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Supplementary Information

Pseudeurglobosins A−F, Six Rearranged [11]-Chaetoglobosins with Immunosuppressive Activities from *Pseudeurotium bakeri* P1-1-1

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Content

Table S1. ^{1}H (400 MHz) and ^{13}C NMR data (100 MHz) for **1**–**2**

	1[a]		**2**[b]	
position	δ_C, type	δ_H (*J* in Hz)	δ_C, type	δ_H (*J* in Hz)
1	173.0, C		174.1, C	
3	53.8, CH	3.54, m	61.6, CH	3.90, m
4	45.2, CH	2.69, d (6.4)	50.8, CH	3.24, br s
5	36.0, CH	2.37, overlapped	127.9, C	
6	141.0, C		135.0, C	
7	123.8, CH	5.75, br s	72.8, CH	4.66, t (7.2)
8	47.2, CH	2.59, overlapped	47.1, CH	2.36, dd (13.5, 10.5)
9	70.8, C		60.9, C	
10	35.8, CH_2	3.05, dd (14.3, 4.2)	34.3, CH_2	3.82, overlapped
		2.79, dd (14.3, 10.1)		
11	13.7, CH_3	1.27, d (7.4)	18.1, CH_3	1.44, s
12	19.9, CH_3	1.72, s	23.4, CH_3	1.92, s
13	41.0, CH	2.89, t (8.8)	46.0, CH	3.67, m
14	40.3, CH	2.37, overlapped	81.8, CH	5.12, overlapped
15	37.1, CH_2	2.05, m	39.2, CH_2	2.41, dd (13.6, 7.5)
		1.22, m		1.71, dd (13.6, 4.9)
16	30.0, CH	1.92, m	23.4, CH	1.96, m
17	47.3, CH_2	2.59, overlapped	36.9, CH_2	2.17, dd (14.0, 7.0)
		1.99, dd (17.1, 10.5)		1.22, dd (14.0, 5.7)
18	213.0, C		79.2, CH	3.95, br d (7.0)
19	44.6, CH	3.08, t (7.8)	42.7, CH	3.27, m
20	50.4, CH	3.47, t (7.8)	44.5, CH_2	2.93, dd (16.2, 13.1)
				2.83, dd (16.2, 4.8)
21	212.5, C		212.2, C	
22	27.2, CH_3	1.01, d (6.2)	23.8, CH_3	1.14, d (7.5)
2'	127.8, CH	6.86, br s	125.1, CH	7.45, br s
3'	111.5, C		113.0, C	
4'	127.1, C		129.2, C	
5'	118.2, CH	7.57, d (7.8)	119.8, CH	8.03, d (7.6)
6'	119.4, CH	7.14, t (7.8)	119.8, CH	7.29, t (7.6)
7'	122.1, CH	7.22, t (7.8)	122.3, CH	7.32, t (7.6)
8'	111.9, CH	7.48, d (7.8)	112.6, CH	7.62, d (7.6)
9'	136.6, C		138.2, C	
7-OH				6.74, d (7.2)
2-NH		6.62, br s		9.34, br s
1'-NH		8.51, br s		11.94, br s

[a]In $CDCl_3$. [b]In Pyridine-d_5.

Table S2. ^{1}H (400 MHz) and ^{13}C NMR data (100 MHz) for **3**

	3[c]		**3**[d]	
position	δ_C, type	δ_H (*J* in Hz)	δ_C, type	δ_H (*J* in Hz)
1	174.8, C		171.8, C	
3	61.4, CH	3.46, dd (9.2, 5.5)	59.0, CH	3.30, dd (9.4, 5.0)
4	51.2, CH	2.85, br s	49.5, CH	2.71, br s
5	129.2, C		127.6, C	
6	134.2, C		132.7, C	
7	77.6, CH	3.96, d (10.6)	75.2, CH	3.78, overlapped
8	52.4, CH	2.43, dd (13.4, 10.6)	50.9, CH	2.31, dd (13.5, 10.5)
9	57.5, C		55.4, C	
10	34.3, CH_2	3.31, dd (13.5, 9.2)	33.1, CH_2	3.17, dd (13.2, 9.4)
		3.17, dd (13.5, 5.5)		3.01, dd (13.2, 5.0)
11	16.5, CH_3	0.93, s	16.0, CH_3	0.83, s
12	13.4, CH_3	1.63, s	13.3, CH_3	1.54, s
13	43.4, CH	2.71, dt (13.4, 10.7)	41.8, CH	2.57, dt (13.5, 10.7)
14	83.8, CH	4.32, t (10.7)	81.3, CH	4.17, t (10.7)
15	44.9, CH_2	2.12, overlapped	43.7, CH_2	2.01, overlapped
		1.26, m		1.22, m
16	26.0, CH	2.12, overlapped	24.5, CH	2.01, overlapped
17	43.8, CH_2	2.04, m	42.7, CH_2	1.90, dd (14.2, 8.1)
		1.33, m		1.22, m
18	71.1, CH	3.90, dd (8.0, 3.3)	68.6, CH	3.78, overlapped
19	37.2, CH	2.58, m	35.6, CH	2.42, m
20	43.4, CH_2	3.03, dd (16.5, 13.1)	42.6, CH_2	2.99, dd (16.5, 13.2)
		2.31, dd (16.5, 4.8)		2.16, dd (16.5, 4.8)
21	213.3, C		212.4, C	
22	24.2, CH_3	1.00, d (6.6)	23.7, CH_3	0.93, d (6.5)
2'	124.7, CH	7.12, br s	123.9, CH	7.18, br d (2.3)
3'	111.8, C		110.3, C	
4'	129.1, C		127.5, C	
5'	119.4, CH	7.59, d (7.9)	118.1, CH	7.52, d (8.0)
6'	119.9, CH	7.01, t (7.9)	118.4, CH	6.98, t (8.0)
7'	122.4, CH	7.09, t (7.9)	120.9, CH	7.06, t (8.0)
8'	112.4, CH	7.35, d (7.9)	111.5, CH	7.34, d (8.0)
9'	138.2, C		136.2, C	
18-OH				4.76, d (4.2)
2-NH				8.25, br s
1'-NH				10.89, br s

[c]In CD_3OD. [d]In DMSO-d_6

Table S3. ^{1}H (400 MHz) and ^{13}C NMR data (100 MHz) for **4**–**6**

	4[a]		**5**[a]		**6**[c]	
position	δ_C, type	δ_H (*J* in Hz)	δ_C, type	δ_H (*J* in Hz)	δ_C, type	δ_H (*J* in Hz)
1	172.5, C		171.6, C		174.8, C	
3	59.3, CH	3.55, dd (9.1, 5.8)	58.7, CH	3.61, dd (9.5, 5.1)	55.5, CH	3.43, ddd (8.4, 5.7, 2.2)
4	50.9, CH	2.86, br s	47.8, CH	3.35, br s	46.7, CH	3.29, dd (6.0, 2.2)
5	127.1, C		127.2, C		35.4, CH	2.10, m
6	134.2, C		133.3, C		142.0, C	
7	76.5, CH	4.09, d (10.7)	76.9, CH	4.21, d (10.6)	124.8, CH	5.38, br s
8	50.8, CH	2.49, dd (13.3, 10.7)	54.4, CH	1.95, dd (12.7, 10.6)	47.8, CH	2.13, br d (11.4)
9	56.1, C		58.2, C		67.9, C	
10	34.4, CH_2	3.30, dd (14.0, 9.1)	34.3, CH_2	3.10, dd (14.3, 5.1)	34.9, CH_2	2.84, dd (13.8, 5.7)
		3.22, dd (14.0, 5.8)		2.89, dd (14.3, 9.5)		2.68, dd (13.8, 8.4)
11	17.5, CH_3	1.50, s	17.1, CH_3	1.53, s	13.2, CH_3	0.56, d (7.2)
12	13.5, CH_3	1.75, s	13.4, CH_3	1.70, s	19.8, CH_3	1.59, s
13	42.3, CH	2.79, td (13.3, 9.8)	39.6, CH	2.98, td (12.7, 9.4)	43.3, CH	3.82, td (11.4, 9.4)
14	83.4, CH	3.97, t (9.8)	85.9, CH	3.70, ddd (11.3, 9.4, 4.0)	139.3, CH	5.31, m
15	44.1, CH_2	2.19, br d (11.8)	42.9, CH_2	2.18, br d (11.8)	118.5, CH_2	4.98, dd (11.3, 1.7)
		1.43, q (11.8)		1.49, q (11.8)		4.95, dd (4.6, 1.7)
16	34.4, CH	1.57, m	27.6, CH	1.84, m	145.9, CH	6.90, dq (15.6, 6.8)
17	36.4, CH_2	1.78, overlapped	52.8, CH_2	2.67, dd (16.1, 11.2)	133.1, CH	6.29, dq (15.6, 1.7)
		1.19, m		2.48, t (16.3)		
18	32.9, CH_2	1.78, overlapped	213.1, C		201.4, C	
		1.23, m				
19	30.9, CH	2.66, m	55.8, CH	2.54, t (10.1)	61.6, CH	3.03, t (11.1)
20	45.9, CH_2	2.49, dd (16.5, 6.1)	74.4, CH	4.95, d (10.1)	75.5, CH	5.32, d (11.1)
		2.45, dd (16.5, 11.7)				
21	210.9, C		202.5, C		206.1, C	
22	23.8, CH_3	0.98, d (6.5)	24.4, CH_3	1.06, d (6.8)	18.5, CH_3	1.87, dd (6.8, 1.6)
2'	123.1, CH	7.08, br d (2.3)	123.0, CH	6.99, br d (2.2)	124.7, CH	7.11, br s
3'	112.0, C		111.1, C		111.7, C	
4'	127.4, C		127.1, C		128.9, C	
5'	118.8, CH	7.58, d (7.9)	118.3, CH	7.56, d (7.8)	119.3, CH	7.61, d (8.0)
6'	119.8, CH	7.12, t (7.9)	119.5, CH	7.11, t (7.8)	119.8, CH	6.98, t (8.0)
7'	122.4, CH	7.20, t (7.9)	122.2, CH	7.19, t (7.8)	122.4, CH	7.04, t (8.0)
8'	111.4, CH	7.36, d (7.9)	111.7, CH	7.40, d (7.8)	112.4, CH	7.30, d (8.0)
9'	136.6, C		136.5, C		137.9, C	
2-NH		5.89, br s		7.23, br s		
1'-NH		8.17, br s		8.72, br s		

[a]In $CDCl_3$. [c]In CD_3OD

Table S4. ^{1}H (400 MHz) data for the (*S*)- and (*R*)-MTPA esters of **6**

	(*S*)-MTPA ester[c]	**(*R*)-MTPA ester**[c]	$\Delta\delta^{S-R}$
position	δ_H (*J* in Hz)	δ_H (*J* in Hz)	
3	3.48, m	3.50, m	- 0.02
4	3.34, overlapped	3.34, overlapped	0
5	2.18, m	2.20, m	- 0.02
7	5.44, br s	5.44, br s	0
8	2.30, br d (11.4)	2.31, br d (11.4)	- 0.01
10	2.92, dd (13.9, 5.7)	2.92, dd (13.9, 5.7)	0
	2.76, dd (13.9, 8.4)	2.76, dd (13.9, 8.4)	0
11	0.71, d (7.2)	0.71, d (7.2)	0
12	1.67, s	1.67, s	0
13	3.89, td (11.4, 9.5)	3.85, td (11.4, 9.5)	+ 0.04
14	5.40, m	5.40, m	0
15	5.08, dd (11.2, 1.8)	5.04, dd (11.2, 1.8)	+ 0.04
	5.04, br s	5.00, br s	+ 0.04
16	6.92, dq (15.6, 6.8)	6.67, dq (15.7, 6.9)	+ 0.25
17	6.22, dq (15.6, 1.8)	5.89, dq (15.7, 1.8)	+ 0.33
19	3.51, t (11.2)	3.45, t (11.2)	+ 0.06
20	6.61, d (11.2)	6.61, d (11.2)	0
22	1.87, dd (6.8, 1.6)	1.72, dd (6.9, 1.6)	+ 0.15
2'	7.16, br s	7.16, br s	0
5'	7.66, d (8.0)	7.66, d (8.0)	0
6'	7.04, t (8.0)	7.04, t (8.0)	0
7'	7.10, t (8.0)	7.10, t (8.0)	0
8'	7.34, d (8.0)	7.34, d (8.0)	0

[c] **In CD_3OD**

Table S5. Immunosuppressive Effects of Compounds **1**–**5** on Murine Lymphocyte Proliferation Induced by ConA (5 μg/mL) or LPS (20 μg/mL)

Compounds	**ConA-induced T-cell proliferation**	**LPS-induced B-cell proliferation**
	IC_{50}(μM) ± SD	IC_{50}(μM) ± SD
1	6.0 ± 0.9	10.8 ± 0.3
2	> 50.0	> 50.0
3	> 50.0	> 50.0
4	> 50.0	> 50.0
5	19 ± 0.5	32 ± 1.1
CsA	0.2 ± 0.3	NT[a]
MMF	[a]NT	0.6 ± 0.7

[a]NT: not tested.

Table S6. Cytotoxicity of **1**–**6** against seven Human Cancer Cell Lines

Compounds (50 μM)	**Cell viability (%)**						
	A549	A427	HCT116	HT-29	HepG2	MCF-7	Hela
1	66.2 ± 1.3	74.5 ± 0.9	74.1 ± 2.3	70.1 ± 1.4	82.3 ± 1.0	84.5 ± 3.1	73.4 ± 1.1
2	80.3 ± 1.4	77.8 ± 2.2	68.9 ± 2.6	93.8 ± 2.3	89.0 ± 2.5	80.2 ± 2.2	81.2 ± 2.7
3	86.9 ± 0.6	78.5 ± 1.1	85.7 ± 1.5	102.0 ± 0.6	88.5 ± 1.6	75.8 ± 1.7	68.0 ± 2.1
4	67.4 ± 0.6	96.3 ± 1.1	61.4 ± 0.4	61.5 ± 0.8	90.1 ± 1.9	81.6 ± 1.4	70.5 ± 1.0
5	70.9 ± 1.2	66.4 ± 0.8	67.1 ± 0.3	82.7 ± 2.1	70.4 ± 3.2	81.4 ± 1.3	76.7 ± 1.5
6	42.6 ± 1.8	31.6± 1.4	28.3 ± 1.9	51.8 ± 1.7	71.8 ± 1.4	68.9 ± 1.1	59.7 ± 2.2
Doxorubicin hydrochloride	3.2 ± 0.8	1.3 ± 0.5	2.2 ± 0.9	2.5 ± 1.4	2.6 ± 0.2	1.7 ± 0.8	1.3 ± 0.5

Doxorubicin hydrochloride was applied as a positive control.

The cell viability (showed as means ± SEM), were normalized and depicted as a percentage of the control group, which is set to 100%.

X-ray Crystallographic data for compounds 2–5.

*Crystallographic data for pseudeurglobosin B (**2**):* $C_{29}H_{34}N_2O_4$, M = 474.58, orthorhombic, space group $P2_12_12_1$ (no. 19), a = 7.69617(11) Å, b = 17.1438(3) Å, c = 18.2154(3) Å, α = 90°, β = 98.1710(14)°, γ = 90°, V = 2403.37(6) Å^3, T = 99.98(10) K, Z = 4, μ(Cu Kα) = 0.698 mm^{-1}, *Dcalc* = 1.312 g/cm^3, 32691 reflections measured (7.08° ≤ 2θ ≤ 148.006°), 4811 unique (R_{int} = 0.0561, R_{sigma} = 0.0315) which were used in all calculations. The final R_1 was 0.0378 ($I > 2\sigma(I)$) and wR_2 was 0.0975 (all data). The goodness of fit on F^2 was 1.054. Flack parameter = −0.17(11).

*Crystallographic data for pseudeurglobosin C (**3**)*: $C_{29}H_{36}N_2O_5$, M = 492.60, orthorhombic, space group $P2_12_12_1$ (no. 19), a = 11.91695(4) Å, b = 13.87123(6) Å, c = 15.20036(6) Å, α = 90°, β = 91.3759(5)°, γ = 90°, V = 2512.660(17) Å^3, Z = 4, T = 100.00(10) K, μ(Cu Kα) = 0.716 mm^{-1}, *Dcalc* = 1.302 g/cm^3, 66071reflections measured (8.63°≤ 2θ ≤ 147.854°), 5083 unique (R_{int} = 0.0329, R_{sigma} = 0.0122) which were used in all calculations. The final R_1 was 0.0271 ($I > 2\sigma(I)$) and wR_2 was 0.0723 (all data). The goodness of fit on F^2 was 1.058. The Flack parameter was 0.03(3).

*Crystallographic data for pseudeurglobosin D (**4**)*: $C_{30.5}H_{35.5}Cl_{4.5}N_2O_3$, M = 637.63, monoclinic, space group $P2_1$ (no.4), a = 9.1280(2) Å, b =12.6160(2) Å, c = 26.8390(2) Å, α = 90°, β = 99.5200(4)°, γ = 90°, V = 3048.18(9) Å^3, Z = 4, T = 100.00(10) K, μ(Cu Kα) = 4.213 mm^{-1}, *Dcalc* = 1.389 g/cm^3, 74838 reflections measured (6.678° ≤ 2θ ≤ 147.96°), 12235 unique (R_{int} = 0.0394, R_{sigma} = 0.0232) which was used in all calculations. The final R_1 was 0.0502 ($I > 2\sigma(I)$) and wR_2 was 0.1313 (all data). The goodness of fit on F^2 was 1.057. The Flack parameter was 0.018(3).

*Crystallographic data for pseudeurglobosin E (**5**)*: $C_{29}H_{32}N_2O_5$, M = 488.57, orthorhombic, space group $P2_12_12_1$ (no. 19), a = 9.4476(2) Å, b = 23.1865(4) Å, c = 39.8892(7) Å, α = β = γ = 90°, V = 8738.0(3) Å^3, Z = 12, T = 99.99(10) K, μ(Cu Kα) = 0.617 mm^{-1}, *Dcalc* = 1.114 g/cm^3, 53113 reflections measured (5.844° ≤ 2θ ≤ 147.962°), 17186 unique (R_{int} = 0.0579, R_{sigma} = 0.0650) which were used in all calculations. The final R_1 was 0.0601 ($I > 2\sigma(I)$) and wR_2 was 0.1654 (all data). The goodness of fit on F^2 was 1.031. The Flack parameter was −0.07(9).

Supplementary immunoblotting images.

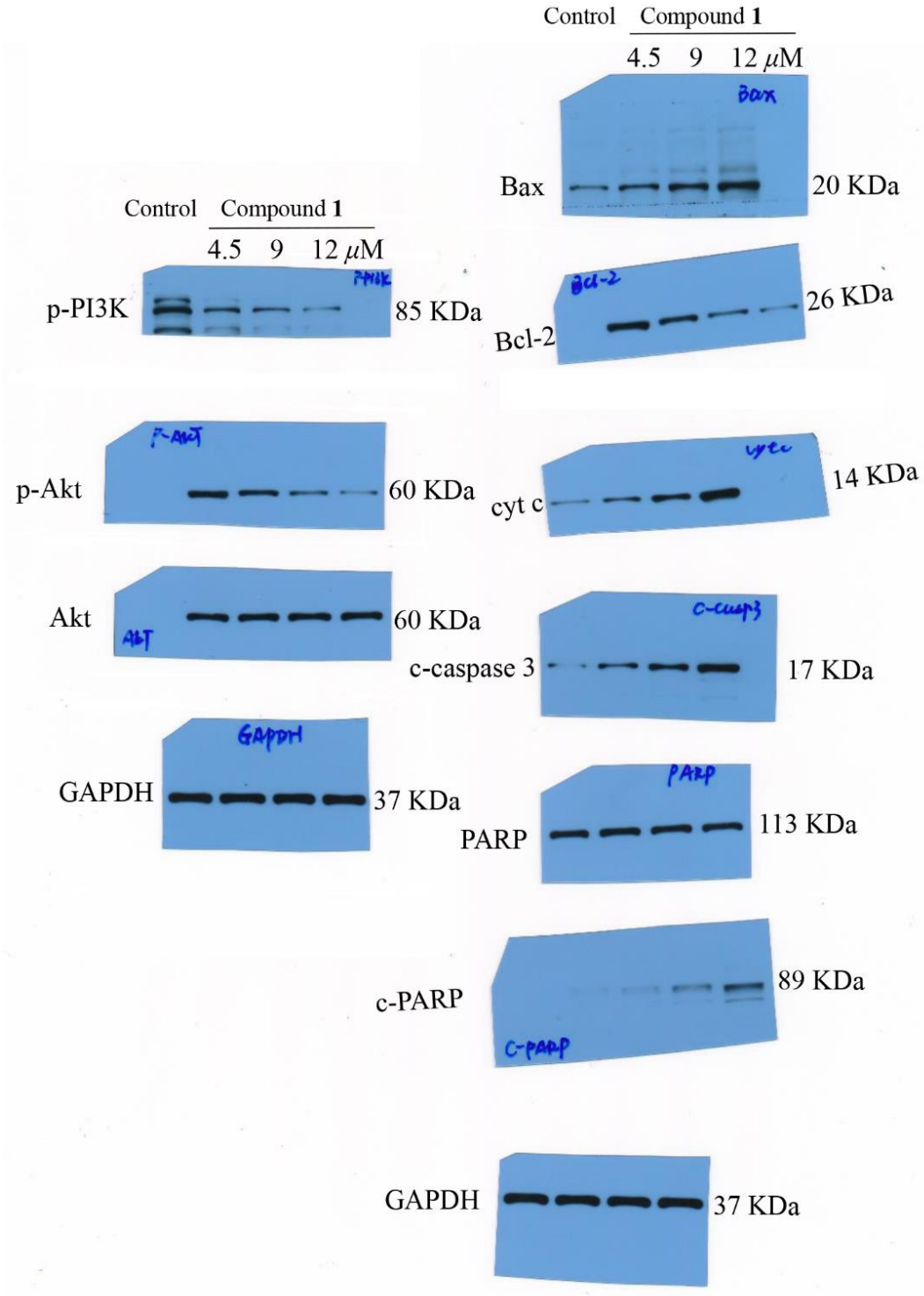


Fig. S1. Raw blot images for Bax, Bcl-2, cytochrome c, cleaved caspase 3, uncleaved PARP, cleaved PARP, *p*-PI3K, *p*-Akt, Akt, and GAPDH.

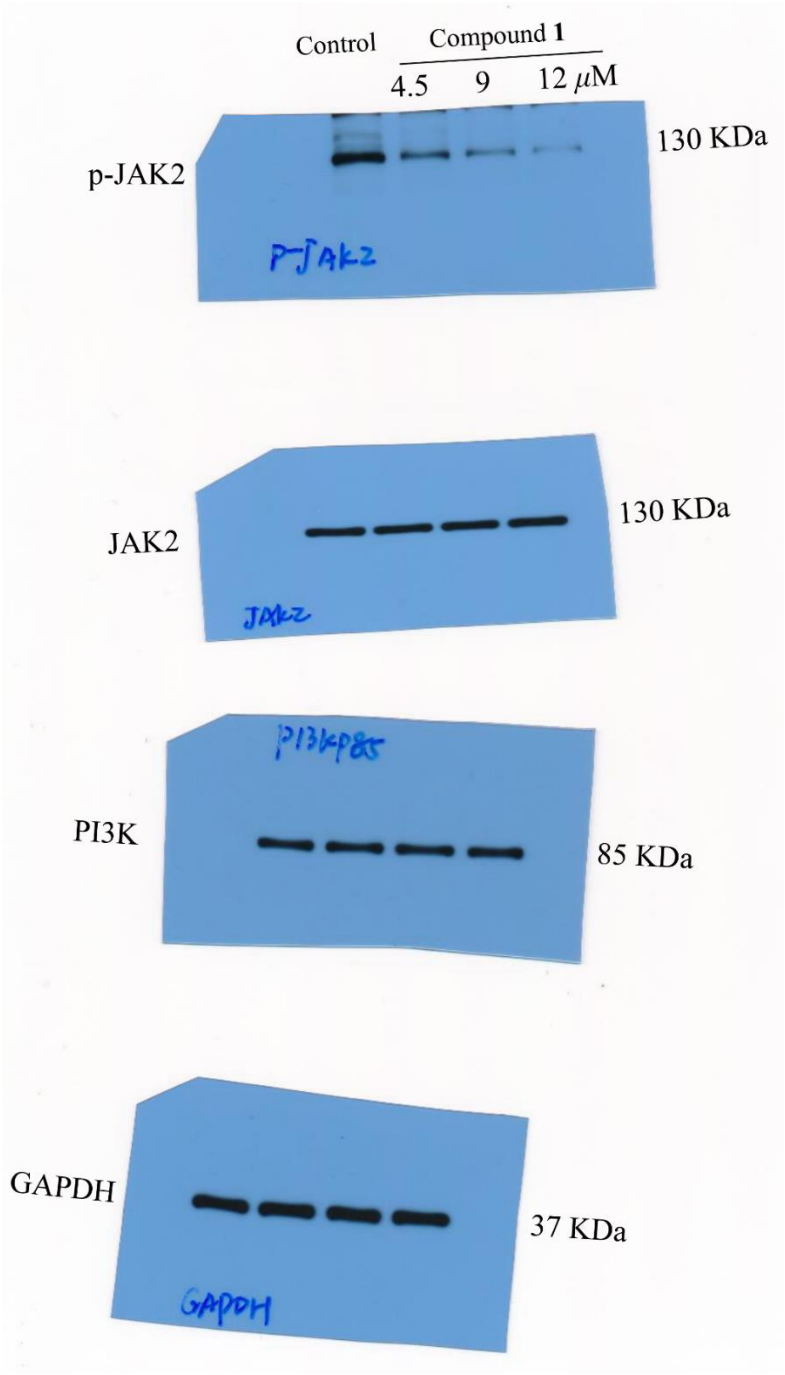


Fig. S2. Raw blot images for *p*-JAK2, JAK2, PI3K, and GAPDH.

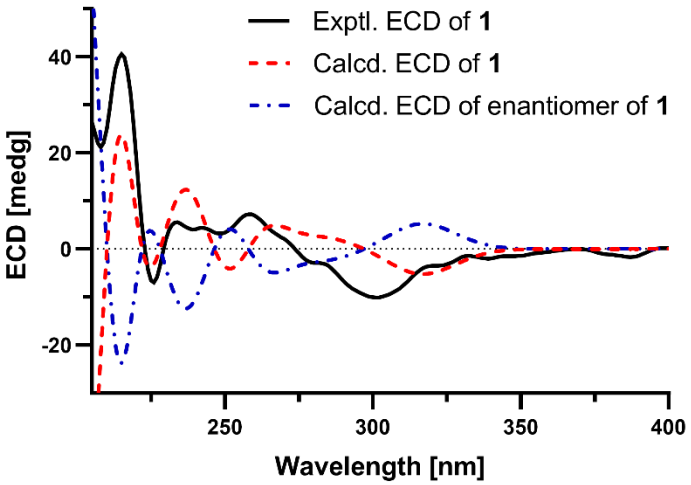


Fig. S3. Experimental ECD spectra of **1** and its enantionmer.

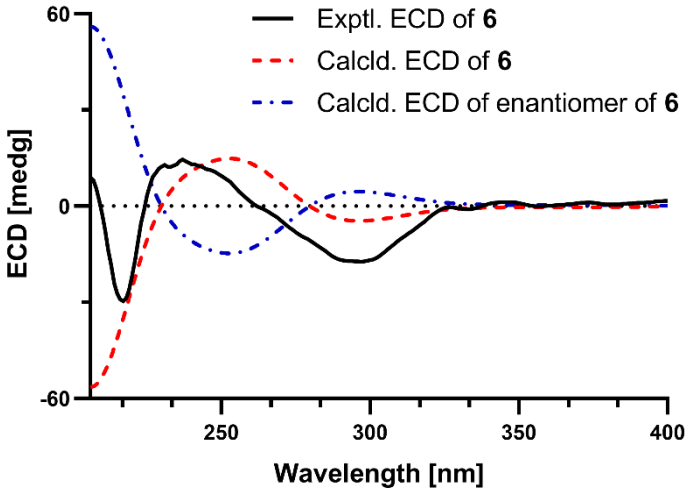


Fig. S4. Experimental ECD spectra of **6** and its enantionmer.

Computational ECD data of 1, 6 and their enantionmers.

Table S7. Important thermodynamic parameters (a.u.) and Boltzmann distribution of the optimized compound **1** at B3LYP/6-311+G(d,p)//B3LYP/6-31G(d) level in methanol

Conformation	Internal Energy	%
1	-1459.342989	60.08%
2	-1459.341805	17.03%
3	-1459.341790	16.85%
4	-1459.340645	5.04%

Table S8. Important thermodynamic parameters (a.u.) and Boltzmann distribution of the optimized the enantionmer of compound **1** at B3LYP/6-311+G(d,p)//B3LYP/6-31G(d) level in methanol

Conformation	Internal Energy	%
1	-1459.342989	60.40%
2	-1459.341805	17.12%
3	-1459.341790	16.94%
4	-1459.340645	5.01%

Table S9. Important thermodynamic parameters (a.u.) and Boltzmann distribution of the optimized compound **6** at B3LYP/6-311+G(d,p)//B3LYP/6-31G(d) level in methanol

Conformation	Internal Energy	%
1	-1534.578567	42.26%
2	-1534.577769	18.11%
3	-1534.577660	16.12%
4	-1534.577033	8.27%
5	-1534.577030	8.27%
6	-1534.576323	3.90%
7	-1534.575681	1.98%

Table S10. Important thermodynamic parameters (a.u.) and Boltzmann distribution of the optimized the enantionmer of compound **6** at B3LYP/6-311+G(d,p)//B3LYP/6-31G(d) level in methanol

Conformation	Internal Energy	%
1	-1534.578566	41.92%
2	-1534.577770	17.97%
3	-1534.577659	15.99%
4	-1534.577032	8.20%
5	-1534.577030	8.20%
6	-1534.576322	3.87%
7	-1534.575681	1.96%

Table S11. Optimized coordinates of compound **1** at B3LYP/6-31G(d) level in methanol

Conformation 1							
Atom	**X**	**Y**	**Z**	**Atom**	**X**	**Y**	**Z**
C	7.008	0.663	-0.466	O	-0.5	-0.457	2.244
C	7.768	-0.228	0.323	H	7.481	1.557	-0.862
C	5.668	0.413	-0.742	H	8.813	-0.006	0.523
C	7.204	-1.386	0.849	H	5.096	1.106	-1.354
C	5.066	-0.749	-0.224	H	7.788	-2.073	1.454
C	5.855	-1.634	0.568	H	-1.662	2.971	1.658

C	-1.205	2.571	0.755	H	3	-3.218	0.585
C	3.782	-2.49	0.412	H	-6.982	-2.227	-0.76
C	3.742	-1.32	-0.311	H	-5.936	-2.332	0.652
C	-0.104	3.115	0.207	H	-5.145	-0.295	1.835
C	-4.962	-1.658	-1.108	H	-5.799	1.298	1.48
C	-1.352	-0.919	-0.599	H	-2.087	1.611	-0.916
C	0.075	-0.079	1.226	H	-0.396	2.593	-1.823
C	-6.191	-1.701	-0.215	H	-3.599	-0.23	-1.862
C	-5.473	0.359	1.014	H	-2.882	-1.763	0.695
C	-1.758	1.337	0.102	H	-4.477	1.587	-0.468
C	0.413	2.468	-1.085	H	-2.876	0.542	1.821
C	-3.951	-0.55	-0.877	H	0.531	0.496	-1.977
C	-2.726	-0.884	0.064	H	-6.929	0.293	-0.572
C	-4.3	0.647	0.066	H	2.59	1.234	-0.163
C	-2.898	0.512	0.731	H	1.621	4.12	1.053
C	0.56	0.904	-0.961	H	0.06	4.66	1.697
C	-6.649	-0.322	0.297	H	0.591	5.167	0.084
C	1.869	0.419	-0.268	H	2.511	3.151	-1.037
C	-0.593	0.326	-0.114	H	1.431	4.165	-1.993
C	0.575	4.327	0.79	H	1.946	2.595	-2.619
C	1.649	3.13	-1.71	H	-7.647	-1.054	2.093
C	-7.879	-0.455	1.203	H	-8.708	-0.943	0.678
C	2.548	-0.749	-1.022	H	-8.224	0.529	1.541
N	1.411	0.025	1.058	H	2.841	-0.373	-2.012
N	5.042	-2.682	0.94	H	1.797	-1.529	-1.19
O	-4.774	-2.494	-1.98	H	2.048	-0.308	1.771
O	-0.944	-1.757	-1.379	H	5.324	-3.476	1.496
Conformation 2							
Atom	**X**	**Y**	**Z**	**Atom**	**X**	**Y**	**Z**
C	4.217	-3.351	1.068	O	-0.022	-0.468	1.995
C	5.606	-3.333	1.319	H	3.619	-4.176	1.445
C	3.604	-2.331	0.348	H	6.057	-4.144	1.885
C	6.41	-2.298	0.852	H	2.534	-2.358	0.161
C	4.388	-1.266	-0.137	H	7.48	-2.284	1.041
C	5.789	-1.274	0.127	H	-1.765	2.731	2.169
C	-1.318	2.602	1.185	H	5.535	1.482	-1.604
C	5.311	0.564	-1.077	H	-5.179	-2.936	0.204
C	4.105	-0.077	-0.91	H	-6.337	-2.712	-1.104
C	-0.361	3.424	0.72	H	-5.571	0.4	1.825
C	-4.471	-1.733	-1.395	H	-4.638	-1.09	1.785
C	-0.996	-0.527	-0.851	H	-2.16	1.856	-0.611
C	0.405	0.186	1.046	H	-0.714	3.28	-1.362
C	-5.601	-2.186	-0.486	H	-3.406	0.032	-1.854

C	-5.135	-0.344	1.147	H	-2.284	-1.859	0.287
C	-1.714	1.446	0.312	H	-4.478	1.329	-0.067
C	0.155	3.148	-0.698	H	-2.553	0.144	1.874
C	-3.634	-0.546	-0.954	H	0.509	1.445	-1.991
C	-2.31	-0.856	-0.149	H	-6.686	-0.327	-0.348
C	-4.105	0.345	0.239	H	2.573	2.141	-0.168
C	-2.654	0.327	0.803	H	-0.338	4.646	2.492
C	0.556	1.639	-0.914	H	1.236	4.528	1.685
C	-6.237	-1.055	0.346	H	-0.022	5.549	1
C	1.976	1.255	-0.4	H	1.538	3.838	-2.226
C	-0.42	0.717	-0.156	H	0.821	5.14	-1.271
C	0.154	4.596	1.515	H	2.116	4.157	-0.585
C	1.222	4.123	-1.216	H	-7.826	-0.788	1.814
C	-7.348	-1.598	1.251	H	-8.123	-2.108	0.666
C	2.769	0.394	-1.413	H	-6.946	-2.319	1.974
N	1.691	0.544	0.841	H	2.909	1.005	-2.314
N	6.319	-0.144	-0.456	H	2.14	-0.457	-1.704
O	-4.224	-2.308	-2.445	H	2.423	0.205	1.453
O	-0.505	-1.123	-1.79	H	7.295	0.115	-0.456
Conformation 3							
Atom	**X**	**Y**	**Z**	**Atom**	**X**	**Y**	**Z**
C	6.924	0.401	0.395	O	-1.233	1.404	2.634
C	7.472	-0.452	-0.588	H	7.535	1.2	0.805
C	5.619	0.232	0.845	H	8.495	-0.296	-0.92
C	6.728	-1.491	-1.137	H	5.212	0.894	1.605
C	4.837	-0.808	0.307	H	7.149	-2.151	-1.89
C	5.414	-1.658	-0.681	H	-1.768	3.499	-0.274
C	-1.113	2.668	-0.528	H	2.445	-2.991	-0.418
C	3.311	-2.354	-0.296	H	-6.676	-2.594	-0.404
C	3.489	-1.274	0.537	H	-6.124	-1.705	1.012
C	0.161	2.854	-0.918	H	-5.5	0.702	0.868
C	-4.595	-2.149	-0.391	H	-5.844	1.664	-0.562
C	-1.267	-0.883	0.656	H	-1.568	0.788	-1.395
C	-0.346	1.084	1.846	H	0.438	1.153	-2.145
C	-6.033	-1.766	-0.085	H	-2.912	-1.35	-1.389
C	-5.497	0.677	-0.232	H	-3.211	-0.878	1.629
C	-1.59	1.251	-0.393	H	-3.981	0.827	-1.775
C	0.962	1.597	-1.283	H	-3.25	1.614	1.004
C	-3.587	-1.032	-0.589	H	1.089	-0.48	-0.68
C	-2.761	-0.578	0.679	H	-6.413	-0.498	-1.788
C	-4.071	0.445	-0.752	H	2.645	1.342	0.793
C	-2.955	0.9	0.233	H	1.658	4.335	-0.407
C	0.871	0.47	-0.183	H	0.053	4.998	-0.764

C	-6.472	-0.418	-0.691	H	1.103	4.429	-2.074
C	1.845	0.633	1.019	H	3.008	2.379	-1.018
C	-0.541	0.454	0.441	H	2.404	2.446	-2.675
C	0.773	4.224	-1.047	H	2.898	0.898	-1.978
C	2.4	1.848	-1.757	H	-8.028	0.01	0.774
C	-7.922	-0.095	-0.313	H	-8.605	-0.887	-0.642
C	2.478	-0.703	1.489	H	-8.247	0.845	-0.774
N	0.985	1.197	2.054	H	1.667	-1.423	1.647
N	4.458	-2.587	-1.028	H	2.944	-0.525	2.468
O	-4.245	-3.318	-0.464	H	1.337	1.495	2.956
O	-0.751	-1.979	0.758	H	4.578	-3.333	-1.697
Conformation 4							
Atom	**X**	**Y**	**Z**	**Atom**	**X**	**Y**	**Z**
C	3.428	-3.482	-0.765	O	-1.276	2.114	2.39
C	4.719	-3.558	-1.333	H	2.72	-4.285	-0.949
C	3.05	-2.4	0.023	H	4.984	-4.417	-1.944
C	5.658	-2.554	-1.122	H	2.052	-2.35	0.451
C	3.977	-1.365	0.253	H	6.653	-2.61	-1.555
C	5.274	-1.466	-0.327	H	-1.905	3.523	-0.898
C	-1.131	2.761	-0.96	H	5.569	1.364	1.272
C	5.182	0.443	0.858	H	-5.936	-3.116	0.02
C	3.94	-0.132	1.008	H	-5.579	-1.908	1.252
C	0.127	3.046	-1.341	H	-5.29	0.495	0.665
C	-3.938	-2.385	-0.01	H	-5.682	1.112	-0.934
C	-0.887	-0.482	0.903	H	-1.282	0.704	-1.449
C	-0.308	1.782	1.71	H	0.698	1.195	-2.189
C	-5.428	-2.16	0.189	H	-2.319	-1.544	-1.076
C	-5.223	0.265	-0.409	H	-2.874	-0.572	1.783
C	-1.423	1.343	-0.56	H	-3.658	0.341	-1.908
C	1.107	1.868	-1.42	H	-3.196	1.733	0.684
C	-3.081	-1.188	-0.376	H	1.477	-0.008	-0.408
C	-2.406	-0.392	0.811	H	-5.889	-1.298	-1.733
C	-3.752	0.147	-0.834	H	2.666	2.291	0.717
C	-2.766	0.933	0.078	H	1.385	4.794	-1.102
C	1.103	0.977	-0.118	H	-0.274	5.142	-1.622
C	-6.014	-1.025	-0.674	H	0.908	4.482	-2.766
C	1.973	1.516	1.056	H	3.013	2.969	-1.259
C	-0.33	0.877	0.449	H	2.502	2.621	-2.912
C	0.557	4.437	-1.727	H	3.157	1.328	-1.9
C	2.524	2.222	-1.893	H	-7.687	-0.558	0.644
C	-7.512	-0.848	-0.401	H	-8.063	-1.777	-0.587
C	2.789	0.427	1.799	H	-7.938	-0.067	-1.042
N	0.979	2.121	1.938	H	2.103	-0.376	2.091

N	5.981	-0.348	0.057	H	3.164	0.876	2.728
O	-3.432	-3.489	0.129	H	1.23	2.639	2.772
O	-0.244	-1.454	1.25	H	6.94	-0.146	-0.186

Table S12. Optimized the coordinates of enantionmer of compound **1** at B3LYP/6-31G(d) level in methanol

Conformation 1							
Atom	**X**	**Y**	**Z**	**Atom**	**X**	**Y**	**Z**
C	-7.007	0.664	-0.465	O	0.499	-0.456	2.245
C	-7.767	-0.227	0.324	H	-7.479	1.559	-0.861
C	-5.667	0.413	-0.742	H	-8.812	-0.004	0.523
C	-7.204	-1.385	0.849	H	-5.095	1.106	-1.353
C	-5.066	-0.749	-0.223	H	-7.788	-2.073	1.454
C	-5.855	-1.634	0.568	H	1.662	2.972	1.657
C	1.205	2.571	0.755	H	-3.001	-3.219	0.584
C	-3.782	-2.491	0.411	H	5.936	-2.332	0.653
C	-3.741	-1.321	-0.311	H	6.982	-2.228	-0.76
C	0.103	3.115	0.207	H	5.799	1.299	1.479
C	4.962	-1.658	-1.108	H	5.145	-0.294	1.835
C	1.352	-0.919	-0.599	H	2.087	1.611	-0.916
C	-0.076	-0.078	1.226	H	0.395	2.592	-1.823
C	6.19	-1.701	-0.215	H	3.599	-0.23	-1.862
C	5.474	0.36	1.014	H	2.882	-1.763	0.695
C	1.758	1.337	0.102	H	4.476	1.588	-0.469
C	-0.413	2.467	-1.085	H	2.876	0.543	1.821
C	3.951	-0.55	-0.877	H	-0.531	0.496	-1.977
C	2.726	-0.884	0.064	H	6.929	0.293	-0.572
C	4.3	0.647	0.066	H	-2.591	1.234	-0.164
C	2.898	0.512	0.731	H	-0.591	5.167	0.083
C	-0.56	0.904	-0.961	H	-0.06	4.659	1.697
C	6.649	-0.322	0.297	H	-1.621	4.121	1.052
C	-1.869	0.419	-0.269	H	-2.512	3.15	-1.037
C	0.593	0.326	-0.114	H	-1.947	2.595	-2.619
C	-0.575	4.327	0.79	H	-1.432	4.164	-1.993
C	-1.649	3.13	-1.71	H	7.647	-1.053	2.093
C	7.879	-0.454	1.203	H	8.224	0.529	1.541
C	-2.548	-0.75	-1.022	H	8.708	-0.942	0.678
N	-1.411	0.025	1.058	H	-1.796	-1.53	-1.19
N	-5.043	-2.683	0.94	H	-2.84	-0.374	-2.013
O	4.774	-2.494	-1.98	H	-2.048	-0.308	1.771
O	0.943	-1.758	-1.378	H	-5.324	-3.476	1.496
Conformation 2							
Atom	**X**	**Y**	**Z**	**Atom**	**X**	**Y**	**Z**

C	-4.217	-3.35	1.068	O	0.022	-0.468	1.995
C	-5.606	-3.333	1.319	H	-3.619	-4.176	1.445
C	-3.604	-2.331	0.348	H	-6.057	-4.144	1.886
C	-6.41	-2.298	0.852	H	-2.534	-2.358	0.162
C	-4.388	-1.266	-0.136	H	-7.48	-2.284	1.041
C	-5.789	-1.274	0.127	H	1.765	2.731	2.169
C	1.318	2.602	1.185	H	-5.535	1.481	-1.605
C	-5.311	0.564	-1.077	H	5.18	-2.935	0.204
C	-4.105	-0.077	-0.91	H	6.338	-2.712	-1.104
C	0.361	3.424	0.72	H	5.571	0.4	1.825
C	4.47	-1.734	-1.394	H	4.638	-1.089	1.785
C	0.996	-0.527	-0.851	H	2.16	1.856	-0.611
C	-0.405	0.186	1.046	H	0.714	3.28	-1.362
C	5.601	-2.186	-0.486	H	3.406	0.032	-1.855
C	5.135	-0.343	1.147	H	2.284	-1.859	0.287
C	1.714	1.446	0.312	H	4.478	1.329	-0.068
C	-0.156	3.148	-0.698	H	2.553	0.144	1.874
C	3.634	-0.547	-0.954	H	-0.509	1.445	-1.991
C	2.31	-0.856	-0.149	H	6.686	-0.327	-0.349
C	4.105	0.345	0.239	H	-2.573	2.141	-0.168
C	2.654	0.327	0.803	H	0.022	5.549	1
C	-0.556	1.639	-0.915	H	0.338	4.646	2.492
C	6.237	-1.054	0.345	H	-1.236	4.528	1.685
C	-1.976	1.255	-0.4	H	-2.116	4.157	-0.584
C	0.42	0.717	-0.156	H	-1.538	3.838	-2.226
C	-0.154	4.596	1.515	H	-0.822	5.14	-1.271
C	-1.222	4.123	-1.216	H	6.946	-2.318	1.974
C	7.348	-1.598	1.251	H	7.827	-0.788	1.813
C	-2.769	0.394	-1.413	H	8.124	-2.107	0.666
N	-1.691	0.544	0.841	H	-2.14	-0.457	-1.704
N	-6.319	-0.144	-0.457	H	-2.909	1.005	-2.314
O	4.223	-2.31	-2.444	H	-2.423	0.205	1.453
O	0.506	-1.123	-1.79	H	-7.295	0.114	-0.456
Conformation 3							
Atom	**X**	**Y**	**Z**	**Atom**	**X**	**Y**	**Z**
C	-6.924	0.401	0.395	O	1.233	1.404	2.635
C	-7.472	-0.452	-0.588	H	-7.535	1.201	0.805
C	-5.619	0.232	0.845	H	-8.495	-0.296	-0.92
C	-6.727	-1.491	-1.137	H	-5.212	0.894	1.605
C	-4.837	-0.808	0.307	H	-7.149	-2.151	-1.89
C	-5.414	-1.658	-0.681	H	1.768	3.499	-0.274
C	1.113	2.668	-0.528	H	-2.445	-2.991	-0.418
C	-3.311	-2.354	-0.296	H	6.124	-1.705	1.012

C	-3.489	-1.274	0.537	H	6.676	-2.594	-0.404
C	-0.161	2.854	-0.918	H	5.844	1.664	-0.562
C	4.595	-2.149	-0.392	H	5.5	0.702	0.868
C	1.267	-0.883	0.656	H	1.568	0.788	-1.395
C	0.346	1.084	1.846	H	-0.438	1.153	-2.145
C	6.033	-1.766	-0.085	H	2.912	-1.35	-1.389
C	5.497	0.677	-0.232	H	3.211	-0.879	1.629
C	1.59	1.251	-0.393	H	3.981	0.827	-1.775
C	-0.962	1.597	-1.283	H	3.25	1.614	1.004
C	3.587	-1.032	-0.589	H	-1.089	-0.48	-0.68
C	2.761	-0.578	0.679	H	6.413	-0.497	-1.787
C	4.071	0.445	-0.752	H	-2.646	1.342	0.793
C	2.955	0.9	0.233	H	-1.103	4.429	-2.074
C	-0.871	0.47	-0.183	H	-0.053	4.998	-0.764
C	6.472	-0.418	-0.691	H	-1.658	4.335	-0.407
C	-1.845	0.633	1.019	H	-3.008	2.378	-1.018
C	0.541	0.454	0.441	H	-2.899	0.898	-1.978
C	-0.773	4.224	-1.047	H	-2.404	2.446	-2.675
C	-2.4	1.848	-1.757	H	8.028	0.01	0.774
C	7.922	-0.094	-0.313	H	8.247	0.845	-0.774
C	-2.478	-0.703	1.489	H	8.605	-0.886	-0.642
N	-0.985	1.197	2.054	H	-2.944	-0.525	2.468
N	-4.458	-2.587	-1.028	H	-1.667	-1.423	1.647
O	4.245	-3.318	-0.464	H	-1.337	1.495	2.956
O	0.751	-1.979	0.758	H	-4.578	-3.334	-1.697
Conformation 4							
Atom	**X**	**Y**	**Z**	**Atom**	**X**	**Y**	**Z**
C	-3.428	-3.482	-0.765	O	1.276	2.114	2.39
C	-4.719	-3.558	-1.332	H	-2.72	-4.285	-0.949
C	-3.05	-2.4	0.023	H	-4.985	-4.416	-1.944
C	-5.658	-2.554	-1.122	H	-2.052	-2.35	0.451
C	-3.977	-1.365	0.254	H	-6.653	-2.61	-1.555
C	-5.274	-1.466	-0.327	H	1.905	3.523	-0.898
C	1.131	2.761	-0.96	H	-5.569	1.364	1.272
C	-5.182	0.443	0.858	H	5.579	-1.909	1.252
C	-3.94	-0.132	1.008	H	5.936	-3.116	0.02
C	-0.127	3.046	-1.341	H	5.682	1.112	-0.934
C	3.938	-2.385	-0.01	H	5.29	0.495	0.665
C	0.887	-0.482	0.903	H	1.282	0.704	-1.449
C	0.308	1.782	1.71	H	-0.698	1.195	-2.189
C	5.428	-2.161	0.189	H	2.319	-1.544	-1.076
C	5.223	0.265	-0.409	H	2.874	-0.572	1.783
C	1.423	1.343	-0.56	H	3.658	0.342	-1.908

