

Supporting Information

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Cytotoxic Diterpenoids from *Scoparia dulcis*

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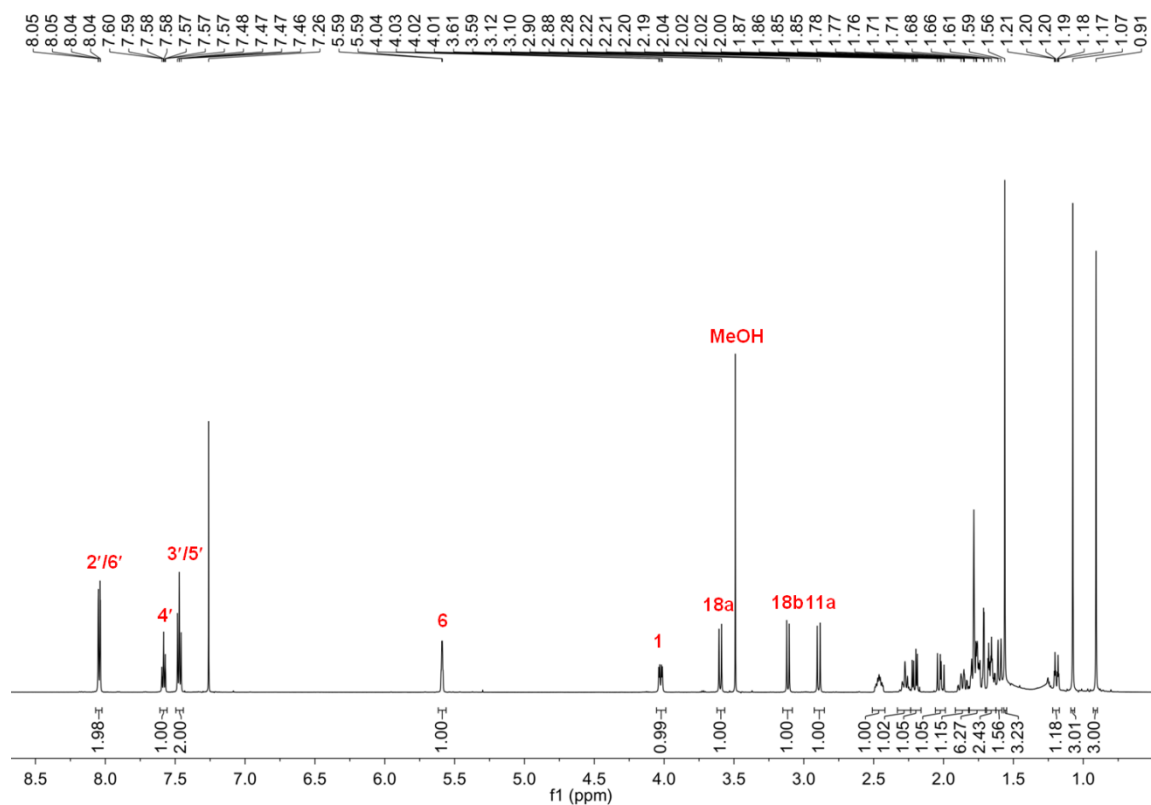


Figure S1: ^1H NMR spectrum (full) of **1** in CDCl_3 .

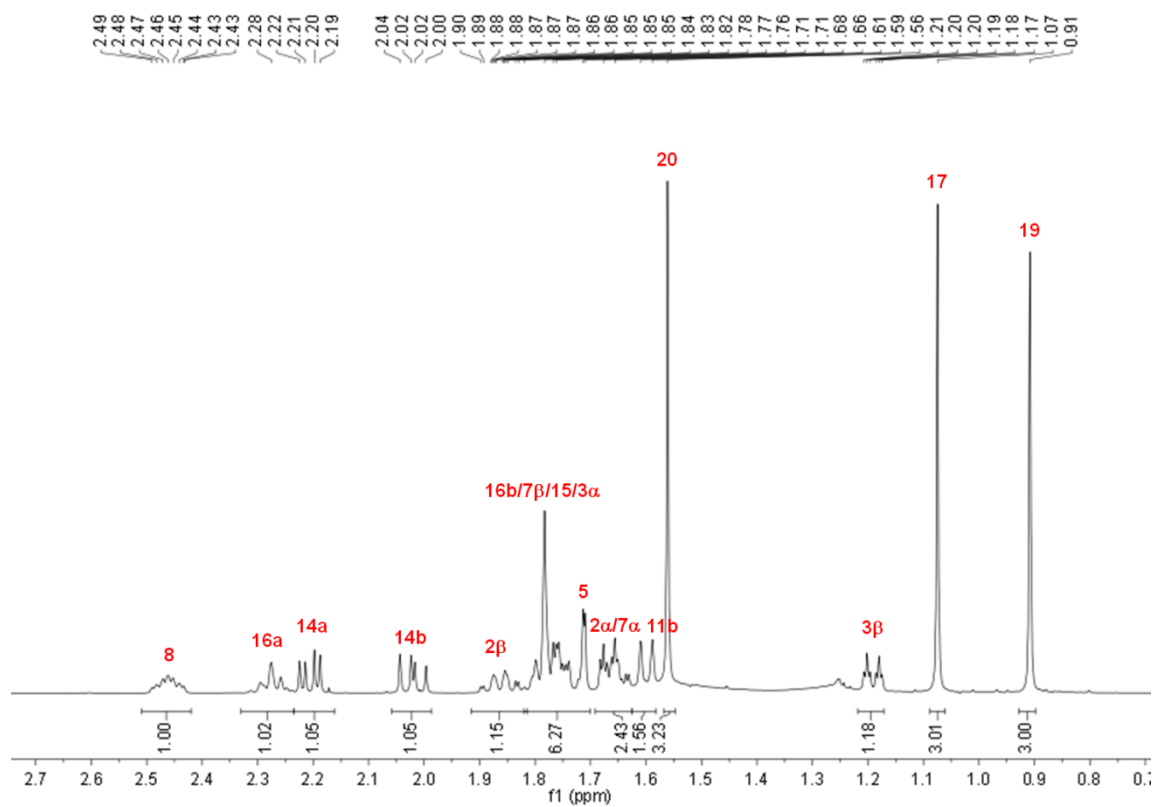


Figure S2: ^1H NMR spectrum (magnified) of **1** in CDCl_3 .

