

SUPPORTING INFORMATION

Synthesis of Cobalt Bis(Dicarbollide) – Curcumin Conjugates for Potential Use in Boron Neutron Capture Therapy

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¹H, ¹¹B and ¹³C NMR, IR and high-resolution mass spectra of compounds **4-7**

Display Report

Analysis Info

Analysis Name D:\Data\Chizhov\INEOS\Druzina\da-043_&clb-.d
Method tune_wide_neg.m
Sample Name /CHIZ DA-043
Comment CH3OH 100 %, dil. 200, calibrant added

Acquisition Date 24.05.2022 16:09:46

Operator BDAL@DE
Instrument / Ser# maXis 43

Acquisition Parameter

Source Type	ESI	Ion Polarity	Negative	Set Nebulizer	0.4 Bar
Focus	Active			Set Dry Heater	180 °C
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Scan End	3000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste

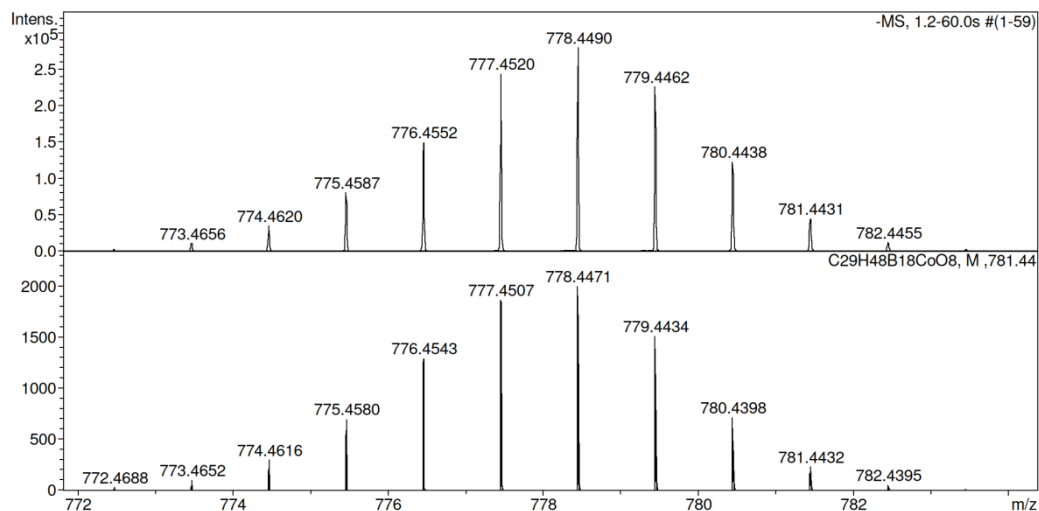
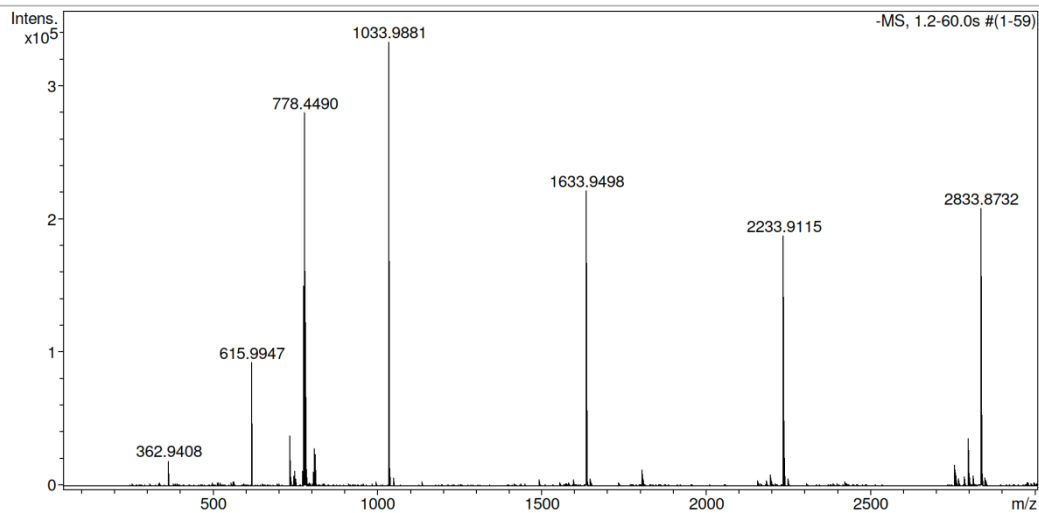


Figure S1. ESI-HRMS spectrum of compound **4**

Display Report

Analysis Info

Analysis Name D:\Data\Chizhov\INEOS\Druzina\da-042_&clblow-.d
Method tune_low_neg_1050.m
Sample Name /CHIZ DA-042
Comment CH3OH 100 %, dil. 200, calibrant added

Acquisition Date 24.05.2022 16:01:27

Operator BDAL@DE
Instrument / Ser# maXis 43

Acquisition Parameter

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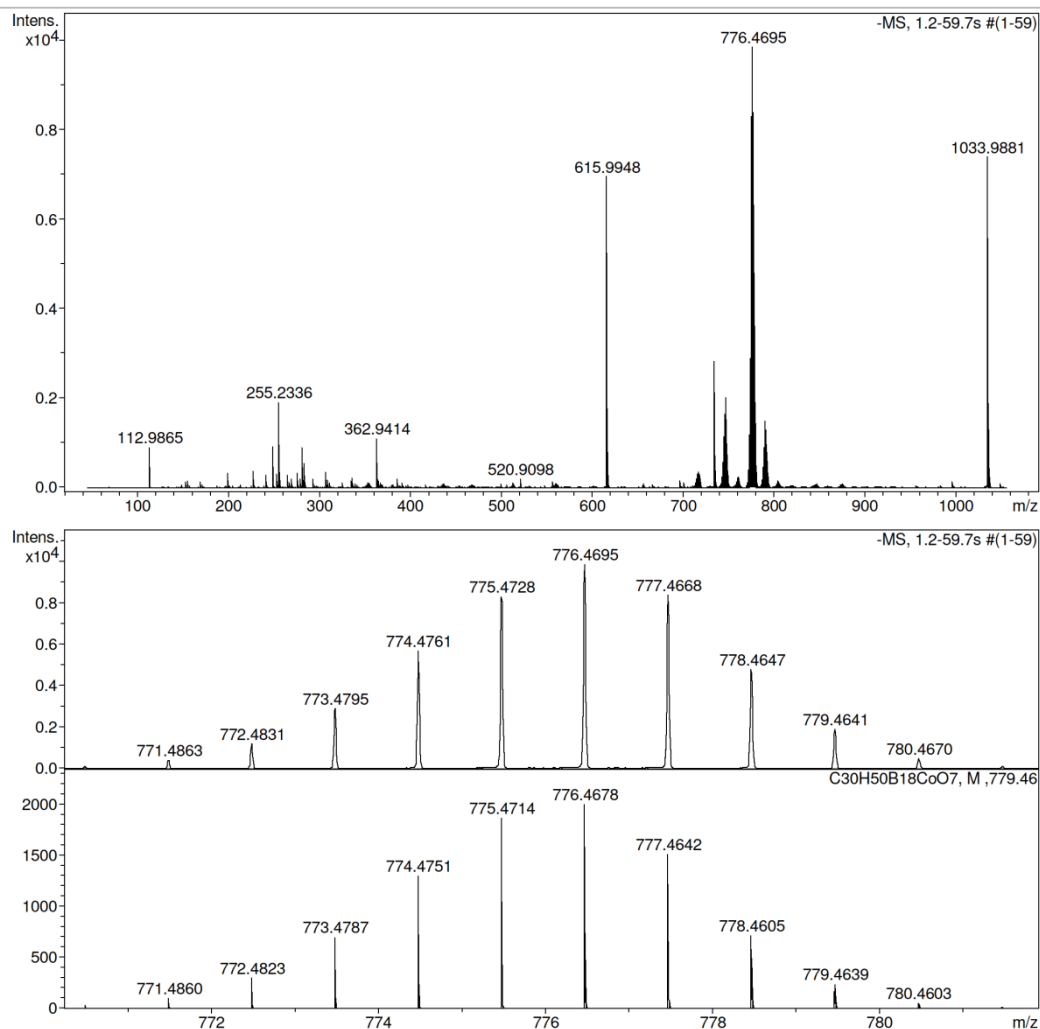


Figure S2. ESI-HRMS spectrum of compound 5

Display Report

Analysis Info

Analysis Name D:\Data\Chizhov\INEOS\Druzina\da-044_&clb-.d
Method tune_wide_neg.m
Sample Name /CHIZ DA-044
Comment CH3OH 100 %, dil. 200, calibrant added

Acquisition Date 24.05.2022 16:17:44

Operator BDAL@DE
Instrument / Ser# maXis 43

Acquisition Parameter

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Focus	Active			Set Dry Heater	180 °C
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Scan End	3000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste

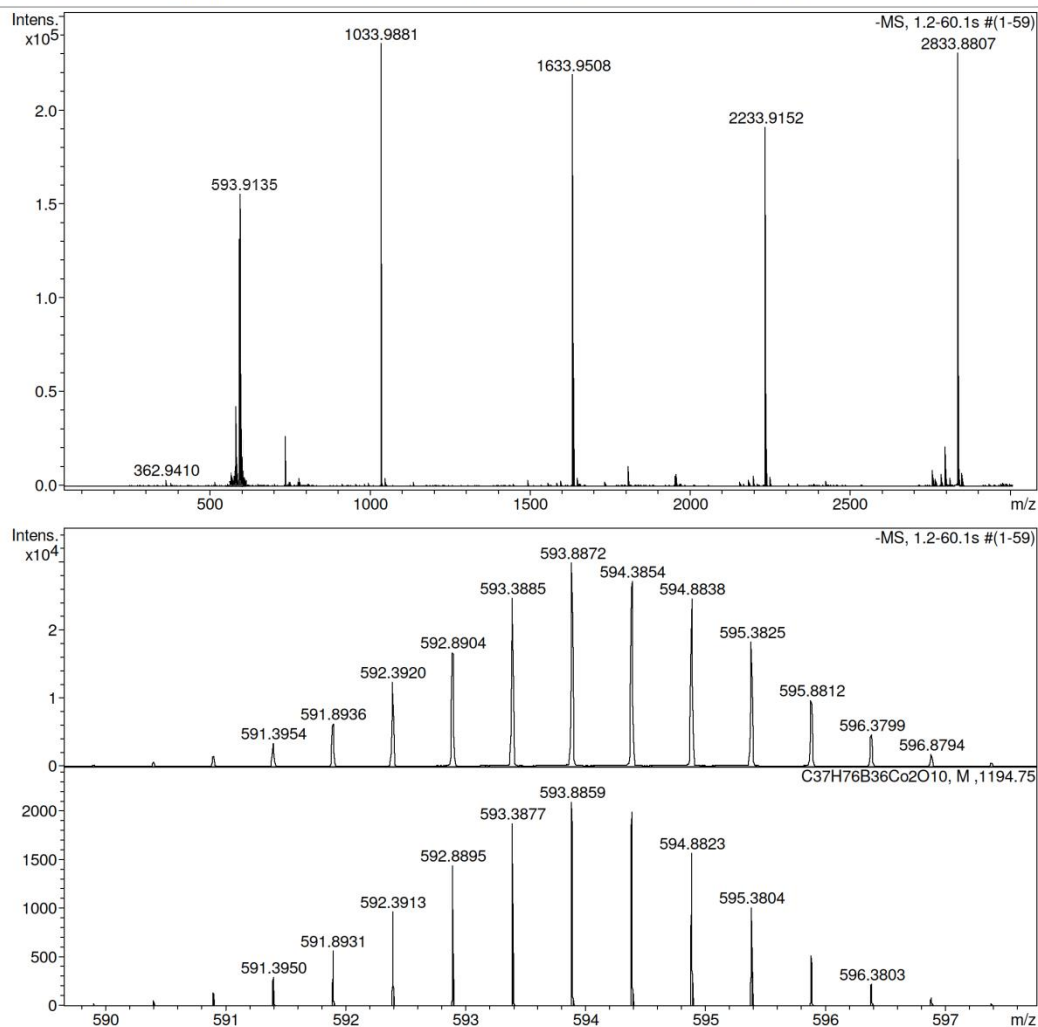


Figure S3. ESI-HRMS spectrum of compound 6

Display Report

Analysis Info

Analysis Name D:\Data\Chizhov\INEOS\Bregadze\Druzina\Jan_17_2022\da-045-2_&clb-.d
Method tune_wide_neg.m
Sample Name /CHIZ DA-045-2
Comment CH3CN 100 %, dil. 20, calibrant added

