

Supporting Information

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A New Antibacterial Diterpene with a Fused 6-5-6-6 Ring System, Trichodermanin I, Isolated from the Soil-Derived Fungus *Trichoderma atroviride* YD-13

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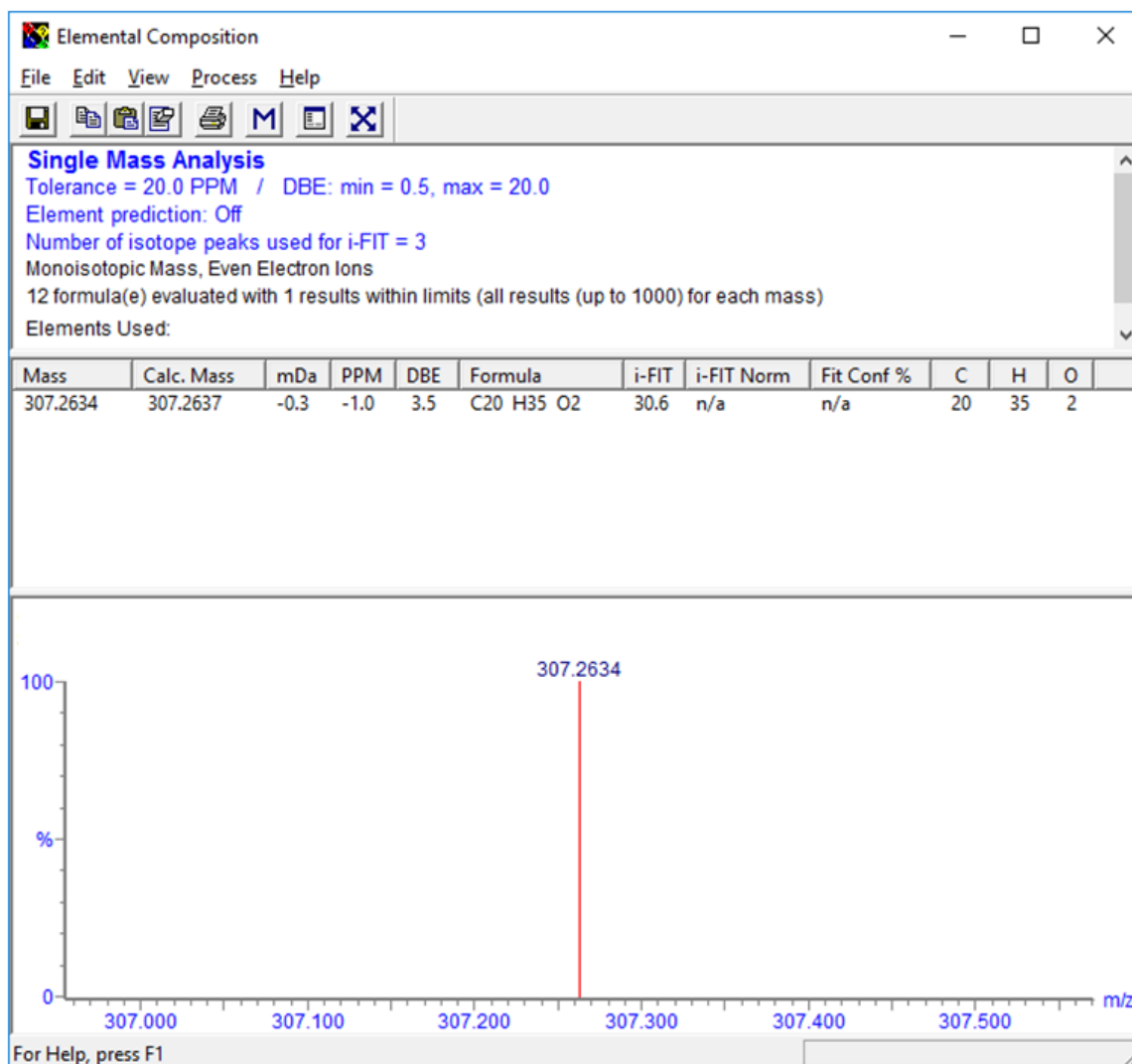


