Synthesis and photophysical properties of novel oxadiazole substituted BODIPY fluorophores

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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 (δ) 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:

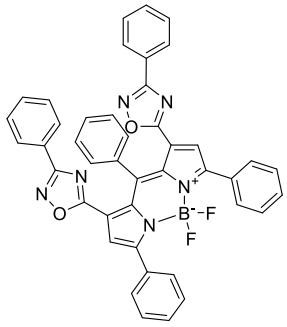
In 25 mL 2 neck round bottom flask 3-phenyl-5-(5-phenyl-1*H*-pyrrol-3-yl)-1,2,4-oxadiazole (1 equiv.) was degassed by argon for 10 min. Then aldehyde (0.5 equiv.) was added and again purged by argon for 10 min. Then few drops of TFA was added and stirred at 120ºC for 2 hours. The reaction progress was 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.

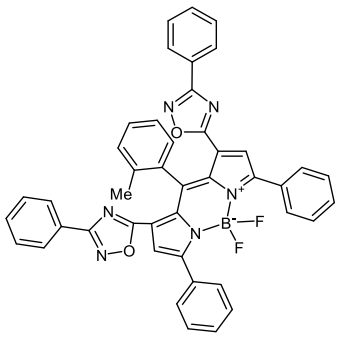
Entry	Solvent	Catalyst	Temp (°C)	Base	Time	Yield (%)[a]
1	DCM	TFA	25	-	-	NR
2	DCM	TFA	reflux	Et_3N	10 days	Trace
3	DCE	TFA	25	-	-	NR
4	DCE	TFA	reflux	Et_3N	7 days	Trace
5	DCE	5 mol% PPTS	25	-	-	NR [1]
6	DCE	10 mol% PPTS	reflux	-	7 days	trace[b]
7	toluene	10% mol I_2	reflux	-	8 days	trace [2][b]
8	Solv. 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.

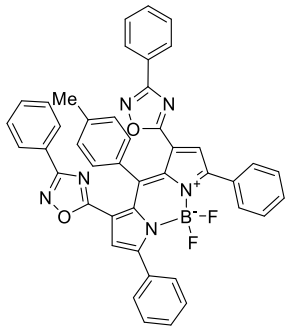
3. NMR and HRMS characterization data



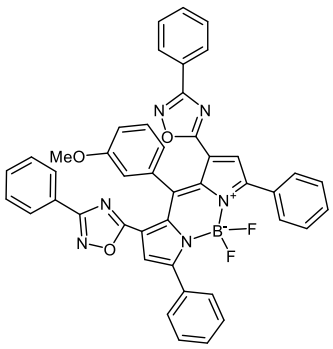
5,5'-(5,5-Difluoro-3,7,10-triphenyl-5*H*-4λ^4,5λ^4-dipyrrolo[1,2-*c*:2',1'-*f*][1,3,2]diazaborinine-1,9-diyl)bis(3-phenyl-1,2,4-oxadiazole) (3a). (262 mg, 0.37 mmol, 37%) dark purple solid, mp = 261– 263 °C. ^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.91–7.89 (m, 4H), 7.80–7.79 (m, 4H), 7.50–7.47 (m, 6H), 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.



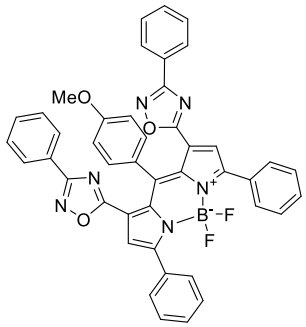
5,5'-(5,5-Difluoro-3,7-diphenyl-10-(*o*-tolyl)-5*H*-4λ^4,5λ^4-dipyrrolo[1,2-*c*:2',1'-*f*][1,3,2]diazaborinine-1,9-diyl)bis(3-phenyl-1,2,4-oxadiazole) (3b). (217 mg, 0.30 mmol, 30%)burgundy solid, mp › 300 °C. ^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.92–7.90 (m, 4H), 7.81–7.79 (m, 4H), 7.50–7.48 (m, 6H), 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.



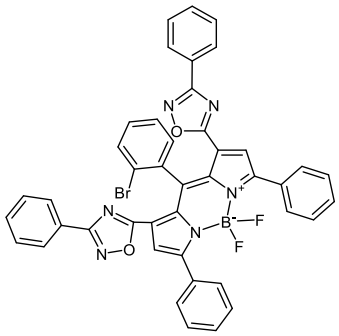
5,5'-(5,5-Difluoro-3,7-diphenyl-10-(*p*-tolyl)-5*H*-4λ^4,5λ^4-dipyrrolo[1,2-*c*:2',1'-*f*][1,3,2]diazaborinine-1,9-diyl)bis(3-phenyl-1,2,4-oxadiazole) (3c). (310 mg, 0.43 mmol, 43%) burgundy solid, mp = 240–242 °C. ^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.90–7.88 (m, 4H), 7.78 (d, *J* = 8.0 Hz, 4H), 7.49–7.46 (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.



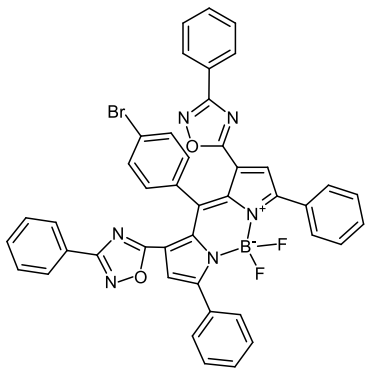
5,5'-(5,5-Difluoro-10-(3-methoxyphenyl)-3,7-diphenyl-5*H*-4λ^4,5λ^4-dipyrrolo[1,2-*c*:2',1'-*f*][1,3,2]diazaborinine-1,9-diyl)bis(3-phenyl-1,2,4-oxadiazole) (3d). (303 mg, 0.41 mmol, 41%) dark purple solid, mp = 228–230 °C. ^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.90–7.89 (m, 4H), 7.81 (d, *J* = 7.3 Hz, 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.



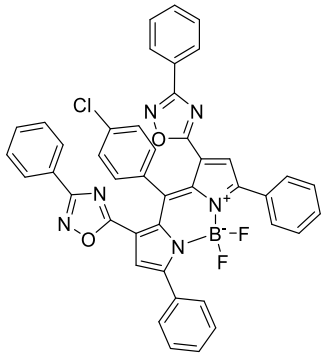
5,5'-(5,5-Difluoro-10-(4-methoxyphenyl)-3,7-diphenyl-5*H*-4λ^4,5λ^4-dipyrrolo[1,2-*c*:2',1'-*f*][1,3,2]diazaborinine-1,9-diyl)bis(3-phenyl-1,2,4-oxadiazole) (3e). (413 mg, 0.56 mmol, 56%) amorphous mass. ^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.89–7.88 (m, 4H), 7.81 (d, *J* = 7.9 Hz, 4H), 7.48–7.47 (m, 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.



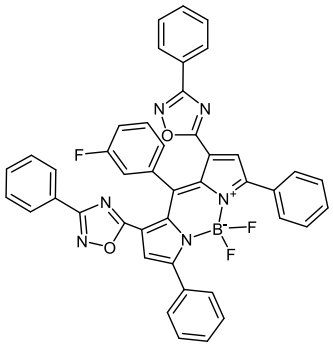
5,5'-(10-(2-bromophenyl)-5,5-difluoro-3,7-diphenyl-5*H*-4λ^4,5λ^4-dipyrrolo[1,2-*c*:2',1'-*f*][1,3,2]diazaborinine-1,9-diyl)bis(3-phenyl-1,2,4-oxadiazole) (3f). (228 mg, 0.29 mmol, 29%) dark blue solid, mp = 158–160 °C. ^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.93–7.91 (m, 4H), 7.83 (d, *J* = 7.2 Hz, 4H), 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.



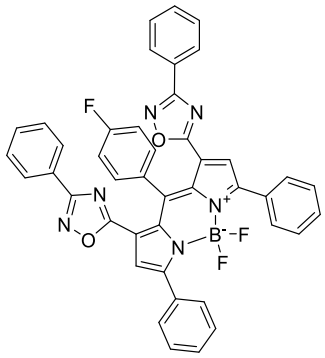
5,5'-(10-(4-bromophenyl)-5,5-difluoro-3,7-diphenyl-5*H*-4λ^4,5λ^4-dipyrrolo[1,2-*c*:2',1'-*f*][1,3,2]diazaborinine-1,9-diyl)bis(3-phenyl-1,2,4-oxadiazole) (3g). (126 mg, 0.16 mmol, 16%) dark blue solid, mp = 197–198 °C. ^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.90–7.89 (m, 4H), 7.83–7.81 (m, 4H), 7.50–7.49 (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**

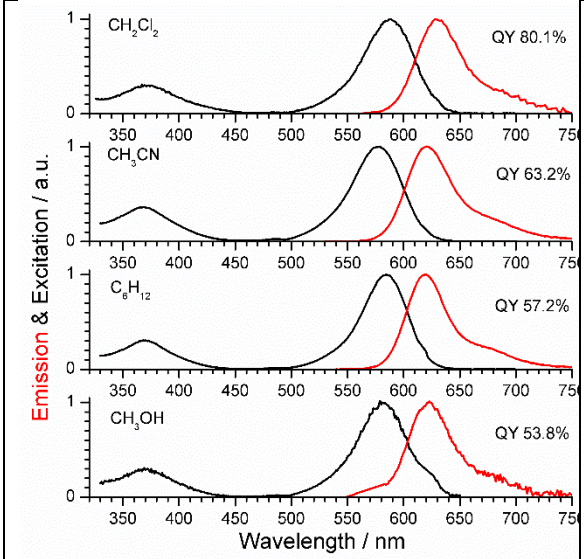


Fig. S2 Compound **3b**

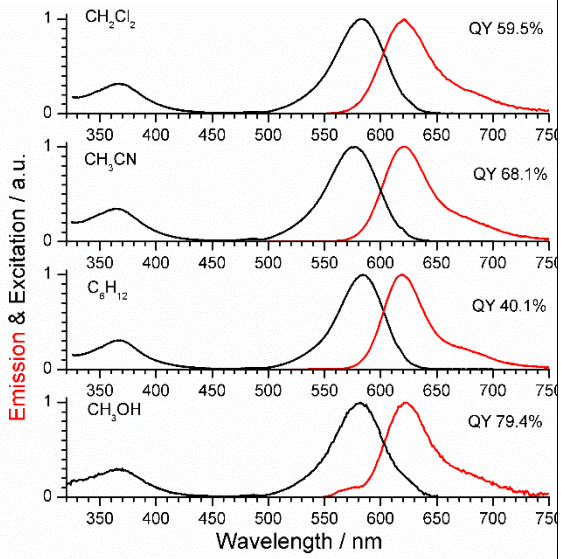


Fig. S3 Compound **3c**

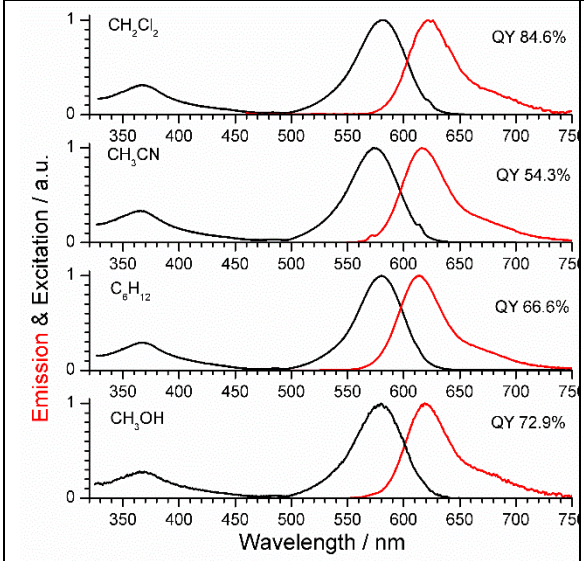


Fig. S4 Compound **3d**

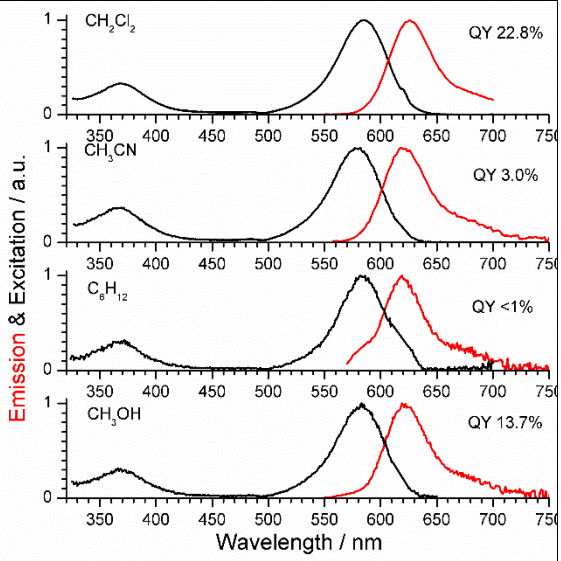


Fig. S5 Compound **3e**

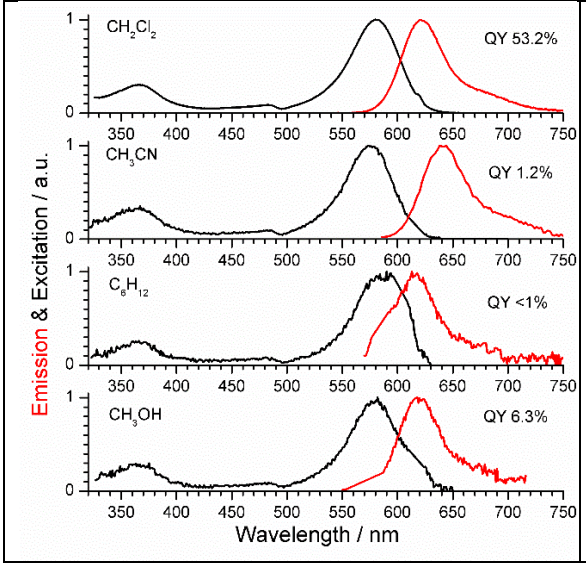


Fig. S6 Compound **3f**

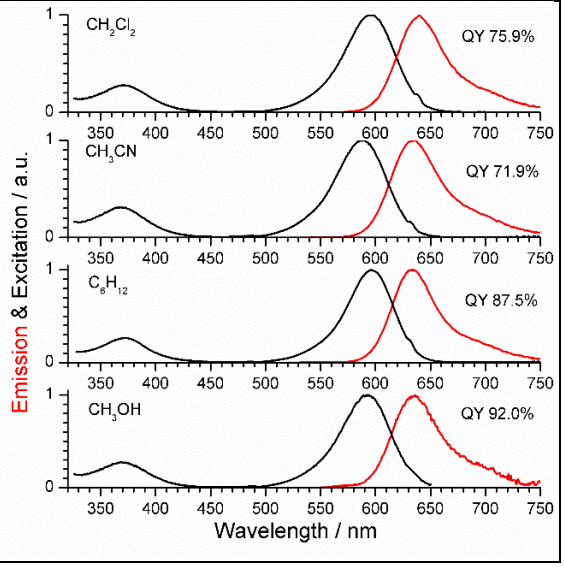


Fig. S7 Compound **3g**

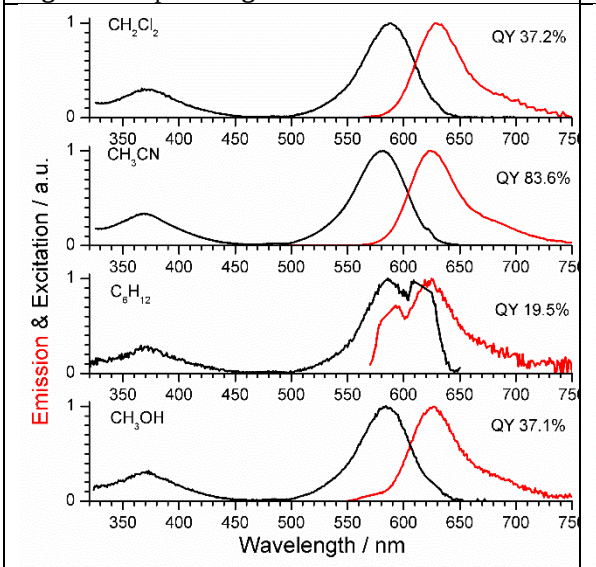


Fig. S8 Compound **3h**

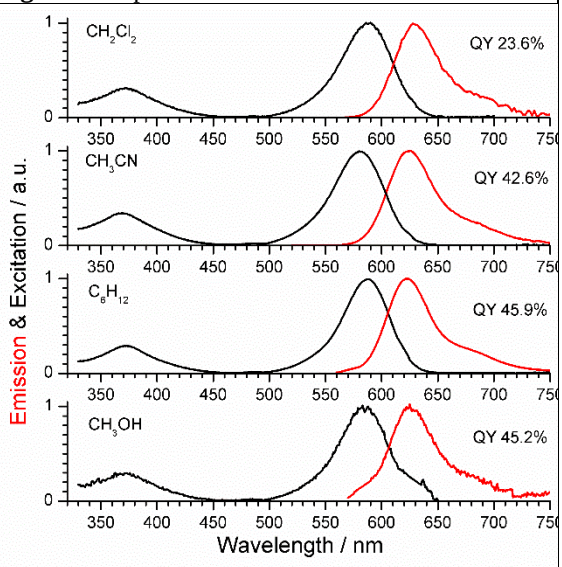


Fig. S9 Compound **3i**

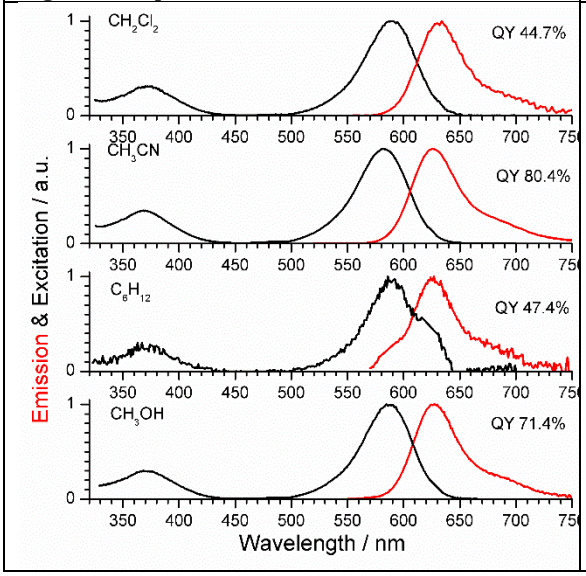
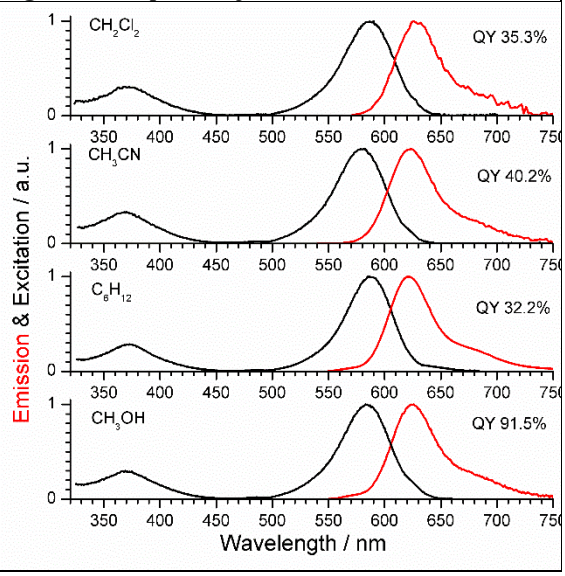


Fig. S10 Compound **3j**



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. λ_{ex} **3a** and (**4**)[a]	$\Delta\lambda_{ex}$[b]	Calc. $\Delta\lambda_{ex(\mathbf{3a}\text{-}\mathbf{4})}$ 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 λ_{ex} values for **3a** and **4** (in parenthesis) to be compared with the experimental λ_{ex} of 588 and 561 nm for **3a** and **4**, respectively (see Fig. 3 of the text).
b) Variation between experimental and calculated λ_{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.

