SUPPORTING INFORMATION FOR:

Structures of New Alkaloids from Rain Forest Trees *Galbulimima belgraveana* and *Galbulimima baccata* in Papua New Guinea, Indonesia, and Northern Australia

Ping Lan*[†], Anthony J. Herlt[‡], Anthony C. Willis[‡], Walter C. Taylor[§,※],

and Lewis N. Mander[*‡]

[†] *Department of Food Science and Engineering, Jinan University, Guangzhou, 510632, China*

[‡] *Research School of Chemistry, Australian National University, Canberra ACT 2601, Australia*

[§] *School of Chemistry, University of Sydney, NSW 2006, Australia*

[※] *Deceased January 1, 2009.*

lew.mander@anu.edu.au

ping.lan@jnu.edu.cn

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Crystallographic Studies

Crystallographic Data for Compounds 14-19 and 26.

Compound 14: $C_{24}H_{33}NO_5$, M = 415.53, T = 150 K, triclinic, space group $P1$, Z = 2, a = 8.3874(3) Å, b = 10.6644(6) Å, c = 13.5952(7) Å; α = 69.268(5)°, β = 89.374(4)°, γ = 71.779(4)°; V = 1073.44(10) Å^3, D_x = 1.286 Mg m^{-3}, 5411 unique data ($2\theta_{max}$ = 144.6°), R = 0.047 [for 5307 reflections with $I > 2.0\sigma(I)$]; Rw = 0.129 (all data), S = 1.02, Flack parameter 0.0(2).

Compound 15 hydrochloride salt: $C_{21}H_{30}NO_2^+Cl^-$, M = 363.93, T = 150 K, monoclinic, space group $P2_1$, Z = 2, a = 10.1135(3) Å, b = 8.7052(1) Å, c = 11.4139(3) Å; β = 113.189(3)° ;V = 923.70(4) Å^3, D_x = 1.308 Mg m^{-3}, 3051 unique data ($2\theta_{max}$ = 144.4°), R = 0.031 [for 2974 reflections with $I > 2.0\sigma(I)$]; Rw = 0.084 (all data), S = 1.00, Flack parameter 0.01(1).

Compound 16 hydrochloride salt: $C_{22}H_{32}NO_4^+Cl^-$, M = 409.95, T = 150 K, orthorhombic, space group $P2_12_12_1$, Z = 8, a = 9.0105(1) Å, b = 13.7999(1) Å, c = 33.4435(2) Å; V = 4158.50(6) Å^3, D_x = 1.310 Mg m^{-3}, 8204 unique data ($2\theta_{max}$ = 144.6°), R = 0.033 [for 7985 reflections with $I > 2.0\sigma(I)$]; Rw = 0.082 (all data), S = 1.03, Flack parameter 0.01(1).

Compound 17: $C_{21}H_{31}NO_2$•0.512(H_2O)•0.488(CH_3OH), M = 354.35, T = 150 K, orthorhombic, space group $P2_12_12_1$, Z = 4, a = 7.8673(2) Å, b = 9.5188(2) Å, c = 26.3409(5) Å; V = 1972.60(8) Å^3, D_x = 1.193 Mg m^{-3}, 3889 unique data ($2\theta_{max}$ = 144.6°), R = 0.031 [for 3769 reflections with $I > 2.0\sigma(I)$]; Rw = 0.079 (all data), S = 1.00, Flack parameter 0.04(18).

Compound 18 hydrochloride salt: $C_{21}H_{32}NO_2^+Cl^-$, M = 365.94, T = 150 K, orthorhombic, space group $P2_12_12_1$, Z = 4, a = 7.4614(1) Å, b = 9.6133(1) Å, c = 28.5458(2) Å; V = 2047.55(4) Å^3, D_x = 1.187 Mg m^{-3}, 4040 unique data ($2\theta_{max}$ = 144.8°), R = 0.024 [for 3978 reflections with $I > 2.0\sigma(I)$]; Rw = 0.061 (all data), S = 1.01, Flack parameter 0.001(8).

Compound 19 hydrochloride salt: $C_{22}H_{30}NO_4^+Cl^-$, M = 407.94, T = 150 K, orthorhombic, space group $P2_12_12_1$, Z = 4, a = 8.5727(3) Å, b = 9.0053(4) Å, c = 26.1687(10) Å; V = 2020.22(14) Å^3, D_x = 1.341 Mg m^{-3}, 3937 unique data ($2\theta_{max}$ = 144.0°), R = 0.065 [for 3797 reflections with $I > 2.0\sigma(I)$]; Rw = 0.182 (all data), S = 1.02, Flack parameter 0.03(3).

Compound 26: $2(C_{21}H_{31}NO_3)\bullet C_4H_8O_2$, M = 779.06, T = 150 K, orthorhombic, space group $P2_12_12_1$, Z = 4, a = 12.7070(6) Å, b = 18.7410(10) Å, c = 19.0369(8) Å; V = 4533.5(4) Å^3, D_x = 1.141 Mg m^{-3}, 4900 unique data ($2\theta_{max}$ = 144.0°), R = 0.067 [for 3819 reflections with $I > 2.0\sigma(I)$]; Rw = 0.171 (all data), S = 0.99.

Structure Determination

Images were measured on an Agilent SuperNova CCD diffractometer (CuKα, mirror monochromator, λ 1.54184 Å) and data extracted using the CrysAlis package.[1] Structure solution was by direct methods (SIR92).[2] The structures of compounds **14-19** and **26** were refined using the CRYSTALS program package.[3] Atomic coordinates, bond lengths and angles, and displacement parameters for compounds **14-19** and **26** have been deposited at the Cambridge Crystallographic Data Centre (CCDC nos. 1587050, 1587051, 1587052, 1587053, 1587054, 1587055 and 1587056 for compounds **14-19** and **26**, respectively). These data can be obtained free-of-charge via www.ccdc.cam.ac.uk/data_request/cif, by emailing data_request@ccdc.cam.ac.uk, or by contacting The Cambridge Crystallographic Data Centre, 12 Union Road, Cambridge CB2 1EZ, UK; fax: +44 1223 336033.

References

1. CrysAlisPro, Agilent Technologies, Version 1.171.37.33d (release 23-04-2014 CrysAlis171.NET) (compiled 23 April 2014, 17:37:27).

2. SIR92. A. Altomare, G. Cascarano, C. Giacovazzo, A. Guagliardi, M. C. Burla, G. Polidori, and M. Camalli, M. *J. Appl. Crystallogr.*, 1994, **27**, 435.

3. P. W. Betteridge, J. R. Carruthers, R. I. Cooper, K. Prout, and D. J. Watkin, *J. Appl. Crystallogr*., 2003, **36**, 1487.

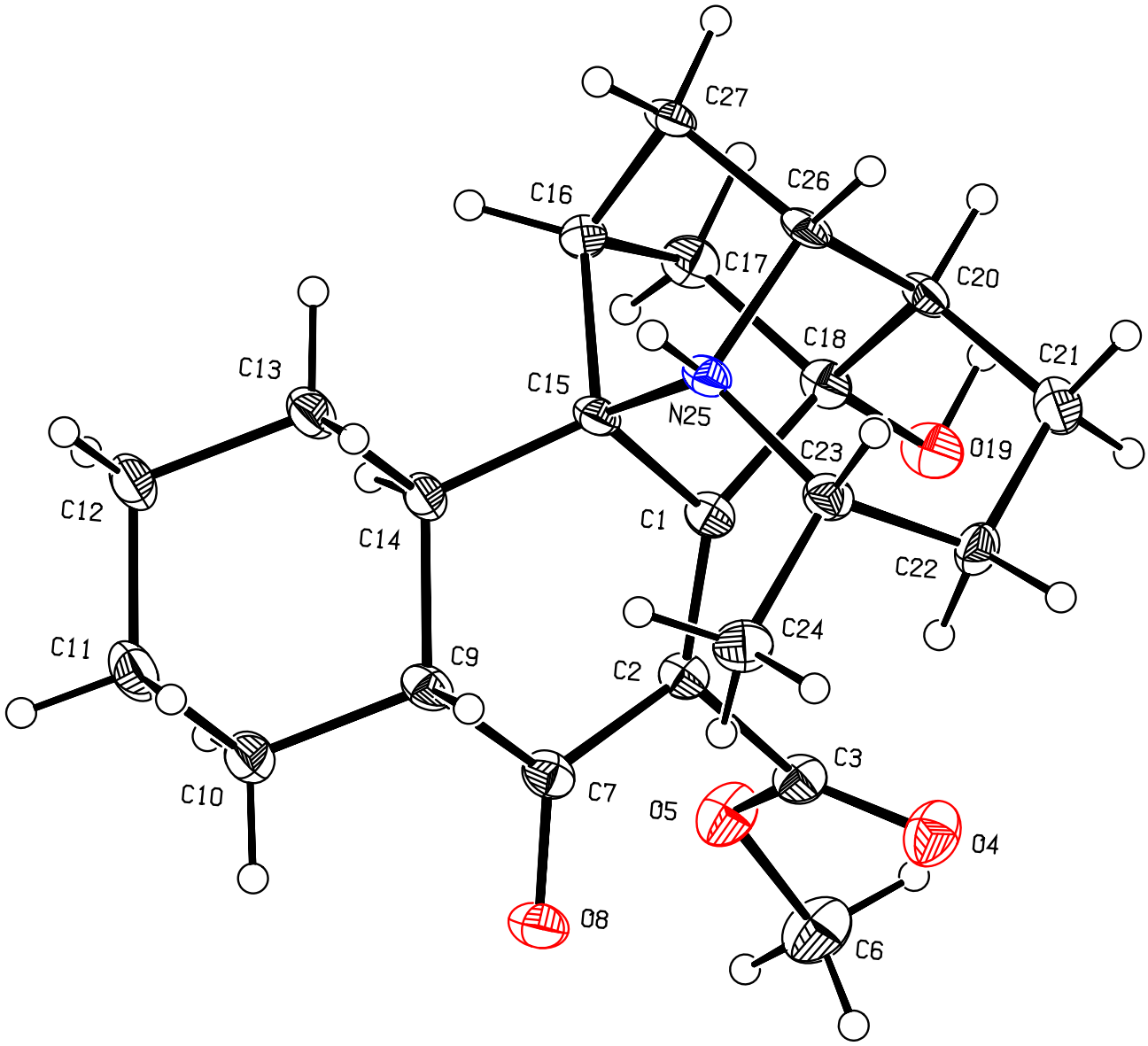

Figure S1: Structure of compound **14** (CCDC 1587050) with labelling of selected atoms. Anisotropic displacement ellipsoids show 30% probability levels. Hydrogen atoms are drawn as circles with small radii.

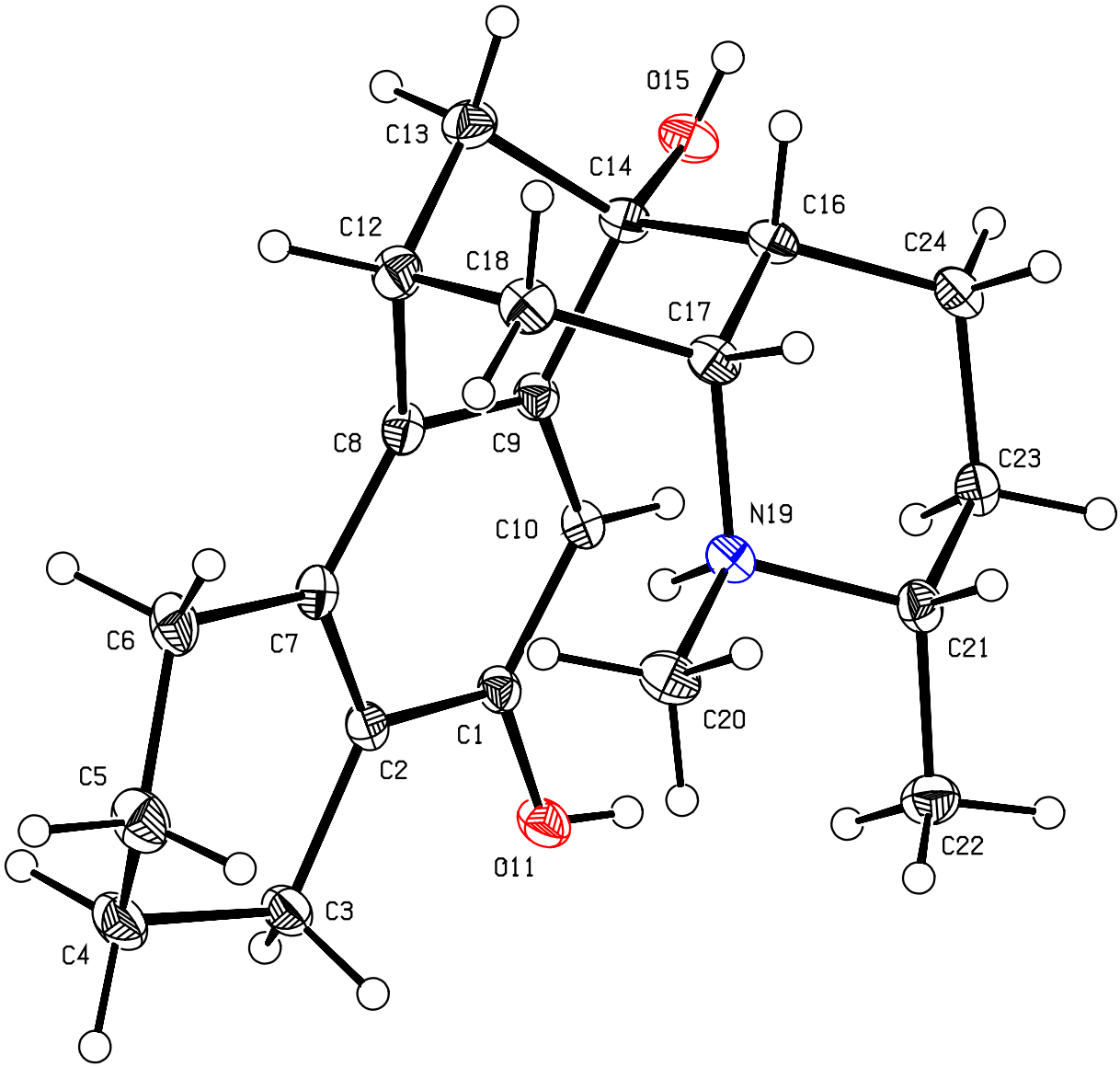

Figure S2: Structure of compound **15** (CCDC 1587051) with labelling of selected atoms. Anisotropic displacement ellipsoids show 30% probability levels. Hydrogen atoms are drawn as circles with small radii.

