SUPPLEMENTARY MATERIAL

A New Depsidone Derivative from Mangrove Sediment Derived Fungus *Lasiodiplodia theobromae*

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Abstract

A new depsidone derivative botryorhodine I (**1**), along with eight known compounds (**2-9**) were obtained from solid rice cultures of the fungal strain, *Lasiodiplodia theobromae* M4.2-2 isolated from a mangrove sediment sample. The structures of the isolated compounds were elucidated on the basis of 1D and 2D NMR analysis as well as by HRESIMS. All compounds were evaluated for their cytotoxic potential against the mouse lymphoma cell line L5178Y as well as for their antibacterial activities against a panel of Gram-positive and Gram-negative bacterial strains. Compound **3** revealed potent cytotoxic activity with an IC_{50} of 7.3 μM whereas compound **7** showed selective anti-bacterial activity against different *S. aureus* and *E. faecium* bacterial strains with MIC value of 25 µg/ml.

Keywords: *Lasiodiplodia theobromae*; fungi; mangrove sediment; depsidones; botryorhodines; biological activity

Table of Contents

Table S1: NMR data of compound **1** measured in methanol-d_4 (^{1}H at 600 MHz and ^{13}C at 150 MHz).

Position	δ_C, type	δ_H (J in Hz)
1	113.8, C	
2	162.8, C	
3	117.1, C	
4	162.4, C	
5	116.2, CH	6.61, s
6	145.8, C	
7	165.9, C	
8	54.8, CH_2	4.95, s
9	21.4, CH_3	2.41, s
1`	113.9, CH	6.43, s
2`	144.5, C	
3`	135.1, C	
4`	135.5, C	
5`	144.4, C	
6`	120.6, C	
7`	16.4, CH_3	2.35, s

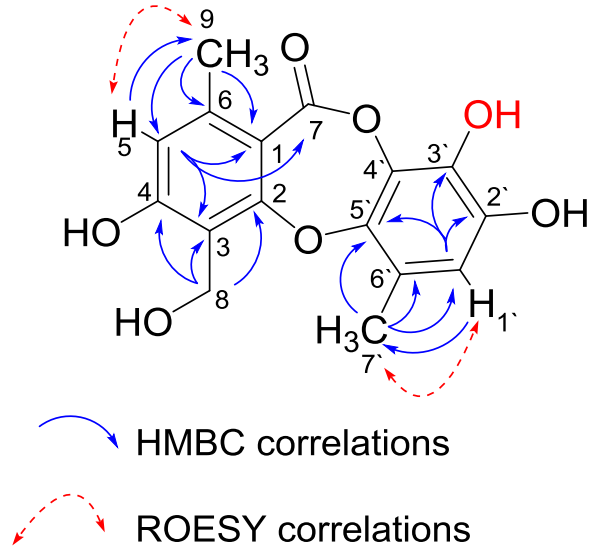

Figure S1: HMBC and ROESY correlations of compound **1**.

Table S2: Measured and reported optical rotation values for compounds **7**-**9**

Compound	Measured optical rotation	Reported optical rotation (reference)
(+)-(*R*)-de-*O*-methyl-lasiodiplodin (7)	$[\alpha]_D$ + 30.7° (c 0.58, MeOH)	$[\alpha]_D$ +35.5° (c 0.58, MeOH) (Xu et al. 2014)
(-)-(*R*)-nordinone (8)	$[\alpha]_D$ - 46.6° (c 0.12, MeOH)	$[\alpha]_D$ -49.3° (c 0.12, MeOH) Renamed lasicicol (Xu et al. 2014)
(-)-(*R*)-mellein (9)	$[\alpha]_D$ -89.2° (c 1.0, EtOH) $[\alpha]_D$ -109.4° (c 1.0, $CHC1_3$)	$[\alpha]_D$ -92.5° (c 1.0, EtOH) (Aldridge et al. 1971) $[\alpha]_D$ -100° (c 1.0, $CHC1_3$) (Schulz et al. 1995)

