

Supporting Information

Hybrid Isoprenoids from a Reeds Rhizosphere Soil

Derived Actinomycete *Streptomyces* sp. CHQ-64

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Experimental details

General Experimental Procedures. Specific rotations were obtained on a JASCO P-1020 digital polarimeter. UV spectra were recorded on Beckman DU 640 spectrophotometer. CD spectra were measured on JASCO J-715 spectropolarimeter. IR spectra were taken on a Nicolet Nexus 470 spectrophotometer in KBr discs. NMR spectra were recorded on a JEOL JNM-ECP 600 spectrometer using TMS as internal standard, and chemical shifts were recorded as δ values. ESIMS utilized on a Waters Q-TOF Ultima Global mass spectrometer and a Thermo Scientific LTQ Orbitrap XL mass spectrometer. Semipreparative HPLC was performed using an ODS column [HPLC (YMC-Pack ODS-A, 10 \times 250 mm, 5 μ m, 4 mL/min)]. TLC and column chromatography (CC) were performed on plates precoated with silica gel GF254 (10–40 μ m) and over silica gel (200–300 mesh, Qingdao Marine Chemical Factory), and Sephadex LH-20 (Amersham Biosciences), respectively. Vacuum-liquid chromatography (VLC) was carried out over silica gel H (Qingdao Marine Chemical Factory). Marimum salt used is made from the evaporation of sea water collected in Laizhou Bay (Weifang Haisheng Chemical Factory).

Actinomycete Material. The actinomycete Chq64, was isolated from reeds rhizosphere soil collected from the mangrove conservation area of Guangdong province, China, July 2008. NCBI BLAST analysis of the partial 16S rDNA sequence of Chq-64 indicates that this strain is affiliated with the genus *Streptomyces* (GenBank accession No. JQ405211). The voucher specimen is deposited in our laboratory at -80°C . The producing strain was prepared on ISP-2 agar slants at 3.3% salt concentration and stored at 4°C .

Fermentation and Extraction. The bacterium (strain Chq-64) was incubated on a rotatory shaker at 147 rpm and 28°C for 7 days in four hundreds of 500 mL Erlenmeyer

flasks each containing 150 mL of liquid medium composed of soluble starch 1%, yeast extract 1%, KH_2PO_4 0.05%, corn syrup 0.3%, glucose 2%, $\text{MgSO}_4 \cdot 7\text{H}_2\text{O}$ 0.05%, beef extract 0.3%, CaCO_3 0.2% and sea-water then adjusting its pH to 7.0. After 7 days of cultivation, 60 L of whole broth was extracted with EtOAc (50 L \times 3). The EtOAc extract was concentrated under reduced pressure to give a dark brown gum (35.5 g).

Purification. The crude extract (35.5 g) was subjected by vacuum liquid chromatography over a silica gel (200–300 mesh) column using stepwise gradient elution with the mixtures of petroleum ether- CHCl_3 -MeOH to give eight fractions. Fraction 1 was rechromatographed on a silica gel column, eluted with petroleum ether/acetone, to provide fourteen subfractions (fractions 1.1-1.14). Fraction 1.13 was further purified on Sephadex LH-20 and semipreparative HPLC (85% MeOH/ H_2O , 4.0 mL/min) to give compound **1** (10 mg, $t_R = 27.8$ min). Fraction 1.12 was purified by repeated ODS CC to afford eight subfractions (fractions 1.12.1-1.12.8). Compound **2** (17 mg, $t_R = 27.8$ min) and Compound **3** (20 mg, $t_R = 20.3$ min) was obtained from fraction 1.12.7 by semipreparative HPLC (85% MeOH/ H_2O , 4.0 mL/min).

Indotertine A (1): Indotertine A (**1**): colorless, amorphous solid; $[\alpha]_D^{20} +21.8$ (c 0.15, MeOH); ECD (MeOH) λ [nm] ($\Delta\epsilon$): 292 (+0.7), 274 (+0.6), 243 (+5.6), 224 (+0.1), 213(+4.4), 198(-8.5); IR (KBr) ν_{max} : 3423, 2925, 1668, 1607, 1461, 1403, 1300 cm^{-1} ; UV (MeOH) λ_{max} (log ϵ): 208 (1.41), 202 (1.11); ^1H and ^{13}C NMR data, see Table S3; HRESIMS m/z : 504.3583 $[\text{M} + \text{H}]^+$ (calcd for $\text{C}_{32}\text{H}_{46}\text{N}_3\text{O}_2$, 504.3585)

Drimentine F (2): colorless, amorphous solid; $[\alpha]_D^{20} -135.2$ (c 0.10, MeOH); ECD (MeOH) λ [nm]($\Delta\epsilon$): 332 (-0.4), 297 (-2.2), 269 (-1.1), 241 (-5.3), 220 (-0.9), 206 (-27.4); IR (KBr) ν_{max} 3367, 2925, 1670, 1606, 1487, 1454, 1303 cm^{-1} ; UV (MeOH) λ_{max} (log ϵ)

209 (1.68), 243 (1.27); ^1H and ^{13}C NMR data, see Table S3. HRESIMS m/z 504.3590 [$\text{M} + \text{H}$] $^+$ (calcd for $\text{C}_{32}\text{H}_{46}\text{N}_3\text{O}_2$, 504.3585).

Drimentine G (3): colorless, amorphous solid; $[\alpha]_{\text{D}}^{20}$ -86.1 (c 0.10, MeOH); ECD (MeOH) $\lambda[\text{nm}](\Delta\epsilon)$: 325 (+0.6), 299 (-1.0), 270 (+0.5), 245 (-4.0), 220 (+2.6), 196 (-19.8); IR (KBr) ν_{max} 3448, 1668, 1460, 1112, cm^{-1} ; UV (MeOH) λ_{max} ($\log \epsilon$) 209 (1.69), 243 (1.25); ^1H and ^{13}C NMR data, see Table S3 HRESIMS m/z 490.3446 [$\text{M} + \text{H}$] $^+$ (calcd for $\text{C}_{31}\text{H}_{44}\text{N}_3\text{O}_2$, 490.3434).

X-ray crystal data for 2 (Cu $K\alpha$ radiation): Colorless crystals of **2** were obtained in the solvent of methanol. Crystallographic data (excluding structure factors) for **2** (Cu $K\alpha$ radiation), has been deposited with the Cambridge Crystallographic Data Center as supplementary publication numbers CCDC 878440. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.

Crystal data for 2 (Cu $K\alpha$ radiation): monoclinic, $\text{C}_{32}\text{H}_{45}\text{O}_2\text{N}_3$, space group P2_1 with $a = 10.22590(10)$ Å, $b = 7.33470(10)$ Å, $c = 19.3434(3)$ Å, $V = 1419.94(3)$ Å 3 , $Z = 2$, $D_{\text{calcd}} = 1.178$ mg/m 3 , $\mu = 0.568$ mm $^{-1}$, and $F(000) = 548$. Crystal size: $0.36 \times 0.24 \times 0.24$ mm 3 . Independent reflections: 4628 with $R_{\text{int}} = 0.0200$. The final agreement factors are $R_1 = 0.0308$ and $wR_2 = 0.0820$ [$I > 2\sigma(I)$].

Cytotoxic assays. Cytotoxicity was assayed by the MTT method. In the assay, HCT-8, Bel-7402, BGC-823, A549 and A2780 cell lines were grown in RPMI-1640 supplemented with 10% FBS under a humidified atmosphere of 5% CO_2 and 95% air at 37 °C. Cell suspensions, 200 μL , at a density of 5×10^4 cell mL $^{-1}$ were plated in 96-well microtiter plates and incubated for 24 h. The test compounds were prepared at different

concentrations with each drug 4-5 dose groups and at least 3 parallel hole. Then, 2 μ L of the test solutions (in MeOH) were added to each well and further incubated for 72 h. The MTT solution (20 μ L, 5 mg/mL in IPMI-1640 medium) was then added to each well and incubated for 4 h. Old medium containing MTT (150 μ L) was then gently replaced by DMSO and pipetted to dissolve any formazan crystals formed. Absorbance was then determined on a Spectra Max Plus plate reader at 540 nm. Taxol was used as the positive control. Three times were repeated.

Table S1. Cytotoxicity of compounds **1-3** for five human tumor cell lines

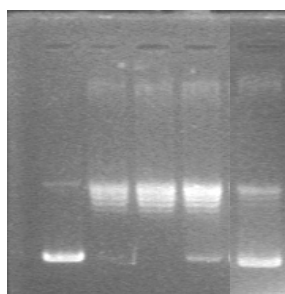
Compound	IC ₅₀ (μ M)				
	HCT-8	Bel-7402	BGC-823	A549	A2780
1	>10	>10	>10	>10	>10
2	>10	>10	>10	>10	>10
3	2.81 \pm 0.09	1.38 \pm 0.27	>10	1.01 \pm 0.04	2.54 \pm 0.18
Taxol	0.051	0.006	< 0.001	0.016	< 0.001

Topoisomerase I mediated DNA cleavage assay. Topoisomerases I were assayed by relaxation of supercoiled plasmid DNA. Relaxation of 250 ng of supercoiled by topoisomerase I (2 U) was performed in 20 μ L of topoisomerase I relaxation buffer [10mM Tris-HCl, pH 7.9, 1 mM EDTA, 150 mM NaCl, 0.1% (w/v) BSA, 0.1 mM spermidine, 5% (v/v) glycerol] in the presence and absence of varying amounts of the test compounds, dissolved in dimethyl sulfoxide (5% (v/v) final concentration). Reactions were started by addition of DNA. Control groups were either DNA alone or DNA treated with topoisomerase. After 30 min at 37°C, the reaction was terminated by addition of 1% (w/v) SDS and digested with 50 mg/mL proteinase K at 55°C for 30 min. DNA was extracted with an equal volume of chloroform/isoamyl alcohol (24:1) and separated on 1% (w/v) agarose gel in Tris-acetate-EDTA (TAE) buffer (40 mM Tris-acetate, pH 8.0,

and 2 mM EDTA) at 2 V/cm for 3.5 h. Gels were stained with 5 mg/mL ethidium bromide, destained, and photographed using Polaroid 665 film or a gel-imaging system for numerical quantification by densitometry scanning (Herolab, Wiesloch, Germany).

The effect of **3** on topoisomerases was investigated using a conventional plasmid DNA relaxation assay. HCPT, a well-known Topo I inhibitor, was employed as a positive control. Compound **3** was found slightly inhibited the DNA relaxation activity of Topo I at the concentration of 100 μ M.

Figure S1. Effect of compound **3** on Topo I-mediated supercoiled pBR322 relaxation



Topo I	-	+	+	+	+
pBR322	+	+	+	+	+
DMSO	-	-	+	+	+
3 (100 μ M)	-	-	-	+	-
HCPT (10 μ M)	-	-	-	-	+

The ATPase activity of H_{Sp}90 assay. Histidine-tagged yeast H_{Sp}90 was transformed into *E. coli* and purified (190%) by metal affinity, gel filtration, and ion-exchange chromatography. The assay buffer was 100 mM Tris-HCl, 20 mM KCl, 6 mM MgCl₂, pH 7.4. 5 μ L of each compound solution was added to each well (equivalent to a final concentration of 10 μ M) of 96-well assay plate. A 10 μ L aliquot of ATP solution was added to each well to give a final assay concentration of 5 μ mol/L. Just before use, H_{Sp}90 protein was thawed on ice and suspended in chilled assay buffer to a stock concentration of 0.22 μ mol/L, and the solution was kept on ice. The incubation was started by adding 10 μ L of the stock H_{Sp}90 to each well. The plates were shaken approximately 2 min and

incubated for 3 h at 37 °C. To stop the incubation, 80 μ L of the malachite green reagent (the malachite green reagent was prepared and contained malachite green (0.0812%, w/v), polyvinyl alcohol (2.32%, w/v; dissolves with difficulty and requires heating), ammonium molybdate (5.72%, w/v, in 6 M HCl), and AR water, mixed in the ratio 2:1:1:2) was added to each well and the plate shaken again. Following the addition of 10 μ L of 34% sodium citrate to each well, the plate was shaken once more and left to stand at room temperature for about 15 min, and the absorbance at 620 nm was measured.

It is now clear that H_{Sp}90 has intrinsic ATPase activity and that ATP binding and hydrolysis is essential for the activity of H_{Sp}90. Inhibition of the ATPase activity of H_{Sp}90 leads to antitumor activity in vitro and in vivo. The positive control of geldanamycin at 10 μ M produced 72.25% inhibition of the H_{Sp}90 ATPase activity, but the activity of compound **3** wasn't found markedly at 10 μ M.

Table S2. The inhibitory rate of compound **3** on Hsp90 ATPase (%)

compound	Inhibition rate (%)
3 (10 μ M)	19.51
17AAG (10 μ M)	72.25

Computational section

Mixed torsional/low mode conformational searches were carried out by means of the Macromodel 9.7.211¹ software using Merck Molecular Force Field (MMFF) with implicit solvent model for chloroform. Geometry reoptimizations [B3LYP/6-31G(d) level of theory] and TDDFT calculations were performed with Gaussian 09² using various functionals (B3LYP, BH&HLYP, PBE0) and TZVP basis set. ECD spectra were generated

as the sum of Gaussians³ with 3600 cm⁻¹ half-height width (corresponding to ca. 23 nm at 250 nm), using dipole-velocity computed rotational strengths. Boltzmann distributions were estimated from the ZPVE corrected B3LYP/6-31G(d) energies. The MOLEKEL⁴ software package was used for visualization of the results.

Table S3. Cartesian coordinates of compound **1** for the lowest energy reoptimized MMFF conformers calculated at B3LYP/6-31G(d) level of theory in vacuo.

