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**QSAR modeling for anti-human African trypanosomiasis activity of substituted 2-Phenylimidazopyridines**

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[View Journal Impact](#)**Abstract**

In the present work, sixty substituted 2-Phenylimidazopyridines previously reported with potent antihuman 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 ( $CC_{\text{ext}} = 0.81-0.92$ ). The QSAR analysis reveals that the HAT activity has good correlation with the presence of five membered rings in the molecule. (C) 2016 Elsevier B.V. All rights reserved.

**Keywords**

**Author Keywords:** Anti-HAT activity; QSAR; Substituted 2-Phenylimidazopyridines

**KeyWords Plus:** DIFFERENT VALIDATION CRITERIA; REAL EXTERNAL PREDICTIVITY; ANTIMALARIAL ACTIVITY; SYNTHETIC PRODIGININES; TAUTOMERISM; POLYPHENOLS; INHIBITORS; QSAR/QSPR; ANALOGS

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