

Article

Costatone C – a New Halogenated Monoterpene from the New Zealand Red Alga “*Plocamium angustum*”

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Table S1 – NMR data (600 MHz for ^1H , 150 MHz for ^{13}C , CD_3OD) of **7**

position	^{13}C (δ)	^1H (δ , mult., J in Hz)	COSY	HMBC
1	117.5	6.28 (quin, 1.4)	3, 9	2, 3, 9
2	138.5			
3	73.8	4.22 (dd, 11.7, 2.6)	1, 4, 9	1, 2, 4, 5, 7, 9
4	39.1	2.45 (dt, 12.9, 11.9)	3, 4, 5	2, 3, 5
		2.15 (ddd, 12.9, 4.4, 2.7)	3, 4, 5	3, 5
5	54.5	4.75 (dd, 12.0, 4.4)	4	3, 4, 6, 10
6	73.6			
7	83.4	4.29 (dd, 11.7, 3.9)	8	3, 6, 5, 8, 10
8	29.0	3.94 (t, 11.6)	7, 8	6, 7
		3.73 (dd, 11.6, 3.9)	7, 8	7
9	13.1	1.84 (d, 1.4)	1, 3	1, 2, 3
10	28.9	1.70 (s)		5, 6, 7

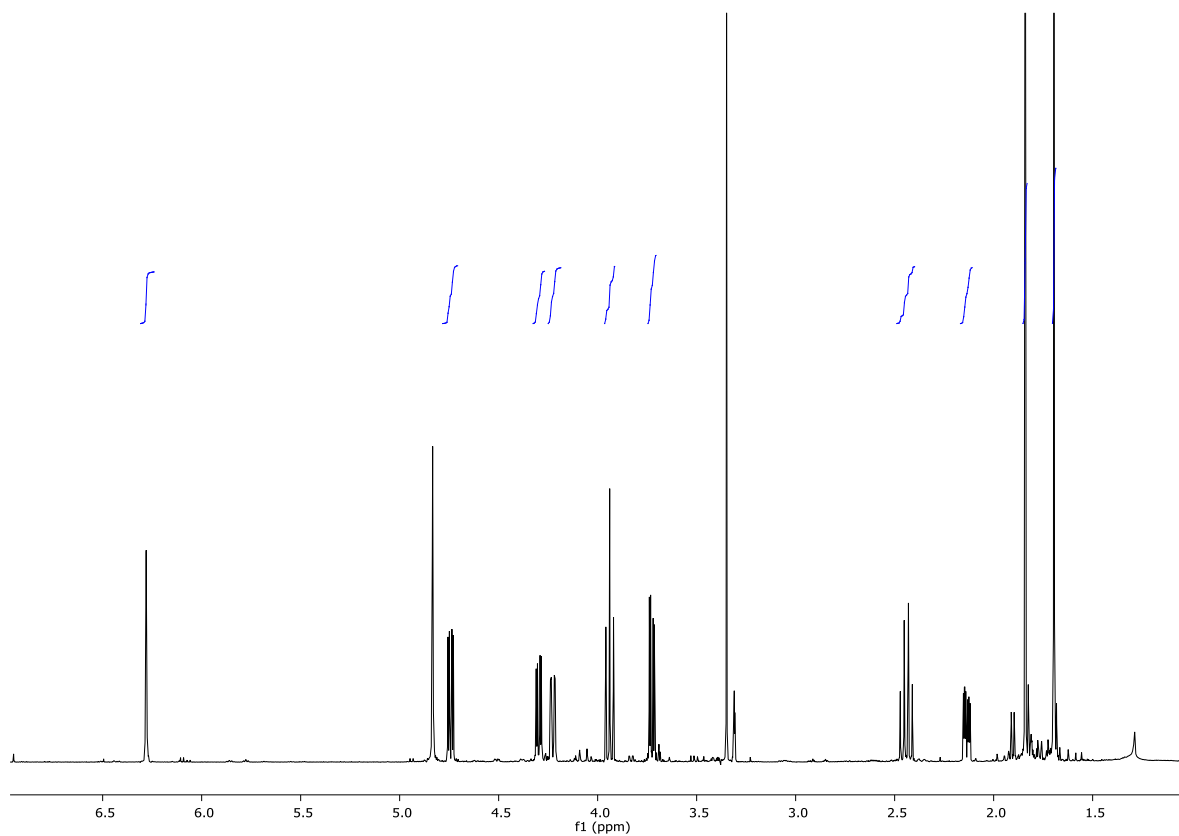
Figure S1 – ^1H Spectrum (600 MHz, CD_3OD) of **7**

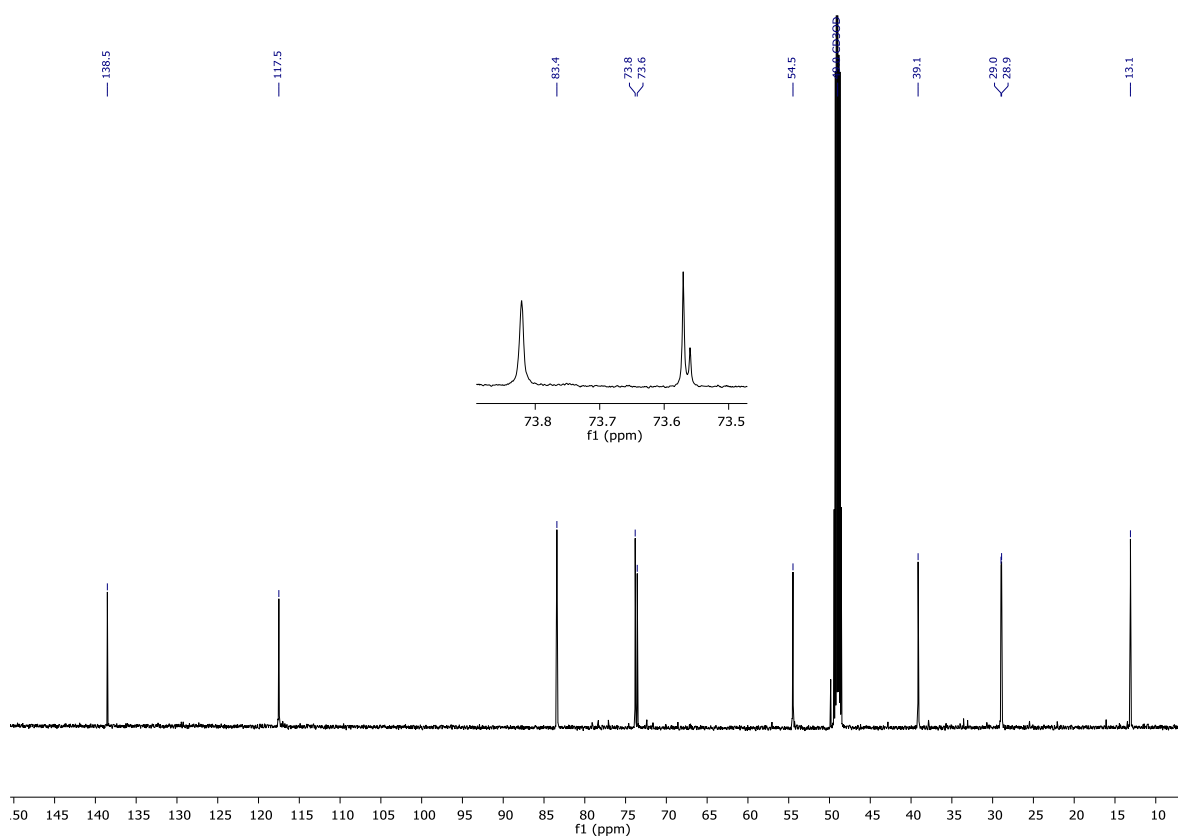
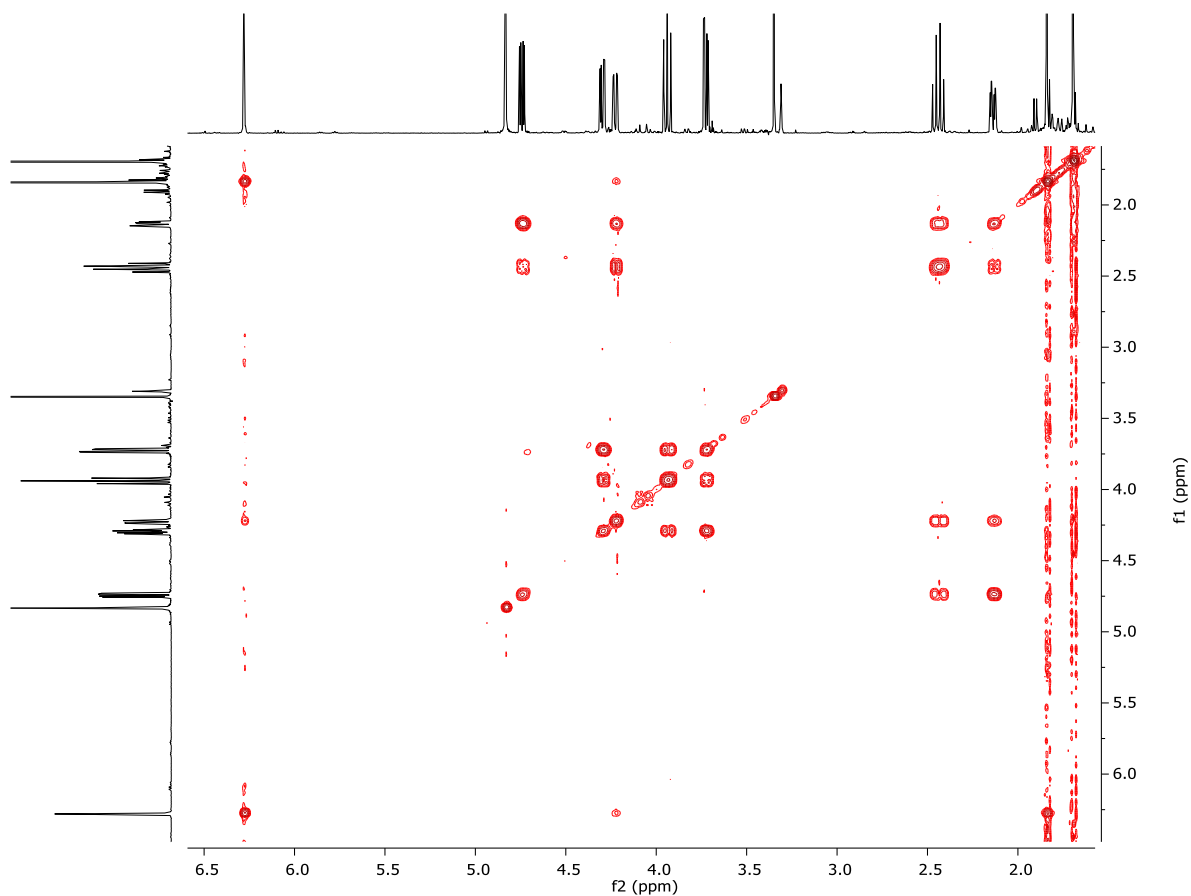
Figure S2 – ^{13}C Spectrum (150 MHz, CD_3OD) of **7**Figure S3 – COSY Spectrum (600 MHz, CD_3OD) of **7**

