

Supporting Information

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A New Ergosterol-Type Steroid Isolated from the *Nicotiana tabacum*-Derived Endophytic Fungus *Aspergillus* sp. TE-65L

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Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
443.3145	443.3161	-1.6	-3.6	7.5	547.2	n/a	n/a	C ₂₈ H ₄₃ O ₄

AO-20

20210119-014 32 (0.092) AM2 (Ar,22000.0,0.00,0.00); ABS; Cm (32.44-61.116)

1: TOF MS ES-
2.18e6

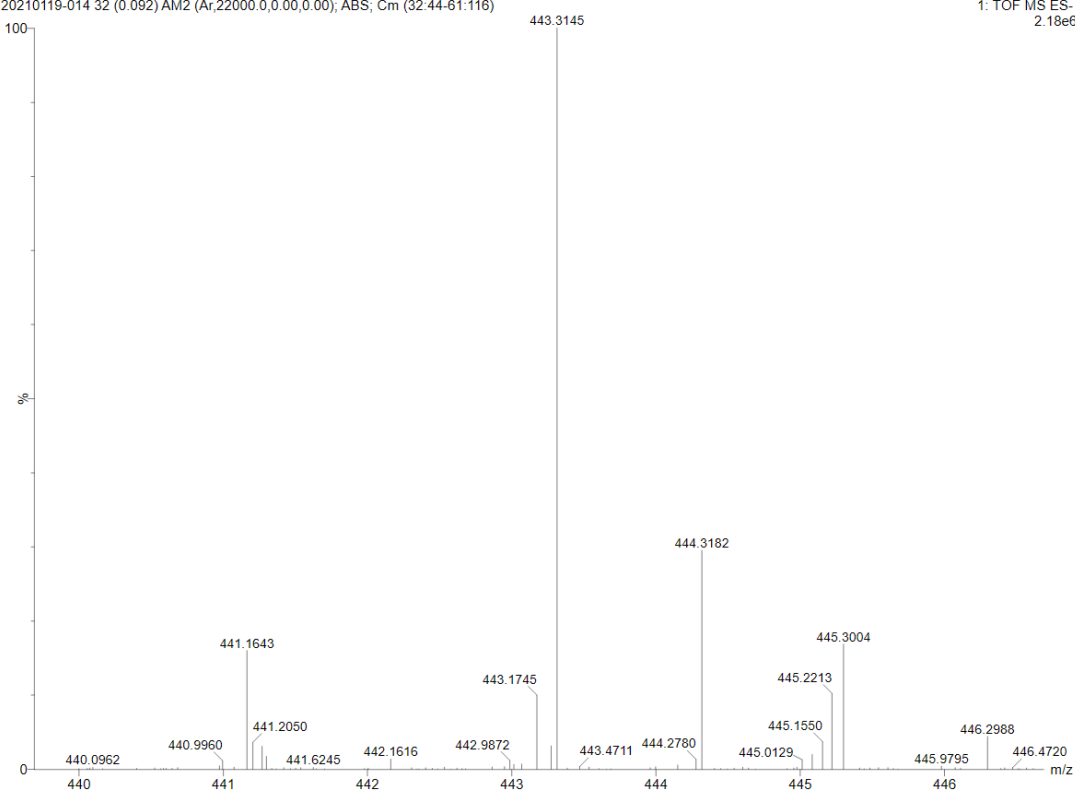


Figure S1: HRESIMS spectrum of 1

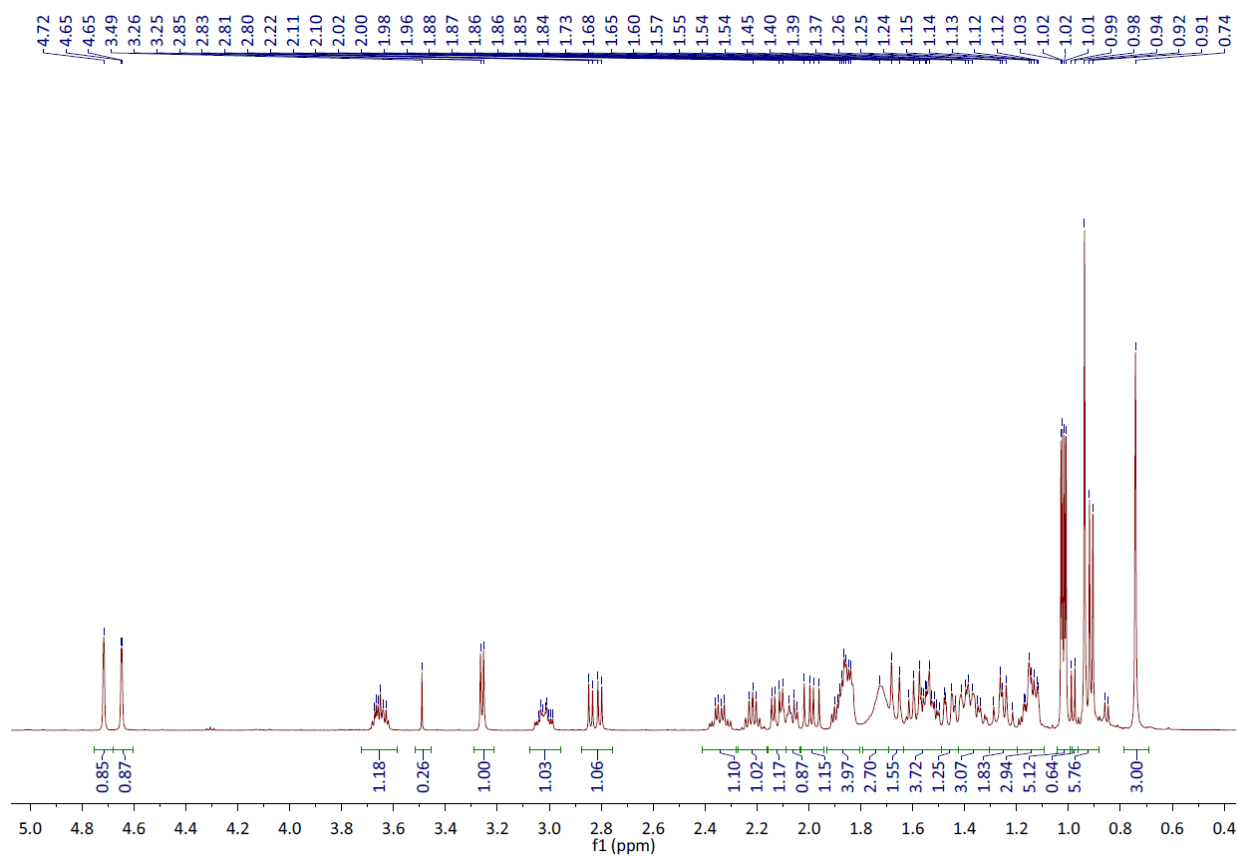


