

SUPPORTING INFORMATION

Synthesis and structure of *nido*-carboranyl azide and its “click” reactions

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¹H, ¹¹B and ¹³C NMR, IR and high-resolution mass spectra of compounds **2,3,5,10-12**

Display Report

Analysis Info

Analysis Name D:\Data\Chizhov\INEOS\Laskova\da-030_&clblow.d
Method tune_low_1550.m
Sample Name /CHIZ DA-030
Comment CH3CN 100 %, dil. 20, calibrant added

Acquisition Date 29.09.2020 13:58:17

Operator BDAL@DE
Instrument maXis 43

Acquisition Parameter

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Focus	Not active	Set Capillary	4500 V	Set Dry Heater	180 °C
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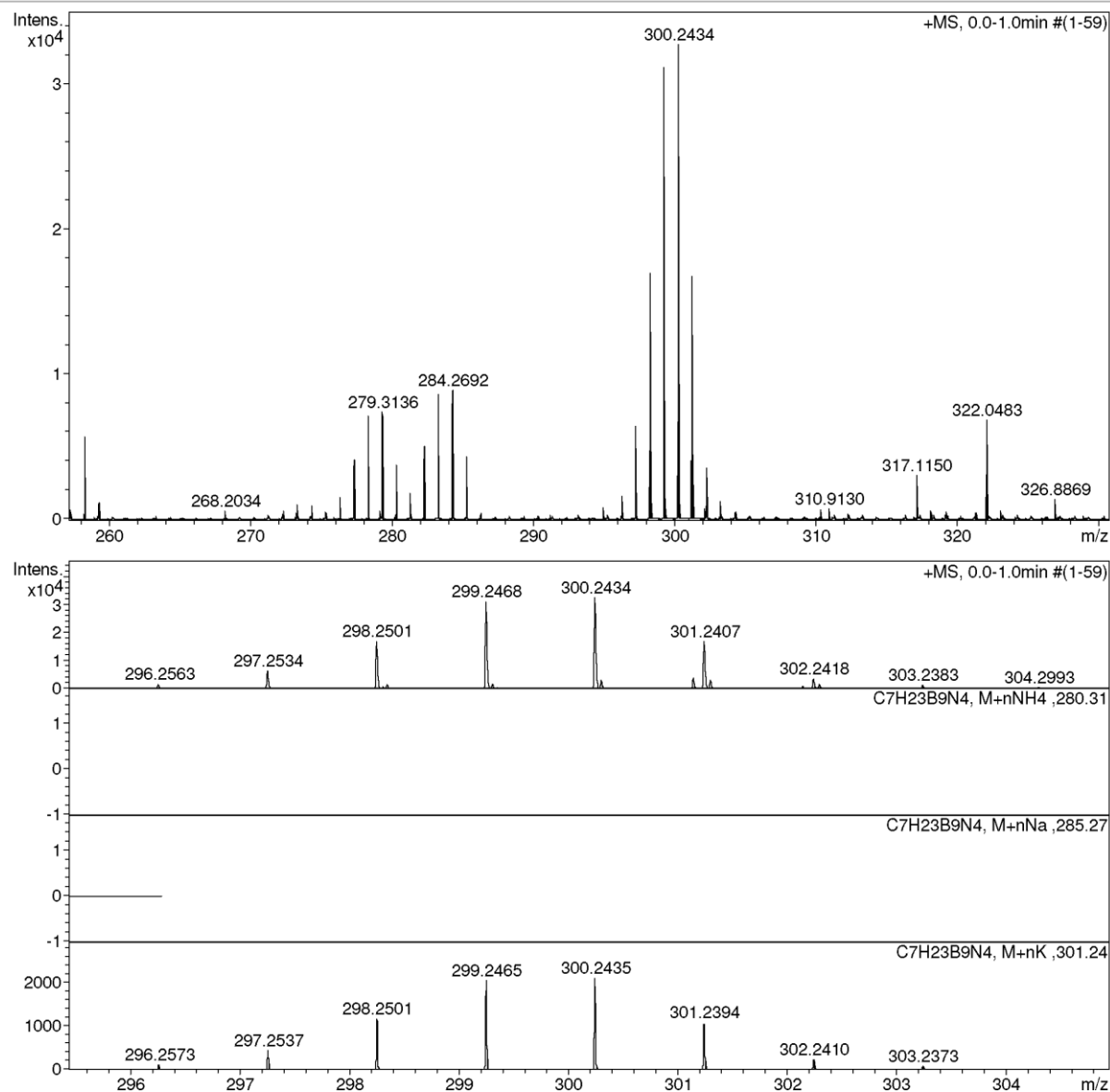


Figure S1. ESI-HRMS spectrum of compound 2

Display Report

Analysis Info

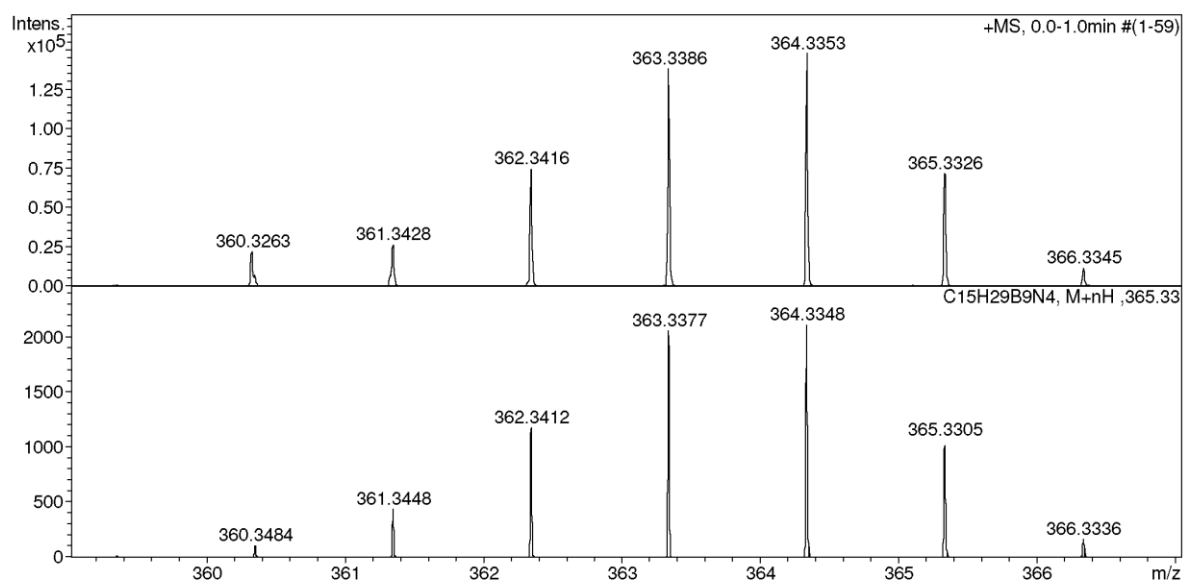
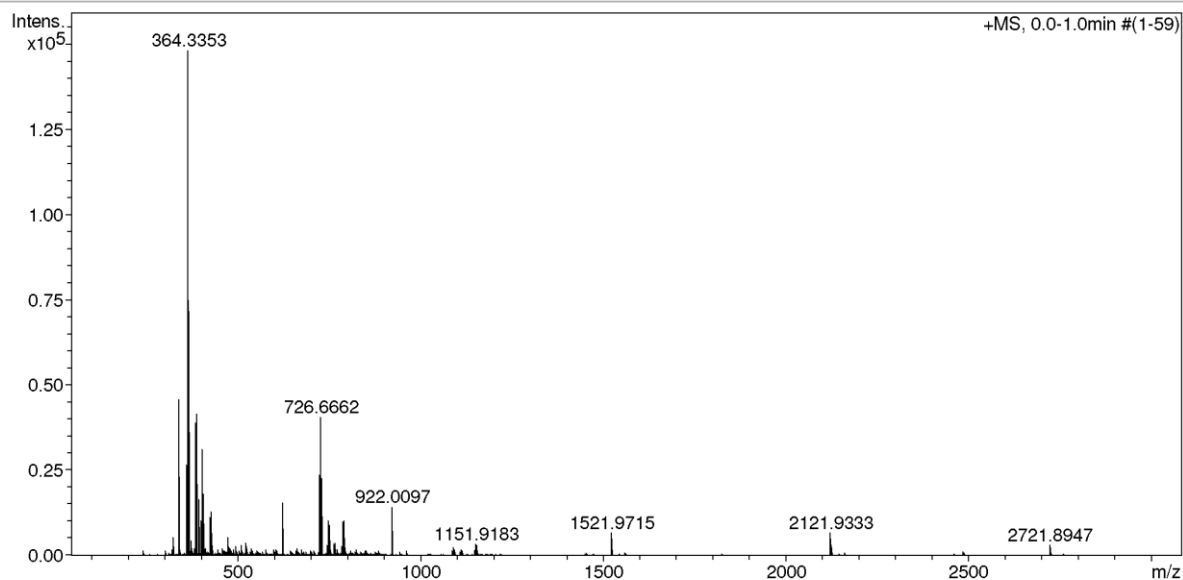
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Method tune_wide.m
Sample Name /CHIZ DA-035
Comment CH3CN !00 %, dil. 200, calibrant added

Acquisition Date 29.09.2020 14:26:58

Operator BDAL@DE
Instrument maXis 43

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.5 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 °C
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Scan End	3000 m/z	Set Collision Cell RF	1200.0 Vpp	Set Divert Valve	Waste



C₁₅H₂₉B₉N₄, M+nH, 365.33

Figure S2. ESI-HRMS spectrum of compound 3

Display Report

Analysis Info

Analysis Name D:\Data\Chizhov\INEOS\Laskova\da-037_&clb.d
Method tune_wide.m
Sample Name /CHIZ DA-037
Comment CH3CN 100 %, dil. 200, calibrant added

Acquisition Date 29.09.2020 14:35:42

Operator BDAL@DE
Instrument maXis 43

Acquisition Parameter

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Scan End	3000 m/z	Set Collision Cell RF	1200.0 Vpp	Set Divert Valve	Waste

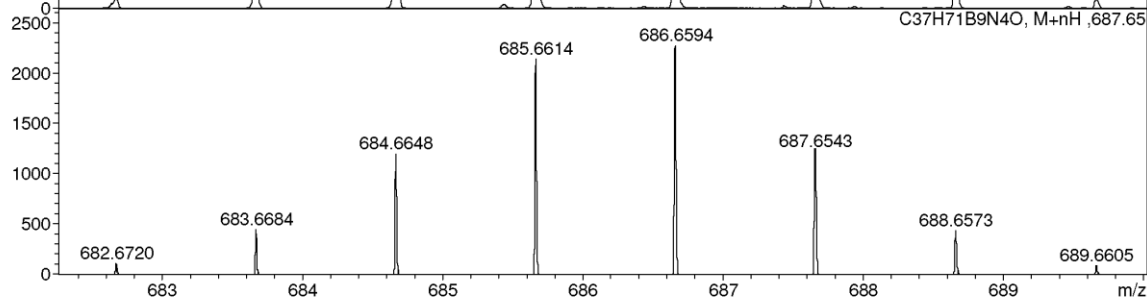
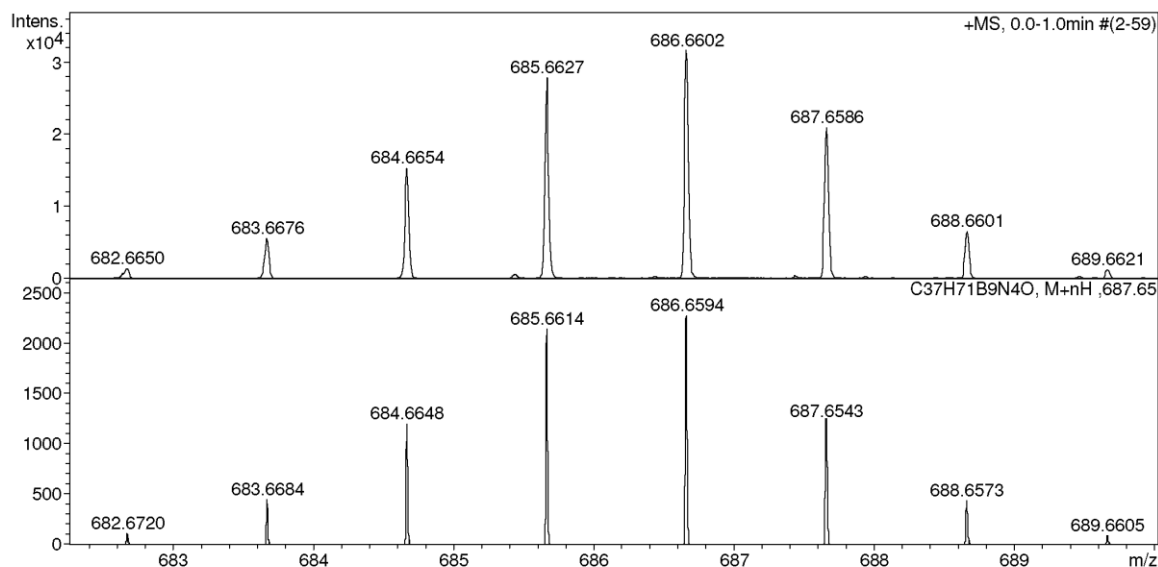
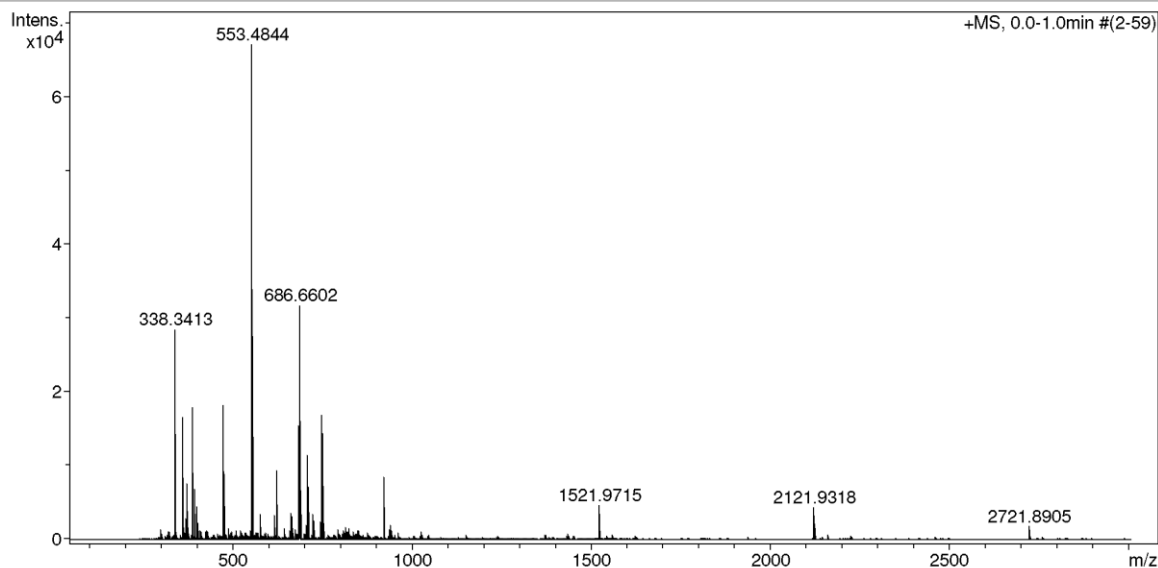


Figure S3. ESI-HRMS spectrum of compound 5

Display Report

Analysis Info

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Method tune_wide.m
Sample Name /CHIZ DA-032
Comment CH3CN 100 %, dil. 20, calibrant added

Acquisition Date 29.09.2020 14:11:16

Operator BDAL@DE
Instrument maXis 43

Acquisition Parameter

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Scan End	3000 m/z	Set Collision Cell RF	1200.0 Vpp	Set Divert Valve	Waste