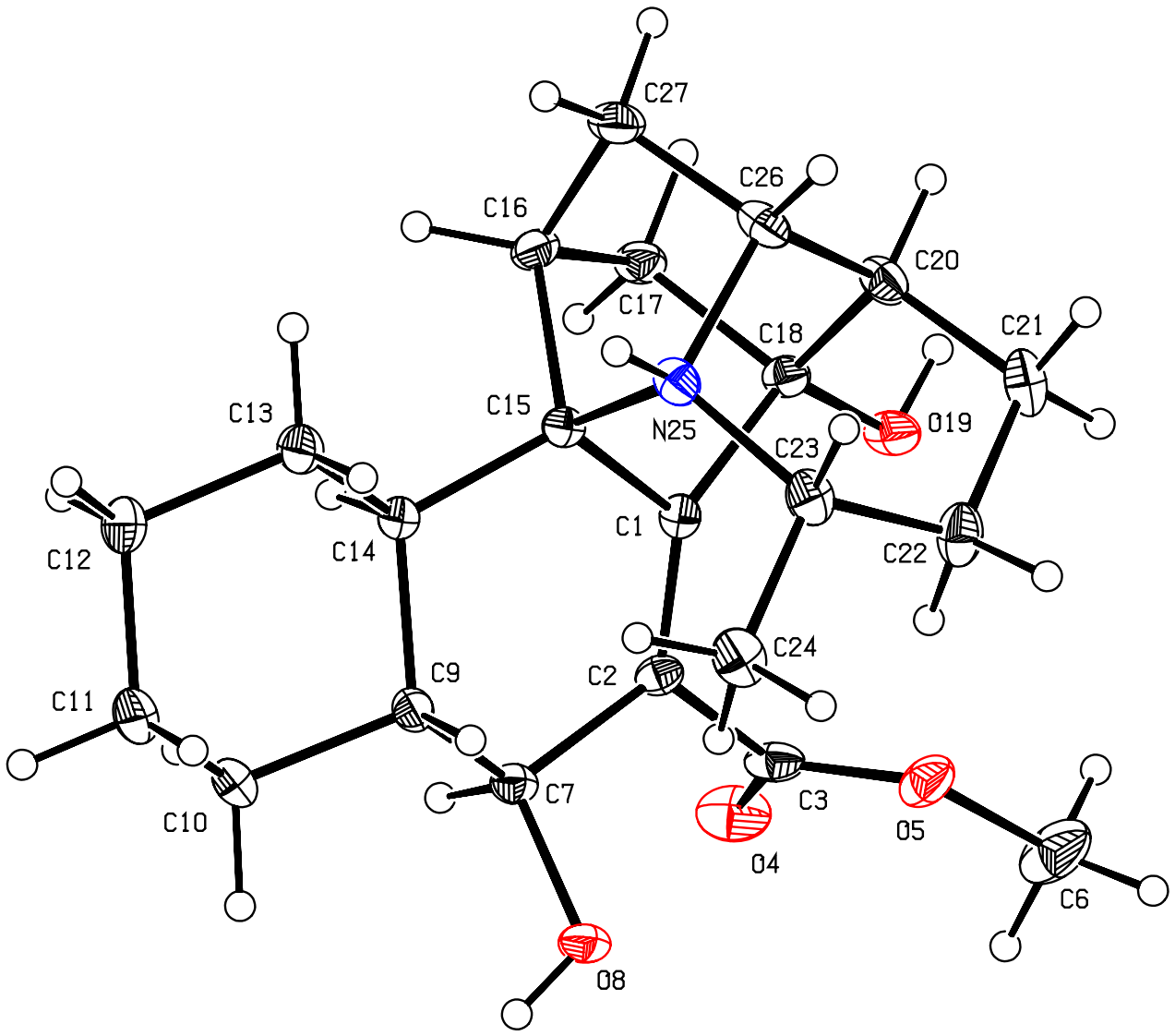

Figure S3: Structure of compound **16** (CCDC 1587052) with labelling of selected atoms. Anisotropic displacement ellipsoids show 30% probability levels. Hydrogen atoms are drawn as circles with small radii.

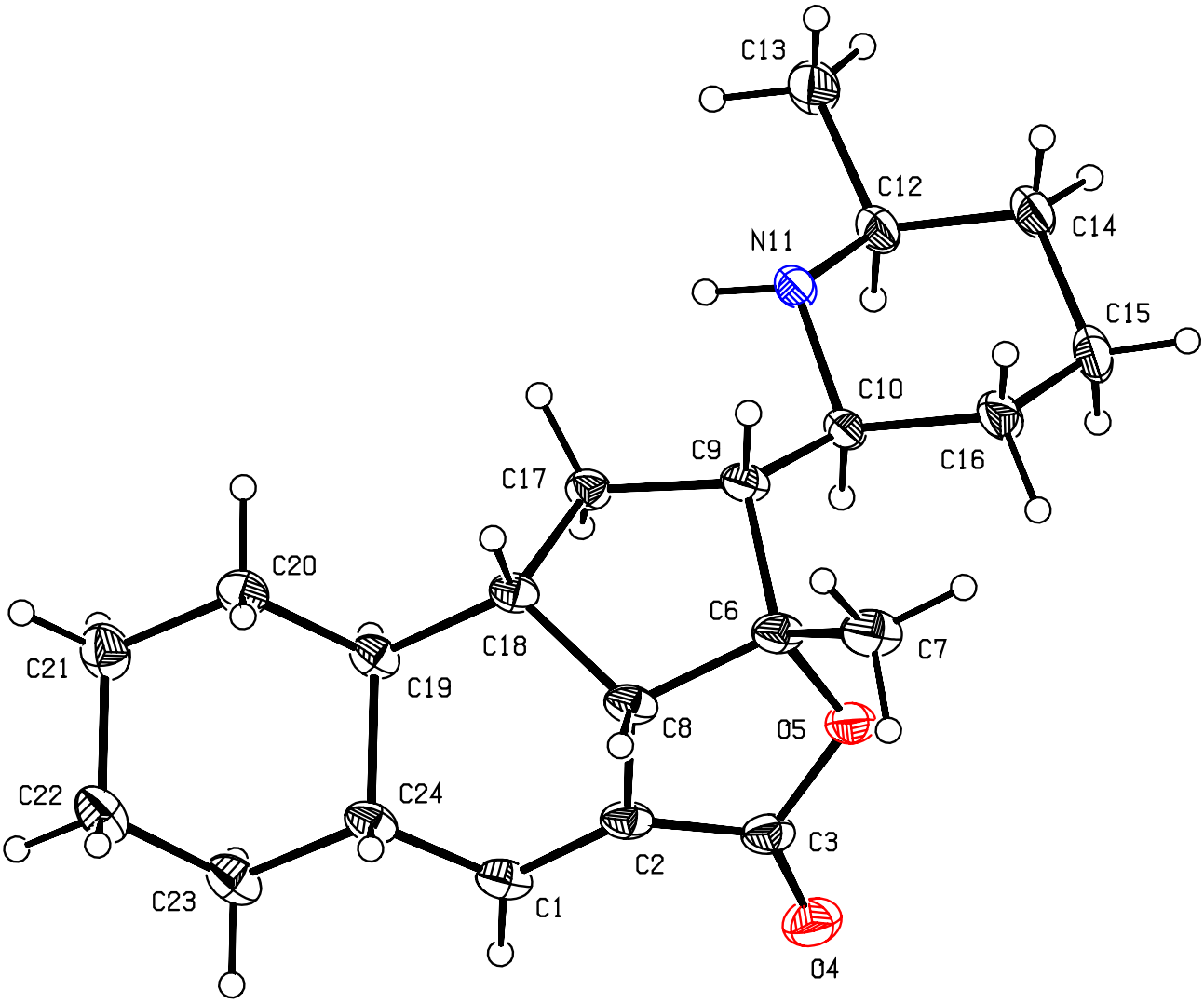

Figure S4: Structure of compound **17** (CCDC 1587053) with labelling of selected atoms. Anisotropic displacement ellipsoids show 30% probability levels. Hydrogen atoms are drawn as circles with small radii.

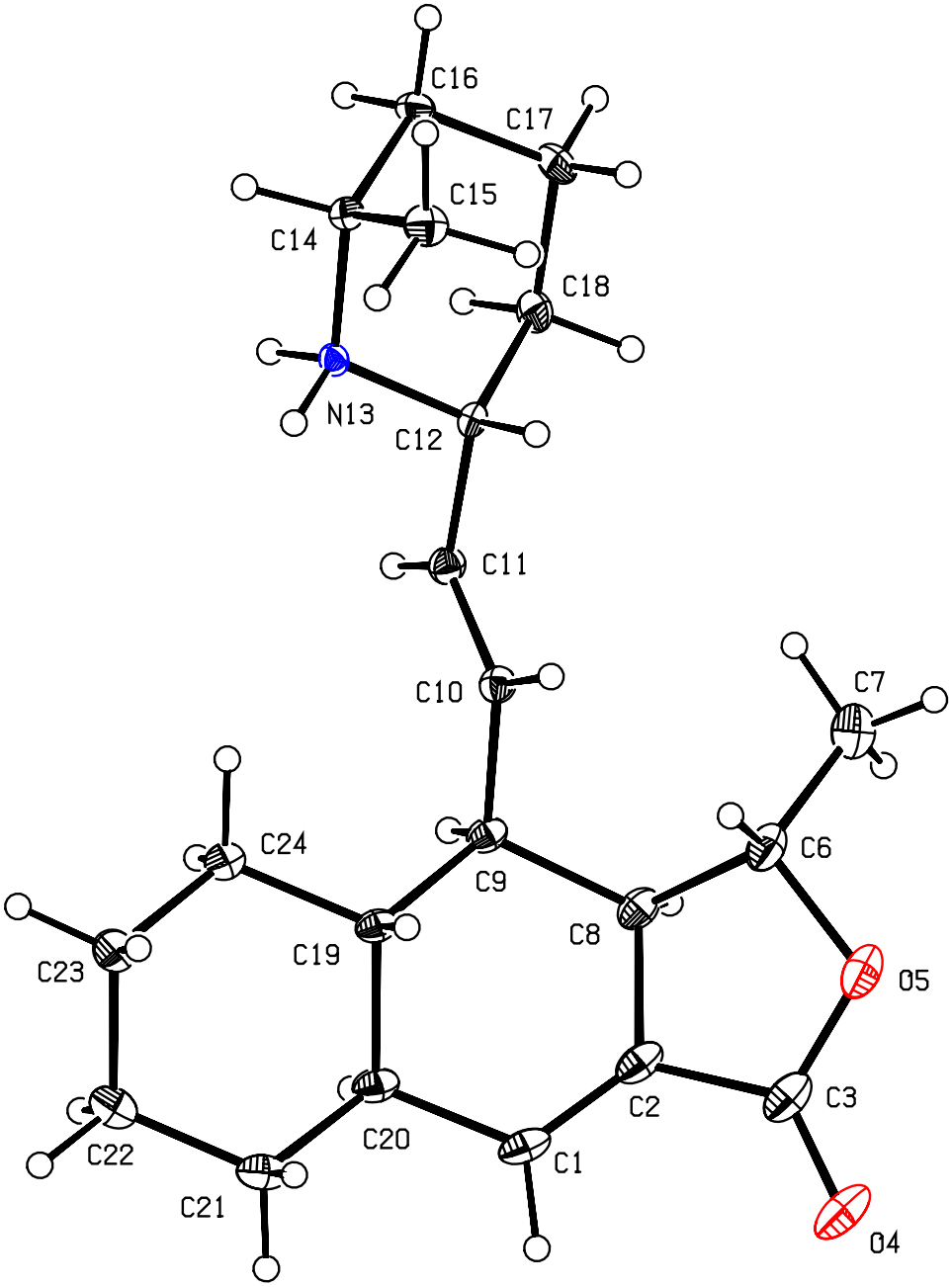

Figure S5: Structure of compound **18** (CCDC 1587054) with labelling of selected atoms. Anisotropic displacement ellipsoids show 30% probability levels. Hydrogen atoms are drawn as circles with small radii.

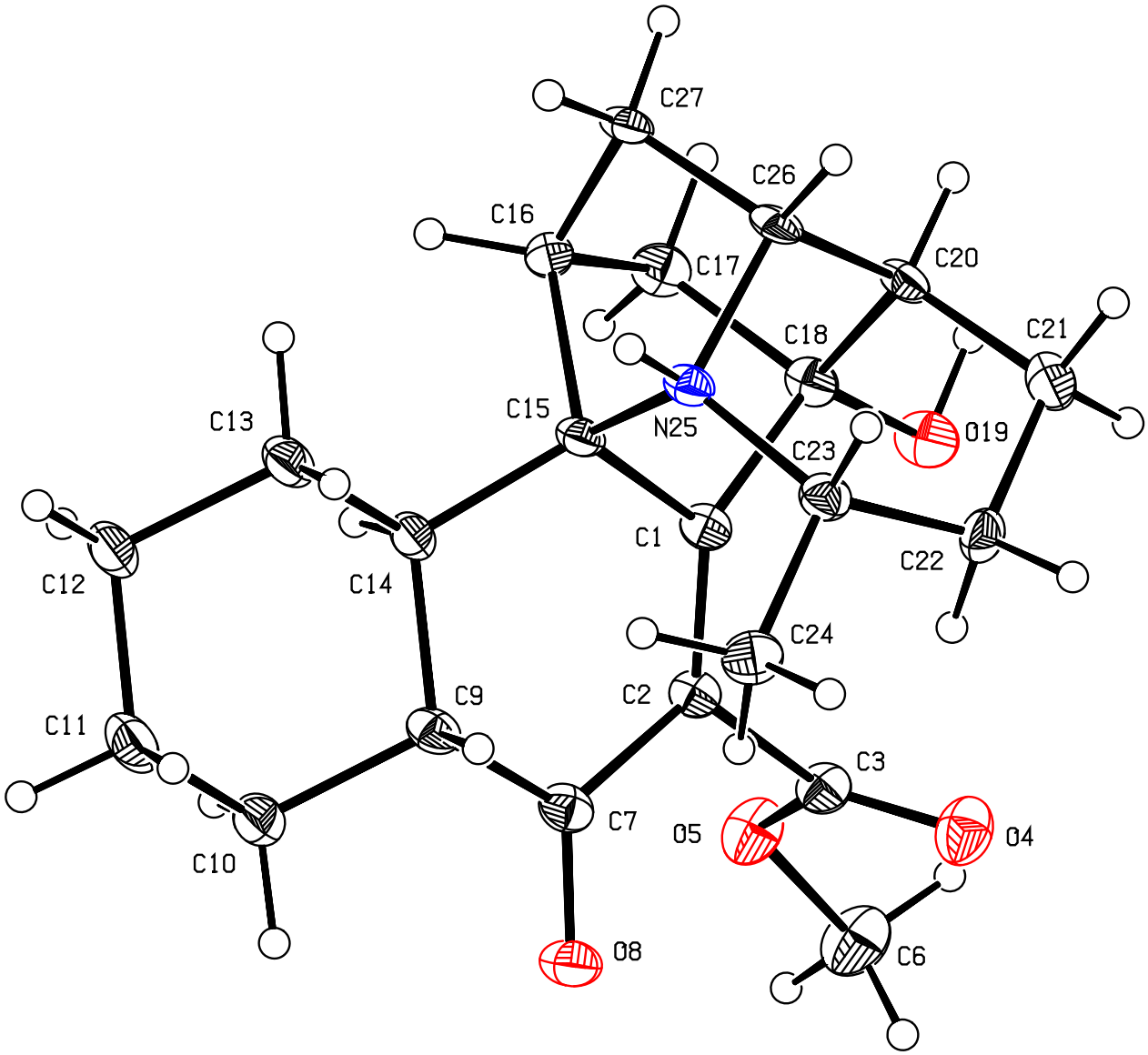

Figure S6: Structure of compound **19** (CCDC 1587055) with labelling of selected atoms. Anisotropic displacement ellipsoids show 30% probability levels. Hydrogen atoms are drawn as circles with small radii.

