Fluorescent Boron Complexes Based on New *N,O*-Chelates as promising candidates for Flow Cytometry

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1. Experimenal Section

General Information and Materials

^{1}H, ^{19}F, ^{11}B, and ^{13}C NMR spectra were recorded on a Bruker Avance II (Karlsruhe, Germany) spectrometer at 400 MHz for ^{1}H, 100 MHz for ^{13}C, 128 MHz for ^{11}B, and 376 MHz for ^{19}F NMR. Chemical shifts are reported in parts per million (ppm) relative to tetramethysilane (0 ppm) in ^{1}H NMR and residual solvent signals in ^{13}C (internal references), and relative to $BF_3{\cdot}OEt_2$ in ^{11}B and $CFCl_3$ in ^{19}F NMR spectra (external references). Coupling constants (*J*) values are given in Hertz (Hz). Signal splitting patterns are described as singlet (s), doublet (d), triplet (t), quartet (q), sextet (sext), quintet (quin), multiplet (m), broad (br), doublet of doublets (dd), and doublet of triplets (dt), in addition to AA'XX' for the spin system of *para*-substituted benzenes with two different substituents. The major isomer signal is highlighted with an asterisk (*). ^{13}C NMR signal patterns for several compounds were analyzed using an attached proton test (APT) and described as follows: + for secondary or quaternary carbon atoms (positive signals); – for primary or tertiary carbon atoms (negative signals). Mass spectra were recorded with a Shimadzu GCMS-QP 2010 “Ultra” (Kyoto, Japan) mass spectrometer using electron impact (EI) ionization (40–200 °C, 70 eV). $[M]^+$ denotes the molecular ion. Fourier-transform infrared (FTIR) spectra were obtained using a Bruker Alpha (NPVO, ZnSe) spectrometer (Ettlingen, Germany).

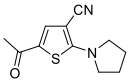
Elemental analyses were performed using a CHNS/O analyzer PerkinElmer 2400 Series II instrument (Shelton, CT USA). Melting points were determined on a Stuart SMP3 apparatus (Staffordshire, ST15 OSA, UK). The reactions were monitored by analytical thin-layer chromatography (TLC) on aluminum-backed silica gel plates (Sorbfil UV–254). Components were visualized using short wavelength UV light (254 nm). Solvents were dried and distilled according to common procedures. All solvents were of spectroscopic grade. All reactants were obtained from Acros Organics and used without further purification.

Preparation and Characterization of New Compounds

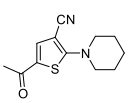
Thiophenes **3a-d** were synthesized according to a procedure described in our previous papers.[1, 2] Dimethylaminoacryloylthiophenes **4a-d** were prepared according literature technique.[3] Arylaminoprop-2-enethioamide **2a-k** were obtained from the corresponding arylamine and dimethylaminopropene thioamide according to the previously described procedure.[4]

Synthesis of BF_2 complexes 1a-k: DIPA (5.0 mmol) and $BF_3{\cdot}OEt_2$ (15.0 mmol) were added to a cold solution of enamine (1.0 mmol) in CH_2Cl_2 (2.5 mL). The resultant mixture was stirred at room temperature for 1–6 h. After reaction completion, the solvent was removed under vacuum and the product was purified by column chromatography using petroleum ether/ethyl acetate mixed solvent as the eluent.

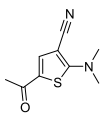
5-Acetyl-2-(pyrrolidin-1-yl)thiophene-3-carbonitrile 3b. Beige powder (0.375 g, 65%); m.p. 200-201 °C; IR (ATR, ZnSe) ν_{max}/cm^{-1}: 2963, 2922, 2883, 2200, 1637; ^{1}H NMR (400 MHz, DMSO-d_6, Me_4Si): δ_H 7.82 (1 H, s, CH), 3.66-3.62 (4 H, m, $2CH_2$), 2.36 (3 H, s, Me), 2.13-2.10 (4 H, m, $2CH_2$); ^{13}C NMR (100 MHz, DMSO-d_6): δ_C 188.2, 165.4, 138.1, 125.4, 117.0, 82.7, 51.9 (2C), 25.4 (2C), 24.8; MS (EI) m/z (%): 220 (M+, 100); Found: C, 59.7; H, 5.6; N, 12.5. Calc. for $C_{11}H_{12}N_2OS$: C, 59.98; H, 5.49; N, 12.72%.



5-Acetyl-2-(piperidin-1-yl)thiophene-3-carbonitrile 3c. Beige powder (0.380 g, 68%); m.p. 94-96 °C; IR (ATR, ZnSe) ν_{max}/cm^{-1}: 2940, 2881, 2202, 1641; ^{1}H NMR (400 MHz, DMSO-d_6, Me_4Si): δ_H 7.99 (1 H, s, CH), 3.67-3.63 (4 H, m, $2CH_2$), 2.38 (3 H, s, Me), 1.67-1.65 (6 H, m, $3CH_2$); ^{13}C NMR (100 MHz, DMSO-d_6): δ_C 188.4, 169.1, 137.9, 125.9, 116.4, 84.4, 51.7 (2C), 24.8, 24.5 (2C), 22.6; MS (EI) m/z (%): 234 (M+, 100); Found: C, 61.3; H, 6.3; N, 12.2. Calc. for $C_{12}H_{14}N_2OS$: C, 61.51; H, 6.02; N, 11.96%.



5-Acetyl-2-(dimethylamino)thiophene-3-carbonitrile 3d. Light-beige crystals (0.280 g, 58%); m.p. 176-178 °C; IR (ATR, ZnSe) ν_{max}/cm^{-1}: 3035, 2934, 2860, 2206, 1635; ^{1}H NMR (400 MHz, DMSO-d_6, Me_4Si): δ_H 7.78 (1 H, s, CH), 3.34 (6 H, s, NMe_2), 2.36 (3 H, s, Me); ^{13}C NMR (100 MHz, DMSO-d_6): δ_C 188.4, 169.0, 138.5, 125.6, 117.0, 83.1, 43.1 (2C), 24.8; MS (EI) m/z (%): 194 (M+, 74); Found: C, 55.3; H, 5.3; N, 14.7. Calc. for $C_9H_{10}N_2OS$: C, 55.65; H, 5.19; N, 14.42%.



5-(3-(Dimethylamino)acryloyl)-2-morpholinothiophene-3-carbonitrile 4a. Light-beige powder (0.235 g, 98%); m.p. 175-177 °C; IR (ATR, ZnSe) ν_{max}/cm^{-1}: 2955, 2916, 2862, 2808, 2204, 1630; ^1H NMR (400 MHz, DMSO-d_6, Me_4Si): δ_H 8.84 (1 H, s, CH), 7.57 (1 H, d, J = 12.3 Hz, CH), 5.74 (1 H, d, J = 12.3 Hz, CH), 3.78-3.75 (4 H, m, $2CH_2$), 3.53-3.51 (4 H, m, $2CH_2$), 3.11 (3 H, br s, Me), 2.89 (3 H, br s, Me); ^{13}C NMR (100 MHz, DMSO-d_6): δ_C 177.8, 168.4, 152.8, 132.2, 130.5, 116.7, 89.5, 85.7, 65.1 (2C), 50.1 (2C), 44.3, 37.1; MS (EI) m/z (%): 98 (M^+, 100); 291 (M^+, 47); Found: C, 57.6; H, 6.0; N, 14.4. Calc. for $C_{14}H_{17}N_3O_2S$: C, 57.71; H, 5.88; N, 14.42%.

5-(3-(Dimethylamino)acryloyl)-2-(pyrrolidin-1-yl)thiophene-3-carbonitrile 4b. Yellow powder (0.250 g, 90%); m.p. 237-239 °C; IR (ATR, ZnSe) ν_{max}/cm^{-1}: 2957, 2927, 2855, 2811, 2197, 1630; ^1H NMR (400 MHz, DMSO-d_6, Me_4Si): δ_H 7.59 (1 H, s, CH), 7.50 (1 H, d, J = 12.4 Hz, CH), 5.58 (1 H, d, J = 12.4 Hz, CH), 3.61 (4 H, m, $2CH_2$), 3.07 (3 H, br s, Me), 2.95 (3 H, br s, Me), 2.10 (4 H, m, $2CH_2$); ^{13}C NMR (100 MHz, $CDCl_3$): δ_C 177.5, 168.4, 152.6, 131.0, 129.7, 118.0, 89.9, 82.8, 51.7 (2C), 44.9, 37.3, 25.9 (2C); MS (EI) m/z (%): 275 (M+, 51); Found: C, 60.8; H, 6.4; N, 15.0. Calc. for $C_{14}H_{17}N_3OS$: C, 61.06; H, 6.22; N, 15.26%.

5-(3-(Dimethylamino)acryloyl)-2-(piperidin-1-yl)thiophene-3-carbonitrile 4c. Light peach color powder (0.260 g, 89%); m.p. 135-137 °C; IR (ATR, ZnSe) ν_{max}/cm^{-1}: 2990, 2853, 2810, 2197, 1633; ^1H NMR (400 MHz, DMSO-d_6, Me_4Si): δ_H 7.61 (1 H, s, CH), 7.52 (1 H, d, J = 12.3 Hz, CH), 5.61 (1 H, d, J = 12.3 Hz, CH), 3.61-3.57 (4 H, m, $2CH_2$), 3.11 (3 H, br s, Me), 2.92 (3 H, br s, Me), 1.74-1.69 (6 H, m, $3CH_2$); ^{13}C NMR (100 MHz, DMSO-d_6): δ_C 177.9, 168.0, 152.5, 130.9, 130.8, 117.0, 89.5, 84.5, 51.6 (2C), 44.3, 37.0, 24.7 (2C), 22.9; MS (EI) m/z (%): 289 (M+, 56); Found: C, 62.0; H, 6.8; N, 14.2. Calc. for $C_{15}H_{19}N_3OS$: C, 62.26; H, 6.62; N, 14.52%.

2-(Dimethylamino)-5-(3-(dimethylamino)acryloyl)thiophene-3-carbonitrile 4d. Beige powder (0.225 g, 90%); m.p. 194-196 °C; IR (ATR, ZnSe) ν_{max}/cm^{-1}: 3026, 2923, 2875, 2809, 2201, 1628; ^1H NMR (400 MHz, DMSO-d_6, Me_4Si): δ_H 7.56 (1 H, s, CH), 7.51 (1 H, d, J = 12.4 Hz, CH), 5.58 (1 H, d, J = 12.4 Hz, CH), 3.29 (6 H, s, 2Me), 3.11 (3 H, br s, Me), 2.94 (3 H, br s, Me); ^{13}C NMR (100 MHz, $CDCl_3$): δ_C 179.6, 168.5, 152.8, 131.2, 130.5, 117.8, 90.2, 84.2, 43.4 (4C); MS (EI) m/z (%): 249 (M+, 52); Found: C, 57.5; H, 6.3; N, 16.3. Calc. for $C_{12}H_{15}N_3OS$: C, 57.81; H, 6.06; N, 16.58%.

