

Supplementary Materials:

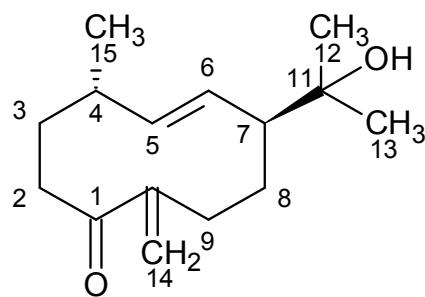


Table S1. ^1H and ^{13}C chemical shifts (δ in ppm) and HMBC correlations of litseagermacrane (1).

Position	δC (ppm), type of atom	δH (ppm), mult. (J in Hz)	HMBC correlations
1	206.0, C		
2	37.4, CH_2	2.30, m 2.83, m	1, 3, 4 1, 3, 4
3	36.8, CH_2	1.80, m 2.01, m	2, 4 2, 4
4	40.6, CH	2.08, m	2, 5, 6
5	142.7, CH	5.00, dd (15.27, 9.33)	4, 6, 7, 15
6	130.1, CH	5.05, dd (15.40, 9.46)	4, 5, 7
7	56.9, CH	1.92, m	5, 6, 8, 9, 11, 12, 13
8	32.7, CH_2	1.30, m 1.35, m	6, 7, 9, 10, 11 6, 7, 9, 10, 11
9	28.7, CH_2	2.25, m 2.55, t (13.00)	7, 10, 14 7, 8, 10, 14
10	155.0, C		
11	71.6, C		
12	26.7, CH_3	1.09, s	7, 11, 13
13	26.7, CH_3	1.13, s	7, 11, 12
14	119.7, CH_2	5.50, s 5.64, s	1, 9, 10 1, 9, 10
15	20.6, CH_3	0.97, d (6.00)	3, 4, 5

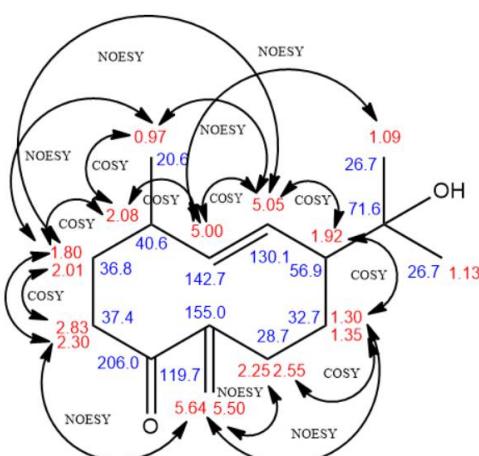
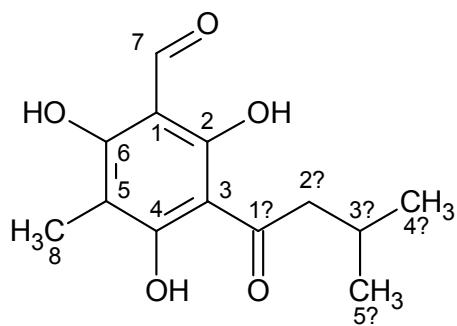


Figure S1. COSY and NOESY scheme of litseagermacrane (1).



Grandinol

Table S2. ¹H and ¹³C chemical shifts (δ in ppm) and HMBC correlations of grandinol (2).

Position	δ C (ppm), type of atom	δ H (ppm), mult. (J in Hz)	HMBC correlations
1	102.8, C		
2	167.7, C		
3	103.9, C		
4	171.4, C		
5	100.5, C		
6	160.9, C		
7	191.2, CHO	10.12, s	2
8	6.16, CH ₃	2.05, s	4, 5, 6
1'	206.6, C		
2'	52.7, CH ₂	3.01, 2H, d (6.55)	1', 3', 4', 5'
3'	24.9, CH	2.27, m	2', 4', 5'
4'	22.6, CH ₃	0.99, d (6.55)	2', 3', 5'
5'	22.6, CH ₃	0.99, d (6.55)	2', 3', 4'
2-OH		14.34, s	1, 2, 3
4-OH		15.46, s	3, 4, 5

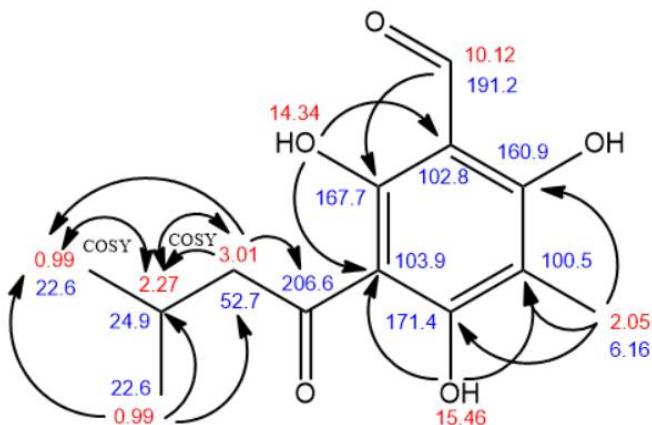
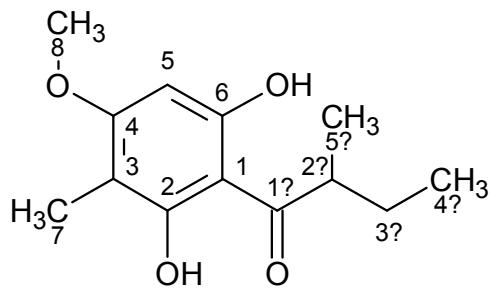


Figure S2. HMBC and COSY scheme of grandinol (2)



Pulverulentone B

Table S3. ^1H and ^{13}C chemical shifts (δ in ppm) and HMBC correlations of pulverulentone B (3).

