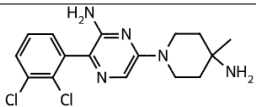
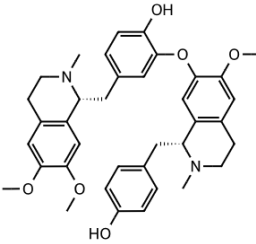
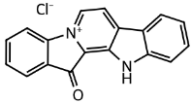
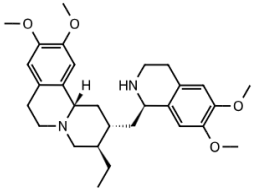
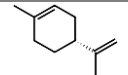
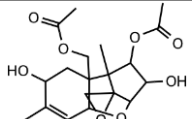
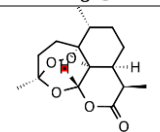
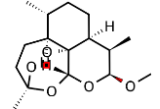
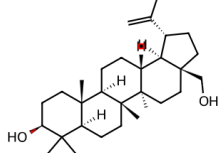
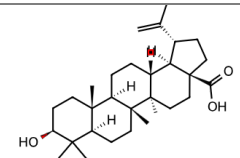
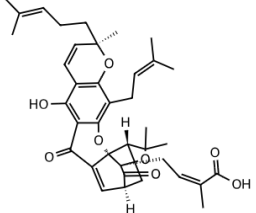
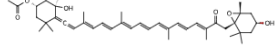
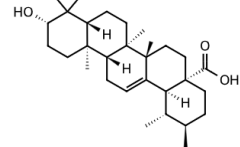
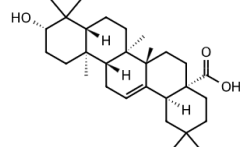
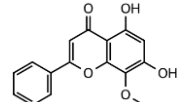
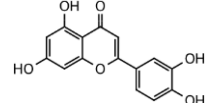
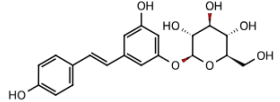
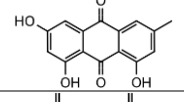
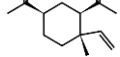
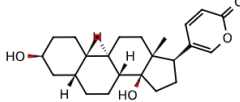
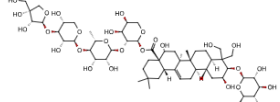
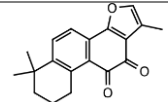
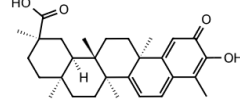
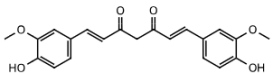
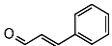
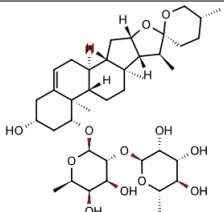
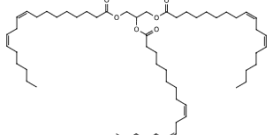
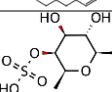
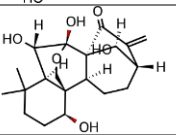
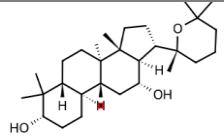
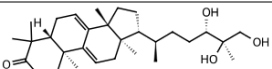
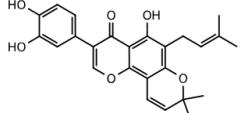
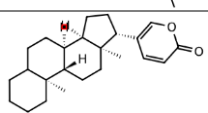
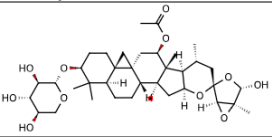
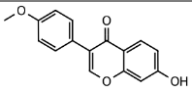
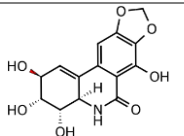
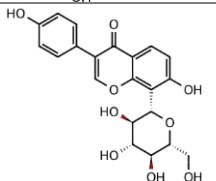
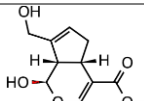
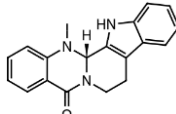
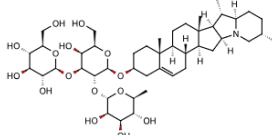
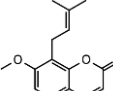
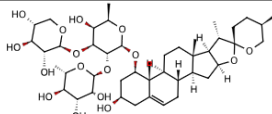
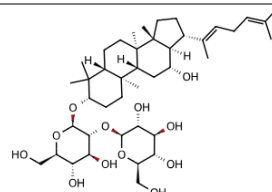
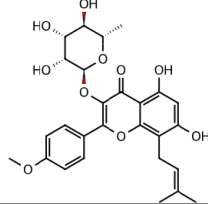
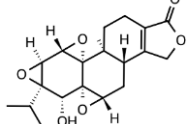
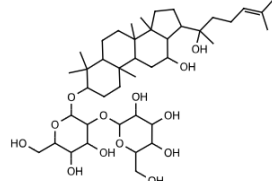
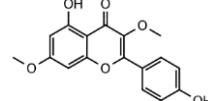
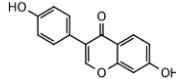
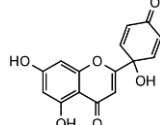


