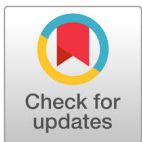


SUPPLEMENTARY MATERIAL



ation and characterization of a dihydrostilbene from the aerial parts of *Indigofera conferta*

Maryam Isah^{a*}, Asmau N. Hamza^b, Nkiruka Theresa Nnadozie^c, Edward Ayakeme Bebe^c, Nasir
Iddeen^d, Aliyu M. Musa^b

^aDepartment of Science Laboratory Technology, Federal University of Lafia, Nasarawa, Nigeria.

^bDepartment of Pharmaceutical and Medicinal Chemistry, Ahmadu Bello University, Zaria, Nigeria

^cDepartment of Chemistry, Federal University of Lafia, Nigeria

^dDepartment of Chemistry, Ahmadu Bello University, Zaria, Nigeria

*Corresponding author. E-mail: Maryamisah01@gmail.com

ORCID ID: 0000-0001-8728-4090

Tel: +2349060516221

ABSTRACT

Indigofera conferta, an annual herb widely distributed in Northeastern and Western Nigeria, is used ethnomedicinally in the treatment of inflammation, pain, sore feet, and snakebite. Despite its ethnomedicinal uses, the phytochemical constituents of this species remain unexplored. The methanol extract of the aerial parts of *I. conferta* was separated by chromatography on silica gel to afford a compound from the chloroform fraction. The structure of the compound was elucidated based on UV, FT-IR, 1D and 2D NMR (¹H, ¹³C, HSQC, and HMBC) spectra and comparison with previously reported literature data. The compound was assigned as 3,5-dimethoxy-4'-O-(2,3-dihydroxy-3-methylbutyl)-dihydrostilbene. This report documents the first isolation of this compound from *I. conferta* and therefore contributes to the phytochemical and chemotaxonomic knowledge of the genus *Indigofera*.

Keywords: *Indigofera conferta*, Isolation, Characterization, Dihydrostilbene

Unassigned and assigned Spectra of compound R1: 3,5-dimethoxy-4'-O-(2,3-dihydroxy-3-methylbutyl)-dihydrostilbene