Figure S1: HRESIMS spectrum of **1**

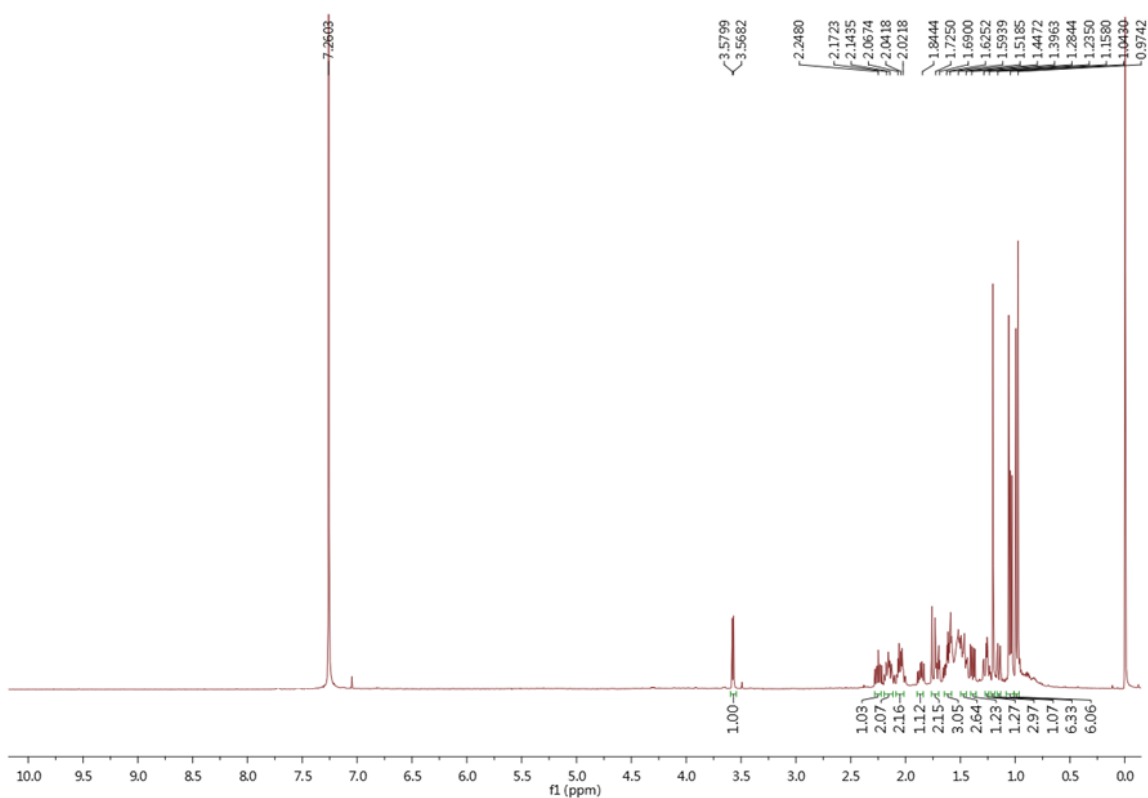


Figure S2: $^1\text{H-NMR}$ (500 MHz, CDCl_3) spectrum of **1**

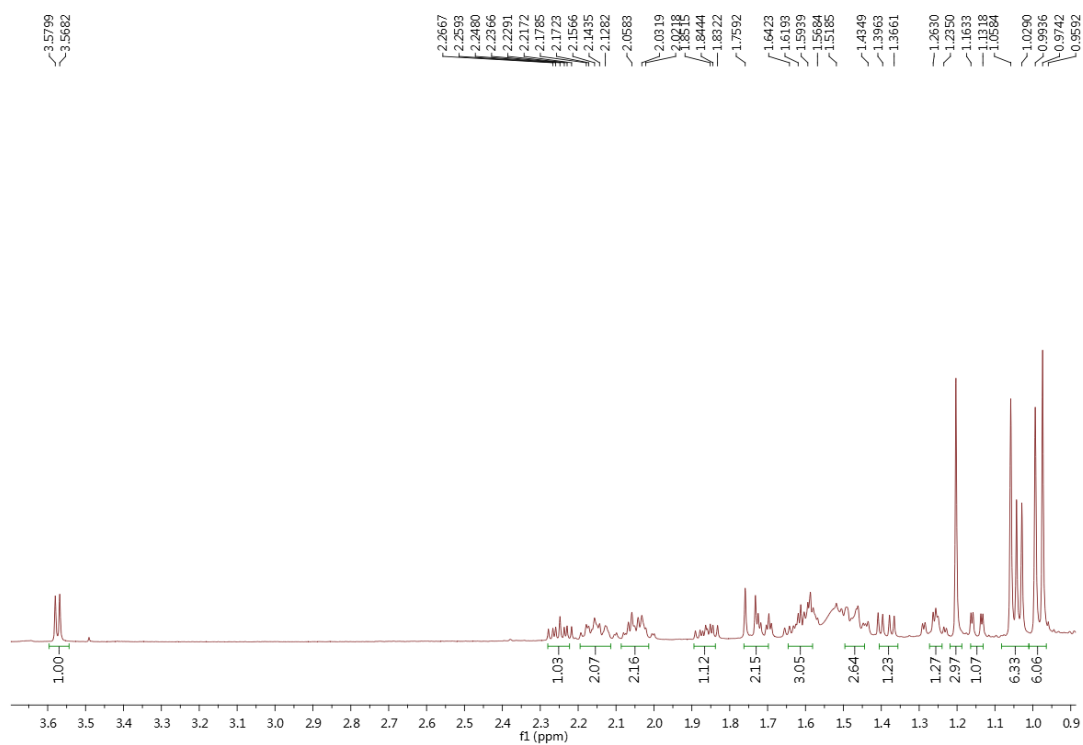


Figure S3: Enlarged $^1\text{H-NMR}$ (500 MHz, CDCl_3) spectrum of **1**