Figure S2: ^1H NMR (500 MHz, CDCl_3) spectrum of **1**

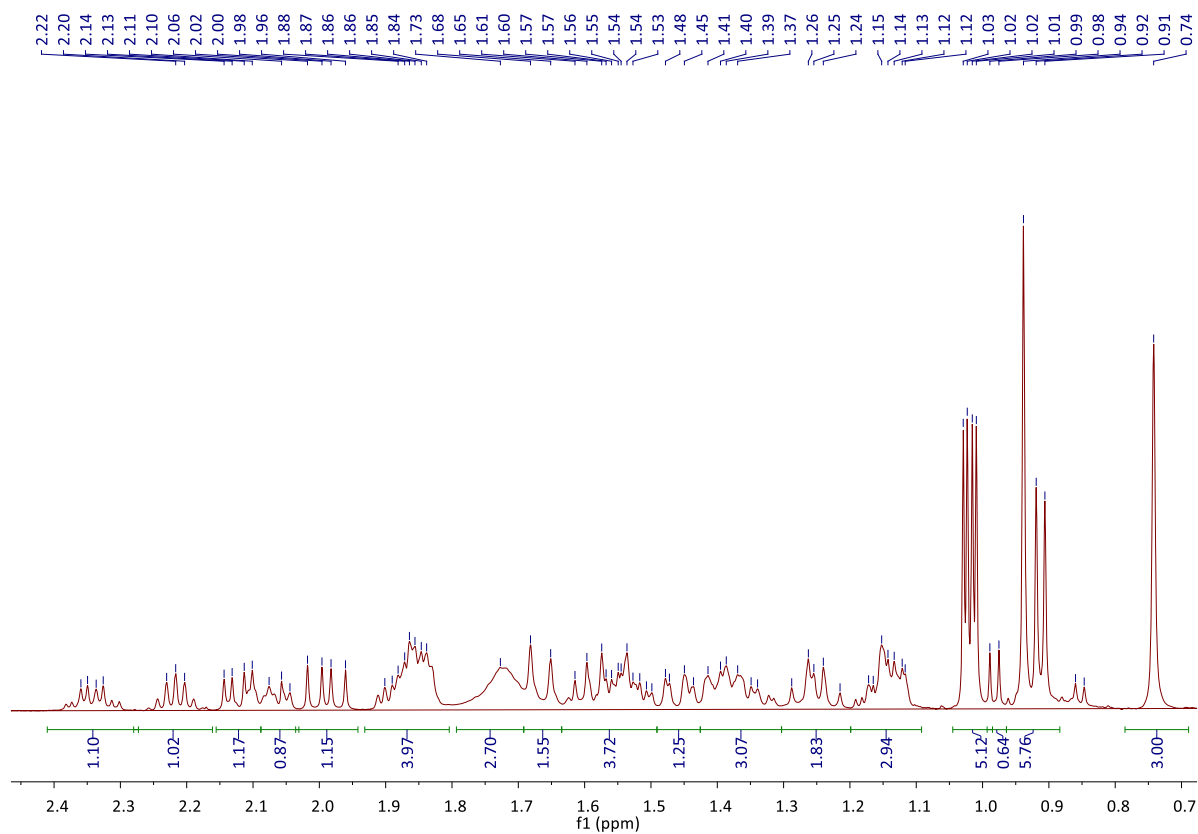


Figure S3: Enlarged ^1H NMR (500 MHz, CDCl_3) spectrum of **1**

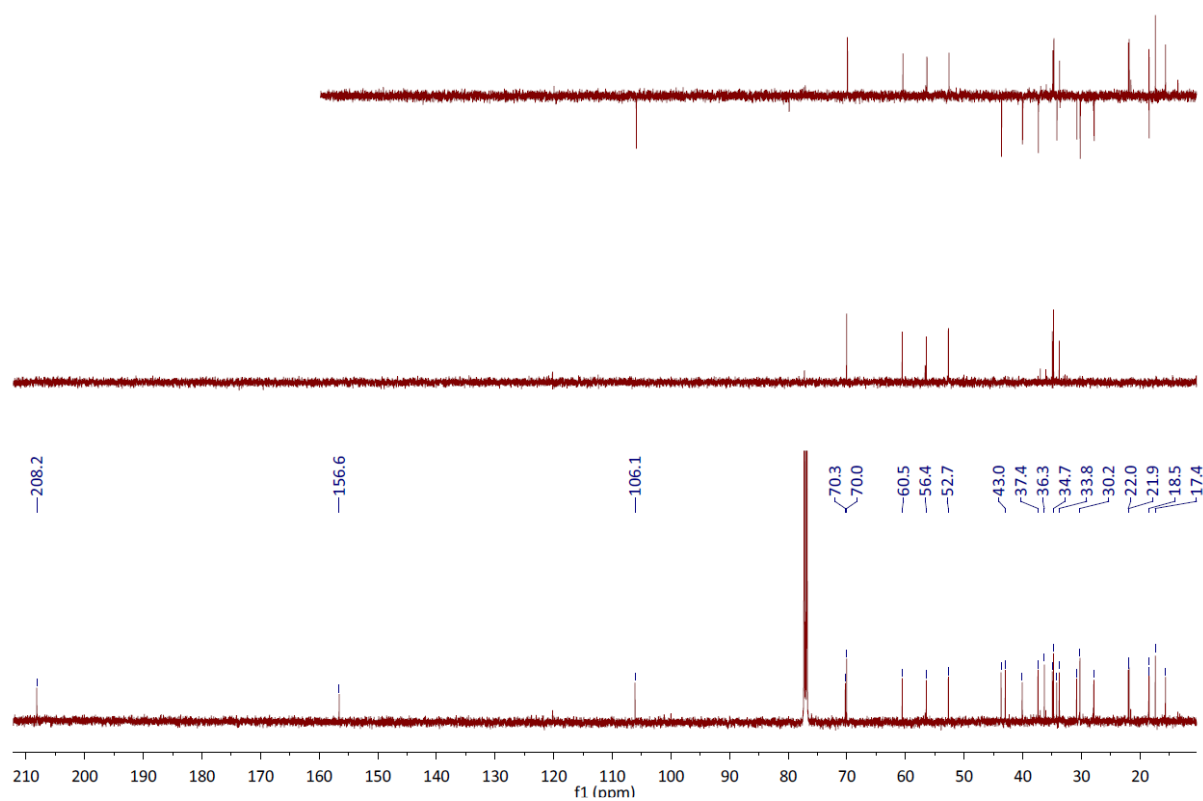


Figure S4: ^{13}C NMR and DEPT (125 MHz, CDCl_3) spectra of **1**

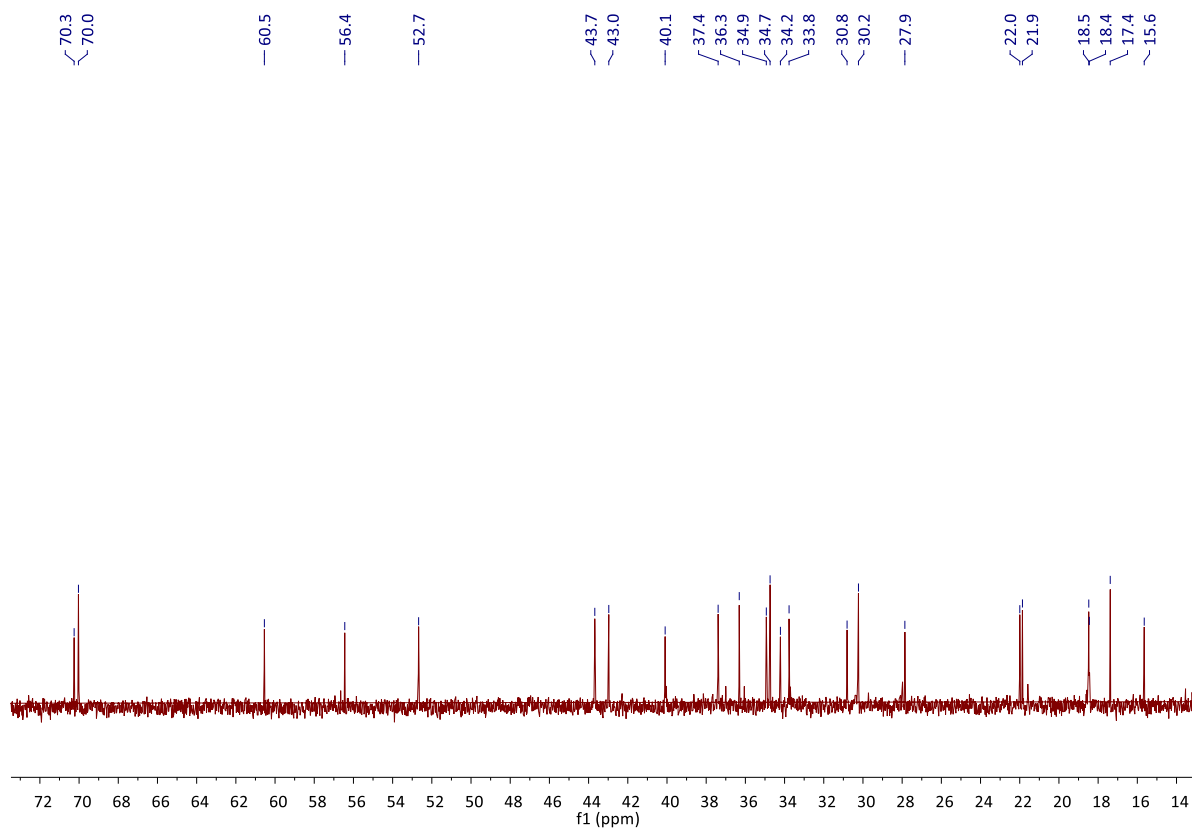