Compound 1 Conformer A		Standard Orientation (Ångstroms)		
I	Atom	X	Y	Z
1	C	0.711113	2.705028	-0.67636
2	C	0.803969	4.094834	-0.65132
3	C	0.434503	4.758611	0.524343
4	C	-0.00662	4.050127	1.644269
5	C	-0.0887	2.651004	1.604536
6	C	0.2624	1.981318	0.438556
7	C	0.313131	0.491645	0.121438
8	C	0.394443	0.520851	-1.43955
9	N	1.077379	1.824812	-1.72007
10	C	-0.9211	-0.3092	0.588497
11	C	-2.27176	0.125256	-0.01016
12	C	-2.14548	0.427155	-1.4922
13	C	-0.95891	0.514855	-2.10654
14	C	-3.43507	-0.90691	0.285993
15	C	-4.74813	-0.31454	-0.34538
16	C	-4.59395	-0.20507	-1.87321
17	C	-3.42863	0.727011	-2.23485
18	C	-3.61816	-1.01989	1.819373
19	C	-4.89665	-1.75829	2.229213
20	C	-6.13112	-1.05545	1.660135
21	C	-6.1232	-0.92838	0.116482
22	C	-7.25486	0.054251	-0.26703
23	C	-6.4756	-2.29165	-0.52053
24	C	1.552003	-0.19212	0.783662
25	C	2.935022	0.490368	0.672965
26	C	3.884034	-0.12759	1.70355
27	N	5.074813	-0.63581	1.274362
28	C	5.454444	-0.85851	-0.12808
29	C	4.631403	-0.03743	-1.12203
30	N	3.479607	0.515196	-0.67667
31	O	3.567168	-0.10255	2.891279
32	O	5.017021	0.086804	-2.28258
33	C	5.473663	-2.37858	-0.49386
34	C	4.068578	-2.99146	-0.55208
35	C	6.26358	-2.65304	-1.78185
36	C	6.003473	-1.10471	2.301456
37	C	-3.05936	-2.28955	-0.30281
38	H	1.02706	-0.28883	-1.82262
39	H	2.819038	1.52826	1.012236
40	H	-4.78904	0.720677	0.03423
41	H	-2.57482	1.06296	0.48363
42	H	1.150773	4.650336	-1.51889
43	H	0.493492	5.843222	0.561725
44	H	-0.28617	4.583117	2.548369
45	H	-0.42865	2.100613	2.478642
46	H	0.9126	2.181228	-2.65799
47	H	-0.73308	-1.35981	0.33928
48	H	-0.96875	-0.25993	1.681707

49	H	-0.93826	0.717566	-3.17984
50	H	-5.50966	0.186072	-2.32934
51	H	-4.42821	-1.19446	-2.31454
52	H	-3.72867	1.75483	-1.97266
53	H	-3.24841	0.727428	-3.31684
54	H	-2.74734	-1.51557	2.264769
55	H	-3.65292	-0.00635	2.248296
56	H	-4.96368	-1.79544	3.324149
57	H	-4.85695	-2.80274	1.89343
58	H	-6.18435	-0.04629	2.096046
59	H	-7.04863	-1.57261	1.973056
60	H	-7.41204	0.109406	-1.34975
61	H	-8.20221	-0.26971	0.181108
62	H	-7.04569	1.067994	0.096223
63	H	-6.37143	-2.27175	-1.61059
64	H	-5.86654	-3.11638	-0.14114
65	H	-7.52075	-2.54018	-0.29802
66	H	1.352383	-0.26909	1.857749
67	H	1.631179	-1.21542	0.393697
68	H	6.481922	-0.48928	-0.24248
69	H	2.957971	1.079243	-1.35133
70	H	6.014333	-2.86623	0.328953
71	H	4.132522	-4.07381	-0.71076
72	H	3.51395	-2.82771	0.378953
73	H	3.485813	-2.5701	-1.3798
74	H	6.333302	-3.73366	-1.954
75	H	7.283872	-2.25711	-1.71414
76	H	5.78705	-2.18624	-2.64681
77	H	5.820814	-2.14997	2.57922
78	H	7.026756	-1.01236	1.924861
79	H	5.877862	-0.49148	3.194182
80	H	-2.30479	-2.78645	0.316038
81	H	-3.91405	-2.96446	-0.35955
82	H	-2.64454	-2.20275	-1.31236

B3LYP Energy = -1561.24793532 a.u.; E+ZPVE = -1560.518878 a.u.

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Table S4. ¹H and ¹³C NMR Data for Compounds **1-3** (600, 150 MHz, DMSO-*d*6, TMS, δppm)

<i>position</i>	1		<i>position</i>	2		3	
	δ _C	δ _H (<i>J</i> in Hz)		δ _C	δ _H (<i>J</i> in Hz)	δ _C	δ _H (<i>J</i> in Hz)
1			1	166.2 s		170.0, qC	
2	63.3, CH	3.88, d (1.6)	2				6.20, brs
3	46.9, qC		3	67.7 d	3.82, brs	60.5, CH	3.86, brs
4	131.2, qC		4	163.8 s		165.8, qC	
5	123.3, CH	7.02, d (7.1)	5				
6	121.3, CH	6.87, ddd (7.7, 7.1, 1.1)	5a	78.5 d	5.59, s	78.9, CH	5.43, s
7	128.2, CH	7.05, ddd (7.1, 7.7, 1.1)	6	NH	4.82, s		5.06, brs
8	112.3, CH	6.68, d (7.7)	6a	149.3 s		149.0, qC	
9	149.2, qC		7	108.8 d	6.56, d (7.7)	109.4, CH	6.59, d (7.7)
10	121.6, CH	5.06, d (2.2)	8	128.8 d	7.05, dd (7.7,7.1)	128.8, CH	7.07, dd (7.2,7.7)
11	141.3, qC		9	119.3 d	6.76, dd (7.1, 7.7)	119.4, CH	6.77, dd (7.7, 7.2)
12	34.4, CH ₂	2.21, m 1.89, m	10	123.8 d	7.08, d (7.7)	123.4, CH	7.08, d (7.2)
13	21.7, CH ₂	1.46, m 1.25, m	10a	131.8, qC		132.0, qC	
14	53.6, CH	0.93, dd (2.2,12.6)	10b	56.3, qC		55.6, qC	
15	33.4, qC		11	41.6, CH ₂	2.51, dd (5.0,12.7) 2.11, dd (12.1,12.7)	39.0, CH ₂	2.55, dd (5.8,12.5), 2.13, dd (12.1,12.5)
16	41.9, CH ₂	1.40, brd (13.2) 1.14, m	11a	58.3, CH	3.94, dd (4.9,12.1)	58.8, CH	3.90, dd (5.8,11.2)
17	19.0, CH ₂	1.46, m	12	30.4, CH ₂	1.91, d (6.1)	29.9, CH ₂	1.89, d (6.6)
18	39.7, CH ₂	1.76, brd (12.1) 1.03, m	13	52.6, CH	1.46, m	52.4, CH	1.52, m
19	37.4, qC		14	149.6, qC		149.6, qC	
20	47.6, CH	1.70, m	15	39.1, CH ₂	2.40, m 1.87, dt (4.4,12.7)	38.9, CH ₂	2.40, m 1.96, dt (4.9,12.7)
21	30.4, CH ₂	a: 2.13, dd (5.0,13.8) b: 1.53, m	16	24.5, CH ₂	1.70, m, 1.28, m	24.4, CH ₂	1.72, m 1.29, m
22	50.5, CH ₂	a: 2.33, dd (1.7,13.7) b: 1.89, m	16a	55.9, CH	0.95, dd (2.2,12.7)	55.6, CH	1.00, dd (2.2,12.7)
23	53.8, CH	3.22, d (11.6)	17	33.7, qC		33.7, qC	
24	167.3, qC		18	42.0, CH ₂	1.32, m 1.12, m	42.0, CH ₂	1.34, brd (13.1) 1.12, m
26	67.7, CH	3.66, d (4.4)	19	19.3, CH ₂	1.50, m 1.40, m	19.3, CH ₂	1.46, m
27	165.8, qC		20	38.4, CH ₂	1.69, m 0.81, m	38.4, CH ₂	1.69, m , 0.81, m
28		8.59, d (2.2)	20a	40.2, qC		40.2, qC	
29	15.2, CH ₃	0.78, s	21	107.7, CH ₂	4.91, s 4.74, s	107.3, CH ₂	4.87, s 4.70, s
30	33.7, CH ₃	0.82, s	22	33.7, CH ₃	0.83, s	33.6, CH ₃	0.84, s
31	22.2, CH ₃	0.84, s	23	21.8, CH ₃	0.76, s	21.8, CH ₃	0.76, s
32	31.6, CH	2.31, m	24	14.6, CH ₃	0.60, s	14.6, CH ₃	0.60, s
33	18.6, CH ₃	1.04, d (7.1)	25	31.3, CH	2.34, m	28.7, CH	2.59, m
34	19.7, CH ₃	1.16, d (6.6)	26	19.6, CH ₃	1.22, d (6.1)	19.1, CH ₃	1.05, d (7.1)
35	34.8, CH ₃	2.90, s	27	16.7, CH ₃	0.93, d (6.1)	16.1, CH ₃	0.94, d (7.1)
			28- NMe	33.7, CH ₃	2.91, s		

Figure S2. CD curves of compounds **2** and **3**.

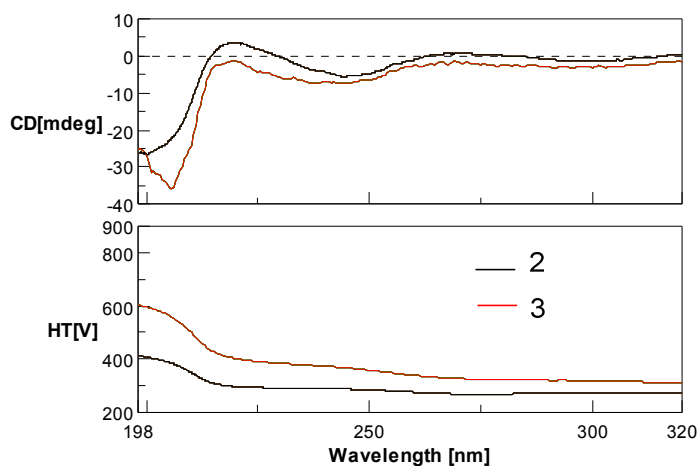
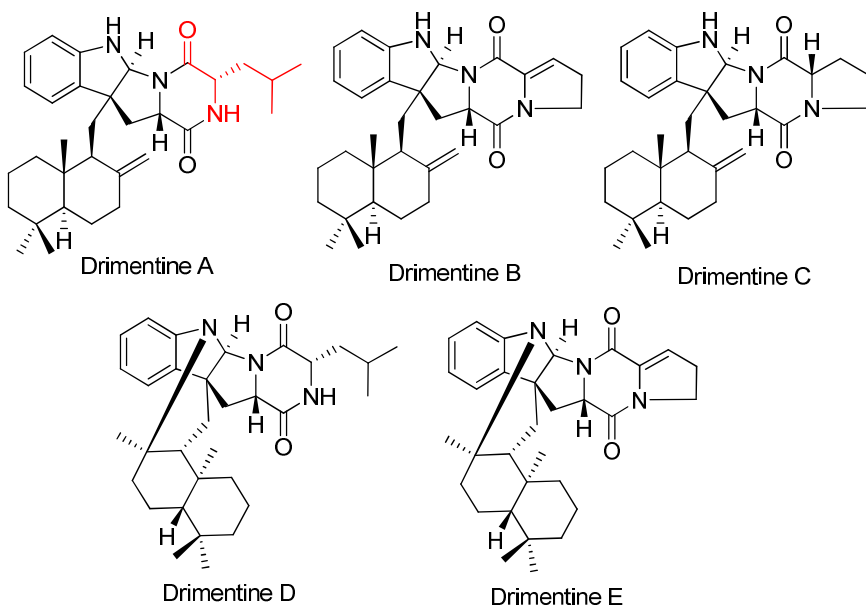


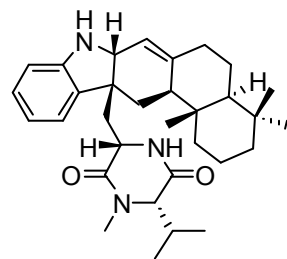
Figure S3. Structures of drimentines A-E in ref 12 .



The planar structure elucidation of compound 1: Compound **1** was obtained as a colorless amorphous powder. Analysis of the COSY correlations established the connectivities of H-5/H-6/H-7/H-8, H-2/H-10, H-20/H-21, H-12/H-13/H-14, H-16/H-17/H-18, H-22/H-23/NH-28, and H-26/H-32/H-33(H-34), as seven fragments. The 2,3-disubstituted indol ring was established by the HMBC correlations from H-7 (δ_H

7.02) to C-9 (δ_C 149.2), from H-8 (δ_H 6.68) to C-4 (δ_C 131.2), from H-5 (δ_H 7.02) to C-3 (δ_C 46.9) and from H-2 (δ_H 3.88) to C-9 and C-4. The drimane-sesquiterpene fragment was assigned on the basis of HMBC correlations from the geminal dimethyls H₃-30 (δ_H 0.82, s) and H₃-31 (δ_H 0.84, s) to C-14 (δ_C 53.6), C-15 (δ_C 33.4), and C-16 (δ_C 41.9), together with the correlations from H₃-29 (δ_H 0.78, s) to C-14, C-19 (δ_C 37.4) and C-20 (δ_C 47.6), from H-18 (δ_H 1.76, 1.03) to C-14, from H-17 (δ_H 1.46) to C-19, from H-20 (δ_H 1.70) to C-10 (δ_C 121.6) and C-11 (δ_C 141.3). The hydrogenated naphtho[2,1-b]carbazole moiety was deduced by the analysis of the COSY correlations (H-2/H-10) and HMBC correlations from H-21 (δ_H 2.13, 1.53) to C-2 (δ_C 63.3). The diketopiperazine unit was established by HMBC correlations from NH-28 (δ_H 8.59) to C-26 (δ_C 67.8) and C-27 (δ_C 165.8), from the methyl hydrogens at H₃-35 (δ_H 3.88) to C-24 (δ_C 167.3) and C-26 and from H-23 (δ_H 3.22) to C-24. Thus, the planar structure of compound **1** could be established by the HMBC correlations from H-22 (δ_H 2.33, 1.89) to C-2, C-3, C-4, C-21 (δ_C 30.4), and C-24.

