

Supplementary data

New spirobisanaphthalenes from an endolichenic fungus strain CGMCC 3.15192

and their anticancer effects through the P53-P21 pathway

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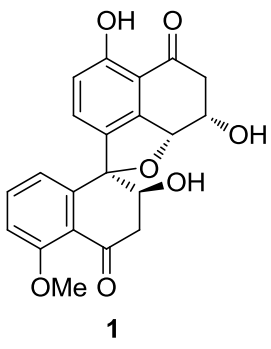
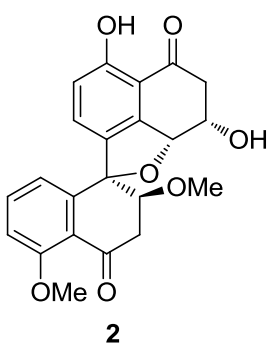
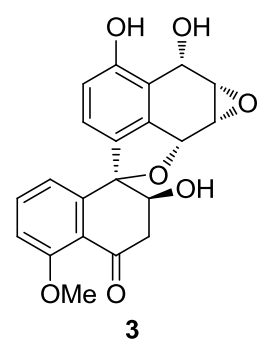
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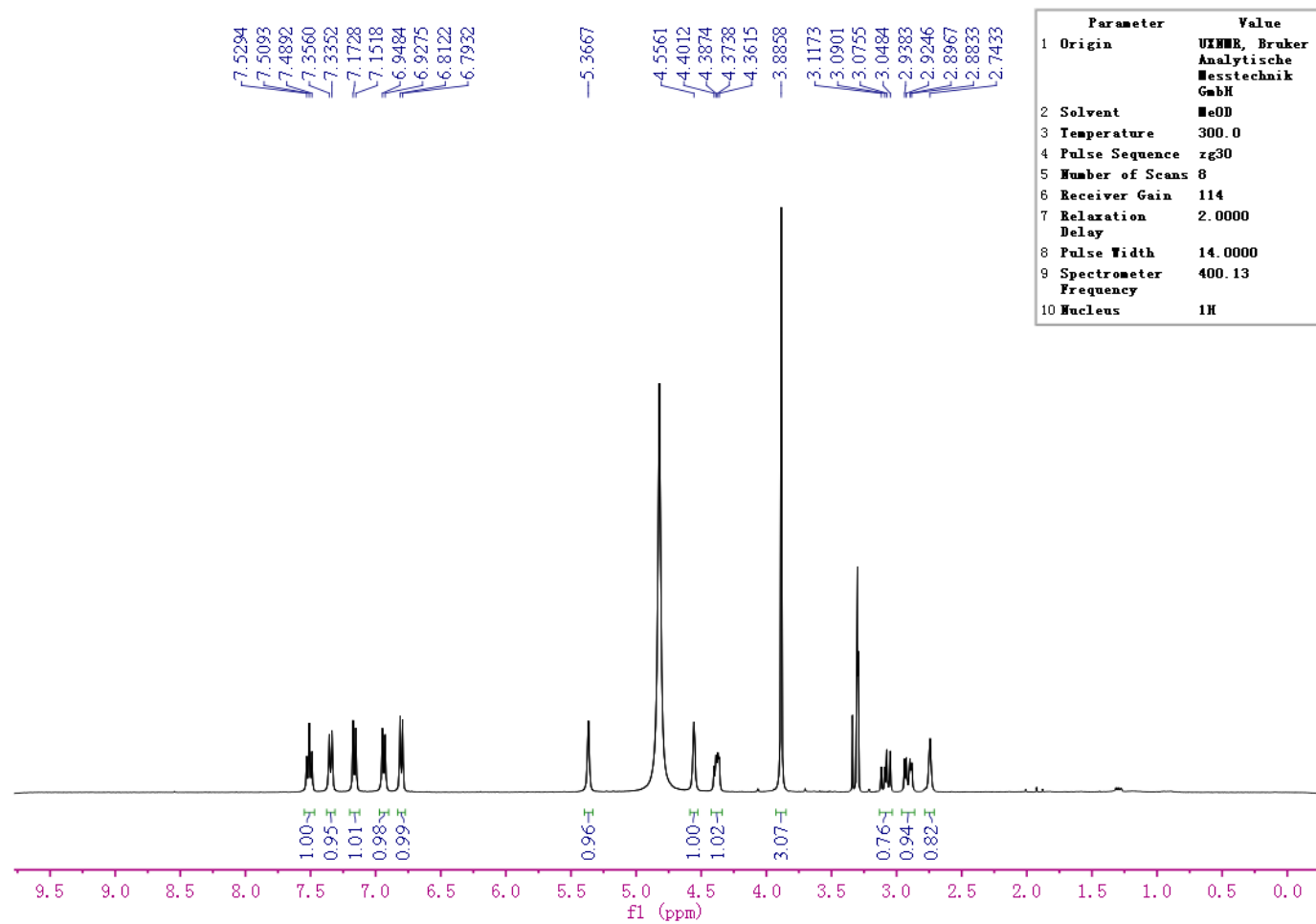


