

## SUPPORTING INFORMATION

### New Boron Containing Acridines: Synthesis and Preliminary Biological Study

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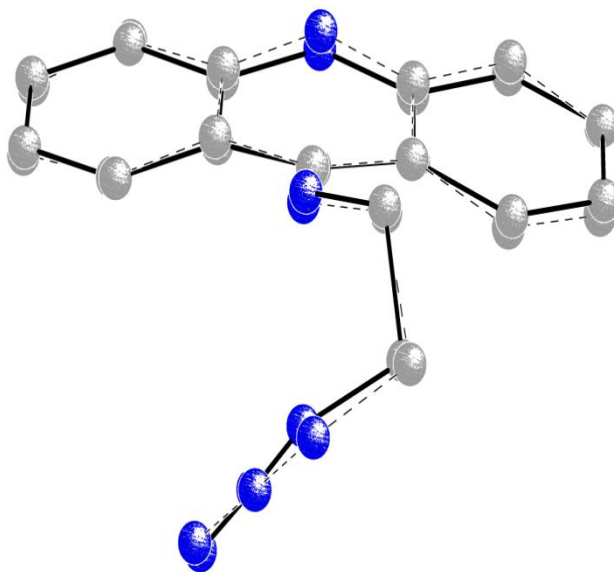
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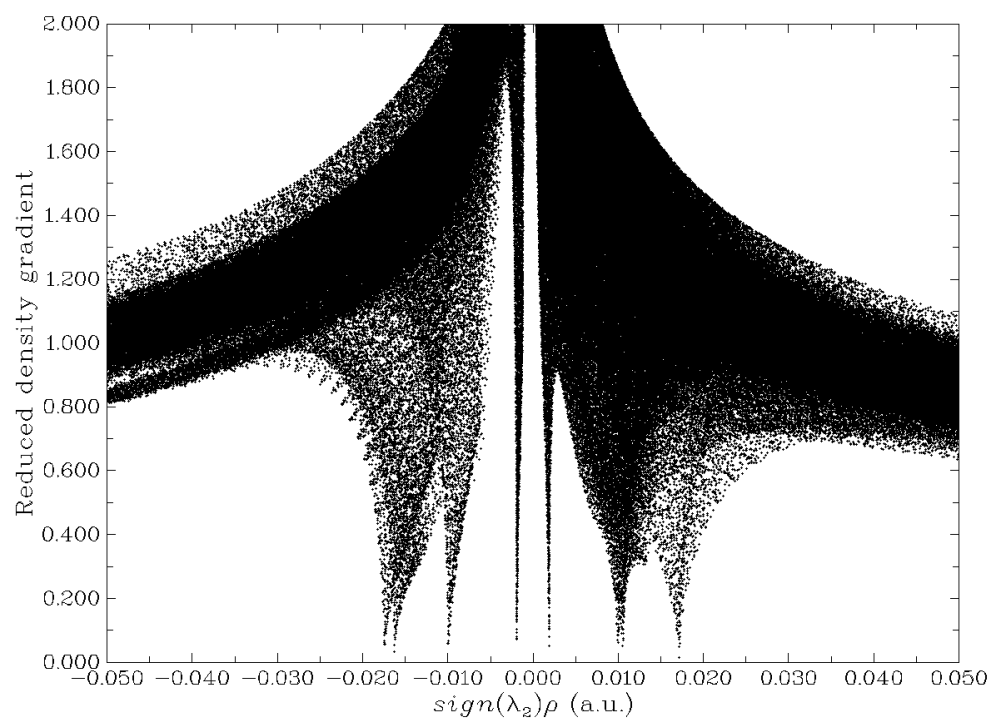
<sup>5</sup> Basic Department of Chemistry of Innovative Materials and Technologies, G.V. Plekhanov Russian University of Economics, 36 Stremyannyi Line, Moscow 117997, Russia; sivaev@ineos.ac.ru (I.B.S.).

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† Dedicated to John Kennedy on the occasion of his 80th Jubilee and in recognition of his outstanding contributions to inorganic and organometallic chemistry.

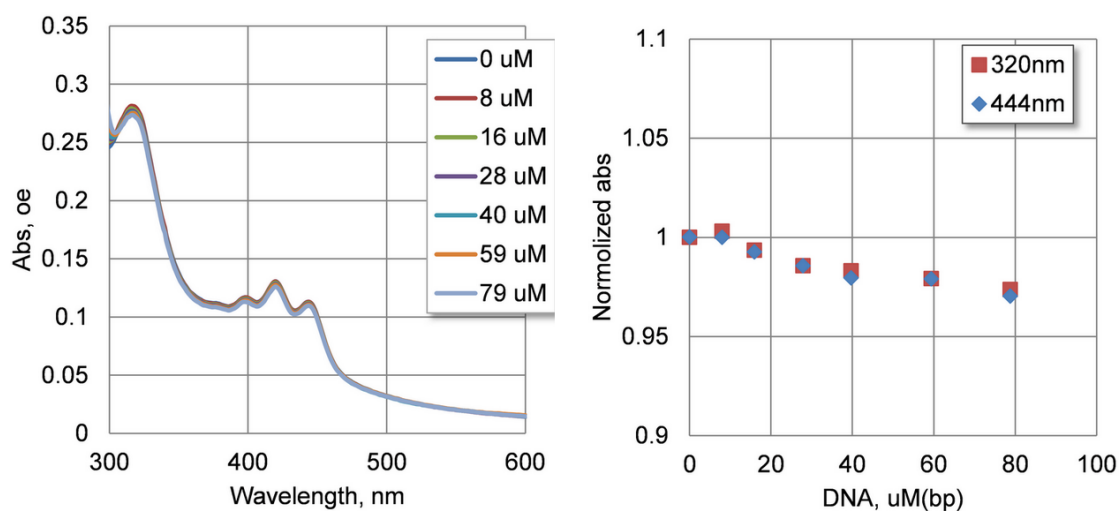


**Figure S1.** The best root-mean-square overlap for the isolated optimized (full lines) and crystal (dashed lines) structure of the substituted acridinium cation from **2**.

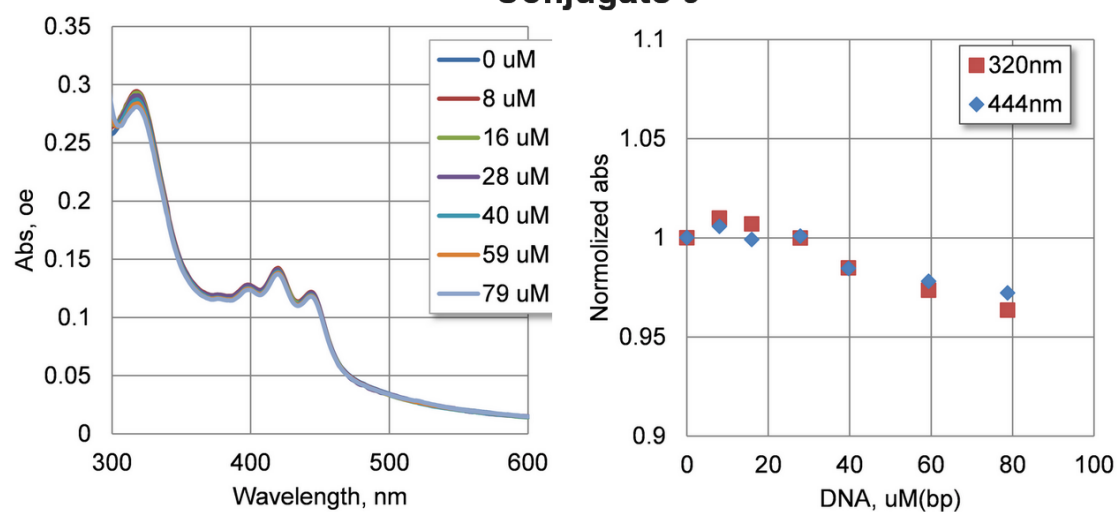


**Figure S2.** The  $\text{RDG}/\text{sign}(\lambda_2)\cdot q(\mathbf{r})$  in the area of substituent in the isolated optimized cation from **2**.

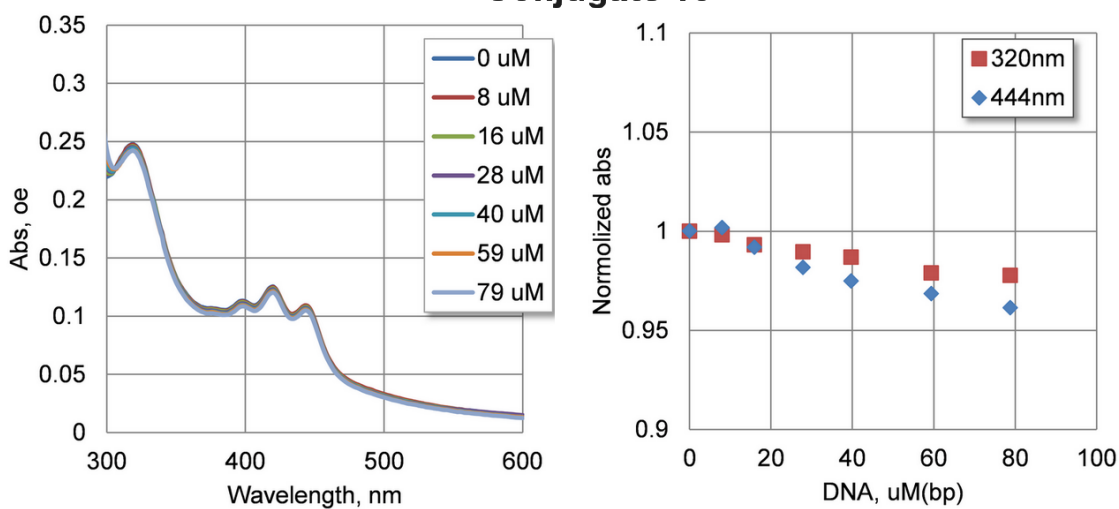
### Conjugate 7



### Conjugate 9



### Conjugate 10



**Figure S3.** Changes of absorbance spectra upon DNA interaction for conjugates 7,9,10. 5 mkM compounds in 10 mM potassium phosphate buffer pH=8.0 and a calf thymus DNA in the range 0-80  $\mu\text{M}$  (b.p.).

$^1\text{H}$ ,  $^{11}\text{B}\{^1\text{H}\}$ ,  $^{11}\text{B}$  and  $^{13}\text{C}\{^1\text{H}\}$  NMR, IR and high-resolution mass spectra of compounds **2**, **7-10**

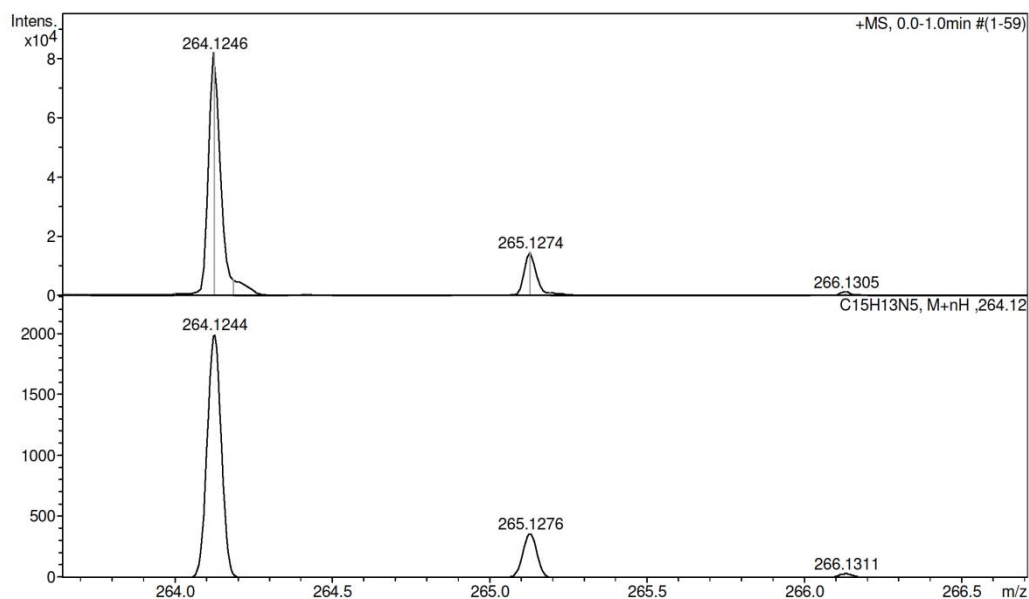
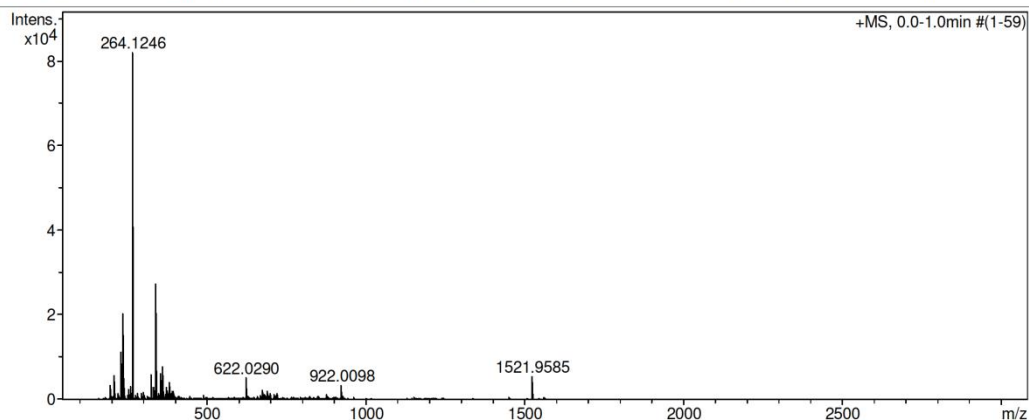
## Display Report

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Sample Name	/CHIZ DA-059	Instrument / Ser#	micrOTOF 10248
Comment	CH <sub>3</sub> CN 100 %, dil. 200, calibrant added		

### Acquisition Parameter

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**Figure S4.** ESI-HRMS spectrum of compound **2**

## Display Report

### Analysis Info

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Acquisition Date 18.04.2023 17:40:18