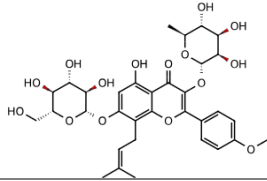
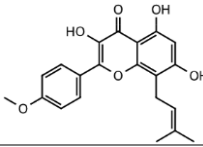
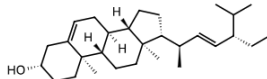
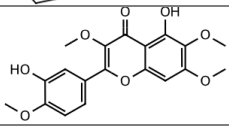
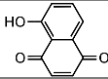
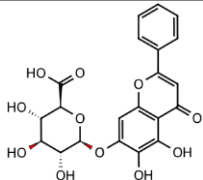
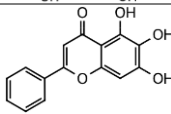
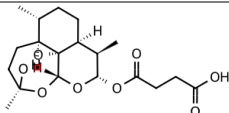
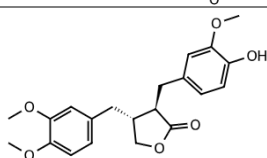
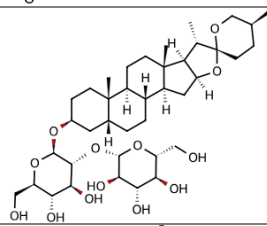
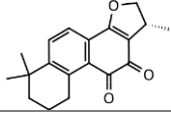
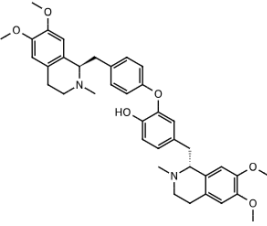
Supplementary Data 1. Binding Affinity Scores and Physicochemical Properties of SHP2 Inhibitor Candidates Based on HyperLab Docking. This supplementary dataset presents the predicted binding affinities of 127 natural compounds and reference inhibitors against the SHP2 allosteric site (PDB ID: 5EHR), calculated using the HyperLab docking platform. Included are each compound's chemical formula, molecular weight, LogP, and topological polar surface area (TPSA). Lower binding energy values (kcal/mol) indicate higher predicted affinity. Compounds with docking failure are marked as "Fail."

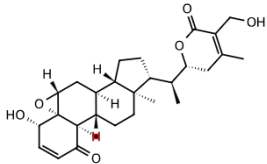
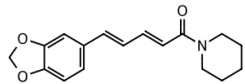
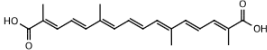
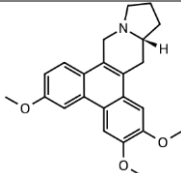
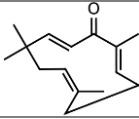
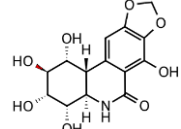
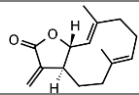
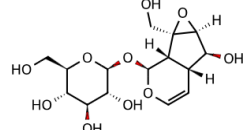
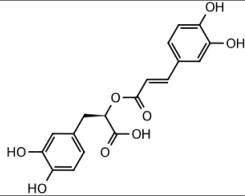
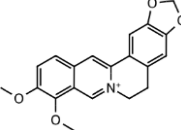
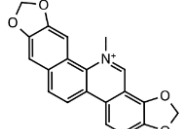
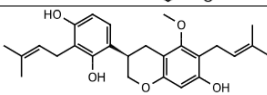
Compound	Structure	Binding score (kcal/mol)	Chemical formula	Molecular weight (g/mol)	LogP	TPSA (Å ²)
SHP009 (positive control)		-10.3	C ₁₆ H ₁₉ Cl ₂ N ₅	352.3	3.4	81
Liensinine		-6.0	C ₃₇ H ₄₂ N ₂ O ₆	610.8	6.5	84
Fascaplysin		-2.7	C ₁₈ H ₁₁ ClN ₂ O	306.8	0.1	37
Emetine		-4.6	C ₂₉ H ₄₀ N ₂ O ₄	480.6	4.9	52
D-limonene		-3.7	C ₁₀ H ₁₆	136.2	3.3	0
Sesquiterpene (AMDT)		-2.9	C ₁₉ H ₂₆ O ₈	382.4	0.1	115
Artemisinin		-1.4	C ₁₅ H ₂₂ O ₅	282.3	2.4	54
Artemether		-2.0	C ₁₆ H ₂₆ O ₅	298.4	2.8	46
Betulin		-3.2	C ₃₀ H ₅₀ O ₂	442.7	7	40

