

Supplementary Materials

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Table S1. Anti-proliferation effect on WI26 of compounds **1**, **2** and xiamenmycin.

	Compound 1 (15 µg/mL)	Compound 2 (30 µg/mL)	Xiamenmycin (30 µg/mL)
1 day	13.8%	12.8%	10%
2 day	18.2%	15%	14.9%
3 day	28.6%	27.8%	18.9%
4 day	30%	28.5%	20%
5 day	33.7%	30.3%	25.4%
6 day	38%	31.2%	28.5%

Figure S1. HRESIMS spectra of compound **1**.**Elemental Composition Report****Page 1****Single Mass Analysis**

Tolerance = 10.0 mDa / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

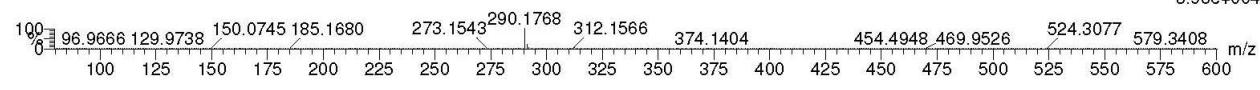
144 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Elements Used:

C: 0-30 H: 0-50 N: 0-2 O: 0-20

2-4-2

XX_Y05775_03 379 (8.480) Cm (379)

1: TOF MS ES+
3.98e+004Minimum: -1.5
Maximum: 10.0 100.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
290.1768	290.1756	1.2	4.1	6.5	33.3	n/a	n/a	C17 H24 N 03

Elemental Composition Report**Page 1****Single Mass Analysis**

Tolerance = 10.0 mDa / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Odd and Even Electron Ions

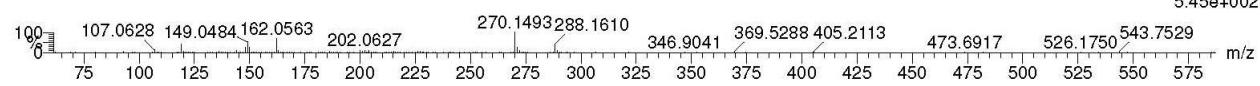
144 formula(e) evaluated with 7 results within limits (up to 50 closest results for each mass)

Elements Used:

C: 0-30 H: 0-50 N: 0-2 O: 0-20

Fr.F-2-4-Z-F-2-4-2

2013031222 668 (3.866) Cm (667.668)

1: TOF MSMS 288.19ES-
5.45e+002Minimum: -1.5
Maximum: 10.0 100.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
288.1610	288.1600	1.0	3.5	7.5	15.2	1.702	18.23	C17 H22 N 03
	288.1626	-1.6	-5.6	12.0	14.7	1.234	29.11	C20 H20 N2
	288.1573	3.7	12.8	3.0	16.0	2.508	8.14	C14 H24 O6
	288.1658	-4.8	-16.7	-1.5	17.1	3.641	2.62	C10 H26 N 08
	288.1685	-7.5	-26.0	3.0	16.3	2.789	6.15	C13 H24 N2 O5
	288.1533	7.7	26.7	-1.0	17.3	3.856	2.12	C9 H24 N2 O8
	288.1514	9.6	33.3	12.0	14.6	1.090	33.63	C21 H20 O

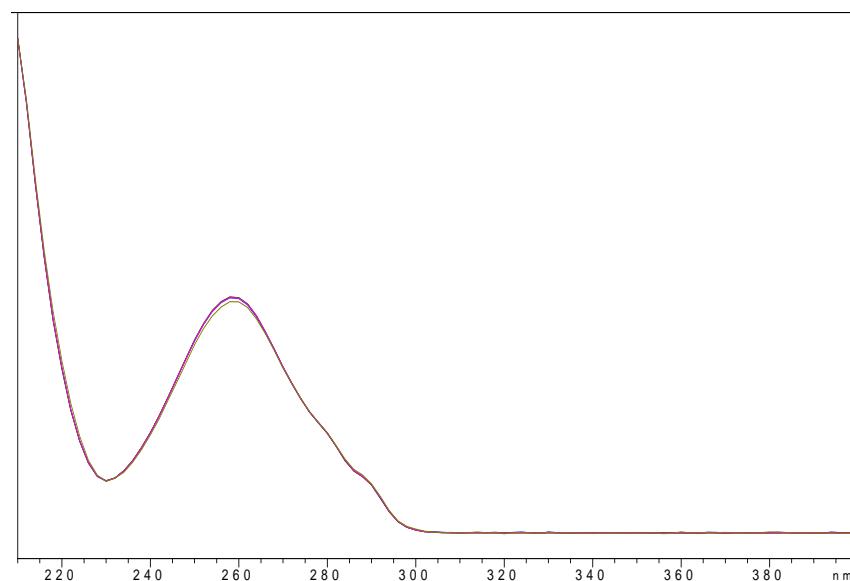
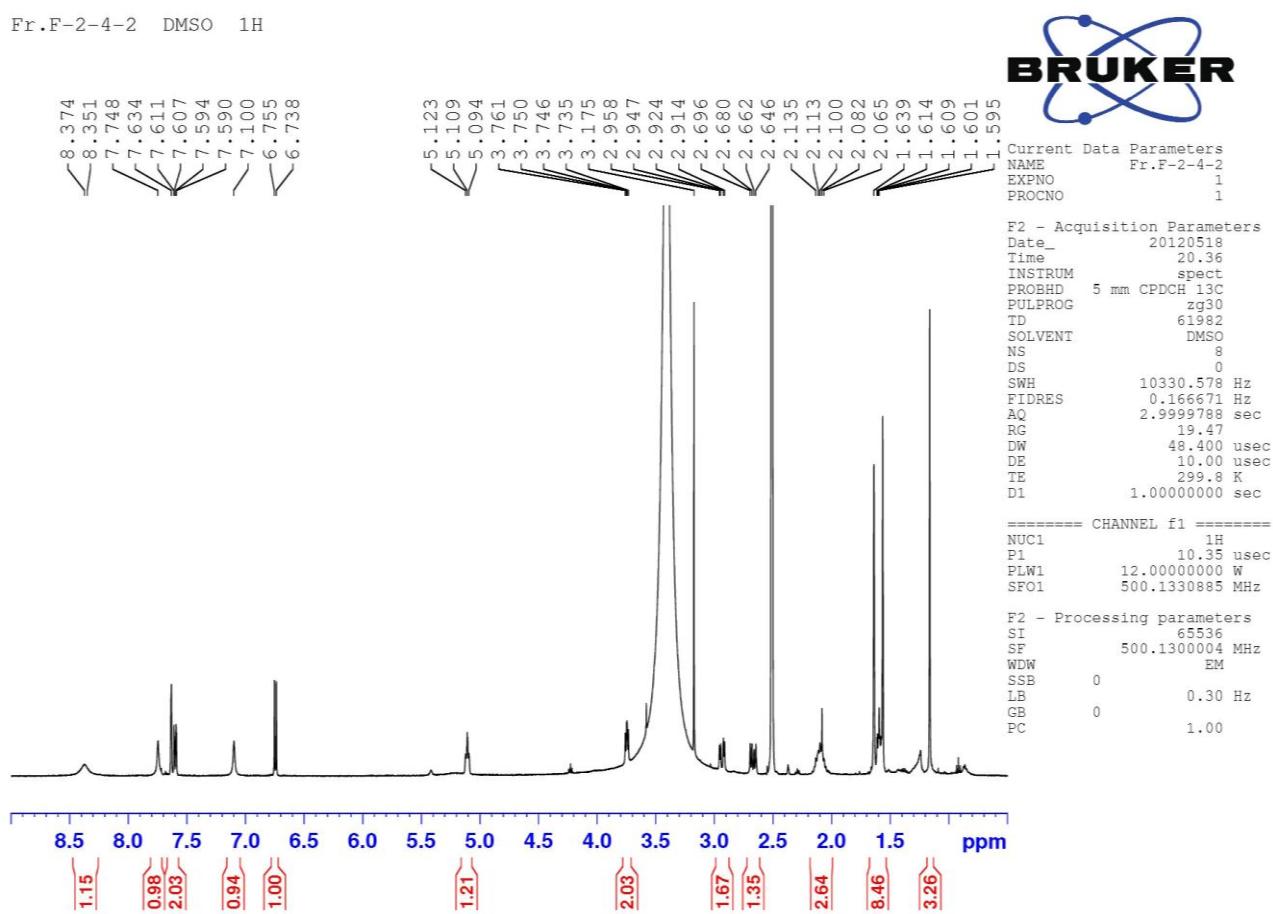
Figure S2. UV spectra of compound **1** (online detection by HPLC).**Figure S3.** ^1H NMR spectrum of compound **1** in $\text{DMSO}-d_6$.

