Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information for

Dicarabrol A, dicarabrone C and dipulchellin A, unique sesquiterpene lactone dimers from *Carpesium abrotanoides* †

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Experimental Section

X-ray crystallographic analyses.

Table S1. X-ray crystallographic data for dipulchellin A (**3**)

Experimental Section

X-ray crystallographic analyses. Dipulchellin A (**3**) was crystallized from acetone at room temperature. The X-ray crystallographic data was obtained on a Bruker SMART CCD detector employing graphite monochromated Cu-Kα radiation (λ = 1.54178 Å) (operated in the φ-ω scan mode). The structure was solved by direct method using SHELXS-97 program and refined with full-matrix least-squares calculations on $F2$ using SHELXL-97. Crystallographic data for **3** (key parameters see Table S1) have been deposited at the Cambridge Crystallographic Data Centre (Deposition No.: CCDC 1479445). Copies of these data can be obtained free of charge via the internet at www.ccdc.cam.ac.uk/conts/retrieving.html or on application to CCDC, 12 Union Road, Cambridge CB2 1EZ, UK [Tel: (+44) 1223-336-408; Fax: (+44) 1223-336-033; E-mail: deposit@ccdc.cam.ac.uk].

Table S1. X-ray crystallographic data for dipulchellin A (**3**)

Crystal data	
$C_{34}H_{44}O_7$	$F(000)$ = 1216
M_r = 564.69	D_x = 1.221 Mg m^{-3}
Orthorhombic, $P2_12_12_1$	Cu $K\alpha$ radiation, λ = 1.54178 Å
a = 10.4583 (1) Å	μ = 0.68 mm^{-1}
b = 13.3200 (2) Å	T = 296 K
c = 22.0536 (3) Å	Plate, colourless
V = 3072.17 (7) Å^3	0.15 × 0.1 × 0.05 mm
Z = 4	
Data collection	
Radiation source: fine-focus sealed tube	R_{int} = 0.034

graphite	$\theta_{max} = 67.7°$, $\theta_{min} = 3.9°$
40986 measured reflections	$h = -10 \rightarrow 12$
5469 independent reflections	$k = -15 \rightarrow 14$
5246 reflections with $I > 2\sigma(I)$	$l = -26 \rightarrow 25$
Refinement	
Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.099$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.308$	$w = 1/[\sigma^2(F_o^2) + (0.2P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.54$	$(\Delta/\sigma)_{max} = 0.179$
5469 reflections	$\Delta\rangle_{max} = 0.93$ e Å^{-3}
377 parameters	$\Delta\rangle_{min} = -1.14$ e Å^{-3}
22 restraints	Absolute structure: Flack H D (1983), Acta Cryst. A39, 876-881
Primary atom site location: structure-invariant direct methods	Flack parameter: 0.1 (4)