Fig. S1 ¹H-NMR spectrum of the new compound **1**

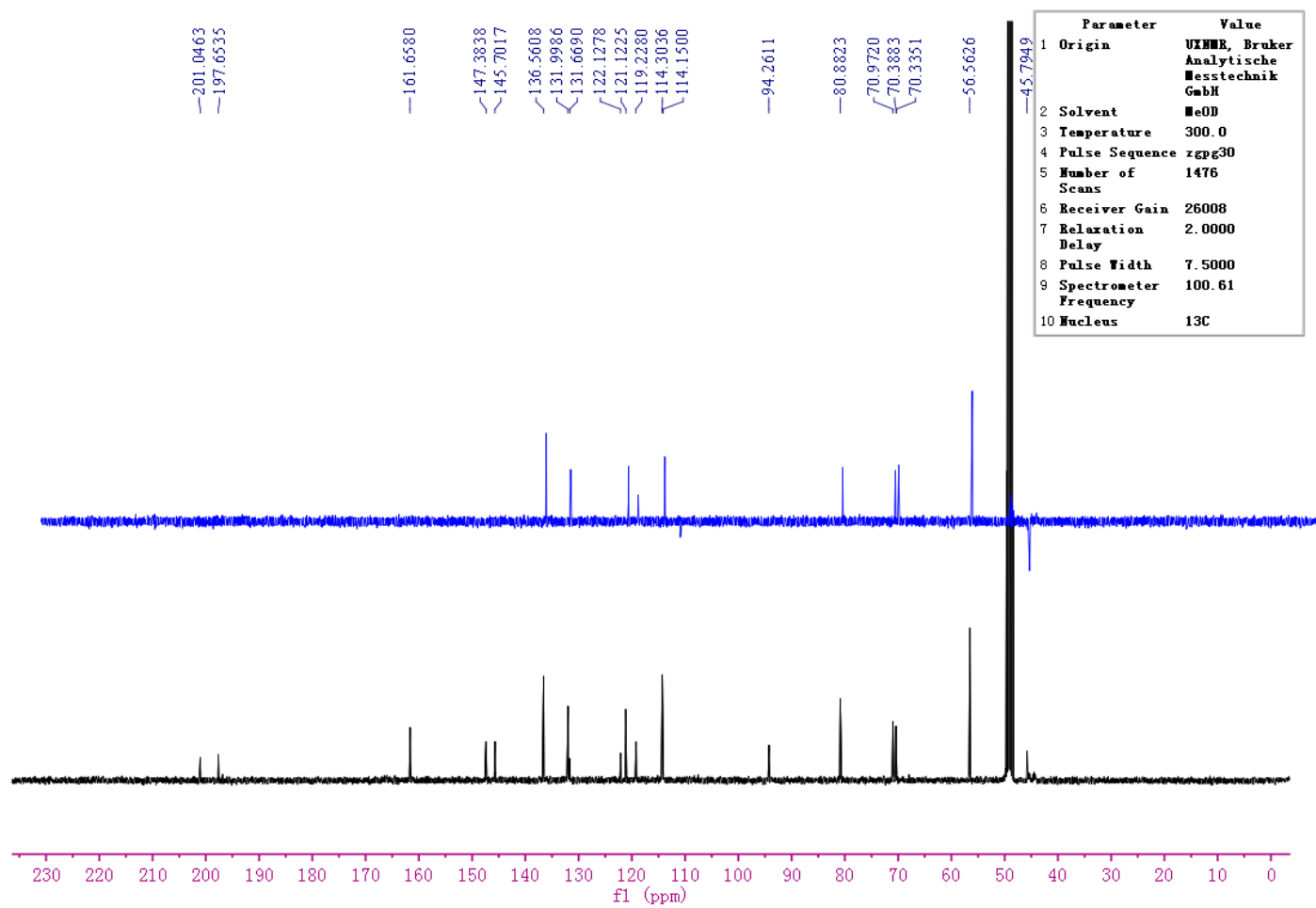


Fig. S2 ^{13}C -NMR & DEPT-135 spectrum of the new compound **1**

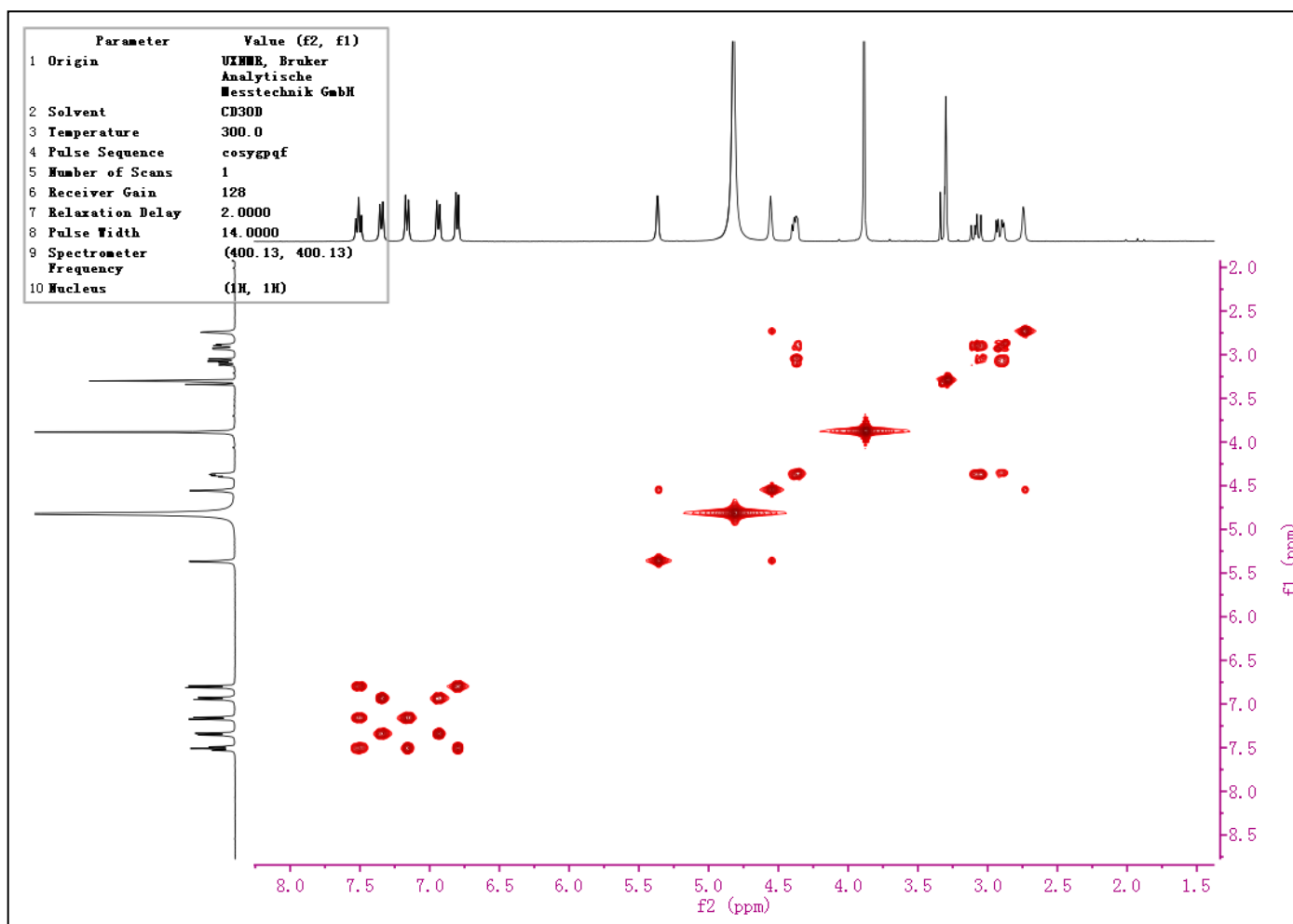


Fig. S3 ^1H - ^1H COSY spectrum of the new compound **1**

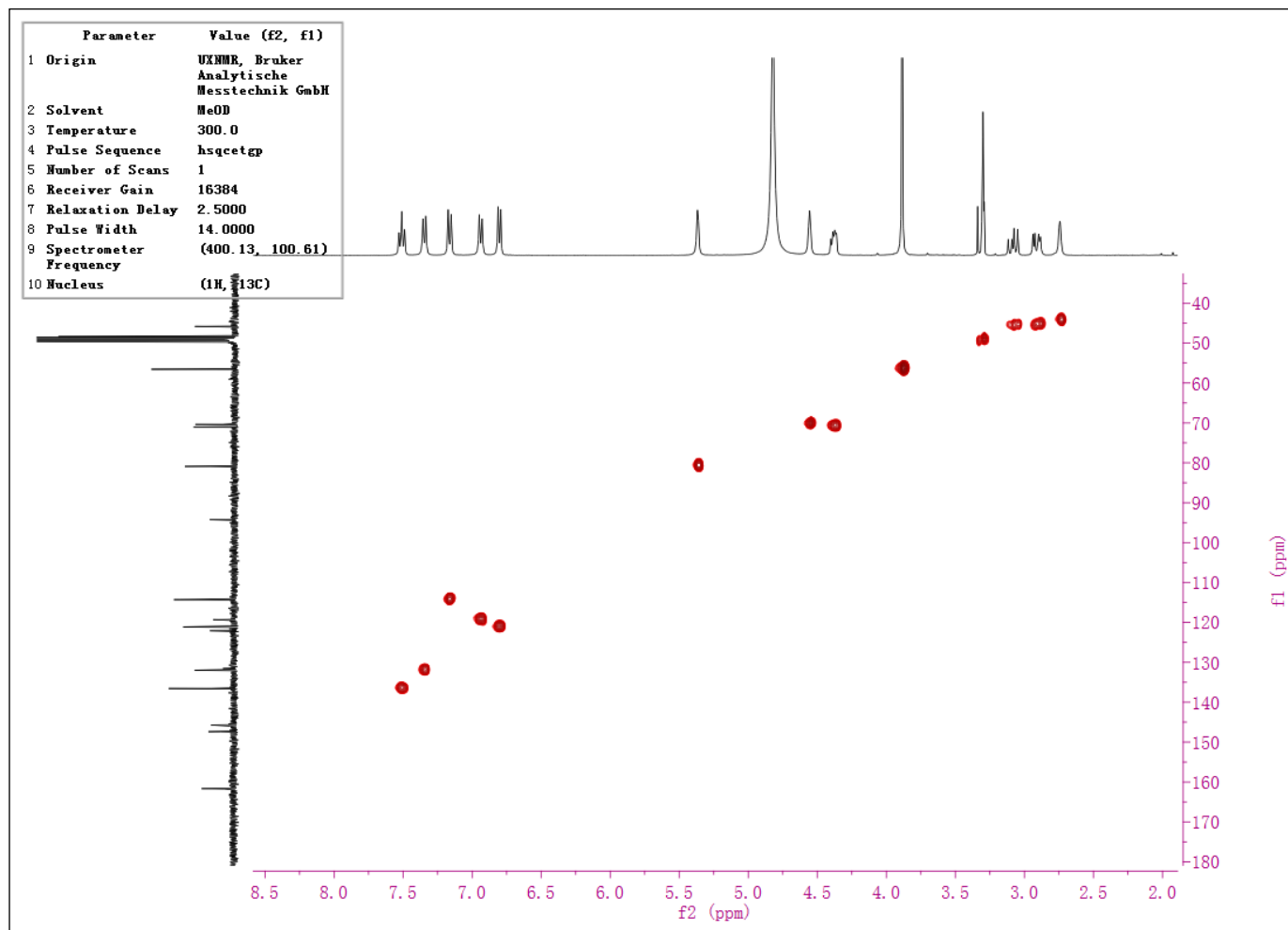


Fig. S4 HSQC spectrum of the new compound 1

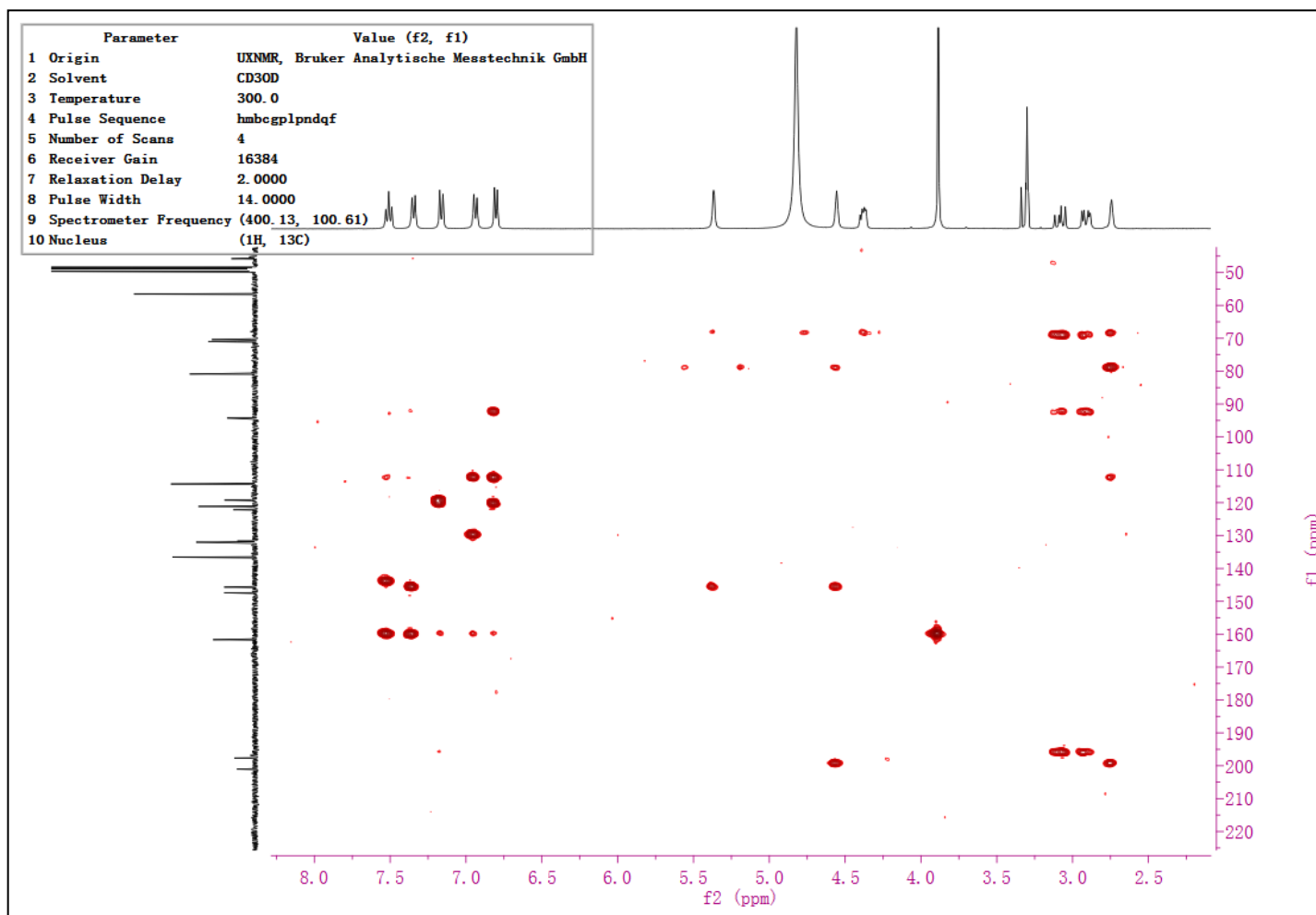


Fig. S5 HMBC spectrum of the new compound **1**

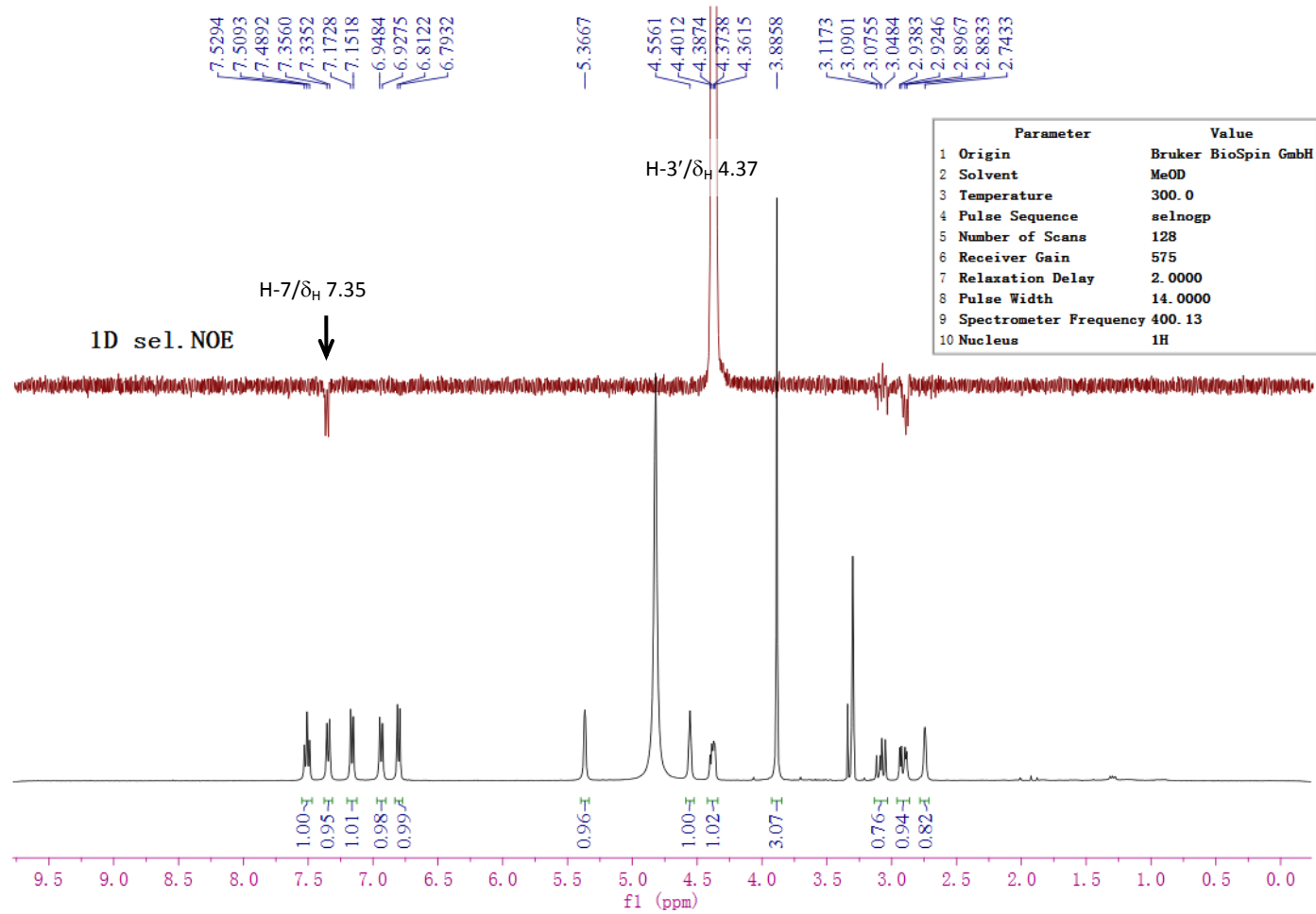


Fig. S6-1 1D sel. Gr. NOE spectrum of the new compound **1**

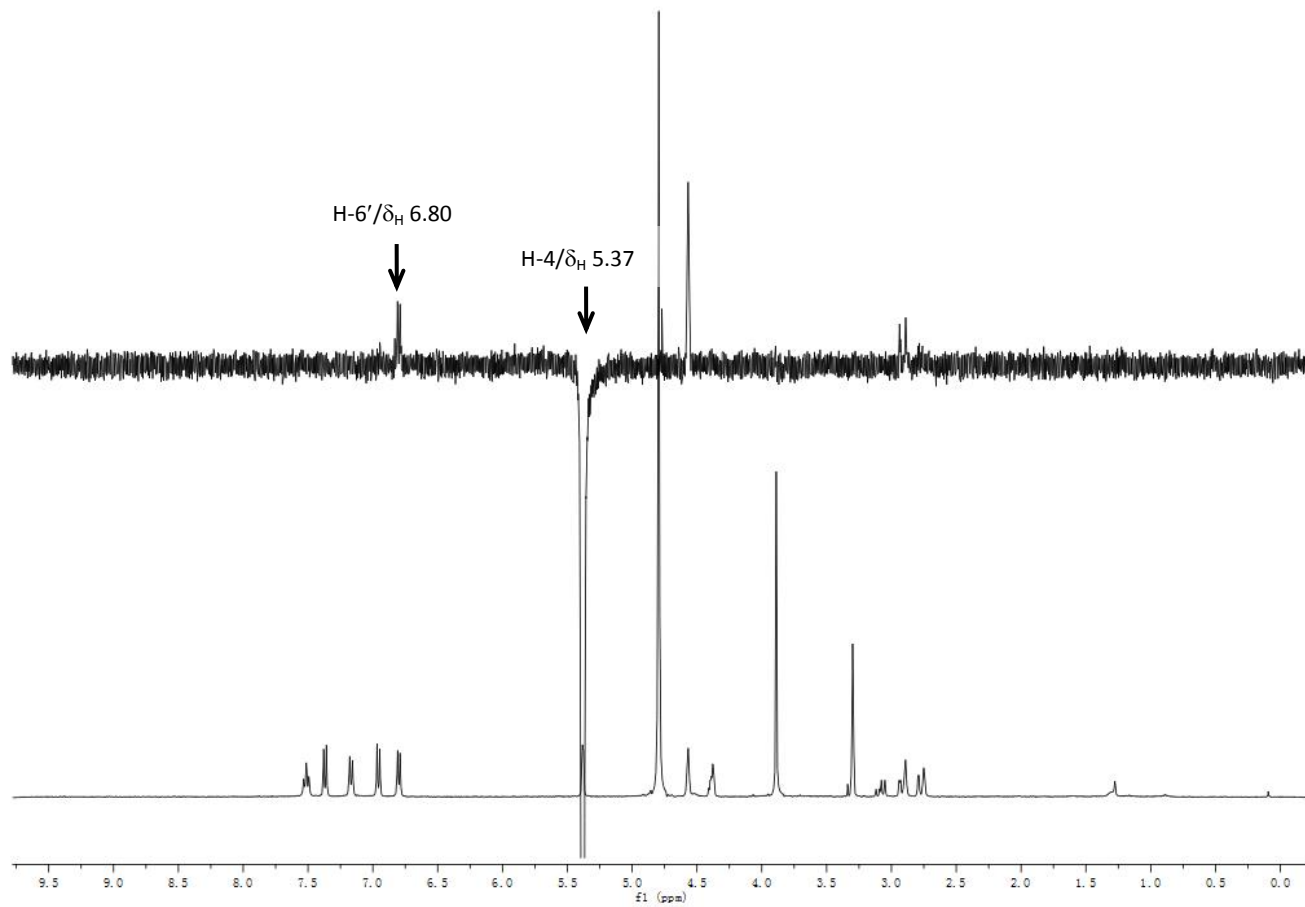


Fig. S6-2 1D sel. Gr. NOE spectrum of the new compound **1**

Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