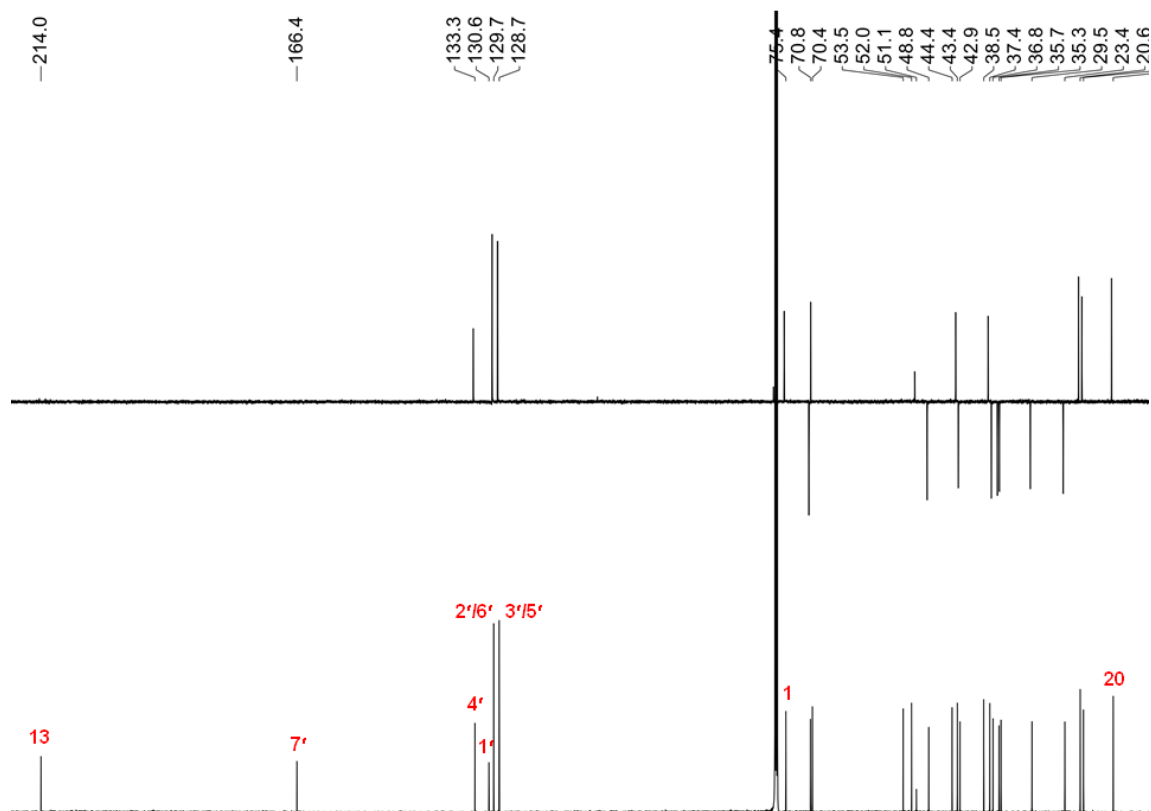


Figure S3: ^{13}C and DEPT 135 NMR spectra (full) of **1** in CDCl_3 .

