

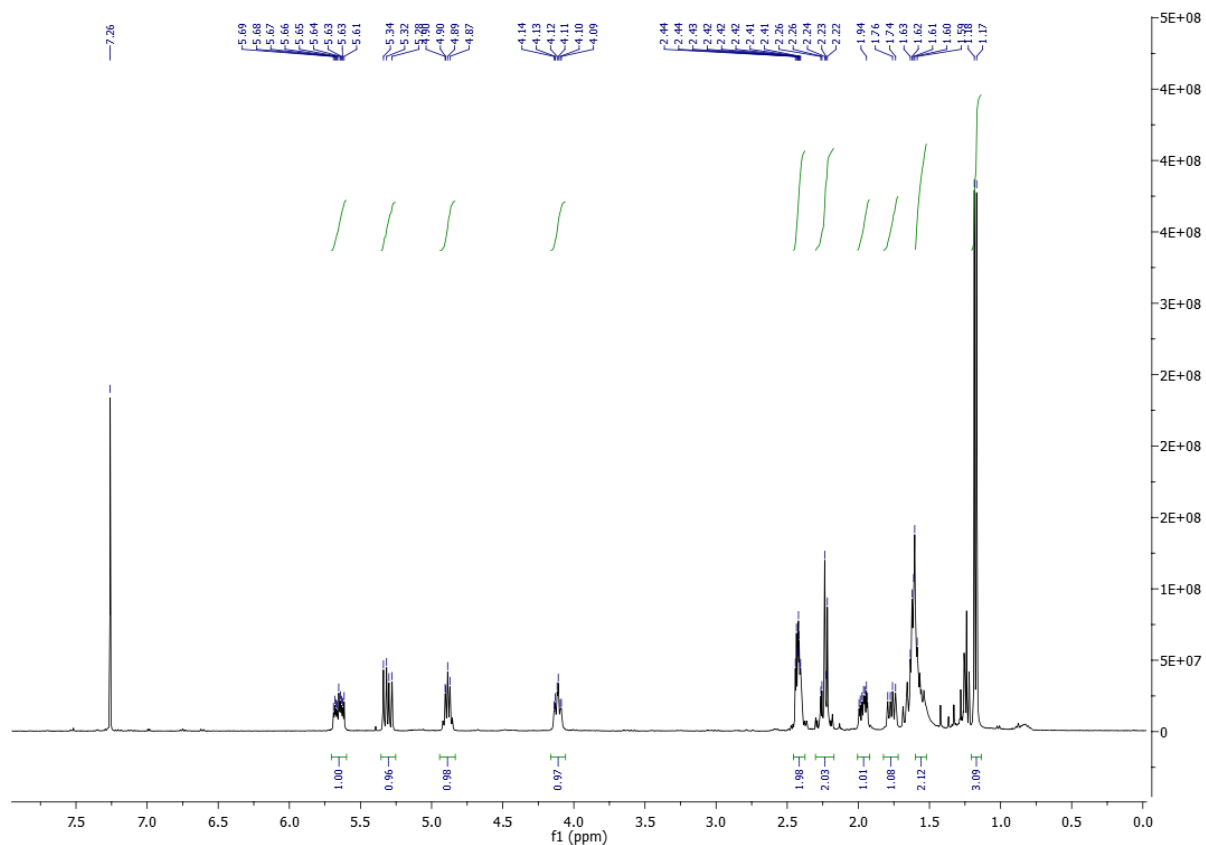
## **SUPPORTING INFORMATION**

**Truncatenolide a Bioactive Disubstituted Nonenolide Produced by *Colletotrichum truncatum*, the Causal Agent of Anthracnose of Soybean in Argentina. Fungal Antagonism and SAR Studies**

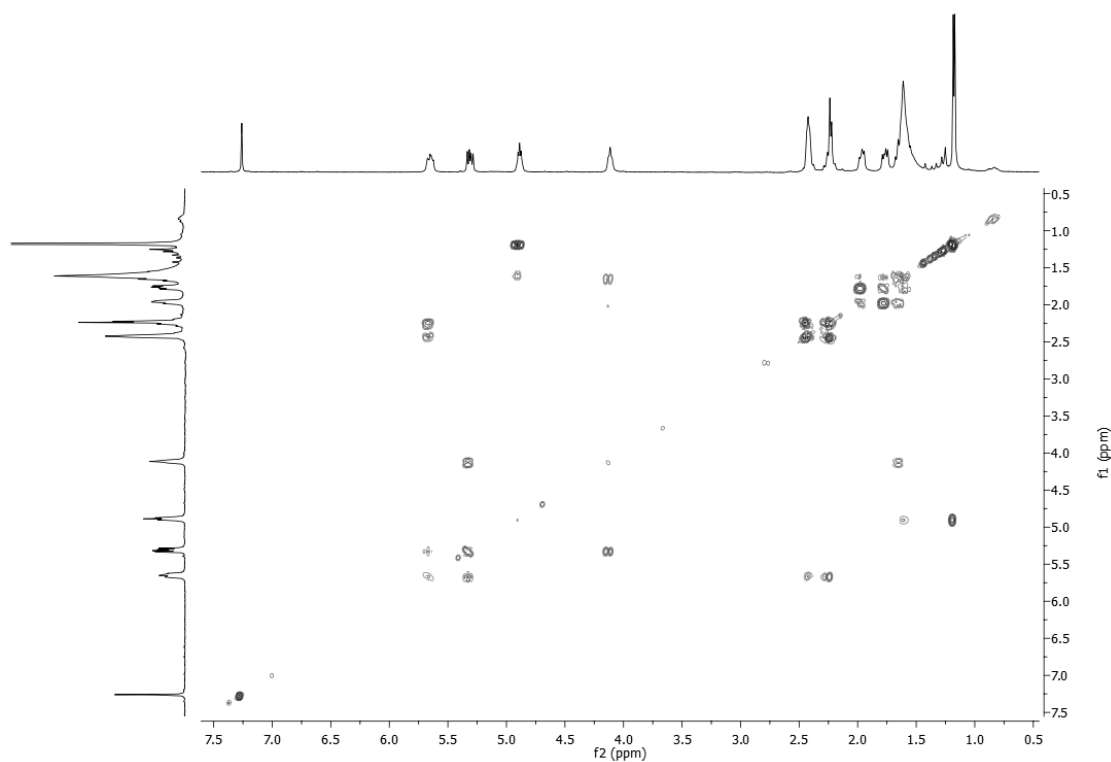
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## Supporting Information List

