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Supplementary Materials

Indian Medicinal Plant-Derived Phytochemicals as Potential Antidotes for Snakebite: A Pharmacoinformatic Study of Atrolysin Inhibitors

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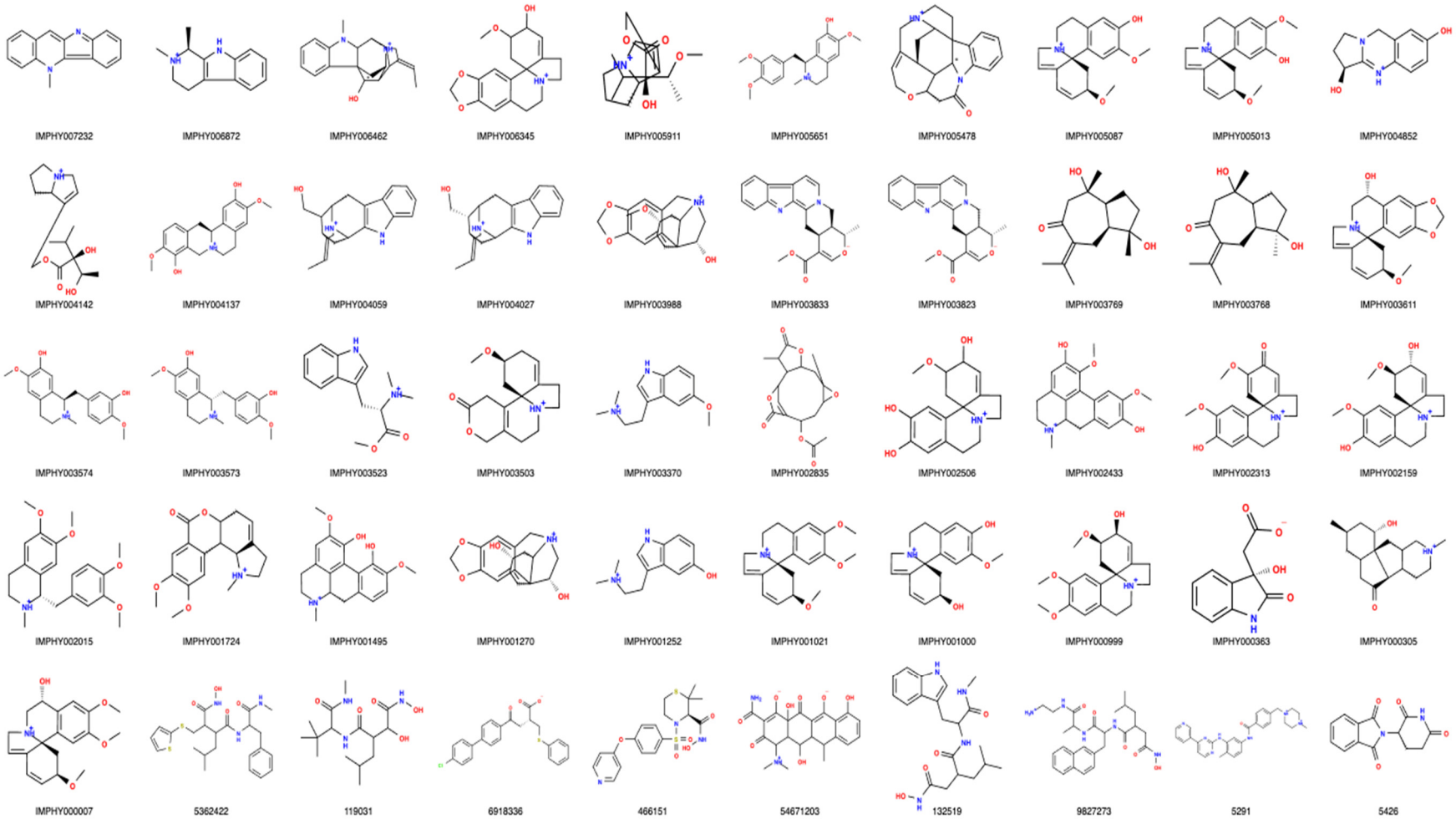
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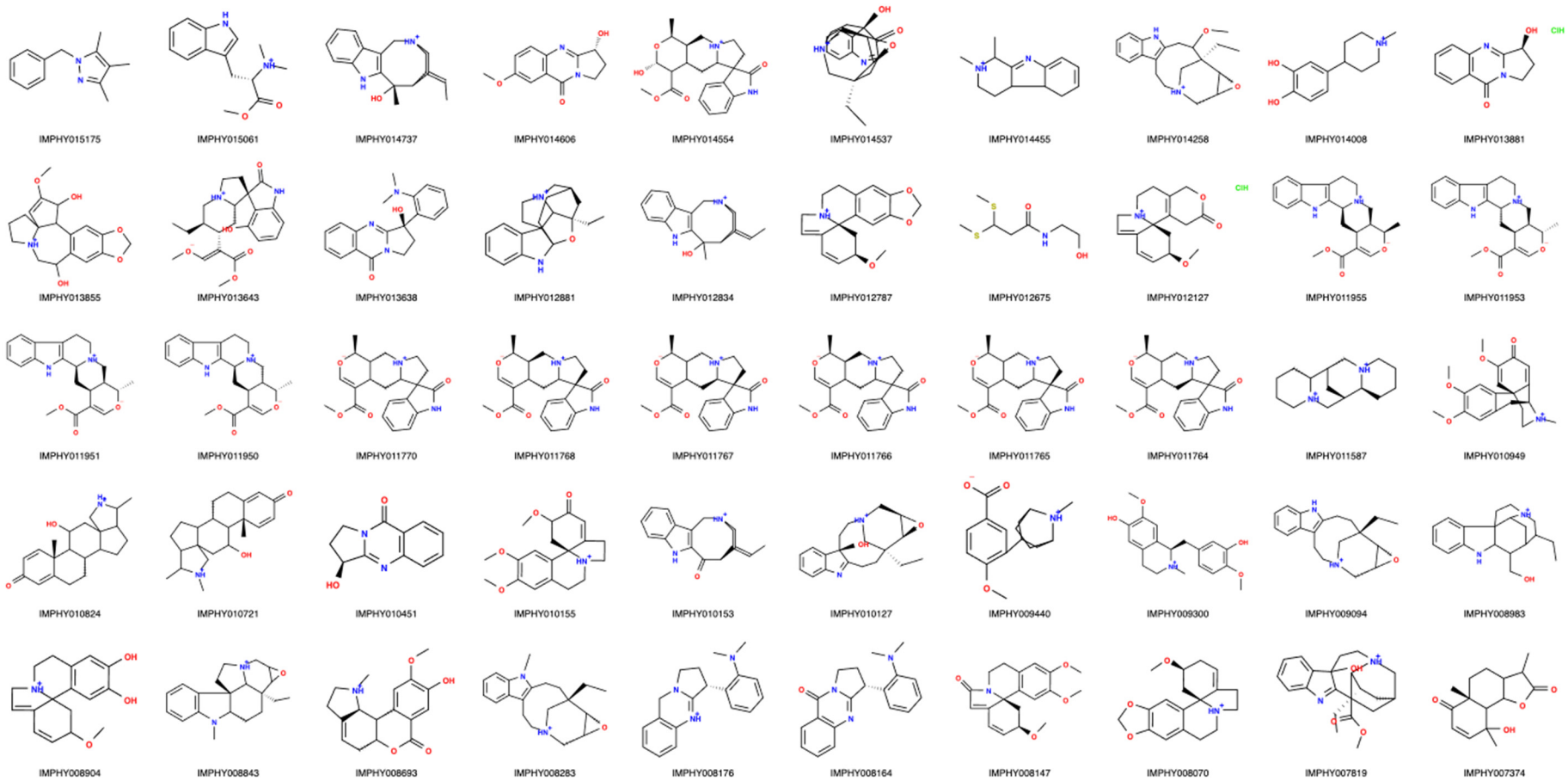