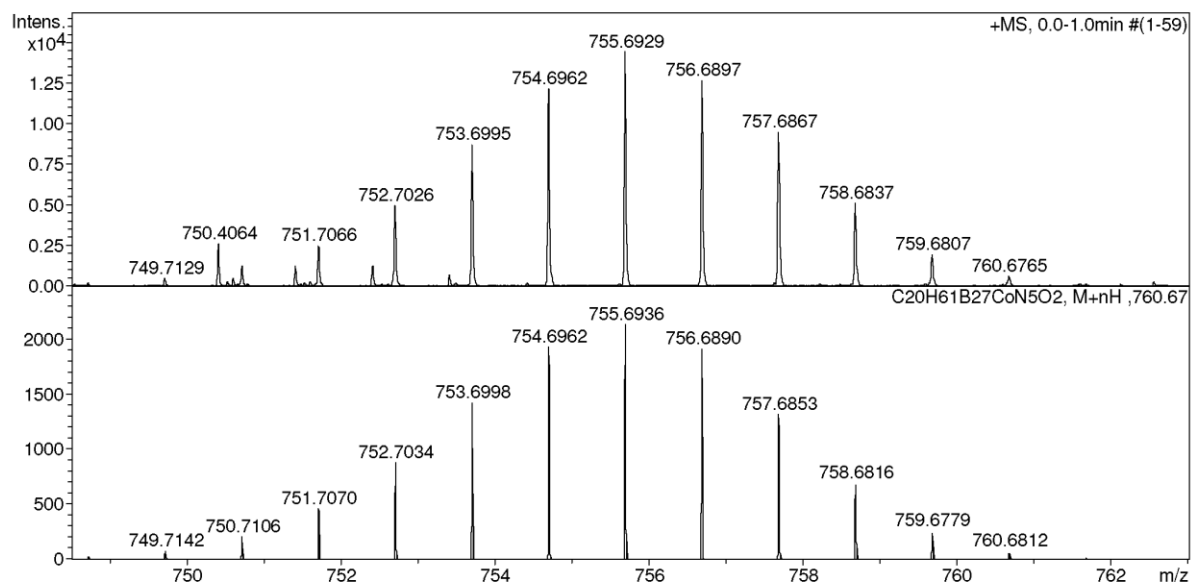
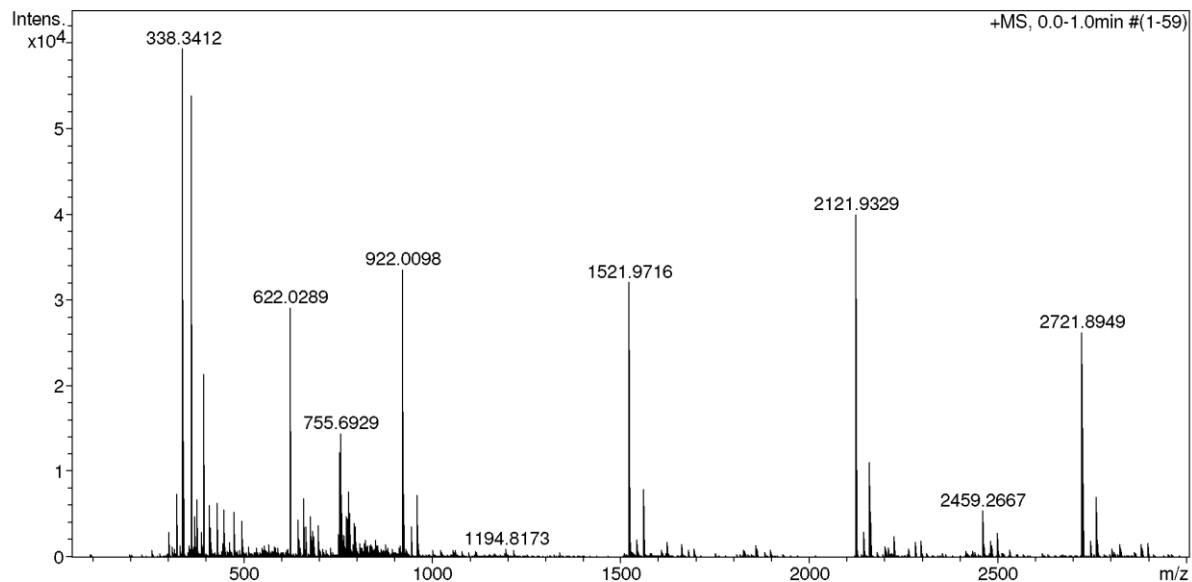


Figure S4. ESI-HRMS spectrum of compound 10

Display Report

Analysis Info

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Method tune_wide.m
Sample Name /CHIZ DA-033
Comment CH3CN !00 %, dil. 20, calibrant added

Acquisition Date 29.09.2020 14:15:00

Operator BDAL@DE
Instrument maXis 43

Acquisition Parameter

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Scan End	3000 m/z	Set Collision Cell RF	1200.0 Vpp	Set Divert Valve	Waste

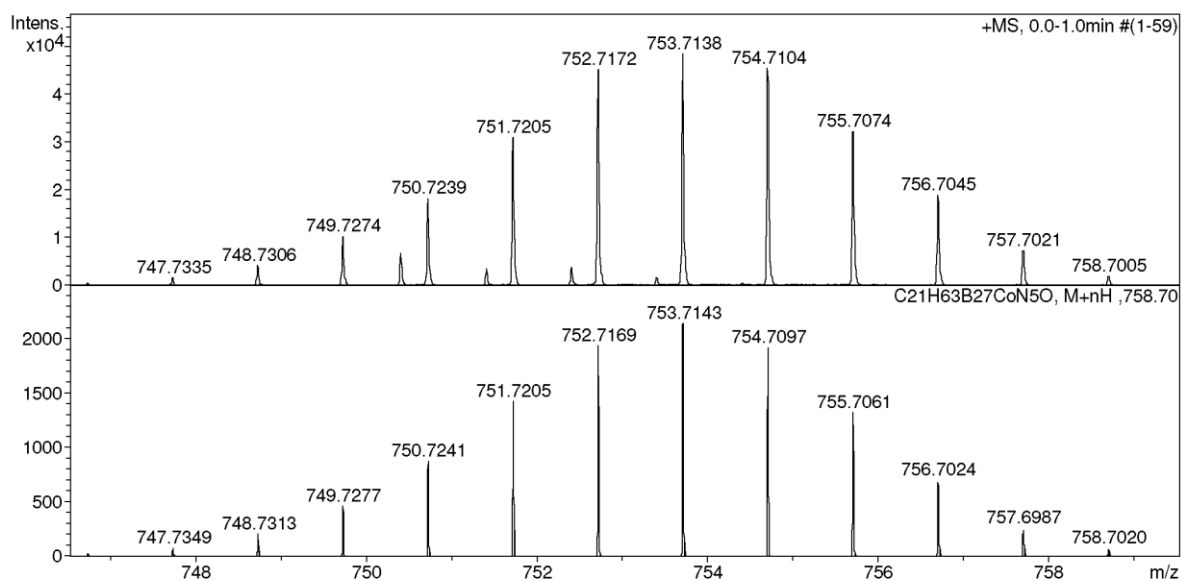
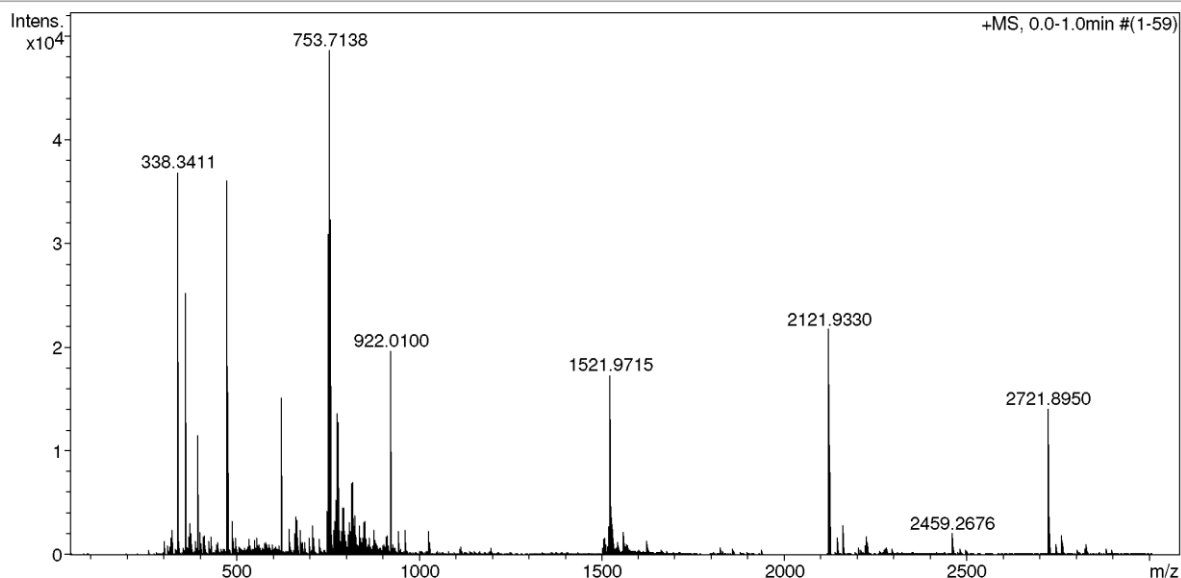


Figure S5. ESI-HRMS spectrum of compound 11

Display Report

Analysis Info

Analysis Name D:\Data\Chizhov\INEOS\Laskova\da-034_&clb.d
Method tune_wide.m
Sample Name /CHIZ DA-034
Comment CH3CN 100 %, dil. 20, calibrant added

Acquisition Date 29.09.2020 14:22:18

Operator BDAL@DE
Instrument maXis 43

Acquisition Parameter

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Scan End	3000 m/z	Set Collision Cell RF	1200.0 Vpp	Set Divert Valve	Waste

