

# Supplementary Materials for

## New Acyclic Cytotoxic Jasplakinolide Derivative from the Marine Sponge *Jaspis splendens*

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## ABSTRACT

A new acyclic jasplakinolide congener (**2**), another acyclic derivative requiring revision (**4**), together with two jasplakinolide derivatives including the parent compound jasplakinolide (**1**) were isolated from the Indonesian marine sponge *Jaspis splendens*. The chemical structures of the new and known compounds were unambiguously elucidated based on HRESIMS and exhaustive 1D and 2D NMR spectral analysis as well as comparison of their NMR data with those of jasplakinolide (**1**). The isolated jasplakinolides inhibited the growth of the mouse lymphoma (L5178Y) cells *in vitro* with IC<sub>50</sub> values in the low micromolar to nanomolar range.

**Keywords:** *Jaspis splendens*, jasplakinolide Z<sub>6</sub>, jasplakinolide Z<sub>5a</sub>, cytotoxic activity.

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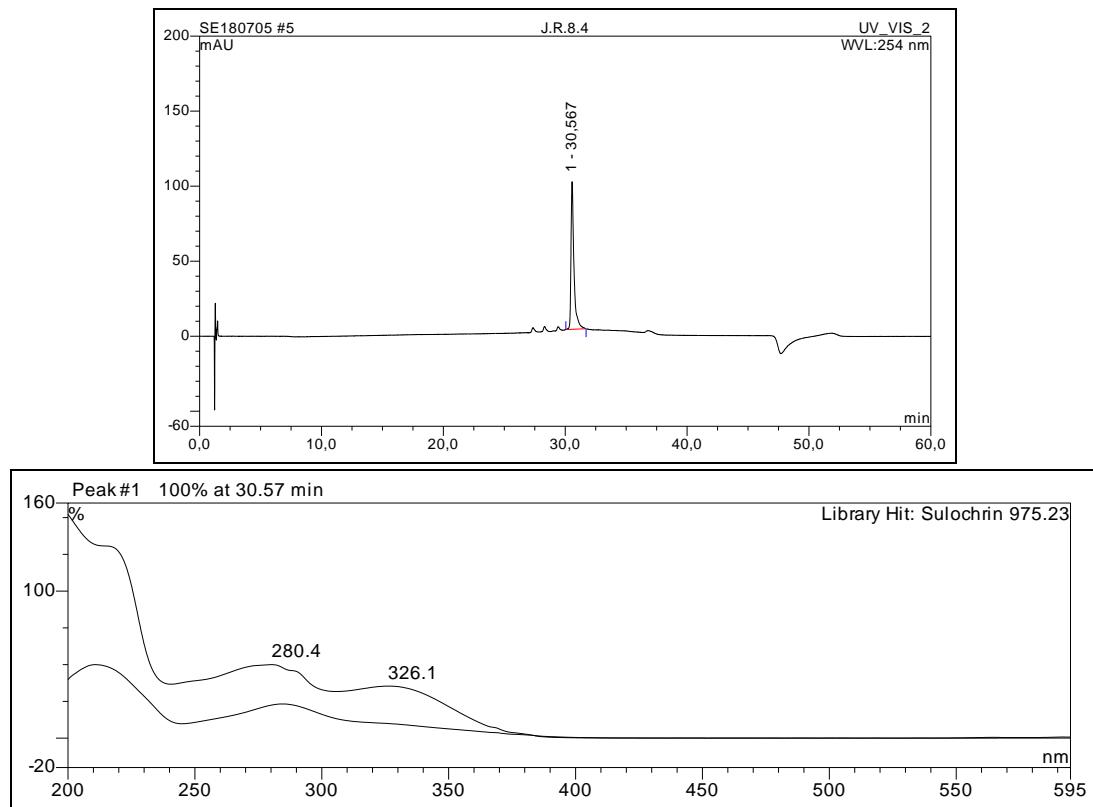


Figure S1. HPLC chromatogram of 2

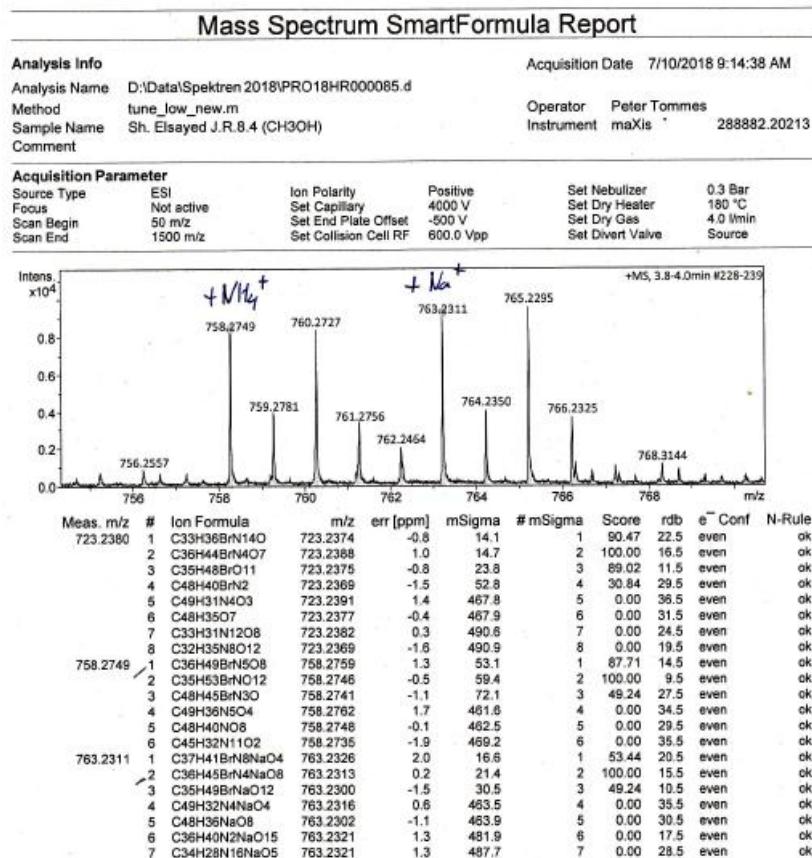


Figure S2. HRESIMS spectrum of 2

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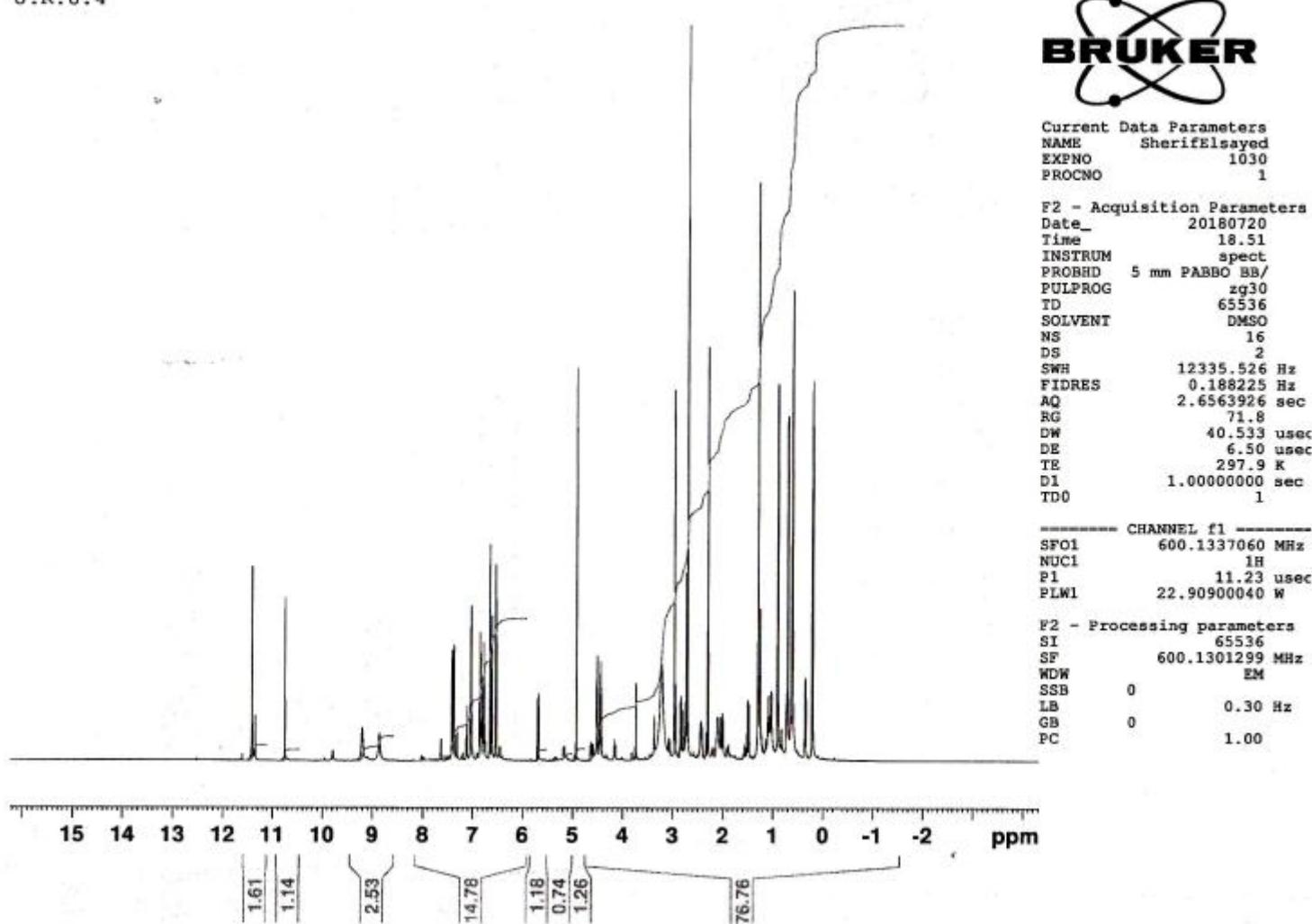


