

Sesquiterpenoids from the Sunflower family as potential anti-inflammatory candidates: A review

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Cheng Chen and Zheling Feng contributed equally to this work.

Table S1. Molecular descriptors of anti-inflammation sesquiterpenoids from Asteraceae plants.

No	Formula	MW	Stereogenic Centers	#H-bond acceptors	#H-bond donors	#Rotatable bonds	rings	Fraction Csp3
1	C ₁₇ H ₂₂ O ₅	306.35	6	5	0	2	3	0.71
2	C ₁₅ H ₂₀ O ₄	264.32	6	4	1	0	3	0.73
3	C ₁₅ H ₂₀ O ₃	248.32	5	3	0	0	3	0.73
4	C ₁₅ H ₂₀ O ₃	248.32	5	3	1	0	3	0.67
5	C ₁₅ H ₂₀ O ₃	248.32	5	3	1	0	3	0.67
6	C ₁₅ H ₂₂ O ₃	250.33	5	3	1	0	3	0.8
7	C ₁₅ H ₂₂ O ₃	250.33	5	3	1	0	3	0.8
8	C ₁₅ H ₂₀ O ₃	248.32	6	3	0	0	4	0.8
9	C ₁₅ H ₂₀ O ₃	248.32	5	3	1	0	3	0.67
10	C ₁₅ H ₁₈ O ₃	246.3	4	3	0	0	3	0.6
11	C ₃₂ H ₄₀ O ₈	552.66	13	8	2	2	8	0.72
12	C ₃₂ H ₄₀ O ₉	568.65	13	9	2	3	8	0.72
13	C ₃₈ H ₅₂ O ₉	652.81	12	9	1	11	7	0.74
14	C ₃₄ H ₄₄ O ₉	596.71	11	9	1	8	7	0.71
15	C ₃₄ H ₄₄ O ₉	596.71	11	9	1	8	7	0.71
16	C ₃₆ H ₄₈ O ₉	624.76	11	9	1	9	7	0.72
17	C ₃₇ H ₅₀ O ₉	638.79	12	9	1	10	7	0.73
18	C ₃₇ H ₅₀ O ₉	638.79	11	9	1	10	7	0.73
19	C ₃₂ H ₄₀ O ₇	536.66	10	7	1	6	7	0.66
20	C ₃₄ H ₄₄ O ₉	596.71	11	9	1	8	7	0.71
21	C ₃₄ H ₄₆ O ₈	582.72	12	8	1	7	7	0.76
22	C ₃₂ H ₄₄ O ₈	556.69	12	8	2	6	7	0.78
23	C ₃₂ H ₄₄ O ₇	540.69	11	7	1	6	7	0.78
24	C ₃₂ H ₄₄ O ₈	556.69	12	8	2	6	7	0.78
25	C ₃₂ H ₄₂ O ₈	554.67	12	8	2	5	7	0.72
26	C ₃₄ H ₄₂ O ₁₀	610.69	12	10	1	7	7	0.68
27	C ₃₂ H ₄₀ O ₈	552.66	11	8	1	5	7	0.69

28	C ₃₂ H ₄₀ O ₈	552.66	11	8	1	5	7	0.69
29	C ₁₅ H ₁₈ O ₄	262.3	5	4	1	0	4	0.67
30	C ₁₅ H ₂₀ O ₄	264.32	5	4	2	0	3	0.67
31	C ₁₅ H ₁₉ ClO ₃	282.76	5	3	1	0	3	0.67
32	C ₃₅ H ₄₀ O ₈	588.69	11	8	1	3	8	0.6
33	C ₃₀ H ₄₀ O ₅	480.64	11	5	1	0	8	0.8
34	C ₃₀ H ₄₀ O ₇	512.63	15	7	2	0	8	0.83
35	C ₃₀ H ₄₀ O ₆	496.64	15	6	1	0	8	0.87
36	C ₂₉ H ₃₈ O ₅	466.61	9	5	2	4	5	0.69
37	C ₃₀ H ₄₀ O ₅	480.64	9	5	2	4	5	0.7
38	C ₃₀ H ₄₀ O ₆	496.64	9	6	3	4	5	0.7
39	C ₃₀ H ₄₀ O ₅	480.64	8	5	2	4	6	0.7
40	C ₃₀ H ₄₀ O ₆	496.64	9	6	3	4	6	0.7
41	C ₃₀ H ₄₀ O ₅	480.64	8	5	2	4	6	0.7
42	C ₃₀ H ₄₂ O ₅	482.65	10	5	2	2	7	0.8
43	C ₃₀ H ₄₂ O ₆	498.65	11	6	3	2	7	0.8
44	C ₃₀ H ₄₂ O ₆	498.65	11	6	3	2	7	0.8
45	C ₃₀ H ₄₀ O ₆	496.64	8	6	2	6	4	0.63
46	C ₃₀ H ₄₂ O ₆	498.65	8	6	2	6	4	0.7
47	C ₃₀ H ₃₈ O ₇	510.62	7	7	2	7	4	0.6
48	C ₁₅ H ₁₆ O ₄	260.29	3	4	1	1	3	0.47
49	C ₁₅ H ₁₆ O ₅	276.28	4	5	2	1	3	0.47
50	C ₁₅ H ₁₈ O ₄	262.3	5	4	1	0	3	0.6
51	C ₂₃ H ₂₂ O ₇	410.42	4	7	2	5	4	0.35
52	C ₃₀ H ₃₄ O ₇	506.59	11	7	2	0	7	0.63
53	C ₃₀ H ₃₆ O ₇	508.6	12	7	1	0	7	0.73
54	C ₃₀ H ₃₂ O ₈	520.57	10	8	0	0	7	0.6
55	C ₃₀ H ₃₄ O ₈	522.59	9	8	1	6	5	0.57
56	C ₄₀ H ₄₄ O ₁₂	716.77	12	12	1	8	7	0.55
57	C ₃₂ H ₄₀ O ₅	504.66	10	5	0	4	6	0.66

