

Supplementary Data

Digyaindoleacid A: 2-(1-(4-Hydroxyphenyl)-3-oxobut-1-en-2-yloxy)-3-(1*H*-indol-3-yl)propanoic Acid, a Novel Indole Alkaloid

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Figure S1. *Paenibacillus* sp. DE2SH (GenBank Accession Number: MH091697) growing on ISP2 agar plates at pH 5.5.



Figure S2. HRESI-LC-MS data for pure Digyaindoleacid A (**1**).

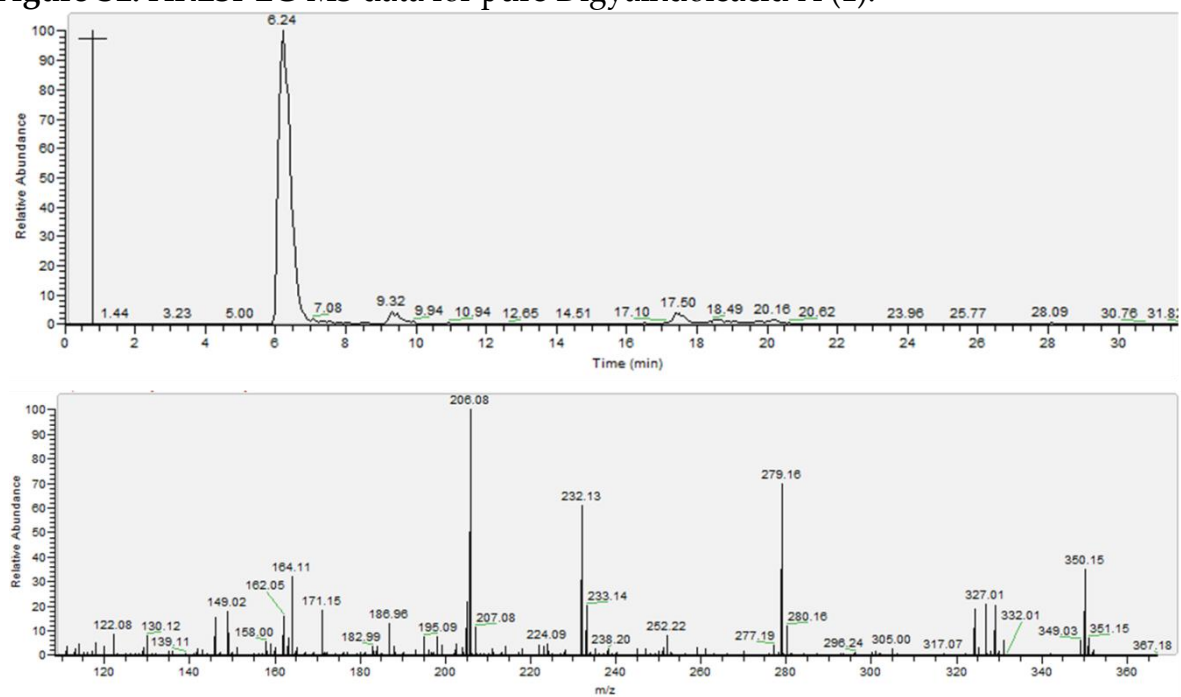


Figure S3. Proposed plausible structures for mass spectrometry fragments of Digya-indoleacid A (**1**).