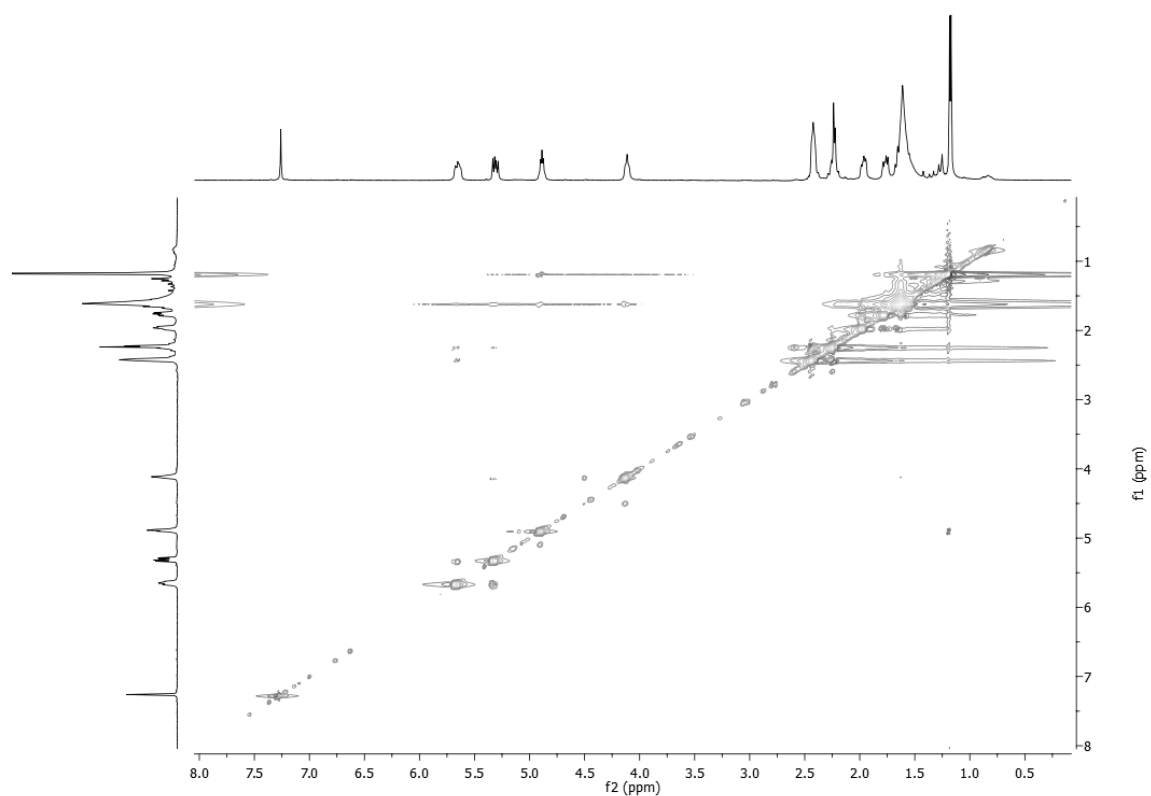
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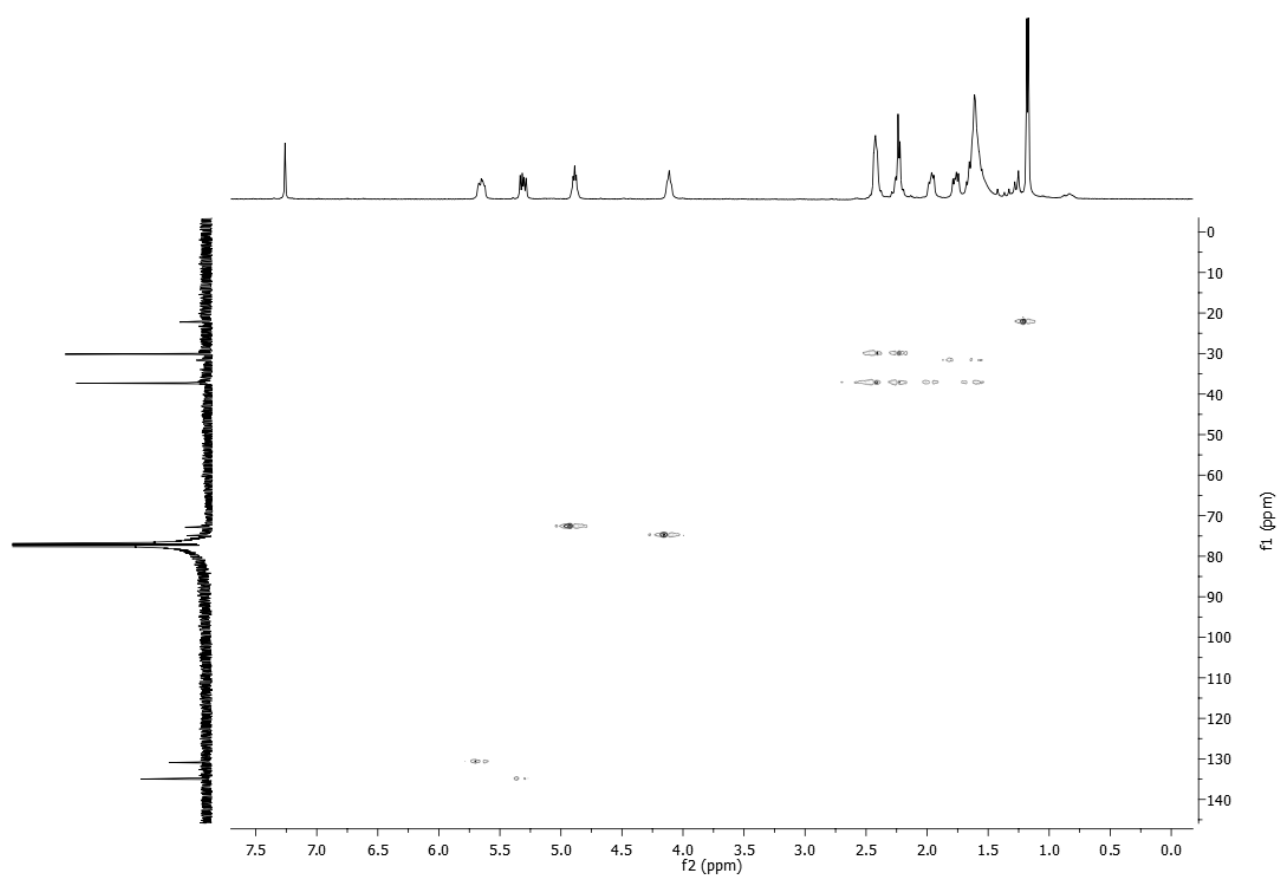
**Figure S1.**  $^1\text{H}$  NMR spectrum of trucantenolide, **1** ( $\text{CDCl}_3$ , 400 MHz).



