

Supporting Information

Synthesis of A-ring quinolones, nine-membered oxolactams and spiroindoles by oxidative transformations of 2,3-indolotriterpenoids

Elmira F. Khusnutdinova,^a Oxana B. Kazakova,^{a*} Alexander N. Lobov,^a Olga S. Kukovinets,^a Kyrill Yu. Suponitsky,^b Craig B. Meyers,^c Mark N. Prichard^d

^aUfa Institute of Chemistry – Subdivision of the Ufa Federal Research Centre of Russian Academy of Sciences, Ufa 450054, Russian Federation. Fax: +73472356066.

^bA.N. Nesmeyanov Institute of Organoelement Compounds, Russian Academy of Sciences, Moscow 119334, Russian Federation.

^cPenn State College of Medicine, Hershey, PA 17033, USA.

^dUniversity of Alabama at Birmingham, Birmingham, AL 35233, USA.

E-mail: obf@anrb.ru;

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1. Instrumentation

1D and 2D NMR spectra were recorded at 298 K on a Bruker *Avance III* 500 MHz instrument with PABBO X{ ^1H } direct detection probe in deuterated chloroform (Cambridge Isotope Laboratories, Inc., degree of deuteration 99.8%). Chemical shifts for carbon and proton are reported in parts per million (ppm) referenced to 0.0 ppm of tetramethylsilane as the internal standard.

The ^1H NMR spectra were acquired with a spectral width of 5.6 kHz and 32k data points and 8 scans, providing a digital resolution of ca. 0.5 Hz (^1H 90° pulse width = 11.5 μs). For $^{13}\text{C}\{^1\text{H}\}$ NMR spectra (WALTZ-16), a spectral width of 29.7 kHz was used with 64k data points and required quantity of scans (^{13}C 90° pulse width = 9.7 μs). Gradient selected $\{^1\text{H}, ^{13}\text{C}\}$ HSQC spectra were recorded using the Bruker sequence hsqcetgp. These data were collected with 4096 x 512 data points with 2 scans for each increment. The delay d4 was set to 1.72 ms. Gradient selected $\{^1\text{H}, ^{13}\text{C}\}$ HMBC spectra (hmbcgpndqf) were collected with 4096 x 512 data points with 4 scans for each increment. The delay d6 was set to 71.4 ms. Spectral widths of 6.0 and 29.7 kHz were used in the *F2* (^1H) and *F1* (^{13}C) domains, respectively. $\{^1\text{H}, ^{13}\text{C}\}$ HSQC and HMBC data were processed using a sine window in the *F2* and *F1* dimensions. $\{^1\text{H}, ^1\text{H}\}$ gs-COSY data were collected with 4K x 512 data points with 2 scans for each increment. For the $\{^1\text{H}, ^1\text{H}\}$ NOESY NMR experiments, the solution was degassed to remove any dissolved oxygen. The following parameters and procedures are commonly employed: spectral width 6.0 kHz, 4K data matrix and 256 time increments of 2 transients each, mixing time 0.5s. Fourier transformations were carried out with zero-filling using the shifted sine-bell apodization function in both dimensions.

2. NMR Spectra

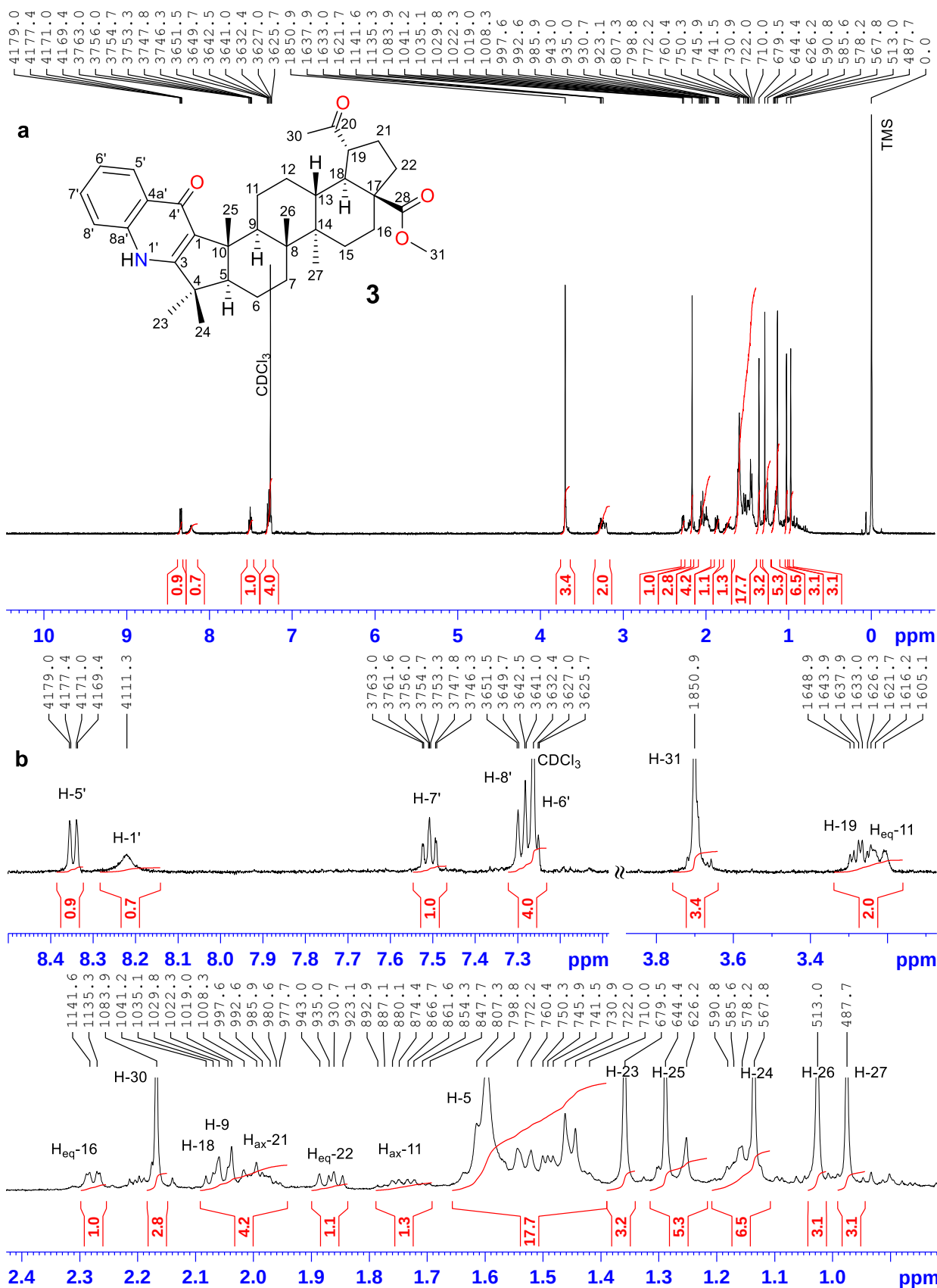


Table S1. Complete numerical listings of ^1H NMR peaks of compound **3** in CDCl_3 .

Peak	$\nu(\text{F1})$ [ppm]	$\nu(\text{F1})$ [Hz]	Intensity [rel]	Half width [Hz]
1	8.36	4179	0.39	1.8
2	8.35	4177.4	0.35	1.2
3	8.34	4171	0.38	3.4
4	8.34	4169.4	0.37	1.2
5	8.22	4111.3	0.14	0.6
6	7.52	3763	0.22	1.2
7	7.52	3761.6	0.21	1.2
8	7.51	3756	0.33	1.2
9	7.51	3754.7	0.43	3.7
10	7.5	3753.3	0.28	0.9
11	7.49	3747.8	0.27	1.8
12	7.49	3746.3	0.22	1.2
13	7.3	3651.5	0.37	1.2
14	7.3	3649.7	0.45	1.2
15	7.28	3642.5	0.62	1.5
16	7.28	3641	0.56	0.9
17	7.26	3632.4	4.4	1.2
18	7.25	3627	0.26	3.1
19	7.25	3625.7	0.24	0.9
20	3.7	1850.9	4.14	1.5
21	3.3	1648.9	0.14	2.7
22	3.29	1643.9	0.17	4
23	3.27	1637.9	0.25	4
24	3.27	1633	0.25	4.3
25	3.25	1626.3	0.17	0.6
26	3.24	1621.7	0.22	4
27	3.23	1616.2	0.17	0.6
28	3.21	1605.1	0.18	1.2
29	2.28	1141.6	0.29	3.4
30	2.27	1135.3	0.3	2.7
31	2.17	1083.9	3.89	1.8
32	2.08	1041.2	0.23	3.1
33	2.07	1035.1	0.28	2.7
34	2.06	1029.8	0.53	5.2
35	2.04	1022.3	0.36	1.8
36	2.04	1019	0.69	4.3
37	2.02	1008.3	0.32	4.3
38	1.99	997.6	0.44	7.3
39	1.98	992.6	0.29	3.4
40	1.97	985.9	0.23	2.7
41	1.96	980.6	0.14	1.2
42	1.95	977.7	0.12	0.9
43	1.89	943	0.26	3.4
44	1.87	935	0.24	3.4
45	1.86	930.7	0.3	3.7
46	1.85	923.1	0.23	3.1

47	1.79	892.9	0.09	0.9
48	1.77	887.1	0.09	0.6
49	1.76	880.1	0.15	1.2
50	1.75	874.4	0.17	2.1
51	1.73	866.7	0.17	2.7
52	1.72	861.6	0.17	1.5
53	1.71	854.3	0.12	2.1
54	1.7	847.7	0.11	0.6
55	1.61	807.3	1.06	3.7
56	1.6	798.8	1.97	11.9
57	1.54	772.2	0.66	10.4
58	1.52	760.4	0.64	9.2
59	1.5	750.3	0.55	5.8
60	1.49	745.9	0.55	4.6
61	1.48	741.5	0.55	6.1
62	1.46	730.9	1.22	7
63	1.44	722	0.98	6.1
64	1.42	710	0.28	0.6
65	1.36	679.5	2.86	2.4
66	1.29	644.4	3.63	1.8
67	1.25	626.2	0.83	4.6
68	1.18	590.8	0.38	1.8
69	1.17	585.6	0.45	1.5
70	1.16	578.2	0.7	4.6
71	1.14	567.8	3.64	2.1
72	1.03	513	2.96	2.7
73	0.98	487.7	3.03	2.1
74	0	0	12.46	2.1

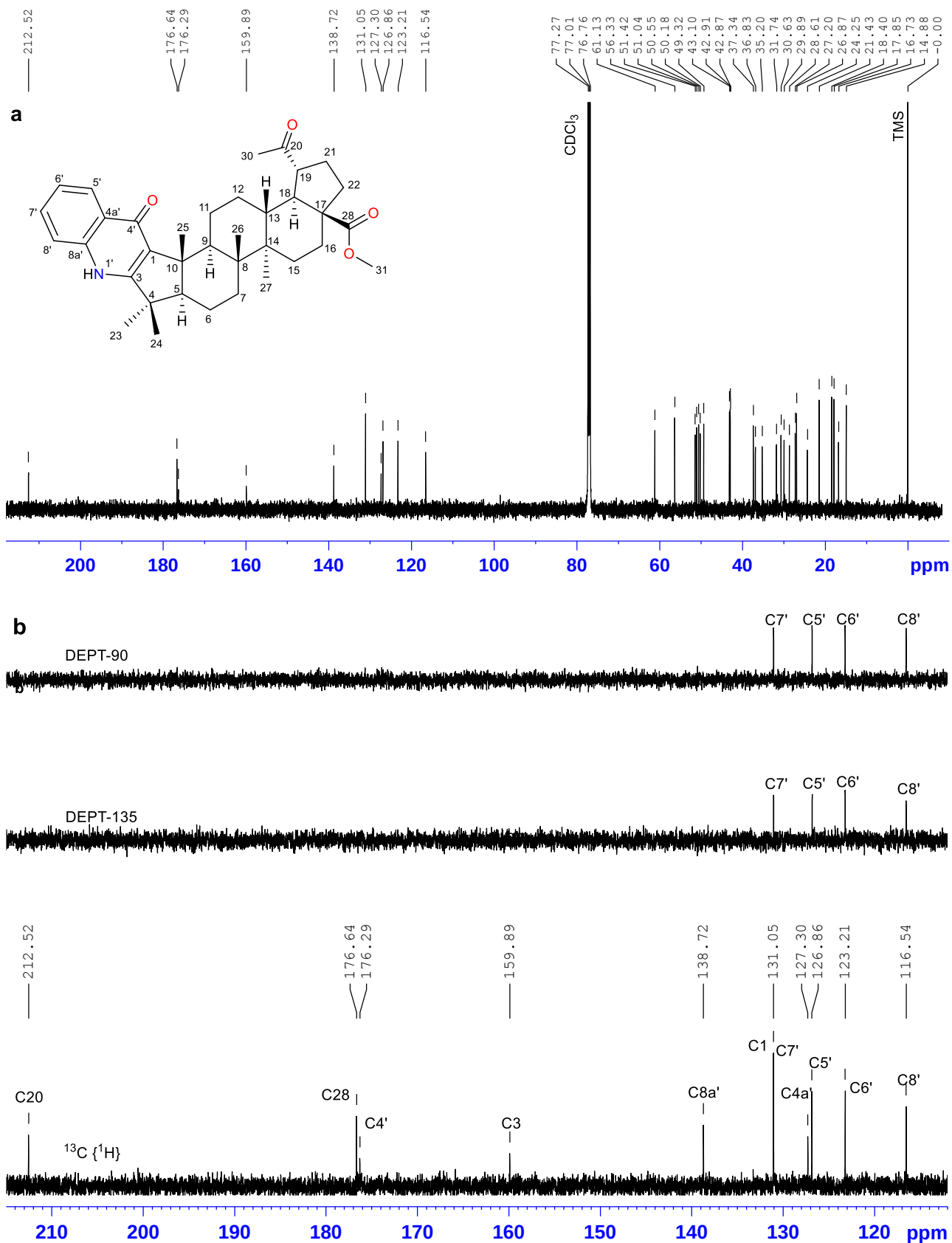


Figure S2. (a) Complete $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of compound **3** in CDCl_3 . (b) Downfield area of annotated $^{13}\text{C}\{^1\text{H}\}$ NMR and DEPT-135, DEPT-90 spectra of compound **3** in CDCl_3 .

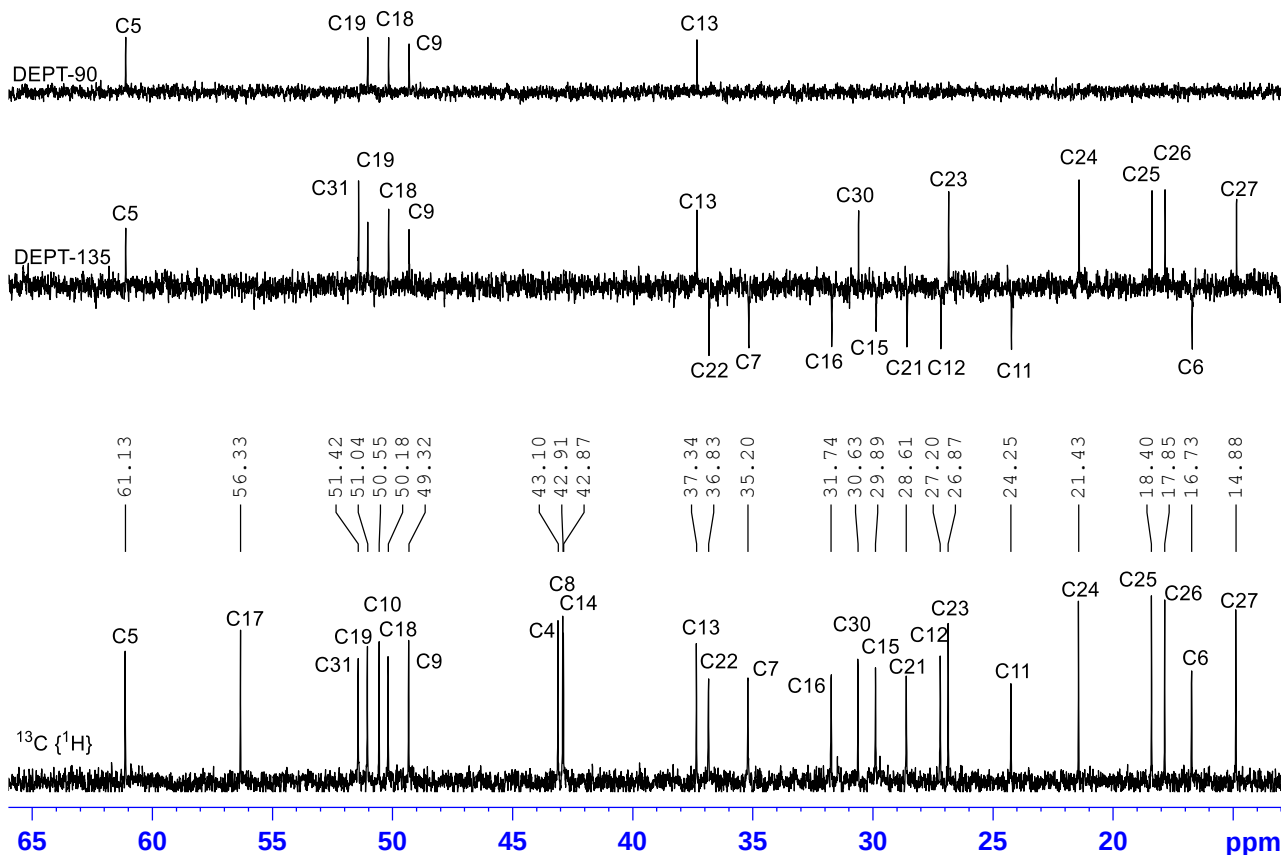


Figure S3. Upfield area of annotated $^{13}\text{C}\{^1\text{H}\}$ NMR and DEPT-135, DEPT-90 spectra of compound **3** in CDCl_3 .

Table S2. Complete numerical listings of ^{13}C NMR peaks of compound **3** in CDCl_3 .

Peak	$\nu(\text{F1})$ [ppm]	$\nu(\text{F1})$ [Hz]	Intensity [rel]	Half width [Hz]
1	212.52	26726.6	0.1	2.7
2	176.64	22214.2	0.14	0.9
3	176.29	22169.3	0.06	2.7
4	159.89	20107.9	0.06	2.7
5	138.72	17445.4	0.13	0.9
6	131.05	16481	0.26	1.8
7	127.3	16009	0.1	1.8
8	126.86	15954.2	0.19	1.8
9	123.21	15494.6	0.19	1.8
10	116.54	14656	0.16	1.8
11	77.27	9717	13.32	2.7
12	77.01	9685.1	13.5	2.7
13	76.76	9653.1	13.49	2.7
14	61.13	7687.2	0.22	0.9
15	56.33	7083.3	0.25	0.9
16	51.42	6466.9	0.21	0.9
17	51.04	6418.7	0.22	1.8
18	50.55	6357.6	0.23	0.9
19	50.18	6310.2	0.21	0.9
20	49.32	6202.4	0.23	1.8
21	43.1	5420.4	0.27	0.9

22	42.91	5395.8	0.27	0.9
23	42.87	5391.2	0.25	0.9
24	37.34	4695.5	0.23	1.8
25	36.83	4632.2	0.17	2.7
26	35.2	4426.2	0.18	2.7
27	31.74	3991.1	0.18	2.7
28	30.63	3851.4	0.21	0.9
29	29.89	3759.4	0.19	1.8
30	28.61	3597.8	0.18	1.8
31	27.2	3420.3	0.21	1.8
32	26.87	3378.7	0.26	0.9
33	24.25	3050	0.16	1.8
34	21.43	2695.6	0.3	0.9
35	18.4	2314	0.31	0.9
36	17.85	2245	0.3	0.9
37	16.73	2103.7	0.19	1.8
38	14.88	1871.8	0.28	0.9
39	0	0	1.29	0.9

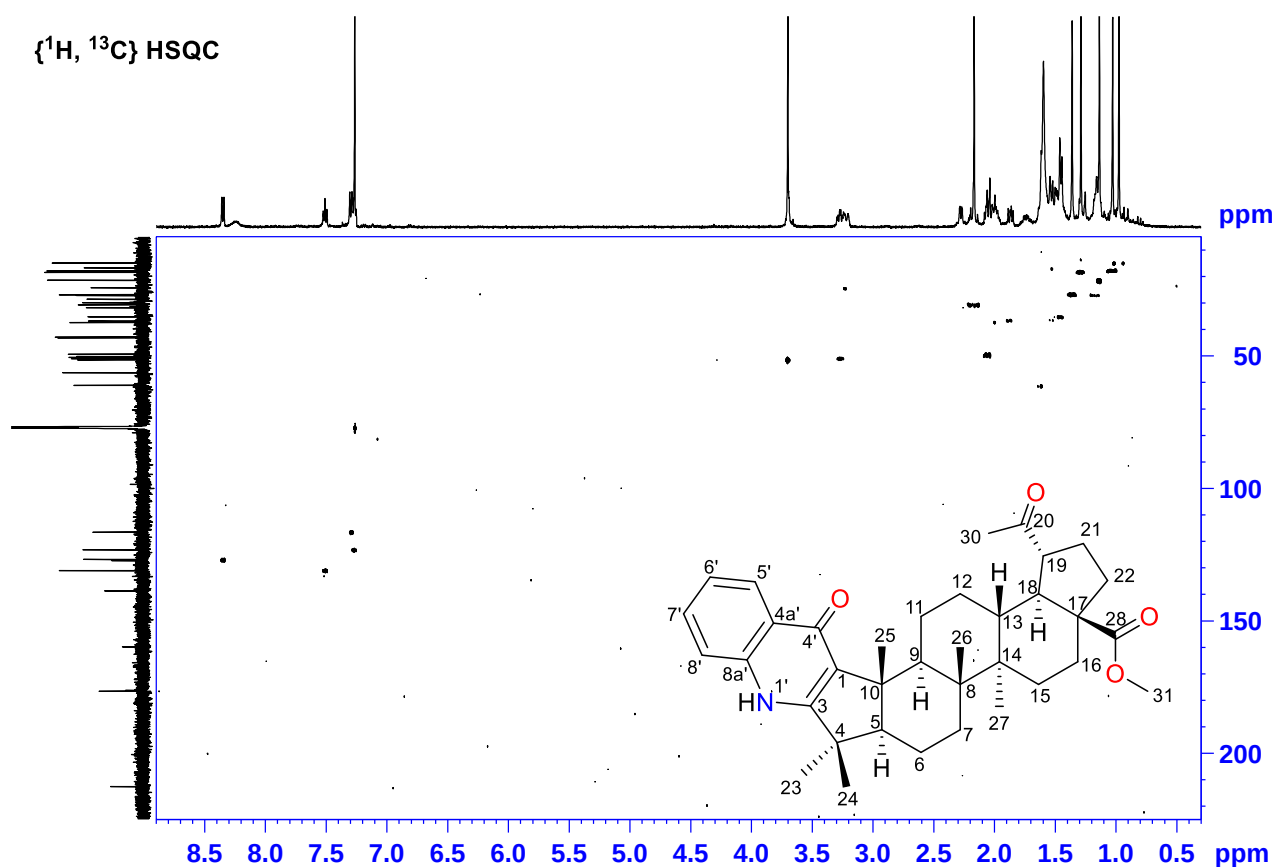
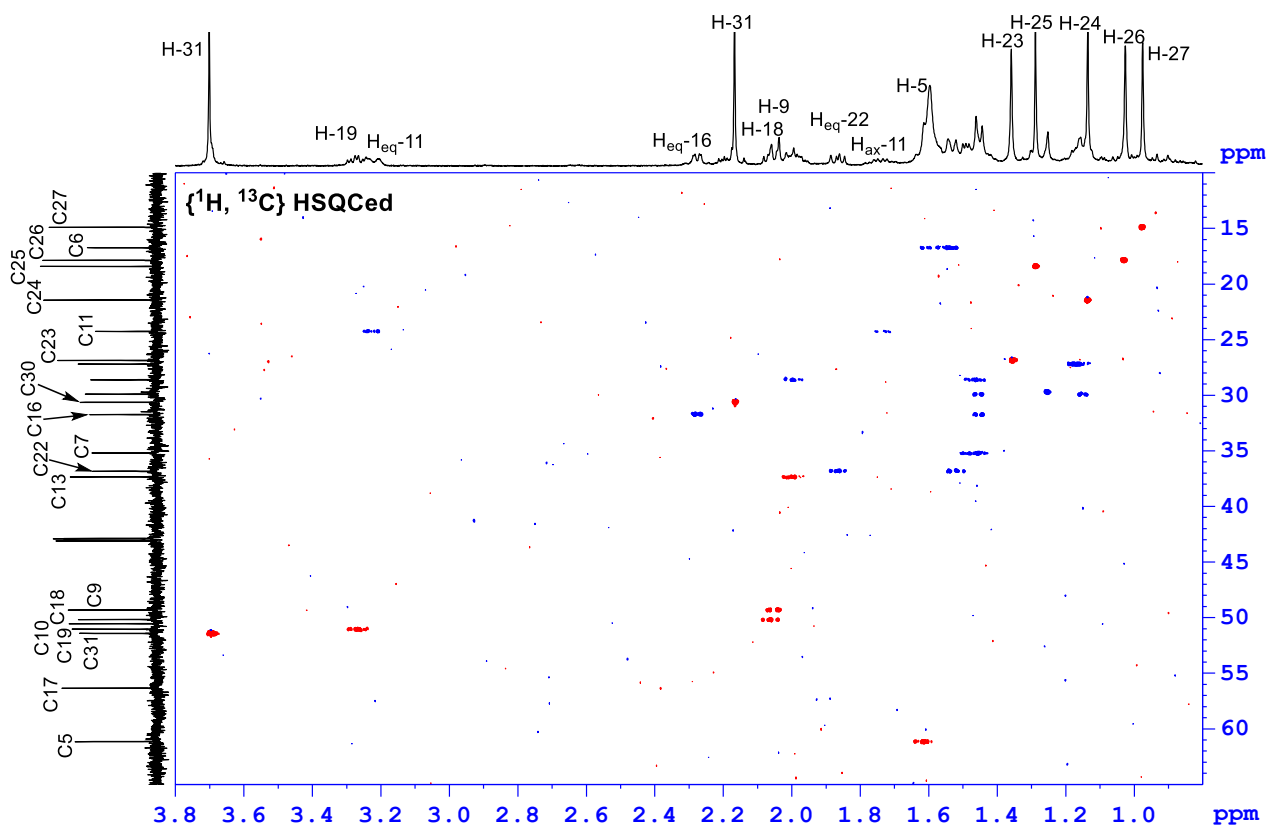
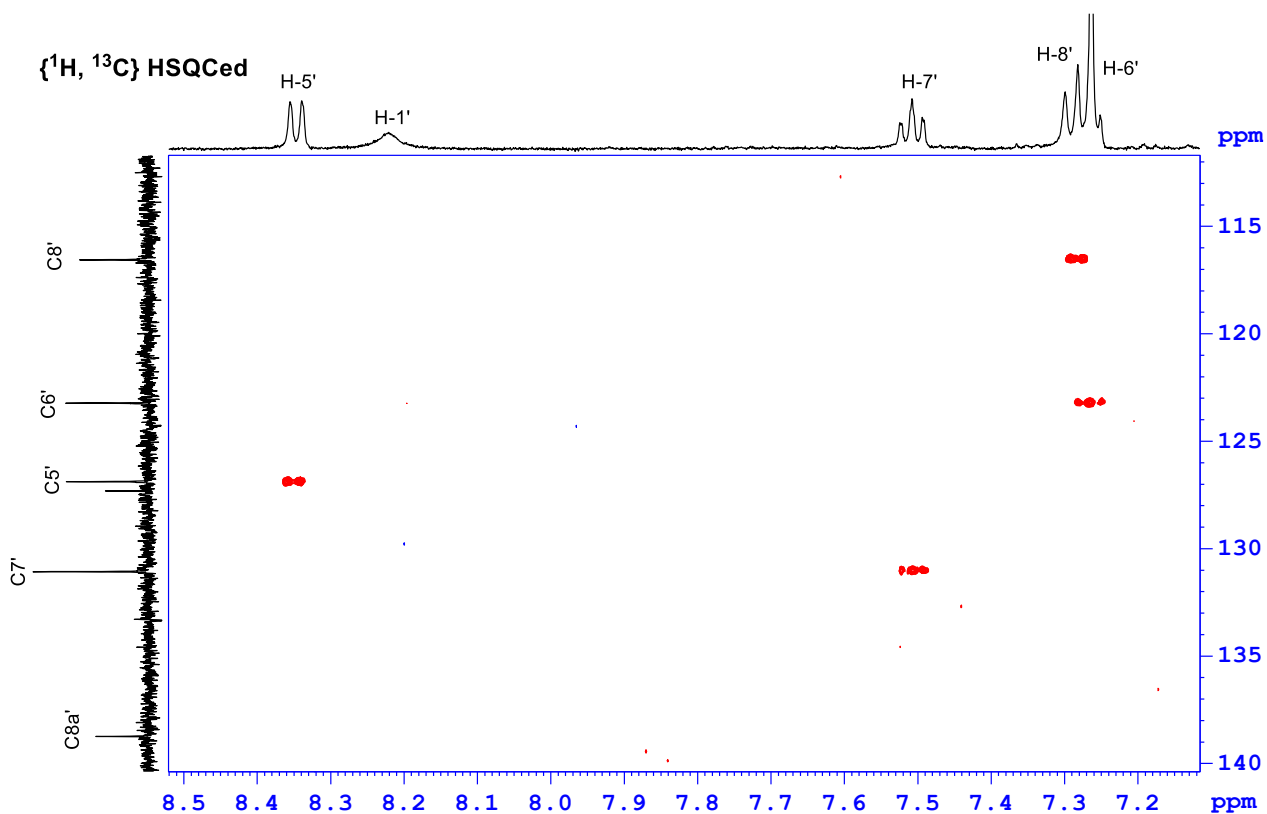


Figure S4. Complete $\{^1\text{H}, ^{13}\text{C}\}$ HSQC NMR spectrum of compound **3** in CDCl_3 .



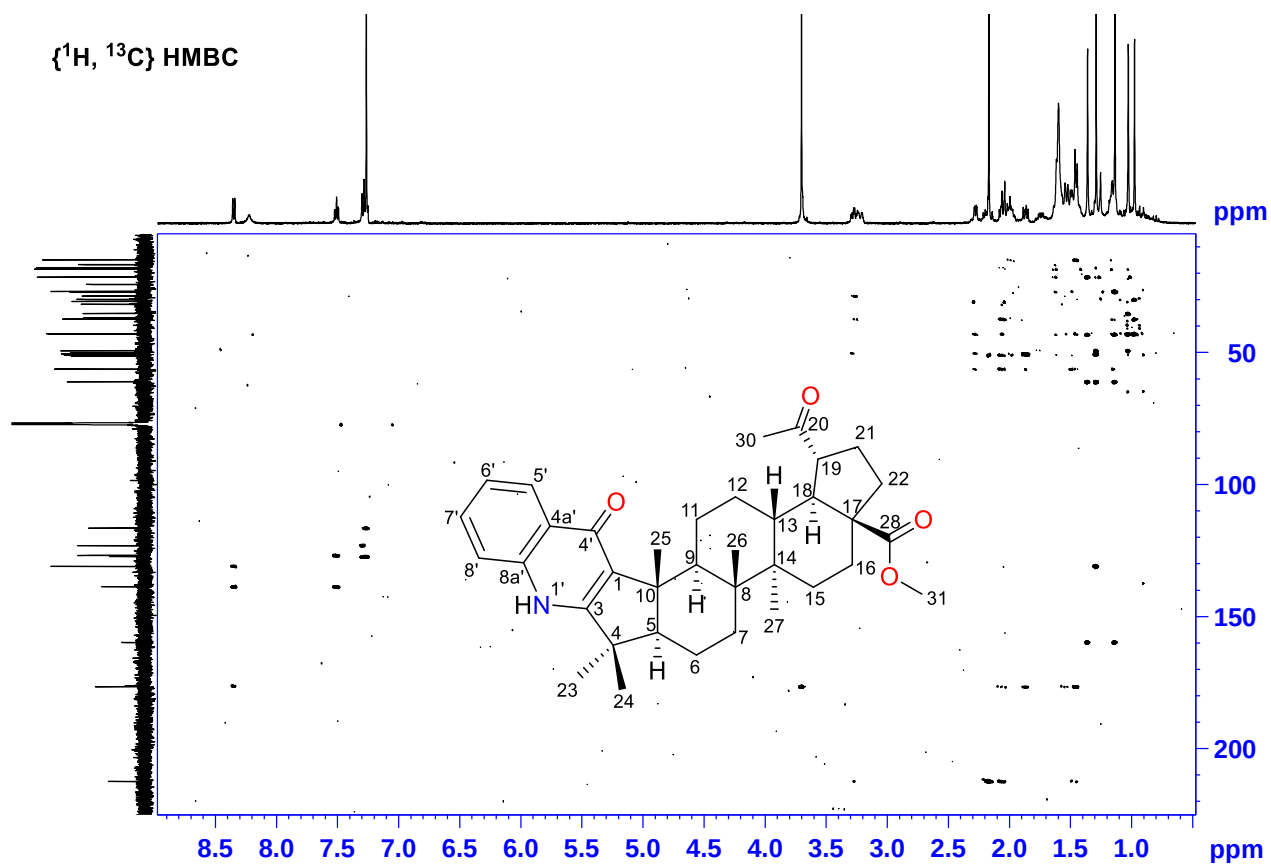


Figure S7. Complete $\{^1\text{H}, ^{13}\text{C}\}$ HMBC NMR spectrum of compound **3** in CDCl_3 .

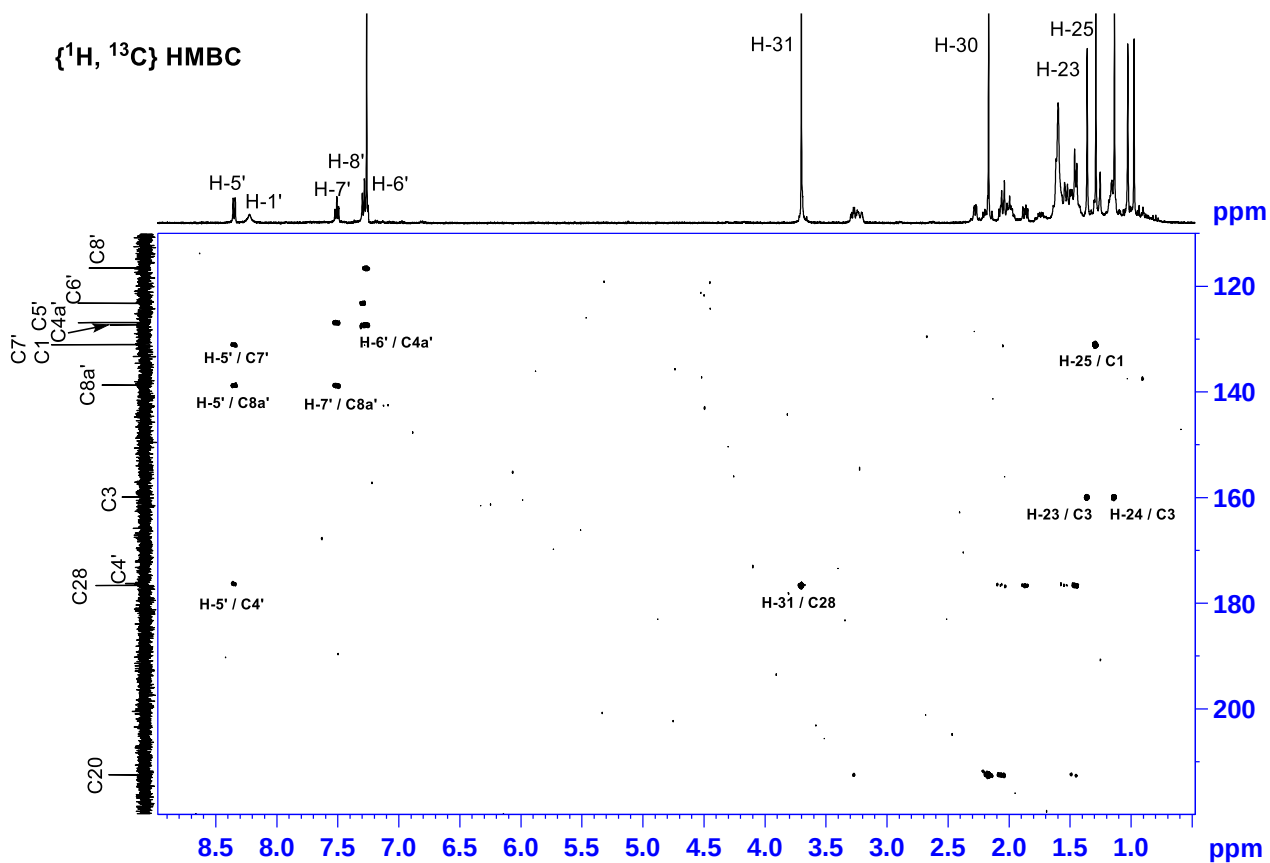


Figure S8. Downfield area of annotated $\{^1\text{H}, ^{13}\text{C}\}$ HMBC NMR spectrum of compound **3** in CDCl_3 .

$\{^1\text{H}, ^1\text{H}\}$ COSY

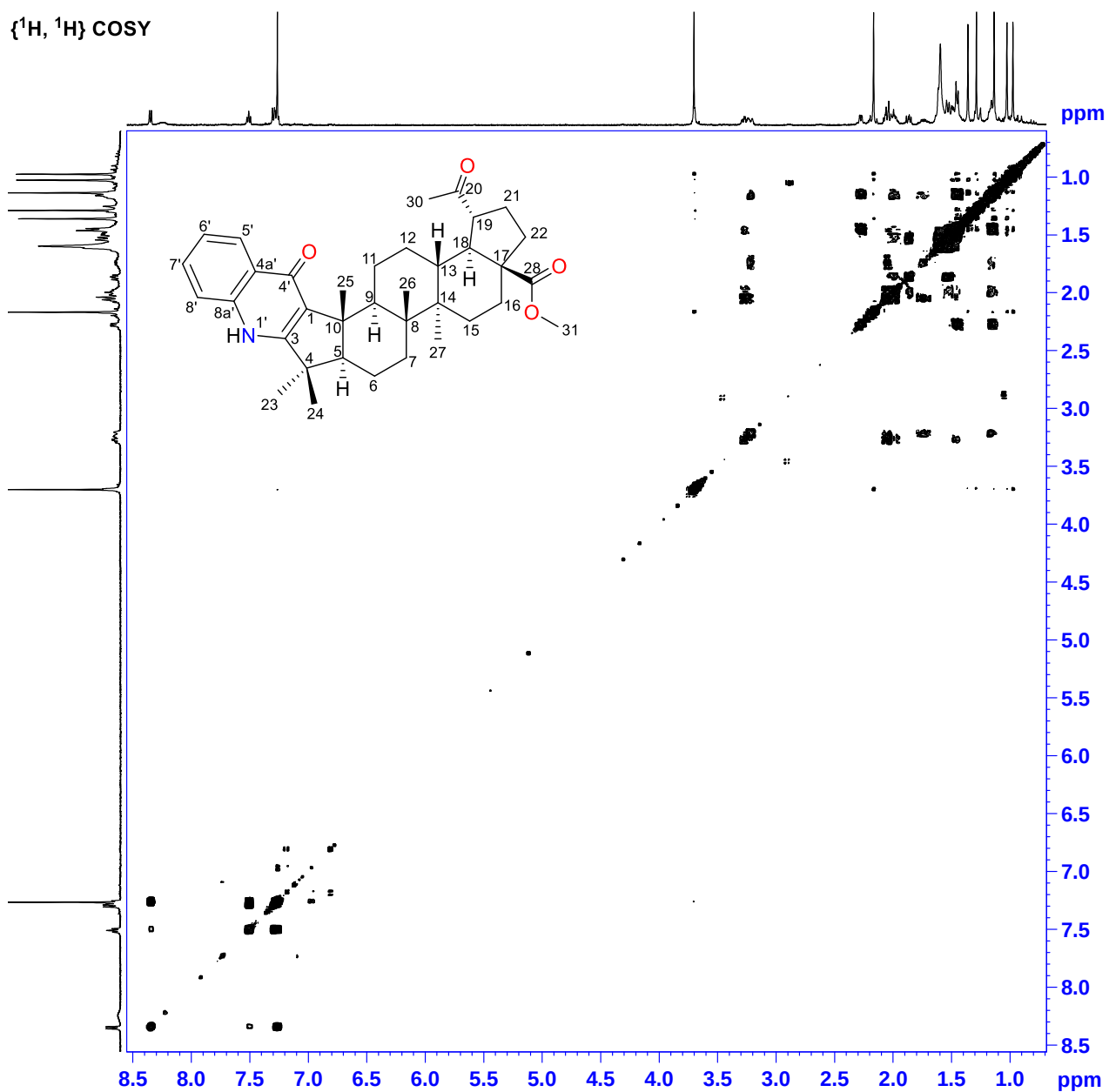


Figure S9. Complete $\{^1\text{H}, ^1\text{H}\}$ COSY NMR spectrum of compound **3** in CDCl_3 .

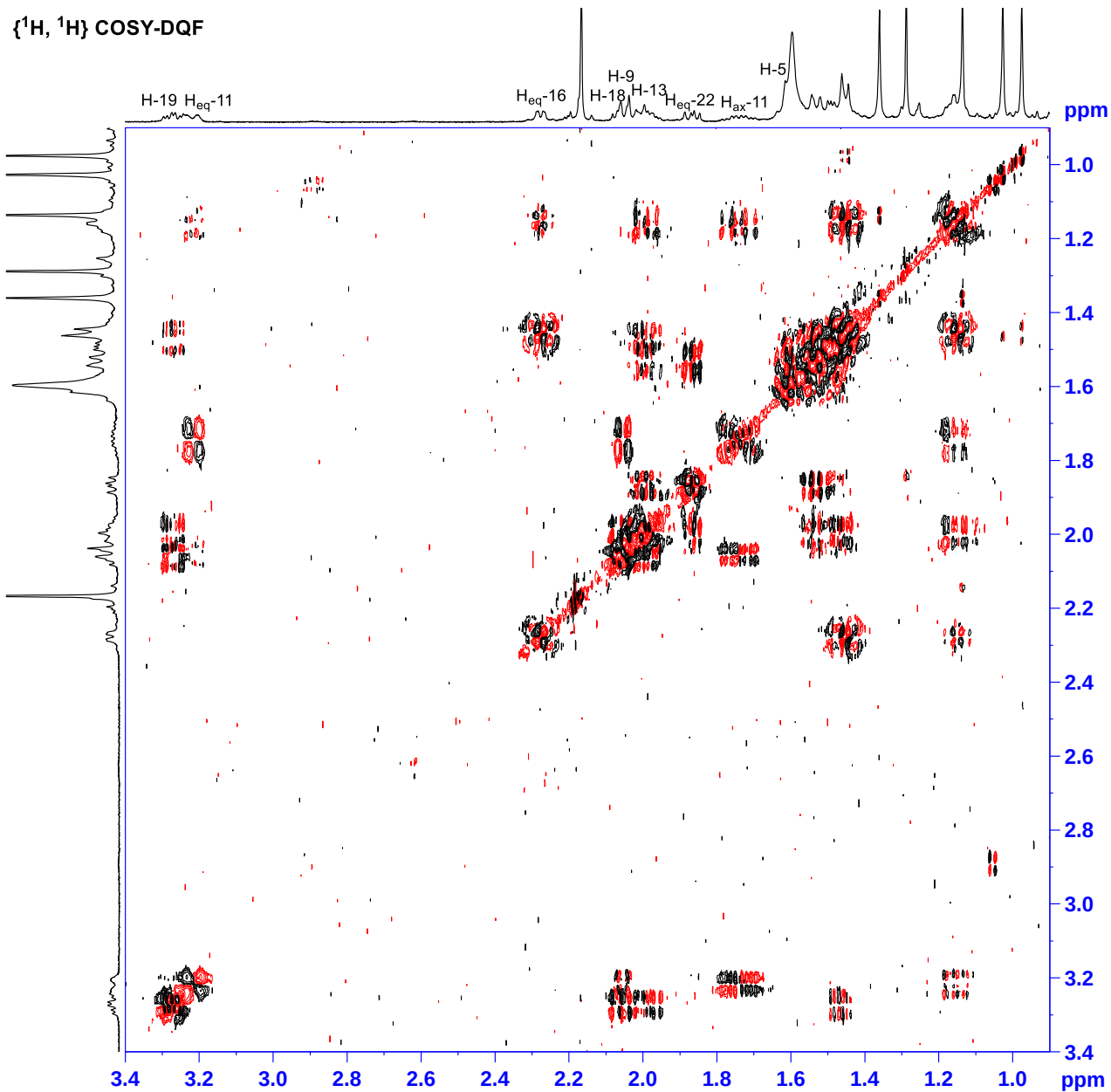


Figure S10. Upfield area of $\{^1\text{H}, ^1\text{H}\}$ COSY-DQF NMR spectrum of compound **3** in CDCl_3 .

$\{^1\text{H}, ^1\text{H}\}$ NOESY

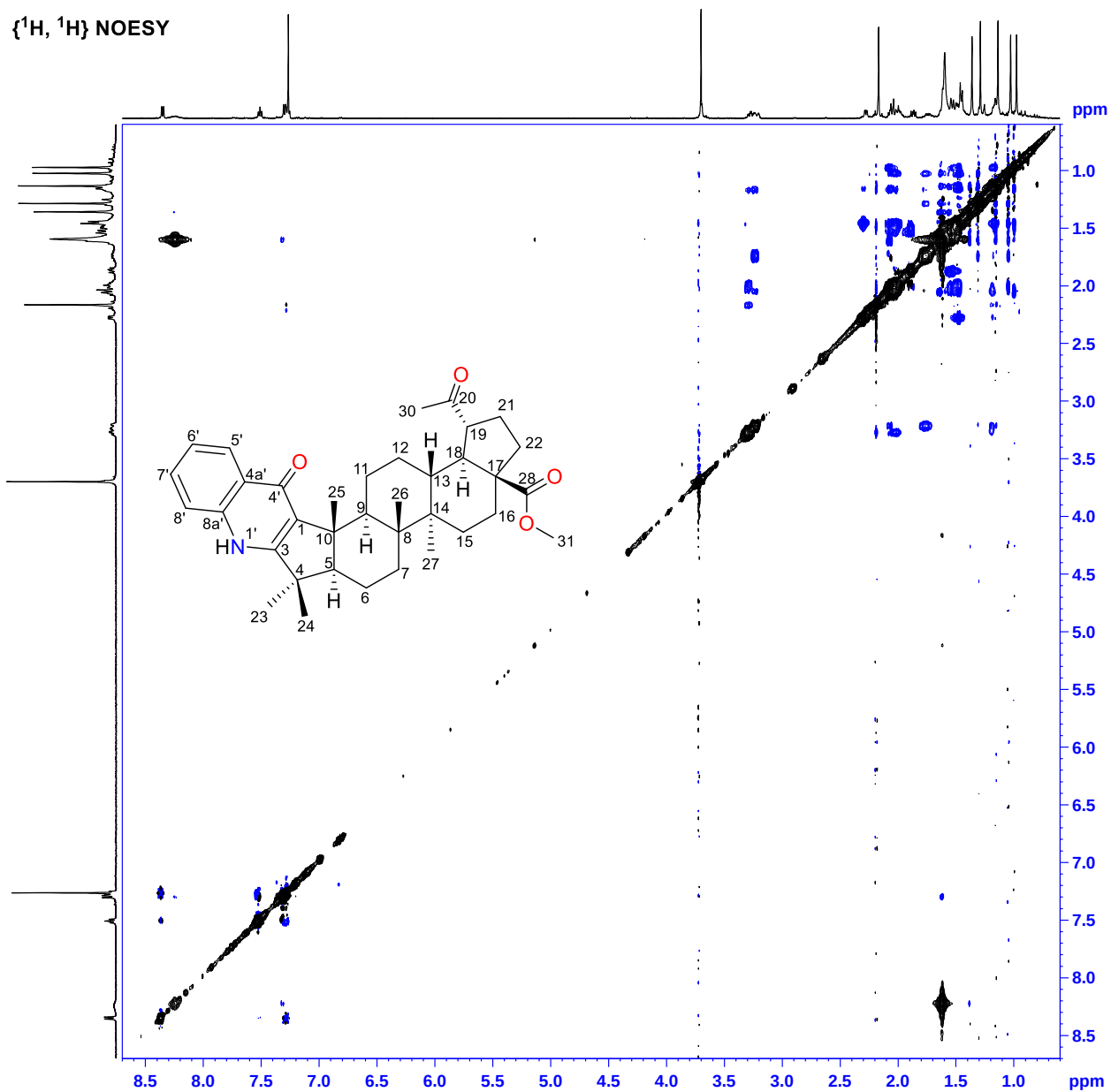


Figure S11. Complete $\{^1\text{H}, ^1\text{H}\}$ NOESY NMR spectrum of compound **3** in CDCl_3 .

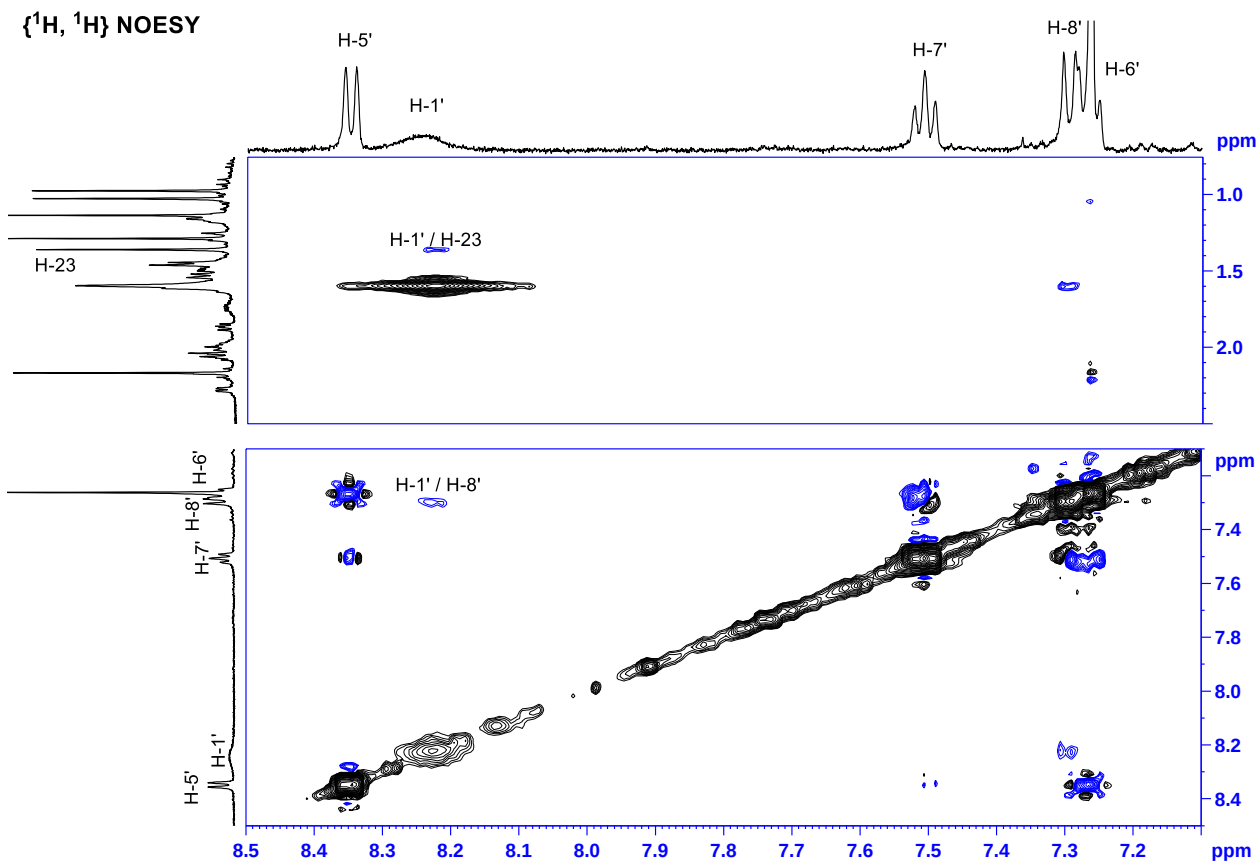


Figure S12. Detailed and annotated $\{^1\text{H}, ^1\text{H}\}$ NOESY NMR spectrum of compound **3** in CDCl_3 .

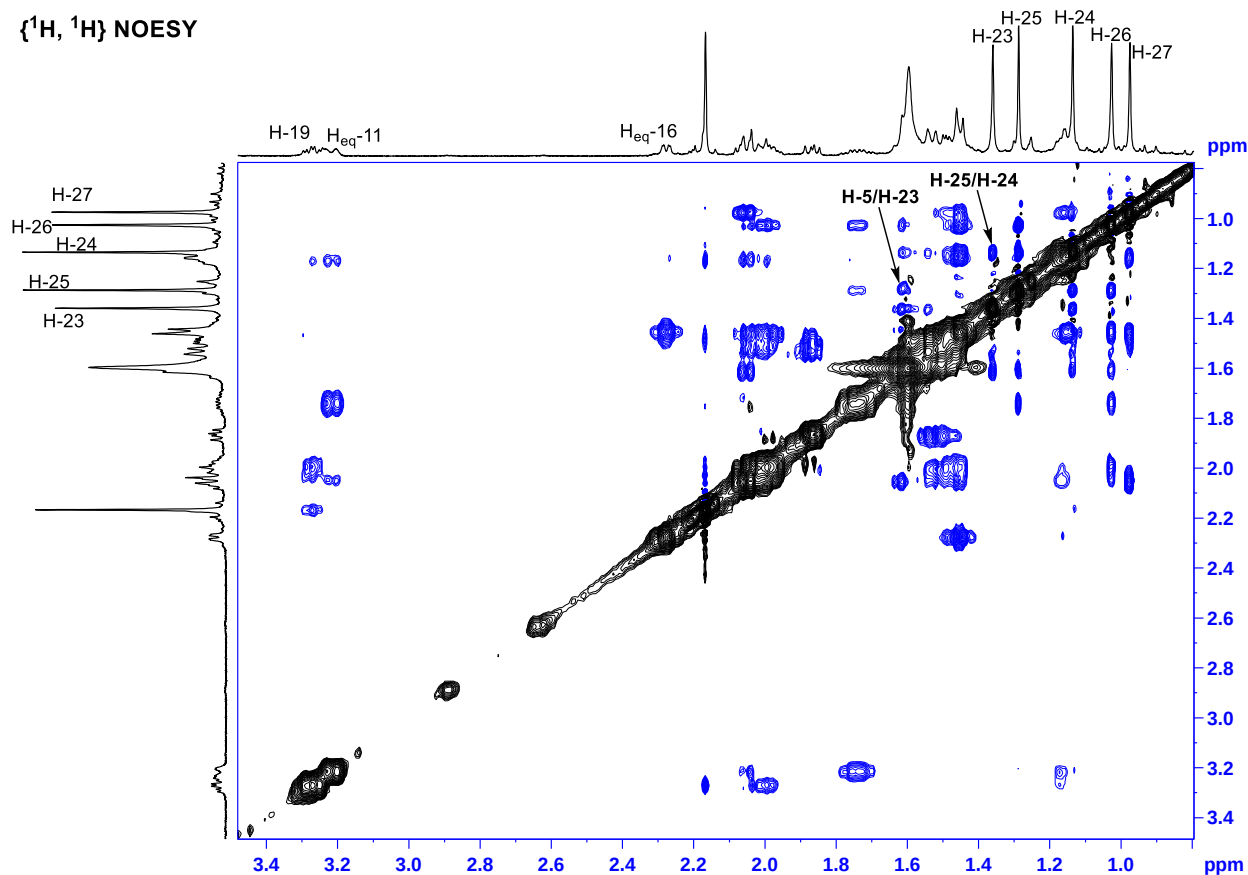


Figure S13. Upfield area of $\{^1\text{H}, ^1\text{H}\}$ NOESY NMR spectrum of compound **3** in CDCl_3 .