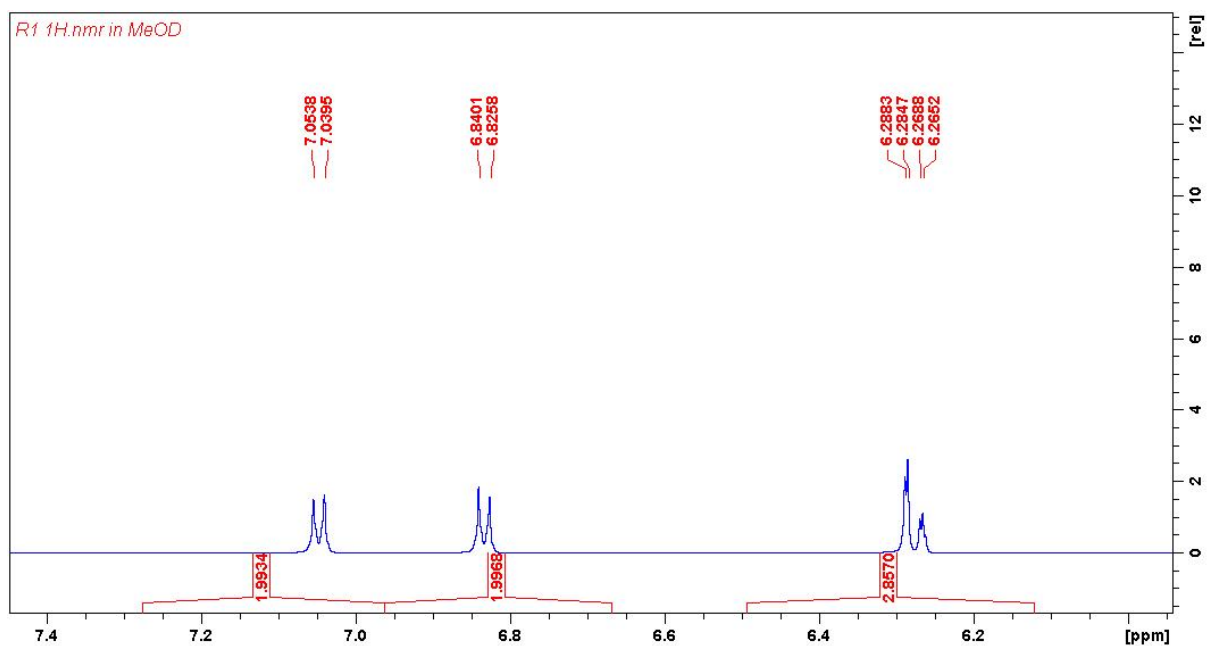


Figure S1a. Expanded ¹H NMR of Aromatic Region of Compound R1

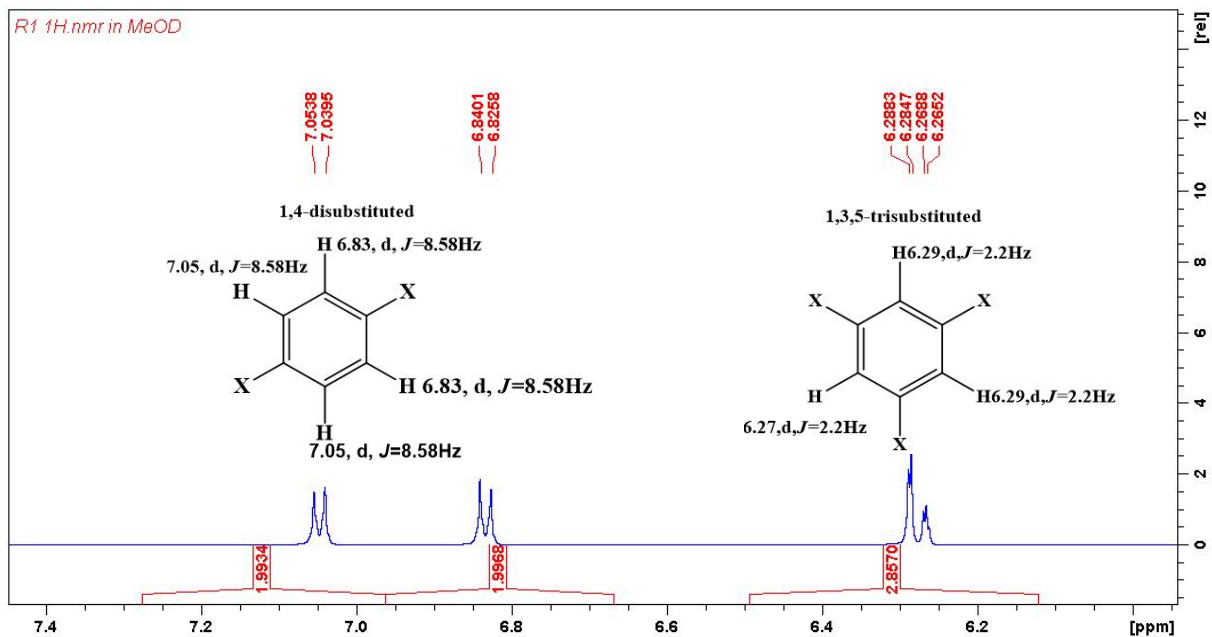


Figure S1b. Expanded ¹H NMR of Aromatic Region of Compound R1 (assigned)