C	-1.107	1.868	-1.42	H	3.196	1.733	0.684
C	3.081	-1.188	-0.376	H	-1.477	-0.009	-0.408
C	2.406	-0.392	0.811	H	5.889	-1.298	-1.733
C	3.752	0.147	-0.834	H	-2.666	2.291	0.717
C	2.766	0.933	0.078	H	-0.908	4.482	-2.766
C	-1.103	0.977	-0.118	H	0.274	5.142	-1.622
C	6.015	-1.025	-0.674	H	-1.385	4.794	-1.102
C	-1.973	1.516	1.056	H	-3.013	2.969	-1.26
C	0.33	0.877	0.449	H	-3.157	1.328	-1.9
C	-0.557	4.437	-1.727	H	-2.501	2.621	-2.912
C	-2.524	2.222	-1.893	H	7.687	-0.558	0.644
C	7.512	-0.848	-0.4	H	7.938	-0.067	-1.041
C	-2.789	0.427	1.799	H	8.063	-1.777	-0.587
N	-0.979	2.121	1.938	H	-3.163	0.876	2.728
N	-5.981	-0.348	0.057	H	-2.103	-0.376	2.091
O	3.432	-3.489	0.129	H	-1.23	2.639	2.772
O	0.244	-1.454	1.25	H	-6.94	-0.146	-0.185

Table S13. Optimized the coordinates of compound **1** at B3LYP/6-31G(d) level in methanol

Conformation 1							
Atom	**X**	**Y**	**Z**	**Atom**	**X**	**Y**	**Z**
C	-7.043	0.86	0.057	O	3.172	-2.396	1.511
C	-7.778	-0.038	-0.746	H	-7.493	1.806	0.346
C	-5.755	0.554	0.482	H	-8.782	0.229	-1.063
C	-7.242	-1.261	-1.135	H	-5.202	1.254	1.104
C	-5.181	-0.674	0.102	H	-7.808	-1.956	-1.751
C	-5.945	-1.566	-0.704	H	1.363	2.801	-1.548
C	0.954	2.433	-0.609	H	-3.211	-3.311	-0.327
C	-3.956	-2.528	-0.283	H	5.132	3.095	-2.072
C	-3.911	-1.312	0.36	H	4.159	1.751	-2.891
C	-0.165	2.944	-0.072	H	6.192	-0.179	1.144
C	1.309	-0.897	1.224	H	4.217	2.472	0.102
C	0.044	-0.45	-0.88	H	7.143	-1.795	-1.278
C	4.427	2.274	-1.976	H	1.971	1.685	1.101
C	6.141	-0.739	0.213	H	0.206	2.53	1.977
C	3.919	1.922	-0.793	H	2.338	-1.932	-0.325
C	7.254	-1.242	-0.346	H	2.691	0.339	-1.536
C	4.81	-0.927	-0.403	H	3.912	0.127	1.265
C	1.659	1.312	0.11	H	-0.702	0.369	2.156
C	-0.603	2.33	1.257	H	-2.526	1.079	0.014
C	2.595	-1.454	0.631	H	-0.475	4.367	-1.657
C	2.946	0.788	-0.573	H	-1.977	3.776	-0.923

C	3.595	-0.315	0.312	H	-0.988	4.947	-0.062
C	-0.657	0.774	1.141	H	8.659	-0.543	1.137
C	-1.89	0.25	0.342	H	9.074	-2.102	0.381
C	0.598	0.189	0.426	H	9.292	-0.614	-0.526
C	-0.939	4.064	-0.713	H	-2.096	2.418	2.833
C	8.637	-1.11	0.202	H	-1.738	3.986	2.101
C	-1.873	2.921	1.885	H	-2.754	2.828	1.241
C	-2.757	-0.75	1.141	H	-3.123	-0.228	2.035
N	-1.299	-0.366	-0.836	H	-2.107	-1.56	1.493
N	-5.17	-2.684	-0.922	H	-1.864	-0.778	-1.569
O	0.921	-1.314	2.307	H	-5.446	-3.498	-1.451
O	0.702	-0.959	-1.786	H	2.574	-2.422	2.285
O	4.642	-1.544	-1.451				
Conformation 2							
Atom	**X**	**Y**	**Z**	**Atom**	**X**	**Y**	**Z**
C	-6.898	0.606	-0.508	O	3.199	-1.689	2.432
C	-7.531	-0.507	-1.102	H	-7.405	1.568	-0.509
C	-5.642	0.491	0.077	H	-8.512	-0.387	-1.552
C	-6.921	-1.758	-1.119	H	-5.169	1.357	0.534
C	-4.996	-0.759	0.073	H	-7.408	-2.616	-1.573
C	-5.657	-1.869	-0.528	H	1.55	2.577	-1.901
C	1.071	2.426	-0.937	H	-2.906	-3.305	0.489
C	-3.679	-2.579	0.274	H	5.338	2.892	-2.193
C	-3.731	-1.239	0.581	H	4.423	1.39	-2.769
C	-0.103	3	-0.629	H	3.996	-1.811	-1.185
C	1.351	-0.336	1.68	H	4.302	2.717	0.009
C	0.252	-0.473	-0.562	H	6.991	-2.025	-0.594
C	4.634	2.096	-1.968	H	1.972	2.15	0.972
C	4.952	-1.614	-0.705	H	0.099	3.114	1.48
C	4.059	1.99	-0.768	H	2.45	-1.714	0.509
C	6.059	-2.259	-1.108	H	2.889	0.266	-1.233
C	4.994	-0.619	0.393	H	3.92	0.718	1.629
C	1.74	1.54	0.082	H	-0.757	1.028	2.12
C	-0.64	2.708	0.77	H	-2.44	1.092	-0.235
C	2.67	-1.004	1.317	H	-1.853	3.518	-1.8
C	3.081	0.91	-0.371	H	-0.307	3.989	-2.531
C	3.675	0.056	0.79	H	-0.976	4.907	-1.169
C	-0.644	1.17	1.042	H	6.509	-4.228	-1.82
C	-1.792	0.403	0.316	H	5.148	-3.447	-2.664
C	0.679	0.485	0.586	H	6.828	-2.95	-2.982
C	-0.846	3.898	-1.582	H	-2.796	3.08	0.471
C	6.125	-3.273	-2.203	H	-1.889	4.464	1.083
C	-1.975	3.373	1.133	H	-2.262	3.112	2.158

C	-2.669	-0.435	1.276	H	-3.126	0.257	1.995
N	-1.09	-0.436	-0.645	H	-2.01	-1.097	1.851
N	-4.827	-2.961	-0.39	H	-1.582	-1.042	-1.29
O	0.917	-0.451	2.818	H	-5.03	-3.898	-0.706
O	0.996	-1.158	-1.264	H	2.585	-1.494	3.168
O	6.033	-0.323	0.975				
Conformation 3							
Atom	**X**	**Y**	**Z**	**Atom**	**X**	**Y**	**Z**
C	-4.368	-3.493	-0.749	O	2.542	-2.12	1.985
C	-5.698	-3.439	-1.219	H	-3.789	-4.401	-0.897
C	-3.79	-2.407	-0.103	H	-6.122	-4.304	-1.722
C	-6.476	-2.299	-1.048	H	-2.765	-2.463	0.255
C	-4.549	-1.235	0.084	H	-7.501	-2.256	-1.407
C	-5.891	-1.208	-0.396	H	1.571	2.65	-2.014
C	1.143	2.547	-1.019	H	-5.68	1.772	0.92
C	-5.454	0.771	0.579	H	5.297	2.125	-2.627
C	-4.291	0.045	0.705	H	4.056	0.858	-3.159
C	0.159	3.348	-0.581	H	5.905	-0.57	1.136
C	0.972	-0.383	1.424	H	4.391	2.105	-0.363
C	-0.281	-0.118	-0.722	H	6.439	-2.797	-0.898
C	4.46	1.483	-2.365	H	2.082	1.957	0.794
C	5.71	-1.294	0.348	H	0.537	3.263	1.506
C	3.955	1.462	-1.13	H	1.726	-1.87	0.1
C	6.692	-2.09	-0.109	H	2.426	0.024	-1.535
C	4.336	-1.37	-0.191	H	3.712	0.13	1.244
C	1.665	1.468	-0.103	H	-0.74	1.38	2.102
C	-0.325	3.086	0.844	H	-2.491	2.004	-0.129
C	2.107	-1.273	0.941	H	0.042	4.482	-2.407
C	2.803	0.594	-0.682	H	-1.509	4.325	-1.562
C	3.281	-0.421	0.399	H	-0.29	5.434	-0.948
C	-0.665	1.573	1.028	H	8.379	-3.083	0.756
C	-2.005	1.148	0.351	H	8.794	-1.879	-0.453
C	0.433	0.642	0.433	H	8.271	-1.353	1.167
C	-0.428	4.452	-1.419	H	-1.697	3.748	2.392
C	8.105	-2.09	0.375	H	-1.114	5.051	1.352
C	-1.441	4.007	1.358	H	-2.357	3.946	0.762
C	-3.013	0.517	1.34	H	-3.236	1.275	2.101
N	-1.584	0.218	-0.687	H	-2.511	-0.31	1.859
N	-6.411	0.029	-0.081	H	-2.238	-0.205	-1.334
O	0.567	-0.5	2.573	H	-7.351	0.338	-0.278
O	0.237	-0.9	-1.517	H	1.992	-1.877	2.756
O	4.011	-2.151	-1.082				

Conformation 4							
Atom	**X**	**Y**	**Z**	**Atom**	**X**	**Y**	**Z**
C	-4.209	-3.603	-0.094	O	2.817	-1.331	2.742
C	-5.463	-3.659	-0.74	H	-3.647	-4.521	0.055
C	-3.683	-2.396	0.352	H	-5.847	-4.617	-1.08
C	-6.217	-2.509	-0.948	H	-2.717	-2.37	0.849
C	-4.419	-1.211	0.154	H	-7.184	-2.549	-1.442
C	-5.685	-1.295	-0.496	H	1.682	2.396	-2.229
C	1.226	2.456	-1.244	H	-5.545	1.911	0.098
C	-5.311	0.857	0.037	H	5.42	1.929	-2.697
C	-4.201	0.179	0.485	H	4.234	0.537	-2.985
C	0.195	3.276	-0.987	H	3.338	-2.257	-0.826
C	1.165	0.133	1.773	H	4.497	2.295	-0.469
C	-0.019	-0.241	-0.406	H	6.288	-2.902	-0.319
C	4.605	1.315	-2.321	H	2.148	2.282	0.661
C	4.345	-2.154	-0.427	H	0.49	3.594	1.095
C	4.091	1.506	-1.104	H	1.971	-1.609	0.881
C	5.295	-3.05	-0.744	H	2.63	-0.043	-1.238
C	4.631	-1.004	0.464	H	3.883	0.697	1.47
C	1.777	1.605	-0.128	H	-0.774	1.77	1.958
C	-0.332	3.252	0.447	H	-2.274	1.873	-0.563
C	2.343	-0.8	1.523	H	0.092	4.046	-2.995
C	2.969	0.692	-0.504	H	-1.479	3.98	-2.174
C	3.476	-0.045	0.773	H	-0.323	5.235	-1.748
C	-0.61	1.779	0.877	H	4.088	-4.309	-2.016
C	-1.863	1.171	0.172	H	5.802	-4.191	-2.483
C	0.578	0.828	0.55	H	5.349	-5.162	-1.091
C	-0.409	4.178	-2.031	H	-1.797	4.11	1.801
C	5.11	-4.236	-1.632	H	-1.252	5.225	0.544
C	-1.517	4.182	0.744	H	-2.404	3.948	0.146
C	-2.997	0.787	1.15	H	-3.291	1.701	1.681
N	-1.332	0.019	-0.541	H	-2.586	0.103	1.904
N	-6.199	-0.018	-0.553	H	-1.916	-0.581	-1.112
O	0.785	0.325	2.919	H	-7.095	0.238	-0.942
O	0.584	-1.173	-0.94	H	2.29	-0.887	3.437
O	5.742	-0.802	0.943				
Conformation 5							
Atom	**X**	**Y**	**Z**	**Atom**	**X**	**Y**	**Z**
C	6.949	0.603	0.782	O	-2.975	-2.803	0.208
C	7.635	0.035	-0.313	H	7.45	1.348	1.395
C	5.646	0.224	1.088	H	8.652	0.35	-0.527
C	7.034	-0.925	-1.121	H	5.131	0.668	1.937
C	5.008	-0.742	0.288	H	7.561	-1.365	-1.962

C	5.722	-1.303	-0.809	H	-1.508	3.304	0.11
C	-0.889	2.504	-0.288	H	2.895	-2.918	-1.059
C	3.683	-2.25	-0.74	H	-5.2	3.574	-0.879
C	3.704	-1.363	0.312	H	-4.677	3.035	0.814
C	0.398	2.698	-0.618	H	-5.647	-1.074	-1.764
C	-1.104	-1.293	0.083	H	-3.772	1.875	-1.892
C	-0.42	0.407	1.785	H	-7.47	-1.017	0.697
C	-4.602	2.906	-0.264	H	-1.444	0.854	-1.518
C	-5.947	-0.963	-0.725	H	0.597	1.208	-2.108
C	-3.817	1.973	-0.805	H	-2.642	-1.269	1.556
C	-7.228	-1.138	-0.359	H	-3.055	1.218	1.044
C	-4.897	-0.624	0.259	H	-3.422	-0.687	-1.327
C	-1.483	1.127	-0.449	H	1.203	-0.645	-0.848
C	1.129	1.482	-1.183	H	2.573	1.054	0.991
C	-2.56	-1.48	0.481	H	1.957	3.967	0.19
C	-2.965	1	-0.024	H	0.4	4.778	-0.061
C	-3.459	-0.457	-0.255	H	1.453	4.402	-1.438
C	0.948	0.236	-0.254	H	-9.139	-0.722	-1.229
C	1.84	0.243	1.024	H	-8.024	-1.591	-2.314
C	-0.517	0.101	0.262	H	-8.825	-2.429	-0.961
C	1.085	4.029	-0.473	H	3.225	2.042	-0.773
C	-8.354	-1.489	-1.275	H	2.648	2.472	-2.385
C	2.589	1.711	-1.599	H	3.018	0.786	-1.996
C	2.587	-1.092	1.278	H	1.855	-1.907	1.243
N	0.887	0.515	2.093	H	2.981	-1.064	2.304
N	4.886	-2.216	-1.416	H	1.17	0.66	3.055
O	-0.485	-2.242	-0.38	H	5.12	-2.788	-2.214
O	-1.357	0.526	2.572	H	-2.195	-3.239	-0.19
O	-5.129	-0.476	1.457				
Conformation 6							
Atom	**X**	**Y**	**Z**	**Atom**	**X**	**Y**	**Z**
C	6.73	0.545	1.475	O	-2.952	-2.831	-0.954
C	7.567	0.192	0.394	H	7.123	1.177	2.266
C	5.416	0.095	1.541	H	8.59	0.559	0.369
C	7.108	-0.618	-0.639	H	4.784	0.371	2.381
C	4.919	-0.725	0.51	H	7.752	-0.892	-1.471
C	5.785	-1.069	-0.568	H	-1.633	3.2	0.246
C	-0.954	2.484	-0.213	H	3.078	-2.667	-1.452
C	3.793	-2.051	-0.924	H	-5.182	3.648	-1.073
C	3.649	-1.364	0.259	H	-4.803	2.85	0.554
C	0.356	2.738	-0.358	H	-4.686	-0.629	1.459
C	-1.118	-1.311	-0.59	H	-3.666	2.112	-2.213
C	-0.693	0.023	1.487	H	-7.389	-1.166	0.127

C	-4.635	2.888	-0.52	H	-1.342	1.081	-1.77
C	-5.413	-0.78	0.664	H	0.752	1.53	-2.051
C	-3.803	2.043	-1.132	H	-2.76	-1.624	0.708
C	-6.701	-1.022	0.96	H	-3.204	1.004	0.635
C	-4.942	-0.708	-0.741	H	-3.313	-0.465	-2.064
C	-1.497	1.158	-0.681	H	1.27	-0.51	-1.057
C	1.173	1.643	-1.039	H	2.342	0.872	1.206
C	-2.599	-1.592	-0.378	H	0.249	4.687	0.55
C	-3.014	0.955	-0.441	H	1.79	3.854	0.823
C	-3.45	-0.441	-0.976	H	1.45	4.565	-0.749
C	0.919	0.256	-0.361	H	-8.07	-0.367	2.47
C	1.646	0.053	1.002	H	-7.741	-2.092	2.495
C	-0.593	0.019	-0.065	H	-6.516	-0.955	3.11
C	0.991	4.027	0.09	H	2.79	2.835	-1.869
C	-7.273	-1.111	2.336	H	3.198	2.126	-0.304
C	2.663	1.946	-1.242	H	3.154	1.108	-1.747
C	2.414	-1.291	1.109	H	1.726	-2.101	0.842
N	0.56	0.104	1.973	H	2.68	-1.441	2.165
N	5.067	-1.876	-1.425	H	0.719	0.064	2.973
O	-0.436	-2.129	-1.193	H	5.419	-2.292	-2.275
O	-1.723	-0.039	2.159	H	-2.135	-3.157	-1.383
O	-5.698	-0.847	-1.697				
Conformation 7							
Atom	**X**	**Y**	**Z**	**Atom**	**X**	**Y**	**Z**
C	4.145	-3.168	-1.271	O	-2.373	-2.667	0.991
C	5.471	-2.992	-1.72	H	3.562	-4.003	-1.652
C	3.572	-2.295	-0.353	H	5.89	-3.691	-2.439
C	6.253	-1.938	-1.258	H	2.547	-2.44	-0.022
C	4.335	-1.216	0.135	H	7.275	-1.8	-1.599
C	5.674	-1.061	-0.332	H	-1.736	3.357	-0.665
C	-0.98	2.587	-0.801	H	5.486	1.449	1.746
C	5.252	0.579	1.146	H	-5.323	2.787	-1.892
C	4.087	-0.151	1.08	H	-4.901	2.781	-0.09
C	0.293	2.886	-1.102	H	-5.074	-1.836	-1.589
C	-0.716	-0.971	0.57	H	-3.582	1.137	-2.336
C	-0.425	1.19	1.782	H	-7.103	-1.51	0.683
C	-4.702	2.399	-1.089	H	-1.19	0.611	-1.57
C	-5.476	-1.552	-0.619	H	0.83	1.112	-2.126
C	-3.746	1.496	-1.318	H	-2.381	-0.803	1.887
C	-6.756	-1.815	-0.305	H	-3.071	1.365	0.706
C	-4.566	-0.878	0.33	H	-2.944	-1.116	-1.087
C	-1.365	1.14	-0.618	H	1.557	-0.237	-0.386
C	1.231	1.694	-1.281	H	2.501	2.083	0.999

C	-2.167	-1.272	0.917	H	-0.037	5.014	-1.121
C	-2.85	0.899	-0.258	H	1.587	4.545	-0.583
C	-3.118	-0.628	-0.12	H	1.177	4.466	-2.292
C	1.135	0.716	-0.063	H	-7.318	-2.764	-2.161
C	1.899	1.194	1.211	H	-8.136	-3.4	-0.711
C	-0.34	0.494	0.393	H	-8.615	-1.841	-1.363
C	0.777	4.3	-1.283	H	3.266	1.117	-1.775
C	-7.748	-2.492	-1.192	H	2.704	2.565	-2.622
C	2.677	2.034	-1.665	H	3.181	2.665	-0.926
C	2.826	0.128	1.852	H	2.25	-0.794	1.99
N	0.823	1.563	2.124	H	3.088	0.486	2.857
N	6.2	0.044	0.299	H	0.995	1.995	3.024
O	0.065	-1.903	0.428	H	7.141	0.392	0.188
O	-1.438	1.365	2.456	H	-1.506	-3.067	0.777
O	-4.921	-0.509	1.447				

Table S14. Optimized the coordinates of enantionmer of compound **6** at B3LYP/6-31G(d) level in methanol

Conformation 1							
Atom	**X**	**Y**	**Z**	**Atom**	**X**	**Y**	**Z**
C	7.043	0.86	0.057	O	-3.173	-2.396	1.512
C	7.778	-0.038	-0.746	H	7.494	1.806	0.346
C	5.755	0.554	0.482	H	8.783	0.229	-1.063
C	7.242	-1.261	-1.136	H	5.202	1.254	1.104
C	5.181	-0.674	0.102	H	7.808	-1.956	-1.751
C	5.945	-1.566	-0.705	H	-1.362	2.8	-1.548
C	-0.954	2.433	-0.61	H	3.211	-3.311	-0.328
C	3.956	-2.527	-0.284	H	-5.132	3.095	-2.073
C	3.911	-1.312	0.36	H	-4.158	1.75	-2.892
C	0.165	2.944	-0.072	H	-6.192	-0.179	1.144
C	-1.309	-0.897	1.225	H	-4.217	2.472	0.102
C	-0.044	-0.451	-0.88	H	-7.143	-1.795	-1.279
C	-4.427	2.273	-1.976	H	-1.971	1.685	1.1
C	-6.141	-0.739	0.213	H	-0.207	2.53	1.977
C	-3.919	1.922	-0.793	H	-2.338	-1.932	-0.325
C	-7.254	-1.242	-0.346	H	-2.691	0.339	-1.536
C	-4.81	-0.927	-0.402	H	-3.912	0.128	1.265
C	-1.659	1.312	0.11	H	0.702	0.368	2.156
C	0.603	2.33	1.257	H	2.526	1.079	0.014
C	-2.595	-1.454	0.631	H	0.988	4.947	-0.062
C	-2.946	0.788	-0.573	H	0.475	4.366	-1.657
C	-3.595	-0.315	0.313	H	1.978	3.776	-0.923
C	0.657	0.774	1.141	H	-9.075	-2.101	0.38

C	1.89	0.25	0.342	H	-8.659	-0.543	1.137
C	-0.598	0.189	0.426	H	-9.292	-0.613	-0.526
C	0.939	4.064	-0.713	H	2.754	2.827	1.241
C	-8.637	-1.11	0.202	H	2.096	2.418	2.833
C	1.873	2.921	1.885	H	1.738	3.986	2.1
C	2.757	-0.75	1.141	H	2.107	-1.56	1.494
N	1.299	-0.367	-0.836	H	3.124	-0.228	2.035
N	5.169	-2.684	-0.922	H	1.864	-0.778	-1.569
O	-0.921	-1.314	2.307	H	5.446	-3.497	-1.452
O	-0.702	-0.959	-1.786	H	-2.575	-2.422	2.286
O	-4.642	-1.544	-1.451				
Conformation 2							
Atom	**X**	**Y**	**Z**	**Atom**	**X**	**Y**	**Z**
C	6.899	0.606	-0.507	O	-3.2	-1.688	2.432
C	7.531	-0.507	-1.101	H	7.405	1.568	-0.508
C	5.643	0.491	0.077	H	8.513	-0.387	-1.551
C	6.922	-1.757	-1.119	H	5.17	1.357	0.534
C	4.997	-0.759	0.073	H	7.408	-2.616	-1.573
C	5.657	-1.869	-0.528	H	-1.549	2.576	-1.902
C	-1.07	2.426	-0.937	H	2.907	-3.305	0.489
C	3.679	-2.579	0.273	H	-5.337	2.892	-2.195
C	3.732	-1.239	0.581	H	-4.422	1.39	-2.77
C	0.103	3	-0.63	H	-3.996	-1.812	-1.184
C	-1.351	-0.336	1.681	H	-4.302	2.717	0.008
C	-0.252	-0.474	-0.561	H	-6.992	-2.024	-0.595
C	-4.633	2.096	-1.969	H	-1.972	2.15	0.972
C	-4.952	-1.614	-0.705	H	-0.098	3.114	1.479
C	-4.059	1.989	-0.769	H	-2.45	-1.714	0.51
C	-6.059	-2.259	-1.108	H	-2.889	0.266	-1.233
C	-4.994	-0.619	0.393	H	-3.92	0.718	1.629
C	-1.74	1.54	0.082	H	0.757	1.028	2.12
C	0.64	2.707	0.77	H	2.44	1.092	-0.235
C	-2.67	-1.004	1.317	H	0.976	4.906	-1.17
C	-3.081	0.91	-0.371	H	0.308	3.988	-2.531
C	-3.675	0.056	0.79	H	1.853	3.518	-1.8
C	0.644	1.169	1.042	H	-6.827	-2.949	-2.983
C	1.792	0.403	0.316	H	-5.148	-3.448	-2.663
C	-0.679	0.484	0.587	H	-6.509	-4.227	-1.821
C	0.846	3.897	-1.583	H	2.796	3.079	0.471
C	-6.125	-3.272	-2.203	H	2.262	3.112	2.158
C	1.975	3.373	1.133	H	1.889	4.463	1.083
C	2.669	-0.435	1.276	H	2.011	-1.097	1.851
N	1.09	-0.436	-0.645	H	3.127	0.258	1.994

N	4.827	-2.961	-0.39	H	1.582	-1.043	-1.29
O	-0.917	-0.449	2.818	H	5.03	-3.898	-0.707
O	-0.996	-1.159	-1.263	H	-2.586	-1.493	3.169
O	-6.033	-0.323	0.975				
Conformation 3							
Atom	**X**	**Y**	**Z**	**Atom**	**X**	**Y**	**Z**
C	4.368	-3.493	-0.75	O	-2.542	-2.12	1.984
C	5.698	-3.439	-1.22	H	3.788	-4.401	-0.897
C	3.789	-2.407	-0.103	H	6.122	-4.304	-1.723
C	6.476	-2.299	-1.048	H	2.764	-2.463	0.254
C	4.548	-1.235	0.084	H	7.501	-2.256	-1.406
C	5.891	-1.208	-0.396	H	-1.57	2.65	-2.014
C	-1.143	2.547	-1.02	H	5.68	1.772	0.921
C	5.454	0.77	0.58	H	-5.297	2.125	-2.628
C	4.291	0.045	0.705	H	-4.056	0.858	-3.16
C	-0.159	3.348	-0.581	H	-5.904	-0.571	1.137
C	-0.972	-0.383	1.423	H	-4.391	2.105	-0.363
C	0.281	-0.118	-0.722	H	-6.44	-2.797	-0.898
C	-4.459	1.483	-2.366	H	-2.082	1.957	0.794
C	-5.71	-1.294	0.348	H	-0.537	3.263	1.506
C	-3.955	1.462	-1.13	H	-1.727	-1.869	0.099
C	-6.692	-2.09	-0.108	H	-2.426	0.024	-1.535
C	-4.336	-1.369	-0.191	H	-3.712	0.131	1.244
C	-1.665	1.469	-0.104	H	0.74	1.38	2.102
C	0.325	3.086	0.844	H	2.492	2.004	-0.129
C	-2.107	-1.273	0.94	H	-0.042	4.483	-2.407
C	-2.803	0.594	-0.682	H	0.29	5.434	-0.948
C	-3.281	-0.42	0.399	H	1.509	4.325	-1.562
C	0.665	1.573	1.028	H	-8.27	-1.355	1.168
C	2.005	1.149	0.352	H	-8.794	-1.879	-0.452
C	-0.433	0.642	0.432	H	-8.379	-3.084	0.756
C	0.428	4.452	-1.419	H	1.697	3.748	2.392
C	-8.104	-2.091	0.376	H	1.113	5.052	1.352
C	1.44	4.007	1.359	H	2.357	3.947	0.762
C	3.012	0.517	1.34	H	2.511	-0.311	1.859
N	1.585	0.218	-0.687	H	3.236	1.275	2.101
N	6.411	0.028	-0.081	H	2.239	-0.205	-1.334
O	-0.567	-0.5	2.572	H	7.351	0.338	-0.278
O	-0.237	-0.9	-1.517	H	-1.992	-1.877	2.756
O	-4.012	-2.15	-1.082				
Conformation 4							
Atom	**X**	**Y**	**Z**	**Atom**	**X**	**Y**	**Z**
C	4.209	-3.603	-0.095	O	-2.816	-1.331	2.742

C	5.463	-3.659	-0.741	H	3.646	-4.521	0.054
C	3.683	-2.396	0.352	H	5.847	-4.617	-1.08
C	6.217	-2.509	-0.948	H	2.717	-2.37	0.849
C	4.419	-1.211	0.154	H	7.184	-2.549	-1.441
C	5.685	-1.295	-0.495	H	-1.683	2.396	-2.229
C	-1.226	2.456	-1.244	H	5.545	1.911	0.099
C	5.311	0.857	0.037	H	-5.421	1.928	-2.696
C	4.201	0.179	0.486	H	-4.235	0.536	-2.984
C	-0.195	3.276	-0.987	H	-3.338	-2.257	-0.825
C	-1.165	0.133	1.773	H	-4.496	2.296	-0.468
C	0.019	-0.241	-0.407	H	-6.288	-2.901	-0.319
C	-4.606	1.315	-2.32	H	-2.148	2.282	0.661
C	-4.345	-2.155	-0.427	H	-0.49	3.594	1.095
C	-4.091	1.506	-1.104	H	-1.971	-1.609	0.881
C	-5.295	-3.05	-0.744	H	-2.63	-0.043	-1.238
C	-4.631	-1.005	0.465	H	-3.882	0.697	1.471
C	-1.777	1.605	-0.128	H	0.774	1.771	1.958
C	0.332	3.253	0.446	H	2.274	1.873	-0.562
C	-2.342	-0.8	1.523	H	0.323	5.235	-1.748
C	-2.969	0.692	-0.504	H	-0.093	4.046	-2.995
C	-3.475	-0.045	0.773	H	1.478	3.98	-2.175
C	0.61	1.78	0.876	H	-5.802	-4.19	-2.484
C	1.863	1.172	0.172	H	-4.088	-4.309	-2.016
C	-0.578	0.828	0.55	H	-5.35	-5.161	-1.092
C	0.408	4.178	-2.031	H	2.404	3.948	0.145
C	-5.11	-4.236	-1.632	H	1.797	4.11	1.8
C	1.517	4.182	0.743	H	1.252	5.225	0.543
C	2.997	0.787	1.15	H	2.585	0.103	1.904
N	1.332	0.019	-0.542	H	3.291	1.7	1.682
N	6.199	-0.018	-0.552	H	1.916	-0.581	-1.112
O	-0.785	0.325	2.919	H	7.095	0.238	-0.941
O	-0.584	-1.173	-0.94	H	-2.29	-0.887	3.437
O	-5.742	-0.802	0.944				
Conformation 5							
Atom	**X**	**Y**	**Z**	**Atom**	**X**	**Y**	**Z**
C	-6.949	0.603	0.783	O	2.975	-2.803	0.208
C	-7.635	0.034	-0.312	H	-7.45	1.348	1.395
C	-5.646	0.224	1.088	H	-8.653	0.35	-0.527
C	-7.034	-0.925	-1.12	H	-5.131	0.668	1.937
C	-5.008	-0.742	0.288	H	-7.562	-1.365	-1.962
C	-5.722	-1.303	-0.809	H	1.508	3.304	0.11
C	0.889	2.504	-0.288	H	-2.895	-2.918	-1.059
C	-3.683	-2.25	-0.74	H	5.2	3.574	-0.878

C	-3.704	-1.363	0.312	H	4.678	3.035	0.814
C	-0.398	2.698	-0.618	H	5.647	-1.075	-1.764
C	1.104	-1.293	0.083	H	3.772	1.875	-1.892
C	0.42	0.407	1.785	H	7.47	-1.016	0.697
C	4.602	2.906	-0.264	H	1.444	0.854	-1.518
C	5.947	-0.964	-0.724	H	-0.597	1.208	-2.109
C	3.817	1.973	-0.805	H	2.642	-1.269	1.556
C	7.228	-1.139	-0.358	H	3.055	1.218	1.044
C	4.897	-0.624	0.26	H	3.422	-0.687	-1.327
C	1.483	1.127	-0.449	H	-1.203	-0.645	-0.848
C	-1.129	1.482	-1.183	H	-2.573	1.054	0.99
C	2.56	-1.48	0.481	H	-1.453	4.402	-1.438
C	2.965	1	-0.024	H	-0.4	4.778	-0.061
C	3.459	-0.457	-0.255	H	-1.957	3.967	0.19
C	-0.948	0.236	-0.254	H	8.825	-2.429	-0.96
C	-1.84	0.244	1.023	H	8.024	-1.592	-2.313
C	0.517	0.102	0.262	H	9.139	-0.722	-1.229
C	-1.085	4.029	-0.473	H	-3.225	2.043	-0.773
C	8.354	-1.489	-1.275	H	-3.018	0.786	-1.996
C	-2.589	1.712	-1.599	H	-2.648	2.472	-2.385
C	-2.587	-1.092	1.278	H	-2.98	-1.064	2.304
N	-0.887	0.515	2.093	H	-1.855	-1.907	1.243
N	-4.886	-2.216	-1.416	H	-1.17	0.66	3.055
O	0.485	-2.242	-0.38	H	-5.12	-2.788	-2.214
O	1.357	0.526	2.572	H	2.195	-3.239	-0.19
O	5.129	-0.475	1.457				
Conformation 6							
Atom	**X**	**Y**	**Z**	**Atom**	**X**	**Y**	**Z**
C	-6.73	0.545	1.475	O	2.952	-2.831	-0.955
C	-7.567	0.193	0.394	H	-7.123	1.178	2.267
C	-5.416	0.095	1.541	H	-8.59	0.56	0.369
C	-7.108	-0.618	-0.639	H	-4.784	0.371	2.381
C	-4.919	-0.724	0.51	H	-7.752	-0.892	-1.47
C	-5.785	-1.069	-0.568	H	1.632	3.199	0.246
C	0.954	2.484	-0.213	H	-3.078	-2.668	-1.451
C	-3.793	-2.051	-0.924	H	5.182	3.648	-1.073
C	-3.649	-1.364	0.259	H	4.803	2.85	0.553
C	-0.356	2.738	-0.359	H	4.685	-0.63	1.459
C	1.118	-1.311	-0.591	H	3.666	2.111	-2.213
C	0.693	0.022	1.487	H	7.389	-1.164	0.129
C	4.635	2.888	-0.521	H	1.342	1.08	-1.771
C	5.412	-0.78	0.664	H	-0.752	1.529	-2.051
C	3.803	2.042	-1.132	H	2.76	-1.625	0.708

C	6.7	-1.021	0.961	H	3.205	1.004	0.635
C	4.942	-0.708	-0.74	H	3.314	-0.465	-2.064
C	1.498	1.158	-0.681	H	-1.27	-0.51	-1.057
C	-1.173	1.642	-1.039	H	-2.341	0.872	1.206
C	2.599	-1.593	-0.378	H	-1.45	4.565	-0.75
C	3.014	0.955	-0.441	H	-0.249	4.687	0.549
C	3.451	-0.441	-0.977	H	-1.79	3.853	0.822
C	-0.918	0.255	-0.361	H	8.069	-0.365	2.471
C	-1.646	0.053	1.002	H	6.514	-0.954	3.111
C	0.593	0.018	-0.065	H	7.741	-2.09	2.496
C	-0.991	4.026	0.09	H	-3.198	2.125	-0.305
C	7.273	-1.109	2.338	H	-3.154	1.108	-1.748
C	-2.663	1.946	-1.243	H	-2.79	2.835	-1.869
C	-2.414	-1.291	1.11	H	-2.68	-1.44	2.166
N	-0.559	0.104	1.973	H	-1.726	-2.101	0.842
N	-5.067	-1.876	-1.425	H	-0.719	0.064	2.973
O	0.436	-2.129	-1.193	H	-5.419	-2.292	-2.274
O	1.723	-0.04	2.158	H	2.135	-3.157	-1.384
O	5.699	-0.848	-1.696				
Conformation 7							
Atom	**X**	**Y**	**Z**	**Atom**	**X**	**Y**	**Z**
C	-4.145	-3.168	-1.271	O	2.373	-2.667	0.991
C	-5.471	-2.992	-1.72	H	-3.562	-4.003	-1.652
C	-3.572	-2.295	-0.353	H	-5.89	-3.691	-2.439
C	-6.253	-1.938	-1.258	H	-2.547	-2.44	-0.022
C	-4.335	-1.216	0.135	H	-7.275	-1.8	-1.599
C	-5.674	-1.061	-0.332	H	1.736	3.357	-0.665
C	0.98	2.587	-0.801	H	-5.486	1.449	1.746
C	-5.252	0.579	1.146	H	5.323	2.787	-1.892
C	-4.087	-0.151	1.08	H	4.901	2.781	-0.09
C	-0.293	2.886	-1.102	H	5.074	-1.836	-1.589
C	0.716	-0.971	0.57	H	3.582	1.137	-2.336
C	0.425	1.19	1.782	H	7.103	-1.51	0.683
C	4.702	2.399	-1.089	H	1.19	0.611	-1.57
C	5.476	-1.552	-0.619	H	-0.83	1.112	-2.126
C	3.746	1.496	-1.318	H	2.381	-0.803	1.887
C	6.756	-1.815	-0.305	H	3.071	1.365	0.706
C	4.566	-0.878	0.33	H	2.944	-1.116	-1.087
C	1.365	1.141	-0.618	H	-1.557	-0.237	-0.386
C	-1.231	1.694	-1.281	H	-2.501	2.083	0.999
C	2.167	-1.272	0.917	H	-1.177	4.466	-2.292
C	2.85	0.899	-0.258	H	0.037	5.014	-1.121
C	3.118	-0.628	-0.12	H	-1.587	4.545	-0.583

C	-1.135	0.716	-0.063	H	8.136	-3.4	-0.711
C	-1.899	1.194	1.211	H	7.318	-2.764	-2.161
C	0.34	0.494	0.393	H	8.615	-1.841	-1.363
C	-0.777	4.3	-1.283	H	-3.181	2.665	-0.926
C	7.748	-2.492	-1.192	H	-3.266	1.117	-1.775
C	-2.677	2.034	-1.665	H	-2.704	2.565	-2.622
C	-2.826	0.128	1.852	H	-3.088	0.486	2.857
N	-0.823	1.563	2.124	H	-2.25	-0.794	1.99
N	-6.2	0.044	0.299	H	-0.995	1.995	3.024
O	-0.065	-1.903	0.428	H	-7.141	0.392	0.188
O	1.438	1.365	2.456	H	1.506	-3.067	0.777
O	4.921	-0.509	1.447				

Fig. S5. ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **1**.

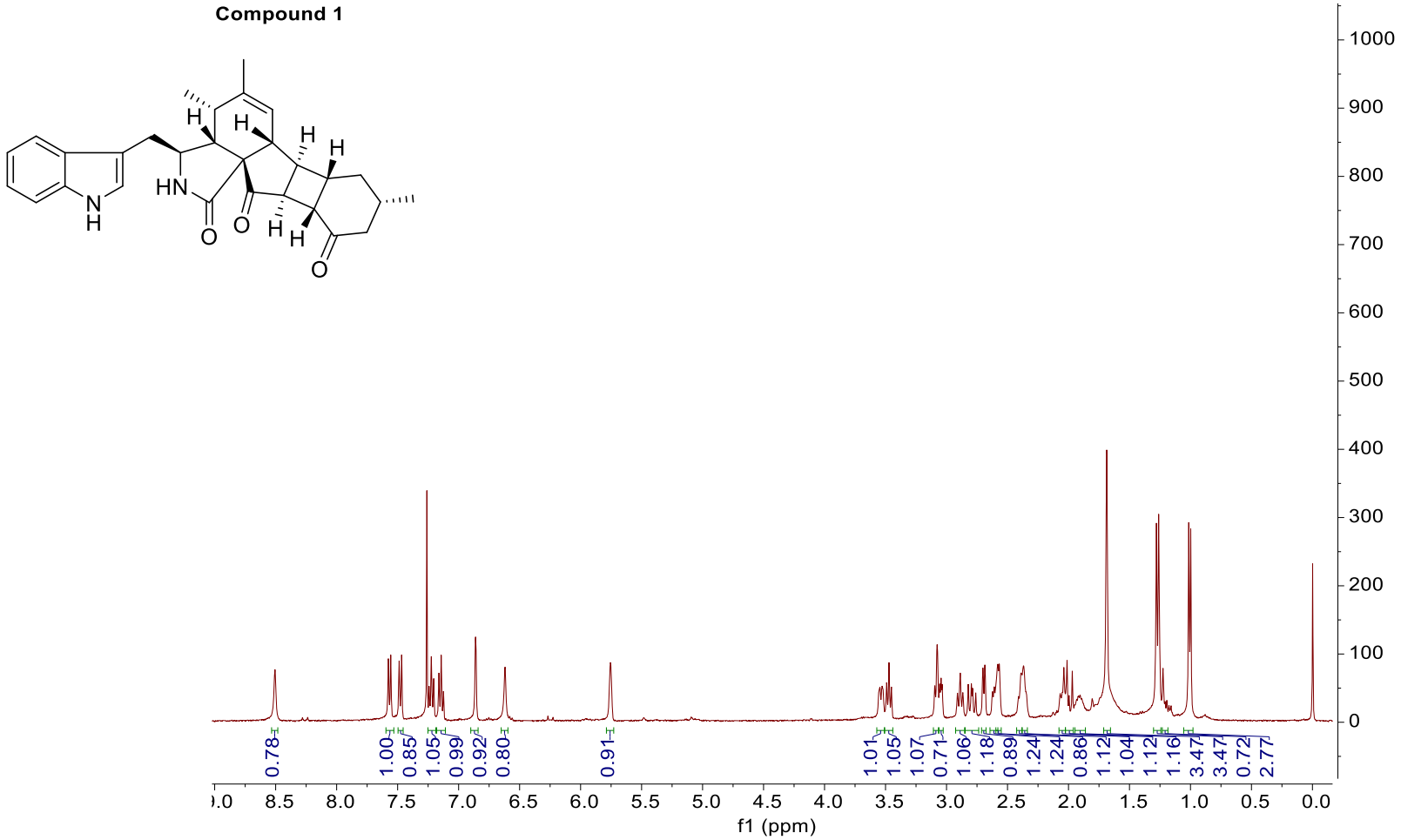
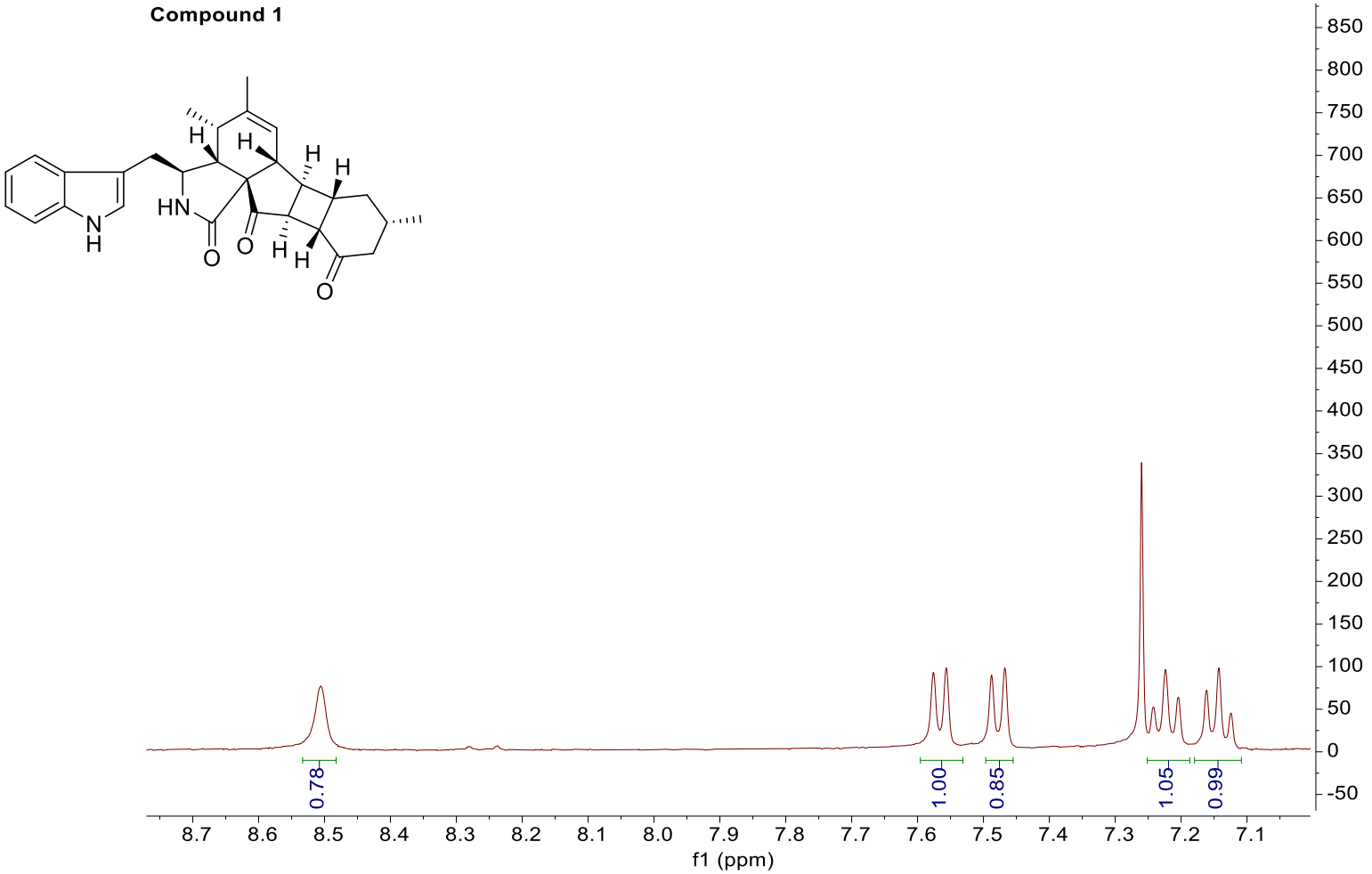
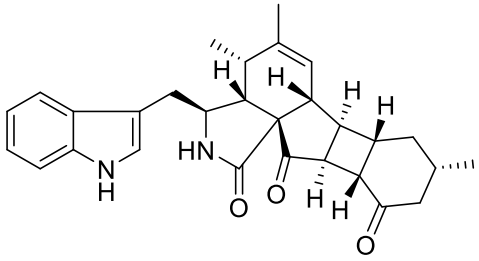


Fig. S6. Enlarged ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **1**.