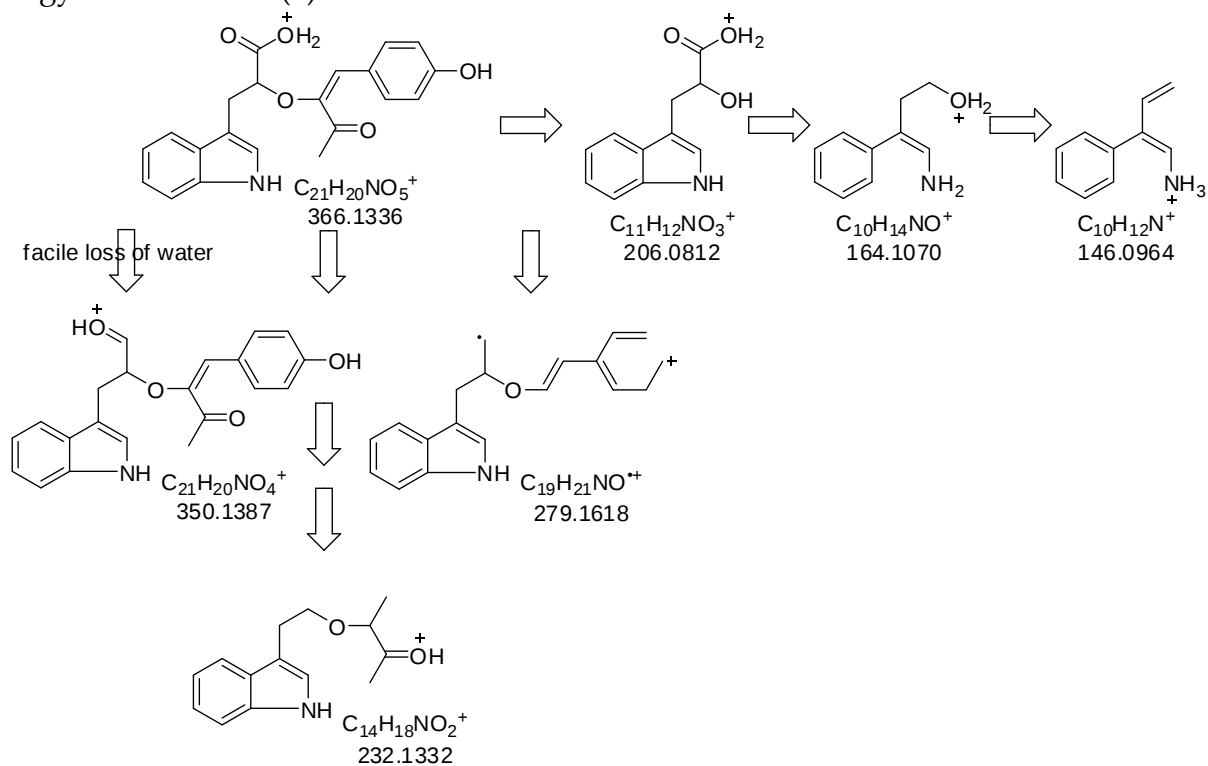


Figure S4. ^{13}C -NMR spectrum of Digyaindoleacid A (1) in DMSO- d_6 .

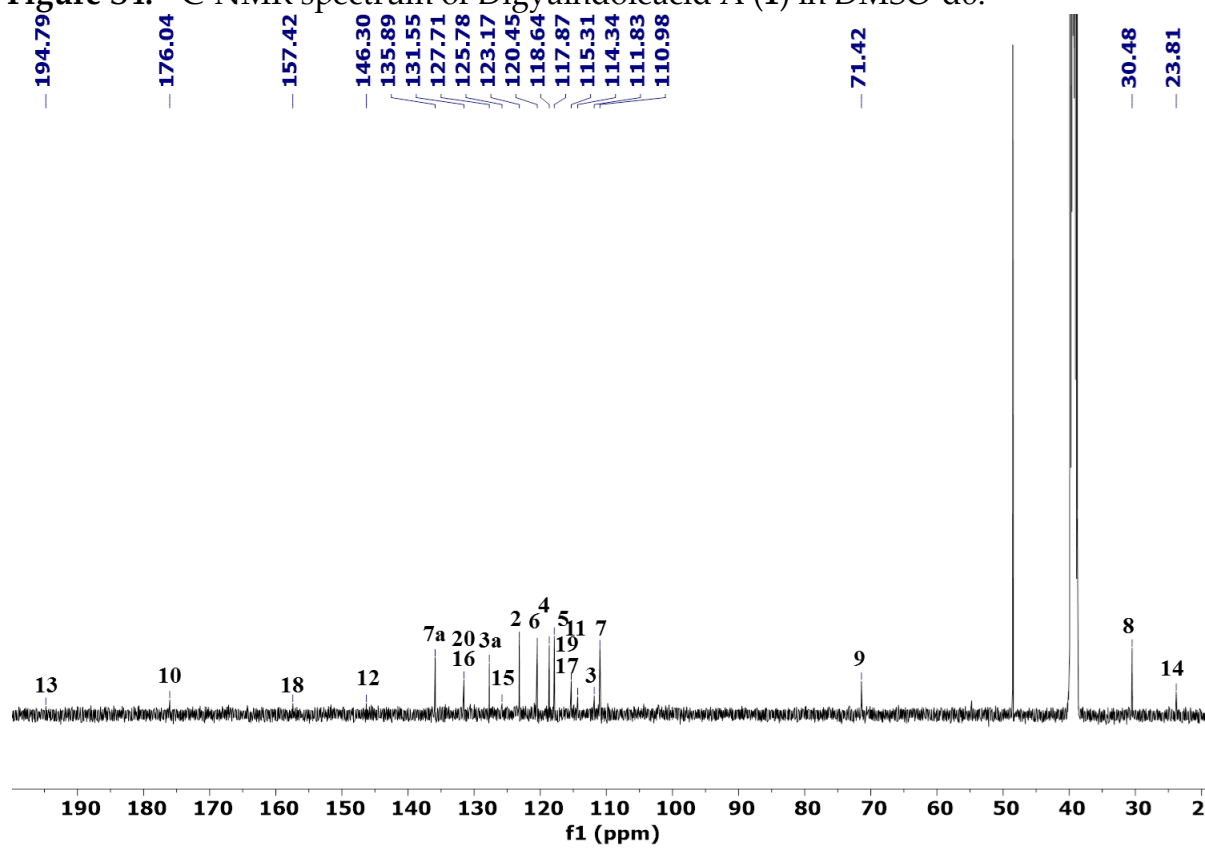


Figure S5. DEPT¹³⁵ spectrum of Digyaindoleacid A (1) in DMSO-d₆.

