بسم الله الرحمن الرحيم

SUDAN UNIVERSTY OF SCIENCE AND TECHNOLOGY

COLLEGE OF GRADUATE STUDIES

Preparation of Some 4- diazo (hetero aryl)phenyl pyrazole and 2-diazo(hetero aryl) phenyl dimedone derivatives

تحضير بعض مشتقات 4- دايا زو (هيتيروياريل) فينيل بيرازولو 2 - دايزو(هيتيرو اريل) فينيل دايميدون

A Thesis submitted for the full of the requirement of the Degree of Doctor of Philosophy in Chemistry

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2016

DEDICTION

This study work is dedicated to my

Mother & Father Souls

Husband

Brother

Sisters

Friends

Acknowledgment

I thanks and grateful Allah who granted me heath and patience to accomplish this work successfully.

I would like to express my sincere and appreciation to my supervisor Prof. Dr. Ahmed Elsadig Mohammed Saeed, who has given me the idea and much of his time for suggestion and supervision of this work.

Iam greatly indebted to my Co- supervisor Dr. Amna Bint Wahab Elrashid Mohammed Hussein and notable assistance this work could never been done. I would like to like to express my thanks and gratitude to any person help and work with me in this work, and during the whole period, this thanks especially to staff in Sudan university lab and technical staff in college of science.

And my deeply thanks to my family, brothers, sisters and husband for their helps to complied the work.

Abstract

In the present work fifty six a new α, β - unsaturated carbonyl compounds and their cyclization reactions with varieties reagent (hydrazine derivatives, hydroxylamine and thio urea) pyrazole, isoxazole and thiopyrimidine derivatives were prepared. A process of the preparation of α, β – unsaturated carbonyl compounds by coupling to diazotized a *p*-aminoacetophenone with 1.3 di carbonyl compounds (ethyl acetoacetate, acetyl acetone, bezoylacetone and dimedone) in presence sodium acetate and ethanol (C-N) bond was formed. Some of the resultant compounds reacted with hydrazine derivatives lead to cyclized to the pyrazole derivatives and condensed with aromatic aldehyde give the synthesis α, β – unsaturated carbonyl. Later were prepared directly from some resultant of the coupling with dimedone in presence basic media sodium hydroxide at room temperature . The reaction progress for all synthesized compounds was checked by (TLC) technique , meting point, and yield percentage. The structure of synthesized compounds were confirmed by spectroscopic instruments IR, some of synthesized compound were confirmed by UV, ^{I}H-NMR, ^{13}C-NMR, MS.

الخلاصة

هذا العمل هدف الى تحضير عد د من المركبات الفا بيتا الغير المشبعة مع دراسة تفاعلاتها الحلقية مع مختلف المواد (مشتقات الهيدازاين، هيدروكسيل امين و الثيويوريا) تؤدى الى تحضير البيرازولات، الايزواكزولات و ثيو بيراميدينات وعدد مركبات الفا وبيتا فى هذه الدراسة حوالى خمسة و ستون مركب .

الطرق التى حضرت بها مركبات الفا بيتا الغير مشبعة هى تحويل مركب البارا امينواسيتوفينون الى ملح ديزونييوم ثم تفاعل هذا الملح مع مركبات 1,3 - ثنائى كربونيل (اثايل أ سيتواستيت أستيل أسيتون بنزوايل أسيتون و الدايميدون) تكونت الرابطة -C)(Nفى وجود أسيتات الصوديوم بعض من هذه المركبات تفاعلت مشتقات الهيدرازين قادت لتكوين المركبات الحلقية البيرازولات ثم كثفت الاخيرة مع بعض الالدهيدات الروماتية فتكونت مركبات الفا بيتا الغير مشبعة الكربونيل، اما المركبات الناتجة من الديميدون كثفت مباشرة مع الادهيدات الاروماتية لتكوين مركيات الفا بيتا الكربونيل الغير مشبعة فى الوسط القاعدى هيدروكسيد الصوديوم فى درجة حرارة الغرفة و جميع المركبات الحلقية تم تحديد تركيبها بي (TLC) ودرجة الأنصهار و النسبة المئويه الوزنية وبعض المركبات تم تحديد تركيبها بواسطة جهاز الشعة البنفسجية، الرنين النووي المغنطيسى والأشعه تحت الحمراء وجهاز مطياف الكتلة .

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List of abbreviations

s	singlet
d	doublet
m	multiplied
δ	Chemical shift
g	gram
Ar	Aryl group
m.p	Melting point
arom	Aromatic
TLC	Thin layer chromatography
vib	vibration
solv	Solvent
st	Stretching
Recy	Recrystallization
℃	Degree centigrade
ml	Millimeter
tem	Temperature
IR	Infrared spectroscopic

^{1}H-NMR	Proton nuclear magnetic resonance
UV	Ultraviolet spectroscopy
DMSO	Dimethylsulfide
MS	Mass spectroscopy

CHAPTER ONE

INTRODUCTION

1. 1. α, β - Unsaturated carbonyl compounds

α, β- unsaturated carbonyl compounds containing the reactive keto ethylenic group (-CO – CH=CH). These are coloured compounds because of the presence of chromophore (- CO – CH=CH-), which depends in the presence of other auxochromes. The chemistry of α, β - unsaturated carbonyl compounds has generated intensive scientific studies throughout the world. Especial interest has been focused on the synthesis and biodynamic activities of α, β -unsaturated carbonyl compounds (Baddily and Toda., 1944, Hyamh*etal.,* 2010,Bakesh Mani and AbddulWahab.,2003).The name α, β - unsaturated carbonyl compoundsare also known as benzlaceto phenone or benzyidene acetophenone. In chalcones two aromatic rings are linked by an aliphatic three carbon chain. α, β - unsaturated carbonyl compounds bear very good synthon so that variety of novel heterocycles with good pharmaceutical profile can be designed(Pande and Saxene.,1987).

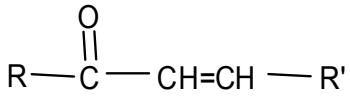


Fig.1.1. structure of α, β - unsaturated carbonyl compound

1.1.1. Synthesis of α, β - unsaturated carbonyl compounds

α, β - unsaturated carbonyl compounds were synthesized by different methods including, Aldol condensation, Claisen-Schmidt condensation, Friedel- Craft acylation, Witting reaction and Allan-Robinson condensation (Brown *et al.,* 1994).

1.1.1. 1. Aldol condensation :

Under the influence of dilute base or acid, two molecules of aldehyde may combine to form β- hydroxy aldehyde in a reaction known aldol condensation,C- C bond formed from a compound contain hydrogen atom, the acidity of alpha hydrogen decrease from aldehyde to ketone to ester. *(*Zhao *et al.,* 2005 *)*.

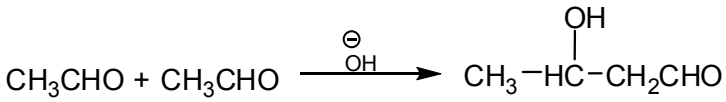


Fig.1.2 . β- hydroxy group structure

1.1.1.2 Claisen-Schmidt reaction

Is the method of synthesis of α, β - unsaturated carbonyl compounds by use of equimolar quantities of a substituted acetophenone with substituted aldehydes in the presence of aqueous alcoholic alkali. The reaction is carried out at about 50℃ for 12-15 hours or at room temperature for one day(Sarkaraetal., 2011,Hero Suwito*et al.,* 2014, Kolb *et al.,* 2011,Sushama*etal*., 2008).

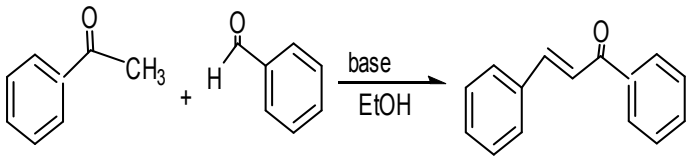


Fig.1.3 Claisen-Schmidt condensation reaction

1.1.1.3. Friedel –Craft Acylation

Besides the Claisen- Schmidt reaction, α, β - unsaturated carbonyl compounds were synthesized by direct Friedel -Crafts Acylation of a phenol. In this approach the phenol becomes the A- ring while the acylation agent provides both the B- ring carbons and the three carbons bridge unit . Friedel - Crafts acylation of 2, 4 –dimethyl - 1, 3, 5- tribenzene with 3-phenylpropionyl chloride gave 2,4,6 - trihydroxy-2,5 dimethyl α, β unsaturated carbonyl compound (Moritani*et al.,* 2000, Sortino*et al.,* 2007, Dominquez *et al,* 2005).

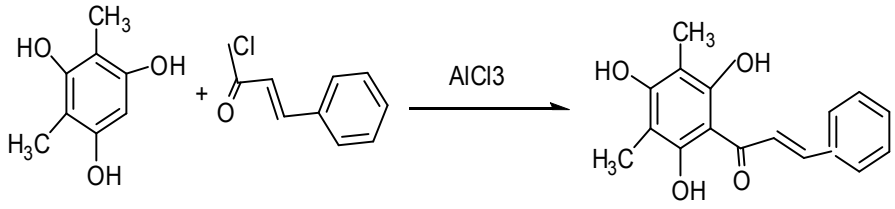


Fig.1.4. Friedel Crafts Acylation reaction

1.1.1.4. Suzuki coupling reaction

Suzuki coupling reaction between benzoyl chloride and phenyl vinyl boronic acid, afforded 3,4,4-trimethoxy chalcones using anhydrous toluene as solvent and catalyzed by teterkis (triphenyl phosphine) palladium and base (EkhlassNassar., 2010).

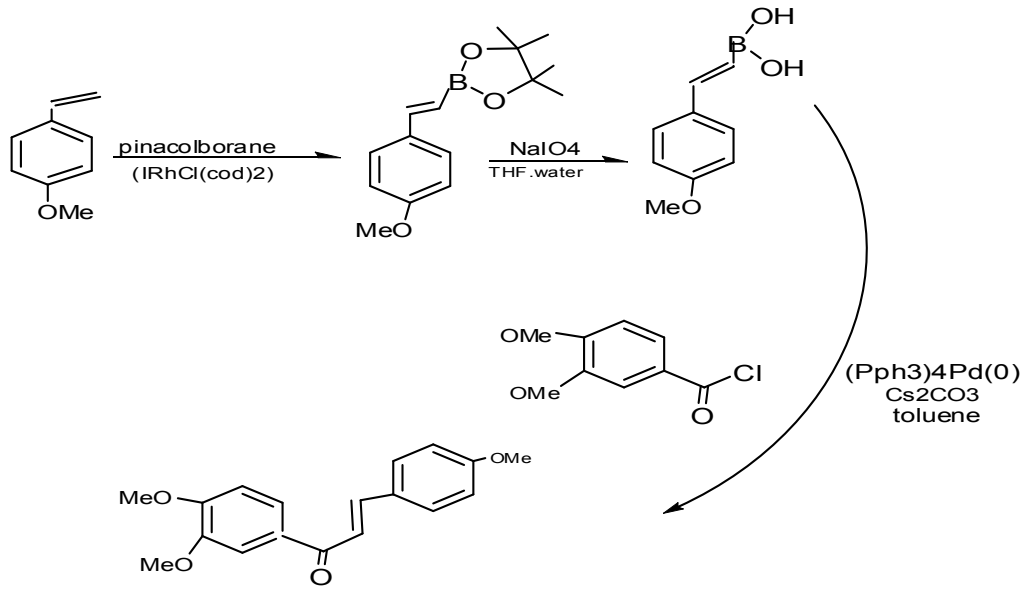


Fig. 1.5 Suzuki coupling reaction

1.1.1.5. Boron trifluorid -etherate reaction.

Several substituted α, β - unsaturated carbonyl compounds were synthesized by use of BF_3- Et_2O. The advantages of this method are high yield, simple work up, short reaction time, no side reactions, and separation is needed to get the products. (Borchhardt*et al.*,2010).

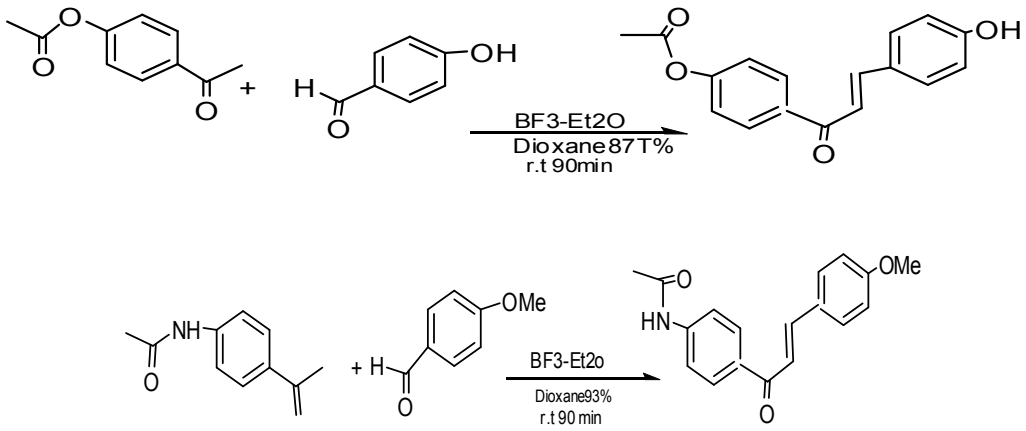


Fig.1.6.BF_3-Et_2O reaction.

1.1.1.6. Microwave Irradiation reaction

The combination of supported reagents and microwave irradiation without the need of solvents proved beneficial since it offers several advantages over conventional heating techniques and accelerates the organic reactions Bhuiyan *etal.,* 2o11). The air- dried paste of 2- hydroxyacetophenone, benzaldehyde and anhydrous K_2CO_3 was subjected to microwave irradiation for 3- 5 minutes to produce 2'-hydroxy α, β - unsaturated carbonyl compounds. This reaction gave a cleaner product with a high yield (80-90%) (Suryawanishi *et al.,* 2008, Deng and Mani., 2006, Shaquiquzzaman et al., 2011).

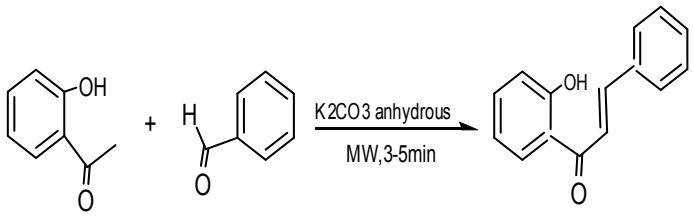


Fig 1.7. Microwave irradiation

1.1.1.7. Von-Konstanecki reaction

This is general method of synthesizing flavones which involves sodium to form 1-(2-methoxyphenyl)-3-phenylpropane-1,3-dioneelimination of water formed flavones (Alka 1987).

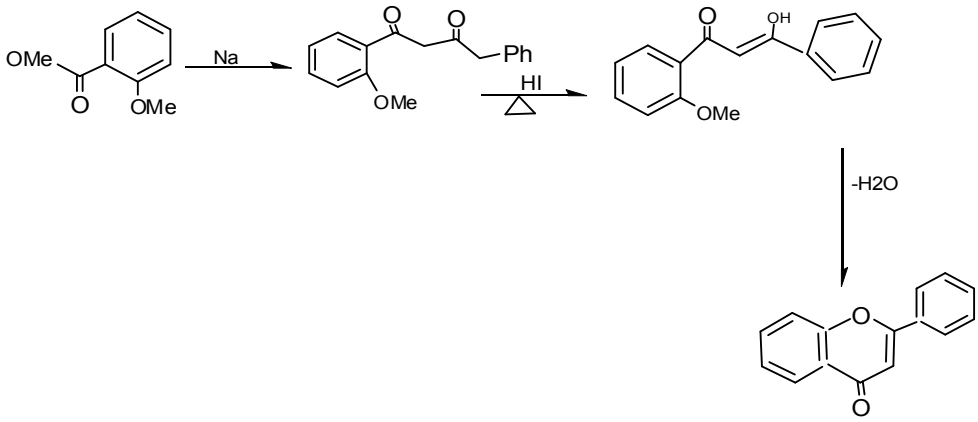


Fig.1.8. synthesis of flavones

1.1.2. Reactions of α, β- unsaturated carbonyl compounds

The α, β - unsaturated carbonyl compounds are very active compounds therefore they react with various reagent to form different compounds, and most important one is the cyclization reaction (Blackman *etal*., 2008, Ashvin*et al.,*2011, Sushama and Usha ., 2008).

1.1.2.1. Reduction of olefinic group

α, β - unsaturated carbonyl compounds have been reduced by hydrogen and platinum to yield saturated carbonyl compounds (Chetana et al., 2009).

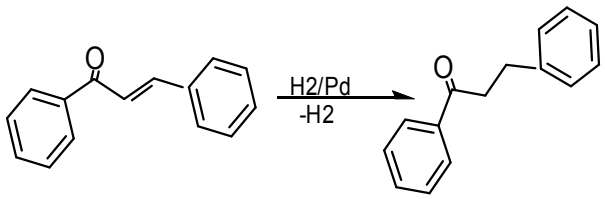


Fig 1.9 reduction of olefin

1.1.2.2. Cyclization reaction

Some novel heterocyclic derivatives such as thiazine's, oxazoles, isoxazole, pyrimidine, pyrazole, oxazole derivatives were synthesized from cyclization

reaction of some α, β - unsaturated carbonyl compoundswith urea, thiourea, hydroxylamine hydrochloride and hydrazine derivative, by condensation in ethanolic basic media(Anees.*etal.,*2010, kalirajan.*etal*.,2009, Bhat *et al.,* 2005).

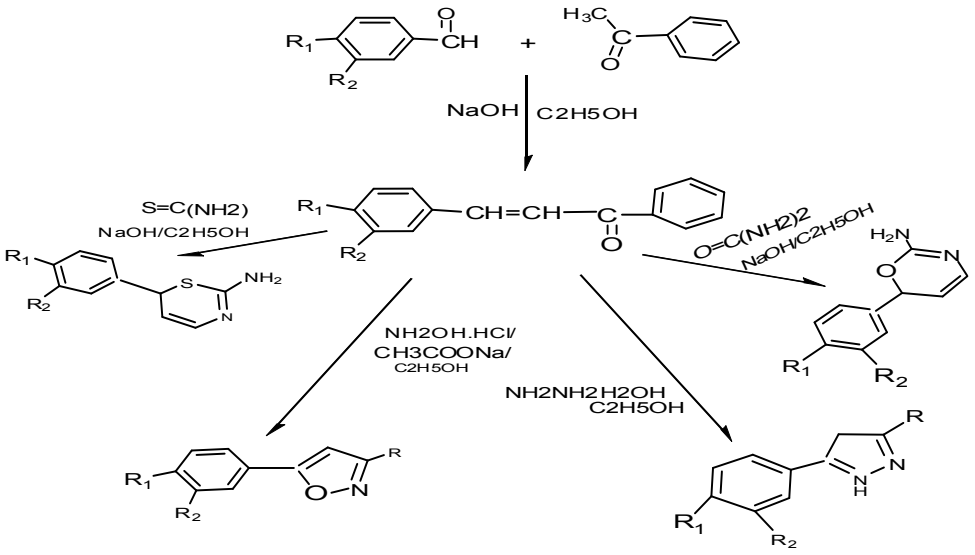


Fig1.10 Cyclization of α, β unsaturated carbonyl compounds

1.2. Pyrimidines

Pyrimidine is a heterocyclic aromatic compound similar to benzene and pyridine containing two nitrogen atoms at position 1 and 3 of six member ring(Brown and Nachod.1955).

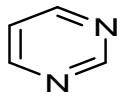
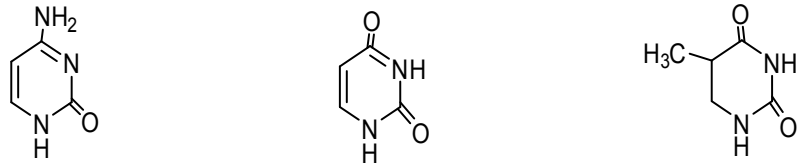


Fig. 1. 11. pyrimidine structure

The four bases commonly found in RNA are divided into two classes: monocyclic compounds and bicyclic compounds, the monocyclic compounds cytosine and uracil are called pyrimidine bases because they

resemble substituted pyrimidine (Norma *etal*.1974). Three nuclei bases found in nucleic acids, cytosine, thymine, and uracil, are pyrimidine derivatives. Other than three major pyrimidine base presented, some minor pyrimidine base can also occur in nucleic acids. These minor pyrimidine's are usually methylated versions of major ones and are postulated to have regulatory functions (Warren., 1997).



Cytosine(C) Uracil(U) Thymine(T)

Fig 1.12. pyrimidine derivatives

1.2.1 Synthesis of pyrimidine derivatives

Various pyrimidine derivatives were synthesized by reaction of chalcones with urea and thiourea under basic condition and ethanol. The synthesized compounds were evaluated for their anti-inflammatory and activity (Vishal *etal.,*2012, EssaAjmi*et al.,* 2015).

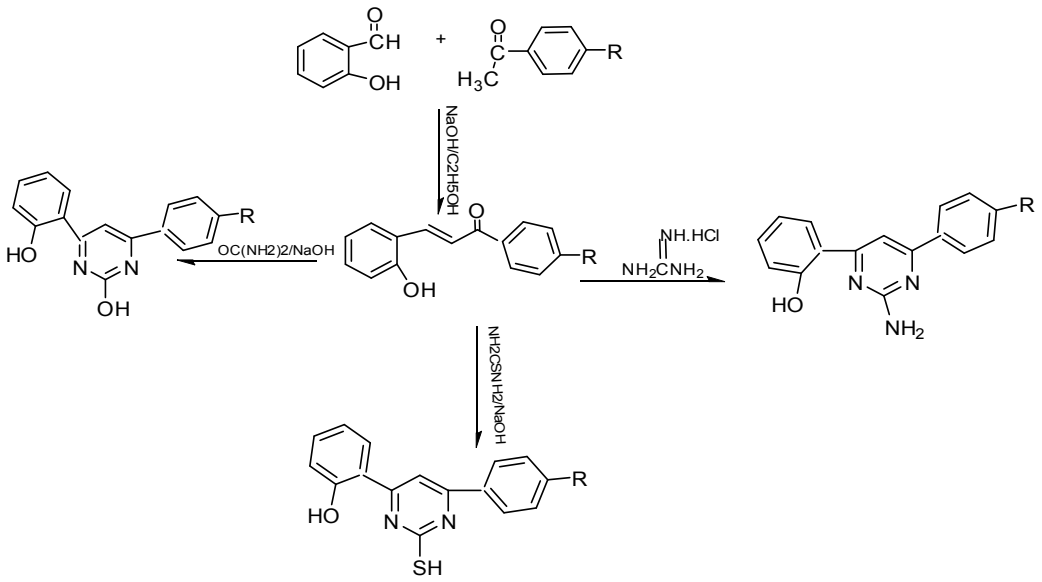


Fig. 1. 13 synthesis of pyrimidine derivative

1.2.2. Biological activities of pyrimidine derivatives

Pyrimidine derivatives are considered to be important for drugs and agricultural chemicals. The use of pyrimidine's is critical to successful treatment of various diseases (Guido *et al.,*2008), pyrimidine derivatives have a good antiflammatory and antimicrobial activities comparable to reference drugs (Xianwen*et al.,* 2014, Shaquiquzzaman*et al.,* 2001, Shaharyar et al., 2014, Vijay *et al*., 2010, Abdel-Wahab *etal.*, 2008, Manish *et al.,* 1998)

1.3.Pyrazoles

Pyrazole is refer to a class of simple aromatic ring of organic compounds of heterocyclic diazole, were π –excessive heterocyclic and contains two nitrogen atoms, in adjacent positions.(Jiang *etal.,* 2009)

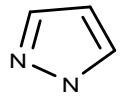


Fig. 1.14. pyrazole structure

Pyrazole ring in incorporated into many of commercially available pharmaceuticals, agrochemicals and dyes tuffs. Some derivatives of pyrazole their activity, analgesic, ant inflammatory and antipyretic (Valla *etal.,* 2006*)*. Pyrazole exist in three partially reduced form differ in positions of double bond.

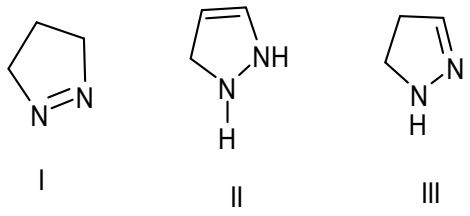


Fig.1.15. Reduced forms of pyrazole

1.3.1. Synthesis of pyrazole derivatives

Pyrazoles were synthesized from 1, 3-diketones, in *situ* from ketones and acid chlorides, were converted into pyrazole by the addition of hydrazine. This method allows a fast and general synthesis of previously inaccessible pyrazole and synthetically demanding pyrazole containing fuse rings.

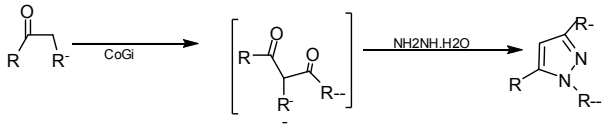


Fig.1.16. synthesis of some pyrazole derivatives

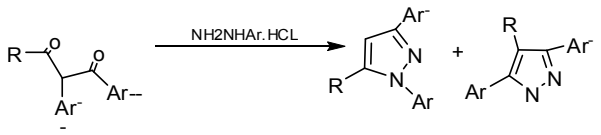


Fig. 1.17. synthesis of pyrazole derivatives.

A highly regioselective synthesis of 1-aryl-3,4,5-substituted pyrazole based on the condensation of 1,3-diketones with aryl hydrazine's proceeds at room temperature in N,N-dimethylacetamide and furnished pyrazole in good yields co(Pradeepkumar.Y*etal.*, 2011). Pyrazole derivatives are prepared by a palladium-catalyzed four component coupling of a terminal alkyne, hydrazine(hydroxylamine), carbon monoxide under ambient pressure, and an aryl iodide(Ahmed *etal.,* 2005, Sandeep *etal.*, 2009).

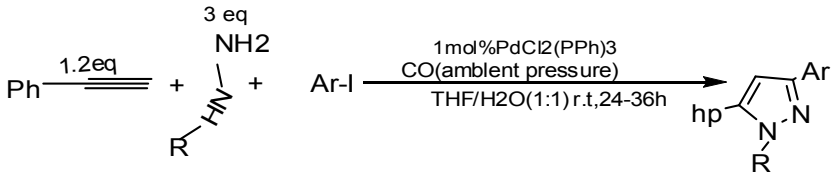


Fig. 1.18. synthesis pyrazole at room temperature

A simple one-pot method allows the synthesis of diversely functionalized N- aryl pyrazoles from aryl nucleophiles, di-tetra -butyl azo di carboxylates, and 1, 3-dicarbonyl or equivalent compounds (Kucukguzel *etal*., 2006).

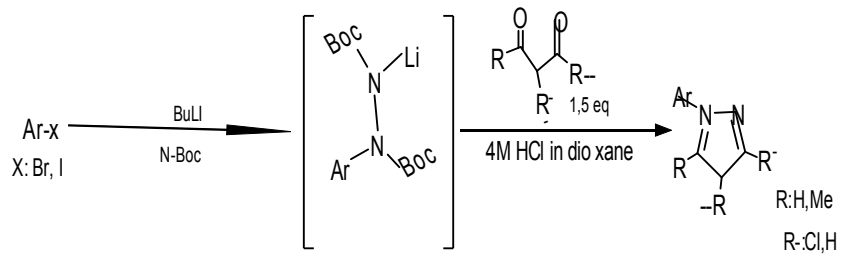


Fig. 1.19. synthesis of pyrazole derivatives from aryl nucleophiles

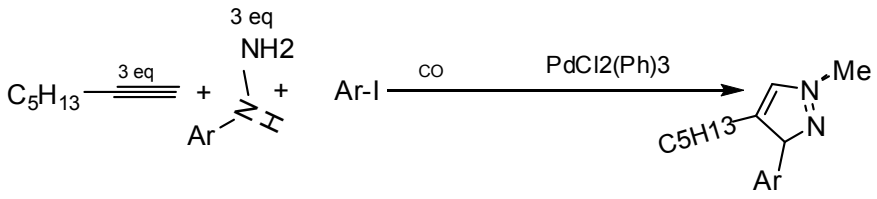


Fig.1.20. synthesis of pyrazole derivatives

A regioselective synthesis of tri-or tetra substituted pyrazoles by the reaction of hydrazones with nitro olefins mediated with strong base such as t- BuOK exhibits a reversed 1,3,4-regioselectivity. Subsequent quenching with strong acids such as TFA is essential to achieve good yields. A stepwise cyclo addition reaction mechanism is proposed

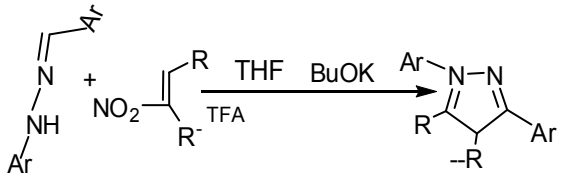


Fig .1.21. synthesis of pyrazole derivative by reaction of olefins with hydrazones

N-aryl hydra zones with nitro olefins allow a regioselective synthesis of 1,3,3-tri-and 1,3,4,5-tetrasubtituted pyrazole ,cyclo addition mechanism*(*Deng and Mani.2006).

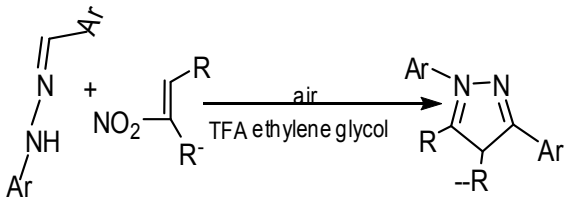


Fig.1.22. synthesis of pyrazole by ethylene glycol

A general methodology for preparation of pyrroles and pyrazole, C-N coupling by use of Cu- catalyzed.

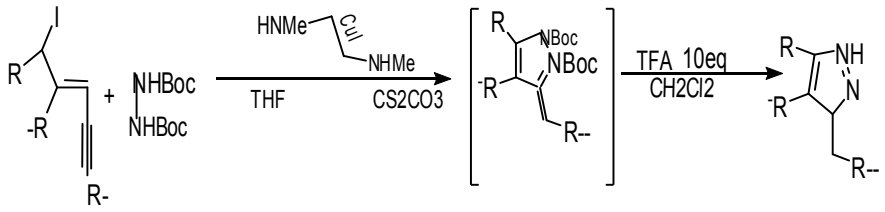


Fig.1.23. synthesis of pyrazole derivatives by C-N coupling

Various 1-acyl-5-hydroxy-4,5-dihydro-1H-pyrazoles were prepared from corresponding 2-alkyn-1-ones, in good yield, dehydration and iodination in presence of Li_2CO_3 at room temperature provide 1-acyl-4-iodo-1H-Payrazoles.

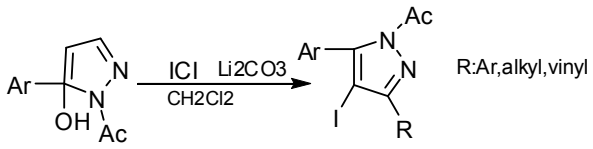


Fig.1.24. synthesis of pyrazole derivatives by dehydration and iodination

A series of 4-substituted 1H pyrazole-5-carboxylates were prepared by cyclo condensation reaction of unsymmetrical amino diketones with tetra - butyl hydrazine hydrochloride or carboxy methyl hydrazine, in good yield (Siles*et al.,* 2006).

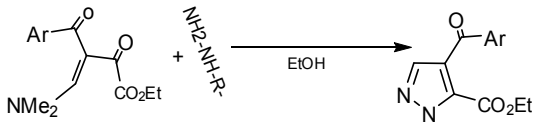


Fig.1.25. synthesis of 4-substituted 1H-pyrazole-5-carboxylates.

1.3.2. Biological activities of pyrazole derivatives

Pharmacological properties, constitute an interesting class of organic chemistry (Suryawanishi et al., 2008). Pyrazole derivatives are used for their analgesic, anti-inflammatory, antiarrhythmic, tranquilizing, and muscle

relaxing, psychoanalytic, and anticonvulsant, monoamine oxidase inhibiting, and antibacterial activities (Fedele *et al.,* 2005)

1.4. Isoxazoles

Isoxazole is a five-membered ring π excessive heterocycle with oxygen (furan-type) and nitrogen (pyridine-type) at position-1and-2 but differs from isoxazole by the presence of N-O bond.

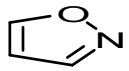


Fig. 1.26. structure of isoxazole

The partially reduced form of isoxazole (dihydroisoxazole) exists in three isomeric form; I,II, III.Isoxazole rings found in some natural product. Isoxazolesform the basis of number of drugs, including the COX-2 inhibitor valdecoxib. (Zoltewicz*et al*.,1978, Seo *et al.,* 2010).

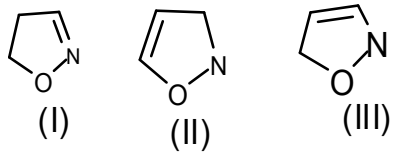


Fig.1.27. isomeric form of isoxazole

1.4.1. Synthesis of isoxazole derivatives

There are various methods available for preparation of isoxazoles. By using of $AlCl_3$-catalyzed on the cyclo isomerization of α, β - acetylenic oximes leads to substituted isoxazoles in very good yields under moderate reaction conditions. The methodology is amenable for the selective synthesis of 3-

substituted ,5-substituted or 3,5-disubstituted isoxazoles (Rajanarendar*et al.,* 2007, Tayaroopa et al., 2013).

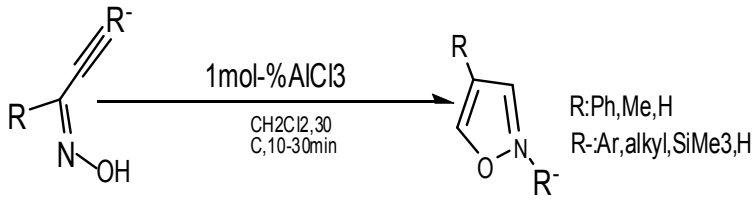


Fig.1.28 3, 5-disubstituted isoxazole

Preparation by using 1,3 dicarbonyl compound and hydroxylamine

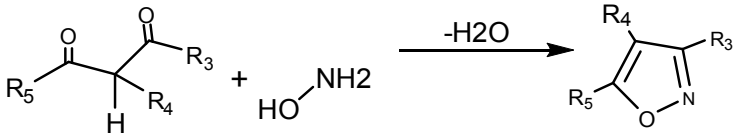


Fig. 1.29. isoxazole derivative

Preparation from the reaction of 1,3-diketones or 1,3 diketo- aldehyde with hydroxyl amine as nuchleophlic character.

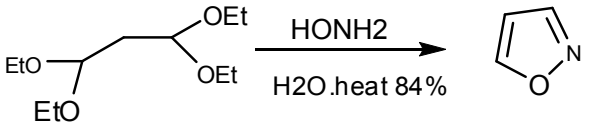


Fig 1.30 resultant isoxazole from nuchleophlic reaction

Dipolar cycloaddition of nitrile oxide generated by base – catalyzed elimination of hydrogen halide from halo – oximes or by dehydration of nitro compounds, readily add to alkyl, generating five member ring.

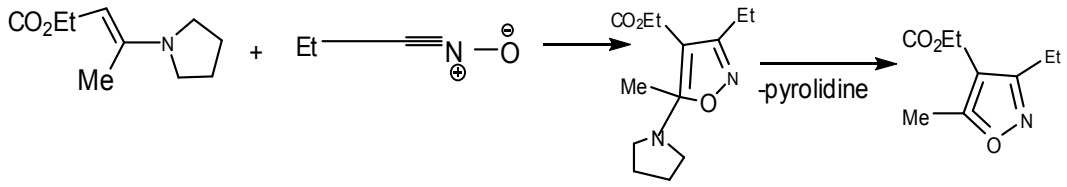


Fig 1.31. cycloaddition of nitrile oxide

Cycloaddition to nitrile oxide and an alkyne generates an aromatics directly, but mixture are sometime obtained.

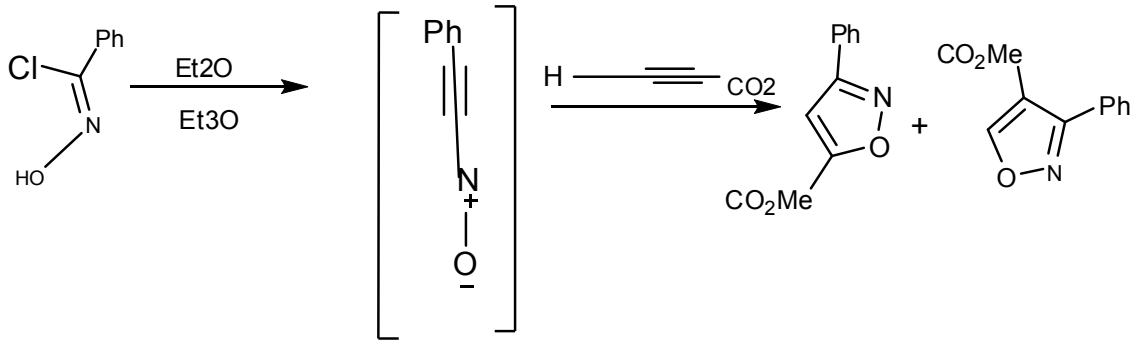


Fig.1.32. preparation of isoxazole derivatives

Anusefulroute to 3-bromo-isoxazoles result on cycloaddition of bromonitrile oxide(Tawalekar et al., 2011)

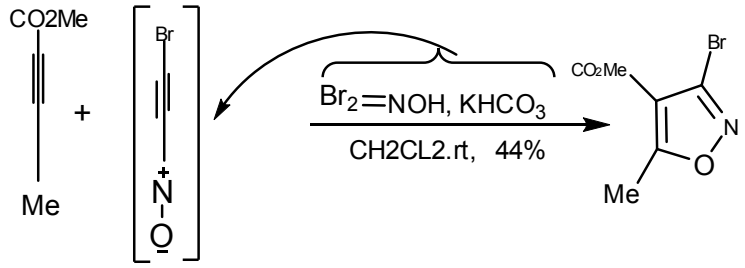


Fig. 1.33. cycloaddition of bromo nitrile oxide

The consecutive Sonogashira coupling of acid chlorides with terminal alkynes, followed by 1,3-dipolar cycloaddition under dielectric heating of in *situ* generated nitrile oxides' from hydroximinoyl chlorides furnishes

isoxazoles in moderate to good yield in the sense of a one-pot three-component reaction(Udupi*etal.,* 1998, Urmila., 2005, Pandely., 2004, Pakesh., 2003).

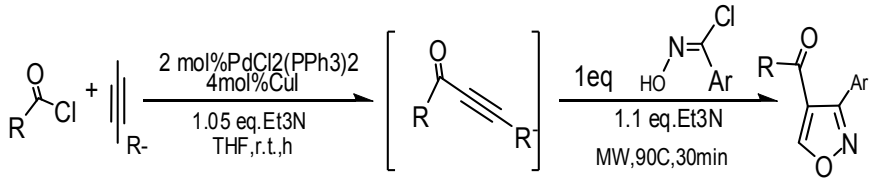


Fig .1.34. 1,3- dipolar cycloaddition

1.4.2. Bioactivities of Isoxazole derivatives

Isoxazole and their derivatives were possess biological activities such as antioxidant, antimicrobial, immunological, antiplatelet, analgesic and acts on human β- drenergic receptor etc. (Abdel-Wahab et al., 2008, Prasad et al., 2005, Maslat et al., 2002, Kucukguzel et al., 2006, Abdelwhab *etal*., 2008, Prasad *etal.*, 2005, Ahluwalia et al., 2006, Abdullah *etal*., 2011, Amila*etal.,* 2012,)

1.5. Aims and objectives:

Pyrazole, isoxazole and pyrimidine derivatives, are associated with a wide range of biological activities as antiflammatory, antimicrobial, antioxidant, cytotoxic, antitumor and anticancer activities. The identification of lead compounds showing pharmacological activity against a biological target and

the progressive optimization of the pharmacological properties and potency of these compounds were one of the focal points of drug discovery.

Pyrazoles and its derivatives occupy a prime position in medicinal pesticide chemistry. Pyrazole analogues have found use as building block in organic synthesis for designing pharmaceutical and agrochemical and as bi functional ligands for metal catalysis. Compound comprising two pyrazole moieties linked by an aliphatic spacer act as bi dentate chelating agents.

The present work aims at:

•Preparation of diazo compounds which coupled with 1,3 dicarbonyl compounds

• Preparation of pyrazole derivatives containing diazo group linkage with aryl keto compounds

• Preparation of α, β - unsaturated carbonyl compounds linkage with pyrazoles by diazo group using Claisen- Schmidt and aldol reaction

• Preparation of heterocyclecompounds from reaction ofα, β - unsaturated carbonyl compounds with hydrazine derivatives, hydroxyl amine and thio urea using Michael reaction

•The project aims to analys both intermediate α, β - unsaturated carbonyl compounds and the final diazoheteroaryl pyrazole derivatives diazo and

hetero dimedone using spectroscopic (UV., IR., ^{1}H- and ^{13}C – NMR) techniques.

CHAPTER TWO

MATERIALSAND METHODS

2.1. Materials and Methods

2.1.1. Chemicals

P- aminoacetophenone, hydroxyl amine hydrochloride, ethyl acetoacetate, phenyl hydrazine, phenyl hydrazinium hydrochloride, hydrazine sulfate, thiourea, dimedone, acetyl acetone, benzaldehyde, bezoylacetone, annisaldehyde, cinnamaldeyde,*O.*nitrobenzaldehyde, salysaldehyde and N,N-dimethylamino benzaldehyde were obtained from LOBA company (India).

2.1.2. Solvents

Chloroform ($CHCl_3$), ethylacetate ($CH_3COOCH_2CH_3$), methanol (CH_3OH), n-Hexane ($CH_3\ (CH_2)_4CH_3$) and petroleum ether were obtained from LOBA (India). Ethanol was obtained from alwtania, Sudan.

2.1.3.Reagents

Concentrated hydrochloric acid (HCl), sodium hydroxide (NaOH), potassium hydroxide (KOH), sodium acetate (CH_3CO_2Na) andsodium nitrite were obtained from LOBA, India.

2.1.4. Thin layer chromatography (TLC):

Thin layer chromatography was carried out using silica gel 60 GF254-precoated(250μ) aluminum plates (Merck) with different mobile phases.

2.1.5. Spectroscopic Instruments

2.1.5.1.(IR) spectrophotometers

The infrared spectrophotometer were recorded using KBr disk byusing IR spectrophotometer, model Perkin Elmer FT IR (4000), USA.

2.1.5.2. Ultraviolet (UV) spectrophotometer

Ulter violet spectral data were obtained using 6505 UV vibspectrophotometer Jenway, England.

2.1.5.3. Nuclear Magnetic Resonance(NMR) spectrometer

^{13}C- and proton ^{1}H nuclear magnetic resonance spectral data were obtained with NMR instrument model (BRUKER, Germany) AMX (400MGZ) spectrophotometer using DMSO as solvent on TMS as internal reference, 200ppm (performed in Cairo University, Egypt).

2.1.5.4 Mass spectrometer (MS):

The mass spectra were run on a AShimadzu. G C. N.Q P. 1000 mass spectrometer at 70 ev(performed in Cairo University**,** Egypt).

2.1.6. General Instruments:

Hot plate with magnetic stirrer. Electronic balance .S.N.O. 1296463,Japan Melting point apparatus, Galleon Kamp.

2.2. Synthetic Methods

2.2.1. Synthesis of 3- di azo-(p-acetyl phenyl) -phenyl butane -1, 3-ones (I-IV)

In a 250-ml one neck, roundbottom flask placed over magnetic stirrer hyphen,*p*-amino acetophenone (0.0025mole, 0.338g) dissolved in concentrated hydrochloric acid (5ml, 32%) was added, and the solution was stirred at room temperature. The solution was cooled to 0- 5℃, sodium nitrite (0.0026 mole, 0.18g in 1-5ml water) was added portionwise at 0-

5℃, and the reaction content was stirred for further one hour at the same temperature. The resulting clear diazonium salt solution was added dropwise over 20 minutes with constant stirring and with frequent addition of ice to a cold (0-5℃) stirred solution of coupling component (0.0032mol) of required 1,3 carbonyl compounds (1,3 diketones) dissolved in 20ml ethanol containing sodium acetate (0.013mol), whilst maintaining temperature at 0-5℃. After addition of the diazonium salt, the mixture was stirred for an additional 3-4 hours at 5-10℃. The precipitated product in each case was separated upon dilution with cold water (30ml) and filtered off, washed with water, air dried and recrystallized from ethanol.

2.2.2. Synthesis of 4- di azo-(p-acetyl phenyl)–pyrazole derivatives (V-XII)

In a 250-ml one neck roundbottom flask placed over a hot plate magnetic stirrer, a mixture of 0.01mole of the required hydrazinederivatives and 0.01 mole of compound (Table 2.2.1) in 25ml (95%) ethanol were added. The mixture was refluxedfor 13-16 hours. The product formed was diluted with cold water and filtered, air dried, recrystallized from ethanol and analyzed by TLC.

2.2.3. Synthesis of 4-diazo-(p-(aryl)-alken-1-on) phenyl)-substituted pyrazole and 2-diazo-p-(aryl)alken-1-on)-phenyl)-5,5-dimethyl-cyclohexane-1,3-diones (XIII- LXVII)

In a 250- ml one neck, roundbottom flask placed over a magnetic stirrer, 0.01moleof required acetylphenyl diazo derivatives (V-XII) and 0.01mole of the target aldehyde, in 10ml of 95% ethanol, were added. Ten ml solution of sodium hydroxide (20%) were added slowly dropwise and the reaction mixture was stirred at room temperature for 24hours. The reaction mixture was allowed tostand overnight,poured into crushed ice or cold water (30ml) and acidified with diluted hydrochloric acid (10%). The precipitate was filtered, washed with cold water, air dried and recrystallized from ethanol and analyzed by TLC. The chemical and physical properties were tabulated in Table (2.3.1).

2.2.4. Synthesis of 4-diazo-(p-(5-(substituted phenyl)-pyrazole-3-yl)-phenyl)–substituted pyrazole derivatives (LXIX-CVI)

In a 250-ml one neck round bottom flask placed over magnetic stirrer placed (0.01mol) of the required α, β - unsaturated carbonyl compounds dissolved in 25-ml ethanol (95%), 0.01mole phenyl hydrazinium hydrochloride chlorideand 0.02mole sodium acetate were added . The reaction mixture was refluxed for 10 hours. The progress of the reaction was monitored on TLC plate. After completion of the reaction, the mixture was cooled , the precipitate that separated out was filtered, washed with water, air dried and recrystallized from ethanol. The chemical and physical properties are showed in Table(2.3.2).

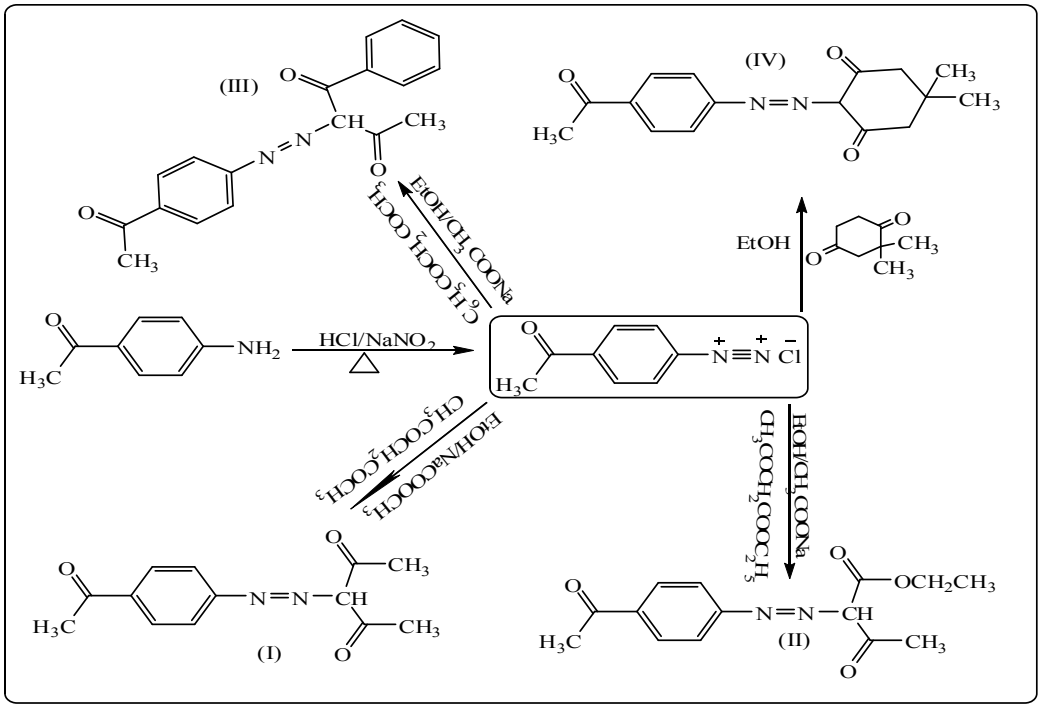
2.2.5. Synthesis of 4-diazo-p-(5-(substituted phenyl)-thiopyrimidine-6-yl)phenyl)-substituted pyrazole derivatives (LXX-CVII)

In a 250ml one neck roundbottom flask maintained over magnetic stirrer were placed (0.01mol) of the required α, β - unsaturated carbonyl compounds dissolved in ethanol (25ml) 95% and thiourea (0.01mol, 0.76g) was added. Solution of KOH (5ml 40%) was added to the reaction mixture and refluxed for 12 hours. The progress of the reaction was monitored on TLC plate. After completion, the reaction mixture was cooled and poured into crushed ice and neutralized with dilute hydrochloric acid (10%). The product which separated out was filtered, washed with water, air dried and recrystallizedfrom ethanol .The chemical and physicalproperties were tabulated in Table (2.3.4).

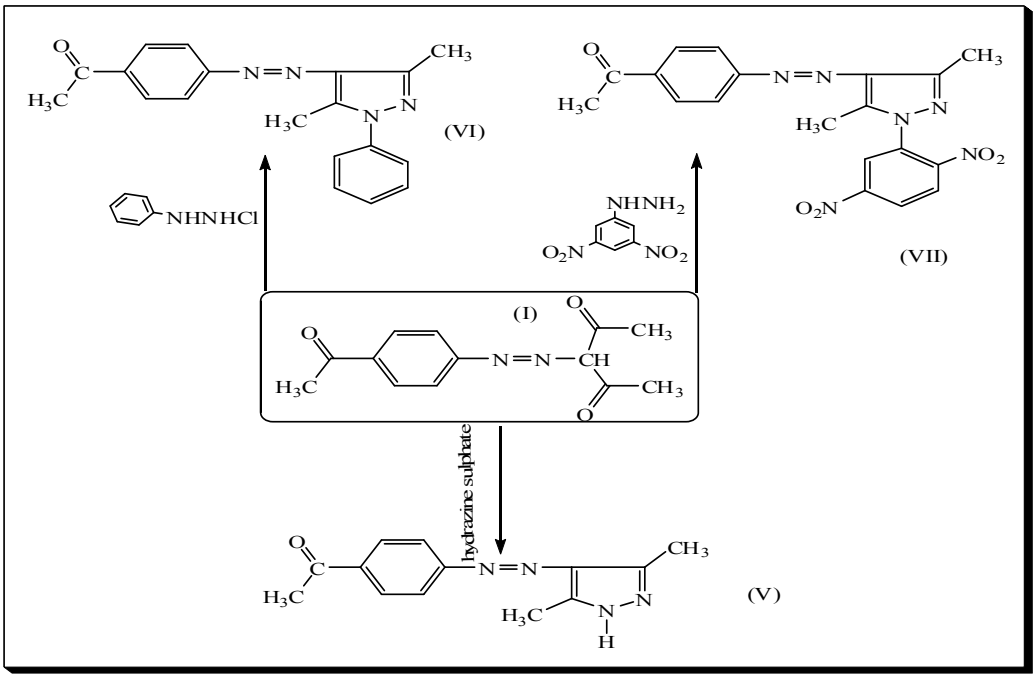
2.2.6. Synthesis of 4-diazo-(p-(5-(substituted phenyl)-isoxazol-5-yl)-phenyl) -substituted pyrazole derivatives (LXVIII-CV)

In a 250-ml one neck round bottom flask maintained over magnetic stirrer were placed(0.01mol) of the required $\alpha, \beta -$ unsaturated carbonyl compounds dissolved in ethanol (25ml) 95%, hydroxide amine hydrochloride (0.01mol) was added . A solution of 40% KOH 0.02 mole was added to the reaction mixture and refluxed for 10-12hours. The progress of the reaction was monitored, on TLC plate. After completion the reaction mixture was cooled and poured into crushed ice and neutralized with dilute hydrochloric acid (10%). The product which separated out was filtered, washed with water,

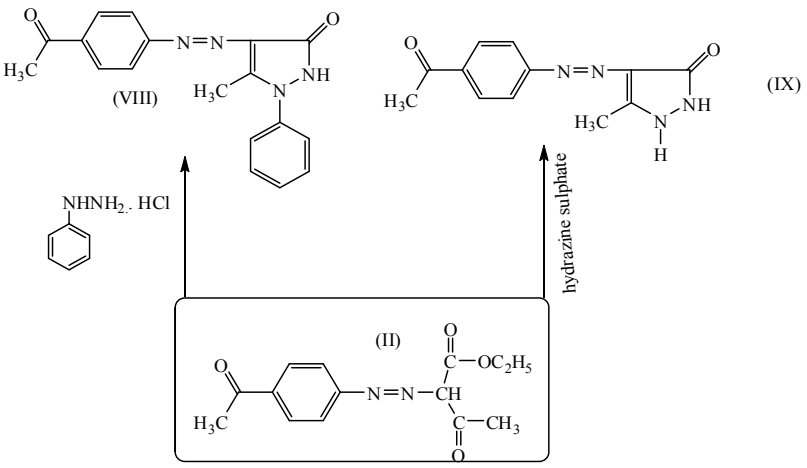
air dried and recrystallized from ethanol. The chemical and physical properties of synthesized compounds were tabulated in Table(2.3.3)



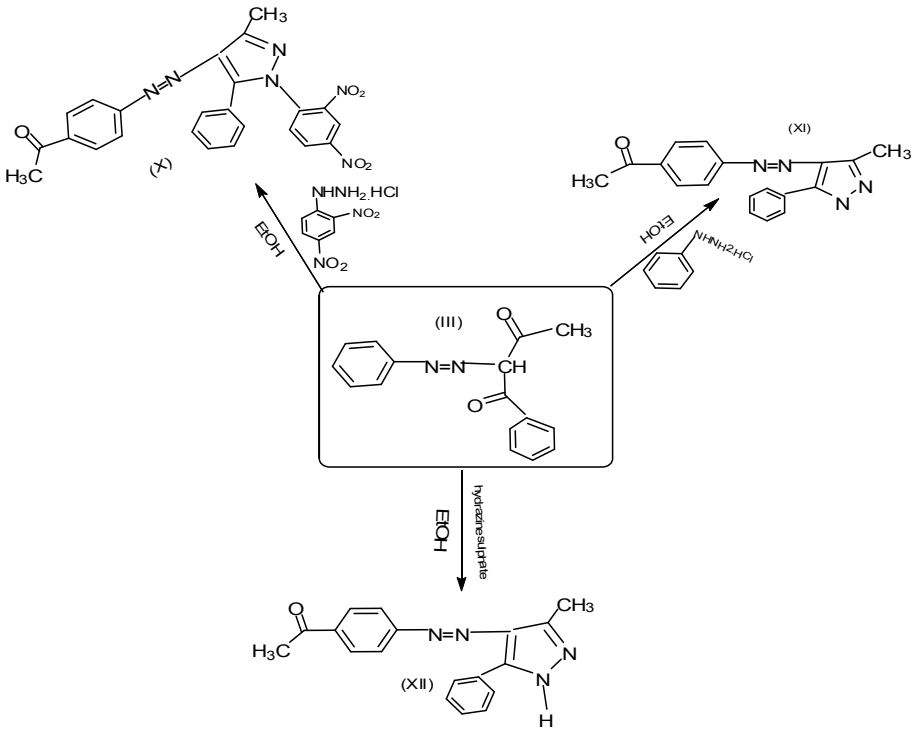
Scheme. 2.1. Chemical structure of the synthesized diazo (acetyl phenyl) 1,3 diones



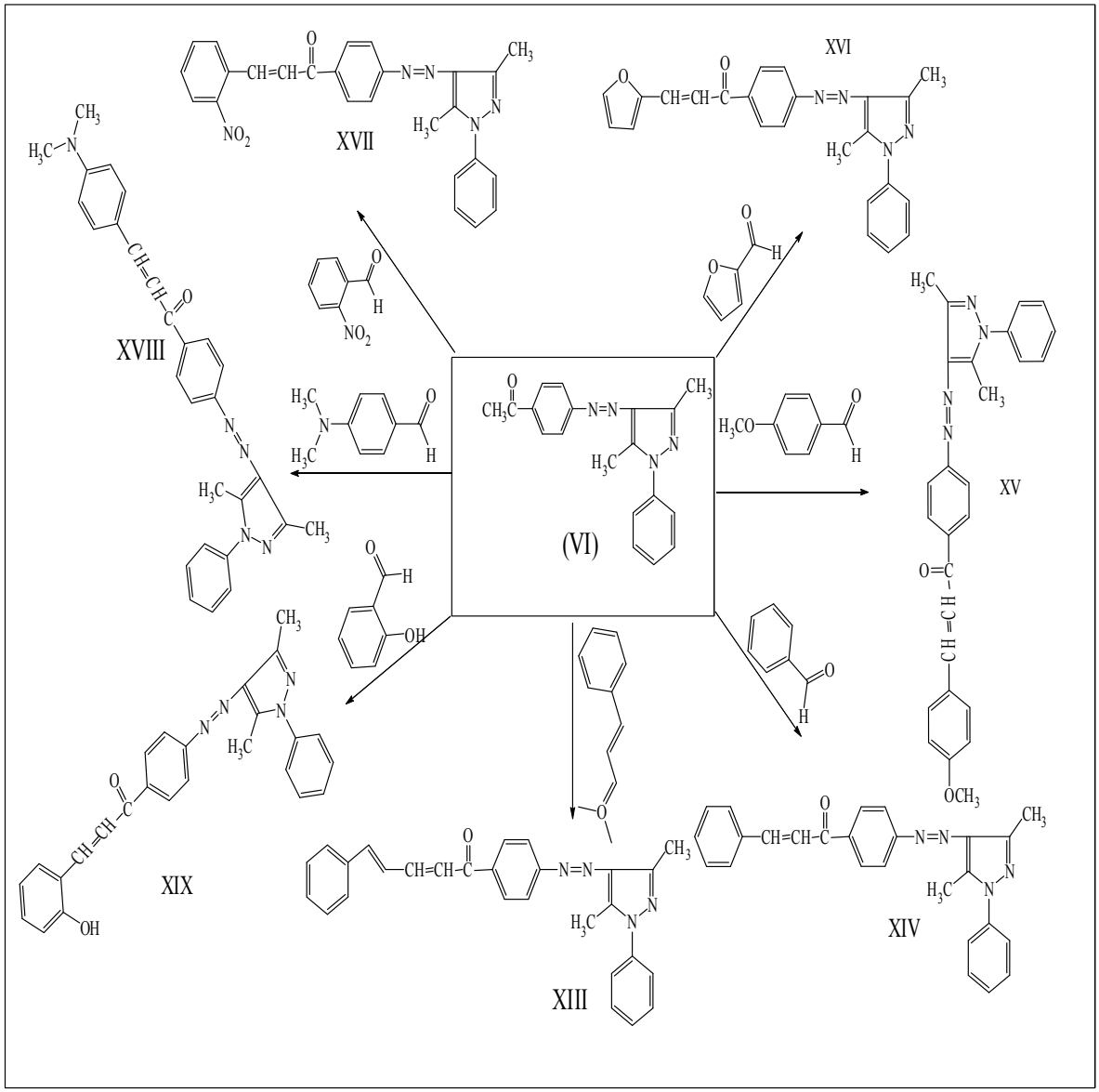
Scheme.2.2. Chemical structure of the synthesized 4 - diazo-(p-acetyl phenyl)-3,5-dimethyl-1- pyrazole derivatives



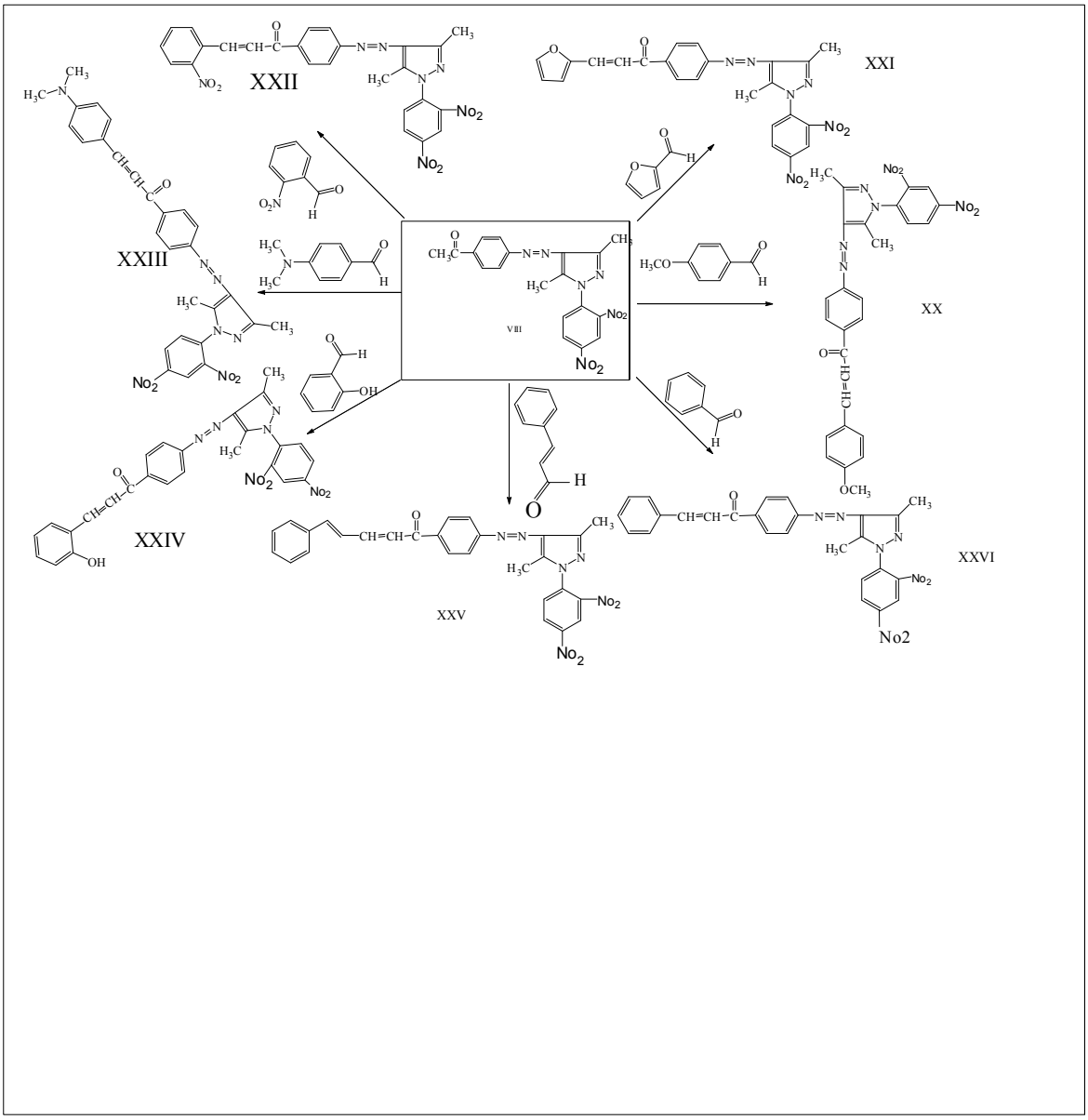
Scheme 2.3. Chemical structure of the synthesized 4-diazo-(p-acetyl phenyl)-5-methyl-1- pyrazole-3-ones derivatives



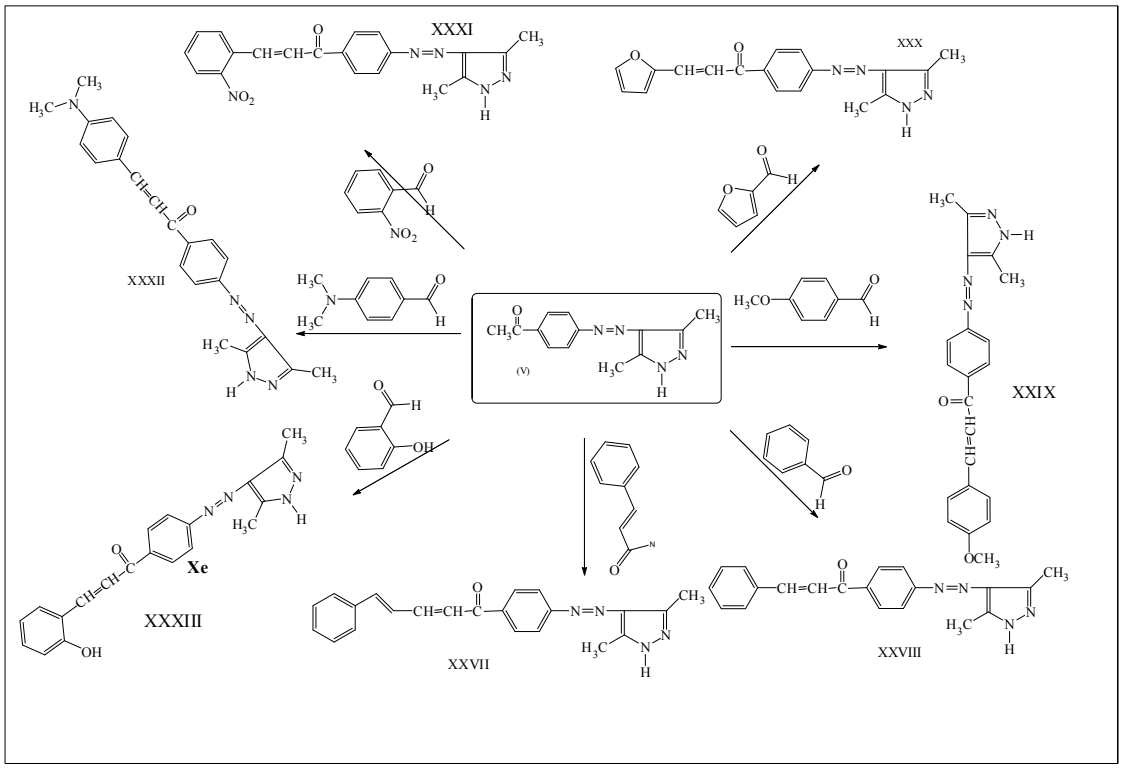
Scheme 2.4. Chemical structure of the synthesized 4- di azo-(p-acetyl phenyl)-3-methyl-5-phenyl-1- pyrazole derivatives



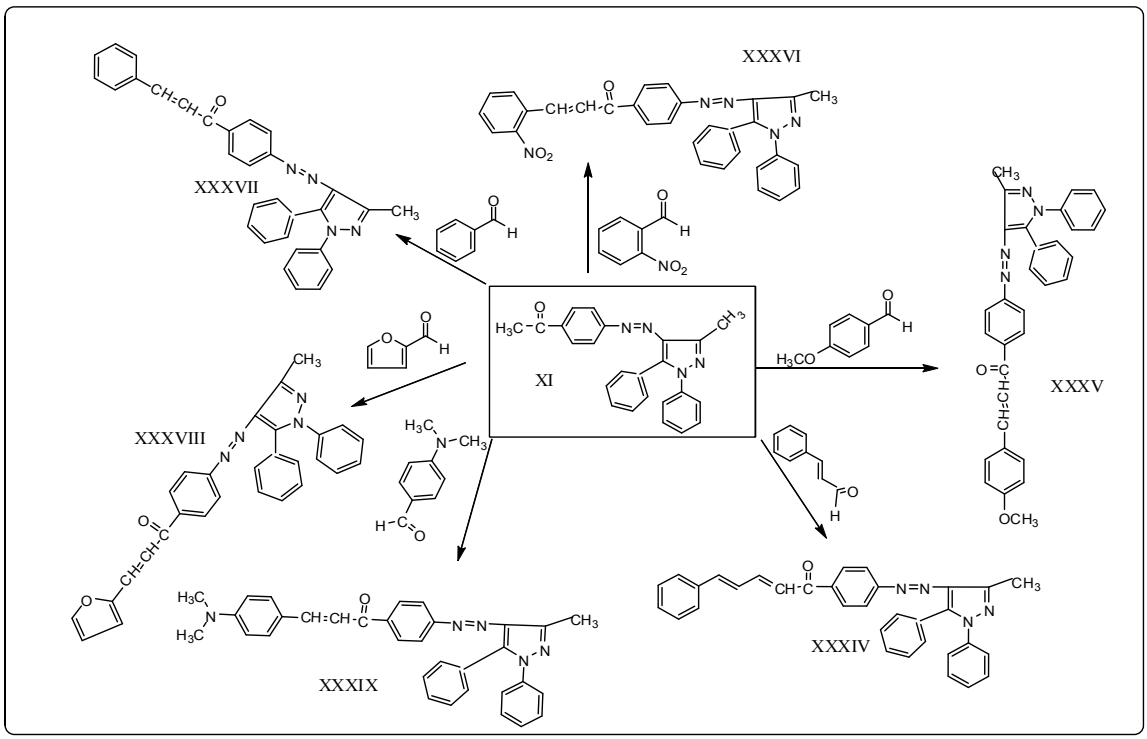
Scheme. 2.5.Chemical structure of the synthesize 4-diazo-(p-(aryl)-alken-1-on)phenyl)-3,5-dimethyl-1-phenyl-pyrazole



