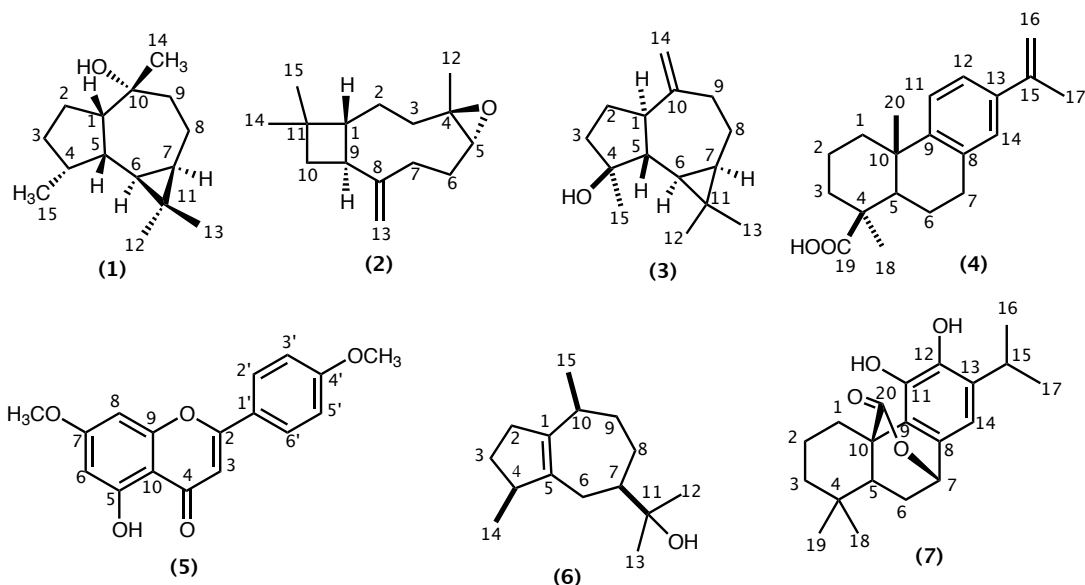


Supplementary material



(-)-Ledol (**1**); $C_{15}H_{26}O$; waxy white powder. $[\alpha]_D^{20} = -5.1$ (c 1.0 in $CHCl_3$). EIMS m/z (%) = 222 (3, M), 204 (53), 189 (40), 162 (24), 161 (100), 149 (18), 148 (33), 147 (53), 136 (10), 135 (21), 134 (14), 133 (52), 123 (16), 122 (56), 121 (45), 120 (19), 119 (61), 117 (13), 115 (10), 111 (18), 109 (46), 108 (26), 107 (83), 106 (26), 105 (92), 96 (12), 95 (39), 94 (21), 93 (70), 92 (16), 91 (76), 83 (13), 82 (23), 81 (51), 80 (11), 79 (54), 77 (35), 69 (41), 67 (37), 65 (13), 55 (35), 53 (17). 1H NMR: see Table S1. ^{13}C NMR: see Table S2.

(-)-Caryophyllene oxide (**2**); $C_{15}H_{24}O$; colourless liquid. EIMS m/z (%) = 220 (4, M), 205 (13), 202 (16), 187 (34), 177 (16), 174 (10), 173 (10), 164 (20), 163 (15), 162 (12), 161 (48), 159 (33), 149 (32), 147 (22), 146 (20), 145 (29), 138 (20), 137 (12), 136 (31), 135 (35), 134 (15), 133 (31), 132 (12), 131 (60), 129 (10), 123 (32), 122 (19), 121 (61), 120 (29), 119 (41), 118 (14), 117 (25), 115 (12), 111 (11), 110 (18), 109 (48), 108 (38), 107 (82), 107 (30), 105 (73), 97 (11), 96 (28), 95 (67), 94 (35), 93 (95), 92 (25), 91 (94), 84 (10), 83 (24), 82 (30), 81 (62), 80 (21), 79 (100), 78 (15), 77 (56), 71 (25), 70 (12), 69 (71), 68 (18), 67 (46), 65 (21), 55 (51), 53 (30). 1H NMR: see Table S1. ^{13}C NMR: see Table S2.

Spathulenol (**3**), $C_{15}H_{24}O$; white powder. EIMS m/z (%) = 220 (15, M), 205 (61), 202 (26), 187 (26), 177 (17), 162 (39), 160 (12), 159 (43), 149 (19), 147 (33), 146 (24), 145 (21), 135 (16), 134 (15), 133 (22), 131 (23), 121 (23), 120 (17), 119 (57), 117 (17), 109 (14), 107 (36), 106 (25), 105 (40), 95 (23), 94 (13), 93 (48), 92 (13), 91 (50), 83 (10), 82 (19), 81 (23), 79 (35), 77 (19), 71 (21), 69 (35), 67 (28), 55 (27), 53 (15), 43 (100), 41 (63). 1H NMR: see table 1.

Angustanoic acid E (**4**); $C_{22}H_{26}O_2$; white powder. ESI-MS $m/z = 323$ $[M+1]$. $[\alpha]_D^{20} = +102.3$ (c 0.6 in $CHCl_3$). 1H NMR: see Table S1. ^{13}C NMR: see Table S2.

5-hydroxy-4',7-dimethoxy flavone (**5**); $C_{17}H_{14}O_5$; yellowish crystals. ESI-MS $m/z = 299$ $[M+1]$. 1H NMR: see Table S1. ^{13}C NMR: see Table S2.