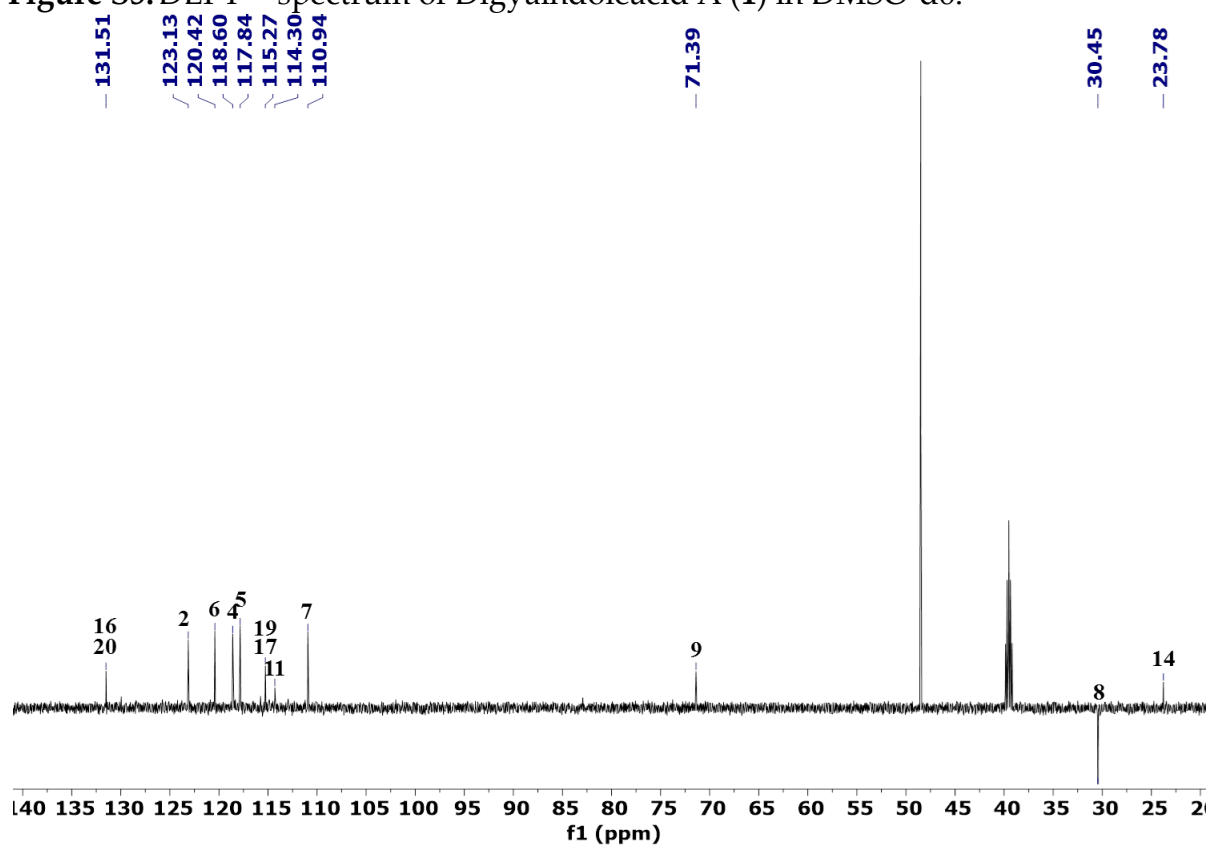


Figure S6. ^1H -NMR spectrum of Digyaindoleacid A (1) in DMSO-d_6 .