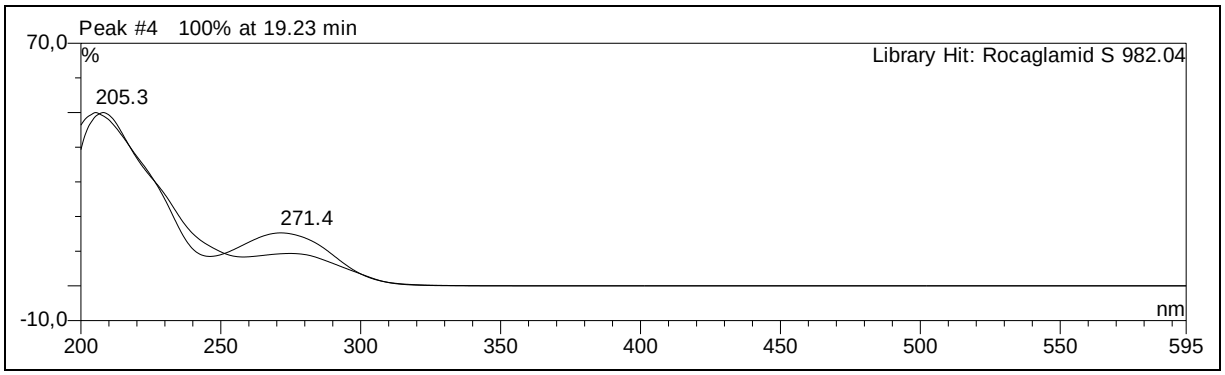

Figure S2: UV spectrum of compound **1**.

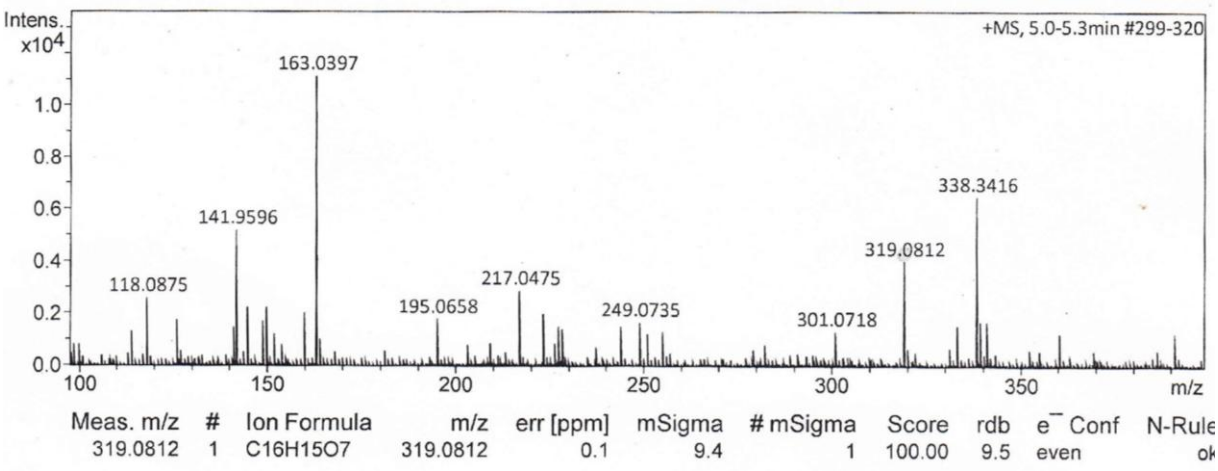

Figure S3: HRESIMS spectrum of compound **1**.