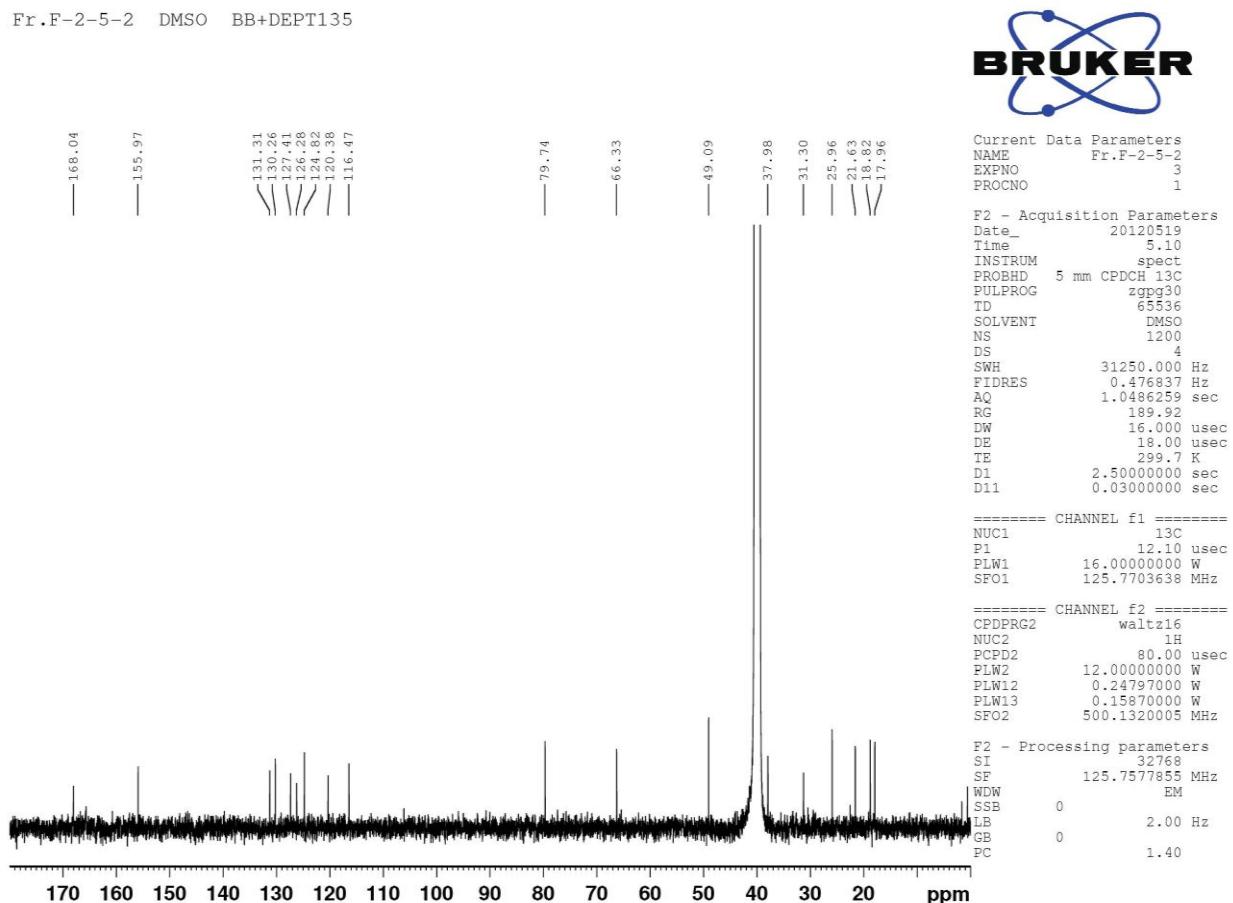
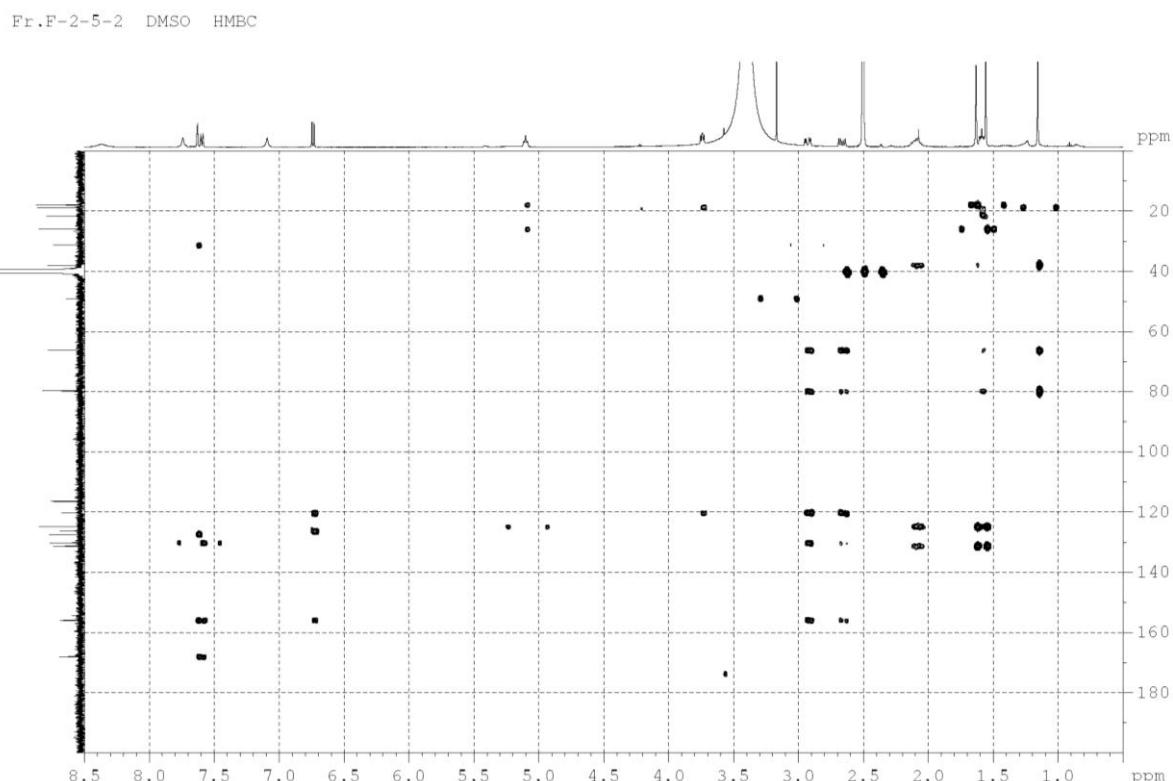
Figure S4. ^{13}C NMR spectrum of compound **1** in $\text{DMSO}-d_6$.**Figure S5.** HMBC spectrum of compound **1** in $\text{DMSO}-d_6$.