Figure S4. ^1H NMR Spectrum (600 MHz) of indotertine A (**1**) in CDCl_3 .



Indotertine A (**1**)

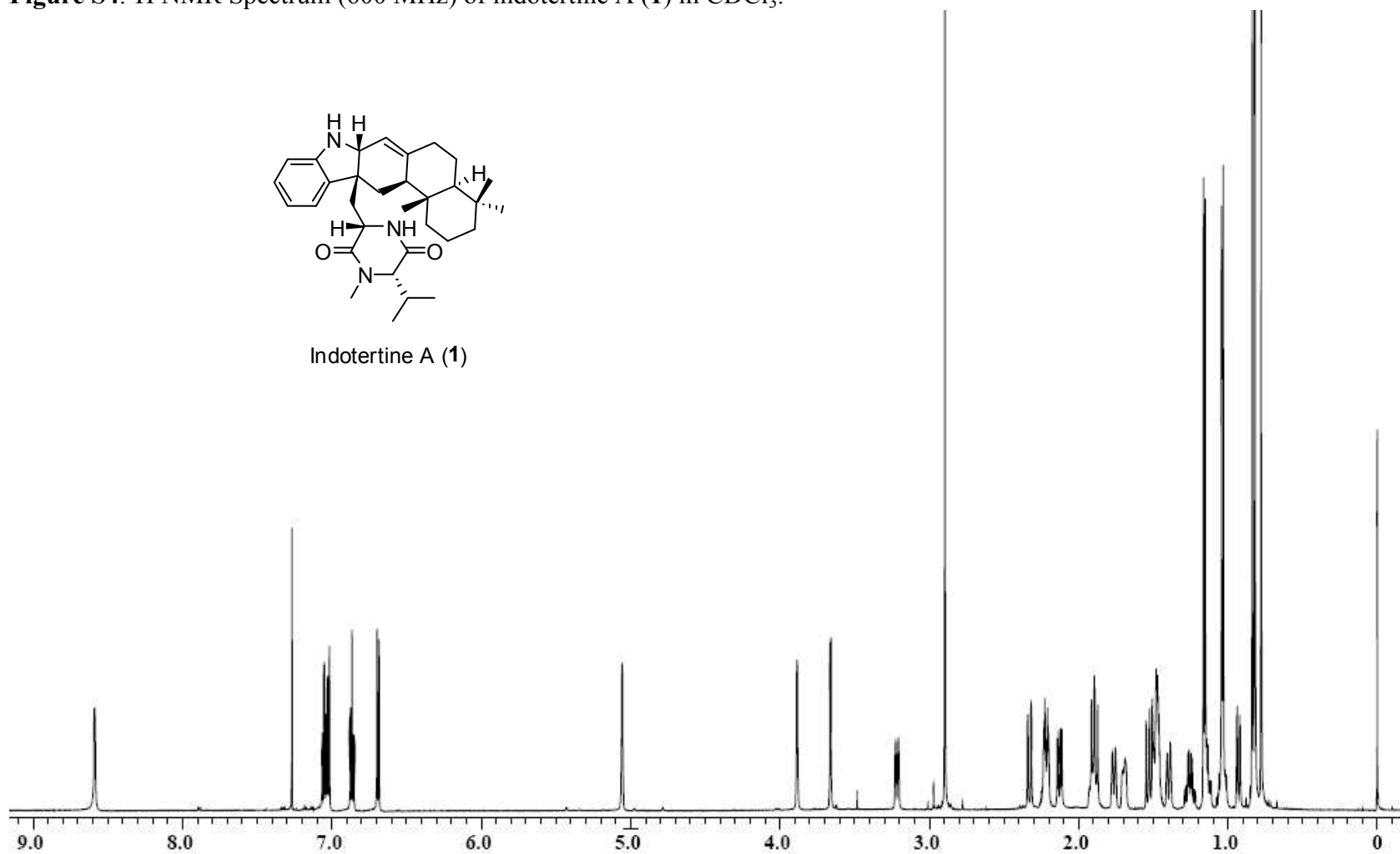


Figure S5. ^{13}C NMR Spectrum (150 MHz) of indotertine A (**1**) in CDCl_3 .

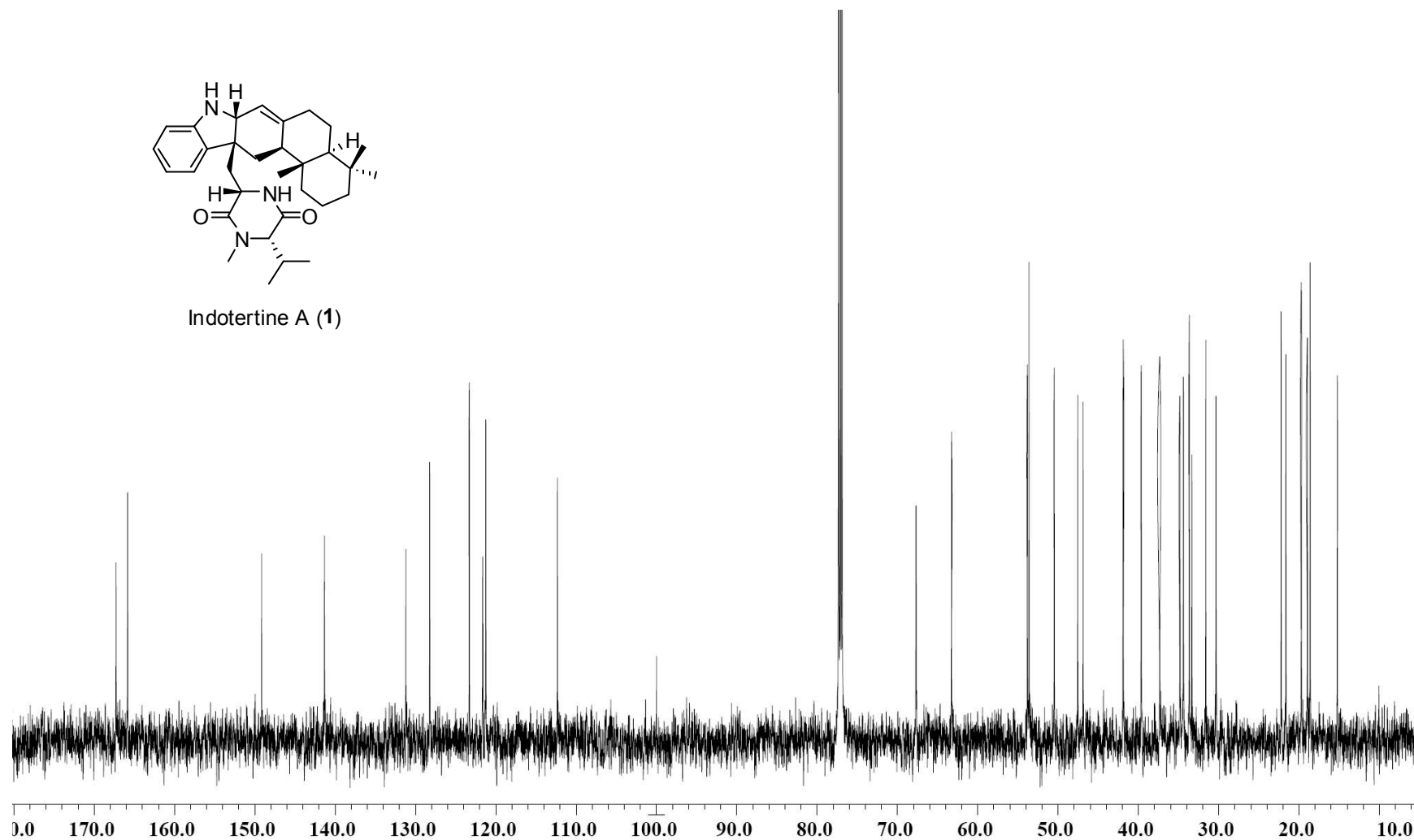


Figure S6. DEPT Spectrum (150 MHz) of indotertine A (**1**) in CDCl₃.

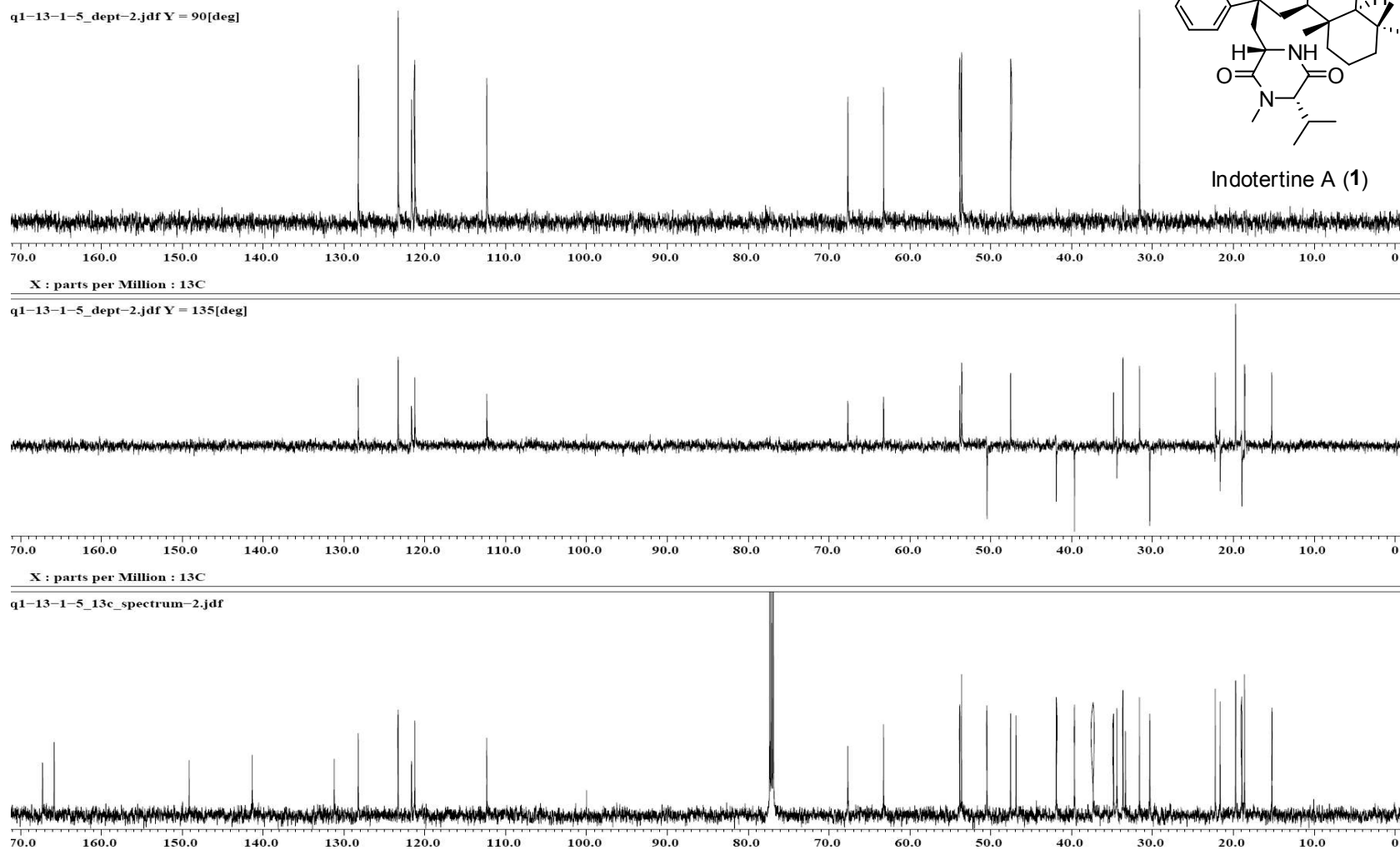


Figure S7. HMQC Spectrum of indotertine A (**1**) in CDCl₃.

