# Synthesis and photophysical properties of novel oxadiazole substituted BODIPY fluorophores

Maria D. Matveeva[a*], Dmitry I. Zhilyaev[b], Almira R.Miftyakhova[b], Pavel Chulkin[c], Patryk Janasik,[c] Leonid G. Voskressensky,[b] Giovanni Talarico,[d*] and Ilya V. Efimov[b]

[a] *A.V. Topchiev Institute of Petrochemical Synthesis, Russian Academy of Sciences, Leninsky pr. 29, 119991, Moscow, Russian Federation*

[b] *Research Center: Molecular Design and Synthesis of Innovative Compounds for Medicine, RUDN University, 117198, Russia, Moscow, Miklukho-Maklaya st, 6*

[c] *Department of Physical Chemistry and Technology of Polymers, Faculty of Chemistry, Silesian University of Technology, Strzody 9,44-100 Gliwice, Poland*

[d] *Dipartimento di Scienze Chimiche, Università di Napoli Federico II, 80126 Napoli, Italy orcid.org/0000-0002-4861-0444*

* *Corresponding author. E-mail address: m.d.matveeva@gmail.com, talarico@unina.it*

**Supporting Information**

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## 1. General information

Reagents were purchased from commercial sources and were used without any additional purification. $^{1}H$ and $^{13}C$ NMR spectra were recorded in Chloroform-*d* solutions at 25ºC, using a 600 MHz NMR spectrometer; peak positions are given in parts per million ($\delta$) referenced to the appropriate solvent residual peak. High-resolution mass spectra were recorded on Bruker maXis QTOF (tandem quarrupole/time-of-flight mass analyzer), equipped with an ESI source. The m/z scanning range was 50–3000. External calibration of the mass scale was carried out using a low-concentration calibration solution "Tuning mix" (Agilent Technologies). Samples were injected using a 500 μL Hamilton RN 1750 syringe (Switzerland). The measurements were carried out in the positive ion mode (+) (grounded spray needle, 4500-V high-voltage capillary; HV End Plate Offset: –500 V). The flow rate during injection was controlled with a syringe pump (3 μL/min). Nitrogen was used as a nebulizer gas (1.0 bar) and dry gas (4.0 L/min, 200°C). The data were processed using the Bruker Data Analysis 4.0 software. The reaction progress was monitored by TLC and the spots were visualized under UV light (254 or 365 nm). Melting points (not corrected) were determined on a SMP-10 apparatus. Solvents were distilled and dried according to standard procedures. The photoluminescence spectra were obtained using Camlin Modular Fluorescence Spectrometer FluoroSENS Pro-11. The concentration of the solutions for photoluminescence study was 1μM in all experiments. The quantum yield was estimated by direct method using an integrating sphere.

## 2. General procedure for the synthesis of BODIPY dyes:

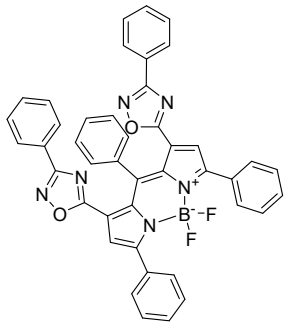
In 25 mL 2 neck round bottom flask 3-phenyl-5-(5-phenyl-1*H*-pyrrol-3-yl)-1,2,4-oxadiazole (1 equiv.) was degassed by argon for 10 min. Then aldehyde (0.5 equiv.) was added and again purged by argon for 10 min. Then few drops of TFA was added and stirred at 120ºC for 2 hours. The reaction progress was controlled by TLC (Sorbfil, 1:3, EtOAc – hexane). After completion of the reaction, the dark green mass was cooled and to the resulting paste, DCM (10.0 mL) was added, followed immediately by the addition of DDQ (1 equiv.). The deep red/purple solution was stirred overnight. After that, DIPEA (10 equiv.) was added and stirred for 30 minutes. Subsequently, reaction mixture was cooled in ice bath and $BF_3 \cdot OEt_2$ (20 equiv.) was added slowly, dropwise, and the mixture was again stirred overnight. Then, the reaction mixture was transferred to a separation funnel, and washed with saturated $Na_2CO_3$ (3 × 20 mL) followed by brine (2 × 20 mL). The organic solvent was removed in vacuo, and the residue was subjected to column chromatography (silica gel, 1:6, EtOAc – hexane) to give the desired product.

**Table S1.** Optimization of reaction conditions.

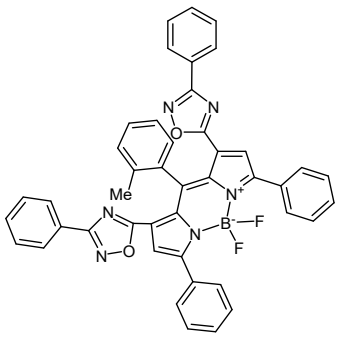
| Entry | Solvent | Catalyst | Temp (°C) | Base | Time | Yield (%)[a] |
|---|---|---|---|---|---|---|
| 1 | DCM | TFA | 25 | - | - | NR |
| 2 | DCM | TFA | reflux | $Et_3N$ | 10 days | Trace |
| 3 | DCE | TFA | 25 | - | - | NR |
| 4 | DCE | TFA | reflux | $Et_3N$ | 7 days | Trace |
| 5 | DCE | 5 mol% PPTS | 25 | - | - | NR [1] |
| 6 | DCE | 10 mol% PPTS | reflux | - | 7 days | trace[b] |
| 7 | toluene | 10% mol $I_2$ | reflux | - | 8 days | trace [2][b] |
| 8 | Solv. free | TFA | 120 | $Et_3N$ | 2h | 32 |
| 9 | Solv. free | TFA | 150 | $Et_3N$ | 2h | 17 |
| 10 | Solv. free | TFA | 200 | $Et_3N$ | 2h | Trace |
| **11** | **Solv. free** | **TFA** | **120** | **DIPEA** | **2h** | **37** |

[a] Isolated yield, after column chromatography [b] After acid-condensation reaction
[b] 1 equiv. pyrrole, 0.5 equiv. aldehyde, a few drops of TFA, 1 equiv. DDQ, 10 equiv. DIPEA, 20 equiv. $BF_3OEt_2$. DCM = dichloromethane; DCE = 1,2-dichloroethane; TFA = trifluoroacetic acid; PPTS = pyridinium *p*-toluenesulfonate; DDQ = 2,3-dichloro-5,6-dicyano-1,4-benzoquinone; DIPEA = *N,N*-diisopropylethylamine; NR = no reaction.

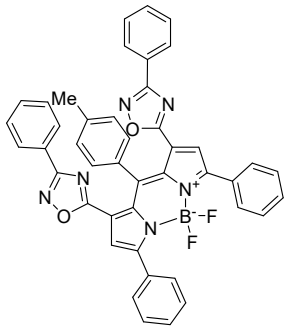
## 3. NMR and HRMS characterization data



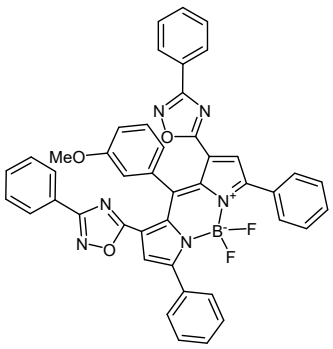
**5,5'-(5,5-Difluoro-3,7,10-triphenyl-5*H*-4λ⁴,5λ⁴-dipyrrolo[1,2-*c*:2',1'-*f*][1,3,2]diazaborinine-1,9-diyl)bis(3-phenyl-1,2,4-oxadiazole)** (3a). (262 mg, 0.37 mmol, 37%) dark purple solid, mp = 261– 263 °C. $^1$H NMR (600 MHz, Chloroform-*d*) δ 7.91–7.89 (m, 4H), 7.80–7.79 (m, 4H), 7.50–7.47 (m, 6H), 7.46–7.45 (m, 1H), 7.45–7.44 (m, 1H), 7.42–7.39 (m, 4H), 7.32–7.31 (m, 2H), 7.09 (s, 2H), 6.97 (t, *J* = 7.7 Hz, 2H), 6.82 (t, *J* = 7.7 Hz, 1H). $^{13}$C NMR (151 MHz, Chloroform-*d*) δ 171.3, 168.3, 158.9, 146.3, 134.35-134.34 (m), 132.3, 131.34, 131.3, 130.7, 130.6, 130.2, 129.8 (t, *J* = 3.7 Hz), 128.8, 128.7, 127.9, 127.5, 126.4, 125.59–125.58 (m). $^{19}$F NMR (565 MHz, Chloroform-*d*) δ -132.21 (q, $J_{F-B}$ = 30.2 Hz). HRMS (ESI) m/z calcd for $C_{43}H_{27}BF_2N_6O_2$ $[M+H]^+$: 709.2337 found 709.2333.



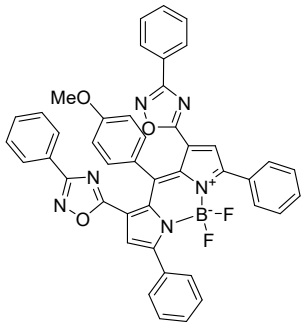
**5,5'-(5,5-Difluoro-3,7-diphenyl-10-(*o*-tolyl)-5*H*-4λ⁴,5λ⁴-dipyrrolo[1,2-*c*:2',1'-*f*][1,3,2]diazaborinine-1,9-diyl)bis(3-phenyl-1,2,4-oxadiazole)** (3b). (217 mg, 0.30 mmol, 30%)burgundy solid, mp › 300 °C. $^1$H NMR (600 MHz, Chloroform-*d*) δ 7.92–7.90 (m, 4H), 7.81–7.79 (m, 4H), 7.50–7.48 (m, 6H), 7.47–7.46 (m, 1H), 7.45–7.44 (m, 1H), 7.42–7.40 (m, 4H), 7.14 (dd, *J* = 7.5, 1.1 Hz, 1H), 7.02 (s, 2H), 6.81 (t, *J* = 7.6 Hz, 1H), 6.74 (d, *J* = 7.7 Hz, 1H), 6.62 (td, *J* = 7.6, 1.3 Hz, 1H), 2.38 (s, 3H). $^{13}$C NMR (151 MHz, Chloroform-*d*) δ 170.9, 168.2, 158.8, 145.8, 137.8, 134.31–134.30 (m), 131.4, 131.3, 130.8, 130.7, 130.4, 130.3, 129.9, 129.8 (t, *J* = 3.7 Hz), 128.8, 128.7, 127.5, 126.4, 125.35–125.33 (m), 125.2, 20.2. $^{19}$F NMR (565 MHz, Chloroform-*d*) δ -131.53–131.85 (m), -133.41-133.73 (m). HRMS (ESI) m/z calcd for $C_{44}H_{29}BF_2N_6O_2$ $[M+H]^+$: 723.2493 found 723.2490.



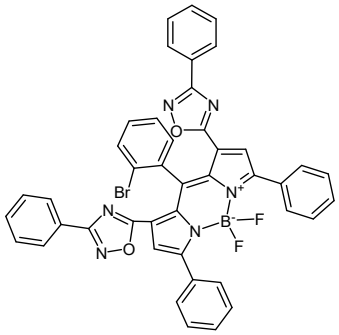
**5,5'-(5,5-Difluoro-3,7-diphenyl-10-(*p*-tolyl)-5*H*-4λ⁴,5λ⁴-dipyrrolo[1,2-*c*:2',1'-*f*][1,3,2]diazaborinine-1,9-diyl)bis(3-phenyl-1,2,4-oxadiazole)** (3c). (310 mg, 0.43 mmol, 43%) burgundy solid, mp = 240–242 °C. $^1$H NMR (600 MHz, Chloroform-*d*) δ 7.90–7.88 (m, 4H), 7.78 (d, *J* = 8.0 Hz, 4H), 7.49–7.46 (m, 6H), 7.46–7.44 (m, 2H), 7.40 (t, *J* = 7.6 Hz, 4H), 7.14 (d, *J* = 6.8 Hz, 2H), 7.07 (s, 2H), 6.70 (d, *J* = 7.4 Hz, 2H), 1.49 (s, 3H). $^{13}$C NMR (151 MHz, Chloroform-*d*) δ 171.2, 168.2, 158.7, 146.7, 141.3, 134.48–134.47 (m), 131.4, 131.3, 130.6, 130.1, 129.8 (t, *J* = 3.6 Hz), 129.75, 128.8, 128.7, 128.6, 128.16–128.13 (m), 127.4, 126.4, 125.24-125.21 (m), 20.5.$^{19}$F NMR (565 MHz, Chloroform-*d*) δ -132.24 (q, $J_{F–B}$ = 30.3 Hz). HRMS (ESI) m/z calcd for $C_{44}H_{29}BF_2N_6O_2$ $[M+H]^+$: 723.2493 found 723.2506.



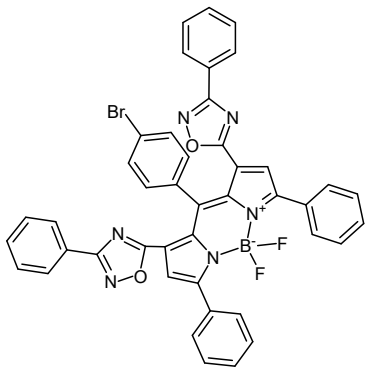
**5,5'-(5,5-Difluoro-10-(3-methoxyphenyl)-3,7-diphenyl-5*H*-4λ⁴,5λ⁴-dipyrrolo[1,2-*c*:2',1'-*f*][1,3,2]diazaborinine-1,9-diyl)bis(3-phenyl-1,2,4-oxadiazole)** (3d). (303 mg, 0.41 mmol, 41%) dark purple solid, mp = 228–230 °C. $^1$H NMR (600 MHz, Chloroform-*d*) δ 7.90–7.89 (m, 4H), 7.81 (d, *J* = 7.3 Hz, 4H), 7.46–7.44 (m, 2H), 7.40 (t, *J* = 7.5 Hz, 4H), 7.07 (s, 2H), 6.86–6.84 (m, 3H), 6.25–6.24 (m, 1H), 3.37 (s, 3H). $^{13}$C NMR (151 MHz, Chloroform-*d*) δ 171.3, 168.3, 158.9, 158.89, 145.9, 134.2, 133.4, 131.34, 131.3, 130.7, 129.8 (t, *J* = 4.2 Hz), 129.1, 128.8, 128.7, 128.25–128.24 (m), 127.5, 126.4, 125.40–125.35 (m), 122.7, 116.0, 54.9. $^{19}$F NMR (565 MHz, Chloroform-*d*) δ -132.22 (q, $J_{F–B}$ = 30.4 Hz). HRMS (ESI) m/z calcd for $C_{44}H_{29}BF_2N_6O_3$ $[M+H]^+$: 739.2442 found 739.2440.



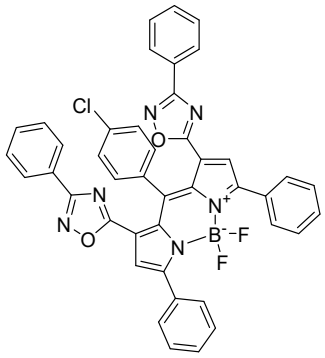
**5,5'-(5,5-Difluoro-10-(4-methoxyphenyl)-3,7-diphenyl-5*H*-4λ⁴,5λ⁴-dipyrrolo[1,2-*c*:2',1'-*f*][1,3,2]diazaborinine-1,9-diyl)bis(3-phenyl-1,2,4-oxadiazole)** (3e). (413 mg, 0.56 mmol, 56%) amorphous mass. $^1$H NMR (600 MHz, Chloroform-*d*) δ 7.89–7.88 (m, 4H), 7.81 (d, *J* = 7.9 Hz, 4H), 7.48–7.47 (m, 6H), 7.45–7.44 (m, 2H), 7.42–7.39 (m, 4H), 7.20 (d, *J* = 8.2 Hz, 2H), 7.09 (s, 2H), 6.41 (d, *J* = 8.2 Hz, 2H), 3.05 (s, 3H). $^{13}$C NMR (151 MHz, Chloroform-*d*) δ 171.4, 168.3, 161.6, 158.5, 146.5, 134.53–134.51 (m), 131.8, 131.4, 131.3, 130.5, 129.8 (t, *J* = 4.1 Hz), 128.8, 128.6, 127.4, 126.4, 125.19–125.16 (m), 125.1, 113.7, 54.7. $^{19}$F NMR (565 MHz, Chloroform-*d*) δ -132.11 (q, $J_{F–B}$ = 30.4 Hz). HRMS (ESI) m/z calcd for $C_{44}H_{29}BF_2N_6O_3$ $[M+H]^+$: 739.2442 found 739.2447.



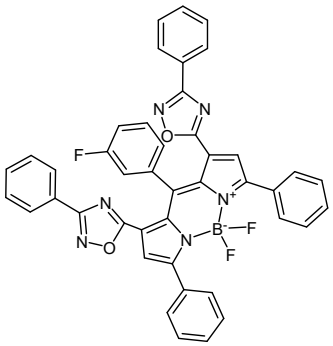
**5,5'-(10-(2-bromophenyl)-5,5-difluoro-3,7-diphenyl-5*H*-4λ⁴,5λ⁴-dipyrrolo[1,2-*c*:2',1'-*f*][1,3,2]diazaborinine-1,9-diyl)bis(3-phenyl-1,2,4-oxadiazole)** (3f). (228 mg, 0.29 mmol, 29%) dark blue solid, mp = 158–160 °C. $^1$H NMR (600 MHz, Chloroform-*d*) δ 7.93–7.91 (m, 4H), 7.83 (d, *J* = 7.2 Hz, 4H), 7.50–7.49 (m, 6H), 7.46–7.45 (m, 2H), 7.41 (t, *J* = 7.4 Hz, 4H), 7.31 (dd, *J* = 7.5, 1.2 Hz, 1H), 7.15 (d, *J* = 7.9 Hz, 1H), 7.09 (s, 2H), 7.00 (t, *J* = 7.6 Hz, 1H), 6.62 (t, *J* = 7.6 Hz, 1H). $^{13}$C NMR (151 MHz, Chloroform-*d*) δ 170.9, 168.3, 159.3, 134.06–134.05 (m), 132.8, 132.6, 132.0, 131.6, 131.4, 131.3, 130.8, 129.8 (t, *J* = 3.7 Hz), 128.9, 128.7, 127.5, 126.8, 126.3, 125.84–125.82 (m), 124.8. $^{19}$F NMR (565 MHz, Chloroform-*d*) δ -132.16–132.91 (m). HRMS (ESI) m/z calcd for $C_{43}H_{26}BBrF_2N_6O_2$ $[M+H]^+$: 787.1442 found 787.1448.



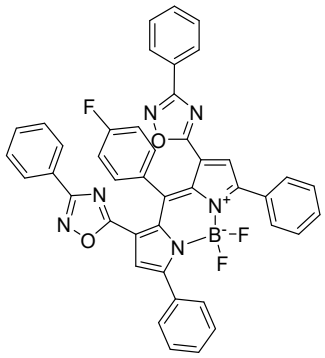
**5,5'-(10-(4-bromophenyl)-5,5-difluoro-3,7-diphenyl-5*H*-4λ⁴,5λ⁴-dipyrrolo[1,2-*c*:2',1'-*f*][1,3,2]diazaborinine-1,9-diyl)bis(3-phenyl-1,2,4-oxadiazole)** (3g). (126 mg, 0.16 mmol, 16%) dark blue solid, mp = 197–198 °C. $^1$H NMR (600 MHz, Chloroform-*d*) δ 7.90–7.89 (m, 4H), 7.83–7.81 (m, 4H), 7.50–7.49 (m, 6H), 7.48–7.47 (m, 2H), 7.43 (t, *J* = 7.4 Hz, 4H), 7.14 (d, *J* = 8.3 Hz, 2H), 7.11 (s, 2H), 7.09 (d, *J* = 8.3 Hz, 2H). $^{13}$C NMR (151 MHz, Chloroform-*d*) δ 171.4, 168.2, 158.4, 154.1, 152.7, 151.5, 149.7, 142.9, 134.6, 131.5, 131.2, 131.0, 130.5, 129.78–129.74 (m), 128.8, 128.6, 128.0, 127.5, 126.5, 125.0, 121.0, 117.5, 116.9. $^{19}$F NMR (565 MHz, Chloroform-*d*) δ -132.18 (q, $J_{F–B}$ = 30.1 Hz). HRMS (ESI) m/z calcd for $C_{43}H_{26}BBrF_2N_6O_2$ $[M+H]^+$: 787.1442 found 787.1449.



**5,5'-(10-(4-chlorophenyl)-5,5-difluoro-3,7-diphenyl-5*H*-4λ$^4$,5λ$^4$-dipyrrolo[1,2-*c*:2',1'-*f*][1,3,2]diazaborinine-1,9-diyl)bis(3-phenyl-1,2,4-oxadiazole)** (3h). (215 mg, 0.29 mmol, 29%) dark blue solid, mp = 276–277 °C. $^1$H NMR (600 MHz, Chloroform-*d*) δ 7.90–7.89 (m, 4H), 7.83–7.81 (m, 4H), 7.50–7.47 (m, 8H), 7.44–7.42 (m, 4H), 7.22 (d, *J* = 8.3 Hz, 2H), 7.11 (s, 2H), 6.93 (d, J = 8.3 Hz, 2H). $^{13}$C NMR (151 MHz, Chloroform-*d*) δ 171.1, 168.5, 159.2, 151.2, 144.59–144.57 (m), 137.4, 134.20–134.18 (m), 131.4 13C NMR (151 MHz, Chloroform-d) δ 144.60 –144.55 (m), 131.41 (d, *J* = 2.9 Hz), 131.2, 130.84, 130.8, 129.8 (t, *J* = 4.2 Hz), 128.9, 128.7, 128.3, 128.08–128.05 (m), 127.5, 126.1, 125.69–125.66 (m). $^{19}$F NMR (565 MHz, Chloroform-*d*) δ -132.17 (q, $J_{F–B}$ = 30.9 Hz). HRMS (ESI) m/z calcd for $C_{43}H_{26}BClF_2N_6O_2$ [M+H]$^+$: 743.1947 found 743.1953.



**5,5'-(5,5-difluoro-10-(3-fluorophenyl)-3,7-diphenyl-5*H*-4λ$^4$,5λ$^4$-dipyrrolo[1,2-*c*:2',1'-*f*][1,3,2]diazaborinine-1,9-diyl)bis(3-phenyl-1,2,4-oxadiazole)** (3i). (225 mg, 0.31 mmol, 31%) burgundy solid, mp = 260–262 °C. $^1$H NMR (600 MHz, Chloroform-*d*) δ 7.90–7.89 (m, 4H), 7.83–7.81 (m, 4H), 7.50–7.48 (m, 6H), 7.47–7.46 (m, 2H), 7.42 (t, *J* = 7.5 Hz, 4H), 7.10 (s, 2H), 7.08–7.07 (m, 2H), 6.94–6.90 (m, 1H), 6.47 (td, *J* = 8.5, 2.4 Hz, 1H). $^{13}$C NMR (151 MHz, Chloroform-*d*) δ 171.1, 168.4, 162.9, 161.2, 159.3, 144.0, 134.2, 134.16, 134.05–134.04 (m), 131.4, 131.2, 130.8, 129.8 (t, *J* = 3.8 Hz), 129.7, 128.9, 128.7, 128.14–128.12 (m), 127.5, 126.2, 126.0 (d, *J* = 3.1 Hz), 125.88–125.79 (m), 117.7, 117.6, 117.4. $^{19}$F NMR (565 MHz, Chloroform-*d*) δ -112.38–112.42 (m), -131.71–132.04 (m), -132.31–132.63 (m). HRMS (ESI) m/z calcd for $C_{43}H_{26}BF_3N_6O_2$ [M+H]$^+$: 727.2242 found 727.2241.



**5,5'-(5,5-difluoro-10-(4-fluorophenyl)-3,7-diphenyl-5*H*-4λ$^4$,5λ$^4$-dipyrrolo[1,2-*c*:2',1'-*f*][1,3,2]diazaborinine-1,9-diyl)bis(3-phenyl-1,2,4-oxadiazole)** (3j). (174 mg, 0.24 mmol, 24%) purple solid, mp = 248–250 °C. $^1$H NMR (600 MHz, Chloroform-*d*) δ 7.90–7.89 (m, 4H), 7.83–7.82 (m, 4H), 7.50–7.47 (m, 8H), 7.44–7.42 (m, 4H), 7.30–7.28 (m, 2H), 7.12 (s, 2H), 6.66 (t, *J* = 8.5 Hz, 1H). $^{13}$C NMR (151 MHz, Chloroform-*d*) δ 13C NMR (151 MHz, Chloroform-d) δ 171.2, 168.5, 159.2, 144.9, 134.37–134.32 (m), 132.3, 132.28, 131.5, 131.2, 130.8, 129.8 (t, *J* = 4.2 Hz), 129.0, 128.7, 128.13–128.08 (m), 127.4, 126.1, 125.75–125.72 (m), 115.5, 115.3. $^{19}$F NMR (565 MHz, Chloroform-*d*) δ -108.80–108.85 (m), -132.17 (q, $J_{F–B}$ = 30.3 Hz). HRMS (ESI) m/z calcd for $C_{43}H_{26}BF_3N_6O_2$ [M+H]$^+$: 727.2242 found 727.2250.