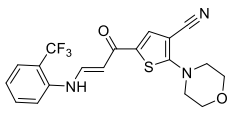
5-(3-((4-Methoxyphenyl)amino)acryloyl)-2-morpholinothiophene-3-carbonitrile 2a. Bright yellow powder (0.325 g, 88%); m.p. 175-177 °C; IR (ATR, ZnSe) ν_{max}/cm^{-1}: 3011, 2980, 2967, 2898, 2834, 2206, 1640; ^1H NMR (400 MHz, DMSO-d_6, Me_4Si): δ_H 11.56* and 9.82 (1 H, both д, J = 12.6 Hz, NH), 7.77* and 7.65 (1 H, both s, CH), 7.90 and 7.62* (1 H, both m, CH), 7.17* and 7.08 (2 H, both d, J = 9.0 Hz, CH_{Ar}), 6.90-6.86 (2 H, m, CH_{Ar}), 6.11 and 5.82* (1 H, both d, J = 7.8 Hz, CH), 3.82-3.79 (4 H, m, $2CH_2$), 3.76* and 3.75 (3 H, both s, OMe), 3.59-3.55 (4 H, m, $2CH_2$); Mixture of two isomers 1:3; ^{13}C NMR (100 MHz, DMSO-d_6): δ_C 180.9*/178.6, 168.9*/168.7, 155.7*/155.2, 145.2*/143.9, 134.3/133.5*, 131.8*/131.1, 131.2/130.0*, 117.5* (2C), 116.6/116.5*, 114.9* (2C), 91.3*, 86.1*/86.0, 55.4*/55.3, 65.1* (2C), 50.1* (2C); MS (EI) m/z (%): 369 (M+, 73); Found: C, 61.5; H, 5.3; N, 11.0. Calc. for $C_{19}H_{19}N_3O_3S$: C, 61.77; H, 5.18; N, 11.37%.

5-(3-((4-Chlorophenyl)amino)acryloyl)-2-morpholinothiophene-3-carbonitrile 2b. Bright yellow powder (0.337 g, 90%); m.p. 227-229 °C; IR (ATR, ZnSe) ν_{max}/cm^{-1}: 2980, 2942, 2873, 2213, 1640; ^1H NMR (400 MHz, DMSO-d_6, Me_4Si): δ_H 11.49* and 10.01 (1 H, both d, J = 12.2 Hz, NH), 7.89* (1 H, s, CH), 7.73-7.68 (1 H, m, CH), 7.35-7.27 (4 H, m, CH_{Ar}), 6.21 and 5.94* (1 H, both d, J = 8.0 Hz, CH), 3.83-3.79 (4 H, m, $2CH_2$), 3.62-3.58 (4 H, m, $2CH_2$); mixture of isomers 1:8; ^{13}C NMR (100 MHz, DMSO-d_6): δ_C 181.2*/178.7, 168.9*/168.7, 143.8*/142.4, 139.9/139.0*, 132.5*/131.7, 130.5*/129.4, 129.0* (2C), 126.6*/125.8, 117.5* (2C), 116.3*/116.2, 96.4/92.7*, 86.0*/85.8, 64.9 (2C), 50.0 (2C); MS (EI) m/z (%): 374 (M+, 88); Found: C, 58.0; H, 4.6; N, 11.0. Calc. for $C_{18}H_{16}ClN_3O_2S$: C, 57.83; H, 4.31; N, 11.24%.

5-(3-((4-Cyanophenyl)amino)acryloyl)-2-morpholinothiophene-3-carbonitrile 2c. Yellow powder (0.340 g, 93%); m.p. 310-311 °C; IR (ATR, ZnSe) ν_{max}/cm^{-1}: 2931, 2904, 2214, 2207, 1643; ^1H NMR (400 MHz, DMSO-d_6, Me_4Si): δ_H 11.56* and 10.28 (1 H, both d, J = 12.1 Hz, NH), 8.19 and 7.92* (1 H, both s, CH), 7.80-7.72 (1 H, m, CH), 7.69* and 7.64 (2 H, both d, J = 8.8 Hz, CH_{Ar}), 7.40* and 7.26 (2 H, both d, J = 8.8 Hz, CHAr), 6.32 and 6.04* (1 H, both d, J = 8.2 Hz, CH), 3.82-3.80 (4 H, m, $2CH_2$), 3.62-3.60 (4 H, m, $2CH_2$); mixture of two isomers 1:3; ^{13}C NMR (100 MHz, DMF-d_7): δ_C 178.3*, 171.7*, 143.7*/142.2, 135.6*, 135.1*/135.0 (2C), 134.7*/133.9, 120.2/120.0*, 117.5*/117.0 (2C), 117.4*; 117.3*/116.8, 101.1/96.2*, 85.3*/84.1, 66.6* (2C), 51.8* (2C); MS (EI) m/z (%): 364 (M+, 100); Found: C, 62.3; H, 4.6; N, 15.0. Calc. for $C_{19}H_{16}N_4O_2S$: C, 62.62; H, 4.43; N, 15.37%.

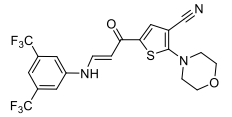
2-Morpholino-5-(3-((4-(trifluoromethyl)phenyl)amino)acryloyl)thiophene-3-carbonitrile 2d. Bright yellow powder (0.358 g, 88%); m.p. 177-179 °C; IR (ATR, ZnSe) ν_{max}/cm^{-1}: 2858, 2206, 1637; ^1H NMR (400 MHz, DMSO-d_6, Me_4Si): δ_H 11.59* and 10.13 (1 H, both d, J = 12.2 Hz, NH), 7.77-7.72* and 8.06-7.79 (1 H, both m, CH), 7.82* and 7.66 (1 H, both s, CH), 7.59-7.53 (2 H, m, CH_{Ar}), 7.37* and 7.26 (2 H, both d, J = 8.5 Hz, CH_{Ar}), 6.27 and 5.96* (1 H, both d, J = 8.1, CH), 3.83-3.81 (4 H, m, $2CH_2$), 3.63-3.60 (4 H, m, $2CH_2$); mixture of two isomers 1:20; ^{19}F NMR (376.5 MHz, DMSO-d_6): δ_F - 61.0; ^{13}C NMR (100 MHz, DMSO-d_6): δ_C 181.7*/179.0, 169.2*/169.0, 144.5/143.1*, 143.6/141.6*, 133.4*/132.4, 130.2/129.1* (2C), 126.7* (m, 2C), 124.5* (q, J = 270.0 Hz), 121.9* (q, J = 32.0 Hz), 116.4*/116.3, 115.9*/115.4, 98.0/93.9*, 85.9*/85.8, 65.0* (2C), 50.0* (2C); MS (EI) m/z (%): 407 (M+, 100); Found: C, 55.7; H, 4.2; N, 10.0. Calc. for $C_{19}H_{16}F_3N_3O_2S$: C, 56.01; H, 3.96; N, 10.31%.

2-Morpholino-5-(3-((2-(trifluoromethyl)phenyl)amino)acryloyl)thiophene-3-carbonitrile 2e. Bright yellow powder (0.370 g, 91%); m.p. 145-147 °C; IR



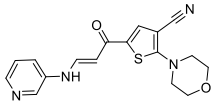
(ATR, ZnSe) ν_{max}/cm^{-1}: 2875, 2844, 2205, 1638; ^1H NMR (400 MHz, DMSO-d_6, Me_4Si): δ_H 12.04 (1 H, d, J = 11.4 Hz, NH), 7.97 (1 H, s CH), 7.81 (1 H, dd, J = 3.1 Hz, 11.2 Hz, H_{Ar}), 7.68-7.62 (3 H, m, H_{Ar}), 7.20 (1 H, t, J = 7.4 Hz, H_{Ar}), 6.08 (1 H, d, J = 8.0 Hz, CH), 3.82-3.80 (4 H, m, $2CH_2$), 3.63-3.61 (4 H, m, $2CH_2$); ^{19}F NMR (376.5 MHz, DMSO-d_6): δ_F - 61.2; ^{13}C NMR (100 MHz, DMSO-d_6): δ_C 182.0, 169.2, 143.6, 138.0, 134.0, 133.8, 128.7, 126.5 (q, J = 5.0 Hz), 124.1 (q, J = 271.0 Hz), 122.6, 116.5, 116.3, 116.0 (q, J = 29.0 Hz), 94.6, 85.9, 64.9 (2C), 50.0 (2C); MS (EI) m/z (%): 407 (M+, 73); Found: C, 55.8; H, 4.2; N, 10.6. Calc. for $C_{19}H_{16}F_3N_3O_2S$: C, 56.01; H, 3.96; N, 10.31%.

5-(3-((3,5-Bis(trifluoromethyl)phenyl)amino)acryloyl)-2-morpholinothiophene-3-carbonitrile 2f. Light yellow crystals (0.430 g, 90%); m.p. 223-225 °C; IR



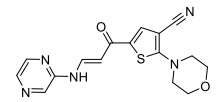
(ATR, ZnSe) ν_{max}/cm^{-1}: 2987, 2868, 2216, 1639; ^1H NMR (400 MHz, DMSO-d_6, Me_4Si): δ_H 11.55* and 10.34 (1 H, both d, J = 12.1 Hz, NH), 8.00* (1 H, s, CH), 8.12 and 7.92* (1 H, both m, CH), 7.99* and 7.73 (2 H, both s, CH_{Ar}), 7.51* and 7.46 (1 H, both s, CH_{Ar}), 6.32 and 6.05* (1 H, both d, J = 8.2 Hz, CH), 3.82-3.80 (4 H, m, $2CH_2$), 3.63-3.61 (4 H, m, $2CH_2$); mixture of two isomers 1:6; ^{19}F NMR (376.5 MHz, DMSO-d_6): δ_F - 62.3*/- 62.4; ^{13}C NMR (100 MHz, DMSO-d_6): δ_C 181.6*/179.0, 169.3*/169.1, 143.2/142.6*, 142.8*/141.6, 133.8*/132.9, 131.3* (q, 2C, J = 33.0 Hz), 130.0/129.0*, 123.0* (q, 2C, J = 272.0 Hz), 116.3*, 116.3*/115.4 (m, 2C), 114.7*/113.9 (t, J = 4.0 Hz), 99.0/94.5*, 85.9*/85.8, 70.0 (2C), 50.0 (2C); MS (EI) m/z (%): 475 (M+, 100); Found: C, 50.2; H, 3.3; N, 8.6. Calc. for $C_{20}H_{15}F_6N_3O_2S$: C, 50.53; H, 3.18; N, 8.84%.

2-Morpholino-5-(3-(pyridin-3-ylamino)acryloyl)thiophene-3-carbonitrile 2g. Yellowish orange powder (0.260 g, 77%); m.p. 225-227 °C; IR (ATR, ZnSe)



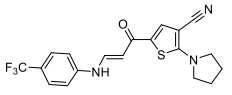
ν_{max}/cm^{-1}: 3093, 3050, 2981, 2928, 2210, 1658; ^1H NMR (400 MHz, DMSO-d_6, Me_4Si): δ_H 11.46 and 10.83 (1 H, both d, J = 12.5 Hz, NH), 8.91 and 8.73 (1 H, both d, J = 2.3 Hz, H_{Ar}), 8.42 and 8.38 (1 H, both d, J = 5.3 Hz, H_{Ar}), 8.33 and 8.22 (1 H, both d, J = 7.4 Hz, H_{Ar}), 8.09-8.03 (1 H, m, CH), 7.85-7.78 (2 H, m, H_{Ar}+CH), 6.46 and 6.14 (1 H, both d, J = 8.3 Hz, CH), 3.80-3.79 (4 H, m, $2CH_2$), 3.63-3.60 (4 H, m, $2CH_2$); mixture of two isomers 1:1; ^{13}C NMR (100 MHz, DMSO-d_6): δ_C 181.7/179.0*, 169.4/169.1*, 142.1/141.0*,140.7*/139.7, 136.1*, 134.6/134.3*, 133.2*/131.6, 130.0/129.7*,129.3/128.7, 129.4*/128.0, 127.0*/126.7, 116.3*, 100.2*/95.5, 85.9/85.8*, 65.0 (2C), 50.0 (2C); MS (EI) m/z (%): 340 (M+, 85); Found: C, 59.7; H, 4.9; N, 16.2. Calc. for $C_{17}H_{16}N_4O_2S$: C, 59.98; H, 4.74; N, 16.46%.