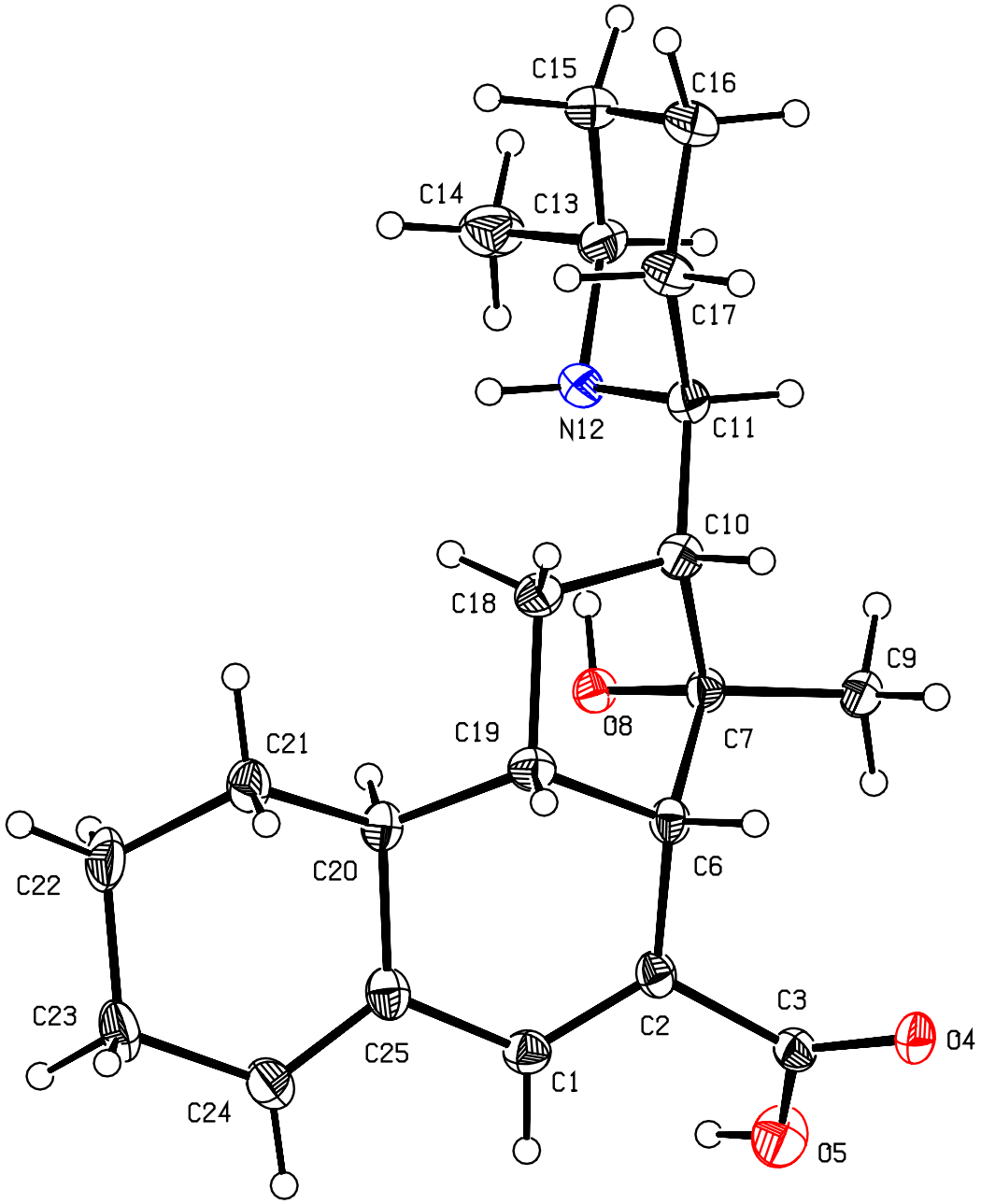

Figure S7: Structure of compound **26** (CCDC 1587056) with labelling of selected atoms. Anisotropic displacement ellipsoids show 30% probability levels. Hydrogen atoms are drawn as circles with small radii.

Figure S8. 400 MHz ^{1}H NMR Spectrum of Compound **14** (Recorded in $CDCl_3$)

GB14 (**14**)

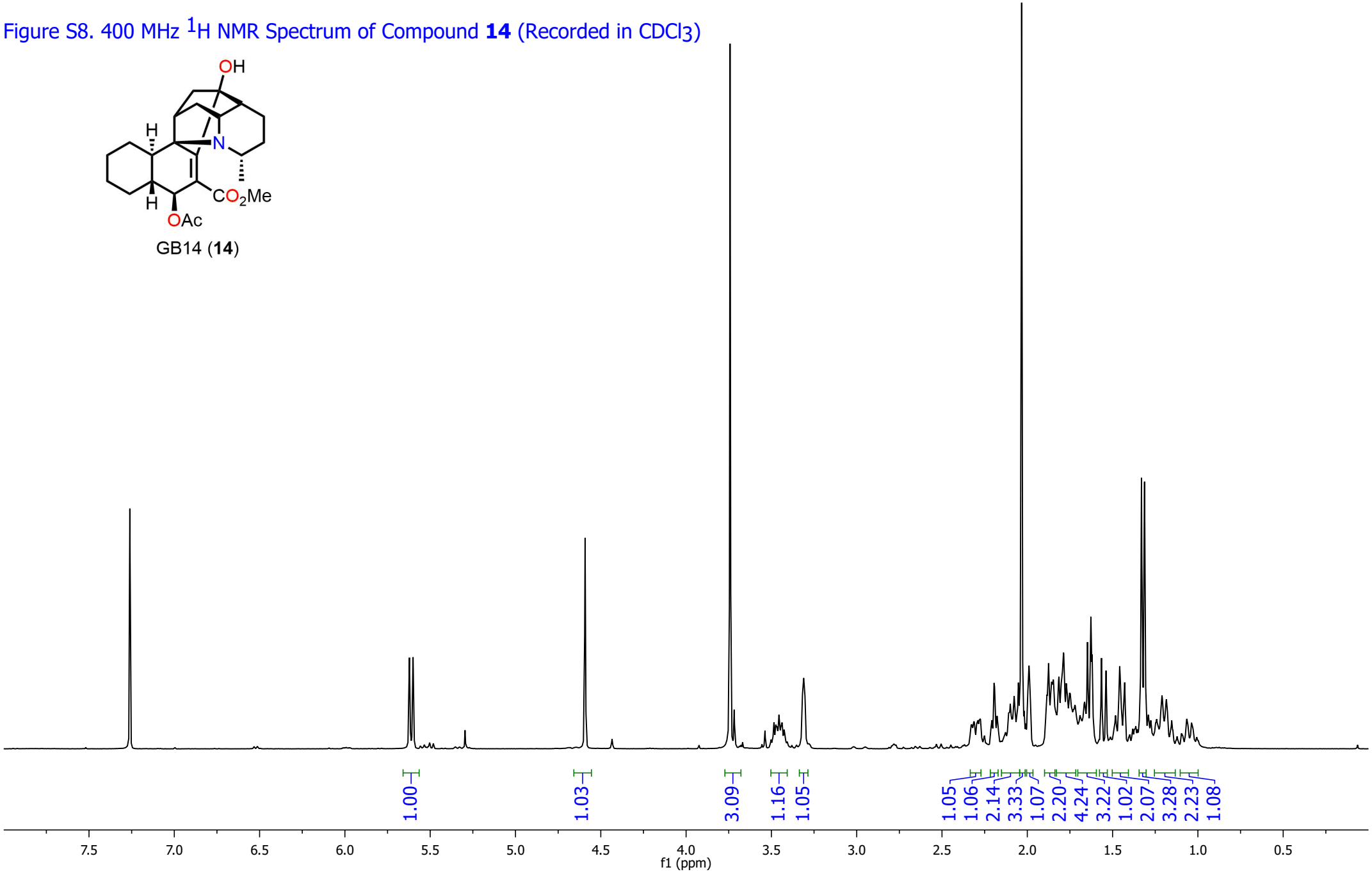

Figure S9. 100 MHz ^{13}C NMR Spectrum of Compound **14** (Recorded in $CDCl_3$)

GB14 (**14**)

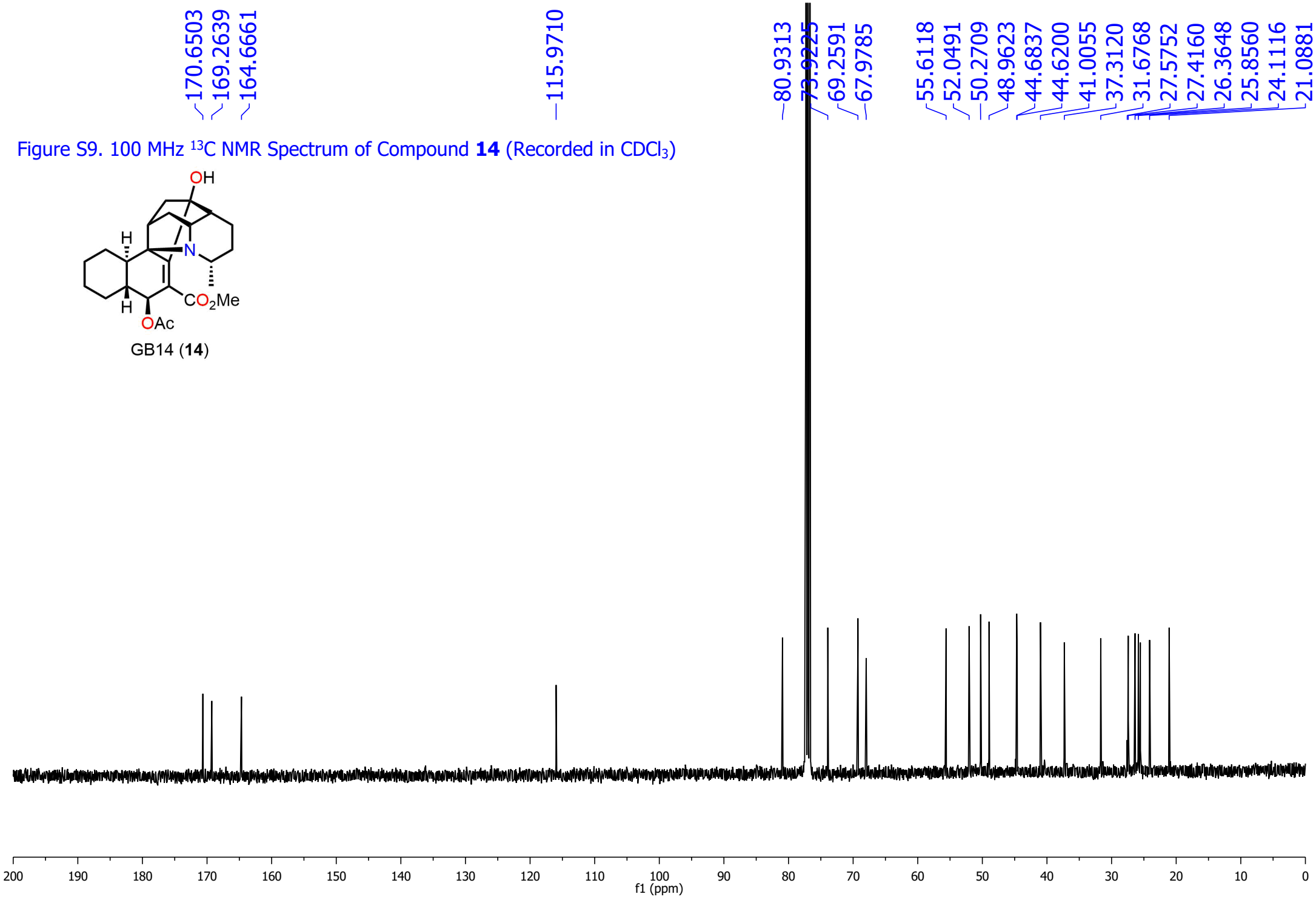

Figure S10. 400 MHz ^{1}H NMR Spectrum of Compound **15** (Recorded in $CDCl_3$)

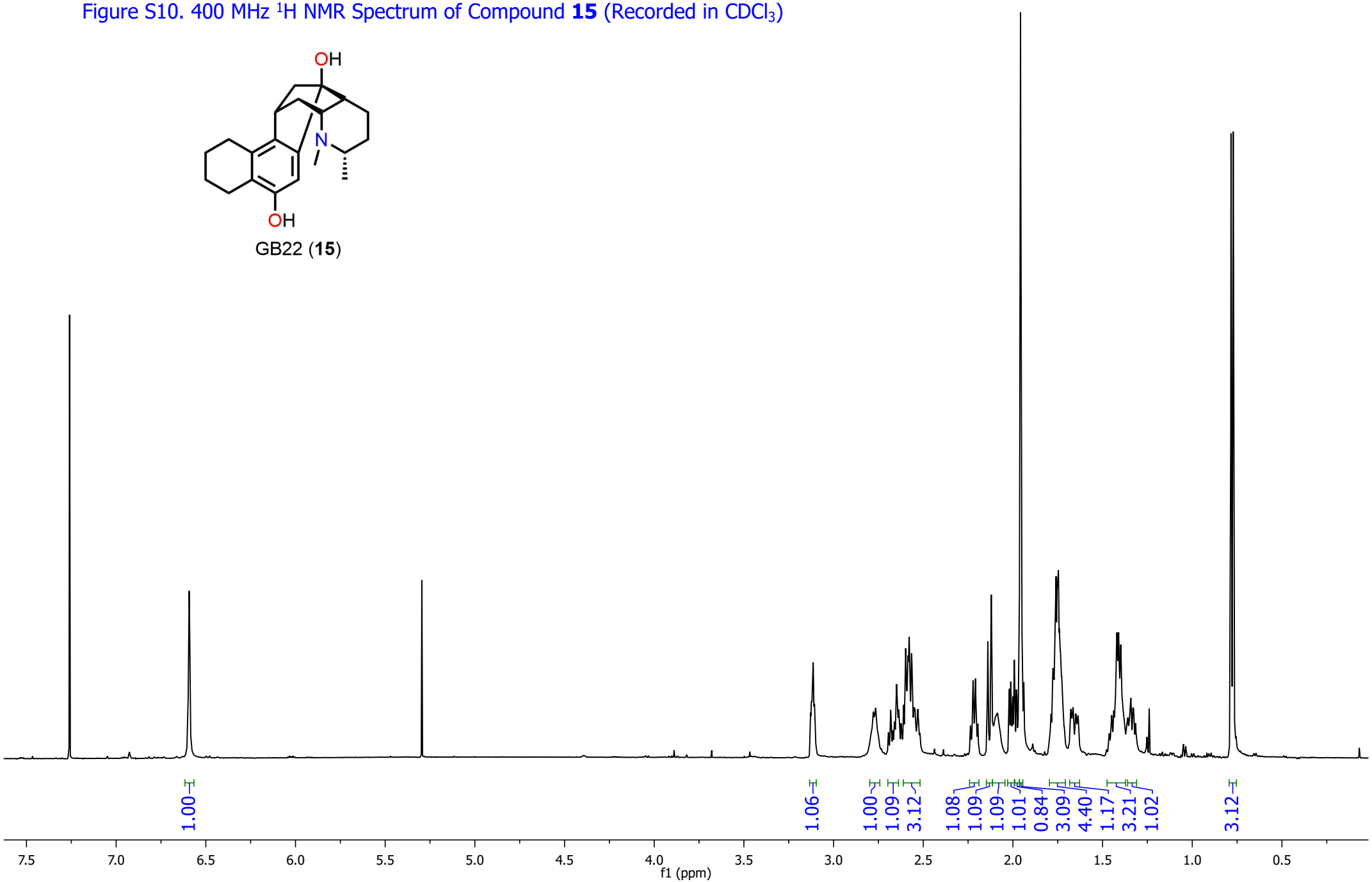

Figure S11. 100 MHz ^{13}C NMR Spectrum of Compound **15** (Recorded in $CDCl_3$)