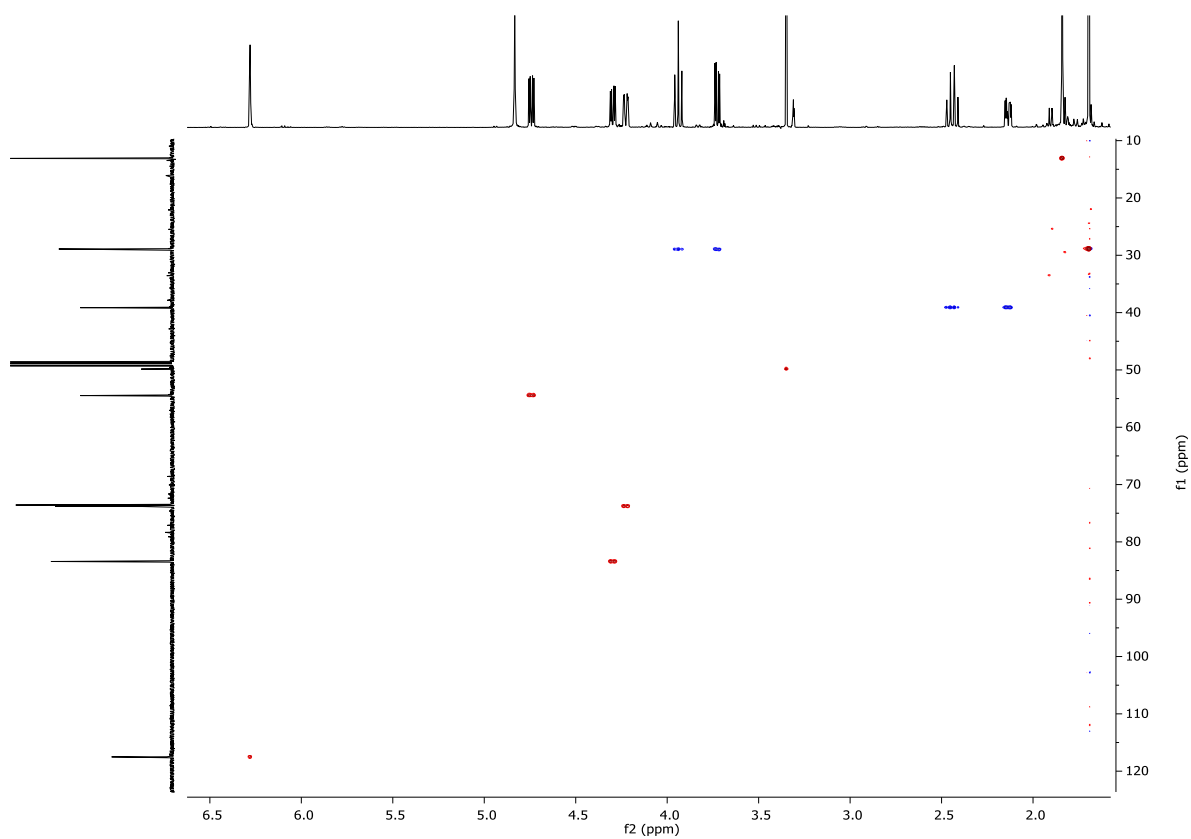
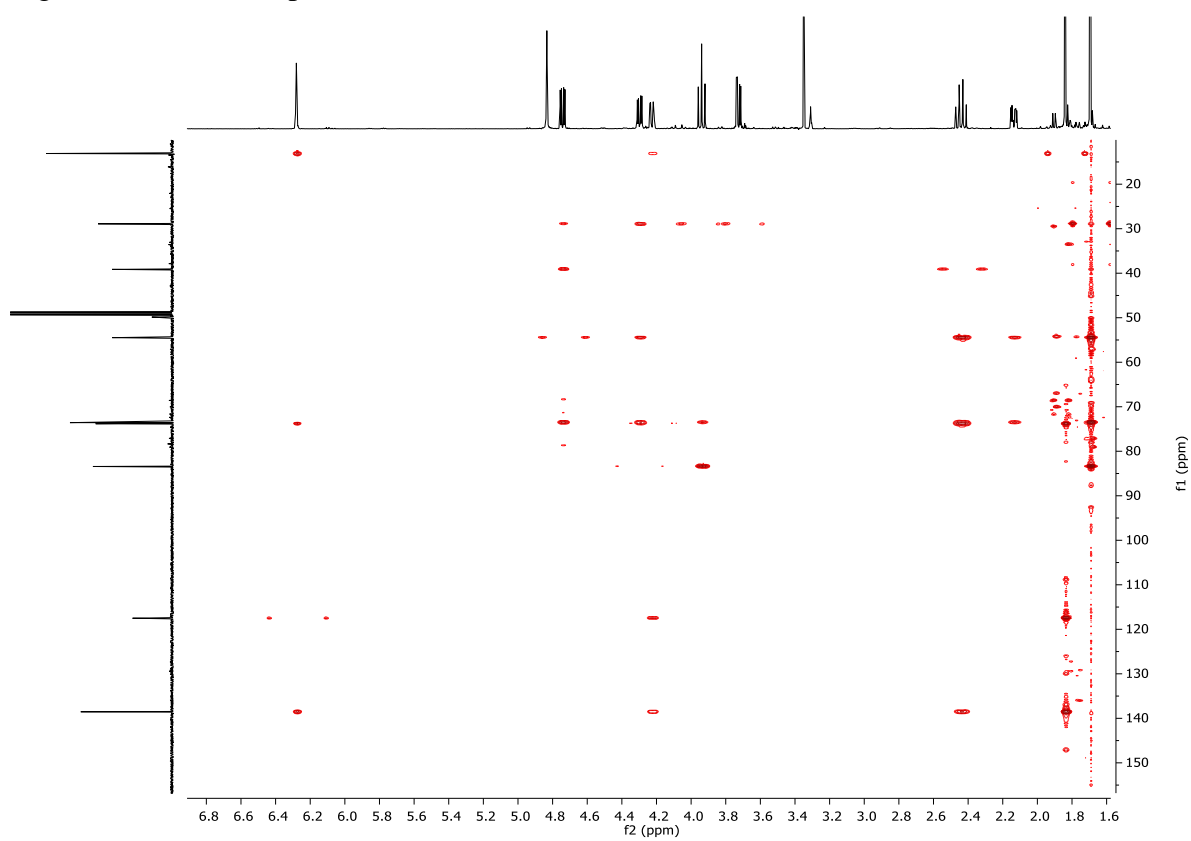
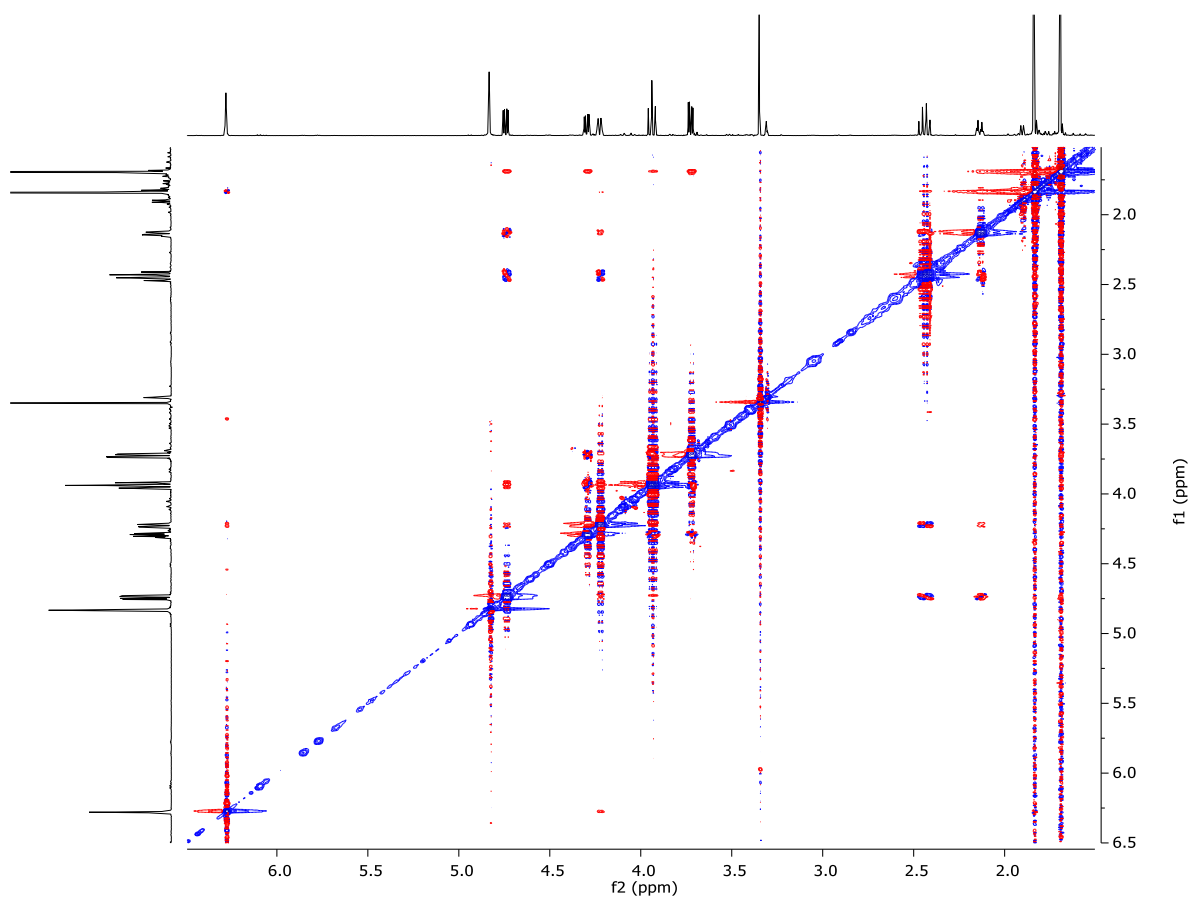
Figure S4 – HSQC Spectrum (600 MHz, CD₃OD) of **7**Figure S5 – HMBC Spectrum (600 MHz, CD₃OD) of **7**