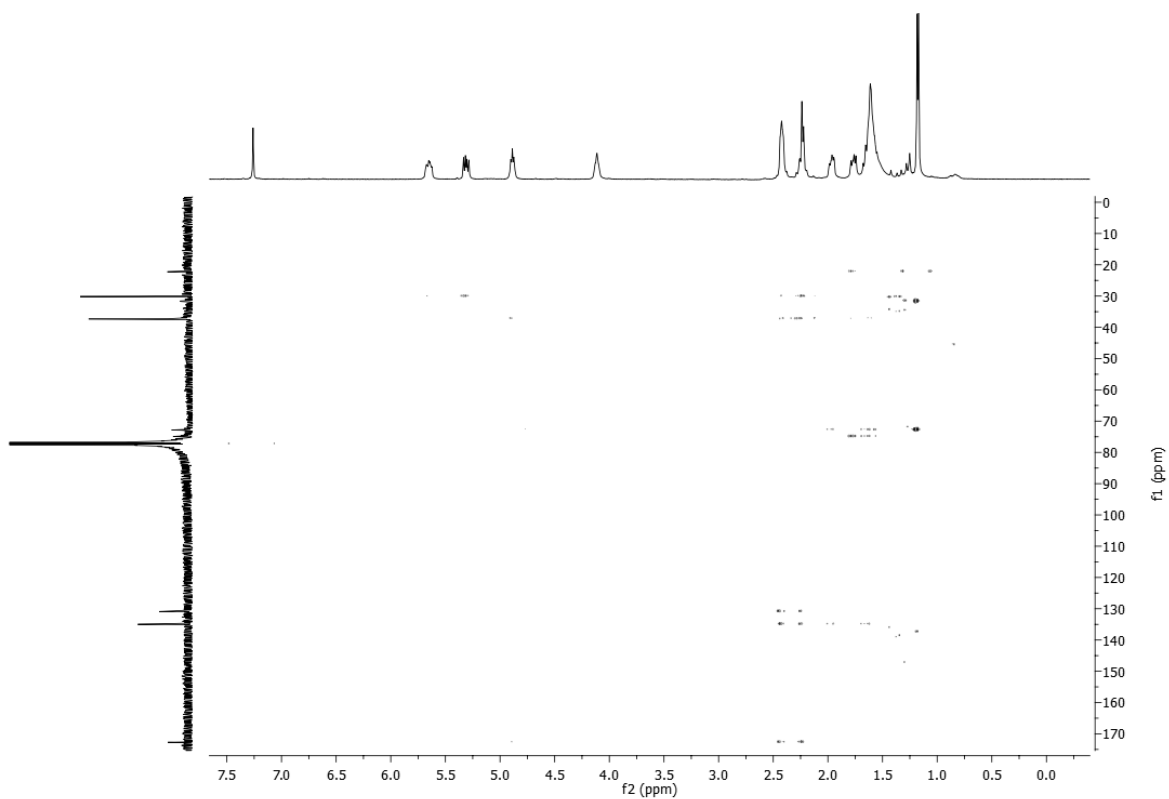
**Figure S2.** COSY spectrum of trucantenolide, **1** ( $\text{CDCl}_3$ , 400 MHz).



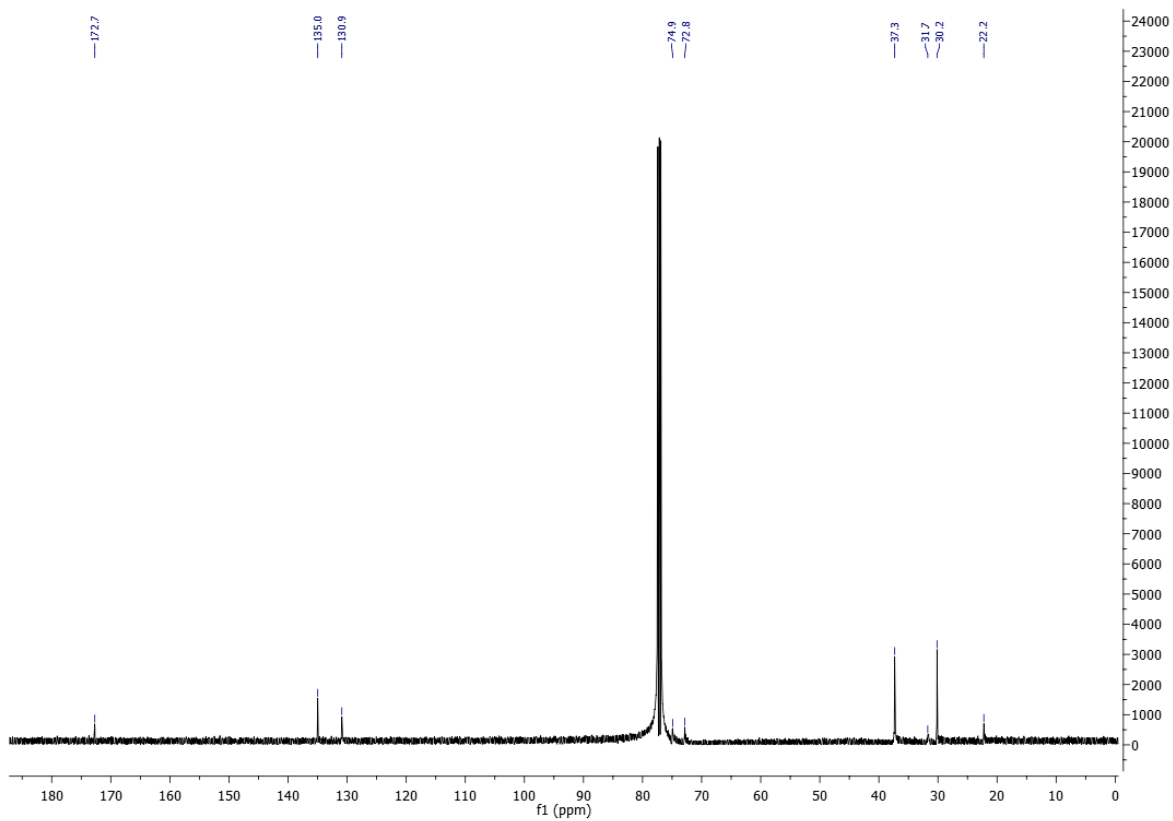
**Figure S3.** NOESY spectrum of trucantenolide, **1** (CDCl<sub>3</sub>, 400 MHz).