Figure S3.  $^1\text{H}$ -NMR spectrum of 2 in  $\text{DMSO}-d_6$

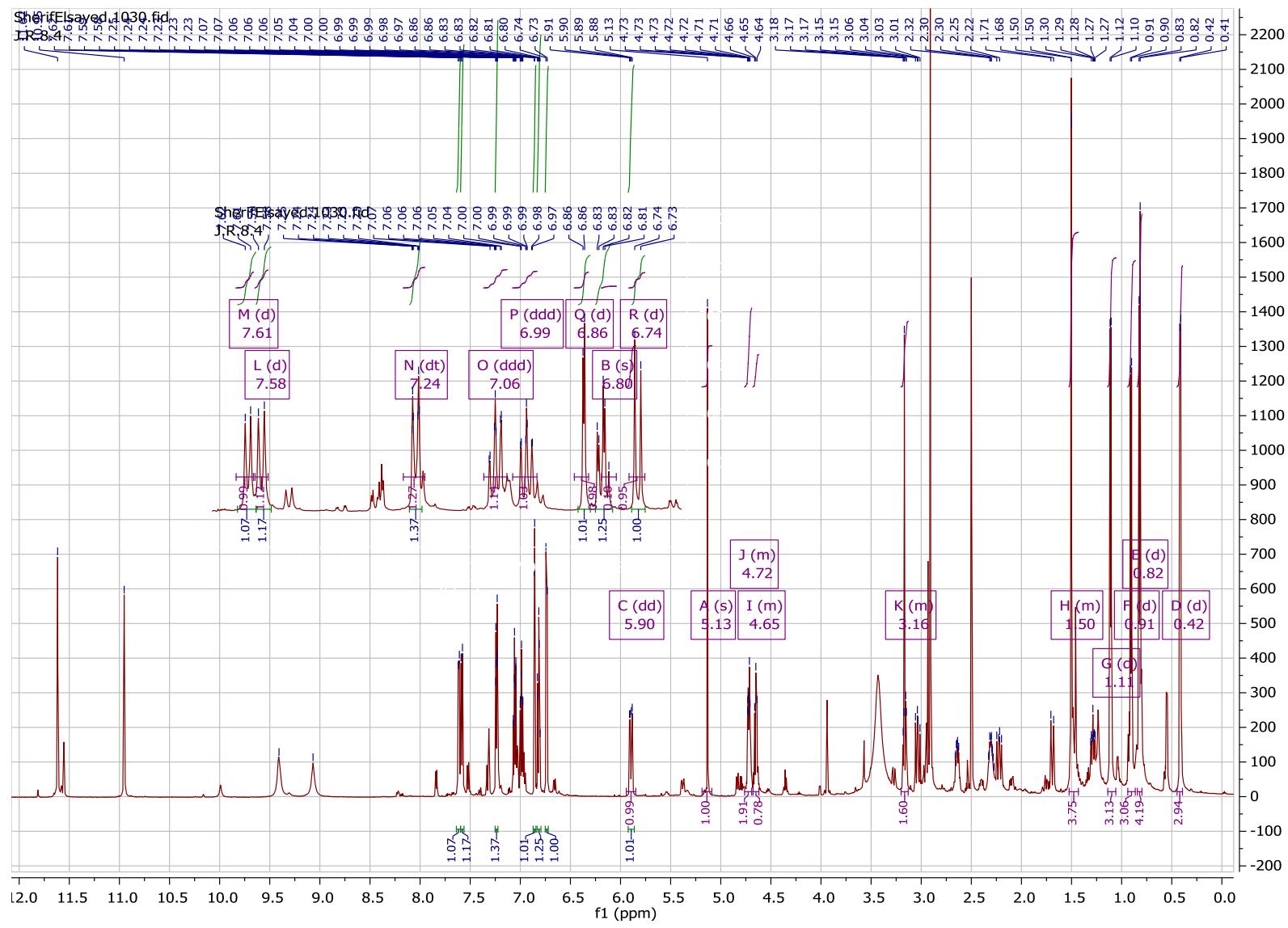
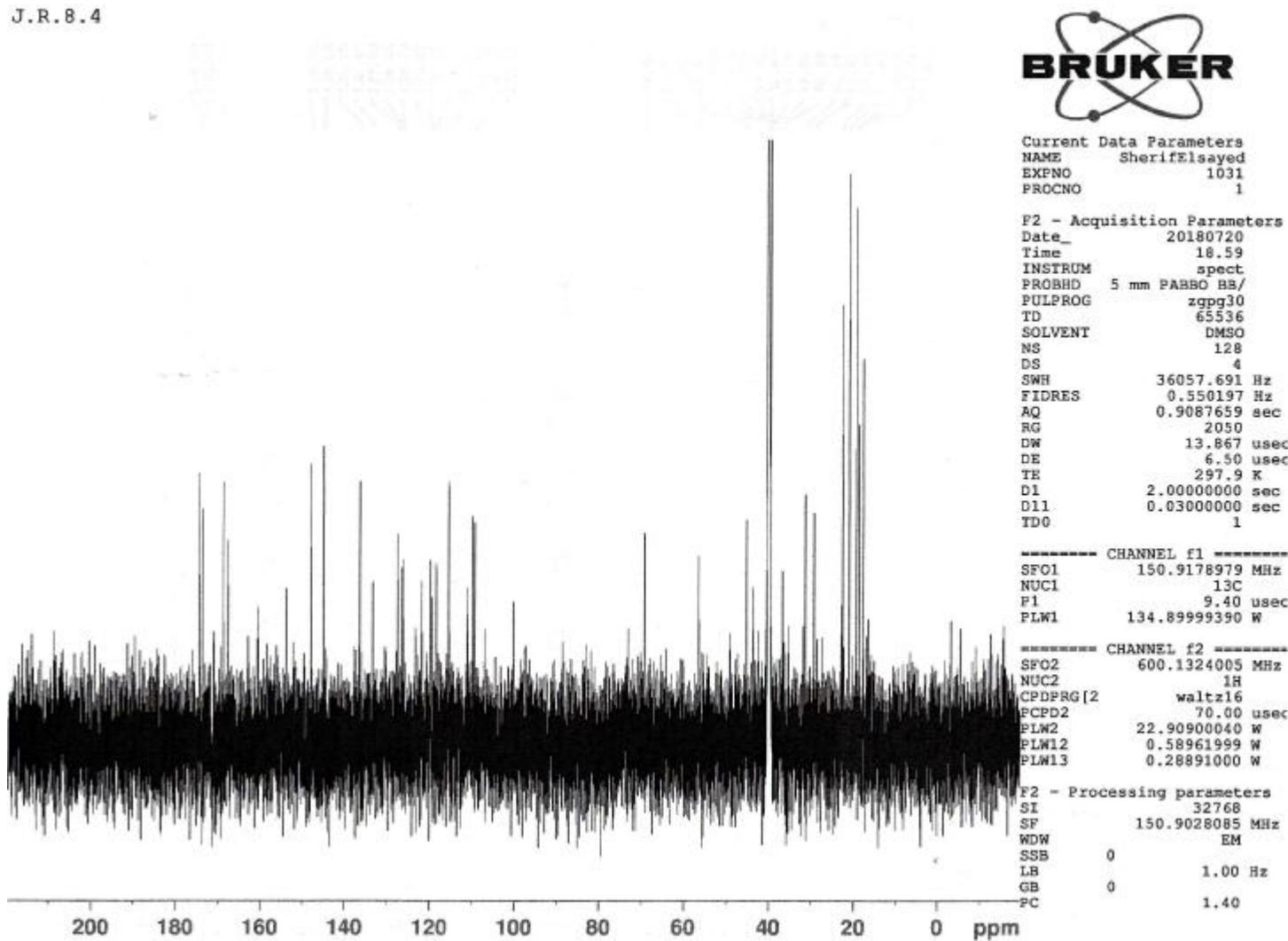