## 4. Photoluminescence data

**Fig. S1** Compound **3a**

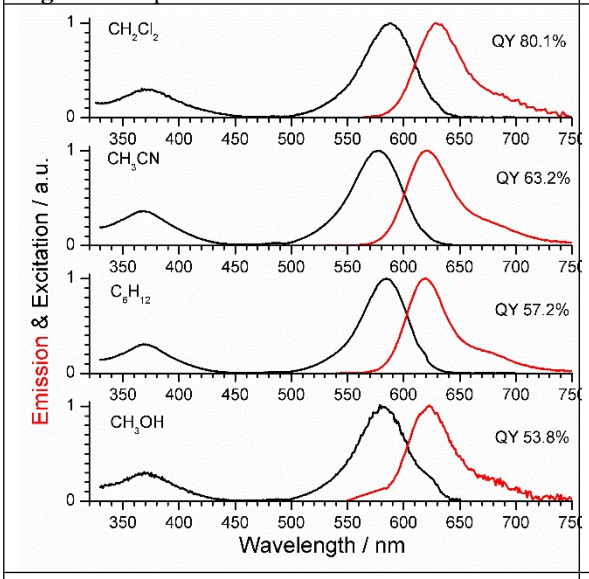



**Fig. S2** Compound **3b**

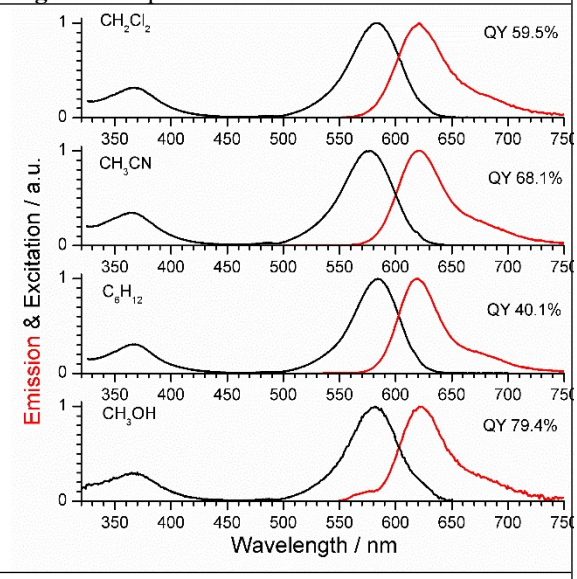



**Fig. S3** Compound **3c**

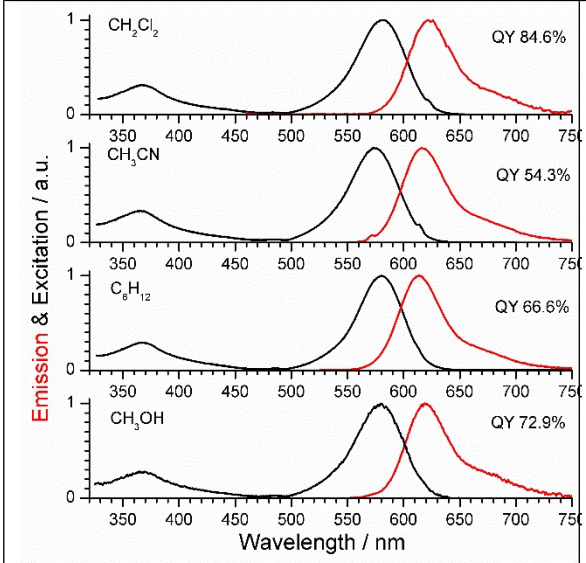



**Fig. S4** Compound **3d**

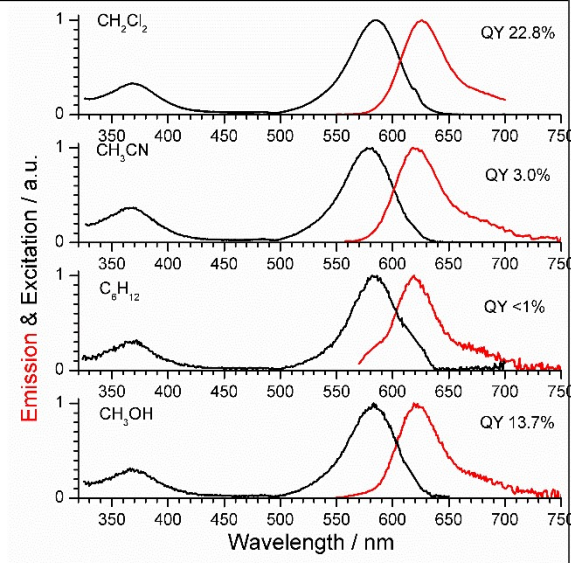



**Fig. S5** Compound **3e**

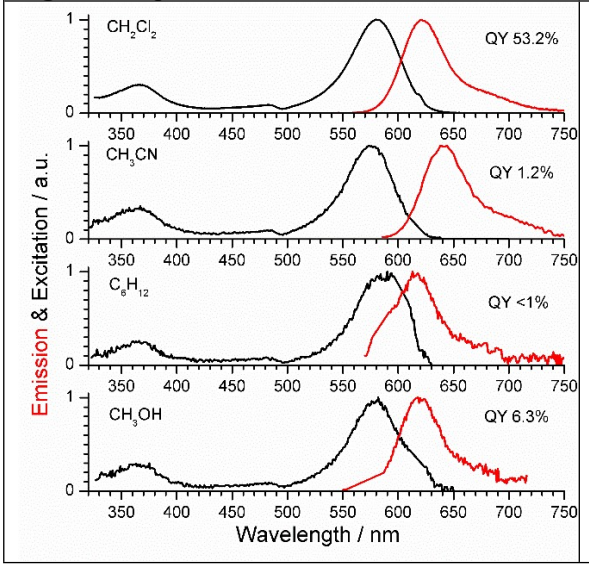



**Fig. S6** Compound **3f**

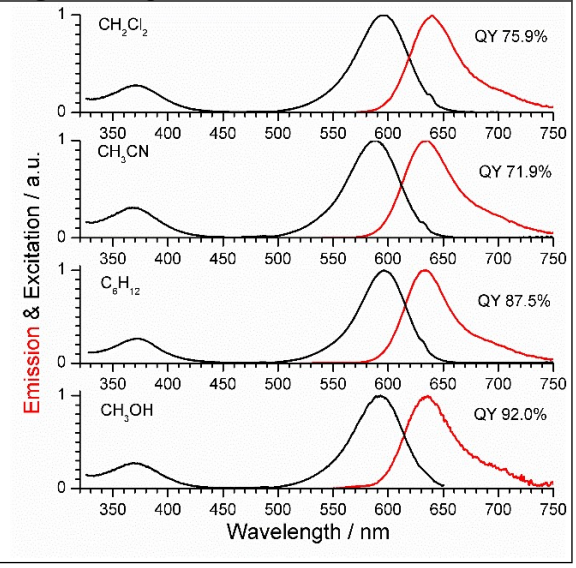


**Fig. S7** Compound **3g**

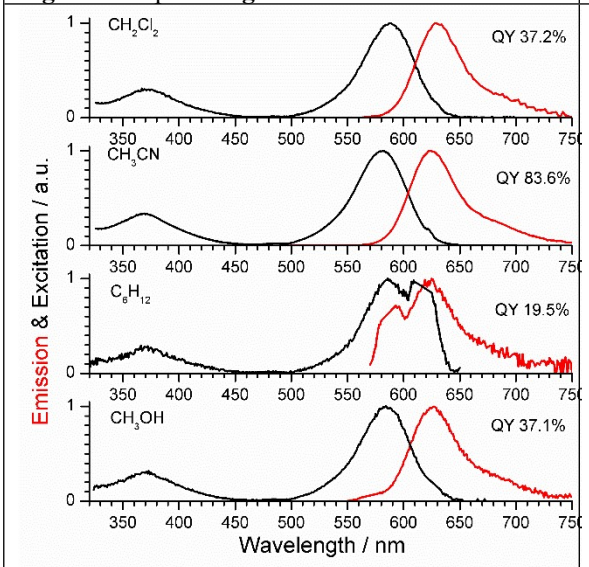



**Fig. S8** Compound **3h**

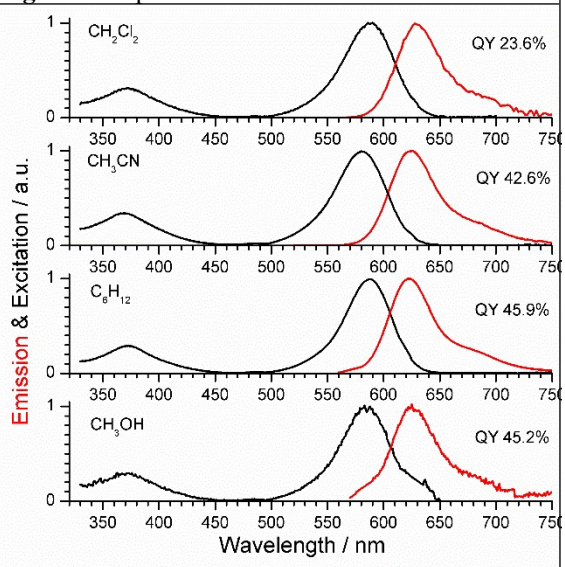



**Fig. S9** Compound **3i**

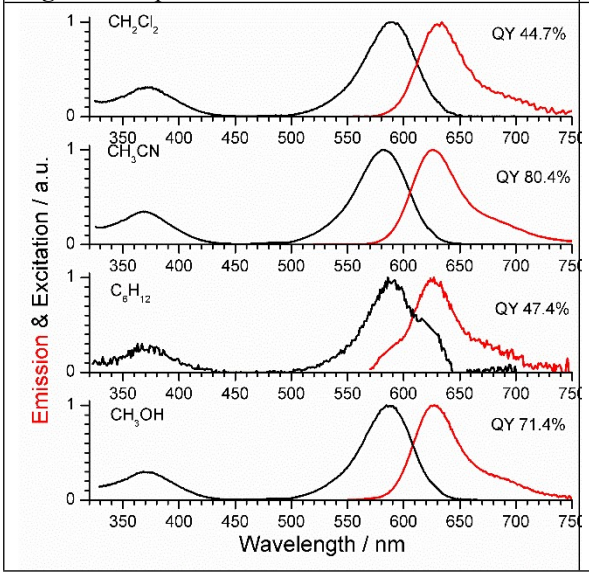
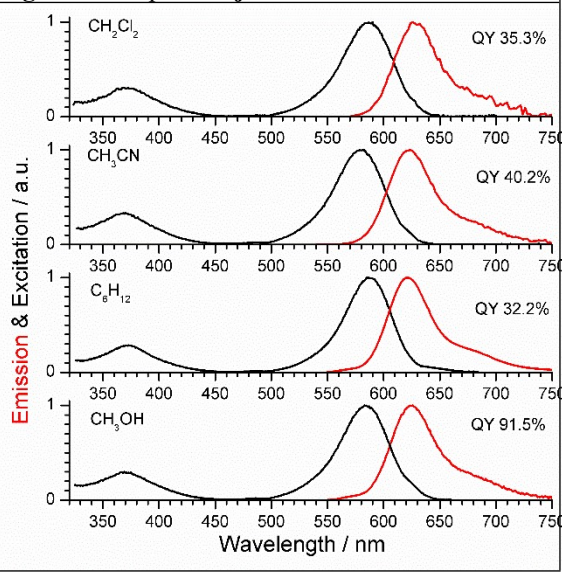



**Fig. S10** Compound **3j**




## 5. Quantum-chemical calculations

DFT and time-dependent density functional theory (TD-DFT) calculations to obtain minimum energy structures in both the ground and excited states for the structures **3a** and **4** were performed by using Gaussian09 set of programs.[3] The ground state was optimized at B3LYP level[4] with 6-31G(d,p) basis set and stationary points were characterized using vibrational analysis - to confirm the minimum nature of the optimized geometries. The effect of dispersion correction[5] was also evaluated on the optimized geometries (empiricaldispersion=gd3bj) and found to be negligible (see Table S2). The excitation spectra for **3a** and **4** structures were simulated by using TD-DFT calculations with a range-separated versions CAM-B3LYP[6] and 6-311+G(d,p) and TZVP basis sets. Solvent effects were treated by the conductor-like polarizable continuum model (CPCM) model[7] adopted in the linear response formalism when used with TD-DFT. According to a general trend of TD-DFT methods[8] we found an overestimation of **3a** and **4** absorption band peaks of about 0.3 eV, (compare the simulated spectra of Fig. S11 with the experimental one of Fig. 3); nevertheless, the yellow-light shift going from **4** to **3a** is well reproduced and the solvent effect was found to be negligible (see Table S2) in agreement with our experimental results. Finally, our TD-DFT analysis revealed that the

maximum of absorption for the S0 ←-S1 transition corresponds to the HOMO and LUMO difference and the MO contributions are reported in Fig. 4 and Fig. S12 for **3a** and **4**, respectively. The near-UV region with maximum at about 360 nm (see Fig. S11) can be attributed to the S0 ←-S2 and S0 ←-S3 transitions with the former more relevant for **3a** and the latter for **4** complexes. DFT and TD-DFT calculations of the structures reported in Table S3 were carried out with B3LYP hybrid functional combined with 6-31G(d) basis set by using ORCA 4.1.1. package programs.[9] Input files and molecular orbital plots were prepared with Gabedit 2.4.7 software.[10] In the case of compounds containing boronic atom, the def2-TZVP basis set[11] was used in combination with CPCM to take into account the effect of the solvent.

**Table S2.** Variability of simulation spectra depending on the computational approach for compounds **3a** and **4** (in parenthesis) compared with the experimental data. Wavelengths in nm.

| Geo | Methods | Calc. $\lambda_{ex}$ **3a** and (**4**)[a] | $\Delta\lambda_{ex}$[b] | Calc. $\Delta\lambda_{ex(\mathbf{3a-4})}$ shift[c] |
|---|---|---|---|---|
| B3LYP/631G(d,p) | CAM-B3LYP/6311G(d,p) | 537 (510) | 51 (51) | 26 |
| | CAM-B3LYP/TZVP | 534 (508) | 53 (53) | 26 |
| D3-B3LYP/631G(d,p) | CAM-B3LYP/6311G(d,p) | 533 (513) | 55 (48) | 20 |
| | CAM-B3LYP/TZVP | 531 (511) | 57 (50) | 20 |
| B3LYP/631G(d,p) | CAM-B3LYP/6311G(d,p) | 538 (510)[d] | - | - |

a) Calculated $\lambda_{ex}$ values for **3a** and **4** (in parenthesis) to be compared with the experimental $\lambda_{ex}$ of 588 and 561 nm for **3a** and **4**, respectively (see Fig. 3 of the text).
b) Variation between experimental and calculated $\lambda_{ex}$ for **3a** and **4** (in parenthesis).
c) Calculated shift going from **4** to **3a**. Values to be compared with the experimental shift of 27 nm.
d) Calculated values using $CH_2Cl_2$ as solvent in a place of THF.

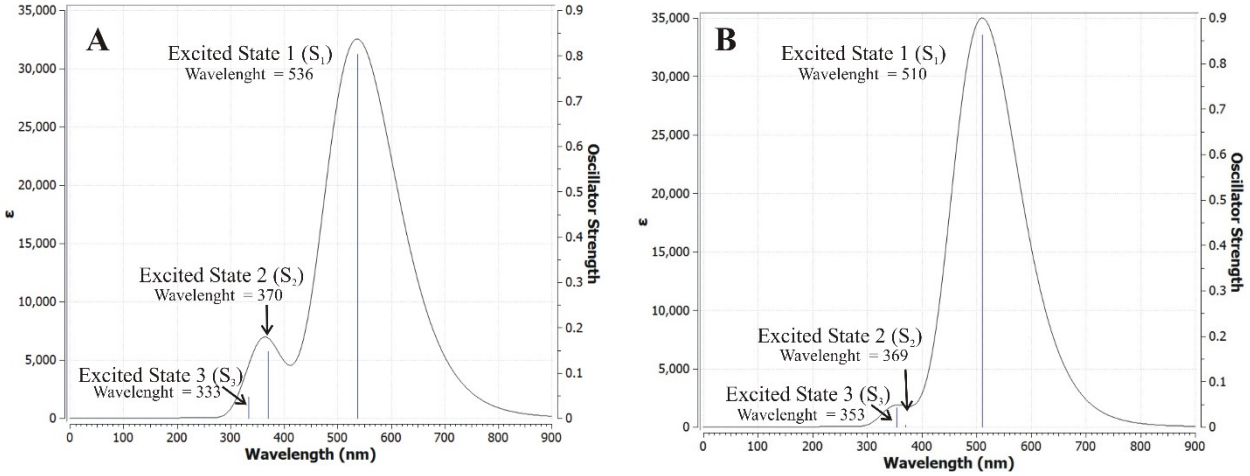



**Fig. S11** TD-DFT (CAM-B3LYP/6311+G(d,p)) **s**imulated spectra for **3a** (A) and **4** (B) in THF as solvent (CPCM model). Wavelenghts in nm.

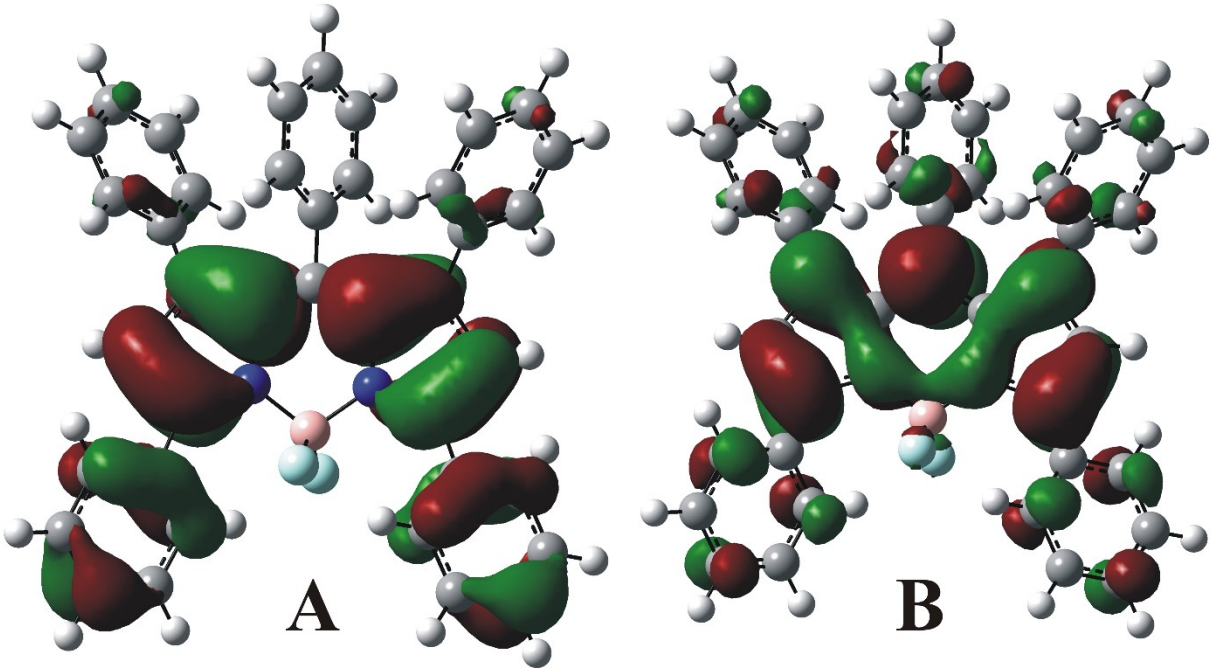



**Fig. S12** HOMO **(A)** and LUMO **(B)** countours calculated at the TD-DFT level for compound **4** corresponding to the S0 ←-S1 transition**.**

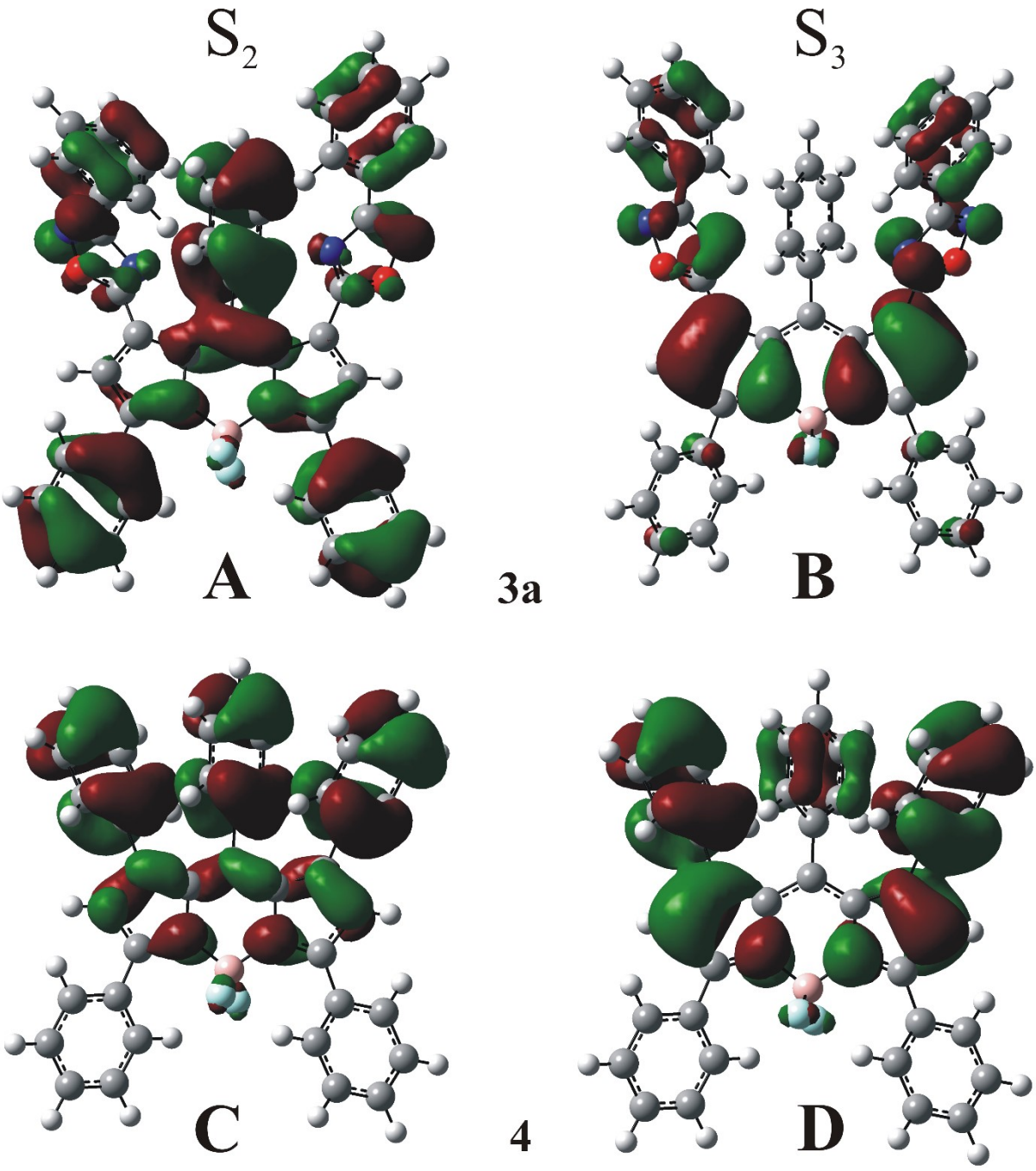



**Fig. S13** TD-DFT analysis (CAM-B3LYP/6311+G(d,p)) of MO contributions for S0 ←-S2 and S0 ←-S3 transitions to the near-UV region (maximum at about 360 nm, see Fig. S11) for complexes **3a** (A, B) and **4** (C, D).

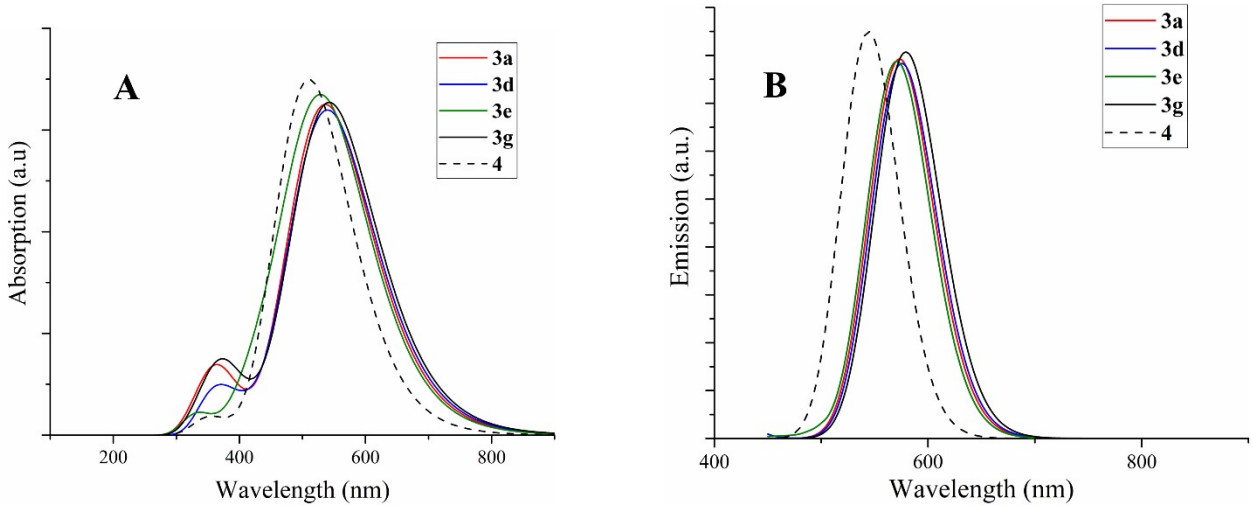



**Fig. S14** TD-DFT (CAM-B3LYP/6311+G(d,p)) simulated spectra for absorption (**A**) and emission (**B**) of selected oxadiazole compounds (**3a**, **3d**, **3e**, **3g**) in THF as solvent. Compound **4** (dotted line) is also reported for comparison.

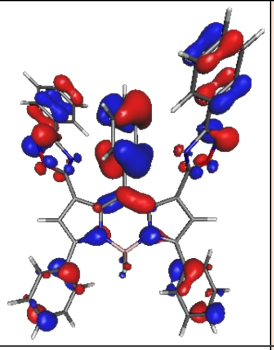
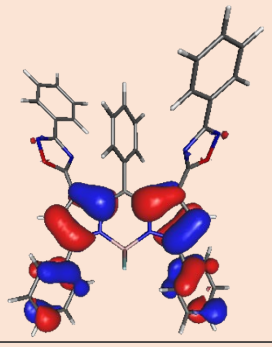
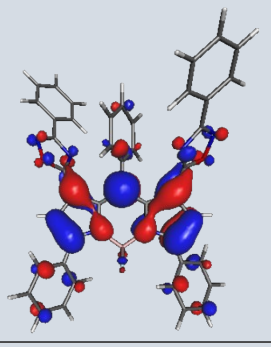
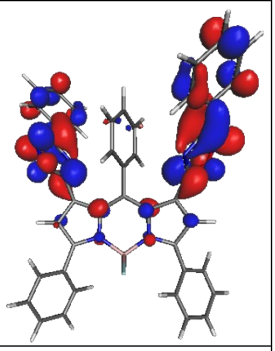
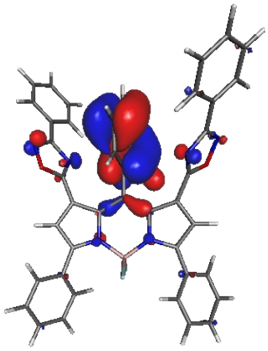
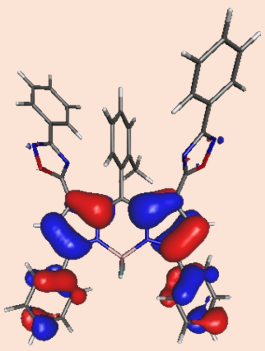
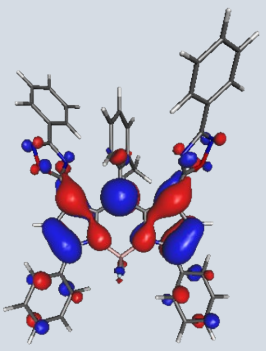
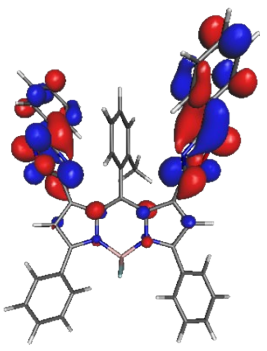
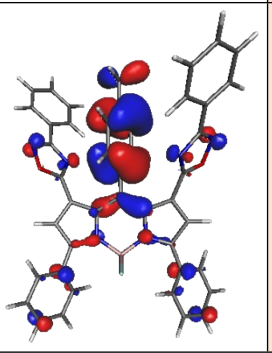
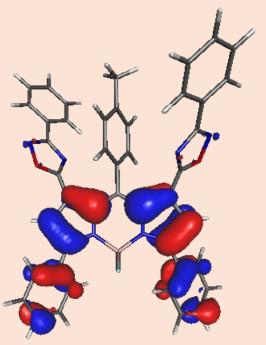
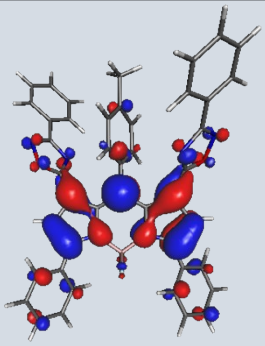
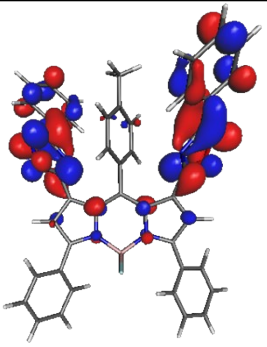
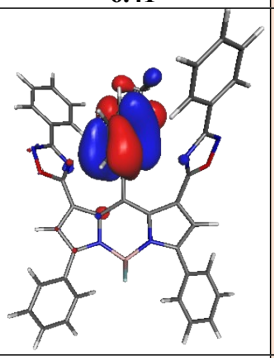
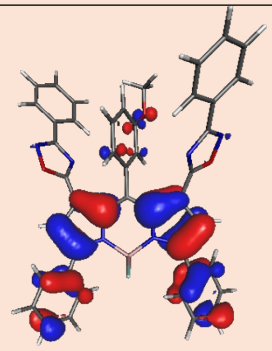
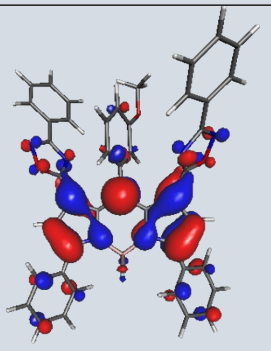
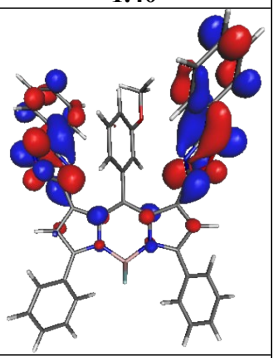
**Table S3.** Calculated main assignments (coefficient), excitation energies *E* (in eV), maximum absorption wavelengths $\lambda_{abs}$ (in nm), the oscillator strength *f*, for selected compounds at the TD-CAM-B3LYP/6-311+G(d,p)//B3LYP/6-31G(d,p) level, by using THF as solvent (CPCM).

