In silico assessment and molecular docking studies of some phyto-triterpenoid for potential disruption of mortalin-p53 interaction

Minh Quan Pham[1,2,*], Thuy Huong Le Thi[1,2], Quoc Long Pham[1,2], Le Thi Le[3], Huy Toan Dao[3], Thanh Le Thi Dang[4], Dung Thuy Nguyen Pham[5,6] and Hai Ha Pham Thi[7,**]

[1] Institute of Natural Products Chemistry, Vietnam Academy of Science and Technology, Hanoi 100000, Vietnam; pham-minh.quan@inpc.vast.vn (M.Q.P.), thuyhuong0102sp2@gmail.com (T.H.L.T.), mar.biochem@fpt.vn (Q.L.P.)

[2] Graduate University of Science and Technology, Vietnam Academy of Science and Technology, Hanoi 100000, Vietnam; pham-minh.quan@inpc.vast.vn (M.Q.P.), thuyhuong0102sp2@gmail.com (T.H.L.T.), mar.biochem@fpt.vn (Q.L.P.)

[3] Hanoi University of Science and Technology, Hanoi 100000, Vietnam; (L.T.L.), (H.T.D.)

[4] Faculty of Chemistry and Environment, Thuyloi University, Hanoi 100000, Vietnam (T.L.T.D.)

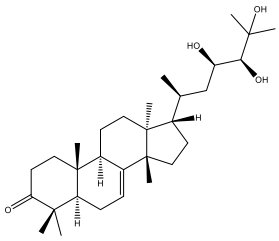
[5] NTT Hi-Tech Institute, Nguyen Tat Thanh University, Ho Chi Minh City 700000, Vietnam; pntdung@nttu.edu.vn (D.T.N.P.)

[6] Center of Excellence for Biochemistry and Natural Products, Nguyen Tat Thanh University, Ho Chi Minh City 700000, Vietnam; pntdung@ntt.edu.vn (D.T.N.P.)

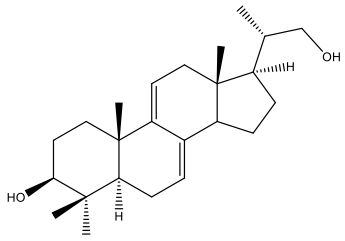
[7] Faculty of Biotechnology, Nguyen Tat Thanh University, Ho Chi Minh City 700000, Vietnam; pthha@ntt.edu.vn (H.H.P.T.)

*, ** Correspondence: * pham-minh.quan@inpc.vast.vn (M.Q.P.); ** pthha@ntt.edu.vn (H.H.P.T.)

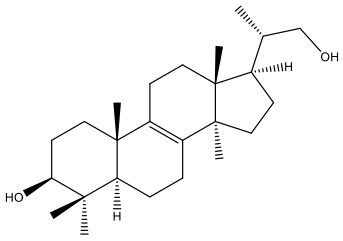
S1. Structure of studied compounds



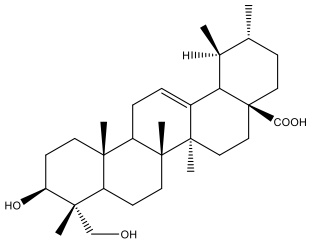
3-oxo-threo-23,24,25-trihydroxytirucall-7-ene (**1**)



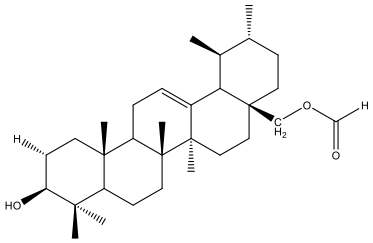
23,24,25,26,27-pentanorlanost-7,9(11)-dien-3β,22-diol (**2**)



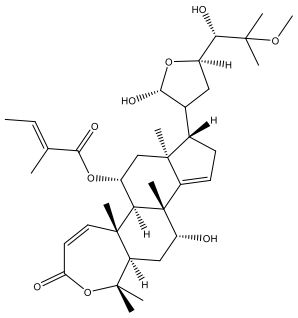
23,24,25,26,27-pentanorlanost-8-en-3β,22-diol (**3**)



