Phytoconstituents from *Turraea obtusifolia* and their antiplasmodial activity

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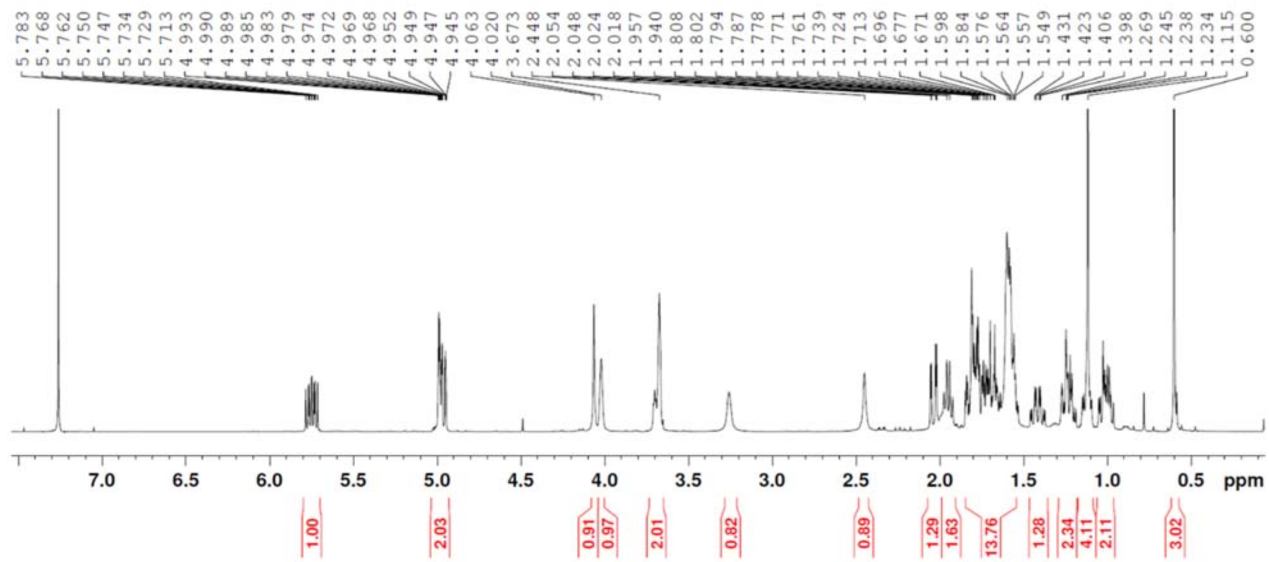

Figure S.I. 1: ^{1}H NMR spectrum of turranin M (**1**) in $CDCl_3$.

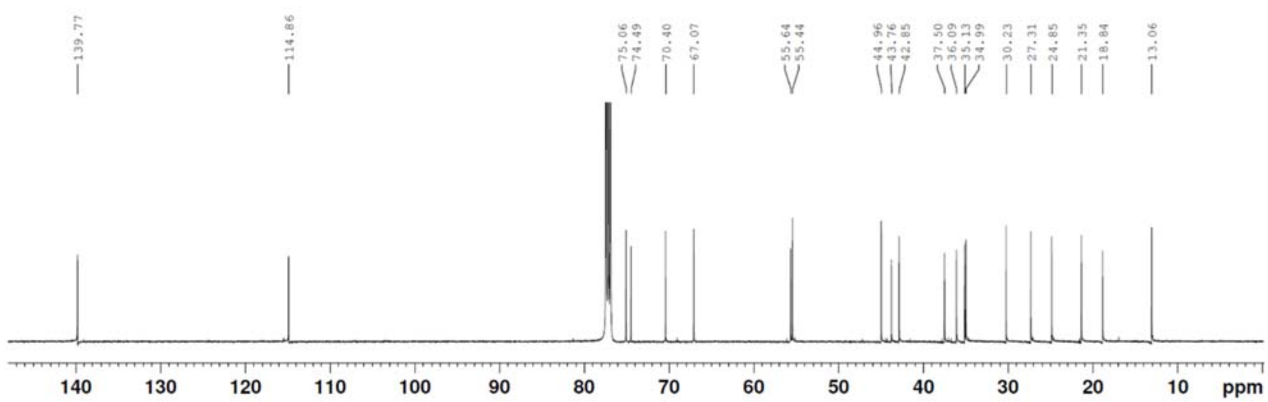

Figure S.I. 2: ^{13}C NMR spectrum of turranin M (**1**) in $CDCl_3$.

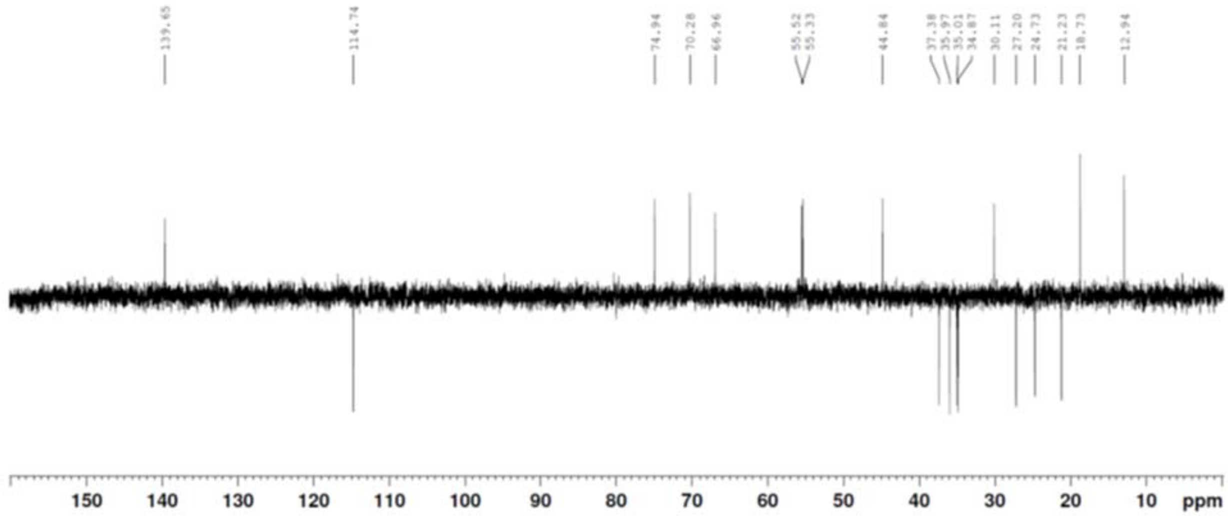

Figure S.I. 3: DEPT-135 spectrum of turranin M (**1**) in $CDCl_3$.