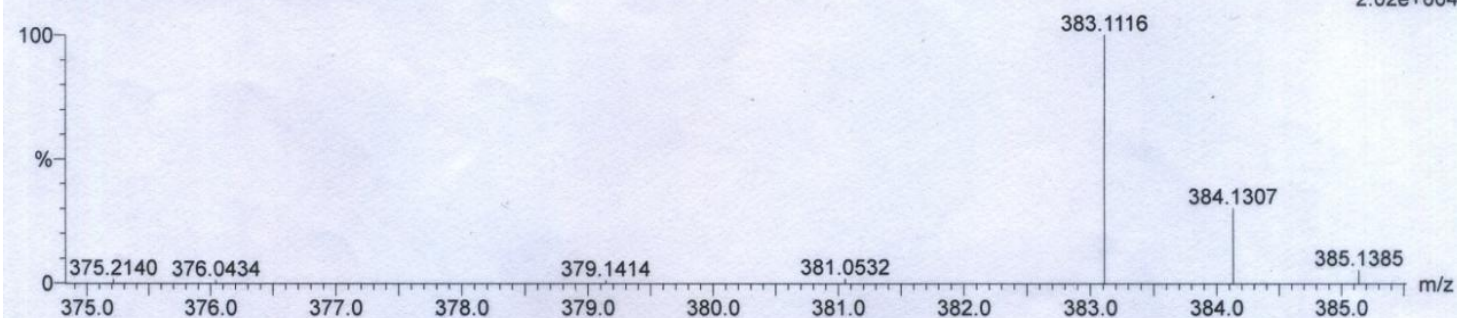
1132 formula(e) evaluated with 6 results within limits (up to 50 best isotopic matches for each mass)

Elements Used:

C: 0-500 H: 0-1000 N: 0-200 O: 0-200

16-18-7-2-w2-b-i-4

20111028-11 44 (0.374) Cm (44:48)



Minimum:				-1.5				
Maximum:		5.0	5.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
383.1116	383.1131	-1.5	-3.9	12.5	28.4	0.424	65.44	<u>C21 H19 O7</u>
	383.1117	-0.1	-0.3	18.5	29.5	1.525	21.76	C18 H11 N10 O
	383.1104	1.2	3.1	13.5	30.1	2.129	11.90	C17 H15 N6 O5
	383.1122	-0.6	-1.6	0.5	33.4	5.490	0.41	C5 H19 N8 O12
	383.1122	-0.6	-1.6	11.5	33.9	5.925	0.27	C3 H7 N22 O2
	383.1109	0.7	1.8	6.5	34.0	6.101	0.22	C2 H11 N18 O6