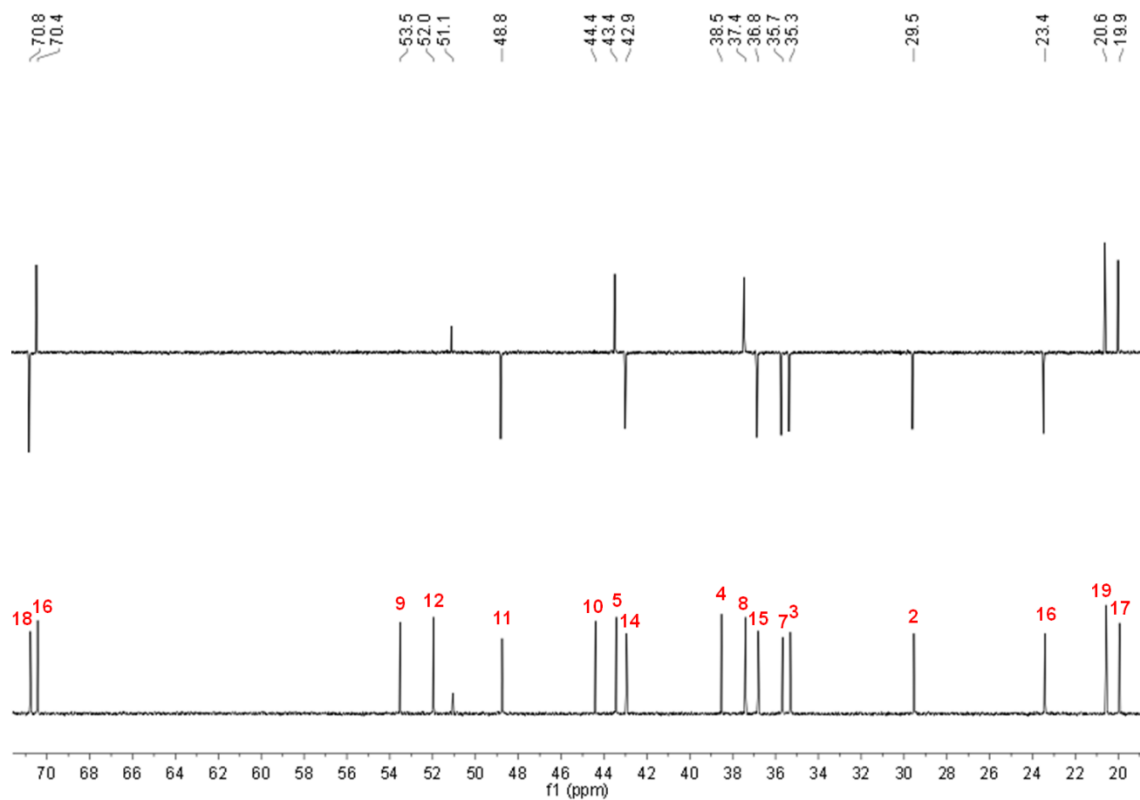


Figure S4: ^{13}C and DEPT 135 NMR spectra (manifold) of **1** in CDCl_3 .

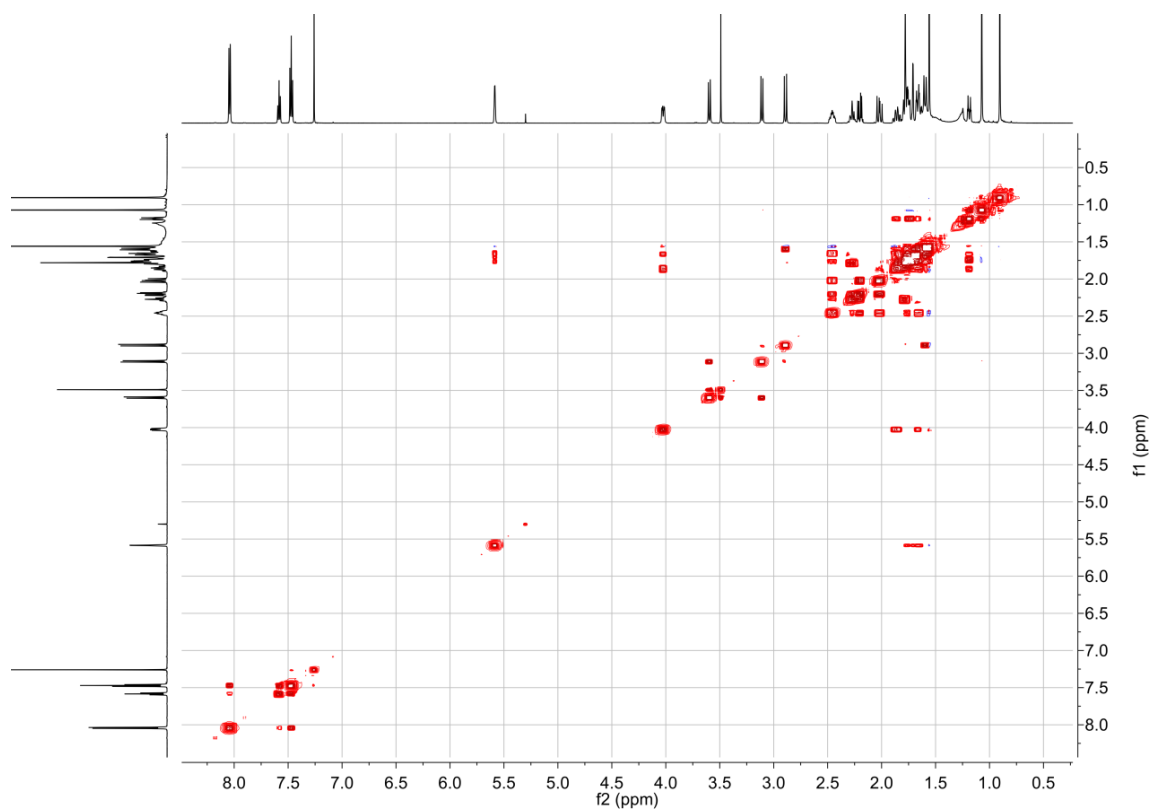


Figure S5: ^1H - ^1H COSY spectrum (full) of **1** in CDCl_3 .