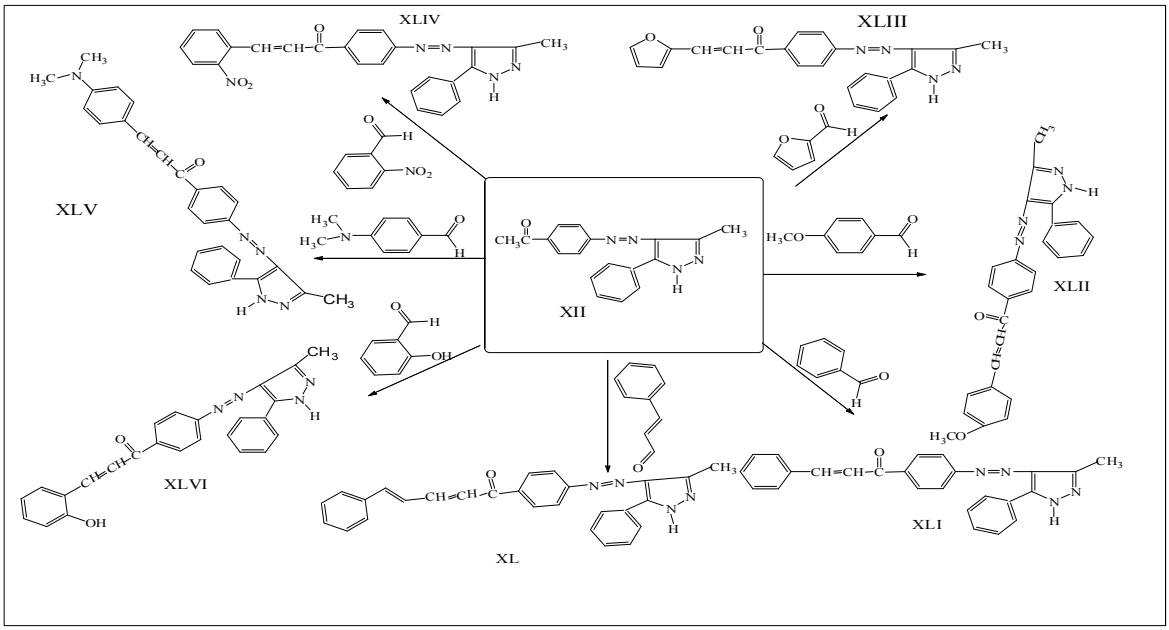
Scheme. 2.6.Chemical structure of the synthesize 4-diazo-(p-(aryl)-alken-1-on)phenyl)-3,5-dimethyl-1-2,4-diphenyl-pyrazole



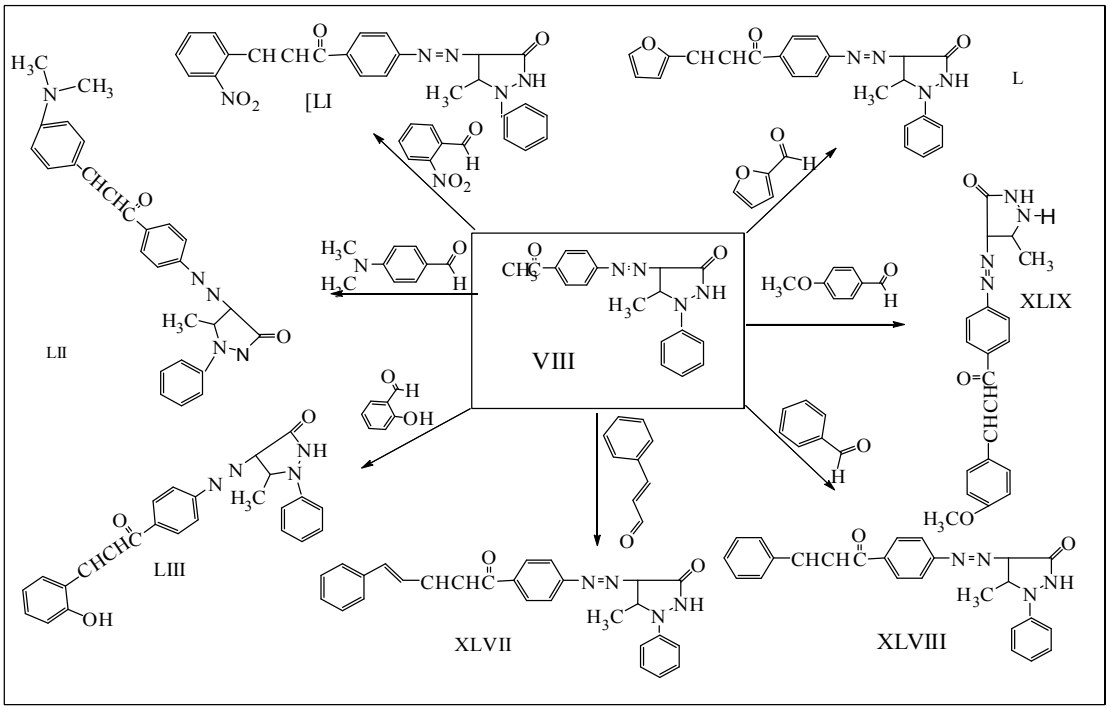
Scheme. 2.7.Chemical structure of the synthesize 4-diazo-(p-(aryl)-alken-1-on)phenyl)-3,5-dimethyl -pyrazole



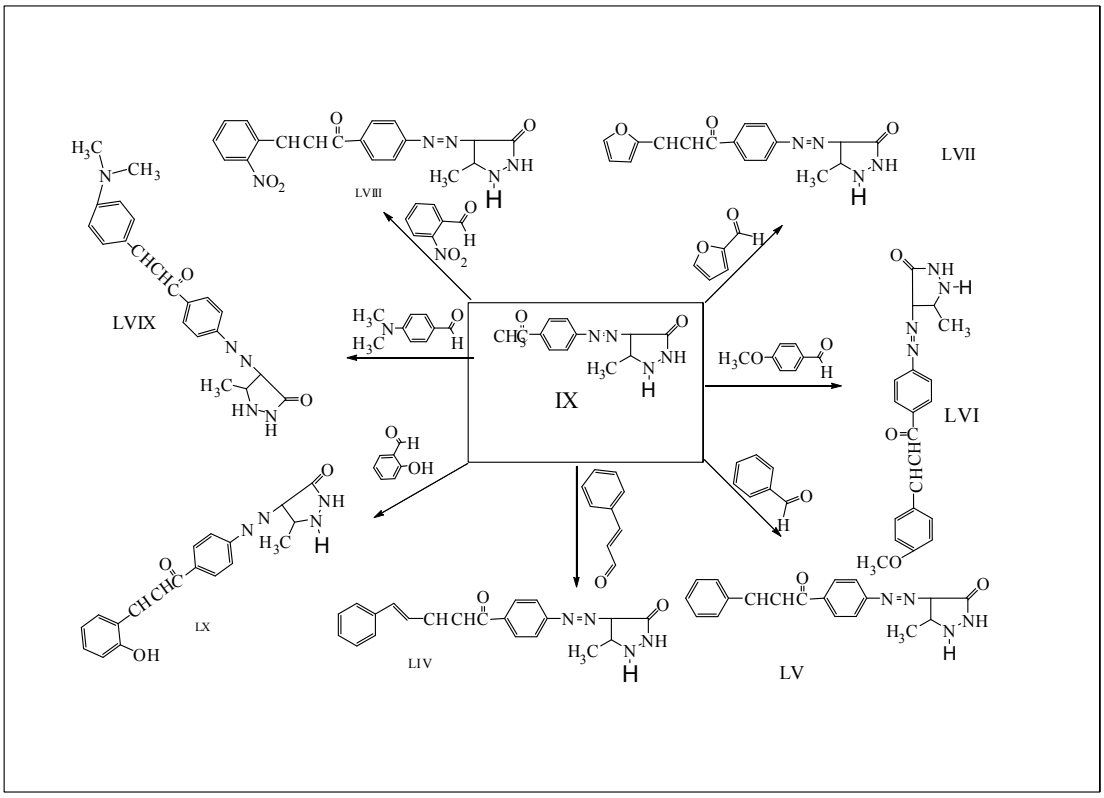
Scheme. 2.8.Chemical structure of the synthesize 4-diazo-(p-(aryl)-alken-1-on)phenyl) -5-methyl-1,3-diphenyl-pyrazole



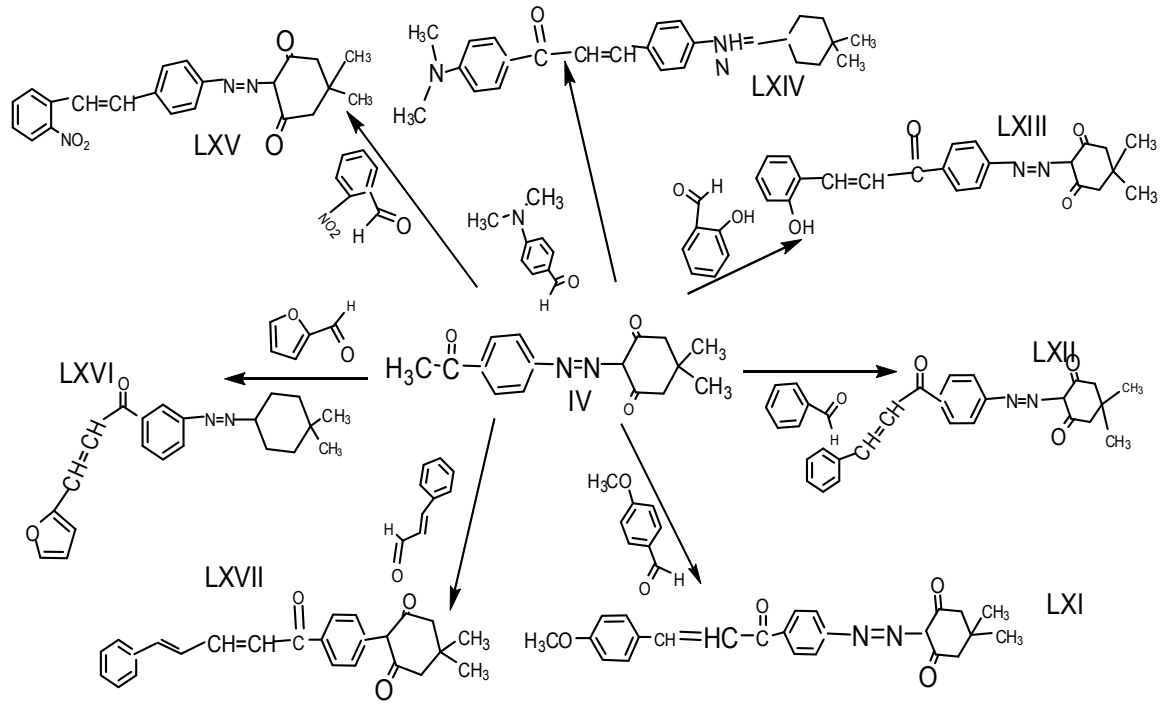
Scheme. 2.9.Chemical structure of the synthesize 4-diazo-(p-(aryl)-alken-1-on)phenyl)-5-dimethyl-3-phenyl-pyrazole



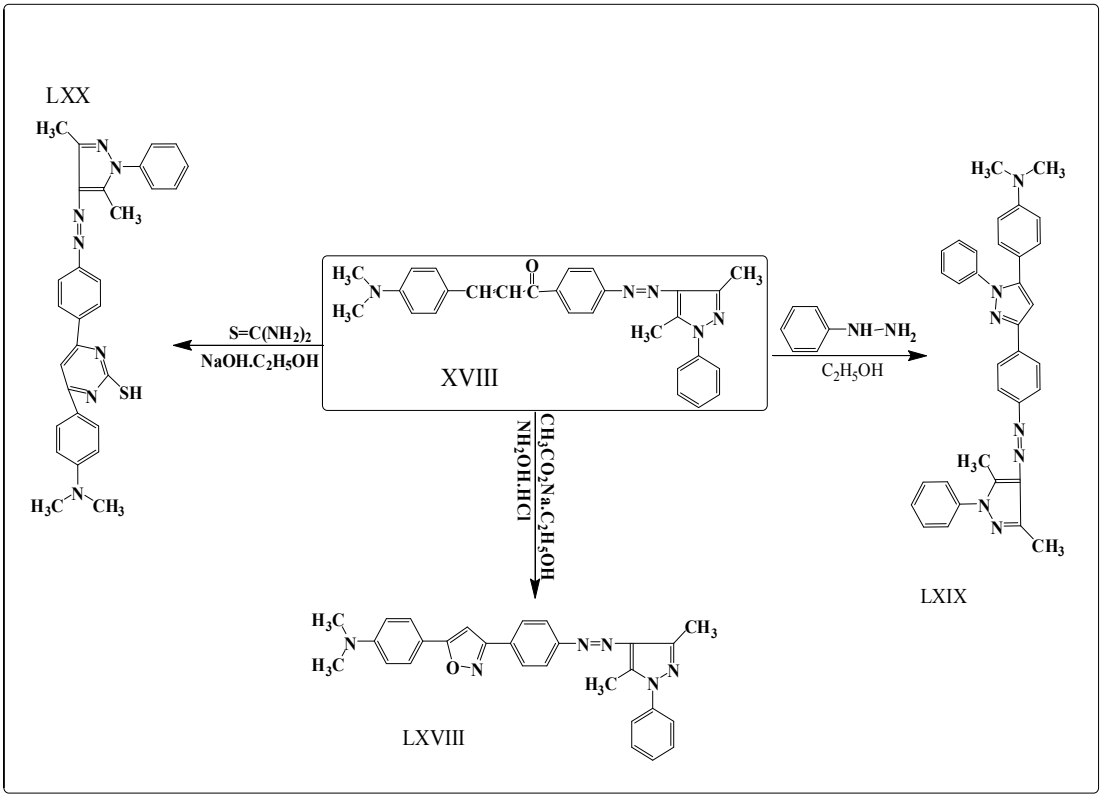
Scheme. 2.10.Chemical structure of the synthesize 4-diazo-(p-(aryl)-alken-1-on)phenyl)-5-methyl-1-phenyl-pyrazol-3-one



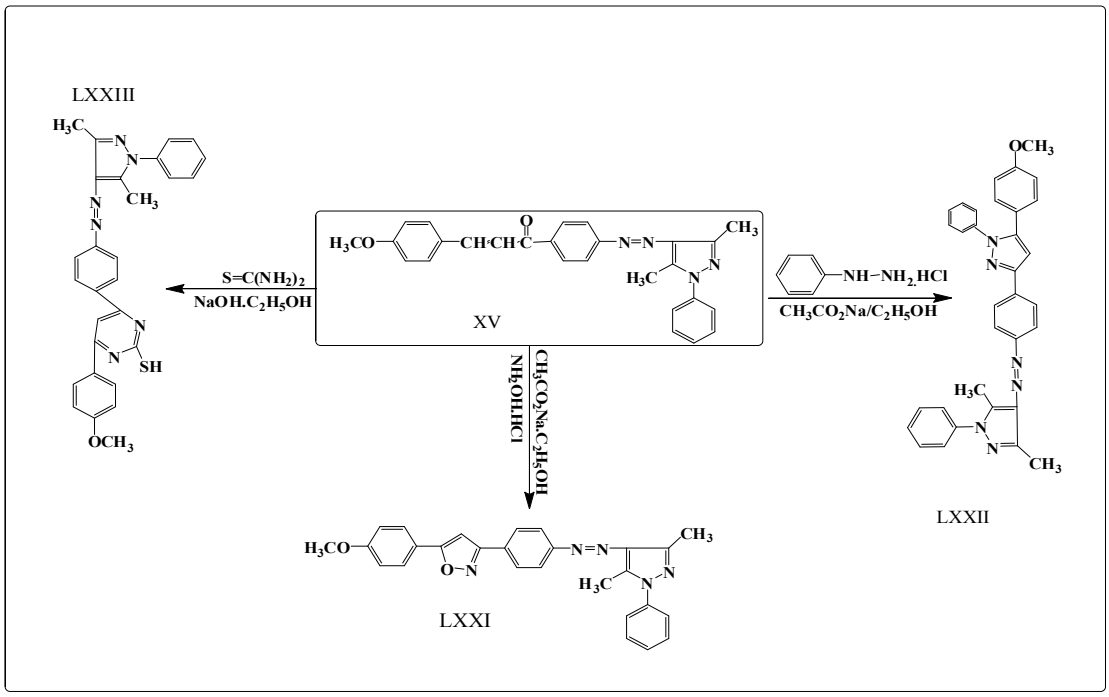
Scheme. 2.11.Chemical structure of the synthesize 4-diazo-(p-(aryl)-alken-1-on)phenyl)-5-methyl-pyrazol-3-ones



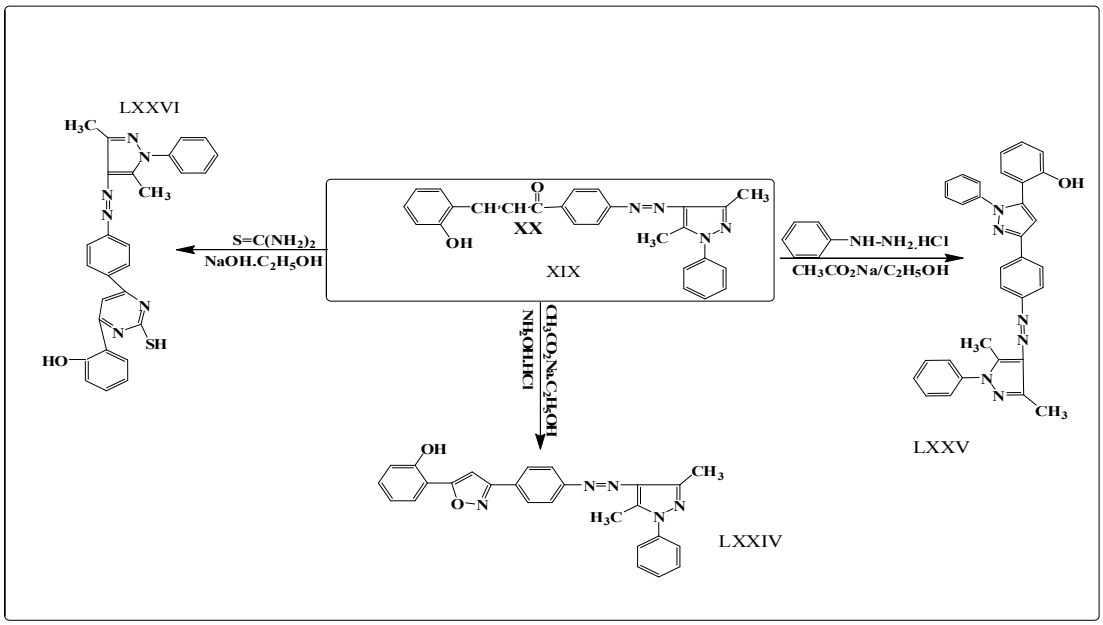
Scheme. 2.12.Chemical structure of the synthesize 4-diazo-(p-(aryl)-alken-1-on)phenyl)-5,5-dimethyl-cyclo hexane-1,3-diones



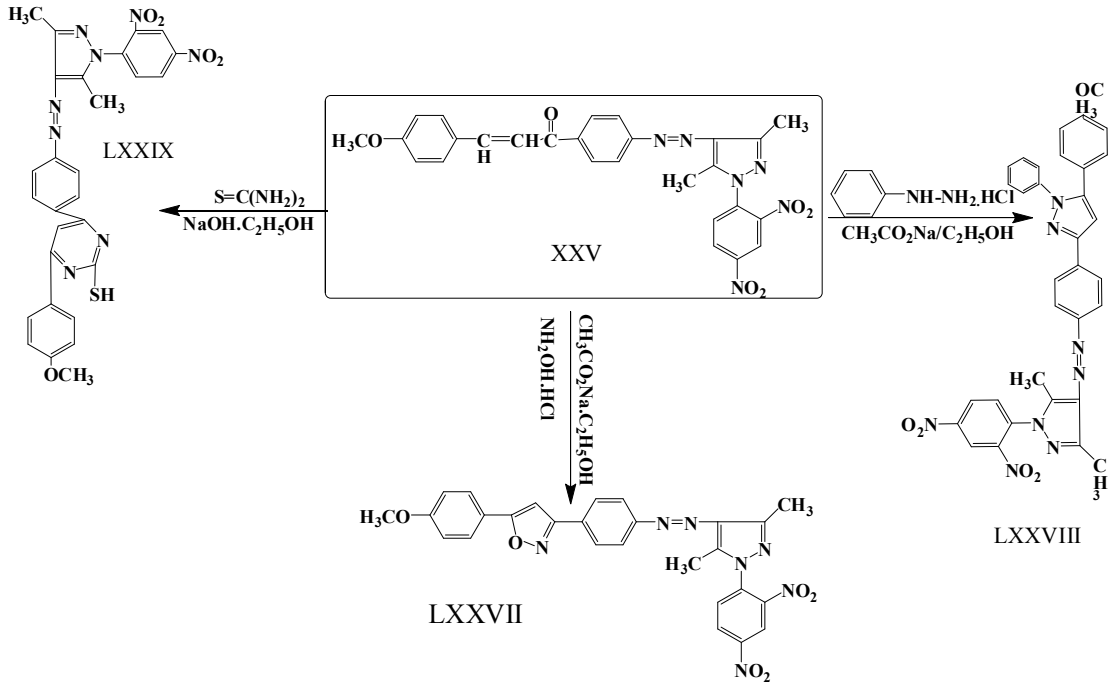
Scheme.2.13. Chemical structure of the synthesized 4-diazo-(p-(5-(p-N,N-dimethyl amino phenyl)-heteroaryl)-3,5-dimethyl-1-phenyl-pyrazol



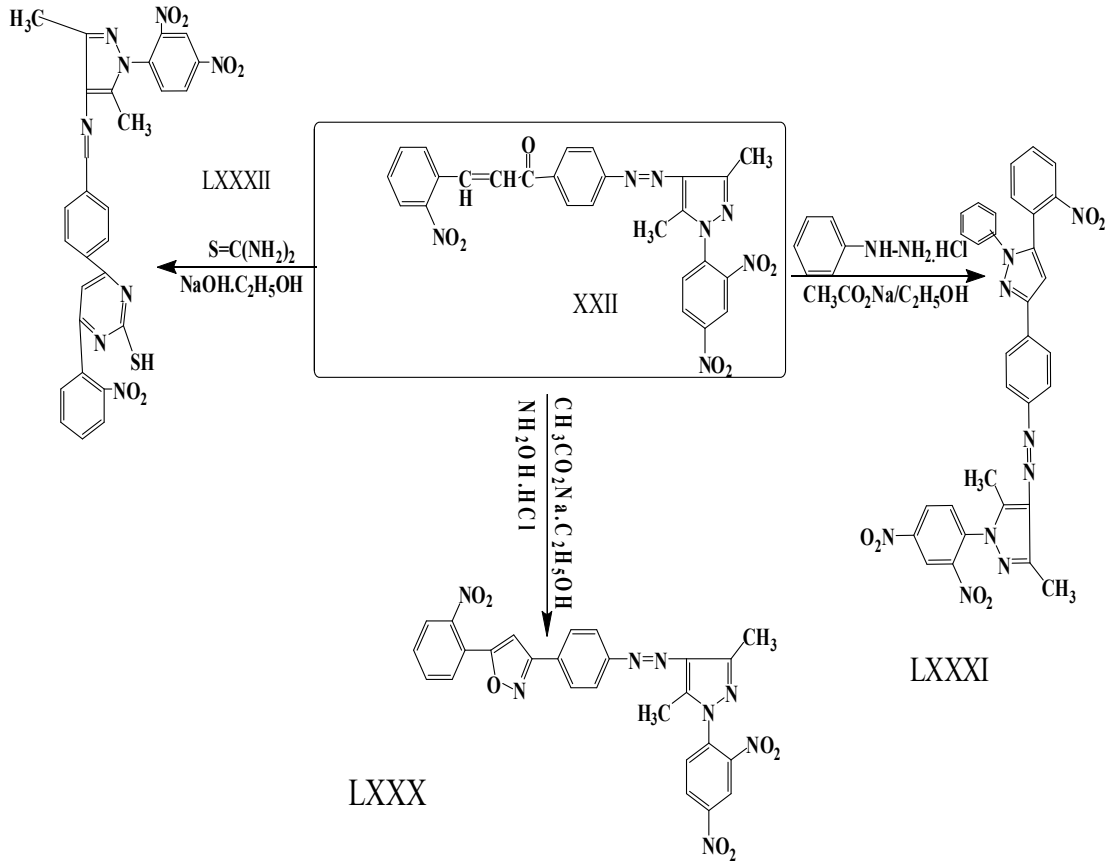
Scheme.2.14.Chemicalstructureof the synthesized 4-diazo-(p-(5-(4-methoxy phenyl)-hetero aryl)-3,5-dimethyl-1-phenyl-pyrazol



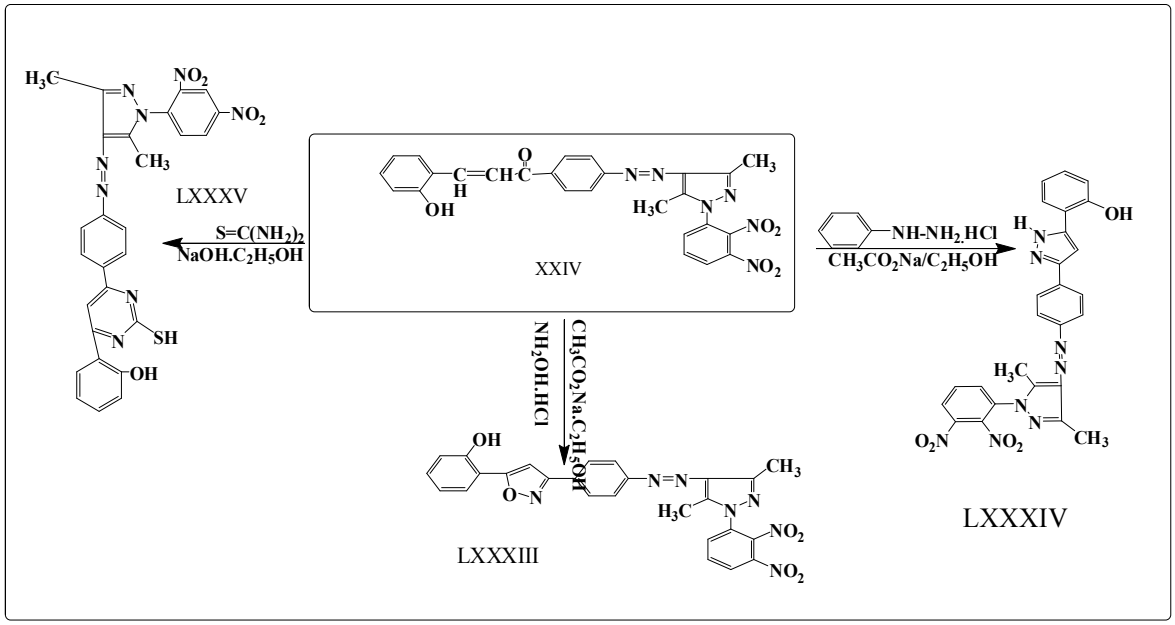
Scheme.2.15.Chemicalstructureof the synthesized 4-diazo-(p-(5-(2-hydroxyphenyl)-heteroaryl)-3,5-dimethyl-1-phenyl-pyrazole



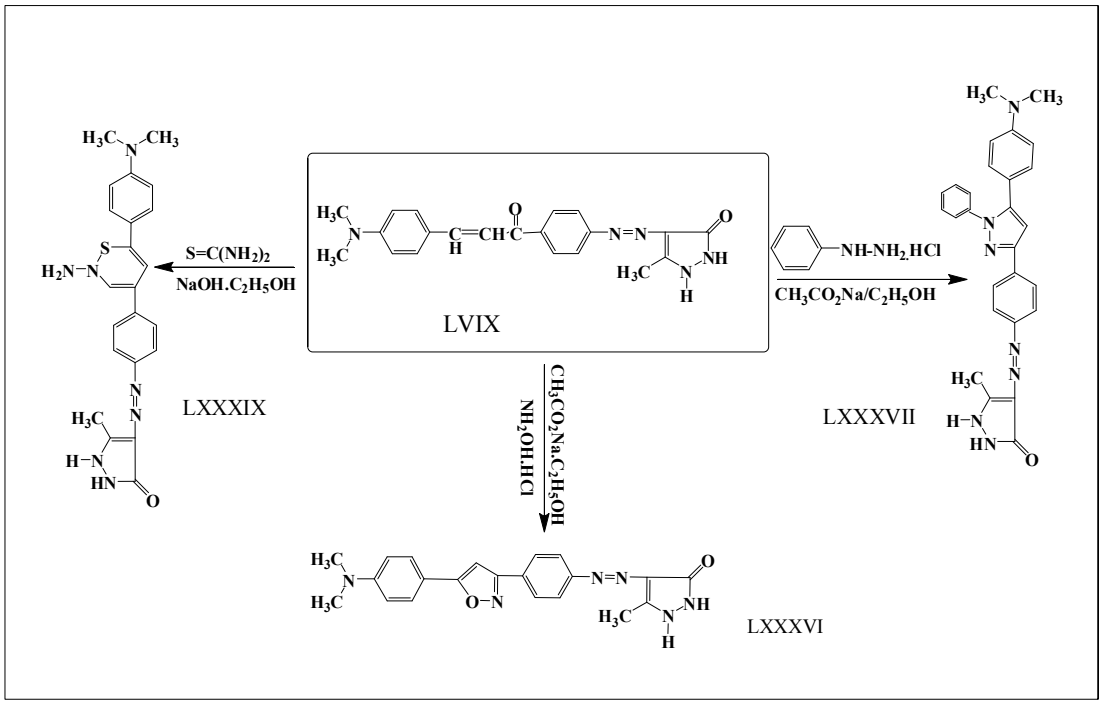
Scheme.2.16.Chemicalstructureof the synthesized 4-diazo-(p-(5-(4-methoxy phenyl)-hetero aryl)-3,5-dimethyl-1-2,4-dinitrophenyl-pyrazole



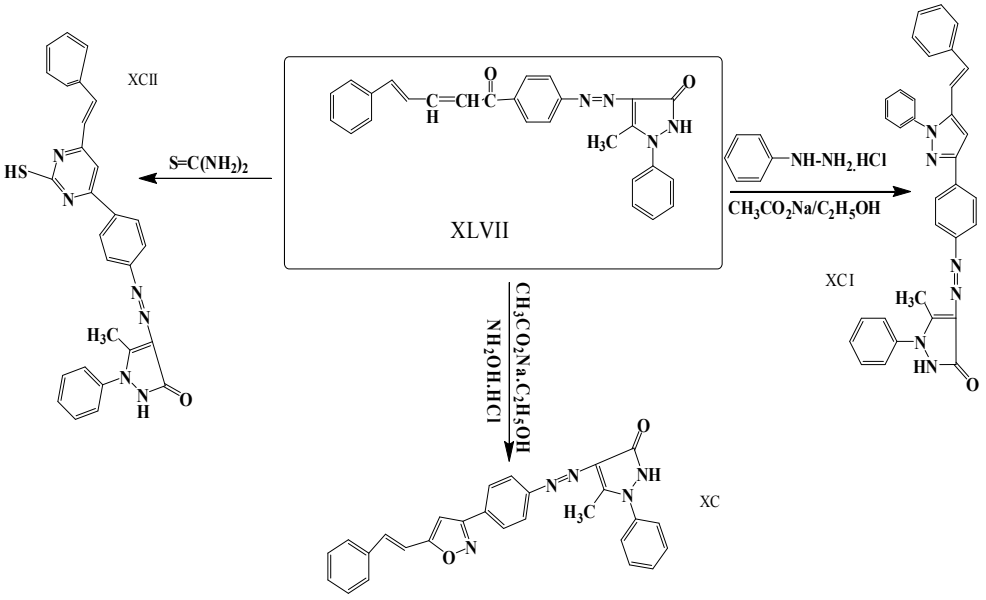
Scheme.2.17.Chemicalstructureof the 4-diazo-(p-(5-(2-nitro phenyl)-hetero aryl)-3,5-dimethyl-1-2,4-dinitrophenyl-pyrazole



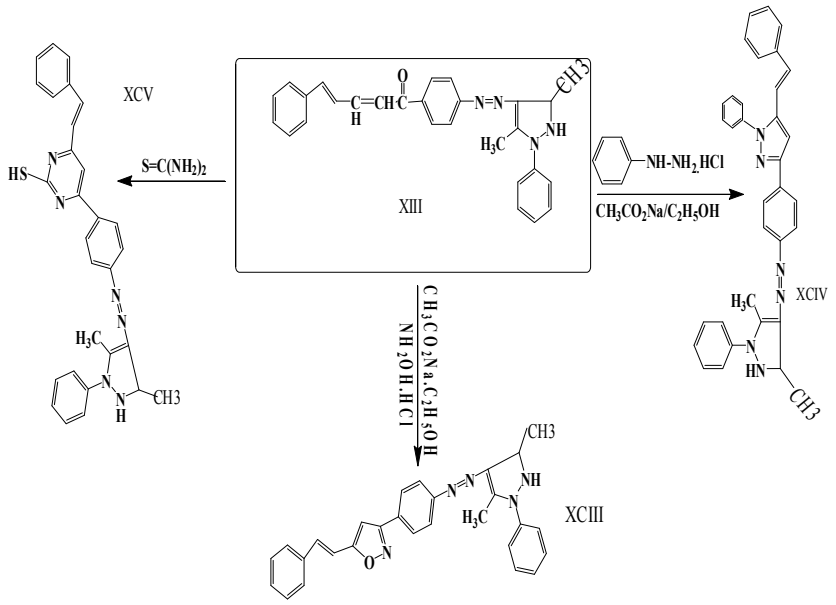
Scheme.2.18.Chemicalstructureof the synthesized 4-diazo-(p-(5-(2-hydroxyphenyl)-heteroaryl)-3,5-dimethyl-1-2,4-dinitrophenyl-pyrazole



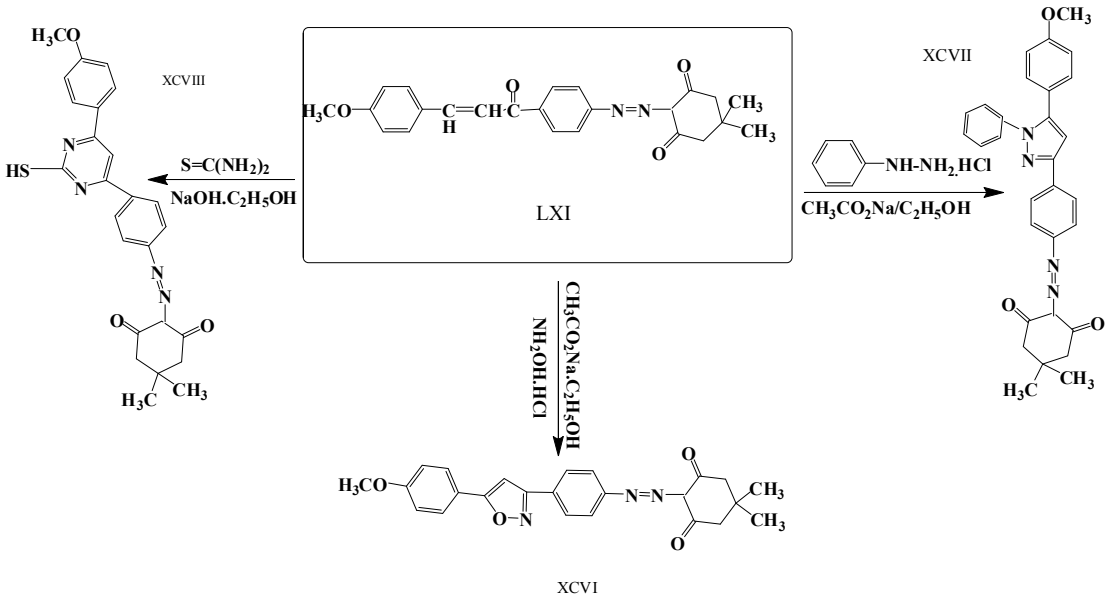
Scheme.2.19. Chemical structure of the synthesized 4-diazo-(p-(5-(p-N,N-dimethylaminophenyl)hetero aryl)-phenyl-5-methyl-pyrazol-3-ones



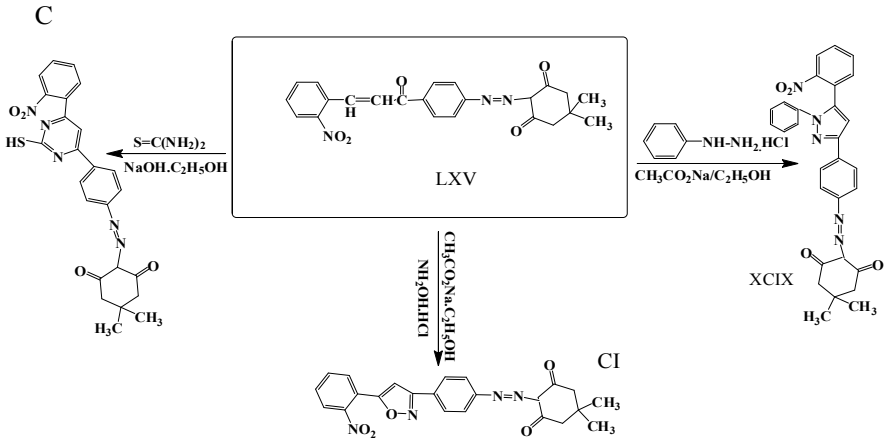
Scheme.2.20. Chemical structure of the synthesized 4-diazo-(p-(5-(2-phenylethenyl))hetero aryl)-phenyl-5-methyl-pyrazol-3-ones



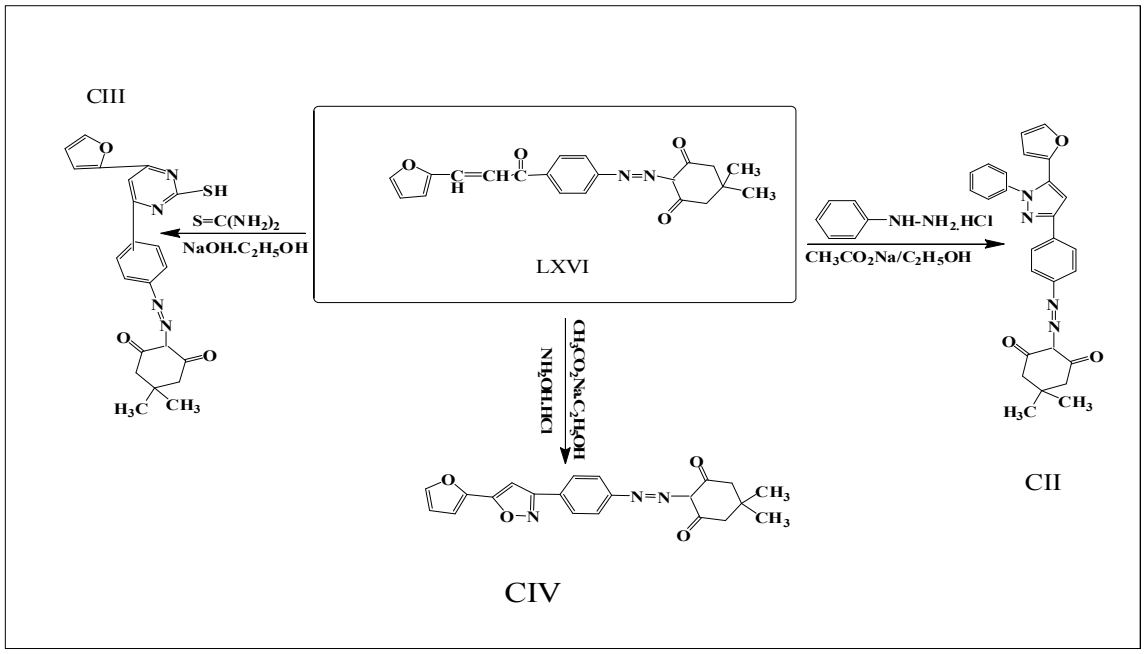
Scheme.2.21. Chemical structure of the synthesized 4-diazo-(p-(5-(2-phenylethenyl))hetero aryl)-phenyl-3,5-dimethyl-1-phenyl pyrazole



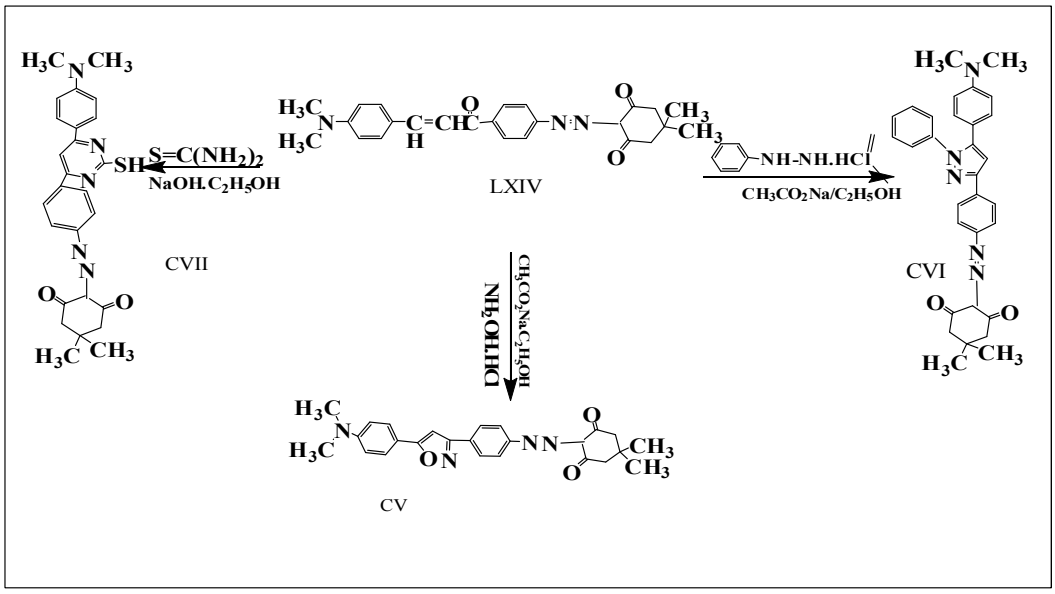
Scheme.2.22. Chemical structure of the synthesized 4-diazo-(p-(5-(4-methoxyphenyl))heteroaryl)-phenyl-3,5-dimethyl-cyclo hexane-1,3-diones



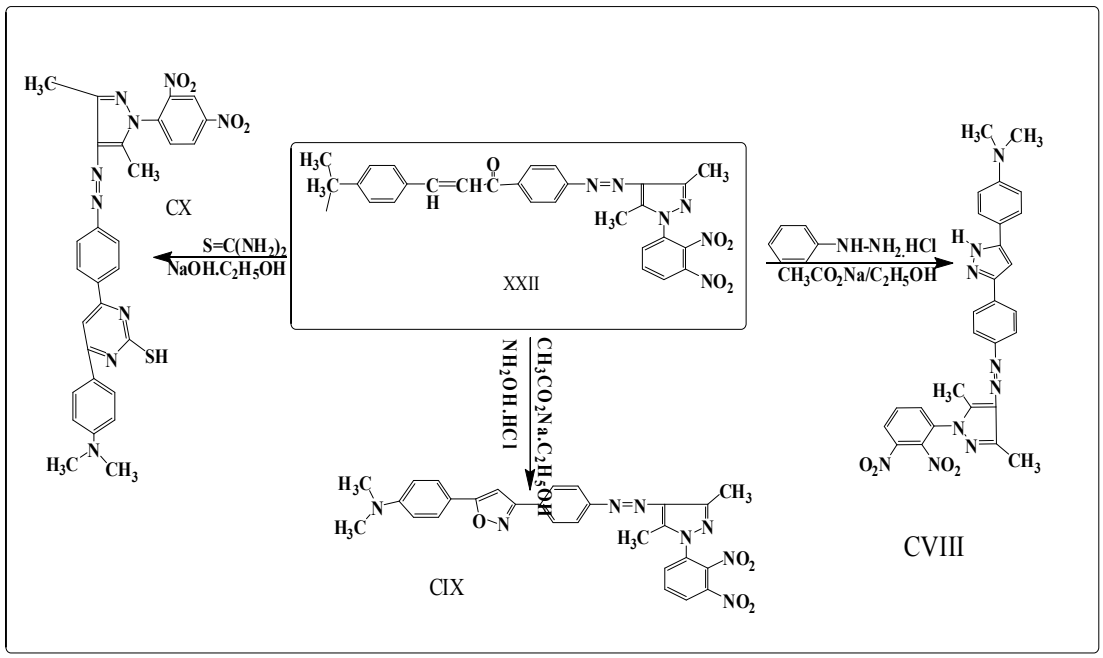
Scheme.2.23. Chemical structure of the synthesized 4-diazo-(p-(5-(2- nitro phenyl))heteroaryl)-phenyl-3,5-dimethyl-cyclo hexane-1,3-diones



Scheme.2.24. Chemical structure of the synthesized 4-diazo-(p-(5-(rural) heteroaryl)-phenyl-3,5-dimethyl-cyclo hexane-1,3-diones



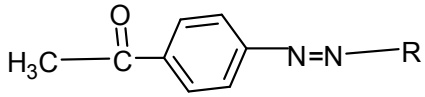
Scheme.2.25. Chemical structure of the synthesized 4-diazo-(p-(5-(p-N,N-dimethylamino phenyl))heteroaryl)-phenyl-3,5-dimethyl-cyclo hexane-1,3-dion



Scheme.2.26.Chemicalstructureof the 4-diazo-(p-(5-(p-N,N-dimethylamino phenyl)-hetero aryl)-3,5-dimethyl-1-2,4-dinitrophenyl-pyrazole

2.2. Chemical names of synthesized compounds

Table2.2.1 Chemical name of synthesis diazo (p-acetyl phenyl)- 1, 3-diones derivatives (I –IV).



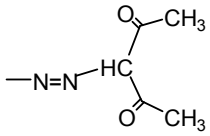
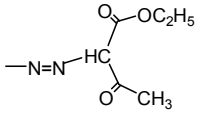
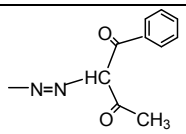
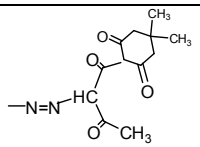
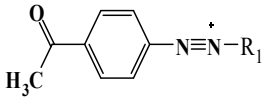
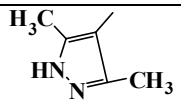
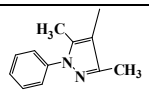
Compound number	**R**	Chemical names
I		diazo-(p-acetylphenyl)pentane-1,3-diones
II		diazo-(p-acetylphenyl)-ethyl acetoacetate
III		diazo-(p-acetyl phenyl)-benzoylacetone
IV		diazo-(p-acetyl phenyl)-dimedone

Table.2.2.2. Chemical name of the 4-diazo-(p-acetyl phenyl)-1- pyrazole derivatives (V- XII)



Comp.No	R_1	Chemical Name
V		4-diazo-(p-acetyl phenyl) -3,5 dimethyl-pyrazole
VI		4- diaozo-(p-acetyl phenyl)-3,5dimethyl-1-phenyl pyrazole

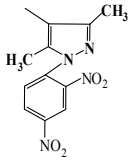
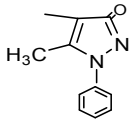
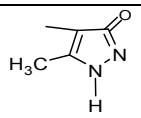
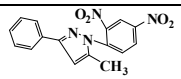
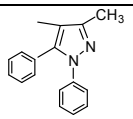
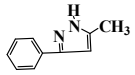
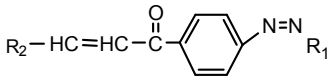
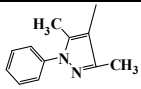
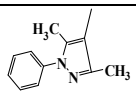
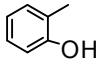
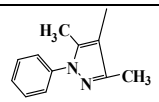
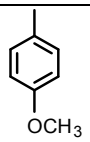
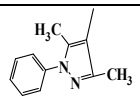
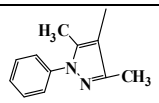
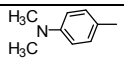
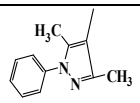
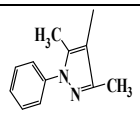
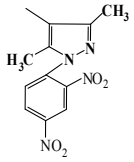
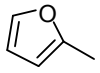
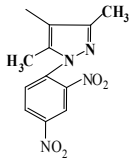
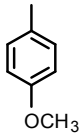
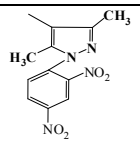
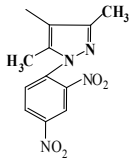
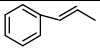
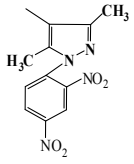
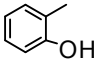
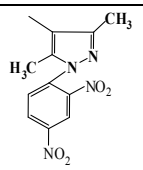
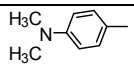
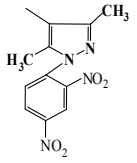
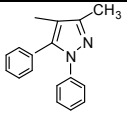
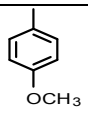
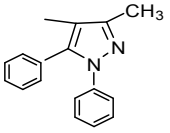
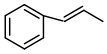
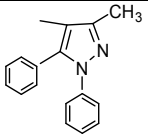
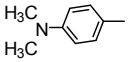
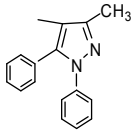
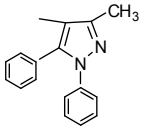
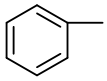
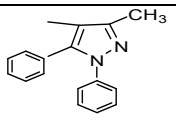
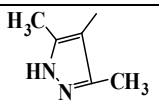
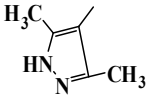
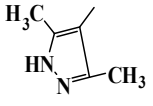
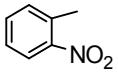
VII		4-diao-(p-acetyl phenyl)-3,5-dimethyl-1-2,4dinitrophenyl pyrazole
VIII		4-diazo(p-acetyl phenyl)-5-meththyl-1-phenyl pyrazole-3-one
IX		4-diazo-(p-acetyl phenyl)-5-methyl pyrazol-3-one
X		4-diazo-(p-acetyl phenyl(-5-methyl-3-2,4 dinitrophenyl-1-phenyl pyrazole
XI		4-diazo-(p-acetyl phenyl)-5-methyl-1,3 phenyl pyrazole
XII		4-diazo-(p-acetyl phenyl)-5-methlpyrazole

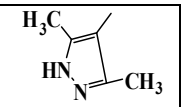
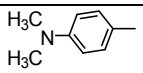
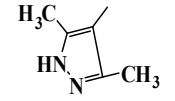
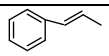
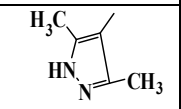
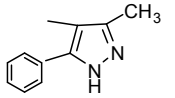
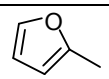
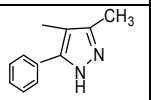
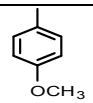
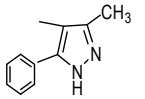
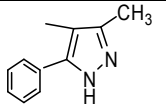
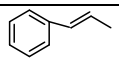
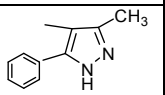
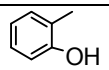
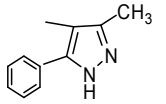
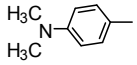
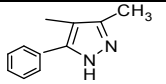
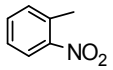
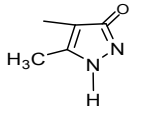
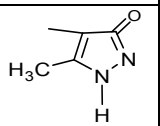
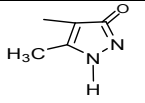
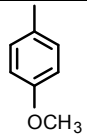
Table 2.2.3. Chemical names of the synthesized compounds (p-(aryl)-alken-1-on)phenyl)-pyrazole derivatives and dimedone (XIII-LXVII)

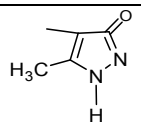
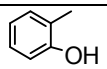
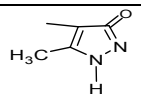
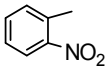
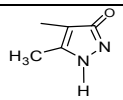
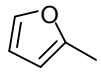
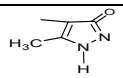
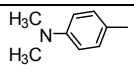
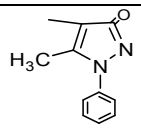
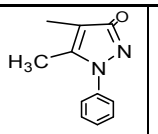
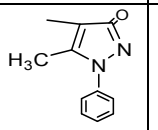
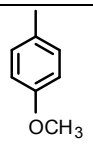
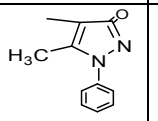
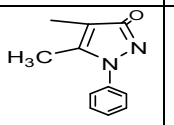
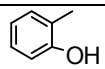
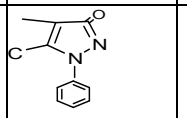
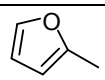
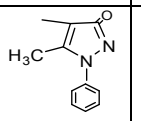
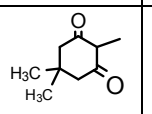
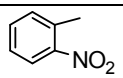


Comp. No	R_1	R_2	Chemical names
XVII			4-diazo-(p(2-nitrophenyl) propen-1-on)phenyl-3,5-dimethyl-1-phenyl pyrazole
XIX			4-diazo-(p-(3-(2-hydroxy) propen-1-on)phenyl-3,5-dimethyl-1-phenyl pyrazole

XV			4-diazo-(p(3(4-methoxy) propen-1-on)phenyl-3,5-dimethyl-1-phenyl pyrazole
XIII			4-diazo-(p-(5-phenyl-pent-2,4-dien-1-on)-phenyl)-3,5-dimethyl-1-phenylpyrazole
XVIII			4-diazo-(p-(3-(p-N,N-dimethyl amino phenyl)-propen-1-on)phenyl)-3,5-dimethyl-1-phenyl pyrazole
XVI			4-diazo-(p-(3-fural)propen-1-on)phenyl)-3,5-dimethyl-1-phenyl pyrazole
XIV			4-(diazo-(p-(3-(phenyl) propen-1-on) phenyl)-3,5-dimethyl-1-phenyl pyrazole
XXI			4-diazo-(p-(3-(fural)-propen-1-on)phenyl)-3,5-dimethyl-1-2,4-dinitro phenyl-pyrazole
XX			4-diazo-(p-(3-(4-methoxyphenyl)-propen-1-on)phenyl)-3,5-dimethyl-1-2,4-dinitro phenyl-pyrazole
XXVI			4-diazo-(p-(3-(phenyl)-propen-1-on)phenyl)-3,5-dimethyl-1-2,4-dinitro phenyl-pyrazole
XXV			4-diazo-(p-(5-phenyl-pent-2,4-dien-1-on) phenyl)-3,5-dimethyl -1-2,4-dinitro-phenyl-pyrazole
XXIV			4-diazo-(p-(3-(2-hydroxy phenyl)-propen-1-on)phenyl)-3,5-dimethyl-1-2,4-dinitro phenyl-pyrazole

XXIII			4-diazo-(p-(3-(p-N,N-dimethyl amino phenyl)-propen-1-on) phenyl)-3,5-dimethyl-1-2,4-dinitro phenyl-pyrazole
XXII			4-diazo-(p-(3-(2-nitro-phenyl)-propen-1-on)phenyl)-3,5-dimethyl-1-2,4-dinitro phenyl-pyrazole
XXXV			4-diazo-(3-(p-(4-methoxy phenyl)-propen-1-on)phenyl)-5-methyl-1,3diphenyl pyrazole
XXXIV			4-diazo-(p-(5-phenyl-pent-2,4dien)phenyl-5-meth-1,3di-phenyl-pyrazole
XXXIX			4-diazo-(p-(3-(p-N,N-dimethyl amino phenyl)-propen-1-on) phenyl)-5-methyl-1,3 diphenyl-pyrazole
XXXVII I			4-diazo-(p-(3-(fural)-propen-1-on)-phenyl)-5-methyl-1,3-diphenyl-pyrazole
XXXVII			4-diazo-(p-(3-(phenyl)-propen-1-on)-phenyl)-5-methyl-1,3-diphenyl-pyrazol
XXXVI			4-diazo-(p-(3-(2-nitrophenyl)-propen-1-on)-phenyl)-5-methyl-1,3-diphenyl-pyrazol
XXIX			4-diazo-(p-(3(4methoxyphenyl)-propen-1-on)-phenyl)-3,5-dimethyl-pyrazole
XXXIII			4-diazo-(p-(3(2-hydroxyphenyl)-propen-1-on)-phenyl)-3,5-dimethyl-pyrazoe
XXXI			4-diazo-(p-(3(2-nitrophenyl)-propen-1-on)-phenyl)-3,5-dimethyl-pyrazoe

XXXII			4-diazo-(p-(3(p-dimethyl amino2-hydroxy-phenyl)-propen-1-on)-phenyl)-3,5-dimethyl-pyrazole
XXVII			4-diazo-(p-2-hydroxy-4methoxyphenyl)-propen-1-on)-phenyl)-3,5-dimethyl-pyrazoe
XXVII			4-diazo-(p-(phenyl)-propen-1-on)-phenyl)-3,5-dimethyl-pyrazoe
XLIII			4-diazo-(p-(3-(furan)-propen-1-on)phenyl)-3-phenyl-5- methyl -pyrazole
XLII			4-diazo-(p-(3-(4-methoxyphenyl)-propen-1-on)phenyl-5-methyl-3-phenyl-pyrazole
XLI			4-diazo-(p-(3-(phenyl)-propen-1-on)phenyl-5-methyl-3-phenyl-pyrazole
XL			4-diazo-(p-(phenylethenyl)-phenyl)-propen-1-on) phenyl-5-methyl-3-phenyl-pyrazole
XLVI			4-diazo-(p-((2-hydroxyphenyl)-propen-1-on) phenyl-5-methyl-3-phenyl-pyrazole
XLV			4-diazo-(p-((p-N,N-dimethyl amino phenyl)-propen-1-on) phenyl-5-methyl-3-phenyl-pyrazole
XLIV			4-diazo-(p-((2-hydroxy phenyl)-propen-1-on)phenyl-5-methyl-3-phenyl-pyrazole
LIV			4-diazo-(p-(5-phenyl-ethenyl-1-on)-phenyl)-5-methyl-pyrazol-3-one
LV			4-diazo-(p-((phenyl)-propen-1-on)-phenyl)-5-methyl-pyrazol-3-one
LVI			4-diazo-(p-((-4-methpxyphenyl)-propen-1-on)-phenyl)-5-methyl-pyrazol-3-one

LX			4-diazo-(p-((2-hydroxy phenyl)-propen-1-on)-phenyl)-5-methyl-pyrazol-3-one
LVIII			4-diazo-(p-(3(2-nitro-phenyl)-propen-1-on)-phenyl)-5-methyl-pyrazol-3-one
LVII			4-diazo-(p-(3(furan)-propen-1-on)-phenyl)-5-methyl-pyrazol-3-one
LVIX			4-diazo-(p-((p-N,N dimethyl amino phenyl)-propen-1-on)-phenyl)-5-methyl-pyrazol-3-one
XLVII			4-diazo-(p-(-phenyl-pent-2,4-dien-1-on)-phenyl)-5-methyl-1-phenyl-pyrazol-3-one
XLVIII			4-diazo-(p-(phenyl)-propen-1-on)-phenyl)-5-methyl-1-phenyl-pyrazol-3-one
XLIX			4-diazo-(p-((-4-methpxy phenyl)-propen-1-on)-phenyl)-5-methyl-1-phenyl-pyrazol-3-one
LI			4-diazo-(p-((2-nitro-phenyl)-propen-1-on)-phenyl)-5-methyl-1-phenyl-pyrazol-3-one
LIII			4-diazo-(p-((2-hydroxy-phenyl)-propen-1-on)-phenyl)-5-methyl-1-phenyl-pyrazol-3-one
L			4-diazo-(p-(3(furyl)-propen-1-on)-phenyl)-5-methyl-1-phenyl-pyrazol-1,3-ones
LII			4-diazo-(p-((p-N,N-dimethylamino-phenyl)-propen-1-on)-phenyl)-5-methyl-1-phenyl-pyrazol-1,3-one
LXV			2-diazo-(p-((2-nitrophenyl)-propen-1-on)phenyl)-5,5-dimethyl-hexane-1,3-diones

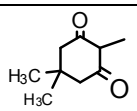
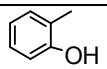
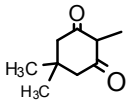
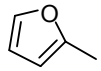
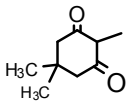
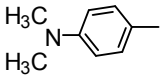
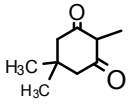
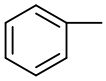
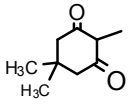
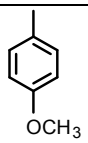
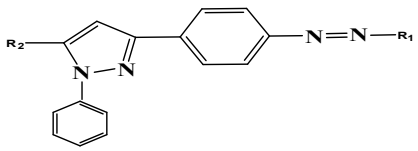
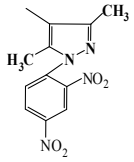
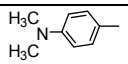
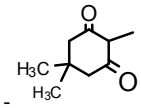
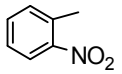
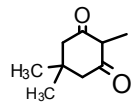
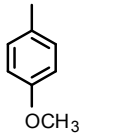
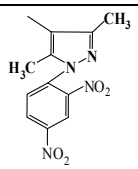
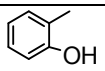
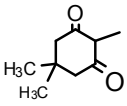
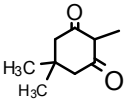
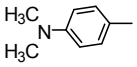
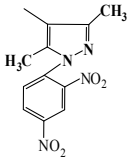
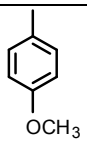
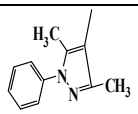
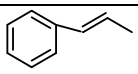
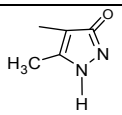
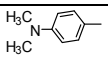
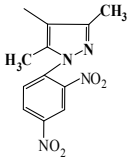
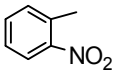
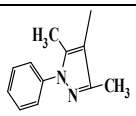
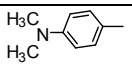
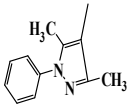
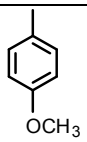
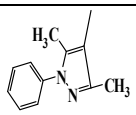
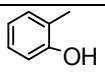
LXIII			2-diazo-(p-((2-hydroxyphenyl)-propen-1-on) phenyl)-5,5-dimethyl-hexane-1,3-diones
LXVI			2-diazo-(p-((furyl)-propen-1-on)phenyl)-5,5-dimethyl-hexane-1,2-diones
LXIV			2-diazo-(p-((p-(N,N-dimethyl aminophenyl)-propen-1-on)-phenyl)-5,5-dimethyl-1,3-diones
LXII			2-diazo-(p-((phenyl)-propen-1-on)-5,5-dimethyl-hexane-1,3-diones
LXI			2-diazo-(p-(4-methoxyphenyl)-propen-1-on)-5,5-dimethyl-1,3-diones

Table. 2.2.4. Chemical names of the synthesizedof pyrazole-derivatives (LXIX-CVI)



Comp.No	R_1	R_2	Chemical names
LXXVIII			4-dizo-(p-(5-(p-N,N-dimethyl amino phenyl)-phenylpyrazol-2-phenyl-3-yl)-phenyl)-3,5-dimethyl-1-2,4-dinitrophenyl-pyrazole
XCIX			4-diazo-(p-(5-(2-nitro phenyl)-phenylpyrazol-2-phenyl-3-yl)-5,5-dimethyl-hexane-1,3-diones
XCVII			4-diazo-(p-(5-(4-methoxyphenyl)-phenyl pyrazol-2-phenyl-3-yl)-5,5-dimethyl-hexane-1,3-diones

LXXXIV			4-dizo-(p-(2-hydroxyphenyl)-phenylpyrazol-2-phenyl-3-yl)-phenyl)-3,5-dimethyl-1-2,4-dinitrophenyl-pyrazole
XVIX			4-diazo-(p-(5-(fural)-phenyl pyrazol-2-phenyl-3-yl)-5,5-dimethyl-hexane-1,3-diones
CVI			4-diazo-(p-(5-(p-(N,N-dimethyl amino phenyl)-phenyl pyrazol –pheny-3-yl)-5,5-dimethyl-hexane-1,3-diones
LXXVIII			4-dizo-(p-(5-(p(4-methoxyphenyl)-phenylpyrazol-2-phenyl-3-yl)-phenyl)-3,5-dimethyl-1-2,4-dinitrophenyl-pyrazole
XCIV			4-diazo-(p-(5-(2-phenyl ethenyl) -pyrazol-2-phenyl-3yl)-phenyl)-3,5-dimethyl-1-2,4-dinitrophenyl-pyrazole
LXXXVII			4-diazo-(p-(5-(N,N- dimethyl amino phenyl)-pyrazol-2-phenyl-3-yl)-phenyl)-5-methyl-pyrazol-3-one
LXXXI			4-dizo-(p-(5-(2-nitrophenyl)-phenyl pyrazol-2-phenyl-3-yl)-phenyl)-3,5-dimethyl-1-2,4-dinitrophenyl-pyrazole
CX			4-diazo-(p-(5-(N,N-dimethyl amino phenyl)-2-phenylpyrazol-3-l)-phenyl)-3,5-dimethyl-1-phenyl-pyrazole
LXXII			4-dizo-(p-(5-(-4-methoxyphenyl)-phenyl pyrazol-2-phenyl-3-yl)-phenyl)-3,5-dimethyl-1-2,4-dinitro phenyl-pyrazole
LXXV			4-dizo-(p-(5-(2-hydroxyphenyl)-phenylpyrazol-2-phenyl-3-yl)-phenyl)-3,5-dimethyl-1-2,4-dinitrophenyl-pyrazole

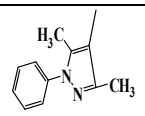
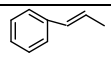
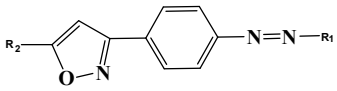
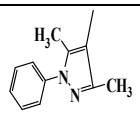
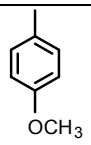
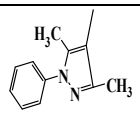
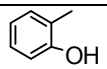
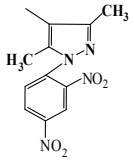
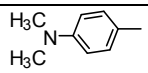
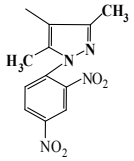
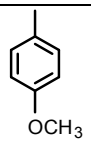
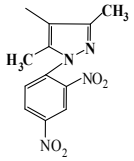
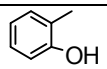
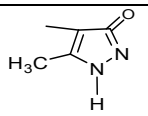
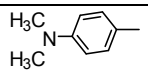
XCIV			4-diazo-(2-phenylethenyl)-pyrazol-2-phenyl-3-yl)-phenyl)-3,5-dimethyl-1-phenyll-pyrazole

Table 2.2.5. Chemical names of the synthesized of isoxazole derivatives(LXVIII-CV)



Comp.No	R_1	R_2	Chemical names
LXXI			4-diazo-(p-(5-(-4-methoxy phenyl)-isoxazol-5-yl)-phenyl)-3,5-dimehyl -1-phenyl pyrazole
LXXIV			4-diazo-(p-(5-(2-hydroxy phenyl)-isoxazol -5-yl)-phenyl)-3,5-dimehyl-1-phenyl pyrazole
CIX			4-diazo-(p-(5-(p-N,N-dimethyl amino phenyl) -isoxazol-5-yl)-phenyl)-3,5-dimehyl -1-2,4-dinirophenyl pyrazol
LXXVII			4-diazo-(p-(5-(-4-mehoxy phenyl)-isoxazol-5-yl)-phenyl)-3,5-dimehyl-1-2,4-dinirophenyl pyrazole
LXXXIII			4-diazo-(p-(5-(2-hydroxy phenyl) -isoxazol-5-yl)-phenyl)-3,5-dimehyl-1-2,4-dinirophenyl pyrazole
LXXXVI			4-diazo-(p-(5-(2-phenylethenyl)-isoxazol-5-yl)-phenyl-5-methyl- pyrazole-3-one

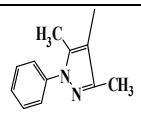
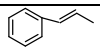
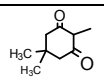
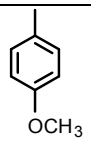
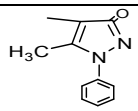
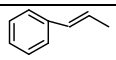
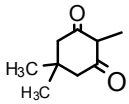
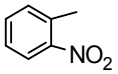
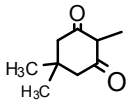
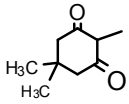
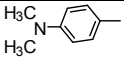
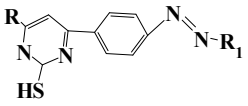
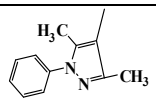
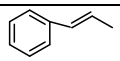
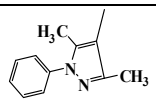
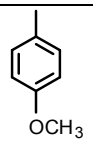
XCIII			4-diazo-(p-(5-(2-phenyl ethenyl) -isoxazol-5-yl)-phenyl)-3,5-dimehyl-1-phenyl pyrazole
XCVI			4-diazo-(p-(5-(-4-methoxy phenyl)-1soxazol-5-yl)-phenyl-5,5-dimethyl -hexane-1,3-diones
XC			4-diazo-(p-(5-(2-phenyl ethenyl) -isoxazol-5-yl)-phenyl)-5-mehyl -1-phenyl pyrazole-1-one
CI			2-diazo-(p-(5-(2-nitro phenyl)-1soxazol-5-yl)-phenyl-5,5-dimethyl-hexane-1,3-diones
CIV			2-diazo-(p-(5-(fural)-1soxazol-5-yl)-phenyl-5,5-dimethyl-hexane-1,3-diones
CV			2-diazo-(p-(5-(p-N,N-dimethyl amino phenyl)-1soxazol-5-yl)-phenyl-5,5-dimethyl-hexane-1,3-diones