Position	δC (ppm), type of atom	δH (ppm), mult. (J in Hz)	HMBC correlations
1	105.5, C		
2	165.0, C		
3	102.8, C		
4	161.0, C		
5	89.7, CH	5.93, s	1, 3, 4, 6
6	159.3, C		
7	7.04, CH_3	2.05, s	2, 3, 4
8	55.2, OCH_3	3.85, s	4
1'	210.2, C		
2'	46.1, CH	3.63, m	1', 5'
3'	27.1, CH_2	1.38, m 1.78, m	1', 2', 4', 5' 1', 2', 4', 5'
4'	12.3, CH_3	0.91, dd (7.67)	2', 3'
5'	16.9, CH_3	1.15, d (6.73)	1', 2', 3'
2-OH		14.34	1, 2, 3
6-OH		12.79	

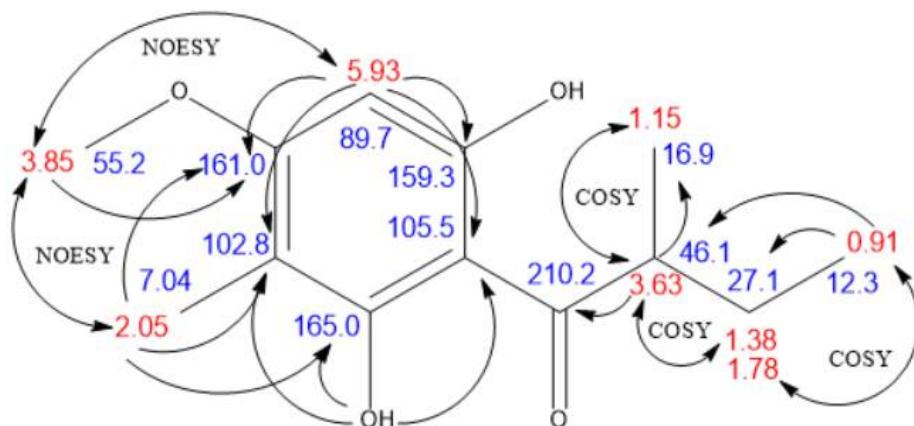
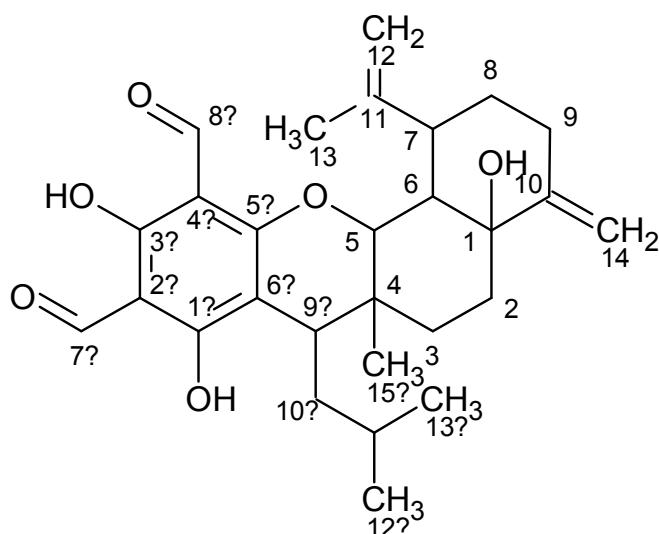


Figure S3. HMBC, COSY, and NOESY scheme of pulverulentone B (3).



Eucalyptal A

Table S4. ^1H and ^{13}C chemical shifts (δ in ppm) and HMBC correlations of eucalyptal A (4).

Position	δC (ppm), type of atom	δH (ppm), mult. (J in Hz)	HMBC correlations
1	73.2, C		
2	30.3, CH_2	2.21, m 2.46, m	1, 4, 6 1, 4, 6
3	29.7, CH_2	1.40, m 1.88, m	1, 4, 5, 15 1, 2, 4, 5, 15
4	35.7, C		
5	75.4, CH	4.07, d (11.64)	6, 15
6	44.6, CH	2.60, dd (2.75, 11.59)	2, 5, 7, 8, 10
7	39.5, CH	3.12, br d (11.97)	5, 6, 11
8	23.4, CH_2	1.79, m 1.96, m	7, 9, 10 9, 11
9	32.1, CH_2	2.41, m 2.66, m	1, 7, 8, 14 1, 7, 8, 14
10	146.5, C		
11	149.4, C		
12	107.8, CH_2	4.72, s 4.84, s	7, 13 7, 13
13	22.3, CH_3	1.87, s	7, 11, 12
14	111.1, CH_2	5.01, s 5.11, s	1, 9 1, 9
15	19.6, CH_3	0.98, s	3, 4, 5, 9'
1'	168.5, C		
2'	104.0, C		
3'	167.1, C		
4'	103.9, C		
5'	162.6, C		
6'	107.5, C		
7'	191.2, CHO	10.15, s	1', 2', 8'
8'	194.9, CHO	9.89, s	3', 4', 7'
9'	37.6, CH	2.49, dd (8.61, 1.80)	5, 5', 6', 10', 11'
10'	42.8, CH_2	1.09, m	6', 9'

		1.32, m	9'
11'	28.4, CH	1.64, m	-
12'	21.6, CH ₃	1.02, d (6.42)	10', 11', 13'
13'	22.7, CH ₃	0.88, d (6.42)	10', 11', 12'
1'-OH		13.29, s	1', 2', 6'
3'-OH		13.75, s	2', 3', 4'

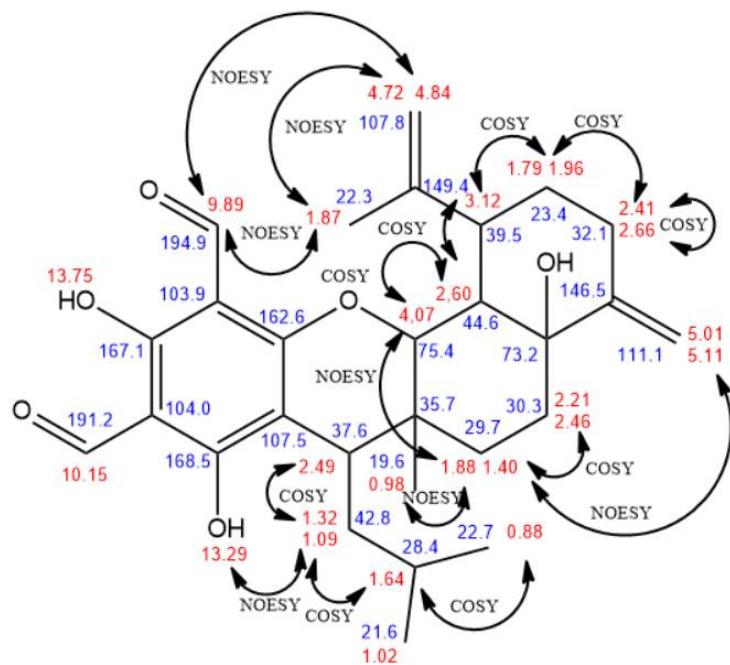
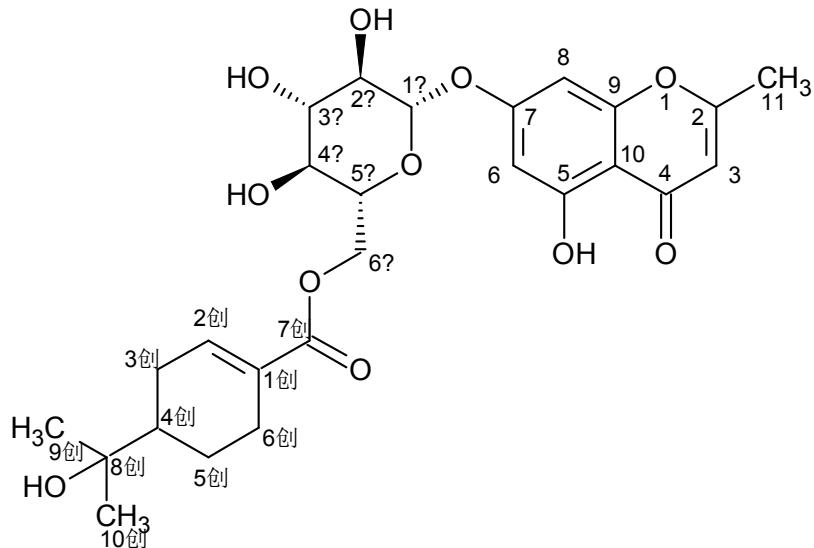


