

Identification of Natural Lead Compounds against Hemagglutinin Esterase Surface Glycoprotein in Human Coronaviruses Investigated via MD Simulation, Principal Component Analysis, Cross-Correlation, H-bond Plot and Mmgbsa

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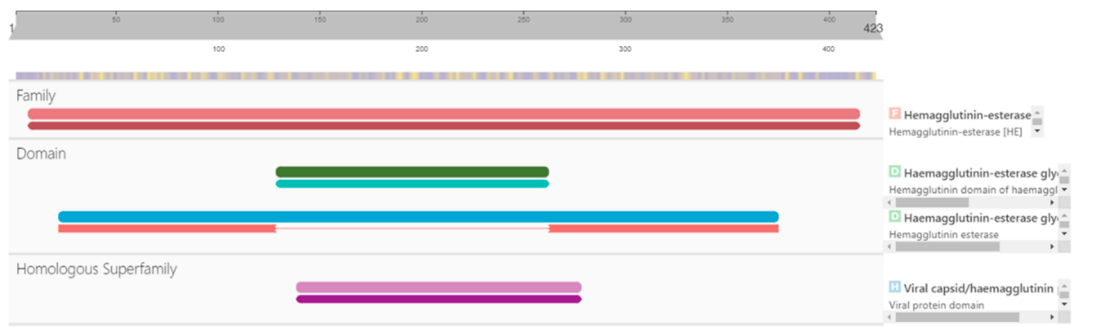


Figure S1. Domain architecture of HE Protein.

Table S1. Calculated values of MMGBSA with different parameters of HE protein- calceolarioside B complex.

Binding Energy Component	Average	Std. Dev.	Std. Err. of Mean
VDWAALS	-46.4165	3.6572	0.2111
EEL	-9.4782	3.4782	0.2008
EGB	23.0200	3.0008	0.1733
ESURF	-4.8051	0.3681	0.0213
DELTA G gas	-55.8948	5.6366	0.3254
DELTA G solv	18.2149	2.8397	0.1639
DELTA TOTAL	-37.6799	3.7919	0.2189

Table S2. (A) 12-Hydroxy-10,13-dimethyl-2,4,5,6,17-dione, (B) AZ628, (C) Telaprevir, (D) Verdinexor, (E) 4-[3-(morpholine-4-carbonyl)-5-[4-(trifluoromethyl)phenyl]pyrazol-1-yl]benzenesulfonamide, (F) 3,4 dihydroxyphenylacetic acid (G) aminomethyl(phenyl)phosphinic acid, (H) 3-[2-(3-cyanatophenoxy)ethoxy]phenyl cyanate, (I) N-[(4,5-difluoro-1H-benzimidazol-2-yl)methyl]-9-(3-fluorophenyl)-2-morpholin-4-ylpurin-6-amine, (J) N-(2-methyl-4-phenylbut-3-en-2-yl)-1-phenylmethanimine, (K) Ruboxistaurin, (L) Daunorubicin, (M) Forsythoside A (N) Turofexorate Isopropyl.

