



Figure S1: Small inhibitor binding with COVID-19 Mpro are highlighted in yellow circles, pdb id given to the corresponding complexes.

Table S1: Inhibitor interacts with SARS-Cov Mpro. The chemical properties of inhibitor are tabulated.

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| Pdb id | Inhibitor Chemical Name | Structure | Formula | Name |
| 6W63 | N-(4-tert-butylphenyl)-N-[(1R)-2-(cyclohexylamino)-2-oxo-1-(pyridin-3-yl)ethyl]-1H-imidazole-4-carboxamide |  | C27H33N5O2 | X77 |
| 6LU7 | N-[(5-methylisoxazol-3-yl)carbonyl]alanyl-l-valyl-n~1~-((1r,2z)-4-(benzyloxy)-4-oxo-1-{[(3r)-2-oxopyrrolidin-3-yl]methyl}but-2-enyl)-l-leucinamide |  | C35H51N6O7 | N3 |
| 5R84 | 2-cyclohexyl-~{N}-pyridin-3-yl-ethanamide |  | C13H18N2O | GWS |
| 5R83 | N-phenyl-N'-pyridin-3-ylurea |  | C12H11N3O | K0G |
| 5R82 | 6-(ethylamino)pyridine-3-carbonitrile |  | C8H9N3 | RZS |
| 5R81 | 1-methyl-3,4-dihydro-2~{H}-quinoline-7-sulfonamide |  | C10H14N2O2S | RZJ |
| 5R80 | methyl 4-sulfamoylbenzoate |  | C8H9NO4S | RZG |
| 5RE4 | N-(4-methylpyridin-3-yl)acetamide |  | C8H10N2O | SZY |
| 5RF1 | 4-bromobenzene-1-sulfonamide |  | C6H6BrNO2S | T5G |
| 5REB | 1-[(thiophen-3-yl)methyl]piperidin-4-ol |  | C10 H15 N O S | T0Y |