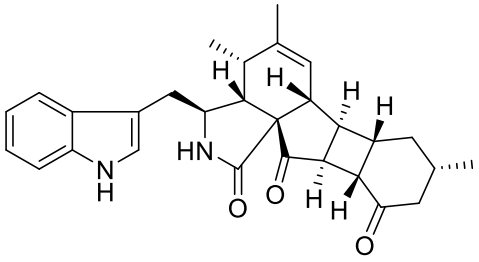


Compound 1


H
H
H
H
HN
N
H
O
O
H
H
O

850
800
750
700
650
600
550
500
450
400
350
300
250
200
150
100
50
0
-50
0.92
0.80
0.91
6.9
6.8
6.7
6.6
6.5
6.4
6.3
6.2
6.1
6.0
5.9
5.8
5.7
5.6
5.5
5.4
5.3
5.2
f1 (ppm)

Compound 1


H
H
H
H
HN
N
H
O
O
H
H
O

850
800
750
700
650
600
550
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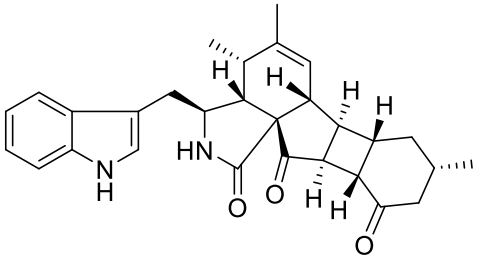
450
400
350
300
250
200
150
100
50
0
-50
1.01
1.05
1.07
0.71
1.06
1.18
0.89
1.24
1.24
0.86
1.12
3.9
3.8
3.7
3.6
3.5
3.4
3.3
3.2
3.1
3.0
2.9
2.8
2.7
2.6
2.5
2.4
2.3
f1 (ppm)

Compound 1


H
H
H
H
HN
N
H
O
O
H
H
O

850
800
750
700
650
600
550
500
450
400
350
300
250
200
150
100
50
0
-50
0.86
1.12
1.04
1.12
1.16
3.47
3.47
0.72
2.77
2.4
2.3
2.2
2.1
2.0
1.9
1.8
1.7
1.6
1.5
1.4
1.3
1.2
1.1
1.0
0.9
0.8
f1 (ppm)

Fig. S7. ^{13}C NMR (100 MHz, $CDCl_3$) spectrum of **1**.

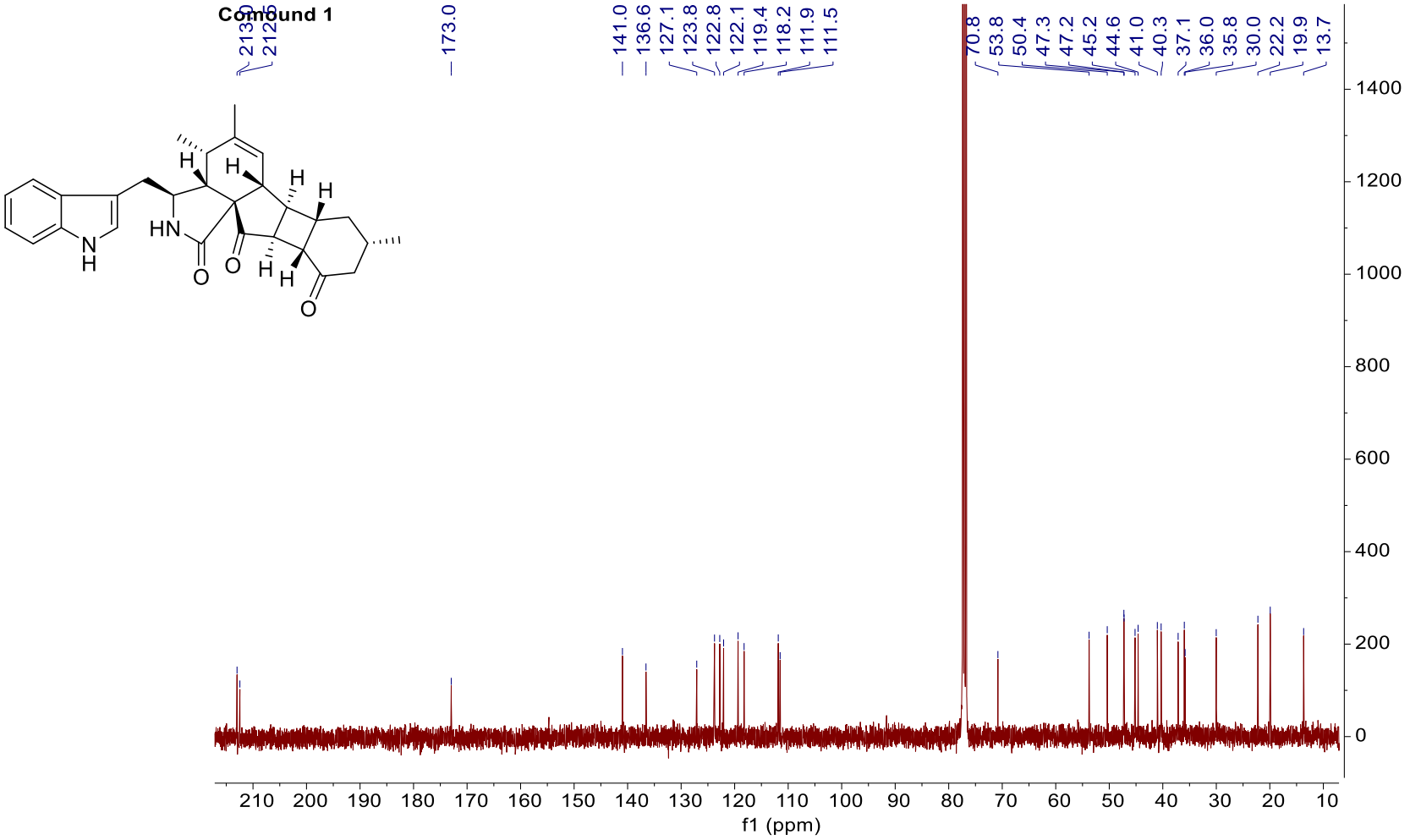


Fig. S8. DEPT-135 (100 MHz, $CDCl_3$) spectrum of **1**.

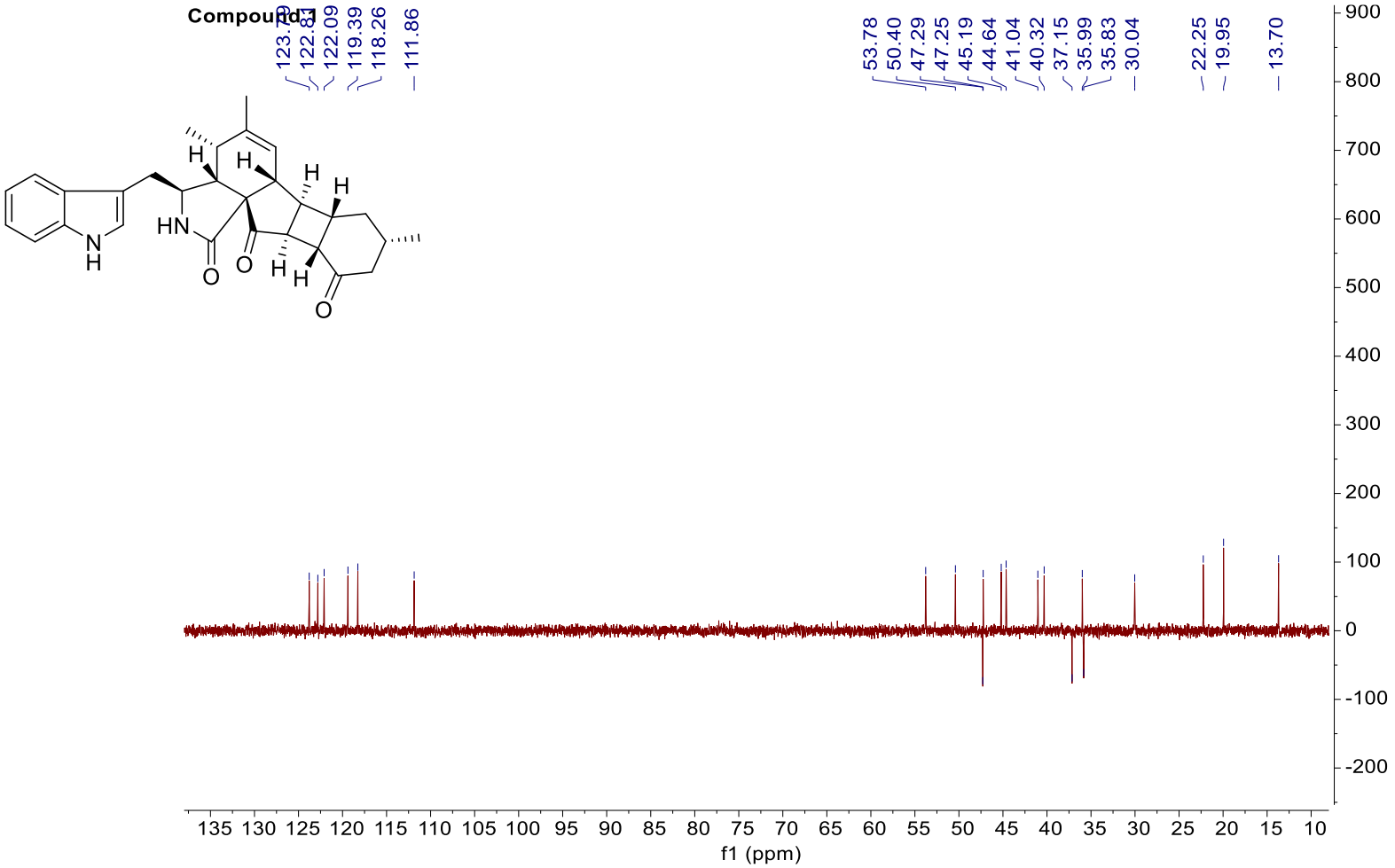


Fig. S9. HSQC spectrum of **1** in $CDCl_3$.

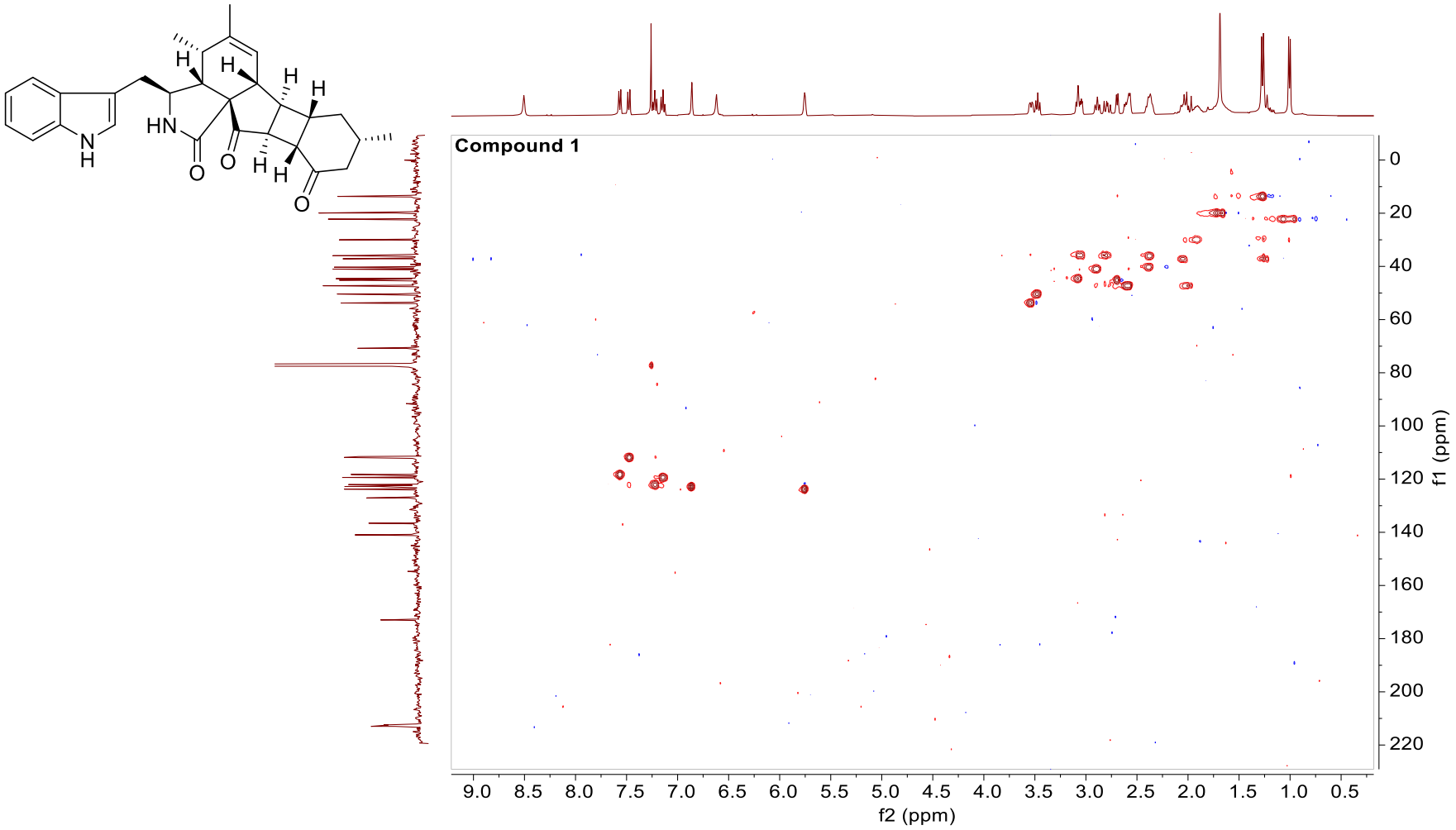


Fig. S10. HMBC spectrum of **1** in $CDCl_3$.

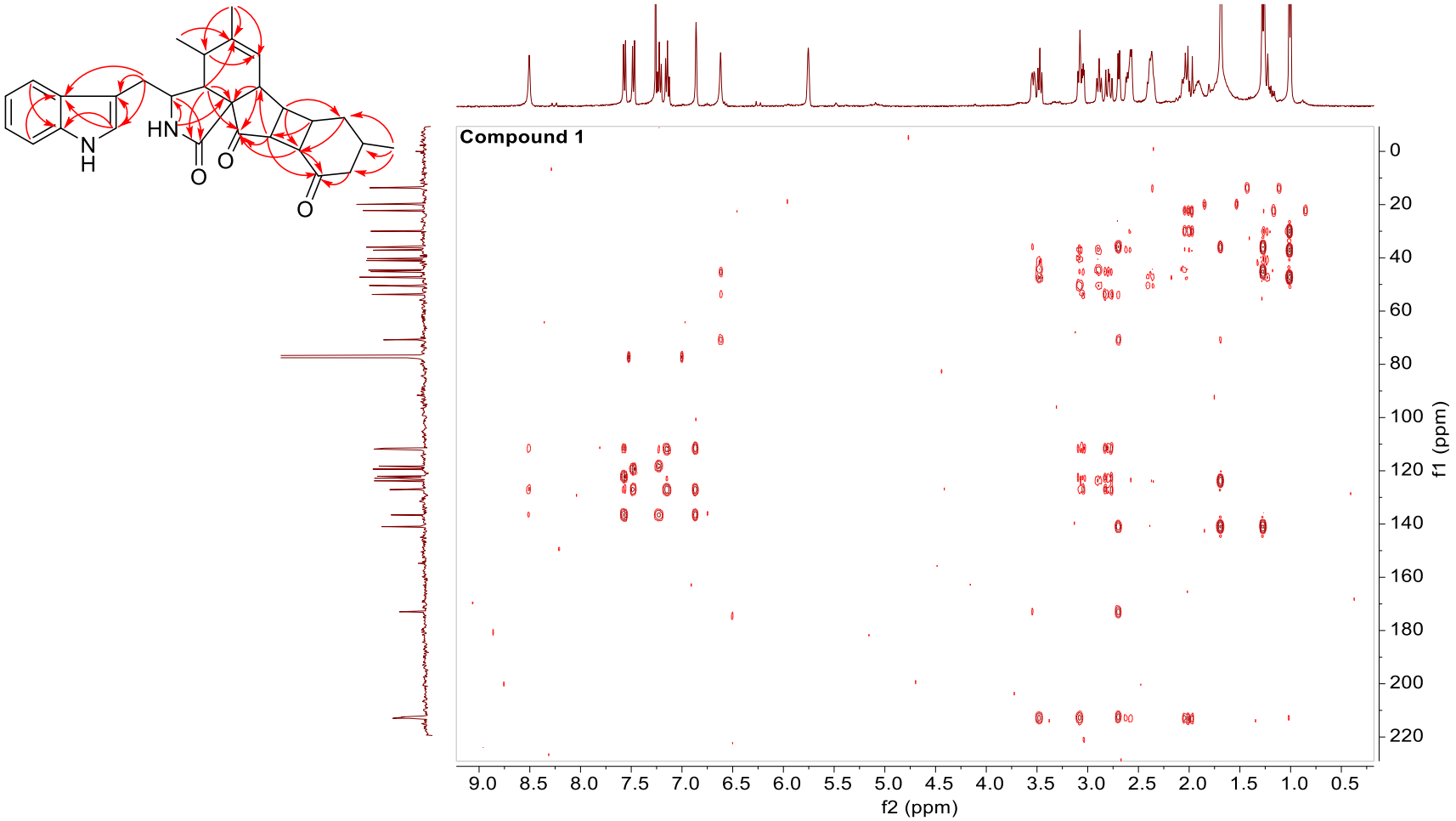


Fig. S11. ^{1}H–^{1}H COSY spectrum of **1** in $CDCl_3$.

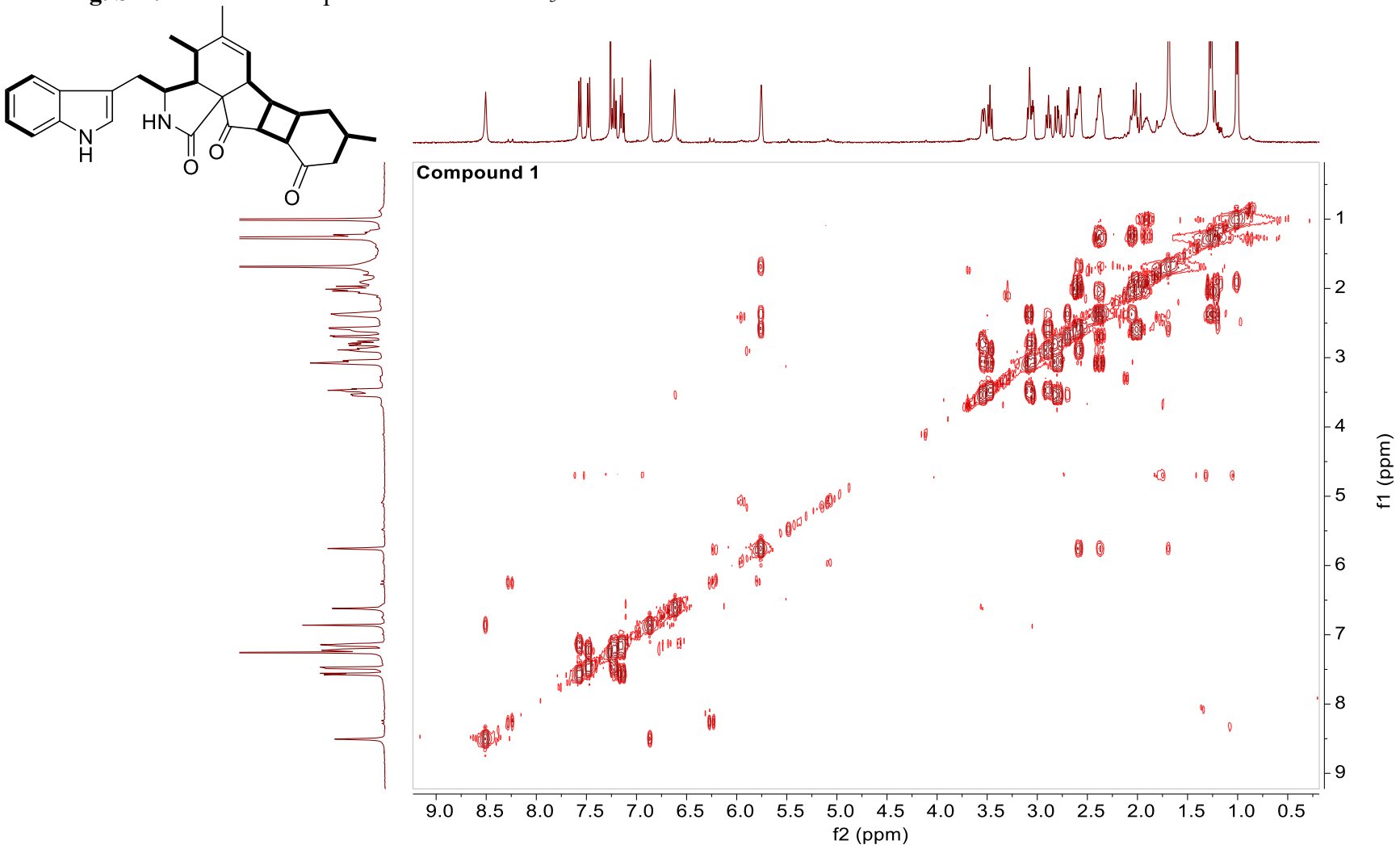


Fig. S12. NOESY spectrum of **1** in $CDCl_3$.

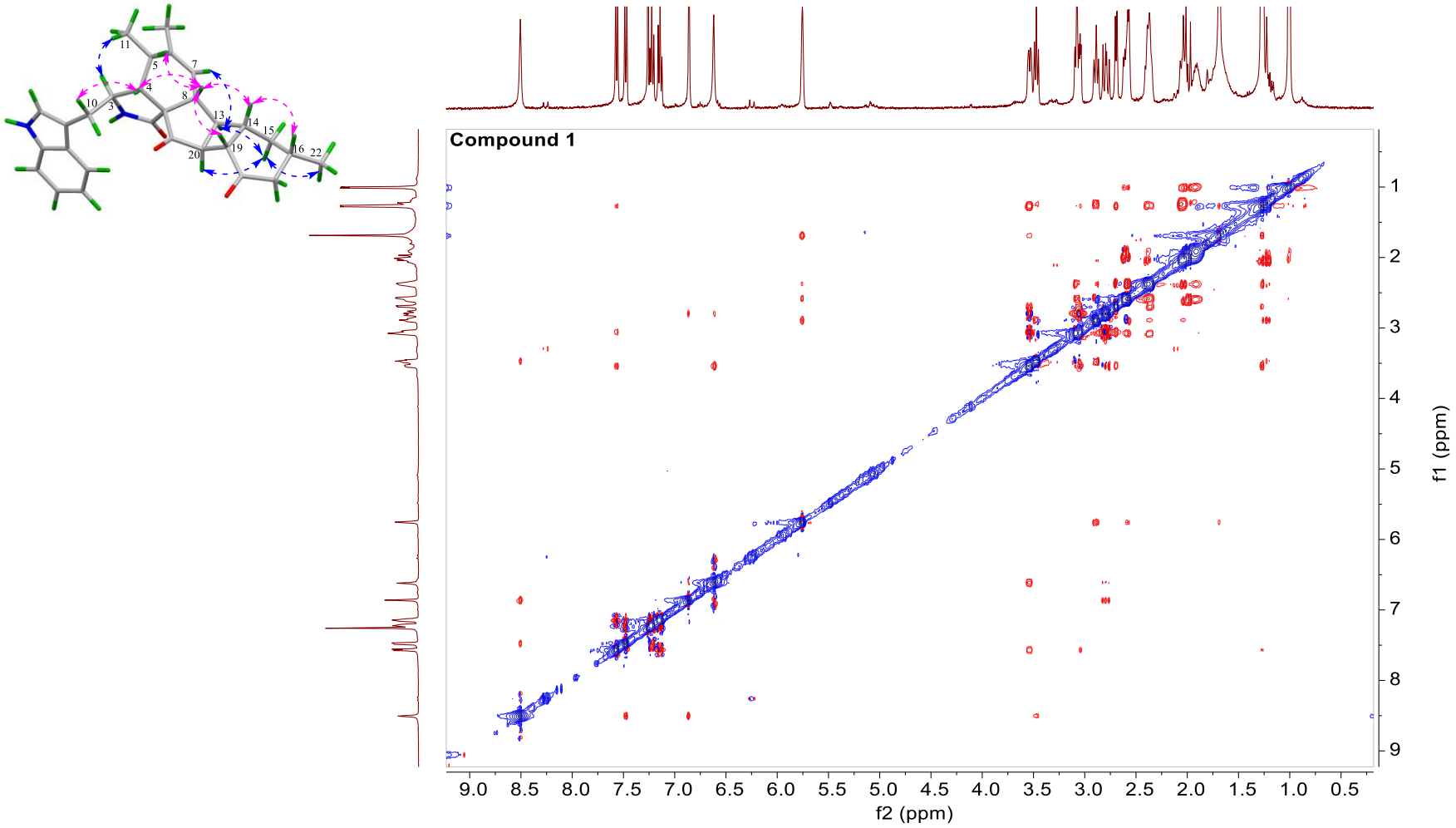


Fig. S13. HRESIMS (+) spectrum of **1**.

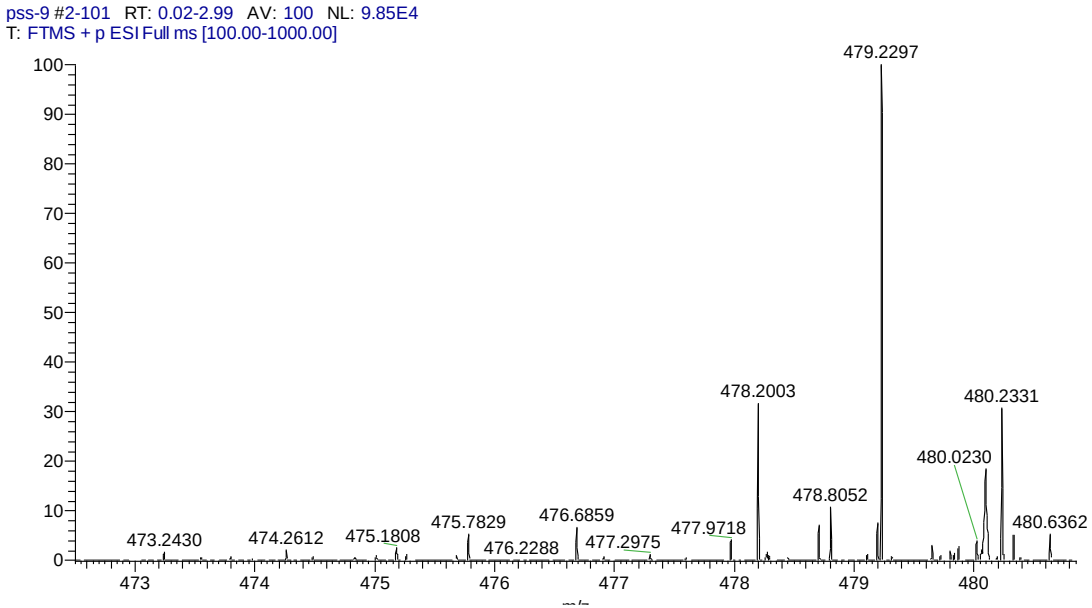


Fig. S14. UV spectrum of **1**.

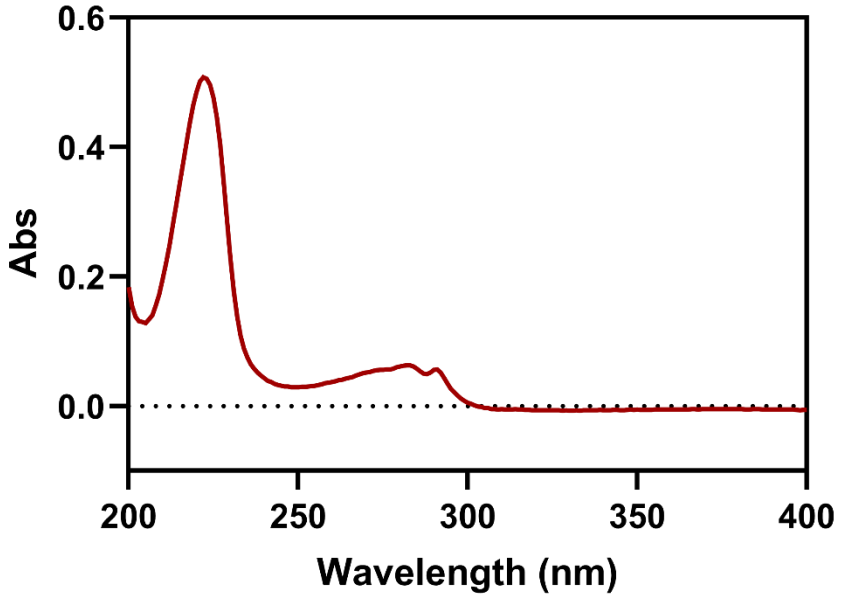


Fig. S15. IR spectrum of **1**.

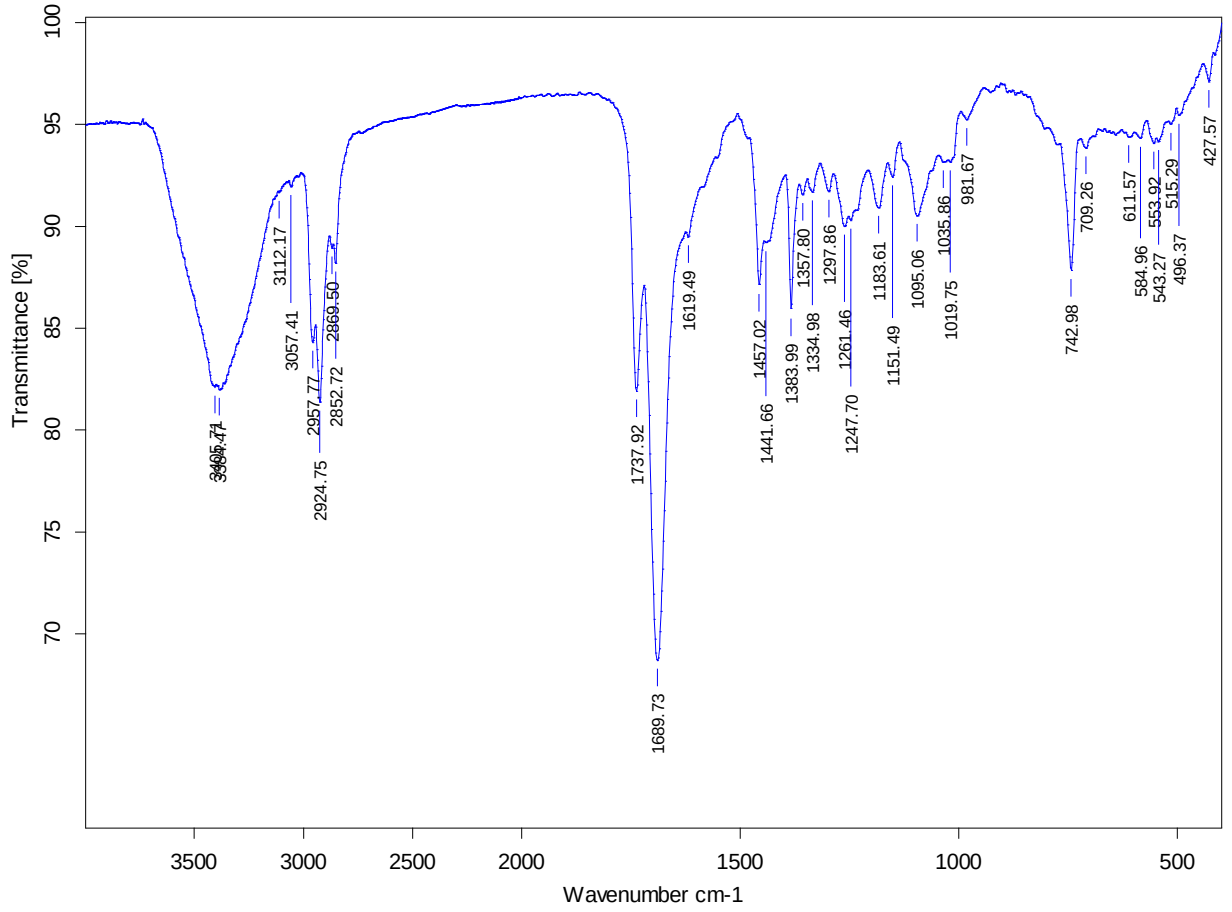


Fig. S16. ^{1}H NMR (400 MHz, Pyridine-d_5) spectrum of **2**.

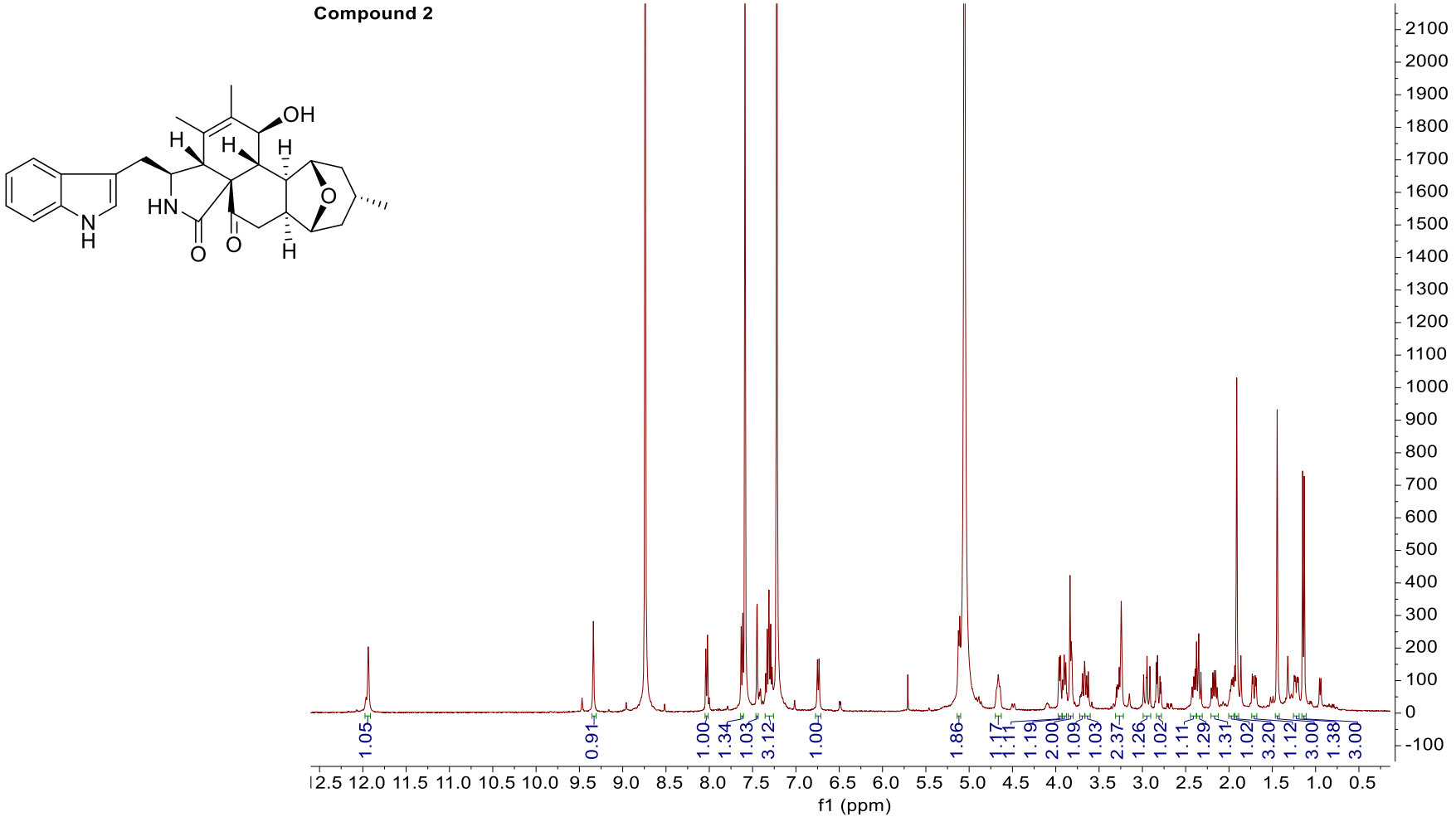
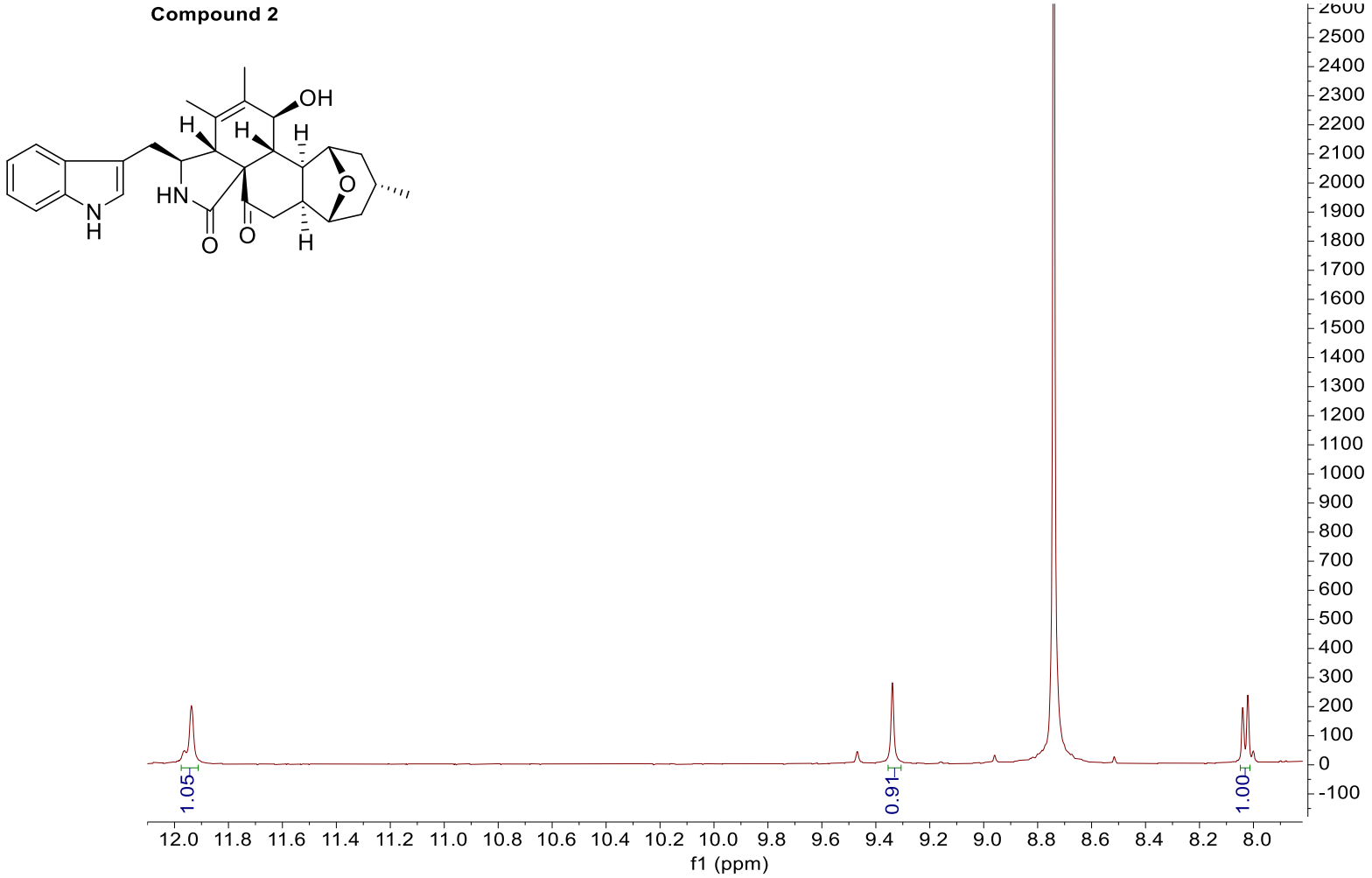
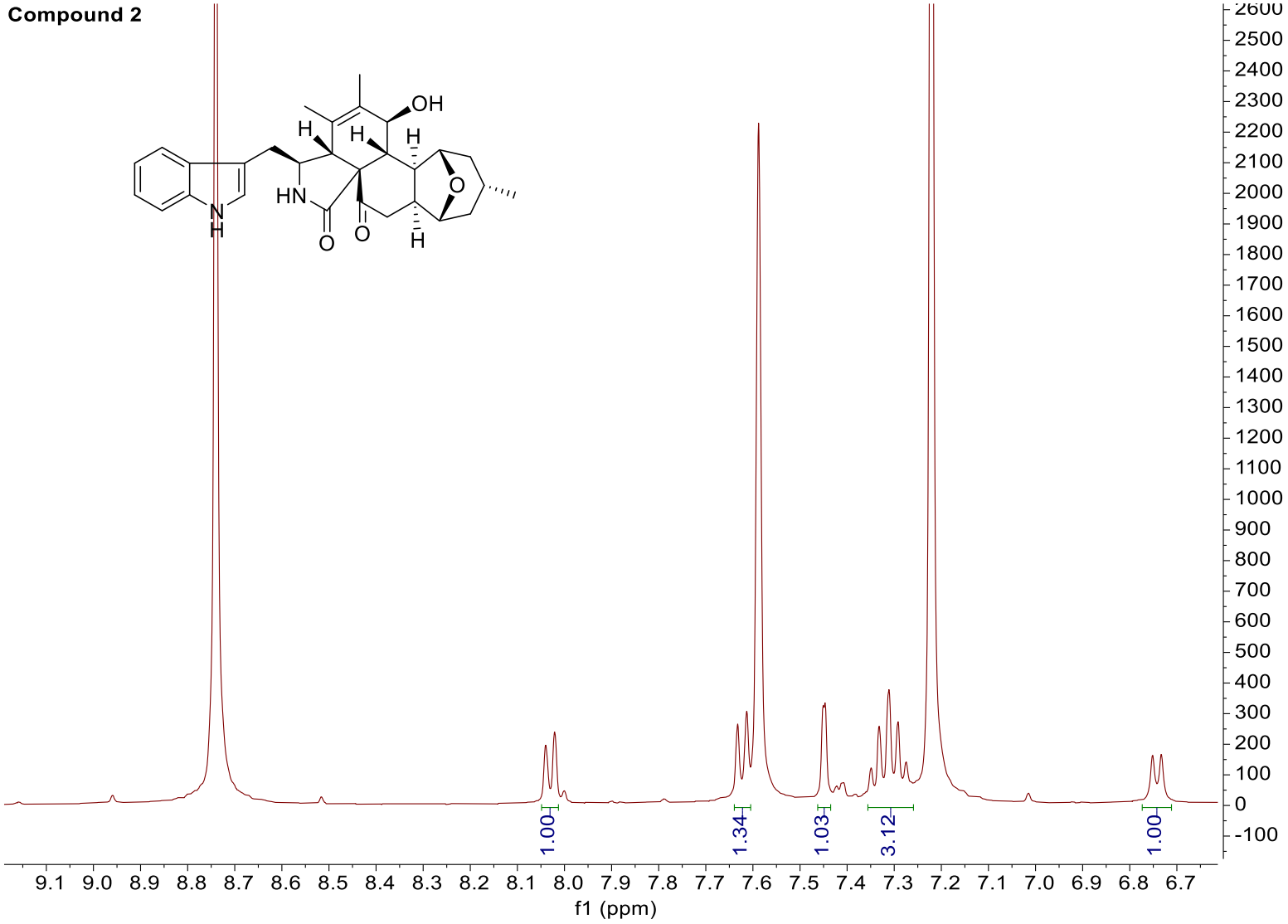
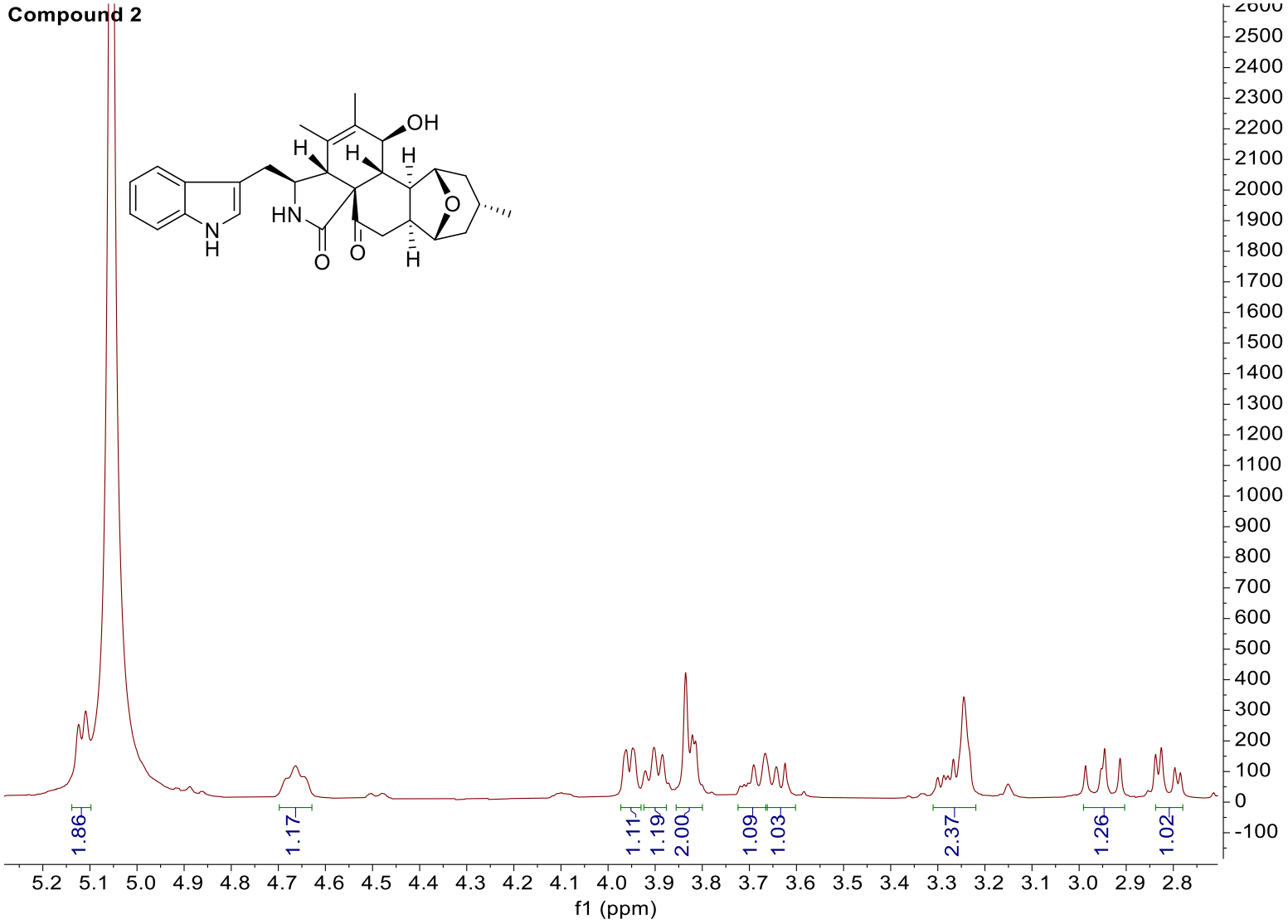


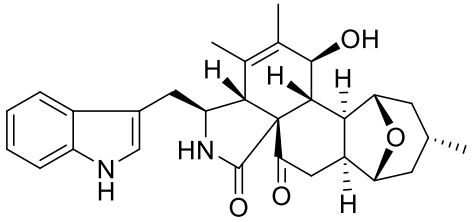
Fig. S17. Enlarged ^{1}H NMR (400 MHz, Pyridine-d_5) spectrum of **2**.




Compound 2
OH
H
H
H
HN
O
O
O
N
H
H
1.00
1.34
1.03
3.12
1.00
9.1 9.0 8.9 8.8 8.7 8.6 8.5 8.4 8.3 8.2 8.1 8.0 7.9 7.8 7.7 7.6 7.5 7.4 7.3 7.2 7.1 7.0 6.9 6.8 6.7
f1 (ppm)
2600 2500 2400 2300 2200 2100 2000 1900 1800 1700 1600 1500 1400 1300 1200 1100 1000 900 800 700 600 500 400 300 200 100 0 -100


Compound 2
OH
H
H
H
HN
O
O
O
N
H
H
1.86
1.17
1.11
1.19
2.00
1.09
1.03
2.37
1.26
1.02
f1 (ppm)

Compound 2


OH
H
H
H
HN
O
O
O
N
H
H

2500
2400
2300
2200
2100
2000
1900
1800
1700
1600
1500
1400
1300
1200
1100
1000
900
800
700
600
500
400
300
200
100
0
-100
1.26
1.02
1.11
1.29
1.31
1.02
3.20
1.12
3.00
1.38
3.00
3.2 3.1 3.0 2.9 2.8 2.7 2.6 2.5 2.4 2.3 2.2 2.1 2.0 1.9 1.8 1.7 1.6 1.5 1.4 1.3 1.2 1.1 1.0 0.9 0.8 0.7
f1 (ppm)

Fig. S18. ^{13}C NMR (100 MHz, Pyridine-d_5) spectrum of **2**.