Fig. S7 HRESIMS spectrum of the new compound 1

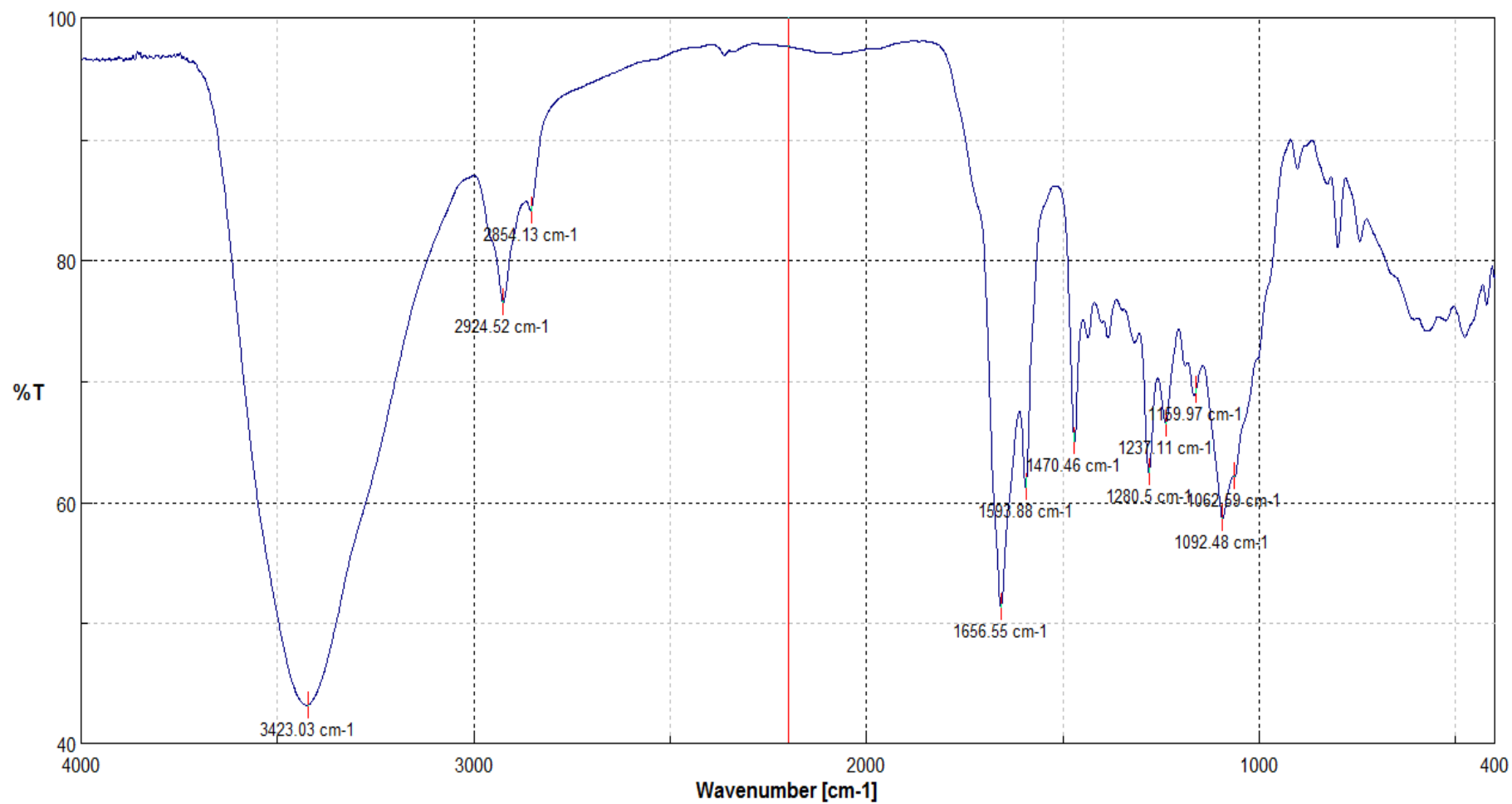


Fig. S8 IR spectrum of the new compound 1

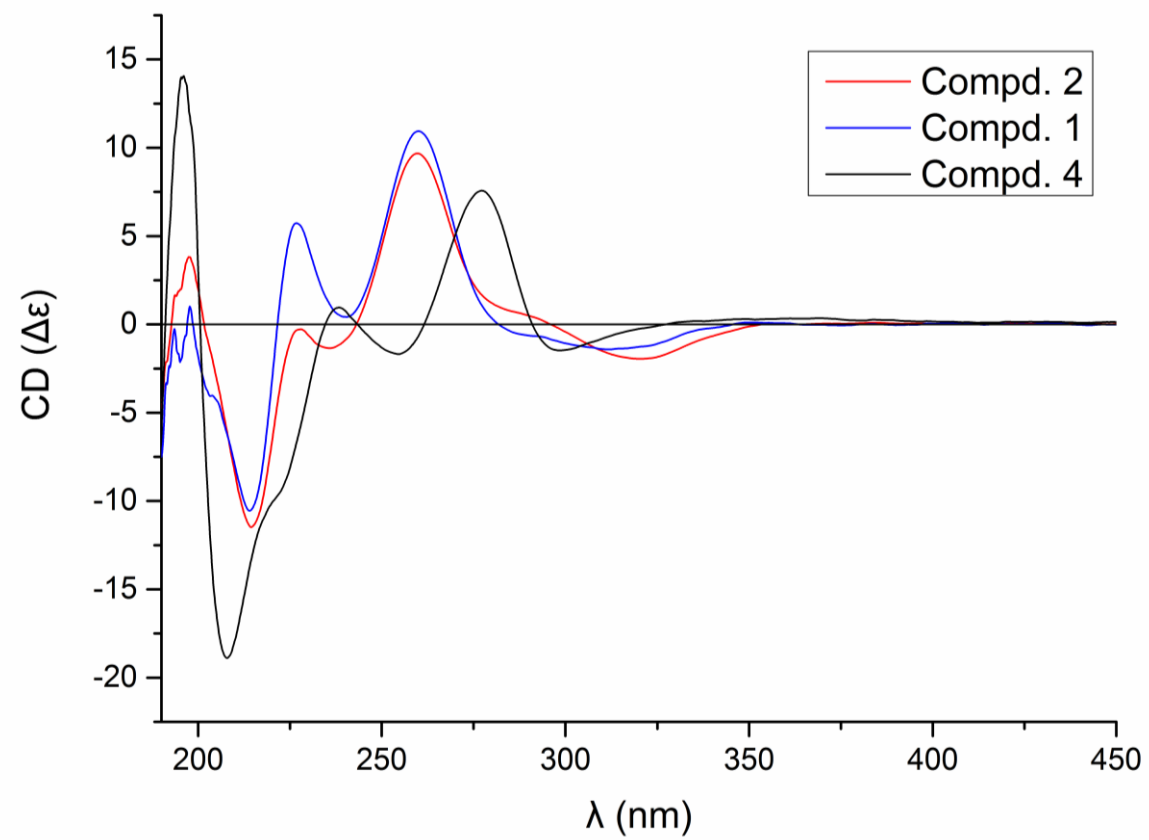


Fig. S9 CD spectrum of the compounds **1** and **2**

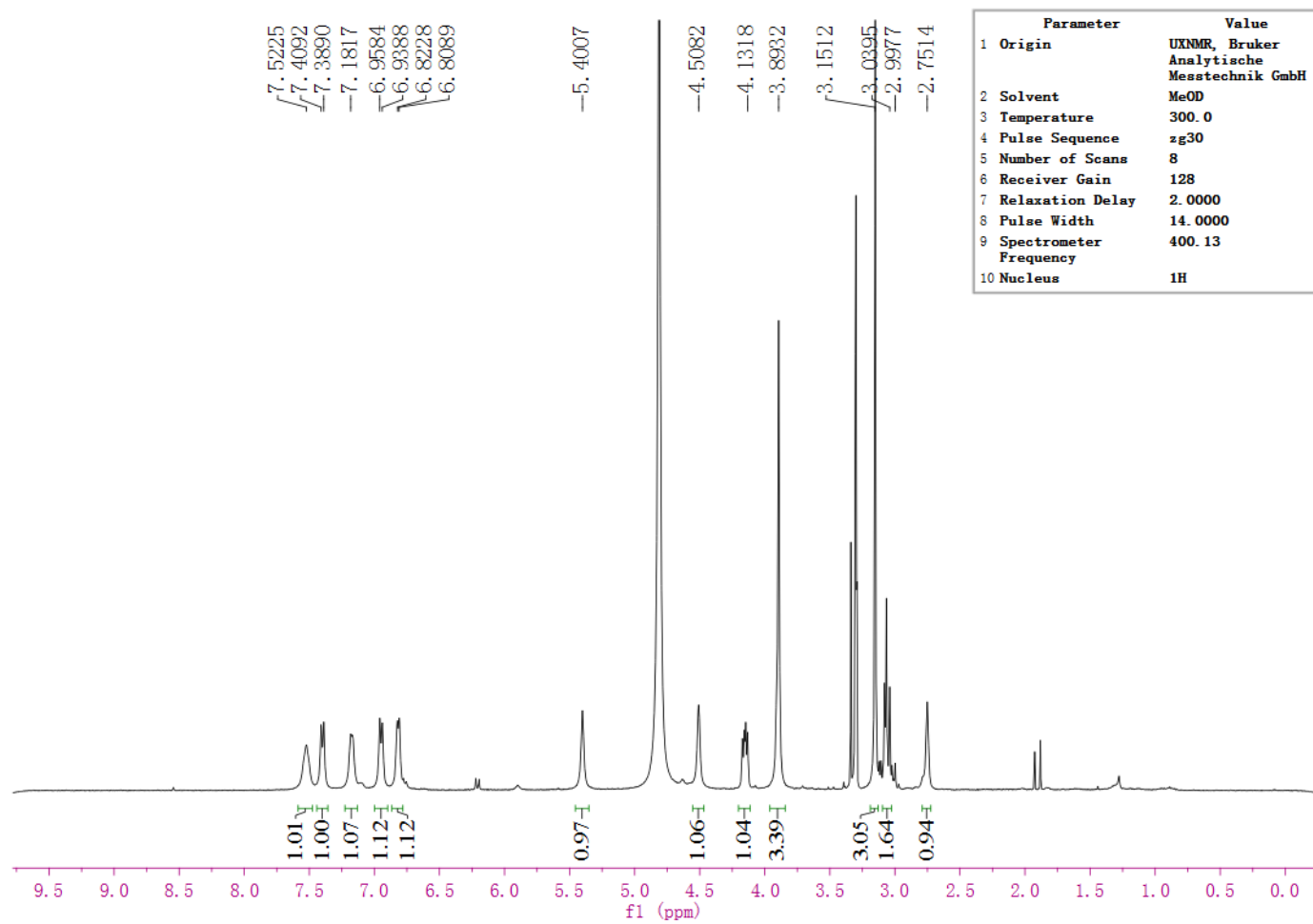


Fig. S10 ¹H-NMR spectrum of the new compound 2

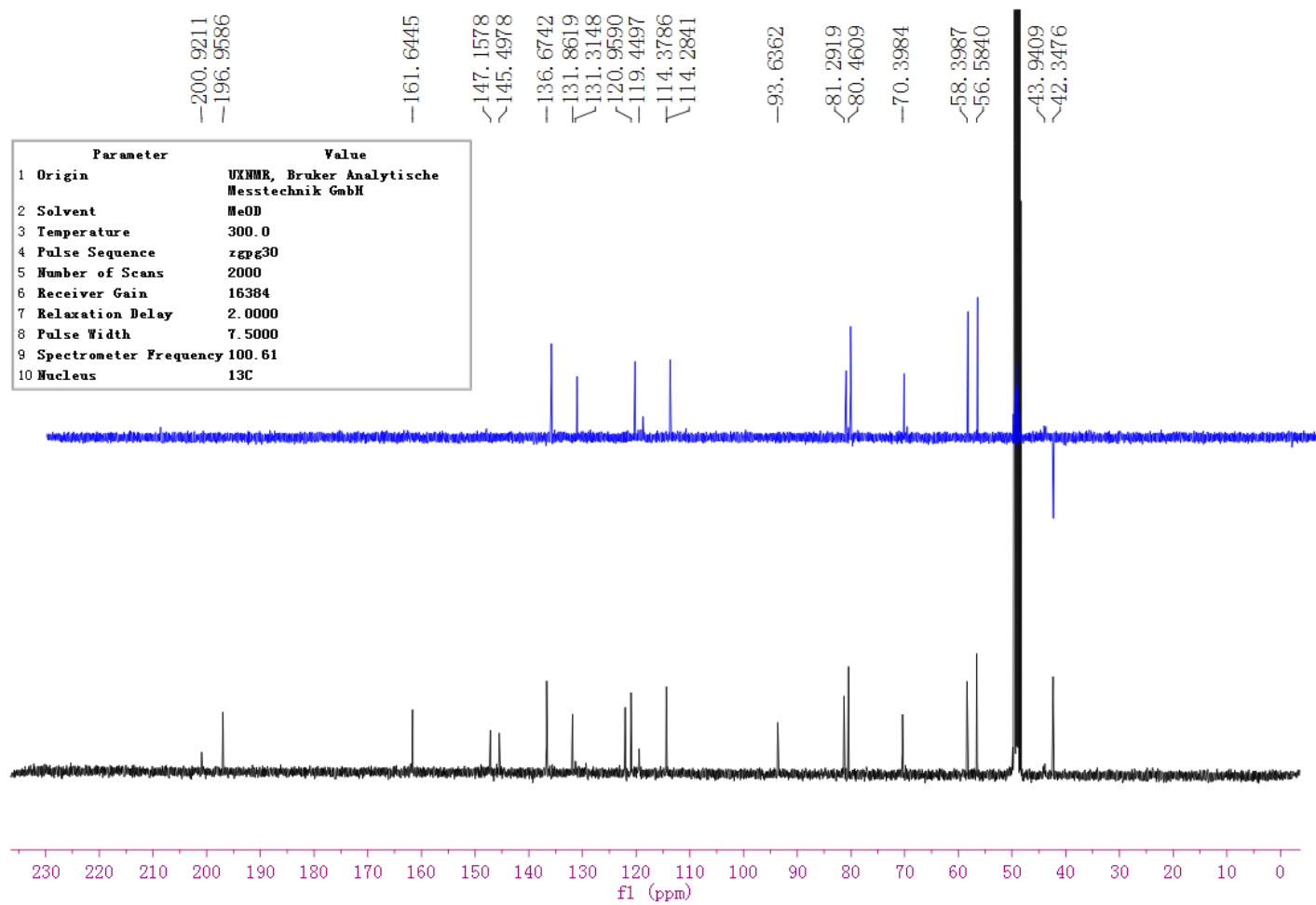


Fig. S11 ¹³C-NMR & DEPT-135 spectrum of the new compound 2

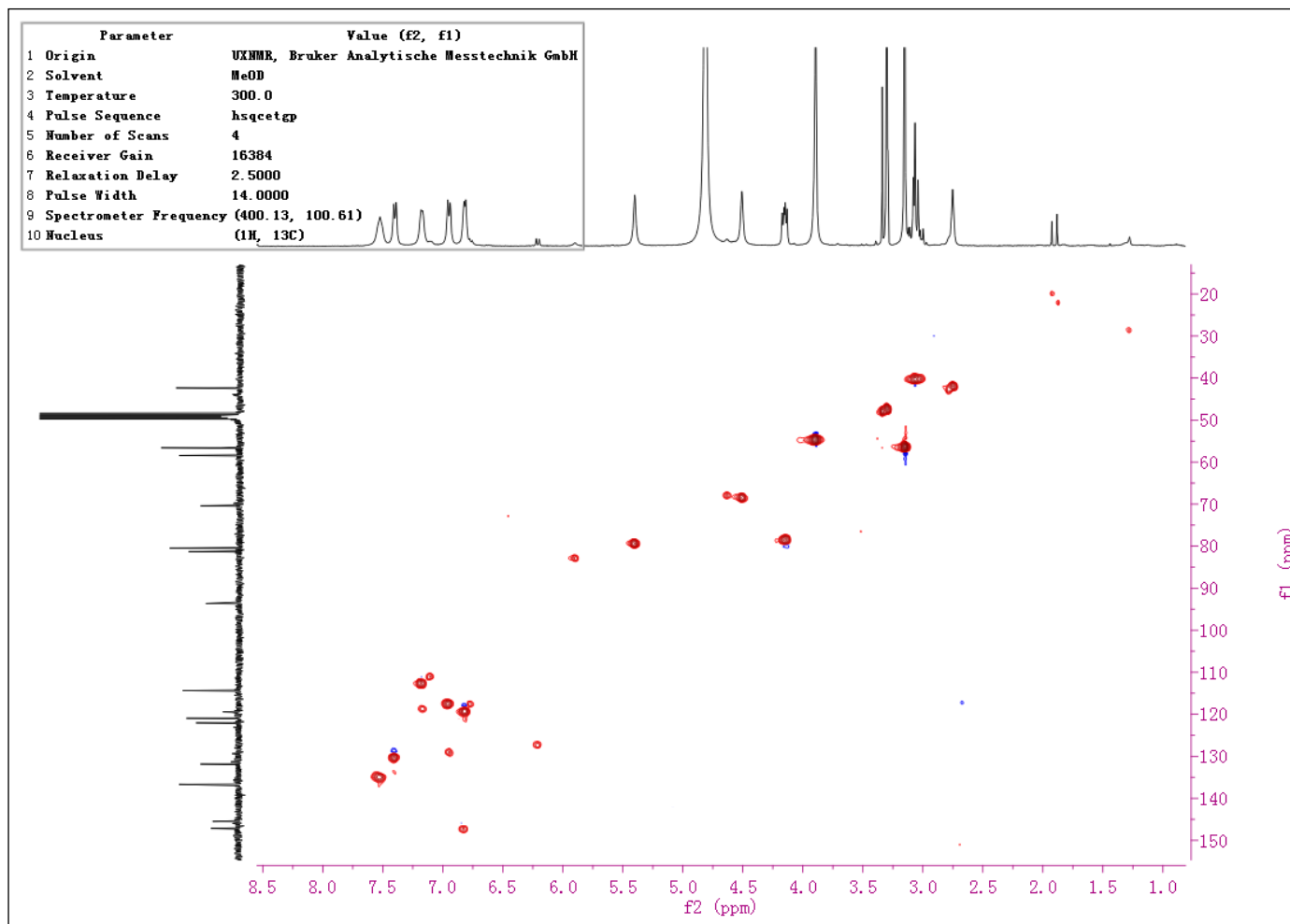


Fig. S13 HSQC spectrum of the new compound 2

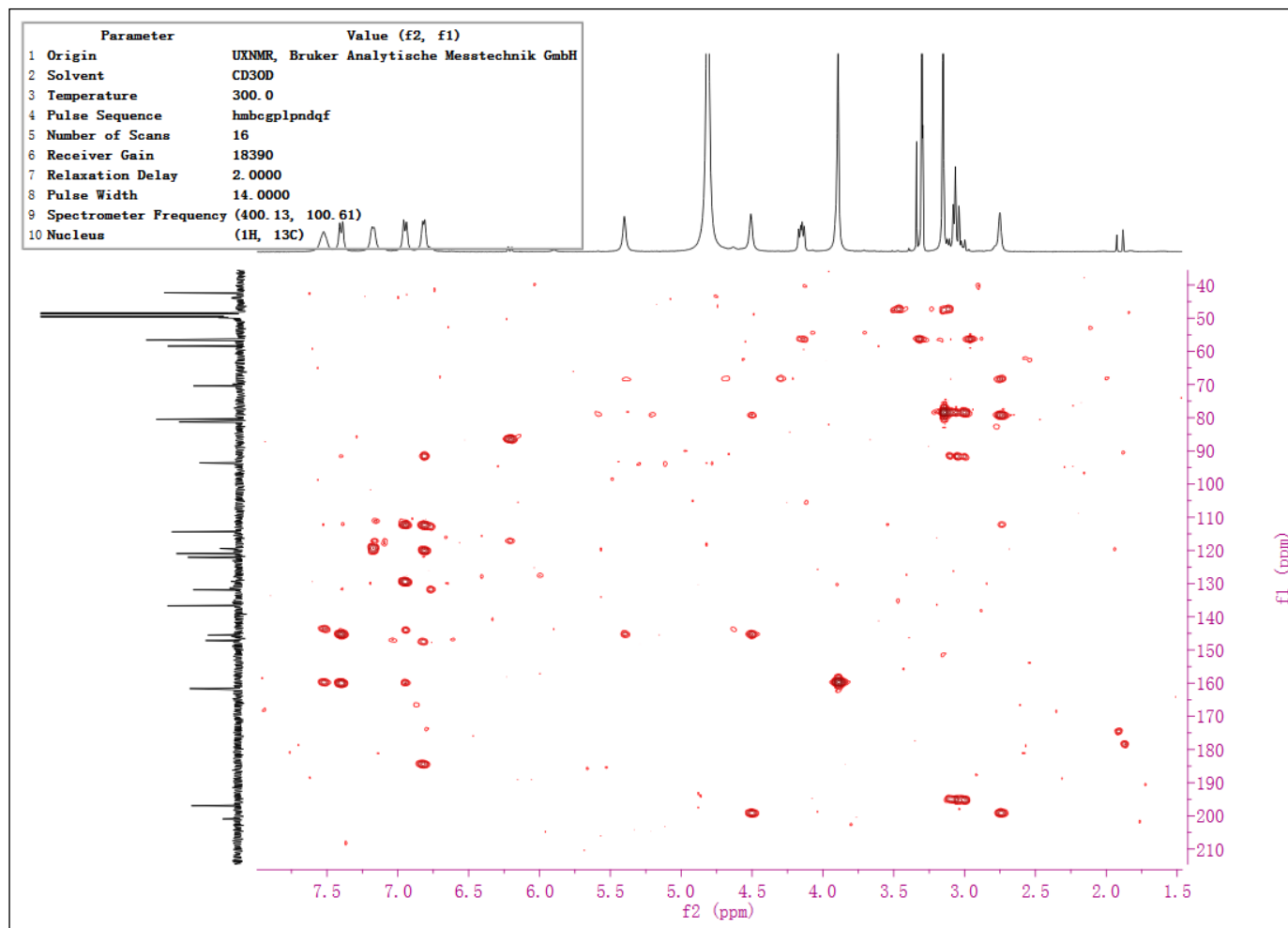


Fig. S14 HMBC spectrum of the new compound 2

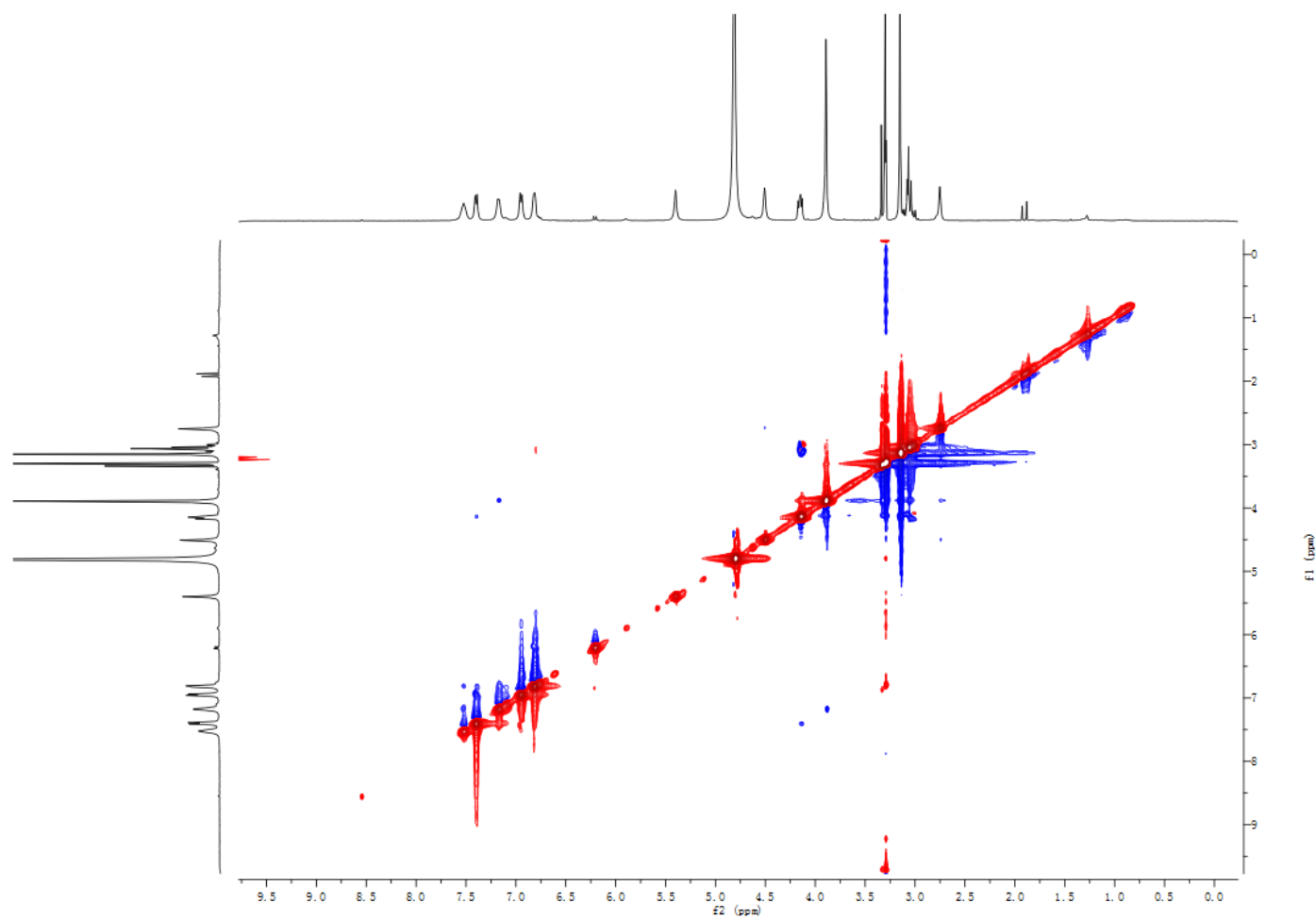


Fig. S15 ROESY spectrum of the new compound **2**

Elemental Composition Report

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