Figure S4. COSY and NOESY scheme of eucalyptal A (**4**).



Cypellocarpin C

Table S5. ^1H and ^{13}C chemical shifts (δ in ppm) and HMBC correlations of cypellocarpin C (5).

Position	δC (ppm), type of atom	δH (ppm), mult. (J in Hz)	HMBC correlations
2	168.5, C		
3	108.5, CH	6.26, s	2, 10
4	182.1, C		
5	162.3, C		
6	99.3, CH	6.43, d (2.00)	5, 7, 8, 10
7	162.4, C		
8	94.5, CH	6.63, d (2.00)	6, 7, 9, 10
9	157.7, C		
10	104.7, C		
11	20.5, CH_3	2.39, s	2, 3
1'	99.3, CH	5.12, dd (3.20, 7.50)	7
2'	73.3, CH	3.27, m	
3'	76.4, CH	3.30, m	
4'	70.4, CH	3.16, m	
5'	74.1, CH	3.78, m	
6'	63.9, CH_2	3.97, dd (7.88, 12.17) 4.42, m	
1''	134.8, C		
2''	140.4, CH	6.91, m	1'', 4'', 7''
3''	27.4, CH_2	1.92, m 2.20, m	
4''	43.8, CH	1.35, m	
5''	23.2, CH_2	1.04, m 1.86, m	
6''	25.2, CH_2	2.01, m 2.36, m	
7''	165.8, C		
8''	70.3, C		
9''	27.1, CH_3	1.04, s	4'', 8'', 10''
10''	27.1, CH_3	1.04, s	4'', 8'', 9''
5-OH		12.84, s	5, 6, 10

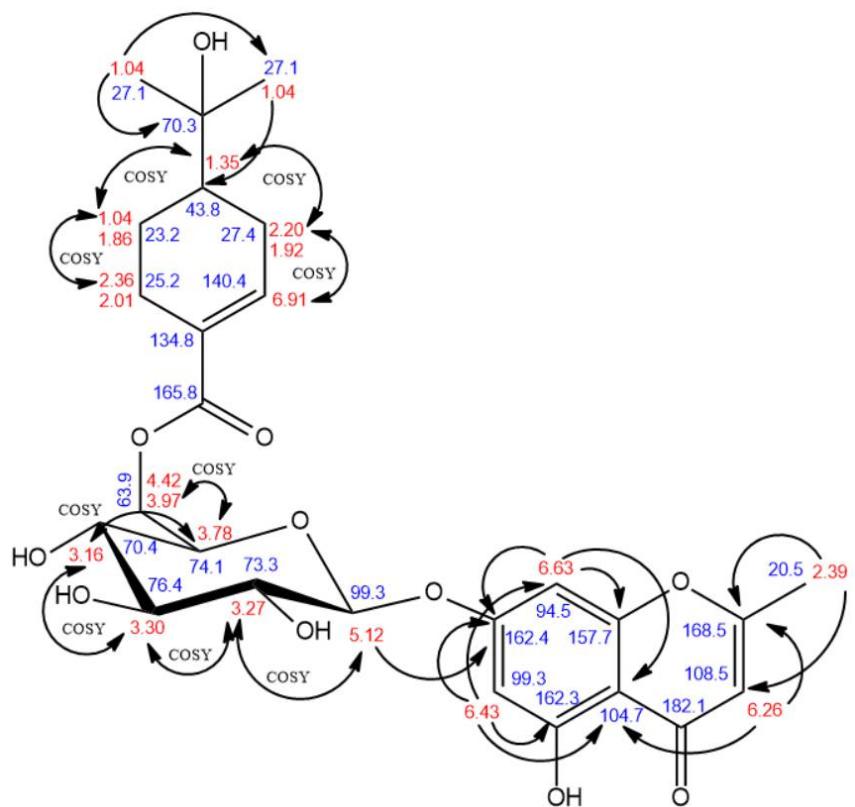
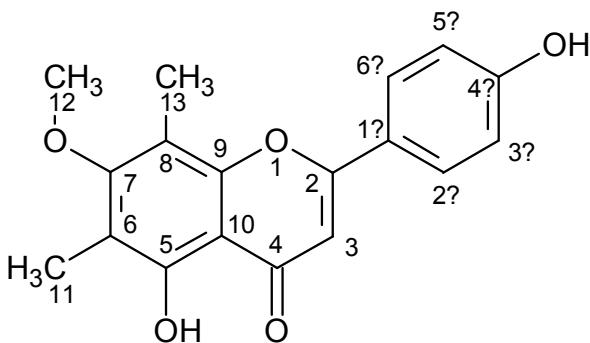


Figure S5. HMBC and COSY scheme of cypellocarpin C (5).



Sideroxylin

Table S6. ^1H and ^{13}C chemical shifts (δ in ppm) and HMBC correlations of sideroxylin (**6**).