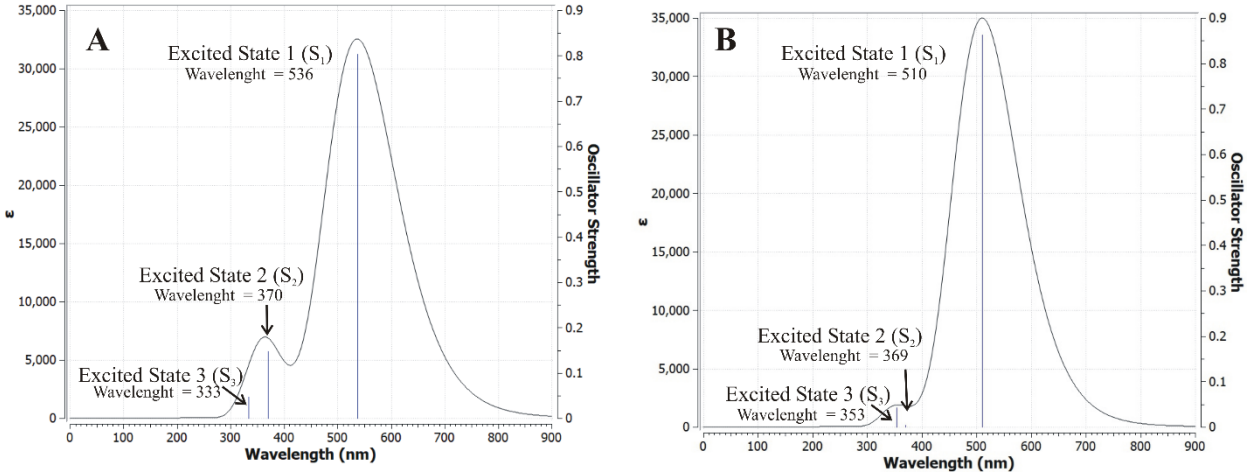


Fig. S11 TD-DFT (CAM-B3LYP/6311+G(d,p)) simulated spectra for **3a** (A) and **4** (B) in THF as solvent (CPCM model). Wavelenghts in nm.

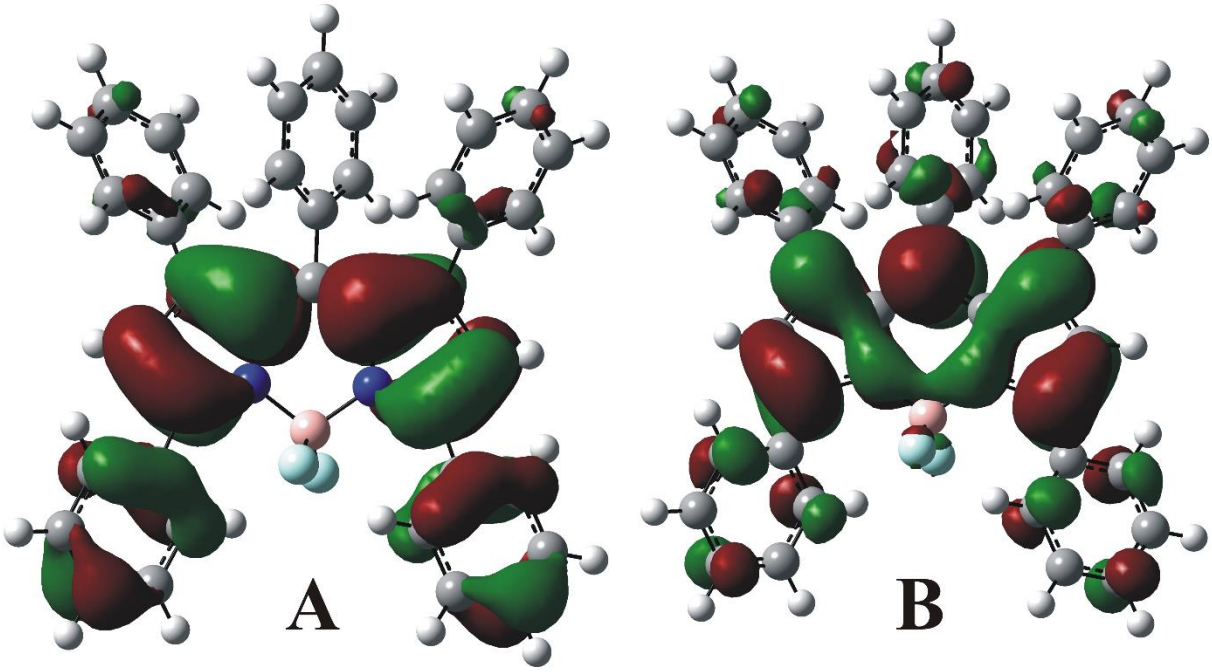


Fig. S12 HOMO **(A)** and LUMO **(B)** countours calculated at the TD-DFT level for compound **4** corresponding to the S0 ←-S1 transition**.**

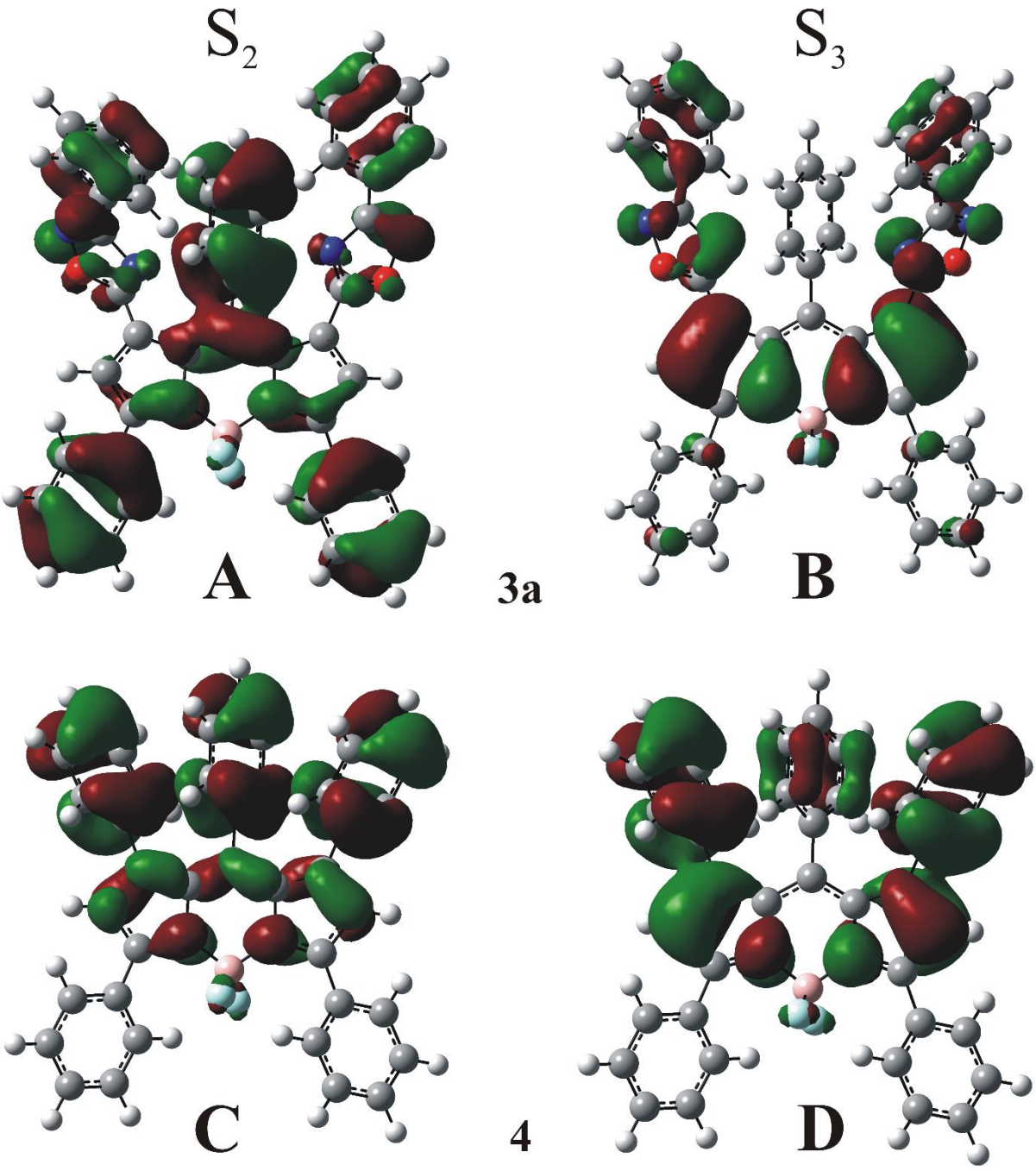


Fig. S13 TD-DFT analysis (CAM-B3LYP/6311+G(d,p)) of MO contributions for S0 ←-S2 and S0 ←-S3 transitions to the near-UV region (maximum at about 360 nm, see Fig. S11) for complexes **3a** (A, B) and **4** (C, D).

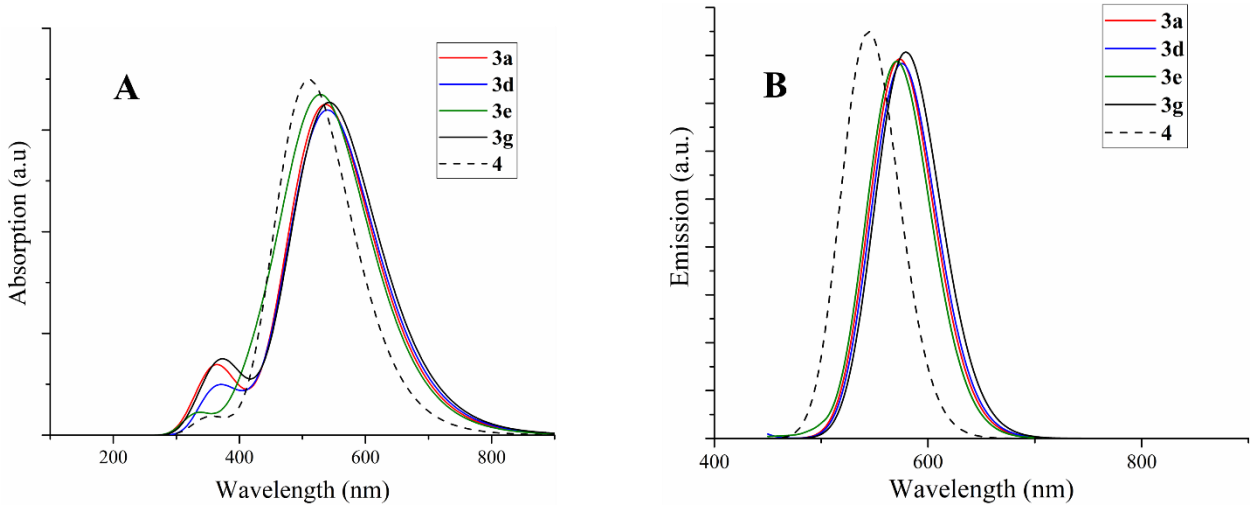


Fig. S14 TD-DFT (CAM-B3LYP/6311+G(d,p)) simulated spectra for absorption (**A**) and emission (**B**) of selected oxadiazole compounds (**3a**, **3d**, **3e**, **3g**) in THF as solvent. Compound **4** (dotted line) is also reported for comparison.

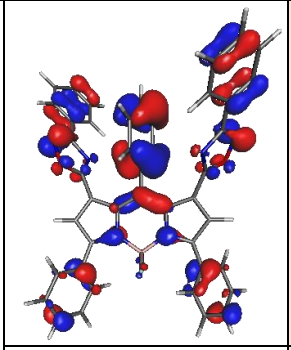
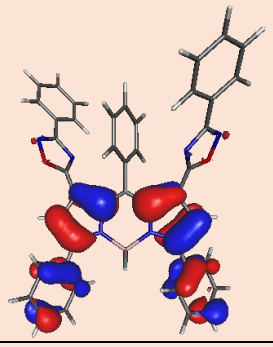
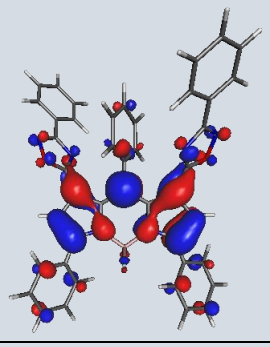
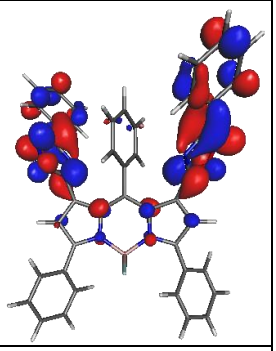
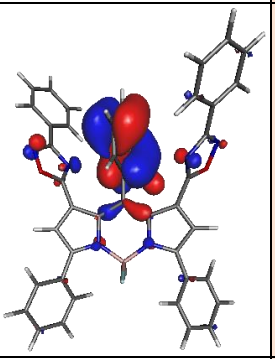
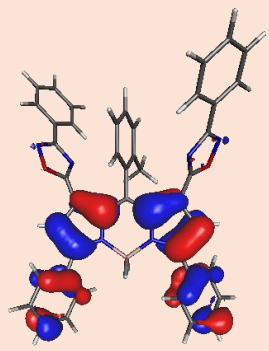
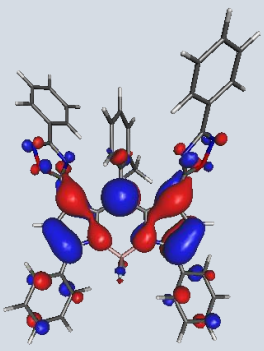
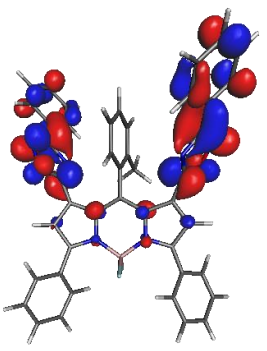
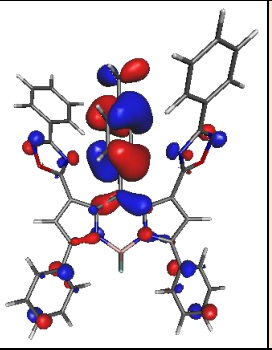
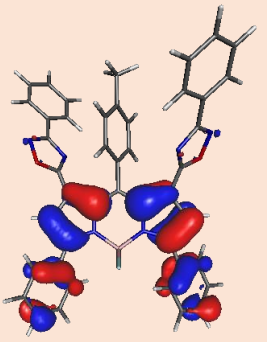
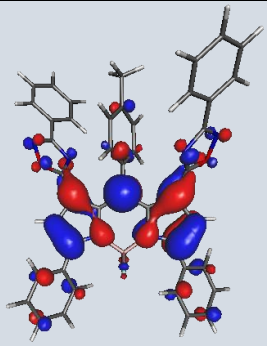
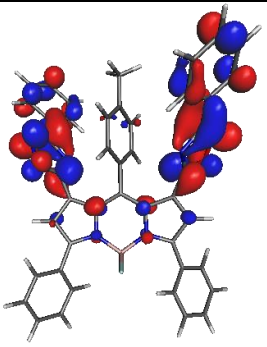
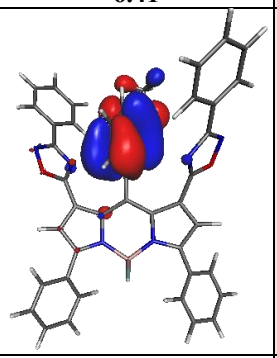
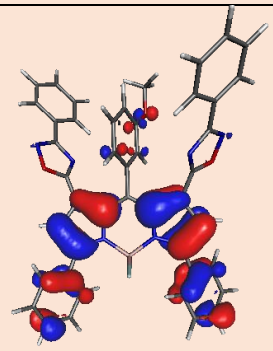
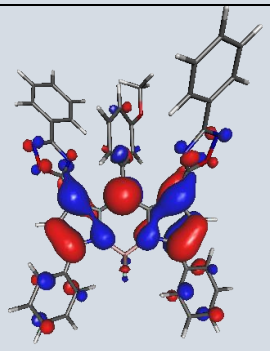
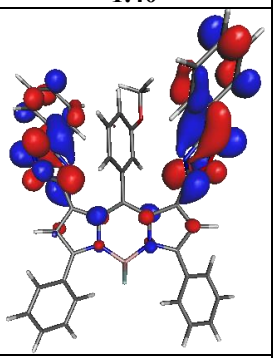
Table S3. Calculated main assignments (coefficient), excitation energies *E* (in eV), maximum absorption wavelengths λ_{abs} (in nm), the oscillator strength *f*, for selected compounds at the TD-CAM-B3LYP/6-311+G(d,p)//B3LYP/6-31G(d,p) level, by using THF as solvent (CPCM).