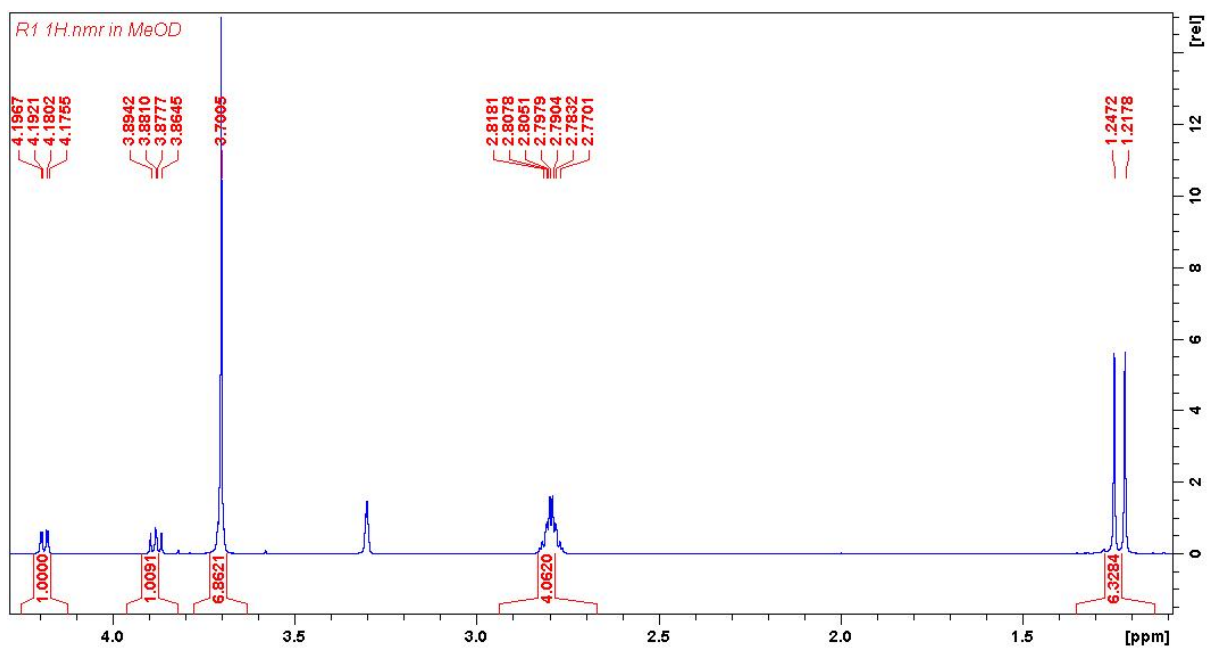


Figure S1c. Expanded ^1H NMR of the Side Chain of Compound R1

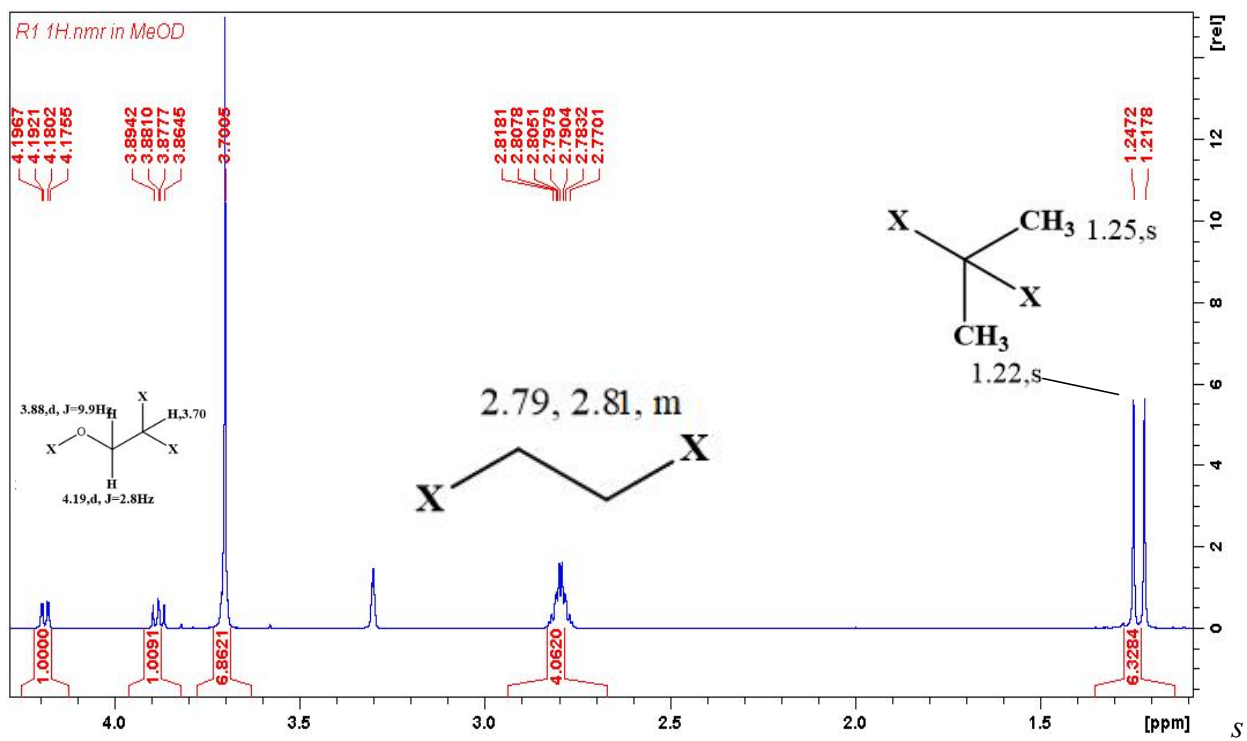


Figure S1d. Expanded ^1H NMR of the Side Chain of Compound R1 (assigned)