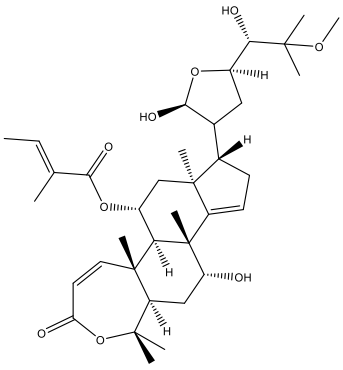
23-hydroxyursolic acid (**4**)



28-formyloxy-3β-hydroxy-urs-12-ene (**5**)



Ailanaltiolide A (**6**)



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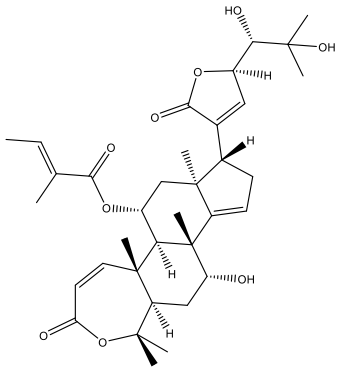
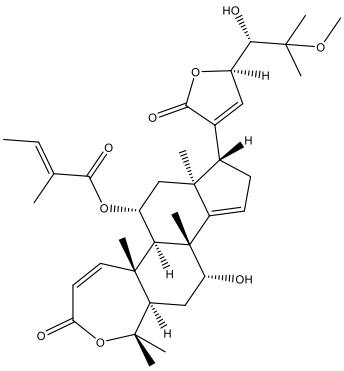


Ailanaltiolide C (**8**)



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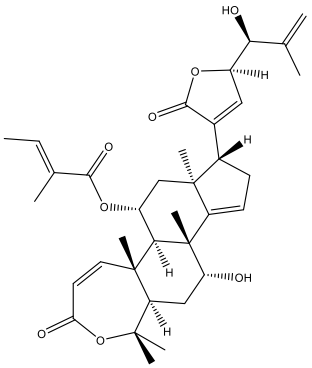
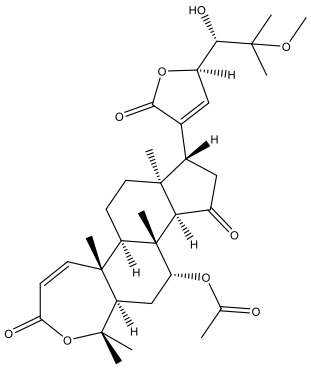


Ailanaltiolide E (**10**)



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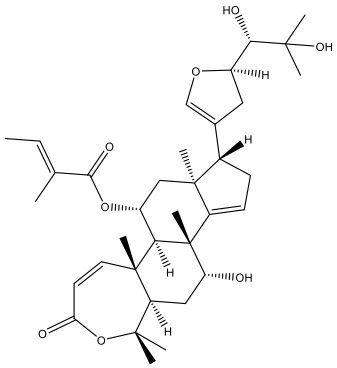

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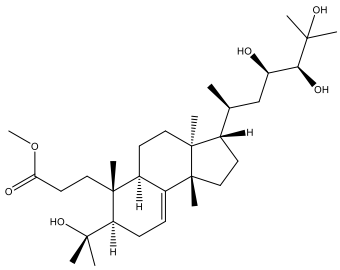

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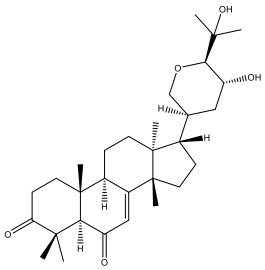

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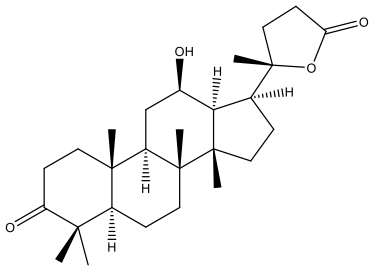

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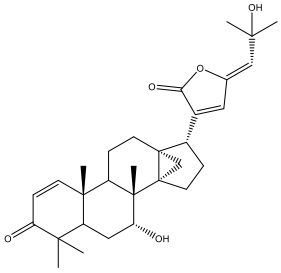
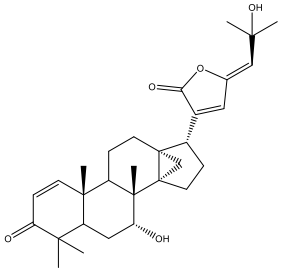