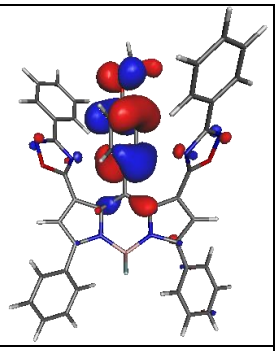
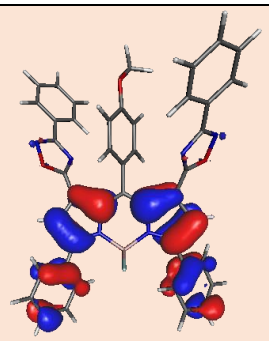
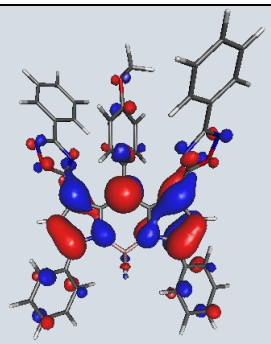
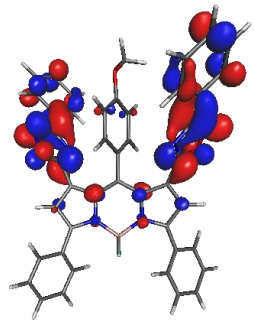
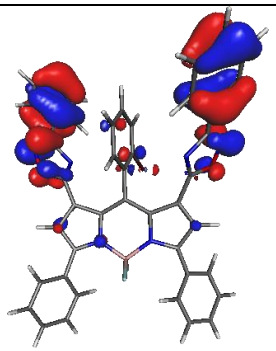
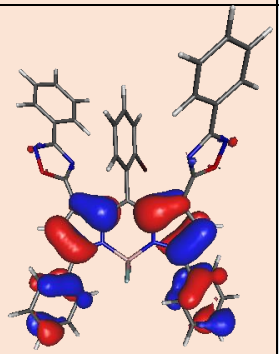
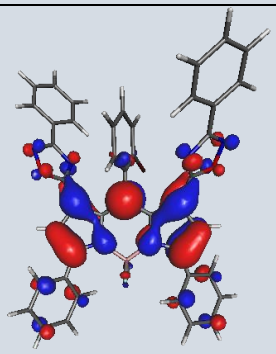
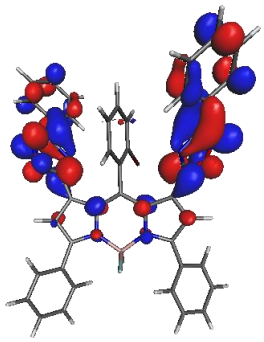
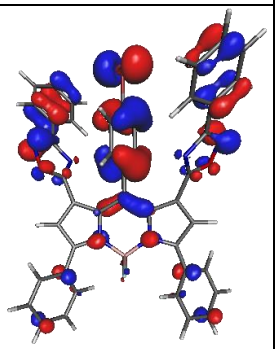
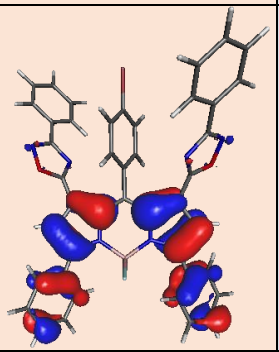
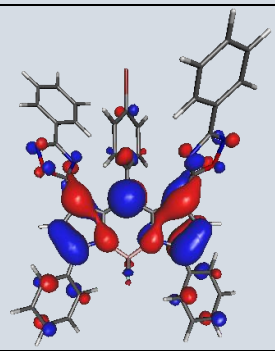
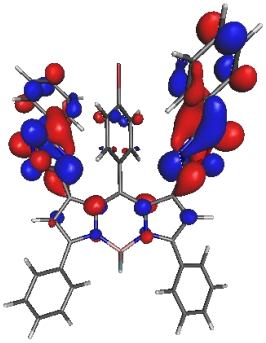
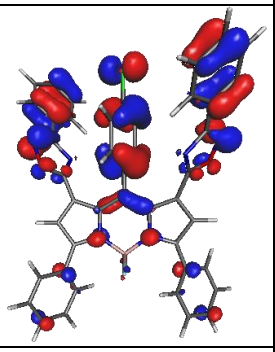
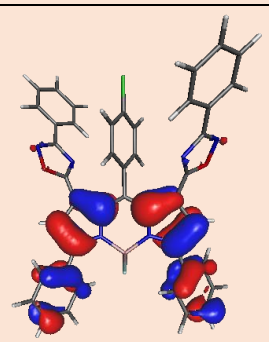
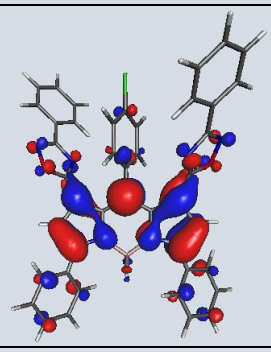
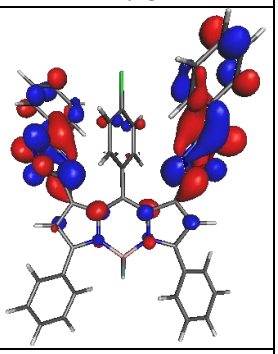
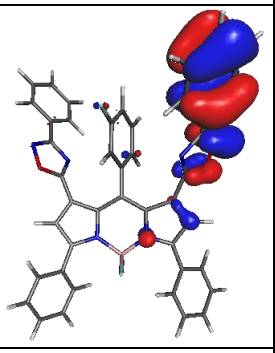
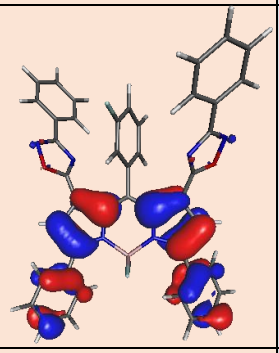
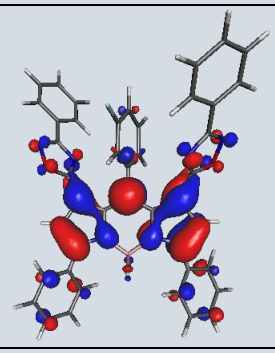
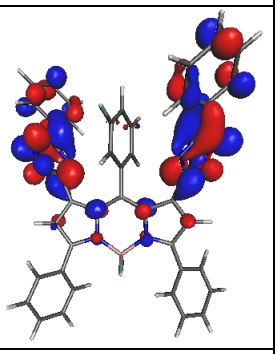
Compounds	Main assignment	*E*	λ_{abs}	*f*
3a	H → L (0.696)	2.3104	536.62	0.8027
3a	H_{-1} → L (0.593)	3.3502	370.09	0.1473
3a	H_{-10} → L (0.586)	3.7130	333.92	0.0476
3d	H → L (0.696)	2.2954	540.14	0.7878
3d	H_{-1} → L (0.6976)	3.0240	410.00	0.0414
3d	H_{-4} → L (0.5909)	3.4189	362.64	0.1038
3e	H → L (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 λ_{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*	λ_{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**

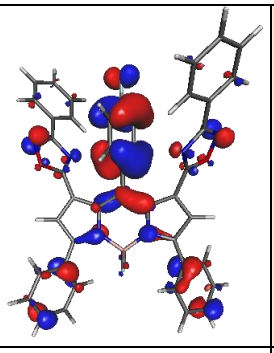
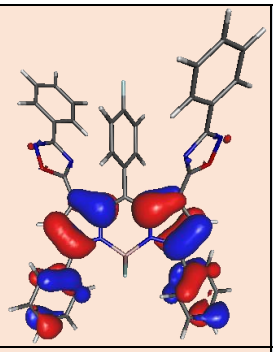
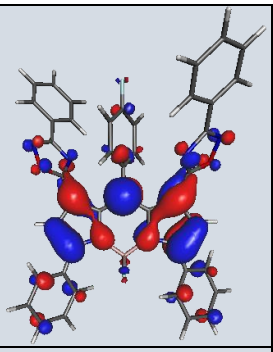
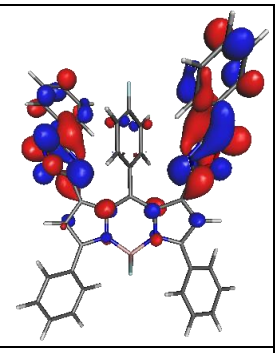
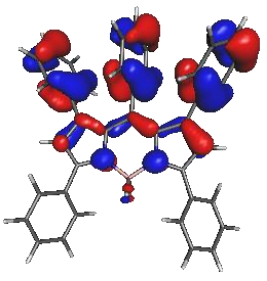
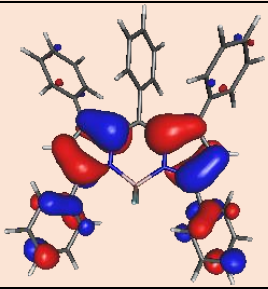
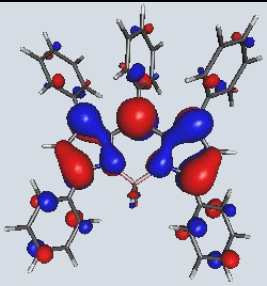
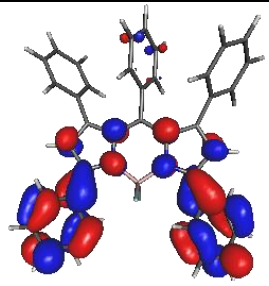
3j				
	-6.55	**-5.76**	**-3.28**	**-1.44**
4				
	-6.08	**-5.38**	**-2.74**	**-0.54**

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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Rabuck, A.D.; Raghavachari, K.; Foresman, J.B.; Ortiz, J.V.; Cui, Q.; Baboul, A.G.;Clifford, S.; Cioslowski, J.; Stefanov, B.B.; Liu, G.; Liashenko, A.; Piskorz, P.; Komaromi, I.; Martin, R.L.; Fox,D.J.; Keith, T.; Al-Laham, M.A.; Peng, C.Y.; Nanayakkara, A.; Challacombe, M.; Gill, P.M.W.; Johnson, B.;Chen, W.; Wong, M.W.; Gonzalez, C.; and Pople, J.A.; Gaussian, Inc., Wallingford CT, 2004, 2004.

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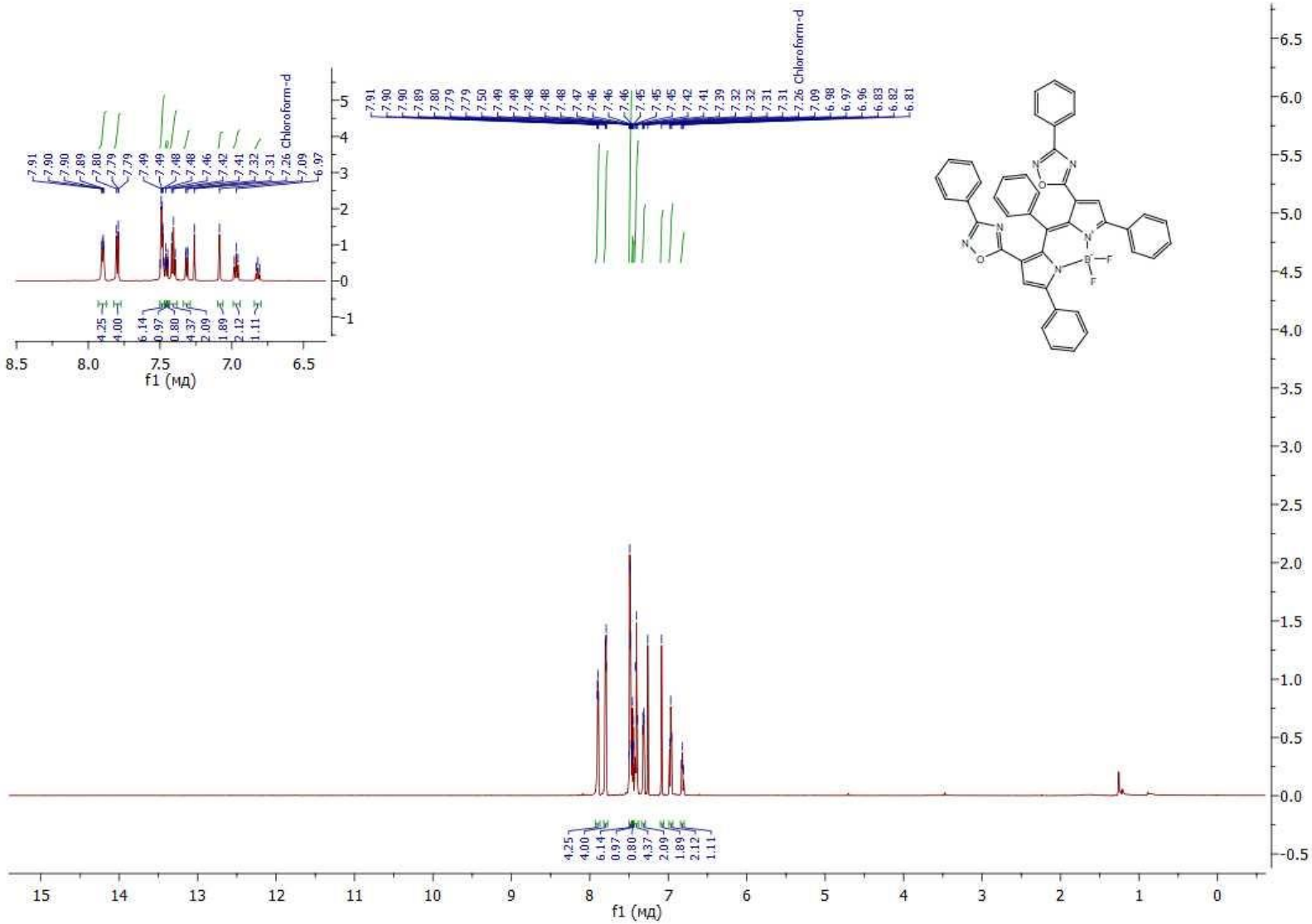
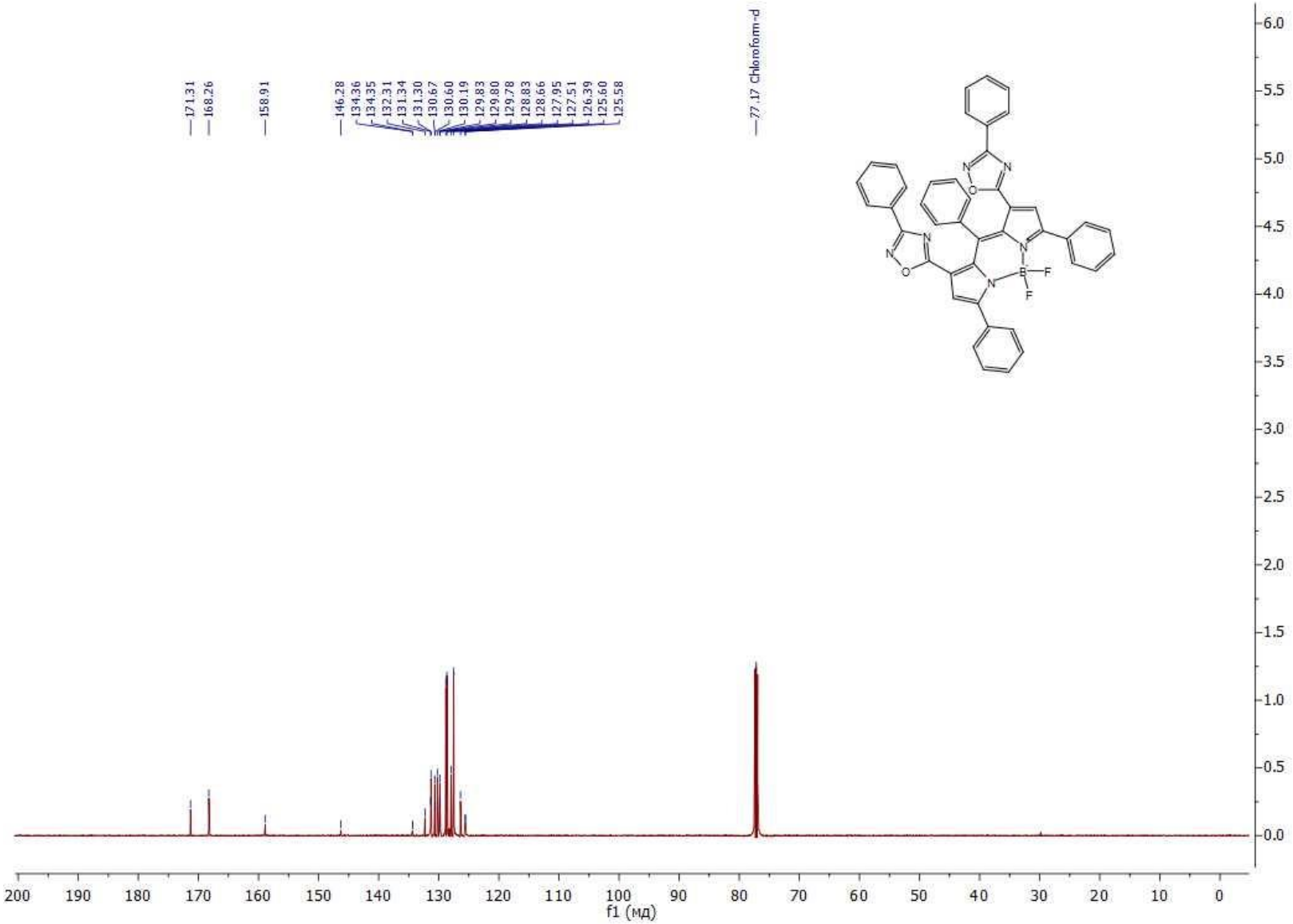
8. NMR spectra for products

