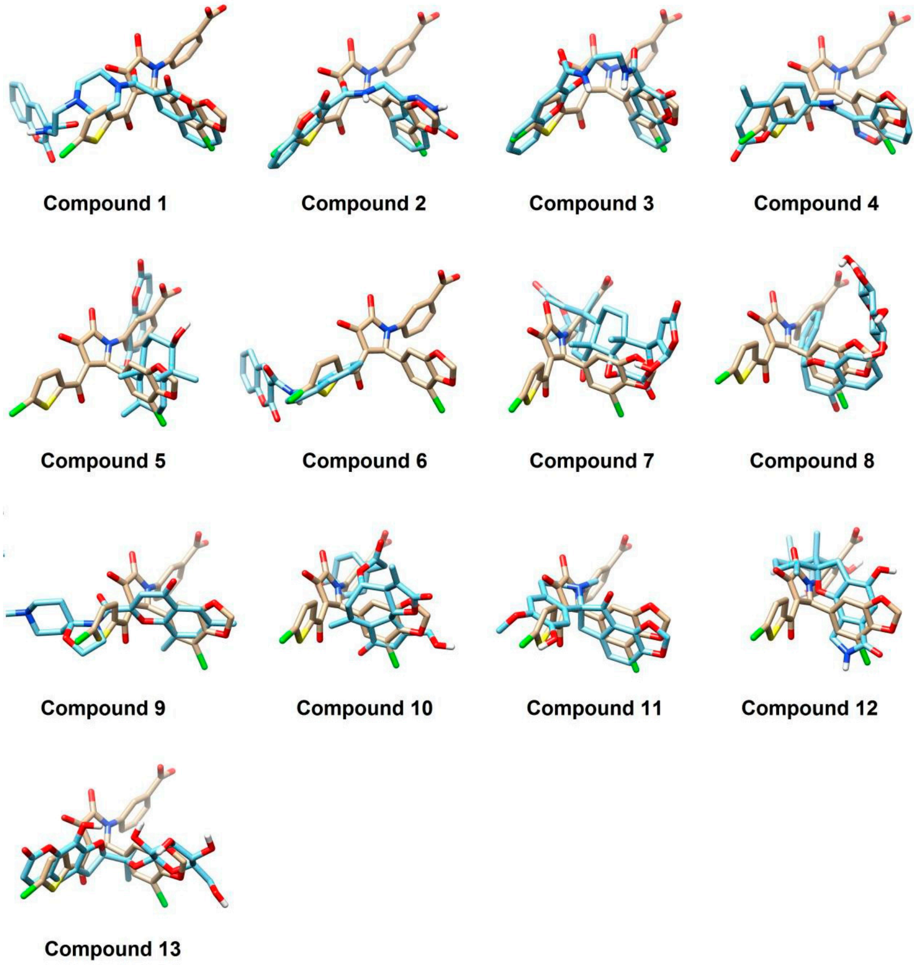
Supplementary Materials: Integrated Computational Approach for Virtual Hit Identification against Ebola Viral Proteins: VP35 and VP40

Muhammad Usman Mirza and Nazia Ikram

Table S1. Autodock vina and DSX score obtained after docking of EBOV-VP35 co-crystalized active compounds against EBOV-Z VP35.

VP35 Inhibitors	PDB ID	AutoDock Vina	DSX-Score
		EBOV-Z VP35 (kcal/mol)	EBOV-Z VP35 (kcal/mol)
VPL57	4IBI	−8	−113.45
VPL58	4IBJ	−7.8	−98.23
VPL48	4IBG	−7.3	−101.321
VPL29	4IBE	−7.2	−98.324
GA017	4IBB	−7.2	−115.2
VPL60	4IBK	−7.2	−97.435
VPL27	4IBD	−7	−102.912
GA246	4IBC	−6.9	−95.82
VPL42	4IBF	−6.8	−6.113

The best autodock vina and DSX score obtained after docking simulations of active compounds against EBOV-Z VP35. The binding energy values are expressed in kcal/mol.



Compound 1 **Compound 2** **Compound 3** **Compound 4**

Compound 5 **Compound 6** **Compound 7** **Compound 8**

Compound 9 **Compound 10** **Compound 11** **Compound 12**

Compound 13

Figure S1. Interactive ligands pose analysis. Superimposition of virtually screen compounds in blue (**1**–**13**) on potent VP35 inhibitor (VPL60) in tan color.