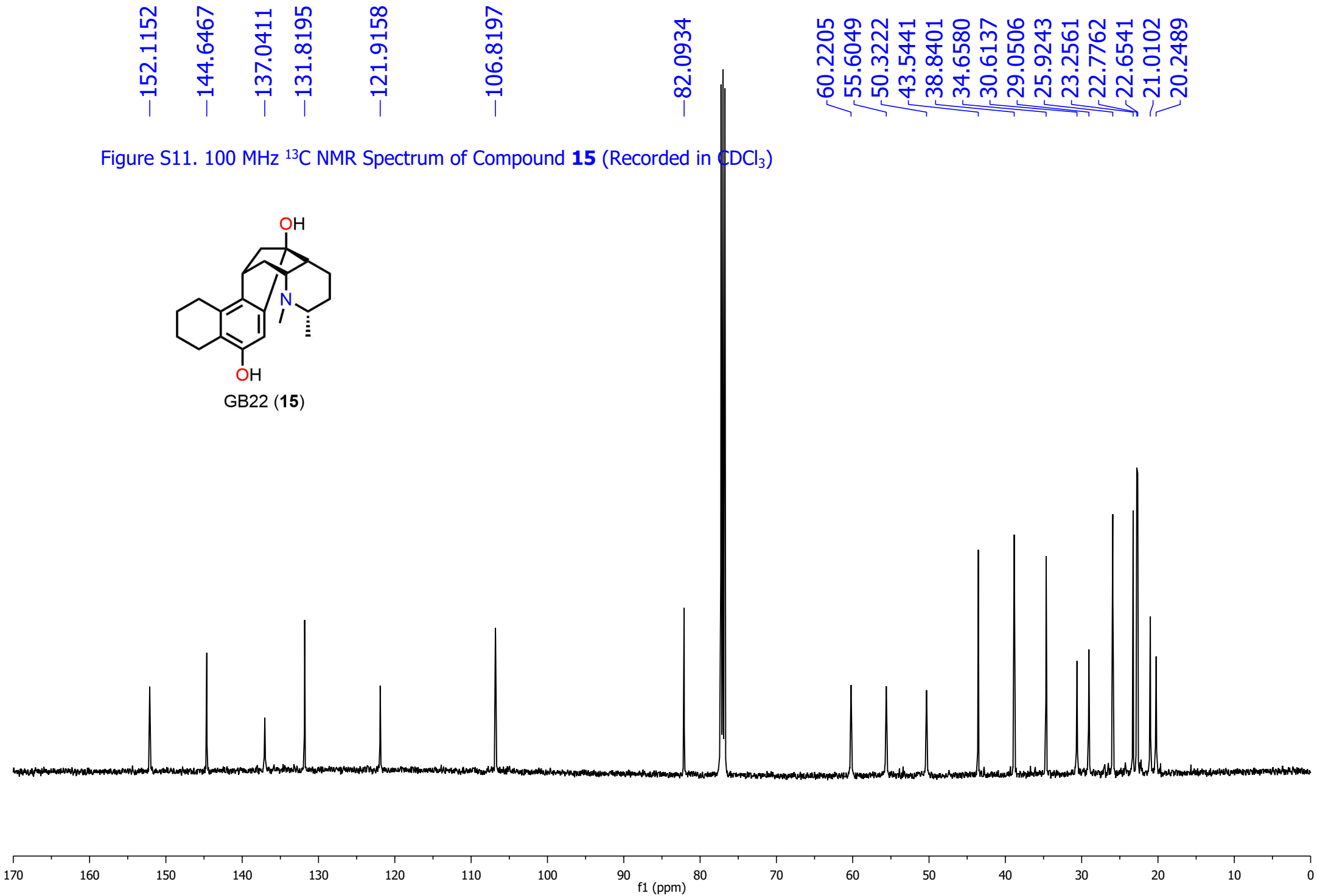

Figure S12. 400 MHz ^{1}H NMR Spectrum of Compound **16** (Recorded in $CDCl_3$)

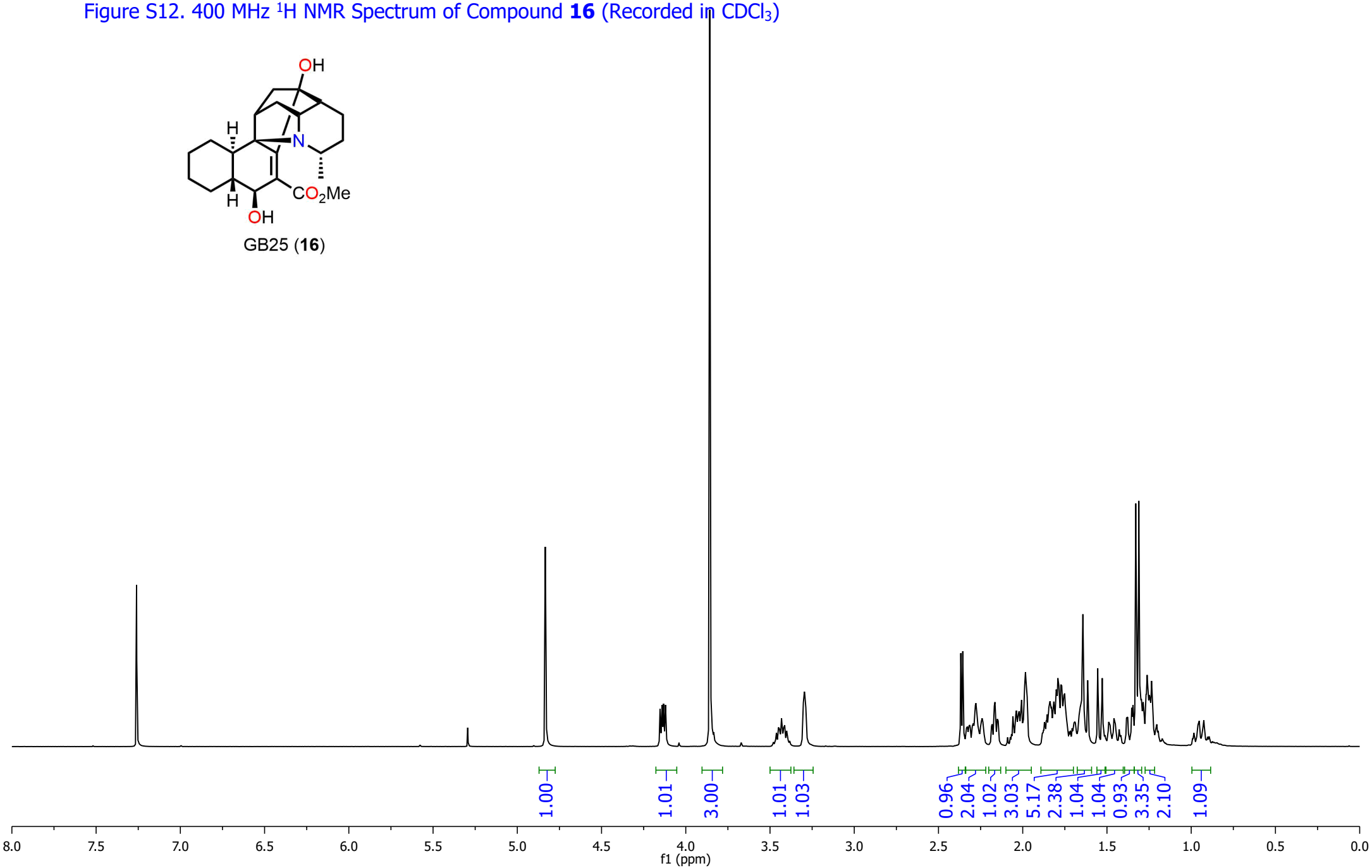

Figure S13. 100 MHz ^{13}C NMR Spectrum of Compound **16** (Recorded in $CDCl_3$)

GB25 (**16**)

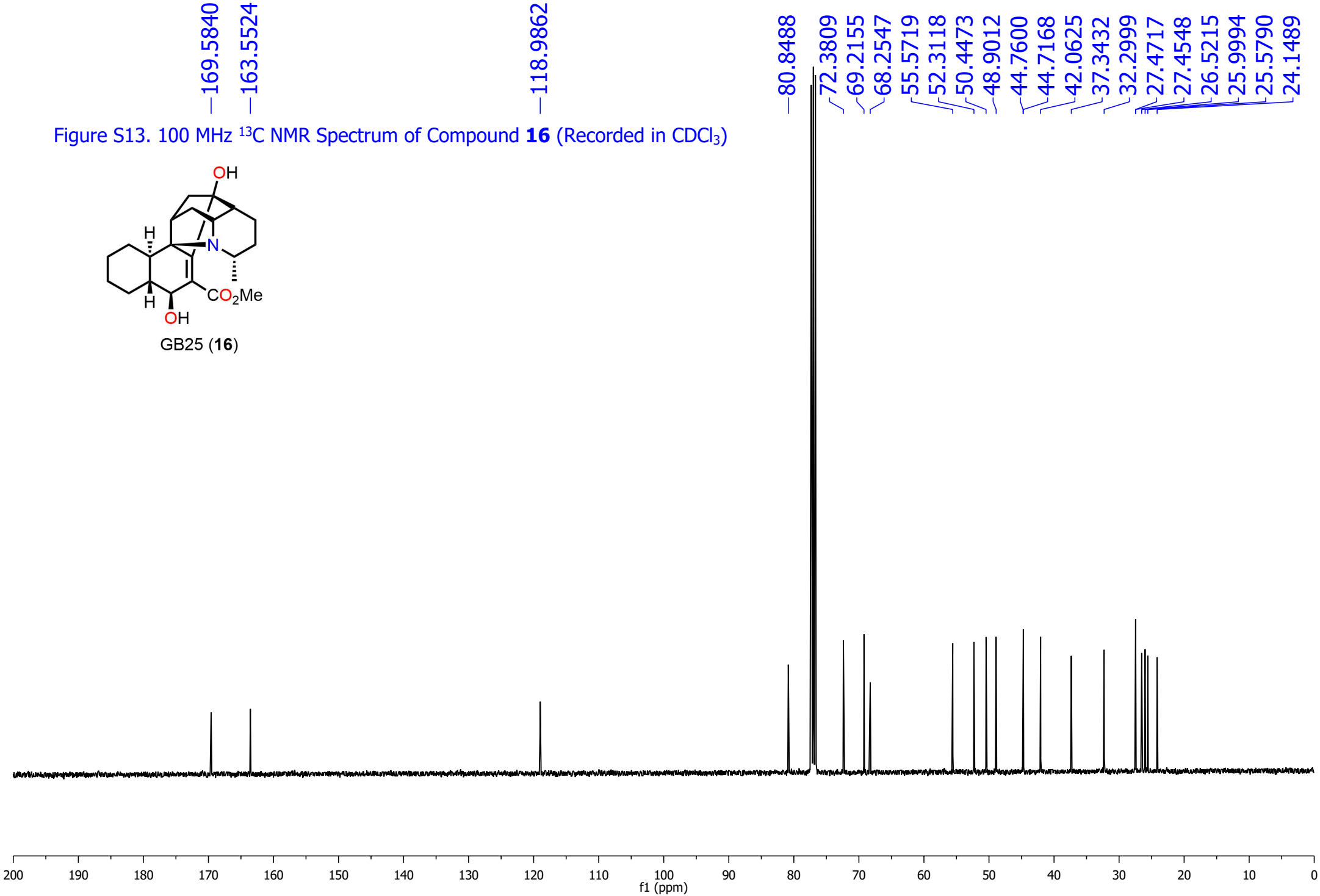

Figure S14. 400 MHz ^{1}H NMR Spectrum of Compound **17** (Recorded in $CDCl_3$)

GB21 (**17**)

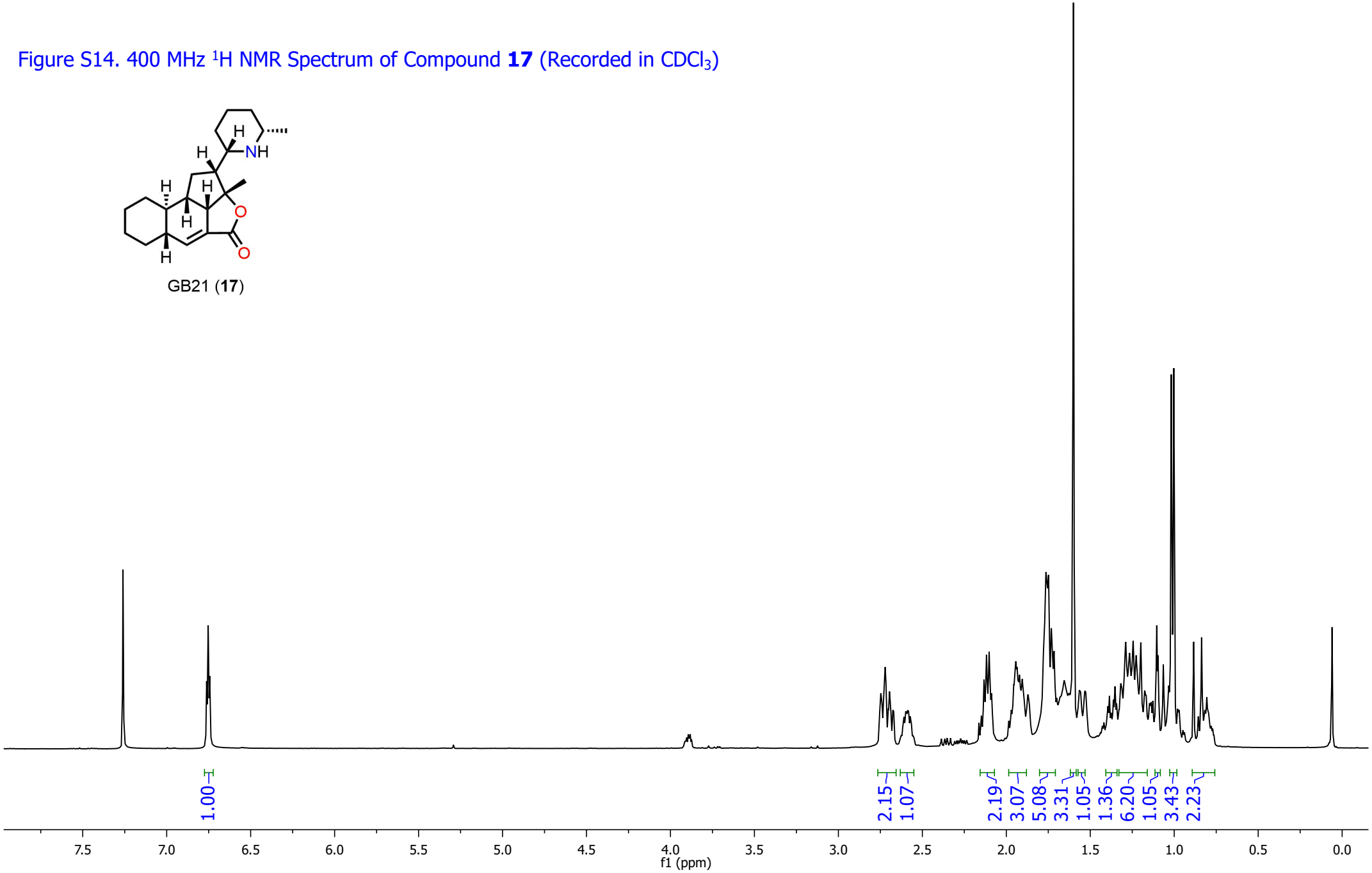

Figure S15. 100 MHz ^{13}C NMR Spectrum of Compound **17** (Recorded in $CDCl_3$)

GB21 (**17**)

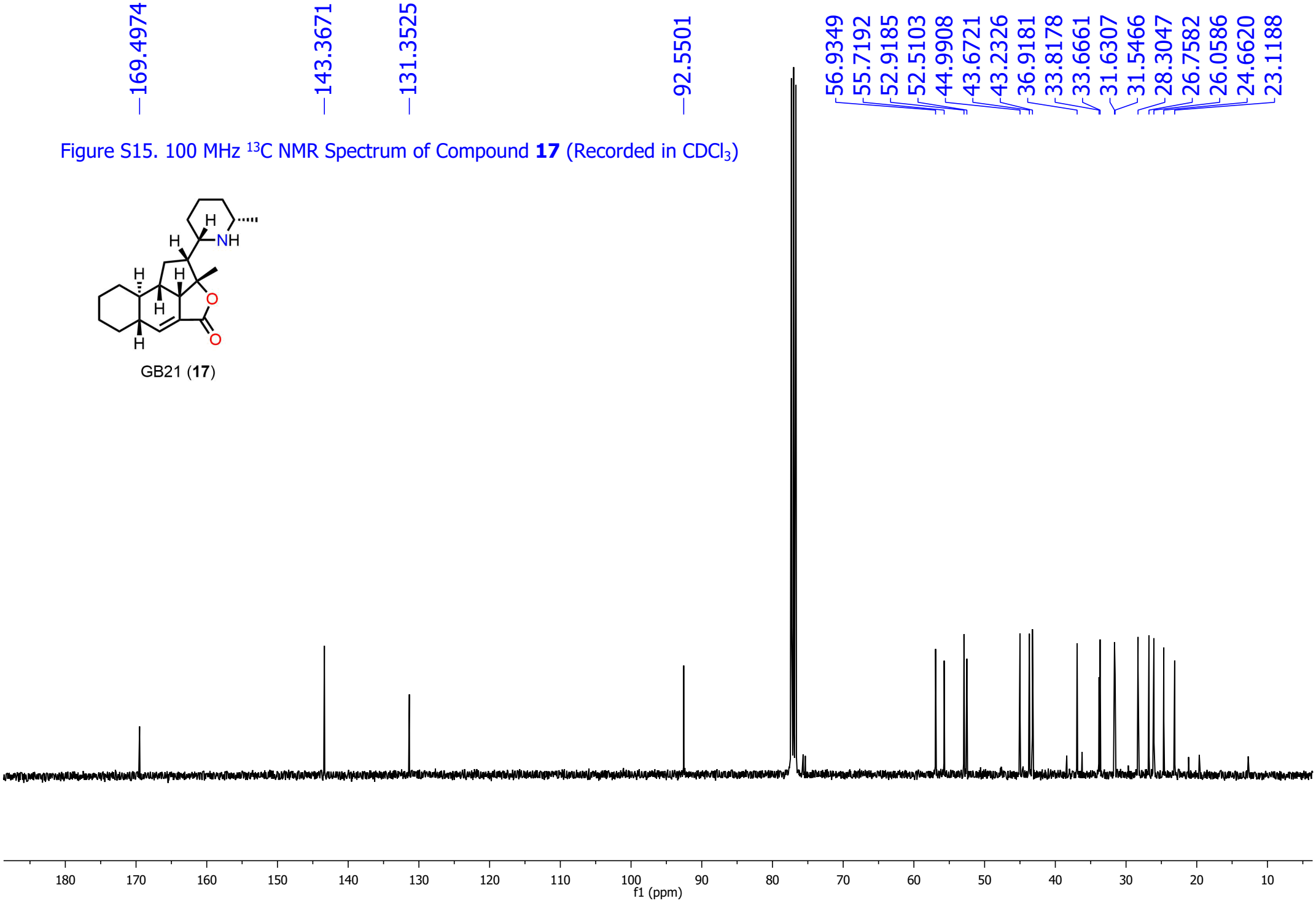

Figure S16. 400 MHz ^{1}H NMR Spectrum of Compound **18** (Recorded in $CDCl_3$)