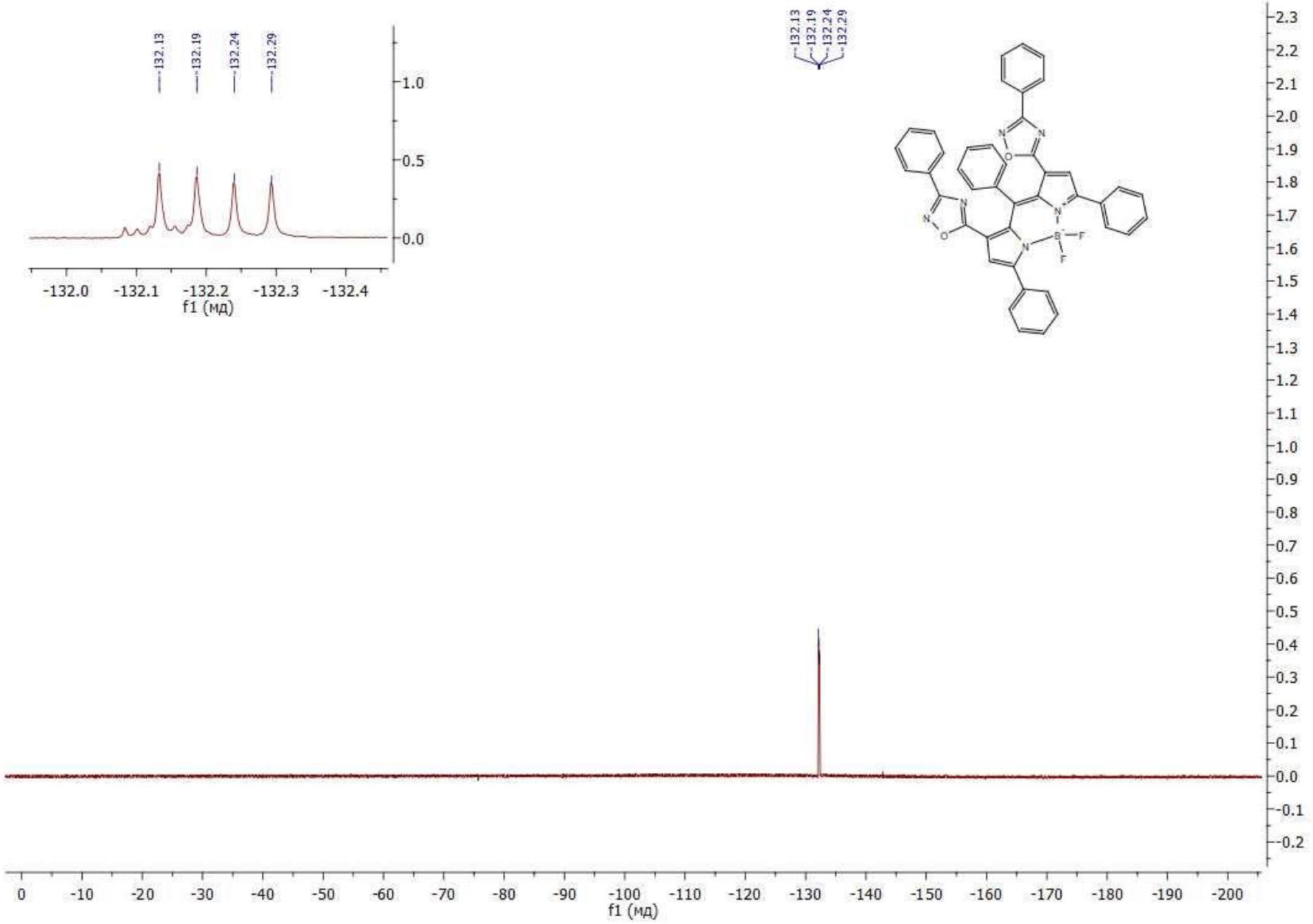
^{1}H NMR spectrum for **3a**



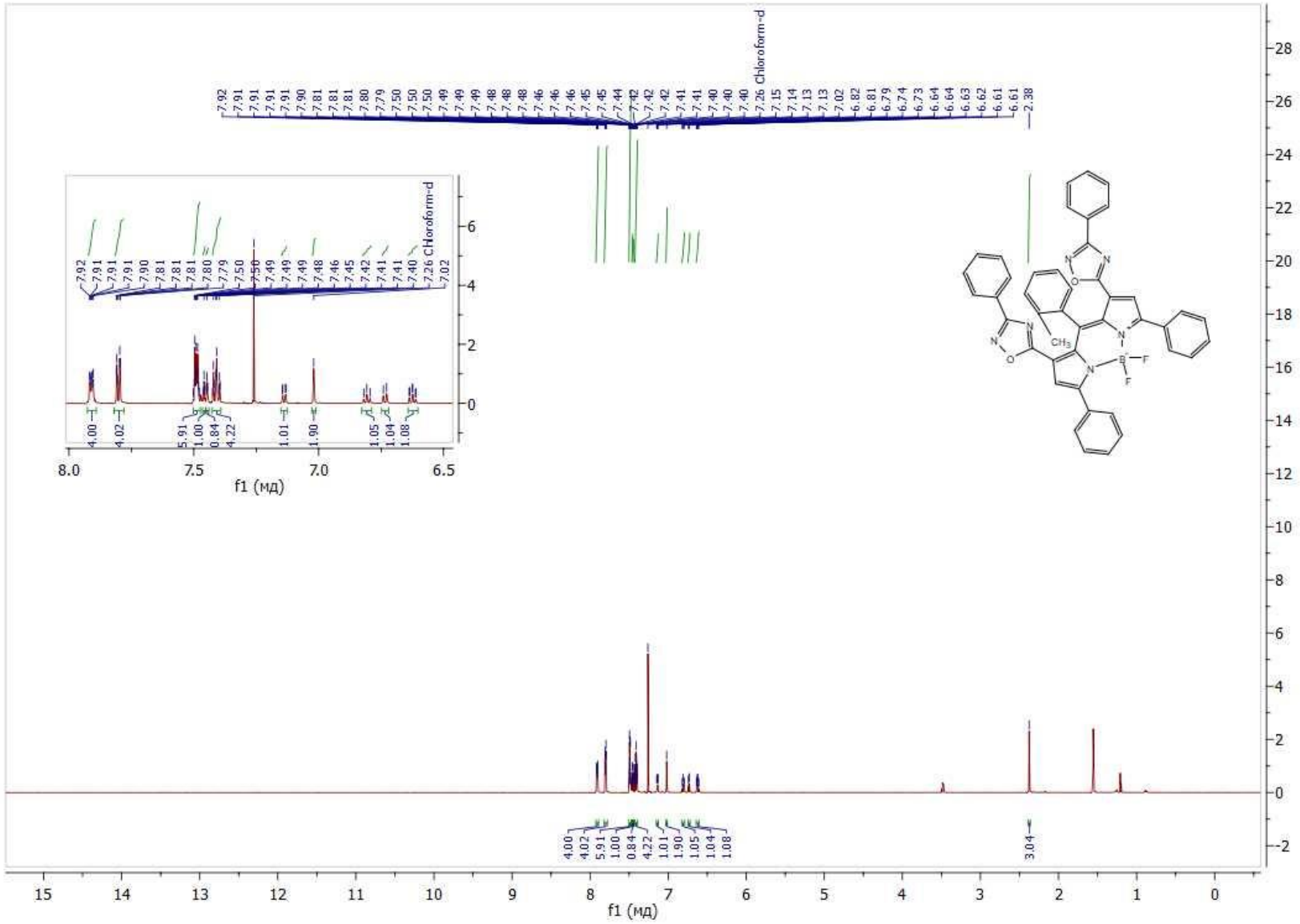
^{13}C NMR spectrum for **3a**



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



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



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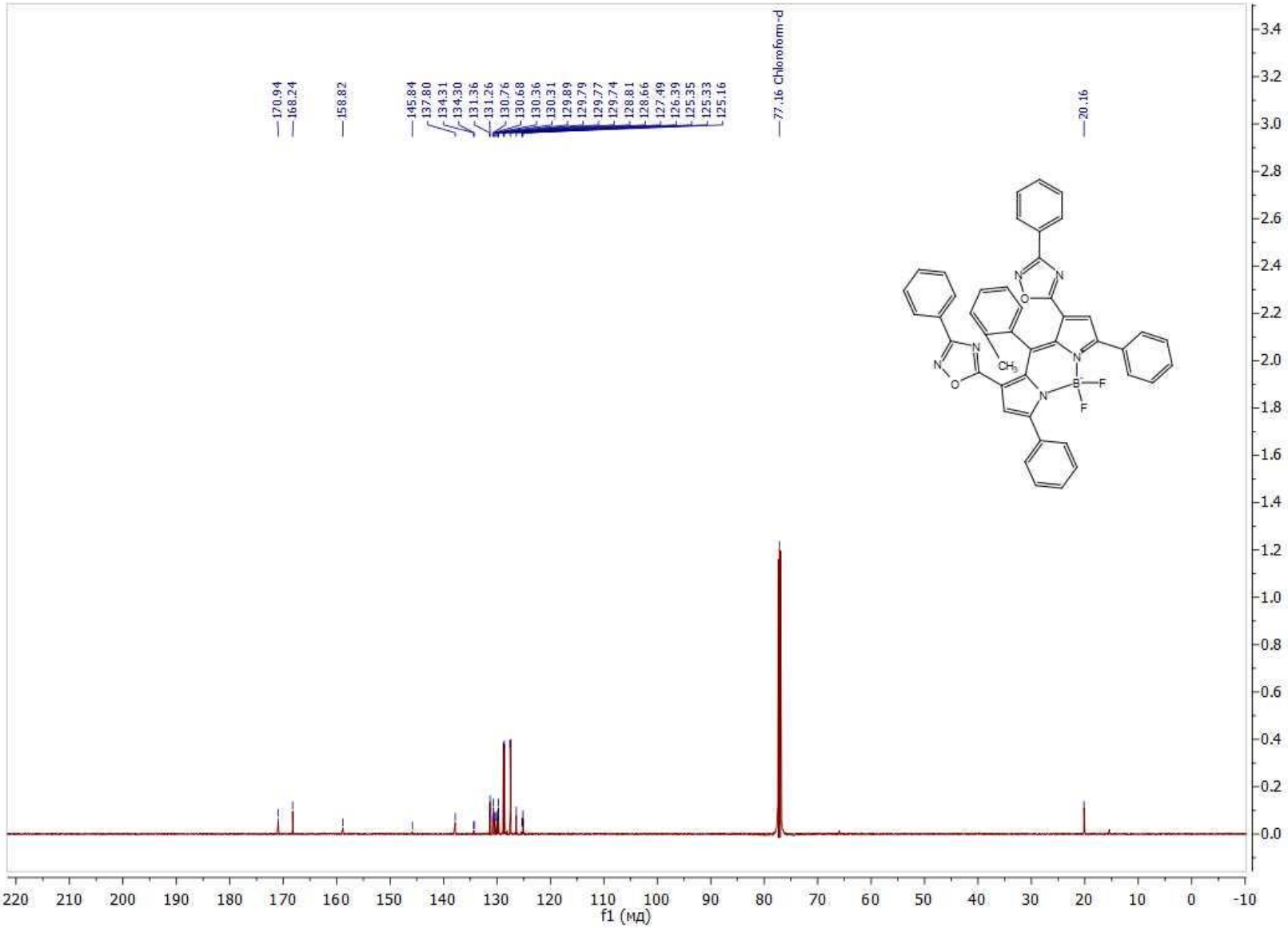

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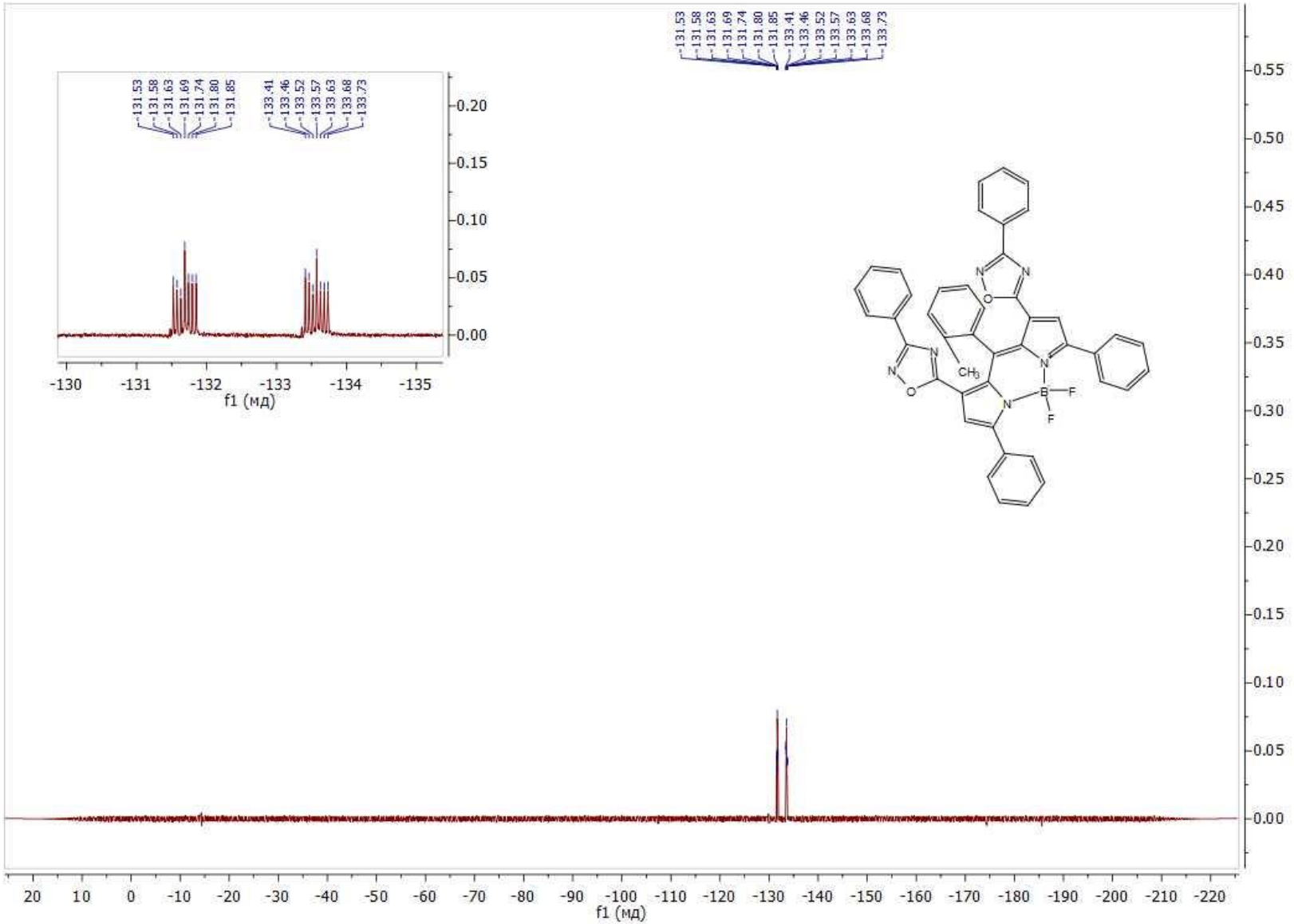

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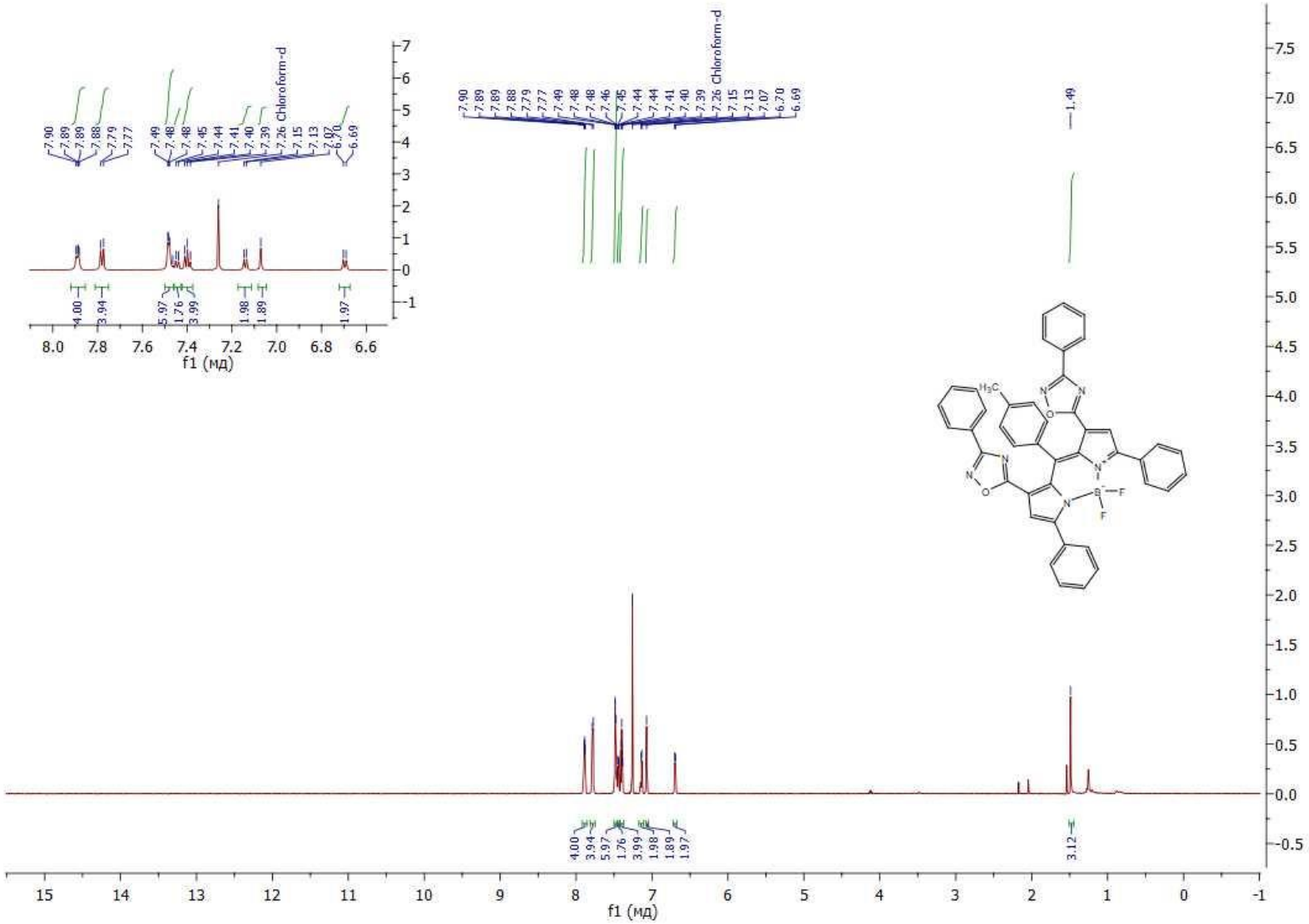
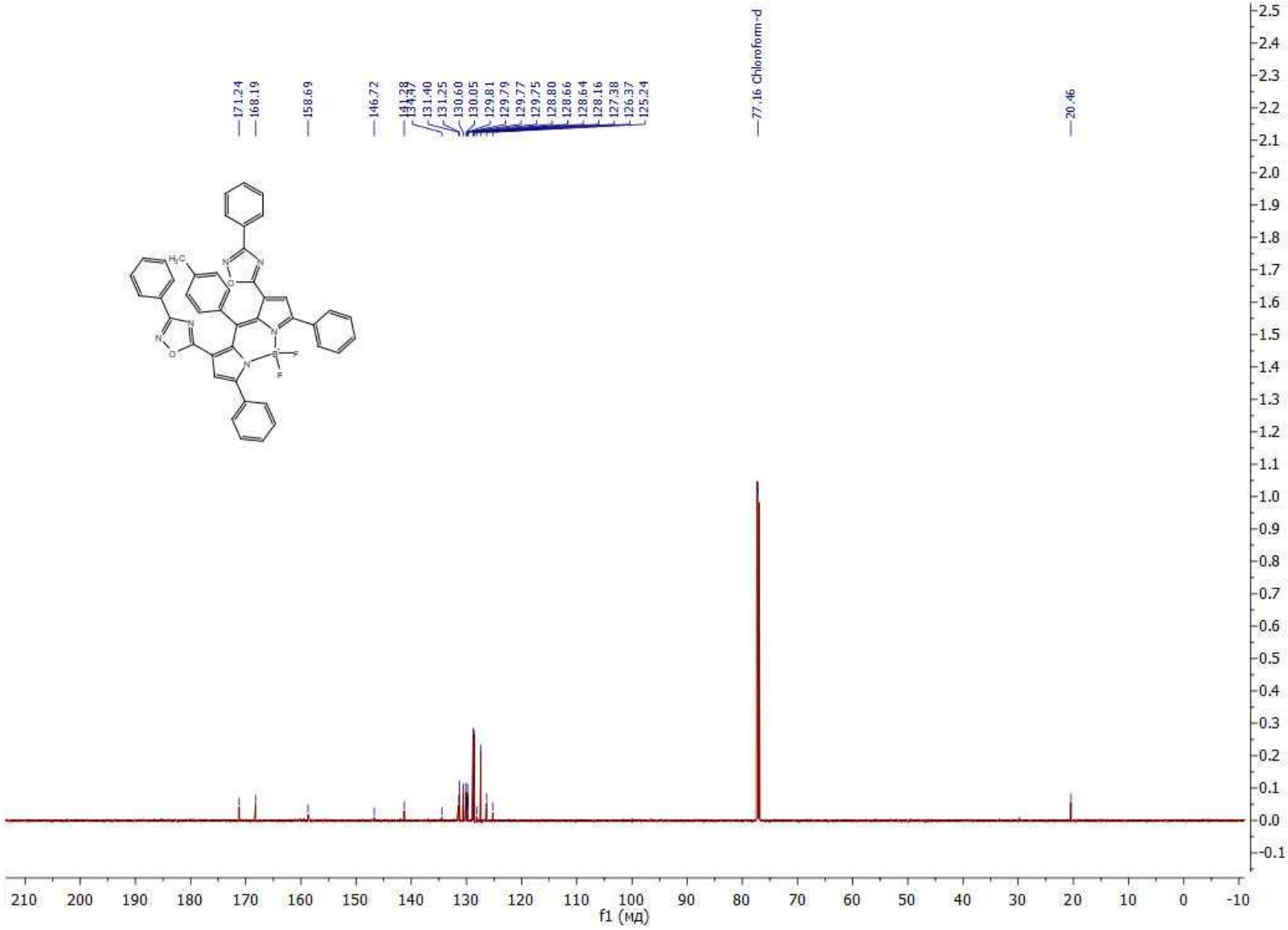
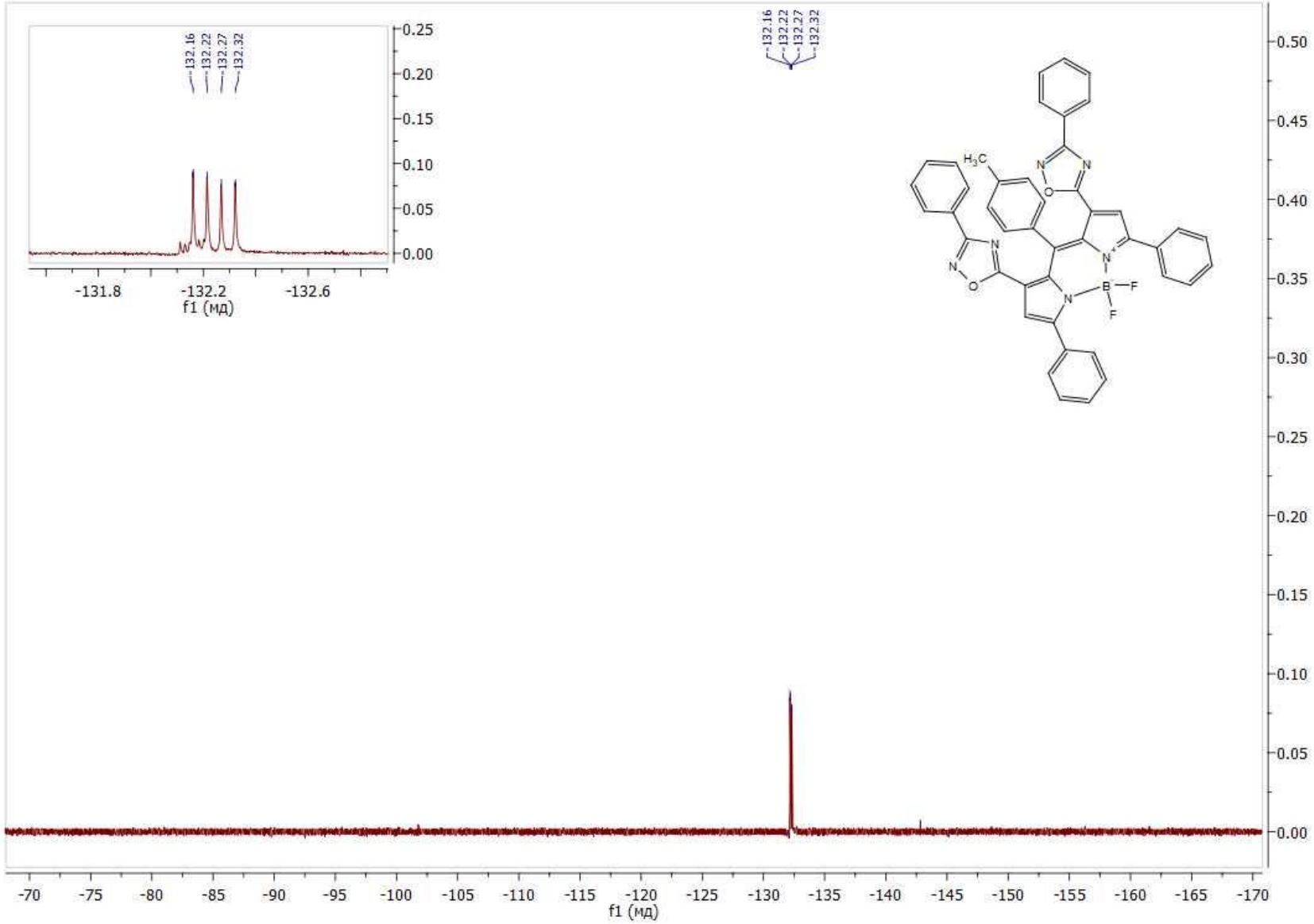


