

Supporting Information

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[Mass Spectrum]

Date : 121219 - Da Kuning - HEAN.10.B (VIAL 7) - 001 Date : 12-Dec-2019 08:51

Instrument : JEOL.MStation JMS-700(2)

Sample :

Note :

Inlet : Direct Ion Mode : EI+

Spectrum Type : Normal Ion [MF-Lines]

RT : 0.37 min Scan# : (419) Time : 226.7 deg.C

BP : m/z 83.0403 Int. : 1930.81 (1919.465)

Output m/z range : 144 to 324 Cut Level : 0.00 %

[Theoretical Ion Distribution]

Molecular Formula : C20 H30 O3

(m/z 318.2195, MW 318.4564, D.S. 6.0)

Base Peak : 318.2195, Averaged MW : 318.4534(a), 318.4542(w)

m/z	INT.
318.2195	100.0000*****
319.2229	22.3590*****
320.2257	2.9773**
321.2284	0.2938
322.2311	0.0230
323.2338	0.0015

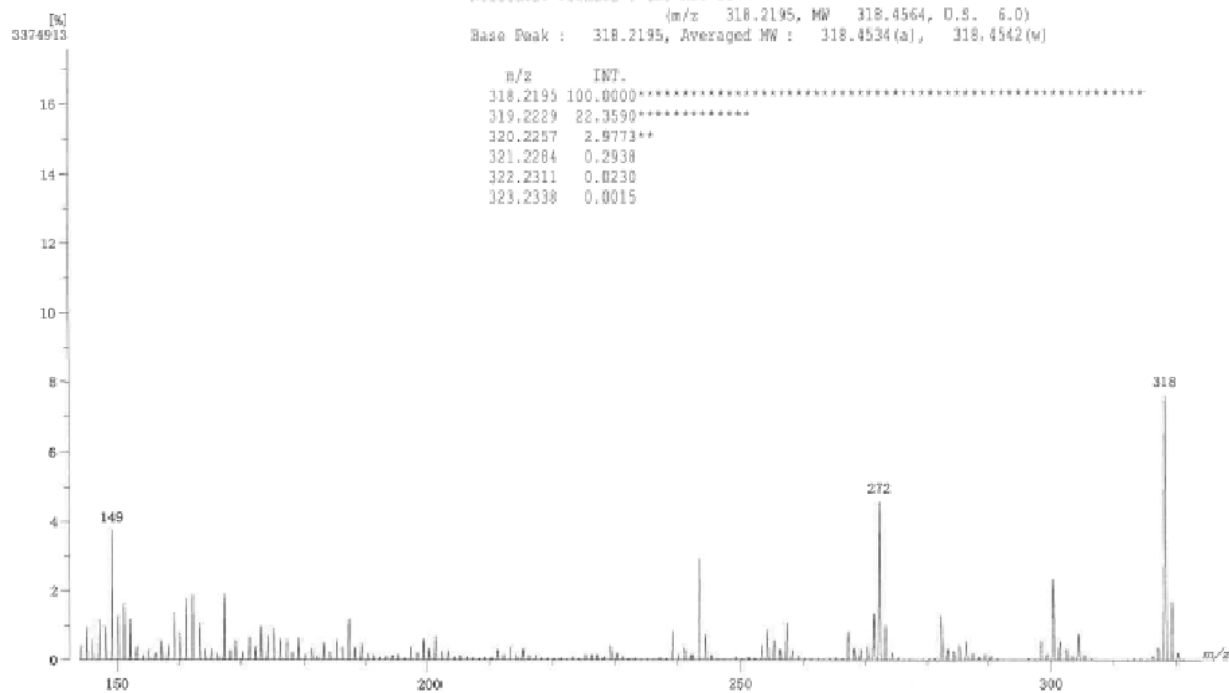


Figure S1: HR-EIMS spectrum of compound **1** [M-H]⁻ ion at $m/z = 319.2229$

IG-JA-PAN76.10.fid
IG-JA-PAN76
PROTON.NIGHT CDCl3 {C:\Bruker\TopSpin3.2} DDU500 22

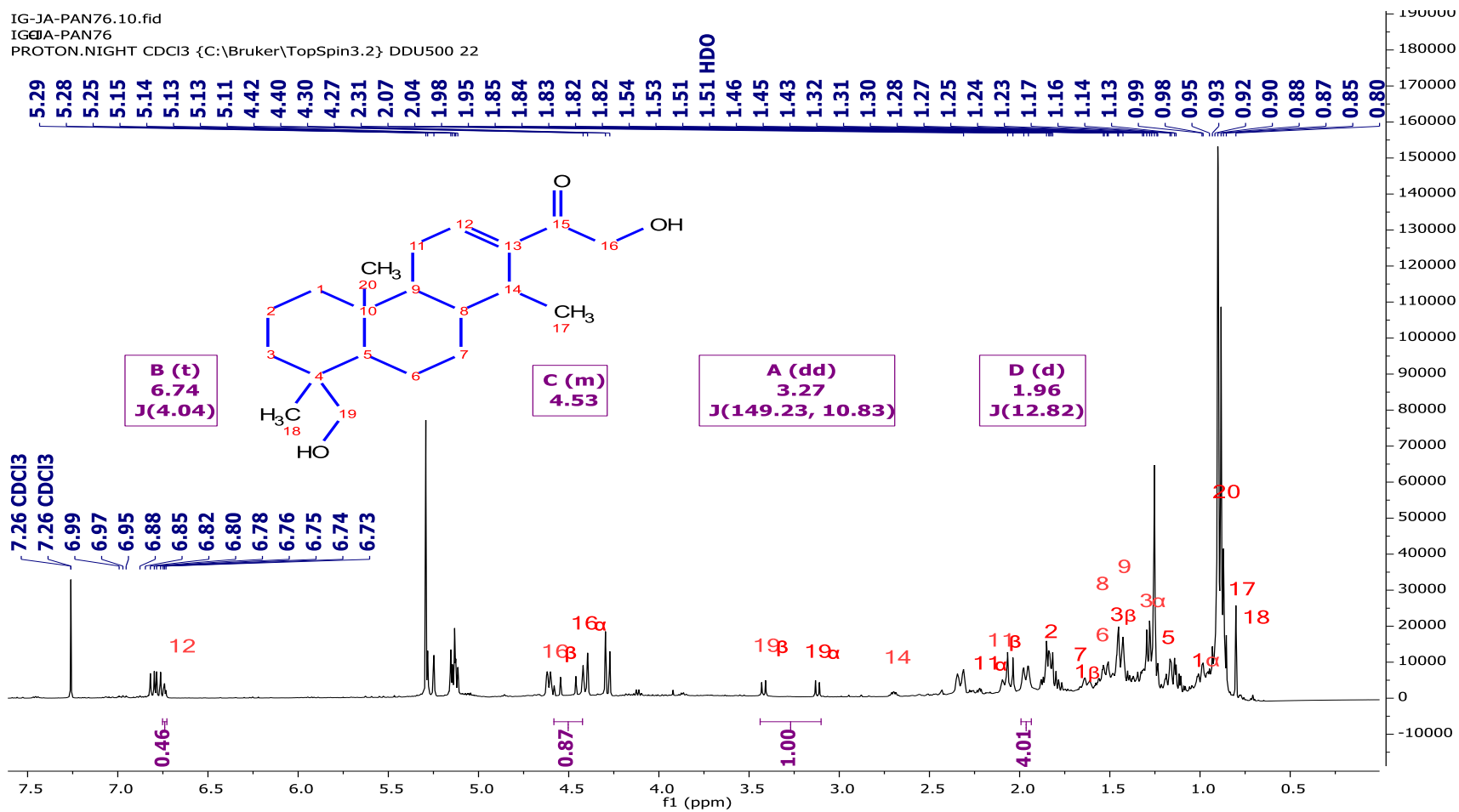


Figure S2: ¹H-NMR (400 MHz, CDCl₃) Spectrum of compound 1

IG-JA-PAN76.10.fid
IG-JA-PAN76
PROTON.NIGHT CDCl3 {C:\Bruker\TopSpin3.2} DDU500 22