Ailanthusin A (**16**)



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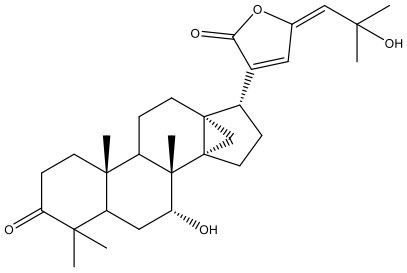

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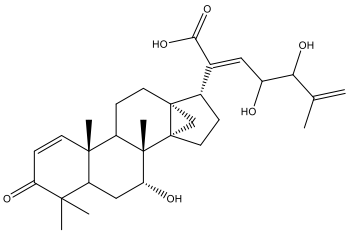

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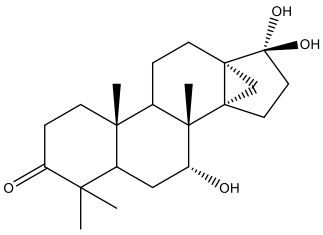

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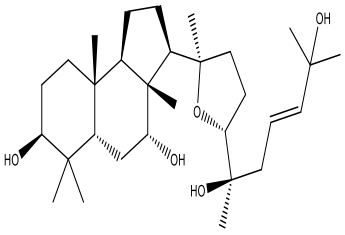

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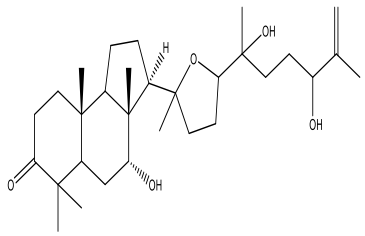

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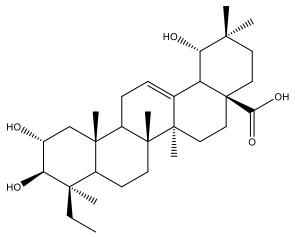
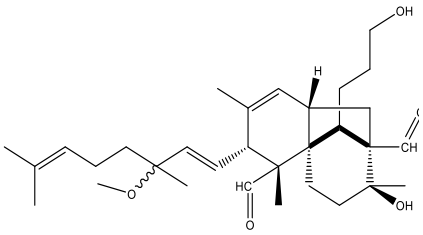


Arjunic acid (**23**)



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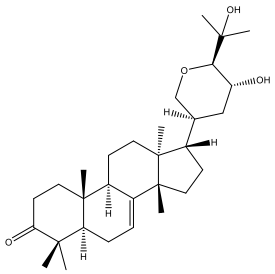
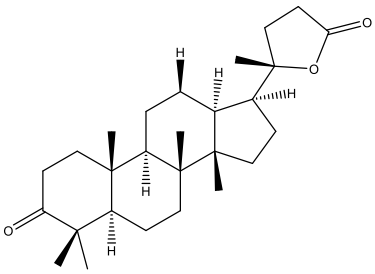


Bourjutinolone A (**25**)



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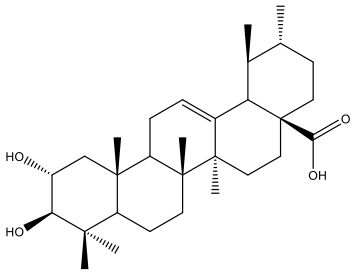

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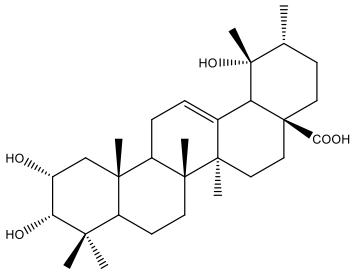

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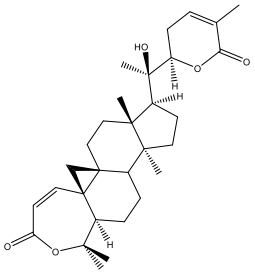
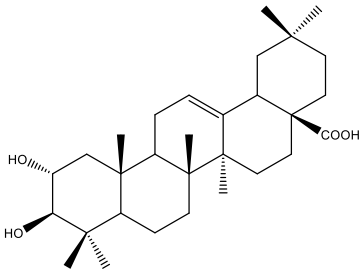
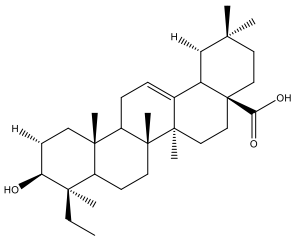