Figure S5: Enlarged ^{13}C NMR (125 MHz, CDCl_3) spectrum of **1**

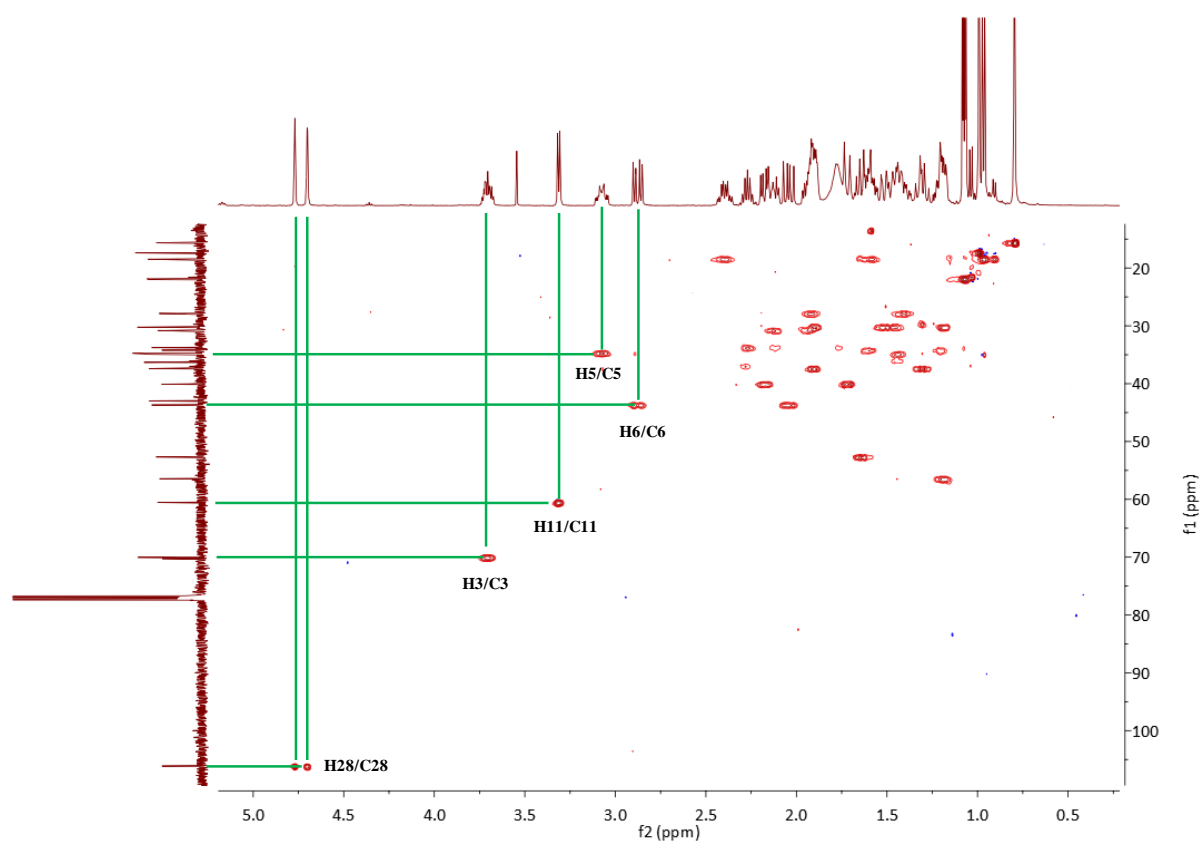


Figure S6: HSQC spectrum of **1**

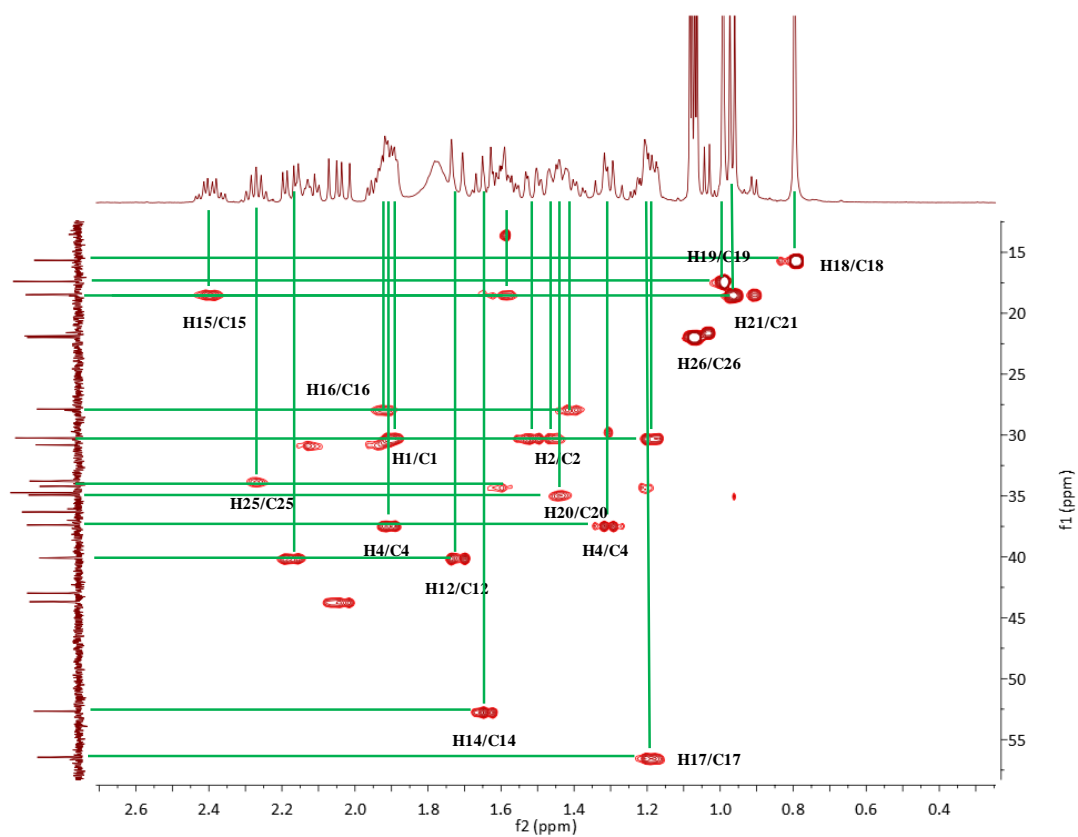


Figure S7: Enlarged HSQC spectrum of **1**

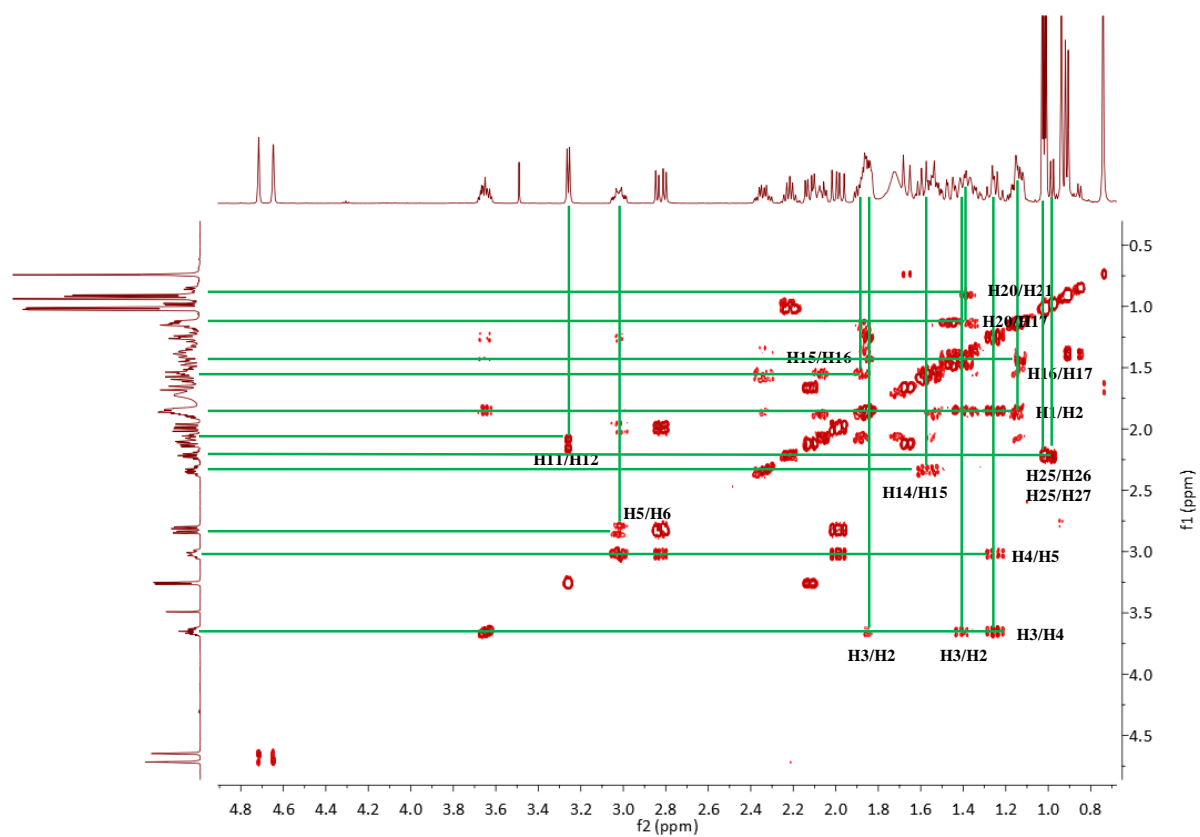


Figure S8: ^1H - ^1H COSY spectrum of **1**