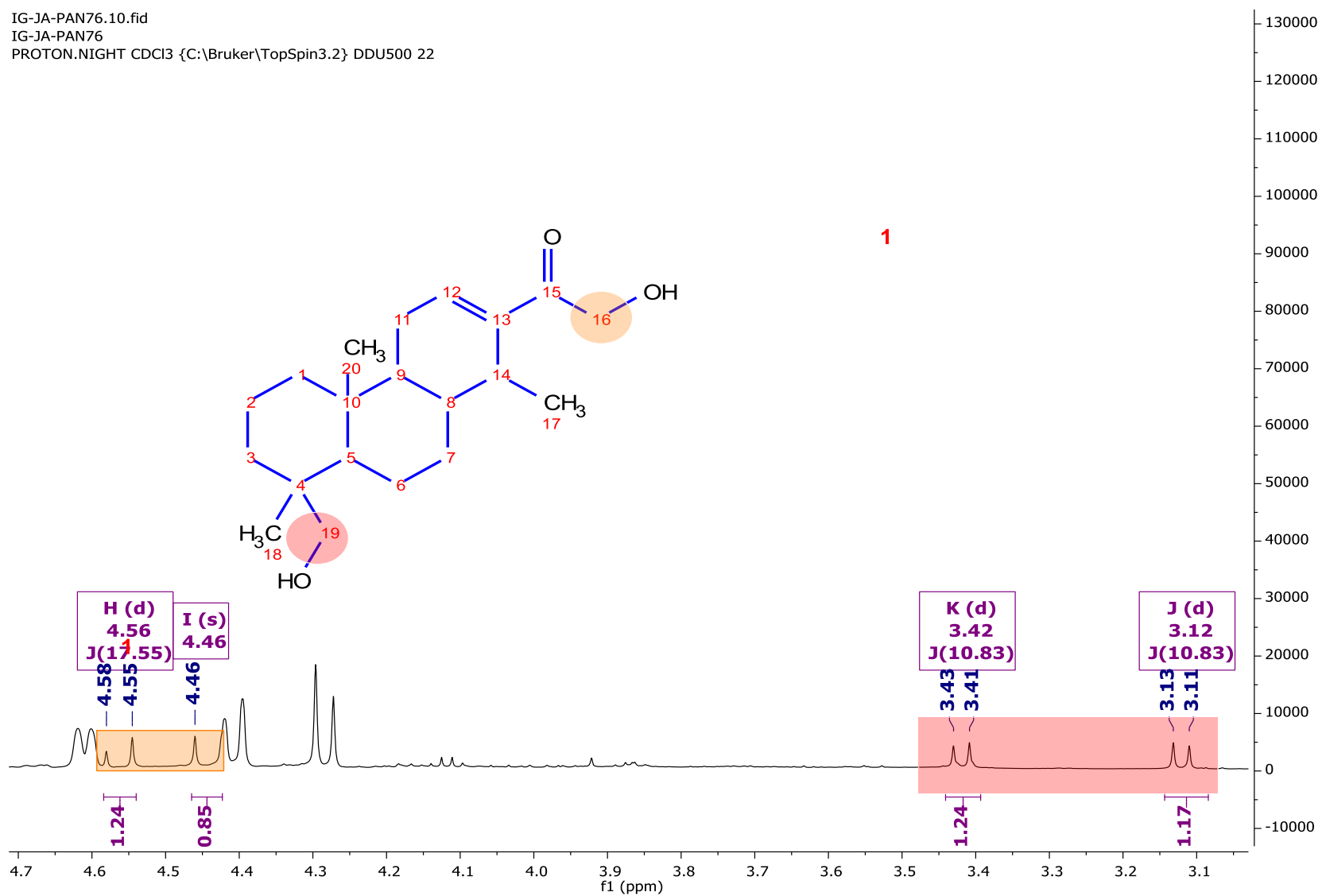


Figure S3: ¹H-NMR (400 MHz, CDCl₃) Spectrum of compound 1 (From δ_{H} 3.1 ppm to δ_{H} 4.7 ppm)

IG-JA-PAN76.10.fid
IG-JA-PAN76
PROTON.NIGHT CDCl3 {C:\Bruker\TopSpin3.2} DDU500 22

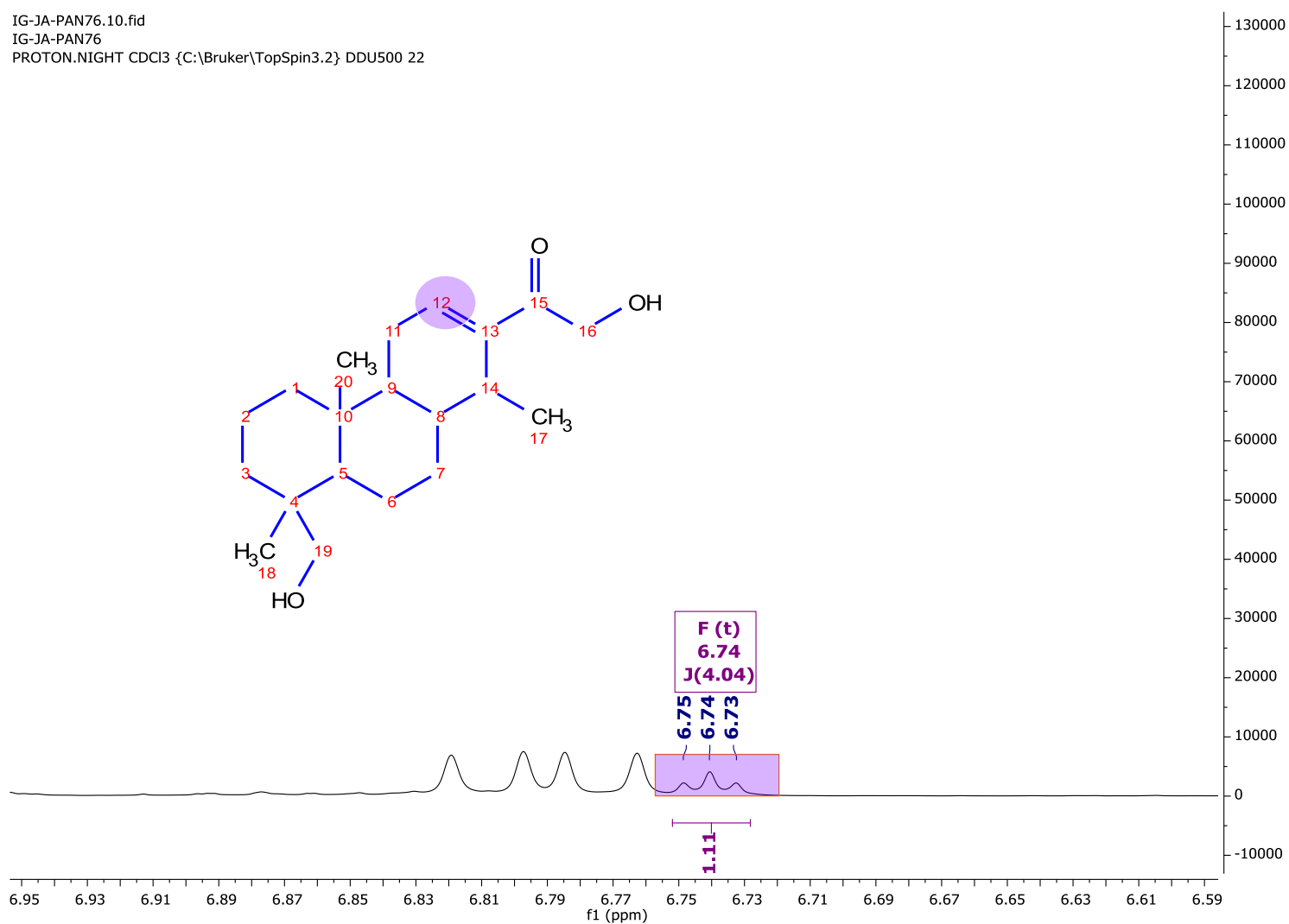


Figure S4: ¹H-NMR (400 MHz, CDCl₃) Spectrum of compound 1 (From δ_{H} 6.6 ppm to δ_{H} 7.0 ppm)

IG-JA-PAN76.10.fid
IG-JA-PAN76
PROTON.NIGHT CDCl3 {C:\Bruker\TopSpin3.2} DDU500 22