Position	δ C (ppm), type of atom	δ H (ppm), mult. (J in Hz)	HMBC correlations
2	164.2, C		
3	103.1, CH	6.89, s	1', 2, 4, 10
4	182.9, C		
5	156.5, C		
6	113.2, C		
7	162.4, C		
8	109.1, C		
9	152.4, C		
10	107.3, C		
11	8.5, CH ₃	2.11, s	5, 6, 7
12	60.8, OCH ₃	3.76, s	7
13	8.6, CH ₃	2.35, s	7, 8, 9
1'	121.6, C		
2'	128.9, CH	7.97, d (8.80)	2, 4', 6'
3'	116.4, CH	6.96, d (8.80)	1', 4', 5'
4'	162.2, C		
5'	116.4, CH	6.96, d (8.80)	1', 3', 4'
6'	128.9, CH	7.97, d (8.80)	2, 2', 4'
5-OH		13.08, s	
4'-OH		10.39, br s	

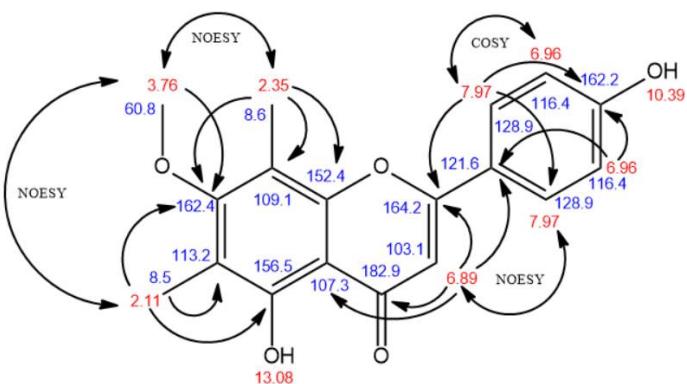
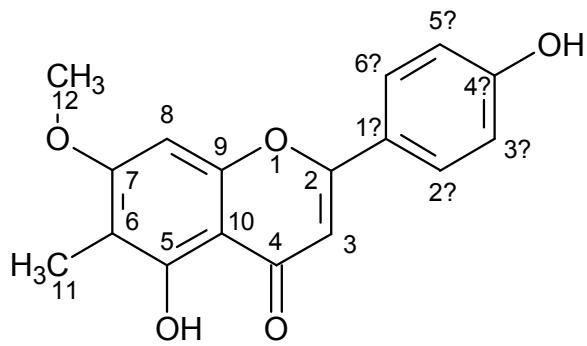


Figure S6. HMBC, COSY, and NOESY scheme of sideroxylin (**6**).



8-Demethylsideroxylin

Table S7. ^1H and ^{13}C chemical shifts (δ in ppm) and HMBC correlations of 8-demethylsideroxylin (7).

Position	δC (ppm), type of atom	δH (ppm), mult. (J in Hz)	HMBC correlations
2	164.3, C		
3	103.1, CH	6.85, s	1', 2, 4, 10
4	182.5, C		
5	158.7, C		
6	107.8, C		
7	163.3, C		
8	89.2, CH	6.87, s	6, 7, 9, 10
9	155.6, C		
10	104.4, C		
11	7.9, CH_3	2.01, s	5, 6, 7
12	56.7, OCH_3	3.93, s	7
1'	121.1, C		
2'	128.8, CH	7.97, d (8.78)	2, 4', 6'
3'	115.6, CH	6.94, d (8.78)	1, 4', 5'
4'	161.1, C		
5'	115.6, CH	6.94, d (8.78)	1', 3', 4'
6'	128.8, CH	7.97, d (8.78)	2, 2', 4'
5-OH		13.11, s	
4'-OH		10.35, br s	

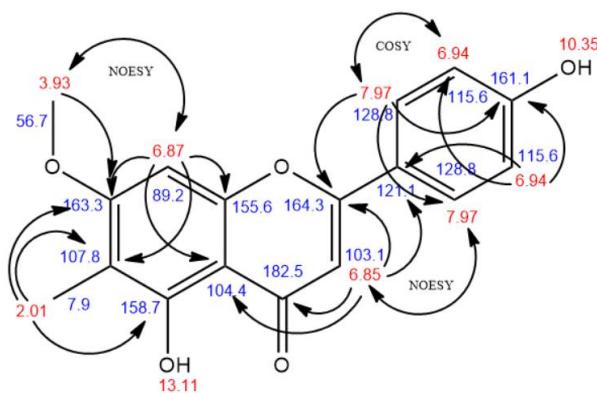
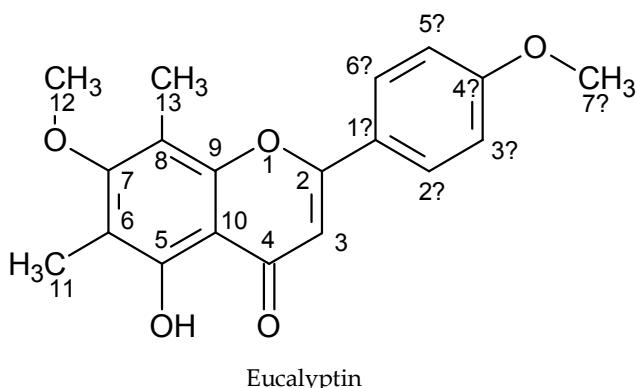


Figure S7. HMBC, COSY, and NOESY scheme of 8-demethylsideroxylin (7).



Eucalyptin

Table S8. ^1H and ^{13}C chemical shifts (δ in ppm) and HMBC correlations of eucalyptin (8).

Position	δC (ppm), type of atom	δH (ppm), mult. (J in Hz)	HMBC correlations
2	163.9, C		
3	103.7, CH	6.64, s	1', 2, 4, 10
4	183.0, C		
5	156.9, C		
6	114.0, C		
7	162.4, C		
8	108.4, C		
9	152.5, C		
10	107.1, C		
11	8.1, CH_3	2.21, s	5, 6, 7
12	61.2, OCH_3	3.81, s	7
13	9.3, CH_3	2.41, s	7, 8, 9
1'	123.6, C		
2'	127.7, CH	7.89, d (8.74)	4', 6'
3'	114.0, CH	7.05, d (8.74)	1', 4', 5'
4'	162.7, C		
5'	114.0, CH	7.05, d (8.74)	1', 3', 4'
6'	127.7, CH	7.89, d (8.74)	2', 4
7'	55.6, OCH_3	3.91, s	4'
5-OH		12.88, br s	