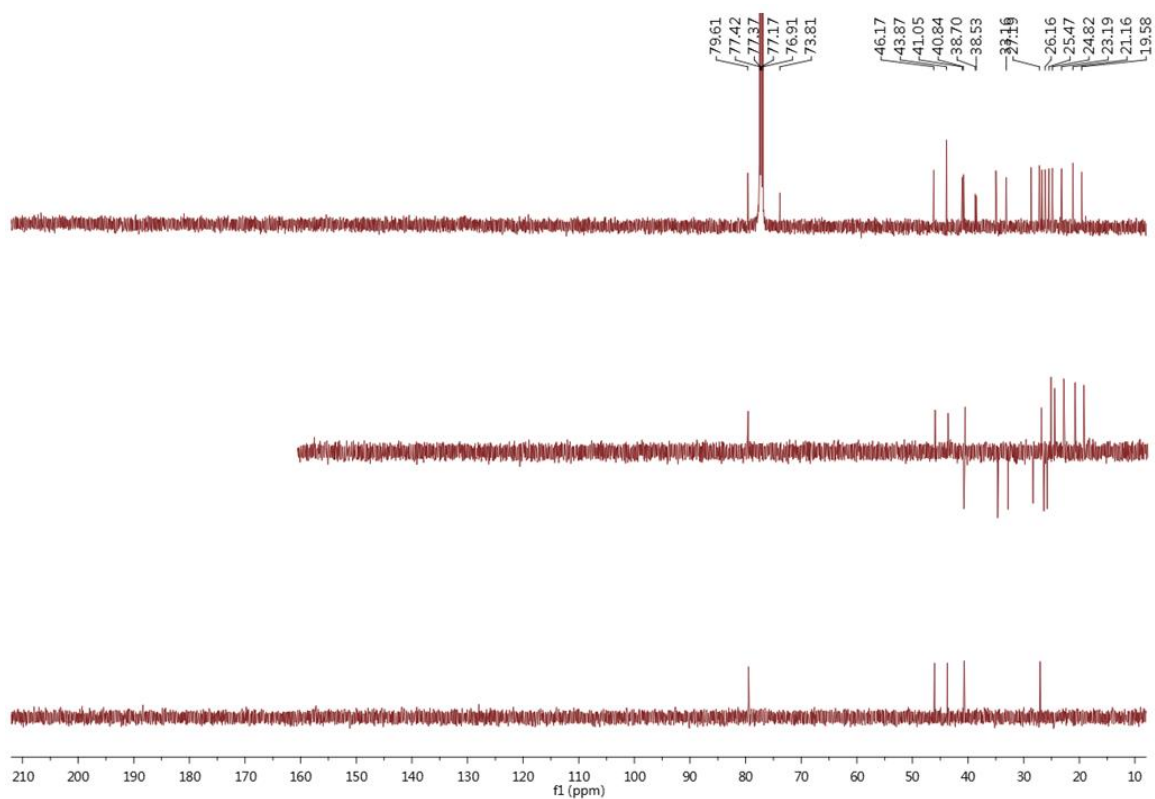


Figure S4: ^{13}C -NMR and DEPT (125 MHz, CDCl_3) spectra of **1**

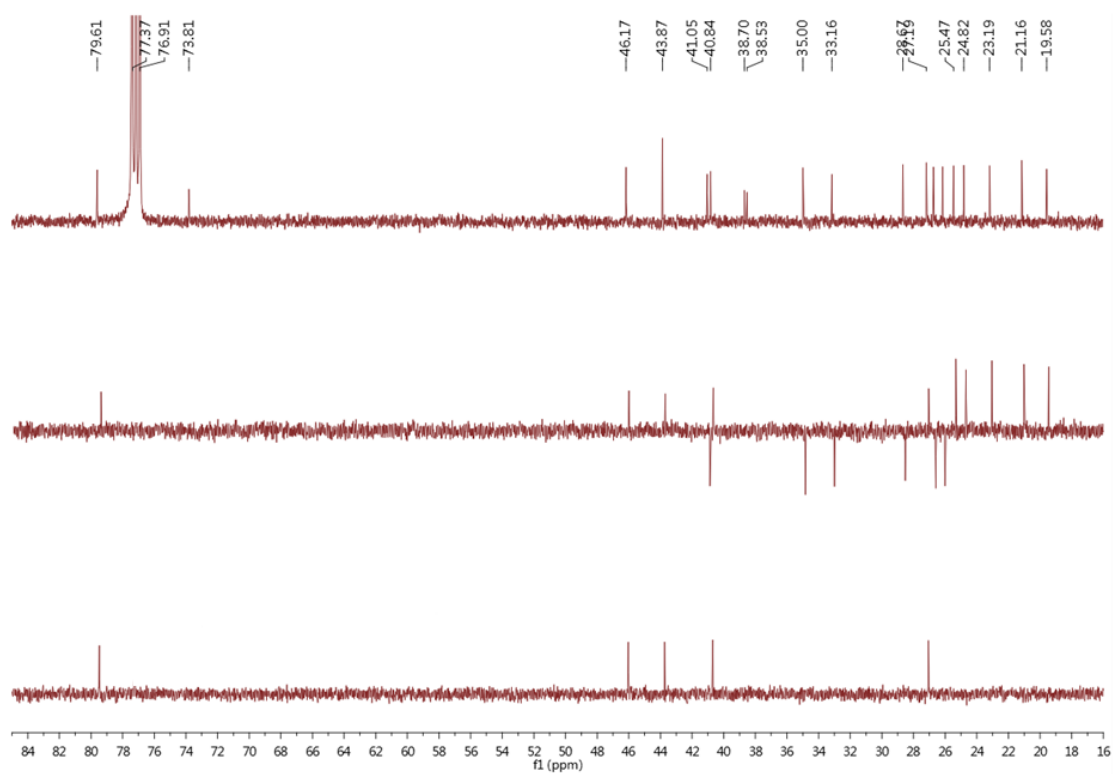


Figure S5: Enlarged ^{13}C -NMR and DEPT (125 MHz, CDCl_3) spectra of **1**

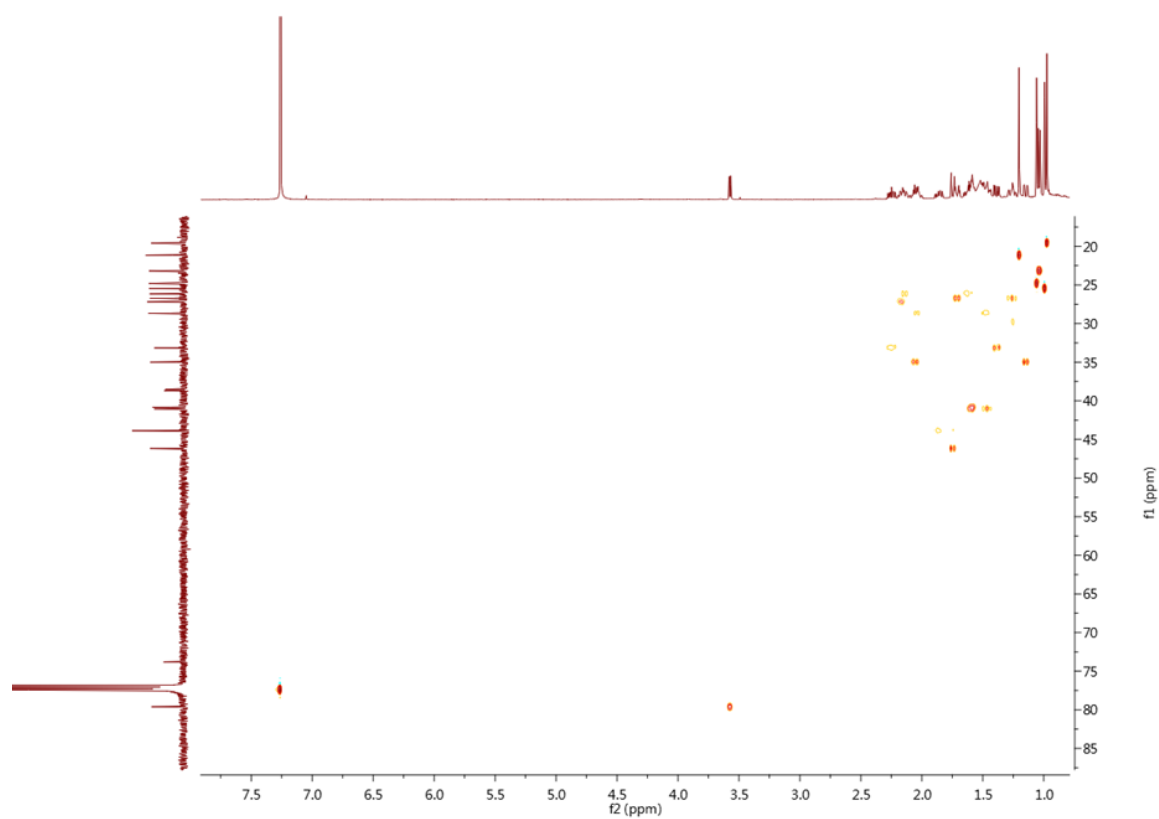