58	C ₃₂ H ₄₀ O ₅	504.66	10	5	0	4	6	0.66
59	C ₃₂ H ₄₂ O ₅	506.67	10	5	0	4	6	0.72
60	C ₃₂ H ₄₂ O ₅	506.67	9	5	0	4	6	0.72
61	C ₃₂ H ₄₂ O ₅	506.67	8	5	0	4	5	0.66
62	C ₃₂ H ₄₂ O ₅	506.67	8	5	0	4	5	0.66
63	C ₃₂ H ₄₄ O ₅	508.69	9	5	0	4	5	0.72
64	C ₃₂ H ₄₂ O ₅	506.67	10	5	0	4	6	0.72
65	C ₃₂ H ₄₂ O ₅	506.67	10	5	1	4	6	0.69
66	C ₂₂ H ₃₂ O ₃	344.49	5	3	0	5	2	0.64
67	C ₂₂ H ₃₂ O ₃	344.49	5	3	0	5	2	0.64
68	C ₂₇ H ₃₈ O ₅	442.59	5	5	0	8	2	0.59
69	C ₂₂ H ₃₂ O ₅	376.49	6	5	0	7	2	0.68
70	C ₂₃ H ₃₄ O ₅	390.51	6	5	0	8	2	0.7
71	C ₂₇ H ₄₀ O ₇	476.6	7	7	0	11	2	0.7
72	C ₂₅ H ₃₆ O ₅	416.55	5	5	0	8	2	0.64
73	C ₂₁ H ₃₂ O ₄	348.48	6	4	1	5	2	0.71
74	C ₂₂ H ₃₄ O ₄	362.5	6	4	1	6	2	0.73
75	C ₂₃ H ₃₆ O ₅	392.53	7	5	1	7	2	0.74
76	C ₂₆ H ₃₆ O ₆	444.56	5	6	0	11	2	0.58
77	C ₂₄ H ₃₂ O ₈	448.51	6	8	0	11	2	0.58
78	C ₂₅ H ₃₄ O ₆	430.53	5	6	0	10	2	0.56
79	C ₂₅ H ₃₄ O ₆	430.53	2	6	1	9	1	0.48
80	C ₂₂ H ₃₀ O ₆	390.47	2	6	1	8	1	0.5
81	C ₁₅ H ₂₀ O ₃	248.32	4	3	0	0	3	0.73
82	C ₁₅ H ₂₂ O ₃	250.33	5	3	1	0	3	0.8
83	C ₁₅ H ₂₀ O ₄	264.32	6	4	1	0	3	0.73
84	C ₁₅ H ₂₂ O ₅	282.33	7	5	0	0	5	0.93
85	C ₁₅ H ₁₆ O ₂	228.29	0	2	1	2	2	0.27
86	C ₁₅ H ₁₈ O	214.3	0	1	1	1	2	0.33
87	C ₁₅ H ₂₀ O ₃	248.32	2	3	2	2	2	0.53

88	C ₁₅ H ₂₄	204.35	2	0	0	0	2	0.73
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Table S2. Biophysicochemical properties of anti-inflammation sesquiterpenoids from Asteraceae plants.