Operator BDAL@DE  
Instrument / Ser# maXis 43

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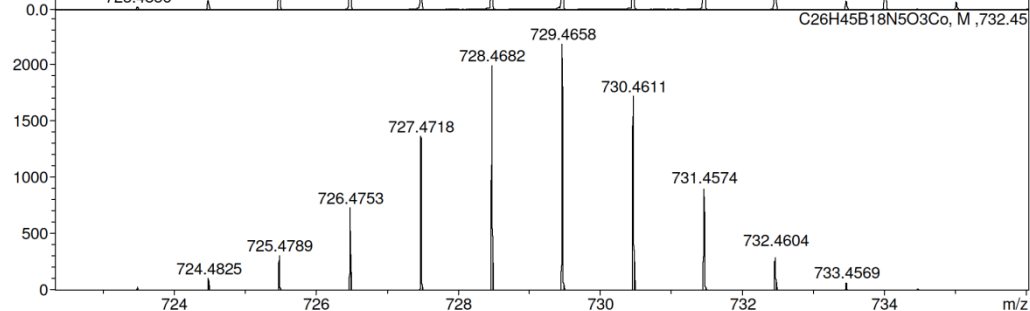
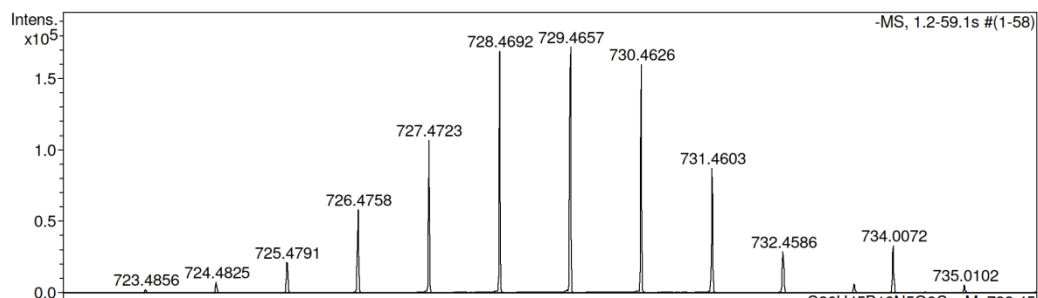
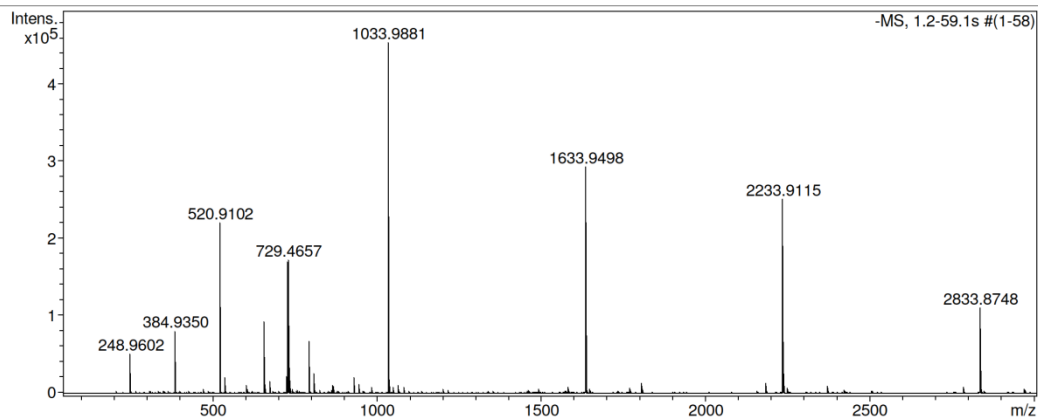


Figure S5. ESI-HRMS spectrum of compound 7

## Display Report

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Acquisition Date 18.04.2023 17:47:37

Operator BDAL@DE  
Instrument / Ser# maXis 43

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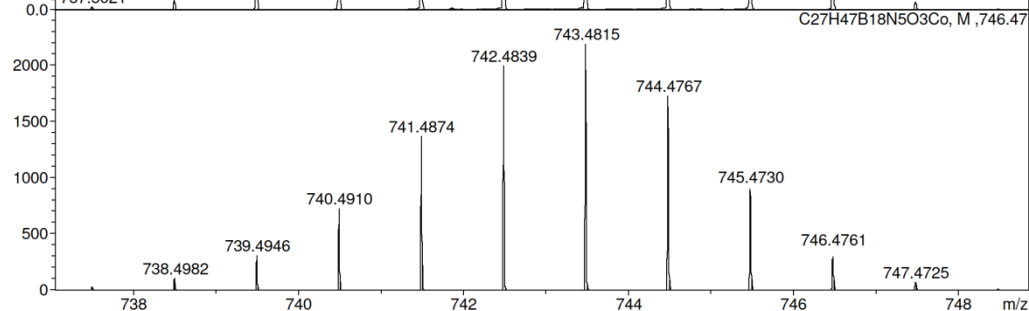
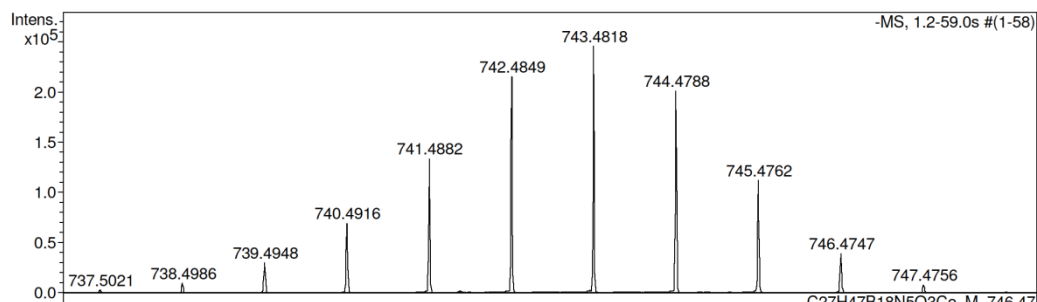
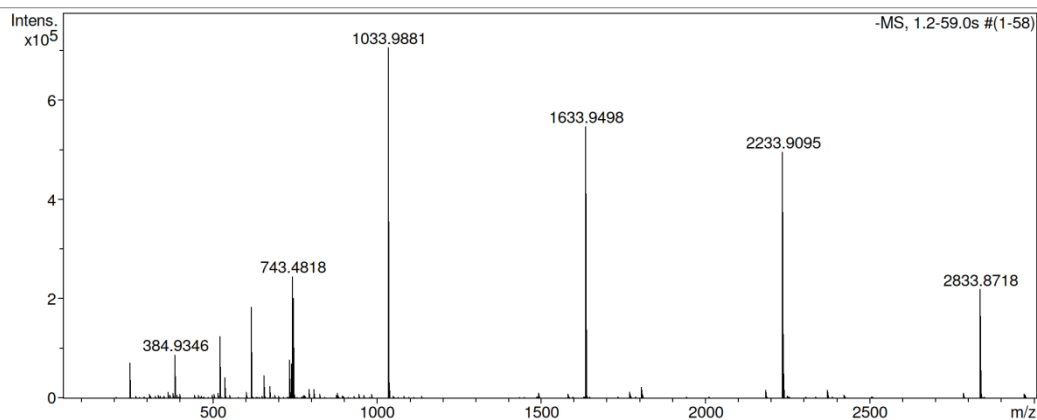


Figure S6. ESI-HRMS spectrum of compound 8

## Display Report

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Acquisition Date 18.04.2023 17:53:03

Operator BDAL@DE  
Instrument / Ser# maXis 43

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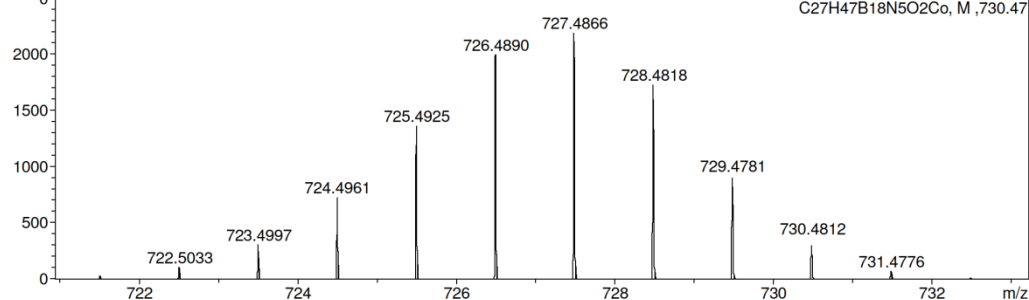
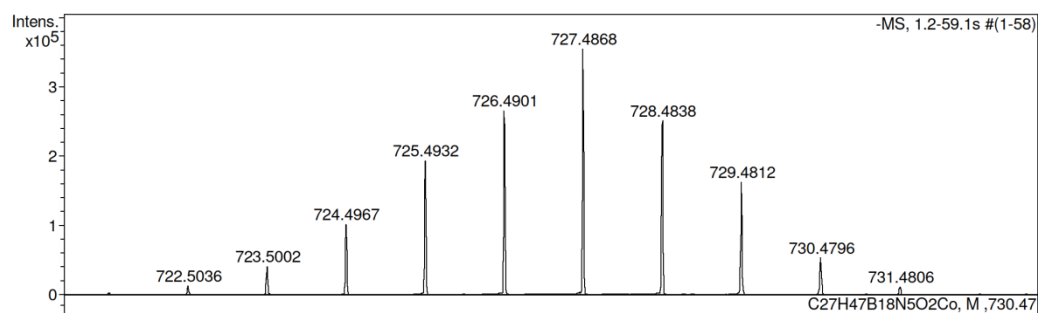
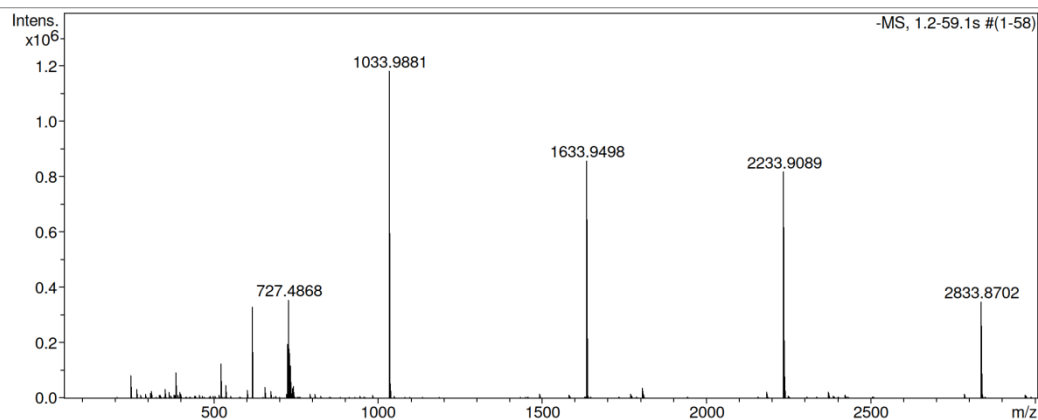


Figure S7. ESI-HRMS spectrum of compound 9

## Display Report

### Analysis Info

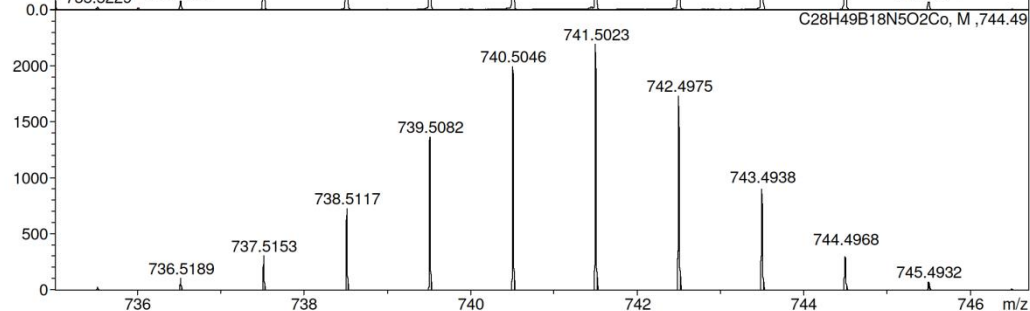
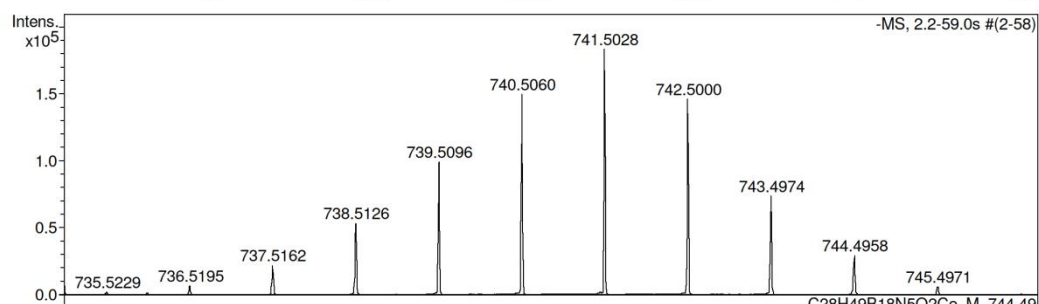
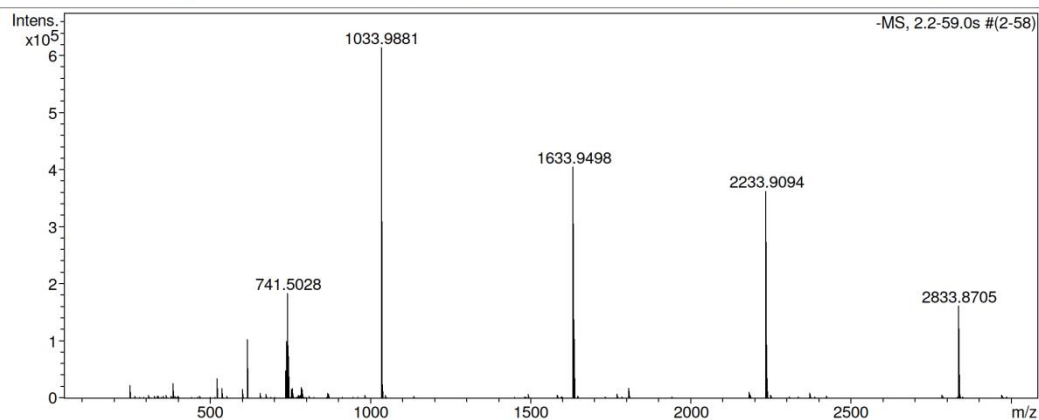
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Acquisition Date 18.04.2023 17:59:10

Operator BDAL@DE  
Instrument / Ser# maXis 43

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Scan Begin	50 m/z	Set Capillary	3000 V	Set Dry Gas	4.0 l/min
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**Figure S8.** ESI-HRMS spectrum of compound 10