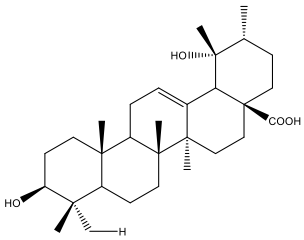
Kadsuphilactone B (**29**)



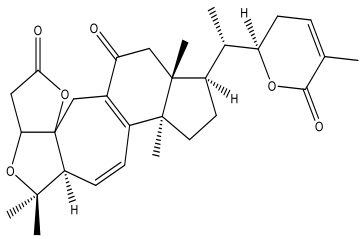
Maslinic acid (**30**)



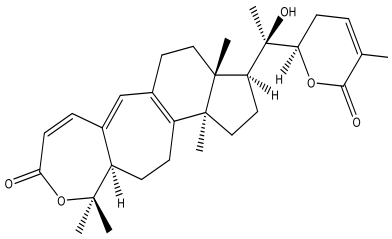
Oleanolic acid (**31**)

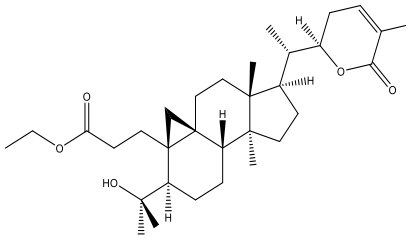


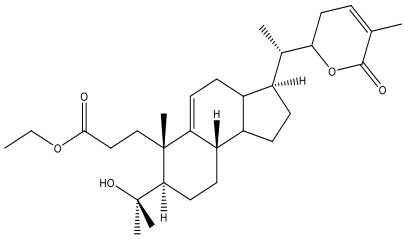
Pomolic acid (**32**)



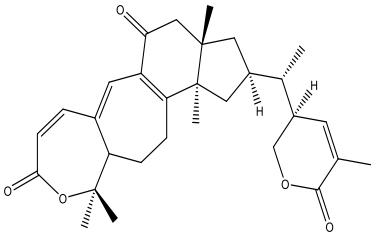
Schinchinenlactone A (**33**)







Schisanlactone C (**34**)



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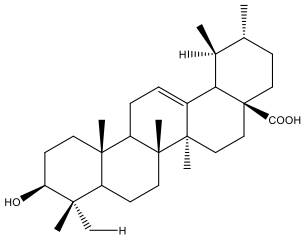
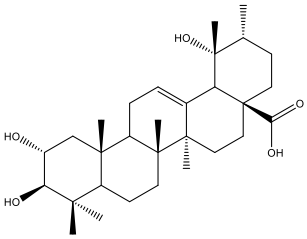
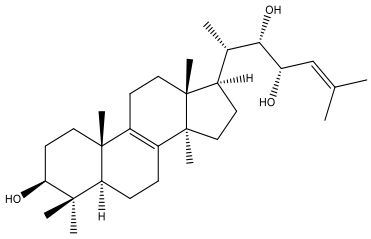


Schisanlactone I (**36**)



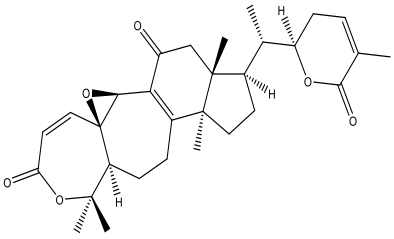
Schisanlactone J (**37**)



Ursolic acid (**38**)

Tormentic acid (**39**)

Lanost-8-en-3β,22S,23S-triol (**40**)



Schisphendilactone B (**41**)

Figure S1. Structure of 41 studied phyto triterpenes

S2. Detailed description for docking studies

Table S1. Pharmacokinetic parameters and toxicity prediction of studied compounds