(-)-Carnosol (**7**); $C_{20}H_{26}O_4$; white crystals. ESI-MS $m/z = 331$ $[M + 1]$. $[\alpha]_D^{20} = -63.0$ (c 0.75 in MeOH). 1H NMR: see table S1. ^{13}C NMR: see table S2.

Table S1. ¹H NMR spectroscopic data for compounds **1-5** and **7** (400 MHz, δ ppm, CDCl₃).

Position	1	2	3	4	5	7
1	2.08 (1H, ddd, <i>J</i> = 9.2, 9.2, 6.4 Hz)	1.75 (1H, ddd, <i>J</i> = 10.3, 10.3, 4.2 Hz)	0.47 (1H, dd, <i>J</i> = 9.6, 11.6 Hz)	1.38 (1H, ddd, <i>J</i> = 13.2, 13.2, 4.0 Hz) 2.28 (1H, m)	-	2.90 (1H, ddd, <i>J</i> = 13.0, 4.8, 1.6 Hz) 2.40 (1H, ddd, <i>J</i> = 13.0, 13.0, 4.4 Hz)
2	1.69 (1H, m) 1.90 (1H, m)	1.45 (1H, m) 1.64 (1H, m)	0.71 (1H, m)	1.62 (1H, m) 2.03 (1H, m)	-	1.68 (1H, m)
3	1.27 (1H, m) 1.71 (1H, m)	2.10 (1H, m) 0.95 (1H, m)	1.01 (1H, m) 1.96 (1H, m)	1.09 (1H, ddd, <i>J</i> = 13.6, 13.6, 4.4 Hz) 2.26 (1H, m)	6.57 (1H, s)	1.55 (1H, ddd, <i>J</i> = 13.4, 4.8, 1.6 Hz) 1.28 (1H, ddd, <i>J</i> = 13.4, 13.4, 3.6 Hz)
4	1.98 (1H, m)	-	2.05 (1H, m) 2.42 (1H, dd, <i>J</i> = 5.2, 13.6 Hz)	-	-	-
5	1.77 (1H, m)	2.85 (1H, dd, <i>J</i> = 10.6, 4.2 Hz)	-	1.57 (1H, dd, <i>J</i> = 12.0, 1.6 Hz)	-	1.73 (1H, dd, <i>J</i> = 10.8, 5.6 Hz)
6	0.33 (1H, dd, <i>J</i> = 9.8, 9.0 Hz)	1.35 (1H, m) 2.25 (1H, m)	2.20 (1H, m)	2.19 (1H, dt, <i>J</i> = 6.0, 1.6 Hz) 2.06 (1H, m)	6.36 (1H, d, <i>J</i> = 2.0 Hz) or 6.48 (1H, d, <i>J</i> = 2.0 Hz)	2.20 (1H, m) 1.69 (1H, m)
7	0.71 (1H, ddd, <i>J</i> = 11.5, 9.0, 5.6 Hz)	2.10 (1H, m) 2.35 (1H, m)	1.64 (1H, m) 1.91 (1H, m)	2.80 (1H, m) 2.92 (1H, dd, <i>J</i> = 16.8, 5.6 Hz)	-	5.37 (1H, dd, <i>J</i> = 4.0, 1.6 Hz)
8	1.85 (2H, m)	-	1.54 (1H, m) 1.77 (1H, m)	-	6.36 (1H, d, <i>J</i> = 2.0 Hz) or 6.48 (1H, d, <i>J</i> = 2.0 Hz)	-
9	1.71 (1H, m) 1.90 (1H, m)	2.60 (1H, dd, <i>J</i> = 10.3, 8.5 Hz)	-	-	-	-
10	-	1.60 (1H, m) 1.69 (1H, m)	1.31 (1H, m)	-	-	-
11	-	-	-	7.22 (1H, d, <i>J</i> = 8.0 Hz)	-	-
12	0.93 (3H, d, <i>J</i> = 6.9 Hz)	1.20 (3H, s)	1.05 (3H, s)	7.24 (1H, d, <i>J</i> = 8.0 Hz)	-	-
13	1.03 (3H, s)	4.86 (1H, d, <i>J</i> = 1.2 Hz)	1.04 (3H, s)	-	-	-

		4.97 (1H, d, $J = 1.2$ Hz)		-	-	-
14	0.98 (3H, s)	1.01 (3H, s)	4.66 (1H, d, $J = 1.3$ Hz) 4.68 (1H, d, $J = 1.3$ Hz)	7.14 (1H, bs)	-	6.64 (H, s)
15	1.14 (3H, s)	0.99 (3H, s)	1.28 (3H, s)	-	-	3.08 (1H, sept, $J = 6.8$ Hz)
16	-	-	-	5.32 (1H, bs) 5.02 (1H, bs)	-	1.22 (3H, d, $J = 7.2$ Hz) or 1.23 (3H, d, $J = 7.2$ Hz)
17	-	-	-	2.12 (3H, s)	-	1.22 (3H, d, $J = 7.2$ Hz) or 1.23 (3H, d, $J = 7.2$ Hz)
18	-	-	-	1.34 (3H, s)	-	0.90 (3H, s)
19	-	-	-	-	-	0.86 (3H, s)
20	-	-	-	1.12 (3H, s)	-	-
2' and 6'	-	-	-	-	7.01 (2H, d, $J = 8.8$ Hz) or 7.84 (2H, d, $J = 8.8$ Hz)	-
3' and 5'	-	-	-	-	7.01 (2H, d, $J = 8.8$ Hz) or 7.84 (2H, d, $J = 8.8$ Hz)	-
4'	-	-	-	-	-	-
-OCH ₃	-	-	-	-	3.88 (3H, s, OCH ₃)	-
-OCH ₃	-	-	-	-	3.89 (3H, s, OCH ₃)	-
-OH (12 or 20)	-	-	-	-	-	5.74 (1H, s)

Table S2. ^{13}C NMR spectroscopic data for compounds 1, 2, 4, 5 and 7 (100 MHz, δ ppm, CDCl_3).

