Document details

Journal of Molecular Structure
Volume 1130, 15 February 2017, Pages 711-718

QSAR modeling for anti-human African trypanosomiasis activity of substituted 2-Phenylimidazopyridines (Article)

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Abstract

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In the present work, sixty substituted 2-Phenylimidazopyridines previously reported with potent anti-human African trypanosomiasis (HAT) activity were selected to build genetic algorithm (GA) based QSAR models to determine the structural features that have significant correlation with the activity. Multiple QSAR models were built using easily interpretable descriptors that are directly associated with the presence or the absence of a structural scaffold, or a specific atom. All the QSAR models have been thoroughly validated according to the OECD principles. All the QSAR models are statistically very robust (R^2 = 0.80–0.87) with high external predictive ability (CCC_{ex} = 0.81–0.92). The QSAR analysis reveals that the HAT activity has good correlation with the presence of five membered rings in the molecule.

SciVal Topic Prominence

Topic: Quantitative Structure-Activity Relationship | Models | quantitative structure-property

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Author keywords

Anti-HAT activity | QSAR | Substituted 2-Phenylimidazopyridines

Indexed keywords

Engineering controlled terms: Genetic algorithms | Molecular graphics | Scaffolds

Engineering uncontrolled terms: Descriptors | Five-membered rings | Good correlations | Predictive abilities | QSAR | QSAR analysis | Structural feature | Substituted 2-Phenylimidazopyridines

Engineering main heading:

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Funding details

Funding sponsor	Funding number	Acronym
Deanship of Scientific Research, King Saud University		

Funding text
The authors would like to extend their sincere appreciation to the Deanship of Scientific Research at King Saud University for its funding this Research (Group No. RG-1435-083). One of the authors VHM is thankful to Dr. Paola Gramatica for providing these software QSARINS-Chem 2.2.1. Appendix A

ISSN: 00222860
CODEN: JMOSB
Source Type: Journal
Original language: English
DOI: 10.1016/j.molstruc.2016.11.012
Document Type: Article
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