

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**

Chhedi Lal Gupta^a, Salman Akhtar^b, Preeti Bajpai^b, K. N. Kandpal^a, G. S. Desai^c,
Ashok K. Tiwari^{a*}

“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