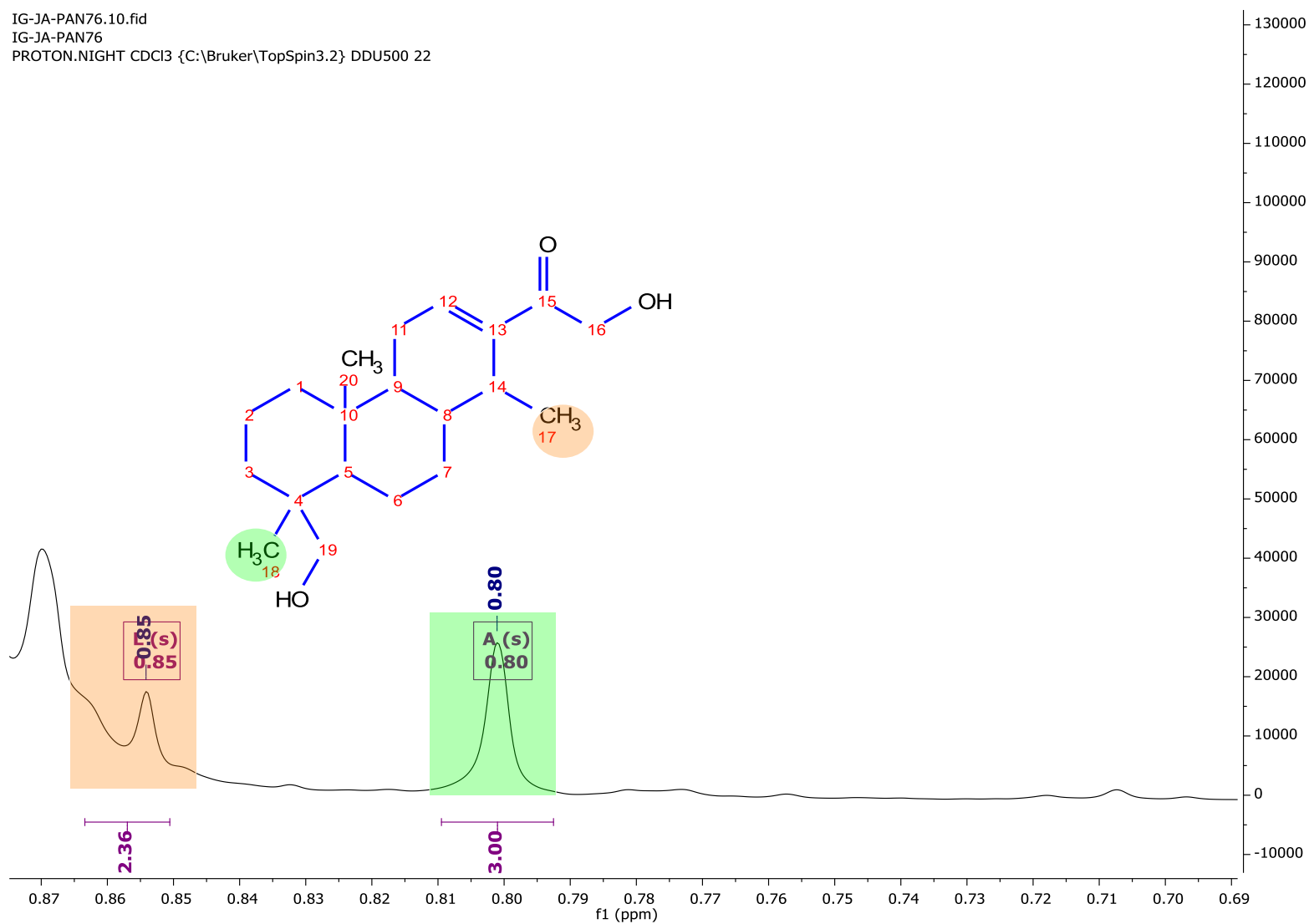


Figure S5: ¹H-NMR (400 MHz, CDCl₃) Spectrum of compound 1 (From δ_H 0.69 ppm to δ_H 0.87 ppm)

IG-JA-PAN76.11.fid
IG-JA-PAN76
DEPTQ_NIGHT CDCl3 {C:\Bruker\TopSpin3.2} DDU500 22

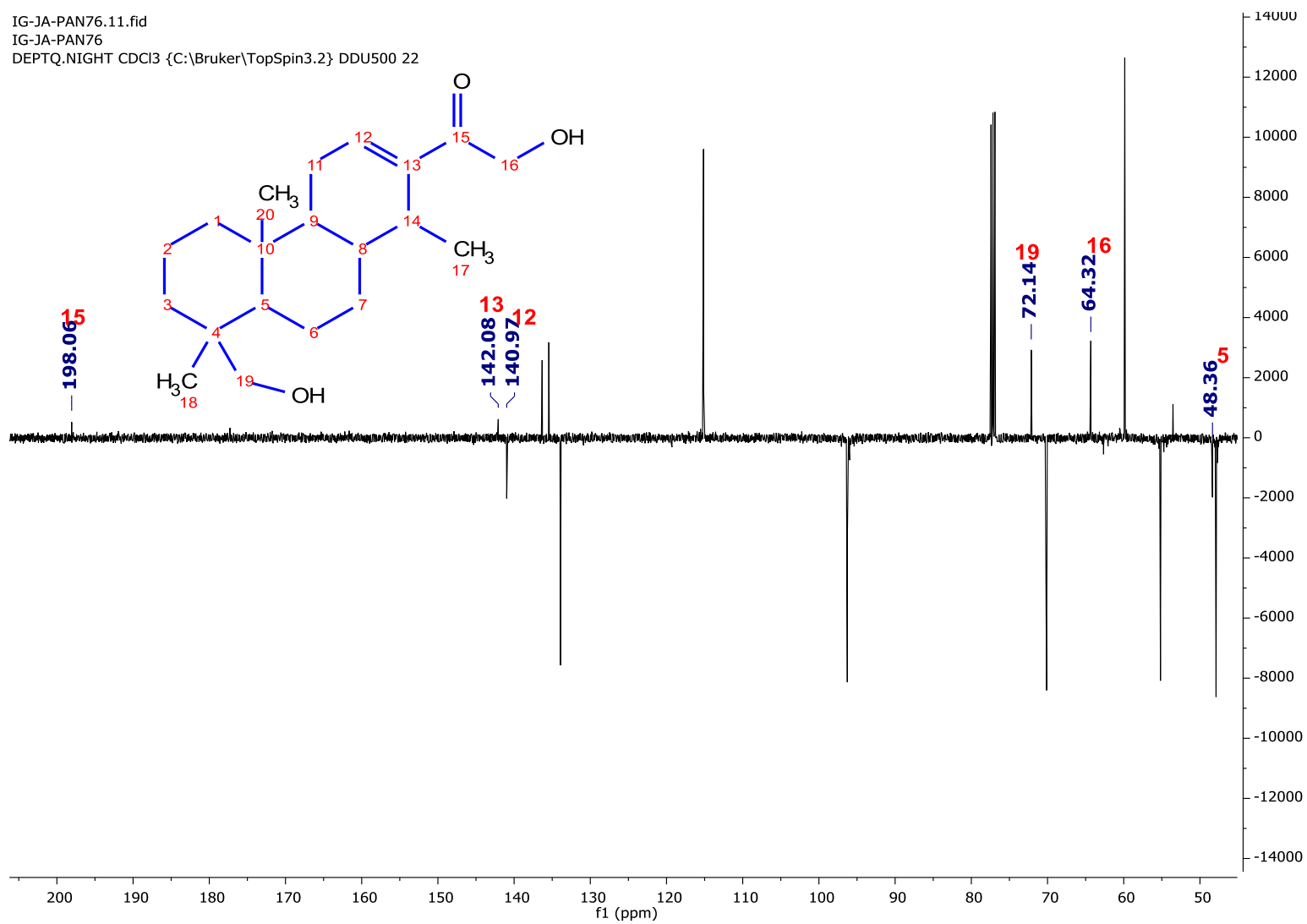


Figure S6: DEPTq135 (100 MHz, CDCl₃) Spectrum of compound 1 (From δ_C 50 ppm to δ_C 200 ppm)

IG-JA-PAN76.11.fid
IG-JA-PAN76
DEPTQ.NIGHT CDCl3 {C:\Bruker\TopSpin3.2} DDU500 22

