

SUPPLEMENTARY MATERIAL**Atalantums H-K from the peels of *Atalantia monophylla* and their Cytotoxicity**

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ABSTRACT

Four new benzoyltyramines, atalantums H-K (**1-4**) and seven known compounds were isolated from the peels of *Atalantia monophylla*. All compounds were tested for cytotoxicity against HeLa, HCT116 and MCF-7 cell lines, as well as normal cells (Vero cells). Compound **5** showed cytotoxicity against HeLa, HCT116 and MCF-7 cell lines with IC₅₀ values ranging from 16-25 µg/mL but was inactive against Vero cells. Compound **6** also showed interesting results as compound **5** with IC₅₀ values ranging from 15-18 µg/mL and an IC₅₀ value of 80.20 µg/mL against Vero cells. This means compounds **5** and **6** can be used as lead compounds for anticancer agents.

KEYWORDS *Atalantia monophylla*; atalantum; benzoyltyramine

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Table S1. ^1H NMR spectroscopic data of compounds **1–4** (CDCl_3 , δ in ppm)

position	1	2	3	4
1	4.54, d (4.0)	4.57, d (8.0)	4.57, d (8.0)	4.53, d (8.0)
2	5.76, t (8.0)	5.83, t (8.0)	5.83, t (8.0)	5.72, t (4.0)
4	4.27, dd (8.0, 4.0)	5.42, dd (8.0, 4.0)	5.42, dd (8.0, 4.0)	4.89, dd (8.0, 4.0)
5	1.58, m	1.78, m	1.79, m	1.78, m
6	3.64, t (8.0)	3.35 dd (8.0, 4.0)	3.35 dd (8.0, 4.0)	4.12, t (8.0)
8	1.10, s	1.09, s	1.08, s	1.13, s
9	1.09, s	1.07, s	1.07, s	1.12, s
10	1.72, s	1.73, s	1.73, s	1.70, s
2', 6'	6.84, d (8.0)	6.85, d (8.0)	6.84, d (8.0)	6.83, d (8.0)
3', 5'	7.12, d (8.0)	7.13, d (8.0)	7.13, d (8.0)	7.11, d (8.0)
7'	2.84, t (8.0)	2.86, t (8.0)	2.86, t (8.0)	2.83, t (8.0)
8'	3.65, m	3.68, m	3.67, m	3.63, m
2'', 6''	7.66, d (8.0)	7.69, d (8.0)	7.69, d (8.0)	7.68, d (8.0)
3'', 5''	7.38, t (8.0)	7.41, t (8.0)	7.40, t (8.0)	7.37, t (8.0)
4''	7.46, t (8.0)	7.47, t (8.0)	7.48, t (8.0)	7.44, t (8.0)
2'''	-	2.28, t (8.0)	2.28, t (8.0)	2.30, t (8.0)
3'''	-	1.60, m	1.60, m	1.60, m
CH ₂ (4'''-15''')	-	1.25, m	1.25, m	1.24, m
CH ₃ (14''' or 16''')	-	0.87, t (8.0)	0.87, t (8.0)	0.86, t (8.0)
7-OMe	3.20, s	3.18, s	3.18, s	3.20, s
NH	6.39, br t (8.0)	6.16, br t (8.0)	6.19, br t (8.0)	6.40, br t (8.0)

Table S2. ^{13}C NMR spectroscopic data of compounds **1–4** (CDCl_3 , δ in ppm)

position	1	2	3	4
1	64.0	64.5	64.5	64.6
2	120.3	124.5	124.5	121.7
3	141.3	137.3	137.3	141.3
4	76.5	77.1	77.1	74.6
5	35.1	34.4	34.4	34.7
6	76.9	74.1	74.1	75.5
7	76.5	77.1	77.1	76.3
8	19.6	20.5	20.5	22.2
9	18.7	19.5	19.5	20.6
10	11.8	12.6	12.6	12.3
7-OMe	48.6	49.3	49.3	49.8
1'	156.8	157.5	157.5	157.5
2', 6'	114.3	115.1, 115.2	115.1, 115.2	115.0
3', 5'	129.2	129.9	129.9	129.8
4'	130.4	131.2	131.2	131.0
7'	34.1	34.9	34.9	35.3
8'	40.6	41.4	41.4	41.4
9'	167.2	167.6	167.6	167.5
1''	133.9	134.8	134.8	134.7
2'', 6''	126.2	126.9	126.9	126.9
3'', 5''	128.0	128.7	128.7	128.6
4''	130.8	131.5	131.5	131.4
1'''	-	172.9	172.9	173.7
2'''	-	34.8	34.8	34.9
3'''	-	25.1	25.1	25.1
4'''-13''' or 4'''-15'''	-	32.1, 29.8-29.3, 22.8	32.1, 29.8-29.3, 22.8	32.0, 29.7-29.3, 22.7
14''' or 16'''	-	14.3	14.3	14.2

Table S3. Cytotoxicity of isolated compounds (IC_{50} , $\mu\text{g/mL}$)

compound	Hela cells	HCT116 cells	MCF-7 cells	Vero cells
5	19.09 ± 2.83	16.02 ± 0.10	25.89 ± 3.49	> 100
6	15.03 ± 0.46	16.65 ± 3.21	18.33 ± 0.31	80.20 ± 4.35
7	22.44 ± 2.59	19.75 ± 0.44	16.18 ± 1.10	25.20 ± 1.41
10	20.06 ± 2.42	35.74 ± 2.02	24.44 ± 1.12	50.60 ± 2.19
The other	inactive	inactive	inactive	inactive
cisplatin	6.65 ± 0.12	4.93 ± 0.77	10.42 ± 0.85	6.55 ± 0.81

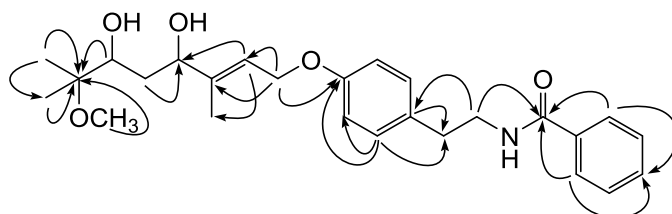


Figure S1. The HMBC correlations of compound **1**.

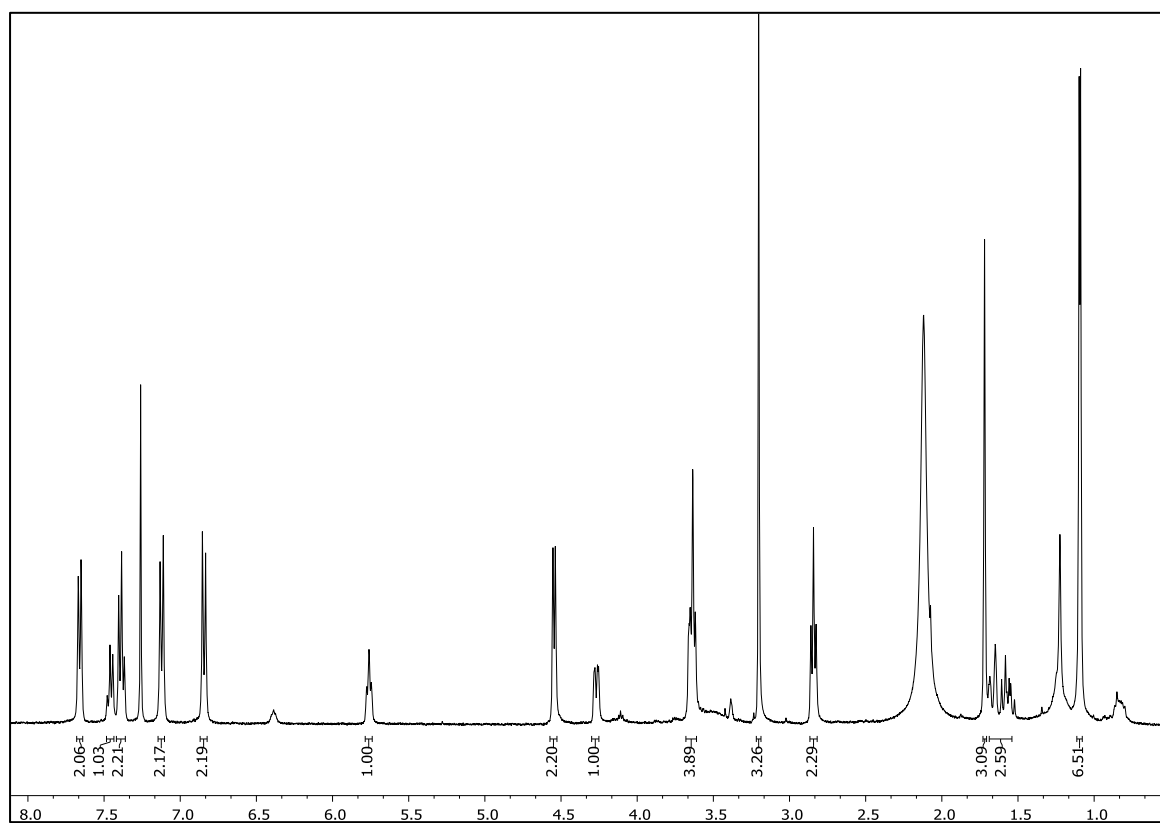
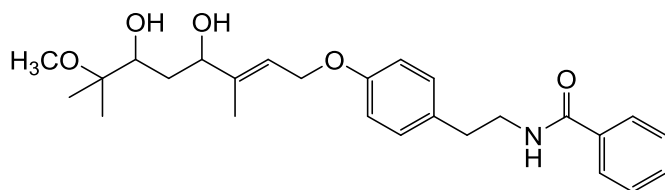


Figure S2. ^1H NMR (400 MHz, CDCl_3) spectrum of atalantum H (**1**)