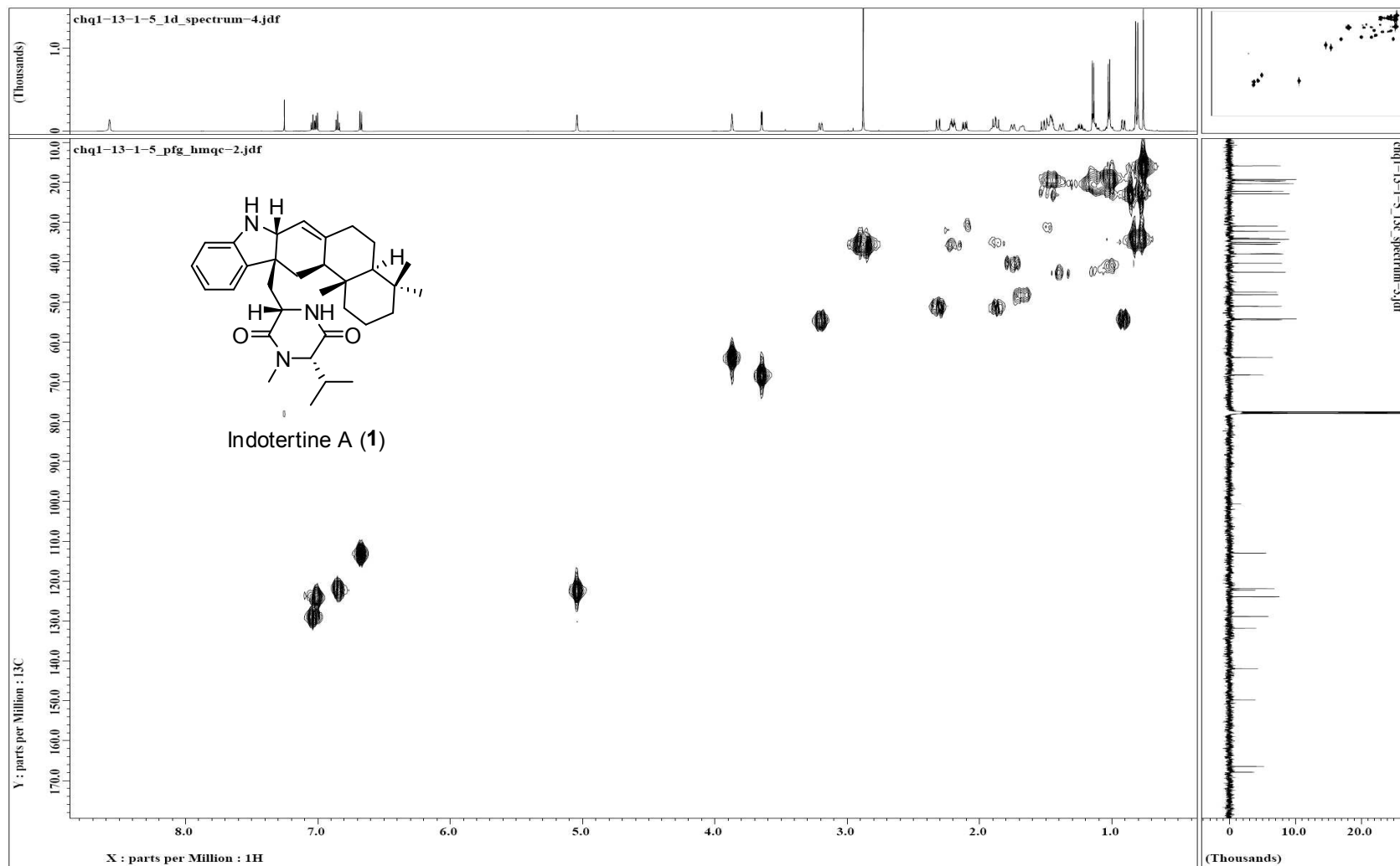


Figure S8. ^1H - ^1H COSY Spectrum of indotertine A (**1**) in CDCl_3 .

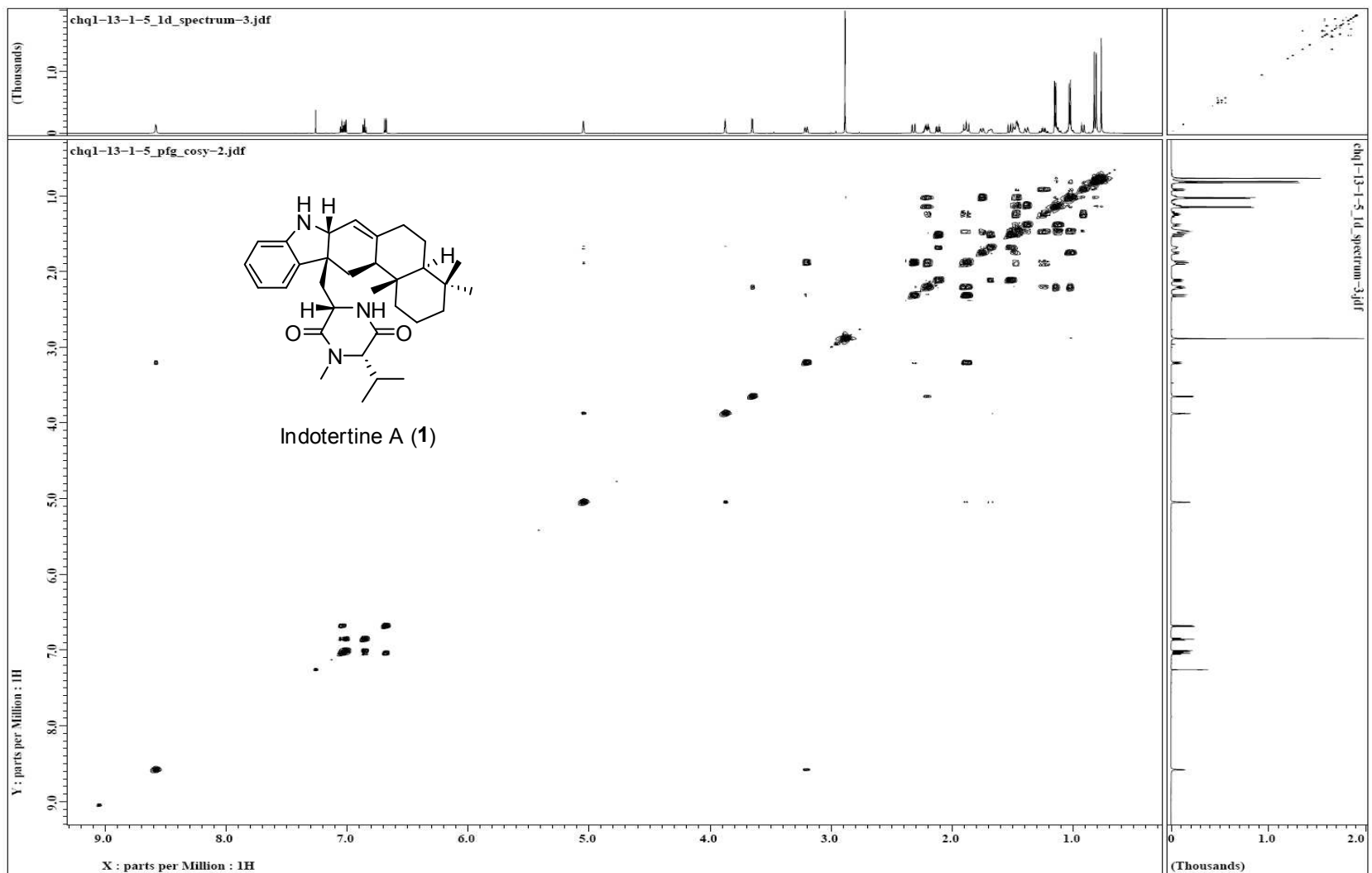


Figure S9. HMBC Spectrum of indotertine A (**1**) in CDCl₃.

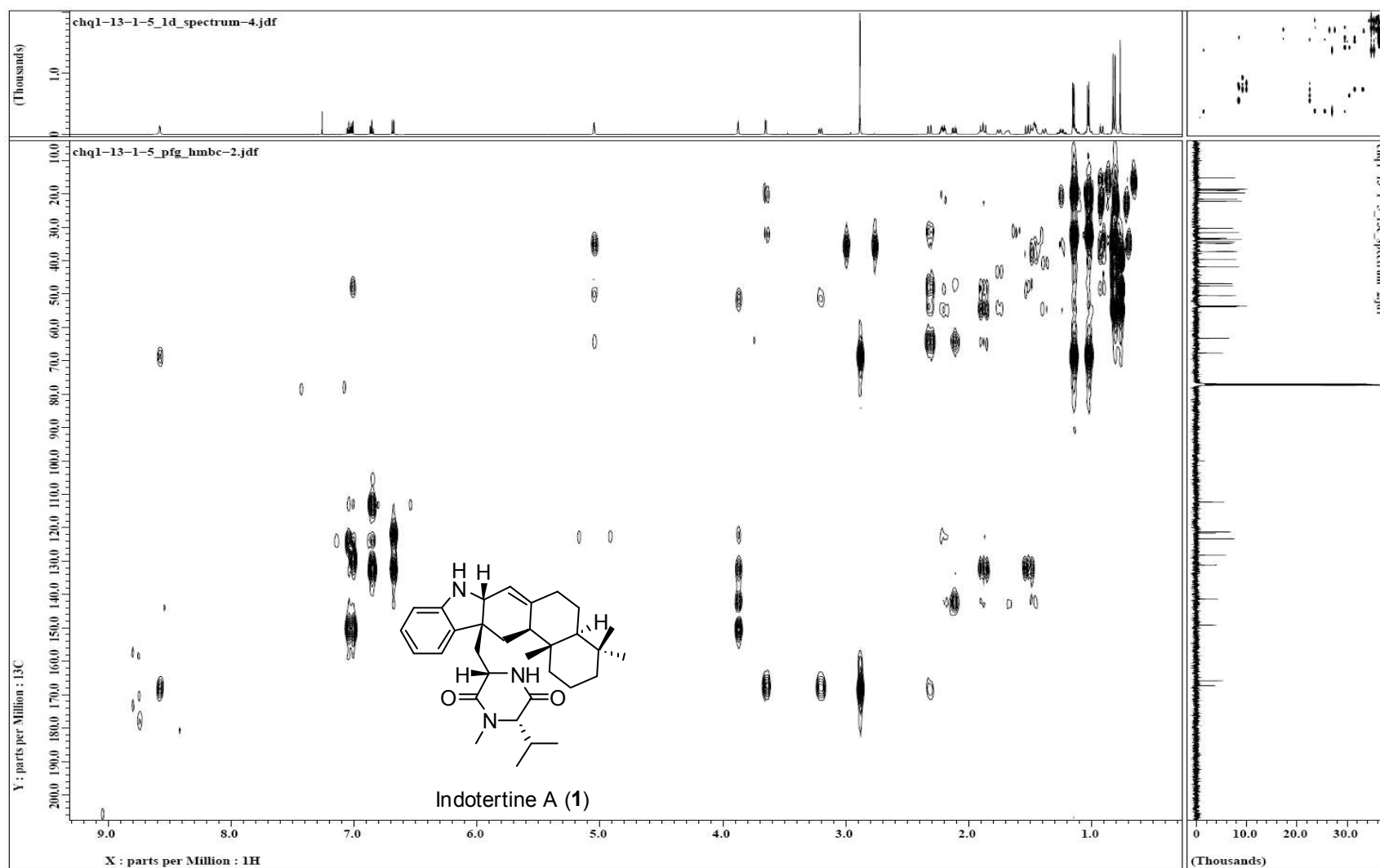


Figure S10. HRESIMS Spectrum of indotertine A (**1**).

20120507-chq-1-13-1-5_120507113528 #5-6 RT: 0.08-0.11 AV: 2 NL: 3.99E7
T: FTMS + p ESI Full ms [100.00-1000.00]