1239 formula(e) evaluated with 8 results within limits (up to 50 best isotopic matches for each mass)

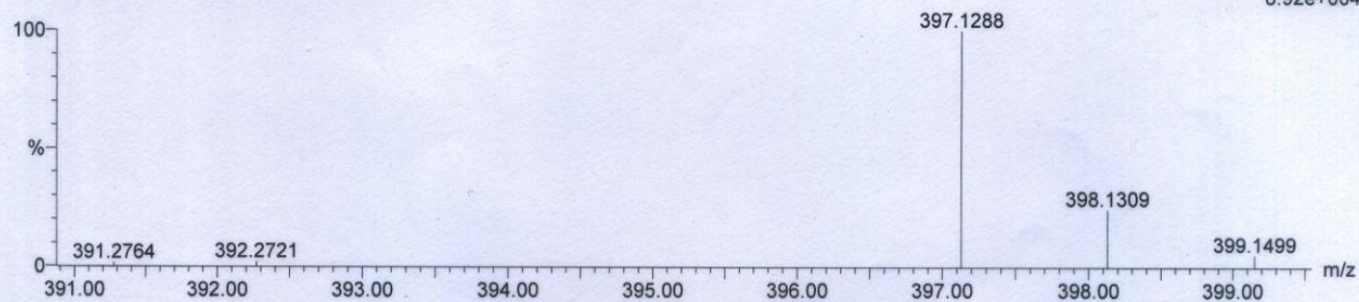
Elements Used:

C: 0-500 H: 0-1000 N: 0-200 O: 0-200

16-18-7-2-w2-b-g-3

20111028-13 58 (0.479) Cm (57:62)

1: TOF MS ES+
8.92e+004



Minimum: -1.5
Maximum: 5.0 5.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
397.1288	397.1287	0.1	0.3	12.5	25.6	0.052	94.91	<u>C22 H21 O7</u>
	397.1301	-1.3	-3.3	17.5	28.7	3.177	4.17	C23 H17 N4 O3
	397.1274	1.4	3.5	18.5	30.2	4.729	0.88	C19 H13 N10 O
	397.1306	-1.8	-4.5	10.5	34.6	9.075	0.01	C8 H13 N16 O4
	397.1306	-1.8	-4.5	-0.5	34.6	9.111	0.01	C10 H25 N2 O14
	397.1292	-0.4	-1.0	5.5	35.0	9.439	0.01	C7 H17 N12 O8
	397.1279	0.9	2.3	0.5	35.5	9.966	0.00	C6 H21 N8 O12
	397.1279	0.9	2.3	11.5	36.0	10.436	0.00	C4 H9 N22 O2