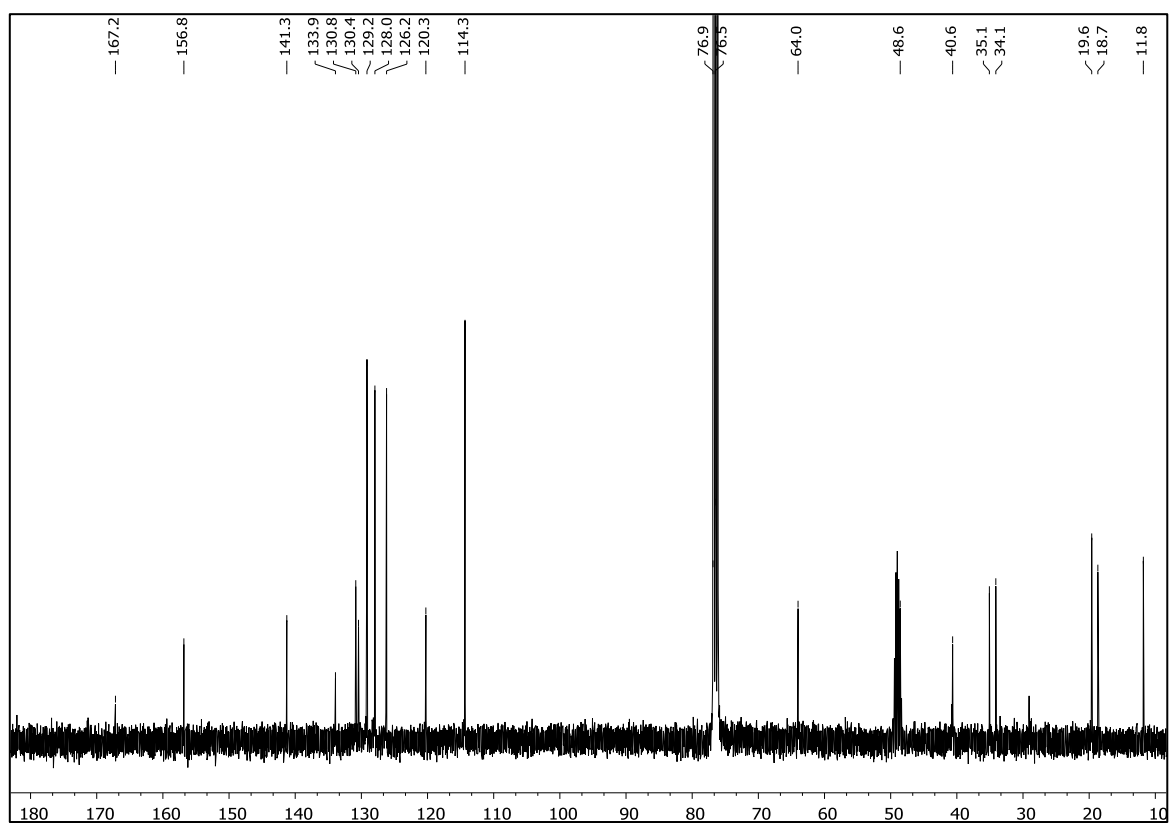


Figure S3. ¹³C NMR (100 MHz, CDCl₃) spectrum of atalantum H (1)

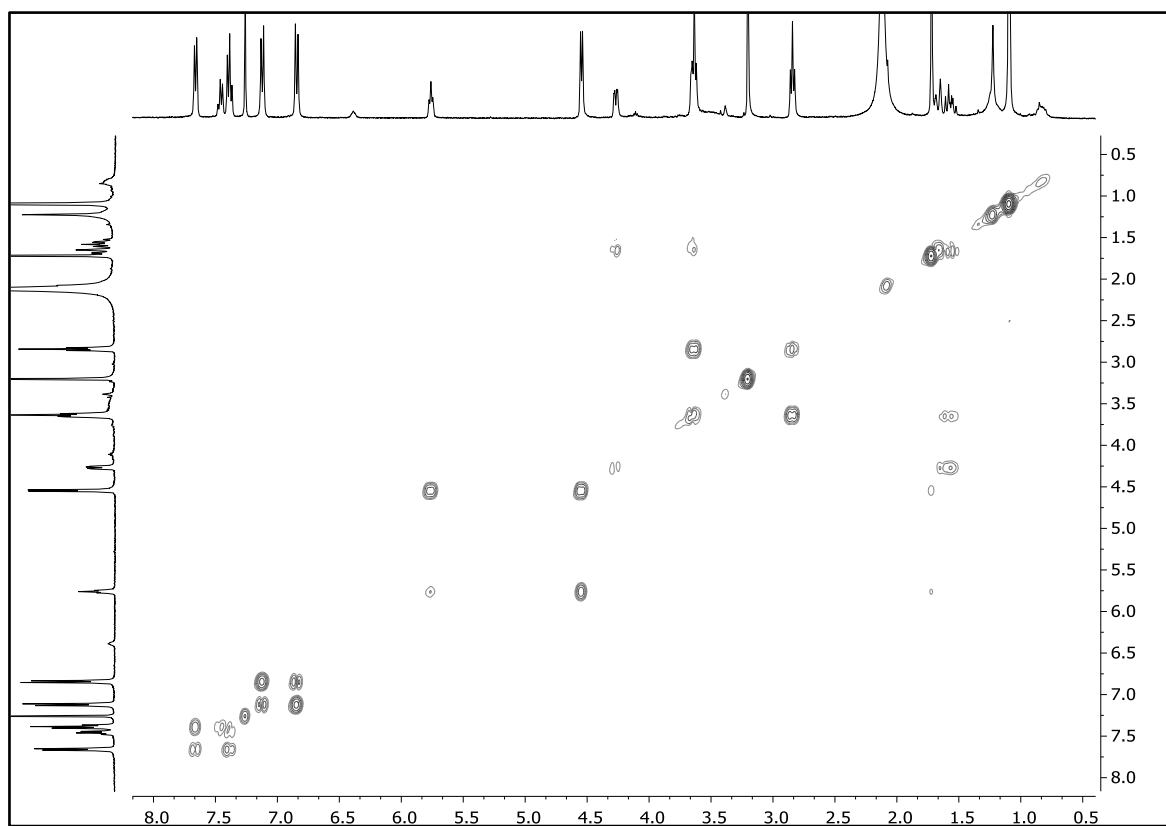


Figure S4. COSY spectrum of atalantum H (1)

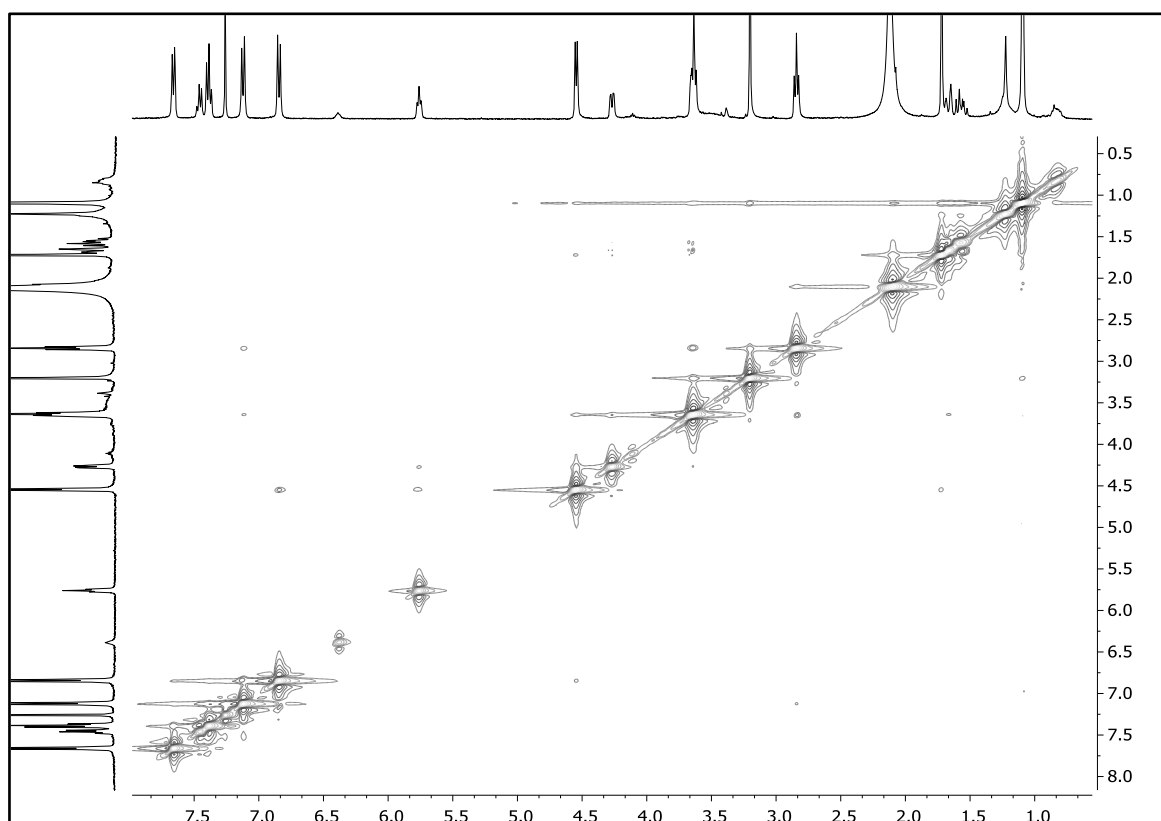


Figure S5. NOESY spectrum of atalantum H (**1**)

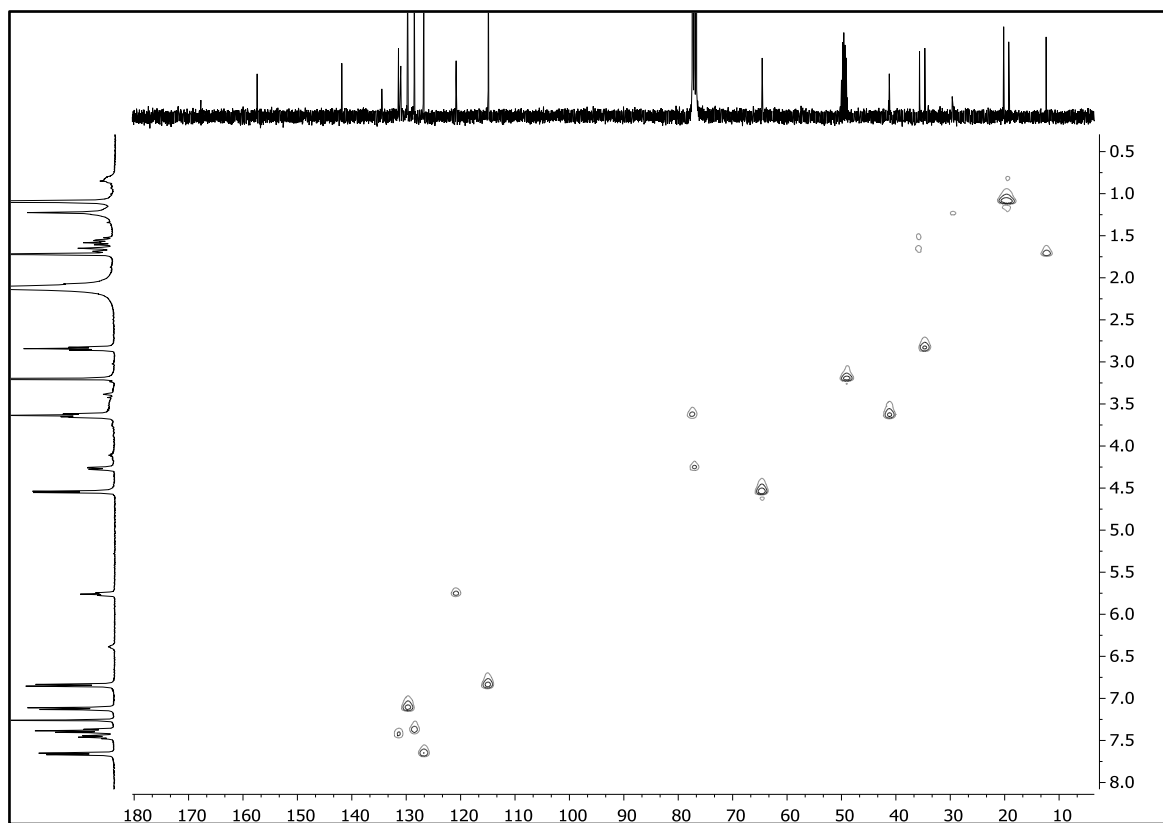


Figure S6. HMQC spectrum of atalantum H (**1**)