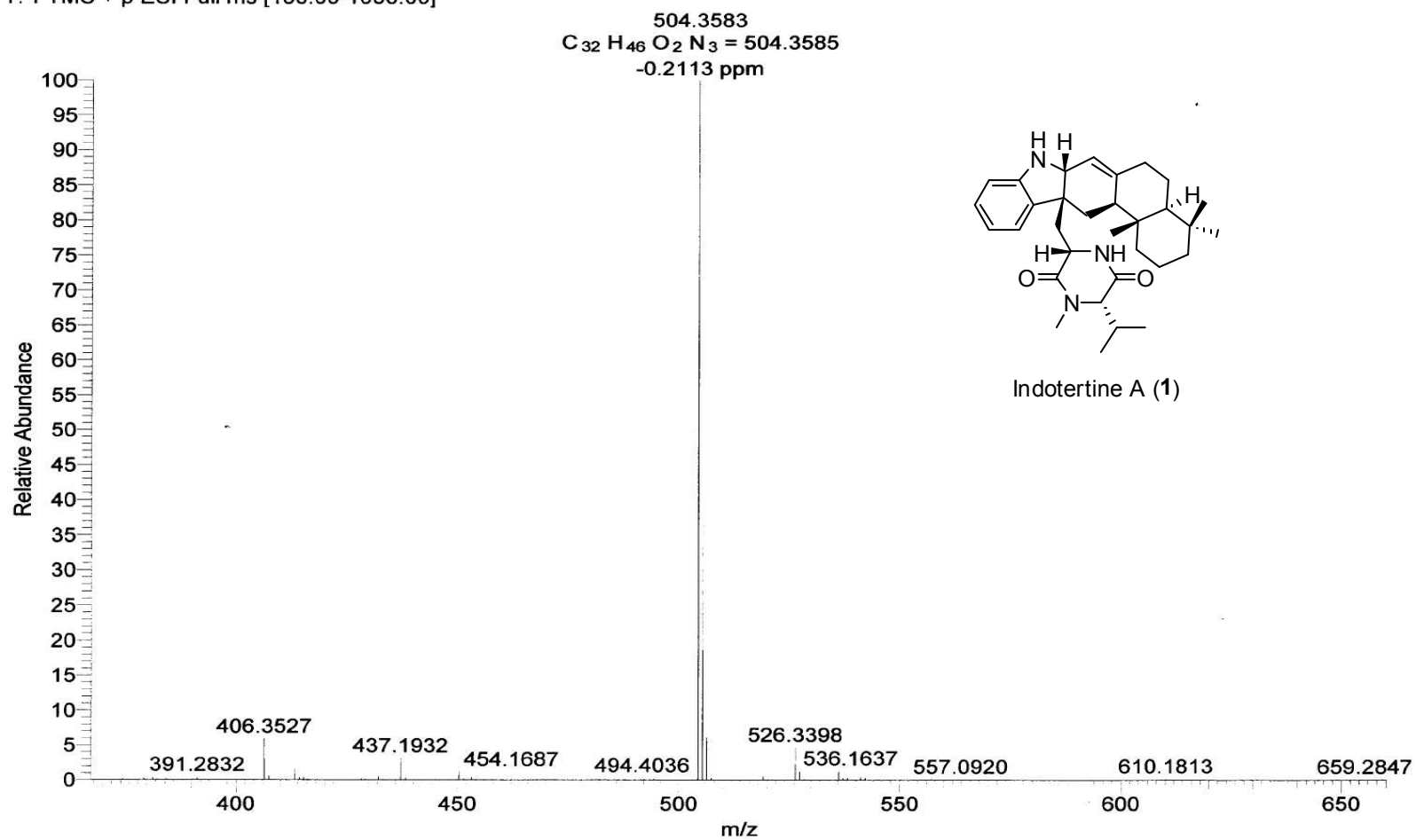
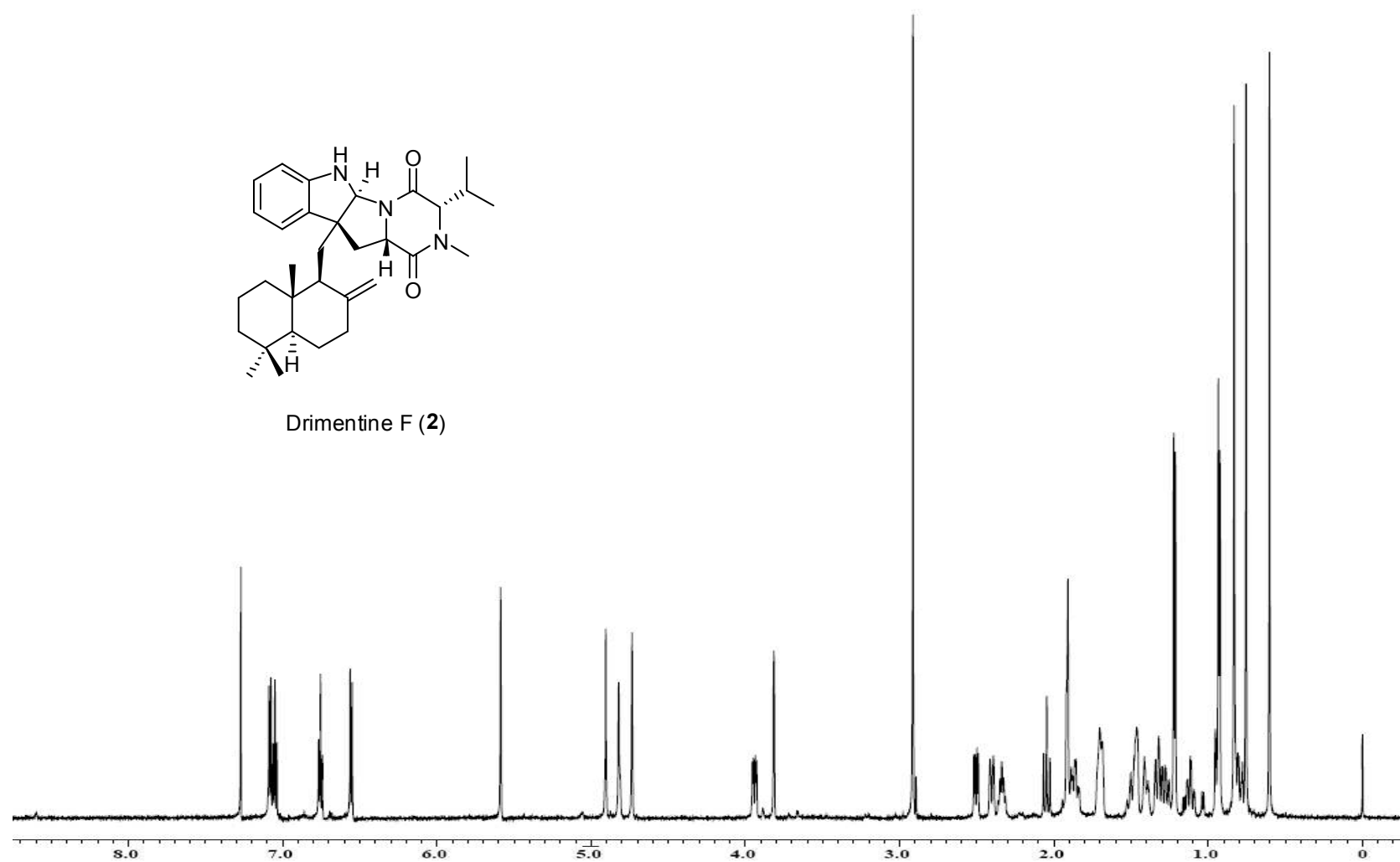
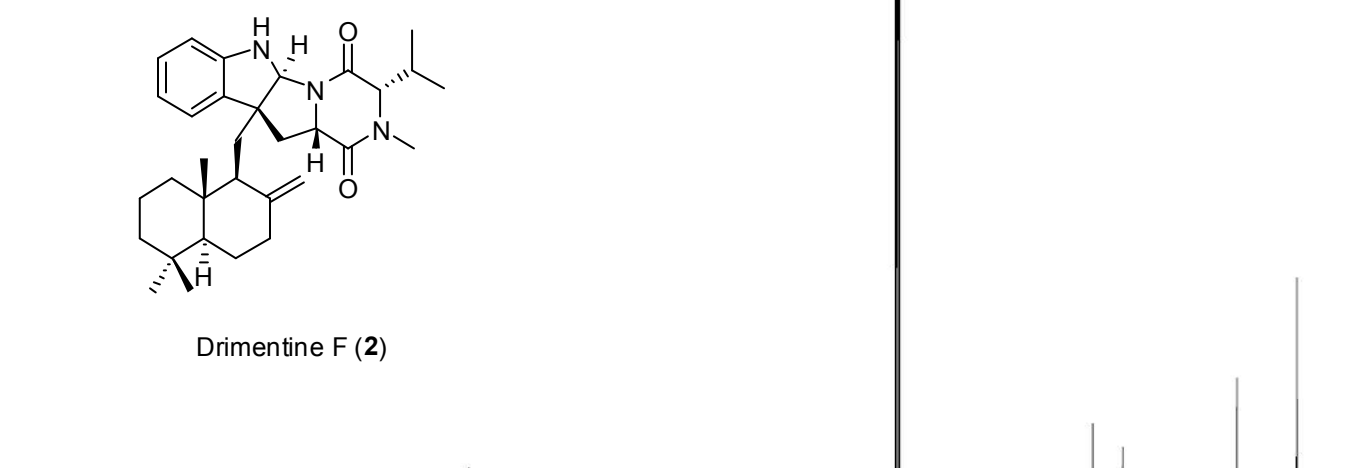


Figure S11. ^1H NMR Spectrum (600 MHz) of drimentine F (**2**) in CDCl_3 .




The chemical structure of Drimentine F (2) is shown above its ¹³C NMR spectrum. The structure is a complex polycyclic molecule featuring a tricyclic core with a benzene ring, a cyclohexane ring, and a cyclohexene ring. It includes a quinuclidine-like system with a carbonyl group and a methyl group. The spectrum displays numerous peaks across the chemical shift range from 10.0 to 190.0 ppm, with a prominent solvent peak at approximately 77.0 ppm.

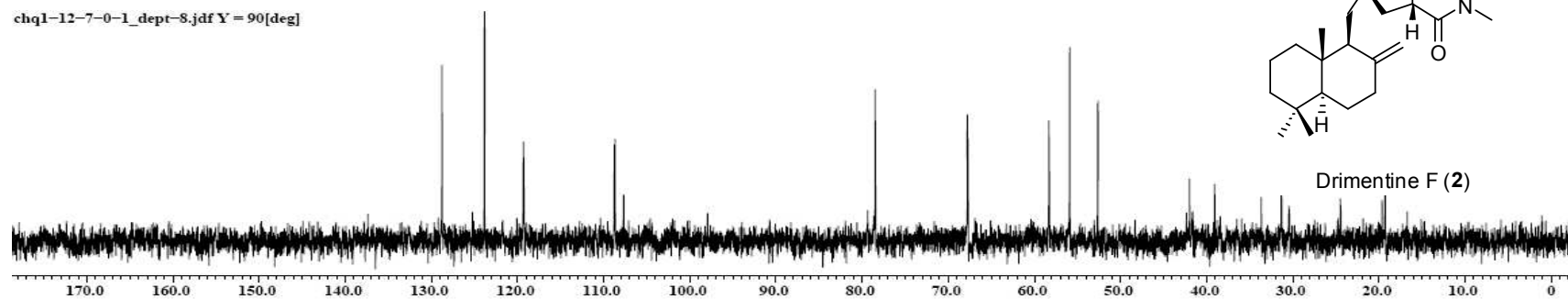
Drimentine F (2)

¹³C NMR spectrum (ppm):

Chemical Shift (ppm)
185.0
175.0
165.0
155.0
145.0
135.0
125.0
115.0
105.0
95.0
85.0
77.0
65.0
55.0
45.0
35.0
25.0
15.0

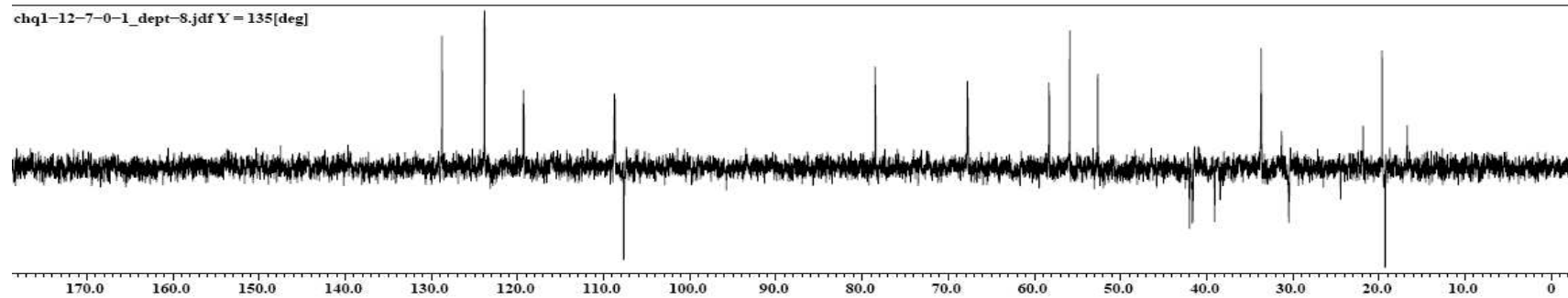
Figure S13. DEPT Spectrum (150 MHz) of drimentine F (**2**) in CDCl₃.

chq1-12-7-0-1_dept-8.jdf Y = 90[deg]



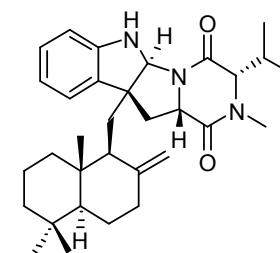
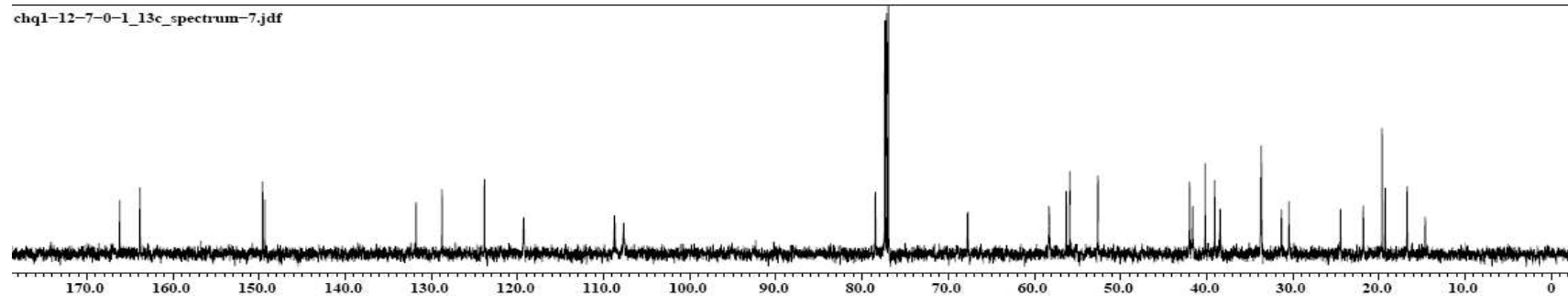
X : parts per Million : 13C

chq1-12-7-0-1_dept-8.jdf Y = 135[deg]



X : parts per Million : 13C

chq1-12-7-0-1_13c_spectrum-7.jdf



Drimentine F (**2**)

Figure S14. HMQC Spectrum of drimentine F (**2**) in CDCl₃.

