

Supporting Information

Rec. Nat. Prod. 17:6 (2023) 1080-1084

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

Xin-Rong Huang^{1,2}, Chao-Nan Jiang², Tong Si^{1,*}, Peng Zhang^{2,*},
and Zhong-Feng Zhang^{2,*}

¹ College of Agronomy, Qingdao Agricultural University, Qingdao 266109, China

² Tobacco Research Institute, Chinese Academy of Agricultural Sciences, Qingdao 266101, China

Table of Contents	Page
Figure S1: HRESIMS spectrum of 1	2
Figure S2: ¹ H NMR (500 MHz, CDCl ₃) spectrum of 1	3
Figure S3: Enlarged ¹ H NMR (500 MHz, CDCl ₃) spectrum of 1	4
Figure S4: ¹³ C NMR and DEPT (125 MHz, CDCl ₃) spectra of 1	5
Figure S5: Enlarged ¹³ C NMR (125 MHz, CDCl ₃) spectrum of 1	6
Figure S6: HSQC spectrum of 1	7
Figure S7: Enlarged HSQC spectrum of 1	8
Figure S8: ¹ H- ¹ H COSY spectrum of 1	9
Figure S9: HMBC spectrum of 1	10
Figure S10: Enlarged HMBC spectrum of 1	11
Figure S11: NOESY spectrum of 1	12
Figure S12: Enlarged NOESY spectrum of 1	13
Figure S13: Scifinder search results of 1	14

*Corresponding author: E-mail: tongsi@qau.edu.cn (T. Si); zhangpeng@caas.cn (P. Zhang); zhangzhongfeng@caas.cn (Z.F. Zhang)

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

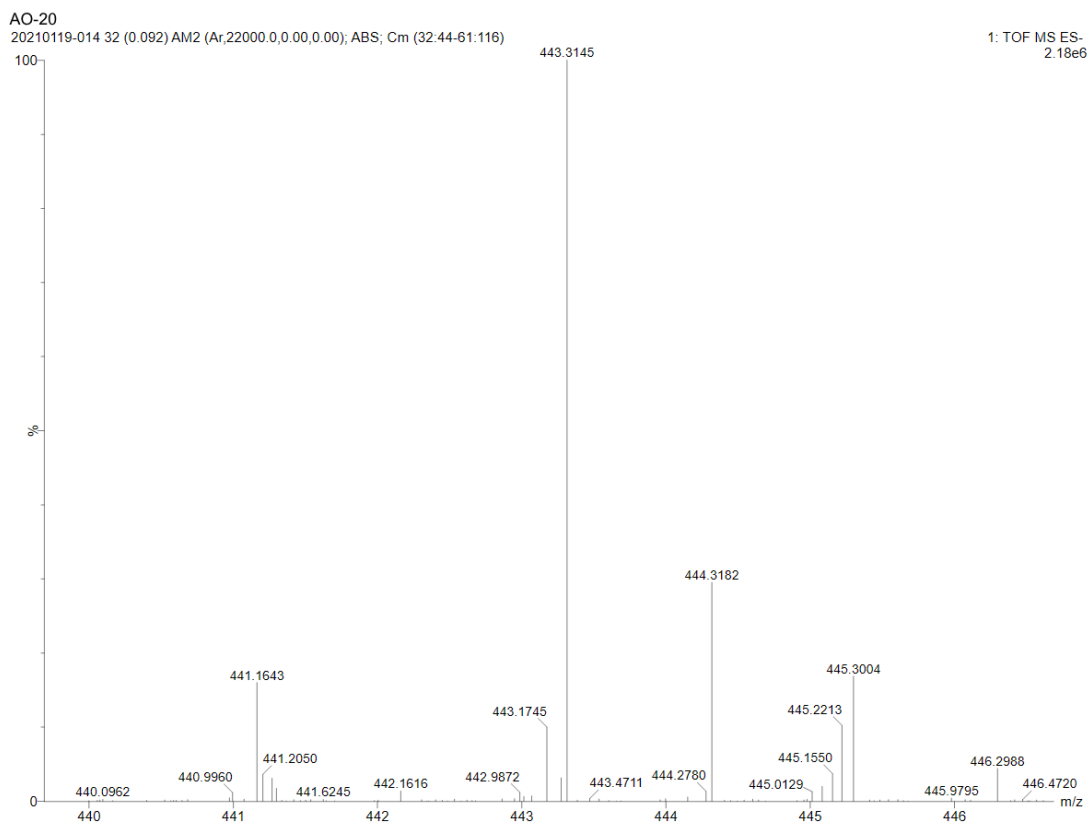
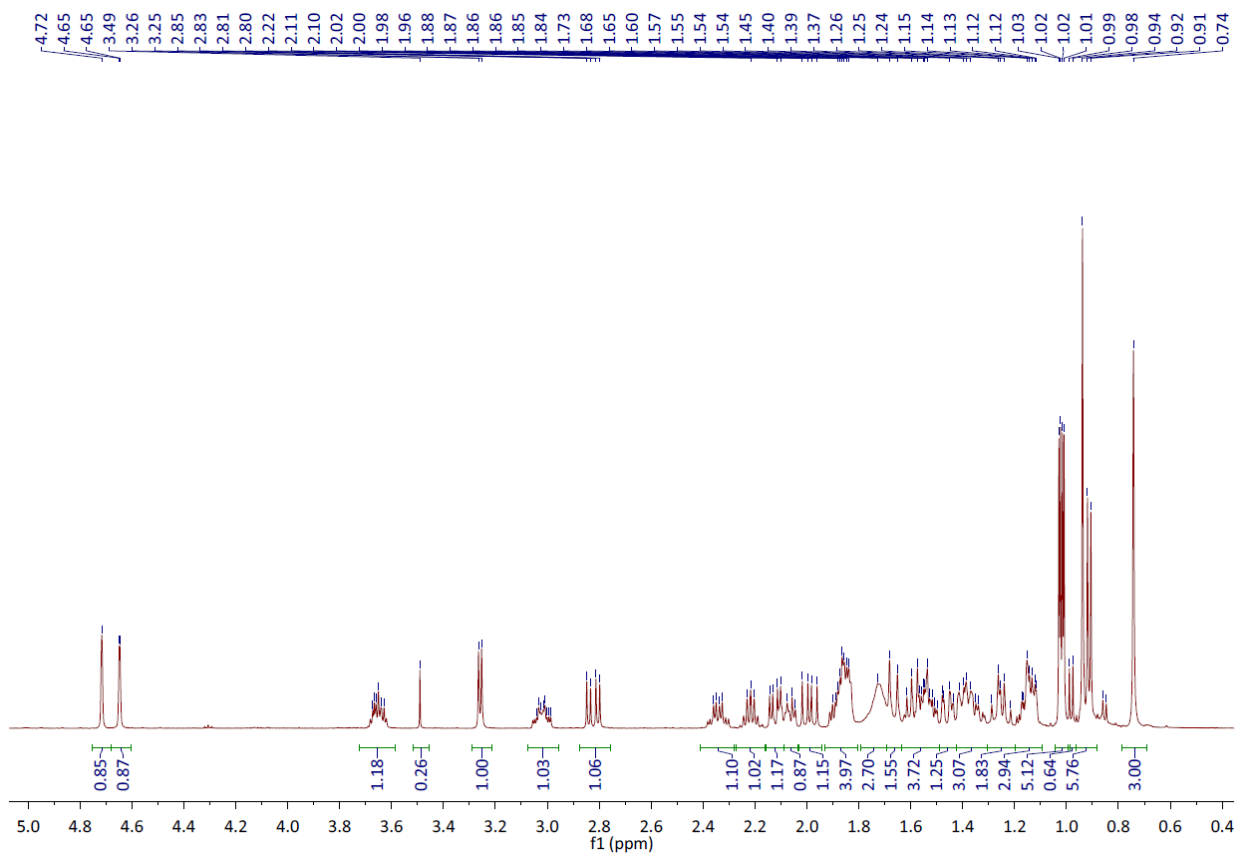


