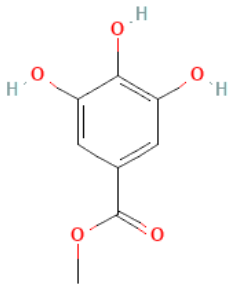
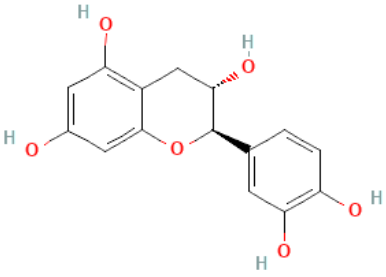
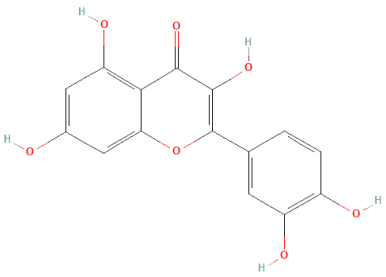
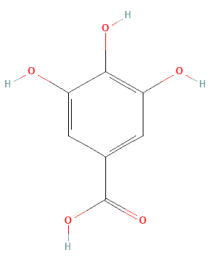
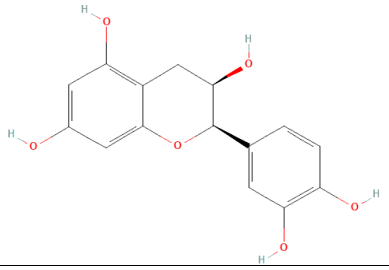
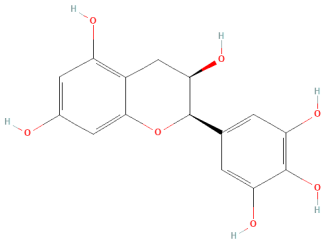
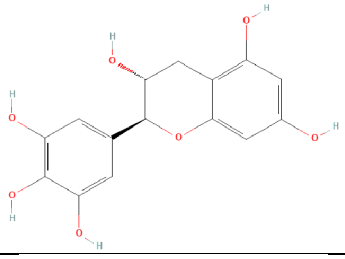
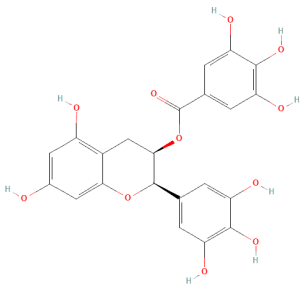
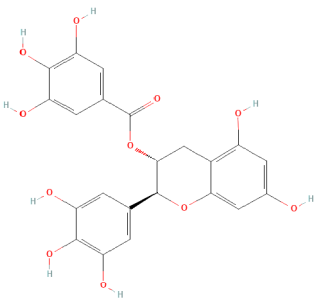
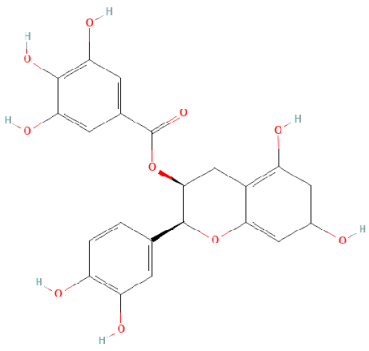
Computational Molecular Docking and Molecular Dynamics Simulations of Potential Inhibitors from the *Cistus incanus* (Cistaceae) against Ebola virus

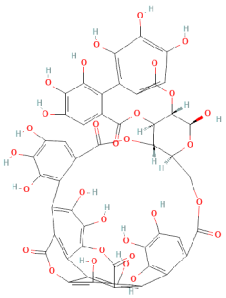
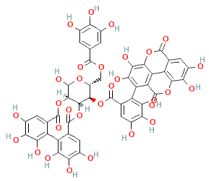
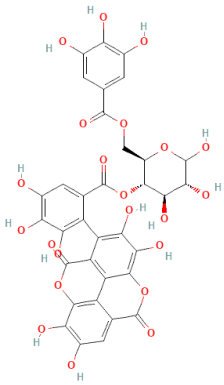
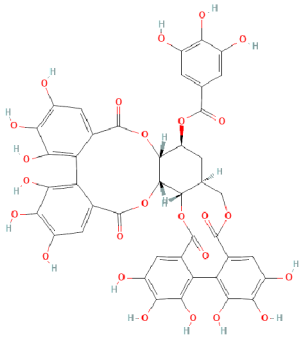
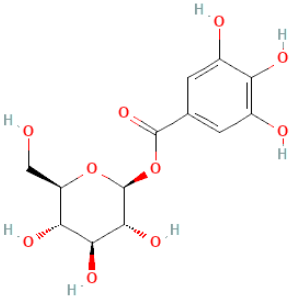
Wafa Hourani [1], Balakumar Chandrasekaran [2,*], Sankar Muthumanickam [3] and Pandi Boomi [3]