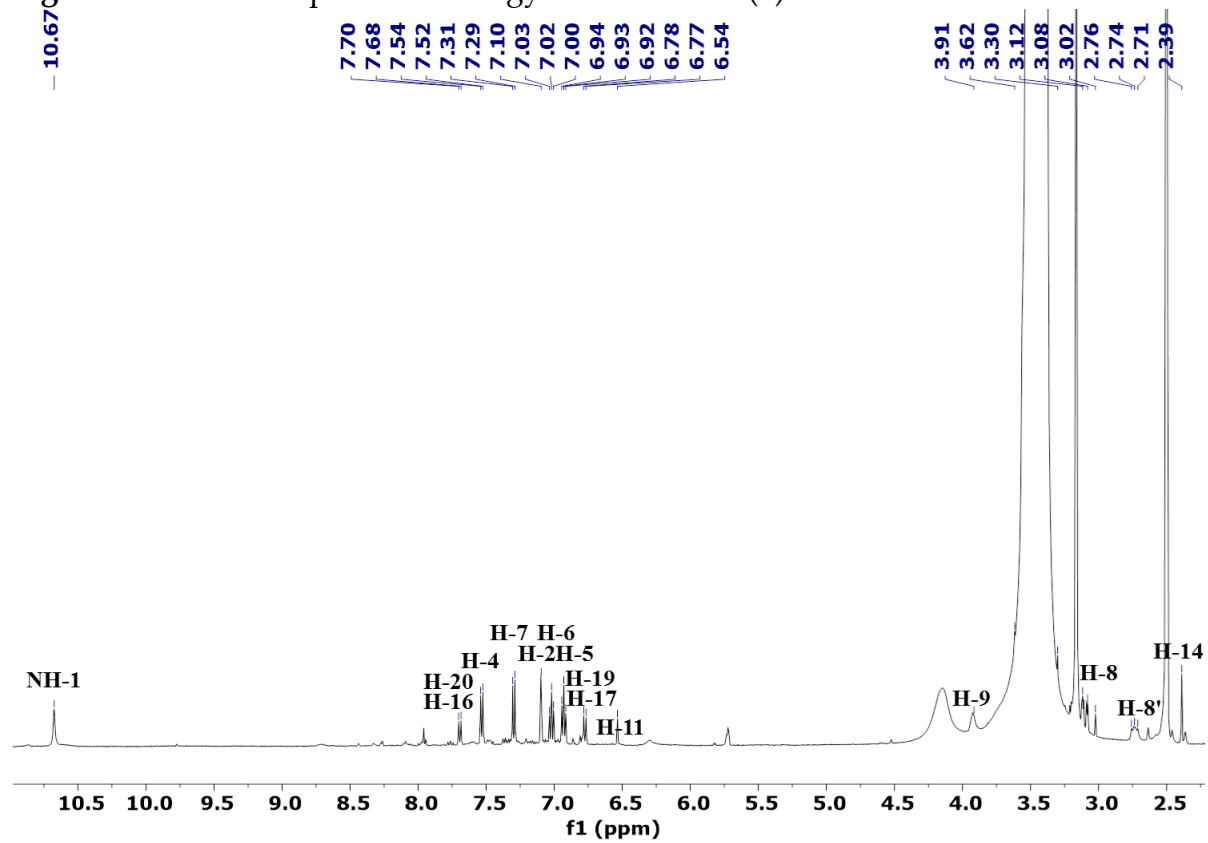


Figure S7. HSQC spectrum of Digyaindoleacid A (**1**) in DMSO-d₆.

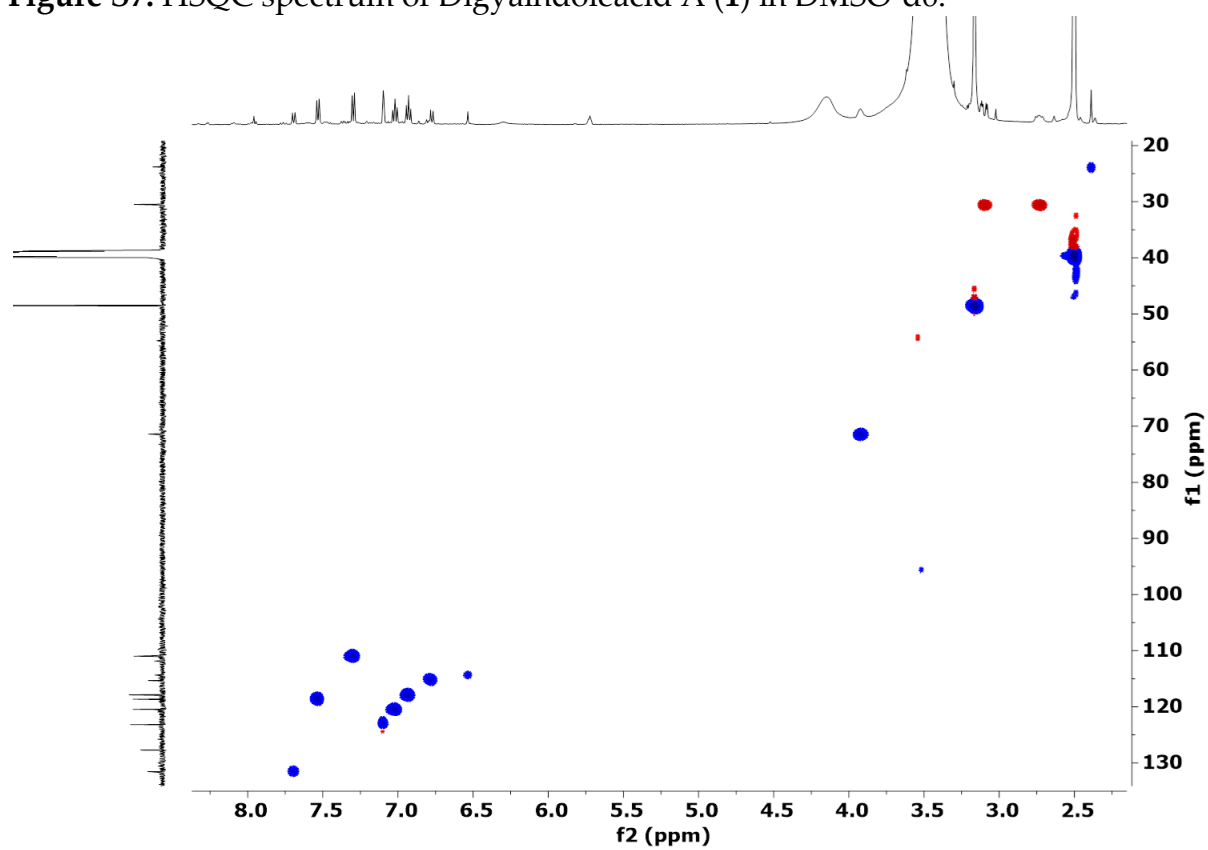


Figure S8. COSY spectrum of Digyaindoleacid A (**1**) in DMSO-d₆.