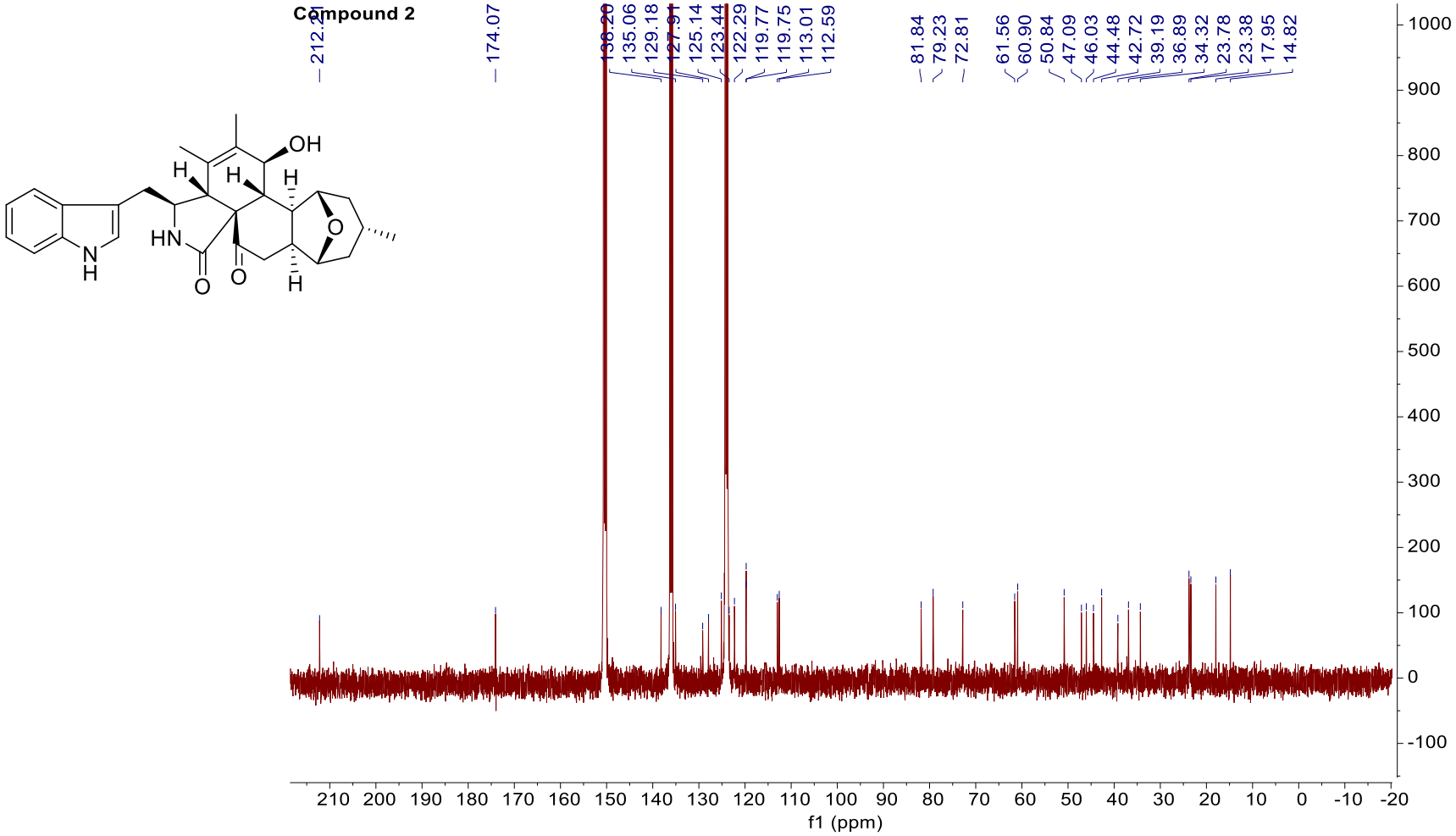


Fig. S19. DEPT-135 (100 MHz, Pyridine-d_5) spectrum of **2**.

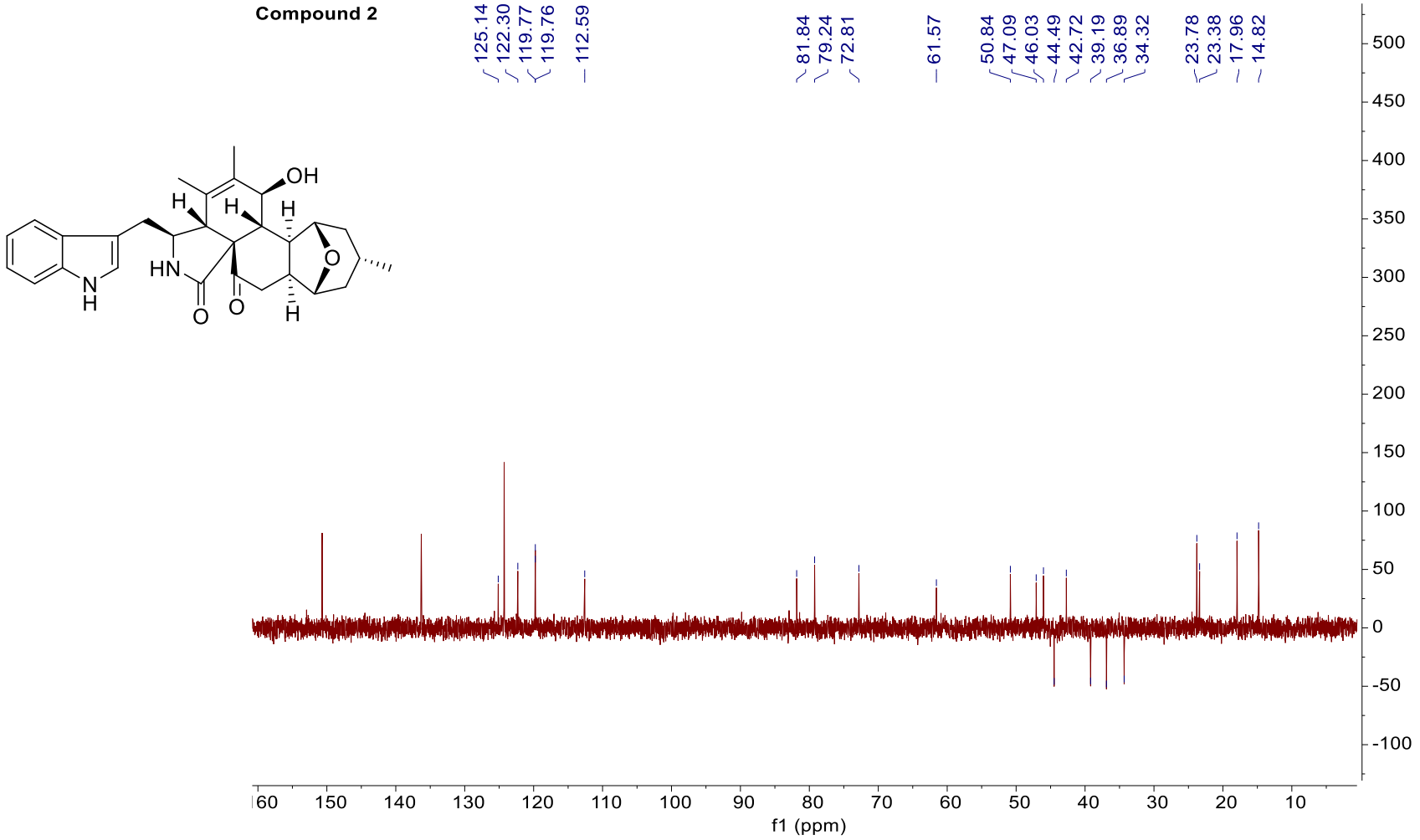


Fig. S20. HSQC spectrum of **2** in Pyridine-d_5.

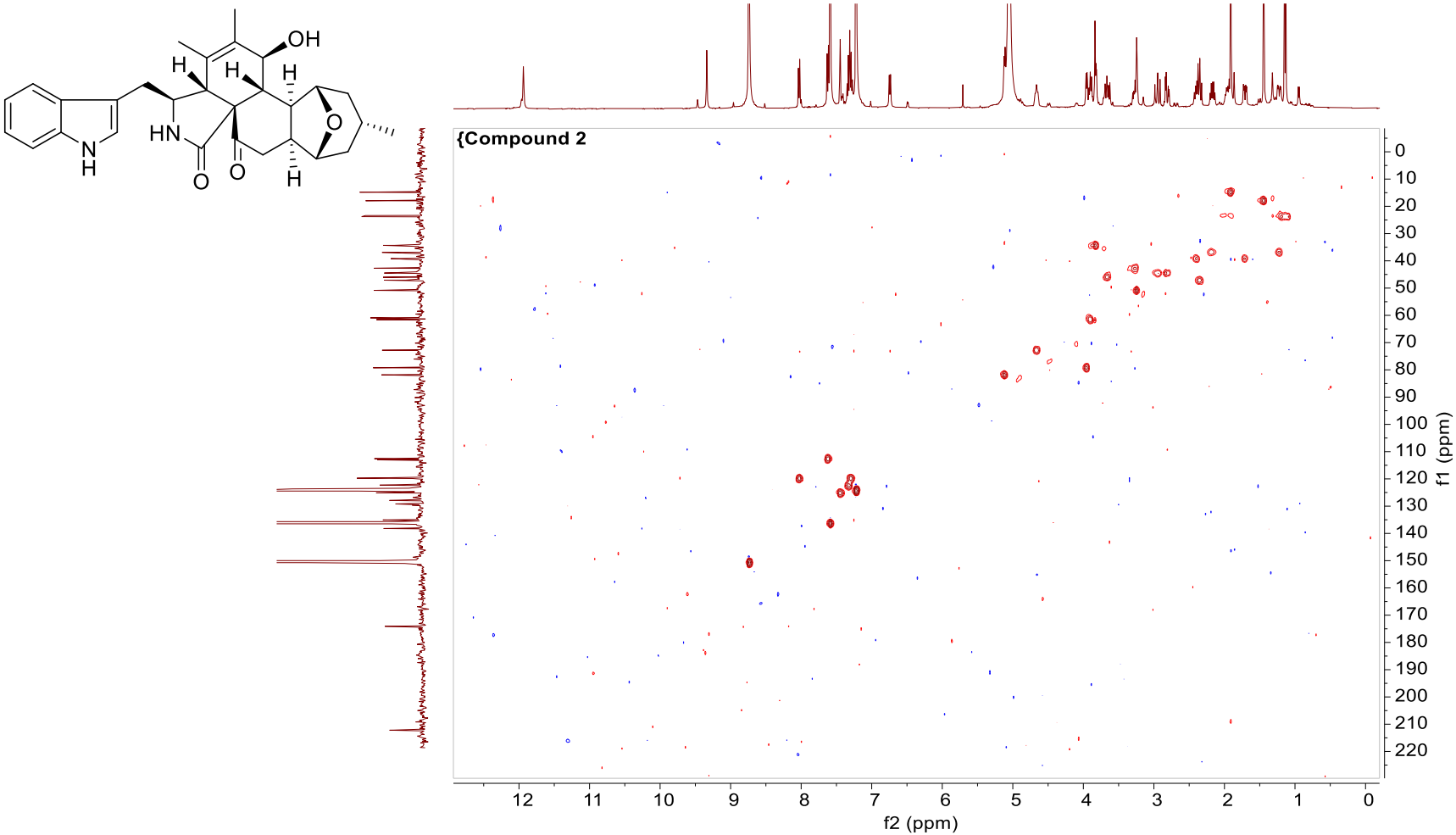


Fig. S21. HMBC spectrum of **2** in Pyridine-d_5.

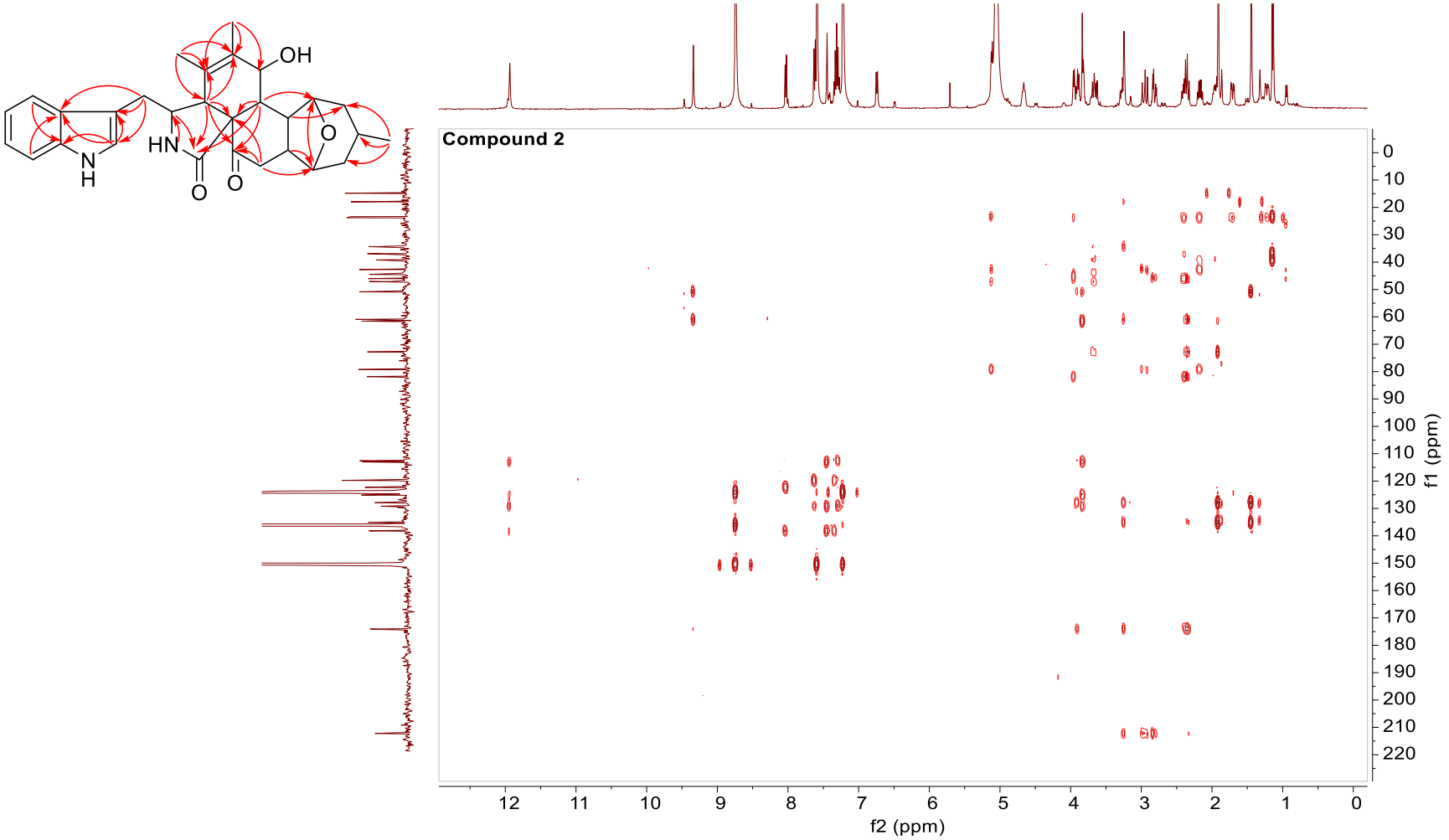


Fig. S22. ^{1}H–^{1}H COSY spectrum of **2** in Pyridine-d_5.

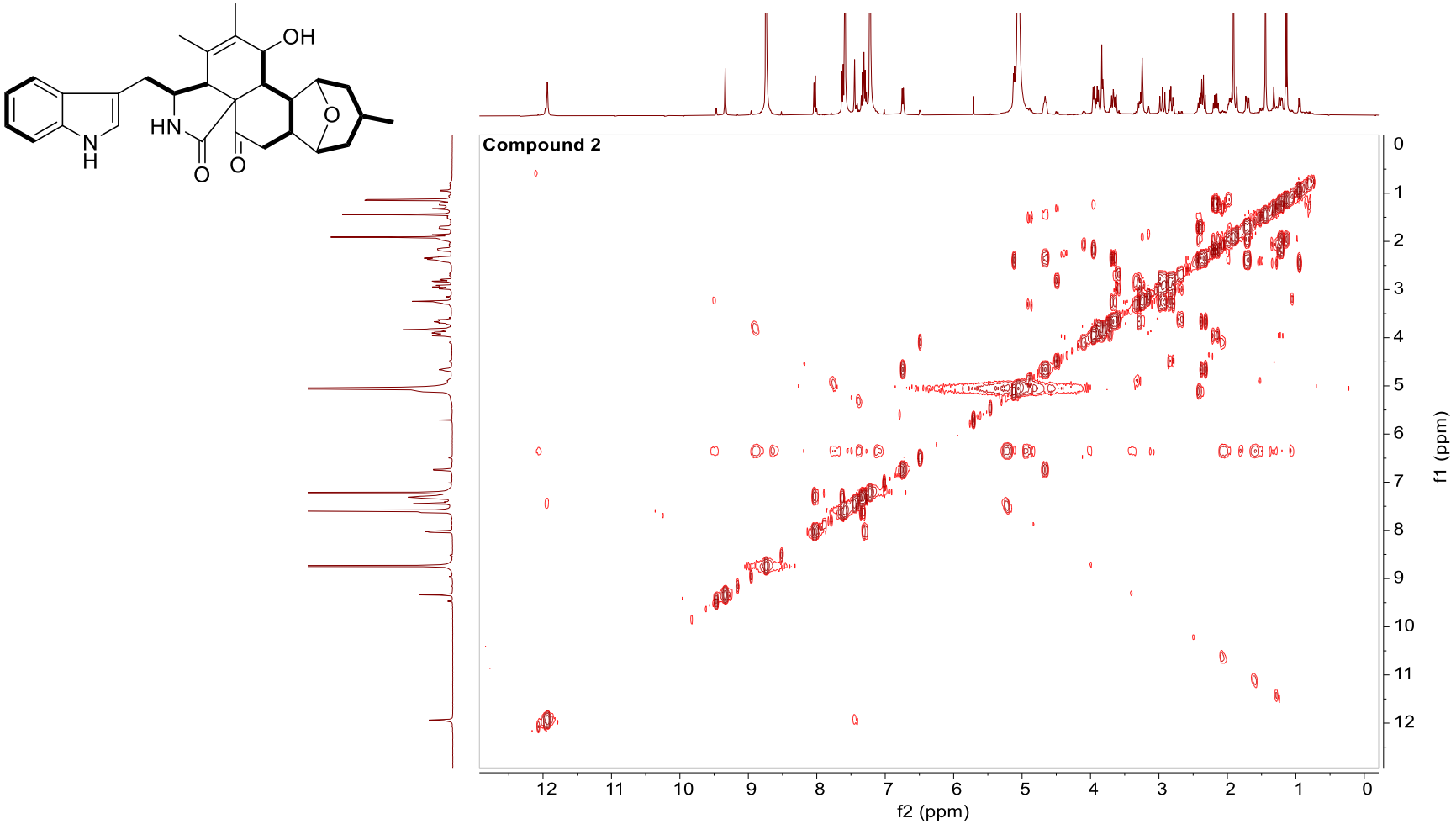


Fig. S23. NOESY spectrum of **2** in Pyridine-d_5.

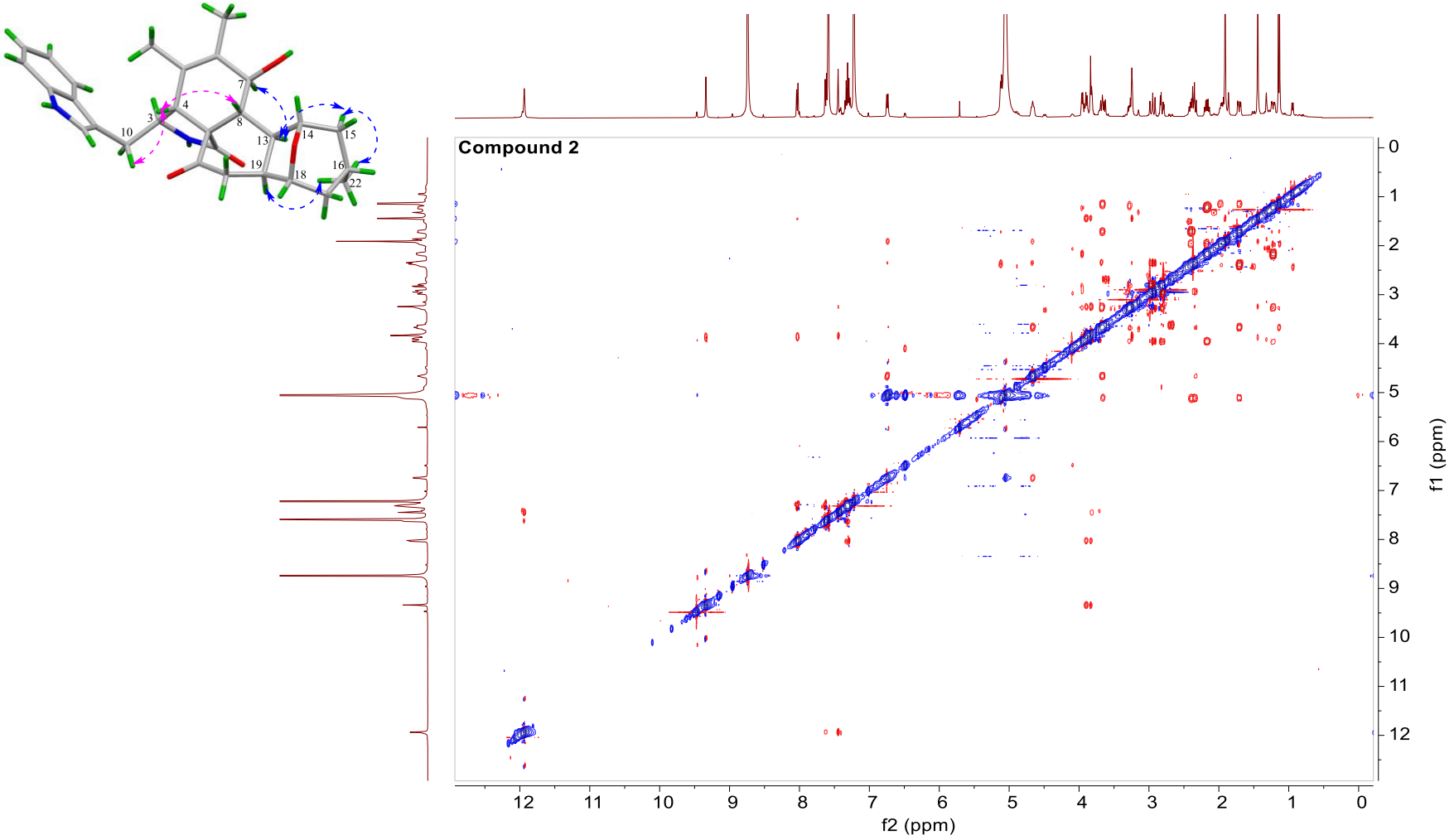


Fig. S24. HRESIMS (+) spectrum of **2**.

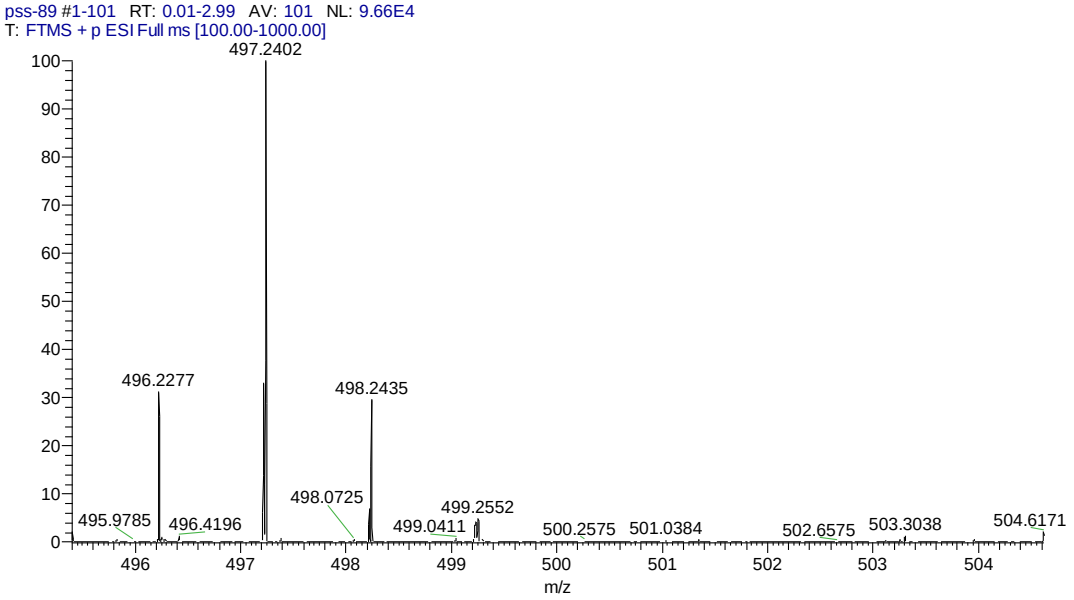


Fig. S25. UV spectrum of **2**.

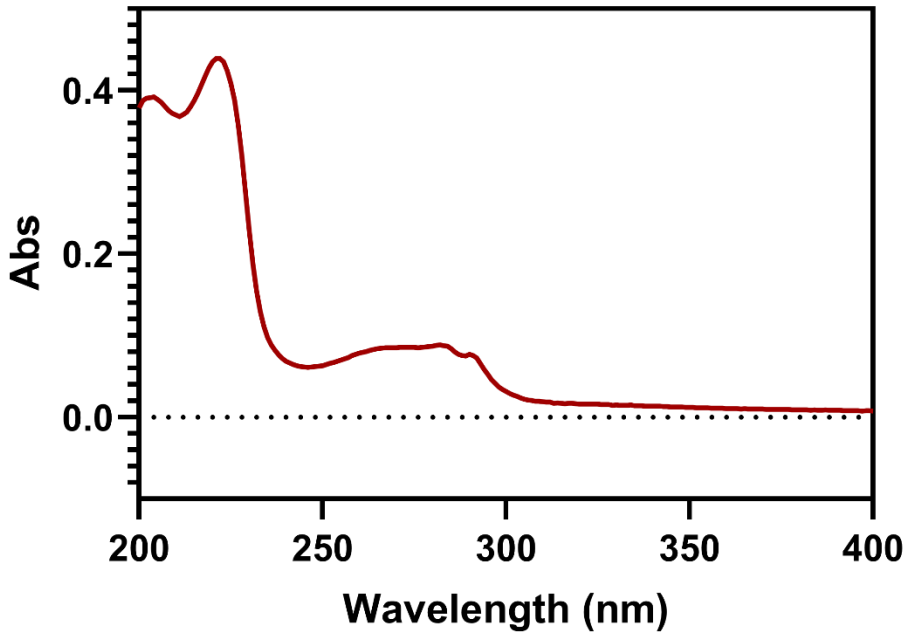


Fig. S26. IR spectrum of **2**.

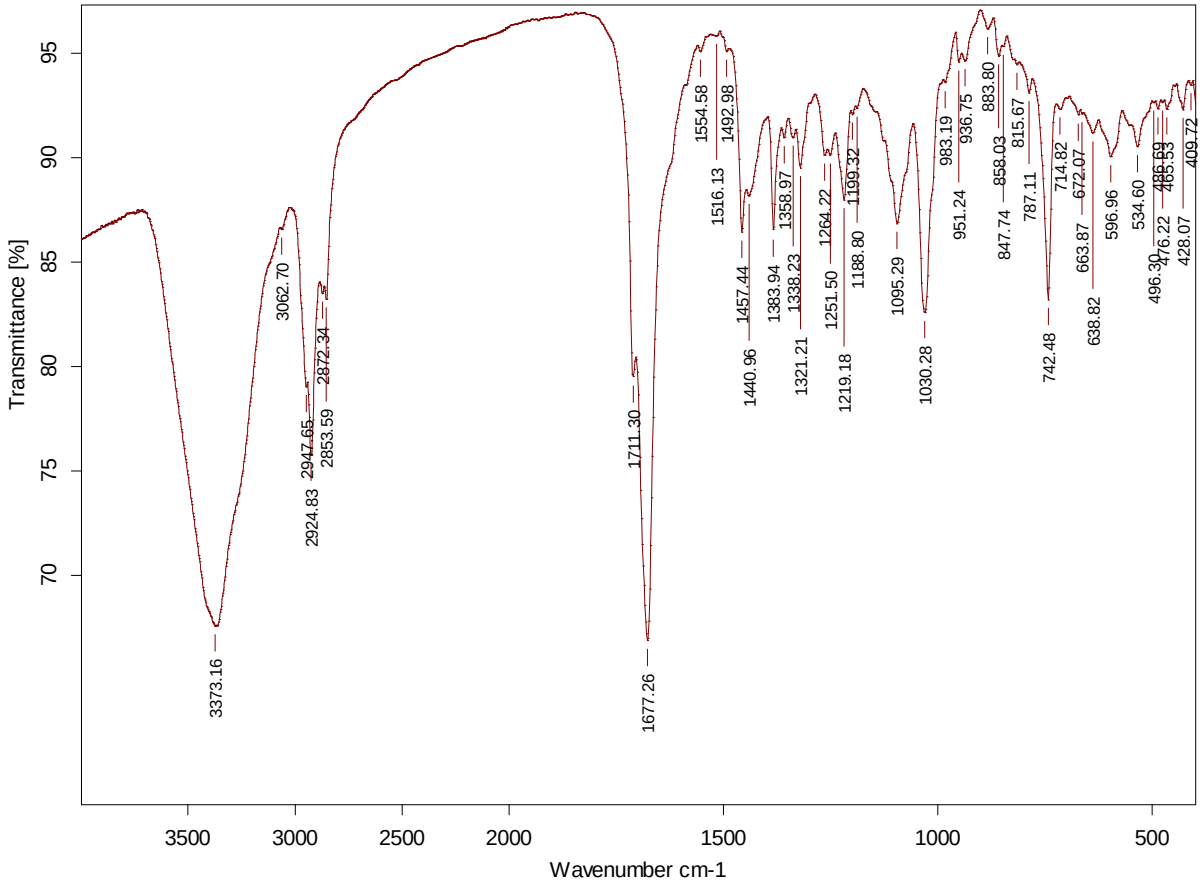


Fig. S27. ECD spectrum of **2**.

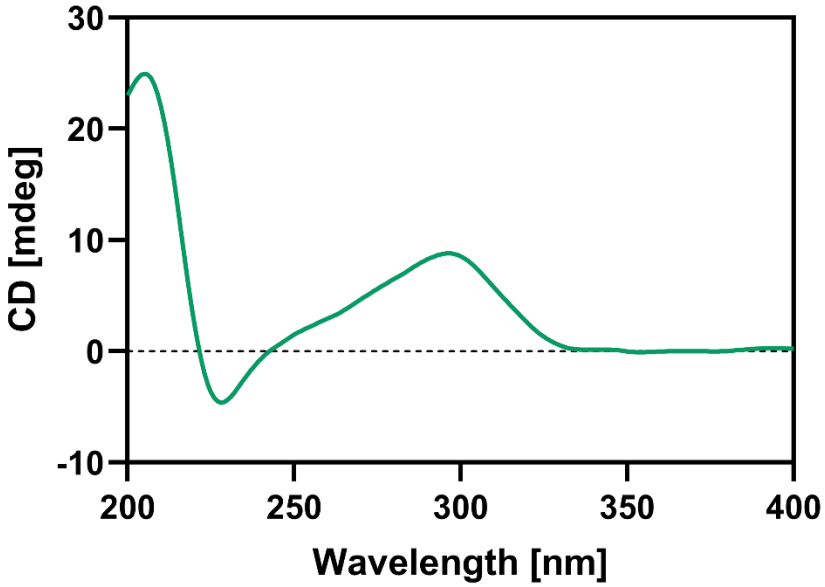


Fig. S28. ^{1}H NMR (400 MHz, DMSO-d_6) spectrum of **3**.

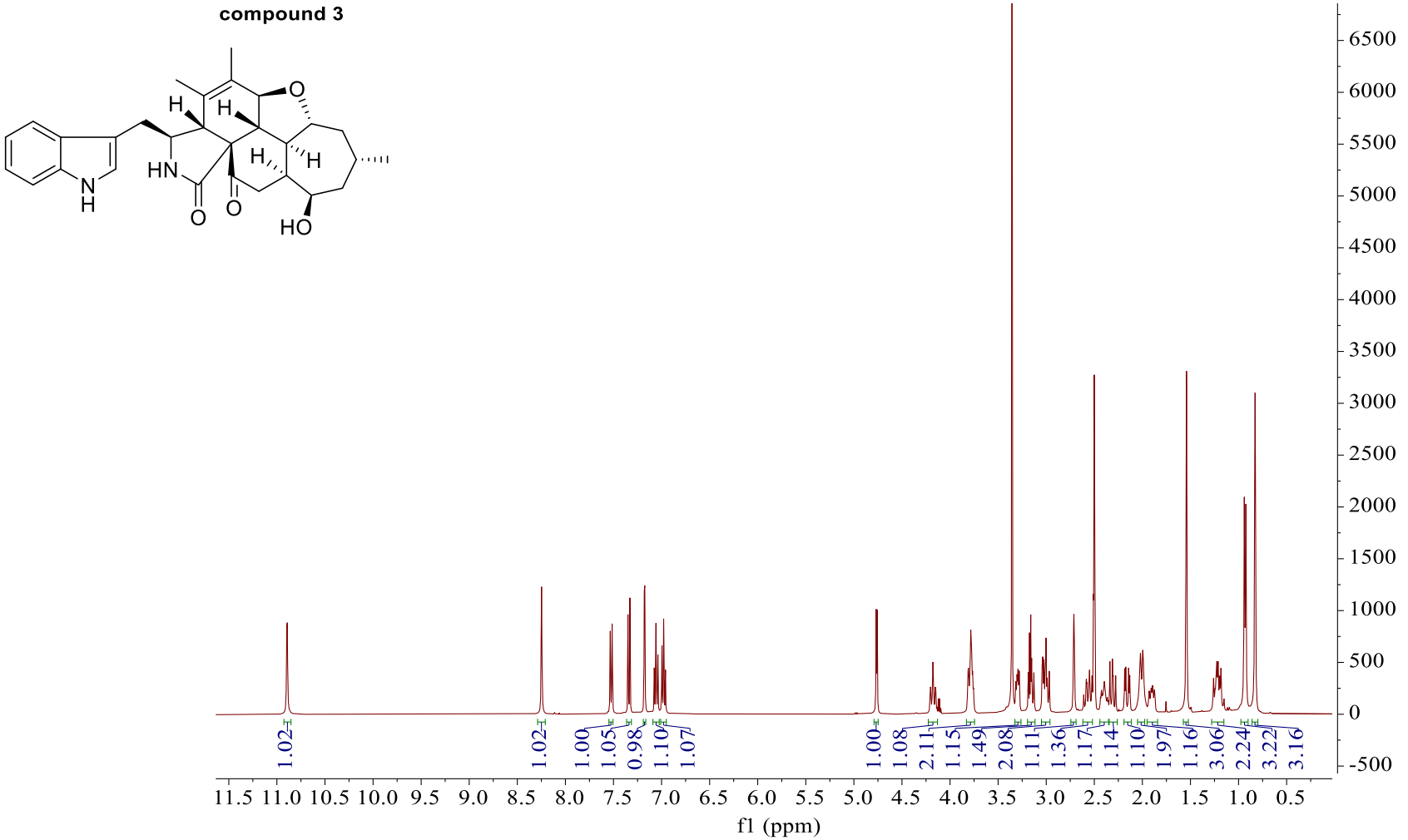
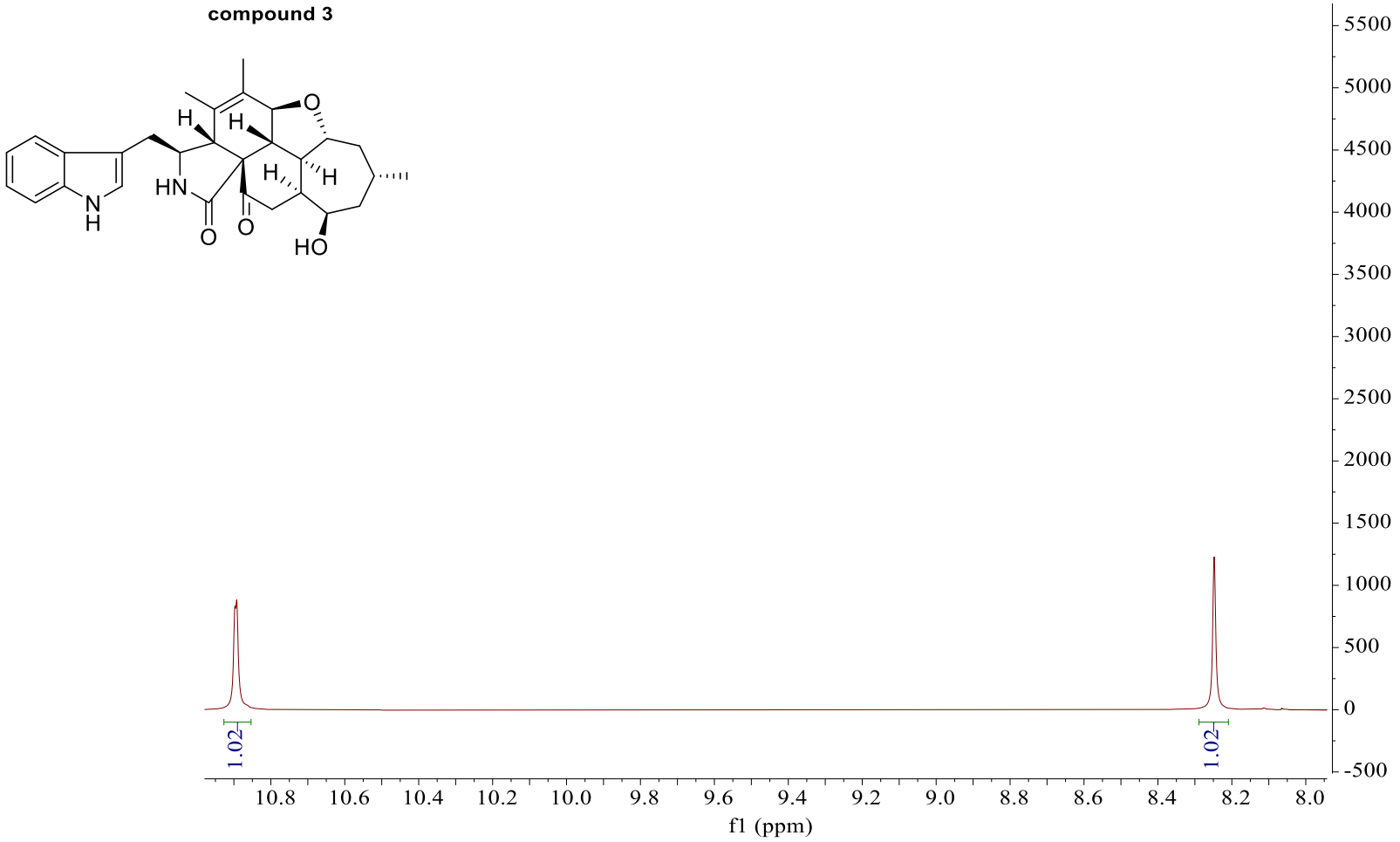
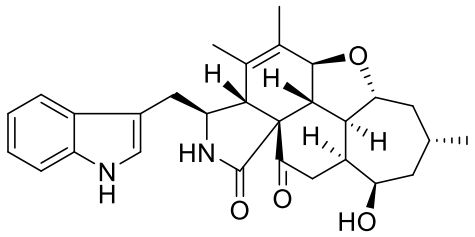


Fig. S29. Enlarged ^{1}H NMR (400 MHz, DMSO-d_6) spectrum of **3**.

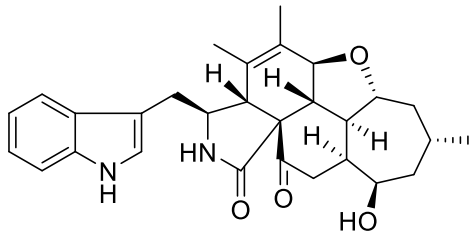


compound 3

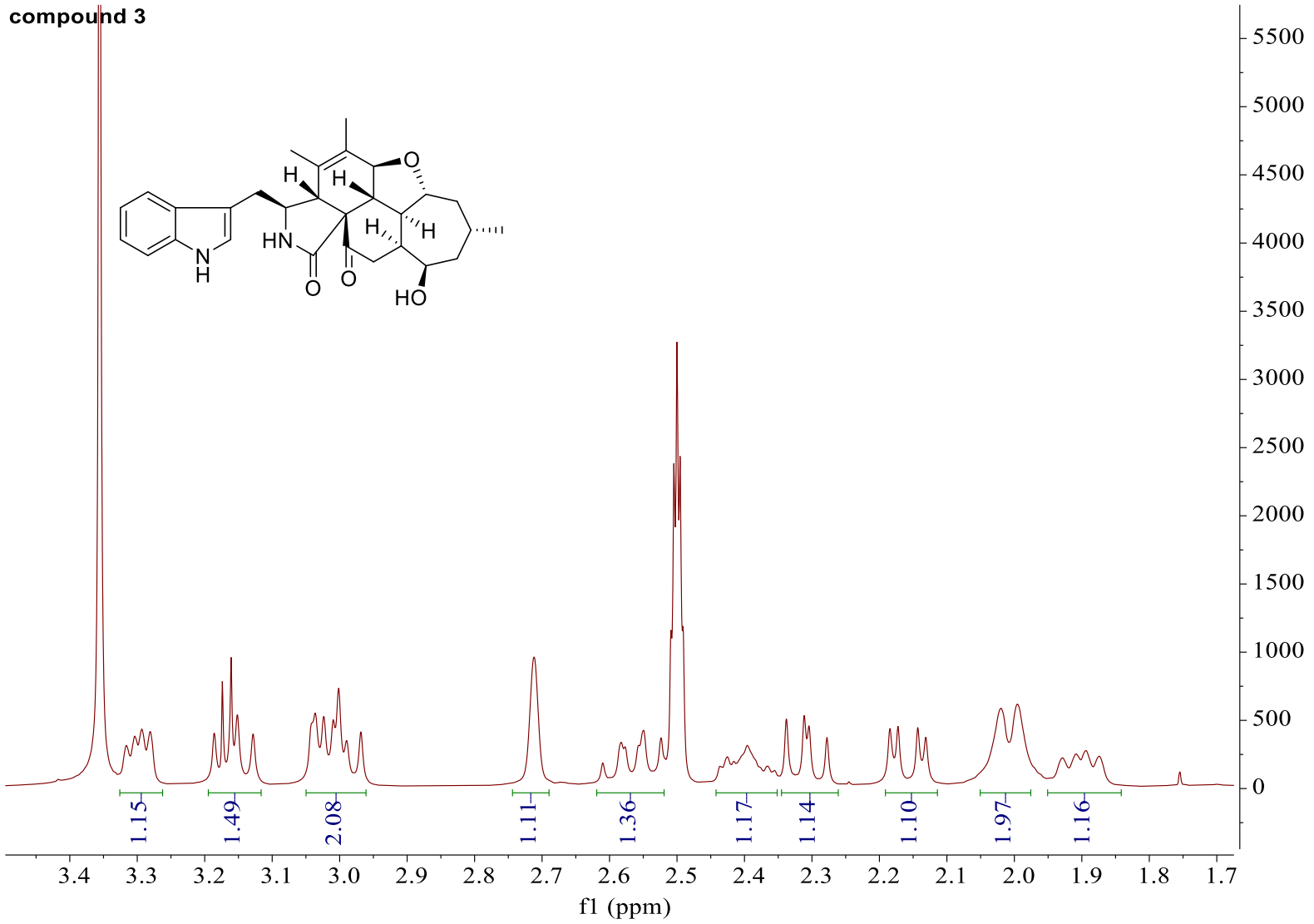

H
H
O
H
H
HN
N
H
O
O
HO

5500
5000
4500
4000
3500
3000
2500
2000
1500
1000
500
0
1.02
1.00
1.05
0.98
1.10
1.07
8.4
8.3
8.2
8.1
8.0
7.9
7.8
7.7
7.6
7.5
7.4
7.3
7.2
7.1
7.0
6.9
6.8
6.7
f1 (ppm)

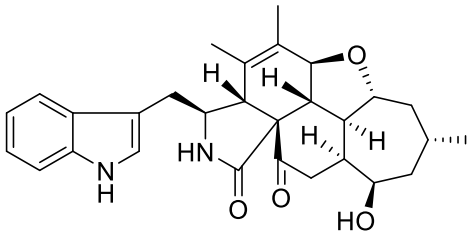
compound 3


H
H
O
H
H
HN
N
H
O
O
HO

5500
5000
4500
4000
3500
3000
2500
2000
1500
1000
500
0
-500
1.00
1.08
2.11
1.15
1.49
4.8
4.7
4.6
4.5
4.4
4.3
4.2
4.1
4.0
3.9
3.8
3.7
3.6
3.5
3.4
3.3
3.2
3.1
f1 (ppm)


compound 3
5500
5000
4500
4000
3500
3000
2500
2000
1500
1000
500
0
1.15
1.49
2.08
1.11
1.36
1.17
1.14
1.10
1.97
1.16
3.4
3.3
3.2
3.1
3.0
2.9
2.8
2.7
2.6
2.5
2.4
2.3
2.2
2.1
2.0
1.9
1.8
1.7
f1 (ppm)

compound 3


H
H
O
H
H
HN
N
H
O
O
HO

5500
5000
4500
4000
3500
3000
2500
2000
1500
1000
500
0
-500
1.17
1.14
1.10
1.97
1.16
3.06
2.24
3.22
3.16
2.4
2.3
2.2
2.1
2.0
1.9
1.8
1.7
1.6
1.5
1.4
1.3
1.2
1.1
1.0
0.9
0.8
0.7
f1 (ppm)

Fig. S30. ^{13}C NMR (100 MHz, DMSO-d_6) spectrum of **3**.