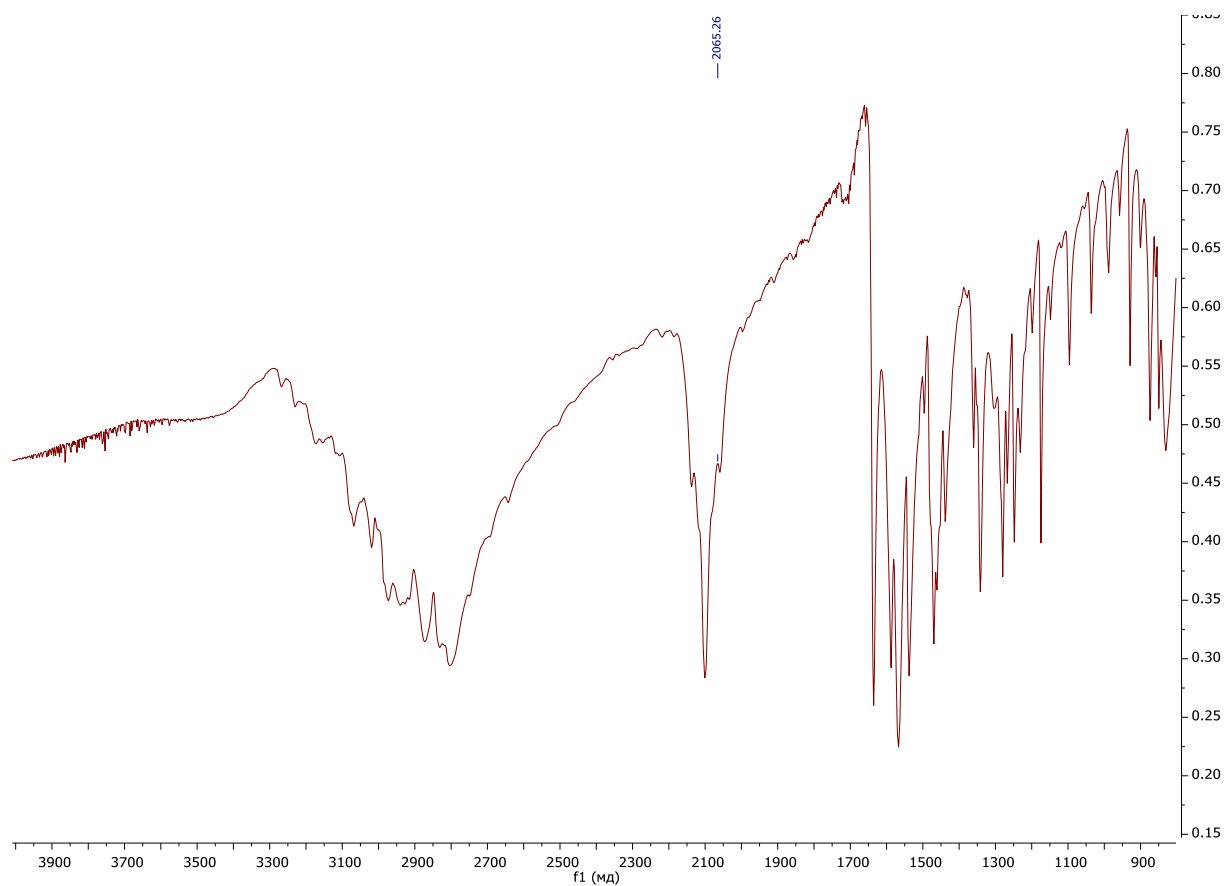


Figure S9. IR spectrum of compound 2

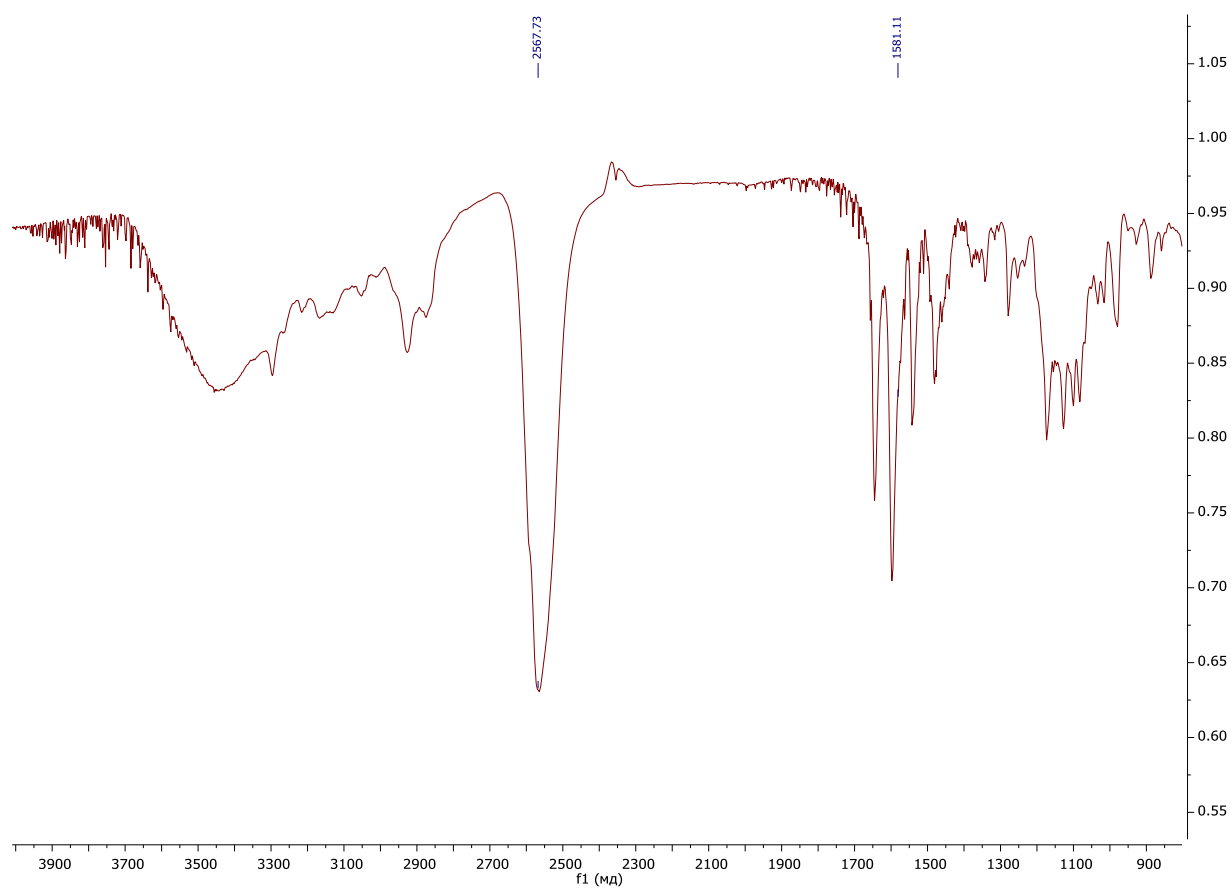
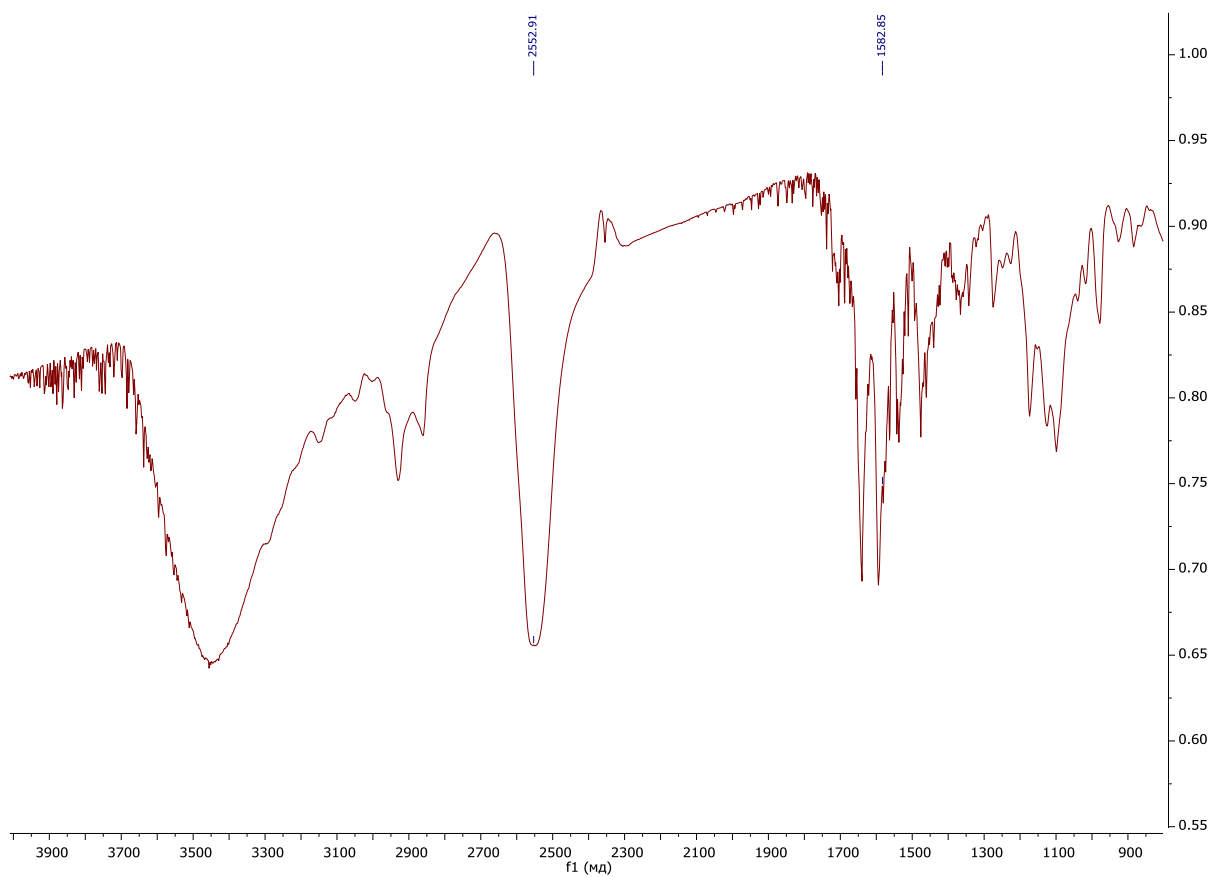
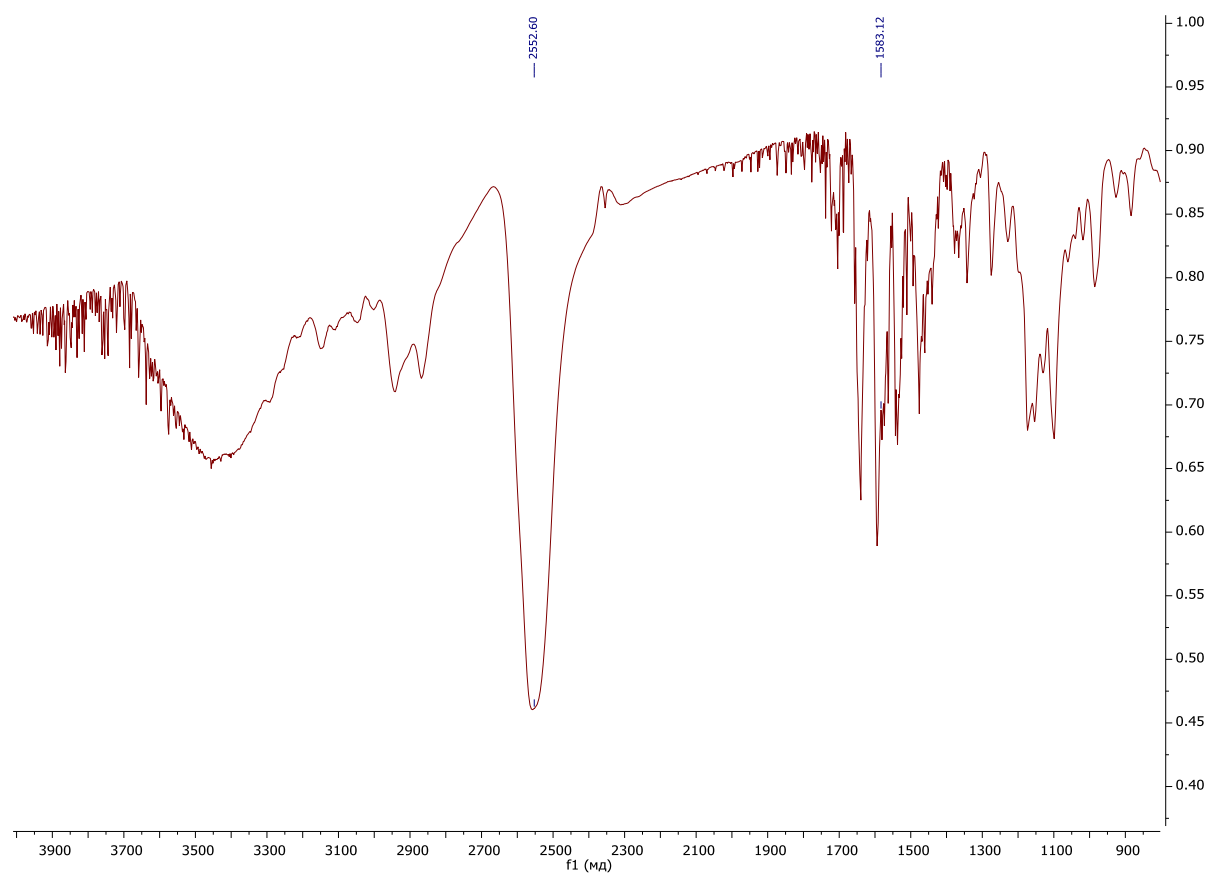