Figure S6: HSQC spectrum of **1**

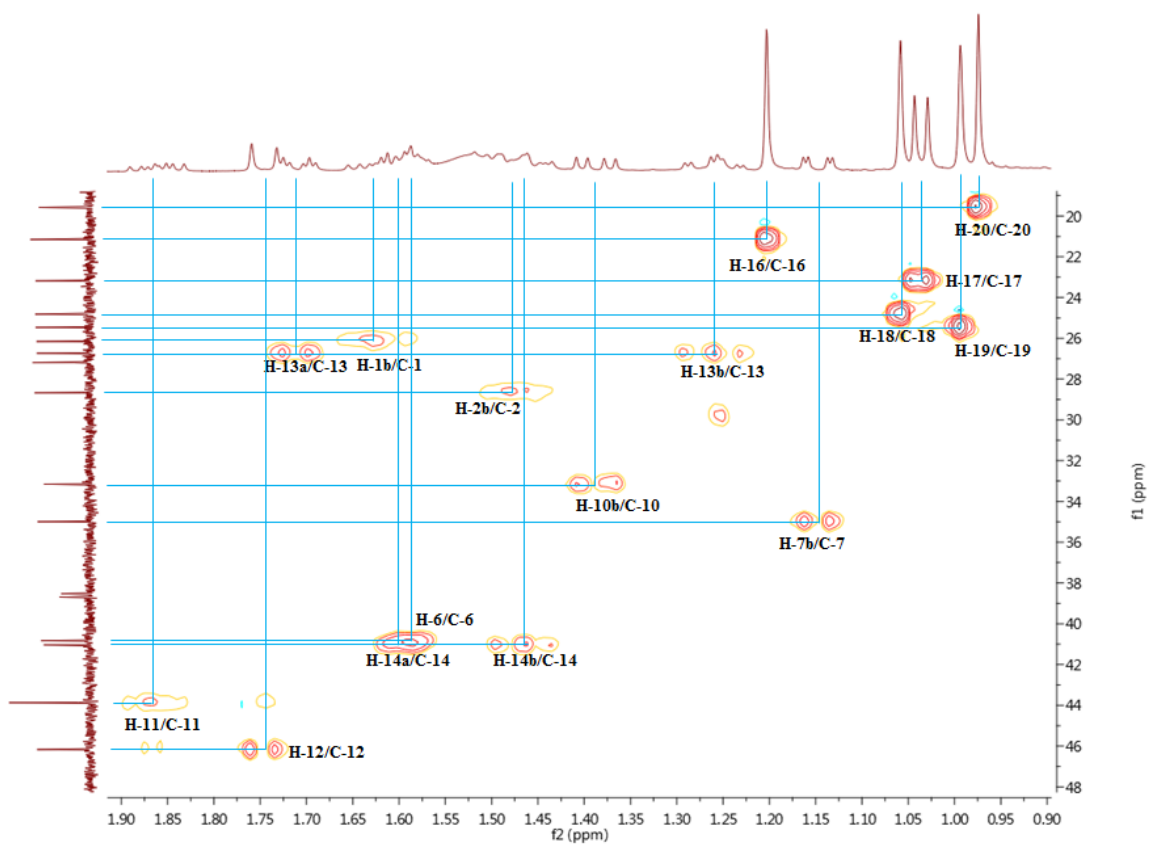


Figure S7: Enlarged HSQC spectrum of **1**

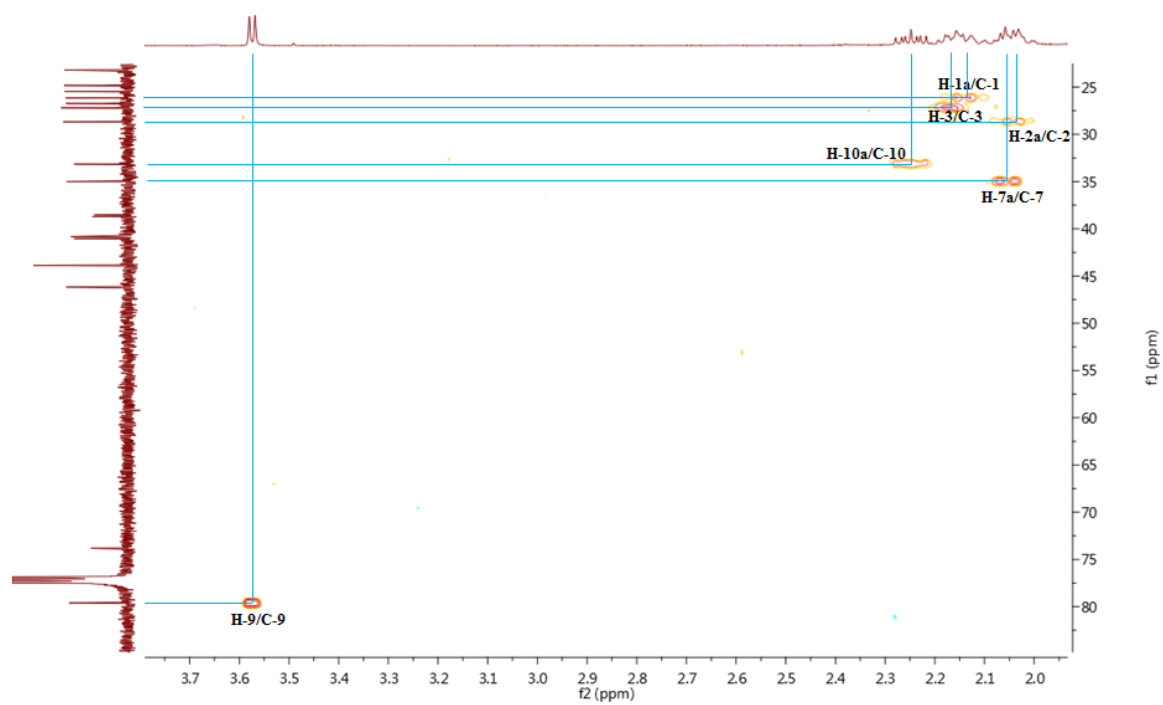


Figure S8: Enlarged HSQC spectrum of **1**

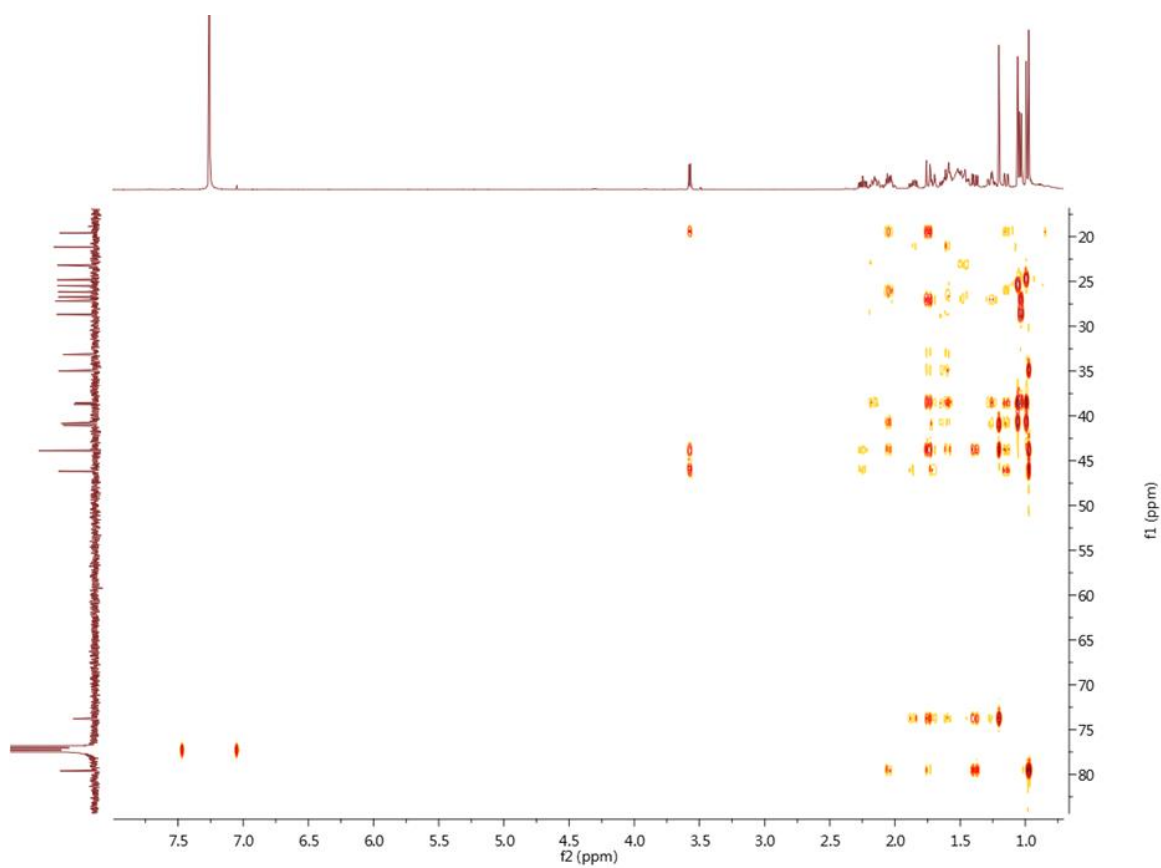


Figure S9: HMBC spectrum of **1**