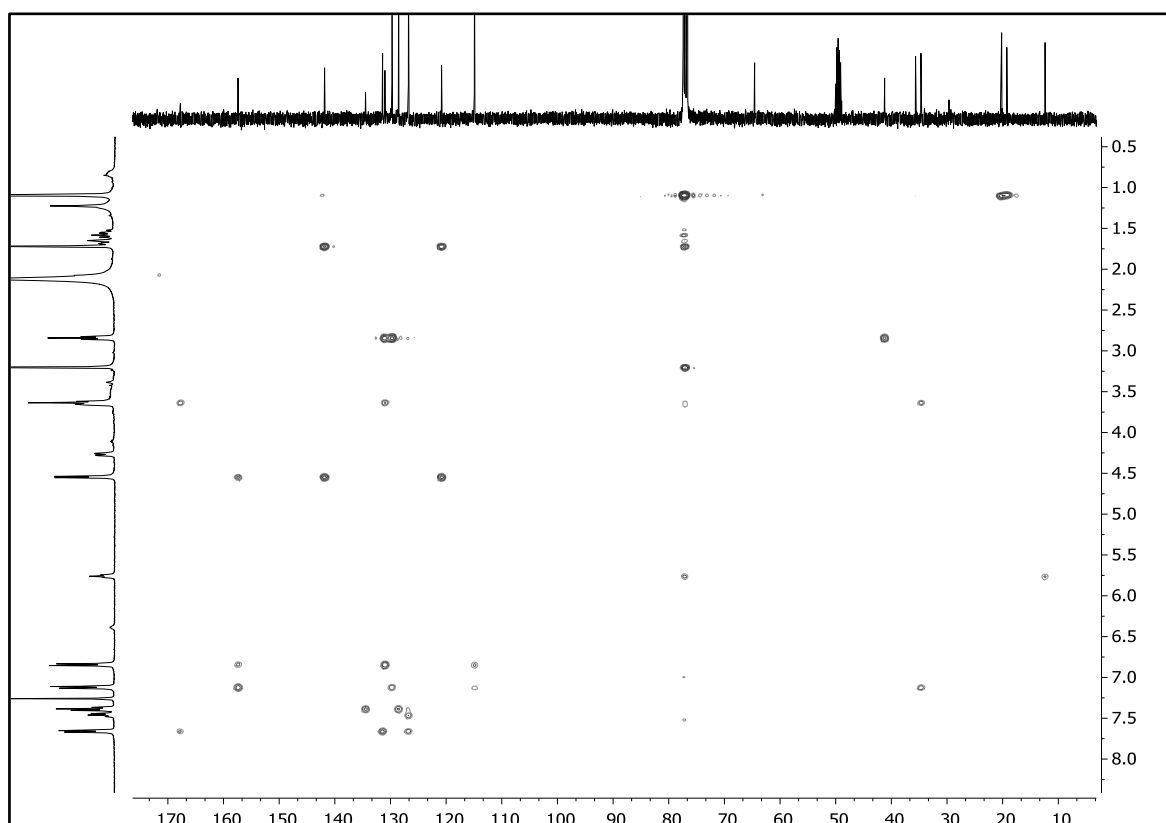


Figure S7. HMBC spectrum of atalantum H (**1**)

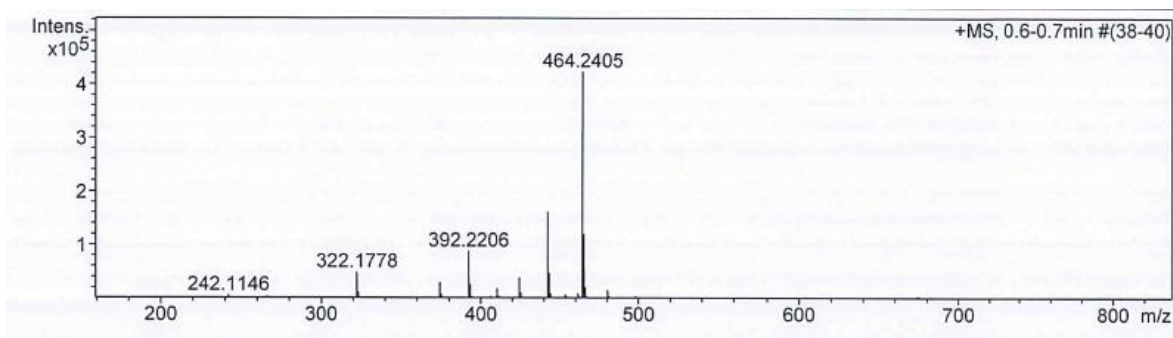


Figure S8. MS spectrum of atalantum H (**1**)

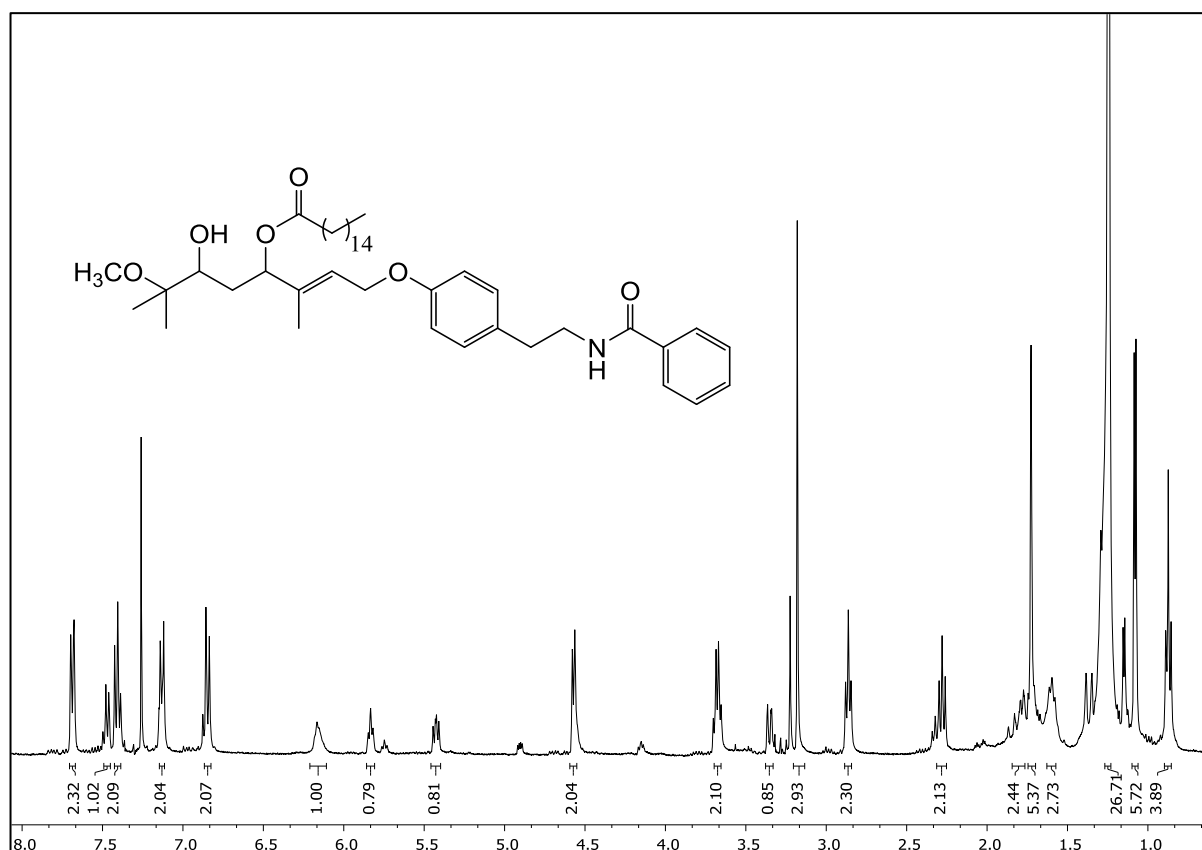


Figure S9. ¹H NMR (400 MHz, CDCl₃) spectrum of atalantum I (2)

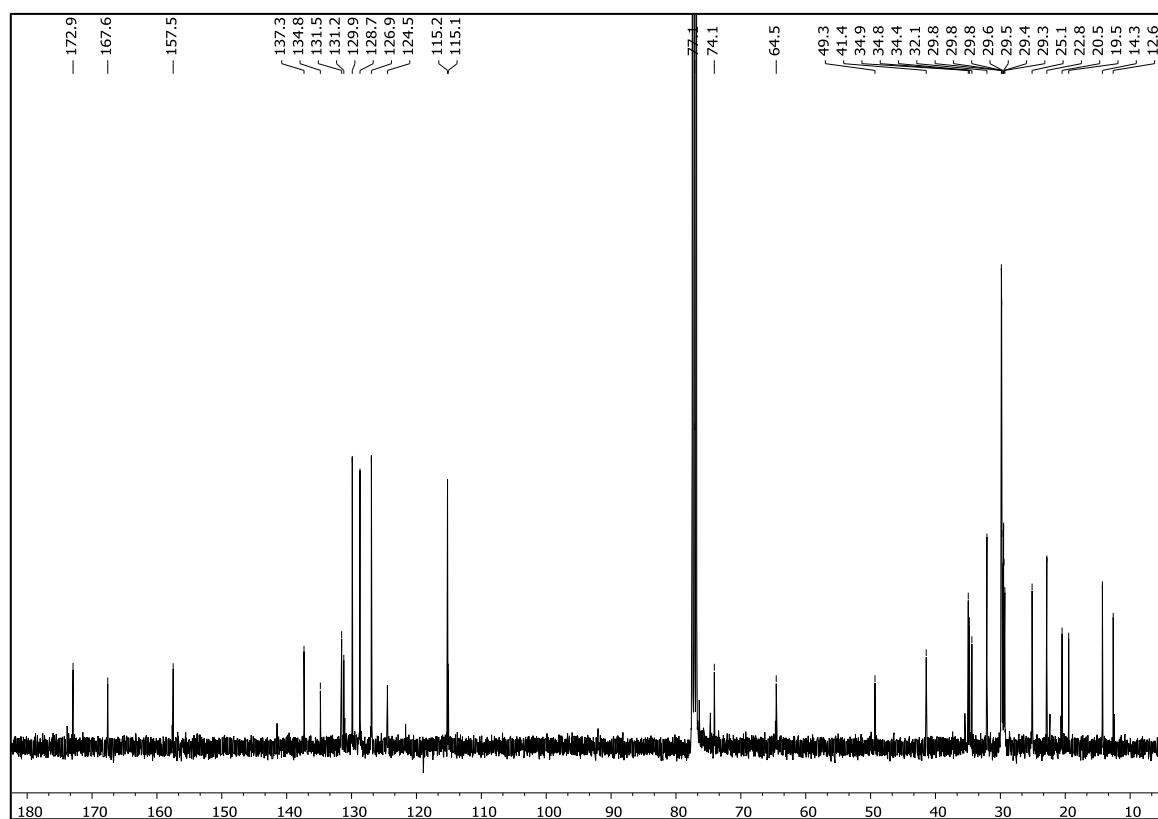


Figure S10. ¹³C NMR (100 MHz, CDCl₃) spectrum of atalantum I (2)

