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SUPPORTING INFORMATION

Title: Dichrocephones A and B, Two Cytotoxic Sesquiterpenoids with the Unique [3.3.3] Propellane Nucleus Skeleton from *Dichrocephala benthamii* C. B. Clarke†

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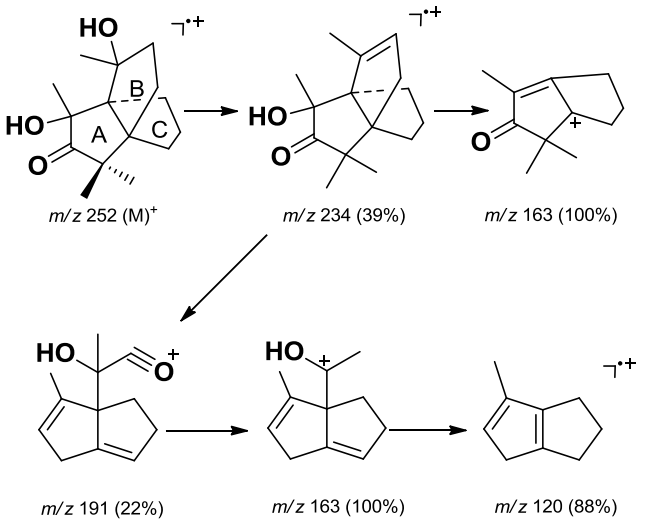


Fig. S1. The EIMS fragments of Dichrocephone A (**1**)

Experimental Section

General: Optical rotations were measured on a Perkin-Elmer 241 polarimeter; UV data were recorded on a Beckman Coulter DU 800 spectrometer; CD spectra were recorded on a JASCO J-815 spectropolarimeter; IR data were recorded using the Shimadzu FTIR-8400S spectrophotometer; ^{1}H and ^{13}C NMR data were acquired with the Bruker 600 and Varian Inova 600 spectrometer using solvent signals (CD_3COCD_3 δ_H 2.05/δ_C 29.8, 206.3) as references, The HSQC and HMBC experiments were optimized for 145.0 and 8.0 Hz respectively; EIMS data were recorded on a GCMS-QP 2010 Shimadzu spectrometer; HRESIMS data were acquired using a LTQ Orbitrap XL; HREIMS data were measured with a Micromass Autospec-Ultima ETOF spectrometer.

Plant Material: The whole plant of *D. benthamii* was collected from Xishuangbanna County, Yunnan Province of People's Republic of China in October 2008. The sample was identified by C. Z. Peng and the voucher specimen (No. DB2008) has been deposited in the Herbarium of the Institute of Medicinal Plant Development, Chinese Academy of Medical Sciences, Beijing.

Extraction and Isolation: The air-dried and chopped whole plant of *D. benthamii* (20 kg) were extracted with 95% EtOH (3 × 80 L) to afford a crude extract (1.7 kg) after evaporation under vacuum. The residue was subject to the diatomaceous silica and eluted successively with petroleum ether, CH_2Cl_2, EtOAc and MeOH. The petroleum ether extract (275 g) was subject to silica gel column chromatography (CC) (2.0 kg, 80–100 mesh), using petroleum ether–Me_2CO gradient elution (50:1–0:1) to afford six corresponding fractions (A, B, C, D, E, F). Fraction B was fractionated over silica gel CC (1.0 kg, 80–100 mesh) using petroleum ether–Me_2CO (1:0–0:1) as the elution to give three fractions (B-1, B-2, B-3). B-2 (73 g) was further fractionated over silica gel CC (2.1 kg, 100–200 mesh) using petroleum ether–EtOAc elution (1:0–0:1) to give six fractions (B-21, B-22, B-23, B-24, B-25, B-26). Compound **2** (9 mg) was isolated from B-24 by further chromatography over silica gel CC (100 g, 200–300 mesh), using petroleum ether–Me_2CO (50:1) elution. Fraction C (43 g) was fractionated over silica gel CC (1.2 kg, 100–200 mesh) using petroleum ether–Me_2CO elution (30:1) to give six fractions (C-1, C-2, C-3, C-4, C-5, C-6). Compound **1** (5 mg) was isolated from fraction C-4 by applying Sephadex LH-20, using CH_2Cl_2–MeOH (1:1) elution.

Dichrocephone A (1): colorless oil, $[\alpha]_D^{25}$ – 63.3 (c 0.18, MeOH); UV (MeOH) λ_{max} (log ε) 199 (1.8); IR (KBr) ν_{max} 3480, 2955, 2926, 2871, 1727, 1464, 1378, 1073 cm^{-1}; EIMS *m/z* (%): 252 $[M]^+$ (7), 234 (39), 206 (7), 191 (22), 177 (34), 163 (100), 149 (25), 120 (88), 107 (27), 71 (66), 58 (90); HREIMS *m/z* 234.1611 $[M - H_2O]^+$ (calcd for $[M - H_2O]^+$, 234.1620); ^{1}H-NMR (600 MHz, CD_3COCD_3) and ^{13}C-NMR (150 MHz, CD_3COCD_3) see Table 1.

Dichrocephone B (2): colorless oil, $[\alpha]_D^{25}$ – 8.0 (c 0.19, MeOH); UV (MeOH) λ_{max} (log ε) 210 (1.3); IR (KBr) ν_{max} 2955, 2925, 2853, 1733, 1275, 1260 cm^{-1}; EIMS *m/z* (%): 234 $[M]^+$ (5), 206 (11), 191 (7), 178 (16), 163 (71), 148 (75), 133 (23), 121 (45), 107 (59), 91 (61), 71 (64), 57 (100); HRESIMS *m/z* 257.1511 $[M + Na]^+$ (calcd for $C_{15}H_{22}O_2Na$, 257.1518); ^{1}H-NMR (600 MHz, CD_3COCD_3) and ^{13}C-NMR (150 MHz, CD_3COCD_3) see Table 1.

MTT Assay: The assay was performed in triplicate. In a 96-well plate, each well was plated with 10^4 cells. After cell attachment overnight, the medium was removed, and each well was treated with 50 μL of medium containing 0.2% DMSO, or appropriate concentrations of the test compounds, or the positive control 5-fluorouracil (10 mg/mL as stock solution of a compound in DMSO and serial dilutions; the test compounds showed good solubility in DMSO and did not precipitate when added to the cells). Cells were treated at 37 °C for 4 h in a humidified incubator and an atmosphere containing 5% CO_2 and then allowed to grow for another 48 h after the medium was changed to fresh Dulbecco's modified Eagle medium (DMEM). The medium was removed from the wells, and in the dark, 50 μL of a solution containing 0.5 mg/mL MTT (Sigma) dissolved in serum-free medium or phosphate-buffered saline (PBS) was added and then incubated at 37 °C for 3 h. Upon removal of MTT/medium, 100 μL of DMSO was added to each well and agitated at 60 rpm for 5 min to dissolve the precipitate. The assay plate was measured at 540 nm using a microplate reader. The cytotoxic activities of dichrocephones A (**1**) and B (**2**) were evaluated against human HeLa, KB, A549 cell lines, and 5-fluorouracil was used as positive control (IC_{50} values 5.9, 6.1, 6.9 μM).

Computational Details

All quantum-chemical calculations have been performed on **1a** by the Gaussian03 package, [1] on an IBM cluster machine located at the High Performance Computing Centre of Peking Union Medical College. A systematic conformational analysis for **1a** was carried out via the Molecular Operating Environment (MOE) software package using the MMFF94 force field. The obtained conformers (**1aC1** – **1aC6**) were further optimized and verified as the true minima of potential energy surface using TDDFT at B3LYP/6-31G(d) basis set level. Conductor-like polarizable continuum model (CPCM) was adopted to consider solvent effects using the dielectric constant of methanol (ε = 32.6). The 20 lowest electronic transitions were calculated and the rotational strengths of each electronic excitation were given using both dipole length and dipole velocity representations. ECD spectra were stimulated using a Gaussian function with a half-bandwidth of 0.3 eV. Equilibrium populations of conformers at 298.15 K were calculated from their relative free energies (ΔG) using Boltzmann statistics. The overall ECD spectra were then generated according to Boltzmann weighting of each conformer.

1. Frisch MJ, Trucks GW, Schlegel HB, Scuseria GE, Robb MA, Cheeseman JR, Montgomery JJA, Vreven T, Kudin KN, Burant JC, Millam JM, Iyengar SS, Tomasi J, Barone V, Mennucci B, Cossi M, Scalmani G, Rega N, Petersson GA, Nakatsuji H, Hada M, Ehara M, Toyota K, Fukuda R, Hasegawa J, Ishida M, Nakajima T, Honda Y, Kitao O, Nakai H, Klene M, Li X, Knox JE, Hratchian HP, Cross JB, Bakken V, Adamo C, Jaramillo J, Gomperts R, Stratmann RE, Yazyev O, Austin AJ, Cammi R, Pomelli C, Ochterski JW, Ayala PY, Morokuma K, Voth GA, Salvador P, Dannenberg JJ, Zakrzewski VG, Dapprich S, Daniels AD, Strain MC, Farkas O, Malick DK, Rabuck AD, Raghavachari K, Foresman JB, Ortiz JV, Cui Q, Baboul AG, Clifford S, Cioslowski J, Stefanov BB, Liu G, Liashenko A, Piskorz P, Komaromi I, Martin RL, Fox D J, Keith T, Al-Laham MA, Peng CY, Nanayakkara A, Challacombe M, Gill PMW, Johnson B, Chen W, Wong M W, Gonzalez C, and Pople JA. Gaussian 03, Revision E.03, Gaussian, Inc., Wallingford CT, 2004.

Fig. S2. EIMS Spectrum of Dichrocephone **A** (**1**)

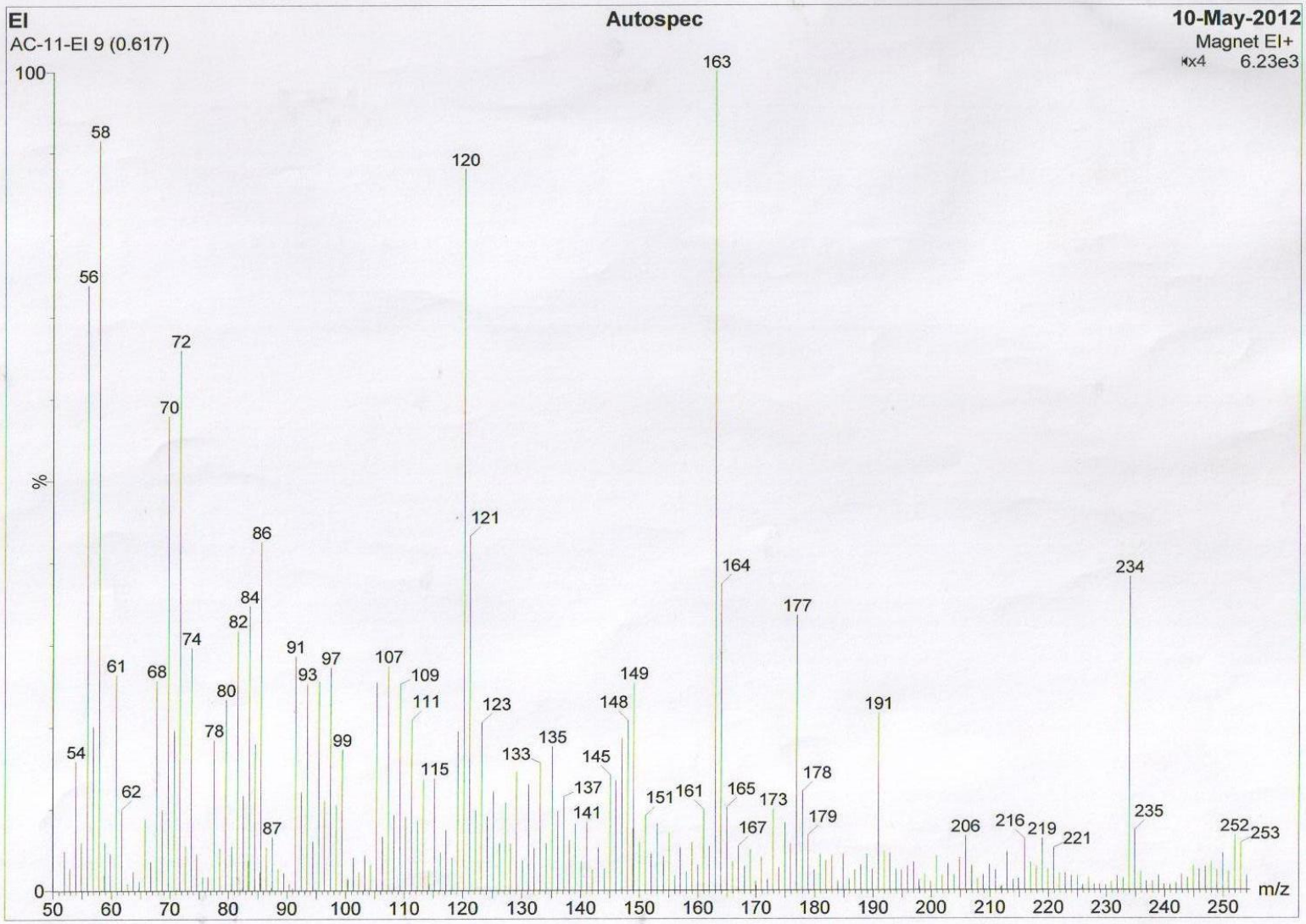
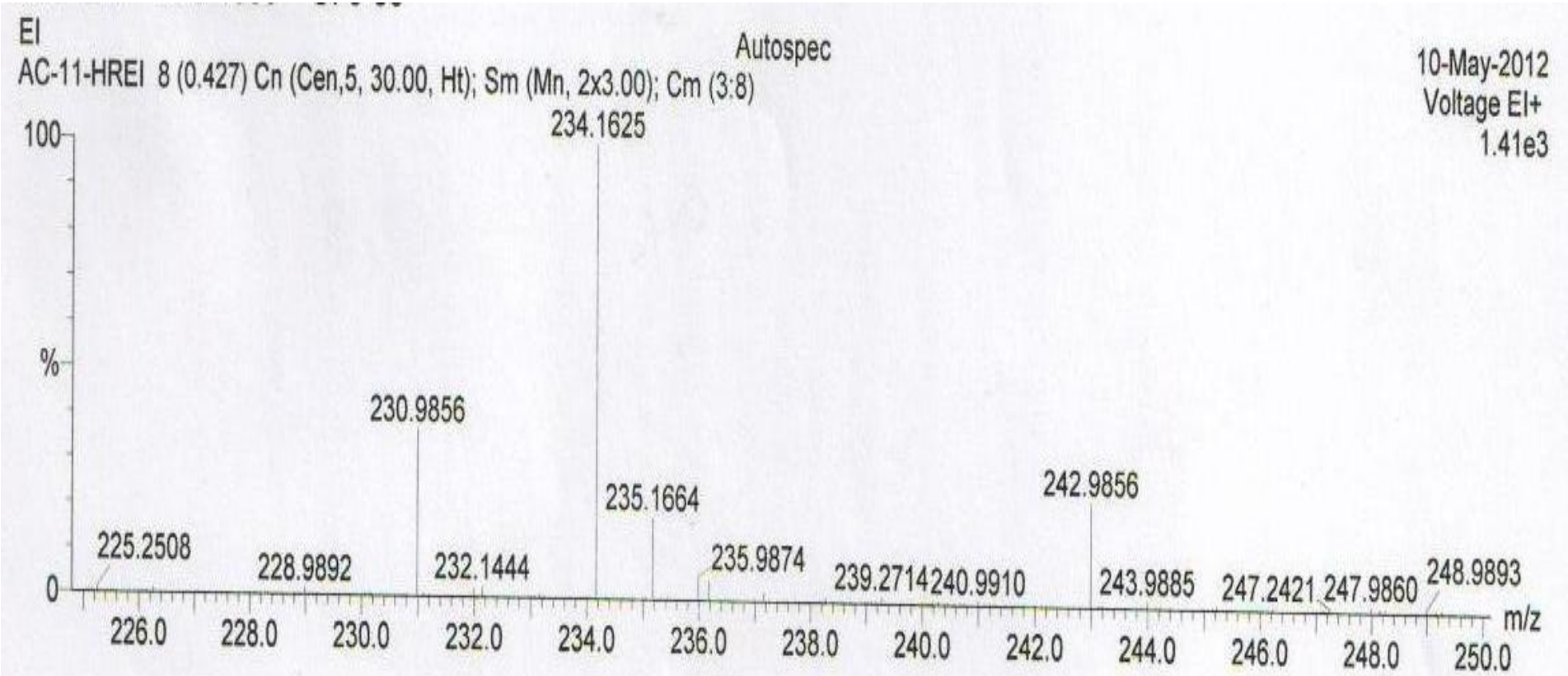