Figure S3a.  $^1\text{H}$ -NMR spectrum of **2** in  $\text{DMSO}-d_6$

Figure S4.  $^{13}\text{C}$ -NMR spectrum of **2** in  $\text{DMSO}-d_6$

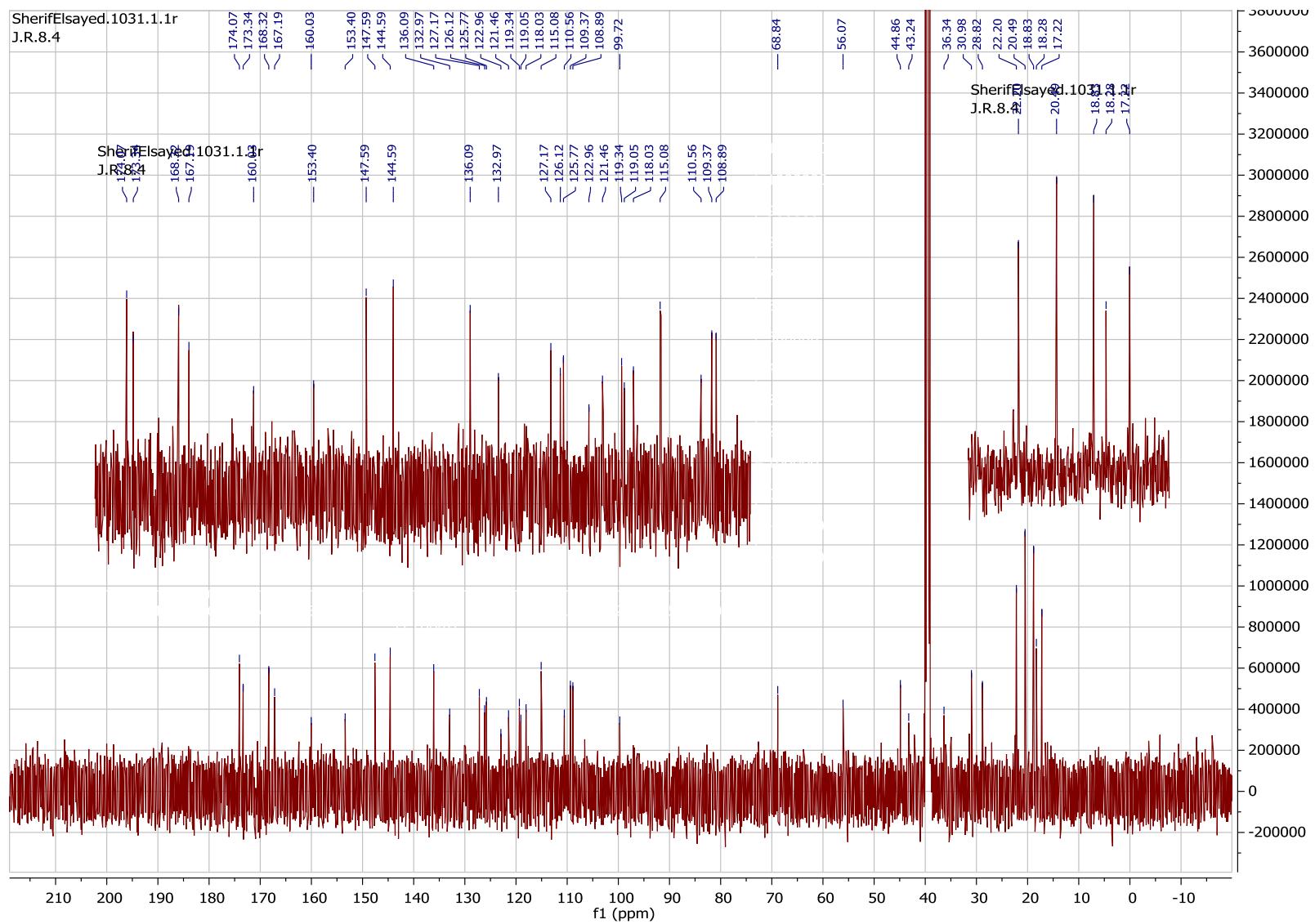
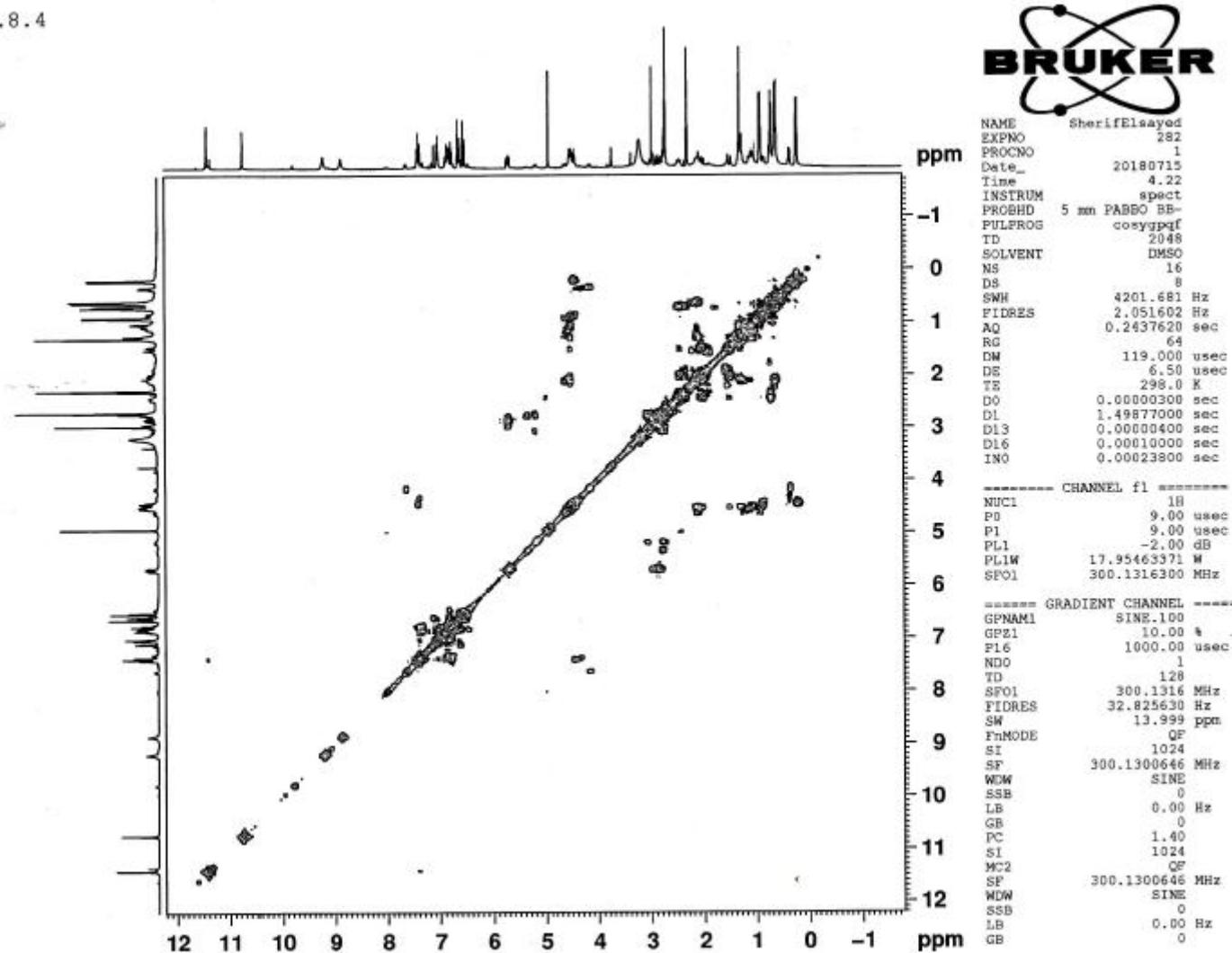


Figure S4a.  $^{13}\text{C}$ -NMR spectrum of **2** in  $\text{DMSO}-d_6$

Figure S5.  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of **2** in  $\text{DMSO}-d_6$

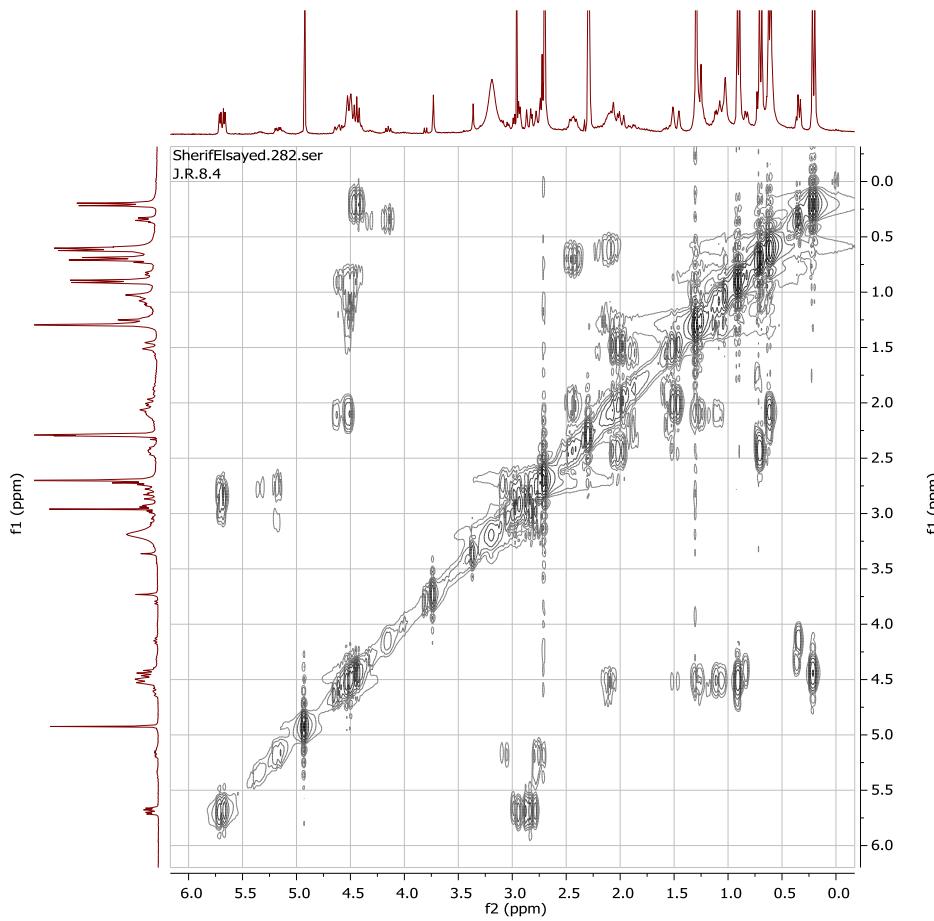
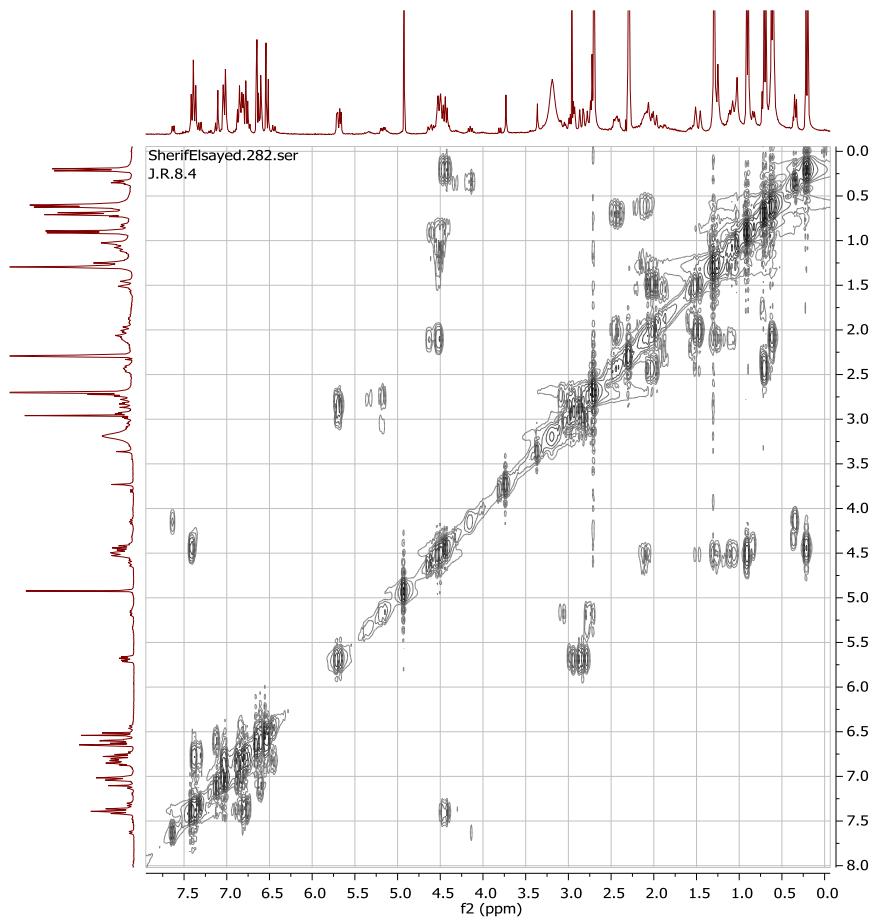
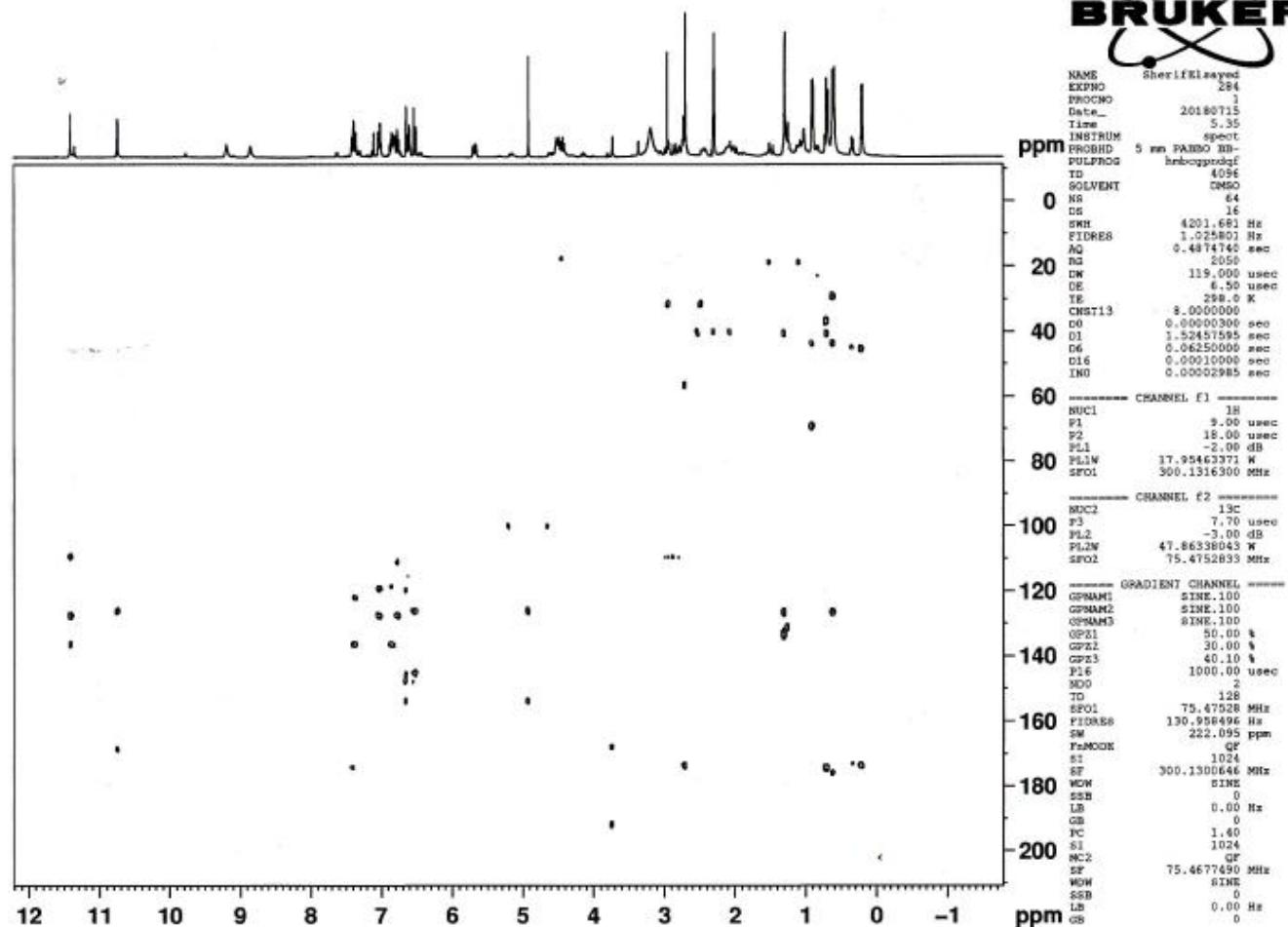