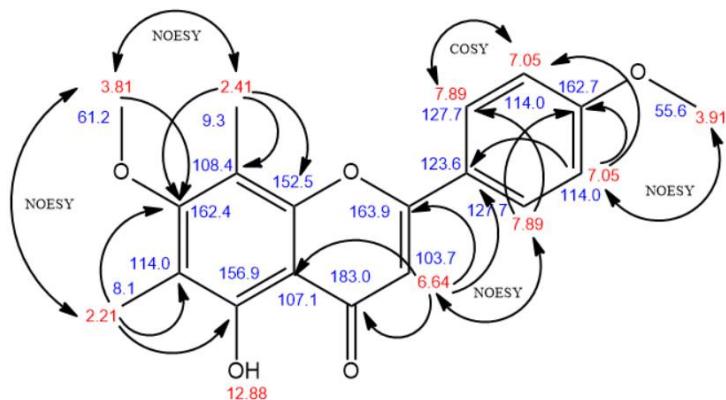
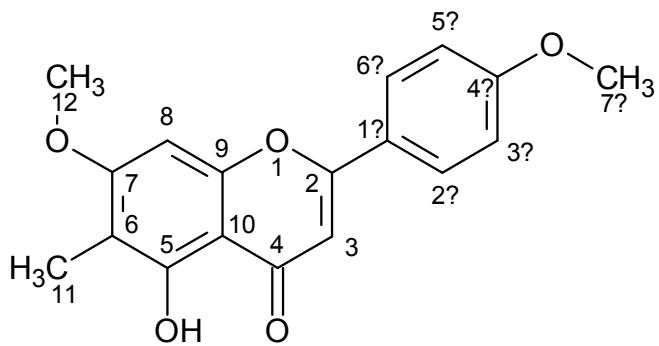


Figure S8. HMBC, COSY, and NOESY scheme of eucalyptin (8).



8-Demethyleucalyptin

Table S9. ^1H and ^{13}C chemical shifts (δ in ppm) and HMBC correlations of 8-demethyleucalyptin (9).

Position	δC (ppm), type of atom	δH (ppm), mult. (J in Hz)	HMBC correlations
2	163.3, C		
3	104.4, CH	6.61, s	1', 2, 4, 10
4	182.4, C		
5	157.9, C		
6	108.9, C		
7	162.4, C		
8	89.2, CH	6.51, s	6, 7, 9, 10
9	155.9, C		
10	105.1, C		
11	7.2, CH_3	2.13, s	5, 6, 7
12	55.7, OCH_3	3.94, s	7
1'	123.8, C		
2'	127.8, CH	7.86, d (8.92)	4', 6'
3'	114.3, CH	7.03, d (8.92)	1', 4', 5'
4'	162.1, C		
5'	114.3, CH	7.03, d (8.92)	1', 3', 4'
6'	127.8, CH	7.86, d (8.92)	2', 4'
7'	55.3, OCH_3	3.91, s	4'

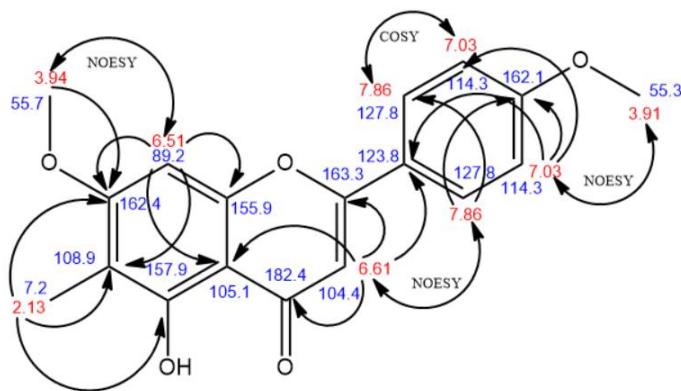
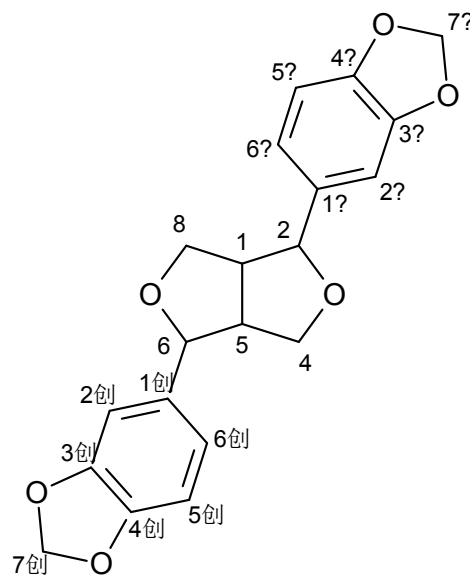


Figure S9. HMBC, COSY, and NOESY scheme of 8-demethyleucalyptin (9).



Sesamin

Table S10. ^1H and ^{13}C chemical shifts (δ in ppm) and HMBC correlations of sesamin (**10**).

Position	δC (ppm), type of atom	δH (ppm), mult. (J in Hz)	HMBC correlations
1	54.2, CH	3.06, m	
2	85.6, CH	4.73, d (4.39)	1, 8, 1', 2', 6'
4	71.5, CH_2	3.89, m 4.24, m	6 5, 6
5	54.2, CH	3.06, m	
6	85.6, CH	4.73, d (4.39)	4, 5, 1'', 2'', 6''
8	71.5, CH_2	3.89, m 4.24, m	2 1, 2
1'	134.2, C		
2'	106.0, CH	6.86, d (1.23)	2, 4', 6'
3'	147.6, C		
4'	146.3, C		
5'	107.9, CH	6.78, obscured	1', 3'
6'	119.1, CH	6.80, obscured	1', 2', 4'
7'	100.6, CH_2	5.96, 2H, s	3', 4'
1''	134.2, C		
2''	106.0, CH	6.86, d (1.23)	6, 4'', 6''
3''	147.6, C		
4''	146.3, C		
5''	107.9, CH	6.78, obscured	1'', 3''
6''	119.1, CH	6.80, obscured	1'', 2'', 4''
7''	100.6, CH_2	5.96, 2H, s	3'', 4''

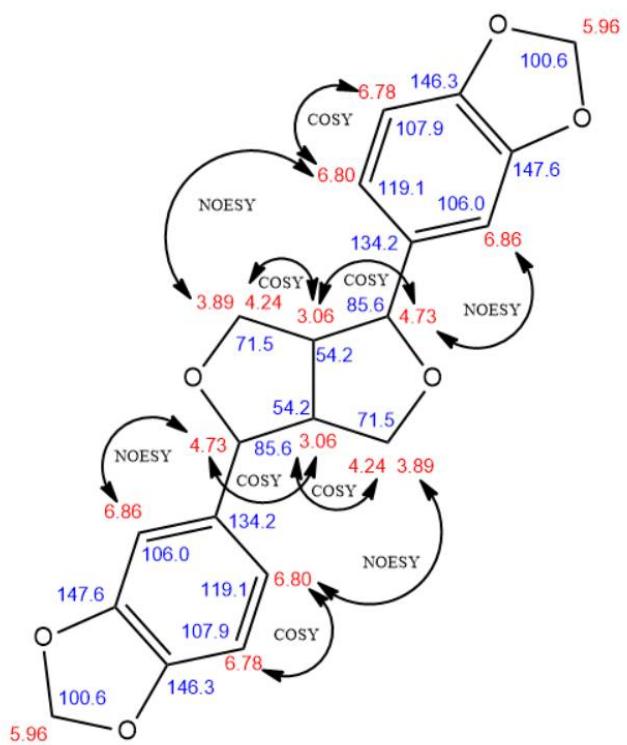


Figure S10. COSY and NOESY scheme of sesamin (10).