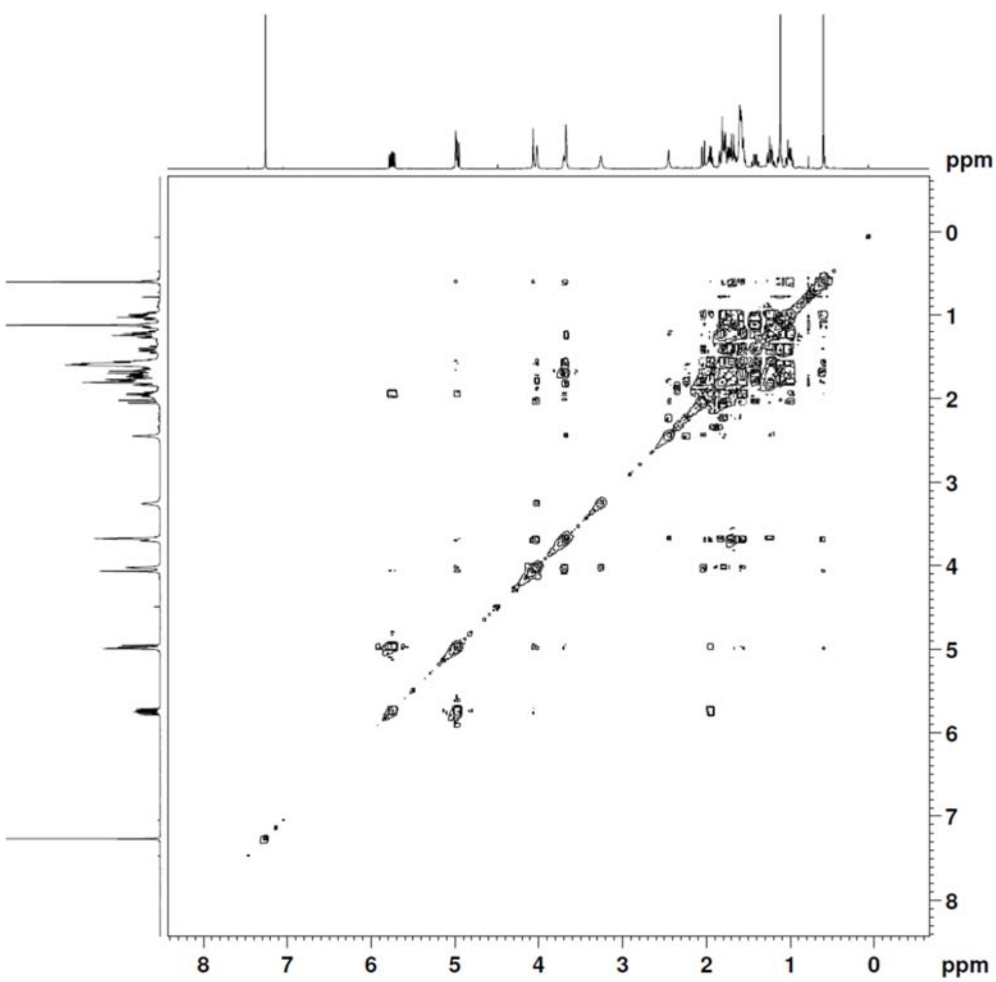

Figure S.I. 4: ^{1}H-^{1}H COSY spectrum of turranin M (**1**) in $CDCl_3$.

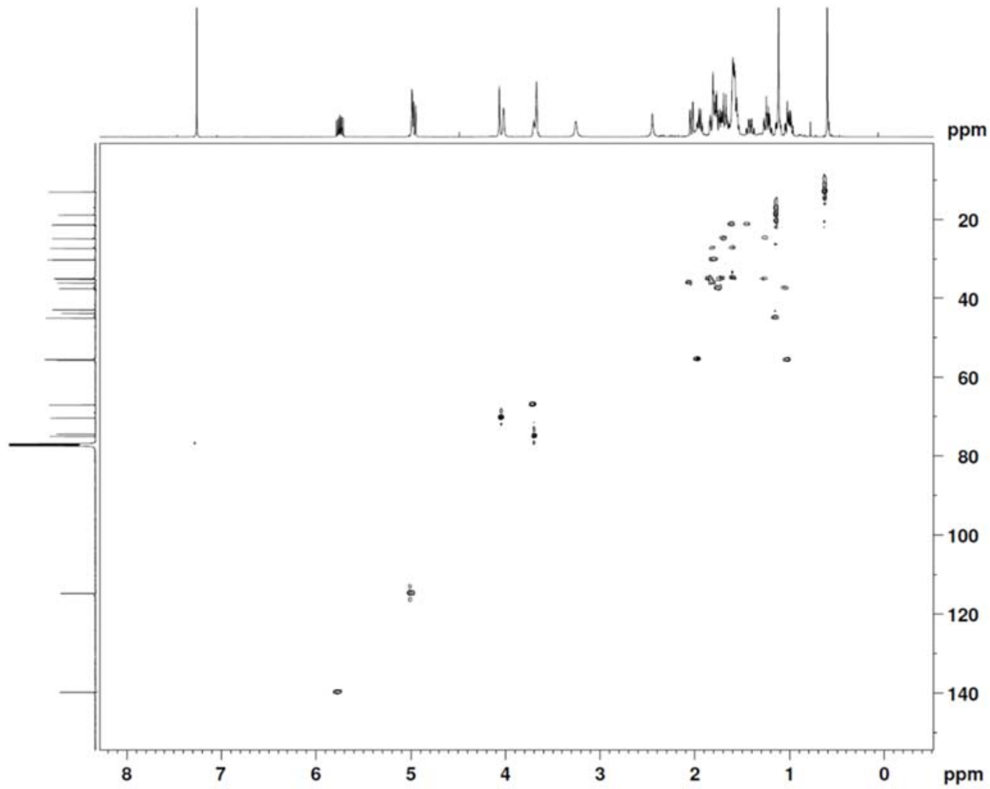

Figure S.I. 5: ^{1}H-^{13}C HSQC spectrum of turranin M (**1**) in $CDCl_3$.

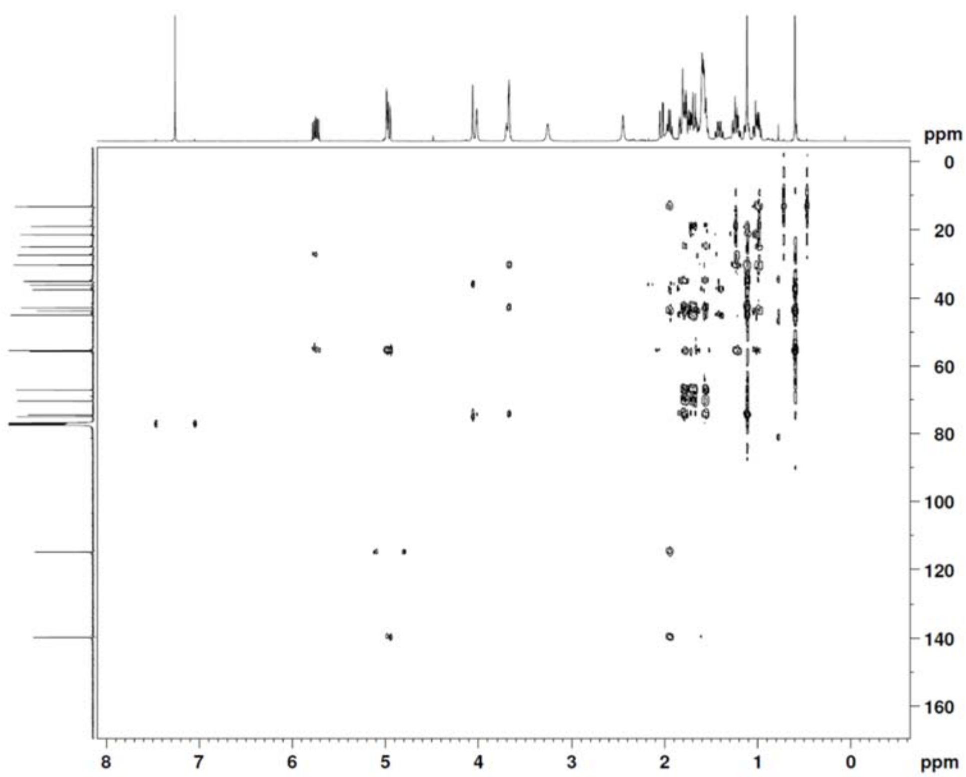

Figure S.I. 6: ^{1}H-^{13}C HMBC spectrum of turranin M (**1**) in $CDCl_3$.

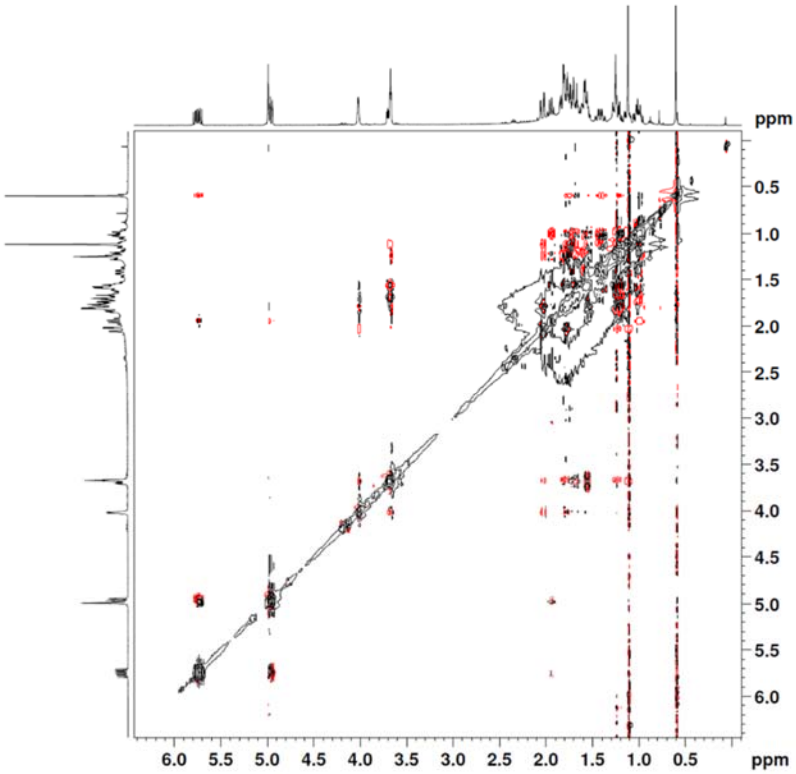

Figure S.I. 7: NOESY spectrum of turranin M (**1**) in $CDCl_3$.

