Electronic Supplementary Material (ESI) for Molecular Systems Design & Engineering.

Designing Novel Inhibitors Derivatives Targeting SARS-CoV-2 M^{pro} Enzyme: A Deep Learning and Structure Biology Approach

Tushar Joshi[#a], Shalini Mathpal[#a], Priyanka Sharma[b], Akshay Abraham[c], Rajadurai Vijay Solomon*[c], Subhash Chandra*[d]

[a]Department of Biotechnology, Bhimtal Campus, Bhimtal 263136, Kumaun University, Uttarakhand, India
[b]Department of Botany, Kumaun University, DSB Campus, Nainital 263001, Uttarakhand, India
[c]Department of Chemistry, Madras Christian College (Autonomous), [Affiliated to University of Madras], Tambaram East, Chennai 600 059, Tamil Nadu, India
[d]Computational Biology & Biotechnology Laboratory, Department of Botany, SSJ University, Almora 263601, Uttarakhand, India

[#] Tushar Joshi and Shalini Mathpal contributed equally to this work.

Corresponding authors*:

1- Subhash Chandra*

Mailing address: Computational Biology & Biotechnology Laboratory, Department of Botany, Soban Singh University, Almora 263601, Uttarakhand, India

E-mail: scjnu@yahoo.co.in

2- Rajadurai Vijay Solomon*

Department of Chemistry, Madras Christian College (Autonomous), [Affiliated to University of Madras], Tambaram East, Chennai 600 059, Tamil Nadu, India

Email: vjsolo@gmail.com

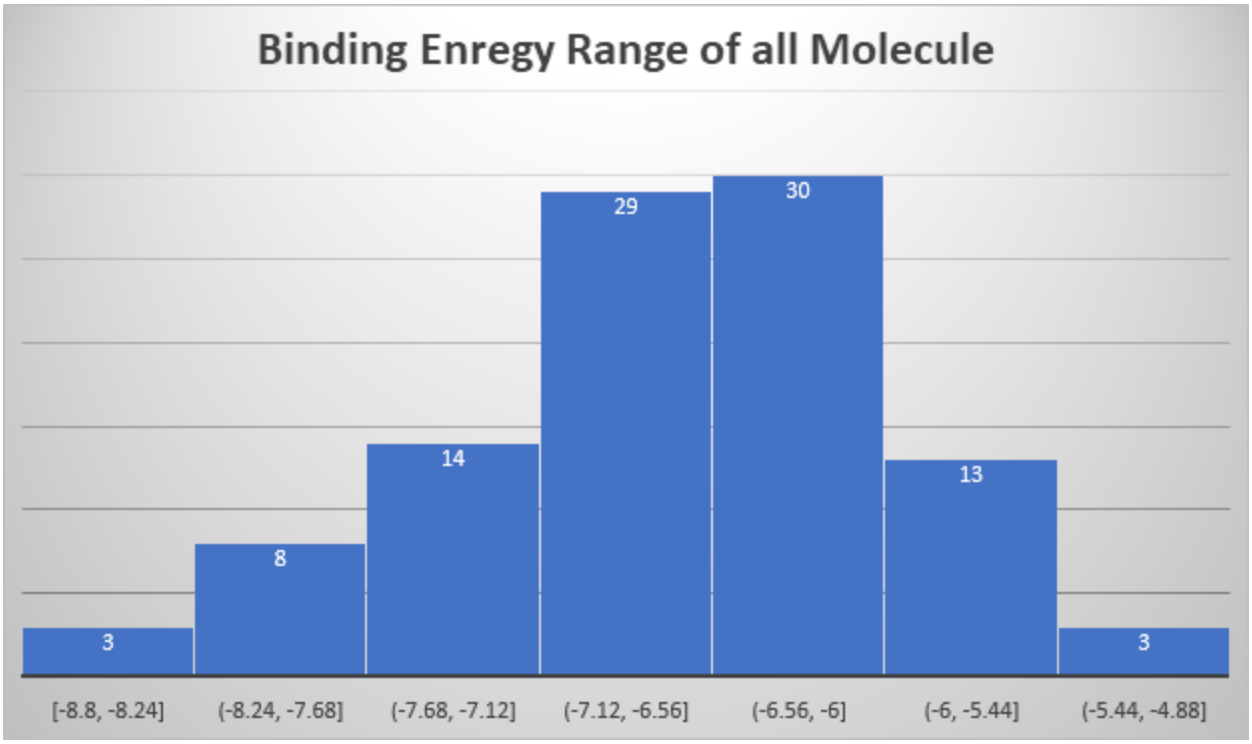

Figure S1: Binding energy range of all designed molecules after Molecular Docking study

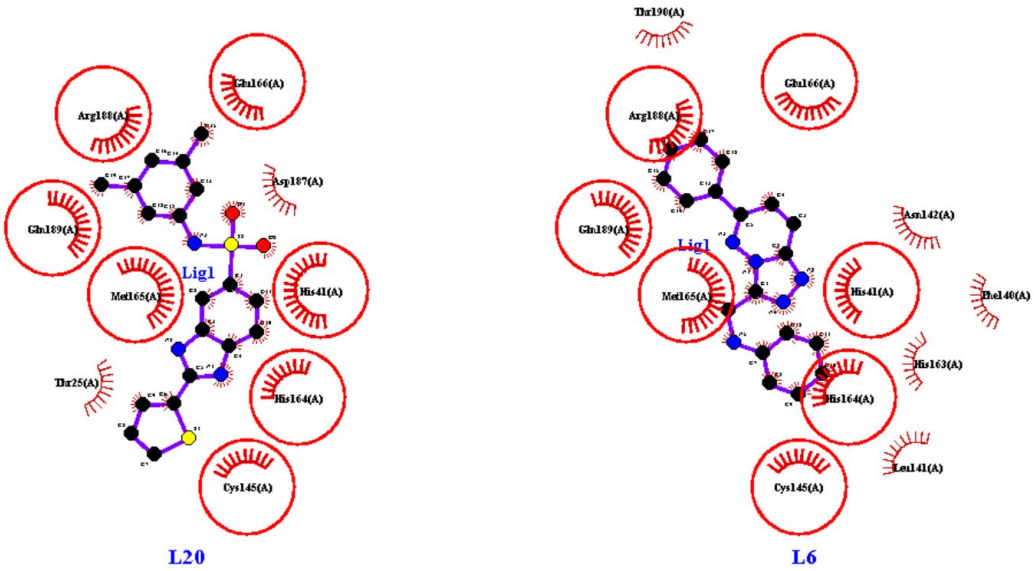

Figure S2: 2D interaction of L20 and L6 compounds showing Hydrophobic Bonds with Mpro.