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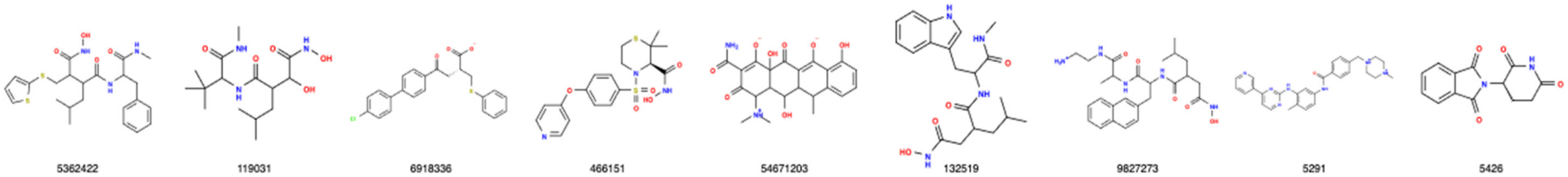
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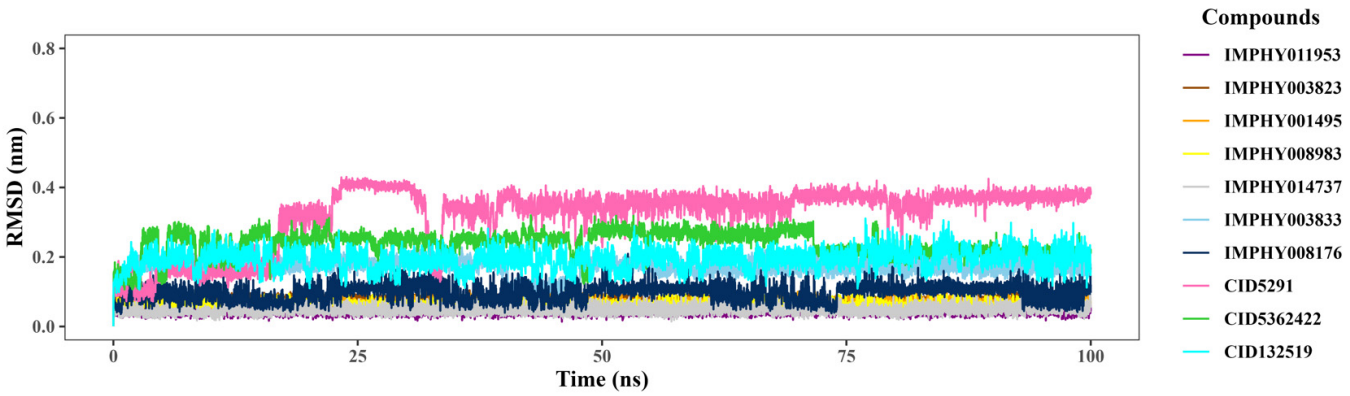

