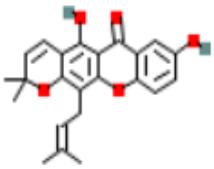
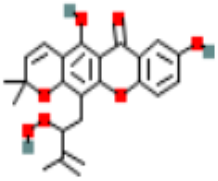
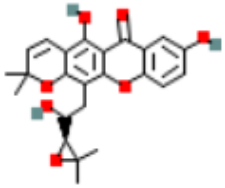
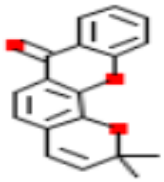
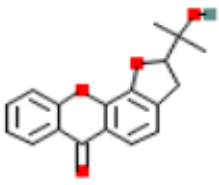
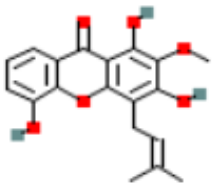
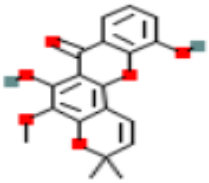
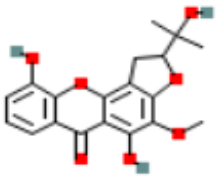
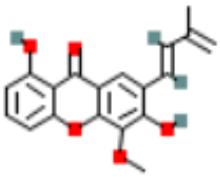
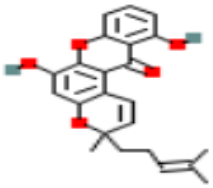
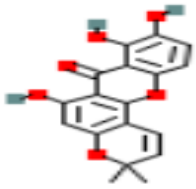
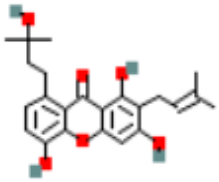
Tables

Table 1. Binding energies and interactions of xanthone derivatives against main protease (PDB: 6Y84).

Compound	PubChem ID	2D Structure	Binding energy	Dissociation constant (KI)	Interacting amino acids
Brasixanthone B	CID_10362269		-8.81	350.95 nM	Thr26
Brasixanthone C	CID_10001590		-9.09	215.77 nM	His163, Thr26
Brasixanthone D	CID_70678720		-8.29	845.06 nM	His163
Caledonixanthone B	CID_ 493293		-8.24	914.93 nM	---
Caledonixanthone C	CID_ 493294		-8.42	669.77 nM	Glu166

Caledonixanthone D	CID_ 5464633		-7.36	4.02 µM	Leu141, Ser144
Caledonixanthone E	CID_ 5464634		-7.63	2.53 µM	Glu166
Caledonixanthone F	CID_ 5464635		-8.03	1.3 µM	Gly143, Cys145, His163
Globulixanthone A	CID_ 5323527		-7.76	2.06 µM	---
Globulixanthone B	CID_10452251		-8.35	753.06 nM	Leu141, Gly143
Globulixanthone C	CID_ 5317656		-6.94	8.14 µM	---
Nigrolineaxanthone N	CID_ 5323589		-8.35	755.8 nM	His41, His163

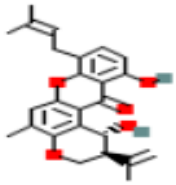
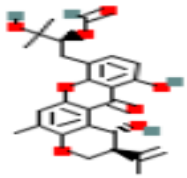
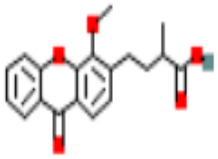
Shamixanthone	CID_15596091		-8.38	715.25 nM	Gly143
Varixanthone	CID_10096170		-7.80	1.91 µM	---
Teysmannic acid	CID_56612721		-8.13	1.1 µM	Asn142, Glu166

Table 2. Results of the phytochemical molecules druglikeness properties.

Drug likeliness properties / Phytochemicals	MW g/mol	Concensus Log Po/w	No. of H-bond Acceptors	No. of H-bond Donors	Molar Refractivity	Lipinski	Veber	Bioavailability Score	Synthetic accessibility (SA)	TPSA (Å^2)	No of rotatable bonds	solubility (mg/ml)
Brasixanthone B	378.42	4.37	5	2	111.8	Yes	Yes	0.55	4.11	79.90	2	3.93e-04
Brasixanthone C	410.42	3.67	7	3	114.53	Yes	Yes	0.55	4.61	109.36	4	1.65e-03
Brasixanthone D	424.44	3.28	7	3	117.53	Yes	Yes	0.55	4.94	112.66	3	5.03e-03
Caledonixanthone B	278.30	3.60	3	0	84.11	Yes	Yes	0.55	3.45	39.44	0	8.61e-03
Caledonixanthone C	296.32	2.93	4	1	84.5	Yes	Yes	0.55	3.65	59.67	1	3.30e-02
Caledonixanthone D	342.34	3.20	6	3	96.27	Yes	Yes	0.55	3.51	100.13	3	4.12e-03
Caledonixanthone E	340.33	2.93	6	2	94.65	Yes	Yes	0.55	3.85	89.13	1	7.99e-03
Caledonixanthone F	358.34	2.31	7	3	95.49	Yes	Yes	0.55	4.05	109.36	2	2.98e-02
Globulixanthone A	324.33	3.56	5	2	94.57	Yes	Yes	0.55	3.52	79.90	3	2.45e-03
Globulixanthone B	378.42	4.44	5	2	111.72	Yes	Yes	0.55	4.49	79.90	3	4.38e-04
Globulixanthone C	326.30	2.67	6	3	90.18	Yes	Yes	0.55	3.68	100.13	0	1.25e-02
Nigrolineaxanthone	398.45	3.90	6	4	115	Yes	Yes	0.55	3.83	111.13	5	1.43e-03

N												
Shamixanthone	406.47	4.62	5	2	119.96	Yes	Yes	0.55	4.80	79.90	3	2.53e-04
Teysmannic acid	326.34	3.25	5	1	92.45	Yes	Yes	0.55	3.43	76.74	5	1.85e-02
Varixanthone	468.50	3.32	8	3	128.11	Yes	Yes	0.55	5.20	126.43	6	2.72e-03

Table 3. Free binding energy calculations of main protease and natural xanthone compounds (Shamixanthone, Brasixanthone B and Brasixanthone C).

S.no	Compounds	Van der energy (kJ/mol)	Electrostatic energy (kJ/mol)	Polar solvation energy (KJ/mol)	SASA energy (kJ/mol)	Binding energy (kJ/mol)
1	Shamixanthone	4832.073 +/- 96.433	-35.344 +/- 7.311	90.996 +/- 10.03	-15.517 +/- 0.853	4872.208 +/- 96.811
2	Brasixanthone B	4399.778 +/- 96.831	-44.625 +/- 10.760	118.177 +/- 14.092	-17.025 +/- 1.002	4456.305 +/- 98.17
3	Brasixanthone C	4856.322 +/- 101.790	-0.793 +/- 3.966	46.065 +/- 9.105	-12.834 +/- 0.891	4888.760 +/- 102.053