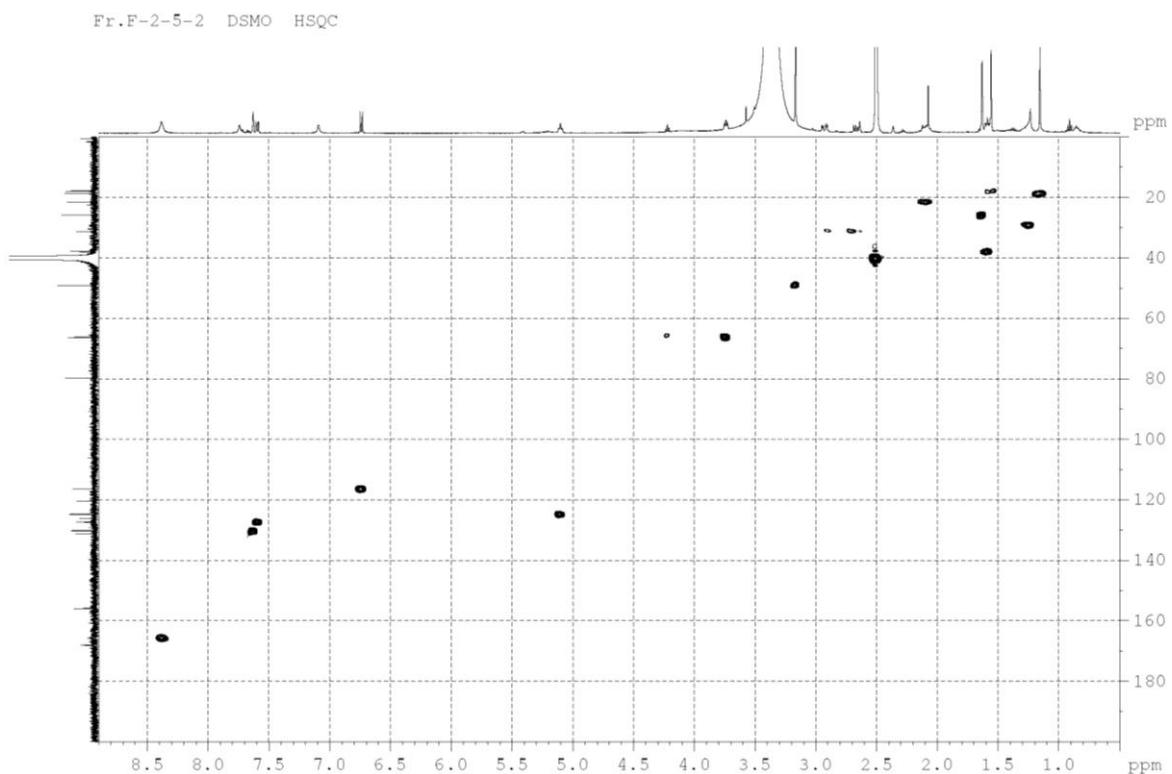
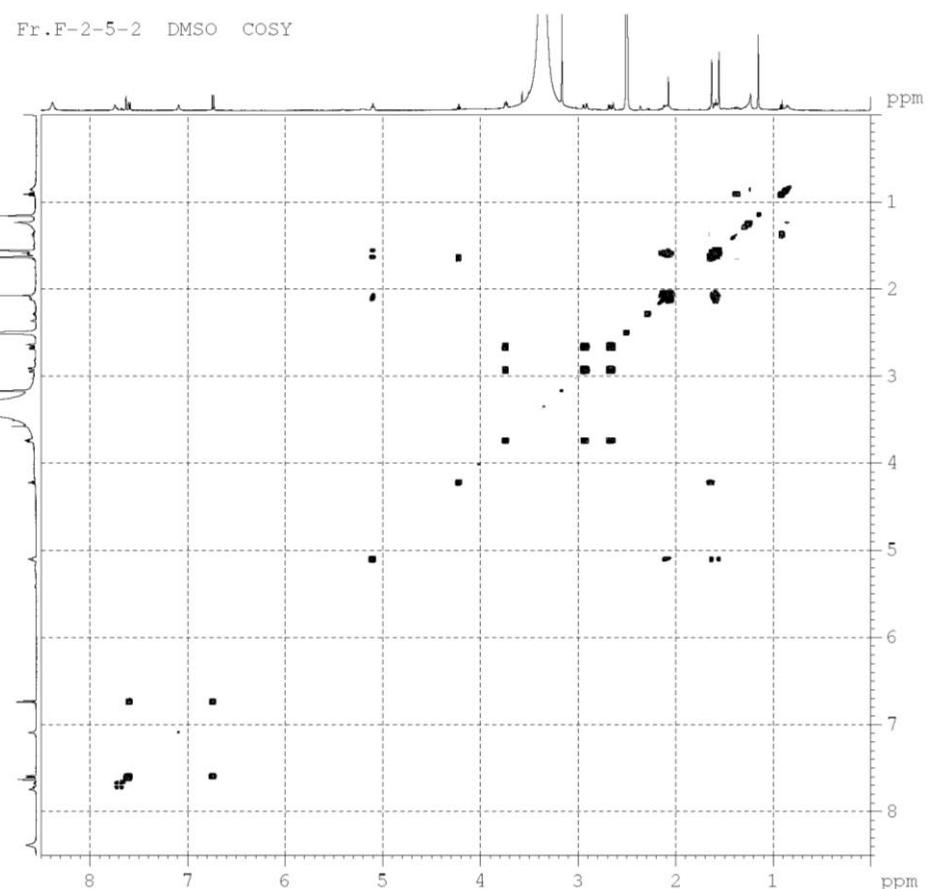
Figure S6. HSQC spectrum of compound **1** in DMSO-*d*₆.**Figure S7.** COSY spectrum of compound **1** in DMSO-*d*₆.