Acquisition Date 17.01.2022 19:26:09
Operator BDAL@DE
Instrument / Ser# microTOF 10248

Acquisition Parameter

Source Type	ESI	Ion Polarity	Negative	Set Nebulizer	0.4 Bar
Focus	Not active			Set Dry Heater	180 °C
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Scan End	3000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste

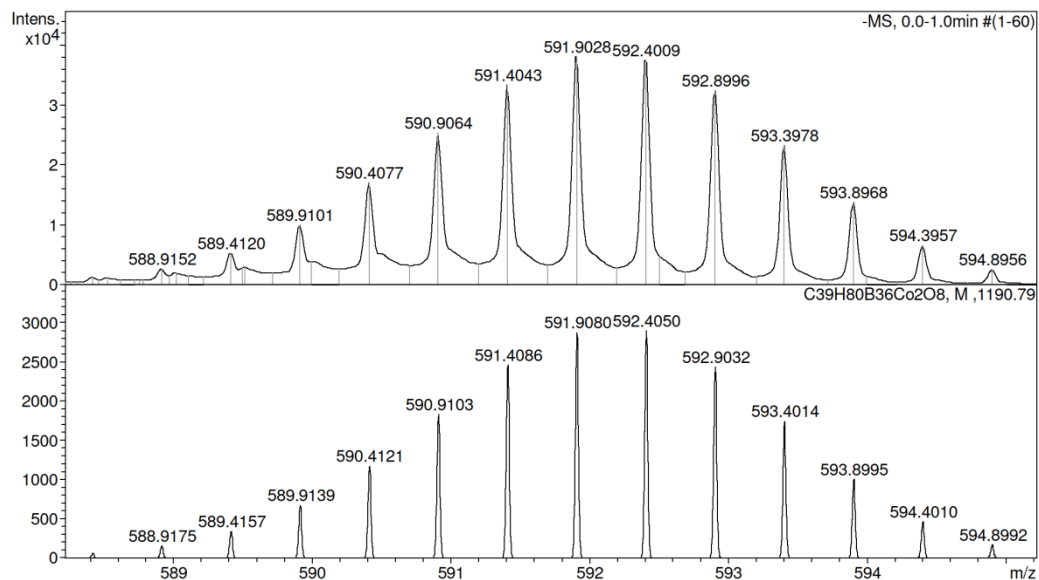
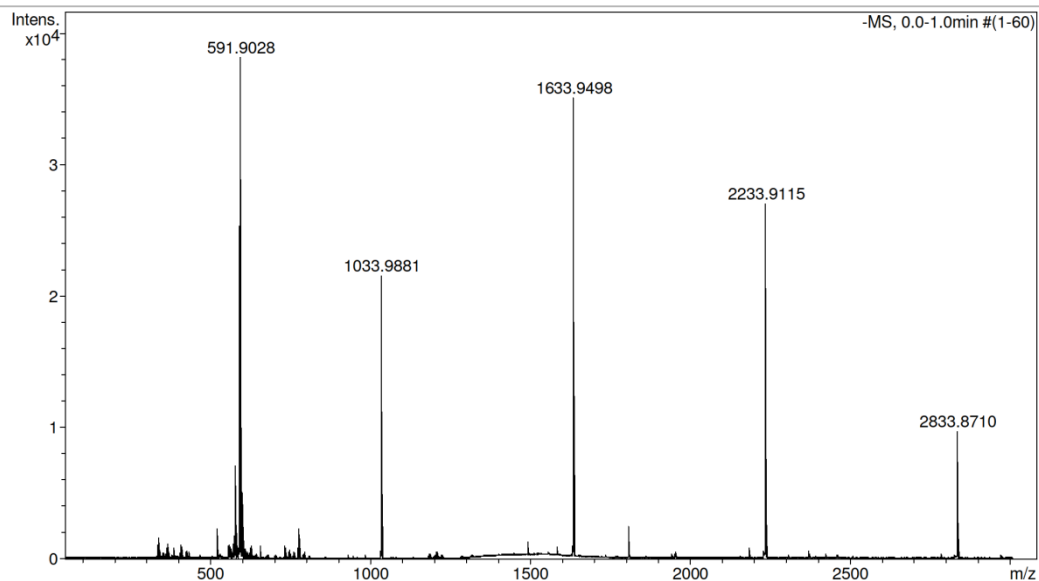