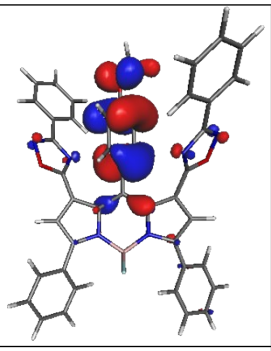
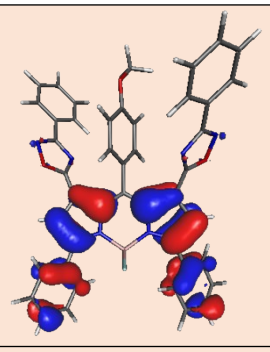
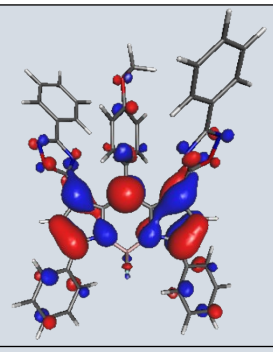
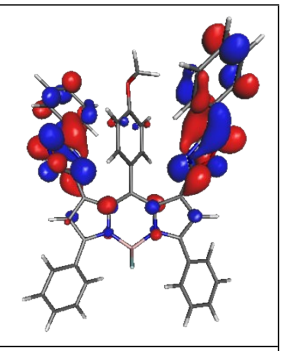
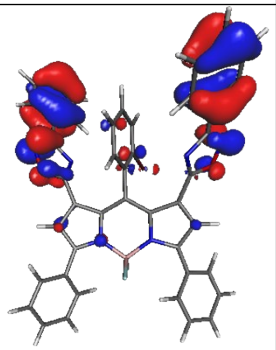
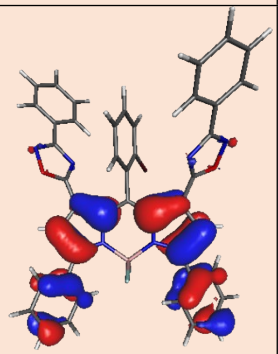
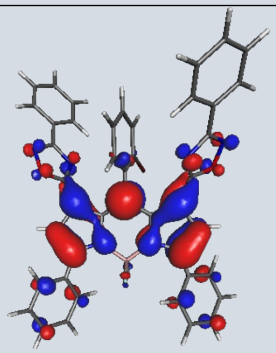
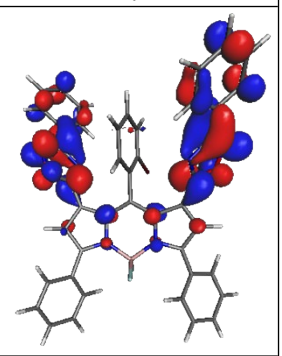
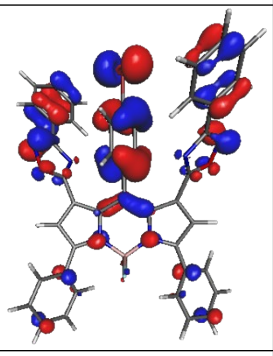
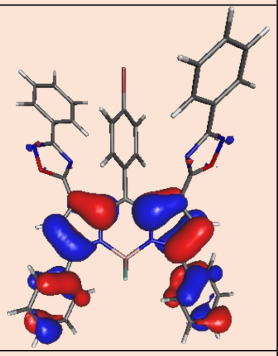
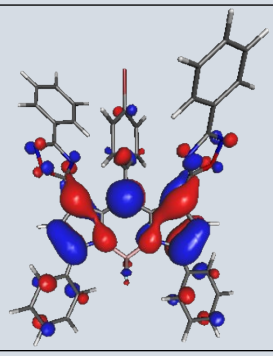
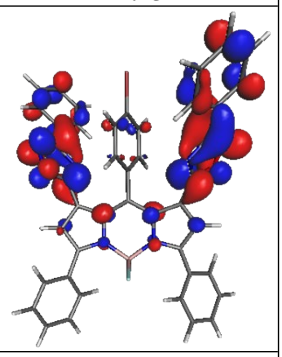
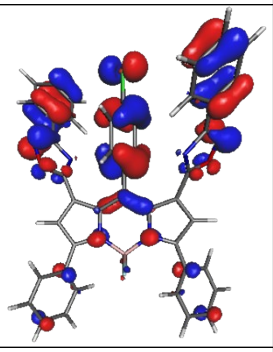
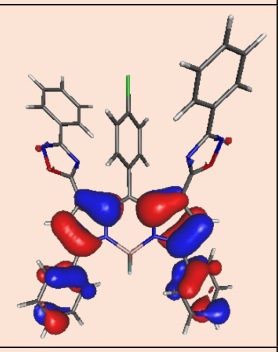
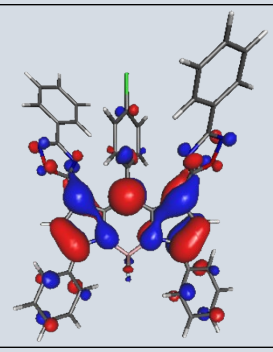
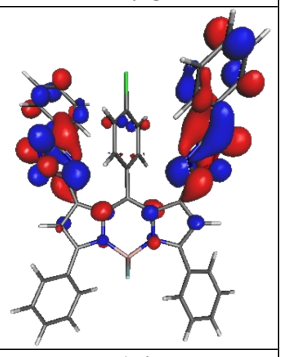
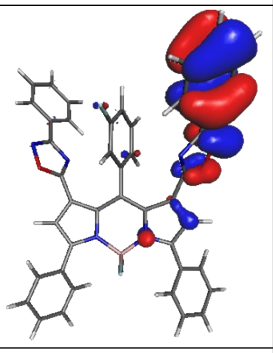
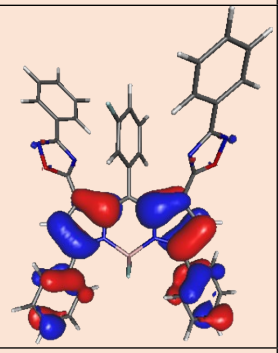
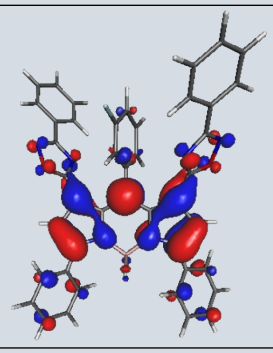
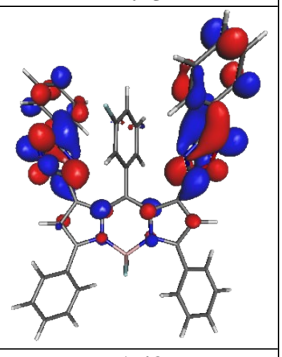
| Compounds | Main assignment | *E* | $\lambda_{abs}$ | *f* |
|---|---|---|---|---|
| **3a** | H → L (0.696) | 2.3104 | 536.62 | 0.8027 |
| **3a** | $H_{-1}$ → L (0.593) | 3.3502 | 370.09 | 0.1473 |
| **3a** | $H_{-10}$ → L (0.586) | 3.7130 | 333.92 | 0.0476 |
| **3d** | H → L (0.696) | 2.2954 | 540.14 | 0.7878 |
| **3d** | $H_{-1}$ → L (0.6976) | 3.0240 | 410.00 | 0.0414 |
| **3d** | $H_{-4}$ → L (0.5909) | 3.4189 | 362.64 | 0.1038 |
| **3e** | H → L (0.6954) | 2.3218 | 534.00 | 0.7907 |
| **3e** | $H_{-1}$ → L (0.6905) | 2.8373 | 436.98 | 0.1766 |
| **3e** | $H_{-10}$ → L (0.5745) | 3.7068 | 334.48 | 0.0535 |
| **3g** | H → L (0.6956) | 2.2846 | 542.69 | 0.8073 |
| **3g** | $H_{-1}$ → L (0.6732) | 3.2707 | 379.08 | 0.1591 |
| **3g** | $H_{-10}$ → L (0.5169) | 3.6422 | 340.41 | 0.0529 |
| **4** | H → L (0.6965) | 2.4287 | 510.49 | 0.8634 |
| **4** | $H_{-1}$ → L (0.6886) | 3.3556 | 369.49 | 0.0039 |
| **4** | $H_{-11}$ → L (0.14859) | 3.5117 | 353.06 | 0.0420 |

**Table S4.** Calculated main assignments (coefficient), excitation energies *E* (in eV), maximum emission wavelengths $\lambda_{em}$ (in nm), the oscillator strength *f*, for selected compounds at the TD-CAM-B3LYP/6-311+G(d,p)//TD-CAM-B3LYP/6-31G(d,p) level, by using THF as solvent (CPCM).

| Compounds | Main assignment | *E* | $\lambda_{em}$ | *f* |
|---|---|---|---|---|
| **3a** | H ← L (0.6969) | 2.1620 | 573.48 | 0.7815 |
| **3d** | H ← L (0.6969) | 2.1540 | 575.60 | 0.7723 |
| **3e** | H ← L (0.6967) | 2.1720 | 570.83 | 0.7768 |
| **3g** | H ← L (0.6969) | 2.1402 | 579.32 | 0.7957 |
| **4** | H ← L (0.6977) | 2.2775 | 544.40 | 0.8385 |

**Table S5.** DFT/TD-DFT calculations for **3a-3j** compounds.

| Compound | HOMO-1 / eV | HOMO / eV | LUMO / eV | LUMO+1 / eV |
|---|---|---|---|---|
| **3a** |  |  |  |  |
| | **-6.59** | **-5.74** | **-3.24** | **-1.41** |
| **3b** |  |  |  |  |
| | **-6.50** | **-5.74** | **-3.24** | **-1.39** |
| **3c** |  |  |  |  |
| | **-6.41** | **-5.73** | **-3.22** | **-1.40** |
| **3d** |  |  |  |  |
| | **-6.06** | **-5.72** | **-3.24** | **-1.40** |

| | | | | |
|---|---|---|---|---|
| **3e** |  |  |  |  |
| | **-6.00** | **-5.72** | **-3.20** | **-1.41** |
| **3f** |  |  |  |  |
| | **-6.63** | **-5.76** | **-3.34** | **-1.45** |
| **3g** |  |  |  |  |
| | **-6.58** | **-5.78** | **-3.31** | **-1.45** |
| **3h** |  |  |  |  |
| | **-6.59** | **-5.77** | **-3.33** | **-1.45** |
| **3i** |  |  |  |  |
| | **-6.63** | **-5.76** | **-3.30** | **-1.43** |

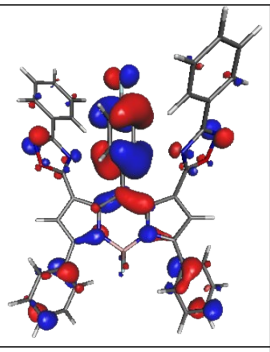
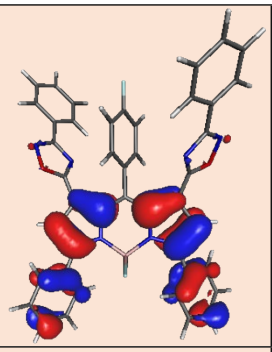
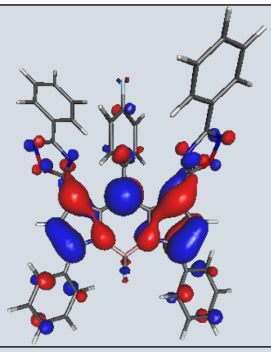
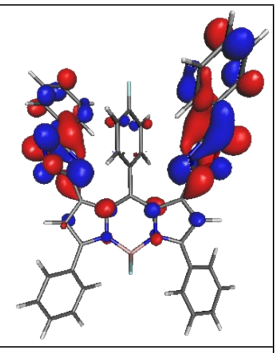
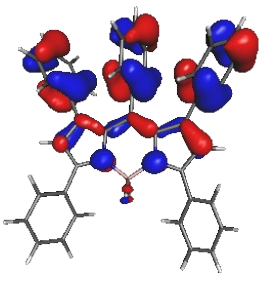
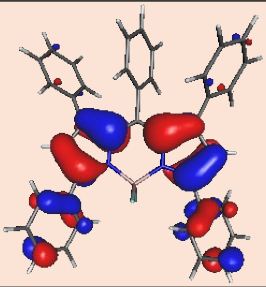
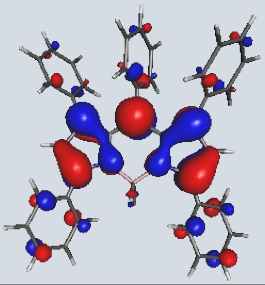
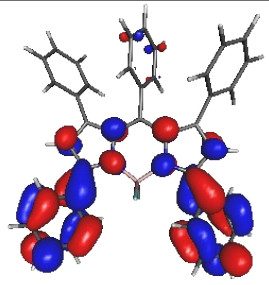
| | | | | |
|---|---|---|---|---|
| **3j** |  |  |  |  |
| | **-6.55** | **-5.76** | **-3.28** | **-1.44** |
| **4** |  |  |  |  |
| | **-6.08** | **-5.38** | **-2.74** | **-0.54** |