Fig. S16 HRESIMS spectrum of the new compound 2

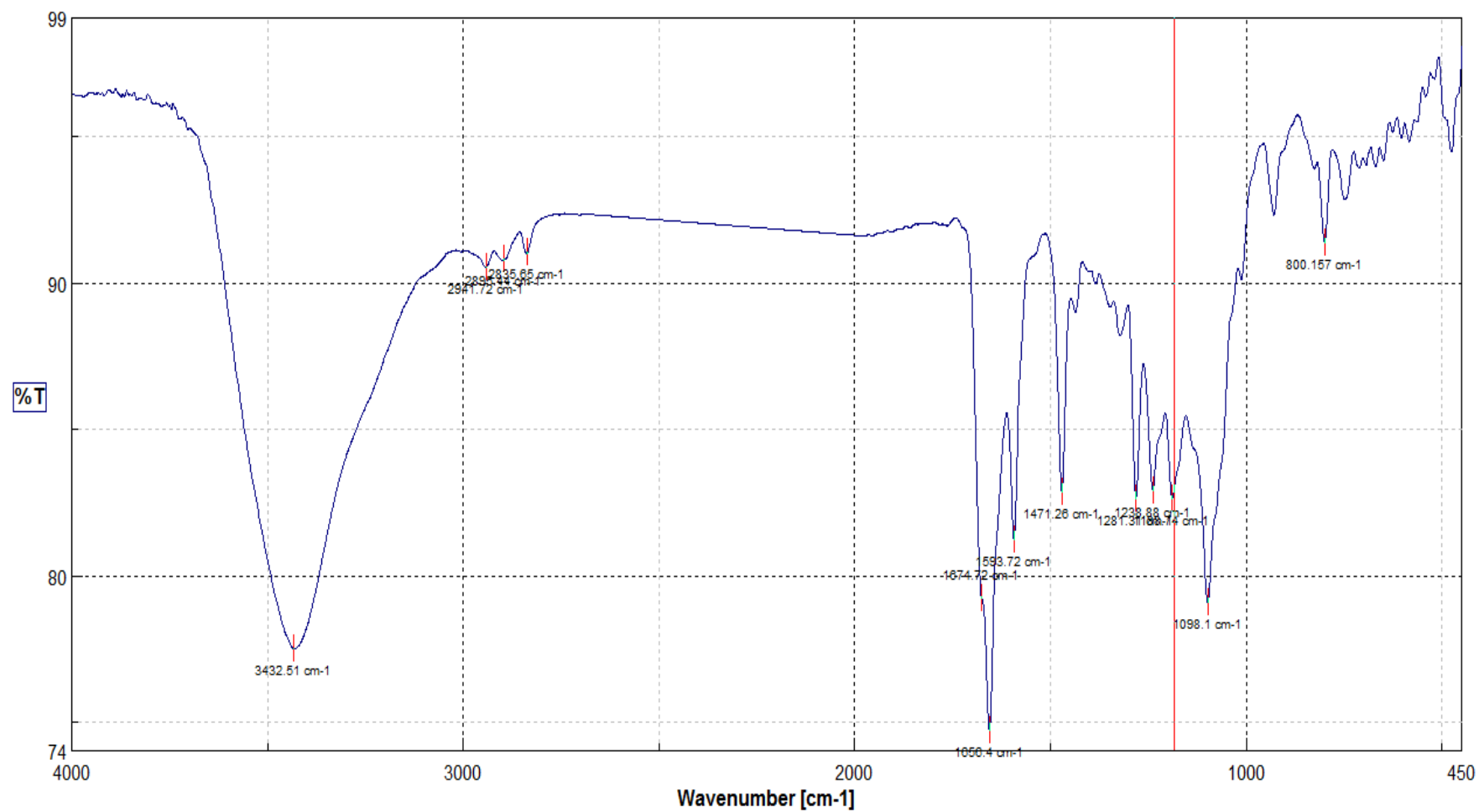


Fig. S17 IR spectrum of the new compound 2

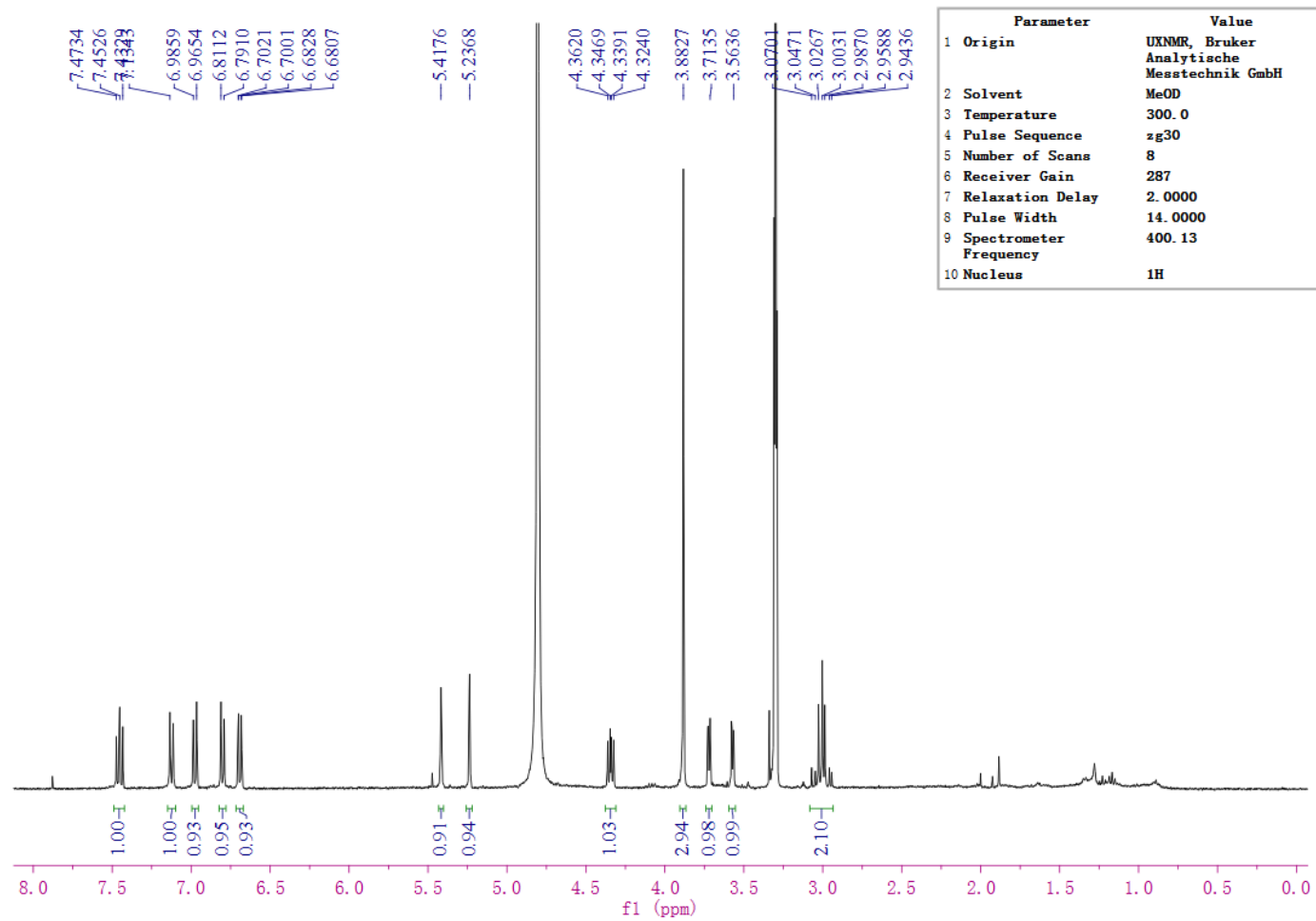


Fig. S18 ¹H-NMR spectrum of the new compound **3**

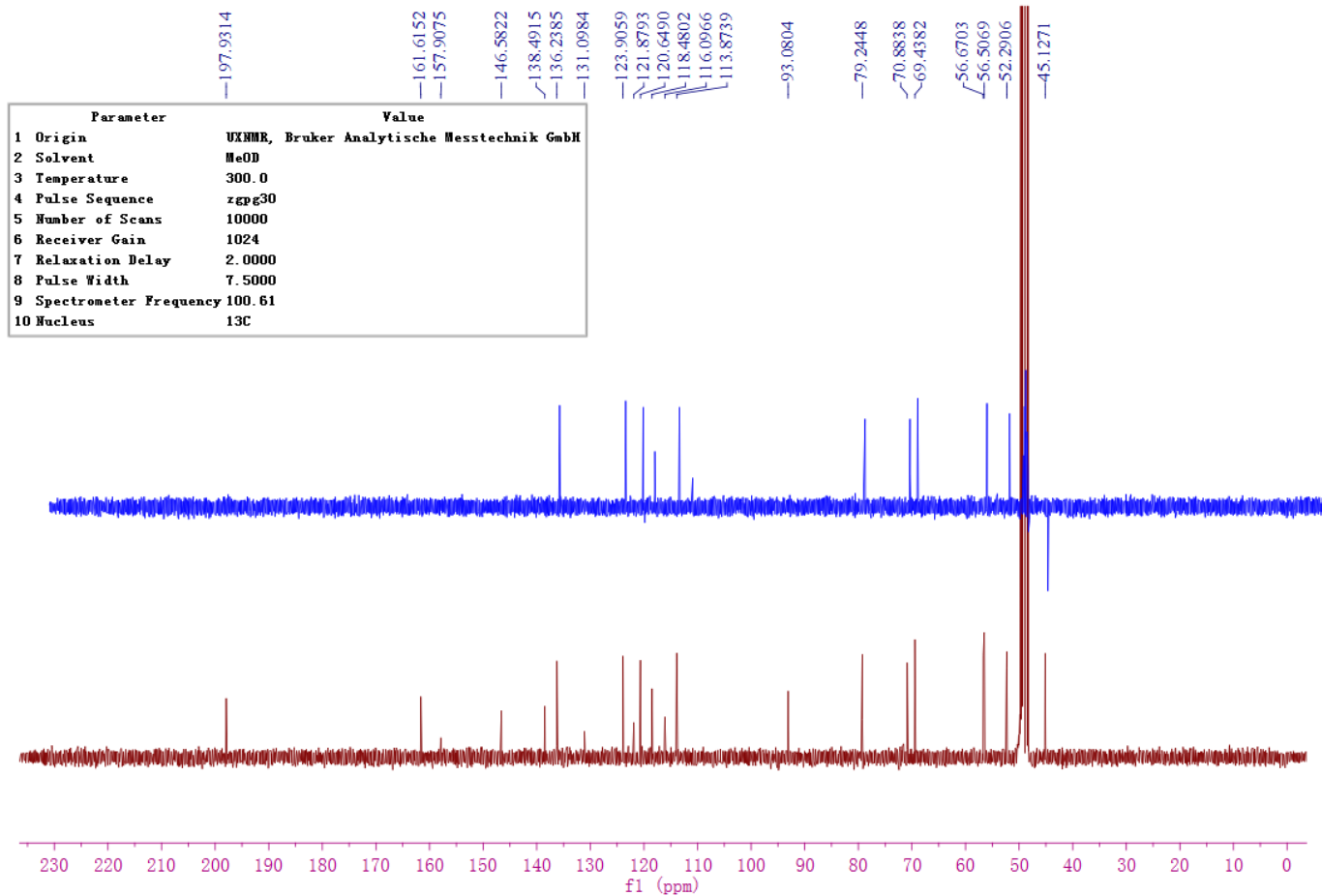


Fig. S19 ^{13}C -NMR & DEPT-135 spectrum of the new compound **3**

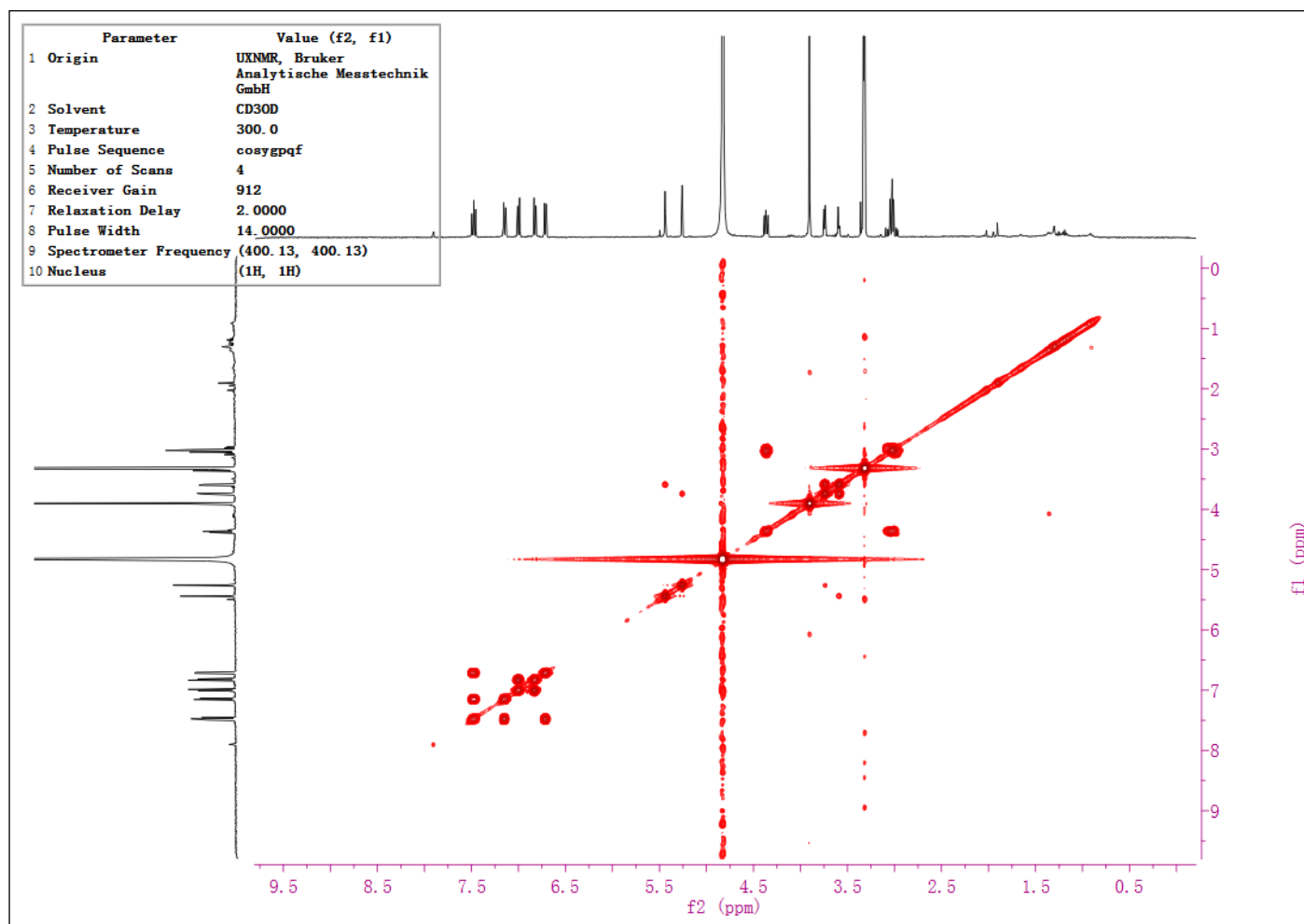


Fig. S20 ^1H - ^1H COSY spectrum of the new compound **3**

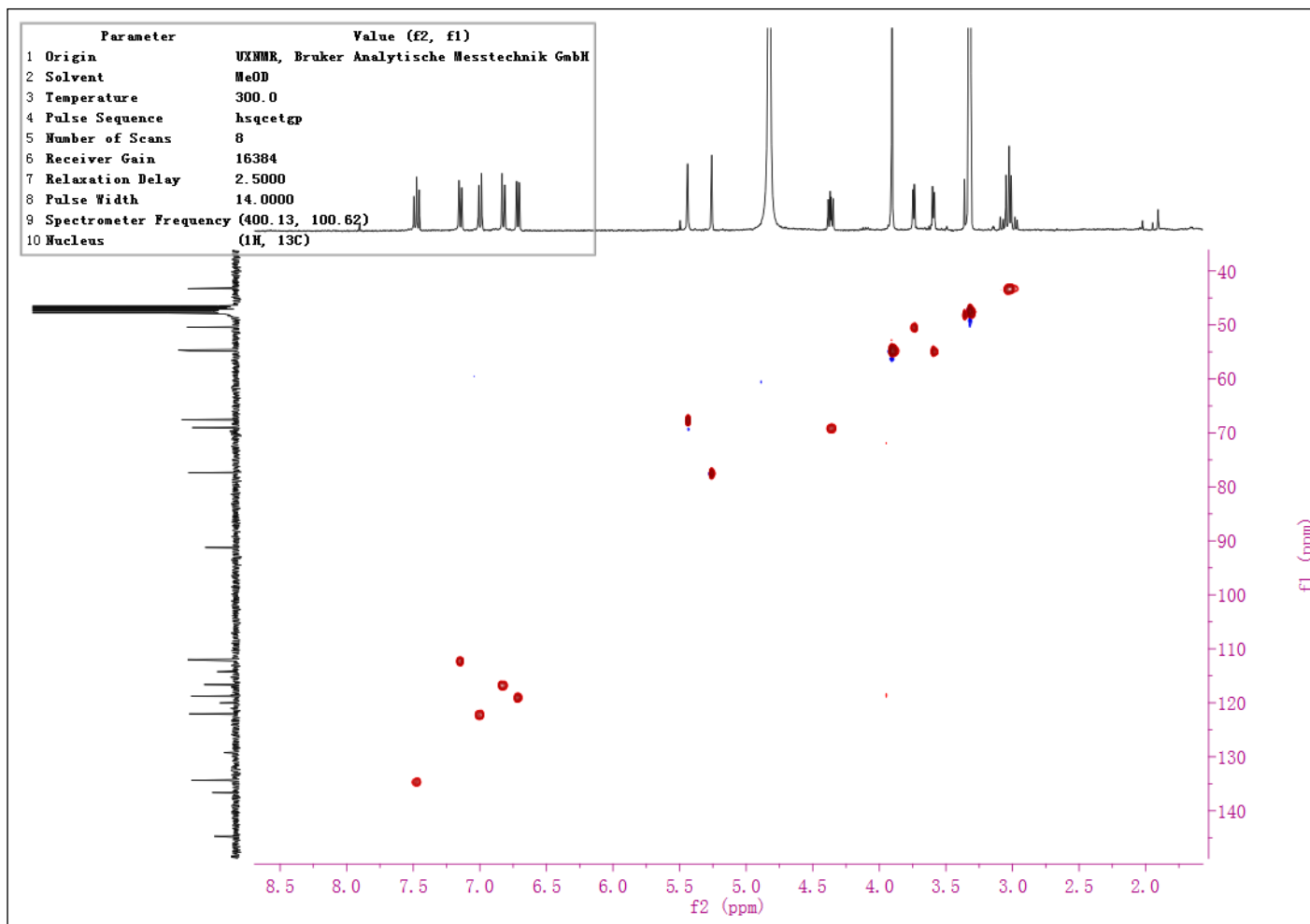


Fig. S21 HSQC spectrum of the new compound **3**

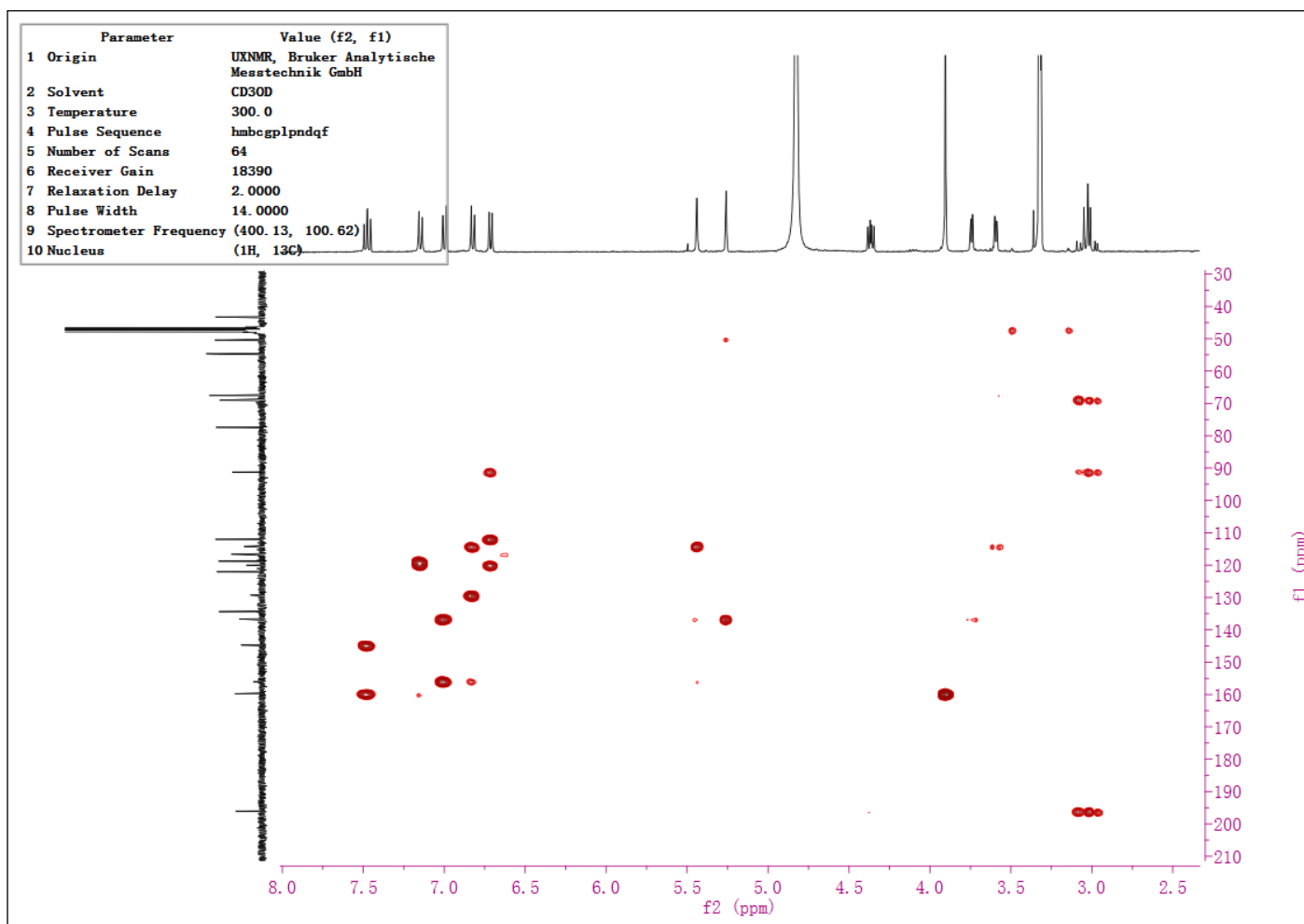


Fig. S22 HMBC spectrum of the new compound **3**