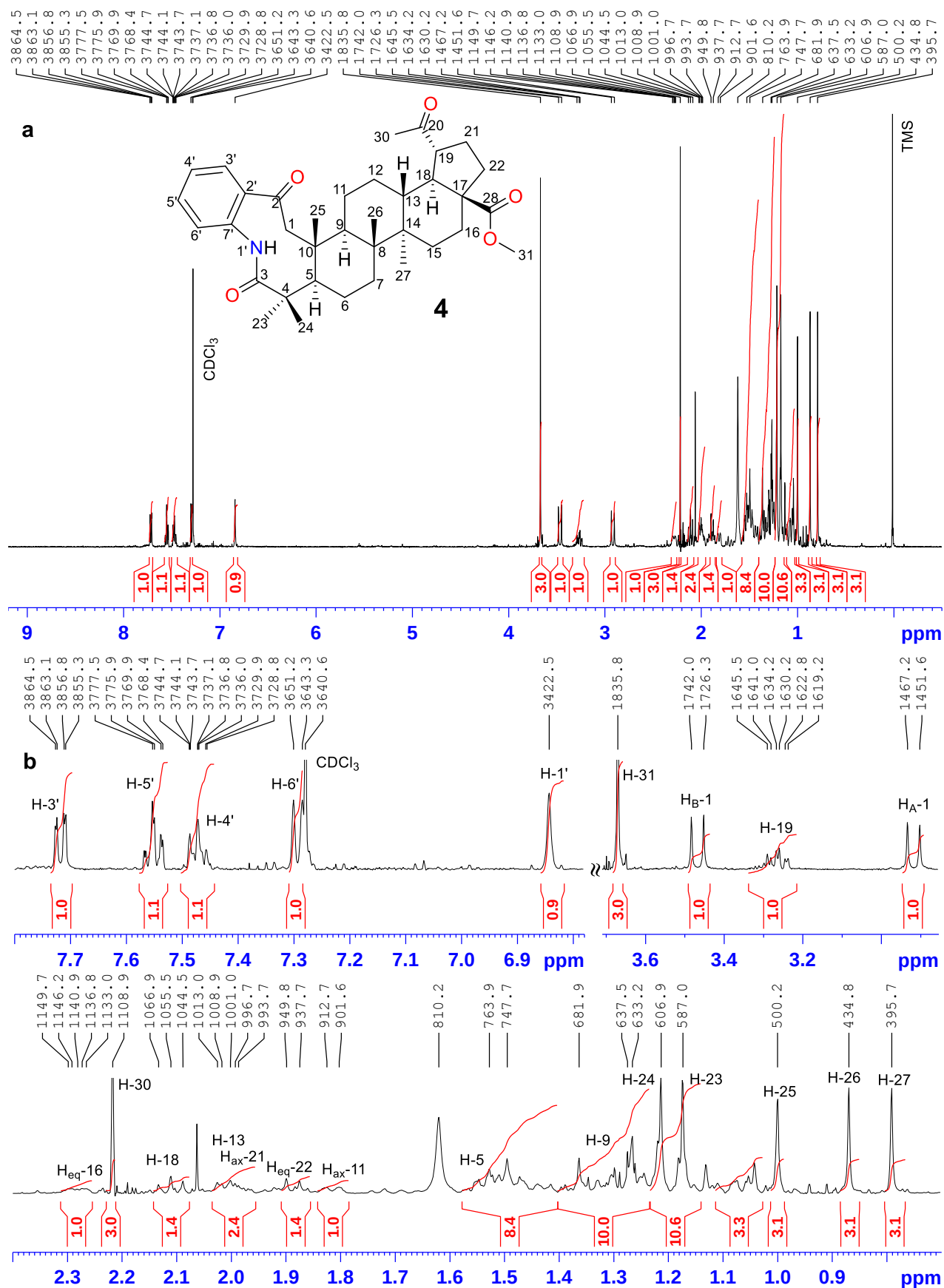


Table S3. Complete numerical listings of ¹H NMR peaks of compound **4** in CDCl₃.

Peak	ν(F1) [ppm]	ν(F1) [Hz]	Intensity [rel]	Half width [Hz]
1	7.73	3864.5	0.61	1.2
2	7.72	3863.1	0.69	1.2
3	7.71	3856.8	0.75	1.2
4	7.71	3855.3	0.75	1.8
5	7.55	3777.5	0.9	1.8
6	7.55	3775.9	0.7	1.2
7	7.54	3769.9	0.49	1.8
8	7.53	3768.4	0.39	1.2
9	7.49	3744.7	0.55	1.8
10	7.49	3744.1	0.47	1.8
11	7.49	3743.7	0.62	1.8
12	7.47	3737.1	0.79	2.4
13	7.47	3736.8	0.66	2.4
14	7.47	3736	0.75	2.4
15	7.46	3729.9	0.39	2.4
16	7.46	3728.8	0.37	2.4
17	7.3	3651.2	0.92	2.4
18	7.28	3643.3	0.92	3.1
19	7.28	3640.6	6.08	0.6
20	6.84	3422.5	1.01	3.1
21	3.67	1835.8	8.05	0.6
22	3.48	1742	0.85	1.2
23	3.45	1726.3	0.9	1.8
24	3.29	1645.5	0.25	1.8
25	3.28	1641	0.2	1.8
26	3.27	1634.2	0.31	3.1
27	3.26	1630.2	0.35	3.1
28	3.24	1622.8	0.18	3.1
29	3.24	1619.2	0.18	2.4
30	2.93	1467.2	0.77	1.8
31	2.9	1451.6	0.73	1.8
32	2.3	1149.7	0.22	4.3
33	2.29	1146.2	0.22	4.9
34	2.28	1140.9	0.2	2.4
35	2.27	1136.8	0.24	4.3
36	2.27	1133	0.22	5.5
37	2.22	1108.9	8.74	0.6
38	2.13	1066.9	0.42	3.1
39	2.11	1055.5	0.82	1.8
40	2.09	1044.5	0.59	1.8
41	2.03	1013	0.52	4.9
42	2.02	1008.9	0.46	3.7
43	2	1001	0.62	5.5
44	1.99	996.7	0.47	3.7
45	1.99	993.7	0.37	4.9
46	1.9	949.8	0.7	2.4

47	1.87	937.7	0.58	2.4
48	1.82	912.7	0.29	4.9
49	1.8	901.6	0.3	8.5
50	1.62	810.2	3.63	5.5
51	1.55	775.6	0.58	4.3
52	1.55	773.5	0.67	3.1
53	1.53	763.9	1.17	4.9
54	1.52	761.1	0.88	3.7
55	1.51	754.9	0.89	6.1
56	1.5	747.7	1.65	4.9
57	1.47	736.2	0.79	9.2
58	1.44	719.6	0.45	9.2
59	1.42	707.7	0.44	7.9
60	1.36	681.9	1.68	2.4
61	1.35	673.4	0.78	1.2
62	1.33	664.7	0.63	5.5
63	1.3	651.9	0.89	4.3
64	1.3	649.3	1.23	1.8
65	1.29	644.7	1.01	0.6
66	1.27	637.5	2.03	1.2
67	1.27	633.2	2.76	3.1
68	1.21	606.9	5.57	1.8
69	1.17	587	5.54	1.8
70	1.11	555	0.49	6.1
71	1.08	540.2	0.56	4.9
72	1.07	537.3	0.61	3.1
73	1.06	529.1	0.58	1.8
74	1.05	526.7	0.82	4.3
75	1	500.2	4.57	1.8
76	0.87	434.8	5.08	1.8
77	0.79	395.7	5.01	1.8
78	0	0	0.07	3.1

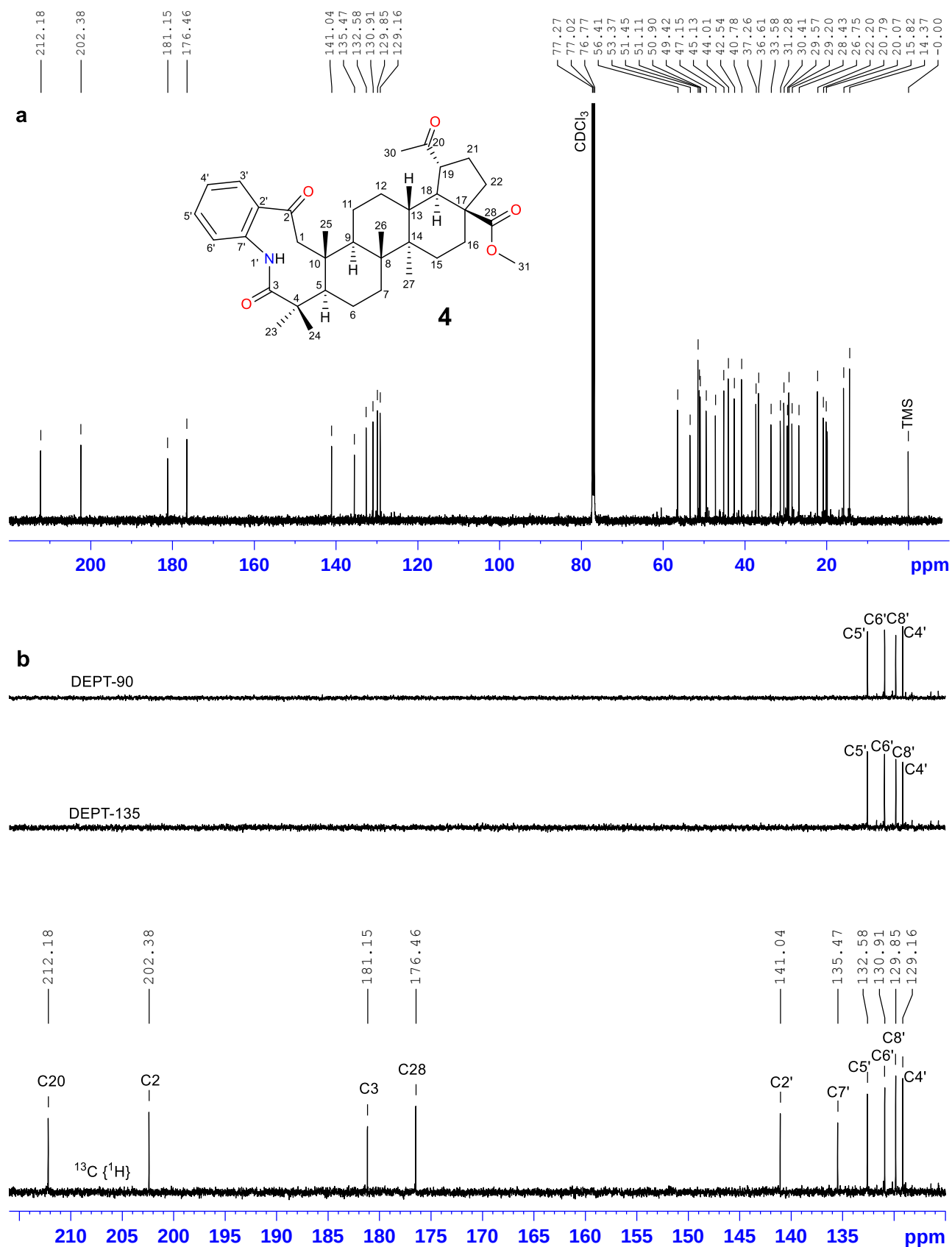


Figure S15. (a) Complete $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of compound **4** in CDCl_3 . (b) Downfield area of annotated $^{13}\text{C}\{^1\text{H}\}$ NMR and DEPT-135, DEPT-90 spectra of compound **4** in CDCl_3 .

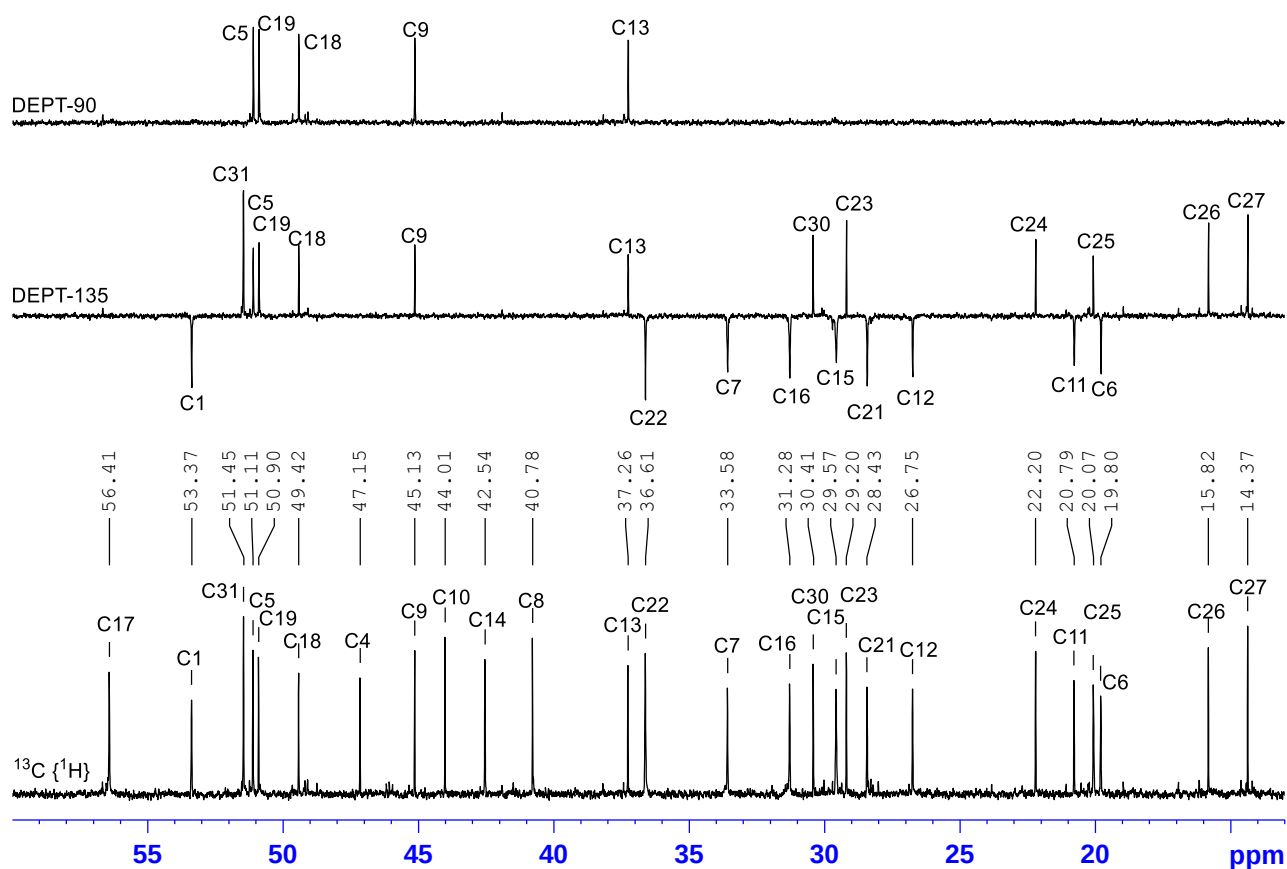


Figure S16. Upfield area of annotated $^{13}\text{C}\{^1\text{H}\}$ NMR and DEPT-135, DEPT-90 spectra of compound **4** in CDCl_3 .

Table S4. Complete numerical listings of ^{13}C NMR peaks of compound **4** in CDCl_3 .

Peak	$\nu(\text{F1})$ [ppm]	$\nu(\text{F1})$ [Hz]	Intensity [rel]	Half width [Hz]
1	212.18	26683	0.41	2.7
2	202.38	25451.1	0.44	1.8
3	181.15	22781.4	0.38	0.9
4	176.46	22190.7	0.48	0.9
5	141.04	17737.4	0.43	0.9
6	135.47	17036	0.39	0.9
7	132.58	16673.2	0.55	2.7
8	130.91	16463.3	0.58	1.8
9	129.85	16329.6	0.64	1.8
10	129.16	16243.3	0.63	1.8
11	77.27	9717.7	12.97	1.8
12	77.02	9685.8	13.5	1.8
13	76.77	9653.9	13.45	1.8
14	56.41	7094.5	0.64	1.8
15	53.37	6712	0.5	1.8
16	51.45	6470.5	0.94	1.8
17	51.11	6426.9	0.76	1.8
18	50.9	6400.5	0.72	1.8
19	49.42	6214.5	0.65	0.9
20	47.15	5929.7	0.63	0.9
21	45.13	5675.6	0.76	0.9

22	44.01	5534.9	0.83	0.9
23	42.54	5349.4	0.73	0.9
24	40.78	5128	0.82	0.9
25	37.26	4685.4	0.7	0.9
26	36.61	4604.3	0.76	2.7
27	33.58	4222.5	0.56	1.8
28	31.28	3933.8	0.58	3.6
29	30.41	3824.3	0.71	0.9
30	29.57	3719.2	0.55	3.6
31	29.2	3671.8	0.76	1.8
32	28.43	3575.7	0.56	1.8
33	26.75	3364.2	0.55	1.8
34	22.2	2792.4	0.8	1.8
35	20.79	2613.9	0.6	1.8
36	20.07	2524.1	0.58	3.6
37	19.8	2490.2	0.52	2.7
38	15.82	1990	0.77	0.9
39	14.37	1807.4	0.88	1.8
40	0	0	0.4	0.9

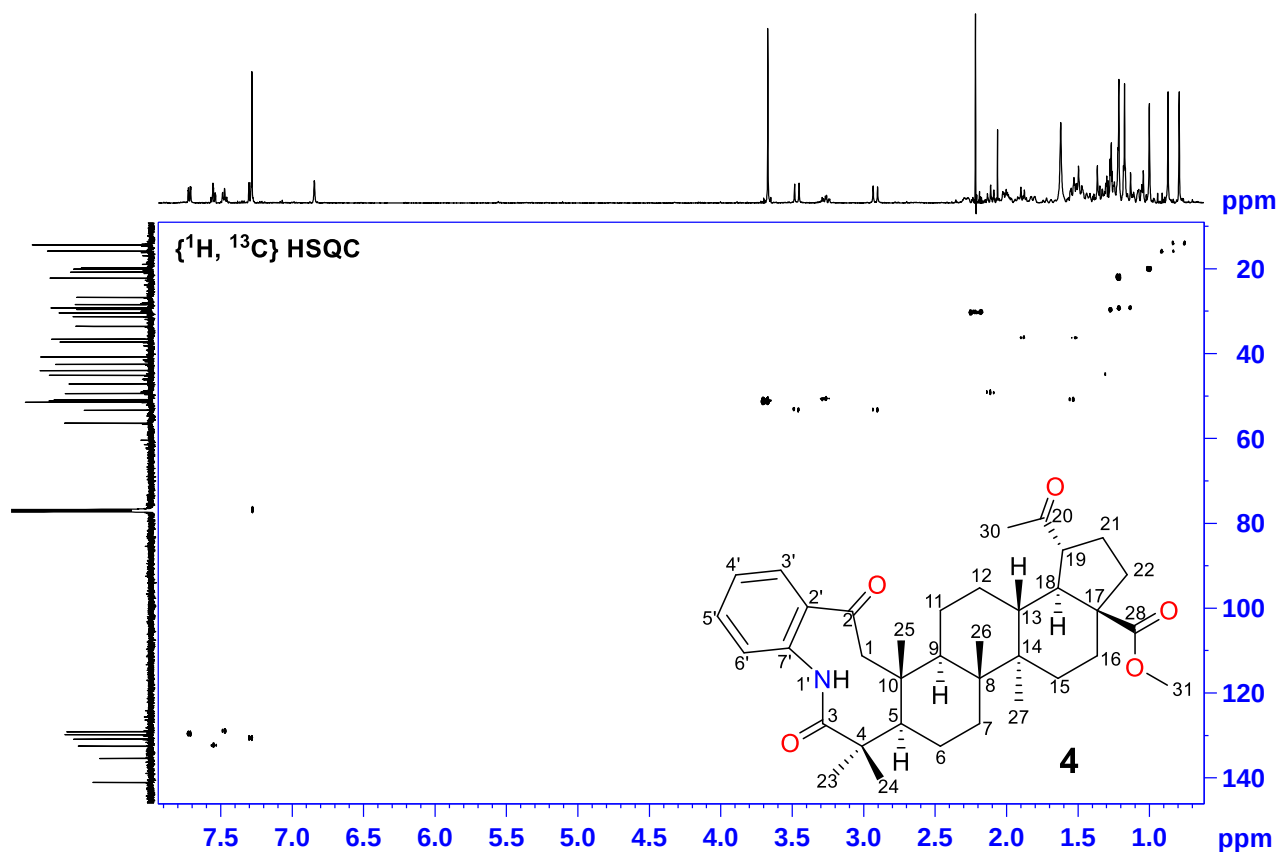


Figure S17. Complete $\{^1\text{H}, ^{13}\text{C}\}$ HSQC NMR spectrum of compound **4** in CDCl_3 .

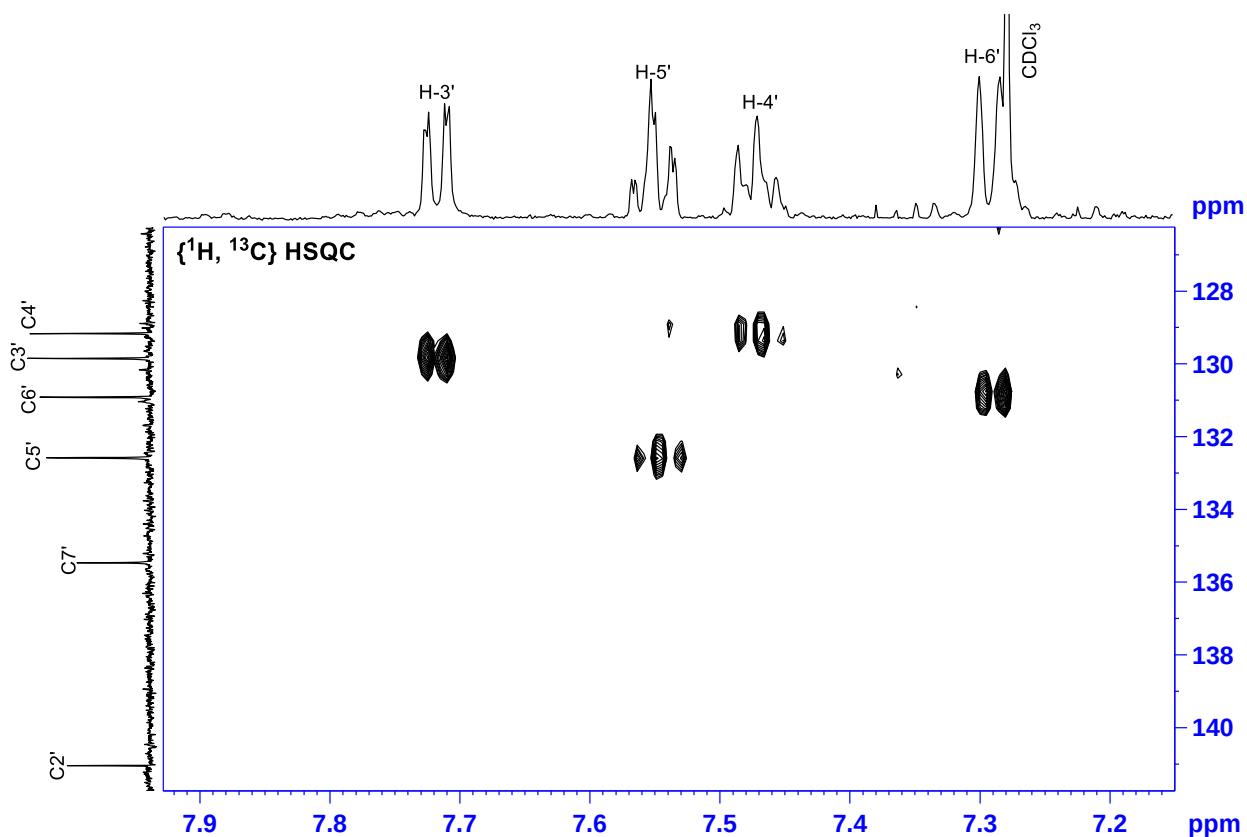


Figure S18. Downfield area of $\{^1\text{H}, ^{13}\text{C}\}$ HSQC NMR spectrum of compound **4** in CDCl_3 .

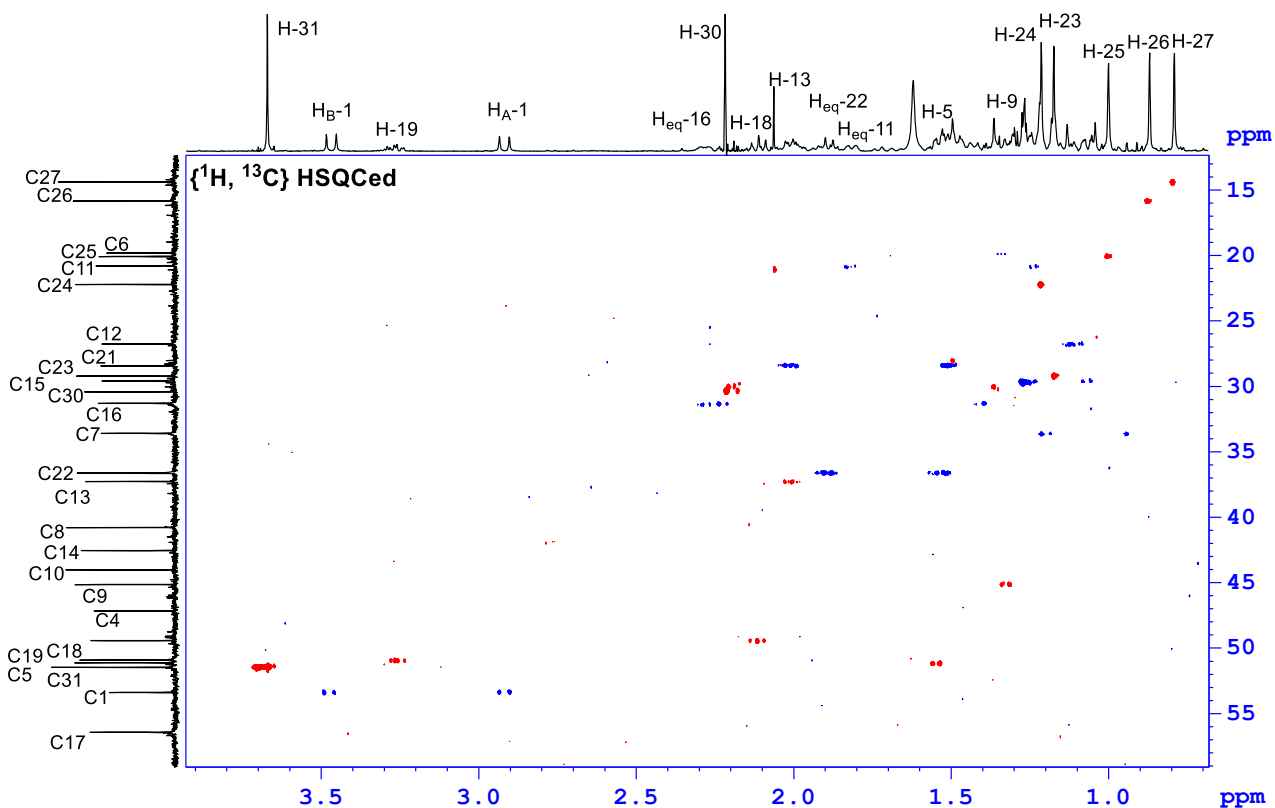


Figure S19. Upfield area of $\{^1\text{H}, ^{13}\text{C}\}$ HSQC multiplicity edited NMR spectrum of compound **4** in CDCl_3 .

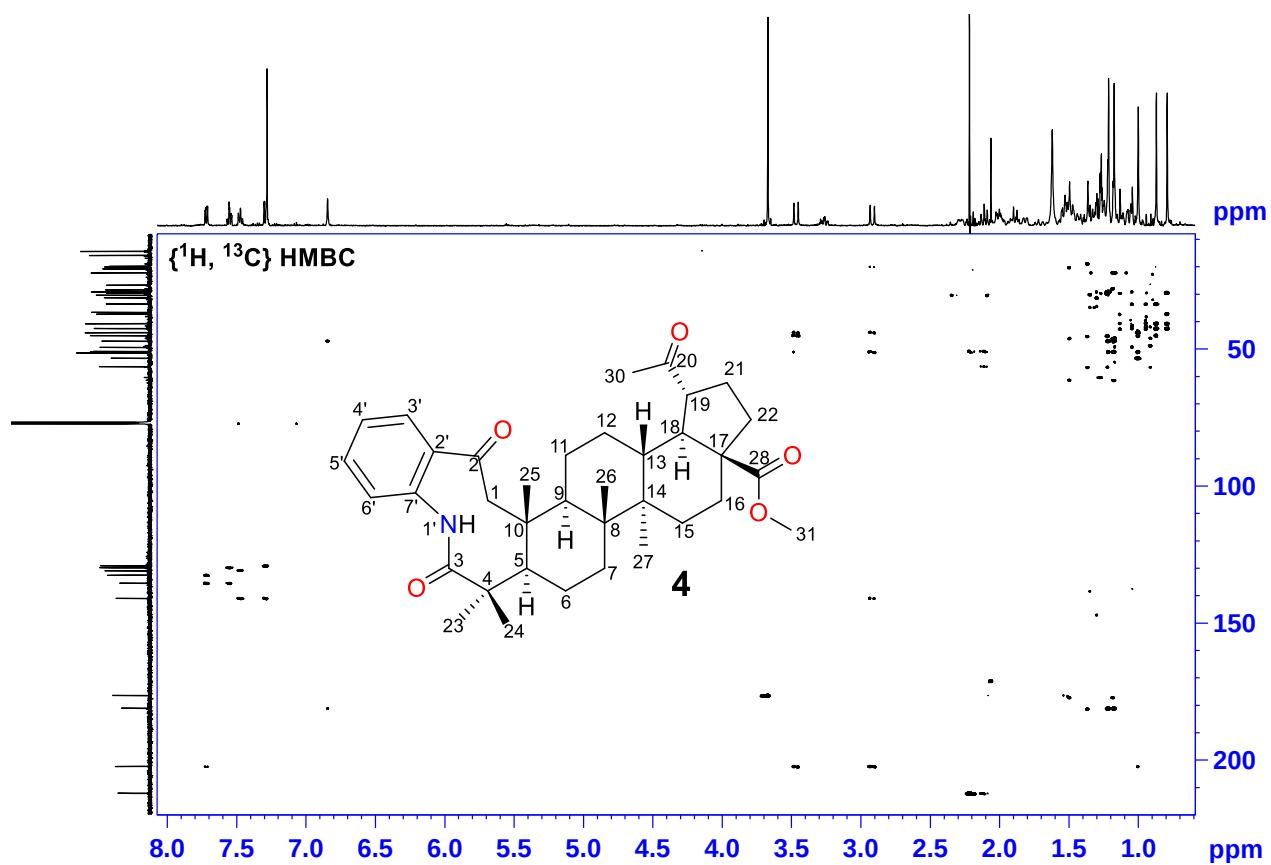


Figure S20. Complete $\{^1\text{H}, ^{13}\text{C}\}$ HMBC NMR spectrum of compound **4** in CDCl_3 .

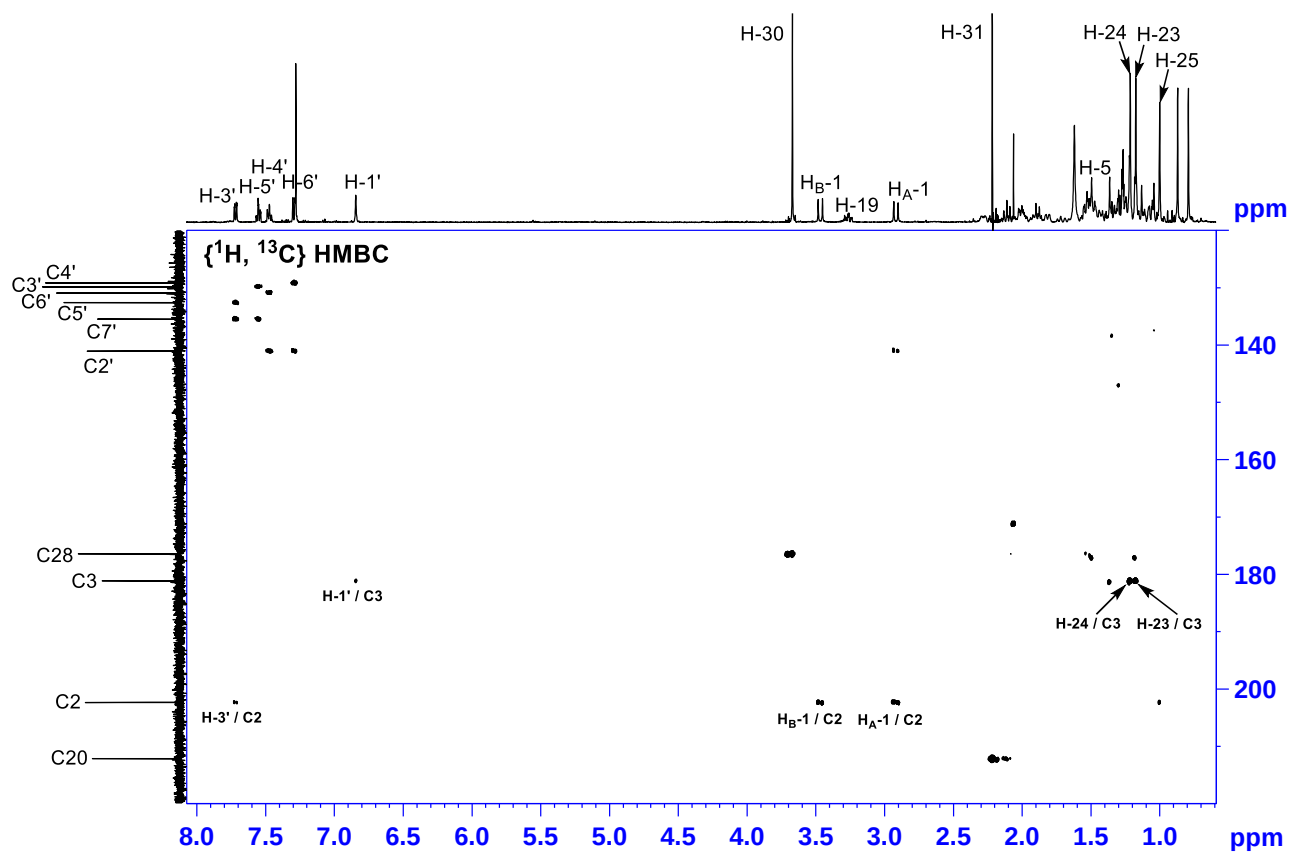


Figure S21. Downfield area of annotated $\{^1\text{H}, ^{13}\text{C}\}$ HMBC NMR spectrum of compound **4** in CDCl_3 .

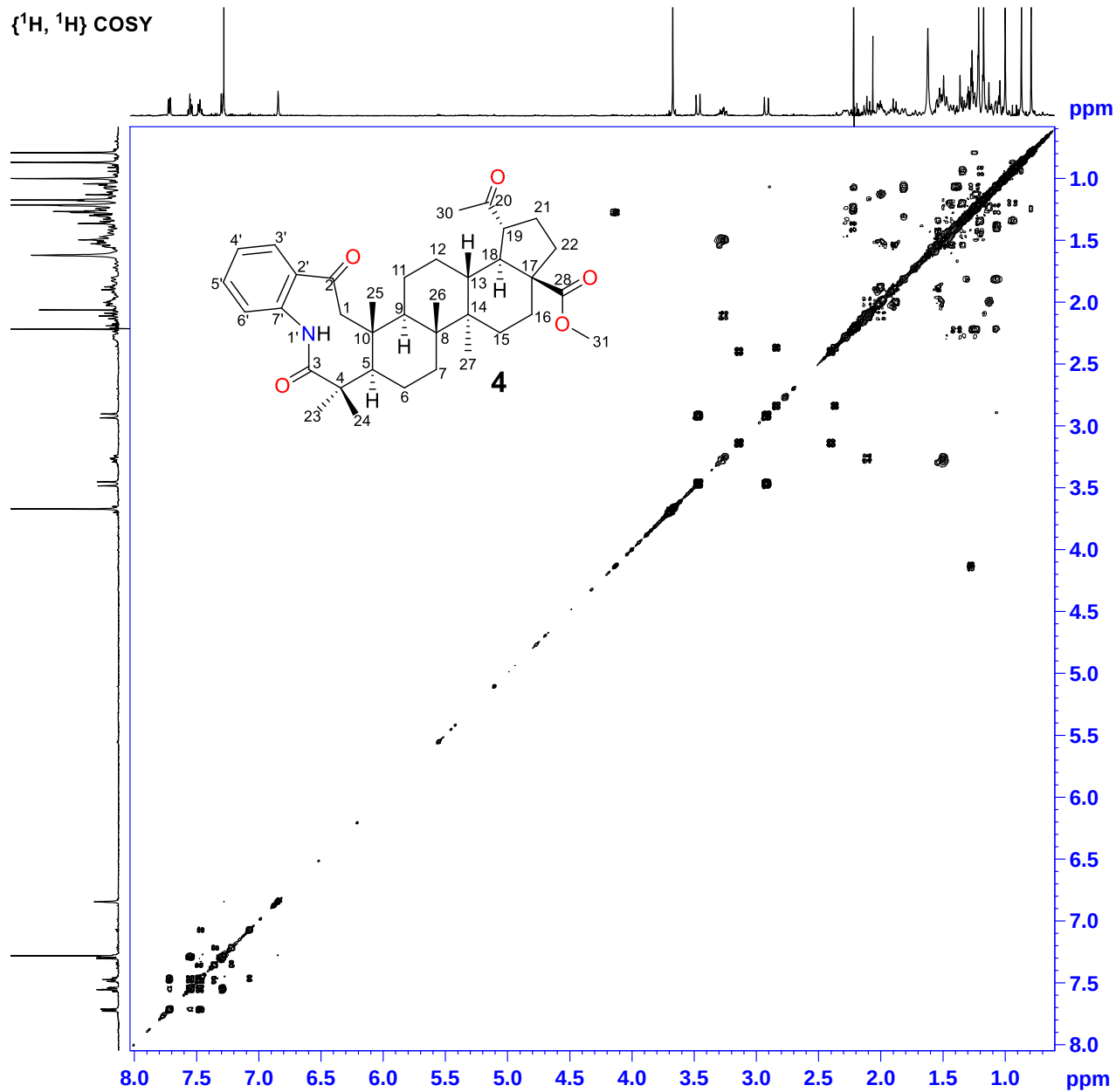


Figure S22. Complete $\{^1\text{H}, ^1\text{H}\}$ COSY NMR spectrum of compound **4** in CDCl_3 .

$\{^1\text{H}, ^1\text{H}\}$ COSY-DQF

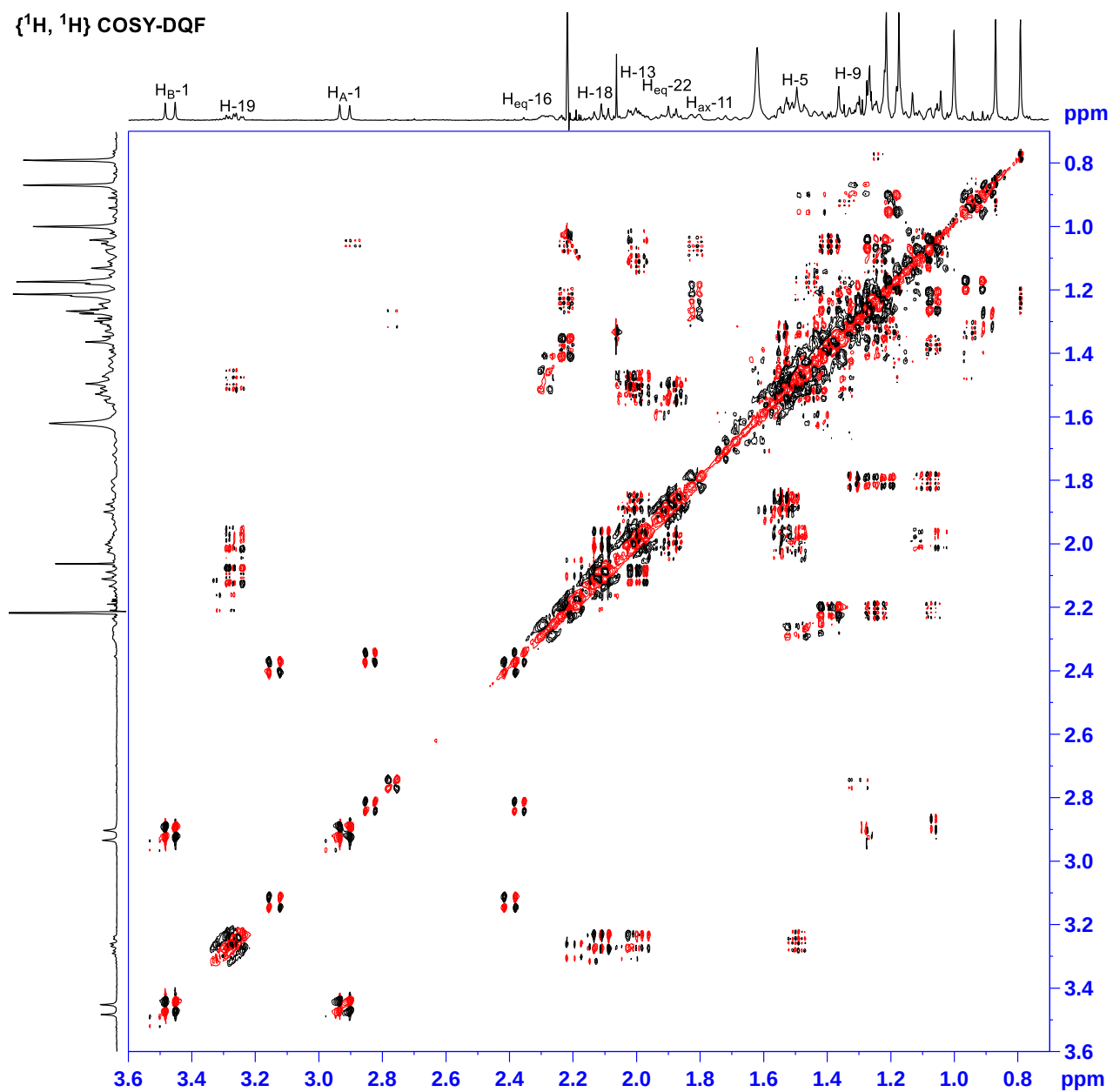


Figure S23. Upfield area of $\{^1\text{H}, ^1\text{H}\}$ COSY-DQF NMR spectrum of compound **4** in CDCl_3 .

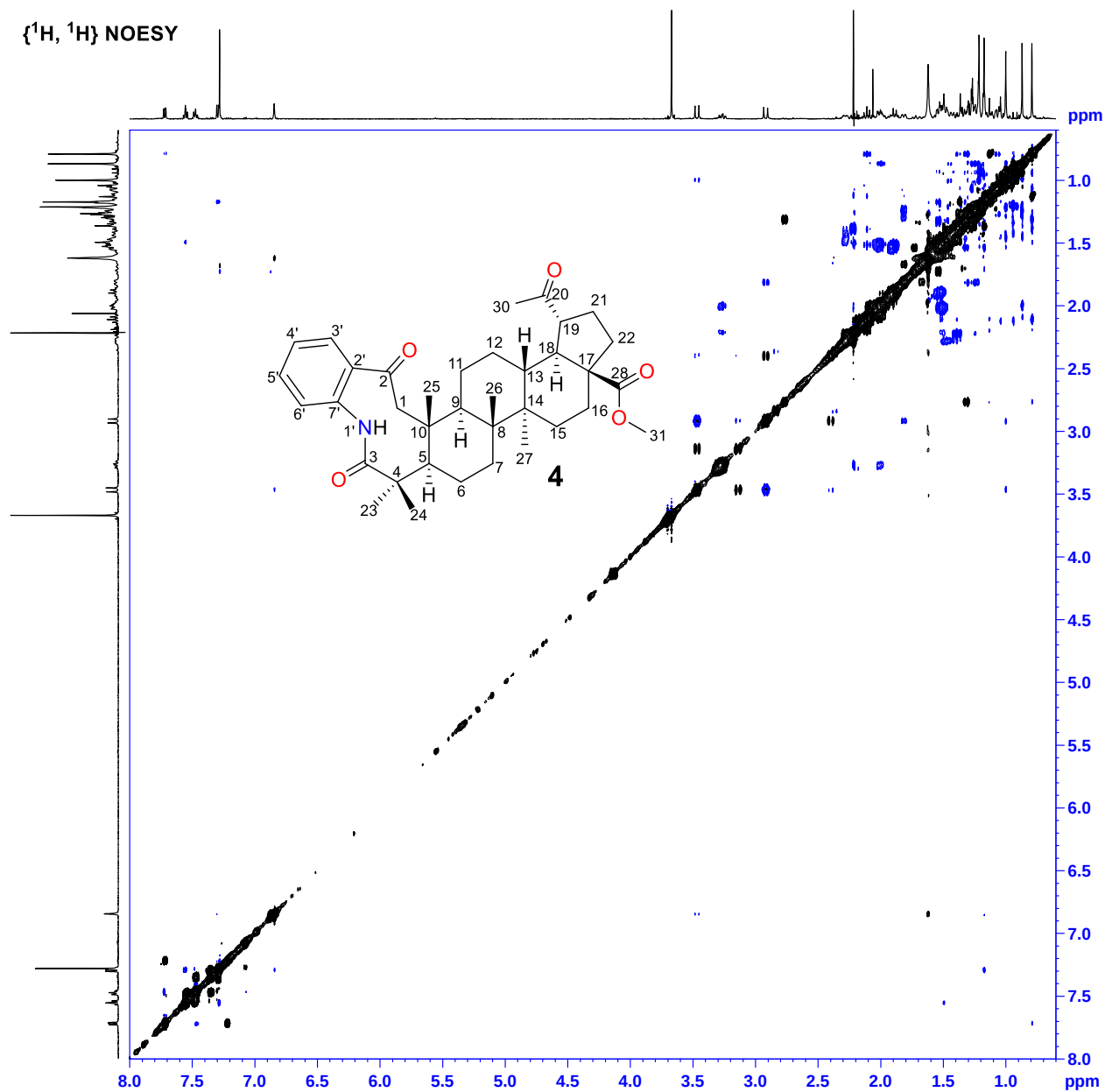


Figure S24. Complete $\{^1\text{H}, ^1\text{H}\}$ NOESY NMR spectrum of compound **4** in CDCl_3 .

$\{^1\text{H}, ^1\text{H}\}$ NOESY

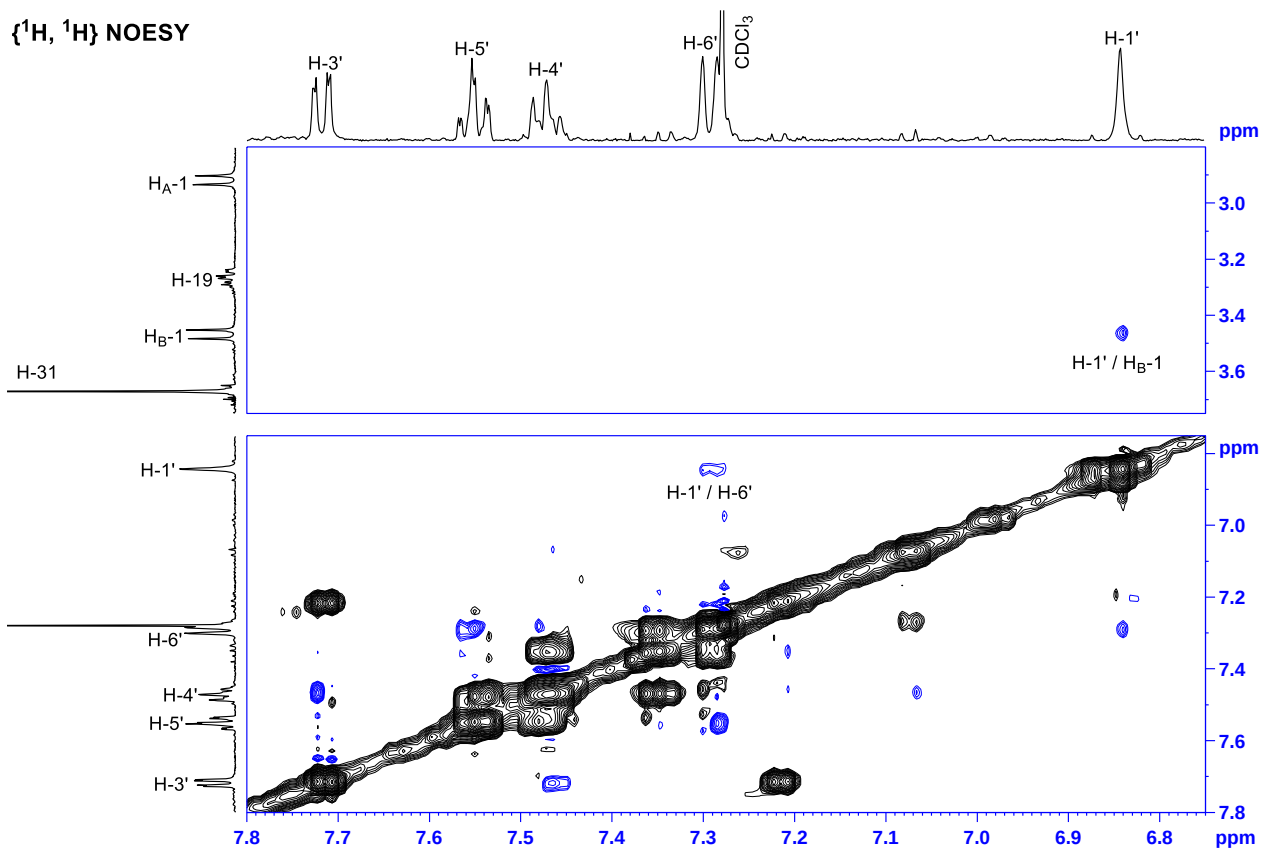


Figure S25. Detailed and annotated $\{^1\text{H}, ^1\text{H}\}$ NOESY NMR spectrum of compound **4** in CDCl_3 .

$\{^1\text{H}, ^1\text{H}\}$ NOESY

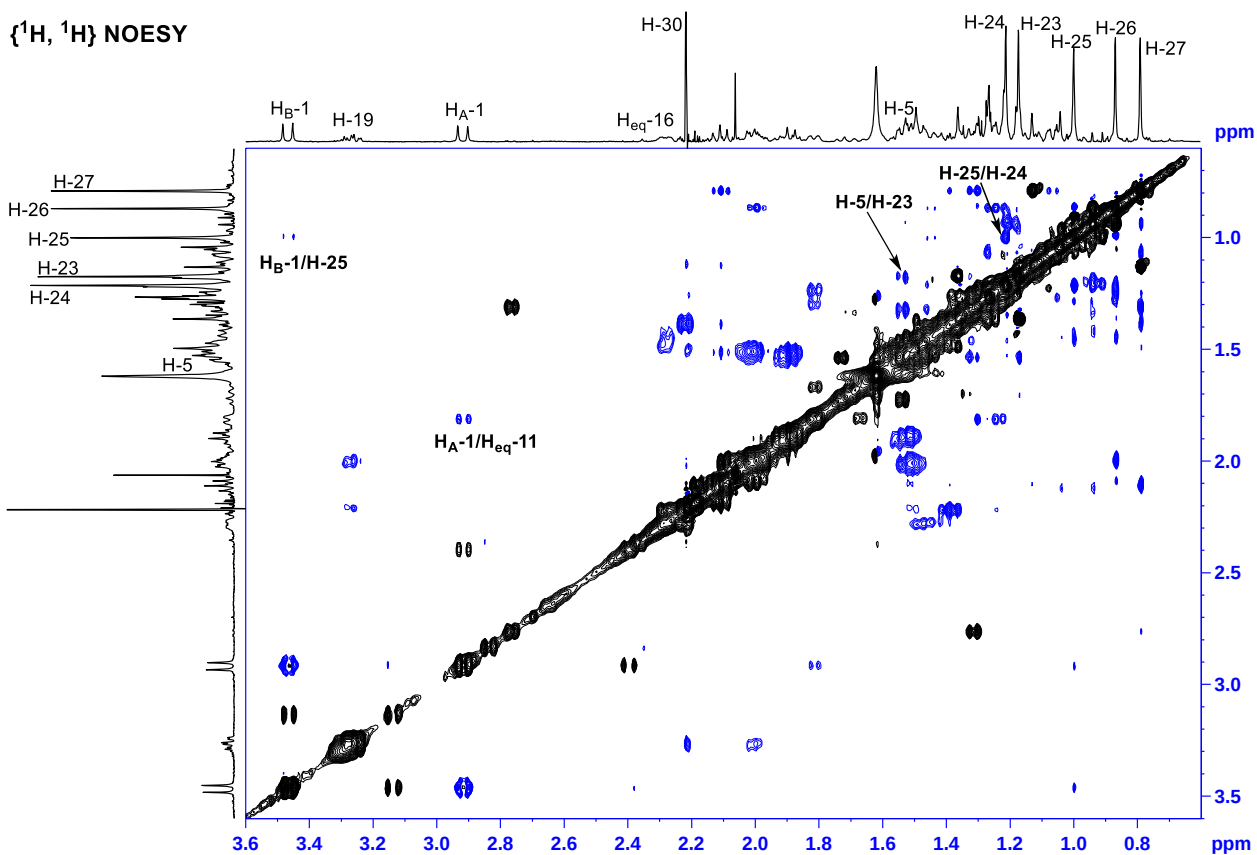


Figure S26. Upfield area of $\{^1\text{H}, ^1\text{H}\}$ NOESY NMR spectrum of compound **4** in CDCl_3 .

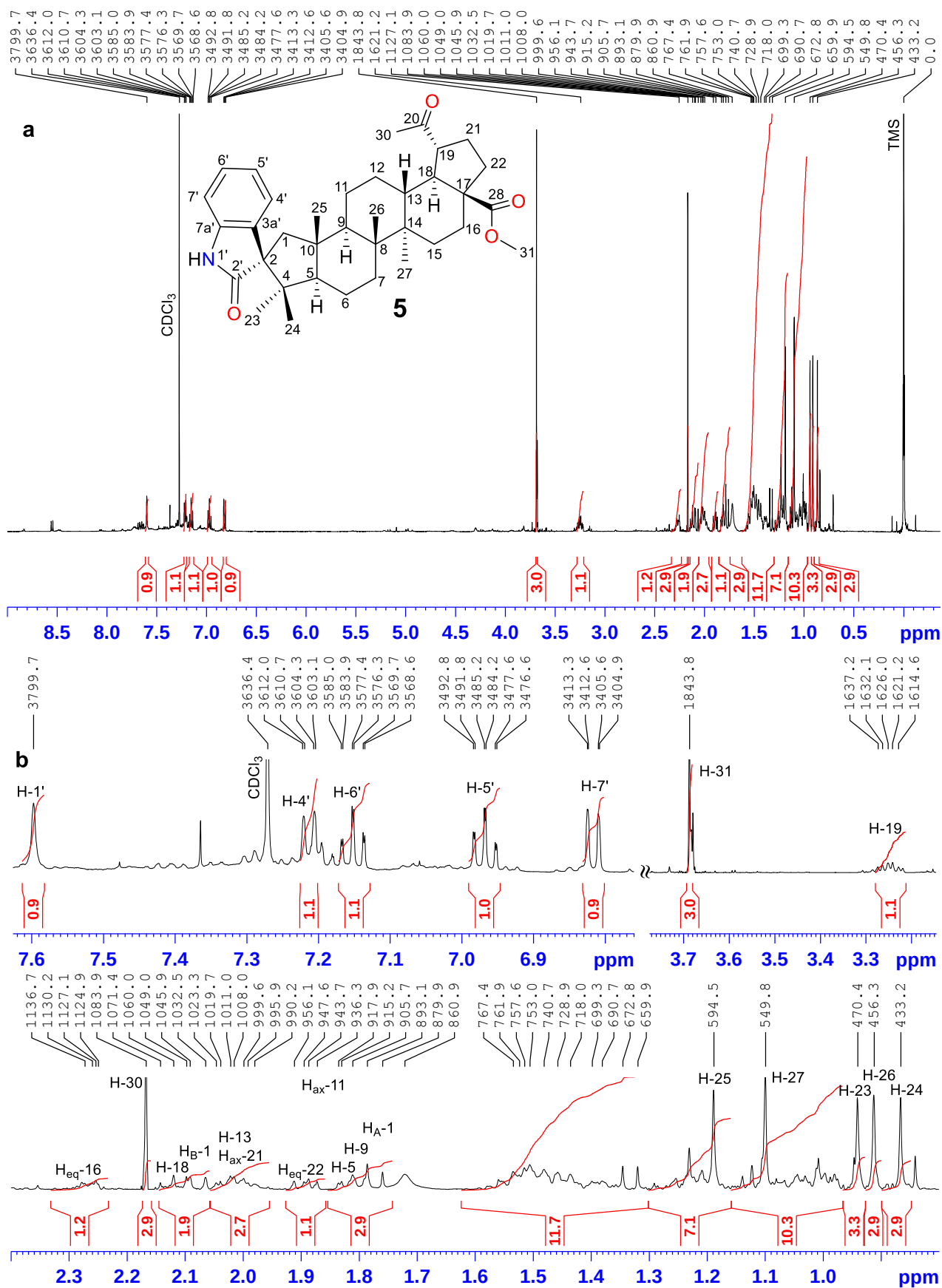


Figure S27. (a) Complete ^1H NMR spectrum of compound **5** in CDCl_3 . (b) Detailed and annotated ^1H NMR spectrum of compound **5** in CDCl_3 .