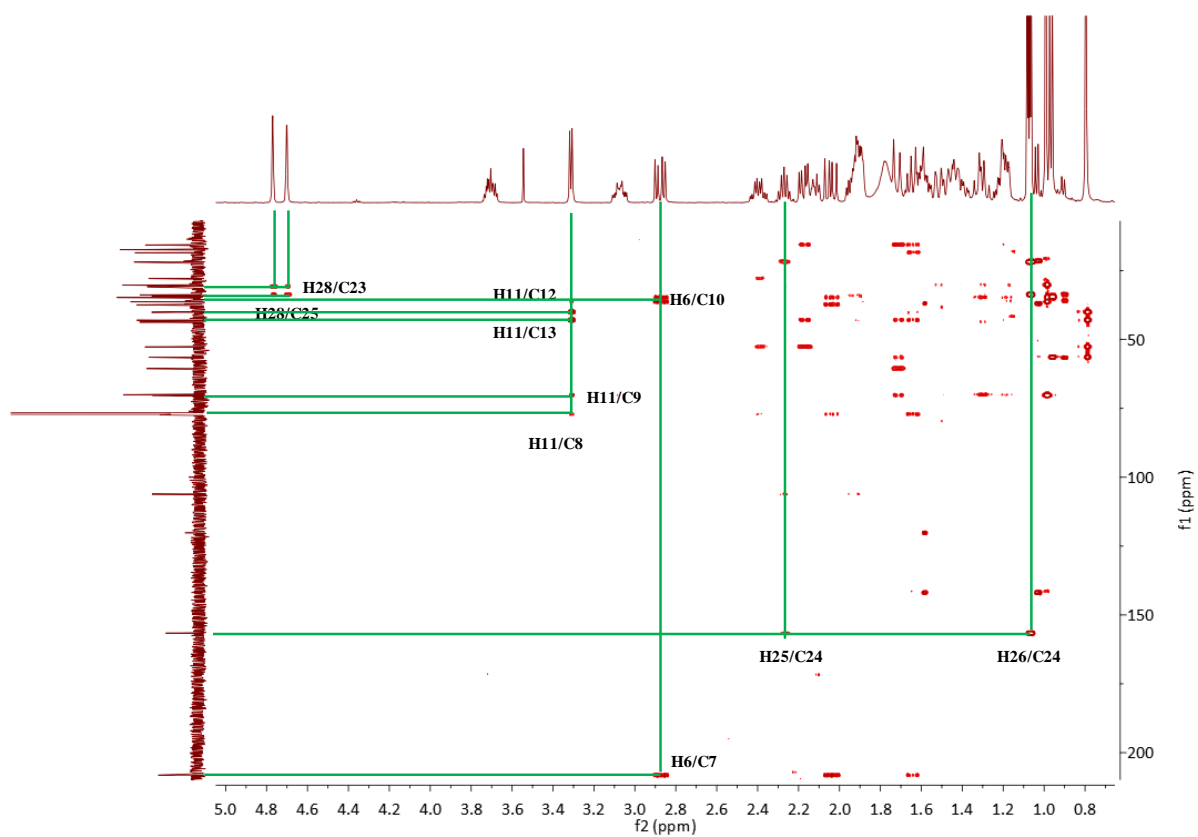


Figure S9: HMBC spectrum of **1**

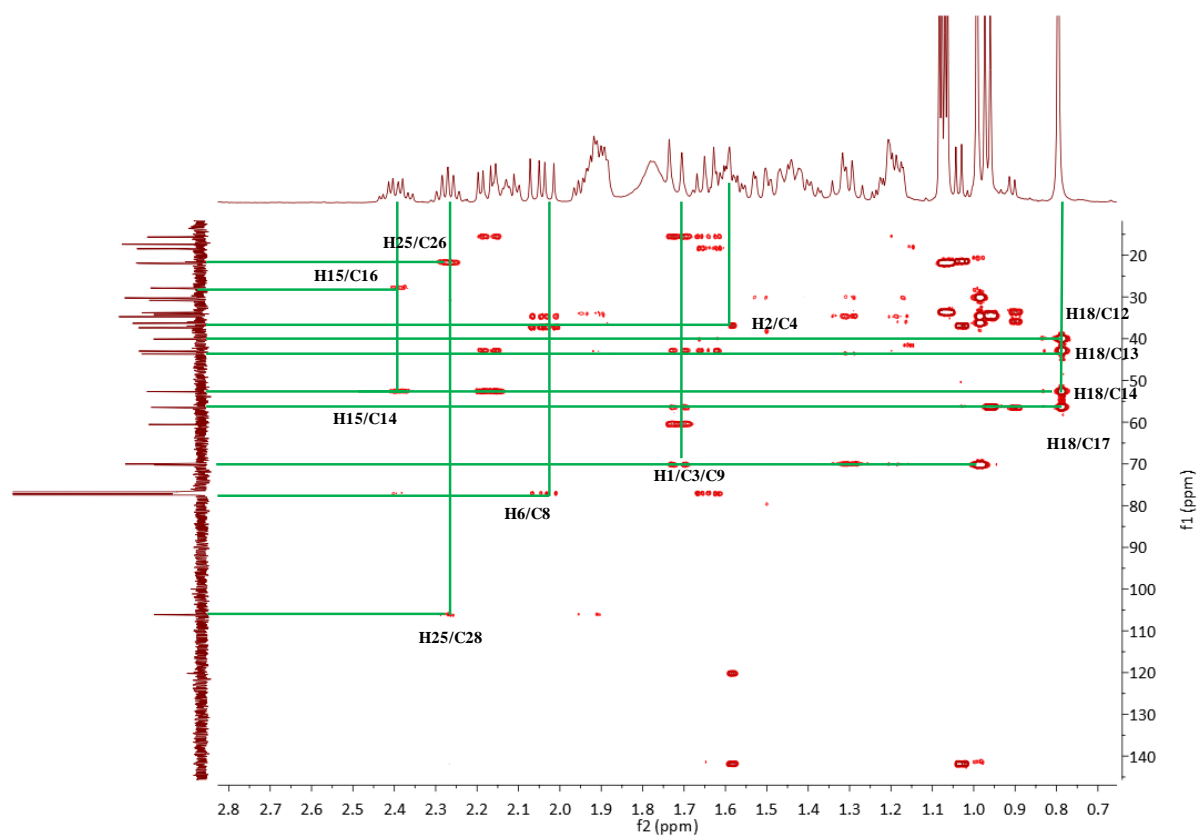


Figure S10: Enlarged HMBC spectrum of **1**

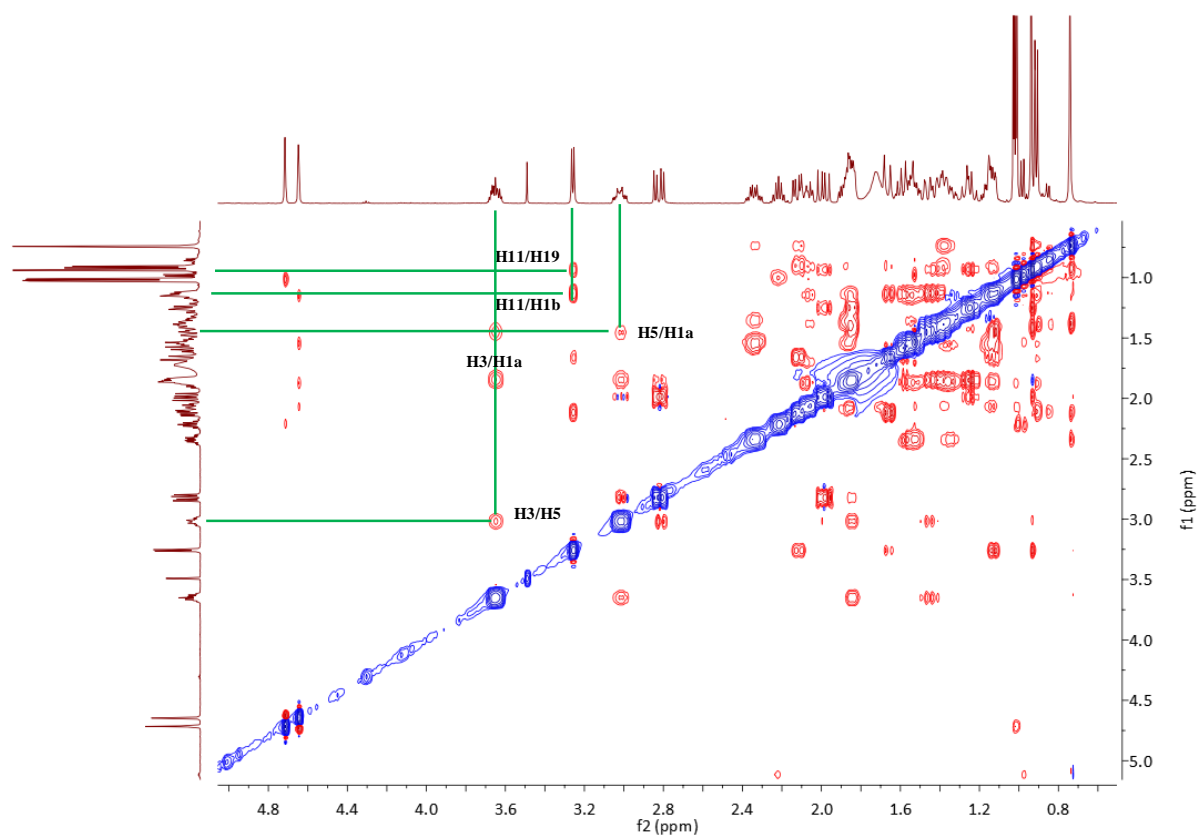


Figure S11: NOESY spectrum of **1**

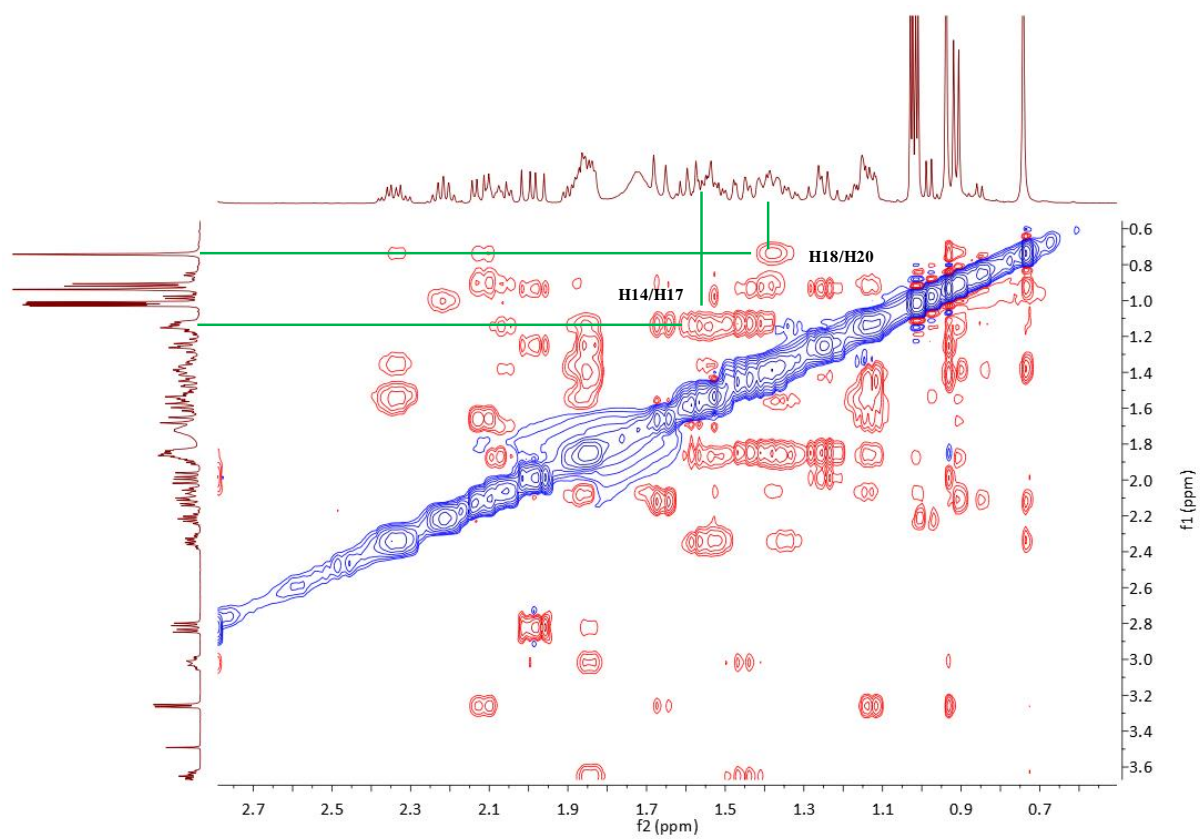