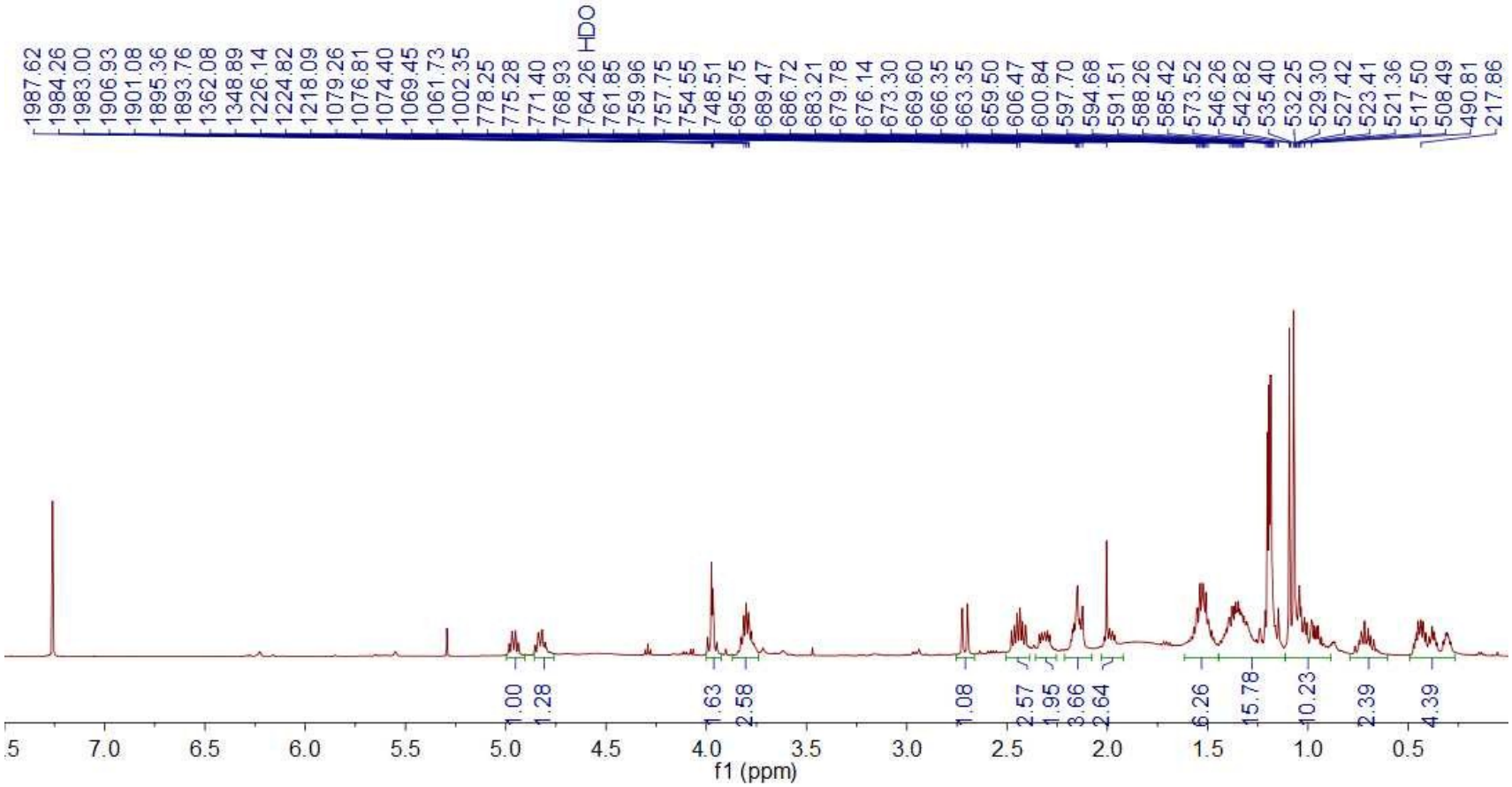


Figure S1. ^{1}H NMR spectrum of dicarabrol A (**1**) in $CDCl_3$

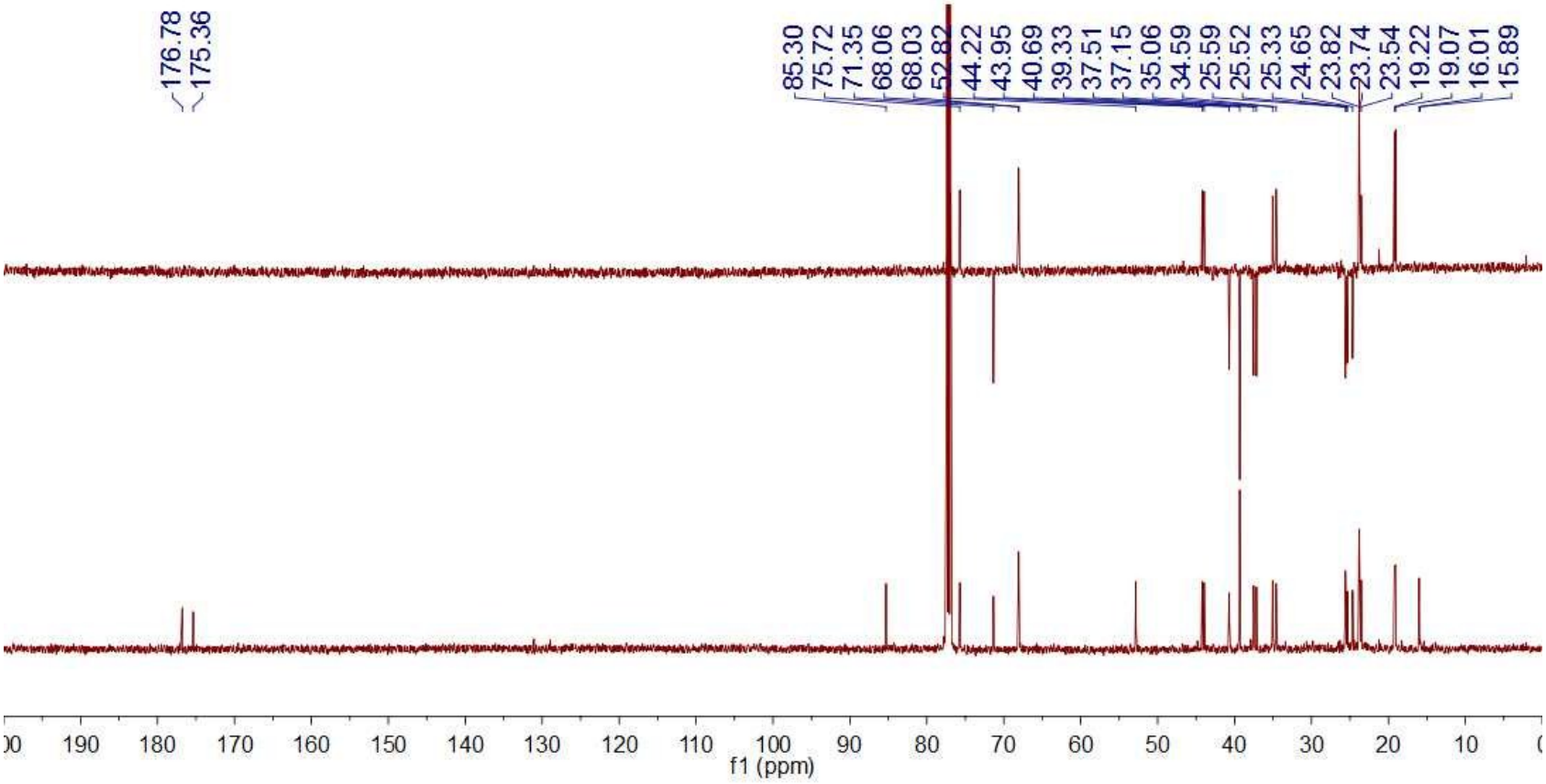


Figure S2. ^{13}C NMR spectrum of dicarabrol A (**1**) in $CDCl_3$

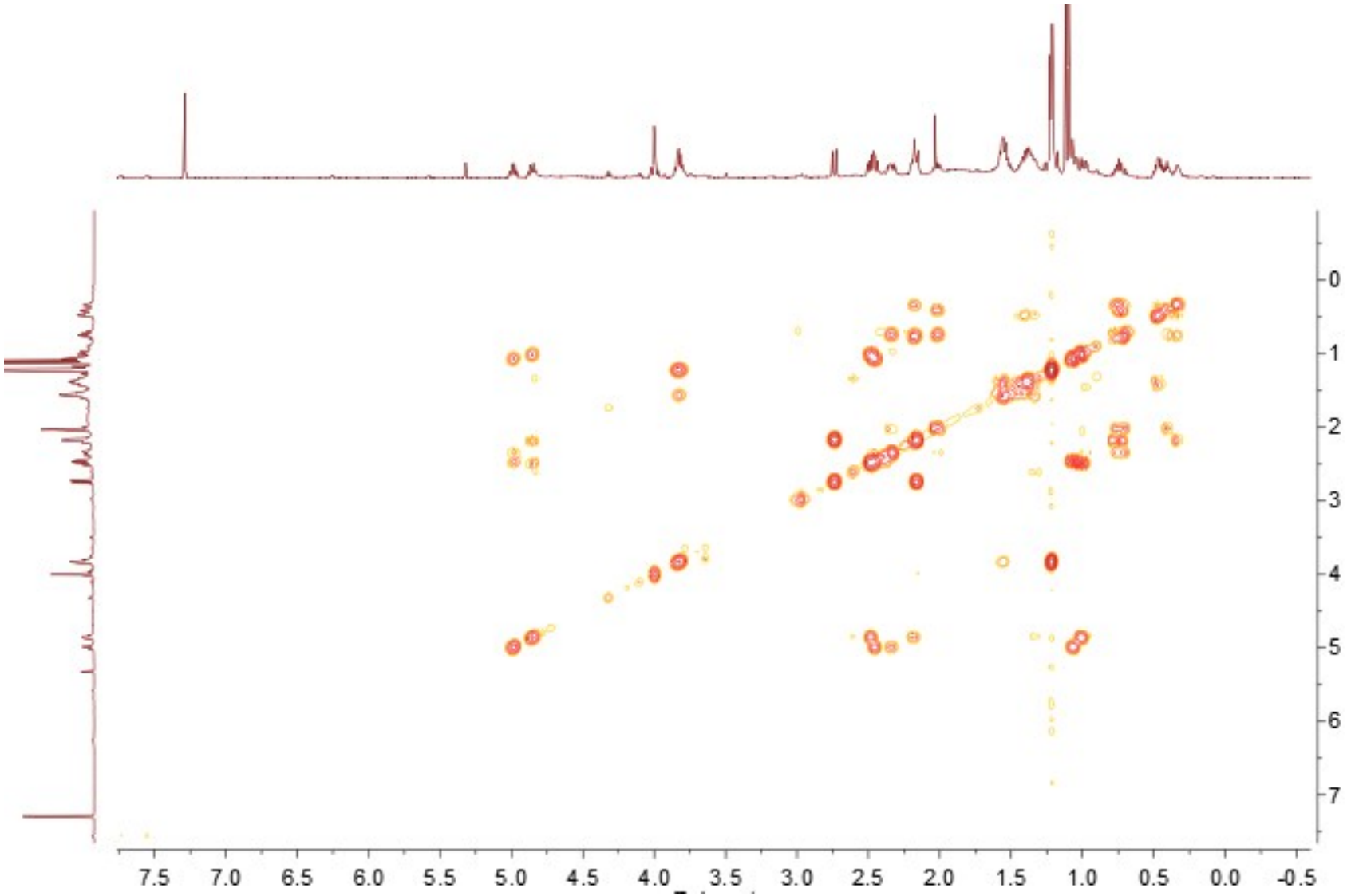


Figure S3. ^{1}H-^{1}H COSY spectrum of dicarabrol A (**1**) in $CDCl_3$

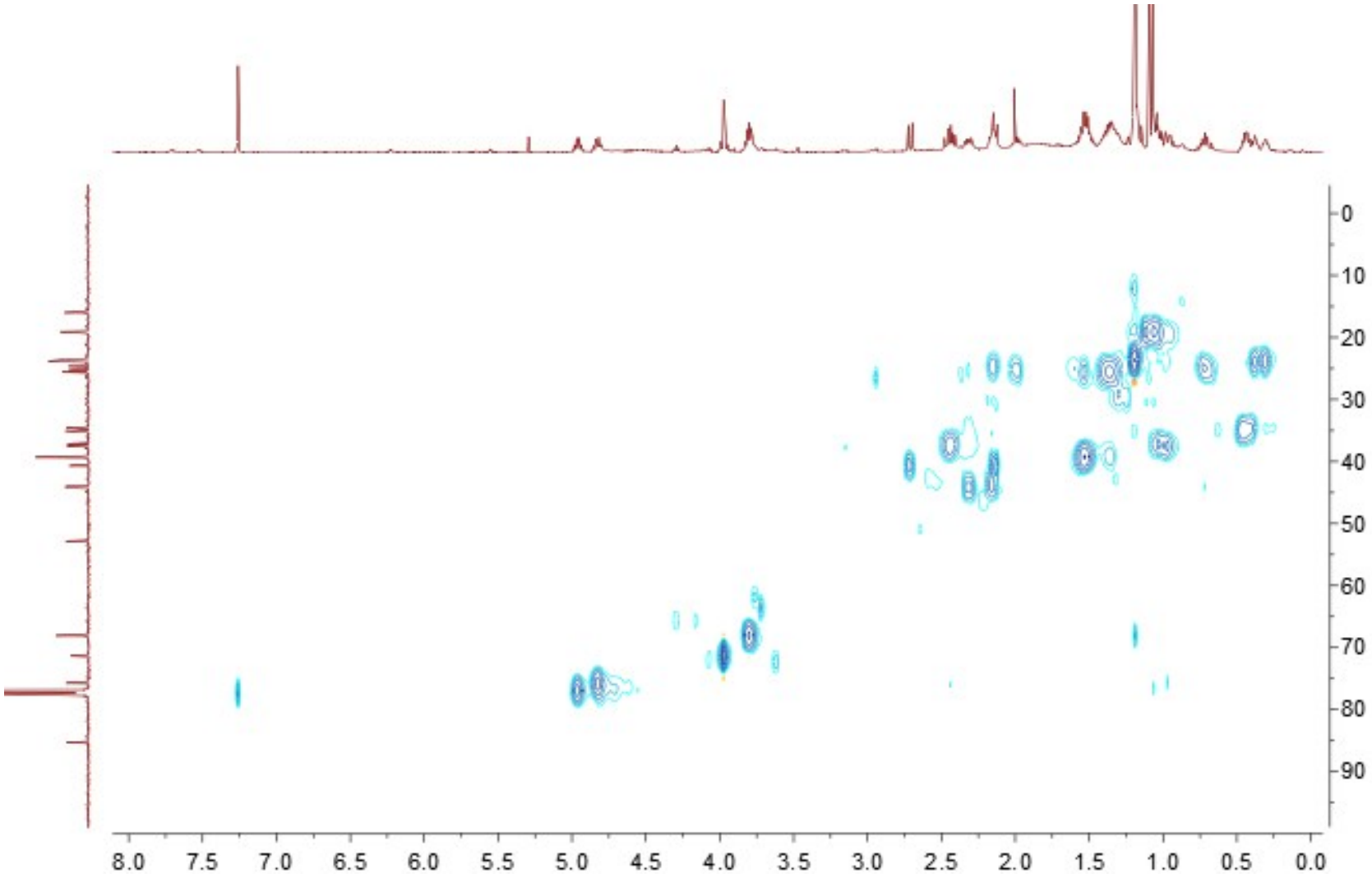


Figure S4. HSQC spectrum of dicarabrol A (**1**) in $CDCl_3$