Table S5. Complete numerical listings of ^1H NMR peaks of compound **5** in CDCl_3 .

Peak	$\nu(\text{F1})$ [ppm]	$\nu(\text{F1})$ [Hz]	Intensity [rel]	Half width [Hz]
1	7.6	3799.7	0.11	3.3
2	7.27	3636.4	1.49	0.6
3	7.22	3612	0.08	0.9
4	7.22	3611.2	0.09	3.1
5	7.22	3610.7	0.08	1.3
6	7.21	3604.3	0.09	1.5
7	7.21	3603.7	0.09	3.1
8	7.2	3603.1	0.09	0.9
9	7.17	3585	0.05	1.1
10	7.17	3583.9	0.05	1.1
11	7.15	3577.4	0.1	1.1
12	7.15	3576.3	0.1	0.9
13	7.14	3569.7	0.06	1.1
14	7.14	3568.6	0.06	0.9
15	6.98	3492.8	0.06	1.1
16	6.98	3491.8	0.06	1.1
17	6.97	3485.2	0.1	1.1
18	6.97	3484.2	0.1	0.9
19	6.95	3477.6	0.05	1.1
20	6.95	3476.6	0.04	0.9
21	6.82	3413.3	0.1	1.1
22	6.82	3412.9	0.1	1.1
23	6.82	3412.6	0.09	1.1
24	6.81	3405.6	0.09	1.1
25	6.81	3404.9	0.08	1.1
26	3.69	1843.8	1.21	0.7
27	3.27	1637.2	0.03	3.3
28	3.26	1632.1	0.04	2.6
29	3.25	1626	0.04	3.5
30	3.24	1621.2	0.05	2.6
31	3.23	1614.6	0.03	2.9
32	3.22	1610	0.02	2.4
33	2.28	1139.2	0.04	2.9
34	2.27	1136.7	0.03	3.5
35	2.26	1131.8	0.03	2.4
36	2.26	1130.2	0.03	5.1
37	2.25	1127.1	0.05	3.7
38	2.25	1124.9	0.03	1.3
39	2.17	1083.9	1.02	1.1
40	2.14	1071.4	0.04	1.5
41	2.12	1060	0.08	2.4
42	2.1	1049	0.07	2.4
43	2.09	1045.9	0.07	3.1
44	2.06	1032.5	0.07	2.6
45	2.05	1023.3	0.04	3.5
46	2.04	1019.7	0.05	4.4
47	2.02	1011	0.07	4.6
48	2.02	1008	0.07	3.9
49	2	999.6	0.06	4.2

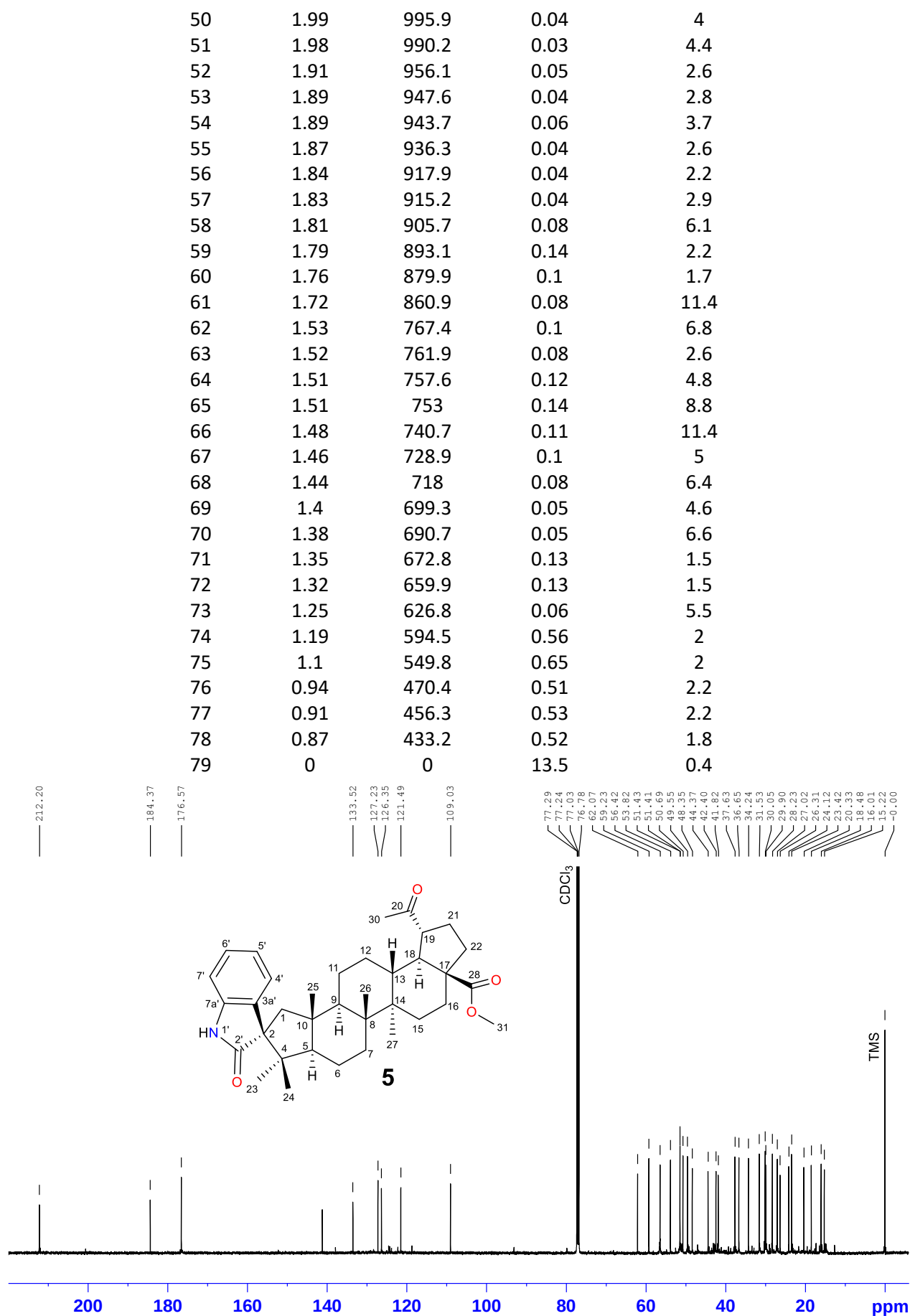


Figure S28. Complete $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of compound **5** in CDCl_3 .

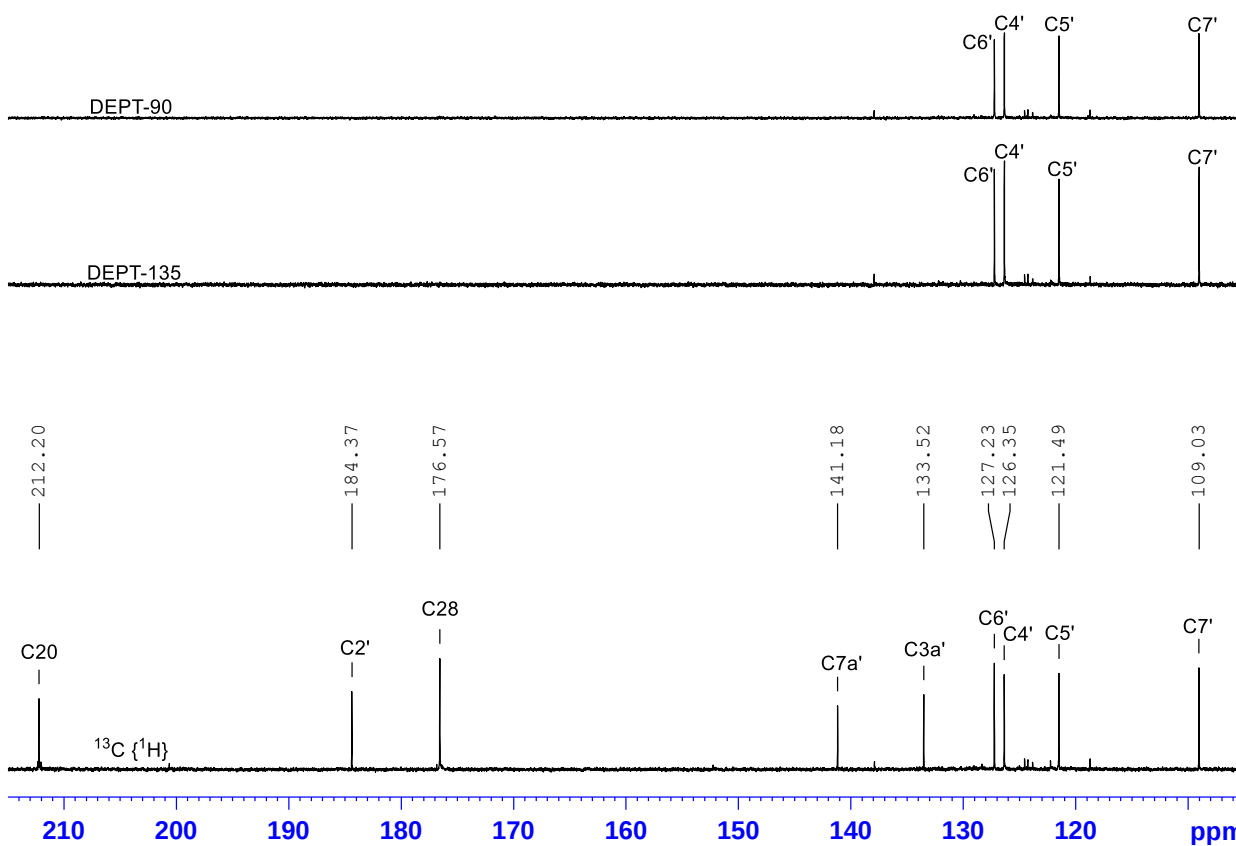


Figure S29. Downfield area of annotated $^{13}\text{C}\{^1\text{H}\}$ NMR and DEPT-135, DEPT-90 spectra of compound **5** in CDCl_3 .

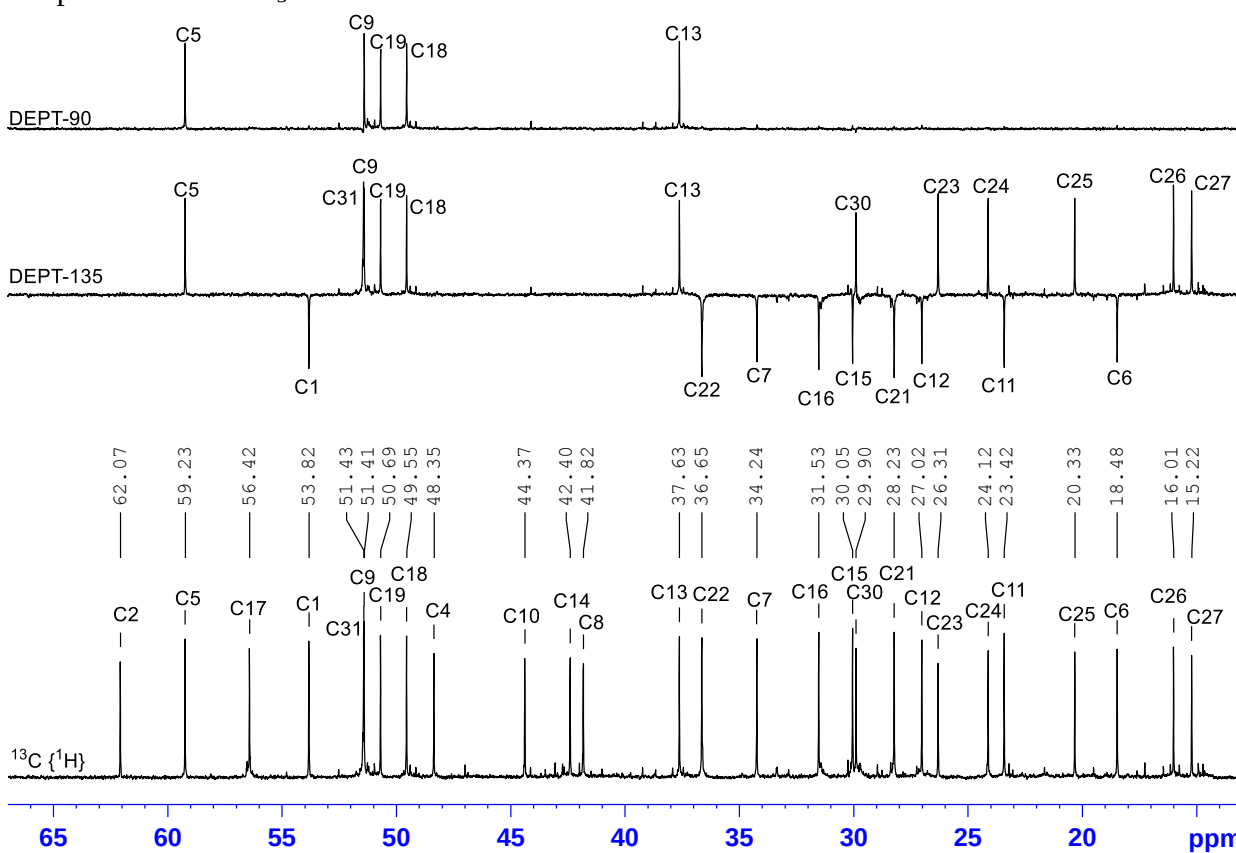


Figure S30. Upfield area of annotated $^{13}\text{C}\{^1\text{H}\}$ NMR and DEPT-135, DEPT-90 spectra of compound **5** in CDCl_3 .

Table S6. Complete numerical listings of ^{13}C NMR peaks of compound **5** in CDCl_3 .

Peak	$\nu(\text{F1})$ [ppm]	$\nu(\text{F1})$ [Hz]	Intensity [rel]	Half width [Hz]
1	212.2	26686	1.03	0.9
2	184.37	23186	1.07	0.9
3	176.57	22205.1	1.53	1.8
4	141.18	17755	0.95	0.9
5	133.52	16790.8	1.04	0.9
6	127.23	16000.8	1.47	1.8
7	126.35	15889.4	1.37	0.9
8	121.49	15278.2	1.4	0.9
9	109.03	13710.9	1.41	1.8
10	77.29	9719.3	13.1	1.8
11	77.24	9713.1	1.23	2.7
12	77.03	9687.4	13.5	1.8
13	76.78	9655.5	13.18	1.8
14	62.07	7805.5	1.6	1.8
15	59.23	7449.3	1.93	1.8
16	56.42	7095.2	1.78	1.8
17	53.82	6768.4	1.89	1.8
18	51.43	6467.6	1.96	1.8
19	51.41	6464.9	2.16	2.7
20	50.68	6374	1.96	1.8
21	49.55	6231.3	1.96	1.8
22	48.35	6080.7	1.71	1.8
23	44.37	5580.4	1.65	1.8
24	42.4	5331.5	1.66	1.8
25	41.82	5259.1	1.64	0.9
26	37.63	4732	1.95	1.8
27	36.65	4608.7	1.98	1.8
28	34.24	4306.1	1.92	1.8
29	31.53	3965.4	2	1.8
30	30.05	3779.2	2.06	1.8
31	29.9	3760.1	1.78	0.9
32	28.23	3550.5	2.05	0.9
33	27.02	3398.4	1.91	1.8
34	26.31	3308.7	1.57	1.8
35	24.12	3033.6	1.75	0.9
36	23.42	2945.4	1.99	1.8
37	20.33	2556.8	1.74	0.9
38	18.48	2323.6	1.85	0.9
39	16.01	2013.4	1.8	0.9
40	15.22	1913.7	1.69	0.9
41	0	0	4.53	0.9

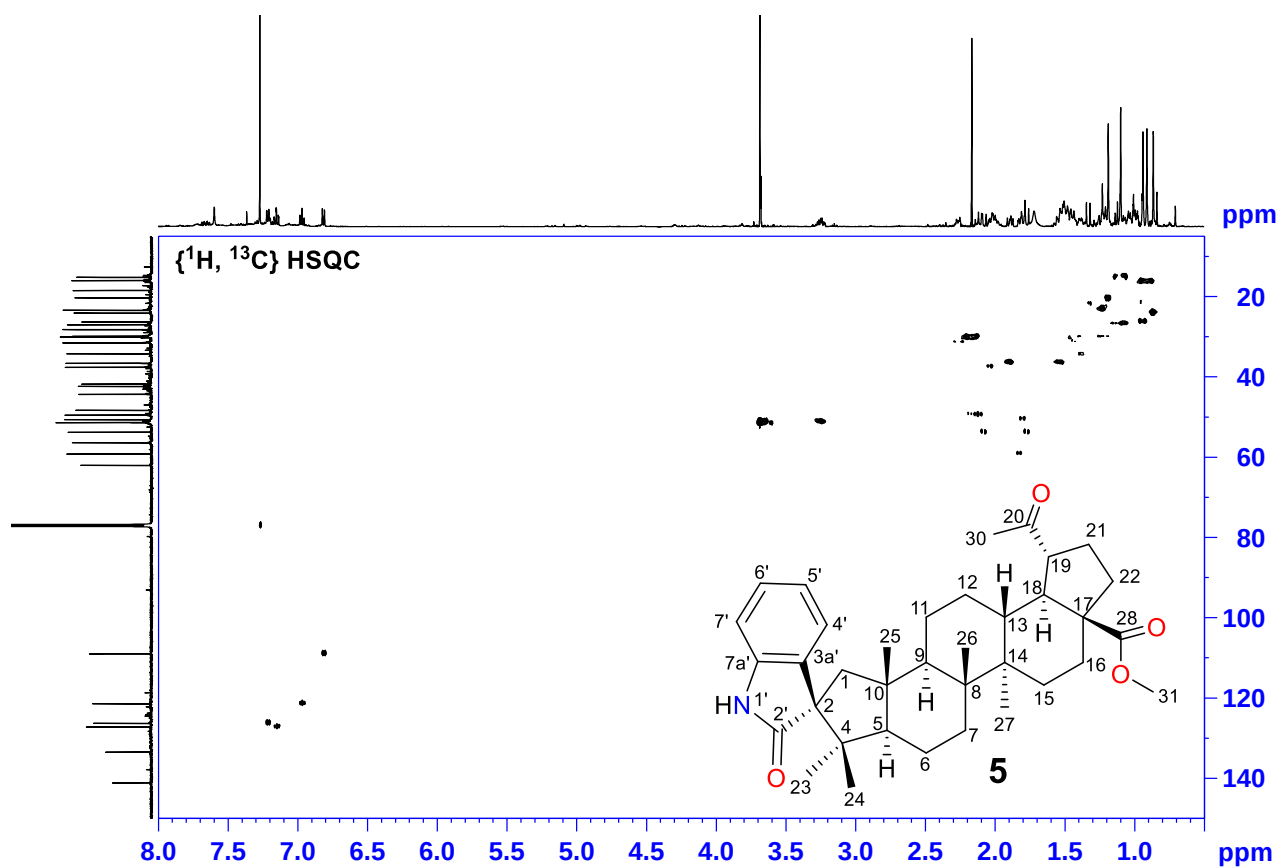


Figure S31. Complete $\{^1\text{H}, ^{13}\text{C}\}$ HSQC NMR spectrum of compound **5** in CDCl_3 .

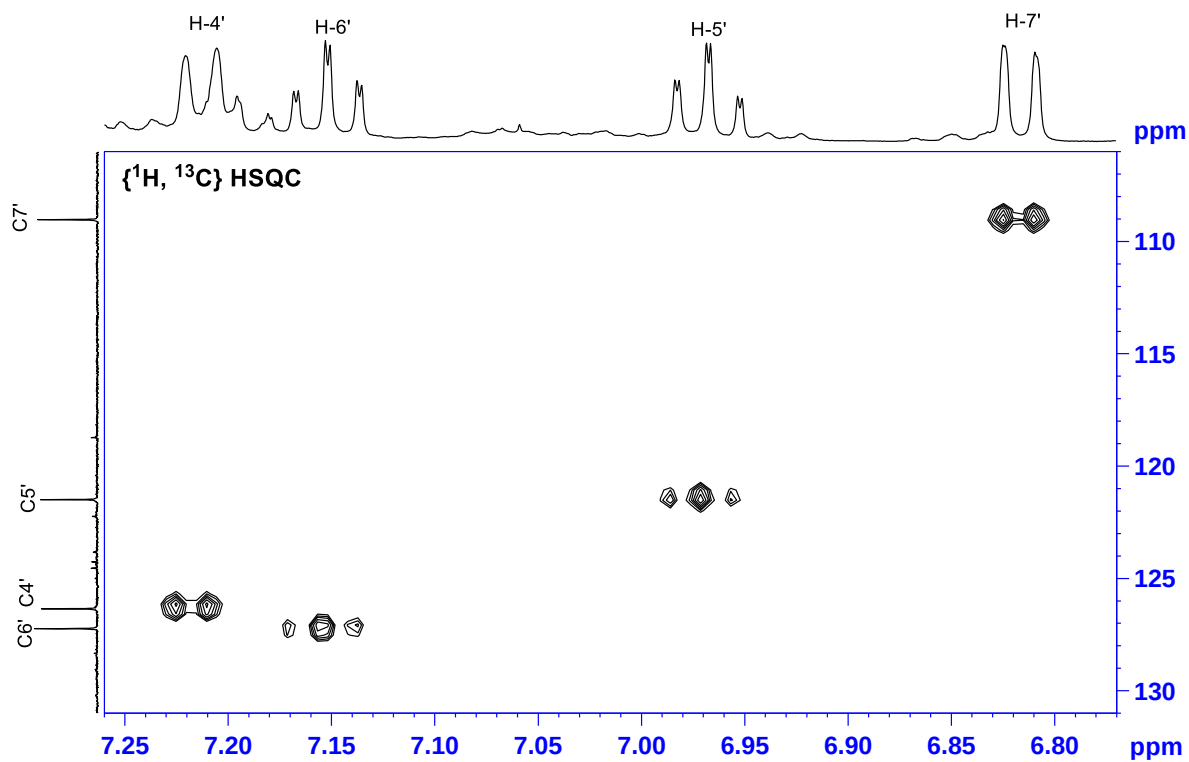


Figure S32. Downfield area of $\{^1\text{H}, ^{13}\text{C}\}$ HSQC NMR spectrum of compound **5** in CDCl_3 .

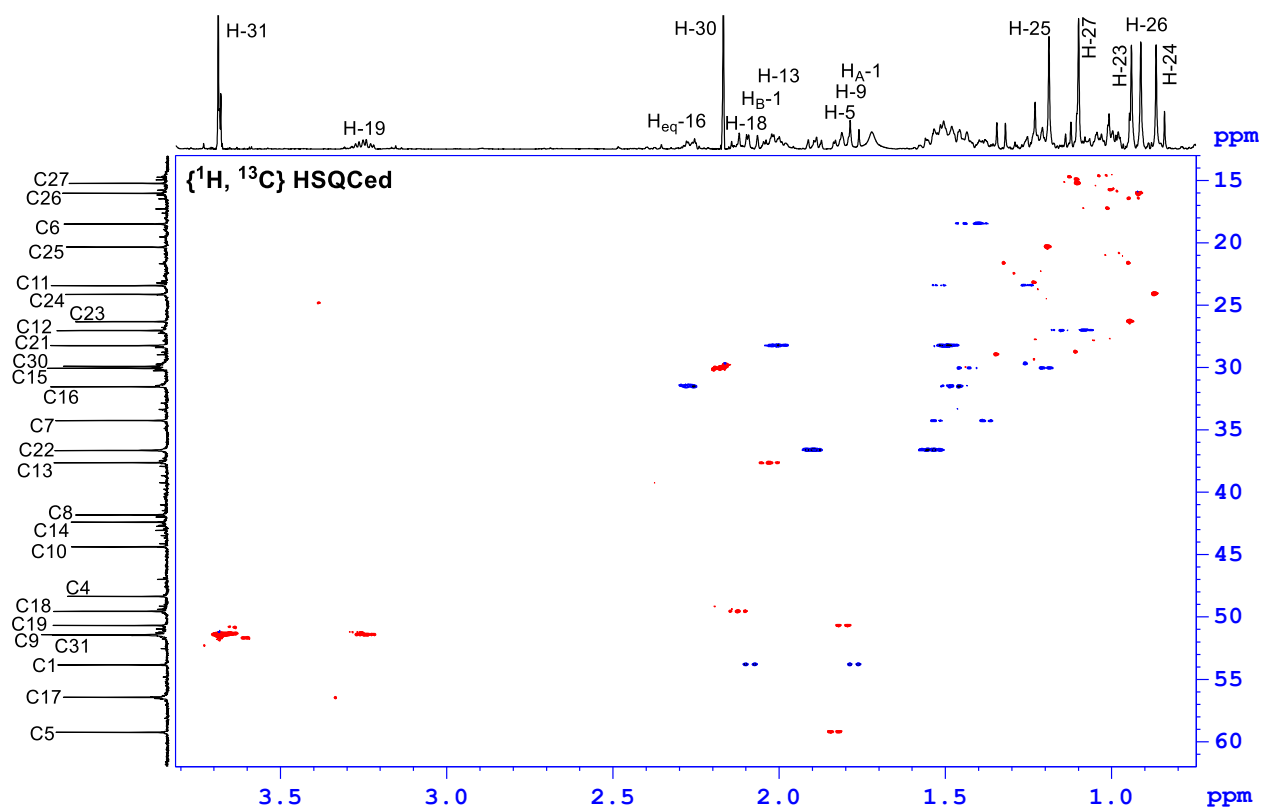


Figure S33. Upfield area of $\{^1\text{H}, ^{13}\text{C}\}$ HSQC multiplicity edited NMR spectrum of compound **5** in CDCl_3 .

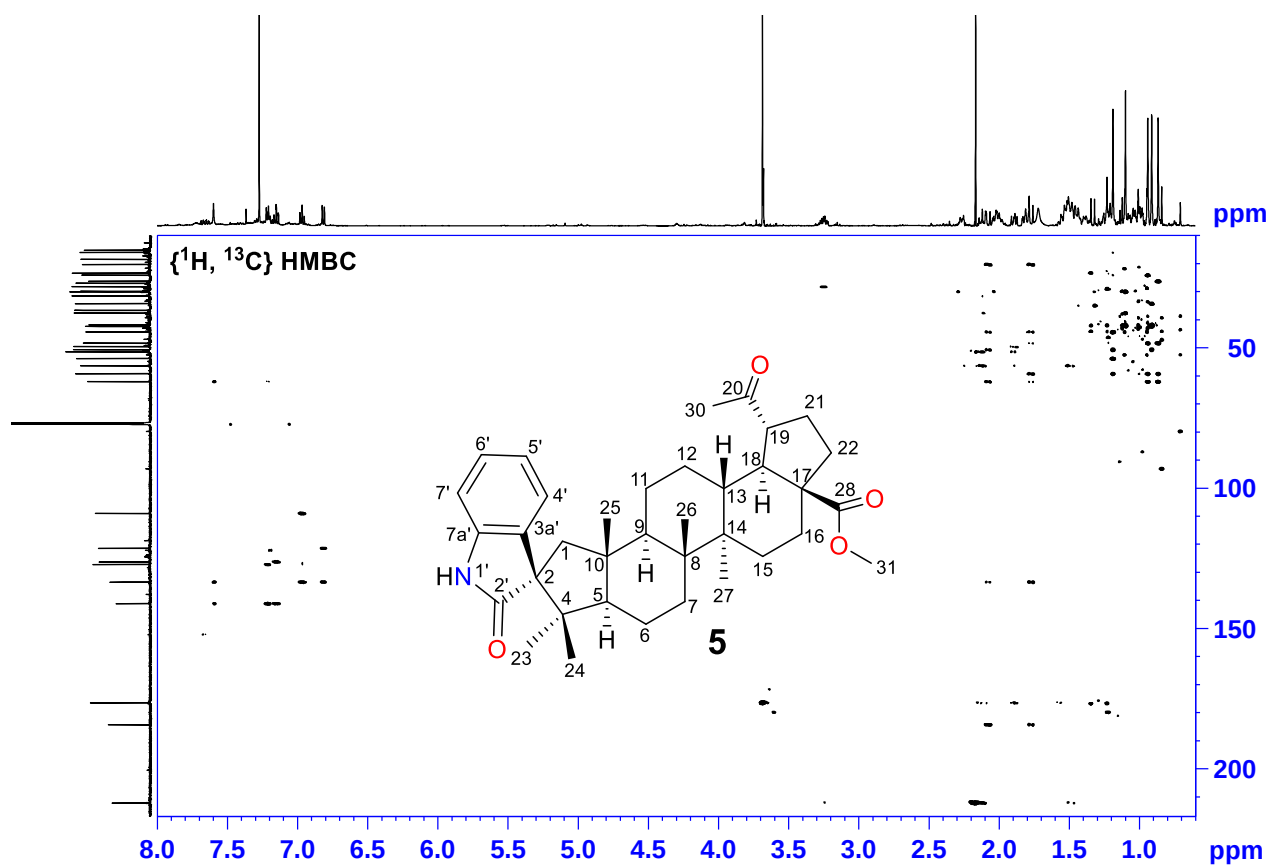


Figure S34. Complete $\{^1\text{H}, ^{13}\text{C}\}$ HMBC NMR spectrum of compound **5** in CDCl_3 .

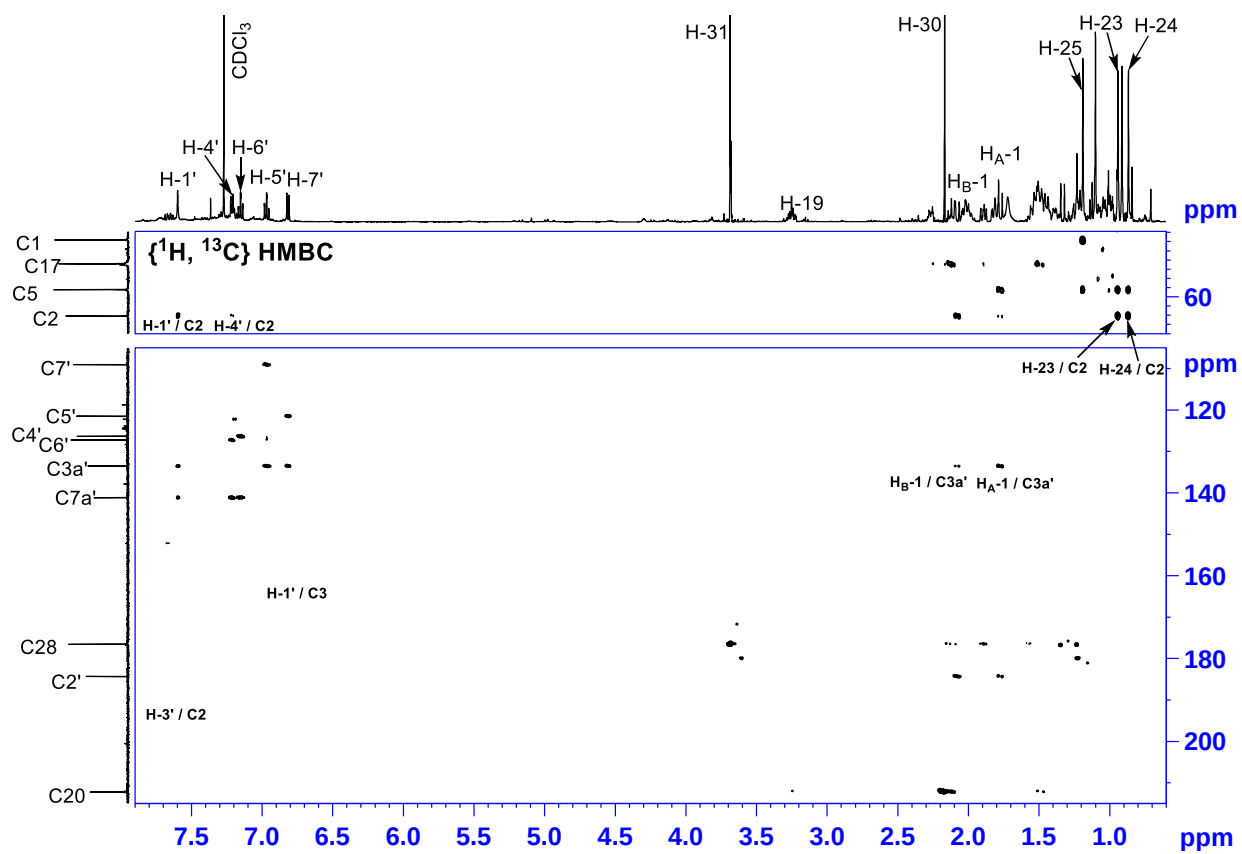


Figure S35. Downfield area of annotated $\{^1\text{H}, ^{13}\text{C}\}$ HMBC NMR spectrum of compound 5 in CDCl_3 .

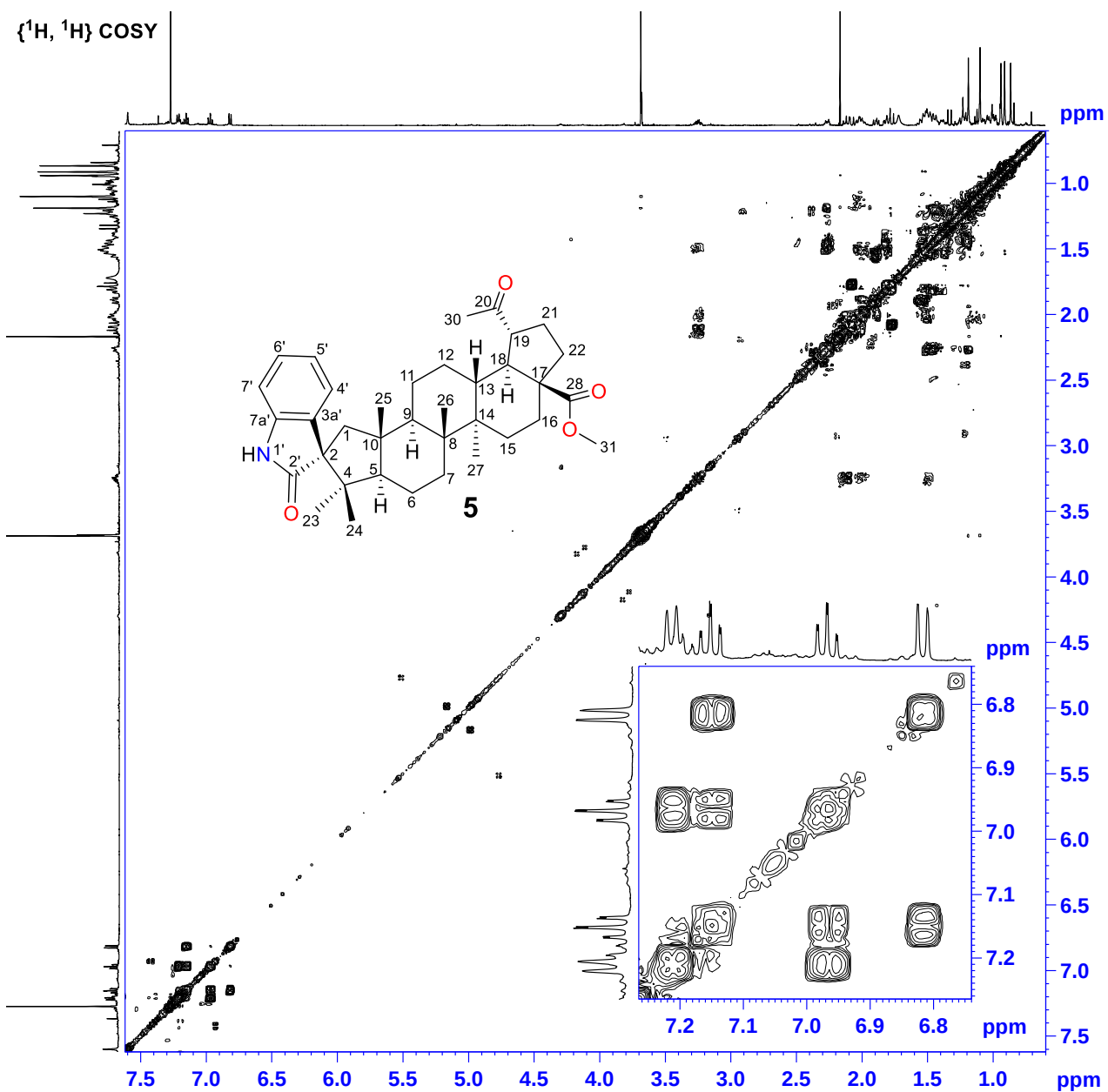


Figure S36. Complete $\{^1\text{H}, ^1\text{H}\}$ COSY NMR spectrum of compound **5** in CDCl_3 .

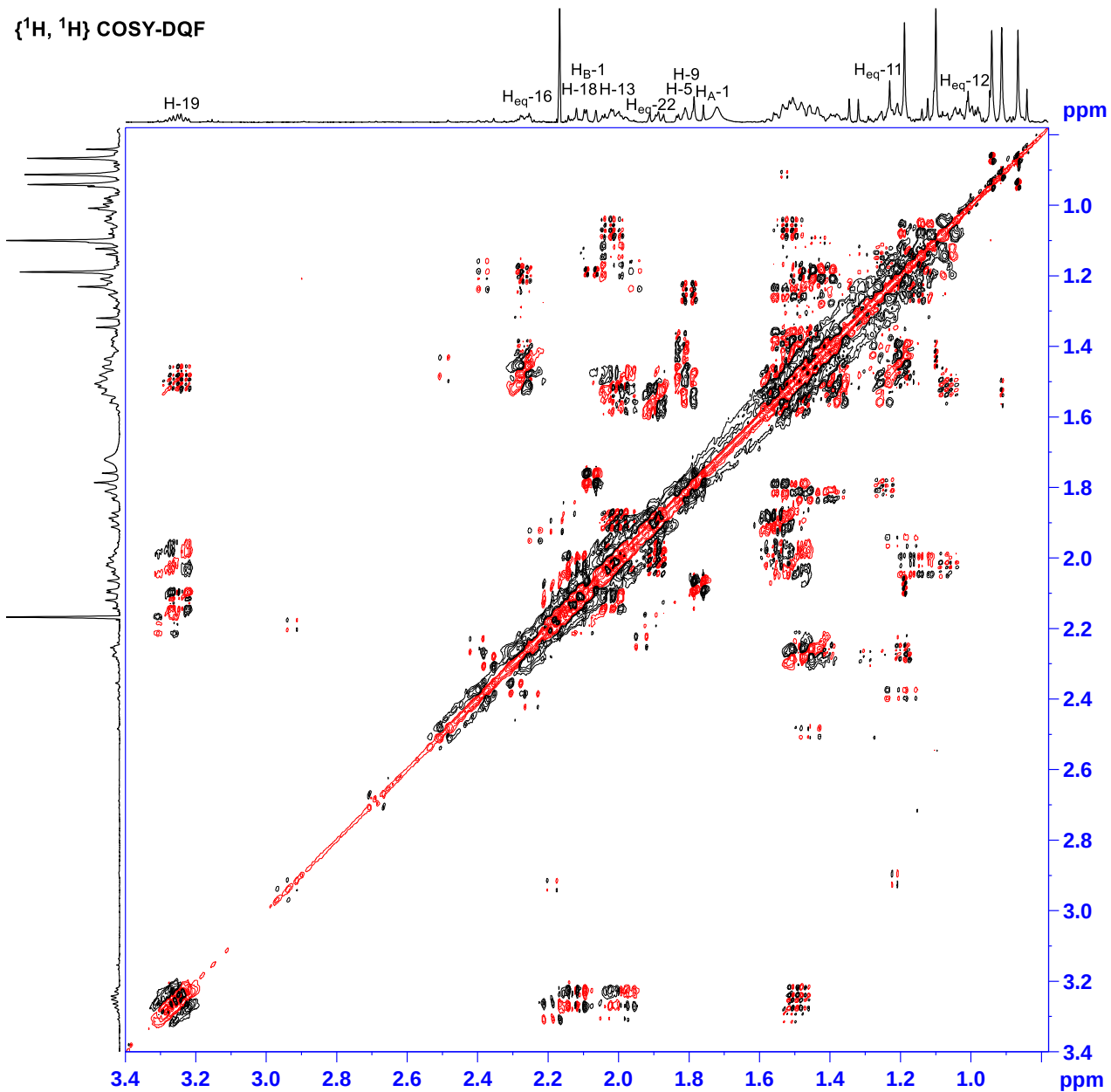


Figure S37. Upfield area of $\{^1\text{H}, ^1\text{H}\}$ COSY-DQF NMR spectrum of compound **5** in CDCl_3 .

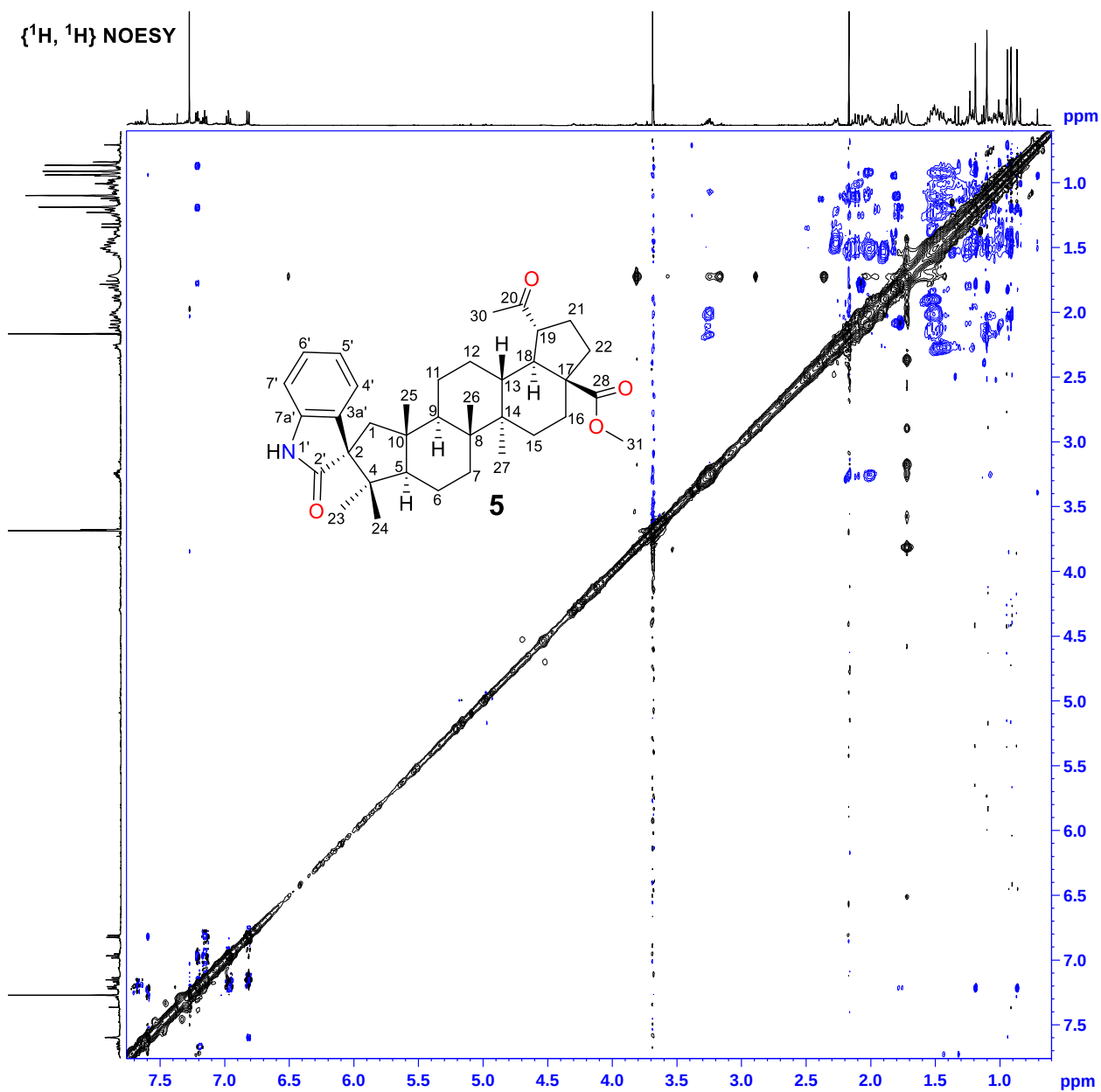


Figure S38. Complete $\{^1\text{H}, ^1\text{H}\}$ NOESY NMR spectrum of compound **5** in CDCl_3 .

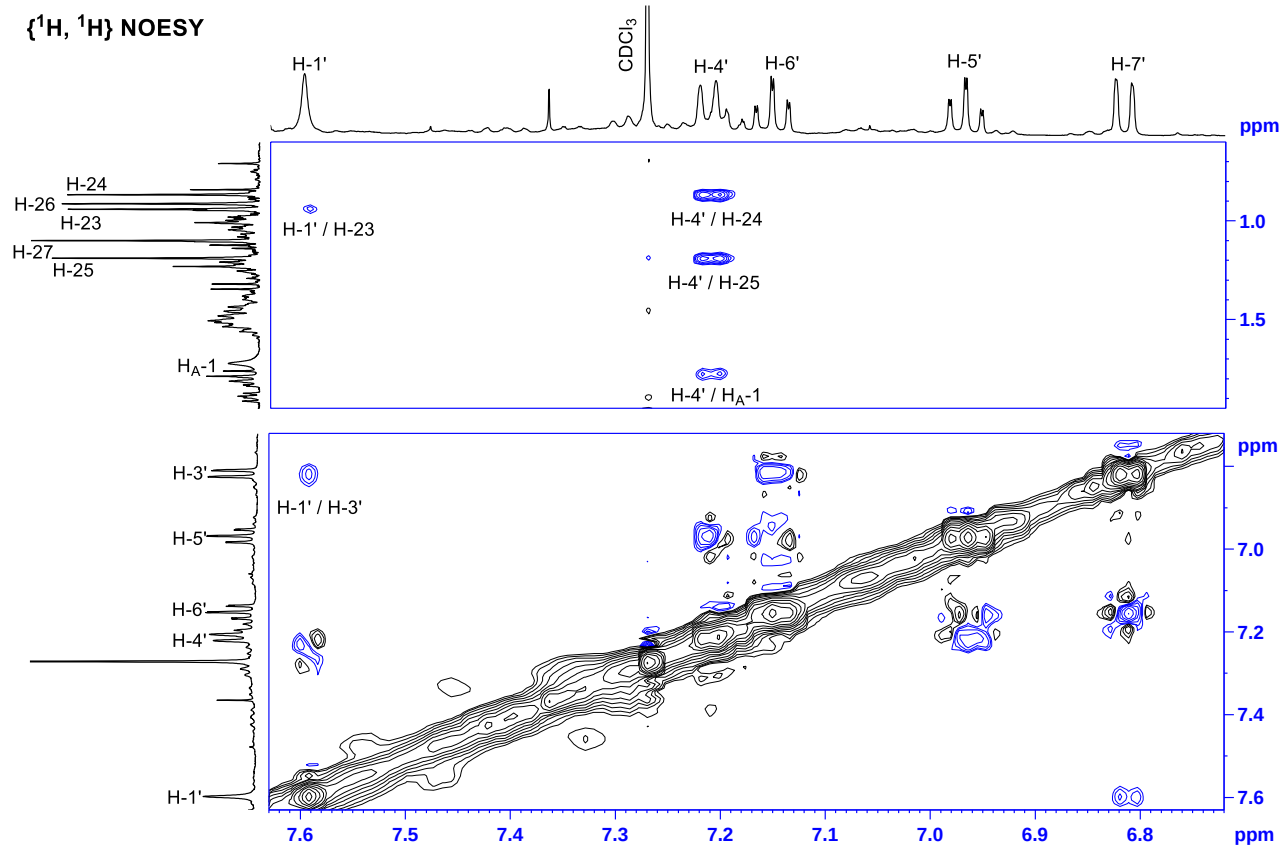


Figure S39. Detailed and annotated $\{^1\text{H}, ^1\text{H}\}$ NOESY NMR spectrum of compound 5 in CDCl_3 .

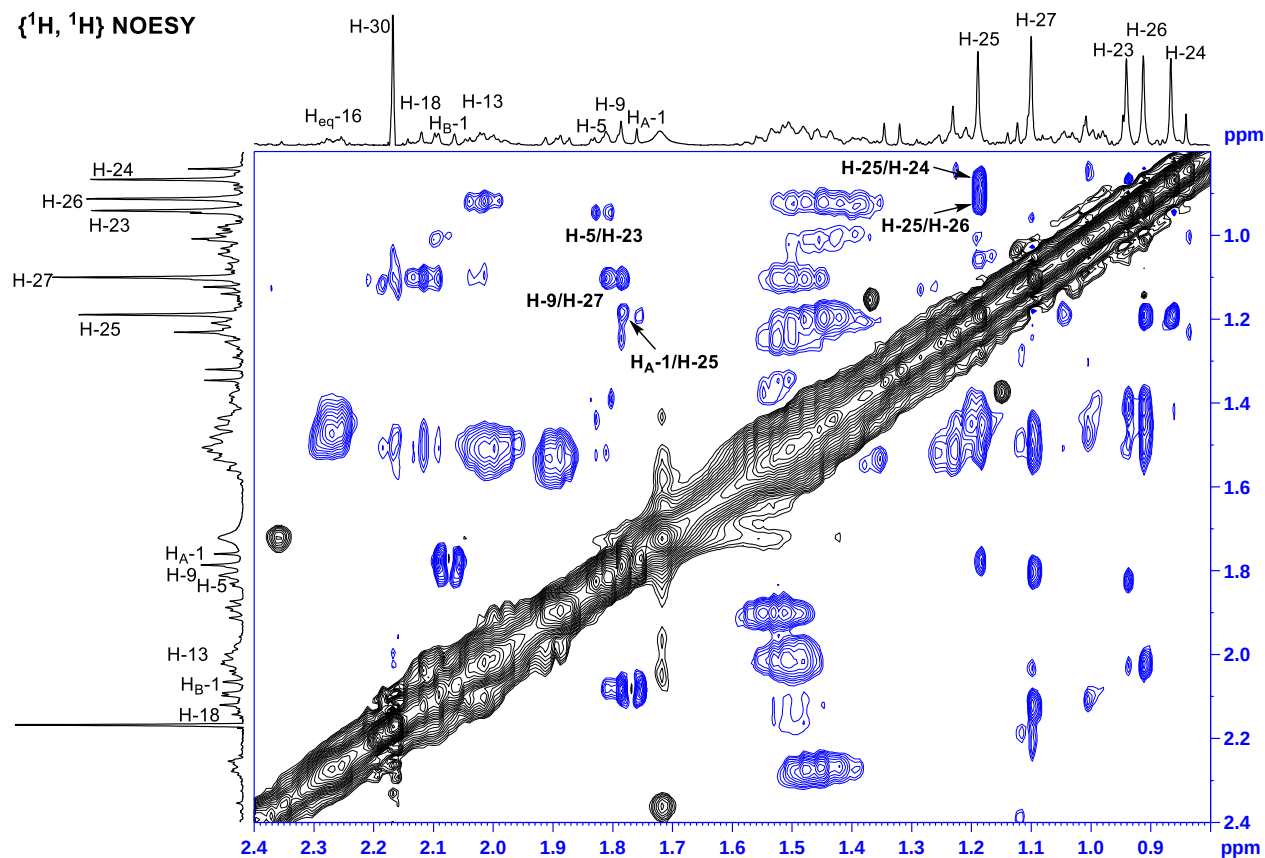


Figure S40. Upfield area of $\{^1\text{H}, ^1\text{H}\}$ NOESY NMR spectrum of compound 5 in CDCl_3 .

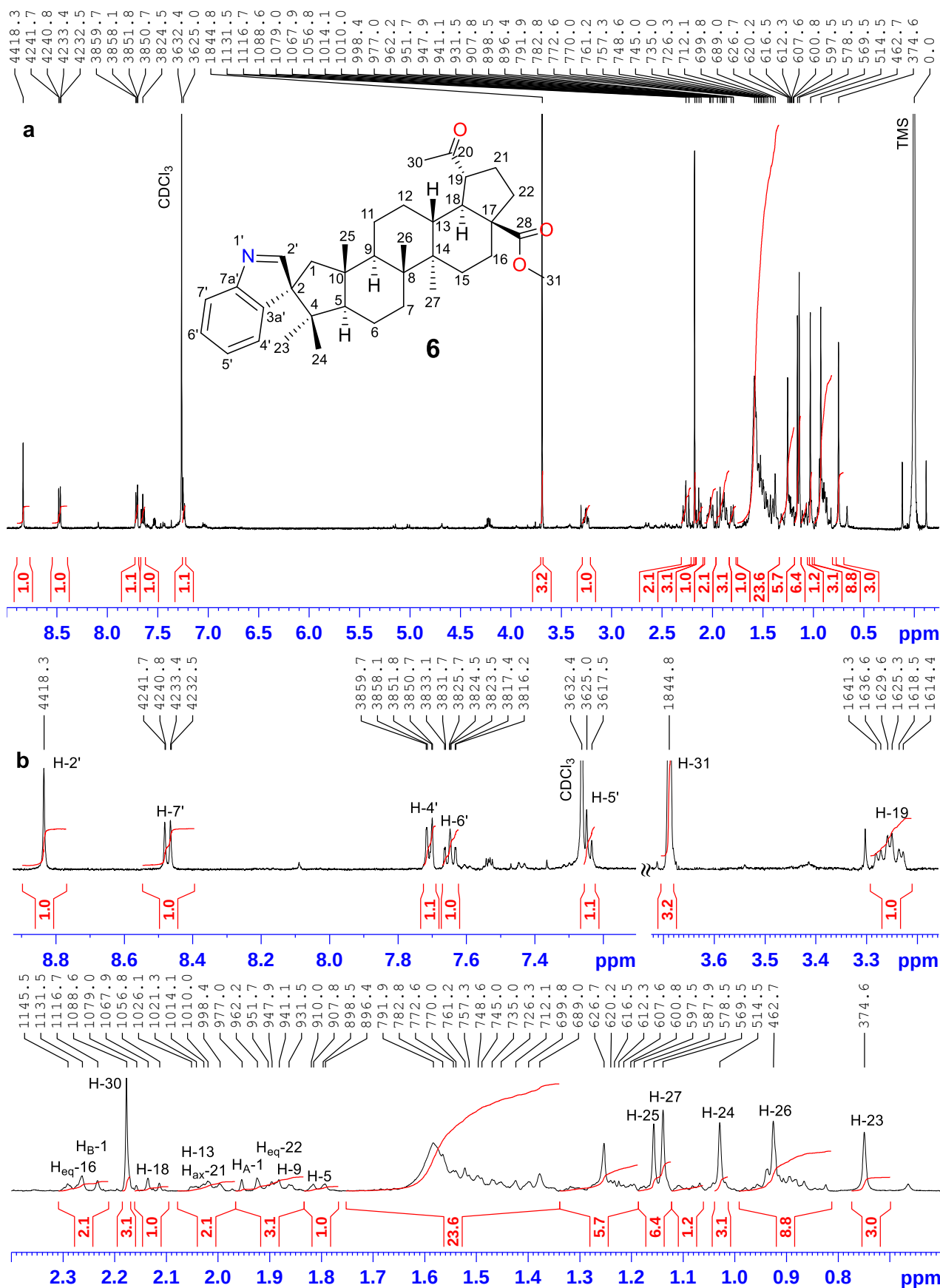


Figure S41. (a) Complete ^1H NMR spectrum of compound 6 in CDCl_3 . (b) Detailed and annotated ^1H NMR spectrum of compound 6 in CDCl_3 .

Table S7. Complete numerical listings of ¹H NMR peaks of compound **6** in CDCl₃.