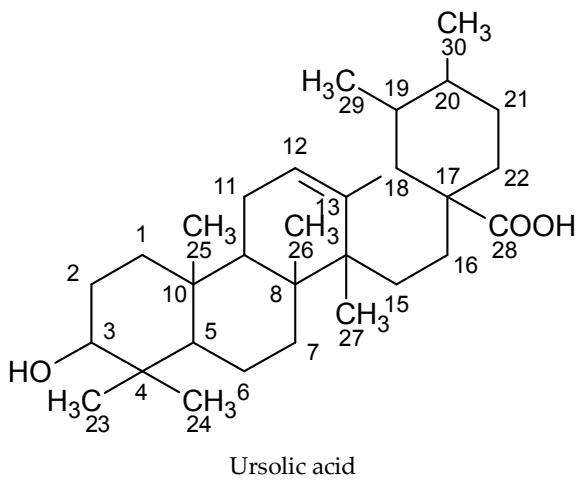


Table S11. ^1H and ^{13}C chemical shifts (δ in ppm) and HMBC correlations of ursolic acid (**11**).

Position	δC (ppm), type of atom	δH (ppm), mult. (J in Hz)	HMBC correlations
1	36.4, CH_2	1.29, m 1.54, m	2, 3, 5, 10
2	27.4, CH_2	1.28, m 1.45, m	
3	77.2, CH	3.00, m	4, 23, 24
4	38.8, C		
5	55.2, CH	0.68, m	
6	18.5, CH_2	1.30, m 1.40, m	
7	32.9, CH_2	1.23, m 1.38, m	
8	39.7, C		
9	47.5, CH	1.45, m	1, 8, 9, 11, 14
10	36.4, C		
11	23.4, CH_2	1.84, 2H, m	
12	124.7, CH	5.13, t (3.02)	9, 11, 14, 18
13	138.6, C		
14	42.1, C		
15	28.4, CH_2	0.74, m 1.79, m	
16	23.8, CH_2	1.50, m 1.92, m	
17	47.6, C		
18	52.7, CH	2.11, d (11.53)	12, 13, 14, 17, 20, 28, 29
19	38.8, CH	1.30, m	
20	39.0, CH	0.92, m	21
21	30.5, CH_2	1.26, m 1.45, m	
22	39.9, CH_2	1.90, m 2.10, m	
23	16.4, CH_3	0.68, s	3, 4, 5, 24
24	28.6, CH_3	0.89, s	3, 4, 5, 23
25	21.5, CH_3	0.87, s	1, 9
26	16.7, CH_3	0.75, s	7, 8, 9, 14

27	23.6, CH ₃	1.04, s	8, 14, 15
28	178.8, C		
29	17.0, C	0.81, obscured	18, 19
30	28.2, C	0.92, obscured	19, 21

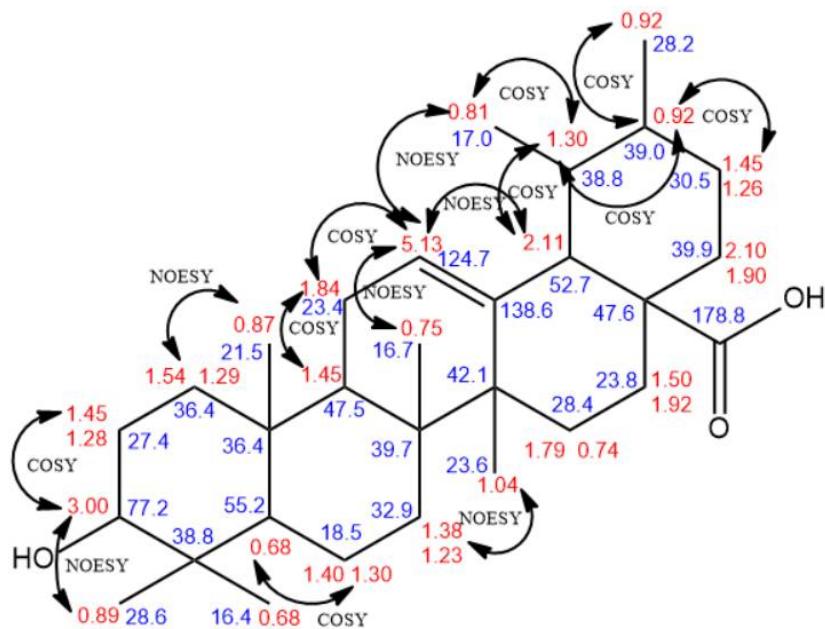
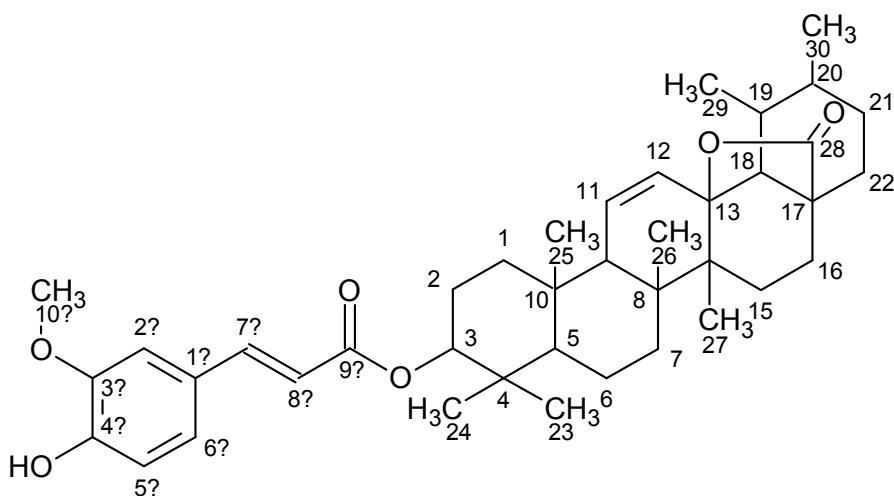


Figure S11. COSY and NOESY scheme of ursolic acid (11).



Tereticornate A

Table S12. ^1H and ^{13}C chemical shifts (δ in ppm) and HMBC correlations of tereticornate A (12).