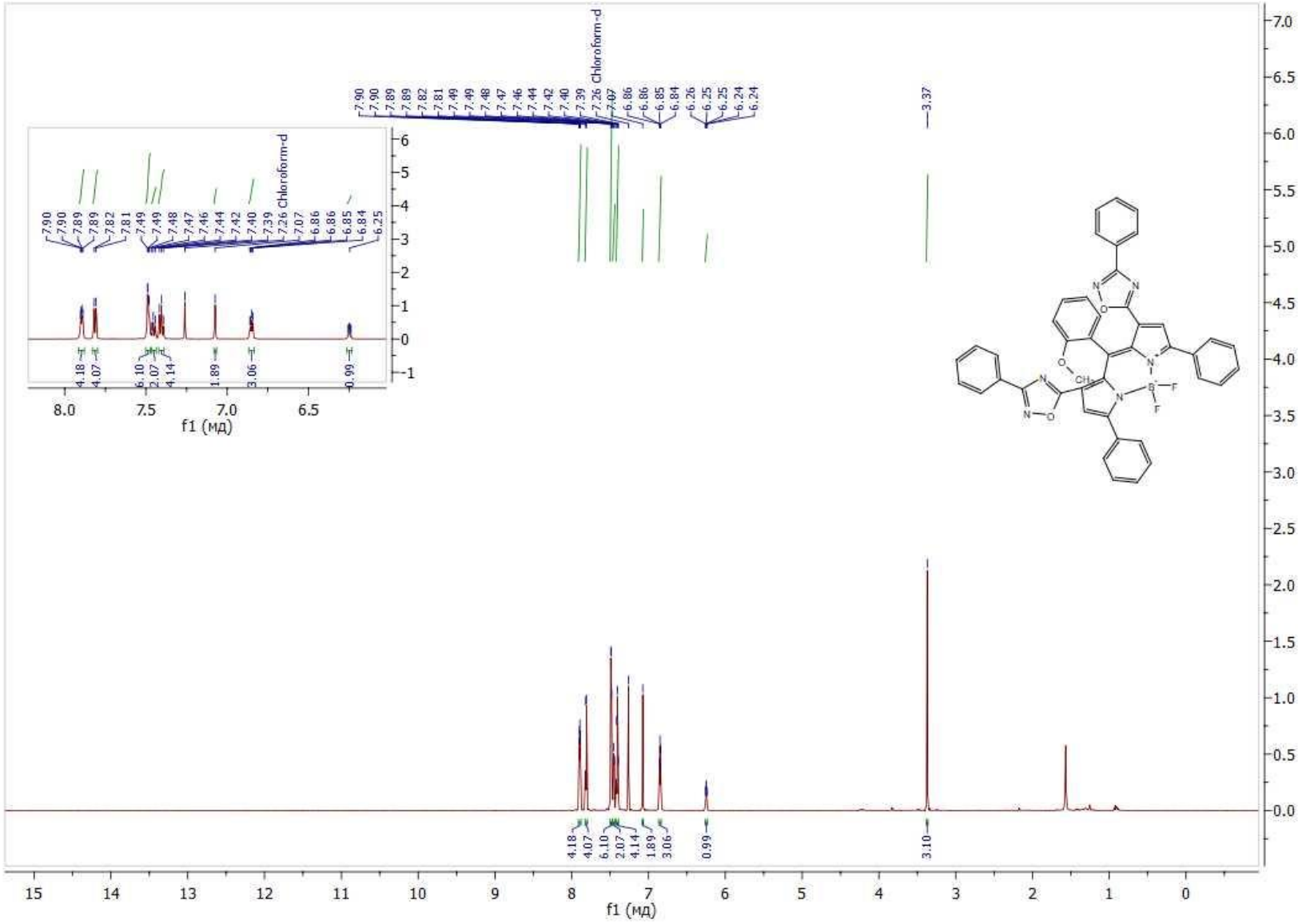
^{13}C NMR spectrum for **3c**



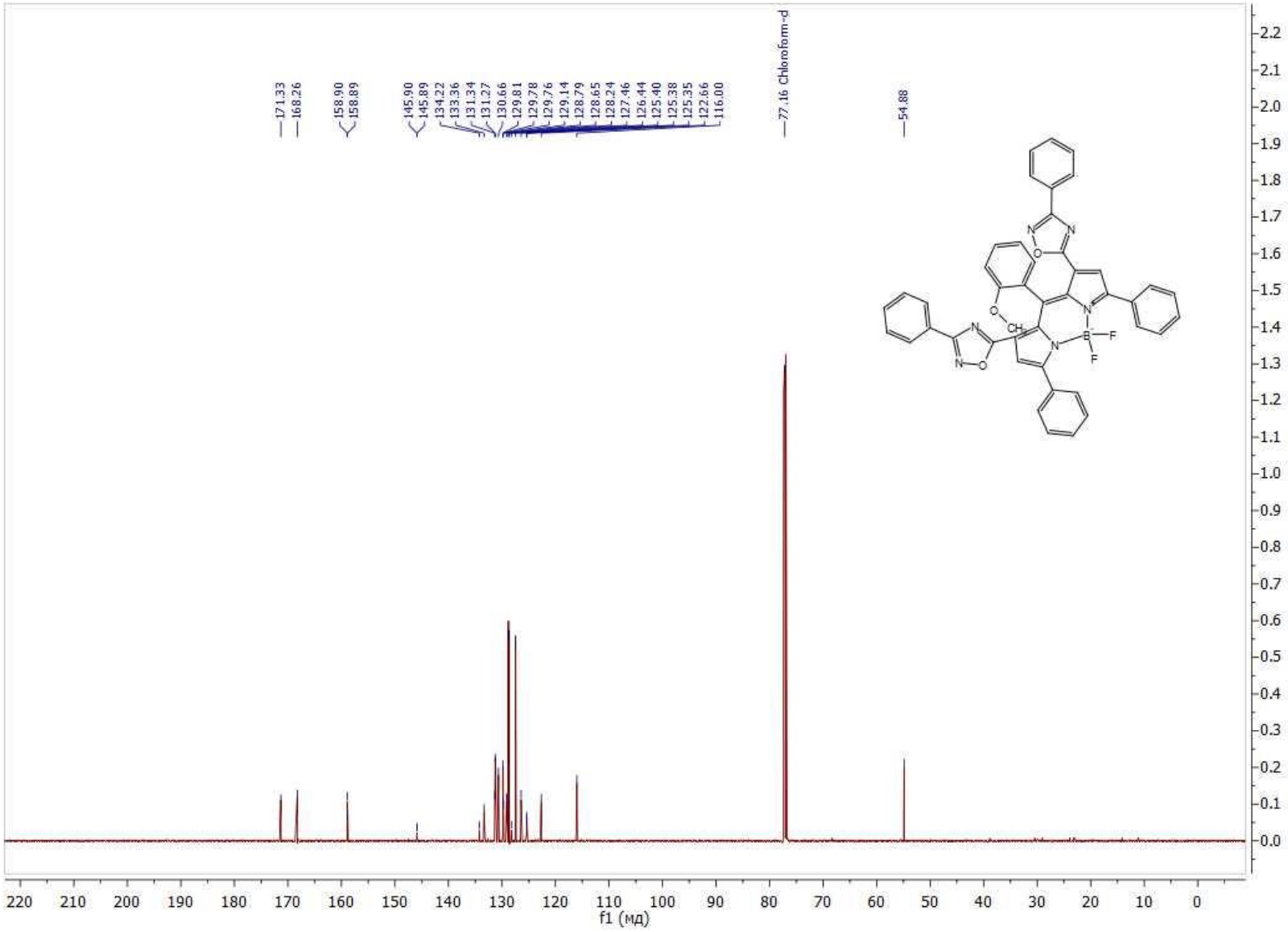
^{19}F NMR spectrum for **3c**



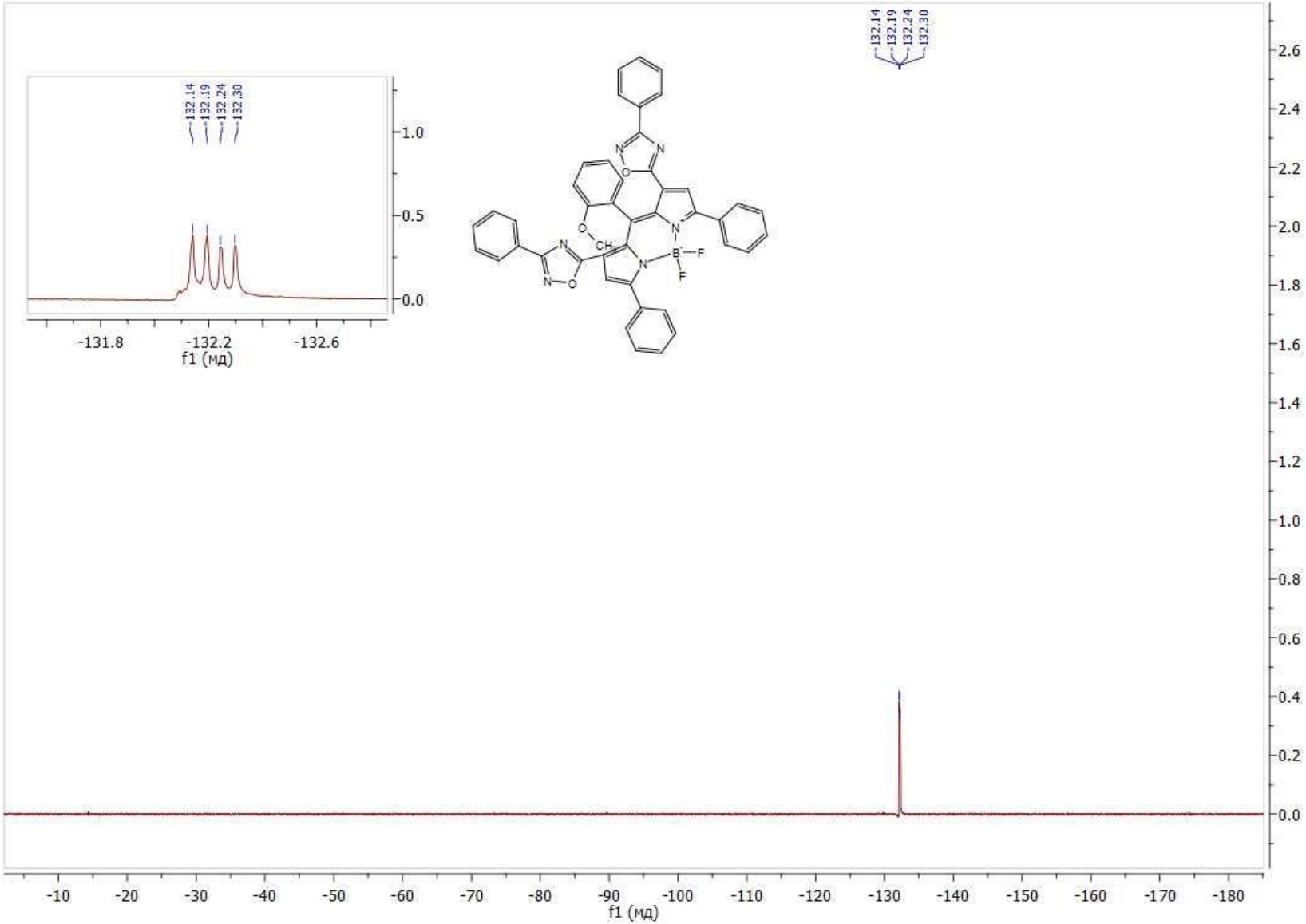
^{1}H NMR spectrum for **3d**



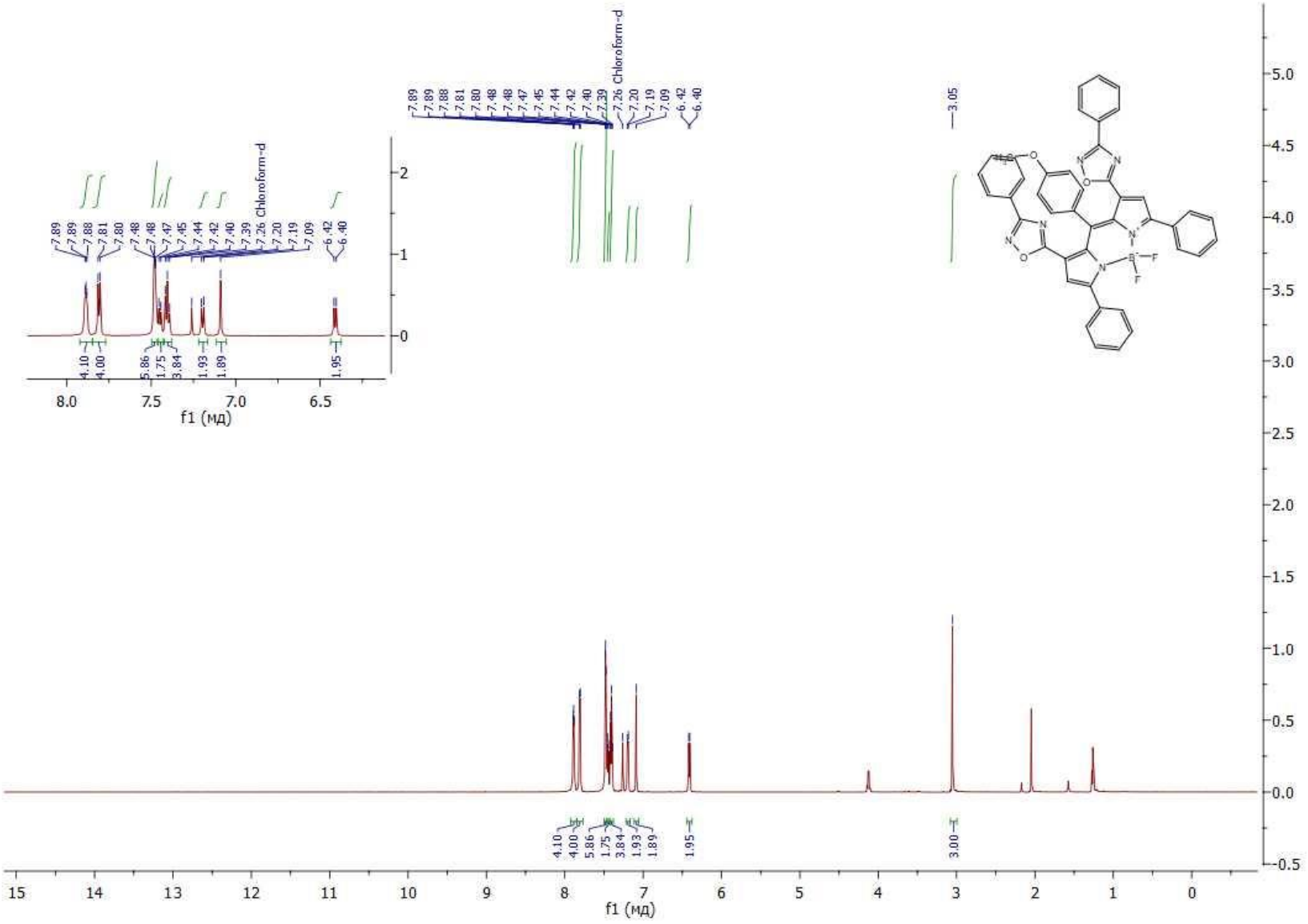
^{13}C NMR spectrum for **3d**