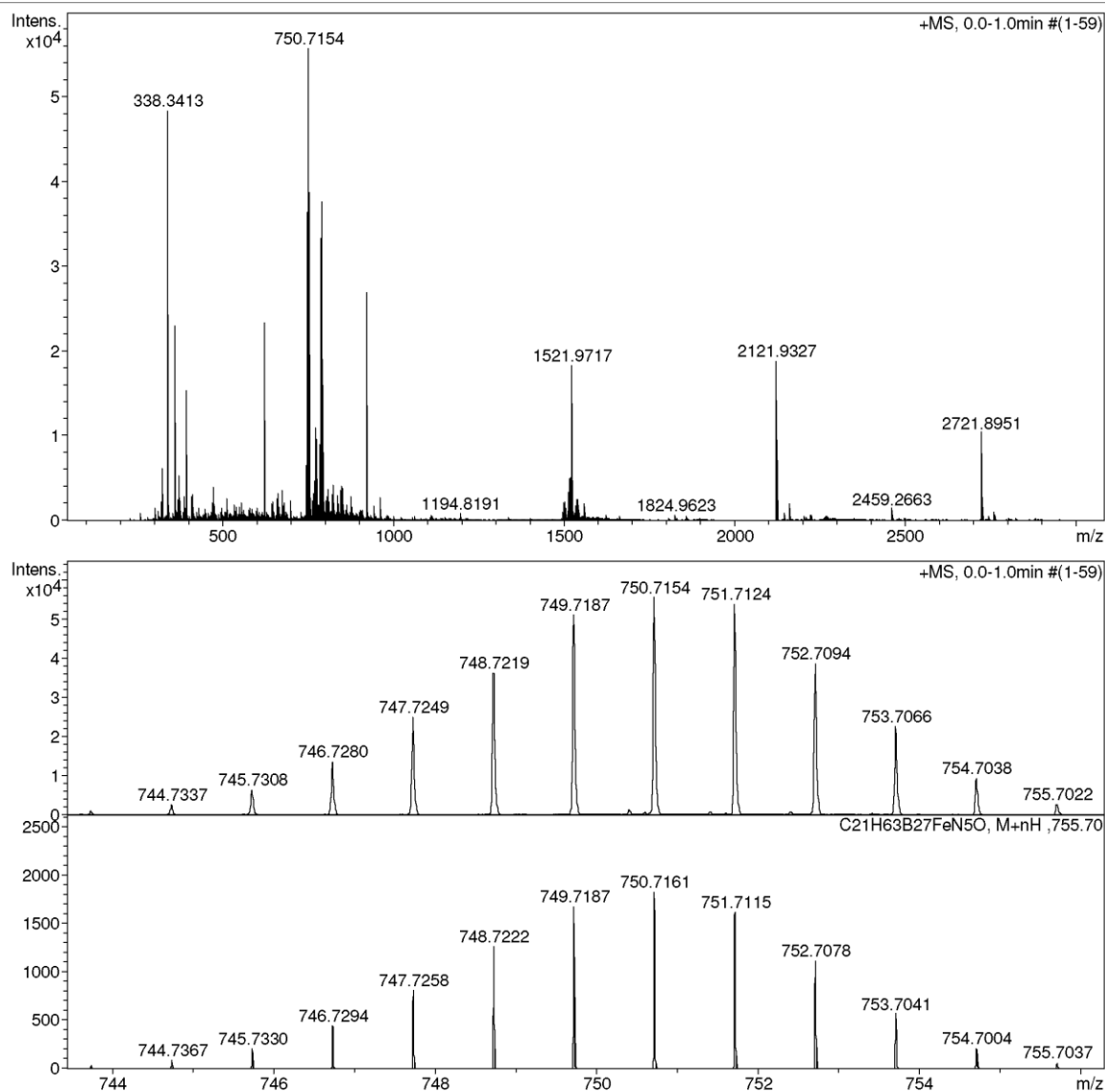


Figure S6. ESI-HRMS spectrum of compound 12

Compound 2

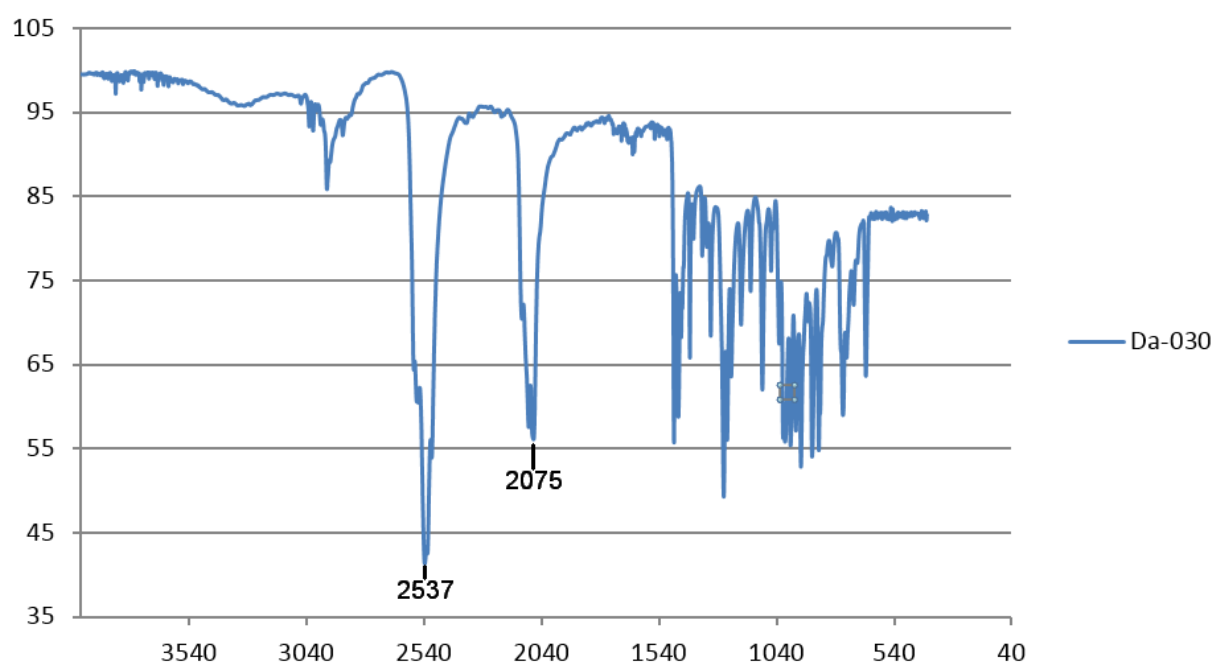


Figure S7. IR spectrum of compound 2

Compound 3

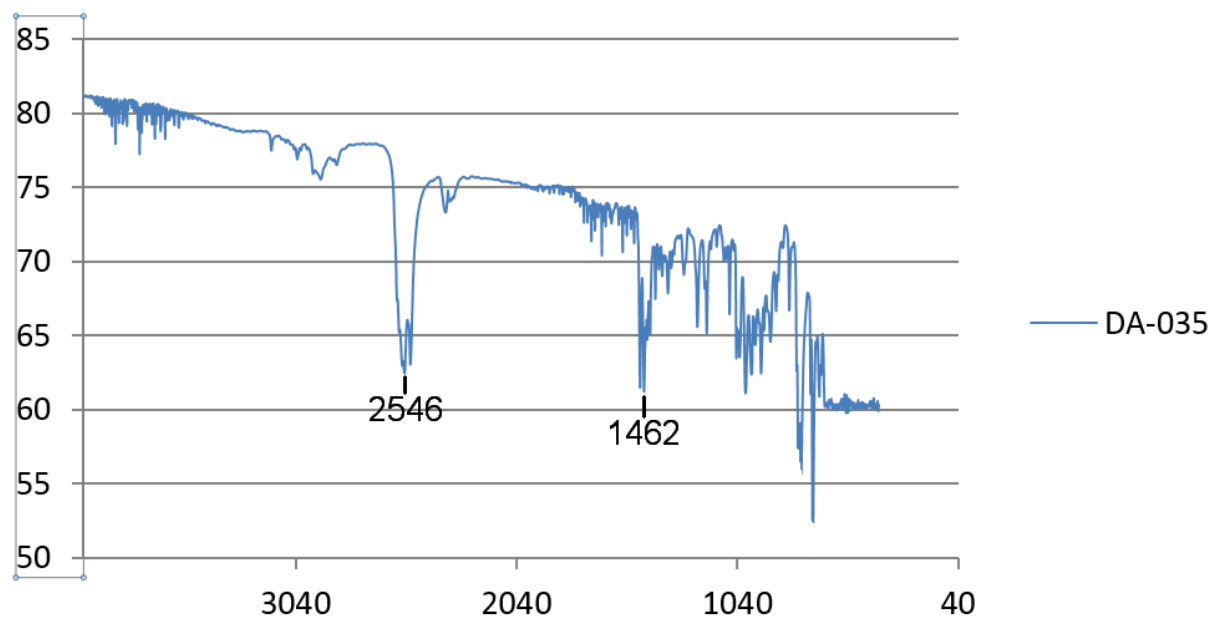


Figure S8. IR spectrum of compound 3

Compound 5

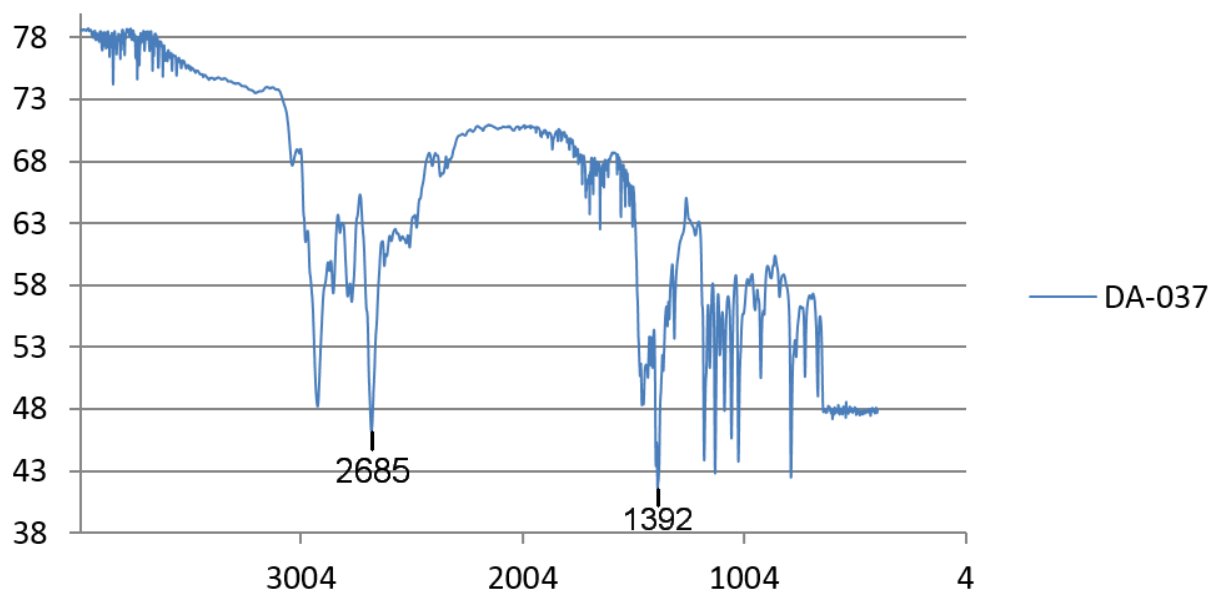


Figure S9. IR spectrum of compound 5

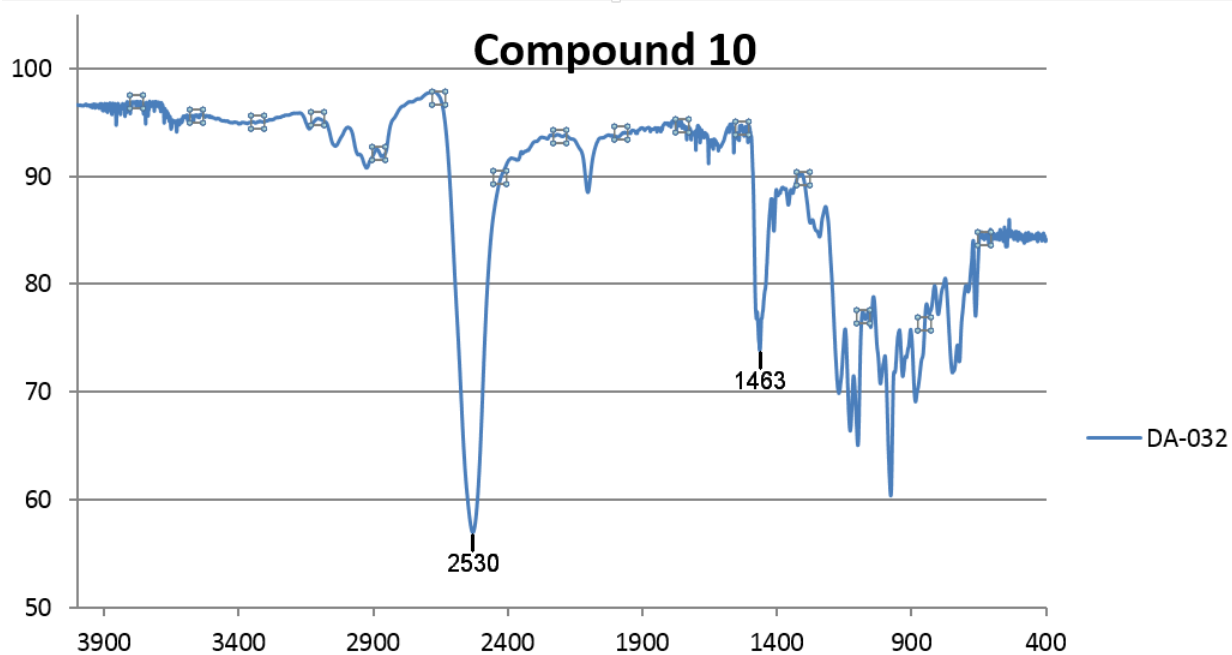


Figure S10. IR spectrum of compound 10

Compound 11

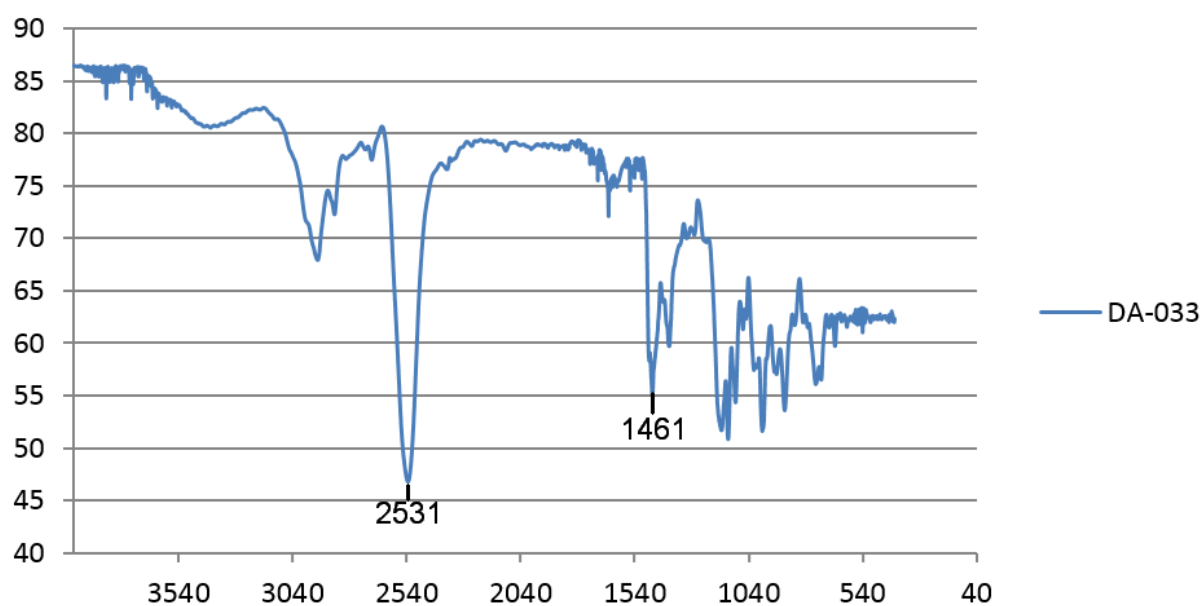