Fig. S3. HREIMS Spectrum of Dichrocephone **A** (**1**)



Minimum:				-2.0		
Maximum:		5.0	10.0	40.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
234.1625	234.1620	0.5	2.1	5.0	11.2	C15 H22 O2

Fig. S4. Experimental ECD spectrum of Dichrocephone **A** (**1**) in methanol and the calculated ECD spectra of (1*S*, 2*R*, 5*S*, 8*R*)-**1a** and (1*R*, 2*S*, 5*R*, 8*S*)-**1b**.

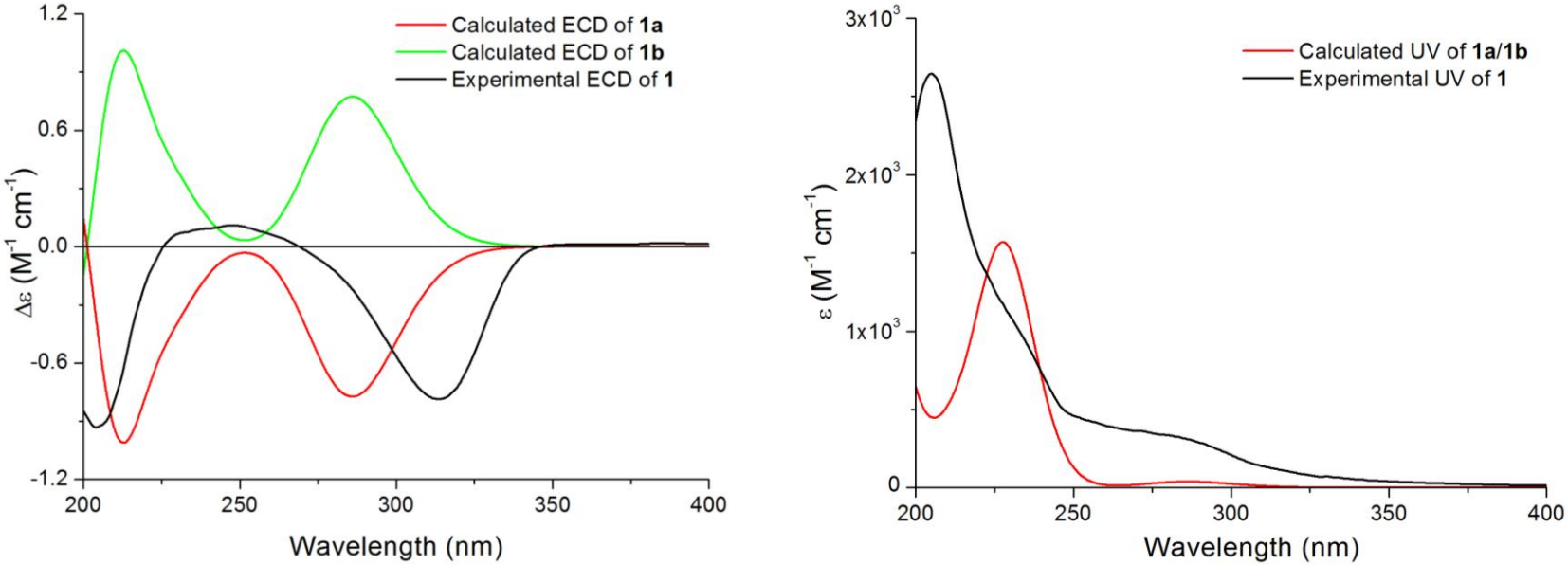


Fig. S5. ^{1}H-NMR Spectrum of Dichrocephone A (**1**; 600 MHz, CD_3COCD_3)

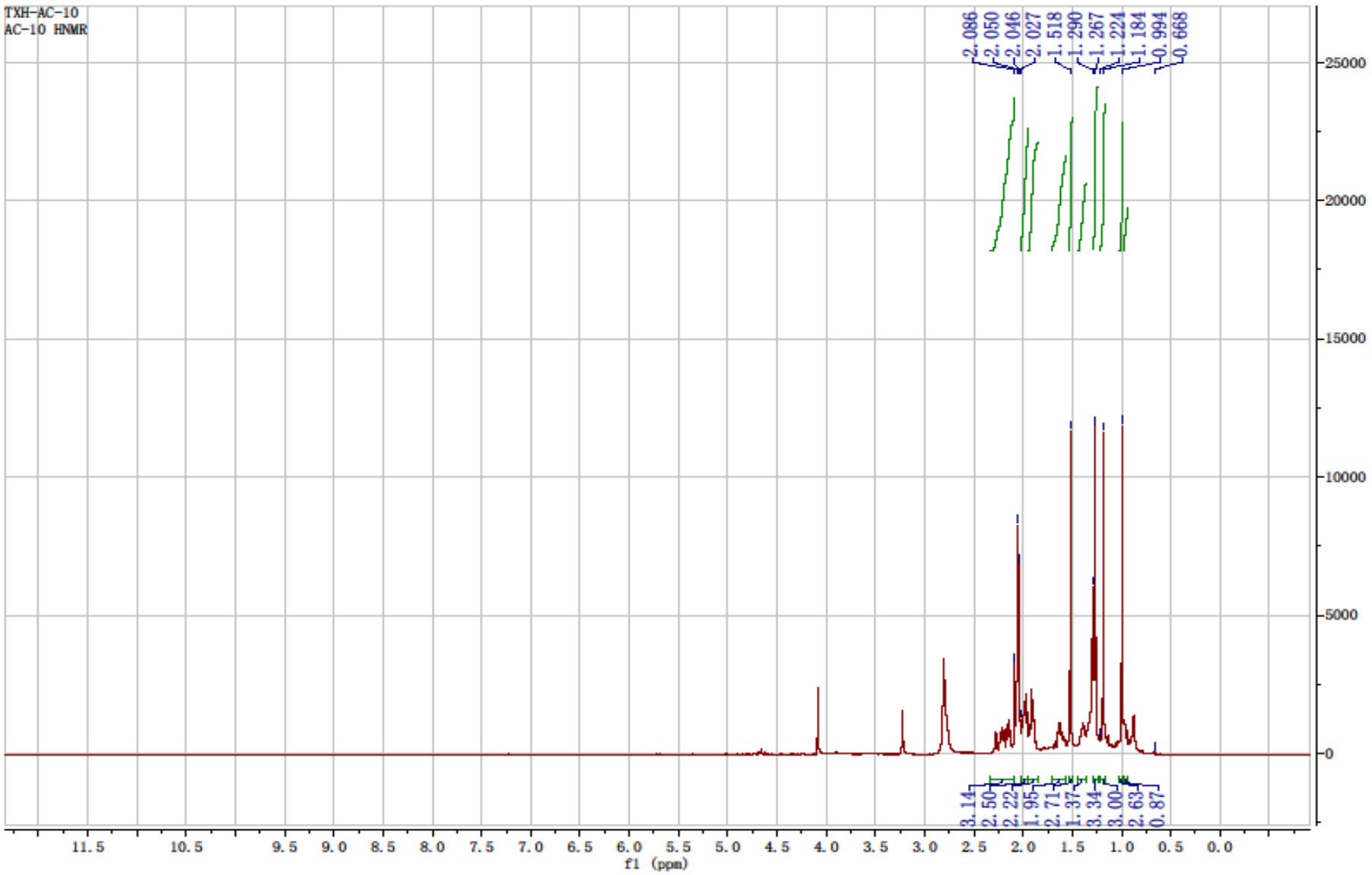


Fig. S6. ^{13}C-NMR Spectrum of Dichrocephone A (**1**; 150 MHz, CD_3COCD_3)

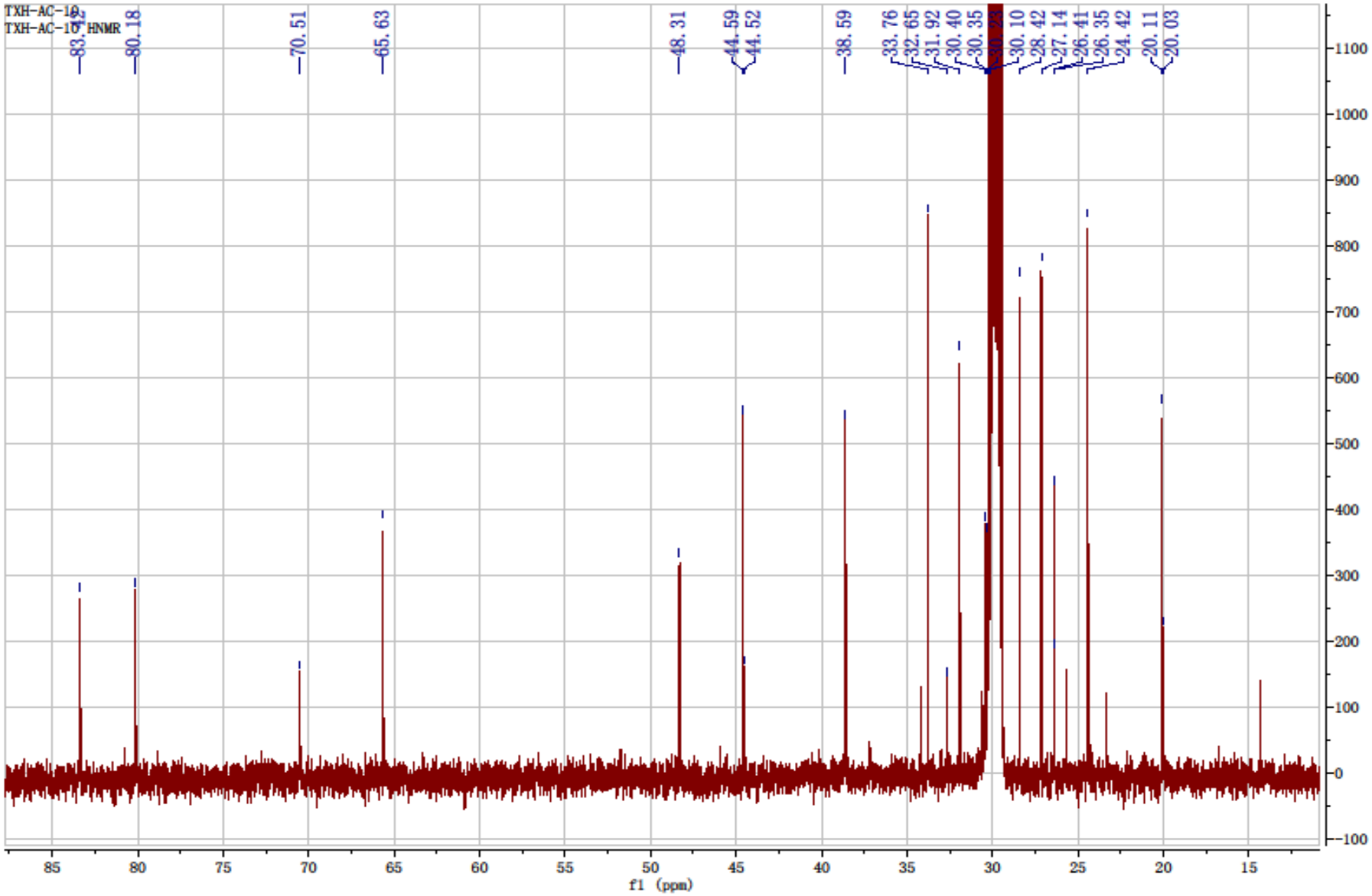


Fig. S7. DEPT Spectrum of Dichrocephone A (**1**; 150 MHz, CD_3COCD_3)