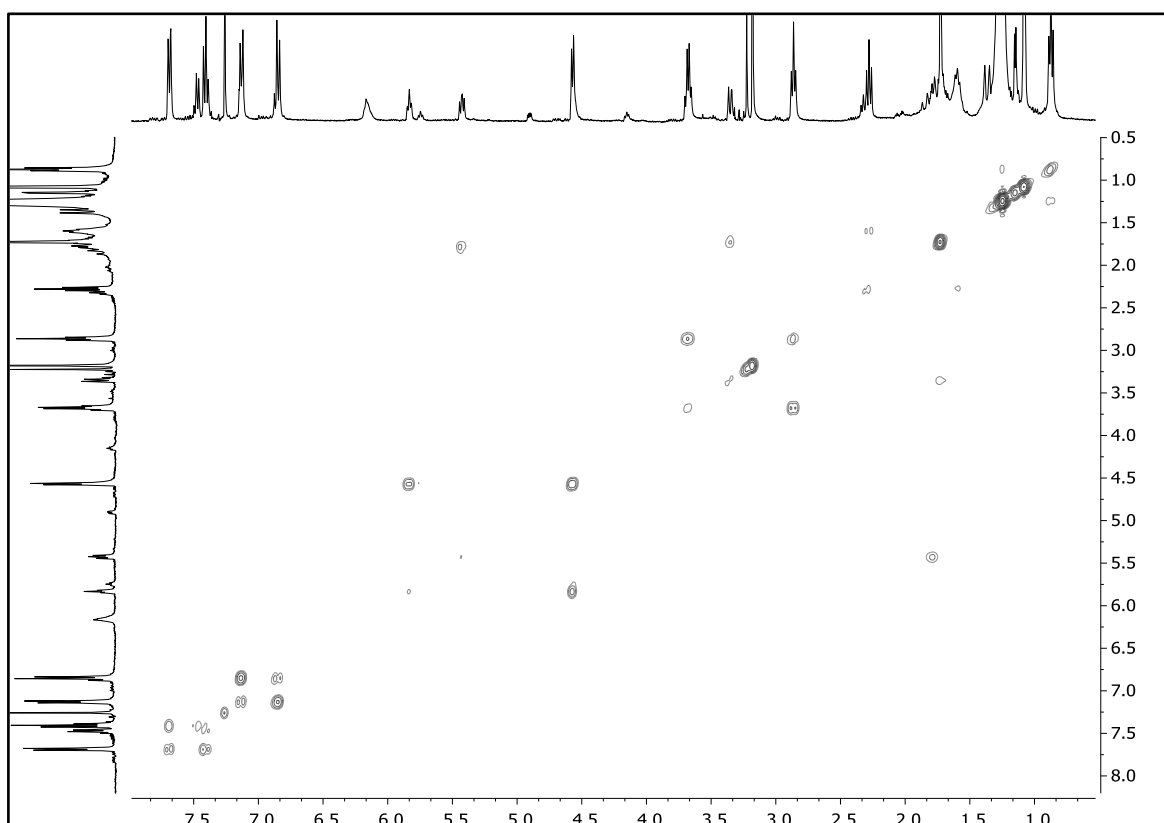


Figure S11. COSY spectrum of atalantum I (2)

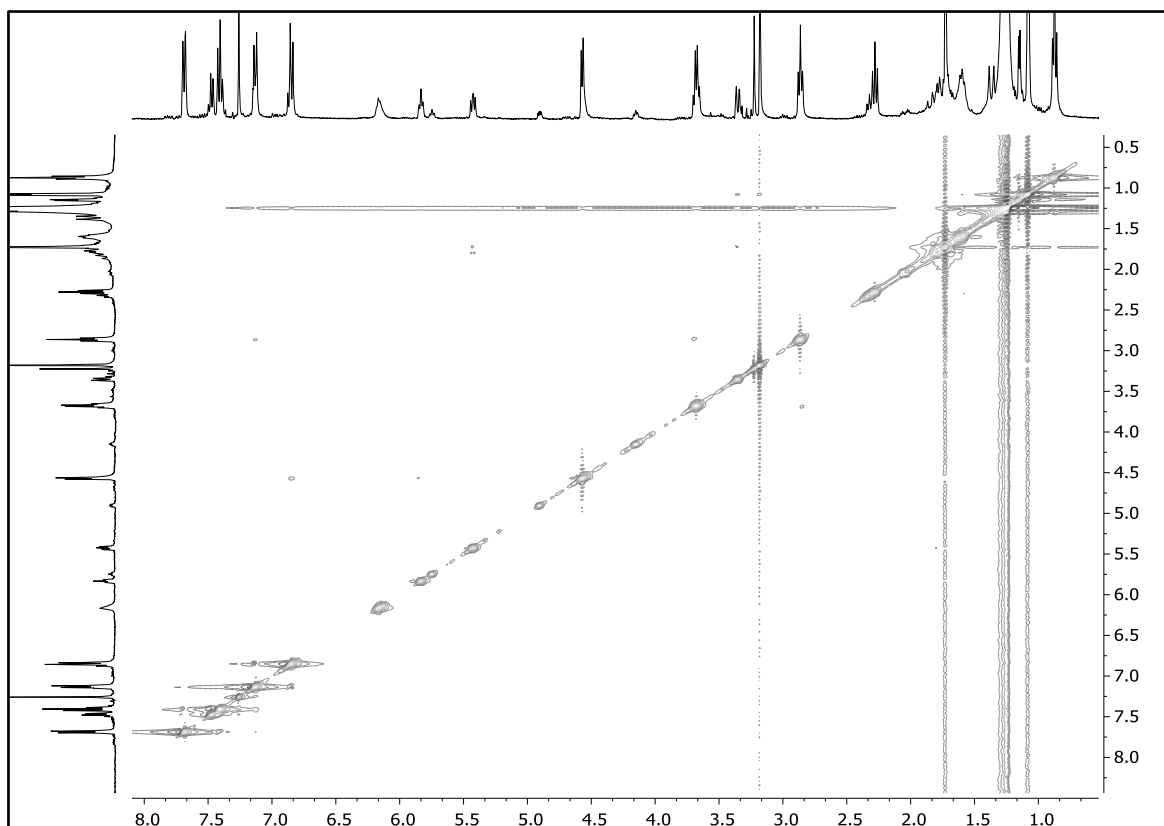


Figure S12. NOESY spectrum of atalantum I (2)

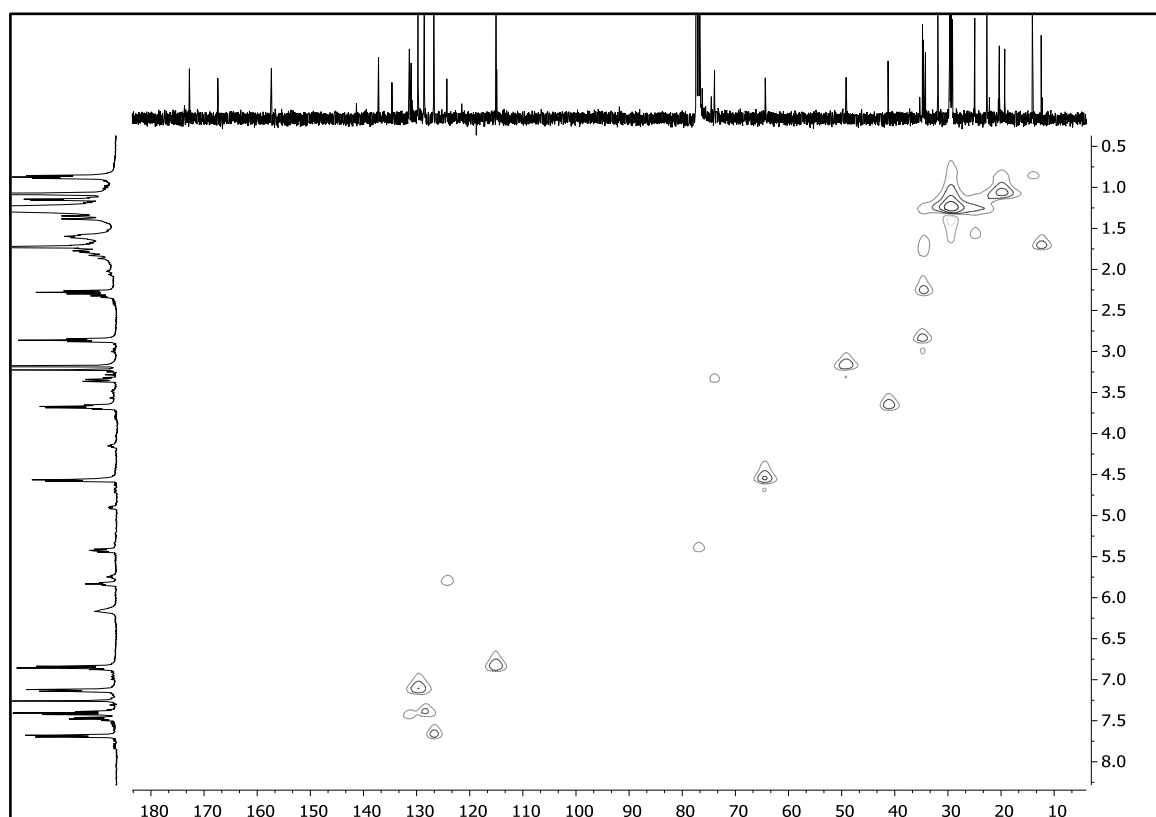


Figure S13. HMQC spectrum of atalantum I (2)