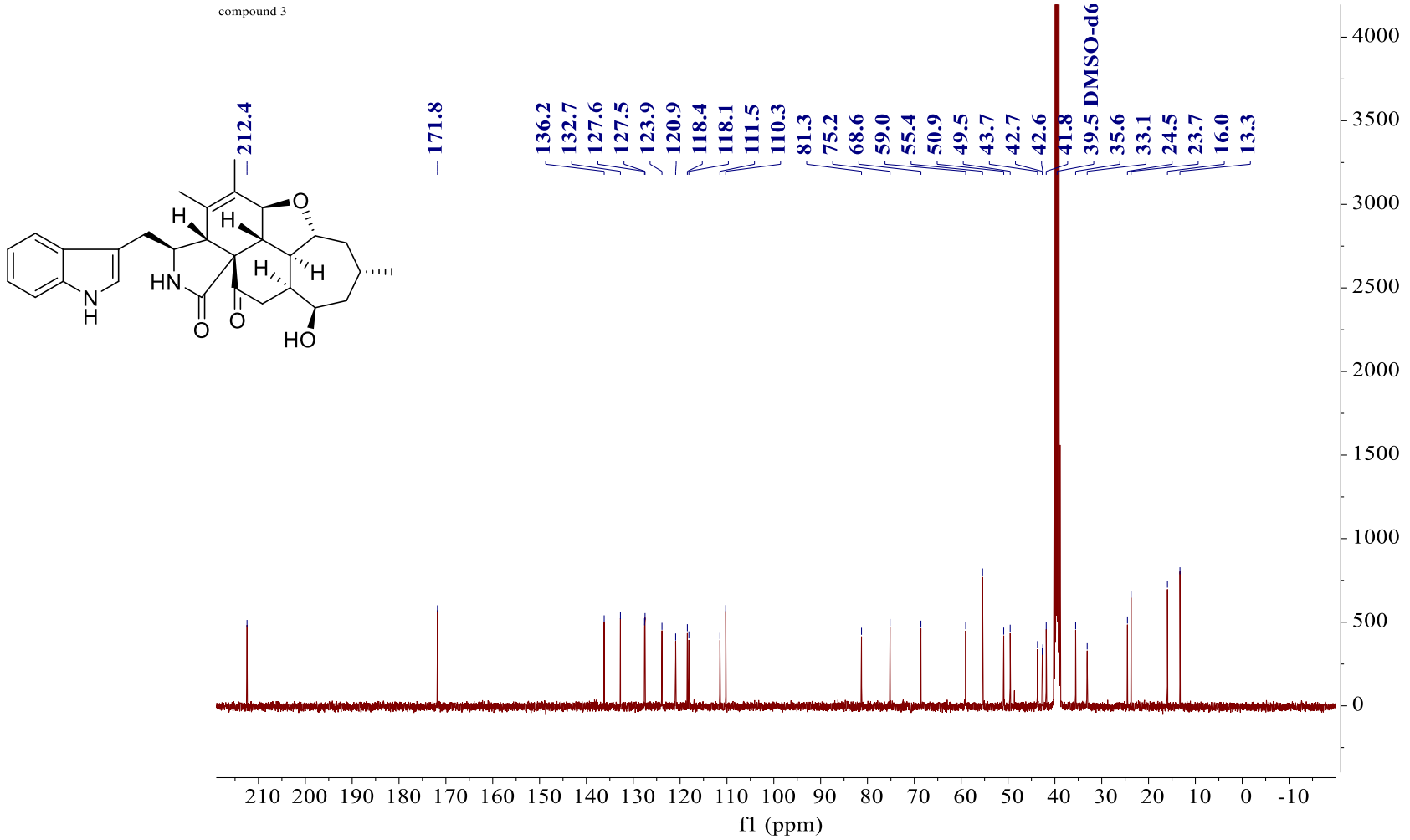


Fig. S31. DEPT-135 (100 MHz, DMSO-d_6) spectrum of **3**.

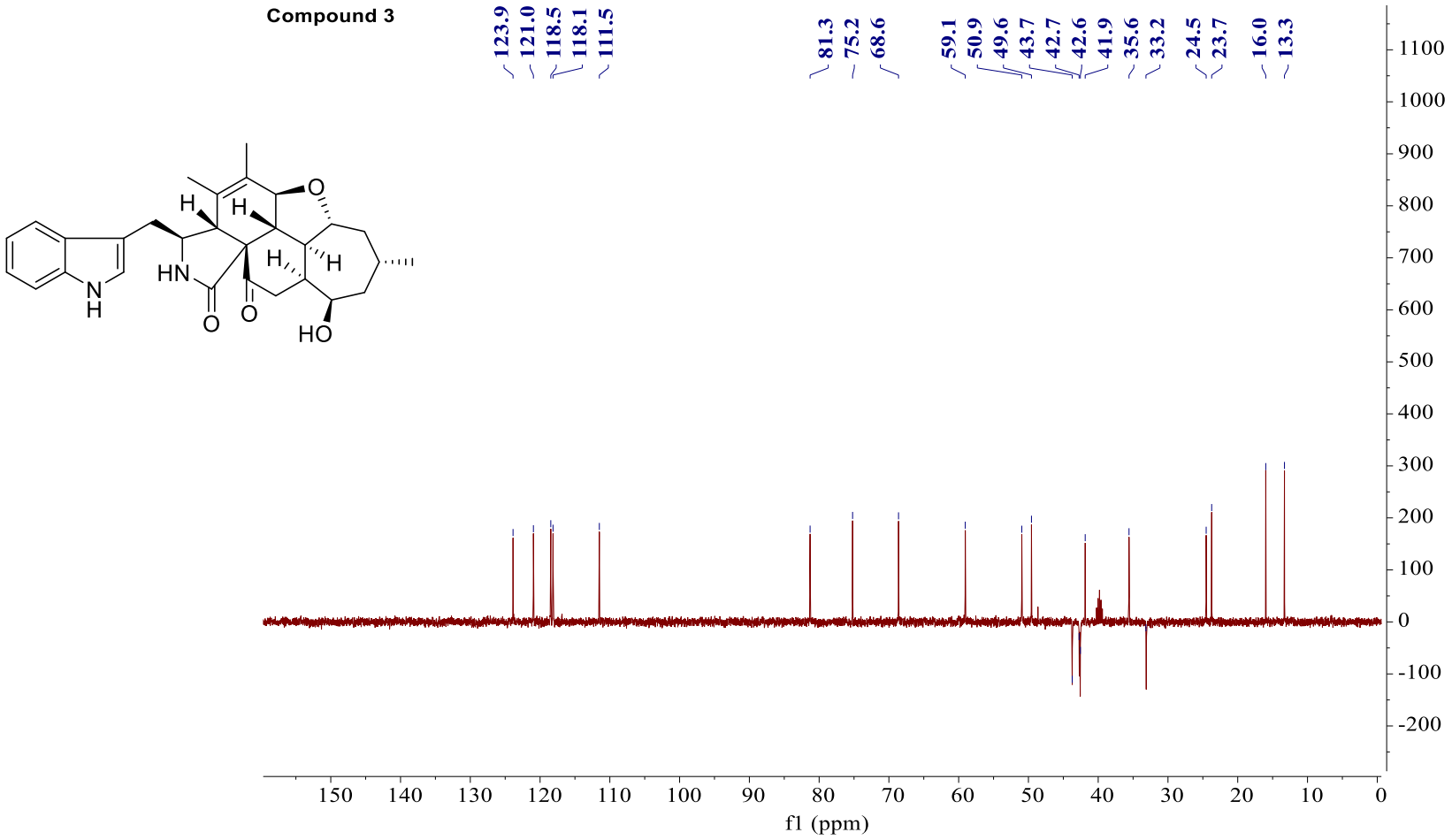


Fig. S32. HSQC spectrum of **3** in DMSO-d_6.

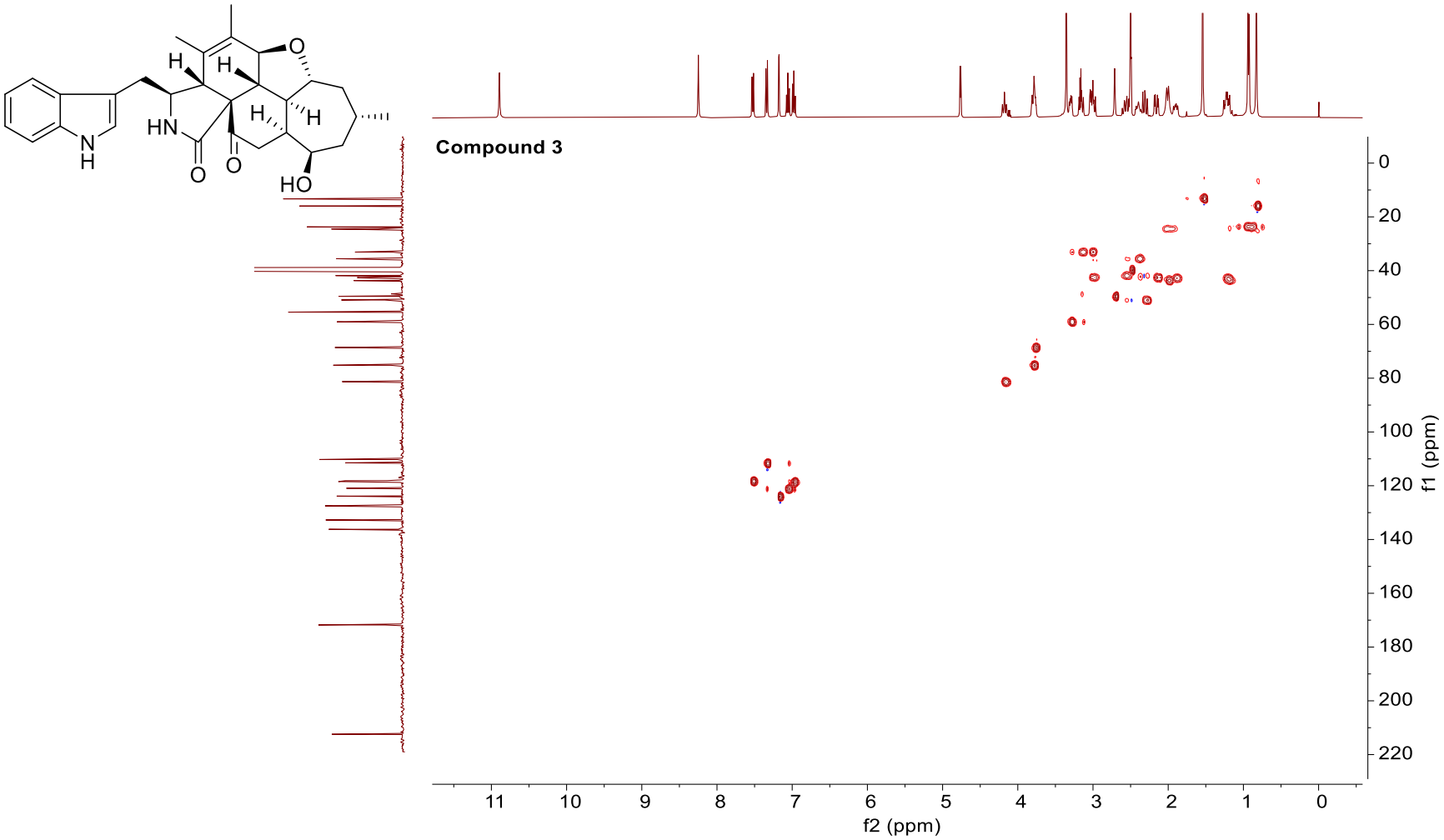


Fig. S33. HMBC spectrum of **3** in DMSO-d_6.

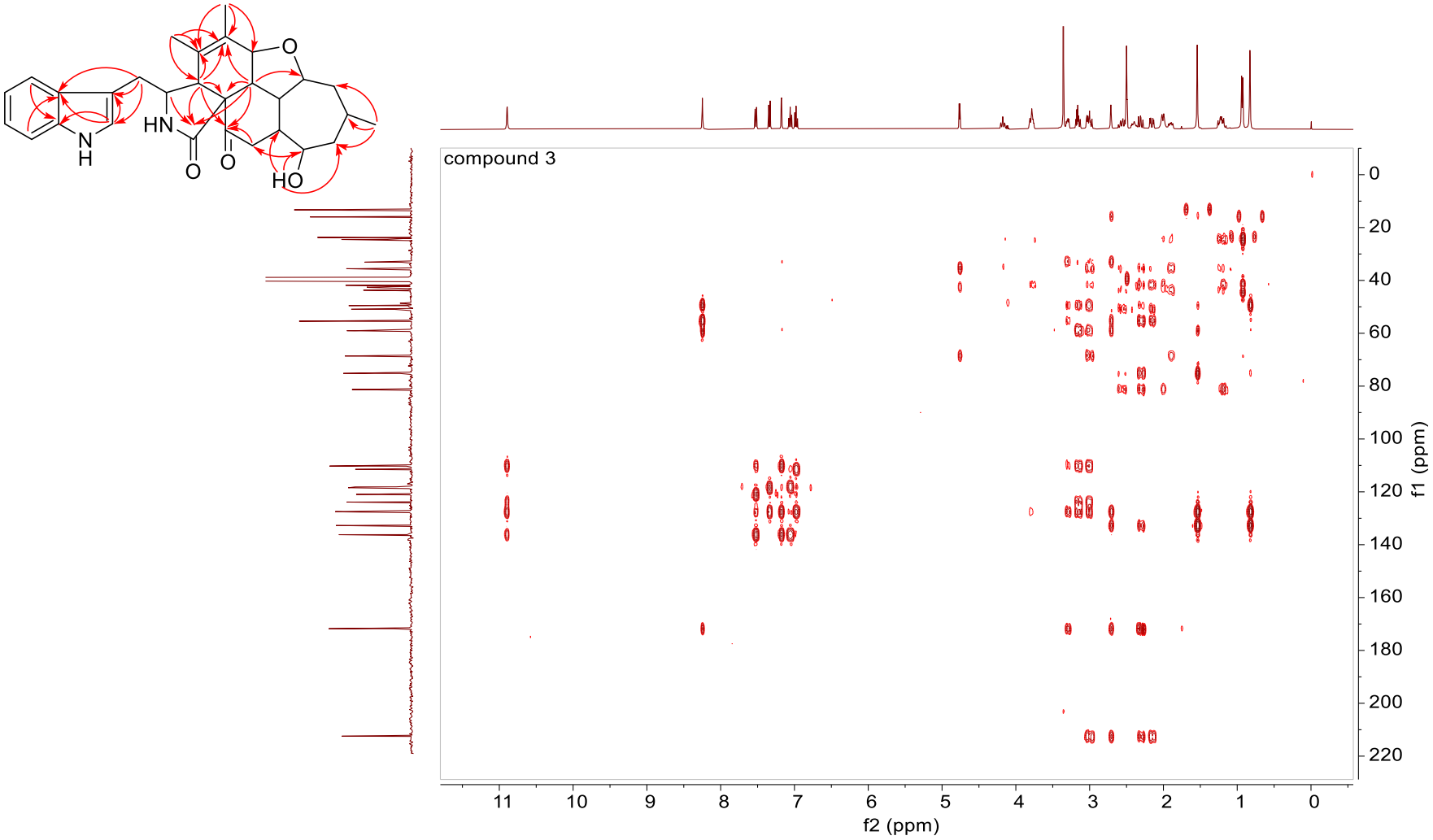


Fig. S34. ^{1}H–^{1}H COSY spectrum of **3** in DMSO-d_6.

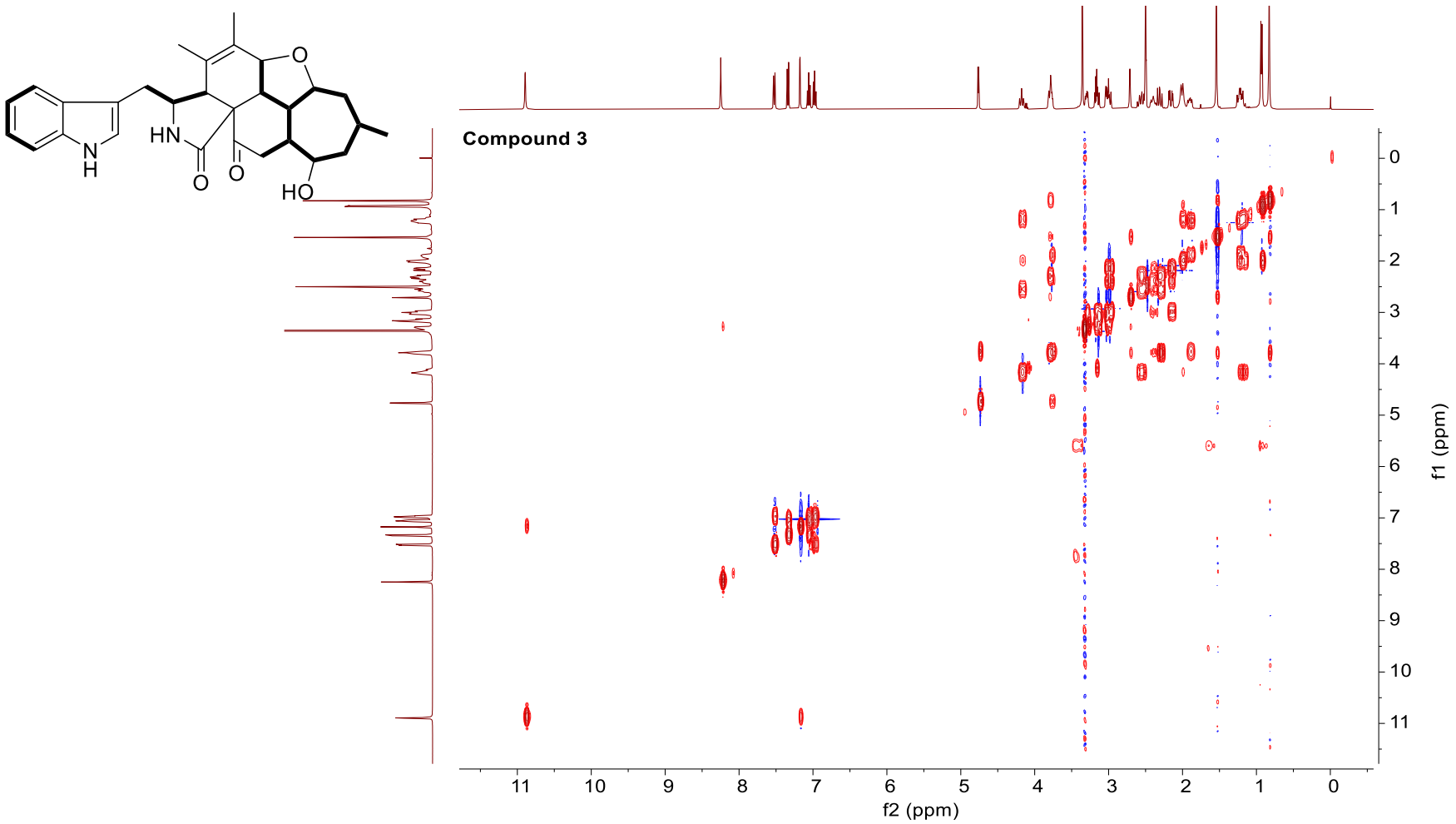


Fig. S35. NOESY spectrum of **3** in DMSO-d_6.

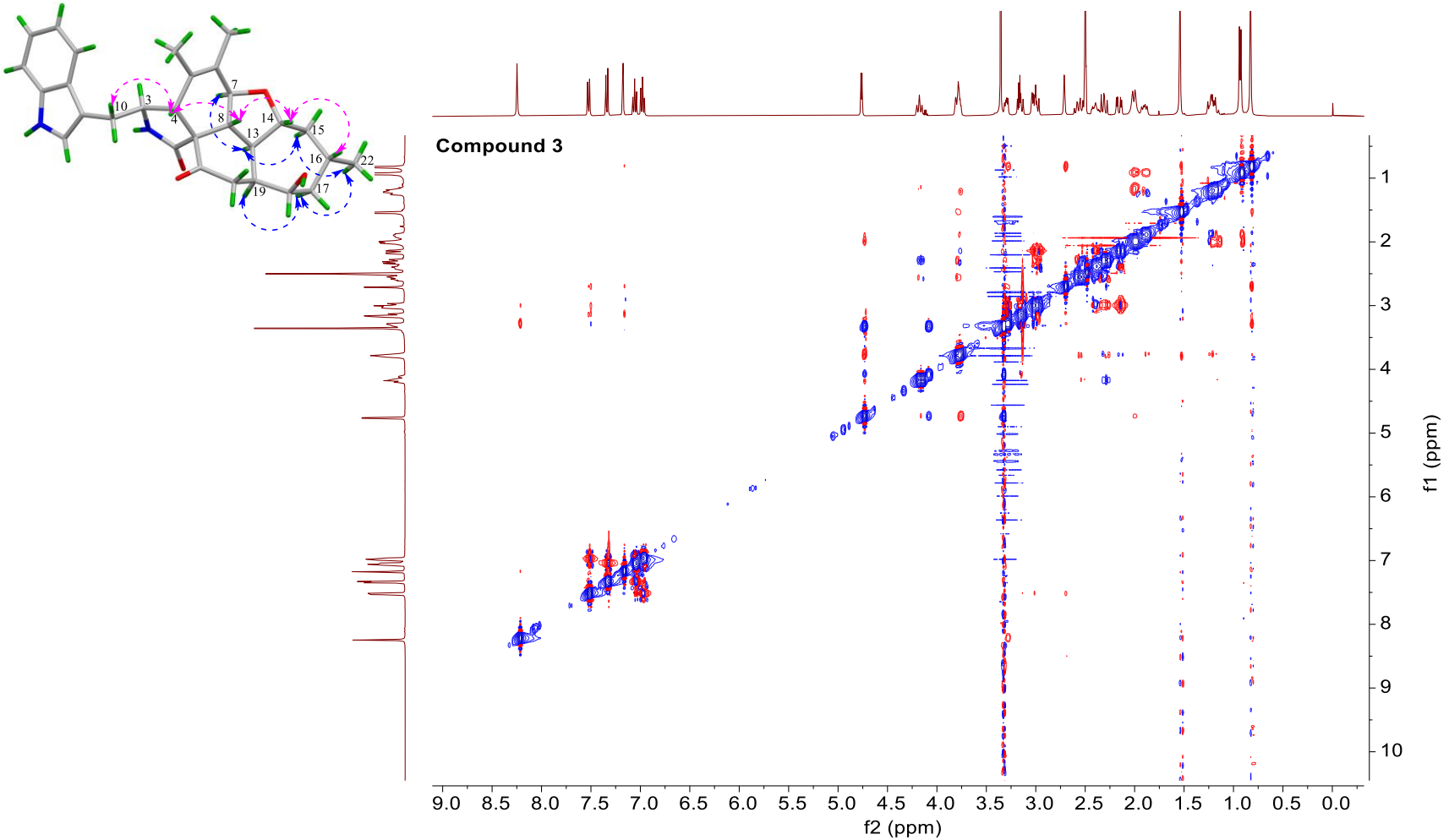


Fig. S36. ^{1}H NMR (400 MHz, CD_3OD) spectrum of **3**.

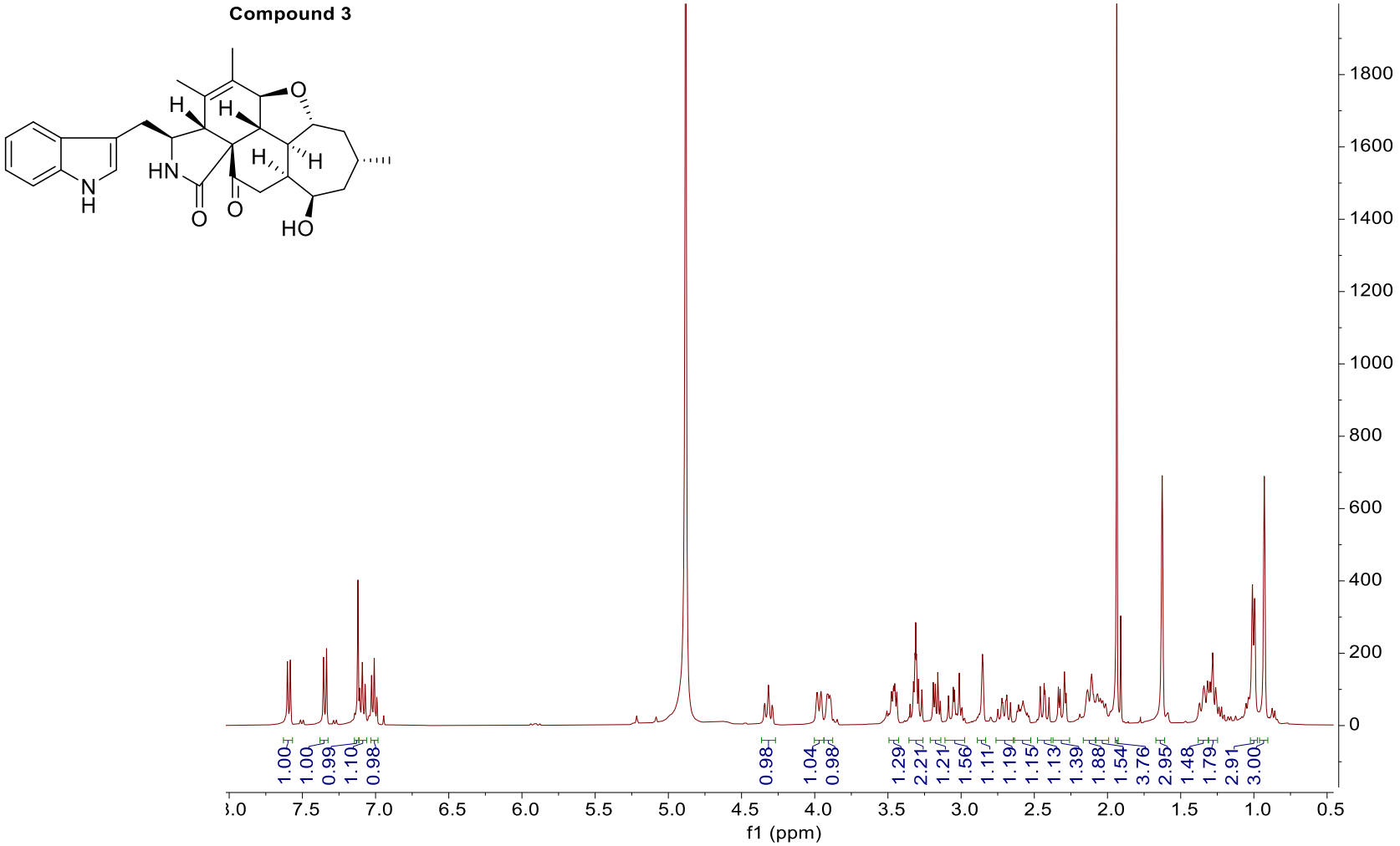


Fig. S37. ^{13}C NMR (100 MHz, CD_3OD) spectrum of **3**.

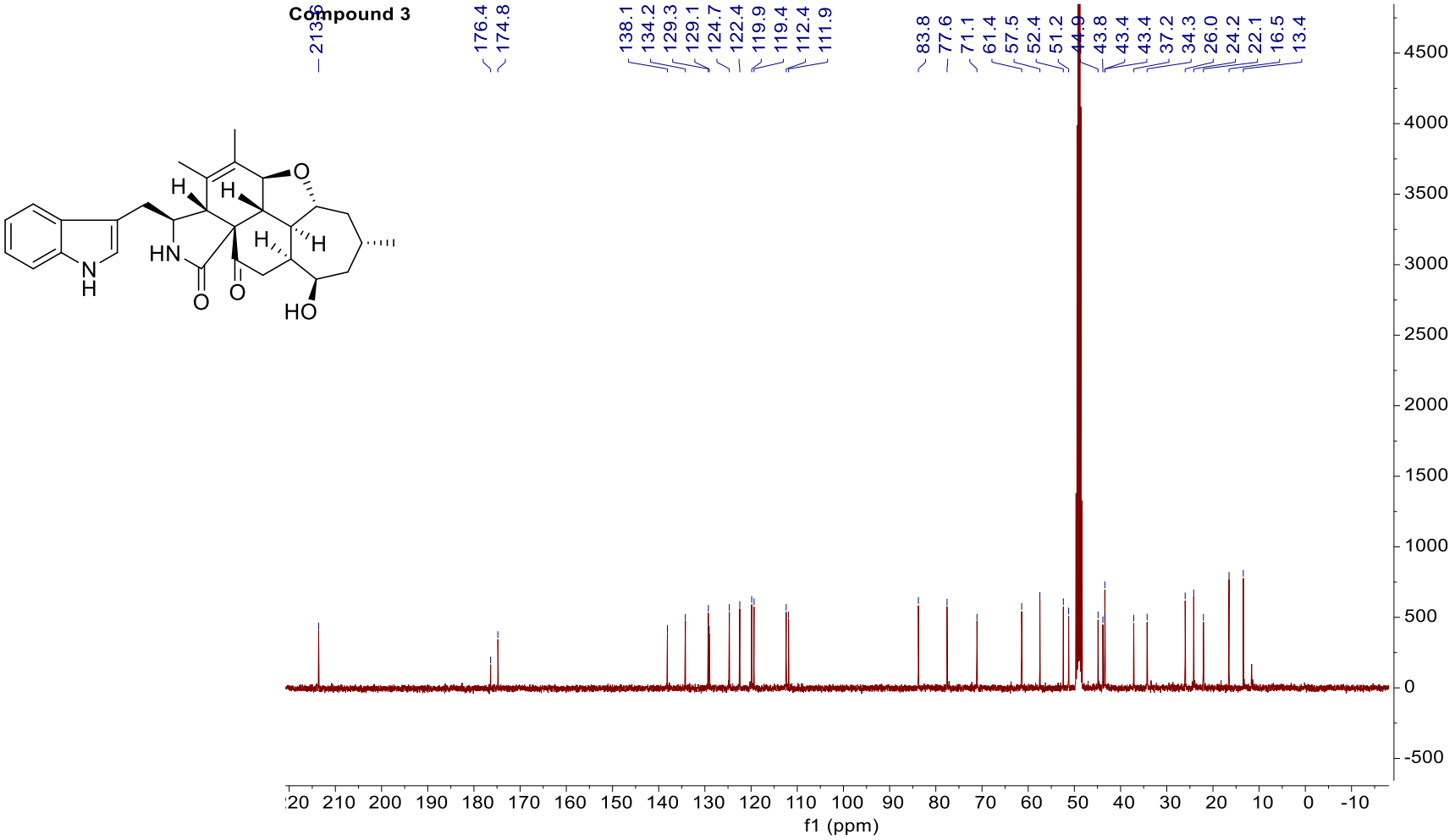


Fig. S38. DEPT-135 (100 MHz, CD_3OD) spectrum of **3**.

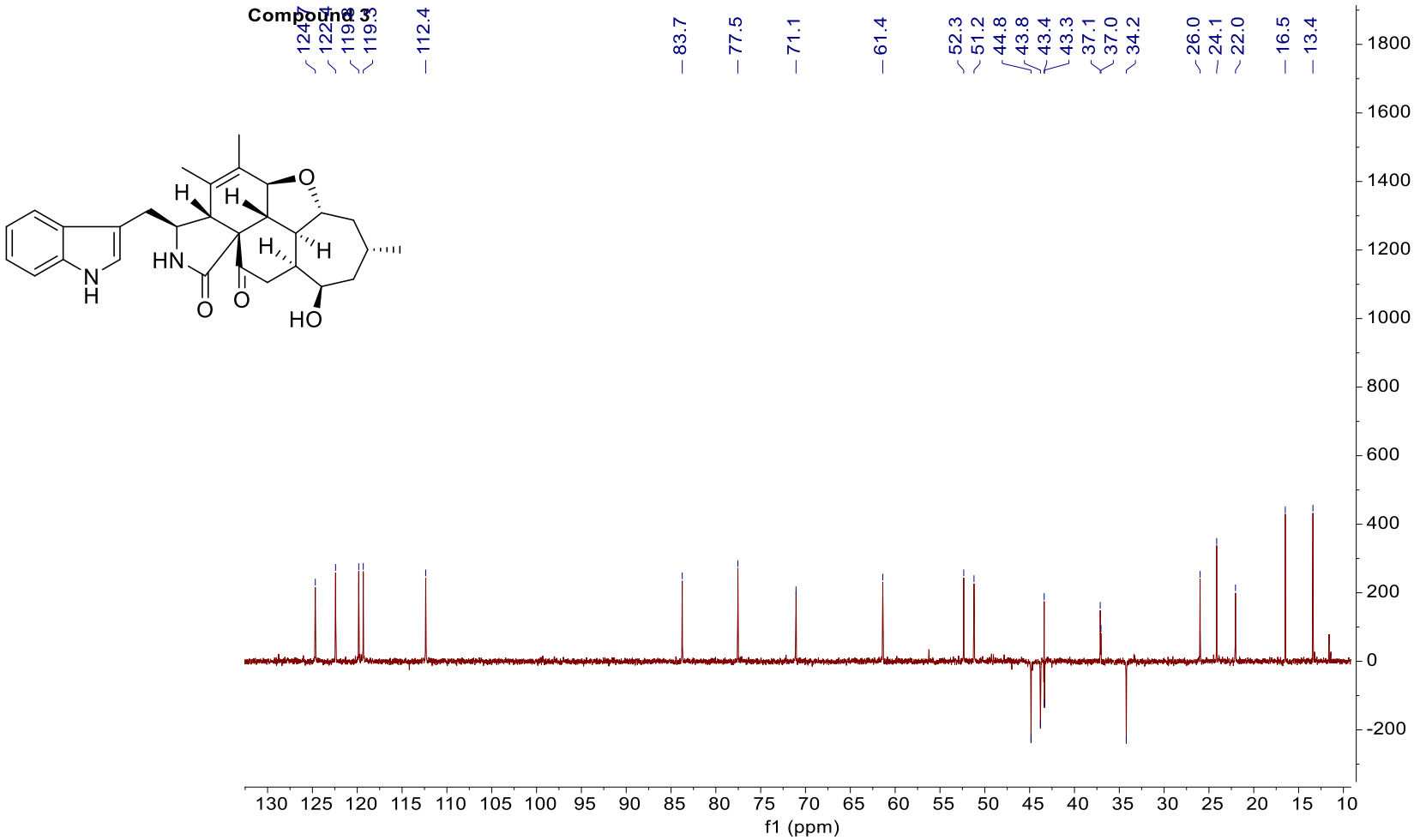


Fig. S39. HSQC spectrum of **3** in CD_3OD.

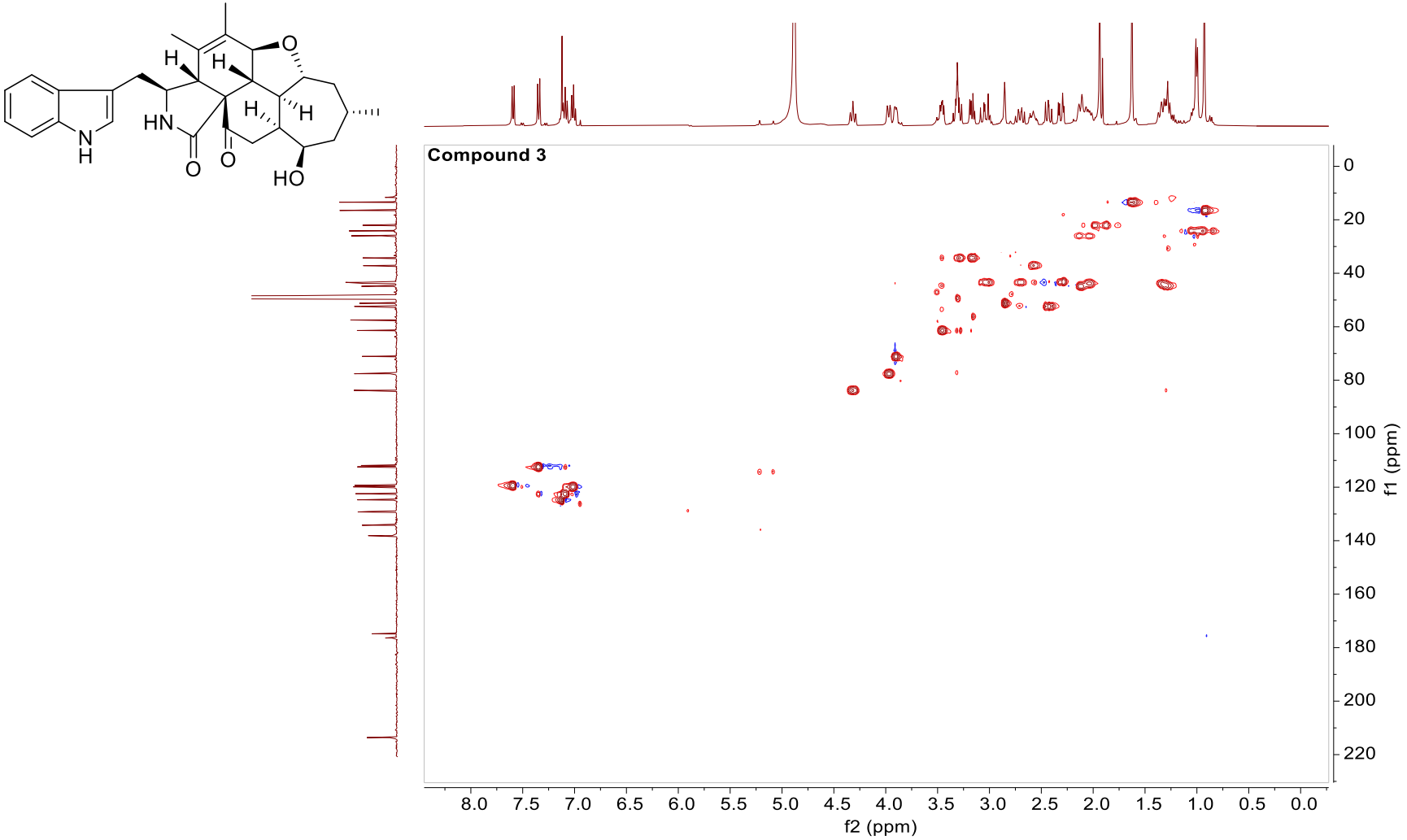


Fig. S40. HMBC spectrum of **3** in CD_3OD.

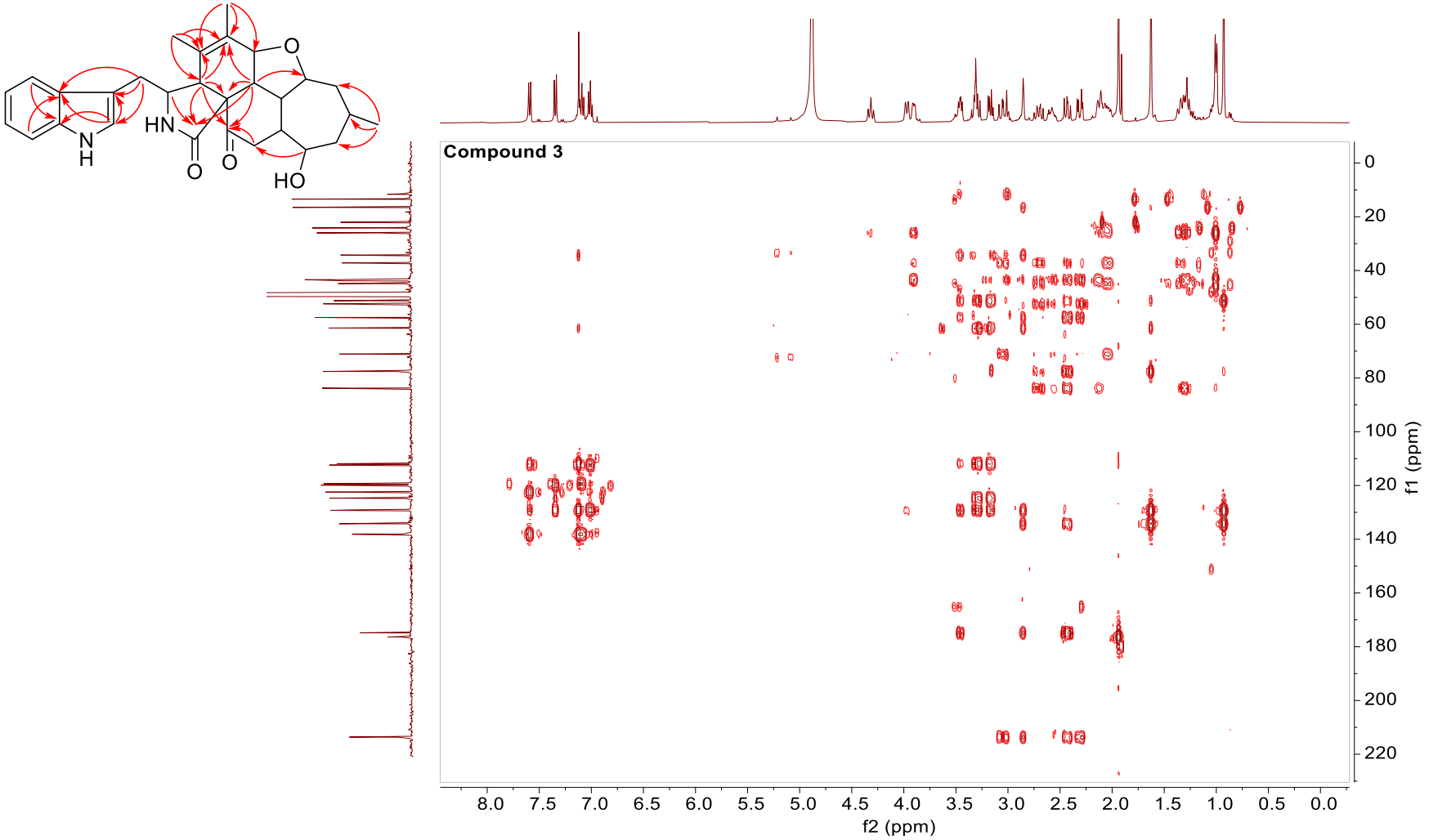


Fig. S41. ^{1}H–^{1}H COSY spectrum of **3** in CD_3OD.

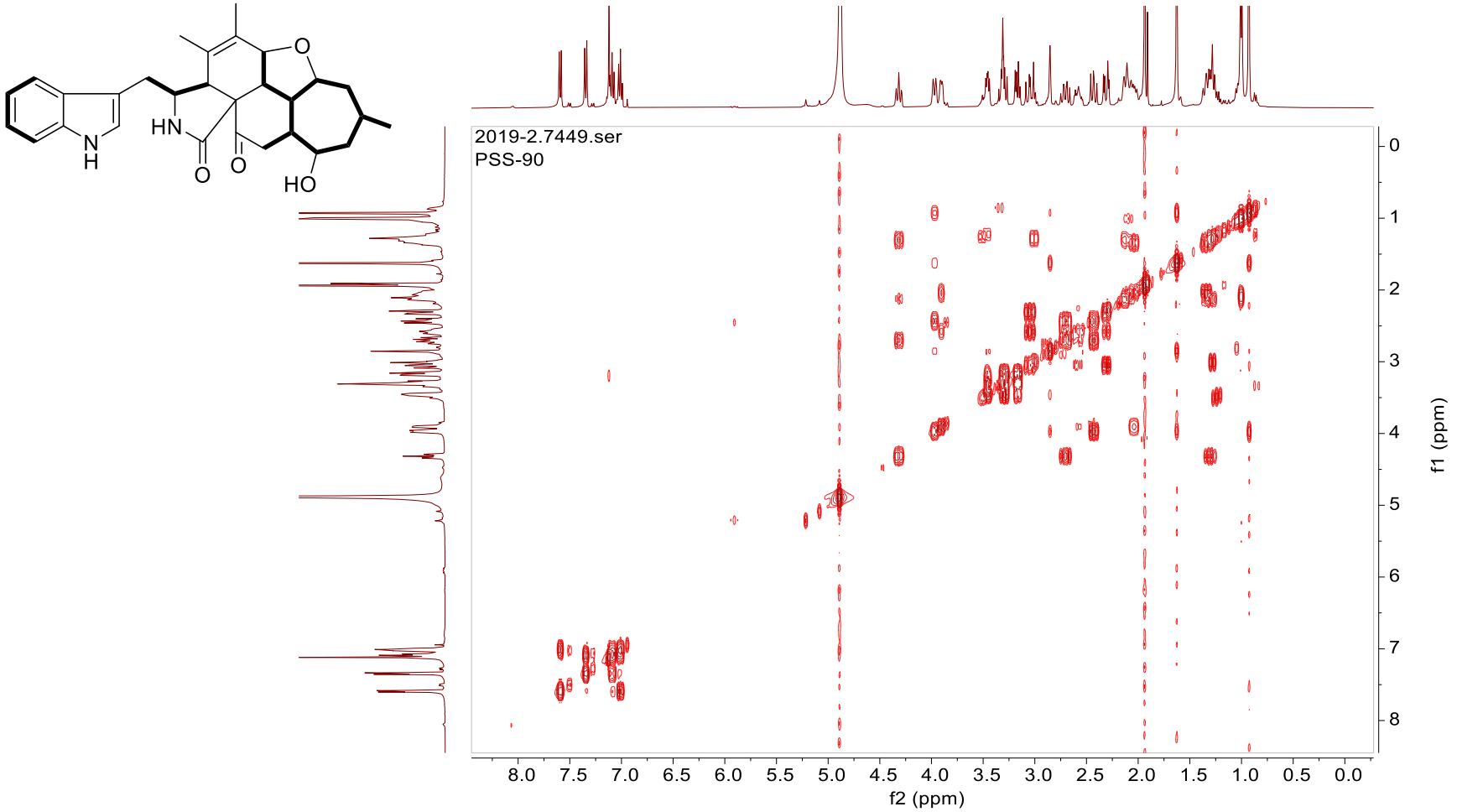


Fig. S42. NOESY spectrum of **3** in CD_3OD.

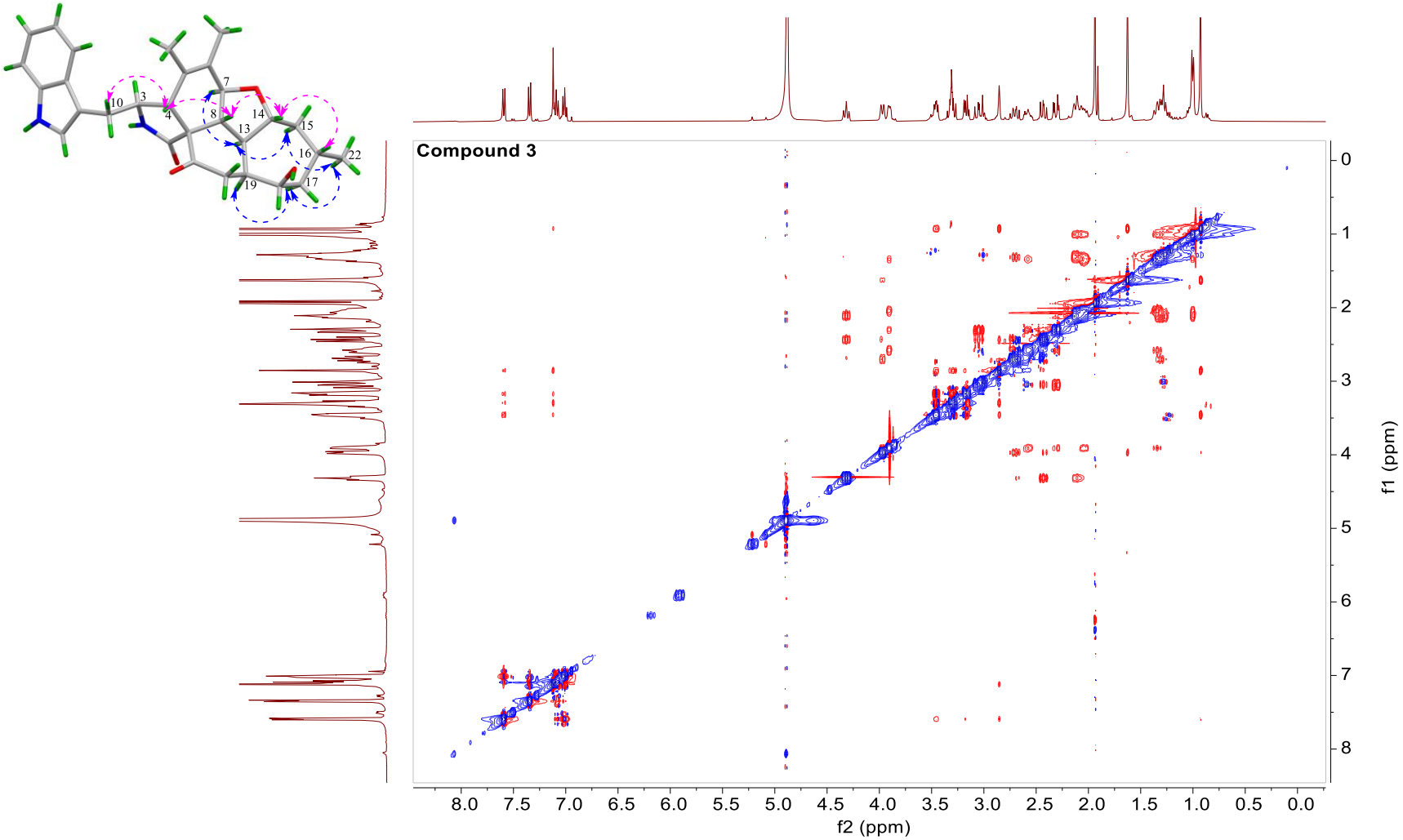


Fig. S43. HRESIMS (+) spectrum of **3**.

