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 AcceptorsnHbD – Number of Hydrogen bond Donors

nRb - Number of Rotatable bonds