Position	1	2	4	5	7
1	53.9	50.9	39.4	-	29.3
2	24.8	27.3	20.0	164.2	19.0
3	31.7	39.3	37.5	104.3	41.1
4	38.6	60.0	44.0	182.5	34.7
5	40.9	63.9	52.9	162.7	45.6
6	23.6	29.9	21.0	98.2	29.9
7	25.1	30.0	32.2	165.6	78.0
8	20.4	152.0	135.2	92.8	132.2
9	39.4	48.9	147.5	157.8	121.7
10	74.7	39.9	38.6	105.7	48.5
11	19.3	34.2	125.6	-	141.9
12	15.5	17.1	123.2	-	141.2
13	28.8	112.9	138.4	-	133.0
14	30.7	21.8	126.2	-	112.4
15	16.1	30.3	143.1	-	27.4
16	-	-	111.8	-	22.6
17	-	-	21.9	-	22.7
18	-	-	28.8	-	31.8
19	-	-	183.1	-	19.8
20	-	-	23.2	-	176.1
1'	-	-	-	123.7	-
2'	-	-	-	128.2	-
3'	-	-	-	114.6	-
4'	-	-	-	162.3	-
5'	-	-	-	114.6	-
6'	-	-	-	128.2	-
7-OMe	-	-	-	55.9	-
4'-OMe	-	-	-	55.7	-

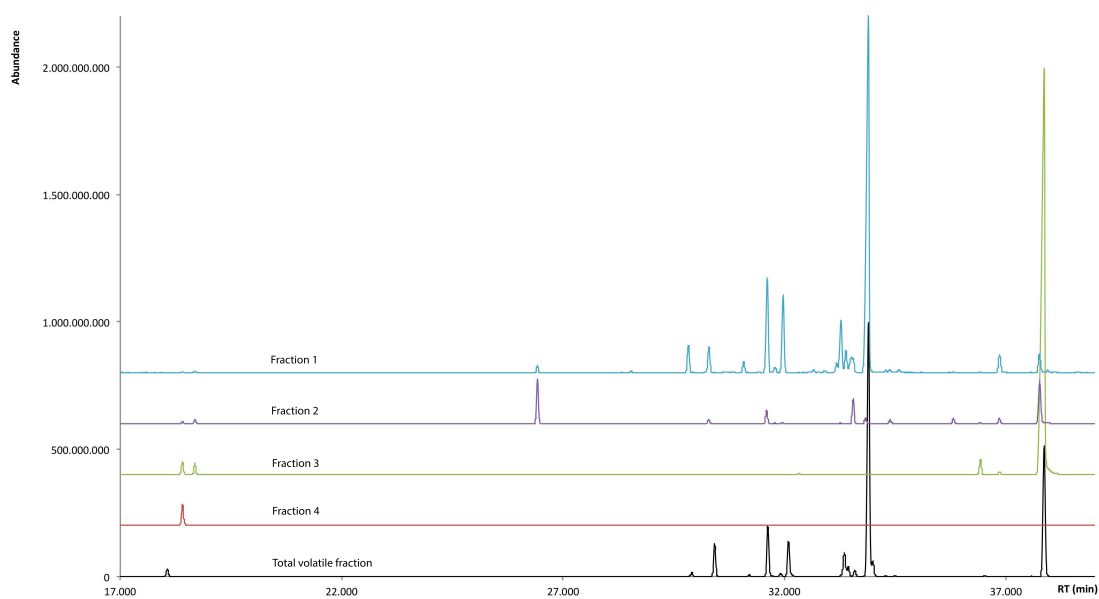


Figure S1. GC-MS comparison of fractions from a preparative TLC analysis of *L. heteromorpha* EO. The fractions represent compounds that can be separated by normal phase liquid chromatography.