Figure S11. IR spectrum of compound 11

Compound 12

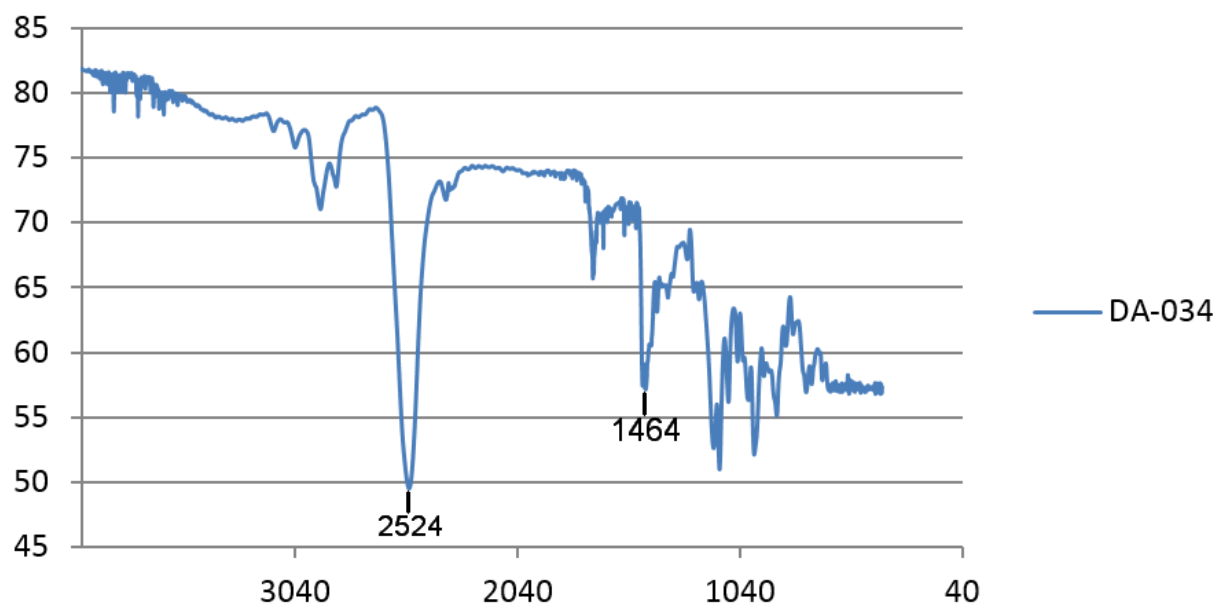


Figure S12. IR spectrum of compound 12

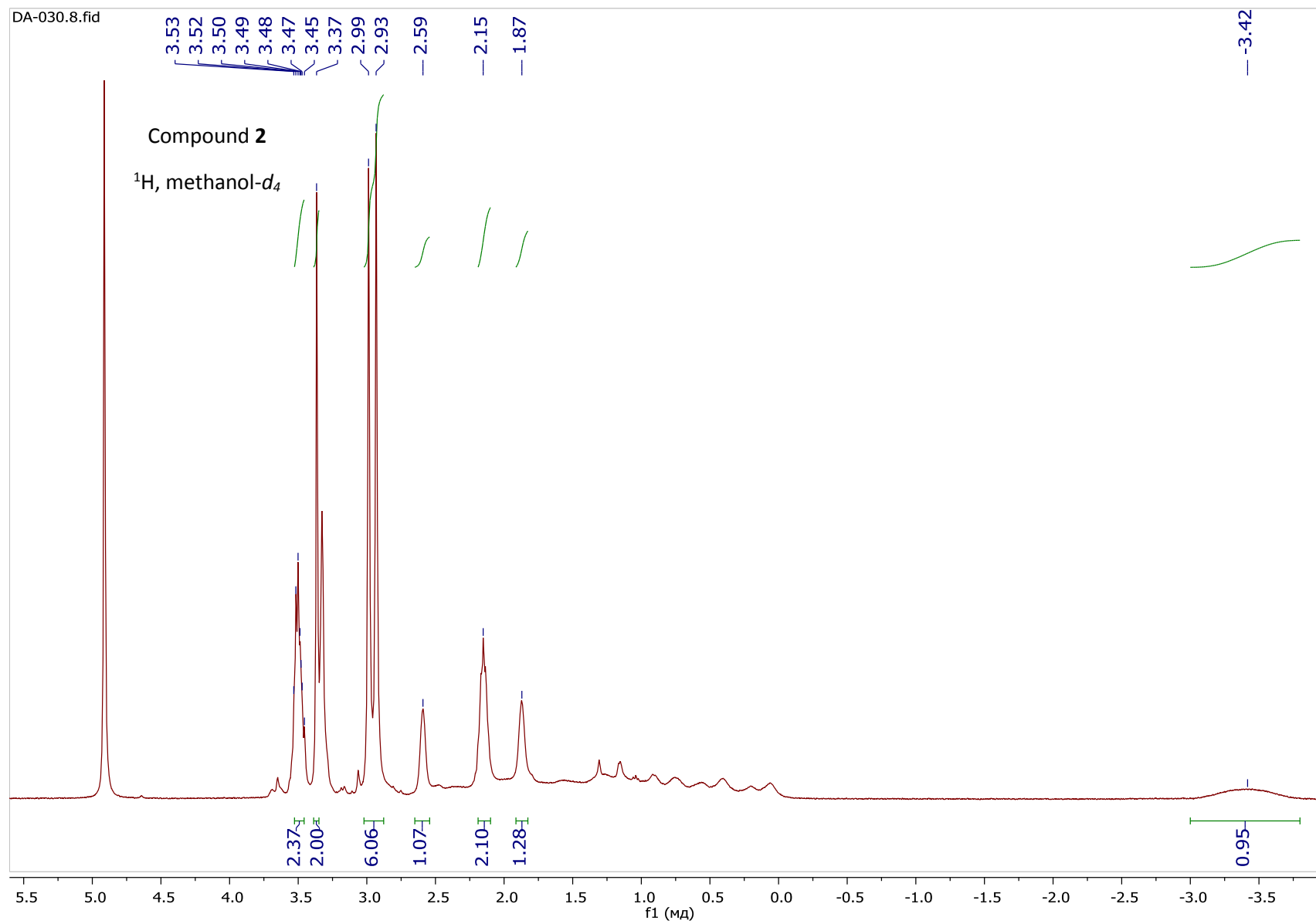


Figure S13. ^1H NMR spectrum of compound **2**

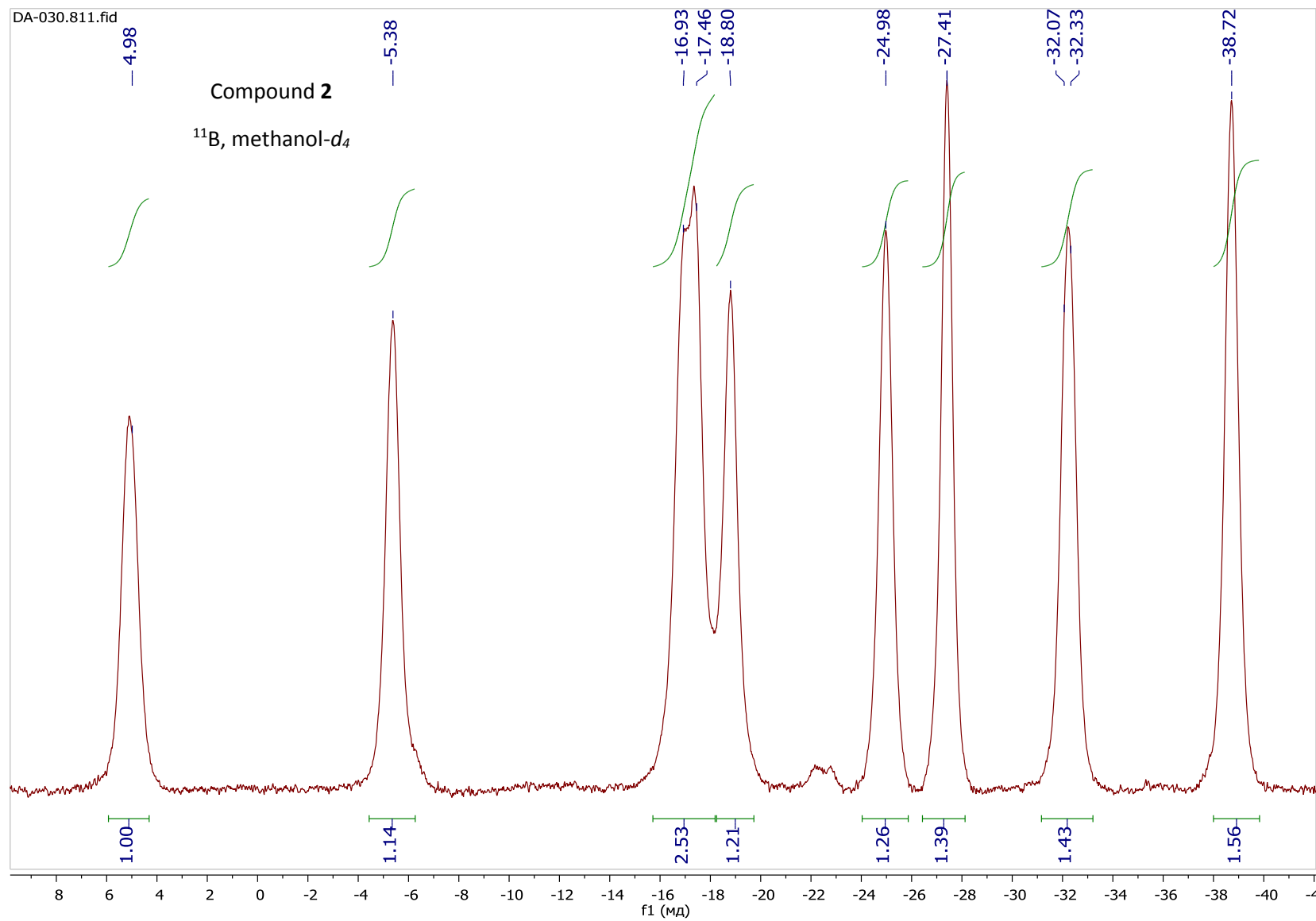


Figure S14. ^{11}B NMR spectrum of compound 2

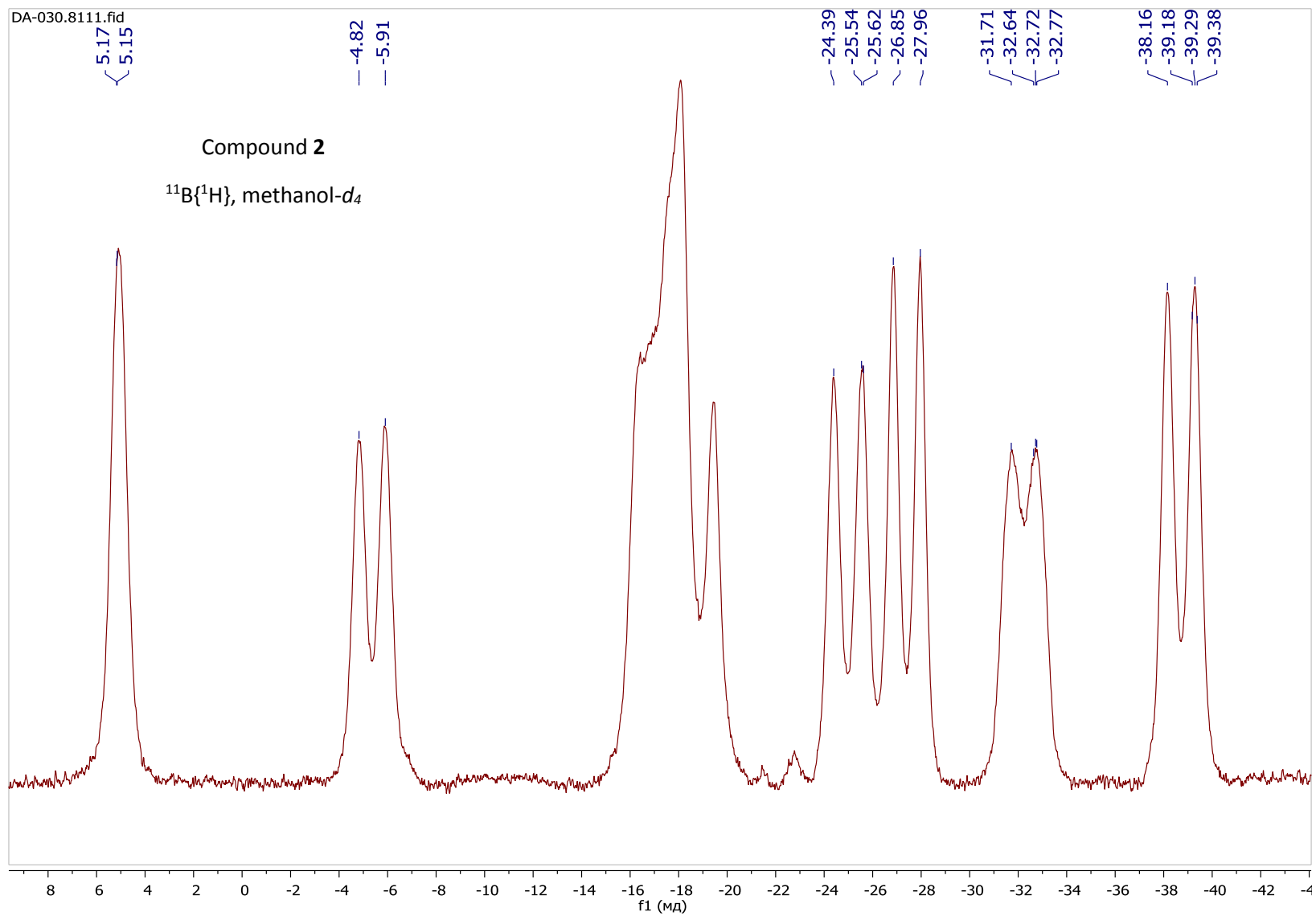


Figure S15. $^{11}\text{B}\{^1\text{H}\}$ NMR spectrum of compound **2**

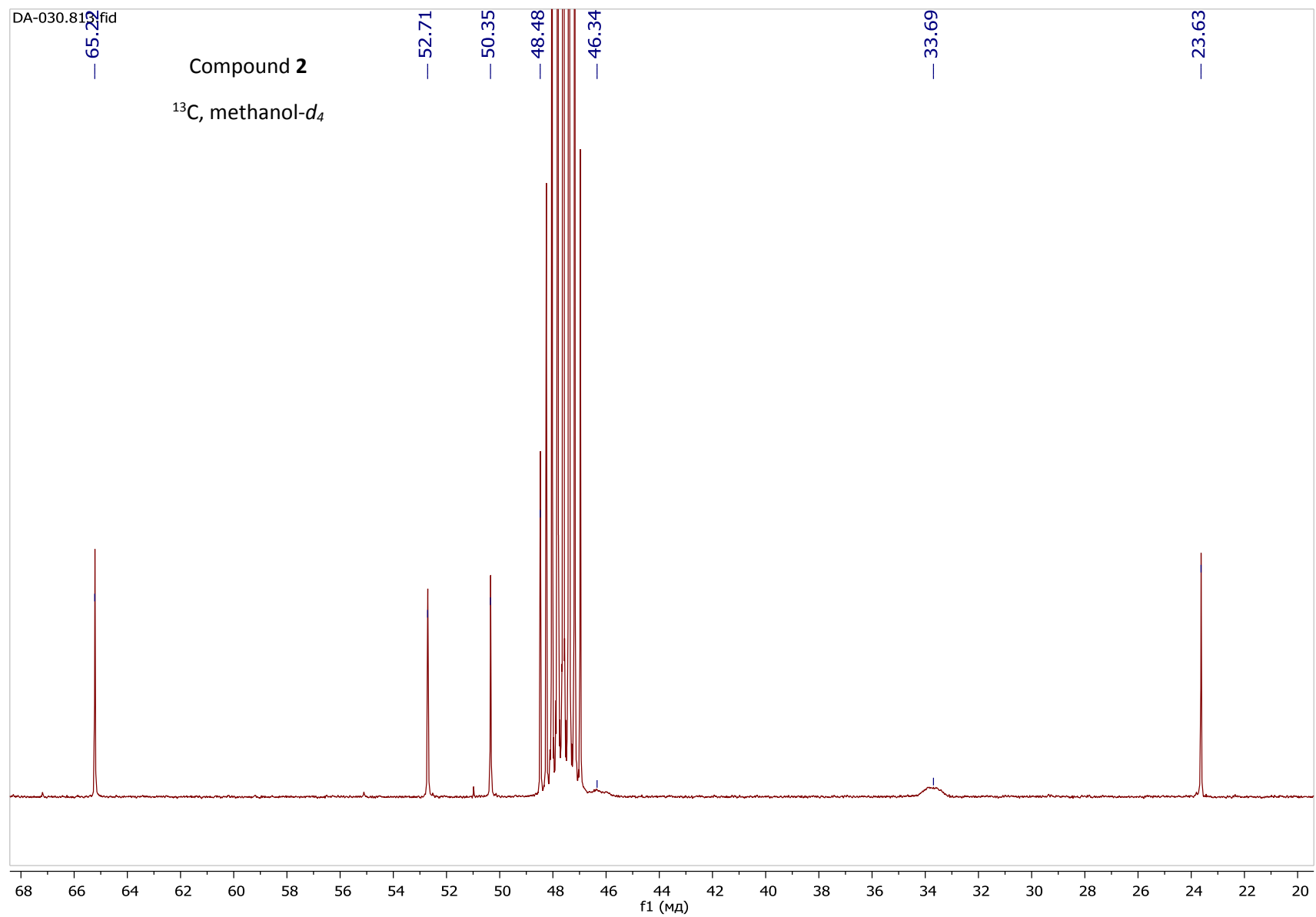