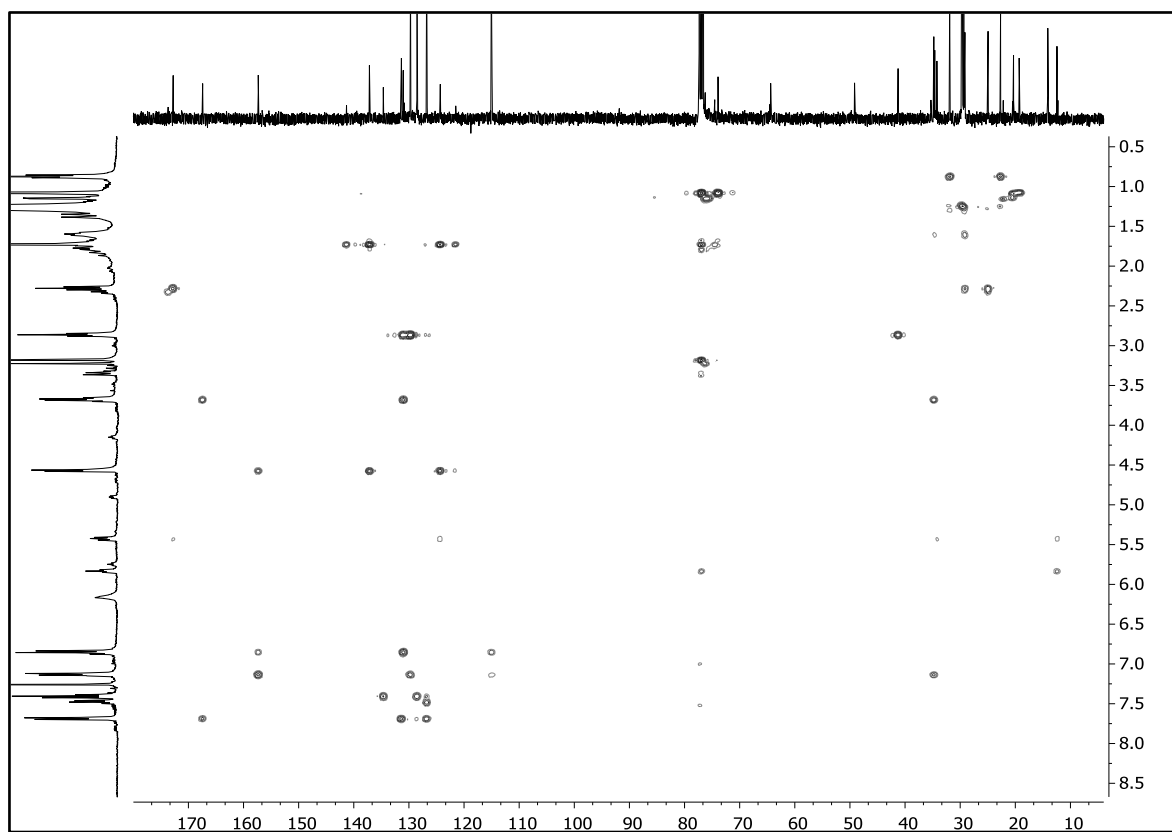


Figure S14. HMBC spectrum of atalantum I (2)

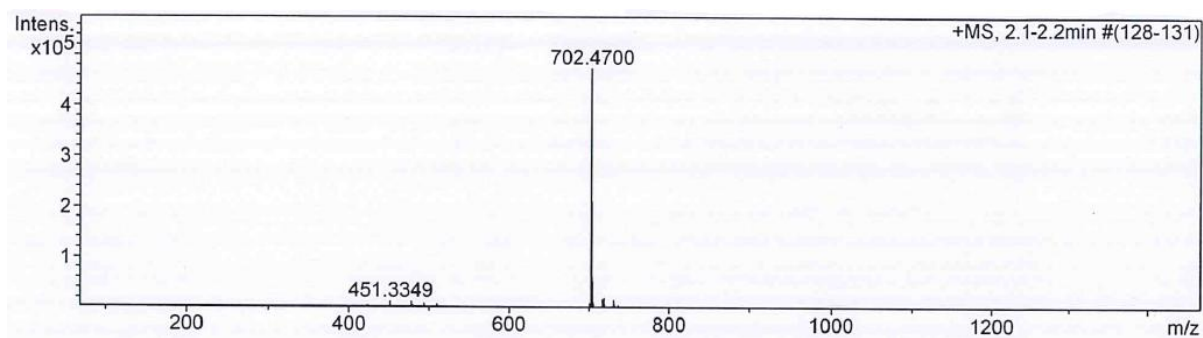


Figure S15. MS spectrum of atalantun I (2)

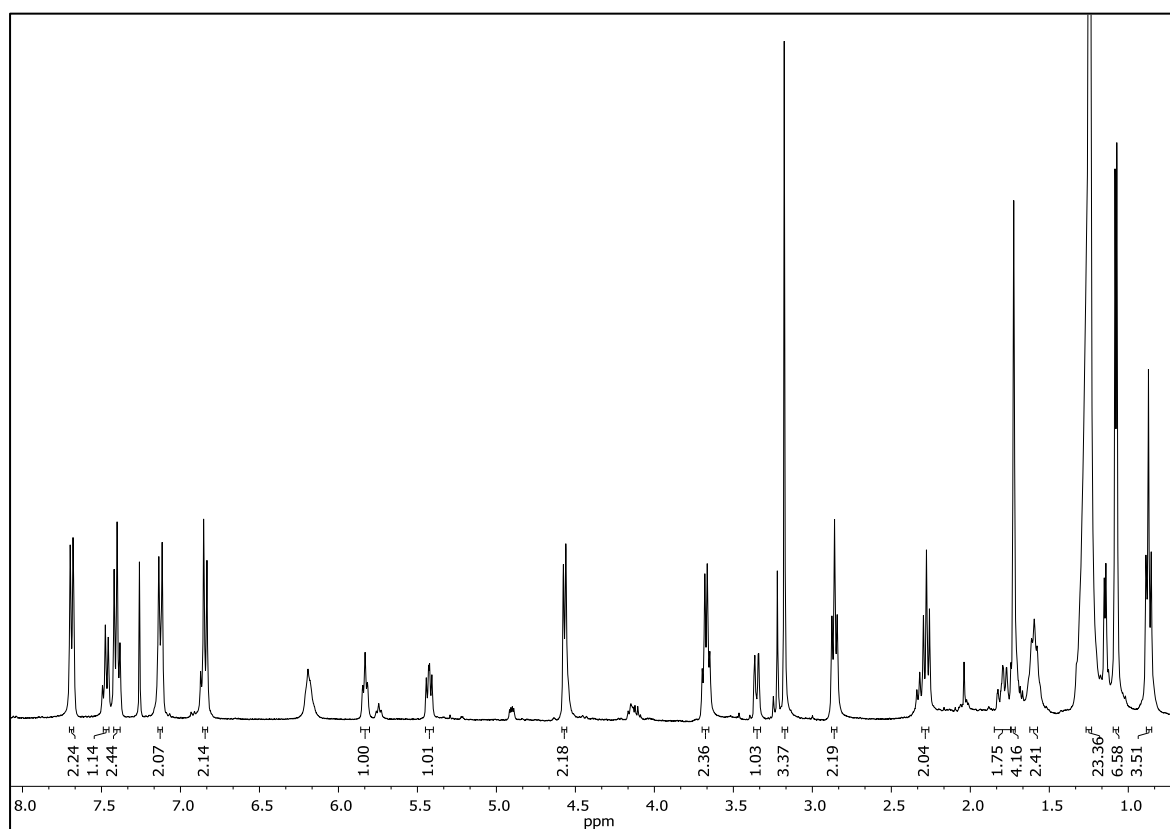
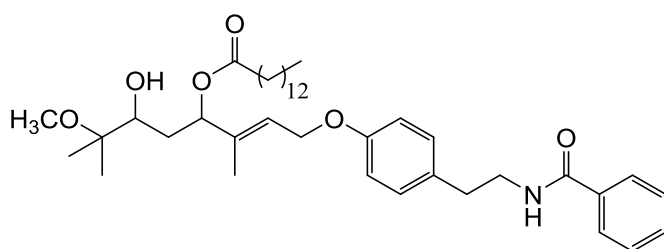


Figure S16. ¹H NMR (400 MHz, CDCl₃) spectrum of atalantun J (3)



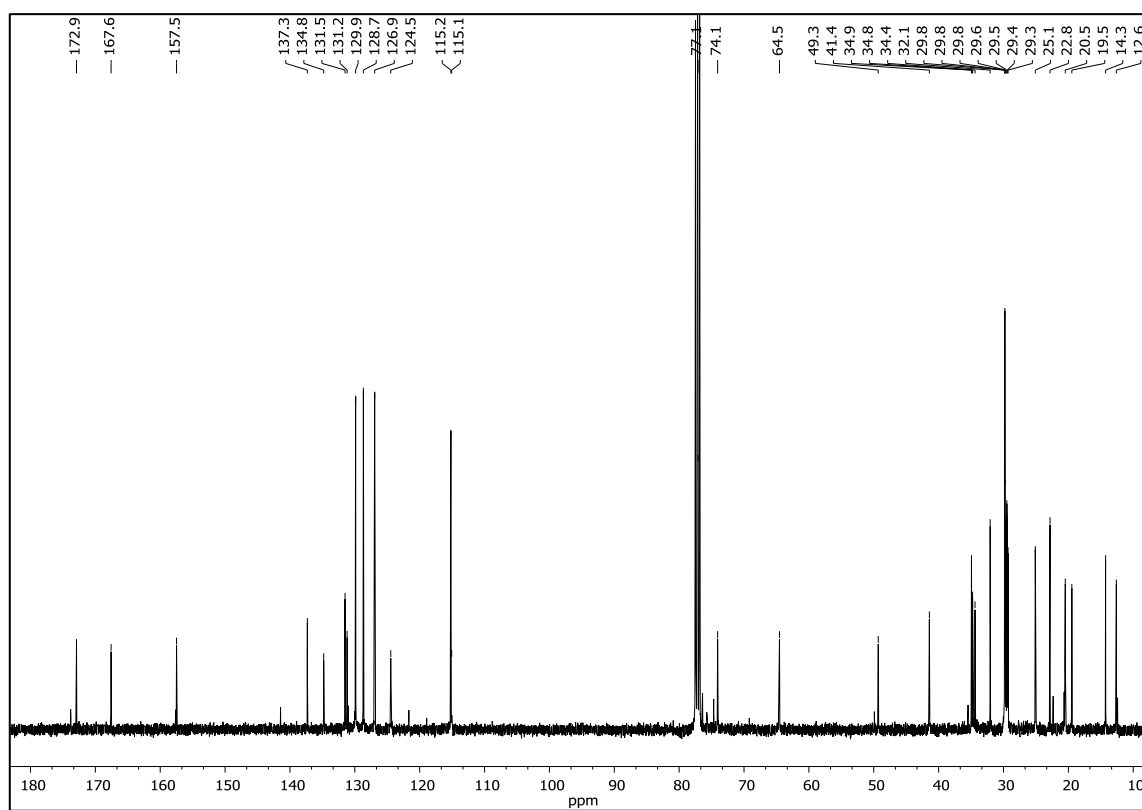


Figure S17. ¹³C NMR (100 MHz, CDCl₃) spectrum of atalantum J (3)