Figure S1: HRESIMS spectrum of 1



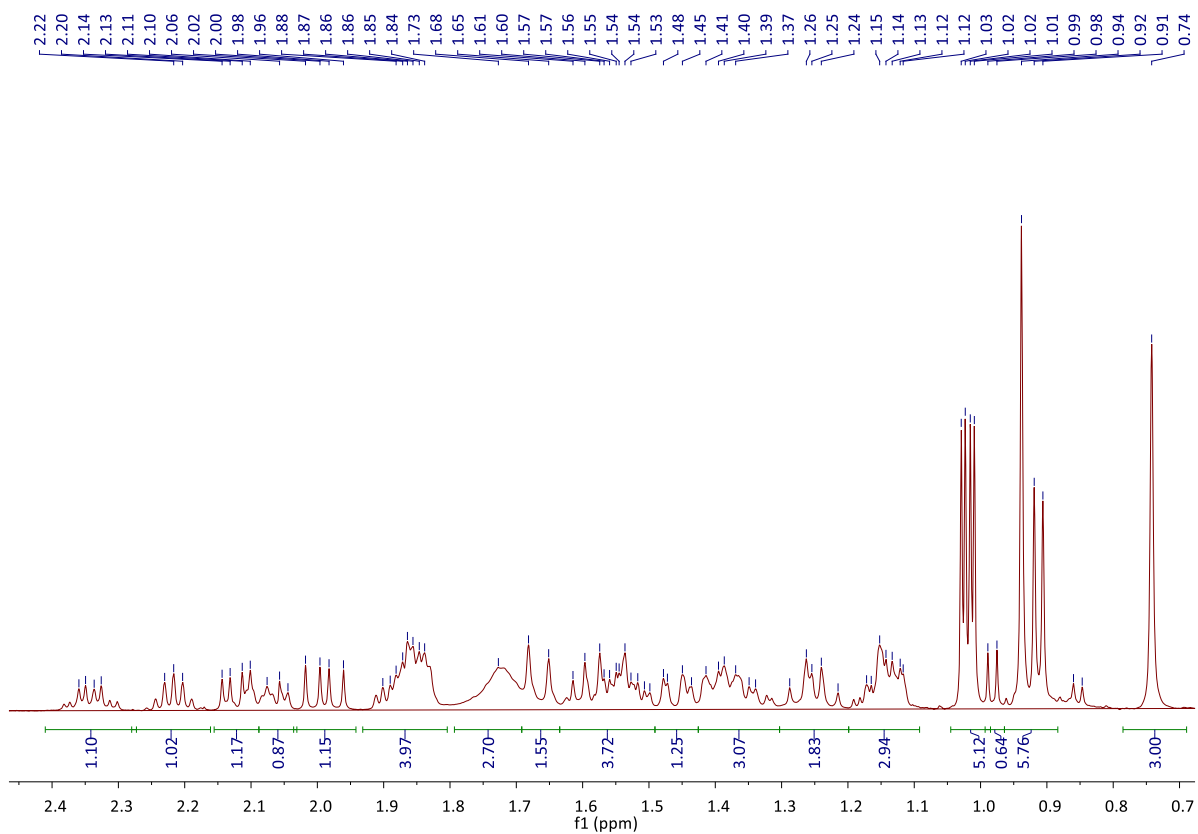


Figure S3: Enlarged ^1H NMR (500 MHz, CDCl_3) spectrum of **1**

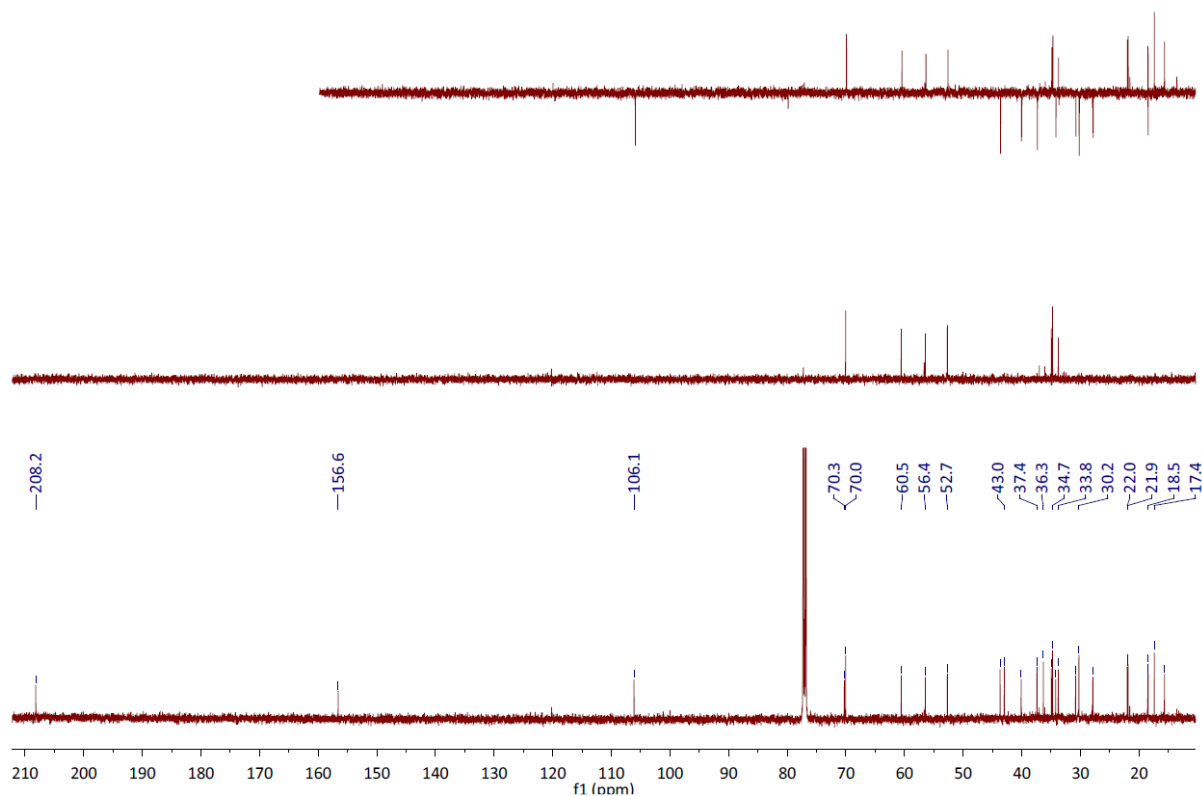


Figure S4: ^{13}C NMR and DEPT (125 MHz, CDCl_3) spectra of **1**

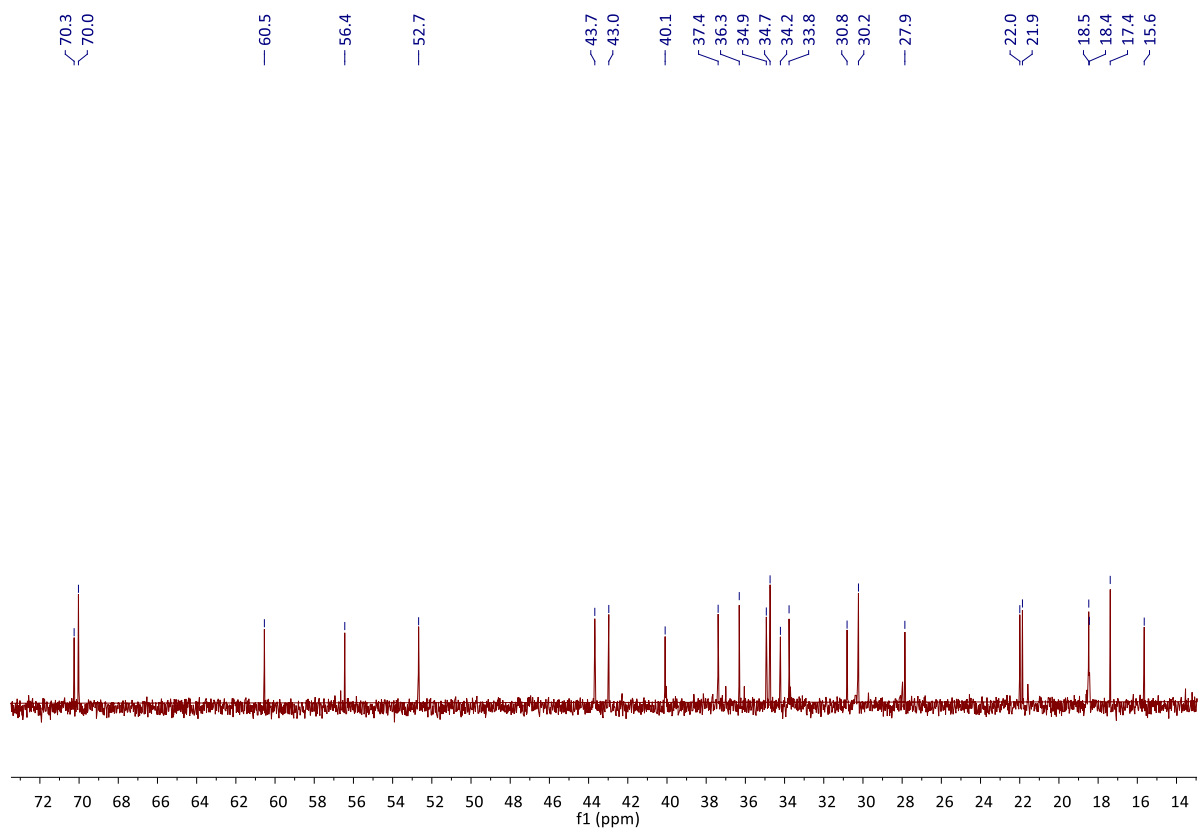