Table.2.2.6.Chemical names of synthesis of pyrimidine derivatives(LXX-CVII)



Comp.NO	R_1	R_2	Chemical name
XCV			4-diazo-(p-(5-(2-phenyl ethenyl)-2-thio pyrimidine-6-yl)-phenyl-3,5-dimethyl-1-phenylpyrazole
LXXIII			4-diazo-(p-(5-(-4-methoxy)-2-thio pyrimidine-6-yl)-phenyl-3,5-dimethyl-1-phenylpyrazole

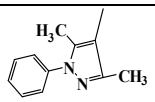
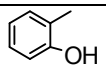
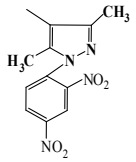
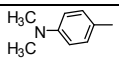
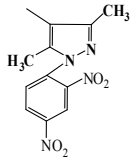
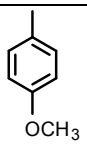
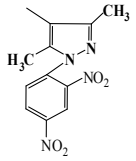
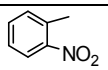
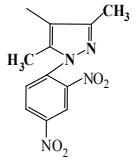
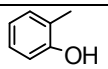
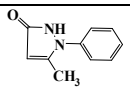
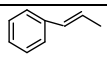
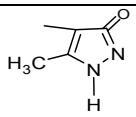
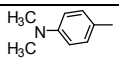
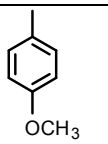
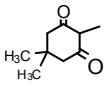
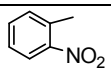
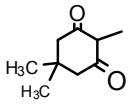
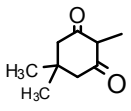
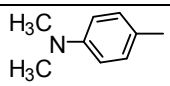
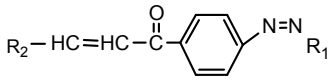
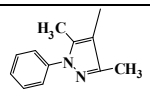
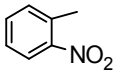
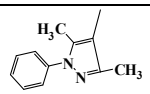
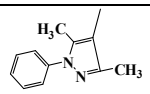
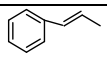
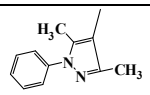
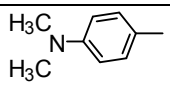
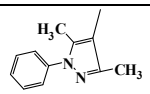
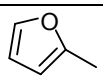
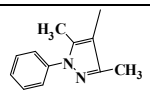
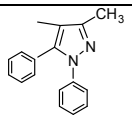
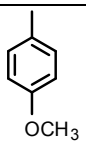
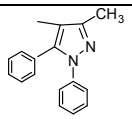
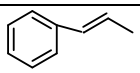
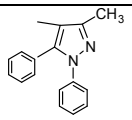
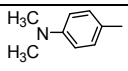
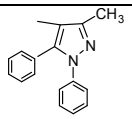
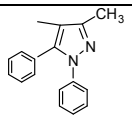
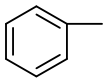
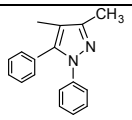
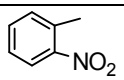
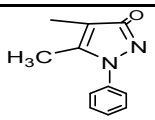
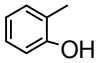
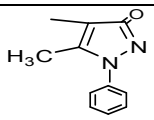
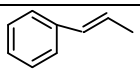
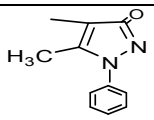
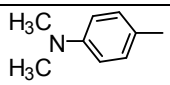
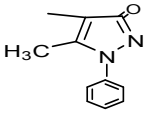
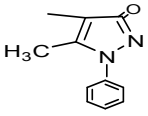
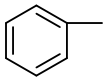
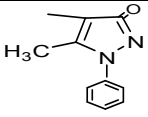
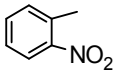
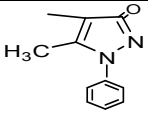
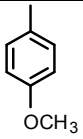
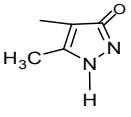
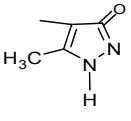
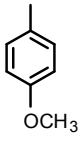
LXXVI			4-diazo-(p-(5-(2-hydroxy)-2-thio pyrimidine-6-yl)-phenyl-3,5-dimethyl-1-phenylpyrazole
CXI			4-diazo-(p-(5-(p-N,N-dimethyl phenyl)-2-thiopyrimidine-6-yl)-phenyl-3,5-dimethyl-1-2,4-diphenylpyrazole
LXXIX			4-diazo-(p-(5-(-4-methoxyphenyl)-2-thio pyrimidine -6-yl)-phenyl-3,5-dimethyl-1-2,4-diphenylpyrazole
LXXXII			4-diazo-(p-(5-(2-nitro phenyl)-2-thio pyrimidine-6-yl)-phenyl -3,5-dimethyl-1-2,4-diphenyl pyrazole
LXXXV			4-diazo-(p-(5-(2-hydroxy phenyl)-2-thio pyrimidine-6-yl)-phenyl-3,5-dimethyl-1-2,4-diphenylpyrazole
XCV			4-diazo-(p-(2-phenylethenyl)-thio pyrimidine-6-yl)-phenyl-5-methyl-1-phenylpyrazol-3-one
LXXXIX			di azo -(p-(5-(p-N,N-dimethyl amino phenyl)-2-thio pyrimidine -6-yl)-phenyl-5-methyl-pyrazol-3-one
XCVIII			2-diazo-(p-(5-(-4-methoxyphenyl)-2-thiopyrimidine-6-yl)-phenyl-5,5-dimethyl-hexane-1,3-diones
C			2-diazo-(p-(5-(2-nitro phenyl)-2-thio pyrimidine-6-yl)-phenyl-5,5-dimethyl-hexane-1,3-diones
CIII			2-diazo-(p-(5-(furan)-2-thio pyrimidine-6-yl)-phenyl-5,5-dimethyl-hexane-1,3-diones
CVII			2-diazo-(p-(5-(p-N,N-dimethyl aminophenyl)-2-thiopyrimidine-6-yl)-phenyl-5,5-dimethyl-hexane-1,3-diones

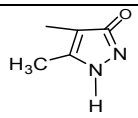
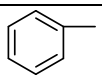
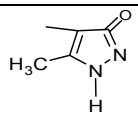
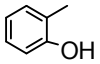
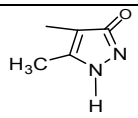
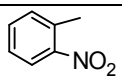
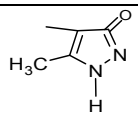
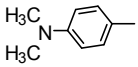
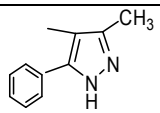
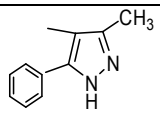
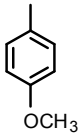
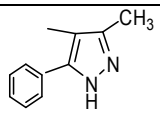
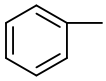
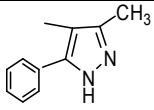
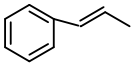
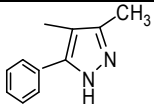
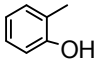
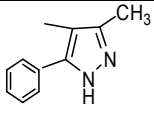
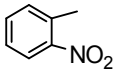
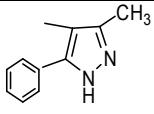
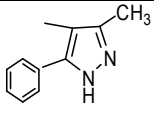
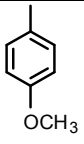
Table 2.3. Reaction conditions of synthesized compounds

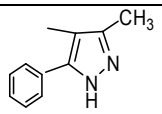
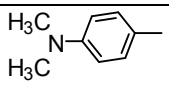
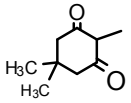
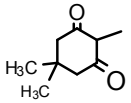
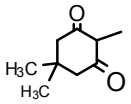
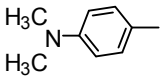
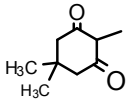
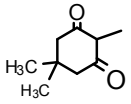
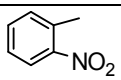
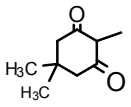
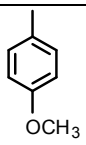
Table 2.3.1.Reaction conditions of α, β- unsaturated carbonyl derivatives



Comp.No	R_1	R_2	Yield%	M.P
XVII			63%	188-189 °C
XIX			75%	152-253 °C
XIII			53%	176-178 °C
XVIII			66%	135-136 °C
XVI			77%	199-200 °C
XIV			94%	190-192 °C
XXXV			89%	72-76 °C
XXVI			92%	208-209 °C
XXIX			42**%**	163-164 °C

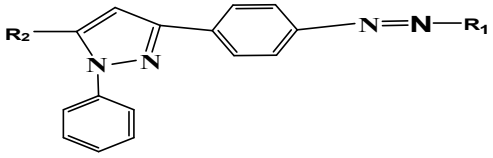
XXXVIII			57%	132-135 °C
XXXVII			63%	87-88 °C
			72%	170-172 °C
LIII			55%	174-175 °C
XLVII			74%	144-145 °C
LII			52%	215-216 °C
L			79%	156-158 °C
XLVIII			67%	245-246 °C
LI			63%	92-93 °C
XLIX			35%s	166-167 °C
LVII			95%	149-150 °C
LVI			72%	180-181 °C

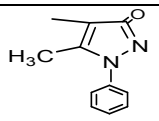
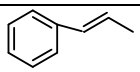
LV			76%	298-299 °C
LX			77%	213-214 °C
LVIII			73%	120-121 °C
LVIX			93%	81-82 °C
XLIII			89%	130-131 °C
XLII			81%	125-126 °C
XLI			95%	121-122 °C
XL			77%	228-229 °C
XLVI			68%	211-213 °C
XLIV			59%	240-241°C
XLIII			79%	205-206 °C
XLII			44%	248-249 °C

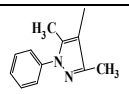
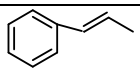
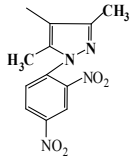
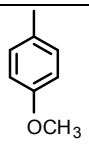
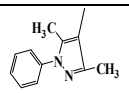
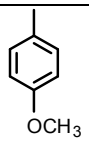
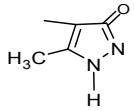
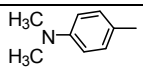
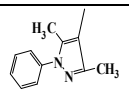
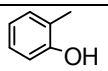
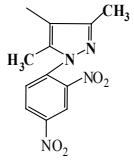
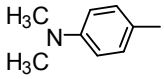
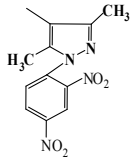
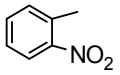
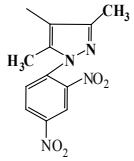
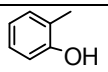
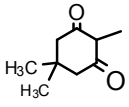
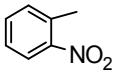
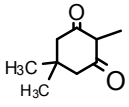
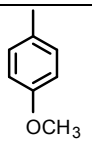
XLV			61%	204-205 °C
LXI			85%	199-201 °C
LXVI			96%	182-183 °C
LXIV			80%	132-133°C
LXII			83%	146-147 °C
LXV			82%	161-162°C
LXI			86%	211-212 °C

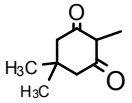
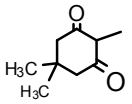
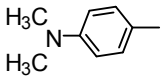
Reaction time: 24 hours, Recrystallized: ethanol, Reaction condition: room temperature.

Table 2.3.2.Reaction condition of synthesized Pyrazole Derivatives.



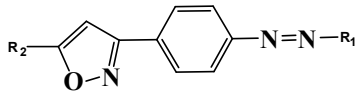
Comp.NO	R_1	R_2	Yield%	m. p
XCI			88%	122-123 °C

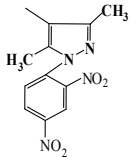
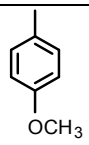
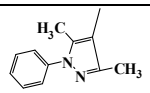
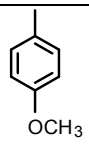
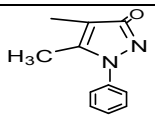
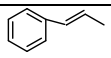
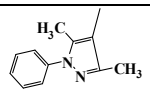
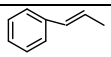
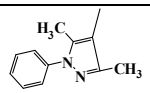
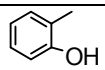
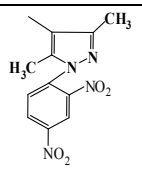
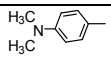
XCV			84%	123-124 °C
LXVIII			63%	145-146°C
LXXII			81%	117-118 °C
LXXXVI			88%	171-172 °C
LXXV			98%	252-253 °C
CX			50%	
LXXX			79%	241-242 °C
LXXXIV			74%	182-183°C
XCIX			89%	241-242°C
XCVII			98%	110-111°C

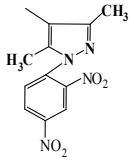
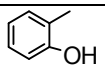
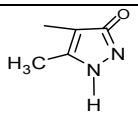
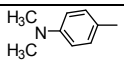
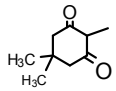
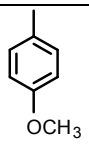
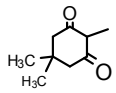
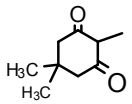
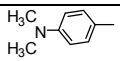
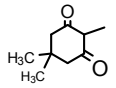
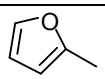
CIII			65%	140-141°C
CVI			86%	149-150°C

Reaction time :13-16 hours, Temperature: 90-100, Recrystallized solvent: ethanol

Table 2.3.3.Reaction condition of synthesized isoxazole derivatives.

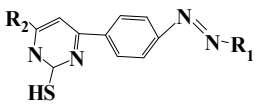


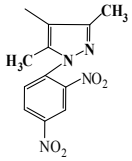
Comp.NO	R1	R3	Yield %	m.p
LXXVII			85%	153-154 °C
LXXI			78%	164-165 °C
XC			81%	116-117 °C
CV			55%	134-135 °C
LXXIV			86%	253-254 °C
CIX			55%	154-155 °C

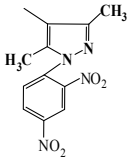
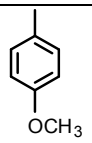
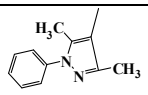
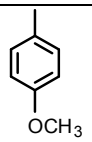
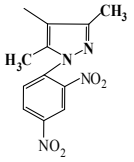
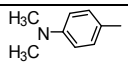
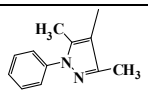
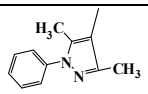
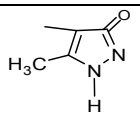
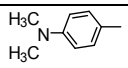
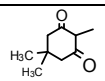
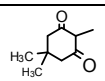
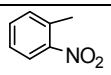
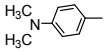
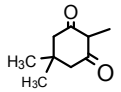
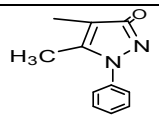
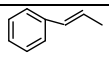
XXXIII			66%	154-155°C
LXXXVII			25%	171-172 °C
XCVI			91%	134-135 °C
CI			77%	189-190°C
CVI			83%	140-142°C
CIV			92%	150- 152 °C

Reaction time: 9-10 hours, Temperature: 90-100, Recrystallized solvent: ethanol

Table 2.3.4. Reaction condition of pyrimidine derivatives:



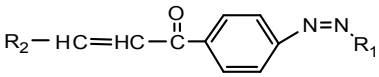
Comp.No	R_1	R_2	Yield%	m.p
LXXXV			63%	126-128°C

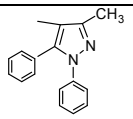
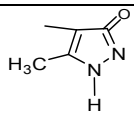
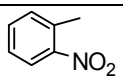
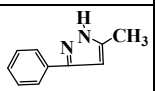
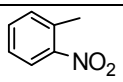
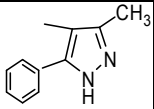
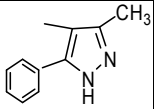
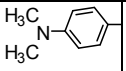
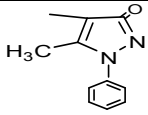
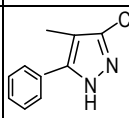
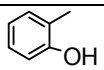
LXXIX			85%	148-149 °C
LXXIII			66%	136-138 °C
CVIII			68%	114-115 °C
XCV			86%	140-141 °C
LXXVI			51%	143-144 °C
LXXXIX			43%	163-164°C
XCVII			83%	161-162°C
C			87%^	253-254°C
CVII			85%	116-115°C
CIII			95%	185-186°C
XCII			56%	145-146°C

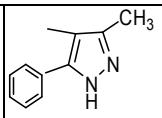
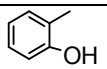
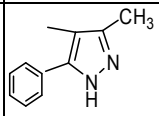
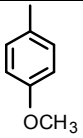
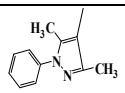
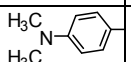
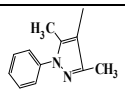
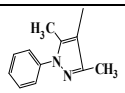
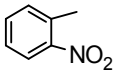
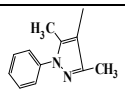
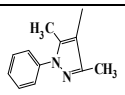
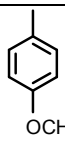
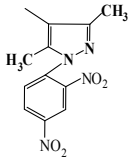
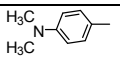
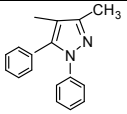
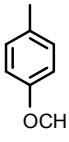
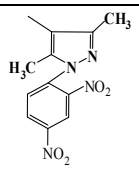
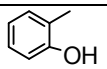
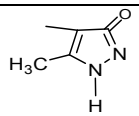
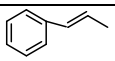
Reaction time: 8-10 hours, Temperature: 90-100, Recrystallized solvent : ethanol

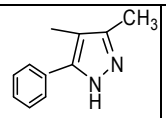
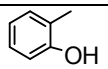
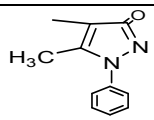
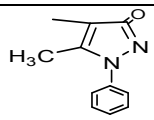
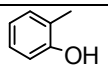
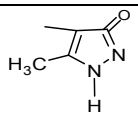
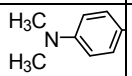
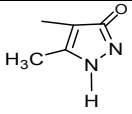
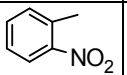
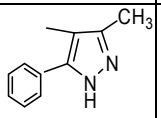
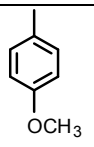
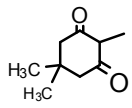
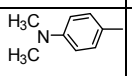
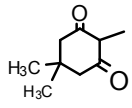
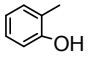
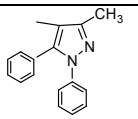
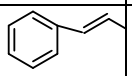
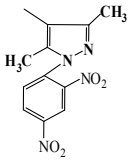
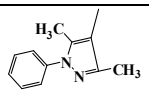
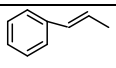
Table 2.4. Infra red spectrum bands of synthesized compounds

Table 2.4.1. Infra red spectrum bands of α, βunsaturated carbonyl derivatives



	R_2	R_3	C=O st.vib	N=N olefin st.vb	C=C arom st.vib	N-N arom st.v.b	C=N arom st.vib	C-N st.vib	Other grops
XXXVII			1695	1659	1539	1017	1594	1344	-
LVIII			1679, 1691	1661	1588	1102	1584	1319	3435(N-H), 1503, 1345(NO_2)
XLIV			1681	1645	1597	1113	1597	1343	1495, 1356
XLI			1694	1655	1560	1042	1592	1331	-
XLV			1693	1669	1566	1052	1569	1337	3448(N-H)
LVII			1693, 1657	1669	1585	1174	1572	1331	1154(C-O)
XIX			1681	1633	1572	1054	1547	1343	3491 (OH), 3441(N-H)

XLVI			1693	1657	1560	1066	1597	1307	3431 (OH) 3232(N-H)
XLII			1693,	1669	1597	1052	1569	1343	1376 (OCH_3)
XVIII			1676	1642	1580	1079	1572	1329	1344 (4-$N(CH_3)$)
XVI			1673	1641	1560	1113	1560	1343	--
XVII			1671	1626	1577	1037	1627	1335	1500, 1335 (NO_2)
XIV			1675	1647	1598	1031	1601	-	--
XV			1673	1634	1577	1111	16 53	1346	1226 (OCH3)
XXIII			1681	1631	1571	1054	1555		1514 (NO_2) 1304 $N(CH_3)_2$
XX			1692	1641	1559	1040	15701	1345	1345(OCH_3
XXIV			1687	1645	1597	1049	1596	1339	3567(OH)
LIV			1681, 1654	1631	1585	1113	1571	1343	3364 (N-H)

XLVI			1687	1648	1572	1029	1646	1343	3386 (OH) 3168 (N-H)
XLVI II			1633, 1670	1638	1567	1036	1569	1332	-
LIII			1612, 1668	1638	1524	1218	1573	1329	3436 (OH)
LVIX			1695, 1674	1624	1572	1014	1572	1325	3468 (N-H)
LVIII			1650, 1676	1624. 25	1578. 68	1042. 27	1627	1343	1499, 1332.(**NO_2**), 3543(N-H)
XLII			1699	1696	1596	1029	1648	1 343	1295. (OCH_3,) (N-H) 3312
LXIV			1715, 1654	1689	1597	1090	13421 643	1342	$N(CH_3)_2$ 1314,1551(C=O)
LXIII			1693, 1655	1681	1585	1042	16453	1331	3305 OH
XXXI V			1693	1681	1585	1054	1645	1319	-
XXVI			1705	1681	1564	1102	1657	1331	-
XXV			1696	1679	1569	1053	1648	1322	-

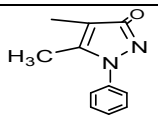
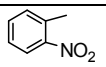
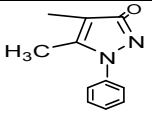
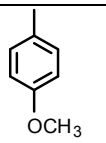
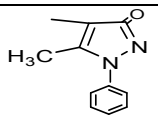
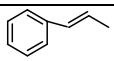
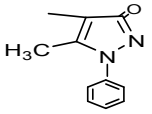
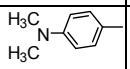
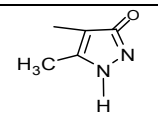
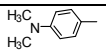
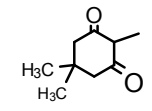
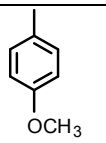
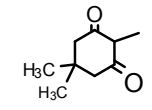
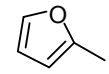
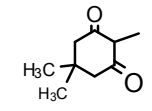
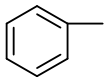
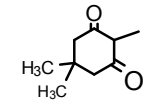
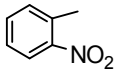
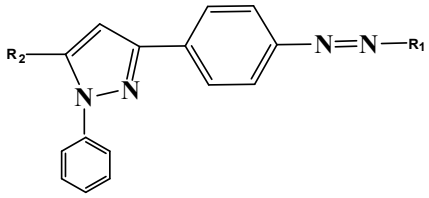
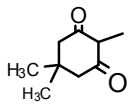
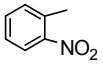
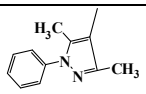
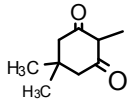
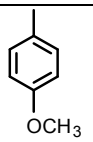
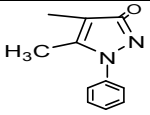
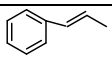
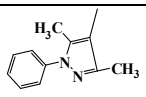
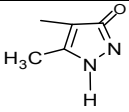
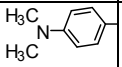
LI			1702, 1665	1654	1574	1046	1631	1346	1510,1369 (NO_2)
XLIX			1651, 1686	1576	1574	1043	1316 1606	1316	1309 (OCH_3)
XLVII			1682, 1663	1657	1581	1052	, 1613	1316	1316
LII			1678, 1653	1641	1564	1054	1630	1329	3284.11(N(CH_3)$_2$)
LVIX			1679, 1616	1576	1585	1113	1331	1331	1364.22(N-H)
LXI			1707, 1674	1621	1553	1014	-	1325	1241 (OCH_3,)
LXVI			1635, 1670	1573	1563	-	-	-	1100(C-O)
LXII			1696, 1664	1685	1564	-	-	-	1212(C-O)
LXV			1640, 1667	1583	1519	-	-	-	1502(NO_2), 1365

Table.2.4.2. 1nfrared spectra of pyrazole derivatives



Comp.No	R_1	R_2	C=C st.vib (arom	C=N st.vib	N-N st.vib	N=N st.vib	C-N st.vib	C-H st.vib	C-H st.vib	Other groups
XCIX			1550	1596	1118	1602	1340	2925	2850	1505, 1456(NO_2), 1662(C=O)
XCV			1506	1575	1101	1664	1263	2920	2804	-
XCVII			1508	1595	1026	1650	1332	2923	2852	1166.80(OCH_3), 1676(C=O)
XCI			1504	1622	1105	1681	1340	2921	2852	1728 (C=O)
LXXV			1562	1641	1118	1689	1313	2923	2854	3440 (OH)
LXXXVI			1506	1595	1066	1610	1367	2921	2852	3384(N-H), 1710(C=O)

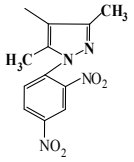
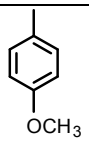
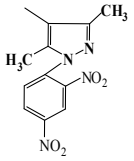
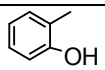
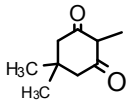
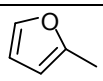
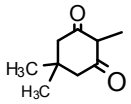
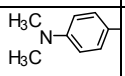
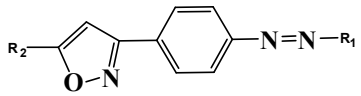
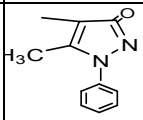
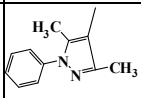
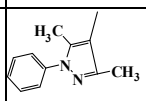
LXVIII			1562	1599	1110	1689	1334	2921	2852	1460,1510 (NO2) 1172 (OCH)
LXXXIV			1510	1600	1039	1653	1332	2925	2825	3284 (OH), 1415, 1315(NO_2)
CII			1502	1550	1164	1606	1230	2923	2854	1708(C=O), 1134(C-O)
CVI			1452	1496	1188	1600	1244	3029	2823	1654(C=O)

Table 2.4.3. Infrared spectrum andsofIsoxazolederivatives



Comp.No	R2	R3	C=C st.vib	C=N st.vib	N-N st.vib	N=N st.vib	C-N st.vib	N-O st.vib	C-H st.vib	C-H st.vib	0ther groups
XC			1494	1550	1155	1658	1338	1070	2923	2854	1708 C=O
LXXIV			1423	1500	1043	1627	1332	1043	2933	2852	3445 (OH)
XCIII			1502	1597	1157	1608	1336	1027	2921	2852	-

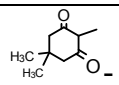
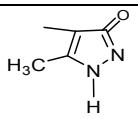
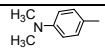
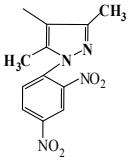
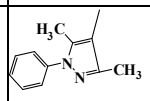
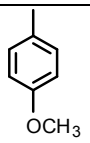
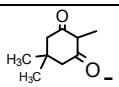
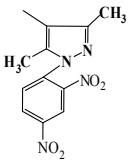
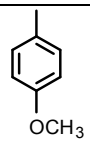
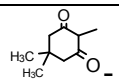
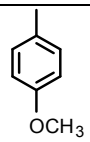
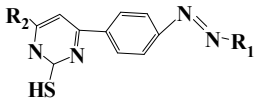
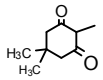
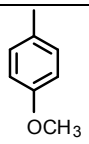
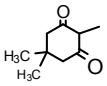
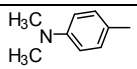
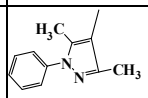
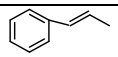
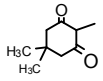
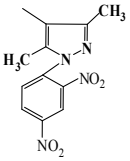
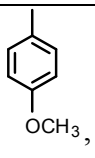
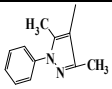
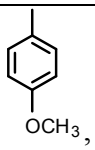
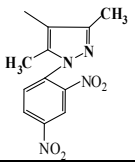
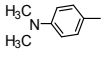
CI			1540	1562	1157	1610	1355	1053	2921	2852	1525, 1417 (-(NO_2), 1675(C=O)
LXXXVII			1537	1598	1161	1664	1365	1031	2921	2850	3622 (N-H), 1708(C=O)
LXXXIII			1517	1595	1166	1622	1265	1185	2927	2852	3383 (OH), 1465, 1342(NO_2)
LXXI			1458	1515	1105	1602	1263	1018	2927	2852	1263 (OCH_3,)
CIV			1456	1514	1174	1602	1043	1043	2927	2852	1656,(C=O), 11149 (C-O)
LXXVII			1502	1616	1175	1676	1244	1114	2921	2850	1209(OCH_3),1458, 1390(NO_2)
XCVI			1413	1508	1172	1605	1334	1027	2921	2850	1296O (CH_3) 1675(C=O)

Table 2.4.4. Infra-red spectrum bands of Pyrimidine derivatives:



Comp.No	R_2	R_3	C=C st.vib	C=N st.vib	N-N st.vib	N=N st.vib	C-N st.vib	S-H st.vib	C-H st.vib	Other groups
XCVII			1355	1460	1170	1652	1334	2848	2925.	1112 (OCH_3), 1698, (C=O)
CVII			1498	1454	1174	1623	1340	2855	2923	3442 (N-H), 1677(C=O)
XCV			1523	1596	1153	1652	1396	2925	3028	-
CIII			1413	1450	1151	1500	1342	2730	2954	1598, 1706(C=O)
LXXIX			1514	1602	1174	1681	1369	2852	2921	1114 $OCH_3$1445, 1367(NO_2)
LXXII			1417	1500	1155	1579	1392	2821	3028	1058 OCH_3
CVIII			1556	1596	1176	1652	1336	2852	2921	-

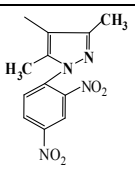
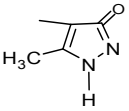
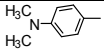
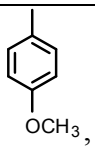
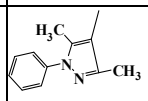
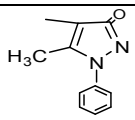
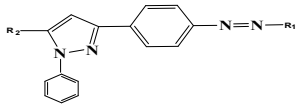
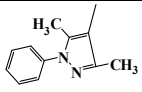
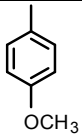
LXXXV			1415	1575	1172	1685	1257	2852	3028	3442 (OH), 1514, 1340 (NO2)
LXXXIX			1498	1577	1153	1602	1389	2852	2921	1718 (C=O)
XCVII			1550	1596	1116	1658	1390	2858	2923	1251OCH_3, 1658(C=O)
LXXVI			1510	1577	1107	1654	1407	2852	2921	3392, (OH)
XCII			1512	1602	1164	1649	1369	2850	2918	C=O 1650

Table 2.5.Ultra violet spectrum bands of synthesized compounds:-

Table 2.5.1. Ultra violet spectrum bands of pyrazole derivatives:



R_1	R_2	R_3	Solvent used	λ (nm)
LXXII			methanol	331.00

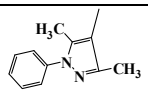
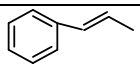
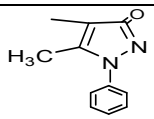
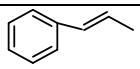
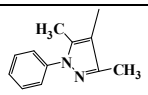
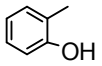
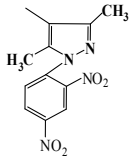
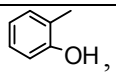
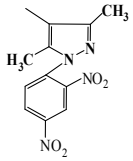
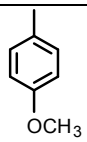
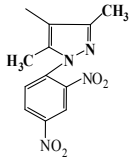
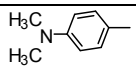
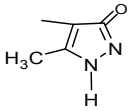
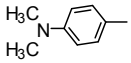
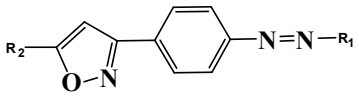
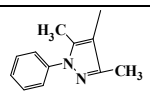
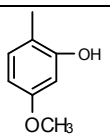
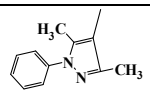
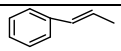
XCV			methanol	334, 295
XCI			methanol	337
LXXV			methanol	343
LXXXIV			methanol	293
LXVIII			methanol	309
XC			methanol	379
LXXXVI			methanol	366, 405

Table 2.5.2 .Ultra violet spectrum bands of Isoxazole derivatives:



Comp.No	R_2	R_3	Solvent used	λ (nm)
LXXI			methanol	355
XCIII			methanol	353

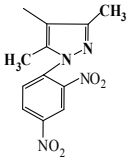
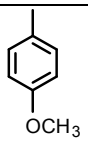
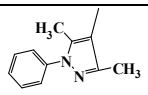
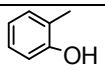
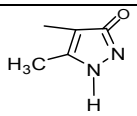
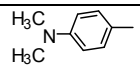
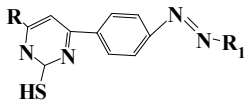
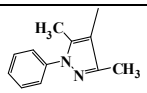
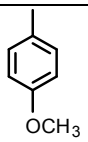
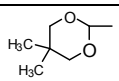
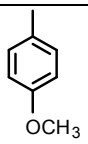
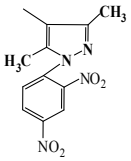
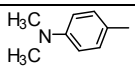
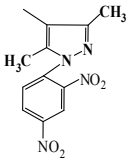
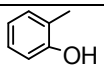
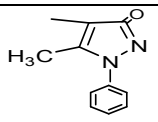
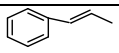
LXXVII			methanol	295
LXXIV			methanol	309, 283
LXXXIII			methanol	309

Table 2.5.3. Ultraviolet spectrum bands of pyrimidine derivatives



Comp.No	R_1	R_2	Solvent used	λ (nm)
LXXIII			methanol	357
XCVII			methanol	396, 294
CVIII			methanol	294
LXXXV			methanol	296.19
XCII			methanol	363, 291

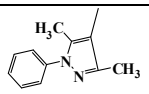
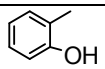
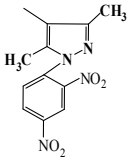
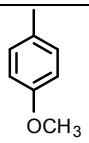
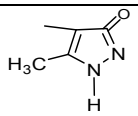
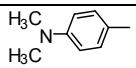
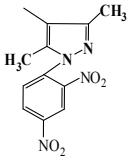
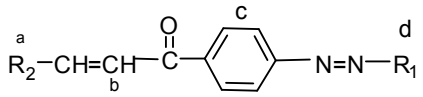
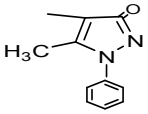
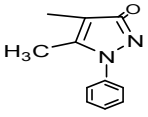
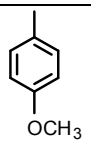
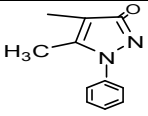
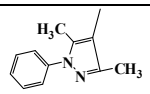
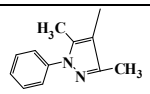
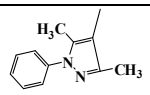
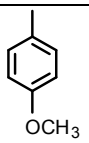
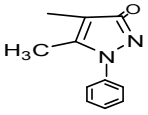
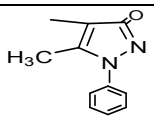
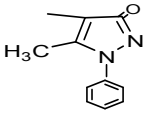
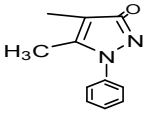
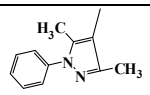
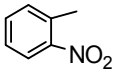
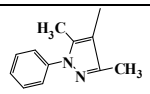
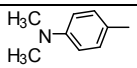
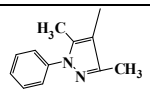
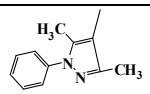
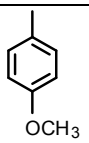
LXXVI			methanol	344, 294
LXXIX			methanol	296
LXXXIX			methanol	296
LXXXV			methanol	303

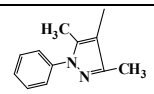
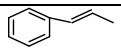
Table.2.6. proton nuclear magnetic resonance spectrum bands of synthesized compounds

Table. 2.6.1.(^{1}H-NMR) spectrum bands of α, β – unsaturated carbonyl derivatives:



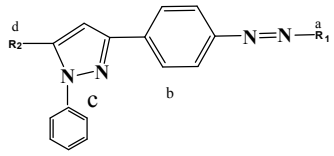
Comp. No	R_1	R_2	Chemical Shifts(ppm)			
			a	b	c	d
LIII			7.20 (m,4H) 2.43(s,1H.OH)	2.50 (d,2H)	6.72-7.10 (m,4H)	7.45 (m,5H), 1.24 (s,3HCH_3)
XLIX			2.50(s,3HOCH_3))7.72 (m,7Ar-H)), 3.41(s1H,OH)	2.40, 2.54 (d,2H)	7.52 m,4H)	7.51 (m,5H), 1.22(s,3H)
XLVII			7.93 (m,5H)	3.70 (d,4H)	7.41 (m,4H)	7.80 (m,5H), 1.13(s,3HCH_3))

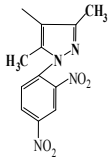
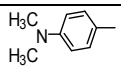
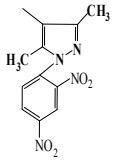
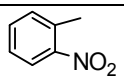
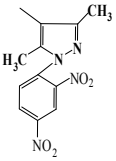
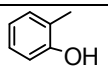
XIV			7.62 (m,5H)	2.34, 2.51 (d,2H)	7.53 (m,4H)	7.89 (m,5H), 1.02,1.92(s,6HCH 3)
XIX			7,53 (m, 5H) 3.40 (s,1H OH)	2.01, 2.43 (d,2H)	7.5 (m,5H)	7.56 (m,5H), 1.13, 0.90 (s,6H CH_3))
XV			7.3 0(m, 3H) 3.13,3H,OCH_3)	2.50, 2.24 d,2H)	7.52 (m,4H)	7.70 (m,5H), 1.12, 098 (s,6HCH_3))
LII			8.1 (m,4H) 3.40(s,6HN(CH_3)$_2$)	2.00,2.40 (d,2H)	7.60 m,4H)	7.83(m,5H)1.40 (s,3HCH_3))
L			6.81, 7.00, 6.45 (d,3H)	2.41, 2.50 (d,2H)	7.20 (m,4H)	7.40-7.60 (m,5H), 1.90 (s,3HCH_3)
LI			7.61 (m,4H)	2.42 (d,2H)	6.70 (m,4H)	7.94 (m,5H), 1.22(s,3HCH_3)
XLVII I			7.4 2(m,5H)	2.07, 2.50 (d,2H)	7.23 m,4H)	7 .70-7.80 (m,5H), 1.22 (s,3HCH_3))
XVII			8.00 (m,4H)	2.50, 2.60 (d,2H)	7.50 (m,4 H)	7.6 (m,5H),1.14,1.01 (s,6HCH_3))
XVIII			7.81 (m ,4H) 3.00 -3.72 (s ,6H)	2.52, 2.60 (d,2H)	7.50 m,4H)	7.63 (m,5H), 0.991.04(s,6HCH_3)
XVI			7.10, 6.35,6.99 (d, 3H furyl)	2.04, 2.62 (d,2H)	7.61 m,4H)	7.92 (m,5H), 0.89,1.04 (s,6HCH_3))
XV			7.63 (m,4H) (s,3H,OCH_3) 3.3 (s,1H)	2.60, 2.50 (d,2H)	7.00 (m,4H)	7.92 (m,5H), 1.04, 1.23(s,6HCH_3))

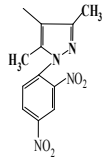
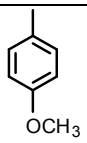
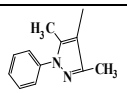
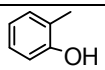
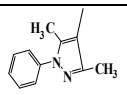
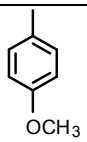
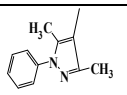
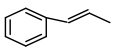
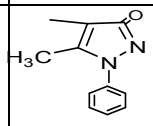
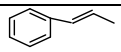
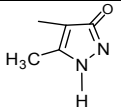
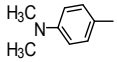
XIII			7.53 (m ,5H) 1.80 (s ,2H)	2.45, 2.15 (d ,2H)	7.1 (m,4H)	7.8(m,5H),1.50, 1.14 s,6HCH$_3$))

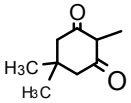
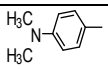
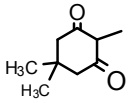
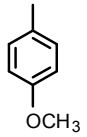
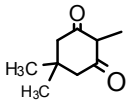
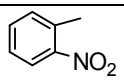
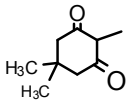
Solvent: DMSO

Table 2.6.2.[1]H-NMR of synthesized pyrazole derivatives



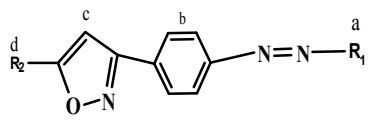
Comp. NO	R1	R2	Chemical shift/ ppm			
			a	b	c	d
CX			1.04, 1.23(s,6HCH$_3$) 7.75(m,3A-H)	8.03-8.23 (d,d,4Ar-H)	6.77(s,1H ,pyrazole ring),6.73 -6.77 (m,5Ar-H)	3.01,3.31 (s,6HN(CH$_3$)),7.67 - 7.7 1 (m, 4Ar-H)
LXXX			7.55 m,3Ar – H), 1.50, 1.61(s,6HCH$_3$)	7.50d,d,4Ar-H)	7.83(m,5 Ar-H), 6.70(s,1H pyrazole ring)	7.40(m,4 A-H)
LXXX IV			8.13(m,3Ar-H), 1.80, 1.67(s,6HCH$_3$)	7.59-7.62 (m,,4Ar-H)	6.22(s,1H ,pyrazol), 7.50-7.56 (m,5Ar-H)	7.87-7.89 (m,4Ar-H), 3.31 (s,1HOH)

LXVIII			7.90(m,3A-H), 2.09, 2.51 (s,6H CH_3)	6.95(m,4Ar-H)	6.54(s,1H,pyrazole), ring7.50(m,5Ar-H)	7.34(m,3Ar-H), 2.51(s,3H OCH_3),)
LXXV			7.50(m,5Ar-H), 2.49, 2.64(s,6HCH_3)	7.90(m,4Ar-H)	7.05(s,1H,pyrazole ring),7.59 (m,5Ar-H)	3.36(s,1H OH),7.80 (m,4Ar-H)
LXXII			2.09(s,6HCH_3),6.50(m,5Ar-H)	7.00(m,4-Ar-H)	6.00(s,1H,pyrazole),6.90(m, 5Ar-H)	2.50(s,3H OCH_3), 7.60(m,3A-H)
XCV			1.20, 1.24 (s,6HCH3),7.50-7.56 (m, 5Ar-H)	7..72-8.12 (d,d,4Ar-H)	6.98 (s,1H,pyrazole ring), 7.12-7.30(m,5Ar-H)	7.60 (m,5Ar-H), 2.08(d,2H,CH=CH)
XCI			7.50(m,5Ar-H), 3.31(s,3HCH_3)	7.93(m,4Ar-H)	6.55(s,1H pyrazole ring),7.00 (5Ar-H)	7.70(m,5Ar-H), 2.33,2.50 (d,2H,CH=CH
LXXXVI			H),2.45(s,3H CH_3)), 3.90(s,1HNH)	7.50(m,4Ar-H2),	6.90(s.1H pyrazol), 6.507.01(m,5Ar-H)	3.50(s,3H CH_3), 7.83-8.06(m,4Ar)

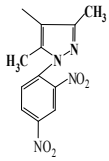
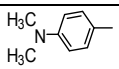
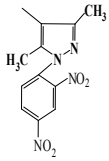
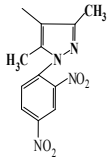
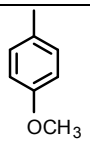
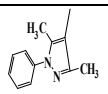
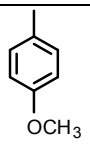
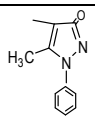
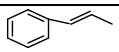
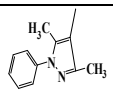
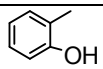
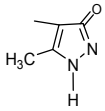
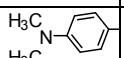
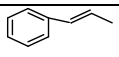
CVI			2.15,2.59(s,4H,cyclohexanediones,0.96, 1.23 (s,6HCH_3)	7.61-7.63(m,4Ar-H)	6.99(s,1H,pyrazole ring)7.12 - 7.15(m,5 Ar-H)	7.73(m,4 Ar-H), 3,31(s,6H NCH_3)
XCVII			2.08 2.67(s,4H,cyclohexane), 1.04, 1.23(s,6HCH_3)	7.01-7.36(m,4Ar-H)	6.71(s,1H,pyrazole),7.01-7.36 (m,5Ar-H)	7.40-8.10(m,3 Ar-H), 3.70(s,3H OCH_3),
XCIX			2.51, 2.67(s,4Hcyclohexanediones),1.04, 1.23(s,6HCH_3)	7.81(m,4Ar-H)	7.67(s,1H,pyrazol), 7.78(m,5 Ar-H)	8.08-8.22(m,4 Ar-H)
CII			2.50,2.70(s,4Hcyclohexne-diones), 1.04, 1.23(s,6HCH_3)	7.86-8.01(m,4Ar-H)	7.71(s,1H pyrazol), 7.41(m,5 Ar-H)	6,79,6.70 ,6.74(d,3 H,furan)

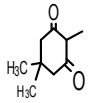
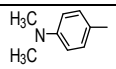
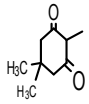
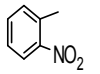
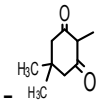
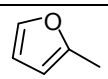
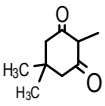
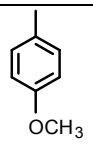
Solvent used DMSO

Table 2.6.3.(^{1}H-NMR) spectrum bands of Isoxazole derivatives:



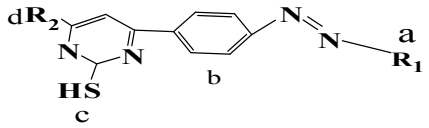
Comp. NO	R2	R3	Chemical shift (ppm)			
			a	b	c	d

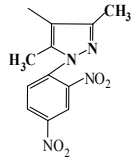
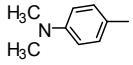
CIX			1.23, 2.50 (s,6HCH$_3$),7.33(m,3Ar-H)	7.16(m,4Ar-H)	6.55(s,1HIsoxazol)	7.50(m,4Ar-H),3.75-3.92(s,6HNCH3)
LXXXIII			1.23, 2.08 (s,3Ar-H), 7.809m,3Ar-H	6.94((m, 4Ar-H)	6.40(s,1Hisoxazol)	7.24(m,4Ar-H),3.34(s,1HOH)
LXXVII			0.85, 1.23 (s,6HCH3), 7.24-7.64 (m,4Ar-H)	7.14 (m,4Ar-H)	6.92(1Hisoxazole)	7.70-7.791(3Ar-H) 3.80(s,3HOCH$_3$)
LXXI			1.68, 2.08 (s,6HCH$_3$), 7.02-7.50 (m,5Ar-H)	7.52-7.72(m4 Ar-H)	7.04(s,1Hisoxazole)	7.78-8.31 (m3Ar-H), 3.57 (s,1HOCH$_3$)
XC			1.23 (s,3HCH$_3$), 7.17-7.33(m,5Ar-H)	7.52-7.62(m,4 Ar-H)	7.00(s,1Hisoxazole)	7.72-8.11(m,5Ar-H),2.50-3.33(d,2aliph-H)
LXXIV			1.62, 2.62 (s,6 CH$_3$), 6.50(m,5Ar-H)	7.58(m,4 Ar-H)	6.63(s,1Hisoxaazole)	7.78(m,4Ar-H),3.36-3.62(s,1HOH)
LXXXVIII			1.53,2.17 (s,3HCH$_3$), 4.00(s,1HNH)	7.00(m,4 Ar-H)	6.50(s,1H isoxazole)	8.00-8.50(m,4Ar-H),3.50-(s,6HNCH$_3$)
CIX			1.23, 2.21 (s,6HCH$_3$), 7.25-7.41 (m,5Ar-H)	7.81-7.82(m,4 Ar-H)	6.90(s,1Hisoxazole)	7.44-7.61(m,5Ar-H),2.66, 23.32(d,2-aliphatic -H)

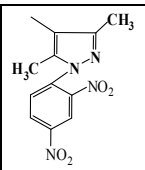
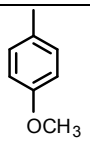
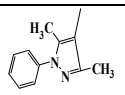
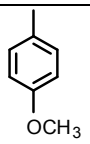
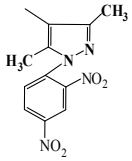
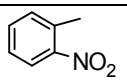
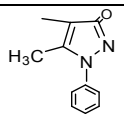
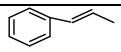
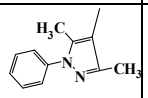
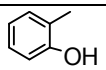
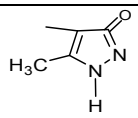
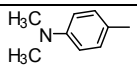
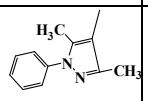
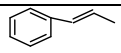
CV			1.05,1.24(s,6HCH3), 2.08, 2.68(s,4Hcyclohexane)	7.69-7.72(m,4Ar-H)	6.76(s,1Hisoxale ring)	8.02-8.05(m,4Ar-H), 3.30(s,6HNCH$_3$)
CI			0.90,1.31(s.6HCH$_3$),2.50-3.31 (s,4alipha-H)	7.76(m,4r-H)	7.53(s,1Hisoxazole ring)	7.76-8.02(m,4Ar-H)
CIV			2.08,2.16 (s,4Hcyclohexane)-H),0.95,1.31(s,6HCH$_3$)	6.98-7.58(m,5Ar-H)	6.23(s,1Hisoxazol)	7.57, 7.14, 7.42 (d,3Ar-H)
XCVI			1.05, 1.23 (s,6HCH$_3$),2.50(s,4 aliphatic-H	6.96(m,4Ar-H)	6.94(s,1Hisoxazol)	7.66-8.01(m,3Ar-H),3.77(s,3HOCH$_3$),

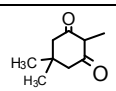
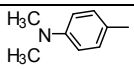
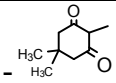
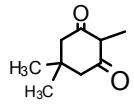
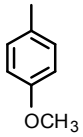
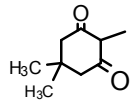
Solvent used DMSO

Table.2.6.4. ^{1}H-NMR Spectrum of synthesis pyrimidine thiol derivatives



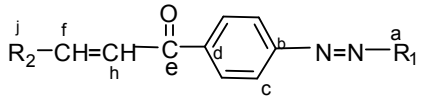
Compound. No	R_1	R_2	Chemical shifts(ppm)			
			a	b	c	d
CVIII			1.23, 2.08 (s,6HCH$_3$) ,7.2(m,3Ar-H)	7.09(m,4Ar-H)	6.86 (s,1H,pyrimidine), ,4.501H-SH)	7.26,7.43(m, 4Ar-H), 3.67(m,6HNCH$_3$)

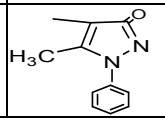
LXXIX			1.23, 2.09 (s,6HCH_3) , 7.207.24(m,3Ar-H)	7.02(m,4A r-H)	6.90 (s,1Hpyri mimidin e), 3.33(s,1 HSH)	7.30, 7.34(m,3ArH) ,2.50(s,3HOC H_3)
LXXIII			0.85,1.35 (s,6HCH_3) , 7.617.70(m,3Ar-H)	7.23, 7.49(m,4A r-H)	6.98 (s1Hpyri midine), 3.33s,1H -SH)	7.72, 8.11(m,3ArH),2.64 (s,3HOCH_3)
LXXXII			1.09, 1.68 (s,6HCH_3) , 7.20-7.39 (m,3Ar-H)	7.50, 7.70(m,4A r-H)	7.10(s,1 Hpyrimi dine),5.4 7(s,1H- SH)	7.89, 8.50(m,4Ar- H)
XCII			0.85, 1.23 (s,3HCH_3) , 7.23 (m,5Ar-H)	7.71-7.98 (m,4 Ar- H)	6.94 (s,1Hpyri midine), 3.31 (s,1H- SH)	7.06- 7.47(m,5Ar- H), 2.33, 2.50(d,2H- aliph)
LXXVI			.0. 89, 1.50(s,6H CH_3)	-	6.56(s, H,pyrim dine), 2.50. s,1H-SH)	3.23(s1HOH)
LXXXIX			1.02 (s,3HCH_3) , 3.309s,1H NH)	6.80-7.30 (m,4Ar-H)	6.80 (s,1Hpyri midine), 4.30(s,1 H-SH)	3.90(s,6HNC H_3), 8.30(m,4Ar- H)
CVIII			1.04, 1.23 (s,6HCH3) ,7.50-7.61 (m,5Ar-H)	7.88(m,4A r-H)	6.90 (s,1H- pyrimidi ne),3.34- 3.57(s,1 H-SH)	7.23- 7.35(m,5Ar- H), 2.50, 2.88(d,2Halip ha)

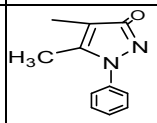
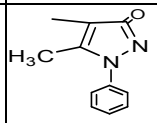
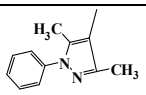
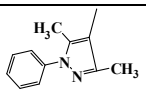
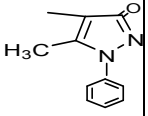
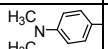
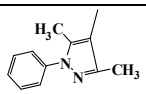
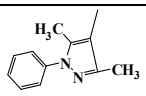
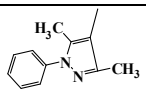
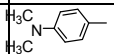
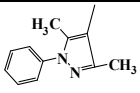
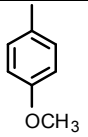
CVII			0.83, 1.23 (s,4Hcyclohexanediones),2.08, 2.59 (s,6HCH_3	6.50,6.88p (m,4Ar-H	3.87 (s,1SH), 6.75 (1Hpyrimidine)	7.05-8.71 (m,4A-H),3.31-(s,6HNCH_3)
C			2.09-2.16ppm(s,4Hcyclohexanediones),2.50-2.65(s,6HCH_3)	7.59-7.75 ppm(m,4Ar-H)	3.31ppm (s,1HSH),6.99 (s,1Hpyrimidine)	7.99-8.02ppm(m,4Ar-H)
XCVII			2.50, 2.65 (s,4Hcyclohexanediones), 1.04, 2.09 (6HCH_3)	7.26 (m,4A-H)	6.76 (s,1Hpyrimidine), 3.80(s,1HSH).	7.30-8.26 (m,3Ar-H),3.80 (s,3HOCH_3)
CIII			2.08, 2.65 (s,4Hcyclohexanediones),0.90-1.59ppm(s,6HCH_3	8.00 (m,4Ar-H)	7.00 (s,1Hpyrimidine), 3.30ppm (s,1HSH) .	**7.99, 7.53, 7.76** (m,3Ar-H)

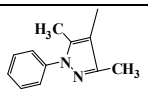
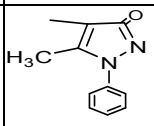
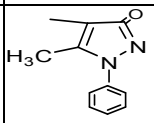
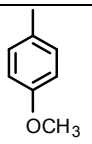
Solvent used DMSO

Table 2.6.5.(^{13}C-NMR) spectrum bands of α, β – unsaturated carbonyl derivative:



Comp .No	R_2	R_3	Chemical shifts(ppm)							
			a	b	c	d	e	h	f	j
LI			4.894, 22.71	114.52	112.69	244.75	133.64	4.062,4.8	49.05	22.71

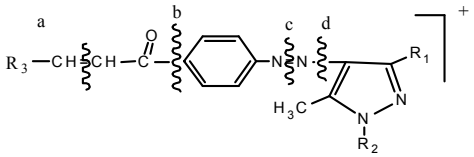
								94		
LIII			26.29	115.77	119.14	222.71	130.31	39.12,39.95	49.60	38.95
XLVII			4.23, 3,4.73	113.66	118.16	167.18, 162.61	131.78	49.66	47.40	-
XV			4.05	142.40	121.63	155.41,	123.74	25.17	37.96	23.43
XIII			4.03	130.93	112.69	223.27	131.79	66.76	36.55	4.87
LII			4.02	129.04.	117.70	23.81	129.04	49.08	23.13	4.92
XVI			25.44	121.83	124.56	132.15	129.32	25.44	38.92	61.98
XIV			38.93	127.07	128.74	129.00	130.93	45.00	40.02	61.96
XVIII			4.62	111.03	162.23	142.23	129.00	23.43	22.13	72.76
XV			24.00	112.69	150.34	131.79	38.97	354.5	39.97	55.64

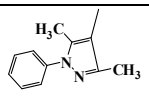
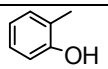
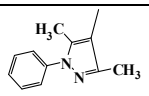
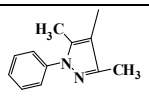
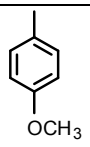
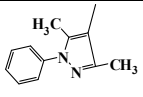
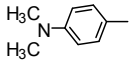
XVII			38.23	121.83	-	-	121.83	39.94	39.27	39.11
L			39.95	114.24	-	-	128.83	-	39.96	-
XLIX			38.97	121.00	128.84	161.23	1298.8	-	65.14	39.97

Solvent used DMSO

Table2.7. Mass spectrum bands of synthesized compounds:

Table 2.7.1. mass spectrum bands of some synthesized α, β- unsaturated carbonyl derivatives:



Comp. No	R_1	R_2	Chemical formula	MW.	M/Z (Relative abundance%)			
					a	b	c	D
XIX			$C_{26}H_{22}N_4O_2$	421.25	-	-	317.20	-
XVII			$C_{26}H_{21}N_5O_3$	434.30	134.10	176.58	261.19	275.15
XV			$C_{27}H_{24}N_4O_3$	421.36	325	139.13	291,21	421.35
XVIII			$C_{28}H_{27}N_5O$	434.17	139.13	176.12	266.22	245.21

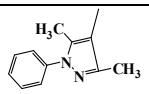
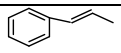
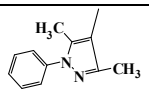
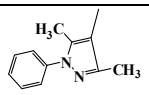
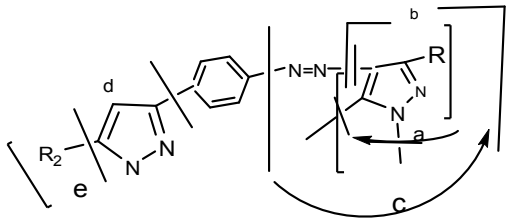
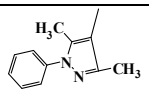
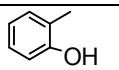
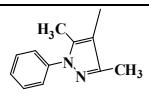
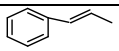
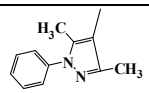
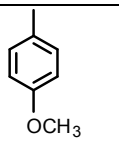
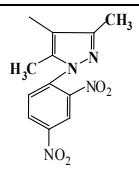
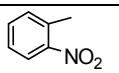
XIII			C28H24NO	386.28	311.27	-	245.22	176.12
XVI			$C_{24}H_{20}N_4O_2$	351.25	319.24	171.11	275.15	213.12
XIV			$C_{26}H_{22}N_4O$	409.28	319.20	-	265.13	176.13

Table 2.7.2.mass spectrum bands of some synthesized pyrazole derivatives:



Com. No	Chemical formula	R_1	R_3	MW calc	MW ,obs	M/z(Relative abundance%)				
						a	b	c	d	e
LXXV	$C_{32}H_{26}N_6O$			510	434(0.06)	77(100)	171(46.27)	199(52.67)	65(11.66)	92(4.94)
XCV	$C_{34}H_{28}N_6$			520	519(0.21)	80(100)	171(18.32)	199(23.80)	64(66.62)	105(7.9)
LXXXII	$C_{33}H_{28}N_6O_2$			540	542 (0.05)	85(46.57)	169(4.12)	199(4.77)	57(100)	125(16.17)
LXXX	$C_{32}H_{23}N_9O_6$			629	552(0.27)	80(100)	266(1.14)	281(1.27)	64(87.38)	119(3.31)

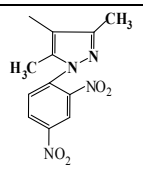
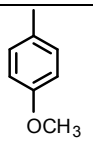
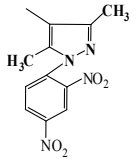
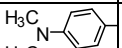
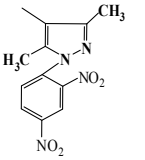
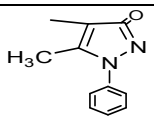
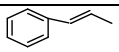
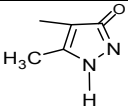
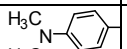
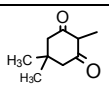
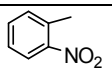
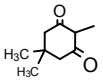
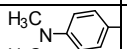
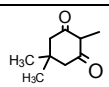
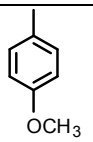
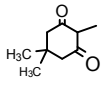
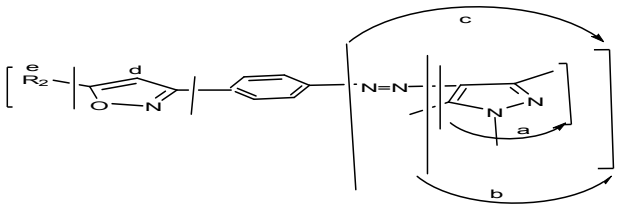
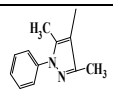
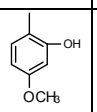
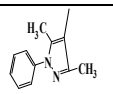
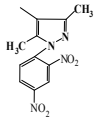
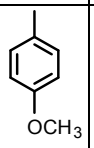
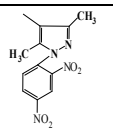
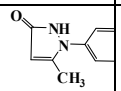
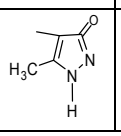
LXVII	$C_{33}H_{26}N_8O_6$			630	629 (0.08)	80(100)	267(0.67)	281(0.65)	64(49.96)	135(7.87)
CX	$C_{34}H_{29}N_9O_4$			627	550(0.35)	77(29.49)	271(29.58)	286(100)	64(22.65)	119(65.39)
LXXXIV	$C_{32}H_{24}N_8O_5$			612	505 (0.16)	80(100)	265(0.7)	281(0.25)	64(3.90)	97(5.5)
XCI	$C_{33}H_{25}N_6O$			521	444(0.04)	80(73.60)	171(0.16)	185(0.17)	64(100)	102(0.13)
LXXXVI	$C_{26}H_{24}N_7O$			462	461 (0.42)	77(72.54)	91(2.25)	105(1.89)	64(12.64)	120(32.92)
XCIX	$C_{29}H_{24}N_5O_4$			506	429(0.28)	80(66.25)	137(0.2.08)	167(1.27)	64(100)	120(3.11)
	$C_{31}H_{30}N_5O_2$			504	427(0.04)	80(100)	(0.13)	167(0.13)	64(63(37)	120(1.11)
XCVII	$C_{30}H_{27}N_4O_4$			507	492(48.00)	80(100)	137(1.83)	165(3.00)	64(51.00)	133(0.65)
CII	$C_{27}H_{23}N_4O_2$			435	358(0.08)	80(100)	137(0.57)	167(0.60)	64(93.70)	63(069)

Table 2.7. 3. mass spectrum of synthesis isoxaz0le derivatives



Comp.no	Molecular forular	R_1	R_2	MW calcl	Mol. obsorved	M/z(Relative abundance%)				
						a	b	c	d	e
LXXI	$C_{27}H_{23}N_5O_3$			465	462(0.41)	80(100)	199(12.50)	171(83.81)	64(99.59)	133(3.40)
LXXIV	$C_{26}H_{21}N_5O_2$			435	435(0.12)	80(100)	199(27.09)	171(23.63)	64(72.24)	106(20.60)
XCIII	$C_{28}H_{23}N_5O$			445	445(0.28)	80(100)	199(5.41)	171(4.51)	64(58)	118(2.85)
LXXVII	$C_{27}H_{21}N_7O_7$			555	555(0.27)	80(100)	288(2.29)	265(8.40)	64(53.82)	133(6.21)
CIX	$C_{28}H_{24}N_8O_5$			552	553(0.35	80(53.65)	289(0.98)	264(2.19)	64(100)	-
XC	$C_{27}H_{20}N_5O_2$			446	448(0.47)	80(100)	190(0.2)	171(0.53)	64(72.24)	118(0.67)
LXXXVII	$C_{21}H_{19}N_6O_2$			387		79(14.96	80(9.85)	109(22.7)	65(6.49)	123(18..02)

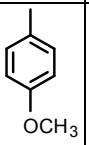
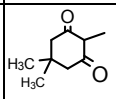
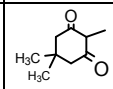
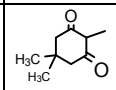
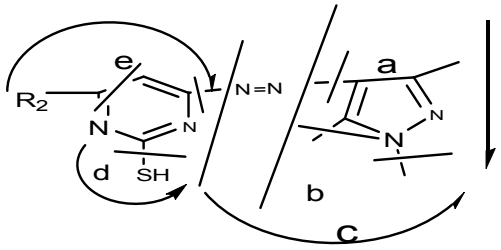
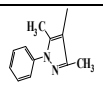
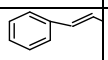
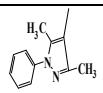
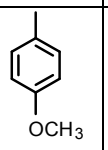
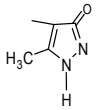
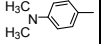
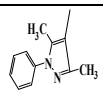
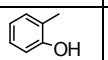
						)				
XCVI	$C_{23}H_{20}N_3O_4$			402	402(3.59)	80(100)	167(4.47)	135(46.86)	64(53.82)	191(14.68)
CI	$C_{23}H_{19}N_4O_5$			431	431(0.25)	80(67.14)	199(1.98)	134(3.44)	64(100)	121(3.82)
	$C_{25}H_{25}N_4O_3$			429	429(0,15)	80(100)	167(1.39)	139(0.43)	64(79.46)	111(1.55)
CIV	$C_{21}H_{18}N_3O_4$			376	377(89.11)	80(100)	167(18.23)	139(28.87)	63(55.98)	123(18.02

Table 2.7.4 mass spectrum bands of synthesized pyrimidine derivatives:



Comp.No	Molecular formula	R_1	R_2	MW (calcul)	MW.observed	M/Z(Relative abundance%)				
						a	b	C	d	e
XCV	$C_{29}H_{24}N_6S$			488	487(0.05)	80(100)	171(0.7)	199(0.8)	64(49.41)	213(0.4)
LXXIII	$C_{28}H_{24}N_6SO_2$			508	506(0.2)	80(100)	171(2.8)	199(3.9)	64(2.8)	239(0.51)
LXXXIX	$C_{22}H_{20}N_7SO$			430	430(.55)	81(41.81)	97(60.00)	125(22.58)	57(100)	129(26.01)
LXXVI	$C_{27}H_{22}N_6SO$			478	477(0.2)	80(65.71)	171(4.53)	199(4.63)	64(100)	203(0.4)

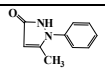
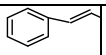
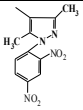
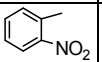
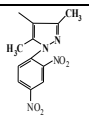
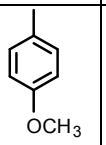
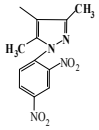
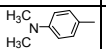
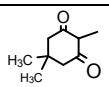
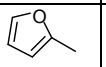
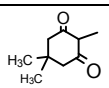
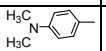
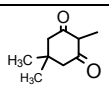
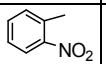
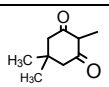
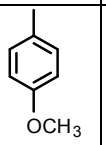
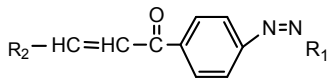
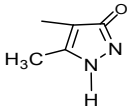
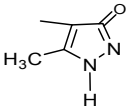
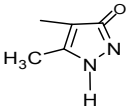
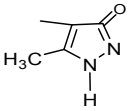
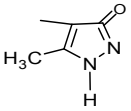
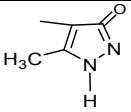
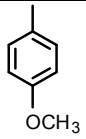
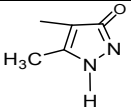
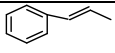
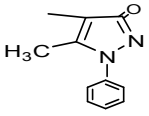
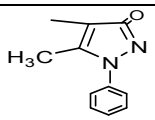
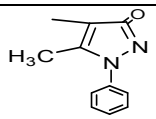
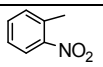
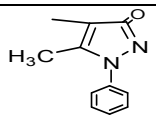
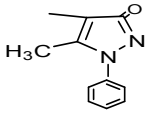
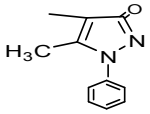
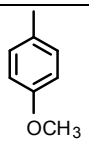
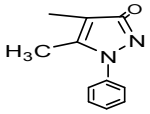
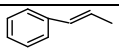
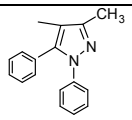
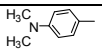
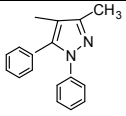
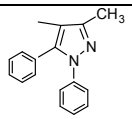
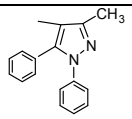
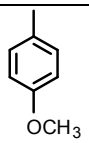
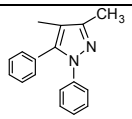
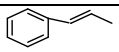
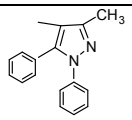
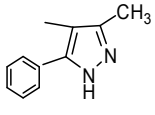
XCII	$C_{28}H_{21}N_6SO$			489	488(0.04)	80	171	185	64	213
LXXXII	$C_{27}H_{19}N_9SO_6$			597	597(0.4)	80(100)	265(0.98)	289(0.55)	64(54.66)	230(0.54)
LXXIX	$C_{28}H_{22}N_8SO_6$			598	598(0.6)	80(100)	260(0.6)	289(0.54)	64(67.52)	234(0.6)
CVIII	$C_{29}H_{25}N_9SO_4$			595	595(0.14)	80(100)	265(0.33)	287(0.3)	64(62.3)	229(0.25)
CIII	$C_{22}H_{19}N_4SO_3$			419	421(0.11)	80(100)	139(1.8)	167(1,7)	64(51.0)	176(0.22)
	$C_{25}H_{23}N_4SO_4$			472	470(0.1)	80(100)	139(0.32)	167(0.3)	64(81.74)	229(0.1)
C	$C_{24}H_{20}N_5SO_4$			474	474(0.22)	80(100)	139(0.8)	167(0.22)	64(58.46)	231(0.2)
XCVII	$C_{25}H_{23}N_4SO_4$			475	460(0.1)	80(100)	1391,74)	167(1.22)	64(49.7) 233(0.12)	