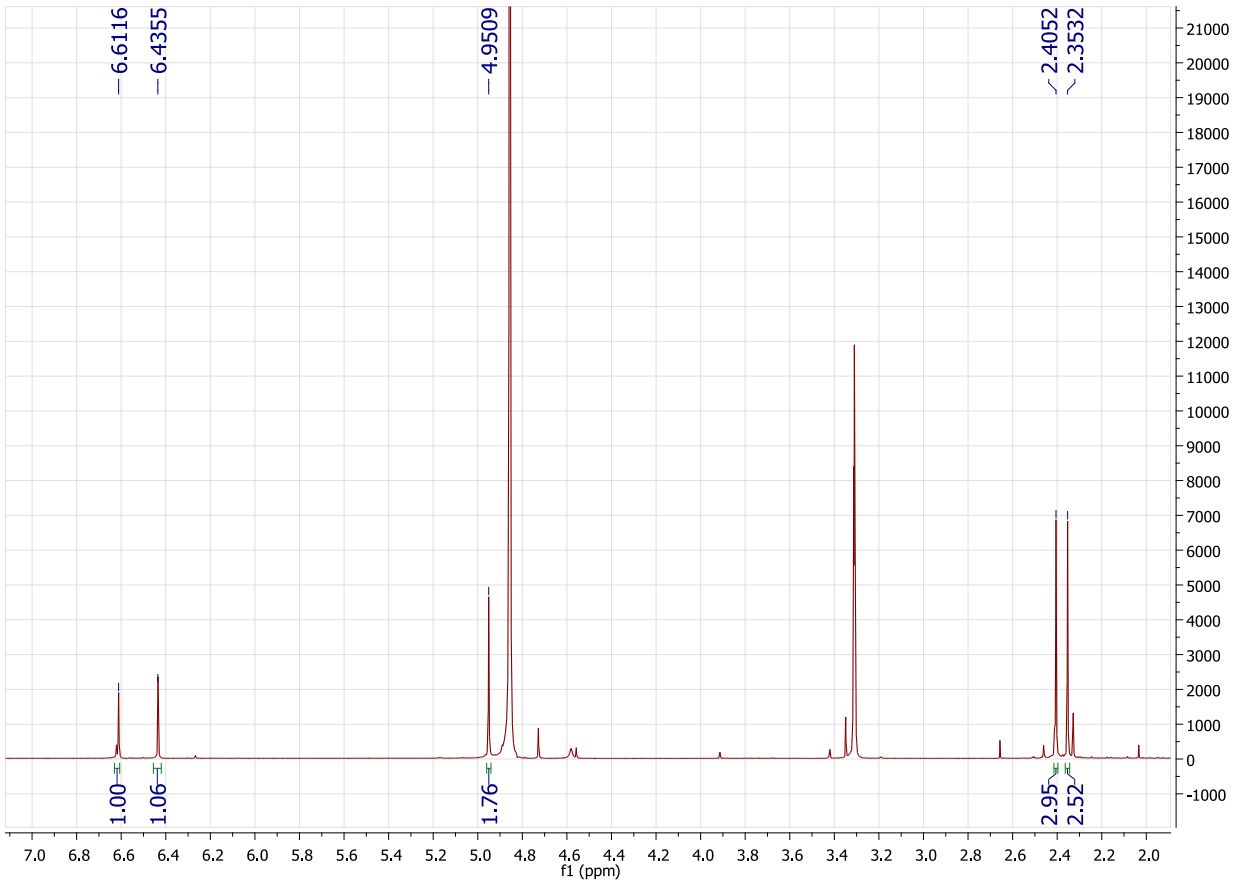

Figure S4: ^{1}H NMR (600 MHz, MeOD) spectrum of compound **1**.