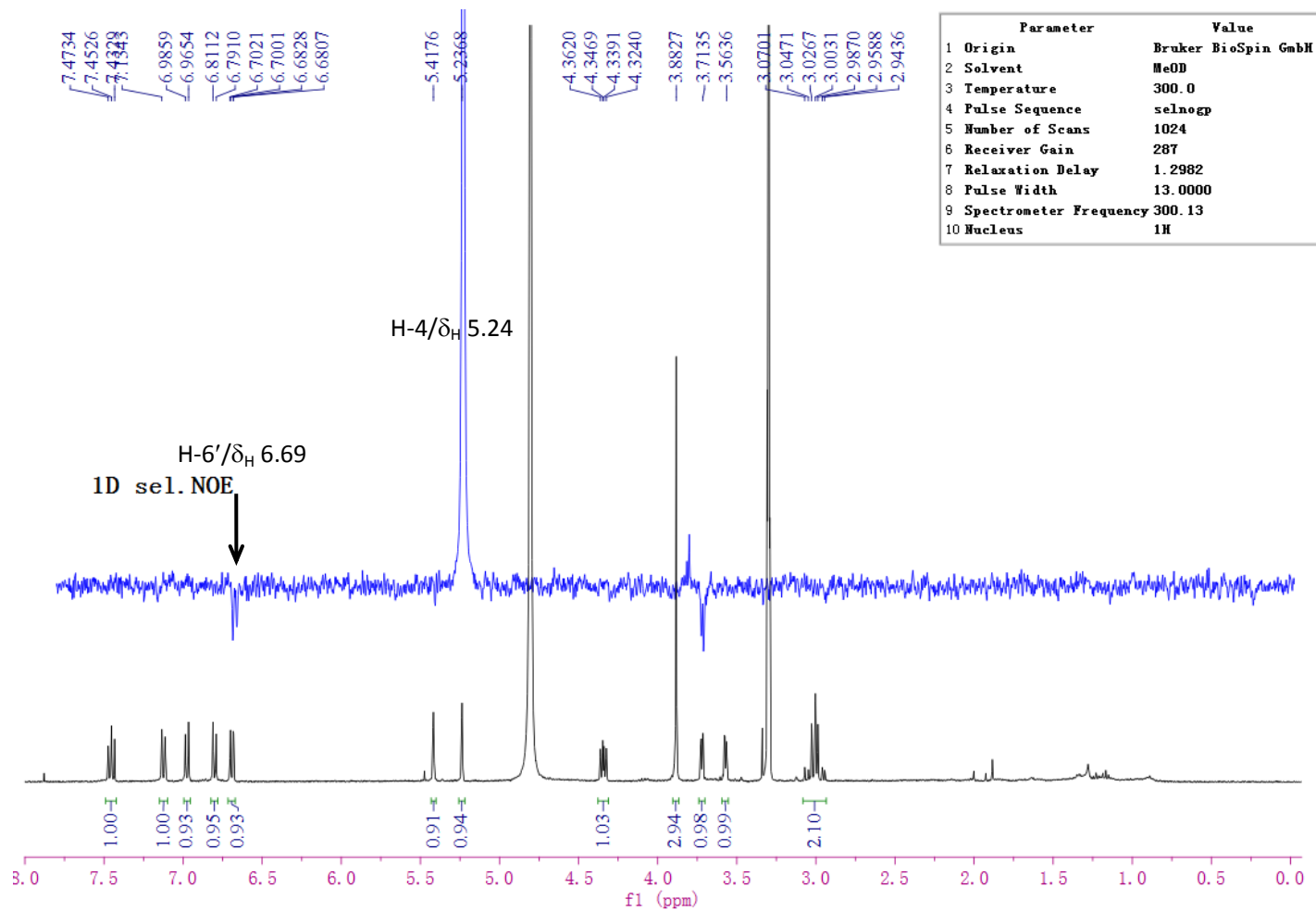


Fig. S23-1 1D sel. Gr. NOE spectrum of the new compound 3

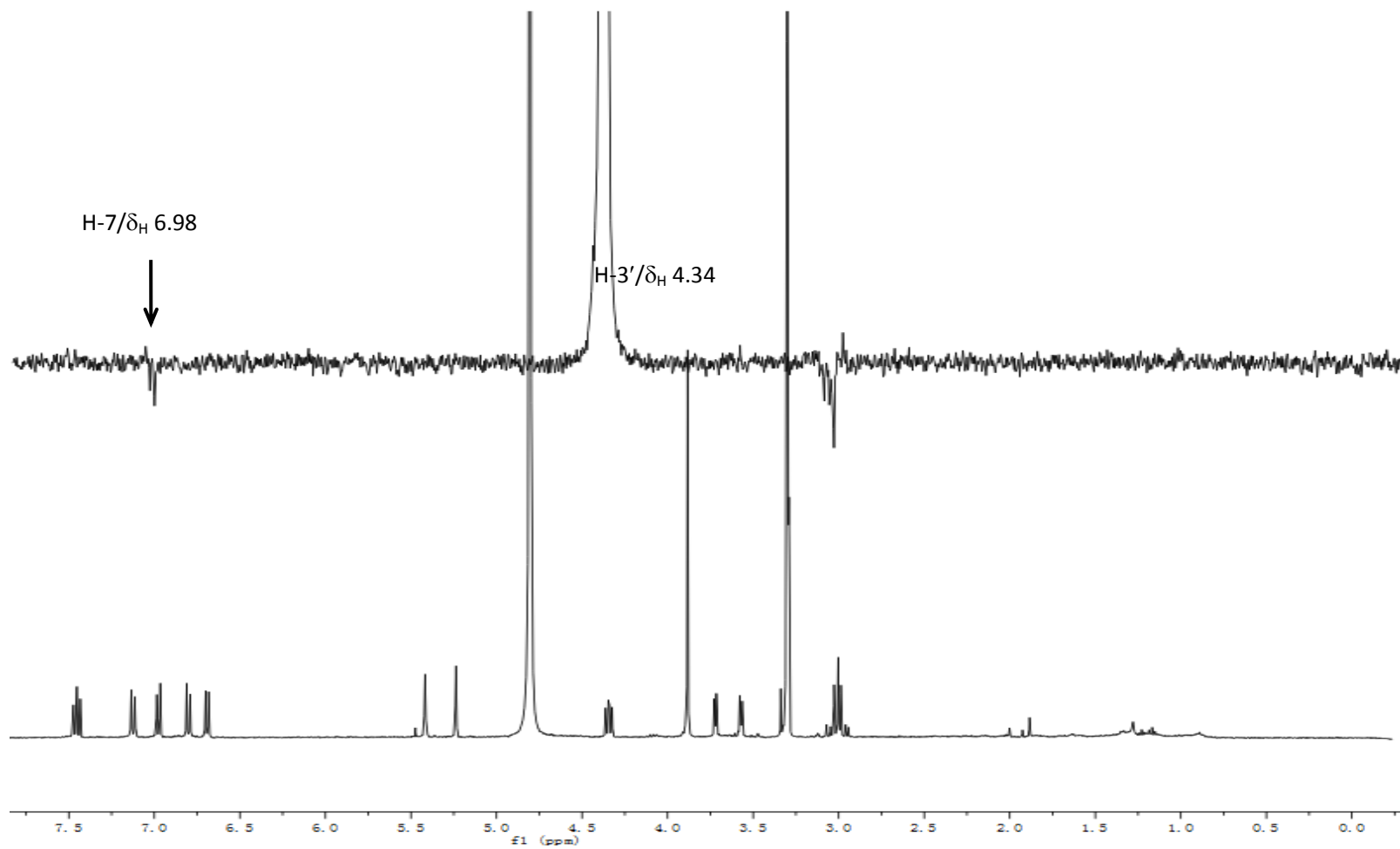


Fig. S23-2 1D sel. Gr. NOE spectrum of the new compound **3**

Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

1132 formula(e) evaluated with 7 results within limits (up to 50 best isotopic matches for each mass)

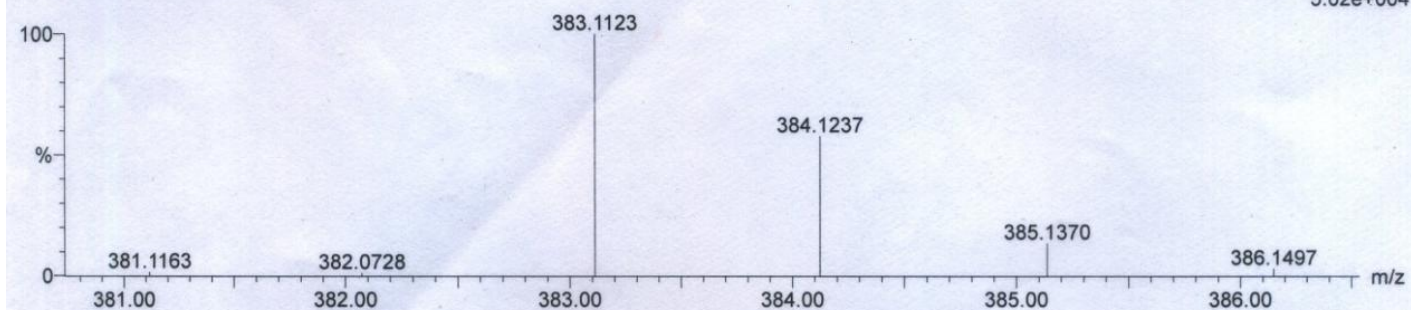
Elements Used:

C: 0-500 H: 0-1000 N: 0-200 O: 0-200

16-18-7-2-w2-b-72-3

20111028-12 40 (0.333) Cm (38:42)

1: TOF MS ES+
5.02e+004



Minimum: -1.5
Maximum: 5.0 5.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