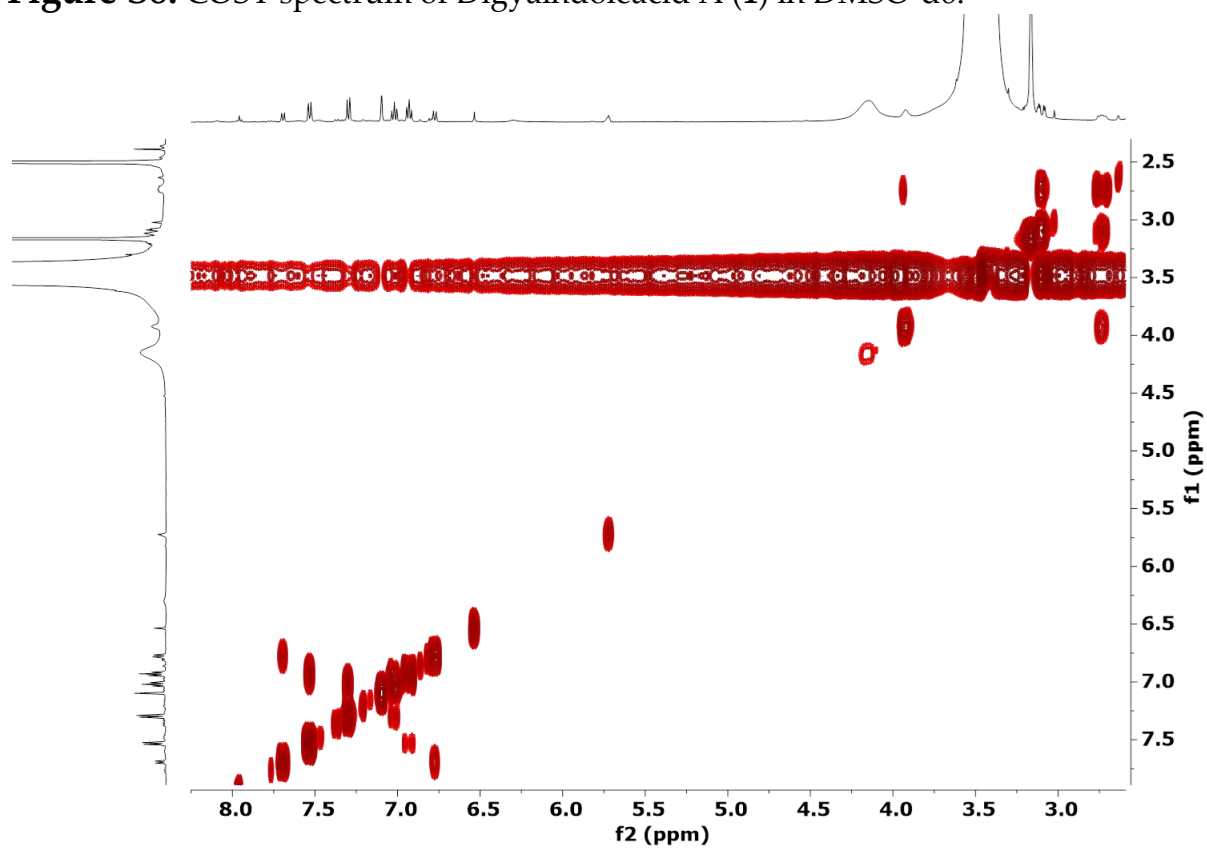


Figure S9. HMBC spectrum of Digyaindoleacid A (1) in DMSO-d₆.