No	MR	TPSA	iLOGP	XLOGP3	WLOGP	MLOGP	Silicos- IT Log P	Consnsus Log P	Ali Log S	ESOL Log S	Silicos- IT LogSw
1	79.53	69.67	2.61	1.7	2.04	2	2.48	2.17	-2.78	-2.68	-2.79
2	69.79	63.6	1.68	1.13	1.47	1.62	2.03	1.59	-2.06	-2.19	-2.15
3	68.63	43.37	2.27	2.1	2.5	2.47	2.94	2.46	-2.64	-2.7	-2.96
4	69.41	46.53	2.45	1.83	2.21	2.47	2.62	2.32	-2.43	-2.53	-2.49
5	69.41	46.53	2.44	1.83	2.21	2.47	2.62	2.31	-2.43	-2.53	-2.49
6	69.89	46.53	2.49	1.94	2.29	2.56	2.35	2.33	-2.54	-2.61	-2.26
7	69.89	46.53	2.49	1.94	2.29	2.56	2.35	2.33	-2.54	-2.61	-2.26
8	67.73	38.83	2.68	2.4	2.45	2.56	3.12	2.64	-2.86	-2.89	-2.79
9	69.41	46.53	2.54	1.83	2.21	2.47	2.62	2.33	-2.43	-2.53	-2.49
10	68.41	43.37	2.24	1.82	2.42	2.38	2.93	2.36	-2.35	-2.51	-2.94
11	145.12	119.36	2.93	2.29	3.41	3.39	3.23	3.05	-4.43	-4.58	-4.07
12	146.65	128.59	3.6	2.58	3.91	3.42	3.06	3.31	-4.93	-4.79	-4.04
13	176.46	125.43	4.55	4.38	5.79	4.42	6.47	5.12	-6.73	-5.92	-6.68
14	157.23	125.43	3.95	2.57	4.37	3.71	4.97	3.91	-4.85	-4.63	-5.51
15	157.23	125.43	3.43	2.57	4.37	3.71	4.97	3.81	-4.85	-4.63	-5.51
16	166.84	125.43	4.3	3.62	5.01	4.07	5.63	4.53	-5.94	-5.4	-5.91
17	171.65	125.43	4.3	3.97	5.4	4.25	6.05	4.79	-6.3	-5.64	-6.29
18	171.65	125.43	3.99	3.84	5.4	4.25	6.05	4.71	-6.17	-5.56	-6.29
19	145.85	99.13	3.52	3.13	4.61	4.1	5.19	4.11	-4.88	-4.74	-5.52
20	157.27	125.43	4.06	2.74	4.37	3.71	4.97	3.97	-5.03	-4.74	-5.51
21	156.62	116.2	3.9	2.42	4.72	3.76	5.14	3.99	-4.5	-4.52	-5.56
22	148.37	119.36	3.68	1.89	4.65	3.47	4.16	3.57	-4.02	-4.09	-4.68
23	146.8	99.13	3.76	3.27	4.91	4.26	5.04	4.25	-5.03	-4.86	-5.5
24	148	119.36	3.83	2.28	3.88	3.47	4.16	3.52	-4.42	-4.33	-4.68

25	147.49	119.36	3.13	2.48	3.66	3.39	3.87	3.3	-4.63	-4.51	-4.33
26	157.43	142.5	2.9	1.53	3.55	2.86	3.84	2.94	-4.13	-4.13	-4.58
27	146.53	116.2	3.97	2.07	4.01	3.31	4.19	3.51	-4.14	-4.24	-4.81
28	146.53	116.2	2.88	2.07	4.01	3.31	4.19	3.29	-4.14	-4.24	-4.81
29	68.46	59.06	2.43	0.64	1.49	1.62	2.59	1.75	-1.46	-1.87	-2.42
30	70.58	66.76	2.14	0.36	1.33	1.62	1.83	1.45	-1.33	-1.71	-1.89
31	74.21	46.53	2.51	1.64	2.57	2.72	2.95	2.48	-2.23	-2.63	-3.07
32	157.67	116.2	3.44	3.82	4.48	3.7	4.7	4.03	-5.96	-5.7	-5.17
33	133.57	72.83	3.79	3.97	5.12	4.77	4.62	4.45	-5.2	-5.32	-5.33
34	135.96	110.13	3.13	1.76	3.06	3.15	2.93	2.81	-3.69	-4.13	-3.83
35	133.61	82.06	0	2.65	4.04	4.04	3.7	2.89	-4.02	-4.59	-4.48
36	132.75	91.67	3.22	5.32	5.67	4.41	4.32	4.59	-7	-5.82	-3.95
37	137.56	91.67	3.24	5.09	6.06	4.6	4.84	4.76	-6.76	-5.76	-4.54
38	138.72	111.9	3.07	3.6	5.17	3.79	4.34	3.99	-5.64	-4.92	-4.17
39	137.56	91.67	2.85	4.76	6.2	4.6	5.23	4.73	-6.42	-5.55	-4.99
40	138.72	111.9	2.79	3.46	5.17	3.79	4.34	3.91	-5.49	-4.83	-4.17
41	137.56	91.67	3.26	4.76	6.2	4.6	5.23	4.81	-6.42	-5.55	-4.99
42	136.47	83.83	3.73	5.16	5.67	4.77	4.86	4.84	-6.67	-5.95	-5.06
43	137.63	104.06	3.26	4	4.64	3.95	3.97	3.97	-5.89	-5.32	-4.24
44	137.67	104.06	3.15	4.16	4.64	3.95	3.97	3.97	-6.05	-5.42	-4.24
45	140.13	100.9	3.97	4.61	5.18	3.71	4.56	4.41	-6.45	-5.43	-4.17
46	140.64	100.9	3.82	5.17	5.4	3.79	4.97	4.63	-7.04	-5.79	-4.64
47	140.37	117.97	3.11	4	4.5	2.83	4.68	3.83	-6.18	-5.06	-4.28
48	69.1	63.6	1.93	0.26	1.31	1.44	2.29	1.45	-1.16	-1.55	-2.36
49	70.26	83.83	1.5	-0.72	0.28	0.61	1.39	0.61	-0.56	-1.03	-1.55
50	69.35	63.6	1.75	0.77	1.39	1.53	2.02	1.49	-1.69	-1.95	-2.13
51	106.51	110.13	1.99	1.1	1.78	1.61	2.88	1.87	-3.01	-2.9	-4.08
52	134.54	110.13	2.24	1.66	2.97	2.91	3.87	2.73	-3.59	-4.03	-4.56
53	134.49	106.97	2.67	1.84	3.33	2.99	3.62	2.89	-3.71	-4.15	-4.55