**Table S6.** Cartesian coordinates for the optimized compounds **3,** calculated at B3LYP/31G(d,p)/CPCM($CCl_2H_2$).

| **3a** | | | | **3b** | | | |
|---|---|---|---|---|---|---|---|
| C | 1.69997 | 1.65547 | 1.26782 | C | 1.64032 | 1.59904 | 1.34395 |
| C | 0.86618 | 0.58968 | 1.57618 | C | 0.80065 | 0.53237 | 1.62821 |
| C | 1.55103 | -0.60683 | 1.25950 | C | 1.48063 | -0.66158 | 1.28889 |
| N | 2.78775 | -0.28682 | 0.78321 | N | 2.72024 | -0.33936 | 0.82387 |
| C | 2.94136 | 1.09808 | 0.82192 | C | 2.87814 | 1.04523 | 0.88311 |
| C | 4.19550 | 1.70199 | 0.60817 | C | 4.13244 | 1.65089 | 0.68739 |
| C | 5.30679 | 0.92162 | 0.23436 | C | 5.25422 | 0.87043 | 0.35025 |
| N | 5.17501 | -0.43745 | -0.04784 | N | 5.14070 | -0.49634 | 0.09611 |
| B | 3.88517 | -1.27060 | 0.25500 | B | 3.83760 | -1.32665 | 0.34571 |
| C | 6.33174 | -0.88441 | -0.61420 | C | 6.31181 | -0.94405 | -0.43804 |
| C | 7.25274 | 0.18709 | -0.66446 | C | 7.22141 | 0.13740 | -0.50095 |
| C | 6.64629 | 1.30145 | -0.10081 | C | 6.59225 | 1.25816 | 0.02194 |
| C | 7.37800 | 2.53346 | 0.17022 | C | 7.29243 | 2.52383 | 0.22289 |
| C | 6.62627 | -2.23322 | -1.12579 | C | 6.63149 | -2.30227 | -0.90708 |
| C | 0.97729 | -1.94826 | 1.45598 | C | 0.89790 | -2.00318 | 1.44915 |
| C | 4.34635 | 3.17070 | 0.77650 | C | 4.27878 | 3.12494 | 0.86925 |
| C | 0.15653 | -2.14110 | 2.58707 | C | 0.05822 | -2.21794 | 2.56211 |
| C | -0.45452 | -3.37067 | 2.82343 | C | -0.56242 | -3.44957 | 2.75946 |
| C | -0.26969 | -4.42847 | 1.92856 | C | -0.36871 | -4.48691 | 1.84269 |
| C | 0.53116 | -4.24426 | 0.79813 | C | 0.45116 | -4.28047 | 0.72977 |
| C | 1.15152 | -3.01870 | 0.55890 | C | 1.08142 | -3.05299 | 0.52985 |
| C | 6.23641 | -3.42236 | -0.48192 | C | 6.23459 | -3.47752 | -0.24231 |
| C | 6.60555 | -4.65955 | -1.00864 | C | 6.62897 | -4.72481 | -0.72503 |
| C | 7.36388 | -4.73745 | -2.17979 | C | 7.41979 | -4.82671 | -1.87259 |
| C | 7.76032 | -3.56288 | -2.82547 | C | 7.82294 | -3.66605 | -2.53897 |
| C | 7.40163 | -2.32306 | -2.30099 | C | 7.43917 | -2.41614 | -2.05820 |
| C | 4.18871 | 3.75639 | 2.04190 | C | 4.28995 | 3.63252 | 2.17602 |
| C | 4.64659 | 3.98023 | -0.32975 | C | 4.39508 | 3.99310 | -0.23841 |
| C | 4.78018 | 5.35936 | -0.17081 | C | 4.54933 | 5.36150 | 0.01790 |
| C | 4.33699 | 5.13436 | 2.19750 | C | 4.43828 | 4.99985 | 2.40501 |
| C | 4.62957 | 5.93829 | 1.09230 | C | 4.57575 | 5.86572 | 1.31969 |
| F | 3.47540 | -1.87119 | -0.93465 | F | 3.48201 | -1.93228 | -0.85847 |
| F | 4.12843 | -2.21338 | 1.25249 | F | 4.03419 | -2.26534 | 1.35760 |
| H | -0.15615 | 0.65219 | 1.91860 | H | 8.24837 | 0.07219 | -0.82913 |
| H | 4.22431 | 5.57923 | 3.18202 | H | -0.22057 | 0.59289 | 1.97426 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| H | 3.97257 | 3.13079 | 2.90281 | H | 4.45082 | 5.38120 | 3.42186 |
| H | 5.00094 | 5.98088 | -1.03367 | H | 4.20026 | 2.94699 | 3.01384 |
| H | 4.75295 | 3.53195 | -1.31333 | H | 4.63596 | 6.04461 | -0.82341 |
| H | 0.01842 | -1.32894 | 3.29440 | H | -0.08748 | -1.42234 | 3.28653 |
| H | -0.74736 | -5.38709 | 2.10960 | H | -0.85402 | -5.44696 | 1.99338 |
| H | -1.07128 | -3.50257 | 3.70788 | H | -1.19395 | -3.59914 | 3.63060 |
| H | 1.75735 | -2.88550 | -0.32688 | H | 1.70405 | -2.90282 | -0.34156 |
| H | 0.67071 | -5.05826 | 0.09197 | H | 0.59819 | -5.07835 | 0.00691 |
| H | 5.66091 | -3.37607 | 0.43219 | H | 5.63167 | -3.41208 | 0.65271 |
| H | 7.70216 | -1.41553 | -2.81523 | H | 7.74555 | -1.52021 | -2.58897 |
| H | 8.34528 | -3.61076 | -3.73932 | H | 8.43286 | -3.73285 | -3.43523 |
| H | 7.64653 | -5.70500 | -2.58425 | H | 7.72210 | -5.80191 | -2.24304 |
| H | 6.30307 | -5.56791 | -0.49569 | H | 6.32048 | -5.62190 | -0.19606 |
| N | 8.86181 | 4.10473 | -0.28192 | N | 8.66614 | 4.14731 | -0.37184 |
| C | 1.24847 | 3.04244 | 1.30810 | C | 1.20820 | 2.98924 | 1.44928 |
| H | 4.74015 | 7.01206 | 1.21523 | H | 4.69561 | 6.93325 | 1.48326 |
| N | 1.27448 | 3.95099 | 0.37531 | N | 1.20443 | 3.92990 | 0.54898 |
| O | 0.59198 | 3.44599 | 2.41699 | O | 0.60524 | 3.36003 | 2.59950 |
| N | 0.16298 | 4.75937 | 2.17271 | N | 0.18201 | 4.68516 | 2.42059 |
| C | 0.59520 | 5.00474 | 0.95176 | C | 0.56392 | 4.97004 | 1.19151 |
| N | 7.49242 | 3.20688 | 1.27959 | N | 7.47138 | 3.21773 | 1.30998 |
| C | 8.42016 | 4.17596 | 0.95811 | C | 8.32863 | 4.21896 | 0.90029 |
| C | 0.36350 | 6.28105 | 0.26064 | C | 0.31690 | 6.27318 | 0.55833 |
| C | 8.88833 | 5.18641 | 1.91771 | C | 8.83481 | 5.26092 | 1.80515 |
| C | 8.27406 | 5.28387 | 3.17569 | C | 8.31913 | 5.35953 | 3.10657 |
| C | 8.71454 | 6.23497 | 4.09644 | C | 8.79578 | 6.34256 | 3.97413 |
| C | 9.76899 | 7.09225 | 3.77037 | C | 9.78891 | 7.23032 | 3.55147 |
| C | 10.38289 | 6.99816 | 2.51636 | C | 10.30531 | 7.13413 | 2.25449 |
| C | -0.41027 | 7.29140 | 0.85696 | C | -0.38048 | 7.28313 | 1.24303 |
| C | -0.62193 | 8.49411 | 0.18617 | C | -0.60794 | 8.51247 | 0.62819 |
| C | -0.06742 | 8.69953 | -1.08196 | C | -0.14499 | 8.74564 | -0.67151 |
| C | 0.70301 | 7.69668 | -1.67704 | C | 0.54844 | 7.74313 | -1.35513 |
| C | 0.92018 | 6.49072 | -1.01008 | C | 0.78061 | 6.51036 | -0.74457 |
| H | -1.22109 | 9.27174 | 0.65118 | H | -1.14725 | 9.28969 | 1.16197 |
| H | -0.84258 | 7.12984 | 1.83903 | H | -0.74070 | 7.10050 | 2.25017 |
| H | 1.52140 | 5.70892 | -1.46167 | H | 1.32025 | 5.72785 | -1.26701 |
| H | 1.13498 | 7.85262 | -2.66102 | H | 0.90893 | 7.92049 | -2.36398 |
| H | -0.23671 | 9.63746 | -1.60347 | H | -0.32573 | 9.70487 | -1.14844 |
| H | 8.23414 | 6.30590 | 5.06793 | H | 8.39101 | 6.41511 | 4.97932 |
| H | 7.45288 | 4.61769 | 3.41798 | H | 7.54488 | 4.66933 | 3.42445 |
| H | 10.11262 | 7.83012 | 4.49001 | H | 10.16088 | 7.99367 | 4.22923 |
| C | 9.94737 | 6.05091 | 1.59189 | C | 9.83295 | 6.15535 | 1.38264 |
| H | 11.20508 | 7.66076 | 2.26142 | H | 11.08019 | 7.82034 | 1.92443 |
| H | 10.42755 | 5.97335 | 0.62157 | H | 10.23766 | 6.07608 | 0.37869 |
| O | 8.17290 | 3.00494 | -0.81462 | O | 7.98198 | 3.01274 | -0.83156 |
| H | 8.27486 | 0.11680 | -1.00638 | C | 4.29158 | 3.49578 | -1.66179 |
| | | | | H | 3.32073 | 3.01689 | -1.83478 |
| | | | | H | 5.06343 | 2.75886 | -1.90617 |
| | | | | H | 4.38709 | 4.32621 | -2.36575 |
| | | **3c** | | | | **3d** | |
| C | 1.67137 | 1.66482 | 1.53703 | C | 1.66437 | 1.71315 | 1.64164 |
| C | 0.84540 | 0.58838 | 1.83147 | C | 0.82687 | 0.62945 | 1.86537 |
| C | 1.53526 | -0.59812 | 1.49126 | C | 1.51932 | -0.54418 | 1.48506 |
| N | 2.76799 | -0.26254 | 1.01463 | N | 2.76340 | -0.19365 | 1.05086 |
| C | 2.91392 | 1.12231 | 1.07619 | C | 2.91361 | 1.18579 | 1.18141 |
| C | 4.16363 | 1.73659 | 0.86223 | C | 4.16899 | 1.80399 | 1.02821 |
| C | 5.27571 | 0.96685 | 0.46752 | C | 5.28837 | 1.05383 | 0.62210 |
| N | 5.14958 | -0.38771 | 0.16339 | N | 5.16772 | -0.28709 | 0.25917 |
| B | 3.86617 | -1.23172 | 0.46086 | B | 3.87678 | -1.14172 | 0.49111 |
| C | 6.30660 | -0.81917 | -0.41513 | C | 6.33440 | -0.69424 | -0.31654 |
| C | 7.22180 | 0.25760 | -0.45060 | C | 7.24930 | 0.38399 | -0.29348 |
| C | 6.61148 | 1.35917 | 0.13428 | C | 6.62884 | 1.46022 | 0.32524 |
| C | 7.33626 | 2.59075 | 0.42588 | C | 7.34471 | 2.68319 | 0.67025 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| C | 6.60518 | -2.15748 | -0.95178 | C | 6.64445 | -2.01009 | -0.89928 |
| C | 0.97031 | -1.94621 | 1.66826 | C | 0.94638 | -1.89620 | 1.58900 |
| C | 4.30879 | 3.20171 | 1.04657 | C | 4.30570 | 3.25934 | 1.30230 |
| C | 0.15803 | -2.16278 | 2.80116 | C | 0.10454 | -2.15879 | 2.69027 |
| C | -0.44484 | -3.39952 | 3.02079 | C | -0.50543 | -3.40224 | 2.84142 |
| C | -0.26008 | -4.44132 | 2.10730 | C | -0.29839 | -4.40491 | 1.88968 |
| C | 0.53254 | -4.23354 | 0.97515 | C | 0.52354 | -4.15111 | 0.78817 |
| C | 1.14456 | -3.00058 | 0.75255 | C | 1.14267 | -2.91130 | 0.63397 |
| C | 6.22231 | -3.35982 | -0.32864 | C | 6.24651 | -3.23564 | -0.33319 |
| C | 6.59464 | -4.58564 | -0.87930 | C | 6.63022 | -4.43920 | -0.92336 |
| C | 7.34954 | -4.63898 | -2.05396 | C | 7.41148 | -4.44729 | -2.08193 |
| C | 7.73913 | -3.45113 | -2.67921 | C | 7.81628 | -3.23623 | -2.65041 |
| C | 7.37700 | -2.22264 | -2.13098 | C | 7.44290 | -2.02989 | -2.06221 |
| C | 4.14332 | 3.78221 | 2.31130 | C | 4.14645 | 3.74588 | 2.61114 |
| C | 4.61221 | 4.02739 | -0.04813 | C | 4.57747 | 4.13984 | 0.25427 |
| C | 4.73252 | 5.40295 | 0.12349 | C | 4.67575 | 5.51738 | 0.49974 |
| C | 4.28269 | 5.15980 | 2.47527 | C | 4.26883 | 5.11212 | 2.84747 |
| C | 4.57181 | 5.99450 | 1.38713 | C | 4.52620 | 6.00701 | 1.80420 |
| F | 3.44944 | -1.81305 | -0.73616 | F | 3.49357 | -1.67824 | -0.73723 |
| F | 4.12031 | -2.19086 | 1.43980 | F | 4.10616 | -2.13616 | 1.44086 |
| H | 8.24305 | 0.19803 | -0.79708 | H | 8.27567 | 0.33968 | -0.62676 |
| H | -0.17563 | 0.63929 | 2.17953 | H | -0.20108 | 0.66919 | 2.19418 |
| H | 4.16286 | 5.59251 | 3.46503 | H | 4.15897 | 5.49568 | 3.85772 |
| H | 3.92799 | 3.15421 | 3.17082 | H | 3.95266 | 3.05897 | 3.42821 |
| H | 4.95303 | 6.02931 | -0.73728 | H | -0.05127 | -1.39114 | 3.44220 |
| H | 0.01973 | -1.36366 | 3.52318 | H | -0.77488 | -5.37427 | 2.00454 |
| H | -0.73129 | -5.40550 | 2.27524 | H | -1.13882 | -3.58815 | 3.70418 |
| H | -1.05506 | -3.54942 | 3.90691 | H | 1.76527 | -2.72471 | -0.23020 |
| H | 1.74395 | -2.84986 | -0.13479 | H | 0.68106 | -4.92128 | 0.03798 |
| H | 0.67227 | -5.03469 | 0.25446 | H | 5.65363 | -3.24422 | 0.57099 |
| H | 5.64948 | -3.33275 | 0.58790 | H | 7.75062 | -1.09348 | -2.51711 |
| H | 7.67204 | -1.30454 | -2.62941 | H | 8.41921 | -3.22950 | -3.55377 |
| H | 8.32121 | -3.47997 | -3.59568 | H | 7.70529 | -5.38904 | -2.53621 |
| H | 7.63481 | -5.59773 | -2.47710 | H | 6.32095 | -5.37651 | -0.47001 |
| H | 6.29738 | -5.50438 | -0.38201 | N | 8.80069 | 4.30382 | 0.31274 |
| N | 8.79914 | 4.18737 | -0.00568 | C | 1.21490 | 3.09578 | 1.76810 |
| C | 1.20997 | 3.04698 | 1.60936 | N | 1.26160 | 4.06690 | 0.90114 |
| N | 1.23977 | 3.98443 | 0.70548 | O | 0.53694 | 3.42433 | 2.88884 |
| O | 0.53666 | 3.41163 | 2.72212 | N | 0.11925 | 4.75426 | 2.72902 |
| N | 0.10118 | 4.72894 | 2.51354 | C | 0.57710 | 5.08172 | 1.53695 |
| C | 0.54625 | 5.01481 | 1.30603 | N | 7.45490 | 3.28561 | 1.81999 |
| N | 7.45720 | 3.23858 | 1.54965 | C | 8.36492 | 4.28859 | 1.55678 |
| C | 8.37127 | 4.22453 | 1.24065 | C | 0.36899 | 6.40656 | 0.93491 |
| C | 0.31643 | 6.31248 | 0.65513 | C | 8.82215 | 5.24296 | 2.57726 |
| C | 8.84046 | 5.21682 | 2.21869 | C | 8.22296 | 5.24012 | 3.84633 |
| C | 8.22834 | 5.28973 | 3.47939 | C | 8.65500 | 6.13611 | 4.82463 |
| C | 8.67072 | 6.22248 | 4.41776 | C | 9.68550 | 7.03809 | 4.54532 |
| C | 9.72489 | 7.08570 | 4.10682 | C | 10.28345 | 7.04472 | 3.28008 |
| C | 10.33631 | 7.01645 | 2.84994 | C | -0.42357 | 7.37133 | 1.57967 |
| C | -0.51529 | 7.27669 | 1.24953 | C | -0.61089 | 8.62280 | 0.99644 |
| C | -0.72253 | 8.50193 | 0.61943 | C | -0.01312 | 8.92294 | -0.23238 |
| C | -0.10533 | 8.77615 | -0.60588 | C | 0.77604 | 7.96563 | -0.87615 |
| C | 0.72325 | 7.81948 | -1.19889 | C | 0.96923 | 6.71106 | -0.29663 |
| C | 0.93526 | 6.59068 | -0.57309 | H | -1.22522 | 9.36434 | 1.49900 |
| H | -1.36778 | 9.24313 | 1.08233 | H | -0.88923 | 7.13645 | 2.53126 |
| H | -0.99635 | 7.06145 | 2.19813 | H | 1.58424 | 5.96477 | -0.78826 |
| H | 1.58119 | 5.84459 | -1.02347 | H | 1.23879 | 8.19397 | -1.83162 |
| H | 1.20310 | 8.02856 | -2.15033 | H | -0.16413 | 9.89834 | -0.68612 |
| H | -0.27137 | 9.73135 | -1.09601 | H | 8.18699 | 6.12929 | 5.80476 |
| H | 8.19214 | 6.27450 | 5.39139 | H | 7.42050 | 4.53979 | 4.05260 |
| H | 7.40734 | 4.61912 | 3.70988 | H | 10.02318 | 7.73210 | 5.30993 |
| H | 10.07058 | 7.80865 | 4.84049 | C | 9.85636 | 6.15281 | 2.29834 |
| C | 9.89882 | 6.08762 | 1.90785 | H | 11.08663 | 7.74240 | 3.06051 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| H | 11.15849 | 7.68348 | 2.60673 | H | 10.32394 | 6.15290 | 1.31884 |
| H | 10.37757 | 6.02848 | 0.93551 | O | 8.12649 | 3.22938 | -0.28599 |
| O | 8.11521 | 3.09325 | -0.55644 | H | 4.68201 | 3.78329 | -0.76556 |
| H | 4.72835 | 3.59241 | -1.03668 | H | 4.60395 | 7.06700 | 2.01564 |
| C | 4.70173 | 7.48873 | 1.55623 | O | 4.91031 | 6.29240 | -0.59616 |
| H | 4.58809 | 7.78467 | 2.60240 | C | 5.01255 | 7.70552 | -0.41574 |
| H | 3.94040 | 8.01613 | 0.96954 | H | 4.07890 | 8.12450 | -0.02316 |
| H | 5.67800 | 7.84322 | 1.20609 | H | 5.20808 | 8.11928 | -1.40568 |
| | | | | H | 5.83919 | 7.96408 | 0.25644 |
| **3e** | | | | **3f** | | | |
| C | 1.70938 | 1.72615 | 1.67331 | C | 1.66142 | 1.66800 | 1.61106 |
| C | 0.86462 | 0.65093 | 1.91755 | C | 0.81075 | 0.59572 | 1.83587 |
| C | 1.54624 | -0.53196 | 1.55089 | C | 1.48828 | -0.58835 | 1.45997 |
| N | 2.79201 | -0.19619 | 1.10743 | N | 2.73734 | -0.25469 | 1.02757 |
| C | 2.95351 | 1.18299 | 1.21975 | C | 2.90493 | 1.12388 | 1.14836 |
| C | 4.21404 | 1.79070 | 1.04637 | C | 4.17406 | 1.71643 | 1.01494 |
| C | 5.31896 | 1.02205 | 0.62759 | C | 5.29477 | 0.94339 | 0.66068 |
| N | 5.17434 | -0.31295 | 0.25495 | N | 5.15750 | -0.39711 | 0.29974 |
| B | 3.88077 | -1.15401 | 0.51699 | B | 3.84310 | -1.22406 | 0.49361 |
| C | 6.33300 | -0.73581 | -0.32777 | C | 6.32867 | -0.83111 | -0.24558 |
| C | 7.26658 | 0.32474 | -0.29592 | C | 7.26457 | 0.22904 | -0.20231 |
| C | 6.66623 | 1.40637 | 0.33593 | C | 6.65130 | 1.32195 | 0.39179 |
| C | 7.40823 | 2.60466 | 0.70977 | C | 7.38745 | 2.53792 | 0.71262 |
| C | 6.61665 | -2.05052 | -0.92781 | C | 6.62533 | -2.15095 | -0.82438 |
| C | 0.96367 | -1.87875 | 1.67592 | C | 0.90094 | -1.93269 | 1.56778 |
| C | 4.37463 | 3.23980 | 1.29971 | C | 4.32776 | 3.17123 | 1.30287 |
| C | 0.13351 | -2.12198 | 2.79032 | C | 0.03350 | -2.17539 | 2.65388 |
| C | -0.48568 | -3.35817 | 2.96288 | C | -0.58441 | -3.41418 | 2.80960 |
| C | -0.29930 | -4.37317 | 2.02005 | C | -0.35939 | -4.43155 | 1.87777 |
| C | 0.51115 | -4.13869 | 0.90592 | C | 0.48783 | -4.19733 | 0.79097 |
| C | 1.13903 | -2.90607 | 0.73016 | C | 1.11389 | -2.96229 | 0.63156 |
| C | 6.20435 | -3.27656 | -0.37341 | C | 6.16029 | -3.37011 | -0.29603 |
| C | 6.56264 | -4.47872 | -0.98248 | C | 6.53174 | -4.57811 | -0.88452 |
| C | 7.33282 | -4.48506 | -2.14837 | C | 7.36649 | -4.59813 | -2.00496 |
| C | 7.75205 | -3.27360 | -2.70531 | C | 7.83748 | -3.39437 | -2.53666 |
| C | 7.40356 | -2.06887 | -2.09859 | C | 7.47684 | -2.18379 | -1.94973 |
| C | 4.15769 | 3.77357 | 2.58397 | C | 4.28562 | 3.60128 | 2.63921 |
| C | 4.73341 | 4.10891 | 0.26059 | C | 4.50350 | 4.14033 | 0.30424 |
| C | 4.30007 | 5.13269 | 2.81731 | C | 4.42490 | 4.94860 | 2.96560 |
| C | 4.63957 | 5.99963 | 1.76297 | C | 4.61214 | 5.89234 | 1.95443 |
| F | 3.45883 | -1.68234 | -0.70283 | F | 3.48118 | -1.74966 | -0.74532 |
| F | 4.12430 | -2.15459 | 1.45674 | F | 4.02878 | -2.22340 | 1.44808 |
| H | 8.29210 | 0.26454 | -0.62951 | H | 8.29768 | 0.16462 | -0.51023 |
| H | -0.16220 | 0.70316 | 2.24820 | H | -0.21569 | 0.64915 | 2.16701 |
| H | 4.14858 | 5.54912 | 3.80809 | H | 4.38992 | 5.25772 | 4.00562 |
| H | 3.89966 | 3.11351 | 3.40647 | H | 4.15625 | 2.86085 | 3.42245 |
| H | -0.00610 | -1.34456 | 3.53546 | H | -0.13422 | -1.39669 | 3.39157 |
| H | -0.78271 | -5.33701 | 2.15149 | H | -0.84126 | -5.39777 | 1.99654 |
| H | -1.10993 | -3.52867 | 3.83544 | H | -1.23672 | -3.58591 | 3.66109 |
| H | 1.75162 | -2.73447 | -0.14424 | H | 1.75522 | -2.79017 | -0.22183 |
| H | 0.65270 | -4.91846 | 0.16242 | H | 0.66000 | -4.98007 | 0.05724 |
| H | 5.62064 | -3.28705 | 0.53661 | H | 5.52719 | -3.37327 | 0.58057 |
| H | 7.72214 | -1.13183 | -2.54469 | H | 7.83501 | -1.25388 | -2.37930 |
| H | 8.34668 | -3.26502 | -3.61415 | H | 8.48204 | -3.39601 | -3.41095 |
| H | 7.60687 | -5.42566 | -2.61721 | H | 7.65019 | -5.54336 | -2.45840 |
| H | 6.24216 | -5.41648 | -0.53786 | H | 6.17064 | -5.50995 | -0.45918 |
| N | 8.91780 | 4.18730 | 0.40340 | N | 8.94138 | 4.06410 | 0.34793 |
| C | 1.26531 | 3.11271 | 1.76492 | C | 1.22568 | 3.05167 | 1.75808 |
| N | 1.33297 | 4.06617 | 0.87976 | N | 1.31906 | 4.05135 | 0.92834 |
| O | 0.57491 | 3.46972 | 2.86926 | O | 0.50242 | 3.34966 | 2.85955 |
| N | 0.16959 | 4.79948 | 2.67636 | N | 0.09848 | 4.68596 | 2.72456 |
| C | 0.64820 | 5.09930 | 1.48519 | C | 0.60996 | 5.04959 | 1.56519 |
| N | 7.50909 | 3.19253 | 1.86830 | N | 7.44996 | 3.21663 | 1.82304 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| C | 8.45302 | 4.17133 | 1.63690 | C | 8.42712 | 4.15478 | 1.55824 |
| C | 0.46367 | 6.41440 | 0.85480 | C | 0.42692 | 6.39142 | 0.99422 |
| C | 8.91250 | 5.10213 | 2.67801 | C | 8.86979 | 5.15141 | 2.54392 |
| C | 8.27981 | 5.10736 | 3.93070 | C | 8.20951 | 5.24595 | 3.77869 |
| C | 8.71358 | 5.98063 | 4.92850 | C | 8.62829 | 6.18181 | 4.72492 |
| C | 9.77901 | 6.85182 | 4.68512 | C | 9.70628 | 7.02685 | 4.44742 |
| C | 10.41046 | 6.85055 | 3.43619 | C | 10.36601 | 6.93568 | 3.21657 |
| C | -0.30545 | 7.41007 | 1.48058 | C | -0.36597 | 7.34840 | 1.65044 |
| C | -0.46880 | 8.65155 | 0.86949 | C | -0.53347 | 8.61443 | 1.09358 |
| C | 0.13012 | 8.91093 | -0.36804 | C | 0.08396 | 8.93671 | -0.12001 |
| C | 0.89595 | 7.92272 | -0.99292 | C | 0.87300 | 7.98715 | -0.77482 |
| C | 1.06442 | 6.67779 | -0.38577 | C | 1.04651 | 6.71825 | -0.22165 |
| H | -1.06471 | 9.41746 | 1.35747 | H | -1.14778 | 9.35014 | 1.60463 |
| H | -0.77108 | 7.20749 | 2.43959 | H | -0.84646 | 7.09666 | 2.59030 |
| H | 1.66009 | 5.90636 | -0.86172 | H | 1.65893 | 5.97606 | -0.72261 |
| H | 1.35950 | 8.11932 | -1.95507 | H | 1.35226 | 8.23304 | -1.71773 |
| H | -0.00186 | 9.87896 | -0.84321 | H | -0.05083 | 9.92405 | -0.55257 |
| H | 8.21948 | 5.98022 | 5.89579 | H | 8.11225 | 6.25059 | 5.67814 |
| H | 7.45049 | 4.43123 | 4.10942 | H | 7.37127 | 4.58856 | 3.98326 |
| H | 10.11795 | 7.52790 | 5.46509 | H | 10.03295 | 7.75262 | 5.18701 |
| C | 9.98185 | 5.98115 | 2.43513 | C | 9.95275 | 6.00341 | 2.26701 |
| H | 11.24096 | 7.52401 | 3.24473 | H | 11.20641 | 7.58857 | 2.99933 |
| H | 10.47532 | 5.97465 | 1.46841 | H | 10.46777 | 5.92847 | 1.31456 |
| O | 8.22664 | 3.13863 | -0.22256 | O | 8.25479 | 2.98398 | -0.22295 |
| O | 4.73254 | 7.31492 | 2.08653 | C | 4.64855 | 5.49078 | 0.61792 |
| C | 5.01905 | 8.25358 | 1.04675 | H | 4.77700 | 6.22049 | -0.17367 |
| H | 5.02949 | 9.23350 | 1.52484 | H | 4.72417 | 6.94468 | 2.19763 |
| H | 4.24455 | 8.23224 | 0.27110 | Br | 4.47714 | 3.65656 | -1.55228 |
| H | 5.99714 | 8.05942 | 0.59215 | | | | |
| C | 4.85586 | 5.48040 | 0.47780 | | | | |
| H | 5.11085 | 6.12791 | -0.35202 | | | | |
| H | 4.88707 | 3.71725 | -0.74061 | | | | |
| **3g** | | | | **3h** | | | |
| C | 1.68041 | 1.68634 | 1.68238 | C | 1.68293 | 1.69153 | 1.68816 |
| C | 0.83375 | 0.61250 | 1.91858 | C | 0.83710 | 0.61763 | 1.92688 |
| C | 1.51129 | -0.57044 | 1.54068 | C | 1.51443 | -0.56538 | 1.54865 |
| N | 2.75623 | -0.23533 | 1.09738 | N | 2.75858 | -0.23027 | 1.10331 |
| C | 2.92277 | 1.14314 | 1.21891 | C | 2.92465 | 1.14847 | 1.22338 |
| C | 4.18689 | 1.74213 | 1.05972 | C | 4.18792 | 1.74807 | 1.06049 |
| C | 5.29664 | 0.97447 | 0.65835 | C | 5.29680 | 0.97993 | 0.65725 |
| N | 5.15467 | -0.36450 | 0.29633 | N | 5.15463 | -0.35885 | 0.29482 |
| B | 3.85256 | -1.20012 | 0.53275 | B | 3.85315 | -1.19449 | 0.53381 |
| C | 6.31390 | -0.79123 | -0.28015 | C | 6.31344 | -0.78476 | -0.28330 |
| C | 7.24683 | 0.27116 | -0.25656 | C | 7.24620 | 0.27785 | -0.25991 |
| C | 6.64549 | 1.35794 | 0.36282 | C | 6.64496 | 1.36388 | 0.36093 |
| C | 7.39124 | 2.56012 | 0.71418 | C | 7.38939 | 2.56605 | 0.71578 |
| C | 6.60203 | -2.11123 | -0.86418 | C | 6.60093 | -2.10413 | -0.86932 |
| C | 0.92322 | -1.91497 | 1.65283 | C | 0.92669 | -1.90997 | 1.66211 |
| C | 4.35047 | 3.19726 | 1.31826 | C | 4.35230 | 3.20364 | 1.31451 |
| C | 0.08498 | -2.16308 | 2.76023 | C | 0.08958 | -2.15790 | 2.77036 |
| C | -0.53936 | -3.39832 | 2.91922 | C | -0.53460 | -3.39312 | 2.93029 |
| C | -0.35120 | -4.40615 | 1.96901 | C | -0.34737 | -4.40130 | 1.98025 |
| C | 0.46667 | -4.16629 | 0.86138 | C | 0.46940 | -4.16164 | 0.87178 |
| C | 1.10082 | -2.93516 | 0.69957 | C | 1.10336 | -2.93048 | 0.70906 |
| C | 6.18630 | -3.33100 | -0.29833 | C | 6.18660 | -3.32461 | -0.30401 |
| C | 6.55021 | -4.53968 | -0.89047 | C | 6.54992 | -4.53252 | -0.89820 |
| C | 7.32870 | -4.55849 | -2.05080 | C | 7.32639 | -4.54976 | -2.05988 |
| C | 7.75110 | -3.35331 | -2.61901 | C | 7.74735 | -3.34384 | -2.62755 |
| C | 7.39795 | -2.14197 | -2.02870 | C | 7.39480 | -2.13327 | -2.03528 |
| C | 4.19479 | 3.70649 | 2.61542 | C | 4.19712 | 3.71856 | 2.60956 |
| C | 4.66056 | 4.07195 | 0.26715 | C | 4.66394 | 4.07410 | 0.26017 |
| C | 4.35118 | 5.06915 | 2.86562 | C | 4.35572 | 5.08150 | 2.85417 |
| C | 4.65463 | 5.91886 | 1.80210 | C | 4.65989 | 5.92780 | 1.78781 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| F | 3.45563 | -1.72986 | -0.69390 | F | 3.45196 | -1.72218 | -0.69249 |
| F | 4.07138 | -2.19736 | 1.48154 | F | 4.07438 | -2.19339 | 1.48026 |
| H | 8.27289 | 0.20882 | -0.58788 | H | 8.27191 | 0.21589 | -0.59240 |
| H | -0.19221 | 0.66527 | 2.25152 | H | -0.18837 | 0.67045 | 2.26136 |
| H | 4.23929 | 5.45748 | 3.87158 | H | 4.24610 | 5.47722 | 3.85783 |
| H | 3.96990 | 3.03647 | 3.43921 | H | 3.97162 | 3.05182 | 3.43575 |
| H | -0.05645 | -1.39111 | 3.51062 | H | -0.05155 | -1.38578 | 3.52065 |
| H | -0.83942 | -5.36895 | 2.08977 | H | -0.83542 | -5.36409 | 2.10176 |
| H | -1.16931 | -3.57377 | 3.78665 | H | -1.16390 | -3.56815 | 3.79826 |
| H | 1.71997 | -2.75887 | -0.16925 | H | 1.72131 | -2.75473 | -0.16073 |
| H | 0.60891 | -4.94053 | 0.11233 | H | 0.61114 | -4.93587 | 0.12261 |
| H | 5.59593 | -3.33143 | 0.60746 | H | 5.59759 | -3.32612 | 0.60266 |
| H | 7.71934 | -1.20995 | -2.48314 | H | 7.71499 | -1.20050 | -2.48903 |
| H | 8.35222 | -3.35517 | -3.52357 | H | 8.34684 | -3.34446 | -3.53319 |
| H | 7.60707 | -5.50418 | -2.50660 | H | 7.60430 | -5.49487 | -2.51716 |
| H | 6.22775 | -5.47261 | -0.43736 | H | 6.22857 | -5.46605 | -0.44552 |
| N | 8.93053 | 4.10859 | 0.38607 | N | 8.91909 | 4.12433 | 0.39001 |
| C | 1.23587 | 3.07069 | 1.79666 | C | 1.23826 | 3.07615 | 1.79996 |
| N | 1.31218 | 4.04333 | 0.93344 | N | 1.30682 | 4.04391 | 0.93066 |
| O | 0.52581 | 3.39955 | 2.89708 | O | 0.53687 | 3.41063 | 2.90420 |
| N | 0.11085 | 4.72853 | 2.72406 | N | 0.11942 | 4.73835 | 2.72696 |
| C | 0.60470 | 5.05738 | 1.54670 | C | 0.60356 | 5.06087 | 1.54385 |
| N | 7.47754 | 3.18529 | 1.85420 | N | 7.48219 | 3.18055 | 1.86100 |
| C | 8.44261 | 4.14105 | 1.61038 | C | 8.44102 | 4.14289 | 1.61847 |
| C | 0.40649 | 6.37882 | 0.93490 | C | 0.39918 | 6.37848 | 0.92580 |
| C | 8.90010 | 5.09565 | 2.63021 | C | 8.90321 | 5.08896 | 2.64412 |
| C | 8.26755 | 5.12808 | 3.88248 | C | 8.28609 | 5.10042 | 3.90439 |
| C | 8.70065 | 6.02347 | 4.86071 | C | 8.72426 | 5.98661 | 4.88865 |
| C | 9.76587 | 6.88916 | 4.59819 | C | 9.77903 | 6.86438 | 4.62404 |
| C | 10.39783 | 6.86013 | 3.34988 | C | 10.39532 | 6.85663 | 3.36759 |
| C | -0.37385 | 7.35654 | 1.57531 | C | -0.36889 | 7.36278 | 1.57090 |
| C | -0.55761 | 8.60181 | 0.97850 | C | -0.55849 | 8.60424 | 0.96798 |
| C | 0.03171 | 8.88270 | -0.25907 | C | 0.01269 | 8.87470 | -0.28039 |
| C | 0.80898 | 7.91274 | -0.89768 | C | 0.77762 | 7.89810 | -0.92376 |
| C | 0.99818 | 6.66428 | -0.30491 | C | 0.97273 | 6.65350 | -0.32484 |
| H | -1.16206 | 9.35393 | 1.47731 | H | -1.15311 | 9.36166 | 1.47057 |
| H | -0.83244 | 7.13666 | 2.53389 | H | -0.81321 | 7.15107 | 2.53798 |
| H | 1.60211 | 5.90677 | -0.79291 | H | 1.56777 | 5.89101 | -0.81602 |
| H | 1.26684 | 8.12711 | -1.85870 | H | 1.22168 | 8.10451 | -1.89296 |
| H | -0.11622 | 9.85379 | -0.72308 | H | -0.13967 | 9.84292 | -0.74897 |
| H | 8.20675 | 6.04390 | 5.82785 | H | 8.24230 | 5.99081 | 5.86201 |
| H | 7.44047 | 4.45358 | 4.07730 | H | 7.46655 | 4.41707 | 4.10023 |
| H | 10.10425 | 7.58276 | 5.36289 | H | 10.12144 | 7.55089 | 5.39331 |
| C | 9.96957 | 5.96904 | 2.36811 | C | 9.96210 | 5.97452 | 2.37990 |
| H | 11.22814 | 7.52949 | 3.14381 | H | 11.21729 | 7.53567 | 3.15964 |
| H | 10.46289 | 5.94212 | 1.40169 | H | 10.44331 | 5.96405 | 1.40708 |
| O | 8.23498 | 3.05161 | -0.21884 | O | 8.22334 | 3.06991 | -0.21934 |
| C | 4.80885 | 5.43833 | 0.50205 | C | 4.81320 | 5.44070 | 0.48984 |
| H | 5.03819 | 6.11271 | -0.31509 | H | 5.04297 | 6.11462 | -0.32801 |
| H | 4.76702 | 3.69125 | -0.74398 | H | 4.77005 | 3.68908 | -0.74929 |
| Br | 4.86509 | 7.79337 | 2.13643 | Cl | 4.85540 | 7.65184 | 2.08719 |
| | | **3i** | | | | **3j** | |
| C | 1.72598 | 1.68891 | 1.70110 | C | 1.68177 | 1.69052 | 1.68535 |
| C | 0.87421 | 0.61975 | 1.93915 | C | 0.83530 | 0.61674 | 1.92370 |
| C | 1.53988 | -0.56575 | 1.54795 | C | 1.51333 | -0.56651 | 1.54818 |
| N | 2.78351 | -0.23725 | 1.09682 | N | 2.75840 | -0.23166 | 1.10458 |
| C | 2.95938 | 1.14000 | 1.22134 | C | 2.92406 | 1.14705 | 1.22347 |
| C | 4.22502 | 1.73066 | 1.05222 | C | 4.18698 | 1.74837 | 1.06010 |
| C | 5.33131 | 0.95524 | 0.65832 | C | 5.29548 | 0.97988 | 0.65499 |
| N | 5.18510 | -0.38585 | 0.30589 | N | 5.15335 | -0.35856 | 0.29164 |
| B | 3.87348 | -1.20977 | 0.53196 | B | 3.85273 | -1.19488 | 0.53317 |
| C | 6.34535 | -0.82141 | -0.26178 | C | 6.31317 | -0.78486 | -0.28462 |
| C | 7.28333 | 0.23674 | -0.23994 | C | 7.24609 | 0.27717 | -0.25905 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| C | 6.68333 | 1.33138 | 0.36682 | C | 6.64412 | 1.36336 | 0.36147 |
| C | 7.43001 | 2.53564 | 0.70957 | C | 7.38762 | 2.56644 | 0.71539 |
| C | 6.62970 | -2.14565 | -0.83825 | C | 6.60093 | -2.10400 | -0.87160 |
| C | 0.94217 | -1.90645 | 1.65297 | C | 0.92611 | -1.91142 | 1.66342 |
| C | 4.40324 | 3.18940 | 1.28730 | C | 4.35019 | 3.20232 | 1.31631 |
| C | 0.10820 | -2.15826 | 2.76261 | C | 0.08860 | -2.15790 | 2.77168 |
| C | -0.52503 | -3.39003 | 2.91345 | C | -0.53467 | -3.39333 | 2.93382 |
| C | -0.35026 | -4.39030 | 1.95273 | C | -0.34583 | -4.40343 | 1.98619 |
| C | 0.46342 | -4.14649 | 0.84284 | C | 0.47148 | -4.16534 | 0.87779 |
| C | 1.10649 | -2.91895 | 0.68921 | C | 1.10424 | -2.93384 | 0.71272 |
| C | 6.20663 | -3.36071 | -0.26782 | C | 6.18601 | -3.32508 | -0.30813 |
| C | 6.56761 | -4.57397 | -0.85252 | C | 6.54927 | -4.53244 | -0.90356 |
| C | 7.35034 | -4.60192 | -2.00976 | C | 7.32653 | -4.54866 | -2.06470 |
| C | 7.77985 | -3.40145 | -2.58256 | C | 7.74820 | -3.34214 | -2.63056 |
| C | 7.42967 | -2.18562 | -1.99974 | C | 7.39544 | -2.13216 | -2.03713 |
| C | 4.31812 | 3.70017 | 2.58874 | C | 4.17892 | 3.71600 | 2.61131 |
| C | 4.67389 | 4.04745 | 0.21131 | C | 4.67523 | 4.07329 | 0.26464 |
| C | 4.52375 | 5.05961 | 2.77895 | C | 4.33483 | 5.07821 | 2.85859 |
| C | 4.78514 | 5.93412 | 1.73024 | C | 4.65099 | 5.91447 | 1.79281 |
| F | 3.47730 | -1.73104 | -0.69858 | F | 3.44950 | -1.72308 | -0.69241 |
| F | 4.07795 | -2.21256 | 1.47811 | F | 4.07648 | -2.19381 | 1.47914 |
| H | 8.31085 | 0.16687 | -0.56523 | H | 8.27226 | 0.21514 | -0.59016 |
| H | -0.14749 | 0.67762 | 2.28416 | H | -0.19059 | 0.66980 | 2.25690 |
| H | 4.13268 | 3.05696 | 3.44207 | H | 4.21731 | 5.49113 | 3.85467 |
| H | -0.02310 | -1.39236 | 3.52104 | H | 3.94353 | 3.04675 | 3.43264 |
| H | -0.84545 | -5.35031 | 2.06711 | H | -0.05356 | -1.38433 | 3.52027 |
| H | -1.15162 | -3.56861 | 3.78266 | H | -0.83295 | -5.36646 | 2.10951 |
| H | 1.72264 | -2.73962 | -0.18120 | H | -1.16433 | -3.56706 | 3.80181 |
| H | 0.59544 | -4.91466 | 0.08569 | H | 1.72270 | -2.75934 | -0.15695 |
| H | 5.61232 | -3.35383 | 0.63531 | H | 0.61464 | -4.94116 | 0.13054 |
| H | 7.75647 | -1.25719 | -2.45766 | H | 5.59652 | -3.32758 | 0.59821 |
| H | 8.38415 | -3.41043 | -3.48496 | H | 7.71607 | -1.19899 | -2.48975 |
| H | 7.62644 | -5.55109 | -2.45970 | H | 8.34831 | -3.34179 | -3.53580 |
| H | 6.23947 | -5.50318 | -0.39587 | H | 7.60444 | -5.49331 | -2.52294 |
| N | 8.98234 | 4.07053 | 0.37697 | H | 6.22722 | -5.46638 | -0.45221 |
| C | 1.29832 | 3.07612 | 1.84327 | N | 8.91442 | 4.12721 | 0.38594 |
| N | 1.36146 | 4.05883 | 0.99074 | C | 1.23961 | 3.07602 | 1.79811 |
| O | 0.62372 | 3.39915 | 2.96787 | N | 1.30739 | 4.04427 | 0.92930 |
| N | 0.22089 | 4.73491 | 2.82392 | O | 0.54602 | 3.41290 | 2.90673 |
| C | 0.68512 | 5.07322 | 1.63726 | N | 0.13538 | 4.74330 | 2.73392 |
| N | 7.50011 | 3.18378 | 1.83813 | C | 0.61484 | 5.06456 | 1.54861 |
| C | 8.47245 | 4.13059 | 1.59126 | N | 7.47853 | 3.18483 | 1.85875 |
| C | 0.48835 | 6.40580 | 1.04933 | C | 8.43436 | 4.14913 | 1.61351 |
| C | 8.91160 | 5.11008 | 2.59606 | C | 0.41867 | 6.38598 | 0.93575 |
| C | 8.20947 | 5.22820 | 3.80582 | C | 8.88978 | 5.10309 | 2.63505 |
| C | 8.62169 | 6.15360 | 4.76516 | C | 8.26816 | 5.12011 | 3.89319 |
| C | 9.73433 | 6.96484 | 4.52634 | C | 8.69840 | 6.01550 | 4.87280 |
| C | 10.43546 | 6.85074 | 3.32060 | C | 9.74948 | 6.89702 | 4.60564 |
| C | -0.24948 | 7.38925 | 1.73009 | C | 10.37016 | 6.88365 | 3.35138 |
| C | -0.43024 | 8.64593 | 1.15644 | C | -0.33625 | 7.37538 | 1.58864 |
| C | 0.11956 | 8.93253 | -0.09795 | C | -0.51598 | 8.62136 | 0.99191 |
| C | 0.85426 | 7.95668 | -0.77698 | C | 0.05197 | 8.89138 | -0.25806 |
| C | 1.04074 | 6.69690 | -0.20739 | C | 0.80371 | 7.90968 | -0.90930 |
| H | -1.00116 | 9.40263 | 1.68673 | C | 0.98915 | 6.66055 | -0.31651 |
| H | -0.67692 | 7.16513 | 2.70194 | H | -1.10020 | 9.38269 | 1.50069 |
| H | 1.61323 | 5.93508 | -0.72561 | H | -0.77779 | 7.16419 | 2.55709 |
| H | 1.28159 | 8.17563 | -1.75093 | H | 1.57435 | 5.89438 | -0.81373 |
| H | -0.02598 | 9.91258 | -0.54348 | H | 1.24521 | 8.11568 | -1.87975 |
| H | 8.07299 | 6.24065 | 5.69841 | H | -0.09259 | 9.86315 | -0.72172 |
| H | 7.34369 | 4.59975 | 3.98348 | H | 8.21302 | 6.02400 | 5.84441 |
| H | 10.05527 | 7.68237 | 5.27639 | H | 7.45110 | 4.43433 | 4.09098 |
| C | 10.02876 | 5.92899 | 2.35791 | H | 10.08542 | 7.59089 | 5.37114 |
| H | 11.30290 | 7.47703 | 3.13354 | C | 9.94496 | 5.99238 | 2.36838 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| H | 10.57593 | 5.83546 | 1.42521 | H | 11.18904 | 7.56576 | 3.14136 |
| O | 8.29406 | 3.00318 | -0.21757 | H | 10.42924 | 5.97798 | 1.39715 |
| C | 4.85337 | 5.41294 | 0.43649 | O | 8.22189 | 3.06897 | -0.22038 |
| H | 5.05281 | 6.07640 | -0.39924 | C | 4.82165 | 5.43933 | 0.49657 |
| H | 4.72592 | 3.64971 | -0.79711 | H | 5.05959 | 6.12873 | -0.30623 |
| F | 4.48264 | 5.54616 | 4.04136 | H | 4.79237 | 3.68633 | -0.74280 |
| H | 4.93534 | 6.98958 | 1.93180 | F | 4.79754 | 7.23691 | 2.02551 |

