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Supplementary material to:

COMPUTATIONAL MODELING AND VALIDATION STUDIES OF 3-D STRUCTURE OF NEURAMINIDASE PROTEIN OF H1N1 INFLUENZA A VIRUS AND SUBSEQUENT IN SILICO ELUCIDATION OF PICEID ANALOGUES AS ITS POTENT INHIBITORS

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"Drug like" properties according to Lipinski's Rule of the two novel compounds screened from docking experiments

Compound (ChemBank ID)	nViol	LogP*	MW	nHbA	nHbD	nRb
2110359	1	1.109	390.384	8	6	**5**
3075417	**1**	**1.093**	**420.409**	**9**	**6**	**6**

The molecular properties of novel compounds were calculated from ChemBank database.

nViol – Number of Violations
LogP* – LogP by Ghose Crippen
MW – Molecular weight
nHbA – Number of Hydrogen bond Acceptors
nHbD – Number of Hydrogen bond Donors
nRb – Number of Rotatable bonds