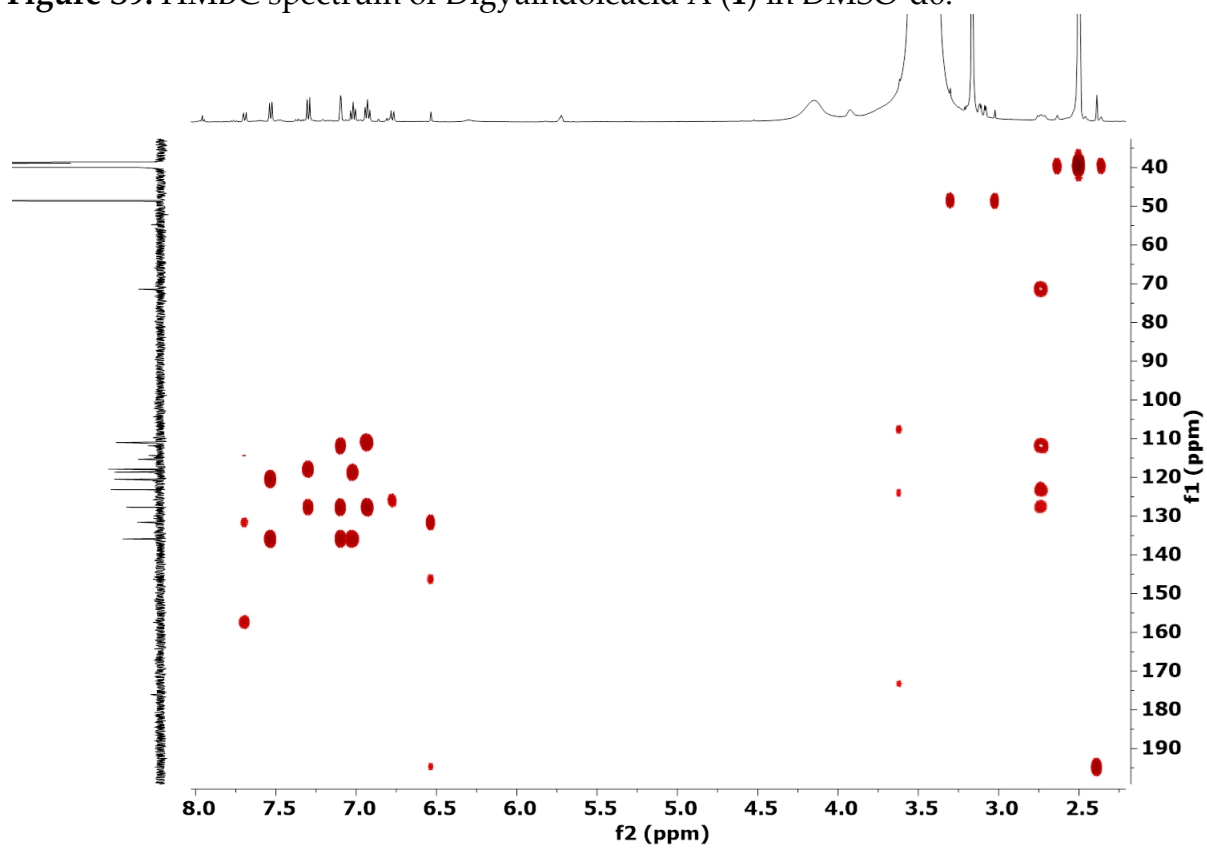


Figure S10. TOCSY spectrum of Digyaindoleacid A (**1**) in DMSO-d₆.

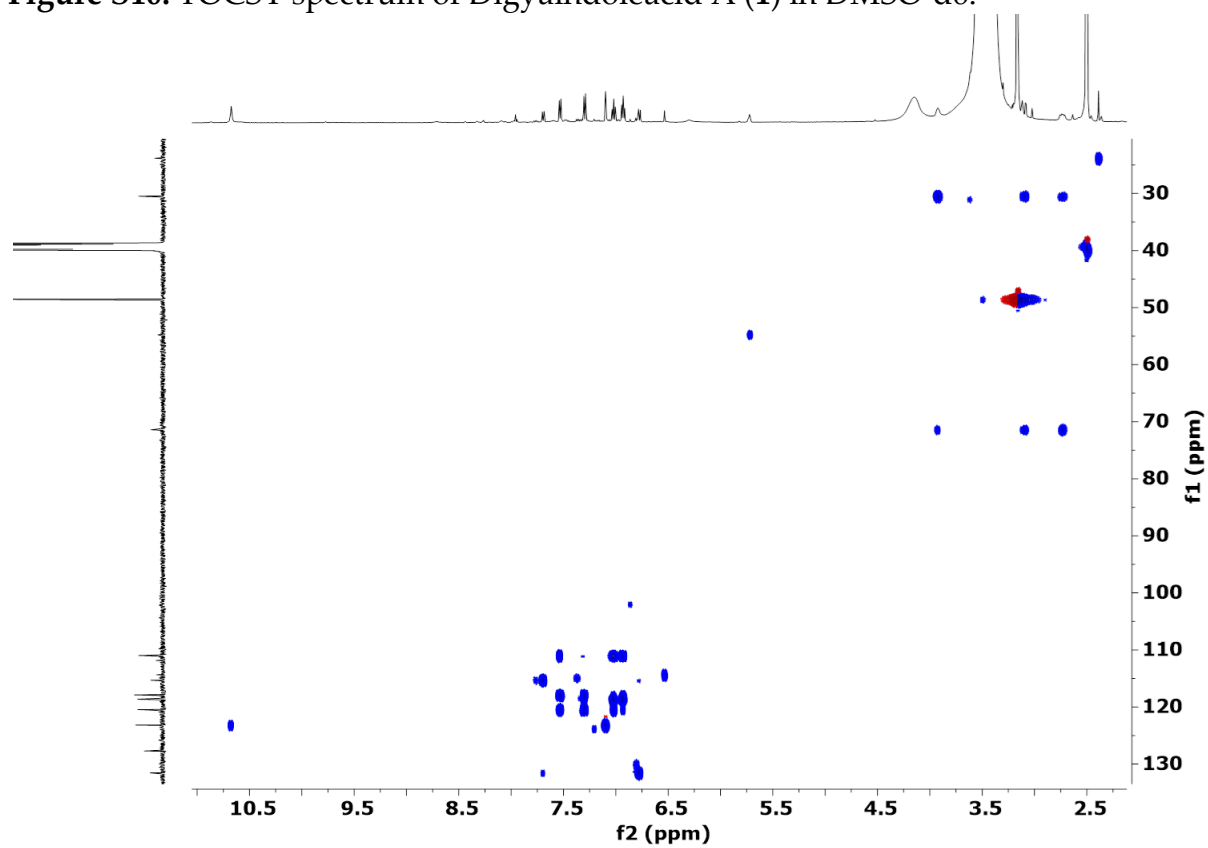


Figure S11. T-ROESY spectrum of Digyaindoleacid A (**1**) in DMSO-d₆.