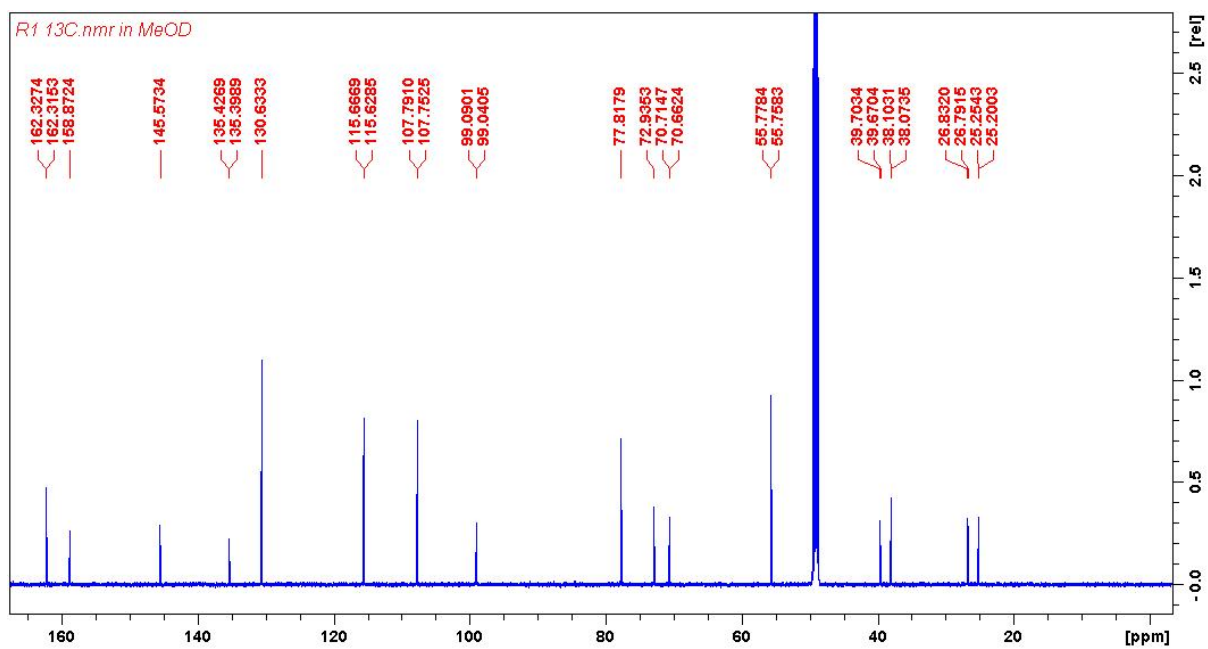


Figure S2a. ¹³C NMR Spectrum of Compound R1

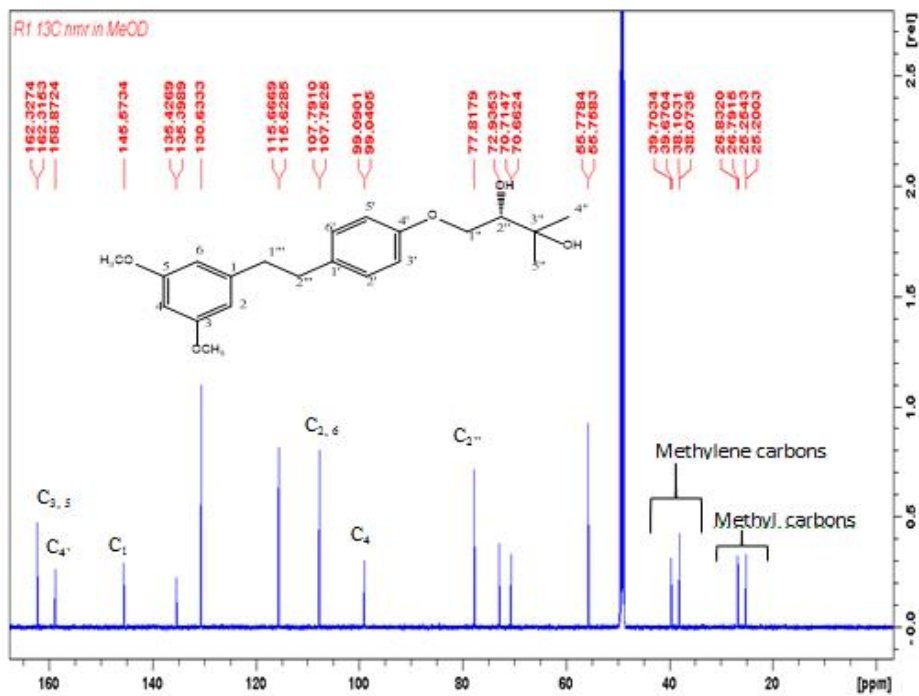


Figure S2b. ¹³C NMR Spectrum of Compound R1 (assigned)