Peak	ν(F1) [ppm]	ν(F1) [Hz]	Intensity [rel]	Half width [Hz]
1	8.83	4418.3	0.08	2.1
2	8.48	4241.7	0.04	2.6
3	8.46	4233.4	0.04	2.4
4	7.72	3859.7	0.03	0.9
5	7.72	3859	0.03	1.5
6	7.71	3858.1	0.03	1.5
7	7.7	3851.8	0.03	1.3
8	7.7	3850.7	0.04	2.8
9	7.66	3833.1	0.02	1.1
10	7.66	3831.7	0.02	1.5
11	7.65	3825.7	0.02	1.1
12	7.65	3824.5	0.03	3.4
13	7.64	3823.5	0.02	1.1
14	7.63	3817.4	0.02	1.5
15	7.63	3816.2	0.02	1.5
16	7.26	3632.4	0.57	0.9
17	7.25	3625	0.05	2.6
18	7.23	3617.5	0.02	2.6
19	3.69	1844.8	0.38	1.3
20	3.28	1641.3	0.01	1.1
21	3.27	1636.6	0.01	1.5
22	3.26	1629.6	0.02	1.7
23	3.25	1625.3	0.02	3.4
24	3.24	1618.5	0.01	1.9
25	3.23	1614.4	0.01	1.9
26	2.29	1145.5	0.02	4.3
27	2.26	1131.5	0.04	4.7
28	2.23	1116.7	0.03	3
29	2.18	1088.6	0.34	1.5
30	2.16	1079	0.02	2.1
31	2.14	1067.9	0.04	2.6
32	2.11	1056.8	0.02	2.1
33	2.05	1026.1	0.01	1.9
34	2.04	1021.3	0.01	1.1
35	2.03	1014.1	0.02	1.5
36	2.02	1010	0.03	3.2
37	1.95	977	0.03	2.4
38	1.92	962.3	0.04	3.8
39	1.9	951.7	0.02	0.4
40	1.9	947.9	0.03	4.1
41	1.88	941.1	0.03	3.4
42	1.86	931.5	0.02	2.4
43	1.82	907.8	0.02	5.3
44	1.79	896.4	0.02	2.8
45	1.58	791.9	0.14	17.1
46	1.57	782.8	0.1	1.7
47	1.54	772.6	0.06	1.1
48	1.54	770	0.06	5.8
49	1.52	761.3	0.07	6.8
50	1.51	757.3	0.05	4.9

51	1.5	748.6	0.04	3
52	1.49	745	0.04	4.1
53	1.47	735	0.03	3.8
54	1.45	726.3	0.03	1.9
55	1.42	712.1	0.03	5.8
56	1.4	699.8	0.03	0.9
57	1.38	689	0.05	5.6
58	1.25	626.7	0.14	3.4
59	1.24	620.2	0.03	1.9
60	1.23	616.5	0.03	3.2
61	1.22	612.3	0.03	3.4
62	1.21	607.6	0.02	1.9
63	1.2	600.8	0.02	3.4
64	1.19	597.5	0.02	3.2
65	1.18	587.9	0.01	2.1
66	1.16	578.5	0.19	2.4
67	1.14	569.5	0.23	2.8
68	1.11	554.1	0.02	1.1
69	1.08	541	0.01	2.6
70	1.07	534	0.02	4.1
71	1.03	514.6	0.2	2.8
72	0.93	462.7	0.2	3.8
73	0.75	374.7	0.17	3
74	0	0	13.5	1.1

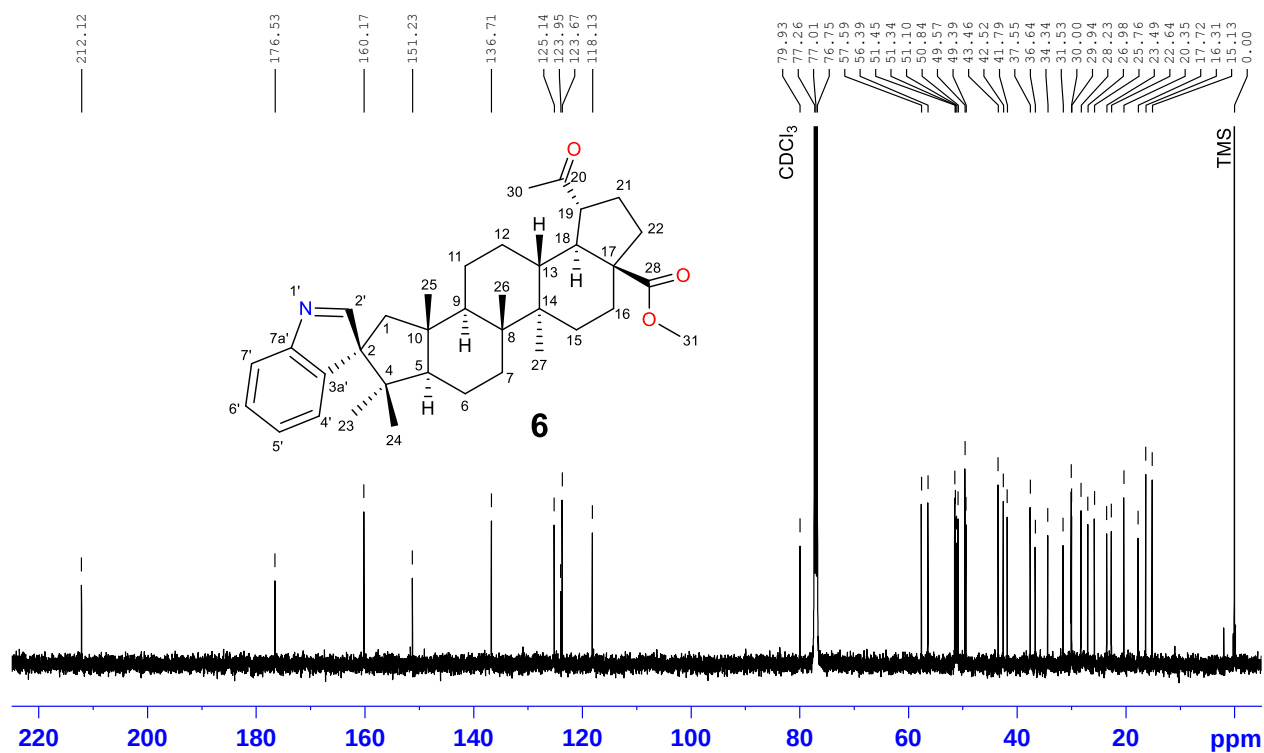


Figure S42. Complete $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of compound **6** in CDCl_3 .

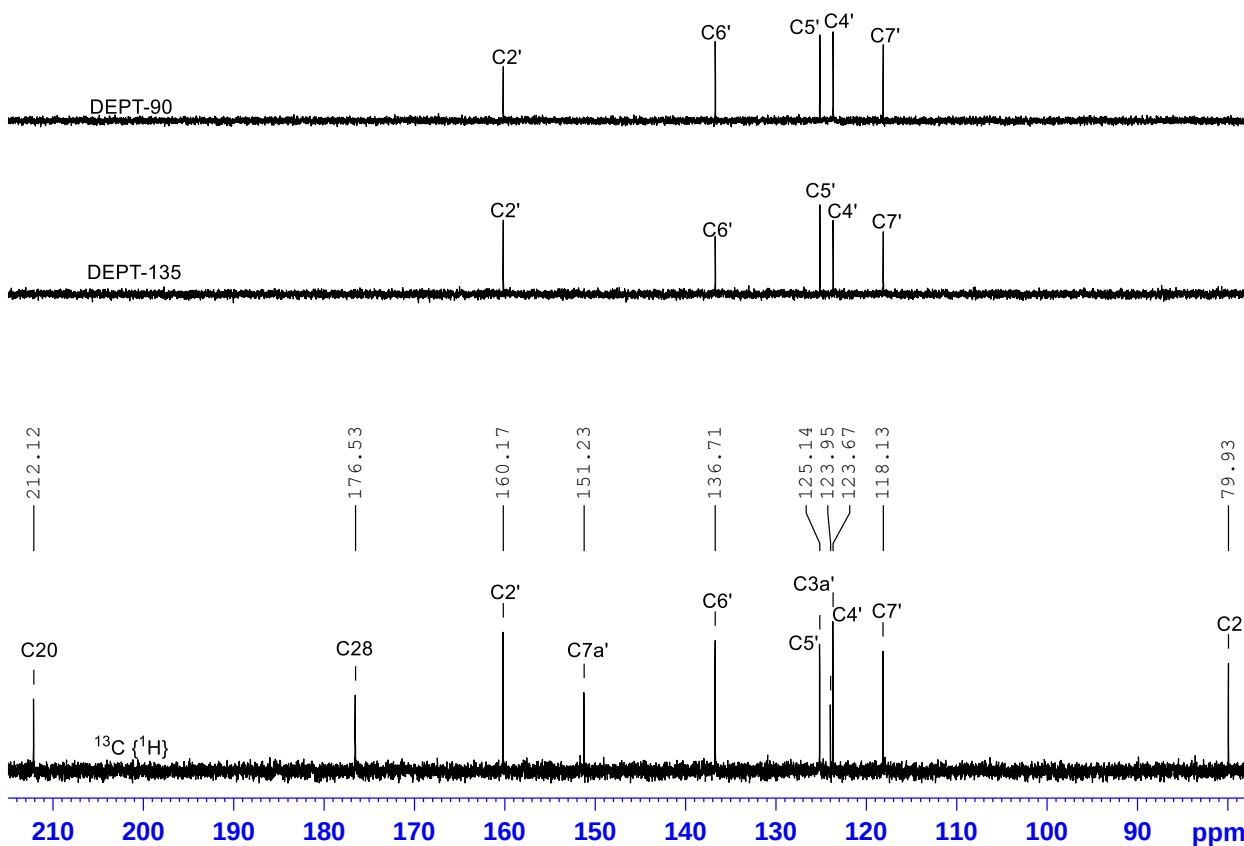


Figure S43. Downfield area of annotated $^{13}\text{C}\{^1\text{H}\}$ NMR and DEPT-135, DEPT-90 spectra of compound **6** in CDCl_3 .

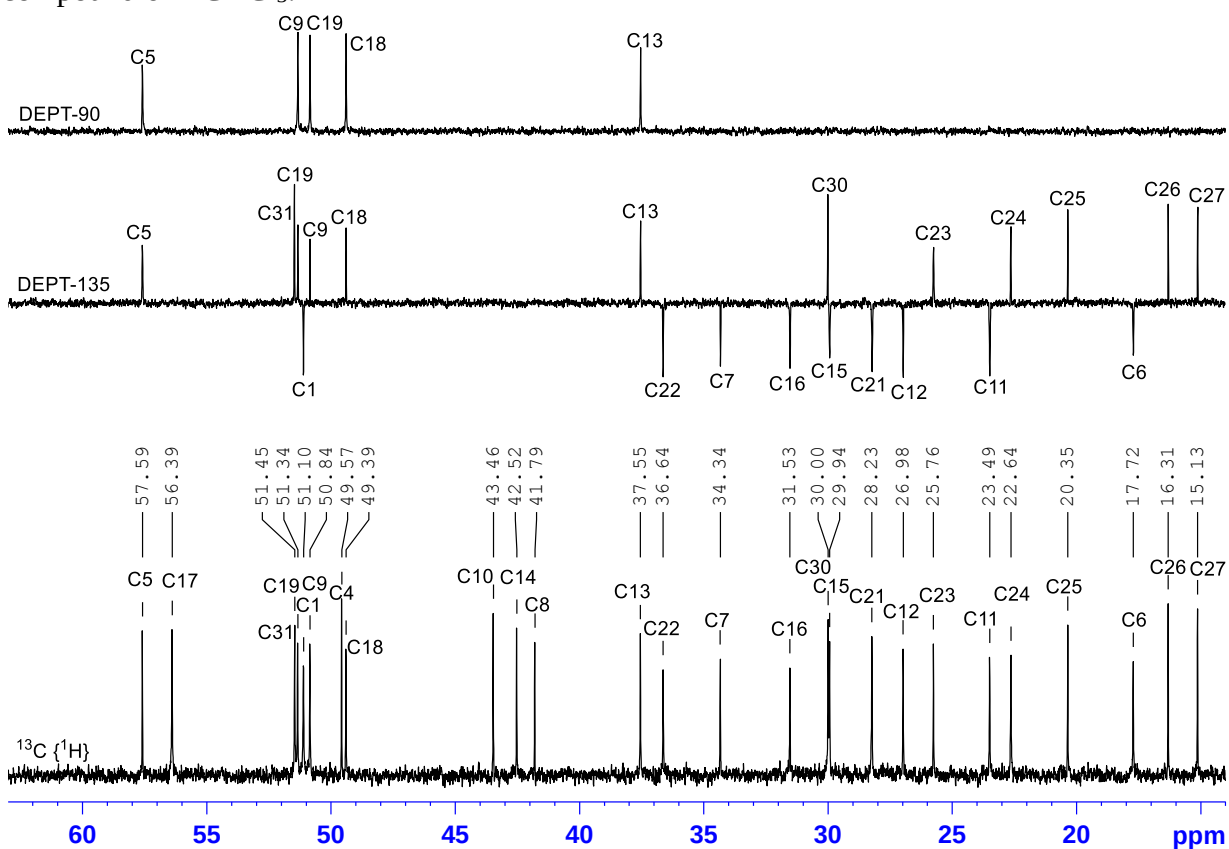


Figure S44. Upfield area of annotated $^{13}\text{C}\{^1\text{H}\}$ NMR and DEPT-135, DEPT-90 spectra of compound **6** in CDCl_3 .

Table S8. Complete numerical listings of ^{13}C NMR peaks of compound **6** in CDCl_3 .

Peak	$\nu(\text{F1})$ [ppm]	$\nu(\text{F1})$ [Hz]	Intensity [rel]	Half width [Hz]
1	212.12	26675.8	0.16	1.8
2	176.53	22199.6	0.17	3.6
3	160.17	20142.6	0.3	1.8
4	151.23	19018.2	0.17	0.9
5	136.71	17191.9	0.29	1.8
6	125.14	15737.5	0.28	1.8
7	123.95	15587.2	0.15	0.9
8	123.67	15552.4	0.32	1.8
9	118.13	14856.1	0.28	0.9
10	79.93	10051.7	0.24	0.9
11	77.26	9716.3	12.94	2.7
12	77.01	9684.3	13.46	1.8
13	76.75	9652.4	13.5	1.8
14	57.59	7241.8	0.32	0.9
15	56.39	7091.5	0.33	2.7
16	51.45	6470.7	0.33	1.8
17	51.34	6456.1	0.29	1.8
18	51.1	6426.6	0.25	3.6
19	50.84	6394.2	0.29	1.8
20	49.57	6233.5	0.39	0.9
21	49.39	6211.5	0.29	0.9
22	43.46	5466	0.35	0.9
23	42.52	5347.6	0.35	0.9
24	41.79	5255.5	0.3	0.9
25	37.55	4722.6	0.32	1.8
26	36.64	4607.4	0.24	2.7
27	34.34	4318.1	0.25	1.8
28	31.53	3965.2	0.25	2.7
29	30	3772.3	0.34	1.8
30	29.94	3764.8	0.29	1.8
31	28.23	3550.7	0.31	2.7
32	26.98	3392.4	0.28	1.8
33	25.76	3239	0.29	1.8
34	23.49	2954.6	0.26	1.8
35	22.64	2847	0.27	2.7
36	20.35	2559.1	0.34	0.9
37	17.72	2228.1	0.25	1.8
38	16.31	2051.1	0.38	0.9
39	15.13	1902.3	0.37	0.9
40	0	0	3.45	0.9

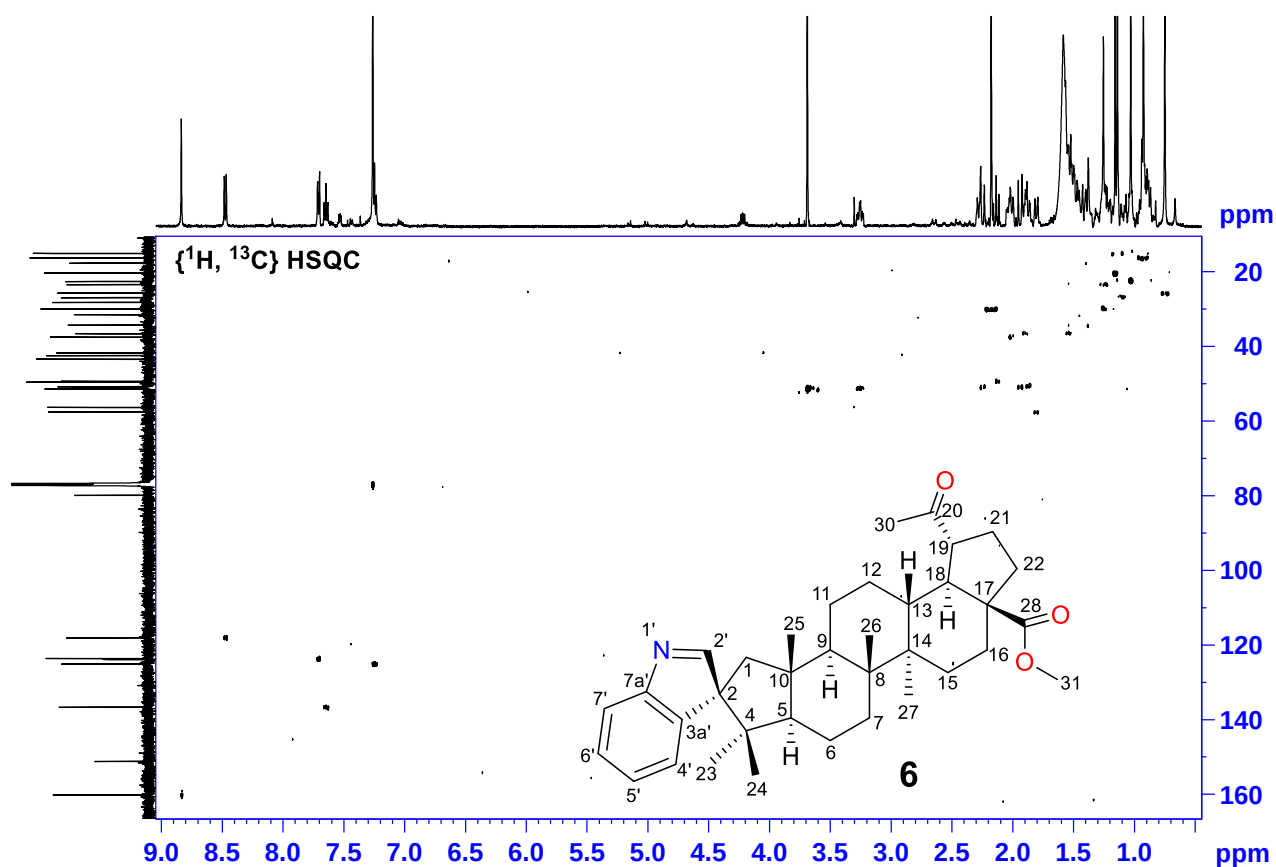


Figure S45. Complete $\{^1\text{H}, ^{13}\text{C}\}$ HSQC NMR spectrum of compound **6** in CDCl_3 .

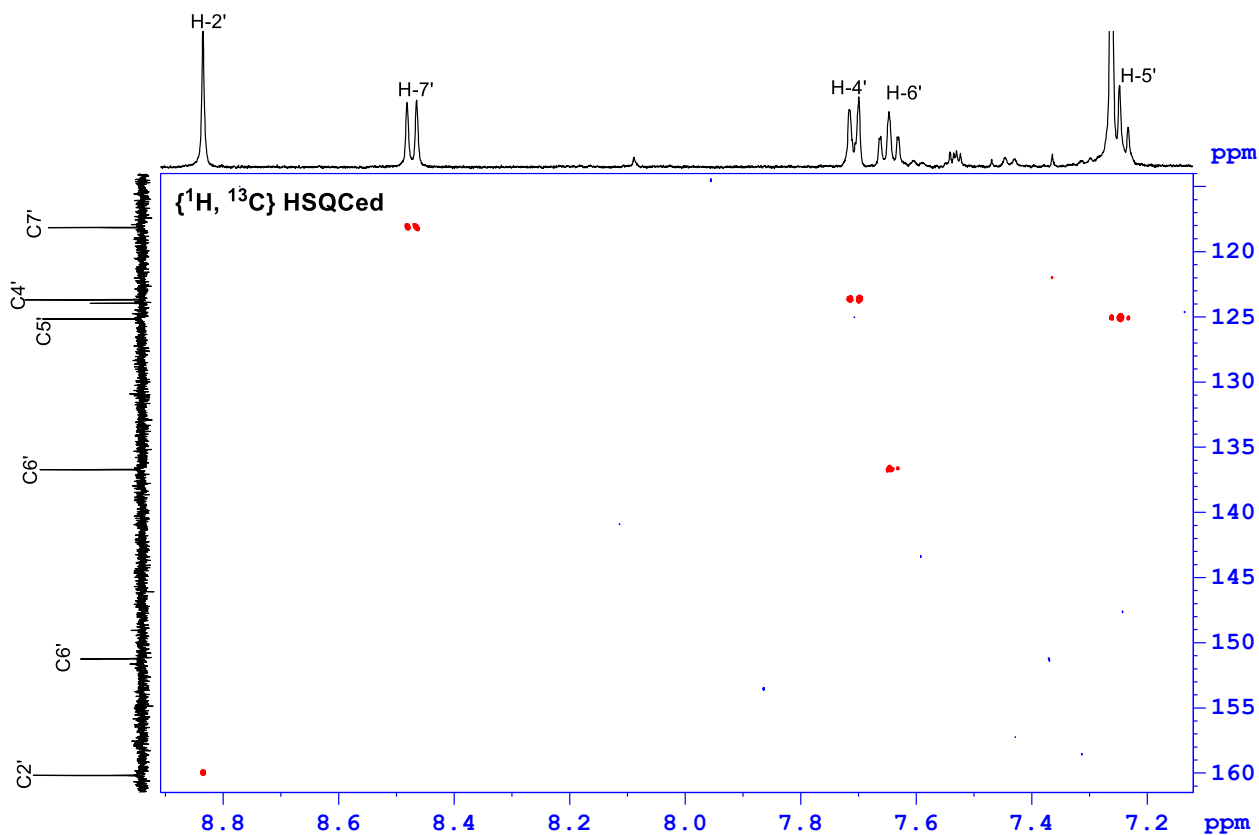


Figure S46. Downfield area of $\{^1\text{H}, ^{13}\text{C}\}$ HSQC multiplicity edited NMR spectrum of compound **6** in CDCl_3 .

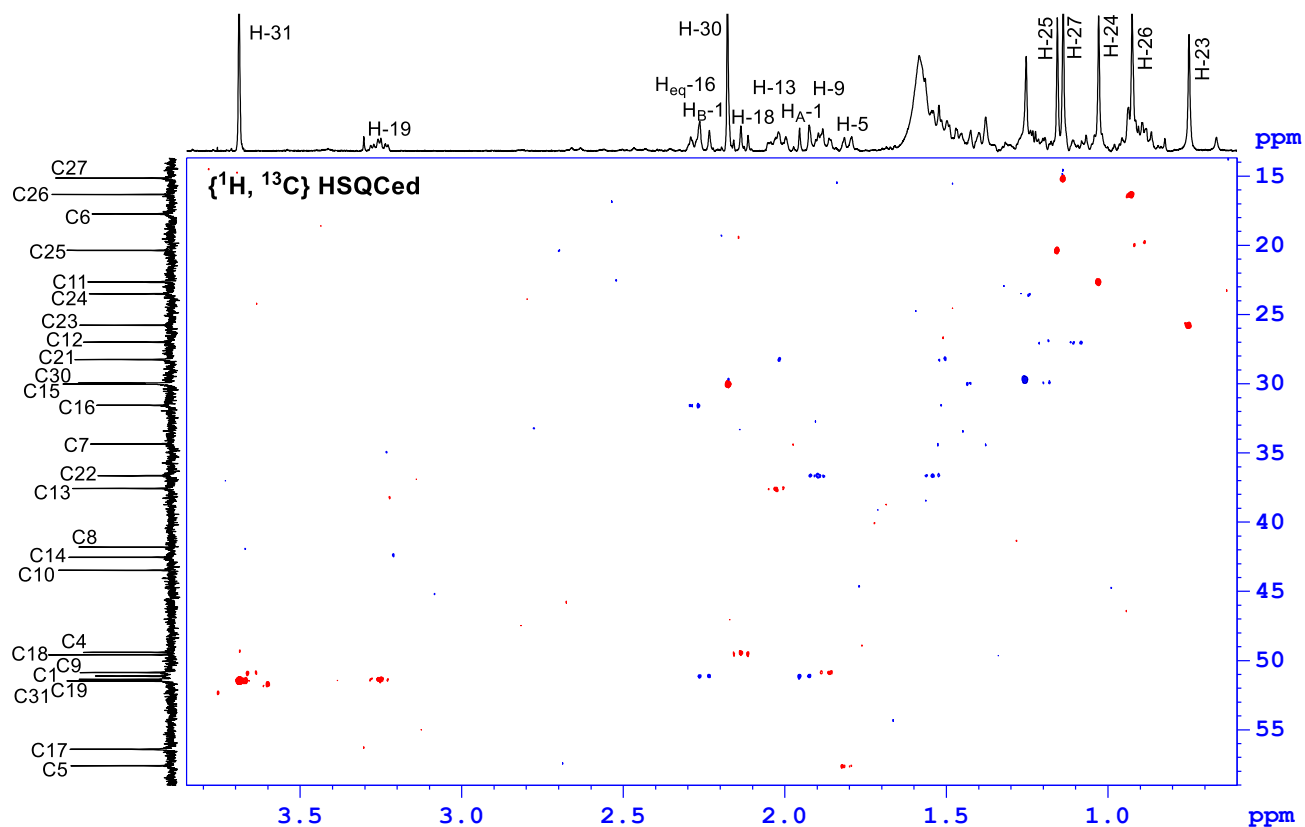


Figure S47. Upfield area of $\{^1\text{H}, ^{13}\text{C}\}$ HSQC multiplicity edited NMR spectrum of compound **6** in CDCl_3 .

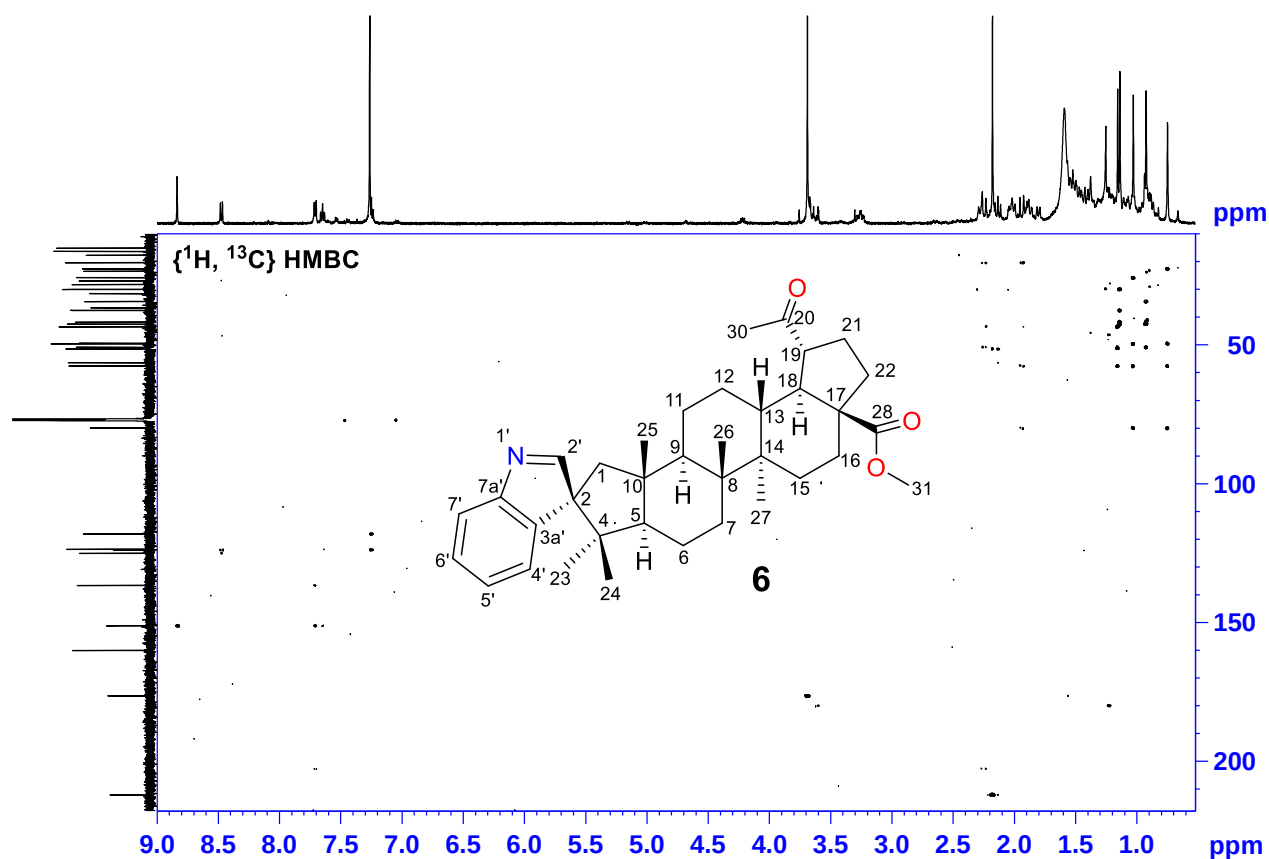


Figure S48. Complete $\{^1\text{H}, ^{13}\text{C}\}$ HMBC NMR spectrum of compound **6** in CDCl_3 .

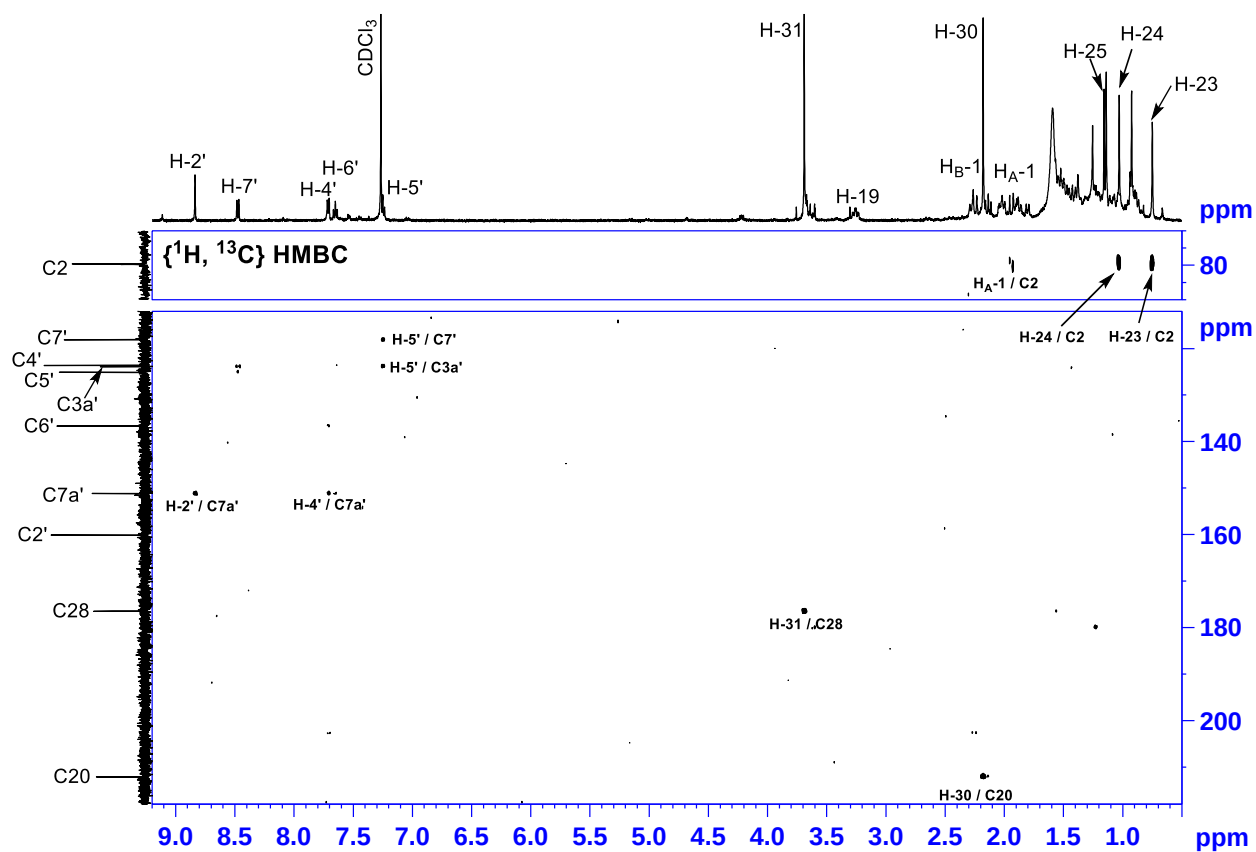


Figure S49. Annotated $\{^1\text{H}, ^{13}\text{C}\}$ HMBC NMR spectrum of compound **6** in CDCl_3 .

$\{^1\text{H}, ^1\text{H}\}$ COSY

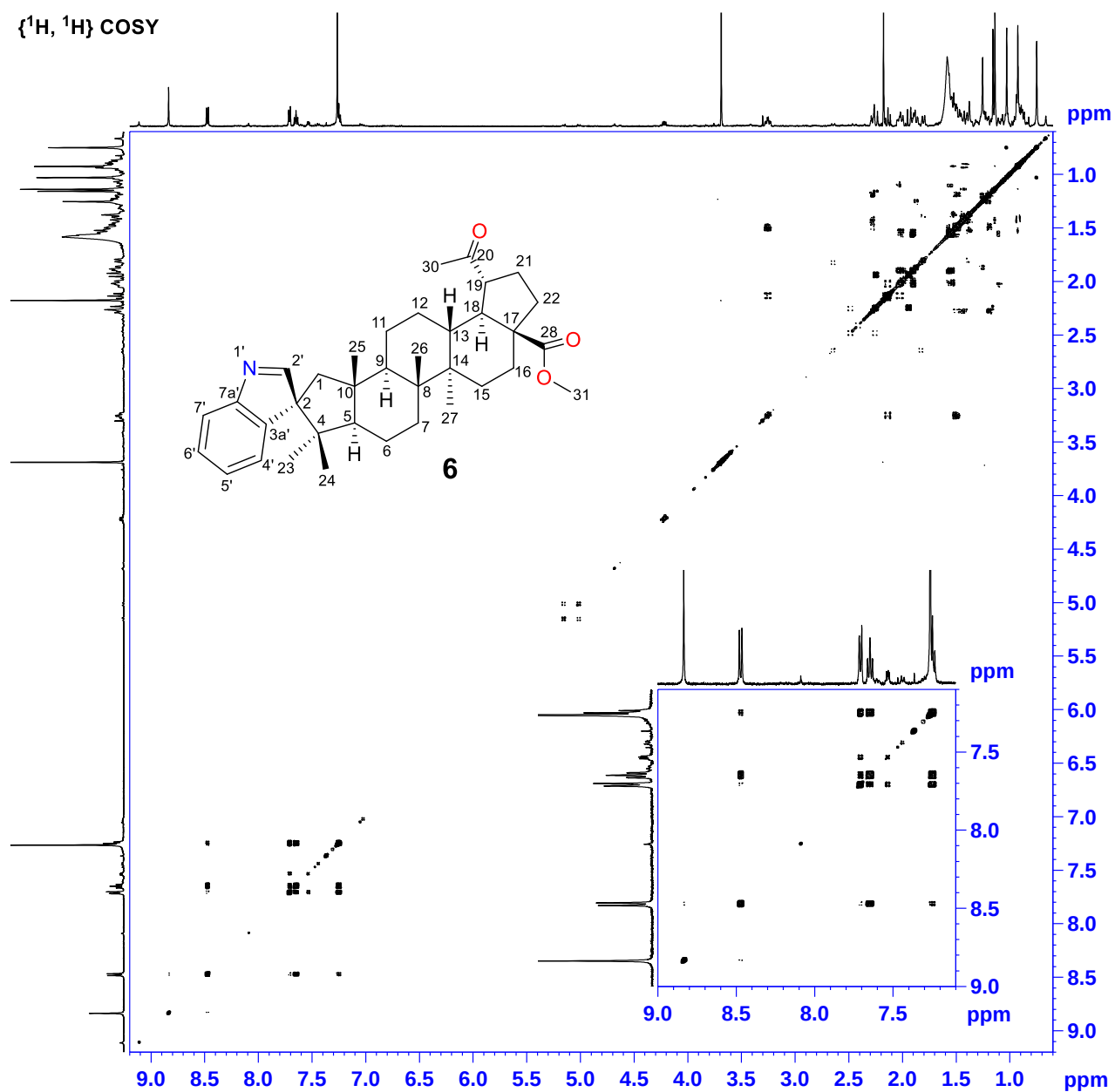


Figure S50. Complete $\{^1\text{H}, ^1\text{H}\}$ COSY NMR spectrum of compound **6** in CDCl_3 .

$\{^1\text{H}, ^1\text{H}\}$ COSY-DQF

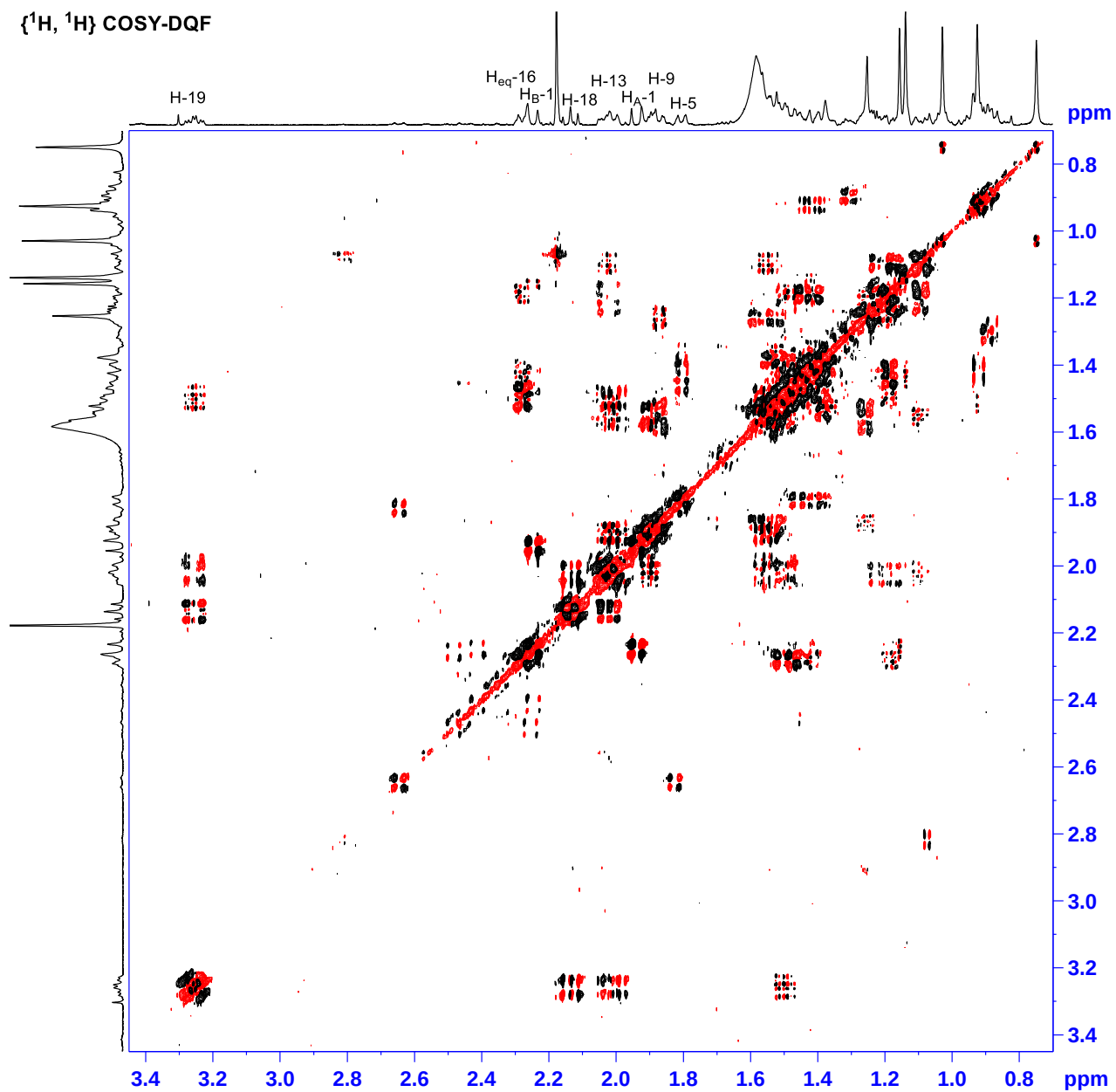


Figure S51. Upfield area of $\{^1\text{H}, ^1\text{H}\}$ COSY-DQF NMR spectrum of compound **6** in CDCl_3 .

$\{^1\text{H}, ^1\text{H}\}$ NOESY

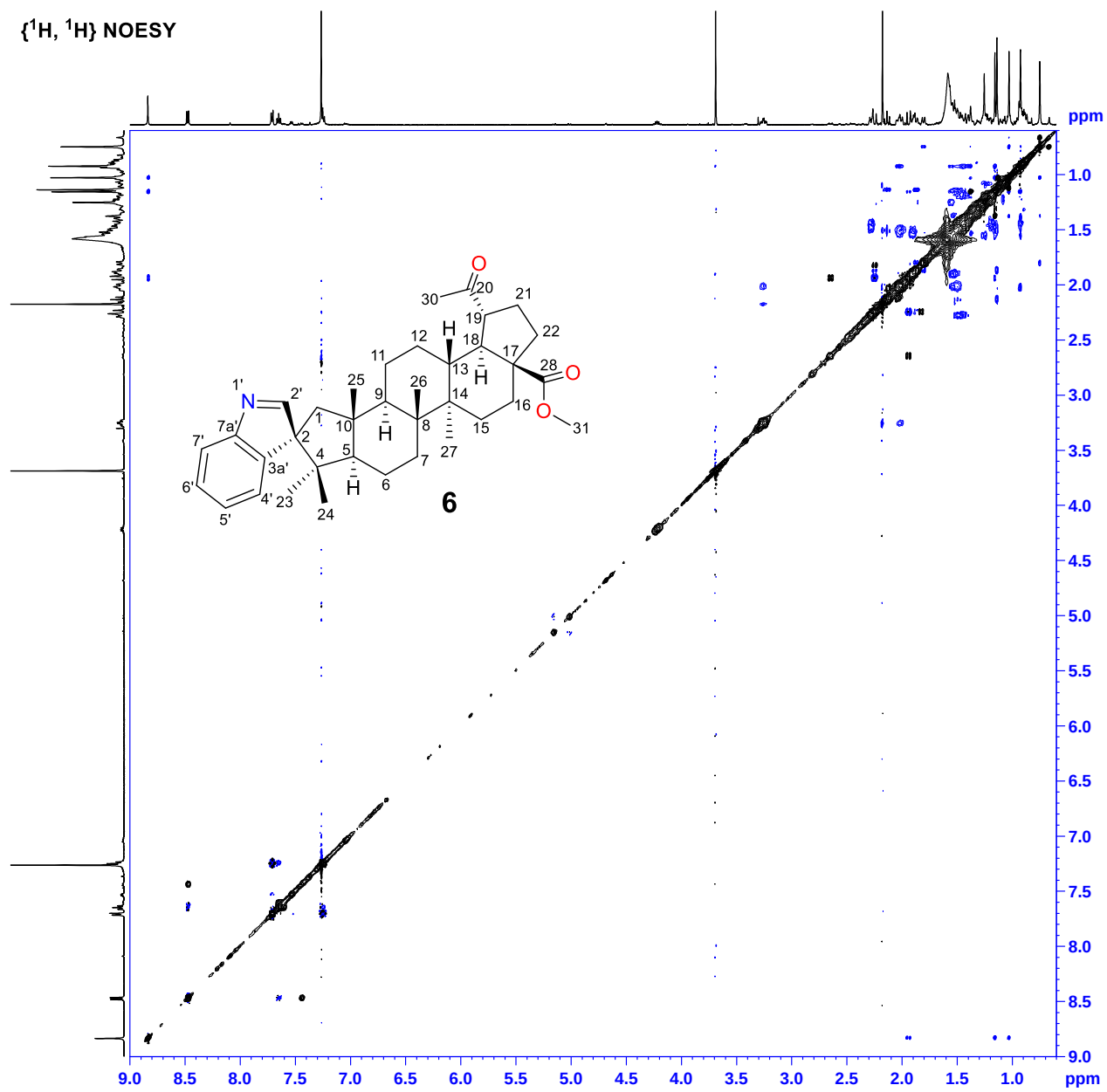


Figure S52. Complete $\{^1\text{H}, ^1\text{H}\}$ NOESY NMR spectrum of compound **6** in CDCl_3 .

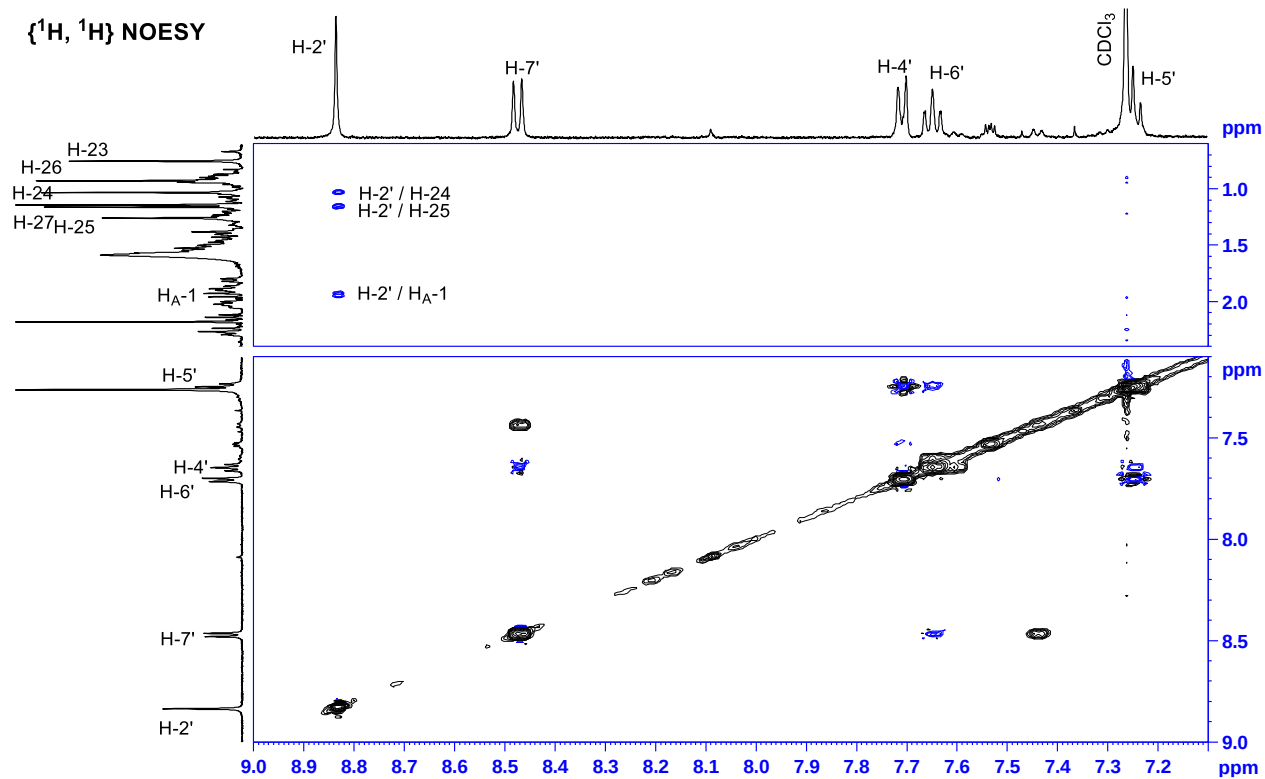


Figure S53. Detailed and annotated $\{^1\text{H}, ^1\text{H}\}$ NOESY NMR spectrum of compound **6** in CDCl_3 .

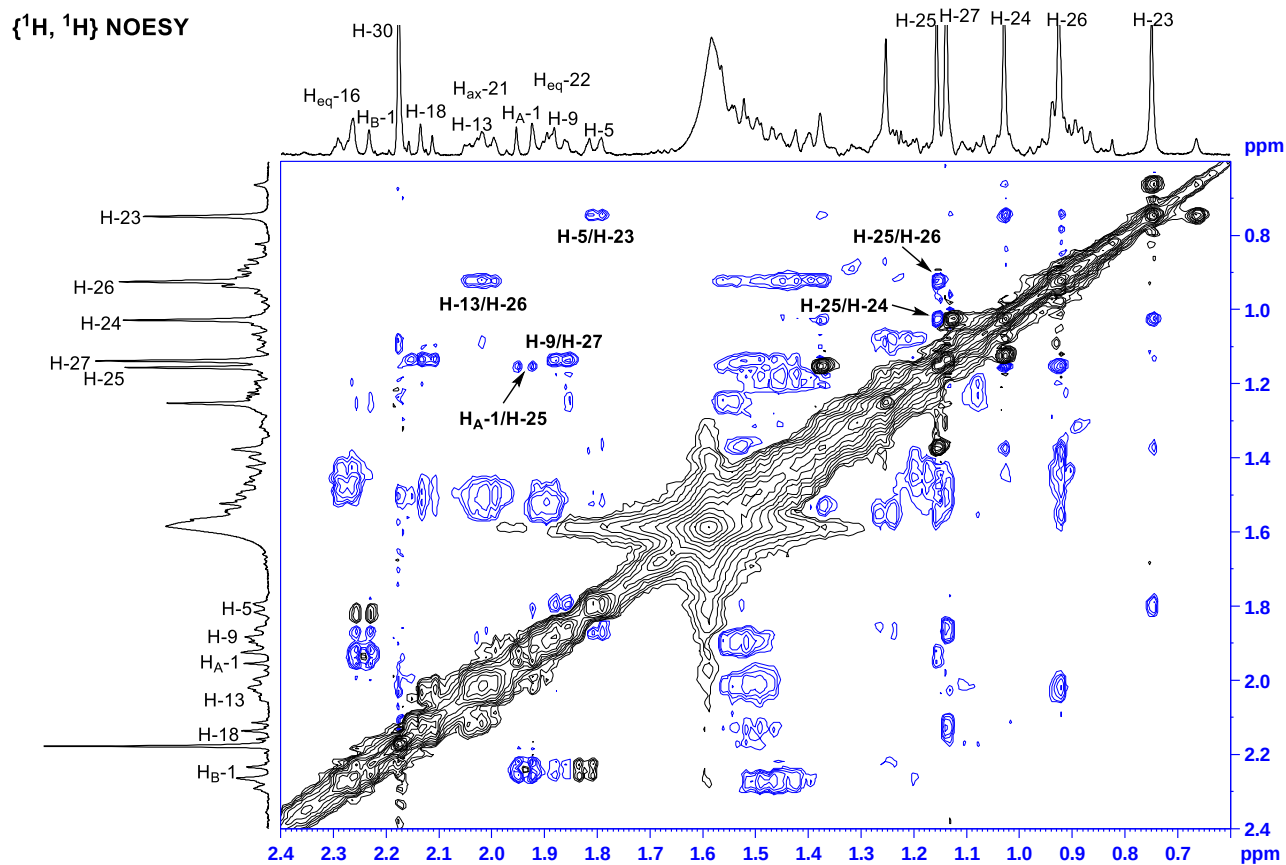


Figure S54. Upfield area of $\{^1\text{H}, ^1\text{H}\}$ NOESY NMR spectrum of compound **6** in CDCl_3 .

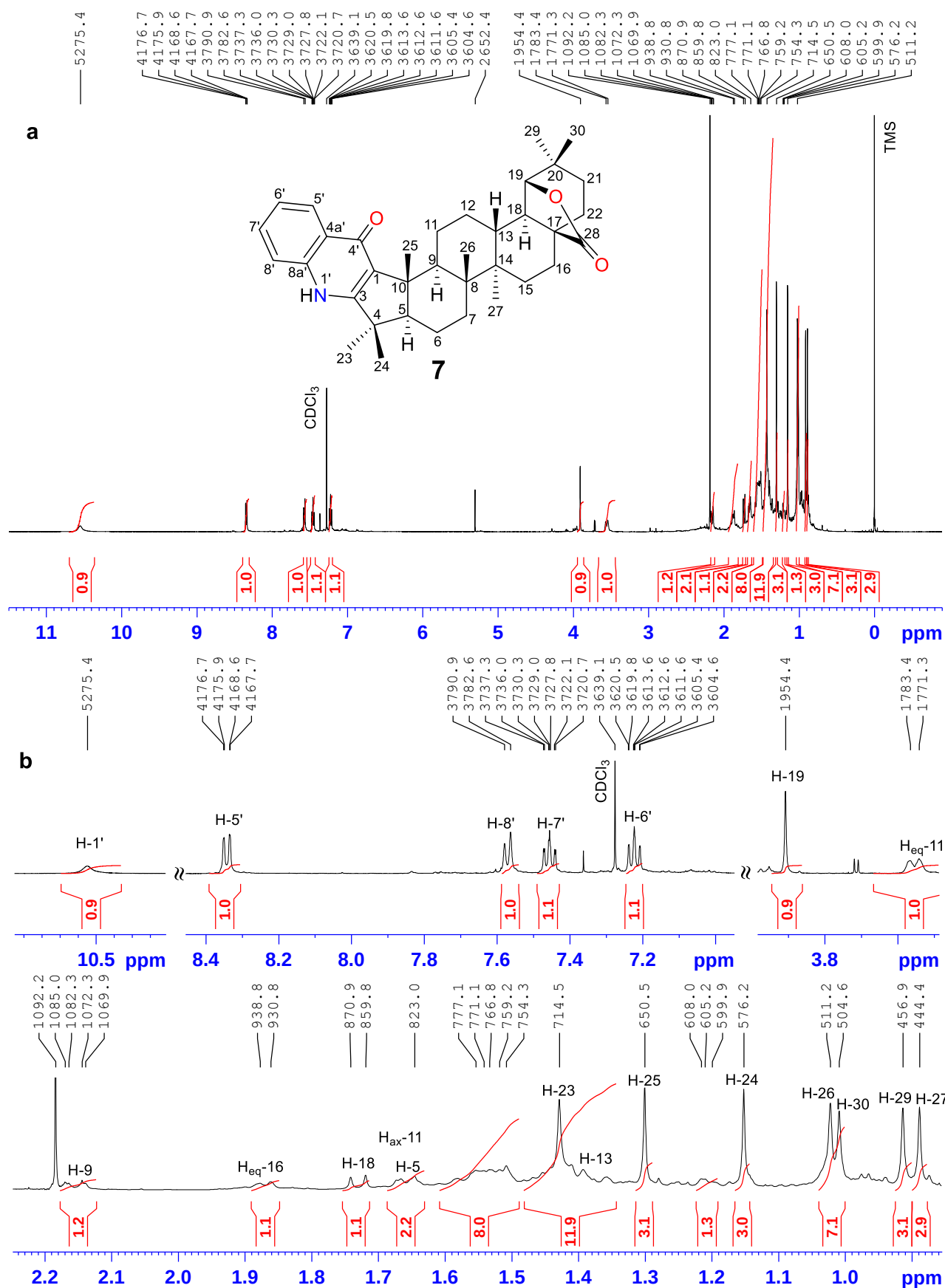
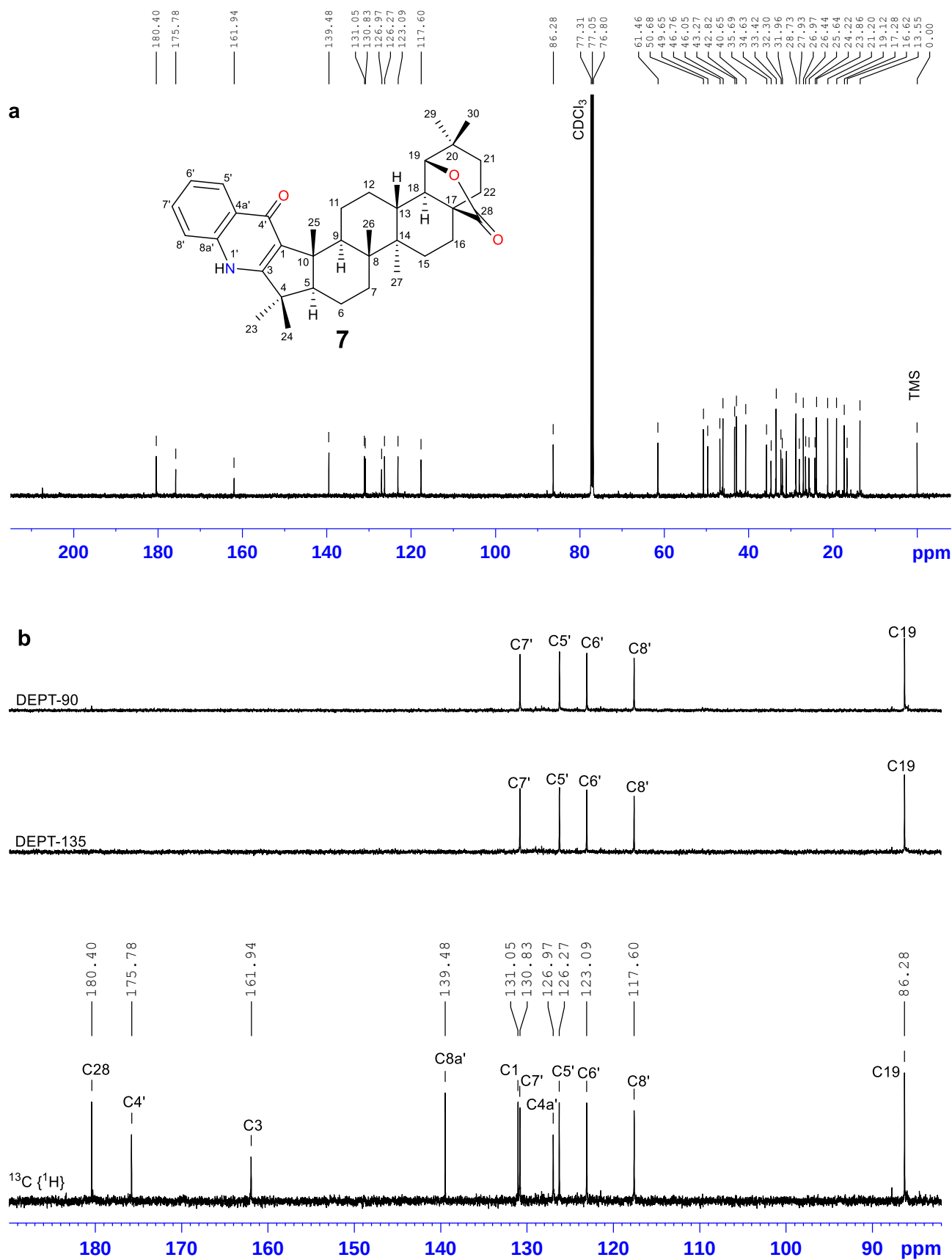


Figure S55. (a) Complete ^1H NMR spectrum of compound **7** in CDCl_3 . (b) Detailed and annotated ^1H NMR spectrum of compound **7** in CDCl_3 .