54	134.85	105.2	2.73	2.66	3.51	3.26	4.12	3.26	-4.52	-4.74	-5.08
55	138.6	124.04	2.94	2.04	3.76	2.78	4.57	3.22	-4.27	-3.97	-4.66
56	184.28	168.8	4.15	3.43	4.08	2.92	4.54	3.82	-6.66	-5.92	-4.37
57	143.87	69.67	4.13	3.99	5.91	4.9	6.23	5.03	-5.15	-5.22	-6.21
58	143.87	69.67	4.16	3.99	5.91	4.9	6.23	5.04	-5.15	-5.22	-6.21
59	144.08	69.67	4.12	4.95	6.13	4.98	6.35	5.3	-6.15	-5.84	-6.43
60	144.08	69.67	4.16	5.05	6.13	4.98	6.35	5.33	-6.25	-5.9	-6.43
61	145.98	69.67	4.13	4.21	6.44	4.9	6.07	5.15	-5.38	-5.37	-6.18
62	145.98	69.67	4.27	4.21	6.44	4.9	6.07	5.18	-5.38	-5.37	-6.18
63	146.46	69.67	4.17	5.29	6.52	4.98	6.08	5.41	-6.5	-6.06	-6.2
64	144.08	69.67	4.19	4.71	6.13	4.98	6.07	5.22	-5.9	-5.68	-6.18
65	144.83	72.83	4.01	4.44	5.7	4.98	5.9	5.01	-5.69	-5.51	-5.74
66	103.44	43.37	4.14	4.87	5.03	3.92	5.04	4.6	-5.52	-4.71	-4.28
67	103.44	43.37	4.14	4.87	5.03	3.92	5.04	4.6	-5.52	-4.71	-4.28
68	128.29	69.67	4.14	4.87	5.52	3.92	5.04	4.6	-5.52	-4.71	-4.28
69	105.46	69.67	3.54	3.45	3.87	3.05	4.05	3.59	-4.59	-3.89	-3.33
70	110.27	69.67	3.9	4.14	4.26	3.27	4.46	4.01	-5.31	-4.34	-3.72
71	130.78	95.97	4.56	5.2	4.44	3.21	4.83	4.45	-6.96	-5.34	-3.92
72	119.41	69.67	4.23	5.54	4.82	3.61	5.12	4.66	-6.76	-5.38	-4.12
73	100.27	63.6	3.5	3.83	3.69	2.94	3.77	3.54	-4.86	-4.08	-3.09
74	105.08	63.6	3.6	4.51	4.08	3.16	4.18	3.91	-5.57	-4.53	-3.48
75	110.97	72.83	3.83	4.49	3.7	2.54	3.87	3.69	-5.74	-4.64	-3.35
76	124.87	82.2	4.71	5.99	4.79	2.92	5.82	4.85	-7.49	-5.64	-4.01
77	117.01	108.5	3.29	3.71	3	1.73	4.16	3.18	-5.68	-4.23	-2.97
78	120.06	82.2	3.29	3.71	4.4	1.73	4.16	3.18	-5.68	-4.23	-2.97
79	121.74	89.9	3.29	3.71	4.65	1.73	4.16	3.18	-5.68	-4.23	-2.97
80	107.79	89.9	3.29	3.71	3.71	1.73	4.16	3.18	-5.68	-4.23	-2.97
81	68.63	43.37	2.3	1.37	2.64	2.47	3.05	2.37	-1.88	-2.24	-3.16
82	69.59	46.53	2.45	1.67	2.44	2.56	2.46	2.32	-2.26	-2.44	-2.46

