Identification of compelling inhibitors of human norovirus 3CL protease to combat gastroenteritis: A structure-based virtual screening and molecular dynamics study

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| Ligand | Affinity (kcal/mol) |
| Sorafenib | **-11.67** |
| YM201636 | **-10.34** |
| LDC4297 | **-9.78** |
| DBeQ | -8.71 |
| KPT-335 | -8.43 |
| CB-5083 | -8.40 |
| Raltegravir | -8.30 |
| OSU\_03012 | -8.10 |
| Salubrinal | -7.65 |
| LY2784544 | -7.51 |
| GNF-2 | -7.44 |
| GSK650394 | -7.36 |
| PD-0332991\_hydrochloride | -7.33 |
| Camptothecine | -7.25 |
| Cinacalcet\_Hydrochloride | -7.25 |
| FR\_180204 | -7.22 |
| Purvalanol\_A | -7.12 |
| FM-381 | -6.54 |
| Dipeptidyl inhibitor 7 | -6.38 |

**Table S1.** Top 20 screened compounds including control (Dipeptidyl inhibitor 7) and their BE with 3CLP.