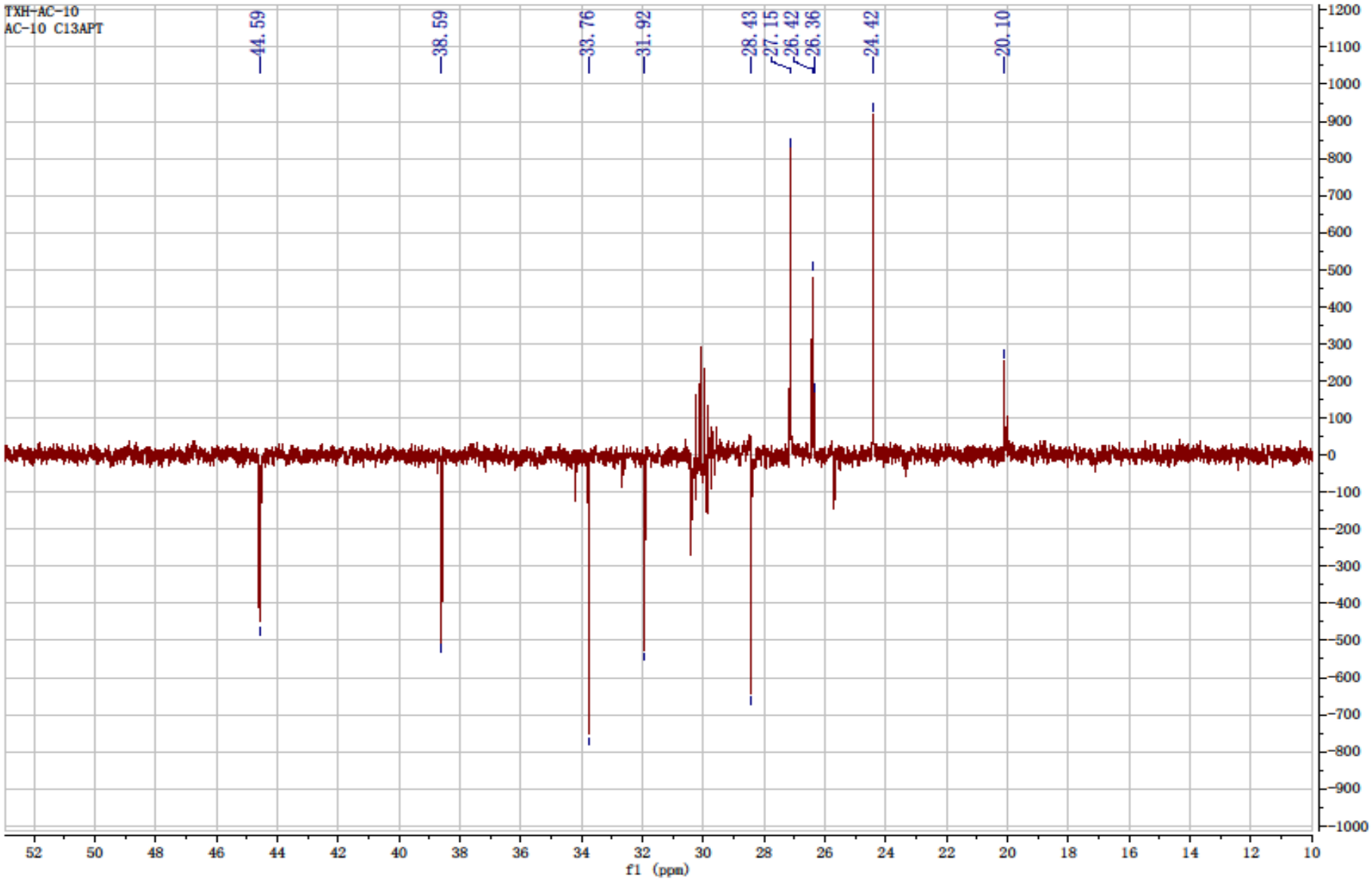


Fig. S8. HSQC Spectrum of Dichrocephone A (**1**; 600 MHz, CD_3COCD_3)

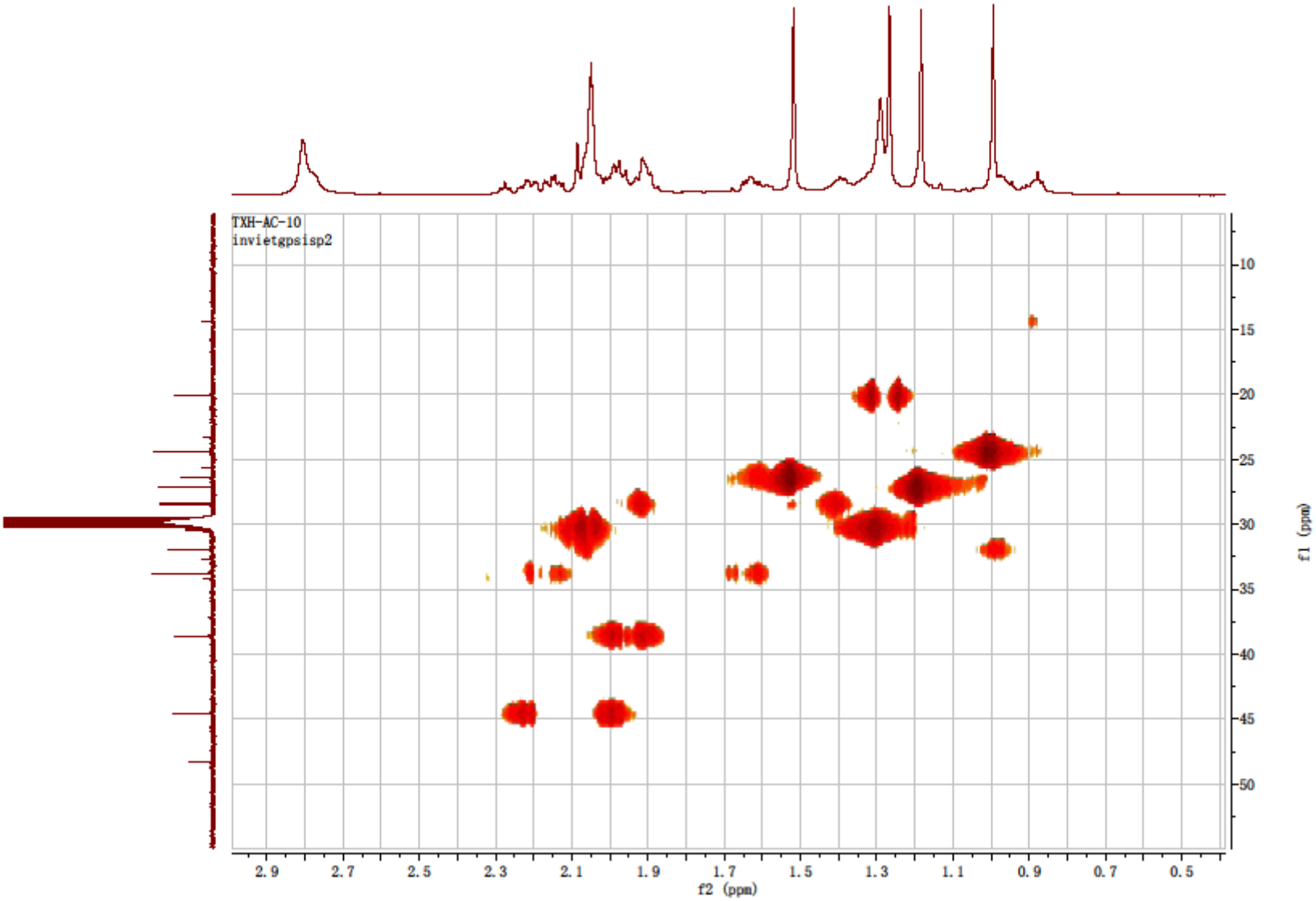


Fig. S9. HMBC Spectrum of Dichrocephone A (**1**; 600 MHz, CD_3COCD_3)

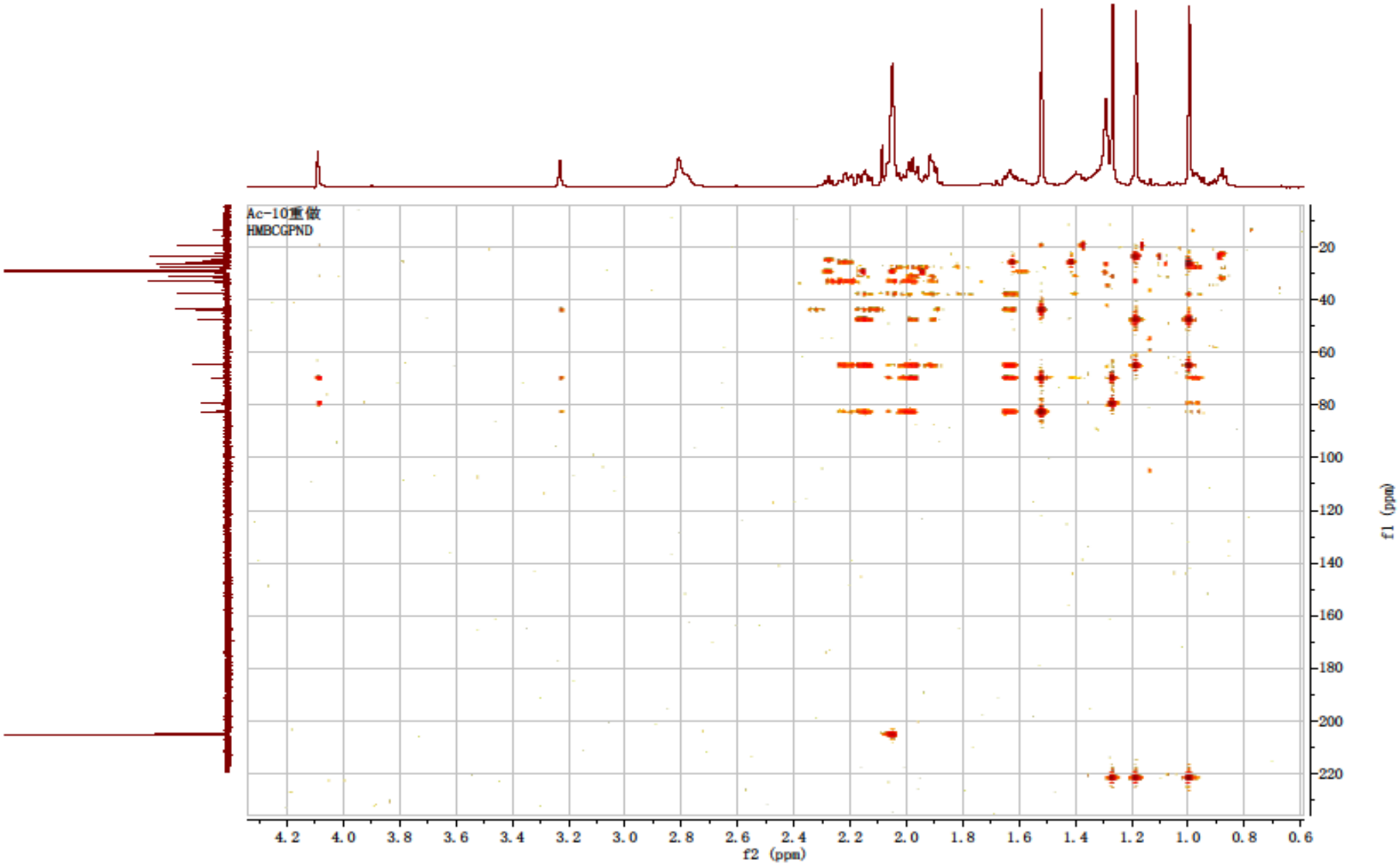


Fig. S10. The magnified HMBC Spectrum of Dichrocephone A (**1**; 600 MHz, CD_3COCD_3)