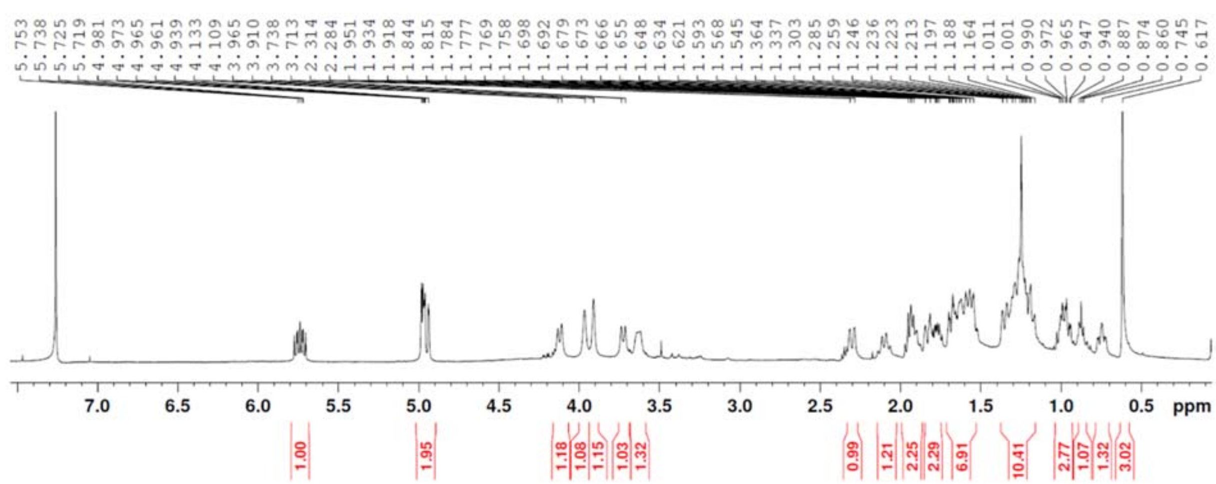

Figure S.I. 8: ^1H NMR spectrum of turranin N (**2**) in $CDCl_3$.

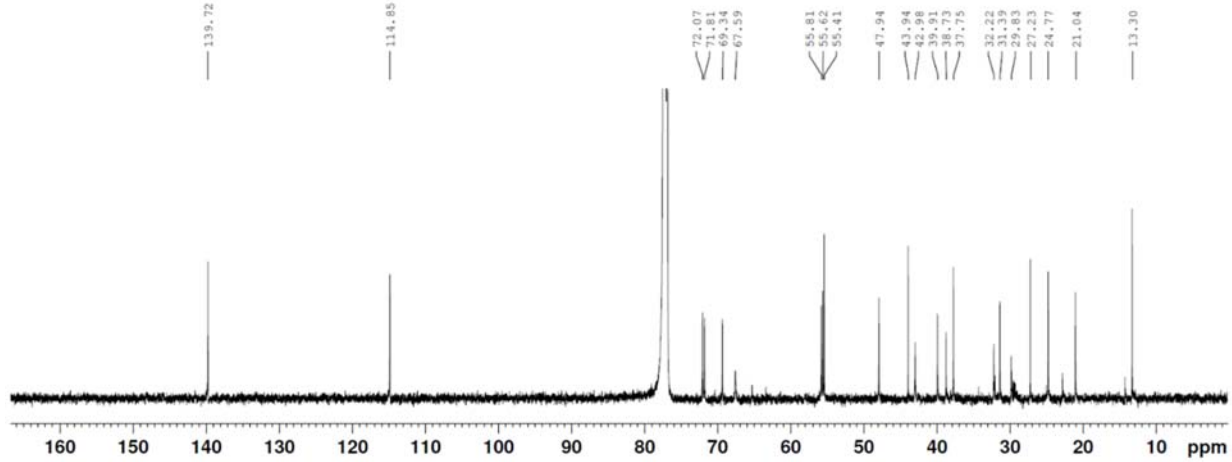

Figure S.I. 9: ^{13}C NMR spectrum of turranin N (**2**) in $CDCl_3$.

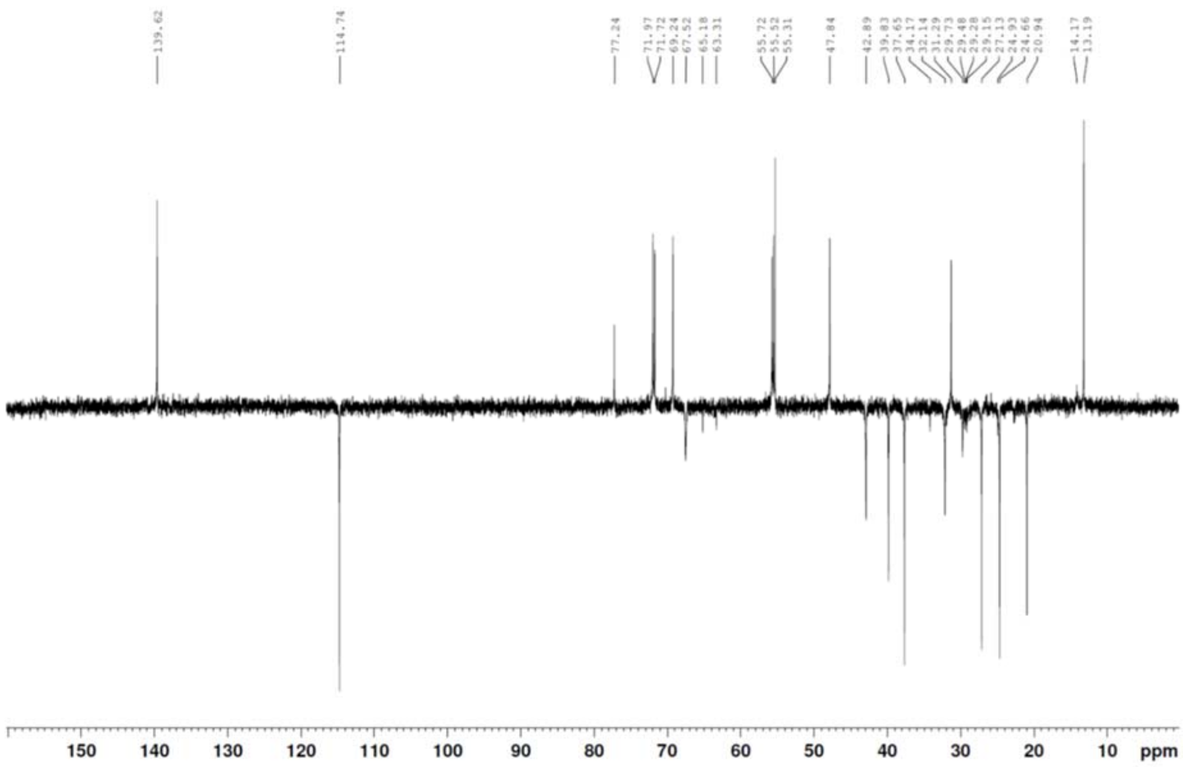

Figure S.I. 10: DEPT-135 spectrum of turranin N (**2**) in $CDCl_3$.