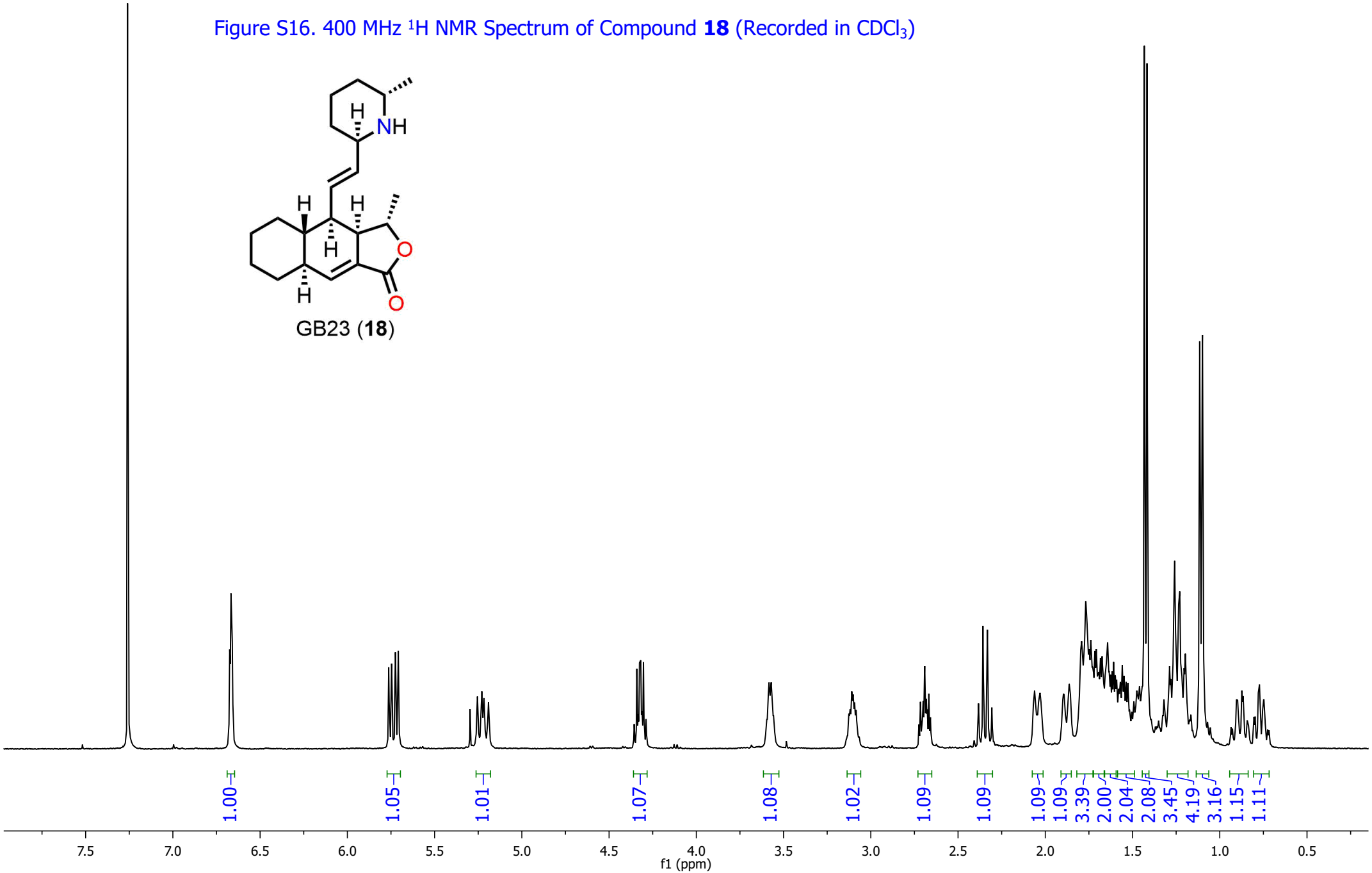

Figure S17. 100 MHz ^{13}C NMR Spectrum of Compound **18** (Recorded in $CDCl_3$)

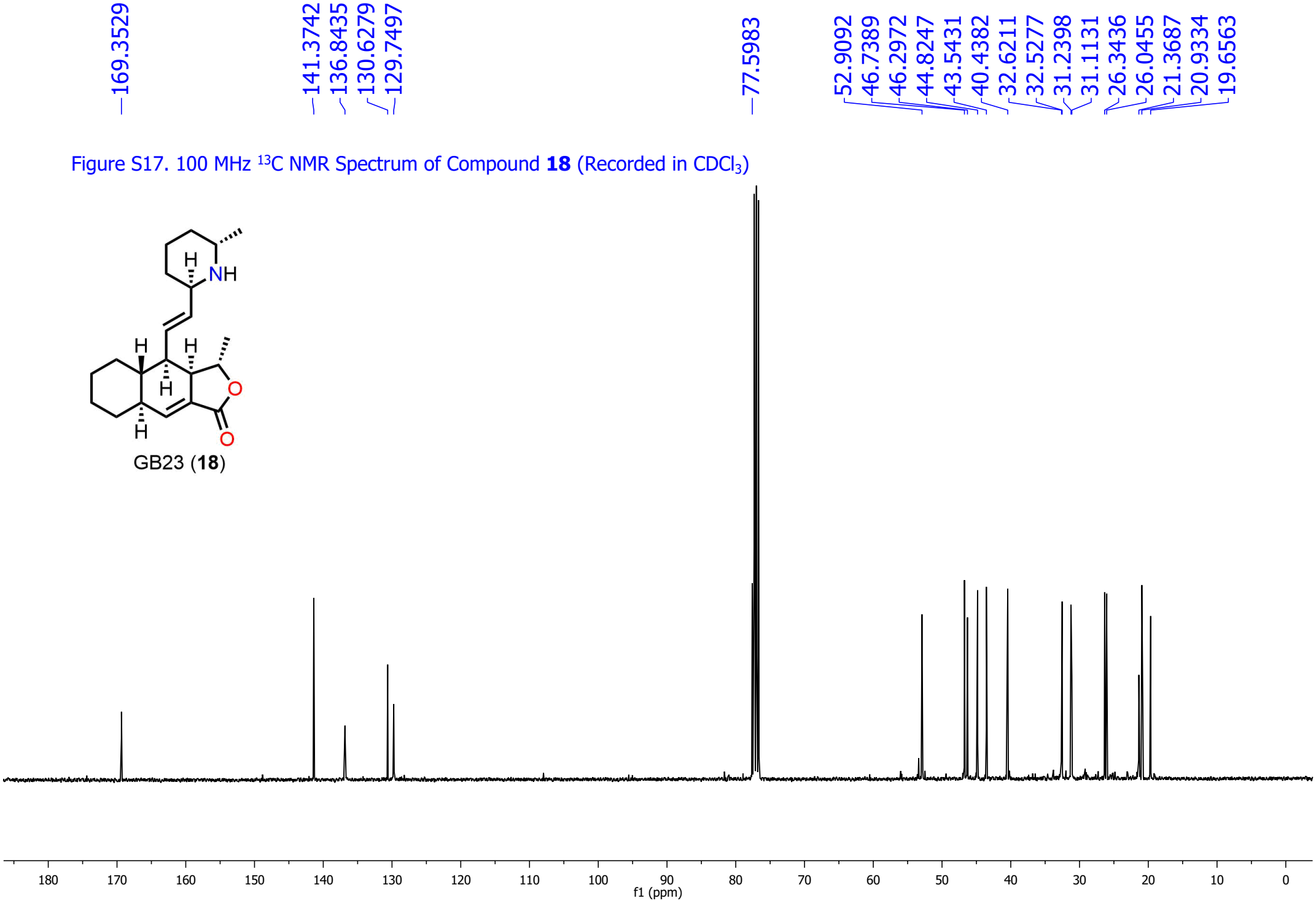

Figure S18. 400 MHz ^{1}H NMR Spectrum of Compound **19** (Recorded in $CDCl_3$)

GB24 (**19**)

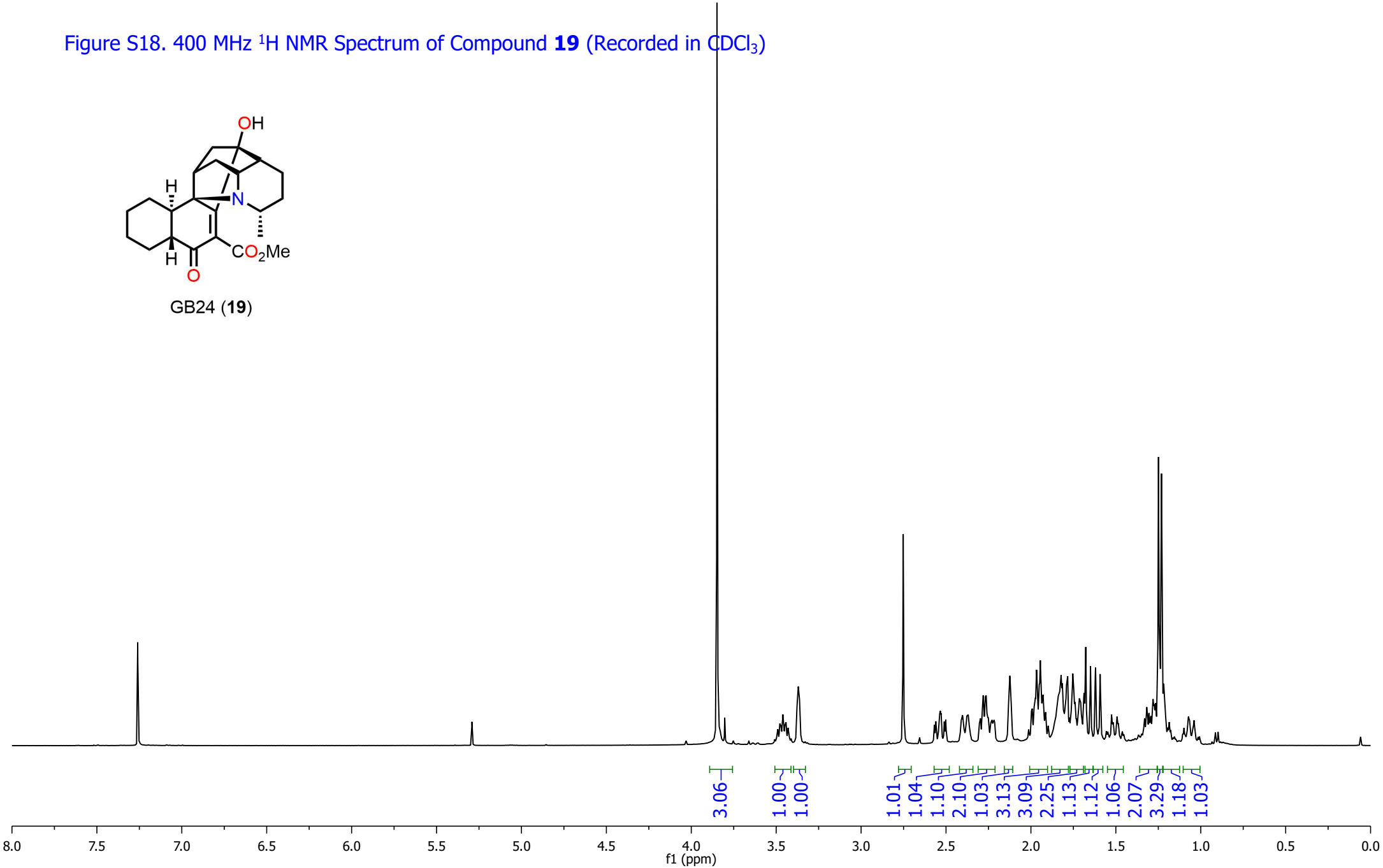

Figure S19. 100 MHz ^{13}C NMR Spectrum of Compound **19** (Recorded in $CDCl_3$)

GB24 (**19**)

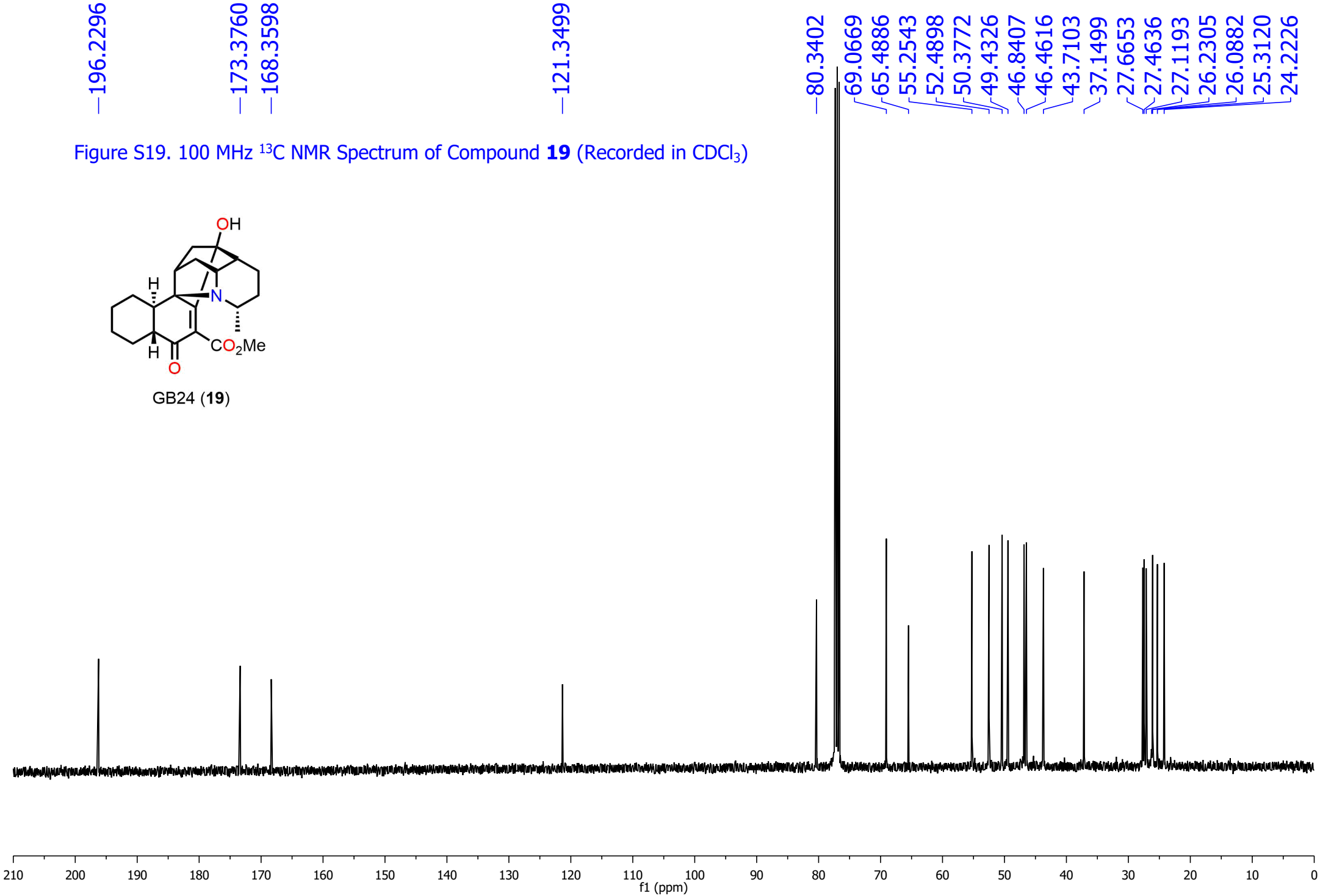

Figure S20. 400 MHz ^{1}H NMR Spectrum of Compound **20** (Recorded in $CDCl_3$)