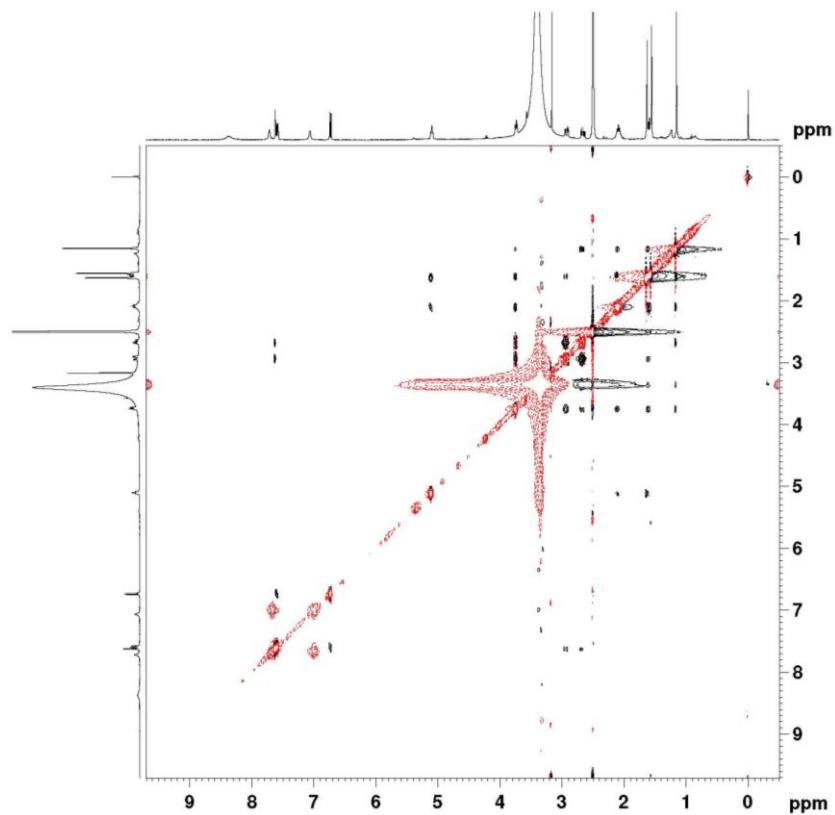
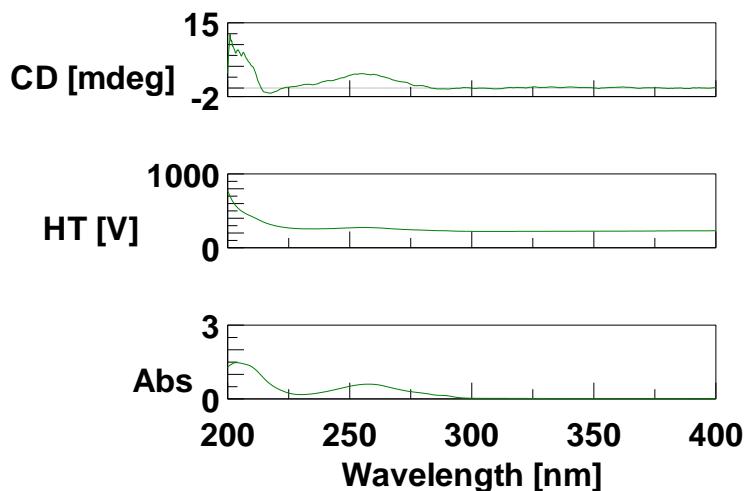
Figure S8. NOSEY spectrum of compound **1** in DMSO-*d*₆.**Figure S9.** CD spectrum of compound **1**.