2-Morpholino-5-(3-(pyrazin-2-ylamino)acryloyl)thiophene-3-carbonitrile 2h. Yellowish orange powder (0.205 g, 60%); m.p. 230-232 °C; IR (ATR, ZnSe)



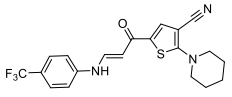
ν_{max}/cm^{-1}: 2214, 1625; ^1H NMR (400 MHz, DMSO-d_6, Me_4Si): δ_H 11.53* and 10.65 (1 H, both d, J = 11.6 Hz, NH), 8.62* and 8.29 (1 H, both br s, H_{Ar}), 8.25 (1 H, m, H_{Ar}), 8.20* and 8.13 (1 H, both d, J = 2.6 Hz, H_{Ar}), 8.44 and 7.98 (1 H, both t, J = 8.5 Hz, CH), 7.99* and 7.82 (1 H, both s, CH), 6.45 and 6.17* (1 H, both d, J = 8.5 Hz, CH), 3.80-3.79 (4 H, m, $2CH_2$), 3.64-3.61 (4 H, m, $2CH_2$); mixture of two isomers 2:3; ^{13}C NMR (100 MHz, DMSO-d_6): δ_C 181.9/179.4*, 169.4/169.1*, 149.2*/148.3, 142.0*/141.9, 139.7/139.4*, 138.2/137.3*, 134.9/124.4*,1 34.2/133.1*, 129.8*/128.8, 116.4*/116.3, 99.7*/95.8, 85.9/85.8*, 65.0* (2C), 50.0* (2C); MS (EI) m/z (%): 341 (M+, 37); Found: C, 55.9; H, 4.6; N, 20.2. Calc. for $C_{16}H_{15}N_5O_2S$: C, 56.29; H, 4.43; N, 20.51%.

2-(Pyrrolidin-1-yl)-5-(3-((4-(trifluoromethyl)phenyl)amino)acryloyl)thiophene-3-carbonitrile 2i. Bright yellow crystals (0.328 g, 84%); m.p. 212-214 °C; IR



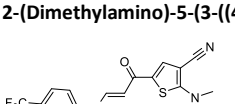
(ATR, ZnSe) ν_{max}/cm^{-1}: 3066, 2980, 2913, 2870, 2203, 1634; ^1H NMR (400 MHz, DMSO-d_6, Me_4Si): δ_H 11.58* and 10.04 (1 H, both d, J = 12.0 Hz, NH), 8.11 and 7.74* (1 H, both s, CH), 7.97 and 6.68* (1 H, both m, CH), 8.58-8.52 (2 H, m, H_{Ar}), 7.33* and 7.24 (2 H, both d, J = 8.5 Hz, H_{Ar}), 6.26 and 5.91* (1 H, both d, J = 8.1 Hz, CH), 3.68-3.65 (4 H, m, $2CH_2$), 2.15-2.11 (4 H, m, $2CH_2$); 1:9 isomer mixture; ^{19}F NMR (376.5 MHz, DMSO-d_6): δ_F - 61.0; ^{13}C NMR (100 MHz, DMSO-d_6): δ_C 181.7*/178.9, 164.9*/164.6, 144.7/143.8*, 142.3*/140.8, 134.2*/133.2, 128.2*/127.2 (2C), 126.7* (m, 2C), 124.5* (q, J = 269.0 Hz), 122.0* (q, J = 32.0 Hz), 117.3/117.2*, 115.8*/115.3, 98.2/94.2*, 82.8*/82.4, 51.8/51.7* (2C), 25.4* (2C); MS (EI) m/z (%): 391 (M+, 100); Found: C, 58.0; H, 4.3; N, 10.5. Calc. for $C_{19}H_{16}F_3N_3OS$: C, 58.30; H, 4.12; N, 10.74%.

2-(Piperidin-1-yl)-5-(3-((4-(trifluoromethyl)phenyl)amino)acryloyl)thiophene-3-carbonitrile 2j. Bright yellow crystals (0.350 g, 86%); m.p. 184-186 °C; IR



(ATR, ZnSe) ν_{max}/cm^{-1}: 3066, 2936, 2853, 2207, 1634; ^1H NMR (400 MHz, DMSO-d_6, Me_4Si): δ_H 11.59 and 10.08 (1 H, both d, J = 12.1 Hz, NH), 8.10 and 7.75* (1 H, both s, CH), 7.99 and 7.58* (1 H, both m, CH), 7.58-7.52 (2 H, m, H_{Ar}), 7.35* and 7.25 (2 H, both d, J = 8.5 Hz, H_{Ar}), 6.26 and 5.93* (1 H, both d, J = 8.1 Hz, CH), 3.73-3.65 (4 H, m, $2CH_2$), 1.78-1.73 (6 H, m, $3CH_2$); mixture of two isomers 1:20; ^{19}F NMR (376.5 MHz, DMSO-d_6): δ_F - 61.0; ^{13}C NMR (100 MHz, DMSO-d_6): δ_C 181.8*/179.0, 168.8/168.6*, 144.6/143.7*, 142.7/141.3*, 134.1*/133.1, 128.9/127.9* (2C), 126.7* (m, 2C), 124.4* (q, J = 270.0 Hz), 121.7* (q, J = 32.0 Hz), 116.8/116.7*,115.9*/115.4, 98.1/94.1*,84.9/84.7*,51.7* (2C), 24.7* (2C), 22.8*; MS (EI) m/z (%): 405 (M+, 100); Found: C, 58.9; H, 4.6; N, 10.1. Calc. for $C_{20}H_{18}F_3N_3OS$: C, 59.25; H, 4.48; N, 10.36%.

2-(Dimethylamino)-5-(3-((4-(trifluoromethyl)phenyl)amino)acryloyl)thiophene-3-carbonitrile 2k. Bright yellow powder (0.325 g, 89%); m.p. 231-233 °C;



IR (ATR, ZnSe) ν_{max}/cm^{-1}: 3279, 3106, 3052, 2981, 2924, 2202, 1651; ^1H NMR (400 MHz, DMSO-d_6, Me_4Si): δ_H 11.50 and 10.20* (1 H, both d, J = 12.7 Hz, NH), 7.97* (1 H, m, CH), 8.03 and 7.75* (1 H, both s, CH), 7.66-7.60 (2 H, m, H_{Ar}), 7.34 and 7.30* (2 H, both d, J = 8.5 Hz, H_{Ar}), 6.31* and 6.02 (1 H, both d, J = 12.7 Hz, CH), 3.30 and 3.29* (3 H, both s, NMe_2); mixture of two isomers 2 : 3; ^{19}F NMR (376.5 MHz, DMSO-d_6): δ_F - 60.2; ^{13}C NMR (100 MHz, DMSO-d_6): δ_C 181.7/178.9*, 168.5/168.3*, 144.7/143.7*, 142.5/141.0*, 134.5/133.5*,

128.4*/127.4 (2C), 126.7* (q, *J* = 4.0, 2C Hz), 124.5* (q, *J* = 270.0 Hz), 121.6* (q, *J* = 32.0 Hz), 117.3*/117.2, /115.8/115.3*, 98.1*/94.1, 83.3/83.0*, 43.1/43.0* (2C); MS (EI) m/z (%): 365 (M+, 75); Found: C, 55.5; H, 4.1; N, 11.3. Calc. for $C_{17}H_{14}F_3N_3OS$: C, 55.88; H, 3.86; N, 11.50%.

5-(2,2-Difluoro-3-(4-methoxyphenyl)-2,3-dihydro-1λ³,3,2λ⁴-oxazaborinin-6-yl)-2-morpho-linothiophene-3-carbonitrile 1a. Orange powder (0.313 g, 75%); m.p. 162-164 °C; IR (ATR, ZnSe) ν_{max}/cm^{-1}: 2969, 2903, 2847, 2210, 1546; ^1H NMR (400 MHz, DMSO-*d*$_6$, Me$_4$Si): δ_H 8.12 (1 H, s, CH), 8.08 (1 H, br s, CH), 7.36 and 6.95 (4 H, AA'XX', *J* = 9.0 Hz, H_{Ar}), 6.32 (1 H, d, *J* = 6.0 Hz, CH), 3.84-3.82 (7 H, m, 2CH$_2$+Me), 3.69-3.67 (4 H, m, 2CH$_2$); ^{19}F NMR (376.5 MHz, DMSO-*d*$_6$): δ_F - 131.7; ^{11}B NMR (128.4 MHz, DMSO-*d*$_6$): δ_B 0.73; ^{13}C NMR (100 MHz, DMSO-*d*$_6$): δ_C 169.1, 165.3, 158.8, 158.4, 136.5, 135.6, 123.9 (2C), 118.7, 116.2, 114.4 (2C), 91.9, 87.2, 65.0 (2C), 55.4, 50.2 (2C); MS (EI) m/z (%): 417 (M+, 100); Found: C, 54.4; H, 4.6; N, 9.8. Calc. for $C_{19}H_{18}BF_2N_3O_2S$: C, 54.70; H, 4.35; N, 10.07%.

5-(3-(4-Chlorophenyl)-2,2-difluoro-2,3-dihydro-1λ³,3,2λ⁴-oxazaborinin-6-yl)-2-morpholino-thiophene-3-carbonitrile 1b. Bright orange powder (0.383 g, 91%); m.p. 245-247 °C; IR (ATR, ZnSe) ν_{max}/cm^{-1}: 3108, 3064, 2962, 2920, 2854, 2210, 1557; ^1H NMR (400 MHz, DMSO-*d*$_6$, Me$_4$Si): δ_H 8.22 (1 H, s, CH), 8.16 (1 H, br s, CH), 7.47-7.42 (4 H, m, CH_{Ar}), 6.39 (1 H, d, *J* = 6.1 Hz, CH), 3.84-3.82 (4 H, m, 2CH$_2$), 3.72-3.69 (4 H, m, 2CH$_2$); ^{19}F NMR (376.5 MHz, DMSO-*d*$_6$): δ_F - 131.5; ^{11}B NMR (128.4 MHz, DMSO-*d*$_6$): δ_B 0.74; ^{13}C NMR (100 MHz, DMSO-*d*$_6$): δ_C 169.5, 166.6, 159.1, 141.3, 137.9, 131.5, 129.2 (2C), 124.4 (2C), 118.2, 116.1, 92.2, 87.4, 65.0 (2C), 50.2 (2C); MS (EI) m/z (%): 421 (M+, 100); Found: C, 51.0; H, 3.7; N, 9.6. Calc. for $C_{18}H_{15}BClF_2N_3O_2S$: C, 51.27; H, 3.59; N, 9.97%.

5-(3-(4-Cyanophenyl)-2,2-difluoro-2,3-dihydro-1λ³,3,2λ⁴-oxazaborinin-6-yl)-2-morpholino-thiophene-3-carbonitrile 1c. Red sparkled crystals (0.397 g, 92%); m.p. 310-312 °C; IR (ATR, ZnSe) ν_{max}/cm^{-1}: 3111, 2918, 2848, 2212, 1575; ^1H NMR (400 MHz, DMSO-*d*$_6$, Me$_4$Si): δ_H: 8.40 (1 H, s, CH), 8.31 (1 H, br s, CH), 7.87 and 7.65 (4 H, AA'XX', *J* = 8.6 Hz, H_{Ar}), 6.52 (1 H, d, *J* = 6.3 Hz, CH), 3.84-3.81 (4 H, m, 2CH$_2$), 3.75-3.72 (4 H, m, 2CH$_2$); ^{19}F NMR (376.5 MHz, $CDCl_3$): δ_F - 131.3; ^{11}B NMR (128.4 MHz, $CDCl_3$): δB 0.81; ^{13}C NMR (DMF-*d*$_7$, *δ*, м.д.): 171.4, 169.6, 159.9, 147.9, 140.0, 134.7 (2C), 124.7 (2C), 119.7, 119.5, 116.9, 111.0, 94.1, 89.7, 66.5 (2C), 52.0 (2C); MS (EI) m/z (%): 412 (M+, 100); Found: C, 55.1; H, 3.8; N, 13.3. Calc. for $C_{19}H_{15}BF_2N_4O_2S$: C, 55.36; H, 3.67; N, 13.59%.