Figure S6 – ROESY Spectrum (600 MHz, CD₃OD) of 7Table S2 – NMR data (600 MHz for ¹H, 150 MHz for ¹³C, CDCl₃) of 7

position	¹³ C (δ)	¹ H (δ, mult., <i>J</i> in Hz)	COSY	HMBC
1	117.3	6.25 (quin, 1.4)	3, 9	2, 3, 9
2	136.7			
3	73.2	4.12 (dd, 11.7, 2.8)	1, 4, 9	1, 2, 5, 9
4	37.7	2.56 (dt, 13.3, 11.9) 2.16 (ddd, 13.3, 4.4, 2.8)	3, 4, 5 3, 4, 5	2, 3, 5, 6 5, 6
5	53.1	4.37 (m, overlap)	4	3, 4, 6, 10
6	71.5			
7	81.7	4.37 (m, overlap)	8	3, 6, 5, 8, 10
8	27.8	3.61 (m)	7	6, 7
9	13.3	1.87 (d, 1.4)	1, 3	1, 2, 3
10	28.6	1.72 (s)		5, 6, 7

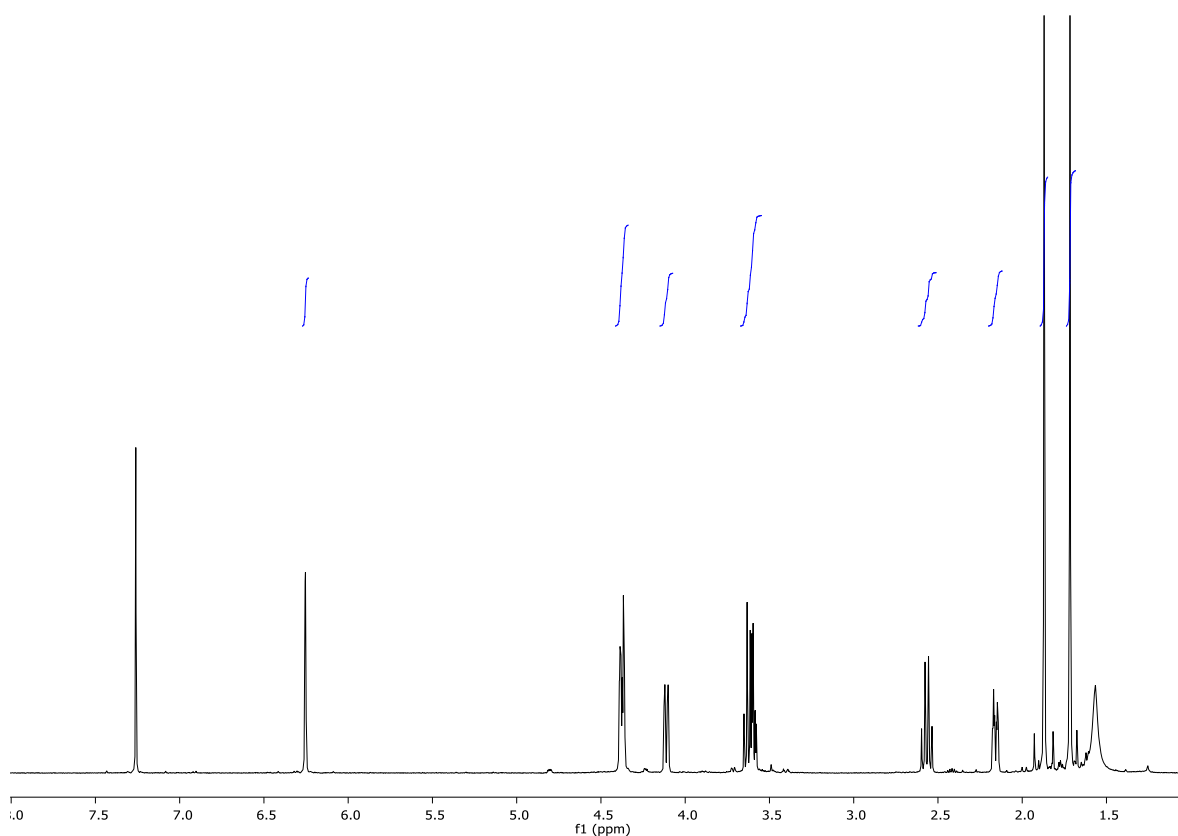
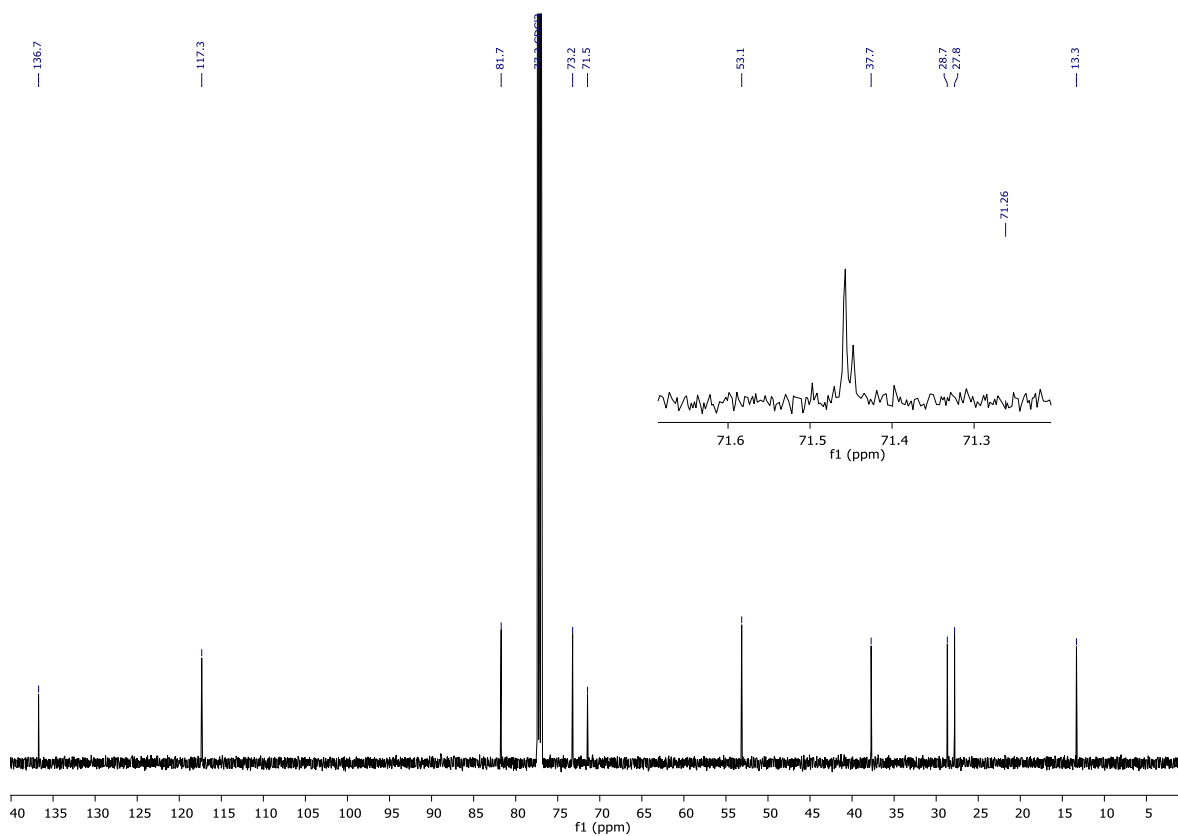
Figure S7 – ^1H Spectrum (600 MHz, CDCl_3) of **7**Figure S8 – ^{13}C Spectrum (150 MHz, CDCl_3) of **7**