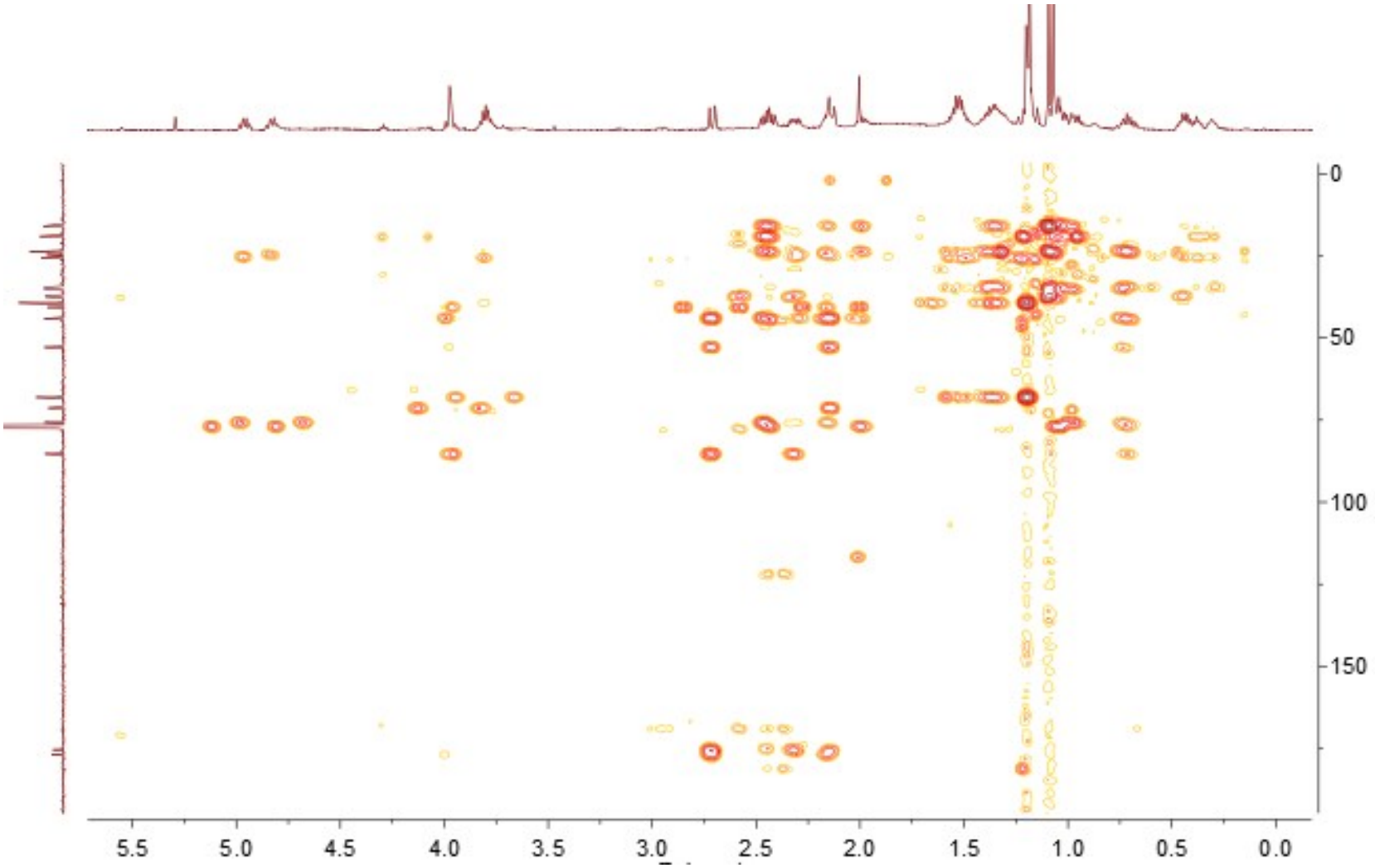


Figure S5. HMBC spectrum of dicarabrol A (**1**) in $CDCl_3$

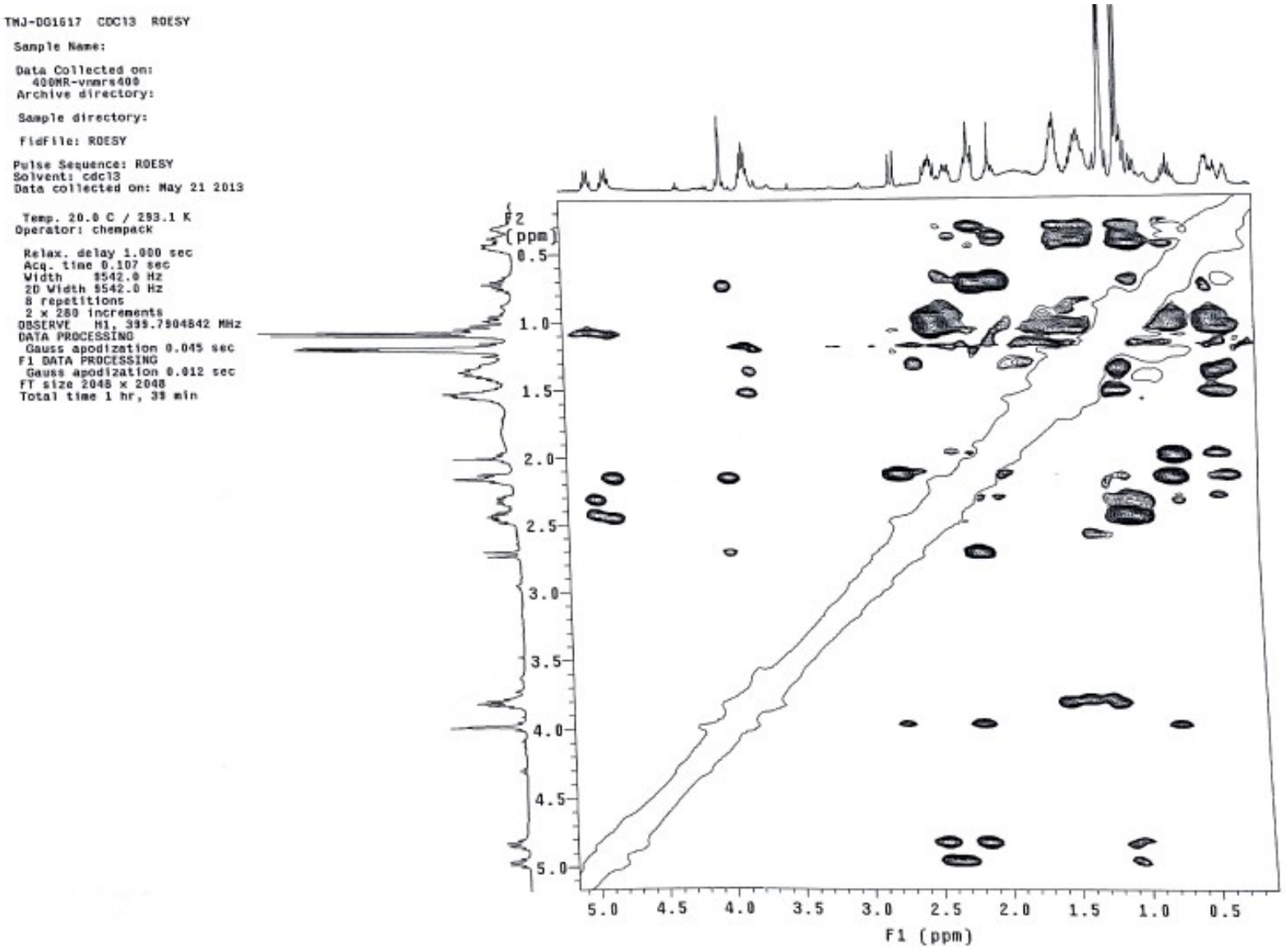


Figure S6. ROESY spectrum of dicarabrol A (**1**) in $CDCl_3$

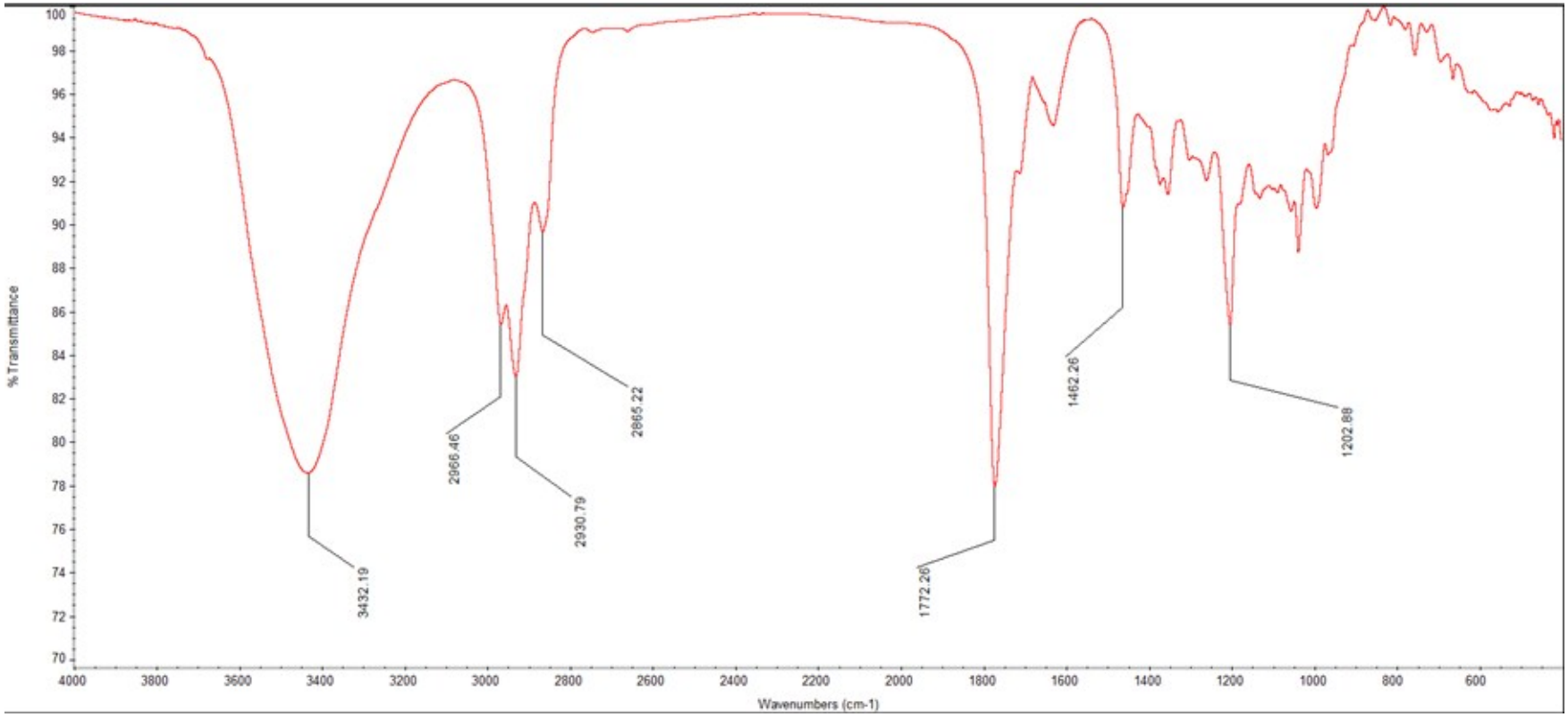


Figure S7. IR spectrum of dicarabrol A (**1**)

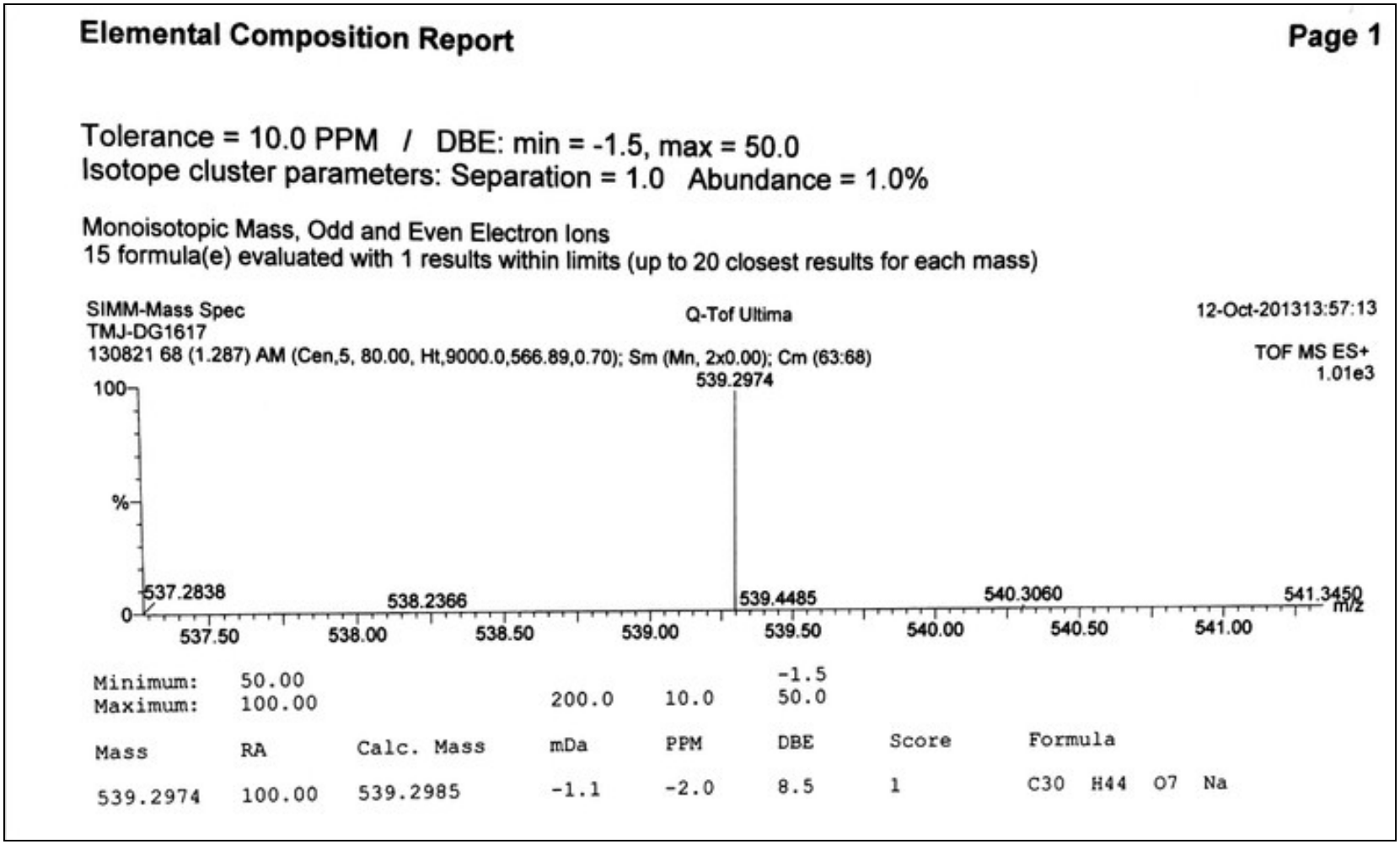


Figure S8. HRESI(+)MS spectrum of dicarabrol A (**1**)