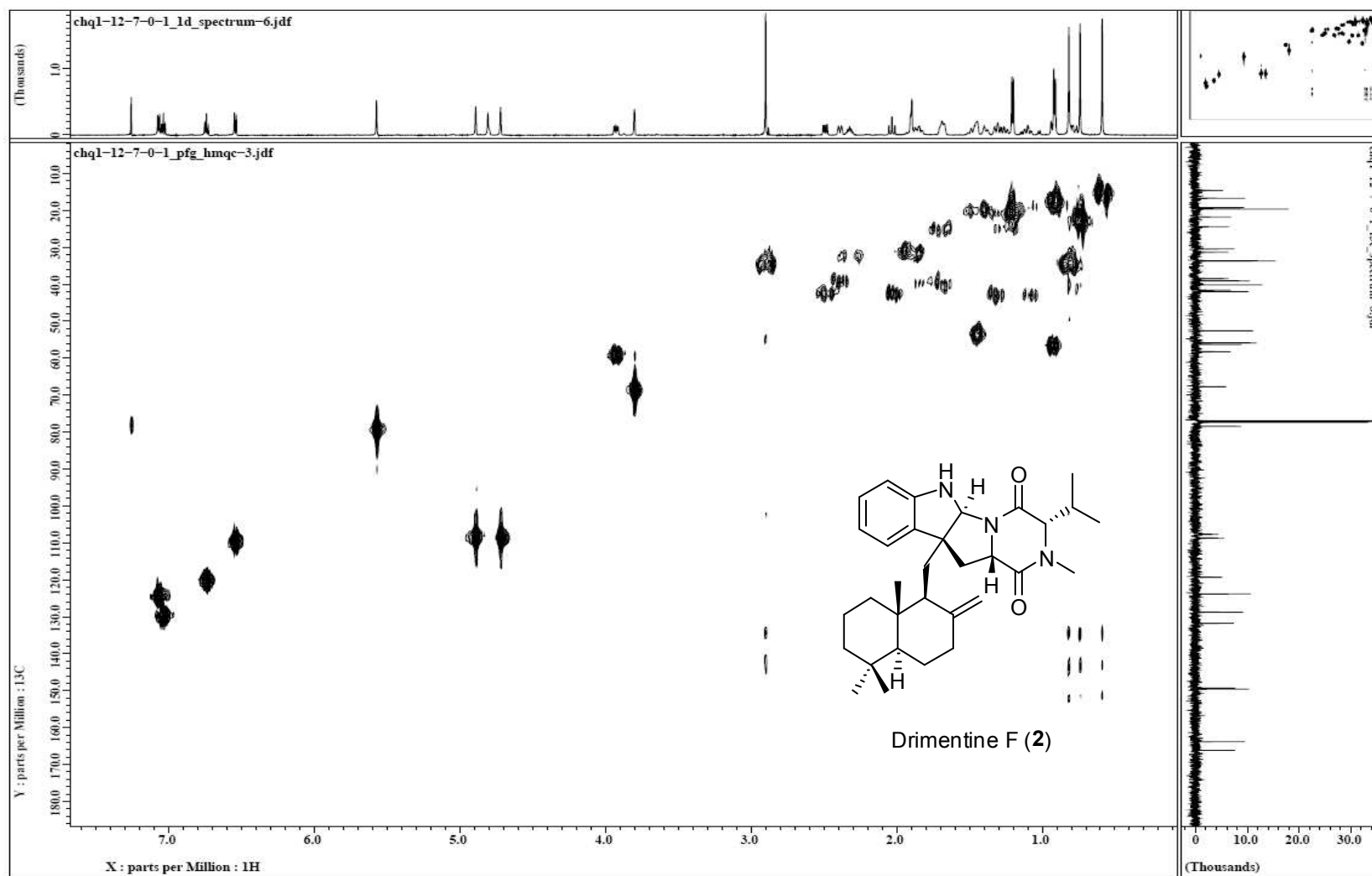


Figure S15. ^1H - ^1H COSY Spectrum of drimentine F (**2**) in CDCl_3 .

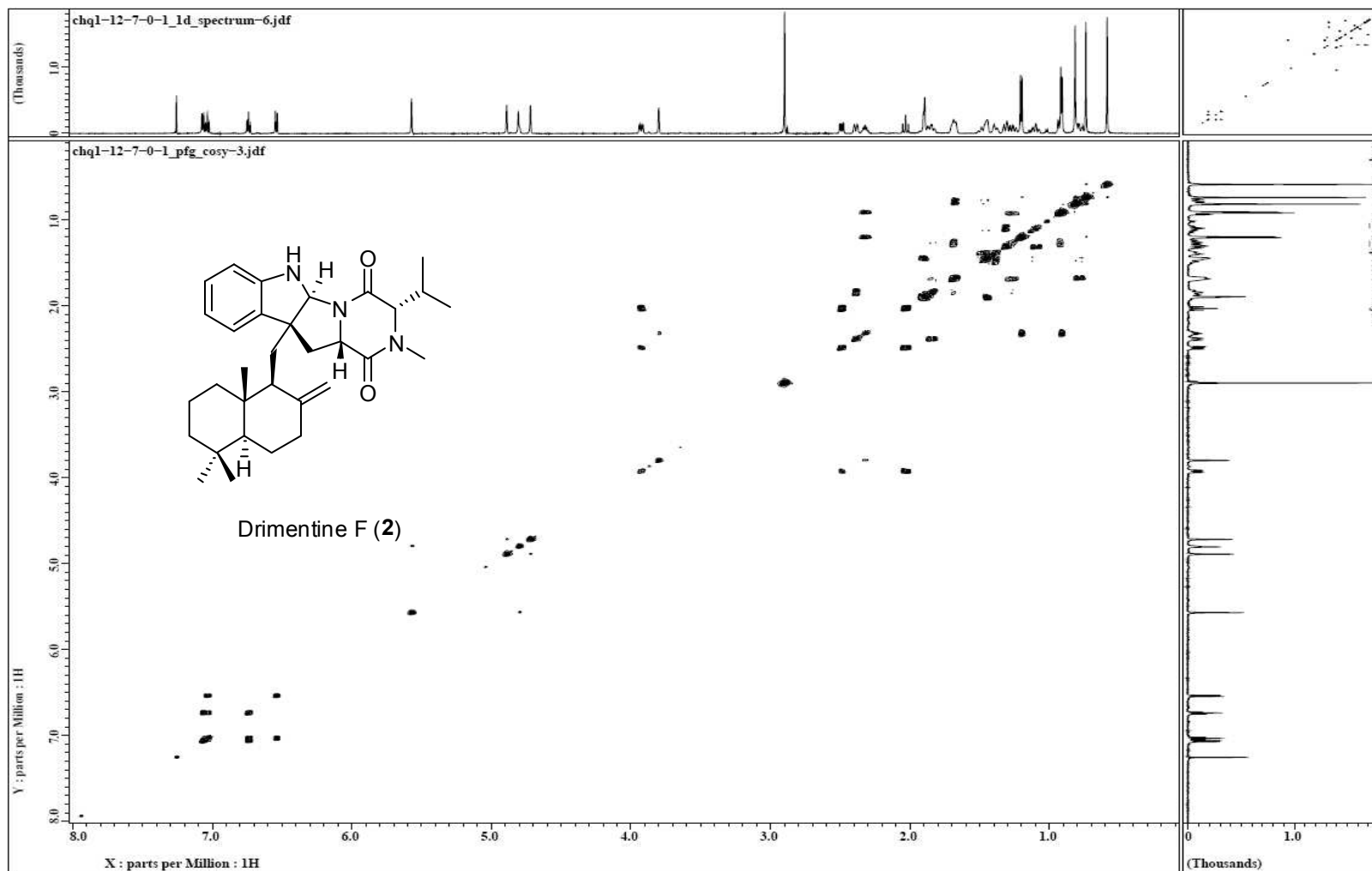


Figure S16. HMBC Spectrum of drimentine F (**2**) in CDCl₃.

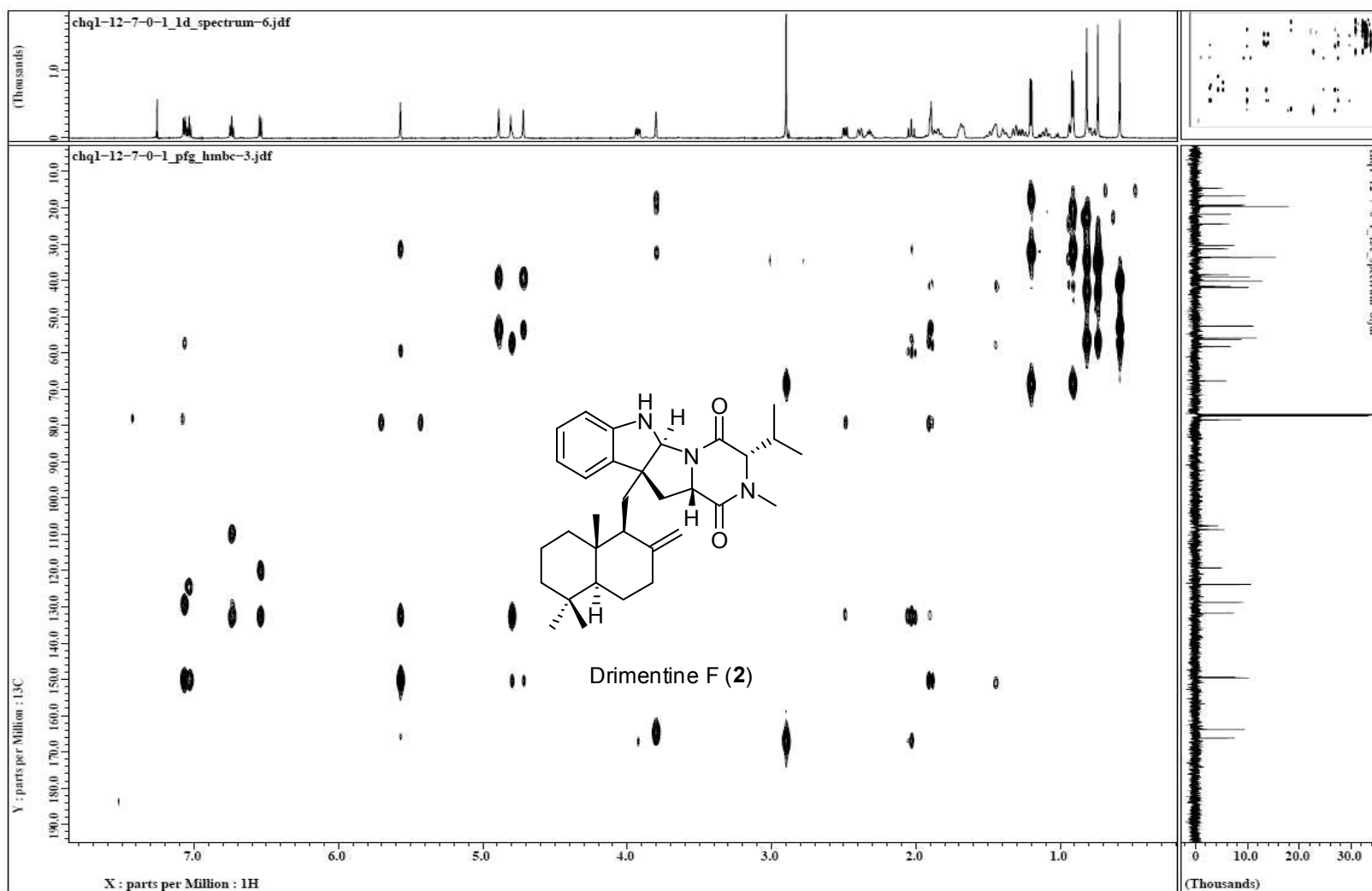


Figure S17. HRESIMS Spectrum of drimentine F (2) .

201111216-CHQ-1-12-7-0-1_111216111025 #9-10 RT: 0.21-0.23 AV: 2 NL: 6.84E7
T: FTMS + p ESI Full ms [100.00-1500.00]

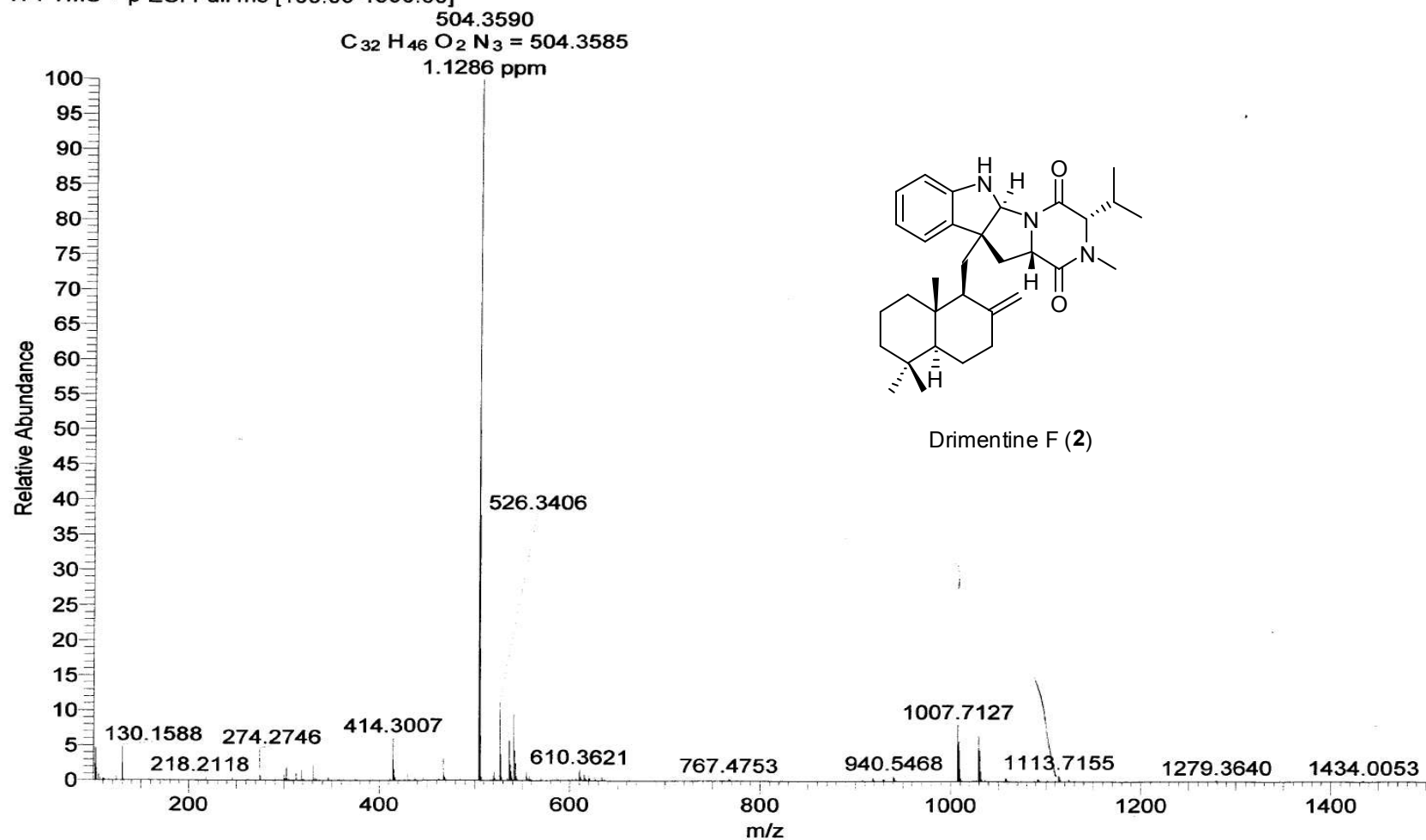


Figure S18. ^1H NMR Spectrum (600 MHz) of drimentine G (**3**) in CDCl_3 .