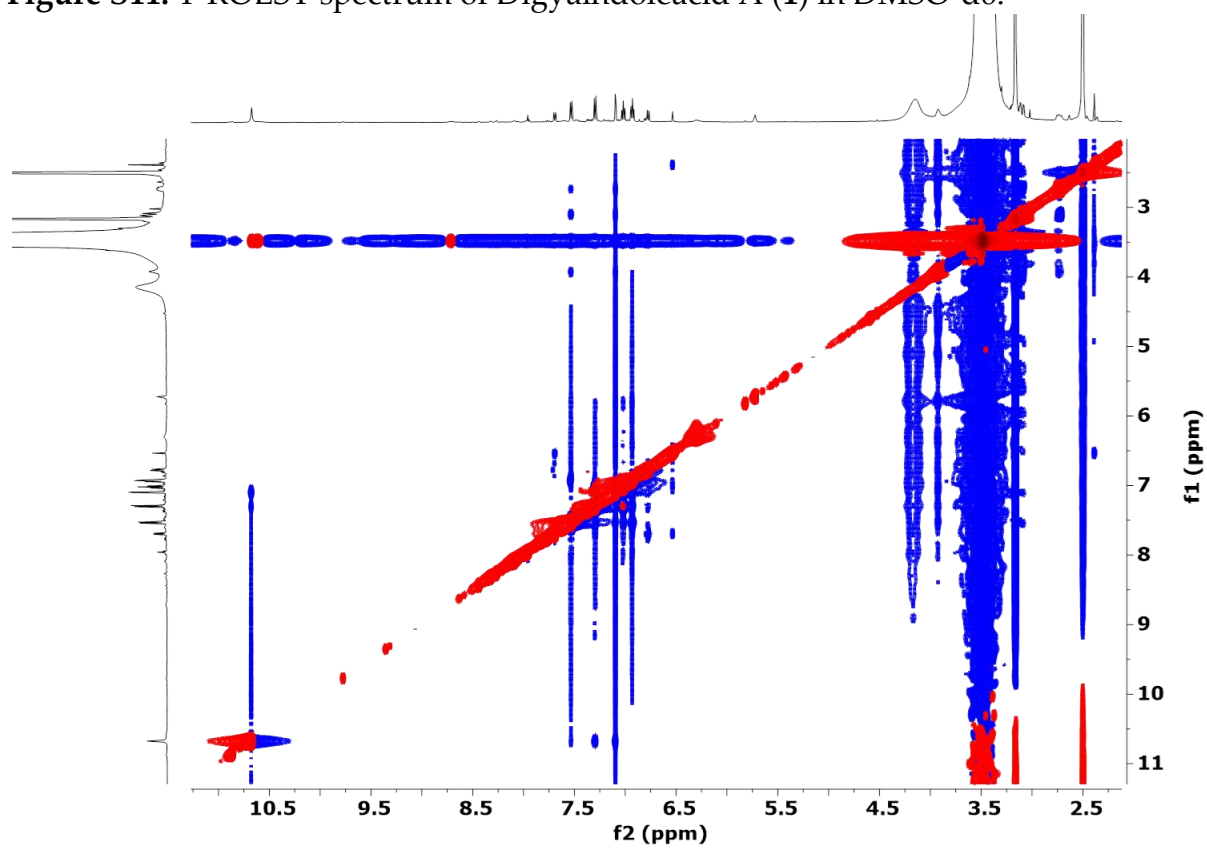


Figure S12. Semi-preparative reverse phase HPLC chromatogram of Digyaindoleacid A (**1**).