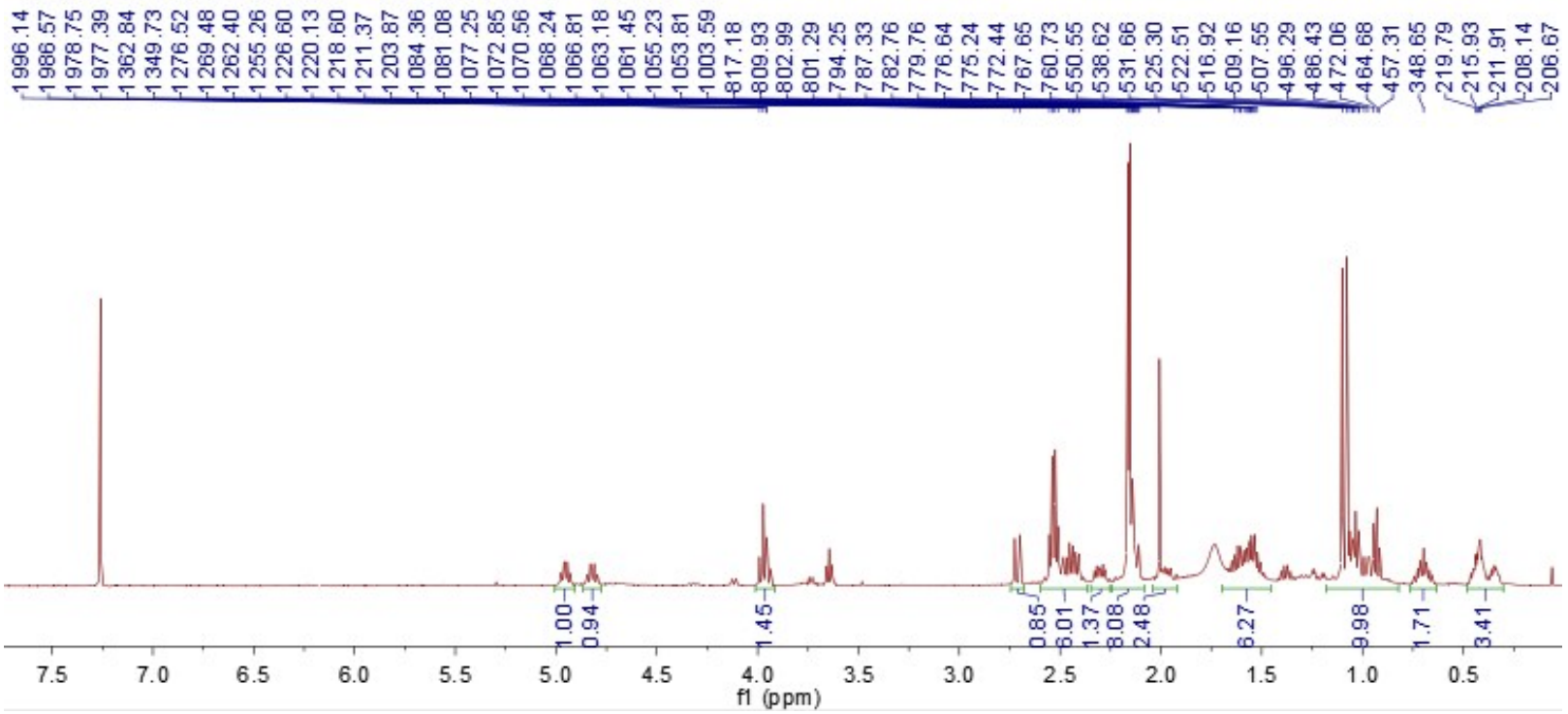


Figure S9. ^{1}H NMR spectrum of dicarabrone C (**2**) in $CDCl_3$

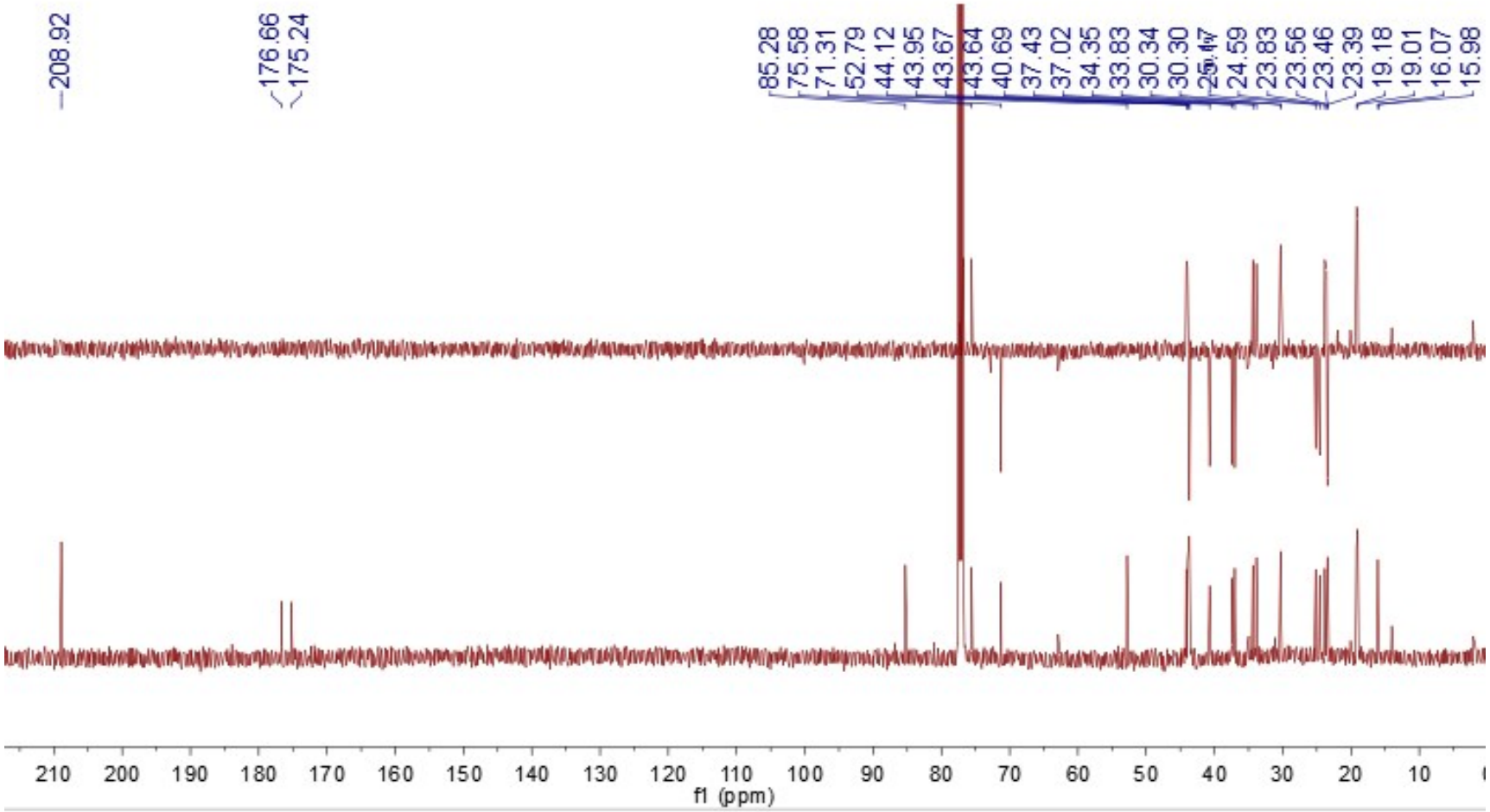


Figure S10. ^{13}C NMR spectrum of dicarabrone C (**2**) in $CDCl_3$

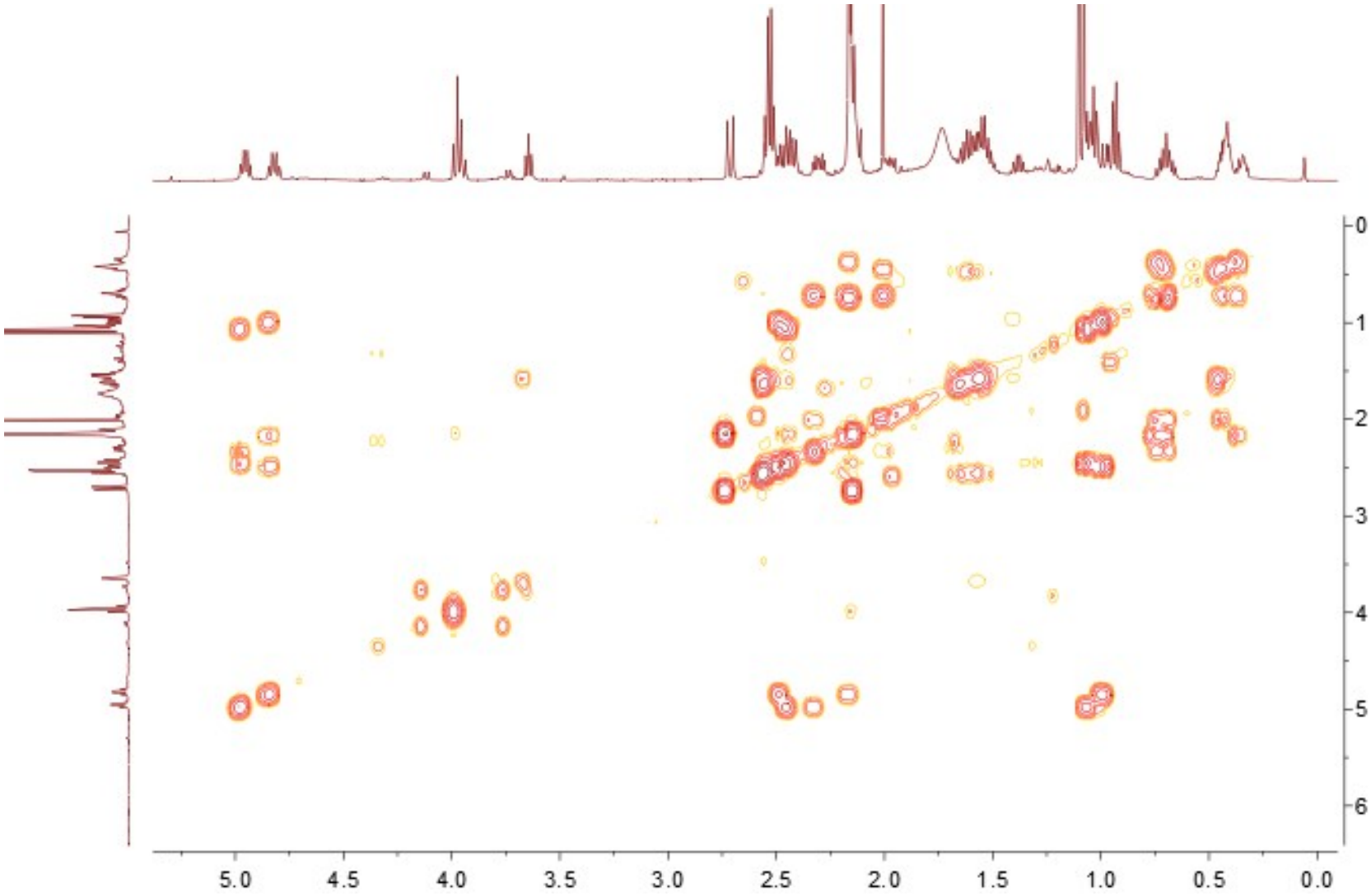


Figure S11. ^{1}H-^{1}H COSY spectrum of dicarabrone C (**2**) in $CDCl_3$

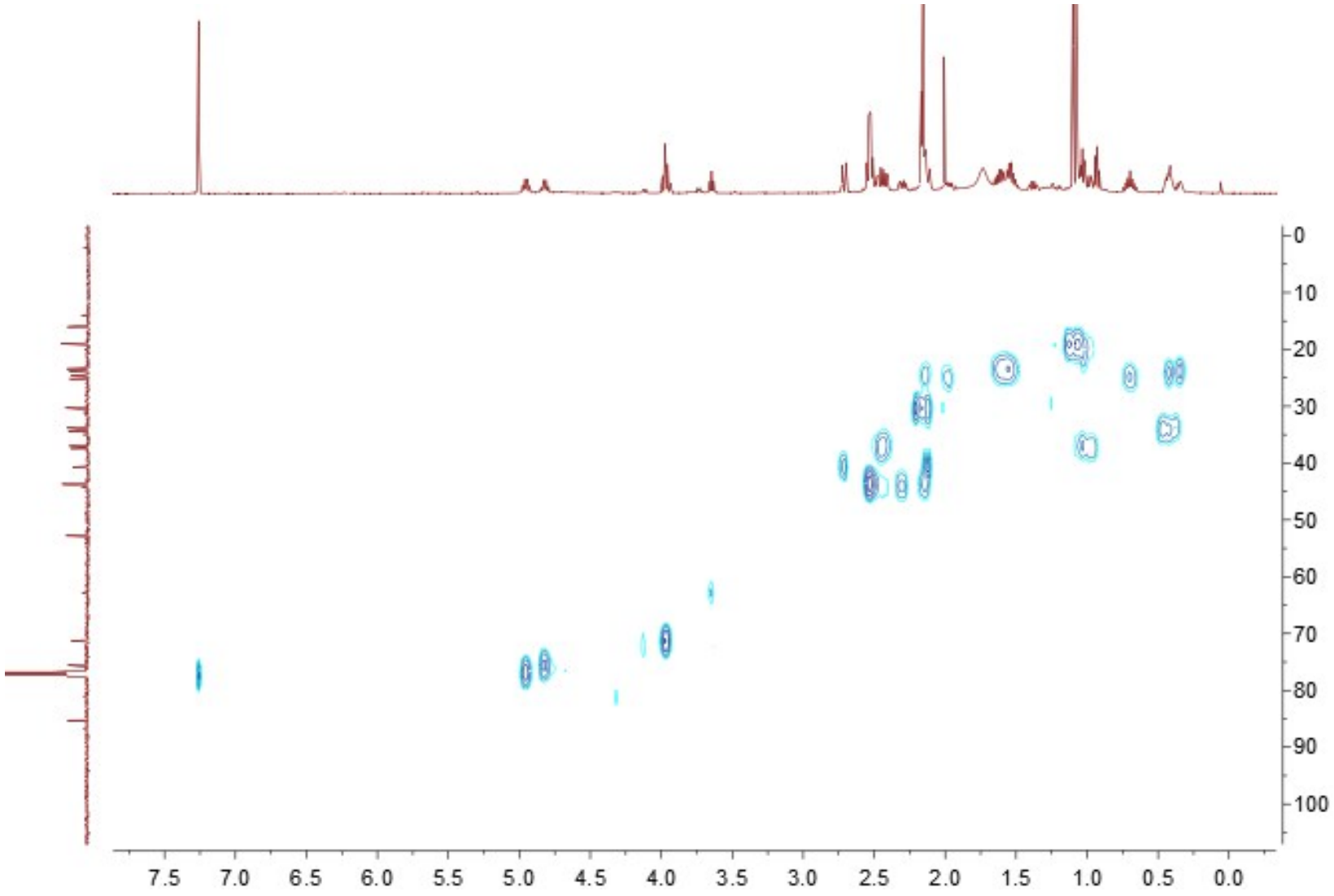


Figure S12. HSQC spectrum of dicarabrone C (**2**) in $CDCl_3$

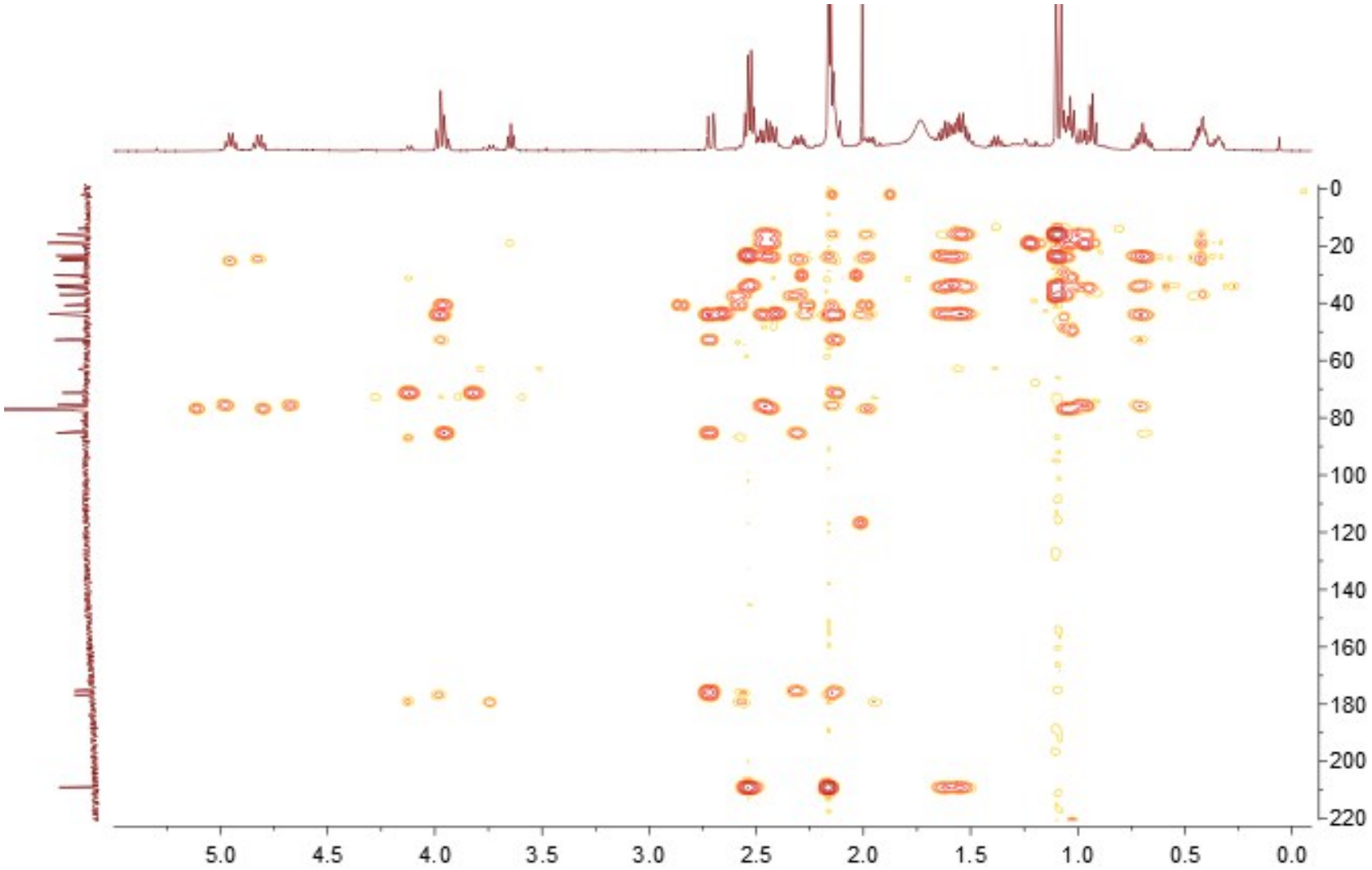


Figure S13. HMBC spectrum of dicarabrone C (**2**) in $CDCl_3$

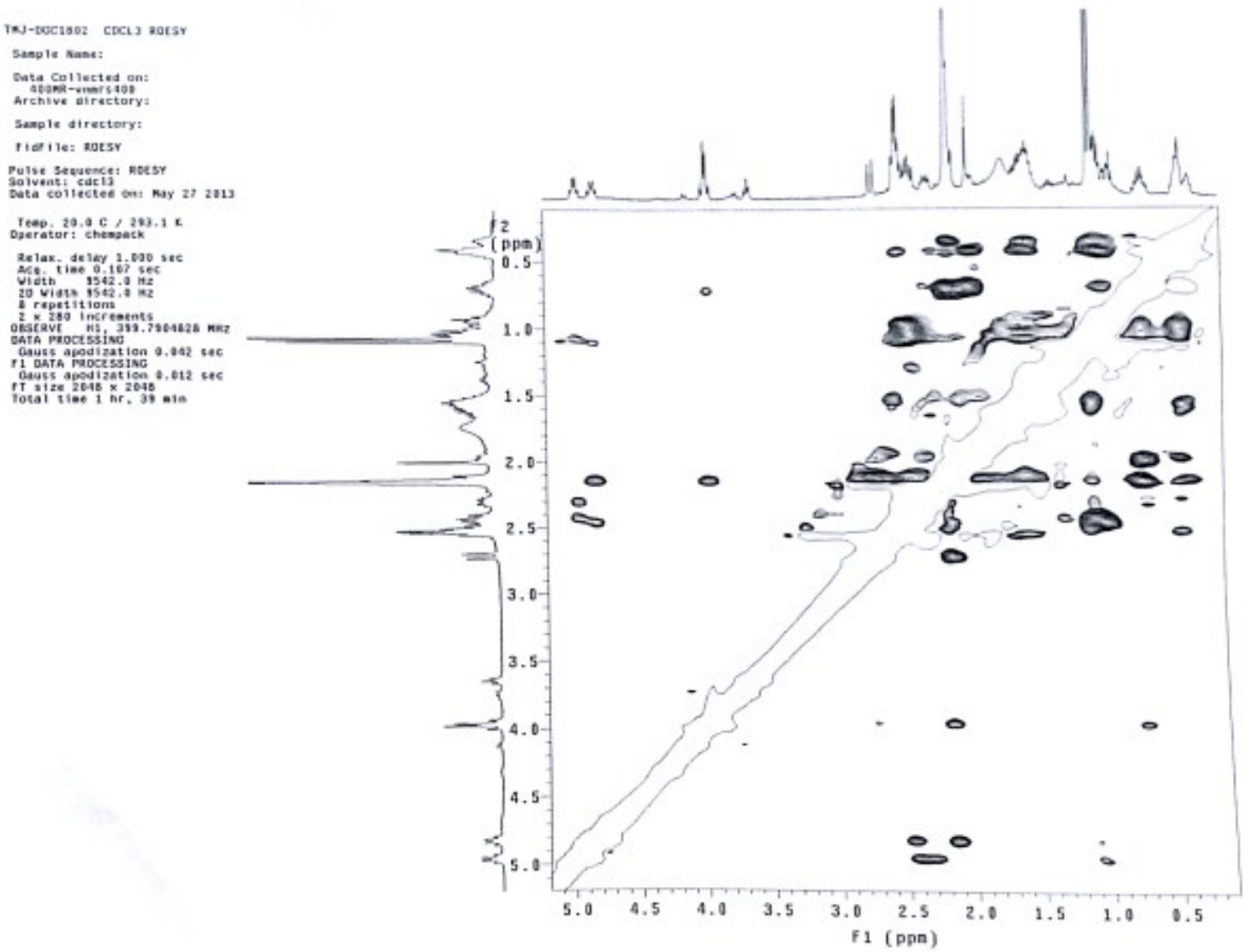


Figure S14. ROESY spectrum of dicarabrone C (**2**) in $CDCl_3$

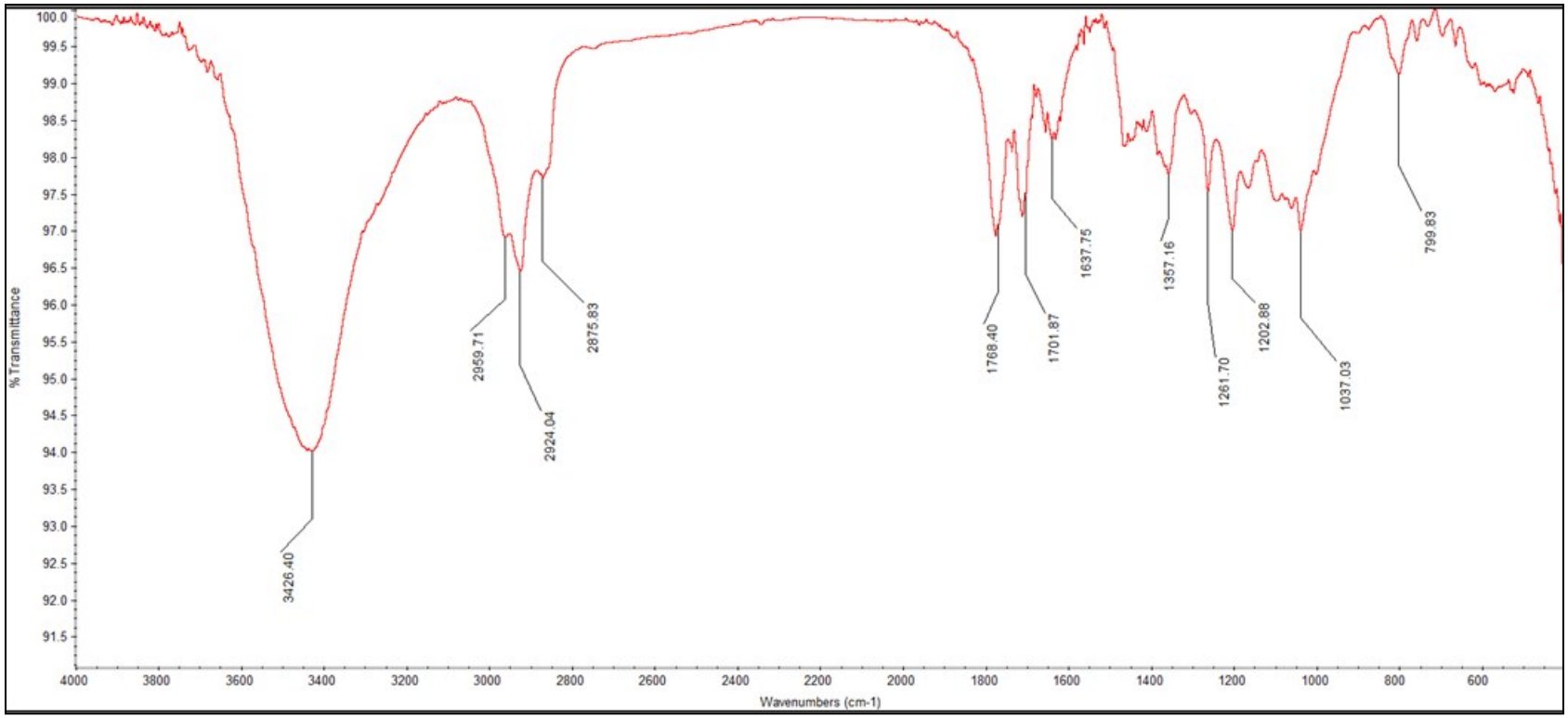


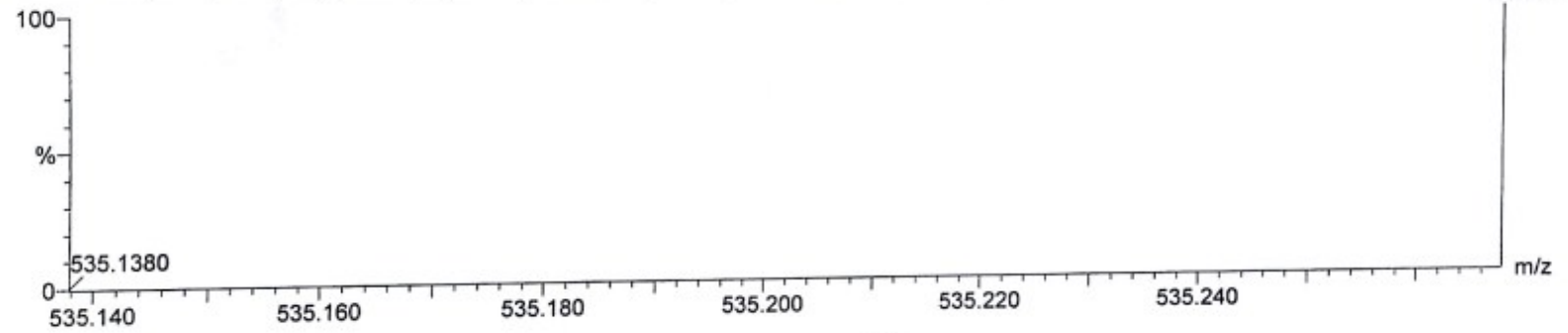
Figure S15. IR spectrum of dicarabrone C (**2**)

Elemental Composition Report **Page 1**

Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0
Isotope cluster parameters: Separation = 1.0 Abundance = 1.0%

Monoisotopic Mass, Odd and Even Electron Ions
36 formula(e) evaluated with 1 results within limits (up to 20 closest results for each mass)

SIMM-Mass Spec Q-Tof Ultima 15-Oct-201315:11:57
TMJ-DGC1802
130881 154 (2.911) AM (Cen,5, 80.00, Ht,9000.0,566.89,0.70); Sm (Mn, 2x0.00); Cm (153:164) TOF MS ES+
3.31e3



Minimum:	50.00				-1.5		
Maximum:	100.00		200.0	10.0	50.0		
Mass	RA	Calc. Mass	mDa	PPM	DBE	Score	Formula
535.2680	100.00	535.2672	0.8	1.5	10.5	1	C30 H40 O7 Na

Figure S16. HRESI(+)MS spectrum of dicarabrone C (**2**)