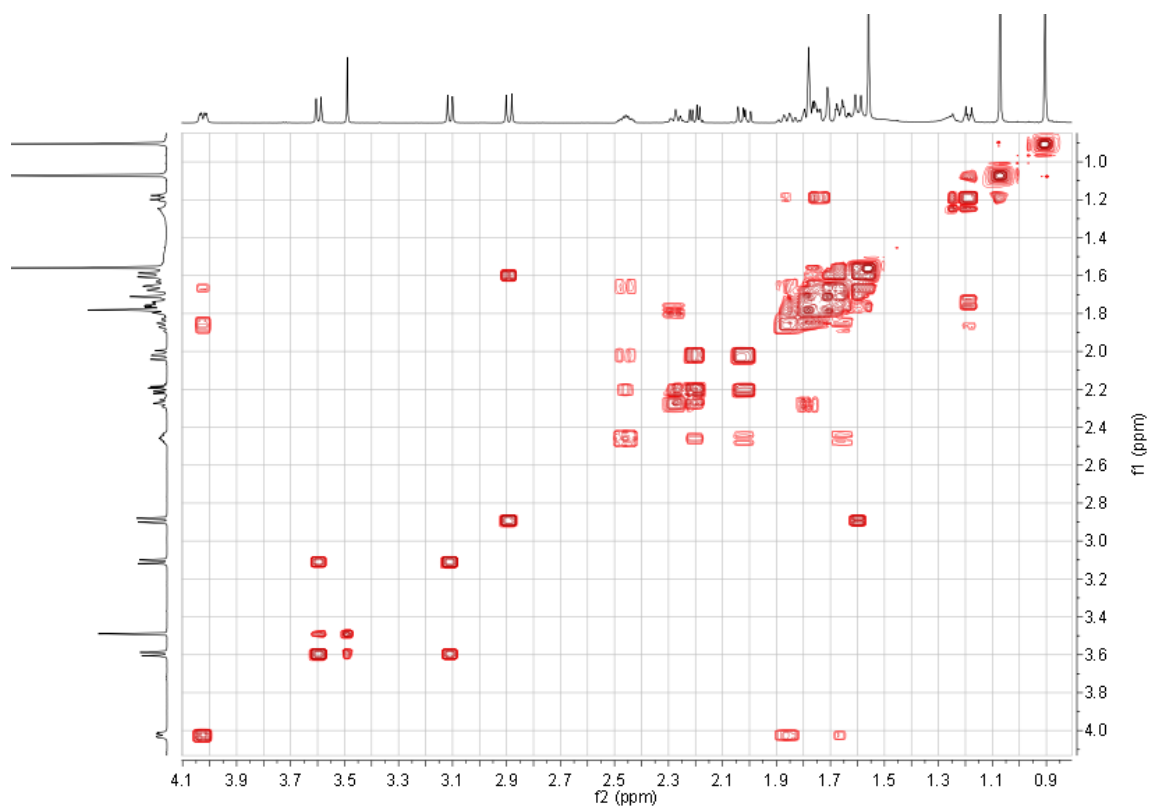


Figure S6: ^1H - ^1H COSY spectrum (magnified) of **1** in CDCl_3 .

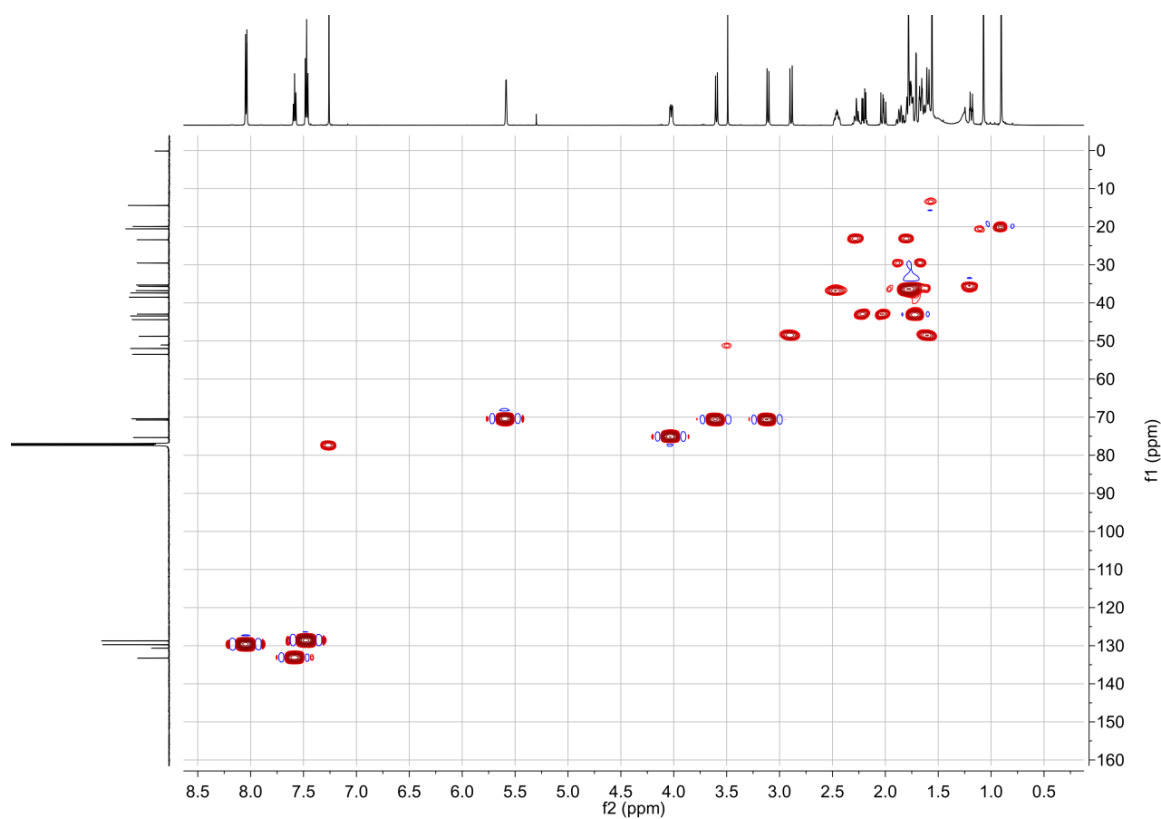


Figure S7: HSQC spectrum (full) of **1** in CDCl₃.