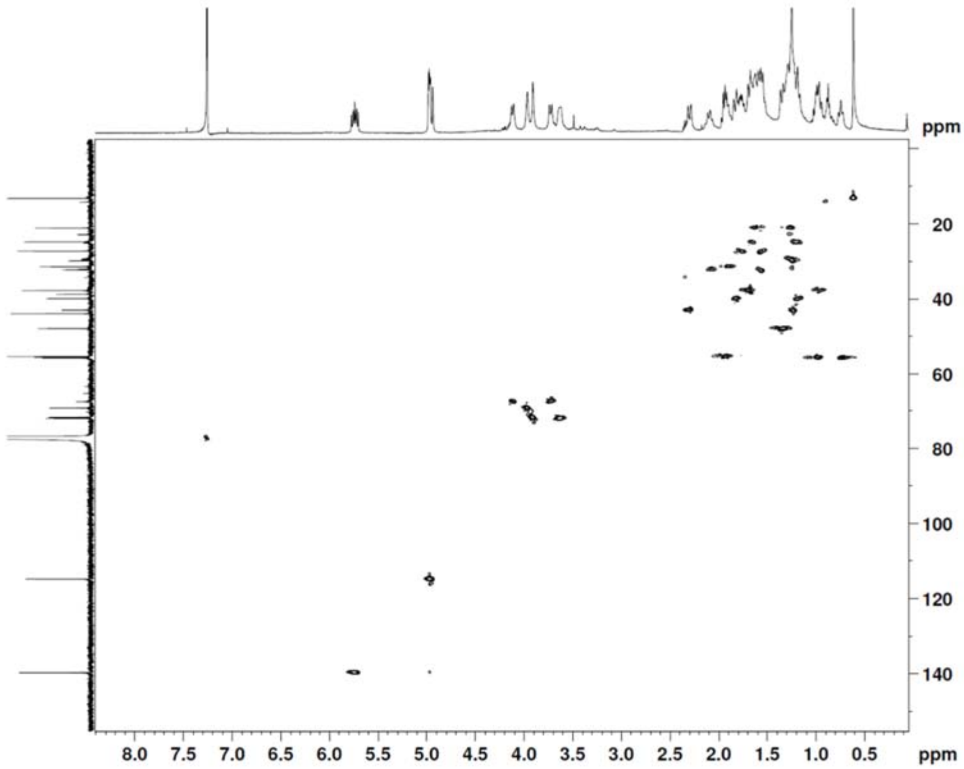

Figure S.I. 11: ^{1}H-^{13}C HSQC spectrum of turranin N (**2**) in $CDCl_3$.

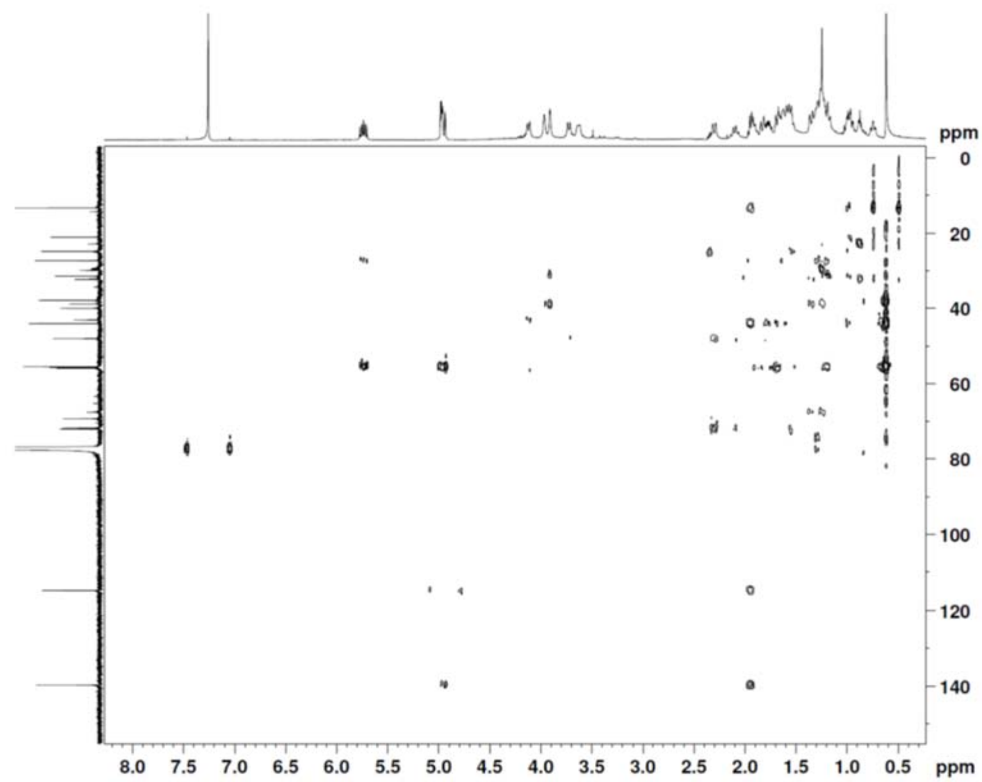

Figure S.I. 12: ^{1}H-^{13}C HMBC spectrum of turranin N (**2**) in $CDCl_3$.

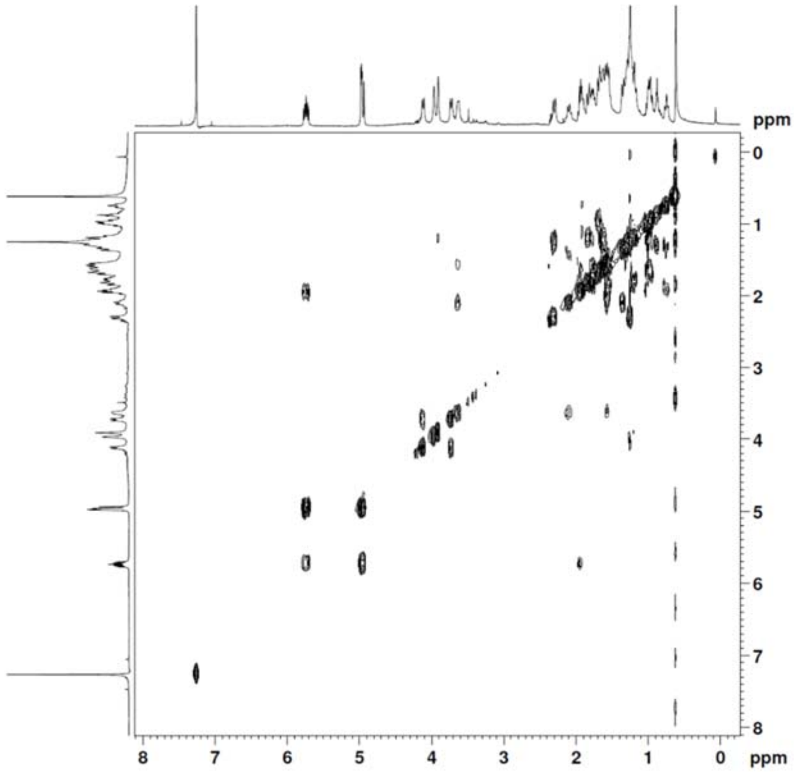

Figure S.I. 13: ^{1}H-^{1}H COSY spectrum of turranin N (**2**) in $CDCl_3$.

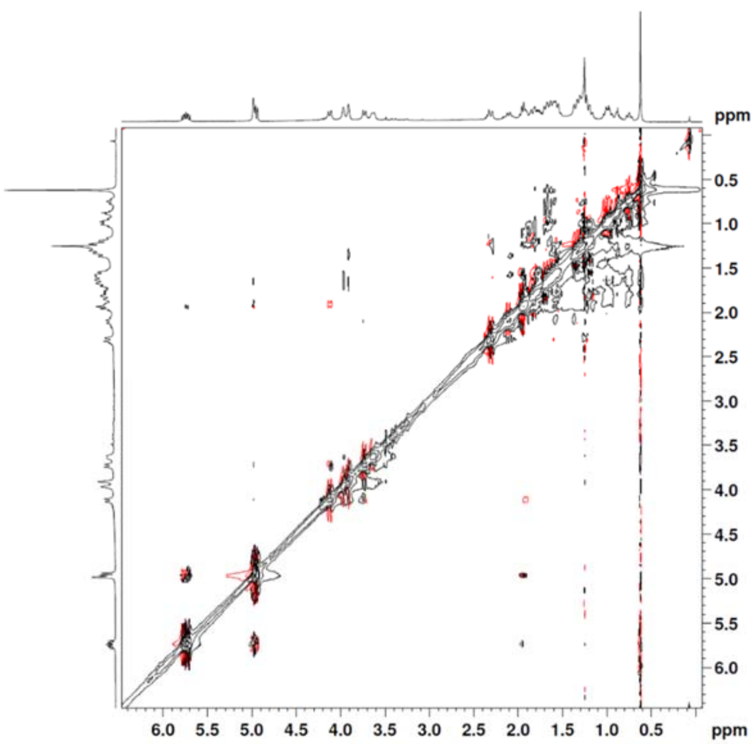

Figure S.I. 14: NOESY spectrum of turranin N (**2**) in $CDCl_3$.