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



^{1}H NMR spectrum for **3e**



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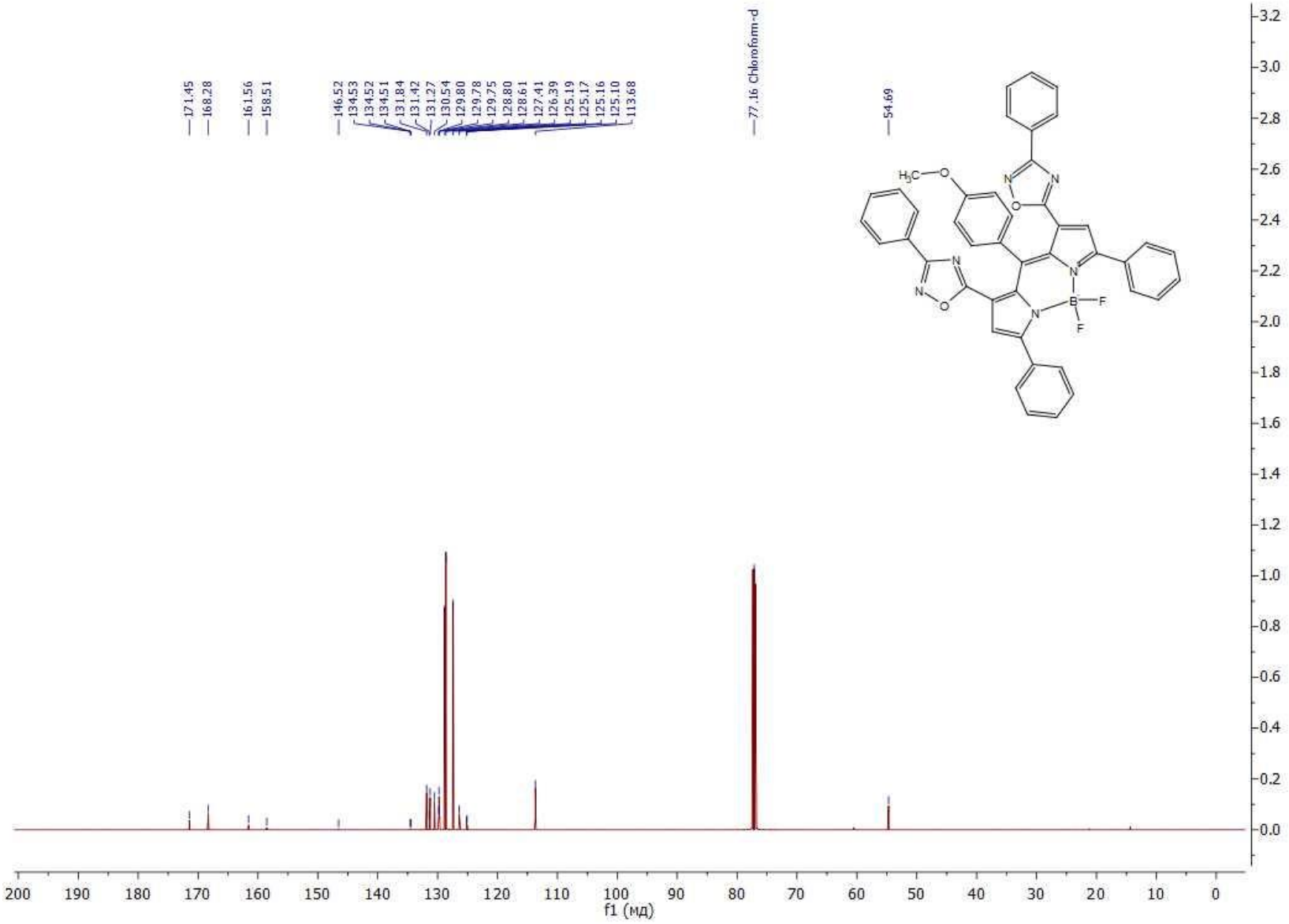
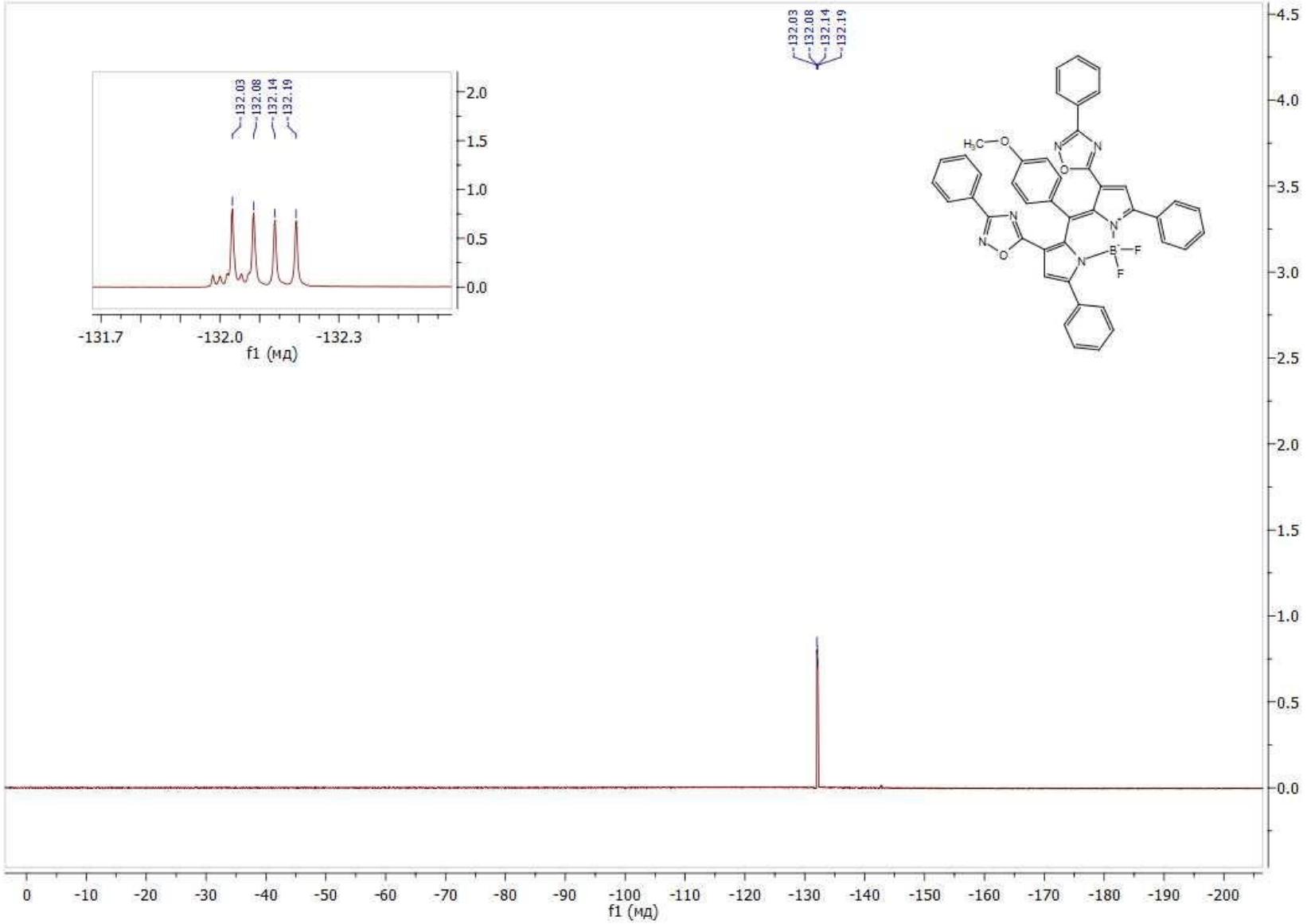
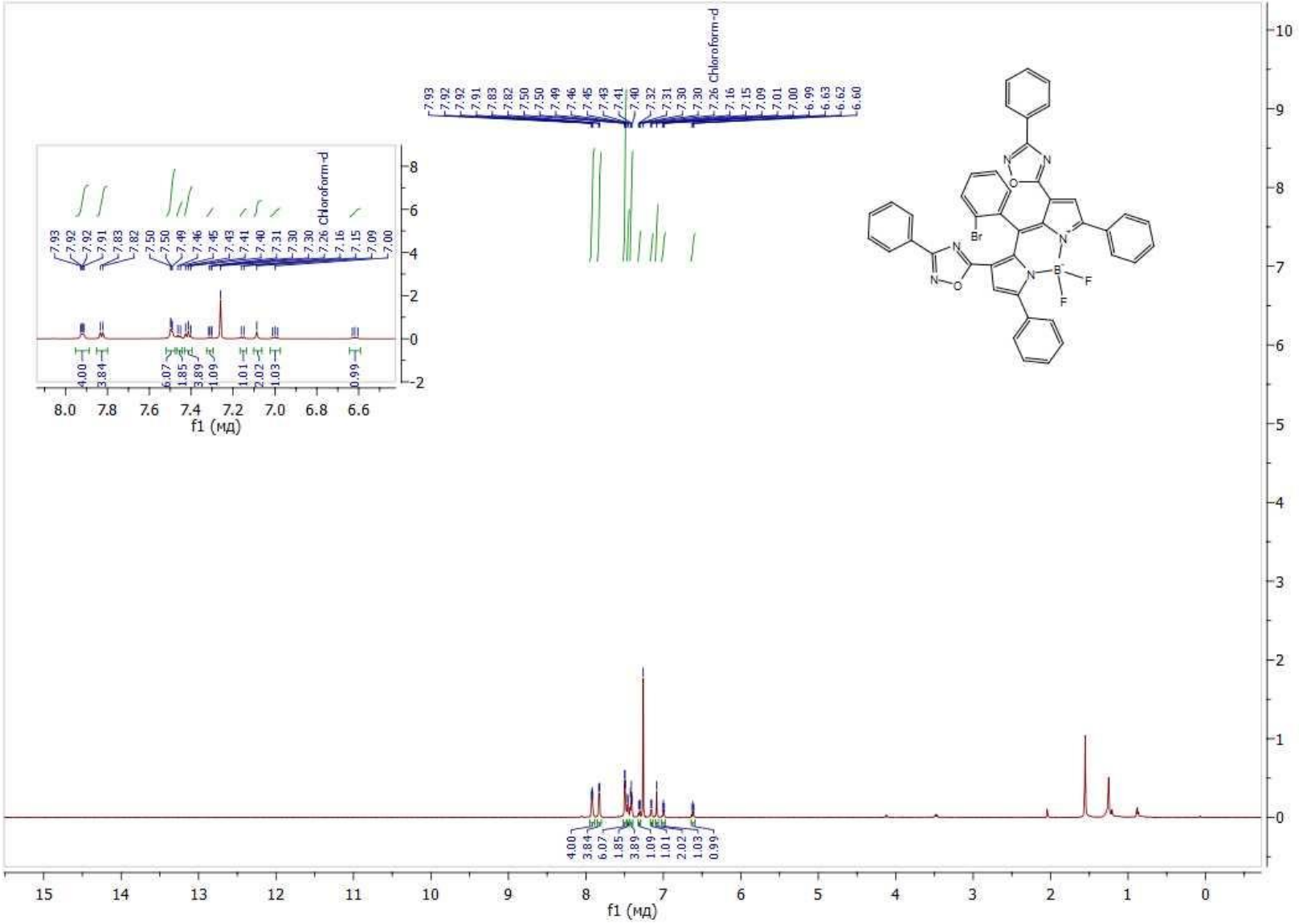