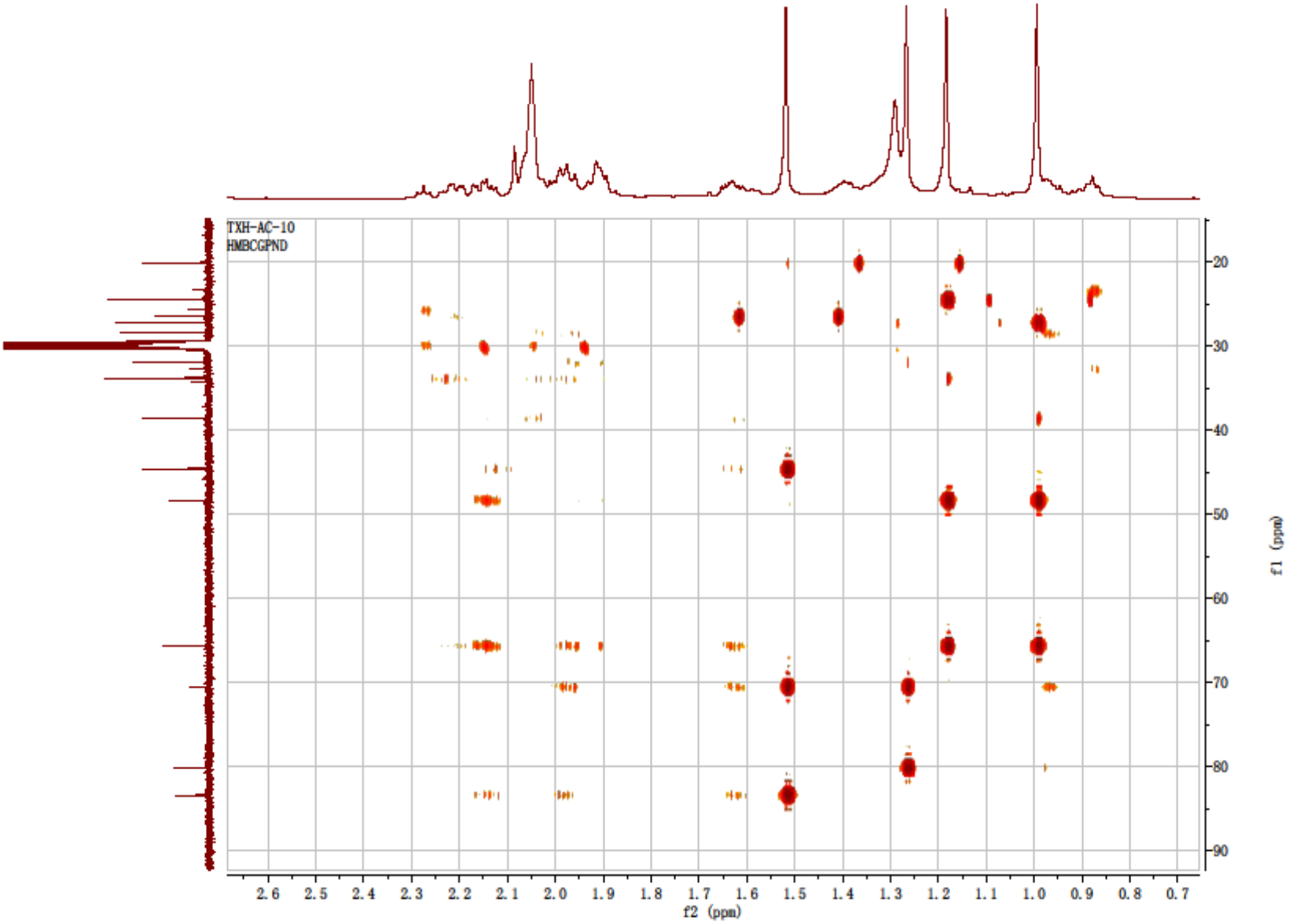


Fig. S11. The magnified HMBC Spectrum of Dichrocephone A (**1**; 600 MHz, CD_3COCD_3)

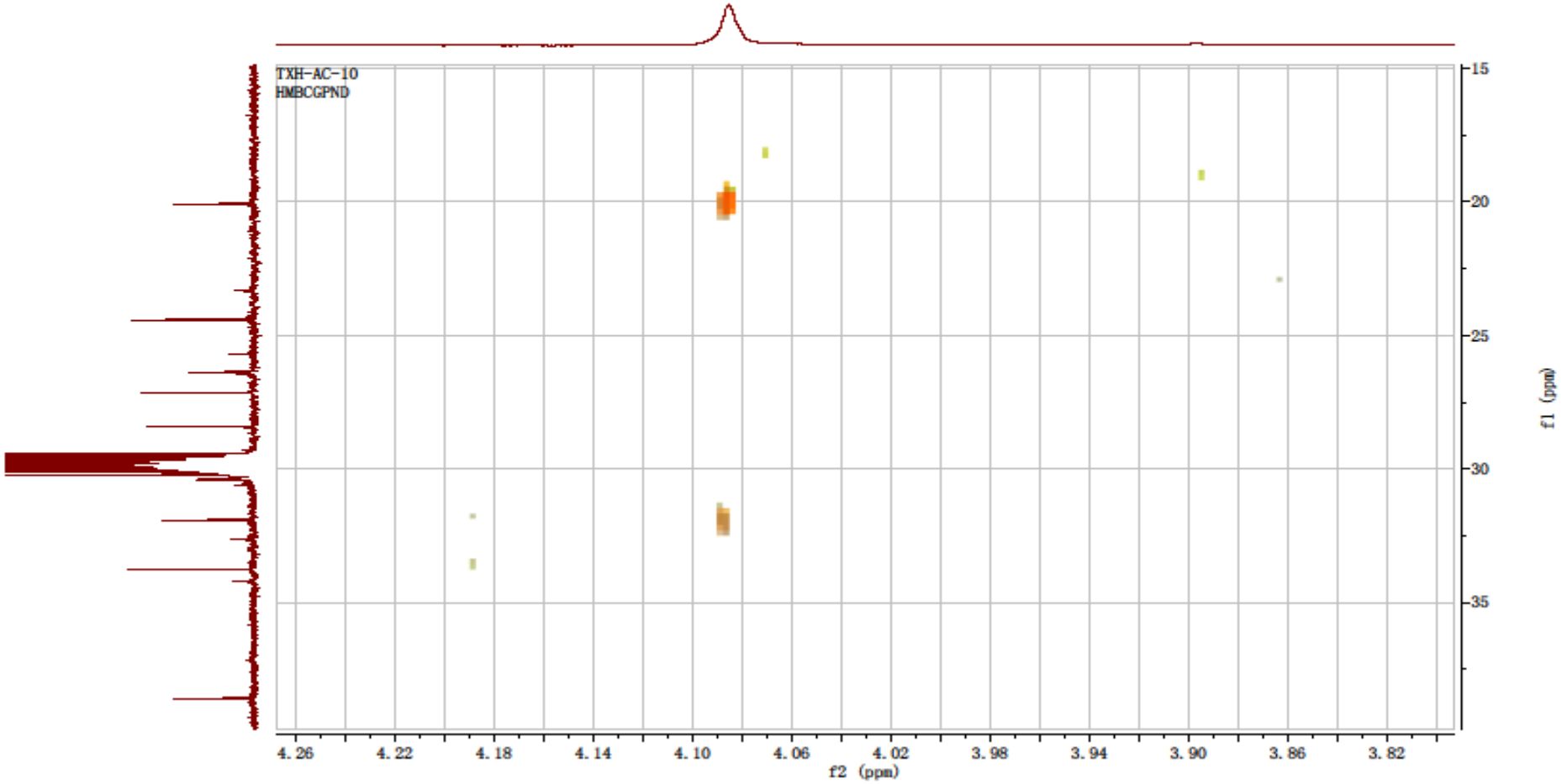


Fig. S12. ROESY Spectrum of Dichrocephone A (**1**; 600 MHz, CD_3COCD_3)

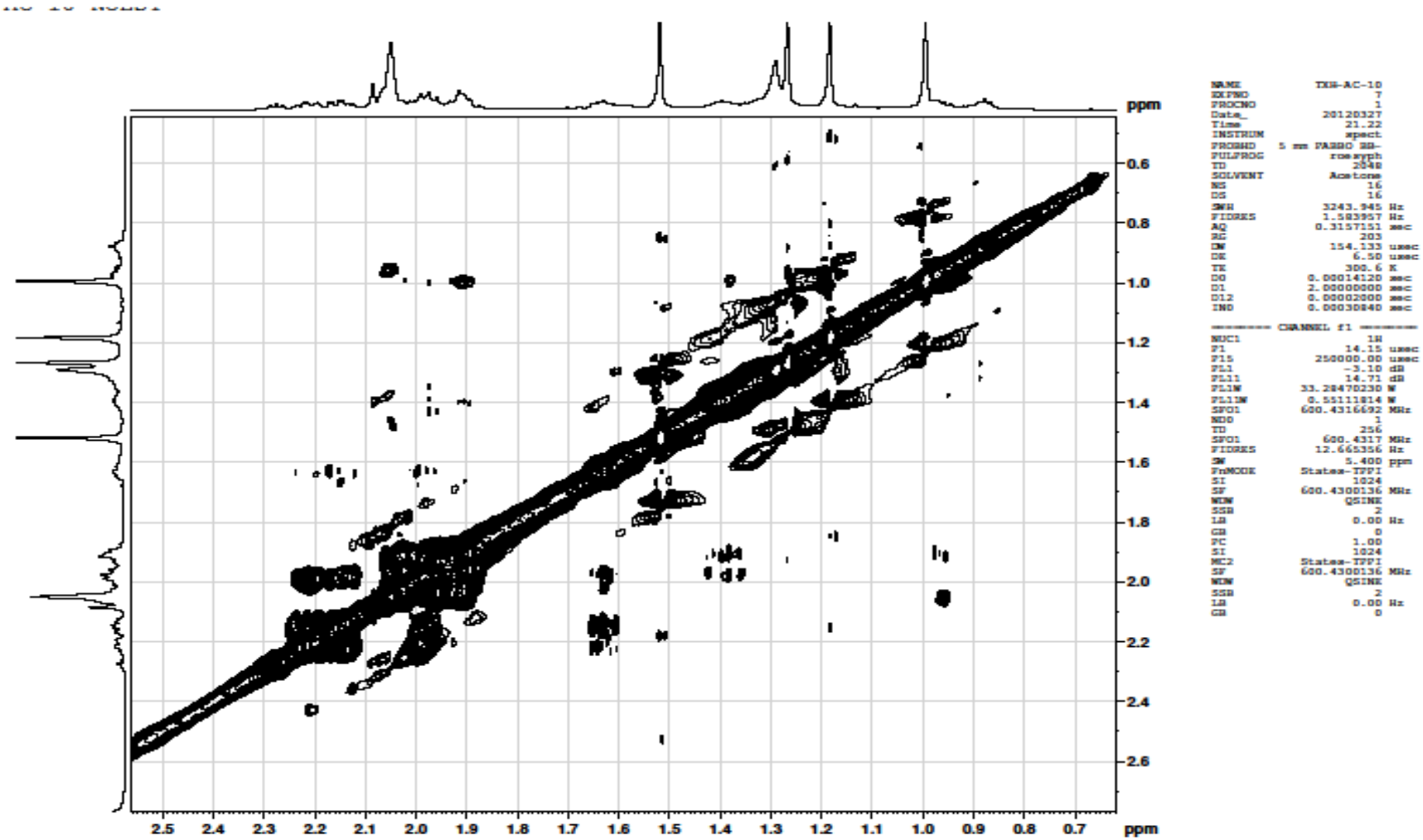


Fig. S13. EIMS Spectrum of Dichrocephone B (**2**)