GB26 (**20**)

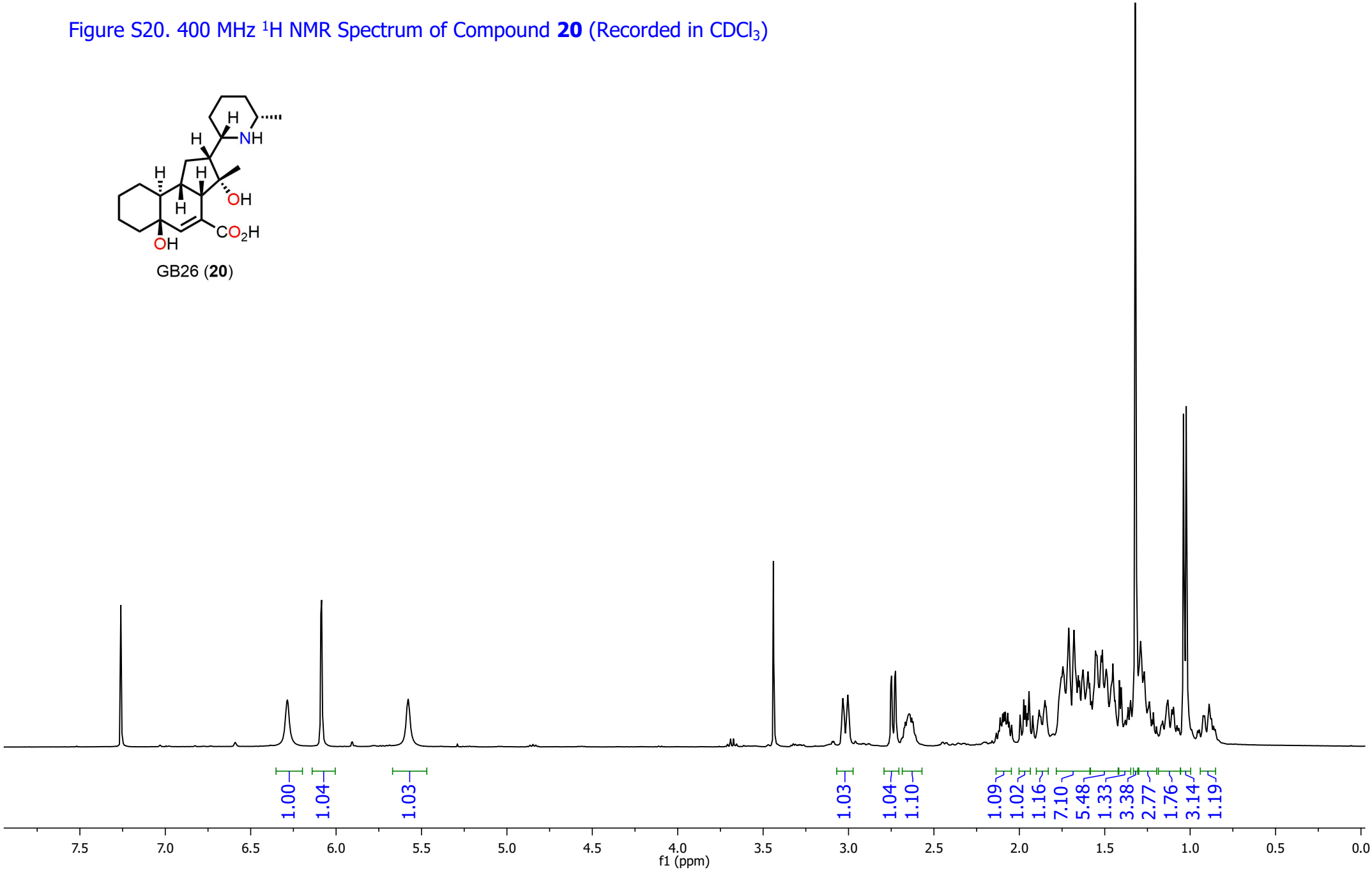

Figure S21. 100 MHz ^{13}C NMR Spectrum of Compound **20** (Recorded in $CDCl_3$)

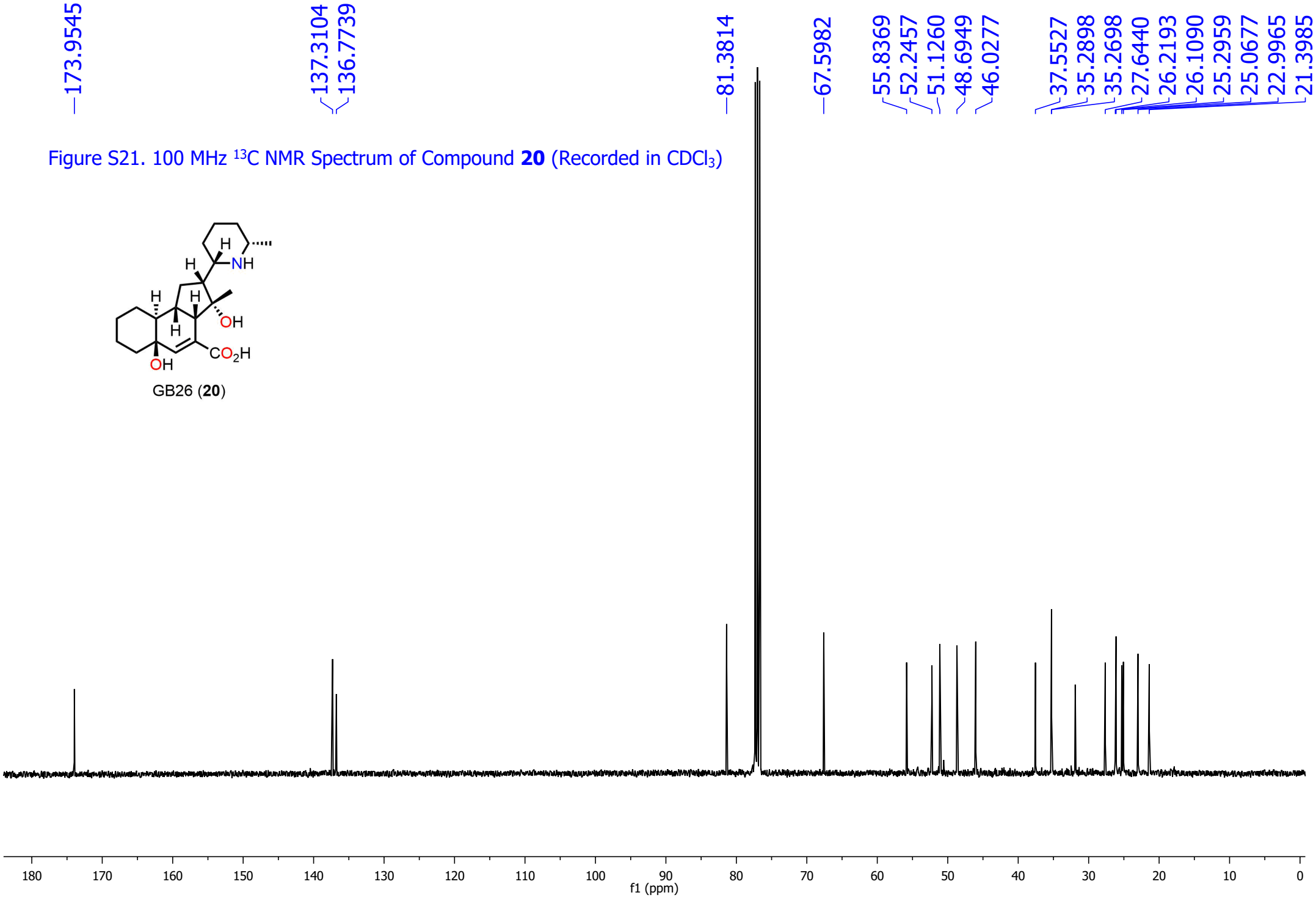

Figure S22. 400 MHz ^{1}H NMR Spectrum of Compound **21** (Recorded in $CDCl_3$)

21

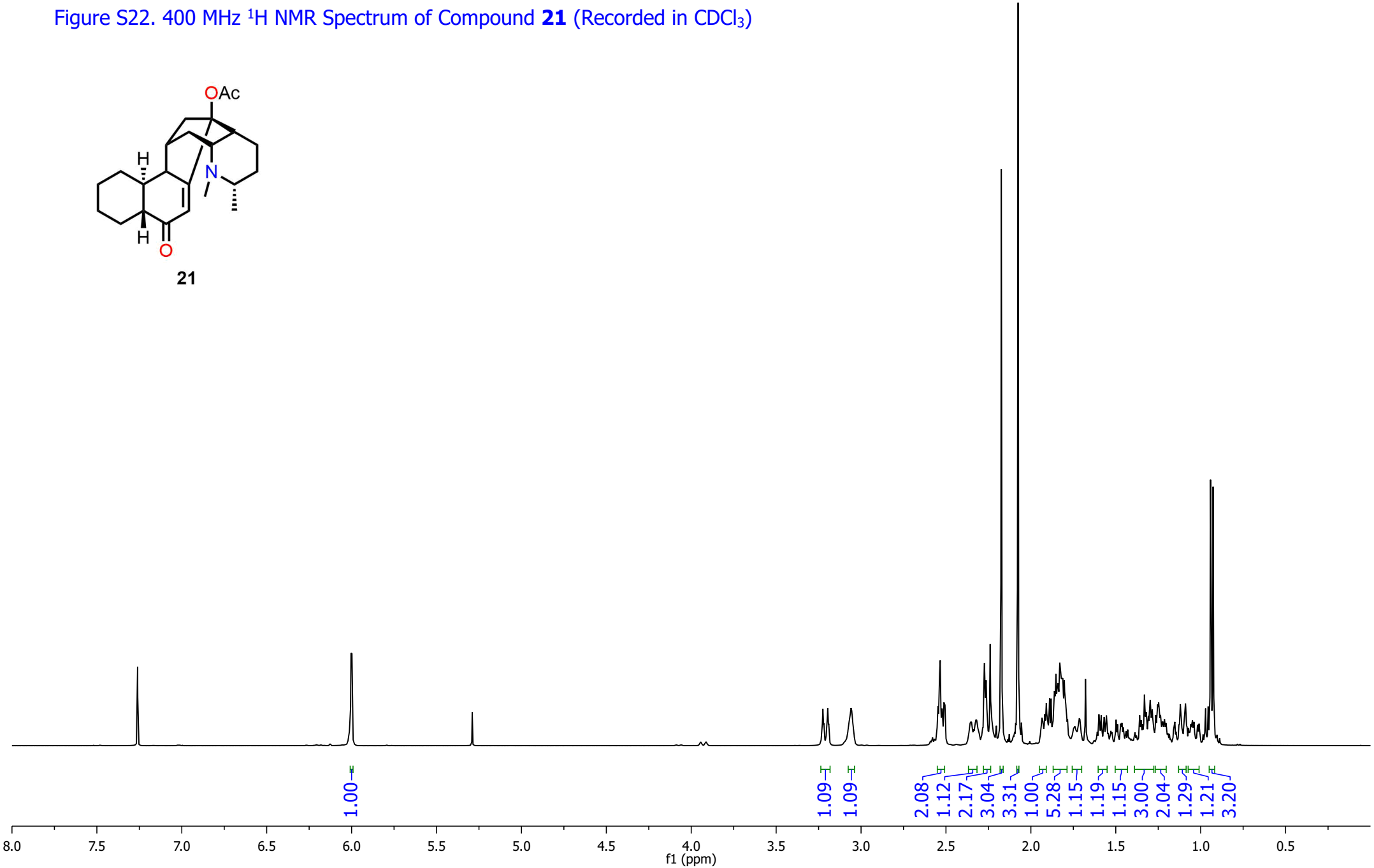

Figure S23. 100 MHz ^{13}C NMR Spectrum of Compound **21** (Recorded in $CDCl_3$)

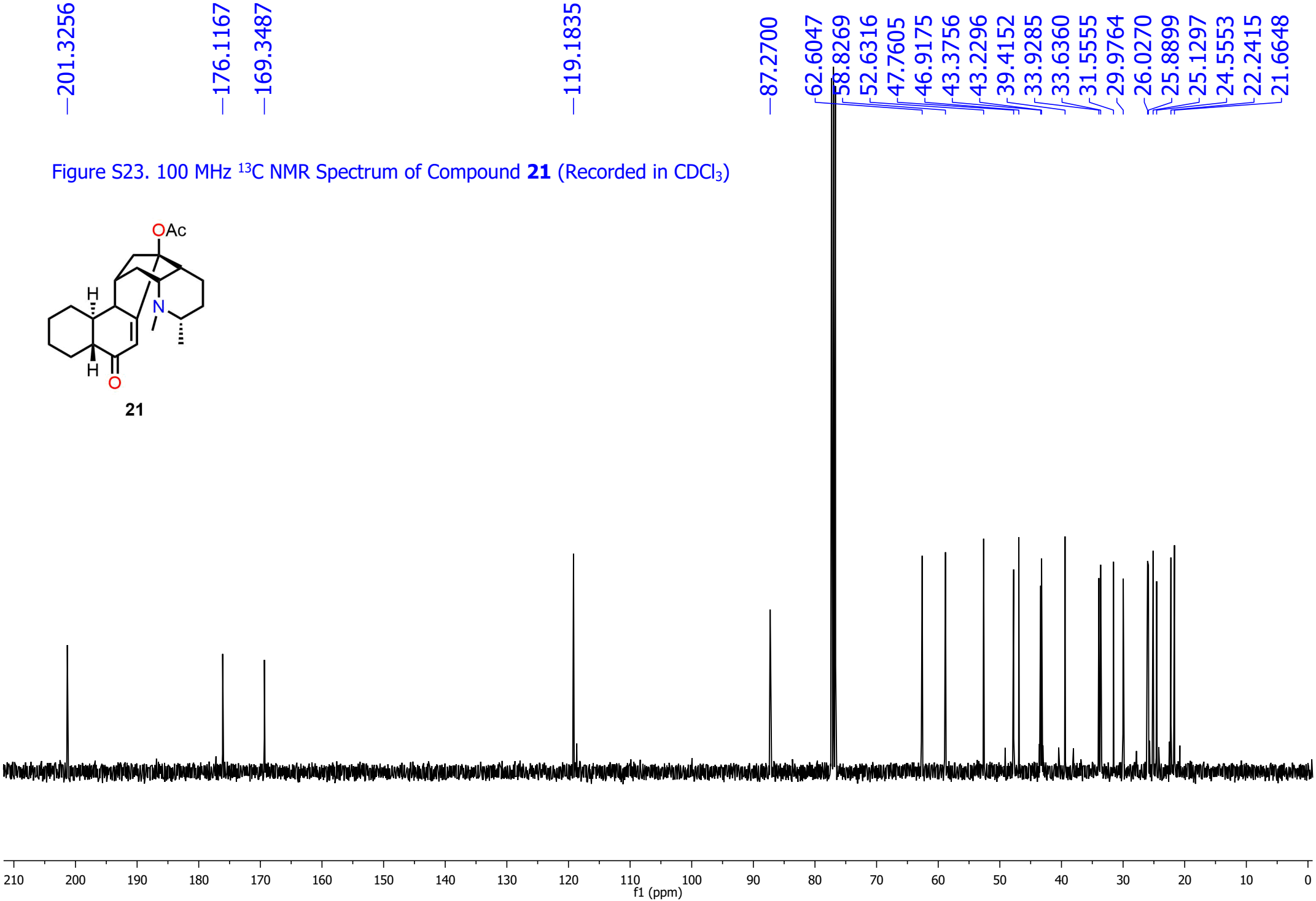

Figure S24. 400 MHz ^{1}H NMR Spectrum of Compound **22** (Recorded in $CDCl_3$)