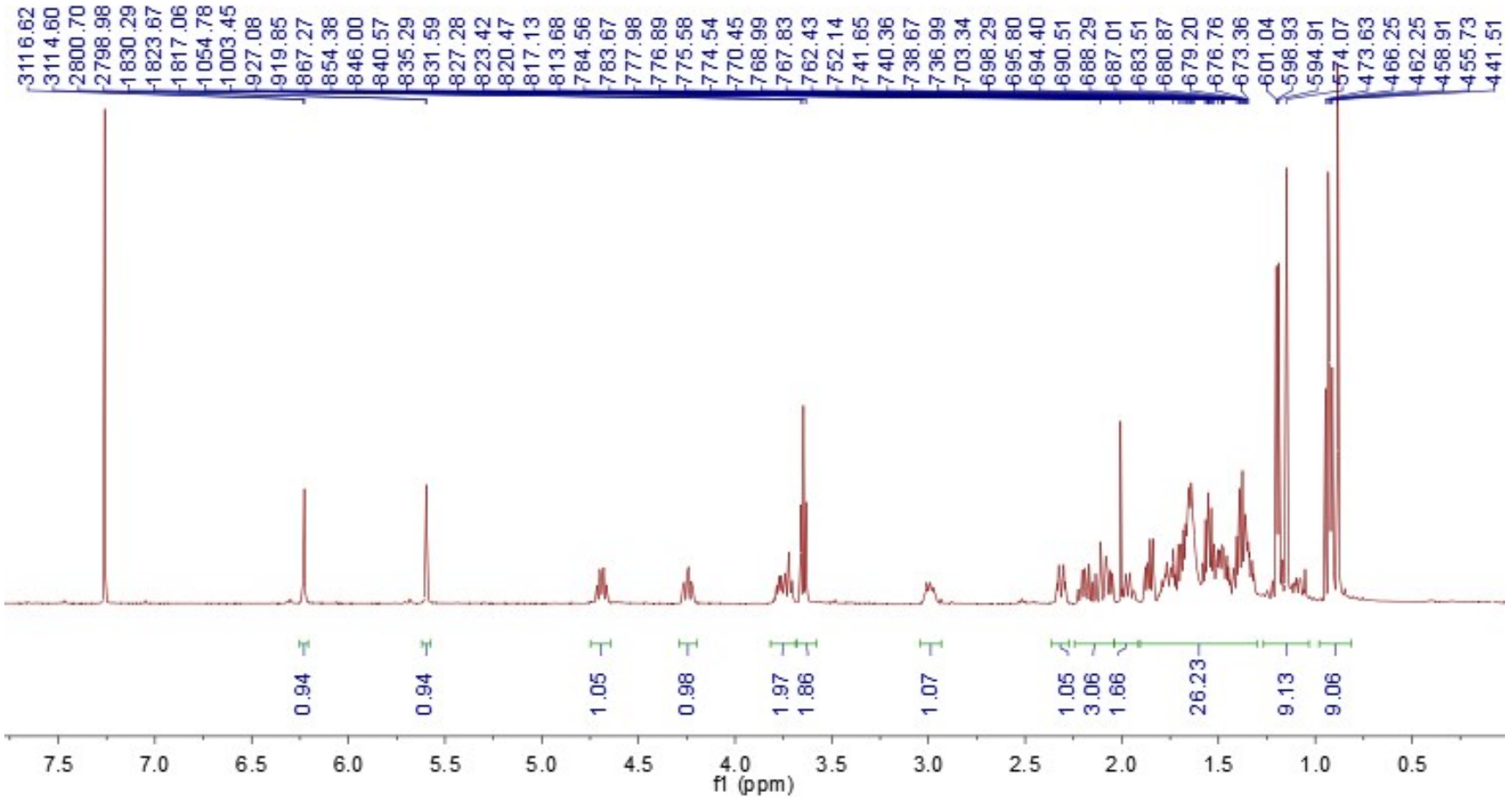


Figure S17. ^{1}H NMR spectrum of dipulchellin A (**3**) in $CDCl_3$

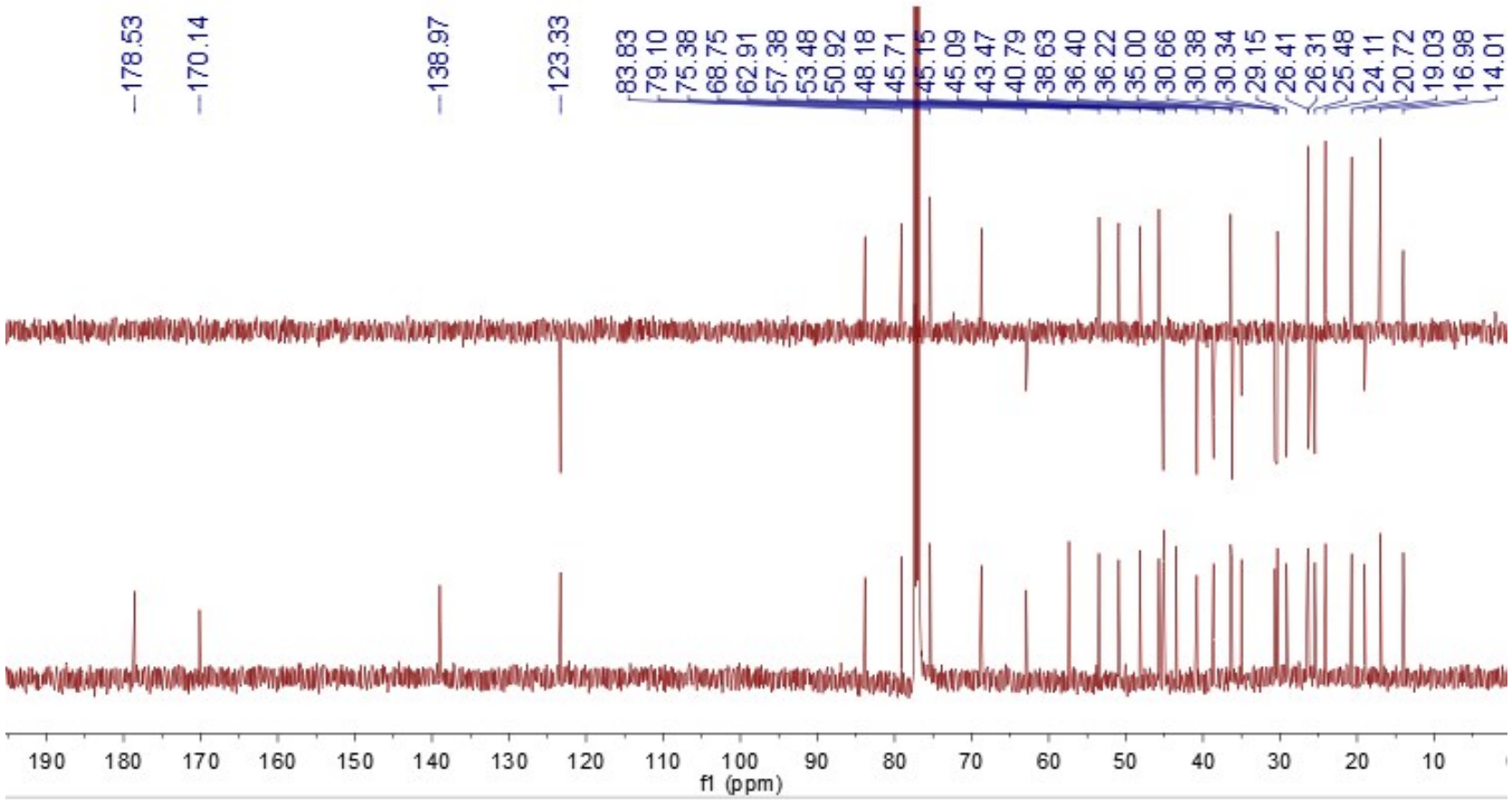


Figure S18. ^{13}C NMR spectrum of dipulchellin A (**3**) in $CDCl_3$

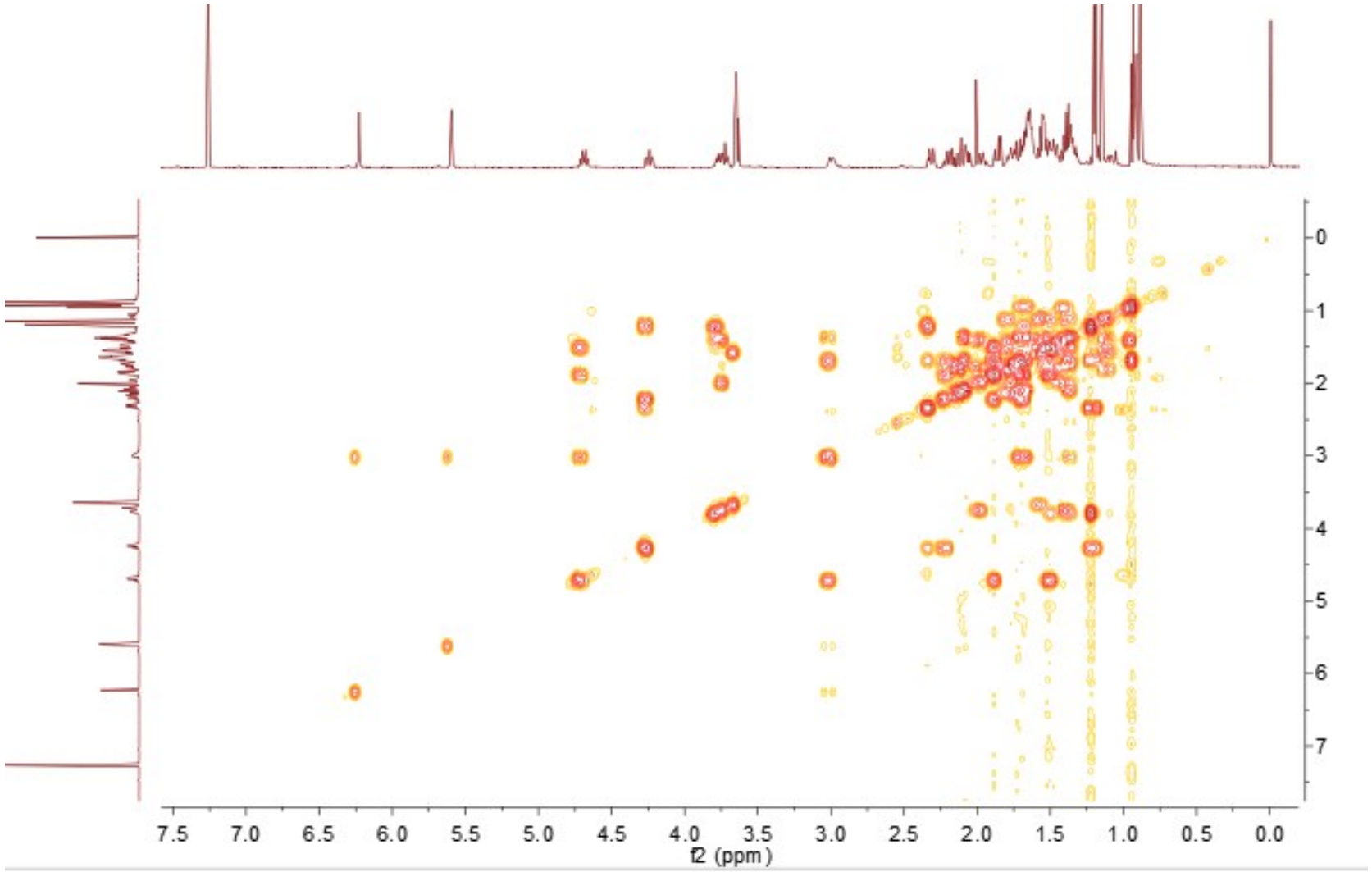