Table S9. Complete numerical listings of ^1H NMR peaks of compound **7** in CDCl_3 .

Peak	$\nu(\text{F1})$ [ppm]	$\nu(\text{F1})$ [Hz]	Intensity [rel]	Half width [Hz]
1	10.55	5275.4	0.11	0.6
2	8.35	4176.7	0.55	1.5
3	8.35	4175.9	0.56	1.7
4	8.34	4168.6	0.61	1.7
5	8.33	4167.7	0.59	1.3
6	7.58	3790.9	0.47	3.4
7	7.56	3782.6	0.64	3.4
8	7.47	3737.3	0.39	1.3
9	7.47	3736	0.39	1.7
10	7.46	3730.3	0.52	1.3
11	7.46	3729	0.67	2.6
12	7.45	3727.8	0.43	1.1
13	7.44	3722.1	0.38	1.5
14	7.44	3720.7	0.37	1.3
15	7.28	3639.1	2.84	0.2
16	7.24	3620.5	0.44	1.1
17	7.24	3619.8	0.45	1.5
18	7.23	3613.6	0.55	1.1
19	7.22	3612.6	0.73	3
20	7.22	3611.6	0.57	1.1
21	7.21	3605.4	0.43	1.3
22	7.21	3604.6	0.43	1.3
23	5.3	2652.4	0.84	0.2
24	3.91	1954.4	1.27	2.4
25	3.57	1783.4	0.2	6.6
26	3.54	1771.3	0.23	10.9
27	2.18	1092.2	13.5	0.2
28	2.17	1085	0.4	2.6
29	2.16	1082.3	0.36	3.4
30	2.14	1072.3	0.5	4.1
31	2.14	1069.9	0.34	2.6
32	1.88	938.8	0.35	10
33	1.86	930.8	0.42	4.7
34	1.74	870.9	0.64	2.8
35	1.72	859.8	0.73	3
36	1.65	823	0.68	11.8
37	1.55	777.1	0.95	12.4
38	1.54	771.1	0.94	3.8
39	1.53	766.8	0.99	2.6
40	1.52	759.2	0.98	5.3
41	1.51	754.3	1.17	8.5
42	1.43	714.5	4.31	3.6
43	1.3	650.5	4.89	1.9
44	1.22	608	0.56	6.6
45	1.21	605.2	0.55	4.3
46	1.2	599.9	0.42	3
47	1.15	576.2	4.77	1.7
48	1.02	511.2	4.13	3.4
49	1.01	504.6	3.76	3.4
50	0.91	456.9	3.91	2.4
51	0.89	444.4	3.94	2.4
52	0	0	8.19	0.4



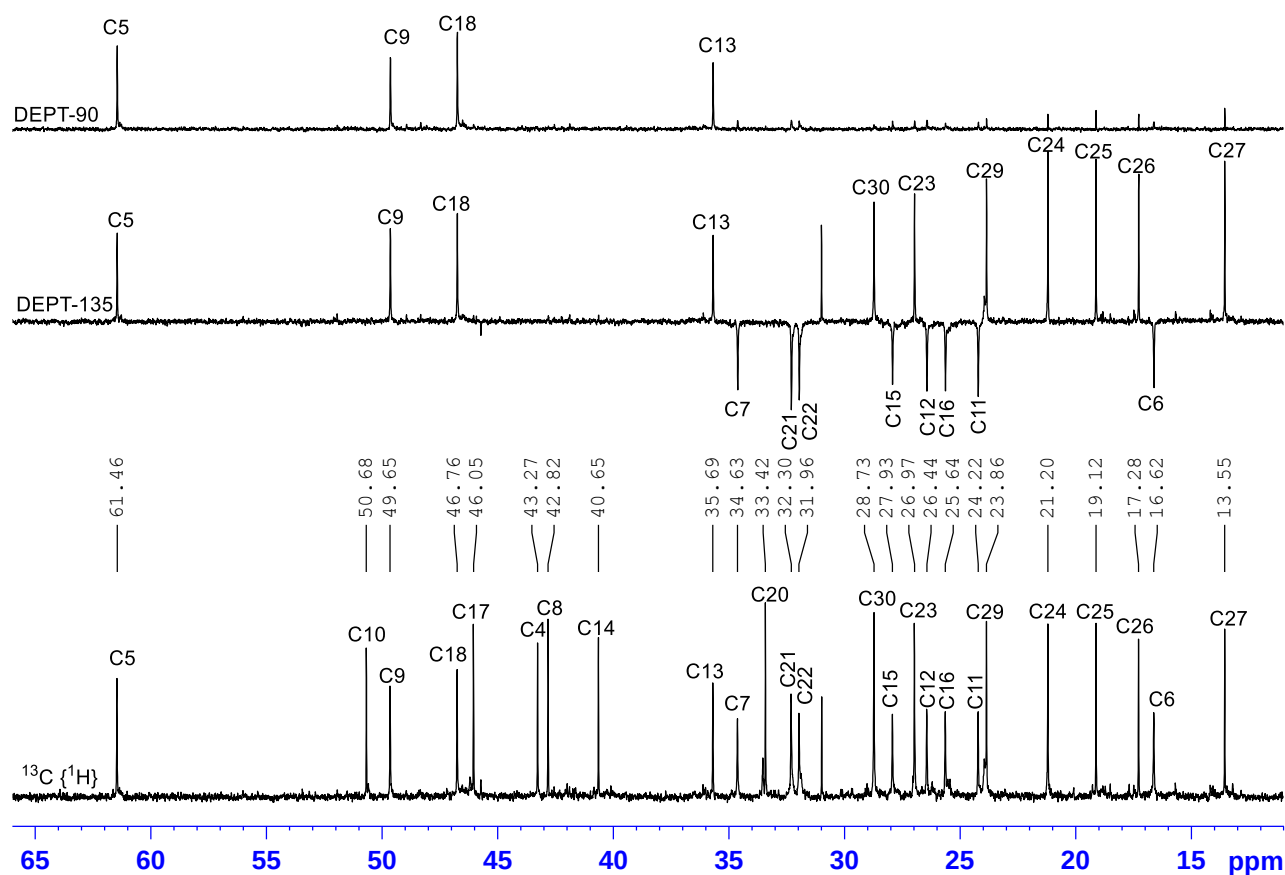


Figure S57. Upfield area of annotated $^{13}\text{C}\{^1\text{H}\}$ NMR and DEPT-135, DEPT-90 spectra of compound **7** in CDCl_3 .

Table S10. Complete numerical listings of ^{13}C NMR peaks of compound **7** in CDCl_3 .

Peak	$\nu(\text{F1})$ [ppm]	$\nu(\text{F1})$ [Hz]	Intensity [rel]	Half width [Hz]
1	180.4	22687.1	0.8	0.9
2	175.78	22105.9	0.52	2.7
3	161.94	20364.8	0.34	5.4
4	139.48	17540.2	0.84	1.8
5	131.05	16480.8	0.8	1.8
6	130.83	16452.8	0.73	2.7
7	126.97	15967.7	0.53	2.7
8	126.27	15879.7	0.78	2.7
9	123.09	15479.4	0.76	3.6
10	117.6	14789.3	0.69	3.6
11	86.28	10850.7	1	2.7
12	77.31	9721.7	13.39	2.7
13	77.05	9689.7	13.5	2.7
14	76.8	9657.7	13.45	1.8
15	61.46	7729.3	1.02	1.8
16	50.68	6374	1.31	0.9
17	49.65	6244.5	0.96	2.7
18	46.76	5880.1	1.09	2.7
19	46.05	5791	1.49	1.8
20	43.27	5441.8	1.39	0.9

21	42.82	5385	1.53	1.8
22	40.65	5111.4	1.41	0.9
23	35.69	4488.7	0.98	1.8
24	34.63	4354.9	0.68	3.6
25	33.42	4202.6	1.67	1.8
26	32.3	4062.6	0.88	4.5
27	31.96	4019.8	0.72	4.5
28	28.73	3612.5	1.61	2.7
29	27.93	3511.9	0.72	4.5
30	26.97	3392.2	1.5	1.8
31	26.44	3325	0.76	3.6
32	25.64	3224.1	0.74	4.5
33	24.22	3045.7	0.74	4.5
34	23.86	3000.5	1.59	2.7
35	21.2	2666.2	1.57	1.8
36	19.12	2404	1.51	1.8
37	17.28	2173	1.42	1.8
38	16.62	2090	0.72	3.6
39	13.55	1704.1	1.46	1.8
40	0	0	1.02	1.8

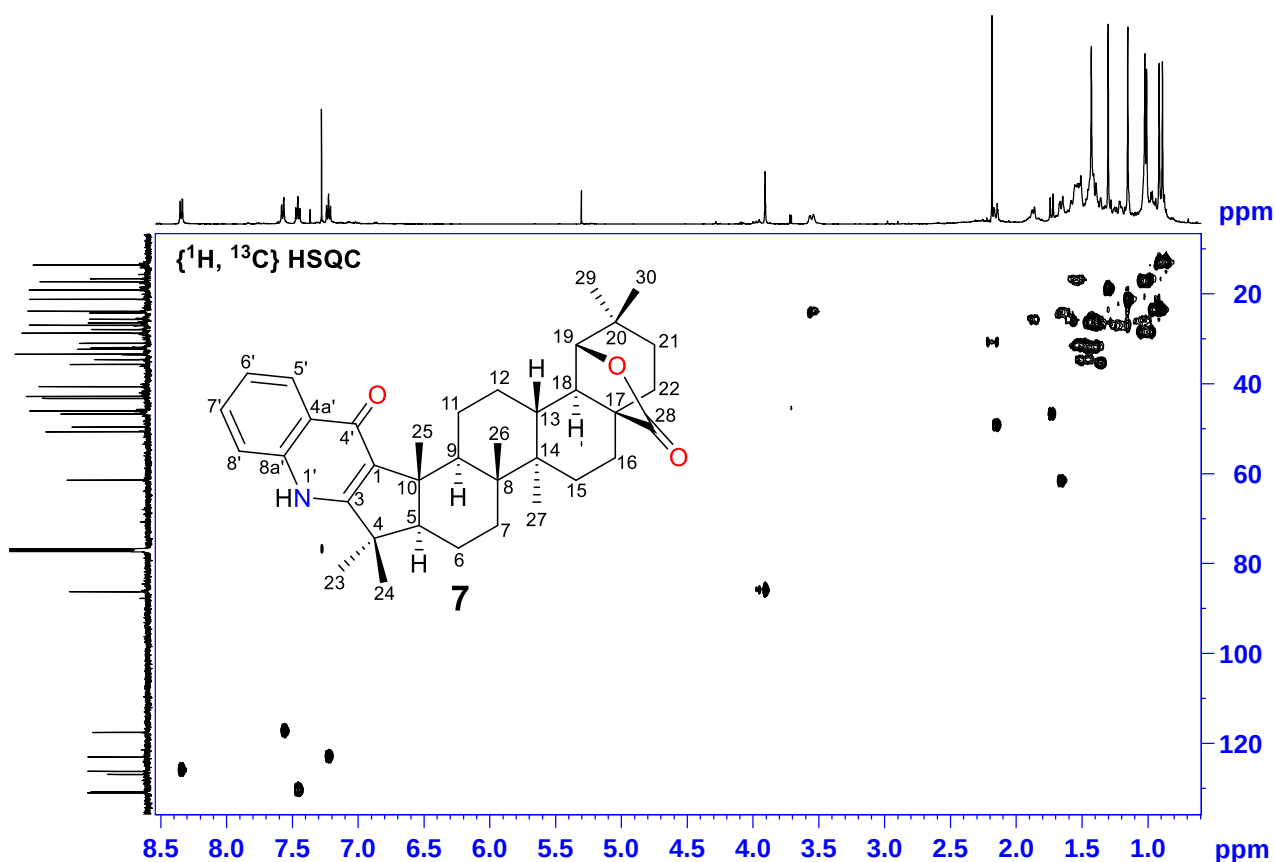


Figure S58. Complete $\{^1\text{H}, ^{13}\text{C}\}$ HSQC NMR spectrum of compound **7** in CDCl_3 .

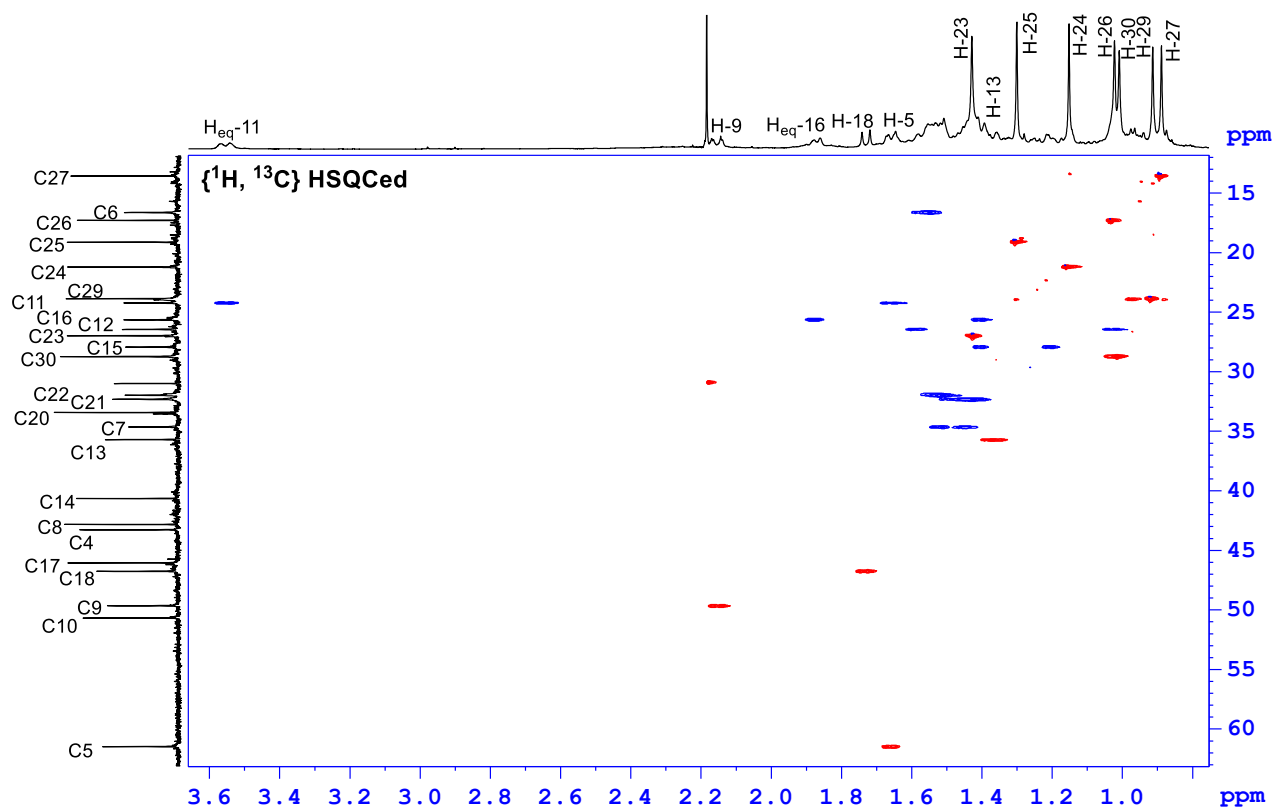


Figure S59. Upfield area of $\{^1\text{H}, ^{13}\text{C}\}$ HSQC multiplicity edited NMR spectrum of compound **7** in CDCl_3 .

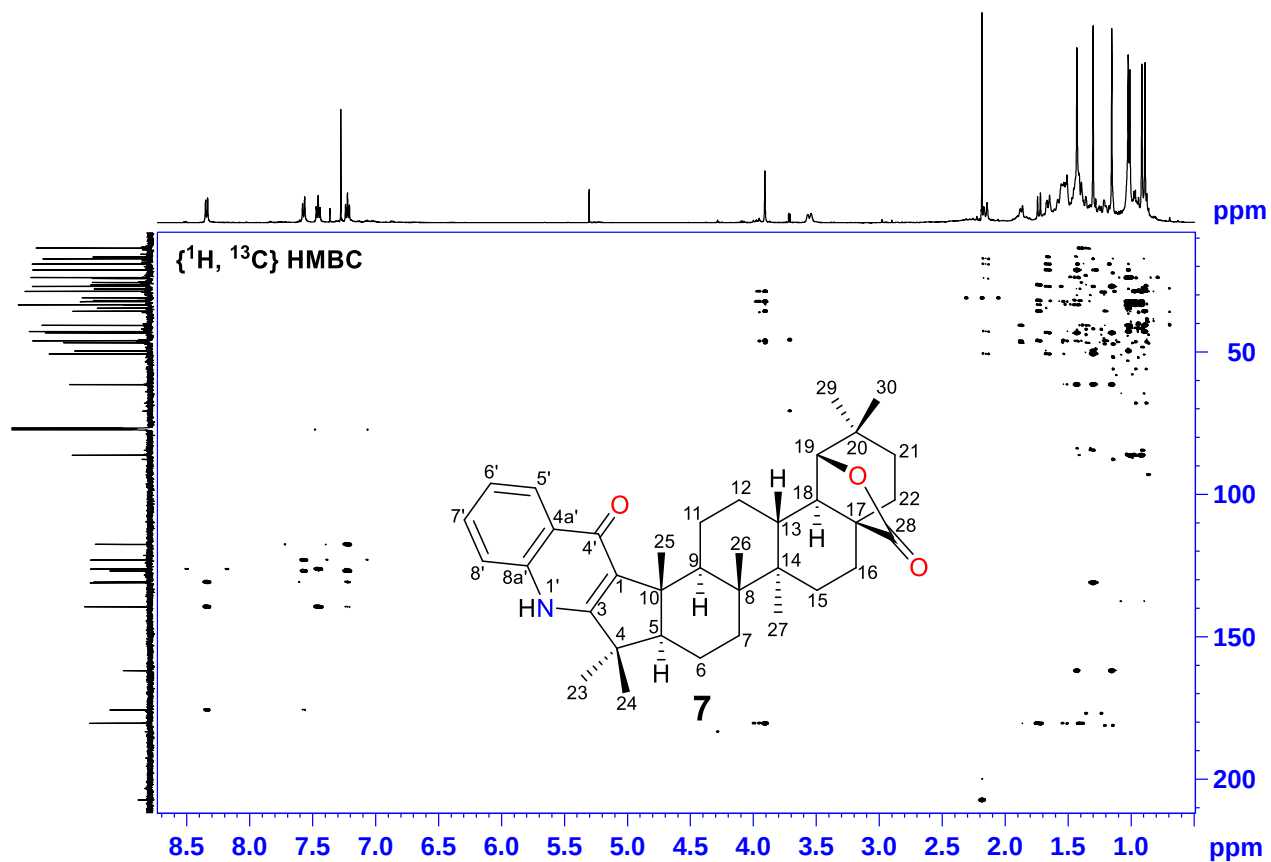


Figure S60. Complete $\{^1\text{H}, ^{13}\text{C}\}$ HMBC NMR spectrum of compound **7** in CDCl_3 .

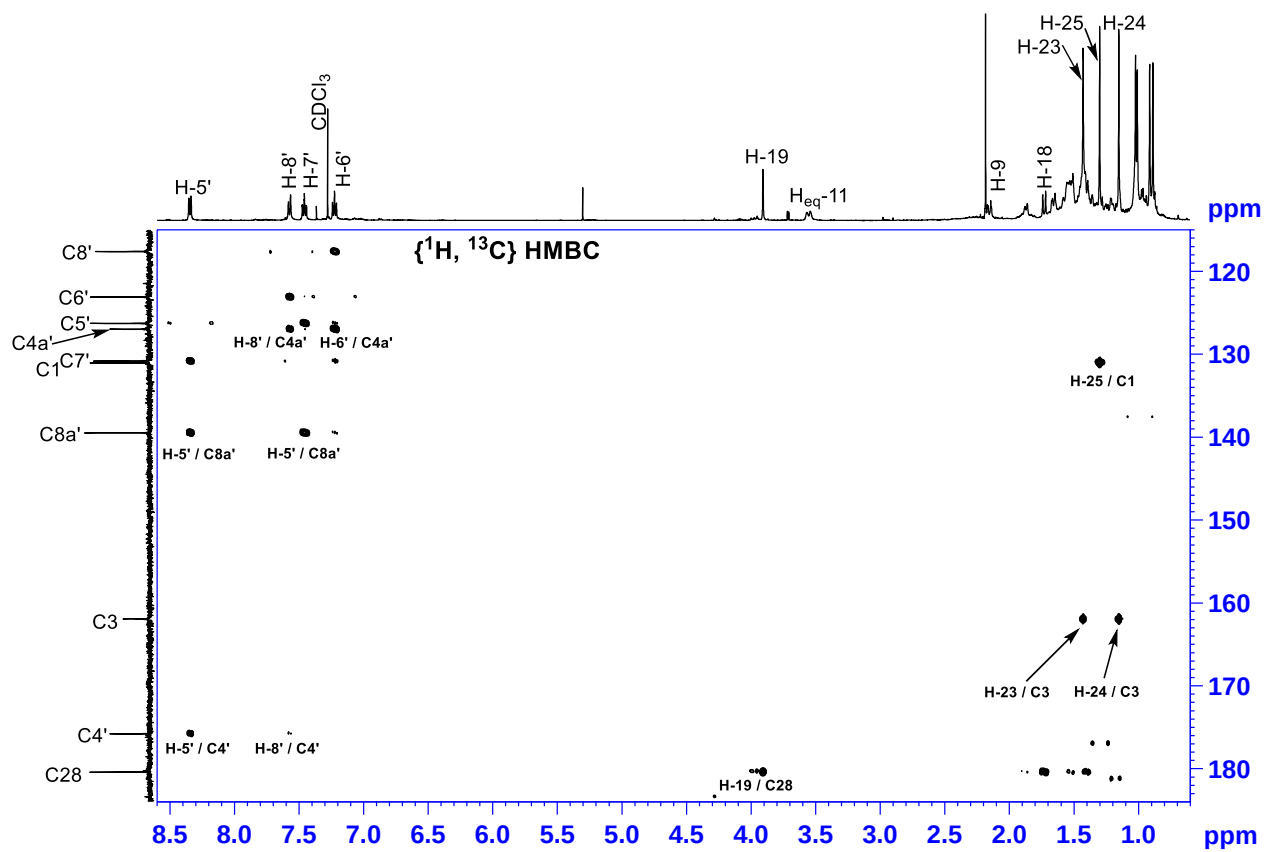


Figure S61. Annotated $\{^1\text{H}, ^{13}\text{C}\}$ HMBC NMR spectrum of compound 7 in CDCl_3 .

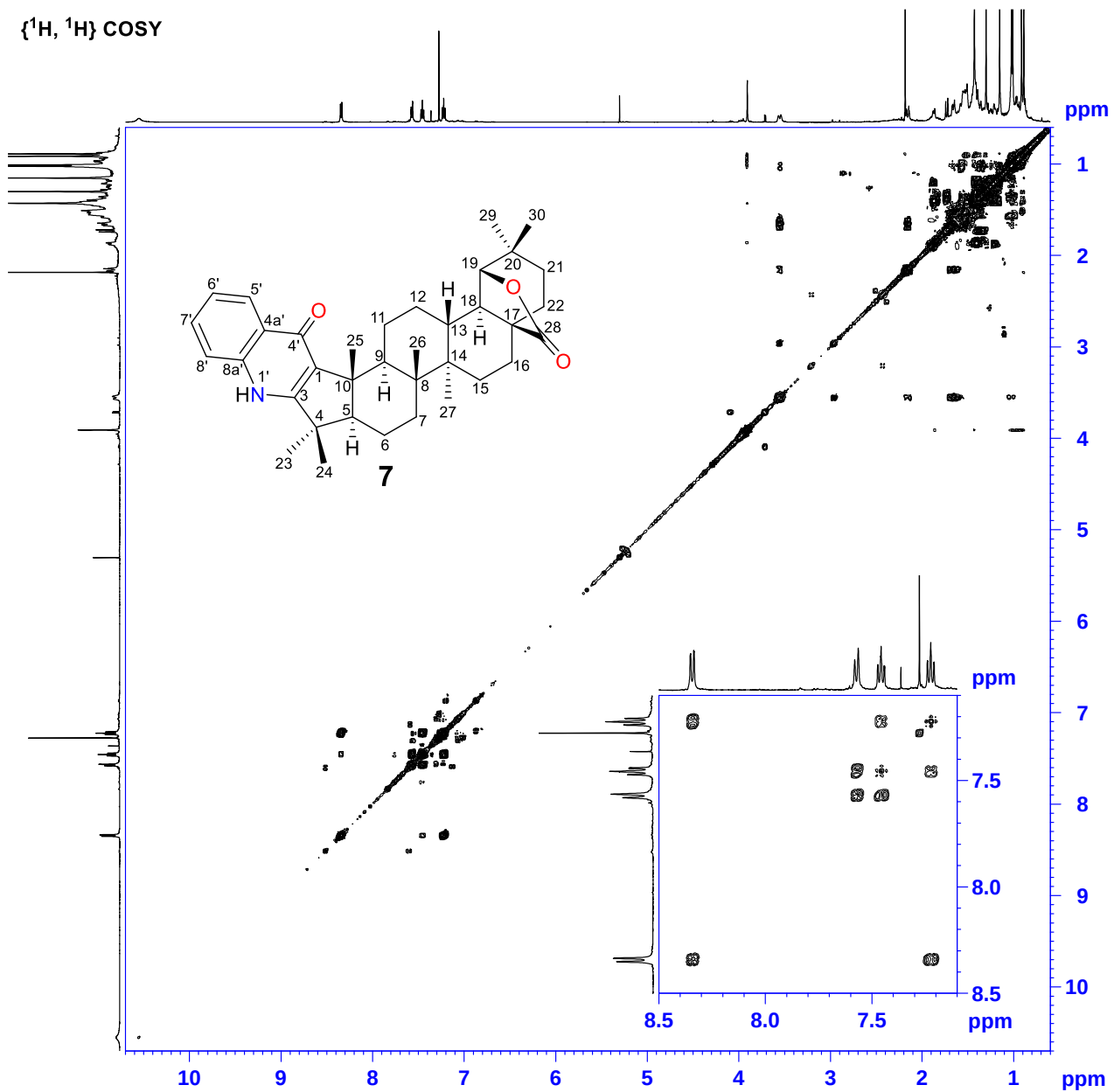


Figure S62. Complete $\{^1\text{H}, ^1\text{H}\}$ COSY NMR spectrum of compound **7** in CDCl_3 .

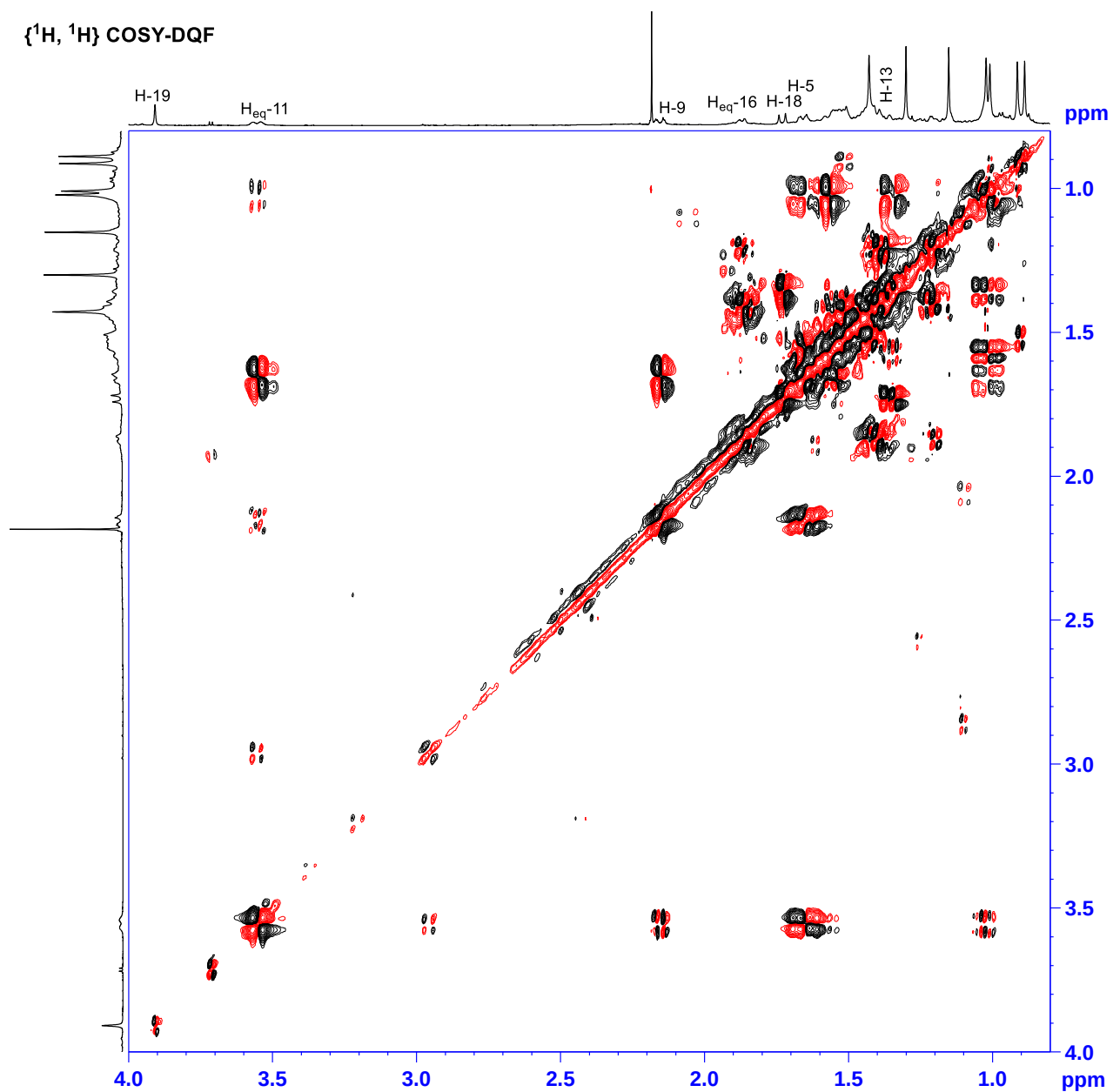


Figure S63. Upfield area of $\{^1\text{H}, ^1\text{H}\}$ COSY-DQF NMR spectrum of compound **7** in CDCl_3 .

$\{^1\text{H}, ^1\text{H}\}$ ROESY

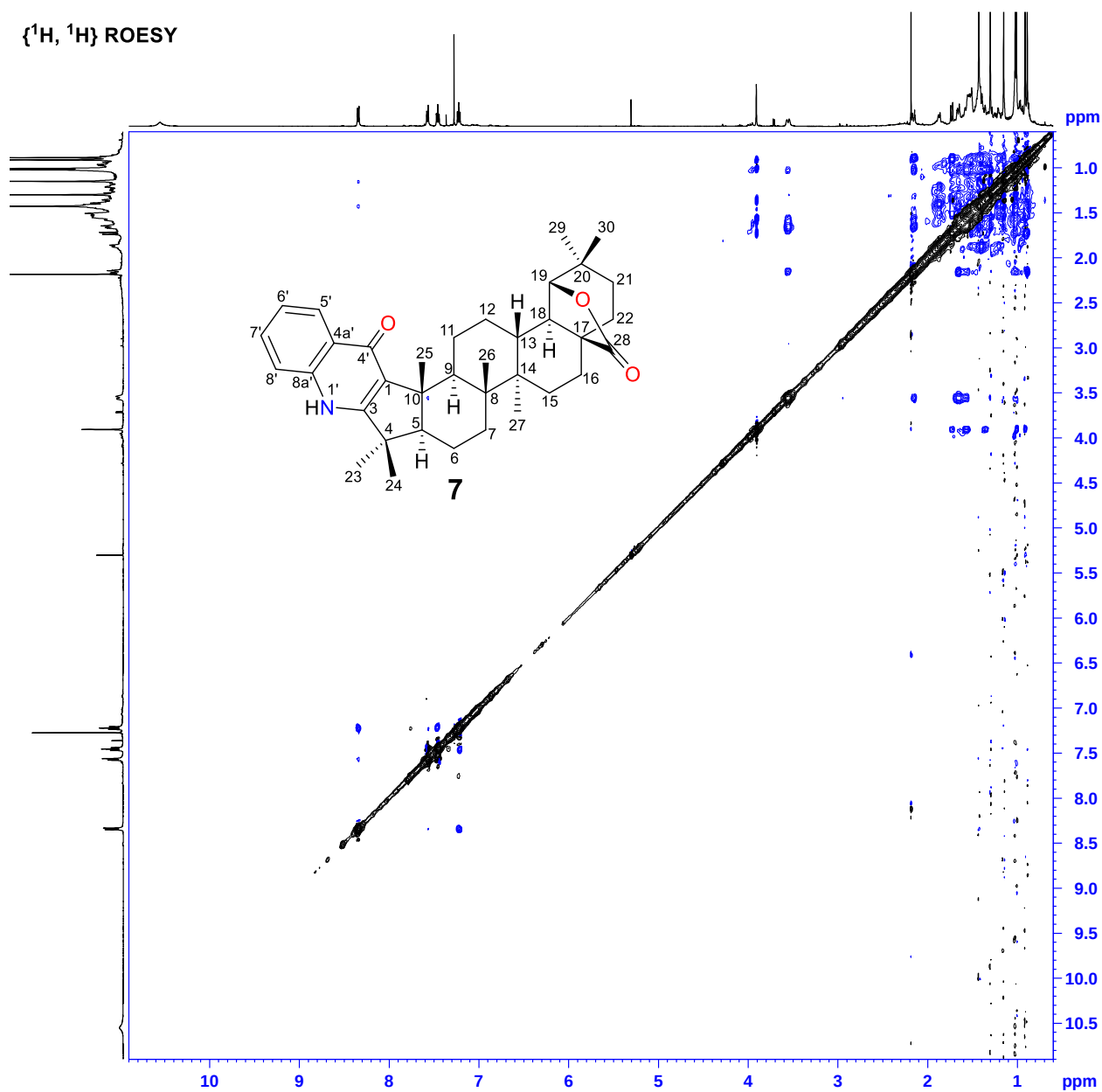


Figure S64. Complete $\{^1\text{H}, ^1\text{H}\}$ ROESY NMR spectrum of compound **7** in CDCl_3 .

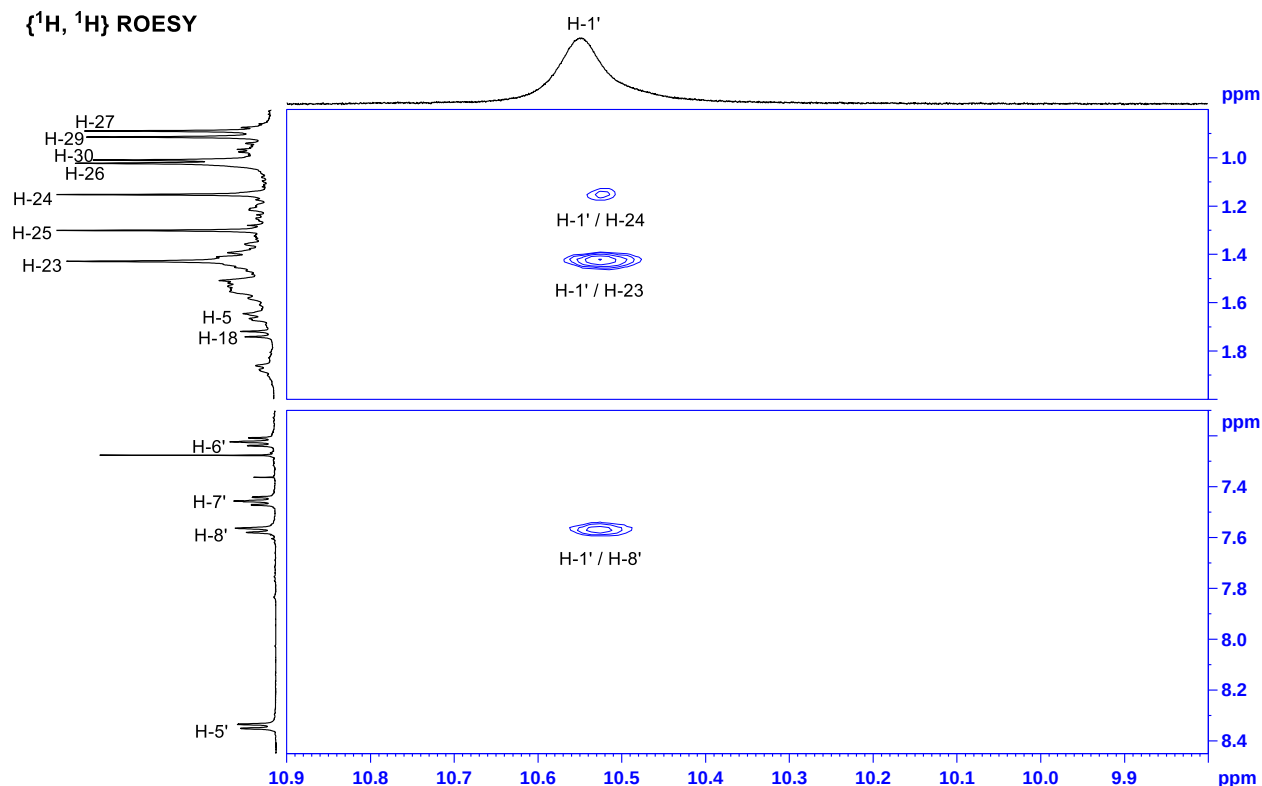


Figure S65. Detailed and annotated $\{^1\text{H}, ^1\text{H}\}$ ROESY NMR spectrum of compound **7** in CDCl_3 .

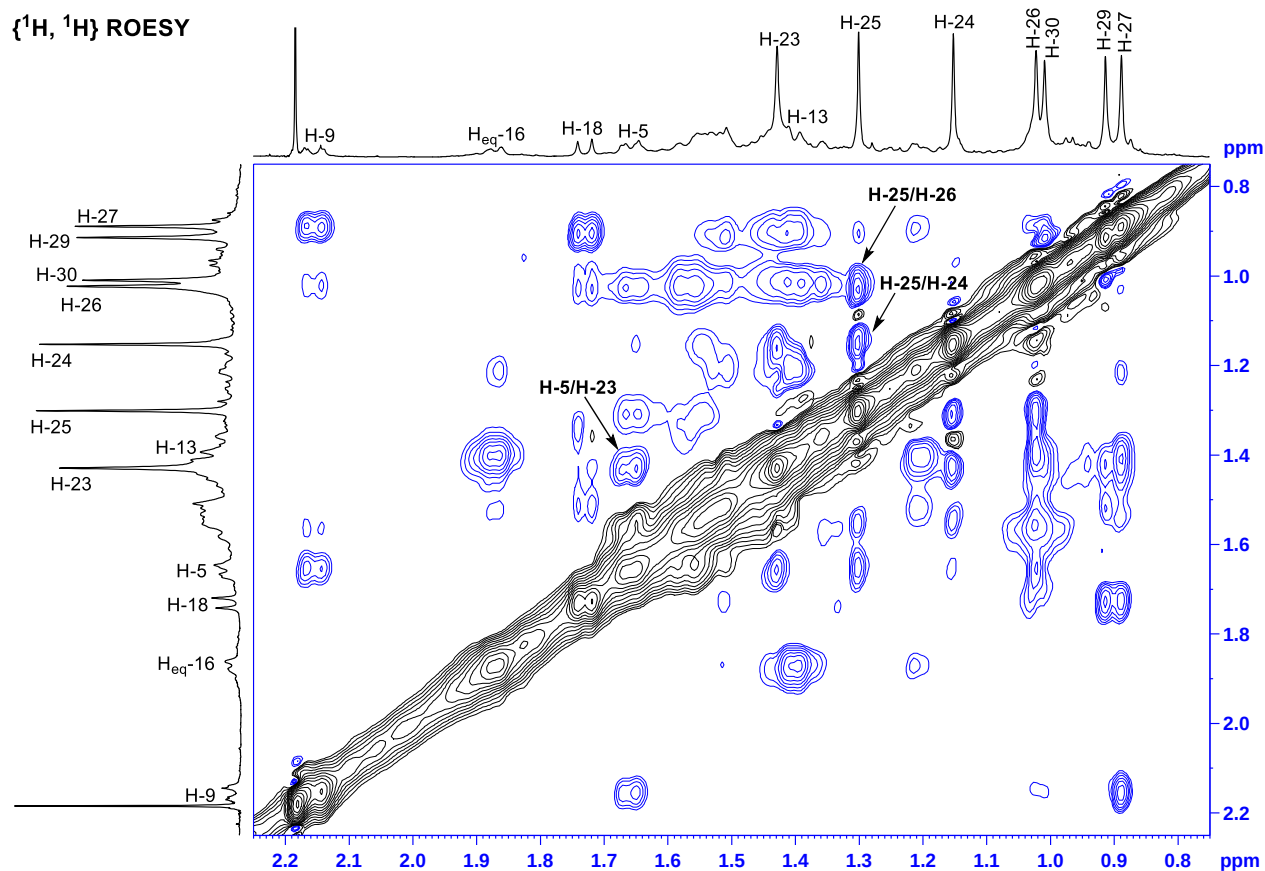


Figure S66. Upfield area of $\{^1\text{H}, ^1\text{H}\}$ ROESY NMR spectrum of compound **7** in CDCl_3 .

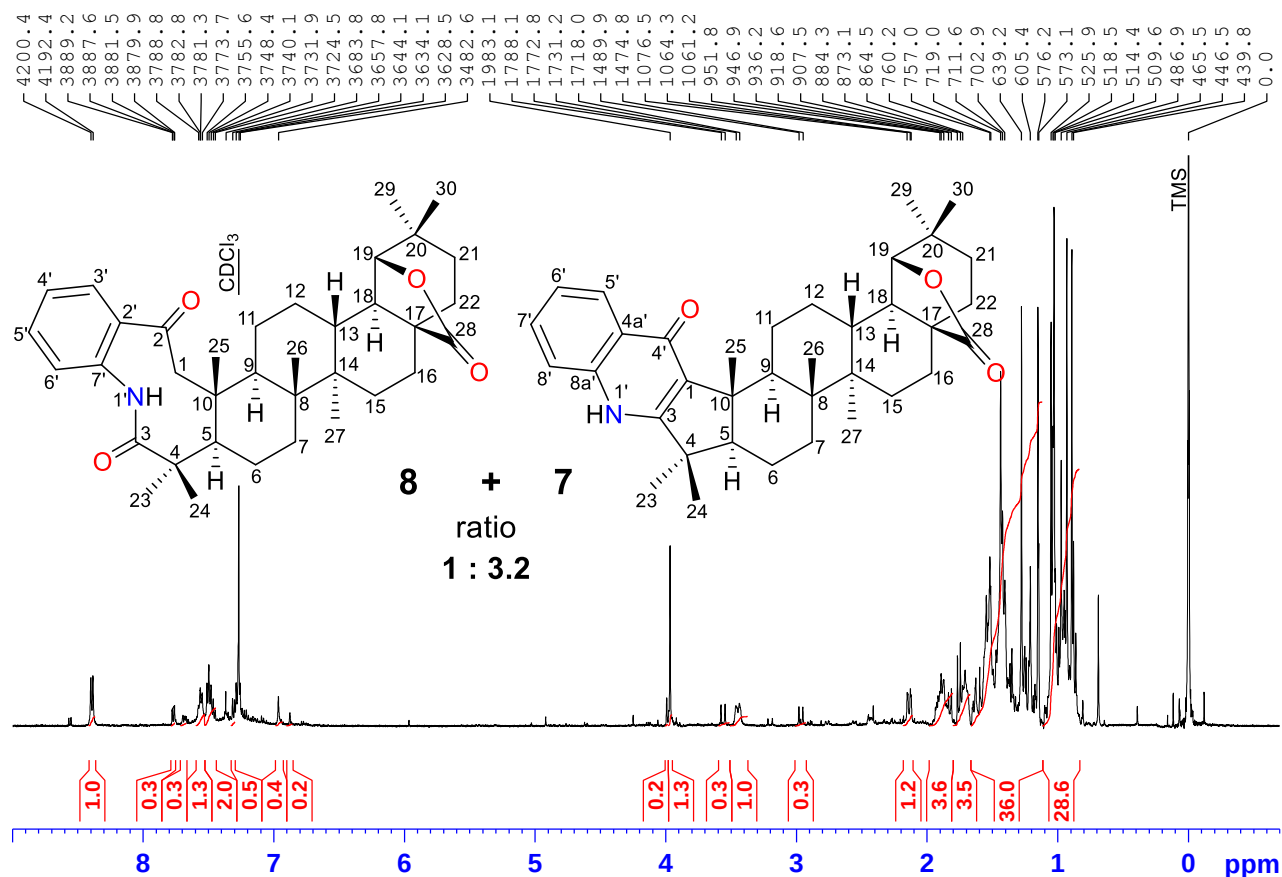


Figure S67. Complete ^1H NMR spectrum of compound **8** in CDCl_3 .

Table S11. Complete numerical listings of ^1H NMR peaks of compound **8** in CDCl_3 .

Peak	$\nu(\text{F1})$ [ppm]	$\nu(\text{F1})$ [Hz]	Intensity [rel]	Half width [Hz]
1	8.57	4284.6	0.01	1.8
2	8.55	4276.3	0.01	2.1
3	8.4	4200.4	0.08	3.7
4	8.38	4192.4	0.09	3.7
5	7.78	3889.2	0.03	1.5
6	7.77	3887.6	0.03	1.8
7	7.76	3881.5	0.03	1.8
8	7.76	3879.9	0.04	1.5
9	7.69	3847.6	0.02	2.4
10	7.68	3839.8	0.02	4
11	7.58	3788.8	0.04	2.4
12	7.56	3782.8	0.06	2.4
13	7.56	3781.3	0.07	4
14	7.55	3773.7	0.06	3.1
15	7.51	3755.6	0.07	3.4
16	7.49	3748.4	0.1	4.6
17	7.48	3740.1	0.07	4.9
18	7.46	3731.9	0.05	3.4
19	7.45	3724.5	0.03	4.9
20	7.37	3683.8	0.06	0.9
21	7.31	3657.8	0.05	3.4
22	7.29	3644.1	0.07	4.6
23	7.27	3634.1	0.85	0.9

24	7.26	3628.5	0.07	4
25	6.96	3482.6	0.05	4.3
26	6.87	3438.3	0.02	3.7
27	3.97	1983.1	0.31	2.1
28	3.58	1788.1	0.04	1.8
29	3.54	1772.8	0.04	2.1
30	3.46	1731.2	0.03	0.9
31	3.44	1718	0.04	3.4
32	2.98	1489.9	0.03	2.4
33	2.95	1474.8	0.03	2.4
34	2.15	1076.5	0.06	2.7
35	2.15	1074.5	0.05	0.6
36	2.13	1064.3	0.06	4
37	2.12	1061.2	0.05	2.4
38	1.94	968.5	0.03	2.7
39	1.92	962.5	0.04	4.6
40	1.92	958.4	0.05	3.1
41	1.9	951.8	0.06	2.4
42	1.89	946.9	0.09	3.4
43	1.87	936.2	0.08	5.2
44	1.86	928.3	0.04	2.4
45	1.84	918.6	0.06	3.4
46	1.81	907.5	0.06	3.4
47	1.77	884.3	0.12	2.1
48	1.75	873.1	0.14	2.4
49	1.71	855.1	0.1	7.9
50	1.65	823.8	0.04	5.2
51	1.63	814	0.08	4.6
52	1.55	773.8	0.22	8.9
53	1.53	767.3	0.18	4
54	1.52	760.2	0.29	7.9
55	1.51	757	0.24	4.3
56	1.44	719	0.61	7
57	1.42	711.6	0.37	7.6
58	1.41	702.9	0.25	8.2
59	1.37	683.2	0.11	4
60	1.35	675.7	0.13	4.3
61	1.28	639.2	0.72	2.1
62	1.25	626.5	0.14	6.4
63	1.21	605.4	0.27	4.3
64	1.15	576.2	0.72	2.1
65	1.15	573.1	0.31	1.8
66	1.05	525.9	0.69	2.7
67	1.04	518.5	0.51	4.3
68	1.03	514.4	0.89	4.3
69	1.02	509.6	0.27	3.1
70	0.97	486.9	0.46	3.1
71	0.95	475.6	0.23	4.6
72	0.93	465.5	0.84	2.4
73	0.89	446.5	0.82	2.1
74	0.88	439.8	0.32	2.7
75	0	0	13.5	0.6

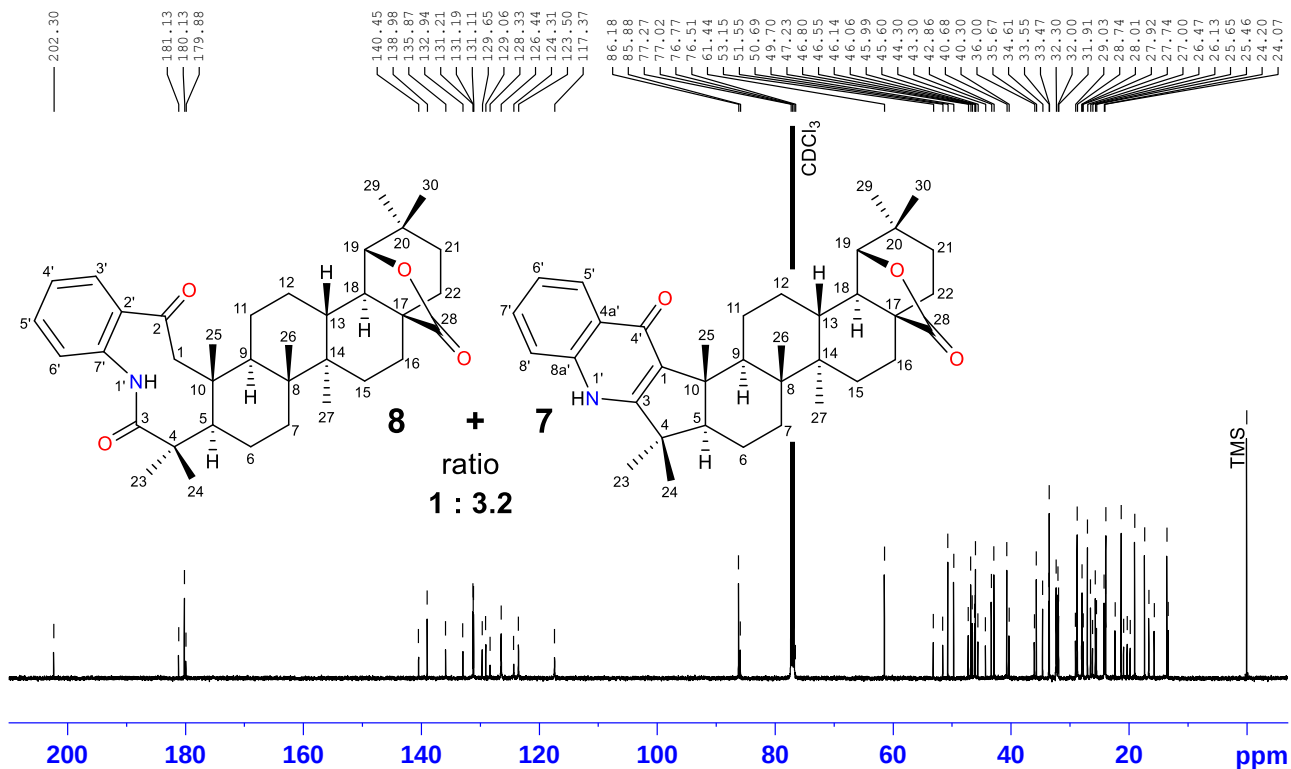


Figure S68. Complete $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of compound **8** in CDCl_3 .

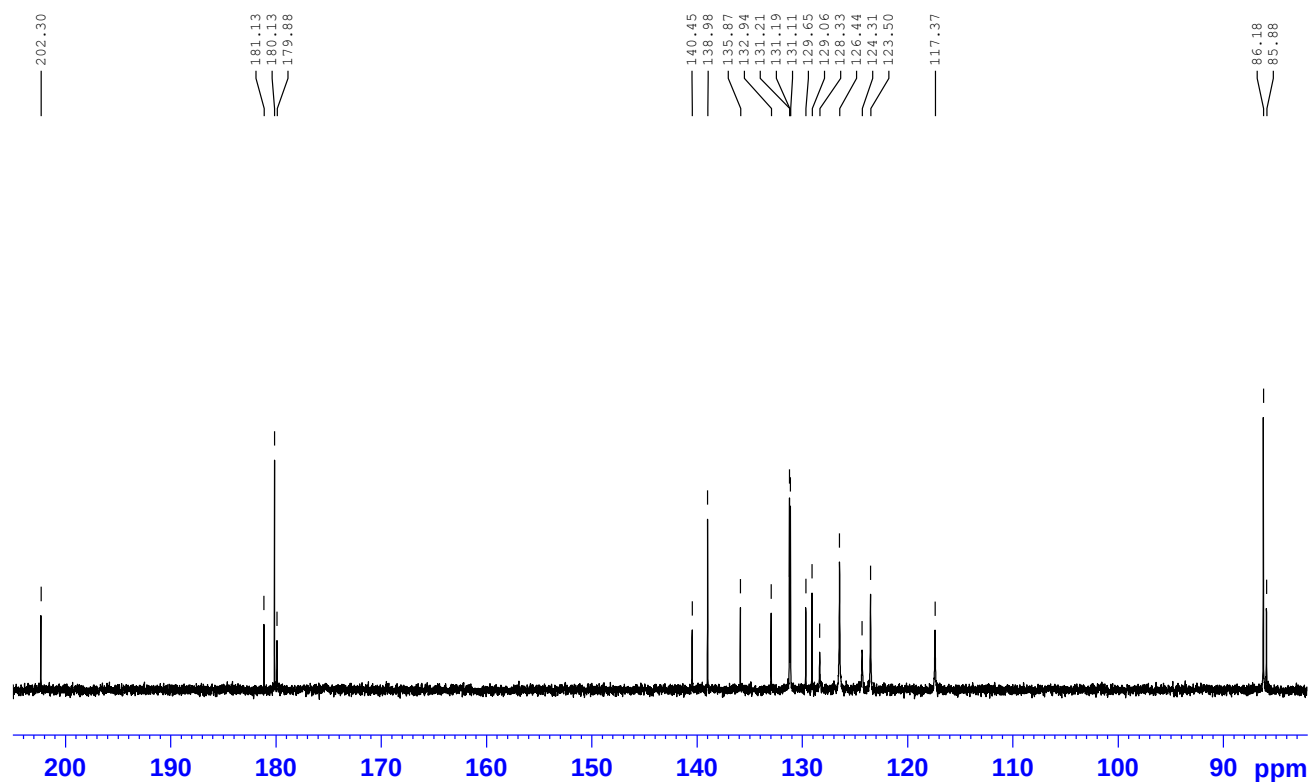


Figure S69. Downfield area of $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of compound **8** in CDCl_3 .

