ملخص باللغة الإنجليزيه
عن الرسالة المقدمة من محمد إبراهيم عبداللطيف حامد

للحصول على درجة الدكتوراه الفلسفة في العلوم الصيدلية (الكيمياءالصيدلية)

وعنوانها

"تشييد والنمذجة الجزيئية لمركبات بنزوبيرونيه وفيوروبنزوبيرونيه ذات فاعلية بيولوجية"

"Synthesis and Molecular Modeling of Benzopyrone and Furobenzopyrone Derivatives with Biological Activity"

The search for new anticonvulsant compounds with potent activity and less toxicity continue to be an area of investigation in medicinal chemistry.

In this study, nine new intermediates and thirty-two target benzopyrone and furobenzopyrone derivativeswere synthesizedin four sets. All the newly target synthesized compounds were subjected to anticonvulsant screening.

This thesis consists of the following parts:

1. Introduction

This section includes a brief literature review on epilepsy and their types. In addition, the different classes of clinically used and other reported antiepileptic agents regarding their mechanism of action were described. Moreover, a literature survey on the different biological activities and methods of synthesis of benzopyrone and furobenzopyroneanalogues were also cited.

2.Aim of the work

This part describes the rationale upon which the newly synthesized compounds were designed to develop new anticonvulsant agents with higher potency and fewer side effects.

3.Theoretical discussion

It deals with the discussion of the experimental methods adopted for the synthesis of designed compounds and the confirmation of their structures by different chemical and spectral analysis.

4.Experimental

This section describes the practical procedures used for the synthesis of the known compounds, new intermediates and new target compounds with their elemental analysis and spectral data (^{1}H-NMR, IR and MS) were described.

5. Biological evaluation

The above mentioned newly synthesized compounds were tested for their anticonvulsant activity using the maximal electroshock (MES) and subcutaneous pentylenetetrazole (*sc*PTZ) screens. Quantitative and neurotoxicity screening have been carried to determine the median effective dose (ED_{50}), median lethal dose (LD_{50}) and protective index (PI)for the active anticonvulsant compounds.

6. Molecular modeling

In this section, molecular modeling simulation studies were conducted by the generation of a validated 3D QSAR pharmacophore model using Discovery Studio 2.5 software, in order to rationalize the relation between the structural features and anticonvulsant activity for the newly significant active compounds.

7.References

This section contains 229 references from 1883 to 2015.