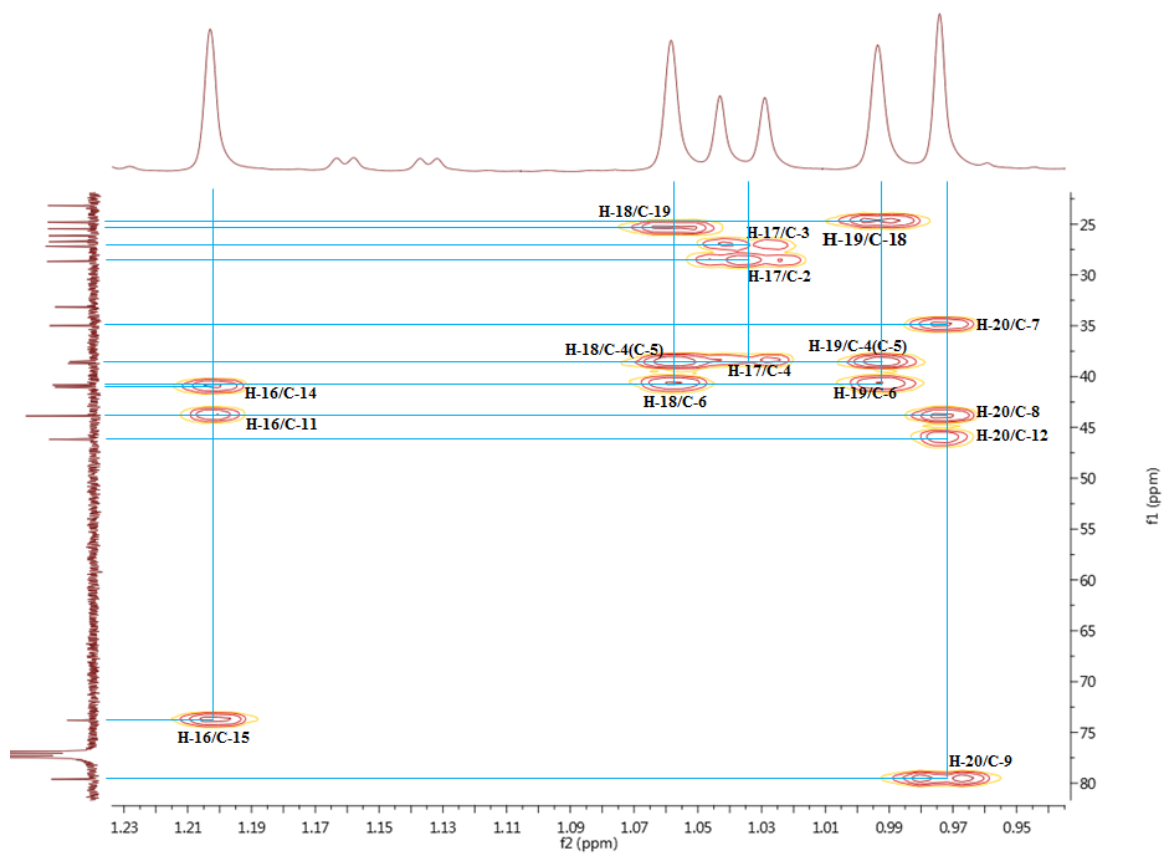


Figure S10: Enlarged HMBC spectrum of **1**

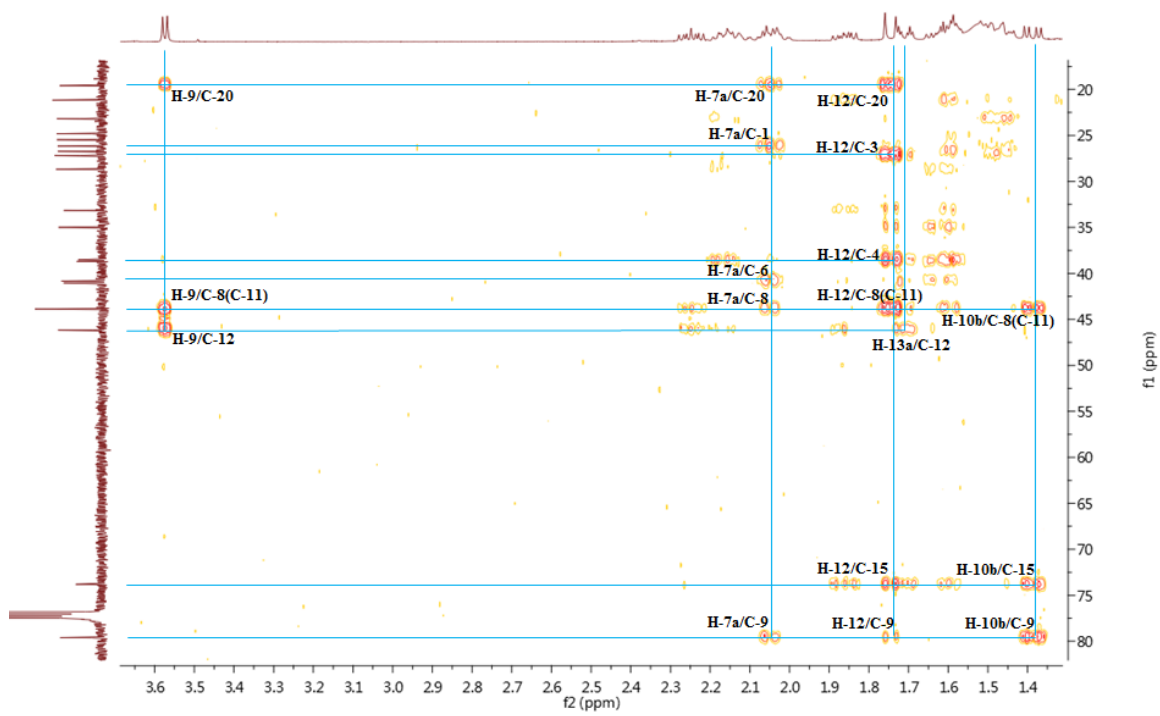


Figure S11: Enlarged HMBC spectrum of **1**

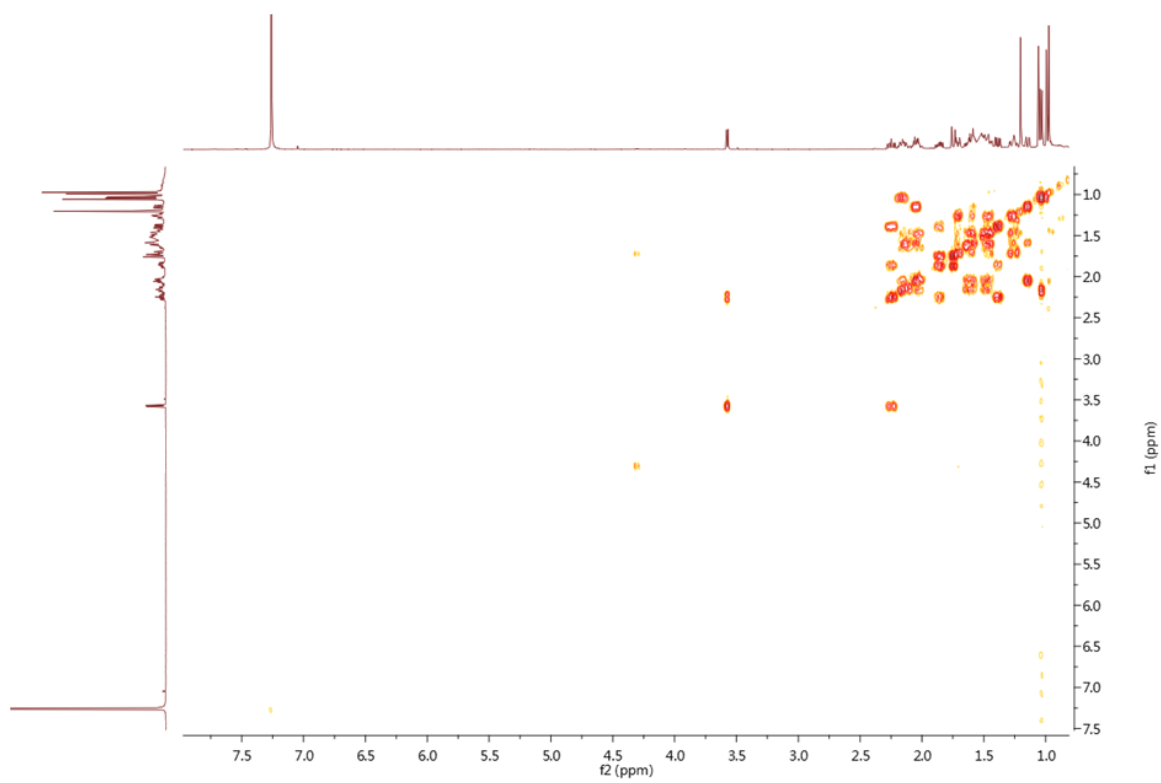


Figure S12: ^1H - ^1H COSY spectrum of **1**