Figure S4. ESI-HRMS spectrum of compound 7

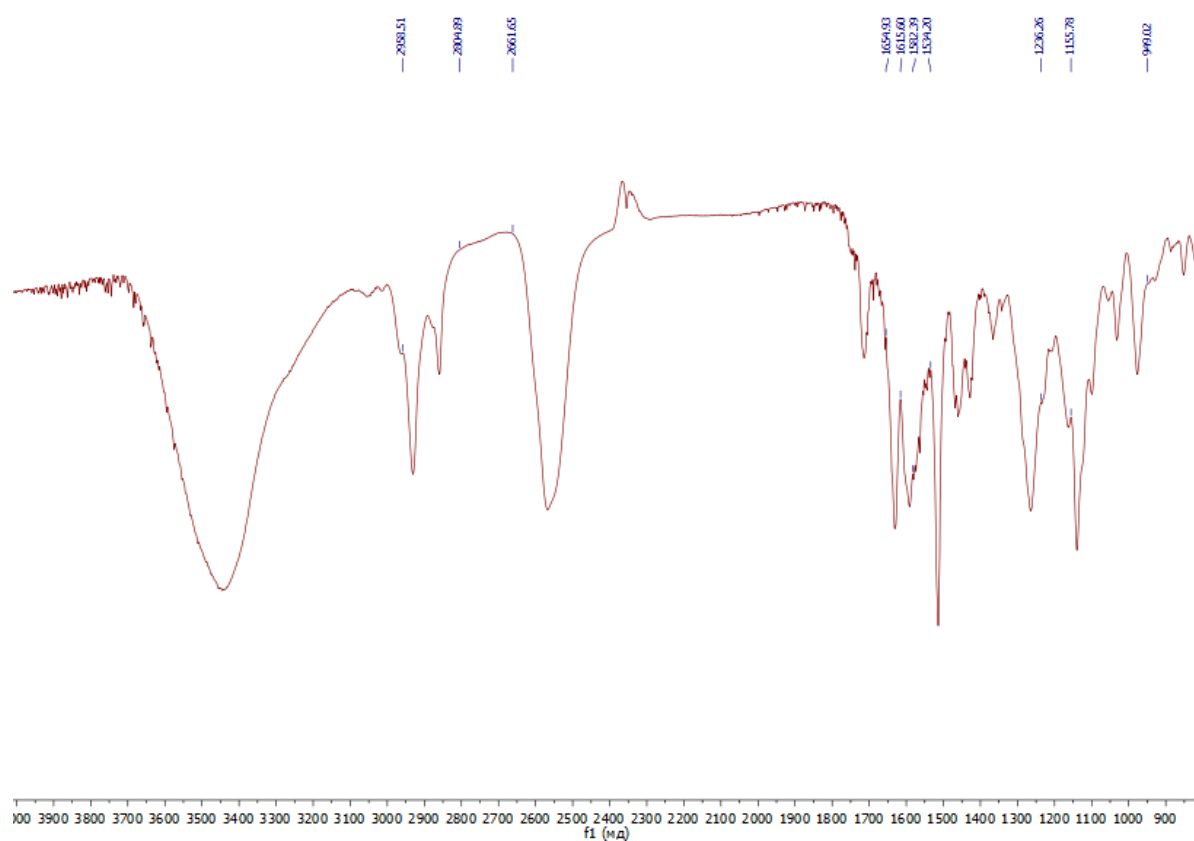


Figure S5. IR spectrum of compound 4

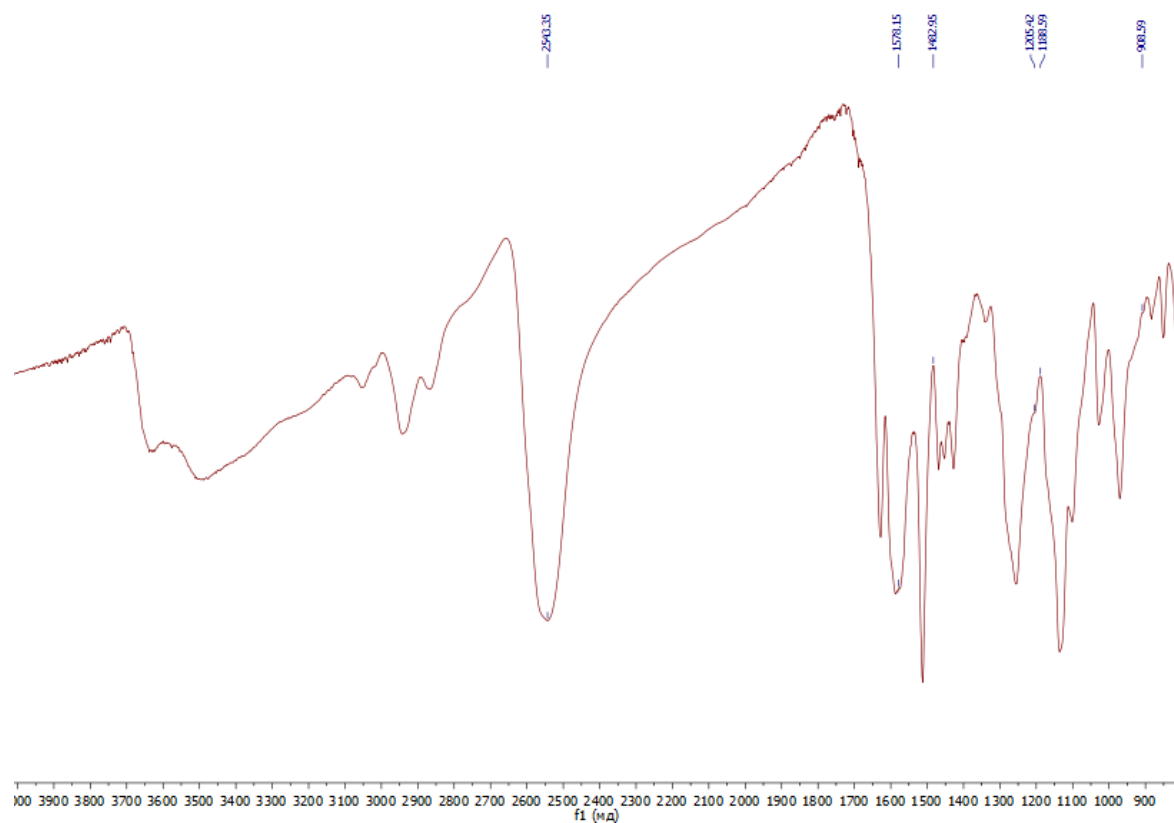


Figure S6. IR spectrum of compound 5

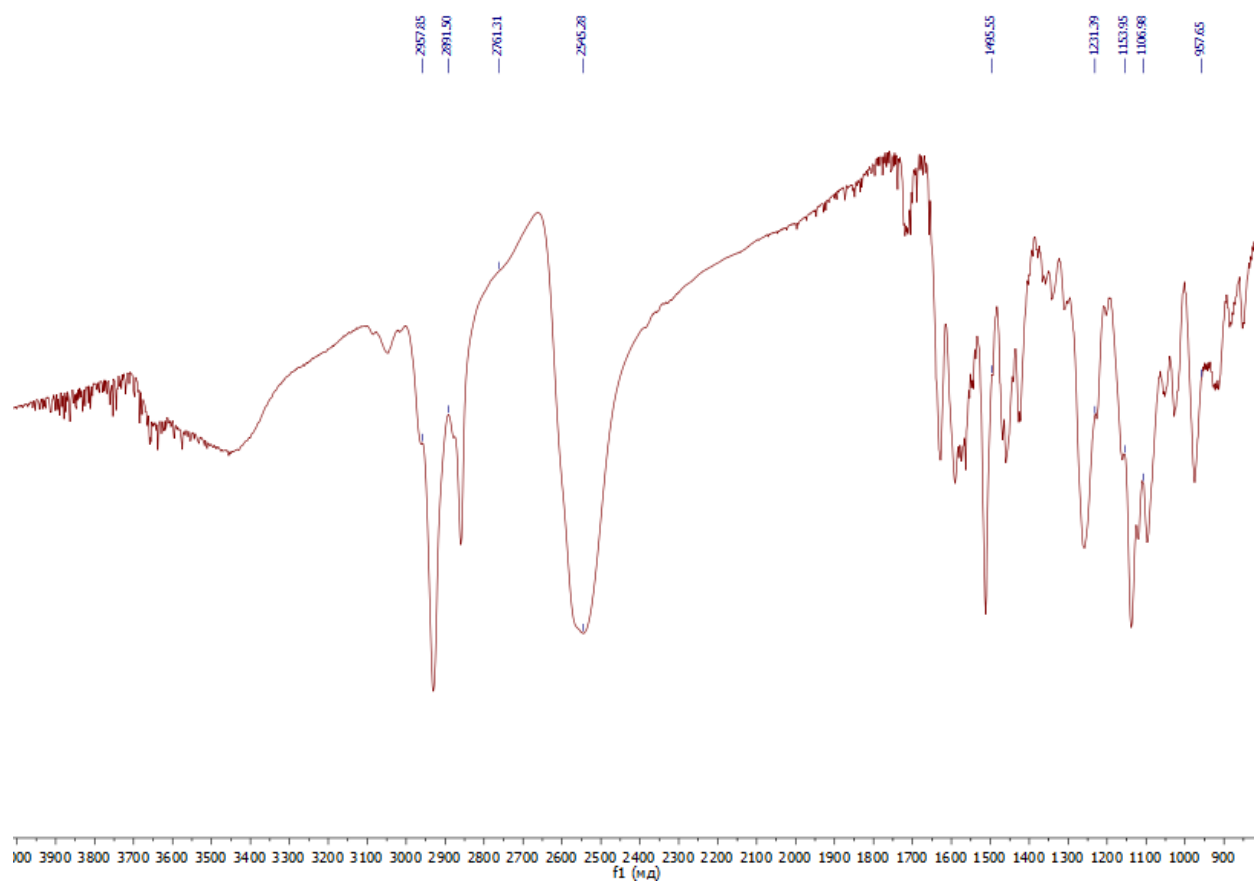


Figure S7. IR spectrum of compound 6

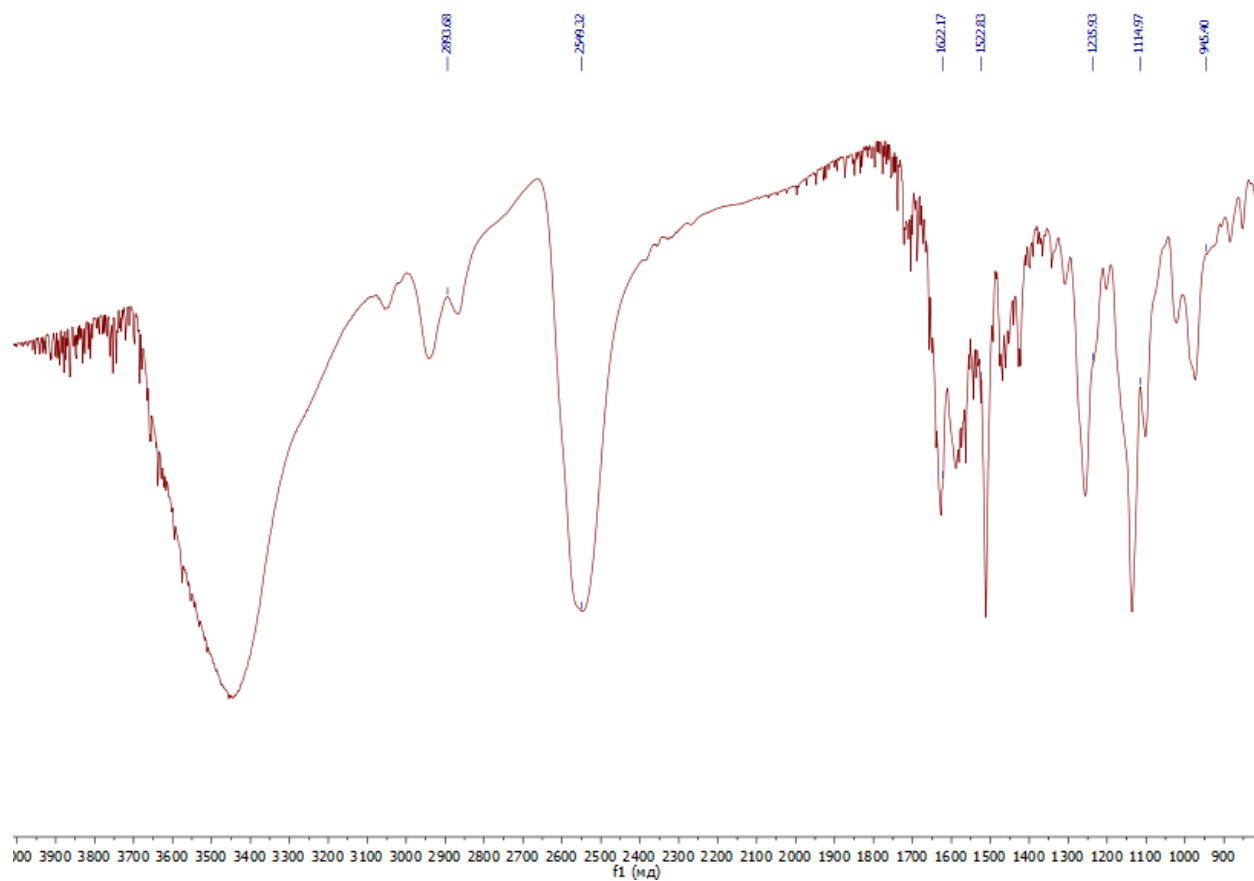