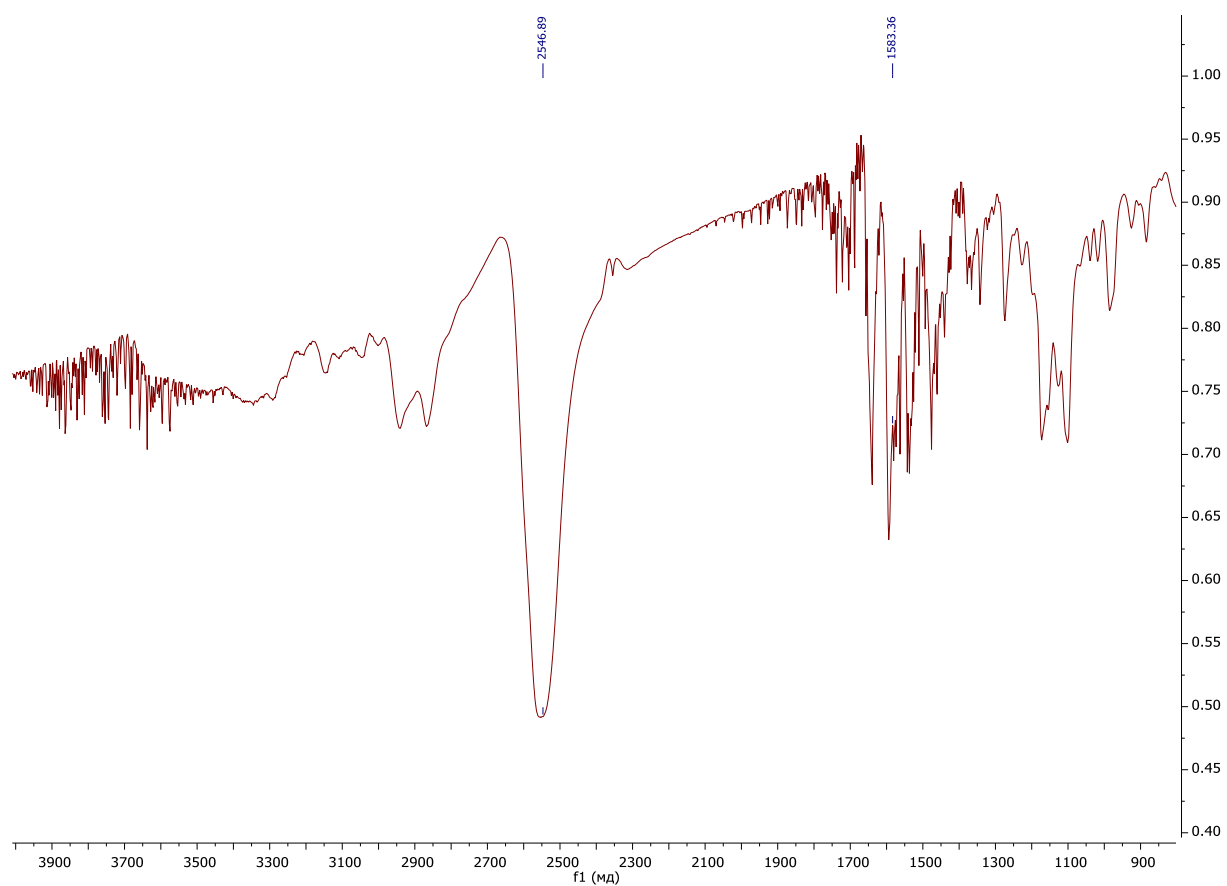
Figure S10. IR spectrum of compound 7



**Figure S11.** IR spectrum of compound **8**



**Figure S12.** IR spectrum of compound **9**



**Figure S13.** IR spectrum of compound **10**

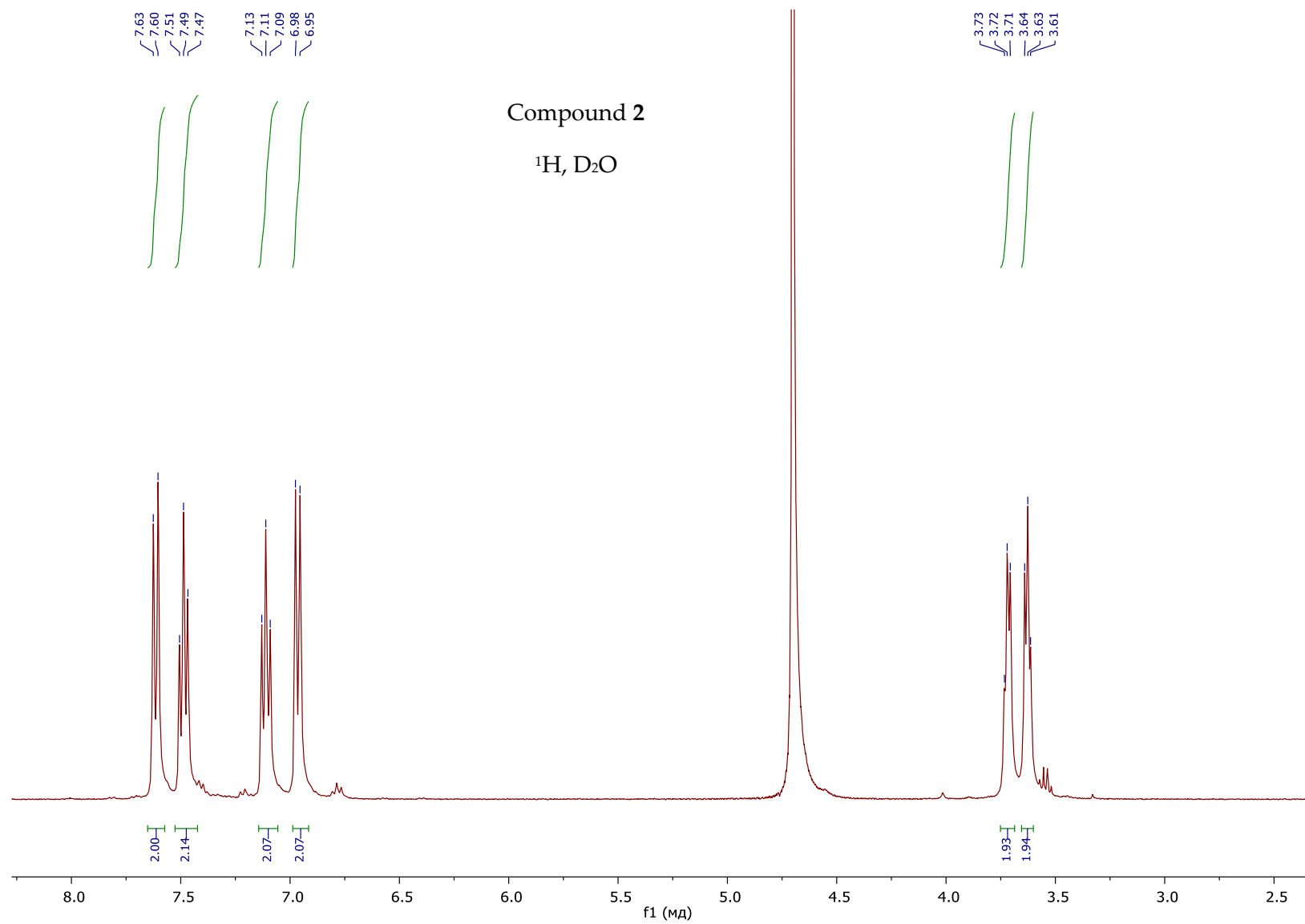


Figure S14.  $^1\text{H}$  NMR spectrum of compound 2

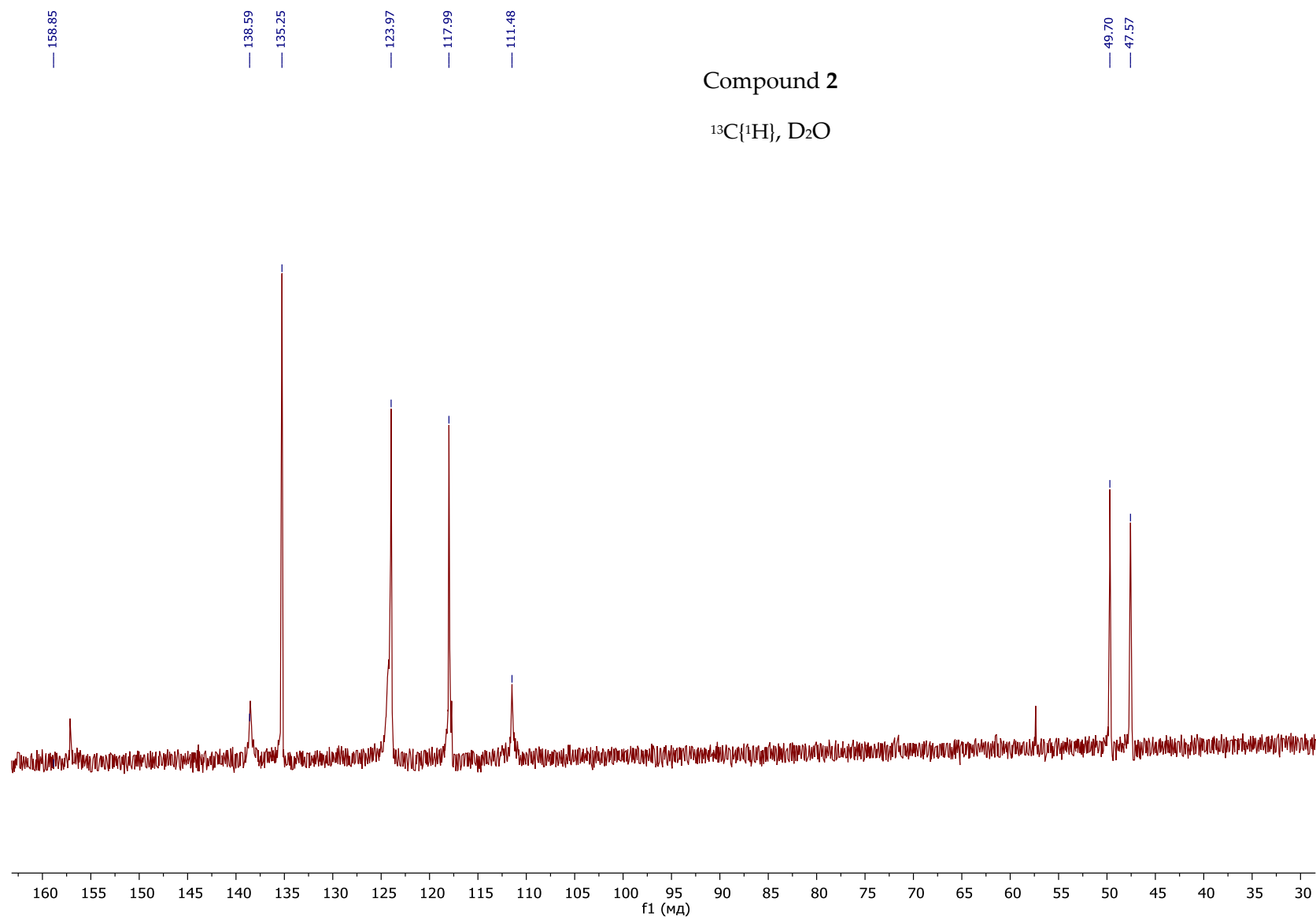


Figure S15.  $^{13}\text{C}\{^1\text{H}\}$  NMR spectrum of compound 2

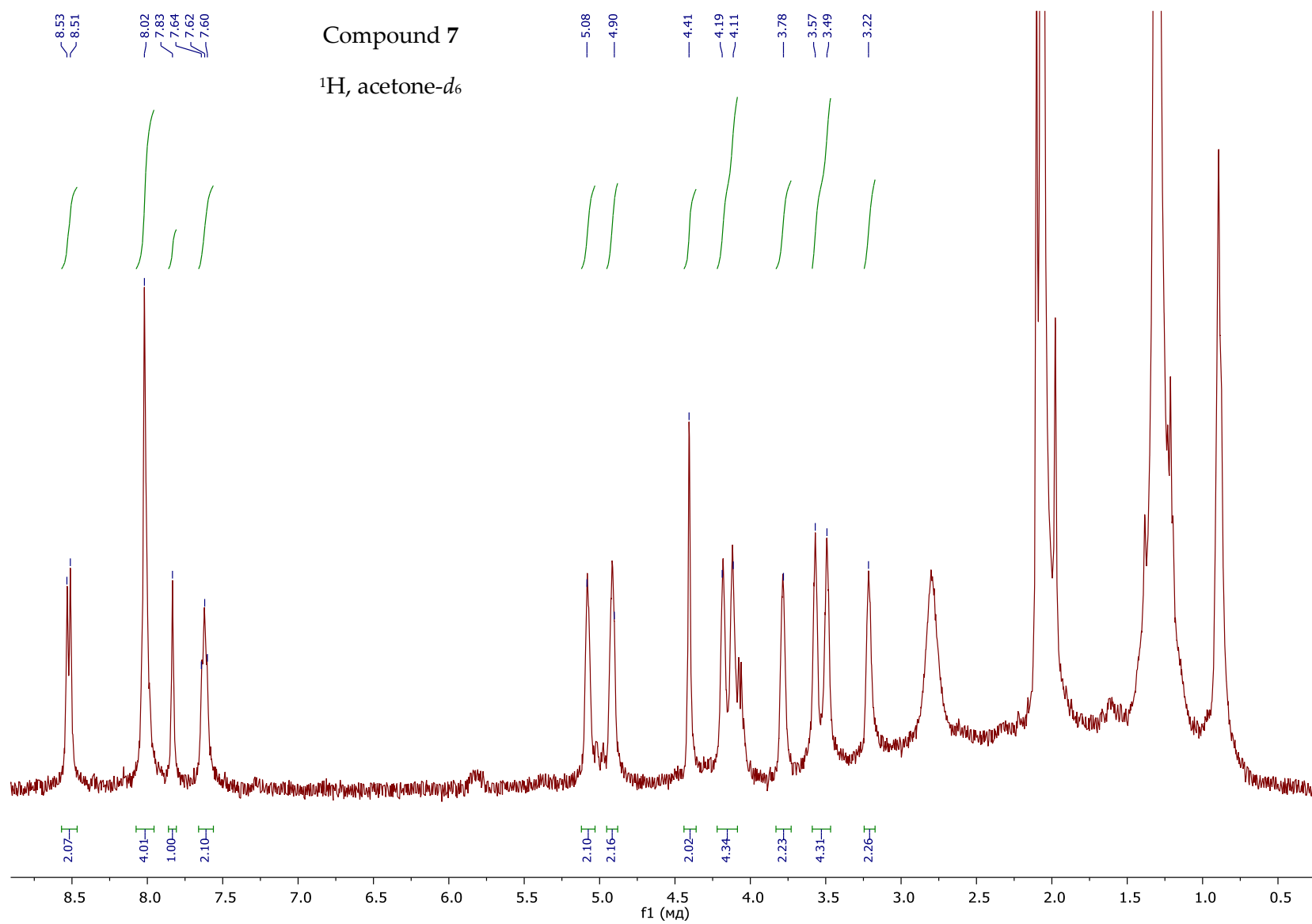
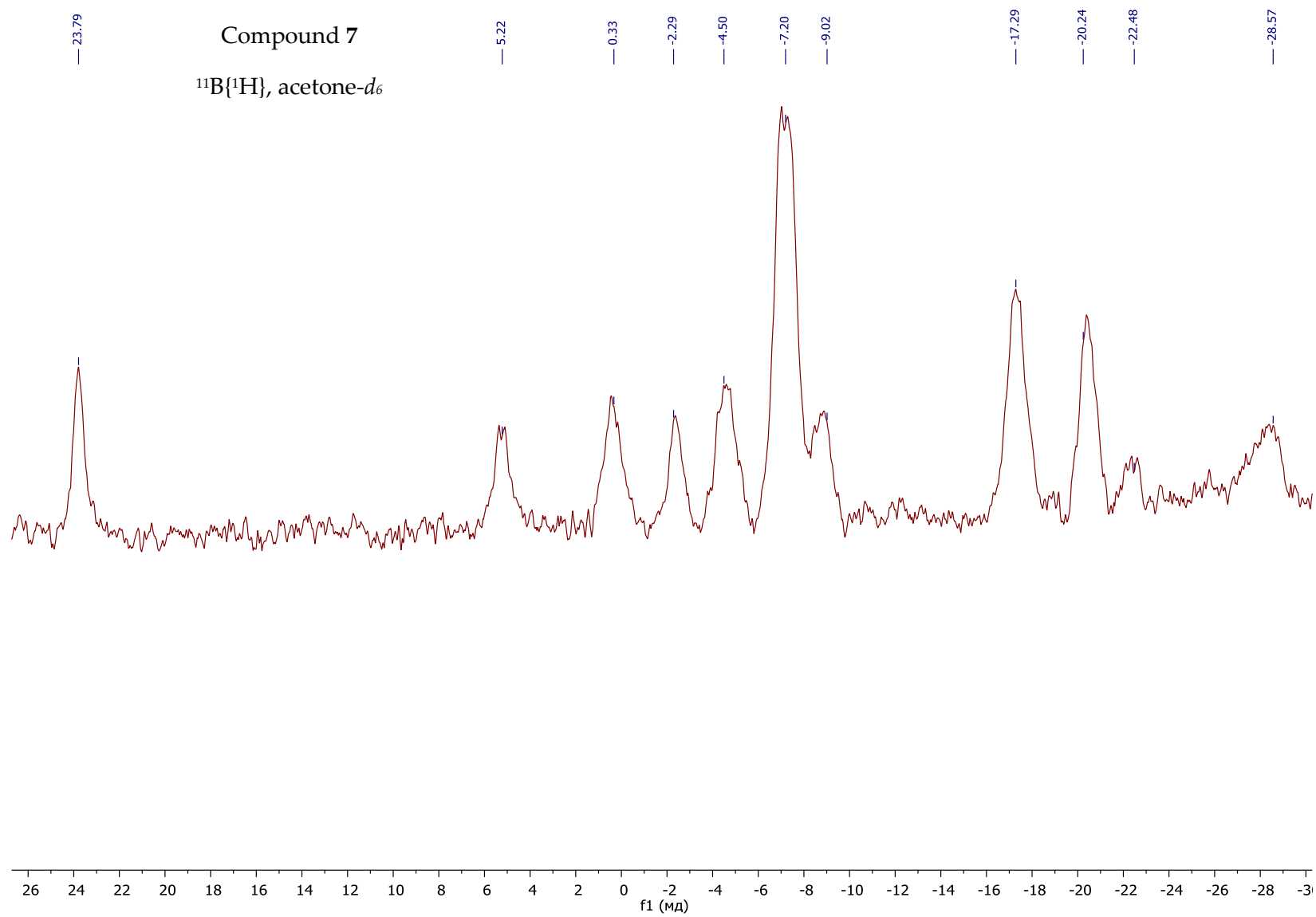