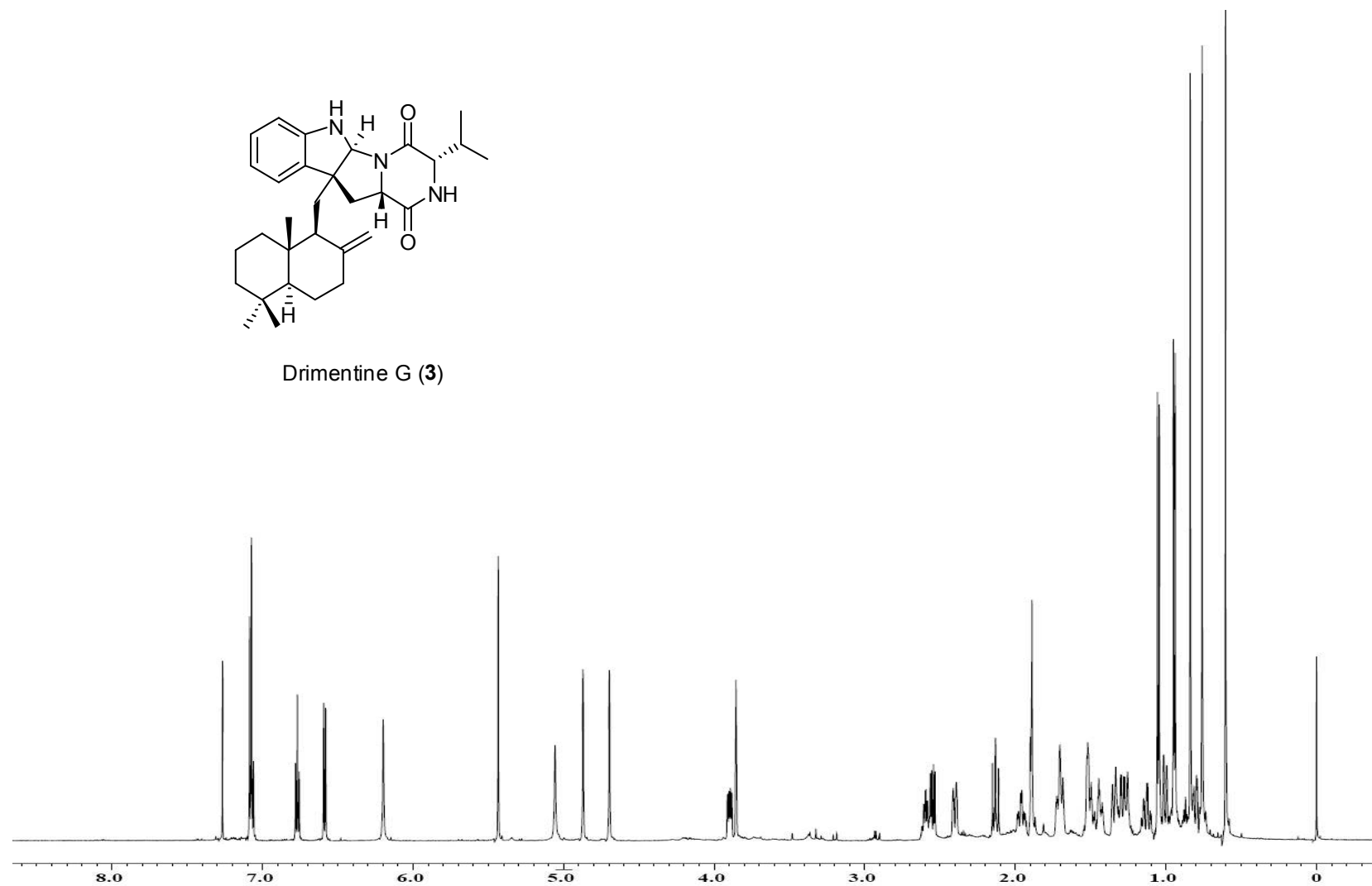


Figure S19. ^{13}C NMR Spectrum (150 MHz) of drimentine G (**3**) in CDCl_3 .

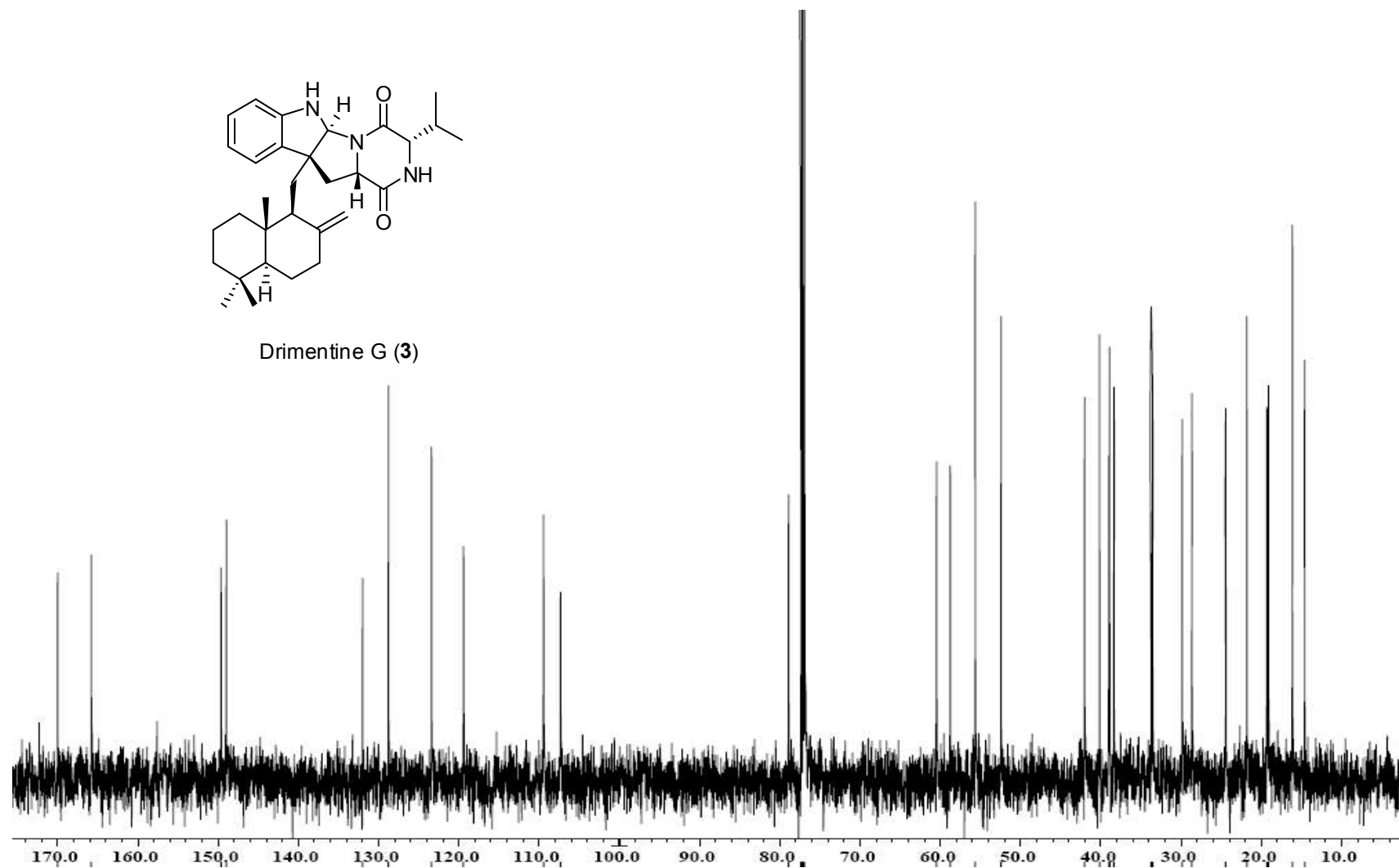
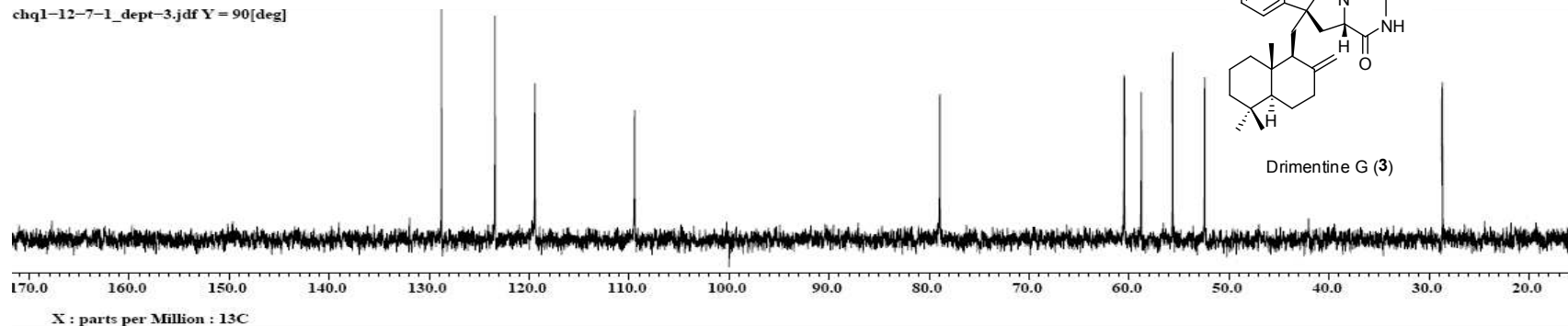
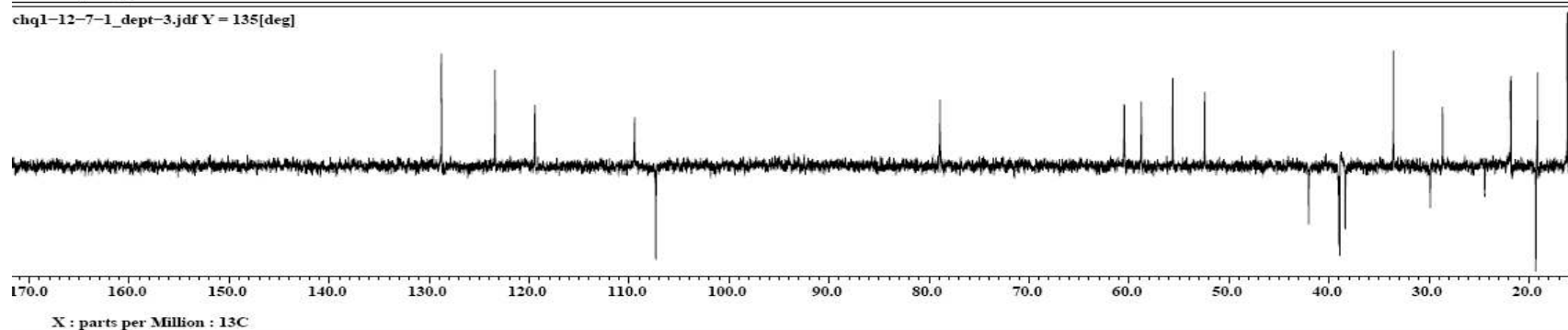


Figure S20. DEPT Spectrum (150 MHz) of drimentine G (**3**) in CDCl₃.

chq1-12-7-1_dept-3.jdf Y = 90[deg]



chq1-12-7-1_dept-3.jdf Y = 135[deg]



chq1-12-7-1_13c_spectrum-3.jdf

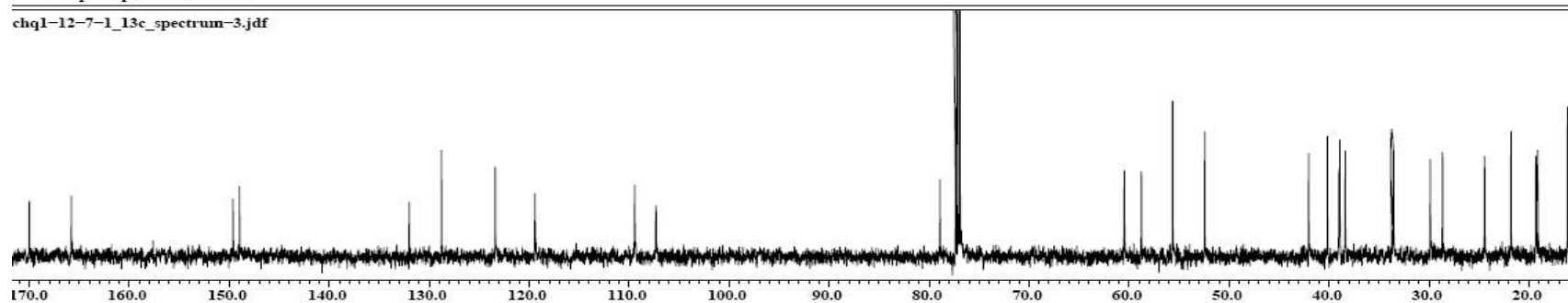


Figure S21. HMQC Spectrum of drimentine G (**3**) in CDCl₃.