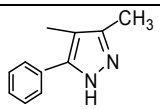
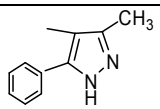
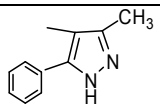
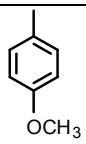
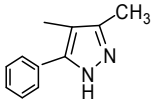
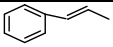
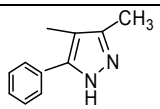
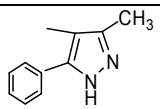
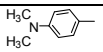
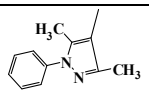
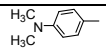
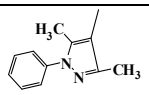
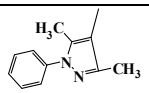
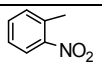
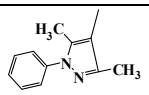
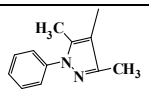
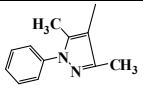
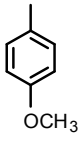
Table2.8. TLC of synthesized compounds:-

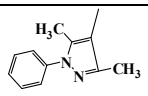
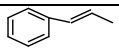
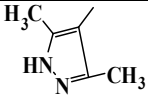
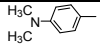
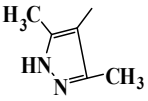
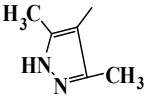
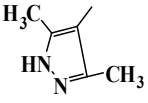
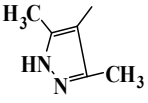
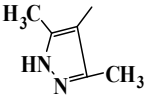
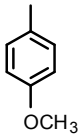
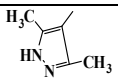
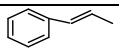
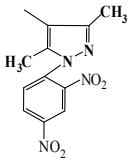
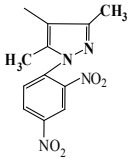
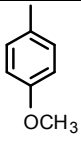
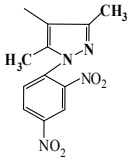
Table 2.8.1.TLC of α, β-unsaturated carbonyl derivatives



Comp.No	R_1	R_3	Solvent used	Rf value
LVIX			Petro.ether.7 : 3 ethyl acetate	0.795
LVII			Petro.ether.7 : 3 ethyl acetate	0.71
LVIII			Petro.ether.7 : 3 ethyl acetate	0.73
LV			Petro.ether.7 : 3 ethyl acetate	0.8
LX			Petro.ether.7 : 3 ethyl acetate	0.63
LVI			Petro.ether.7 : 3 ethyl acetate	0.76
LIV			Petro.ether.7 : 3 ethyl acetate	.070
LII			Petro.ether.7 : 3 ethyl acetate	0.63
L			Petro.ether.7 : 3 ethyl acetate	0.77

LI			Petro.ether.7 : 3 ethyl acetate	0.80
XLVIII			Petro.ether.7 : 3 ethyl acetate	0.83
LIII			Petro.ether.7 : 3 ethyl acetate	0.79
XLIX			Petro.ether.7 : 3 ethyl acetate	0.73
XLVII			Petro.ether.7 : 3 ethyl acetate	0.84
XXXIX			Methanol 9: 1 n-hexane	0.95
XXXVIII			Methanol 9: 1 n-hexane	0.93
XXXVI			Methanol 9: 1 n- hexane	0.85
XXXV			Methanol 9: 1 n- hexane	0.83
XXVI			Methanol 9: 1 n- hexane	0.83
XXXVII			Methanol 9: 1 n- hexane	0.84
XLIV			Chloroform 7: 3 methanol	0.94

XLIII			Chloroform 7: 3 methanol	0.92
XLVI			Chloroform 7: 3 methanol	0.80
XLII			Chloroform 7: 3 methanol	0.93
XL			Chloroform 7: 3 methanol	0.97
XLI			Chloroform 7: 3 methanol	0.73
XLV			Chloroform 7: 3 methanol	
XVIII			chloroform 9.5 : 0.5 methanol	0.70
XXI			chloroform 9.5 : 0.5methanol	0.56
XVII			chloroform 9.5 : 0.5 methanol	0.58
XIV			chloroform 9.5 : 0.5 methanol	0.66
XIX			chloroform 9.5 : 0.5methanol	0.60
XV			chloroform 9.5 : 0.5 methanol	0.68

XIII			chloroform 9.5 : 0.5 methanol	0.53
XXXII			chloroform 9.5 : 0.5 methanol	0.67
XXX			chloroform 9.5 : 0.5 methanol	0.92
XXXI			chloroform 9.5 : 0.5 methanol	0.80
XXVIII			chloroform 9.5 : 0.5 methanol	0.90
XXXIII			chloroform 9.5 : 0.5 methanol	081
XXIX			chloroform 9.5: 0.5: methanol	091
XXVI			chloroform 9.5 : 0.5 methanol	0.85
XXVI			chloroform 9.5 :0.5 methanol	0.97
XX			Methanol 9 : 1 chloroform	0.89
XXIV			Methanol 9 : 1 chloroform	0.85

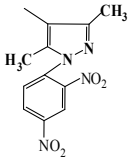
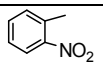
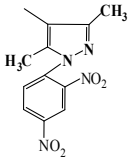
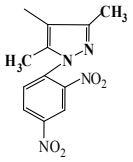
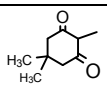
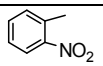
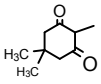
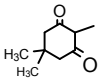
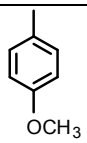
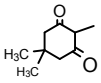
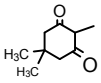
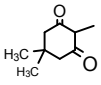
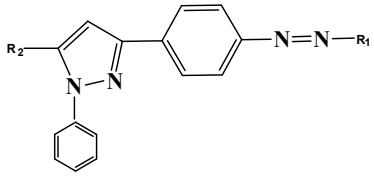
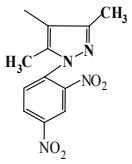
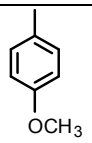
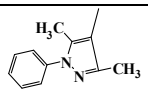
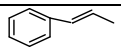
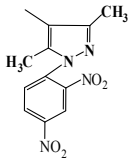
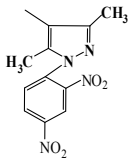
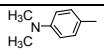
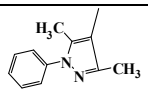
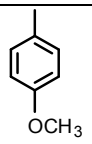
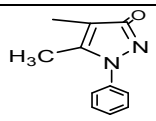
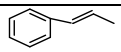
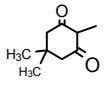
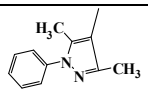
XXII			Methanol 9 : 1 chloroform	0.79
XXI			Methanol 9 : 1 chloroform	0.68
XXIII			Methanol 9 : 1 chloroform	0.94
LXV			Petro.ether.7 : 3 ethyl acetate	0.49
LXVI			Petro.ether.7 : 3 ethyl acetate	0.65
LXI			Petro.ether.7 : 3 ethyl acetate	0.54
LXIII			Petro.ether.7 : 3 ethyl acetate	0.27
LXII			Petro.ether.7 : 3 ethyl acetate	0.66
LXIV			Chloroform 10	0.28

Table 2.8.2.TLC of synthesized pyrazole derivatives



Comp.No	R_1	R_2	Solvent used	Rf. Values
LXVIII			chloroform 9 : 1 methanol	0.90
XCV			chloroform 7 : 3 methanol	0.92
LXXXIV			chloroform 9 : 1 methanol	0.87
CX			Petro.ether.7 : 3 ethyl acetate	0.93
LXXII			Petro.ether.7 : 3 ethyl acetate	0.55
XCI			chloroform 9 : 1 methanol	0.93
CII			chloroform 9 : 1 methanol	0.82
LXXV			ethanol 7 : 3 n-hexane	0.90

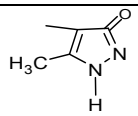
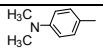
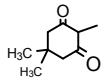
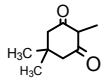
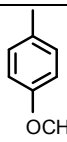
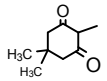
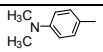
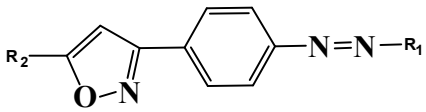
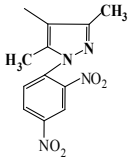
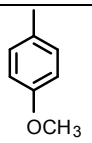
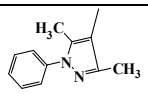
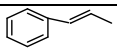
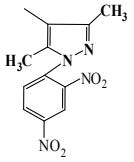
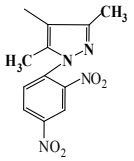
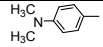
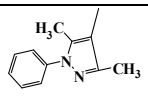
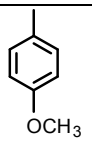
XCI			Ethanol 9 : 1 chloroform	0.95
XCIX			Ethanol 3 : 7chloroform	0.80
XCVII			Ethanol 3 : 7chloroform	0.74
CVI			Chloroform 10	0.23

Table 2.8.3 TLC of synthesized Isoxazole derivatives:



Comp.NO	R2	R3	Solvent system used	Rf. value
LXXVII			chloroform 9: 1 methanol	0.94
XCIII			Chloroform 7: 3methanol	0.86
LXXXIII			chloroform 9: 1 methanol	0.89
CIX			Petro.ether.7: 3ethylacetat	0.87
LXXI			Petro.ether.7:3ethylacetate	0.50

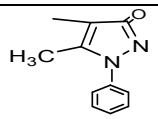
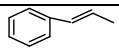
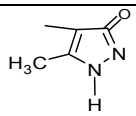
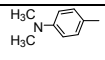
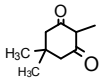
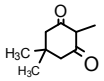
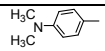
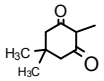
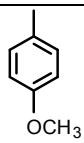
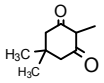
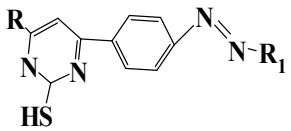
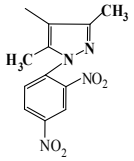
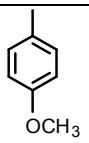
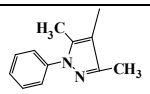
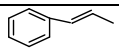
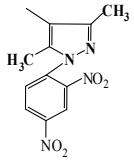
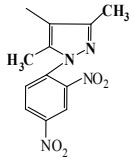
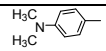
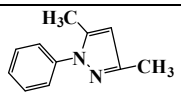
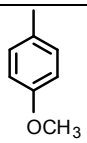
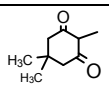
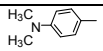
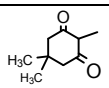
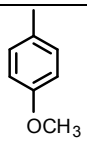
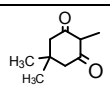
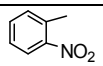
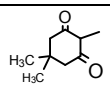
XC			Chloroform 9:1methano	0.91
LXXXVIII			Ethanol 9:1 chloroform	0.82
CI			Ethanol 3: 7chloroform	0.90
CV			Chloroform 10	0.38
XVIC			chloroform 9:1 methanol	0.46
CIV			Chloroform7: 3 ethanol	0.81

Table 2.8.4.TLCofsynthesis pyrimidinederivatives:



Comp.No	R2	R3	Solvent system used	Rf .value
LXXIX			Chloroform 9: 1 methanol	0.81
XCV			chloroform 7: 3methanol	0.82

LXXXV			chloroform 9:1methanol	0.94
CVIII			Petro.ether.7:3ethylacetate	0.83
LXXIII			Petro.ether.7:3ethylacetate	0.65
CVII			Chloroform10	0.62
XCVII			Chloroform 7:3 ethanol	0.85
C			Chloroform 7:3 ethanol	0.58
CIII			chloroform 9 : 1 methanol	0.74

CHAPTER THREE

RESULTS AND DISCUSSIONS

Results and Discussions

3.1 Organic Synthesis:

Organic synthesis is special branch of chemical synthesis and is concerned with the construction of organic compound *via* organic reaction. Organic molecules can often contain a higher level of complexity compared to purely inorganic compounds, so the synthesis of organic compounds has developed into one of the most important branches of organic chemistry.

3.2. Retrosynthetic analysis:

Retrosynthetic analysis is a technique for solving problem in the planning of organic synthesis. This is achieved by transforming a target molecule into simpler precursor structures without assumptions regarding starting materials. Each precursor material is examined using same method. This procedure is repeated until simple or commercially available structures are reaching. Retrosynthetic analysis can done by two methods, disconnection or functional group inter conversion (FGI). Strategiesfollowed in course of this work have been constructed from the appropriated retrosynthetic analysis of the target molecules. The basic α, β - unsaturated carbonyl compound can be disconnected at CH=CH bond (Warren, Smith.2002). The appropriate synthetic equivalent ofproduced synthon. The basic pyrazole, isoxazole and thio pyrimidine derivatives structure can be disconnected at C-N, C-O, C-N bond as in heterocyclic nitrogen, oxygen, nitrogen containing compounds through ring open respectively (Warren, 2000).

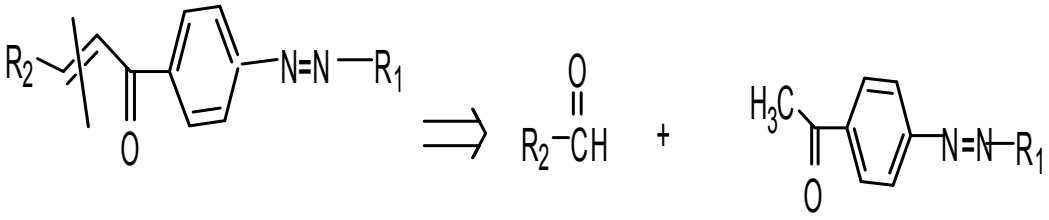


Fig.3.2.1. Retro synthesistic analysis of α, β unsaturated carbonyl derivatives

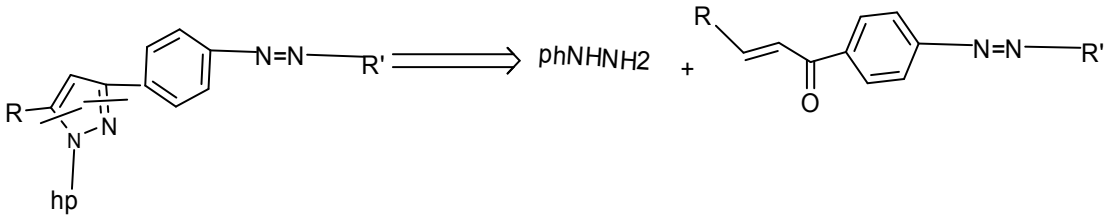


Fig 3.2.2. Retrosynthetic analysis of pyrazole derivatives

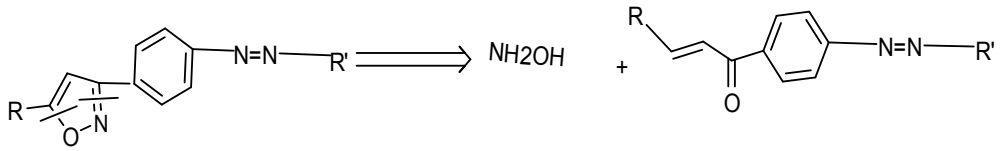


Fig.2.2.3. Retrosynthetic analysis of synthesis isoxazole

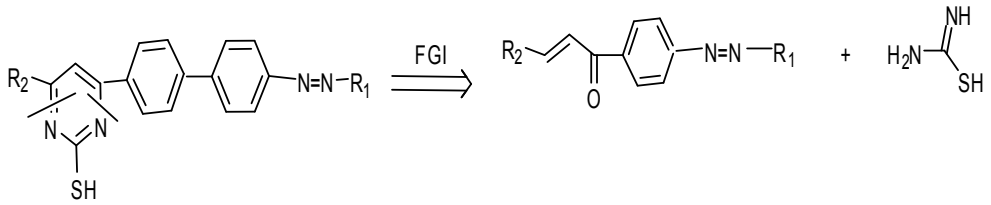


Fig.2.2.4. Retrosynthetic analysis of synthesis pyrimidine derivatives

3.3. Reaction mechanisms

3.3.1. Reaction mechanism of formation of α, β – unsaturated carbonyl compounds

The reaction type followed is Aldol and Claisen-Schmidt reaction, in which aromatic aldehydes condense with aryl ketones. The first step is a condensation involving the nuchleophlic addition of carbanion derived from the methyl ketone to the carbonyl- carbon of aromatic aldehydes. Dehydration of the of β - hydroxy ketone to form the conjugated α, β - unsaturated carbonyl compounds occurs spontaneously (Furniss, 1989).

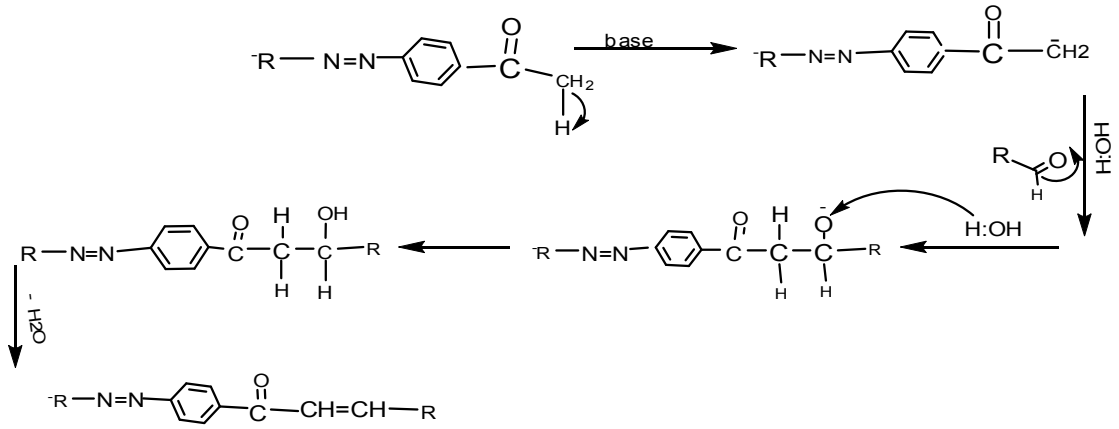


Fig.3.3.1.Reaction mechanism of α, β - unsaturated carbonyl derivatives

3.3.2.Reaction mechanism of formation of pyrazole derivatives:

Payrazoles are heterocyclic compounds contain two nitrogen atoms, were prepared by the cyclization reaction of some α, β - unsaturated compounds, with hydrazine results in formation of pyrazoles, the reaction proceeding *via* the nuchleophlic attack by nitrogen of hydrazine to carbon -carbonyl, followed by protonation the oxygen of carbonyl group . Nuchleophlic attack by another nitrogen of hydrazine to the β- carbon of conjugated unsaturated carbonyl compound . Lead to condensation that followed by dehydration and cyclization (Geissman, 1980).

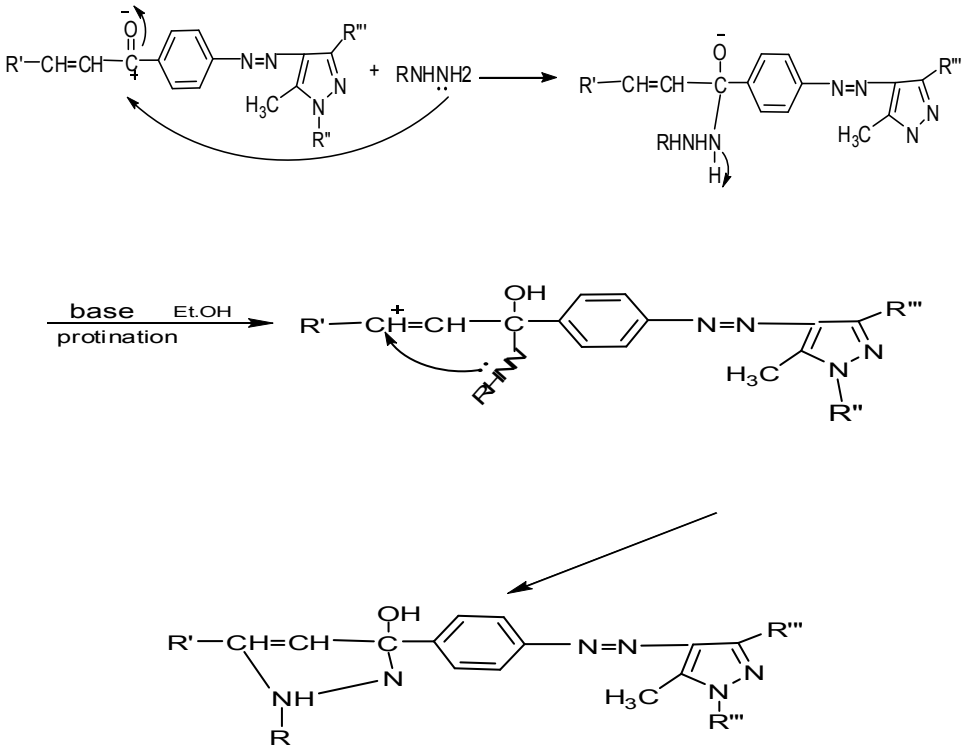


Fig.3.3.1.Reaction mechanism of synthesis pyrazole derivatives

Reaction mechanism of formation of isoxazole derivatives:3. 3.3.

Isoxazole is five membered heterocyclic with oxygen and nitrogen at positions-1and-2, was prepared by most general and widely used method which involved condensation- cyclization of β- diketones with hydroxylamine in presence potassium hydroxide and ethanol. The reaction proceeds *via* the formation intermediate which subsequently on cyclization and dehydration leads to formation of isoxazole. First stepis the reaction by nuchleophlic attack of nitrogen of hydroxylamine to carbon- carbonyl group, step II nuchleophlic attack by oxygen of hydroxyl to electrophilic β- carbon of conjugated α, β-unsaturated compound and protonated the oxygen of carbonyl group, step III condensation the product II, step IV elimination reaction losing two molecule of water lead to cyclization under reflux condition (Michael reaction), (Ballester and Bartlett., 1958).

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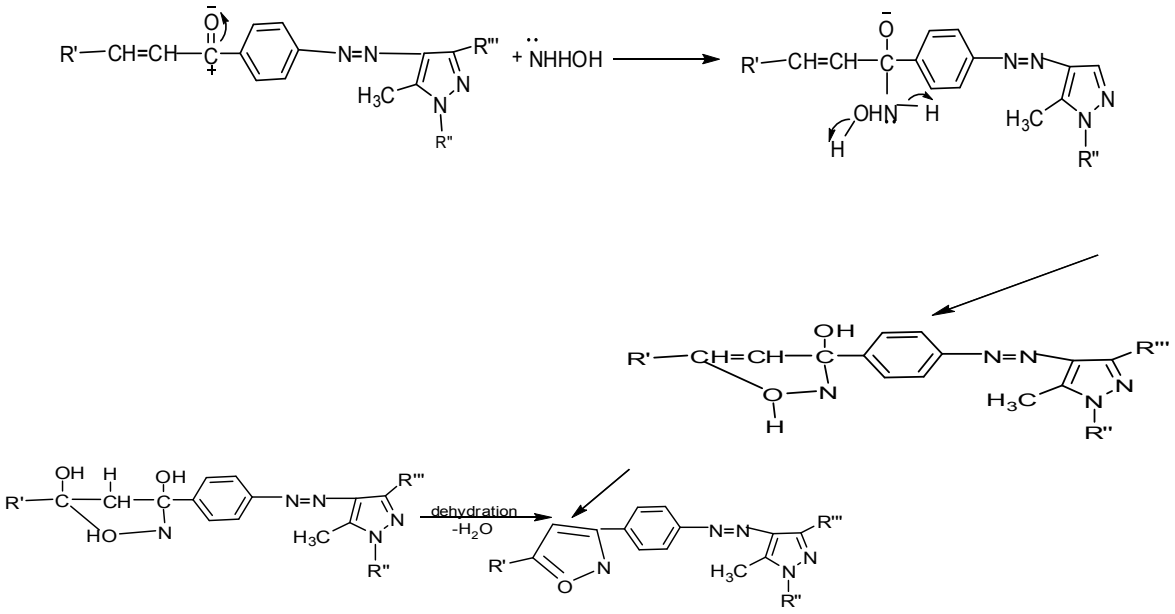
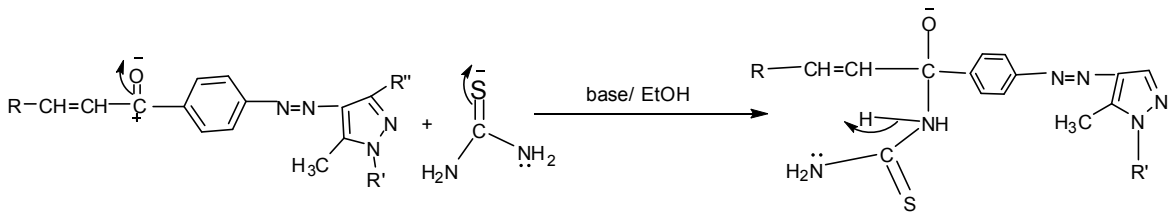


Fig.3.3.3.Reaction mechanism of isoxazole derivatives

3.3.4.Reaction mechanism of formation of thio pyrimidine derivatives:

Pyrimidine derivatives are six membered ring contained two nitrogen atoms at position 1,3, were prepared by the cyclization reaction of some synthesized α, β - unsaturated carbonyl derivatives and thiourea in presence of alkali media. The reaction mechanism was illustrated as flowing. The step (I) nuchleophlic attack by nitrogen of thiourea to carbon-carbonyl which acts as electrophilic character. Step (II) nuchleophlic attack by another nitrogen to β-carbon-conjugated unsaturated compound. Step (III) Step (IV) dehydration elimination the molecule of water Kalirajan *et al.,* 2009).



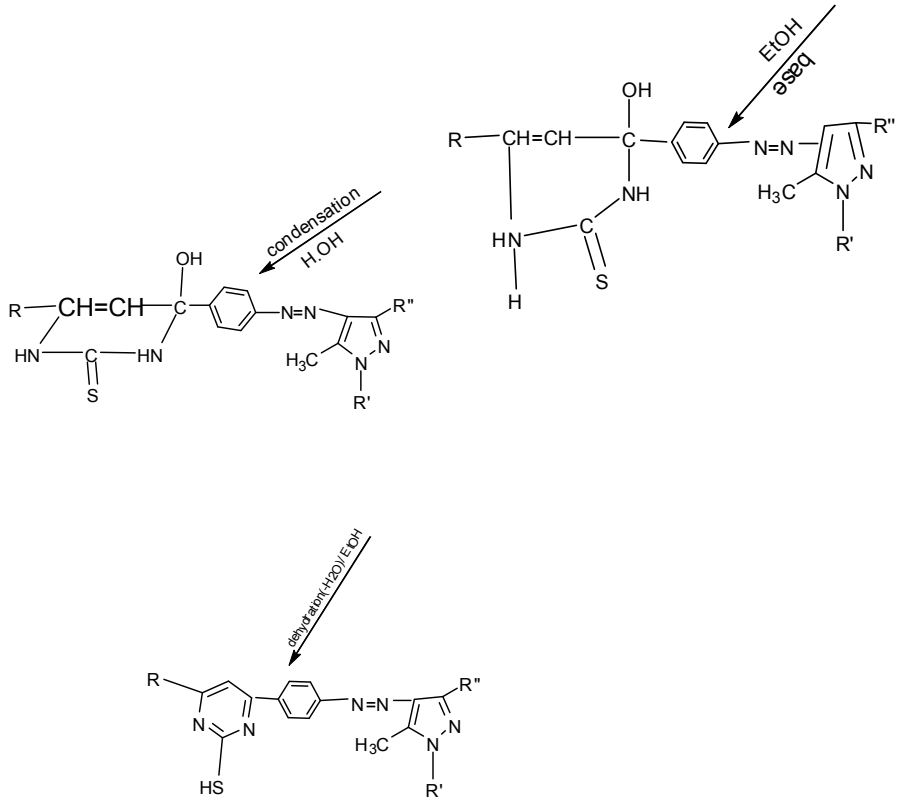


Fig.3.3.4.Reaction mechanism of pyrimidine derivatives

3.4. spectroscopic analysis:

The identification and characterization of the synthetic compounds in this work was carried out by determining their physical properties using (TLC, M.P, IR, UV, ^{1}H and ^{13}C -NMR, MS). The (IR) spectrum bands of synthesized α, β - unsaturated carbonyl derivatives(XIII,LVIII,XLIV, XLV,LVII, XIX, XLVI, XLII, XVII, XVI, XVII, XIV, XIX,XV, XXIII,XX, XXIV,LIV, XLVI, XX, LIII, LVIII, XLI, LI, LXI, XXIV, LXIII, XXLI,LXIILXV,XLVII and LXVII) act as intermediate compounds in this work were tabulated in table (3.1.1.1), C=O carbonyl groups in α, β - unsaturated appear at ranges (1715-1612) cm^{-1}, absorption bands st.vib of C=C olefinic at range (1689-1624)cm^{-1}, C=C aromatic st.vib absorbed

bands showed at (1576-1524) cm^{-1}, N=N olefinic st.vib band appear in range (1667- 1631)cm^{-1} , the range at (1113-1040) cm^{-1} , indicated st.vib absorbed band of N-N , the absorbed band st.vib showed at range(1597--1524) cm^{-1} , were indicated for C=N group, st.vib at range (1355- 1316) cm-1the absorbed band due to C- N group. Compounds LVIII, XLIV, XVII, LVIII, and LI contain nitro group located at *o.*position aldehydic aryl ring their st.vib appear at range 1514- 1332 cm^{-1} due to nitro group. Compounds XIX, XLVI, LIII, LXIII st.vib absorption bands at range 3567- 3431 cm^{-1}, indicated to OH group. Compounds XLII, LXI, XLIX and XLIX contain methoxy group at aldeydic aryl ring therefore st.vib absorption bands appear at regions 1376- 1241cm^{-1}.Compounds LIV, LVIX and XLV contain two methyl groups attached to amino at para position on aldehydic aryl ring our st.vib absorption bands at range 1364- 1315 cm^{-1}. The st.vib absorption bands of IR- spectra for synthesized α, β– unsaturated carbonyl derivatives were tabulated in Table (2.4.1).

Payrazoles derivatives synthesized in this work were prepared as final compound by cyclization reaction of some α, β - unsaturated carbonyl compounds and hydrazine derivatives in presence of sodium acetate as catalyst and ethanol, reflux a mixture eight hours, synthesized pyrazoles have the same structure with difference in R_1, R_2 . I. R spectra of (XCIX, XCV, XCV, XCVII, XCI, LXXV, LXVIII, CII) pyrazole showed st.vib bands in range (1526- 1501 cm^{-1} due to C=C aromatic, the absorption

band wish appeared in ranges (1622 -1550cm^{-1}), were indicated to presence C=N st.vib, the st.vib absorption band seen in the range (1164-1026)cm^{-1} indicated N-N aromatic, the absorption presence in range 1689-1600 cm^{-1} indicated to N=N st.vib absorption band for this group, the st.vib absorption bands showed in the region (2804-2854cm^{-1}), due to C-H asym and at region 3029-2920cm^{-1}due to C- H symmetry. Compounds (XCIX) contains nitro groups at *ortho* position st.vib presence at 15047, 1460cm^{-1}.Compounds(LXXII,LXVIII, XCVII) contained methoxy groups in *para* position their st.vib absorption bands appear at range (1166-1172 cm^{-1}). Compounds (LXXV and LXXXIV) each one of them contain hydroxyl groups in *ortho* position their st.vib band in the range (3440 - 3284 cm^{-1}), compounds (LXIX- CX). The st.vib absorption bands appear (N-N) groups due to presence of pyrazole compounds. Absorption band of IR for synthesized Pyrazole derivatives were tabulated in Table (2.4.2).

Isoxazole derivatives in this study were prepared by cyclization reaction of some synthesized α, β-unsaturated compounds derivatives with hydroxylamine hydrochloride in presence basic media and ethanol. The infra- red spectra of isoxazoles (XC, LXXIV, XCIII, CI, LXXXVII, LXVXII-CIX) showed the st.vib absorption bands in the range 1500-1596cm^{-1}, due to C=C, N-N st.vib bands were showed in the range 1105-1175 cm^{-1}, the st.vib absorption bands showed in the rang 1602-1976 cm^{-1}indicated for N=N, the st.vib absorption bands showed in the region between 1343-

1365 cm^{-1} , were indicated the presence C-N ring, the st.vib absorption bands showed in the range 1185-1017 cm^{-1}, were indicated N-O in the isoxazole ring, the st.vib absorption bands were showed in region 2923-2900 cm^{-1} , indicated the presence of C-H sym, 2854-2852 cm^{-1} , the rang of st.vib absorption band showed indicated C-H asym .The isoxazoles derivatives (LXXI, LXXIV, LXXXIII, XCVI) each of one contain hydroxyl groups their st.vib absorption bands appear in the rang 3445-3383cm^{-1}, the compounds (LXXVII,XCVI) all of these were contain methoxy group in para- position their st.vib absorption band presence in the rang 1241-1296 cm^{-1}, the isoxazole derivative (CIV) contain amino group in para- position their st.vib absorption band presence in the rang 3622cm^{-1}, compound (CI) contains nitro group at ortho position their st.vib appear at 1525,1417cm^{-1}. All absorption bands of infra-red spectra for synthesized isoxazole derivatives were tabulated in Table(2.4.3).

Thiopyrimidine derivatives in this work were prepared as final compounds by cyclization the intermediate some compounds (α, β - unsaturated derivatives) with thiourea in basic media and ethanol under reflux condition. Infra-red spectra bands of derivatives in this study showed st.vib absorption bands in the rang e 1556- 1355cm^{-1} indicated the presence C=C groups, the st.vib absorption bands showed in the range 1602- 1500 cm^{-1}, indicated C=N groups, the st.vib absorption bands in the range 1176-1174 cm^{-1} indicated N-N band, the st.vib absorption bands presence in region

1685- 1500 cm^{-1}, were indicated N=N groups, the st.vib absorption bands showed in the range 1392-1257cm^{-1}, indicated C-N groups, the st.vib absorption bands whish observed in the range 2855-2850 cm^{-1}, indicated the presence S-H groups, the st.vib bands showed in the region 3028-2921 cm^{-1}, indicated C-H groups. Compounds (LXXIII, LXXIX, XCVII) each contains methoxy group in para –position their st.vib absorption bands appear in the range 1058-1051 cm^{-1} due to appearance OCH_3 groups at*para* position. Compounds (LXXVI, LXXXV,) contain hydroxy group at *ortho* position st.vib appear at range 3444 -3392 cm^{-1}. Compounds LXXXV, CVIII and LXXIX contain nitro group at ortho position their st.vib presence at region 1445- 1367 cm^{-1}, due to NO_2 group. The st.vib absorption bands of infra-red spectra for synthesized pyrimidine derivative were tabulated in Table(2.4.4).

The new derivatives compounds (pyrazoles, isoxazole, pyrimidine) in this work were prepared as final compounds by the cyclization reaction of some synthesis α, β - unsaturated carbonyl compounds.

^{1}H-NMR was one of the most powerful technique used in structural elucidation. It provide much information about the different chemical and magnetic environments of protons together with the accurate number in each environment. The value of coupled constants provide an information about which proton coupled to which one. The results were on $\boldsymbol{\delta}$ value (ppm) scale with the signal appear to the left of TMS, the internal ($\boldsymbol{\delta}$ = 00). The 1H-NMR

of synthesized α, β – unsaturated carbonyl compounds XIX, XVII, XV, XVIII, XIII, XVI, XIV, LI, LIII, XLVII, XV,L, XLIX their aromatic protons appear at $\boldsymbol{\delta}$ 6.81- 8.00 the intensity of protons resonating as a multiplied, and conjugated α and β protons displayed two doubled signal at $\boldsymbol{\delta}$ 2.09-2.65 due to two protons of α, β - unsaturated carbonyl compounds. Compounds LIII, XIX contain hydroxy group located at *ortho* position a singlet signal showed as sharp signal at $\boldsymbol{\delta}$ 3.62- 3.80 this due to deshielding can be rationalized on the basis of the lone pair of oxygen atom. Compounds XV, XLIX, XV contain methoxy group at *para* position the Protons resonating as singlet at $\boldsymbol{\delta}$ 3.30- 3.60 the deshielding due to alone pair effect of oxygen atom compared to methyl groups located on pyrazole ring and cyclohexane that appear at $\boldsymbol{\delta}$1.04- 1.92. The ^{1}H-NMR of synthesized α, β- unsaturated carbonyl derivatives were tabulate in Table (2.6.1).

^{1}H - NMR of synthesis pyrazole derivatives were displayed sharp singlet's signal of three protons intensity at $\boldsymbol{\delta}$ 2.09- 2.52 assigned to two methyl groups located on C_3 and C_5 of pyrazole ring and one sharp singlet signal of proton intensity at $\boldsymbol{\delta}$ 6.00- 7.17 located at pyrazole ring. Compounds CX, LXXXVI, CVI contains two methyl group attached to amino group, the protons of methyl group resonating as a singlet at $\boldsymbol{\delta}$ 3.01- 3.50 compared to protons of methyl groups attached to C3, C5 of pyrazole rings the difference in the chemical shift due to the lone pair effect of nitrogen atoms. Compounds

LXXXIV, LXXV contain hydroxy group at *ortho* position displayed one sharp sing lets of one proton intensity at **δ** 3.31- 3.87 the deshielding due to hydrogen bond or alone pair effect of oxygen atom. Compounds LXVIII, LXXII, XCVII contain methoxy group at *para* position therefore displayed one sharp singlet signals at **δ** 2.50-3.70 the deshielding due to rationalized on the basis of lone pair effect of oxygen atoms attached to methyl group. Compounds CVI, XCVII, CIX, CII contain cyclohexane attached two methyl groups at position C_5 and carbonyl groups located at C_1, C_3 1H NMR spectrum displayed one sharp singlet signals at **δ**0.98- 1.23 due to three protons of two methyl groups and two singlet signals of four protons of cyclohexane at **δ** 2.08- 2.67. All synthesis pyrazole derivatives are multiplied at **δ** 6.77 - 8.22. The ^{1}H-NMR of synthesized pyrazole derivatives were tabulated in Table (2.6.2).

1H- NMR of isoxazole derivatives compounds (CIX, LXXXII, LXXVII, LXXI, XC, LXXIV, LXXXVIII, CV, CI, CIV, XCVI) is displayed singlet of one proton intensity at δ6.40- 7.04 assigned to proton of isoxazoles rings and the protons of aromatic rings appear as multiplied intensity at δ 7.02- 8.05. Compounds CIX, LXXXVIII and CI contain amino group located at para position therefore displayed singlet signals of six protons of two methyl groups at δ 3.23- 3.92, compared with methyl groups attached to pyrazole of heteroaryl compounds that appear at δ 0.85- 2.62, the difference intensity

due to nitrogen atom turn resonate at lower field than the methyl attached to carbon and the effect of lone pair (electronegative atom) nitrogen atom causes deshielding of the proton. Compounds LXXXIII, LXXIV contain hydroxy group located at *ortho* position of aldehydic ring which showed at δ 3.23-3.50 this due to hydrogen bonding greater the downfield shift higher δ value of its resonance. The ^{1}H-NMR spectra of synthesized isoxazole derivatives were tabulated in Table (2.6.3).

^{1}H – NMR spectrum of thio pyrimidine derivatives CVII, LXXIX, LXXIII, LXXXII, XCII, LXXVI, LXXXIX, CVIII, CVII, C, XCVII, CIII displayed singlets signal of one proton intensity at δ6.76 – 7.10 due to proton of thio pyrimidine ring beside the proton of SH appear as singlet at δ 3.33-6.47and intensity of protons on aromatic rings showed the multiply asδ7.05 -8.30, the difference in the shifts affect by electrons density and groups attached the ring. Compounds CVII, CVIII, CXXXIX contain two methyl groups attached amino group. Compounds LXXXIX, LXXIII, XCVII contain methoxy group at para position at aldehydic aryl ring were displayed singlets of three protons methyl group intensity at δ 3.31 – 3.90, 2.64 – 3.80 respectively those compared to compounds contain methyl group attached the carbon atom displayed singlets of three proton intensity asδ 0.85 – 2.08. The difference in chemical shift due to lone pair effect of oxygen and

nitrogen atom.The ^{1}H – NMR spectra of synthesized thio pyrimidine derivatives were tabulated in Table (2.6.4).

The mass spectra of synthesis pyrazole, isoxazole and pyrimidine derivatives showed similar cleavage pattern. Cleavage of the side chain of C-C and C-N bond lead to the base peak at m/z 80(100%) due to ($C_4H_3N_2$) ion, further fragmentation appear to gives a characteristic peaks at m/z 171, 64, 137 .

The molecular weight of all synthesized compounds are determined by mass spectra. Some synthesized derivatives characterized by mass spectrometer , therefore their details showed at fowling M, M+1, M+2, M-1.pyrazole the molecular weight absolved at M-77. The MS - spectra of pyrazole, isoxazole and thiopyrimidine derivatives were tabulate in Tables (2.7.2), (2.7.3) and (2.7.4) respectively.

CHAPTER FOUR

CONCLUSIONS AND RECOMMENDATIONS

Conclusions and recommendations

The following points may be concluded from the results of this work :

I. The interaction of diazotized *p*-aminoacetophenone with 1,3 dicarbonyl(benzoyl acetone, ethyl acetoacetate, acetyl acetone and dimedone)in presence of sodium acetate led to formation of diazo (acetyl phenyl)-1,3-dicarbonyl .

II. Synthetic equivalent reaction of hydrazine derivatives and β- di carbonyl diazo compounds, led to usual approach for synthesis of pyrazole derivatives

III. The prepared compounds condensed with aromatic aldehydes in alkali media at room temperature led to formation α, β- unsaturated carbonyl compounds(Claisen- Schmidt reaction). The first condensed involving the nuchleophlic addition of carbanion of methyl of *p*-amino aceto diazo phenyl to the carbonyl- carbon of aromatic aldehydes. Dehydration to formed conjugated unsaturated carbonyl compound.

IV. α, β – unsaturated carbonyl compounds were isolated as intermediated at the high yield and very active compounds, therefore could react with regents to form various compounds(isoxazole, pyrazole and pyrimidine. .et). and were a key intermediate in synthesis of diazo (hetero phenyl)-pyrazoles and diazo(hetero phenyl)-5,5-dimethy cyclohexane-1,3-diones by cyclization.

V. α, β unsaturated carbonyl compounds reacted as electrophile with nuchleophlic attack of hydrazine derivatives, hydroxyl amine and thiourea (Michael addition) by cyclization afford pyrazole, isoxazole and thio urea. The reaction mechanism was Michael reaction which had been shown to proceed by a substituted as well as by an elimination – addition mechanism.

VI. Pyrazole, isoxazole and thio pyrimidine derivatives were final products. Were purified by recrystallization and TLC techniques. The structures of synthesis compounds were characterized by IR, ^{1}H,^{13}C-NMR and mass spectra

VII. The practical advantage of reactions leading to compounds, that were isolated upon cyclization, was that their structures was supported by analytical spectral data

VIII. Further examination of the activity of newly synthesized to examining against bacteria, fungal and cancer is recommended.

CHAPTER FIVE

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CHAPTER SIX

APPENDIXES

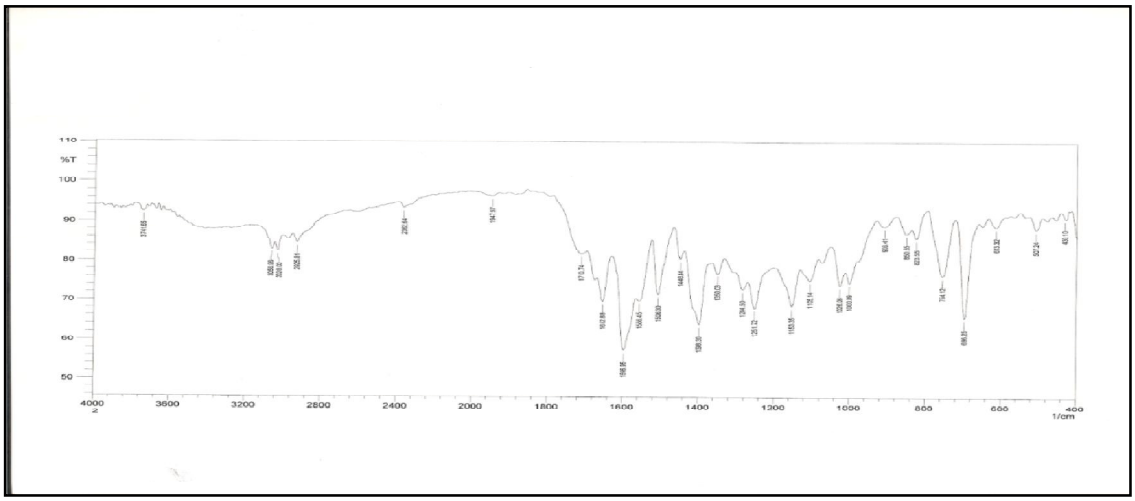

Fig.6.1. IR spectra of synthesis 4-diazo- (4-((p-(5-(-4 -methoxy phenyl) -2-thiopyrimidine-6-yl)-phenyl-3,5-dimethyl-1-phenylpyrazole(LXXIII)

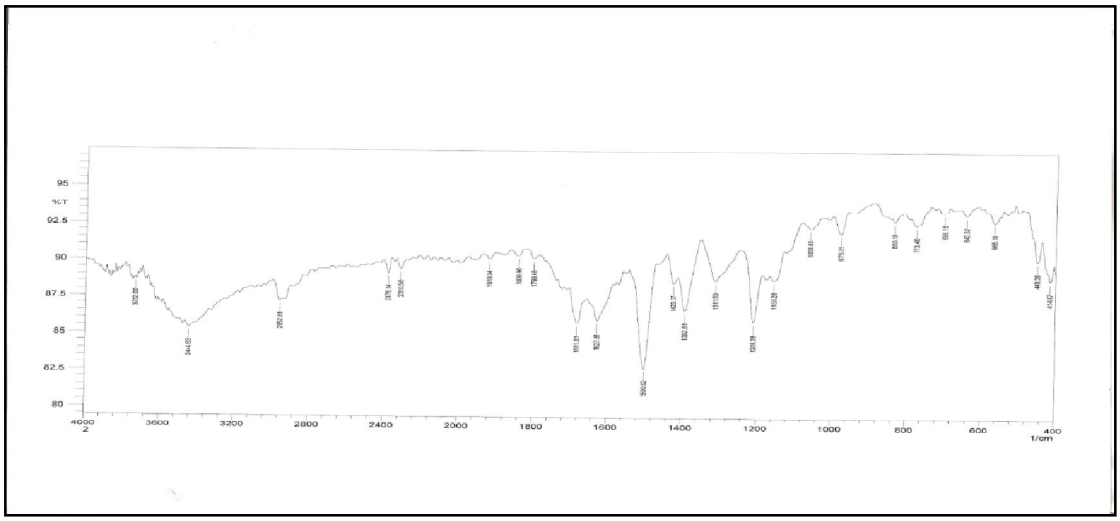

Fig.6.2.IR spectra of synthesis 4-diazo-(p-5-((2-hydroxyphenyl)-isoxazol-5-yl)phenyl-3,5-dimethyl-1-phenylpyrazole (LXXIV)

Fig.6.3.IR spectra of synthesis 4-diazo-(p-5-(4-methoxy phenyl)-pyrazol-3-yl)phenyl-3,5-dimethyl-1-phenylpyrazole(LXXII)

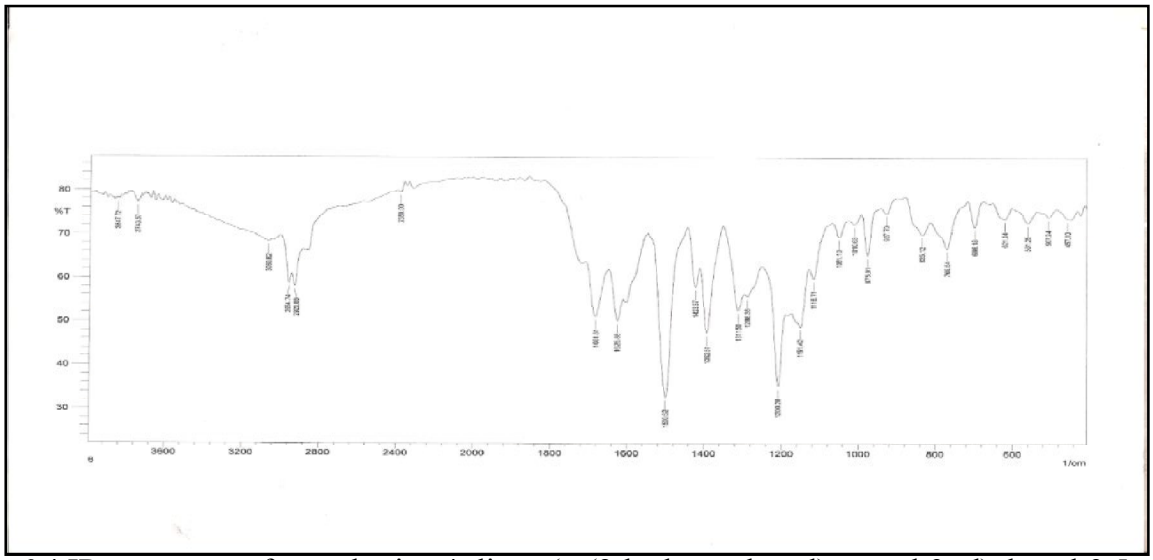

Fig.6.4.IR spectra of synthesis 4-diazo-(p-(2-hydroxyphenyl)-yrazol-3-yl)phenyl-3,5-dimethyl-phenylpyrazole (LXXV)

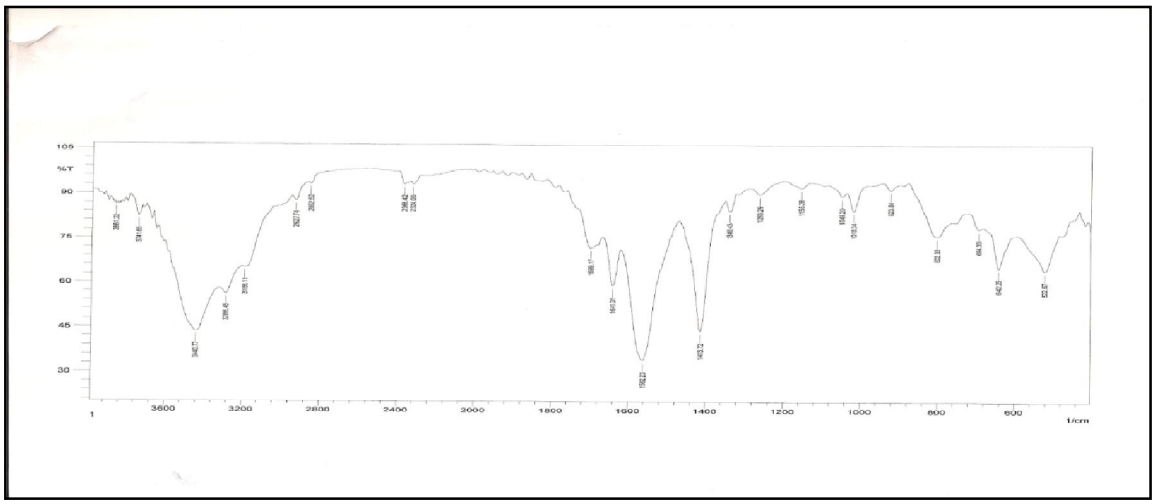

Fig.6.5.IR.spectra of synthesized 4-diazo-(-4-methoxyphenyl) –isoxazol-5-yl)-phenyl-5,5-dimethyl-cyclohexane-1,3-dione(XCVI)

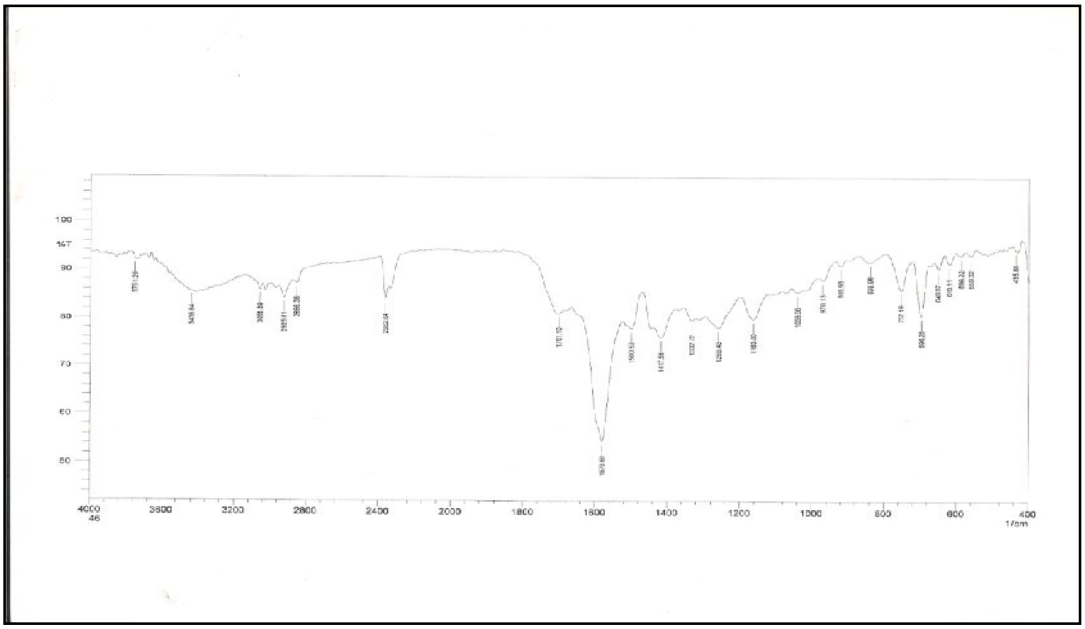

Fig.6.6. IRspectra of synthesis 4-diazo-(p-(5-(p-N,N-dimethyl amino phenyl) -2-thiopyrimidine-6-yl)phenyl-3,5-dimethyl-1-2,4dinitrpphenyl-pyrazol,(CX)

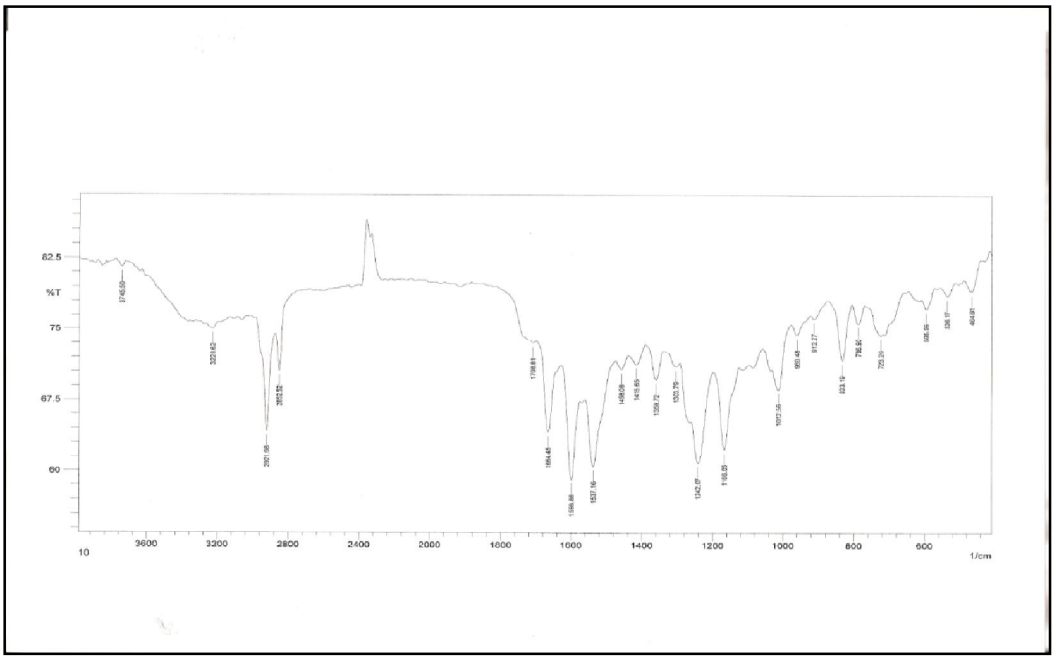

Fig.6.7.IR spectra of synthesis 4-diazo-(p-(5-(p-N,N-dimethylamino) phenyl)- isoxazol- 5-yl)phenyl)diazenyl)-5-methyl-pyrazol-3-one (XC)

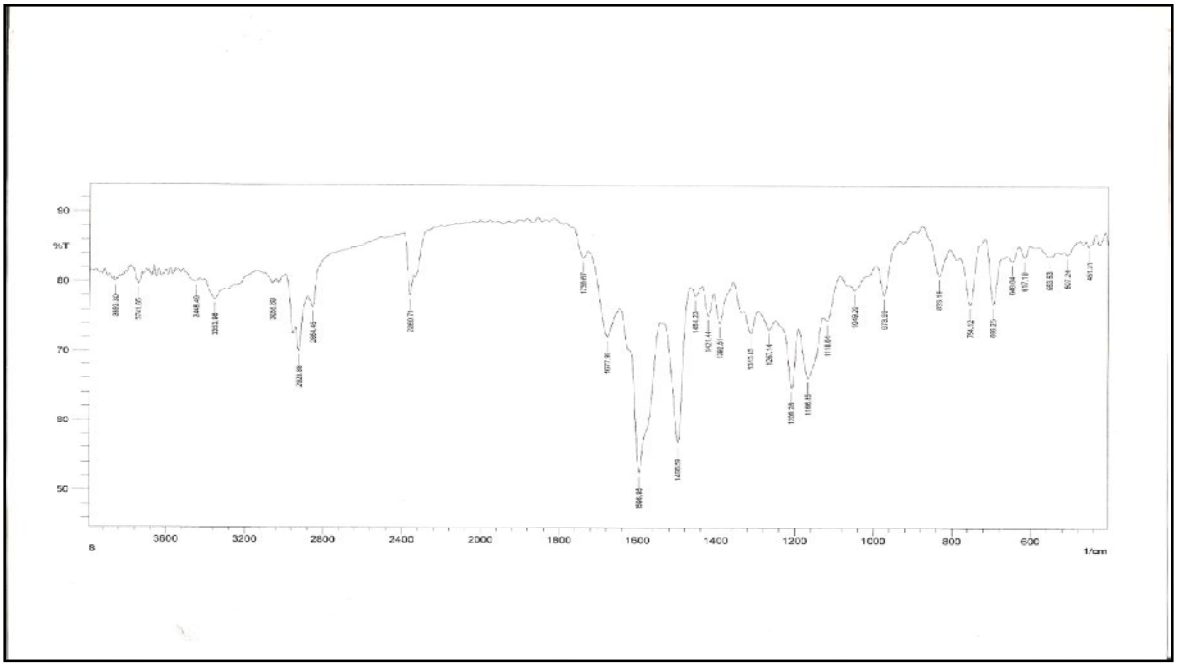

Fig.6.8.IR. spectra of synthesis 4-diazo-(p(5-(p-N,Ndimethyl amino phenyl) –2-thiothiopyrimidine-6-yl)phenyl)- 5,5-dimethylcyclohexane-1,3-dione (CVII)

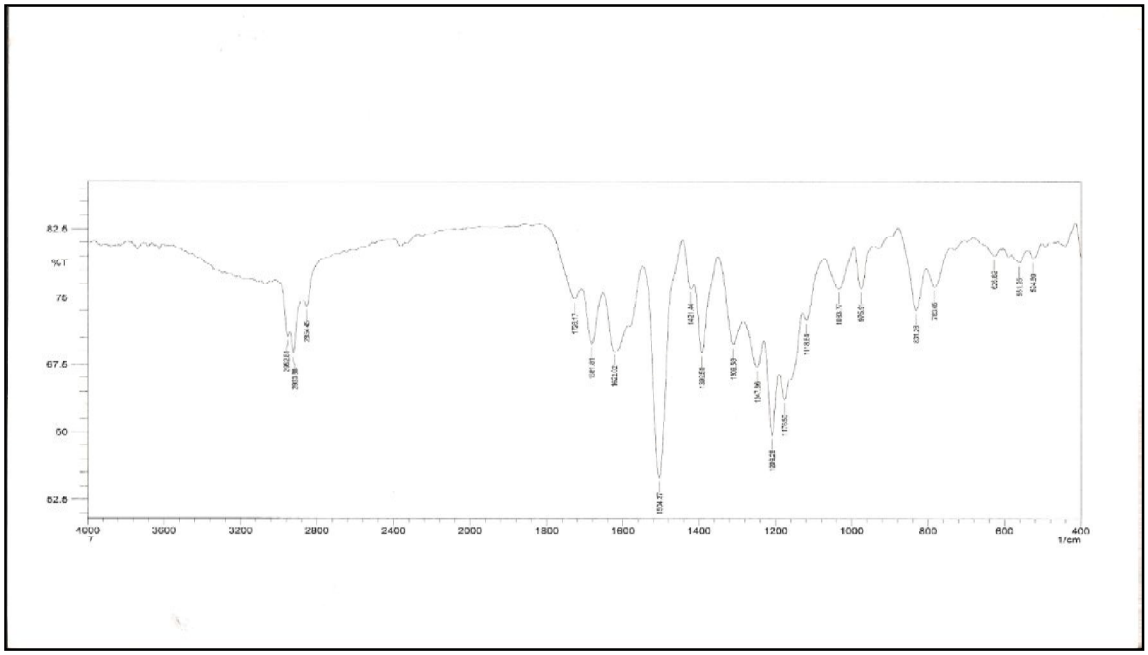

Fig.6.9.IR .spectra of synthesis 4- diazo- (p-(5-(2-phenyl ethenyl) –pyrazol-3-yl) phenyl) -5-methyl -1-phenyl pyrazol-3-one (XCI)

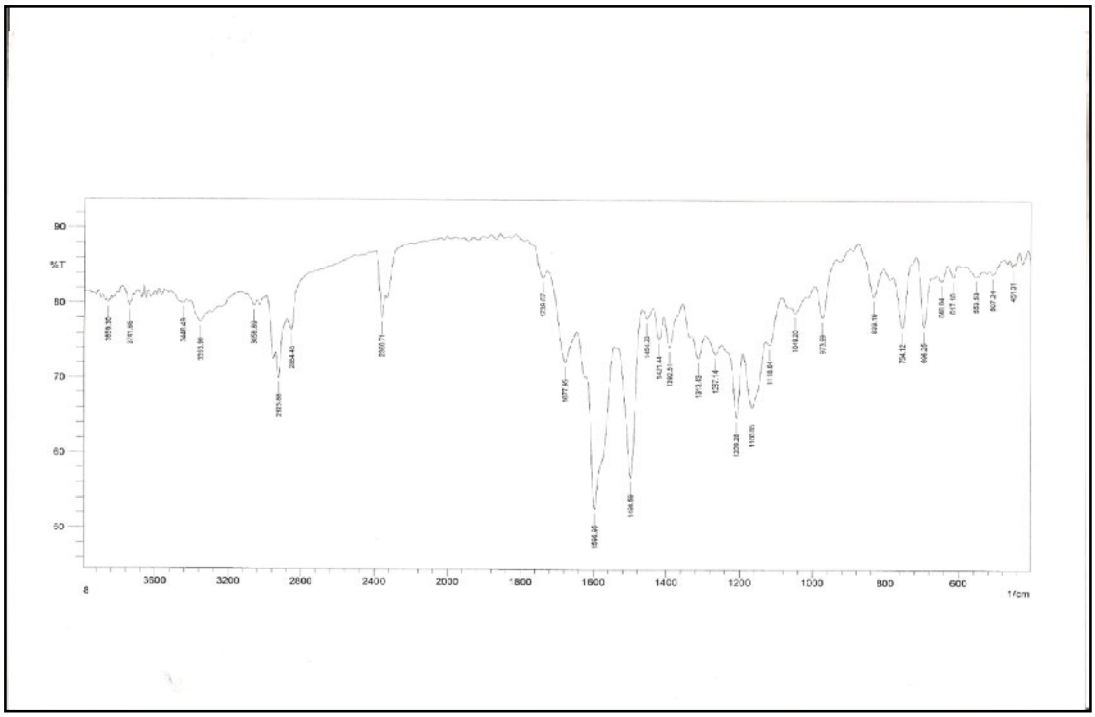

Fig.6.10.IR spectra of synthesis 4-diazo-(p-(5-(p-N,N-dimethyl amino phenyl)-pyrazol -3-yl)-phenyl)-3,5-dimethyl-1-2,4-dinitrphenylpyrazole(CVIII)

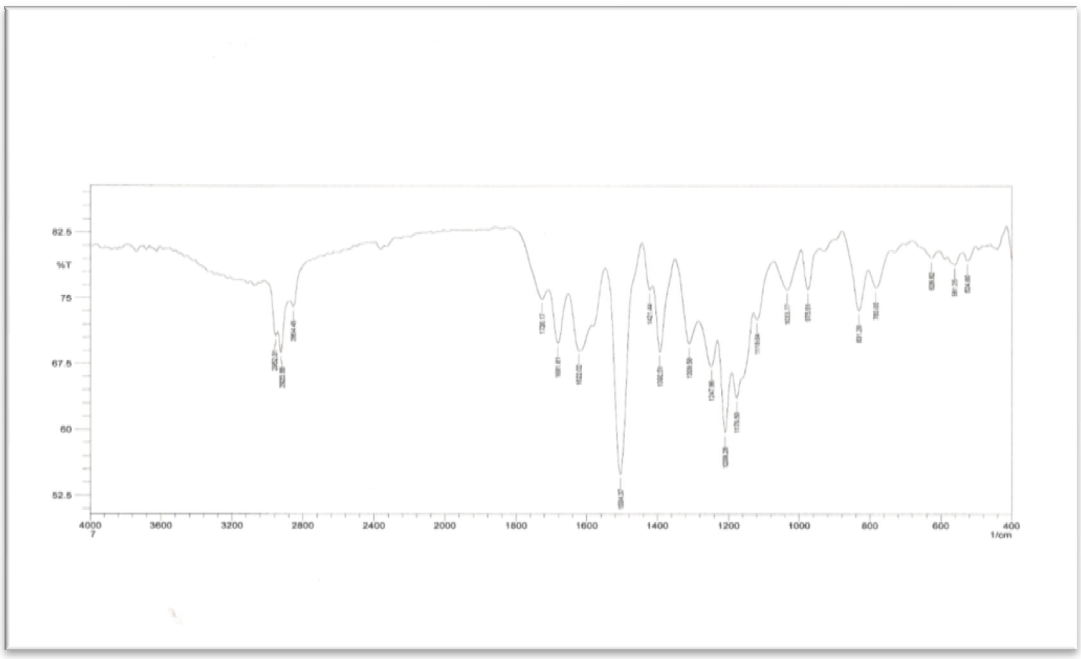

Fig.6.11.IR. spectra of synthesis 4-diazo-(p-(5-(2-phenylethenyl)-isoxazol -5-yl)-phenyl-5-methyl-1-phenylpyrazol-3-one (XC)