Figure S16.  $^1\text{H}$  NMR spectrum of compound 7



**Figure S17.**  $^{11}\text{B}\{^1\text{H}\}$  NMR spectrum of compound 7

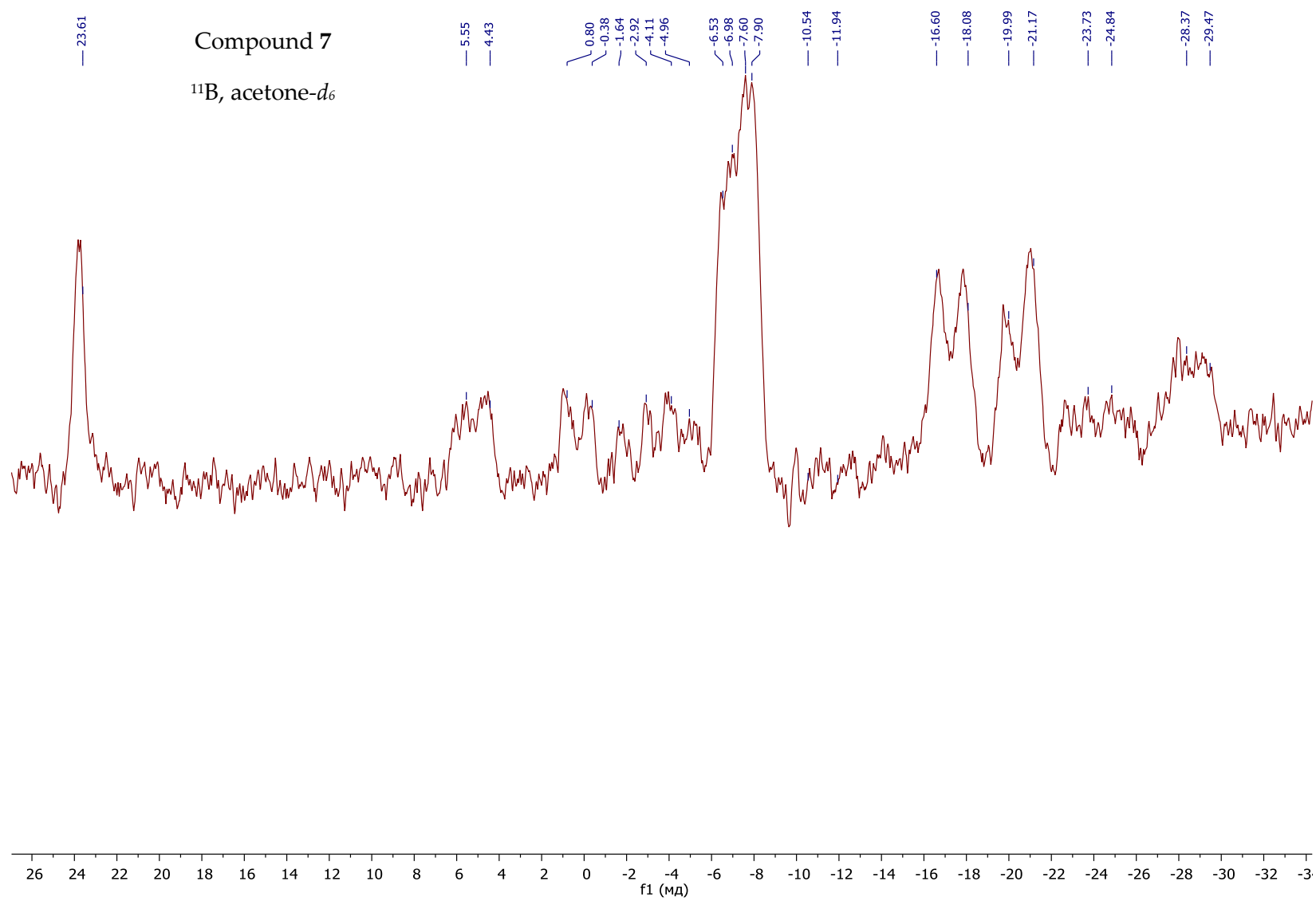


Figure S18.  $^{11}\text{B}$  NMR spectrum of compound 7



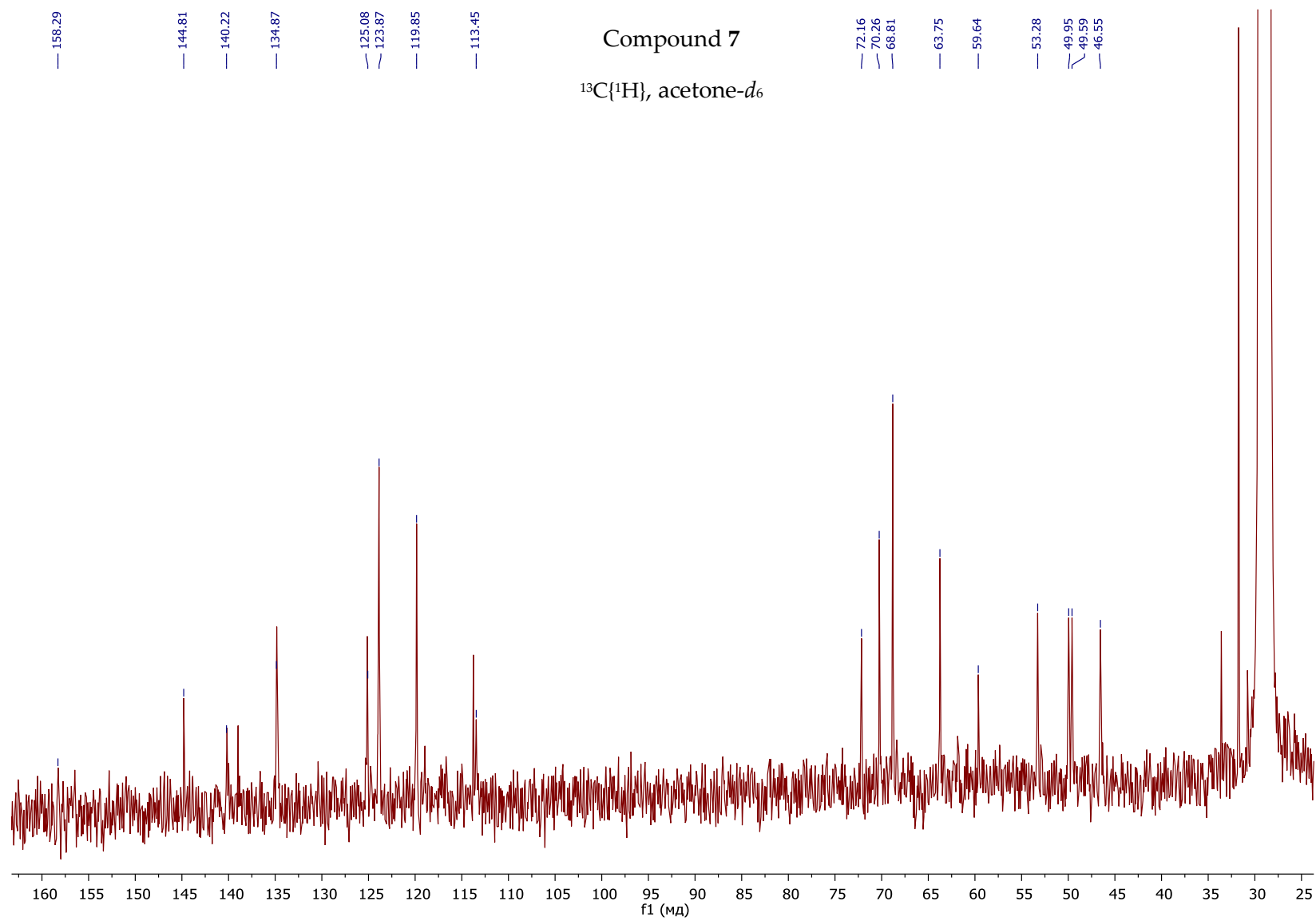


Figure S19.  $^{13}\text{C}\{^1\text{H}\}$  NMR spectrum of compound 7