Figure S19. ^{1}H-^{1}H COSY spectrum of dipulchellin A (**3**) in $CDCl_3$

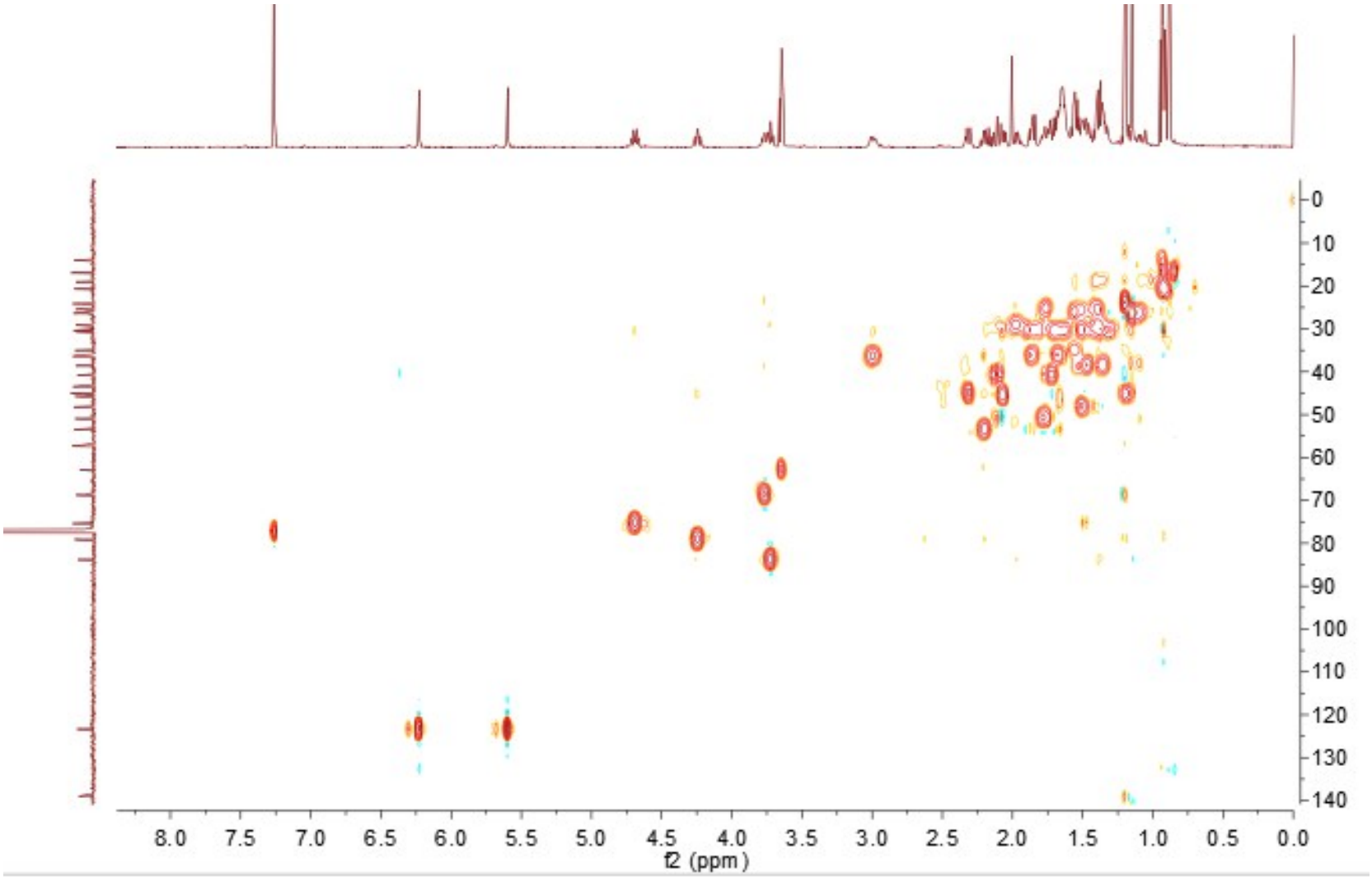


Figure S20. HSQC spectrum of dipulchellin A (**3**) in $CDCl_3$

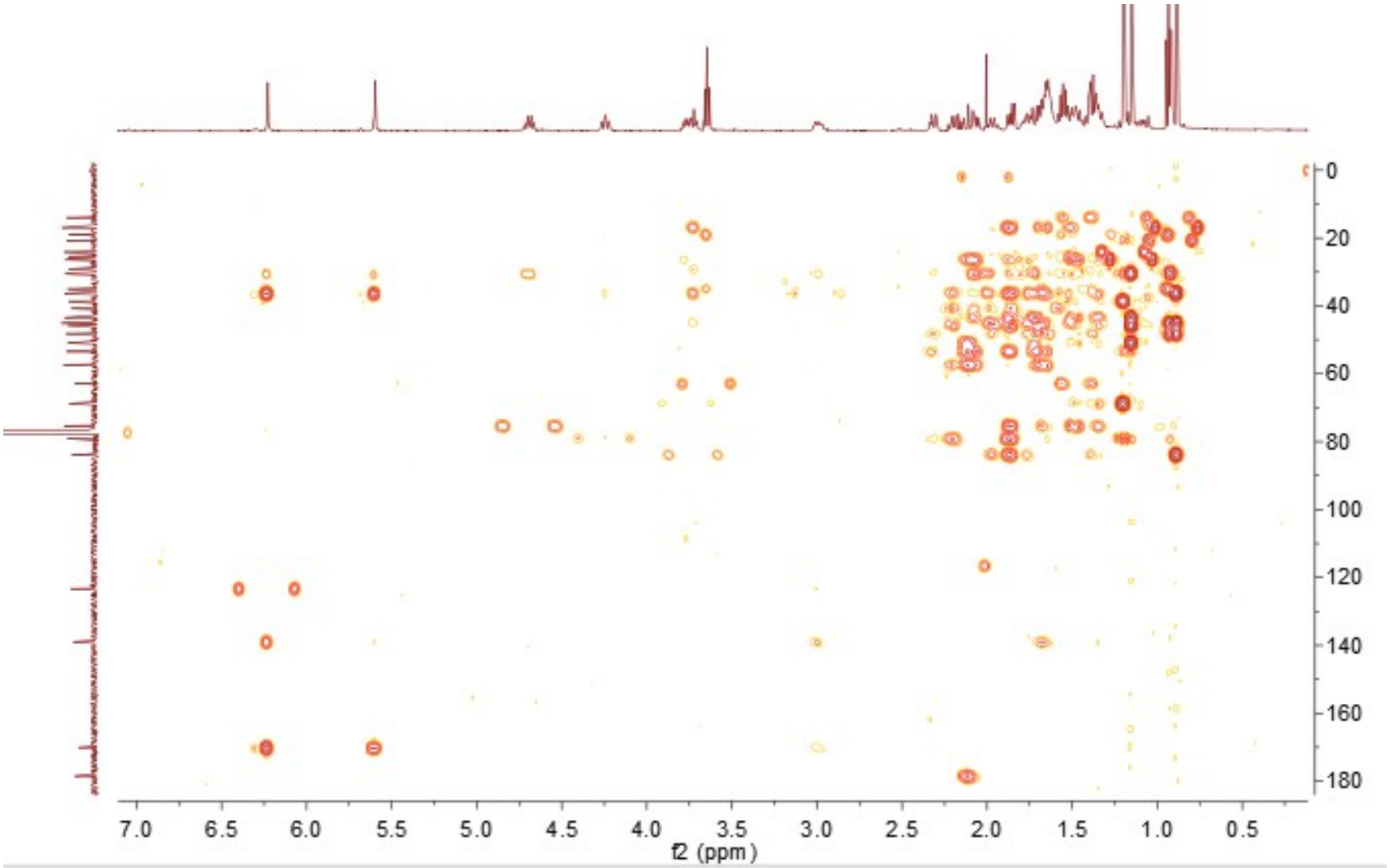


Figure S21. HMBC spectrum of dipulchellin A (**3**) in $CDCl_3$