Position	δC (ppm), type of atom	δH (ppm), mult. (J in Hz)	HMBC correlations
1	31.0, CH_2	1.13, m 1.82, m	
2	25.5, CH_2	1.24, m 1.74, m	
3	80.3, CH	4.66, dd (5.79, 10.50)	9'
4	37.6, C		
5	54.7, CH	0.90, m	10
6	17.5, CH_2	1.64, 2H, m	
7	30.5, CH_2	1.61, m 1.80, m	
8	41.5, C		
9	52.9, CH	2.01, s	10, 12, 14
10	36.9, C		
11	128.8, CH	5.55, dd (2.25, 10.30)	8, 9
12	133.0, CH	5.96, d (10.30)	13, 14
13	89.5, C		
14	41.5, C		
15	25.1, CH_2	1.23, m 1.74, m	
16	22.9, CH_2	1.44, m 2.16, m	28
17	45.0, C		
18	60.4, CH	1.65, m	13, 16, 17, 19
19	40.2, CH	0.92, m	
20	38.1, CH	1.81, m	
21	30.4, CH_2	1.27, m 1.72, m	
22	31.3, CH_2	1.23, m 1.57, m	
23	27.6, CH_3	0.92, s	3, 4, 5, 24
24	16.3, CH_3	0.96, s	3, 4, 5, 23
25	17.8, CH_3	0.98, s	1, 9, 10

26	18.2, CH ₃	1.08, s	7, 9, 14
27	16.2, CH ₃	1.18, s	8, 13, 15
28	180.0, C		
29	19.1, CH ₃	0.95, d (6.13)	18, 19, 20
30	17.6, CH ₃	1.02, d (6.13)	19, 20, 21
1'	126.6, C		
2'	108.9, CH	7.05, s	4', 6'
3'	146.7, C		
4'	147.6, C		
5'	114.5, CH	6.94, d (8.33)	1', 3'
6'	122.6, CH	7.10, d (8.33)	2', 4'
7'	144.3, CH	7.61, d (16.00)	2', 6', 9'
8'	115.9, CH	6.29, d (16.00)	1', 9'
9'	166.7, C		
10'	55.9, OCH ₃	3.95, s	3'

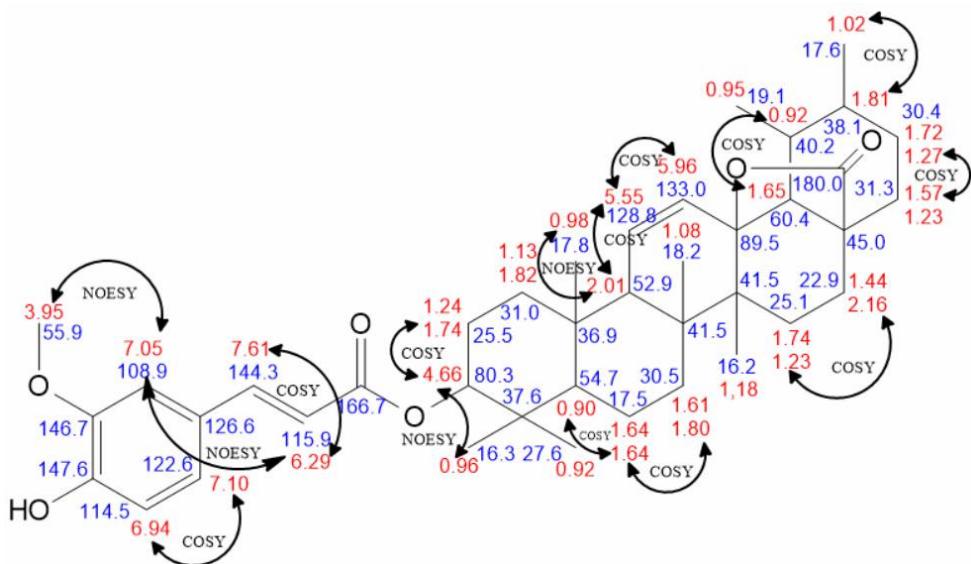
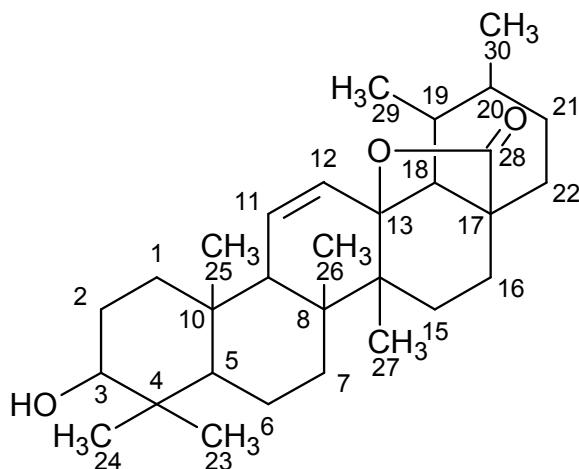


Figure S12. COSY and NOESY scheme of tereticornate A (12).



Ursolic acid lactone

Table S13. ^1H and ^{13}C chemical shifts (δ in ppm) and HMBC correlations of ursolic acid lactone (13a).

Position	δC (ppm), type of atom	δH (ppm), mult. (J in Hz)	HMBC correlations
1	37.3, CH ₂	1.36, m 2.03, m	
2	27.0, CH ₂	1.63, m 1.69, m	
3	78.6, CH	3.23, m	
4	38.5, C		
5	54.3, CH	0.75, m	
6	17.6, CH ₂	1.48, m 1.59, m	
7	30.9, CH ₂	1.63, m 1.82, m	
8	41.3, C		
9	52.4, CH	1.96, m	
10	36.2, C		
11	133.3, CH	5.98, m	8, 10, 13
12	128.6, CH	5.54, m	
13	89.7, C		
14	41.6, C		
15	25.0, CH ₂	1.68, m 1.79, m	
16	22.4, CH ₂	1.40, m 2.15, m	15, 17, 28
17	43.7, C		
18	60.2, CH	1.64, m	12, 13, 17, 19, 29
19	38.3, CH	1.32, m	17, 18
20	38.5, CH	1.78, m	
21	30.4, CH ₂	1.29, m 1.54, m	
22	36.9, CH ₂	1.34, m 1.80, m	
23	14.7, CH ₃	0.78, s	3, 4, 5, 24
24	27.2, CH ₃	0.99, s	3, 4, 5, 23

25	16.8, CH ₃	0.90, s	5, 9, 10
26	19.0, CH ₃	1.06, s	7, 9, 14
27	15.9, CH ₃	1.16, s	8, 13, 15
28	179.7, C		
29	17.8, CH ₃	1.00, obscured	18, 19, 20
30	18.4, CH ₃	0.93, obscured	