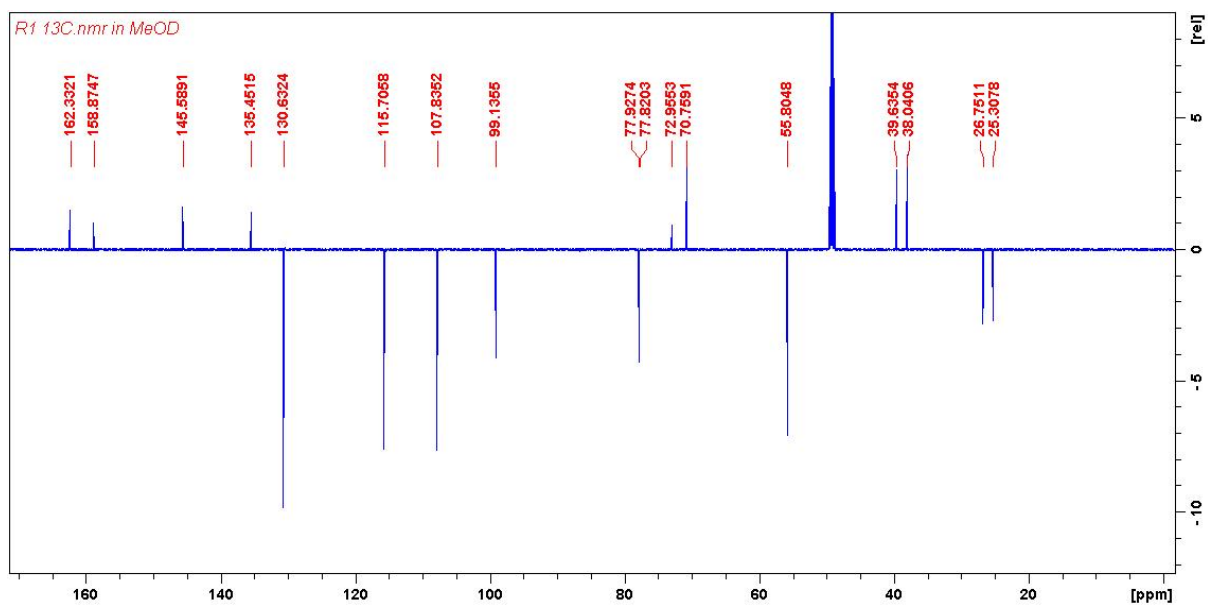


Figure S3a. APT Spectrum of Compound R1

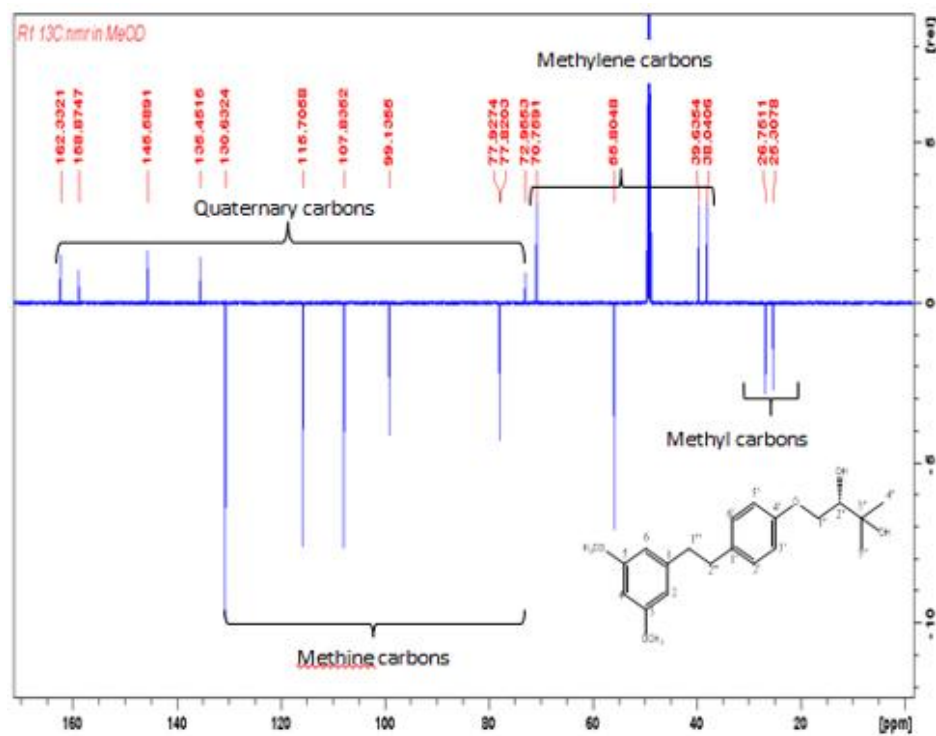


Figure S3b. APT Spectrum of Compound R1 (assigned)