**4**

| | | | |
|---|---|---|---|
| C | 1.69346 | 2.61036 | 0.77729 |
| C | 0.79981 | 1.55218 | 0.90447 |
| C | 1.50734 | 0.33818 | 0.78225 |
| N | 2.82646 | 0.62149 | 0.59134 |
| C | 2.99636 | 2.01284 | 0.63836 |
| C | 4.28994 | 2.57278 | 0.71081 |
| C | 5.44098 | 1.76056 | 0.61964 |
| N | 5.32203 | 0.39059 | 0.34559 |
| B | 3.98143 | -0.39672 | 0.37011 |
| C | 6.55905 | -0.10515 | 0.06211 |
| C | 7.50213 | 0.93489 | 0.19697 |
| C | 6.84109 | 2.09577 | 0.58416 |
| C | 6.91089 | -1.47846 | -0.34231 |
| C | 0.87270 | -0.98881 | 0.88142 |
| C | 4.44287 | 4.04554 | 0.89139 |
| C | -0.18474 | -1.13253 | 1.80437 |
| C | -0.86445 | -2.34251 | 1.93219 |
| C | -0.51014 | -3.43356 | 1.13361 |
| C | 0.52826 | -3.29992 | 0.20797 |
| C | 1.21541 | -2.09297 | 0.07867 |
| C | 6.34324 | -2.63778 | 0.21823 |
| C | 6.77576 | -3.90066 | -0.18563 |
| C | 7.77665 | -4.03633 | -1.15133 |
| C | 8.35108 | -2.89268 | -1.71267 |
| C | 7.92743 | -1.62804 | -1.30898 |
| C | 4.04522 | 4.65510 | 2.08984 |
| C | 4.98662 | 4.83328 | -0.13329 |
| C | 5.12456 | 6.21049 | 0.03684 |
| C | 4.19819 | 6.03034 | 2.26306 |
| C | 4.73503 | 6.81136 | 1.23659 |
| F | 3.84256 | -1.05134 | -0.86025 |
| F | 3.95815 | -1.31221 | 1.43026 |
| H | -0.27399 | 1.63743 | 0.99561 |
| H | 3.89531 | 6.49152 | 3.19904 |
| H | 3.62570 | 4.04892 | 2.88718 |
| H | 5.53893 | 6.81297 | -0.76669 |
| H | 5.29187 | 4.36624 | -1.06479 |
| H | -0.45732 | -0.29509 | 2.43914 |
| H | -1.03845 | -4.37787 | 1.23124 |
| H | -1.66785 | -2.43340 | 2.65806 |
| H | 2.01161 | -2.00121 | -0.64732 |
| H | 0.80478 | -4.14001 | -0.42333 |
| H | 5.57355 | -2.54685 | 0.97253 |
| H | 8.36985 | -0.74523 | -1.75990 |
| H | 9.12712 | -2.98428 | -2.46767 |
| H | 8.10712 | -5.02319 | -1.46244 |
| H | 6.33023 | -4.78414 | 0.26270 |
| H | 4.84983 | 7.88361 | 1.37132 |
| C | 1.23801 | 4.01631 | 0.72269 |
| C | 7.57179 | 3.33133 | 0.93976 |
| C | 7.40370 | 3.95372 | 2.18833 |
| C | 8.17728 | 5.05918 | 2.53969 |
| C | 9.13663 | 5.55940 | 1.65424 |
| C | 9.32197 | 4.94075 | 0.41527 |
| C | 0.34643 | 4.49292 | 1.70022 |

| | | | |
|---|---|---|---|
| C | -0.18063 | 5.78233 | 1.61711 |
| C | 0.16550 | 6.61417 | 0.54897 |
| C | 1.04064 | 6.14557 | -0.43573 |
| C | 1.56981 | 4.85817 | -0.35258 |
| H | -0.86234 | 6.13544 | 2.38655 |
| H | 0.07771 | 3.84988 | 2.53388 |
| H | -0.24611 | 7.61728 | 0.48182 |
| H | 8.03513 | 5.52735 | 3.50978 |
| H | 6.67060 | 3.56273 | 2.88609 |
| H | 9.73654 | 6.42272 | 1.92916 |
| C | 8.55074 | 3.83236 | 0.06364 |
| H | 10.06720 | 5.31999 | -0.27902 |
| H | 8.69416 | 3.35570 | -0.90207 |
| H | 8.57230 | 0.81785 | 0.09898 |
| H | 1.30570 | 6.78173 | -1.27603 |
| H | 2.23500 | 4.49607 | -1.12960 |

**Table S7.**Total energies for the optimized compounds **3,** calculated at B3LYP/31G(d,p)/CPCM($CCl_2H_2$).

| Compound | Total energy / Hatree |
|---|---|
| 3a | -2357.12876368 |
| 3b | -2416.65709432 |
| 3c | -2471.59658013 |
| 3d | -2396.42014345 |
| 3e | -2440.35730430 |
| 3f | -2456.32922605 |
| 3g | -2440.25152207 |
| 3h | -2471.59519117 |
| 3i | -2456.32849846 |
| 3j | -2396.41715296 |
| 4 | -1835.57217178 |

## 6. Acknowlegments

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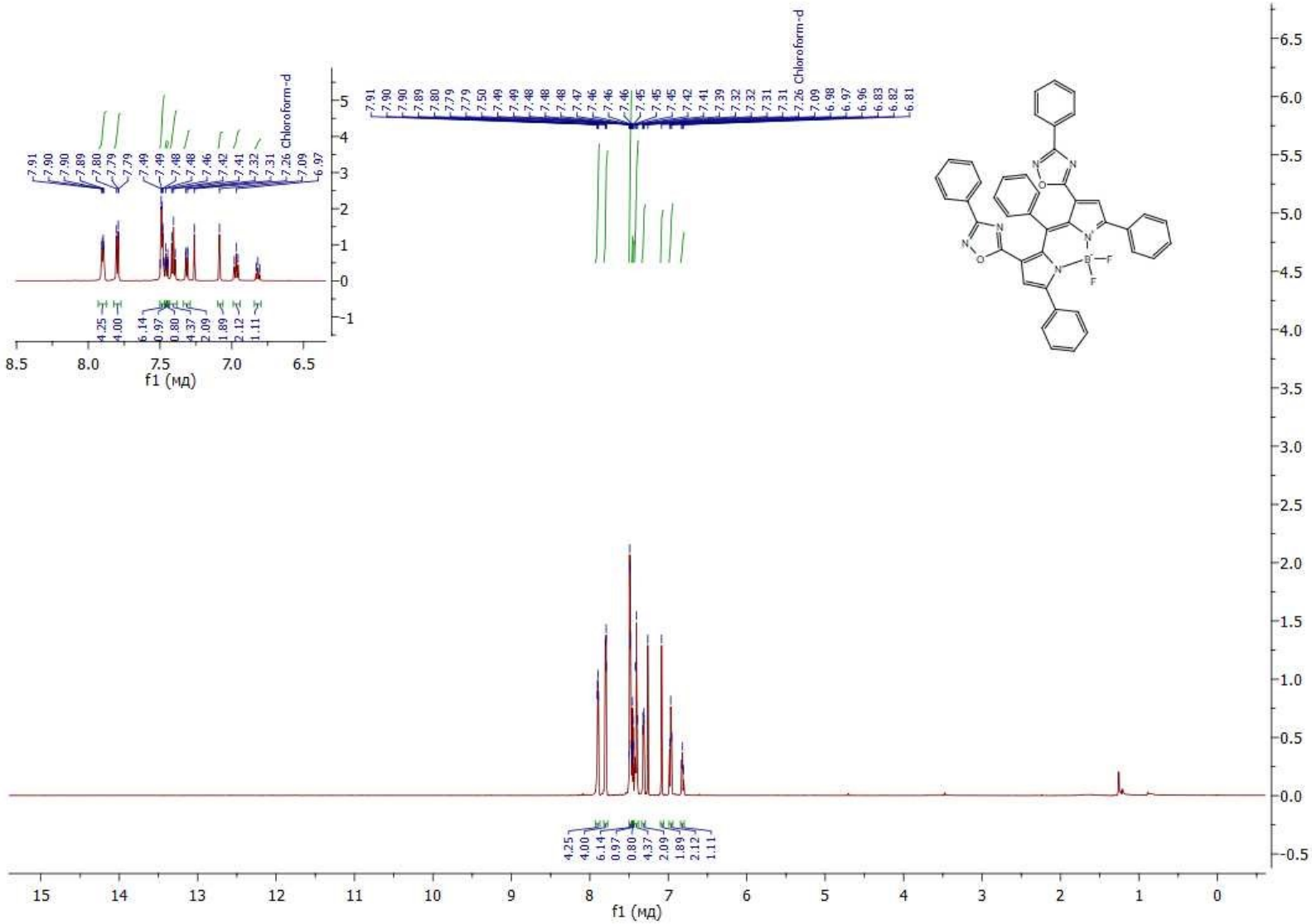
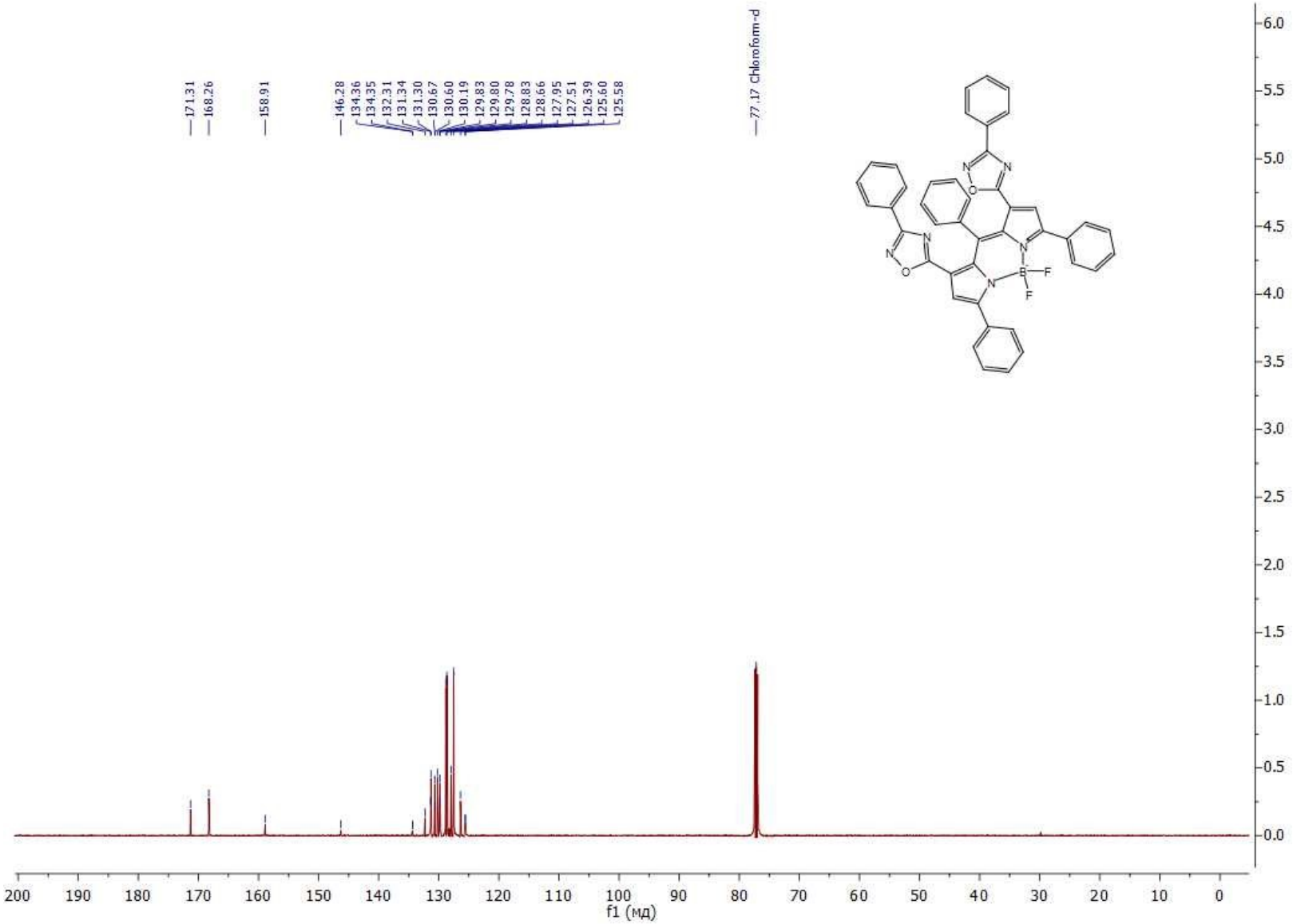
## 8. NMR spectra for products

