الآيـــة

قال تعالى:

(قُلْ هَلْ يَسْتَوِي الَّذِينَ يَعْلَمُونَ وَالَّذِينَ لَا يَعْلَمُونَ ۗ إِنَّمَا يَتَذَكَّرُ أُولُو الْأَلْبَابِ)

صدق الله العظيم

سورة الزمر- الآية (9)

Dedication

I dedicated this work to my

Parents,

Brothers and

Sisters.

Acknowledgment

Firstly praise to almighty Allah, who give me strength to complete this work.

Then I wish to express my gratitude and thanks to prof. Dr. Ahmed Elsadig Mohammed Saeed for his guidance, suggestion, encouragement and support to complete this research.

Thanks also to Sudan University of Science and Technology.

Abstract

In this research 40 derivatives of 1,4-dihydropyridine were designed by using ACD Lab and descriptors were calculated. A QSAR equation was obtained from reported biological activities from literature review. The QSAR equation was used to predict the anti-cancer activity of the designed compound, synthesized compounds (XII) and (XX) showed high value in biological activity measure (TGI) 120 and 48 respectivly.

Docking studies of 1,4-dihydropyridine derivatives as anti-cancer agent were performed to study their efficacy against liver cancer, and according to its results, some of 1,4-dihydropyridine derivatives were prepared the prepared compounds were (I,II,III,IV,V,VI,VII and VIII).

The synthesized compounds were characterized there physical property (melting point) the results of melting point were (175-178), (168-170), (148-151), (252-256), (170-174), (152-156), (204-206) and (211-214) respectively. Chromatographic techniques (TLC) used also to characterized synthesized compounds and instrumentally by using IR spectroscopy and UV spectroscopy. In the Docking process the synthesized compounds were placed in appropriate configuration to interact with receptor (4o6w) which affected HepG2 cells causes liver cancer as a result of interaction of the synthesized compounds with receptor compound (XXXV) AND(XXXVIII) shows activity approximately similar as the standard compound doxorubicin 4 interaction for both

المستخلص

في هذا العمل تم عمل تصميم 40 من مشتقات 1,4 ثنائي هيدروبيريدين باستخدام برنامج أي سي دي لاب ,و تم حساب الواصفات.تم الحصول علي معادلة (العلاقات الكمية للبنية الجزيئة بالفاعلية) من النشاطية الحيوية من الدراسات السابقة. معادلة (العلاقات الكمية للبنية الجزيئة بالفاعلية) المشتقة تم إستخدامها لتوقع نشاط مضاد للسرطان للمركبات المصممة, المركبات المحضرة (XII) و(XX) اظهرت قيمة عالية في مقياس النشاط الحيوي 120 و48 TGI علي التوالي.

دراسات الرسو و لبعض مشتقات 1,4 ثنائي هيدروبيريدين كعامل مضاد للسرطان تم التحقق منها لدراسة فاعليتها ضد سرطان الكبد, ووفقا لنتائجها, تم تحضير بعض مشتقات 1,4 ثنائي هيدروبيريدين (I,II,III,IV,V,VI,VII وVIII) .

المركبات المحضرة تم تشخيصها بخواصها الفيزيائية (درجة الانصهار) وكانت النتيجة (-170 174),(170-168),)(151-148),(256-252),(174-170),(156-152),(206-204) و(211-214) علي التوالي. تقنيات الكروماتوغرافيا (كروماتوغرافيا الطبقة الرقيقة) استخدمت ايضا للتعرف علي المركبات تامحضرة و باستخدام الأجهزة, مطياف الاشعة تحت الحمراء و مطياف الاشعة فوق الابنفسجية.

في عملية الرسو المركبات المحضرة تم وضعها في الترتيب الفراغي المناسب للتداخل مع المستقبل (4o6w) الذي يؤثر على خلايا (HepG2) مما يسبب سرطان الكبد , نتيجة لتداخلات المركبات المحضرة مع المركب المستقبل (XXXV) و(XXXVIII) اظهرت نشاطية قريبة للمركب القياسي دوكسوروبيسين 4 تداخلات لكليهما.

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