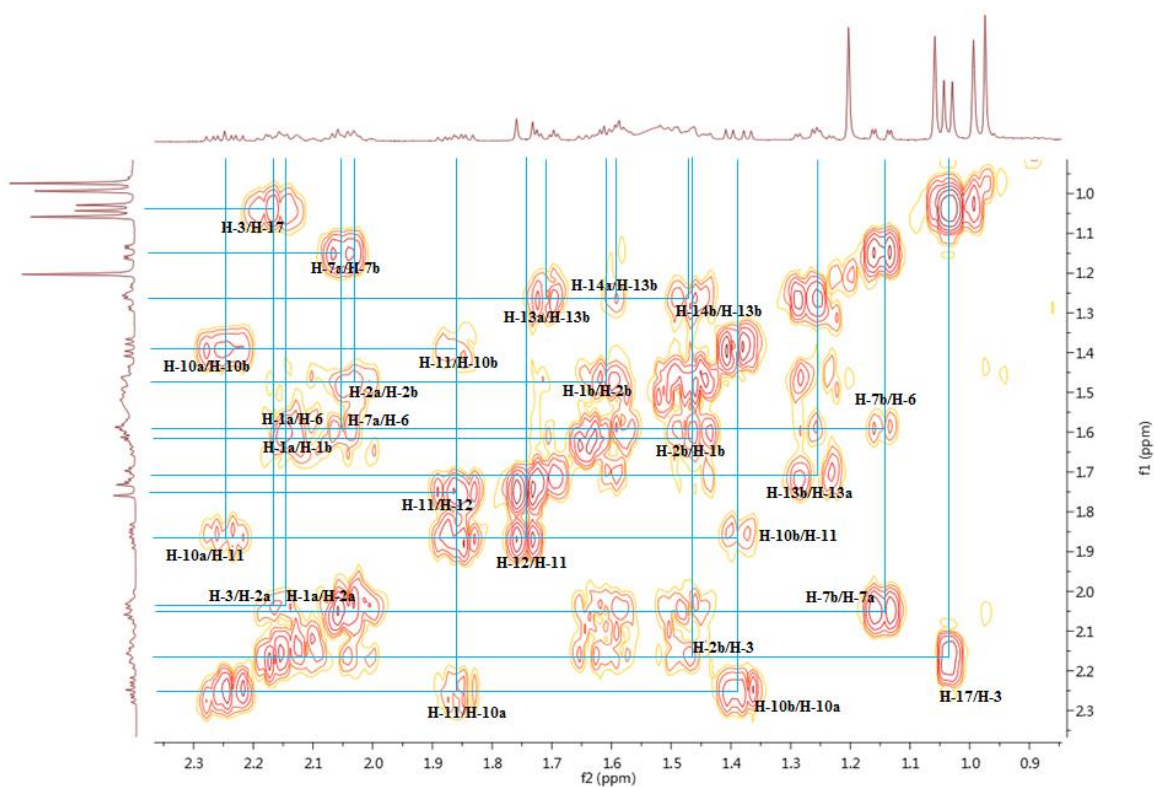


Figure S13: Enlarged ^1H - ^1H COSY spectrum of **1**

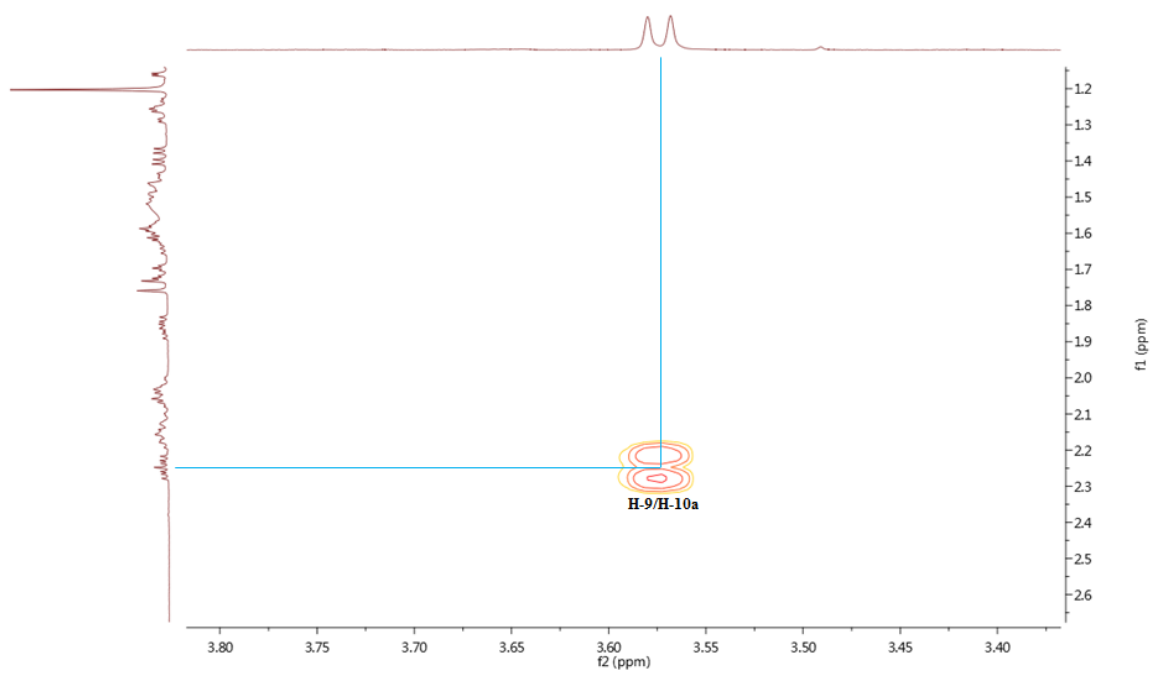


Figure S14: Enlarged ^1H - ^1H COSY spectrum of **1**

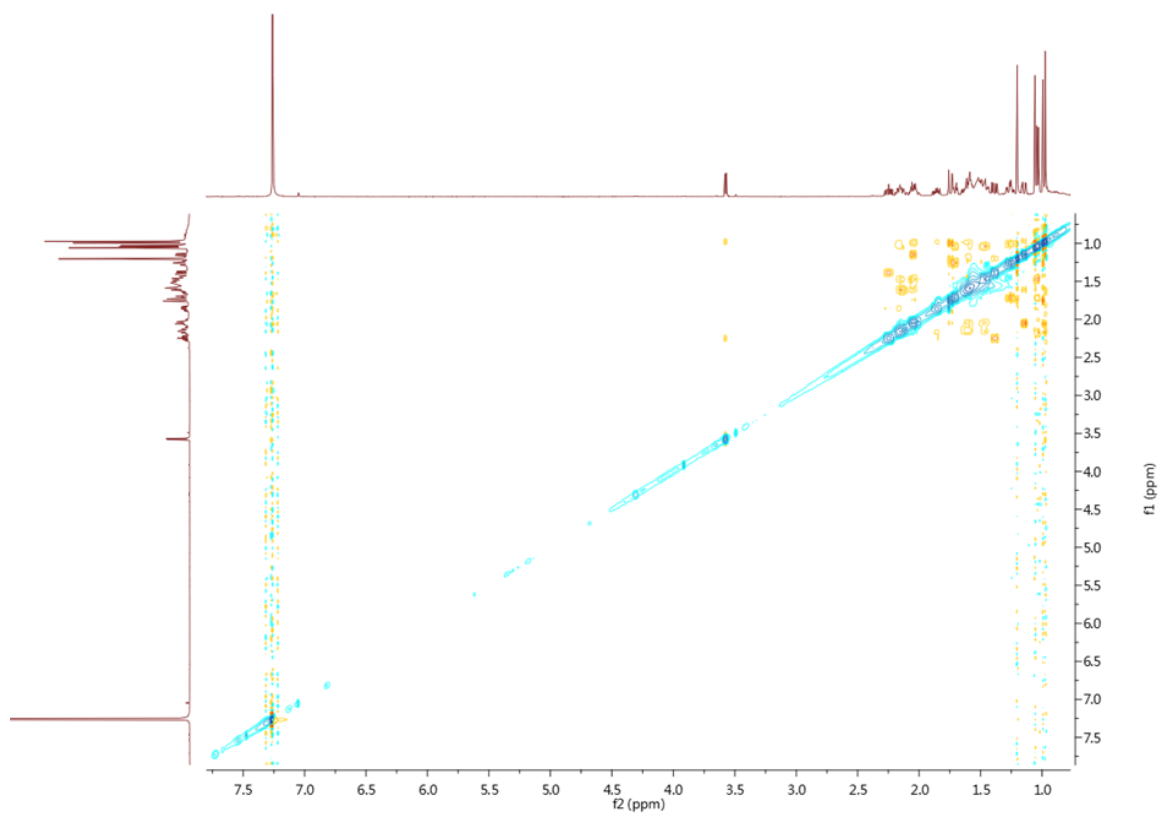


Figure S15: NOESY spectrum of **1**