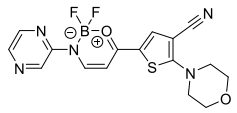
5-(2,2-Difluoro-3-(4-(trifluoromethyl)phenyl)-2,3-dihydro-1λ³,3,2λ⁴-oxazaborinin-6-yl)-2-morpholinothiophene-3-carbonitrile 1d. Orange sparkled powder (0.405 g, 89%); m.p. 274-276 °C; IR (ATR, ZnSe) ν_{max}/cm^{-1}: 3116, 3064, 2978, 2870, 2215, 1552; ^1H NMR (400 MHz, DMSO-*d*$_6$, Me$_4$Si): δ_H 7.82 (1 H, br s, CH), 7.76 (1 H, s, CH), 7.71 and 7.57 (4 H, AA'XX', *J* = 8.4 Hz, H_{Ar}), 6.03 (1 H, d, *J* = 6.1 Hz, CH), 3.93-3.90 (4 H, m, 2CH$_2$), 3.75-3.72 (4 H, m, 2CH$_2$); ^{19}F NMR (376.5 MHz, DMSO-*d*$_6$): δ_F - 62.5 (s, 3F), - 133.3 (br s, 2F); ^{11}B NMR (128.4 MHz, DMSO-*d*$_6$): δ_B 0.93; ^{13}C NMR (100 MHz, DMSO-*d*$_6$): δC 169.6, 167.3, 159.0, 145.7, 138.6, 127.1 (q, *J* = 33.0 Hz), 126.4 (q, 2C, *J* = 4.0 Hz), 124.0 (q, *J* = 270.0 Hz), 123.2 (d, 2C, *J* = 2.0 Hz), 117.9, 115.9, 92.5, 87.6, 64.9 (2C), 50.3 (2C); MS (EI) m/z (%): 455 (M+, 100); Found: C, 49.8; H, 3.5; N, 8.9. Calc. for $C_{19}H_{15}BF_5N_3O_2S$: C, 50.13; H, 3.32; N, 9.23%.

5-(2,2-Difluoro-3-(2-(trifluoromethyl)phenyl)-2,3-dihydro-1λ³,3,2λ⁴-oxazaborinin-6-yl)-2-morpholinothiophene-3-carbonitrile 1e. Yellow powder (0.400 g, 88%); m.p. 98-100 °C; IR (ATR, ZnSe) ν_{max}/cm^{-1}: 2974, 2866, 2212, 1547; ^1H NMR (400 MHz, DMSO-*d*$_6$, Me$_4$Si): δ_H 8.20 (1 H, s, CH), 7.82-7.79 (2 H, m, H_{Ar}+CH), 7.73 (1 H, t, *J* = 7.9 Hz, H_{Ar}), 7.60 (1 H, t, *J* = 7.7 Hz, H_{Ar}), 7.54 (1 H, d, *J* = 7.8 Hz, H_{Ar}), 6.36 (1 H, d, *J* = 6.0 Hz, CH), 3.85-3.83 (4 H, m, 2CH$_2$), 3.73-3.70 (4 H, m, 2CH$_2$); ^{19}F NMR (376.5 MHz, DMSO-*d*$_6$): δ_F - 61.2 (s, 3 F), - 137.7 (br s, 2 F); ^{11}B NMR (128.4 MHz, DMSO-*d*$_6$): δ_B 0.37; ^{13}C NMR (100 MHz, DMSO-*d*$_6$): δ_C 169.6, 167.4, 162.4, 140.0, 138.1, 133.4, 129.0, 127.4 (q, *J* = 5.0 Hz), 125.2 (q, *J* = 30.0 Hz), 123.3 (q, *J* = 272.0 Hz), 118.2, 116.1, 90.9, 87.4, 65.0 (2C), 50.3 (2C); MS (EI) m/z (%): 455 (M+, 100); Found: C, 49.8; H, 3.5; N, 8.9. Calc. for $C_{19}H_{15}BF_5N_3O_2S$: C, 50.13; H, 3.32; N, 9.23%.

5-(3-(3,5-Bis(trifluoromethyl)phenyl)-2,2-difluoro-2,3-dihydro-1λ³,3,2λ⁴-oxazaborinin-6-yl)-2-morpholinothiophene-3-carbonitrile 1f. Bright orange powder (0.382 g, 73%); m.p. 235-237 °C; IR (ATR, ZnSe) ν_{max}/cm^{-1}: 3104, 2993, 2875, 2215, 1534; ^1H NMR (400 MHz, DMSO-*d*$_6$, Me$_4$Si): δ_H 8.55 (1 H, s, CH), 8.46 (1 H, br s, CH), 8.14 (2 H, s, CH_{Ar}), 8.08 (1 H, s, CH_{Ar}), 6.59 (1 H, d, *J* = 6.4 Hz, CH), 3.82-3.80 (4 H, m, 2CH$_2$), 3.76-3.73 (4 H, m, 2CH$_2$); ^{19}F NMR (376.5 MHz, DMSO-*d*$_6$) δ_F - 61.4 (s, 6 F), - 131.4 (br s, 2 F); ^{11}B NMR (128.4 MHz, DMSO-*d*$_6$): δ_B 0.86; ^{13}C NMR (100 MHz, DMSO-*d*$_6$): δ_C 170.0, 168.0, 159.4, 144.1, 139.9, 131.3 (q, 2C, *J* = 33.0 Hz), 123.1 (2C), 120.0, 122.9 (q, 2C, *J* = 271.0 Hz), 117.5, 116.0, 92.7, 87.8, 65.0 (2C), 50.4 (2C); MS (EI) m/z (%): 523 (M+, 100); Found: C, 45.6; H, 2.9; N, 7.8. Calc. for $C_{20}H_{14}BF_8N_3O_2S$: C, 45.91; H, 2.70; N, 8.03%.

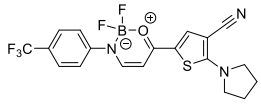
5-(2,2-Difluoro-3-(pyridin-3-yl)-2,3-dihydro-1λ³,3,2λ⁴-oxazaborinin-6-yl)-2-morpholino-thiophene-3-carbonitrile 1g. Scarlet powder (0.345 g, 89%); m.p. 150-152 °C; IR (ATR, ZnSe) ν_{max}/cm^{-1}: 3091, 2997, 2870, 2214, 1541; ^1H NMR (400 MHz, DMSO-*d*$_6$, Me$_4$Si): δ_H 8.89 (1 H, br s, CH), 8.70 (1 H, d, *J* = 4.7 Hz, H_{Ar}), 8.42 (1 H, s, CH), 8.37-8.35 (2 H, m, H_{Ar}), 7.91-7.87 (1 H, m, H_{Ar}), 6.57 (1 H, d, *J* = 6.4 Hz, CH), 3.85-3.82 (4 H, m, 2CH$_2$), 3.77-3.75 (4 H, m, 2CH$_2$); ^{19}F NMR (376.5 MHz, DMSO-*d*$_6$): δ_F - 131.8; ^{11}B NMR (128.4 MHz, DMSO-*d*$_6$): δ_B 0.72; ^{13}C NMR (100 MHz, DMSO-*d*$_6$): δ_C 169.9, 168.0, 158.7, 143.6, 140.1, 139.8, 134.4, 125.7, 117.5, 115.8, 92.9, 87.9, 64.9 (2C), 50.4 (2C); MS (EI) m/z (%): 388 (M+, 33); Found: C, 52.4; H, 4.0; N, 14.1. Calc. for $C_{17}H_{15}BF_2N_4O_2S$: C, 52.60; H, 3.89; N, 14.43%.

5-(2,2-Difluoro-3-(pyrazin-2-yl)-2,3-dihydro-1λ³,3,2λ⁴-oxazaborinin-6-yl)-2-morpholinothio-phene-3-carbonitrile 1h. Red-orange powder (0.276 g, 71%);



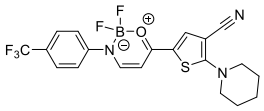
m.p. 204-206 °C; IR (ATR, ZnSe) ν_{max}/cm^{-1}: 3050, 2864, 2210, 1588; ^{1}H NMR (400 MHz, DMSO-d_6, Me_4Si): δ_H 8.87 (1 H, br s, CH), 8.80 (1 H, s, CH), 8.48-8.45 (3 H, m, H_{Ar}), 6.62 (1 H, d, J = 6.8 Hz, CH), 3.85-3.77 (8 H, m, $4CH_2$); ^{19}F NMR (376.5 MHz, DMSO-d_6): δF - 131.6; ^{11}B NMR (128.4 MHz, DMSO-d_6): δ_B 1.05; ^{13}C NMR (100 MHz, DMSO-d_6): δC 170.3, 169.2, 154.7, 148.4, 142.0, 142.0, 141.2, 137.5, 117.1, 115.7, 93.4, 88.3, 64.8 (2C), 50.4 (2C); MS (EI) m/z (%): 389 (M+, 41); Found: C, 49.1; H, 3.9; N, 17.7. Calc. for $C_{16}H_{14}BF_2N_5O_2S$: C, 49.38; H, 3.63; N, 18.00.

5-(2,2-Difluoro-3-(4-(trifluoromethyl)phenyl)-2,3-dihydro-1λ³,3,2λ⁴-oxazaborinin-6-yl)-2-(pyrrolidin-1-yl)thiophene-3-carbonitrile 1i. Red-orange



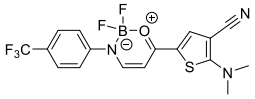
sparcled powder (0.405 g, 92%); m.p. 242-244 °C; IR (ATR, ZnSe) ν_{max}/cm^{-1}: 2983, 2922, 2878, 2209, 1576; ^{1}H NMR (400 MHz, DMSO-d_6, Me_4Si): δ_H 8.31 (1 H, s, CH), 8.18 (1 H, br s, CH), 7.72 and 7.64 (4 H, AA'XX', J = 8.3 Hz, H_{Ar}), 6.40 (1 H, d, J = 6.4 Hz, CH), 3.75-3.72 (4 H, m, $2CH_2$), 2.16-2.14 (4 H, m, $2CH_2$); ^{19}F NMR (376.5 MHz, DMSO-d_6): δ_F -61.3 (3F), - 131.8 (2F); ^{11}B NMR (128.4 MHz, DMSO-d_6): δ_B 0.81; ^{13}C NMR (100 MHz, DMSO-d_6): δ_C 167.5, 165.5, 157.7, 145.9, 139.4, 126.6 (q, J = 32.0 Hz), 126.5 (q, J = 3.7 Hz), 124.0 (q, J = 270.0 Hz), 122.9 (2C), 116.2, 116.0, 92.1, 86.0, 52.2 (2C), 25.3 (2C); MS (EI) m/z (%): 439 (M+, 87); Found: C, 51.6; H, 3.6; N, 9.2. Calc. for $C_{19}H_{15}BF_5N_3OS$: C, 51.96; H, 3.44; N, 9.57%.

5-(2,2-Difluoro-3-(4-(trifluoromethyl)phenyl)-2,3-dihydro-1λ³,3,2λ⁴-oxazaborinin-6-yl)-2-(piperidin-1-yl)thiophene-3-carbonitrile 1j. Bright orange



sparkled powder (0.395 g, 87%); m.p. 315-317 °C; IR (ATR, ZnSe) ν_{max}/cm^{-1}: 3065, 2941, 2858, 2211, 1565; ^{1}H NMR (400 MHz, DMSO-d_6, Me_4Si): δ_H 8.29 (1 H, s, CH), 8.22 (1 H, br s, CH), 7.73 and 7.64 (4 H, AA'XX', J = 8.3 Hz, H_{Ar}), 6.42 (1 H, d, J = 6.2 Hz, CH), 3.79-3.77 (4 H, m, $2CH_2$), 1.77-1.75 (6 H, m, $3CH_2$); ^{19}F NMR (376.5 MHz, DMSO-d_6): δ_F - 61.4 (3F), - 131.7 (2F); ^{11}B NMR (128.4 MHz, DMSO-d_6): δ_B 0.80; ^{13}C NMR (100 MHz, DMSO-d_6): δ_C 169.1, 167.6, 158.4, 145.9, 139.6, 126.9 (q, J = 32.0 Hz), 126.5 (q, J = 3.8 Hz), 124.2 (q, J = 270.0 Hz), 123.1 (2C), 116.6, 116.3, 92.4, 87.0, 52.2 (2C), 24.8 (2C), 22.7; MS (EI) m/z (%): 453 (M+, 88); Found: C, 52.7; H, 3.9; N, 9.0. Calc. for $C_{20}H_{17}BF_5N_3OS$: C, 53.00; H, 3.78; N, 9.27%.