Figure S5: Enlarged ^{13}C NMR (125 MHz, CDCl_3) spectrum of **1**

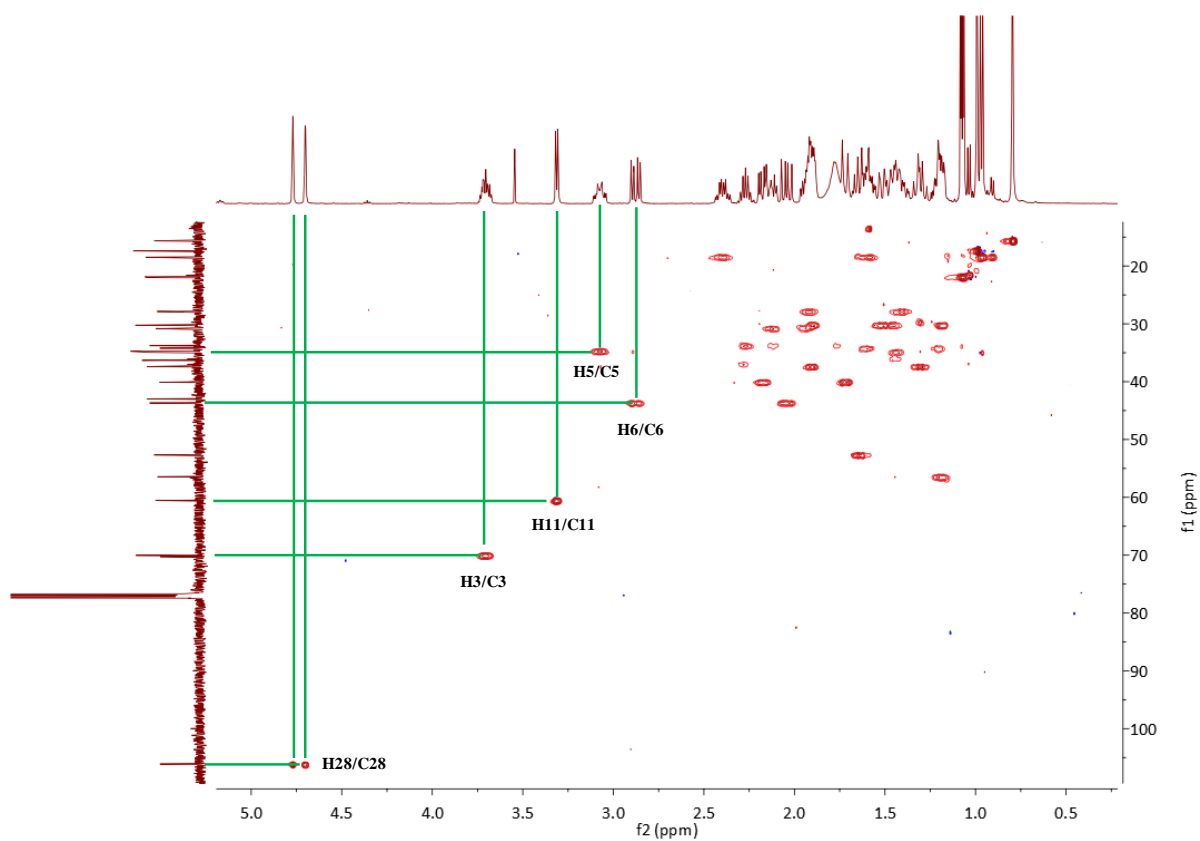


Figure S6: HSQC spectrum of **1**

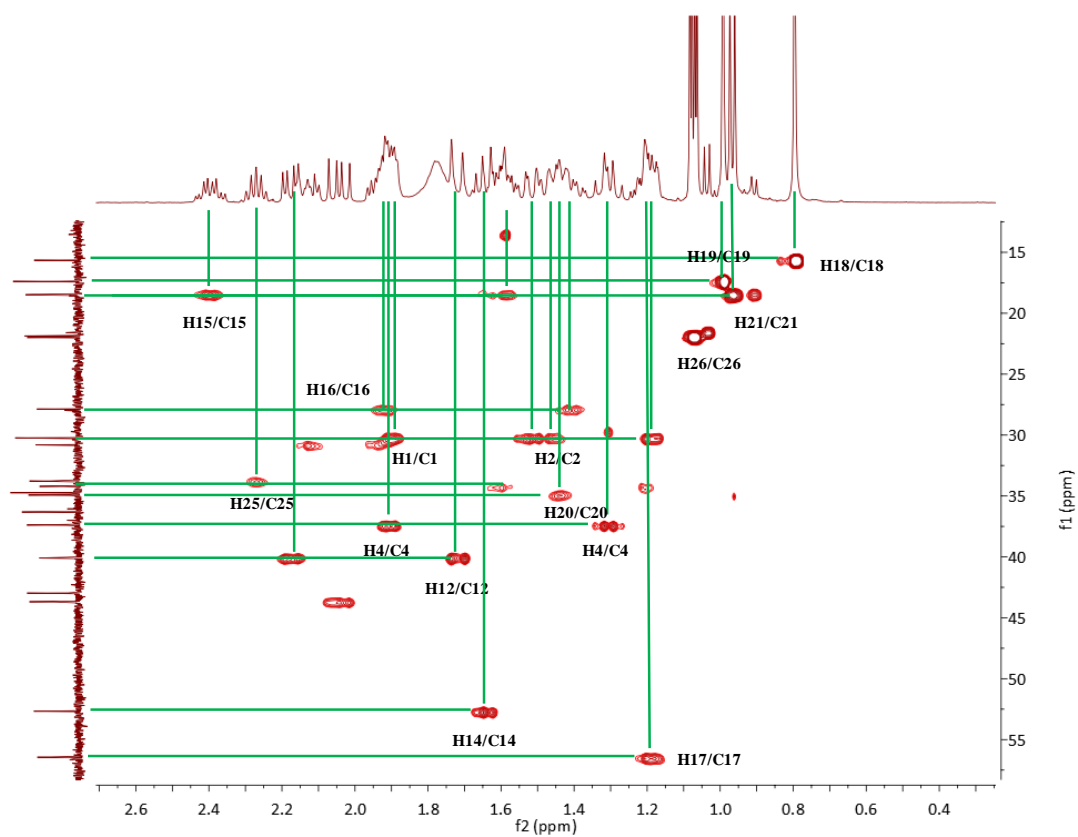


Figure S7: Enlarged HSQC spectrum of **1**

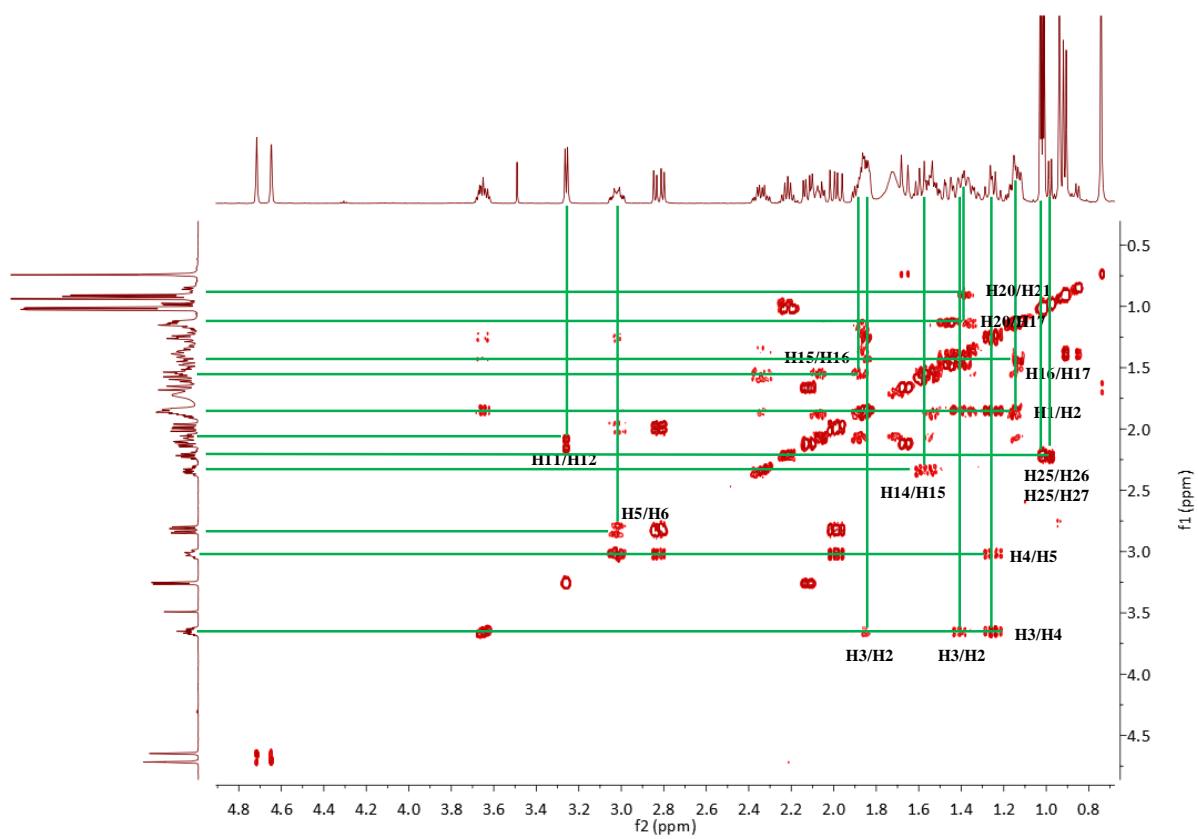


Figure S8: ^1H - ^1H COSY spectrum of **1**

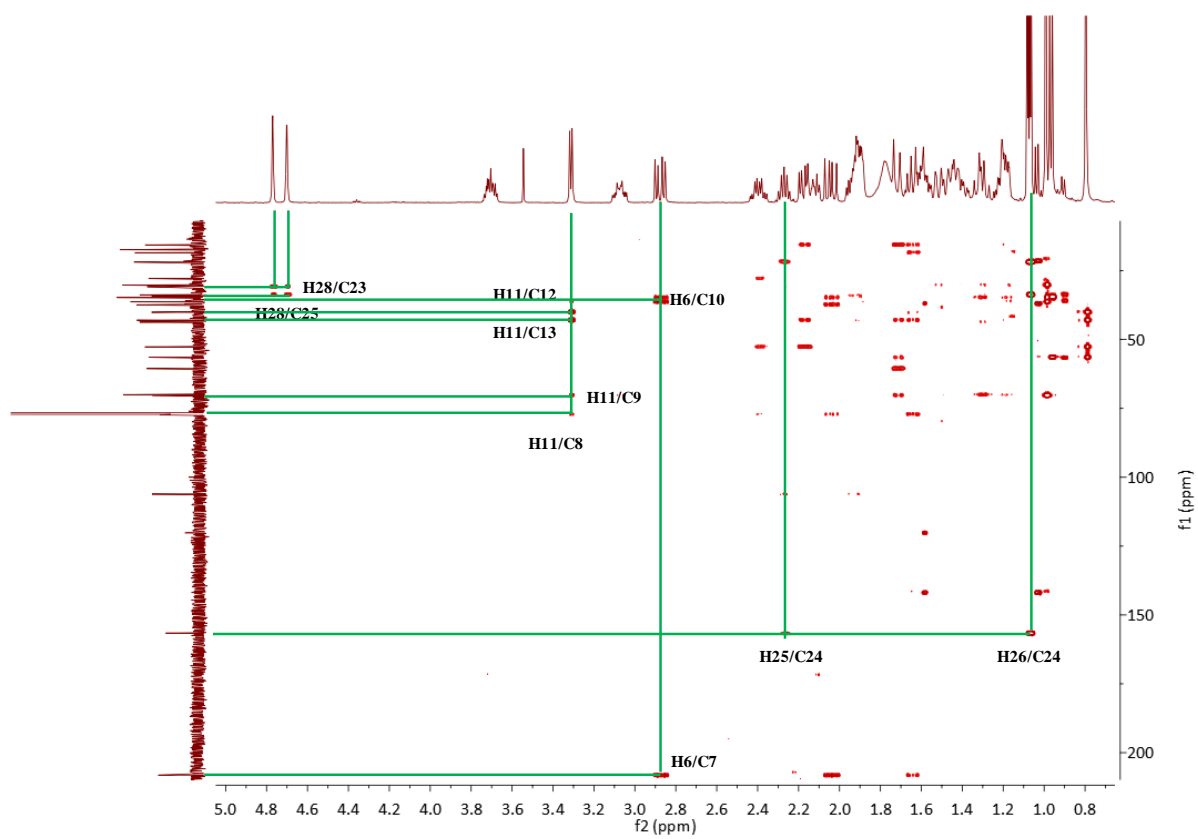