22

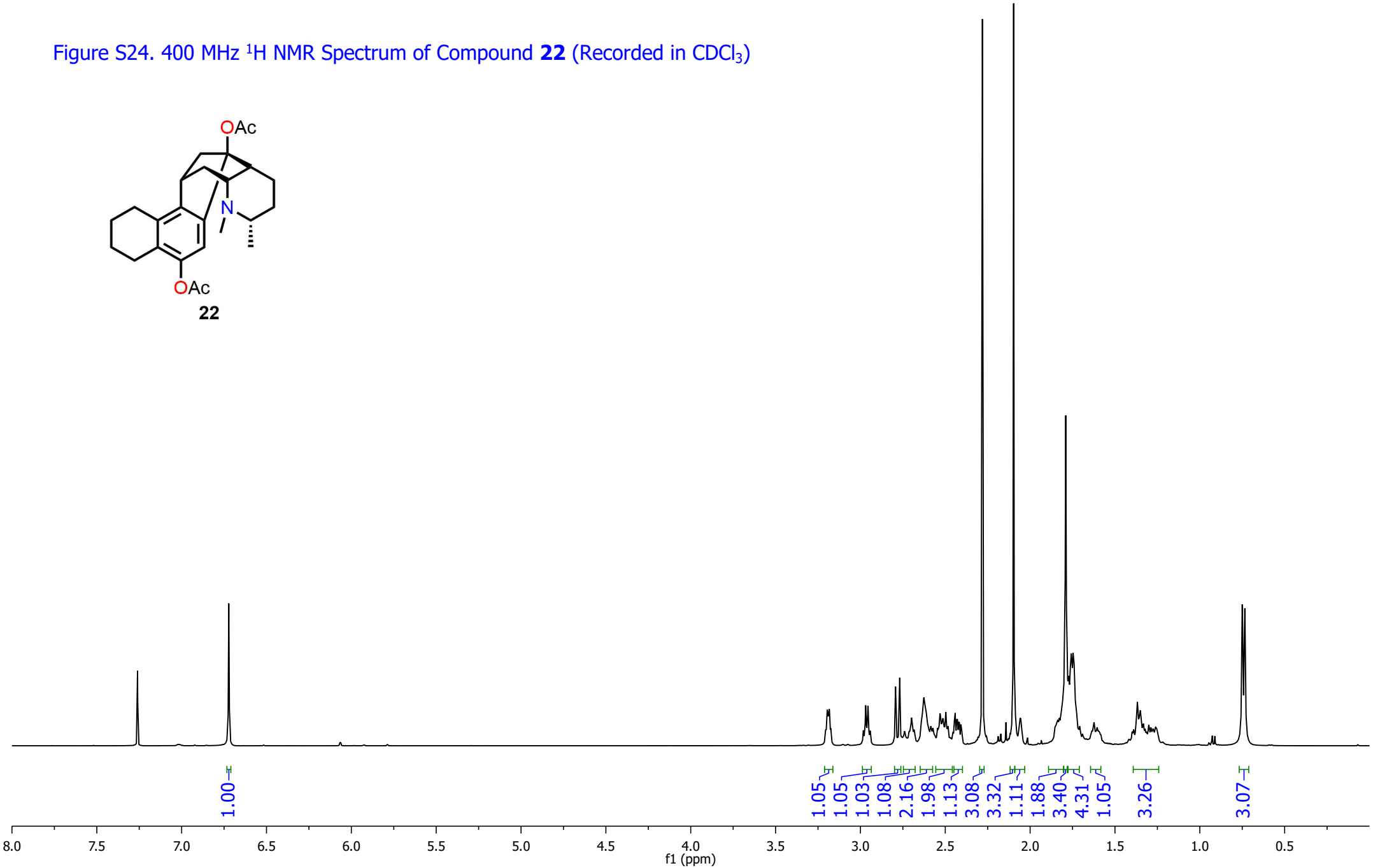

Figure S25. 100 MHz ^{13}C NMR Spectrum of Compound **22** (Recorded in $CDCl_3$)

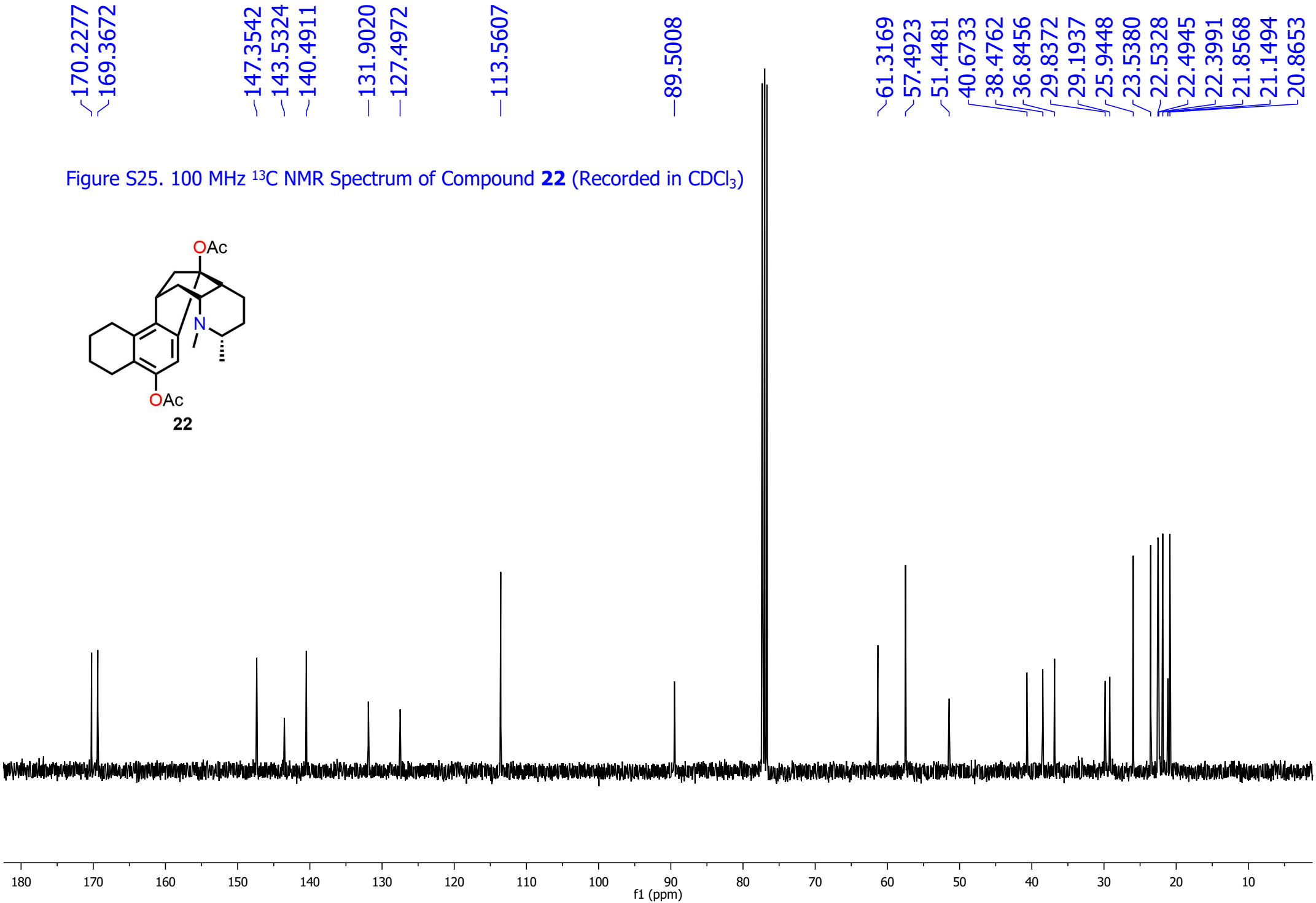

Figure S26. 400 MHz ^{1}H NMR Spectrum of Compound **23** (Recorded in $CDCl_3$)

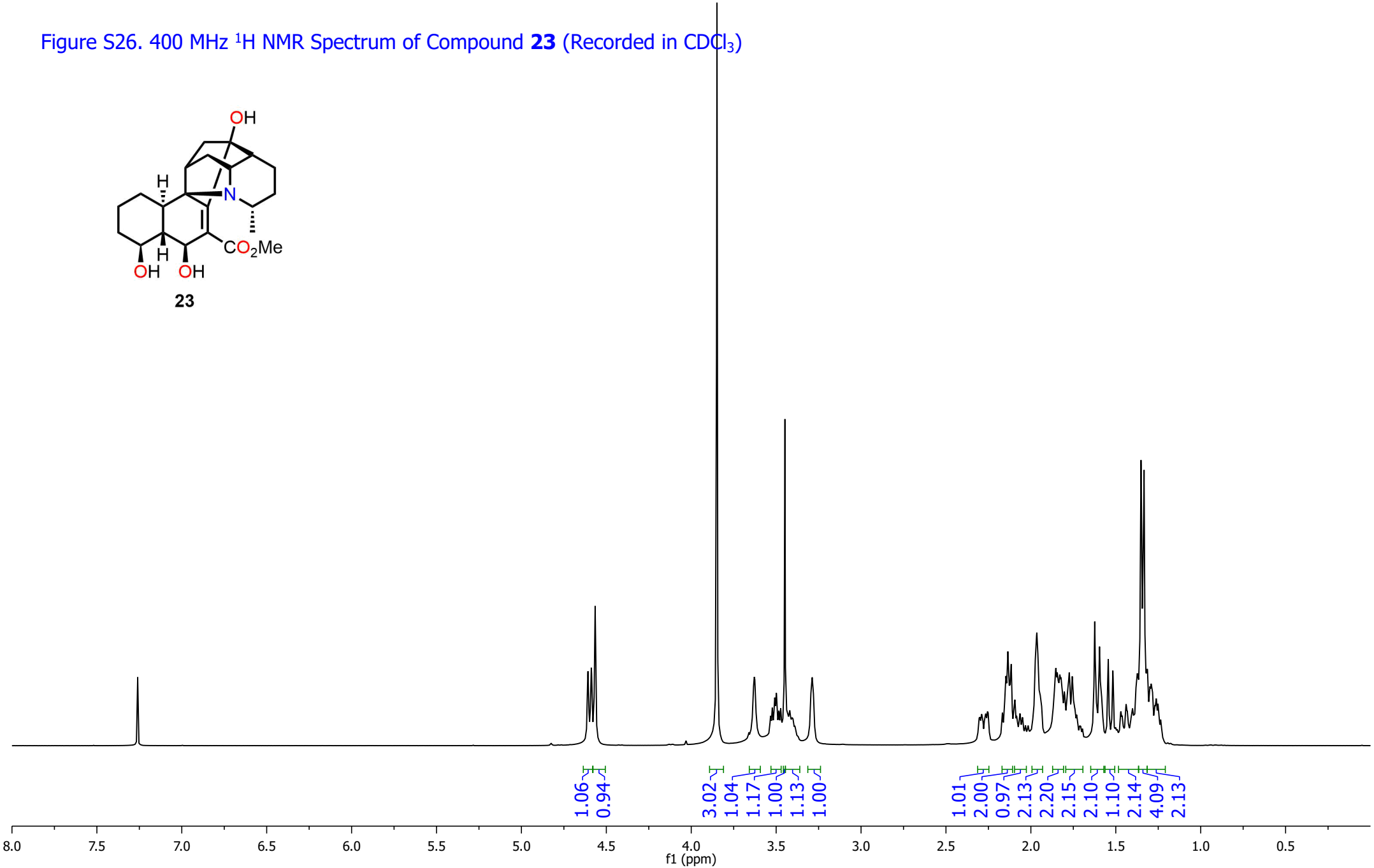

Figure S27. 100 MHz ^{13}C NMR Spectrum of Compound **23** (Recorded in $CDCl_3$)

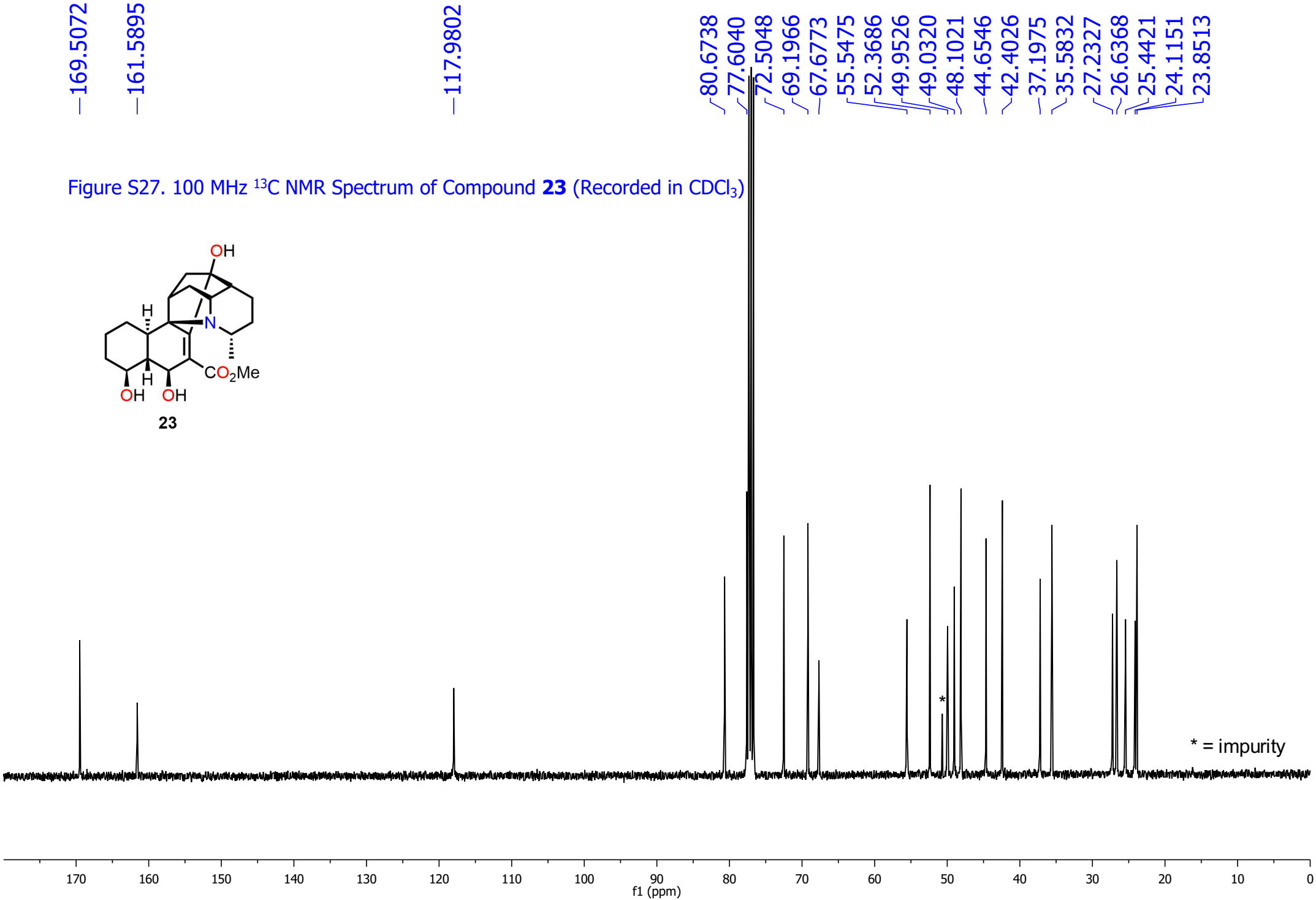

Figure S28. 400 MHz ^{1}H NMR Spectrum of Compound **24** (Recorded in $CDCl_3$)