5-(2,2-Difluoro-3-(4-(trifluoromethyl)phenyl)-2,3-dihydro-1λ³,3,2λ⁴-oxazaborinin-6-yl)-2-(dimethylamino)thiophene-3-carbonitrile 1k. Scarled sparcled



rowder (0.268 g, 65%); m.p. 249-251 °C; IR (ATR, ZnSe) ν_{max}/cm^{-1}: 2932, 2215, 1575; ^{1}H NMR (400 MHz, DMSO-d_6, Me_4Si): δ_H 8.26 (1 H, s, CH), 8.18 (1 H, br s, CH), 7.71 and 7.64 (4 H, AA'XX', J = 8.0 Hz, H_{Ar}), 6.39 (1 H, d, J = 6.5 Hz, CH), 3.42 (6 H, s, NMe_2); ^{19}F NMR (376.5 MHz, DMSO-d_6): δ_F -61.5 (3F), - 131.7 (2F); ^{11}B NMR (128.4 MHz, DMSO-d_6): δ_B 0.78; ^{13}C NMR (100 MHz, DMSO-d_6): δ_C 169.2, 167.6, 158.1, 145.9, 140.0, 126.8 (q, J = 32.0 Hz), 126.4 (q, J = 4.0 Hz), 124.1 (q, J = 270.0 Hz), 123.0 (2C), 116.5, 116.3, 92.2, 86.2, 43.5 (2C); MS (EI) m/z (%): 413 (M+, 78); Found: C, 49.1; H, 3.3; N, 9.9. Calc. for $C_{17}H_{13}BF_5N_3OS$: C, 49.42; H, 3.17; N, 10.17%.

2. NMR spectra for new compounds

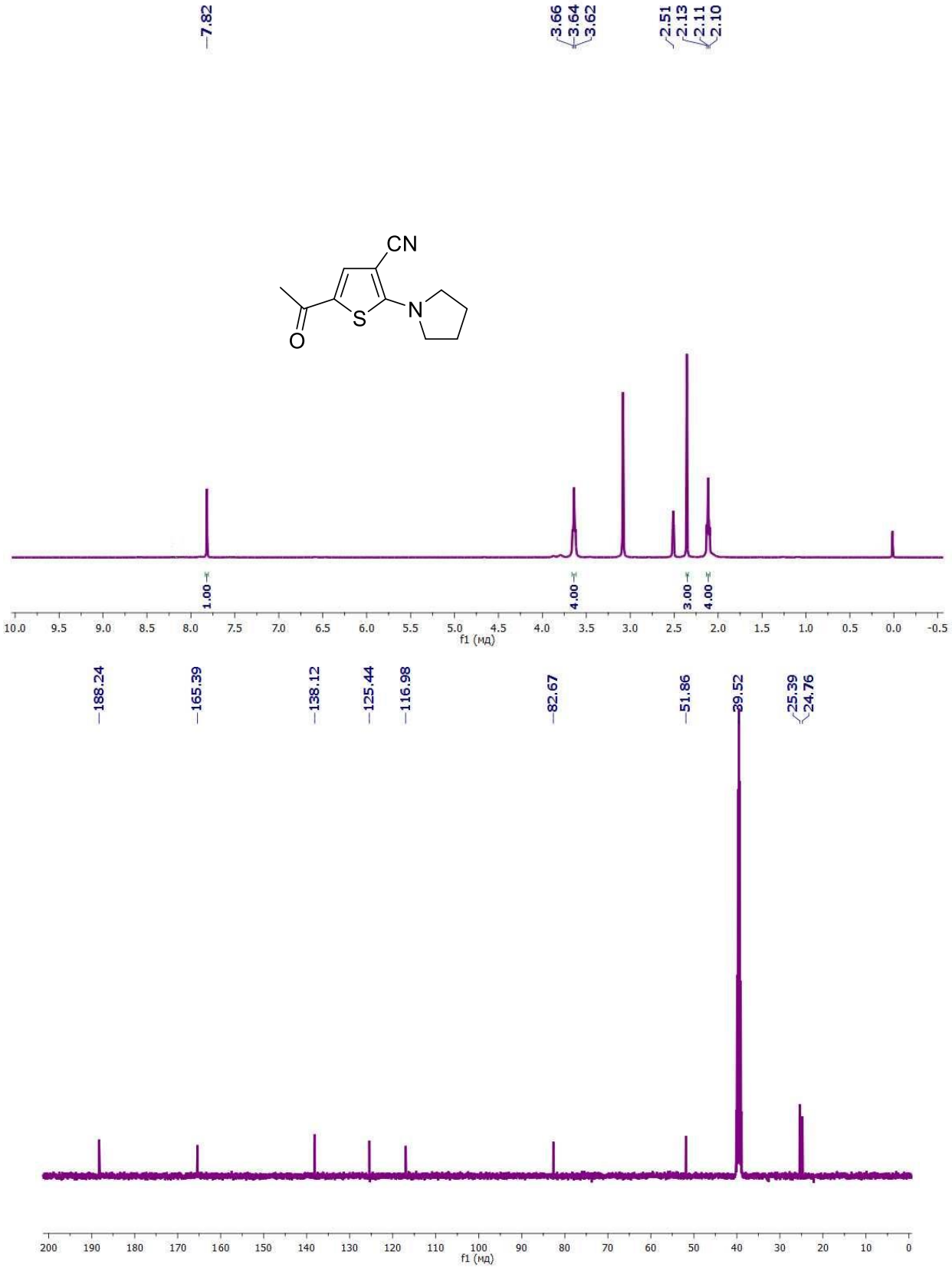


Fig. S1. ^{1}H NMR (400 MHz, DMSO-d_6, TMS) and ^{13}C NMR (100 MHz, DMSO-d_6) spectra of 5-acetyl-2-(pyrrolidin-1-yl)thiophene-3-carbonitrile **3b**.

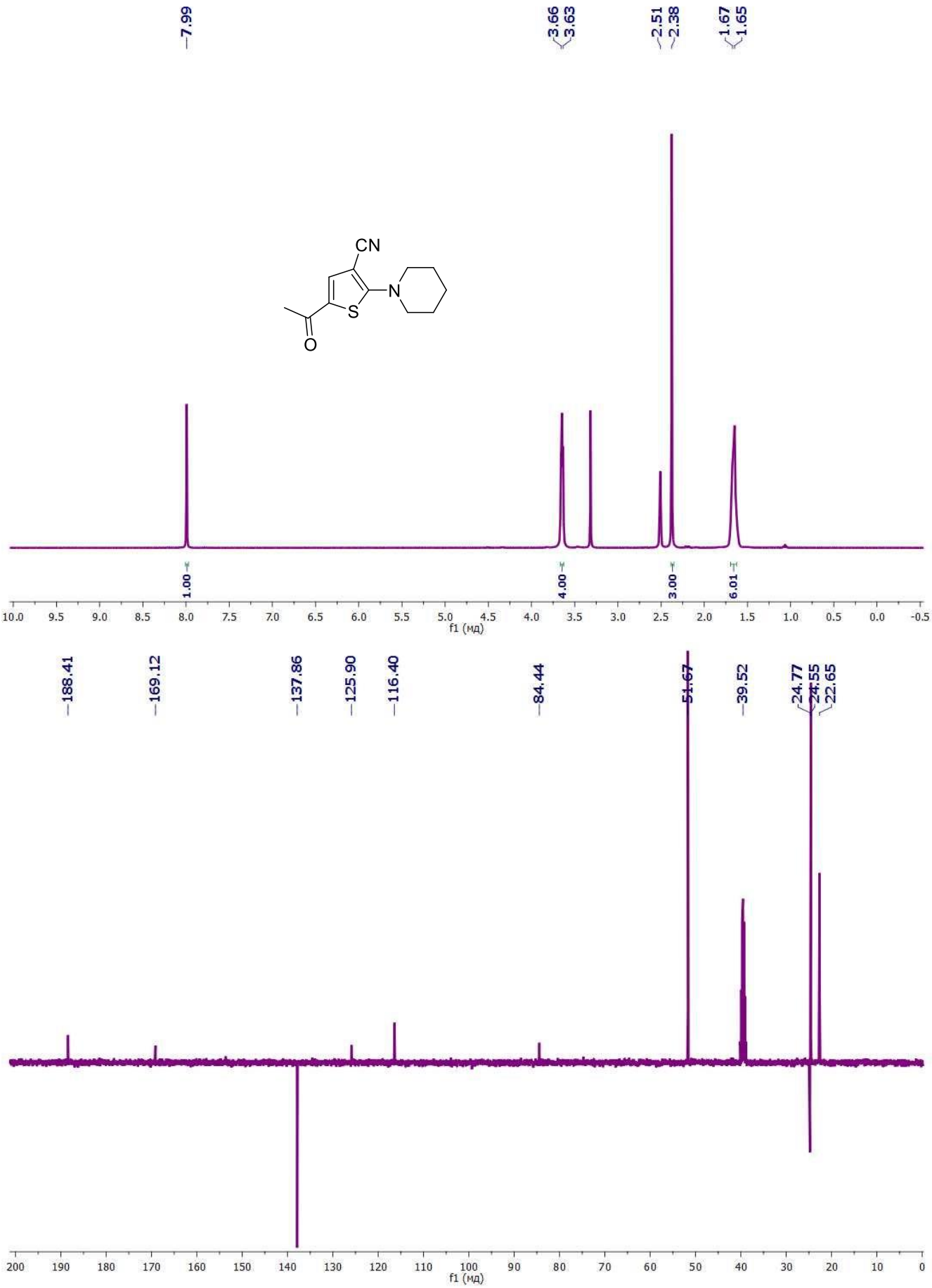


Fig. S2. ^{1}H NMR (400 MHz, DMSO-d_6, TMS) and ^{13}C NMR (100 MHz, DMSO-d_6) spectra of 5-acetyl-2-(piperidin-1-yl)thiophene-3-carbonitrile **3c.**