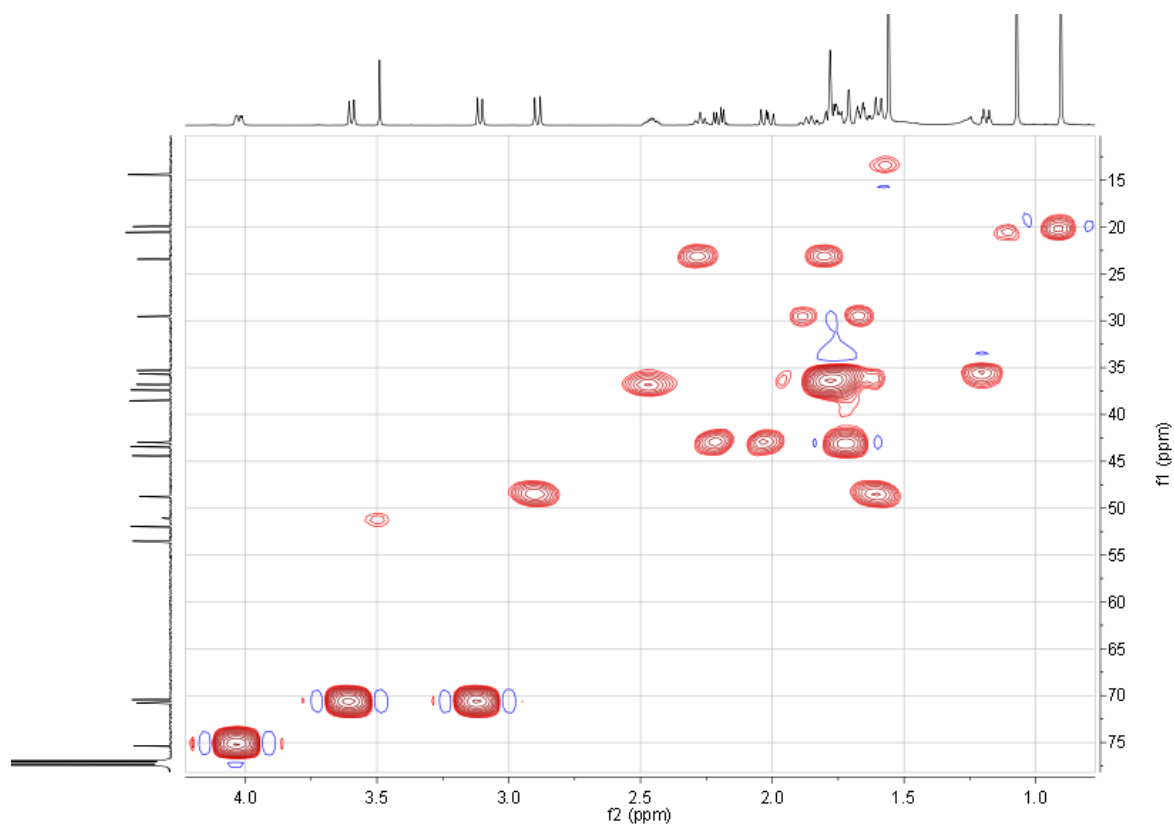


Figure S8: HSQC spectrum (magnified) of **1** in CDCl₃.

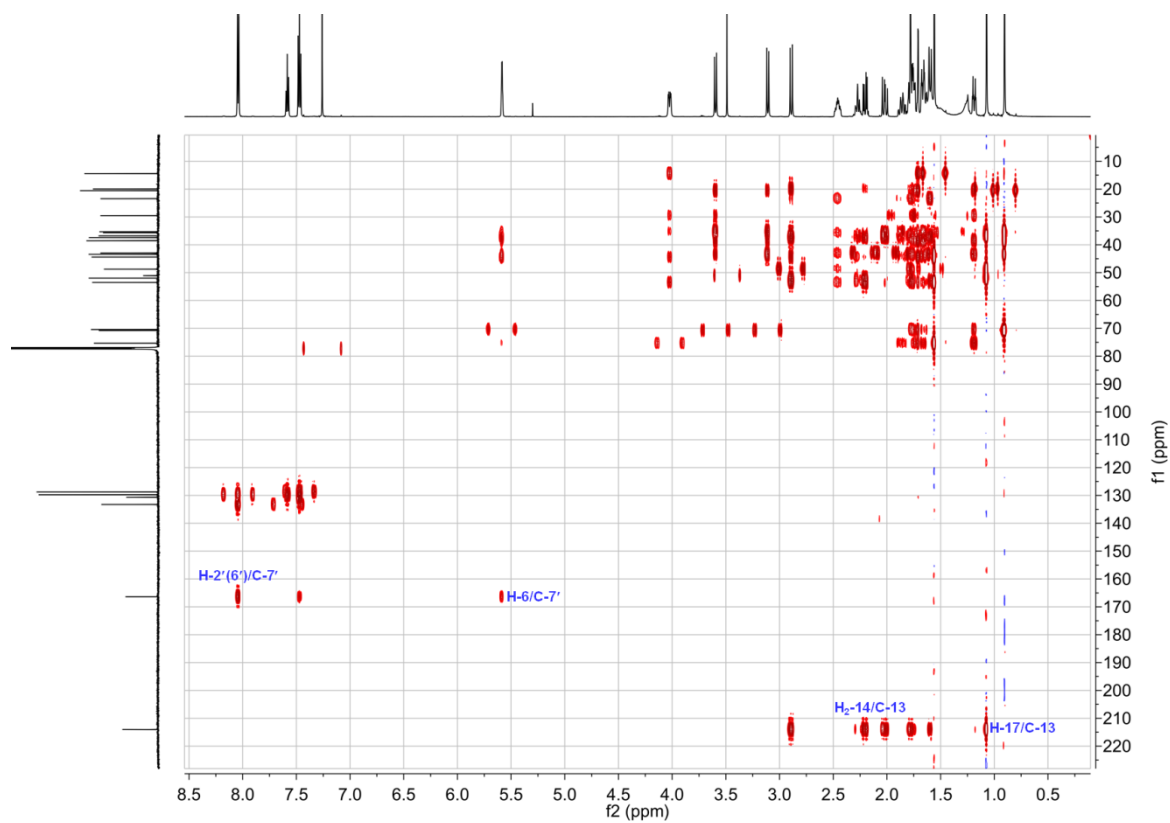


Figure S9: HMBC spectrum (full) of **1** in CDCl₃.