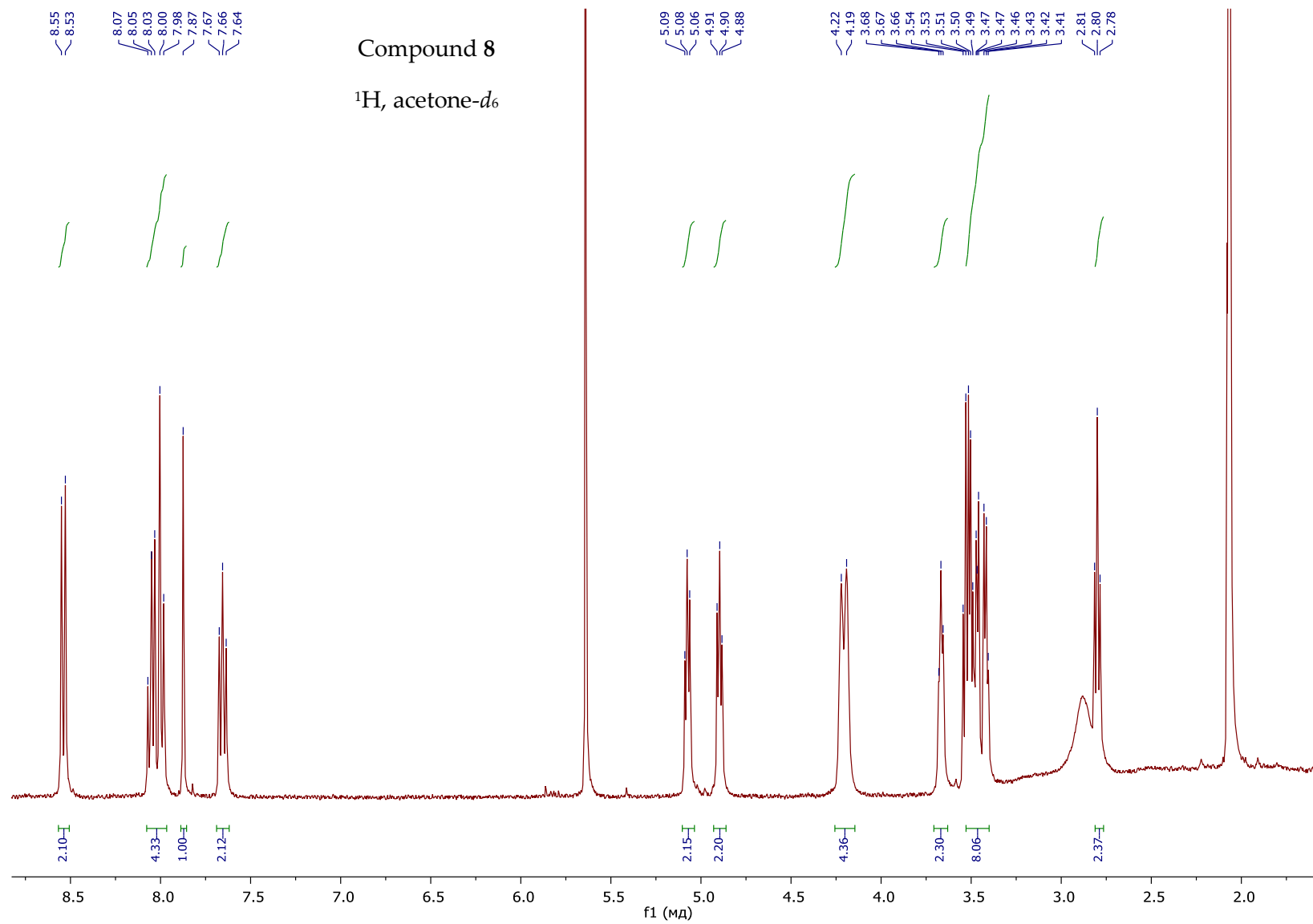
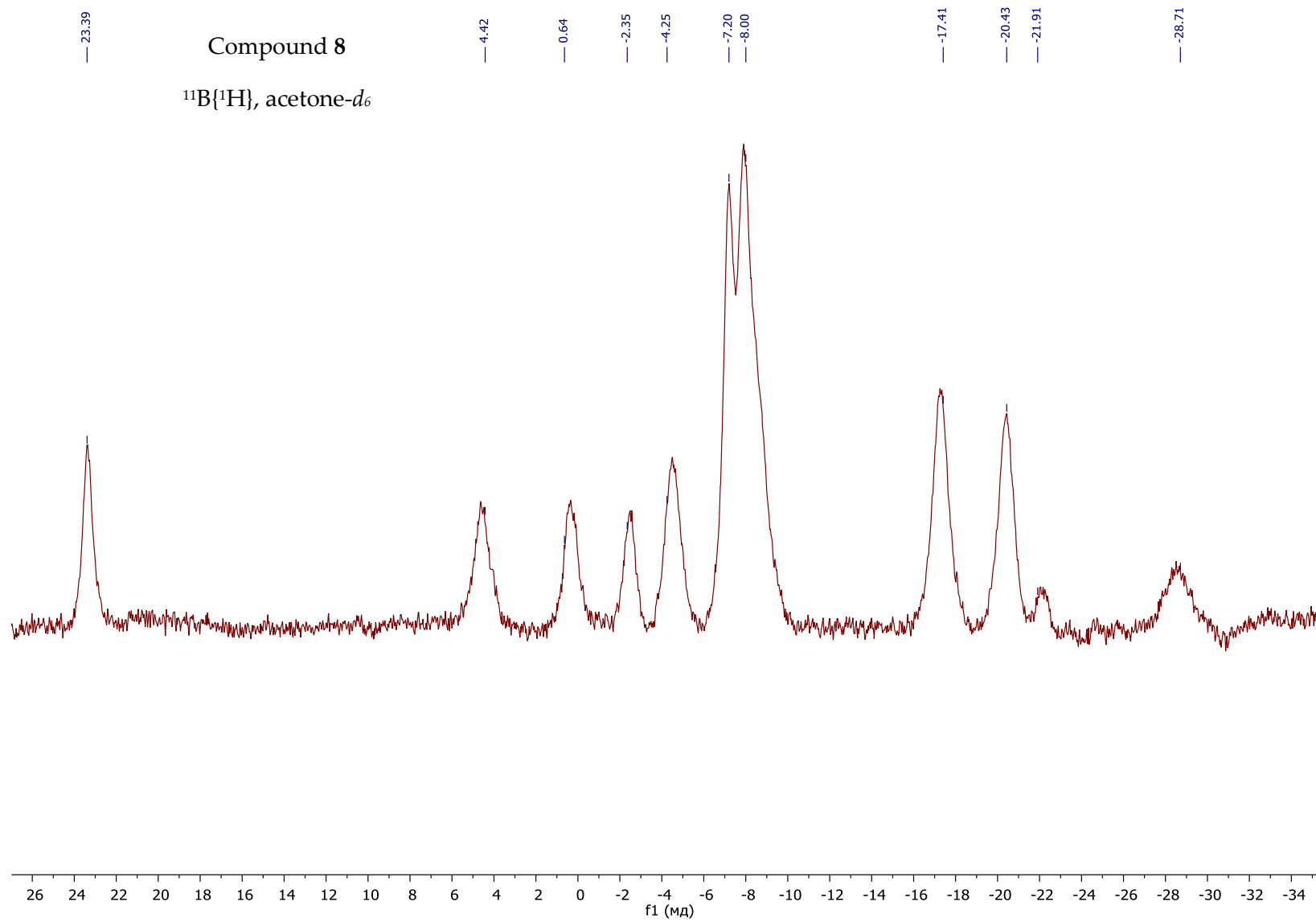


Figure S20.  $^1\text{H}$  NMR spectrum of compound 8



**Figure S21.**  $^{11}\text{B}\{^1\text{H}\}$  NMR spectrum of compound 8

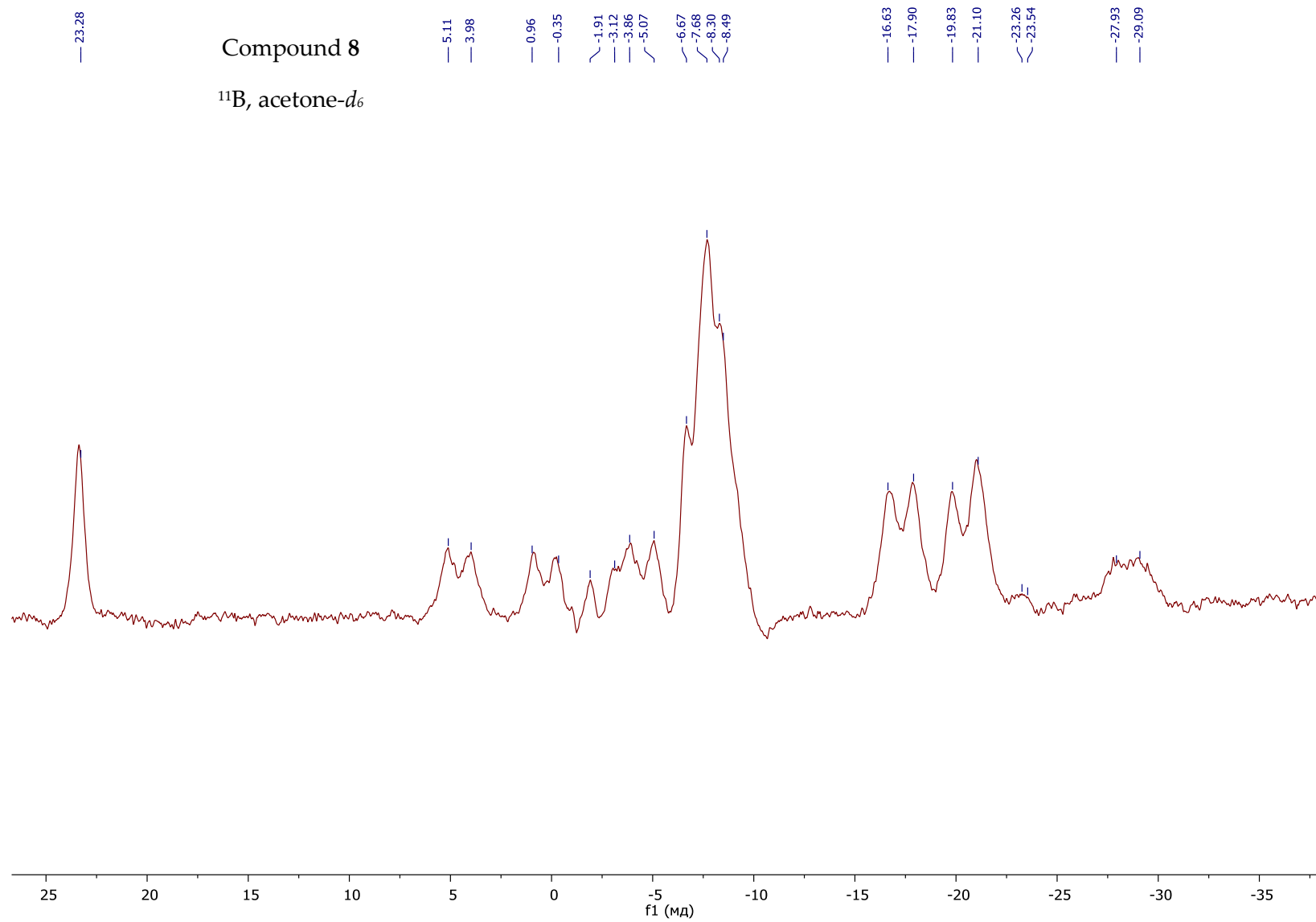
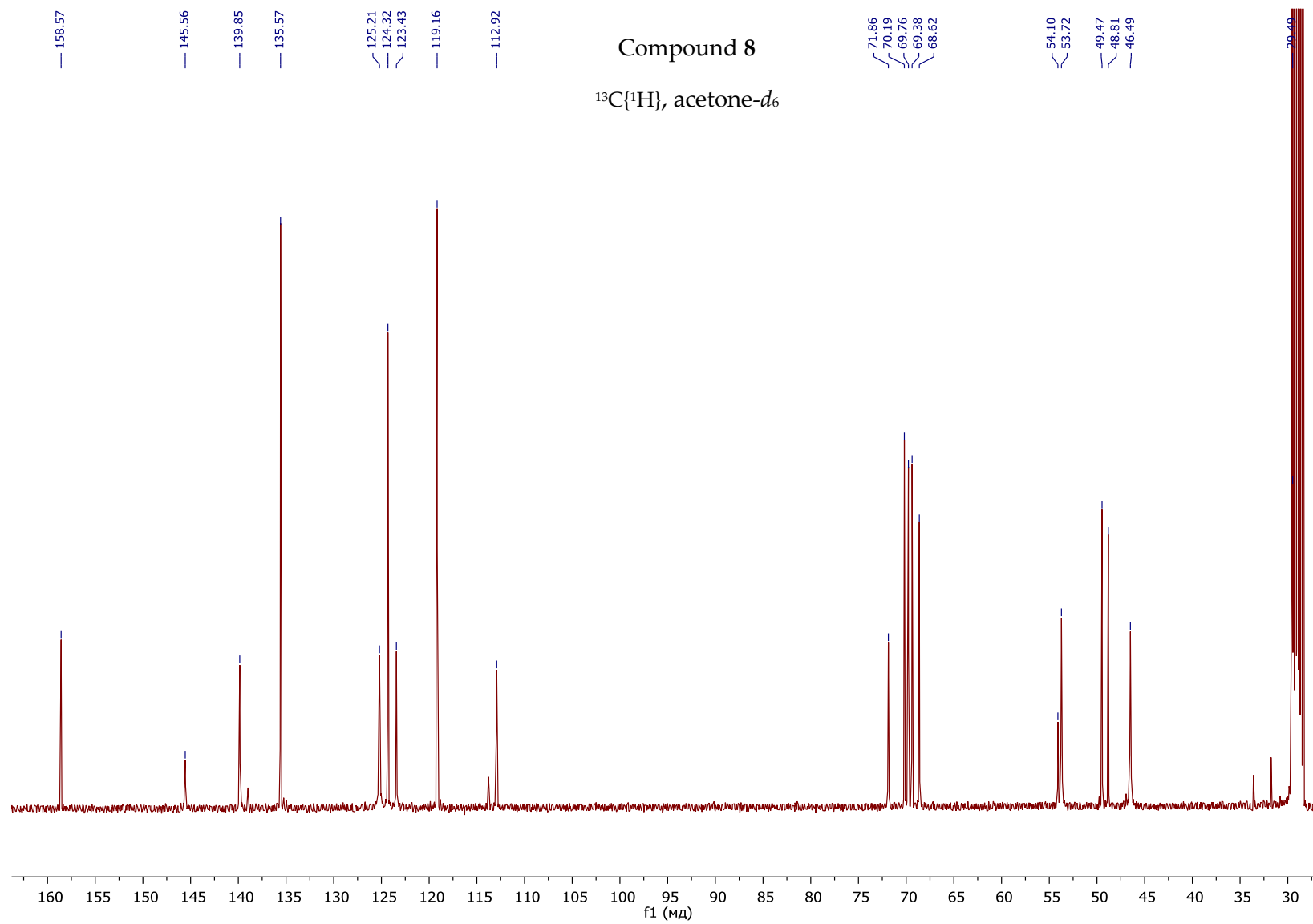