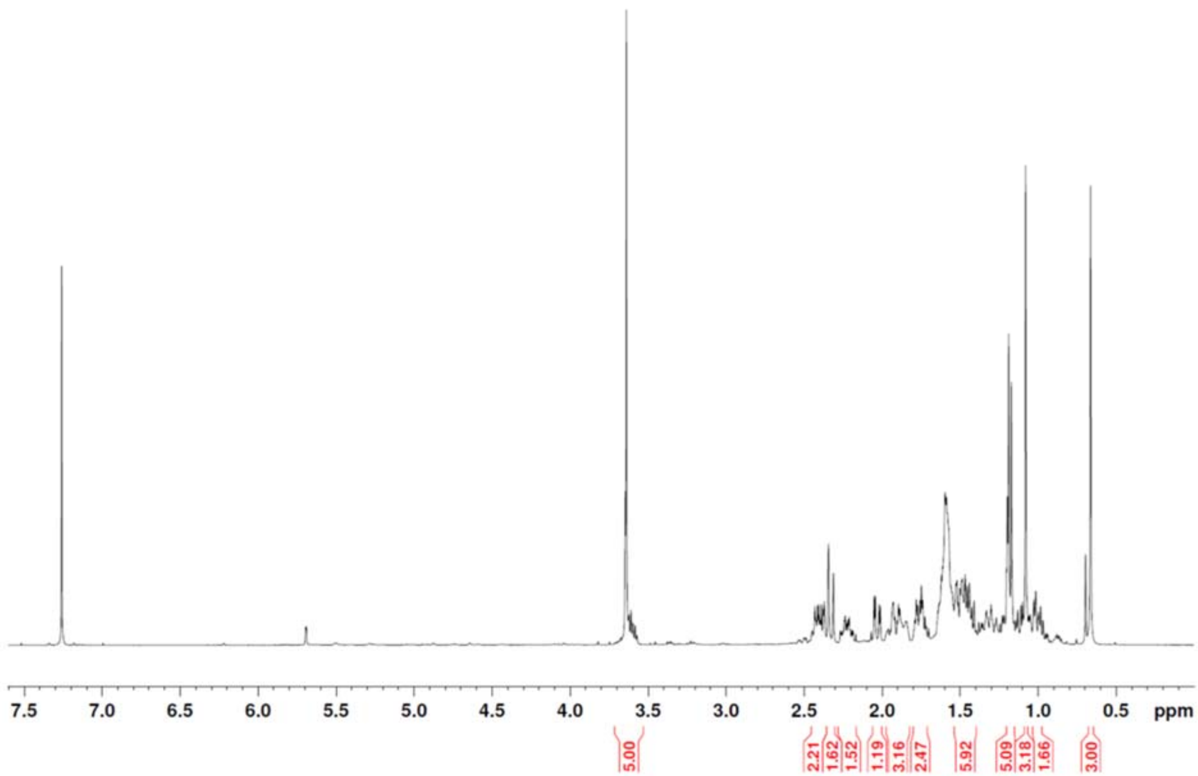

Figure S.I. 15: ^{1}H NMR spectrum of turranin O (**3**) in $CDCl_3$.

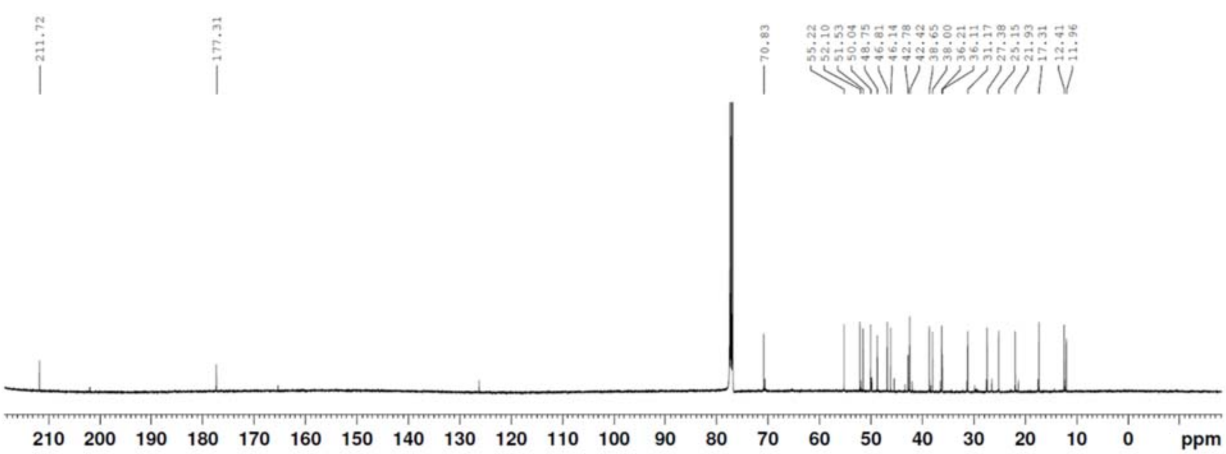

Figure S.I. 16: ^{13}C NMR spectrum of turranin O (**3**) in $CDCl_3$.

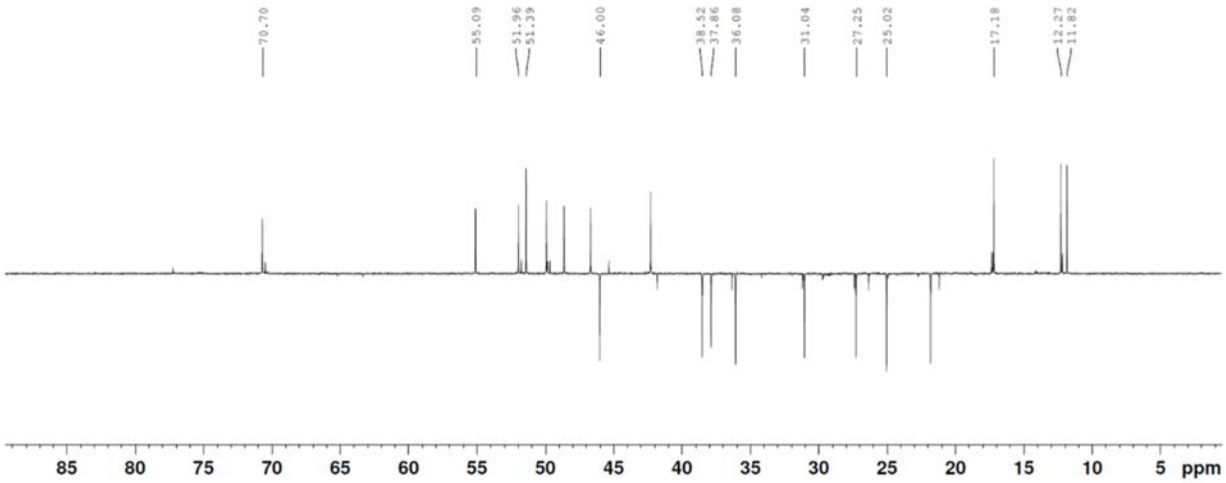

Figure S.I. 17: DEPT-135 spectrum of turranin O (**3**) in $CDCl_3$.