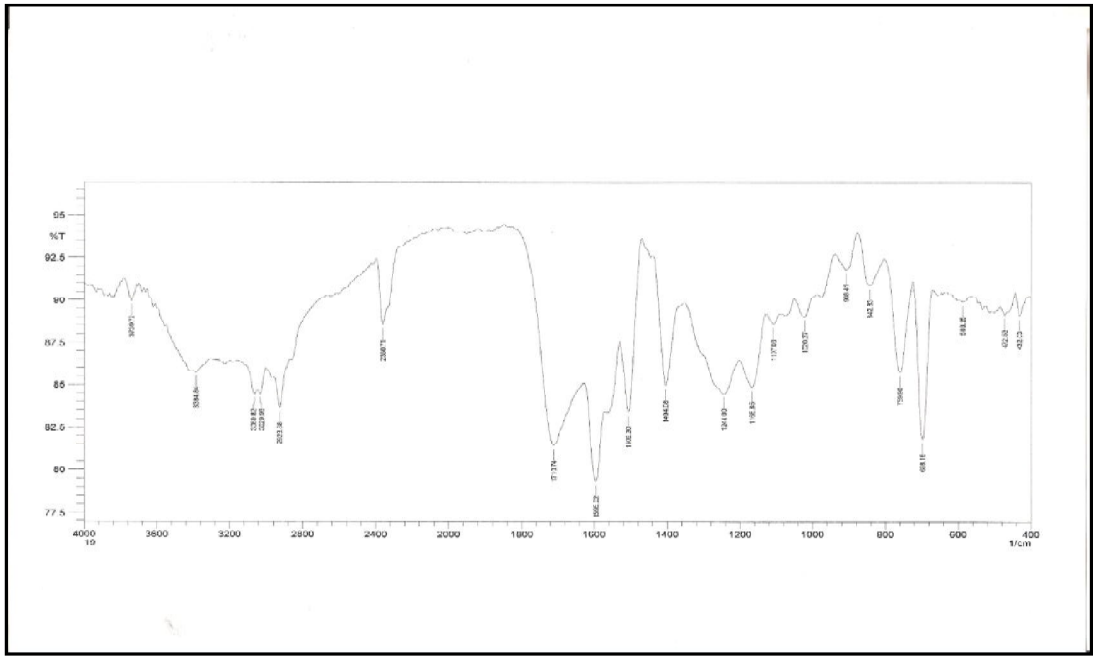

Fig.6.12.IR. spectra of synthesis 4-diazo-(p-(5-(p-N,Ndimethyl amino phenyl) -pyrazol-3-yl)- phenyl)-5-methyl pyrazol-3-one(LXXXVI)

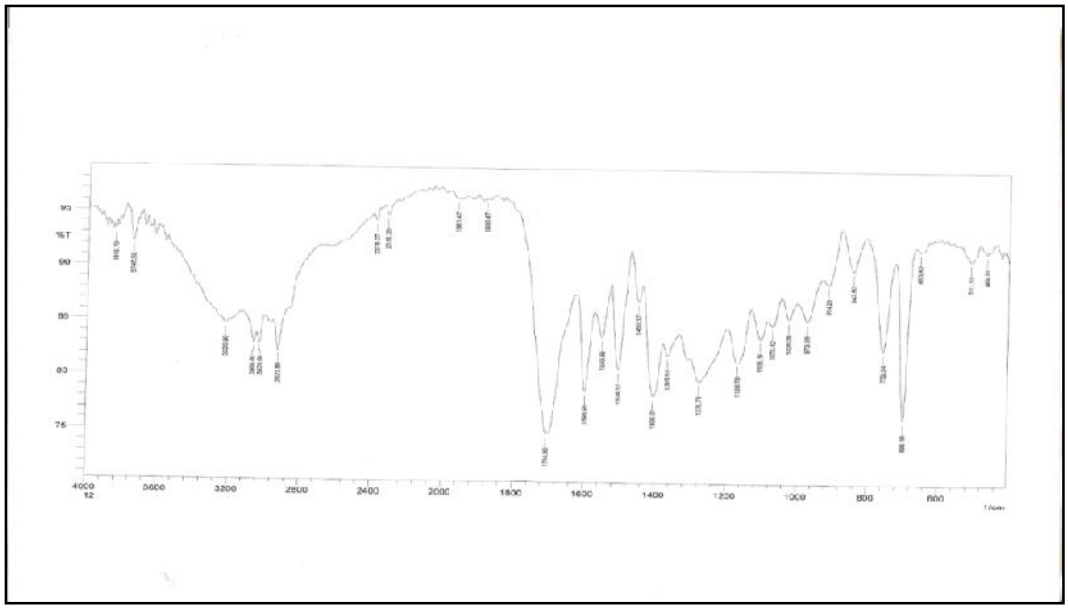

Fig.6.13.IR.spectra of synthesis 4-diazo-(p-(5-(p-N,N-dimethylamino phenyl)-isoxazol-5 -yl)-phenyl)-3,5-dimethyl-1-2,4-dinitrophenylpyrazole(CIX)

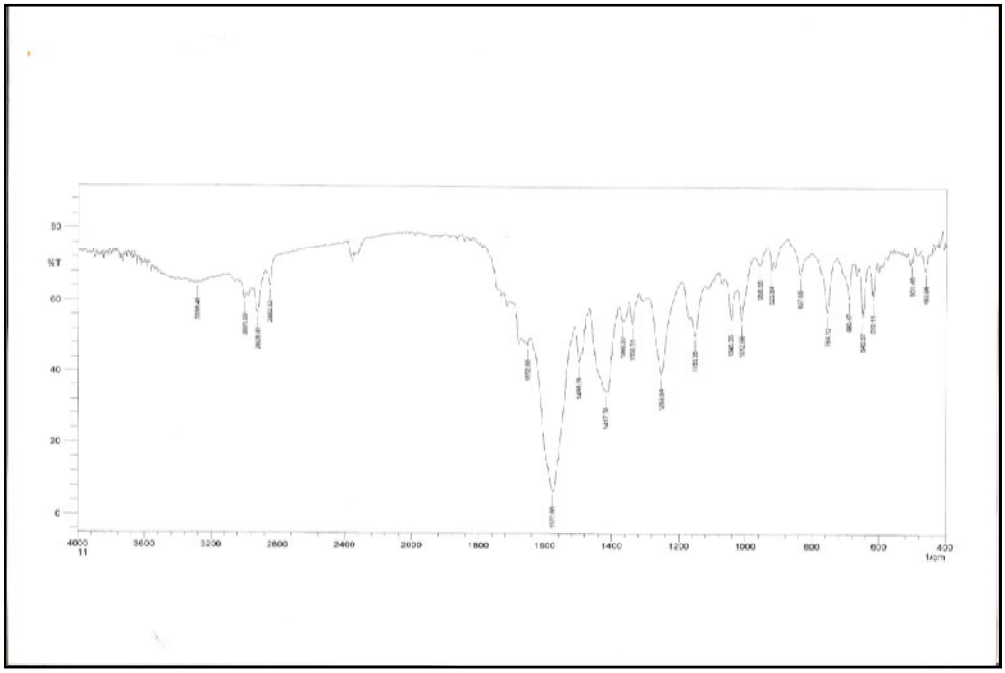

Fig.6.14.IR.spectra of synthesis 4-diazo-(p-(5-(p(N,N-dimethyl amino phenyl)-2thiopyrimidin-6-yl)- phenyl)-5- methyl pyrazo-3-one(LXXXIX)

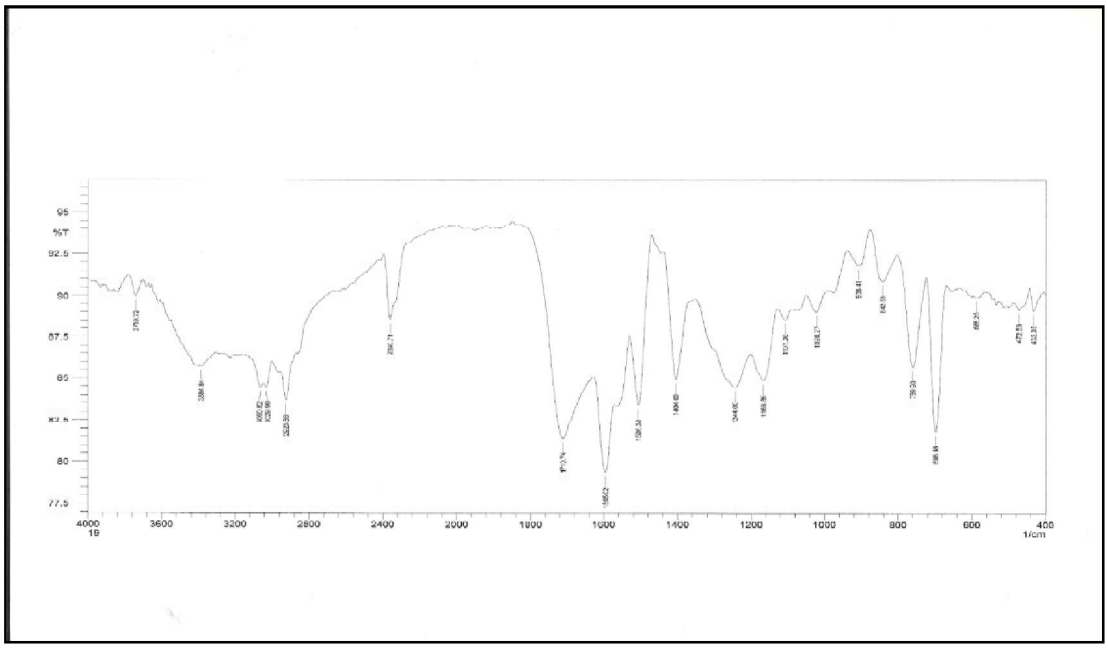

Fig.6.15.IRspectraofsynthesis 4-diazo-(p-(5-(2-hydroxyphenyl) isoxazol-5-yl) -phenyl) -3,5-dimethyl -1-2,4- di nitro phenyl pyrazole(LXXXIII)

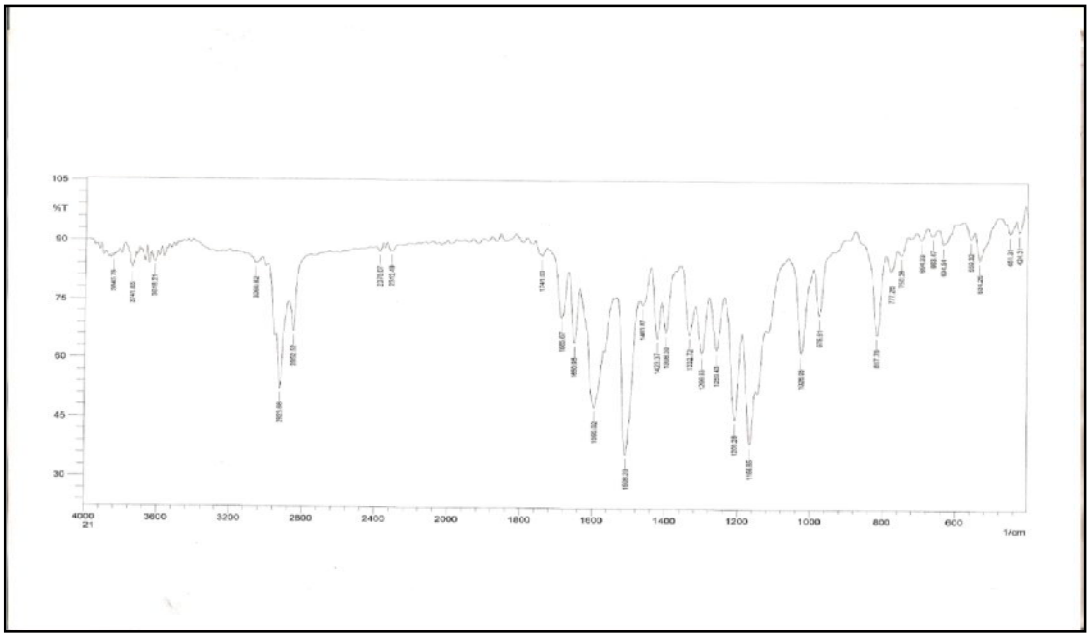

Fig.6.16.IRspectraofsynthesis 4-diazo-(p(5-(4-methoxy phenyl)-pyrazol-3-yl)-phenyl)-5,5-dimethyl-1,3-cyclo hexane-di-one(XCVII)

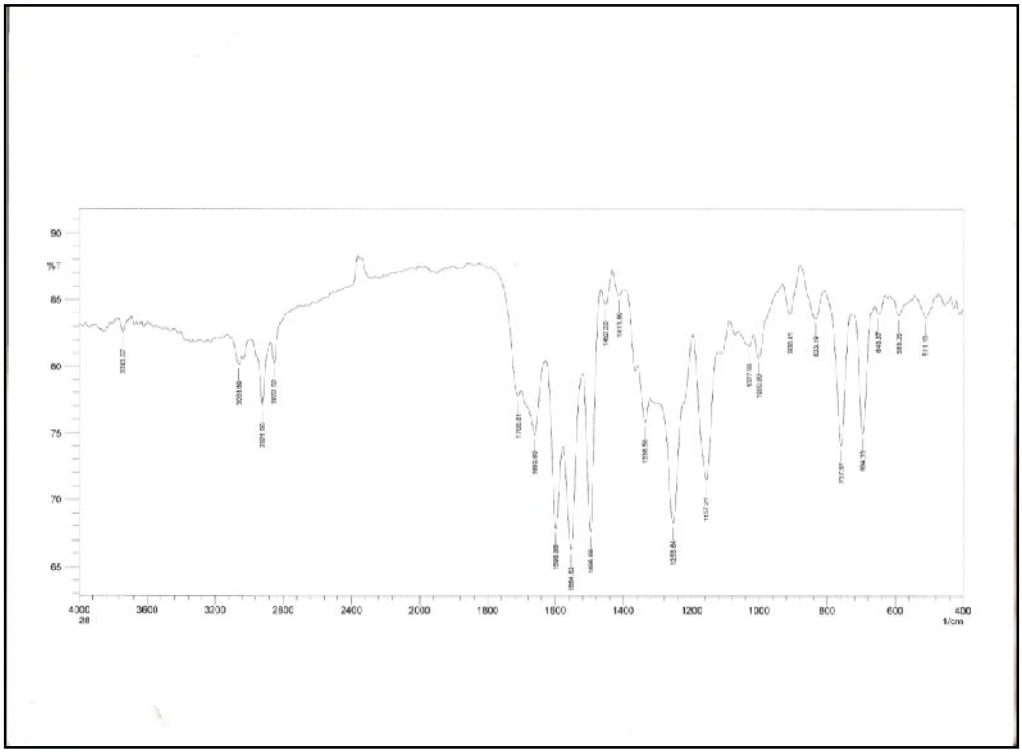

Fig.6.17.IR. spectra of synthesis 4-diazo-(p-(5-(p-N,N-dimethyl amino phenyl)-pyrazol-3-yl)-phenyl)-5,5-dimethyl-cyclohexane-1,3-di-one(CV)

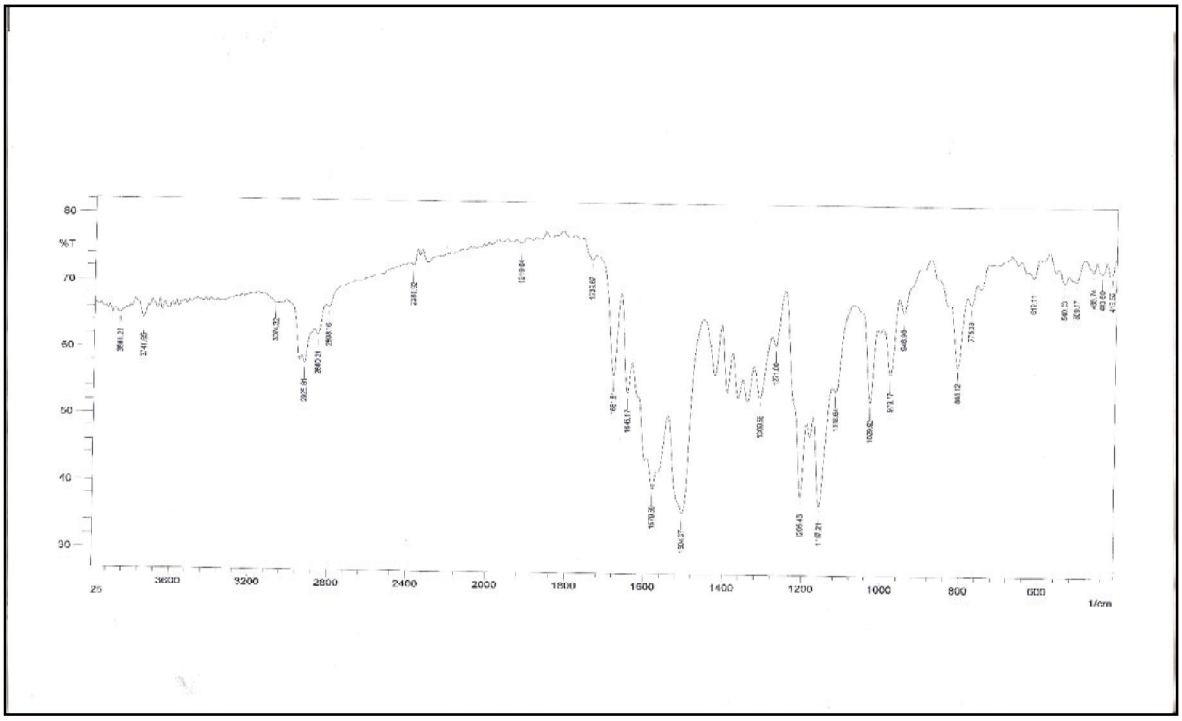

Fig.6.18.IR.spectra of synthesis 4-diazo-(p-(5-(2-phenyl ethenyl)-2-thiopyrimidine-6-yl)-phenyl)-3,5-dimethyl-1-phenylpyrazole (XCV)

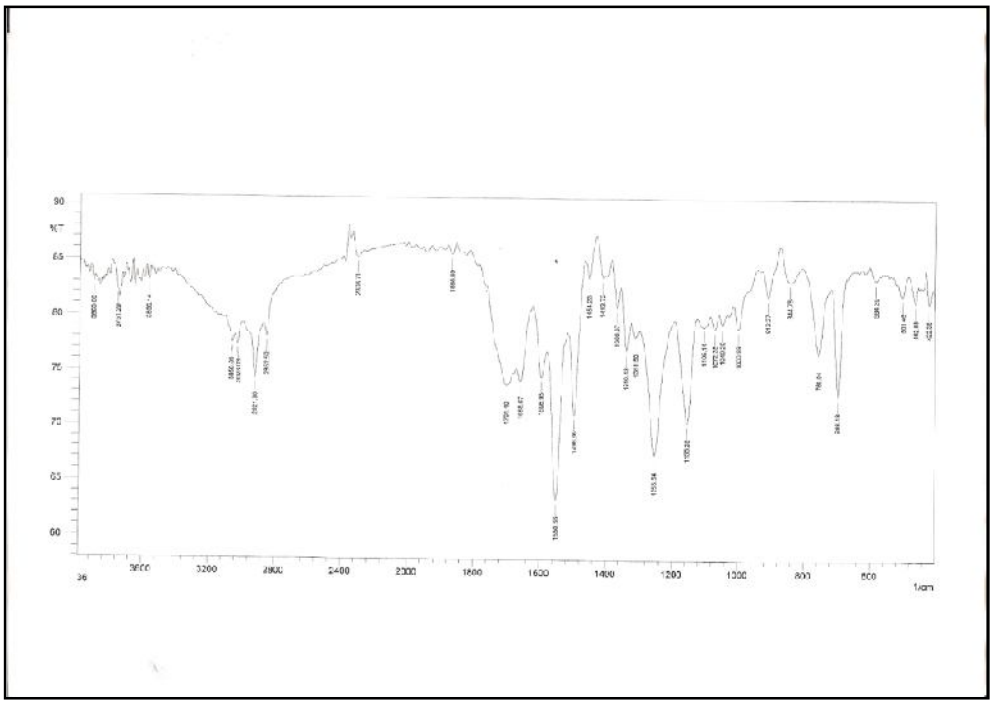

Fig.6.19.IR spectra of synthesis 4-diazo-(p-(5-(p-N,N-dimethyl amino phenyl)-2-thiopyrimidine-6-yl)-phenyl)-5,5-dimethyl-cyclohexane-1,3-dione(CVII

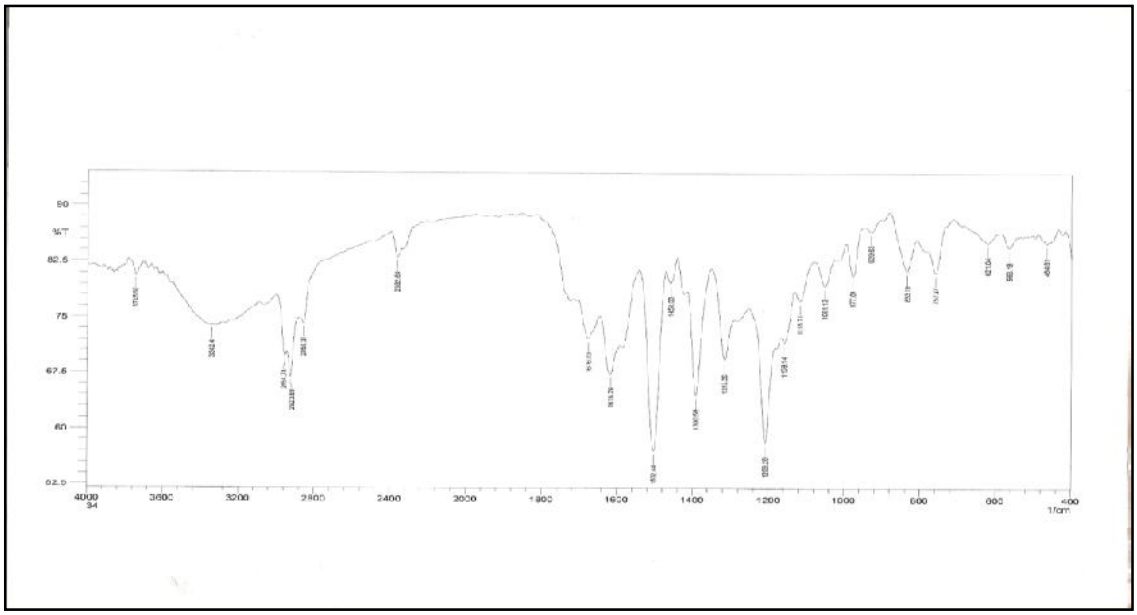

Fig.6.20. IR spectra of synthesis 4-diazo-(p-(5-(-4-methoxy phenyl)-2-thiopyrimidine-6-yl)-phenyl)-5,5-dimethylcyclohexane-1,3-one (XCVII)

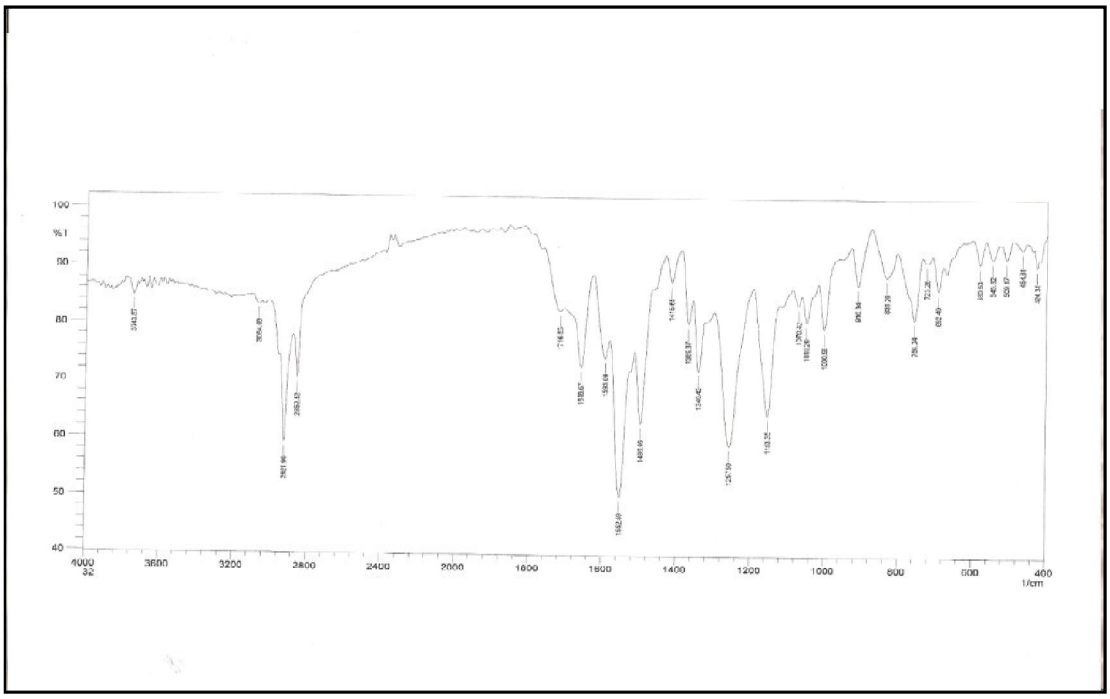

Fig.6.21.IR spectra of synthesis 4-diazo-(p-(5-(2-phenyl ethenyl) -pyrazo-3-yl)-phenyl)-3,5-dimethyl-1-phenylpyrazole(XCV)

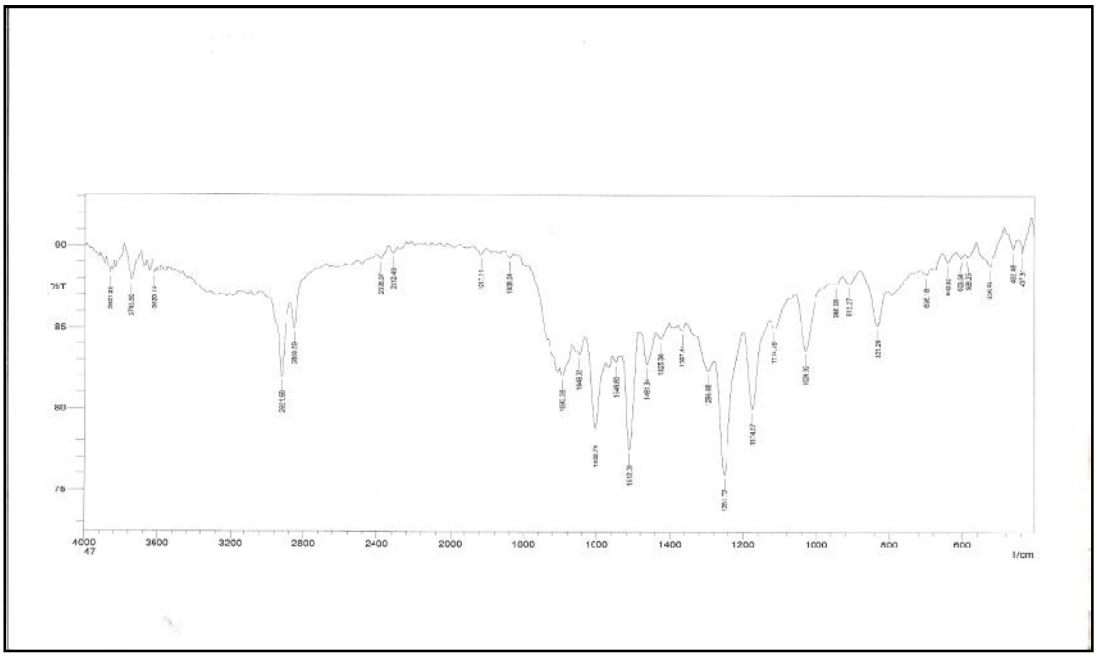

Fig.6.22.IR.spectra of synthesis 4-diazo-(p-(5-(2-phenyl-thenyl)-2-thiopyrimidine-6-yl)-phenyl)-5-methylpyrazol-3-one (XCII)

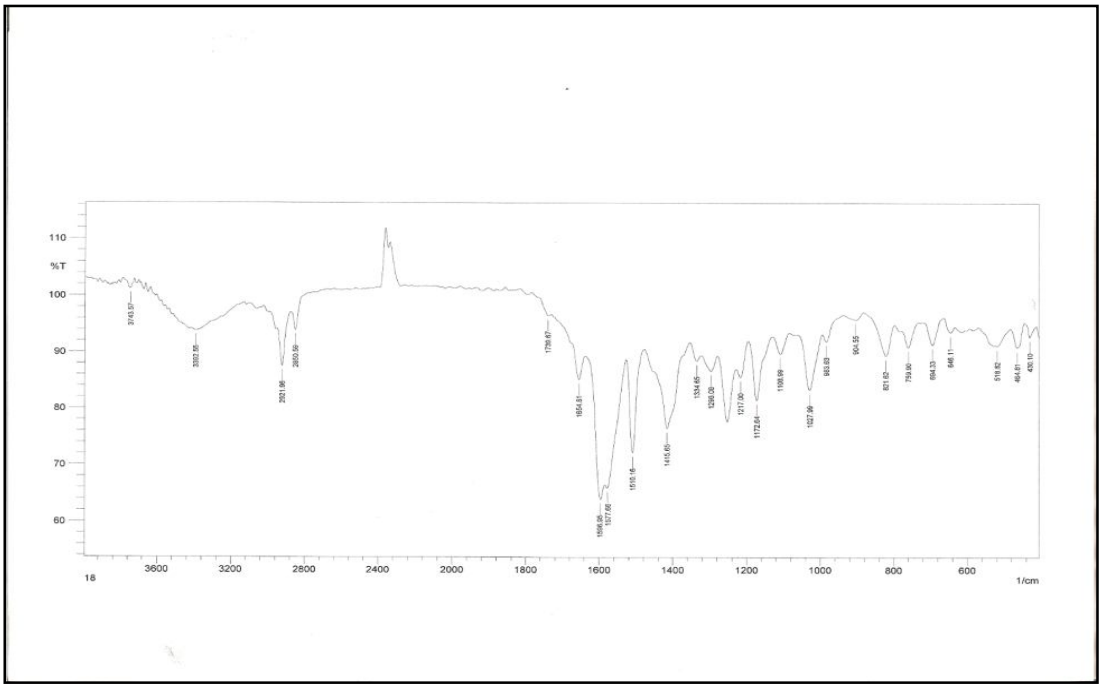

Fig.6.23.IR. spectra of synthesis 4-diazo-(p-(5-(2-hydroxyphenyl)-2-thiopyrimidine-6-yl)-phenyl)-3,5-dimethyl-1-pphenylpyrazole(LXXVI)

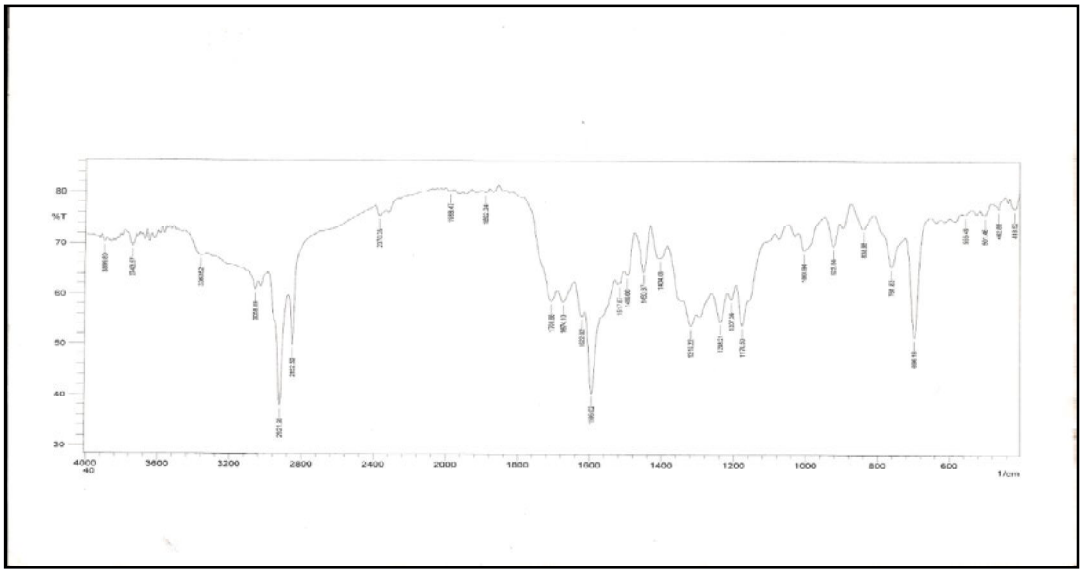

Fig.6.24.IR spectra of synthesis 4-diazo-(p-(5-(2-nitrophenyl)-2-thiopyrimidine-6-yl)-3,5-dimethyl-1-2,4-dinitrpphenylpyrazole(LXXXII)

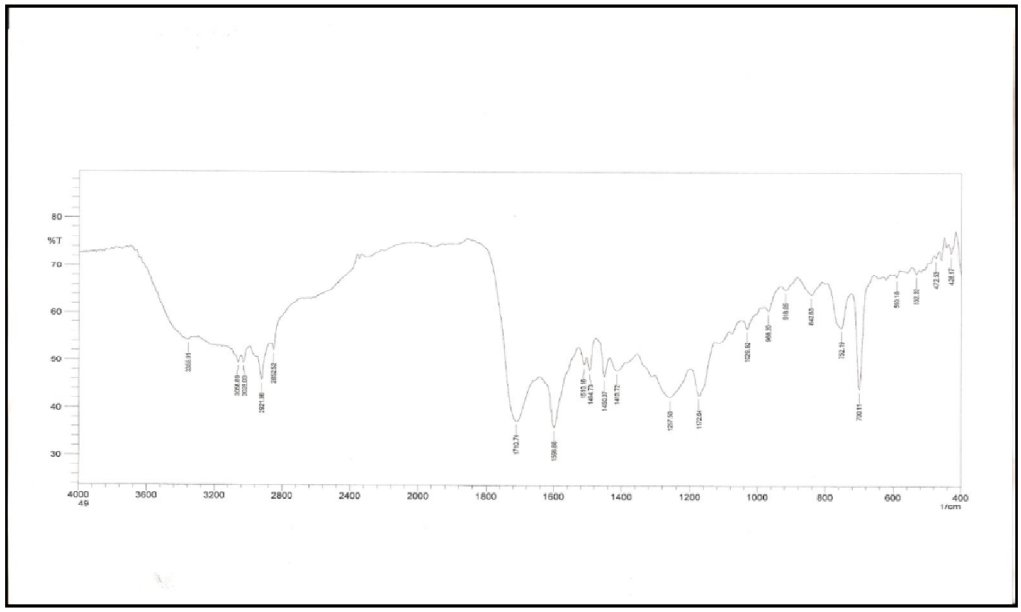

Fig.6.25.IR spectra of synthesis 4-diazo-(p-(5-(-4-methoxy phenyl) -pyrazol-3-yl)-phenyl)-3,5-dimethyl-1-2,4-dinitrophenylpyrazole(LXXXIV)

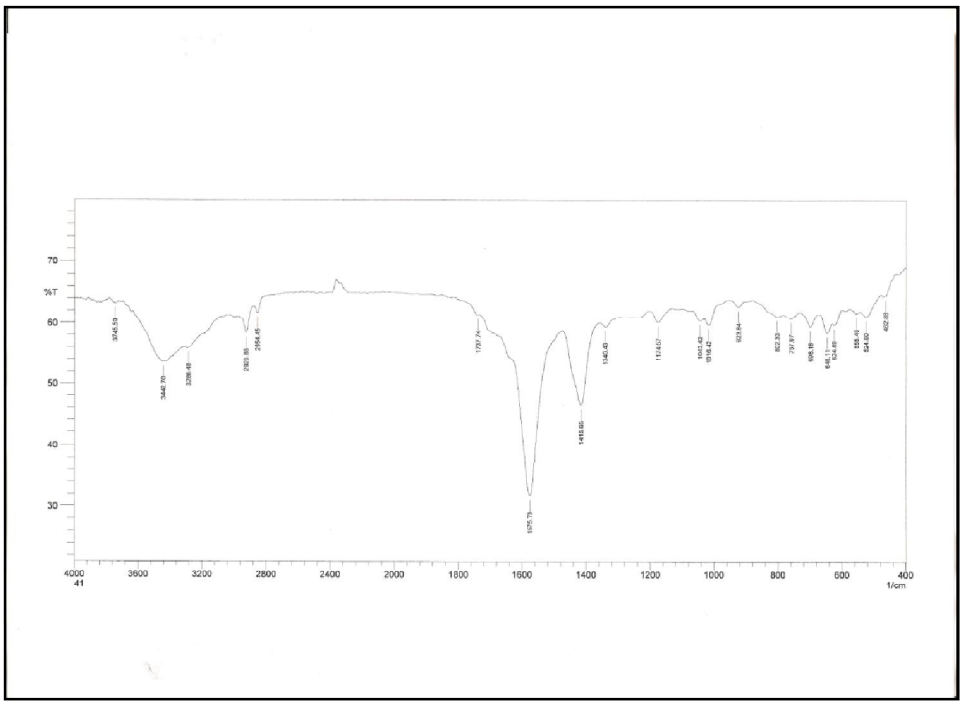

Fig.6.26.IR spectra of synthesis 4-(p-(5-(2-hydroxyphenyl)-phenyl)-2-thiopyrimidine-6-yl)-phenyl)-3,5-dimethyl-1-2,4-nitrophenylpyrazole(LXXXV)

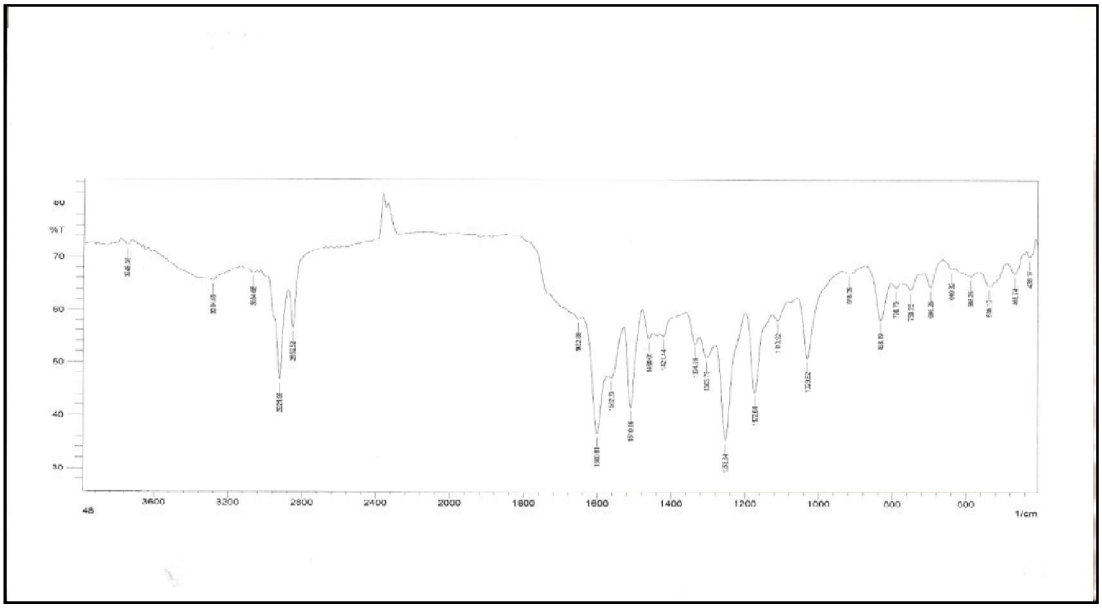

Fig.6.27.IR spectra of synthesis 4-diazo-(p-(5-(2-hydroxyphenyl)-pyrazol-3-yl)-phenyl)-3,5-dimethyl-1-2,4-dinitrophenylpyrazole(LXXXIV)

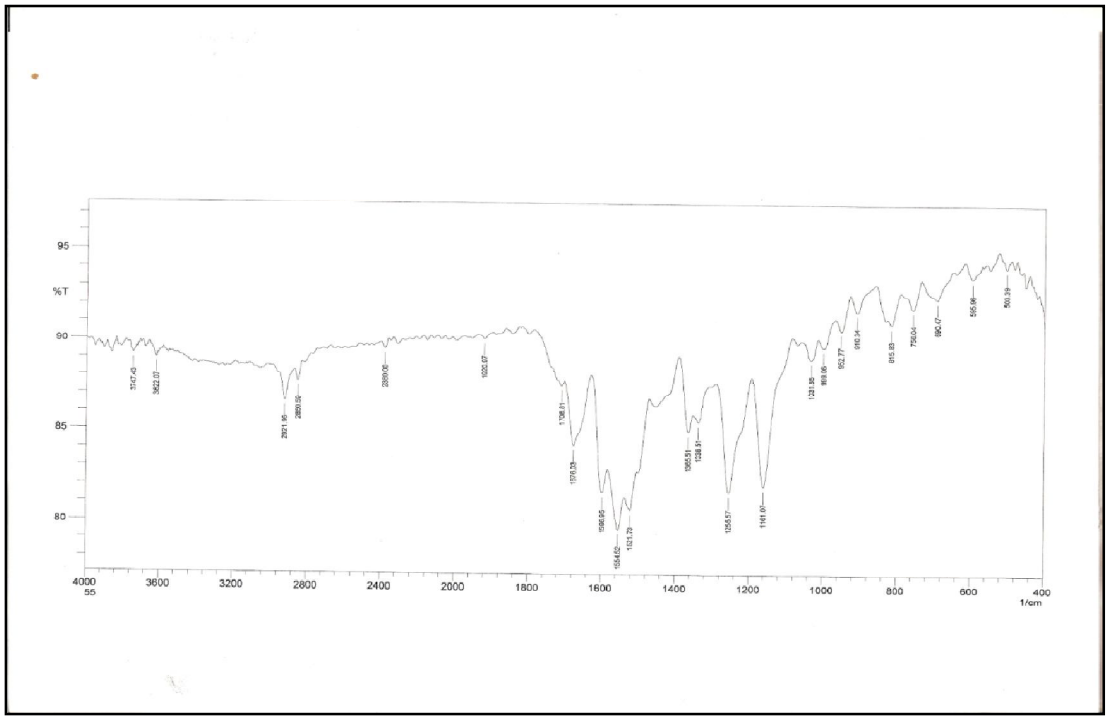

Fig.6.28.IR. spectra of synthesis 4-diazo-(p-(5-(2-nitrophenyl)-pyrazol-3-yl)-phenyl)-3,5-dimethyl-1-2,4-dinitrophenylpyrazole (LXXX)

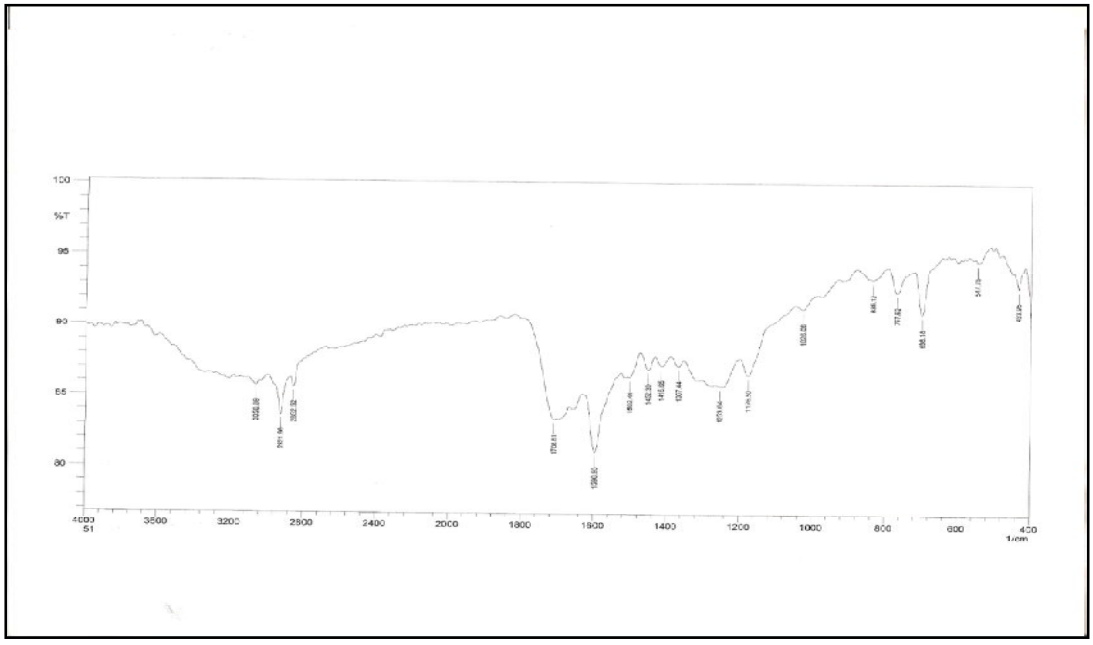

Fig.6.29.IR spectra synthesis 4-diazo-(p-(5-(2-phenyl ethenyl)-isoxazol-5-yl)phenyl)3,5-dimethyl-1-phenylpyrazole (XCIII)

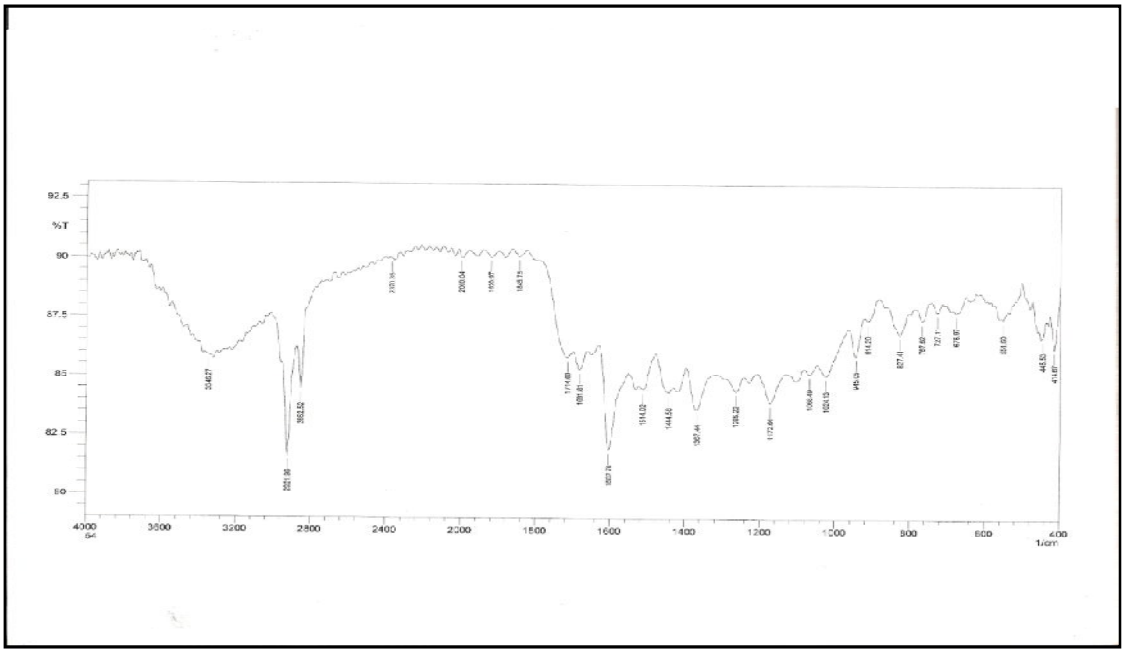

Fig.6.30.IR spectra of synthesis 4-diazo-(p-(5-(2-hydroxy-4-methoxy phenyl)-2-thiopyrimidine-6-yl)-phenyl)-3,5-dimethyl-1-2,4-dintro phenyl pyrazole(LXXIX)

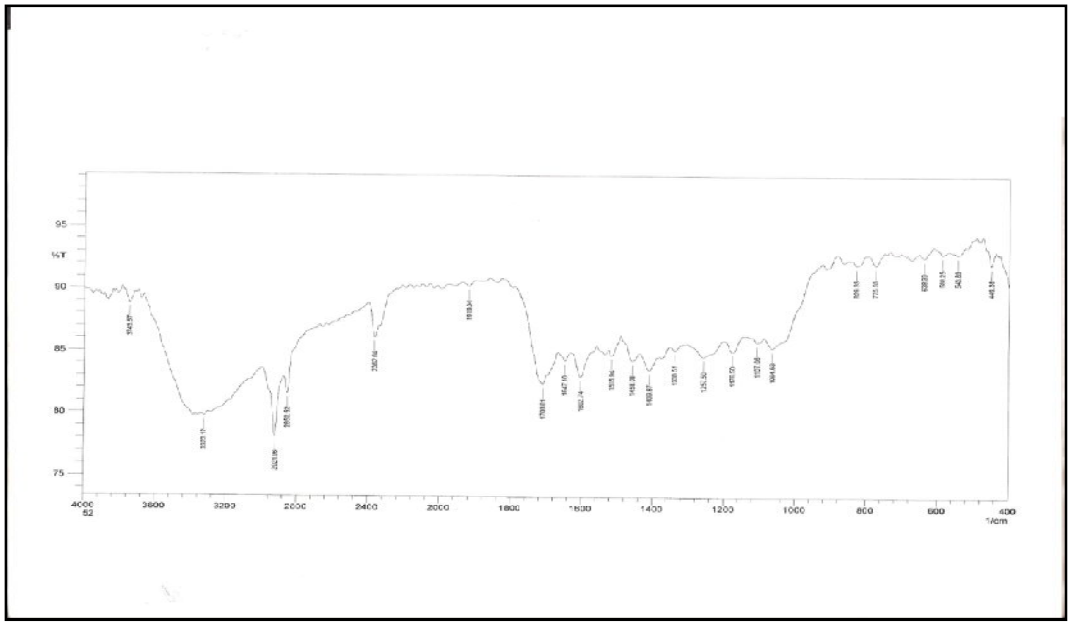

Fig.6.31.IR. spectra of synthesis 4-diazo-(p-(5-(-4-methox y phenyl)-isoxazol-5-yl)-phenyl)-3,5-dimethyl-1-2,4-dinitrophenylpyrazole(LXXVII)

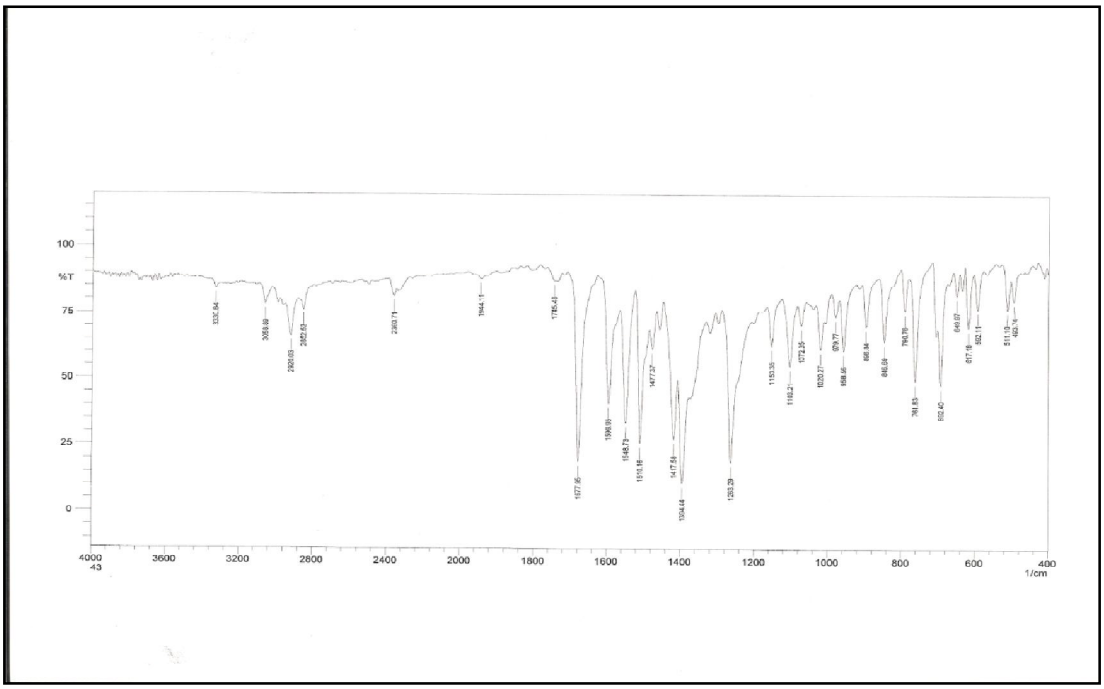

Fig.6.32.IRspectraofsynthesis 4-diazo-(p-(5-(2-nitrophenyl)-2-thio pyrimidine -6-yl)-phenyl)-5,5-dimethyl-cyclohexane-1,3-dione©

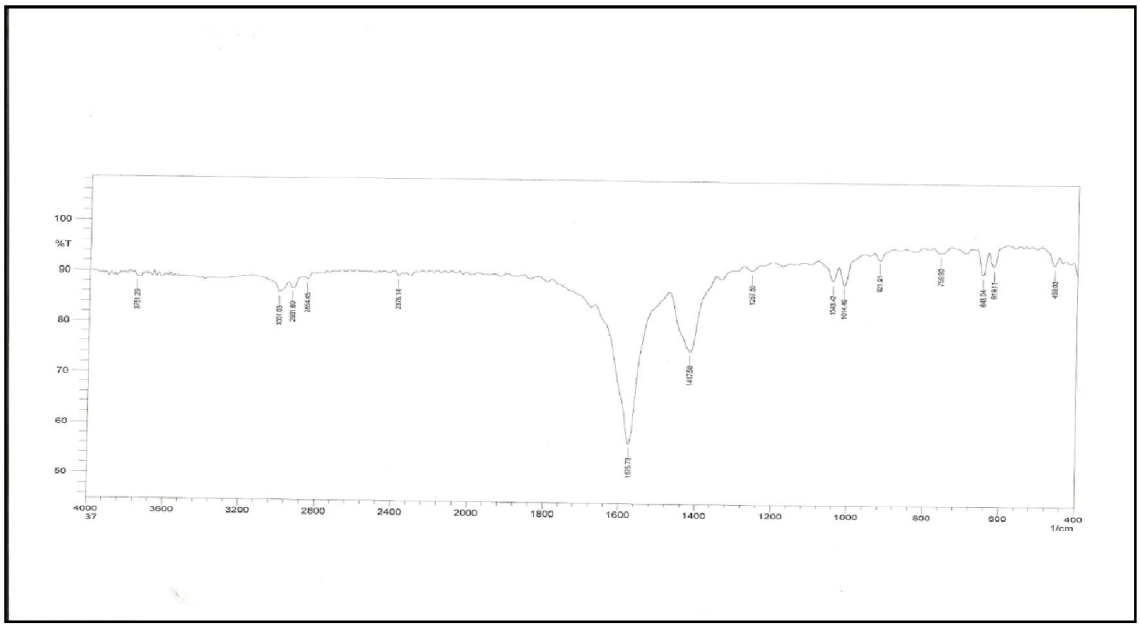

Fig.6.33.IR spectra of synthesis 4-diazo-(p-(5-(2-nitrophenyl)-isoxazol-5-yl)-phenyl)-5,5-dimethyl-cyclohexane-1,3-dione(CI)

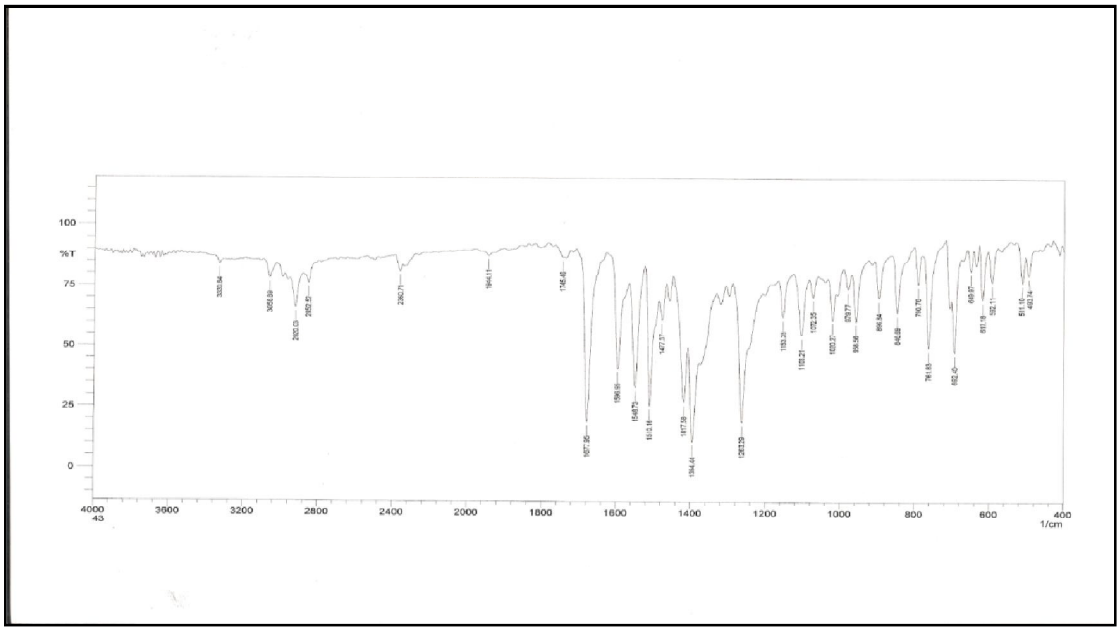

Fig.6.34.IR.spectra of synthesis 4-diazo-(p-(5-(2-nitrophenyl)-pyrazol-3-yl)-phenyl)-5,5-dimethyl-cyclohexane-1,3-dione (XCIX)

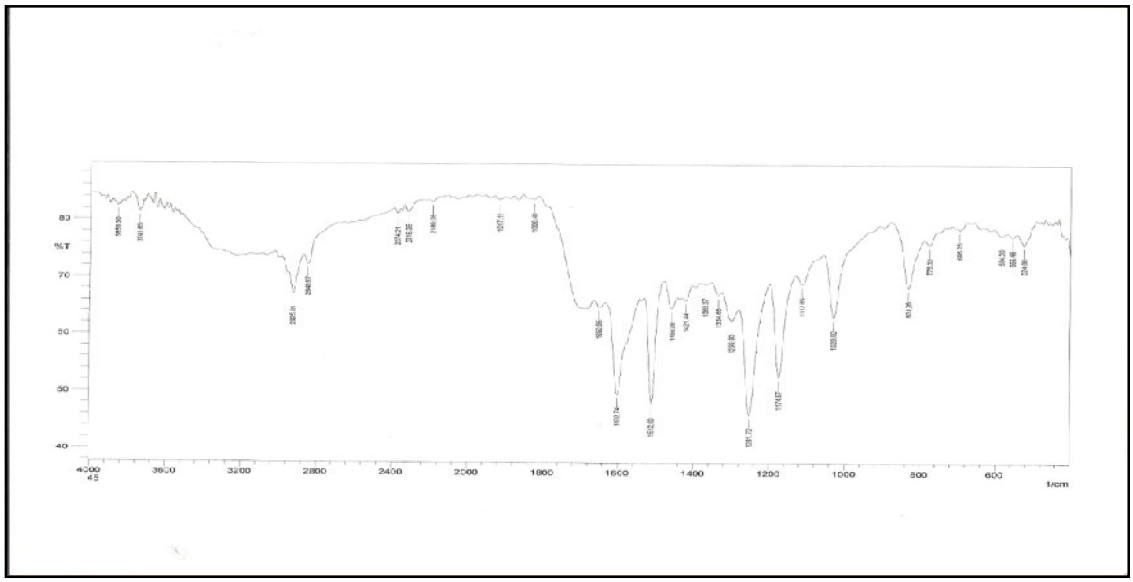

Fig.6.35.IR.spectra of synthesis 4-diazo-(p-(5-(p-N,N-dimethyl amino phenyl)-pyrazol-3-yl)-phenyl)-5,5-dimethylcyclohexane-1,3-dione(CVI)

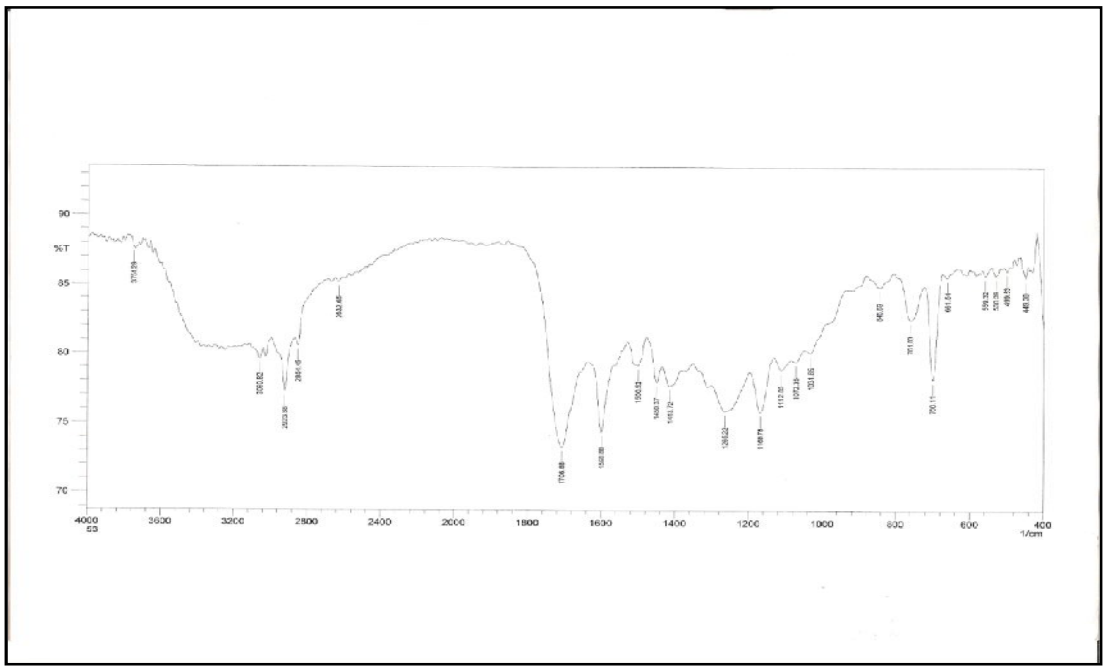

Fig.6.36.IR.spectraofsynthesis 4-diazo-(p-(5-(furan)-2-thiopyrimidine-6-yl)-phenyl)-5,5-dimethylcyclohexane-1,3-dione(CIII)

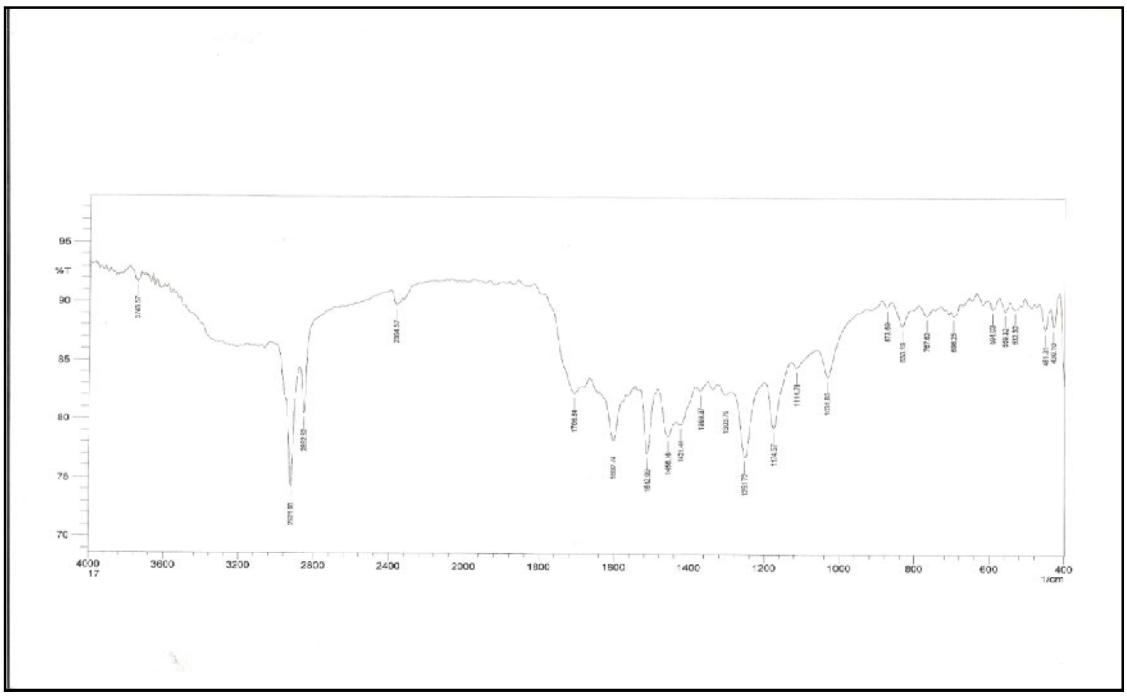

Fig.6.37.IR spectra of synthesis 4-diazo-(p-(5-(furan)-isoxazol-5-yl) phenyl)-5,5-dimethyl-cyclohexane-1,3-dione(CIV)

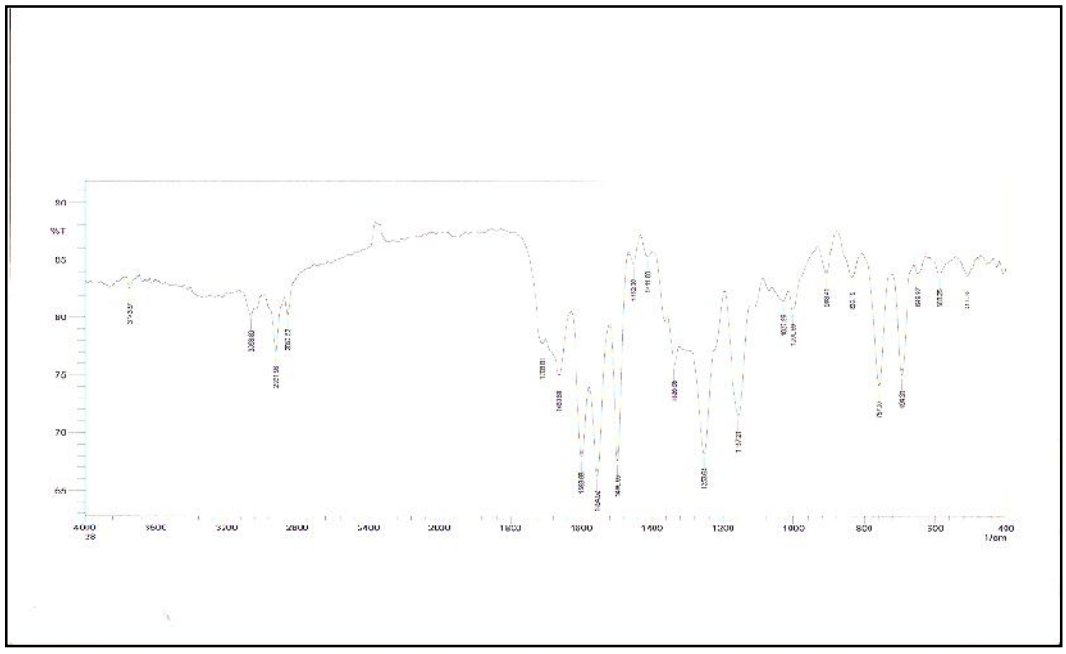

Fig.6.38.IR spectra of synthesized 4-diazo(p-(5-((furan-3-yl)- pyrazol-3-yl)- phenyl)- 5,5-dimethylcyclohexane-1,3-dione(CII)

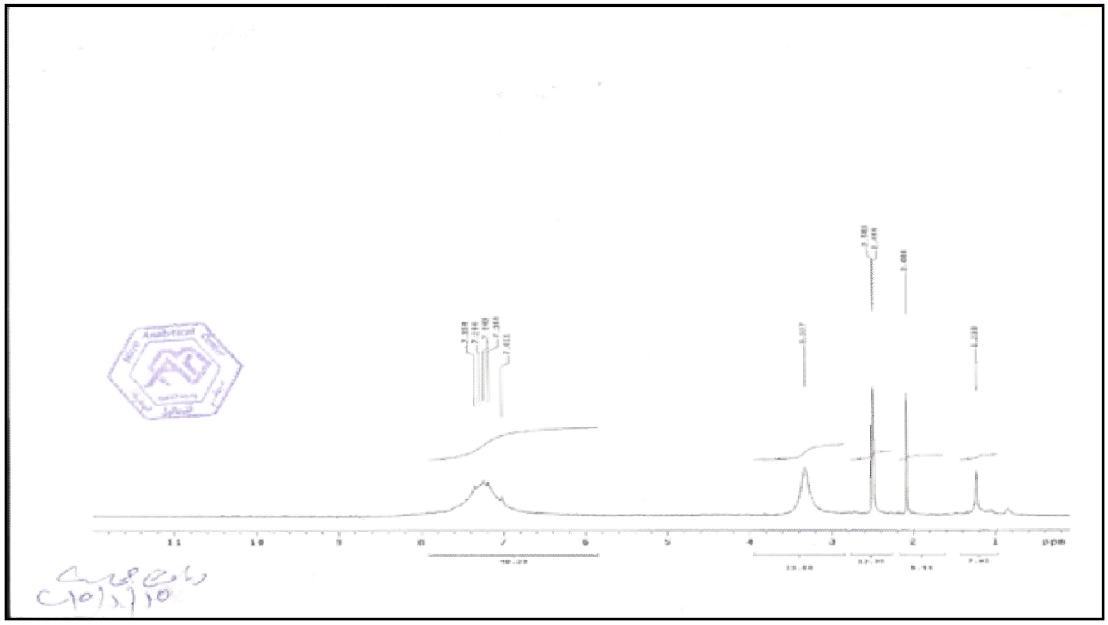

Fig. 6.39.1H-NMR spectra of synthesis 4-diazo-(p-(5-(-4-methox yphenyl)-2-thiopyrimidine-6-yl)-phenyl)-3,5-dimethyl-1-2,4-dinitrophenylpyrazole(LXXIX)