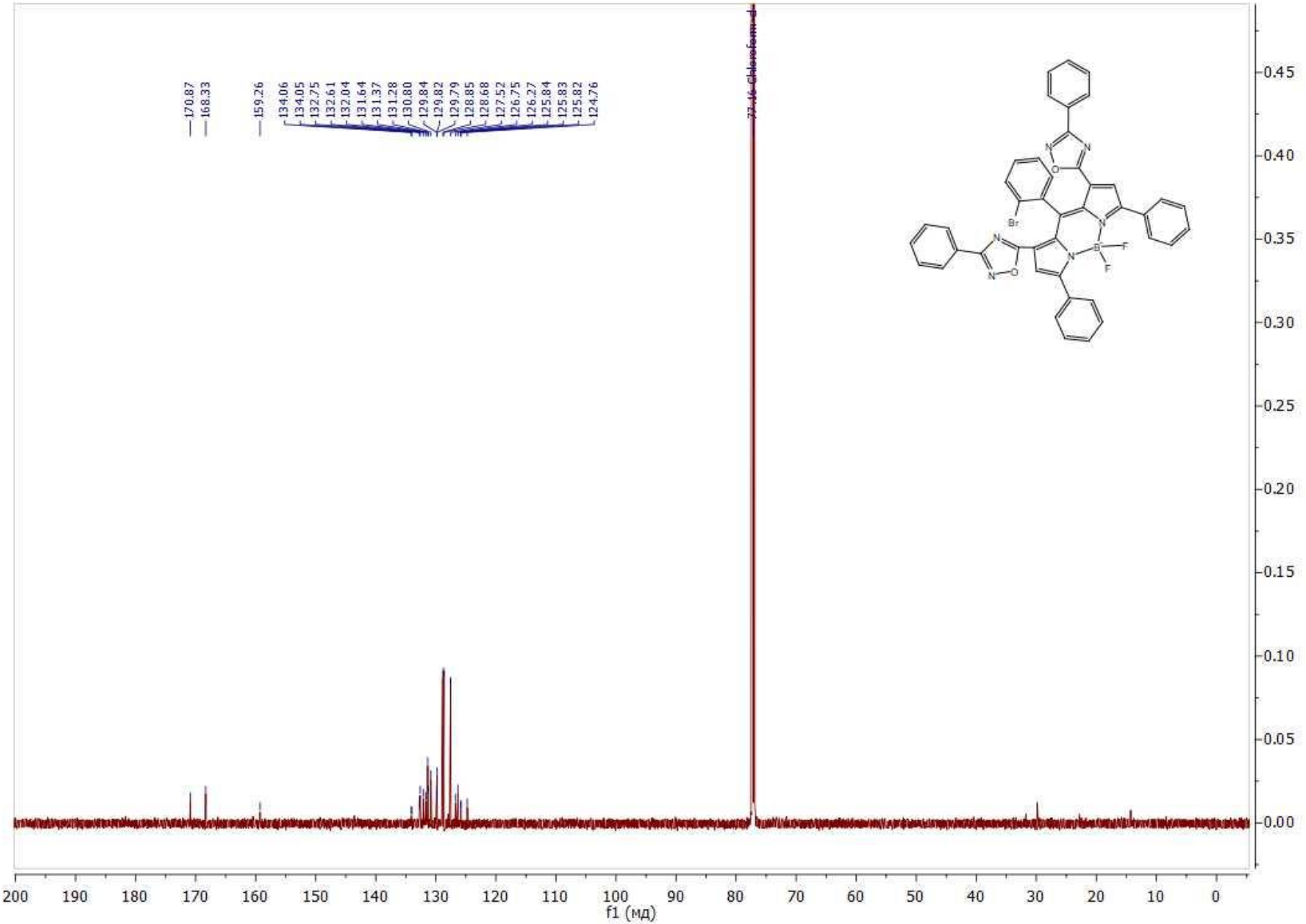
^{19}F NMR spectrum for **3e**



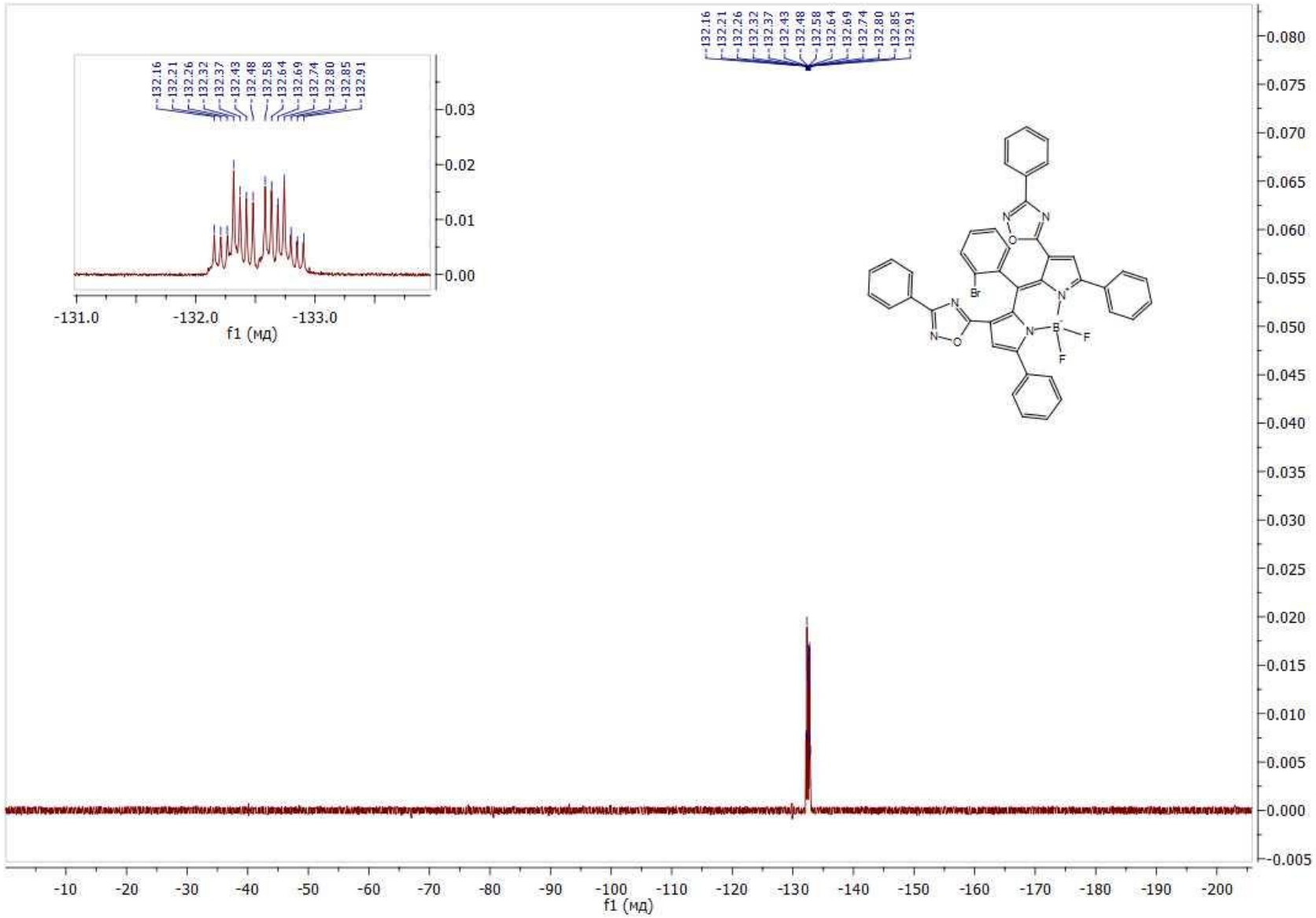
^{1}H NMR spectrum for **3f**



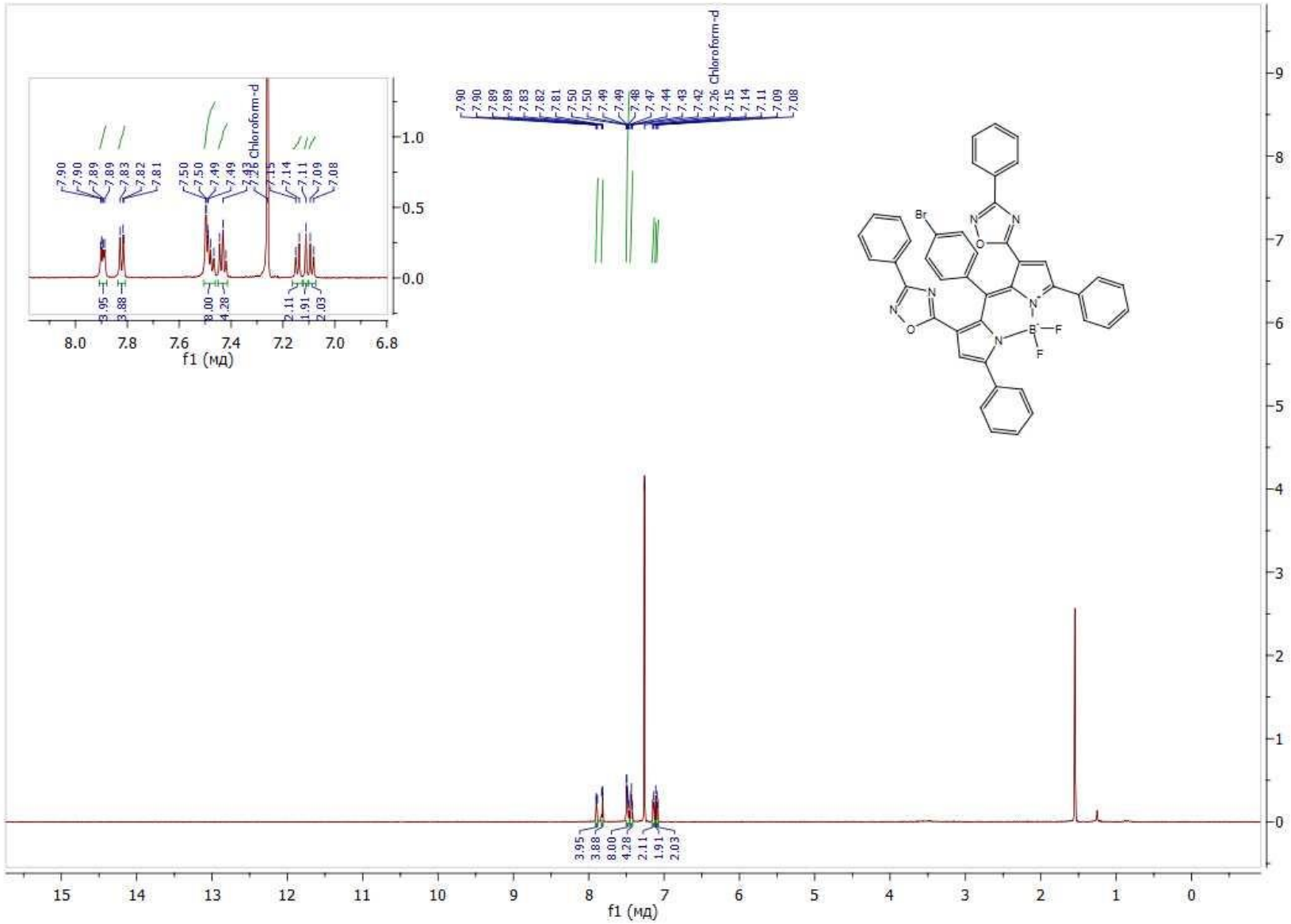
^{13}C NMR spectrum for **3f**



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



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



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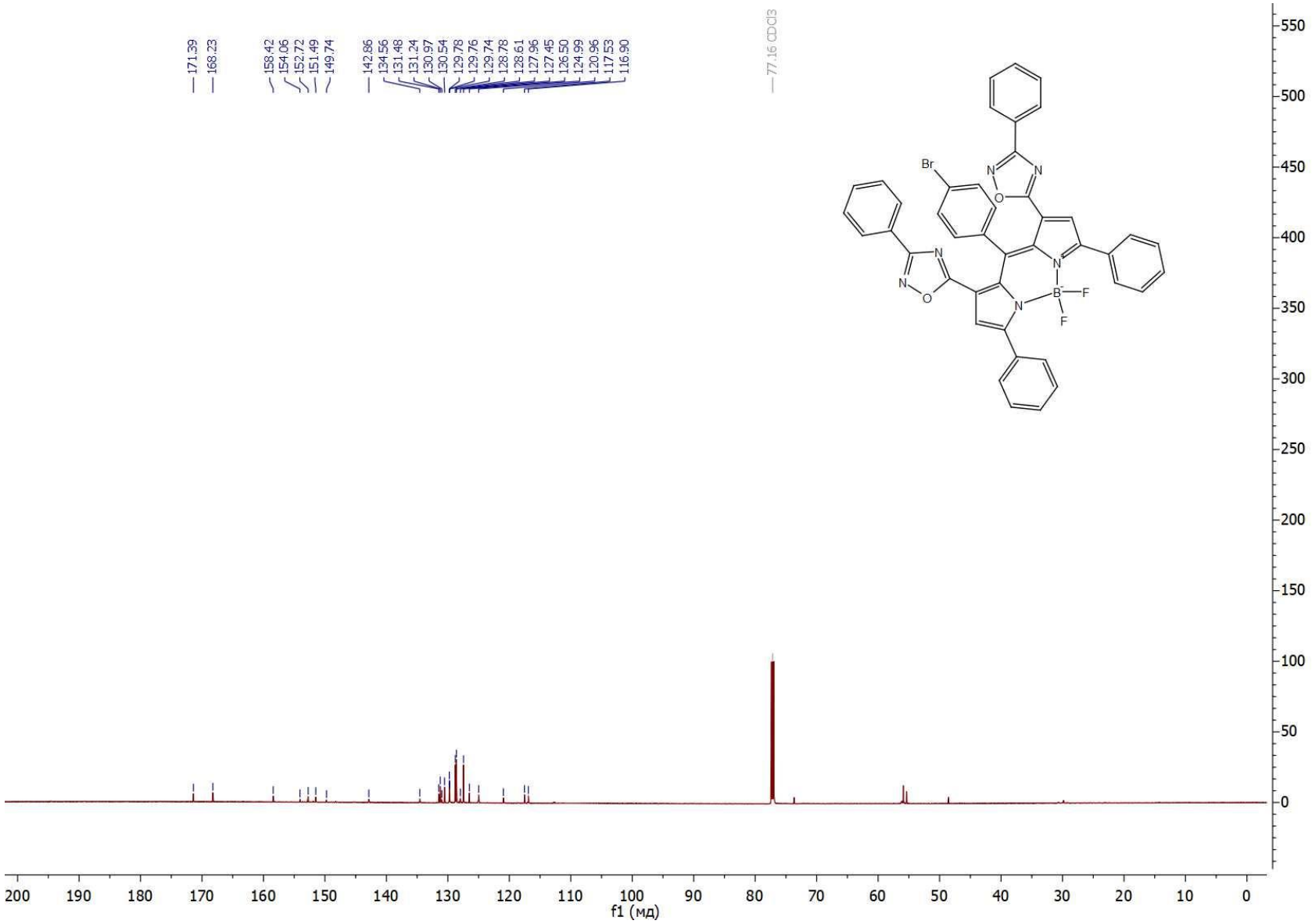

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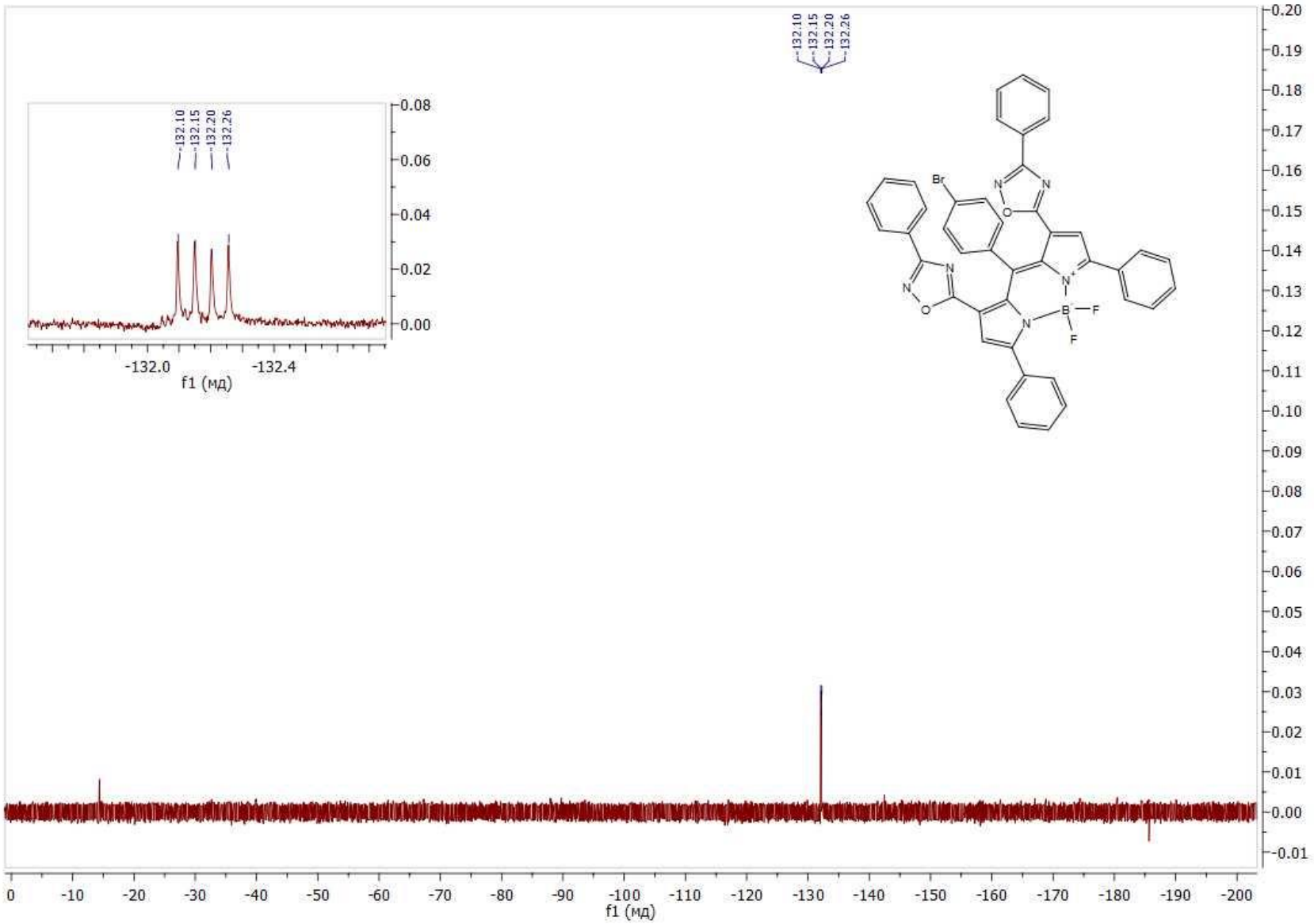
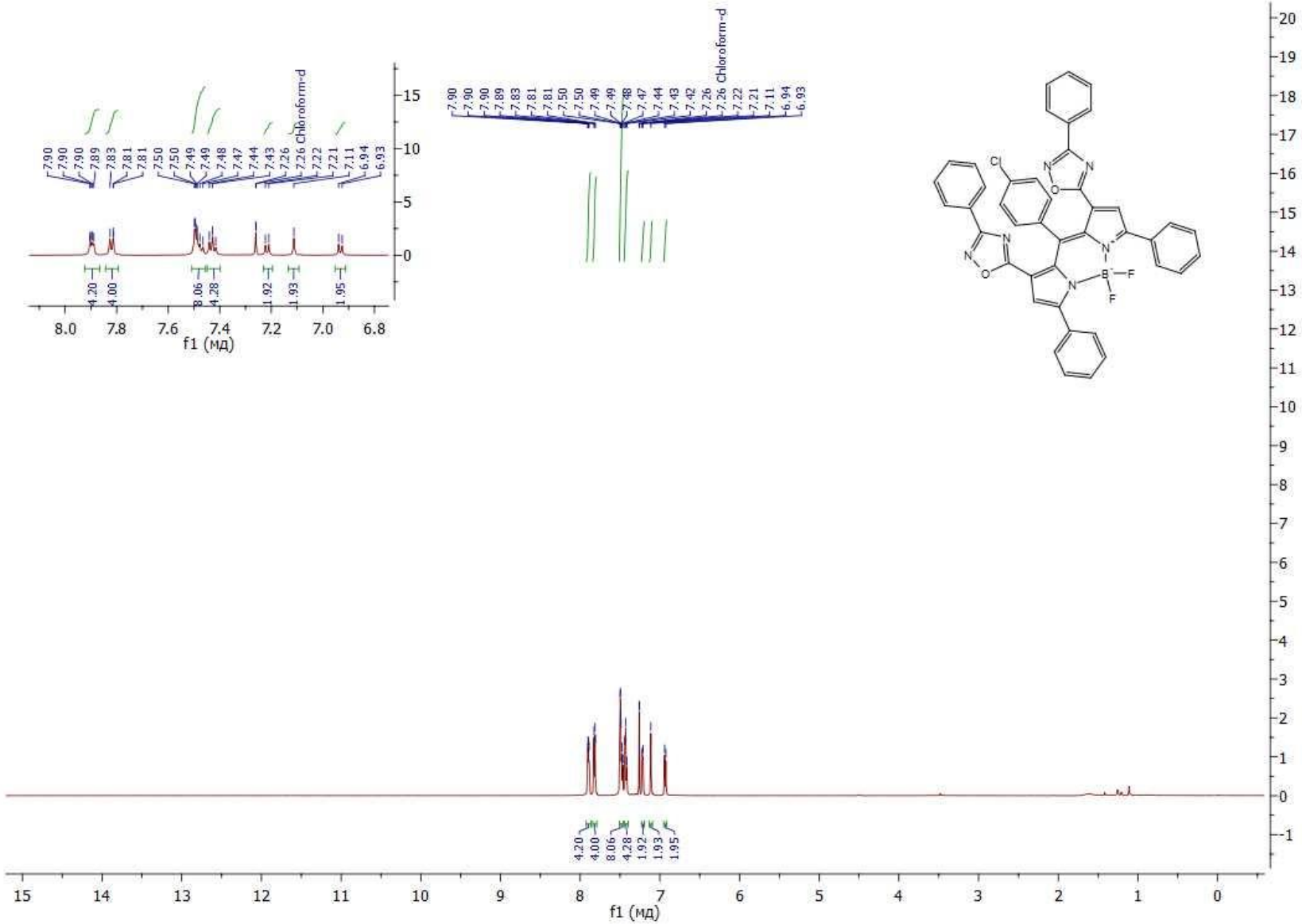
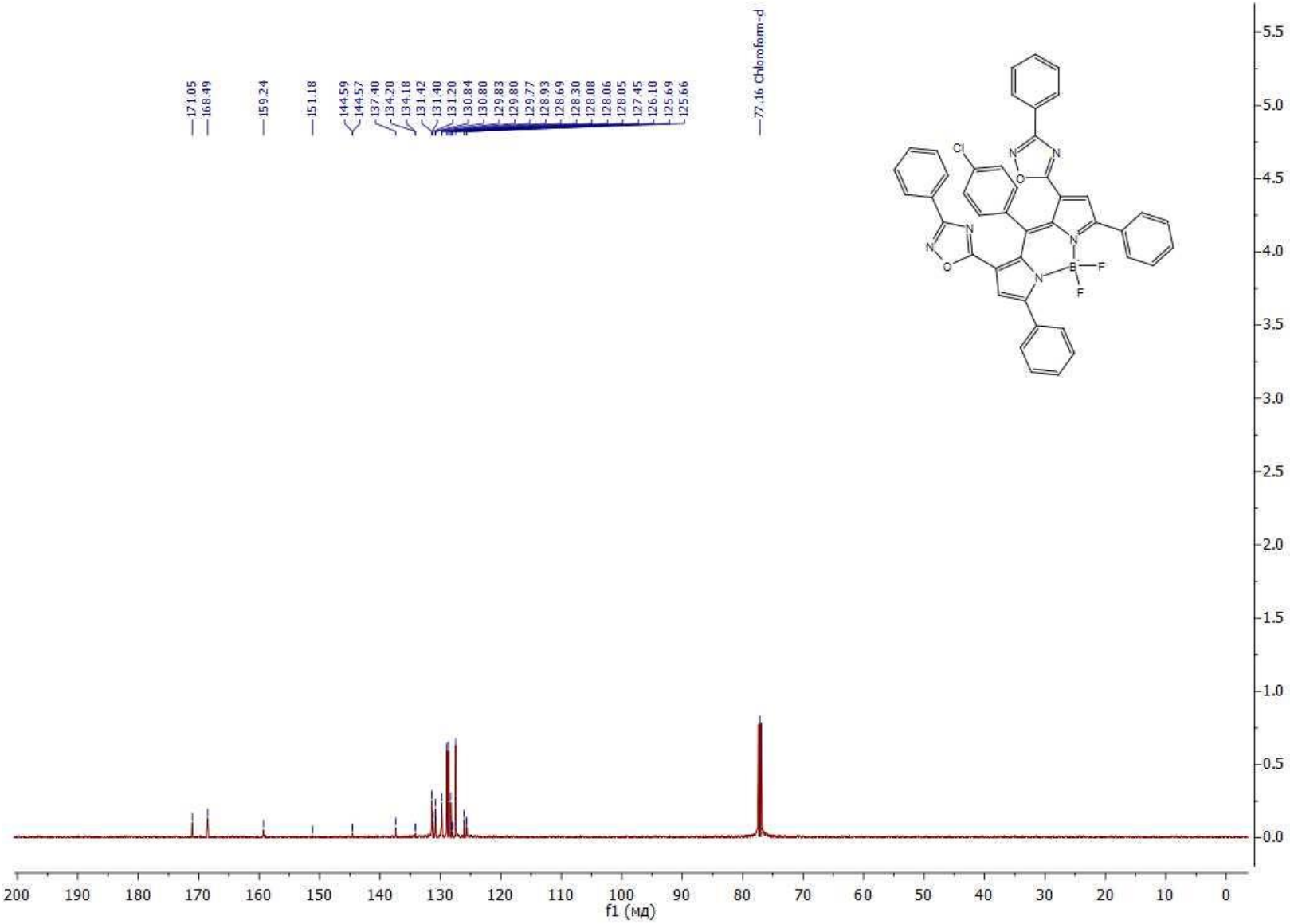