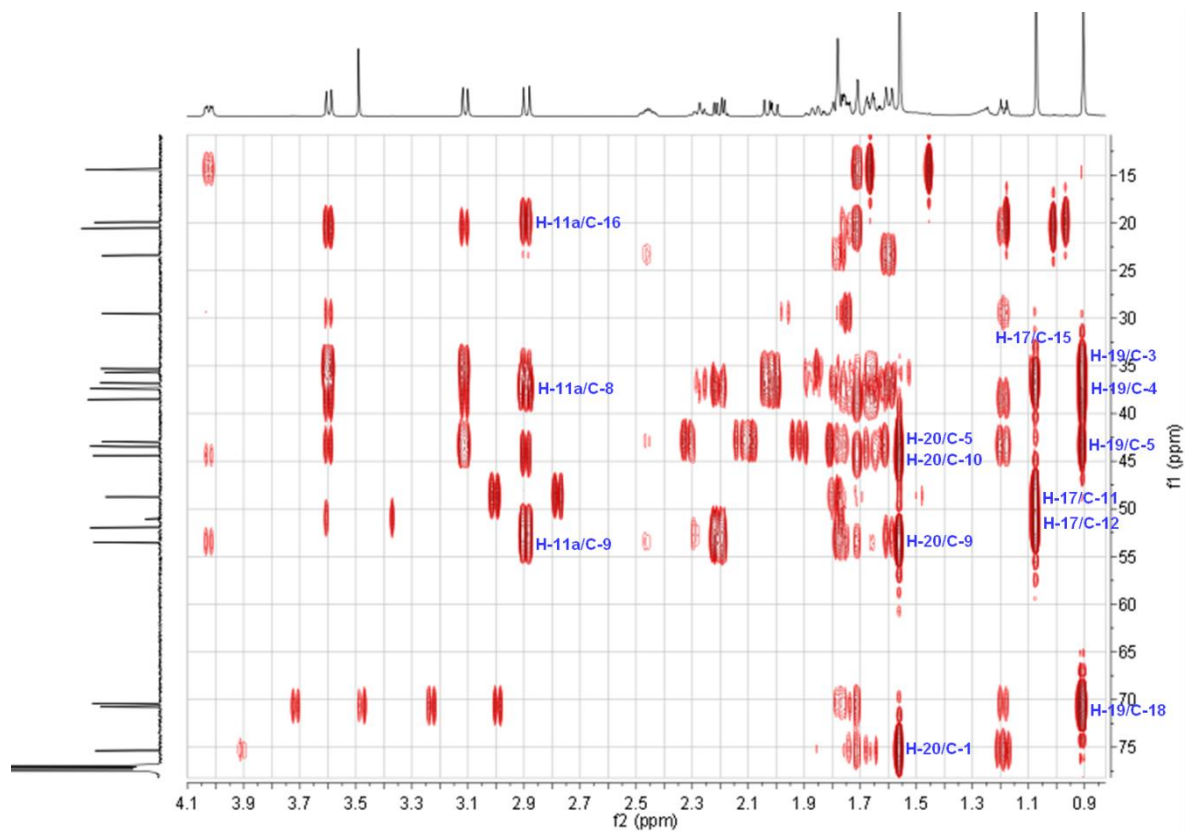


Figure S10: HMBC spectrum (magnified) of **1** in CDCl₃.

