

anti-Nipah: A QSAR based prediction method to identify the inhibitors against Nipah virus

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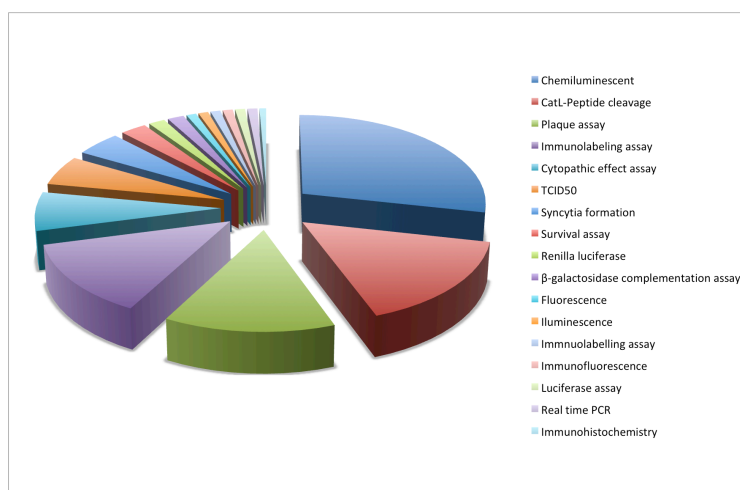
[#] Equal contributions

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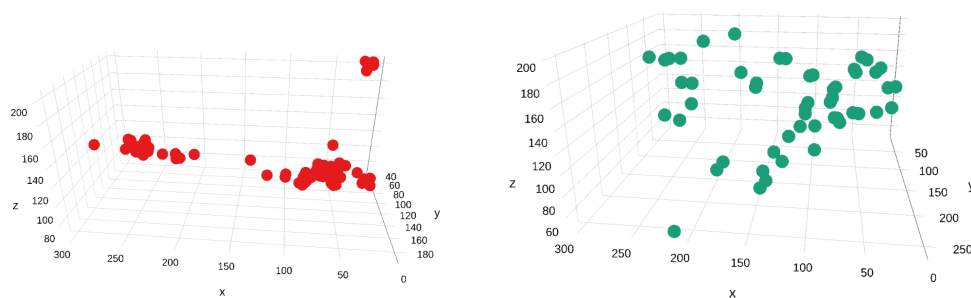
Supplementary Figure S1. Frequency distribution of assays used to check the inhibition of anti-Nipah compounds

Supplementary Figure S2. The principal component of the antiviral and non-antiviral compounds or drugs against NiV. The red spheres (left) represent active compounds and green spheres (right) represent non-active compounds against NiV

Supplementary Table S1. Details of the most relevant descriptors extracted from mRMR feature selection algorithm and used for prediction model development



Supplementary Figure S1. Frequency distribution of assays used to check the inhibition of anti-Nipah compounds



Supplementary Figure S2. The principal component of the antiviral and non-antiviral compounds or drugs against NiV. The red spheres (left) represent active compounds and green spheres (right) represent non-active compounds against NiV.

Supplementary Table S1. Details of the most relevant descriptors extracted from mRMR feature selection algorithm and used for prediction model development

Descriptor Name	Type	Description
FP502	CDK fingerprint	Fingerprint of length 1024 and search depth of 8
FP169	CDK fingerprint	Fingerprint of length 1024 and search depth of 8
KRFP4293	Klekota-Roth fingerprint	Presence of chemical substructures
FP265	CDK fingerprint	Fingerprint of length 1024 and search depth of 8
FP644	CDK fingerprint	Fingerprint of length 1024 and search depth of 8
GATS5e	CDK graph only fingerprint	Specialized version of the Fingerprinter which does not take bond orders into account
GraphFP87	CDK graph only fingerprint Specialized version of the Fingerprinter which does not take bond orders into account	Specialized version of the Fingerprinter which does not take bond orders into account
FP731	CDK fingerprint	Fingerprint of length 1024 and search depth of 8
nsssN	2D	Atom type electrotopological state
ExtFP308	CDK extended fingerprint	Extends the Fingerprinter with additional bits describing ring features
FP490	CDK fingerprint	Fingerprint of length 1024 and search depth of 8
ExtFP857	CDK extended fingerprint	Extends the Fingerprinter with additional bits describing ring features
FP626	CDK fingerprint	Fingerprint of length 1024 and search depth of 8
GraphFP101	CDK graph only fingerprint Specialized version of the Fingerprinter which does not take bond orders into account	Specialized version of the Fingerprinter which does not take bond orders into account

FP541	CDK fingerprint	Fingerprint of length 1024 and search depth of 8
PubchemFP824	Pubchem fingerprint	Pubchem fingerprint
FP551	CDK fingerprint	Fingerprint of length 1024 and search depth of 8
GraphFP980	CDK graph only fingerprint Specialized version of the Fingerprinter which does not take bond orders into account	Specialized version of the Fingerprinter which does not take bond orders into account
ExtFP666	CDK extended fingerprint	Extends the Fingerprinter with additional bits describing ring features
FP172	CDK fingerprint	Fingerprint of length 1024 and search depth of 8