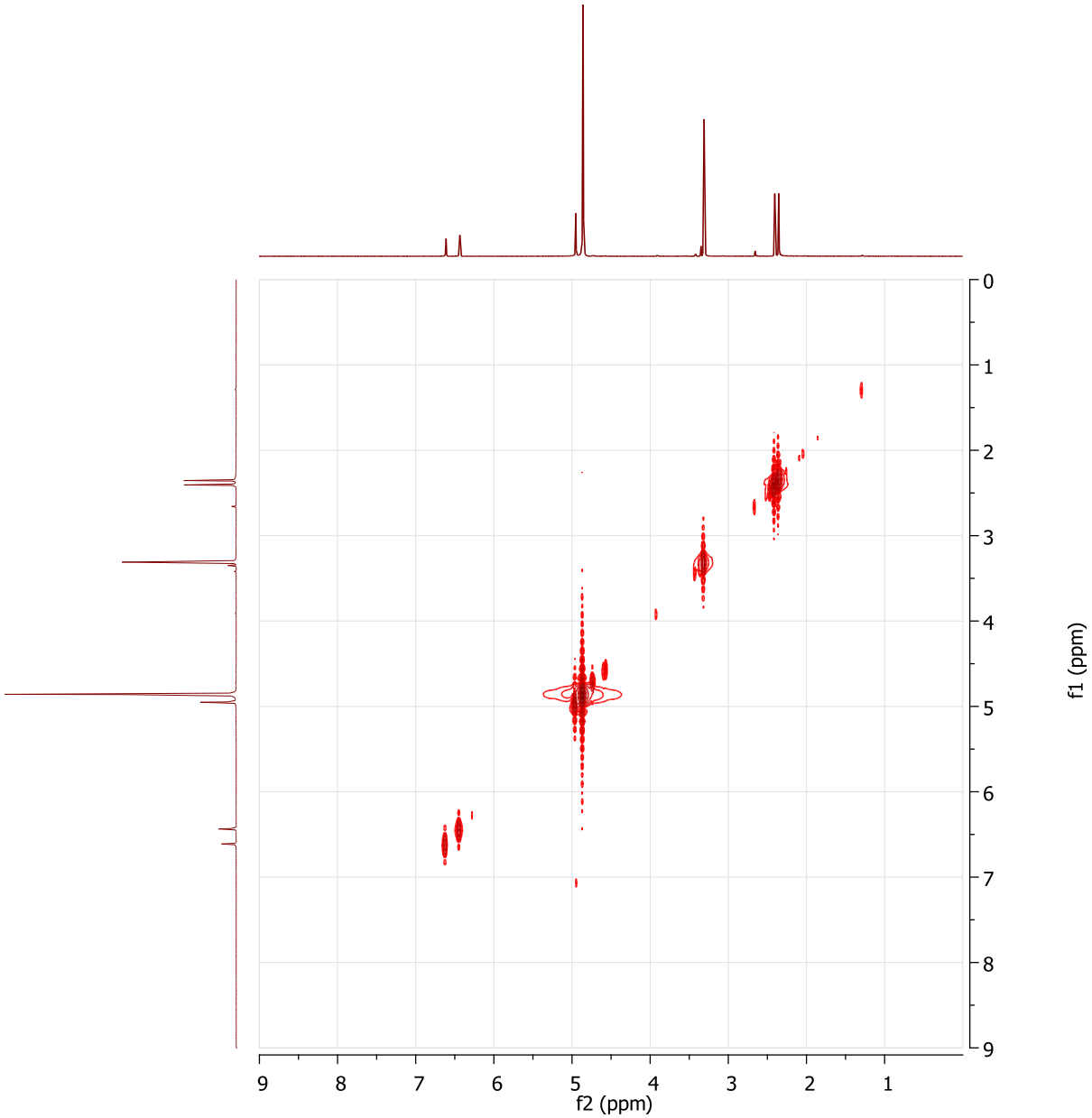

Figure S5: ^{1}H-^{1}H COSY (600 MHz, MeOD) spectrum of compound **1**.