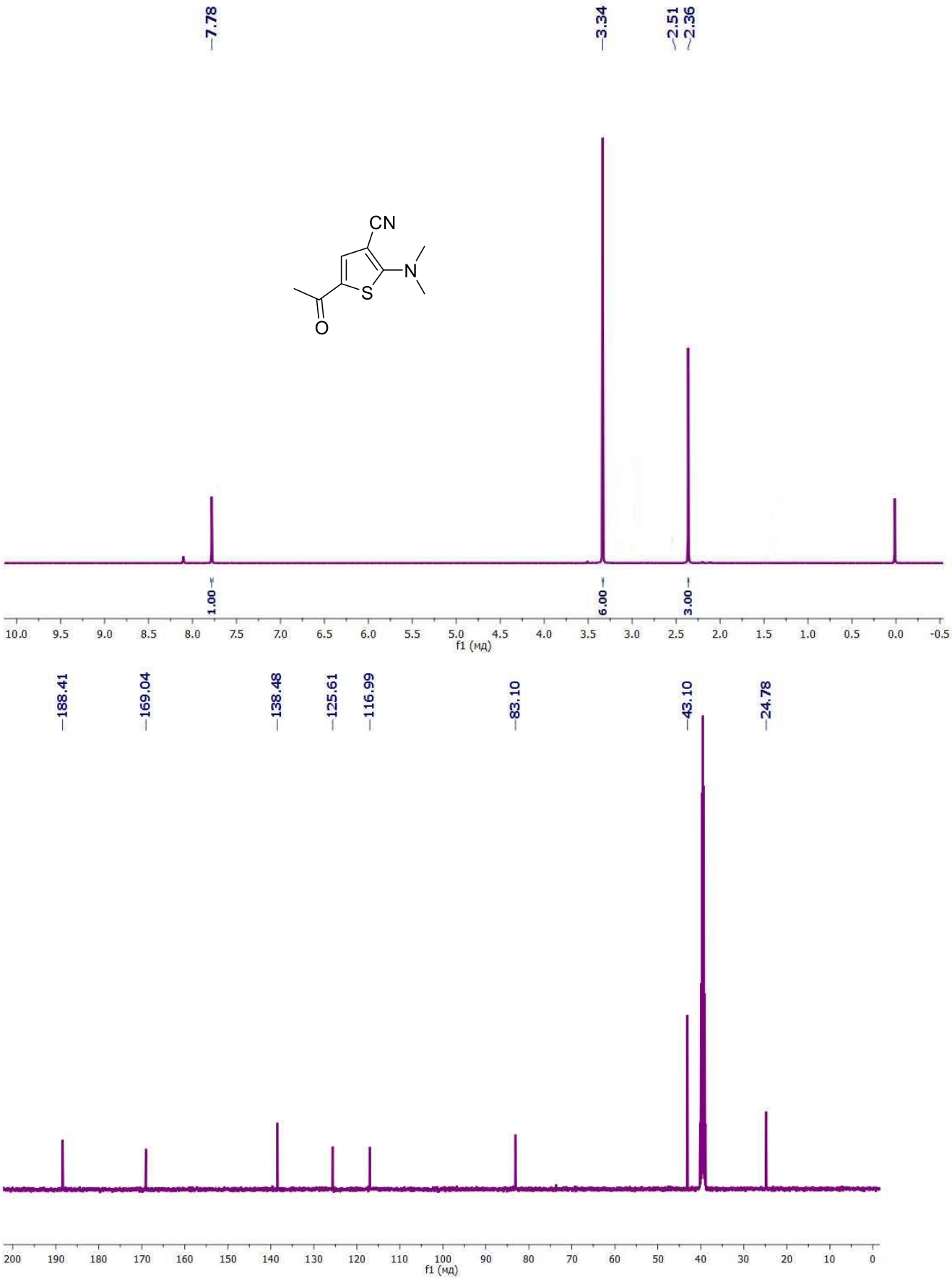
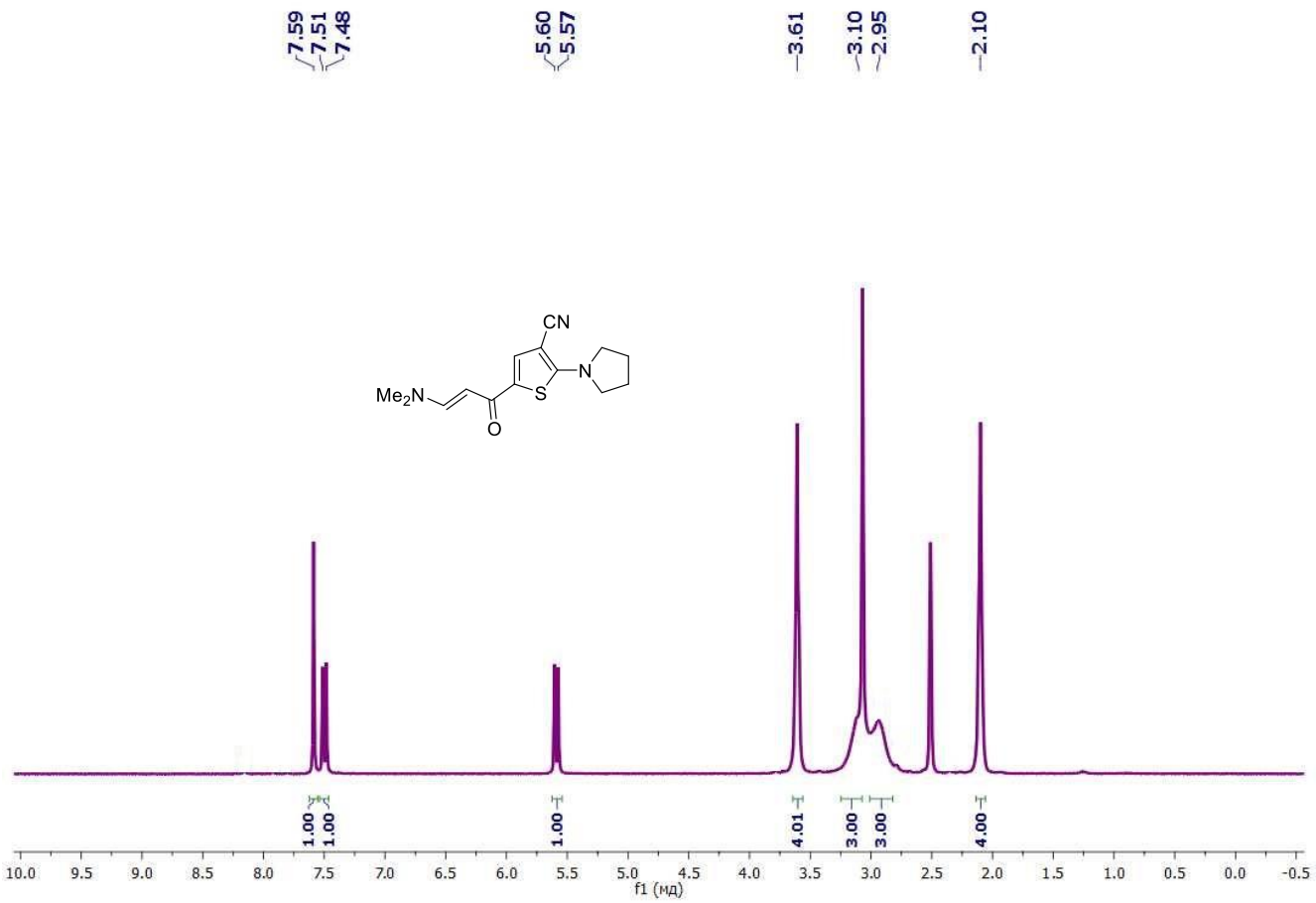
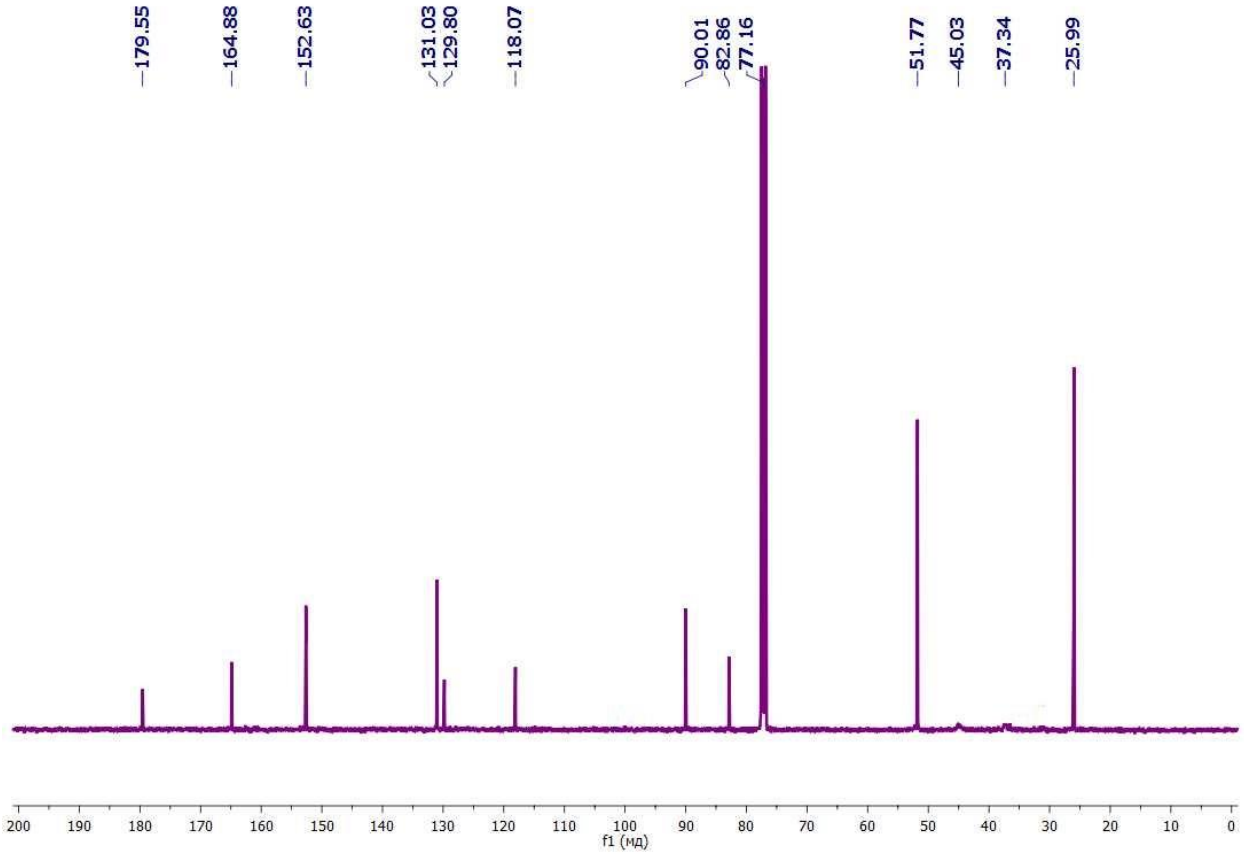


Fig. S3. ^{1}H NMR (400 MHz, DMSO-d_6, TMS) and ^{13}C NMR (100 MHz, DMSO-d_6) spectra of 5-acetyl-2-(dimethylamino)thiophene-3-carbonitrile **3d**.

Fig. S4. ^{1}H NMR (400 MHz, DMSO-d_6, TMS) and ^{13}C NMR (100 MHz, DMSO-d_6) spectra of 5-(3-(dimethylamino)acryloyl)-2-morpholinothiophene-3-carbonitrile **4a**.