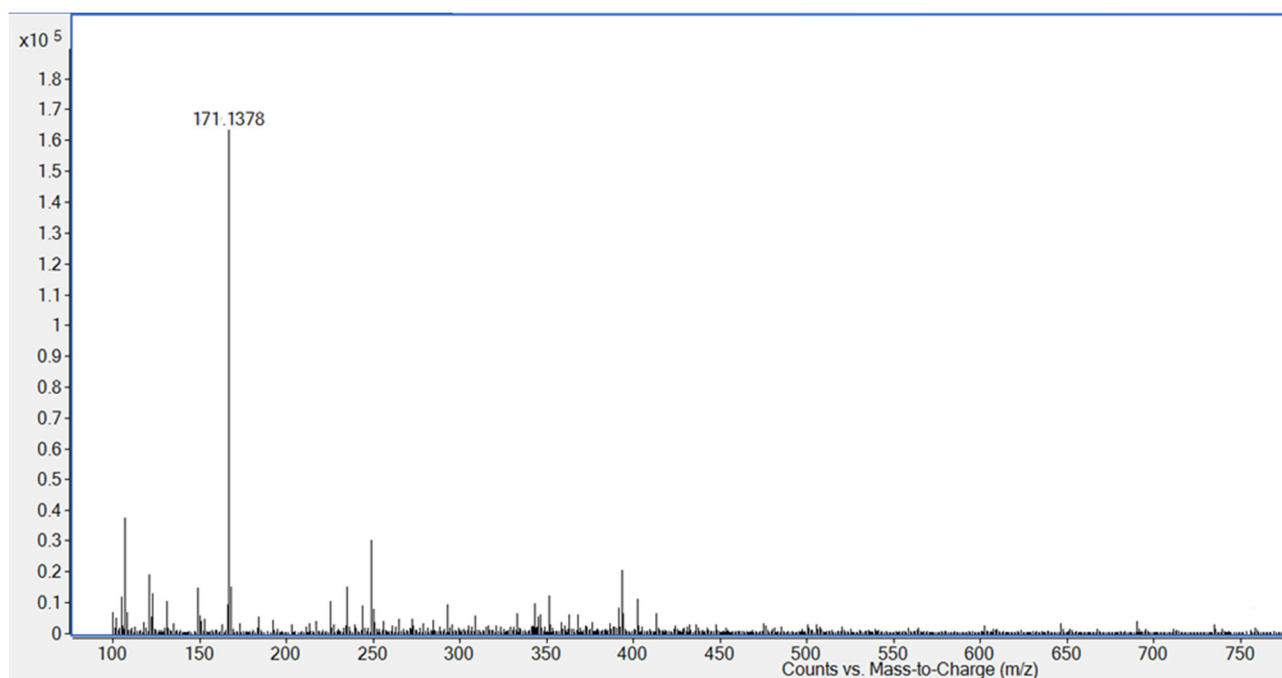
**Figure S4.** HSQC spectrum of of trucantenolide, **1** (CDCl<sub>3</sub>, 400/100 MHz).



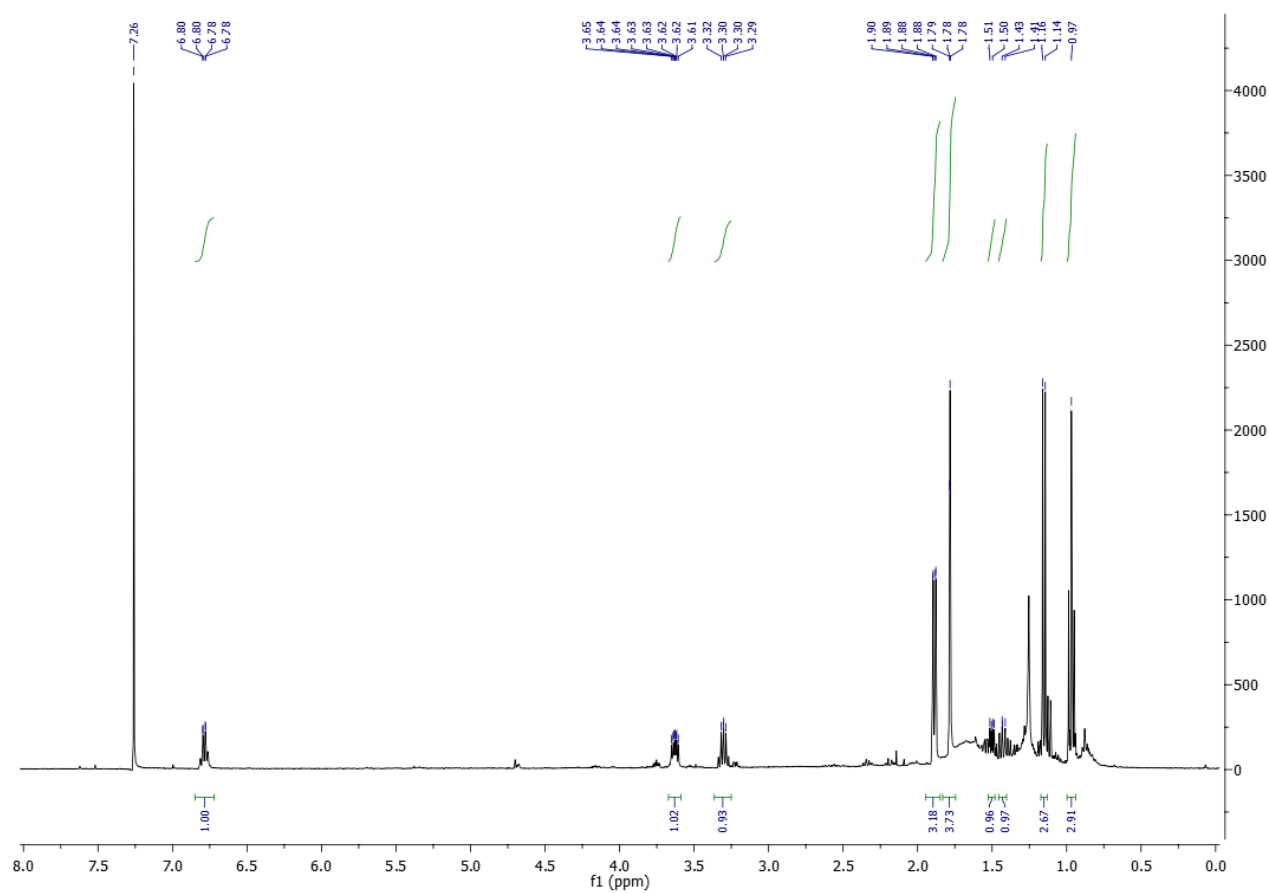
**Figure S5.** HMBC spectrum of of trucantenolide, **1** (CDCl<sub>3</sub>, 400/100 MHz).