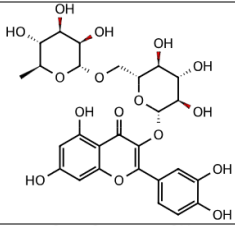
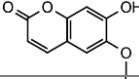
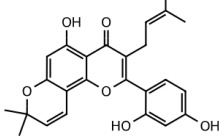
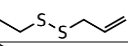
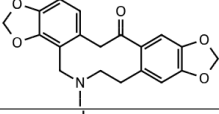
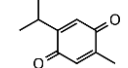
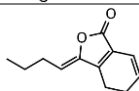
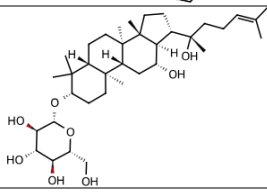
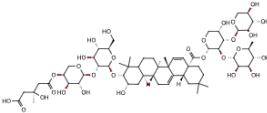
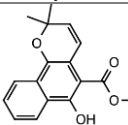
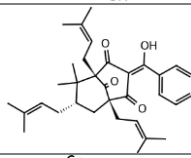
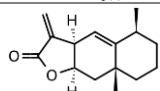
Betulinic Acid		-3.9	C ₃₀ H ₄₈ O ₃	456.7	7.1	58
Gambogic acid		-5.4	C ₃₈ H ₄₄ O ₈	628.8	7.2	119
Fucoxanthin		-6.3	C ₄₂ H ₅₈ O ₆	658.9	8.7	96
Ursolic acid		-3.0	C ₃₀ H ₄₈ O ₃	456.7	7.1	58
Oleanolic acid		-3.9	C ₃₀ H ₄₈ O ₃	456.7	7.2	58
Wogonin		-3.5	C ₁₆ H ₁₂ O ₅	284.3	2.9	80
Luteolin		-4.3	C ₁₅ H ₁₀ O ₆	286.2	2.3	111
Polydatin		-5.0	C ₂₀ H ₂₂ O ₈	390.4	0.4	140
Emodin		-3.4	C ₁₅ H ₁₀ O ₅	270.2	1.9	95
β -elemene		-3.7	C ₁₅ H ₂₄	204.4	4.7	0
Bufalin		-3.6	C ₂₄ H ₃₄ O ₄	386.5	4.2	71
Platycodin-D		Fail	C ₅₇ H ₉₂ O ₂₈	1225.3	-5.4	453
Tanshinone IIA		-2.1	C ₁₉ H ₁₈ O ₃	294.4	4.2	47
Celastrol		-3.5	C ₂₉ H ₃₈ O ₄	450.6	6.7	75