Figure S16. ^{13}C NMR spectrum of compound **2**

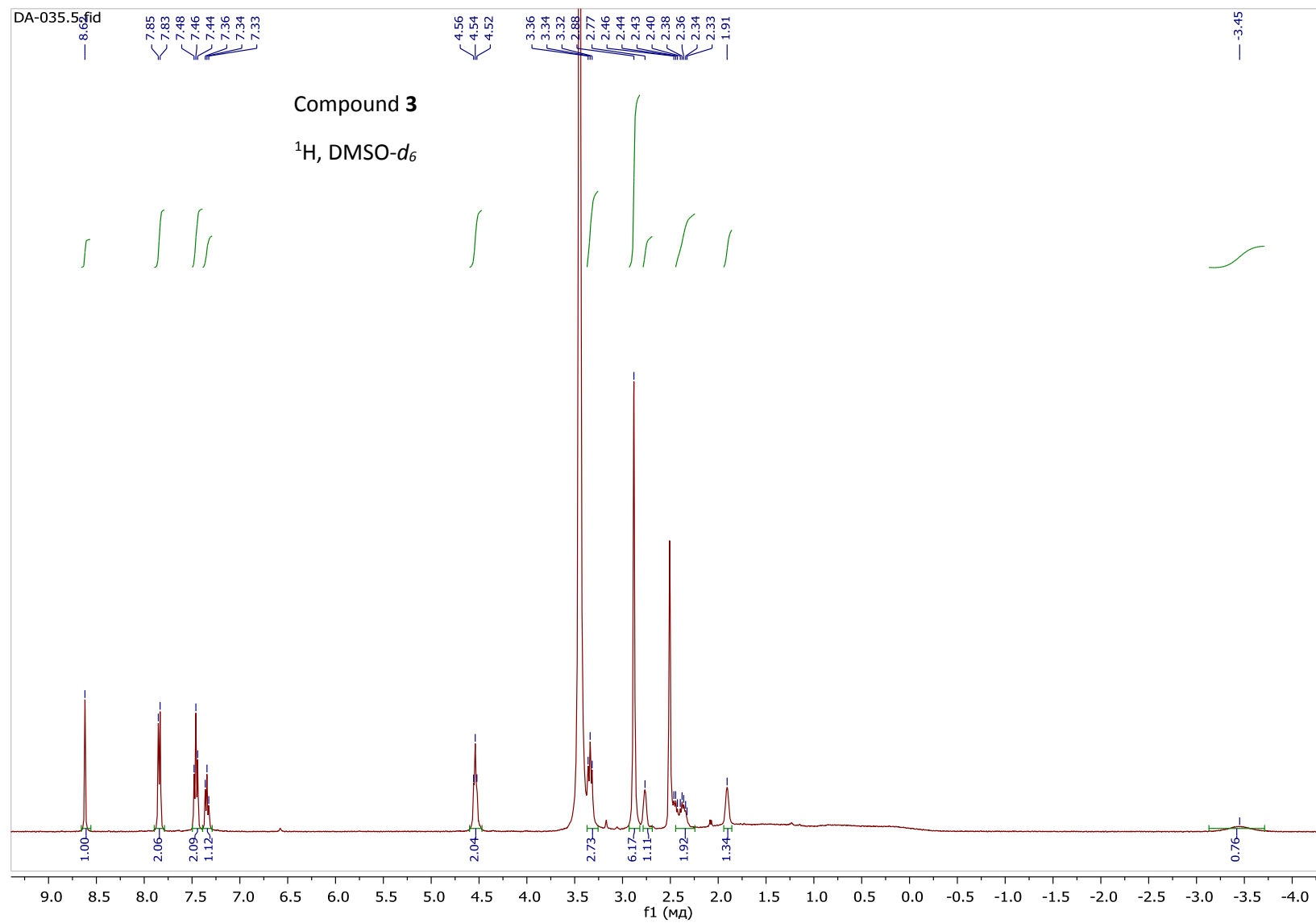


Figure S17. ^1H NMR spectrum of compound **3**

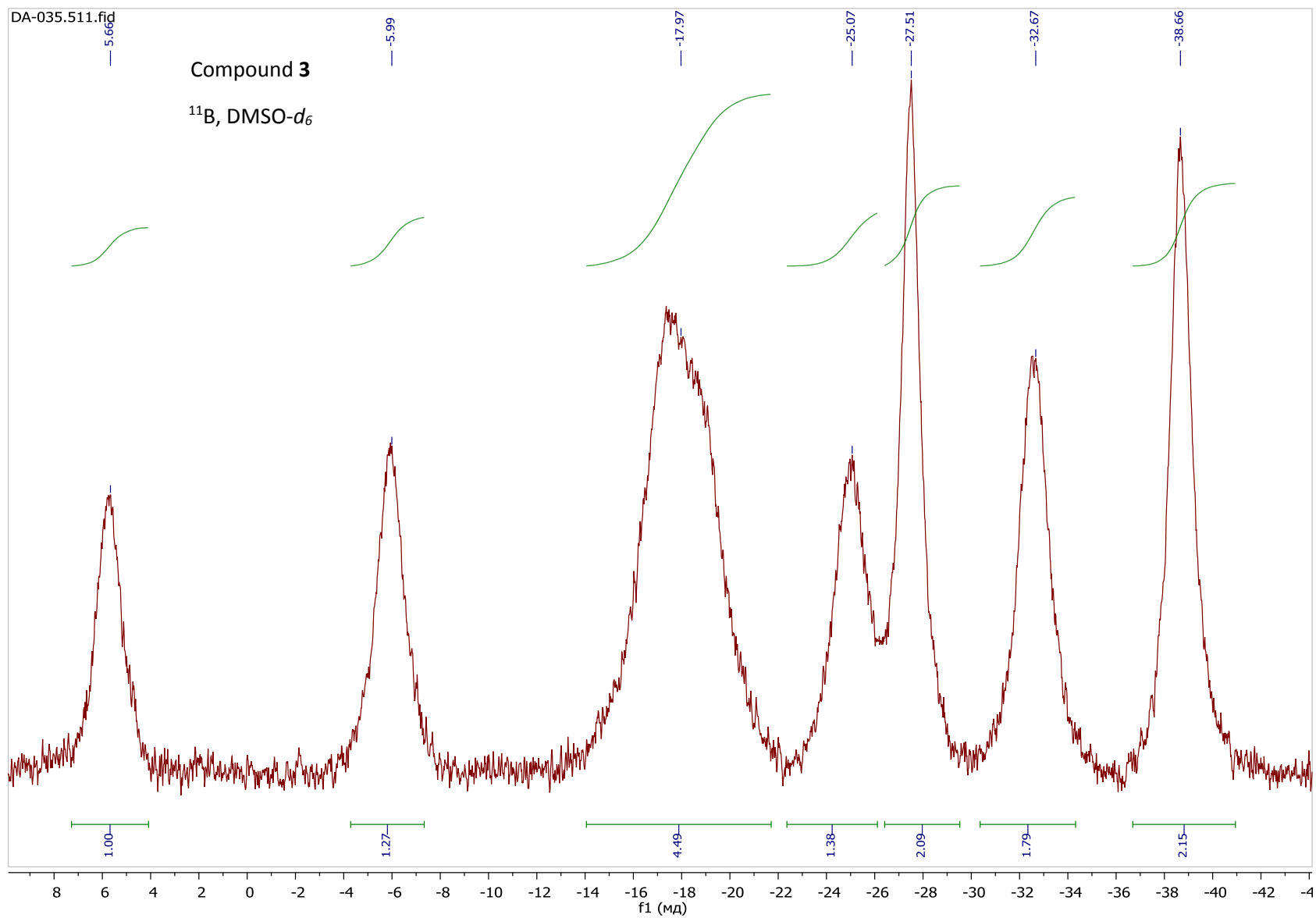


Figure S18. ^{11}B NMR spectrum of compound 3

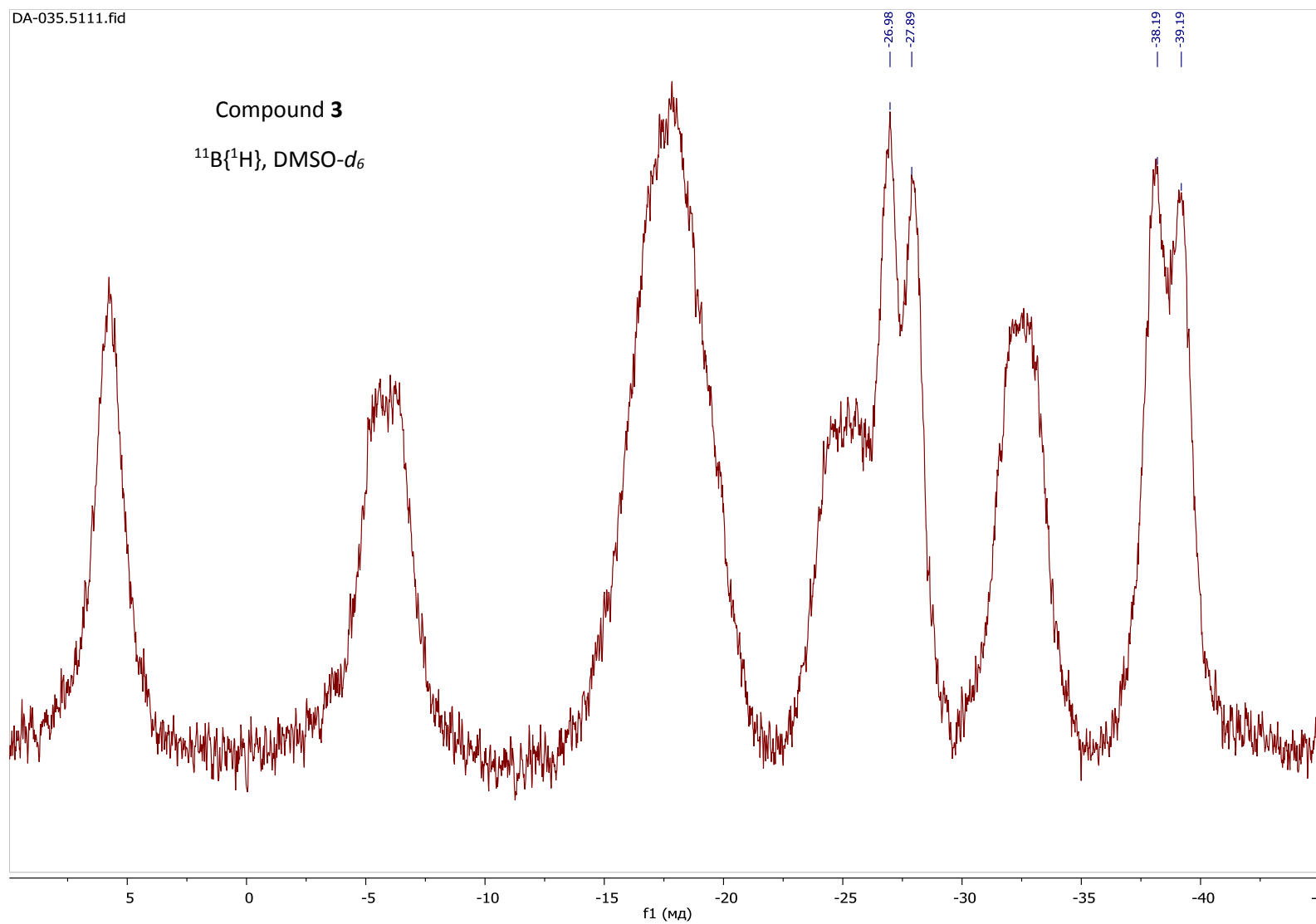


Figure S19. $^{11}\text{B}\{^1\text{H}\}$ NMR spectrum of compound **3**

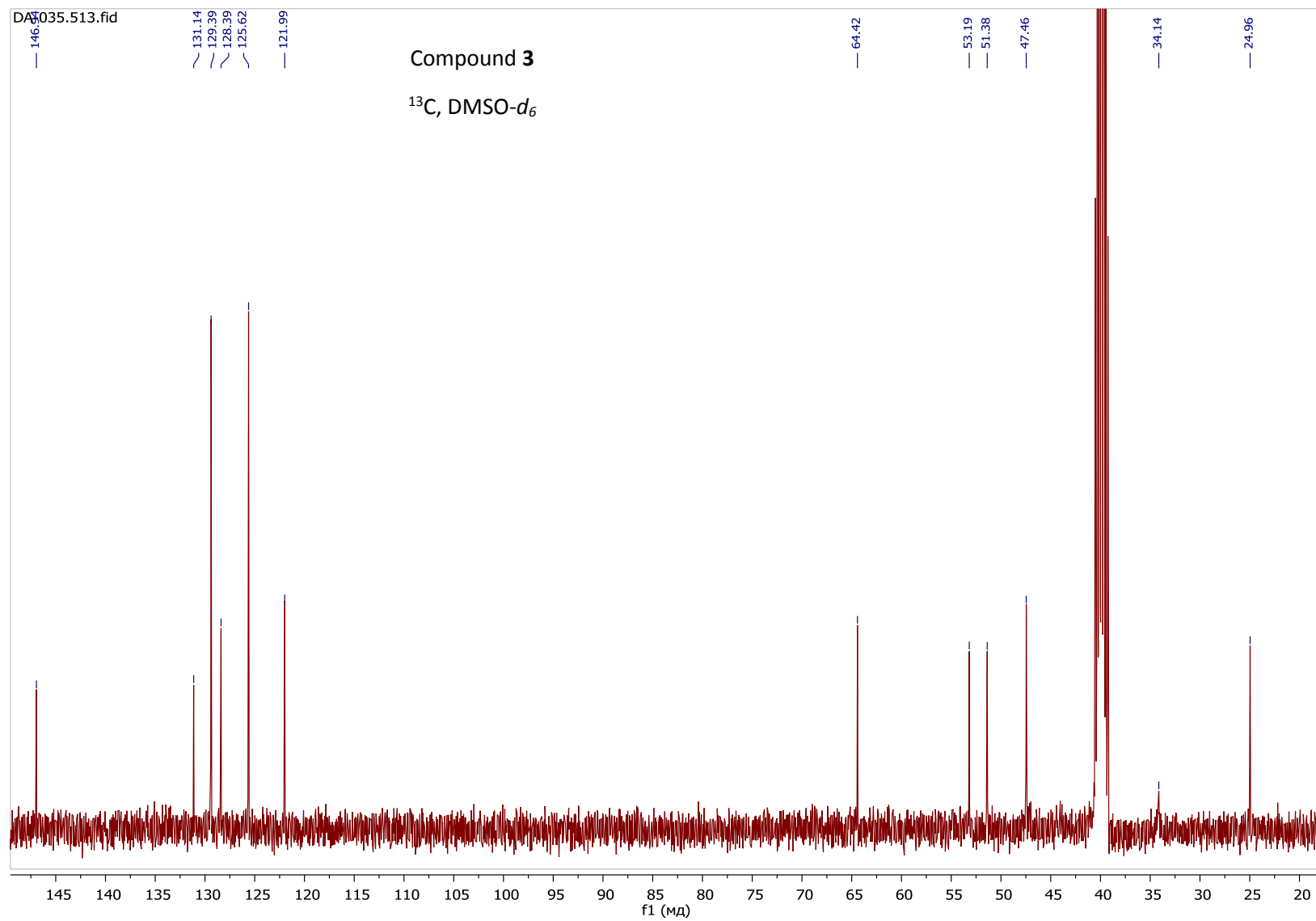


Figure S20. ^{13}C NMR spectrum of compound **3**

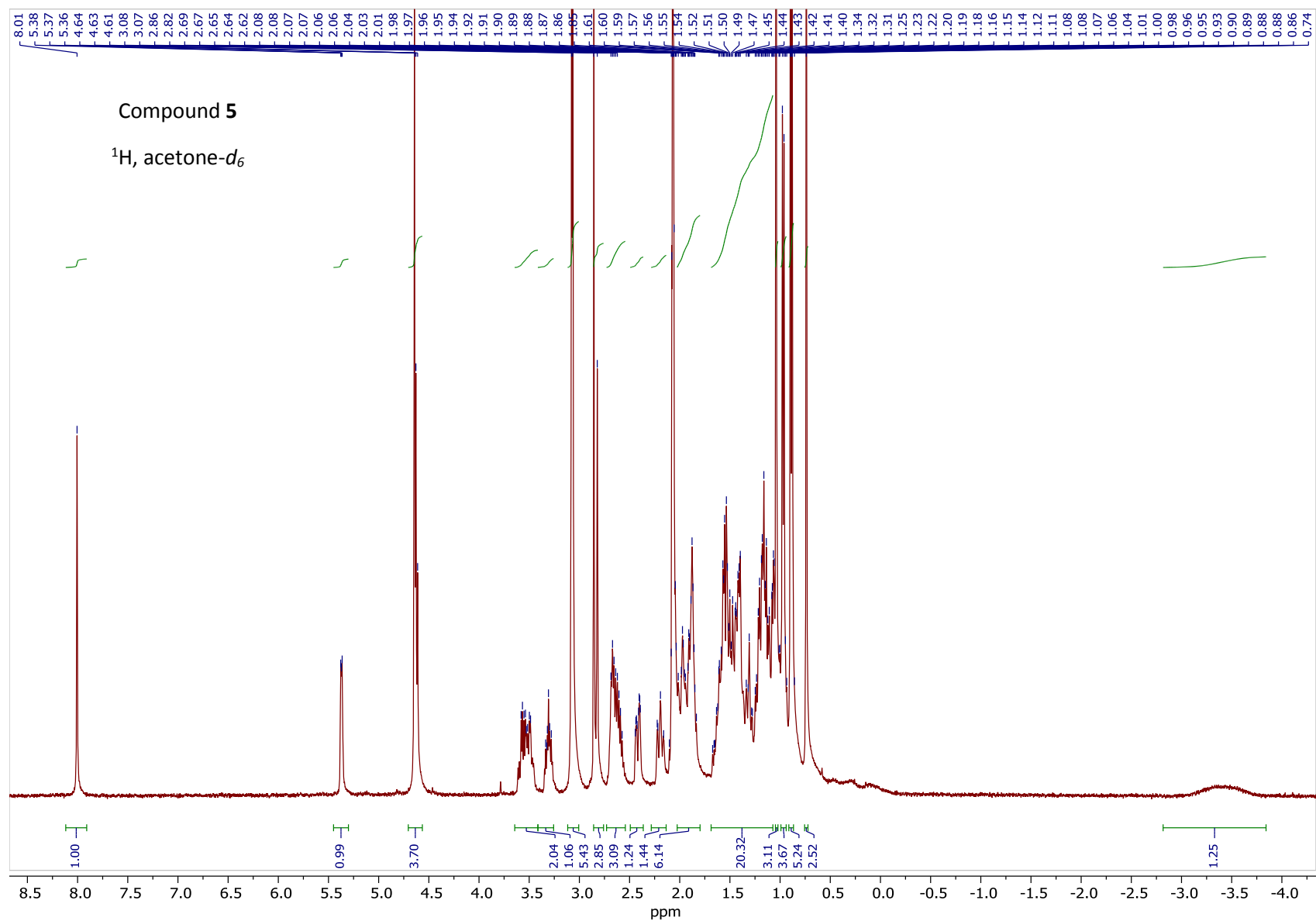