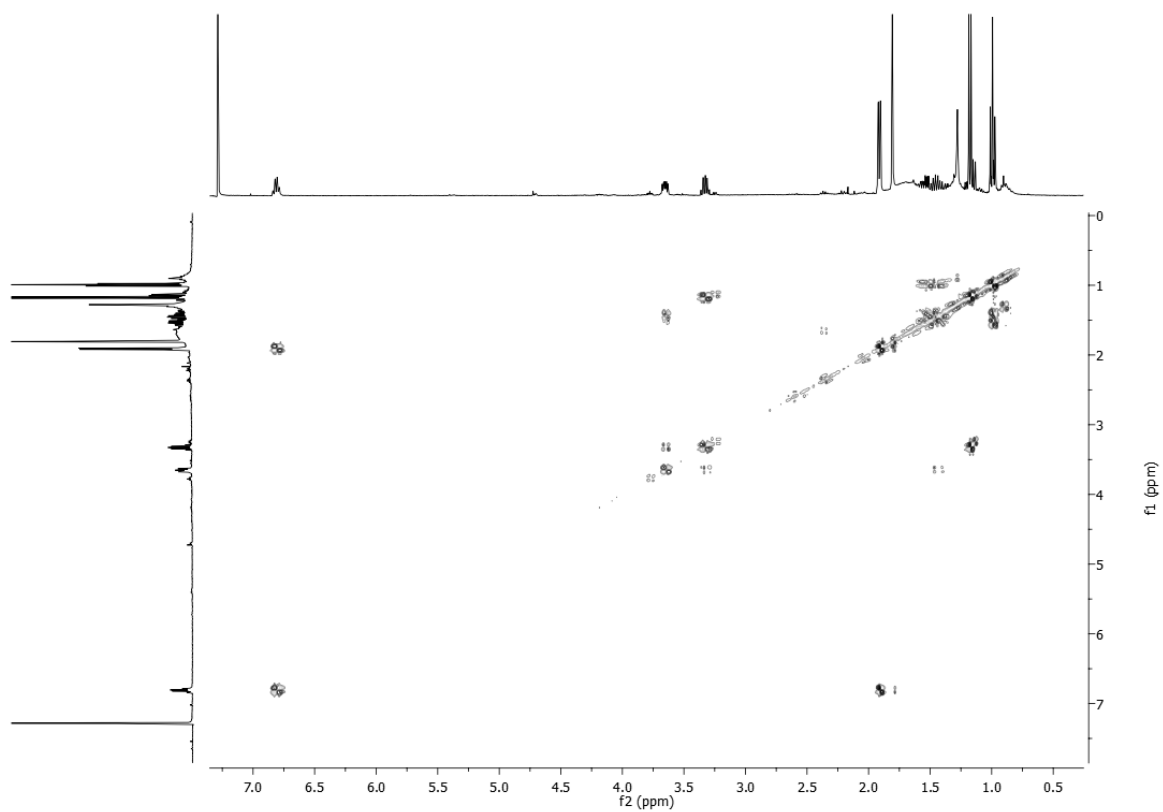
**Figure S6.** <sup>13</sup>C NMR spectrum of trucantenolide, **1** (CDCl<sub>3</sub>, 100 MHz).



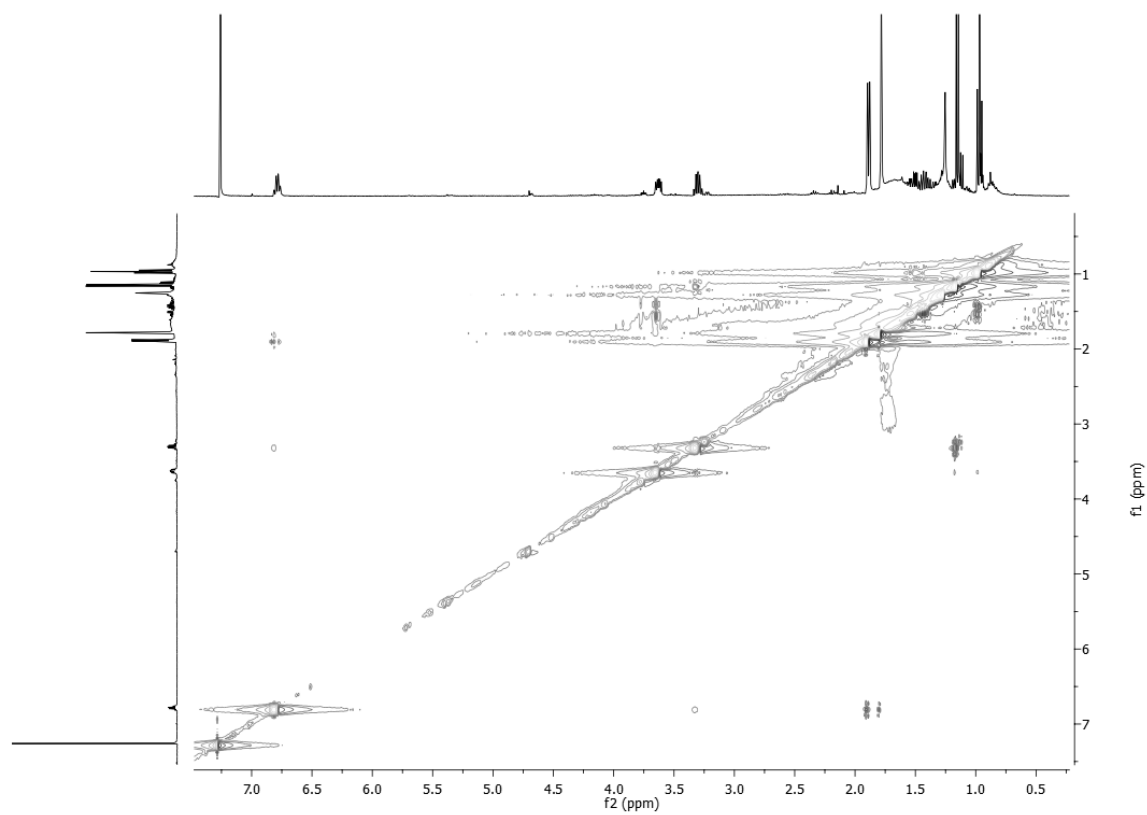
**Figure S7.** HRESI MS spectrum of of truncatenolide, **1** recorded in positive modality.