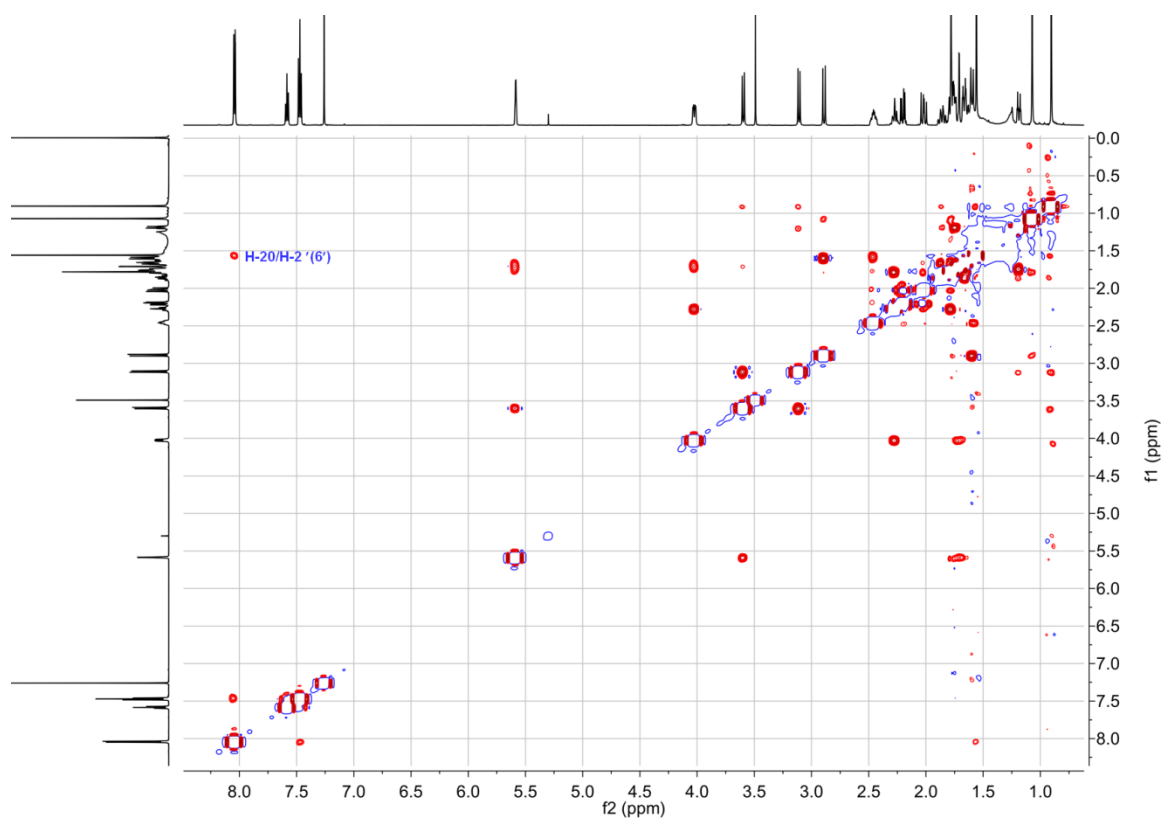


Figure S11: NOESY spectrum (full) of **1** in CDCl₃.

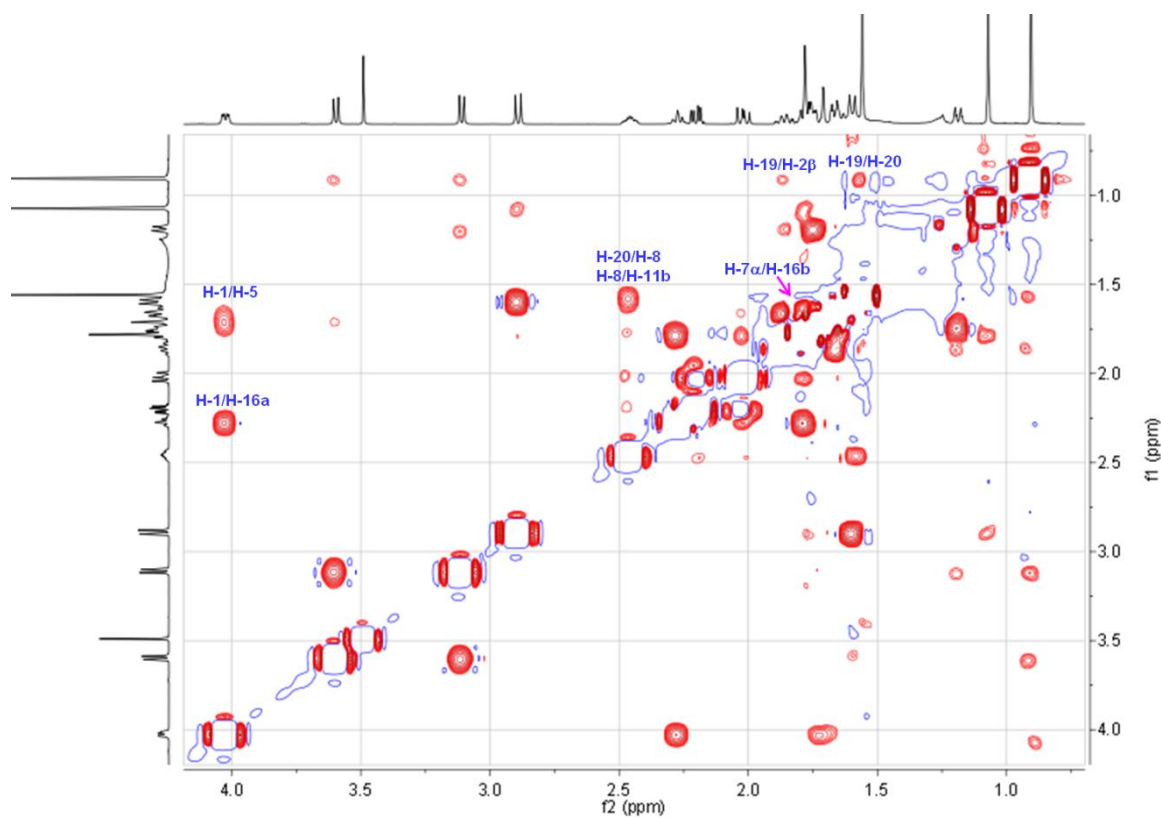


Figure S12: NOESY spectrum (magnified) of **1** in CDCl₃.