Figure S10. HRESIMS spectra of compound 2 (positive mode).

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
406.2210	406.2230	-2.0	-4.9	7.5	23.6	0.280	75.55	C22 H32 N 06
	406.2171	3.9	9.6	16.5	24.7	1.435	23.82	C29 H28 N 0
	406.2288	-7.8	-19.2	-1.5	28.3	5.063	0.63	C15 H36 N 011

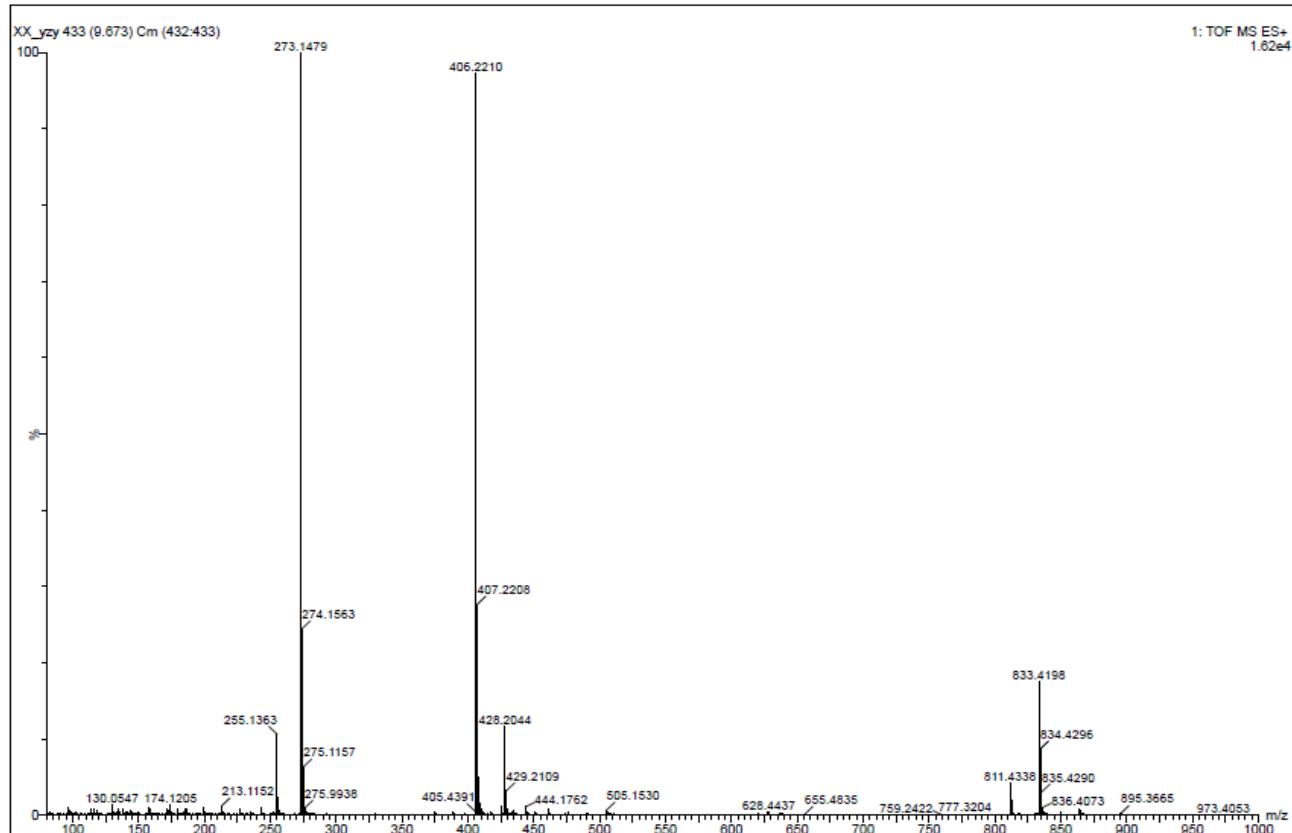
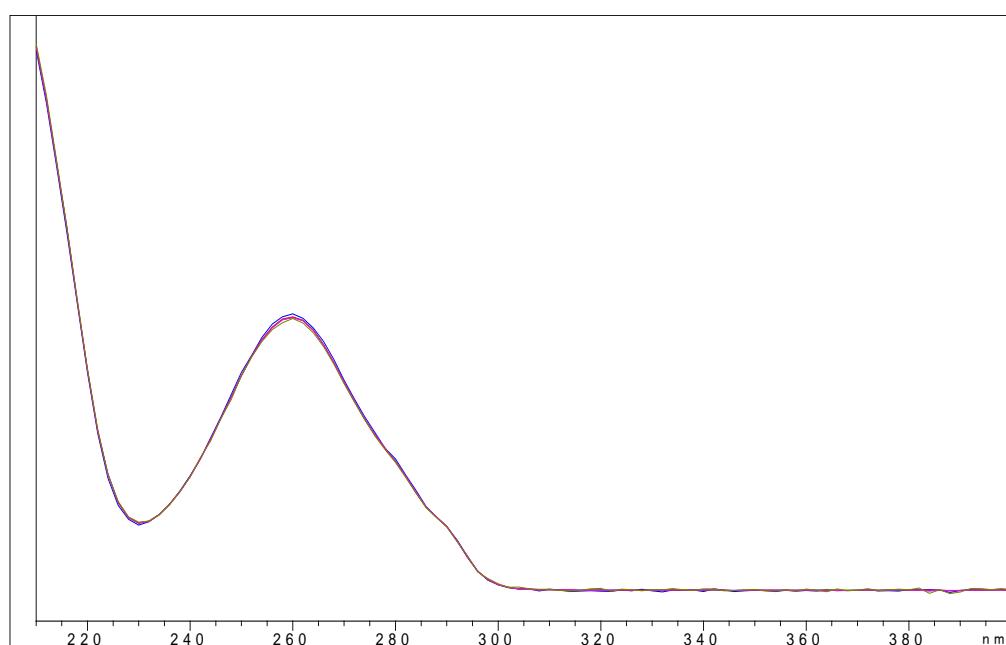
**Figure S11.** UV spectra of compound 2 (online detection by HPLC).