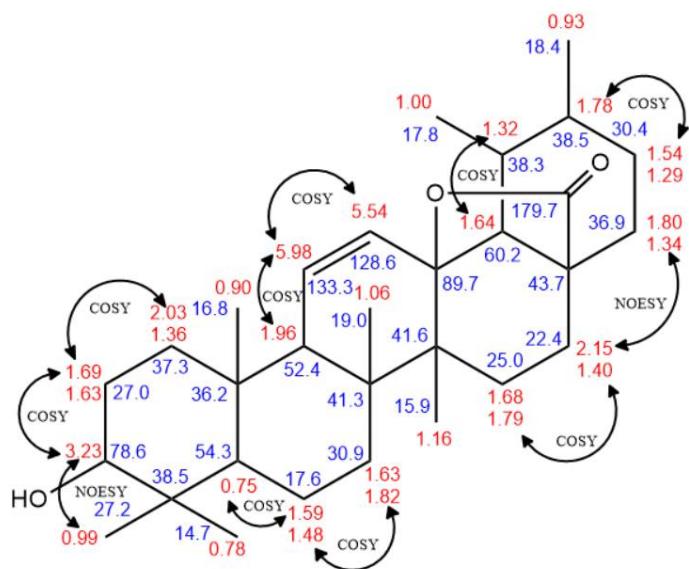
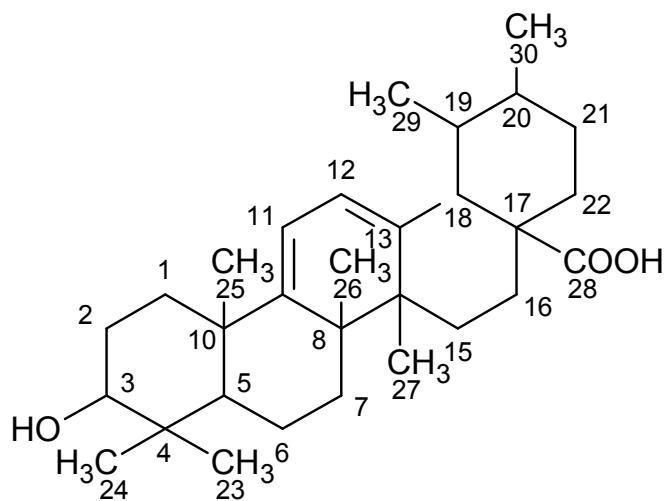


Figure S13. COSY and NOESY scheme of ursolic acid lactone (13a).



3β -hydroxyursa-9(11),12-dien-28-oic acid (loxanic acid)

Table S14. ^1H and ^{13}C chemical shifts (δ in ppm) and HMBC correlations of loxanic acid (**13b**).

Position	δC (ppm), type of atom	δH (ppm), mult. (J in Hz)	HMBC correlations
1	36.4, CH ₂	obsured	
2	27.0, CH ₂	1.63, m 1.69, m	
3	78.6, CH	3.23, m	
4	38.5, C		
5	50.9, CH	0.84, m	
6	17.6, CH ₂	1.48, m 1.59, m	
7	32.1, CH ₂	1.63, m 1.82, m	
8	42.9, C		
9	154.7, C		
10	38.6, C		
11	115.1, CH	5.59, obscured	8, 9, 10, 13
12	123.1, CH	5.52, d (2.63)	9, 11, 14, 18
13	138.6, C		
14	40.6, C		
15	26.9, CH ₂	1.69, m 2.03, m	
16	24.6, CH ₂	1.69, m 1.74, m	
17	47.2, C		
18	50.7, CH	2.32, m	12, 13, 14, 16, 17, 19
19	38.5, CH	1.32, m	
20	38.5, CH	1.78, m	
21	30.4, CH ₂	1.29, m 1.54, m	
22	36.9, CH ₂	1.36, m 2.03, m	28 28
23	15.1, CH ₃	0.79, s	3, 4, 5, 24
24	27.2, CH ₃	1.02, s	3, 4, 5, 23

25	15.9, CH ₃	1.17, s	1, 5, 9, 10
26	21.3, CH ₃	0.98, s	7, 8, 9, 14
27	17.9, CH ₃	0.92, s	8, 13, 14, 15
28	182.2, C		
29	15.1, CH ₃	0.80, obscured	18, 19, 20
30	18.4, CH ₃	0.94, obscured	

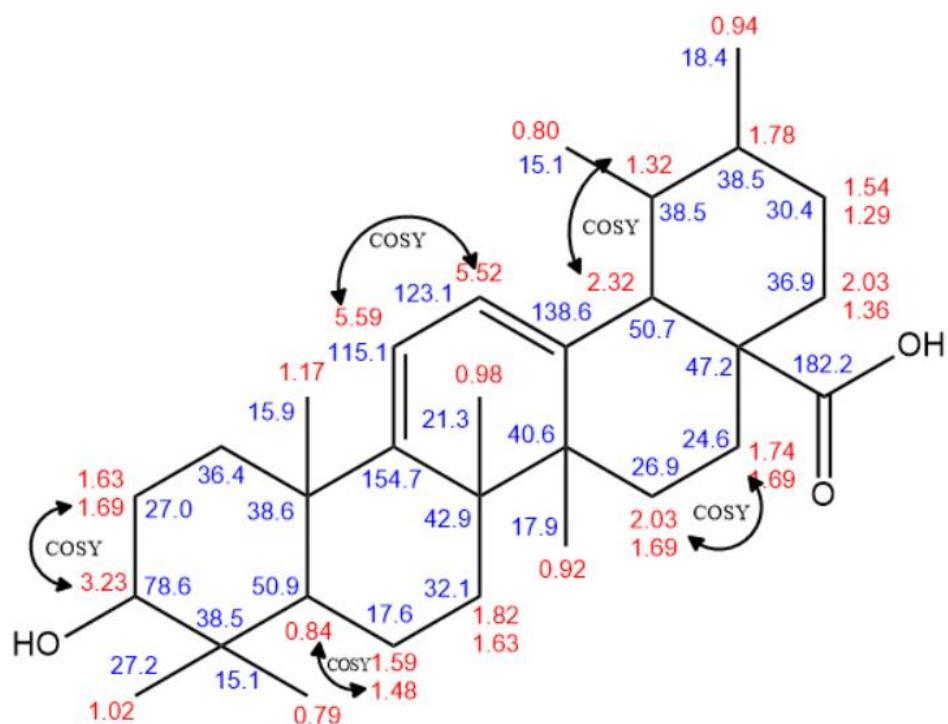


Figure S14. COSY scheme of loxanic acid (13b).