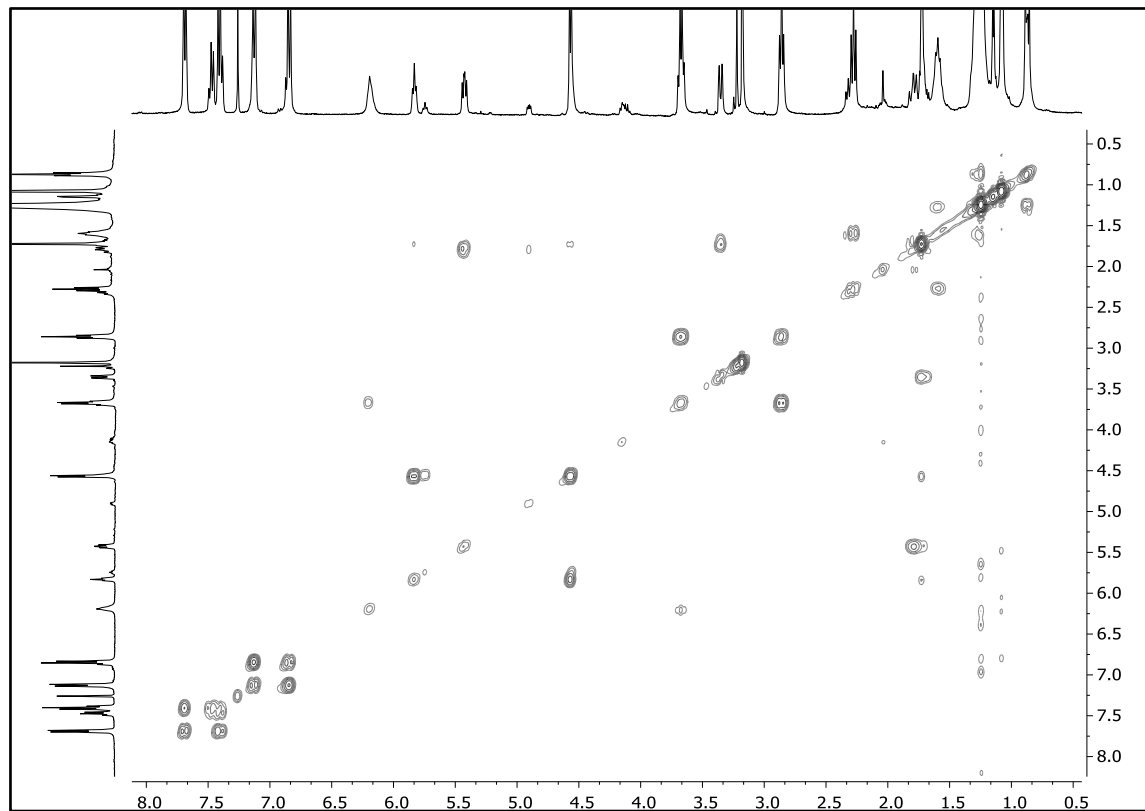


Figure S18. COSY spectrum of atalantum J (3)

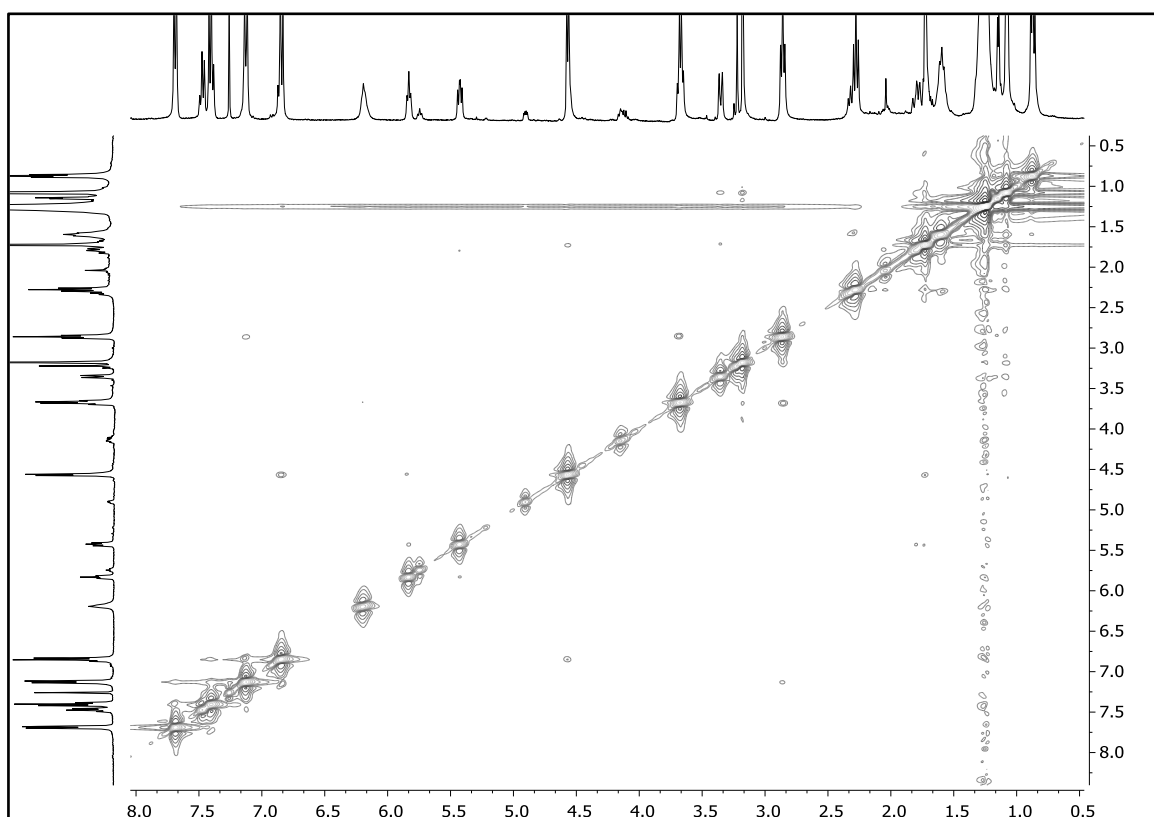


Figure S19. NOESY spectrum of atalantum J (3)

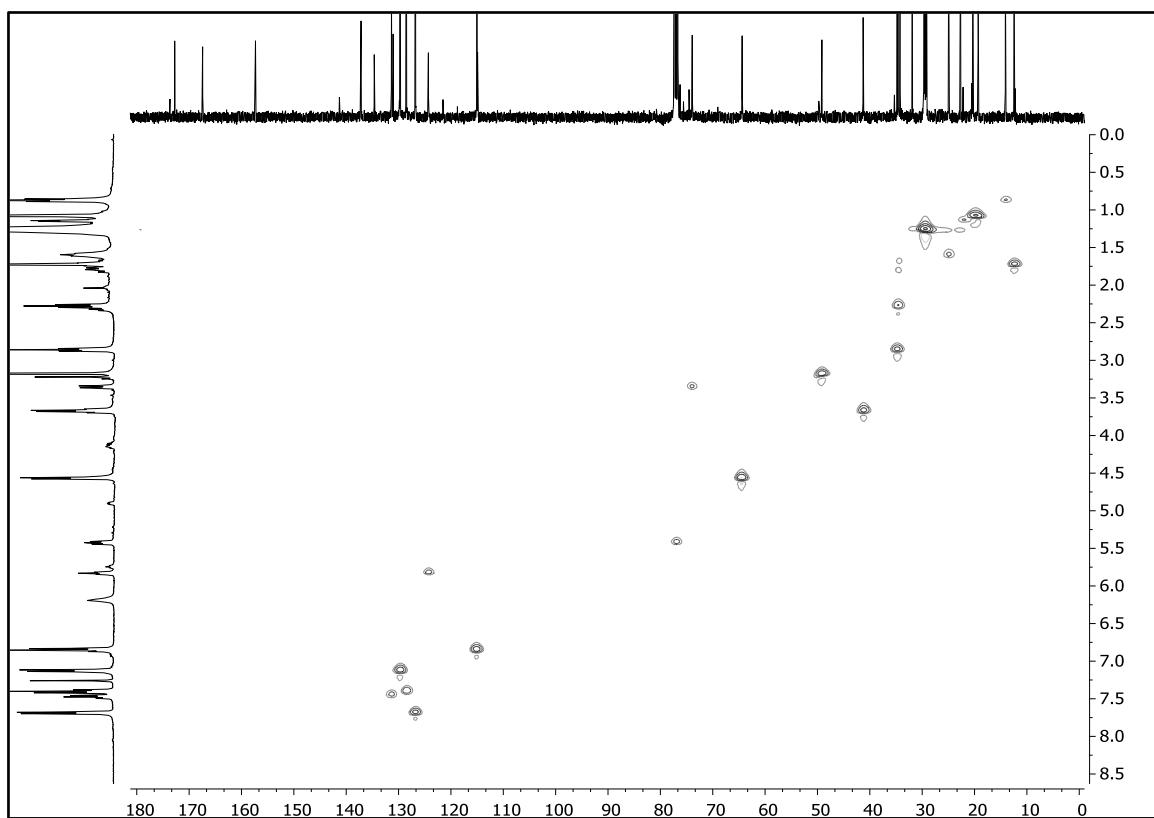


Figure S20. HMQC spectrum of atalantum J (3)

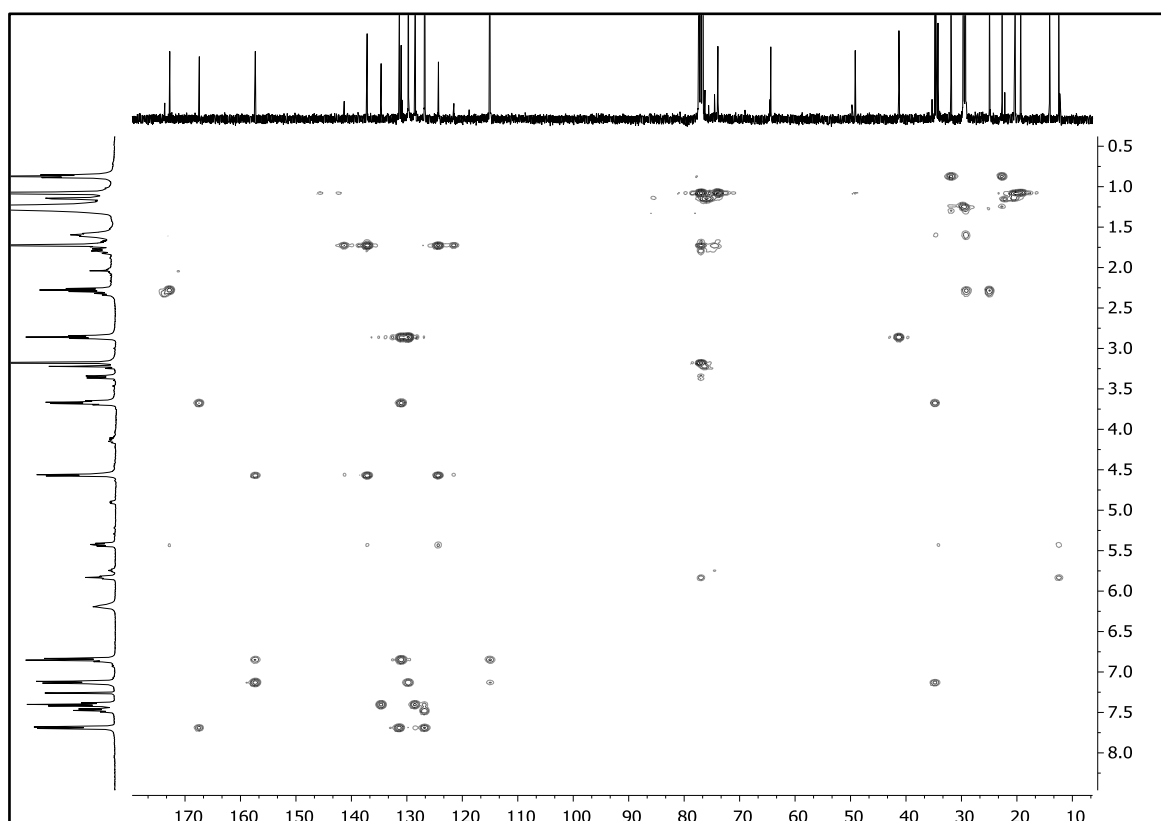


Figure S21. HMBC spectrum of atalantum J (**3**)