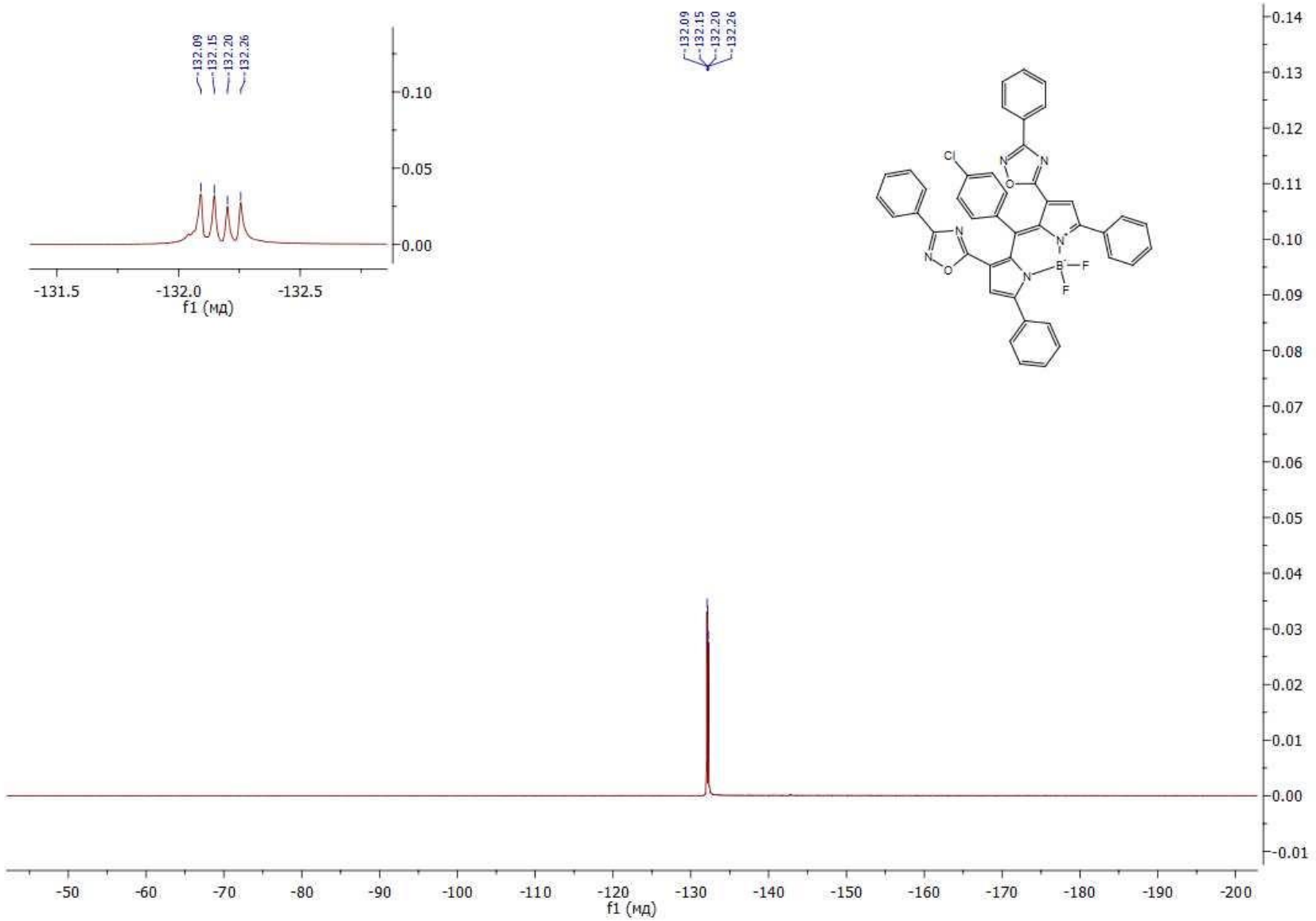
^{1}H NMR spectrum for **3h**



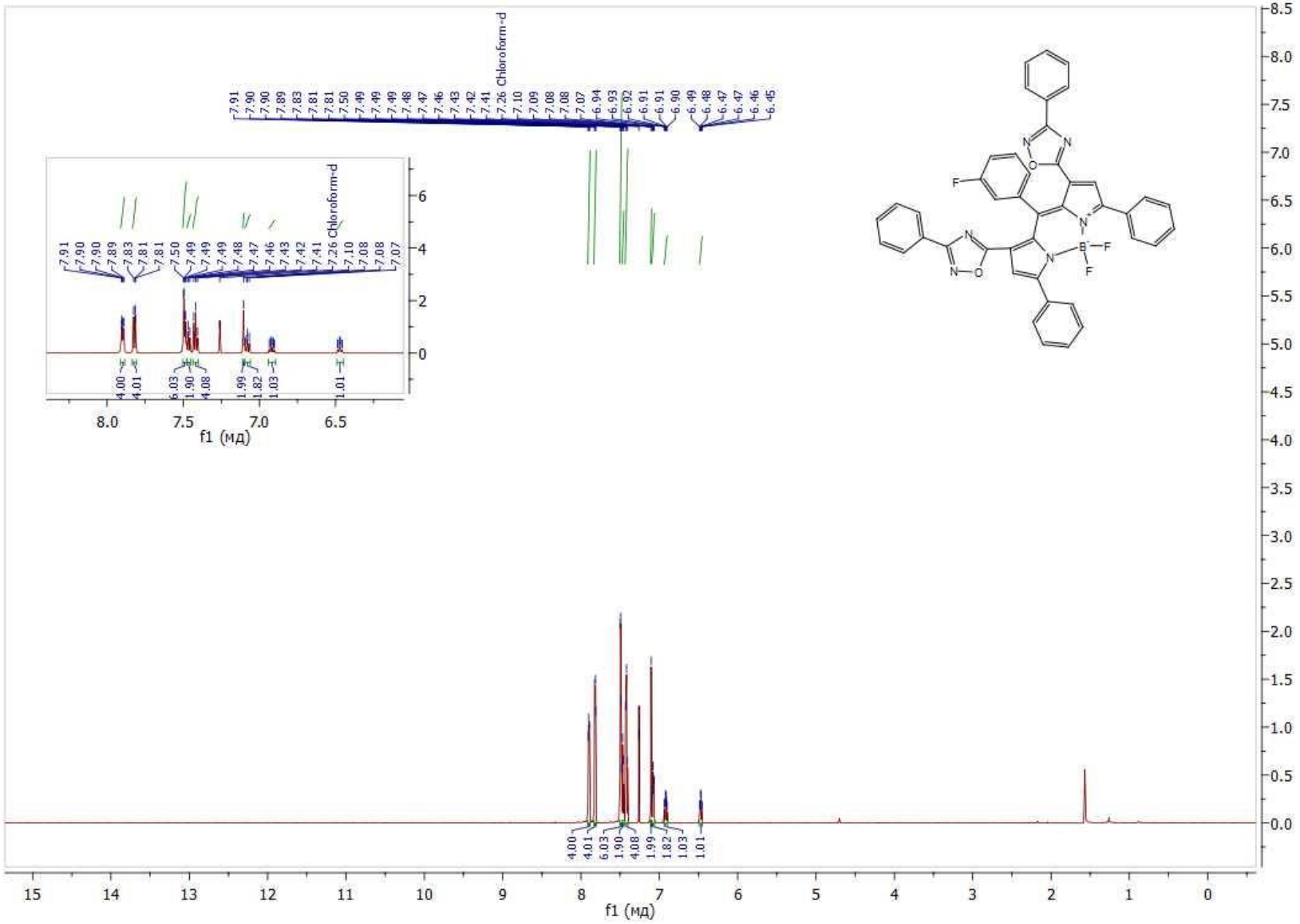
^{13}C NMR spectrum for **3h**



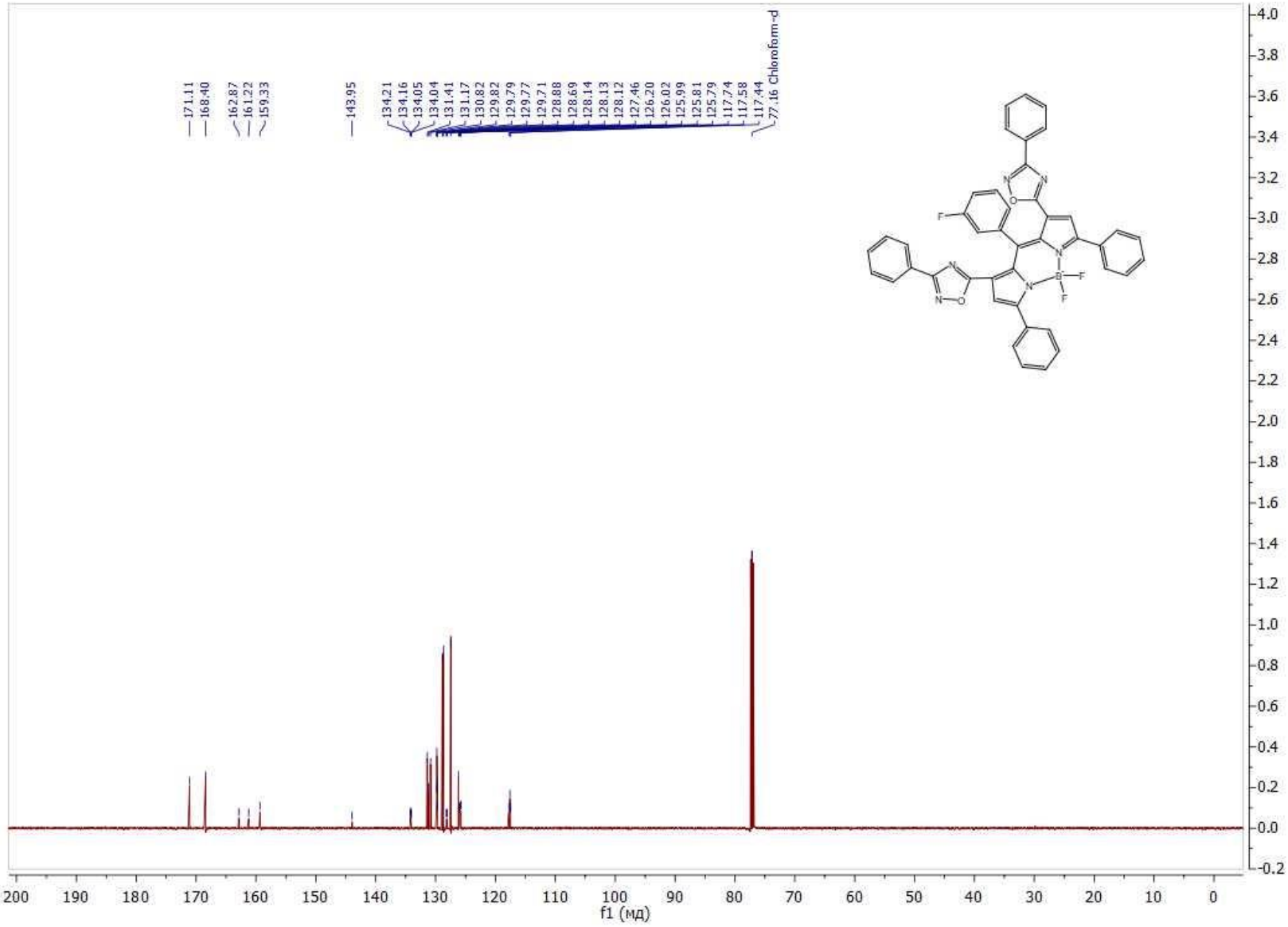
^{19}F NMR spectrum for **3h**



^{1}H NMR spectrum for **3i**



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



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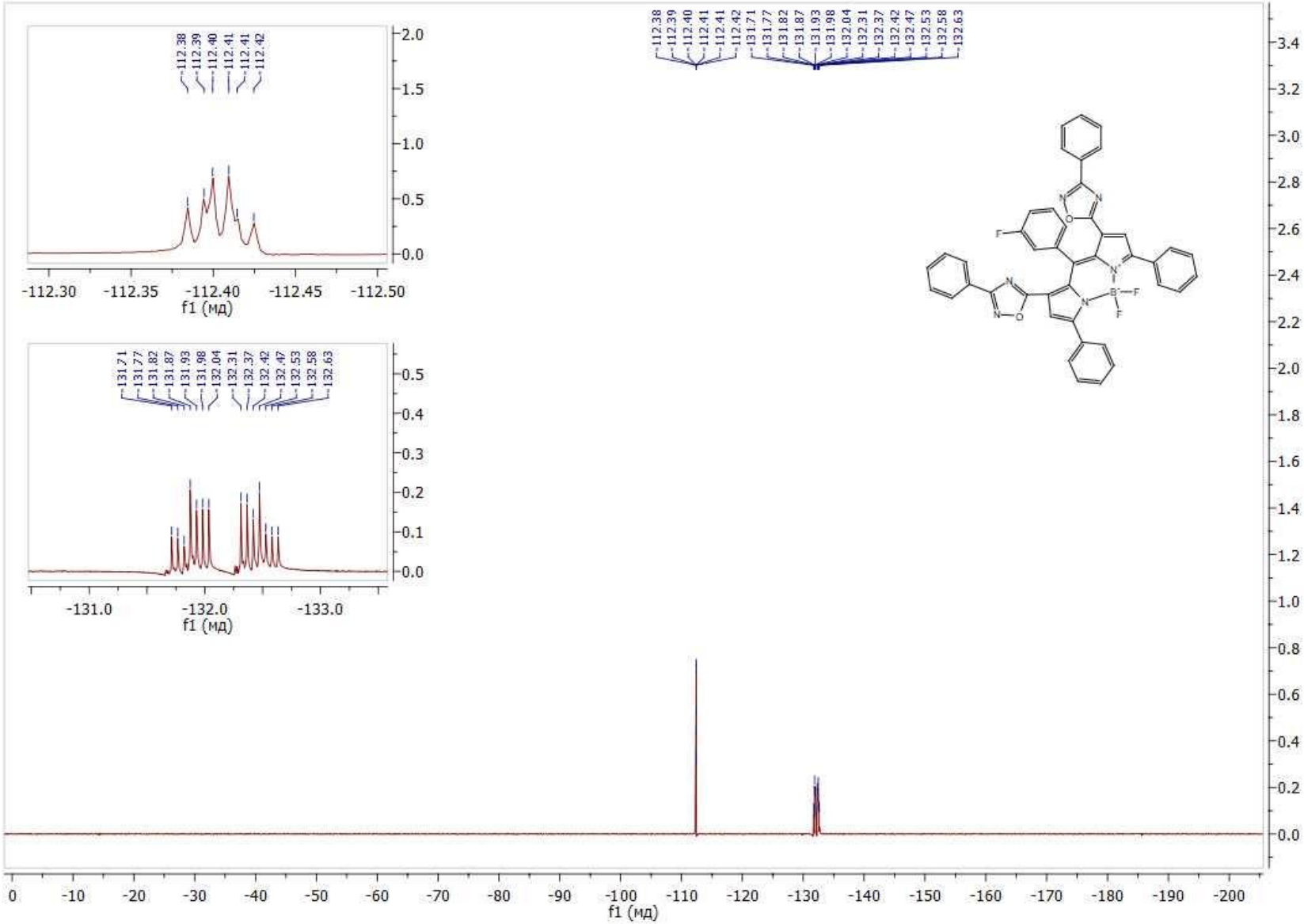
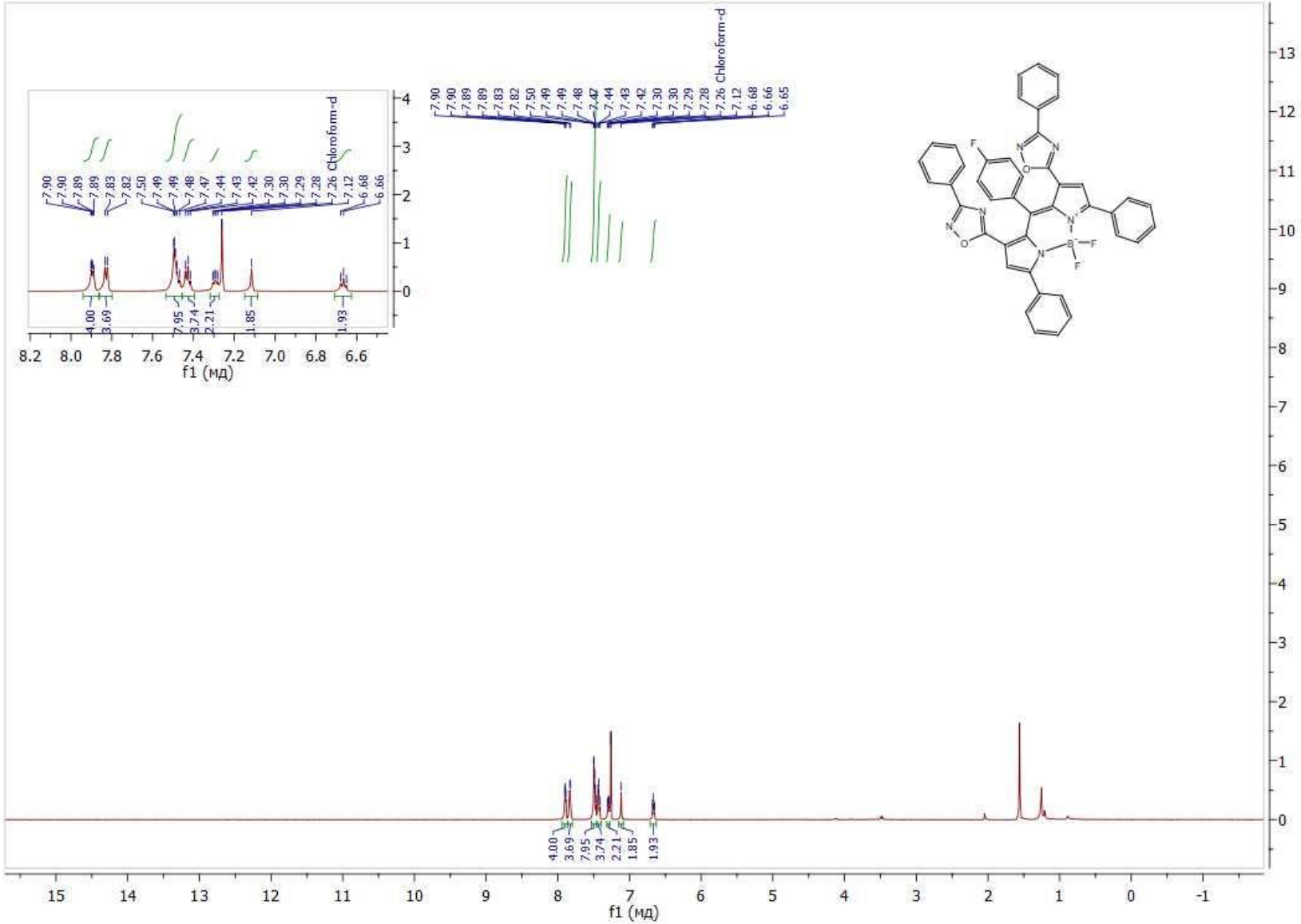


^{1}H NMR spectrum for **3j**



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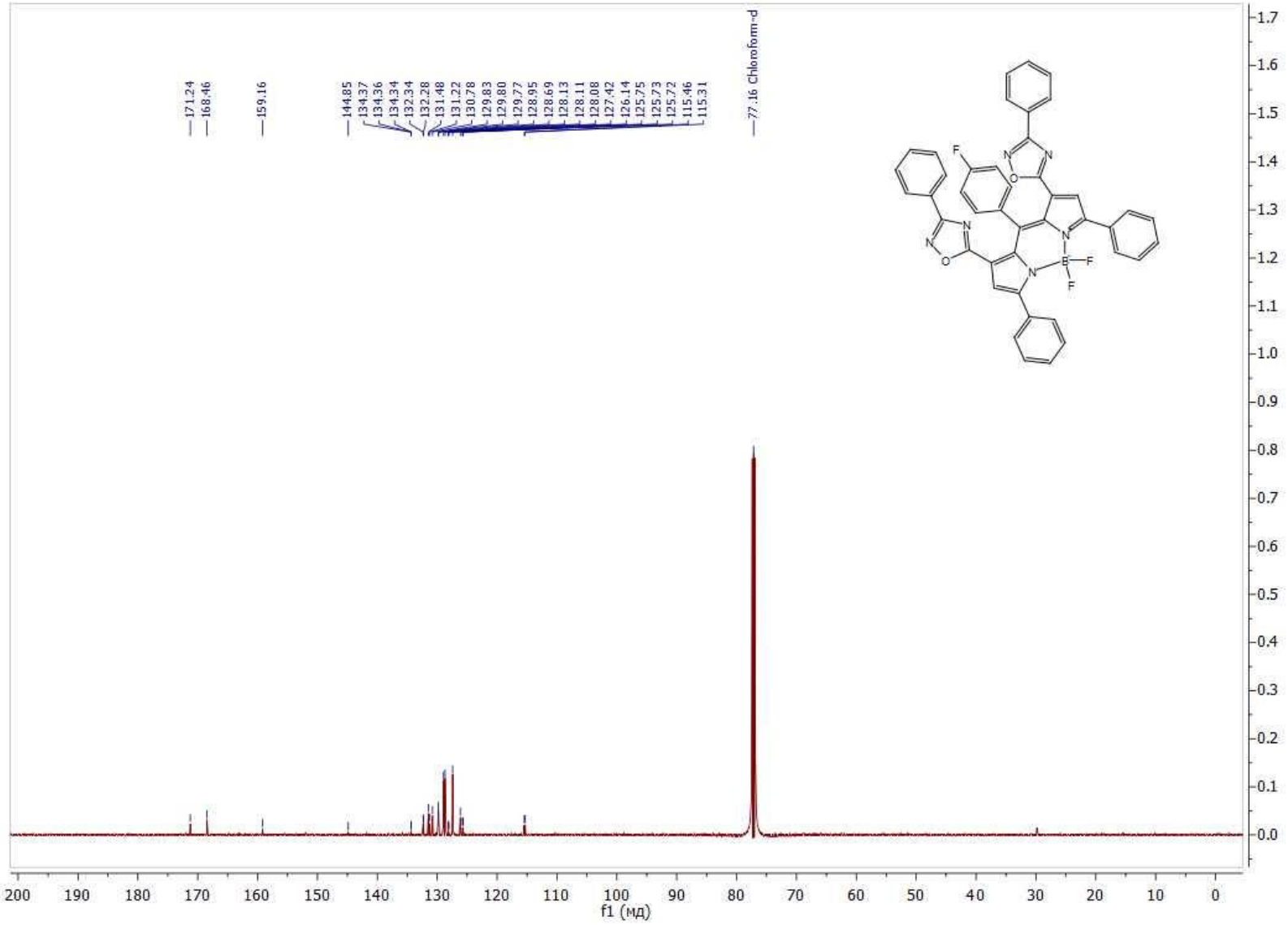

^{19}F NMR spectrum for **3j**