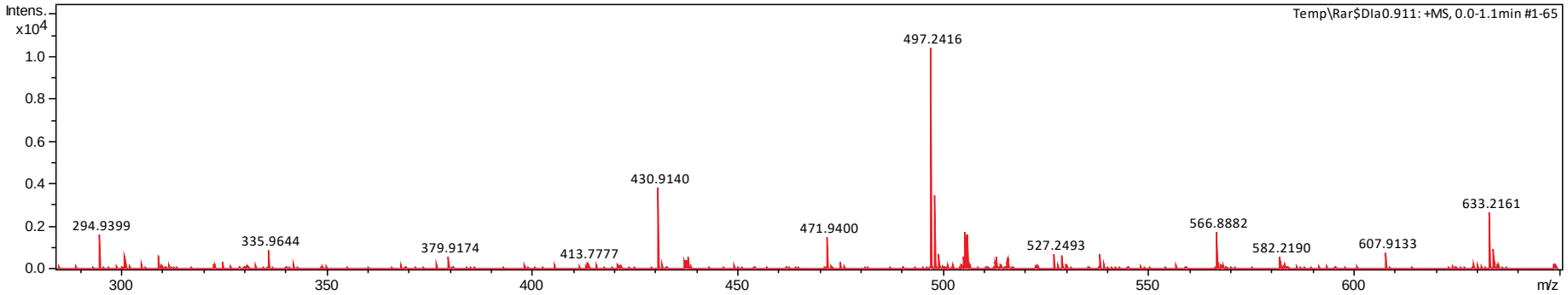


Fig. S44. UV spectrum of **3**.

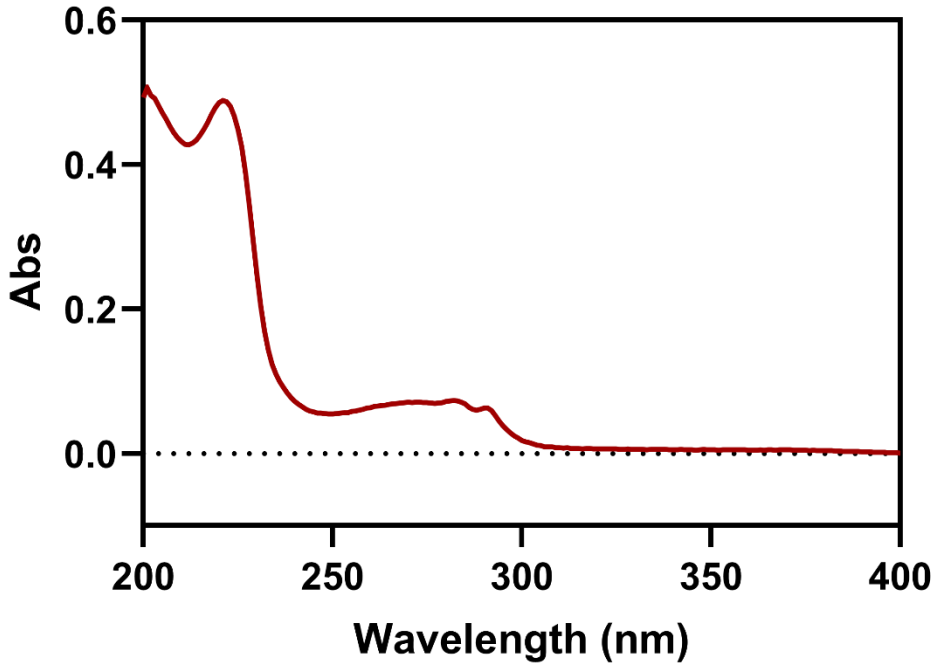


Fig. S45. IR spectrum of **3**.

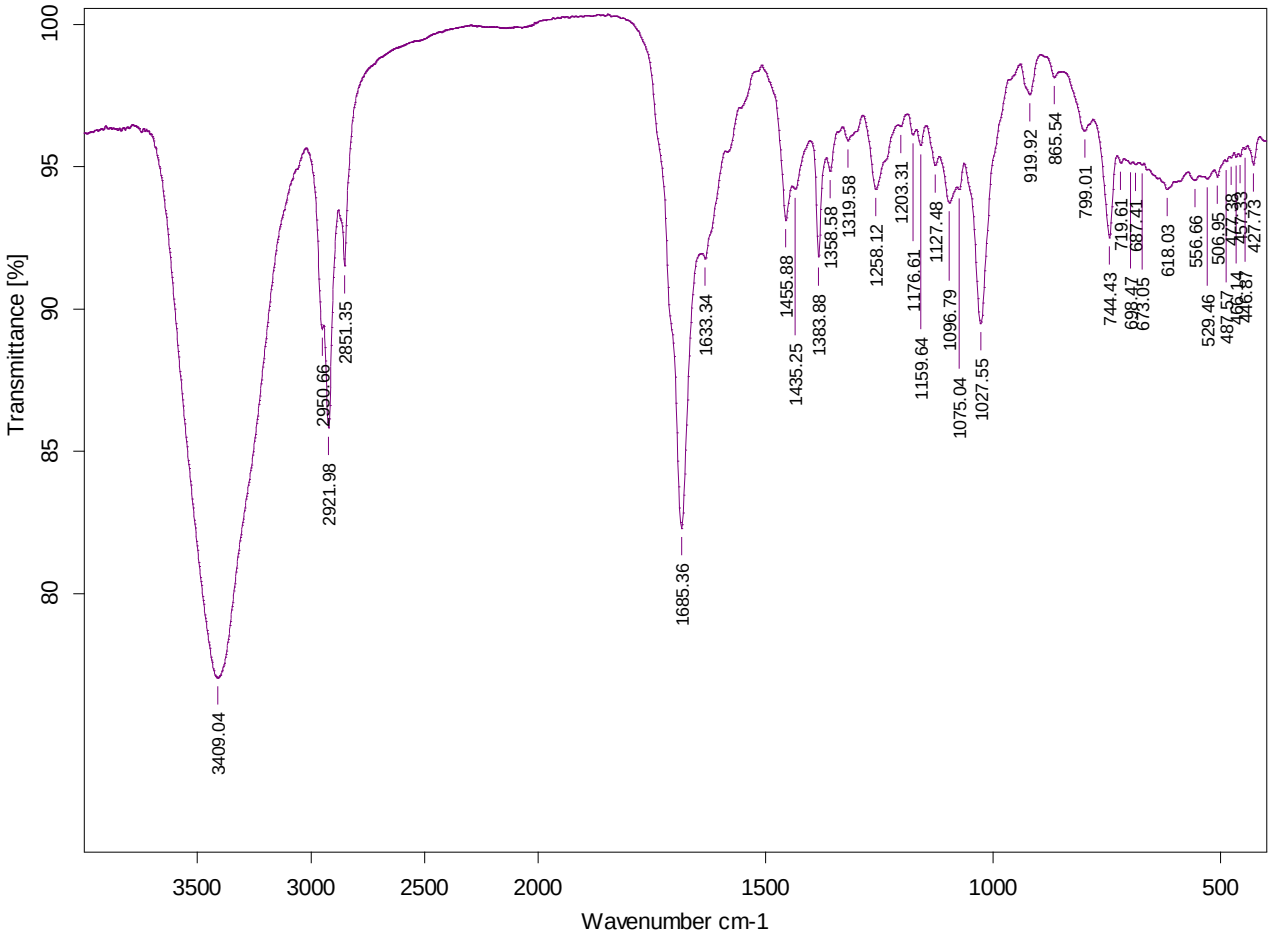


Fig. S46. ECD spectrum of **3**.

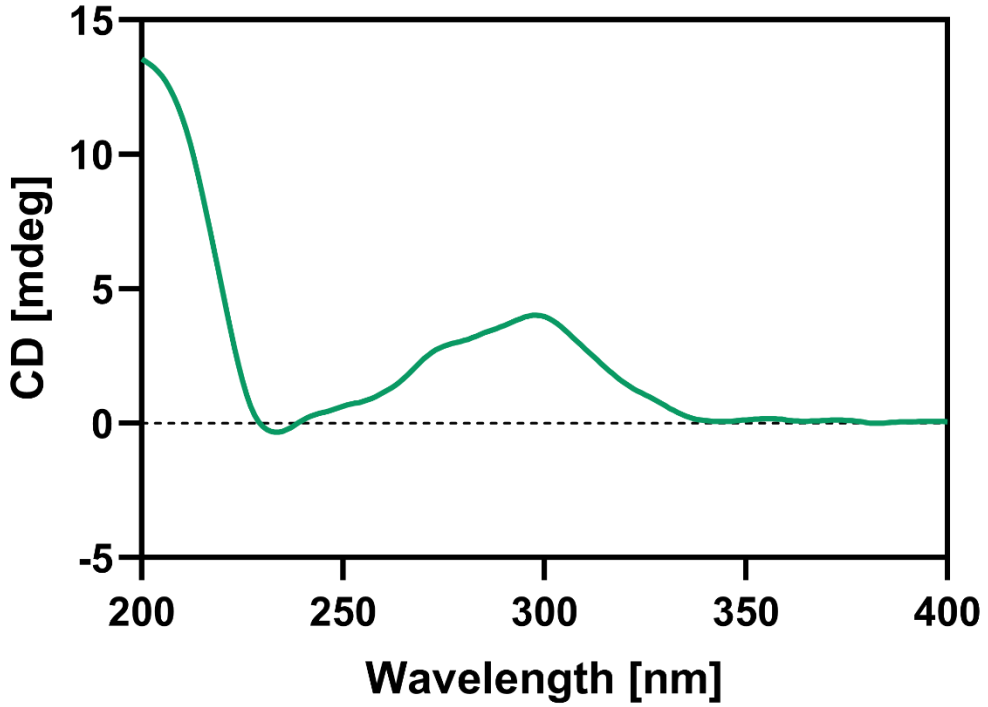


Fig. S47. ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **4**.

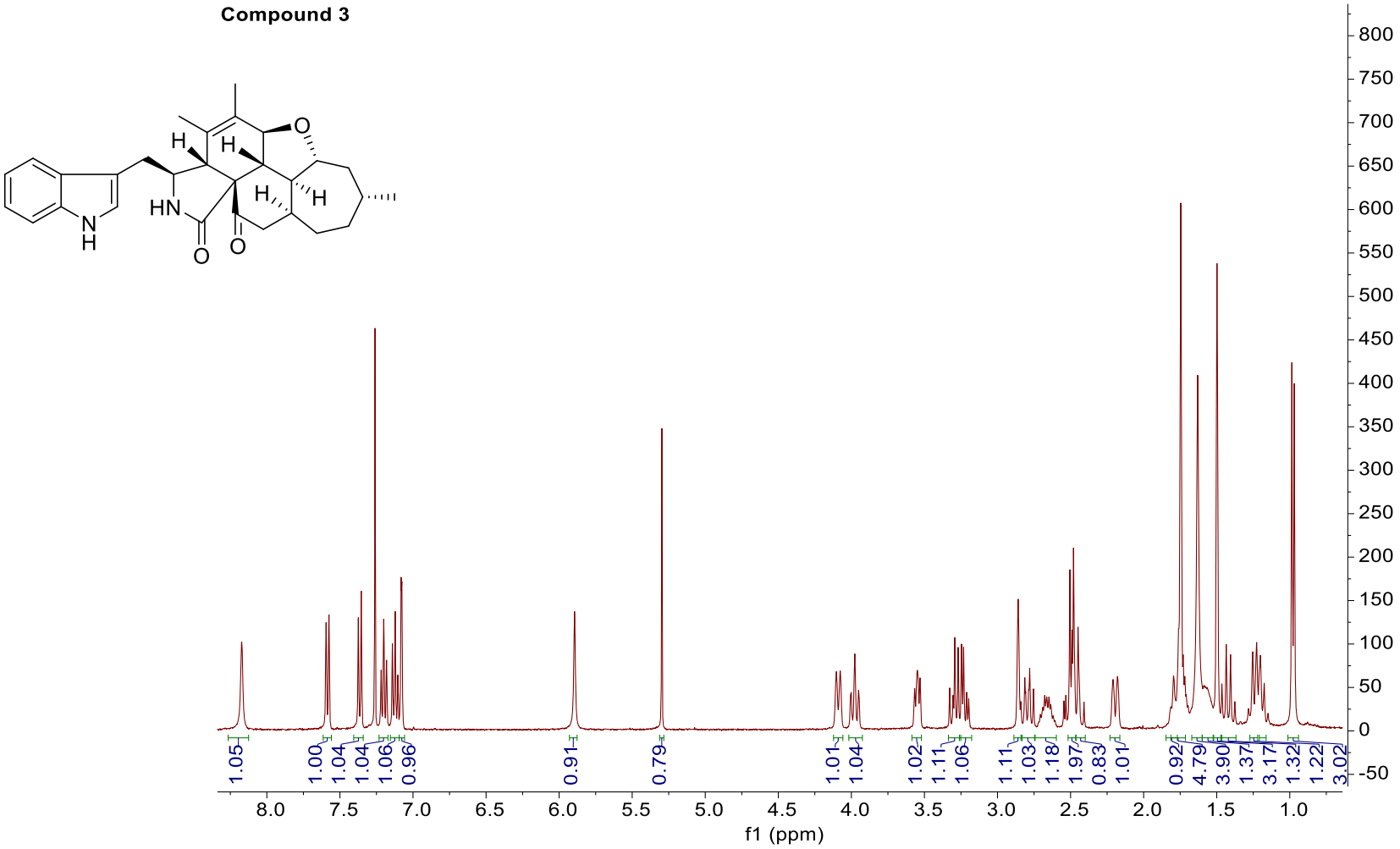
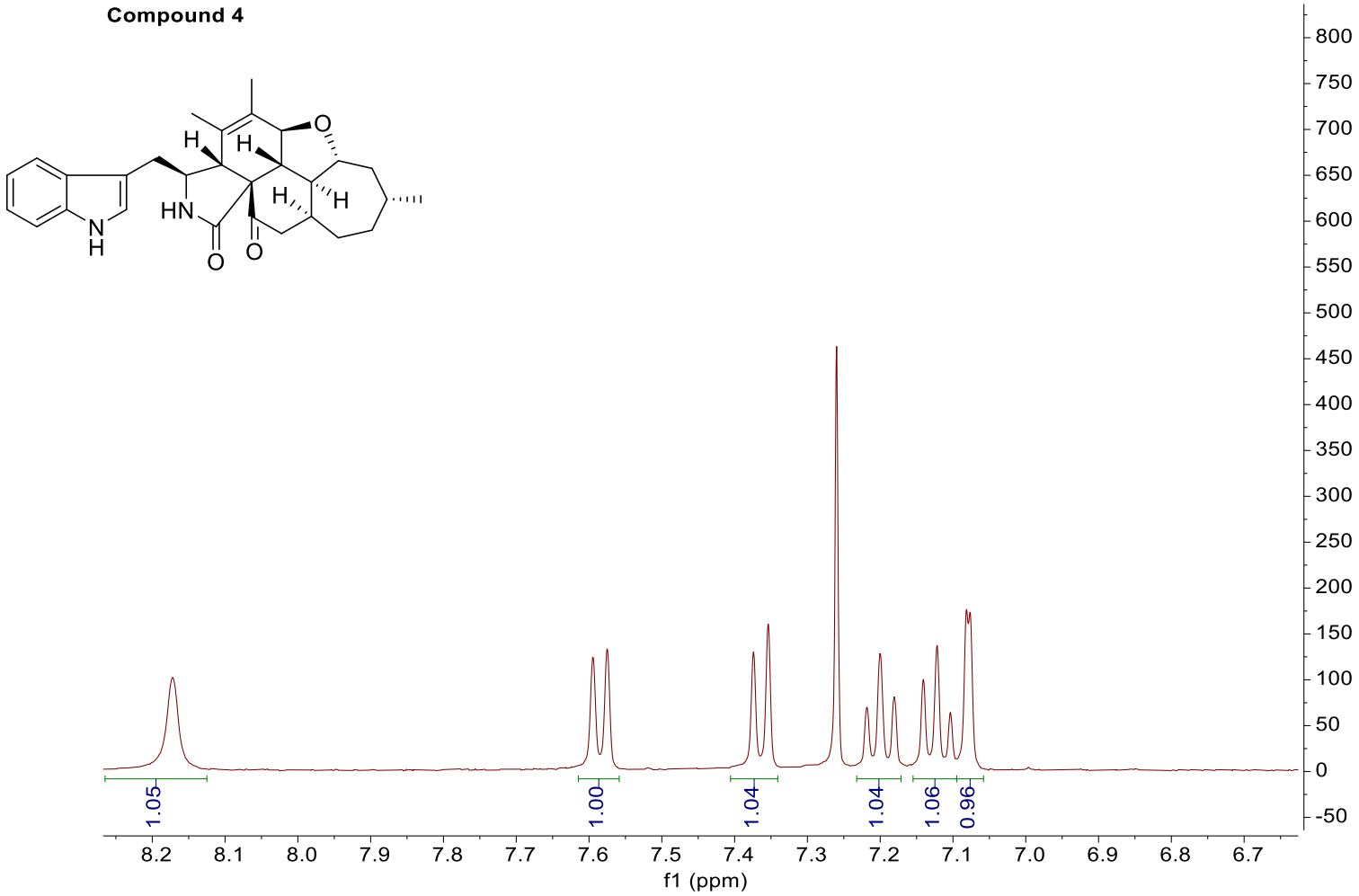
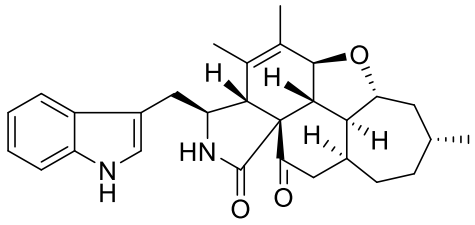


Fig. S48. Enlarged ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **4**.

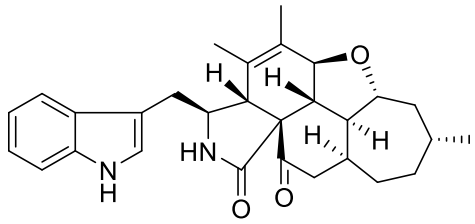


Compound 4


H
H
O
HN
H
H
N
H
O
O

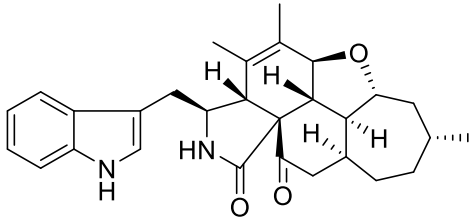
800
750
700
650
600
550
500
450
400
350
300
250
200
150
100
50
0
-50
1.04
1.04
1.06
0.96
0.91
7.4
7.3
7.2
7.1
7.0
6.9
6.8
6.7
6.6
6.5
6.4
6.3
6.2
6.1
6.0
5.9
5.8
f1 (ppm)

Compound 4


H
H
O
H
H
HN
N
H
O
O

800
750
700
650
600
550
500
450
400
350
300
250
200
150
100
50
0
-50
1.01
1.04
1.02
1.11
1.06
1.11
1.03
1.18
4.2
4.1
4.0
3.9
3.8
3.7
3.6
3.5
3.4
3.3
3.2
3.1
3.0
2.9
2.8
2.7
2.6
f1 (ppm)

Compound 4


H
H
O
H
H
HN
N
H
O
O

900
800
700
600
500
400
300
200
100
0
1.97
0.83
1.01
0.92
4.79
3.90
1.37
3.17
1.32
1.22
0.84
3.02
2.5
2.4
2.3
2.2
2.1
2.0
1.9
1.8
1.7
1.6
1.5
1.4
1.3
1.2
1.1
1.0
f1 (ppm)

Fig. S49. ^{13}C NMR (100 MHz, $CDCl_3$) spectrum of **4**.

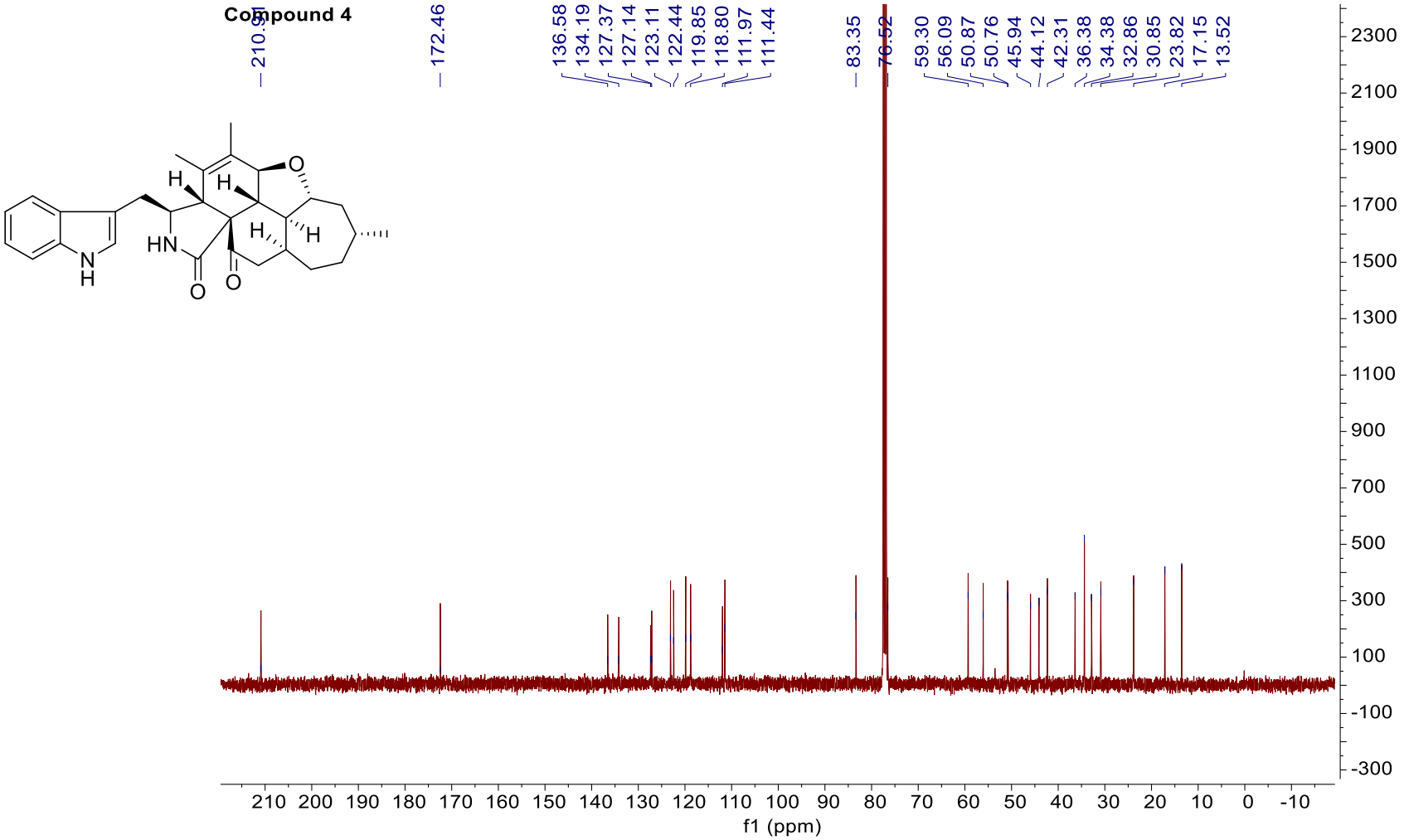


Fig. S50. DEPT-135 (100 MHz, $CDCl_3$) spectrum of **4**.

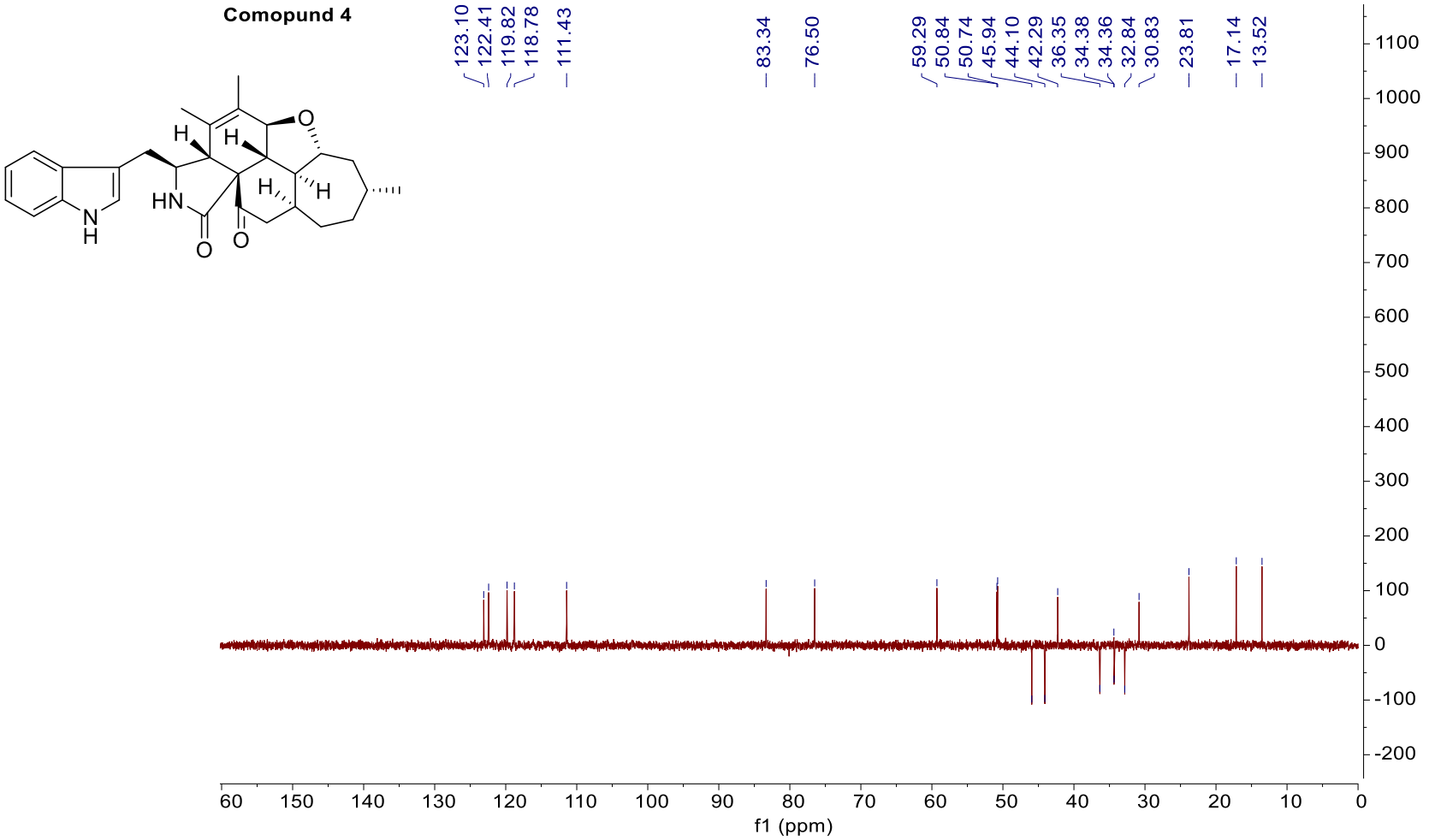


Fig. S51. HSQC spectrum of **4** in $CDCl_3$.

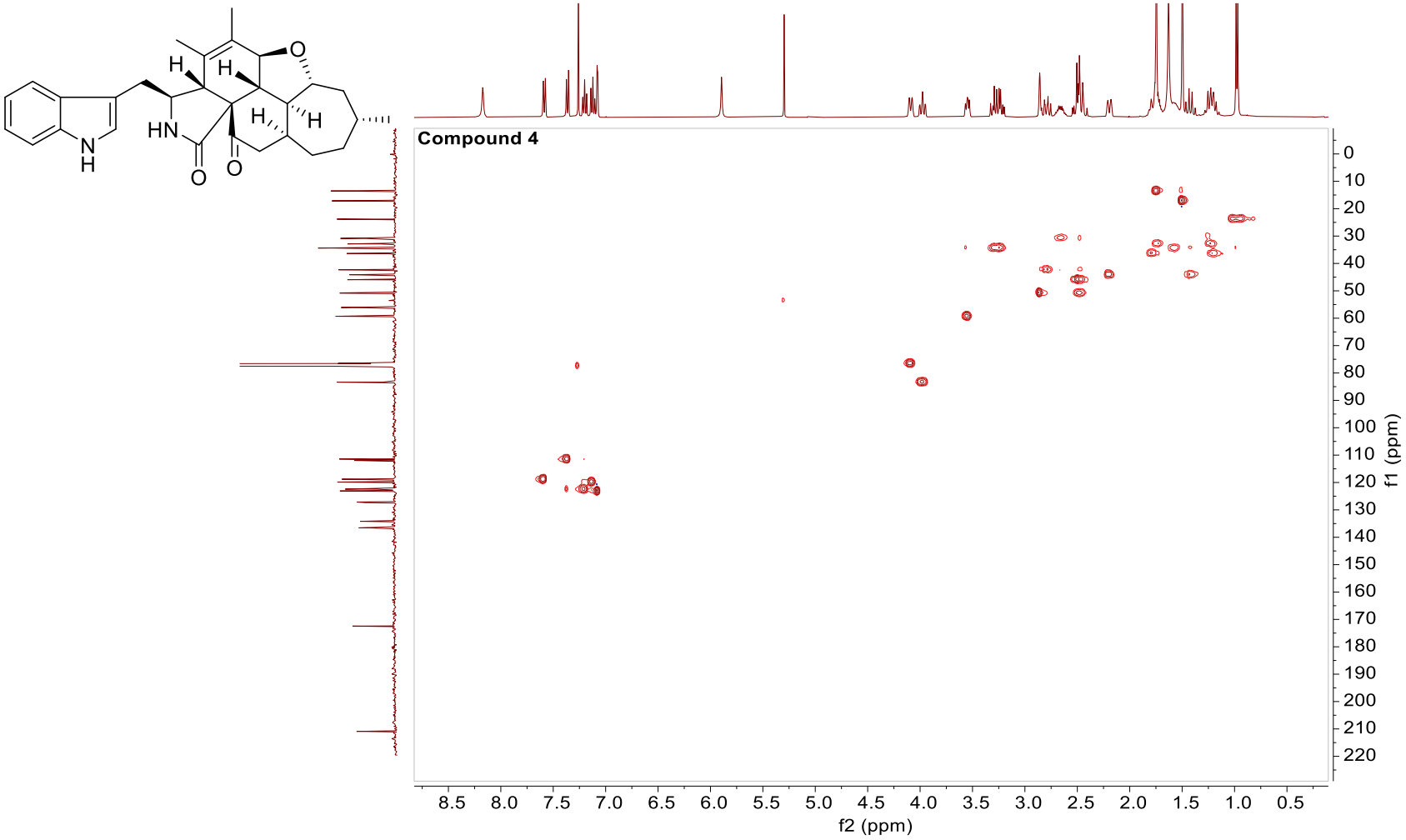


Fig. S52. HMBC spectrum of **4** in $CDCl_3$.

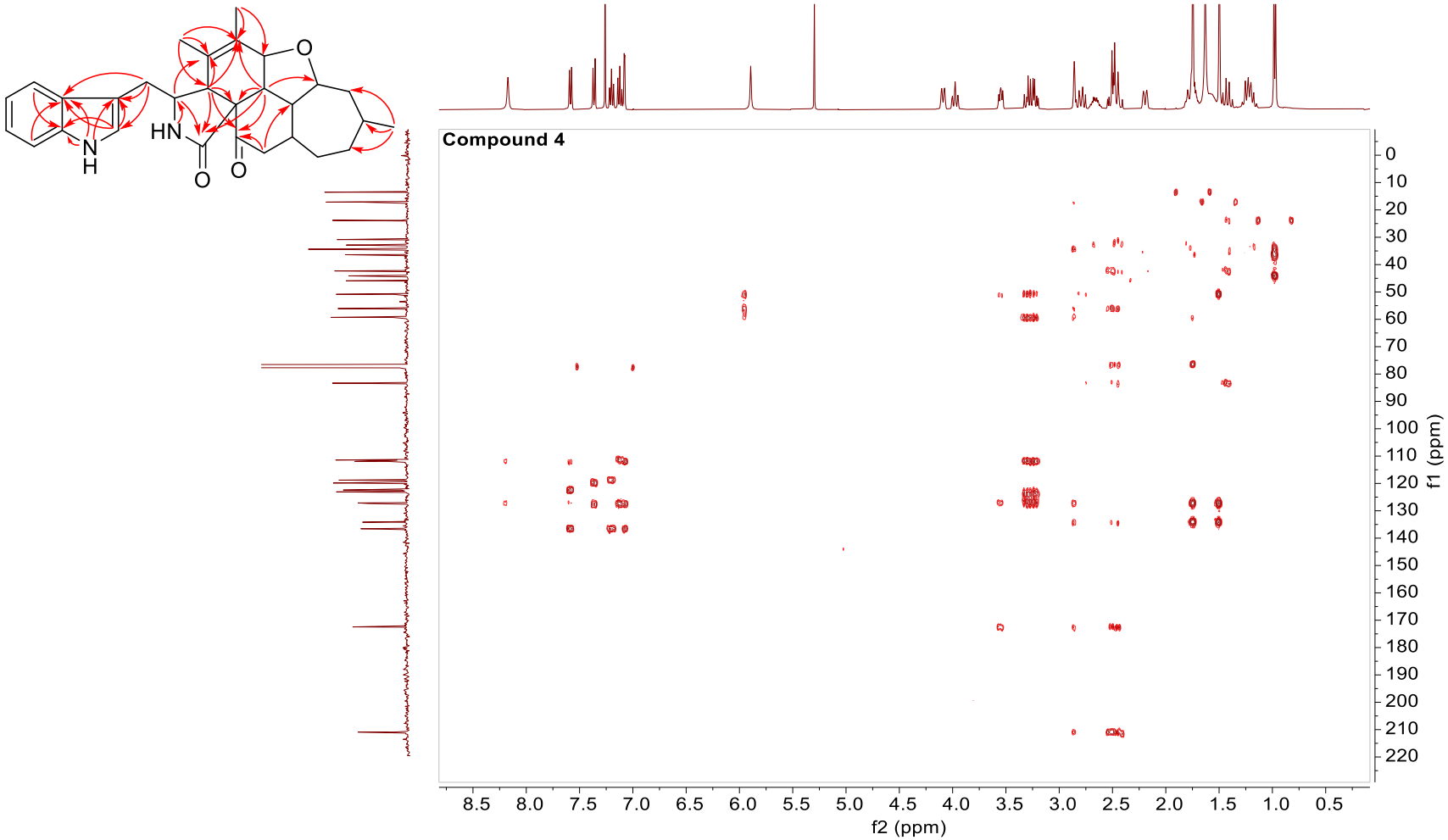


Fig. S53. ^{1}H–^{1}H COSY spectrum of **4** in $CDCl_3$.

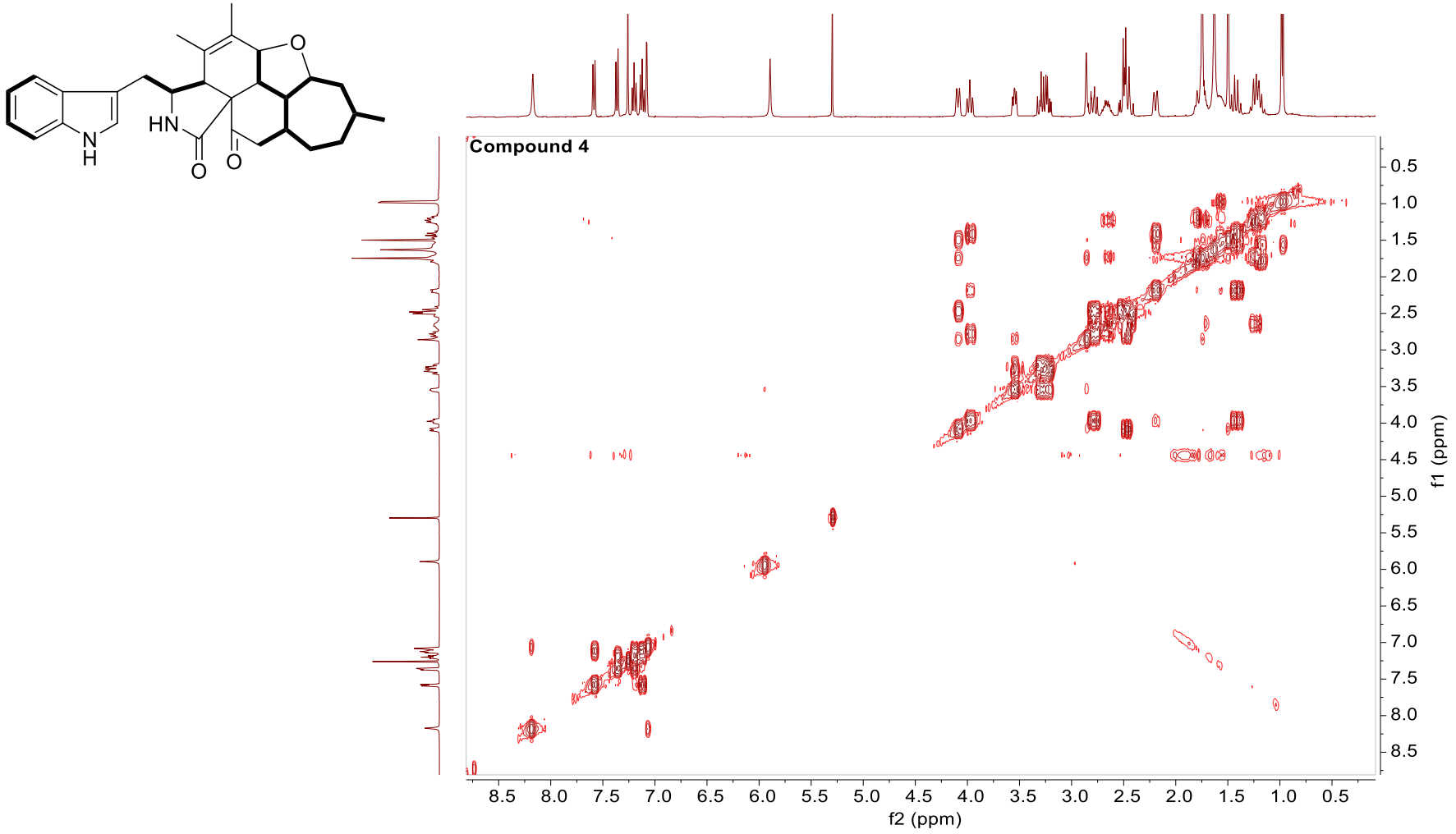


Fig. S54. NOESY spectrum of **4** in $CDCl_3$.

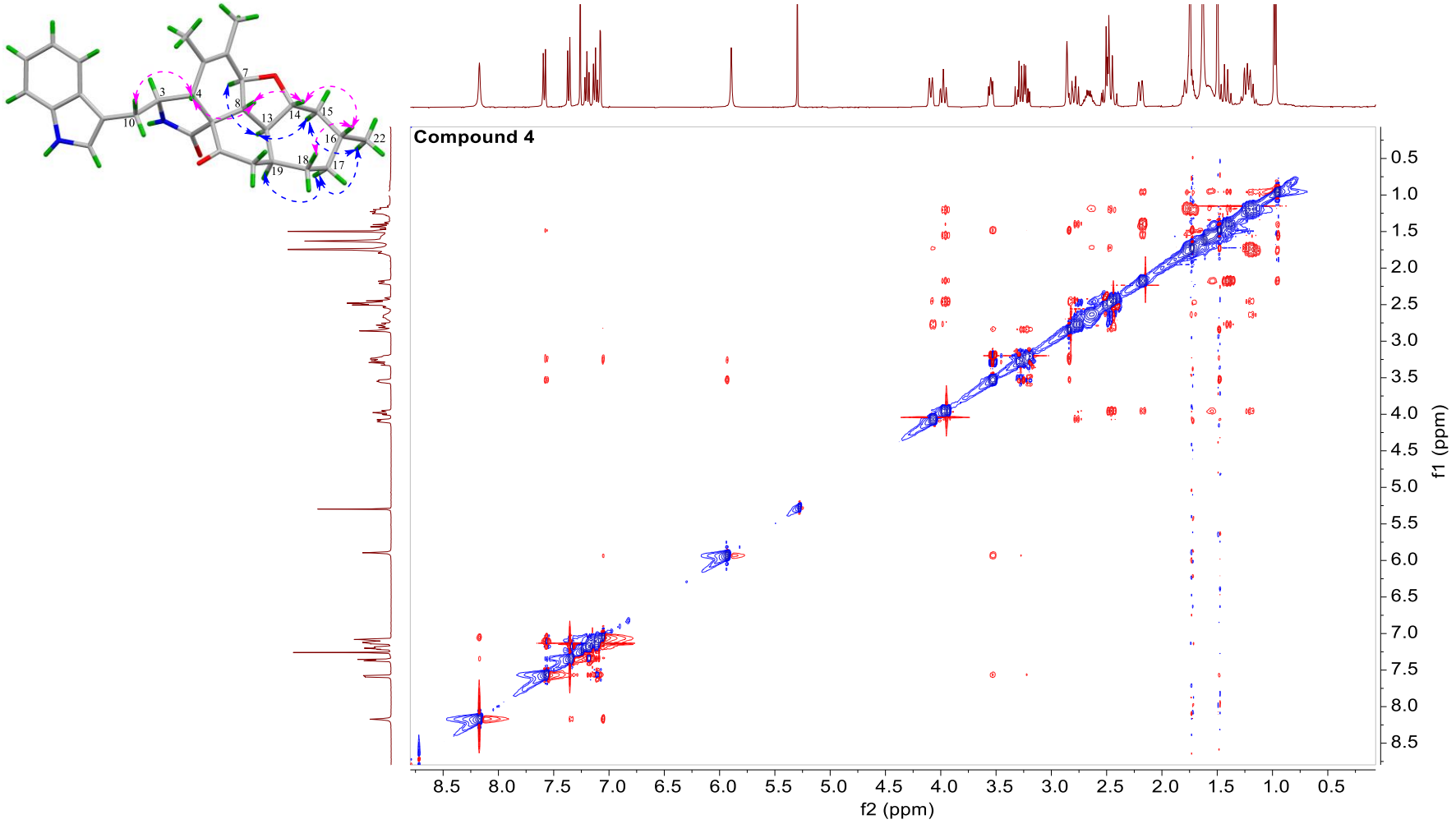


Fig. S55. HRESIMS (+) spectrum of **4**.

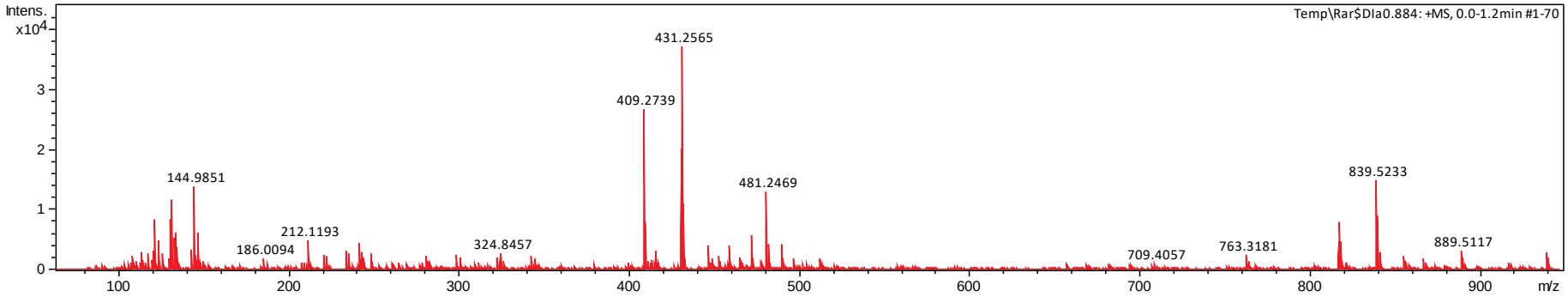


Fig. S56. UV spectrum of **4**.

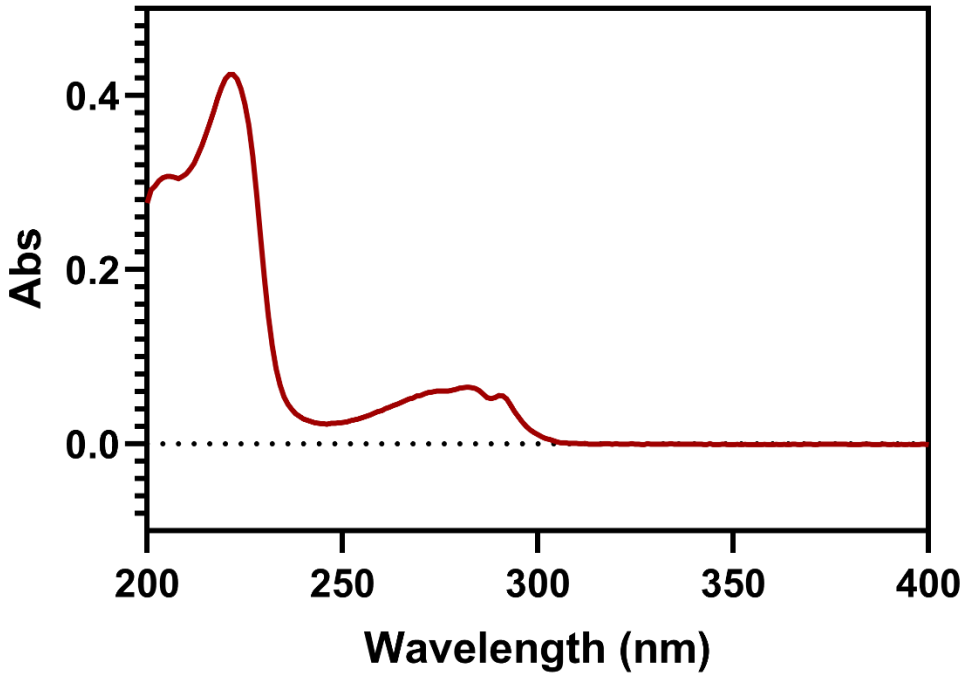


Fig. S57. IR spectrum of **4**.

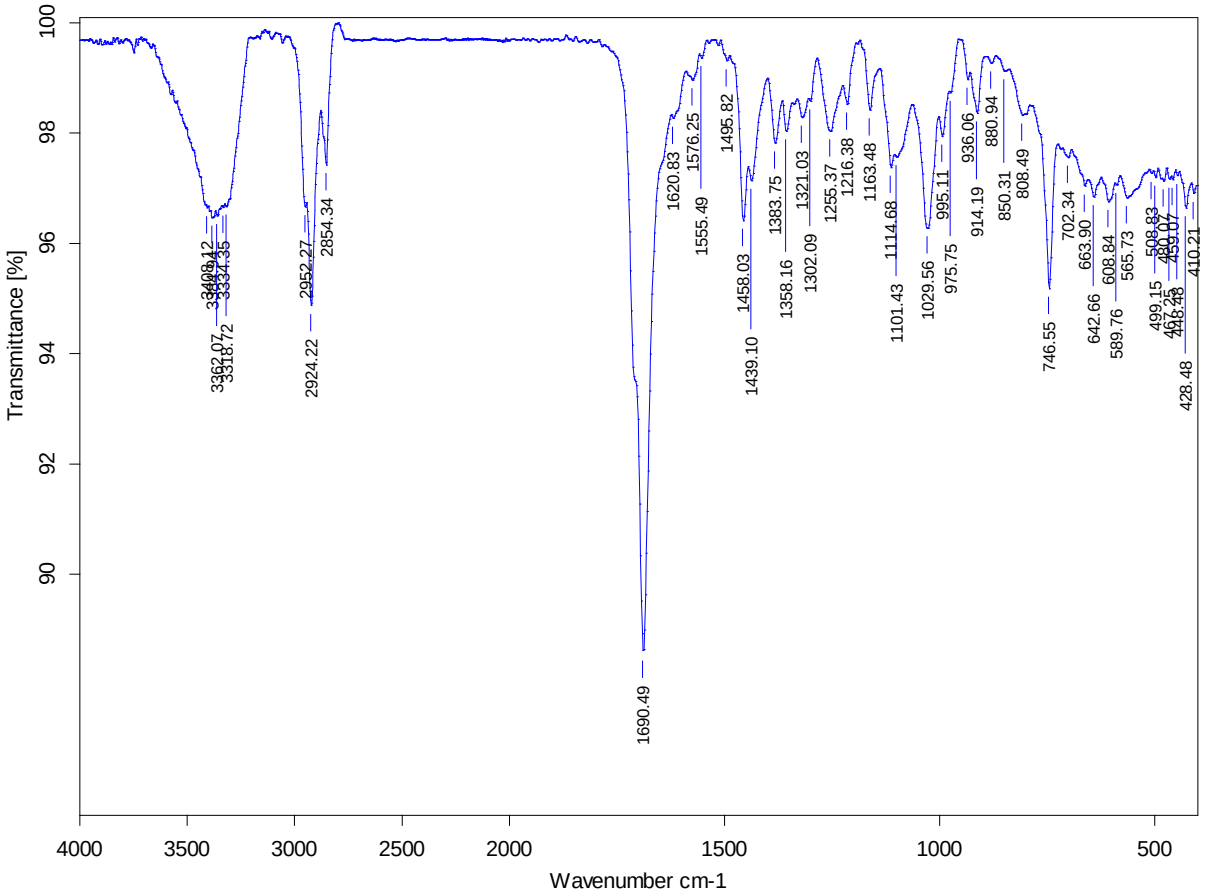


Fig. S58. ECD spectrum of **4**.