Figure S8. IR spectrum of compound 7

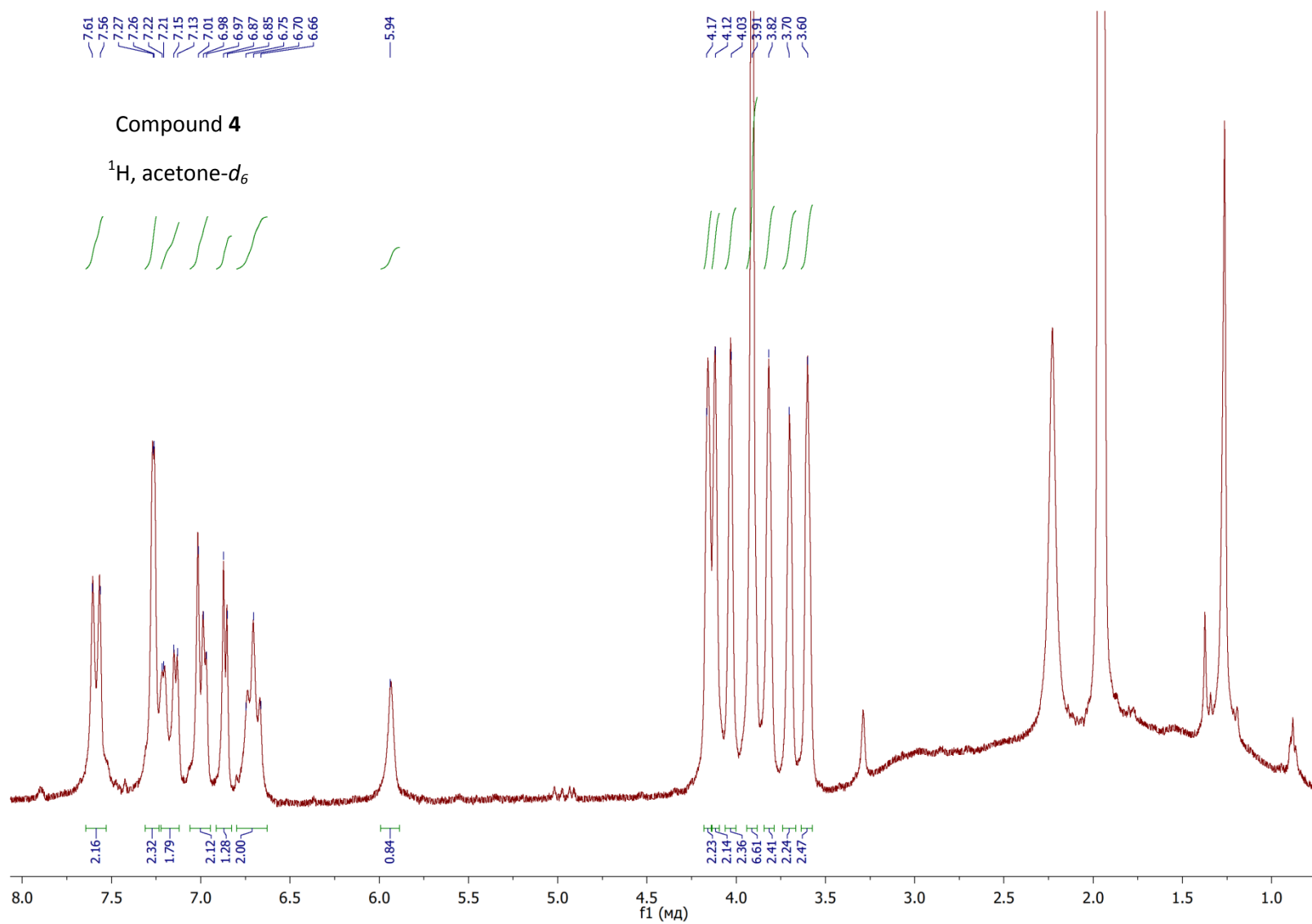


Figure S9. ^1H NMR spectrum of compound **4**

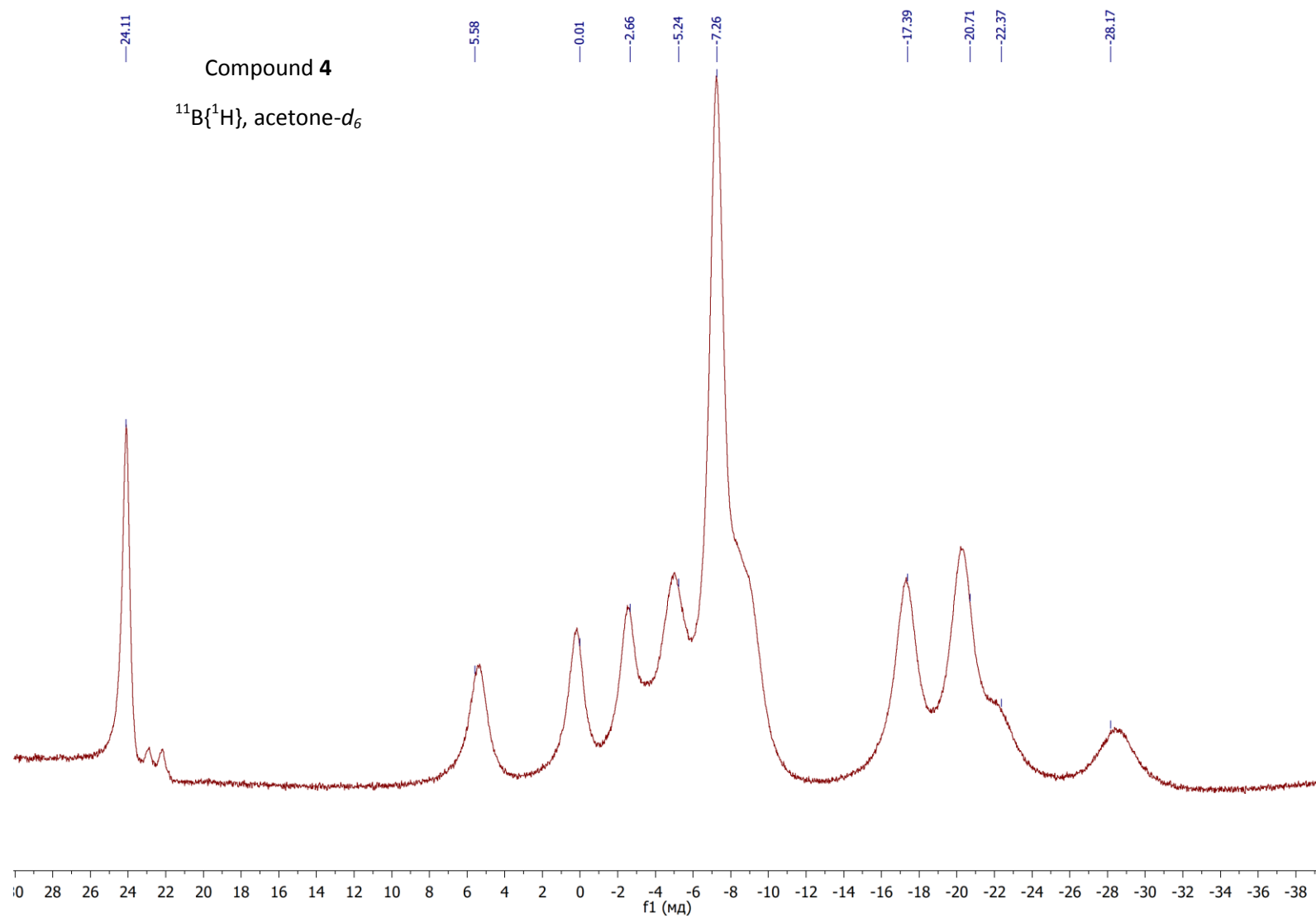


Figure S10. $^{11}\text{B}\{^1\text{H}\}$ NMR spectrum of compound **4**

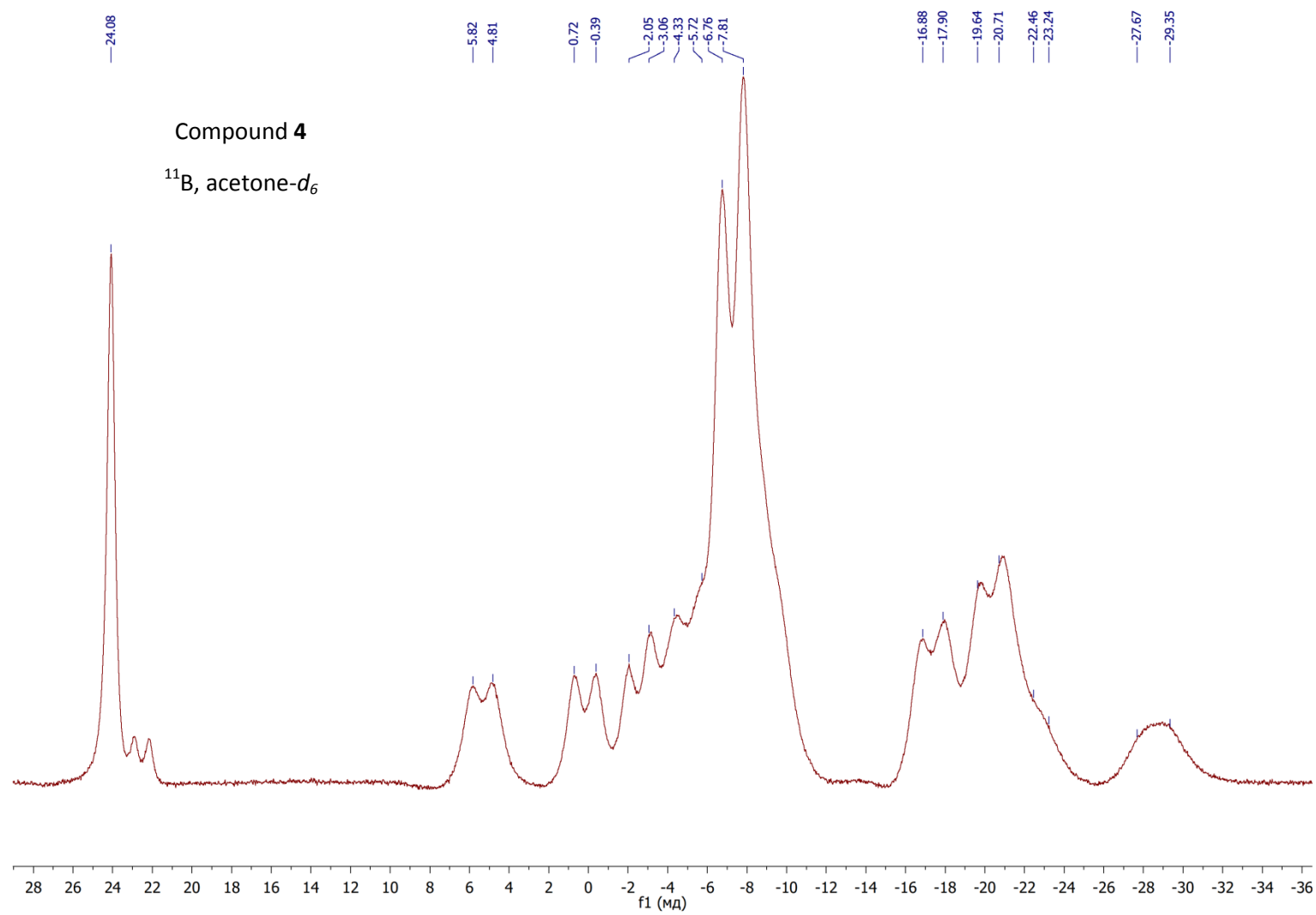