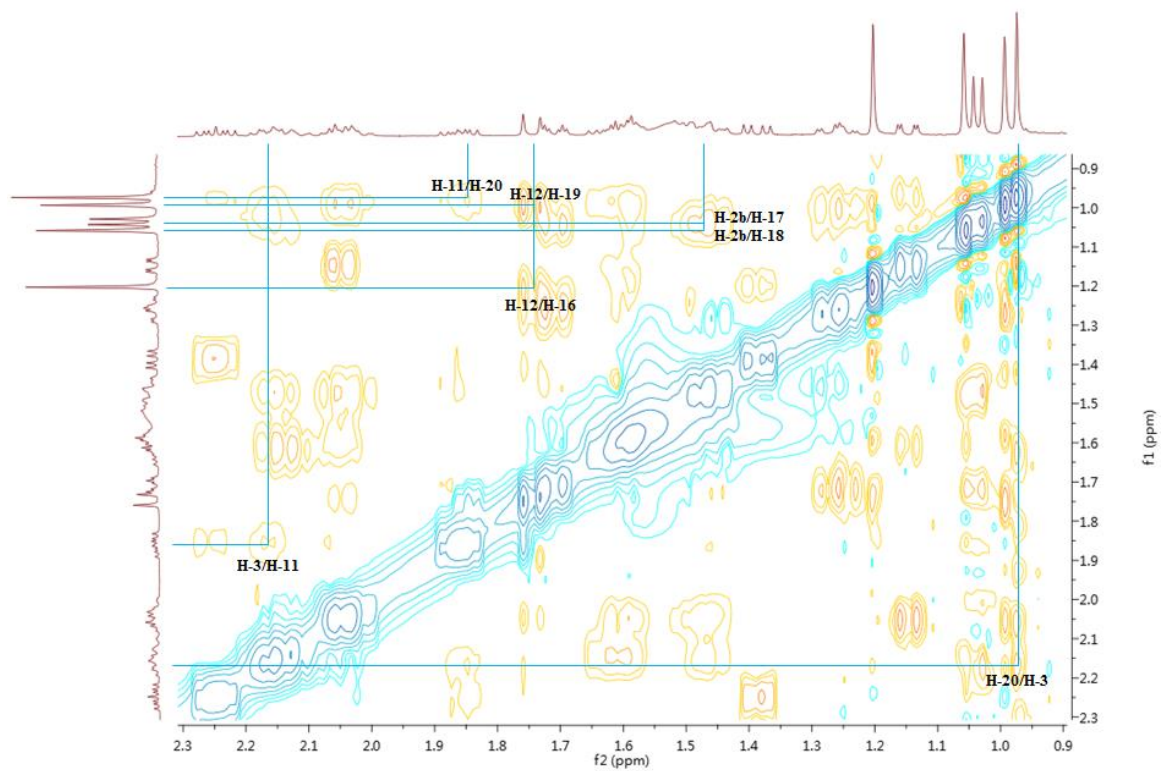


Figure S16: Enlarged NOESY spectrum of **1**

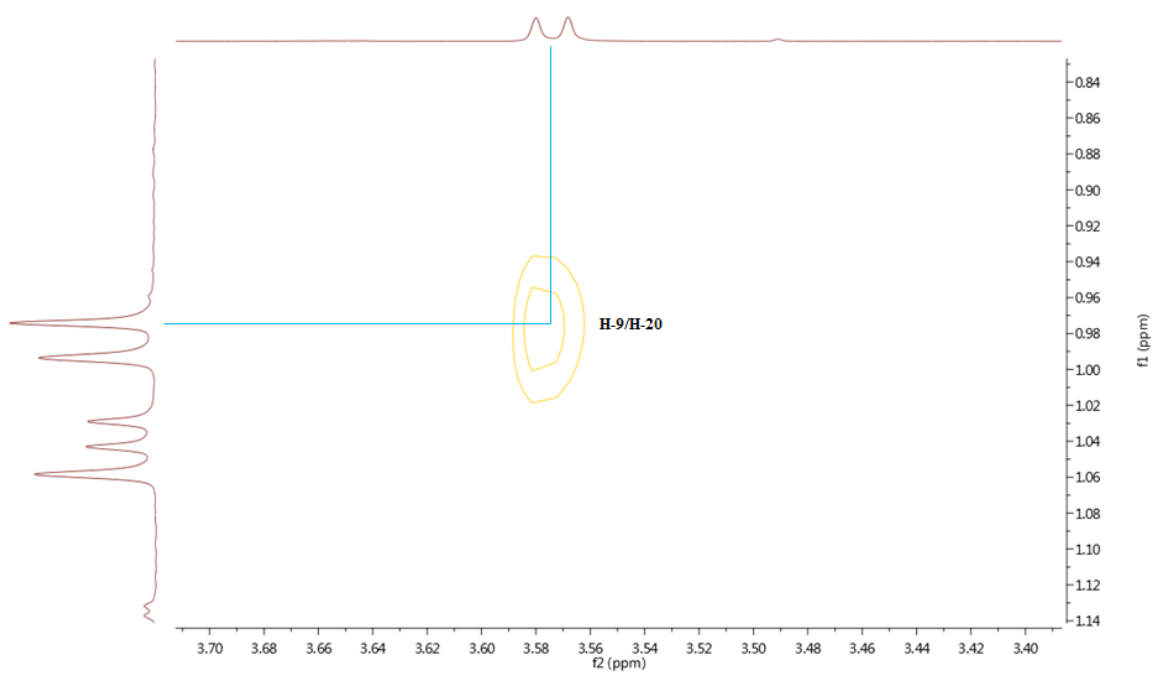




Figure S17: Enlarged NOESY spectrum of **1**

Substances search for drawn structure

References Reactions Suppliers   Save

Structure Match

As Drawn (0)