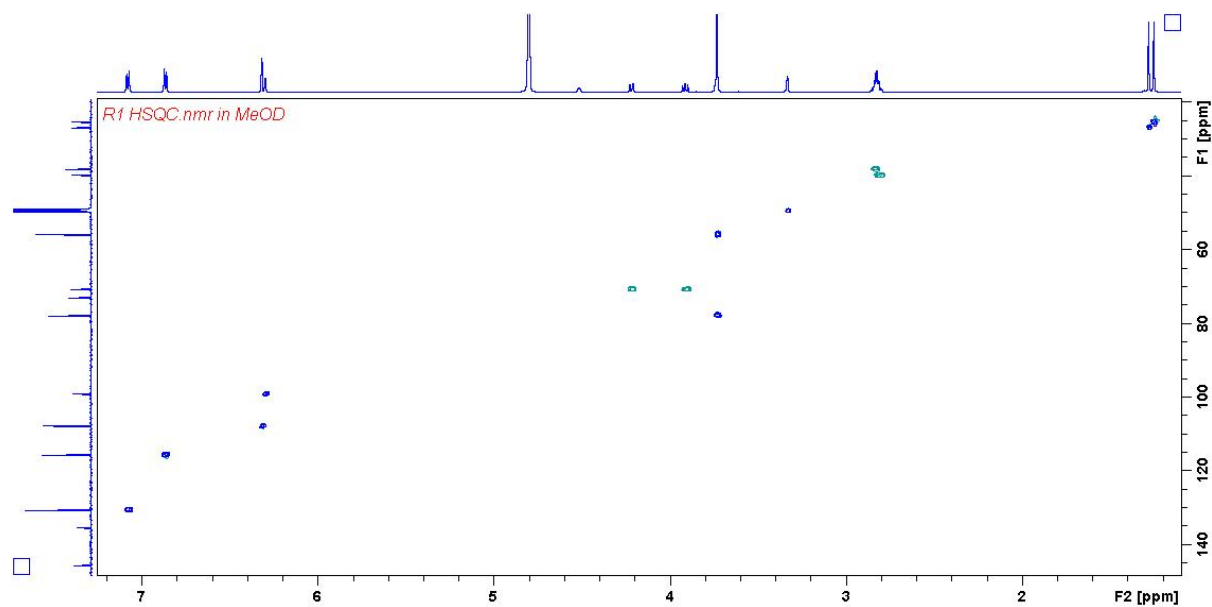


Figure S4a. HSQC Spectrum of Compound R1

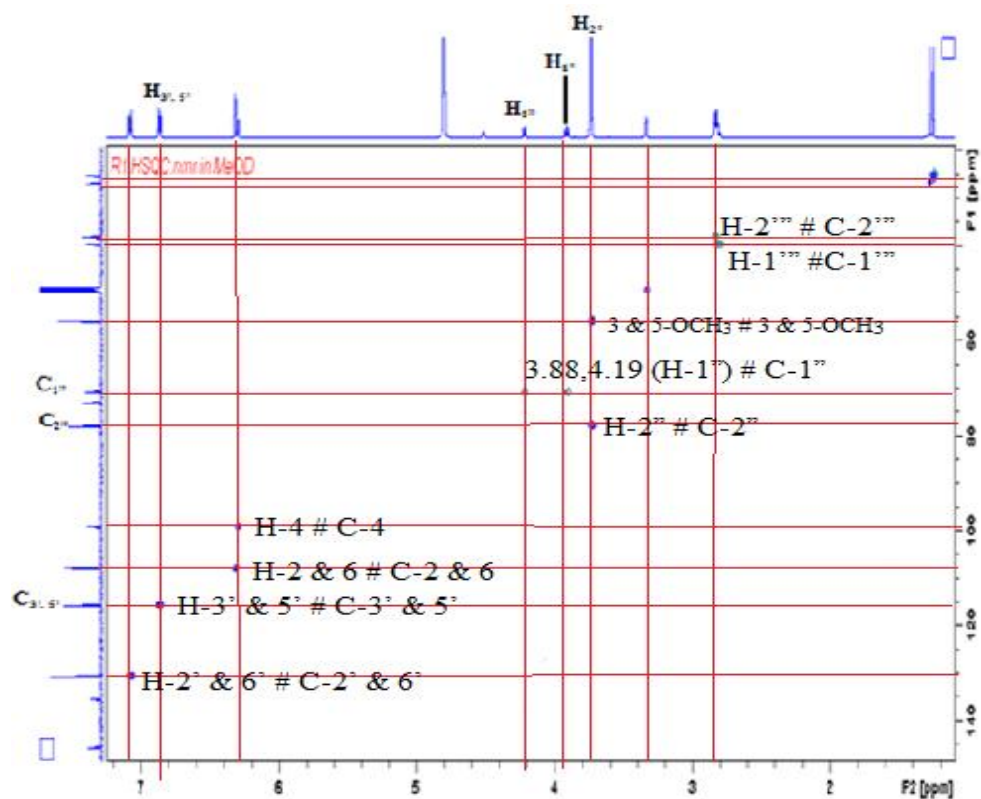


Figure S4b: HSQC Spectrum of Compound R1 (assigned)