Figure S12: Enlarged NOESY spectrum of **1**

Initiating Search

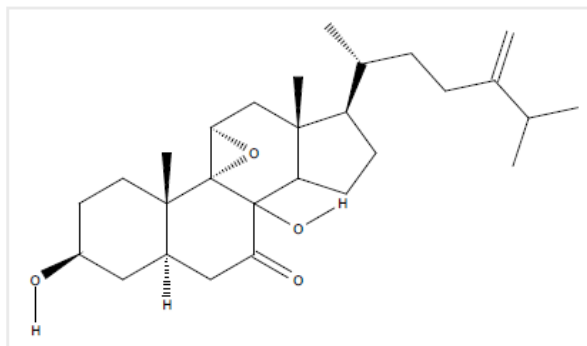
October 11, 2023, 9:09AM

Substances:

Filtered By:

Similarity: 95-98

Number of Components: 1



Structure Match: Similarity

Search Tasks

Task	Search Type	View
Exported: Returned Substance Results + Filters (1)	Substances	View Results

Substances (1)

[View in SciFinderⁿ](#)

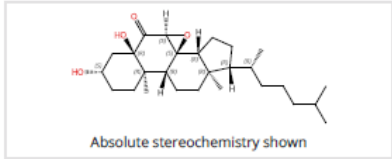
1	Similarity Score: 96		
73792-82-2  Absolute stereochemistry shown C₂₇H₄₄O₄ Cholestan-6-one, 7,8-epoxy-3,5-dihydroxy-, (3β,5α,7α,8α)- <div><div>1 Reference</div><div>1 Reaction</div><div>0 Suppliers</div></div>	Key Physical Properties	Value	Condition
	Molecular Weight	432.64	-
	Boiling Point (Predicted)	552.9±50.0 °C	Press: 760 Torr
	Density (Predicted)	1.13±0.1 g/cm ³	Temp: 20 °C; Press: 760 Torr
	pKa (Predicted)	12.37±0.70	Most Acidic Temp: 25 °C

Figure S13: Scifinder search results of 1