Figure S5a.  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of **2** in  $\text{DMSO}-d_6$

Figure S6. gHMBC spectrum of **2** in DMSO-*d*<sub>6</sub>

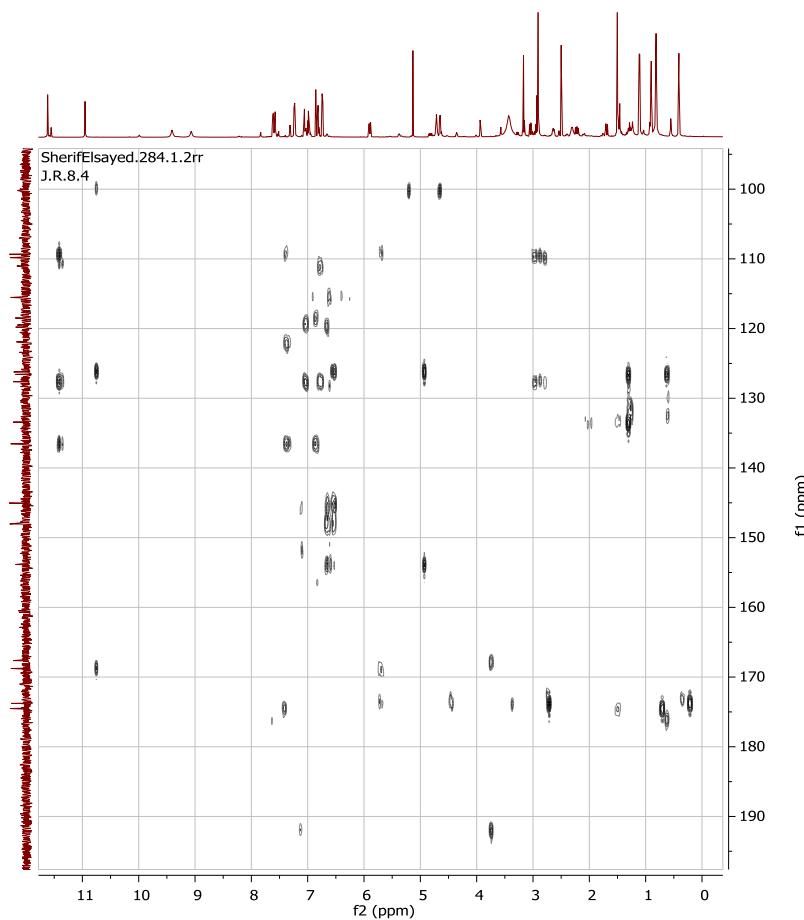
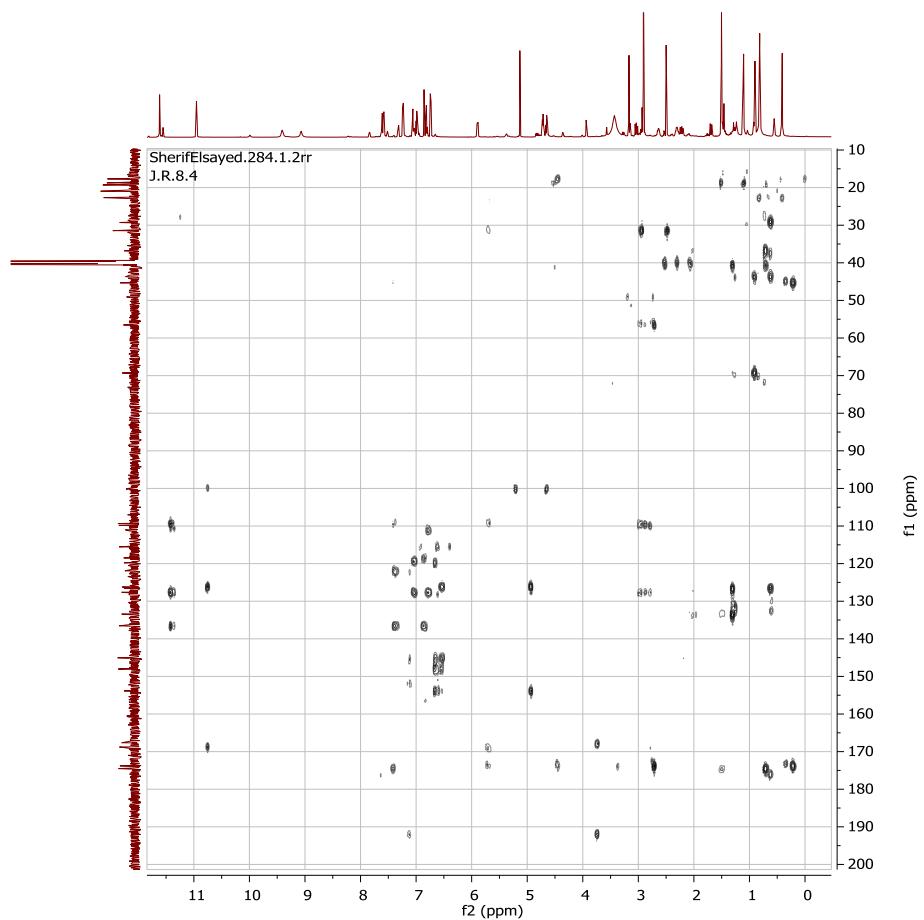


Figure S6a. gHMBC spectrum of **2** in  $\text{DMSO}-d_6$

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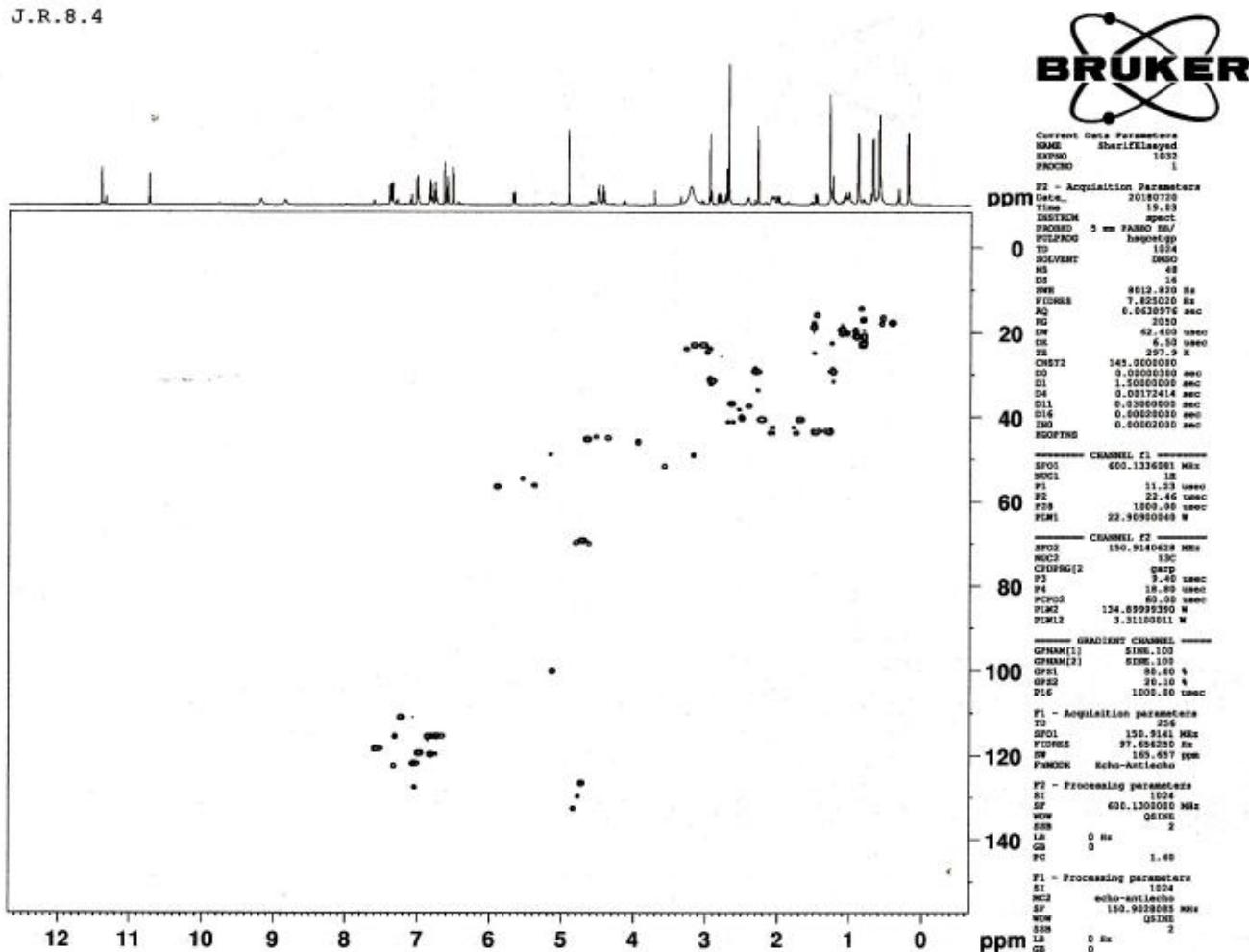