Figure S9: HMBC spectrum of **1**

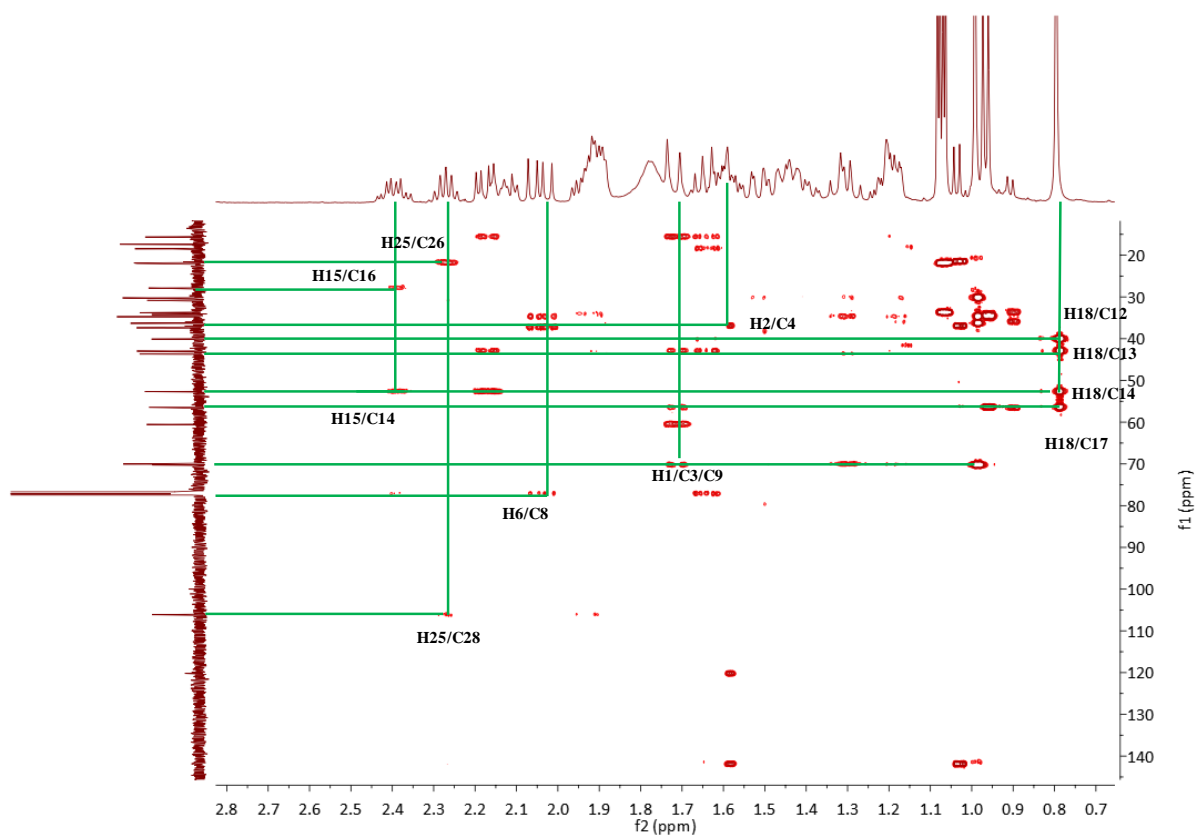


Figure S10: Enlarged HMBC spectrum of **1**

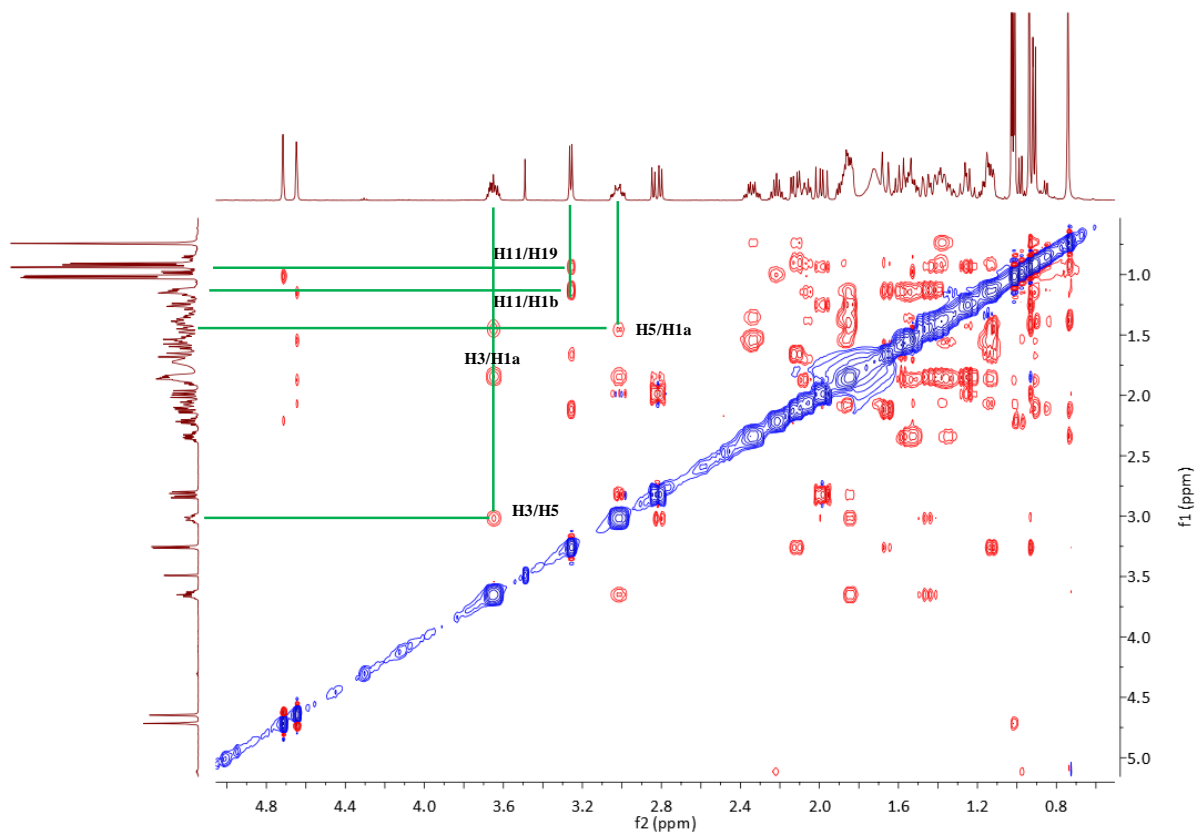


Figure S11: NOESY spectrum of **1**

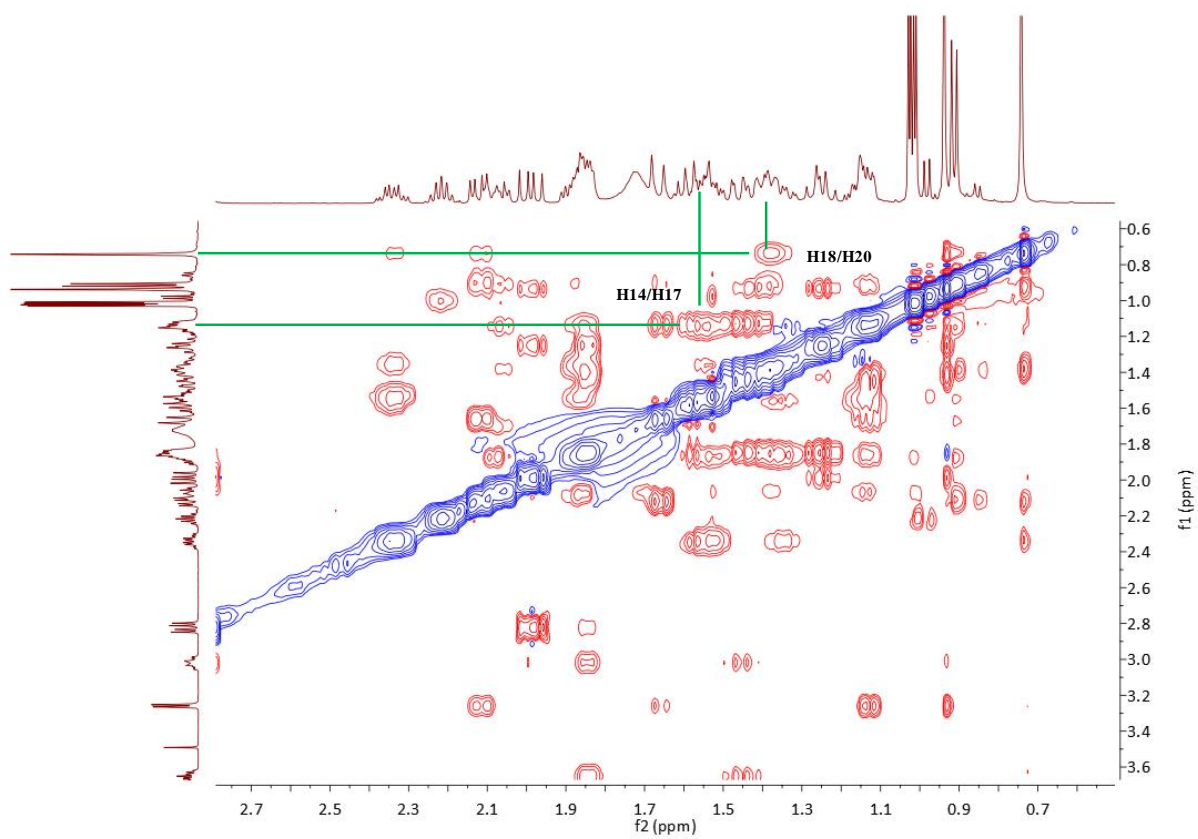


Figure S12: Enlarged NOESY spectrum of **1**