Compound ID	miLogP[a]	TPSA (Å^2)[b]	LD_{50} (mg/kg)	Toxicity prediction[c]
1	5.30	77.75	5010	6
2	5.26	40.46	1190	4
3	5.53	40.46	2000	4
4	5.61	77.75	2000	4
5	7.33	46.53	4800	5
6	5.79	131.76	590	4
7	5.79	131.76	590	4
8	5.52	139.6	400	4
9	6.14	128.6	400	4
10	6.53	119.37	1000	4
11	4.90	125.45	1000	4
12	5.57	122.53	1000	4
13	4.84	107.22	5000	5
14	4.30	83.83	1000	4
15	3.68	63.60	4400	5
16	3.83	87.74	5105	6
17	3.83	87.74	5105	6
18	3.86	87.74	250	3
19	3.52	115.05	9000	6
20	2.35	77.75	1000	4
21	5.04	90.15	6000	6
22	4.97	86.99	5000	5
23	5.23	97.98	2000	4
24	5.90	83.83	1410	4
25	5.40	66.76	1000	4
26	4.59	43.38	4400	5
27	5.87	77.75	2000	4
28	4.93	97.98	2000	4
29	6.02	72.84	7	2
30	5.81	77.75	2000	4
31	7.06	57.53	2000	4
32	5.84	77.75	2000	4
33	3.36	78.92	50	2
34	6.24	72.84	55	3
35	6.56	72.84	333	4
36	6.62	72.84	333	4

37	6.20	69.68	100	3
38	5.52	82.21	1000	4
39	4.93	97.98	2000	4
40	6.55	60.68	667	4
41	6.79	57.53	2000	4
Withanone	**4.15**	**96.36**	**7**	**2**
Withaferin A	**3.86**	**96.36**	**7**	**2**

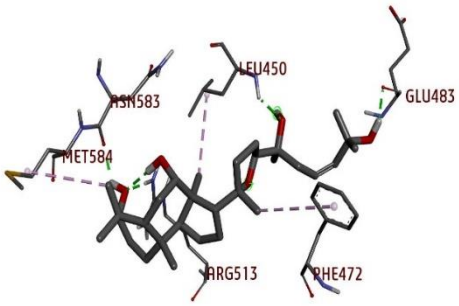
[a] Calculated octanol/water partition coefficient

[b] Molecular total polar surface area

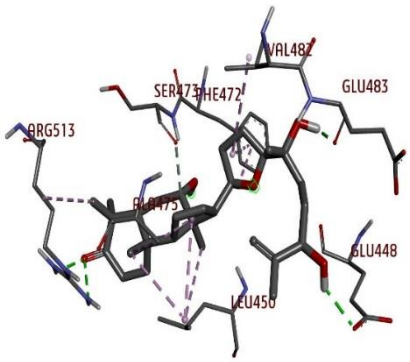
[c] Toxicity prediction class: 1 → 6 (High toxicity to non-toxic)

Table S2. The H-bond interactions between potential compounds and Mortalin model 3N8E

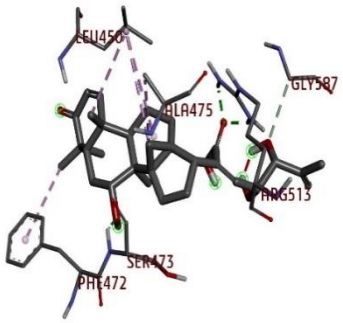
Compound ID	No. of H-bonds	Interacting residues
21	4	Leu450; Glu483; Arg513; Asn583
22	3	Glu448; Glu483; Arg513
19	2	Ser473; Arg513
34	3	Leu450; Arg513
38	3	Thr474; Arg513; Glu580
16	2	Arg513; Asn583
17	1	Gln479
14	4	Leu450; Gly514; Gln517
18	3	Ser473; Arg513; Asn583
Withanone	**3**	**Thr449; Thr455; Arg513**
Withaferin A	**6**	**Phe454; Lys456; Ser473; Thr474; Arg513; Lys576**



