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AntiMalarial Mode of Action (AMMA) Database: Data Selection, Verification and Chemical Space Analysis

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Abstract

© 2018 Wiley-VCH Verlag GmbH & Co. KGaA, Weinheim This paper presents the effort of collecting and curating a data set of 15461 molecules tested against the malaria parasite, with robust activity and mode of action annotations. The set is compiled from in-house experimental data and the public ChEMBL database subsets. We illustrate the usefulness of the dataset by building QSAR models for antimalarial activity and QSPR models for modes of actions, as well as by the analysis of the chemical space with the Generative Topographic Mapping method. The GTM models perform well in prediction of both activity and mode of actions, on par with the classical SVM methods. The visualization of obtained maps helps to understand the distribution of molecules corresponding to different modes of action: molecules with similar targets are located close to each other on the map. Therefore, this analysis may suggest new modes of action for non-annotated or even annotated compounds. In perspective, this can be used as a tool for prediction of both antimalarial activity and target for novel, untested compounds.

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Keywords

Antimalarial compounds, Chemical Space analysis, Generative Topographic Maps, Structure-Property Relationships

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