7.59
7.51
7.48
5.60
5.57
3.61
3.10
2.95
2.10
CN
Me2N
S
N
O
1.00
1.00
1.00
4.01
3.00
3.00
4.00
f1 (мд)


179.55
164.88
152.63
131.03
129.80
118.07
90.01
82.86
77.16
51.77
45.03
37.34
25.99
f1 (мд)

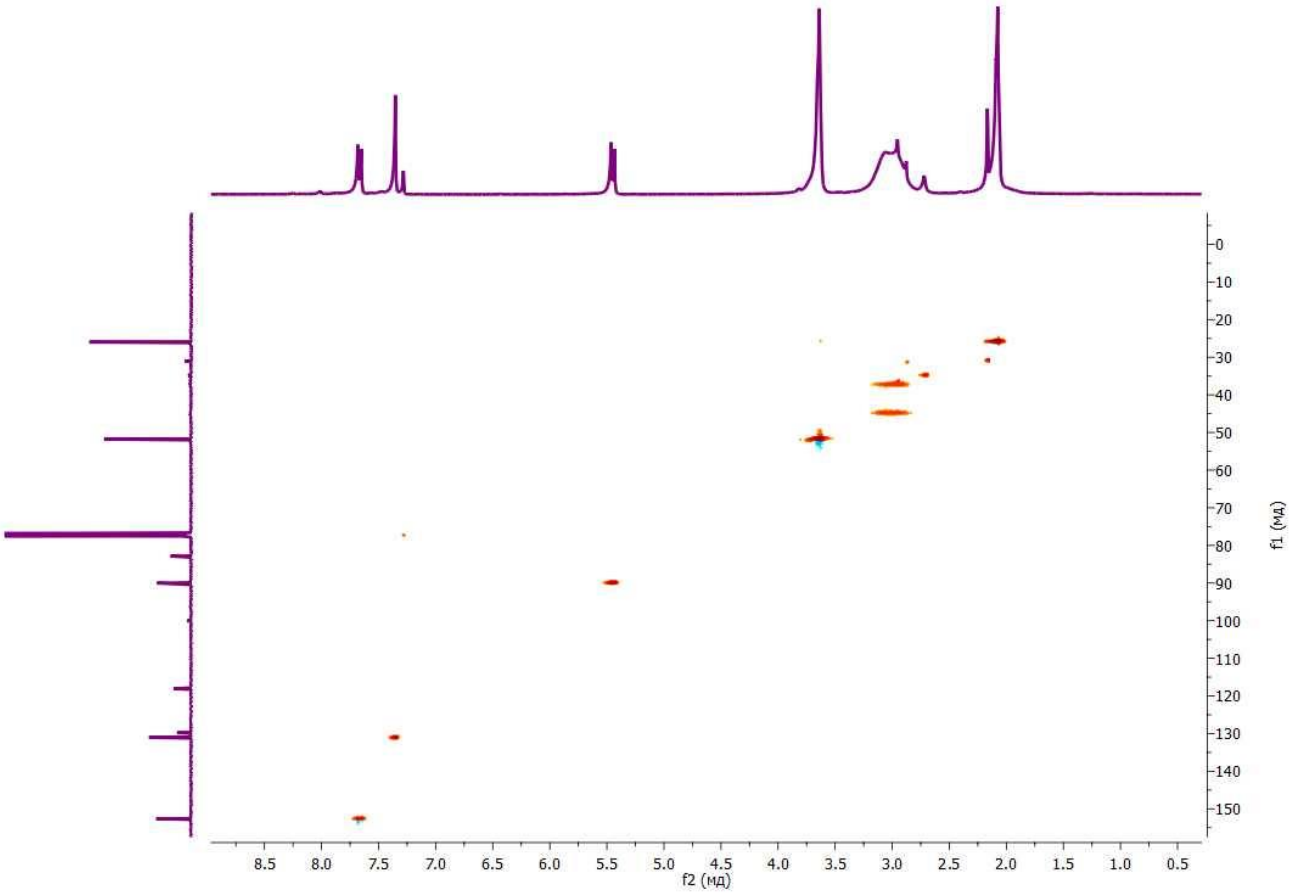


Fig. S5. ^{1}H NMR (400 MHz, DMSO-d_6, TMS) and ^{13}C NMR (100 MHz, DMSO-d_6) spectra of 5-(3-(dimethylamino)acryloyl)-2-(pyrrolidin-1-yl)thiophene-3-carbonitrile **4b.**

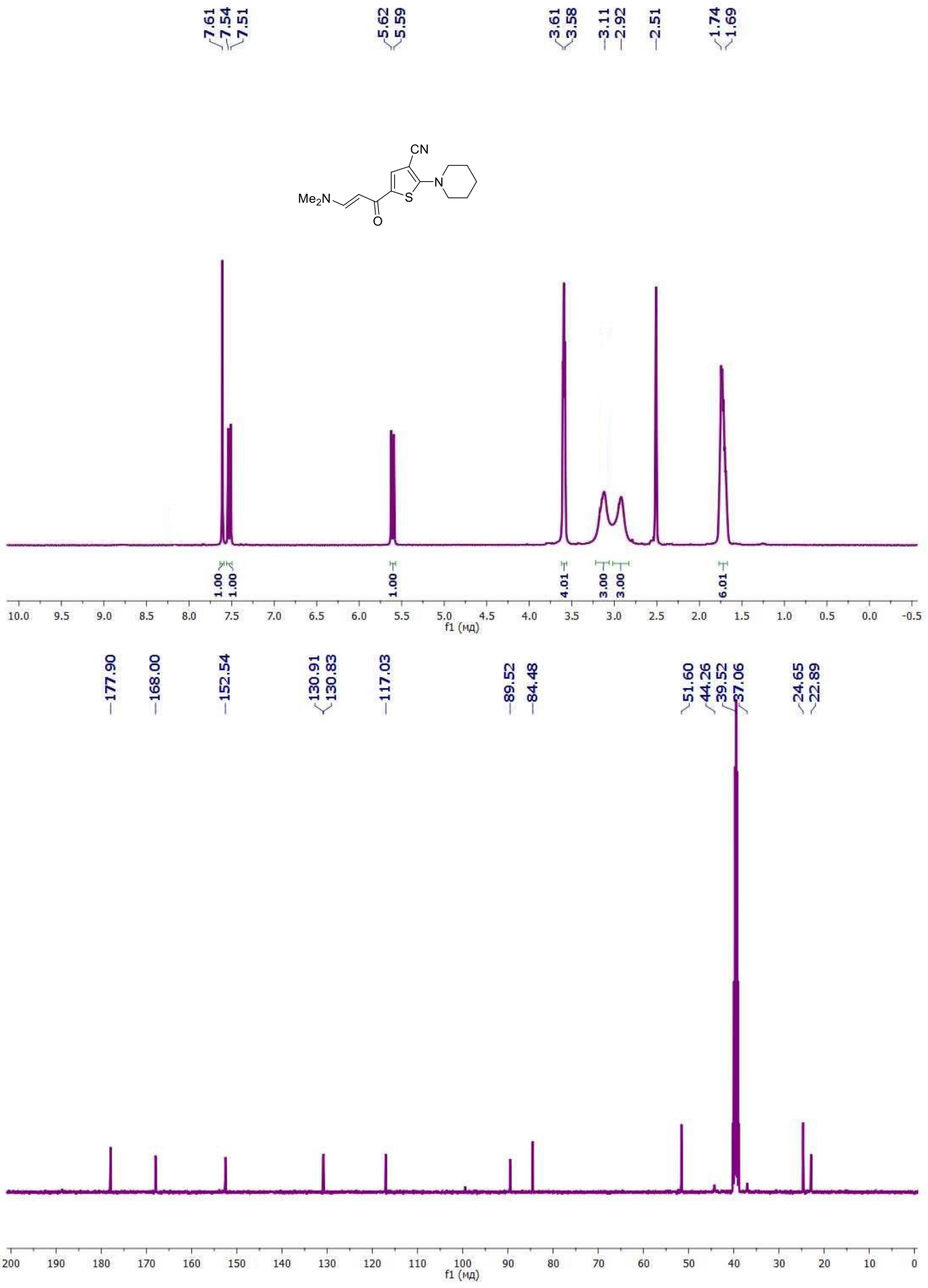


Fig. S6. ^{1}H NMR (400 MHz, DMSO-d_6, TMS) and ^{13}C NMR (100 MHz, DMSO-d_6) spectra of 5-(3-(dimethylamino)acryloyl)-2-(piperidin-1-yl)thiophene-3-carbonitrile **4c.**

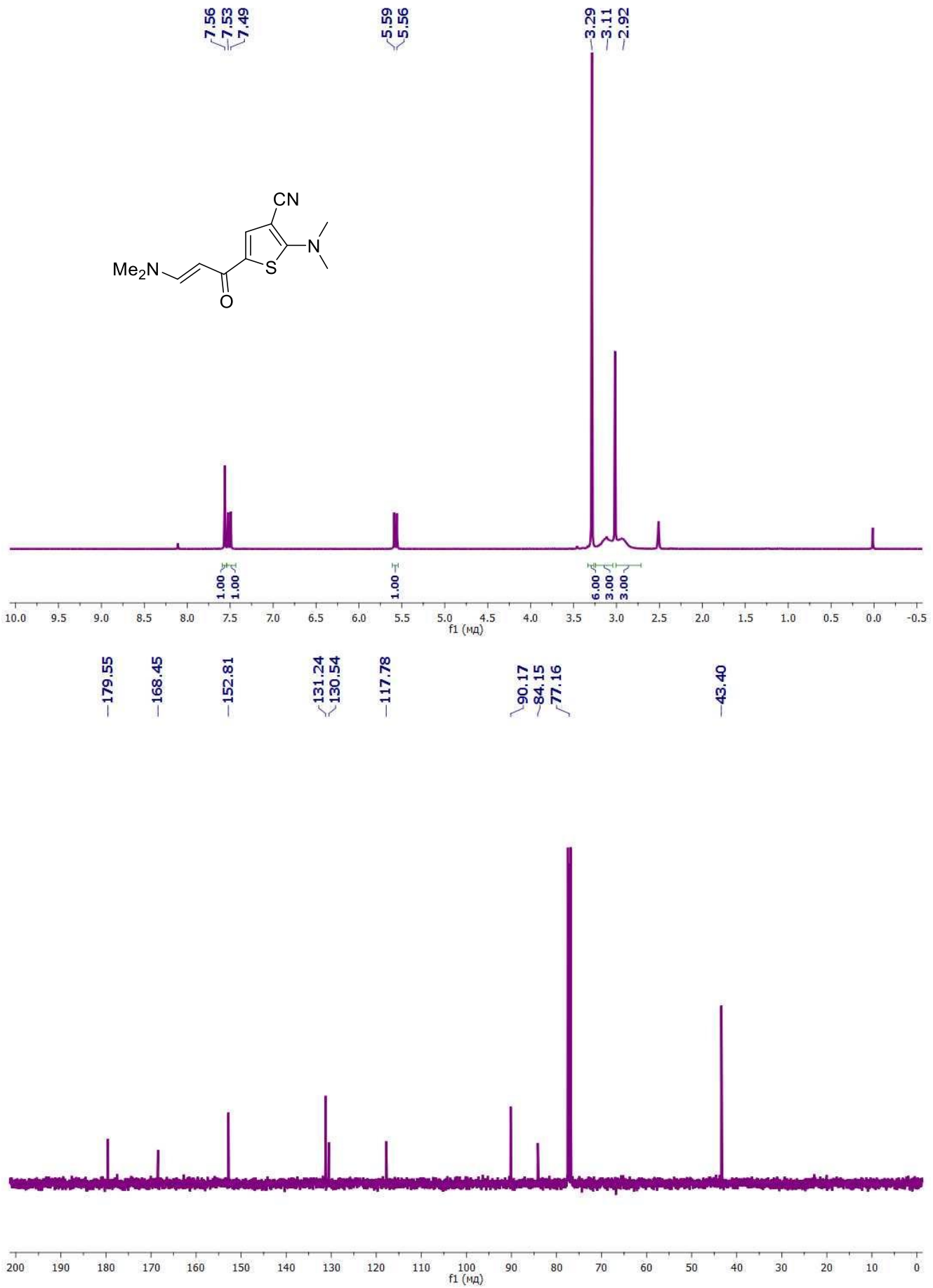


Fig. S7. ^{1}H NMR (400 MHz, DMSO-d_6, TMS) and ^{13}C NMR (100 MHz, DMSO-d_6) spectra of 2-(dimethylamino)-5-(3-(dimethylamino)acryloyl)thiophene-3-carbonitrile **4d.**