83	69.83	63.6	2.08	1.25	1.47	1.62	1.75	1.63	-2.18	-2.27	-1.9
84	70.38	53.99	2.84	2.9	2.39	2.21	1.82	2.43	-3.69	-3.42	-2.03
85	70.9	37.3	2.41	3.77	3.79	2.9	4.16	3.41	-4.25	-3.93	-4.66
86	70.48	20.23	2.75	4.67	4.29	3.91	4.47	4.02	-4.82	-4.51	-5.1
87	71.11	57.53	2.14	2.66	3.02	2.65	2.89	2.67	-3.52	-3.17	-3.28
88	68.78	0	3.22	4.38	4.73	4.63	4.19	4.23	-4.1	-3.87	-3.77

Table S3. Molecular descriptors of marketed drugs.

Drug type	Stereogenic Centers	MW (g/mol)	LogP	#H-bond acceptors	#H-bond donors	Polar surface area (Å ²)	#Rotatable bonds
Natural products	7.6	546.8	0.7	10	5.4	105.3	9.4
Natural derivatives	4.1	436.7	1.7	8.1	3.5	94.1	7.4
Synthetic	0.5	325.2	2.4	4.8	1.6	53.7	5.4
Assumed synthetic	0.8	352.1	3.1	5	1.5	57.2	6.1
Natural products macrocycle	12	1008	1.4	19.4	8.8	211.4	17.5
Natural products polycyclic	4.3	456.7	2.5	8.3	3.5	86.9	7.4

Table S4. Violations of drug-likeness rules by the anti-inflammation sesquiterpenoids from Asteraceae plants. For each compound, the type of violations of each rule was described.

No	Lipinski	Ghose	Veber	Egan	Muegge
1	0	0	0	0	0
2	0	0	0	0	0
3	0	0	0	0	0
4	0	0	0	0	0
5	0	0	0	0	0
6	0	0	0	0	0
7	0	0	0	0	0
8	0	0	0	0	0
9	0	0	0	0	0
10	0	0	0	0	0
11	1	3	0	0	0
12	1	3	0	0	0
13	2	4	1	0	1
14	1	3	0	0	0
15	1	3	0	0	0
16	1	3	0	0	1
17	2	3	0	0	1
18	2	3	0	0	1
19	1	3	0	0	0
20	1	3	0	0	0
21	1	3	0	0	0
22	1	3	0	0	0
23	2	3	0	0	0
24	1	3	0	0	0
25	1	3	0	0	0
26	1	3	1	1	1
27	1	3	0	0	0
28	1	3	0	0	0
29	0	0	0	0	0
30	0	0	0	0	0
31	0	0	0	0	0
32	1	3	0	0	0
33	1	3	0	0	0
34	1	3	0	0	0
35	0	3	0	0	1
36	1	3	0	0	1
37	1	4	0	1	1
38	0	3	0	0	0
39	1	4	0	1	0
40	0	3	0	0	0
41	1	4	0	1	0
42	1	4	0	0	1
43	0	3	0	0	0
44	0	3	0	0	0

45	0	3	0	0	0
46	0	3	0	0	1
47	1	3	0	0	0
48	0	0	0	0	0
49	0	0	0	0	0
50	0	0	0	0	0
51	0	0	0	0	0
52	1	3	0	0	0
53	1	3	0	0	0
54	1	2	0	0	0
55	1	3	0	0	0
56	2	3	1	1	3
57	2	4	0	1	0
58	2	4	0	1	0
59	2	4	0	1	0
60	2	4	0	1	1
61	2	4	0	1	0
62	2	4	0	1	0
63	2	4	0	1	1
64	2	4	0	1	0
65	2	4	0	0	0
66	0	0	0	0	0
67	0	0	0	0	0
68	0	0	0	0	0
69	0	0	0	0	0
70	0	0	0	0	0
71	0	2	1	0	1
72	0	0	0	0	1
73	0	0	0	0	0
74	0	0	0	0	0
75	0	0	0	0	0
76	0	0	1	0	1
77	0	0	1	0	0
78	0	0	1	0	0
79	0	0	1	0	0
80	0	0	1	0	0
81	0	0	0	0	0
82	0	0	0	0	0
83	0	0	0	0	0
84	0	0	0	0	0
85	0	0	0	0	0
86	0	0	0	0	1
87	0	0	0	0	0
88	1	0	0	0	1

MW – molecular weight, MR - molar refractivity, TNA - total number of atoms, PSA – polar surface area, HBA – hydrogen bond acceptor, HBD – hydrogen bond donor, RB - rotatable bonds, LOG P – considered log P value calculated by XLOGP3.