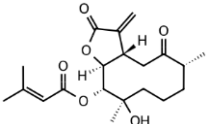
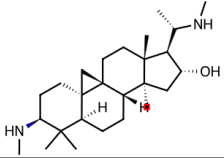
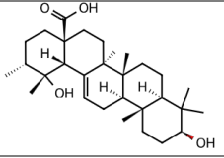
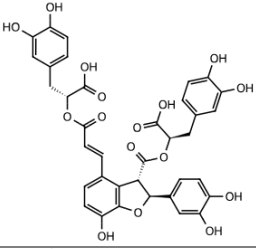
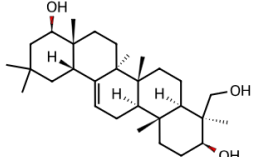
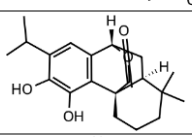
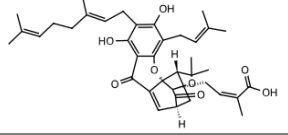
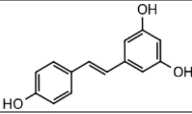
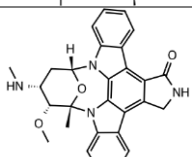
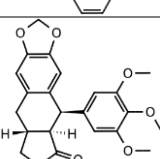
Curcumin		-4.4	C ₂₁ H ₂₀ O ₆	368.4	3.4	93
Cinnamaldehyde		-2.5	C ₉ H ₈ O	132.2	1.9	17
Ophiopogonin B		-3.8	C ₃₉ H ₆₂ O ₁₂	722.9	2.4	177
Trilinolein		Fail	C ₅₇ H ₉₈ O ₆	879.4	17.4	79
Fucoidan		-3.3	C ₇ H ₁₄ O ₇ S	242.2	-1.3	113
Oridonin		-3.8	C ₂₀ H ₂₈ O ₆	364.4	0.4	107
Panaxadiol saponins		-4.6	C ₃₀ H ₅₂ O ₃	460.7	6.7	50
Ganodermanontriol		-4.4	C ₃₀ H ₄₈ O ₄	472.7	5.6	78
Pomiferin		-4.1	C ₂₅ H ₂₄ O ₆	420.5	5.3	100
Bufadienolides		-4.0	C ₂₄ H ₃₄ O ₂	354.5	6.2	30
Actein		-4.1	C ₃₇ H ₅₆ O ₁₁	676.8	3	157
Formononetin		-3.6	C ₁₆ H ₁₂ O ₄	268.3	3.2	60
Narciclasine		-2.9	C ₁₄ H ₁₃ NO ₇	307.3	-1.3	128
Puerarin		-4.0	C ₂₁ H ₂₀ O ₉	416.4	0.4	161

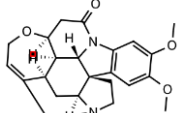
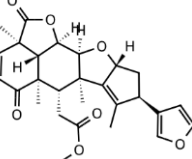
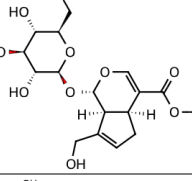
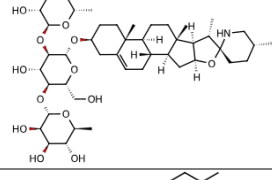
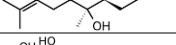
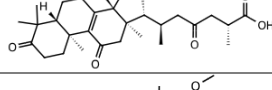
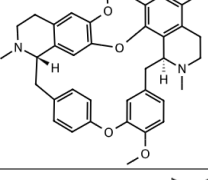
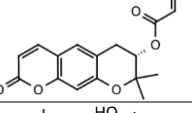
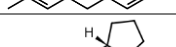
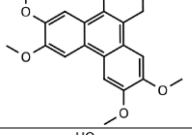
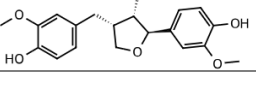
Genipin		-3.3	C11H14O5	226.2	-0.1	76
Evodiamine		-3.0	C19H17N3O	303.4	3.3	39
α -Solanine		+0.8	C45H73NO15	868.1	0.2	241
Osthole		-3.3	C15H16O3	244.3	3.3	39
Ophiopogonin D		-0.6	C44H70O16	855	0.9	236
Ginsenoside Rg5		-5.0	C42H70O12	767	3	199
Icariside II		-4.0	C27H30O10	514.5	2.6	159
Triptolide		-2.7	C20H24O6	360.4	1.1	84
Ginsenoside 20(S)-Rg3		-1.8	C42H72O13	785	2.1	219
Kumatakenin		-3.8	C17H14O6	314.3	2.9	89
Daidzein		-3.5	C15H10O4	254.2	2.9	71
Protoapigenone		-3.8	C15H10O6	286.2	1.1	108