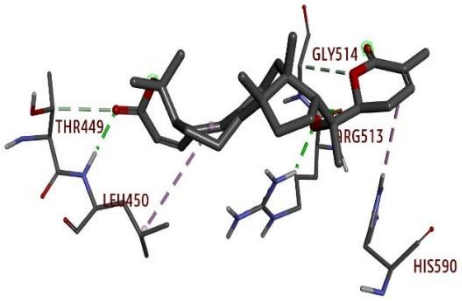
A



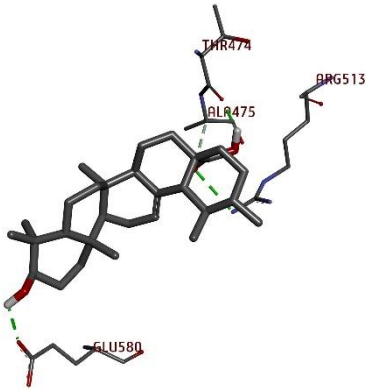
B


LEU450
GLY587
ALA475
ARG513
SER473
PHE472

C


GLY514
THR449
ARG513
LEU450
HIS590

D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ARG513
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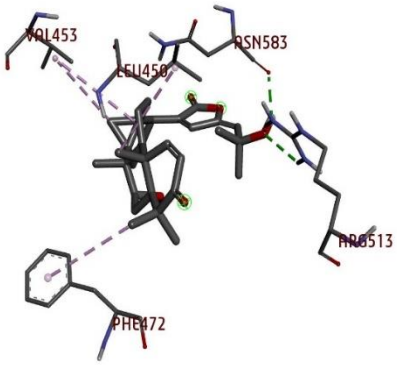
GLU580

E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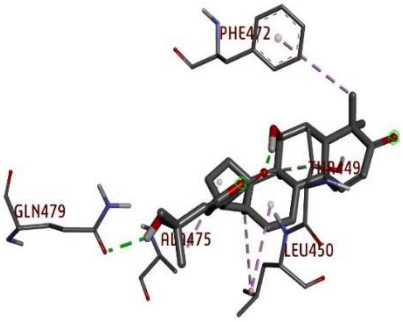
ARG513
PHE472

F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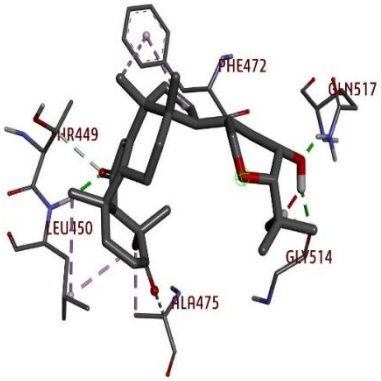
THR449
GLN479
ALA475
LEU450

G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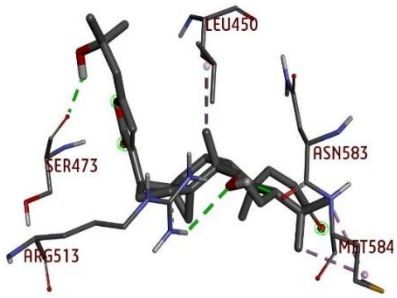
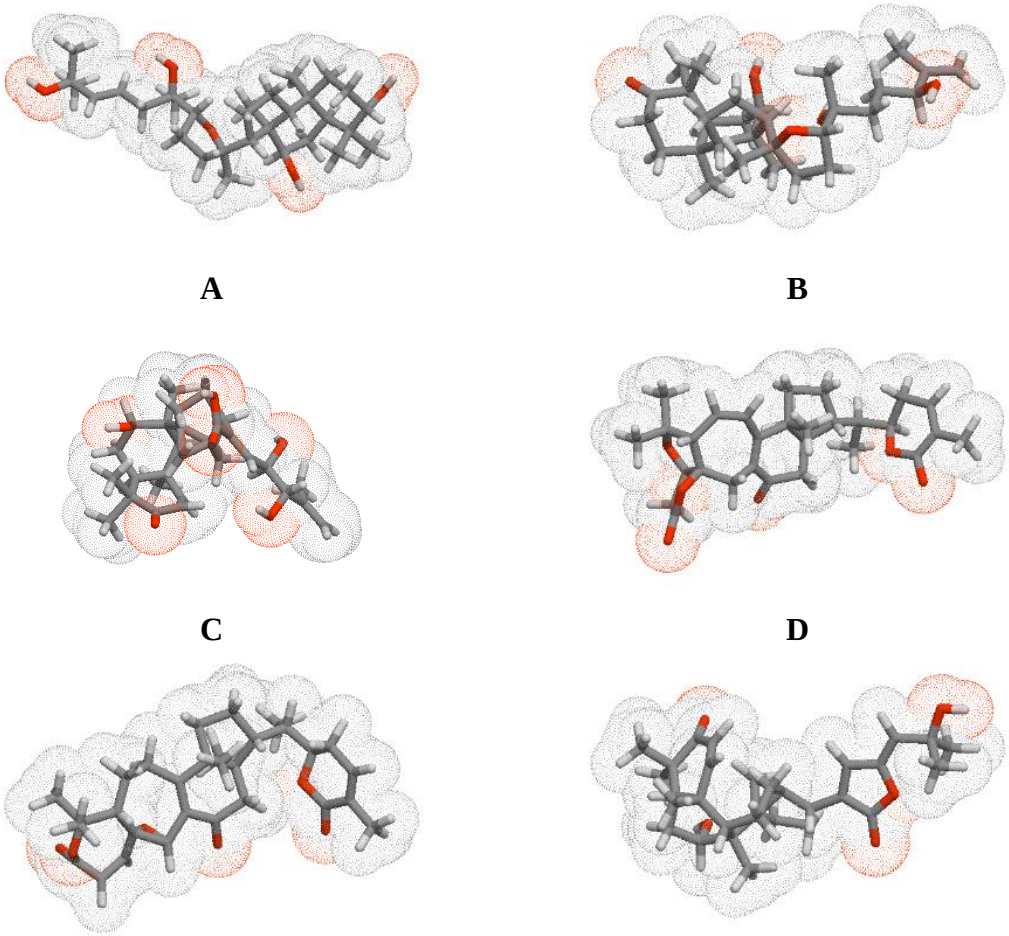
GLN517
THR449
LEU450
GLY514
ALA475