Figure S12. ^1H NMR spectrum of compound **2** in $\text{DMSO}-d_6$.

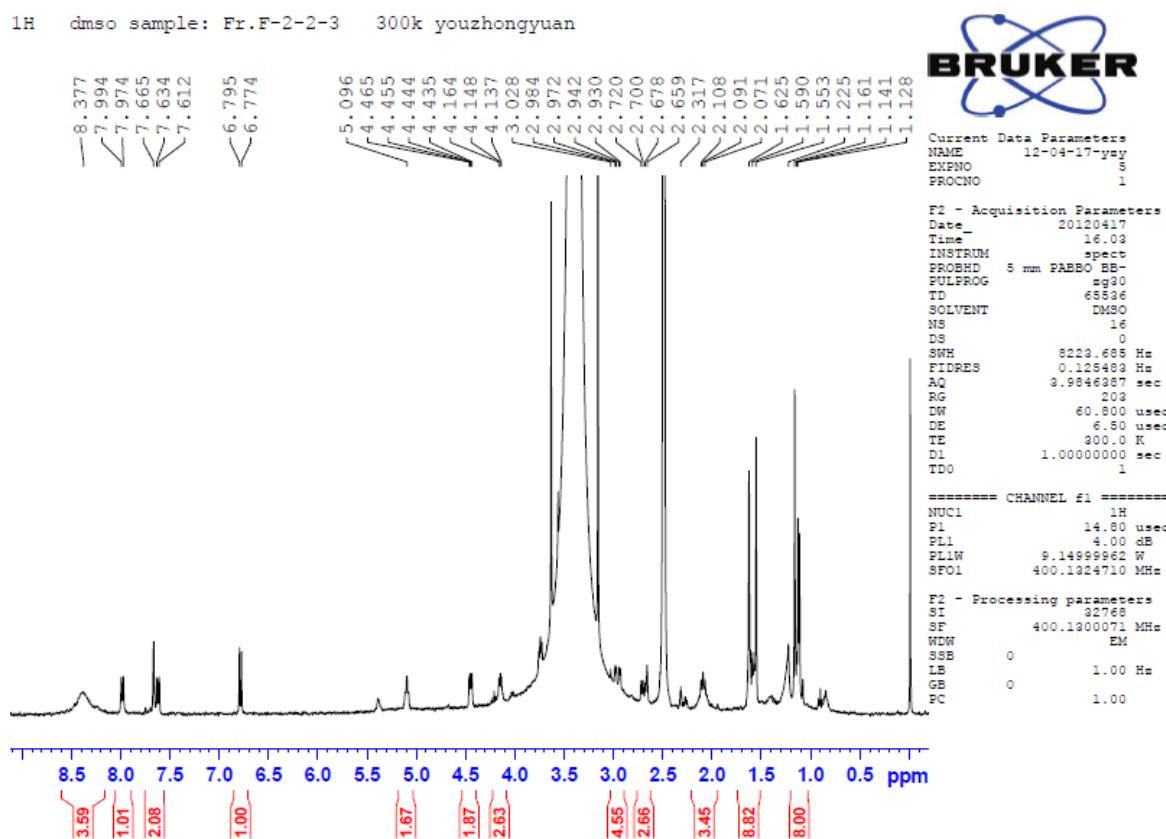


Figure S13. ^{13}C NMR spectrum of compound **2** in $\text{DMSO}-d_6$.