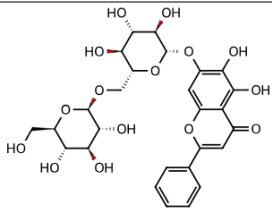
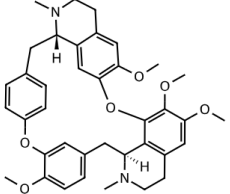
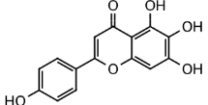
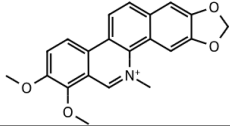
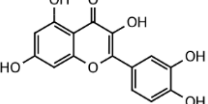
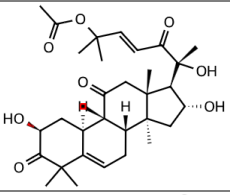
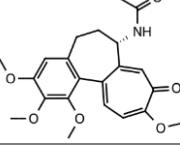
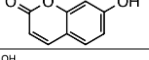
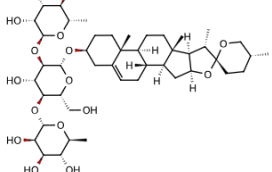
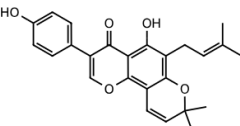
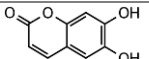
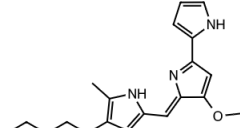
Icariin		-3.4	C33H40O15	676.7	0.1	238
Icaritin		-3.5	C21H20O6	368.4	4.1	100
Stigmasterol		-4.4	C29H48O	412.7	7.8	20
Casticin		-3.3	C19H18O8	374.3	2.9	108
Juglone		-2.8	C10H6O3	174.2	1.3	54
Baicalin		-4.7	C21H18O11	446.4	0.1	187
Baicalein		-4.2	C15H10O5	270.2	2.6	91
Artesunate		-4.0	C19H28O8	384.4	2.6	101
Arctigenin		-4.3	C21H24O6	372.4	3	74
Asparanin A		-0.4	C39H64O13	740.9	1.4	197
Cryptotanshinone		-2.9	C19H20O3	296.4	3.4	43
Dauricine		-5.7	C38H44N2O6	624.8	6.8	73

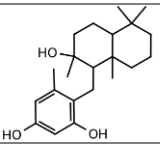
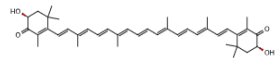
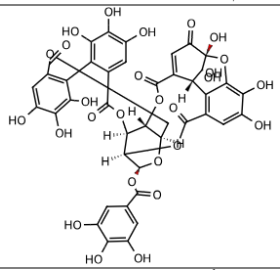
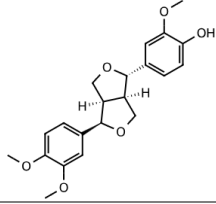
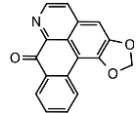
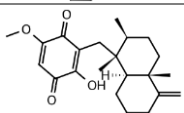
Withaferin A		-4.6	C ₂₈ H ₃₈ O ₆	470.6	3.4	96
Piperine		-3.8	C ₁₇ H ₁₉ NO ₃	285.3	3	39
Crocin		-5.5	C ₂₀ H ₂₄ O ₄	328.4	4.6	75
Antofine		-3.2	C ₂₃ H ₂₅ NO ₃	363.5	4.5	31
Zerumbone		-2.3	C ₁₅ H ₂₂ O	218.3	4.2	17
Pancratistatin		-4.1	C ₁₄ H ₁₅ NO ₈	325.3	-2.2	149
Costunolide		-1.8	C ₁₅ H ₂₀ O ₂	232.3	3.6	26
Catalpol		-3.9	C ₁₅ H ₂₂ O ₁₀	362.3	-3.6	162
Rosmarinic acid		-5.1	C ₁₈ H ₁₆ O ₈	360.3	1.8	145
Berberine		-2.1	C ₂₀ H ₁₈ NO ₄ ⁺	336.4	3.1	41
Sanguinarine		-2.2	C ₂₀ H ₁₄ NO ₄ ⁺	332.3	3.4	41
Licoricidin		-4.8	C ₂₆ H ₃₂ O ₅	424.5	5.5	79