Figure S21. ^1H NMR spectrum of compound 5

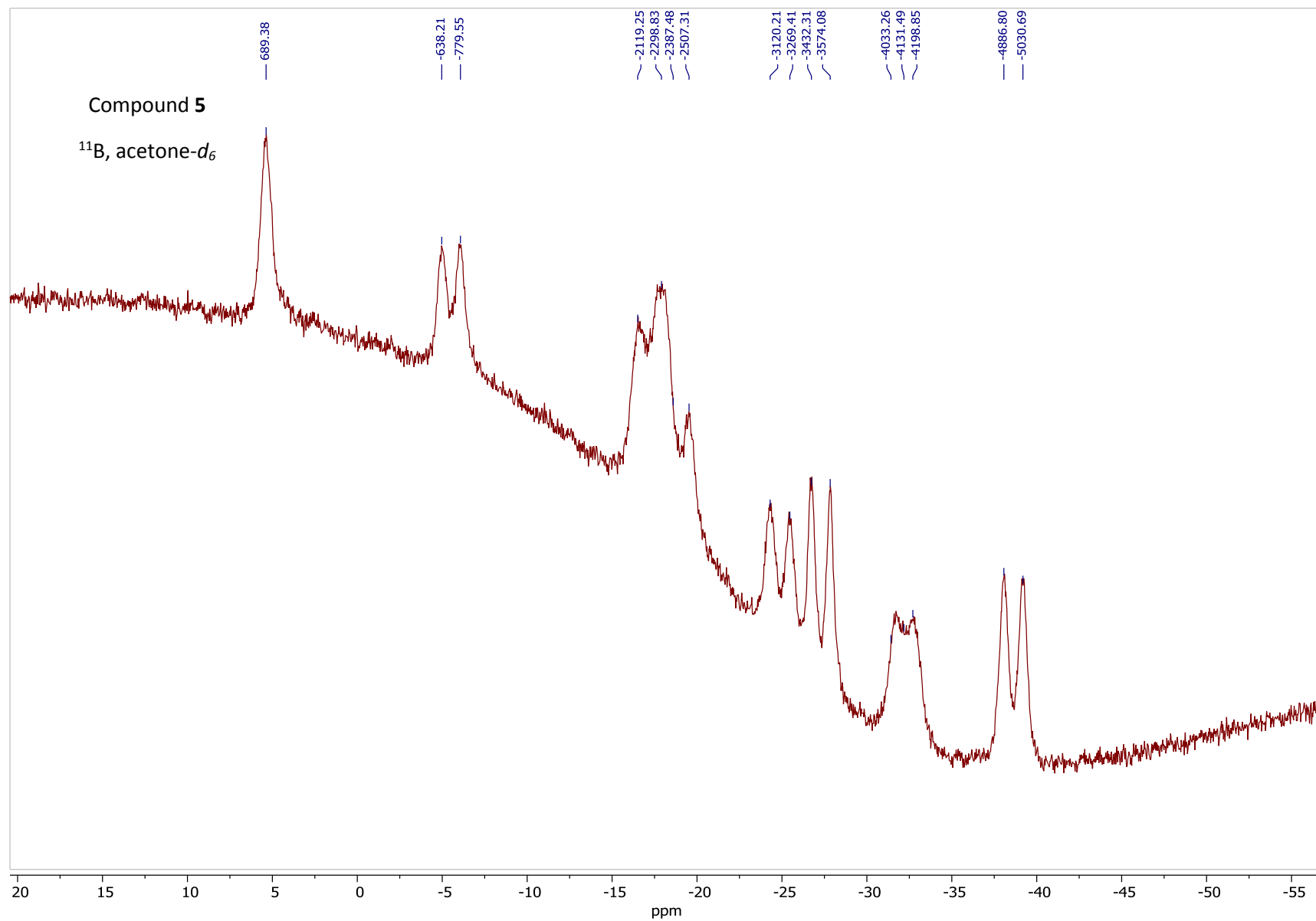


Figure S22. ^{11}B NMR spectrum of compound 5

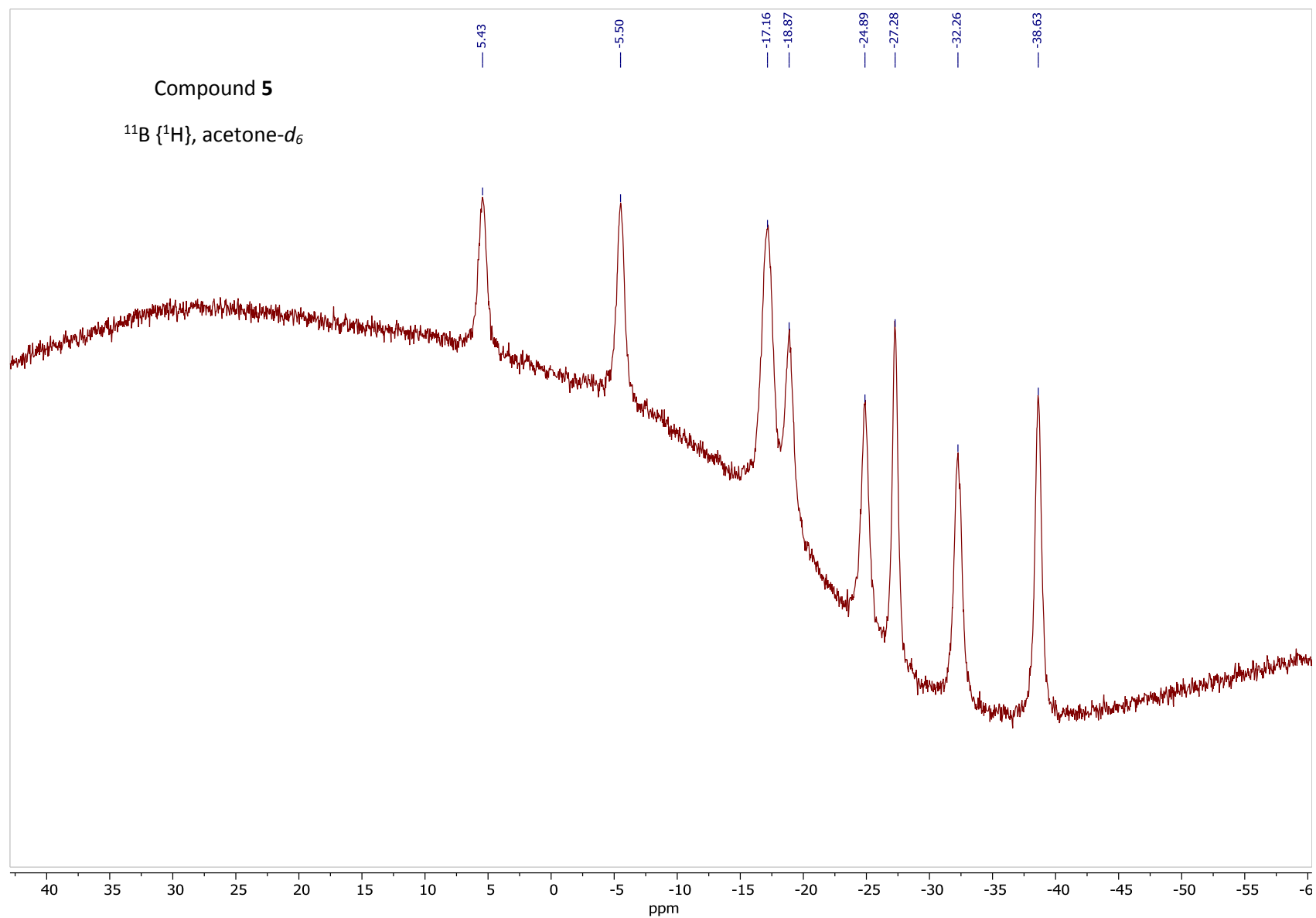


Figure S23. $^{11}\text{B}\{^1\text{H}\}$ NMR spectrum of compound 5

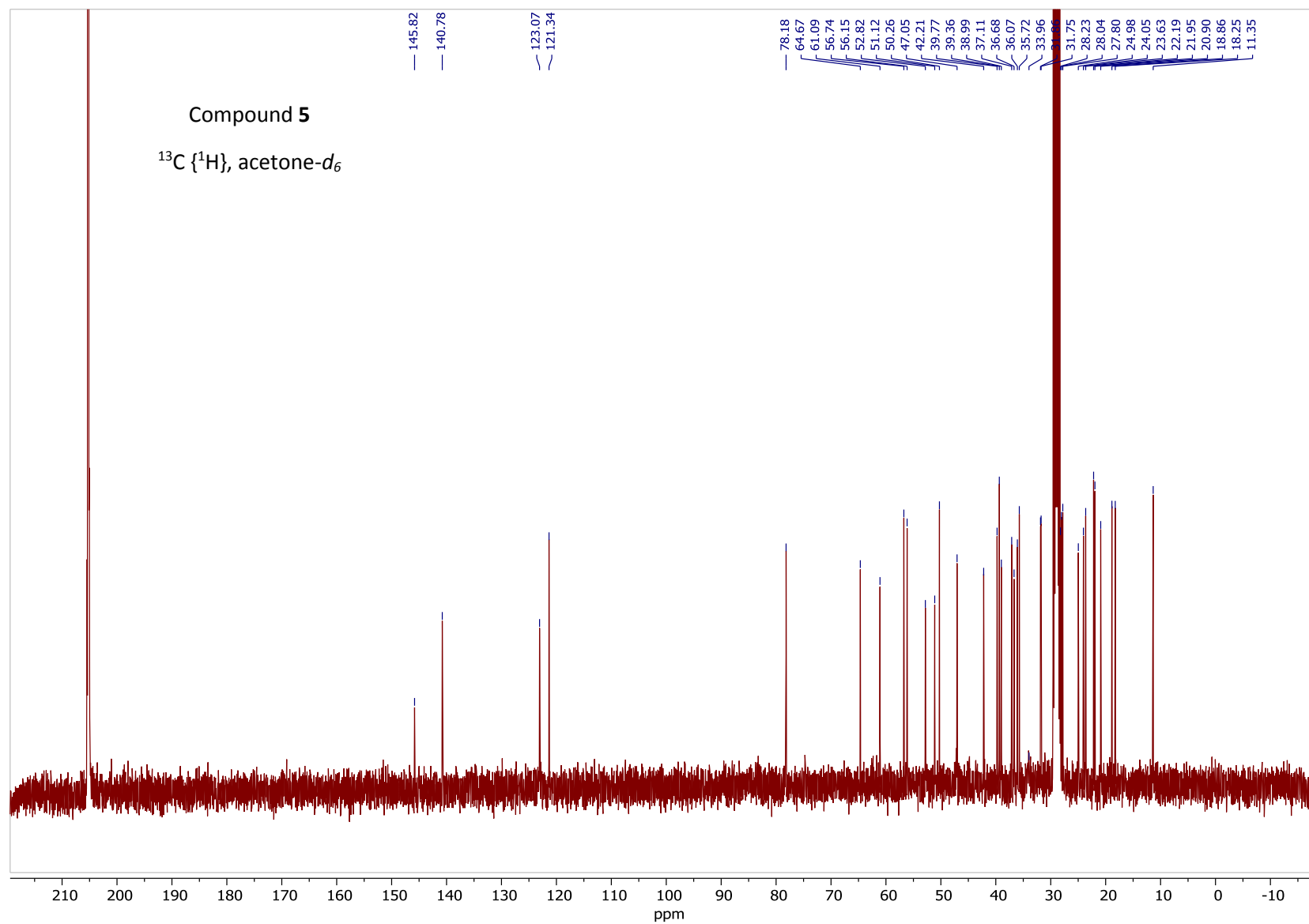


Figure S24. ^{13}C NMR spectrum of compound **5**

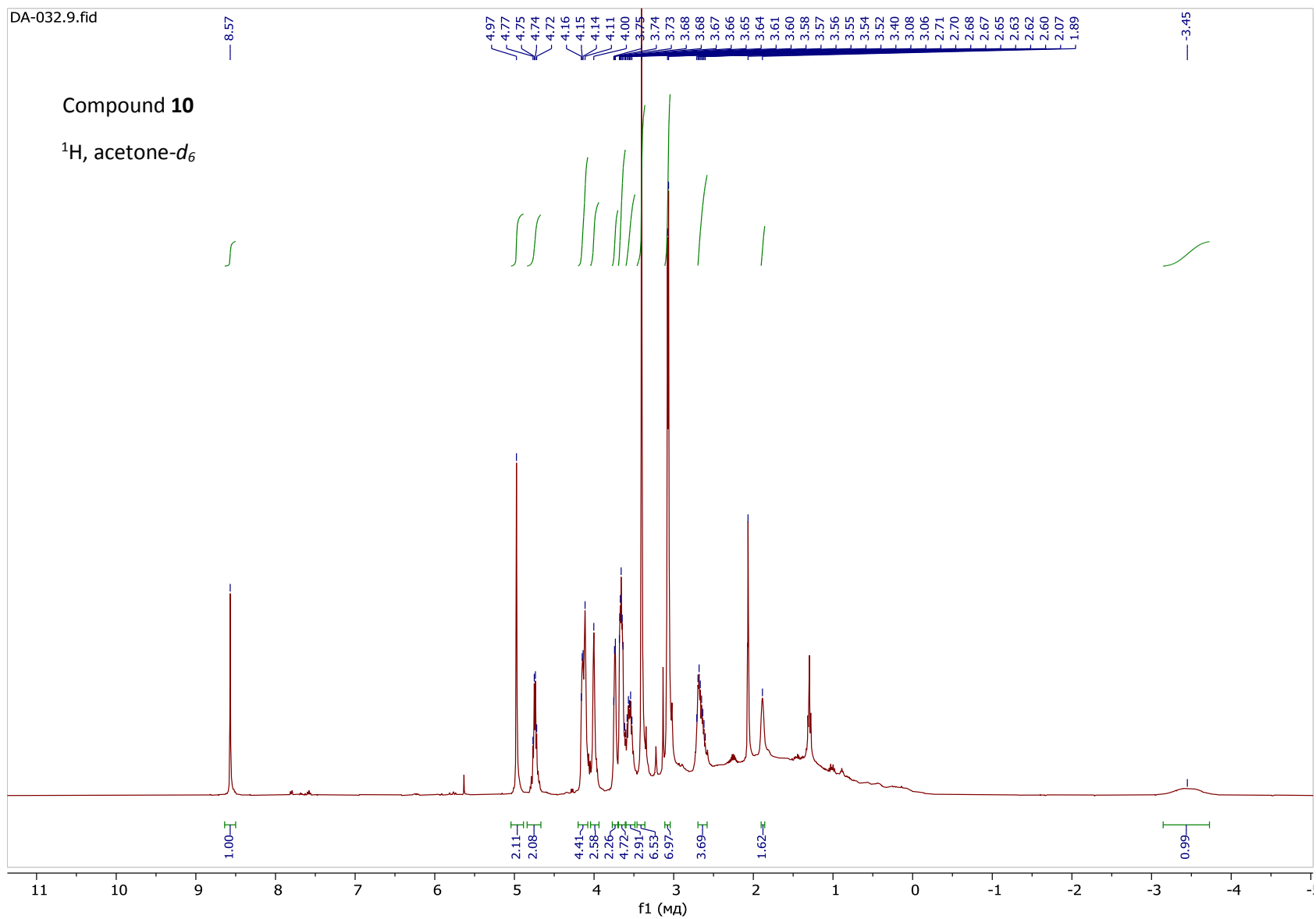


Figure S25. ^1H NMR spectrum of compound **10**

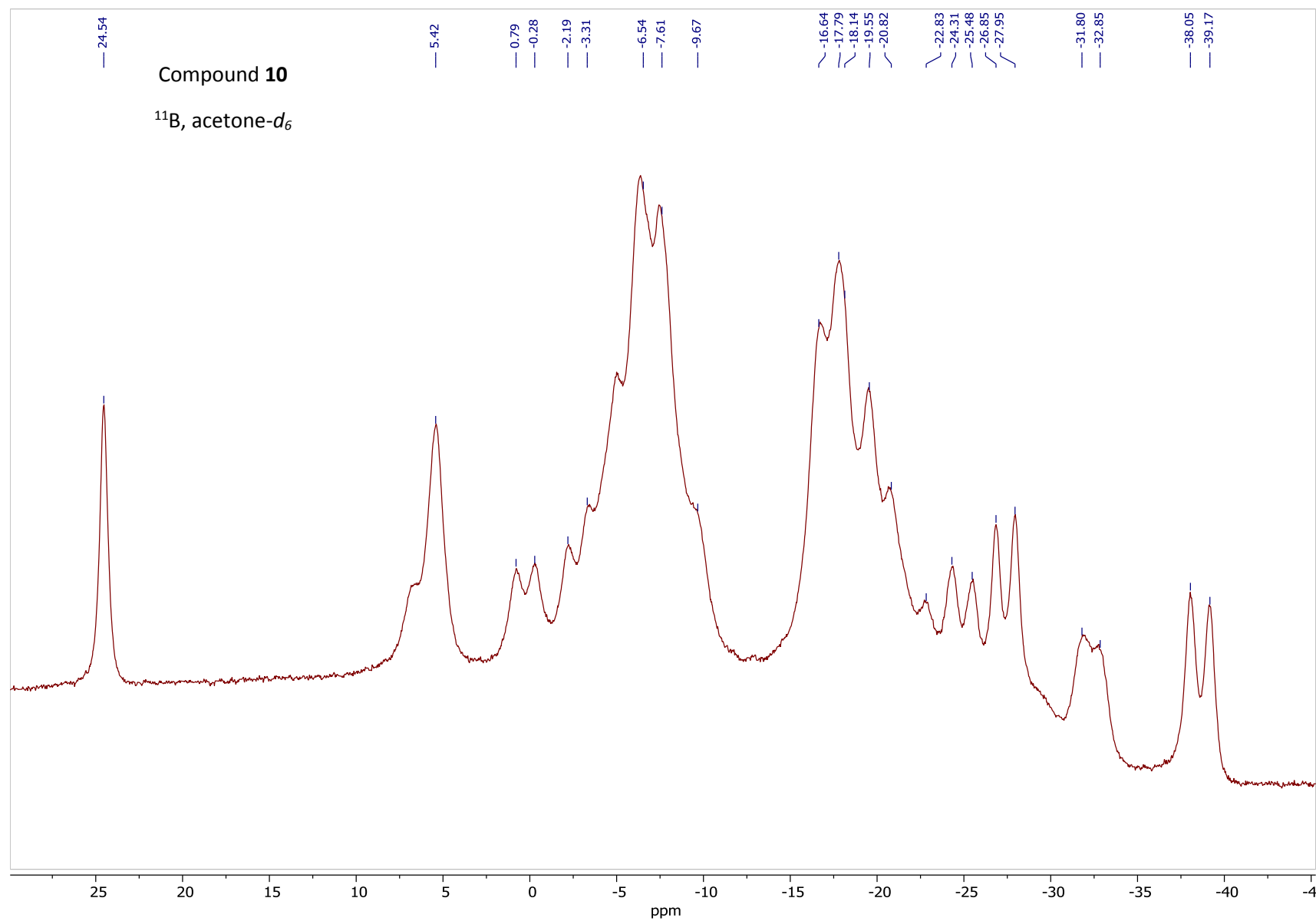