Figure S22.  $^{11}\text{B}$  NMR spectrum of compound 8



**Figure S23.**  $^{13}\text{C}\{^1\text{H}\}$  NMR spectrum of compound 8

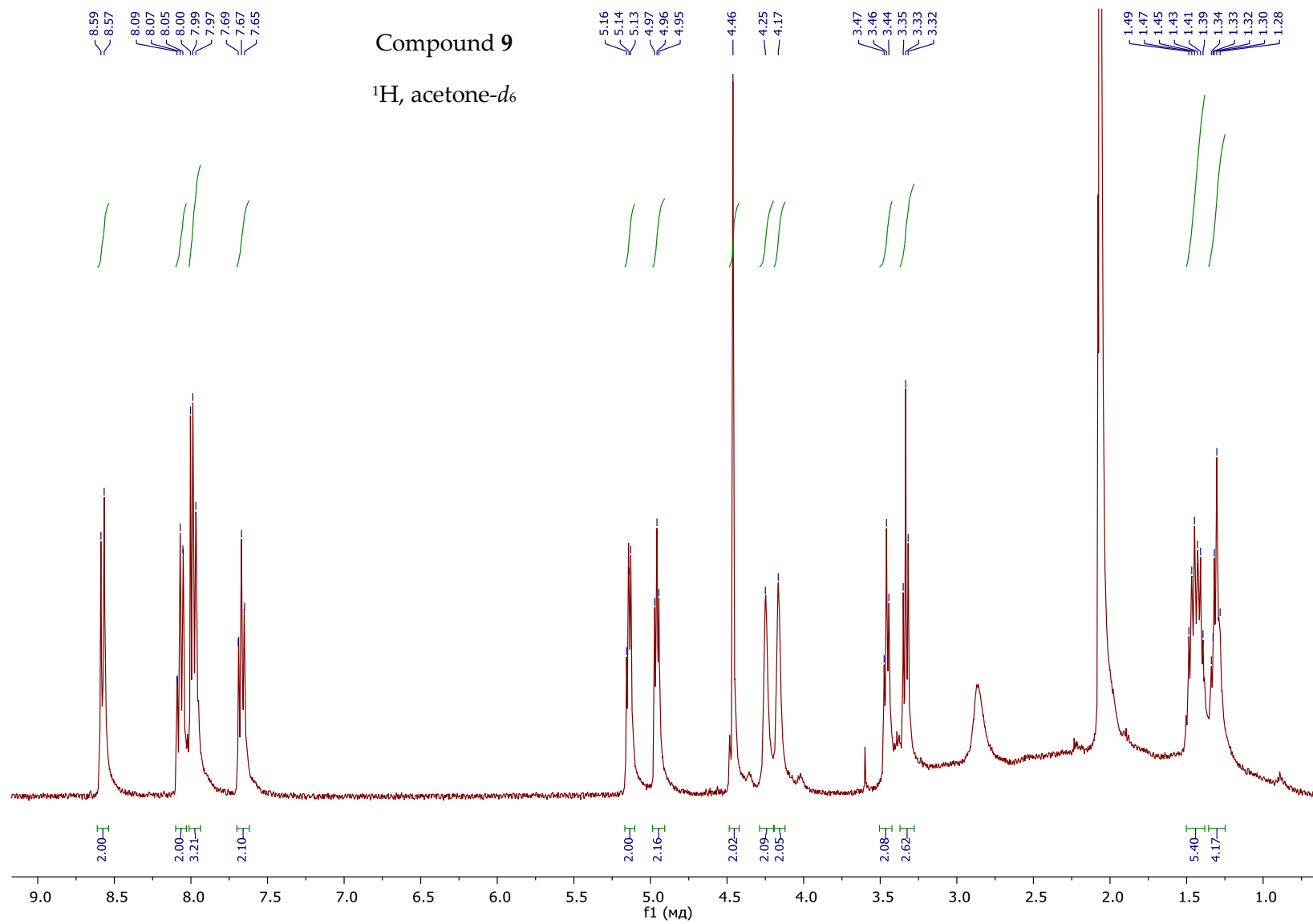
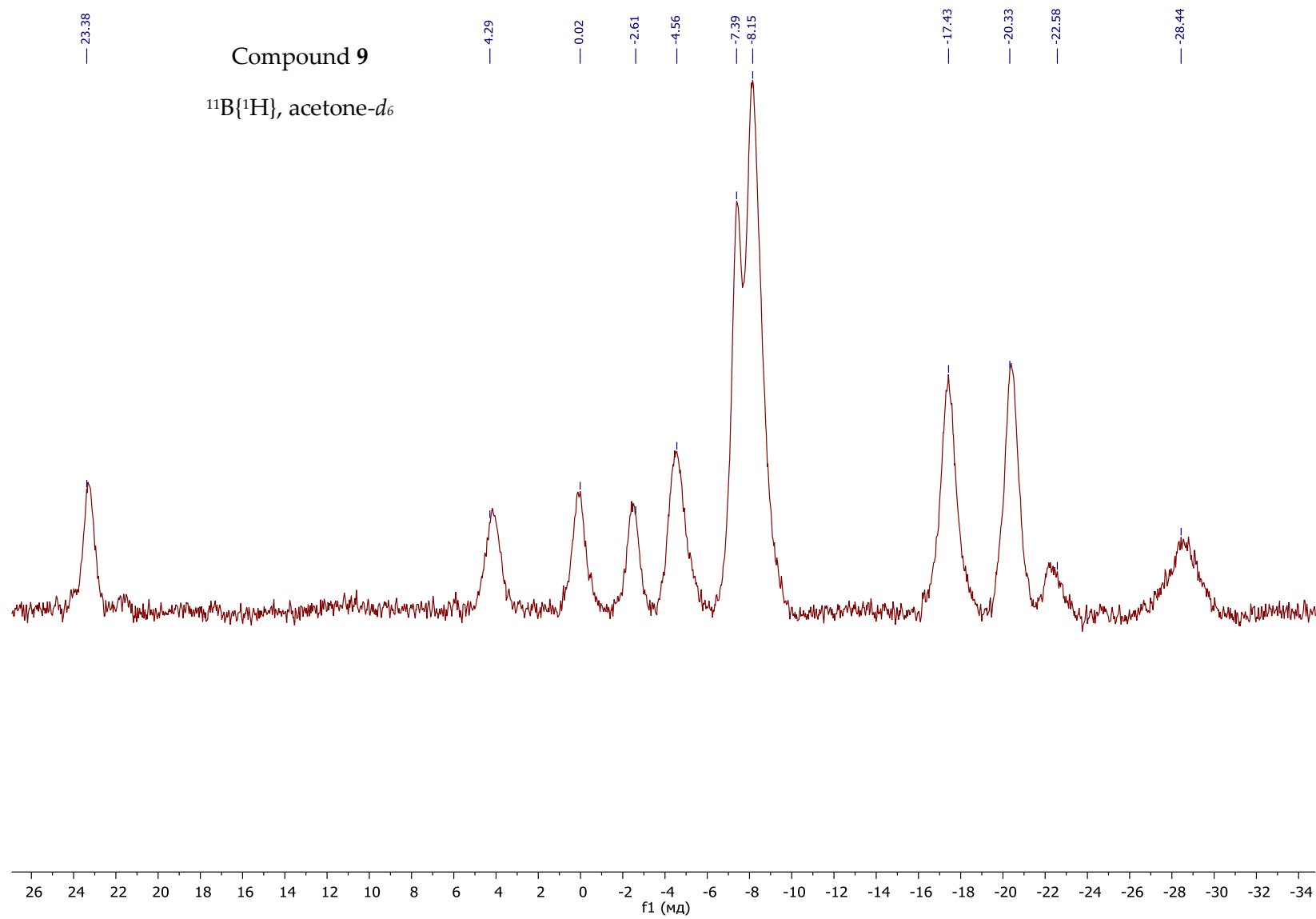


Figure S24.  $^1\text{H}$  NMR spectrum of compound 9



**Figure S25.**  $^{11}\text{B}\{^1\text{H}\}$  NMR spectrum of compound **9**

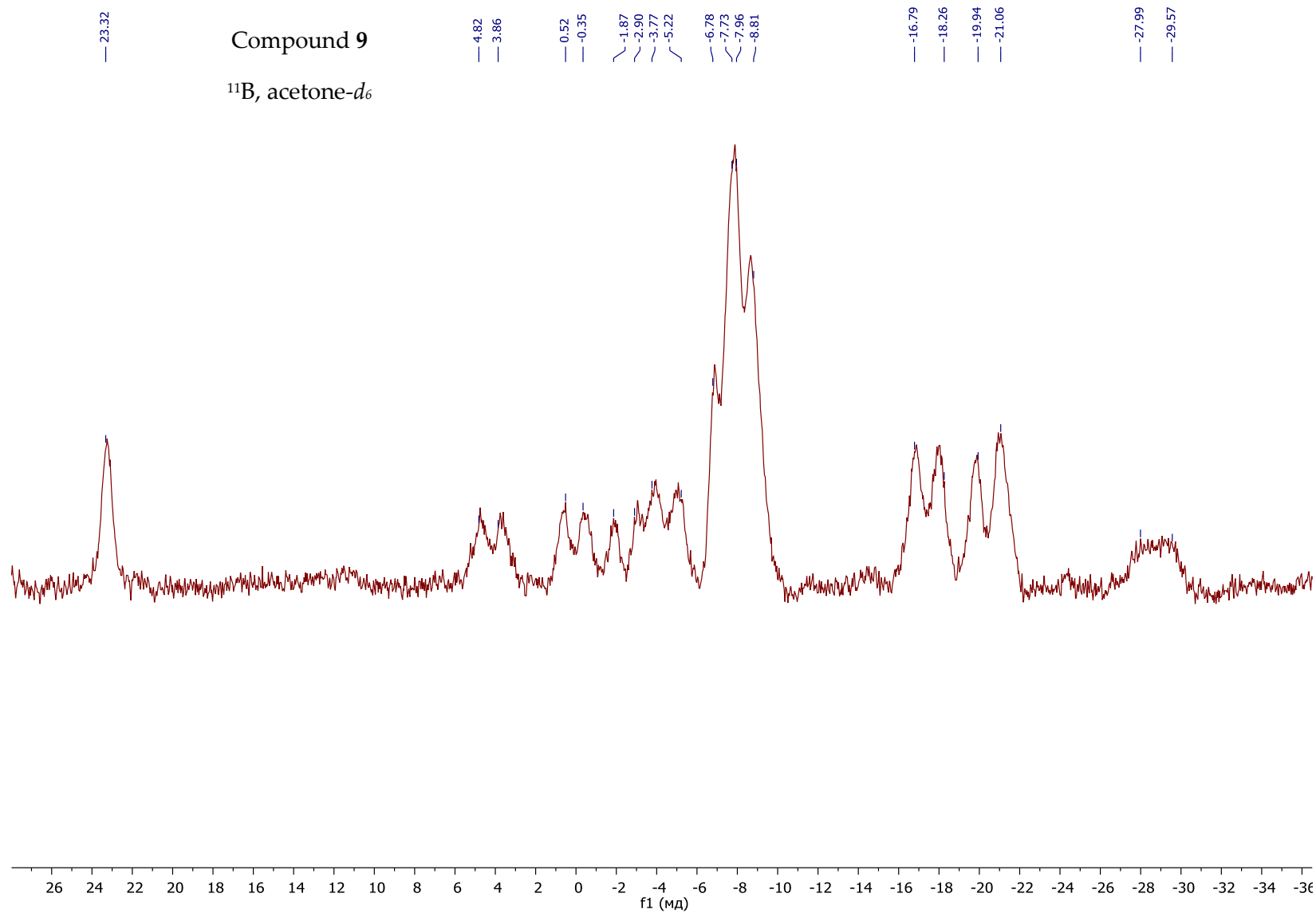
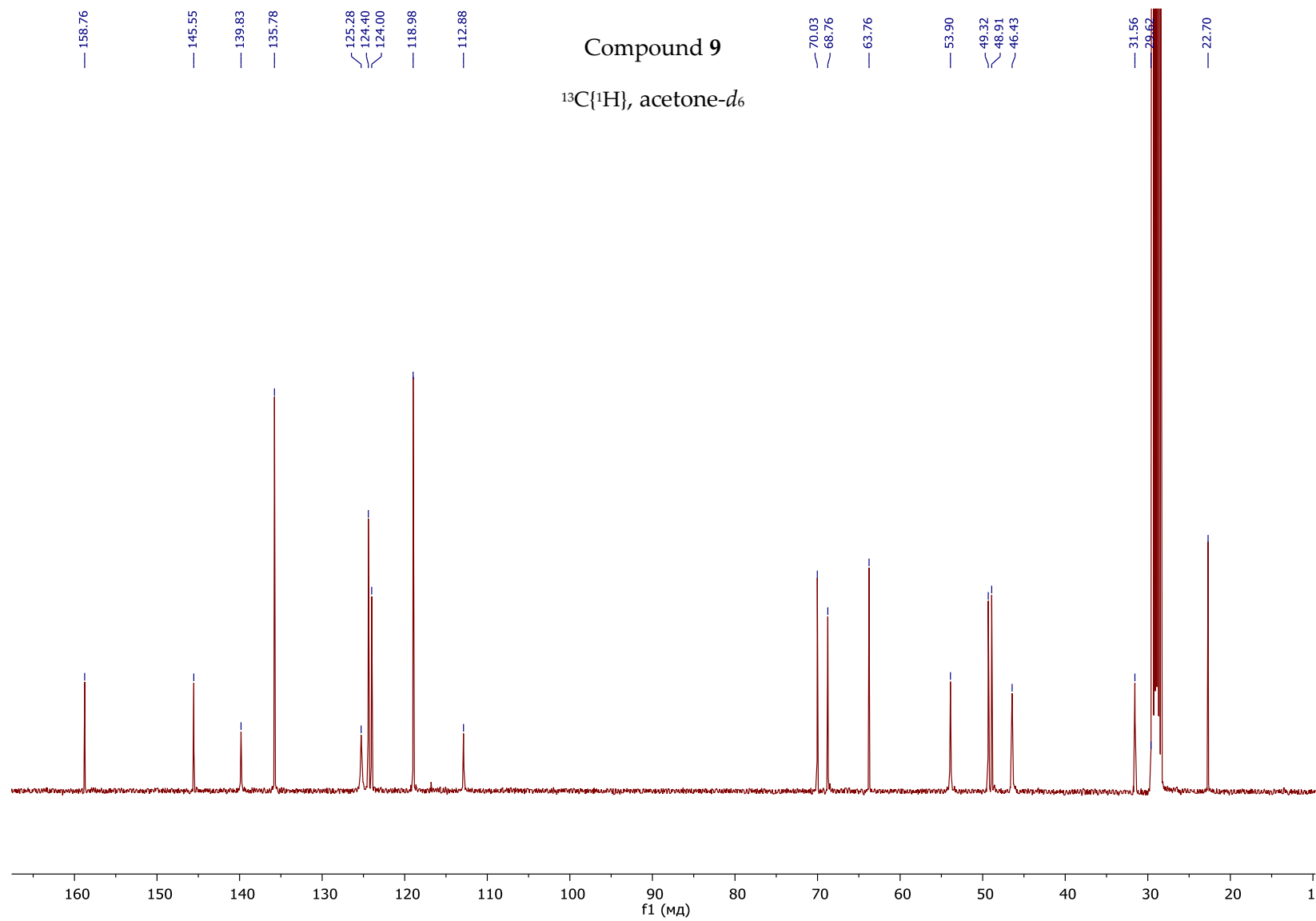