**Figure S8.**  $^1\text{H}$  NMR spectrum of truncatenone, **2** ( $\text{CDCl}_3$ , 400 MHz).



**Figure S9.** COSY spectrum of truncatenone, **2** (CDCl<sub>3</sub>, 400 MHz).



**Figure S10.** NOESY spectrum of truncatenone, **2** (CDCl<sub>3</sub>, 400 MHz).

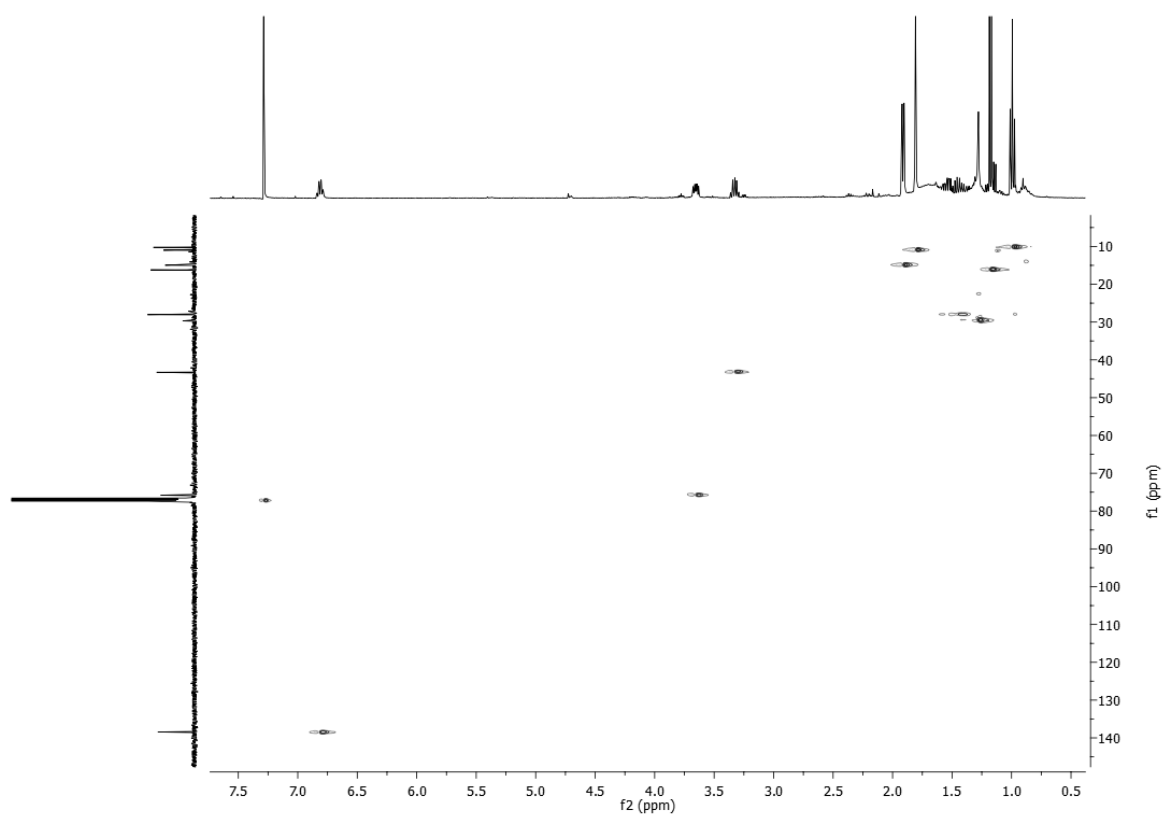


Figure S11. HSQC spectrum of truncatenone, **2** (CDCl<sub>3</sub>, 400/100 MHz).