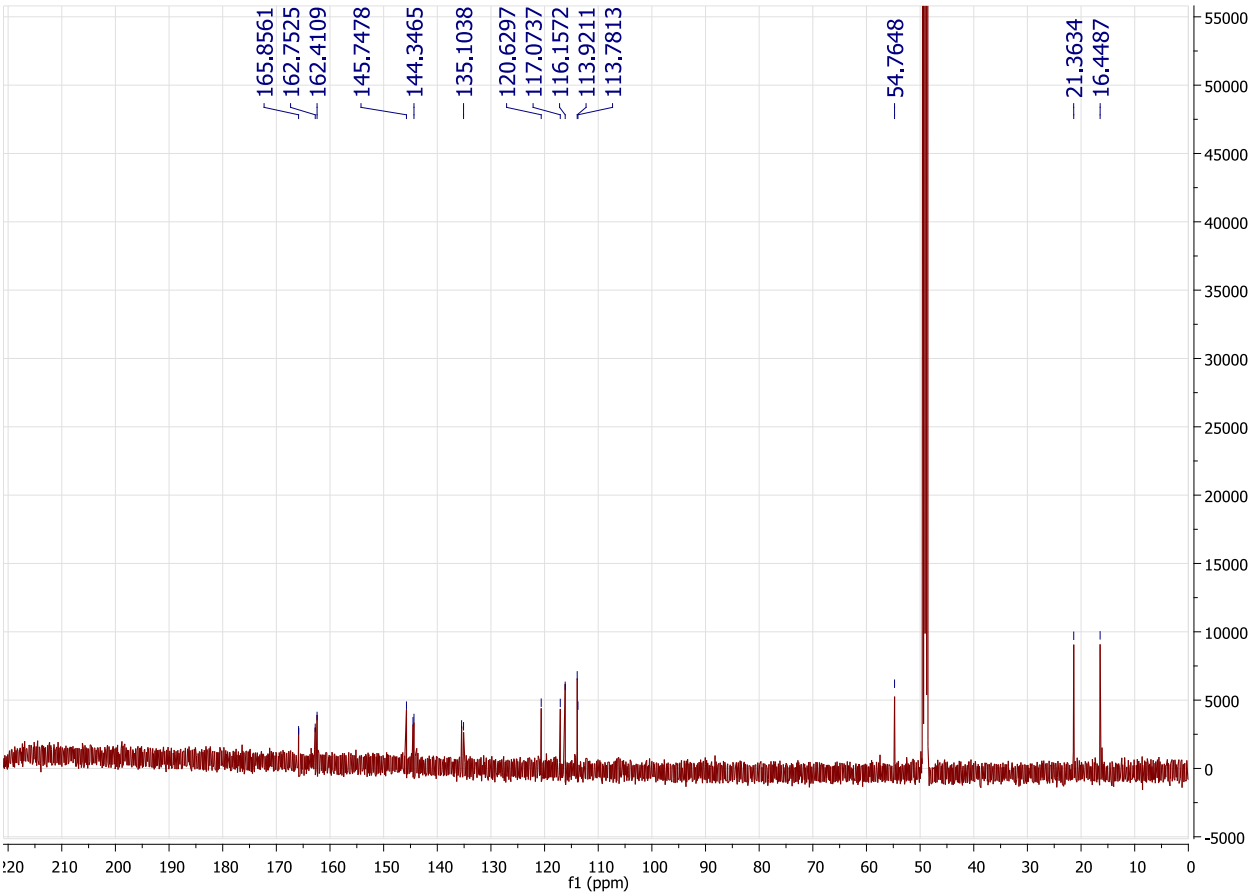

Figure S6: ^{13}C NMR (150 MHz, MeOD) spectrum of compound **1**.