Rutin		-4.7	C ₂₇ H ₃₀ O ₁₆	610.5	-1.7	269
Scopoletin		-2.9	C ₁₀ H ₈ O ₄	192.2	1.5	60
Morusin		-3.4	C ₂₅ H ₂₄ O ₆	420.5	5.3	100
Diallyl disulphide		-3.1	C ₆ H ₁₀ S ₂	146.3	2.7	0
Protopine		-3.2	C ₂₀ H ₁₉ NO ₅	353.4	2.6	57
Thymoquinone		-3.9	C ₁₀ H ₁₂ O ₂	164.2	1.7	34
Z-ligustilide		-4.6	C ₁₂ H ₁₄ O ₂	190.2	2.9	26
Ginsenoside Rh2		-5.1	C ₃₆ H ₆₂ O ₈	622.9	4.3	140
Tubeimoside-1		Fail	C ₆₅ H ₁₀₂ O ₂₉	1319.4	-2.4	456
alpha-Thujone		-3.7	C ₁₀ H ₁₆ O	152.2	2.3	17
Mollugin		-2.6	C ₁₇ H ₁₆ O ₄	284.3	3.5	56
7-epiclusianone		-4.3	C ₃₃ H ₄₂ O ₄	502.7	7.8	71
Selenocysteine		-3.3	C ₃ H ₆ NO ₂ Se	167	-1	63
Alantolactone		-3.2	C ₁₅ H ₂₀ O ₂	232.3	3.2	26

Nepalolide A		-2.1	C ₂₀ H ₂₈ O ₆	364.4	2.5	90
Cyclovirobuxine D		-4.2	C ₂₆ H ₄₆ N ₂ O	402.7	4.6	44
Pomolic acid		-3.5	C ₃₀ H ₄₈ O ₄	472.7	6.2	78
Salvianolic Acid B		-5.8	C ₃₆ H ₃₀ O ₁₆	718.6	3.3	278
Soyasapogenol B		-3.0	C ₃₀ H ₅₀ O ₃	458.7	6.1	61
Carnosol		-3.6	C ₂₀ H ₂₆ O ₄	330.4	4.3	67
Tetramethylpyrazine		-2.0	C ₈ H ₁₂ N ₂	136.2	1.7	26
Gambogenic acid		-5.9	C ₃₈ H ₄₆ O ₈	630.8	7.3	130
Resveratrol		-4.1	C ₁₄ H ₁₂ O ₃	228.2	3	61
Germacrone		-3.1	C ₁₅ H ₂₂ O	218.3	4.4	17
Staurosporine		-4.3	C ₂₈ H ₂₆ N ₄ O ₃	466.5	4.4	69
Deoxypodophyllotoxin		-2.7	C ₂₂ H ₂₂ O ₇	398.4	2.9	72

Brucine		-2.9	C23H26N2O4	394.5	2.1	51
Nimbolide		-3.4	C27H30O7	466.5	3.7	92
Geniposide		-4.0	C17H24O10	388.4	-2.2	155
Solamargine		-2.9	C45H73NO15	868.1	0.8	238
α -bisabolol		-3.7	C15H26O	222.4	4.2	20
Ganoderic acid A		-4.9	C30H44O7	516.7	4.1	129
Hernandezine		-2.9	C39H44N2O7	652.8	7.2	71
Decursin		-3.4	C19H20O5	328.4	3.4	66
Linalool		-3.3	C10H18O	154.3	2.7	20
Tylophorine		-2.9	C24H27NO4	393.5	4.5	40
Lariciresinol		-4.3	C20H24O6	360.4	2.7	88

Oroxin B		-5.3	C27H30O15	594.5	-2.1	249
Tetrandrine		-3.2	C38H42N2O6	622.8	7.2	62
Scutellarein		-3.8	C15H10O6	286.2	2.3	111
Chelerythrine		-2.3	C21H18NO4+	348.4	3.7	41
Quercetin		-3.5	C15H10O7	302.2	2	131
Cucurbitacin B		-5.6	C32H46O8	558.7	3.5	138
Colchicine		-2.4	C22H25NO6	399.4	2.9	83
Umbelliferone		-2.9	C9H6O3	162.1	1.5	50
Dioscin		-1.0	C45H72O16	869.1	1.2	236
Osajin		-4.0	C25H24O5	404.5	5.6	80
Esculetin		-2.9	C9H6O4	178.1	1.2	71
Prodigosin		-4.5	C20H25N3O	323.4	4.8	53

Neolbaconol		-5.5	C22H34O3	346.5	4.9	61
Astaxanthin		-5.9	C40H52O4	596.9	8.9	75
Geraniin		+4.6	C41H28O27	952.6	-1.1	450
Phillygenin		-3.5	C21H24O6	372.4	3.5	66
Liriodenine		-2.6	C17H9NO3	275.3	3.2	48
Ilimaquinone		-3.1	C22H30O4	358.5	4.7	64