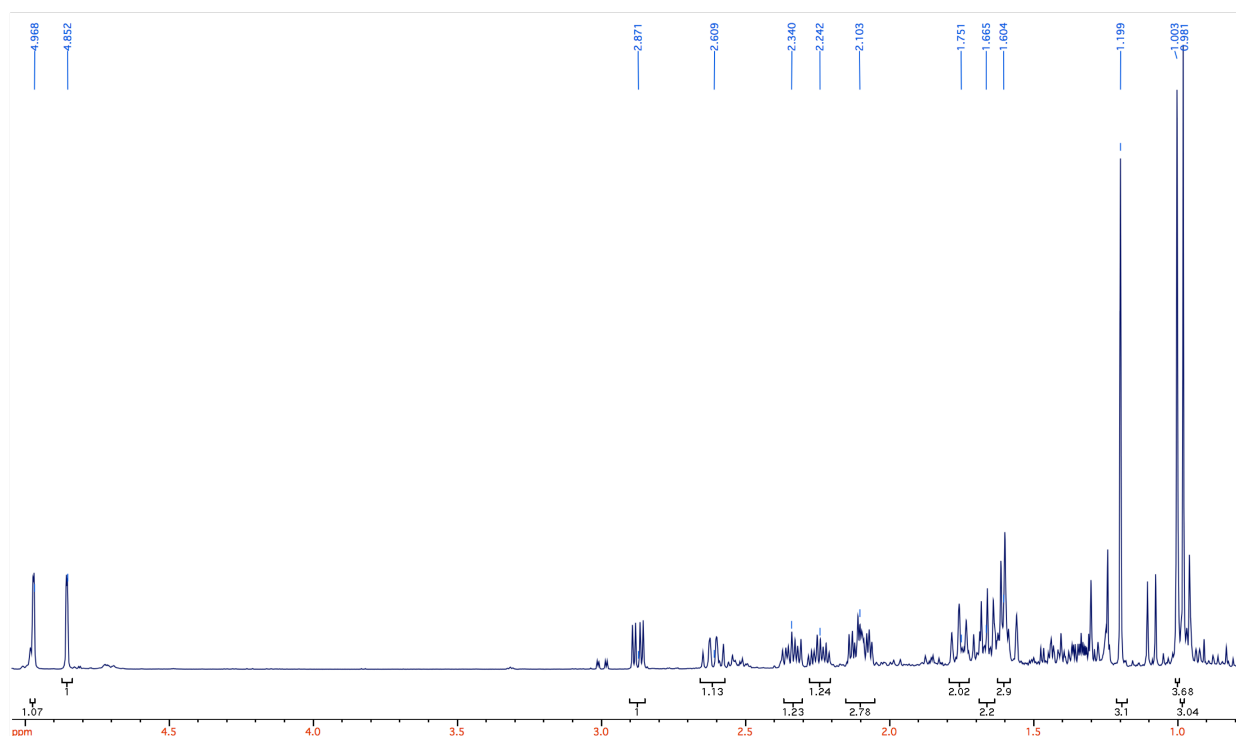


Figure S4. ¹H NMR (400 MHz) spectrum of compound (2) in CDCl₃

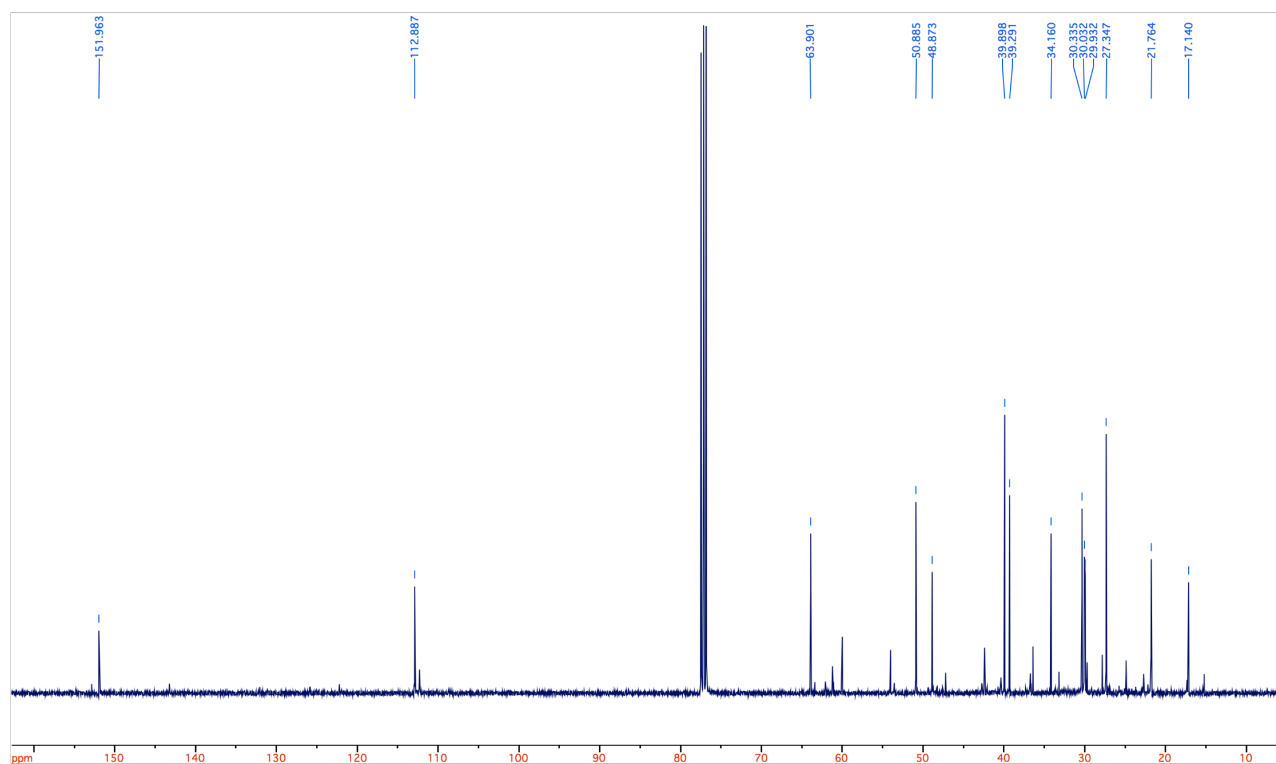


Figure S5. ¹³C NMR (100 MHz) spectrum of compound (2) in CDCl₃