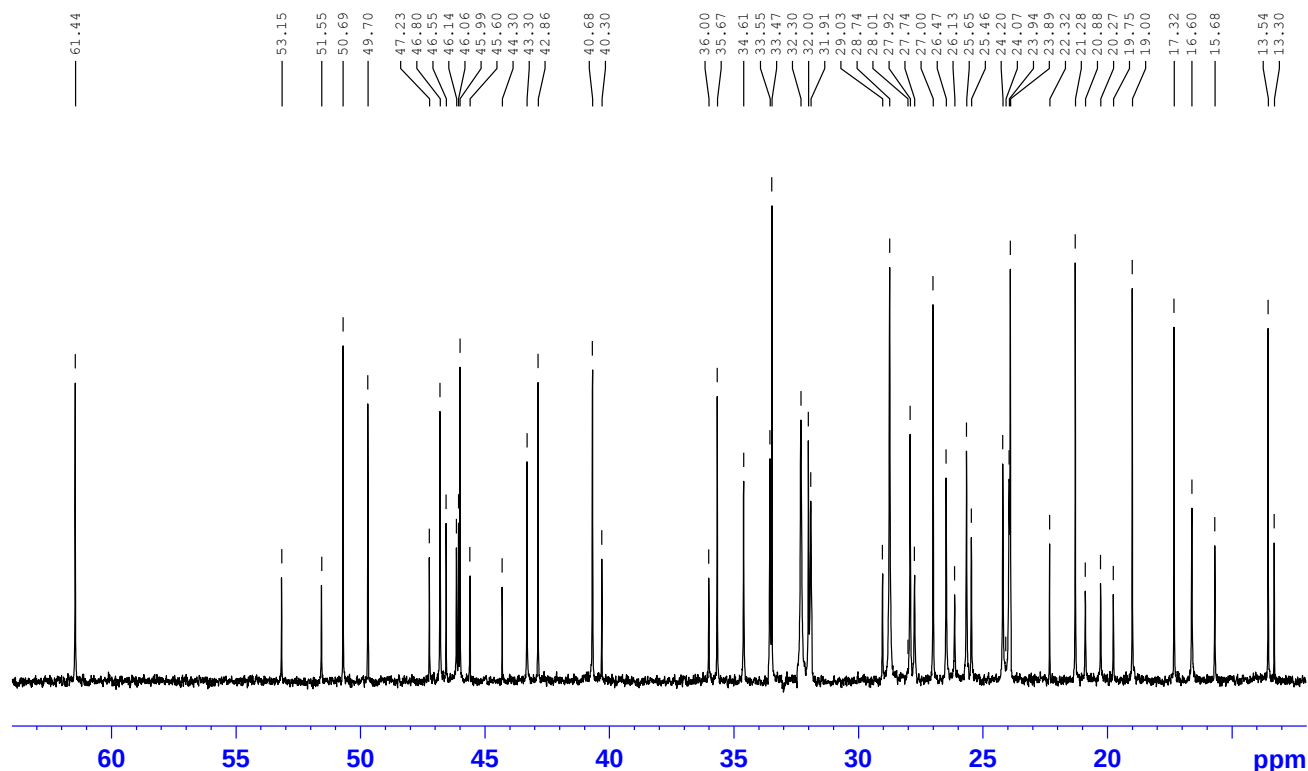


Figure S70. Upfield area of $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of compound **8** in CDCl_3 .

Table S12. Complete numerical listings of ^{13}C NMR peaks of compound **8** in CDCl_3 .

Peak	$\nu(\text{F1})$ [ppm]	$\nu(\text{F1})$ [Hz]	Intensity [rel]	Half width [Hz]
1	202.3	25440.5	0.36	0.9
2	181.13	22778.1	0.33	0.9
3	180.13	22652.1	1.13	0.9
4	179.88	22621.8	0.25	2.7
5	140.45	17662.4	0.3	1.8
6	138.98	17477.9	0.85	0.9
7	135.87	17086.2	0.4	0.9
8	132.94	16717.9	0.39	1.8
9	131.21	16500.2	0.96	2.7
10	131.19	16497.7	0.74	1.8
11	131.11	16488	0.91	2.7
12	129.65	16304.8	0.42	2.7
13	129.06	16229.9	0.48	1.8
14	128.33	16138.7	0.19	6.4
15	126.44	15901.3	0.63	7.3
16	124.31	15632.4	0.2	8.2
17	123.5	15531.3	0.47	6.4
18	117.37	14760.7	0.3	8.2
19	86.18	10837.5	1.34	1.8
20	85.88	10799.9	0.41	2.7
21	77.27	9717.6	13.16	1.8
22	77.02	9685.7	13.5	1.8
23	76.77	9653.8	13.21	1.8
24	76.51	9622.2	0.07	2.7
25	61.44	7726.6	1.46	1.8

26	53.15	6684	0.5	1.8
27	51.55	6482.8	0.5	0.9
28	50.69	6375.2	1.64	0.9
29	49.7	6249.8	1.36	1.8
30	47.23	5939.3	0.6	0.9
31	46.8	5885.3	1.37	0.9
32	46.55	5854.6	0.78	0.9
33	46.14	5802.3	0.67	1.8
34	46.06	5792.1	0.77	0.9
35	45.99	5784.2	1.61	0.9
36	45.6	5734	0.51	1.8
37	44.3	5571.2	0.46	0.9
38	43.3	5445.9	1.08	1.8
39	42.86	5390.1	1.55	0.9
40	40.68	5115.7	1.58	1.8
41	40.3	5068.2	0.6	0.9
42	36	4527.7	0.5	1.8
43	35.67	4485.2	1.4	0.9
44	34.61	4351.9	1	2.7
45	33.55	4218.9	1.09	3.6
46	33.47	4209	2.33	0.9
47	32.3	4062.5	1.28	6.4
48	32	4024.6	1.18	1.8
49	31.91	4012.7	0.88	6.4
50	29.03	3650.6	0.54	1.8
51	28.74	3614.8	2.03	4.5
52	28.01	3522.2	0.06	2.7
53	27.92	3511.3	1.21	2.7
54	27.74	3488.8	0.52	3.6
55	27	3395.1	1.84	1.8
56	26.47	3329	1	2.7
57	26.13	3286.1	0.42	3.6
58	25.65	3226.2	1.12	2.7
59	25.46	3201.6	0.7	1.8
60	24.2	3042.7	1.06	2.7
61	24.07	3027.3	0.07	4.5
62	23.94	3010.6	1	4.5
63	23.89	3004.9	2.07	2.7
64	22.32	2806.6	0.67	0.9
65	21.28	2676.7	2.05	0.9
66	20.88	2625.7	0.44	2.7
67	20.27	2548.5	0.48	1.8
68	19.75	2484.3	0.42	1.8
69	19	2388.9	1.93	0.9
70	17.32	2177.8	1.82	0.9
71	16.6	2088	0.85	2.7
72	15.68	1972	0.66	1.8
73	13.54	1702.8	1.79	0.9
74	13.3	1672.1	0.68	0.9
75	0	0	3.4	0.9

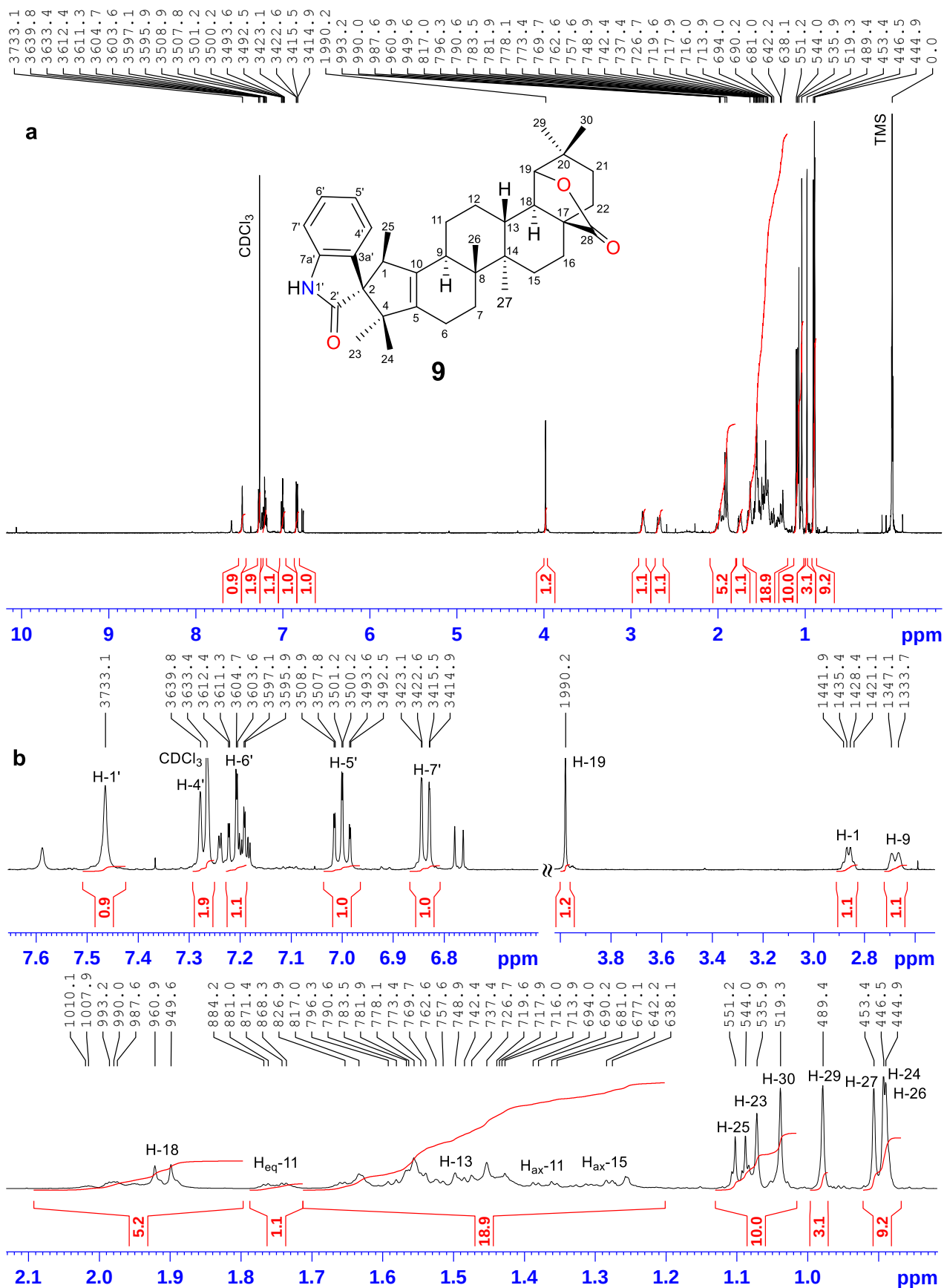
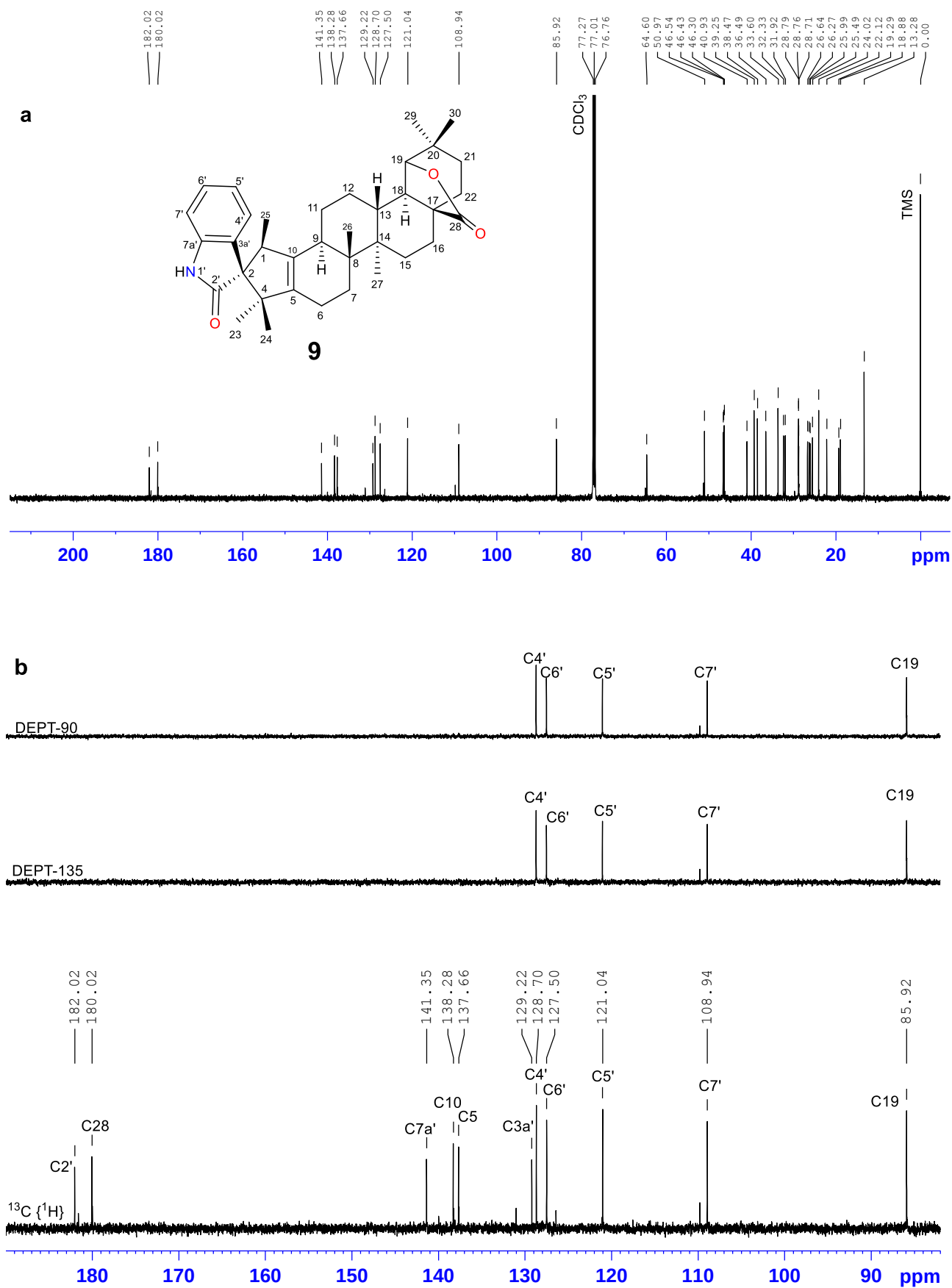


Figure S71. (a) Complete ^1H NMR spectrum of compound **9** in CDCl_3 . (b) Detailed and annotated ^1H NMR spectrum of compound **9** in CDCl_3 .

Table S13. Complete numerical listings of ^1H NMR peaks of compound **9** in CDCl_3 .

Peak	$\nu(\text{F1})$ [ppm]	$\nu(\text{F1})$ [Hz]	Intensity [rel]	Half width [Hz]
1	7.46	3733.1	0.11	3.6
2	7.28	3639.8	0.11	2.6
3	7.26	3633.4	0.87	0.4
4	7.22	3612.4	0.06	1.1
5	7.22	3611.3	0.06	1.1
6	7.21	3604.7	0.14	1.1
7	7.21	3603.6	0.13	1.1
8	7.19	3597.1	0.09	1.1
9	7.19	3595.9	0.08	0.9
10	7.02	3508.9	0.08	1.1
11	7.01	3507.8	0.08	0.9
12	7	3501.2	0.13	0.9
13	7	3500.2	0.13	1.1
14	6.99	3493.6	0.06	1.1
15	6.98	3492.5	0.06	0.9
16	6.84	3423.1	0.12	1.1
17	6.84	3422.6	0.12	1.1
18	6.83	3415.5	0.12	1.1
19	6.83	3414.9	0.11	0.9
20	3.98	1990.2	0.27	2.1
21	2.88	1442.5	0.02	3
22	2.87	1435.1	0.05	4.3
23	2.87	1434.9	0.05	4.3
24	2.86	1428.9	0.05	3.2
25	2.85	1427.8	0.05	3.4
26	2.84	1421.1	0.02	3
27	2.69	1347.1	0.04	4.7
28	2.67	1333.7	0.04	6.4
29	2.02	1010.1	0.02	4.7
30	2.02	1007.9	0.02	2.6
31	1.99	995.5	0.04	2.8
32	1.99	993.2	0.06	2.8
33	1.98	990	0.06	3.2
34	1.97	987.6	0.06	6.4
35	1.95	977	0.04	2.4
36	1.95	975.4	0.04	2.6
37	1.95	973.3	0.04	2.6
38	1.92	960.9	0.2	2.8
39	1.9	949.6	0.21	2.8
40	1.77	884.2	0.04	3.2
41	1.76	881	0.04	4.1
42	1.75	877.6	0.03	2.4
43	1.75	874.9	0.03	2.8
44	1.74	871.4	0.05	3.8
45	1.74	868.3	0.05	5.6
46	1.65	826.9	0.05	3.6

47	1.63	817	0.12	8.8
48	1.59	796.3	0.06	5.1
49	1.58	790.6	0.08	4.1
50	1.57	783.5	0.16	3.6
51	1.56	781.9	0.16	1.7
52	1.56	778.1	0.26	7.1
53	1.55	773.4	0.13	2.1
54	1.54	769.7	0.13	3.8
55	1.52	762.6	0.08	5.6
56	1.51	757.6	0.06	4.7
57	1.5	748.9	0.13	6.6
58	1.48	742.4	0.09	4.3
59	1.47	737.4	0.11	6.8
60	1.45	726.7	0.22	5.1
61	1.44	719.6	0.1	1.9
62	1.44	717.9	0.1	1.5
63	1.43	716	0.1	1.9
64	1.43	713.9	0.13	6.2
65	1.39	694	0.05	3.6
66	1.38	690.2	0.05	3.8
67	1.36	681	0.06	4.1
68	1.35	677.1	0.04	3.2
69	1.31	656.5	0.04	4.7
70	1.31	653	0.04	3.8
71	1.3	649.2	0.03	4.3
72	1.28	642.2	0.07	3.8
73	1.28	638.1	0.07	4.1
74	1.27	635.8	0.05	2.1
75	1.26	628.7	0.1	2.1
76	1.25	627.6	0.1	2.6
77	1.1	551.2	0.45	1.3
78	1.09	544	0.46	1.5
79	1.07	535.9	0.64	1.7
80	1.05	526.5	0.06	1.5
81	1.04	519.3	0.86	1.7
82	1.03	513.9	0.05	1.1
83	1.02	509.9	0.01	1.9
84	0.98	489.4	0.88	1.7
85	0.91	453.4	0.86	1.9
86	0.89	446.5	1.01	1.7
87	0.89	444.9	0.91	1.9
88	0	0	13.5	0.4



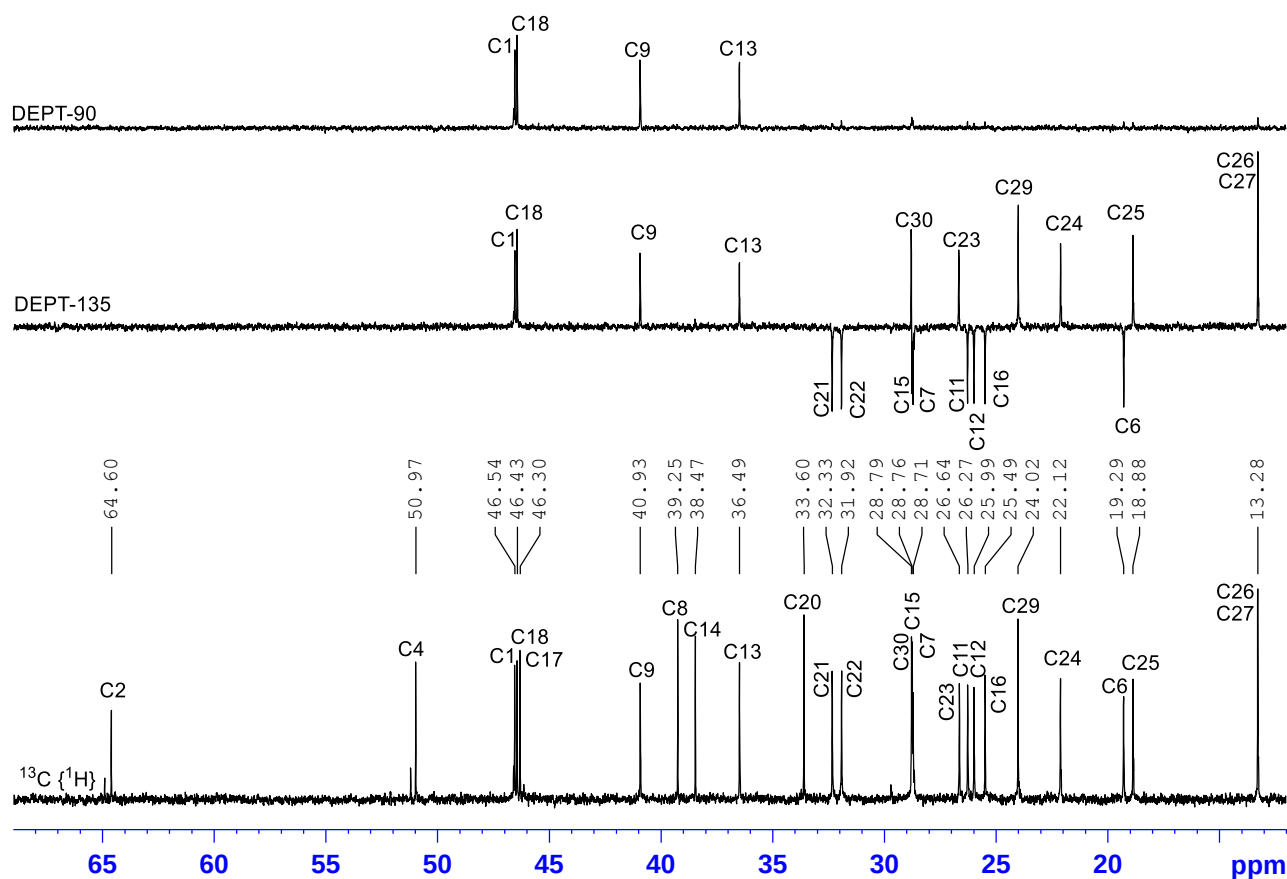


Figure S73. Upfield area of annotated $^{13}\text{C}\{^1\text{H}\}$ NMR and DEPT-135, DEPT-90 spectra of compound **9** in CDCl_3 .

Table S14. Complete numerical listings of ^{13}C NMR peaks of compound **9** in CDCl_3 .

Peak	$\nu(\text{F1})$ [ppm]	$\nu(\text{F1})$ [Hz]	Intensity [rel]	Half width [Hz]
1	182.02	22890.4	0.44	0.9
2	180.02	22639.3	0.49	0.9
3	141.35	17776.4	0.48	0.9
4	138.28	17389.6	0.58	0.9
5	137.66	17312.3	0.56	0.9
6	129.22	16250.6	0.47	0.9
7	128.7	16184.5	0.85	0.9
8	127.5	16034.6	0.75	1.8
9	121.04	15221.6	0.82	0.9
10	108.94	13700.3	0.74	0.9
11	85.92	10804.5	0.83	0.9
12	77.27	9717.1	13.16	2.7
13	77.01	9685.1	13.49	2.7
14	76.76	9653.2	13.5	1.8
15	64.6	8123.6	0.6	0.9
16	50.97	6409.7	0.91	0.9
17	46.54	5852.9	0.89	0.9
18	46.43	5839.4	0.93	1.8
19	46.3	5822	0.99	1.8
20	40.93	5147.4	0.8	0.9

21	39.25	4936.4	1.2	0.9
22	38.47	4837.3	1.1	0.9
23	36.49	4588.4	0.92	0.9
24	33.6	4225.2	1.24	0.9
25	32.33	4066.2	0.86	1.8
26	31.92	4013.7	0.86	1.8
27	28.79	3620.1	1.12	2.7
28	28.76	3616.7	1.05	2.7
29	28.71	3610.8	0.75	2.7
30	26.64	3350.7	0.77	1.8
31	26.27	3303.4	0.76	1.8
32	25.99	3268	0.75	1.8
33	25.49	3205.2	0.83	1.8
34	24.02	3020.1	1.21	0.9
35	22.12	2781.2	0.8	1.8
36	19.29	2426.3	0.7	1.8
37	18.88	2373.7	0.84	0.9
38	13.28	1670.4	1.72	1.8
39	0	0	4.15	0.9

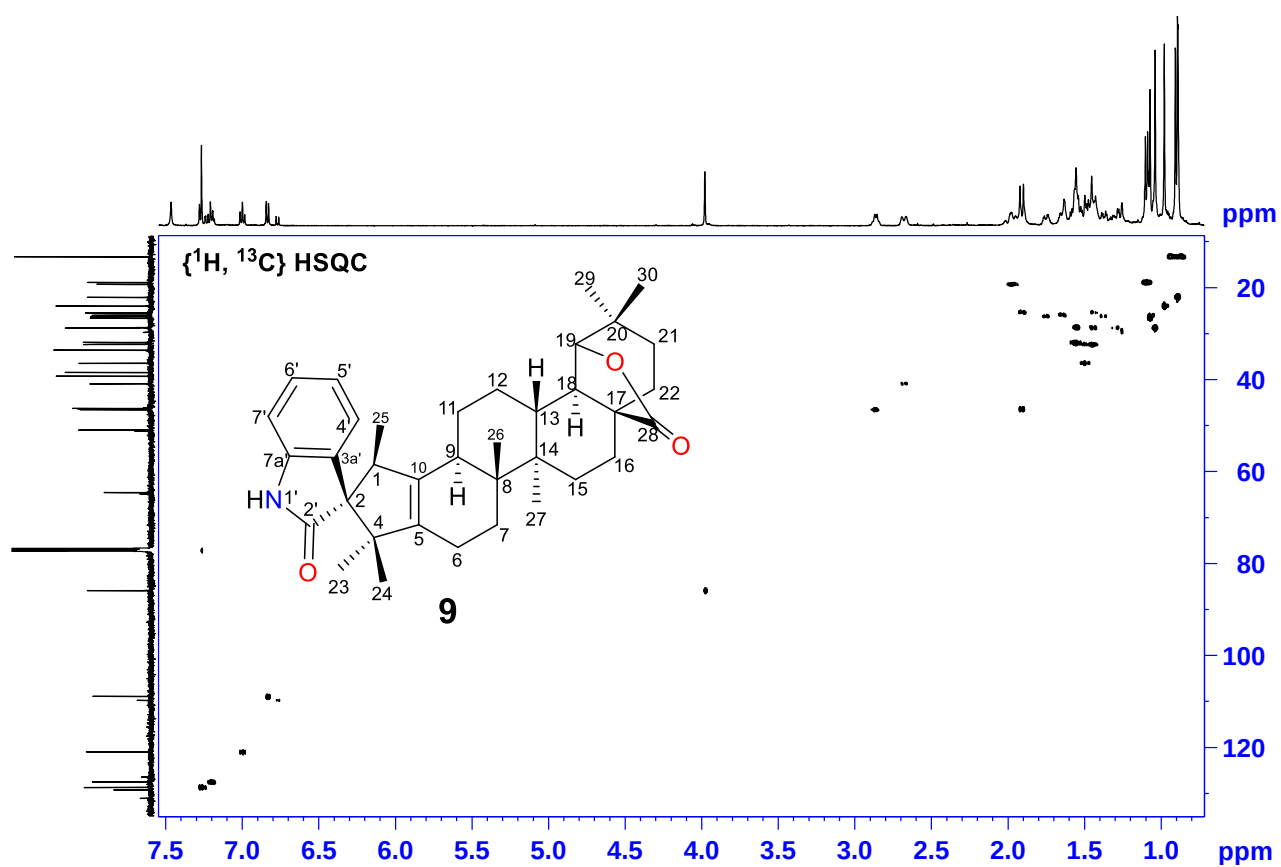


Figure S74. Complete $\{^1\text{H}, ^{13}\text{C}\}$ HSQC NMR spectrum of compound **9** in CDCl_3 .

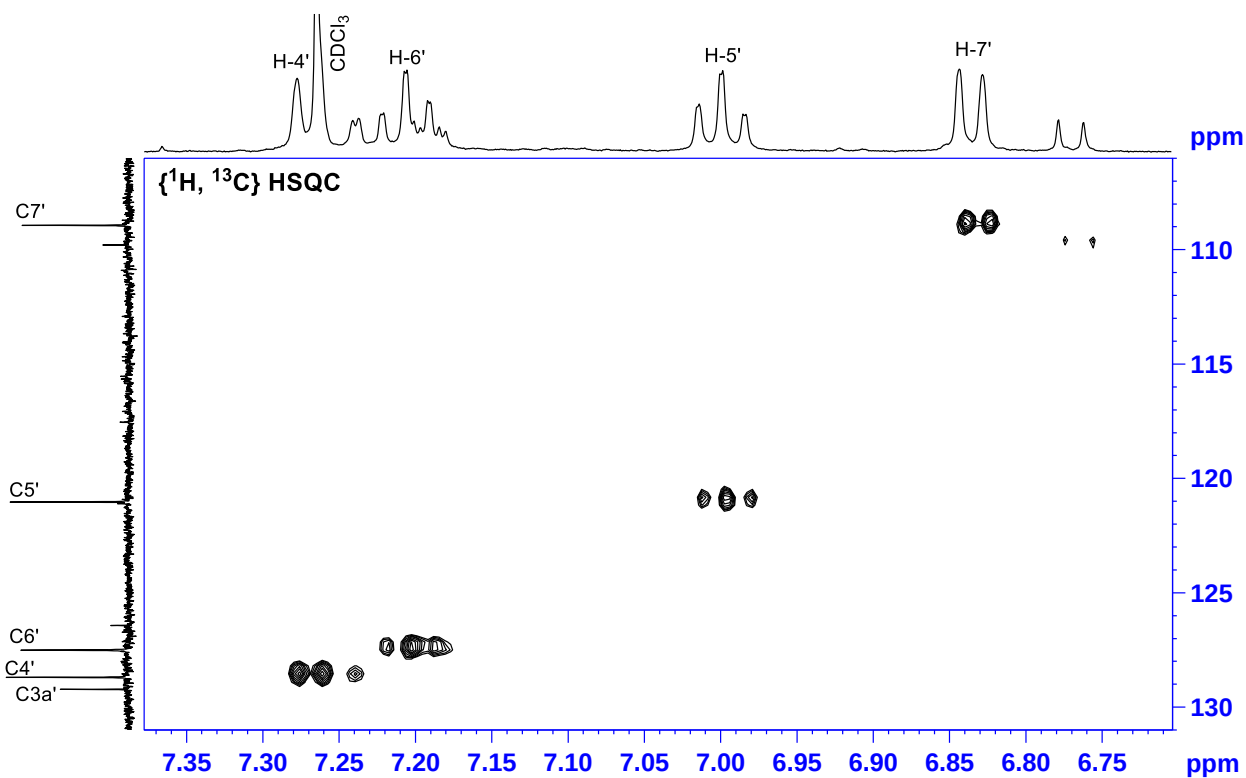


Figure S75. Downfield area of $\{^1\text{H}, ^{13}\text{C}\}$ HSQC NMR spectrum of compound **9** in CDCl_3 .

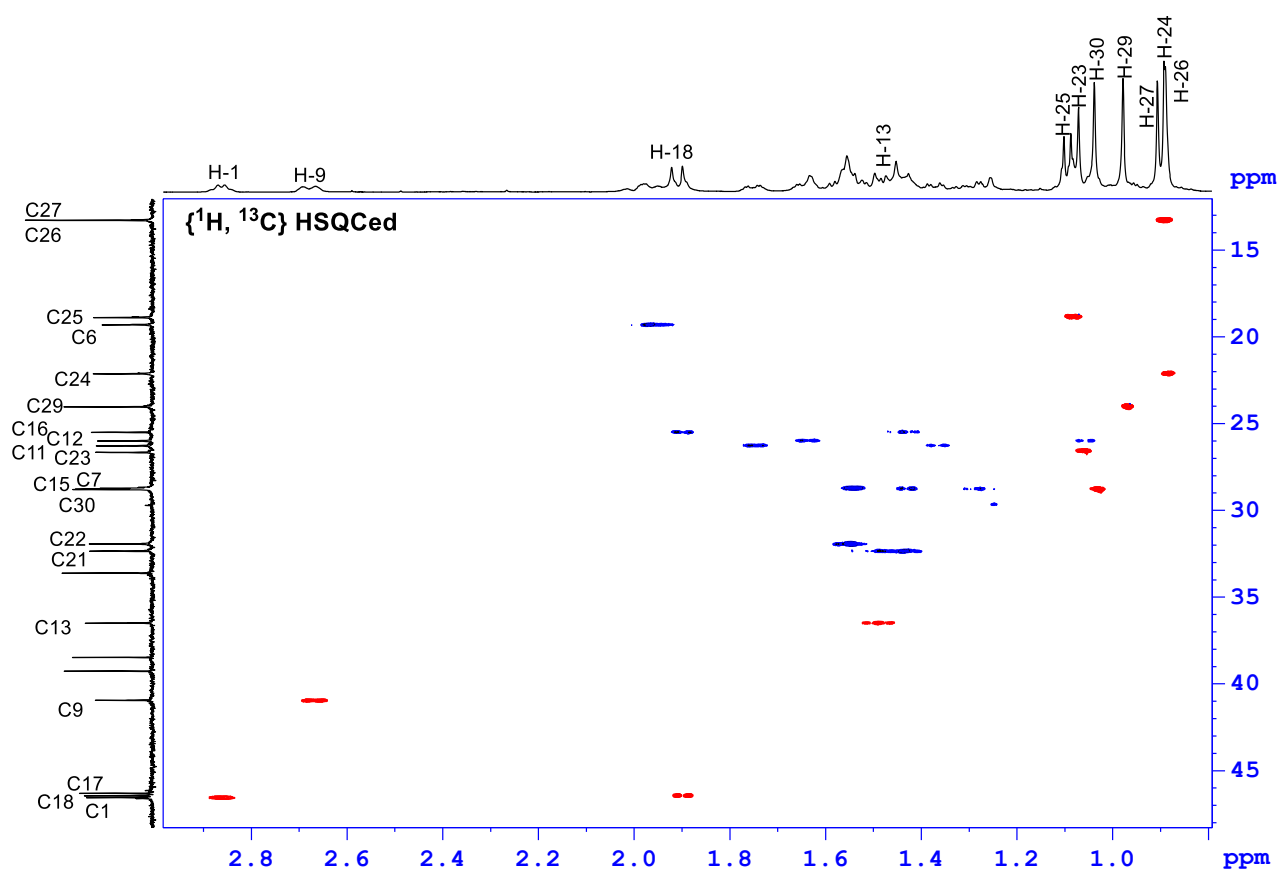


Figure S76. Upfield area of $\{^1\text{H}, ^{13}\text{C}\}$ HSQC multiplicity edited NMR spectrum of compound **9** in CDCl_3 .

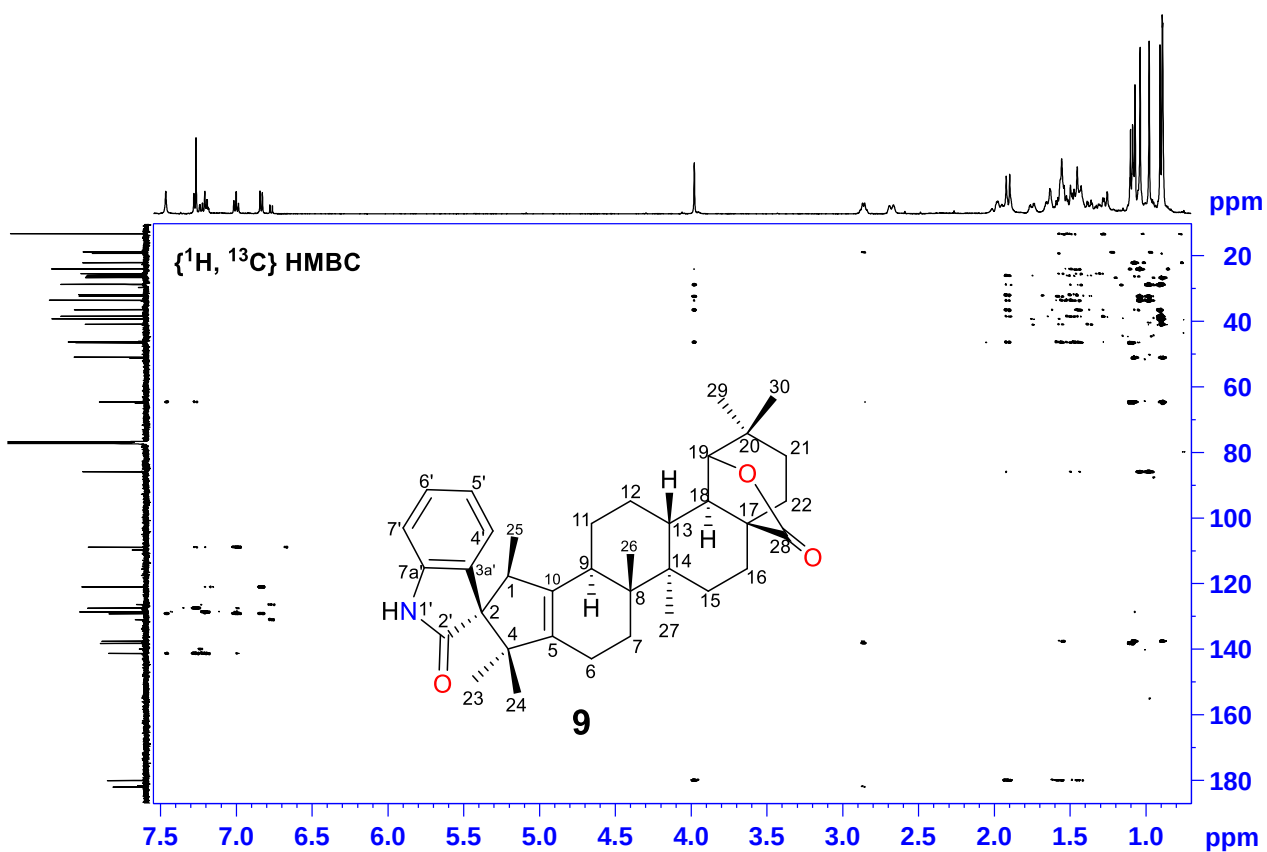


Figure S77. Complete $\{^1\text{H}, ^{13}\text{C}\}$ HMBC NMR spectrum of compound **9** in CDCl_3 .

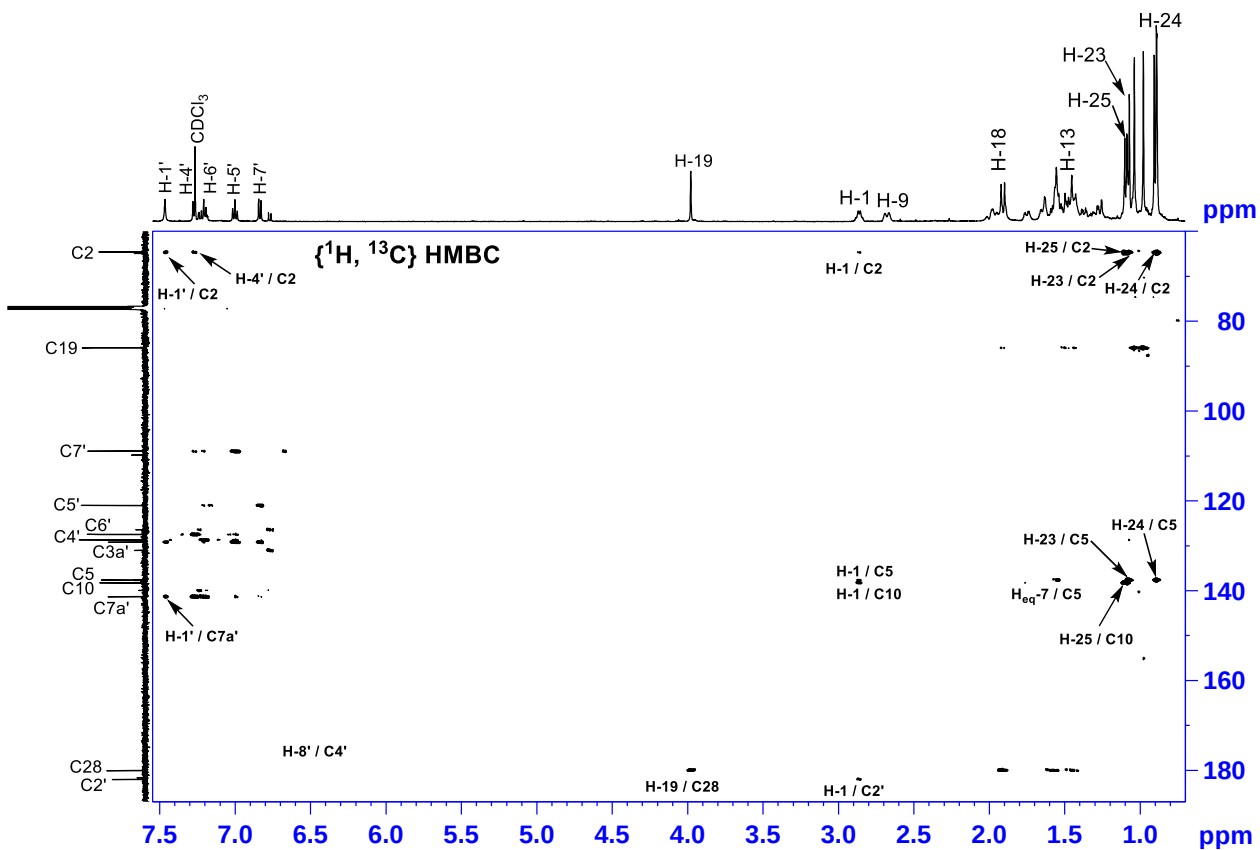


Figure S78. Annotated $\{^1\text{H}, ^{13}\text{C}\}$ HMBC NMR spectrum of compound **9** in CDCl_3 .

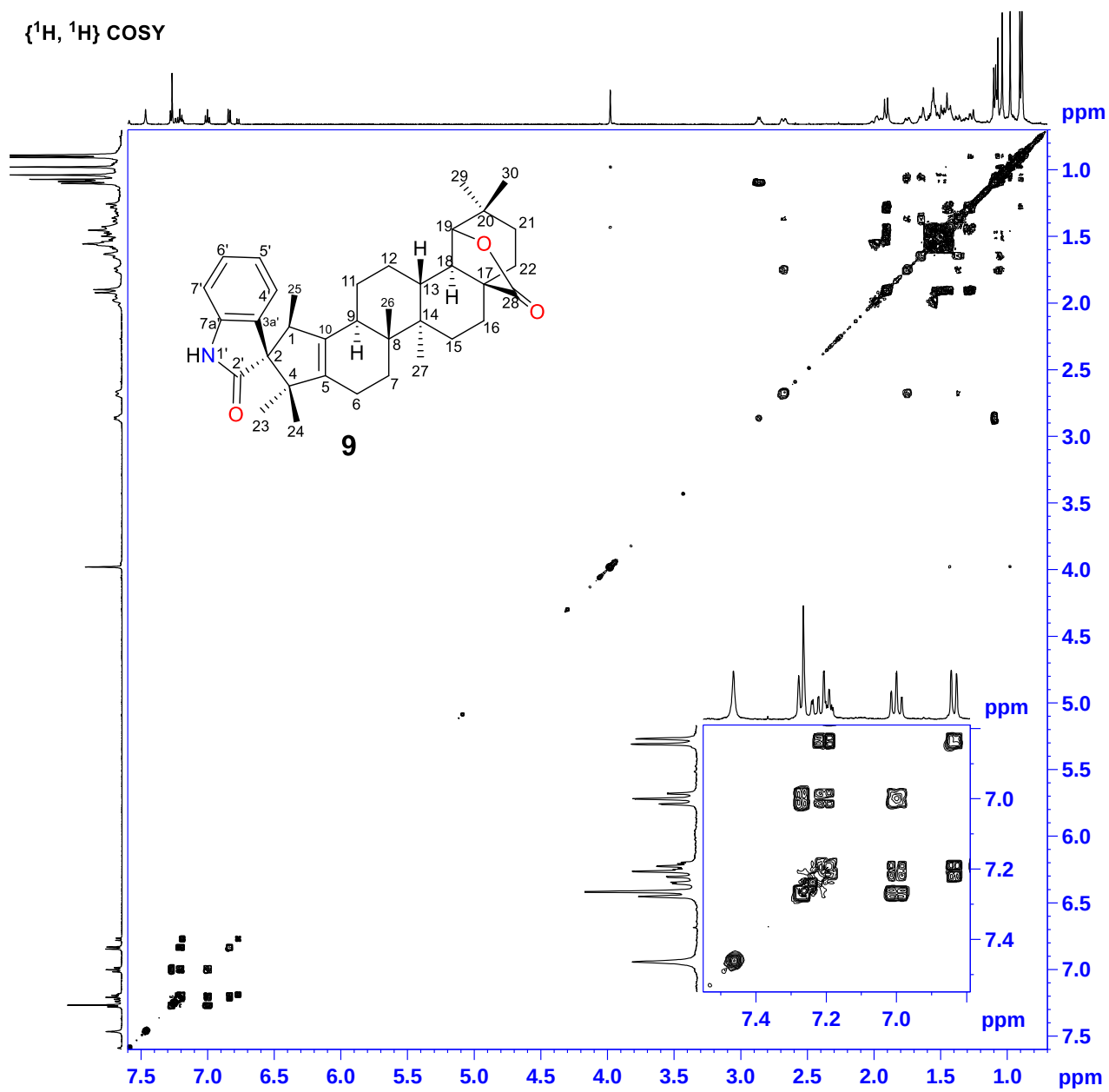


Figure S79. Complete $\{^1\text{H}, ^1\text{H}\}$ COSY NMR spectrum of compound **9** in CDCl_3 .

$\{^1\text{H}, ^1\text{H}\}$ COSY-DQF

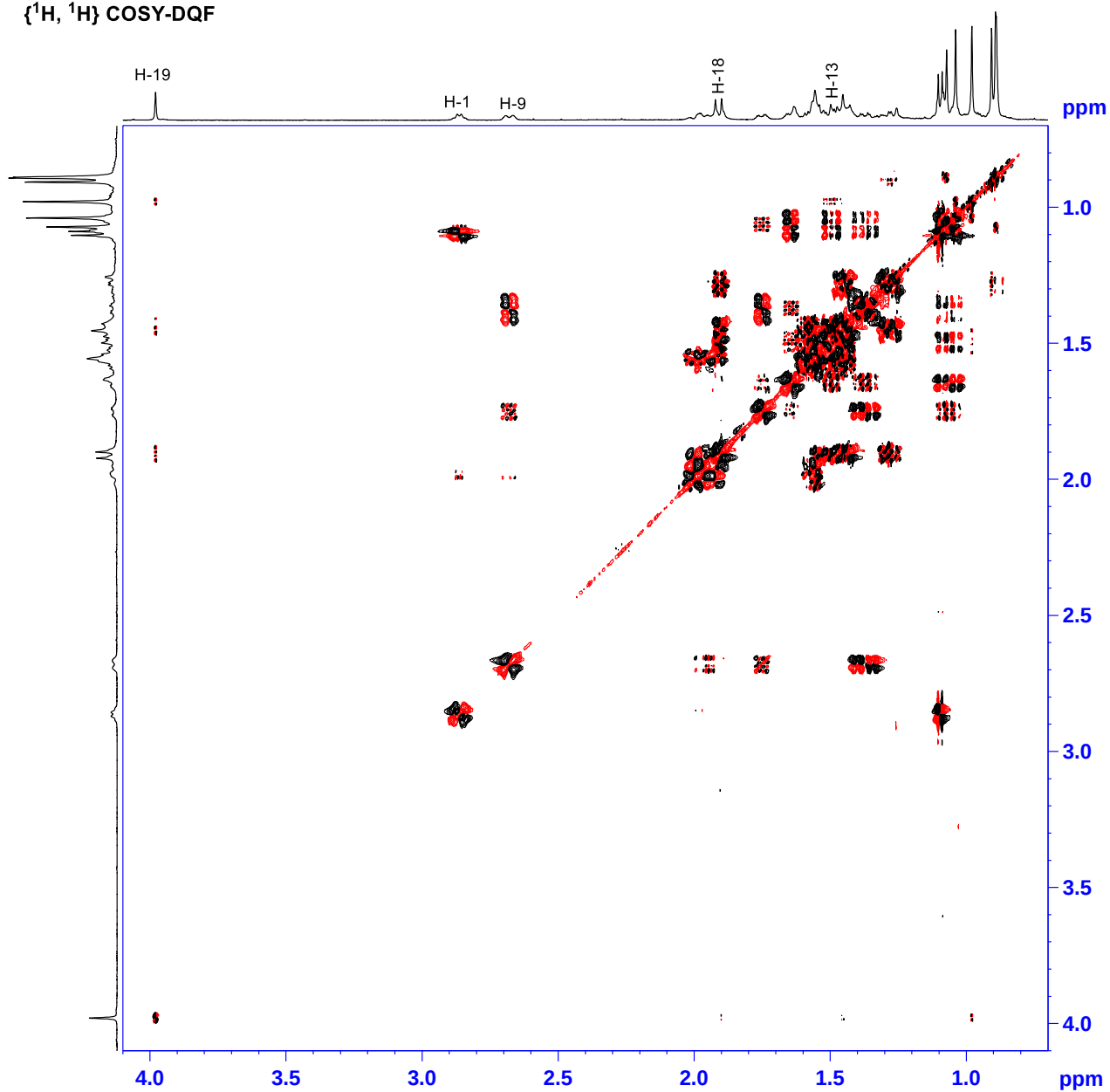


Figure S80. Upfield area of $\{^1\text{H}, ^1\text{H}\}$ COSY-DQF NMR spectrum of compound **9** in CDCl_3 .

$\{^1\text{H}, ^1\text{H}\}$ NOESY

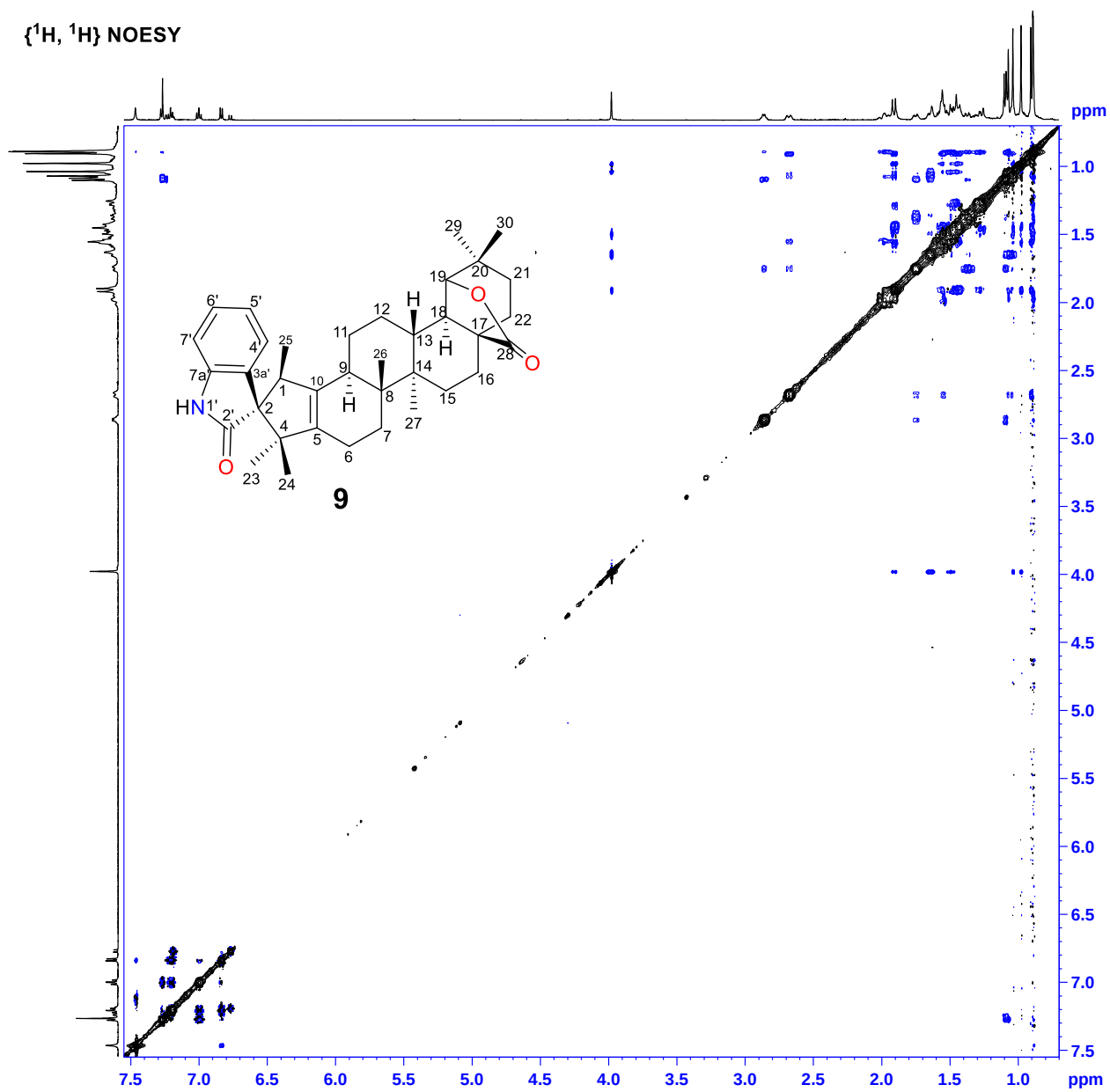


Figure S81. Complete $\{^1\text{H}, ^1\text{H}\}$ NOESY NMR spectrum of compound **9** in CDCl_3 .

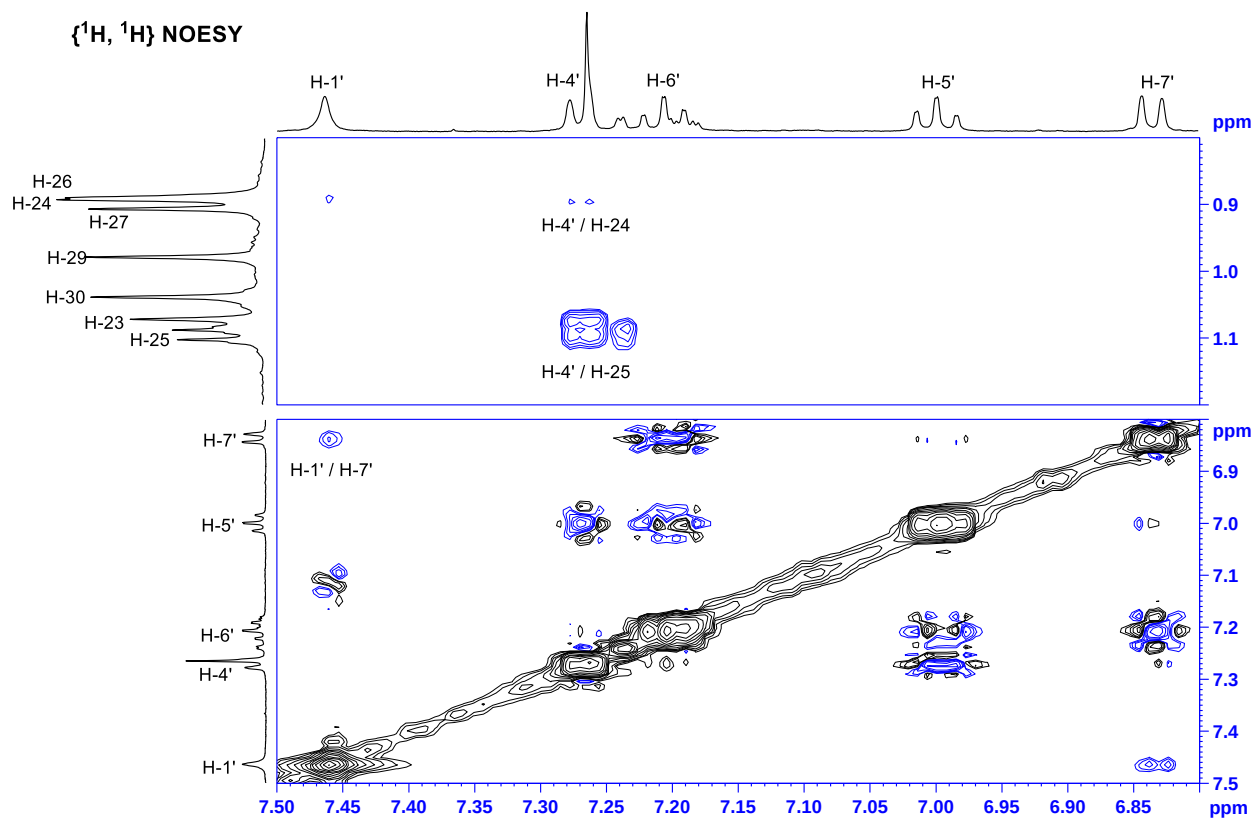


Figure S82. Detailed and annotated $\{^1\text{H}, ^1\text{H}\}$ NOESY NMR spectrum of compound **9** in CDCl_3 .