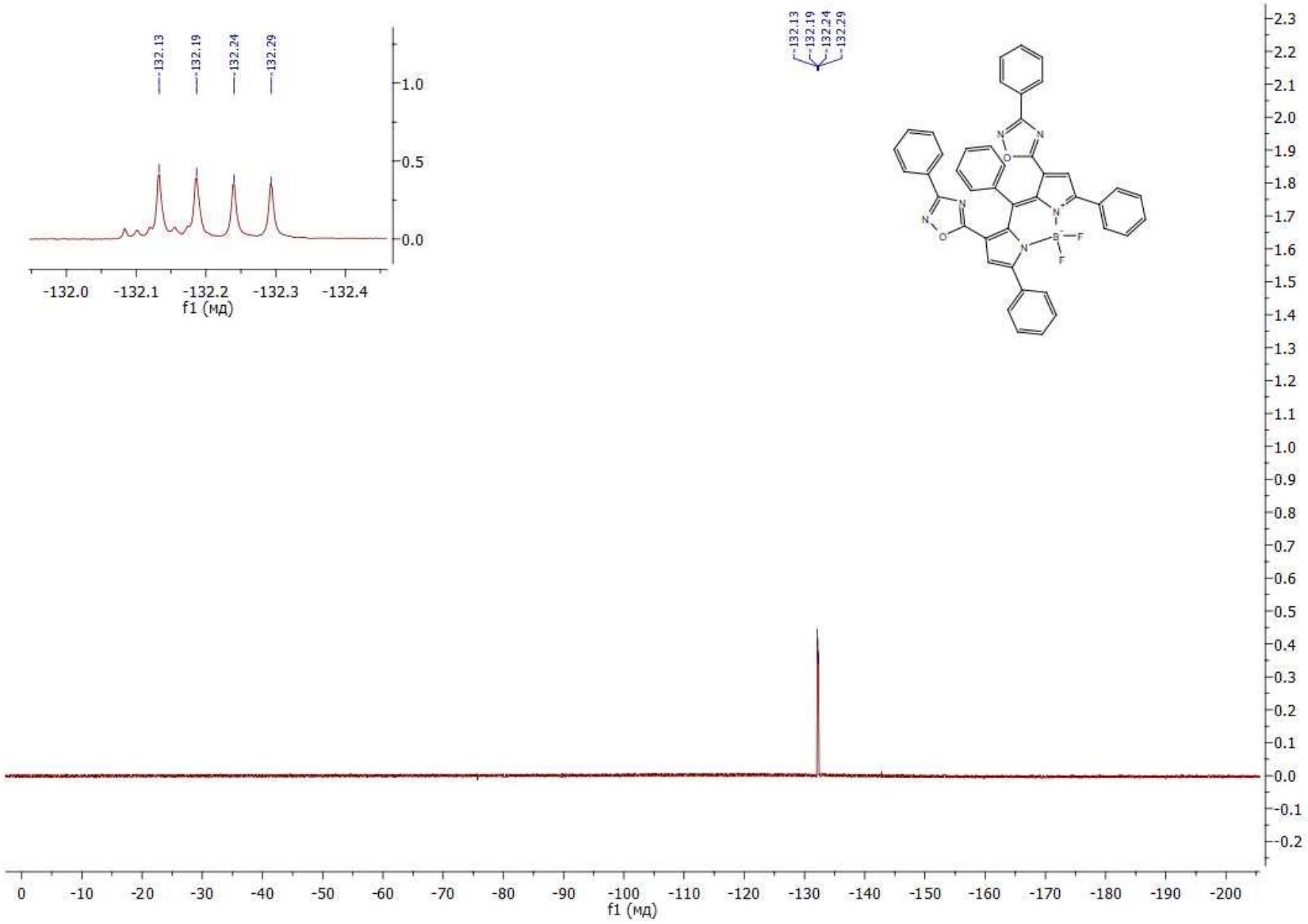
$^{1}$H NMR spectrum for **3a**



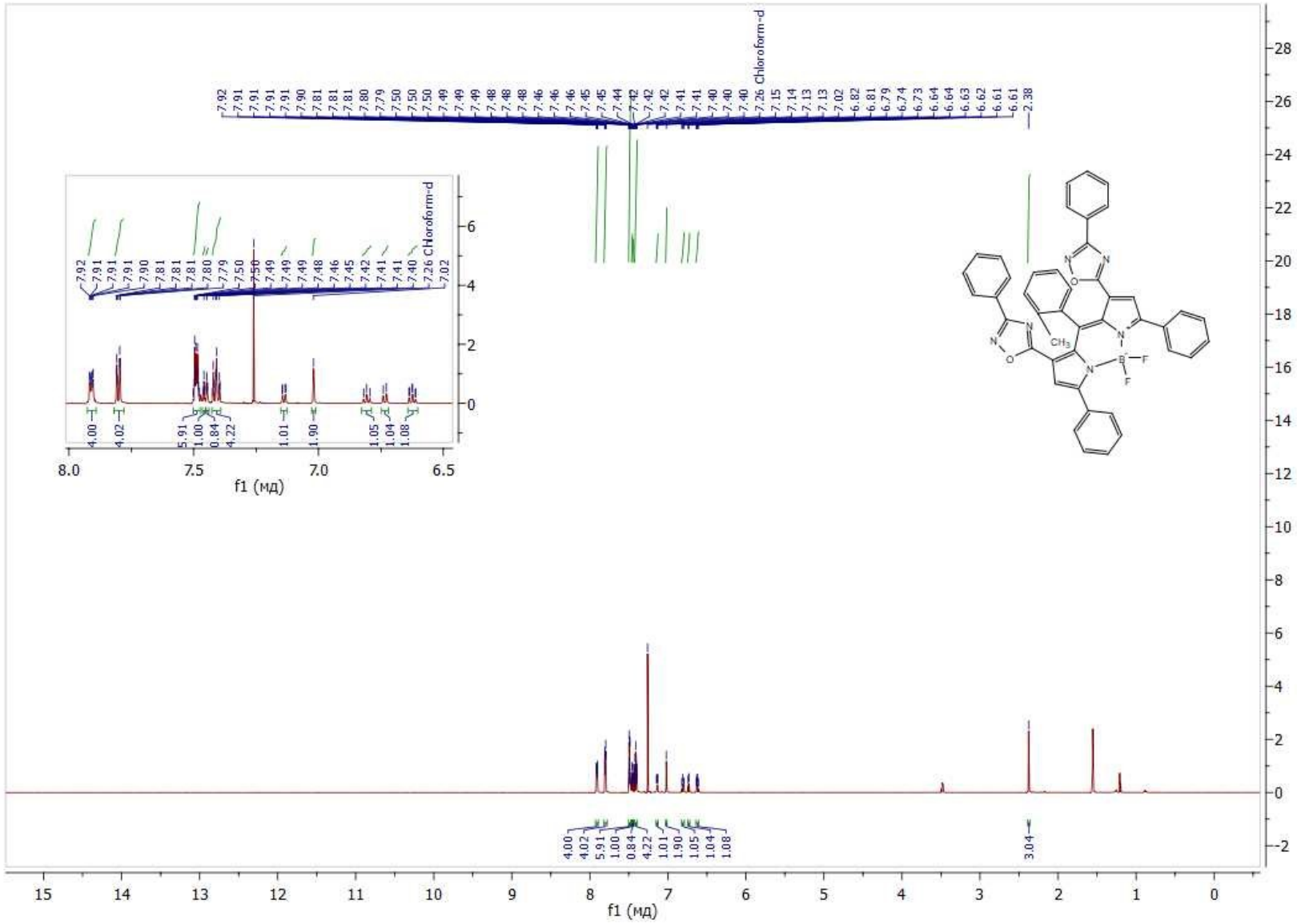
$^{13}$C NMR spectrum for **3a**



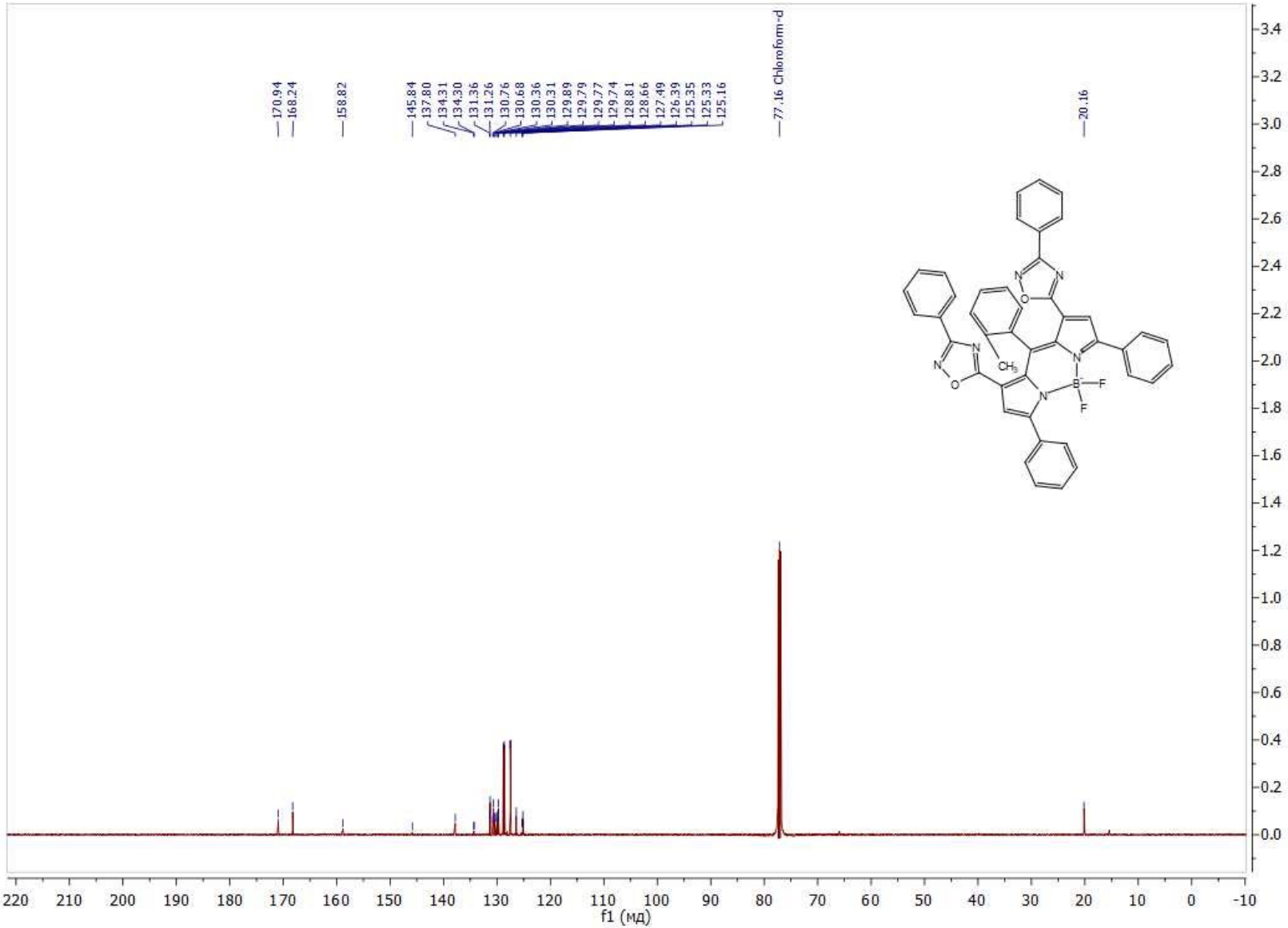
$^{19}$F NMR spectrum for **3a**



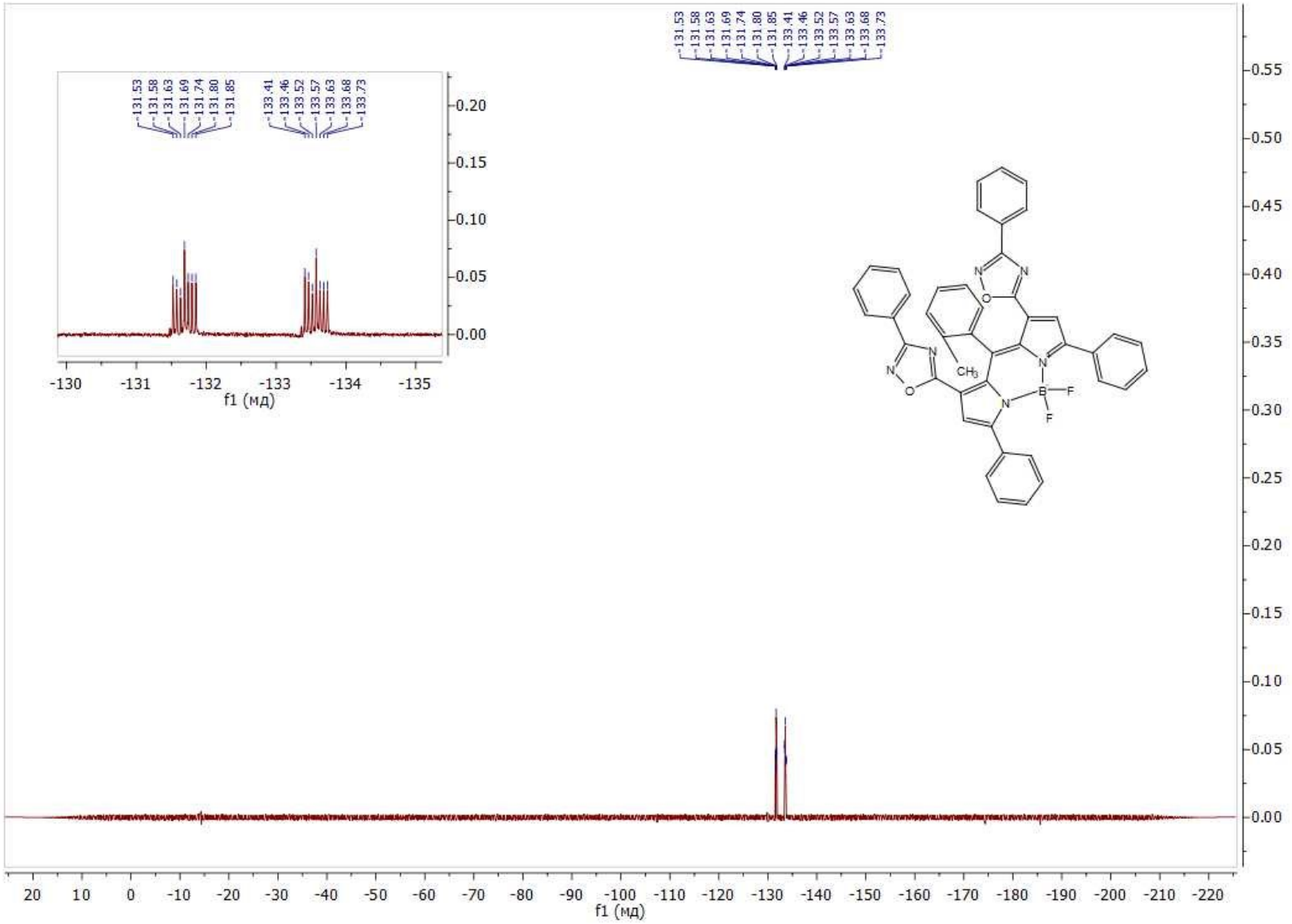
[1]H NMR spectrum for **3b**



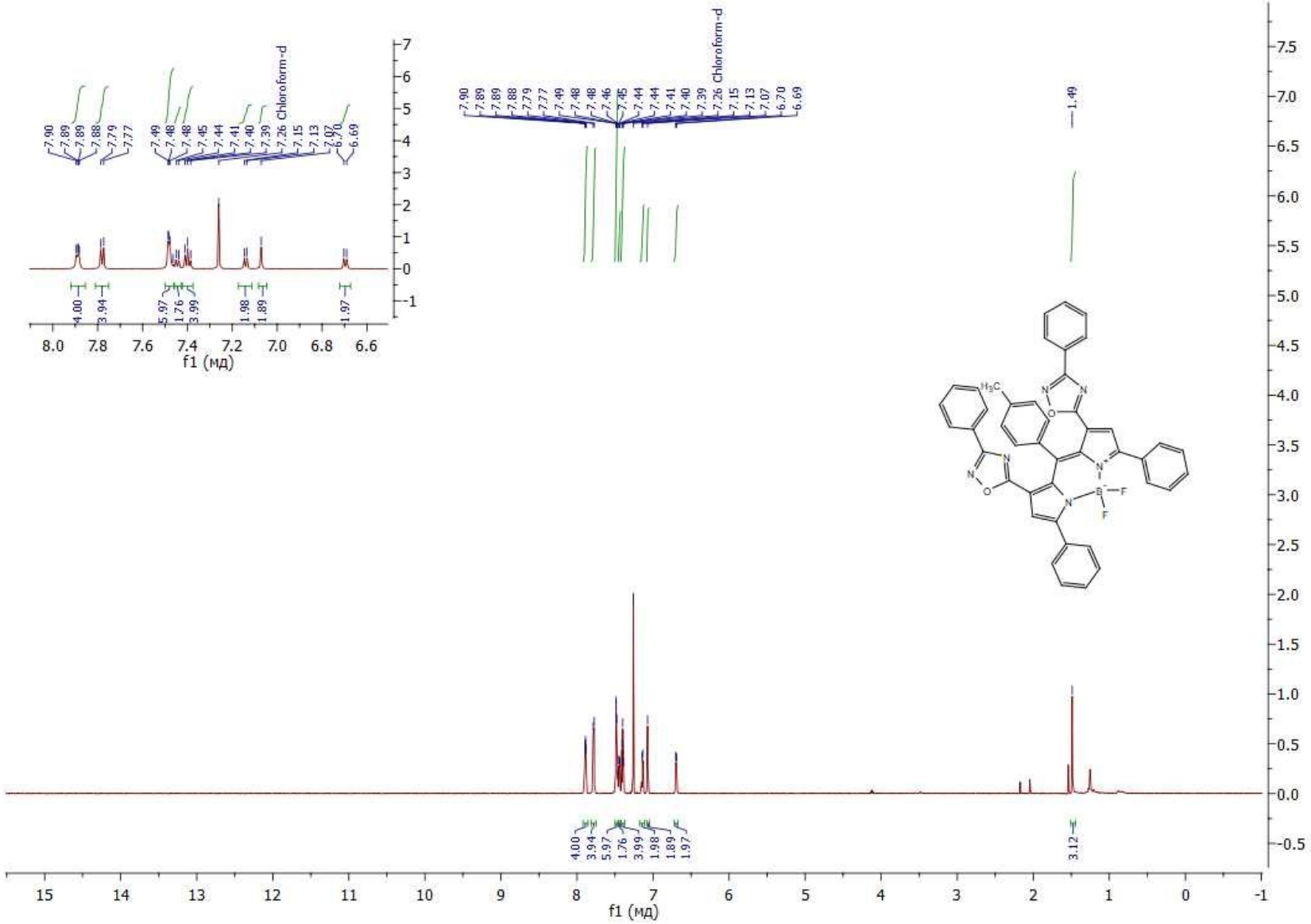
$^{13}$C NMR spectrum for **3b**



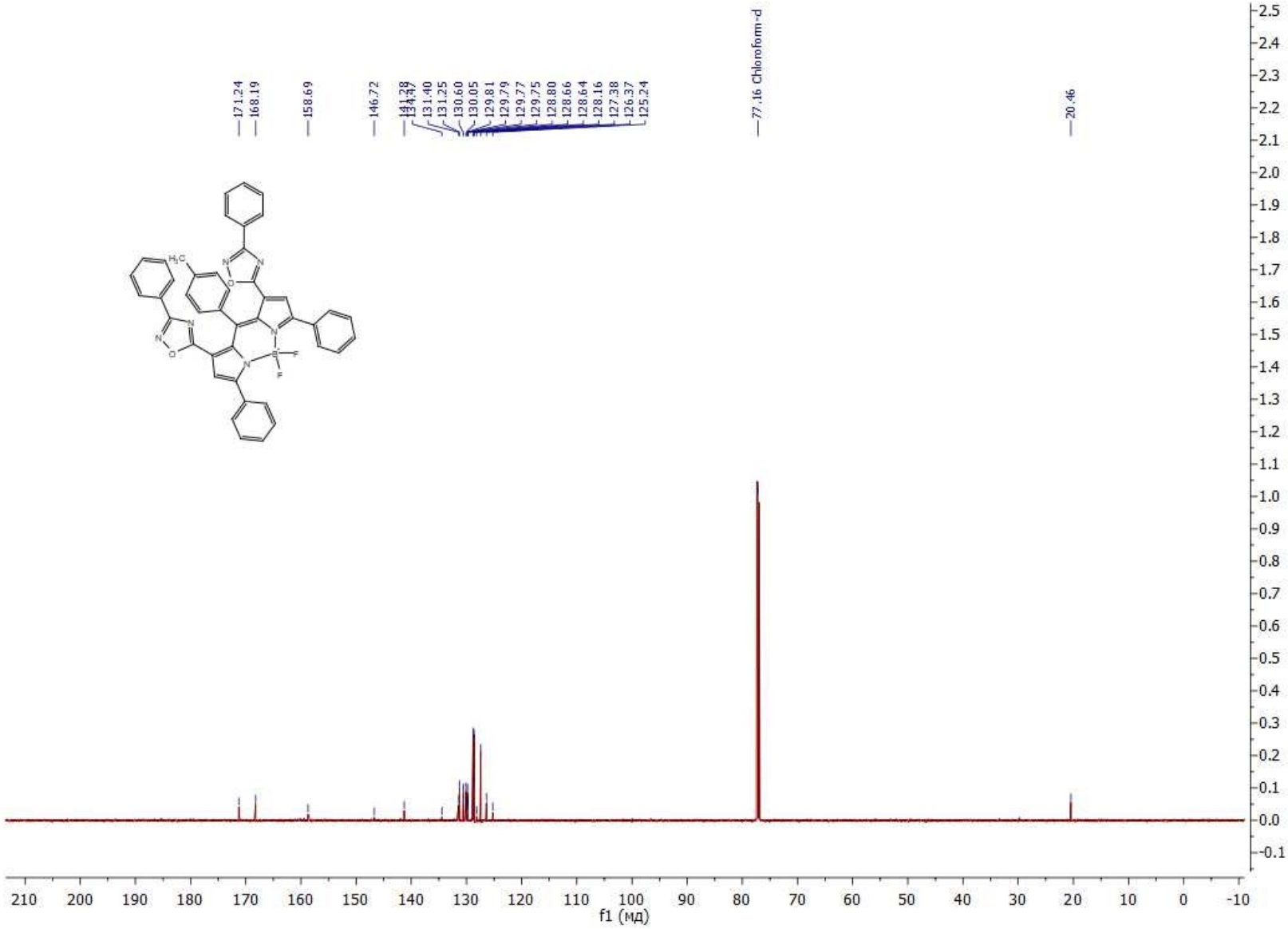
$^{19}$F NMR spectrum for **3b**



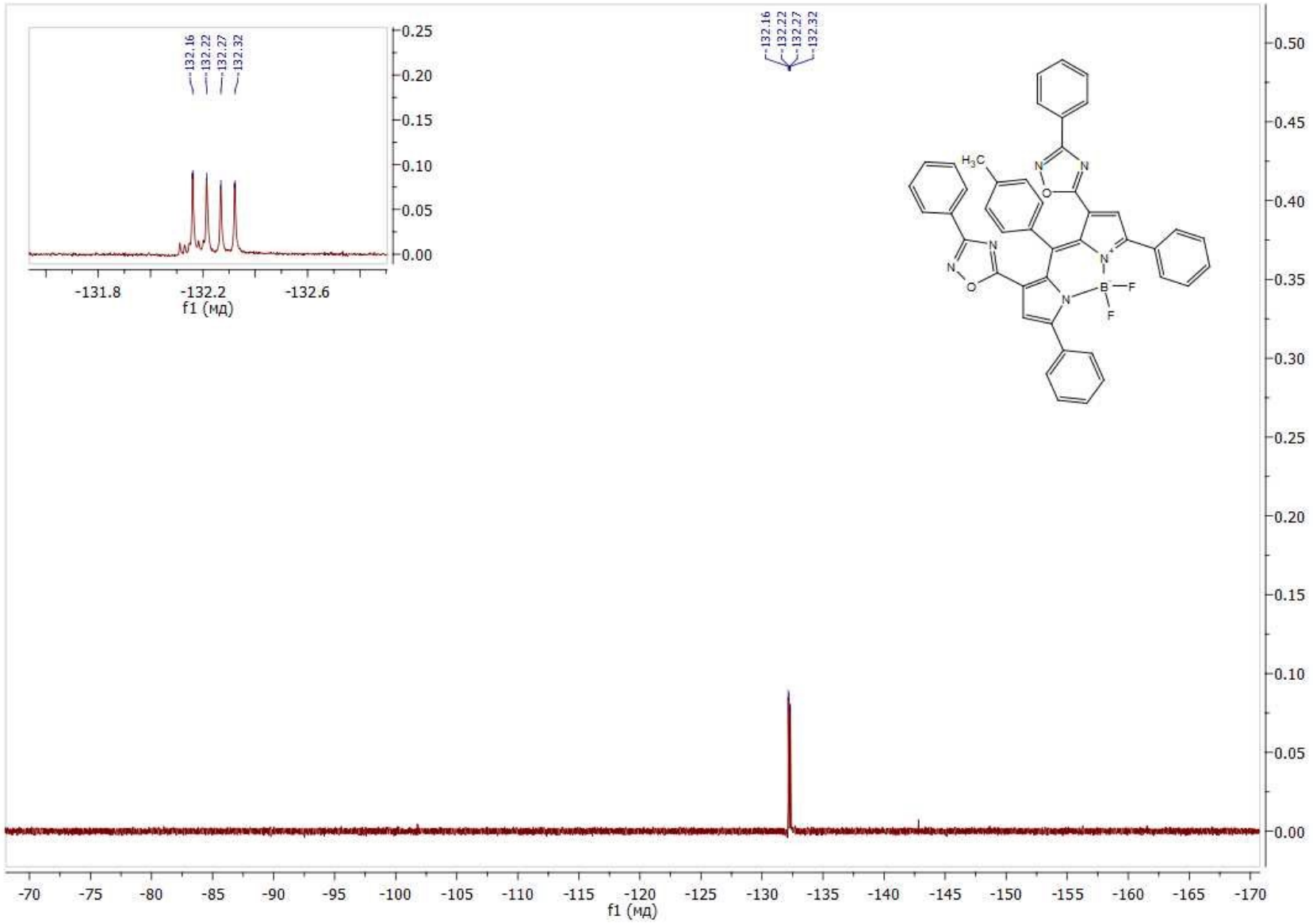
$^{1}$H NMR spectrum for **3c**



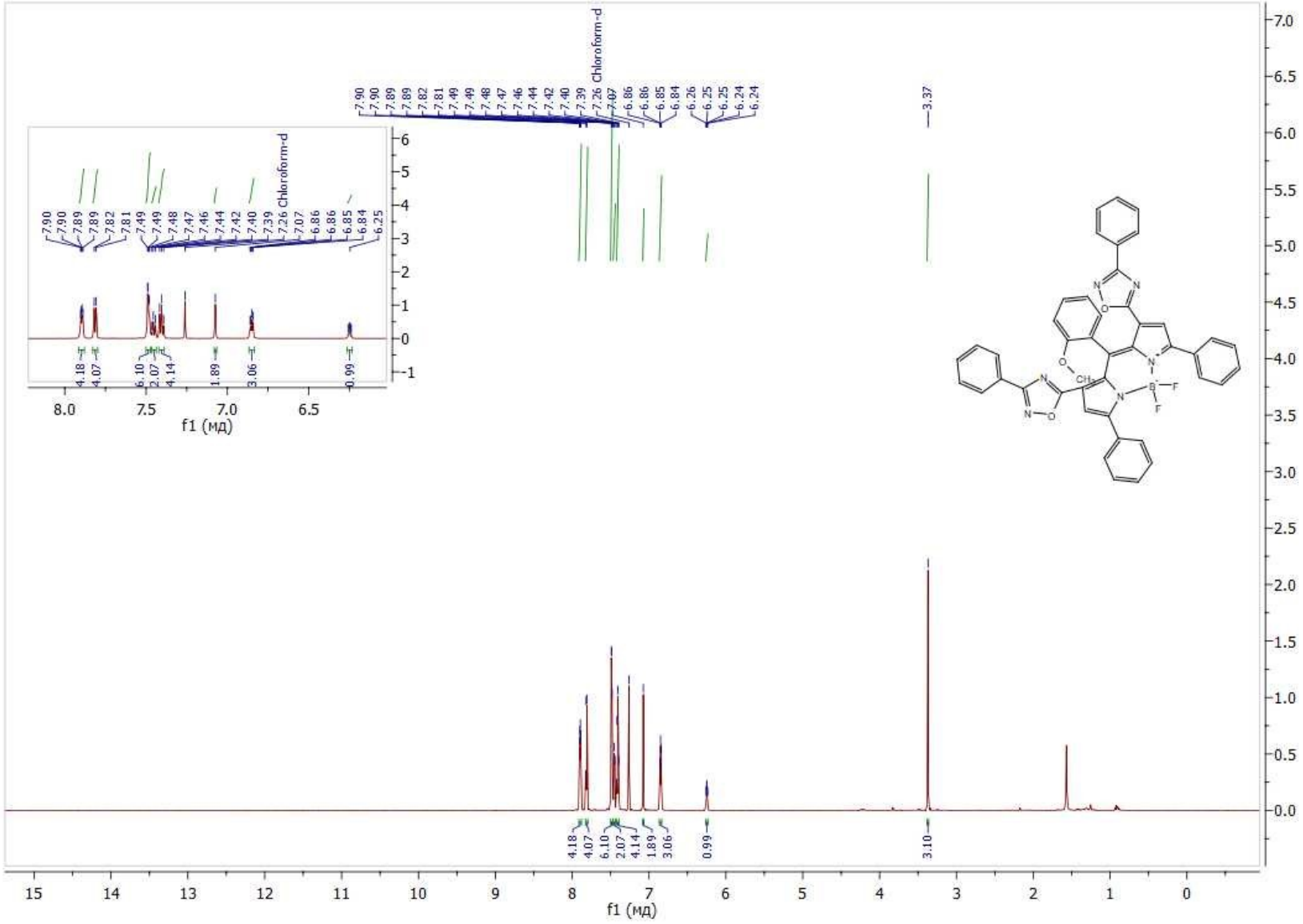
$^{13}$C NMR spectrum for **3c**



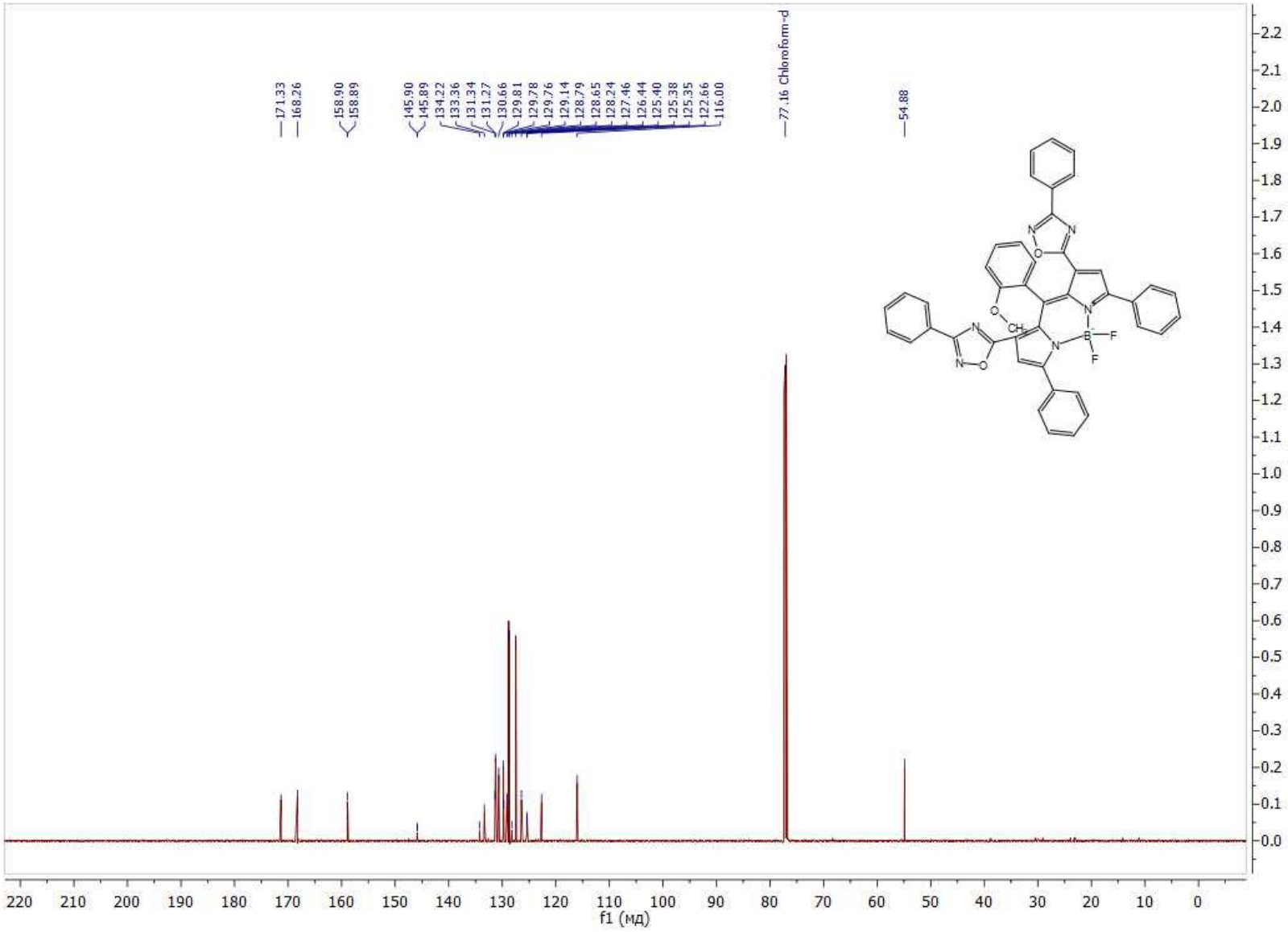
$^{19}$F NMR spectrum for **3c**



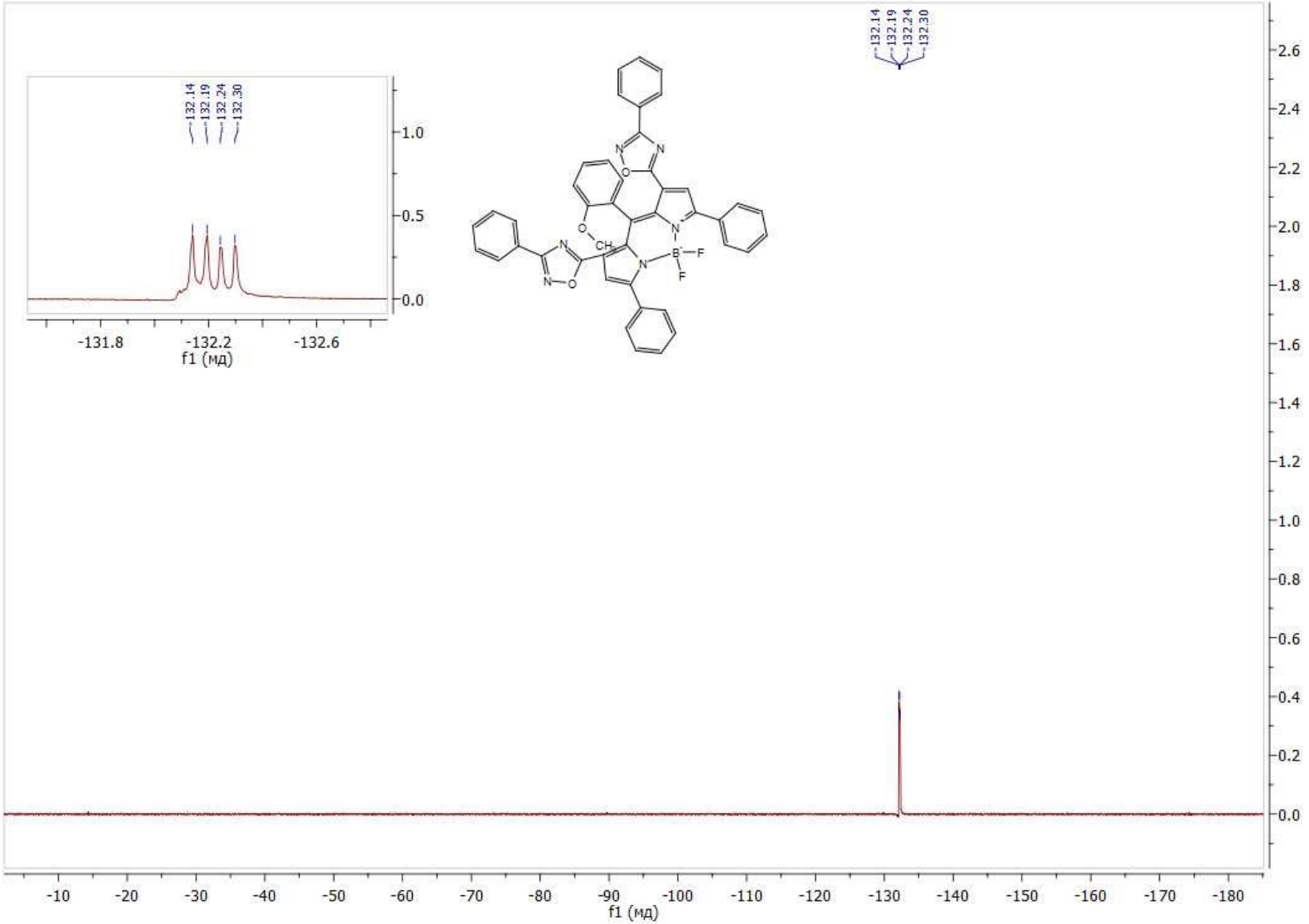