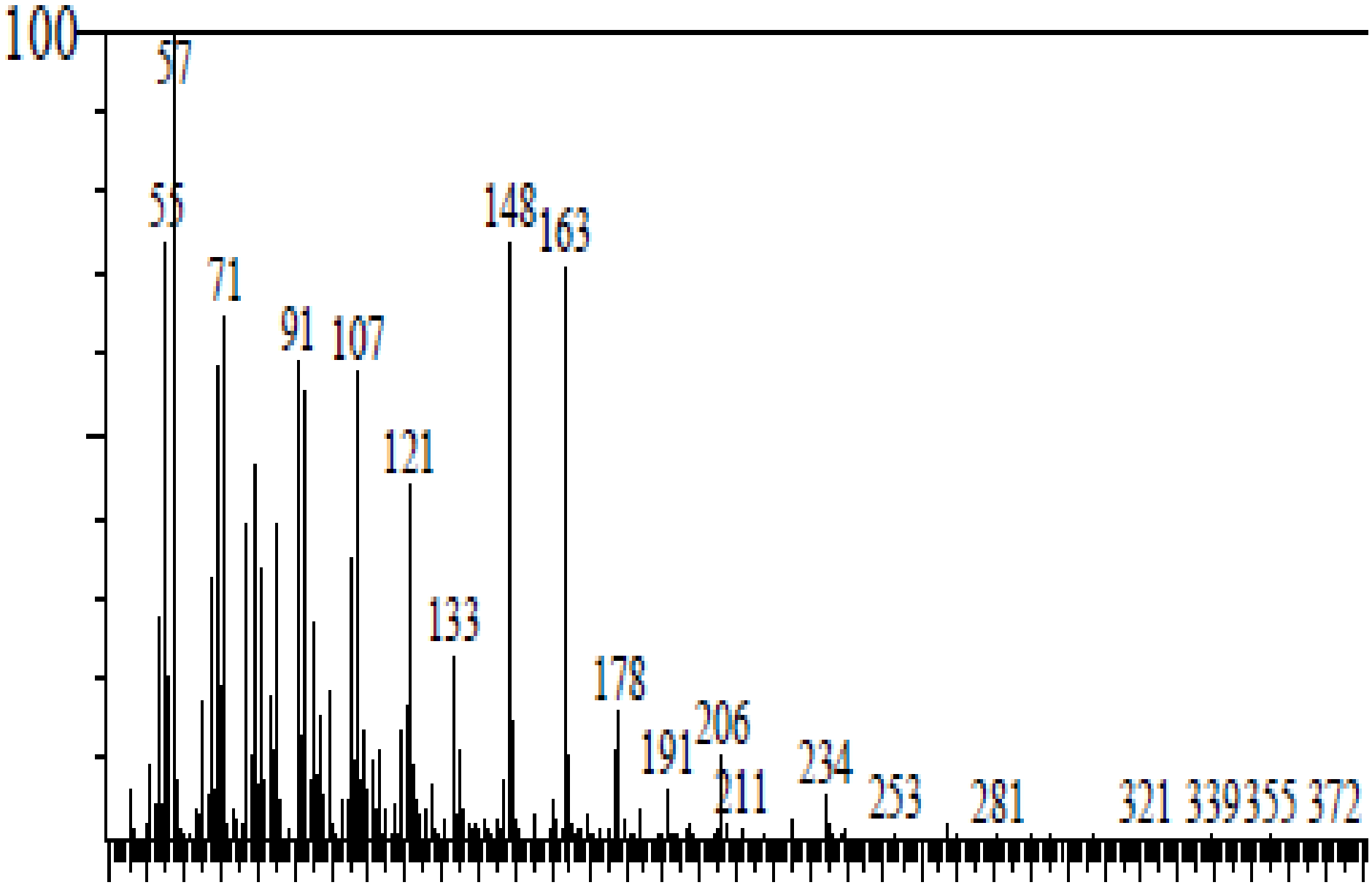


Fig. S14. HRESIMS Spectrum of Dichrocephone B (**2**)

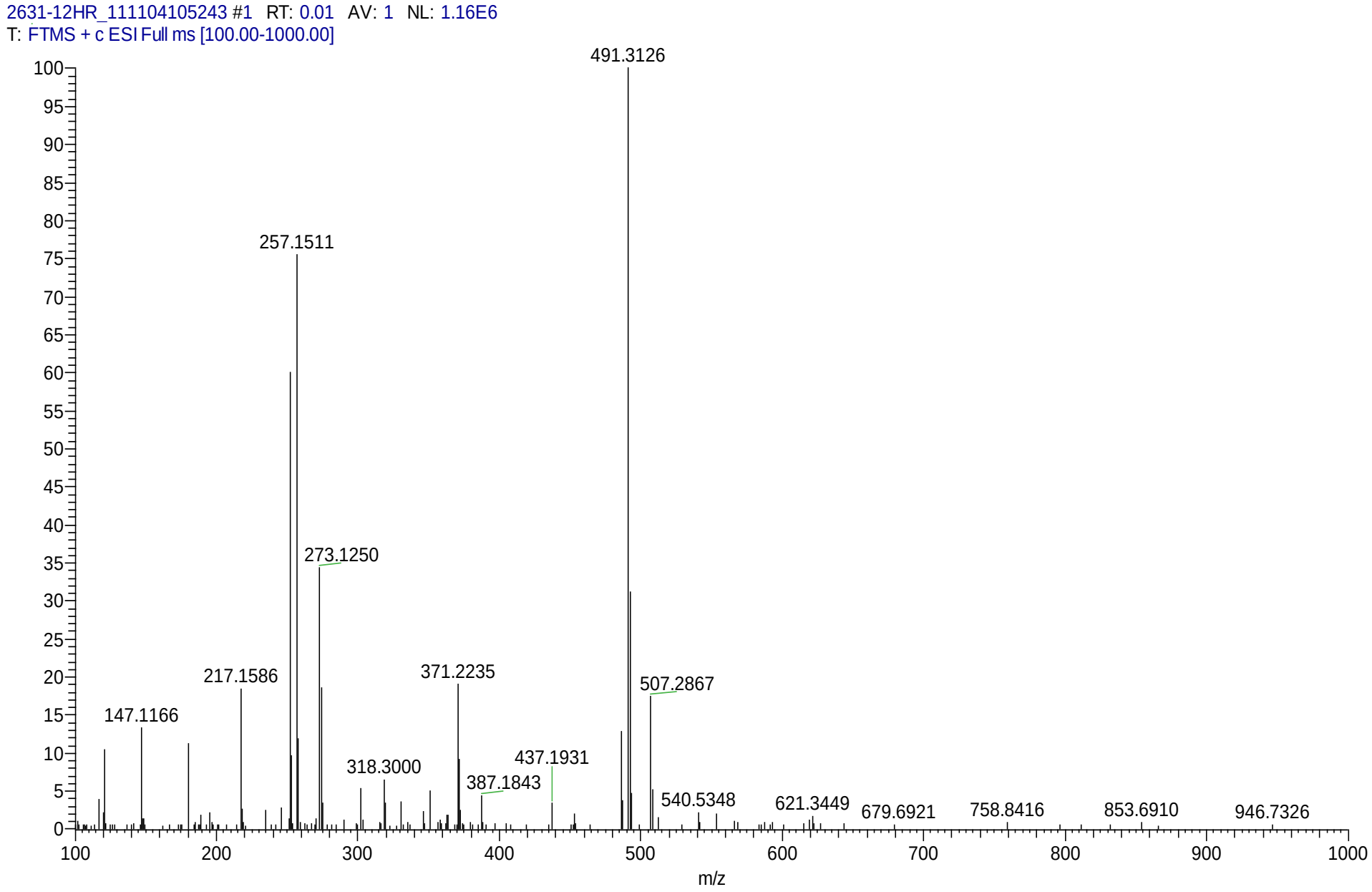


Fig. S15. ^{1}H-NMR Spectrum of Dichrocephone B (**2**; 600 MHz, CD_3COCD_3)

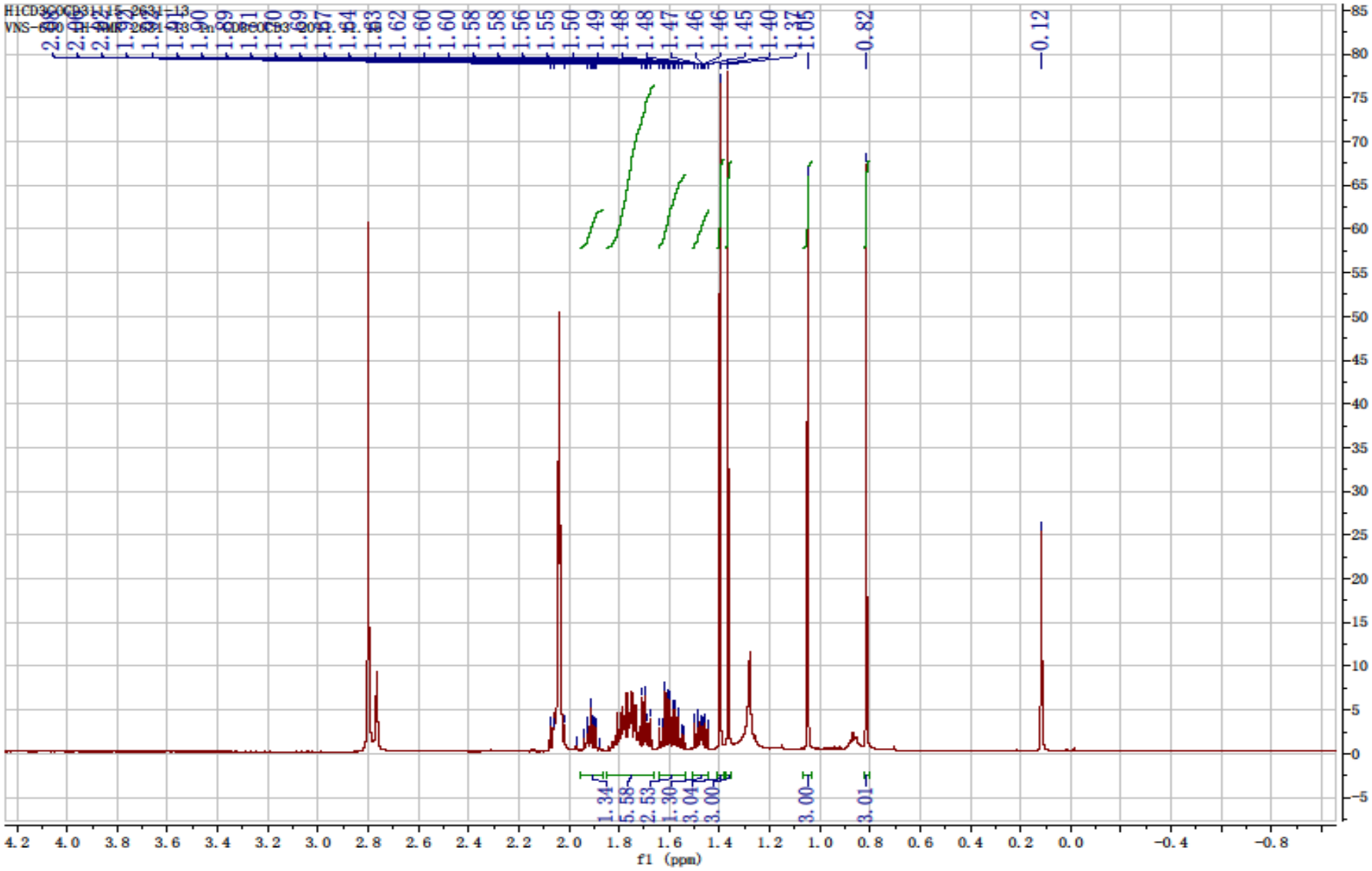


Fig. S16. ^{13}C-NMR Spectrum of Dichrocephone B (**2**; 150 MHz, CD_3COCD_3)

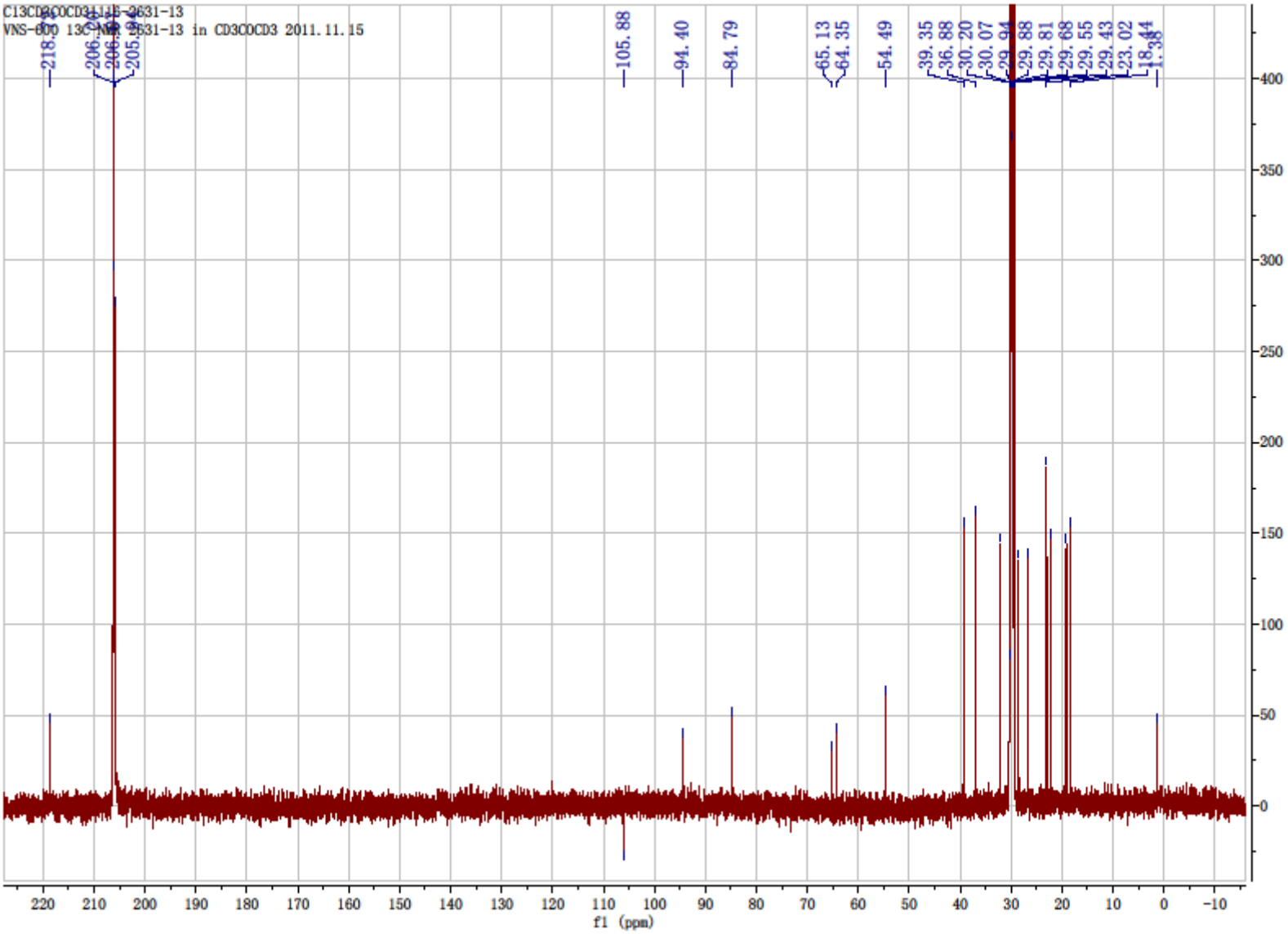


Fig. S17. DEPT Spectrum of Dichrocephone B (**2**; 150 MHz, CD_3COCD_3)