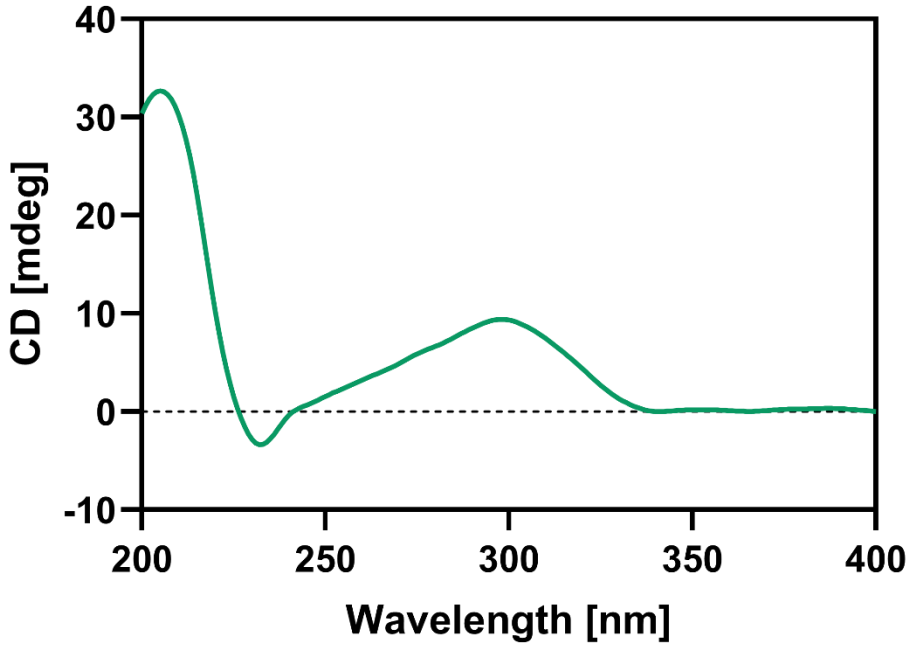


Fig. S59. ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **5**.

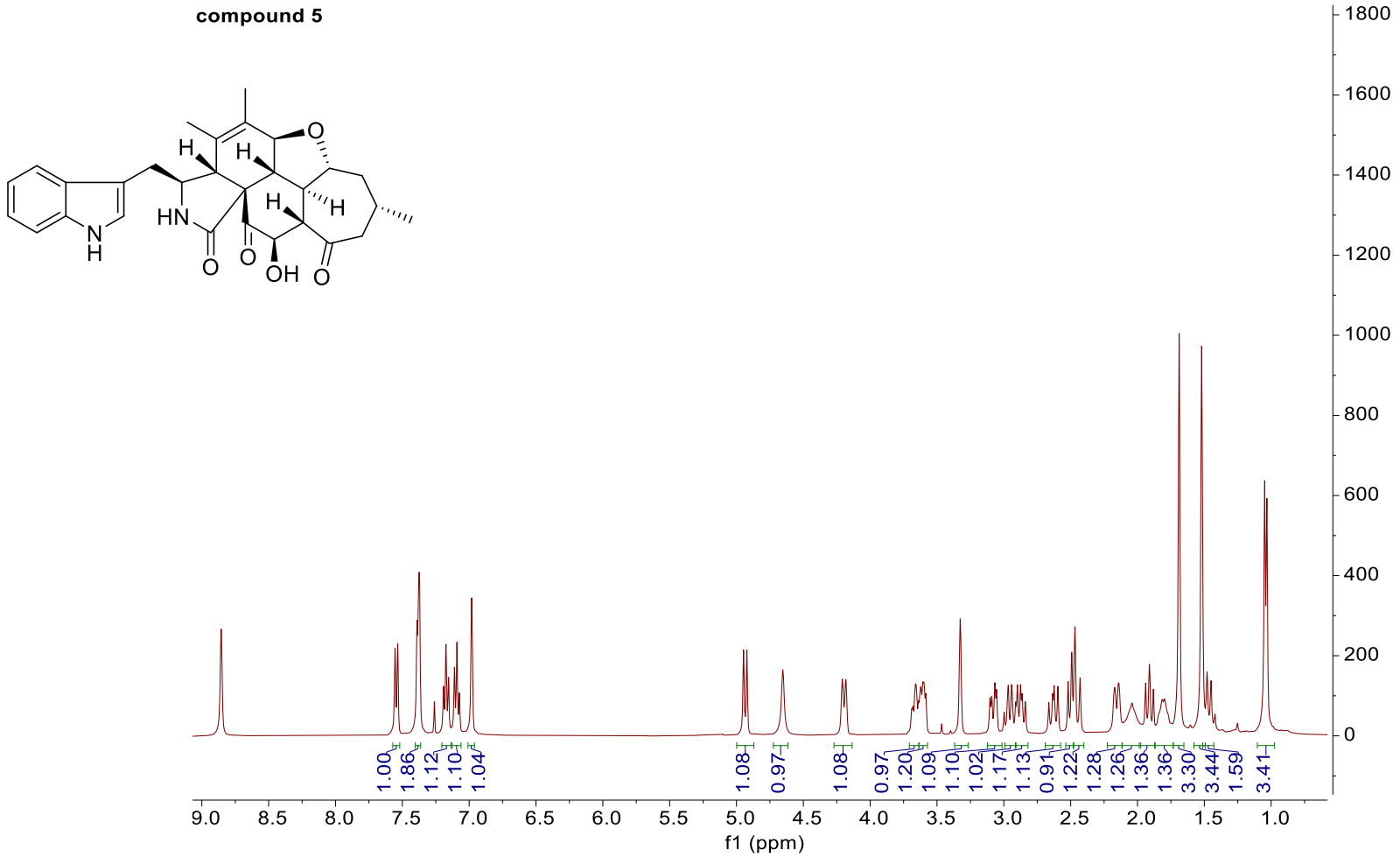
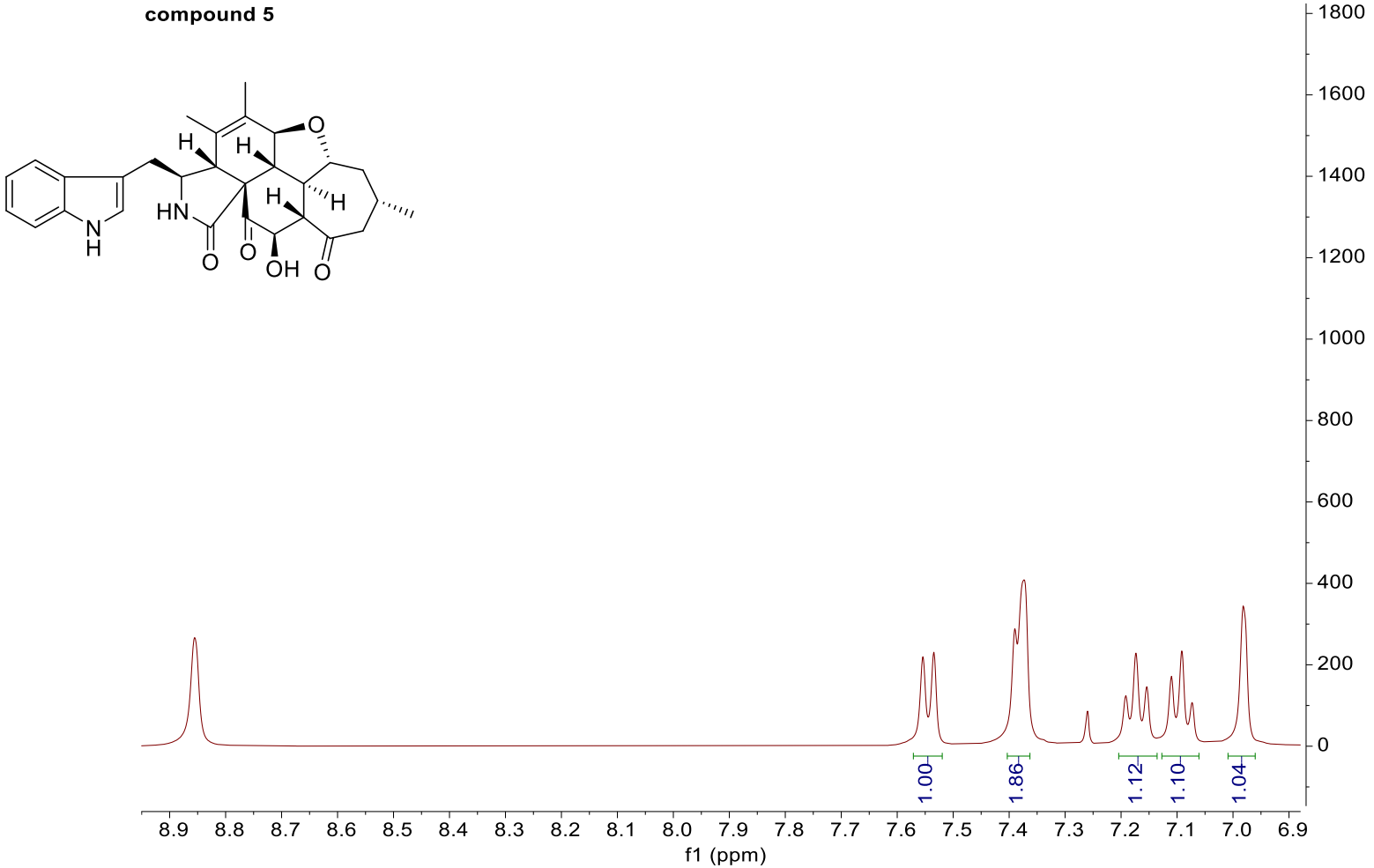
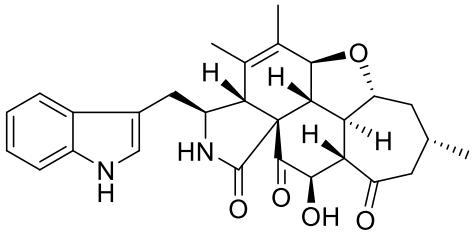


Fig. S60. Enlarged ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **5**.

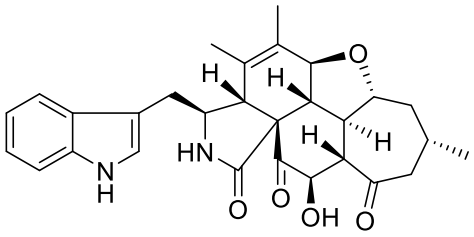


compound 5


H
H
O
H
H
HN
N
H
O
O
OH
O

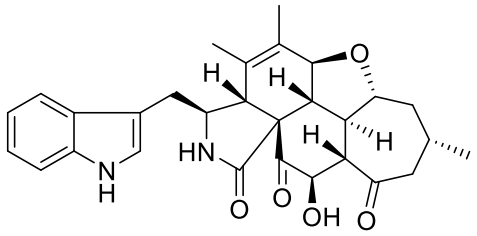
1800
1600
1400
1200
1000
800
600
400
200
0
1.08
0.97
1.08
0.97
1.20
1.09
5.2
5.1
5.0
4.9
4.8
4.7
4.6
4.5
4.4
4.3
4.2
4.1
4.0
3.9
3.8
3.7
3.6
3.5
3.4
3.3
3.2
f1 (ppm)

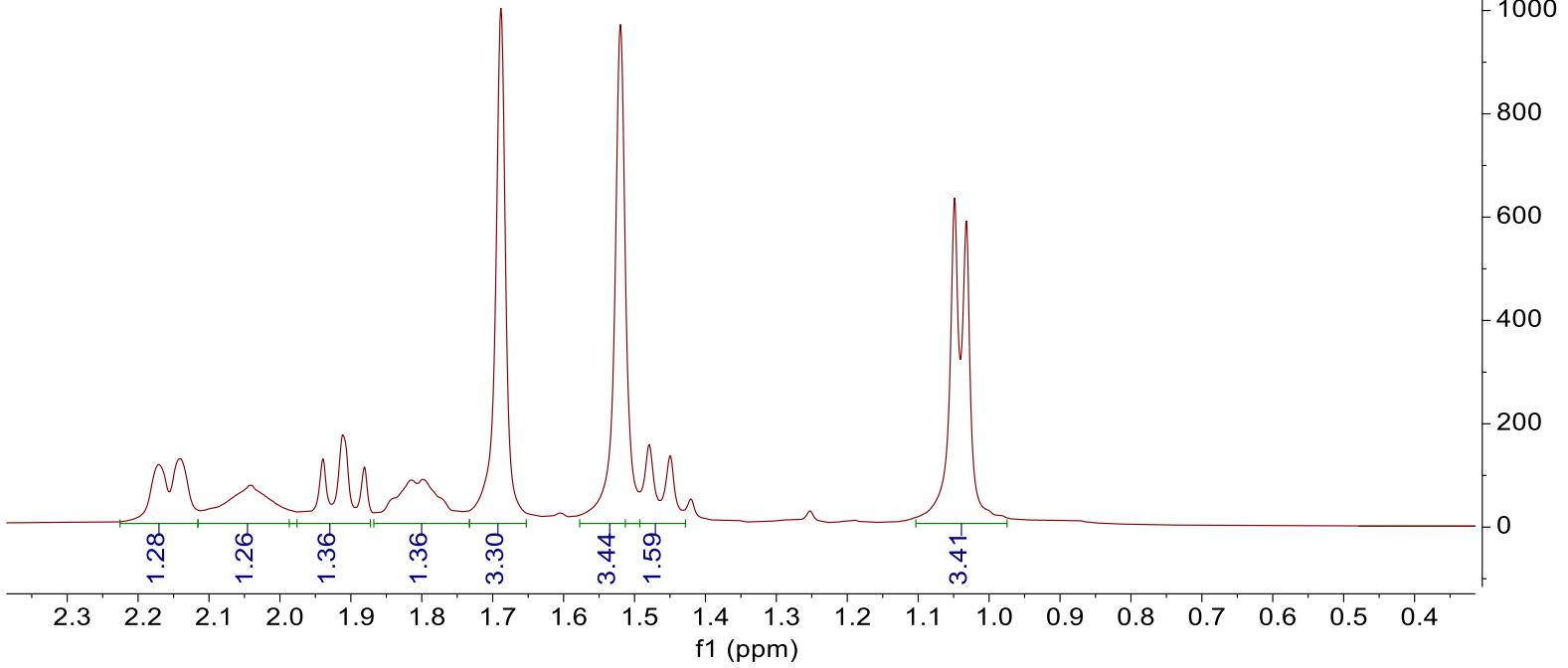
compound 5


H
H
O
H
H
HN
N
H
O
O
OH
O

1800
1600
1400
1200
1000
800
600
400
200
0
1.09
1.10
1.02
1.17
1.13
0.91
1.22
1.28
1.26
1.36
1.36
3.30
3.44
1.59
3.4 3.3 3.2 3.1 3.0 2.9 2.8 2.7 2.6 2.5 2.4 2.3 2.2 2.1 2.0 1.9 1.8 1.7 1.6 1.5 1.4
f1 (ppm)

compound 5


H
H
O
H
H
HN
N
H
O
O
OH
O


1800
1600
1400
1200
1000
800
600
400
200
0
1.28
1.26
1.36
1.36
3.30
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1.59
3.41
2.3
2.2
2.1
2.0
1.9
1.8
1.7
1.6
1.5
1.4
1.3
1.2
1.1
1.0
0.9
0.8
0.7
0.6
0.5
0.4
f1 (ppm)

Fig. S61. ^{13}C NMR (100 MHz, $CDCl_3$) spectrum of **5**.

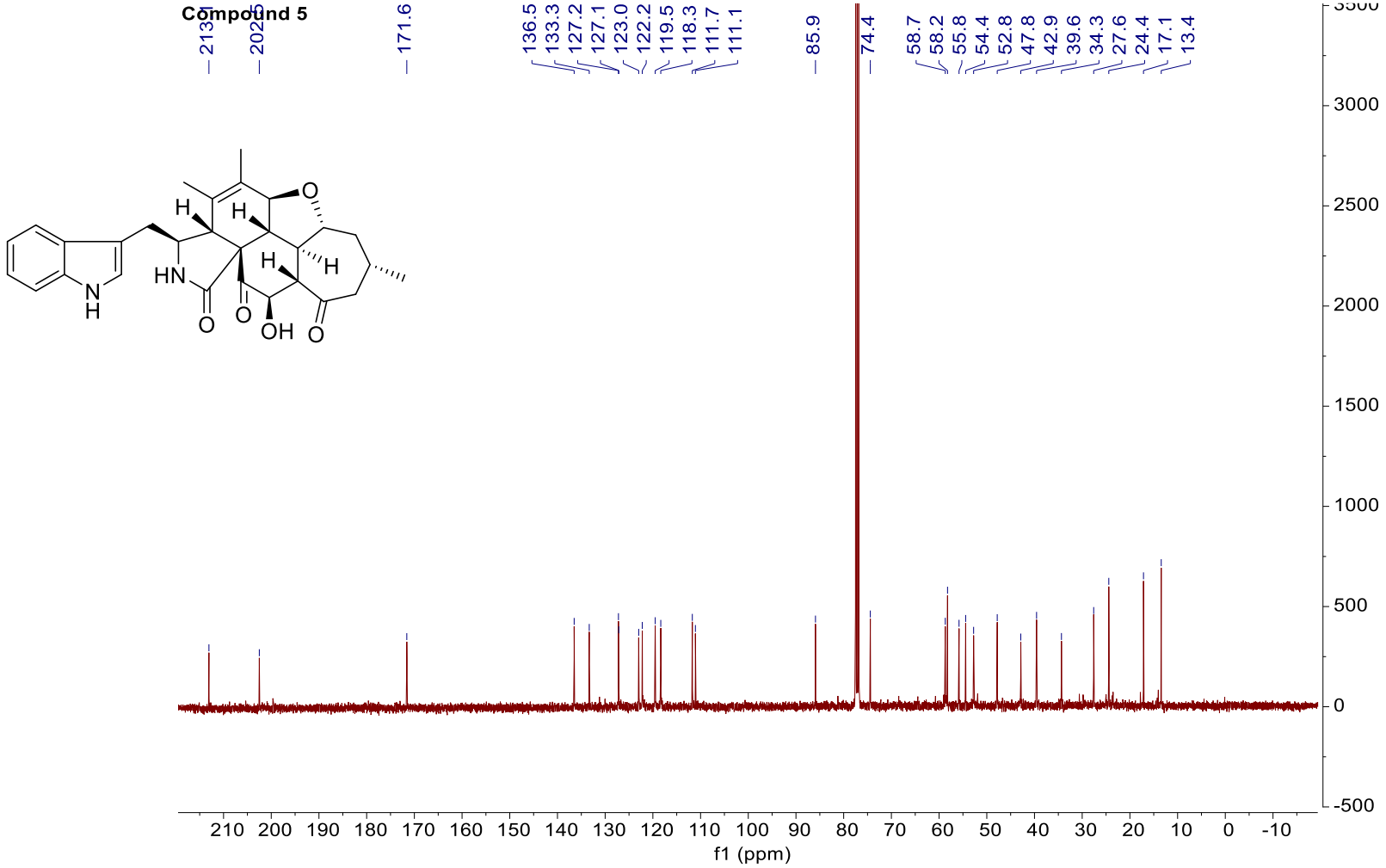


Fig. S62. DEPT-135 (100 MHz, $CDCl_3$) spectrum of **5**.

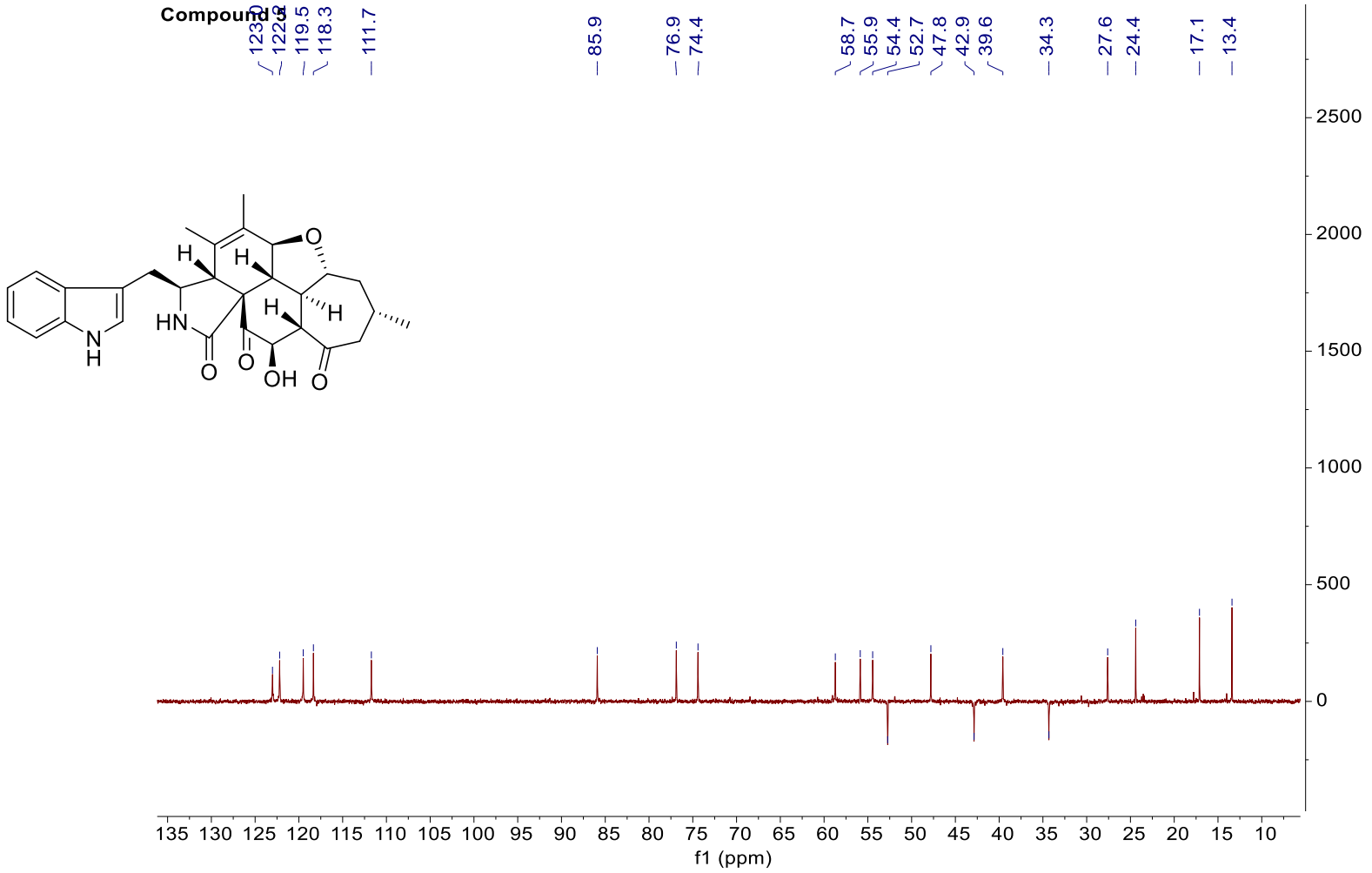


Fig. S63. HSQC spectrum of **5** in $CDCl_3$.

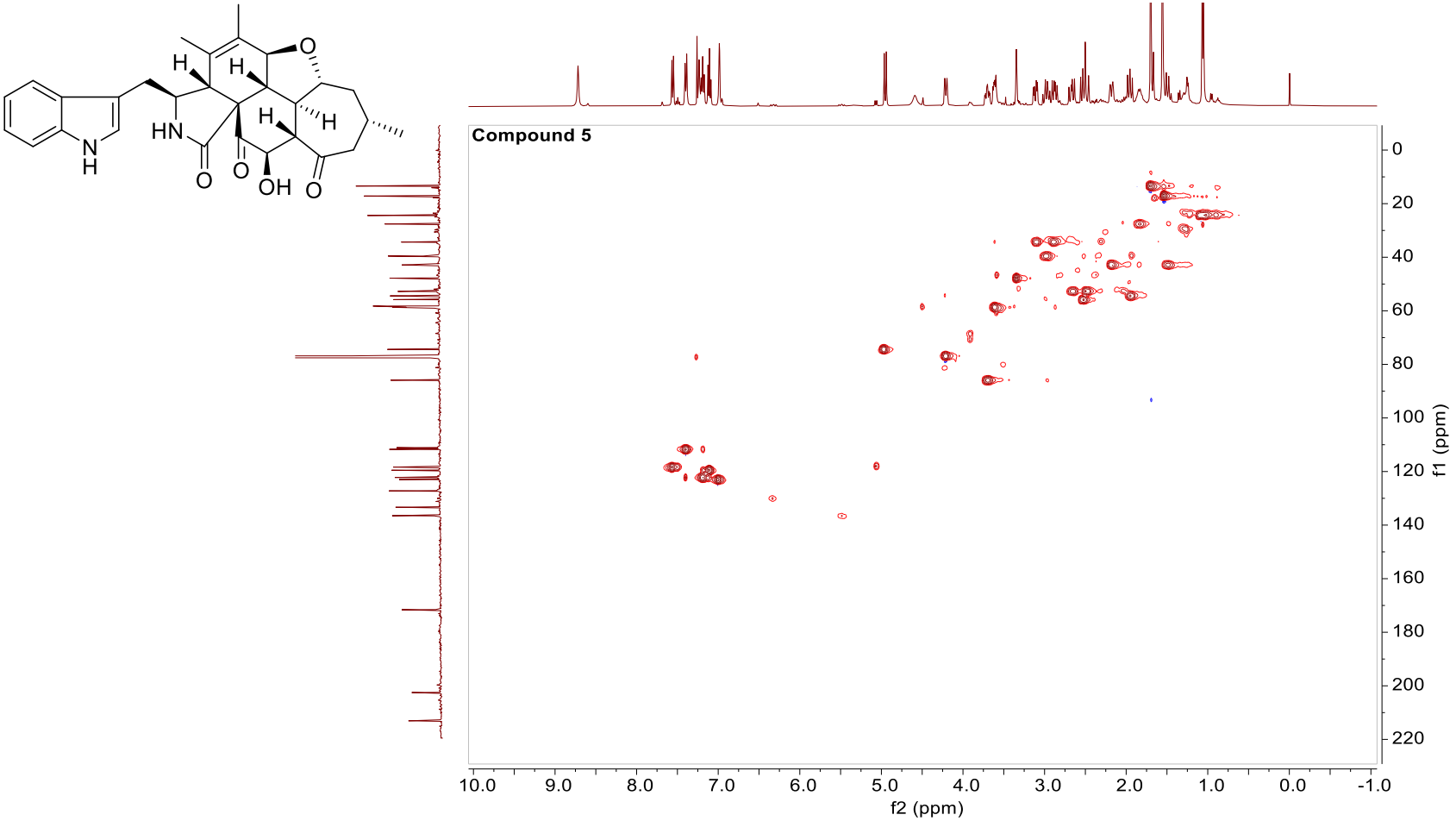


Fig. S64. HMBC spectrum of **5** in $CDCl_3$.

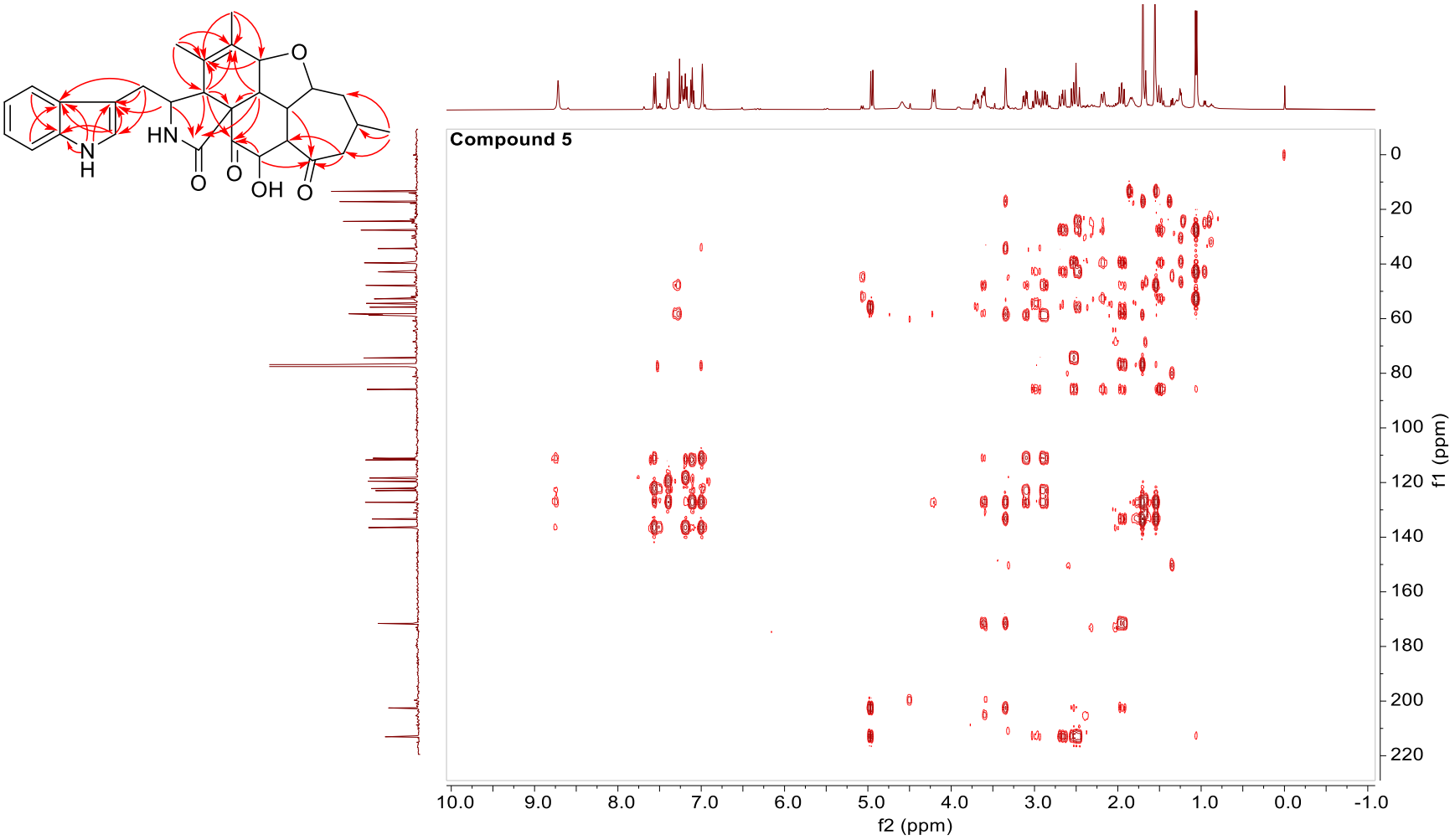


Fig. S65. ^{1}H–^{1}H COSY spectrum of **5** in $CDCl_3$.

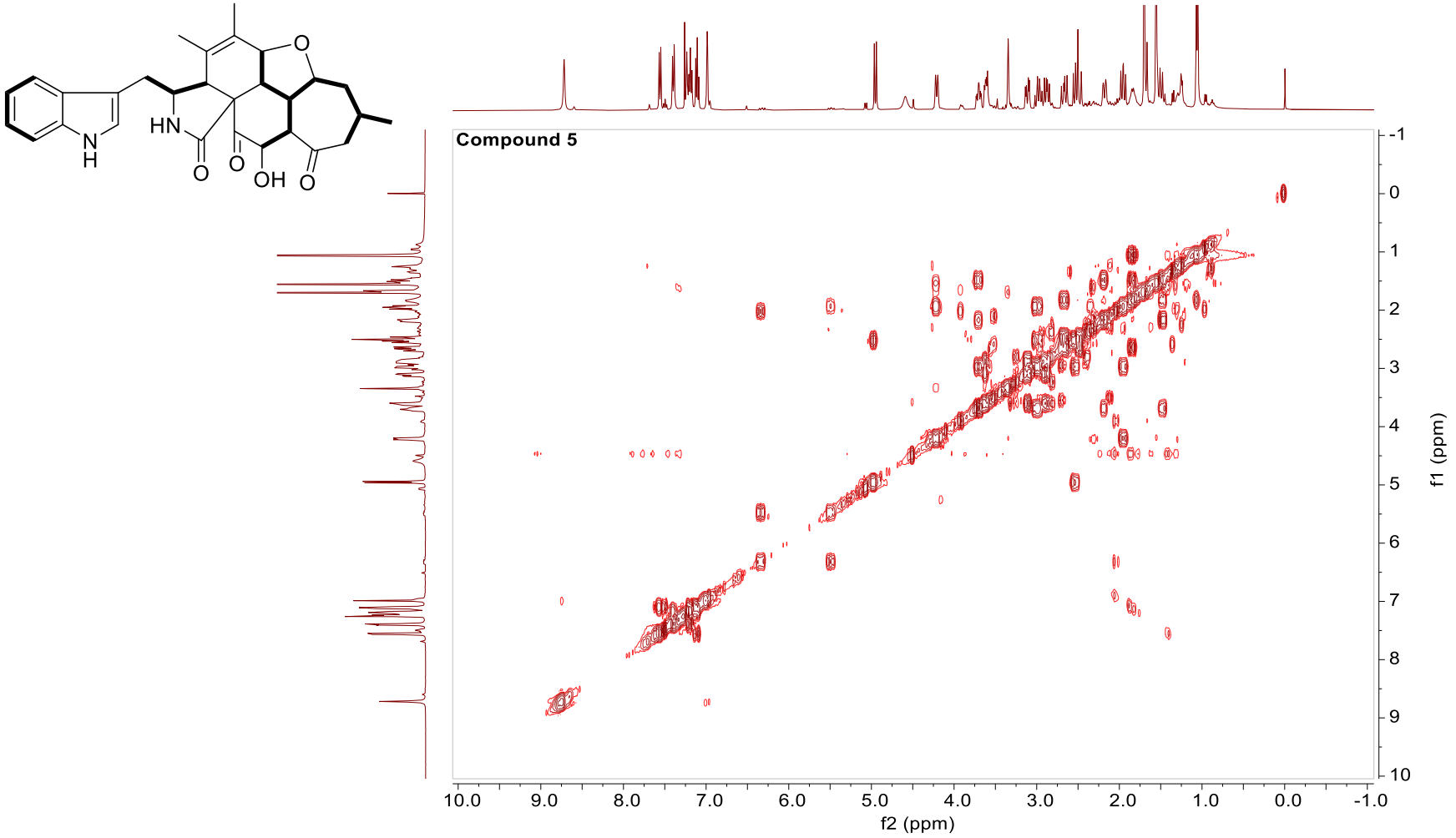


Fig. S66. NOESY spectrum of **5** in $CDCl_3$.

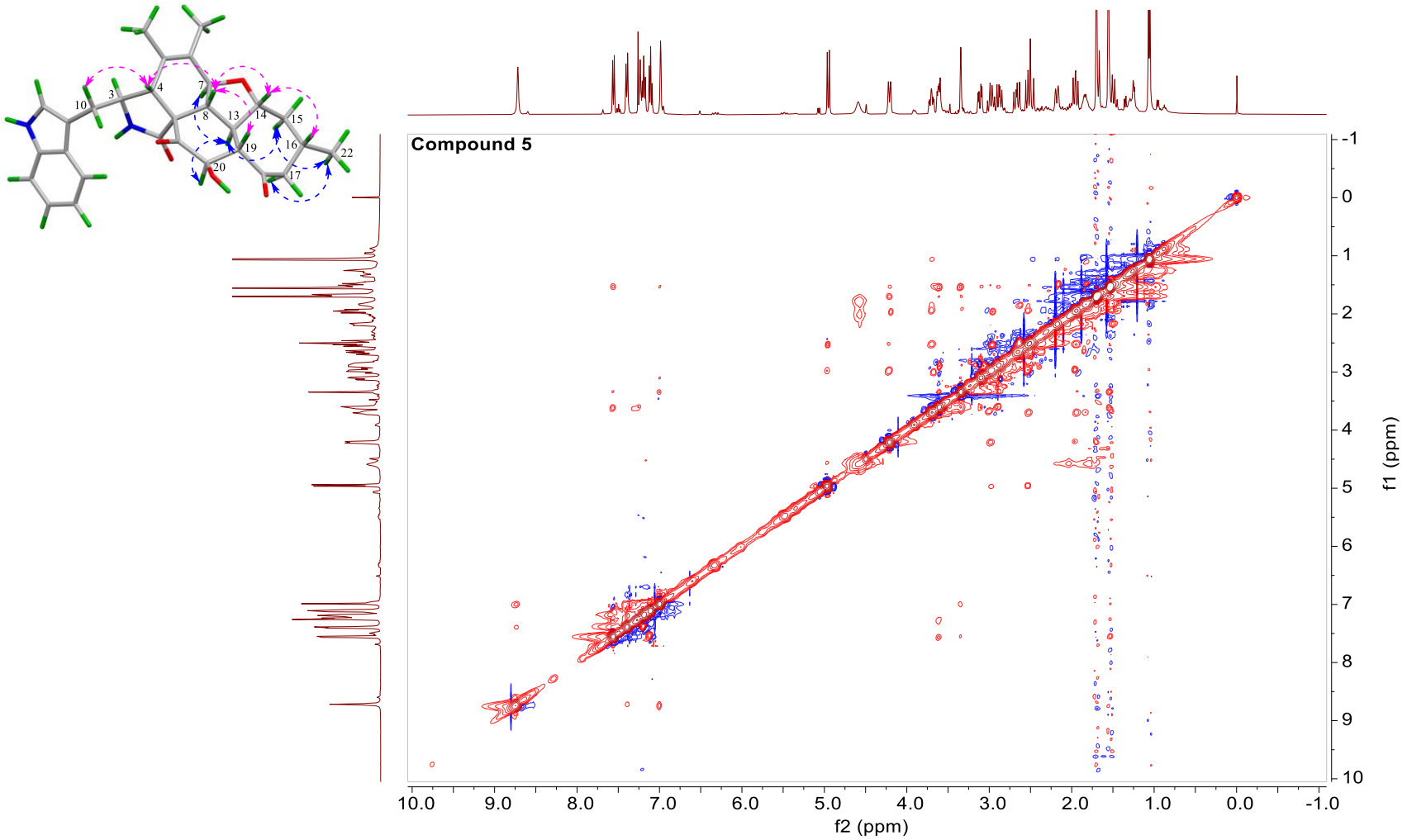


Fig. S67. HRESIMS (+) spectrum of **5**.

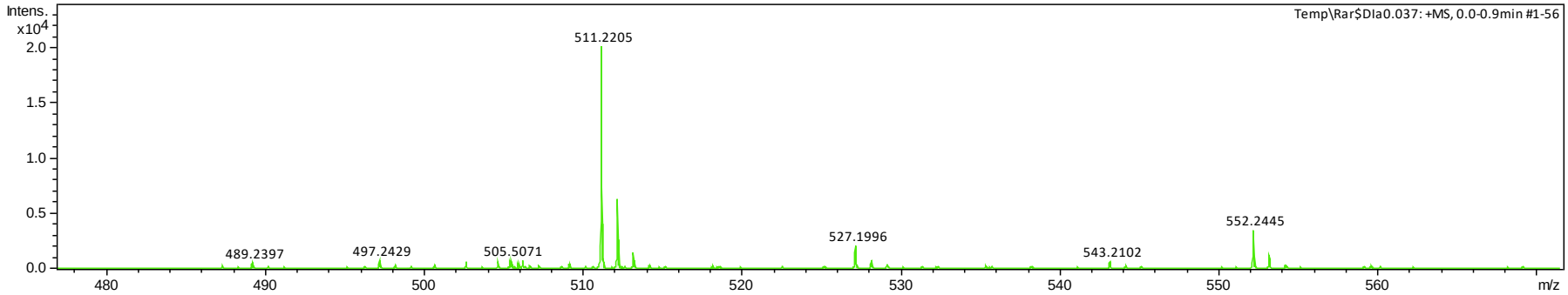


Fig. S68. UV spectrum of **5**.

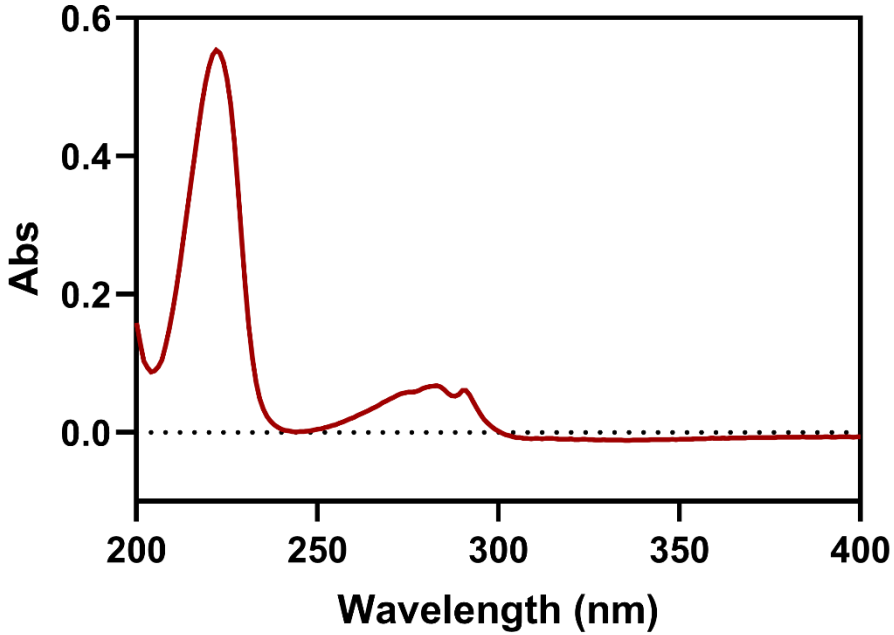


Fig. S69. IR spectrum of **5**.

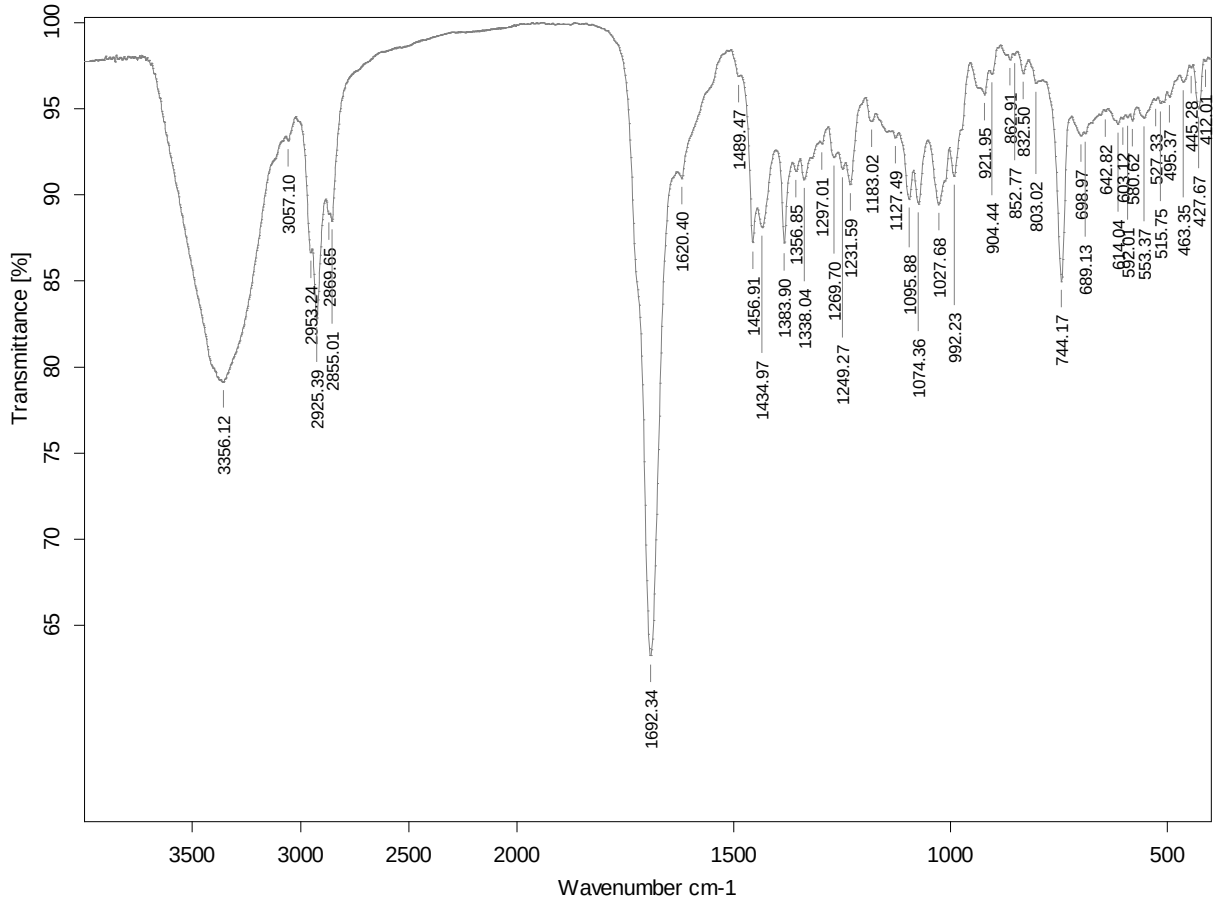


Fig. S70. ECD spectrum of **5**.

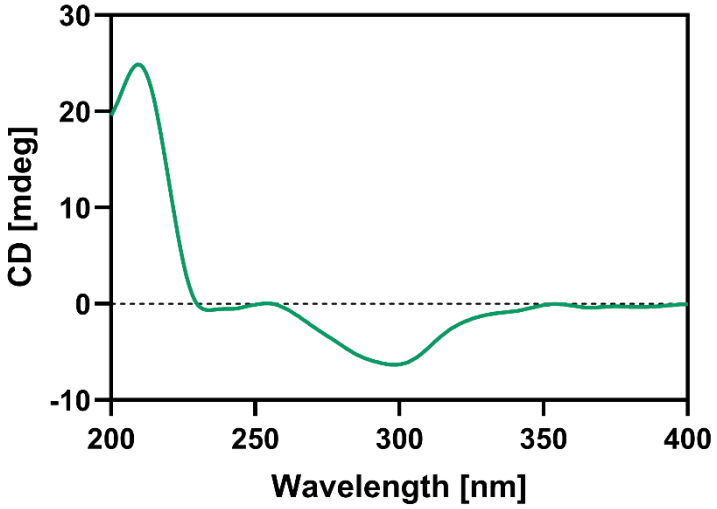


Fig. S71. ^{1}H NMR (400 MHz, CD_3OD) spectrum of **6**.