Initiating Search

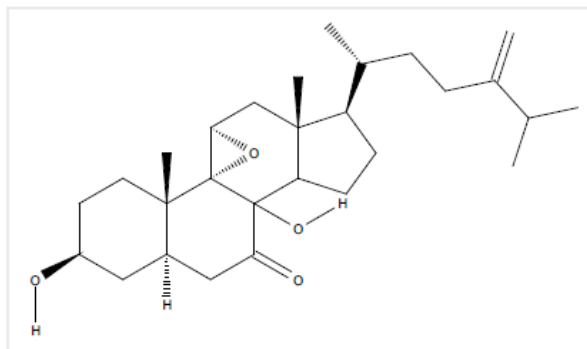
October 11, 2023, 9:09AM

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 SciFinder[®]](#)

1	Similarity Score: 96																
<p>73792-82-2</p> <p>Absolute stereochemistry shown</p> <p>C₂₇H₄₄O₄ Cholestan-6-one, 7,8-epoxy-3,5-dihydroxy-, (3β,5α,7α,8α)-</p> <p>1 Reference 1 Reaction 0 Suppliers</p>	<table border="1"> <thead> <tr> <th>Key Physical Properties</th> <th>Value</th> <th>Condition</th> </tr> </thead> <tbody> <tr> <td>Molecular Weight</td> <td>432.64</td> <td>-</td> </tr> <tr> <td>Boiling Point (Predicted)</td> <td>552.9±50.0 °C</td> <td>Press: 760 Torr</td> </tr> <tr> <td>Density (Predicted)</td> <td>1.13±0.1 g/cm³</td> <td>Temp: 20 °C; Press: 760 Torr</td> </tr> <tr> <td>pKa (Predicted)</td> <td>12.37±0.70</td> <td>Most Acidic Temp: 25 °C</td> </tr> </tbody> </table>	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	
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