24

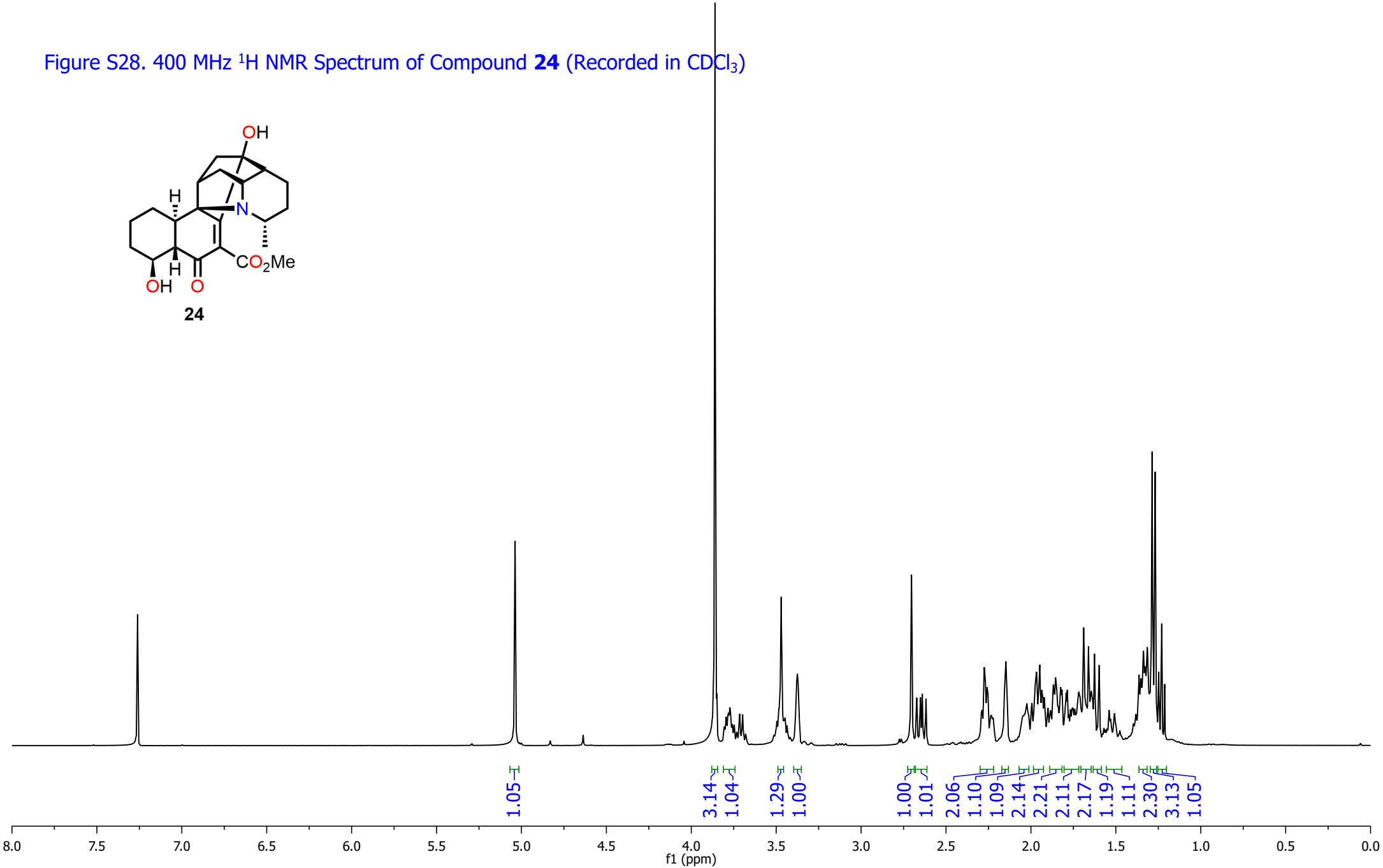

Figure S29. 100 MHz ^{13}C NMR Spectrum of Compound **24** (Recorded in $CDCl_3$)

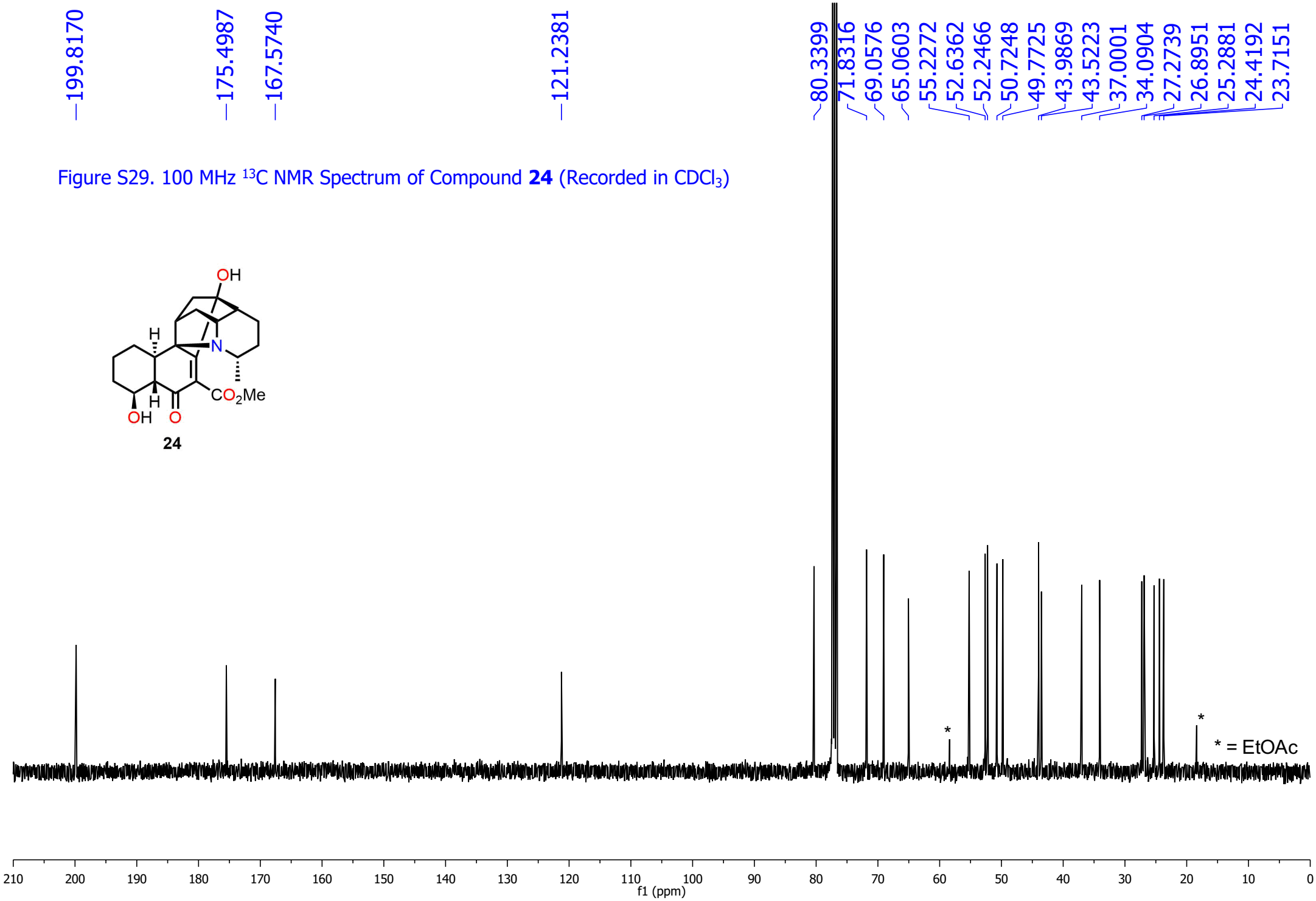

Figure S30. 400 MHz ^{1}H NMR Spectrum of Compound **25** (Recorded in $CDCl_3$)

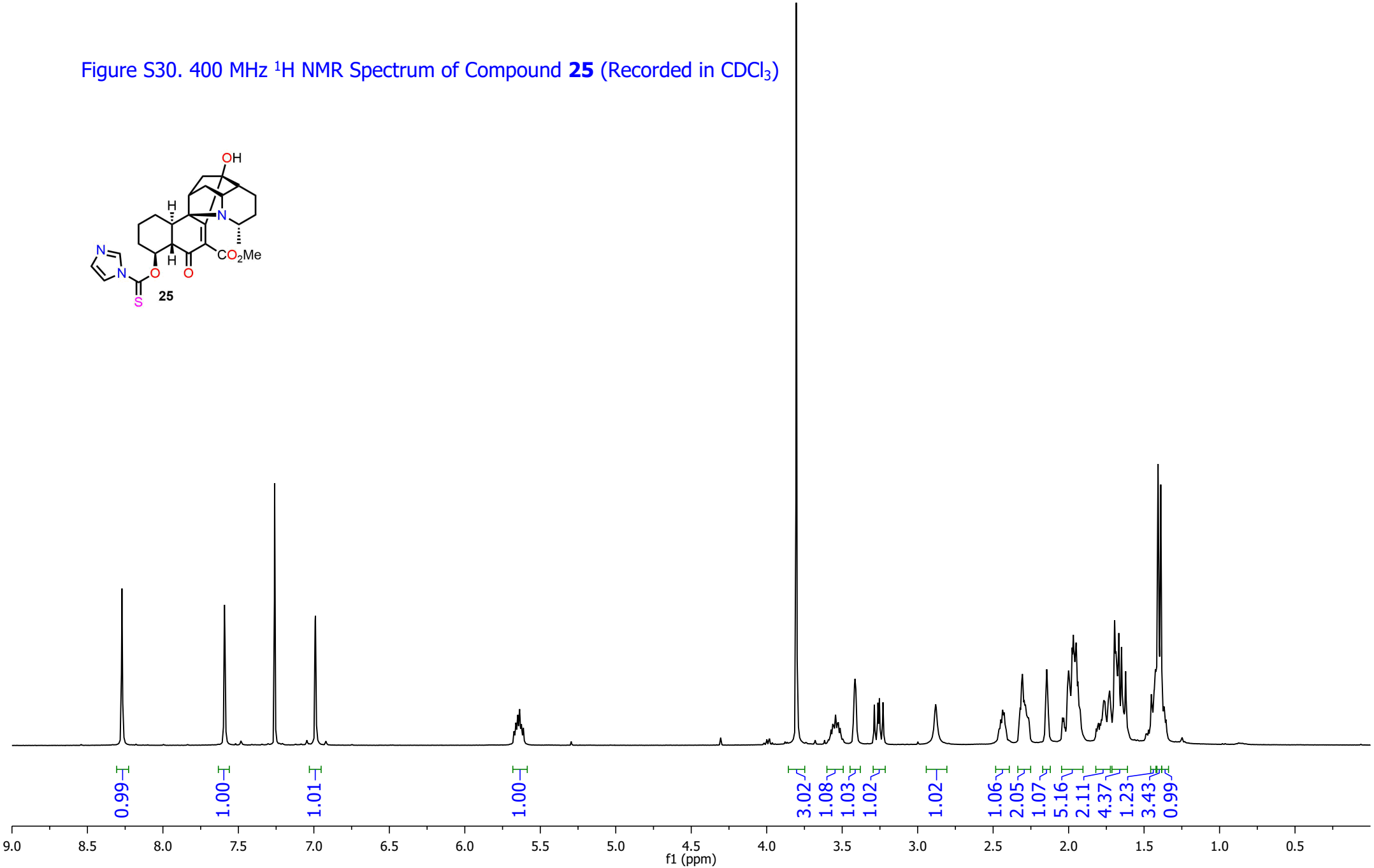
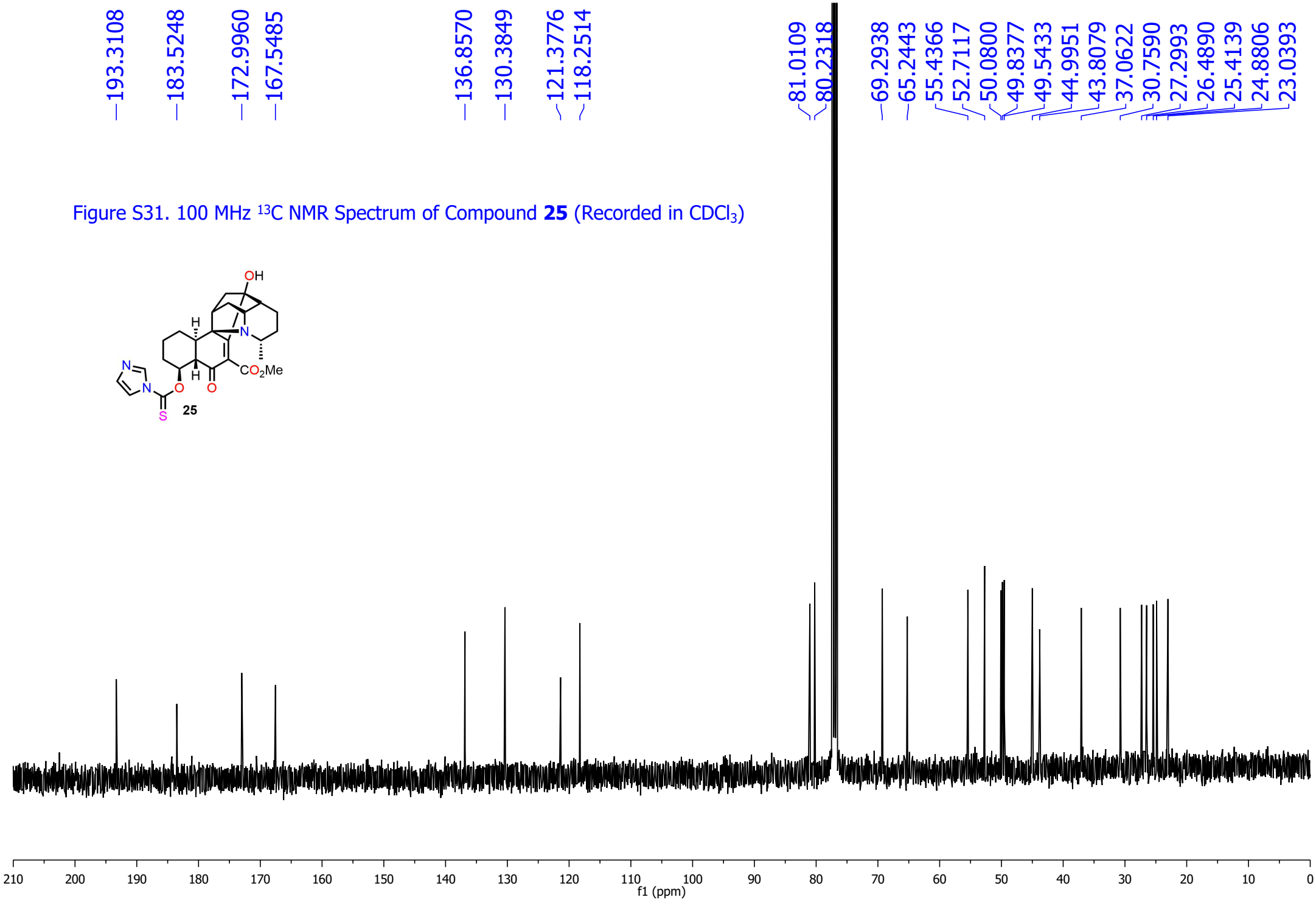
Figure S31. 100 MHz ^{13}C NMR Spectrum of Compound **25** (Recorded in $CDCl_3$)