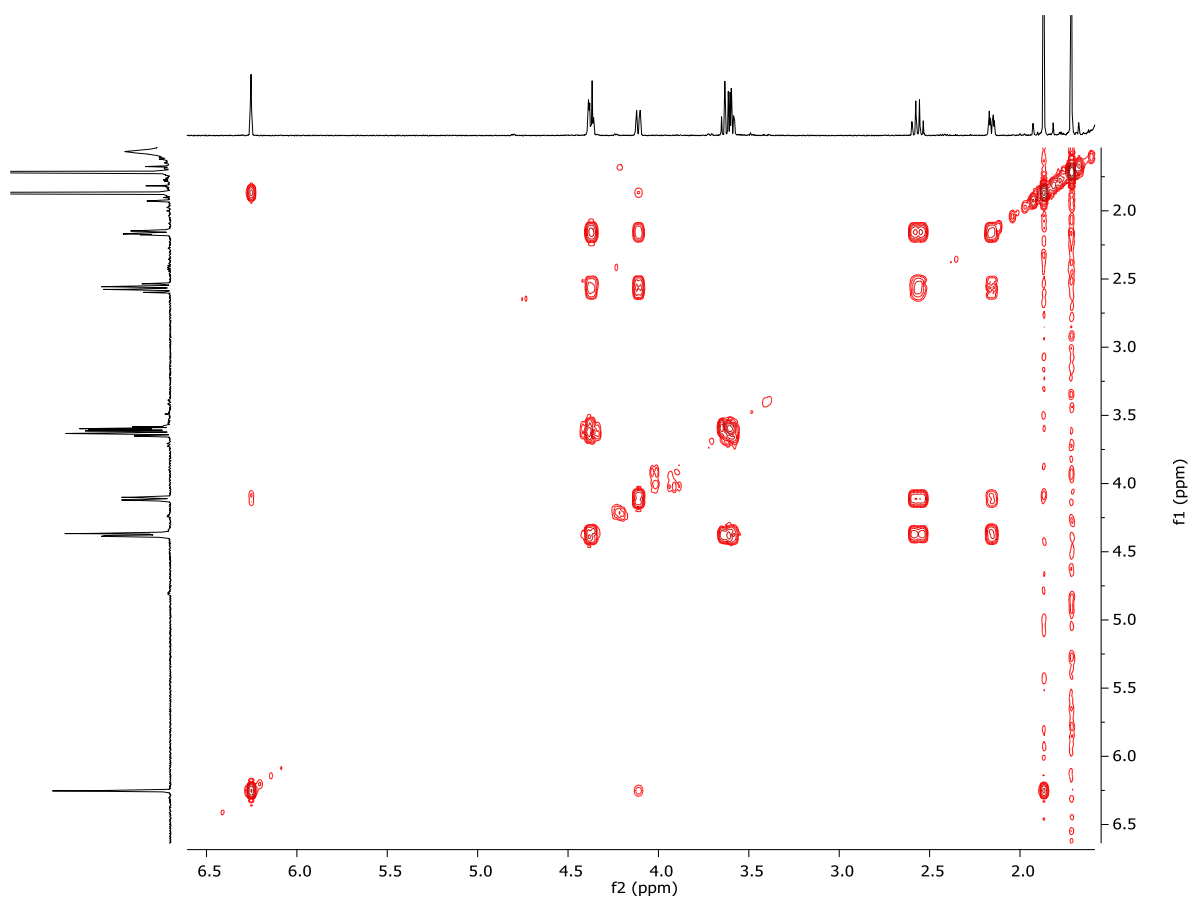
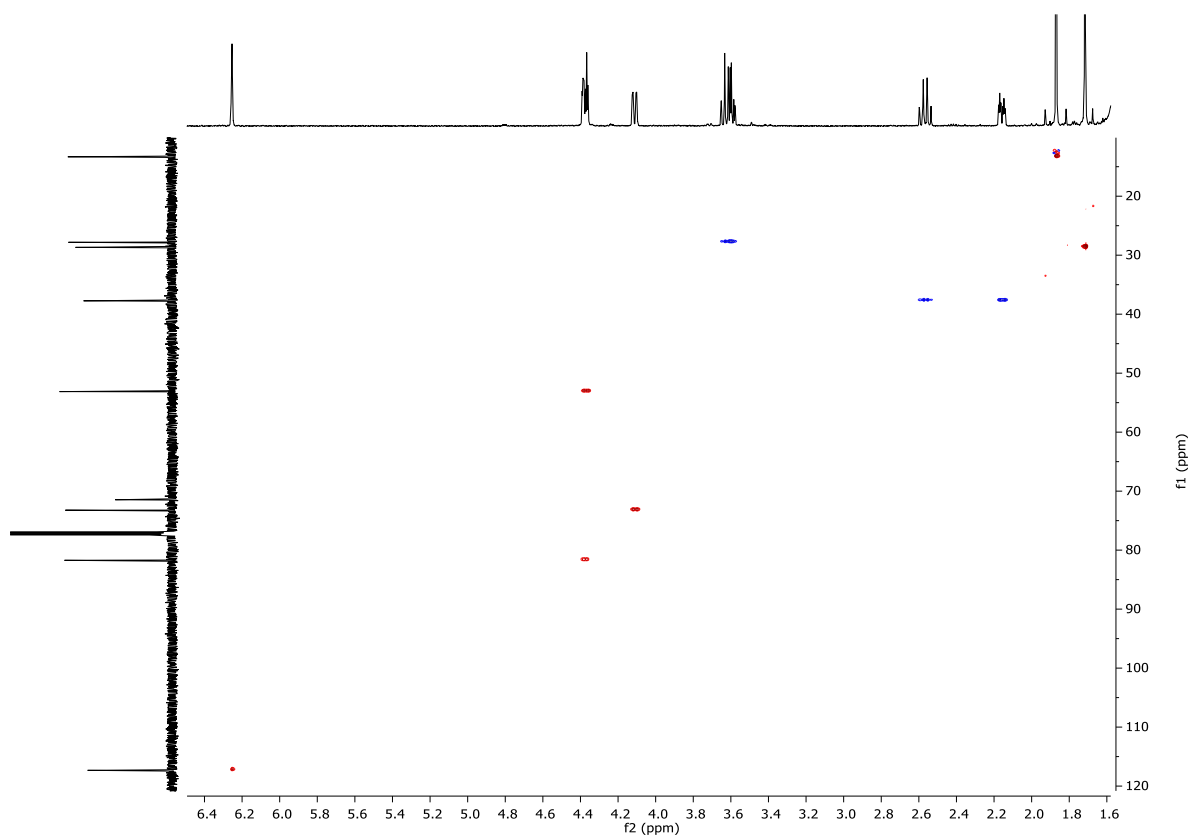
Figure S9 – COSY Spectrum (600 MHz, CDCl₃) of **7**Figure S10 – HSQC Spectrum (600 MHz, CDCl₃) of **7**

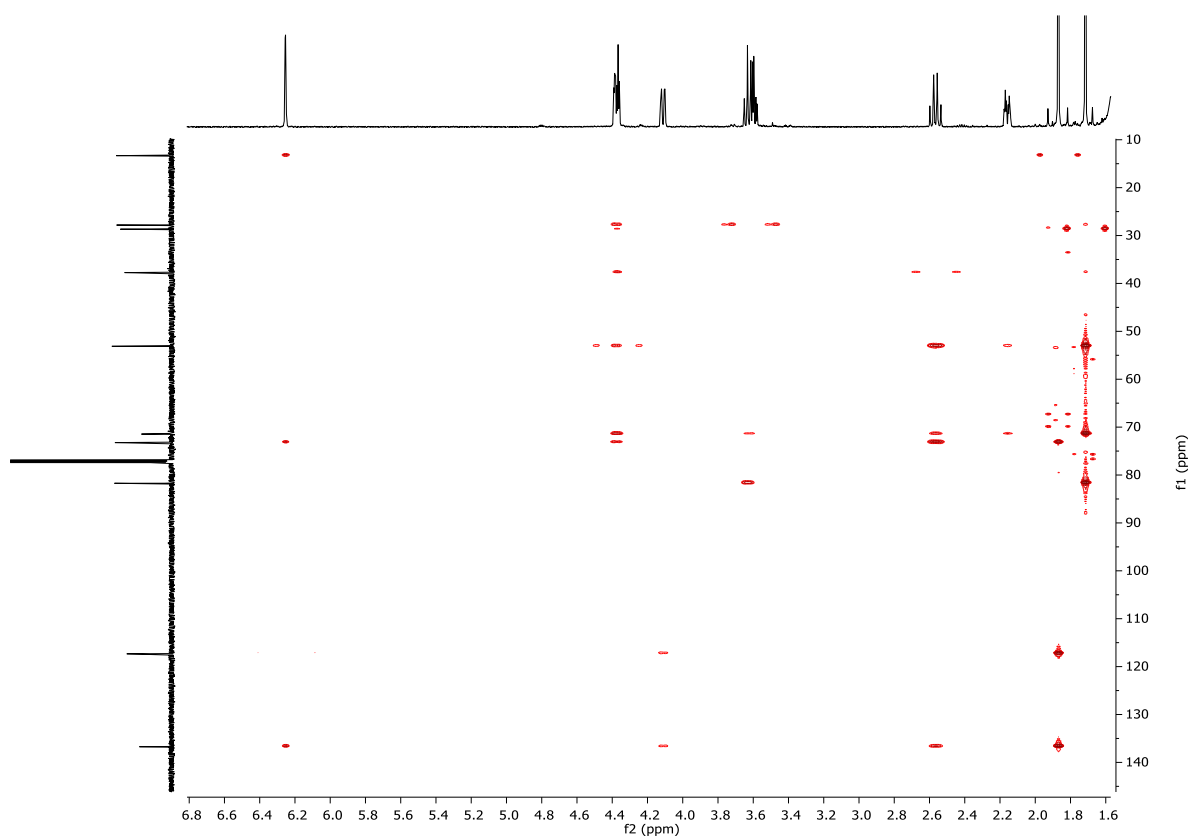
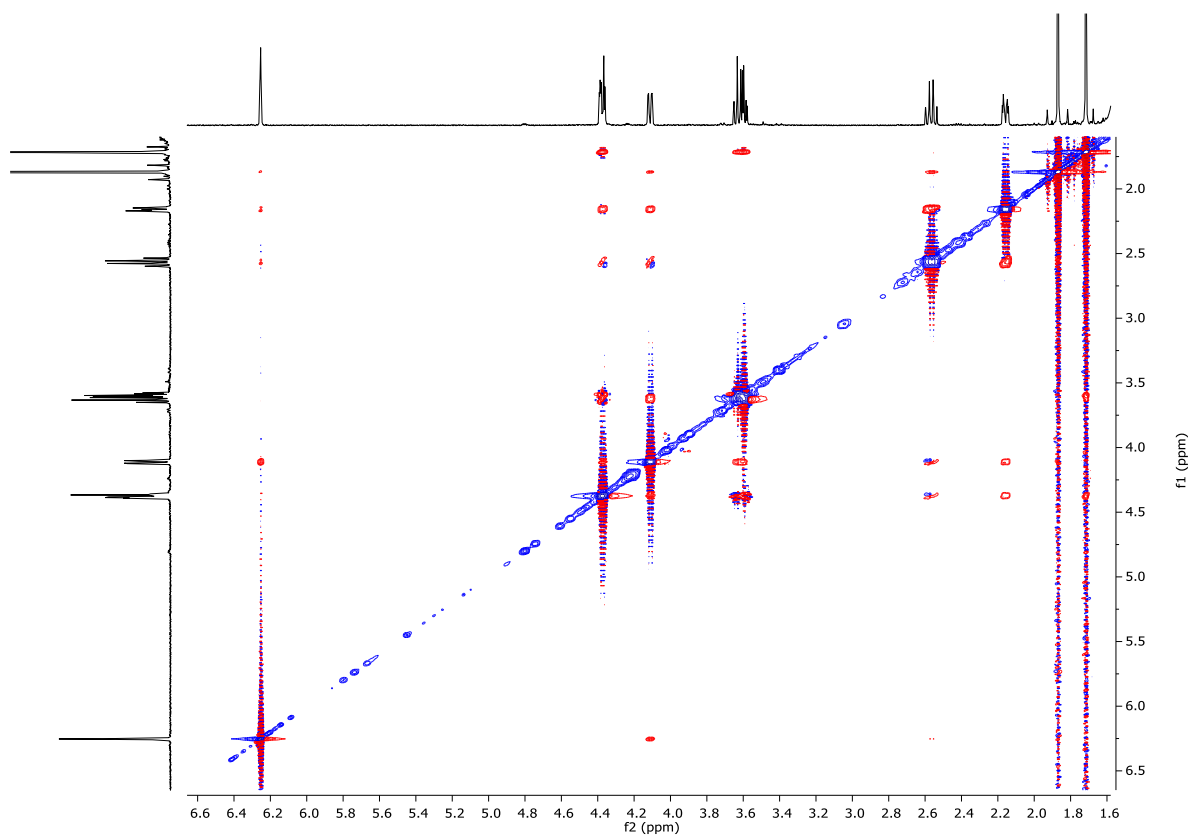
Figure S11 – HMBC Spectrum (600 MHz, CDCl₃) of **7**Figure S12 – NOESY Spectrum (600 MHz, CDCl₃) of **7**