Table S5. Absorption and Metabolism parameters of anti-inflammation sesquiterpenoids from Asteraceae plants.

	GI absorption	BBB permeant	P-gp substrate	CYP1 A2 inhibitor	CYP2C 19 inhibitor	CYP2 C9 inhibitor	CYP2 D6 inhibitor	CYP3 A4 inhibitor
1	High	Yes	No	No	No	No	No	No
2	High	Yes	No	No	No	No	No	No
3	High	Yes	No	No	No	No	No	No
4	High	Yes	No	No	No	No	No	No
5	High	Yes	No	No	No	No	No	No
6	High	Yes	No	No	No	No	No	No
7	High	Yes	No	No	No	No	No	No
8	High	Yes	No	No	No	No	No	No
9	High	Yes	No	No	No	No	No	No
10	High	Yes	No	No	No	No	No	No
11	High	No	Yes	No	No	No	No	No
12	Low	No	Yes	No	No	No	No	No
13	Low	No	Yes	No	No	No	No	No
14	Low	No	Yes	No	No	No	No	No
15	Low	No	Yes	No	No	No	No	No
16	Low	No	Yes	No	No	No	No	No
17	Low	No	Yes	No	No	No	No	No
18	Low	No	Yes	No	No	No	No	No
19	High	No	Yes	No	No	No	No	No
20	Low	No	Yes	No	No	No	No	No
21	High	No	Yes	No	No	No	No	No
22	Low	No	Yes	No	No	No	No	No
23	High	No	Yes	No	No	No	No	No
24	High	No	Yes	No	No	No	No	No
25	High	No	Yes	No	No	No	No	No
26	Low	No	Yes	No	No	No	No	No
27	High	No	Yes	No	No	No	No	No
28	High	No	Yes	No	No	No	No	No
29	High	Yes	Yes	No	No	No	No	No
30	High	Yes	Yes	No	No	No	No	No
31	High	Yes	No	No	No	No	No	No
32	High	No	Yes	No	No	No	No	No
33	High	No	Yes	No	No	No	No	No
34	High	No	Yes	No	No	No	No	No
35	High	No	Yes	No	No	No	No	No
36	High	No	Yes	No	No	Yes	No	No
37	High	No	Yes	No	No	Yes	No	No
38	Low	No	Yes	No	No	Yes	No	Yes
39	Low	No	Yes	No	No	Yes	No	No
40	Low	No	Yes	No	No	No	No	Yes
41	Low	No	Yes	No	No	Yes	No	No
42	High	No	Yes	No	No	No	No	No
43	High	No	Yes	No	No	No	No	No

44	High	No	Yes	No	No	No	No	No
45	High	No	Yes	No	No	Yes	No	Yes
46	High	No	Yes	No	No	Yes	No	Yes
47	High	No	Yes	No	No	Yes	No	Yes
48	High	Yes	No	No	No	No	No	No
49	High	No	No	No	No	No	No	No
50	High	Yes	No	No	No	No	No	No
51	High	No	Yes	No	No	No	No	No
52	High	No	Yes	No	No	No	No	No
53	High	No	Yes	No	No	No	No	No
54	High	No	Yes	No	No	No	No	No
55	High	No	Yes	No	No	No	No	No
56	Low	No	Yes	No	No	Yes	No	No
57	High	No	Yes	No	No	Yes	No	No
58	High	No	Yes	No	No	Yes	No	No
59	High	No	Yes	No	No	Yes	No	No
60	High	No	Yes	No	No	Yes	No	No
61	High	No	Yes	No	No	Yes	No	No
62	High	No	Yes	No	No	Yes	No	No
63	High	No	Yes	No	No	Yes	No	No
64	High	No	Yes	No	No	Yes	No	No
65	High	No	Yes	No	No	Yes	No	No
66	High	Yes	No	No	Yes	Yes	Yes	Yes
67	High	Yes	No	No	Yes	Yes	Yes	Yes
68	High	Yes	No	No	Yes	Yes	Yes	Yes
69	High	Yes	No	No	No	No	Yes	Yes
70	High	Yes	No	No	No	Yes	Yes	Yes
71	High	No	No	No	No	Yes	No	Yes
72	High	Yes	No	No	No	Yes	Yes	Yes
73	High	Yes	No	No	No	No	No	Yes
74	High	Yes	No	No	No	Yes	Yes	Yes
75	High	Yes	No	No	No	No	Yes	Yes
76	High	No	No	No	No	Yes	No	Yes
77	High	No	No	No	No	No	Yes	No
78	High	No	No	No	No	No	Yes	No
79	High	No	No	No	No	No	Yes	No
80	High	No	No	No	No	No	Yes	No
81	High	Yes	No	No	No	No	No	No
82	High	Yes	No	No	No	No	No	No
83	High	Yes	No	No	No	No	No	No
84	High	Yes	No	Yes	No	No	No	No
85	High	Yes	No	Yes	Yes	No	Yes	No
86	High	Yes	No	No	No	No	Yes	No
87	High	Yes	No	No	No	No	Yes	No
88	Low	No	No	No	Yes	Yes	No	No