Figure S11. ^{11}B NMR spectrum of compound **4**

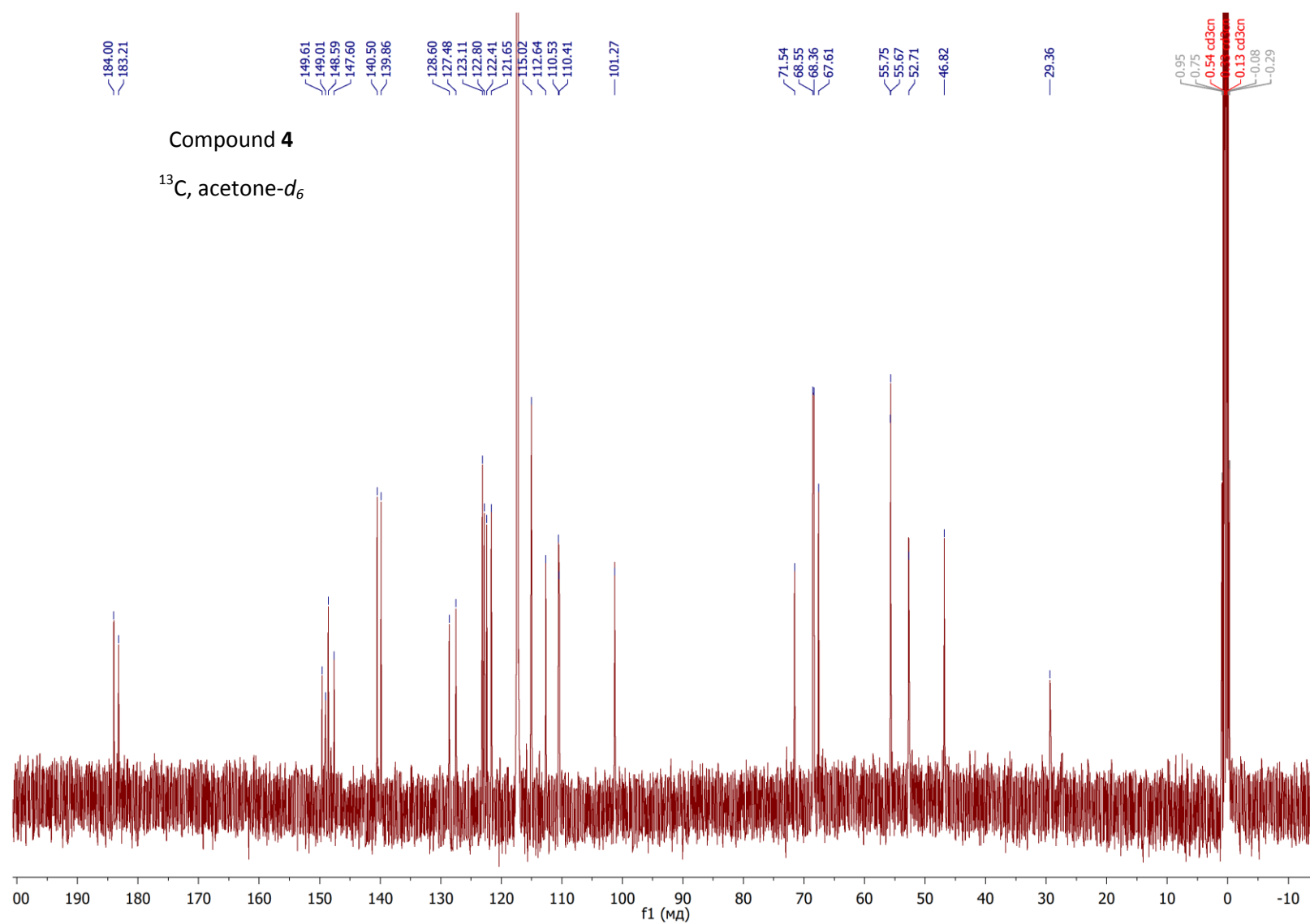


Figure S12. ^{13}C NMR spectrum of compound **4**

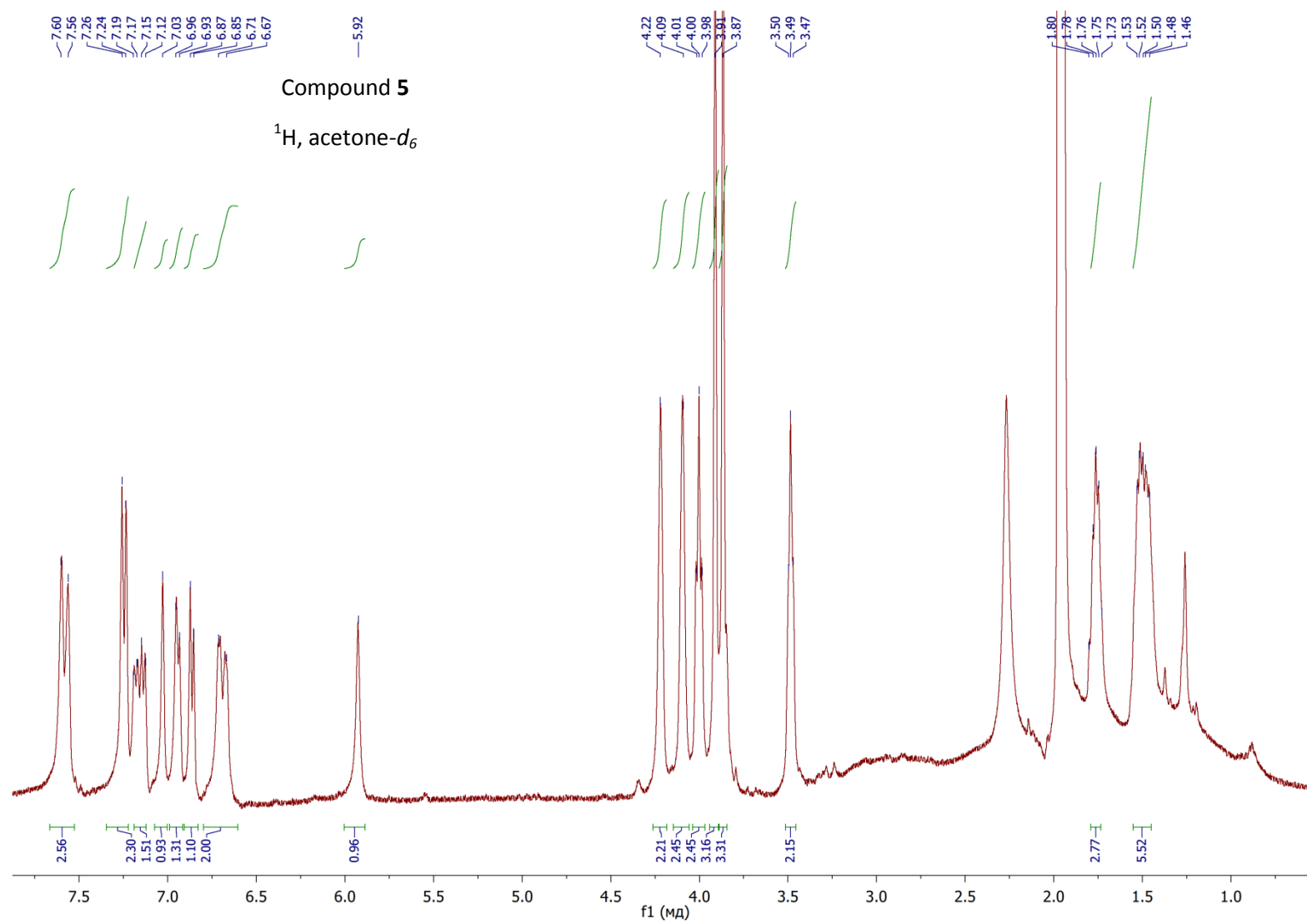


Figure S13. ^1H NMR spectrum of compound **5**

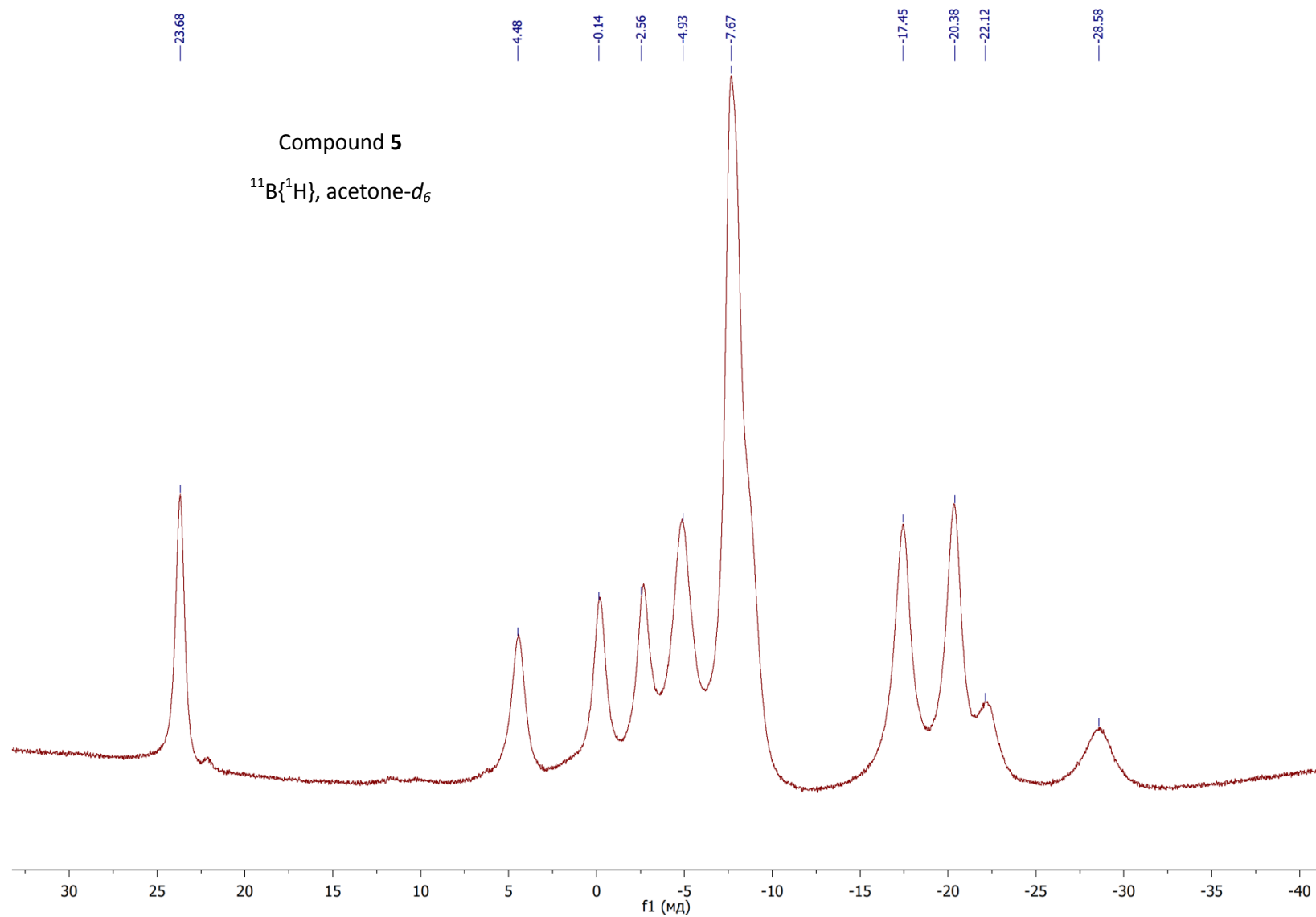


Figure S14. $^{11}\text{B}\{^1\text{H}\}$ NMR spectrum of compound **5**