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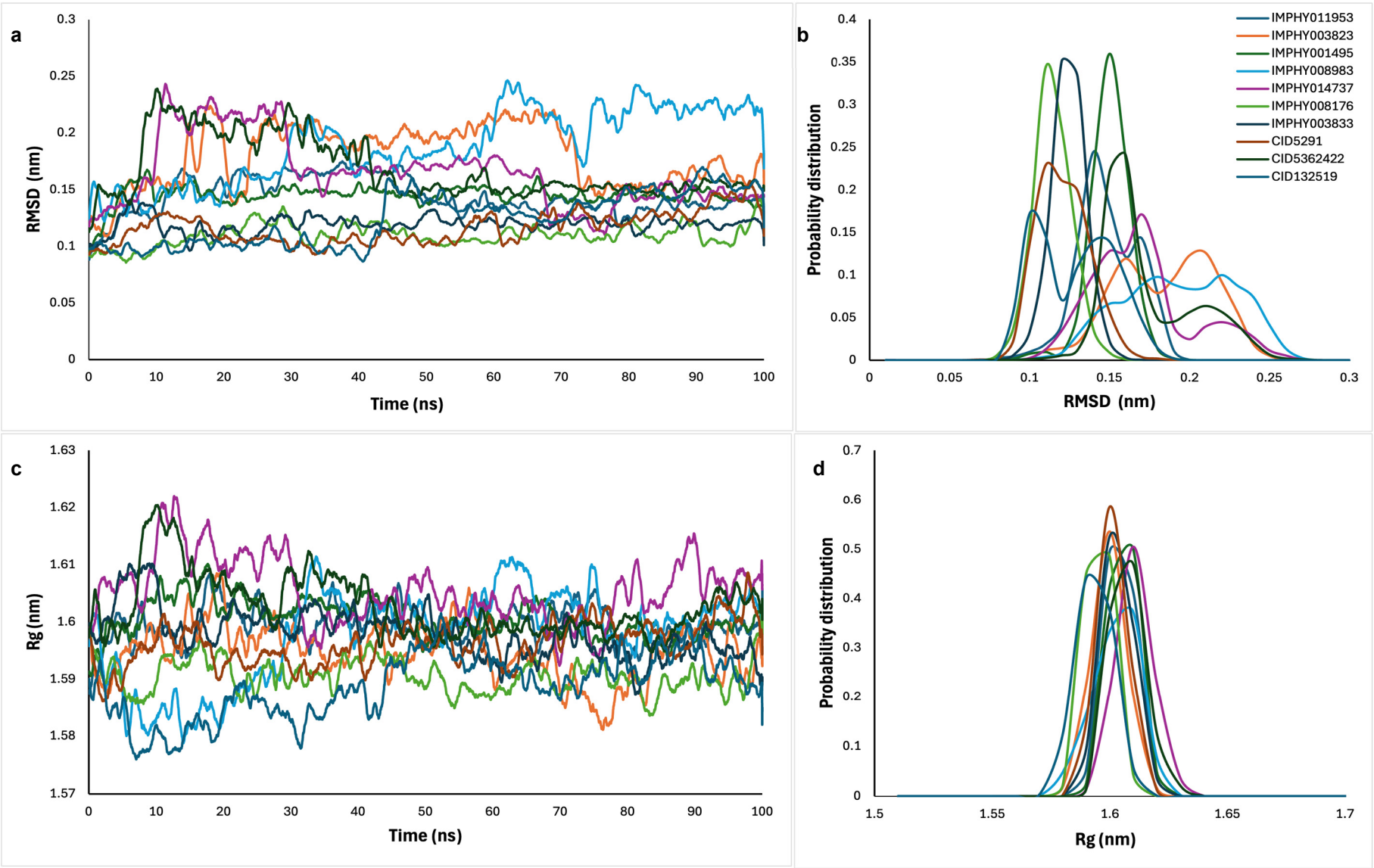
Supplementary .Fig. S1 (cont.)



Supplementary Figure S1. The chemical structure of the selected compound.



Supplementary Figure S2. Ligand RMSD of the compound was recorded for 100ns.


a
RMSD (nm)
Time (ns)
b
Probability distribution
RMSD (nm)
IMPHY011953
IMPHY003823
IMPHY001495
IMPHY008983
IMPHY014737
IMPHY008176
IMPHY003833
CID5291
CID5362422
CID132519
c
Rg (nm)
Time (ns)
d
Probability distribution
Rg (nm)

Supplementary Figure S3. (a) Root Mean Square Deviation (RMSD) moving average for the complexes over 100 ns, (b) RMSD distribution plot for the complexes over 100 ns (c) Radius of Gyration moving average for the complexes over 100 ns , and (d) Radius of Gyration distribution plot for the complexes over 100 ns.