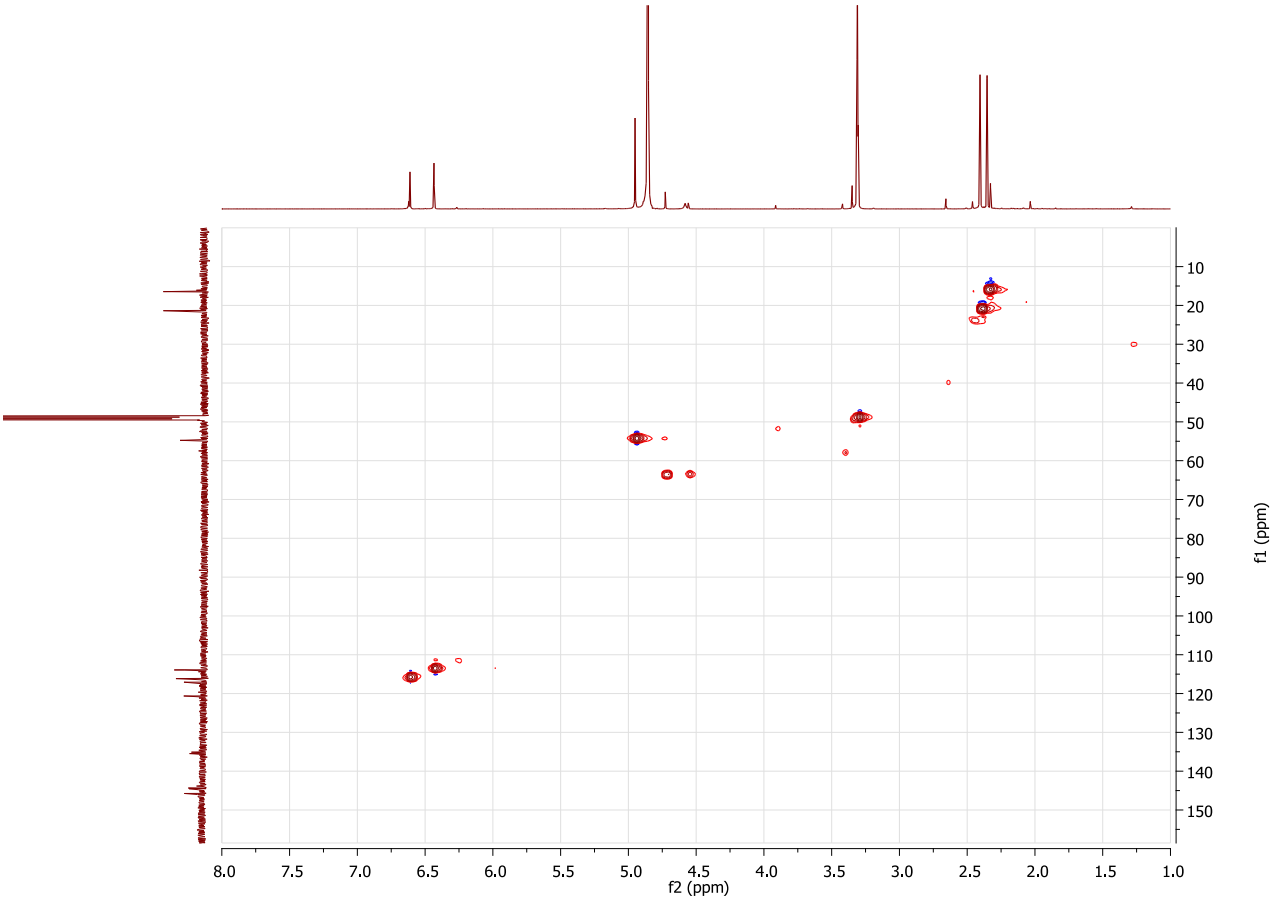

Figure S7: HSQC (600 and 150 MHz, MeOD) spectrum of compound **1**.

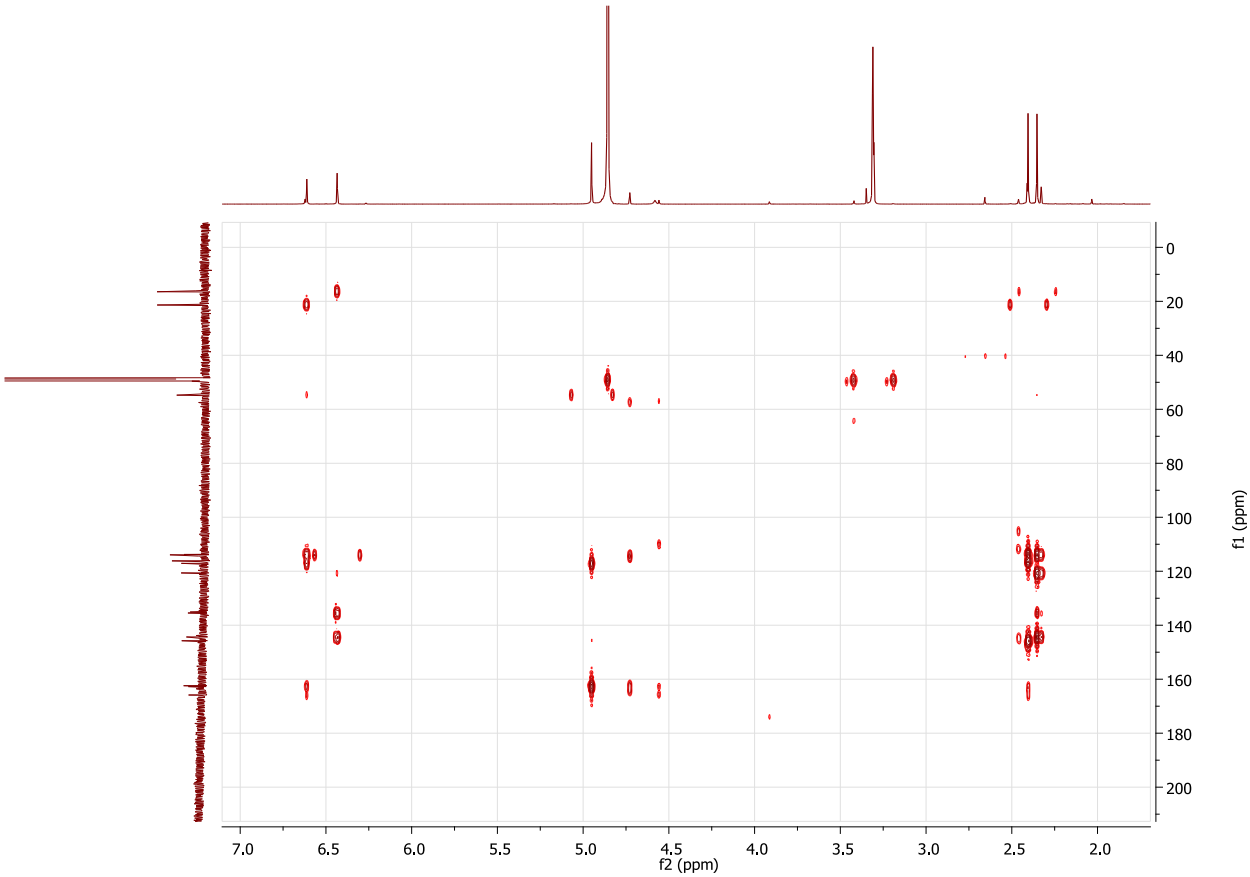

Figure S8: HMBC (600 and 150 MHz, MeOD) spectrum of compound **1**.