$^{1}$H NMR spectrum for **3d**



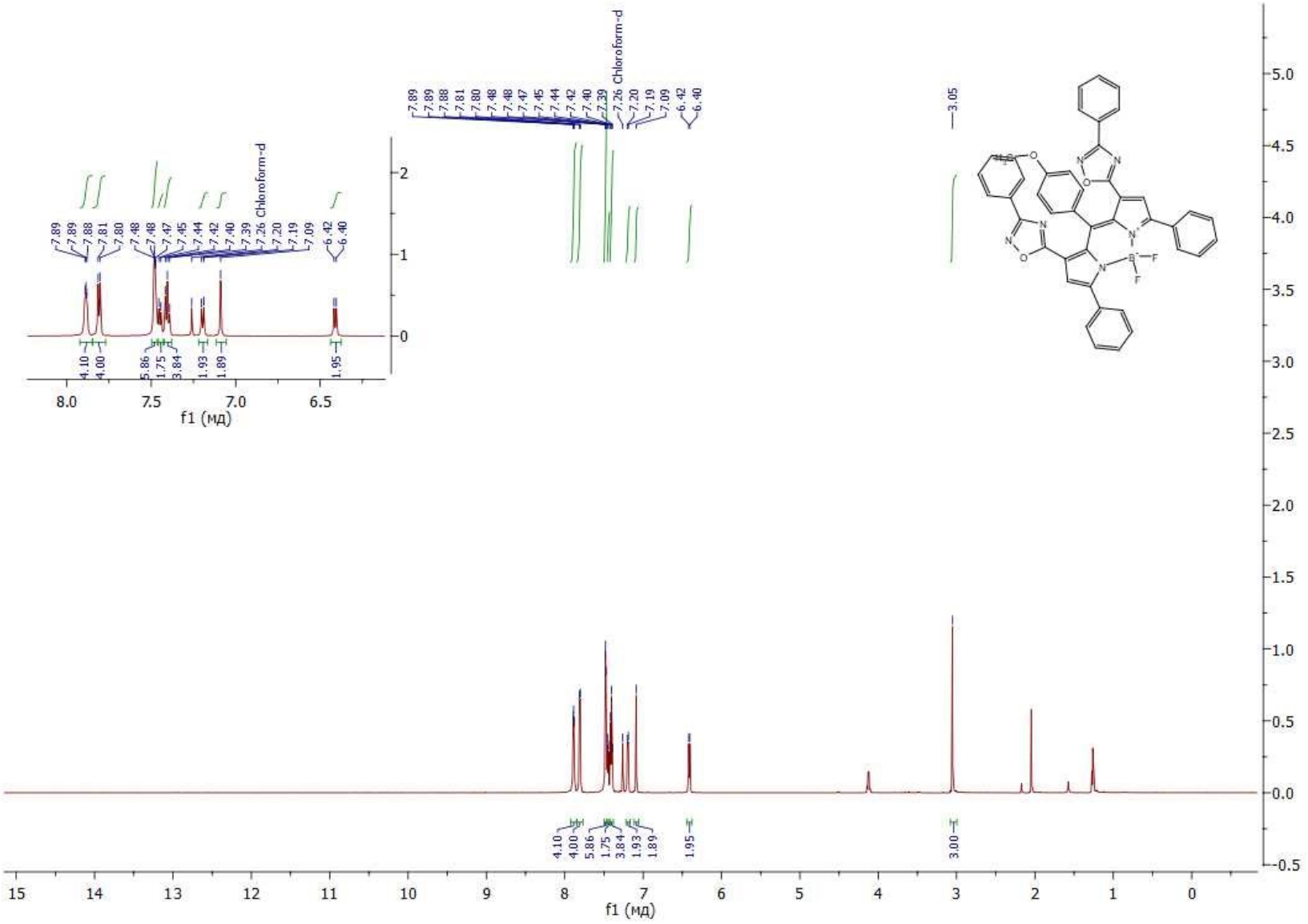
$^{13}$C NMR spectrum for **3d**



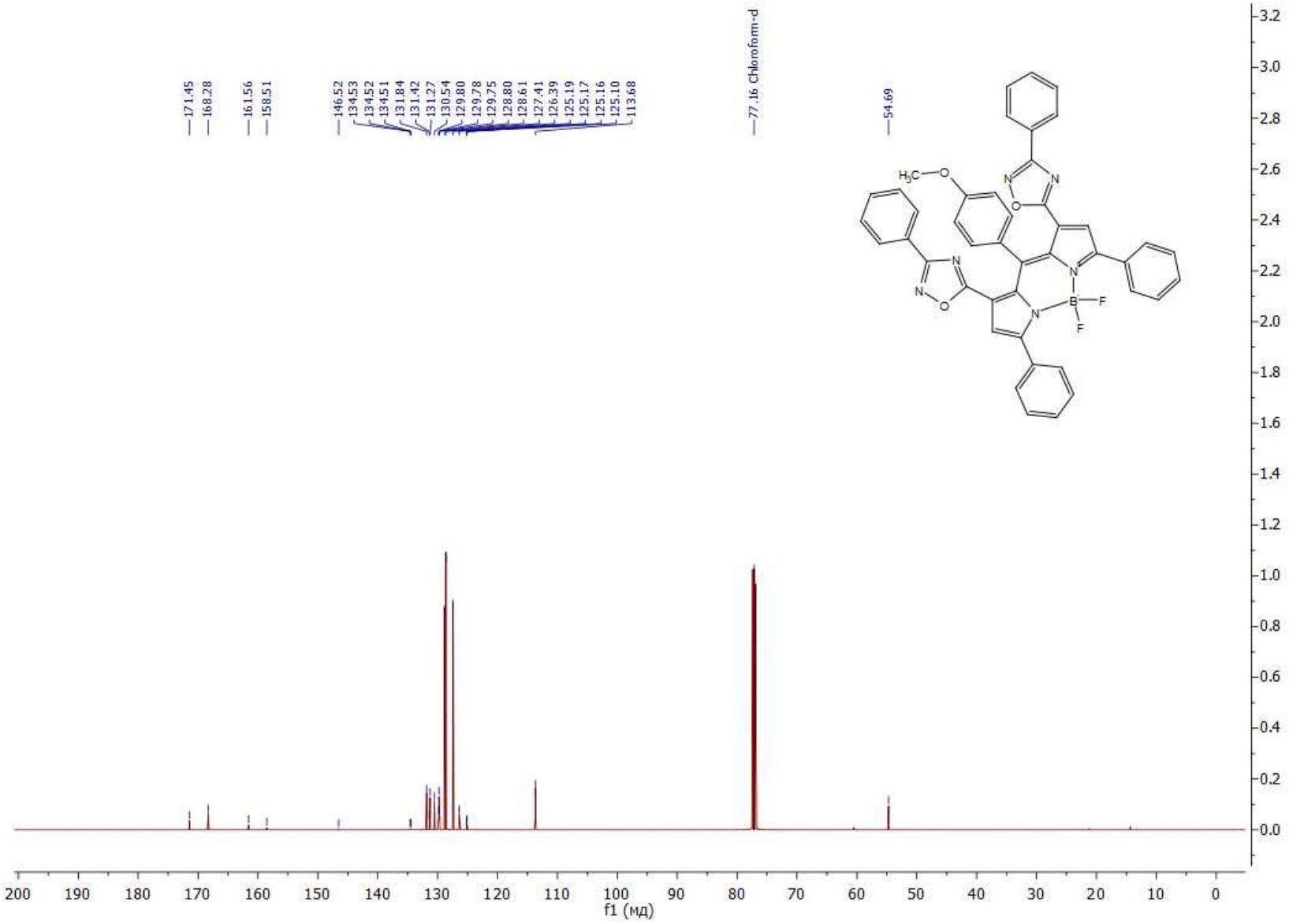
$^{19}$F NMR spectrum for **3d**



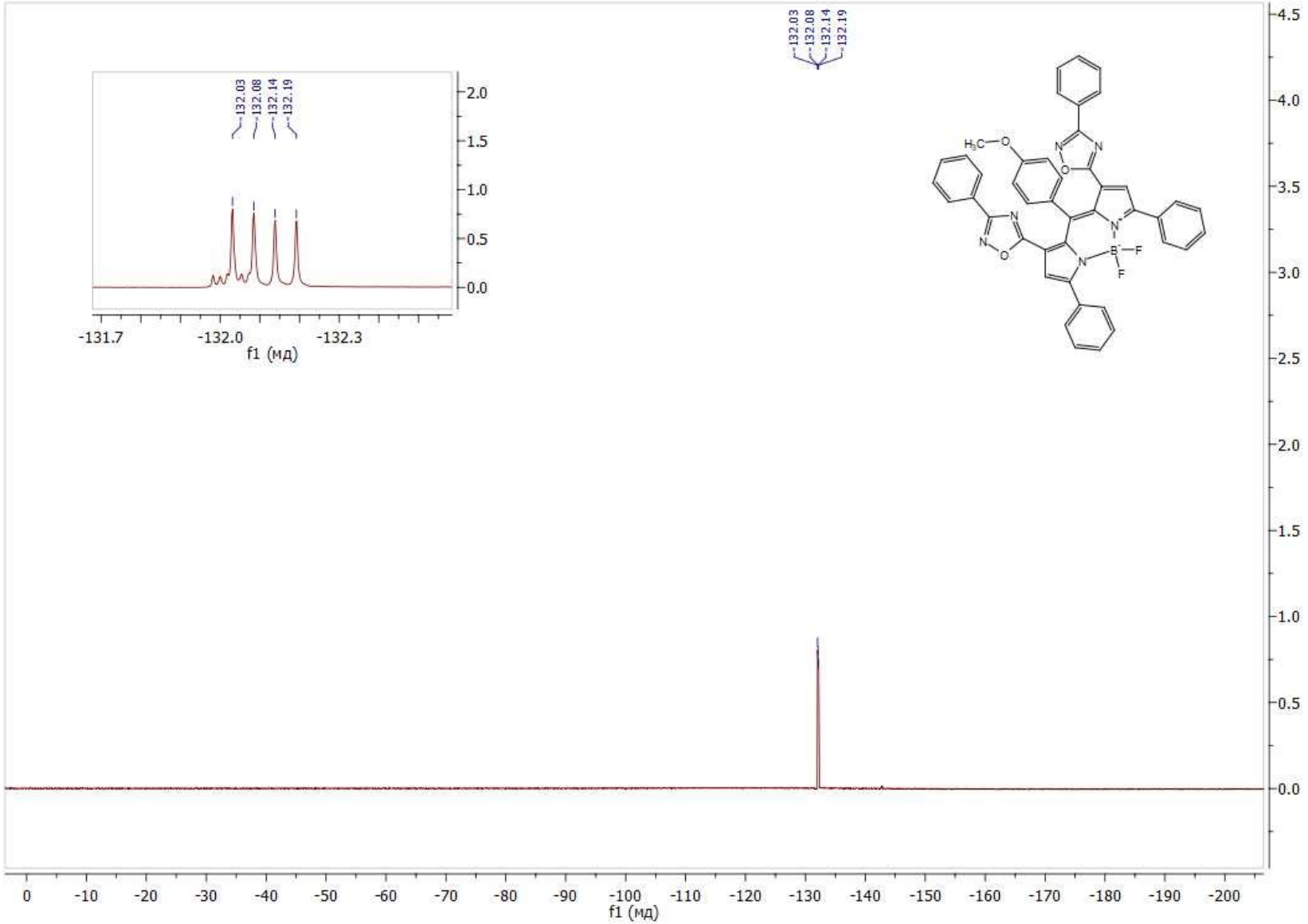
[1]H NMR spectrum for **3e**



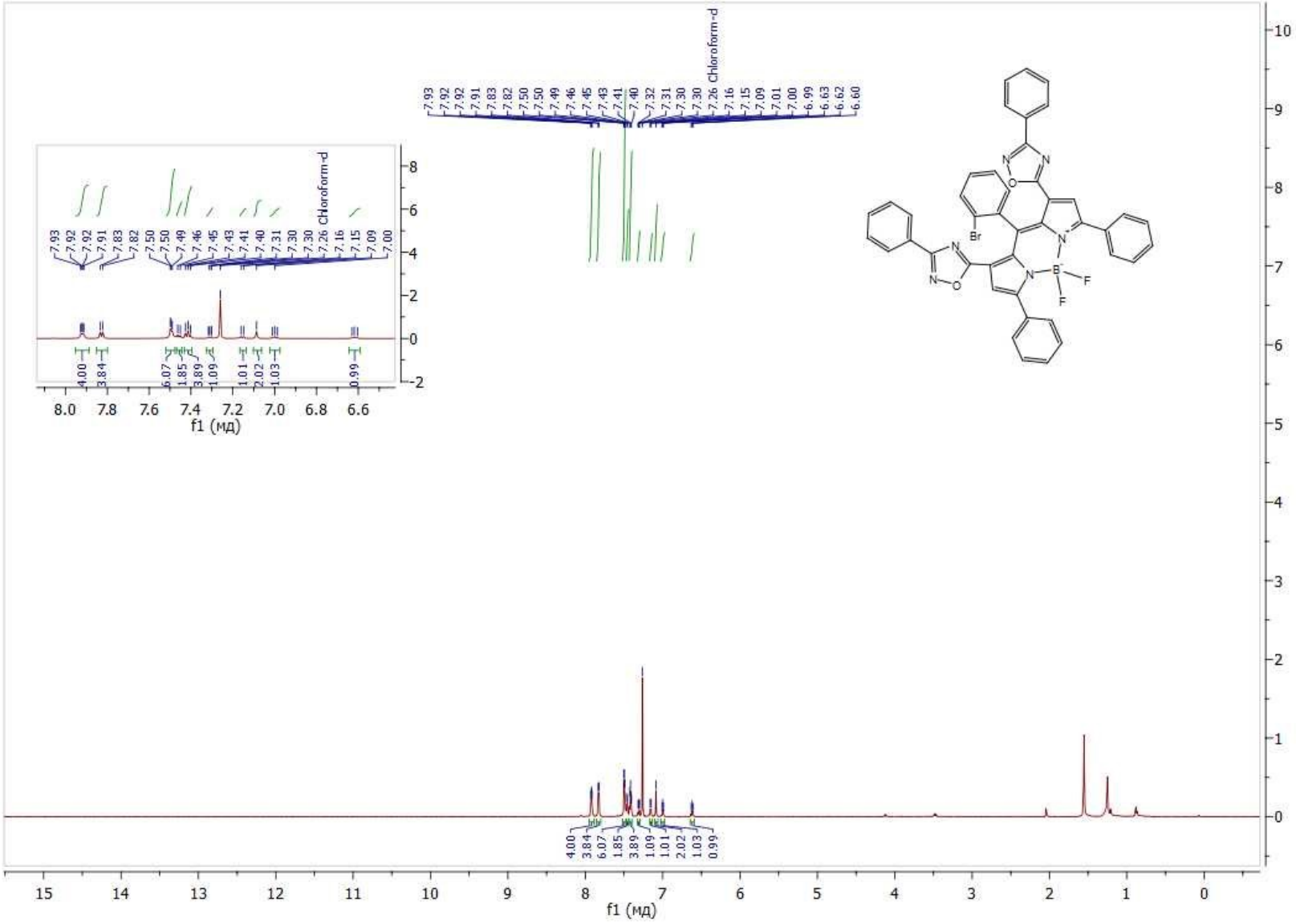
$^{13}$C NMR spectrum for **3e**



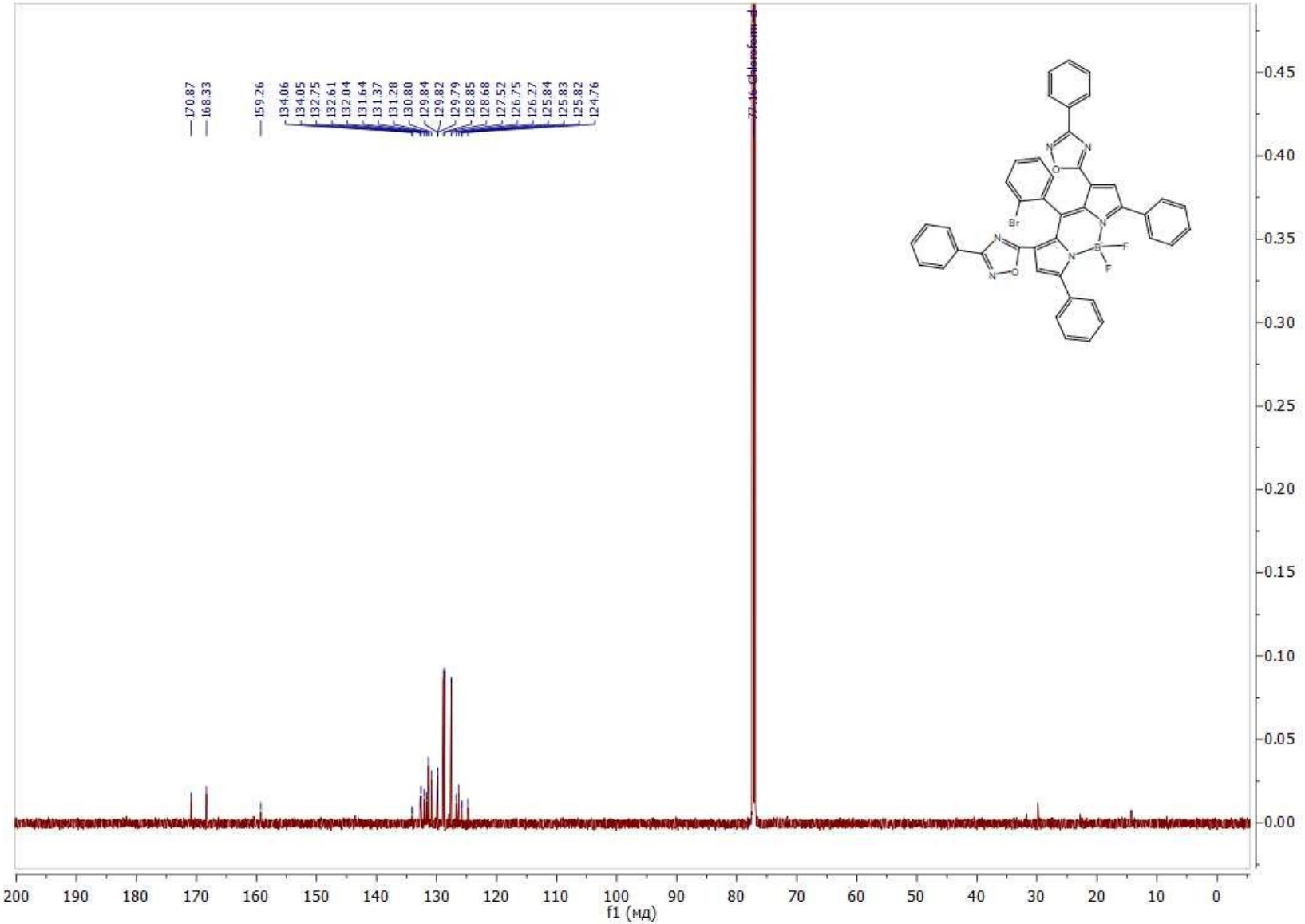
$^{19}$F NMR spectrum for **3e**



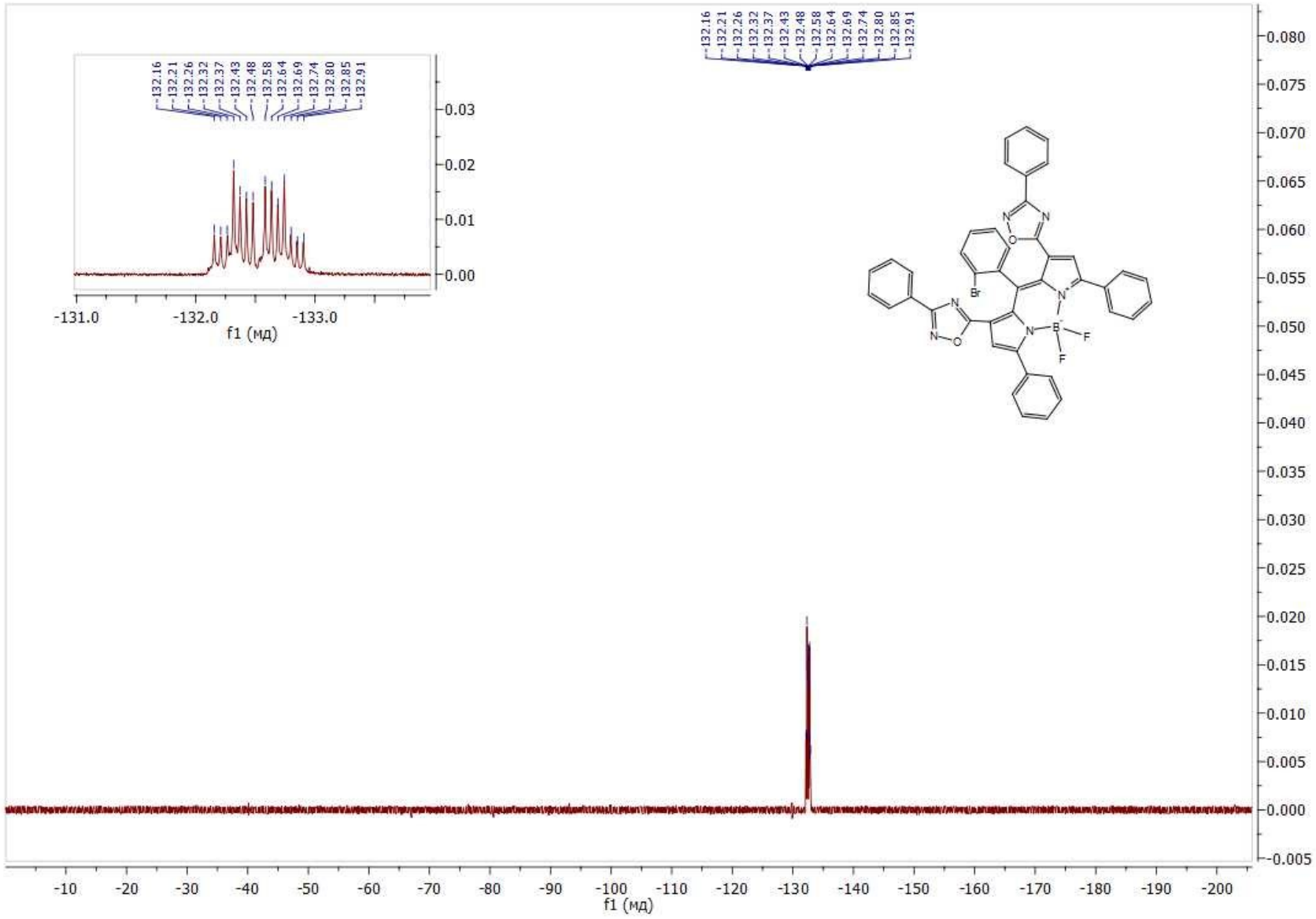
$^{1}$H NMR spectrum for **3f**



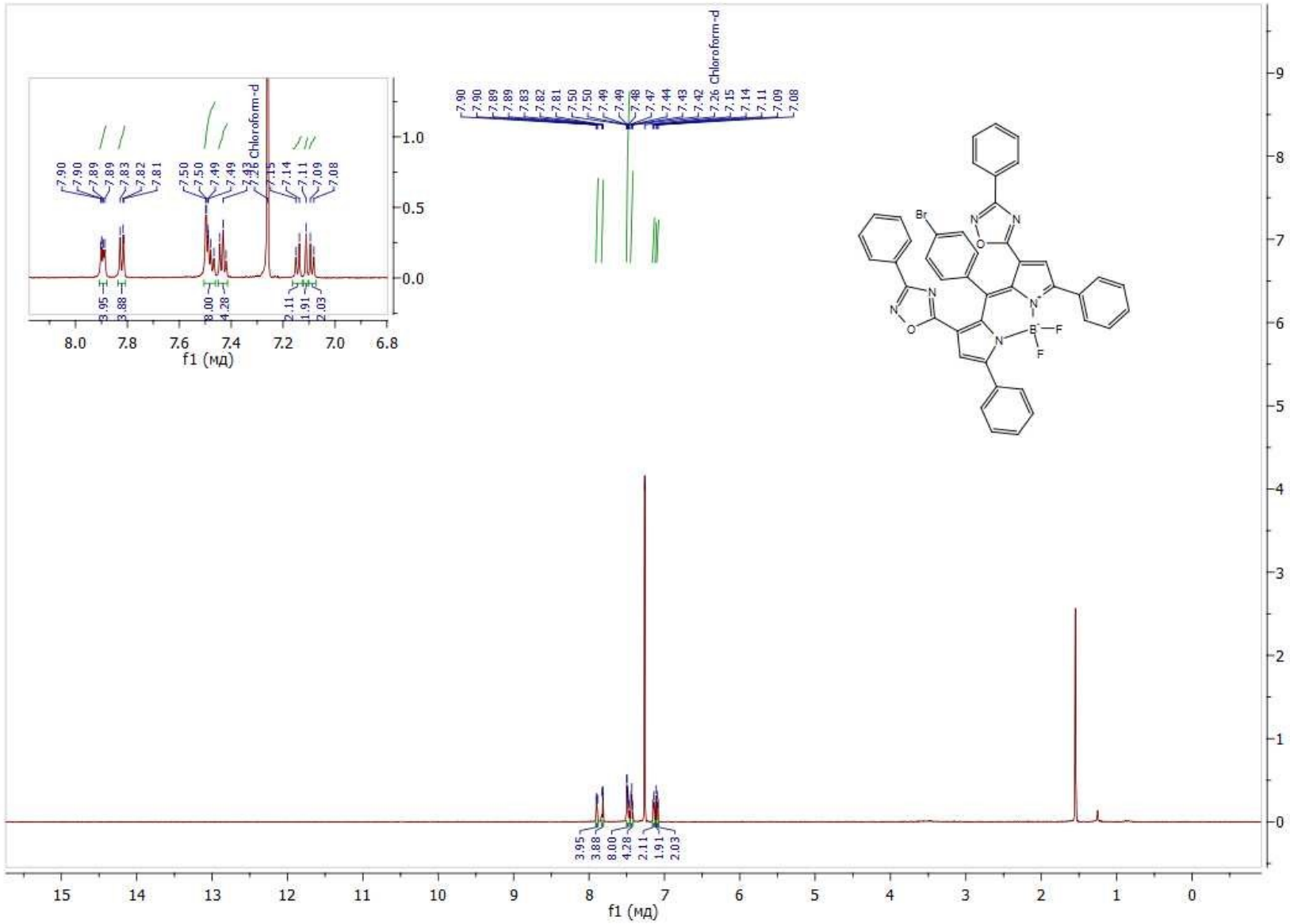
$^{13}$C NMR spectrum for **3f**



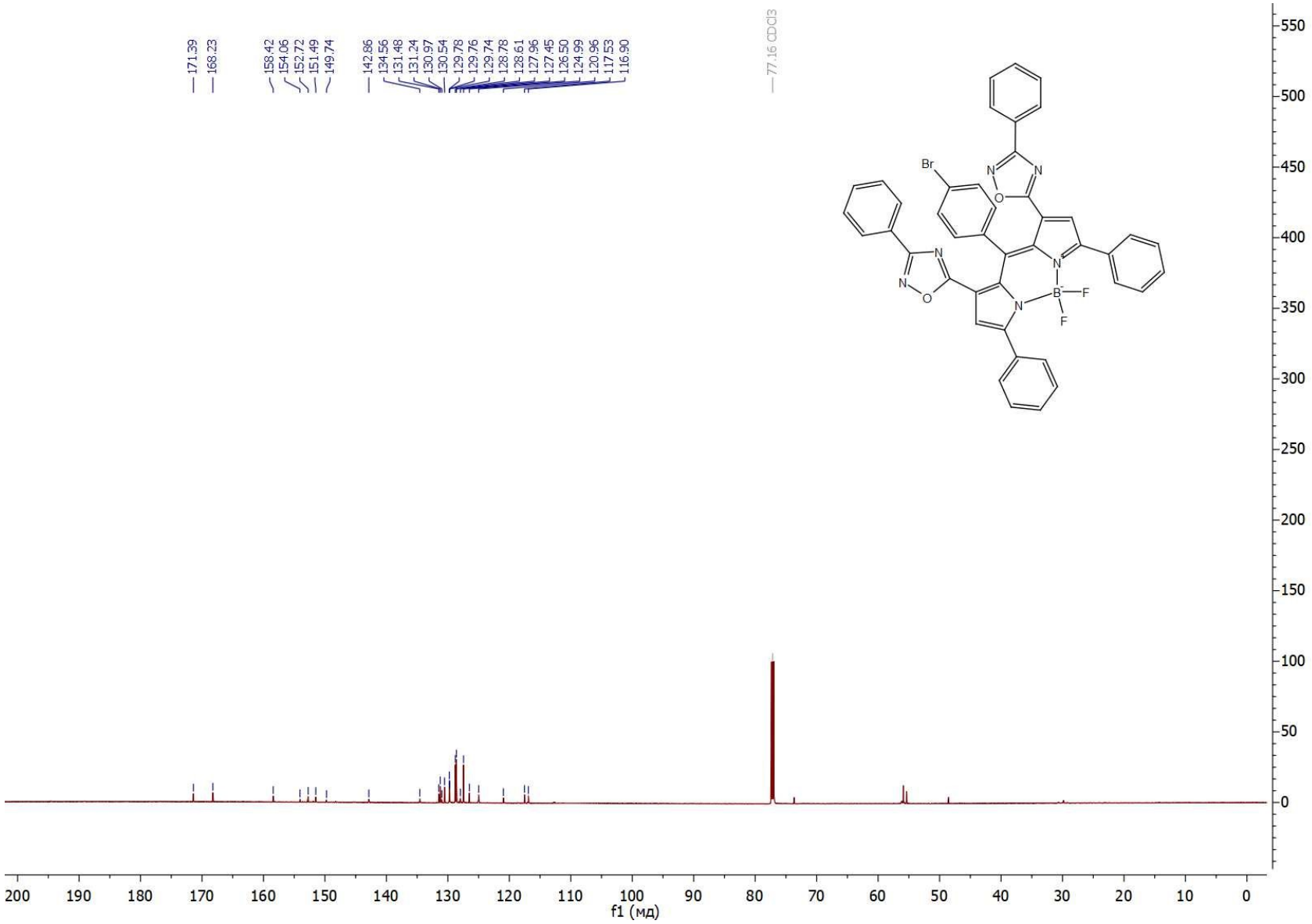
$^{19}$F NMR spectrum for **3f**



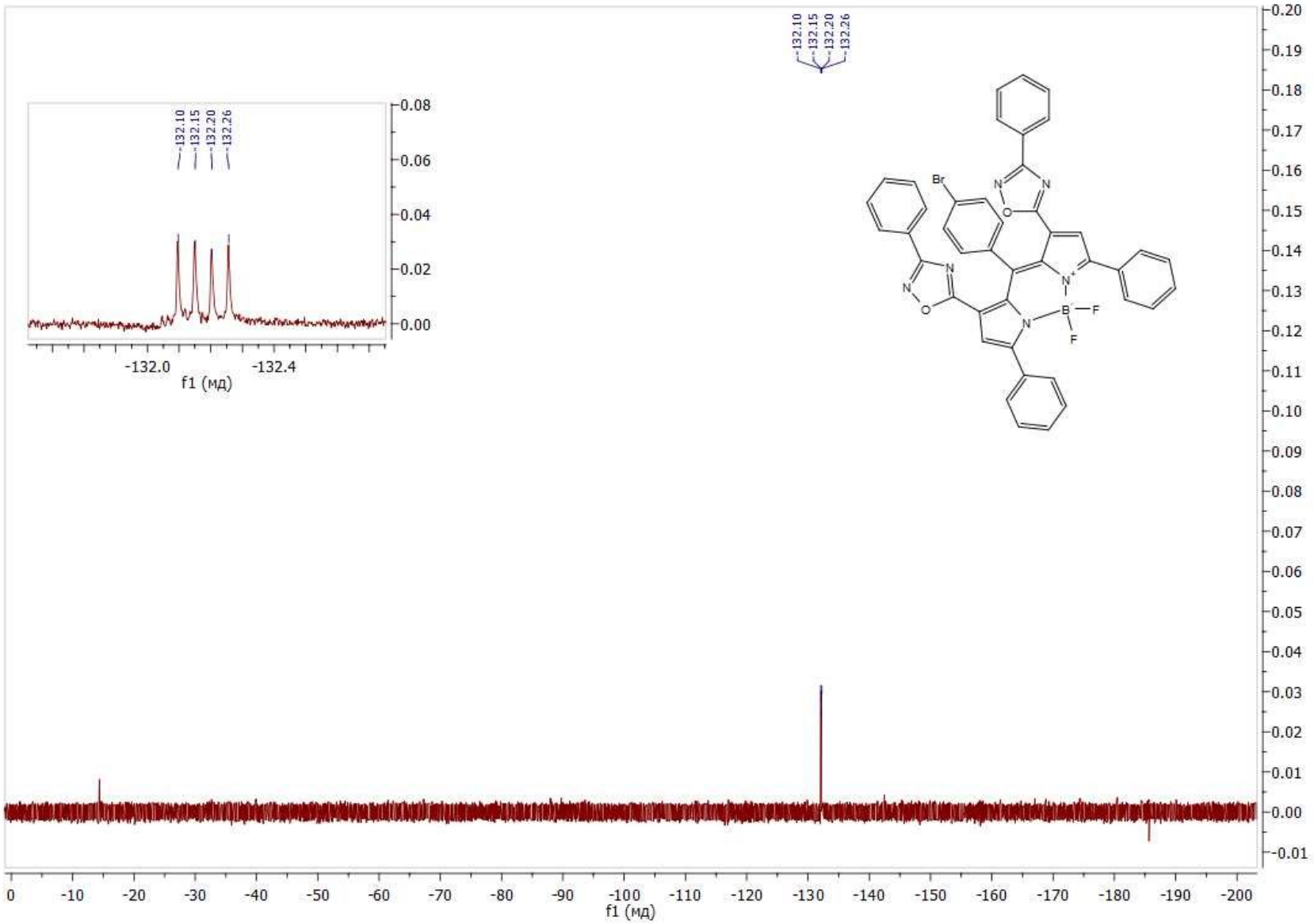
$^{1}$H NMR spectrum for **3g**