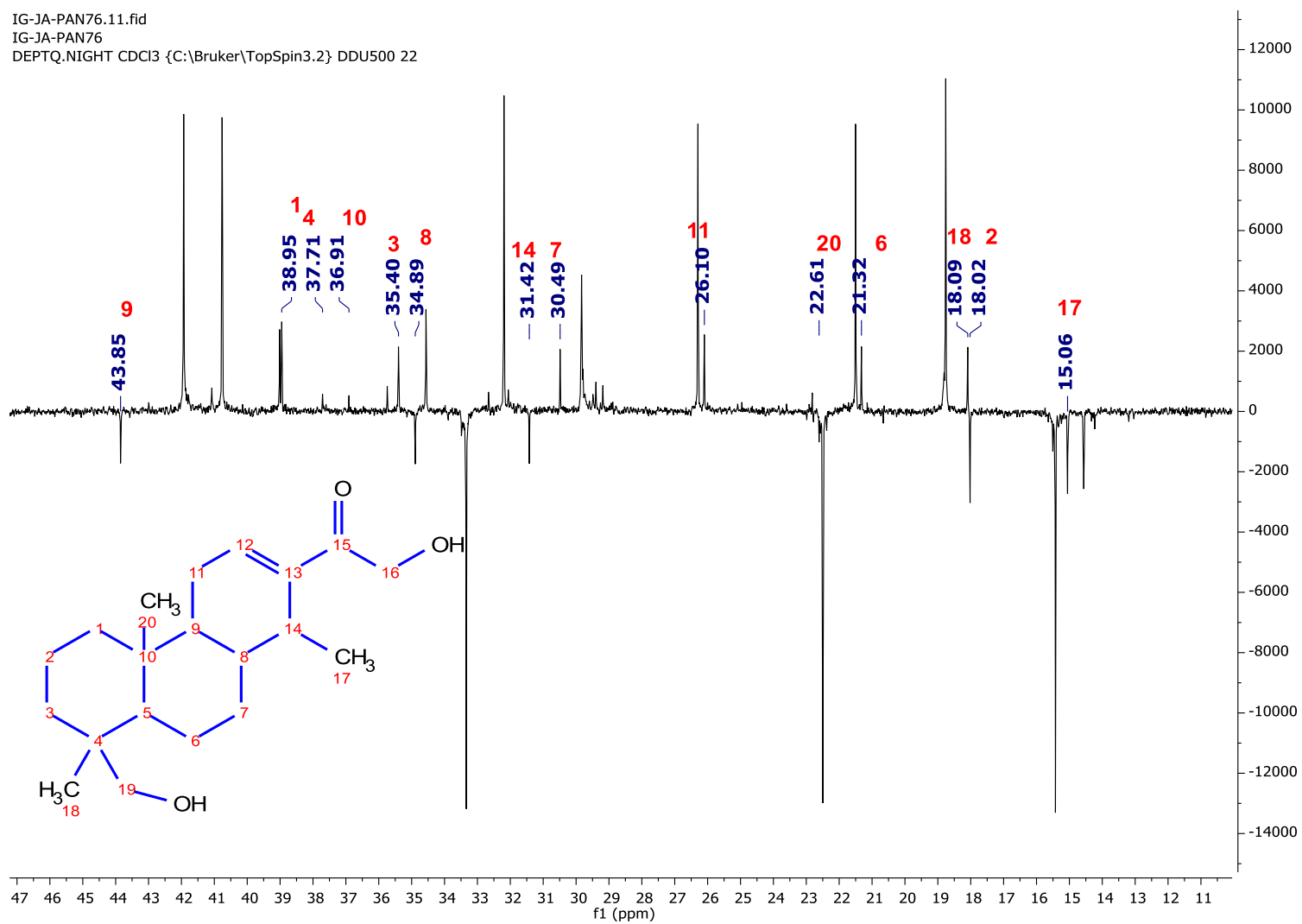


Figure S7: DEPTq135 (100 MHz, CDCl₃) Spectrum of compound 1 (From δ_c 11 ppm to δ_c 47 ppm)