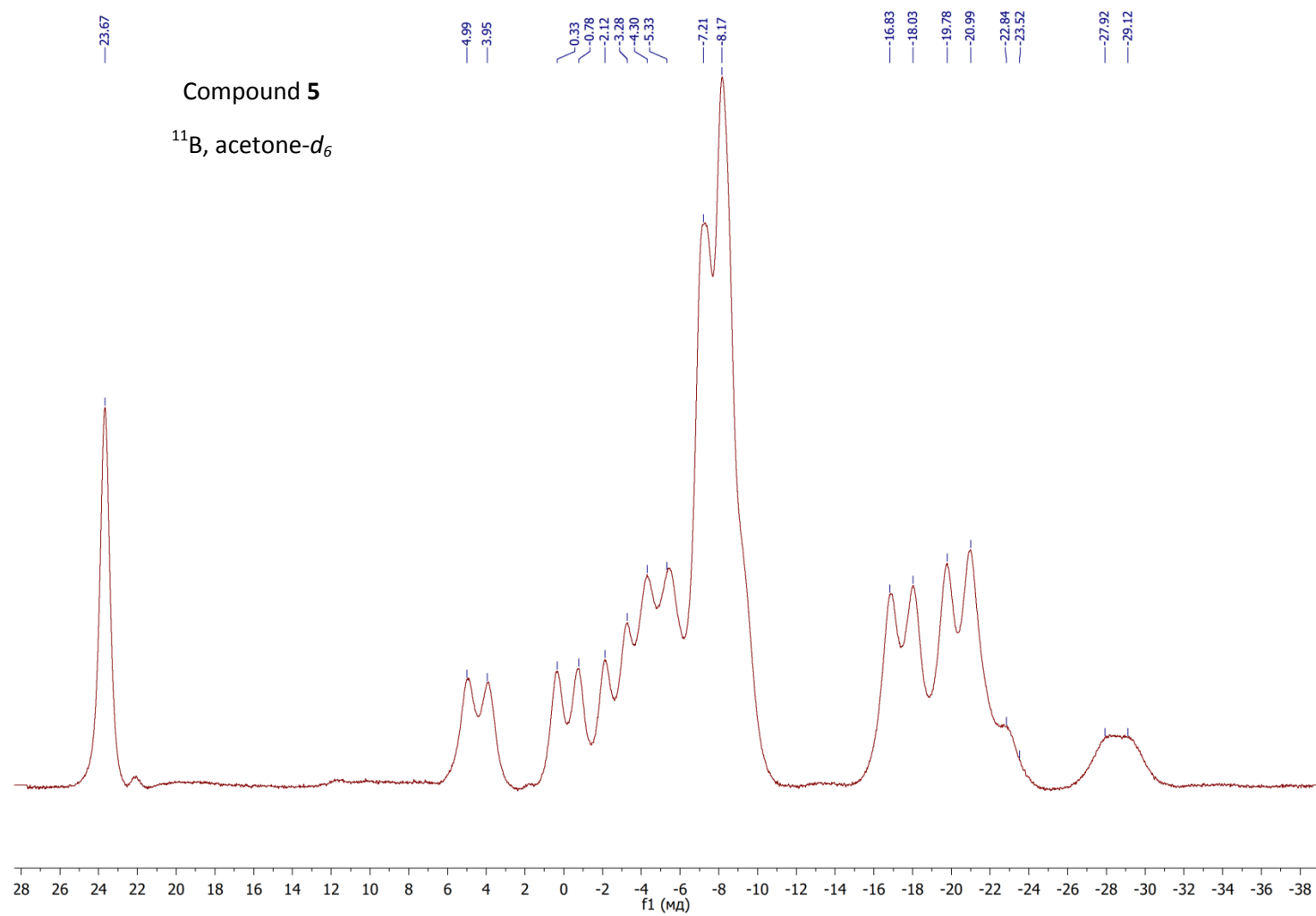


Figure S15. ^{11}B NMR spectrum of compound 5

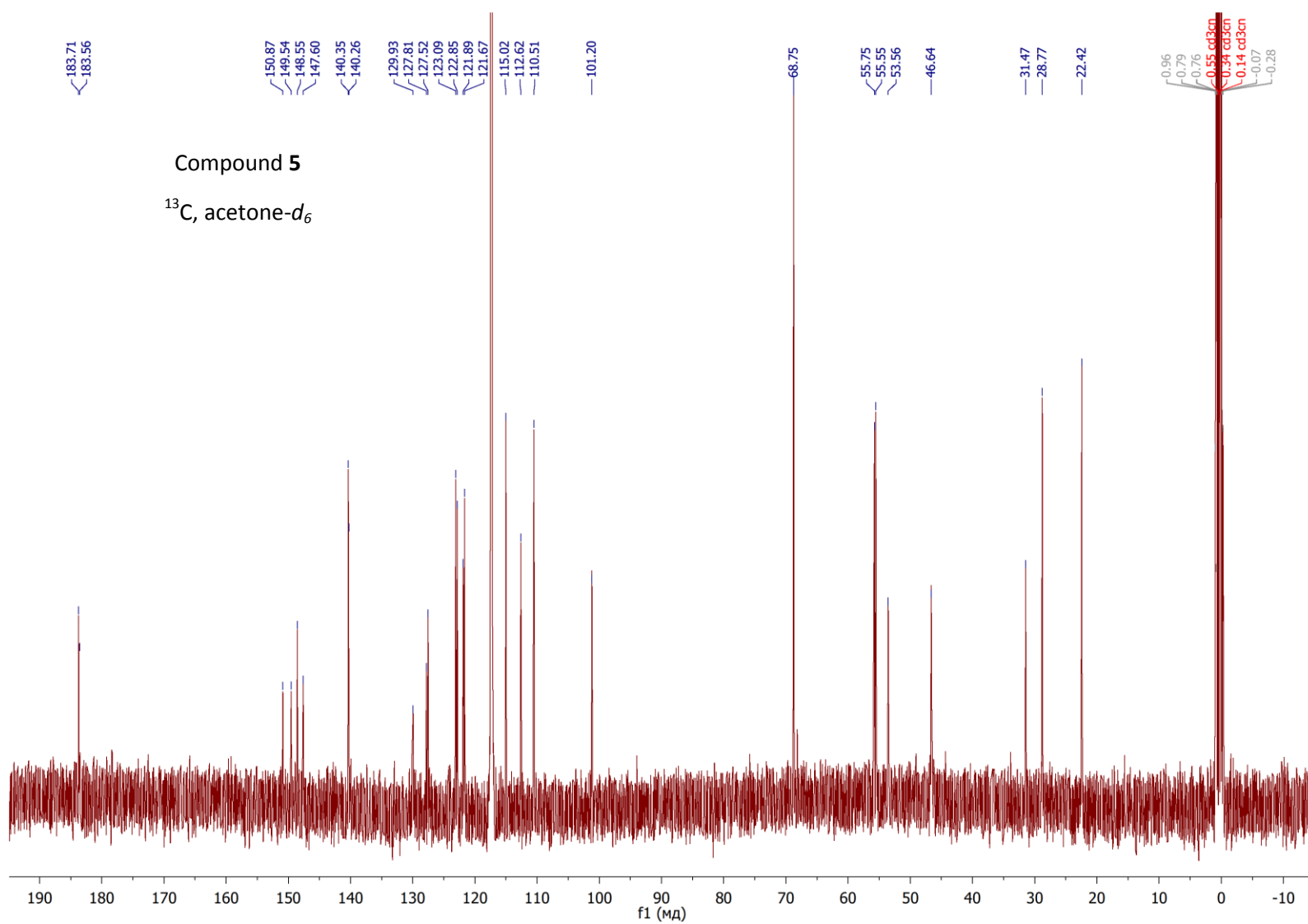


Figure S16. ^{13}C NMR spectrum of compound 5

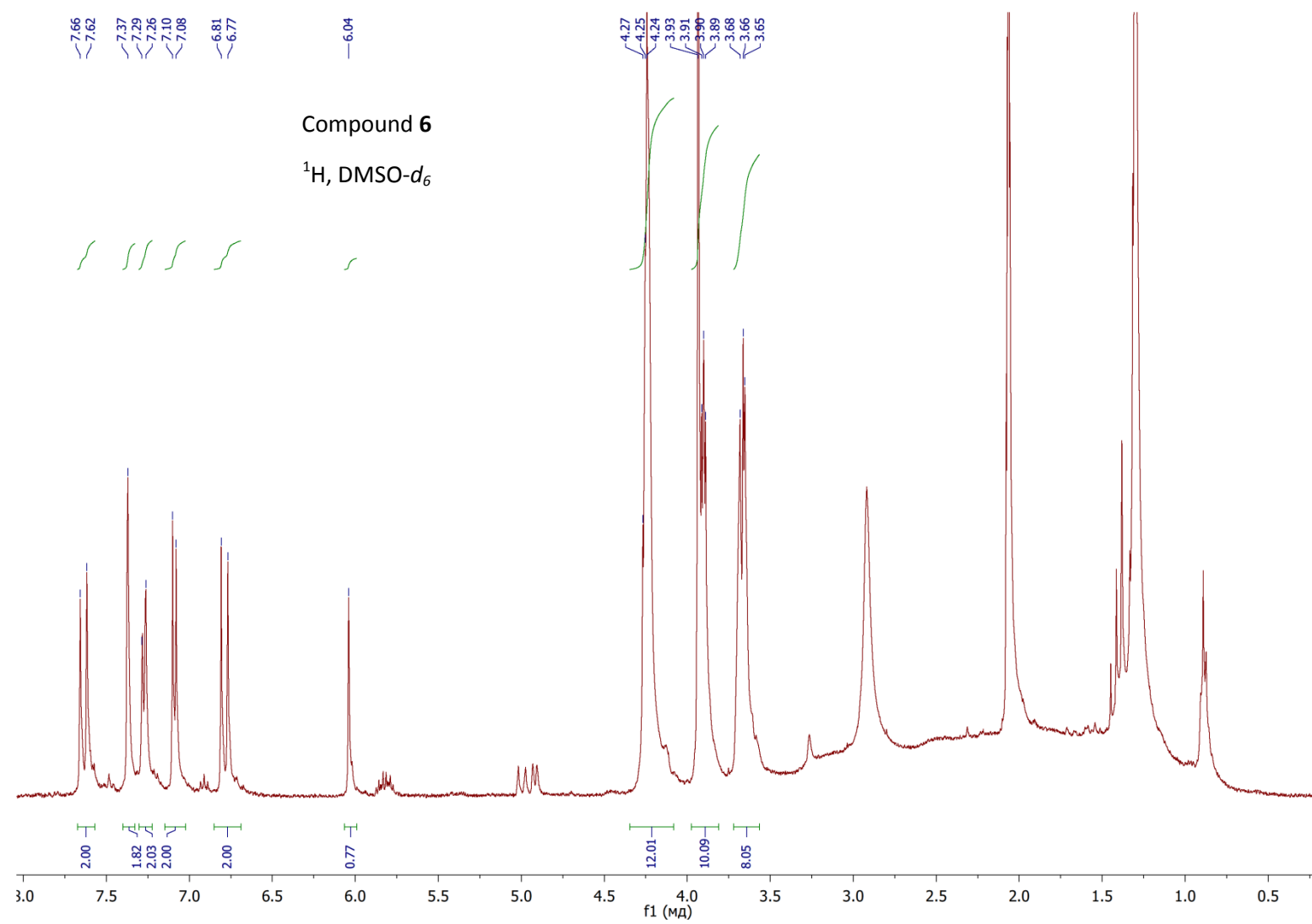


Figure S17. ^1H NMR spectrum of compound **6**

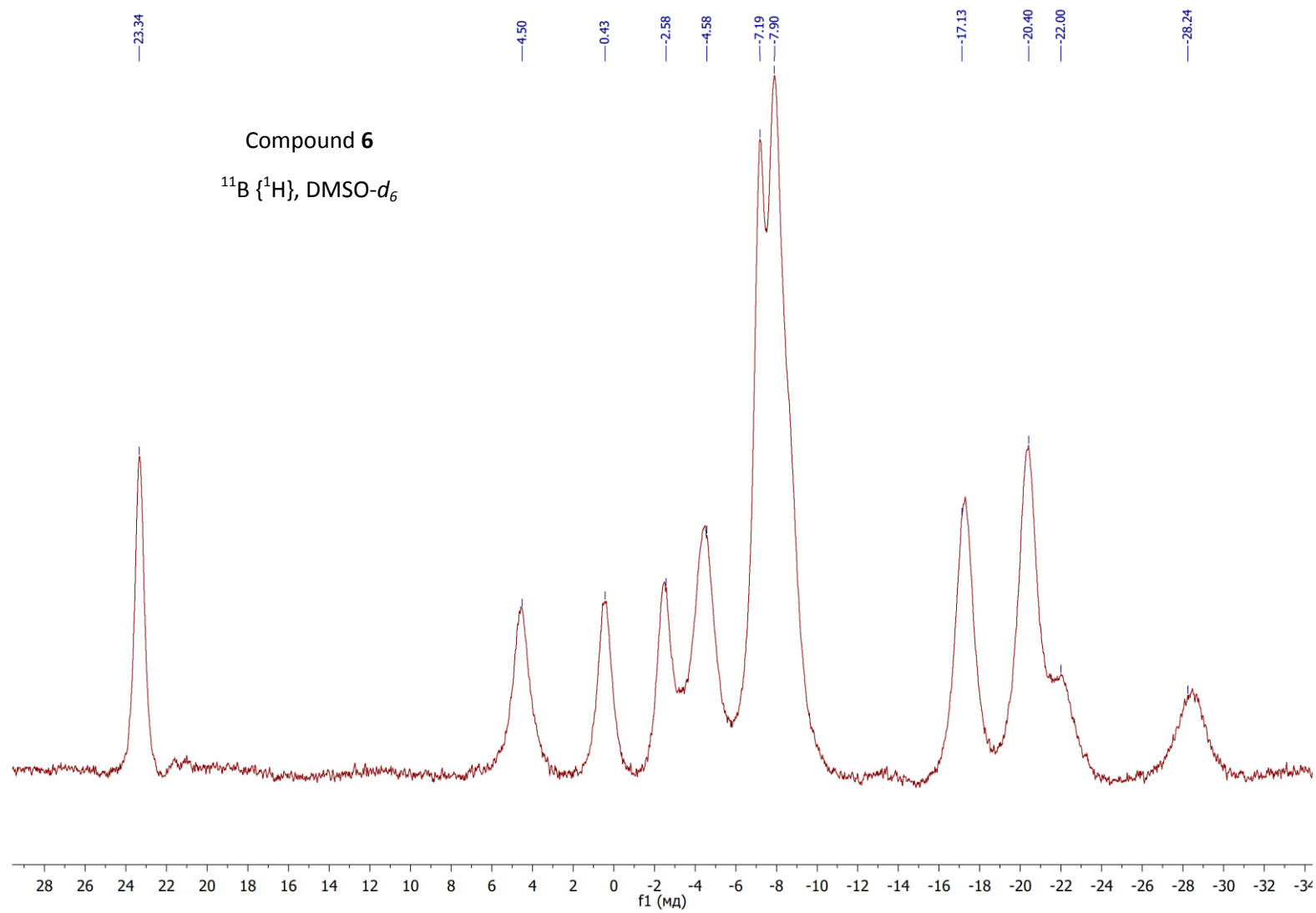