Figure S26.  $^{11}\text{B}$  NMR spectrum of compound **9**





**Figure S27.**  $^{13}\text{C}\{^1\text{H}\}$  NMR spectrum of compound **9**

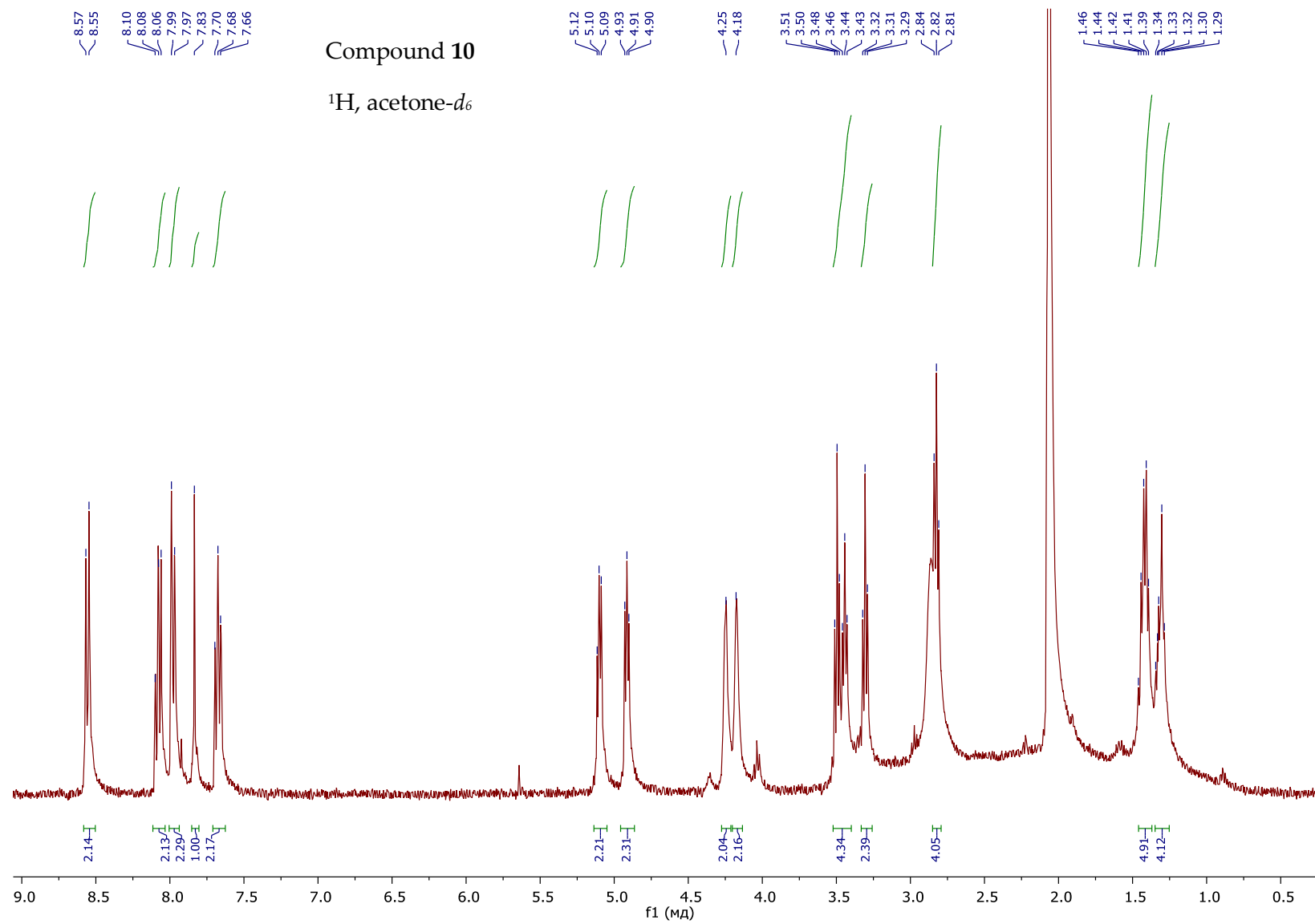


Figure S28.  $^1\text{H}$  NMR spectrum of compound **10**

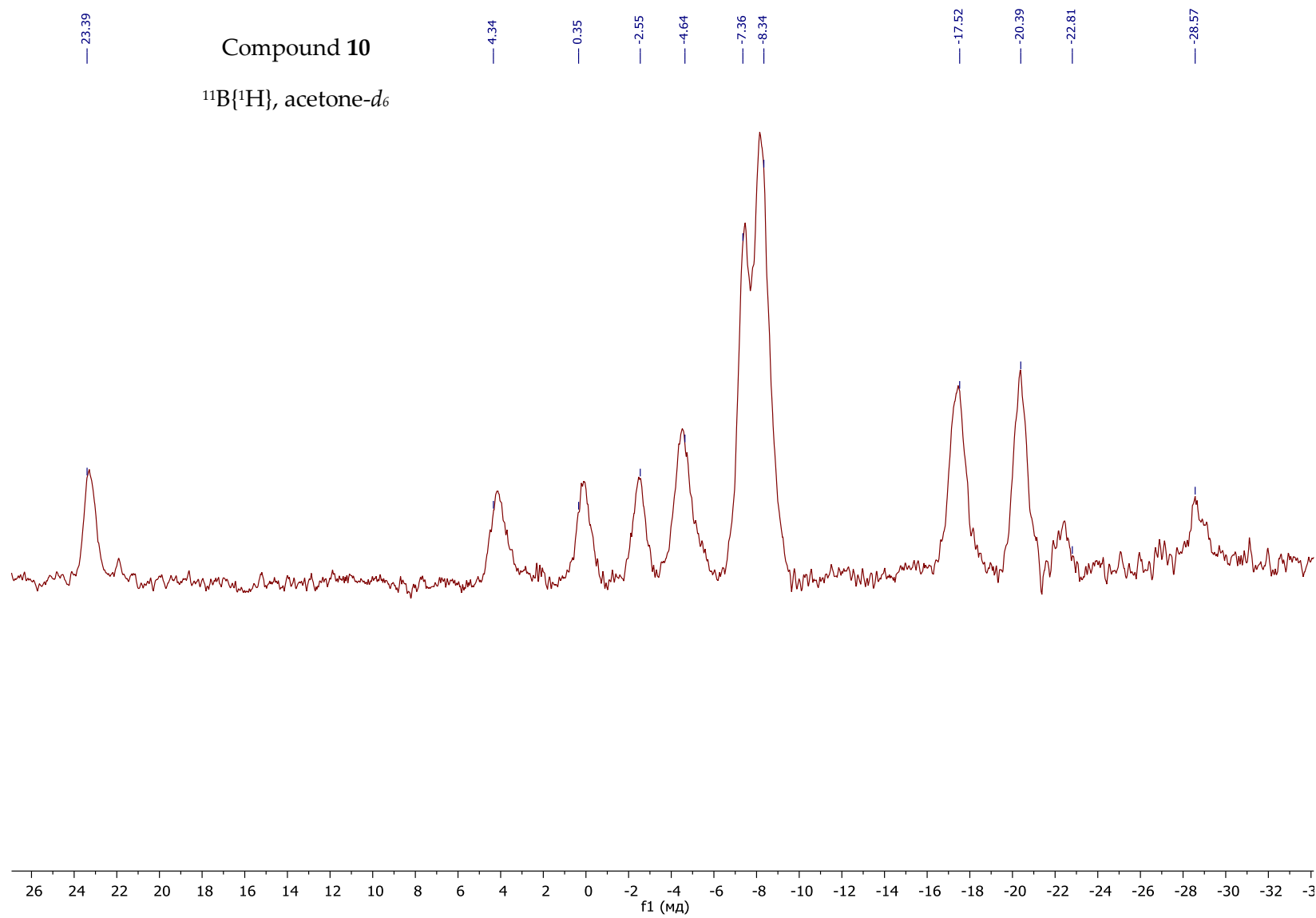
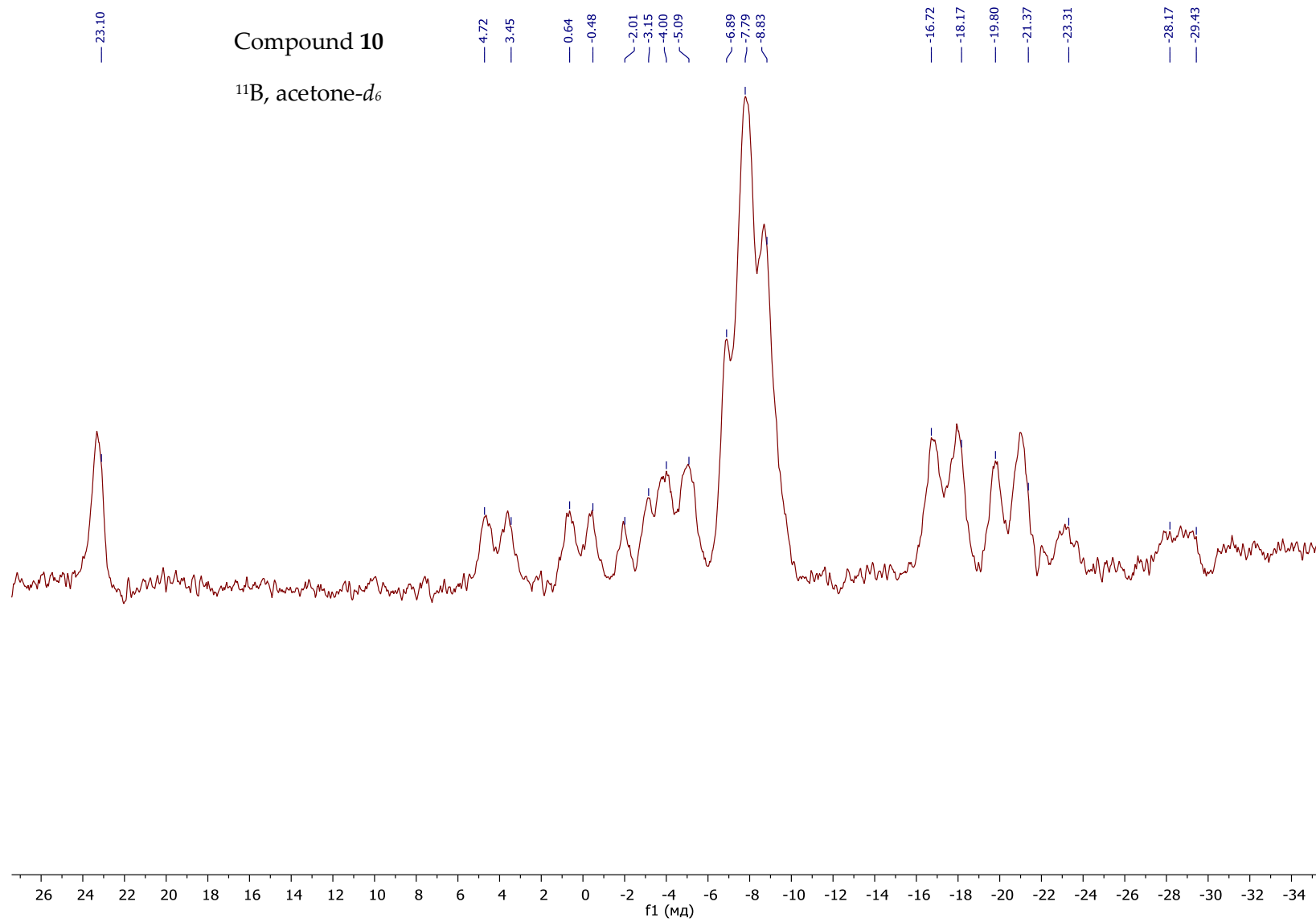


Figure S29.  $^{11}\text{B}\{^1\text{H}\}$  NMR spectrum of compound **10**



**Figure S30.**  $^{11}\text{B}$  NMR spectrum of compound **10**

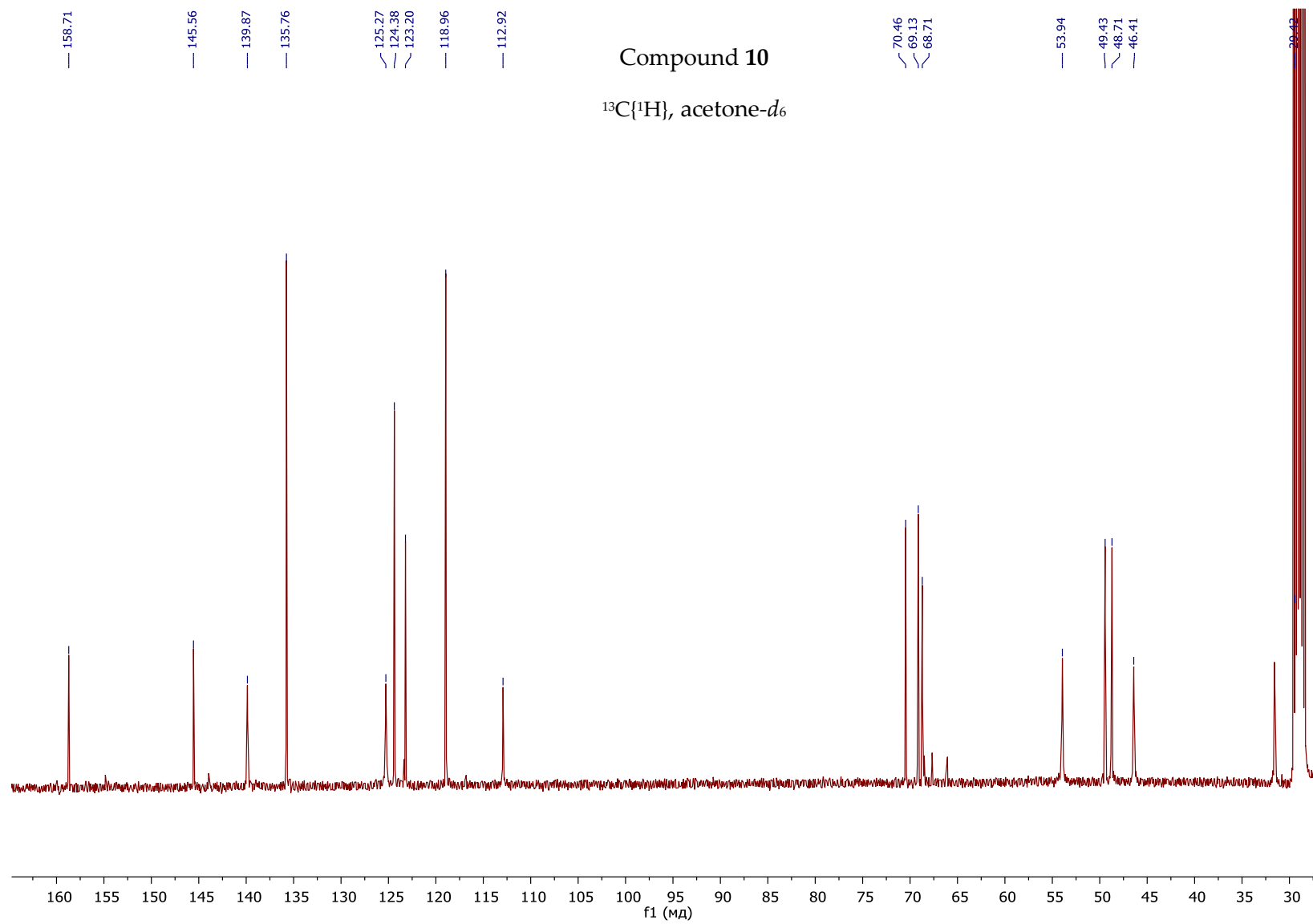


Figure S31.  $^{13}\text{C}\{^1\text{H}\}$  NMR spectrum of compound **10**