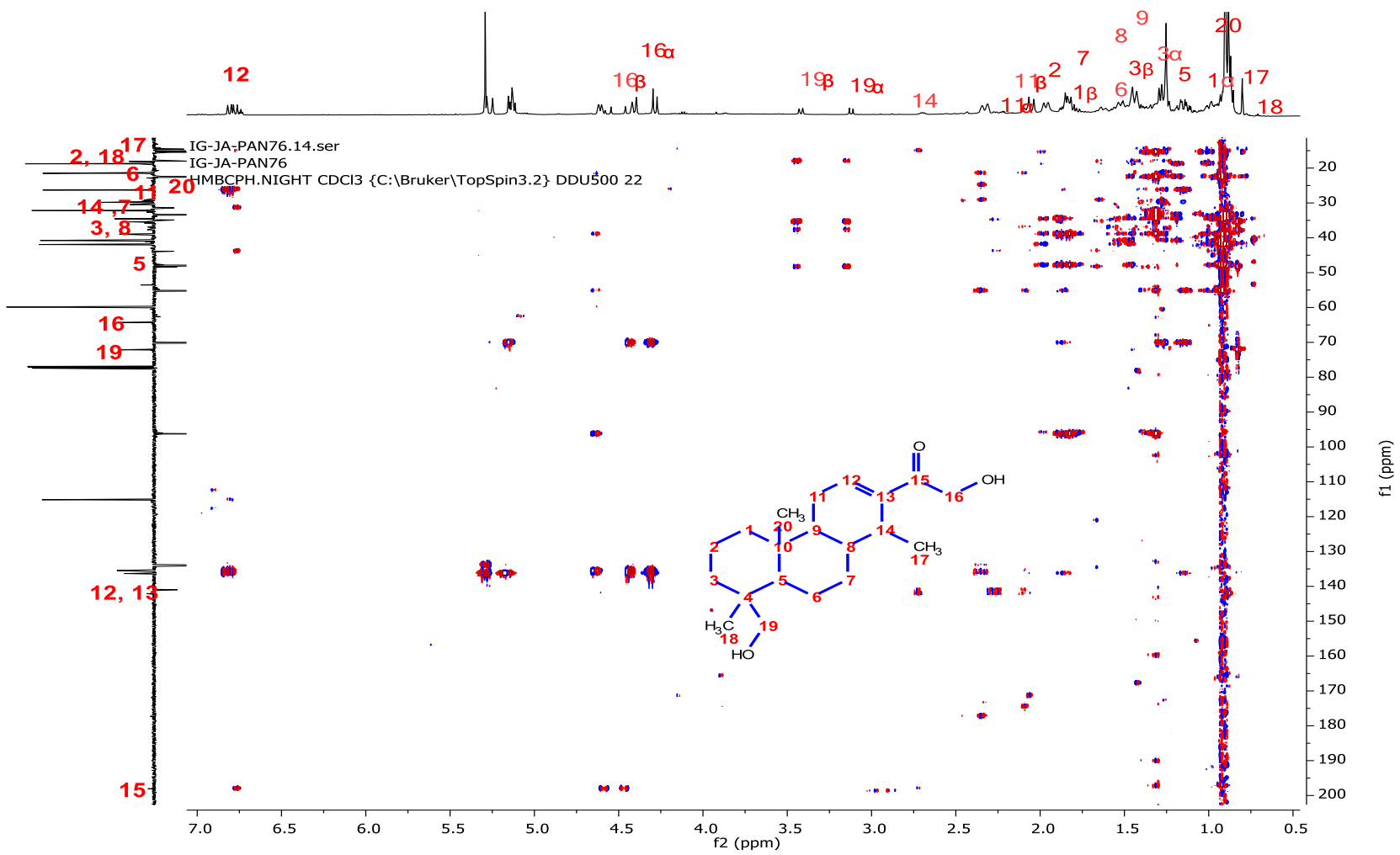


Figure S8: HMBC Spectrum of compound 1

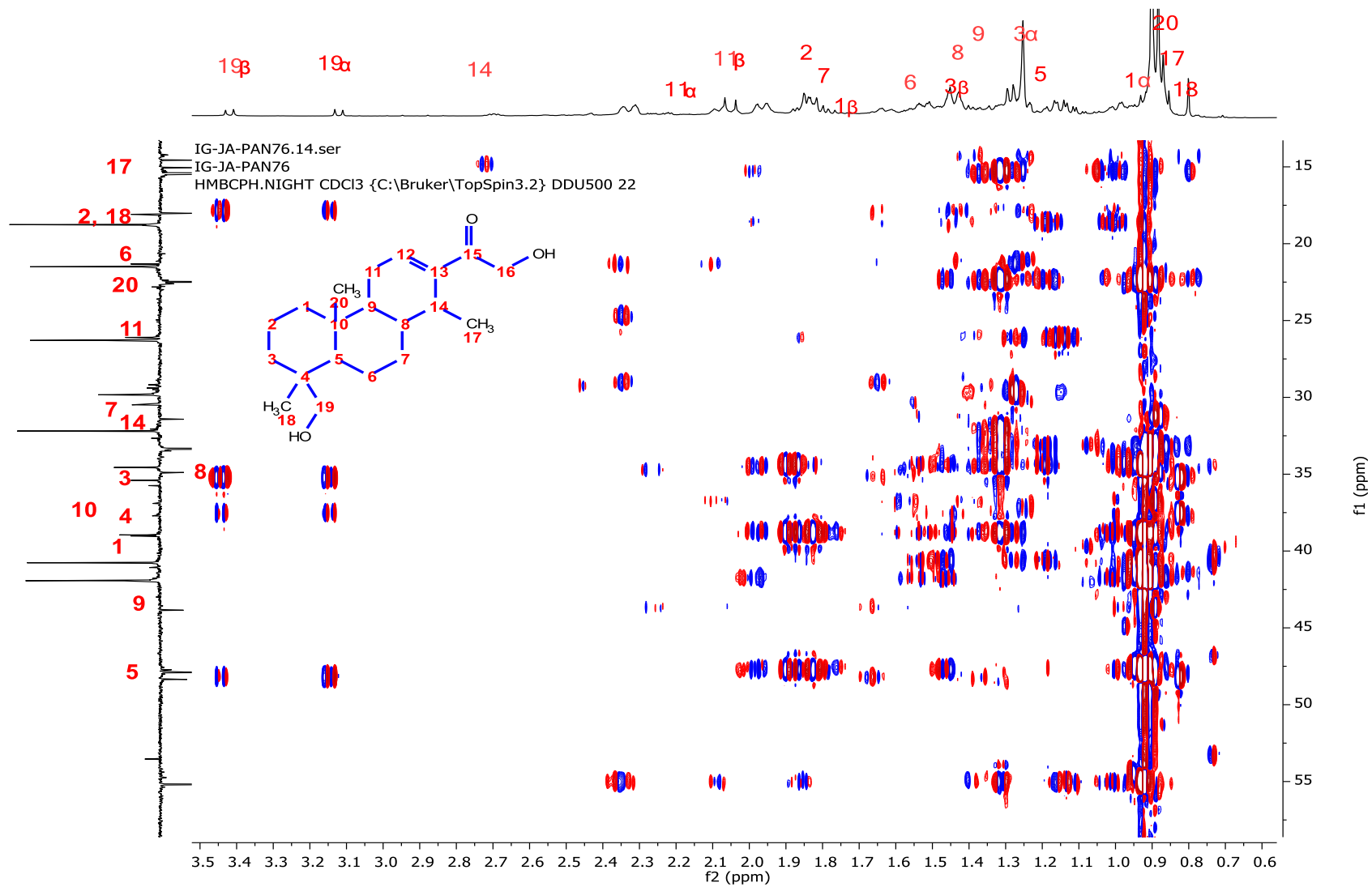


Figure S9: HMBC Spectrum of compound 1 (From δ_H 3.50 ppm to δ_H 0.70 ppm)/(δ_C 15 ppm to δ_C 55 ppm)