Figure S13 – (-)HR-APCI-MS Spectrum of 7

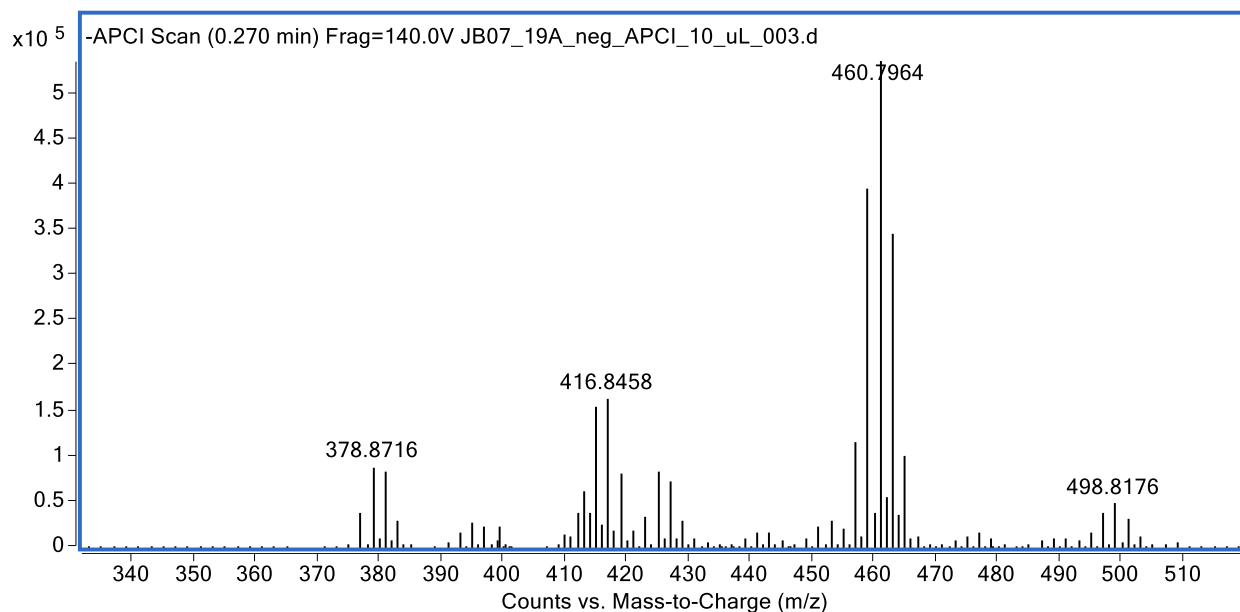


Figure S14 – IR Spectrum (film) of 7

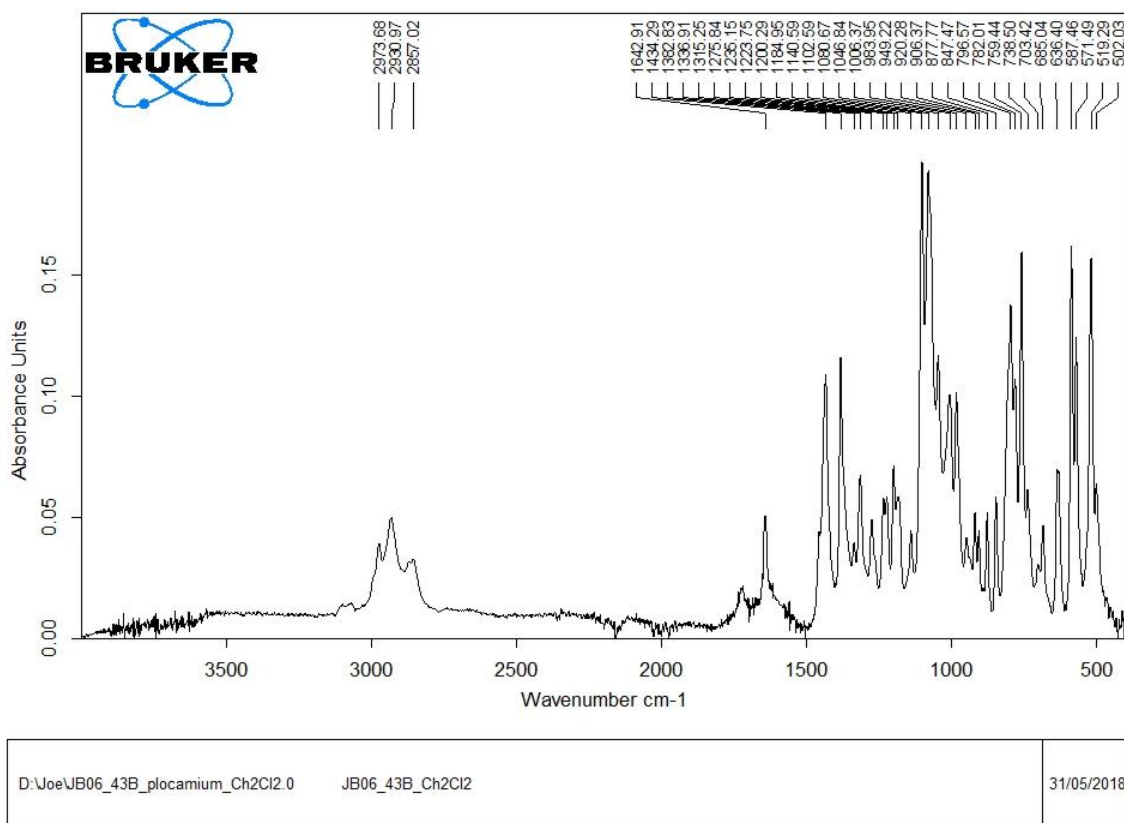


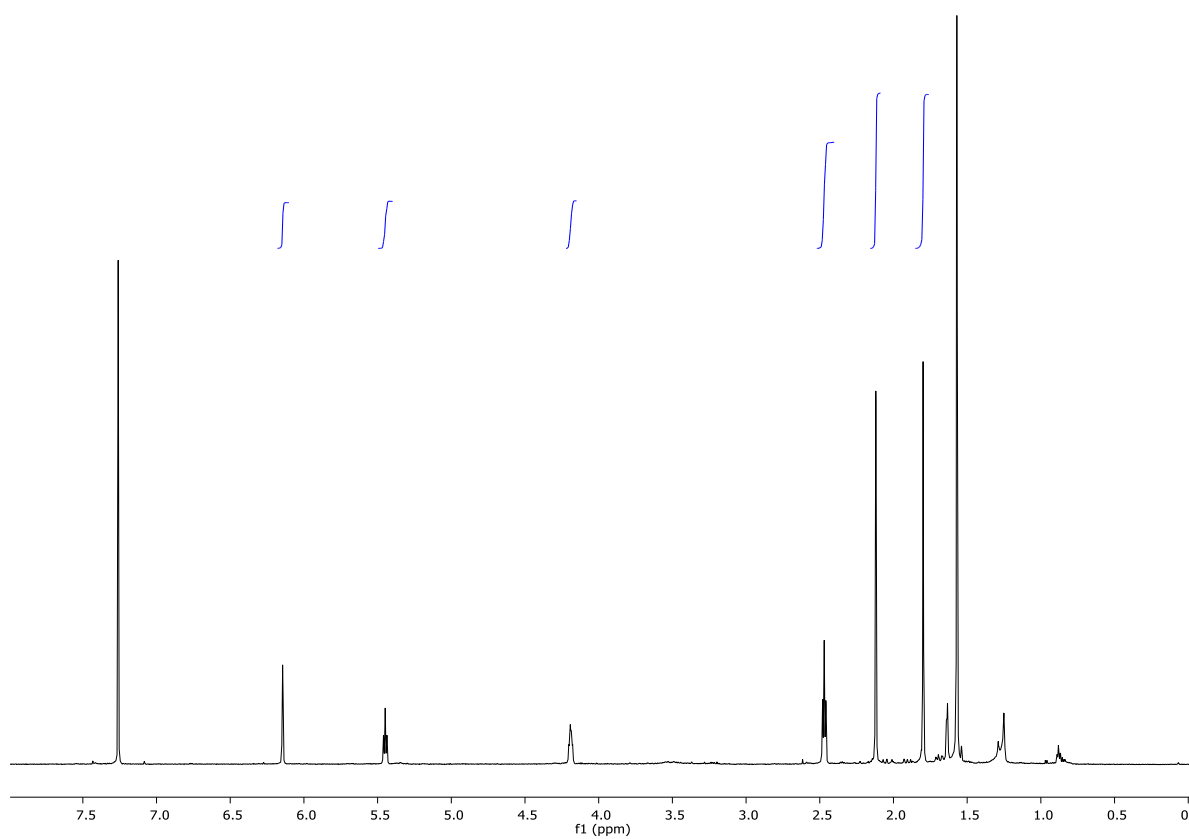
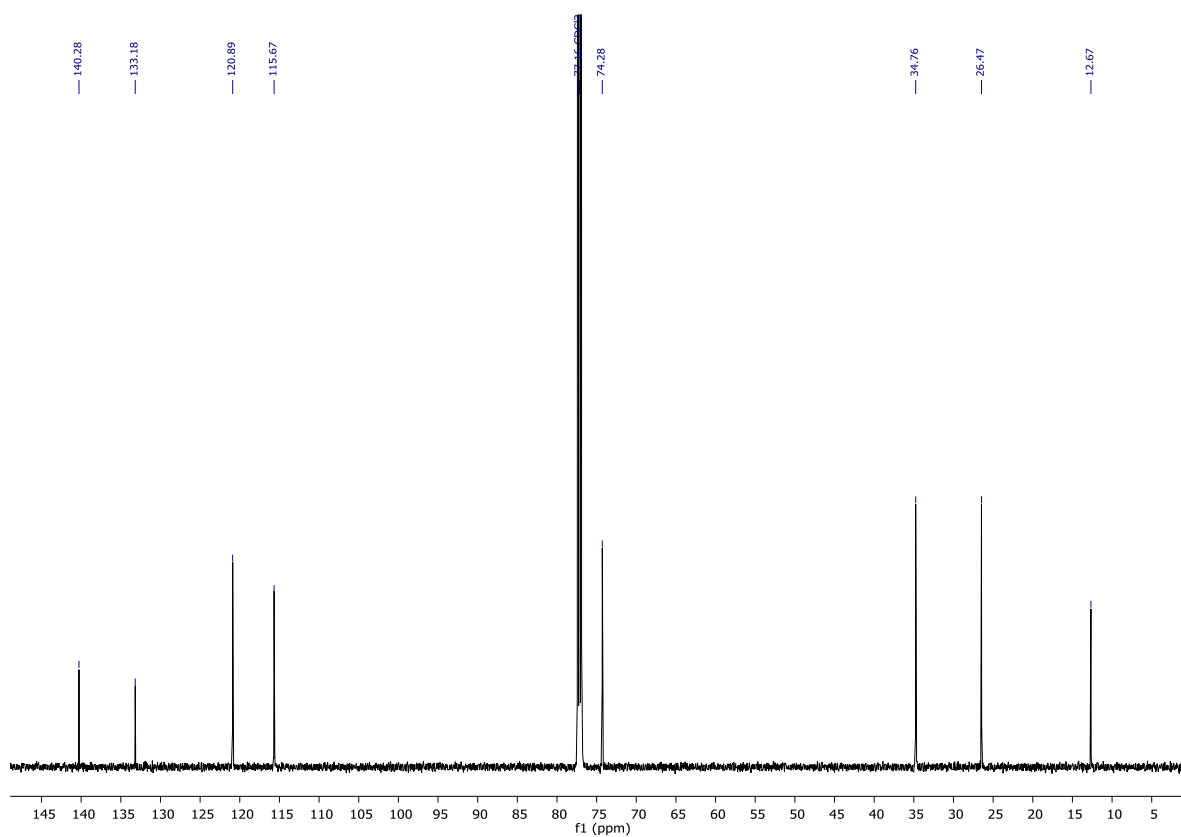
Figure S15 – ^1H Spectrum (600 MHz, CDCl_3) of **8**Figure S16 – ^{13}C Spectrum (150 MHz, CDCl_3) of **8**

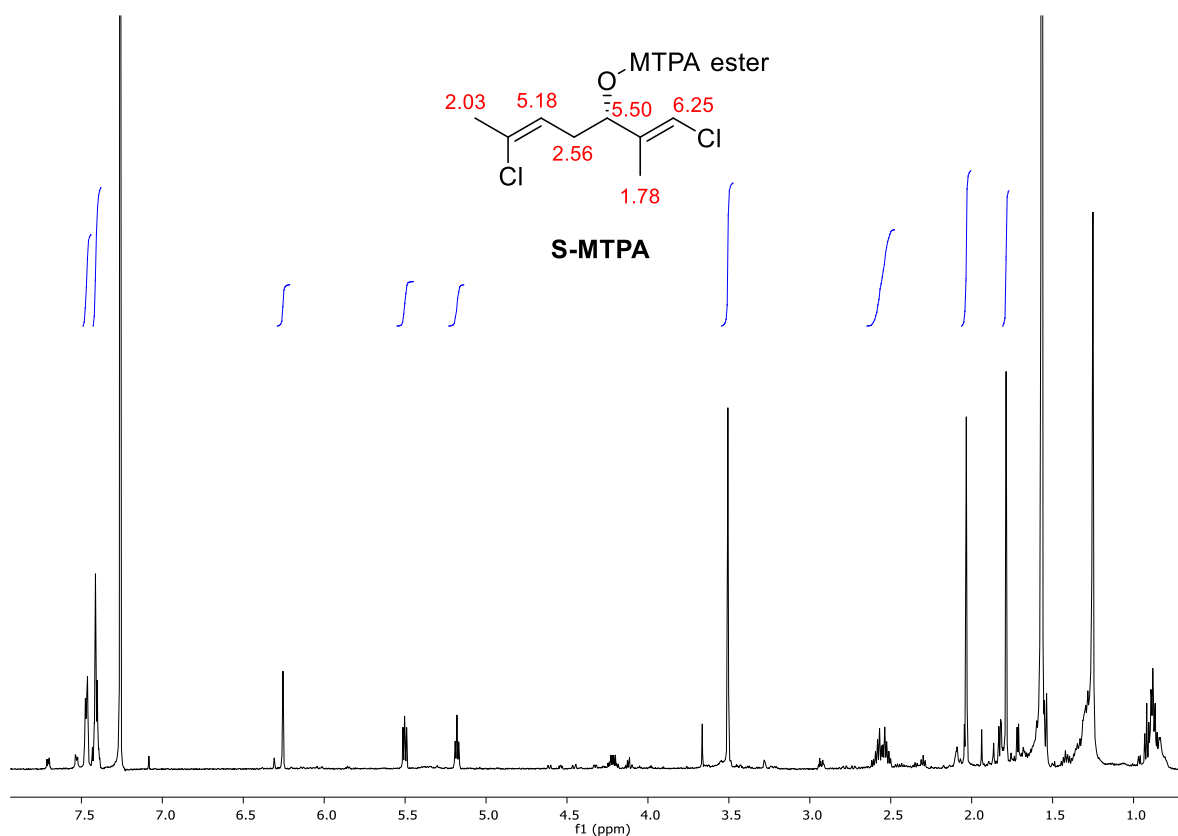
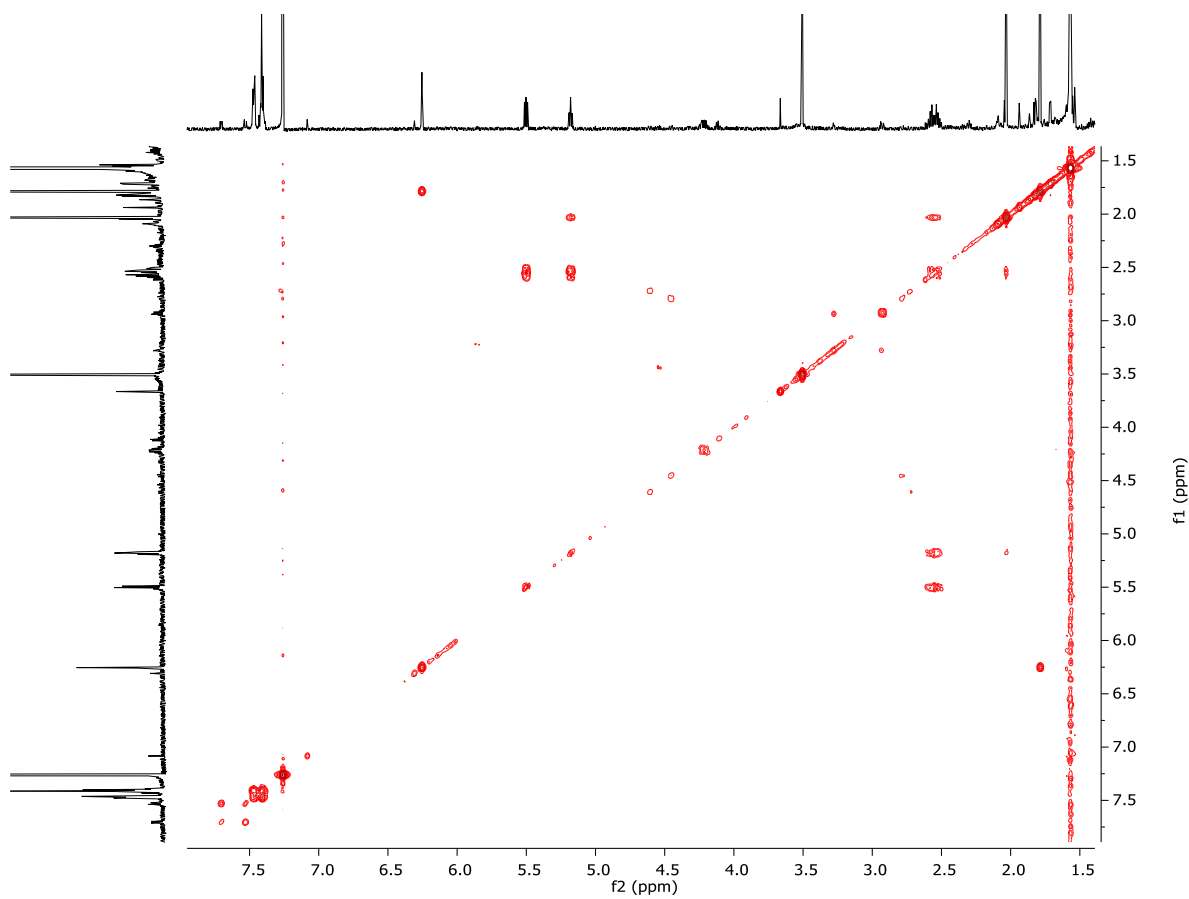
Figure S17 – ^1H Spectrum (600 MHz, CDCl_3) of *S*-MTPA ester of **8** (**12a**)Figure S18 – COSY Spectrum (600 MHz, CDCl_3) of *S*-MTPA ester of **8** (**12a**)