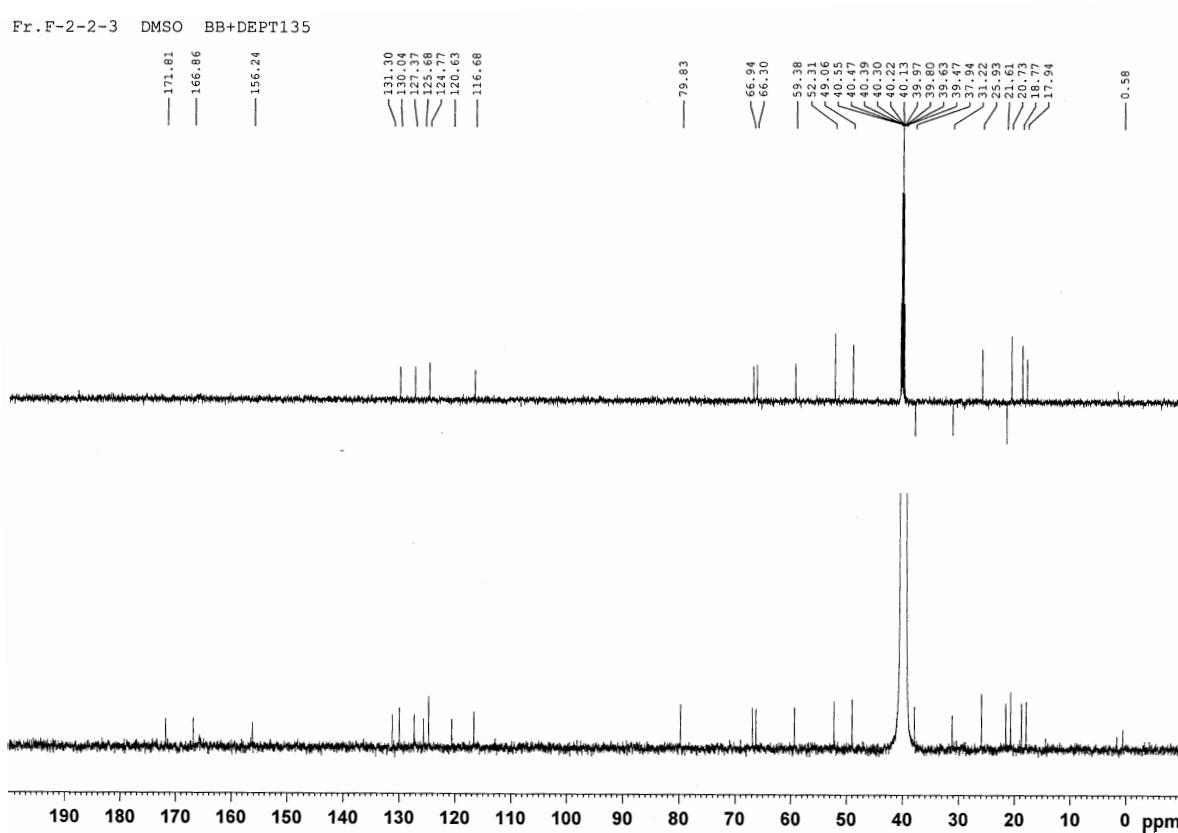


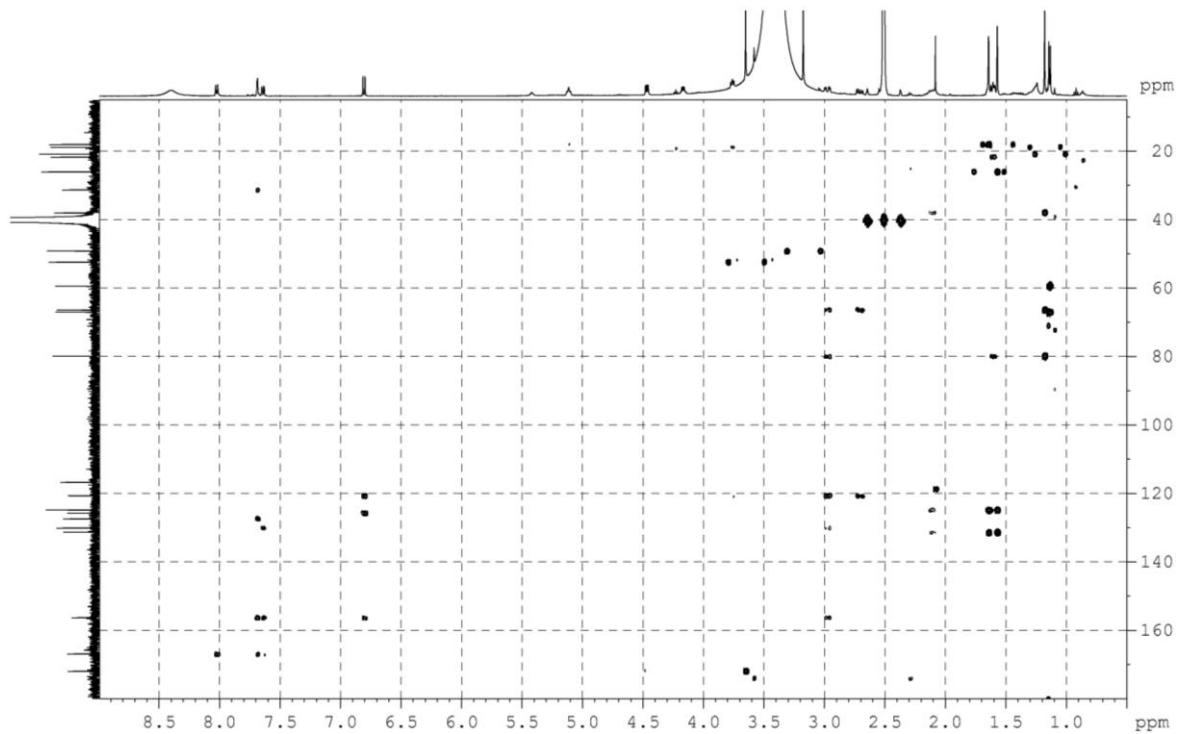
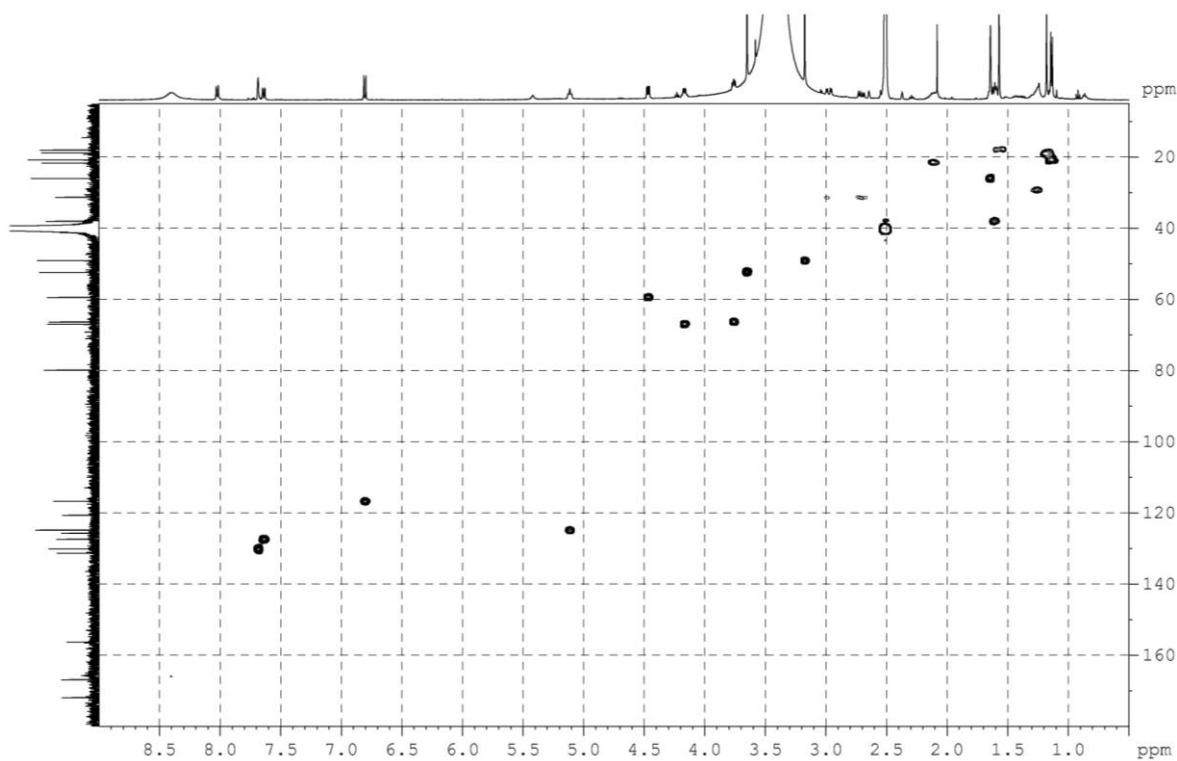
Figure S14. HMBC spectrum of compound **2** in DMSO-*d*₆.**Figure S15.** HMQC spectrum of compound **2** in DMSO-*d*₆.