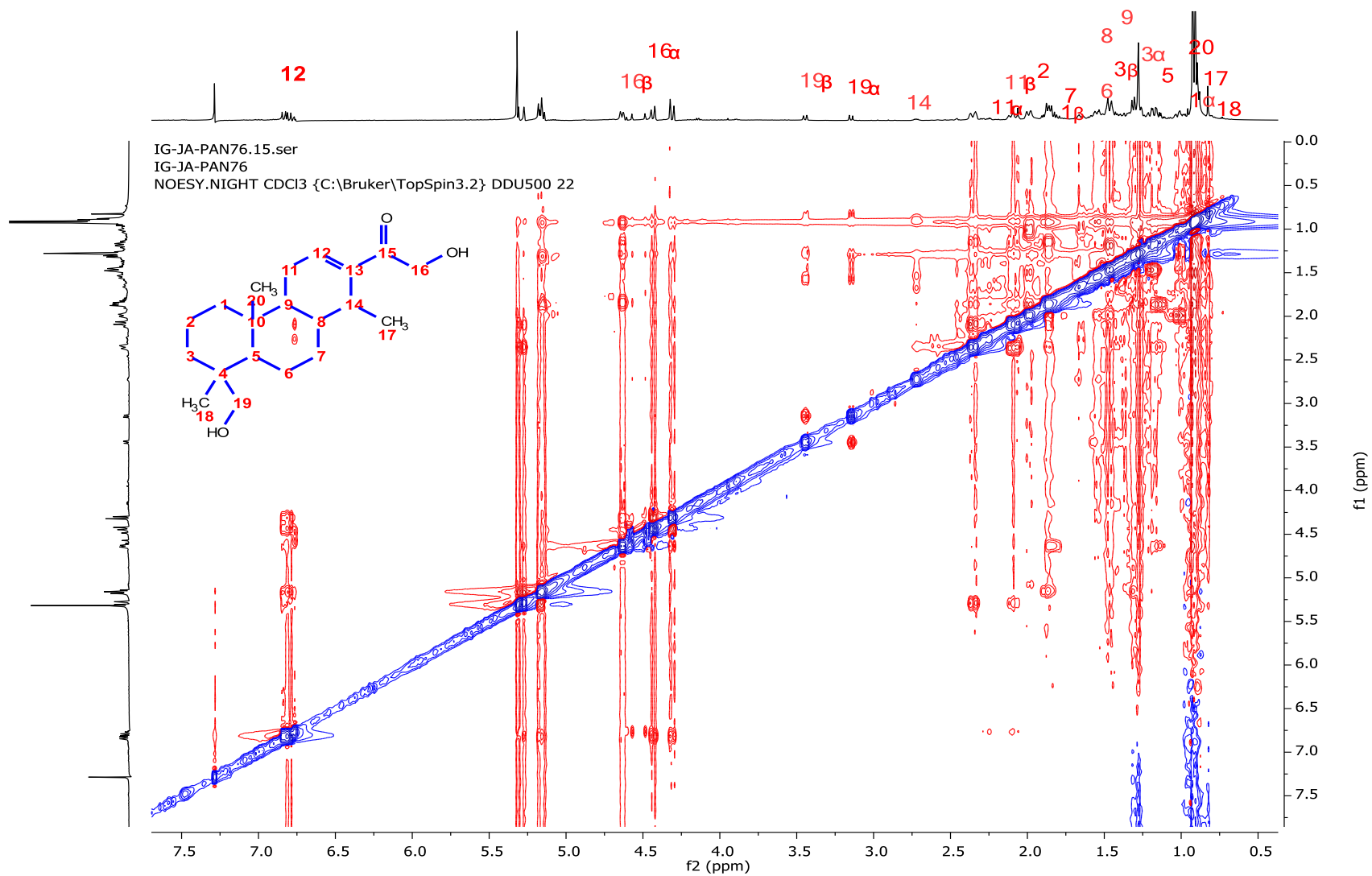


Figure S10: NOESY Spectrum of compound 1

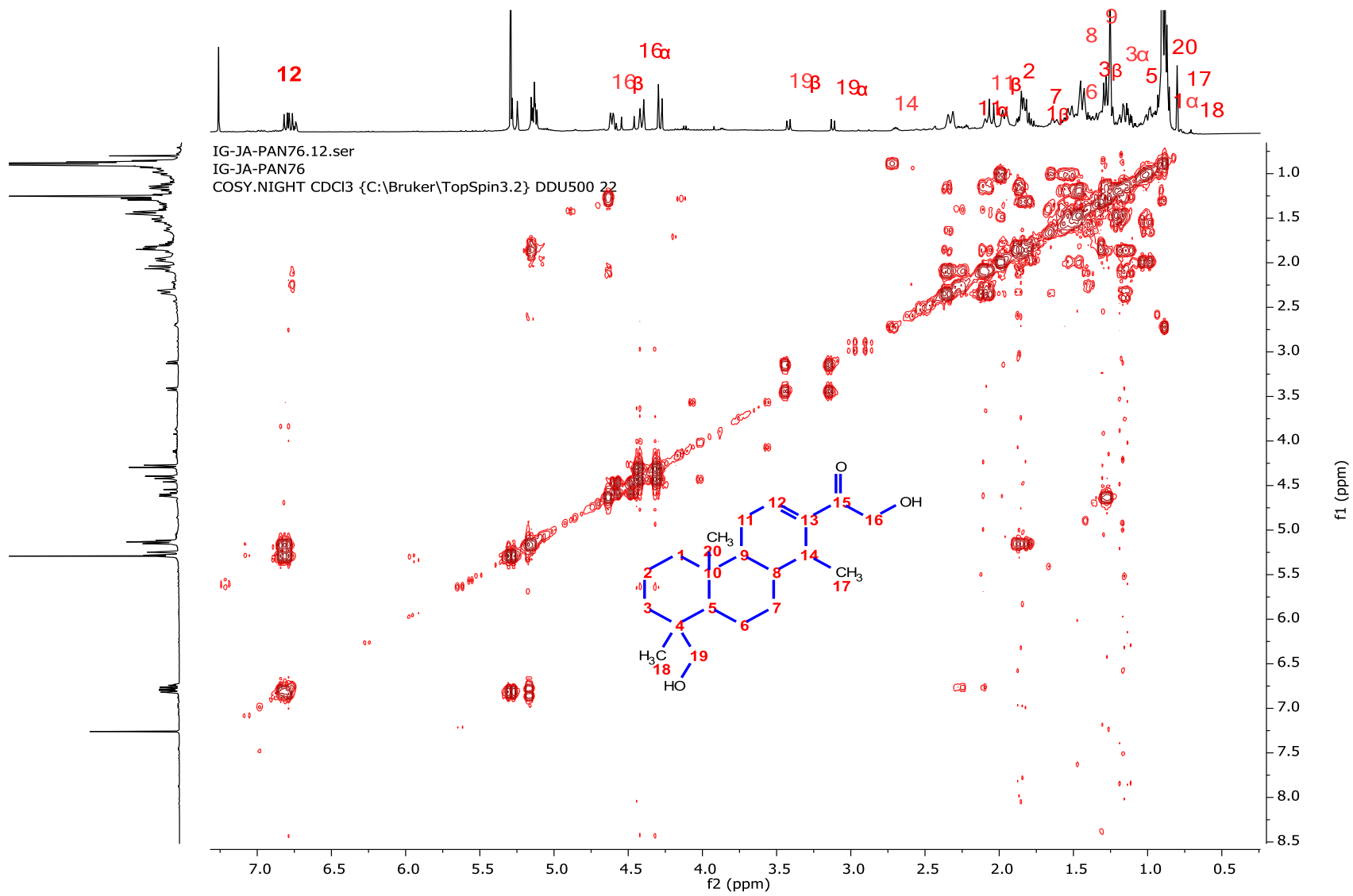


Figure S11: COSY Spectrum of compound 1

[Mass Spectrum]
Data : 171219 - HEAL19 - 001 Date : 17-Dec-2019 07:11
Instrument : JEOL MSStation JMS-1002J
Sample :
Note :
Inlet : Direct Ion Mode : EI+
Spectrum Type : Normal Ion [MP-Linear]
RT : 0.74 min Scan#: (7,14) Temp : 3276.7 degC
BP : m/z 134.1644 Int : 1768.82 (18547440)
Output m/z range : 50 to 454 Cut Level : 0.00 %