Figure S26. ^{11}B NMR spectrum of compound **10**

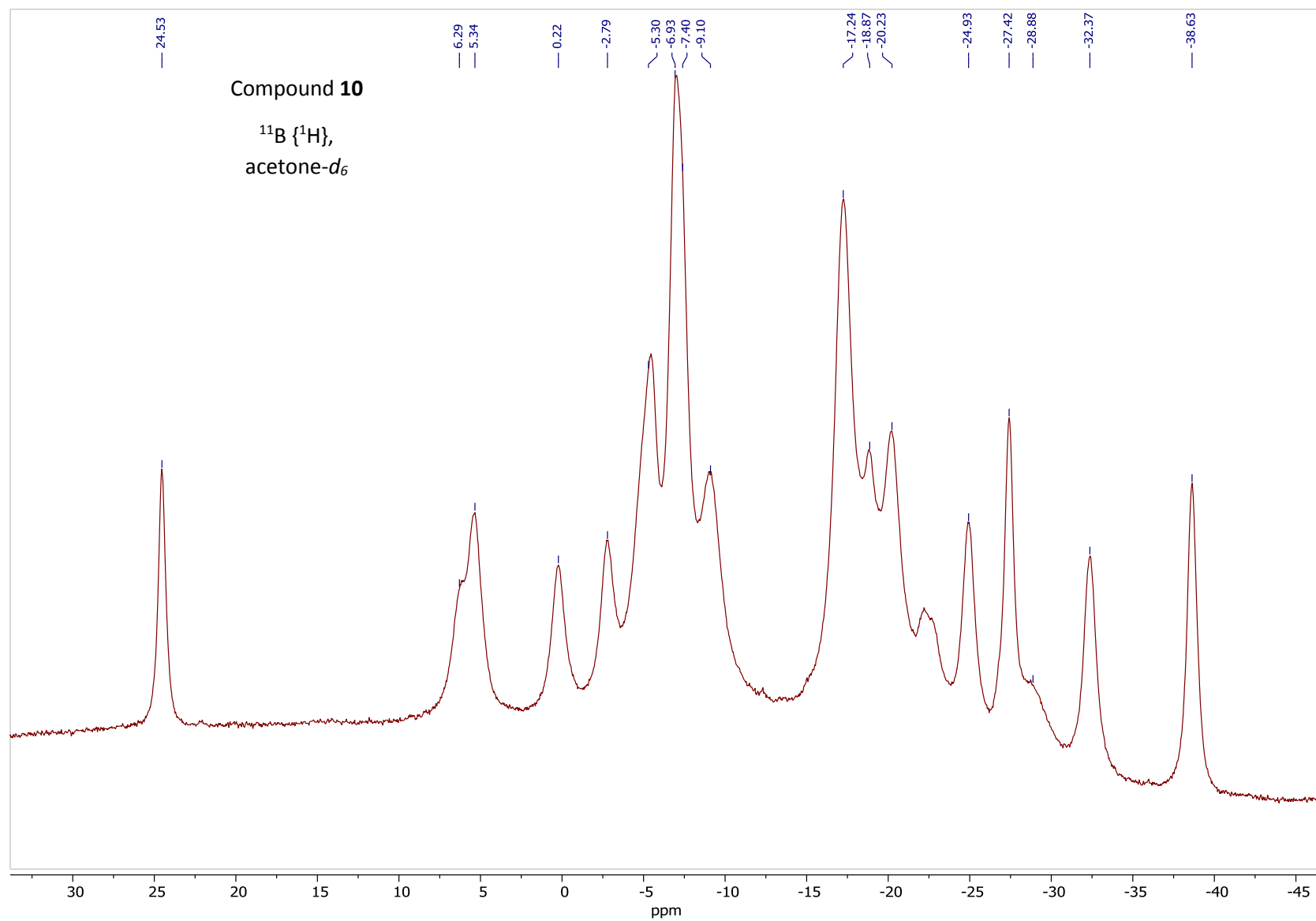


Figure S27. $^{11}\text{B}\{^1\text{H}\}$ NMR spectrum of compound **10**

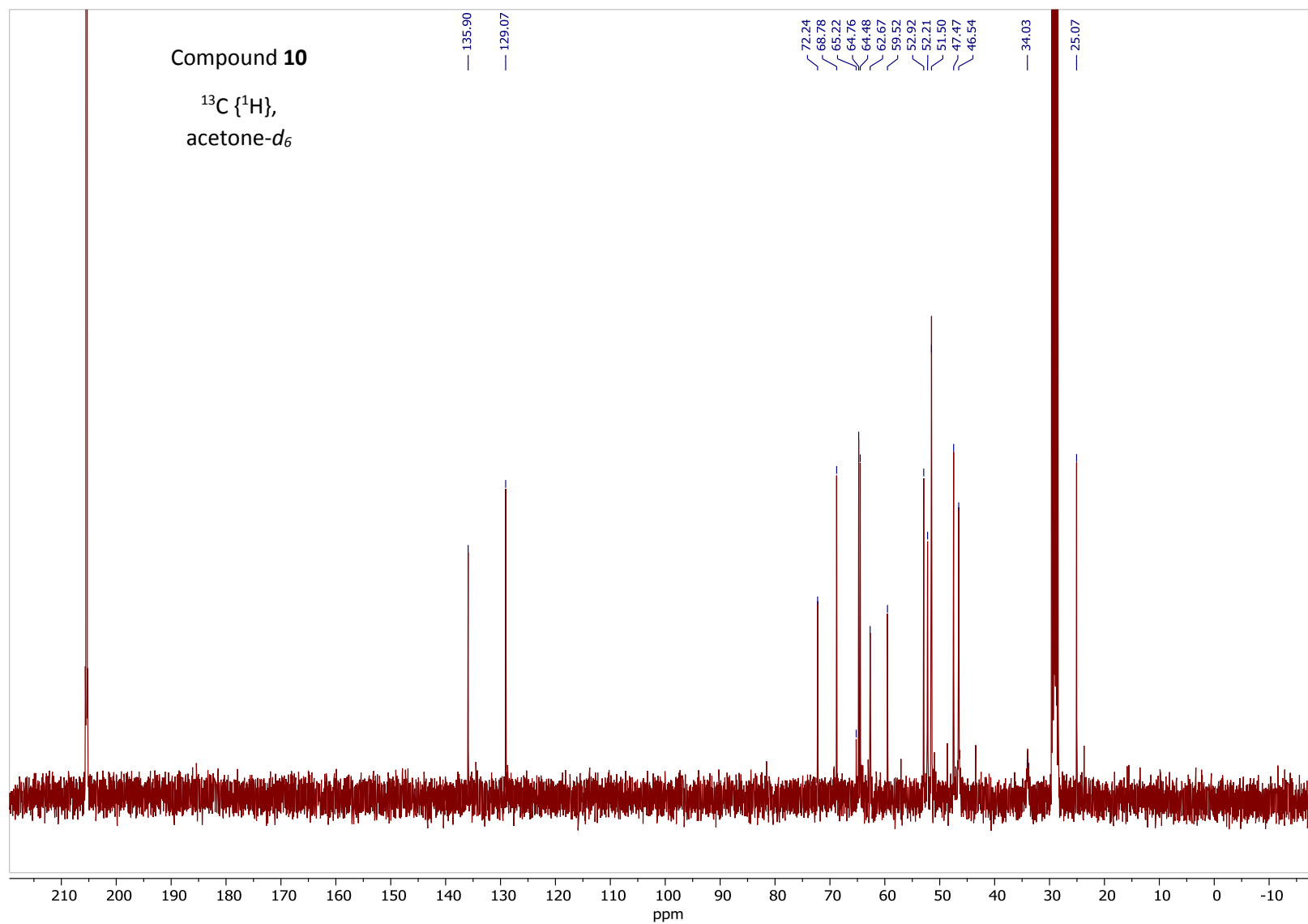


Figure S28. ^{13}C NMR spectrum of compound **10**

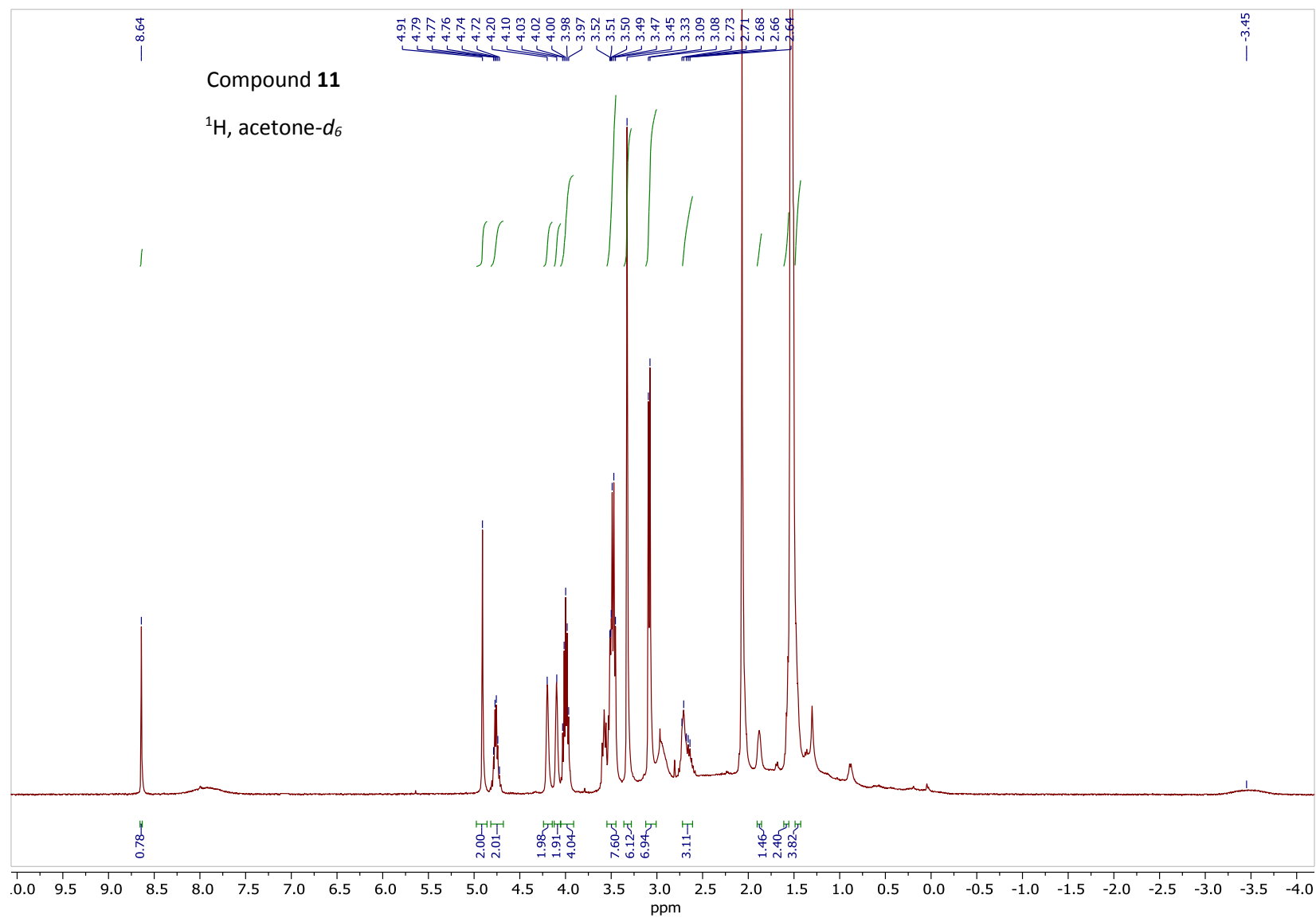


Figure S29. ^1H NMR spectrum of compound **11**

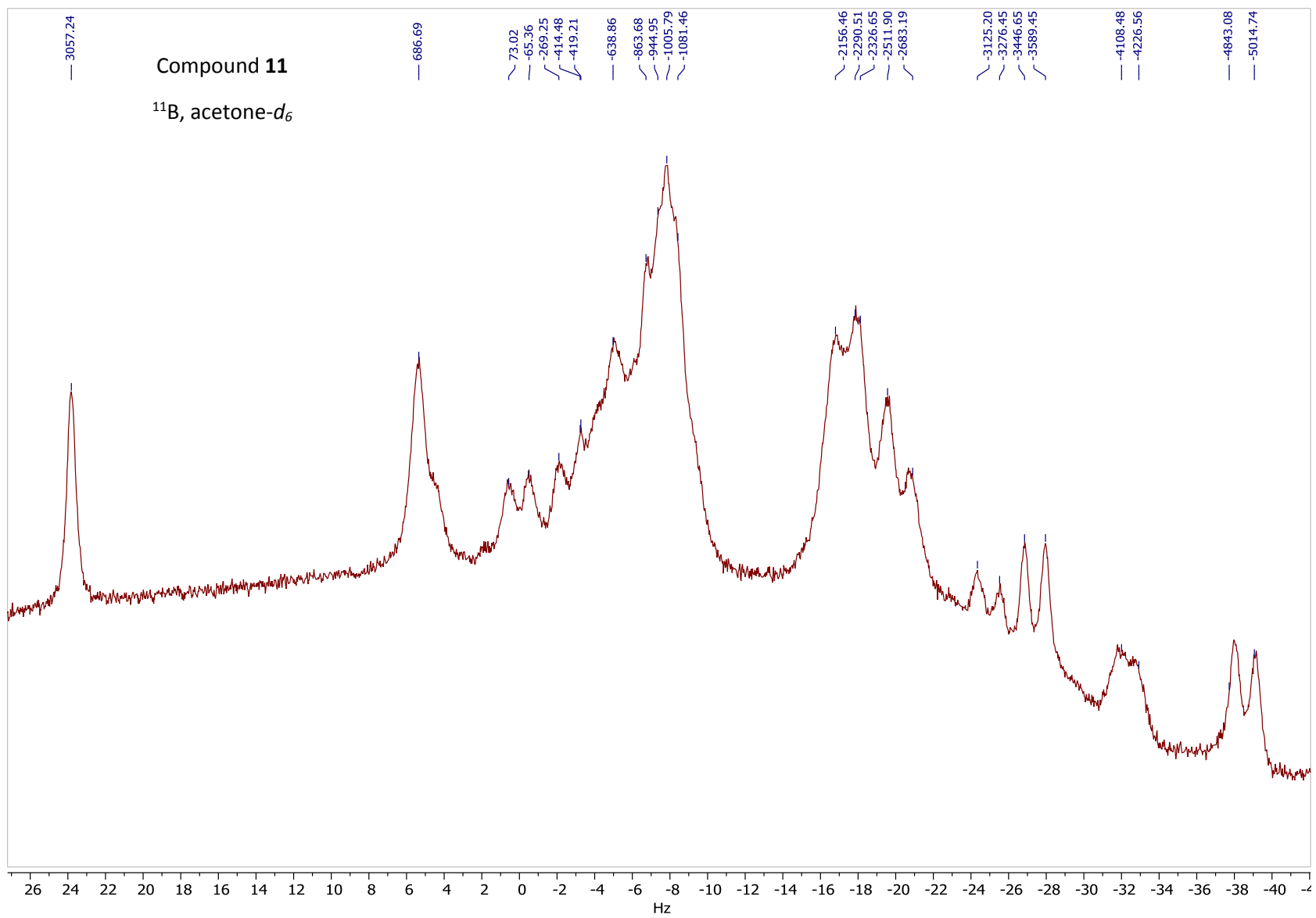


Figure S30. ^{11}B NMR spectrum of compound **11**

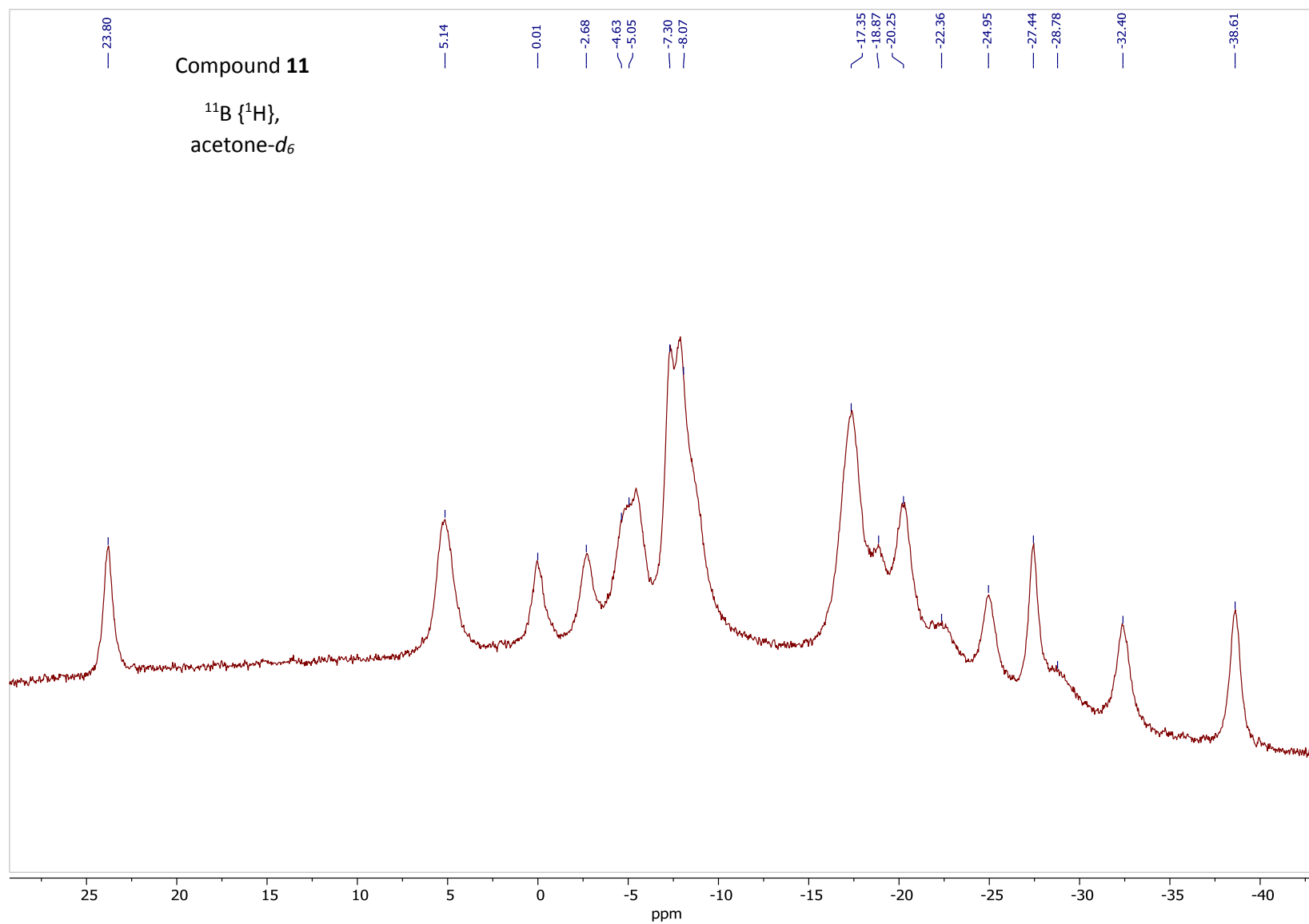