383.1123	383.1131	-0.8	-2.1	12.5	36.9	0.978	37.62	<u>C21 H19 O7</u>
	383.1117	0.6	1.6	18.5	37.3	1.445	23.58	C18 H11 N10 O
	383.1104	1.9	5.0	13.5	37.5	1.622	19.75	C17 H15 N6 O5
	383.1136	-1.3	-3.4	5.5	38.6	2.735	6.49	C6 H15 N12 O8
	383.1122	0.1	0.3	0.5	38.7	2.843	5.82	C5 H19 N8 O12
	383.1109	1.4	3.7	6.5	39.2	3.310	3.65	C2 H11 N18 O6
	383.1122	0.1	0.3	11.5	39.3	3.475	3.09	C3 H7 N22 O2

Fig. S24 HRESIMS spectrum of the new compound 3

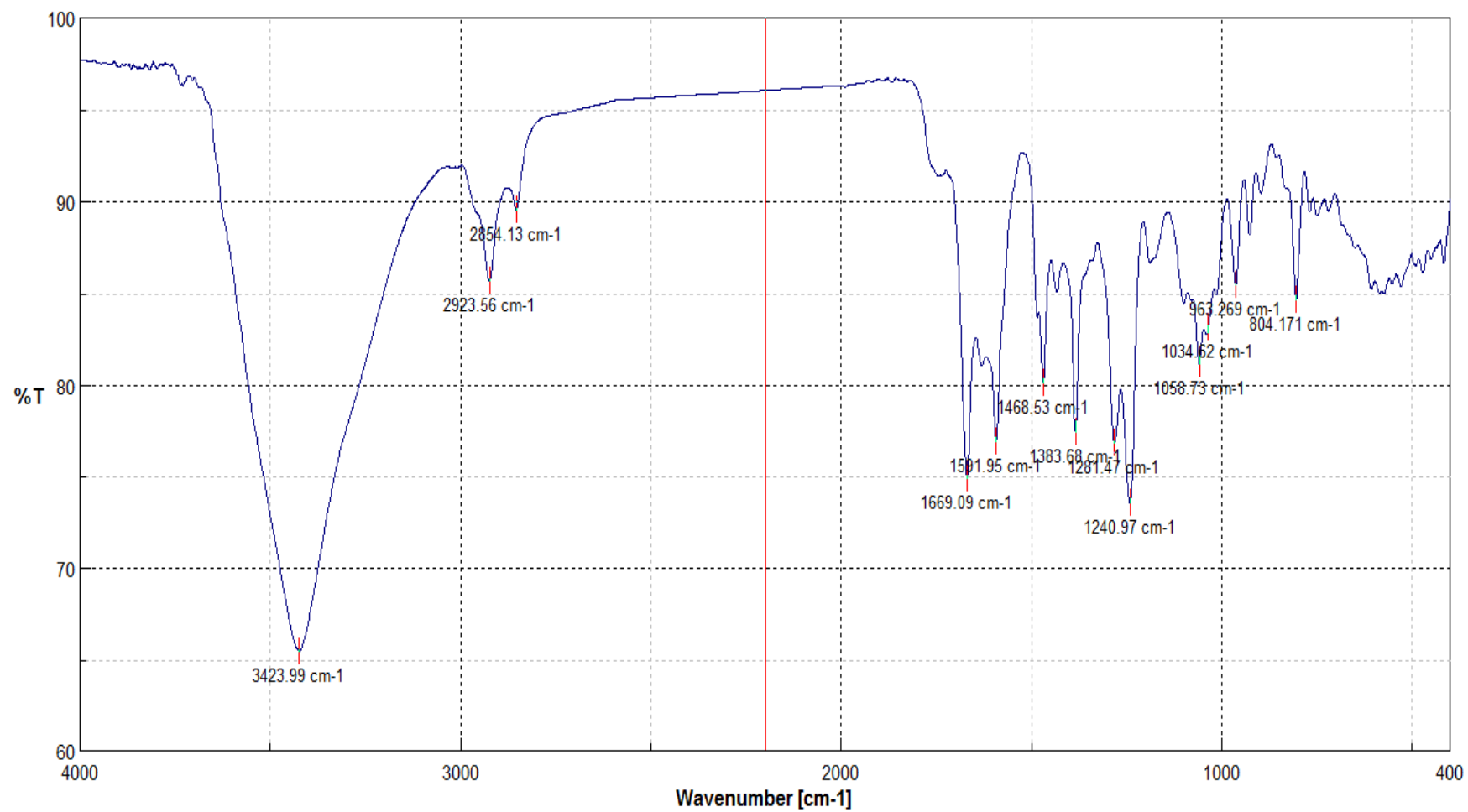


Fig. S25 IR spectrum of the new compound **3**

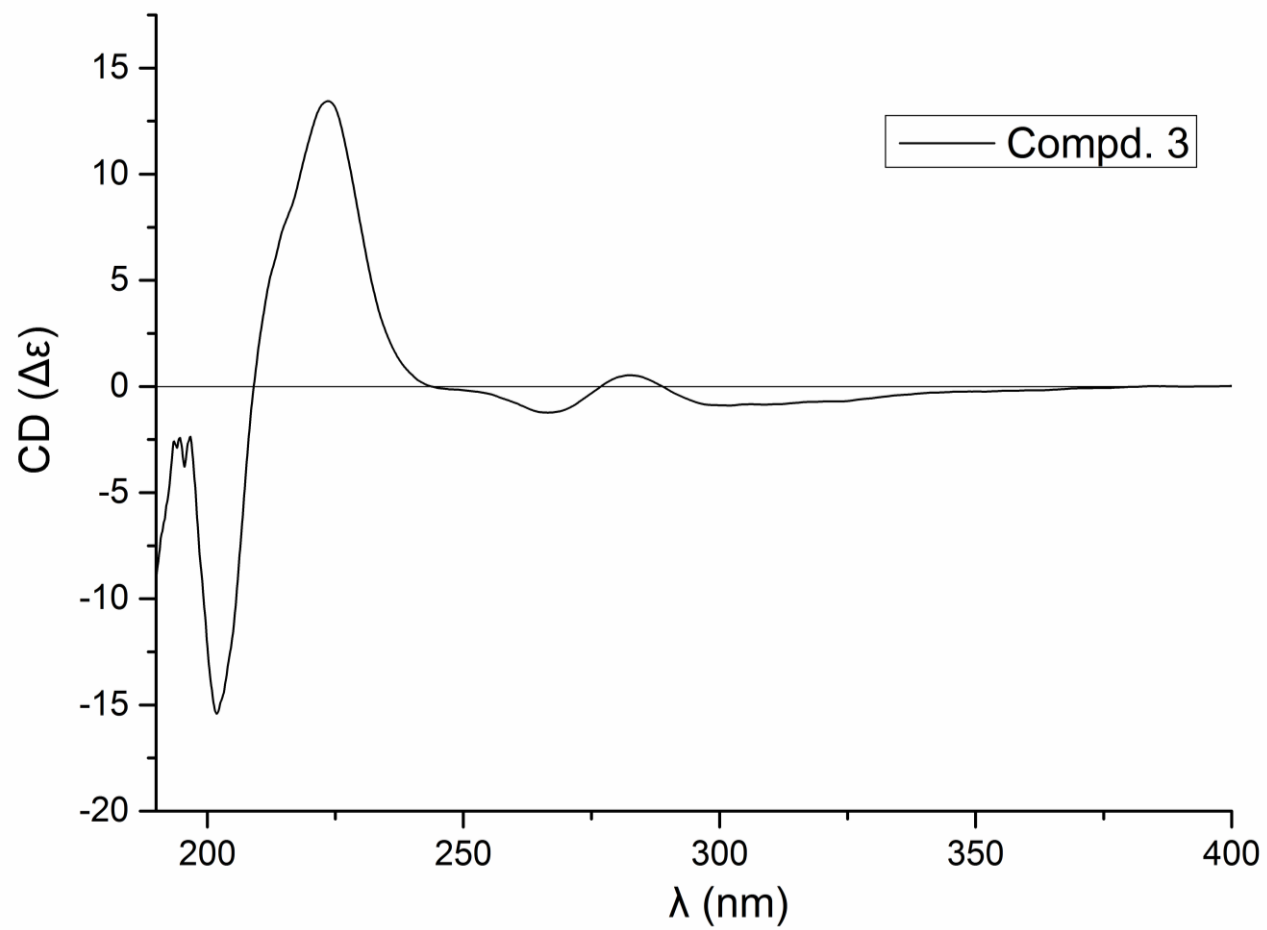


Fig. S26 CD spectrum of the new compound **3**