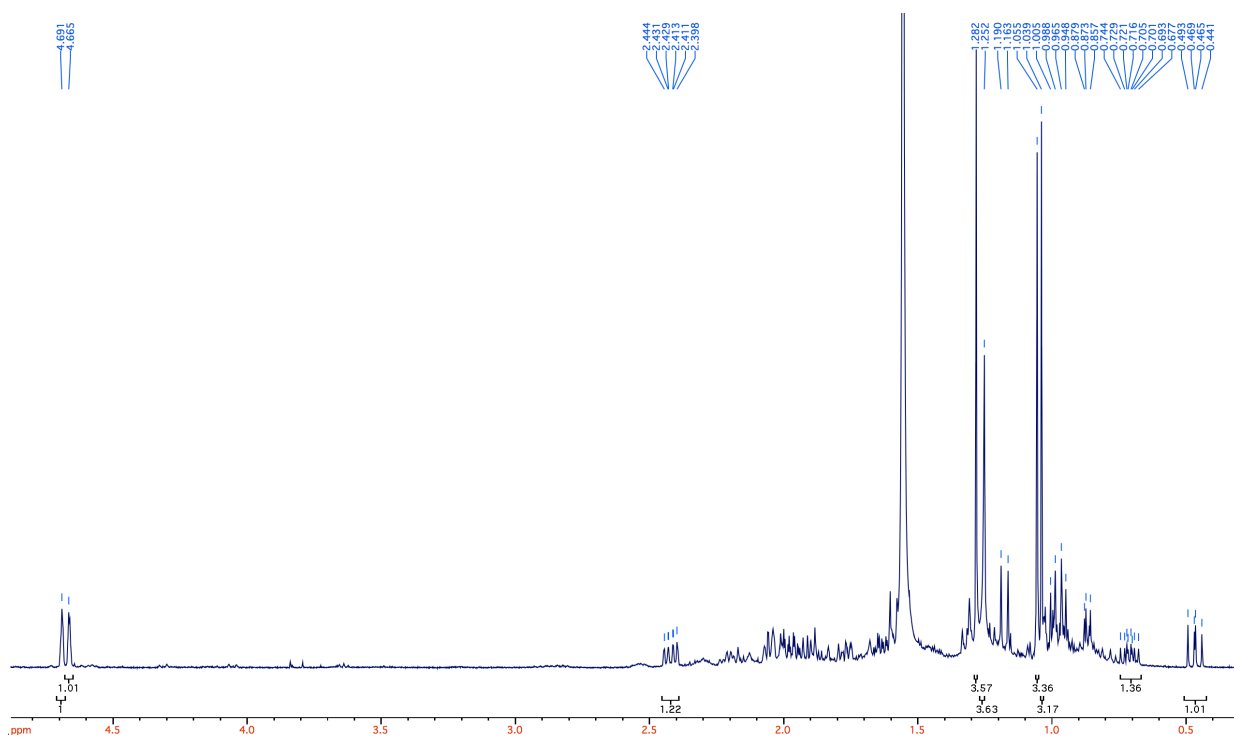


Figure S6. ¹H NMR (400 MHz) spectrum of compound (3) in CDCl₃

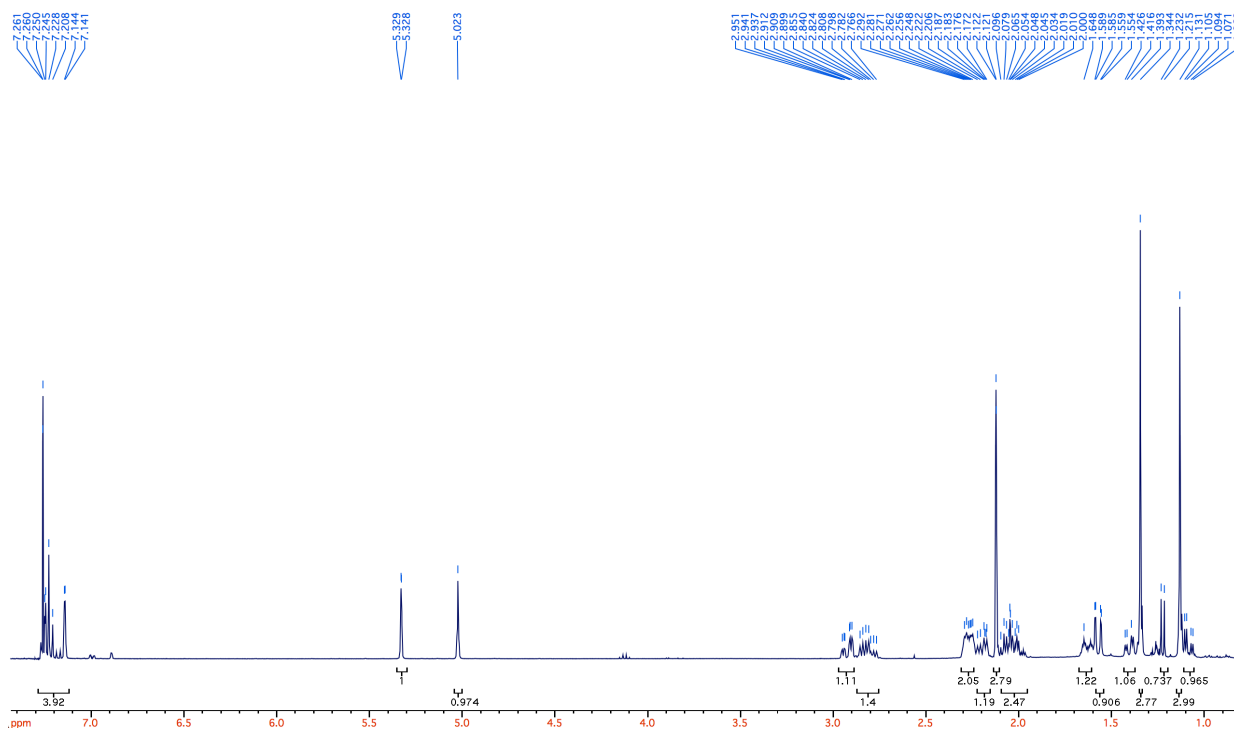