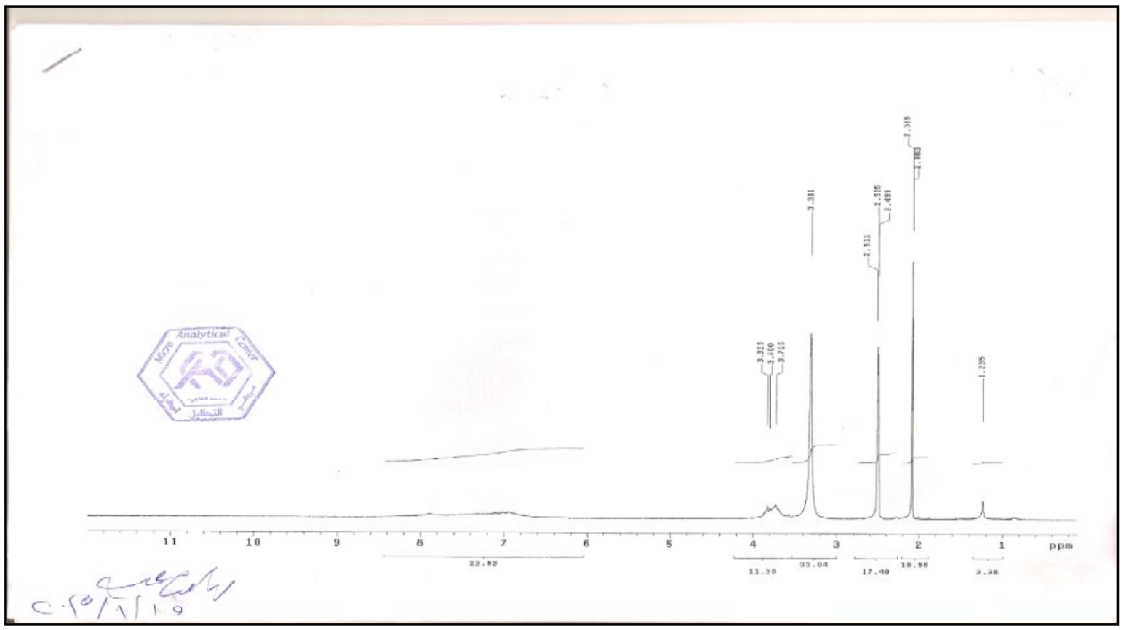

Fig.6.40. 1H-NMR spectra of synthesis 4-diazo-(p-(5-(-4-methoxyphenyl)-pyrazol-3-yl)-phenyl)-3,5-dimethyl-1-2,4-dinitro phenyl pyrazole(LXVIII)

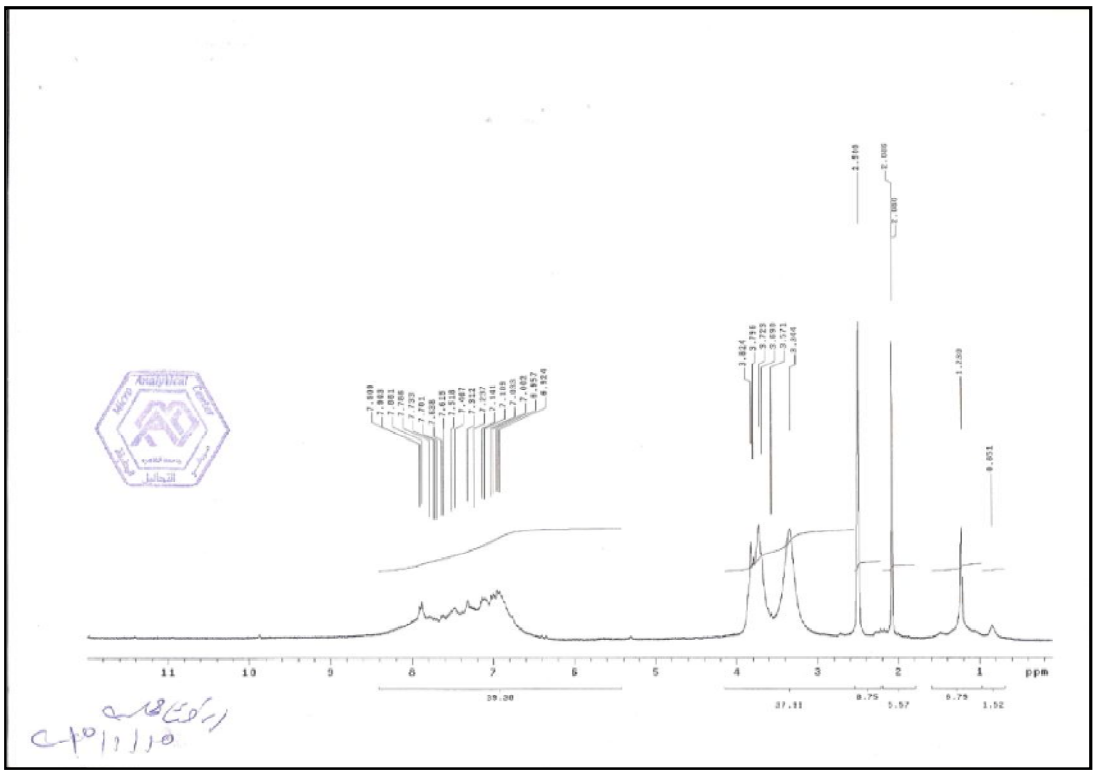

Fig.6.41.1H-NMR spectra of synthesis 4-diazo-(p-(5(-4- methoxy phenyl)isoxazol-5yl)-93,5-dimethyl-1-2,4-dinitrophenyl-pyrazole(LXXVII)

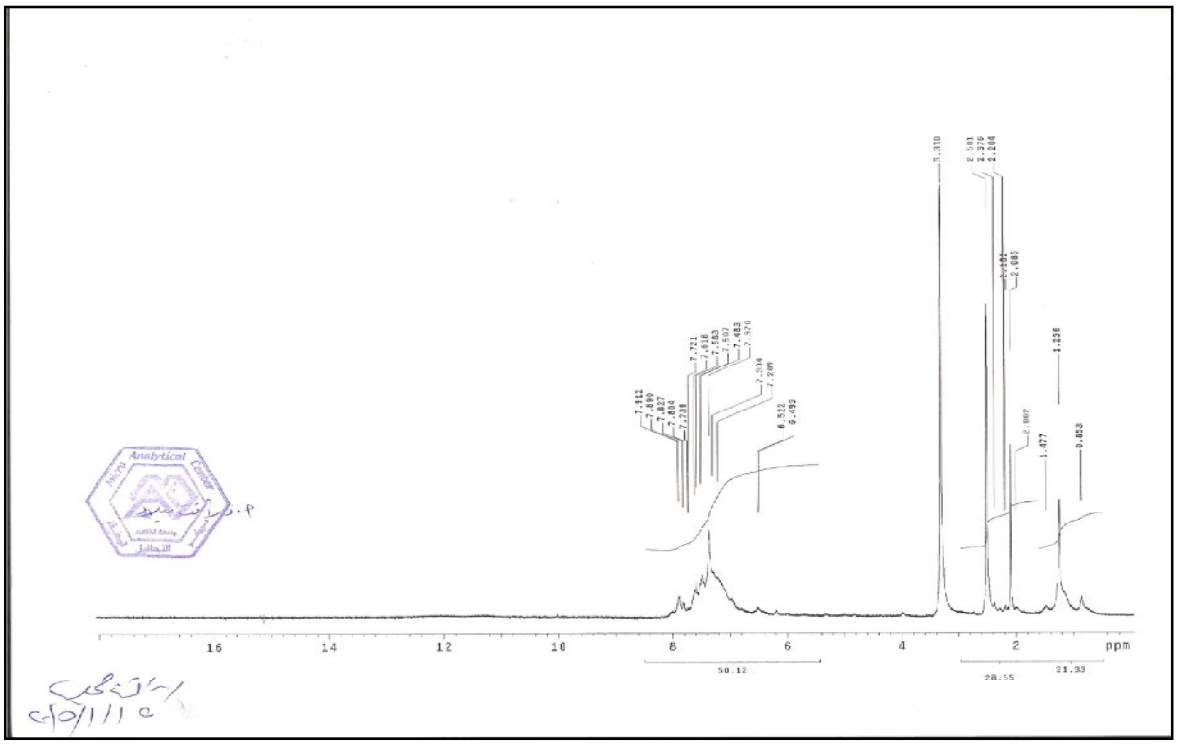

Fig.6.42.[1]H-NMR spectra of synthesis 4-diazo-(p-(5-(2-hydroxyphenyl)-2-thiopyrimidine-6-yl)-3,5-dimethyl-1-2,4-dinitrophenylpyrazole(LXXXV)

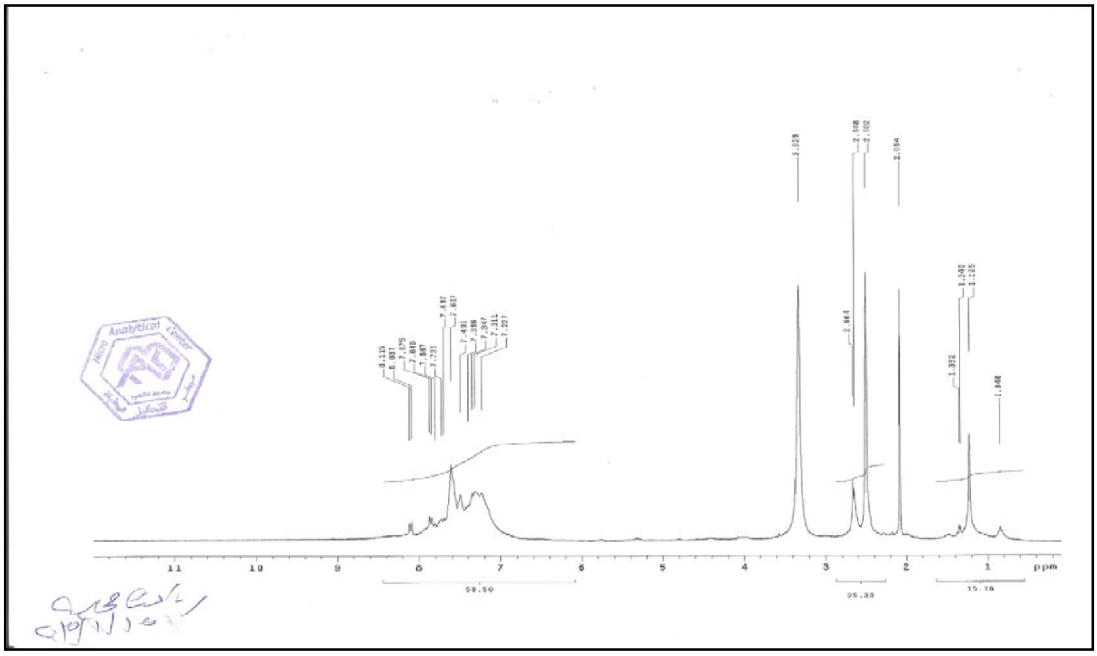

Fig.6.43.1H-NMRspectra of synthesis 4-diazo-(p-(5-(-4-methoxy phenyl)-2-thiopyrimidine-6-yl)-phenyl) -3,5-dimethyl-1-phenylpyrazole (LXXVI)

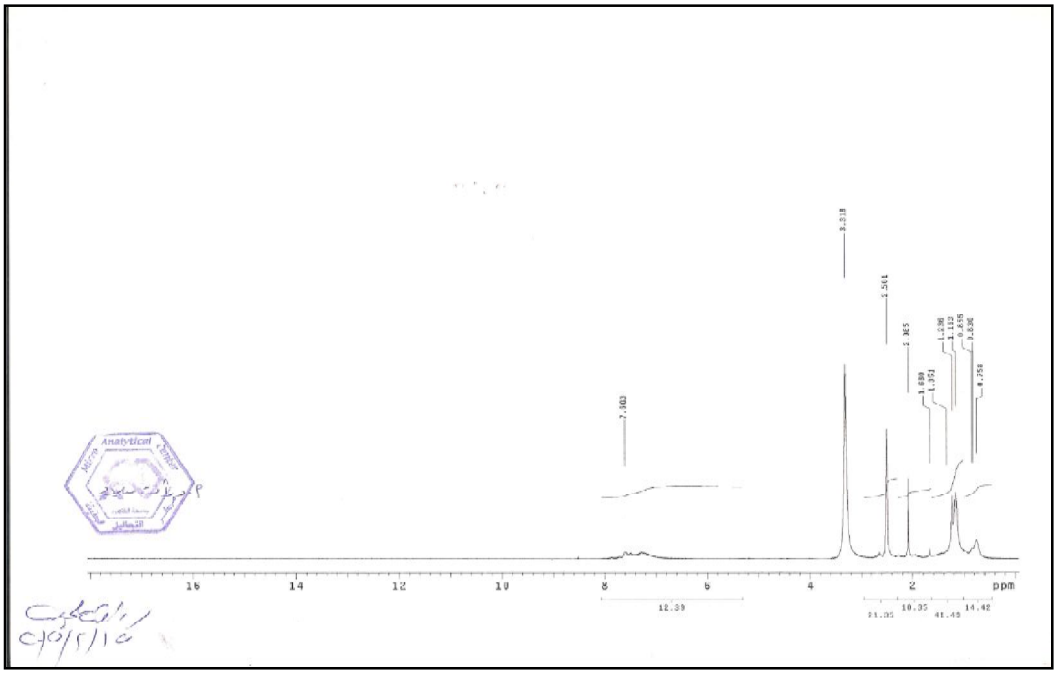

Fig.6.44.1H-NMR spectra of synthesis 4-diazo-(p-(5-(-4-methoxyphenyl)-pyrazol-3-yl)-phenyl)-3,5-dimethyl-1-phenylpyrazole(LXXV)

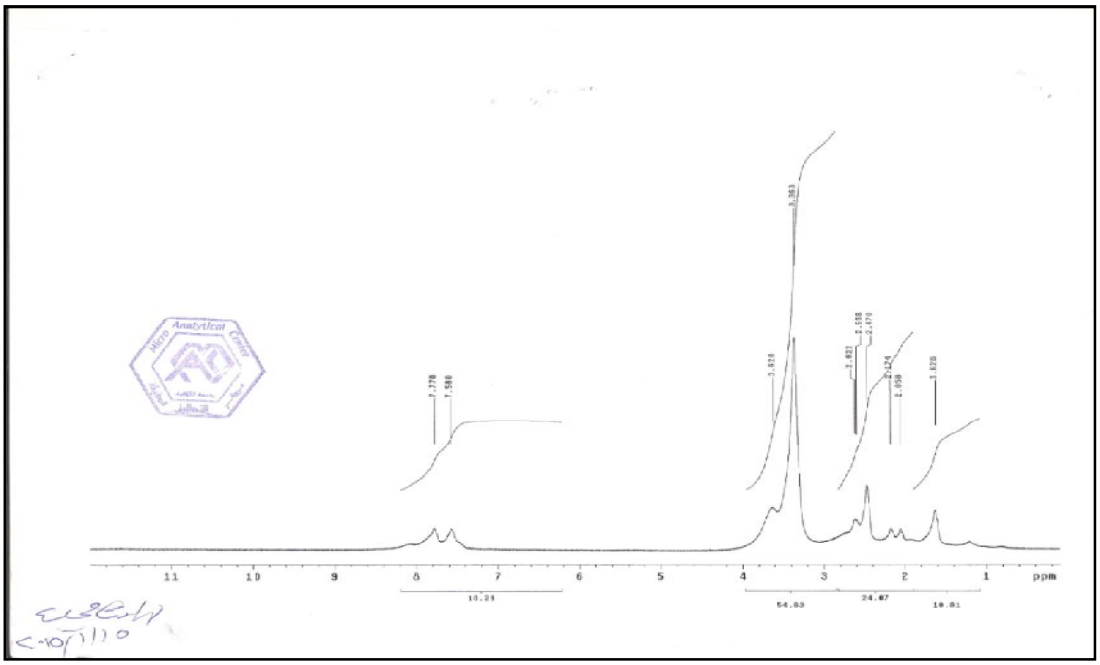

Fig.6.45.1H-NMR spectra of synthesis 4-diazo-(p-(5-(-4-methoxyphenyl)-isoxazol-5-yl)-phenyl)-3,5-dimethyl-1-phenylpyrazole(LXXI))

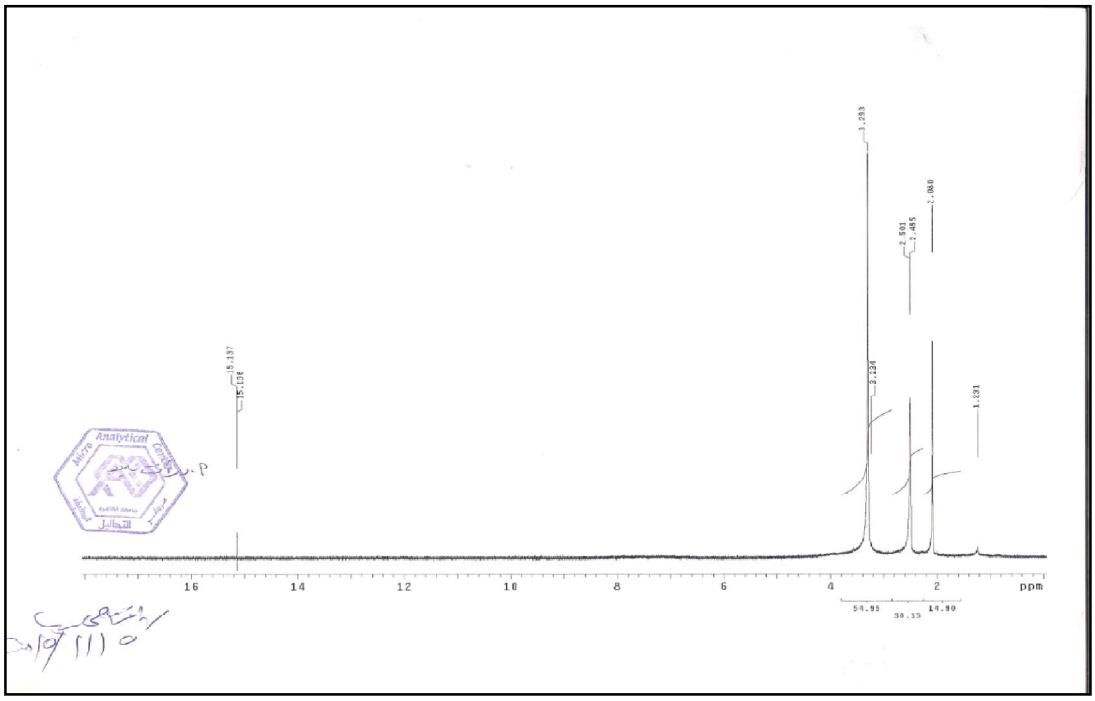

Fig.6.46.1H-NMR spectra of synthesis 4-diazo-(p-(2-hydroxyphenyl)-isoxazol-5-yl)-phenyl)-3,5-dimethyl-1-phenylpyrazole (LXXI)

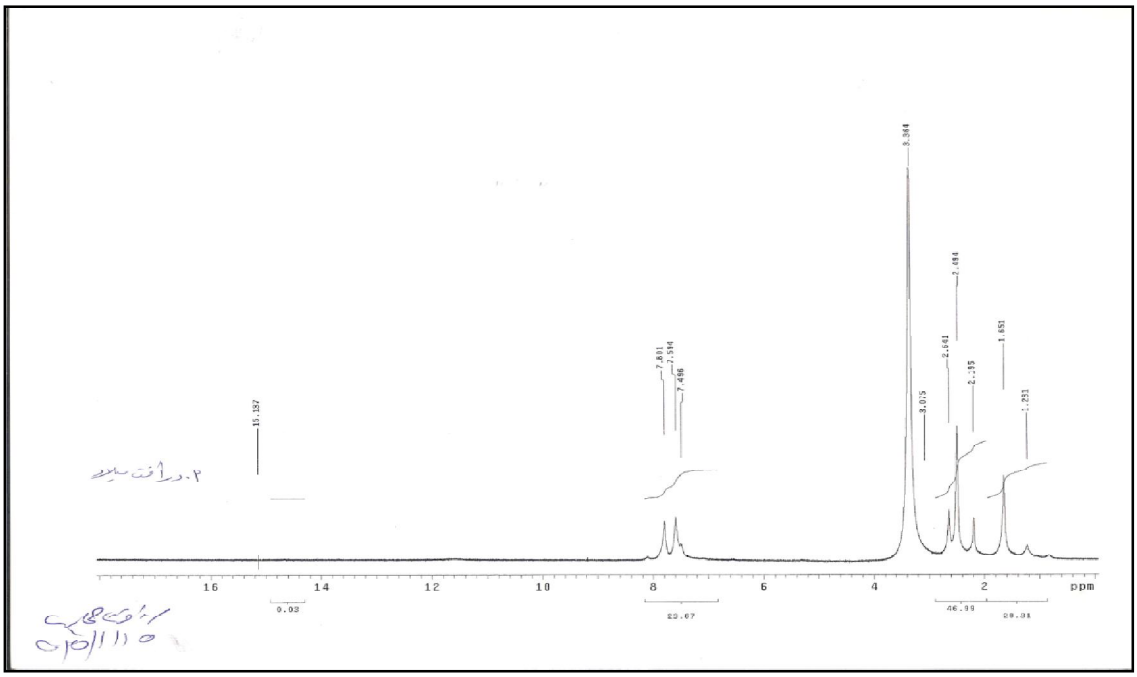

Fig.6.47.1H-NMRspectra of synthesis 4-diazo-(p-(5-(2-hydroxyphenyl)-2-thiopirimidine-6-yl)-phenyl)-3,5-dimethyl-1-phenylpyrazole (LXXIII)

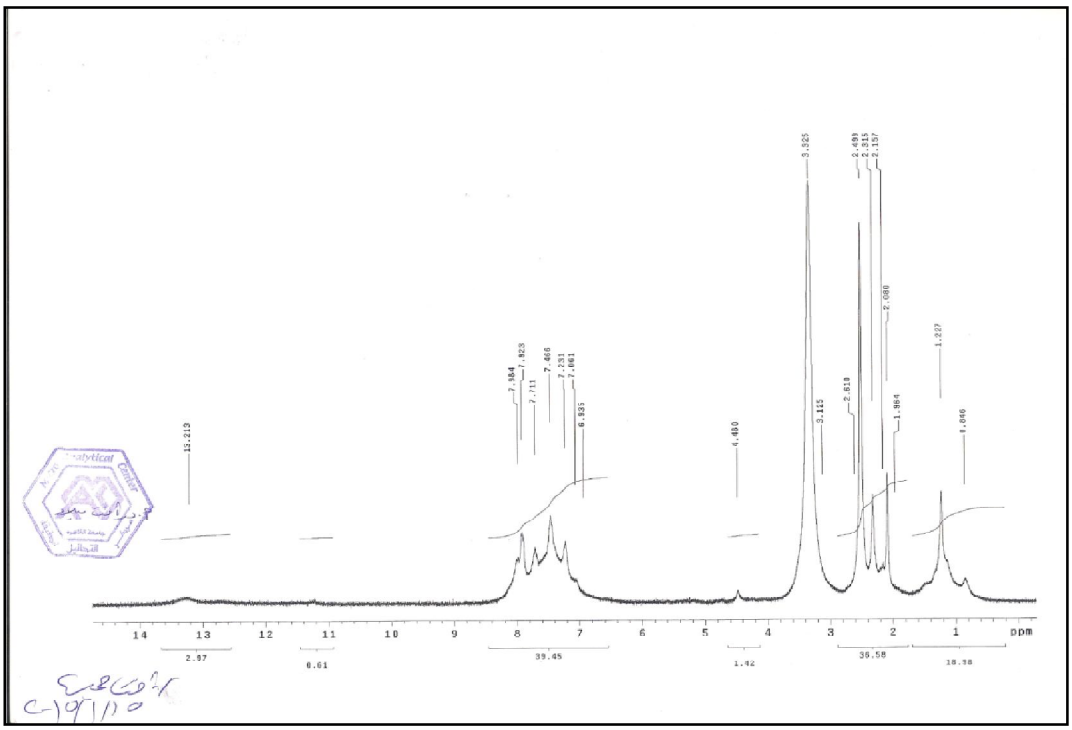

Fig.6.48.1H-NMR.spectra of synthesis 4-diazo-(p-(5-(2-phenyl ethenyl)-2-thiopyrimidine-6-yl)-phenyl)-5-methyl-1-phenyl-pyrazol-3-one (XCII)

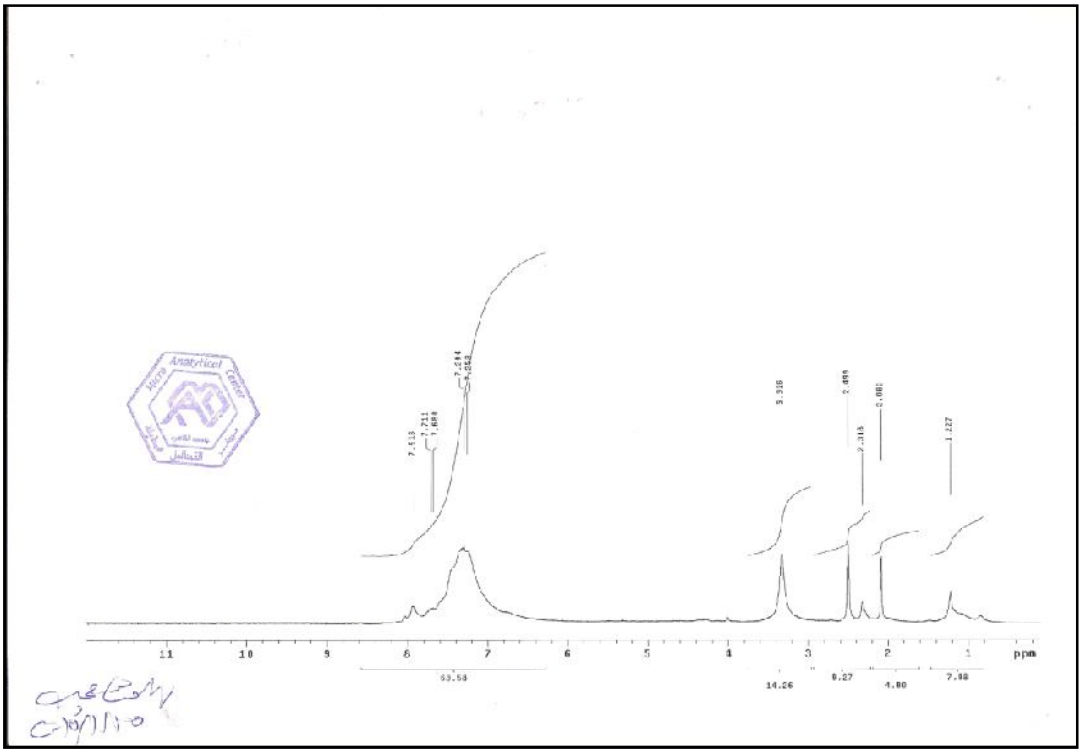

Fig.6.49.1H-NMR.spectra of synthesis 4-diazo-(p-(5-(2-phenyl ethenyl)-isoxazol-5-yl)-phenyl)-5-methyl-1-phenyllpyrazol-3-one(XC)

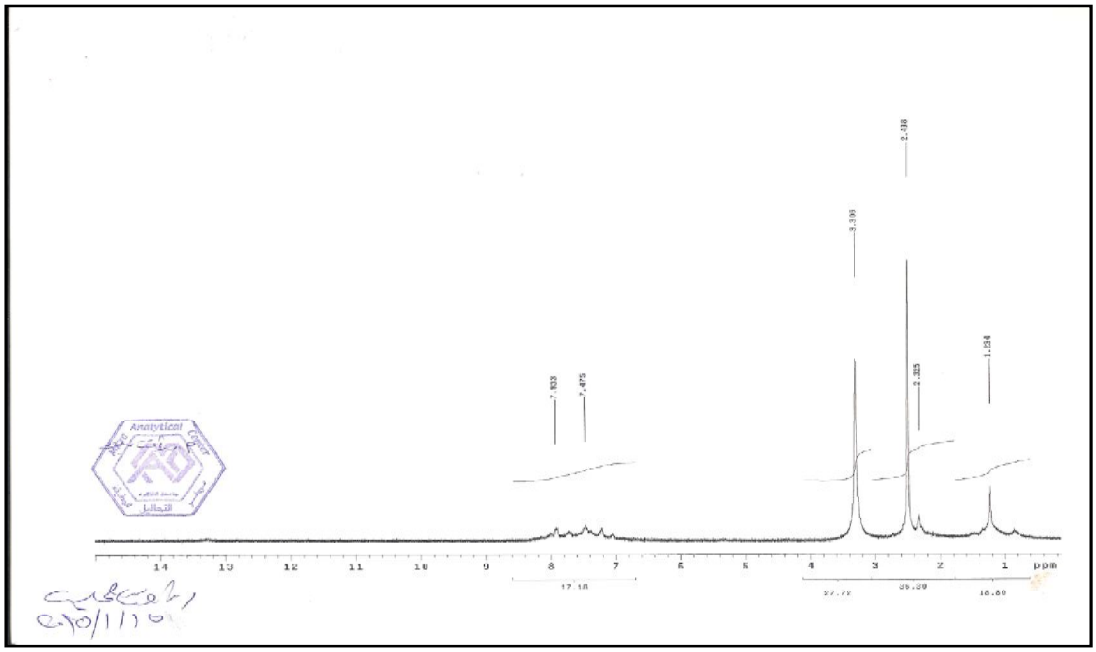

Fig.6.50.1H-NMRspectra of synthesis 4-diazo-(p-(5-(2-phenyl ethenyl)-pyrazol-3-yl)-5-methyl-1-phenylpyrazol-3-one(XCI)

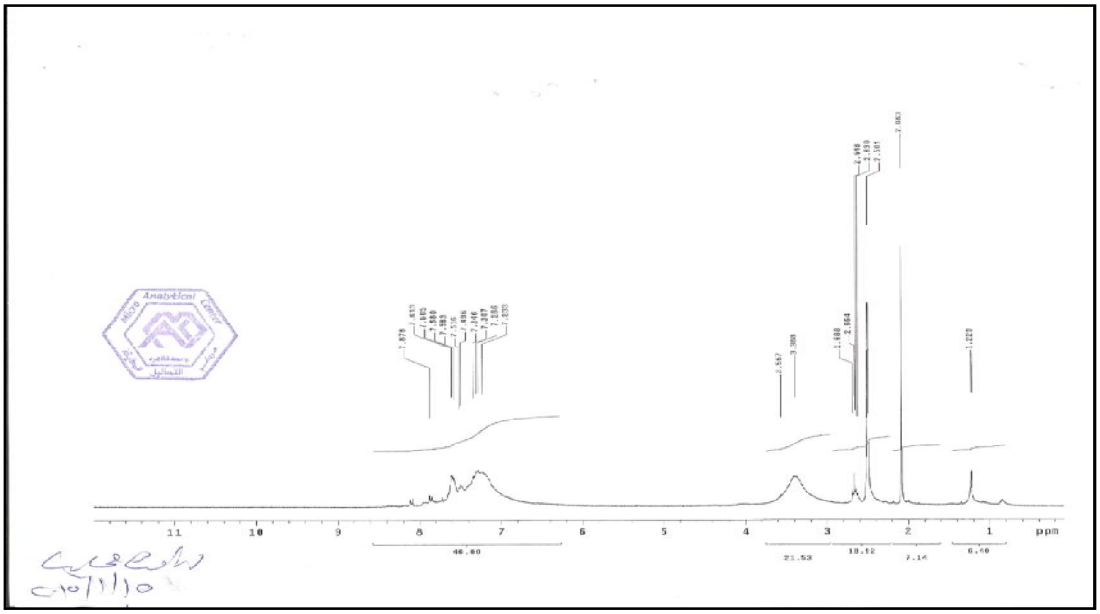

Fig.6.51.1H-NMRspectra of synthesis 4-diazo-(p-(5-(p-N,Ndimethyl aminophenyl)-2-thiopyrimidine-6-yl)-phenyl)-3,5-dimethyl-1-2,4-dinitro phenyl pyrazole (CX)

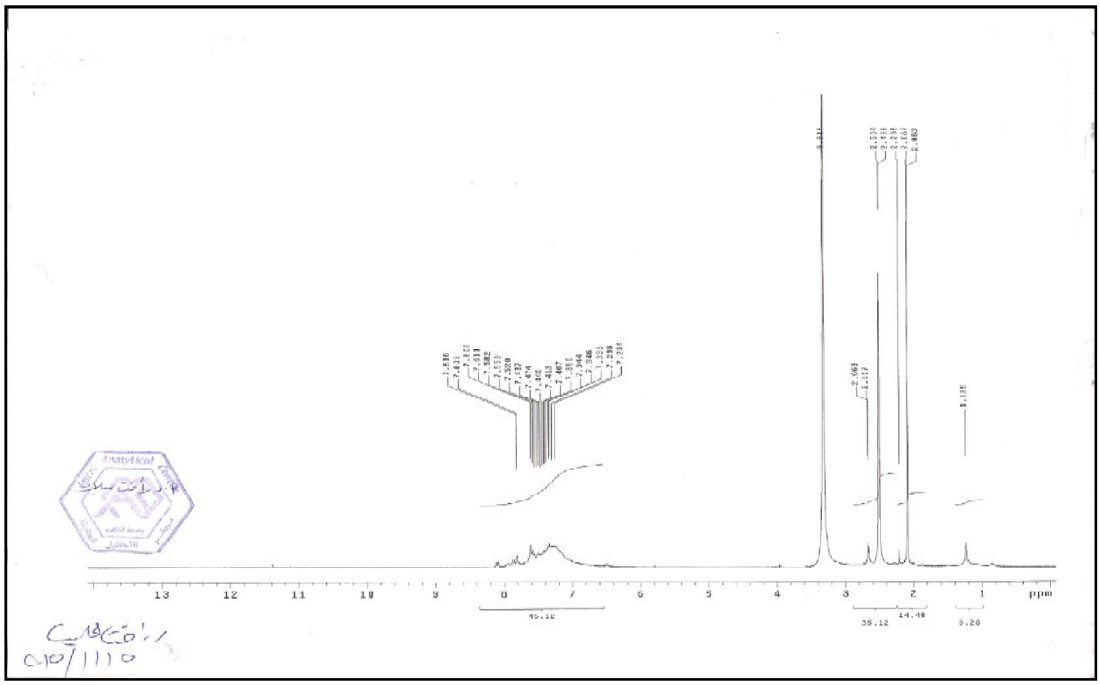

Fig.6.52.1H-NMR spectra of synthesis 4-diazo-(p-(5-(2-phenyl ethenyl)-2-thiopyrimidine-6-yl)-3,5-dimethyl-1-phenylpyrazole(XCV)

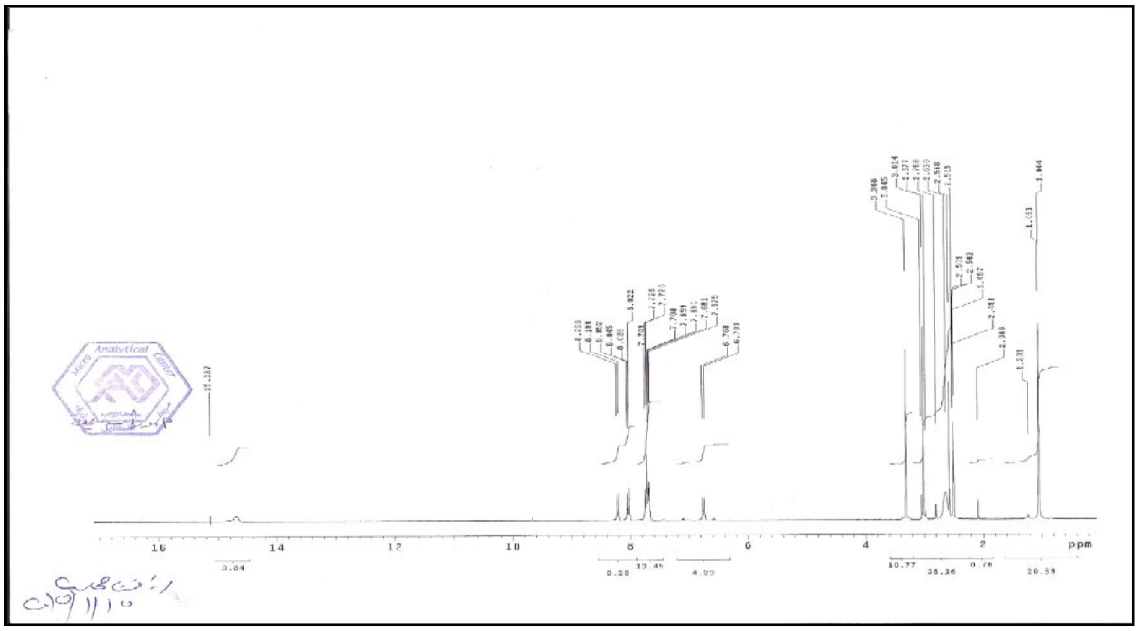

Fig.6.53.1H-NMRspectraof synthesis 4-diazo-(p-(5-(2-phenyl ethenyl)-isoxazol-5-yl)-phenyl)-3,5-dimethyl-1- phenyl pyrazole (XCIII)

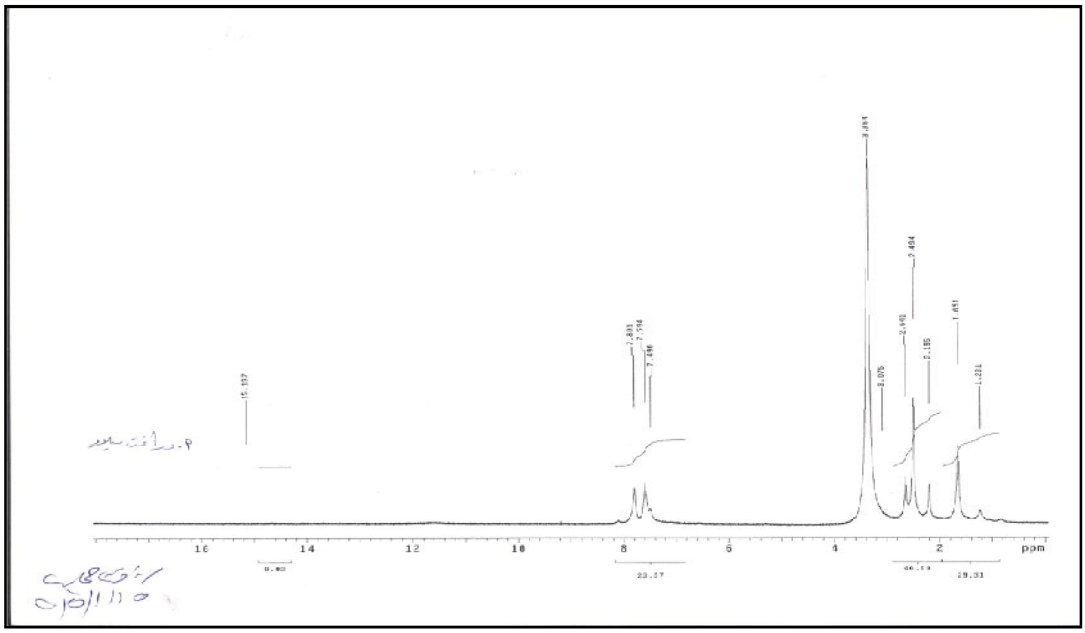

Fig.6.54.1H-NMR spectra of synthesis 4-diazo-(p-(5-(2-phenyl ethenyl)-pyrazol-3-yl)-phenyl)-3,5-dimethyl-1-phenylpyrazole(XCV)

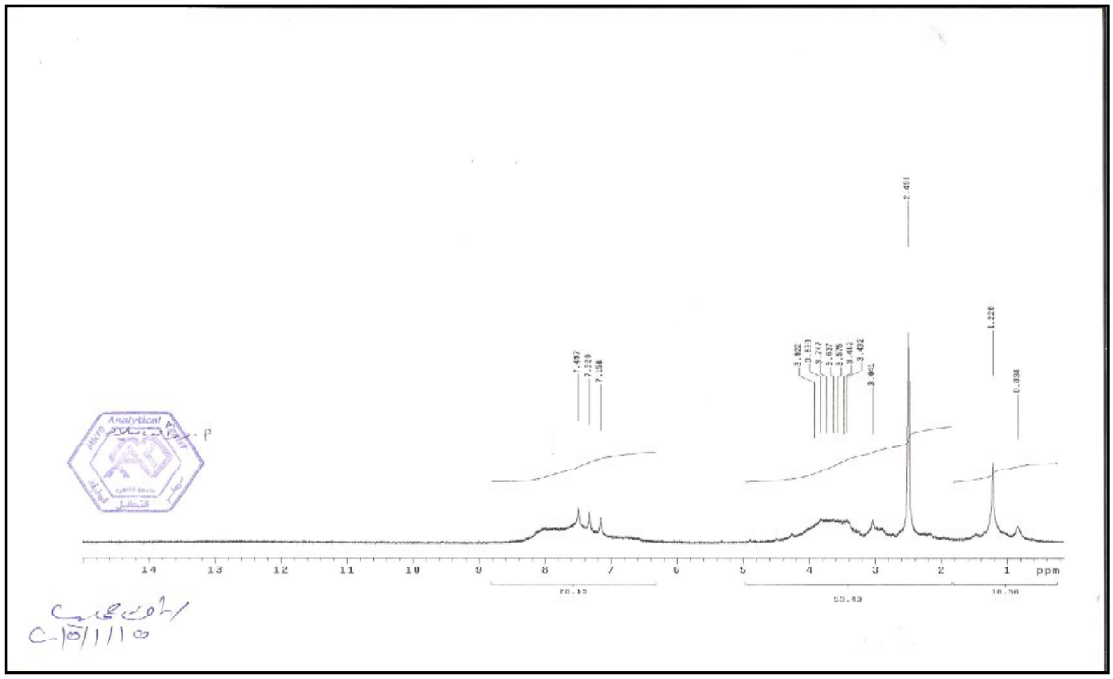

Fig.6.55.1H-NMR spectra of synthesis 4-diazo-(p-(5-(p-N,N-dimethyl aminophenyl)-isoxazol-5-yl)-3,5-dimethyl-1-2,4-dinitrophenylpyrazole(CIX)

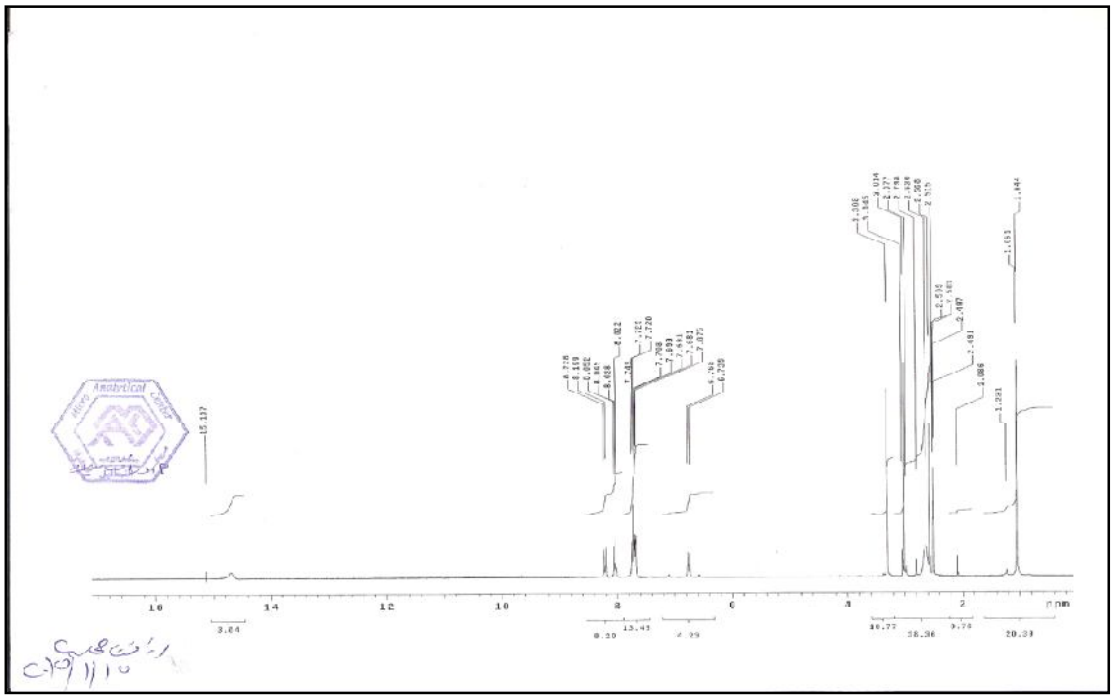

Fig 6.56. 1H-NMR spectra of synthesis 4-diazo-(p-(5-(p-N,N-dimethylaminophenyl)-pyrazol-3-yl)-phenyl)-3,5-dimethyl-1-2,4-dinitrophenylpyrazole(CVIII)

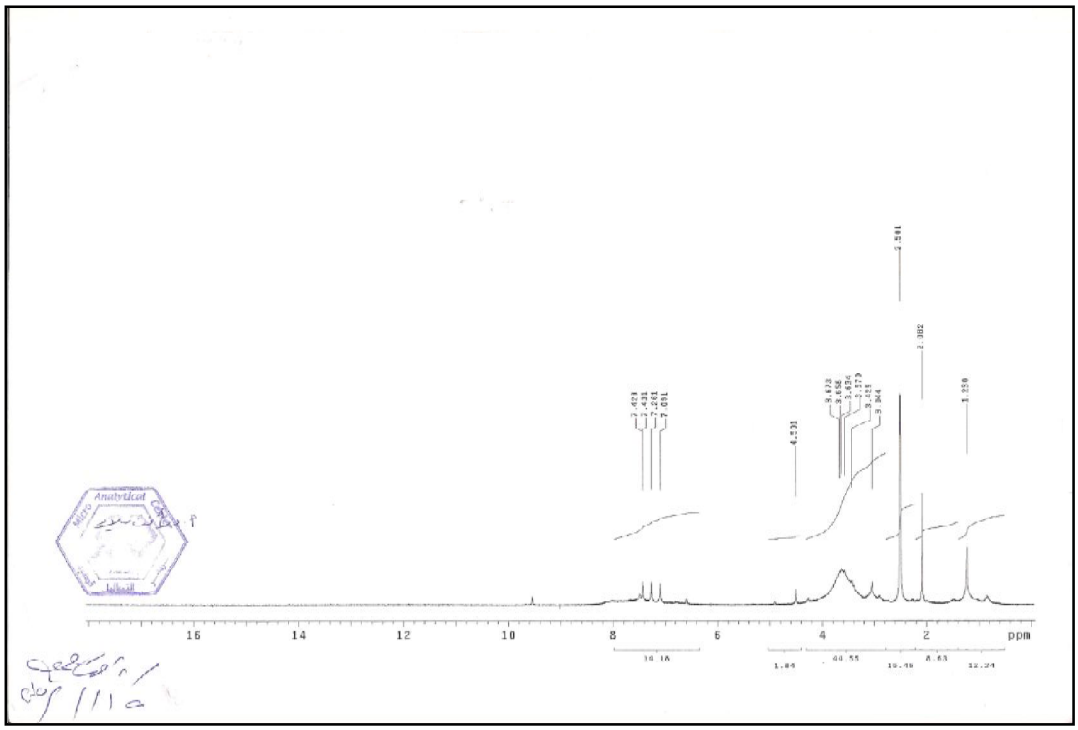

Fig.6.57.1H-NMR spectra of synthesis 4-diazo-(p-(5-(2-hydroxy phenyl)-isoxazol -5-yl)-phenyl)-3,5-dimethyl-1-2,4-dinitrophenyl pyrazole9LXXIV)

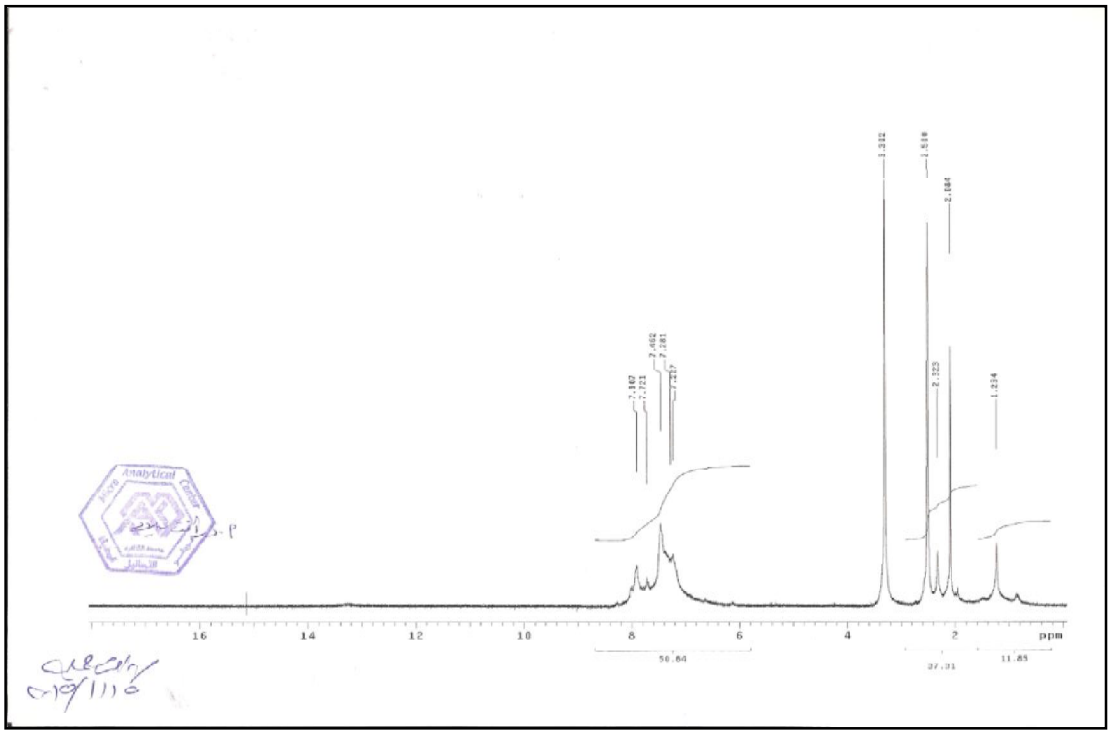

Fig.6.58.1H-NMR spectra of synthesis 4-diazo-(p-(5-(2-hydroxyphenyl)-pyrazol-3-yl)-phenyl)-3,5-dimethyl-1-phenylpyrazole (LXXV)

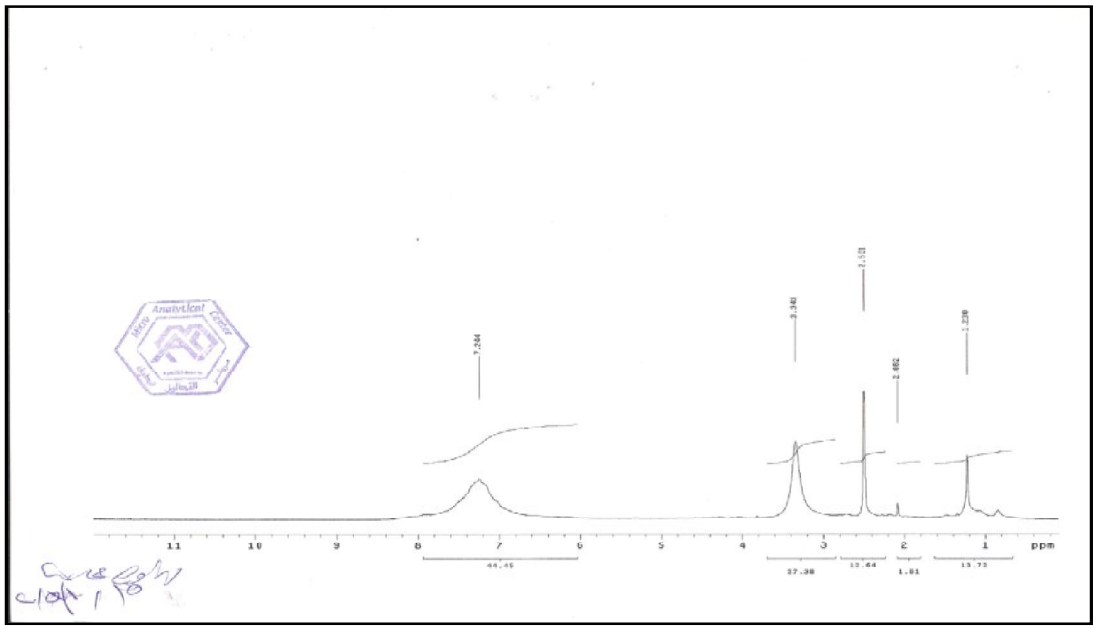

Fig.6.59.1H-NMR spectra of synthesis 4-diazo-(p-(5-(2-hydroxyphenyl)-2-thiopyrimidine-6-yl)-phenyl)-3,5-dimethyl-1-2,4-dinitrophenylpyrazole(LXXXV)

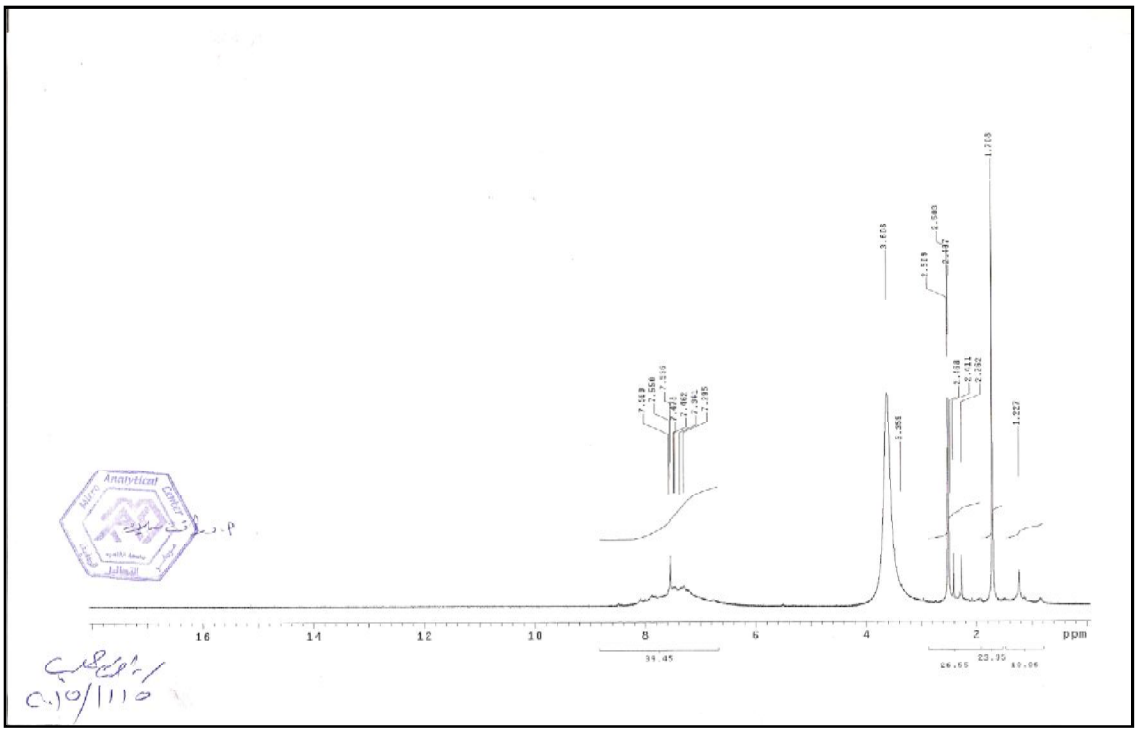

Fig.6.60.1H-NMR spectra of synthesis 4-diazo-(p-(5-(2-nitrophenyl)-pyrazol-3-yl)-3,5-dimethyl-1-2,4-dinitrophenylpyrazole LXXX)

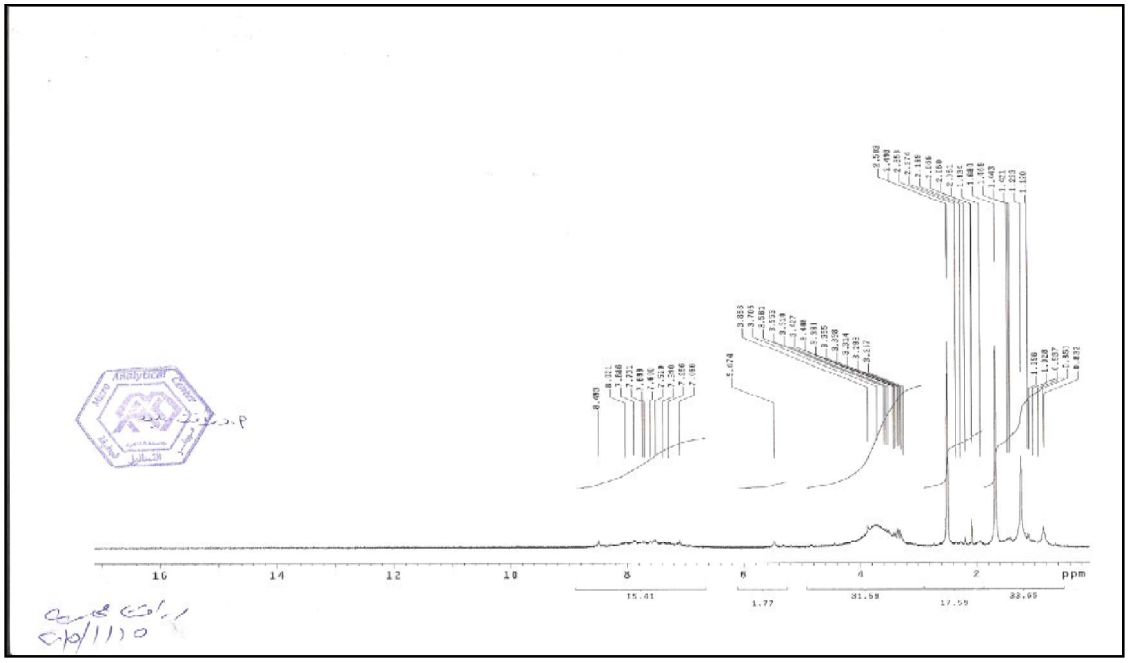

Fig.6.61.1H-NMR spectra of synthesis 4-diazo-(p-(5-(2-nitrophenyl)-2-thiopyrimidine-6-yl)-phenyl)-3,5-dimethyl-1-2,4-dinitrophenylpyrazole(LXXXII)

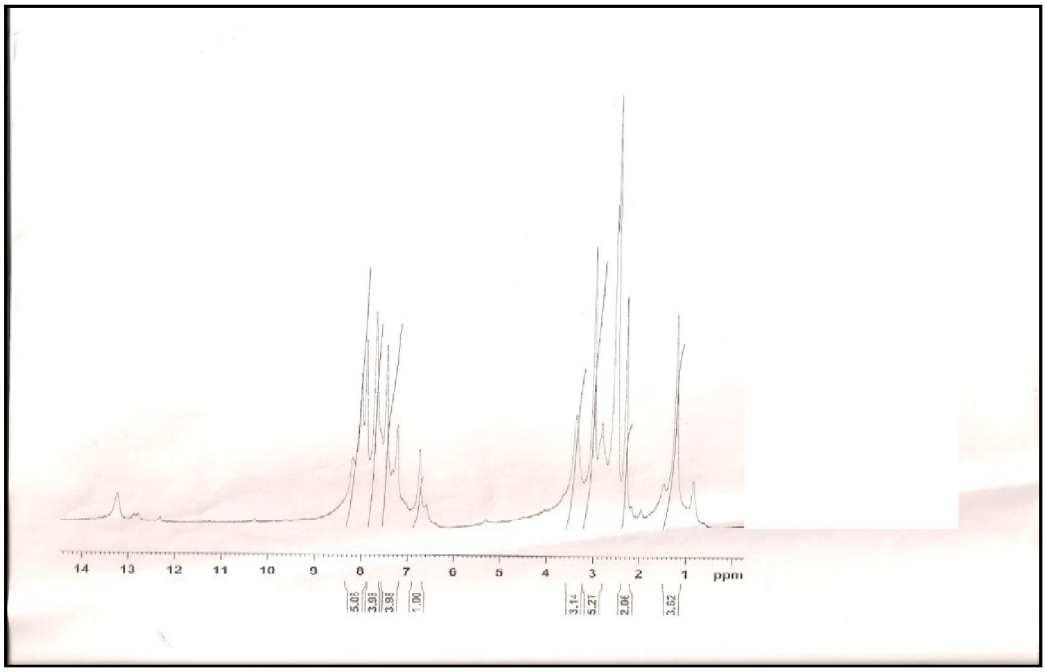

Fig.6.62.1H-NMRspectra of synthesis 4-diazo-(p-(5-(p-N,N-dimethyl amino phenyl)-pyrazol-3-yl)-phenyl)-5-methyl-pyrazol-3-one(LXXXVI)

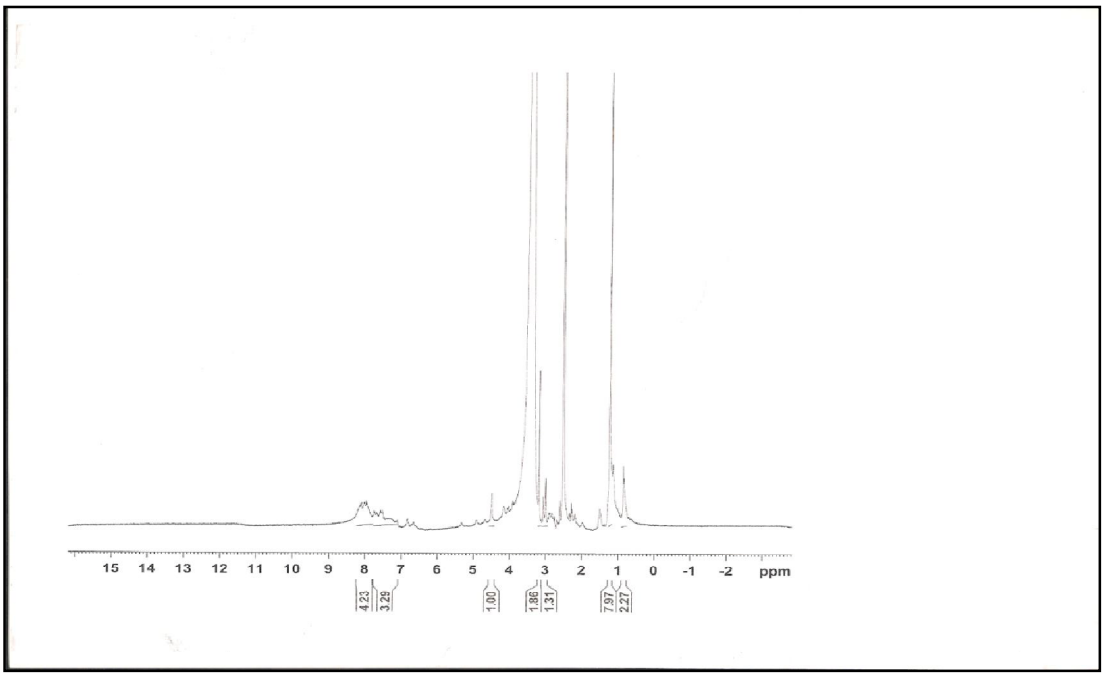

Fig.6.63 1H-NMR spectra of synthesis 4-diazo-(p-(5-(p-N,N-dimethylaminophenyl)-isoxazol-5-yl)-phenyl)-5-methyl-pyrazol-3-one(LXXXVII)

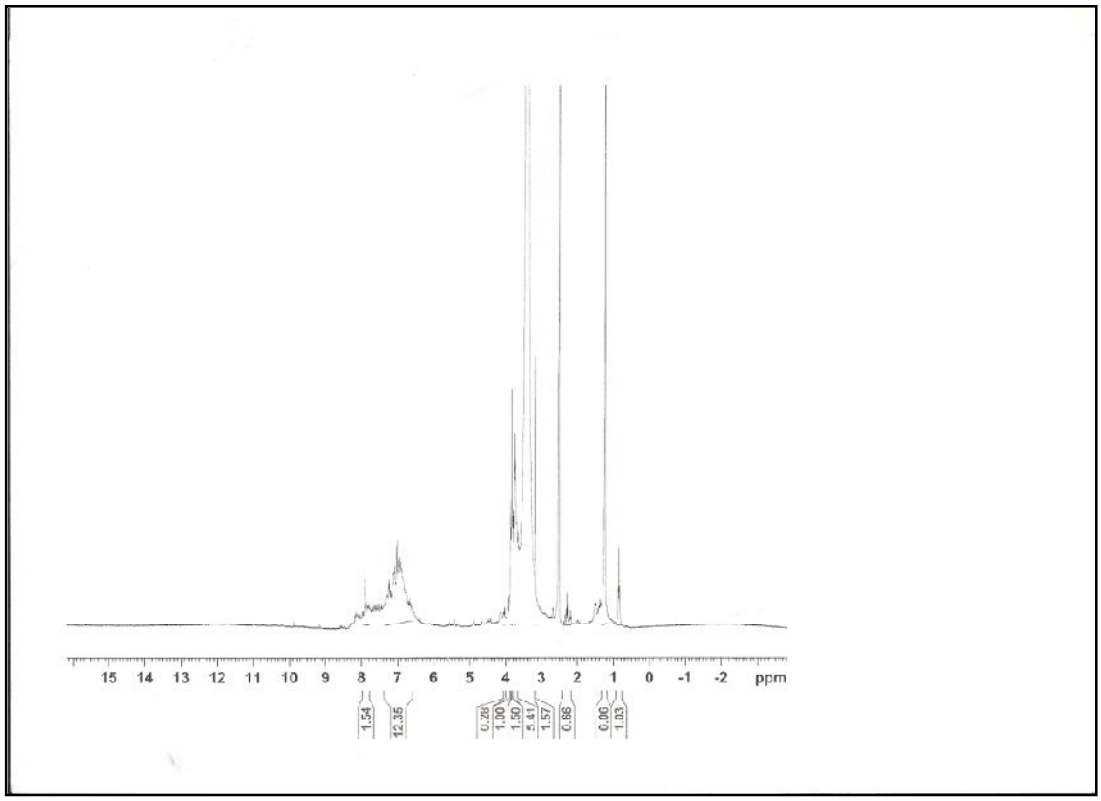

Fig.6.64.1H-NMR spectra of synthesis 4-diazo-(p-(5-(p-N,N-dimethyl amino phenyl)-2-thiopyrimidine-6-yl)-5-methyl-pyrazol-3-one(LXXXIX)

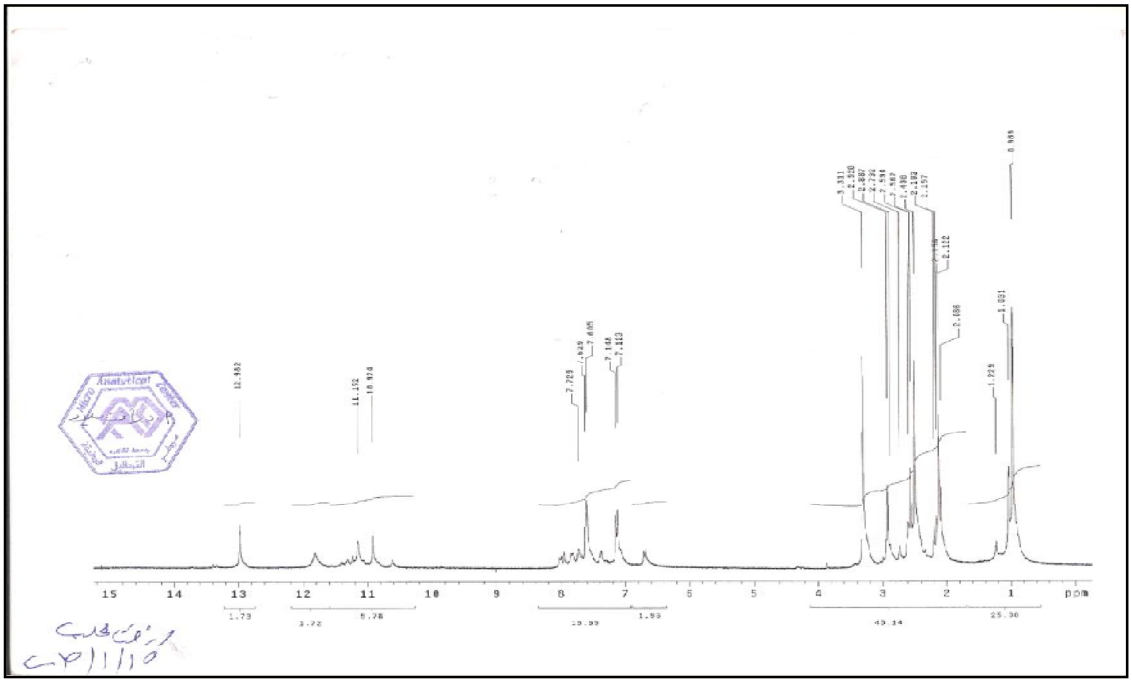

Fig.6.65.1H-NMRspectra of synthesis 4-diazo-(p-(5-(p-N,N-dimethylaminophenyl)-pyrazol-3-yl)-5,5-dimethyl-cyclohexane-1,3-dione(CVI)