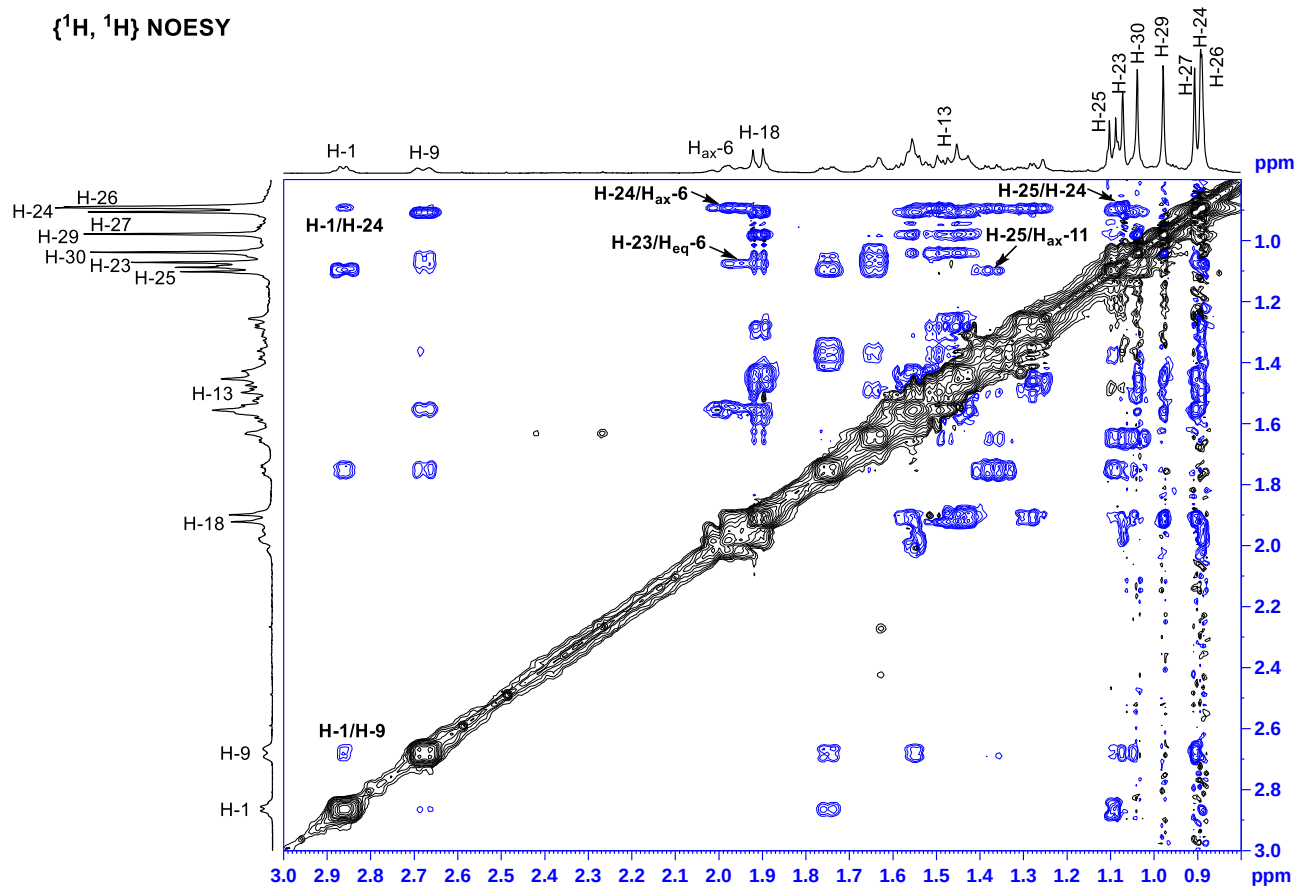


Figure S83. Upfield area of $\{^1\text{H}, ^1\text{H}\}$ NOESY NMR spectrum of compound **9** in CDCl_3 .

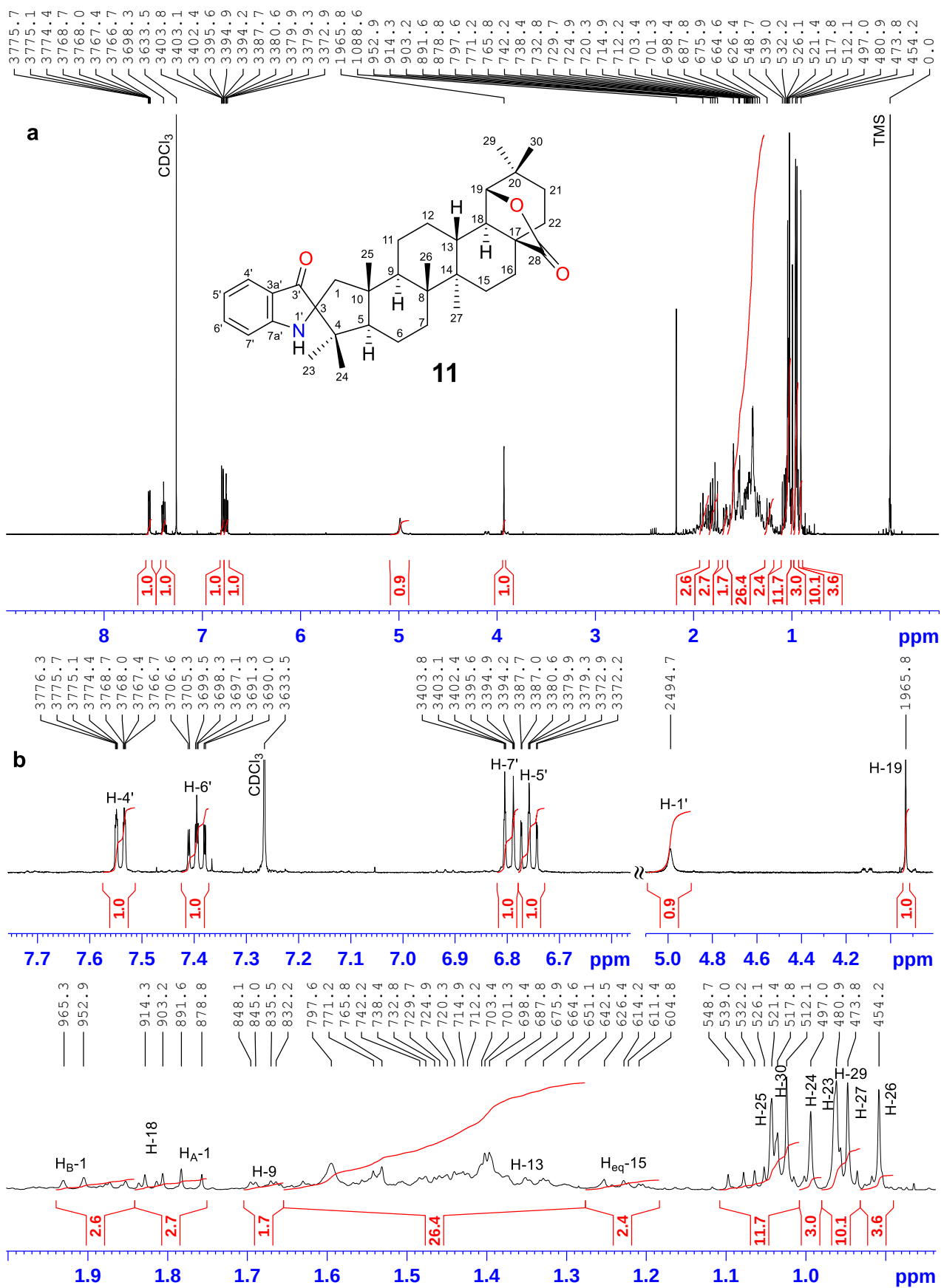


Figure S84. (a) Complete ^1H NMR spectrum of compound **11** in CDCl_3 . (b) Detailed and annotated ^1H NMR spectrum of compound **11** in CDCl_3 .

Table S15. Complete numerical listings of ^1H NMR peaks of compound **11** in CDCl_3 .

Peak	$\nu(\text{F1})$ [ppm]	$\nu(\text{F1})$ [Hz]	Intensity [rel]	Half width [Hz]
1	7.55	3776.3	2.75	0.6
2	7.55	3775.7	3.38	0.6
3	7.55	3775.1	3.66	0.8
4	7.55	3774.4	3.1	0.6
5	7.54	3768.7	2.95	0.6
6	7.53	3768	3.72	0.8
7	7.53	3767.4	3.72	0.8
8	7.53	3766.7	3.08	0.6
9	7.41	3706.6	2.47	0.6
10	7.41	3705.3	2.49	0.6
11	7.4	3699.5	2.83	0.8
12	7.39	3698.3	4.49	0.8
13	7.39	3697.1	2.85	0.8
14	7.38	3691.3	2.82	0.6
15	7.38	3690	2.73	0.6
16	7.27	3633.5	51.12	0.3
17	6.81	3403.8	3.09	0.5
18	6.8	3403.1	5.81	1.1
19	6.8	3402.4	3.58	0.6
20	6.79	3395.6	3.07	0.5
21	6.79	3394.9	5.58	1.1
22	6.79	3394.2	3.35	0.6
23	6.77	3387.7	3	0.8
24	6.77	3387	2.89	0.6
25	6.76	3380.6	3.48	0.5
26	6.76	3379.9	5.15	0.9
27	6.76	3379.3	3.49	0.6
28	6.74	3372.9	2.9	0.8
29	6.74	3372.2	2.73	0.6
30	4.99	2494.7	1.37	0.6
31	3.93	1965.8	7.45	1.8
32	2.18	1088.6	19.36	0.2
33	1.93	965.3	2.68	3.2
34	1.91	952.9	3.5	1.5
35	1.88	938.9	1.61	2.7
36	1.87	936.4	2.26	2.7
37	1.86	929.1	1.34	1.8
38	1.85	926.5	2.5	3.2
39	1.83	914.3	4.43	1.7
40	1.81	903.2	4.74	1.5
41	1.78	891.6	6.12	1.2
42	1.76	878.8	4.49	1.2
43	1.7	848.1	2.25	3.1
44	1.69	845	2.18	3.1
45	1.67	835.5	2.56	4

46	1.66	832.2	2.32	3.2
47	1.63	815.3	2.5	3.7
48	1.62	812	1.73	2.4
49	1.62	808.4	1.56	2.4
50	1.59	797.6	7.69	7.5
51	1.56	778.4	2.82	3.7
52	1.54	771.2	5.48	4.4
53	1.53	765.8	6.71	2.9
54	1.48	742.2	3.54	5.3
55	1.48	738.4	3.85	4.9
56	1.47	732.8	3.62	3.5
57	1.46	729.7	4.03	3.4
58	1.45	724.9	4.39	5
59	1.44	720.3	5.27	4
60	1.43	714.9	5.29	2.6
61	1.42	712.2	4.74	1.7
62	1.41	703.4	7.47	5.5
63	1.4	701.3	10.7	2.9
64	1.4	698.4	10.86	4.9
65	1.38	687.8	4.07	2.9
66	1.35	675.9	3.53	4.6
67	1.33	664.6	3.32	3.2
68	1.3	651.1	1.67	0.9
69	1.28	642.5	1.11	2.1
70	1.25	626.4	3.04	3.7
71	1.23	614.2	2.7	3.4
72	1.22	611.4	2.02	2.9
73	1.21	604.8	1.69	2.7
74	1.2	602.2	1.59	2.4
75	1.04	521.4	26.62	2.1
76	1.02	512.1	34.17	1.4
77	0.99	497	22.95	1.7
78	0.96	482	28.17	1.2
79	0.96	480.9	31.8	3.1
80	0.95	473.8	31.21	1.5
81	0.91	454.2	29.19	1.2
82	0	0	100	0.3

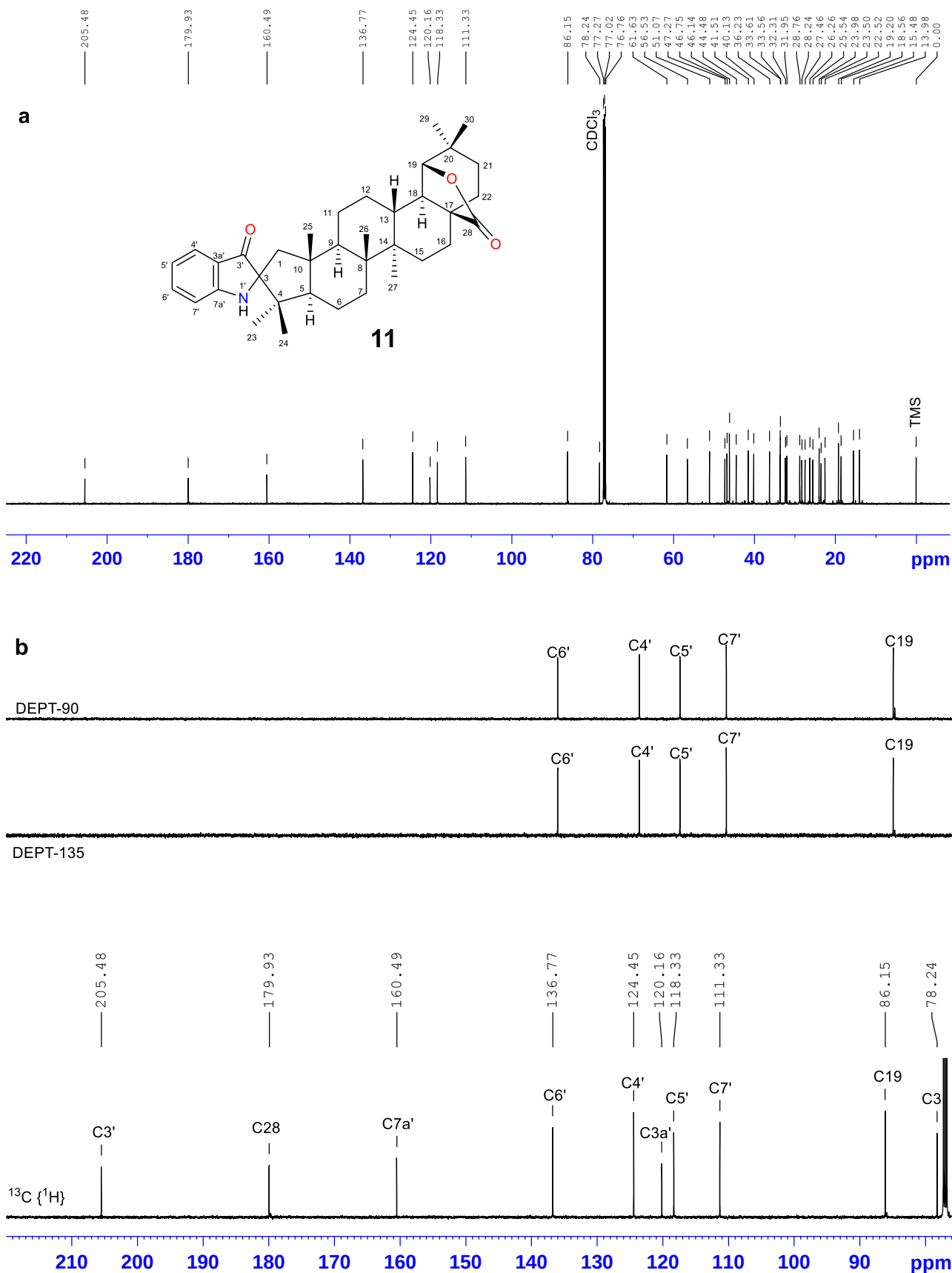


Figure S85. (a) Complete $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of compound **11** in CDCl_3 . (b) Downfield area of annotated $^{13}\text{C}\{^1\text{H}\}$ NMR and DEPT-135, DEPT-90 spectra of compound **11** in CDCl_3 .

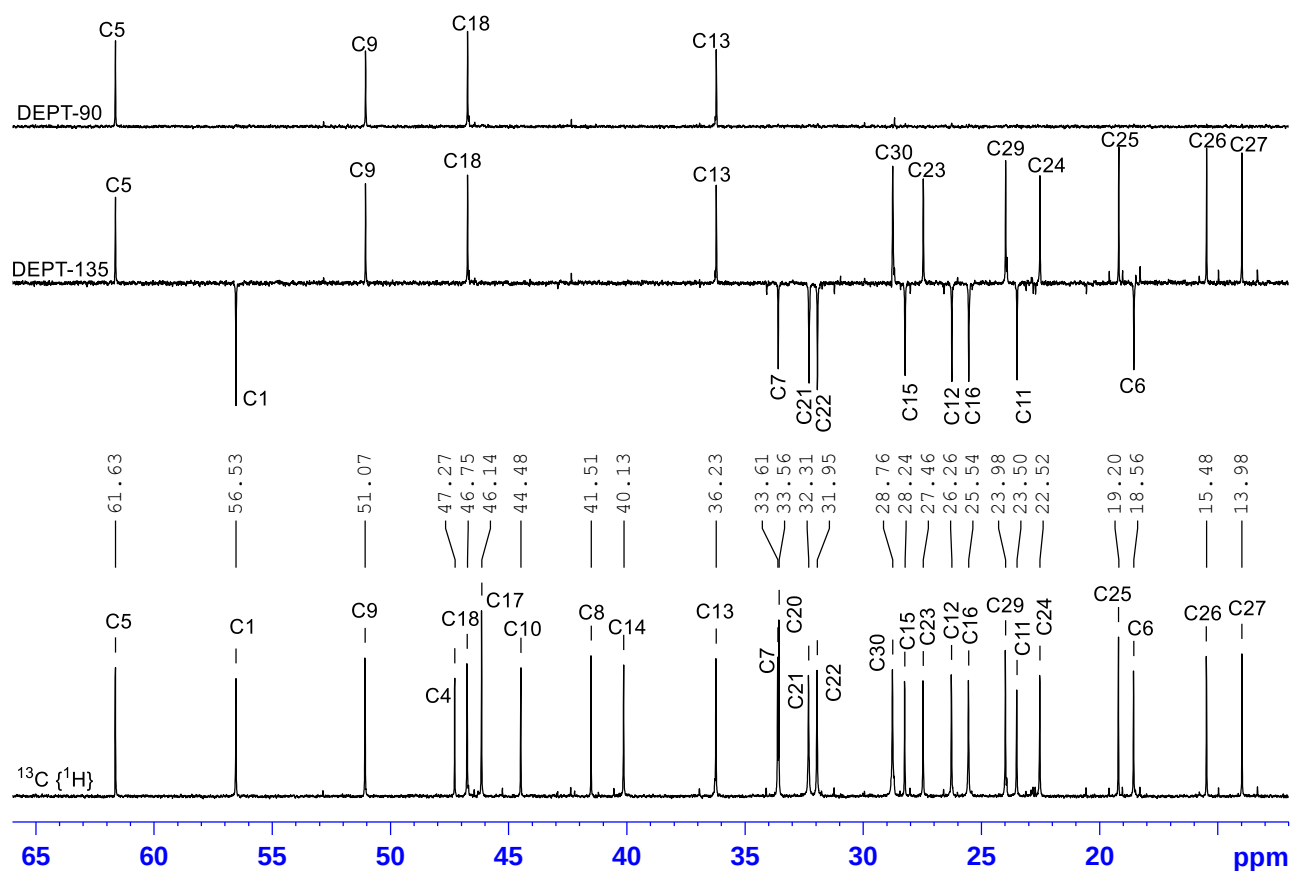


Figure S86. Upfield area of annotated $^{13}\text{C}\{^1\text{H}\}$ NMR and DEPT-135, DEPT-90 spectra of compound **11** in CDCl_3 .

Table S16. Complete numerical listings of ^{13}C NMR peaks of compound **11** in CDCl_3 .

Peak	$\nu(\text{F1})$ [ppm]	$\nu(\text{F1})$ [Hz]	Intensity [rel]	Half width [Hz]
1	205.48	25841	6.32	1.8
2	179.93	22627	6.91	0.9
3	160.49	20182.6	7.45	0.9
4	136.77	17199.7	11.26	1.8
5	124.45	15650.2	13.15	1.8
6	120.16	15111.6	6.72	0.9
7	118.34	14881.5	10.97	1.8
8	111.33	14000.4	12.65	0.9
9	86.15	10833.5	13.54	1.8
10	78.24	9838.8	11.08	0.9
11	77.27	9717.5	98.37	1.8
12	77.02	9685.6	100	1.8
13	76.76	9653.6	98.1	2.7
14	61.63	7750.5	12.95	0.9
15	56.53	7109.1	11.49	1.8
16	51.07	6422.1	13.62	0.9
17	47.27	5944.9	12.07	0.9
18	46.75	5879	13.08	1.8
19	46.14	5802	17.98	1.8
20	44.48	5593.2	12.57	0.9
21	41.51	5219.8	13.6	0.9

22	40.13	5046.4	12.74	1.8
23	36.22	4555.6	13.64	1.8
24	33.61	4226.4	13.81	1.8
25	33.56	4220.1	17.62	0.9
26	32.31	4062.6	11.69	3.6
27	31.95	4017.5	12.32	3.6
28	28.76	3616.4	12.5	4.5
29	28.24	3551	11.52	1.8
30	27.46	3453.2	11.16	1.8
31	26.26	3302.3	11.85	1.8
32	25.54	3211.9	11.42	2.7
33	23.98	3015.4	14.11	1.8
34	23.5	2955	10.83	2.7
35	22.52	2832.5	12.12	2.7
36	19.2	2414.2	15.42	0.9
37	18.56	2333.5	12.2	1.8
38	15.48	1947.1	13.92	0.9
39	13.98	1758.2	14.02	0.9
40	0	0	11.83	1.8

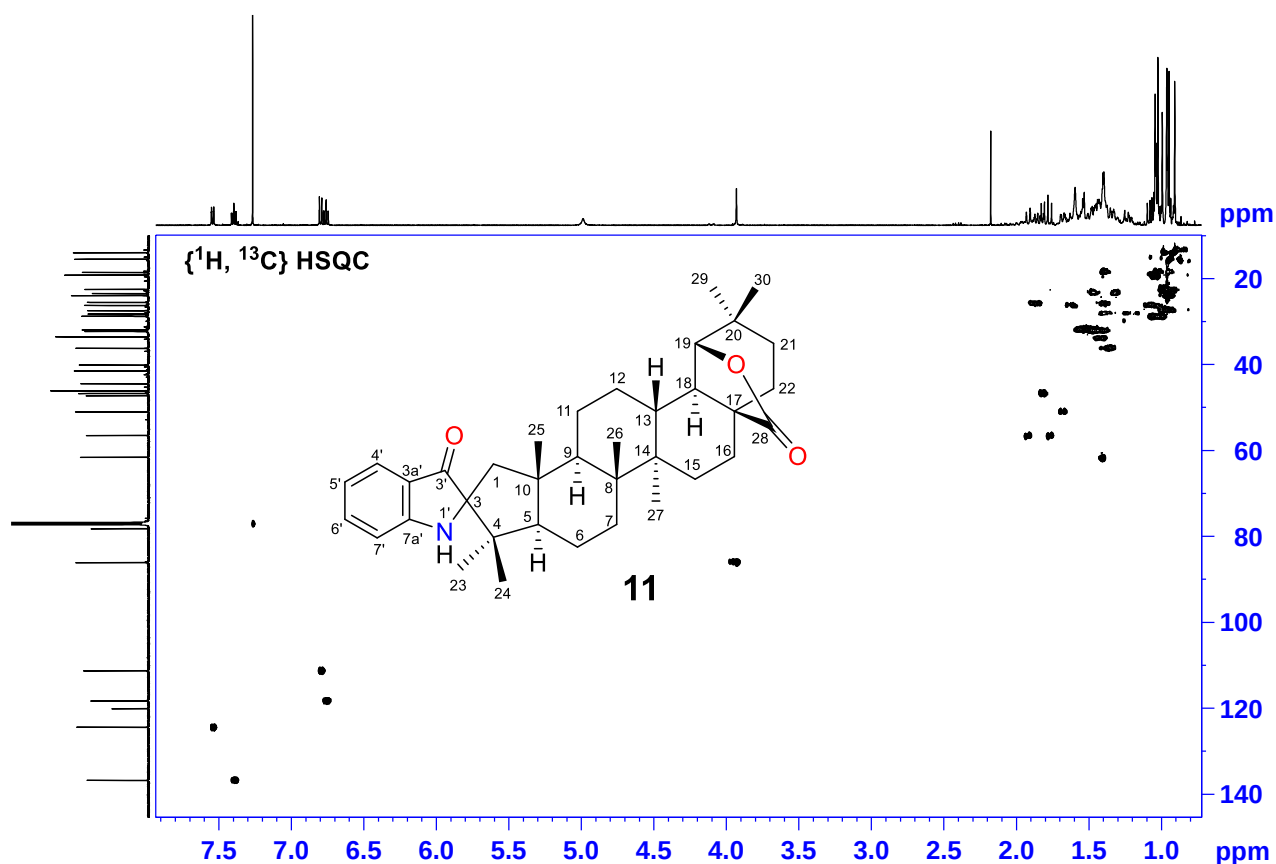


Figure S87. Complete $\{^1\text{H}, ^{13}\text{C}\}$ HSQC NMR spectrum of compound **11** in CDCl_3 .

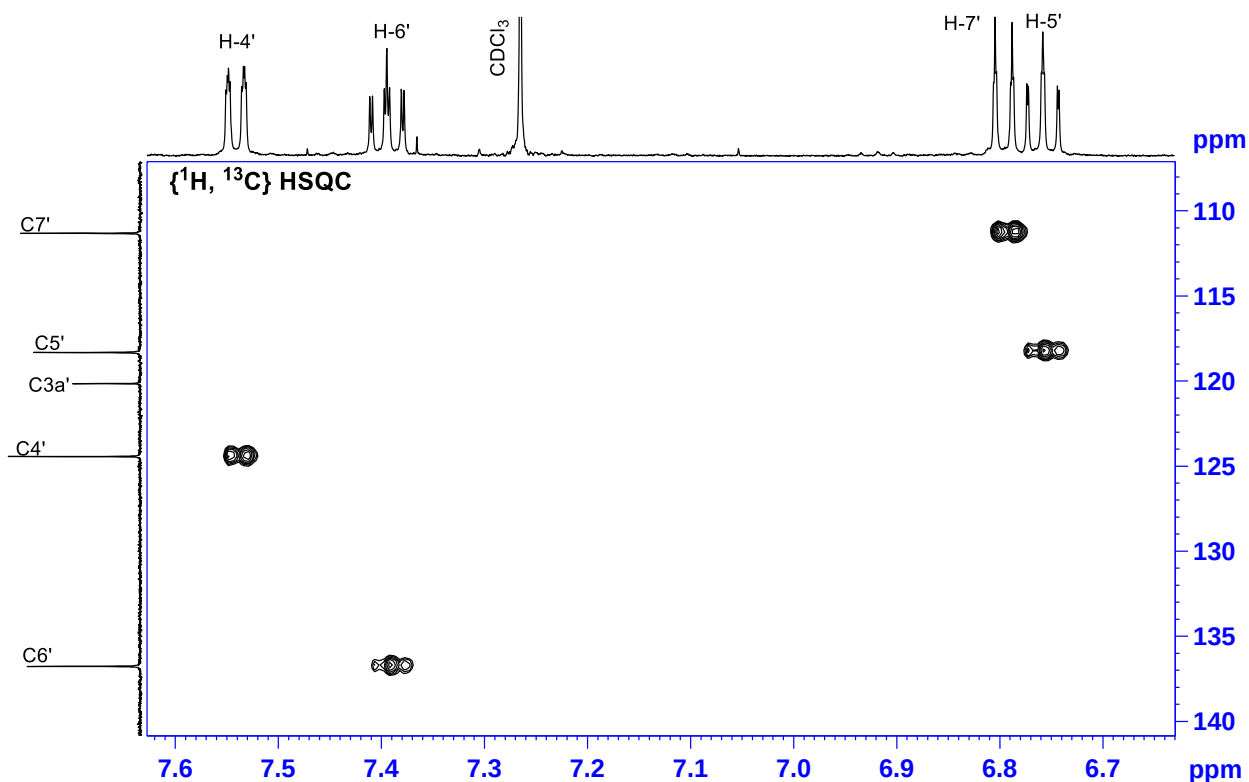


Figure S88. Downfield area of $\{^1\text{H}, ^{13}\text{C}\}$ HSQC NMR spectrum of compound **11** in CDCl_3 .

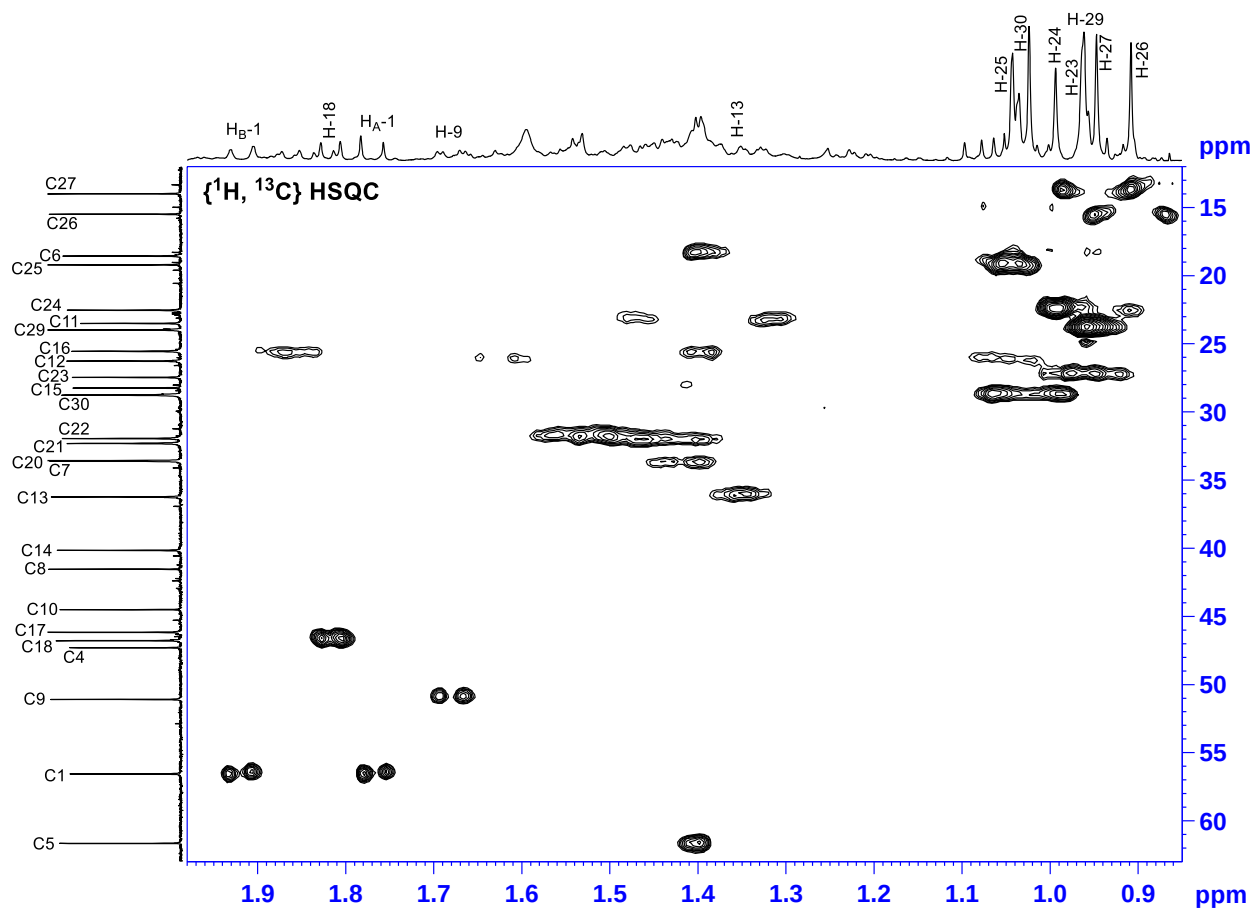


Figure S89. Upfield area of $\{^1\text{H}, ^{13}\text{C}\}$ HSQC multiplicity edited NMR spectrum of compound **11** in CDCl_3 .

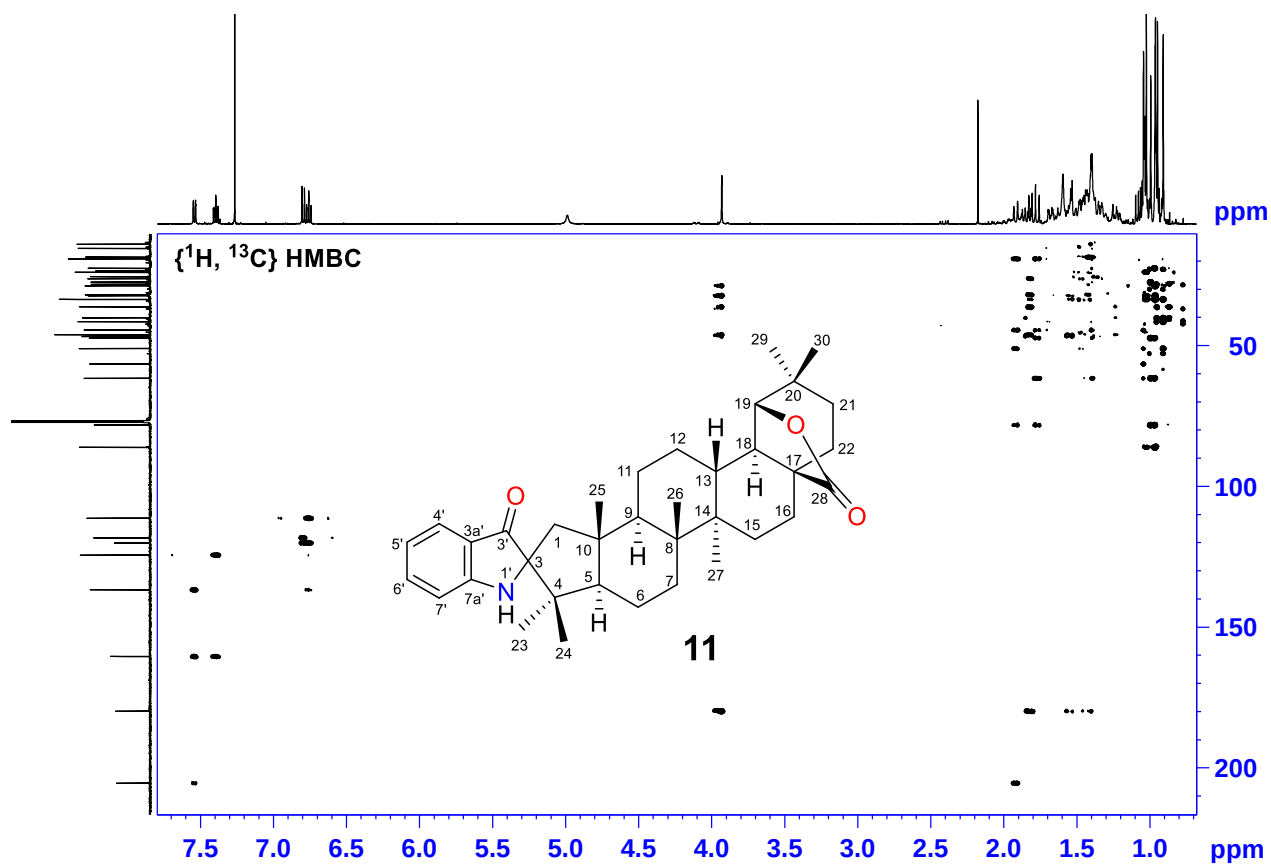


Figure S90. Complete $\{^1\text{H}, ^{13}\text{C}\}$ HMBC NMR spectrum of compound **11** in CDCl_3 .

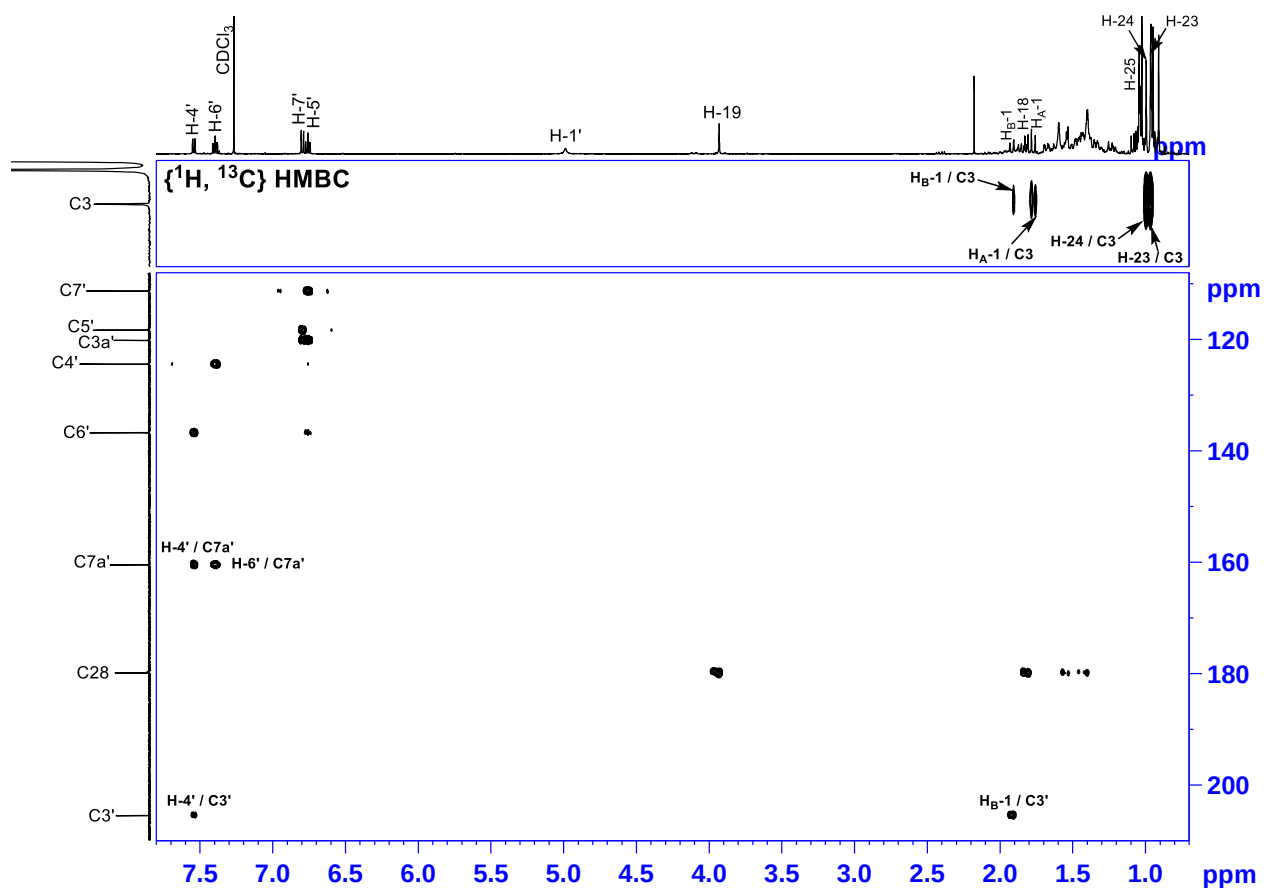


Figure S91. Annotated $\{^1\text{H}, ^{13}\text{C}\}$ HMBC NMR spectrum of compound **11** in CDCl_3 .

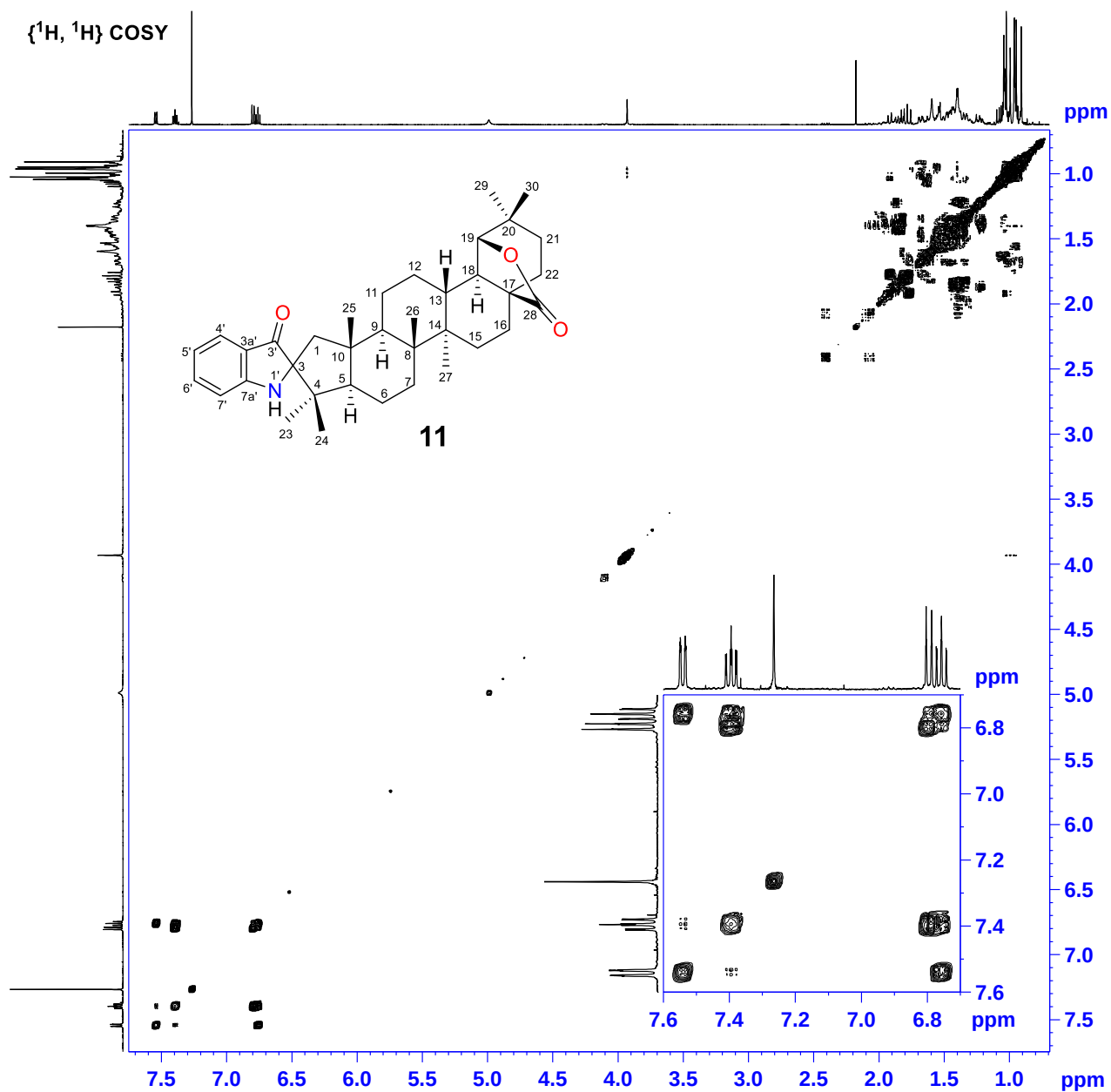


Figure S92. Complete $\{^1\text{H}, ^1\text{H}\}$ COSY NMR spectrum of compound **11** in CDCl_3 .

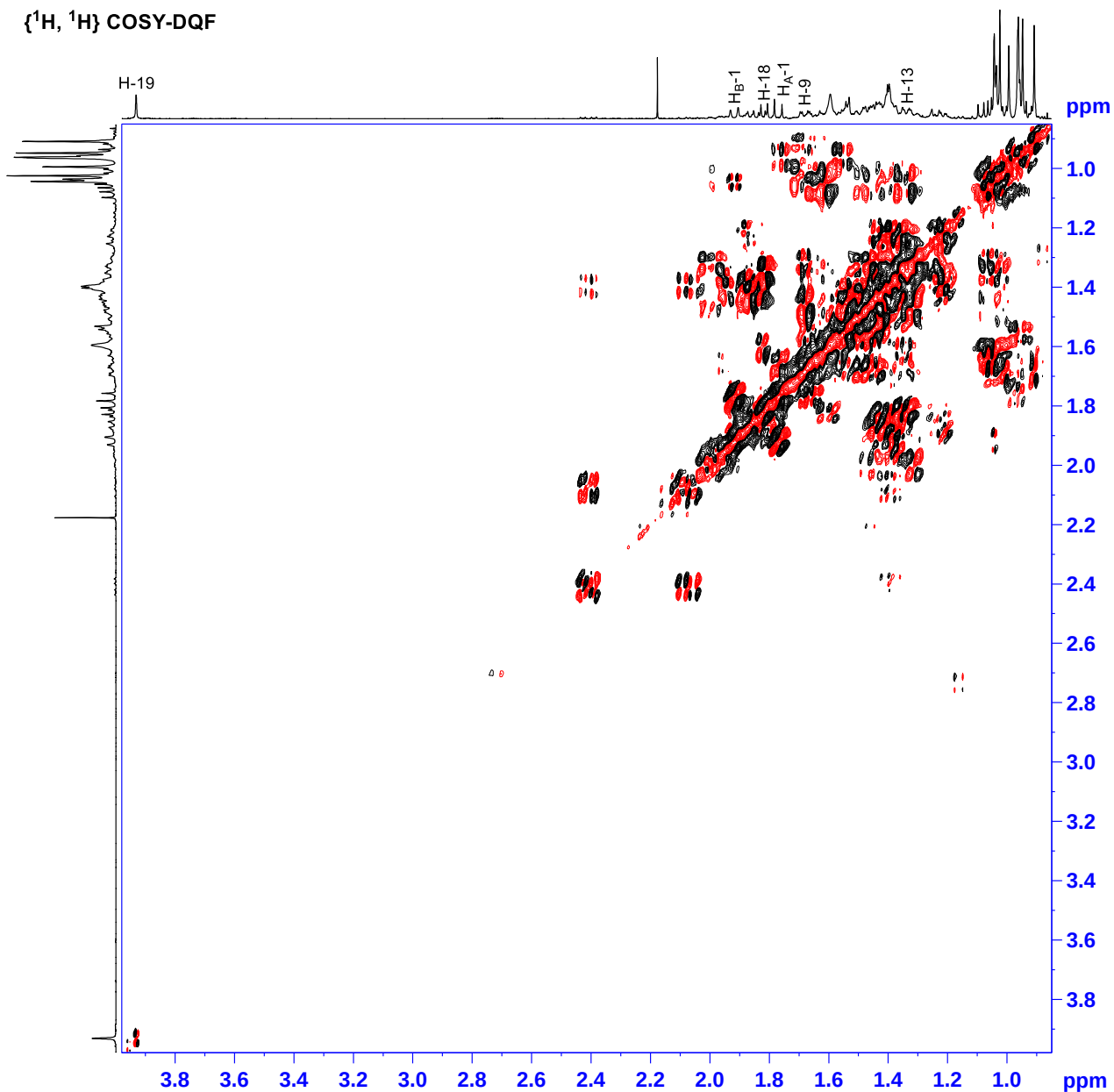


Figure S93. Upfield area of $\{^1\text{H}, ^1\text{H}\}$ COSY-DQF NMR spectrum of compound **11** in CDCl_3 .

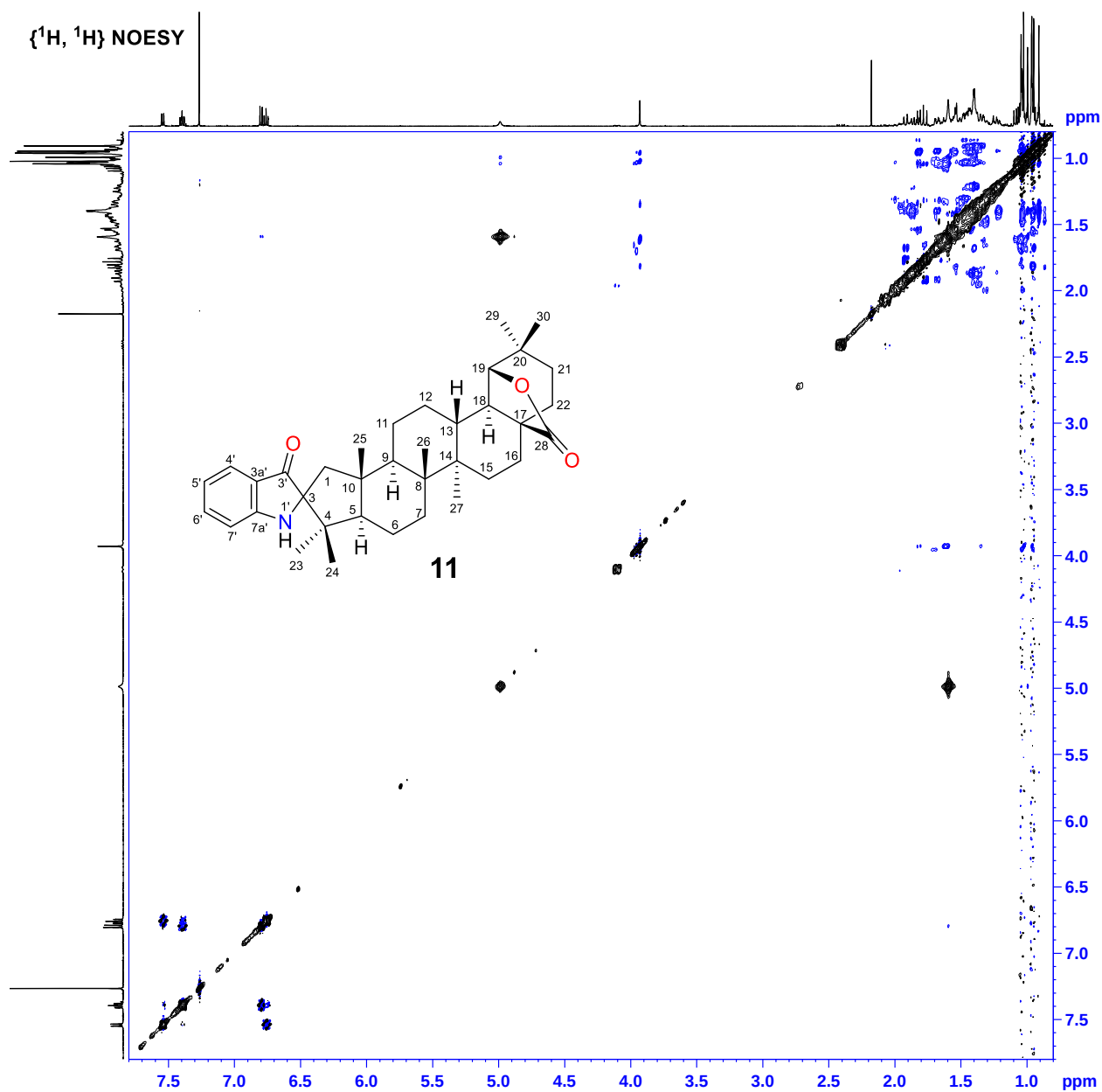


Figure S94. Complete $\{^1\text{H}, ^1\text{H}\}$ NOESY NMR spectrum of compound **11** in CDCl_3 .

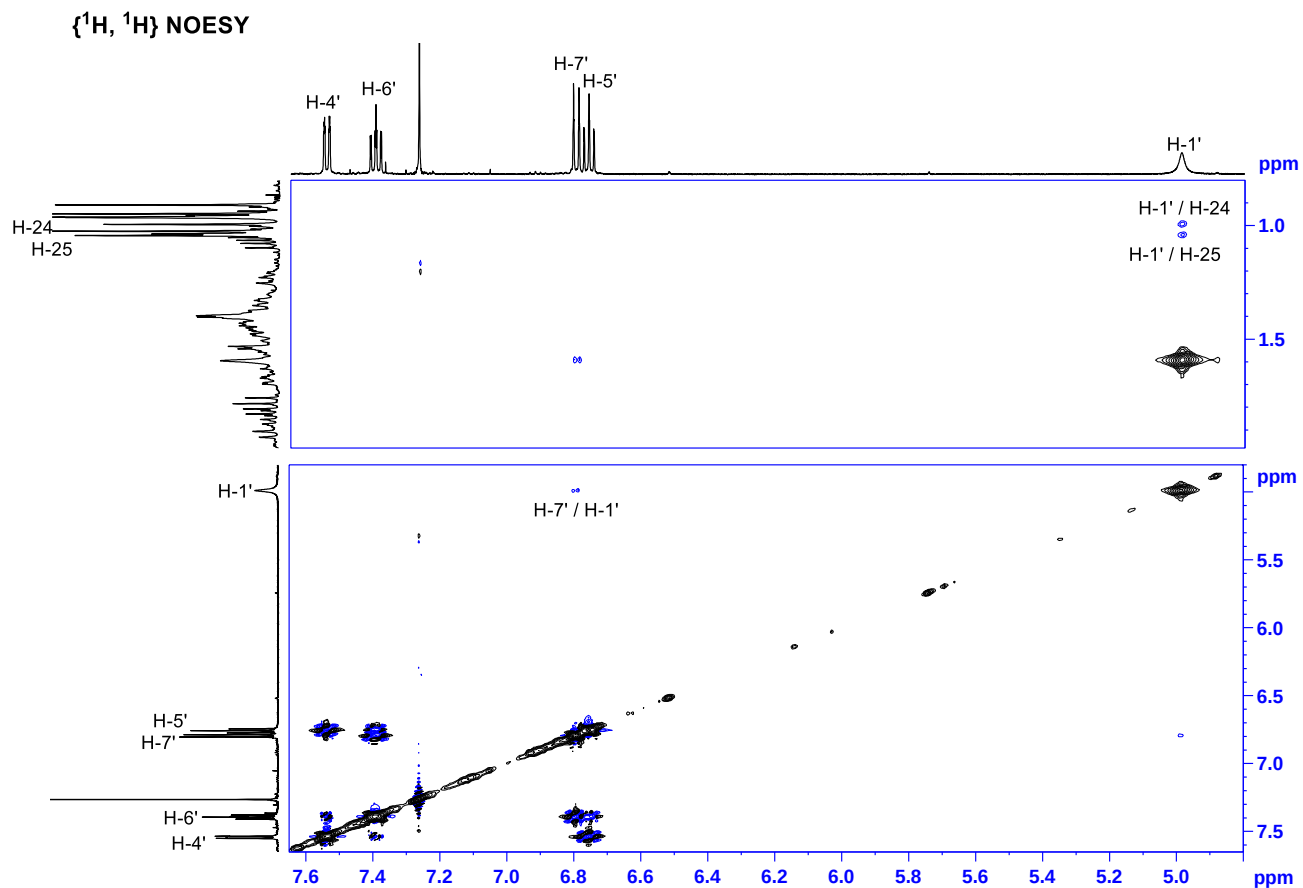


Figure S95. Detailed and annotated $\{^1\text{H}, ^1\text{H}\}$ NOESY NMR spectrum of compound **11** in CDCl_3 .