Figure S7. ¹H NMR (400 MHz) spectrum of compound (4) in CDCl₃

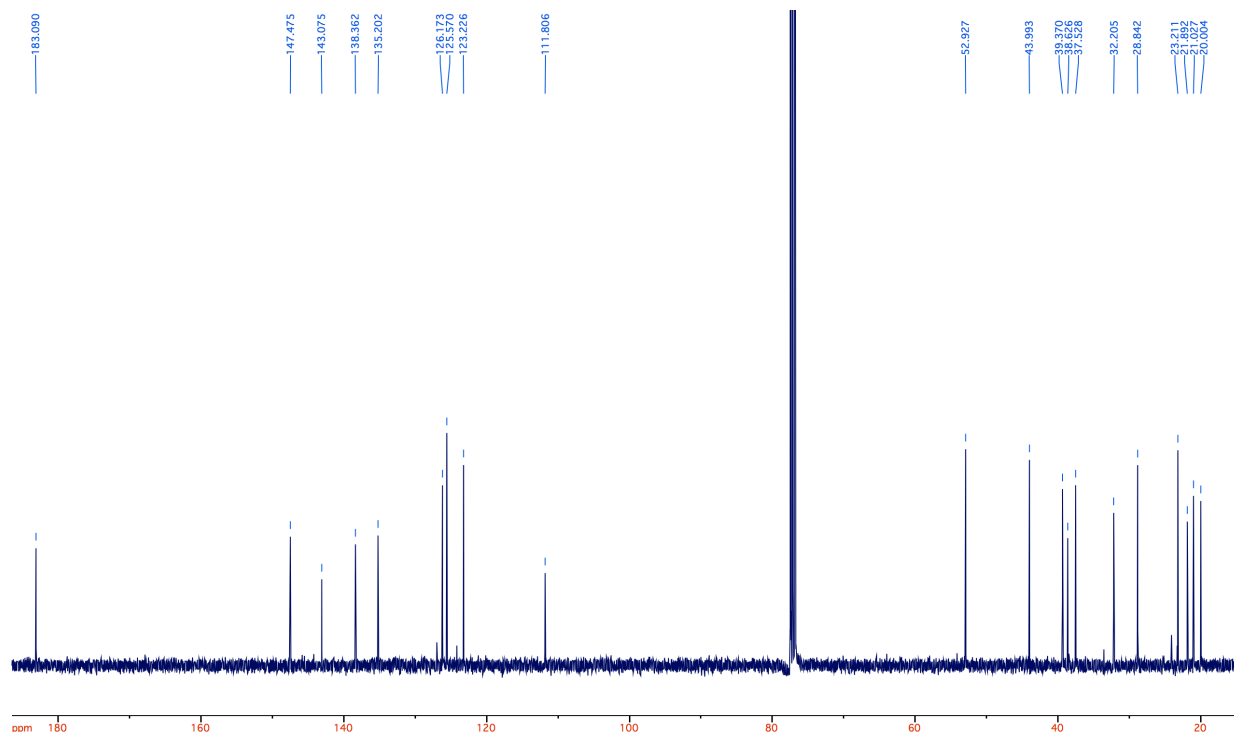


Figure S8. ^{13}C NMR (100 MHz) spectrum of compound (4) in CDCl_3

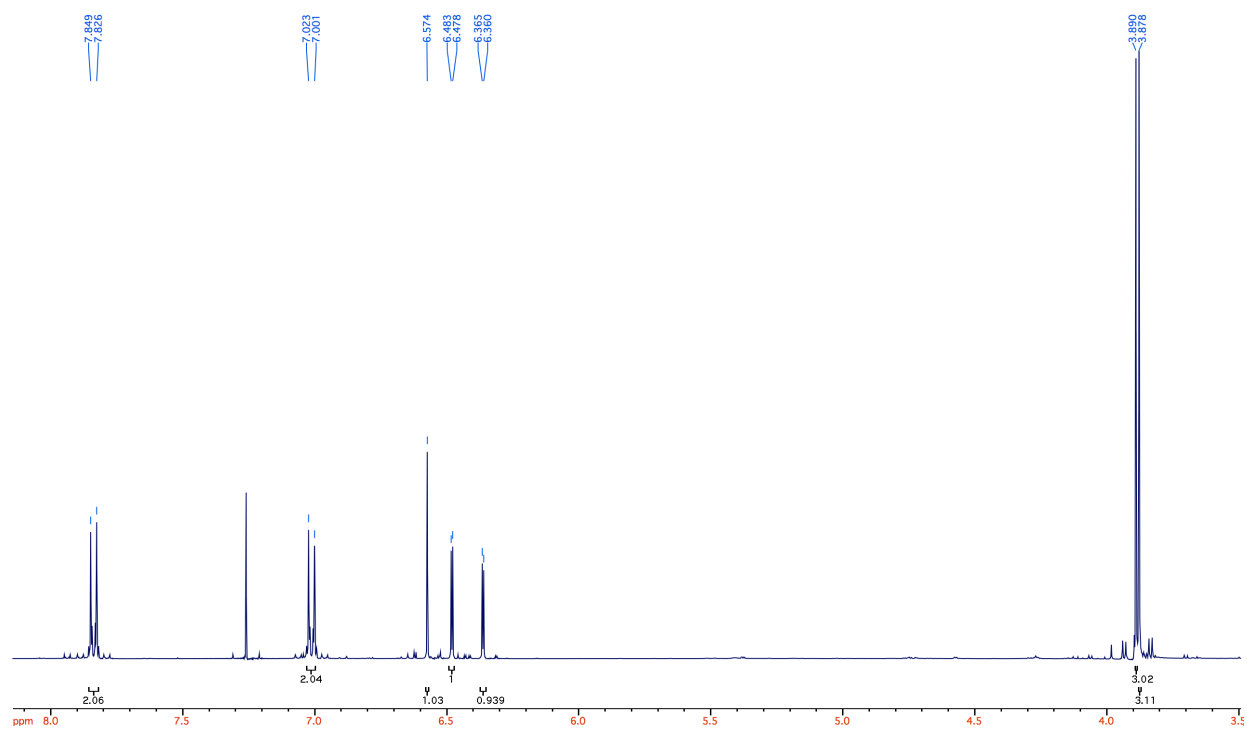