Figure S7. gHMQC spectrum of **2** in DMSO-*d*<sub>6</sub>

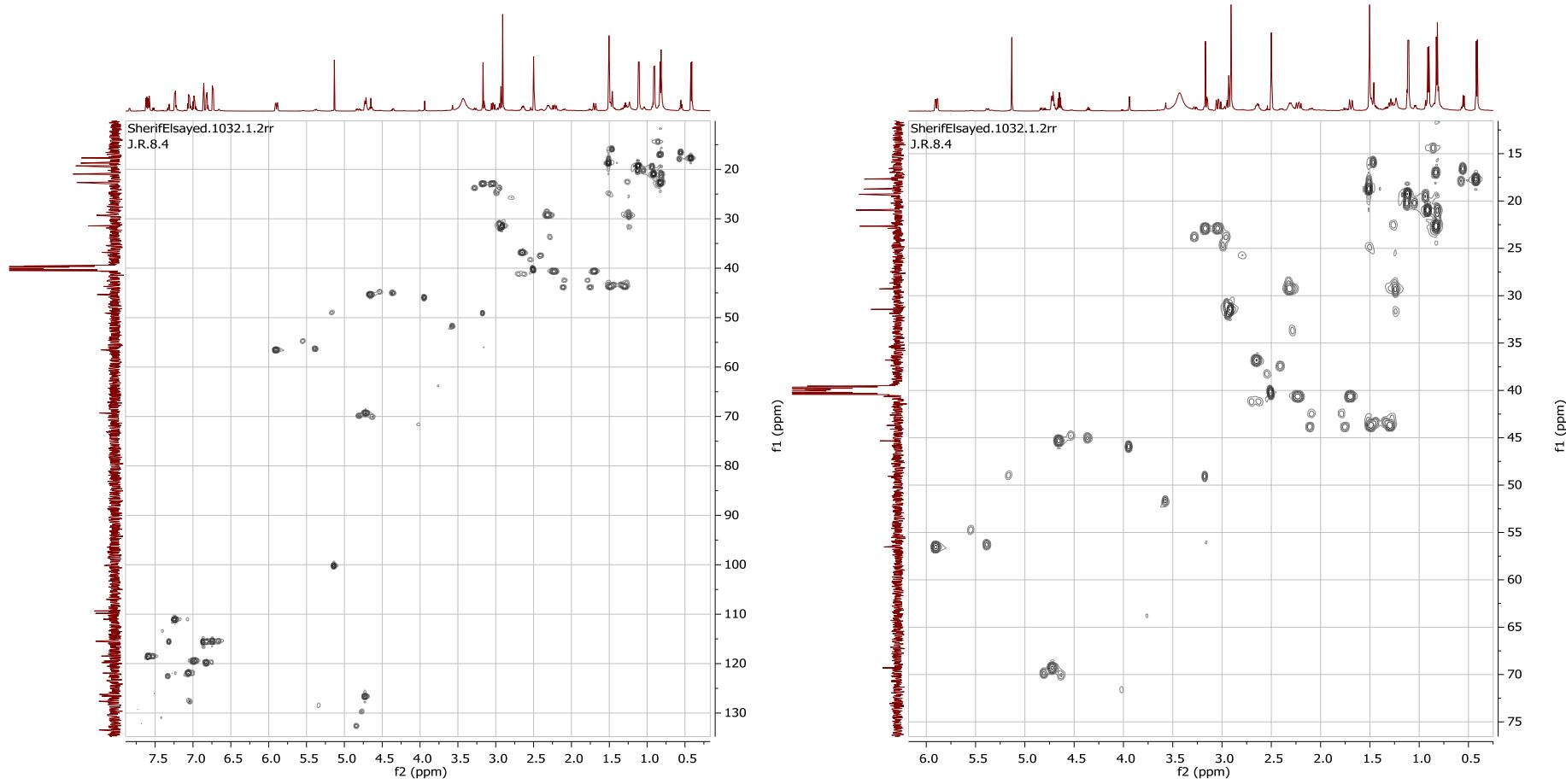


Figure S7a. gHMQC spectrum of **2** in  $\text{DMSO}-d_6$

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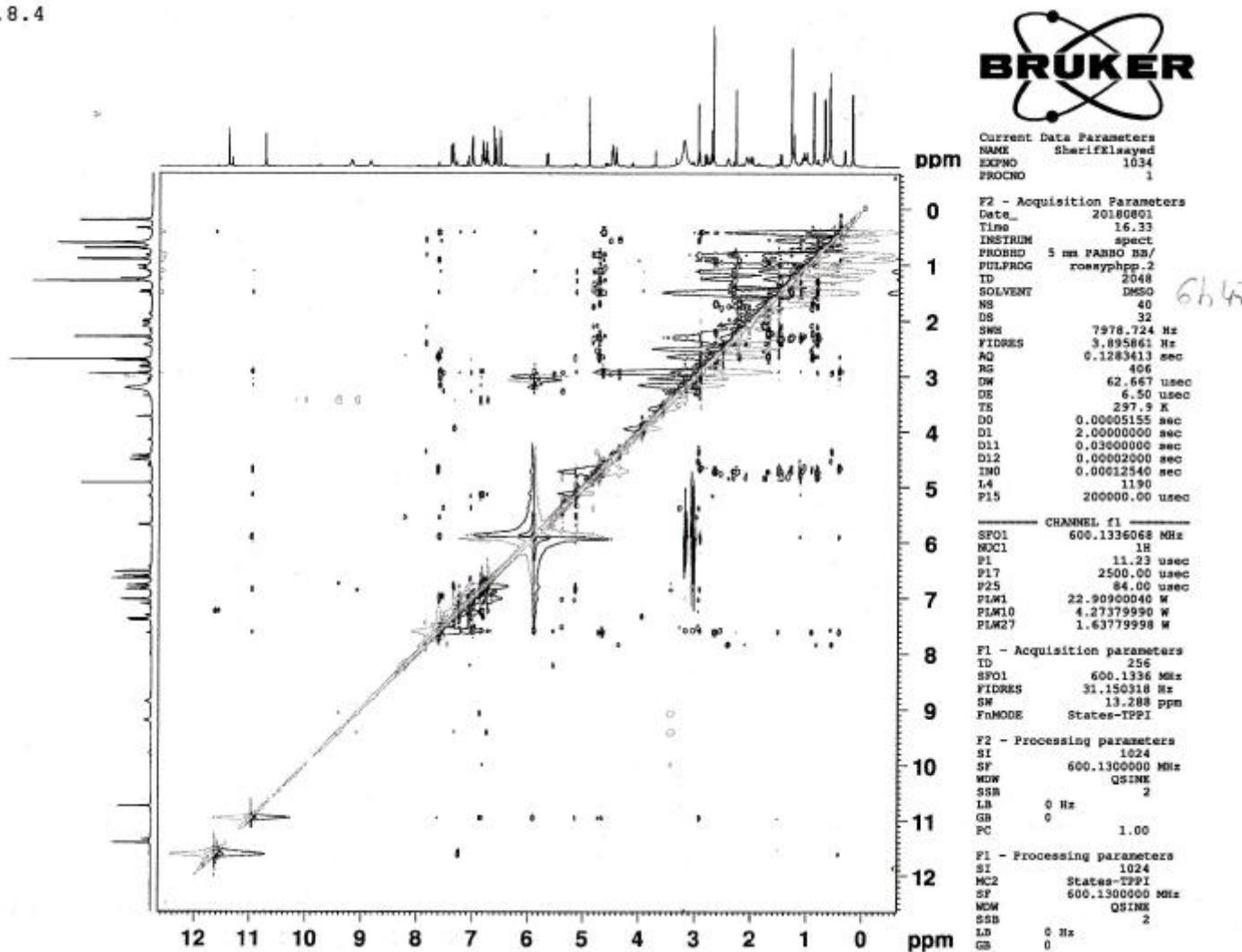