Figure S31. $^{11}\text{B}\{^1\text{H}\}$ NMR spectrum of compound **11**

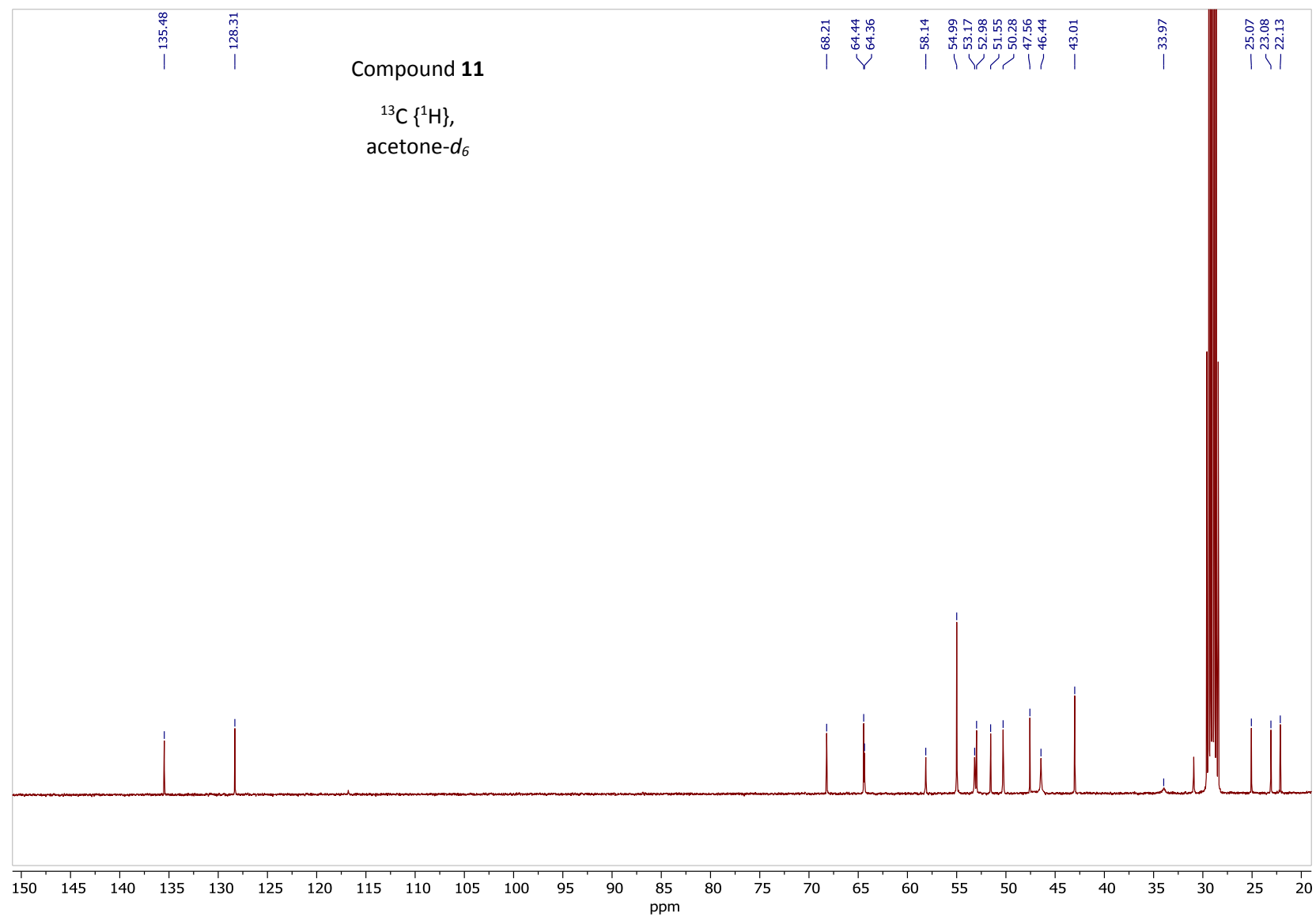


Figure S32. ^{13}C NMR spectrum of compound **11**

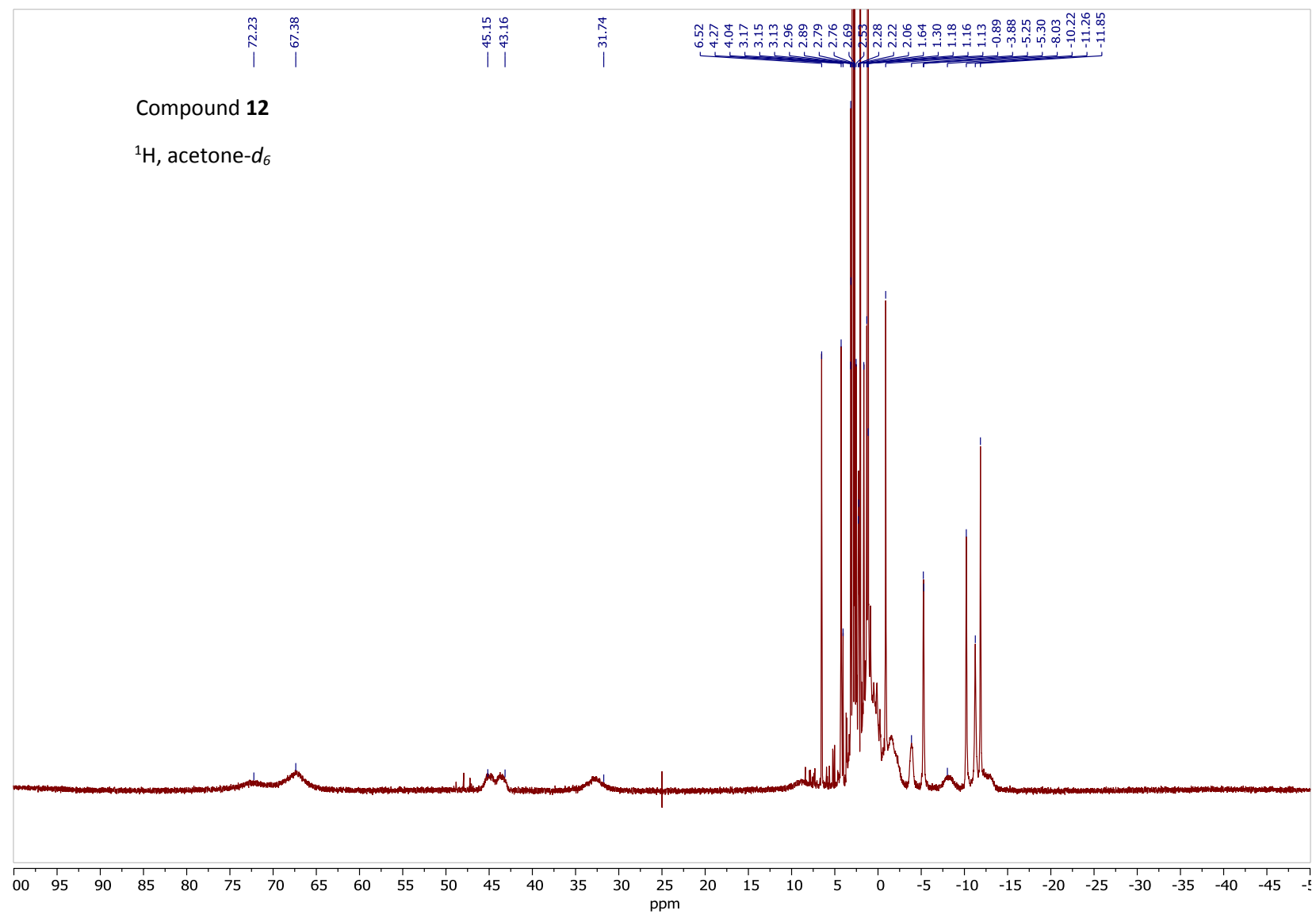


Figure S33. ^1H NMR spectrum of compound **12**

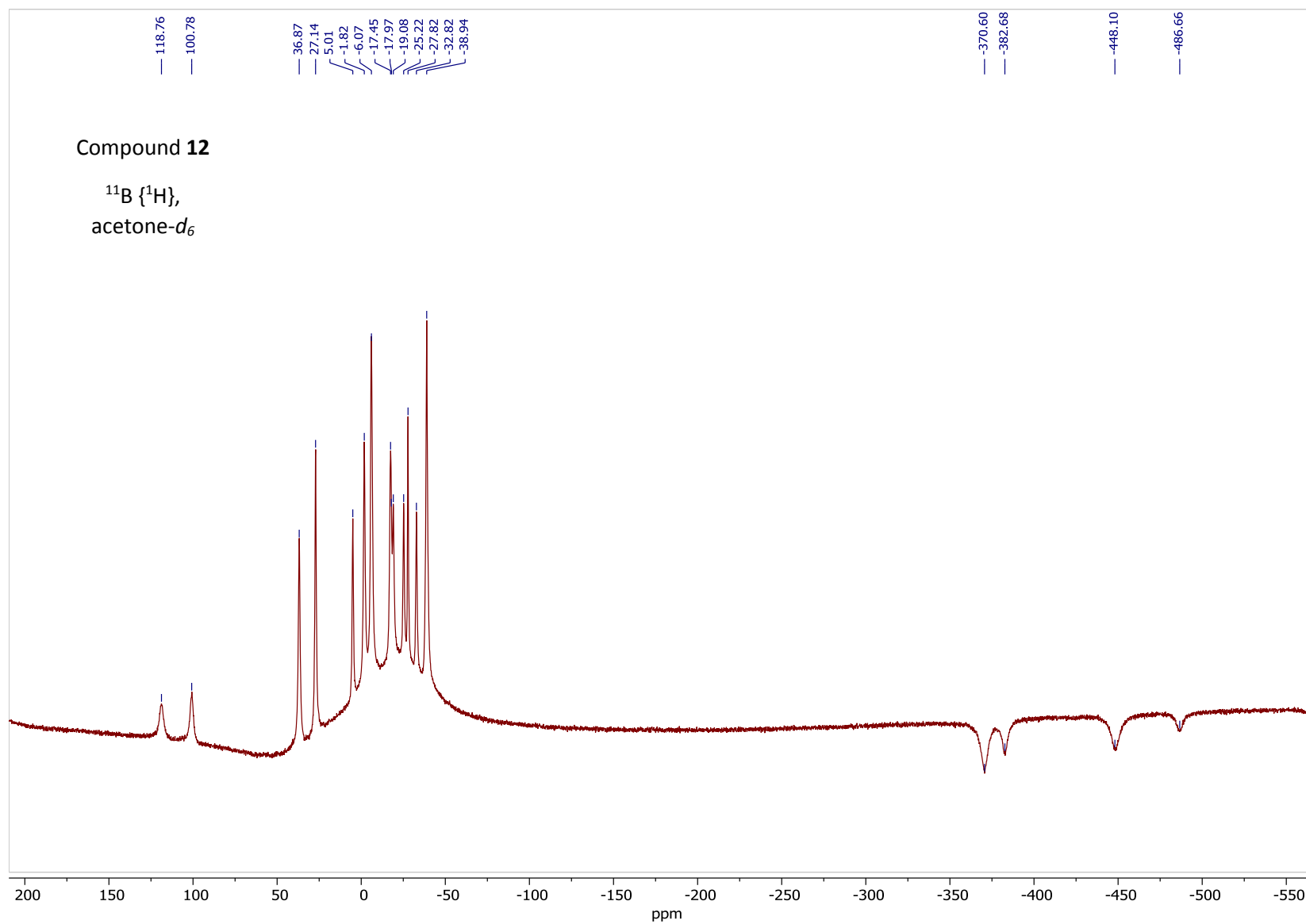


Figure S34. $^{11}\text{B}\{^1\text{H}\}$ NMR spectrum of compound **12**

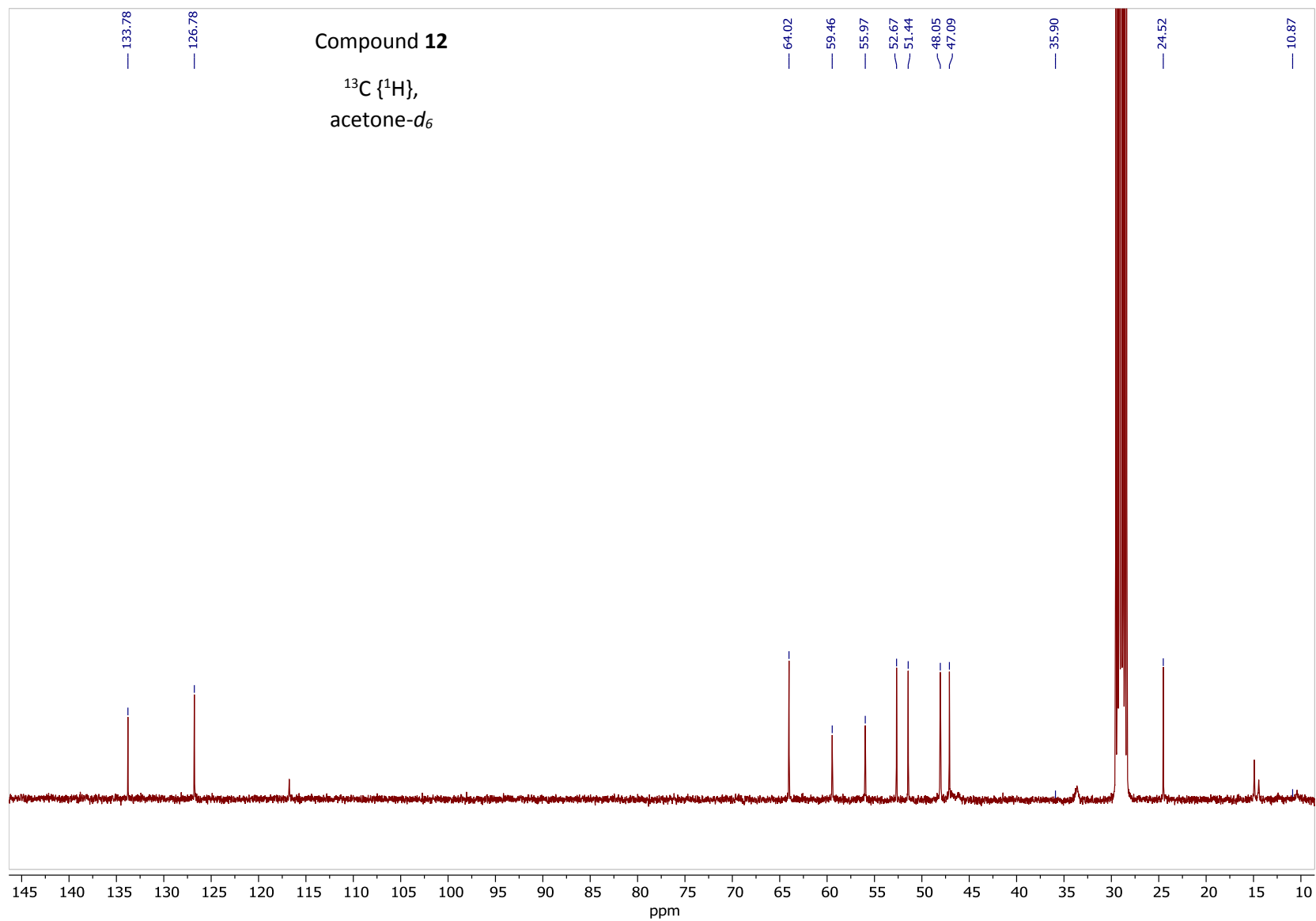


Figure S35. ^{13}C NMR spectrum of compound **12**