Table S6. Toxicity and Drug-likeness analysis of anti-inflammation sesquiterpenoids

from Asteraceae plants.

No	hERG	DILI	Carcinogenicity	Lipinski	Pfizer	GSK	GoldenTriangle
1	0.026	0.874	0.672	Accepted	Accepted	Accepted	Accepted
2	0.032	0.426	0.793	Accepted	Accepted	Accepted	Accepted
3	0.028	0.595	0.863	Accepted	Accepted	Accepted	Accepted
4	0.023	0.654	0.766	Accepted	Accepted	Accepted	Accepted
5	0.023	0.725	0.772	Accepted	Accepted	Accepted	Accepted
6	0.025	0.804	0.47	Accepted	Accepted	Accepted	Accepted
7	0.025	0.804	0.47	Accepted	Accepted	Accepted	Accepted
8	0.07	0.904	0.879	Accepted	Accepted	Accepted	Accepted
9	0.035	0.482	0.859	Accepted	Accepted	Accepted	Accepted
10	0.01	0.899	0.751	Accepted	Accepted	Accepted	Accepted
11	0.031	0.26	0.703	Accepted	Accepted	Rejected	Rejected
12	0.083	0.133	0.773	Accepted	Accepted	Rejected	Rejected
13	0.01	0.889	0.128	Accepted	Accepted	Rejected	Rejected
14	0.05	0.891	0.122	Accepted	Accepted	Rejected	Rejected
15	0.014	0.892	0.19	Accepted	Accepted	Rejected	Rejected
16	0.026	0.91	0.119	Accepted	Accepted	Rejected	Rejected
17	0.031	0.9	0.105	Accepted	Accepted	Rejected	Rejected
18	0.011	0.922	0.124	Accepted	Accepted	Rejected	Rejected

19	0.219	0.489	0.274	Accepted	Accepted	Rejected	Rejected
20	0.047	0.858	0.239	Accepted	Accepted	Rejected	Rejected
21	0.097	0.812	0.061	Accepted	Accepted	Rejected	Rejected
22	0.149	0.698	0.164	Accepted	Accepted	Rejected	Rejected
23	0.268	0.861	0.103	Accepted	Accepted	Rejected	Rejected
24	0.047	0.677	0.268	Accepted	Accepted	Rejected	Rejected
25	0.35	0.842	0.533	Accepted	Accepted	Rejected	Rejected
26	0.032	0.874	0.388	Accepted	Accepted	Rejected	Rejected
27	0.084	0.713	0.865	Accepted	Accepted	Rejected	Rejected
28	0.013	0.709	0.757	Accepted	Accepted	Rejected	Rejected
29	0.022	0.307	0.942	Accepted	Accepted	Accepted	Accepted
30	0.035	0.153	0.175	Accepted	Accepted	Accepted	Accepted
31	0.018	0.162	0.814	Accepted	Rejected	Accepted	Accepted
32	0.009	0.139	0.701	Accepted	Accepted	Rejected	Rejected
33	0.047	0.66	0.828	Accepted	Rejected	Rejected	Accepted
34	0.029	0.788	0.031	Accepted	Accepted	Rejected	Rejected
35	0.413	0.777	0.081	Accepted	Accepted	Rejected	Accepted
36	0.096	0.949	0.442	Accepted	Accepted	Rejected	Accepted
37	0.06	0.923	0.357	Accepted	Accepted	Rejected	Accepted
38	0.025	0.835	0.606	Accepted	Accepted	Rejected	Accepted