Figure S8. ROESY spectrum of **2** in DMSO-*d*6

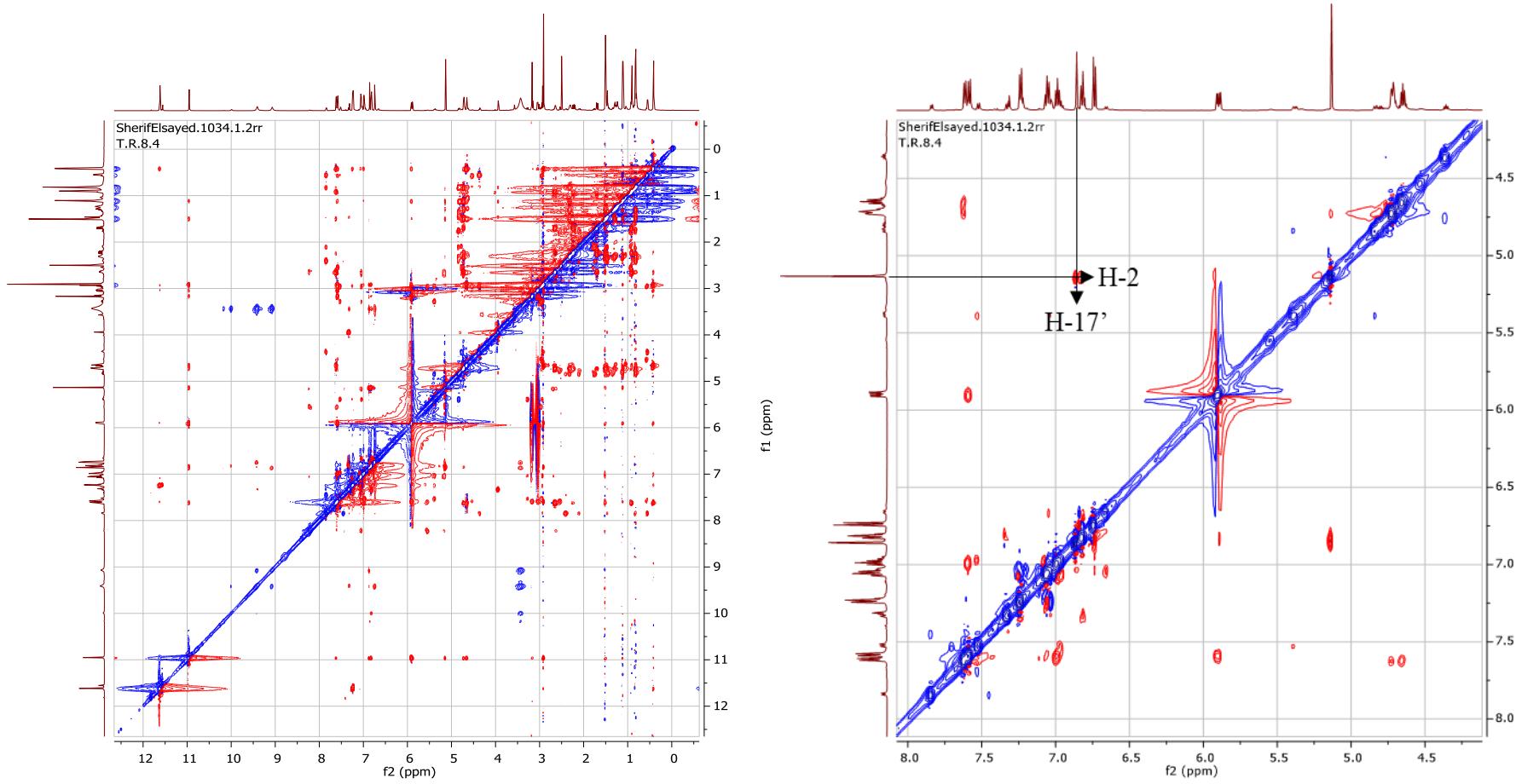


Figure S8a. ROESY spectrum of **2** in  $\text{DMSO}-d_6$

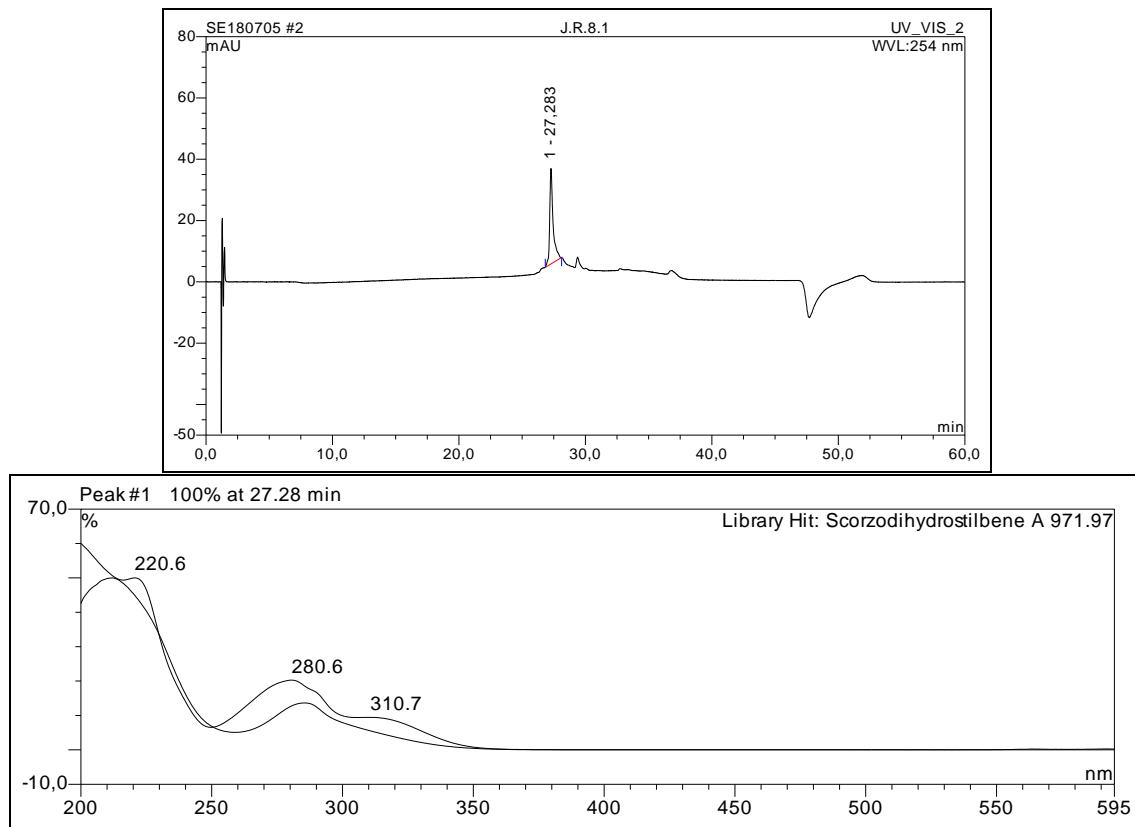


Figure S9. HPLC chromatogram of **4**

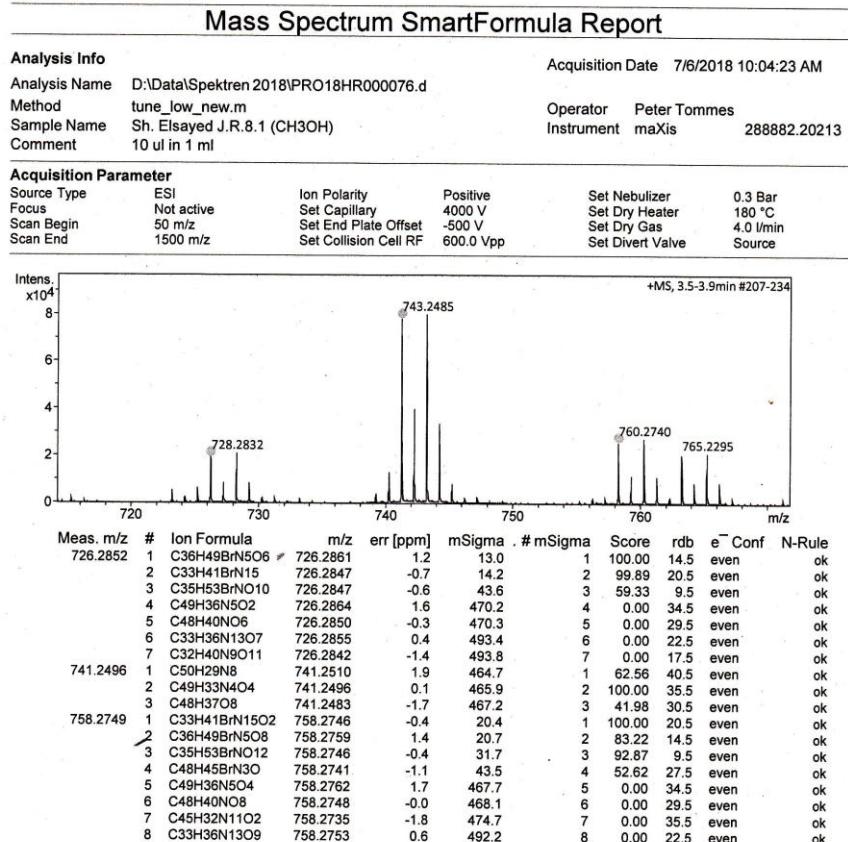
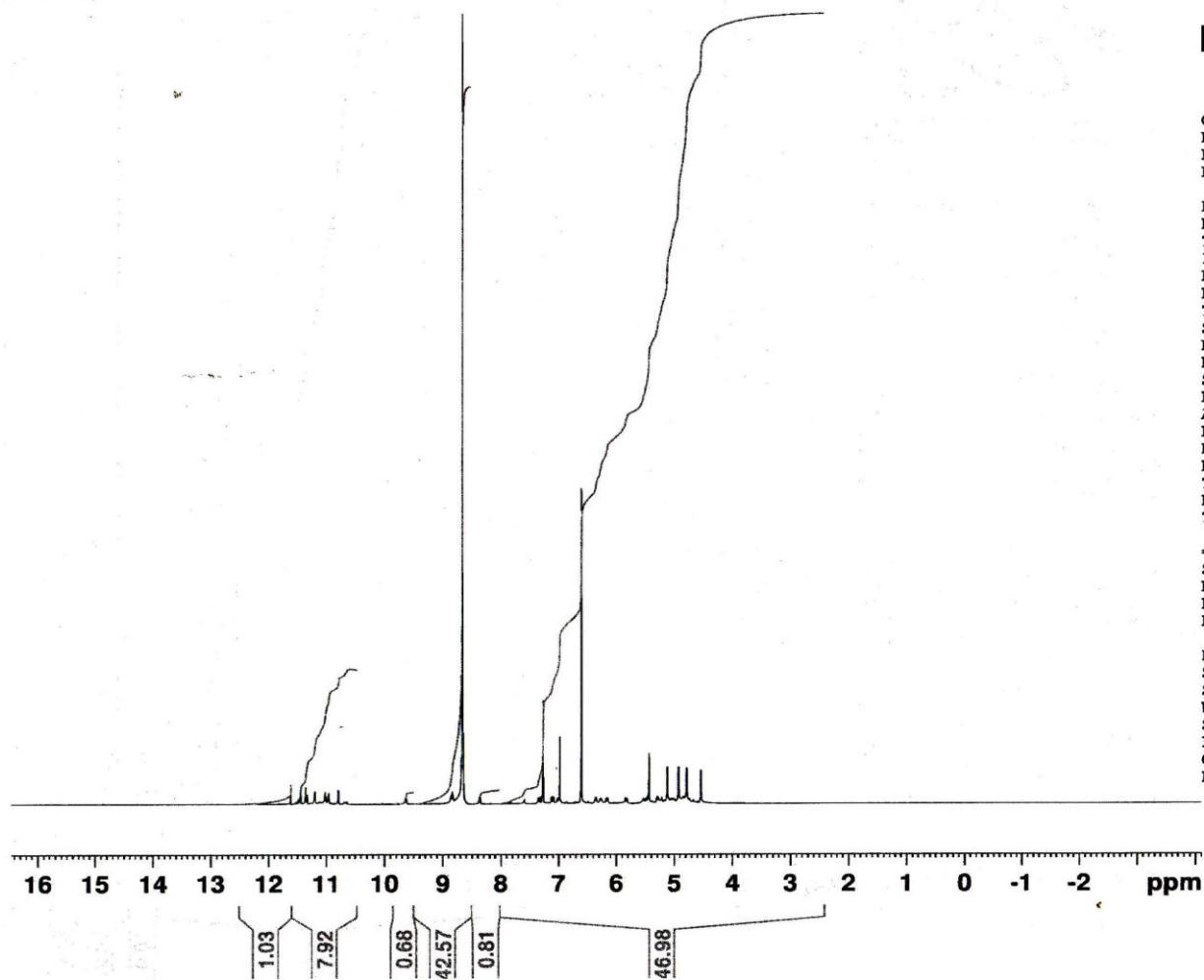