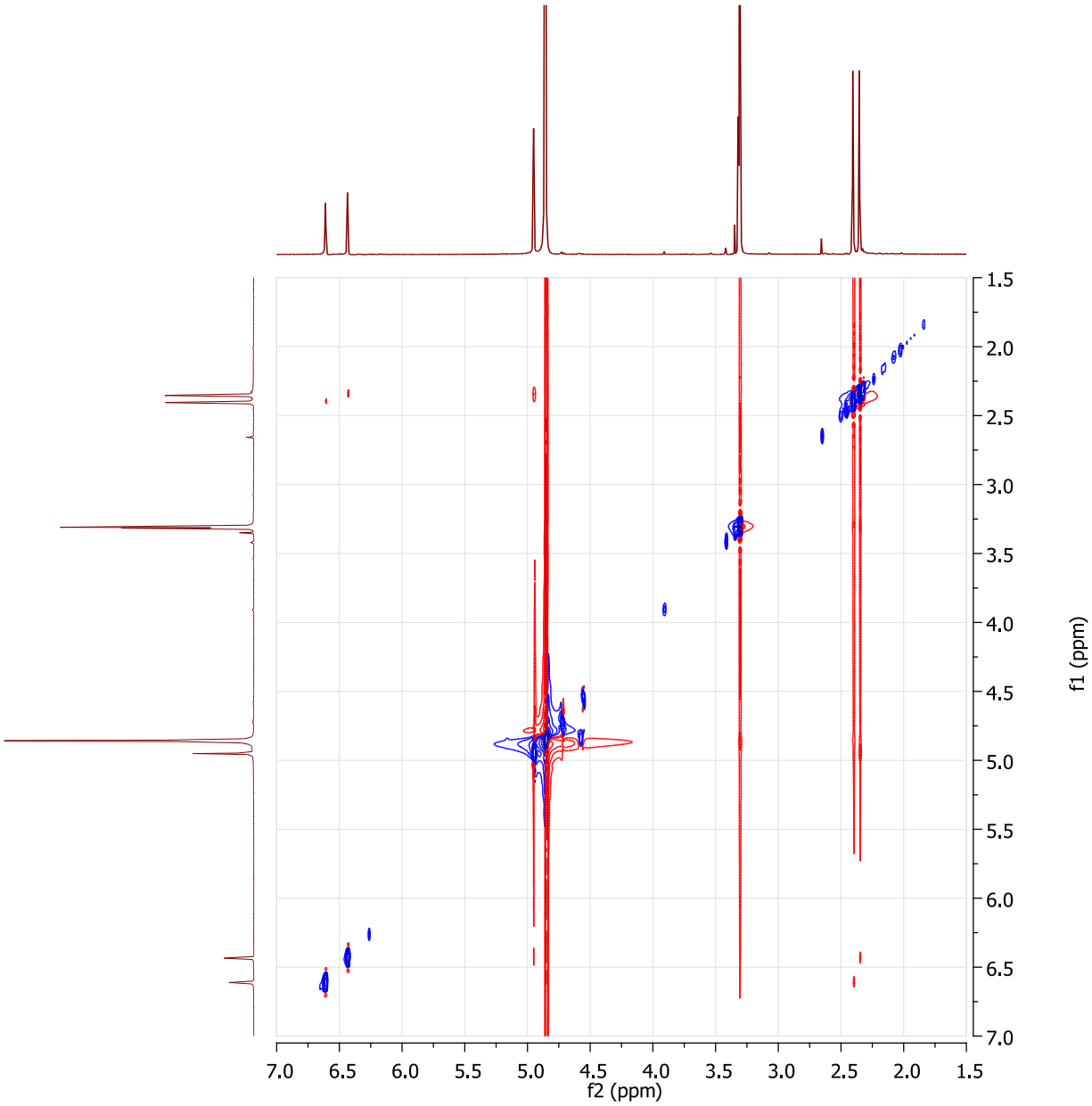

Figure S9: ROESY (600 MHz, MeOD) spectrum of compound **1**.

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