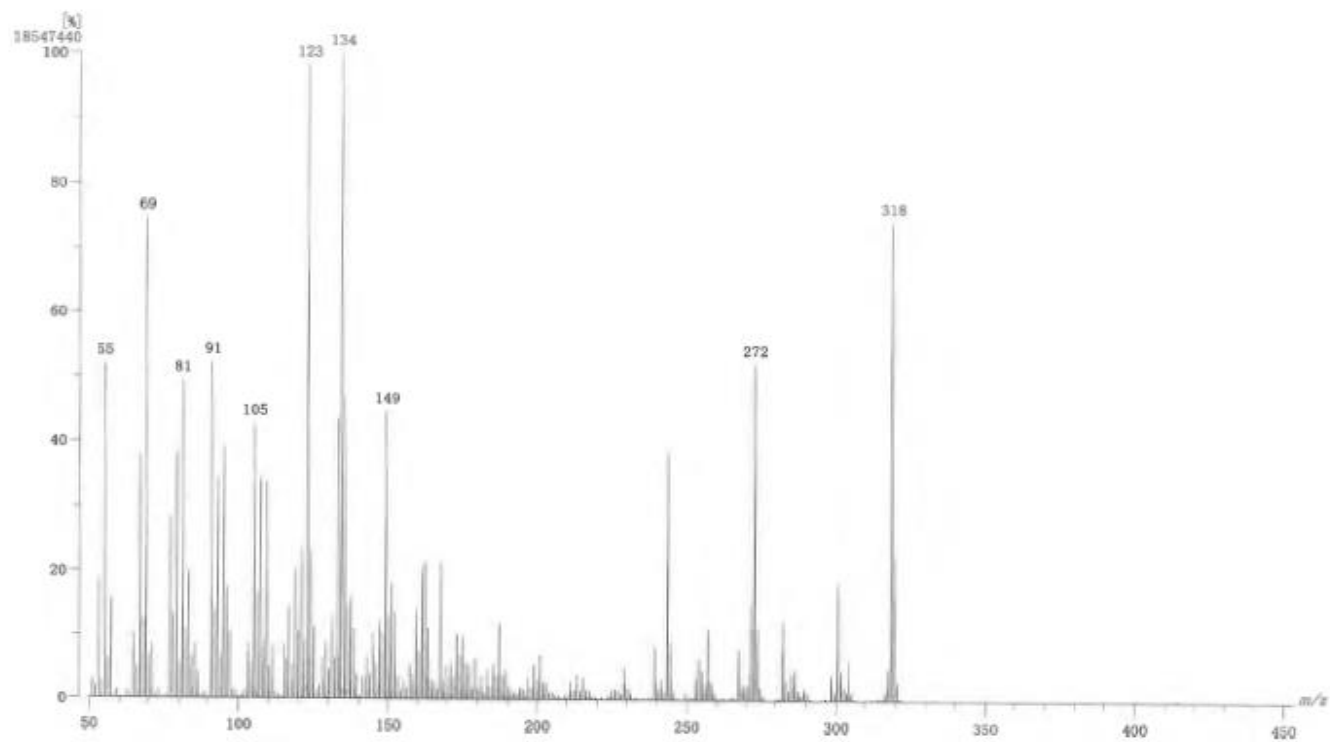


Figure S12: HR-EIMS spectrum of compound **2** at $m/z = 318.2195$

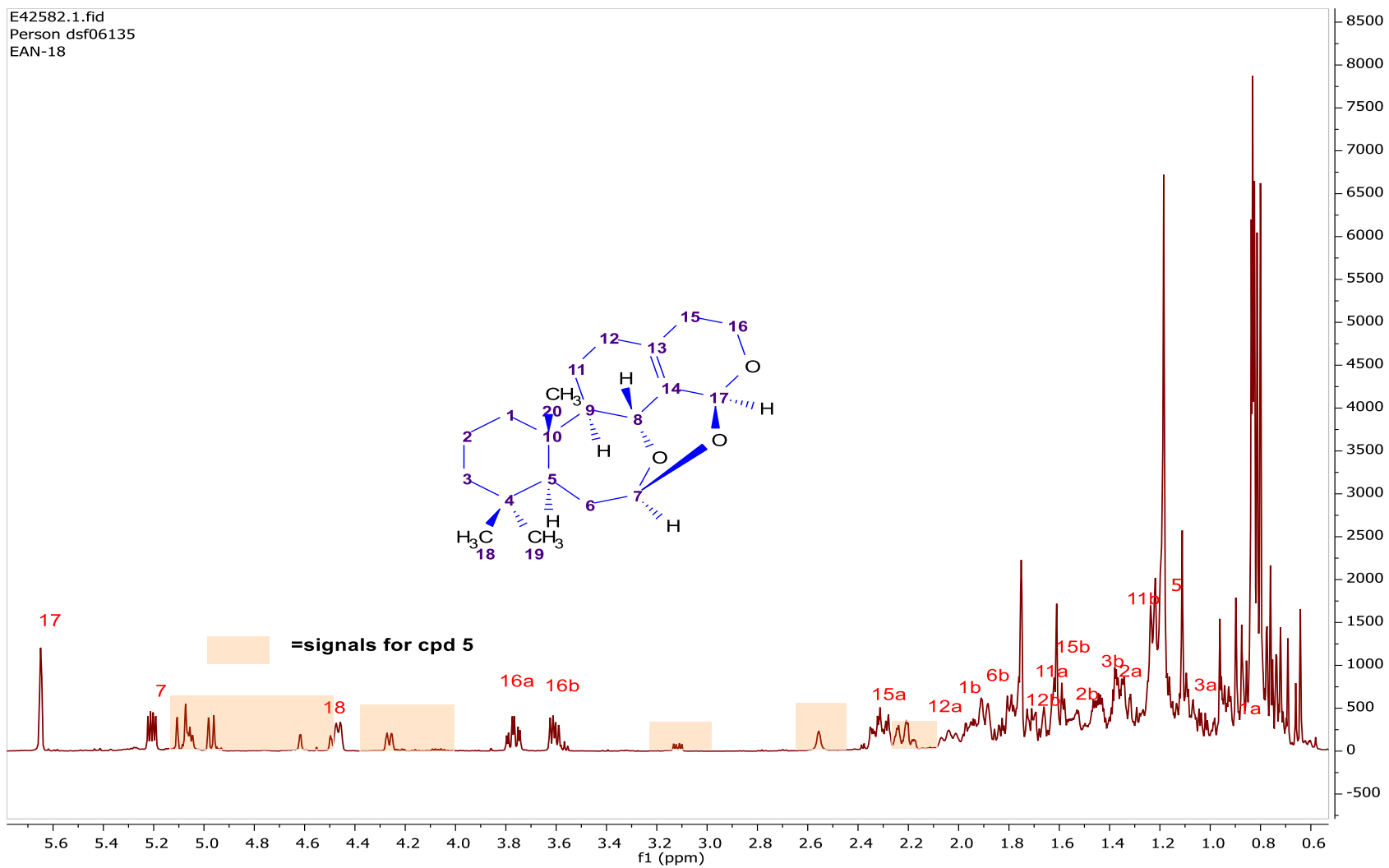


Figure S14: ¹H NMR Spectrum of compound 2 (annotated).