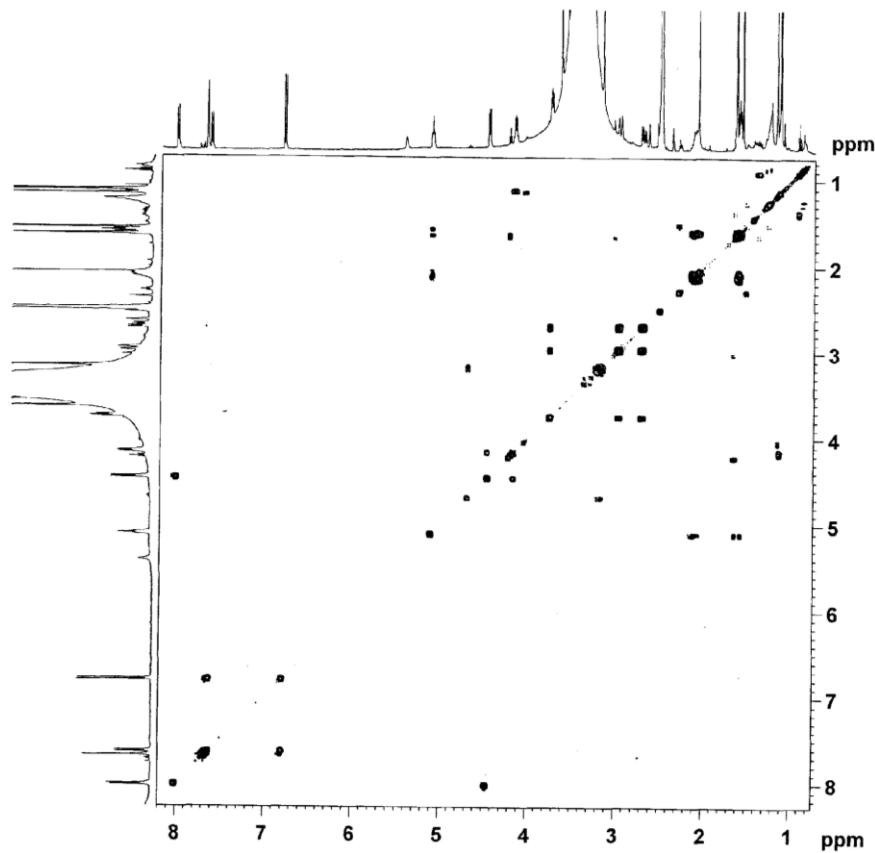
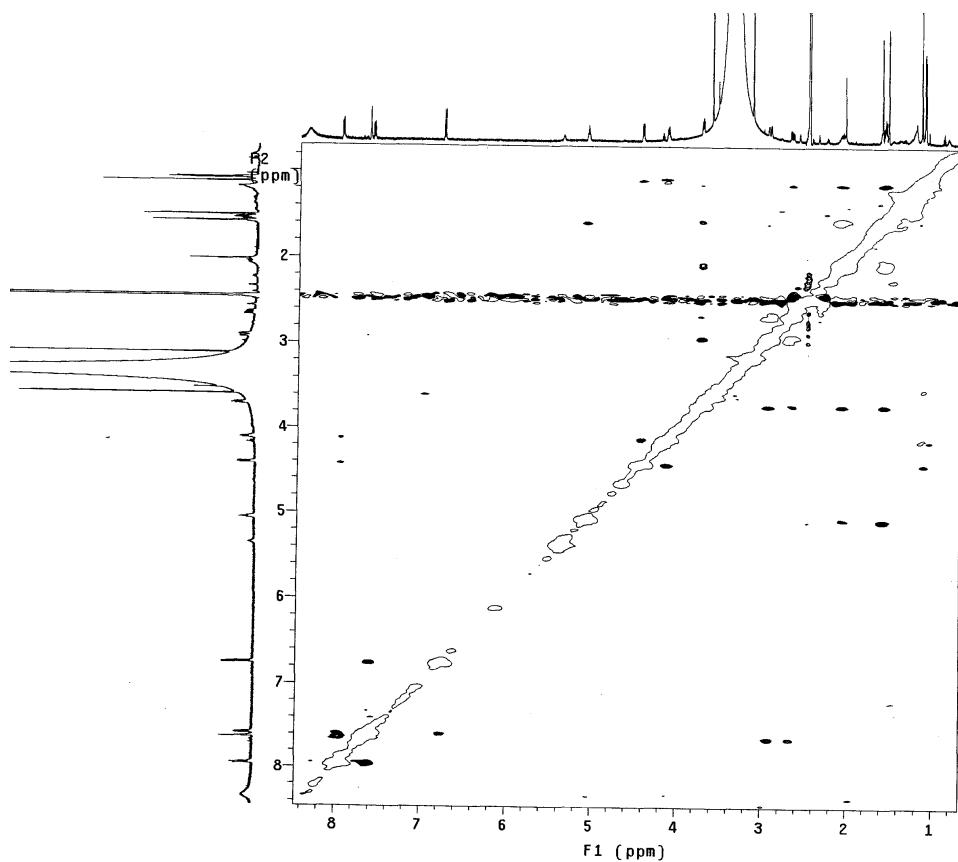
Figure S16. COSY spectrum of compound **2** in $\text{DMSO}-d_6$.**Figure S17.** ROSEY spectrum of compound **2** in $\text{DMSO}-d_6$.

Figure S18. CD spectrum of compound 2.