Figure S18. $^{11}\text{B}\{^1\text{H}\}$ NMR spectrum of compound 6

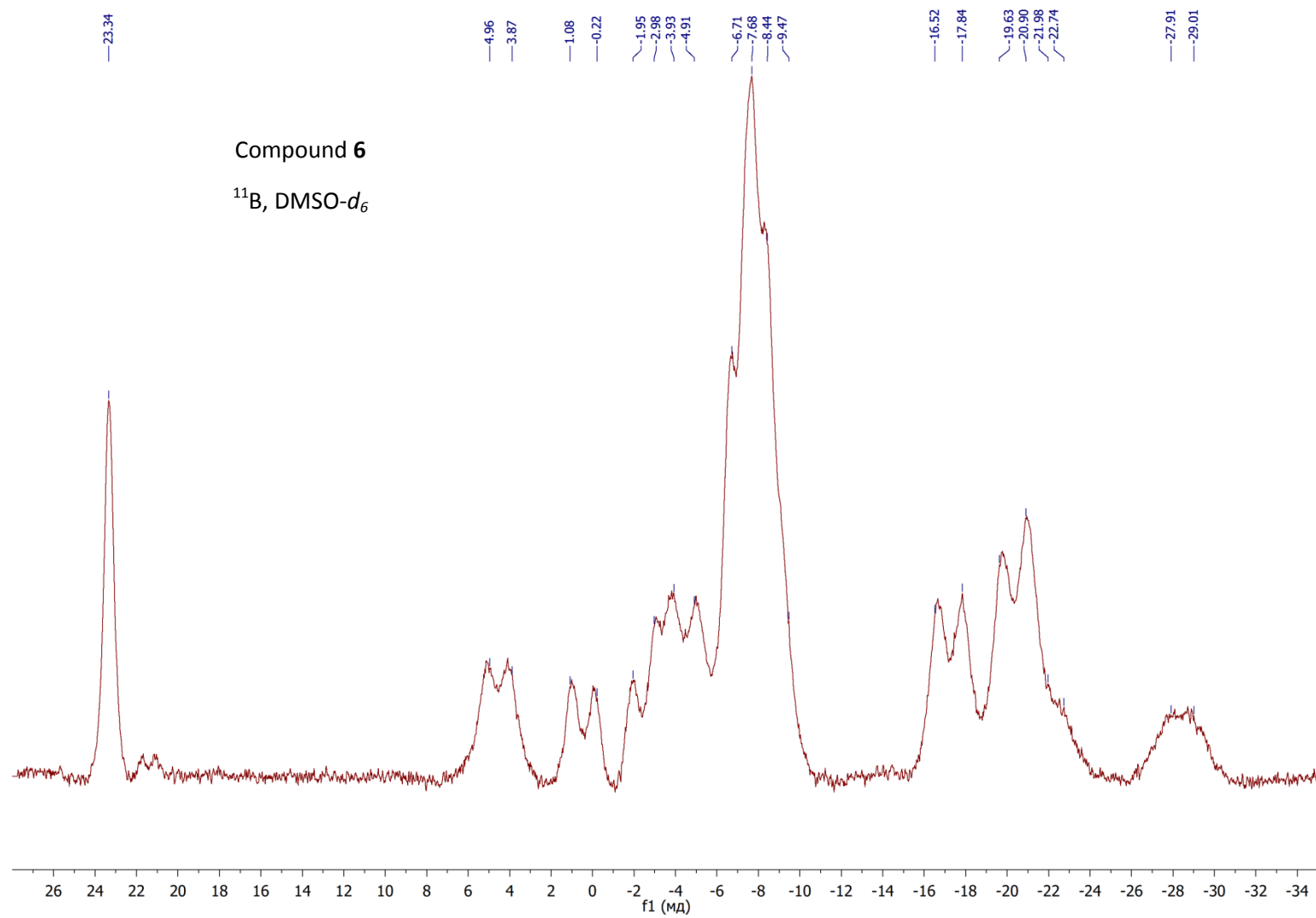


Figure S19. ^{11}B NMR spectrum of compound **6**

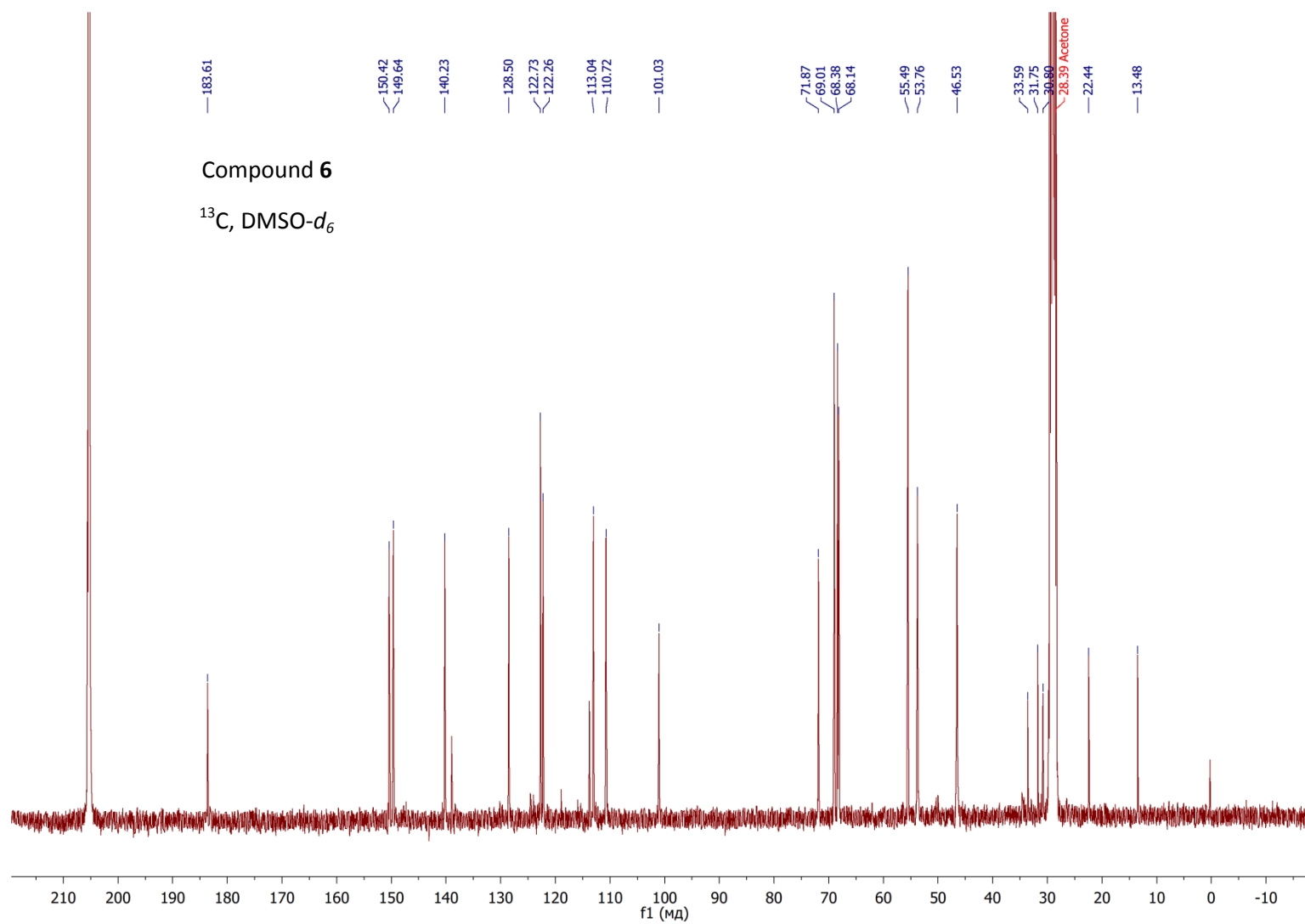


Figure S20. ^{13}C NMR spectrum of compound **6**

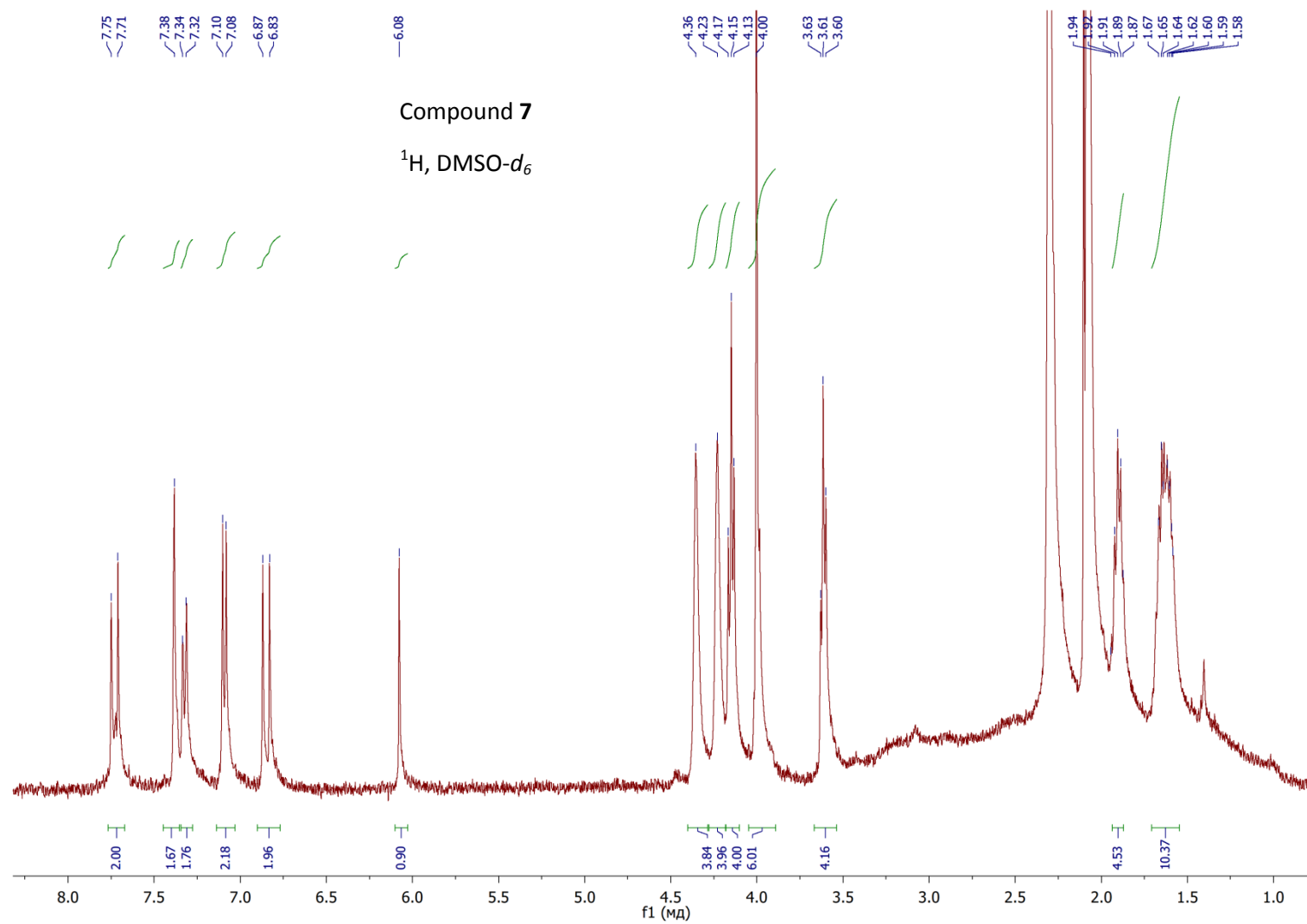