Figure S10. HRESIMS spectrum of **4**

T.R.8.1



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PROCNO 1

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PULPROG zg30  
TD 65536  
SOLVENT CDC13  
NS 64  
DS 2  
SWH 12335.526 Hz  
FIDRES 0.188225 Hz  
AQ 2.6563926 sec  
RG 90.5  
DW 40.533 usec  
DE 6.50 usec  
TE 299.2 K  
D1 1.0000000 sec  
TDO 1

===== CHANNEL f1 =====  
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NUC1 1H  
P1 11.23 usec  
PLW1 22.90900040 W

F2 - Processing parameters  
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SF 600.1300000 MHz  
WDW EM  
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LB 0.30 Hz  
GB 0  
PC 1.00

Figure S11.  $^1\text{H}$ -NMR spectrum of **4** in  $\text{CDCl}_3$

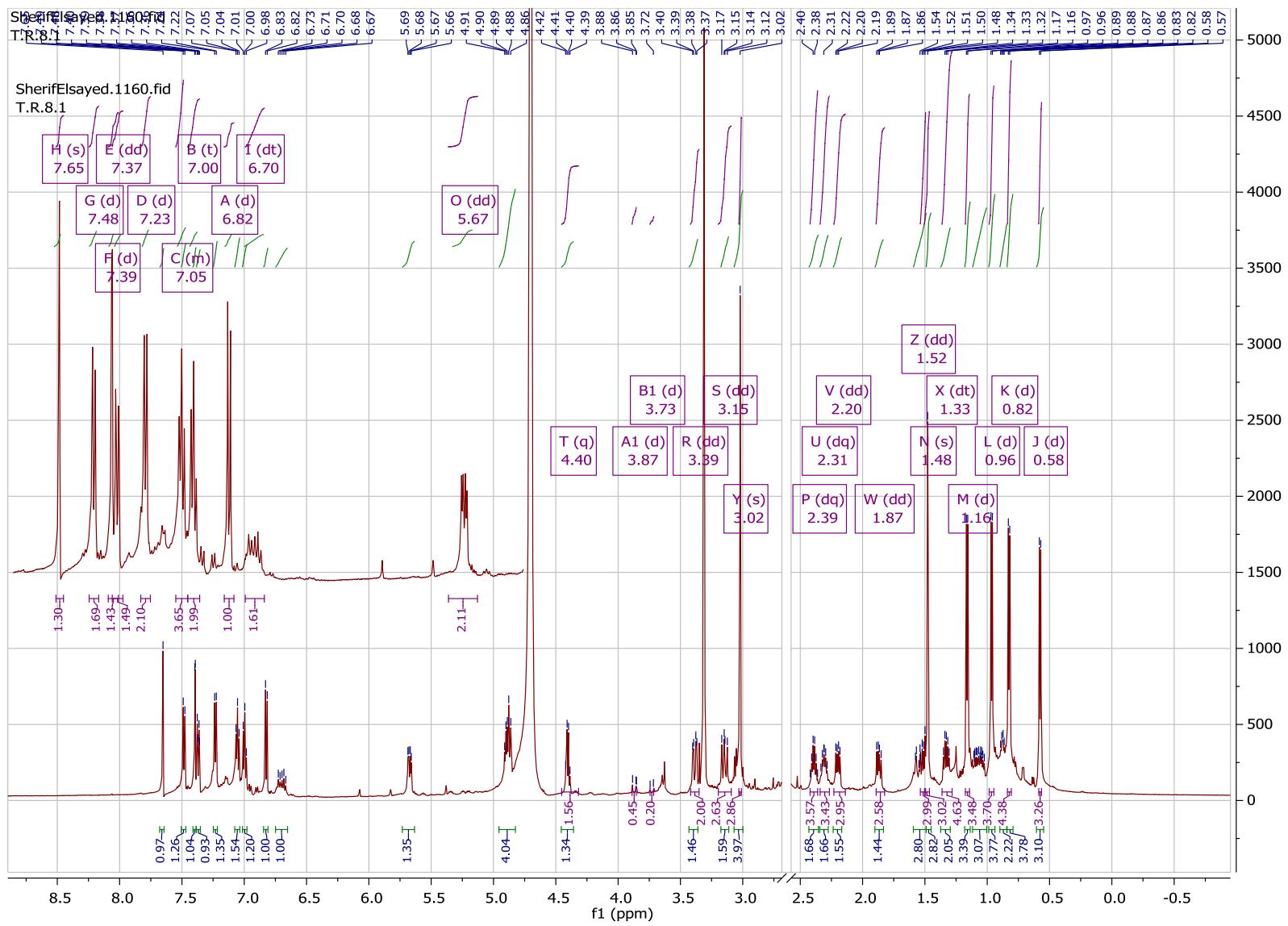


Figure S11a.  $^1\text{H}$ -NMR spectrum of **4** in  $\text{CDCl}_3$

T.R.8.1



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PROCNO 1

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PULPROG zgpg30  
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SOLVENT CDCl3  
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DS 4  
SWH 36057.691 Hz  
FIDRES 0.550197 Hz  
AQ 0.9087659 sec  
RG 2050  
DW 13.867 usec  
DE 6.50 usec  
TE 299.8 K  
D1 2.0000000 sec  
D11 0.03000000 sec  
TD0 1

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NUC1 13C  
P1 9.40 usec  
PLW1 134.89999390 W

----- CHANNEL f2 -----  
SFO2 600.1324005 MHz  
NUC2 1H  
CPDPRG[2] waltz16  
PCPD2 70.00 usec  
PLW2 22.90900040 W  
PLW12 0.58961999 W  
PLW13 0.28891000 W

F2 - Processing parameters  
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GB 0  
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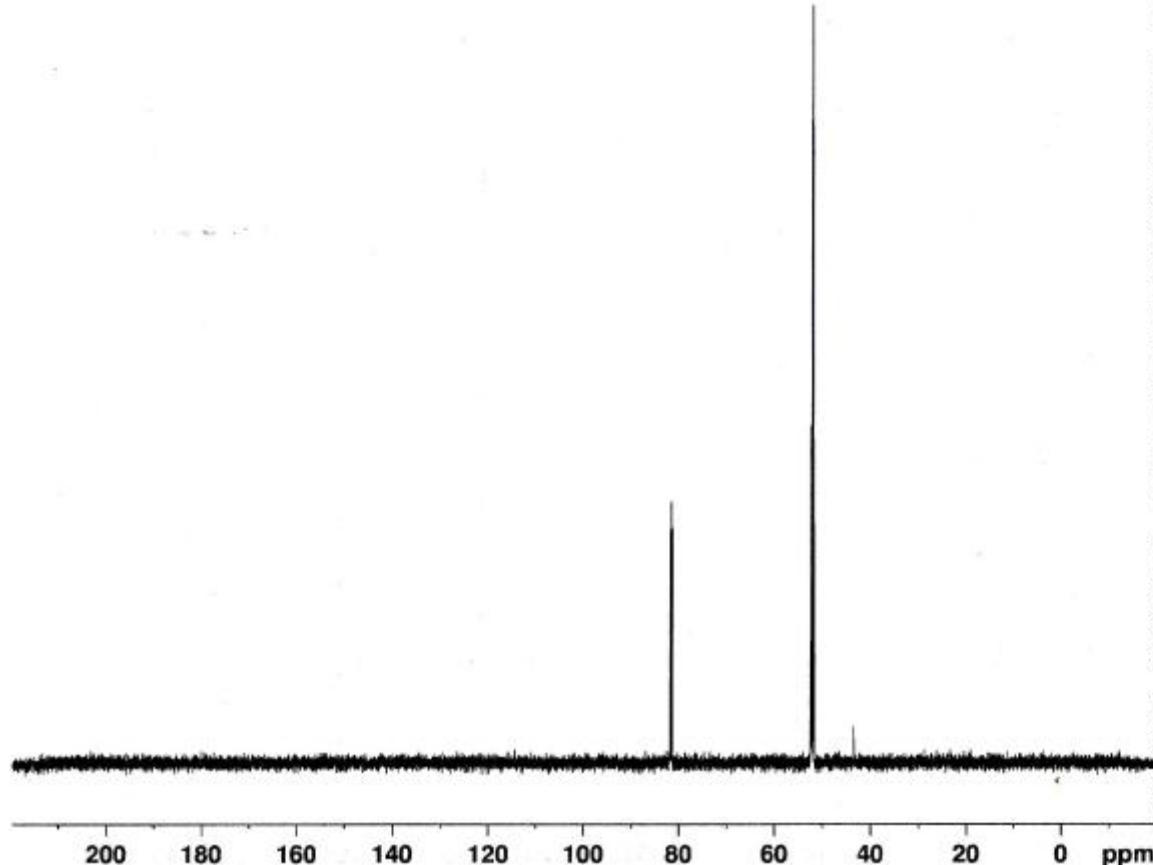