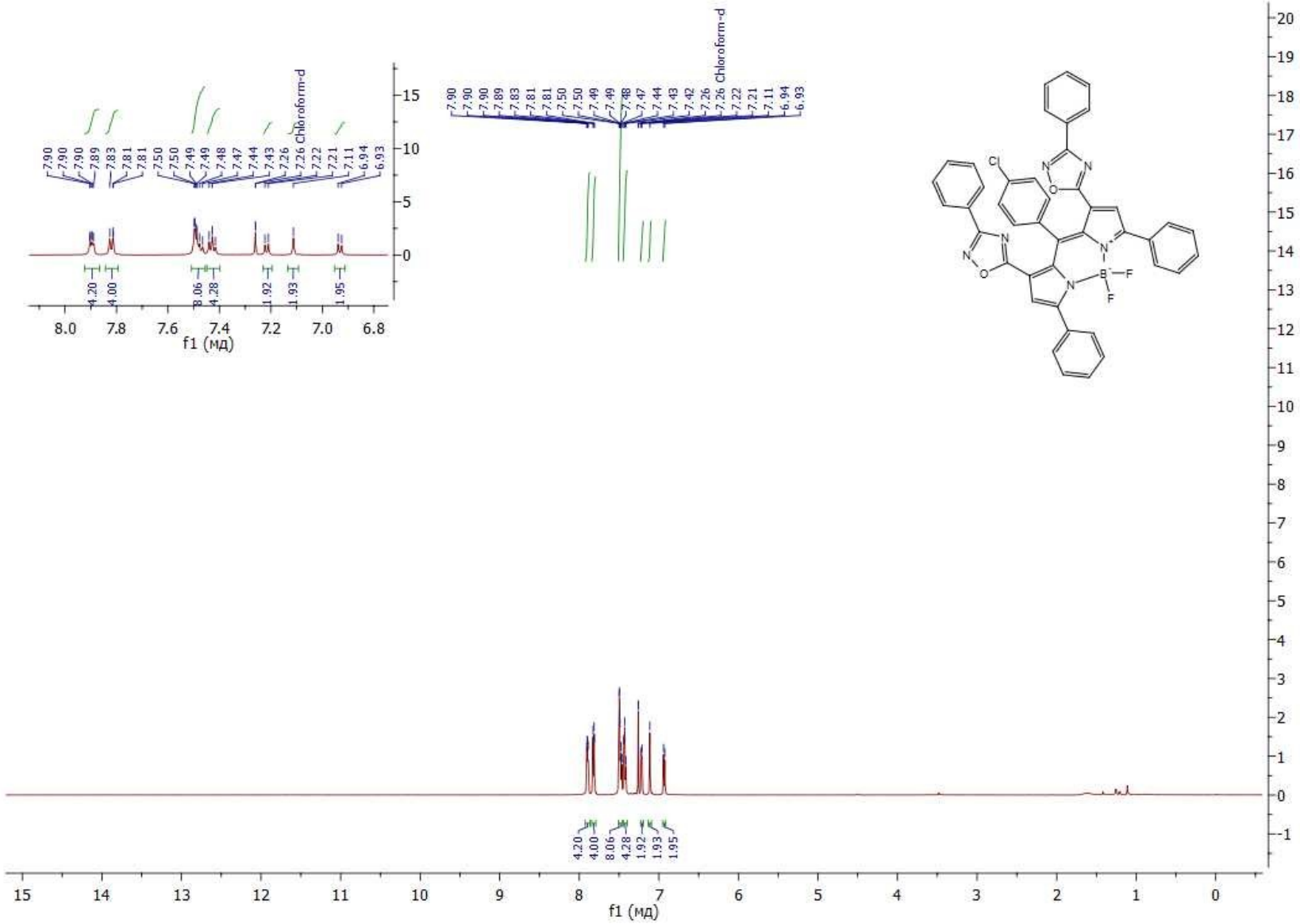
$^{13}$C NMR spectrum for **3g**



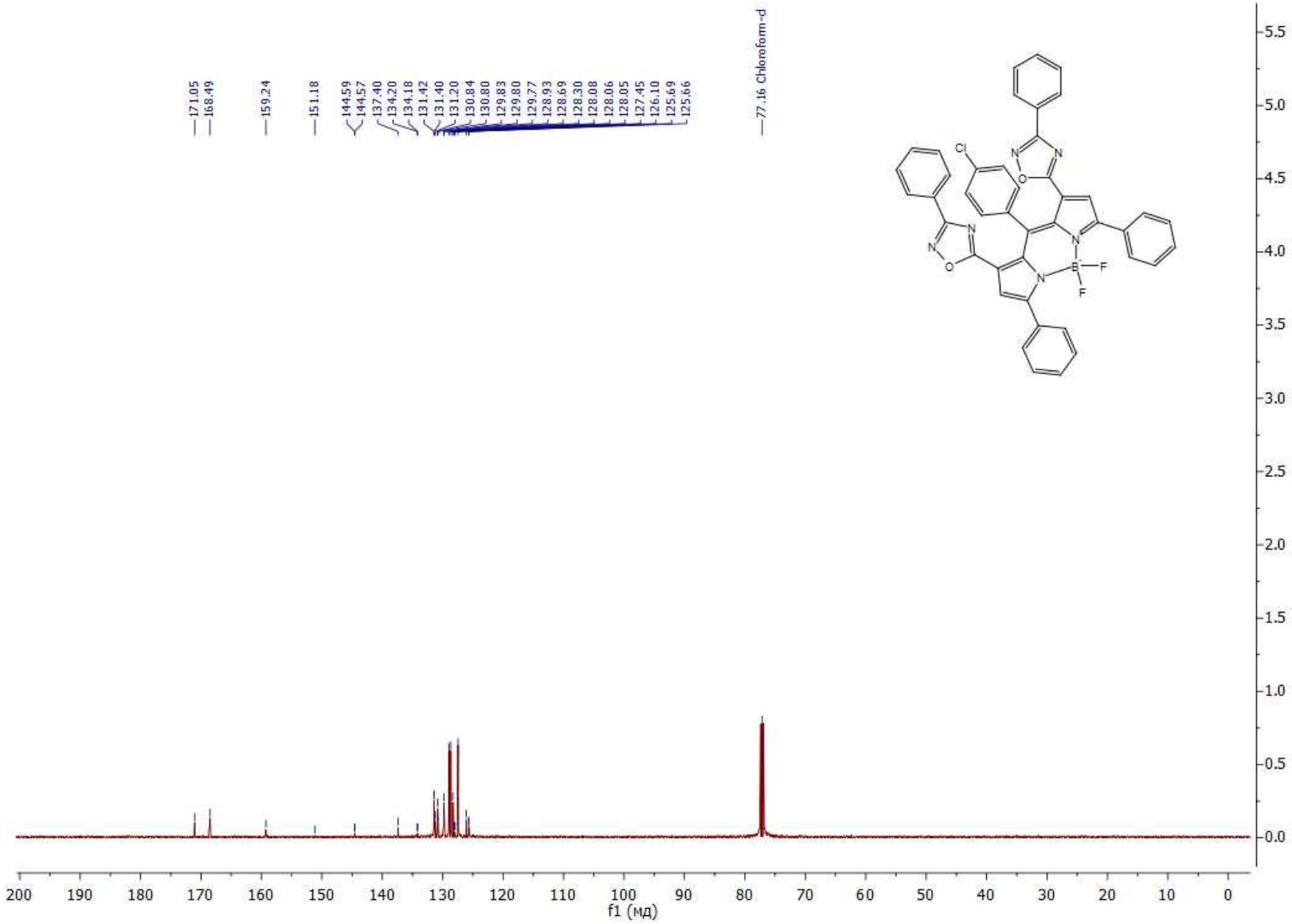
$^{19}$F NMR spectrum for **3g**



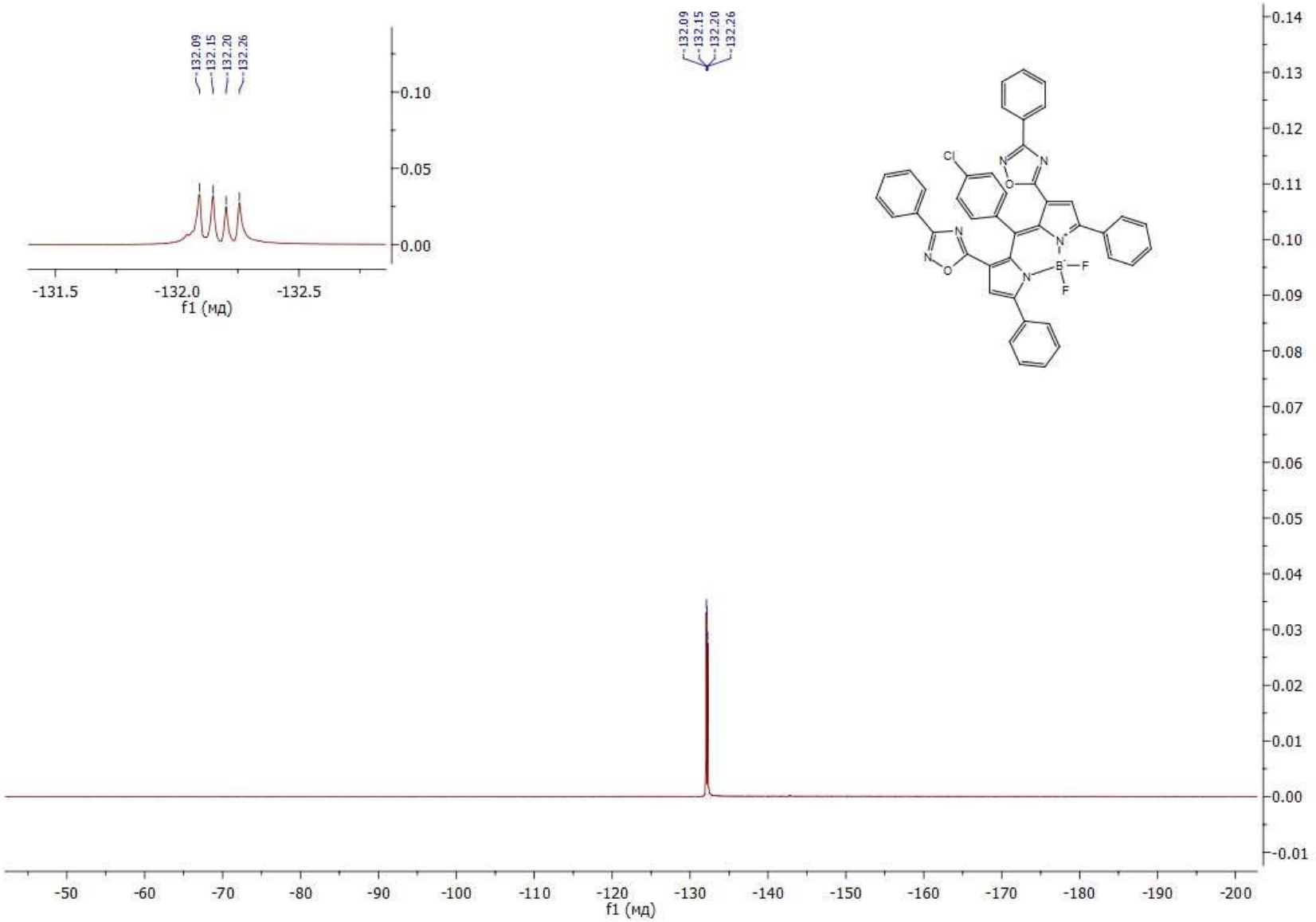
$^{1}$H NMR spectrum for **3h**



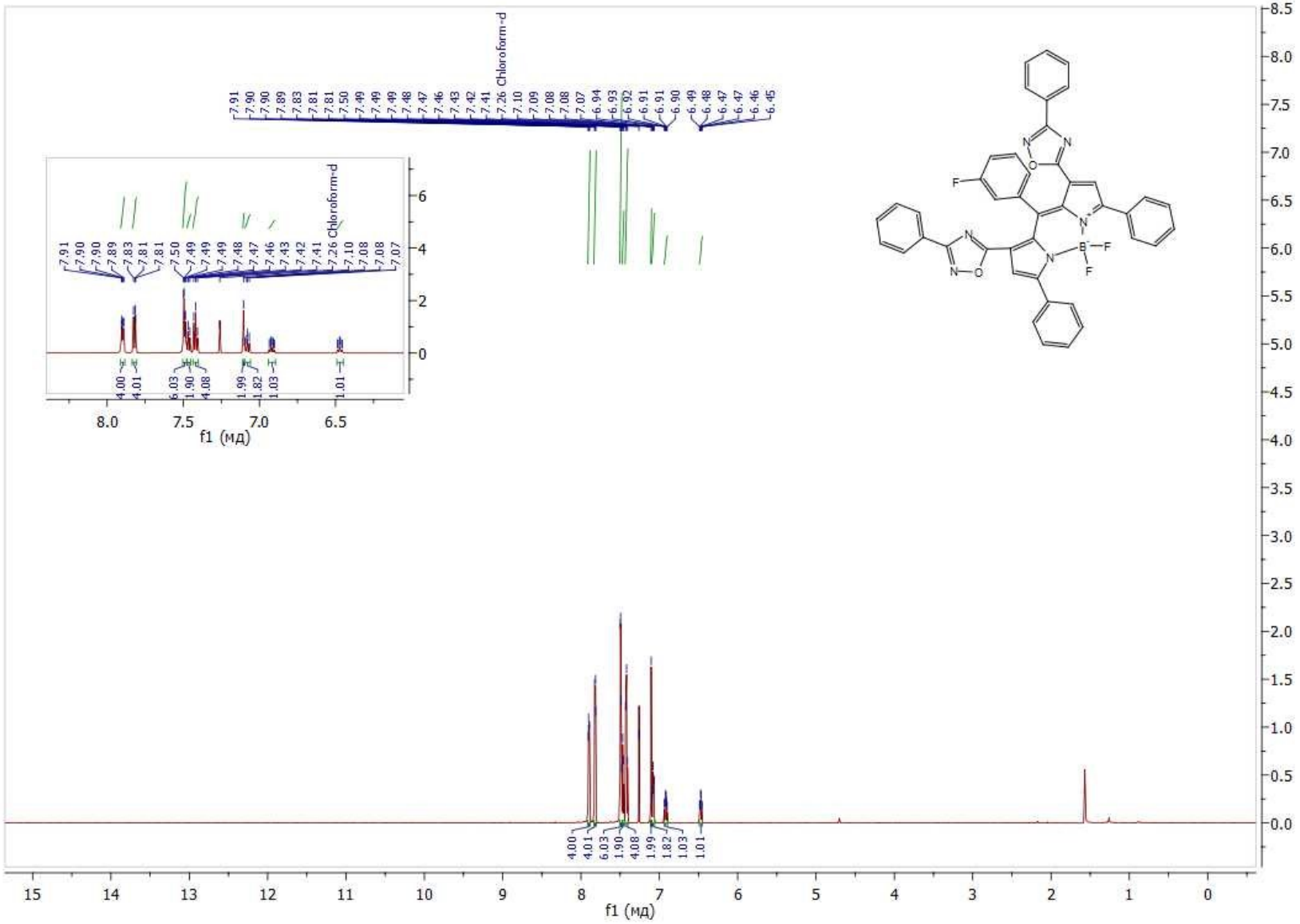
$^{13}$C NMR spectrum for **3h**



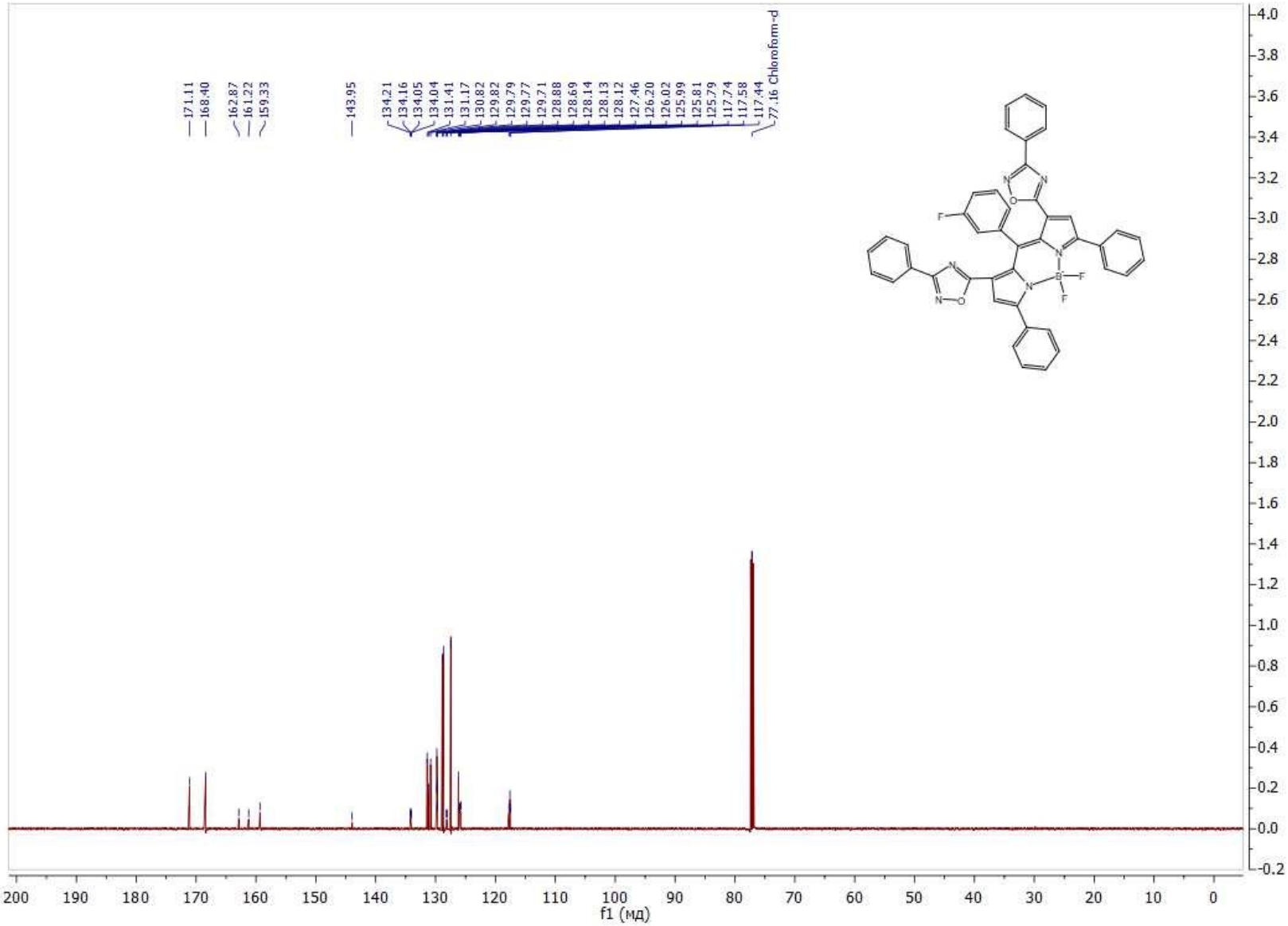
$^{19}$F NMR spectrum for **3h**



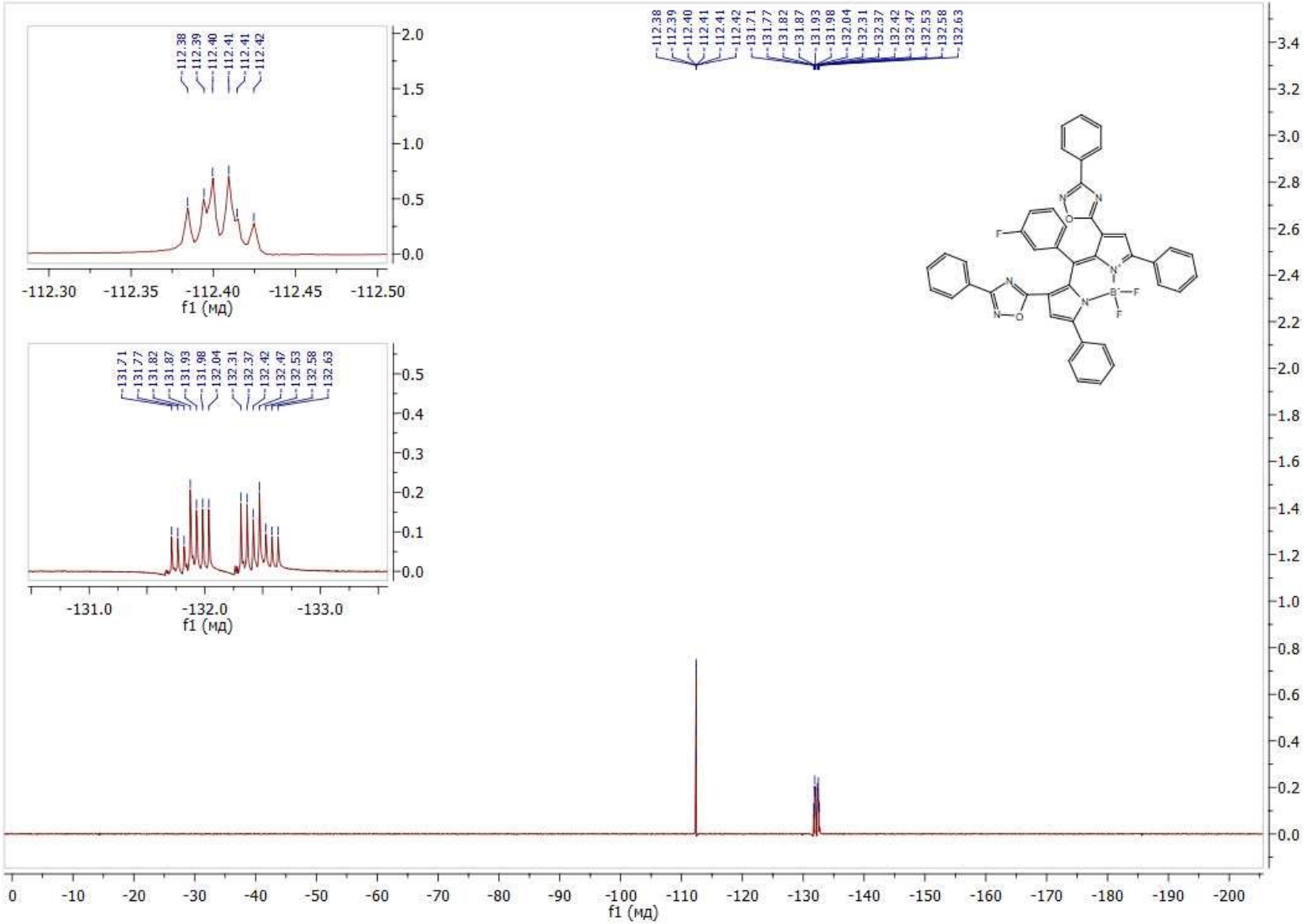
[1]H NMR spectrum for **3i**



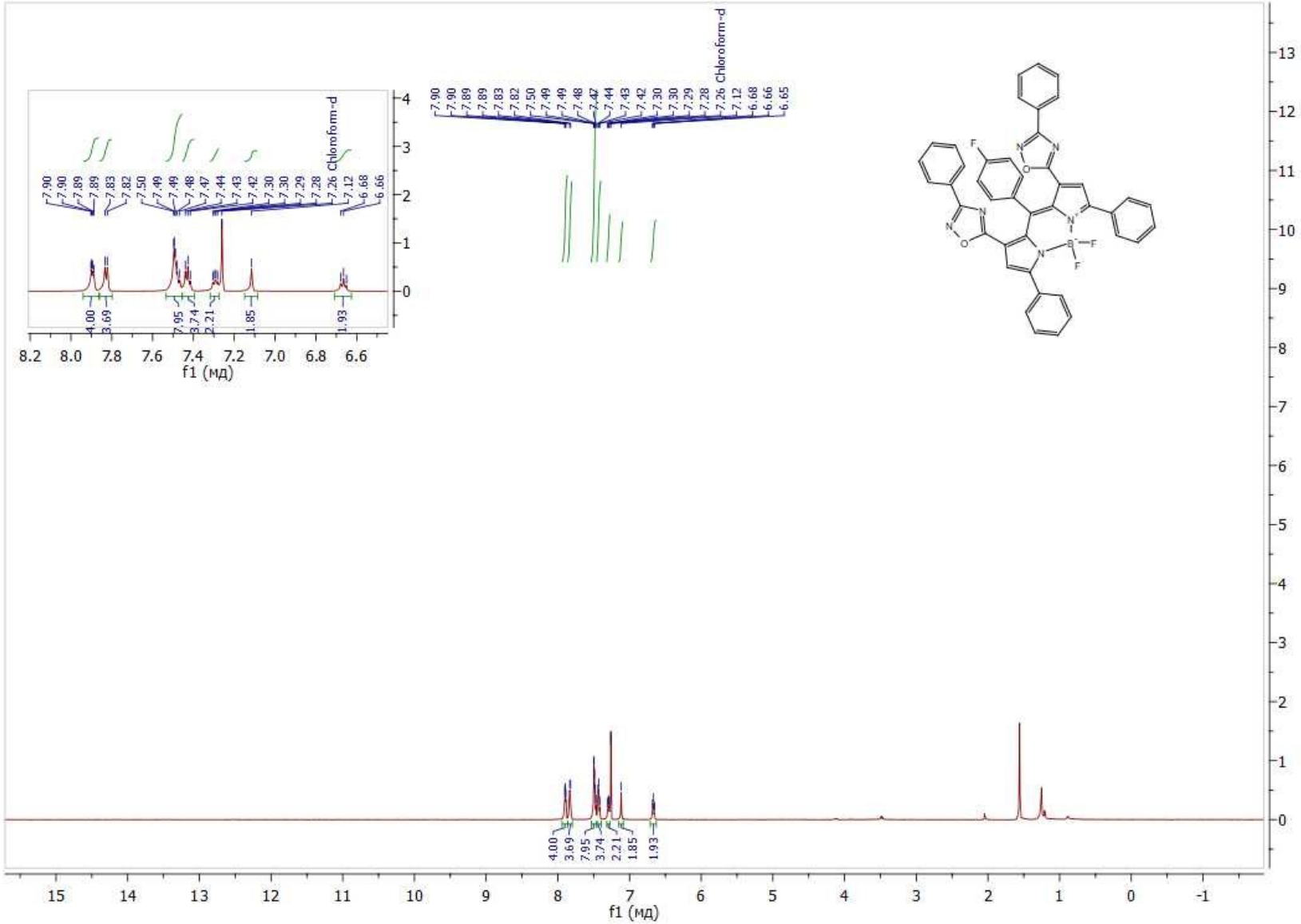
$^{13}$C NMR spectrum for **3i**



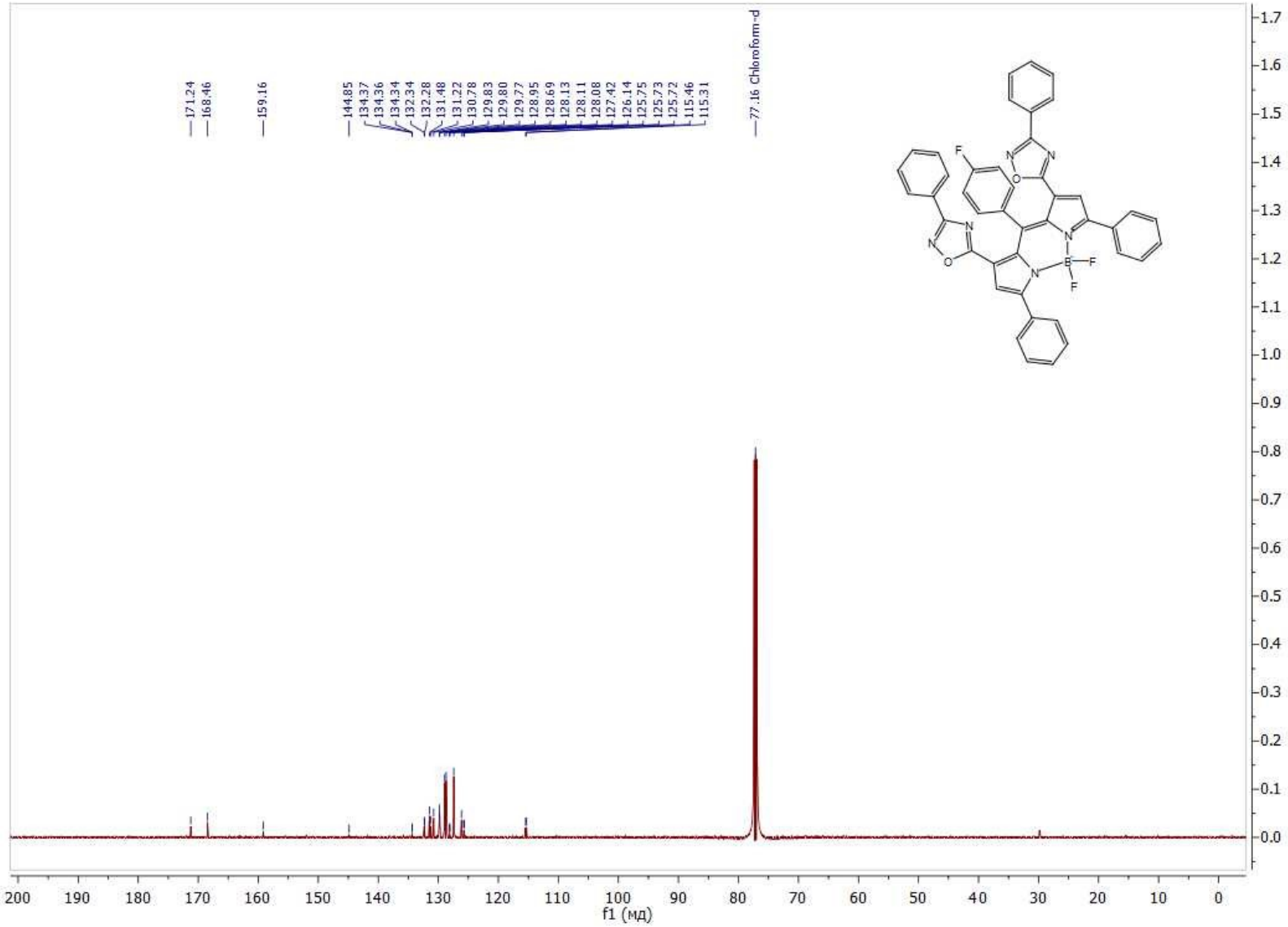
$^{19}$F NMR spectrum for **3i**



$^{1}$H NMR spectrum for **3j**



$^{13}$C NMR spectrum for **3j**



$^{19}$F NMR spectrum for **3j**