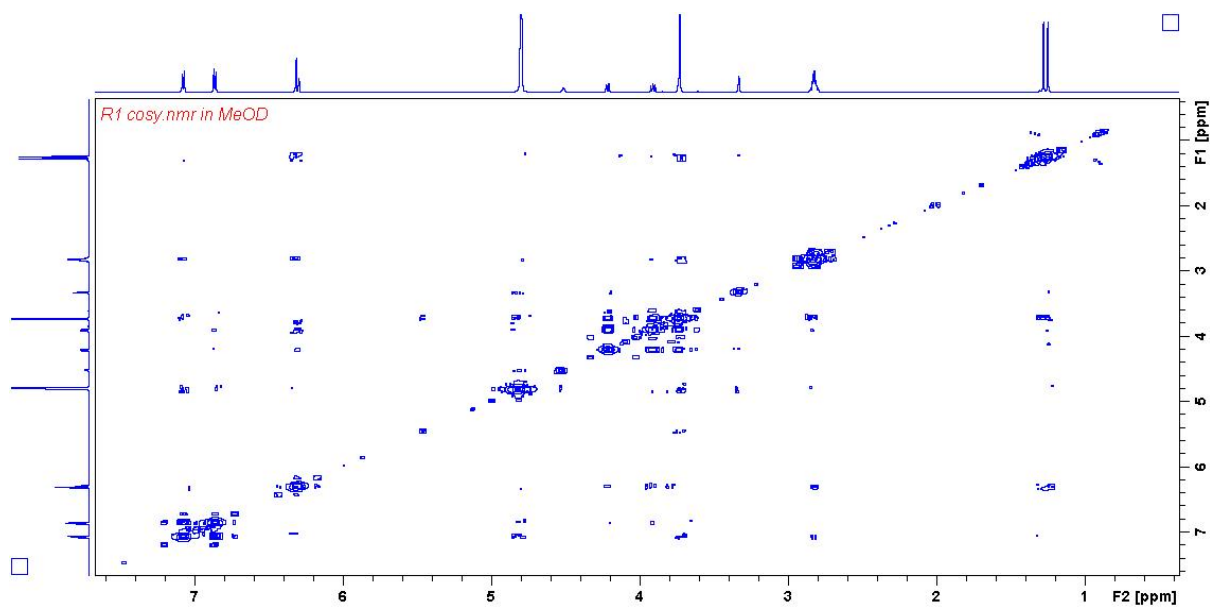


Figure S5a. ^1H - ^1H COSY Spectrum of Compound R1 Showing Important Cross Peaks

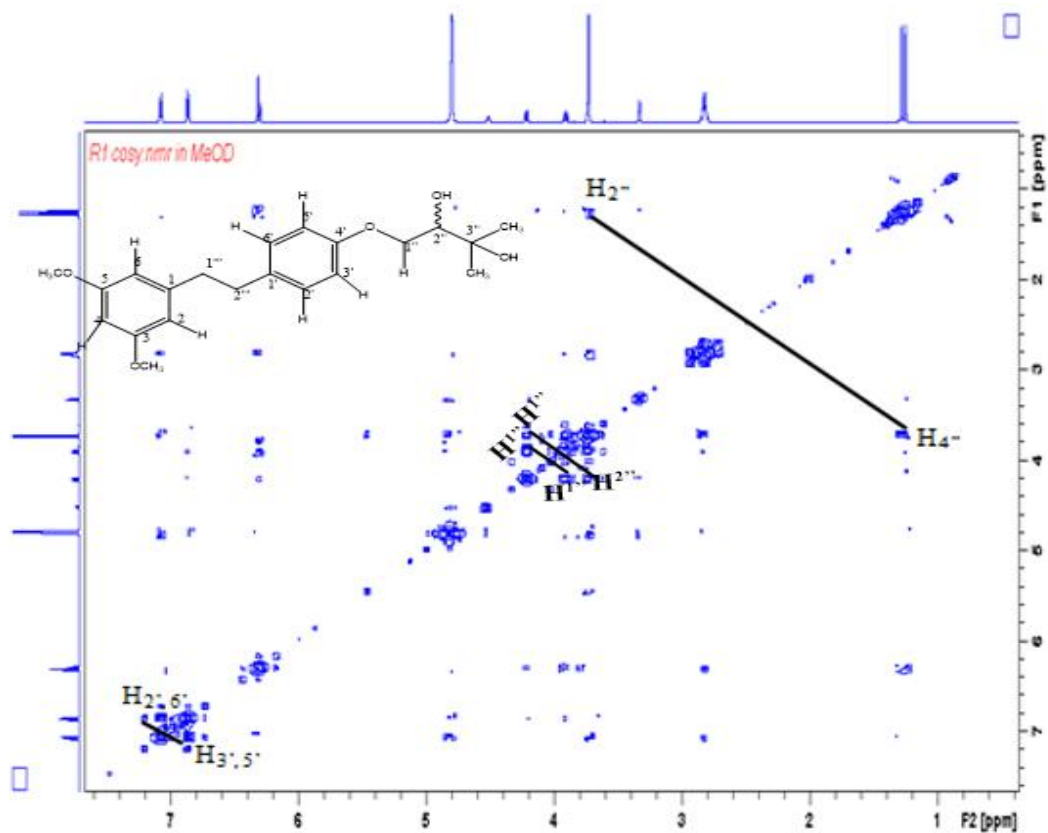


Figure S5b. ^1H - ^1H COSY Spectrum of Compound R1 Showing Important Cross Peaks (assigned)