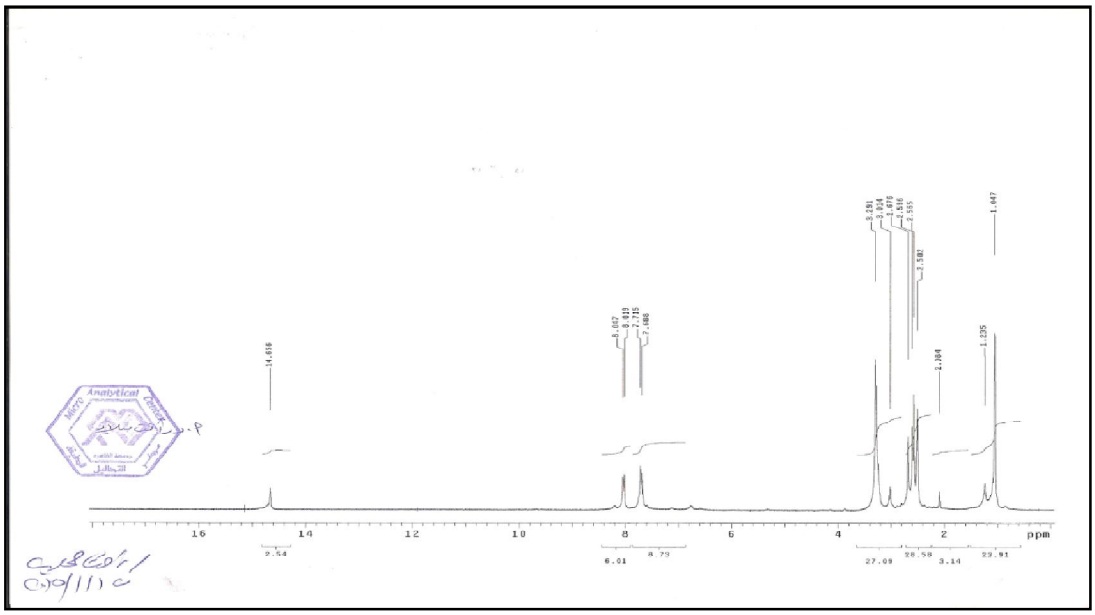

Fig.6.66.1H-NMRspectraofsynthesis 4-diazo-(p-(5-(p-N,N-dimethyl aminophenyl)-isoxaazol-5-yl)-phenyl)-5,5-dimethy-cyclohexane-1,3-dione(CV)

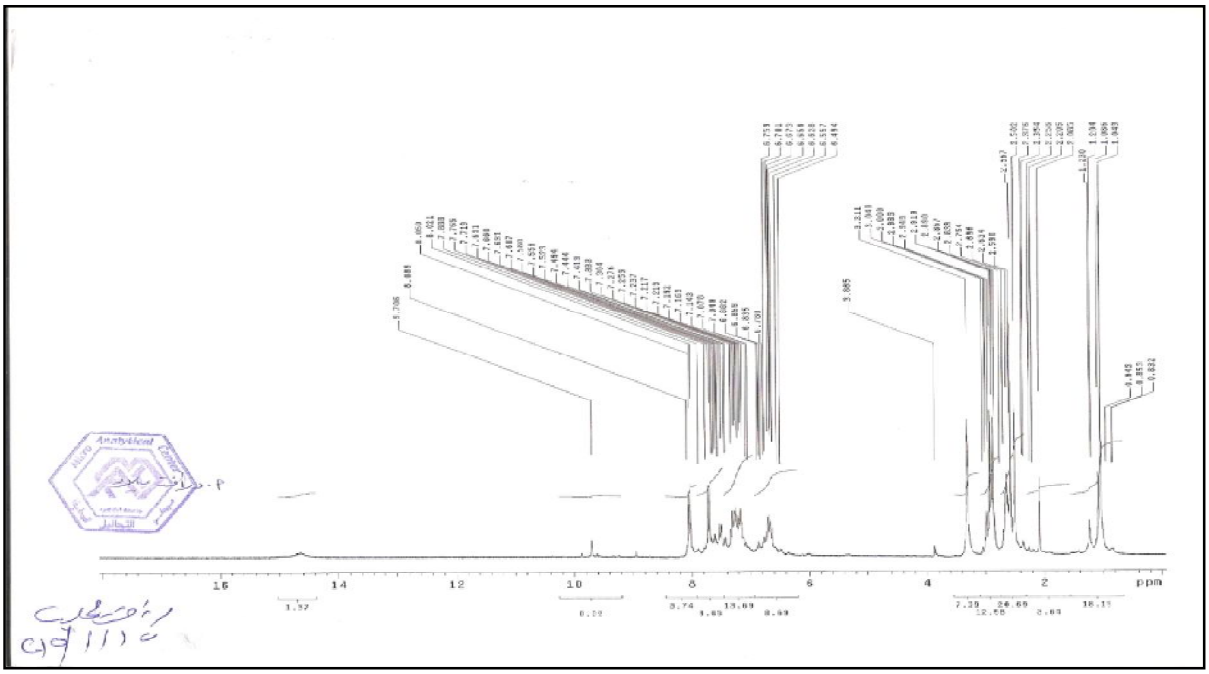

Fig.6.67.1H-NMR spectra of synthesis 4-diazo-(p-(5-(p-N,N-dimethyl aminophenyl)-2-thiopyrimidine-6-yl)-phenyl)-5,5-dimethyl-cyclohexane-1,3-dione(CVIII)

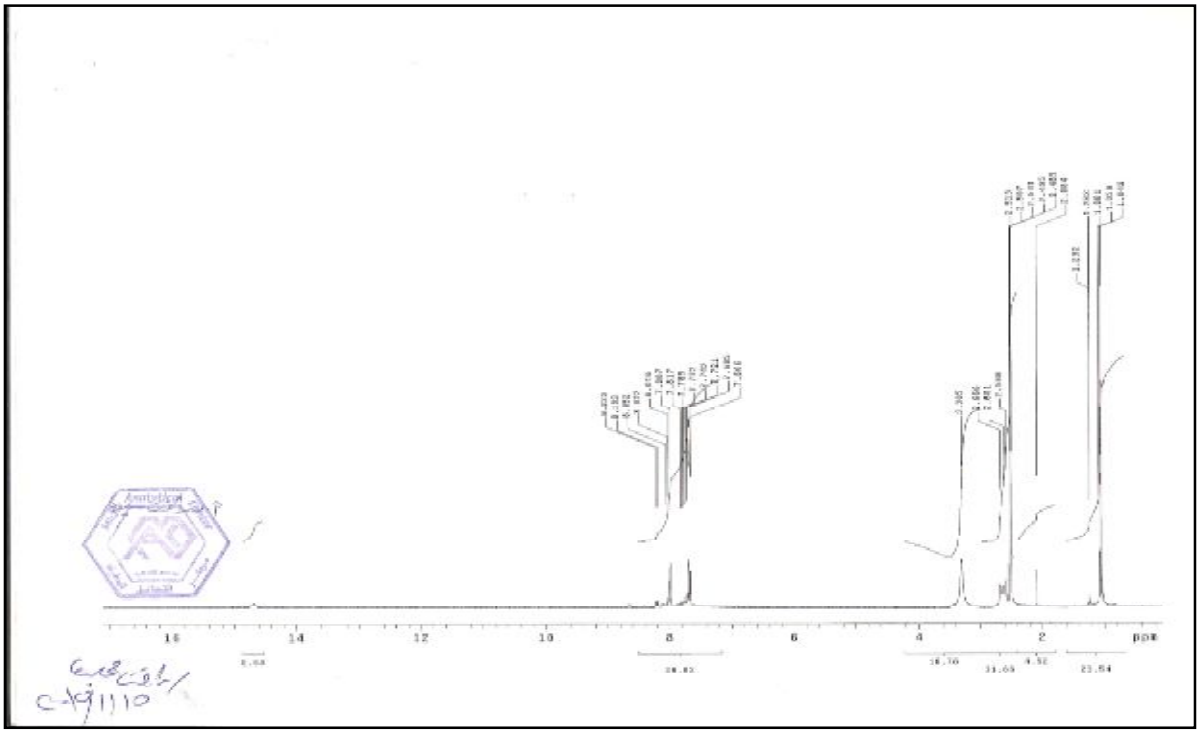

Fig.6.68.1H-NMR spectra of synthesis 4-diazo-(p-(5-(2-nitrophenyl)-pyrazol-3-yl)-phenyl)-5,5-dimethyl-cyclohexane-1,3-dione(XCIX)

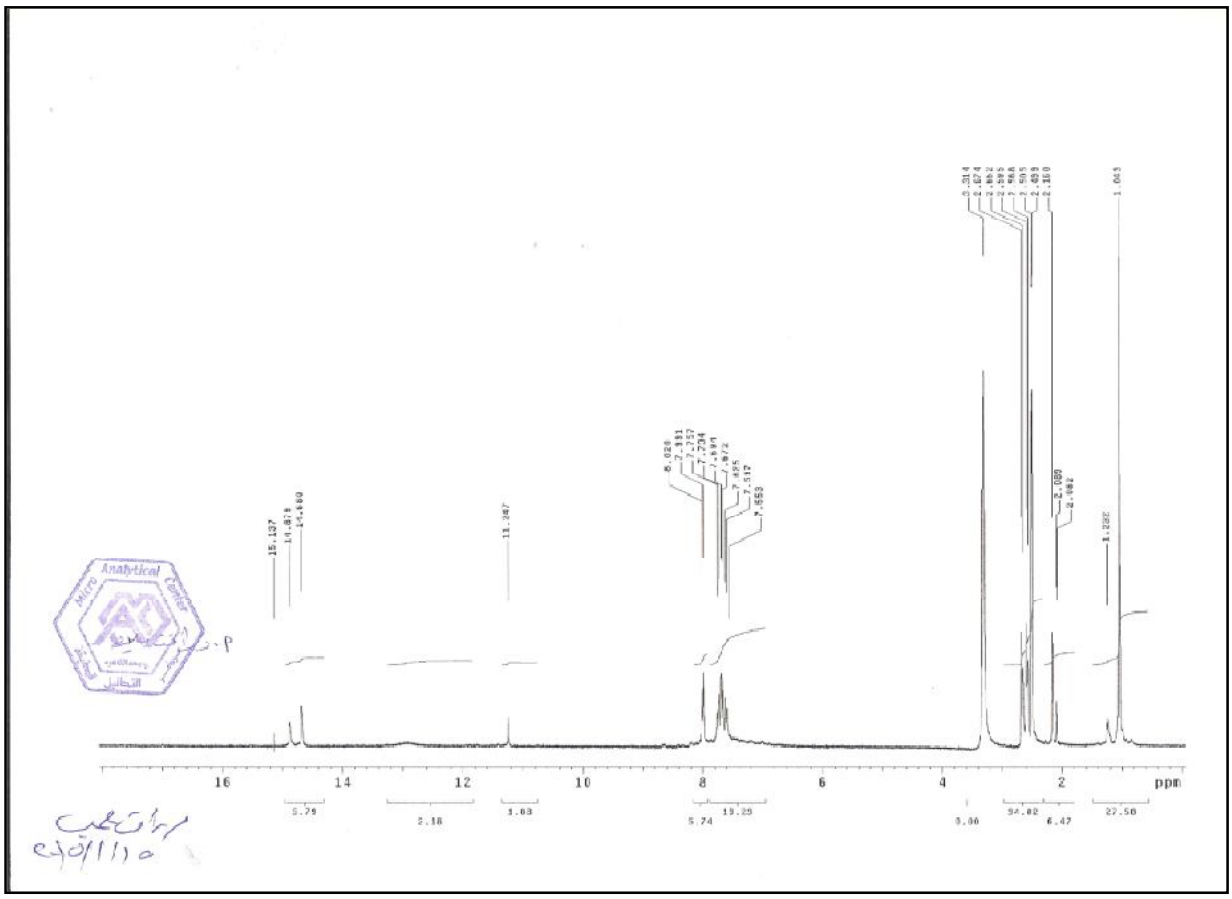

Fig.6.69.1H-NMRspectra of synthesis 4-diazo-(p-(5-(2-nitophenyl)- isoxazol-5-yl)-phenyl)-5,5-dimethyl-cyclohexane-1,3-dione(Cl)

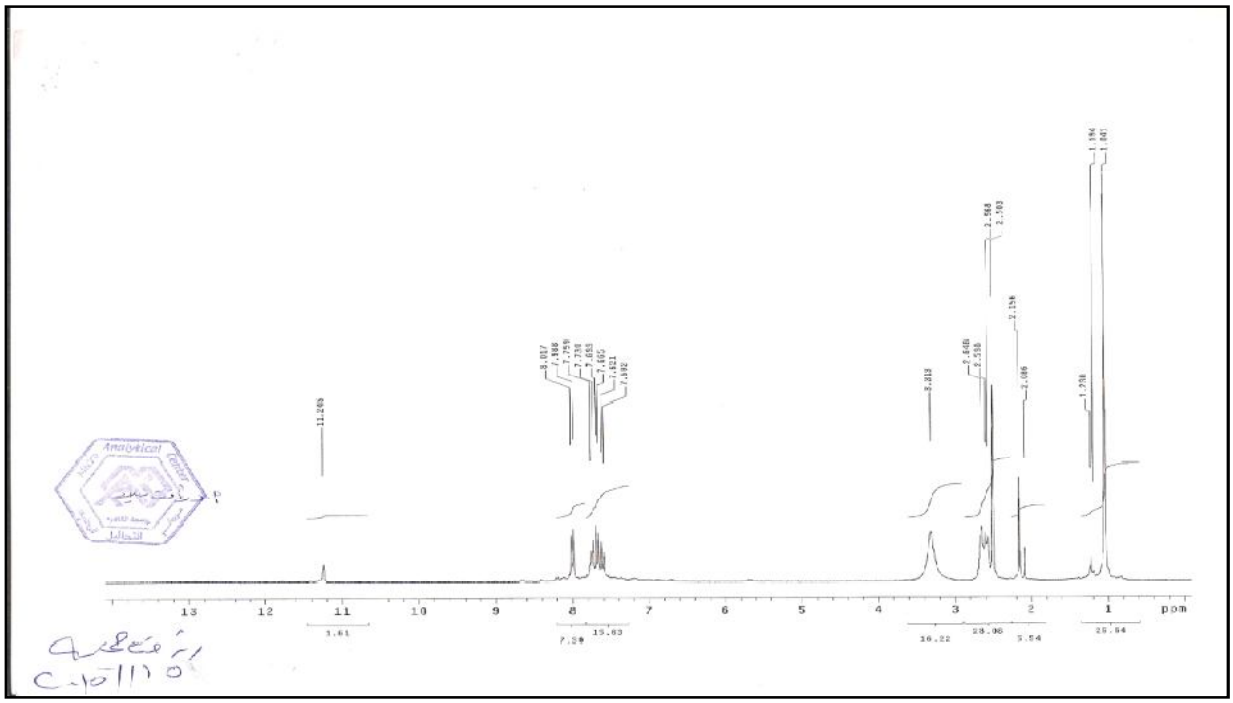

Fig.6.70.1H-NMR spectra of synthesis 4-diazo-(p-(5-(2-nitrophenyl)-2-thiopyrimidine-6-yl)-5,5-dmethyl-cyclohexane-1,3-dione©

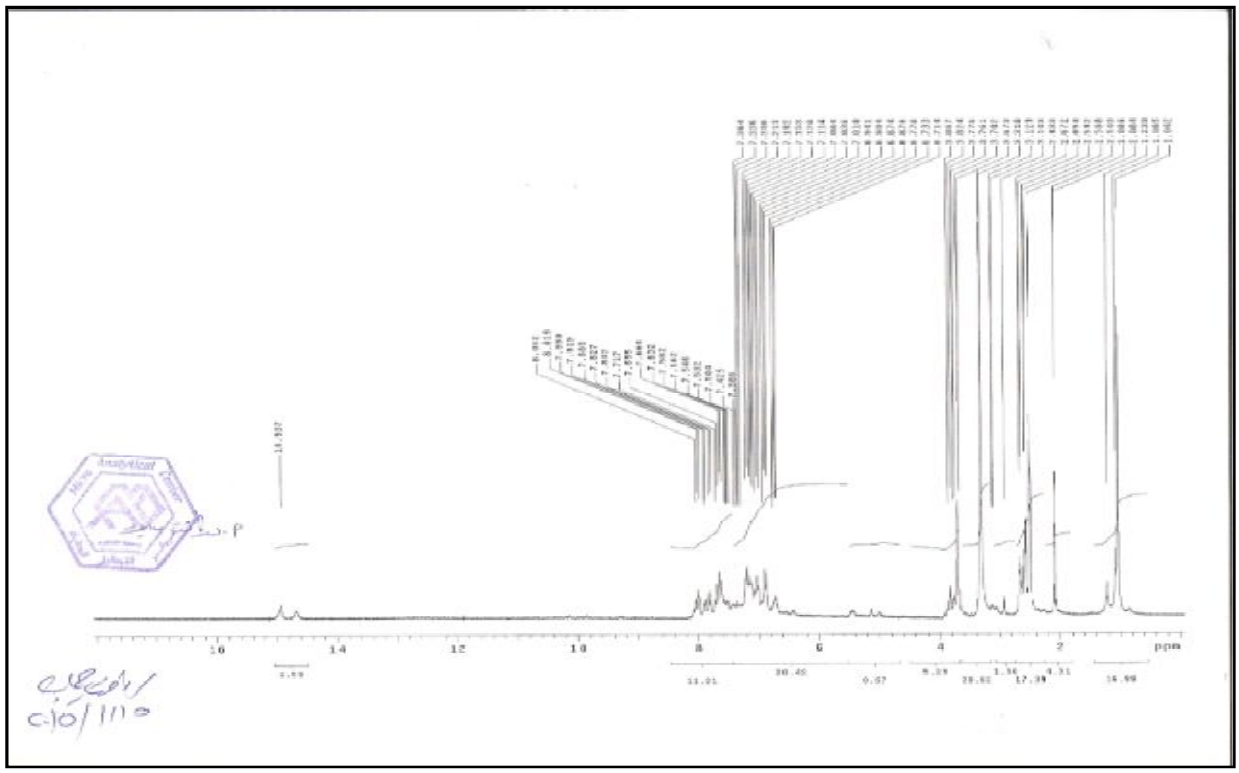

Fig.6.71.1H-NMR. Spectra of synthesis 4-diazo-(p-(5-(-4-methoxyphenyl)-pyrazol-3-yl)-phenyl)-5,5-dimethyl-cyclohexane-1,3-dione(XCVII)

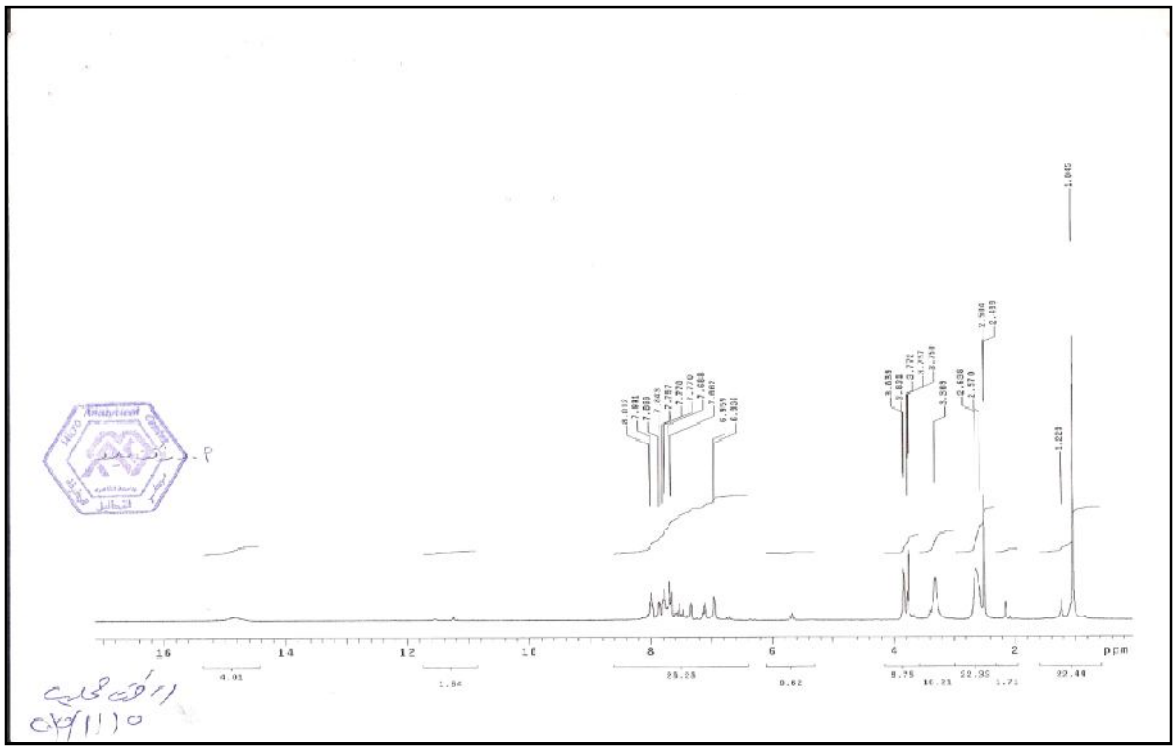

Fig.6.72.1H-NMRspectra of synthesis 4-diazo-(p-(5-(4-methoxy phenyl) isoxazole)-phenyl)5,5-dimethyl-cyclohexane-1,3-dioneXCVI)

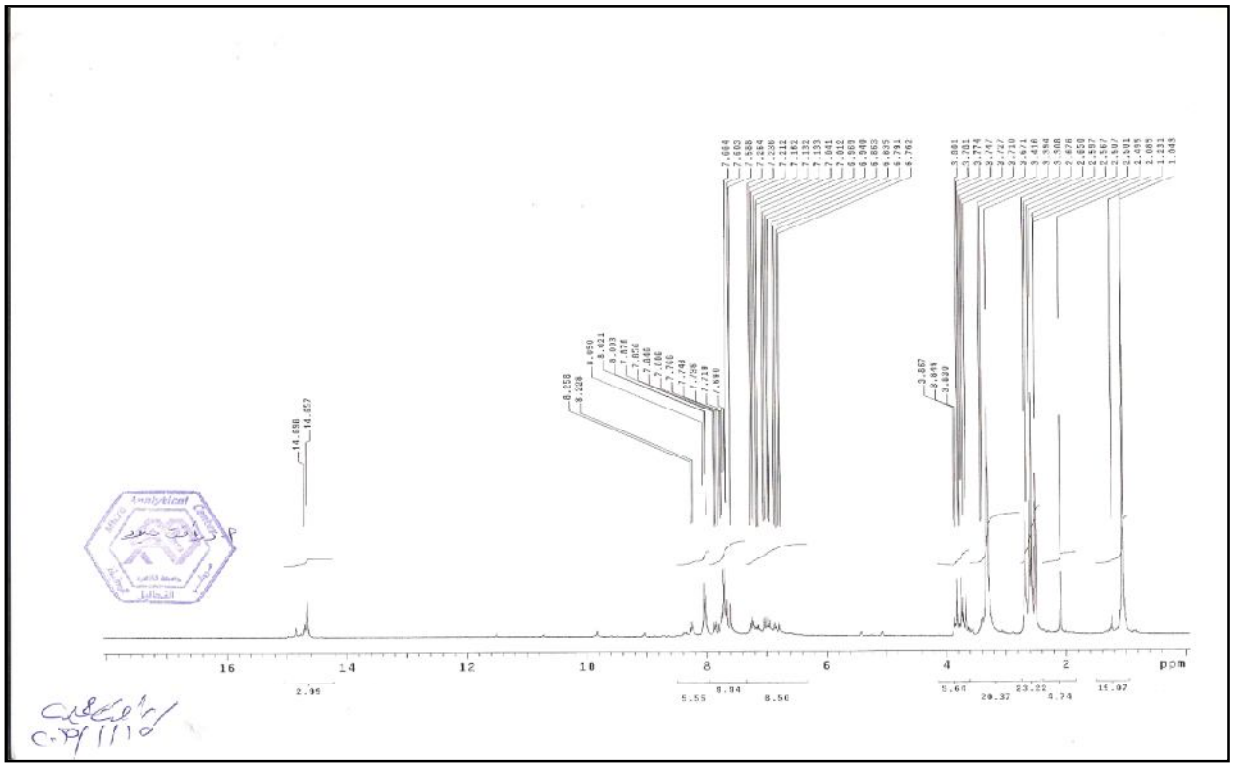

Fig.6. 73.1H-NMRspectraof synthesis 4-diazo-(p-(5-(-4-methoxyphenyl)-2-thiopyrimidine-6-yl)-phenyl)-5,5-dimethyl-cyclohexane-1,3-dione (XCVII)

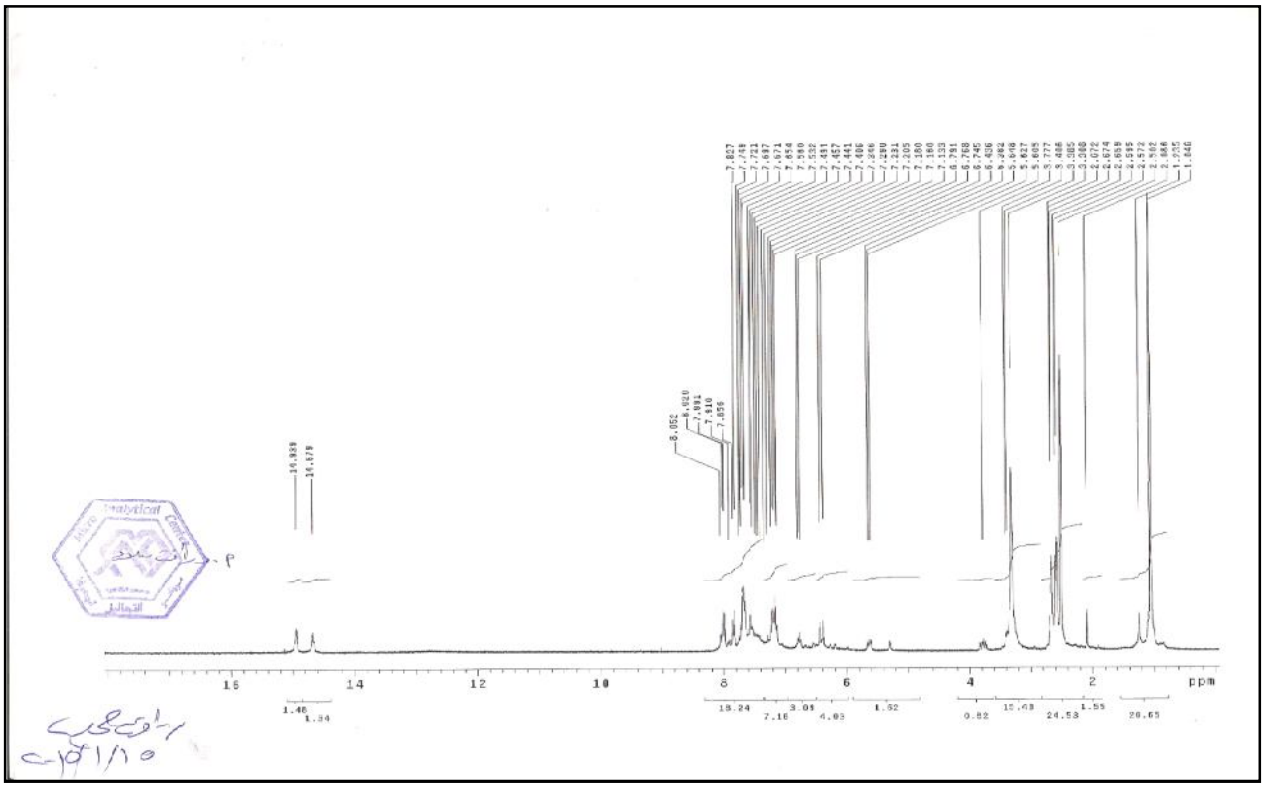

Fig.6.74,1H-NMR spectra of synthesis 4-diazo-(p-(5-(furan)-pyrazol-3-yl)-5,5-dimethyl-cyclohexane-1,3-dione(CII)

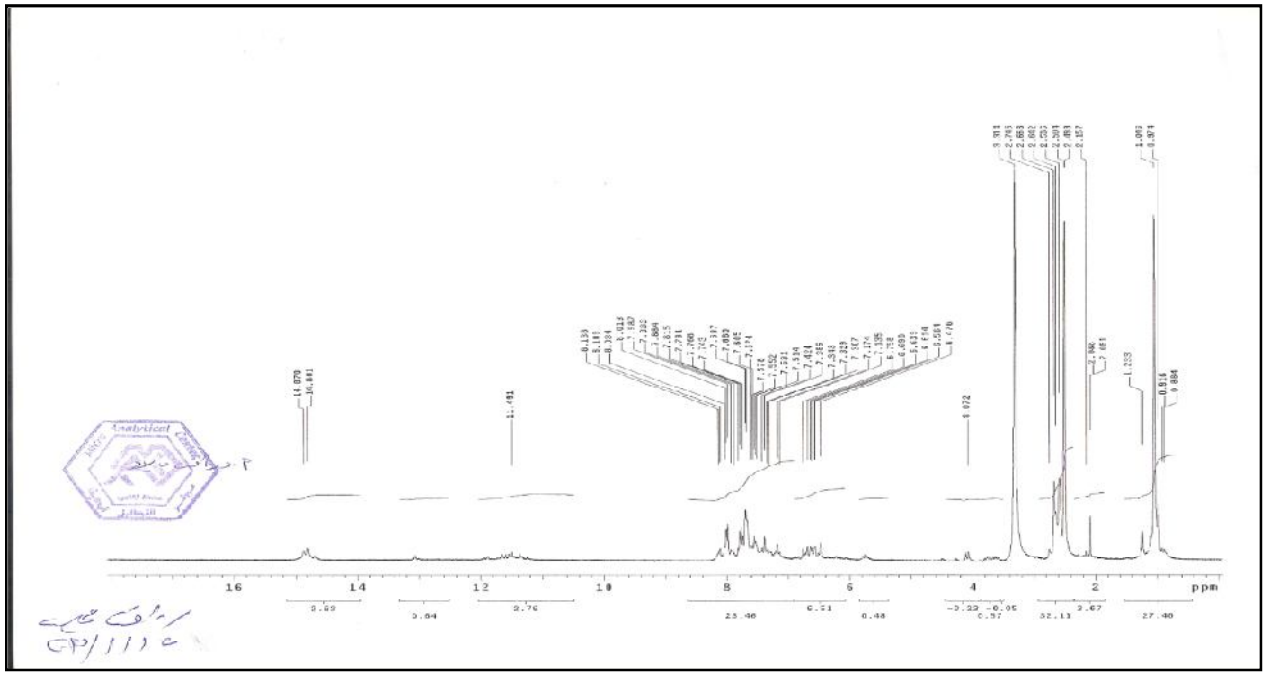

Fig.6.75.1H-NMR spectra of synthesis 4-diazo-(p-(5-(furan)-isoxazol-5-yl)-phenyl)-5,5-dimethyl-cyclohexane-1,3-dione (CIV)

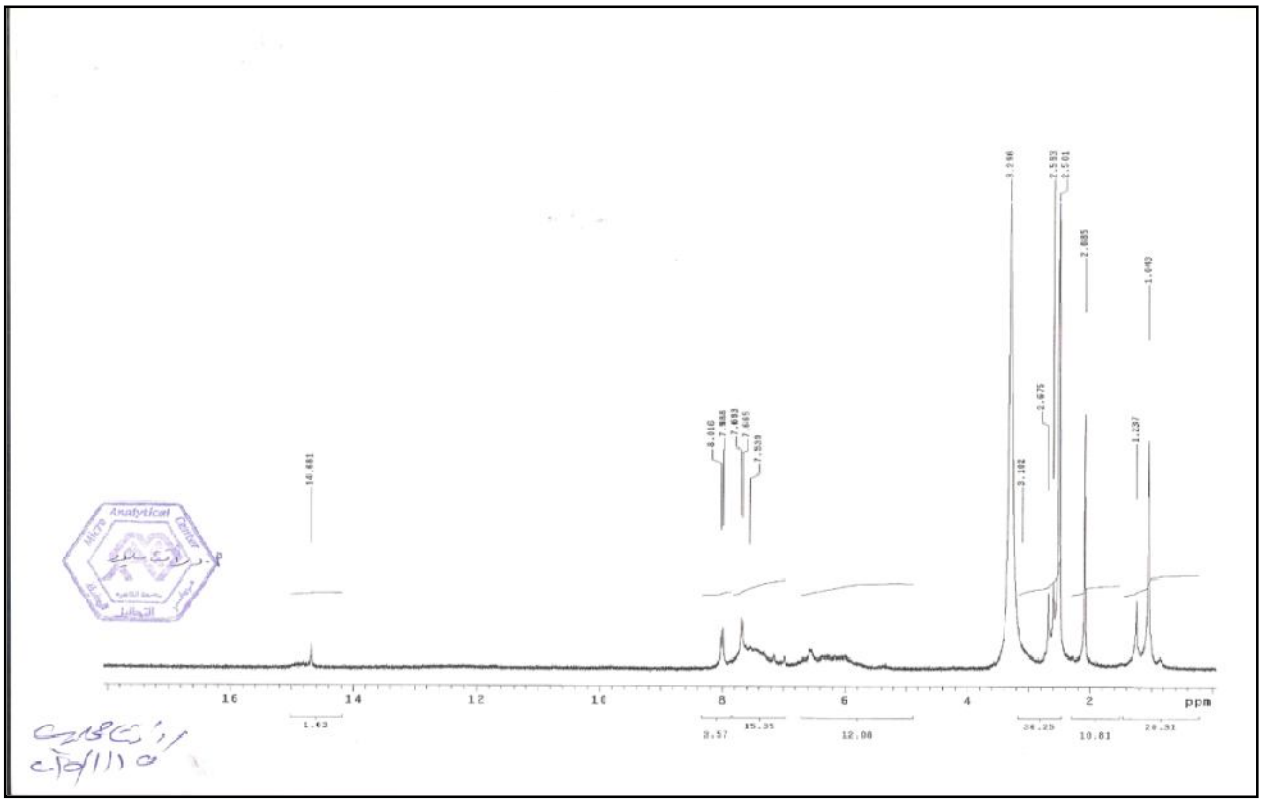

Fig.6.76.1H-NMR spectra of synthesis 4-diazo-(p-(5-(furan)-2-thio pyrimidine-6-yl)-phenyl)-5,5-dimethyl-cyclohexane-1,3-dione (CIII)

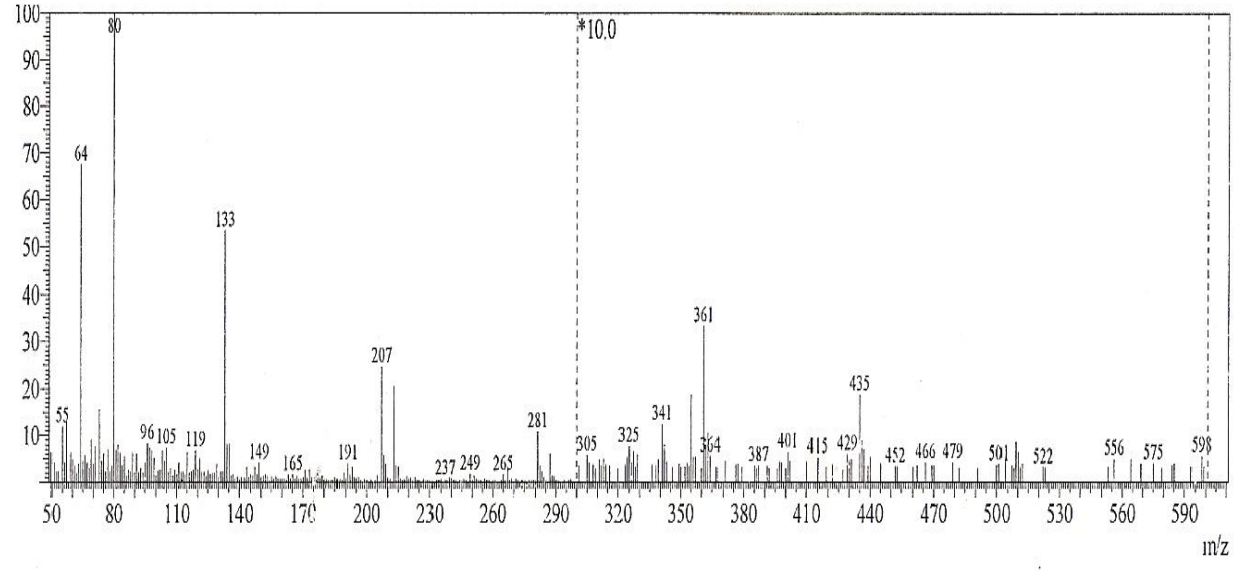

Fig.6.77. MS spectra of synthesis 4-diazo-(p-(5-(-4-methoxyphenyl)-2-thiopyrimidine-6-yl)-phenyl)-3,5-dimethyl-1-2,4-dinitro phenyl pyrazole(LXXIX)

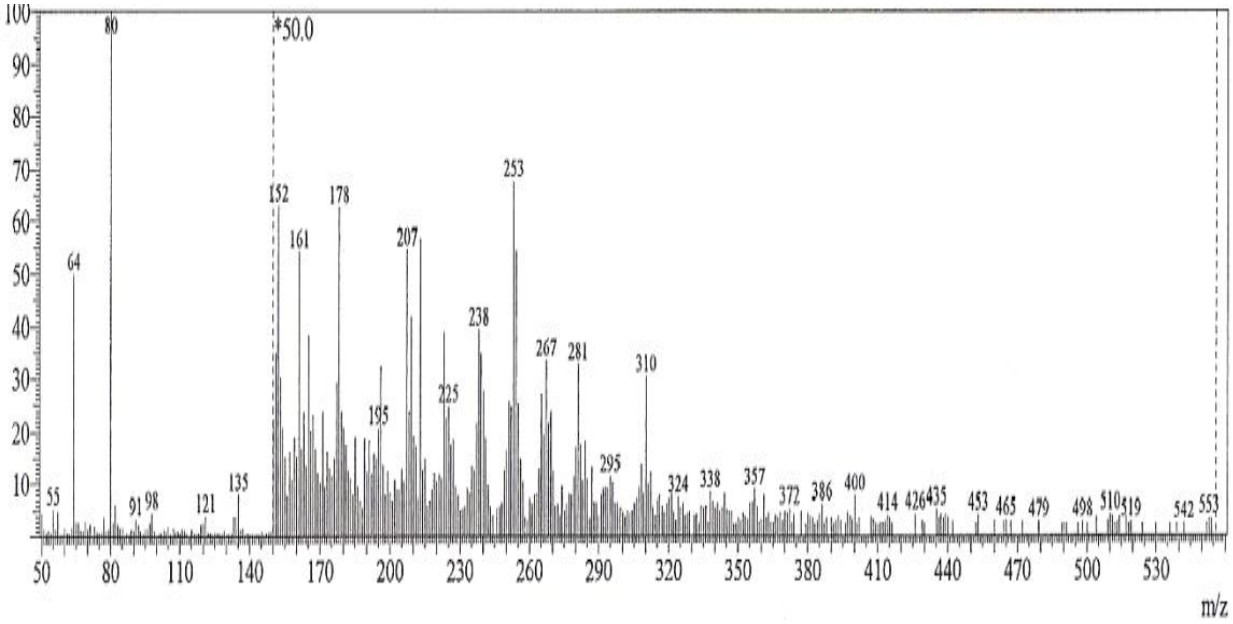

Fig.6.78. MS spectra of synthesis 4-diazo-(p-(5-(4-methoxyphenyl)-pyrazol-3-yl)-phenyl)-3,5-dimethyl-1-2,4-dinitro phenyl pyrazole(LXVIII)

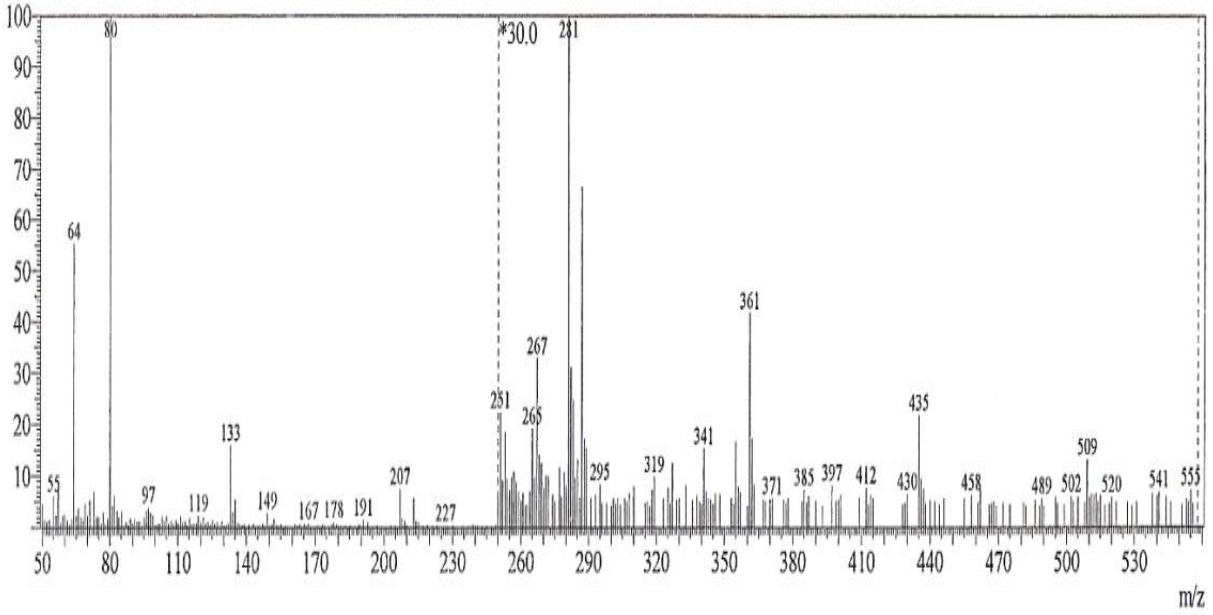

Fig.6.79.MS spectra of synthesis 4-diazo-(p-(5-((4methoxyphenyl)-isoxazol-5 -yl)-phenyl)-3,5-dimethyl-1-2,4-dinitro phenyl pyrazole(LXXVII)

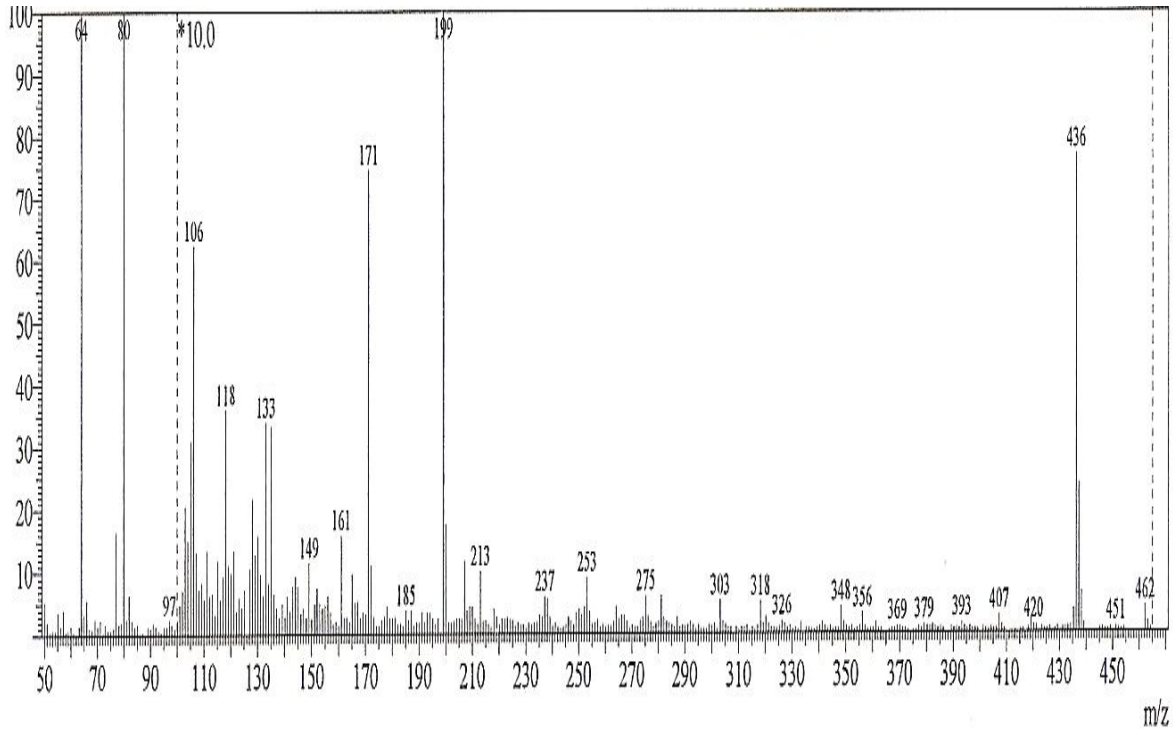

Fig.6.80. MS. spectra of synthesis 4-diazo-(p-(5-(-4-methoxyphenyl)-isoxazol-5-yl)-phenyl)-3,5-dimethyl-1-phenylpyrazole(LXXI)

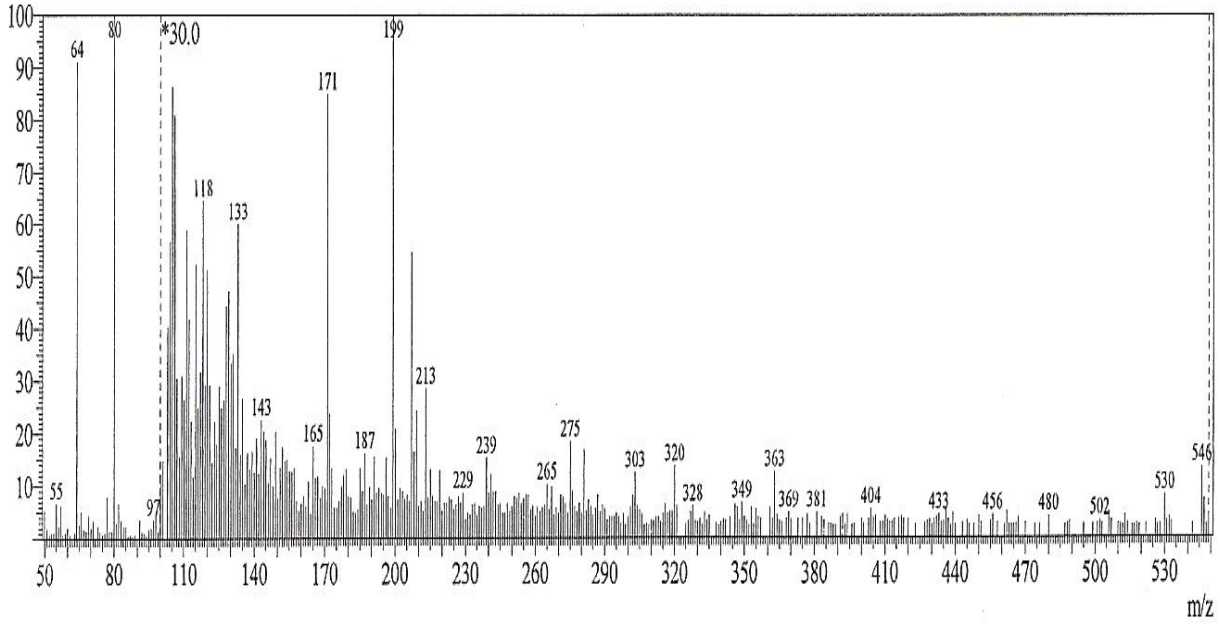

Fig.6.81.MSspectra of synthesis 4-diazo-(p-(5-(2-hydroxyphenyl)-2-thiopyrimidine-6-yl)-phenyl)-3,5-dimethyl-1-phenylpyrazole(LXXVI)

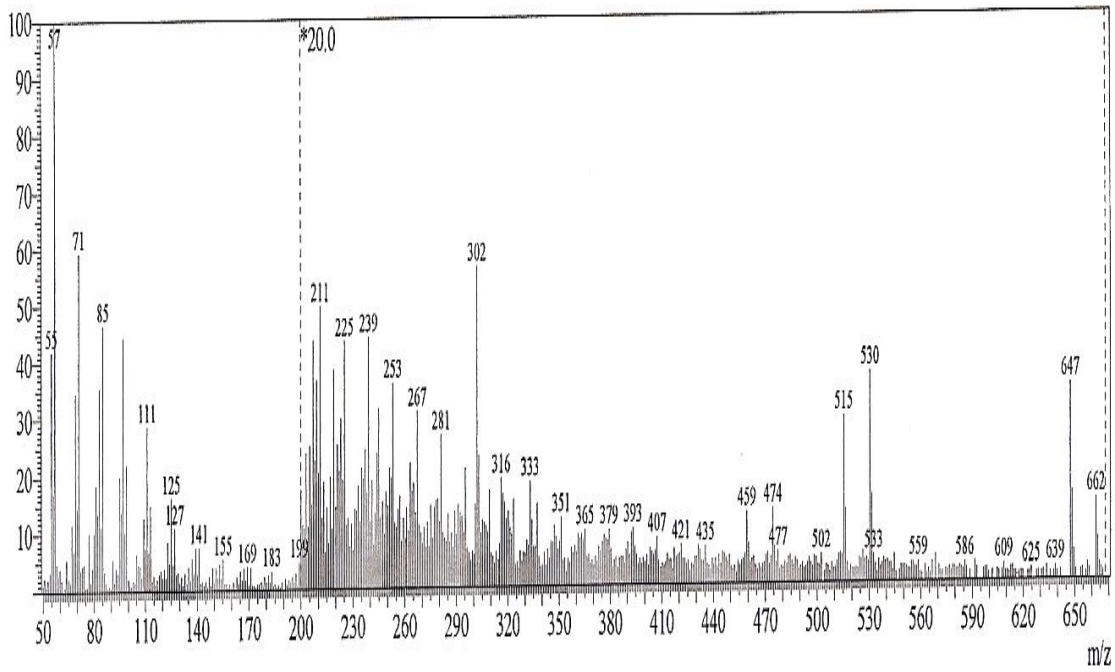

Fig6.82 MSspectra of synthesis 4-diazo(p-(5-(4-methoxyphenyl)-pyrazol-3-yl)-phenyl)-3,5-dimethyl-1-phenylpyrazole9LXXII)

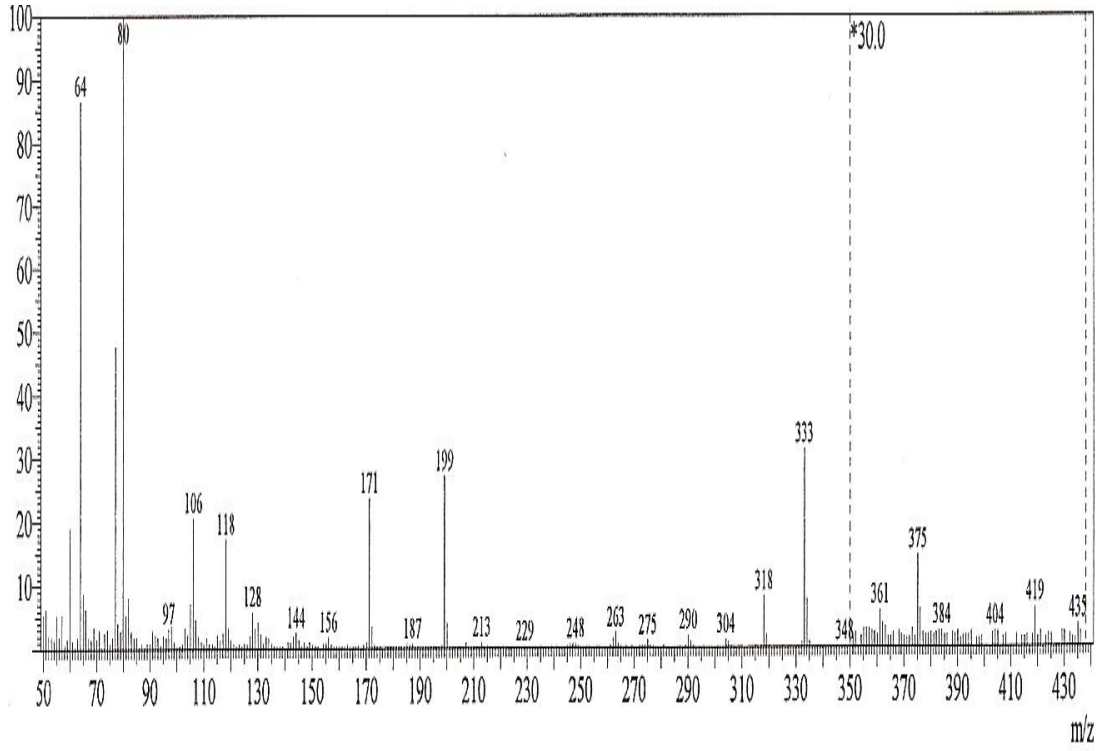

Fig.6.83.MS spectra of synthesis 4-diazo-(p-(5-(2-hydroxyphenyl)-isoxazol-5-yl)-phenyl)-3,5-dimethyl-1-phenylpyrazole(LXXIV)

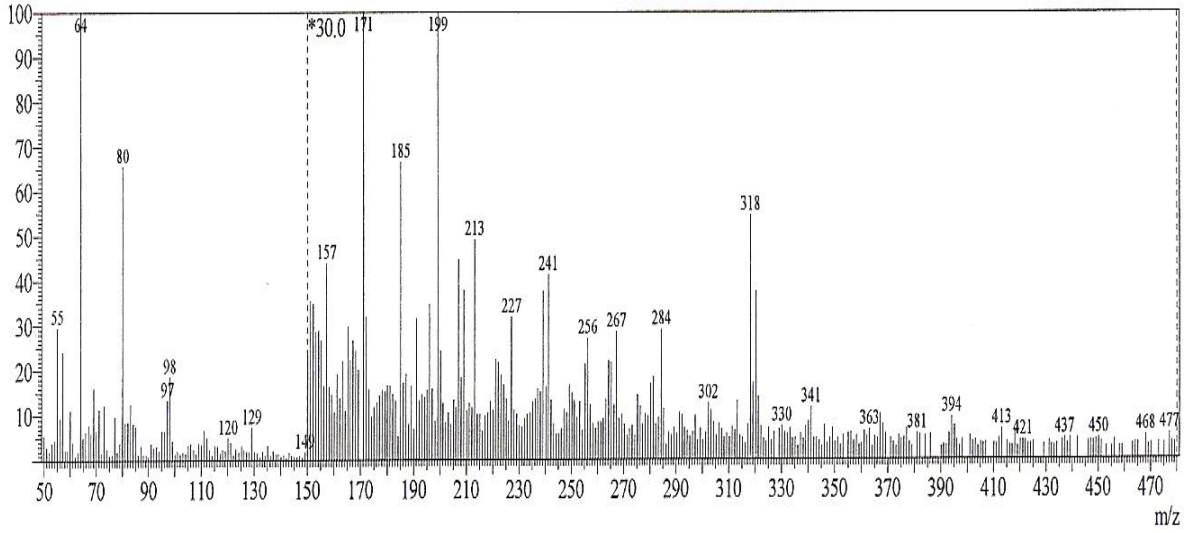

Fig.6.84.MS spectra of synthesis 4-diazo-(p-(5-(2-hydroxy-4-methoxyphenyl)-2-thiopyrimidine-6-yl)-phenyl)-3,5-dimethyl-1-phenylpyrazole(LXXVI)

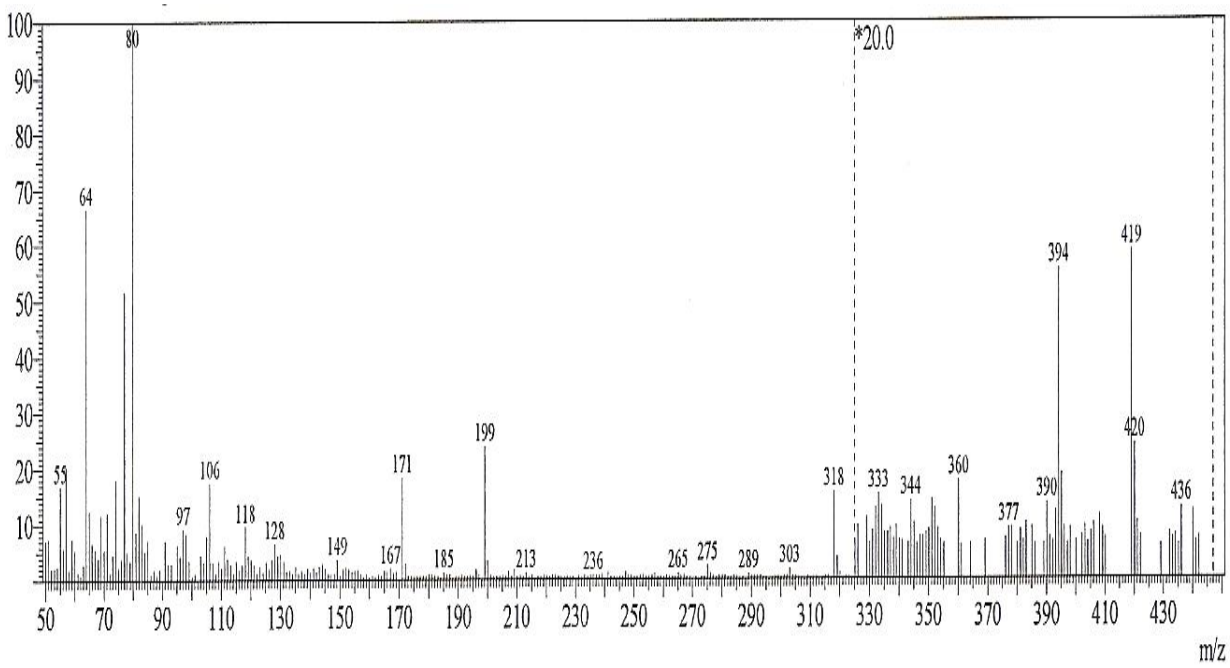

Fig.6.85.MS spectra of synthesis 4-diazo-(p-(5-(2-hydroxyphenyl)-pyrazol-3-yl)-phenyl)-3,5-dimethyl-1-phenylpyrazole(LXXV)

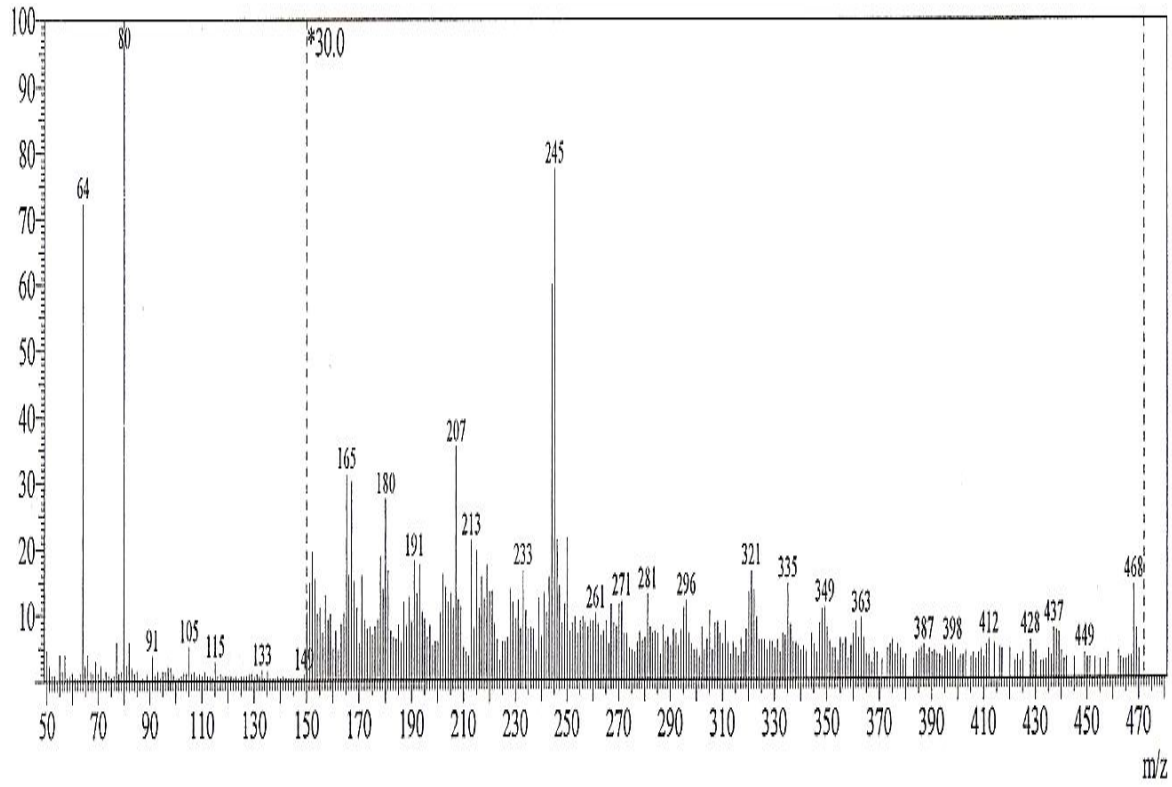

Fig.6.86.MS.spectra of synthesis 4-diazo-(p-(5-(2-phenylethenyl)-isoxazol-5-yl)-phenyl)-5-methyl-1-phenylpyrazol-3-one(XC)

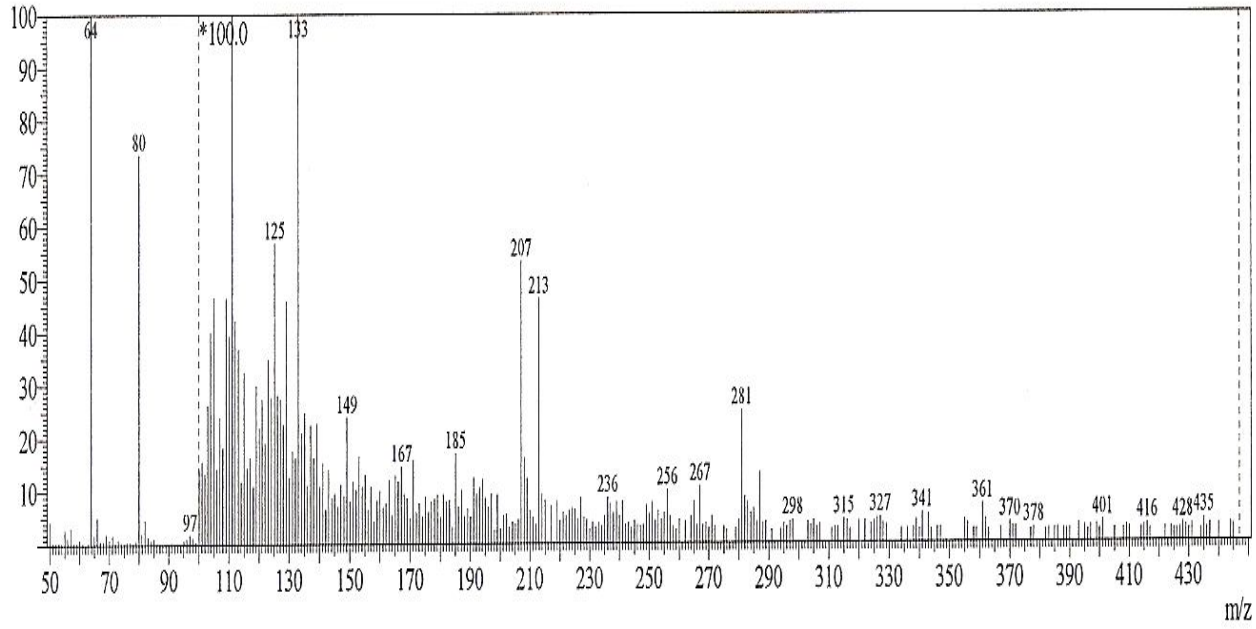

Fig.6.87.MS spectra of synthesis 4-diazo-(p-(5-(2-phenylethenyl)-pyrazol-3 -yl)-phenyl)-5-methyl-1-phenylpyrazol-3-one(XCI)

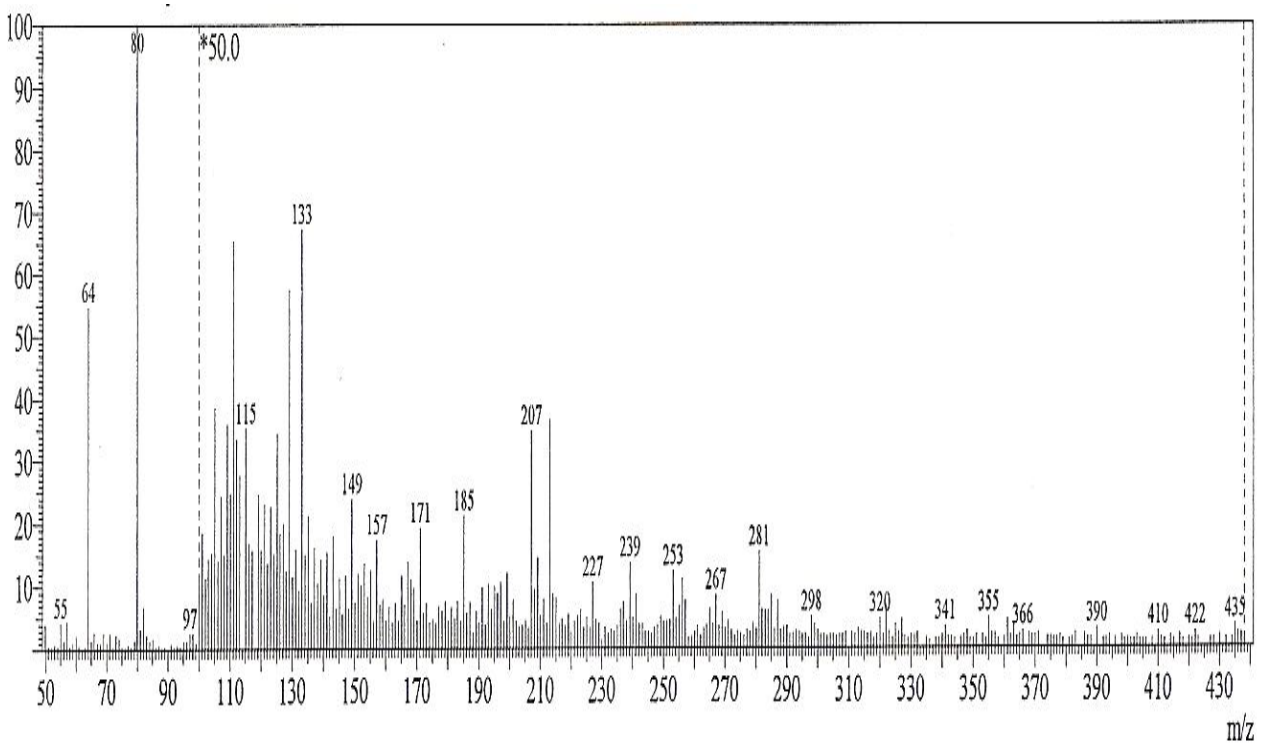

Fig.6.88.MS.spectra of synthesis 4-diazo-(p-(5-(2-phenylethenyl)-2-thiopyrimidine-6 -yl)-phenyl)-5-methyl-1-phenylpyrazol-3-one(XCII)

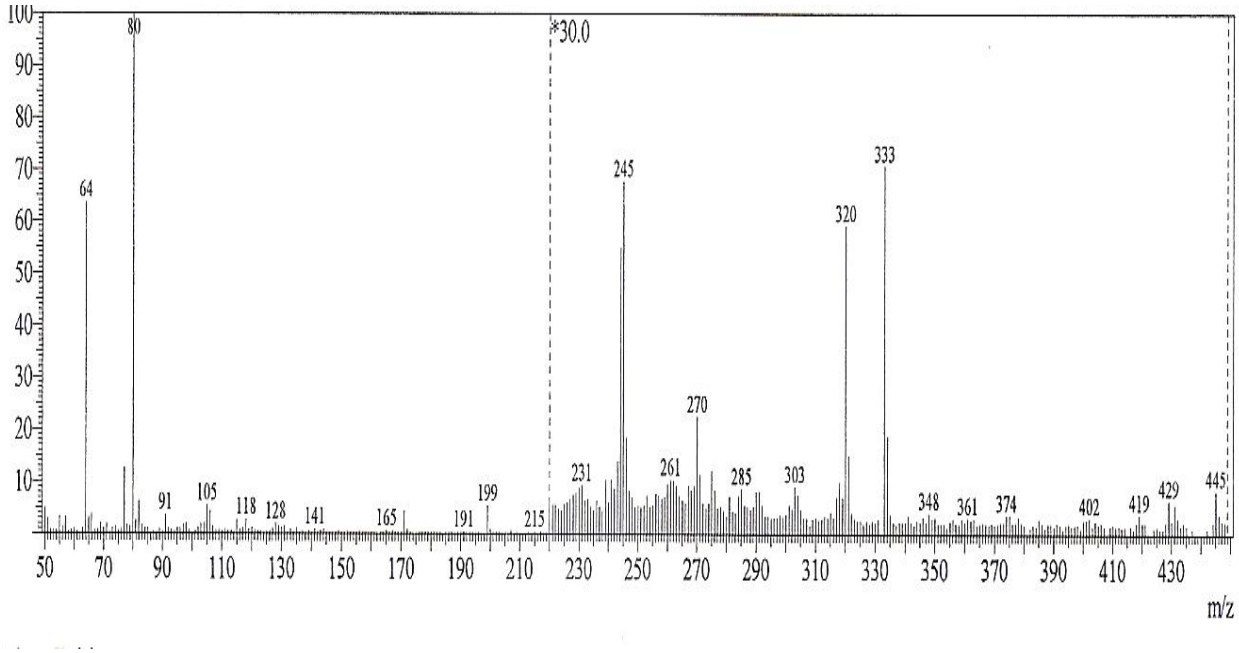

Fig.6.89.MS spectra of synthesis 4-diazo-(p-(5-(2-phenylethenyl)-isoxazo-5 -yl)-phenyl)-3,5-dimethyl-1-phenylpyrazole(XCIII)