Figure S21. ^1H NMR spectrum of compound **7**

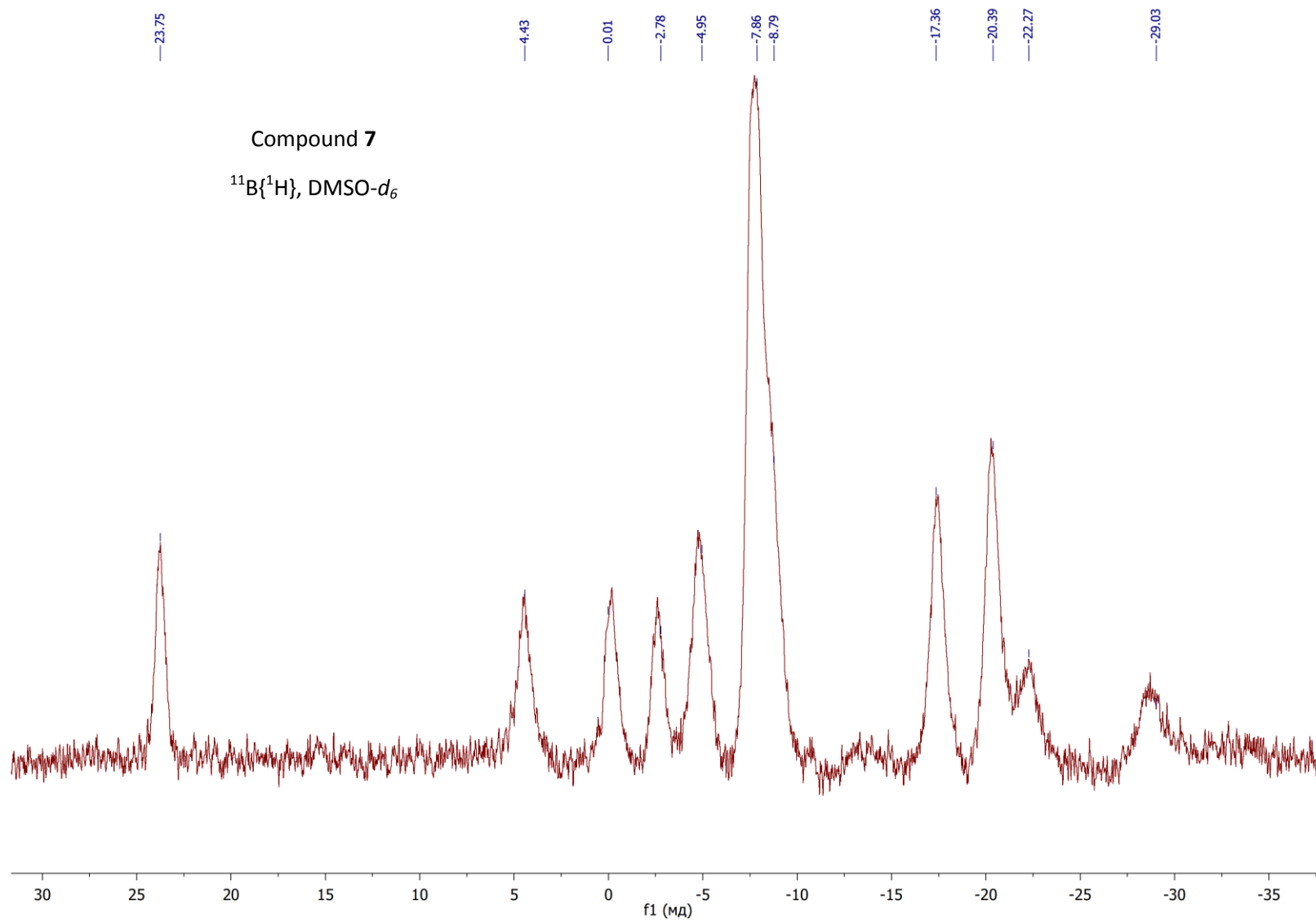


Figure S22. $^{11}\text{B}\{^1\text{H}\}$ NMR spectrum of compound 7

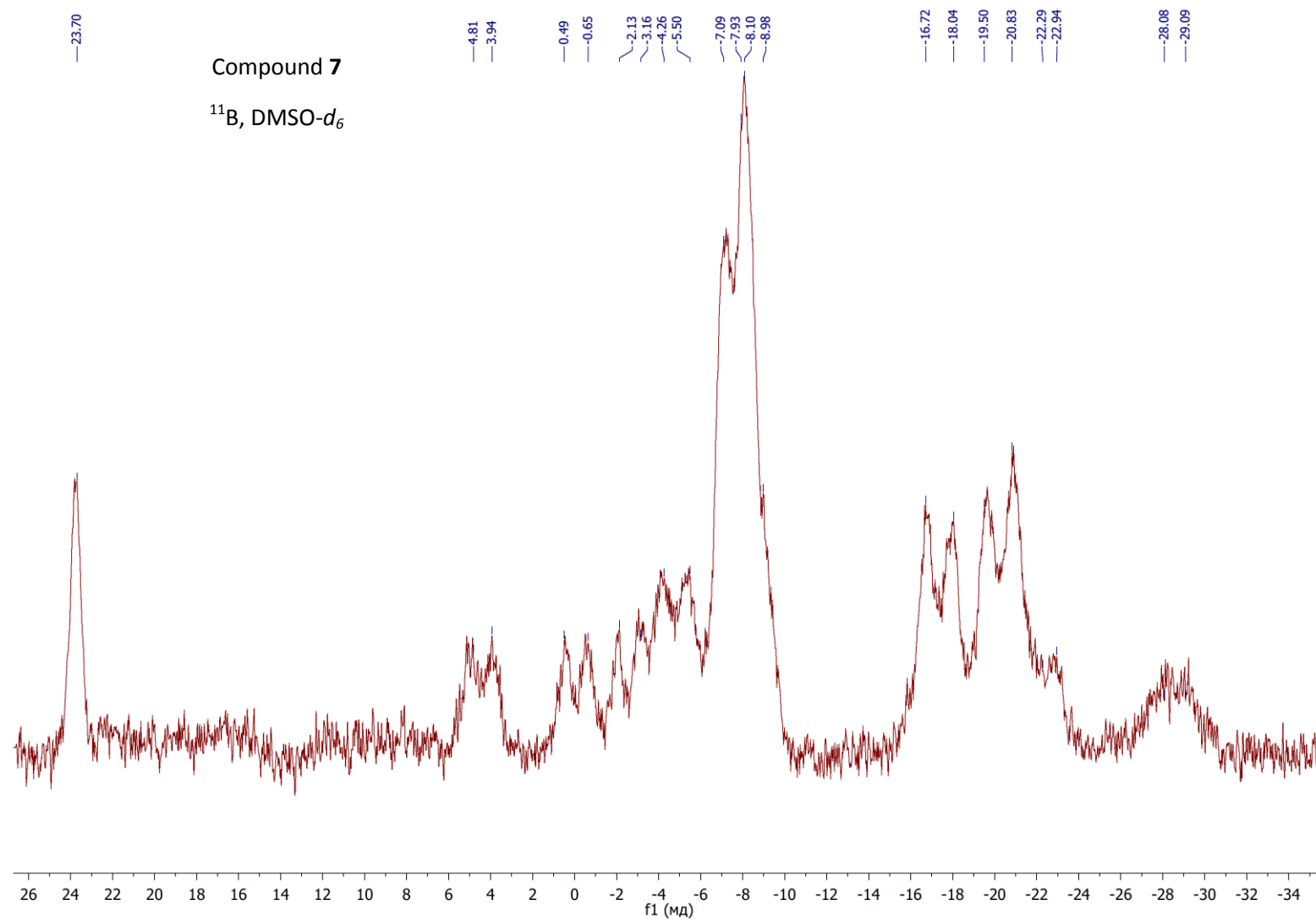


Figure S23. ^{11}B NMR spectrum of compound **7**

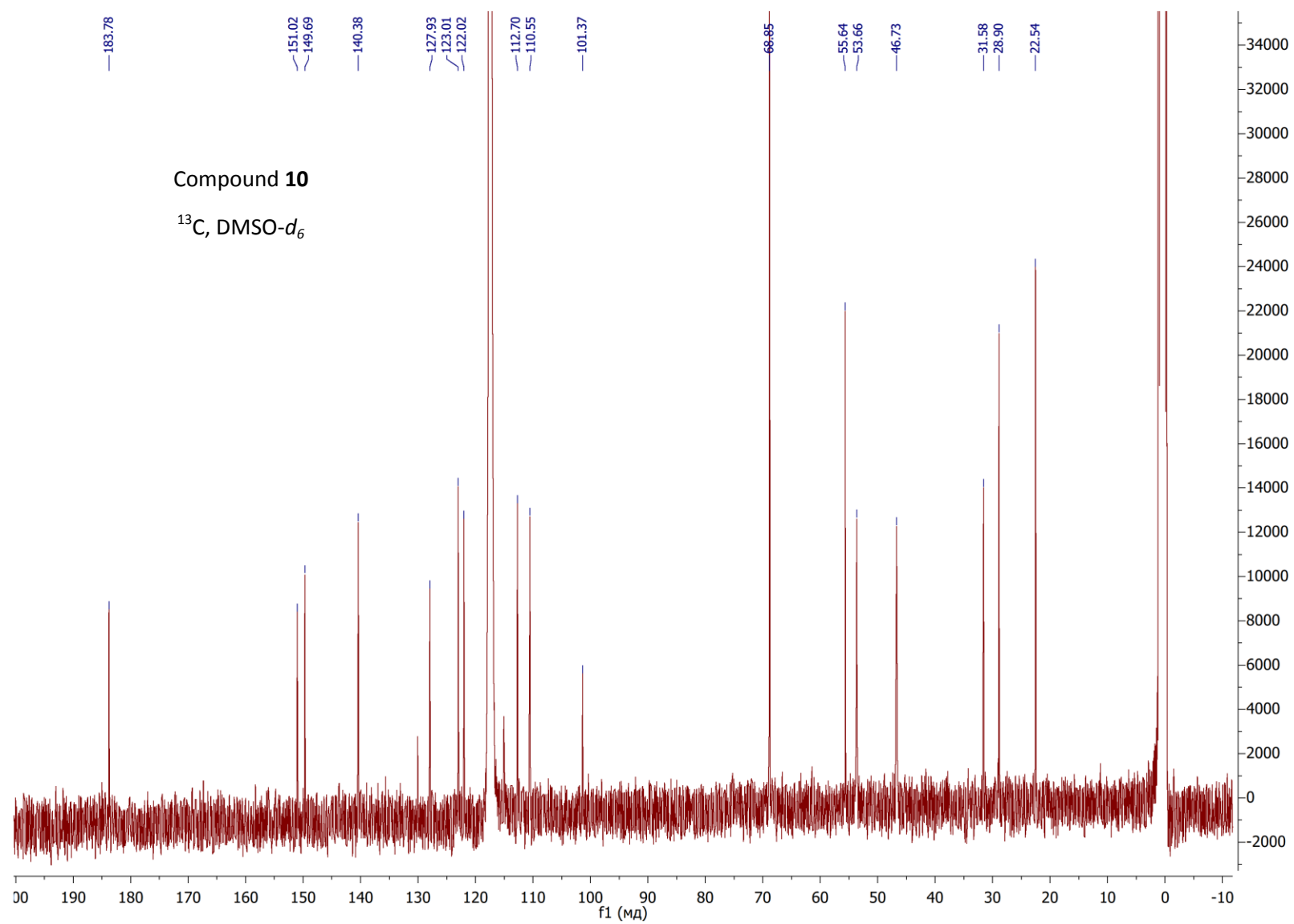


Figure S24. ^{13}C NMR spectrum of compound 7