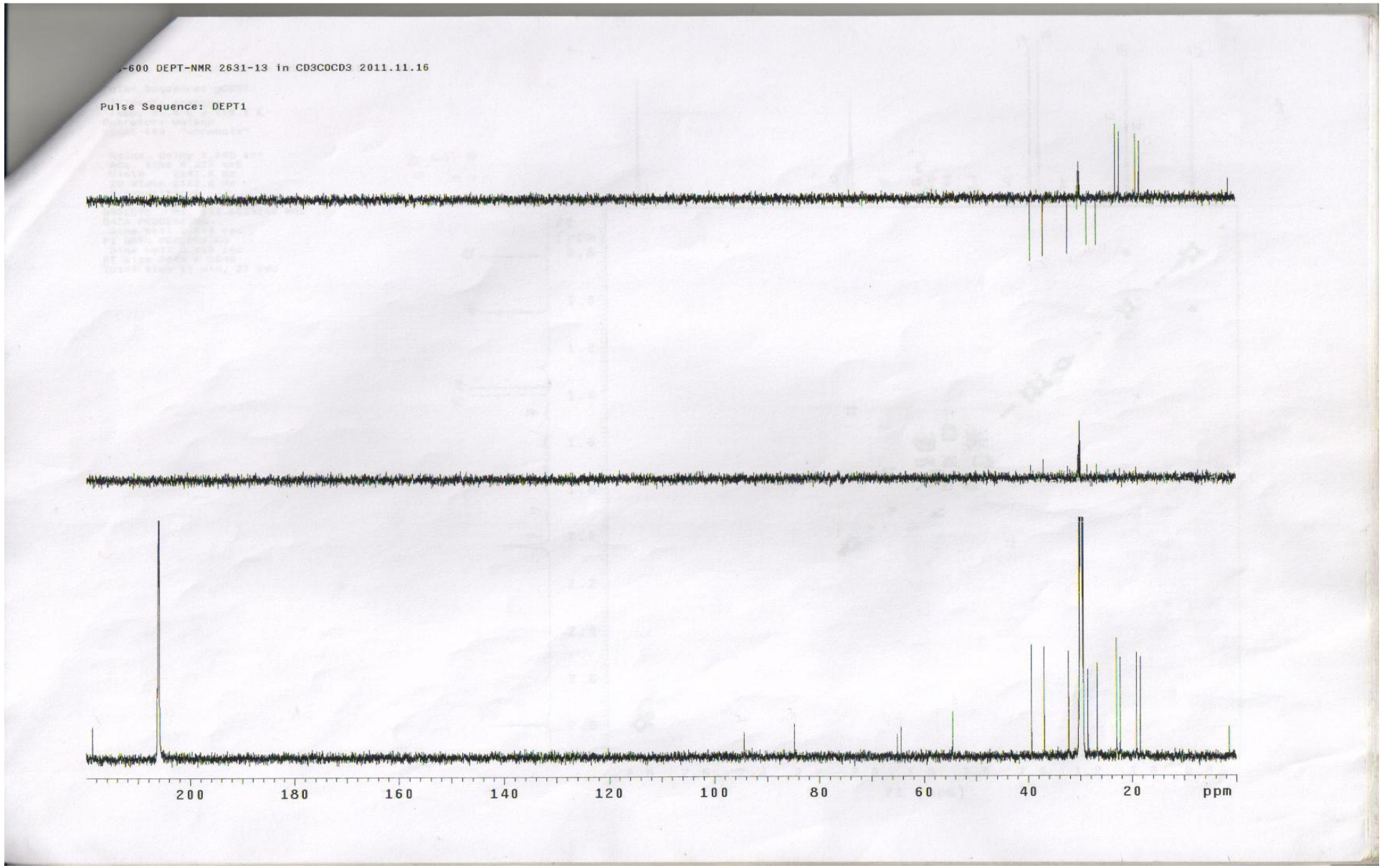


Fig. S18. ^{1}H-^{1}H COSY Spectrum of Dichrocephone B (**2**; 600 MHz, CD_3COCD_3)

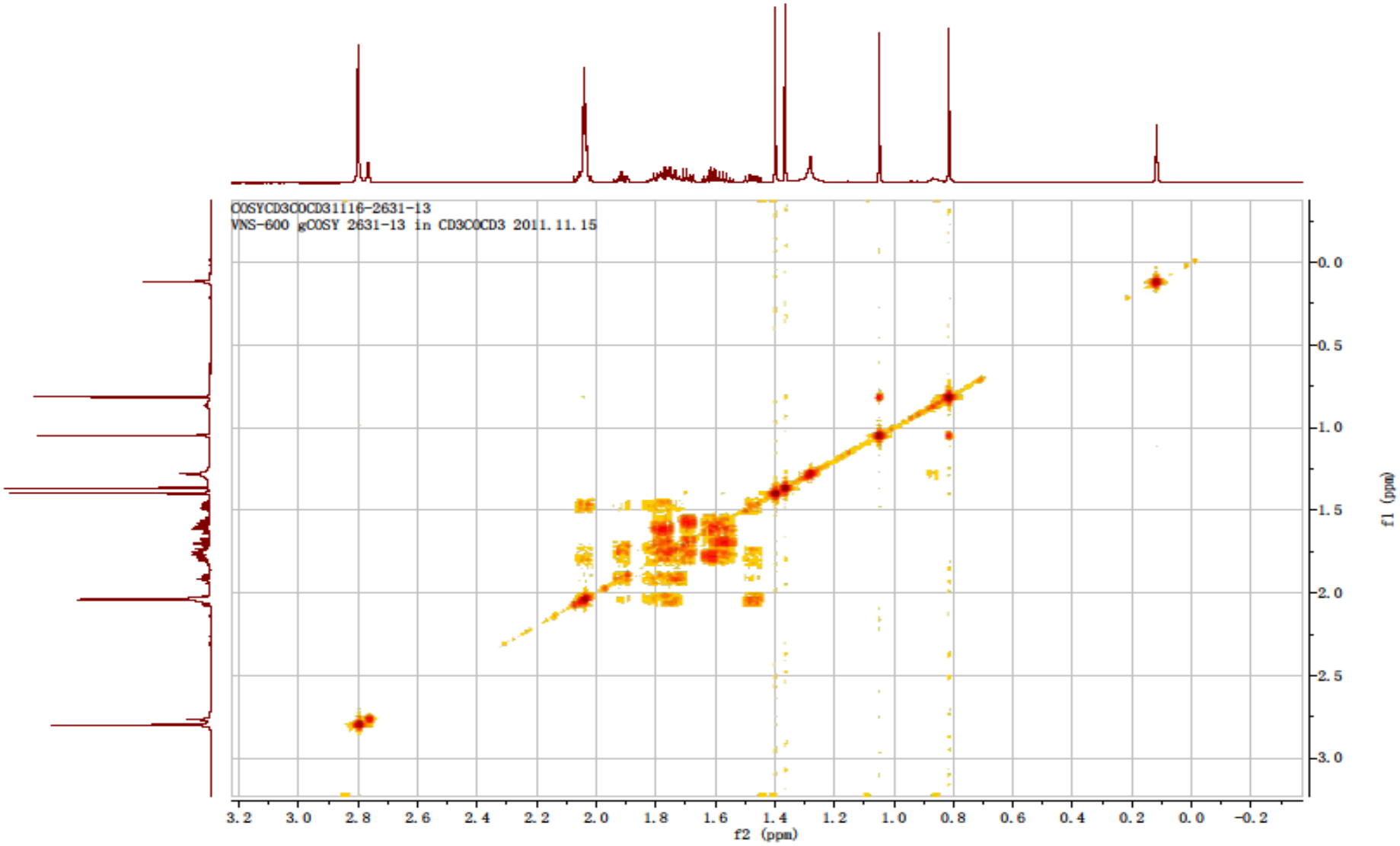


Fig. S19. HSQC Spectrum of Dichrocephone B (**2**; 600 MHz, CD_3COCD_3)

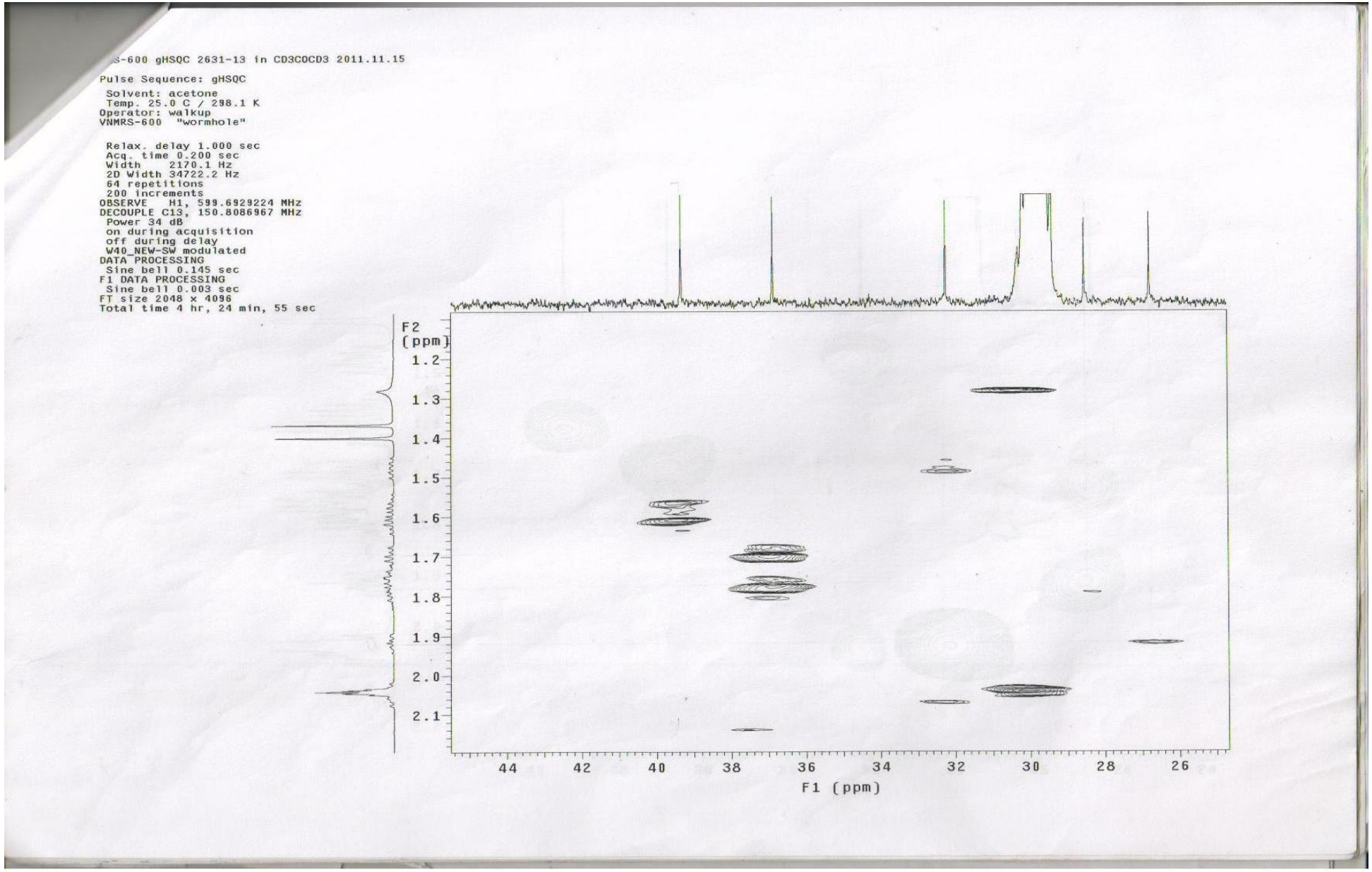


Fig. S20. HMBC Spectrum of Dichrocephone B (**2**; 600 MHz, CD_3COCD_3)