Figure S9. ^1H NMR (400 MHz) spectrum of compound (5) in CDCl_3

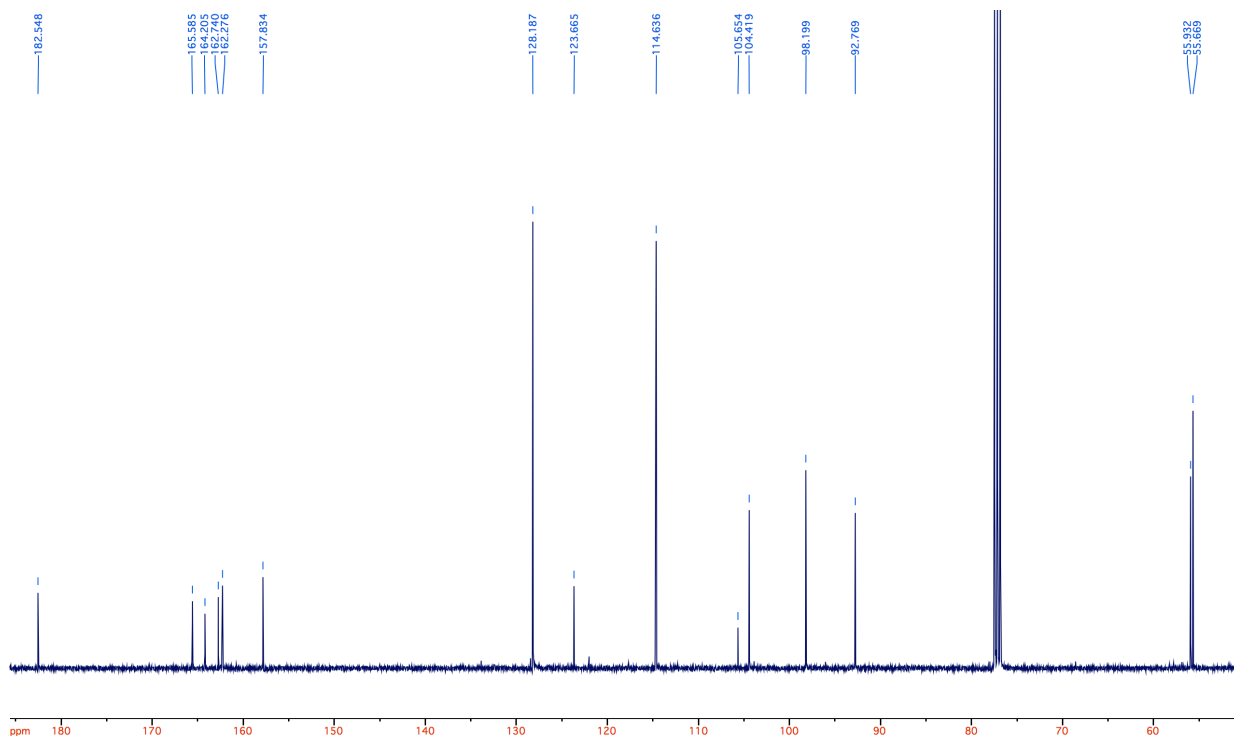


Figure S10. ^{13}C NMR (100 MHz) spectrum of compound (5) in CDCl_3

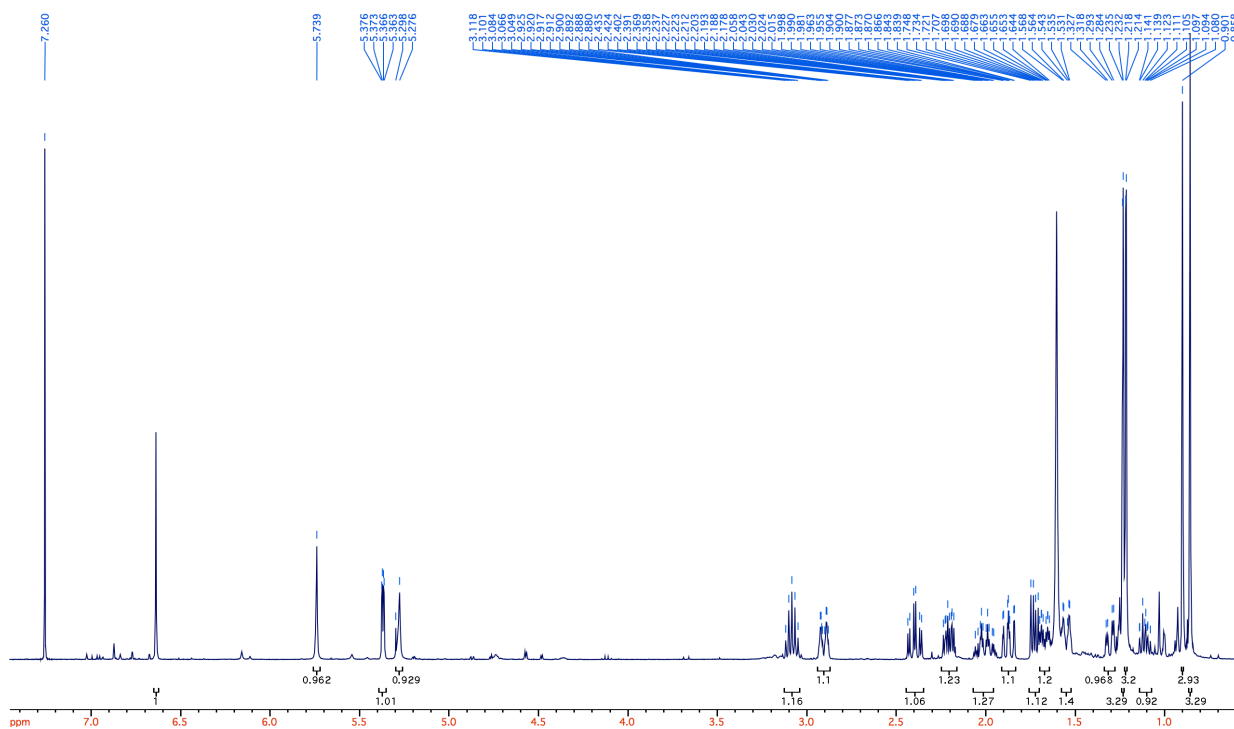