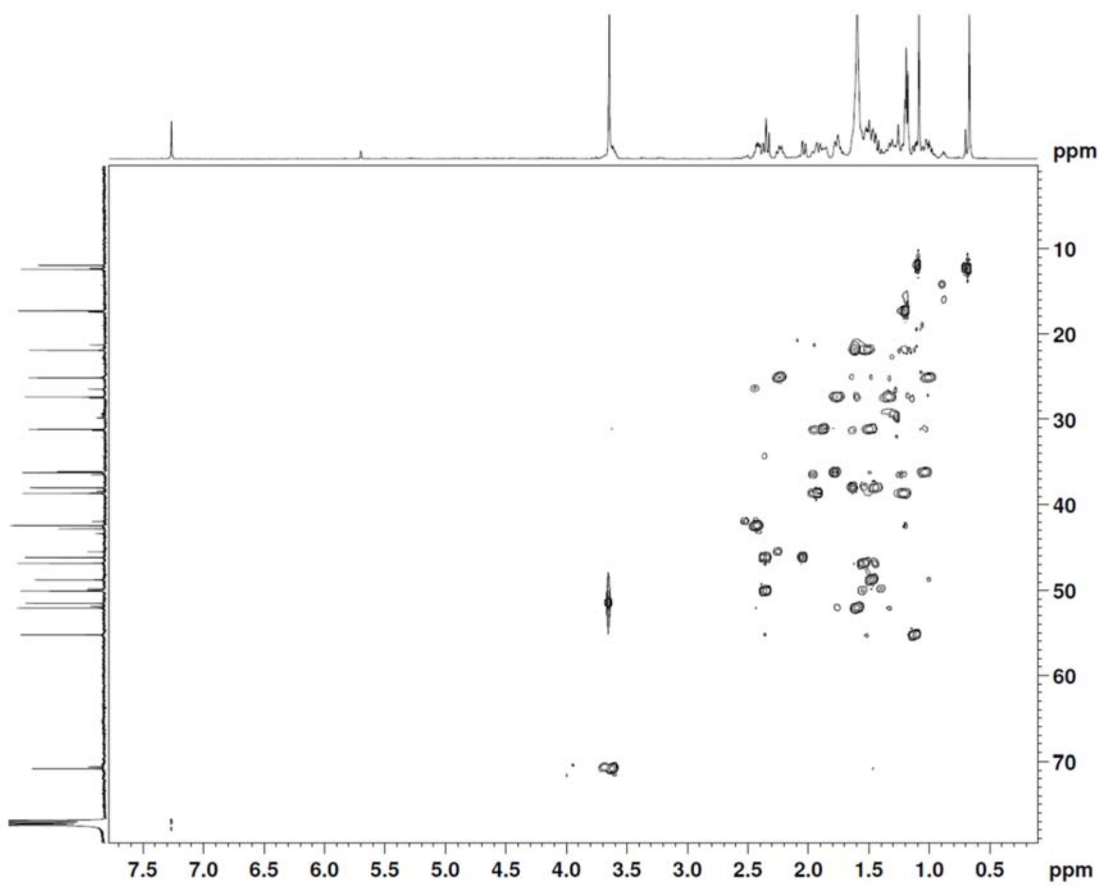

Figure S.I. 18: ^{1}H-^{13}C HSQC spectrum of turranin O (**3**) in $CDCl_3$.

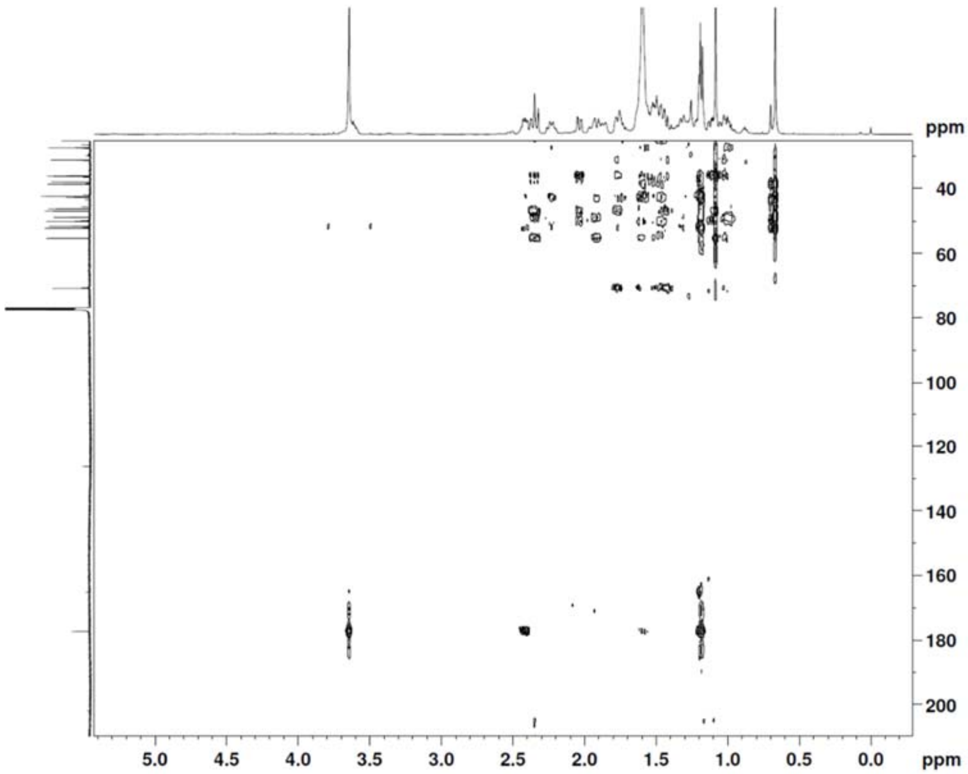

Figure S.I. 19: ^{1}H-^{13}C HMBC spectrum of turranin O (**3**) in $CDCl_3$.

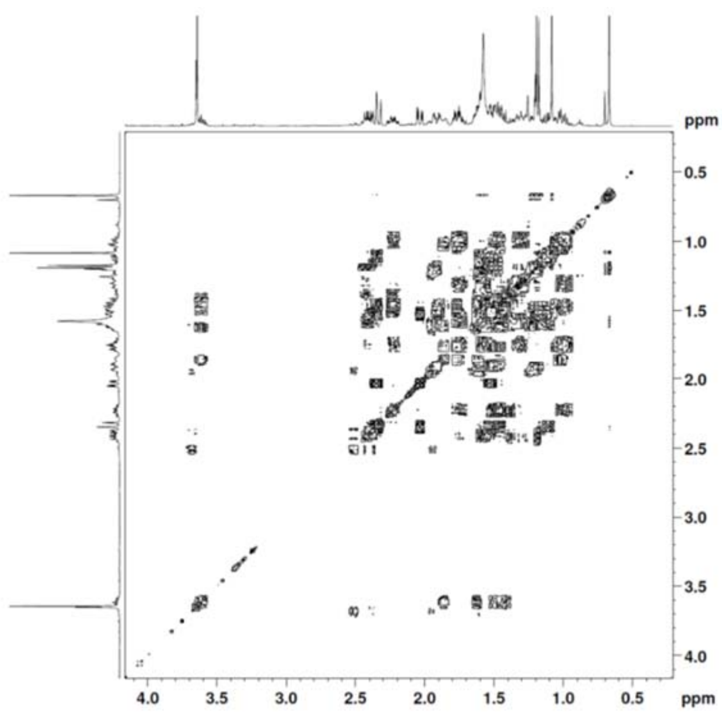

Figure S.I. 20: ^{1}H-^{1}H COSY spectrum of turranin O (**3**) in $CDCl_3$.

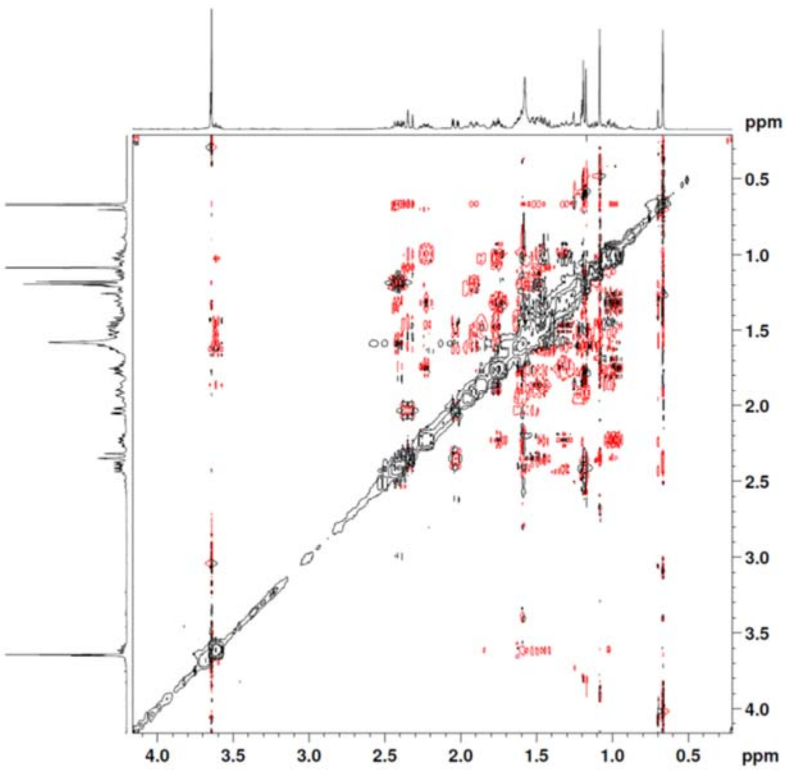

Figure S.I. 21: NOESY spectrum of turranin O (**3**) in $CDCl_3$.