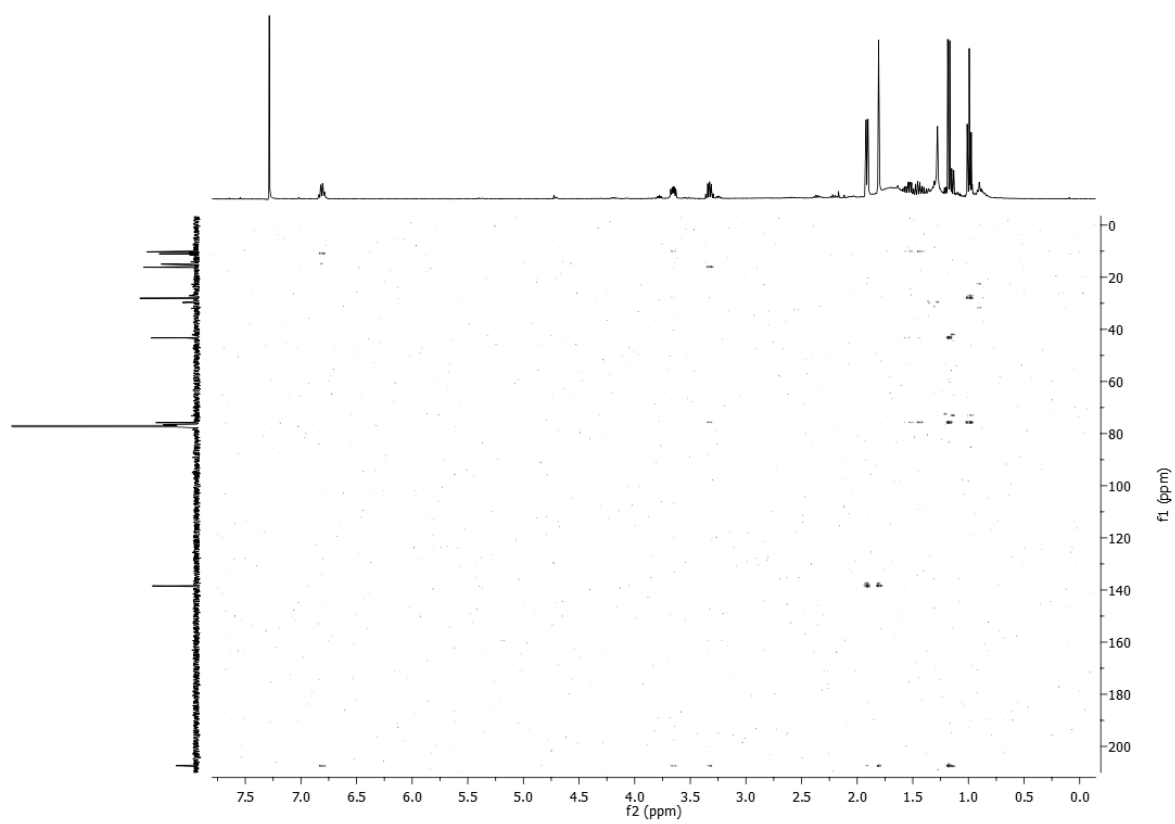
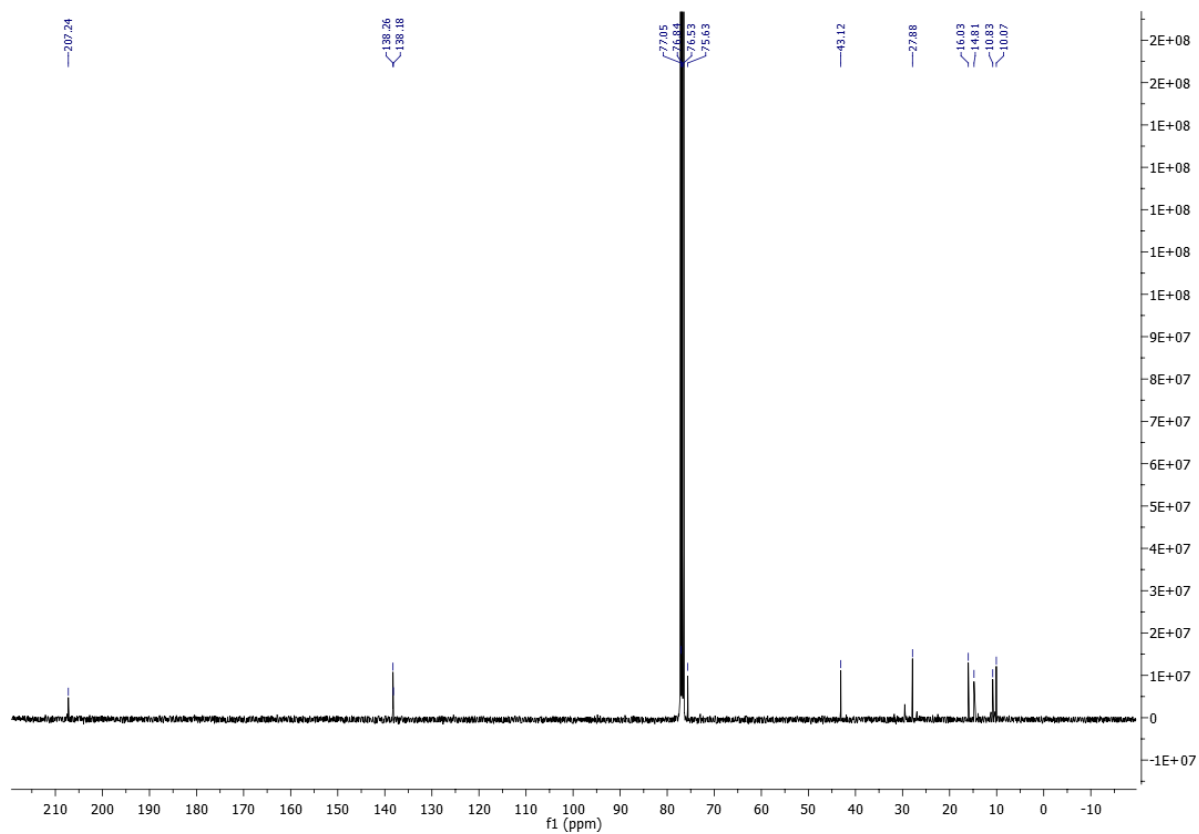
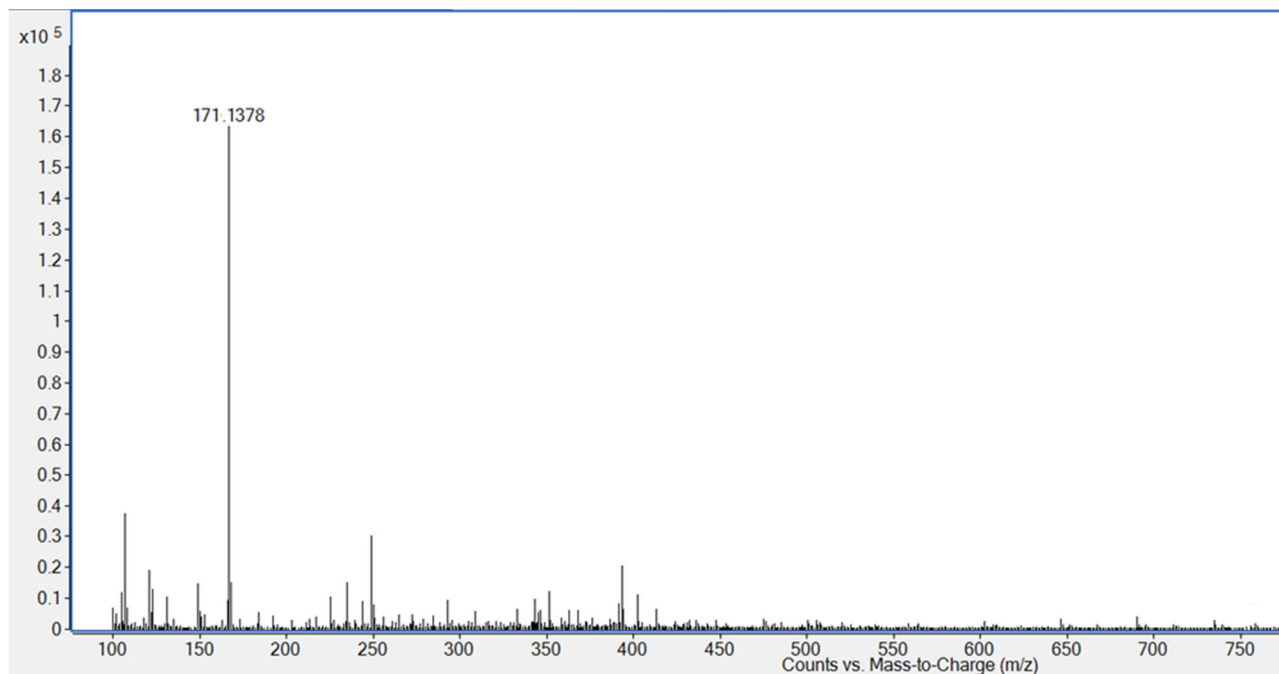


Figure S12. HMBC spectrum of truncatenone, **2** (CDCl<sub>3</sub>, 400/100 MHz).