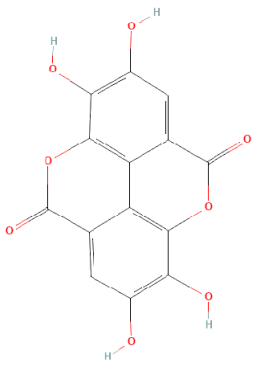
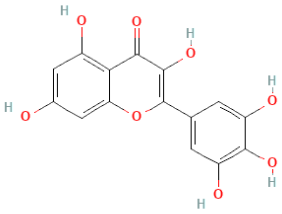
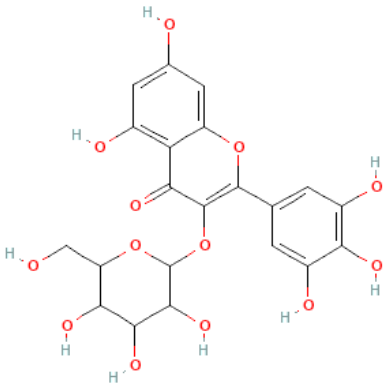
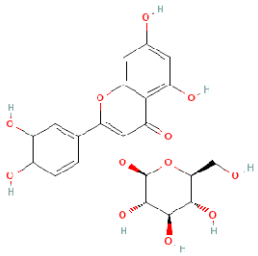
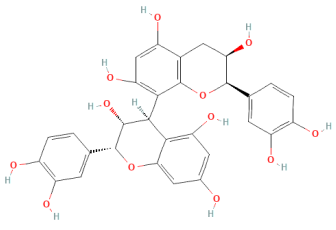
[1]Department of Pharmaceutical Sciences, Faculty of Pharmacy, Philadelphia University, P.O. Box 1, Amman, 19392, Jordan.
[2]Department of Pharmaceutical Sciences, Faculty of Pharmacy, Zarqa University, P.O. Box 2000, Zarqa, 13111, Jordan.
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Table S1. The 2D structures, docking scores, Glide energy and Glide Emodel of phytocompounds of *Cistus incanus*.

Phytocompound	Chemical Structures	Docking Score (kcal/mol)	Glide Energy (kcal/mol)	Glide Emodel (kcal/mol)
Methyl gallate		-9.8	-43.59	-68.71
Catechin		-8.8	-50.02	-65.26
Quercetin		-7.7	-36.8	-44.95
Gallic acid		-5.493	-54.852	-34.4

Epicatechin		-5.265	-31.385	-20.484
Epigallocatechin		-5.245	-41.38	-32.351
Gallo catechin		-4.945	-48.479	-36.852
Epigallocatechin gallate		-4.941	-24.434	-29.657
Gallocatechin gallate		-4.856	-43.221	-29.345
Epicatechin gallate		-4.668	-39.444	-32.962

Punicalagin (isomer b)		-4.656	-40.378	-35.813
Terflavin A (isomer a)		-4.644	-35.917	-27.042
Terflavin A (isomer b)		-4.542	-46.041	-34.9
HHDP-Glc (isomer b)		-4.394	-35.415	-34.342
Monogalloyl glucose		-4.368	-35.164	-35.831

Ellagic acid		-4.361	-28.235	-30.3
Myricetin		-4.35	10000	-26.935
Myricetin-hexo-side gallate		-4.361	-28.235	-30.3
Isoquercitrin (quercetin-3-O-glucoside)		-4.361	-28.235	-30.3
Procyanidin B (di-mer)		-4.343	-51.817	-35.635

