Supplementary Table 1. Bioactivity prediction (druglikeness*) of β-lapachone and its derivatives for specific biological activities

Compound	GPCR ligand	Ion channel modulator	Kinase inhibitor	Nuclear receptor ligand	Protease inhibitor	Enzyme inhibitor
Lapachol	-0.17	0.27	-0.11	0.20	-0.09	0.65
ß-lapachone	-0.08	0.33	-0.25	0.07	0.08	0.45
α-lapachone	-0.24	-0.12	-0.29	0.14	-0.18	0.26
3-iodo-ß-lapachone	-0.13	0.20	-0.21	0.03	0.01	0.50
3-I-α-lapachone	-0.28	-0.24	-0.24	0.09	-0.24	0.32
naphtho[2,1-d]oxazole-4,5-diones	-0.39	-0.21	-0.44	-0.46	-0.54	0.26

*Druglikeness scores were calculated using molinspiration chemoinformatics pharmacological database (https://www.molinspiration.com/cgi-bin/properties).

Supplementary Table 2. Bioactivity prediction (druglikeness*) of resveratrol and its derivatives for specific biological activities

Compound	GPCR ligand	Ion channel modulator	Kinase inhibitor	Nuclear receptor ligand	Protease inhibitor	Enzyme inhibitor
Resveratrol and Methoxylated Resveratrol Derivatives						
Resveratrol	-0.20	0.02	-0.20	0.01	-0.41	0.02
Pterostilbene	-0.13	-0.06	-0.12	0.08	-0.33	0.01
Trimethoxystilbene	-0.14	-0.12	-0.13	-0.02	-0.29	-0.05
Tetramethoxystilbene	-0.08	-0.14	-0.08	0.05	-0.22	-0.07
Pentamethoxystilbene	-0.07	-0.13	-0.02	-0.04	-0.17	-0.05
Hydroxylated Resveratrol Derivatives						
Dihydroxystilbene	-0.27	0.04	-0.27	-0.11	-0.47	-0.01
Tetrahydroxystilbene	-0.16	-0.02	-0.14	0.08	-0.36	0.04
Hexahydroxystilbene	-0.30	0.04	-0.19	-0.19	-0.33	0.05

*Druglikeness scores were calculated using molinspiration chemoinformatics pharmacological database(https://www.molinspiration.com/cgi-bin/properties).

Supplementary Table 3. Chemical and pharmacological properties of Lapachol, β-lapachone and derivatives.

Compound	PubChem CID	Molecular Formula	Molecular Mass (Da)	logP	tPSA (Å^2)	nrotb	Lipinski's rule violations	Molecular volume (Å^3)	Canonical SMILES
Lapachol	3884	$C_{15}H_{14}O_3$	242.27	3.16	54.37	2	0	223.94	CC(=CCC1=C(C2=CC=CC=C2C(=O)C1=O)O)C
ß-lapachone	3885	$C_{15}H_{14}O_3$	242.27	2.95	43.38	0	0	219.96	CC1(CCC2=C(O1)C3=CC=CC=C3C(=O)C2=O)C
α-lapachone	72732	$C_{15}H_{14}O_3$	242.27	2.95	43.38	0	0	219.96	CC1(CCC2=C(O1)C(=O)C3=CC=CC=C3C2=O)C
3-iodo-ß-lapachone	N.A.	$C_{15}H_{13}IO_3$	368.17	3.43	43.38	0	0	243.97	C1=C2C(=CC=C1)C3=C(C(C2=O)=O)CC(C(C)(C)O3)I
3-I-α-lapachone	N.A.	$C_{15}H_{13}IO_3$	368.17	3.43	43.38	0	0	243.97	C1=C2C(=CC=C1)C(C3=C(C2=O)OC(C(C3)I)(C)C)=O
naphtho[2,1-d]oxazole-4,5-diones	N.A.	$C_{13}H_9NO_3$	227.22	2.16	60.17	1	0	227.22	C1(C(C3=C(C2=C1C=CC=C2)OC(=N3)CC)=O)=O

N.A. compounds not available at Pubchem database. logP values, tPSA (topological polar surface area), nrotb (rotatable bonds), Lipinski's rule violations and molecular volume were extracted from molinspiration chemoinformatics pharmacological database(https://www.molinspiration.com/cgi-bin/properties) after insertion of Canonical SMILES representation of each compound. Canonical Smiles were collected from PubChem database.

Supplementary Table 4. Chemical and pharmacological properties of resveratrol and derivatives.

Compound	PubChem CID	Molecular Formula	Molecular Weight	logP	Total polar surface área	Rotatable bonds	Rule of five violations	Molecular volume	Canonical SMILES
Resveratrol and Resveratrol Methoxylated Derivatives									
Resveratrol	445154	C14H12O3	228.24	2.99	60.68	2	0	206.92	C1=CC(=CC=C1C=CC2=CC(=CC(=C2)O)O)O
Pterostilbene	5281727	C16H16O3	256.3	4.06	38.70	4	0	241.98	COC1=CC(=CC(=C1)C=CC2=CC=C(C=C2)O)OC
Trimethoxystilbene	5388063	C17H18O3	270.32	4.59	27.70	5	0	259.51	COC1=CC=C(C=C1)C=CC2=CC(=CC(=C2)OC)OC
Tetramethoxystilbene	5354004	C18H20O4	300.3	4.40	36.94	6	0	285.05	COC1=CC(=C(C=C1)C=CC2=CC(=CC(=C2)OC)OC)OC
Pentamethoxystilbene	9818893	C19H22O5	330.4	4.17	46.17	7	0	310.60	COC1=CC(=CC(=C1)C=CC2=CC(=C(C(=C2)OC)OC)OC)OC
Hydroxylated Resveratrol Derivatives									
Dihydroxystilbene	5282363	C14H12O2	212.24	3.54	40.46	2	0	198.91	C1=CC(=CC=C1C=CC2=CC=C(C=C2)O)O
Tetrahydroxystilbene	5281717	C14H12O4	244.24	2.72	80.91	2	0	214.94	C1=CC(=C(C=C1O)O)C=CC2=CC(=CC(=C2)O)O
Hexahydroxystilbene	129837003	C14H12O6	276.24	3.37	121.37	2	1	230.98	C1=CC=C(C=C1)C=C(C2=C(C(=C(C(=C2O)O)O)O)O)O

logP values, tPSA (topological polar surface area), nrotb (rotatable bonds), Lipinski's rule violations and molecular volume were extracted from molinspiration chemoinformatics pharmacological database(https://www.molinspiration.com/cgi-bin/properties) after insertion of Canonical SMILES representation of each compound. Canonical Smiles were collected from PubChem database.