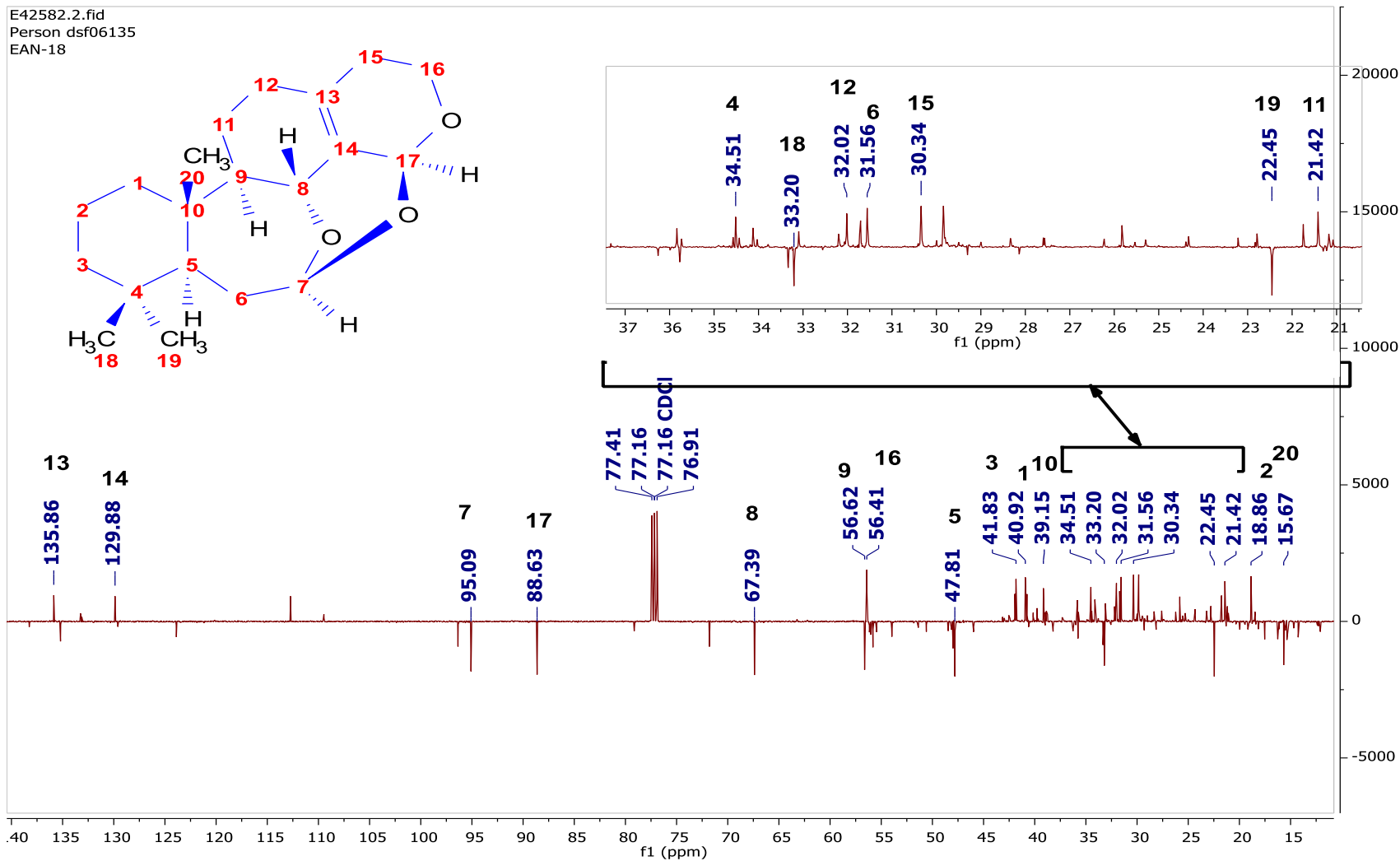


Figure S15: ¹³C DEPTq-135 Spectrum of compound 2

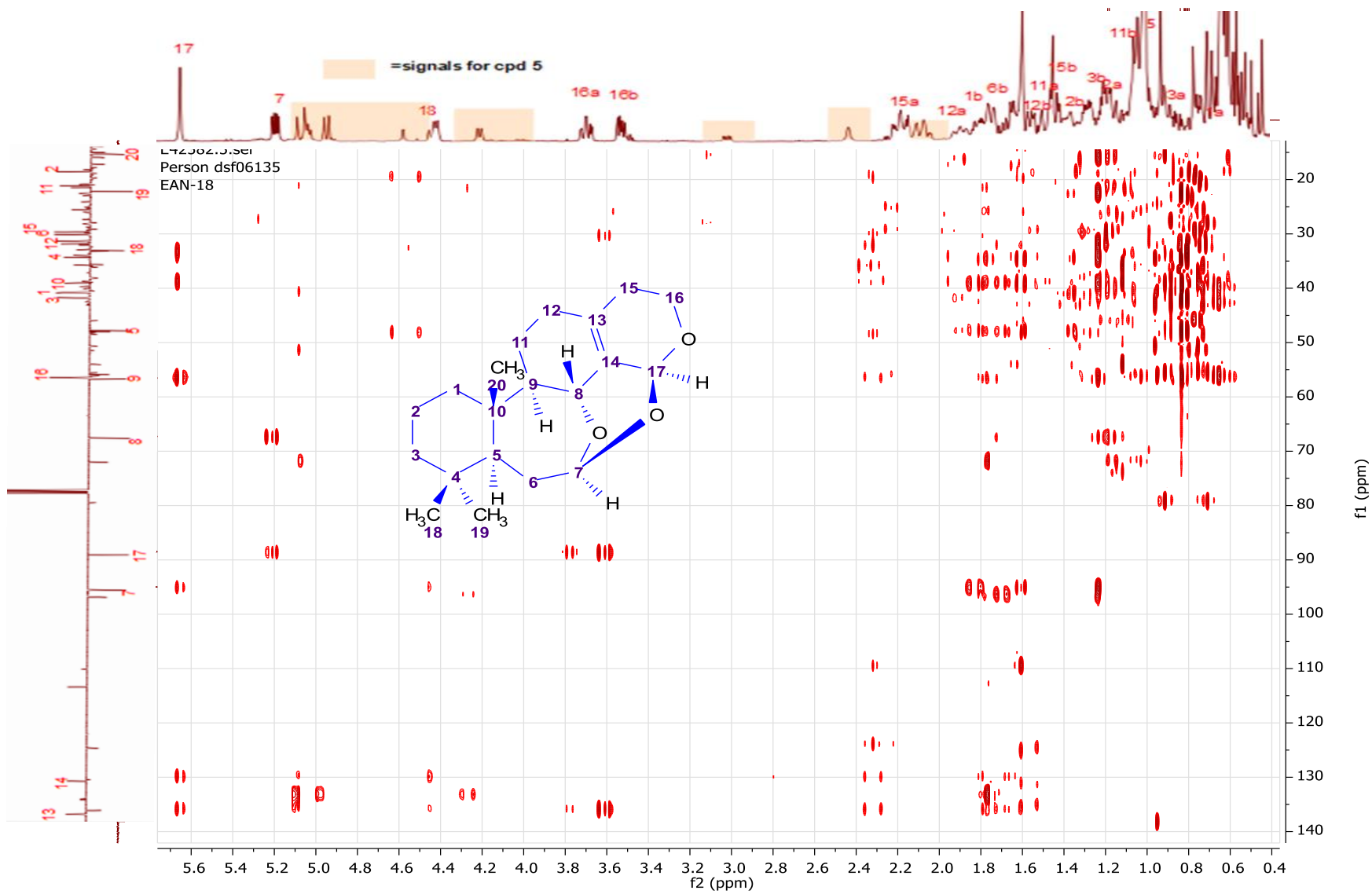


Figure S16: HMBC Spectrum of compound 2

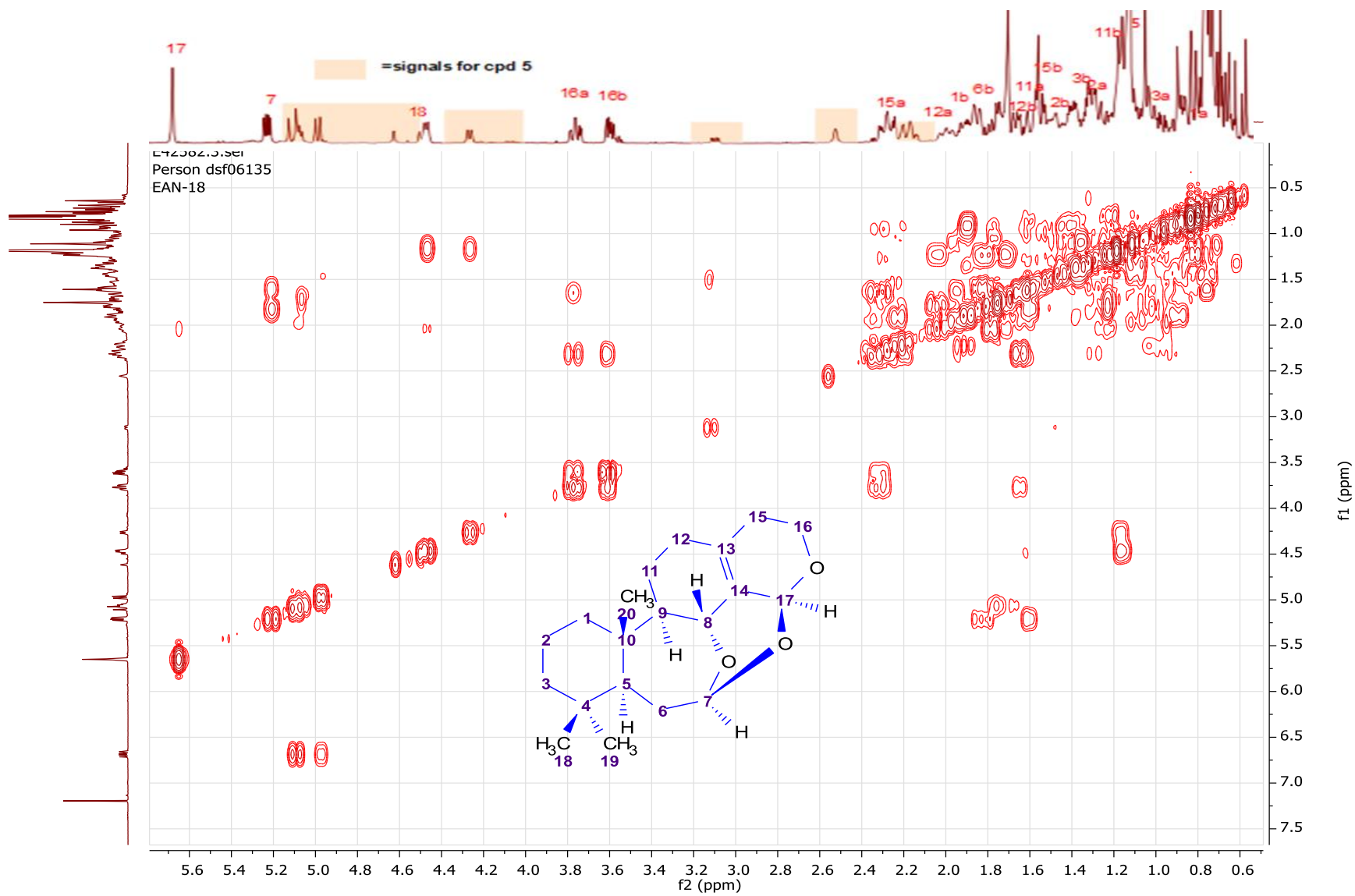


Figure S17: COSY Spectrum of compound 2

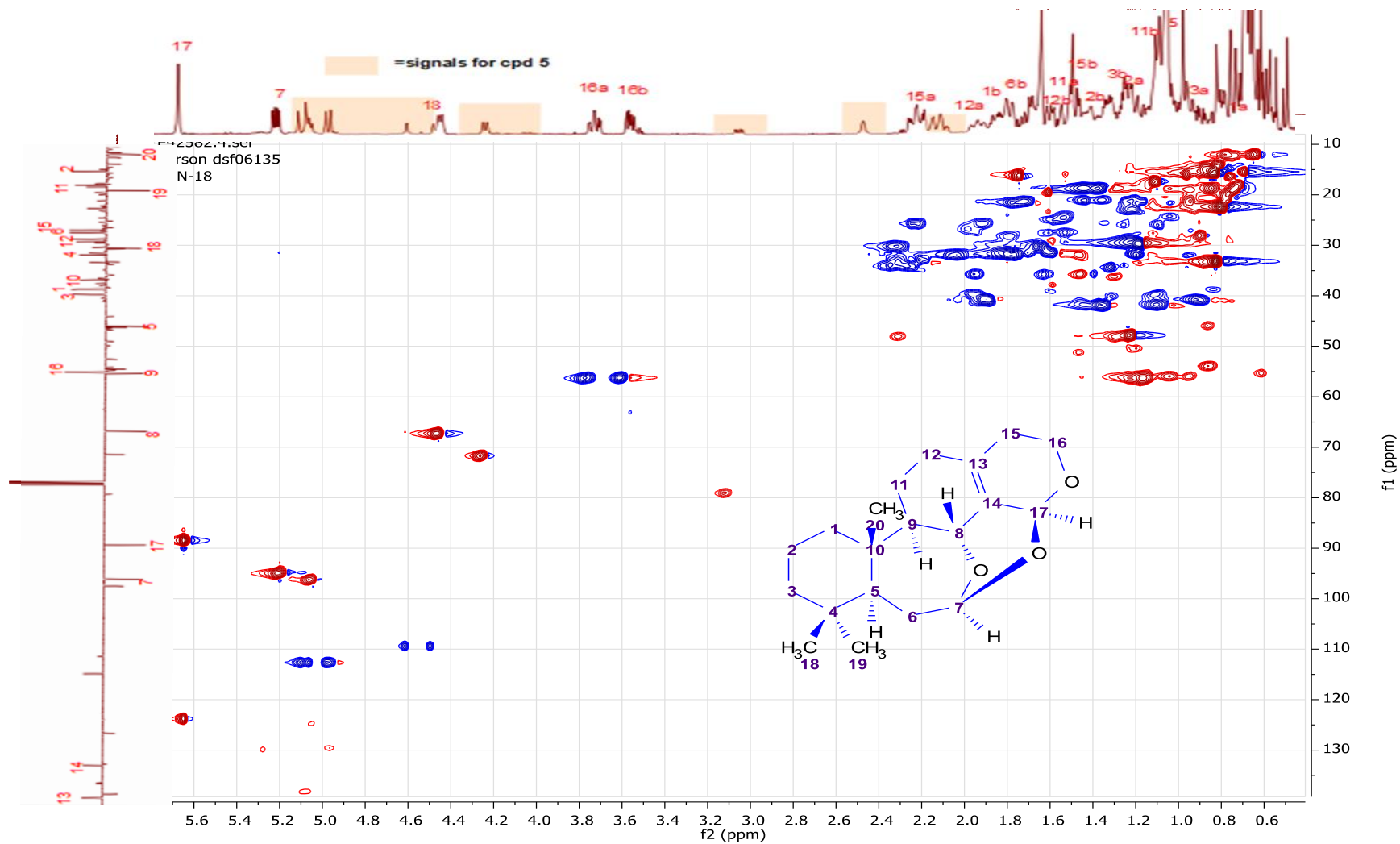


Figure S18: HSQC Spectrum of compound 2