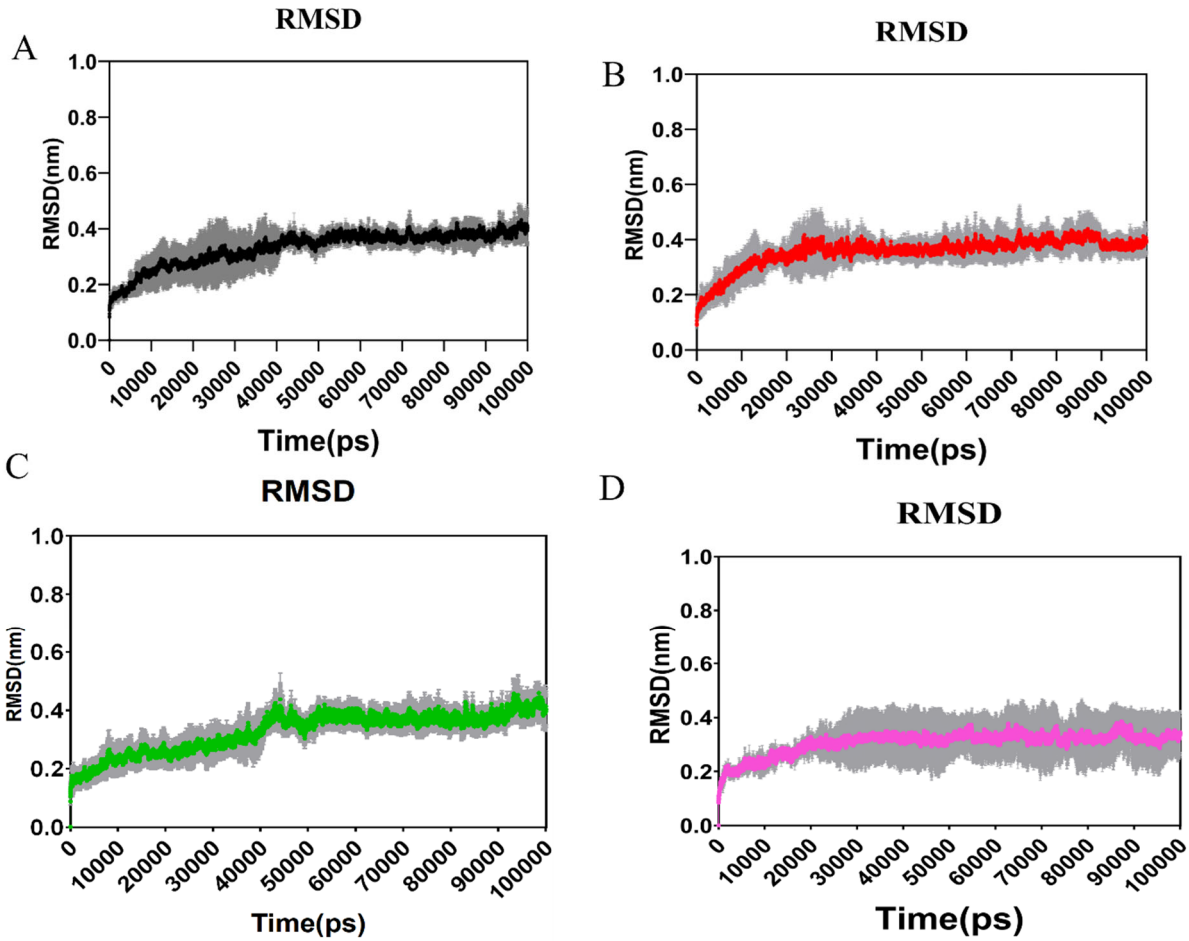


Figure S1. Backbone RMSD of VP40 (A) and ligand RMSD of methyl gallate (B), quercetin (C), and catechin (D) over 100 ns molecular dynamics simulations. Triplicate runs indicate stable systems with low fluctuations (mean ± SD): backbone (0.332 ± 0.026 nm), methyl gallate (0.357 ± 0.041 nm), quercetin (0.307 ± 0.065 nm), and catechin (0.326 ± 0.029 nm).

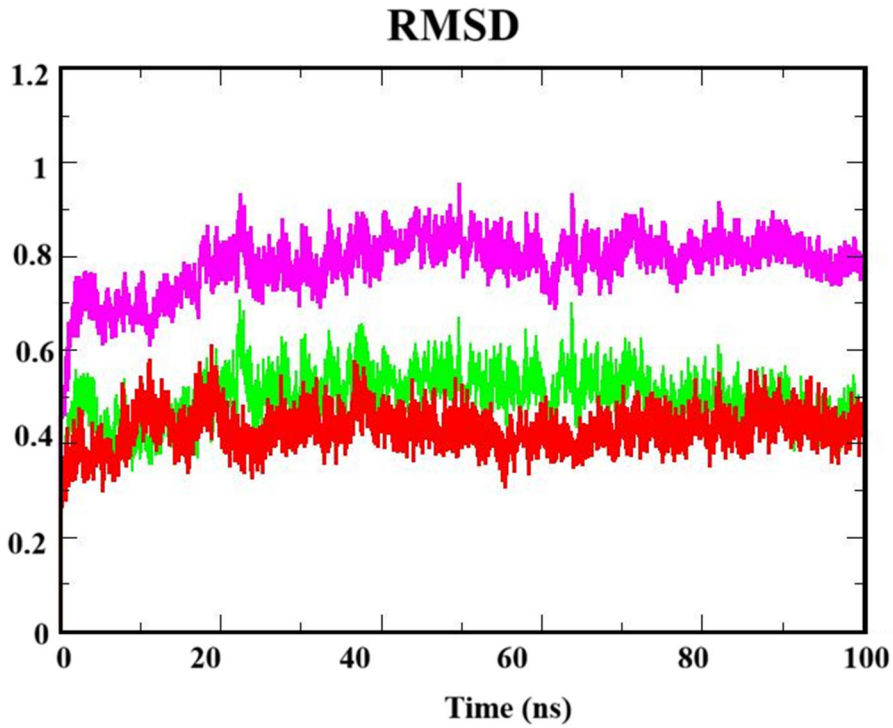


Figure S2. Ligand RMSD within the VP40 binding cavity over the 100 ns MD simulation, illustrating stable ligand positioning and consistent binding orientation.