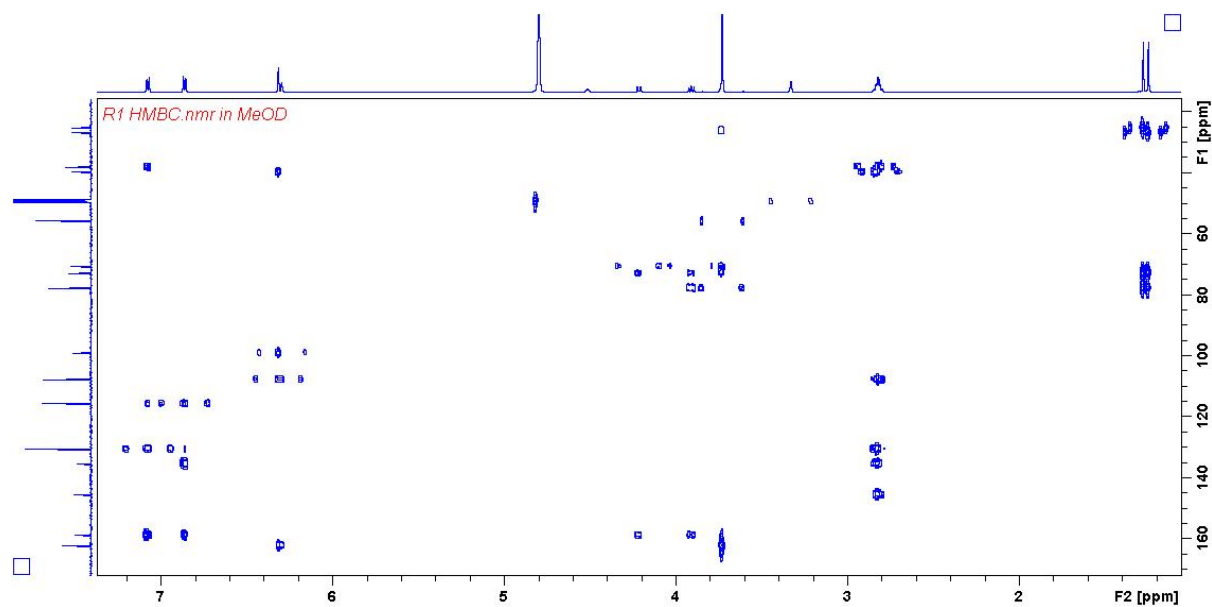


Figure S6a. HMBC Spectrum of Compound R1

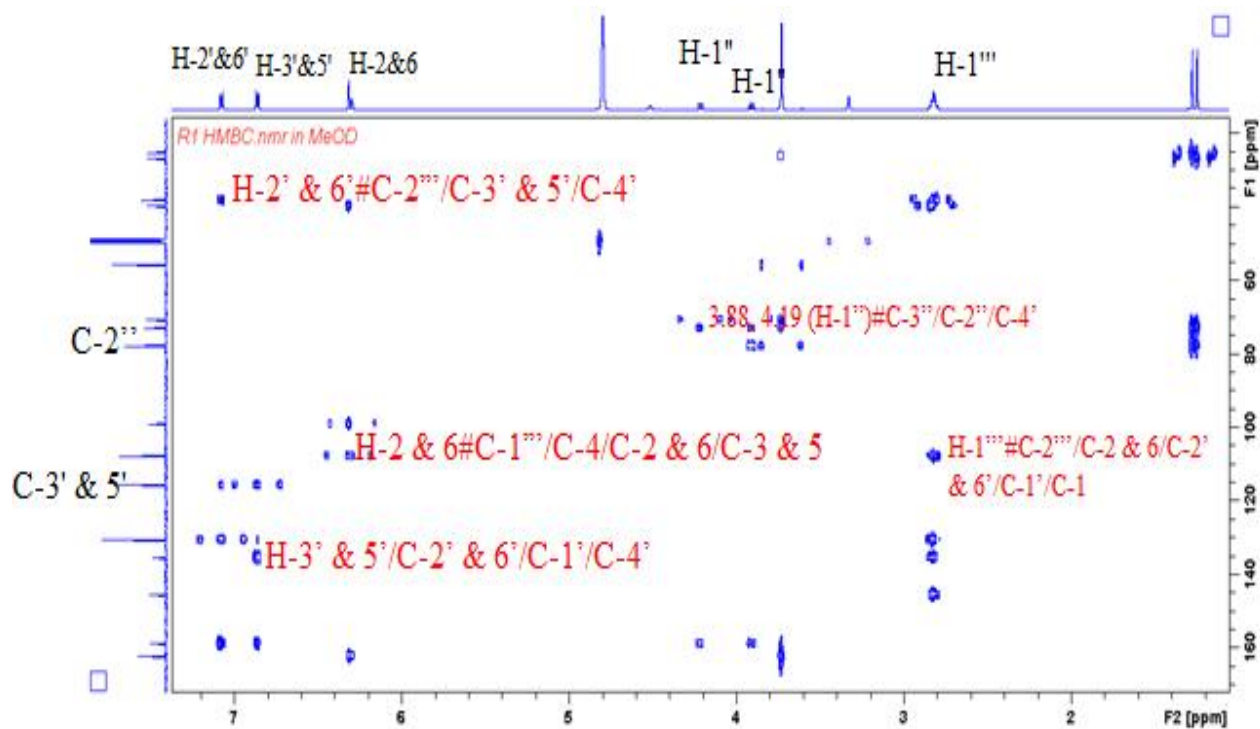


Figure S6b. HMBC Spectrum of Compound R1 (assigned)

Table S1. 1D and 2D NMR Spectral Summary Data for Compound R1

Position	δH , J in Hz	δC	APT	COSY	HMBC
1	-	145.6	C	-	
2, 6	6.29, 2.16 Hz	107.8	CH	-	C-1''', 4, 2&6, 3&5
3, 5	-	162.3	C	-	
4	6.27, 2.16 Hz	99.1	CH	-	C-2&6, 3&5
1'	-	135.4	C	-	
2', 6'	7.05, 8.58 Hz	130.6	CH	H-3' & 5'	C-2''', 3'&5', 4'
3' 5'	6.83, 8.58 Hz	115.7	CH	-	C-2'&6', 1', 4'
4'	158.9	C	-	
1''	3.88,4.19	70.7	CH ₂	H-2''	C-3'', 2'', 4'
2''	3.70	77.8	CH	H-1''', 3''-Me	H- C-1'', 3'', 4'', 3&5
3''	72.9	C	-	
1'''	2.81	39.7	CH ₂	-	C-2''', 2&6, 2'&6', 1', 1
2'''	2.78	38.1	CH ₂	-	C-1''', 2&6, 1
3''-Me (a)	1.22	25.3	CH ₃	-	C-5'', 1'', 3'', 2''
3''-Me (b)	1.25	26.8	CH ₃	-	C-4'', 1'', 3'', 2''
3,5-OMe	3.70	55.8	OCH ₃	-	

C: Carbon, H: Hydrogen, Me: Methyl, OMe: Methoxy, Hz: Hertz, J: Coupling constant

Table S2. ¹H & ¹³C-NMR Data of R1 Compared with those Reported in Literature

Position	δH	δC	δC (Musa <i>et al.</i> , 2008)	δH
1	145.6	145.0
2, 6	6.29	107.8	115.5	6.45
3, 5	162.3	162.3
4	6.27	99.1	99.1	6.49
1'	135.4	135.3
2', 6'	7.05	130.6	130.5	6.94
3' 5'	6.83	115.7	115.6	6.73
4'	158.9	158.1
1''	3.88,4.19	70.7	70.2	3.76,3. 81
2''	3.70	77.8	76.7	3.55
3''	72.9	71.9
1'''	2.81	39.7	39.4	2.81
2'''	2.78	38.1	38.2	2.78
3'''-Me	1.22	25.3	27.1	1.04
	1.25	26.8	26.5	1.15
3,5-OMe	3.70	55.8	55.5	3.36

C: Carbon, H: Hydrogen, Me: Methyl, OMe: Methoxy, Hz: Hertz, J: Coupling constant

References

Musa A, Haruna AK, Ilyas M, Ahmadu A, Gibbons S, Mukhlesur Rahman M. 2008. Dihydrostilbenes from *Indigofera pulchra*. Nat. Prod. Commun. 3(5):805-808, doi: 10.1177/1934578x0800300524.