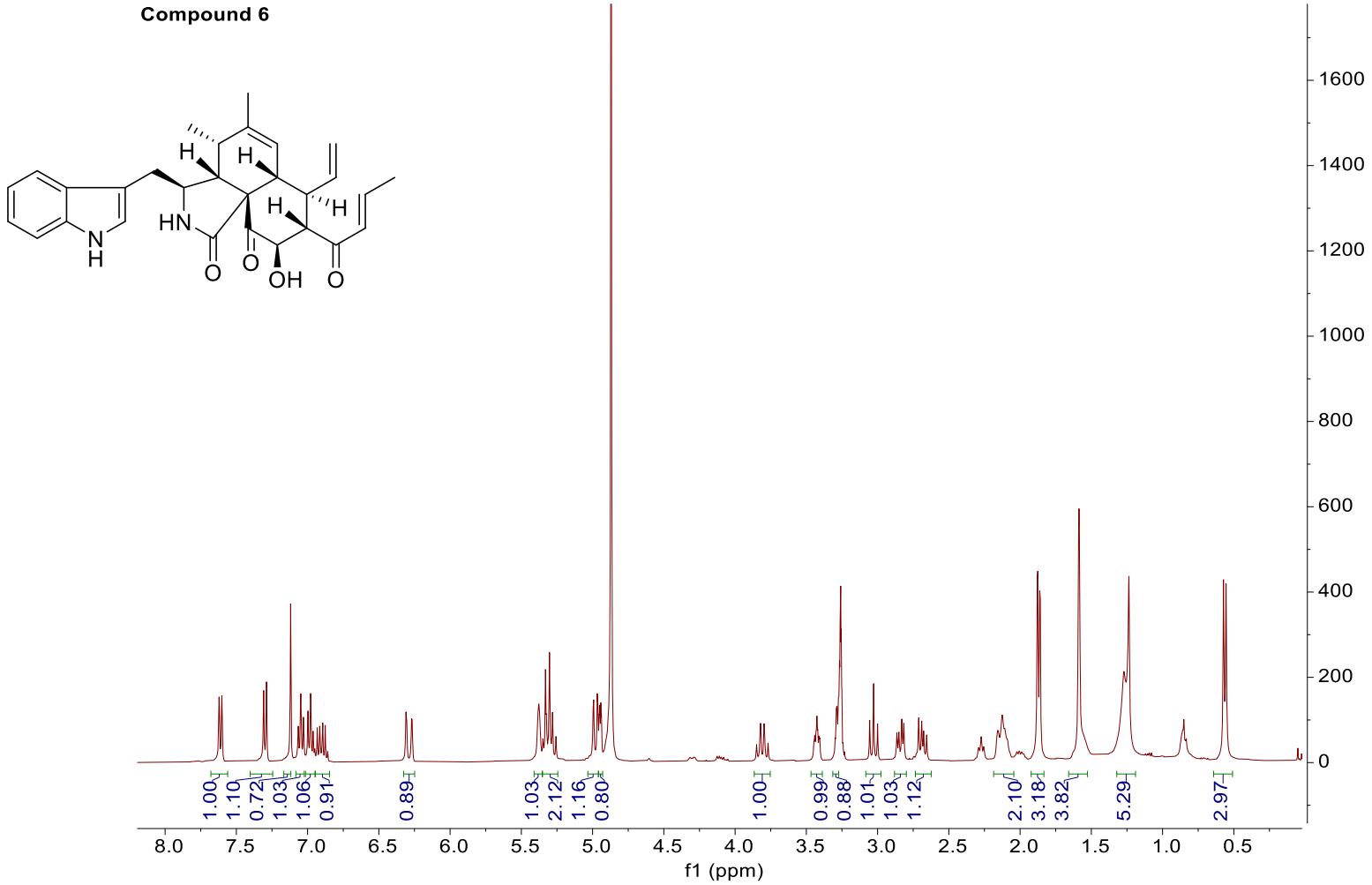
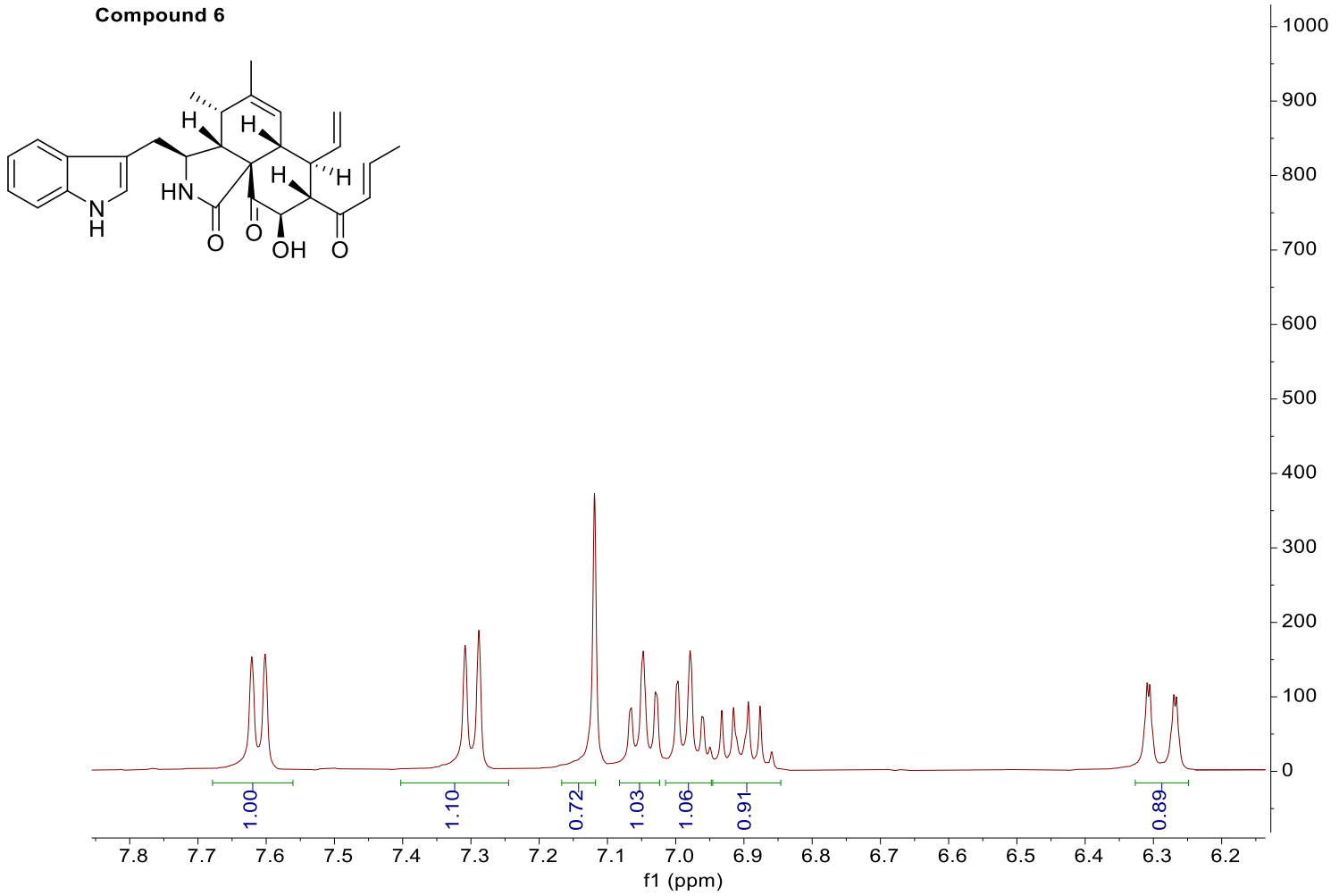
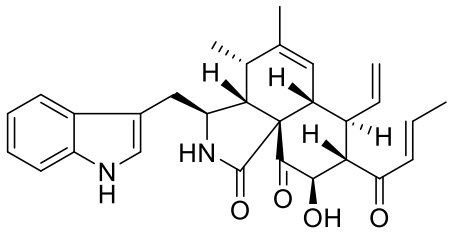


Fig. S72. Enlarged ^{1}H NMR (400 MHz, CD_3OD) spectrum of **6**.

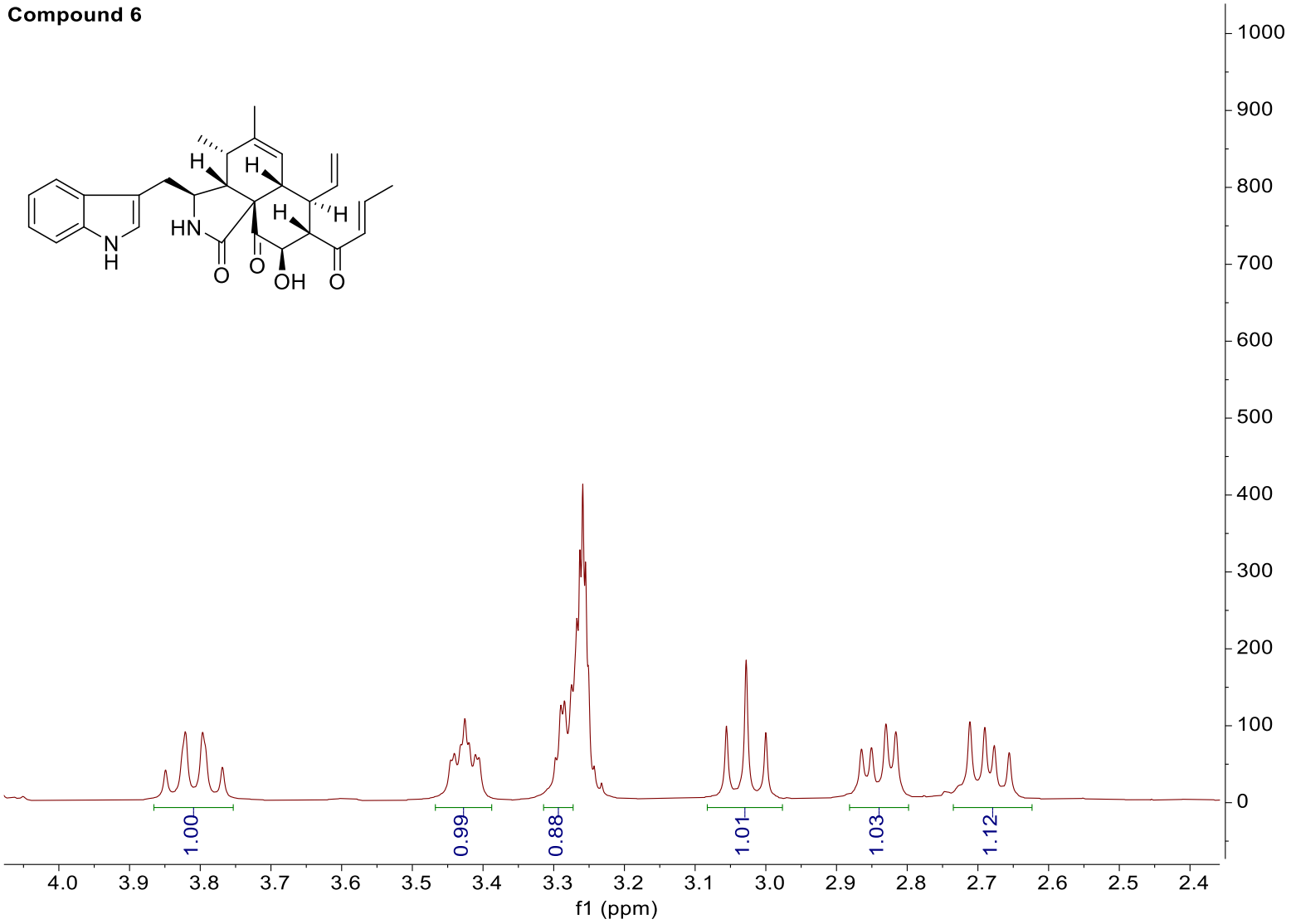


Compound 6

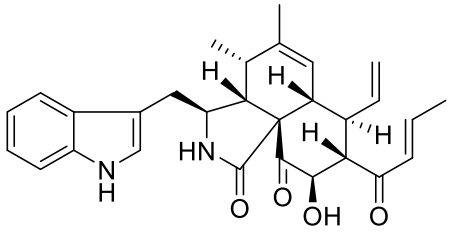

H
H
H
H
HN
N
H
O
O
OH
O

1200
1100
1000
900
800
700
600
500
400
300
200
100
0
0.89
1.03
2.12
1.16
0.80
6.4
6.3
6.2
6.1
6.0
5.9
5.8
5.7
5.6
5.5
5.4
5.3
5.2
5.1
5.0
4.9
4.8
f1 (ppm)

Compound 6


H
H
H
H
HN
N
H
O
O
OH
O
1000
900
800
700
600
500
400
300
200
100
0
1.00
0.99
0.88
1.01
1.03
1.12
4.0
3.9
3.8
3.7
3.6
3.5
3.4
3.3
3.2
3.1
3.0
2.9
2.8
2.7
2.6
2.5
2.4
f1 (ppm)

Compound 6


H
H
H
H
HN
N
H
O
O
OH
O

1200
1100
1000
900
800
700
600
500
400
300
200
100
0
2.10
3.18
3.82
5.29
2.97
2.4
2.3
2.2
2.1
2.0
1.9
1.8
1.7
1.6
1.5
1.4
1.3
1.2
1.1
1.0
0.9
0.8
0.7
0.6
0.5
0.4
f1 (ppm)

Fig. S73. ^{13}C NMR (100 MHz, CD_3OD) spectrum of **6**.

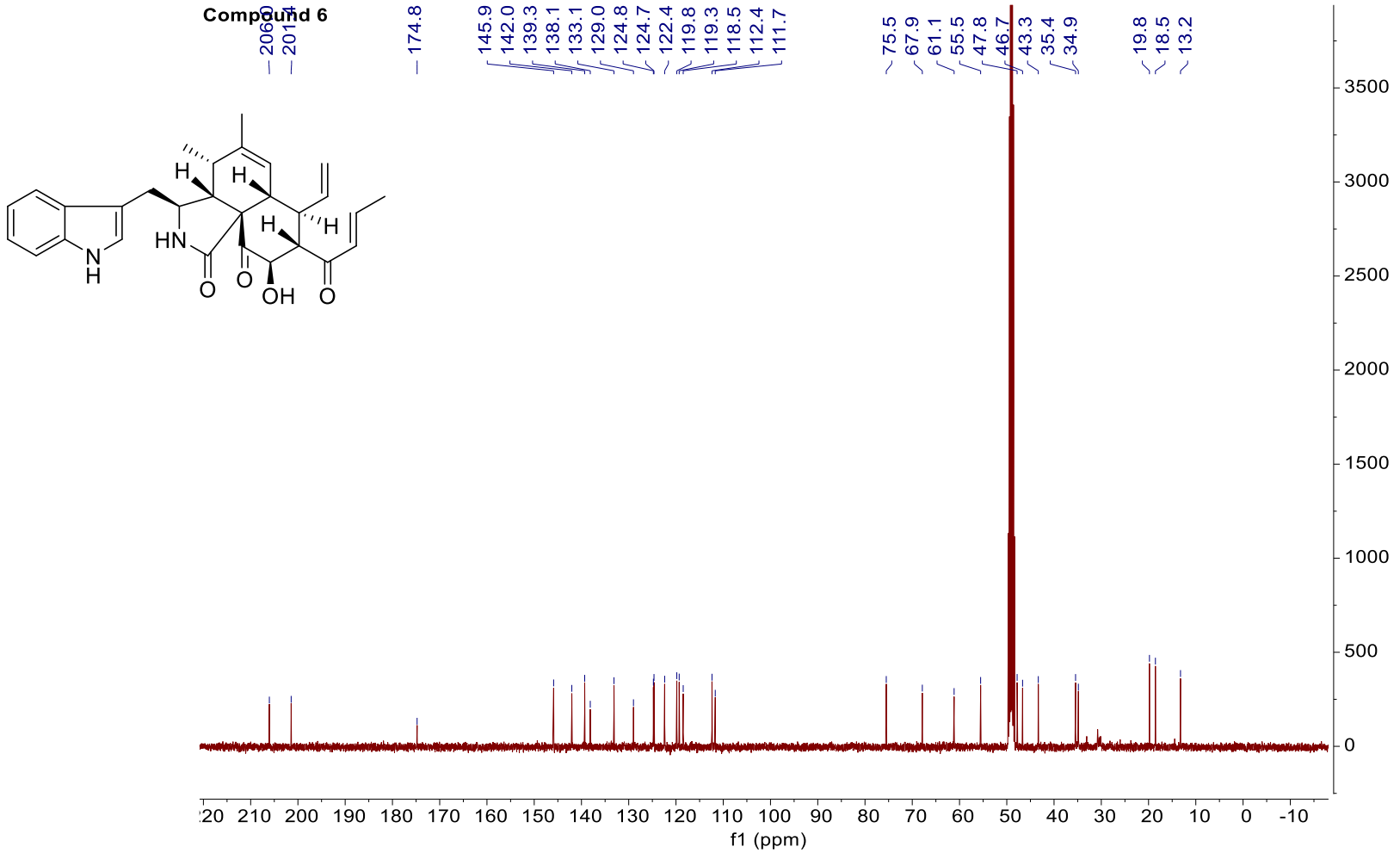


Fig. S74. DEPT-135 (100 MHz, CD_3OD) spectrum of **6**.

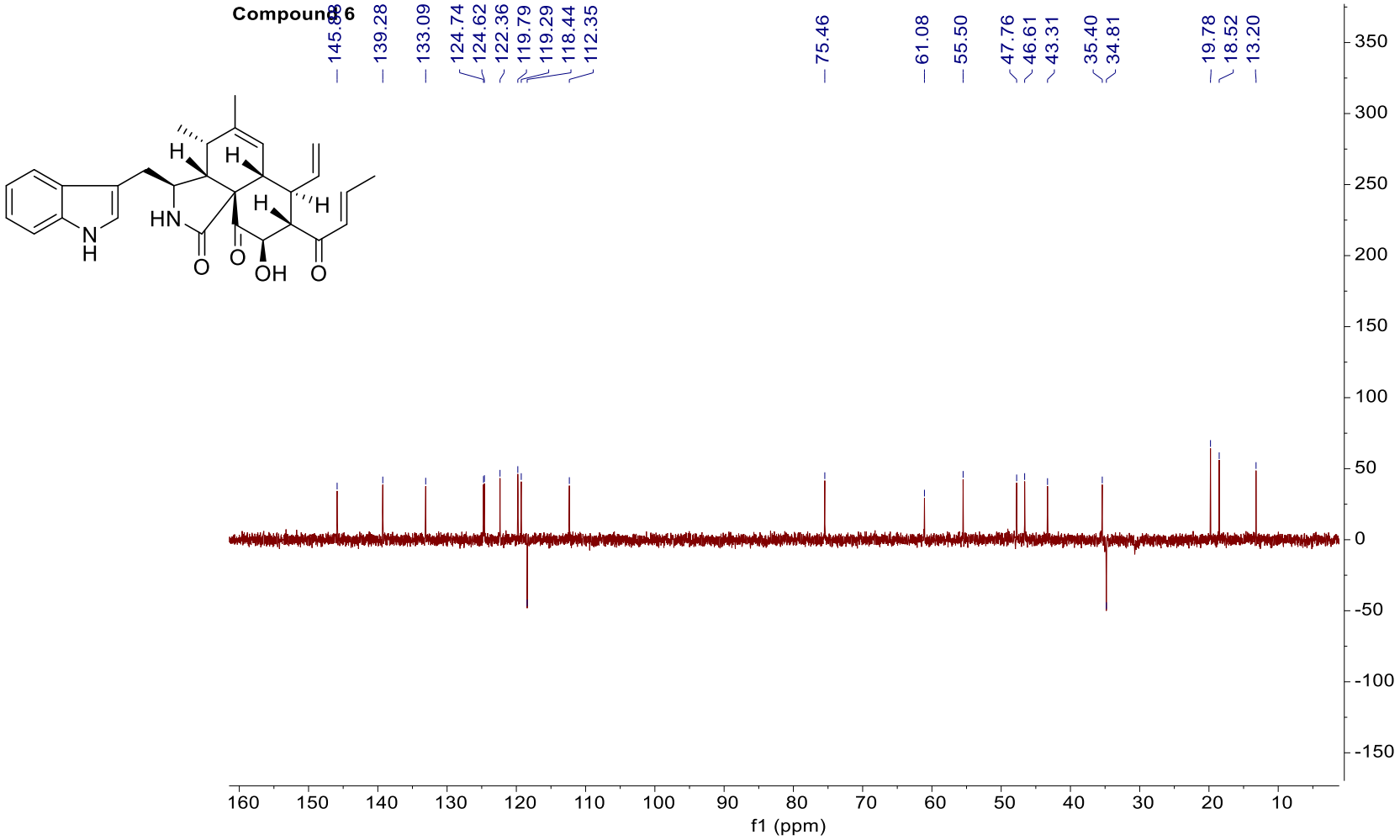


Fig. S75. HSQC spectrum of **6** in CD_3OD.

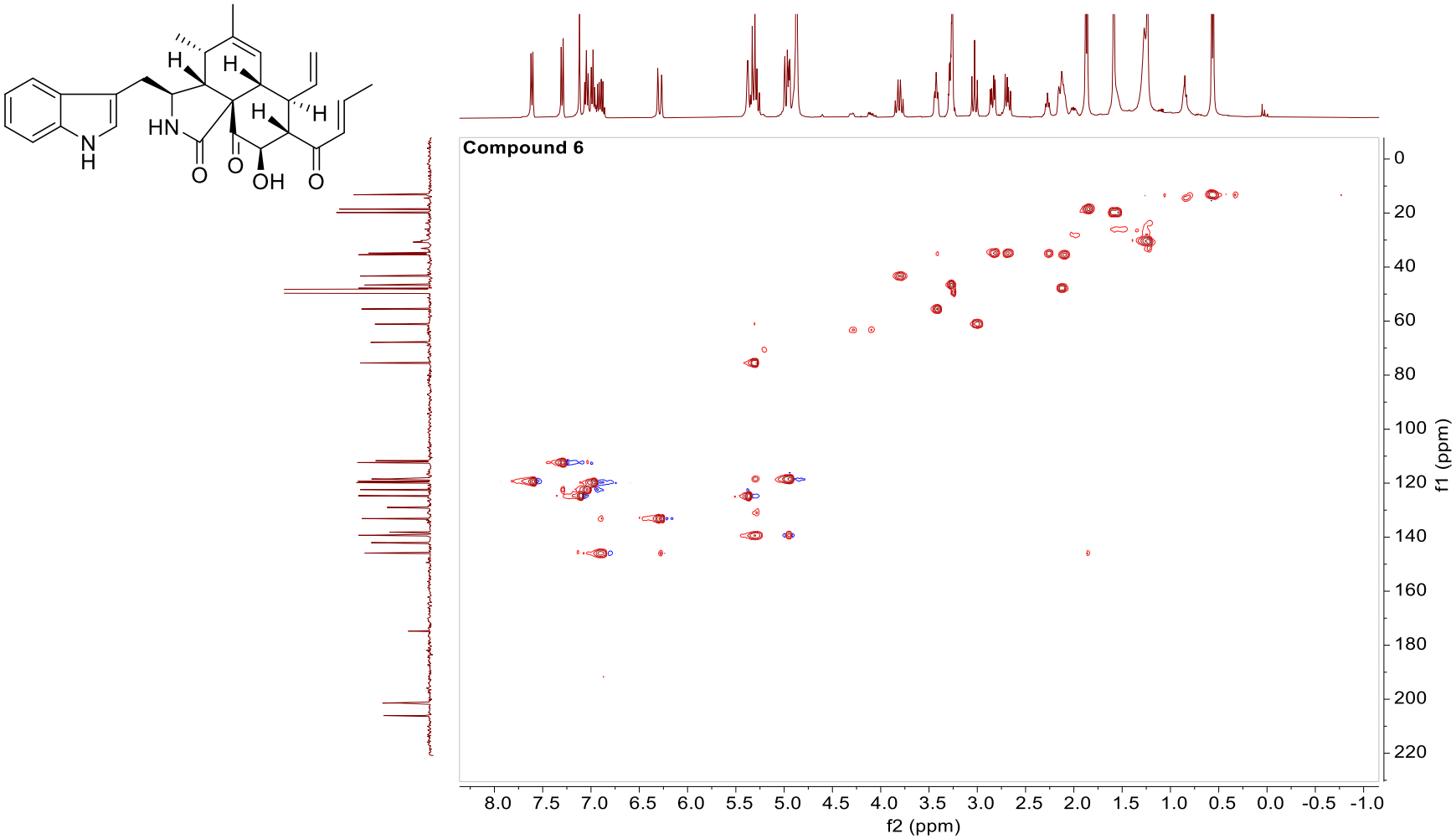


Fig. S76. HMBC spectrum of **6** in CD_3OD.

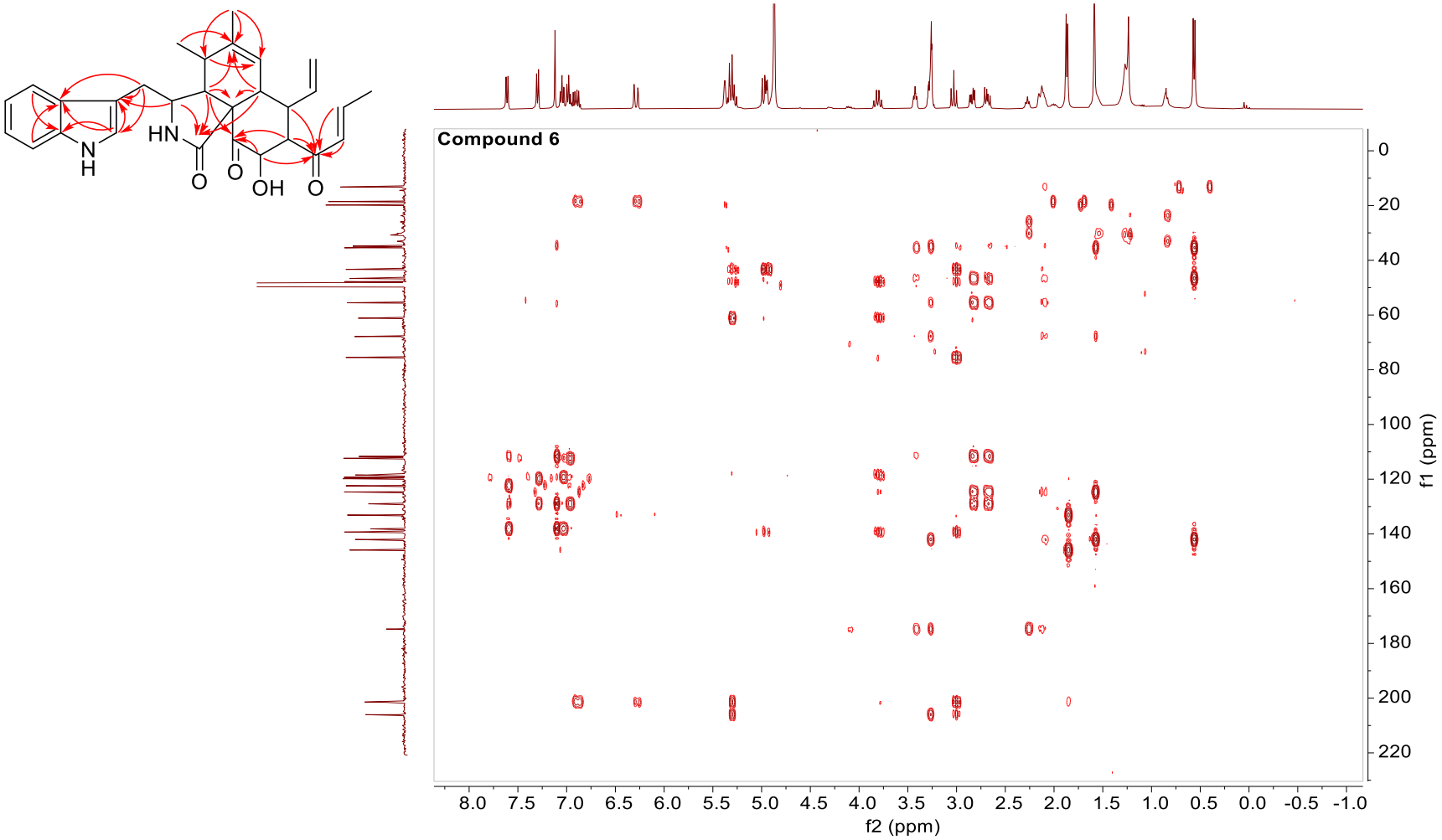


Fig. S77. ^{1}H–^{1}H COSY spectrum of **6** in CD_3OD.

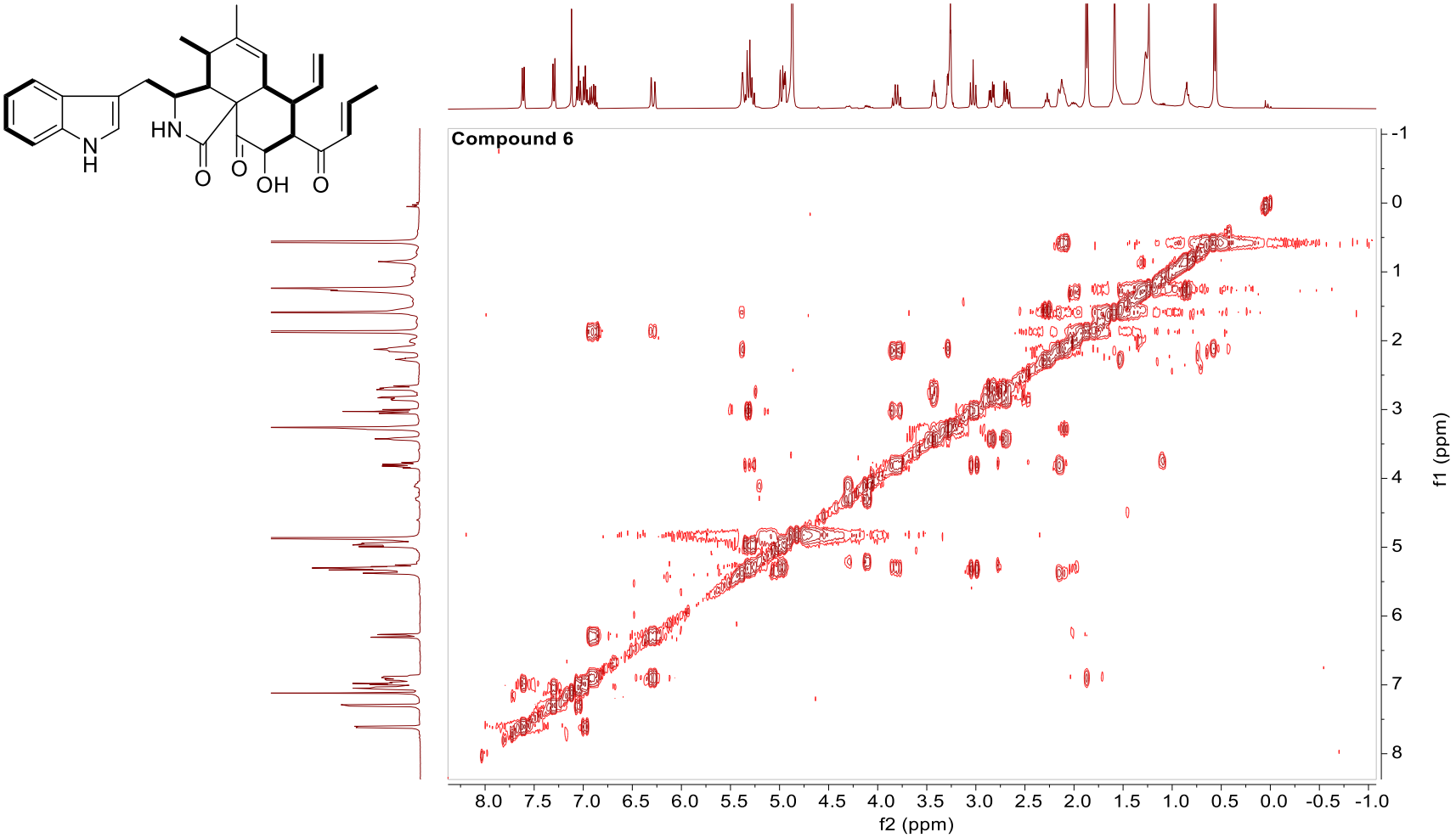


Fig. S78. NOESY spectrum of **6** in CD_3OD.

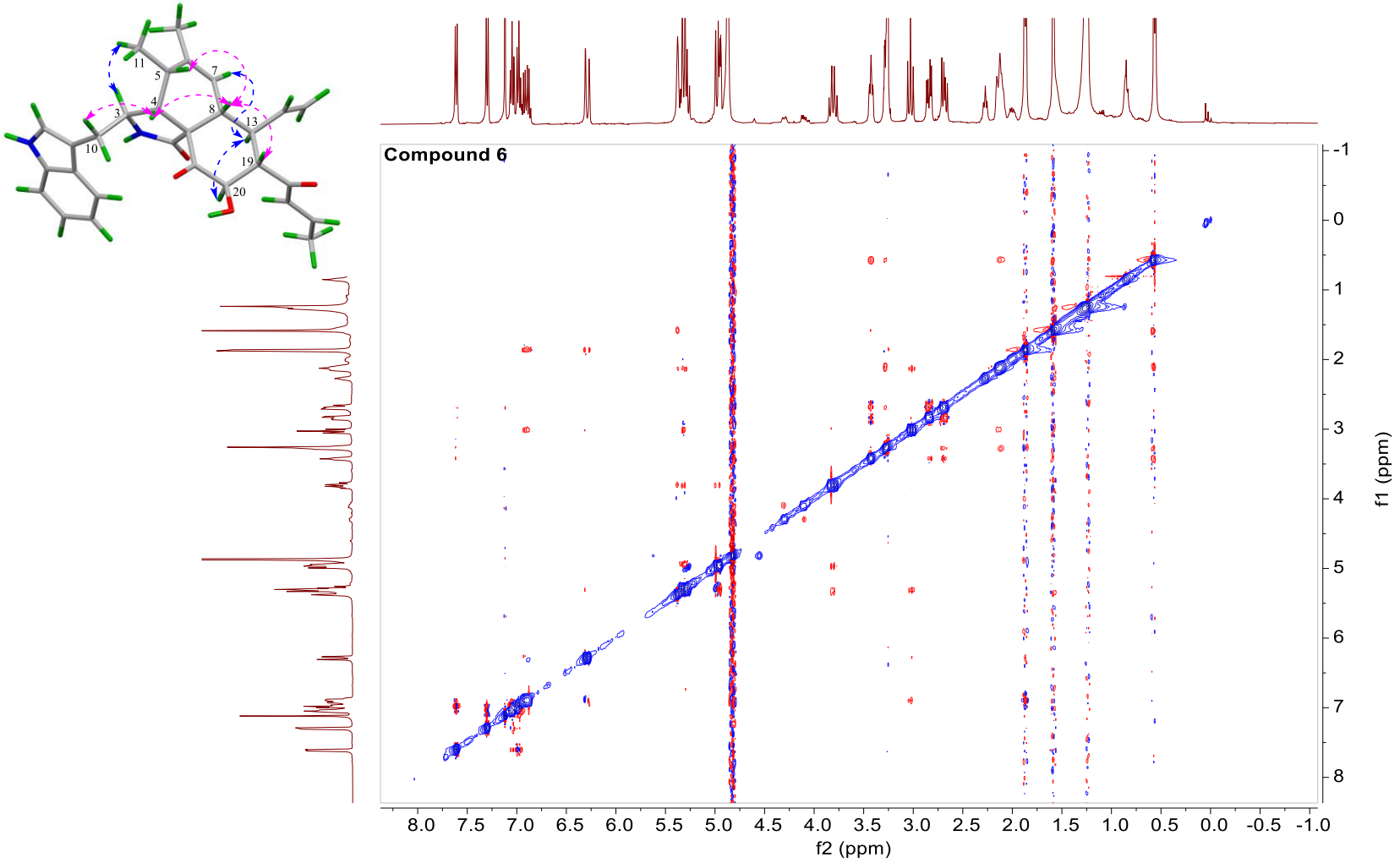


Fig. S79. HRESIMS (+) spectrum of **6.**

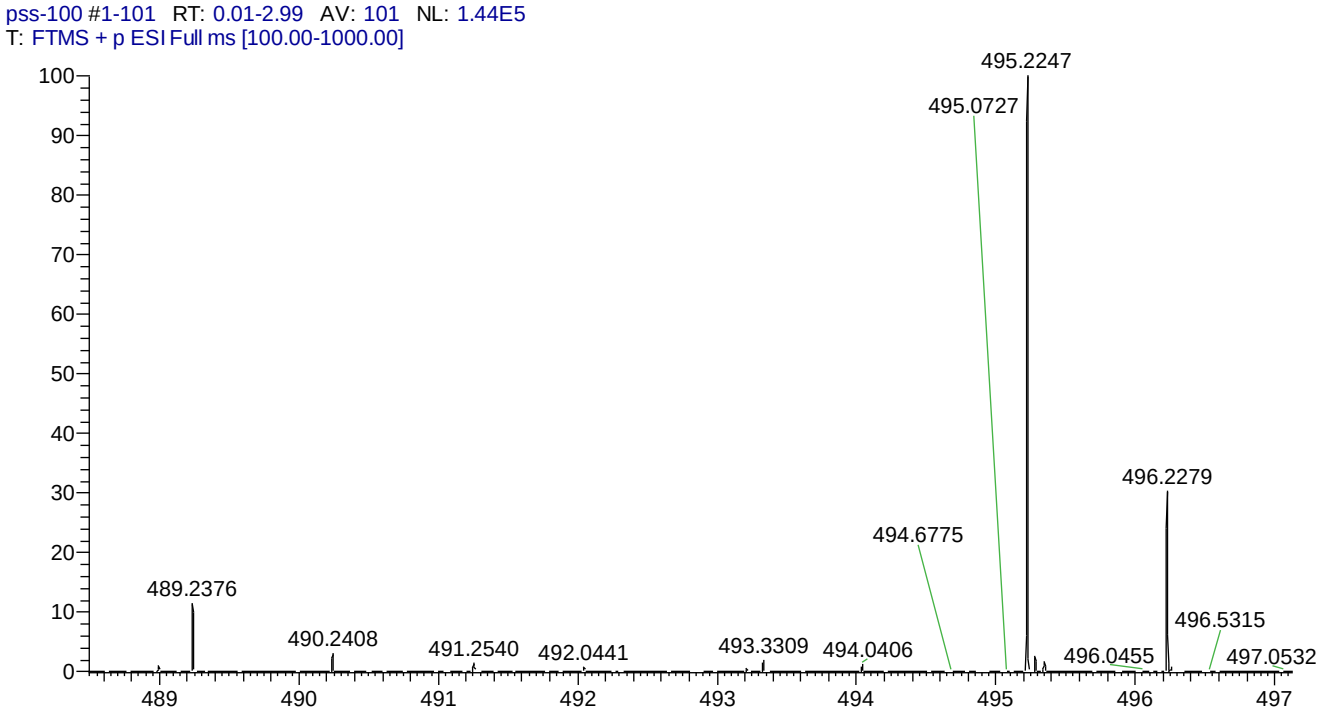


Fig. S80. UV spectrum of **6**.

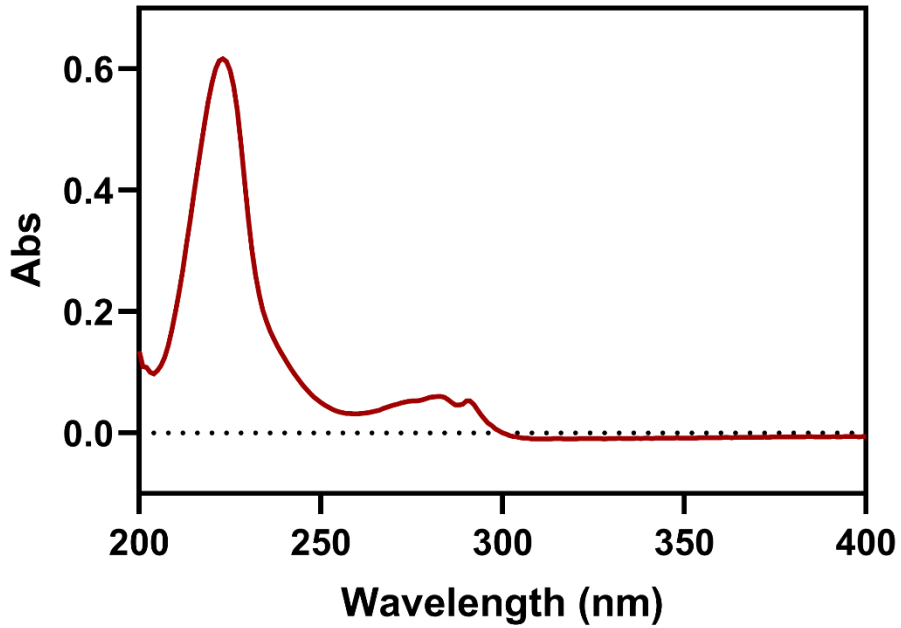


Fig. S81. IR spectrum of **6**.

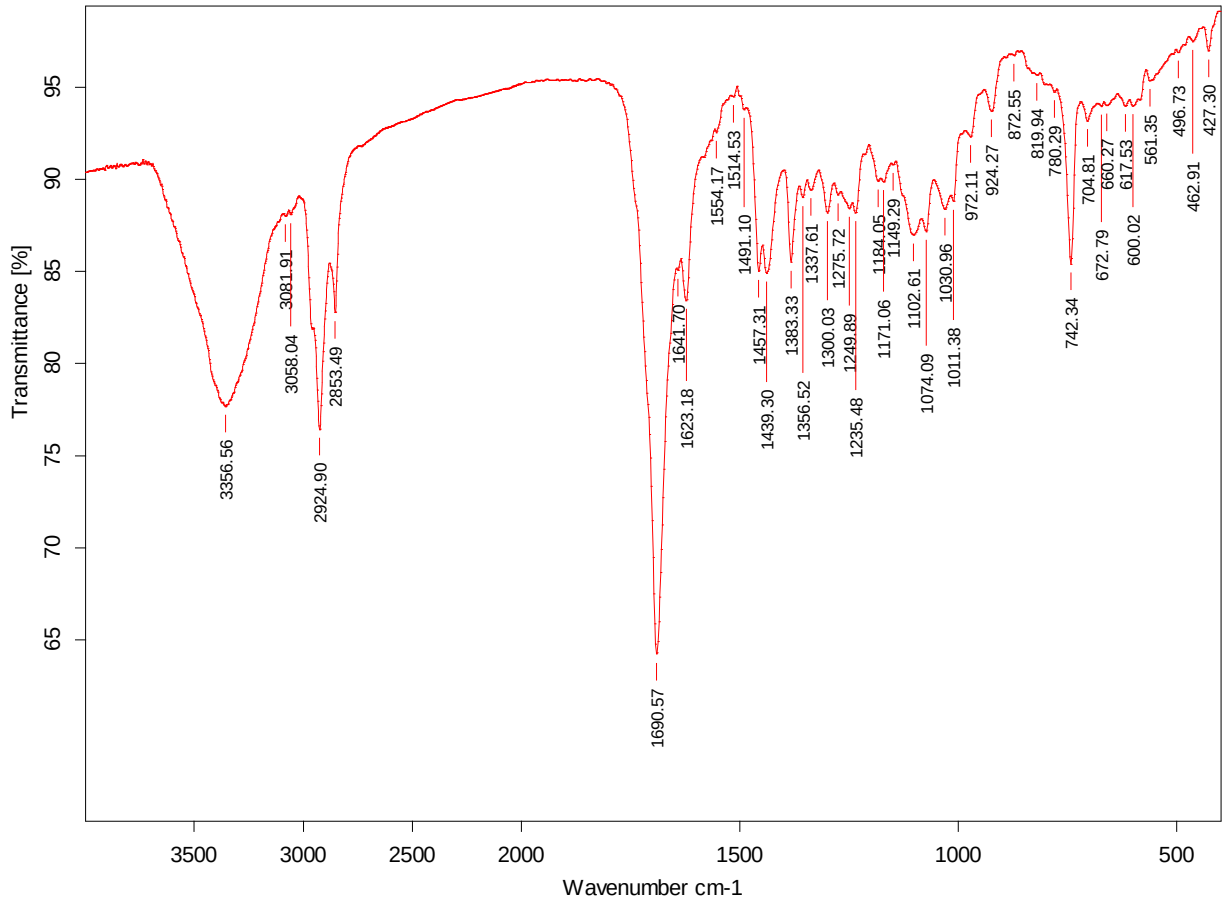


Fig. S82. ^{1}H NMR (400 MHz, CD_3OD) spectrum of *S*-MTPA esters of **6**.

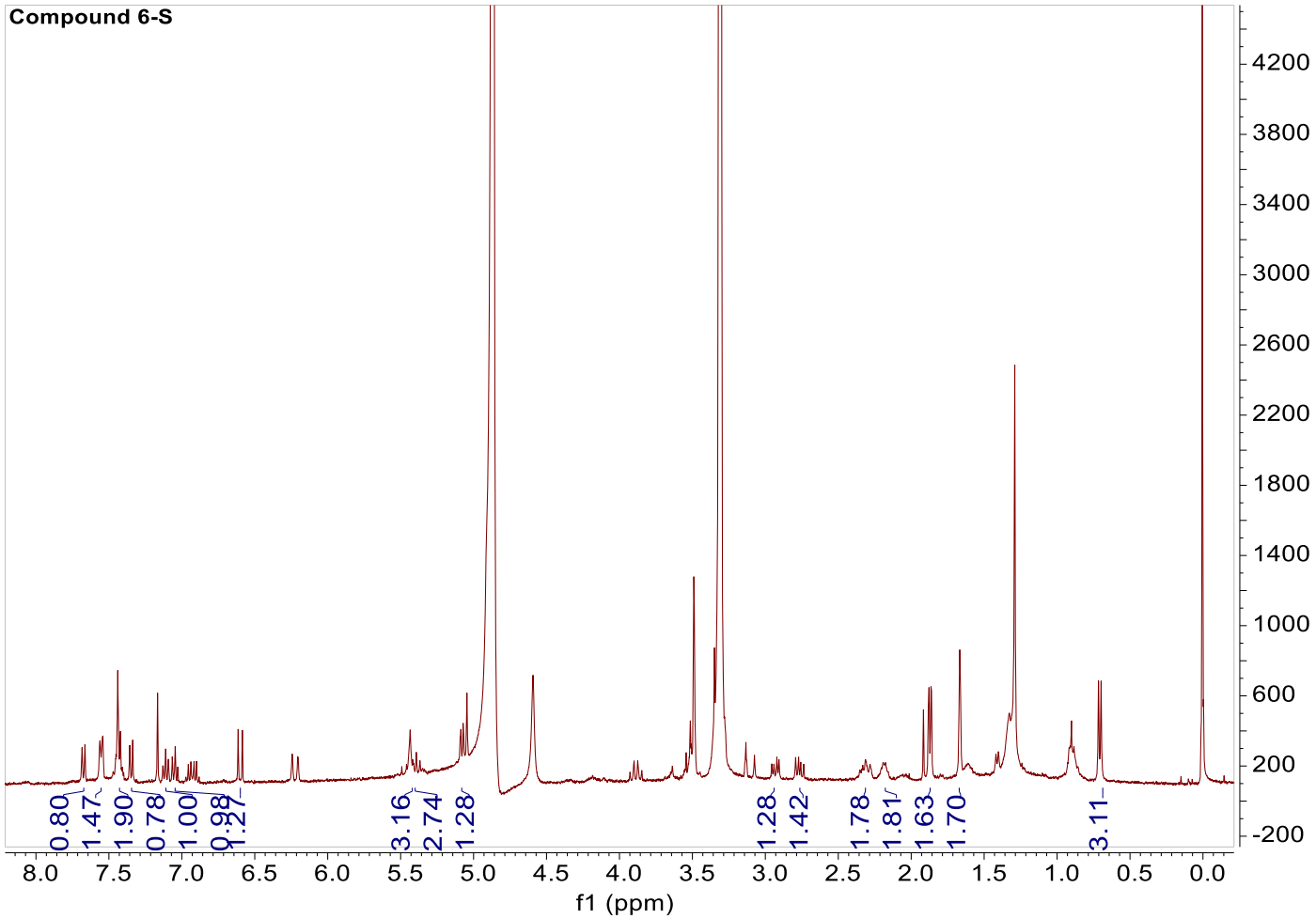


Fig. S83. ^{1}H NMR (400 MHz, CD_3OD) spectrum of *R*-MTPA esters of **6**.