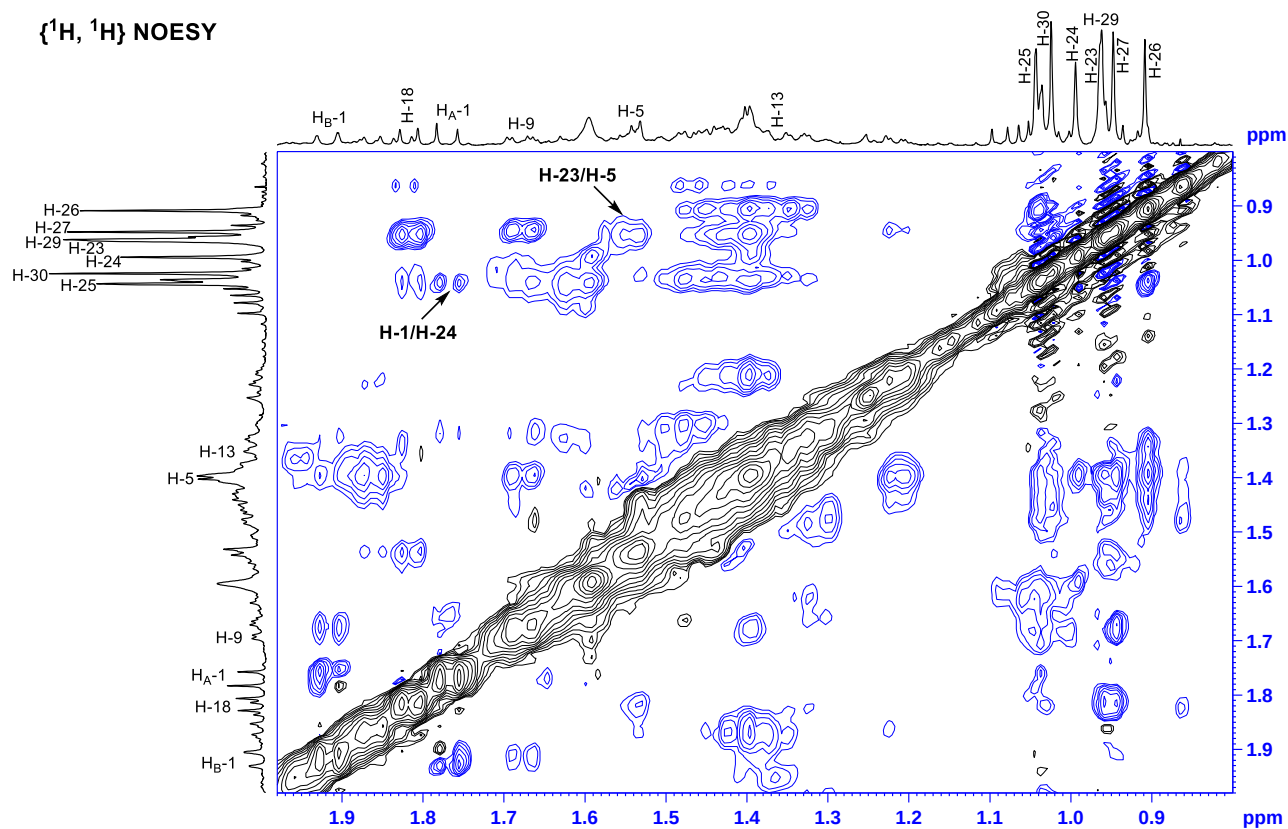
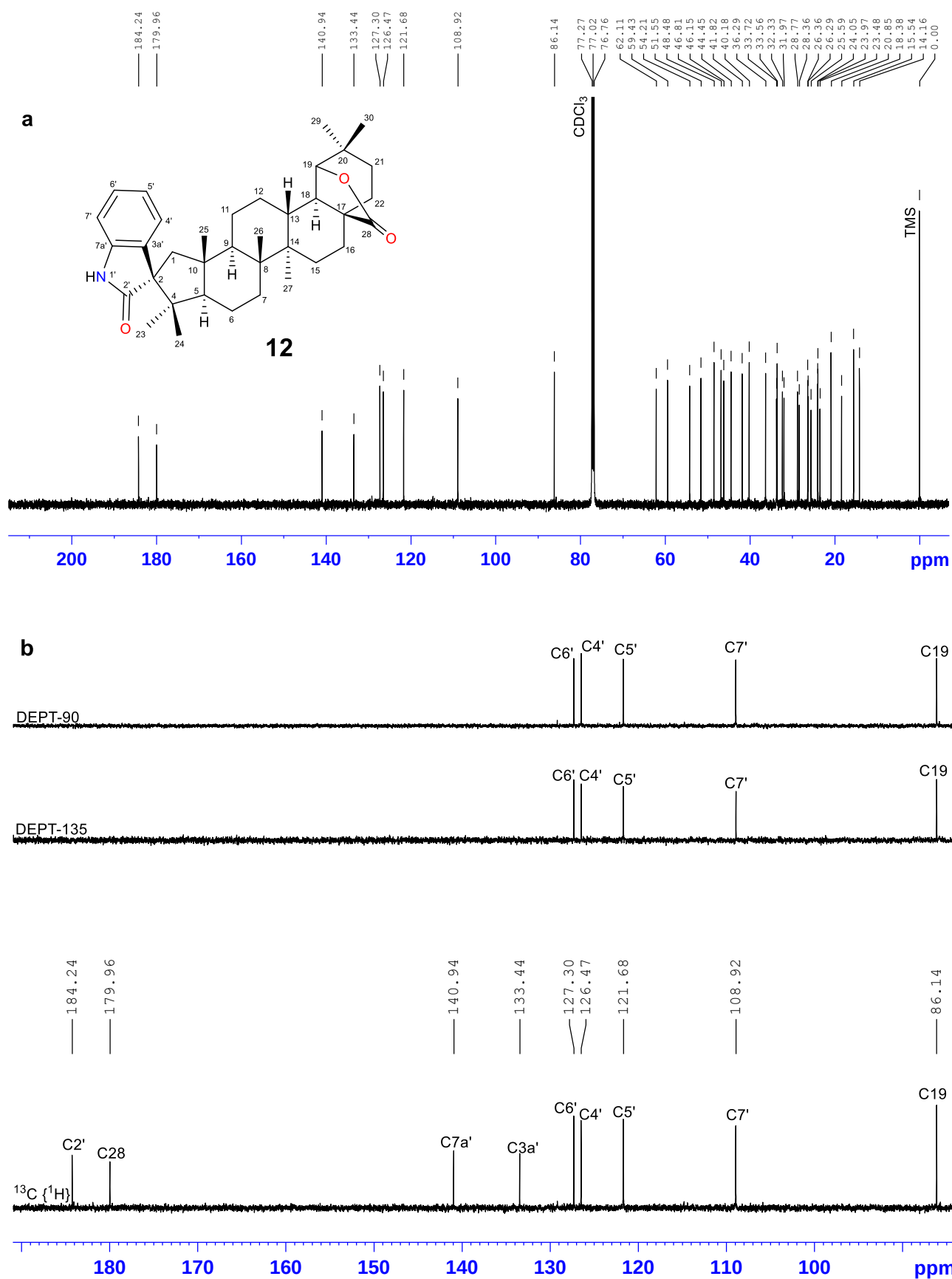


Figure S96. Upfield area of $\{^1\text{H}, ^1\text{H}\}$ NOESY NMR spectrum of compound **11** in CDCl_3 .

Table S17. Complete numerical listings of ^1H NMR peaks of compound **12** in CDCl_3 .

Peak	$\nu(\text{F1})$ [ppm]	$\nu(\text{F1})$ [Hz]	Intensity [rel]	Half width [Hz]
1	7.26	3632.3	7.47	0.3
2	7.24	3623.2	0.48	2.6
3	7.23	3615.6	0.55	2.6
4	7.17	3588	0.34	0.9
5	7.17	3586.9	0.38	1.1
6	7.17	3583.6	0.26	4.1
7	7.16	3580.4	0.81	1.1
8	7.16	3579.2	0.79	0.9
9	7.14	3572.7	0.55	1.1
10	7.14	3571.5	0.49	0.9
11	7.01	3503.5	0.37	0.8
12	7	3502.4	0.4	0.9
13	6.99	3495.9	0.65	0.8
14	6.99	3494.8	0.68	0.9
15	6.97	3488.3	0.3	0.9
16	6.97	3487.2	0.3	0.9
17	6.81	3407	0.57	0.8
18	6.81	3406.5	0.59	1.2
19	6.8	3399.3	0.54	0.9
20	6.8	3398.8	0.53	1.2
21	3.94	1970.2	1.09	2
22	2.15	1074.7	0.4	2.4
23	2.12	1061.5	0.48	2.4
24	1.89	943.3	0.19	3.2
25	1.88	941.3	0.19	2.7
26	1.86	931.5	0.33	2.3
27	1.86	928.1	0.49	2.4
28	1.85	925.3	1.1	2
29	1.83	916.4	0.86	3.5
30	1.82	912.2	1.15	2.1
31	1.81	905.4	0.74	1.5
32	1.65	825	0.09	1.7
33	1.64	821	0.17	3.4
34	1.64	818.3	0.18	2.4
35	1.63	814.9	0.14	1.8
36	1.62	812.1	0.13	2.3
37	1.62	809.2	0.17	2
38	1.61	805.9	0.2	1.2
39	1.61	803.2	0.13	0.8
40	1.57	786.9	3.89	1.4
41	1.57	785.2	3.51	1.4
42	1.54	772.3	0.55	4.9
43	1.53	767.3	0.69	5.8
44	1.52	761	0.27	4.1
45	1.51	754.7	0.31	1.5
46	1.5	752.1	0.3	3.1

47	1.5	748.2	0.28	4.6
48	1.48	740.9	0.46	4.6
49	1.46	730.5	1.11	7.2
50	1.44	722.2	0.52	4.1
51	1.44	718.2	0.78	4.6
52	1.43	715	0.59	3.5
53	1.41	707.4	0.76	3.1
54	1.41	705.9	0.7	4.3
55	1.4	699.8	0.61	7.2
56	1.37	687	0.39	3.2
57	1.37	684	0.38	4.9
58	1.35	675.6	0.44	4.7
59	1.35	673.2	0.7	3.1
60	1.25	622.9	0.22	1.2
61	1.24	621.4	0.38	3.2
62	1.24	619.6	0.3	0.5
63	1.24	618.2	0.27	1.4
64	1.22	611.5	3.57	1.7
65	1.21	607.3	0.23	0.6
66	1.21	605.9	0.21	0.2
67	1.13	567.3	0.09	4.1
68	1.13	562.8	0.1	2.6
69	1.11	554.3	0.21	3.4
70	1.1	550.1	0.22	3.4
71	1.08	541.6	0.21	3.5
72	1.07	537.4	0.2	2.7
73	1.06	528.9	0.18	2
74	1.05	524.6	0.12	2.9
75	1.02	512.5	3.79	1.5
76	0.98	489.8	4.28	1.4
77	0.96	478.5	5.5	0.6
78	0.96	478.1	6.55	1.8
79	0.93	467.2	4.27	1.4
80	0.88	438.3	3.59	1.5
81	0	0	100	0.3



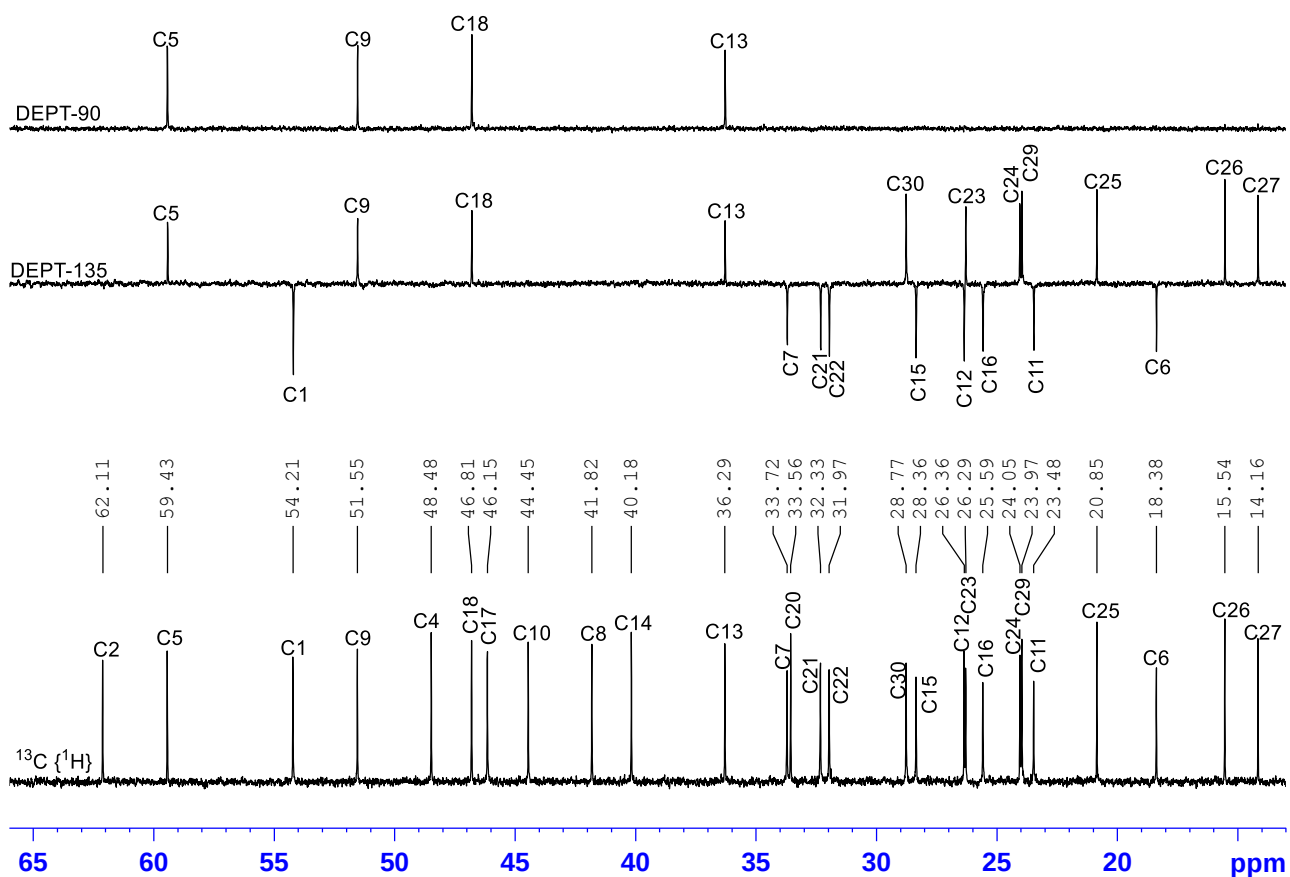


Figure S99. Upfield area of annotated $^{13}\text{C}\{^1\text{H}\}$ NMR and DEPT-135, DEPT-90 spectra of compound **12** in CDCl_3 .

Table S18. Complete numerical listings of ^{13}C NMR peaks of compound **12** in CDCl_3 .

Peak	$\nu(\text{F1})$ [ppm]	$\nu(\text{F1})$ [Hz]	Intensity [rel]	Half width [Hz]
1	184.24	23169.1	2.6	0.9
2	179.96	22630.8	2.33	0.9
3	140.94	17723.9	2.76	0.9
4	133.44	16781.1	2.63	0.9
5	127.3	16009	4.44	1.8
6	126.47	15904.5	4.25	1.8
7	121.68	15302.2	4.33	1.8
8	108.92	13697.3	4.03	1.8
9	86.14	10833	5	0.9
10	77.27	9717.3	99.17	2.7
11	77.02	9685.3	100	2.7
12	76.76	9653.3	98.46	2.7
13	62.11	7811	4.34	0.9
14	59.43	7473.4	4.75	0.9
15	54.21	6817.3	4.45	1.8
16	51.55	6483	4.79	0.9
17	48.48	6097.1	5.32	0.9
18	46.81	5886.5	5.03	1.8
19	46.15	5804.1	4.82	1.8
20	44.45	5590.4	4.97	1.8

21	41.82	5258.9	4.9	0.9
22	40.18	5052.5	5.36	0.9
23	36.29	4564	4.91	1.8
24	33.72	4240.1	4.11	1.8
25	33.56	4220.8	5.29	1.8
26	32.33	4065.7	4.33	2.7
27	31.97	4019.9	3.99	1.8
28	28.77	3618.3	4.31	1.8
29	28.36	3566.3	3.91	1.8
30	26.36	3315.2	4.64	1.8
31	26.29	3306.8	4.12	1.8
32	25.59	3217.5	3.76	1.8
33	24.05	3023.9	4.72	0.9
34	23.97	3013.8	5.17	1.8
35	23.48	2952.2	3.72	1.8
36	20.85	2622.3	5.71	0.9
37	18.38	2311.6	4.07	1.8
38	15.54	1954.6	5.8	0.9
39	14.16	1780.8	5.27	0.9
40	0	0	10.99	0.9

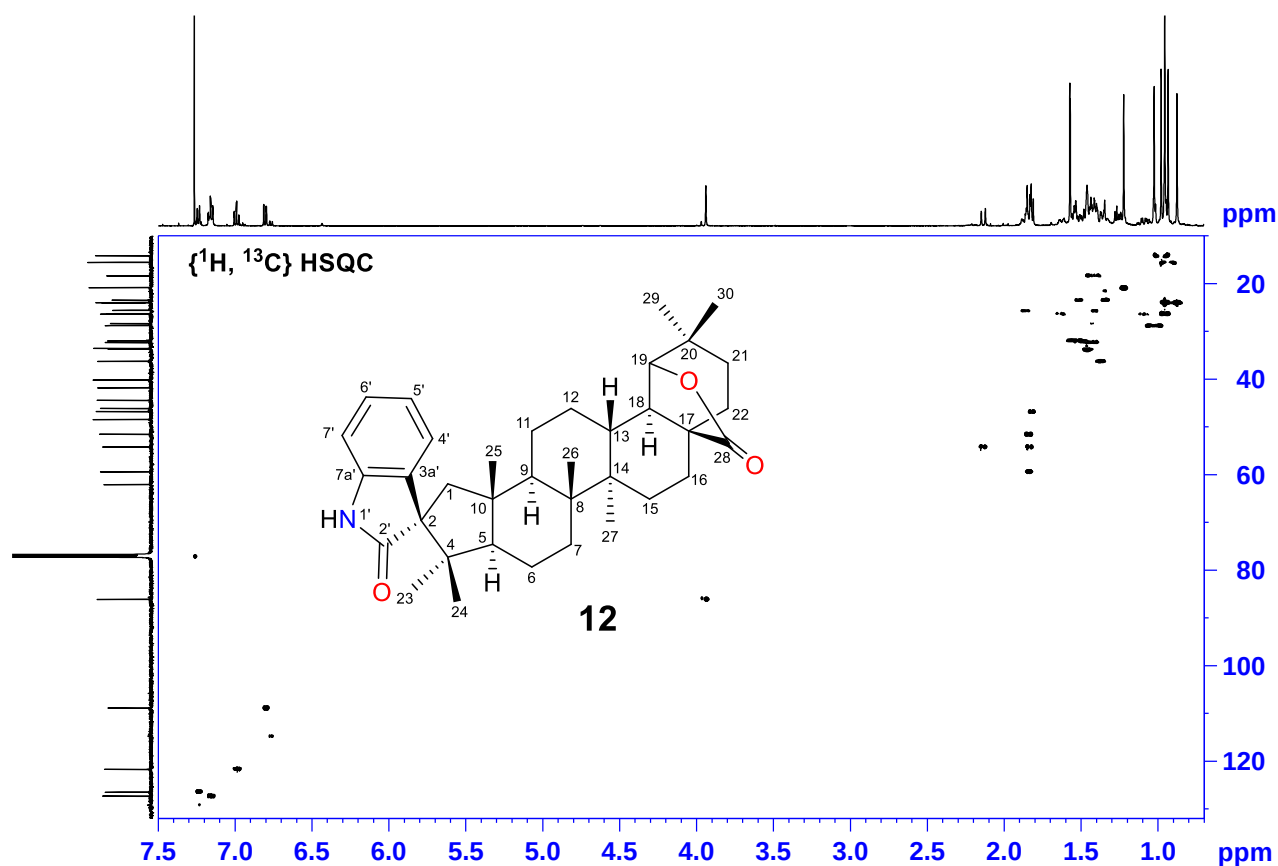


Figure S100. Complete $\{^1\text{H}, ^{13}\text{C}\}$ HSQC NMR spectrum of compound **12** in CDCl_3 .

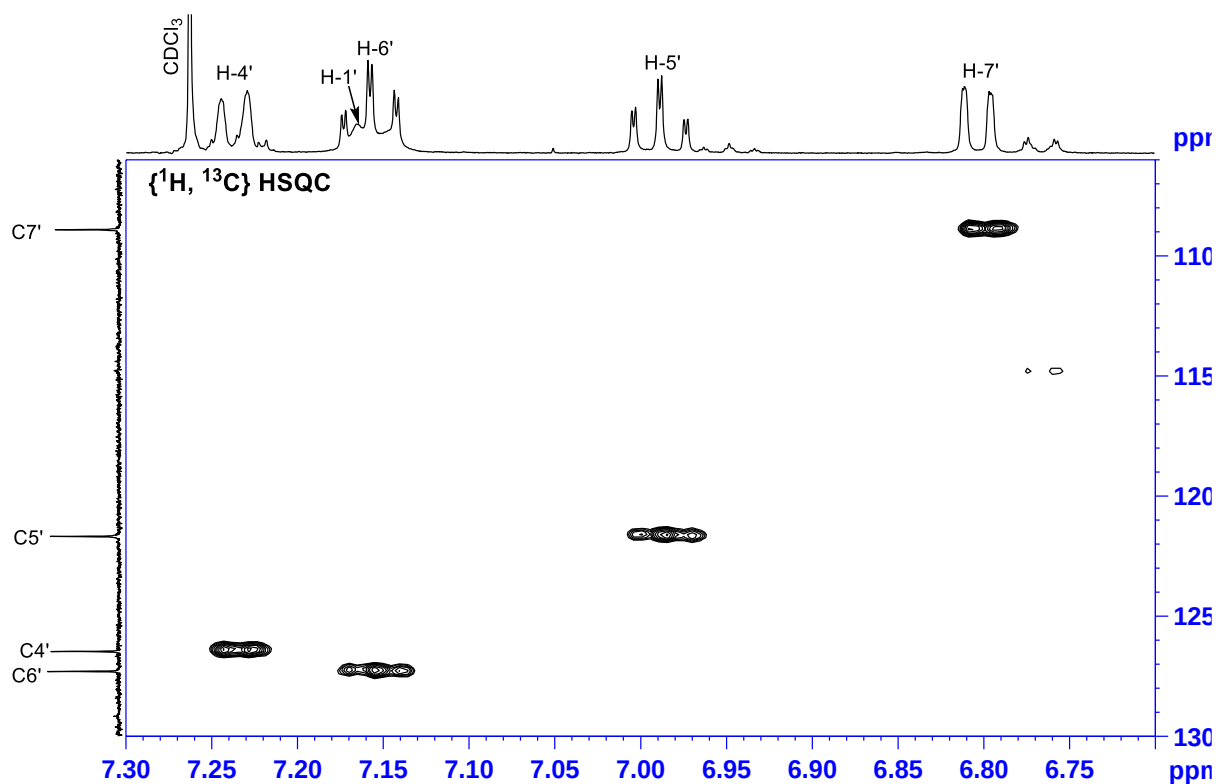


Figure S101. Downfield area of $\{^1\text{H}, ^{13}\text{C}\}$ HSQC NMR spectrum of compound **12** in CDCl_3 .

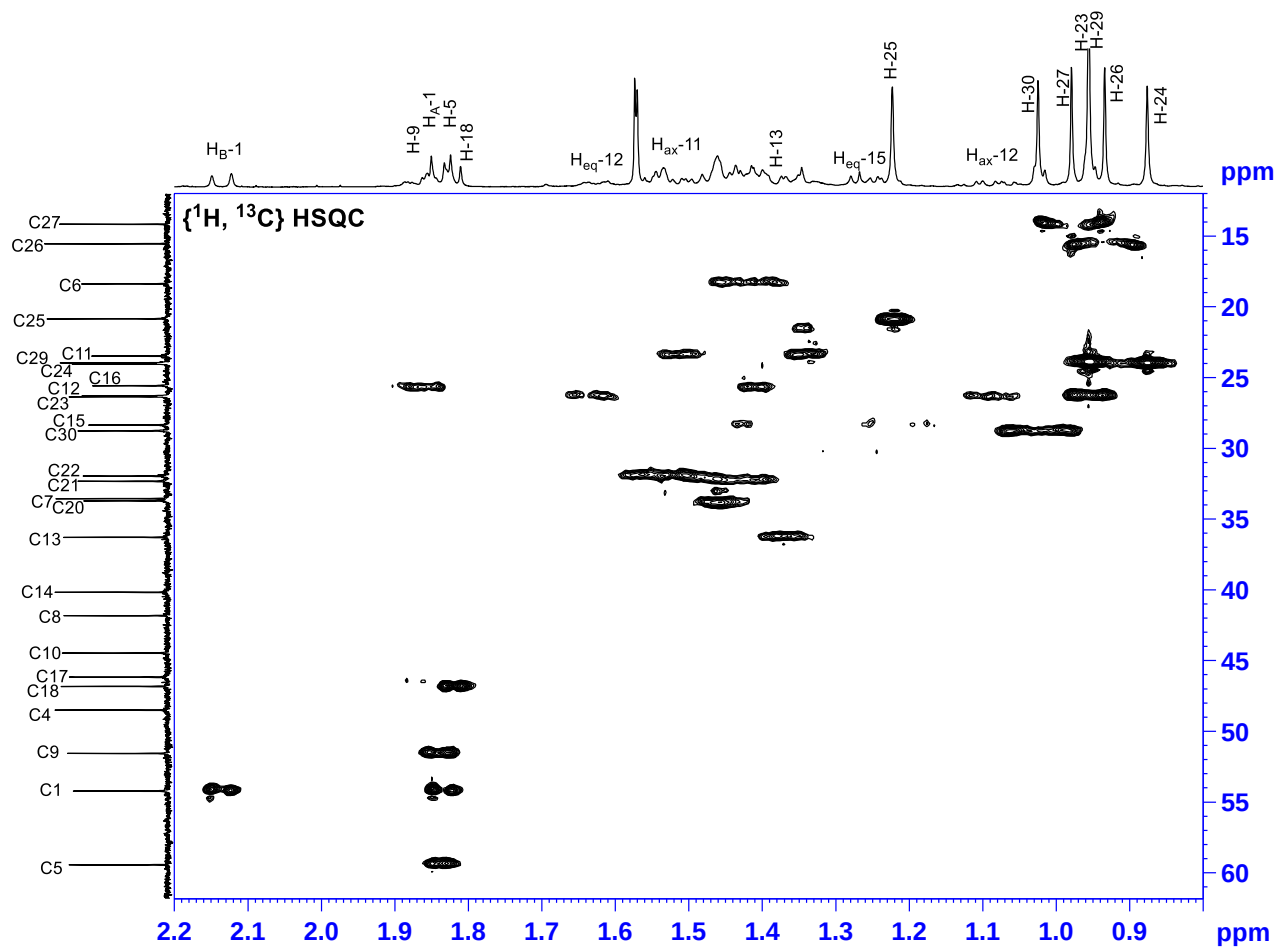


Figure S102. Upfield area of $\{^1\text{H}, ^{13}\text{C}\}$ HSQC multiplicity edited NMR spectrum of compound **12** in CDCl_3 .

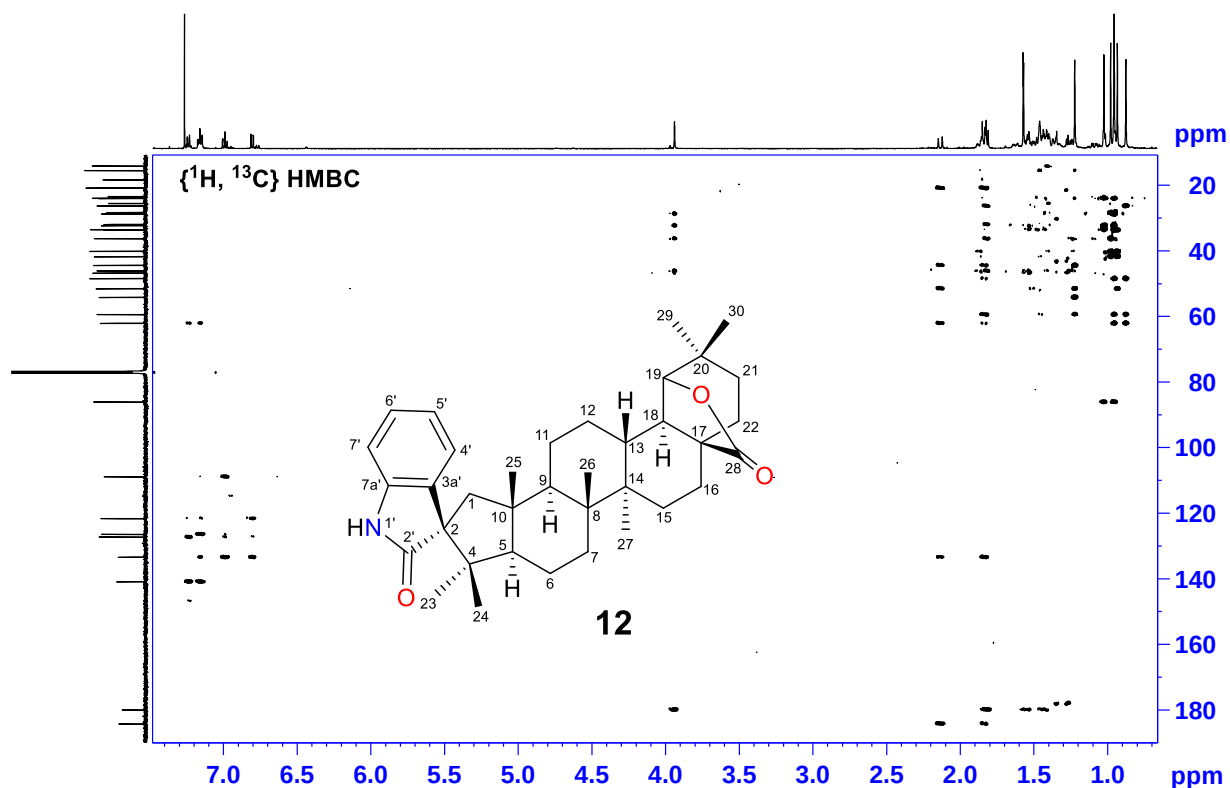


Figure S103. Complete $\{^1\text{H}, ^{13}\text{C}\}$ HMBC NMR spectrum of compound **12** in CDCl_3 .

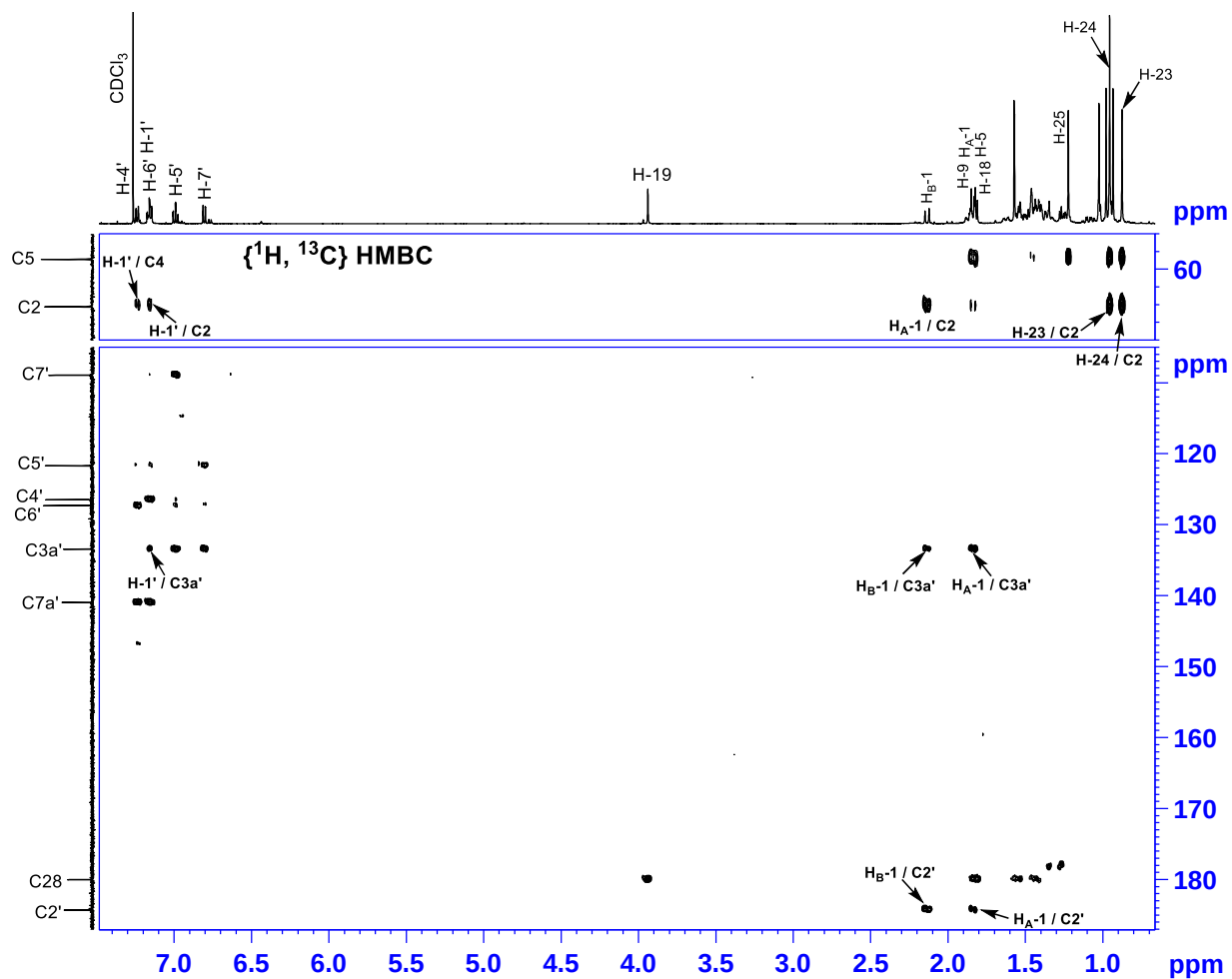


Figure S104. Annotated $\{^1\text{H}, ^{13}\text{C}\}$ HMBC NMR spectrum of compound **12** in CDCl_3 .

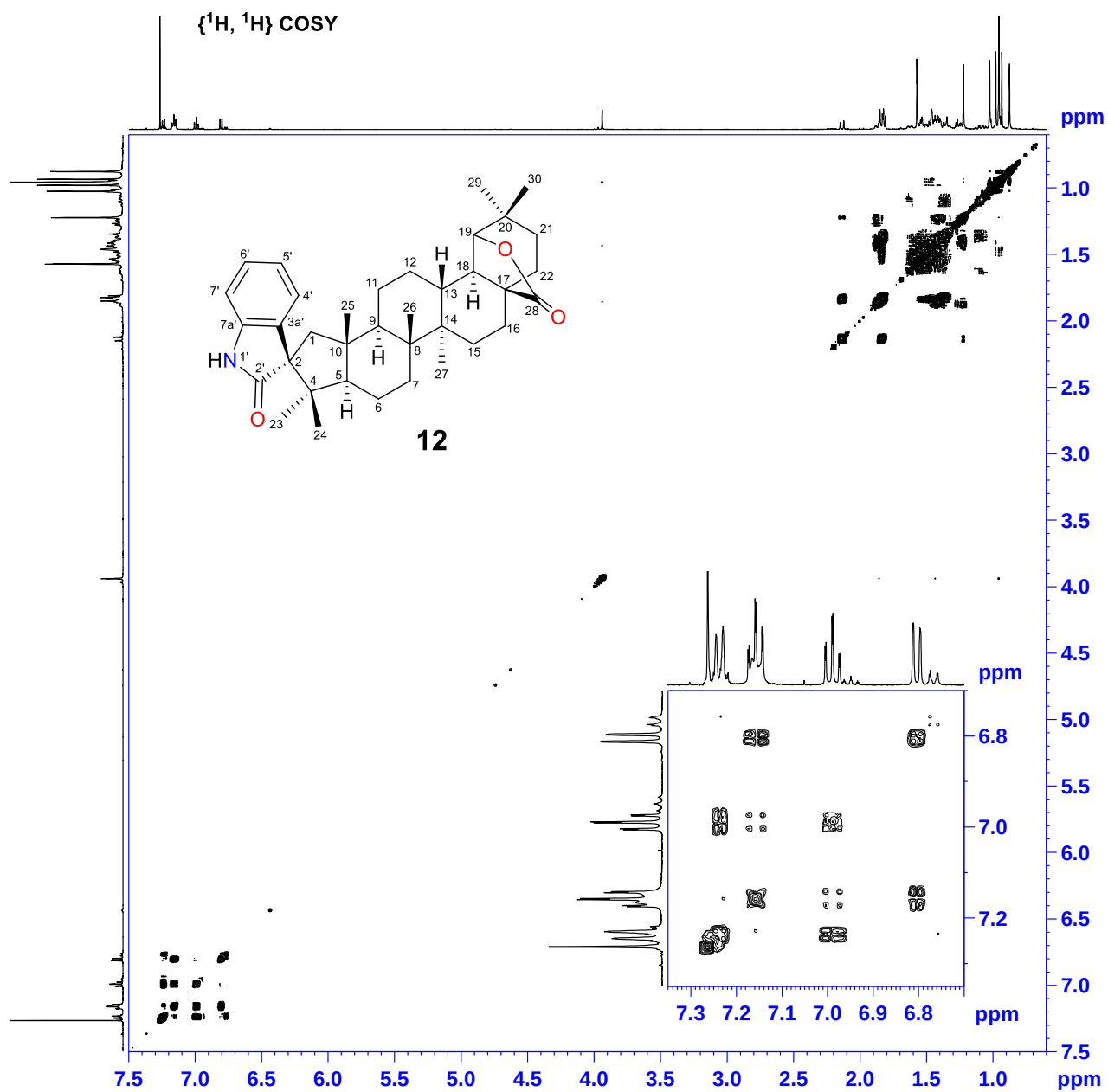


Figure S105. Complete $\{^1\text{H}, ^1\text{H}\}$ COSY NMR spectrum of compound **12** in CDCl_3 .

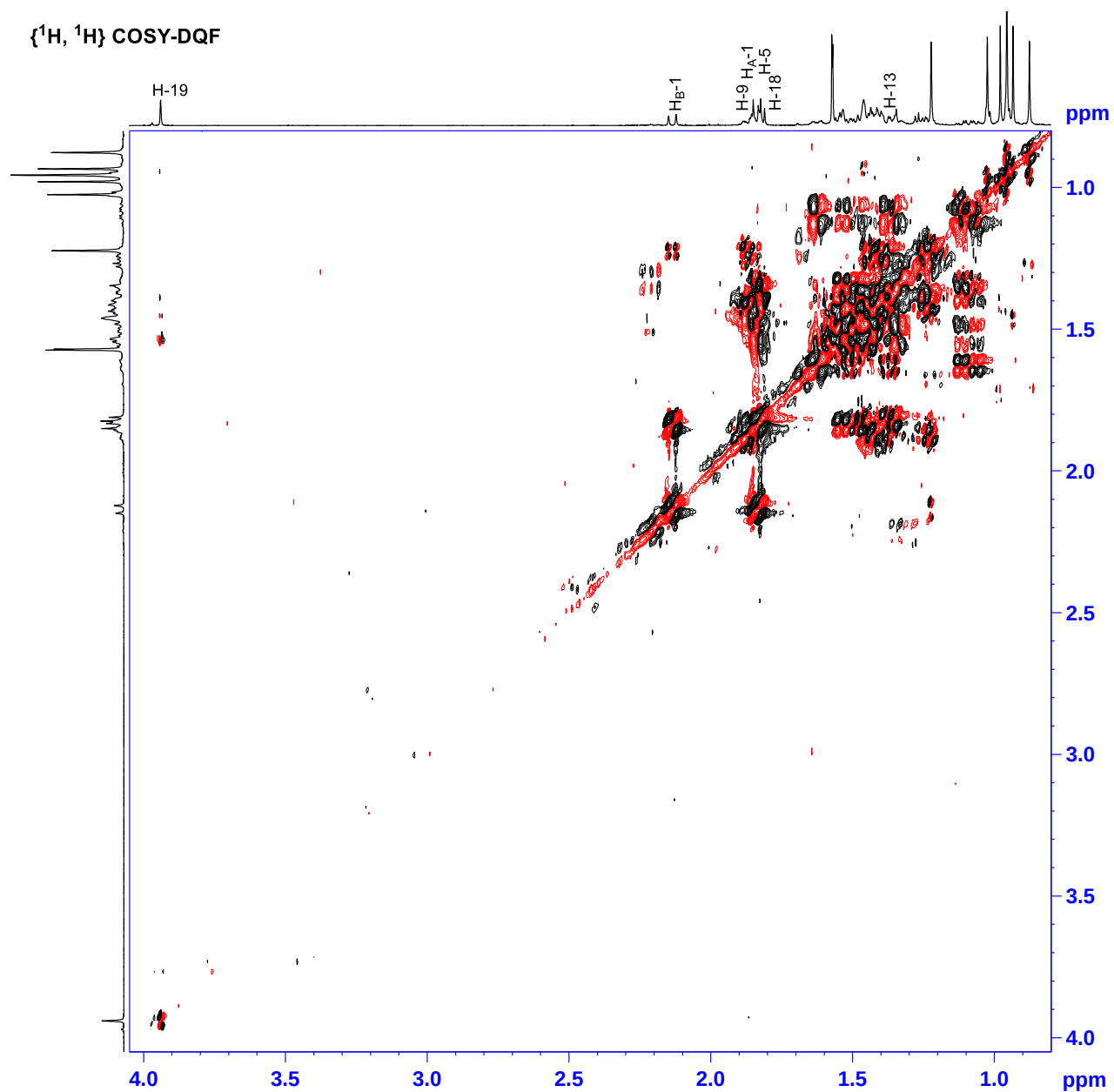


Figure S106. Upfield area of $\{^1\text{H}, ^1\text{H}\}$ COSY-DQF NMR spectrum of compound **12** in CDCl_3 .

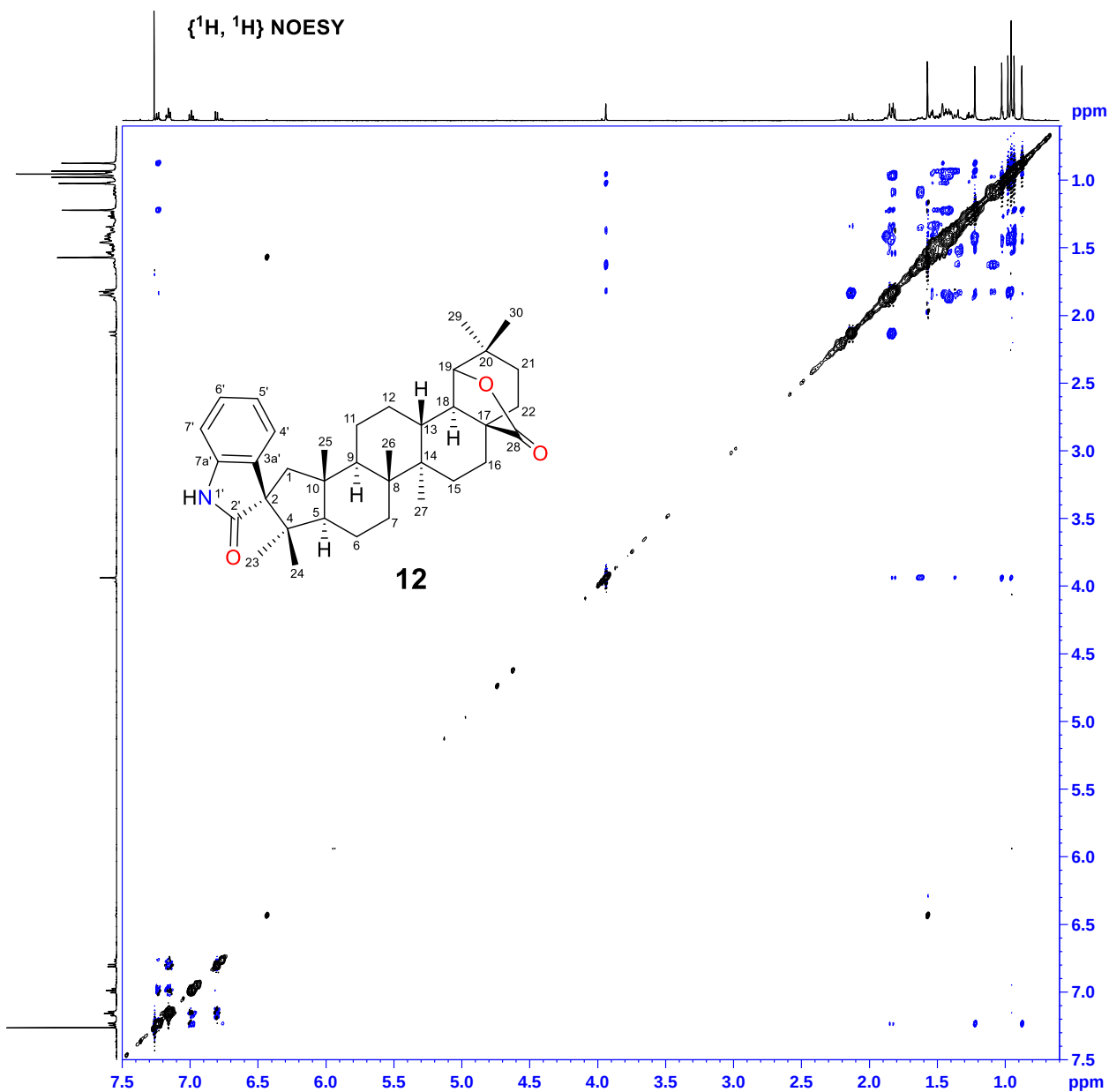


Figure S107. Complete $\{^1\text{H}, ^1\text{H}\}$ NOESY NMR spectrum of compound **12** in CDCl_3 .

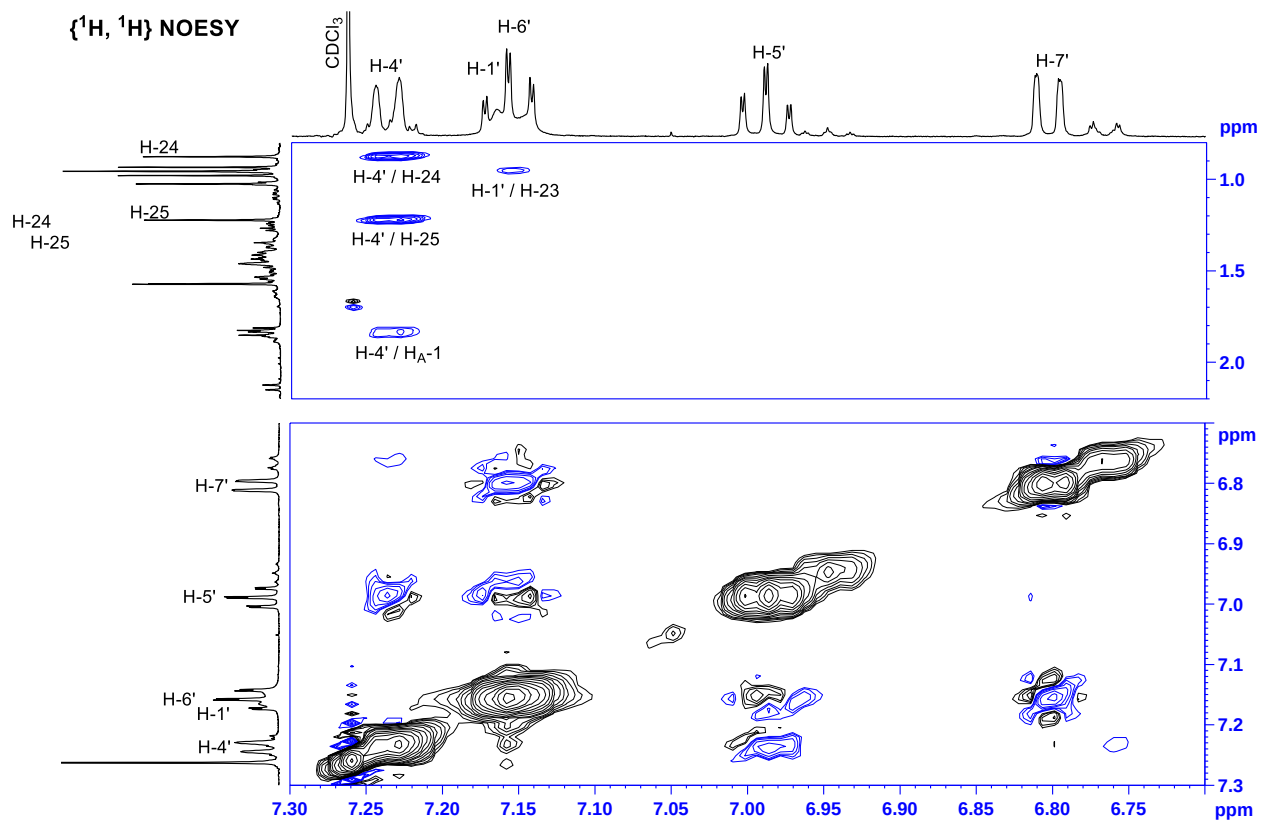


Figure S108. Detailed and annotated $\{^1\text{H}, ^1\text{H}\}$ NOESY NMR spectrum of compound **12** in CDCl₃.

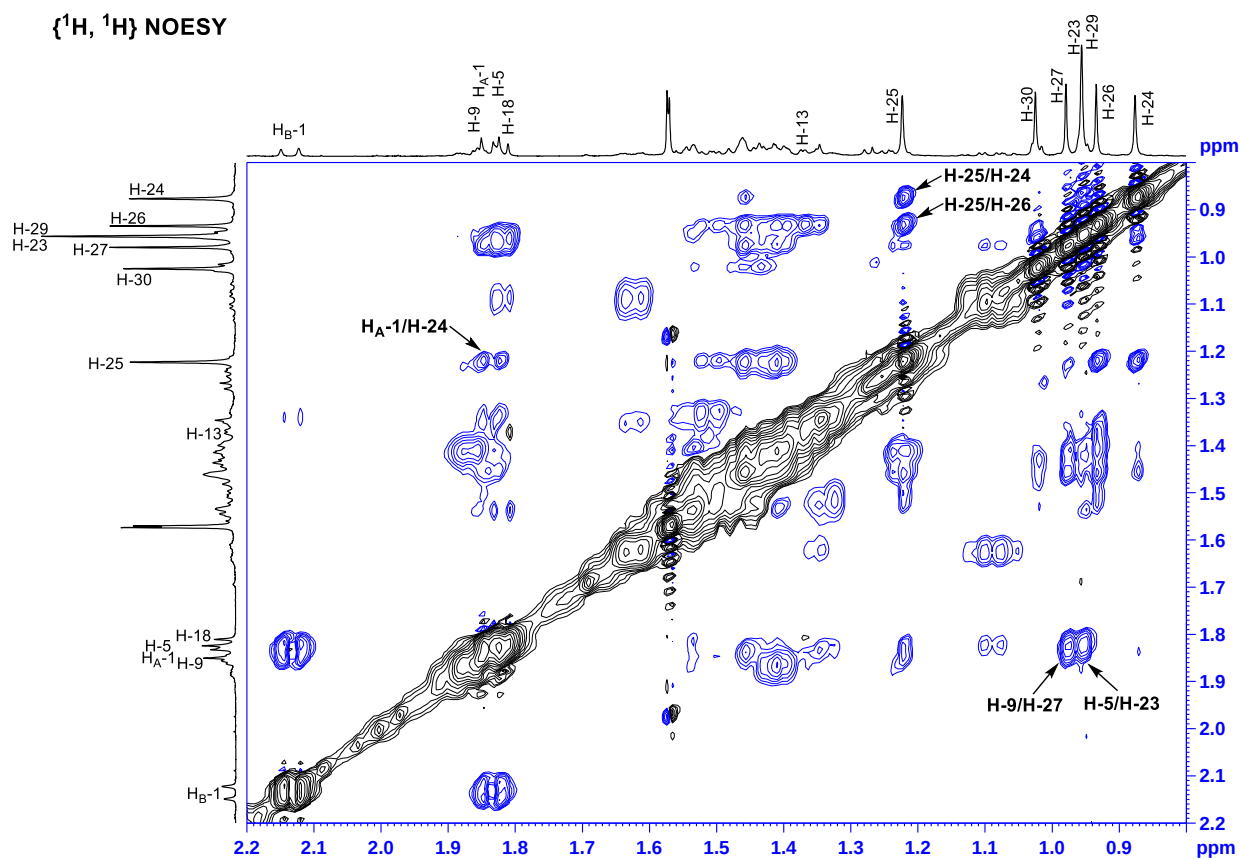


Figure S109. Upfield area of $\{^1\text{H}, ^1\text{H}\}$ NOESY NMR spectrum of compound **12** in CDCl₃.

3. X-Ray Crystal data for compound 11

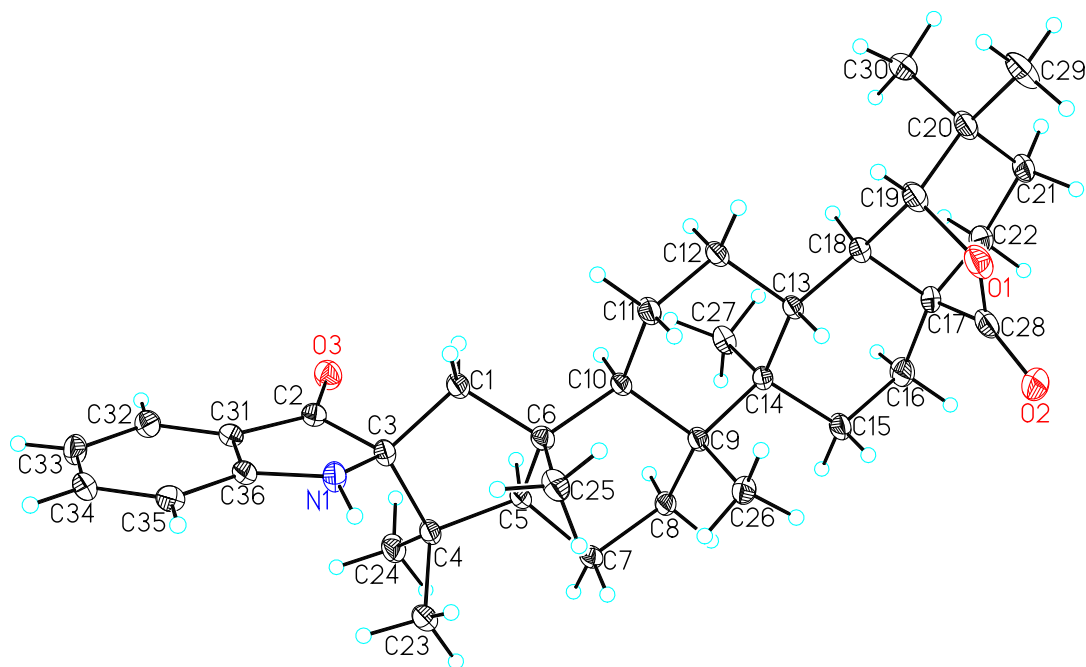


Table 1. Crystal data and structure refinement for F103 (compound 11).

Identification code	f103	
Empirical formula	C ₃₆ H ₄₉ N O ₃	
Formula weight	543.76	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	P 21 21 21	
Unit cell dimensions	a = 7.3603(7) Å	α = 90°.
	b = 16.4621(16) Å	β = 90°.
	c = 24.344(2) Å	γ = 90°.
Volume	2949.6(5) Å ³	

Z	4
Density (calculated)	1.224 Mg/m ³
Absorption coefficient	0.076 mm ⁻¹
F(000)	1184
Crystal size	0.19 x 0.08 x 0.03 mm ³
Theta range for data collection	1.49 to 31.00°.
Index ranges	-10<=h<=10, -23<=k<=23, -35<=l<=35
Reflections collected	39595
Independent reflections	5247 [R(int) = 0.0878]
Completeness to theta = 31.00°	99.8 %
Absorption correction	None
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	5247 / 0 / 368
Goodness-of-fit on F ²	1.049
Final R indices [for 4156 rfln with I>2sigma(I)]	R1 = 0.0443, wR2 = 0.0947
R indices (all data)	R1 = 0.0664, wR2 = 0.1043
Largest diff. peak and hole	0.322 and -0.251 e.Å ⁻³

Table 2. Atomic coordinates (x 10⁴) and equivalent isotropic displacement parameters (Å²x 10³) for F103. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
O(1)	8075(2)	9545(1)	1036(1)	26(1)
O(2)	11087(2)	9714(1)	1037(1)	40(1)
O(3)	3315(2)	15519(1)	1825(1)	22(1)

N(1)	3937(2)	15444(1)	396(1)	18(1)
C(1)	4314(3)	14227(1)	1014(1)	18(1)
C(2)	3459(3)	15661(1)	1333(1)	17(1)
C(3)	4621(3)	15153(1)	929(1)	17(1)
C(4)	6770(3)	15303(1)	1025(1)	17(1)
C(5)	7392(2)	14445(1)	1199(1)	14(1)
C(6)	6171(3)	13828(1)	904(1)	15(1)
C(7)	9394(3)	14217(1)	1181(1)	16(1)
C(8)	9617(3)	13397(1)	1476(1)	17(1)
C(9)	8435(3)	12702(1)	1241(1)	14(1)
C(10)	6408(2)	12998(1)	1201(1)	14(1)
C(11)	5137(3)	12328(1)	995(1)	19(1)
C(12)	5246(3)	11568(1)	1356(1)	20(1)
C(13)	7207(3)	11260(1)	1402(1)	15(1)
C(14)	8498(3)	11927(1)	1633(1)	15(1)
C(15)	10448(3)	11568(1)	1653(1)	21(1)
C(16)	10584(3)	10803(1)	2010(1)	24(1)
C(17)	9234(3)	10158(1)	1831(1)	20(1)
C(18)	7286(3)	10462(1)	1735(1)	16(1)
C(19)	6564(3)	9732(1)	1416(1)	21(1)
C(20)	6207(3)	8980(1)	1780(1)	20(1)
C(21)	8025(3)	8730(1)	2045(1)	23(1)
C(22)	9171(3)	9450(1)	2249(1)	23(1)
C(23)	7730(3)	15628(1)	512(1)	22(1)
C(24)	7185(3)	15906(1)	1494(1)	23(1)

C(25)	6459(3)	13777(1)	276(1)	21(1)
C(26)	9221(3)	12483(1)	673(1)	19(1)
C(27)	7966(3)	12144(1)	2227(1)	20(1)
C(28)	9656(3)	9799(1)	1270(1)	26(1)
C(29)	5474(4)	8282(1)	1430(1)	31(1)
C(30)	4772(3)	9189(1)	2210(1)	24(1)
C(31)	2569(3)	16293(1)	1016(1)	16(1)
C(32)	1515(3)	16963(1)	1177(1)	20(1)
C(33)	814(3)	17461(1)	775(1)	22(1)
C(34)	1131(3)	17282(1)	218(1)	21(1)
C(35)	2154(3)	16624(1)	54(1)	19(1)
C(36)	2904(3)	16132(1)	462(1)	17(1)