Figure S12.  $^{13}\text{C}$ -NMR spectrum of **4** in  $\text{CDCl}_3$

T.R.8.1

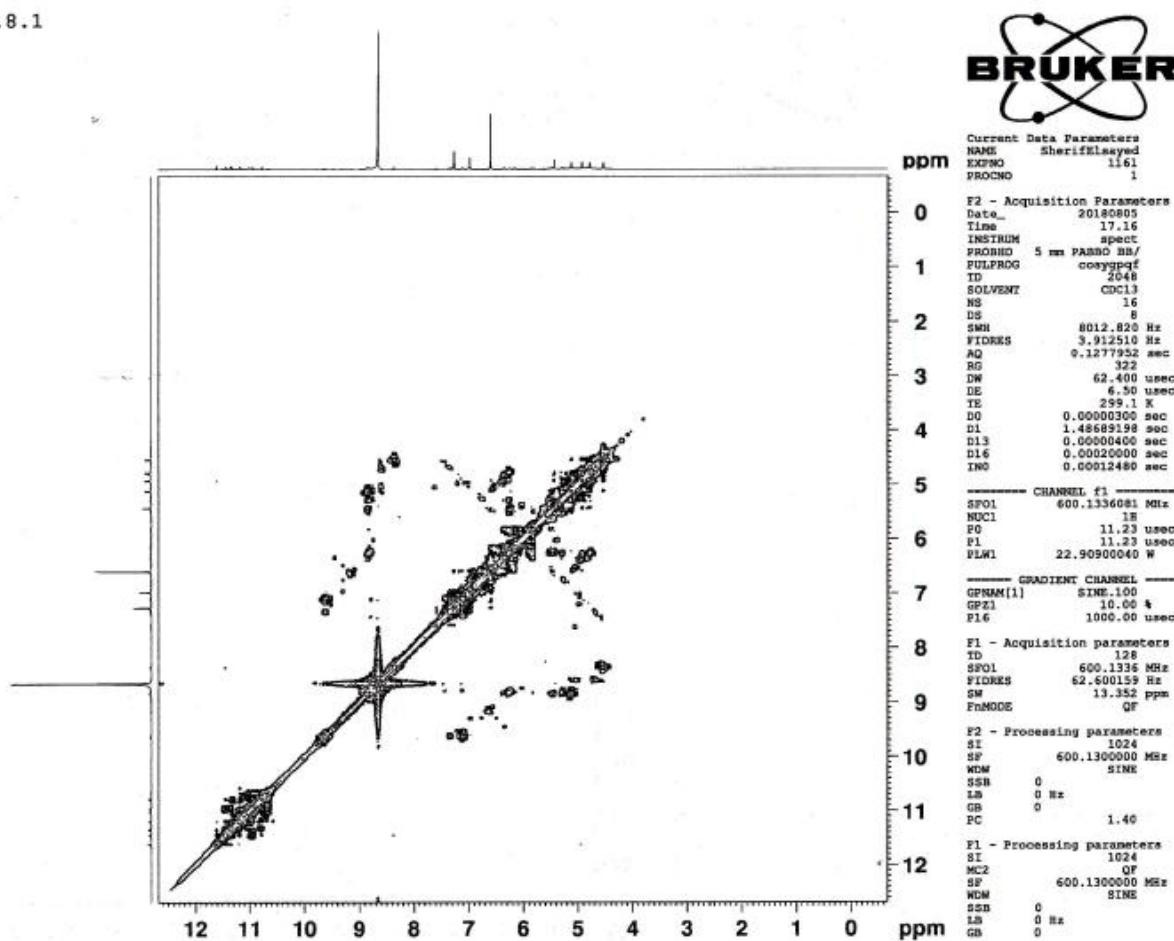


Figure S13.  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of **4** in  $\text{CDCl}_3$

T.R.8.1

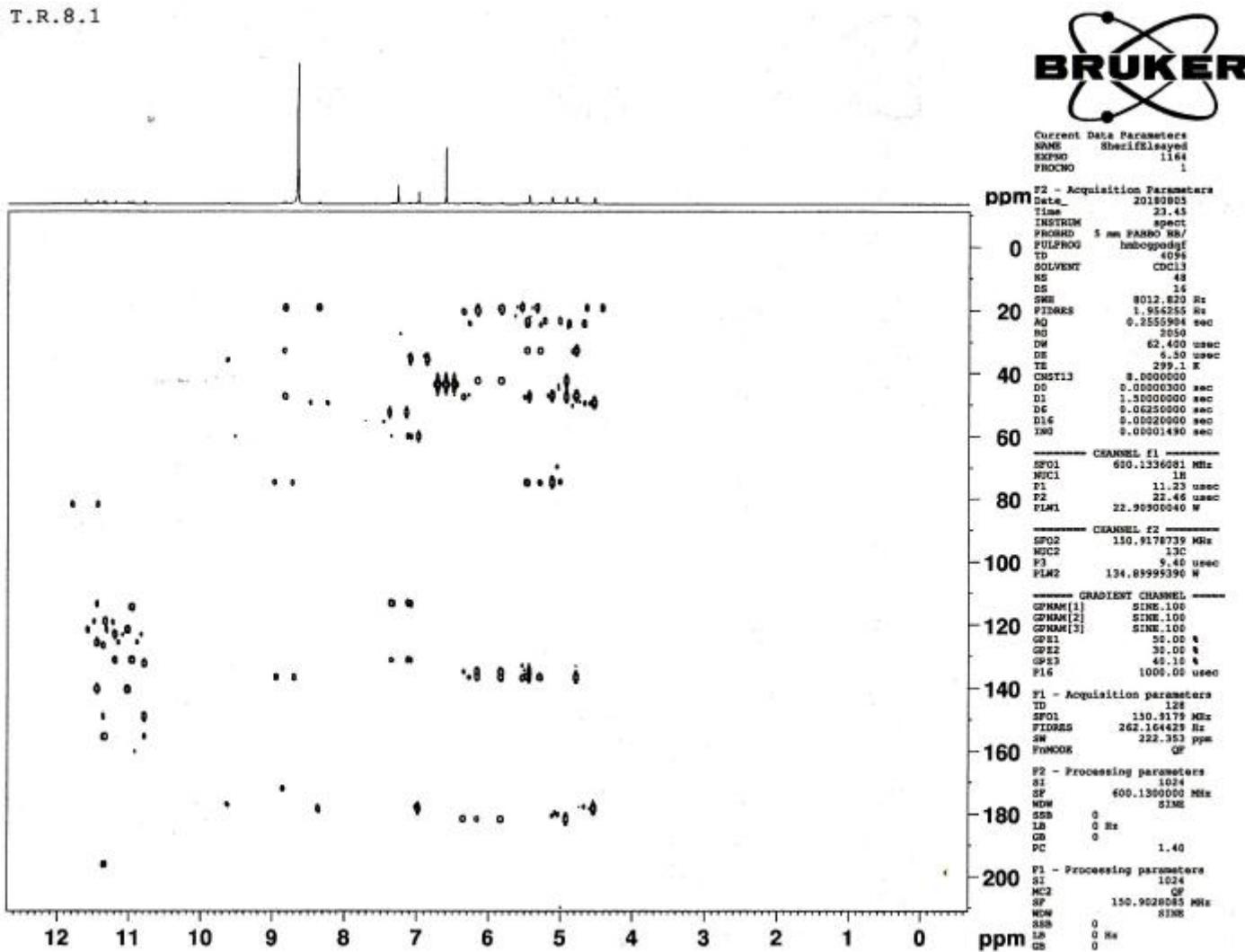


Figure S14. gHMBC spectrum of **4** in  $\text{CDCl}_3$

T.R.8.1

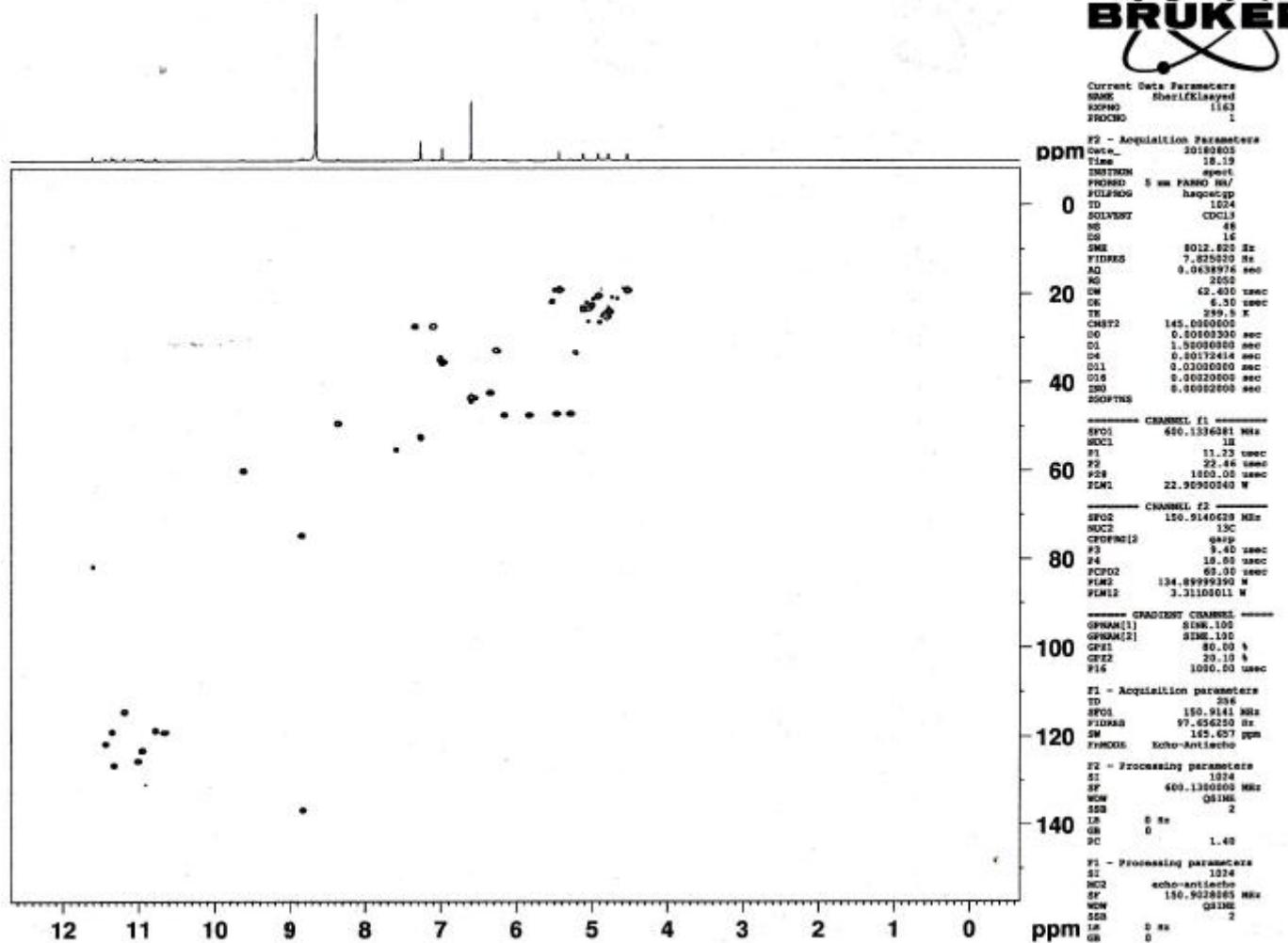


Figure S15. gHMQC spectrum of **4** in CDCl<sub>3</sub>