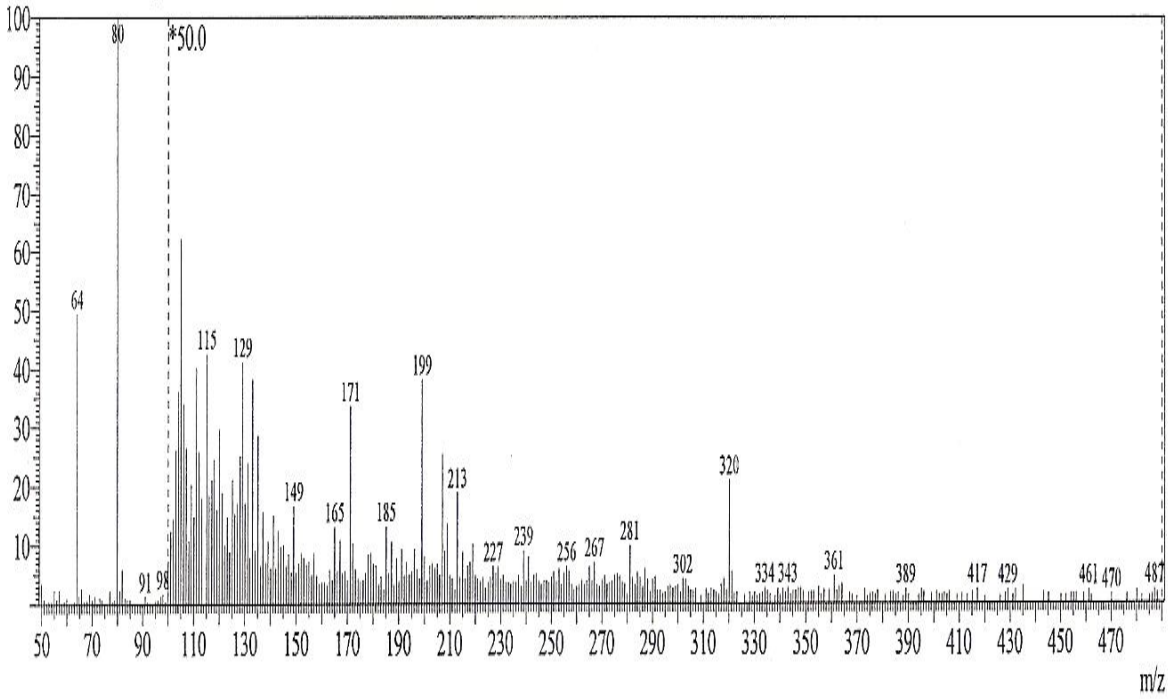

Fig.6.90.MS spectra of synthesis 4-diazo-(p-(5-(2-phenylethenyl)-2-thiopyrimidine-6-yl)-phenyl)-3,5-dimethyl-1-phenylpyrazole(XCV)

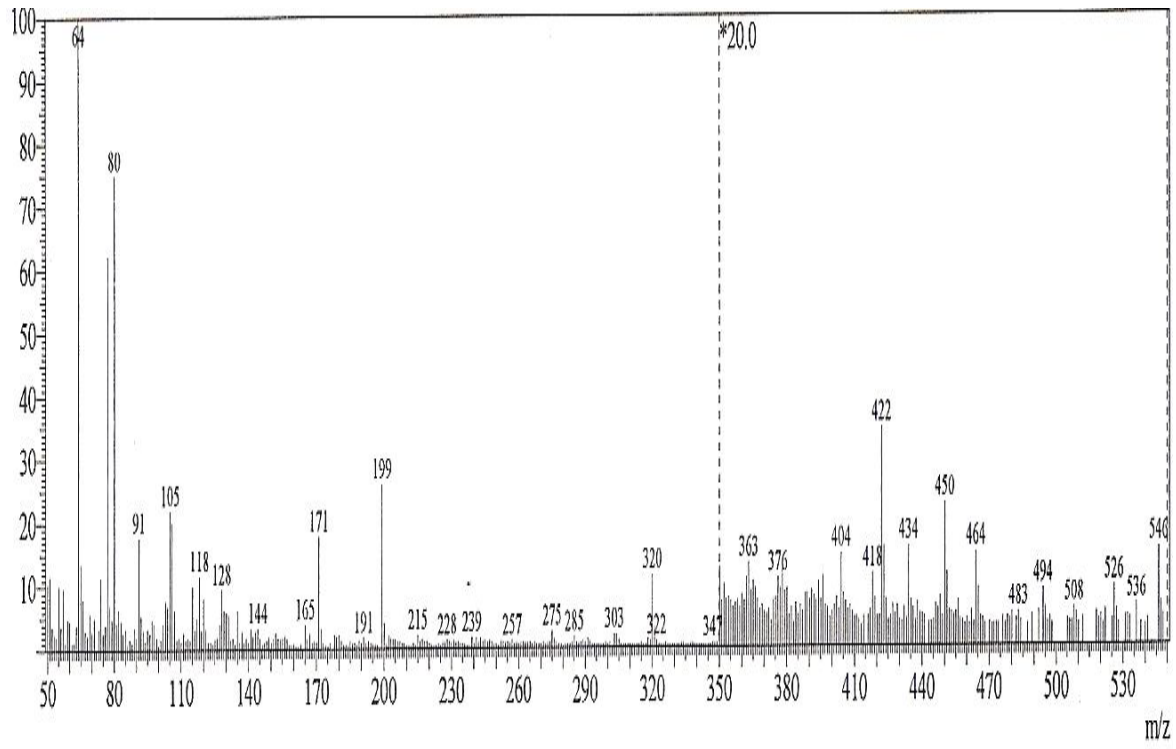

Fig.6.91.MS spectra of synthesis 4-diazo-(p-(5-(2-phenylethenyl)-pyrazol-3 -yl)-phenyl)-3,5-dimethyl-1-phenylpyrazole(XCV)

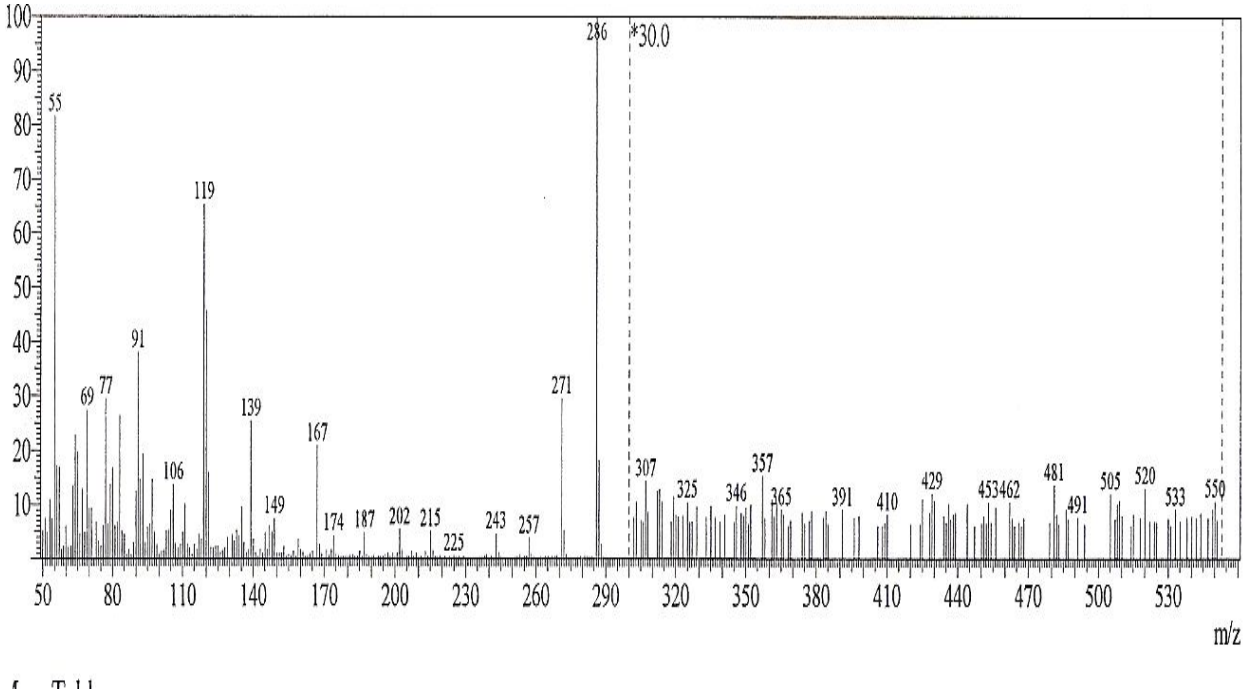

Fig.6.92.MS spectra of synthesis 4-diazo-(p-(5-(P-N,N-dimethylaminophenyl)-pyrazol-3-yl)-phenyl)-3,5-dimethyl-1-2,4-dinitrophenylpyrazole(CVIII)

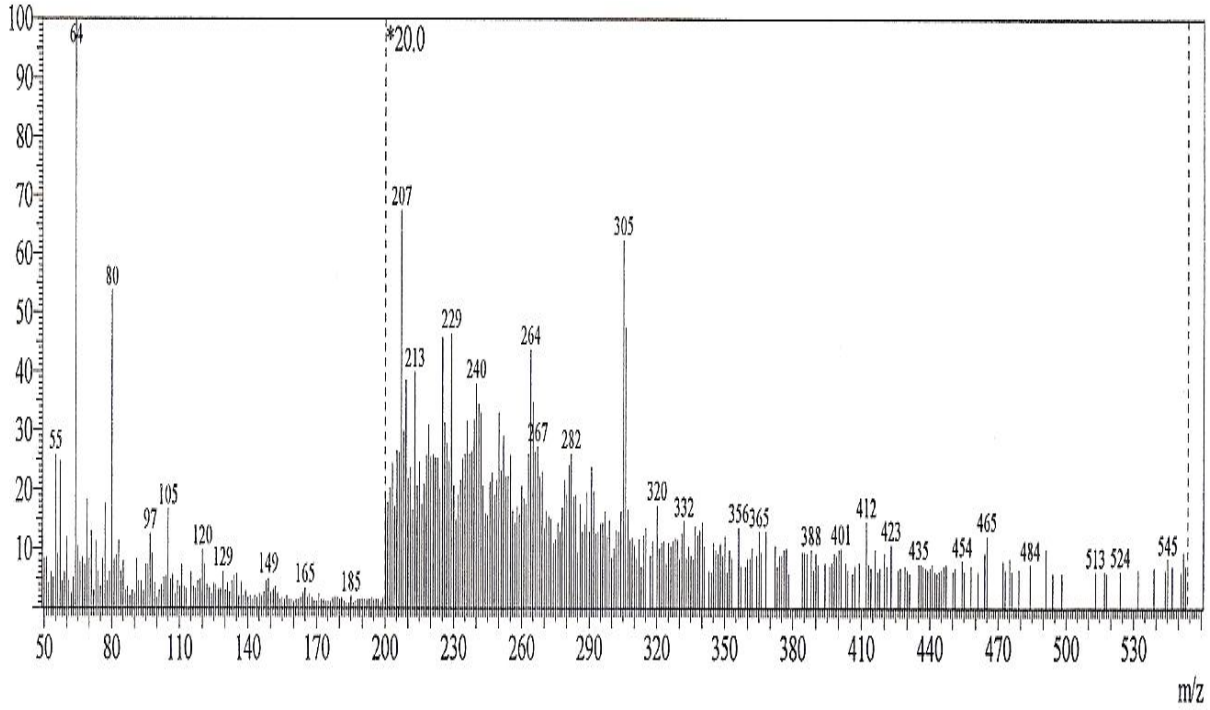

Fig.6.93.MS spectra of synthesis 4-diazo-(p-(5-(P-N,N-dimethyl amino phenyl)-isoxazol-5 -yl)-phenyl)-3,5-dimethyl-1-2,4-dinitro phenyl pyrazole(CIX)

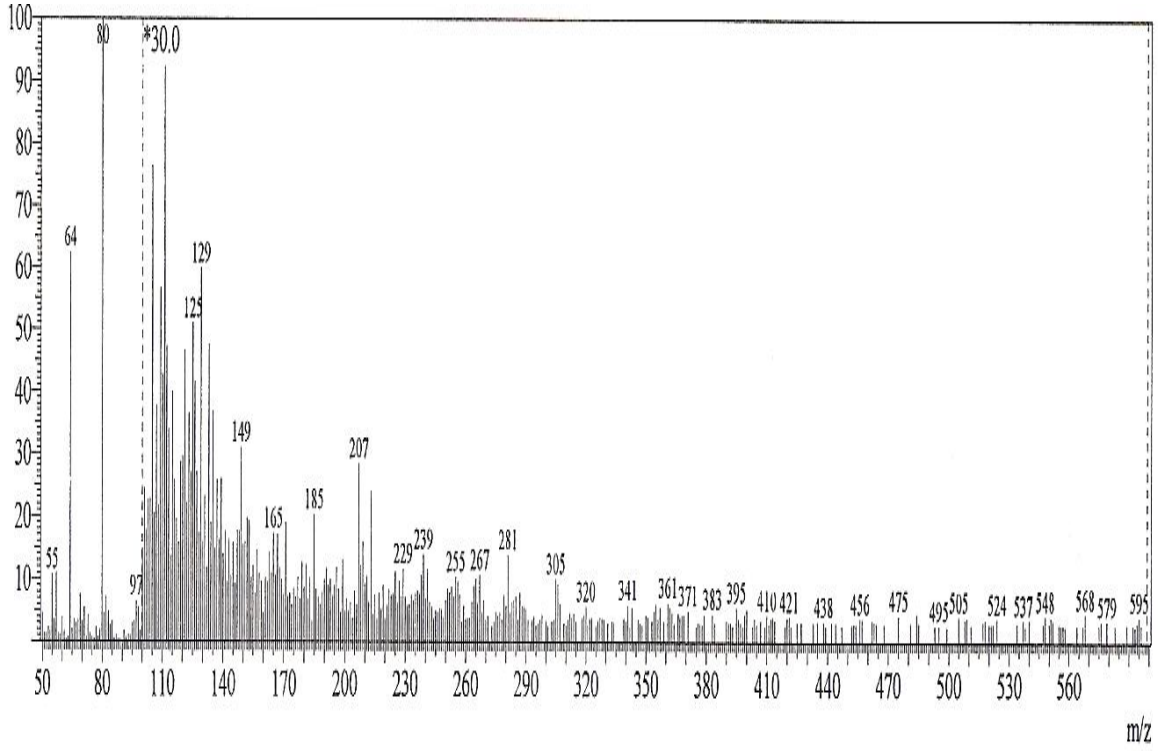

Fig.6.94.MS spectra of synthesis 4-diazo-(p-(5-(P-N,N-dimethylaminophenyl)-2-thiopyrimidine -6-yl)-phenyl)-3,5-dimethyl-1-2,4-dinitrophenylpyrazole(CX)

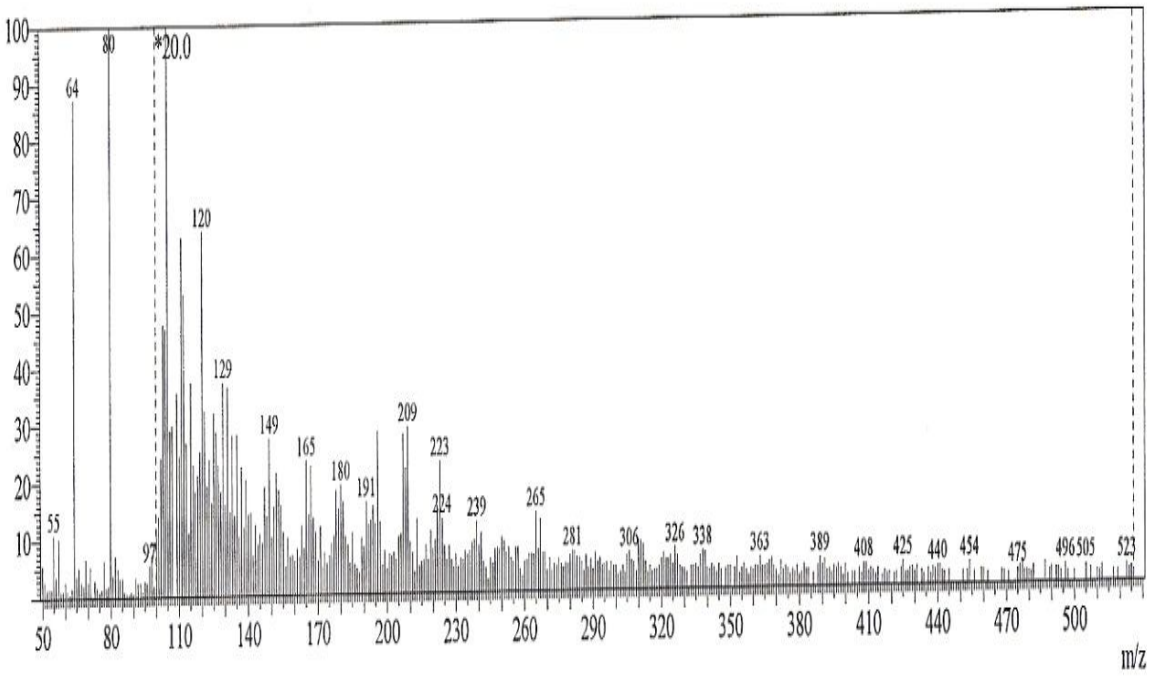

Fig.6.95.MS spectra of synthesis 4-diazo-(p-(5-(2-hydroxyphenyl)-pyrazol-3-yl)-phenyl)-3,5-dimethyl-1-2,4-dinitrophenylpyrazoleLXXXIV)

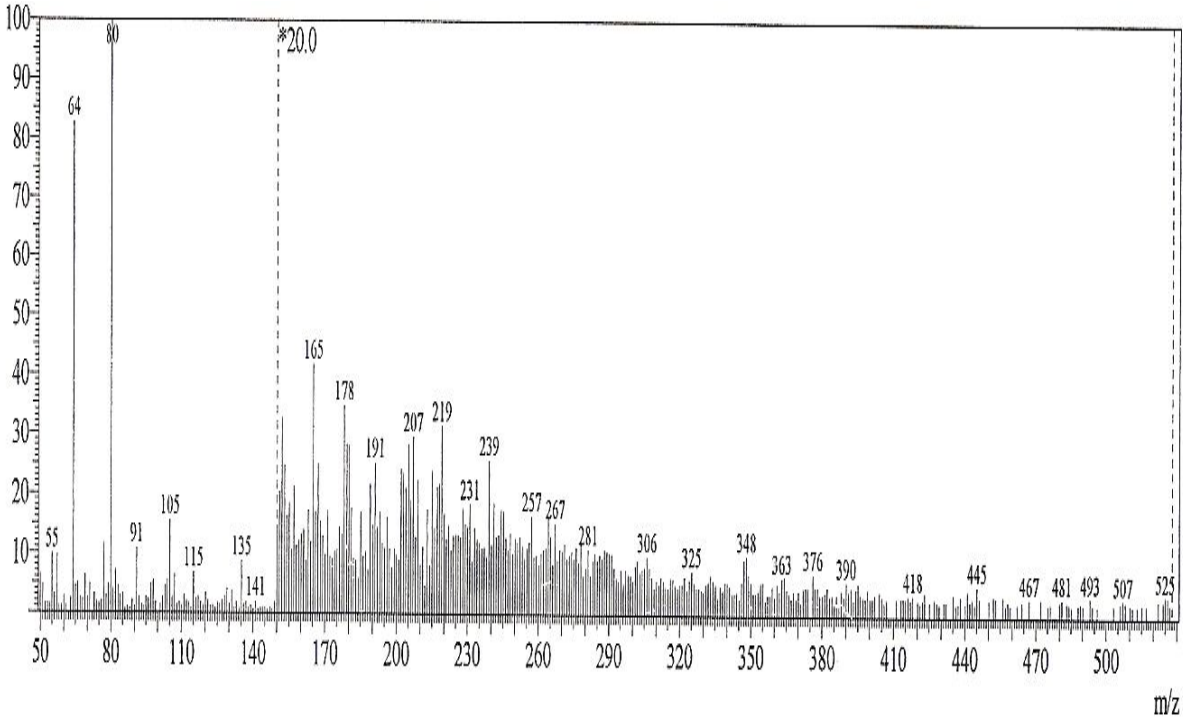

Fig.6.96.MS spectra of synthesis 4-diazo-(p-(5-(2-hydroxyphenyl)-isoxazo-5-yl)-phenyl)-3,5-dimethyl-1-2,4-dinitrophenylpyrazole(LXXXIII)

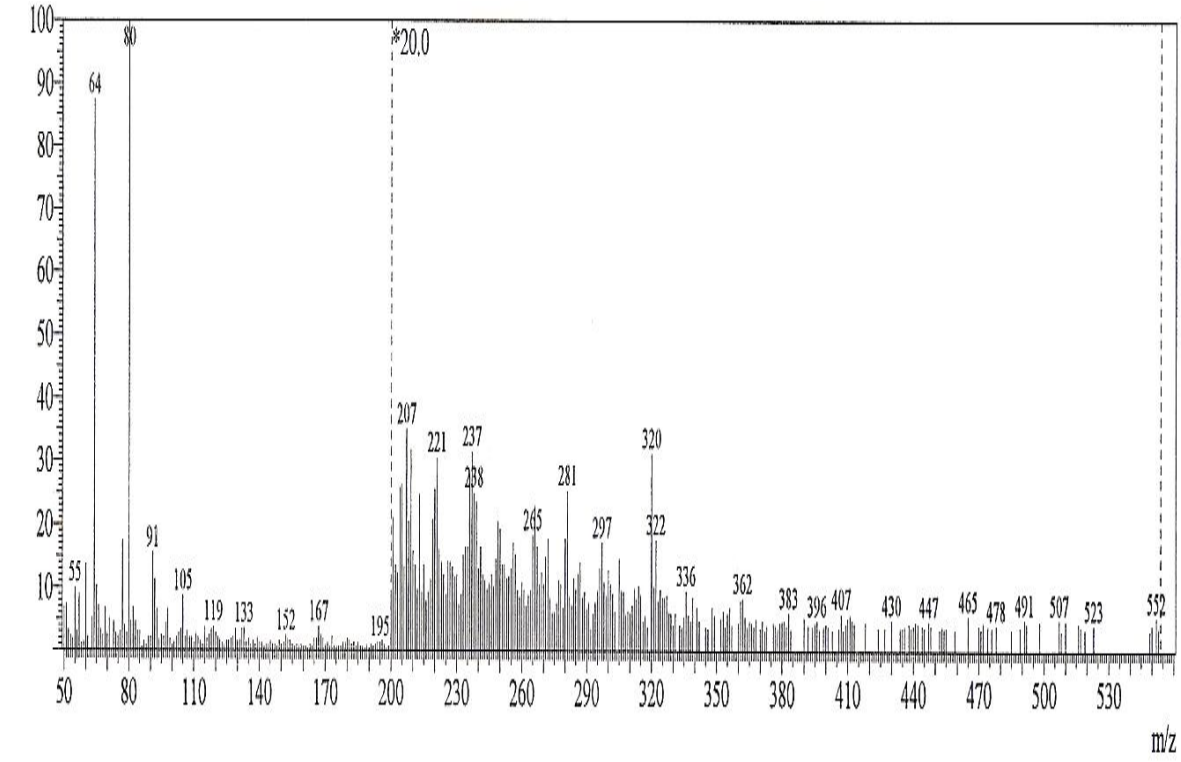

Fig.6.97.MS spectra of synthesis 4-diazo-(p-(5-(2-nitrophenyl)-pyrazol-3-yl)-phenyl)-3,5-dimethyl-1-2,4-dinitrophenylpyrazole(LXXX)

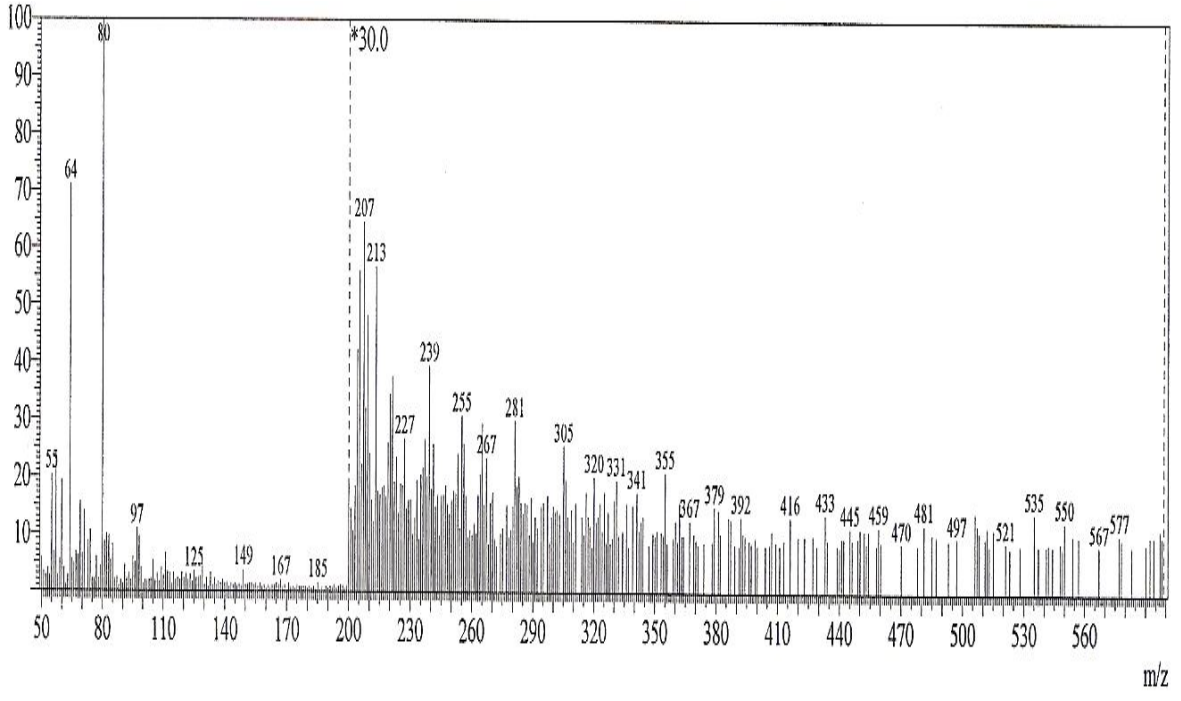

Fig.6.98.MS spectra of synthesis 4-diazo-(p-(5-(2-nitrophenyl)-2-thiopyrimidine-6- yl)-phenyl)-3,5-dimethyl-1-2,4-dinitrophenylpyrazole(LXXXII)

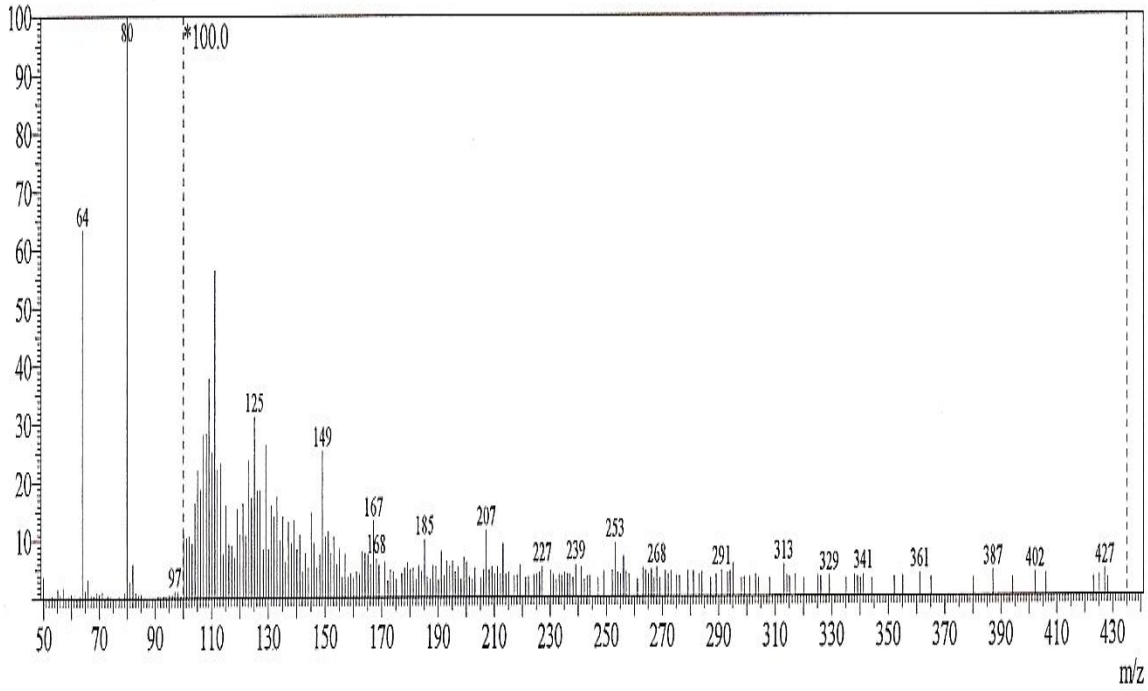

Fig.6.99.MS spectra of synthesis 4-diazo-(p-(5-(p-N,N-dimethyl amino phenyl)-pyrazol-3-yl)-phenyl)-5,5-dimethyl-cyclohexane-1,3-dione(CVII)

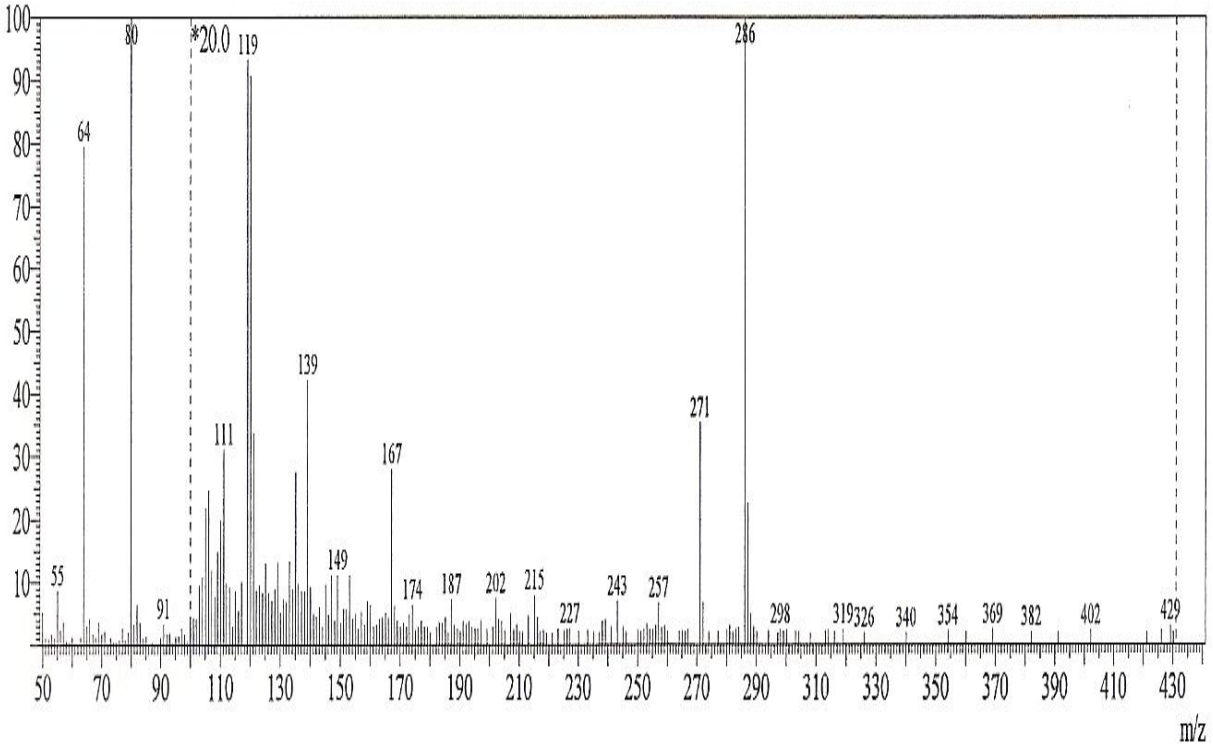

Fig.6.100.MS spectra of synthesis 4-diazo-(p-(5-(p-N,N-dimethyl amino phenyl)-isoxazol-5 -yl)-phenyl)-5,5-dimethyl-cyclohexane-1,3-dione(CV)

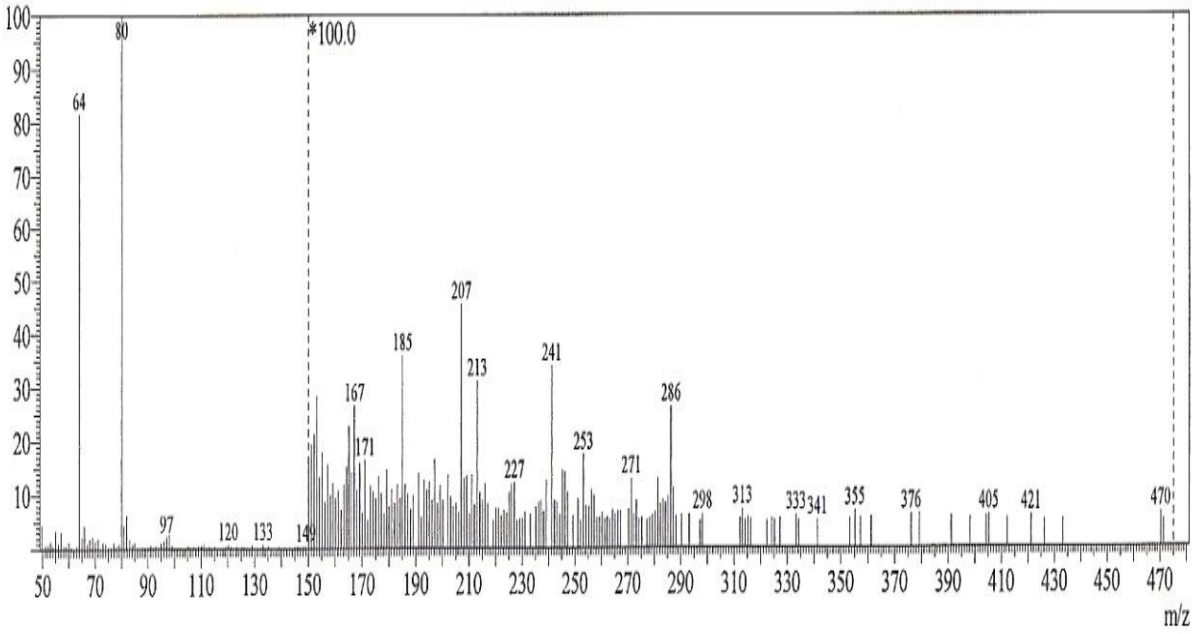

Fig.6.101.MS spectra of synthesis 4-diazo-(p-(5-(p-N,N-dimethyl amino phenyl)-2-thiopyrimidine-6 -yl) -phenyl) -5,5-dimethyl-cyclo hexane -1,3-dione(CVII)

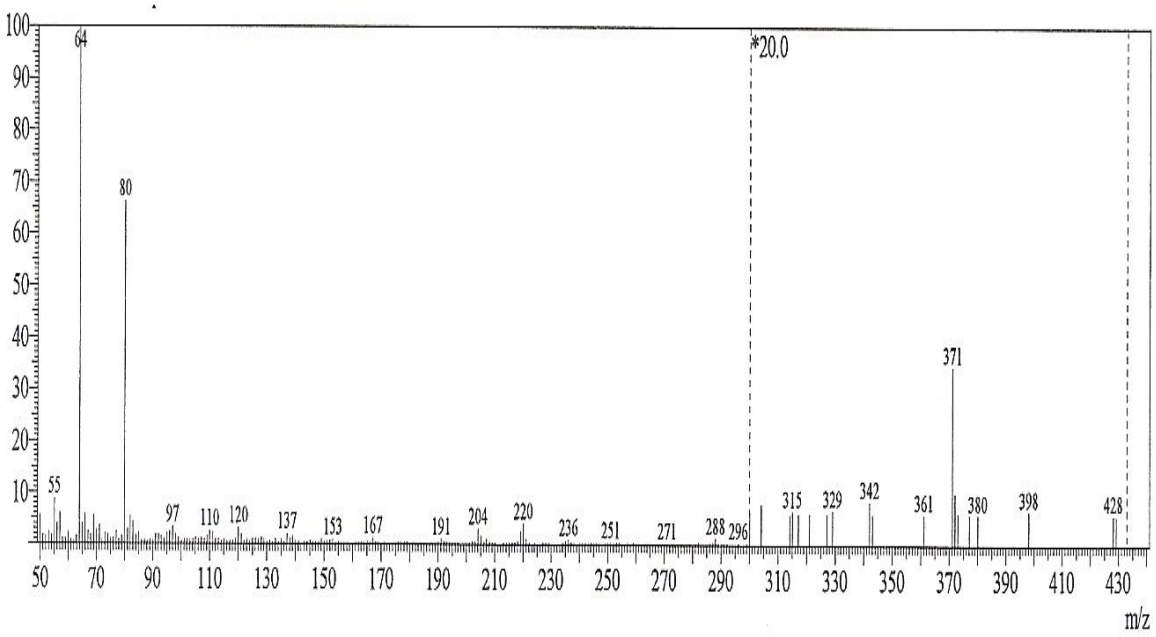

Fig.6.102.MS spectra of synthesis 4-diazo-(p-(5-(2-nitrophenyl)-pyrazol-3-yl)-phenyl)-5,5-dimethyl-cyclohexane-1,3-dione(XCIX)

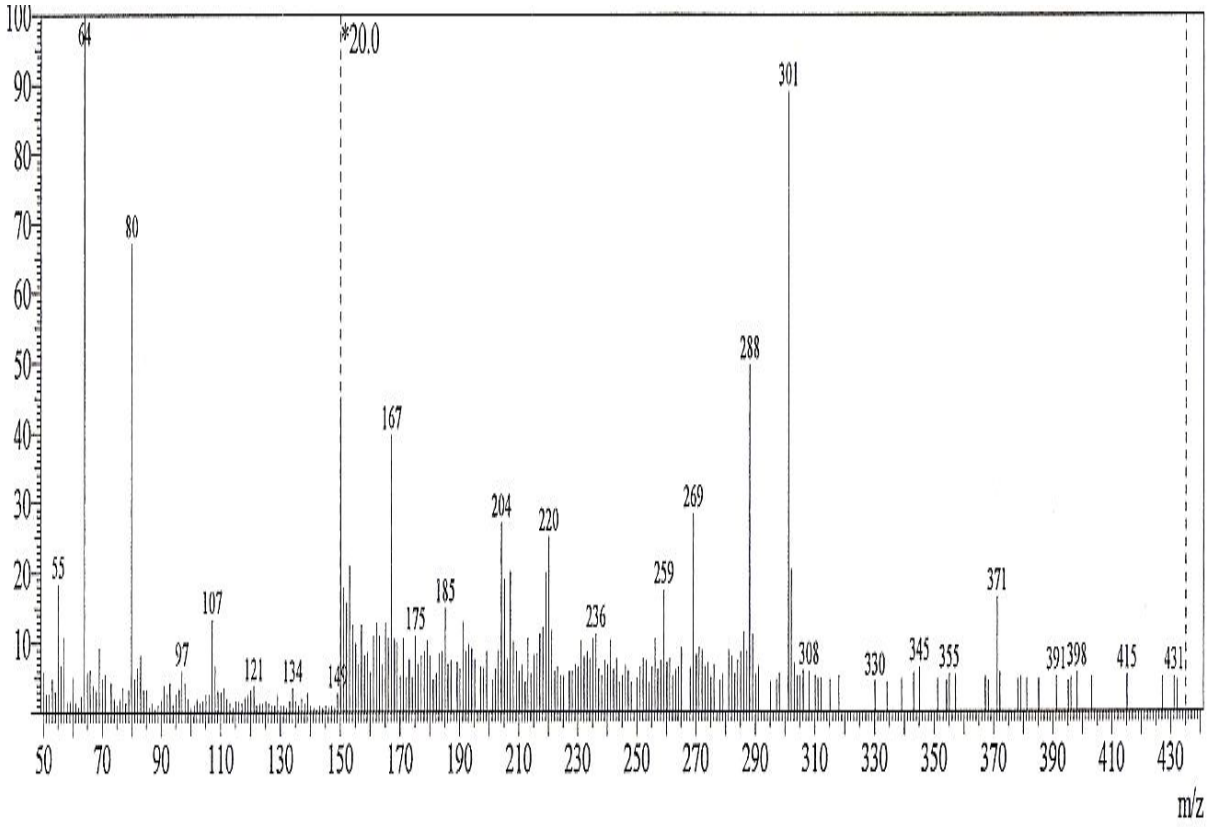

Fig.6.103.MSspectra of synthesis 4-diazo-(p-(5-(2-nitrophenyl)-isoxazol-5 -yl)-phenyl)-5,5-dimethyl-cyclohexane-1,3-dione(CI)

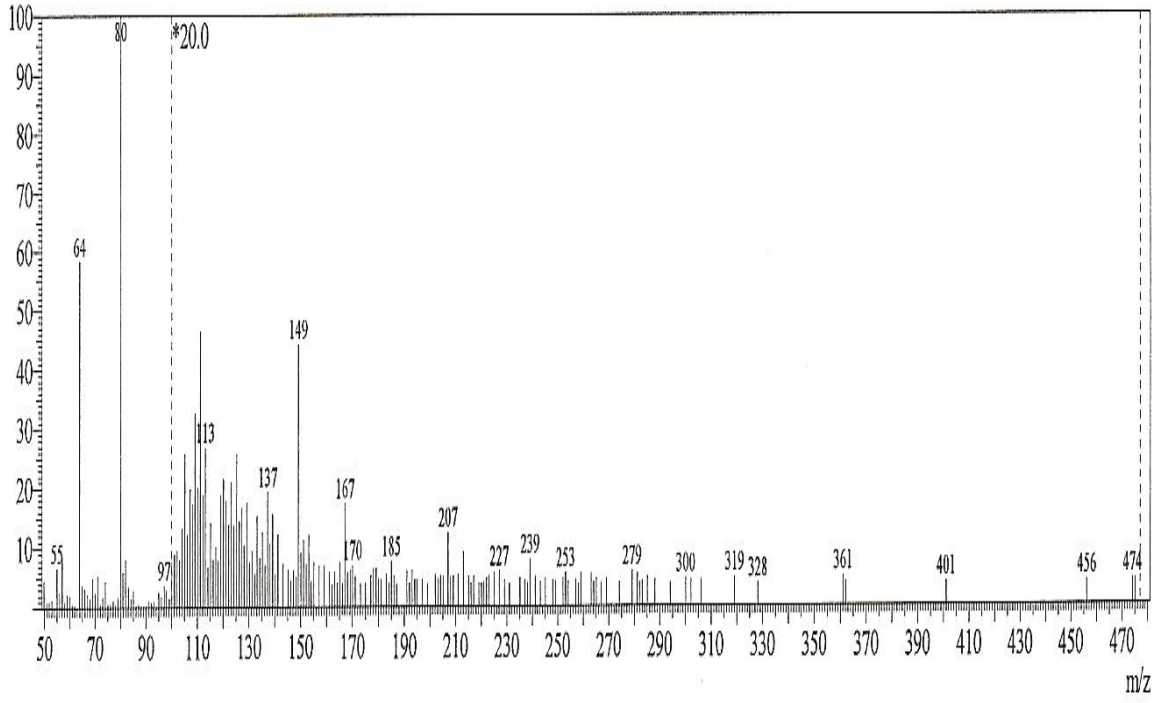

Fig.6.104. MS spectra of synthesis 4-diazo-(p-(5-(2-nitrophenyl)-2thiopyrimidine -6-yl)-phenyl)-5,5-dimethyl-cyclohexane-1,3-dione©

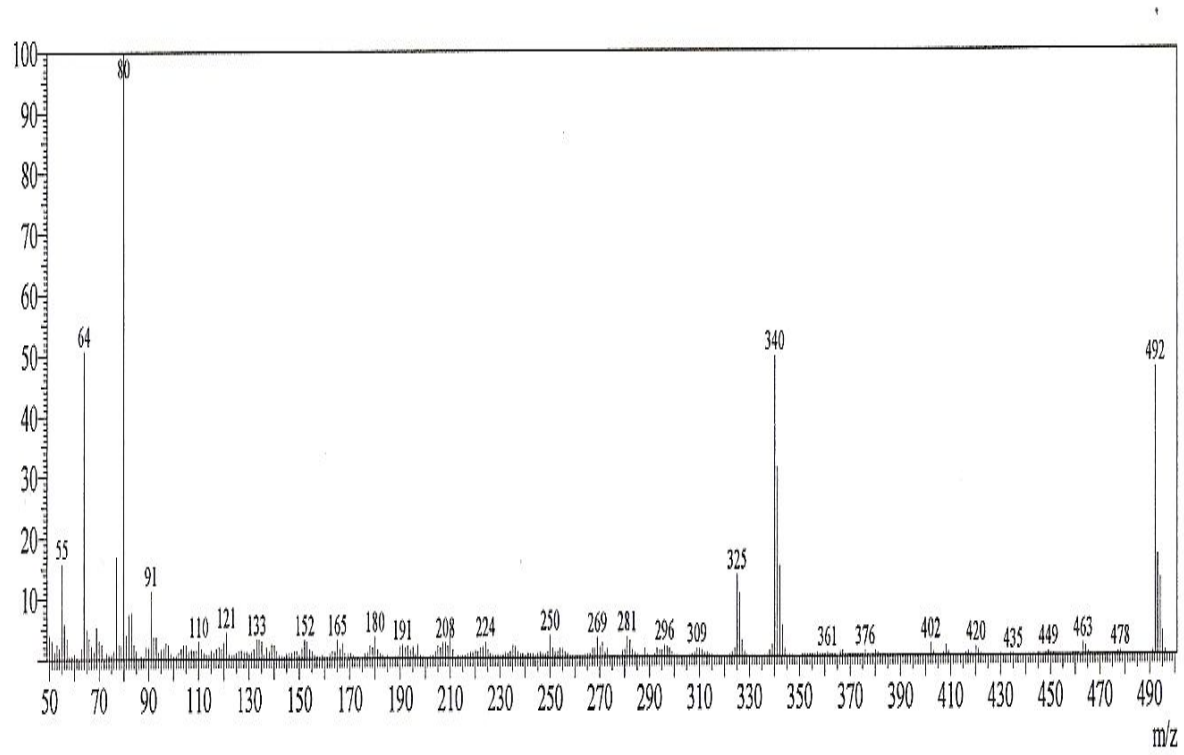

Fig.6.105.MSspectra of synthesis 4-diazo-(p-(5-(4-methoxyphenyl)-pyrazol-3-yl)-phenyl)-5,5-dimethyl-cyclohexane-1,3-dione(XCVII)

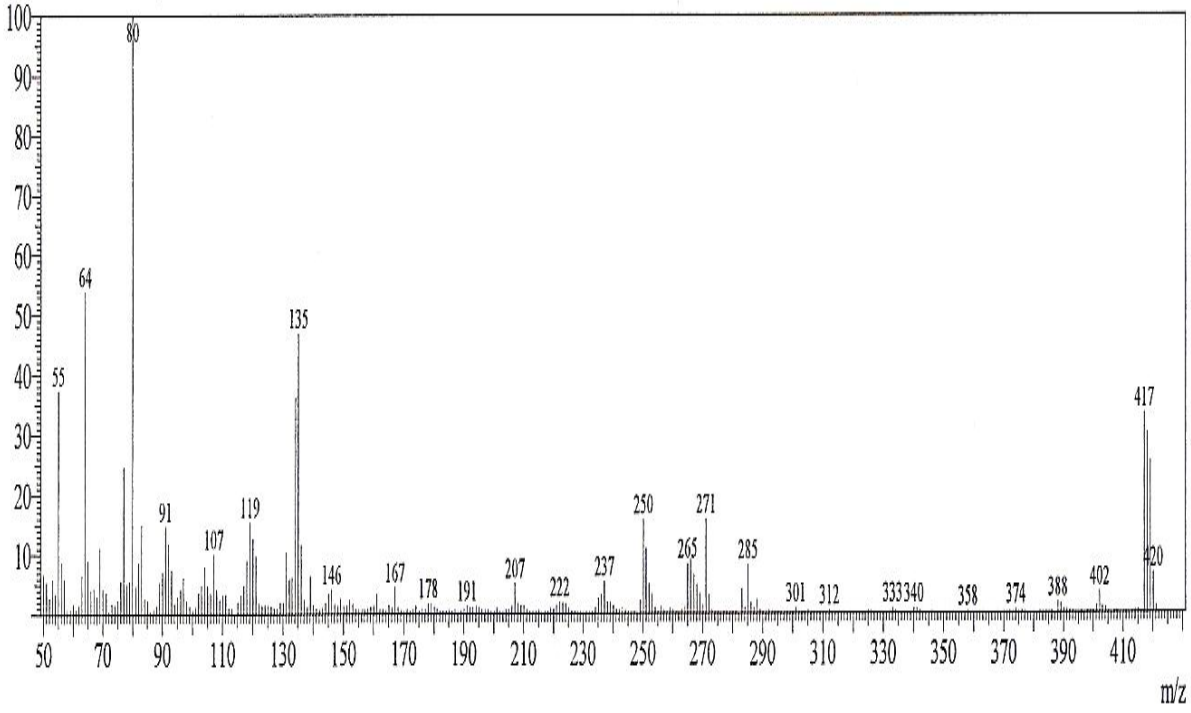

Fig.6.106.MSspectraof of synthesis 4-diazo-(p-(5-(-4-methoxyphenyl)-isoxazol -5-yl)-phenyl)-5,5-dimethyl-cyclohexane-1,3-dione (XCVI)

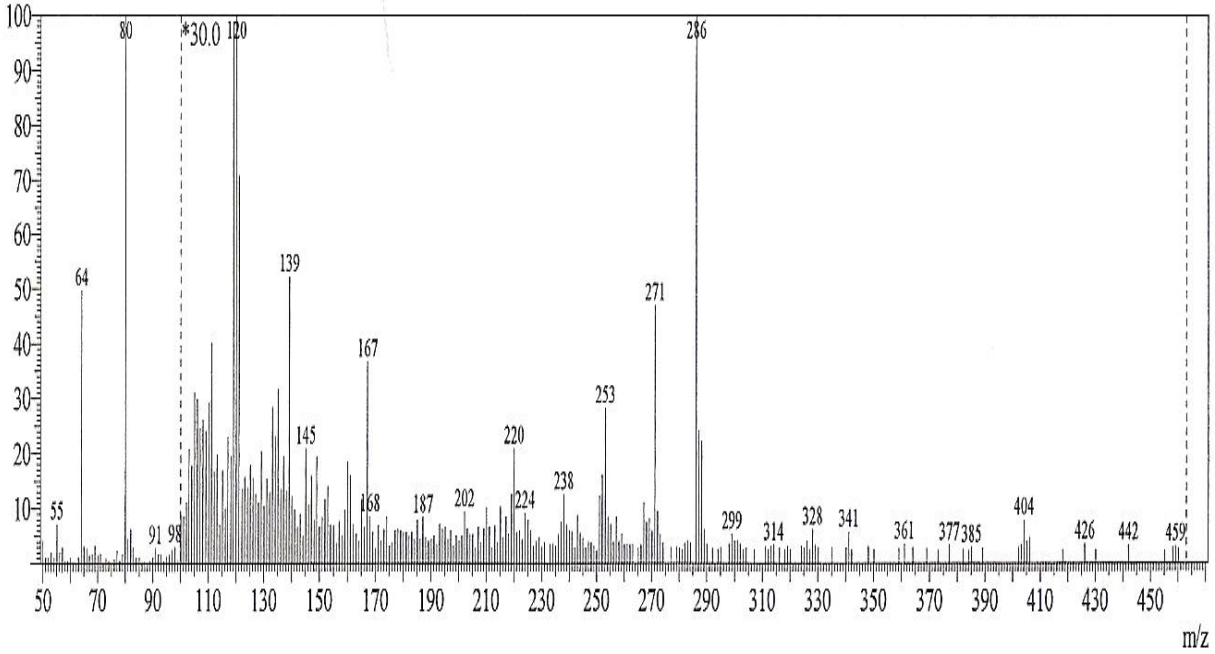

Fig.107.MS of synthesis 4-diazo-(p-(5-(4-methoxyphenyl)-2-thiopyrimidine-6 -yl)-phenyl)-5,5-dimethyl-cyclohexane-1,3-dione (XCVII)

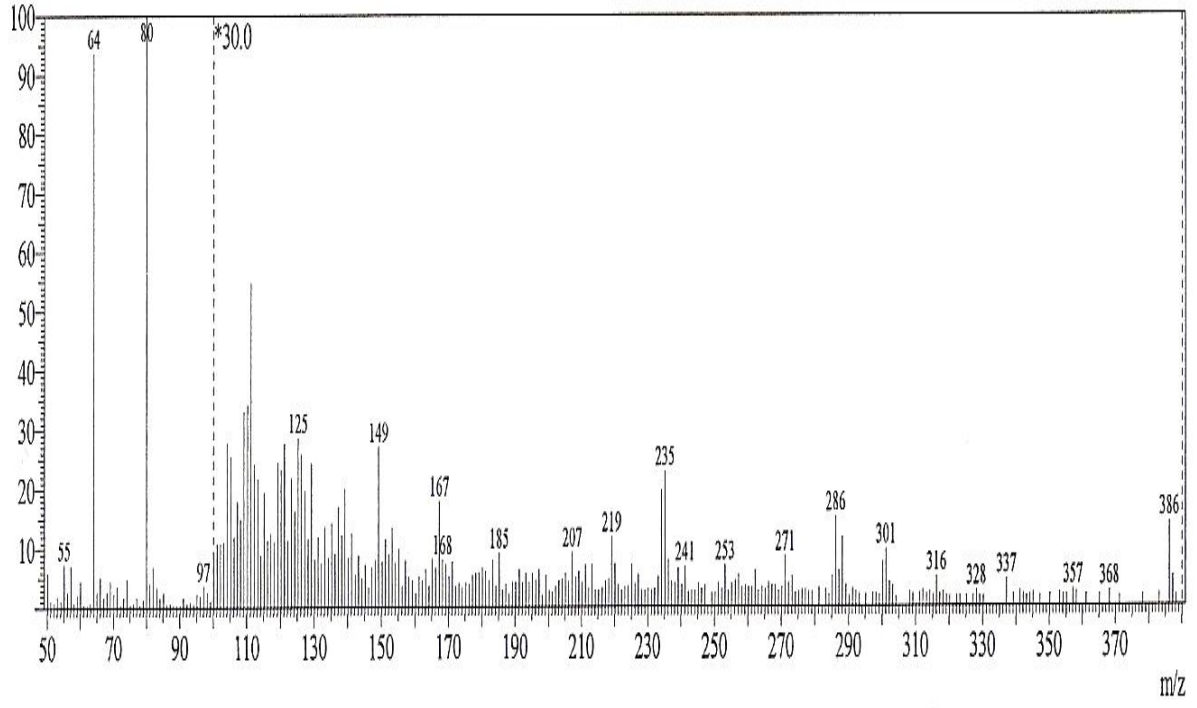

Fig.6.108.MS spectra of synthesis 4-diazo-(p-(5-(furan)-pyrazol-3-yl)-phenyl)-5,5-dimethyl-cyclohexane-1,3-dione(CII)

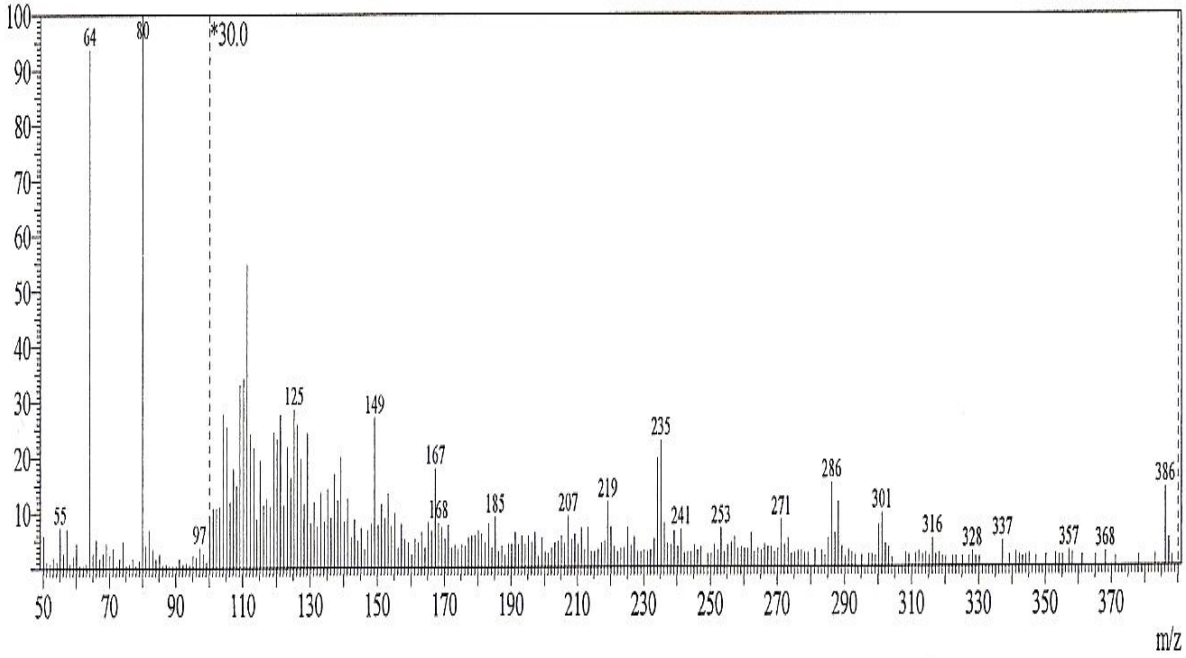

Fig.6.109.MS spectra of synthesis 4-diazo-(p-(5-(furan)-isoxazol -5-yl)-phenyl)-5,5-dimethyl-cyclohexane-1,3-dione(CIV)

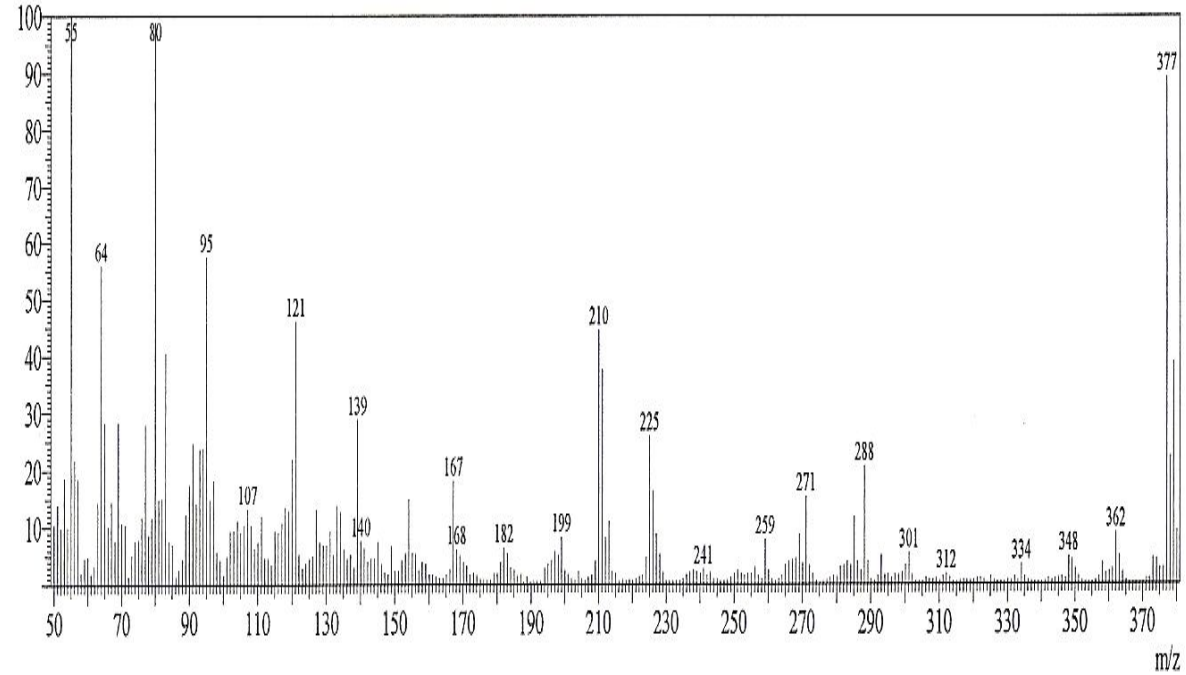

Fig.6.110.MSspectraof synthesis 4-diazo-(p-(5-(furan)-2-thiopyrimidine -6-yl)-phenyl)-5,5-dimethyl-cyclohexane-1,3-dione(CIII)

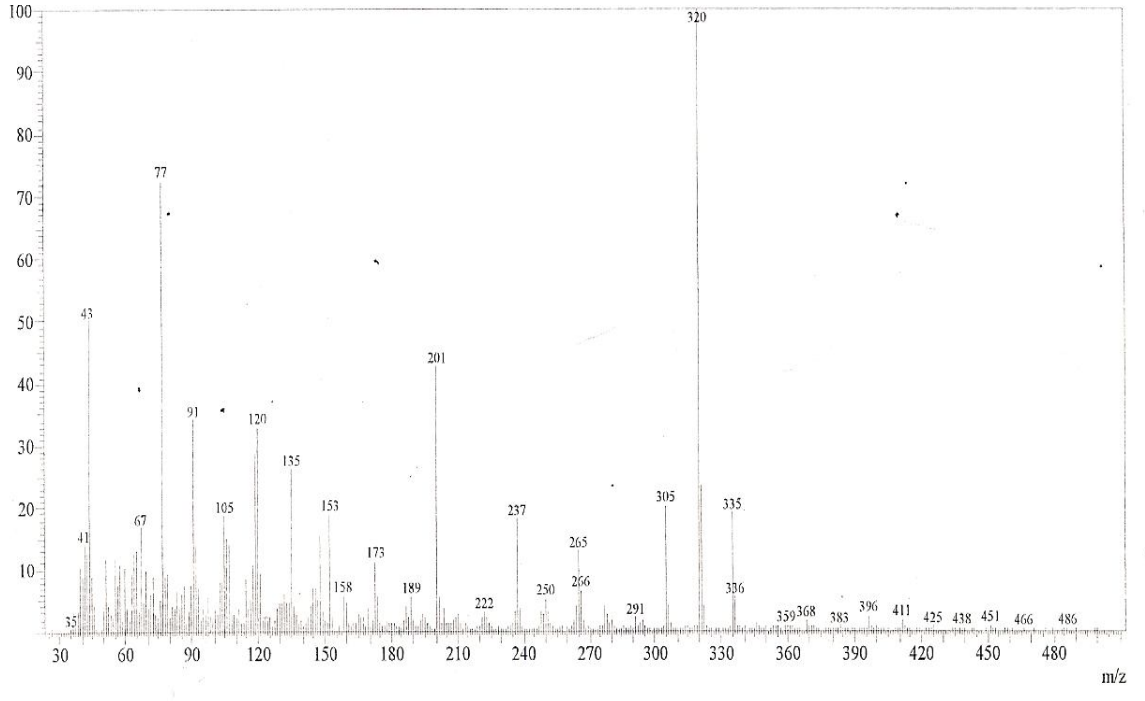

Fig.6.111.MS spectra of synthesis 4-diazo-(p-(5-(p-N,N-dimethyl amino phenyl)-pyrazol-3-yl)-phenyl)-5-methyl-pyrazol-3-one(CVIII)

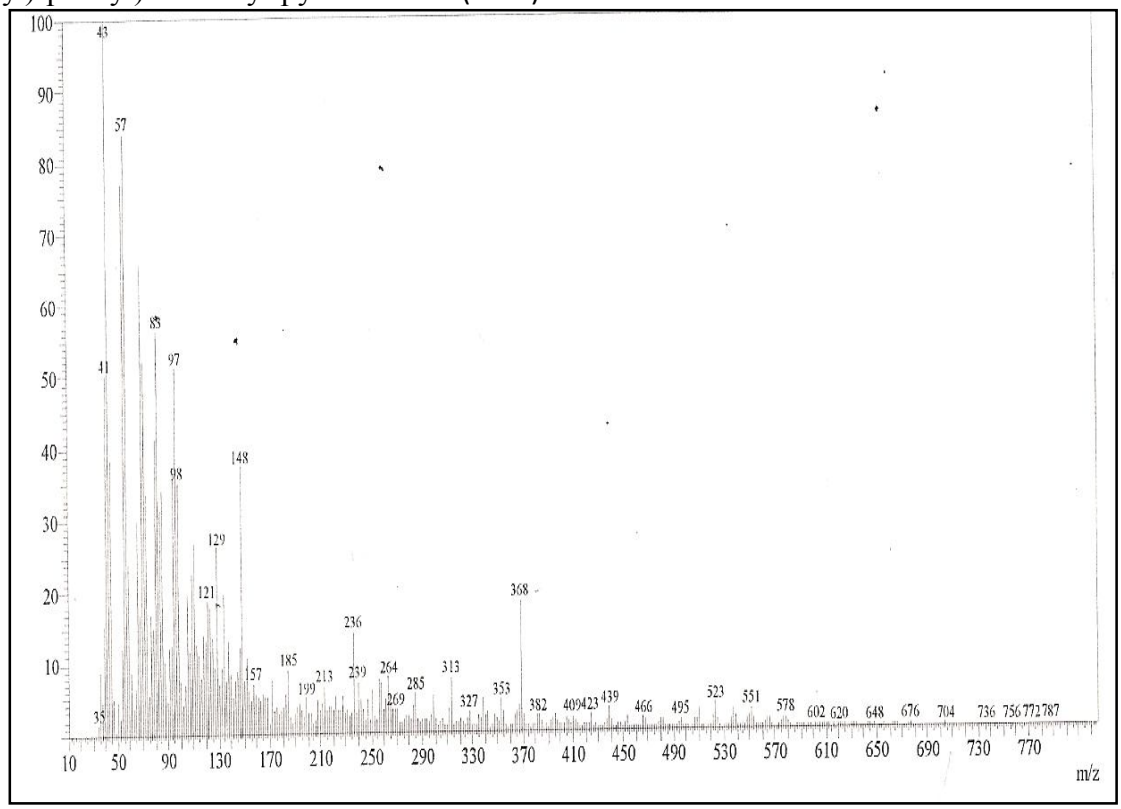

Fig.6.112 .MS spectra of synthesis 4-diazo-(p-(5-(p-N,N-dimethyl amino phenyl)-isoxazol -5-yl)-phenyl)-5-methyl-pyrazol-3-one (CIX)

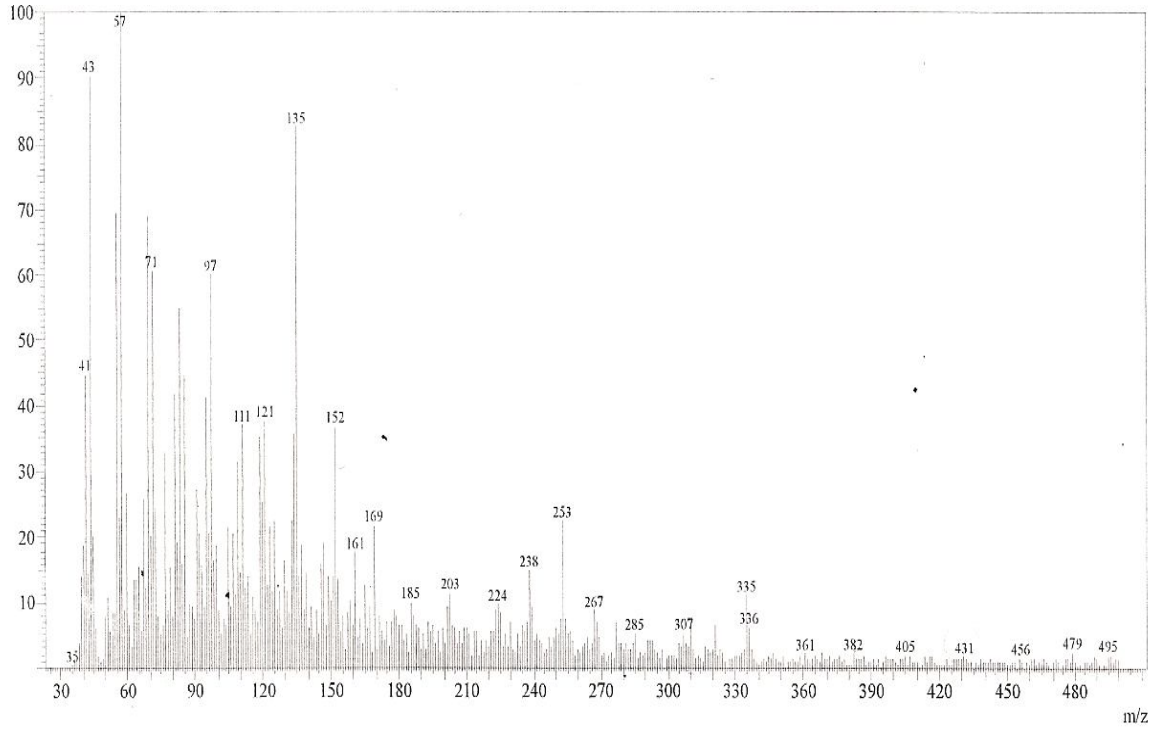

Fig.6.113.MS spectra of synthesis 4-diazo-(p-(5-(p-N,N-dimethyl amino phenyl)-2-thiopyrimidine -6-yl)-phenyl)-5-methyl-pyrazol-3-one(CX)