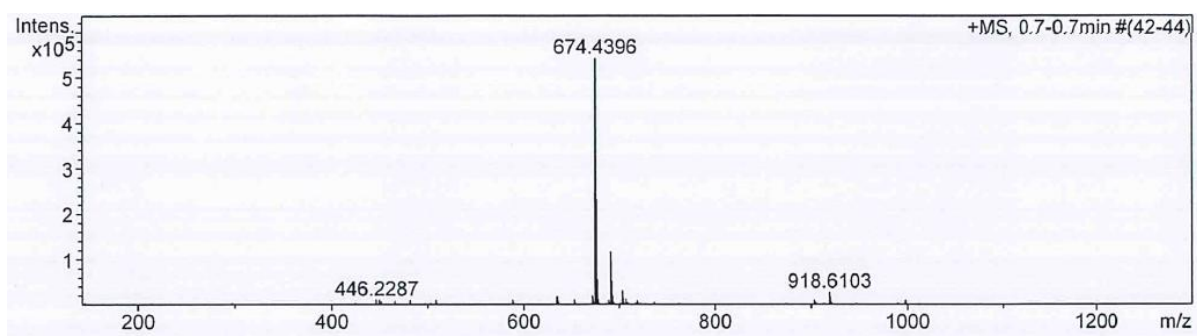


Figure S22. MS spectrum of atalantum J (**3**)

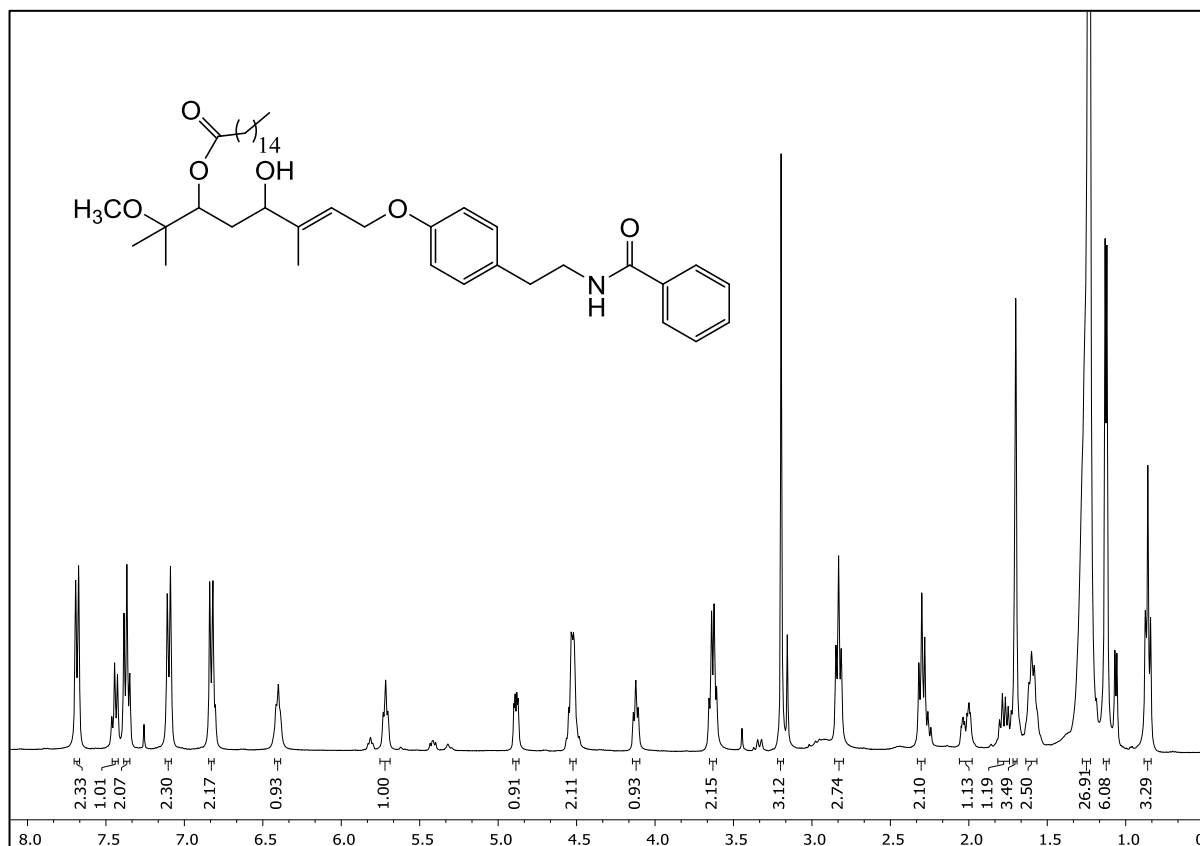


Figure S23. ¹H NMR (400 MHz, CDCl₃) spectrum of atalantum K (4)

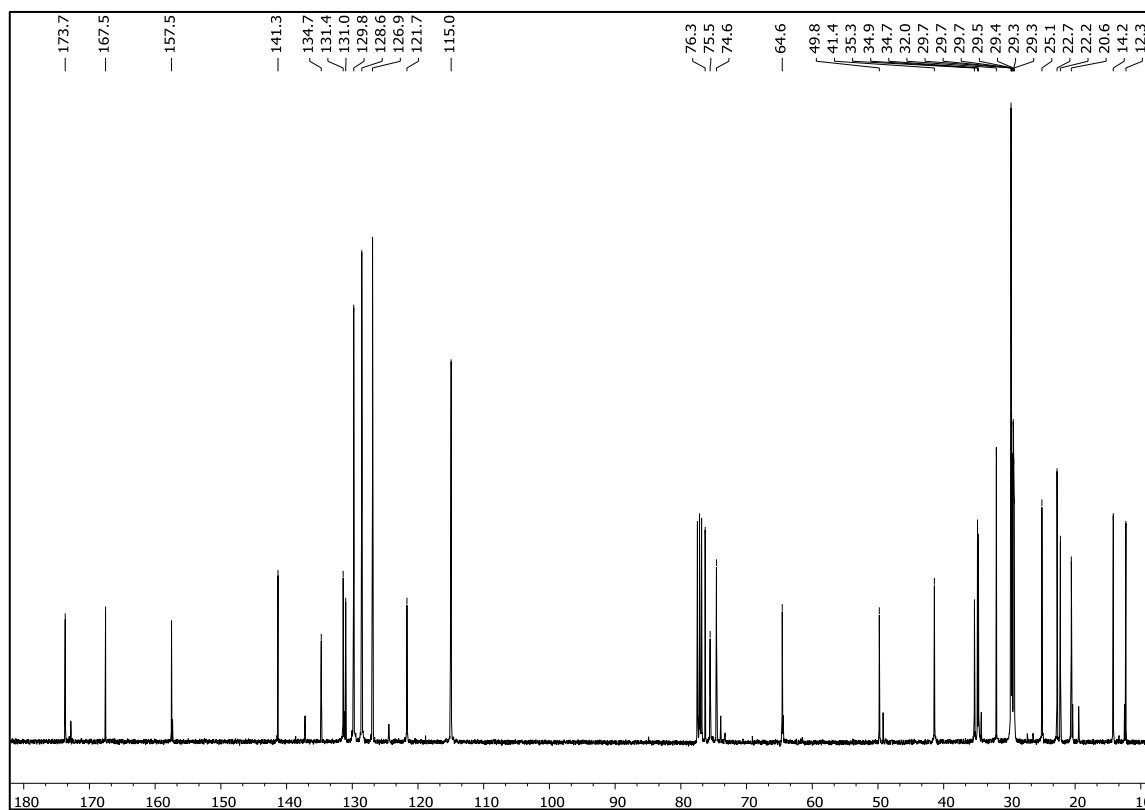


Figure S24. ^{13}C NMR (100 MHz, CDCl_3) spectrum of atalantum K (**4**)

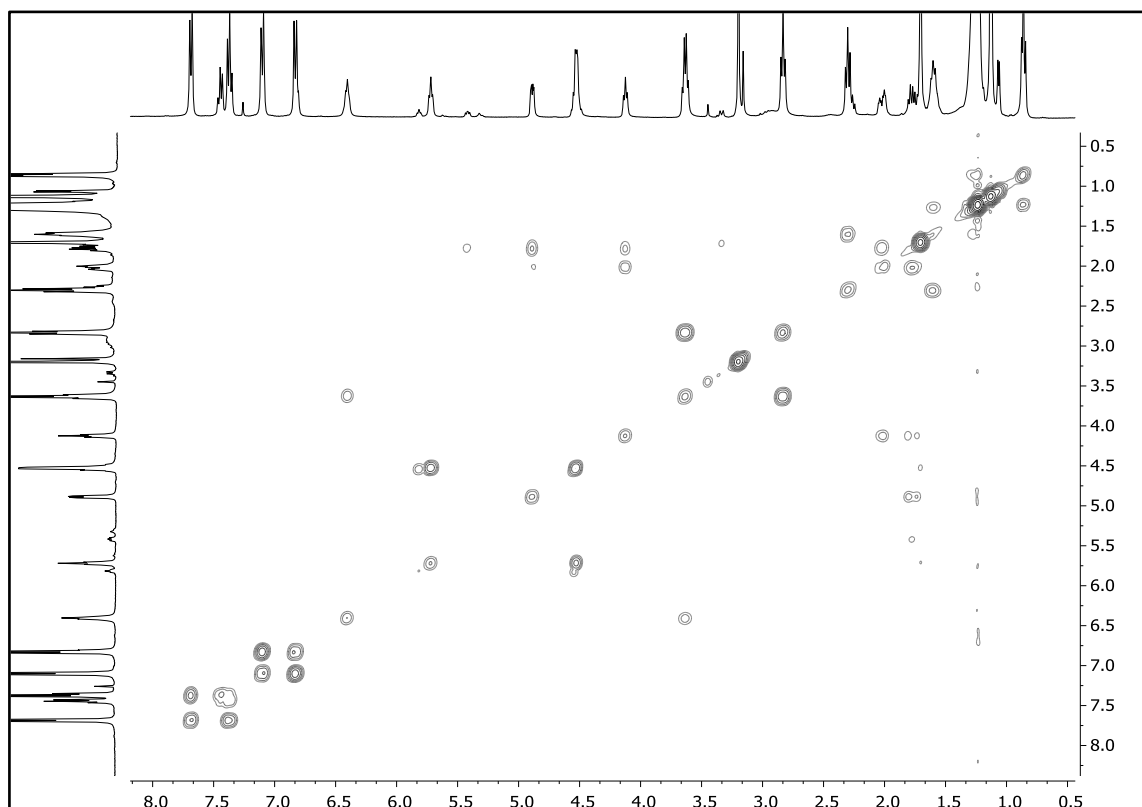


Figure S25. COSY spectrum of atalantum K (**4**)