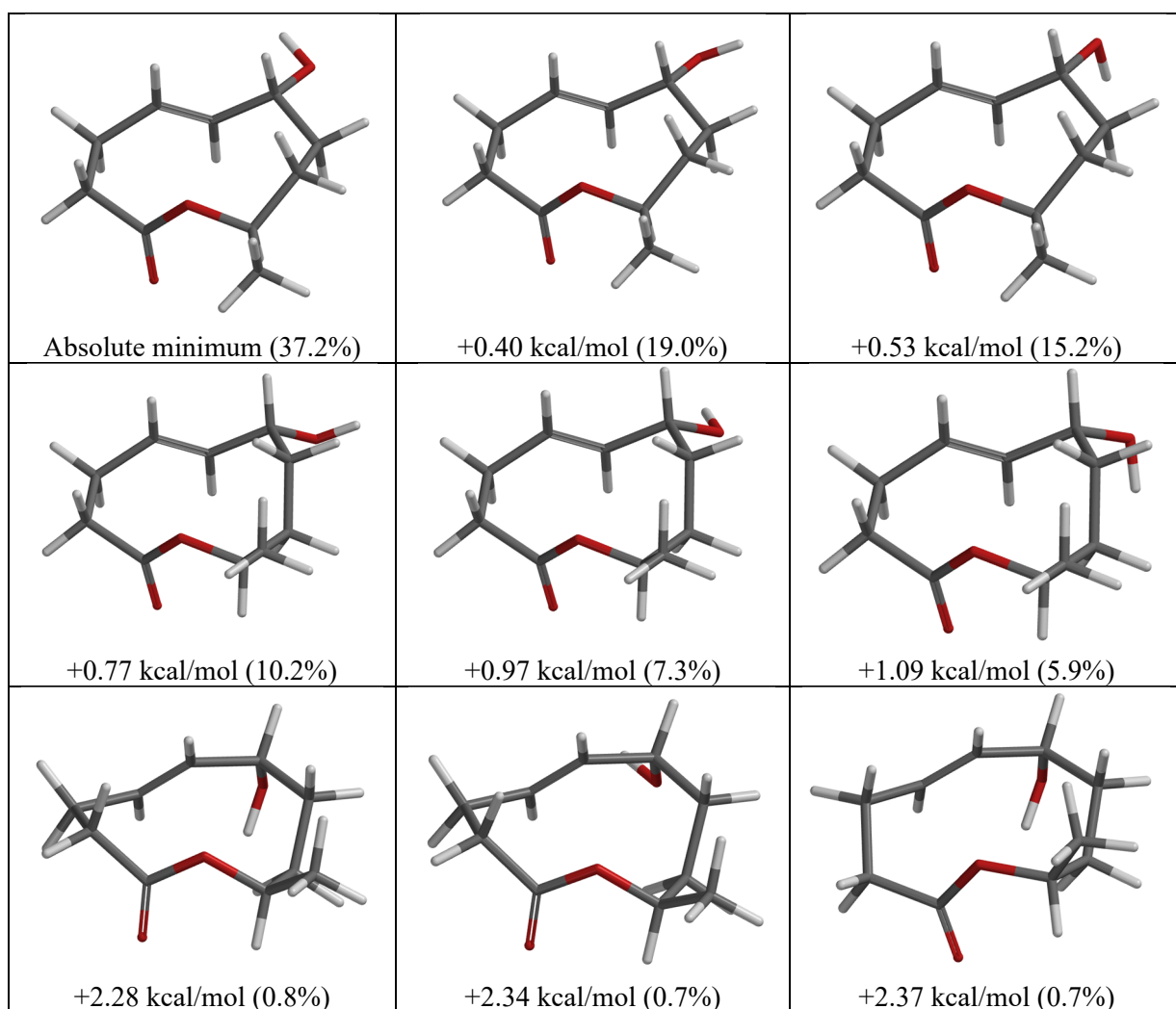




**Figure S13.** <sup>13</sup>C NMR spectrum of truncatenone, **2** (CDCl<sub>3</sub>, 100 MHz).







**Figure S14.** HRESI MS spectrum truncatenone, **2** recorded in positive modality.







**Figure S15.** Low-energy conformers, relative internal energy and Boltzmann population at 300K calculated for compound (7*R*,10*R*)-1 at  $\omega$ B97X-D/6-311+G(d,p) level, including the Solvation Model based on Density (SMD) for acetonitrile.

**Table S1.** Summary of DP4+ test on (7*R*,10*S*)-1 (isomer 1) and (7*R*,10*R*)-1 (isomer 2). See Computational Section (main text) for details.

Functional		Solvent?	Basis Set			Type of Data	
B3LYP		Gas Phase	6-31G(d)			Scaled Shifts	
		DP4+	-	-	-	-	-
Nuclei	sp2?	Experimental	Isomer 1	Isomer 2	Isomer 3	Isomer 4	Isomer 5
C	x	172.7	173.6	173.2			
C		37.3	36.4	36.4			
C		30.2	31.4	31.6			
C	x	130.9	127.6	131.6			
C	x	135	137.6	137.1			
C		74.9	69.6	75.6			
C		37.3	34.9	36.4			
C		31.7	27.7	31.4			
C		72.8	71.6	72.6			
C		22.2	21.2	21.6			
			Isomer 1	Isomer 2			
sDP4+ (H data)			-	-			
sDP4+ (C data)			0.00%		100.00%		
sDP4+ (all data)			0.00%		100.00%		

**Table S2.** Summary of DP4+ test on (5*R*,6*S*)-2 (isomer 1) and (5*S*,6*S*)-2 (isomer 2). See Computational Section (main text) for details.

Functional		Solvent?	Basis Set			Type of Data	
B3LYP		Gas Phase	6-31G(d)			Scaled Shifts	
		DP4+	-	-	-	-	-
Nuclei	sp2?	Experimental	Isomer 1	Isomer 2	Isomer 3	Isomer 4	Isomer 5
C		14.8	17.3	16.8			
C	x	138.3	145.0	143.6			
C	x	138.2	134.6	135.3			
C		10.8	22.4	22.3			
C	x	207.2	212.4	212.0			
C		43.1	45.7	47.4			
C		16	11.1	16.1			
C		75.6	72.1	74.4			
C		27.9	27.7	28.3			
C		10.1	12.3	11.7			
			Isomer 1	Isomer 2			
sDP4+ (H data)			-	-			
sDP4+ (C data)			0.13%		99.87%		
sDP4+ (all data)			0.13%		99.87%		