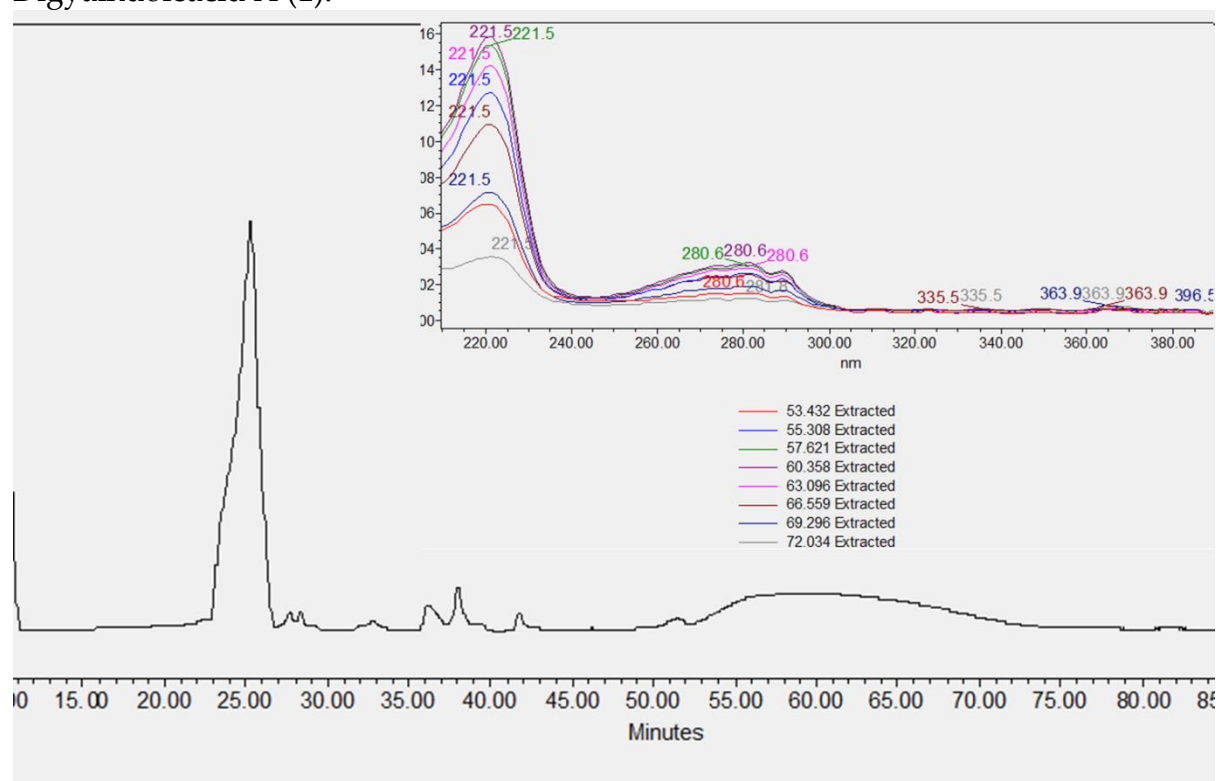


Figure S13. UV spectrum of Digyaindoleacid A (**1**).

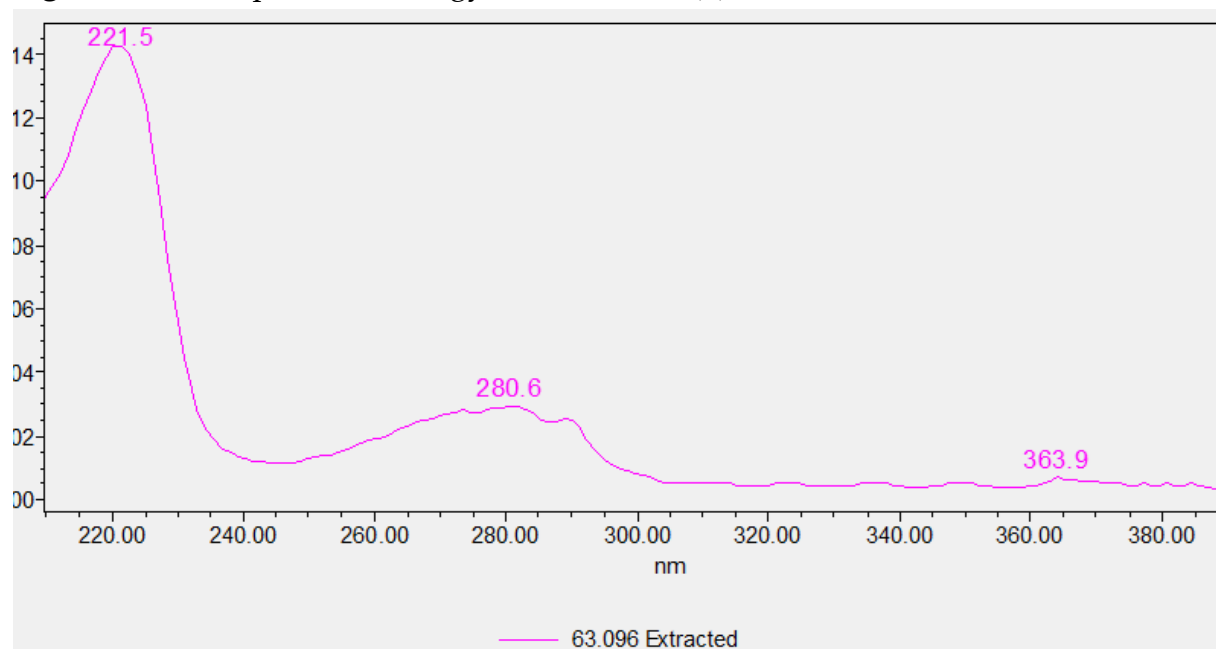


Table S1. Interpretation of peaks in the Infrared absorption spectrum of Digyaindoleacid A (1).

Wavenumber (cm ⁻¹)	Attribute	Absorption	Comment
3367	Broad Strong	O-H stretching	Carboxylic acid and Phenol
2947 2835	Medium	C-H stretching	Alkane
2263 2133	Weak	Aromatic overtones	Aromatics
1740	Medium	C=O stretching	Carboxylic acid
1647	Strong	C=O stretching	α,β -Unsaturated Ketone
1449 1368	Medium	CH ₃ bending CH ₂ bending	Alkanes
1213	Medium	C-O stretch	Carboxylic acid
1112	Medium	C-H bending	Aromatics
1022 993	Sharp Strong	C-O stretching	Ether Alcohol