H



I

Figure S2. Stereoview of the binding mode of nine potential inhibitors of protein Mortalin (PDB ID: 3N8E). (A) Compound 21; (B) Compound 22; (C) Compound 19; (D) Compound 34; (E) Compound 38; (F) Compound 16; (G) Compound 17; (H) Compound 14; (I) Compound 18



A **B**

C **D**

E **F**

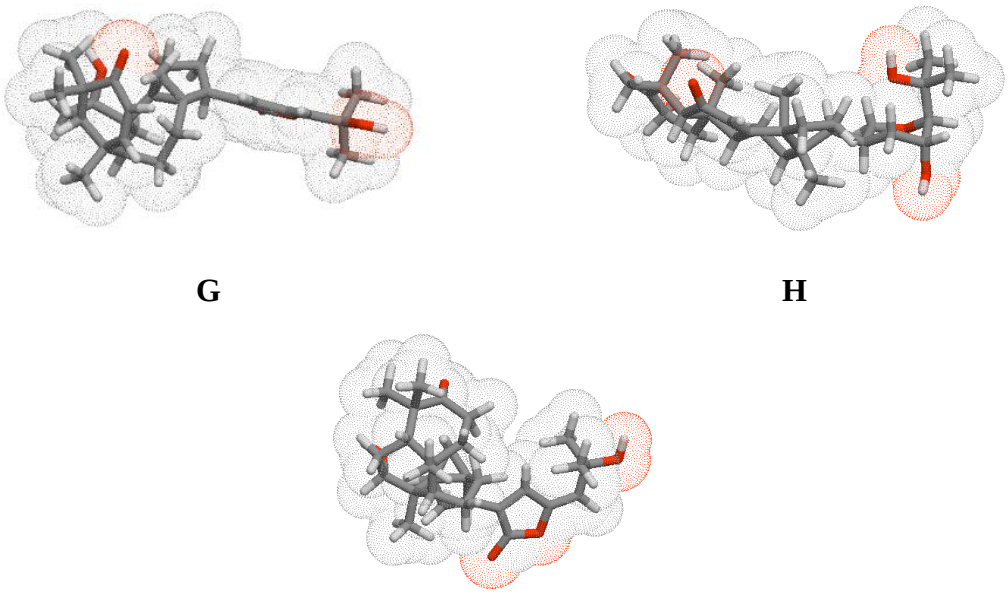


Figure S3. Maps of total polar surface area (TPSA) of nine potential compounds showing the nonpolar area (gray white color) and polar area (red color). (A) Compound 21; (B) Compound 22; (C) Compound 19; (D) Compound 34; (E) Compound 38; (F) Compound 16; (G) Compound 17; (H) Compound 14; (I) Compound 18