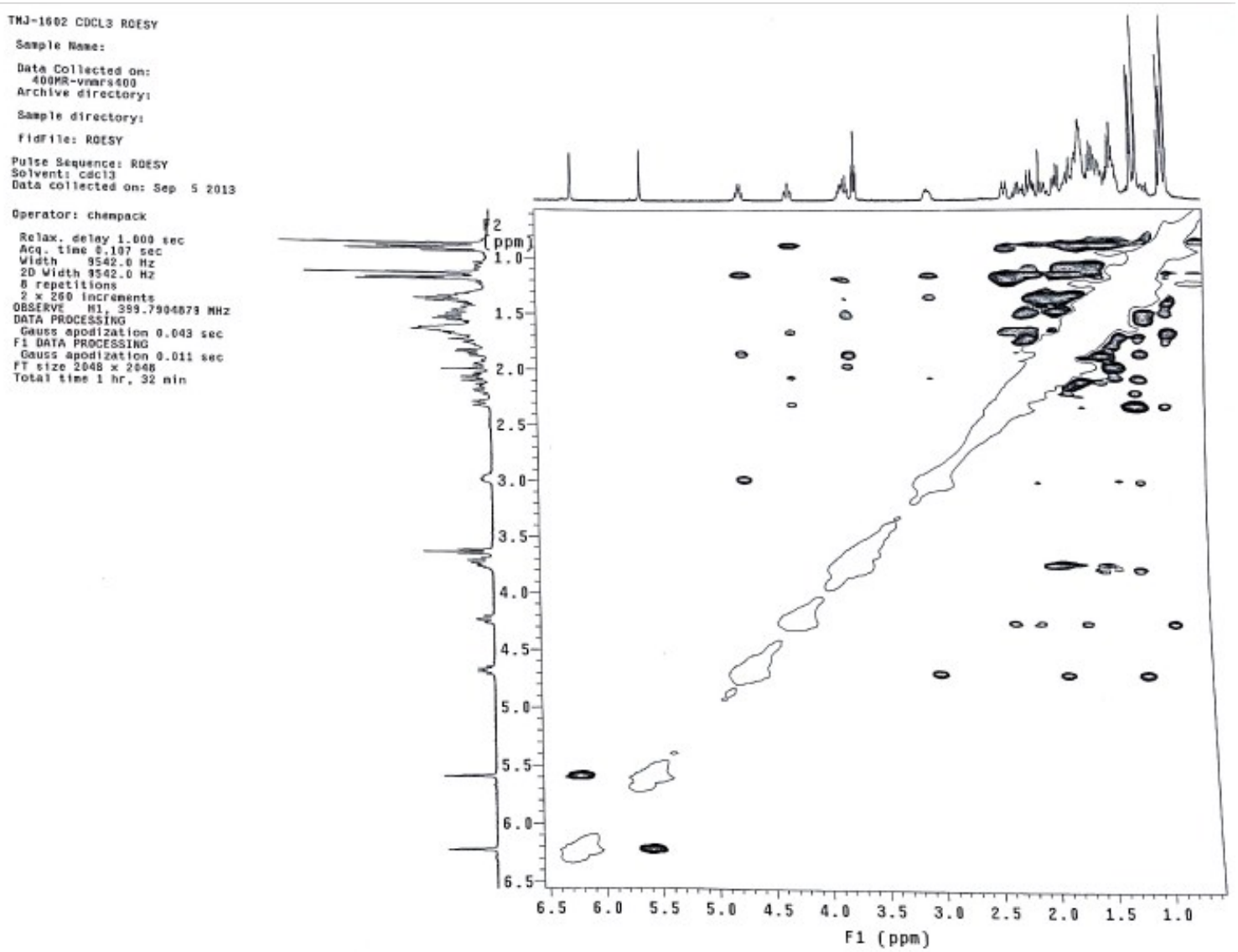


Figure S22. ROESY spectrum of dipulchellin A (**3**) in $CDCl_3$

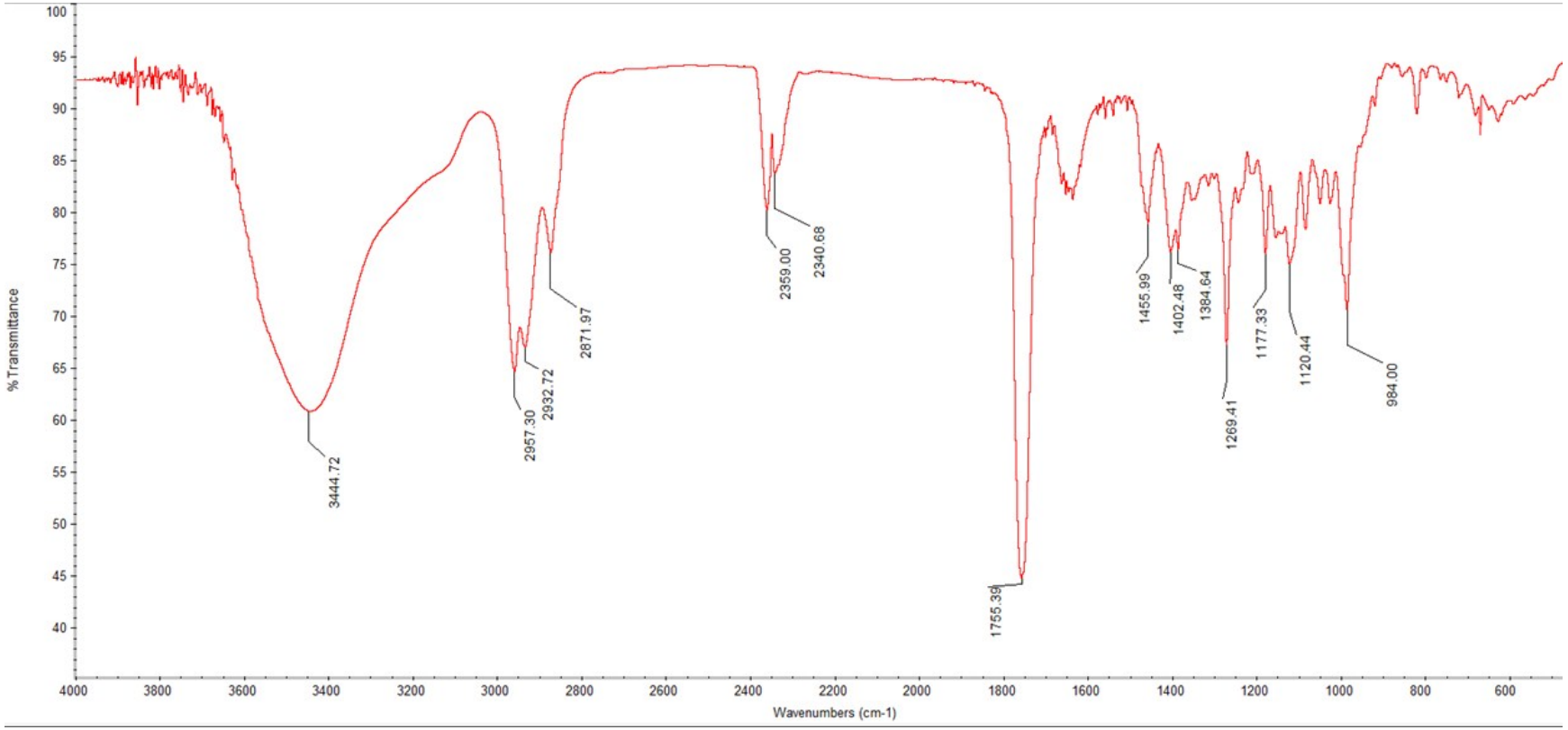


Figure S23. IR spectrum of dipulchellin A (**3**)

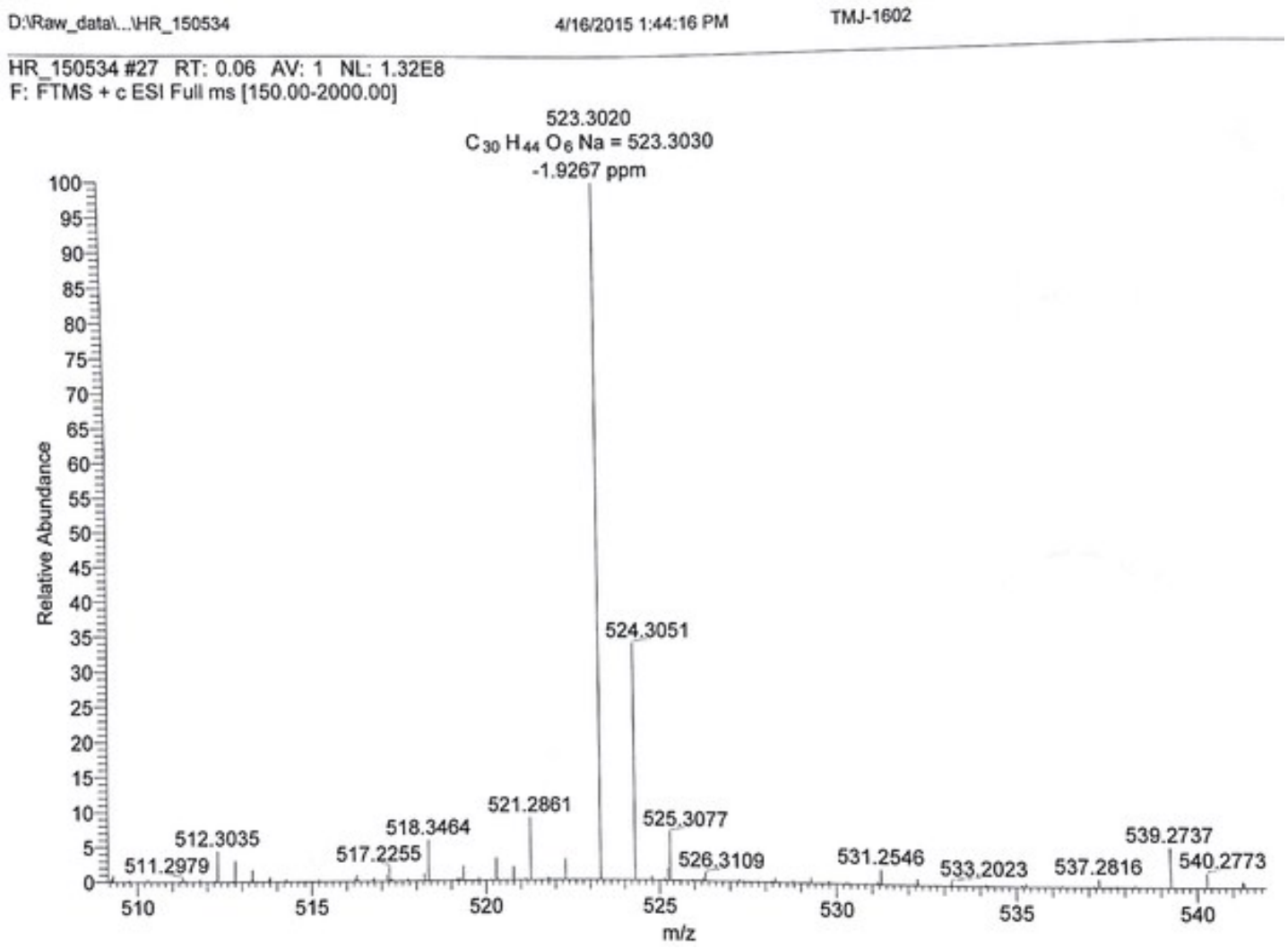


Figure S24. HRESI(+)MS spectrum of dipulchellin A (**3**)