Supplementary table 1: Comparison of ^{1}H (500 MHz) and ^{13}C (125 MHz) NMR data of isolated nymania 1 (**4**) in $CDCl_3$ to the published data (L. Musza et al. 1994).

Position	**Isolated nymania 1 ($CDCl_3$)**		**Data published for nymania 1 in $CDCl_3$ (L. Musza et al. 1994)**	
	δ_H (m, *J* in Hz)	**δ_C**	**δ_H (m, *J* in Hz)**	**δ_C**
1	5.25 (dd, 12.3, 2.8, 1H)	70.7	5.25 (dd, 3.2.12.4, 1H)	70.6
2α	2.03 (dd, 12.3, 3.4, 1H)	39.9	2.03 (dd, 3.2,13.9, 1H)	39.8
2β	2.58 (t, 13.0, 1H)		2.57 (t, 13.2, 1H)	
3		119.6		119.4
4		82.8		82.7
5	2.94 (m, 1H)	48.9	2.95 (d, 10.7, 1H)	48.8
6α	1.72 (m, 1H)	33.8	1.71 (d, 17.8, 1H)	33.6
6β	2.74 (dd, 10.0, 17.6, 1H)		2.73 (dd, 10.0, 17.9, 1H)	
7		175.7		175.6

8		138.8		142.8
9	4.197 (d, 7.1, 1H)	50.7	4.19 (d, 8.2, 1H)	48.6
10		48.8		49.4
11	5.38 (t, 8.7, 1H)	71.4	5.37 (dd, 8.5.10.7, 1H)	71.2
12	6.03 (d, 12.0, 1H)	74.3	6.05 (m, 1H)	74.6
13		49.6		50.6
14		80.9		80.8
15		207.0		207.3
16α	2.94 (m, 1H)	41.8	2.97 (dd, 8.5, 18.8, 1H)	41.6
16β	2.32 (m, 1H)		2.30 (dd, 9.4, 19.2, 1H)	
17	3.98 (t, 9.1, 1H)	35.2	3.97 (dd. 7.4, 9.3, 1H)	35.1
18-CH_3	1.00 (s, 3H)	13.2	1.00 (s, 3H)	13.1
19-CH_3	1.297 (s, 3H)	16.7	1.29 (s, 3H)	16.6
20		123.3		126.3
21	7.20 (s, 3H)	140.7	7.20 (s, 3H)	140.6
22	6.25 (d, 12.0, 1H)	110.7	6.25 (s, 1H)	110.6
23	7.37 (d, 11.8, 1H)	143.1	7.37 (s, 1H)	143.0
28	1.42 (s, 3H)	29.0	1.42 (s, 3H)	28.8
29α	3.65 (d, 8.4, 1H)	73.8	3.64 (d, 8.6, 1H)	73.7
29β	4.12 (d, 8.4, 1H)		4.11 (d, 8.6, 1H)	
30a (E to H-9	6.06 (brs, 1H)	126.4	6.06 (d, 1.4, 1H)	123.2
30b (Z to H-9)	5.98 (s, 1H)		5.98 (d, 1.2, 1H)	
1’		175.1		174.9
2’	3.20 (d, 1.2, 1H)	74.7	3.20 (m, 1H)	74.1
3’	1.5 (m, 1H)	38.3	1.52 (m, 1H)	38.2
4’a	1.16 (m, 1H)	23.3	1.16 (m, 1H)	23.2

4’b	1.08 (m, 1H)		1.08 (m, 1H)	
5’-CH_3	0.86 (dd, 6.7, 12.3, 3H)	15.3	0.86 (d, 4.7, 3H)	15.2
6’-CH_3	0.79 (d, 7.3, 3H)	11.8	0.78 (t, 7.4, 3H)	11.6
1’’		170.0		169.7
1’’-CH_3	2.02 (s, 3H)	21.3	2.02 (s, 3H)	21.1
HCOO	7.94 (s, 1H)	161.1	7.93 (s, 1H)	160.9
7-OCH_3	3.73 (s, 3H)	53.2	3.72 (s, 3H)	53.0
14-OH	4.43 (s, 1H)			

Supplementary table 2: Comparison of ^{1}H (500 MHz) and ^{13}C (125 MHz) NMR data of isolated rubralin B (**5**) in $CDCl_3$ to the published data (Musza et al. 1995).

Position	**Isolated rubralin B ($CDCl_3$)**		**Data published for rubralin B (^{1}H, 360 MHz ^{13}C, 90 MHz) (Musza et al. 1995)**	
	δ_H (m, *J* in Hz)	δ_C	δ_H (m, *J* in Hz)	δ_C
1	4.74 (dd, 3.1, 5.2, 1H)	70.5	4.75 (dd, 3.5, 4.5, 1H)	70.4
2	3.22 (m, 1H)	35.1	3.20 (m, 1H)	35.0
3		168.9		168.5
4		85.3		85.0
5	2.55 (dd, 2.2, 13.2, 1H)	44.5	2.56 (d, 10.9, 1H)	44.4
6α 6β	1.95 (m, 1H) 2.04 (m, 1H)	26.5	1.95 (m, 1H) 2.10 (m, 1H)	26.4
7	5.29 (br q, 1.7, 1H)	75.2	5.29 (m, 1H)	75.2
8		41.5		41.4
9	2.72 (dd, 8.1, 11.7, 1H)	37.3	2.73 (dd, 8.1, 11.7, 1H)	37.2
10		44.2		44.2
11α 11β	1.16 (m, 1H) 2.04 (m, 1H)	25.5	1.30 (m, 1H) 2.07 (m, 1H)	25.4

12	5.05 (t, 8.4, 1H)	76.6	5.06 (t, 8.3, 1H)	76.5
13		51.3		51.2
14		155.1		155.1
15	5.50 (dd, 1.7, 3.6, 1H)	122.5	5.51 (brs, 1H)	122.4
16	2.41 (m, 1H)	36.8	2.41 (m, 1H)	36.7
17	3.02 (dd, 8.0, 10.5, 1H)	49.9	3.03 (dd, 7.9, 10.6, 1H)	49.9
18-CH_3	1.19 (s, 3H)	15.5	1.20 (s, 3H)	15.3
19-CH_3	0.93 (s, 3H)	14.8	0.95 (s, 3H)	14.7
20		124.5		124.1
21	7.18 (brs, 1H)	140.4	7.18 (s, 1H)	140.3
22	6.22 (dd, 0.8, 2.0, 1H)	111.6	6.22 (s, 1H)	111.5
23	7.34 (t, 1.9, 1H)	142.4	7.34 (s, 1H)	142.2
28-CH_3	1.43 (s, 3H)	29.2	1.43 (s, 3H)	29.1
29α 29β	4.04 (d, 12.3, 1H) 4.95 (d, 12.3, 1H)	65.6	4.05 (d, 12.3, 1H) 4.93 (d, 12.3, 1H)	65.6
30	1.25 (s, 3H)	28.3	1.25 (s, 3H)	28.1
1'		174.9		174.7
2'	4.14 (d, 3.8, 1H)	75.1	4.14 (d, 3.8, 1H)	75.5
3'	1.82 (m, 1H)	39.1	1.83 (m, 1H)	39.0
4'	1.29 (m, 1H)	23.8	1.28 (m, 1H)	23.7
5'	0.89 (t, 7.4, 3H)	11.9	0.90 (t, 7.4, 3H)	11.7
6'	1.00 (d, 6.9, 3H)	15.5	1.00 (d, 7.6, 3H)	15.4
1''		174.1		173.9
2''	4.04 (m, 1H)	75.5	4.03 (m, 1H)	75.0
3''	2.09 (m, 1H)	31.9	2.06 (m, 1H)	31.8
4''	1.09 (d, 7.0, 3H)	19.5	1.09 (d, 7.0, 3H)	19.3
5''	0.85 (d, 6.8, 3H)	15.8	0.87 (d, 6.9, 3H)	15.7

1'''		169.6		169.4
1'''-CH_3	2.07 (s, 3H)	20.8	2.07 (s, 3H)	20.6
1''''		171.0		170.8
1''''-CH_3	1.93 (s, 3H)	21.5	1.93 (s, 3H)	21.3

Supplementary table 3: Comparison of ^{1}H (500 MHz) and ^{13}C (125 MHz) NMR data of isolated aphapolynin C (**6**) in $CDCl_3$ to the published data (Zhang et al. 2013).