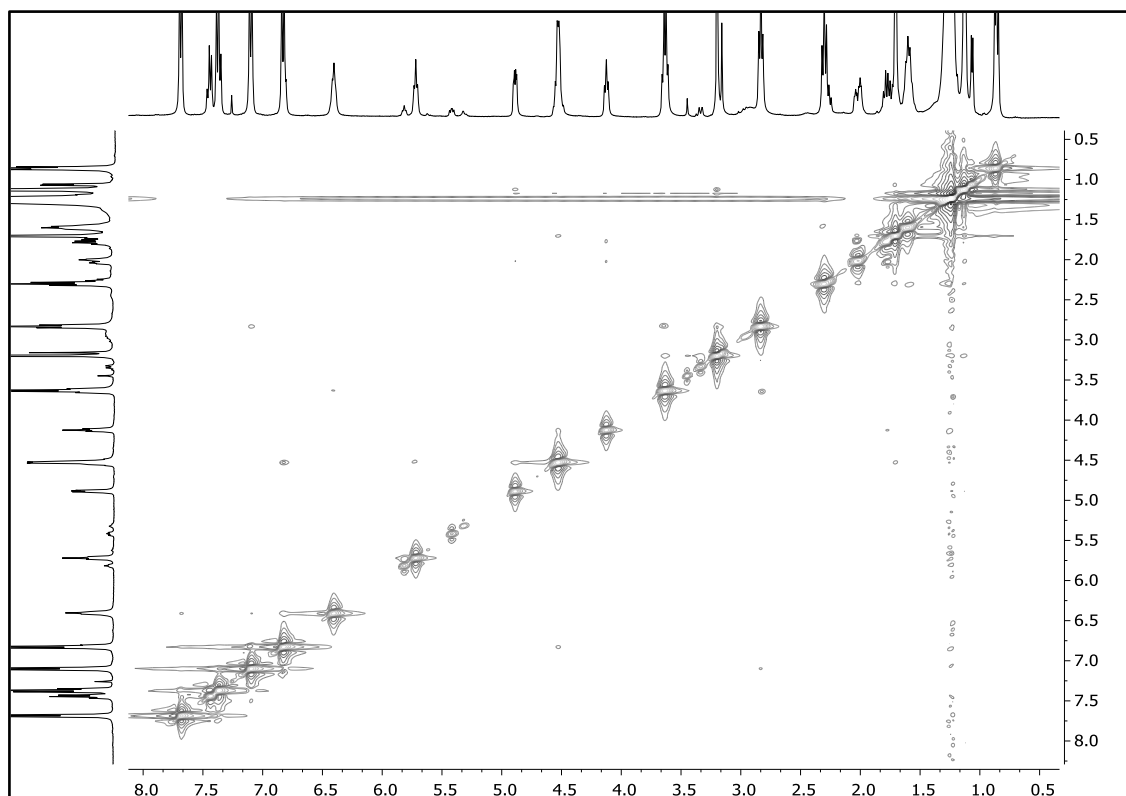


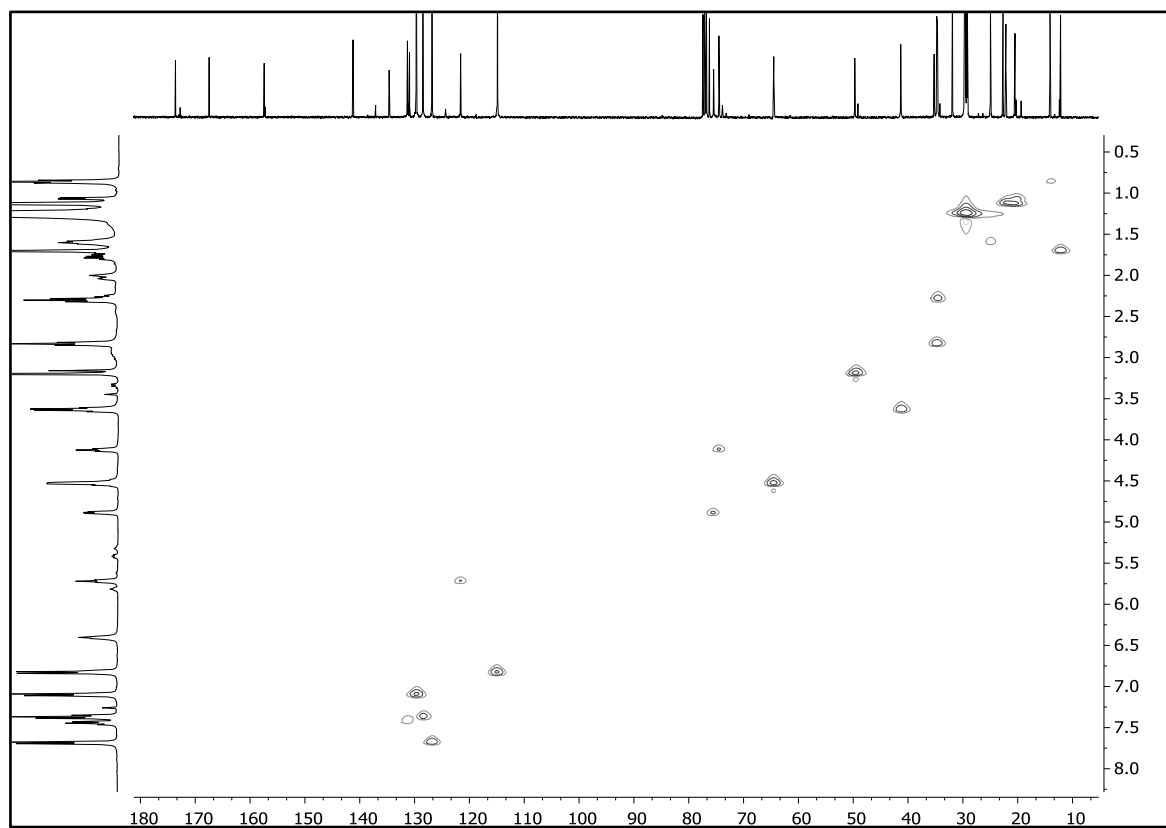
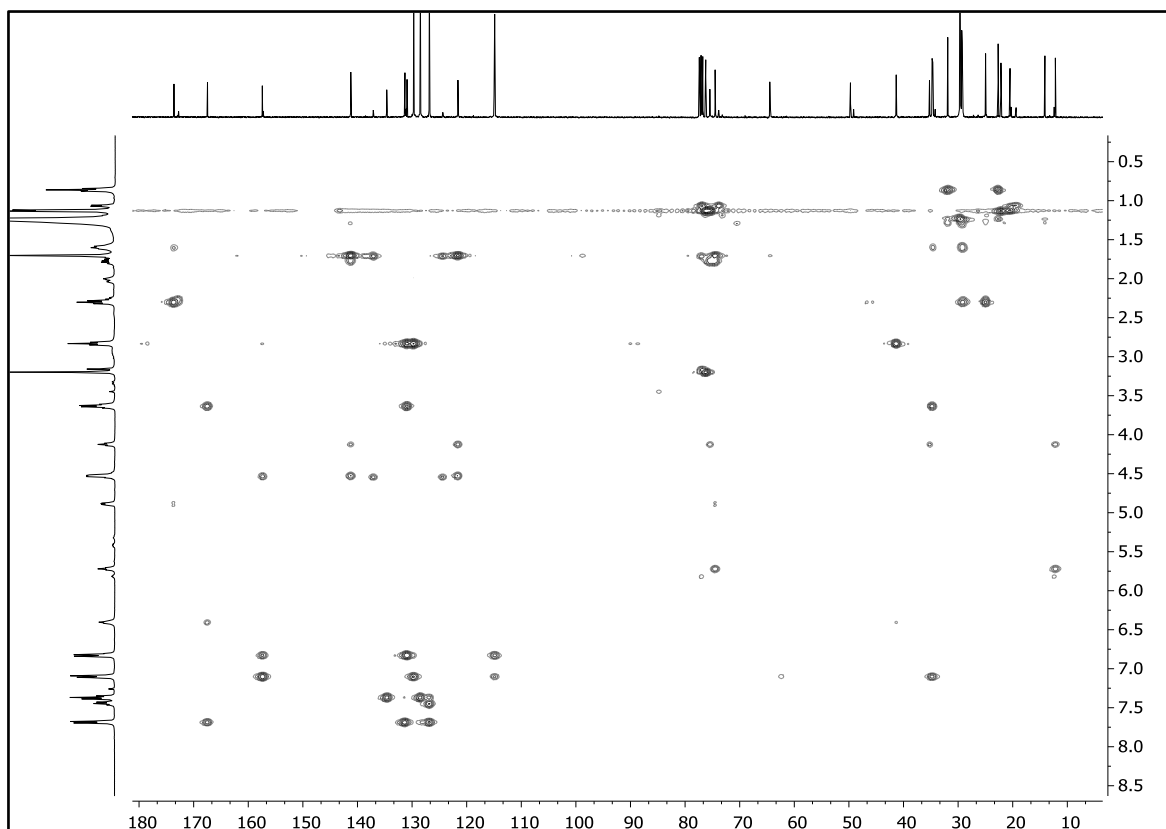
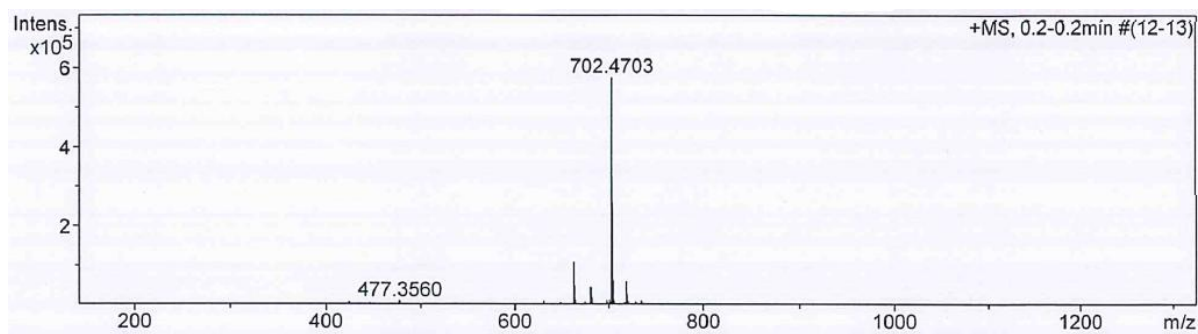
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