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

Masand, V.H.^a, El-Sayed, N.N.E.^{b,f}, Mahajan, D.T.^a, Mercader, A.G.^c, Alafeefy, A.M.^d, Shibi, I.G.^e

^aDepartment of Chemistry, Vidya Bharati College, Camp, Amravati, Maharashtra 444 602, India
^bDepartment of Chemistry, College of Science, "Girls Section", King Saud University, P.O. Box 2457, Riyadh, 11451, Saudi Arabia
^cInstituto de Investigaciones Fisicoquímicas Teóricas y Aplicadas (INIFTA), UNLP, CCT La Plata-CONICET, Diag. 113 y 64, Sucursal 4, C.C. 16, La Plata, 1900, Argentina

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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 ($R^2 = 0.80\text{--}0.87$) with high external predictive ability ($CCC_{ex} = 0.81\text{--}0.92$). The QSAR analysis reveals that the HAT activity has good correlation with the presence of five membered rings in the molecule.
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SciVal Topic Prominence

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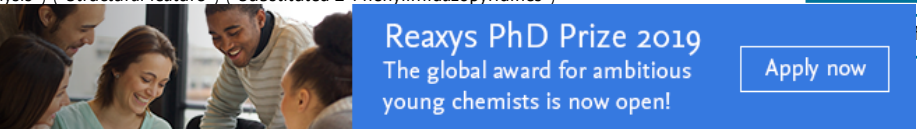
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Muthukumaran, P. , Rajiniraja, M.
(2019) *Journal of Theoretical Biology*
QSAR study of anti-Human African Trypanosomiasis activity for 2-phenylimidazopyridines derivatives using DFT and Lipinski's descriptors
Chtita, S. , Ghamali, M. , Ousaa, A.
(2019) *Heliyon*
Multiple quantitative structure-activity relationships (QSARs) analysis for orally active trypanocidal N-myristoyltransferase inhibitors
Masand, V.H. , El-Sayed, N.N.E. , Bambole, M.U.
(2019) *Journal of Molecular Structure*
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- ☐ 1 Brun, R., Blum, J., Chappuis, F., Burri, C.
Human African trypanosomiasis
(2010) *The Lancet*, 375 (9709), pp. 148-159. Cited 493 times.
doi: 10.1016/S0140-6736(09)60829-1
[View at Publisher](#)
- ☐ 2 Brun, R., Don, R., Jacobs, R.T., Wang, M.Z., Barrett, M.P.
Development of novel drugs for human African trypanosomiasis
(2011) *Future Microbiology*, 6 (6), pp. 677-691. Cited 93 times.
doi: 10.2217/fmb.11.44
[View at Publisher](#)
- ☐ 3 Kennedy, P.G.E.
Clinical features, diagnosis, and treatment of human African trypanosomiasis (sleeping sickness)
(2013) *The Lancet Neurology*, 12 (2), pp. 186-194. Cited 155 times.
doi: 10.1016/S1474-4422(12)70296-X
[View at Publisher](#)
- ☐ 4 Bukhari, S.N.A., Zhang, X., Jantan, I., Zhu, H.-L., Amjad, M.W., Masand, V.H.
Synthesis, molecular modeling, and biological evaluation of novel 1, 3-diphenyl-2-propen-1-one based pyrazolines as anti-inflammatory agents
(2015) *Chemical Biology and Drug Design*, 85 (6), pp. 729-742. Cited 18 times.
<http://www.wiley.com.ezproxy.um.edu.my/bw/journal.asp?ref=1747-0277>
doi: 10.1111/cbdd.12457
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Masand, V.H. , Mahajan, D.T. , Maldhure, A.K.
(2016) *Medicinal Chemistry Research*

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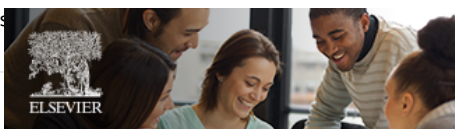
Masand, V.H. , Mahajan, D.T. , Nazeruddin, G.M.
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