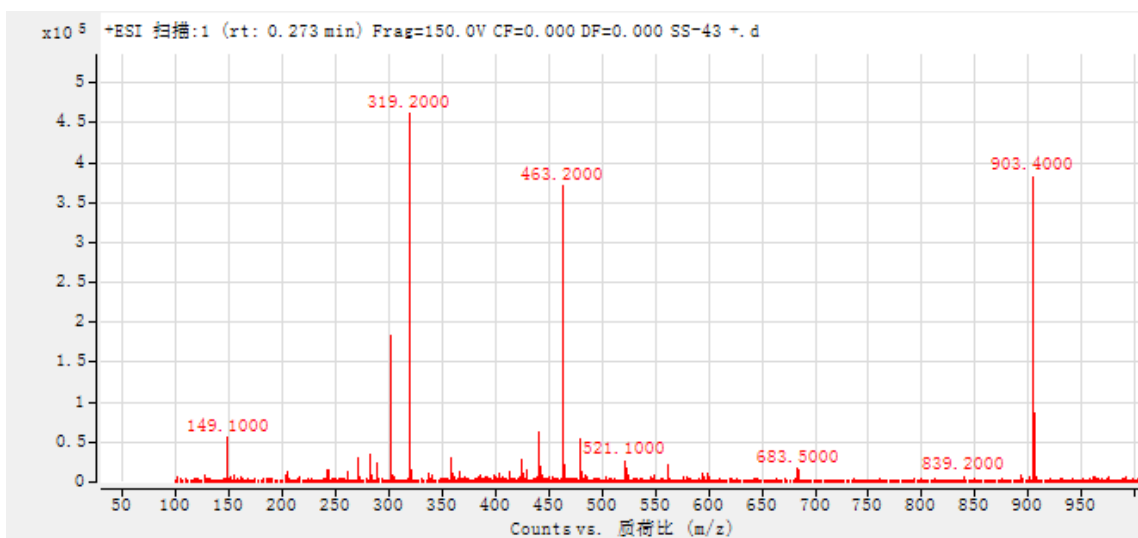


Figure S13: (+)-ESIMS spectrum of 1.

Sample Name	SS-43	Position	P2-C3	Instrument Name	Instrument 1
User Name		Inj Vol	1	InjPosition	
Sample Type	Sample	IRM Calibration Status	Success	Data Filename	SS-43.d
ACQ Method	wss-isocratic elution-Positive.m	Comment		Acquired Time	4/7/2021 10:44:09 AM

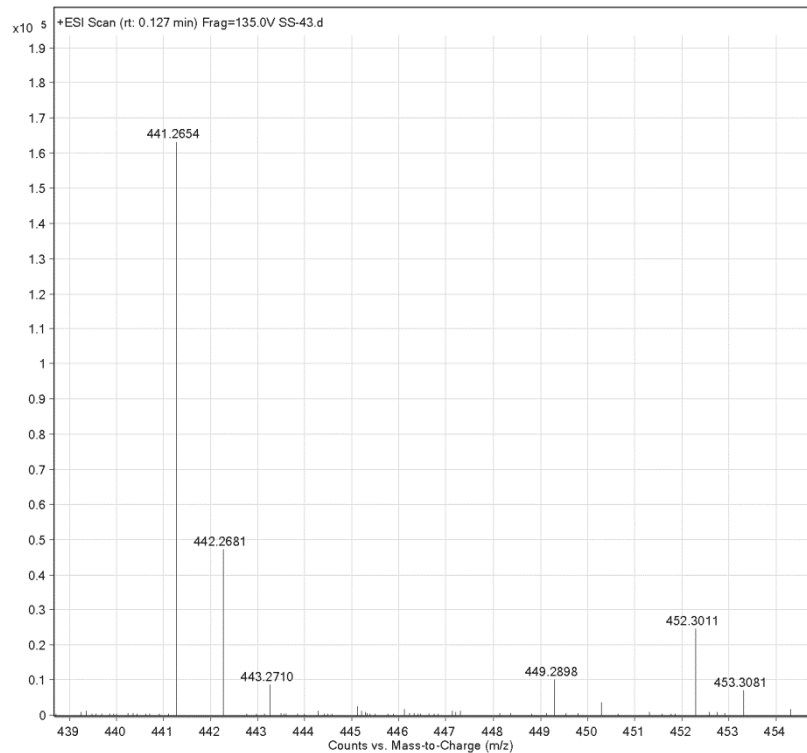


Figure S14: (+)-HR-ESIMS spectrum of 1.

(1) “Exact search” resulted in zero hit.

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No candidates available [Return](#)

Chemical Structure exact

SUBSTANCES

No candidates available

(2) “Similarity search” led to four structures with $\geq 95\%$ similarity to compound 1.

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Chemical Structure similarity

SUBSTANCES

Select All Deselect All

1 of 8 Similarity Candidates Selected

Similarity Range	Substances
<input type="checkbox"/> ≥ 99 (most similar)	0
<input checked="" type="checkbox"/> 95-98	4
<input type="checkbox"/> 90-94	27
<input type="checkbox"/> 85-89	46
<input type="checkbox"/> 80-84	369
<input type="checkbox"/> 75-79	2113
<input type="checkbox"/> 70-74	9701
<input type="checkbox"/> 65-69	32385
<input type="checkbox"/> 0-64 (least similar)	90085

Get Substances

(3) The four structures with $\geq 95\%$ similarity to compound 1.

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Chemical Structure similarity > substances (4)

SUBSTANCES

Analyze | Reference | Get Reactions | Get Commercial Sources | Tools

Sort by: Similarity Score

0 of 4 Substances Selected

Score: 97
 1. 57871A-90-6

Score: 96
 2. 136065-26-9

Score: 95
 3. 166920-09-1

Score: 95
 4. 57871A-91-7

Figure S15 displays the SciFinder search report for compound 1. The report shows the chemical structure of compound 1 and four similar structures with their respective scores and CAS numbers. The structures are: 1. 57871A-90-6 (Score: 97), 2. 136065-26-9 (Score: 96), 3. 166920-09-1 (Score: 95), and 4. 57871A-91-7 (Score: 95). The structures are shown in a grid format, with the first structure being the most similar and the last being the least similar.

Figure S15: SciFinder search report for compound 1.