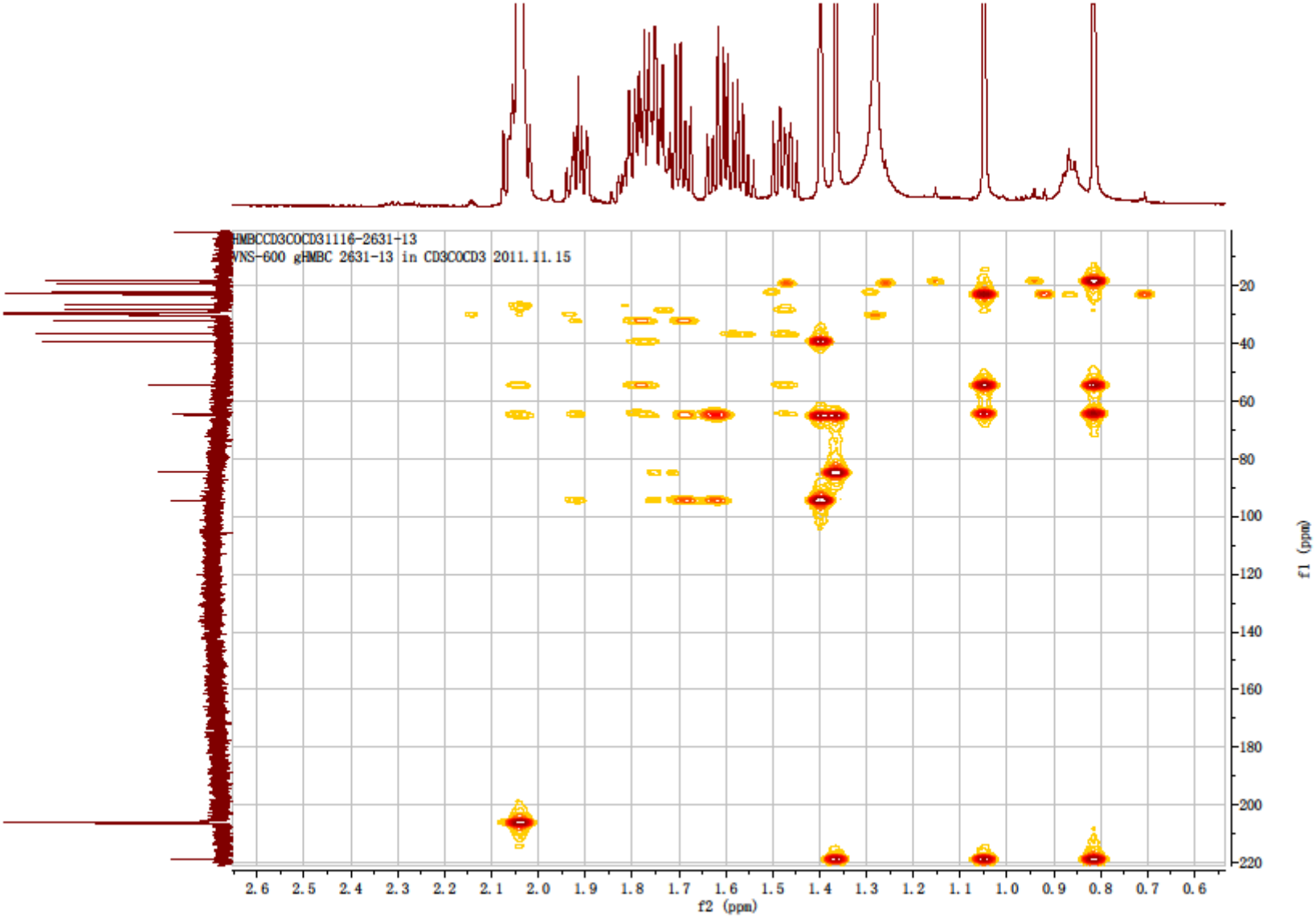


Fig. S21. The magnified HMBC Spectrum of Dichrocephone B (**2**; 600 MHz, CD_3COCD_3)

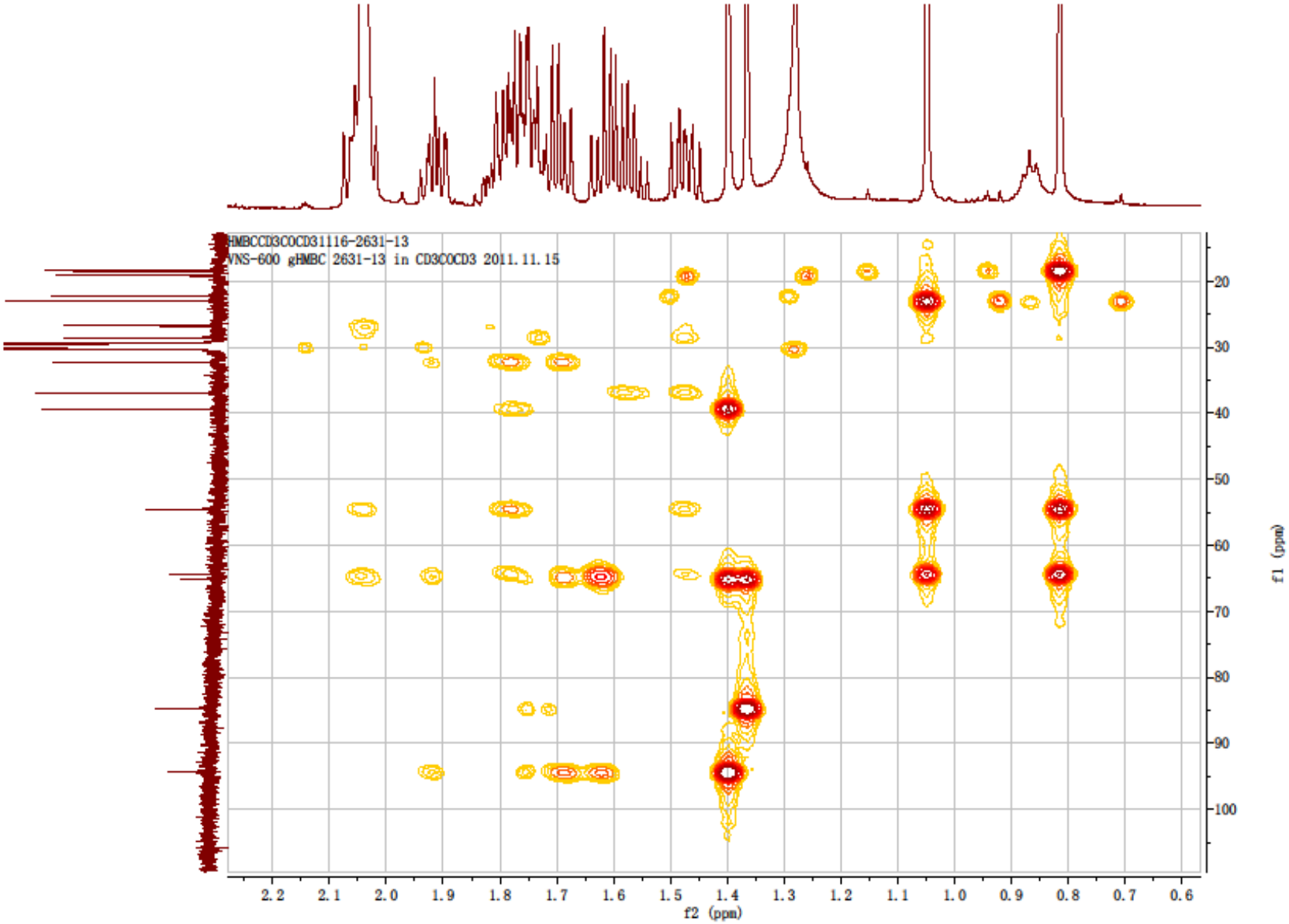


Fig. S22. ROESY Spectrum of Dichrocephone B (**2**; 600 MHz, CD_3COCD_3)

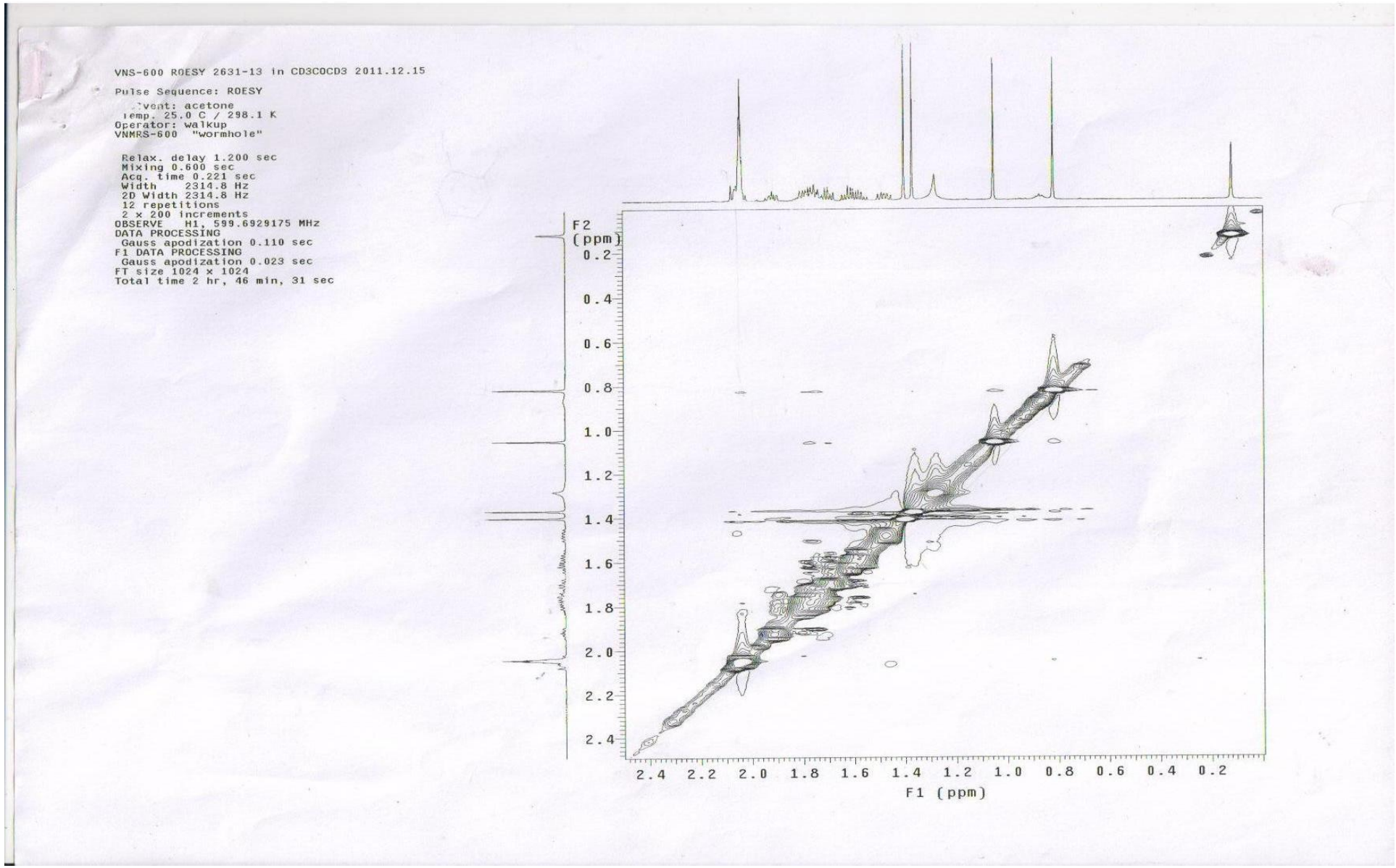
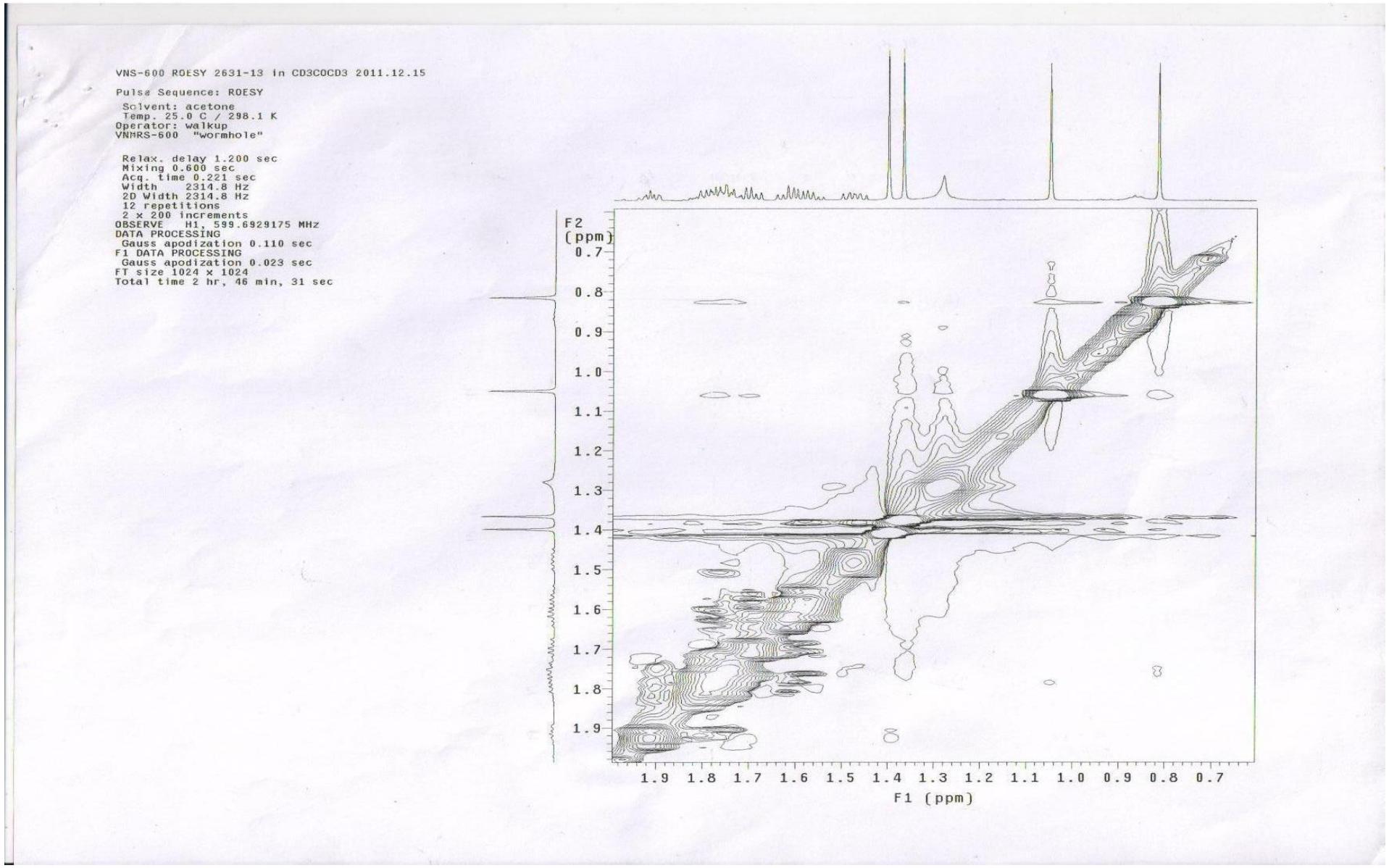