Position	**Isolated Aphapolynin C ($CDCl_3$)**		**Data published for Aphapolynin C in DMSO-*d*$_6$ (^{1}H, 500 MHz ^{13}C, 125 MHz) (Zhang et al. 2013)**	
	δ_H (m, *J* in Hz)	δ_C	δ_H (m, *J* in Hz)	δ_C
1	7.46 (d, 10.4, 1H)	152.3	7.43 (d, 12.0, 1H)	152.9
2	6.07 (d, 12.4, 1H)	120.9	5.96 (d, 12.0, 1H)	119.2
3		171.9		166.9
4		79.1		79.7
5	2.12 (brs, 1H)	50.8	2.37 (brs, 1H)	49.9
6α 6β	2.48 (dd, 15.1, 4.1, 1H) 2.71 (m, 1H)	29.7	2.56 (dd, 15.5, 10.0, 1H) 2.70 (dd, 15.5, 7.5, 1H)	29.8
7		169.3		172.7
8		136.8		138.8
9	3.72 (brs, 1H)	52.4	3.00 (d, 7.5, 1H)	51.9
10				43.4
11	5.66 (brs, 1H)	71.1	5.42 (dd, 10.5, 7.5, 1H)	71.6
12	6.19 (d, 10.2, 1H)	75.6	6.04 (d, 10.5, 1H)	74.7
13		49.5		49.1
14		80.6		79.2
15		207.2		207.5
16α	2.39 (dd, 9.9, 19.4, 1H)	41.8	2.47 (dd, 19.5, 9.5, 1H)	41.2

16β	2.93 (dd, 8.8, 19.4, 1H)		2.76 (dd, 19.5, 9.0, 1H)	
17	3.99 (t, 9.4, 1H)	35.4	3.79 (t, 9.5, 1H)	34.9
18-CH_3	0.96 (s, 3H)	13.5	0.86 (s, 3H)	12.4
19-CH_3	1.02 (s, 3H)	23.0	1.02 (s, 3H)	23.1
20		122.2		123.0
21	7.23 (d, 6.2, 1H)	140.9	7.39 (s, 1H)	140.5
22	6.25 (d,10.6, 1H)	110.3	6.49 (s, 1H)	111.1
23	7.40 (d, 12.0, 1H)	143.5	7.55 (s, 1H)	142.8
28-CH_3	1.68 (s, 3H)	27.3	1.53 (s, 3H)	25.3
29α 29β	4.29 (d, 11.2, 1H) 4.10 (d, 11.4, 1H)	74.4	4.23 (d, 11.5, 1H) 4.16 (d, 11.5, 1H)	73.6
30a 30b	5.99 (s, 1H) 5.35 (s, 1H)	123.6	5.78 (s, 1H) 5.35 (s, 1H)	120.6
1'		175.0		173.3
2'	3.12 (d, 2.6, 1H)	74.9	3.07 (dd, 5.5, 3.5, 1H)	74.2
3'	1.50 (m, 1H)	37.7	1.40 (m, 1H)	37.2
4'	1.16 (m, 1H) 0.96 (m, 1H)	22.8	a = 1.08 (m, 1H) b = 0.96 (m, 1H)	22.8
5'	0.80 (t, 7.0, 3H)	11.5	0.71 (t, 7.5, 5H)	11.3
6'	0.87 (d, 6.8, 3H)	15.4	0.72 (d, 7.0, 3H)	15.4
HCOO	7.92 (s, 1H)	159.7	8.22 (s, 1H)	160.7
14-OH			6.64 (s, 1H)	
2'-OH			4.96 (d, 5.5, 1H)	

Supplementary table 4: Comparison of ^{1}H (500 MHz) and ^{13}C (125 MHz) NMR data of isolated Trichillia substance Tr B (**7**) in $CDCl_3$ to the published data (Gunatilaka et al. 1998).

Position	**Isolated Trichillia substance Tr B ($CDCl_3$)**		**Data published for Trichillia substance Tr B in $CDCl_3$ (^{1}H, 500 MHz ^{13}C, 100.57 MHz) (Gunatilaka et al. 1998)**	
	δ_H (m, *J* in Hz)	δ_C	δ_H (m, *J* in Hz)	δ_C
1	5.00 (brs, 1H)	75.4	5.44 (dd, 6.8, 5.9, 1H)	73.1
2	3.23 (brs, 2H)	37.5	2.05 (dd, 11.8, 9.0, 2H)	41.9
3		169.0		169.7
4		79.2		79.3
5	3.18 (brs, 1H)	42.5	3.18 (dd, 7.7, 3.8, 1H)	38.0
6α 6β	2.57 (d, 4.9, 1H) 2.69 (dd, 4.9, 16.2, 1H)	32.0	2.48 (dd, 9.0, 7.7, 1H) 2.63 (dd, 7.7, 3.8, 1H)	42.2
7		173.2		173.7
8		138.5		138.2
9	3.79 (brs, 1H)	51.4	3.78 (d, 7.4, 1H)	51.3
10		46.0		45.8
11	5.49 (dd, 7.6, 10.2, 1H)	71.0	5.46 (dd, 7.4, 10.3, 1H)	78.1
12	6.12 (d, 10.2, 1H)	73.3	6.16 (d, 10.3, 1H)	71.2
13		49.7		49.6
14		80.9		80.8
15		206.7		206.3
16α 16β	2.41 (dd, 8.7, 18.3, 1H) 2.88 (dd, 8.6, 18.3, 1H)	41.8	2.34 (dd, 8.5, 9.0, 1H) 2.82 (dd, 8.8, 9.0, 1H)	35.0
17	3.95 (t, 8.7, 1H)	35.7	3.95 (t, 8.5, 1H)	37.9
18-CH_3	0.98 (s, 3H)	12.8	0.97 (s, 3H)	12.9
19-CH_3	1.76 (s, 3H)	21.0	1.62 (s, 3H)	22.9

20		122.8		125.2
21	7.23 (brs, 1H)	140.8	7.20 (brs, 1H)	140.6
22	6.29 (brs, 1H)	110.5	6.23 (brs, 1H)	110.3
23	7.40 (brs, 1H)	143.3	7.38 (t, 1H)	143.3
28	1.81 (s, 3H)	23.0	1.81 (s, 3H)	28.5
29α 29β	4.16 (d, 11.1, 1H) 4.24 (d, 11.1, 1H)	78.0	4.22 (dd, 12.0, 2H)	75.5
30a 30b	5.89 (brs, 1H) 5.52 (brs, 1H)	124.0	5.89 (brs, 1H) 5.49 (brs, 1H)	122.5
1'		174.9		174.9
2'	3.08 (brs, 1H)	74.6	3.30 (br d, 1H)	74.6
3'	1.43 (m, 1H)	37.9	1.45 (m, 1H)	37.9
4'	1.11 (m, 1H) 0.96 (m, 1H)	22.8	1.15 (m, 2H)	22.7
5'	0.75 (t, 7.3, 3H)	11.3	0.84 (t, 7.6, 3H)	11.4
6'	0.81 (d, 6.6, 3H)	15.0	0.82 (d, 6.5, 3H)	15.1
HCOO	7.78 (s, 1H)	160.3	7.74 (s, 1H)	
CH_3CO	2.06 (s, 1H)	21.2	1.99 (s, 1H)	
		169.4		

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