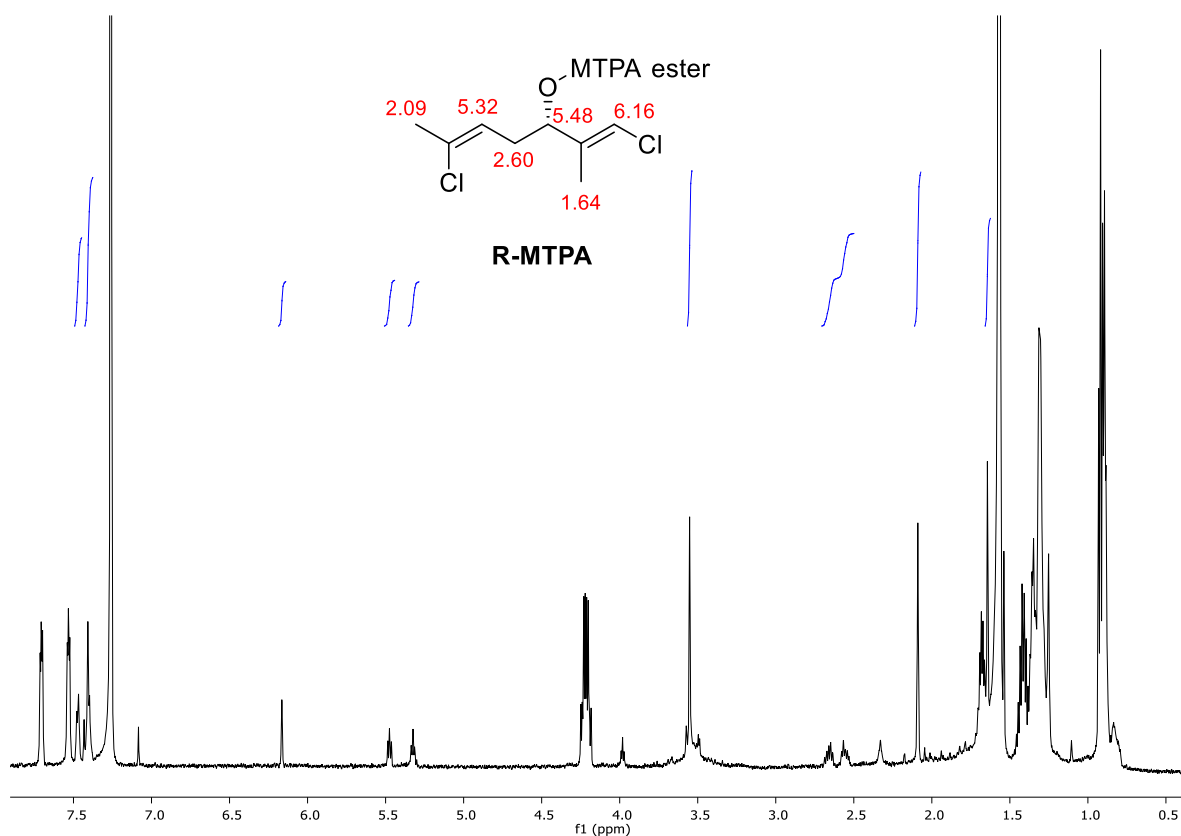
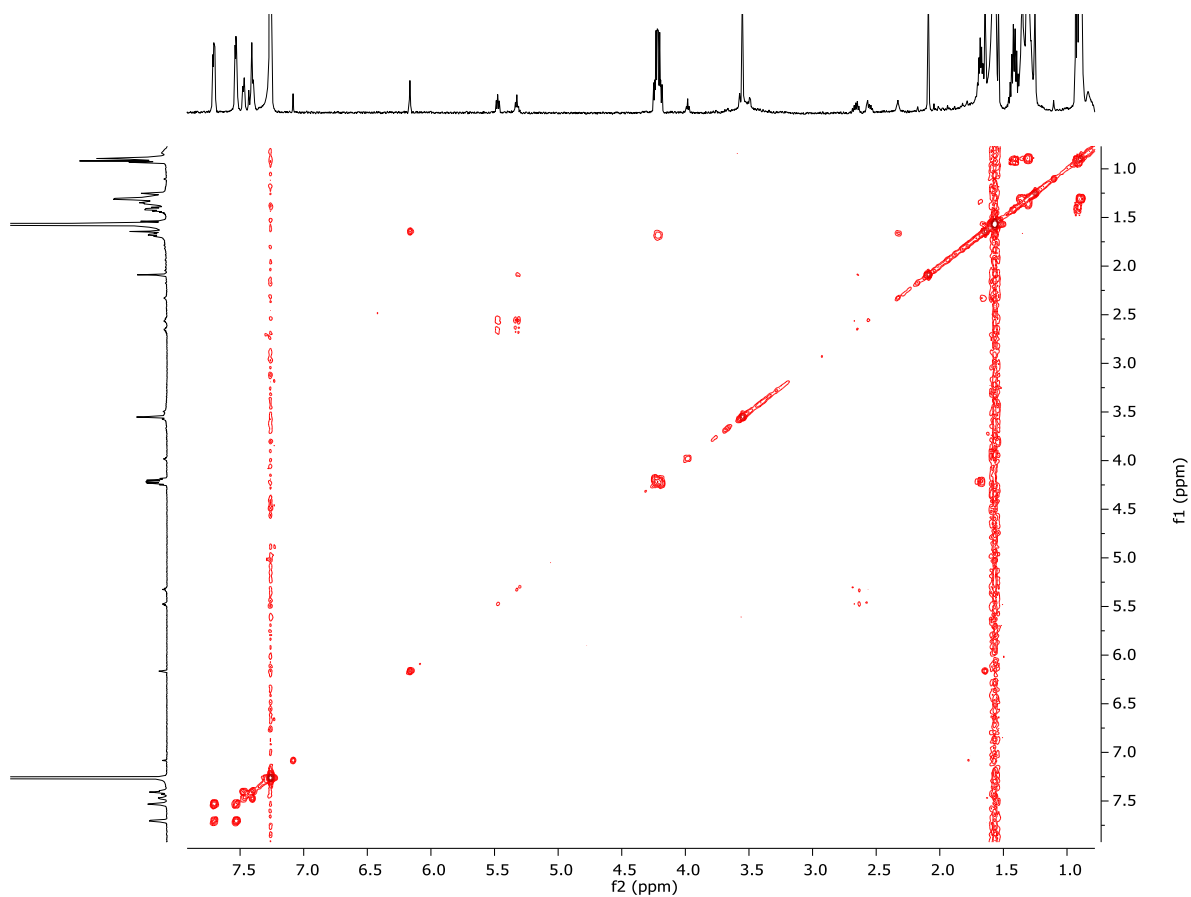
Figure S19 – ^1H Spectrum (600 MHz, CDCl_3) of *R*-MTPA ester of **8** (**12b**)Figure S20 – COSY Spectrum (600 MHz, CDCl_3) of *R*-MTPA ester of **8** (**12b**)

Figure S21 – Antibacterial testing of **7** and **8**. (A) Initial screening for growth inhibition of *P. aeruginosa* (black circles) and *Staphylococcus aureus* (white triangles). Cntl: 1% DMSO control. The individual data points are shown; horizontal lines represents the mean of three replicates. (B) Determination of the minimum inhibitory concentration of **7** towards *S. aureus* (grey bars) and *S. epidermidis* (black bars). The means and standard deviations of three replicates are shown as bars and lines, respectively.