Substructure (0)

Similarity (198K)

Chemscape Analysis

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Filter Behavior

Filter by Exclude

Search Within Results

Similarity

- 95-98 (1)
- 90-94 (18)
- 85-89 (362)
- 80-84 (1,791)
- 75-79 (6,366)

Filtering: Similarity: 3 Selected Number of Components: 1 [Clear All Filters](#)

381 Results

Sort: Relevance View: Partial

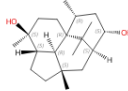
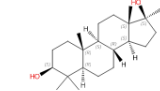
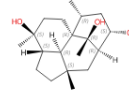

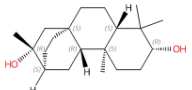
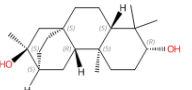
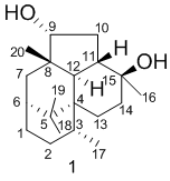
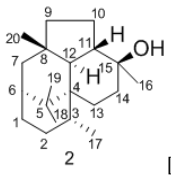
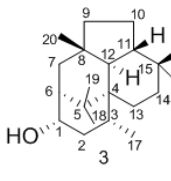
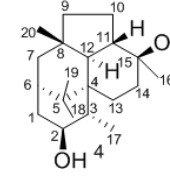
<p><input type="checkbox"/> 1 98</p> <p>1355394-77-2</p>  <p>Absolute stereochemistry shown, Rotation (+)</p> <p>$C_{20}H_{34}O_2$ (2a<i>S</i>,3<i>S</i>,5a<i>R</i>,6<i>R</i>,8<i>S</i>,9<i>S</i>,10a<i>S</i>,10b<i>R</i>)-Dodecahydro-3,6,10a,11,11-pentamethyl-3<i>H</i>-5a,9-me...</p> <p>7 References 53K Reactions 0 Suppliers</p>	<p><input type="checkbox"/> 2 92</p> <p>95221-82-2</p>  <p>Absolute stereochemistry shown</p> <p>$C_{22}H_{38}O_2$ 5<i>α</i>-Androstane-3<i>β</i>,17<i>β</i>-diol, 4,4,17-trimethyl-</p> <p>5 References 0 Reactions 0 Suppliers</p>	<p><input type="checkbox"/> 3 92</p> <p>2933872-44-5</p>  <p>Absolute stereochemistry shown, Rotation (+)</p> <p>$C_{19}H_{32}O_3$</p> <p>1 Reference 8,824 Reactions 0 Suppliers</p>
<p><input type="checkbox"/> 4 92</p> <p>87013-77-2</p>  <p>Absolute stereochemistry shown</p>	<p><input type="checkbox"/> 5 92</p> <p>1818243-49-0</p>  <p>Relative stereochemistry shown</p>	<p><input type="checkbox"/> 6 92</p> <p>1818243-48-9</p>  <p>Relative stereochemistry shown</p>

Figure S18: Scifinder search results of 1

Table S1: ^1H and ^{13}C NMR data of compounds **1-4**

Pos								
	δ_{H} (<i>J</i> in Hz)	δ_{C} , type	δ_{H} (<i>J</i> in Hz)	δ_{C} , type	δ_{H} (<i>J</i> in Hz)	δ_{C} , type	δ_{H} (<i>J</i> in Hz)	δ_{C} , type
1a	2.14, m	26.2, CH ₂	2.09, m	25.7, CH ₂	4.18, dd	72.7, CH	2.54, ddd	36.5, CH ₂
1b	1.63, m		1.61, m				1.68, m	
2a	2.04, m	28.7, CH ₂	2.00, dddd	28.8, CH ₂	2.61, ddd	42.3, CH ₂	4.30, ddd	74.2, CH
2b	1.47, m		1.46, m		1.43, ddd			
3	2.17, m	27.2, CH	2.11, m	26.6, CH	2.01, ddq	27.1, CH	1.98, qd	37.9, CH
4		38.5, C		38.8, C		39.3, C		40.8, C
5		38.7, C		38.7, C		39.6, C		39.0, C
6	1.59, m	40.8, CH	1.48, m	41.1, CH	1.42, m	52.8, CH	1.62, m	41.8, CH
7a	2.05, m	35.0, CH ₂	1.67, dd	43.0, CH ₂	1.74, dd	41.6, CH ₂	1.71, dd	42.5, CH ₂
7b	1.15, dd		1.49, m		1.64, dd		1.56, dd	
8		43.9, C		39.2, C		39.8, C		39.7, C
9a	3.57, d	79.6, CH	1.41, d	43.9, CH ₂	1.43, m	43.9, CH ₂	1.02, m	43.9, CH ₂
9b			1.01, d		1.02, m		1.43, m	
10a	2.25, ddd	33.2, CH ₂	1.78, m	21.6, CH ₂	1.79, m	22.2, CH ₂	1.60, m	21.6, CH ₂
10b	1.39, dd		1.56, m		1.58, m		1.81, m	
11	1.86, ddd	43.9, CH	1.87, ddd	44.4, CH	1.81, ddd	44.6, CH	1.85, m	44.4, CH
12	1.74, d	46.2, CH	1.27, d	52.0, CH	1.28, d	52.2, CH	1.30, d	51.9, CH
13a	1.71, dt	26.7, CH ₂	1.68, m	26.4, CH ₂	1.74, ddd	26.8, CH ₂	1.18, ddd	26.4, CH ₂
13b	1.26, ddd		1.21, ddd		1.24, ddd		1.68, m	
14a	1.59, m	41.0, CH ₂	1.57, ddd	40.8, CH ₂	1.62, ddd	41.4, CH ₂	1.62, m	41.1, CH ₂
14b	1.46, m		1.44, m		1.45, m		1.46, ddd	
15		73.8, C		73.9, C		73.8, C		73.8, C
16	1.20, s	21.2, CH ₃	1.17, s	20.5, CH ₃	1.18, s	21.3, CH ₃	1.18, s	20.4, CH ₃
17	1.04, d	23.2, CH ₃	1.02, d	22.9, CH ₃	1.07, d	23.1, CH ₃	1.19, s	20.4, CH ₃
18	1.06, s	24.8, CH ₃	1.05, s	24.6, CH ₃	0.98, s	26.6, CH ₃	0.95, s	25.3, CH ₃
19	0.99, s	25.5, CH ₃	0.94, s	25.6, CH ₃	1.13, s	25.6, CH ₃	0.96, s	25.4, CH ₃
20	0.97, s	19.6, CH ₃	1.05, s	19.9, CH ₃	0.91, d	20.5, CH ₃	1.13, s	20.3, CH ₃