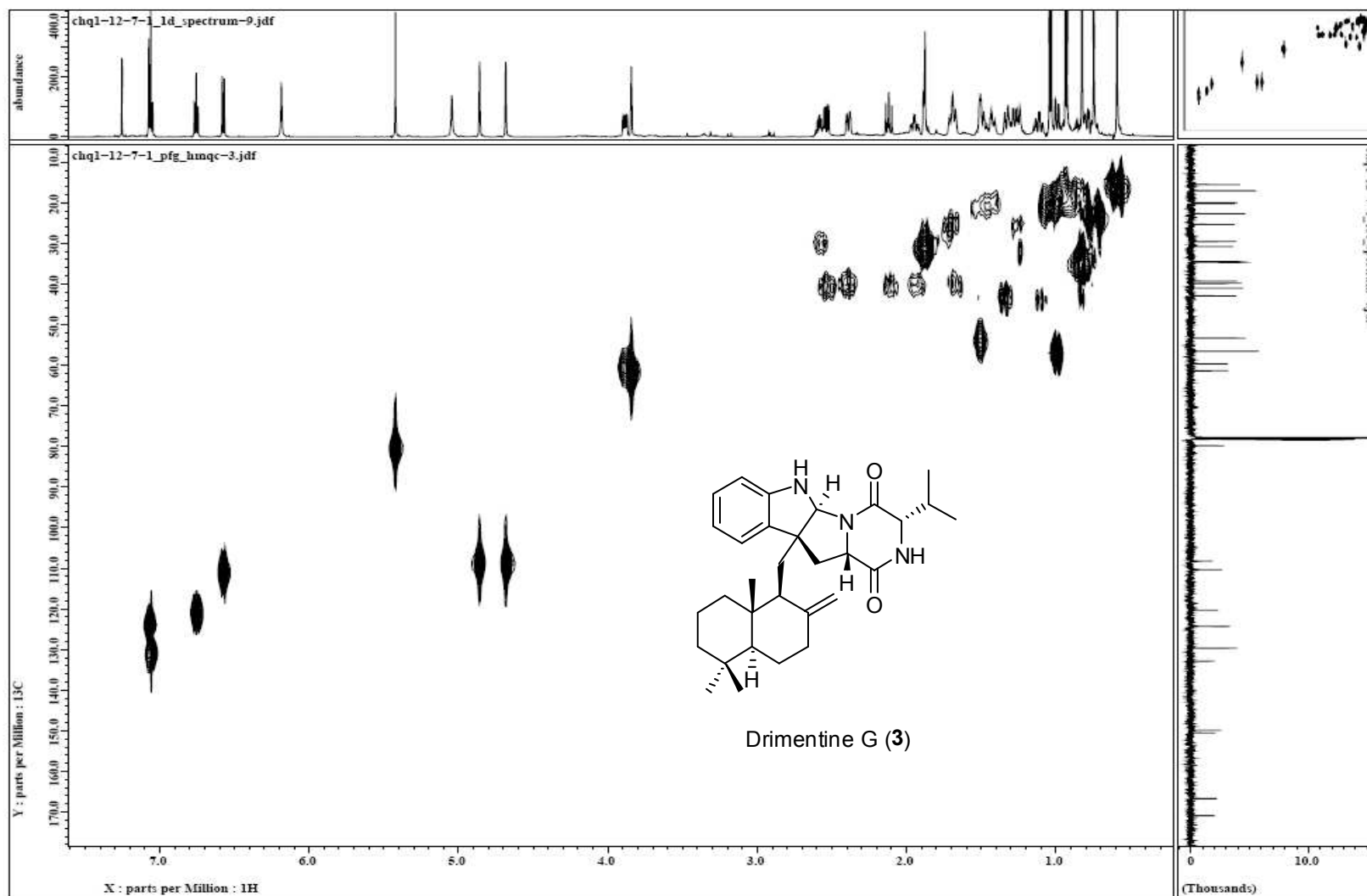


Figure S22. ^1H - ^1H COSY Spectrum of drimentine G (**3**) in CDCl_3 .

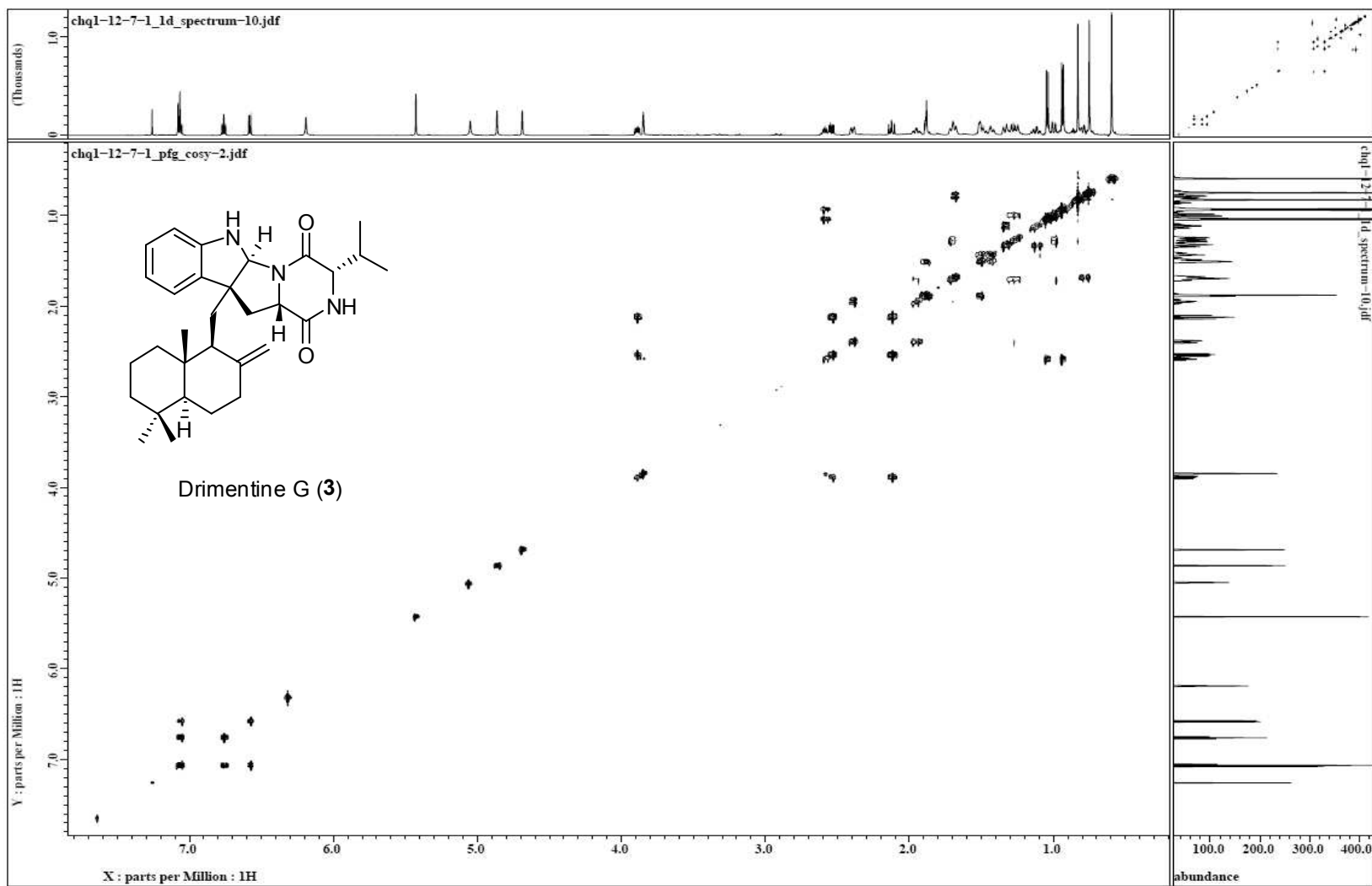


Figure S23. HMBC Spectrum of drimentine G (**3**) in CDCl₃.

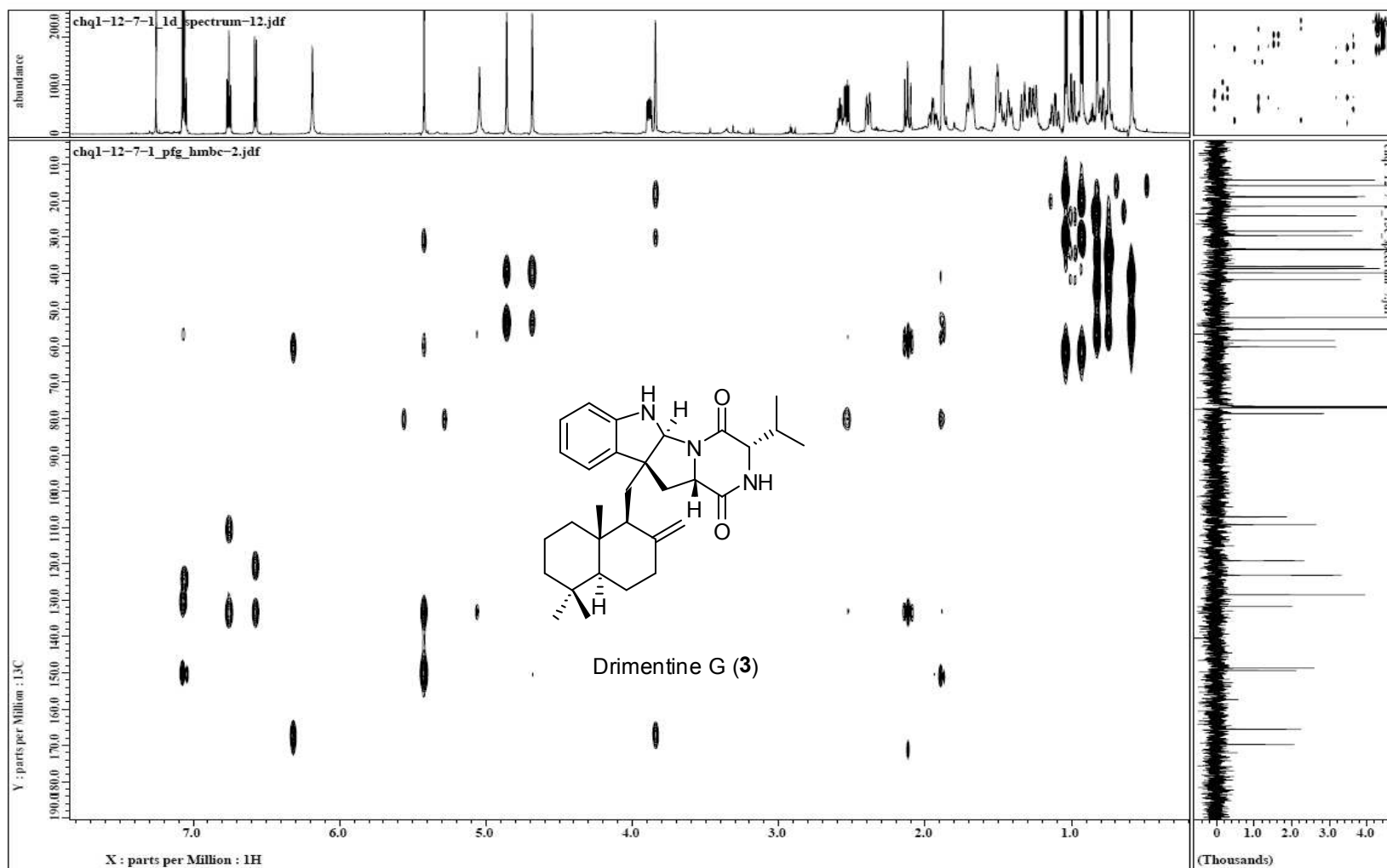


Figure S24. HRESIMS Spectrum of drimentine G (**3**).

Elemental Composition Report

Single Mass Analysis

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

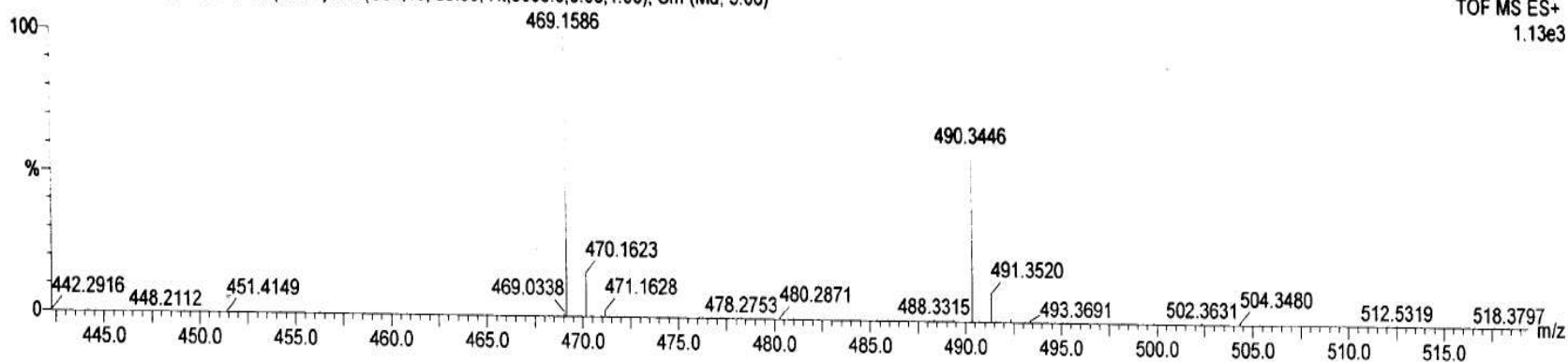
Isotope cluster parameters: Separation = 1.0 Abundance = 1.0%

Monoisotopic Mass, Odd and Even Electron Ions

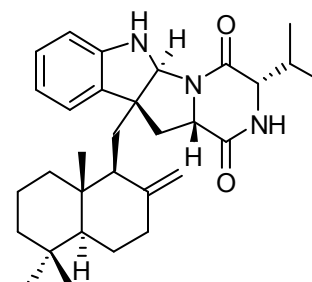
1 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)

HRMSCHQ1-12-7-1

20100928-HRMSCHQ1-12-7-1 94 (3.354) AM (Cen,10, 80.00, Ht,5000.0,0.00,1.00); Sm (Md, 3.00)



Minimum:				-1.5		
Maximum:	200.0	5.0	50.0			
Mass	Calc. Mass	mDa	PPM	DBE	Score	Formula
490.3446	490.3434	1.2	2.5	11.5	1	C31 H44 N3 O2



Drimentine G (**3**)