39	0.01	0.90 3	0.776	Accepted	Accepted	Rejected	Accepted
40	0.006	0.86 8	0.773	Accepted	Accepted	Rejected	Accepted
41	0.011	0.94 9	0.643	Accepted	Accepted	Rejected	Accepted
42	0.741	0.34 2	0.701	Accepted	Accepted	Rejected	Accepted
43	0.315	0.10 3	0.761	Accepted	Accepted	Rejected	Accepted
44	0.055	0.17 1	0.877	Accepted	Accepted	Rejected	Accepted
45	0.17	0.97 3	0.088	Accepted	Accepted	Rejected	Accepted
46	0.023	0.97 6	0.62	Accepted	Accepted	Rejected	Accepted
47	0.019	0.87 6	0.735	Accepted	Accepted	Rejected	Rejected
48	0.002	0.75 1	0.179	Accepted	Accepted	Accepted	Accepted
49	0.004	0.90 1	0.538	Accepted	Accepted	Accepted	Accepted
50	0.039	0.15 2	0.937	Accepted	Accepted	Accepted	Accepted
51	0.006	0.96	0.384	Accepted	Accepted	Rejected	Accepted
52	0.533	0.18 3	0.9	Accepted	Accepted	Rejected	Rejected
53	0.008	0.78 1	0.161	Accepted	Accepted	Rejected	Rejected
54	0.081	0.55 7	0.605	Accepted	Accepted	Rejected	Rejected
55	0.022	0.9	0.507	Accepted	Accepted	Rejected	Rejected
56	0.012	0.95 5	0.032	Rejected	Accepted	Rejected	Rejected
57	0.648	0.79	0.422	Rejected	Rejected	Rejected	Rejected
58	0.479	0.81 5	0.217	Accepted	Rejected	Rejected	Rejected

59	0.779	0.80 1	0.294	Rejecte d	Rejecte d	Rejecte d	Rejected
60	0.292	0.77 4	0.587	Rejecte d	Rejecte d	Rejecte d	Rejected
61	0.478	0.75 2	0.483	Rejecte d	Rejecte d	Rejecte d	Rejected
62	0.368	0.74 9	0.512	Rejecte d	Rejecte d	Rejecte d	Rejected
63	0.675	0.82 7	0.591	Rejecte d	Rejecte d	Rejecte d	Rejected
64	0.822	0.79 7	0.254	Rejecte d	Rejecte d	Rejecte d	Rejected
65	0.722	0.82	0.404	Rejecte d	Rejecte d	Rejecte d	Rejected
66	0.044	0.46 9	0.171	Accepte d	Rejecte d	Rejecte d	Accepted
67	0.044	0.46 9	0.171	Accepte d	Rejecte d	Rejecte d	Accepted
68	0.038	0.57 3	0.049	Accepte d	Rejecte d	Rejecte d	Accepted
69	0.013	0.86 2	0.291	Accepte d	Accepte d	Accepte d	Accepted
70	0.012	0.85 6	0.382	Accepte d	Rejecte d	Accepte d	Accepted
71	0.012	0.94 9	0.107	Accepte d	Accepte d	Rejecte d	Accepted
72	0.057	0.86	0.132	Accepte d	Rejecte d	Rejecte d	Accepted
73	0.018	0.45 1	0.064	Accepte d	Rejecte d	Accepte d	Accepted
74	0.019	0.40 9	0.079	Accepte d	Rejecte d	Accepte d	Accepted
75	0.021	0.88 4	0.036	Accepte d	Rejecte d	Accepte d	Accepted
76	0.01	0.75 3	0.303	Accepte d	Accepte d	Rejecte d	Accepted
77	0.004	0.92	0.151	Accepte d	Accepte d	Rejecte d	Accepted
78	0.011	0.76 6	0.35	Accepte d	Accepte d	Rejecte d	Accepted

79	0.004	0.04 7	0.059	Accepted d	Accepted d	Rejected d	Accepted
80	0.003	0.14 3	0.081	Accepted d	Accepted d	Rejected d	Accepted
81	0.002	0.41 7	0.768	Accepted d	Accepted d	Accepted d	Accepted
82	0.007	0.53 4	0.384	Accepted d	Accepted d	Accepted d	Accepted
83	0.037	0.12 7	0.633	Accepted d	Accepted d	Accepted d	Accepted
84	0.796	0.85 7	0.914	Accepted d	Rejected d	Accepted d	Accepted
85	0.014	0.60 8	0.804	Accepted d	Rejected d	Accepted d	Accepted
86	0.02	0.59 9	0.668	Accepted d	Rejected d	Rejected d	Accepted
87	0.035	0.91 8	0.029	Accepted d	Rejected d	Accepted d	Accepted
88	0.018	0.31 8	0.071	Accepted d	Rejected d	Rejected d	Accepted

Figure S1. BOILED-Egg of anti-inflammation sesquiterpenoids from Asteraceae plants.