Fig. S23. The magnified ROESY Spectrum of Dichrocephone B (**2**; 600 MHz, CD_3COCD_3)



Tab. S1. The atomic coordinates of conformers of **1a** (Å)

1aC1				1aC2			
C	-0.9853	3.0621	0.6355	C	-2.0860	0.7146	1.9009
C	-1.2202	1.8086	1.4743	C	-0.7530	0.1468	1.4223
C	-1.2221	0.6427	0.3914	C	-0.7242	0.5565	-0.1122
C	-1.0392	1.3179	-1.0592	C	-1.9295	1.6130	-0.3503
C	-0.4736	2.7428	-0.7785	C	-2.5429	1.9138	1.0578
C	-2.5637	-0.1625	0.2771	C	-1.0263	-0.6181	-1.0941
C	-2.4980	1.3578	-1.6387	C	-2.9174	0.8412	-1.3074
C	-3.0950	0.0324	-1.1560	C	-1.9654	-0.0208	-2.1478
C	-0.0420	-0.3566	0.4805	C	0.5571	1.3061	-0.5943
C	-0.1033	0.3415	-1.8409	C	-1.2580	2.8317	-1.0407
C	0.0986	-0.9016	-0.9456	C	0.2246	2.8046	-0.6351
O	-1.1644	4.2151	0.9893	O	-2.7668	0.2972	2.8217
O	-0.9978	3.7431	-1.6702	O	-3.9858	1.9385	1.0613
C	-2.6454	1.5700	-3.1506	C	-3.8709	1.7154	-2.1285
C	1.0600	2.8881	-0.7748	C	-2.1082	3.2163	1.7588
C	-2.5298	2.0107	2.2673	C	0.3665	0.7960	2.2843
C	-0.0773	1.7198	2.5226	C	-0.7075	-1.3664	1.7201
O	-3.2420	2.3895	-0.9557	O	-3.6865	-0.1142	-0.5546
H	-3.3034	0.1831	0.9970	H	-1.5523	-1.4342	-0.6021
H	-2.3961	-1.2226	0.4966	H	-0.1053	-1.0311	-1.5200
H	-4.1886	0.0661	-1.2072	H	-2.5202	-0.7808	-2.7082
H	-2.7617	-0.7767	-1.8155	H	-1.4239	0.5983	-2.8725
H	0.8910	0.1437	0.7577	H	0.7885	0.9753	-1.6140
H	-0.2161	-1.1403	1.2269	H	1.4420	1.0788	0.0067
H	0.8646	0.8071	-2.0386	H	-1.7536	3.7803	-0.8133
H	-0.5102	0.0705	-2.8175	H	-1.3146	2.7095	-2.1271
H	1.0662	-1.3860	-1.1173	H	0.3784	3.2714	0.3435
H	-0.6733	-1.6538	-1.1478	H	0.8568	3.3512	-1.3442
H	-0.9690	4.5720	-1.1506	H	-4.2303	1.5999	1.9474
H	-2.1635	2.4992	-3.4672	H	-3.3426	2.3972	-2.8022
H	-3.7125	1.6356	-3.3904	H	-4.5138	2.3114	-1.4726
H	-2.2244	0.7465	-3.7346	H	-4.5113	1.0677	-2.7373
H	1.3218	3.8732	-0.3729	H	-2.5229	3.2179	2.7727
H	1.5664	2.1288	-0.1725	H	-1.0282	3.3445	1.8366
H	1.4377	2.8282	-1.7994	H	-2.5240	4.0733	1.2221
H	-3.3838	2.1558	1.6034	H	0.1328	0.6694	3.3468
H	-2.4329	2.9061	2.8884	H	0.5069	1.8618	2.0938
H	-2.7235	1.1581	2.9270	H	1.3200	0.2933	2.0925
H	-0.1515	2.5669	3.2120	H	-1.5977	-1.8902	1.3650
H	0.9234	1.7428	2.0842	H	-0.6479	-1.5254	2.8013
H	-0.1707	0.7965	3.1041	H	0.1751	-1.8216	1.2586
H	-2.8369	3.2239	-1.2621	H	-4.2118	0.4309	0.0637
1aC3				1aC4			
C	-0.0846	2.0948	1.2451	C	-1.6278	-0.9299	1.5588
C	0.4418	0.6527	1.2971	C	-0.6961	-1.7229	0.6452
C	-0.1182	-0.0119	-0.0318	C	0.0222	-0.6152	-0.2192
C	-1.0409	1.0746	-0.7643	C	-0.9078	0.7051	-0.1461
C	-0.6544	2.4656	-0.1449	C	-1.9931	0.4554	0.9645

C	-1.0599	-1.2499	0.1785	C	0.1881	-0.9073	-1.7399
C	-2.4998	0.6450	-0.3996	C	-1.3856	0.9270	-1.6375
C	-2.4311	-0.8884	-0.4245	C	-0.1745	0.4155	-2.4395
C	0.9461	-0.3674	-1.1014	C	1.3977	-0.1537	0.3666
C	-0.7499	0.8904	-2.2891	C	0.0833	1.8236	0.3012
C	0.1733	-0.3404	-2.4249	C	1.1245	1.1165	1.1762
O	-0.0464	2.8761	2.1754	O	-2.1070	-1.3354	2.6018
O	-1.7300	3.3887	-0.0196	O	-3.3114	0.2911	0.3751
C	-3.6428	1.2183	-1.2439	C	-1.8212	2.3598	-1.9649
C	0.4413	3.2507	-0.8834	C	-2.1519	1.4969	2.0753
C	-0.0367	0.0272	2.6257	C	0.2145	-2.6386	1.4842
C	1.9902	0.7266	1.3818	C	-1.6408	-2.6428	-0.1822
O	-2.6848	1.0846	0.9777	O	-2.4404	0.0348	-2.0346
H	-0.6421	-2.1411	-0.3021	H	-0.4972	-1.6789	-2.0877
H	-1.1696	-1.4965	1.2330	H	1.2037	-1.2437	-1.9760
H	-3.2728	-1.3311	0.1233	H	-0.4489	0.2776	-3.4907
H	-2.5141	-1.2356	-1.4610	H	0.6543	1.1316	-2.4072
H	1.7382	0.3861	-1.1447	H	2.0606	0.1087	-0.4671
H	1.4314	-1.3298	-0.9020	H	1.9140	-0.9322	0.9312
H	-0.2440	1.7705	-2.6911	H	-0.4094	2.6719	0.7810
H	-1.6613	0.7751	-2.8796	H	0.6029	2.2241	-0.5748
H	0.8331	-0.2714	-3.2968	H	0.7209	0.8734	2.1682
H	-0.4169	-1.2568	-2.5452	H	2.0239	1.7218	1.3367
H	-2.3642	2.9556	0.5837	H	-3.9074	-0.0286	1.0740
H	-3.6274	0.8414	-2.2700	H	-1.0403	3.0997	-1.7656
H	-3.5989	2.3095	-1.2713	H	-2.7079	2.6317	-1.3801
H	-4.6042	0.9187	-0.8071	H	-2.0876	2.4208	-3.0255
H	0.7509	4.0884	-0.2513	H	-2.8831	1.1193	2.7979
H	1.3204	2.6447	-1.1174	H	-1.2275	1.6882	2.6239
H	0.0401	3.6590	-1.8161	H	-2.5221	2.4386	1.6601
H	0.3711	-0.9814	2.7570	H	-0.3938	-3.3867	2.0014
H	-1.1260	-0.0166	2.6869	H	0.7755	-2.0938	2.2490
H	0.3179	0.6485	3.4533	H	0.9283	-3.1644	0.8407
H	2.4455	1.2988	0.5693	H	-1.0502	-3.3459	-0.7792
H	2.4230	-0.2797	1.3712	H	-2.2852	-2.0724	-0.8536
H	2.2752	1.2121	2.3205	H	-2.2663	-3.2260	0.5019
H	-3.5366	0.7401	1.2932	H	-3.1235	0.0871	-1.3412
1aC5				1aC6			
C	-2.7101	0.8519	0.7290	C	0.4939	2.6547	-0.2190
C	-2.2226	-0.4322	0.0318	C	-0.1532	2.2405	1.1172
C	-1.3483	0.1000	-1.1800	C	-1.1720	1.0951	0.7058
C	-1.1397	1.6450	-0.9271	C	-0.8924	0.7884	-0.8232
C	-2.3890	2.0930	-0.1293	C	-0.3379	2.1287	-1.4067
C	-2.0045	0.0346	-2.5801	C	-2.6757	1.4539	0.7397
C	-0.9799	2.3172	-2.3681	C	-2.2786	0.2984	-1.4245
C	-1.3407	1.1737	-3.3735	C	-3.3091	0.4882	-0.2743
C	0.0990	-0.4691	-1.2272	C	-0.9240	-0.2652	1.4245
C	0.1147	1.6928	-0.0132	C	0.2272	-0.2859	-0.7705
C	1.0009	0.4807	-0.3963	C	0.0112	-1.1116	0.5209
O	-3.3268	0.8924	1.7762	O	1.4998	3.3266	-0.3274
O	-3.5385	2.1253	-1.0353	O	-1.3393	3.1595	-1.5008

C	0.4119	2.8768	-2.6759	C	-2.3070	-1.1309	-1.9735
C	-2.3123	3.4013	0.6432	C	0.4383	2.0438	-2.7181
C	-1.4627	-1.2703	1.0873	C	0.9784	1.8146	2.0784
C	-3.4643	-1.2600	-0.3820	C	-0.8189	3.4977	1.7319
O	-1.8320	3.4599	-2.5370	O	-2.6061	1.1682	-2.5476
H	-3.0773	0.2173	-2.5155	H	-2.8370	2.4804	0.4083
H	-1.8648	-0.9426	-3.0578	H	-3.1132	1.3507	1.7397
H	-1.9879	1.5722	-4.1614	H	-4.2656	0.8539	-0.6664
H	-0.4291	0.8174	-3.8671	H	-3.5149	-0.4828	0.1893
H	0.4435	-0.4908	-2.2660	H	-1.8766	-0.7862	1.5618
H	0.1466	-1.5038	-0.8775	H	-0.5182	-0.1284	2.4291
H	-0.1934	1.5895	1.0350	H	1.1985	0.2200	-0.7075
H	0.6465	2.6462	-0.0732	H	0.2744	-0.9044	-1.6710
H	1.3933	-0.0088	0.5014	H	0.9692	-1.3255	1.0070
H	1.8738	0.7948	-0.9774	H	-0.4417	-2.0838	0.2999
H	-4.3012	2.4436	-0.5222	H	-2.0612	2.7449	-2.0195
H	0.4103	3.2577	-3.7031	H	-3.3236	-1.3665	-2.3145
H	1.1949	2.1189	-2.5980	H	-2.0386	-1.8728	-1.2170
H	0.6577	3.7110	-2.0114	H	-1.6323	-1.2376	-2.8283
H	-1.4701	3.4131	1.3399	H	1.2422	1.3029	-2.6831
H	-2.2016	4.2336	-0.0561	H	-0.2416	1.7804	-3.5334
H	-3.2255	3.5381	1.2341	H	0.8852	3.0197	-2.9301
H	-2.1065	-1.4033	1.9620	H	1.7223	2.6154	2.1212
H	-0.5369	-0.7974	1.4258	H	1.4927	0.9043	1.7559
H	-1.2168	-2.2619	0.6940	H	0.5949	1.6520	3.0910
H	-4.1596	-0.6926	-1.0041	H	-1.3564	3.2325	2.6495
H	-4.0039	-1.5797	0.5156	H	-1.5152	3.9776	1.0422
H	-3.1564	-2.1558	-0.9329	H	-0.0451	4.2286	1.9902
H	-2.7268	3.1772	-2.2677	H	-3.5081	0.9513	-2.8346