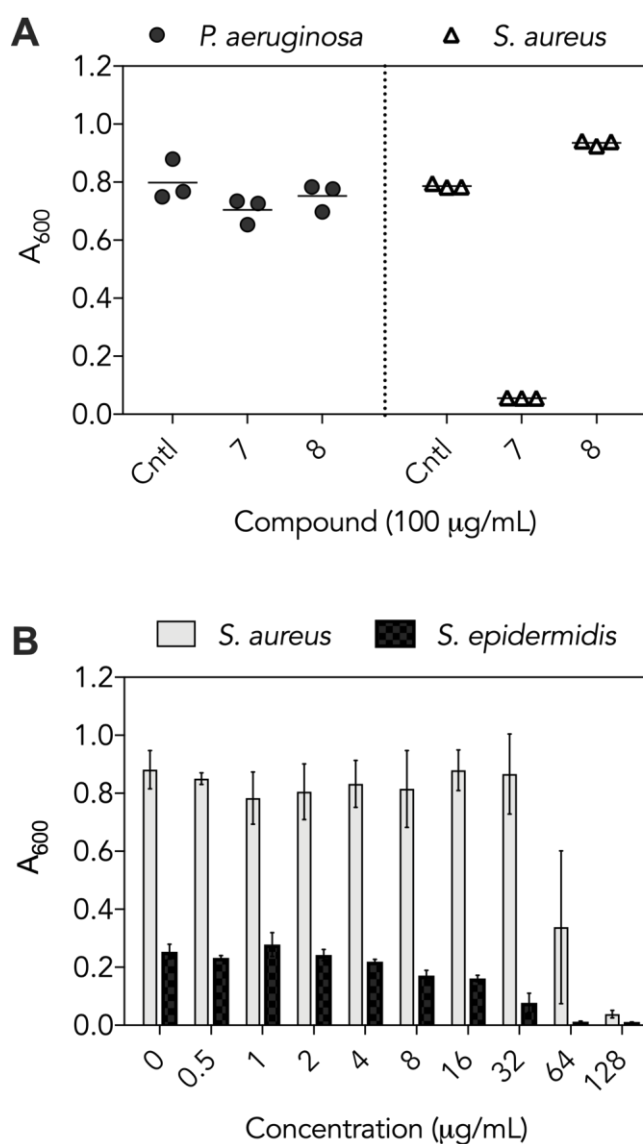


Figure S22 – Phylogenetic analysis (maximum-likelihood) of *Plocamium* species based on COI data. Bootstrap values >50% on branches shown. Scale bar = substitutions/site

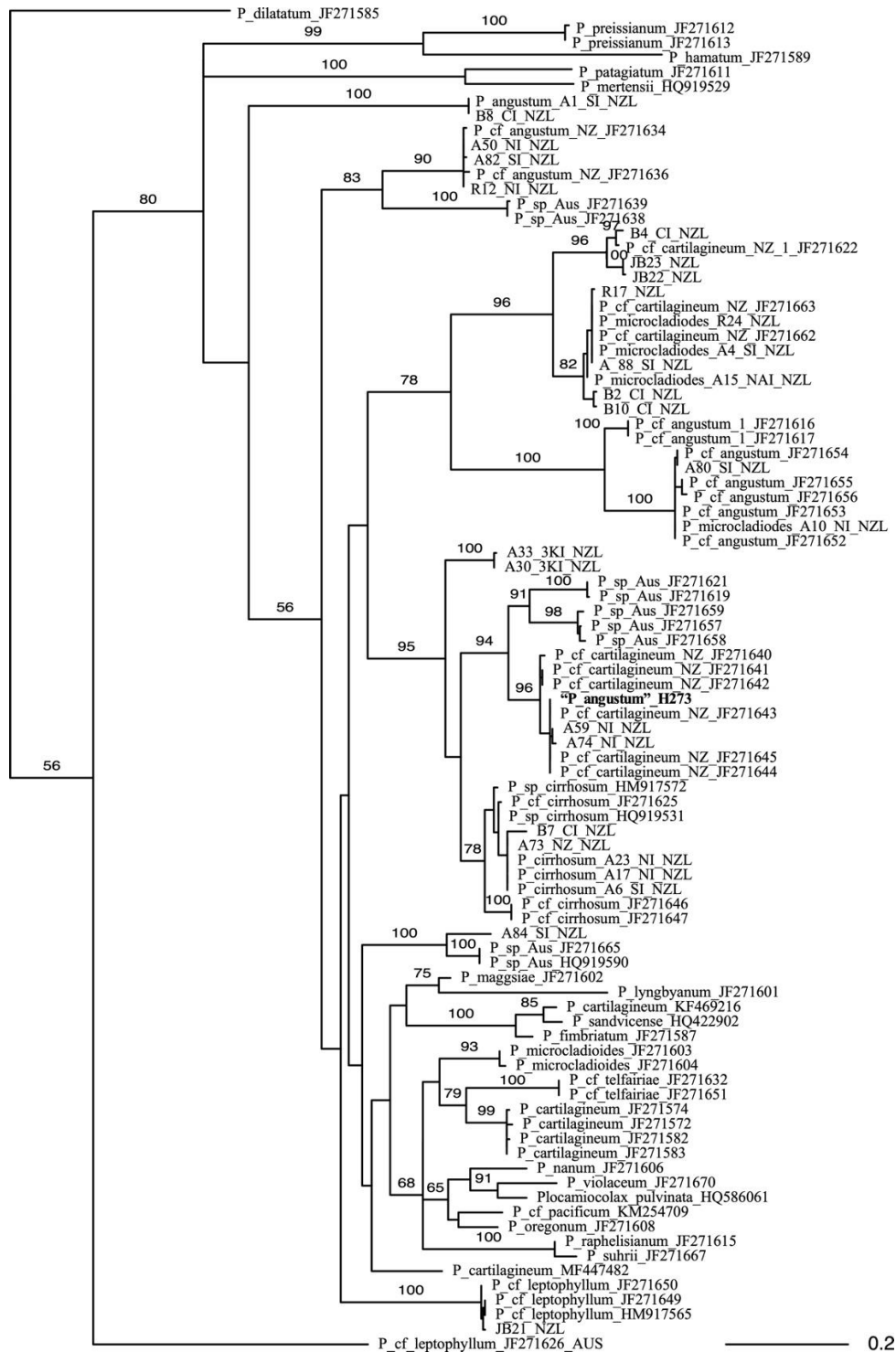


Figure S23 - Comparison of experimental ECD spectrum with calculated unscaled, calculated with only intensity scaling, and calculated with both intensity and frequency scaling (Figure 3 in the manuscript). Due to the much lower intensity of the calculated values, the values were multiplied by 20. The frequency was shifted 7 nm to the left for the calculated spectrum to compare with the experimental spectrum whose data was available for 190-280 nm.

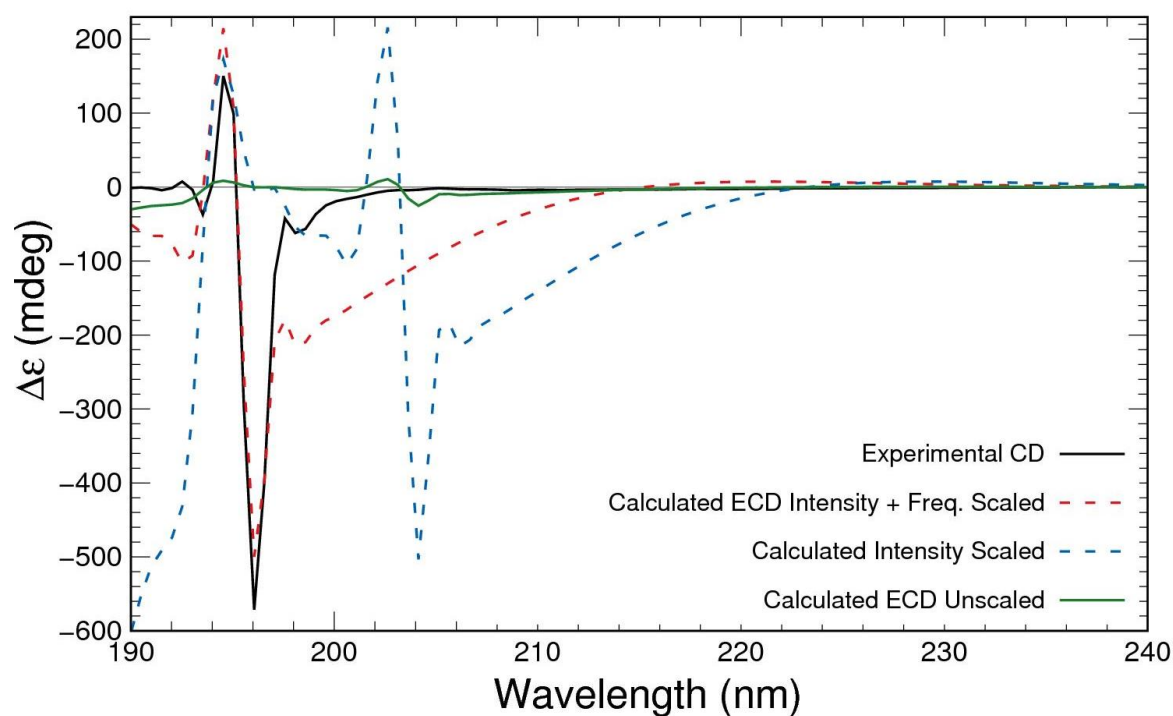


Figure S24 – Relative energies of all computed conformers of costatone C (7).