Figure S11. ^1H NMR (400 MHz) spectrum of compound (7) in CDCl_3

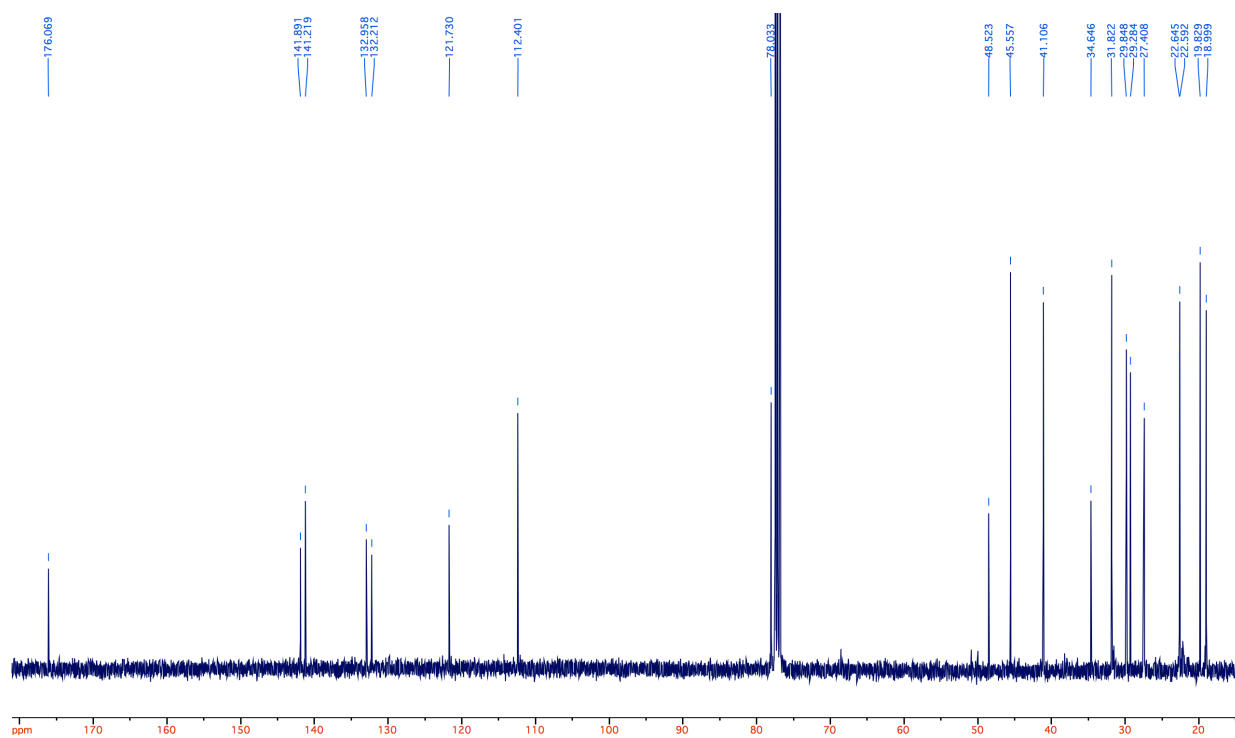


Figure S12. ^{13}C NMR (100 MHz) spectrum of compound (7) in CDCl_3