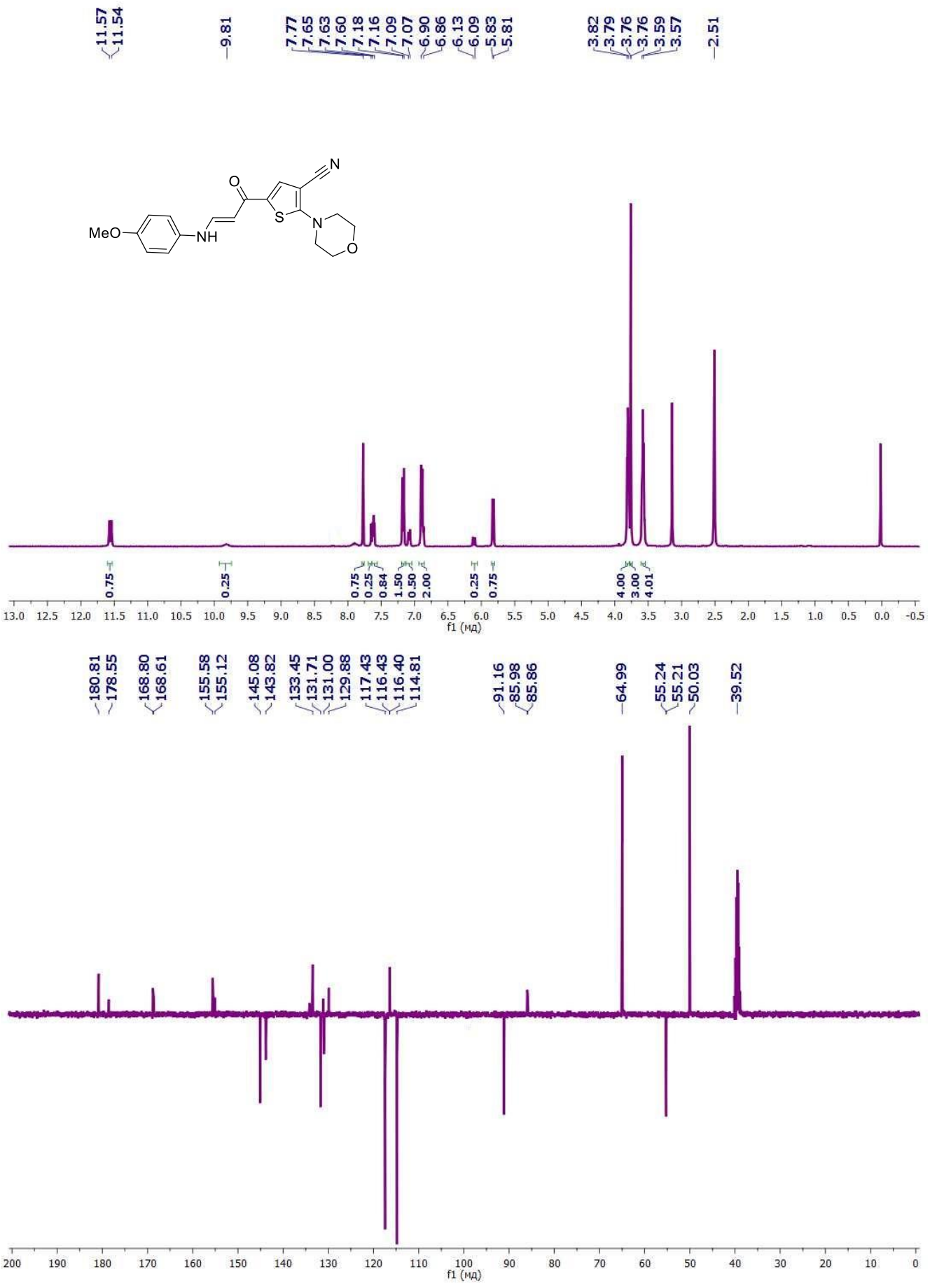


Fig. S8. ^{1}H NMR (400 MHz, DMSO-d_6, TMS) and ^{13}C NMR (100 MHz, DMSO-d_6) spectra of 5-(3-((4-methoxyphenyl)amino)acryloyl)-2-morpholinothiophene-3-carbonitrile **2a.**

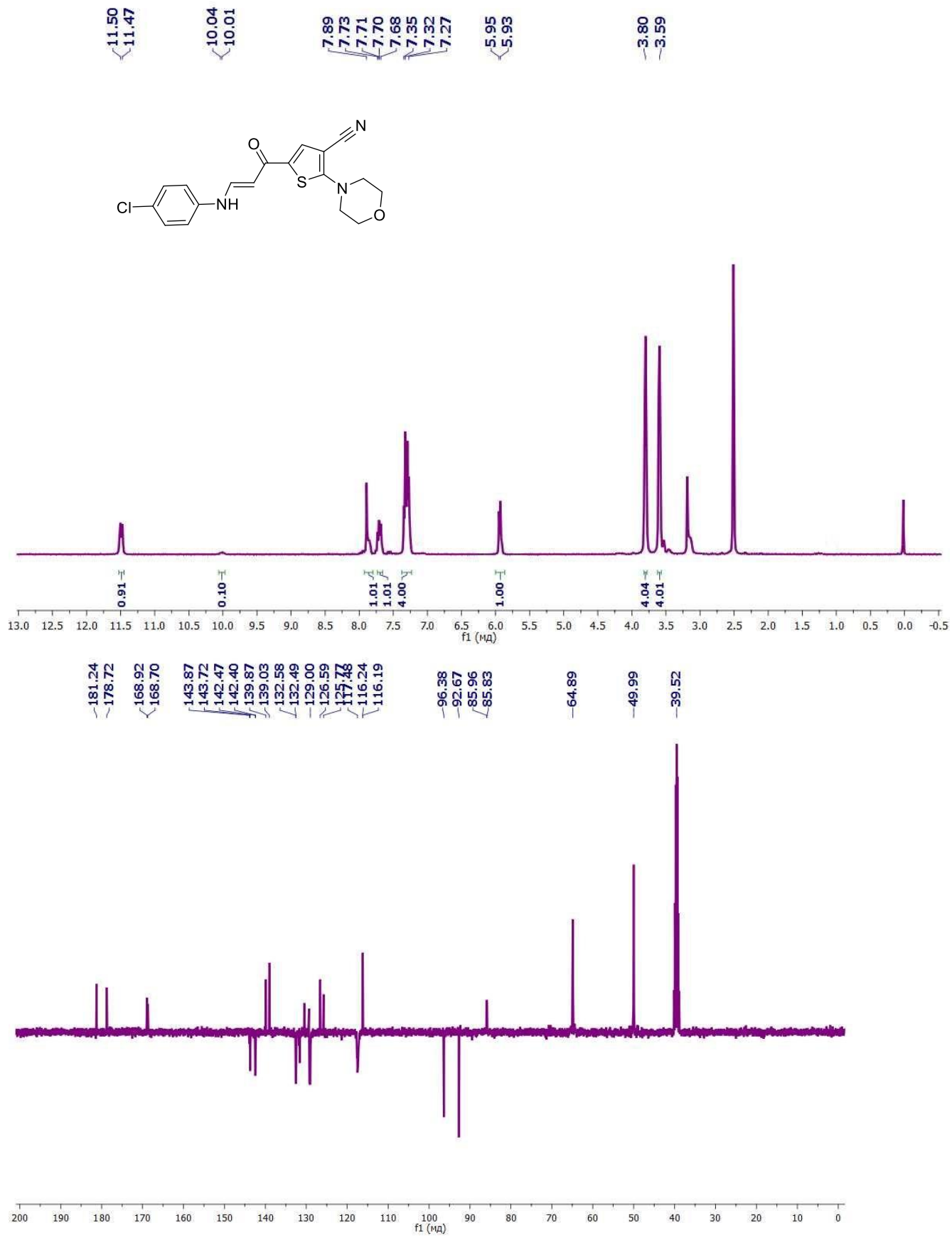


Fig. S9. ^{1}H NMR (400 MHz, DMSO-d_6, TMS) and ^{13}C NMR (100 MHz, DMSO-d_6) spectra of 5-(3-((4-chlorophenyl)amino)acryloyl)-2-morpholinothiophene-3-carbonitrile **2b.**

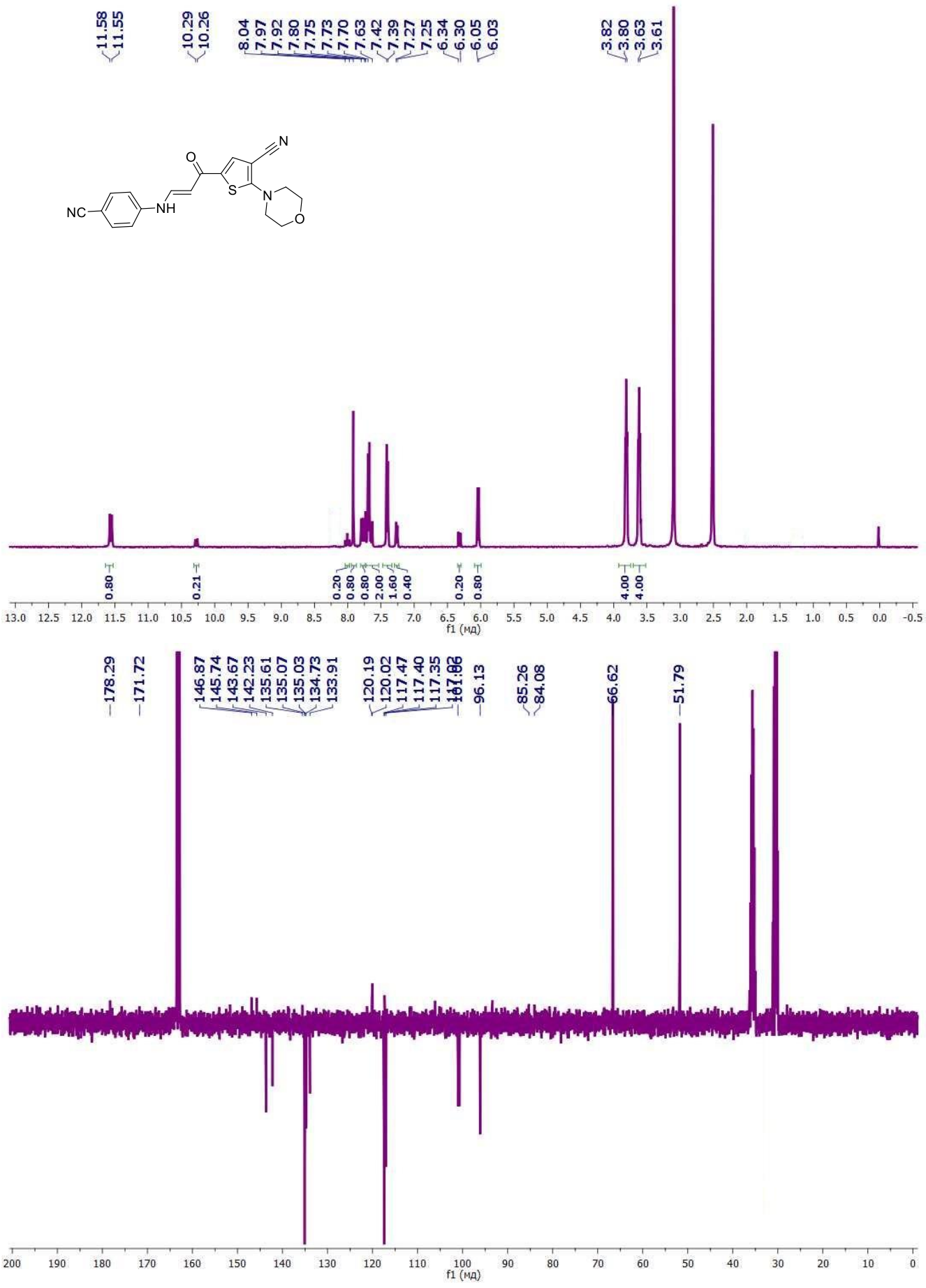


Fig. S10. ^{1}H NMR (400 MHz, DMSO-d_6, TMS) and ^{13}C NMR (100 MHz, DMSO-d_6) spectra of 5-(3-((4-cyanophenyl)amino)acryloyl)-2-morpholinothiophene-3-carbonitrile **2c.**

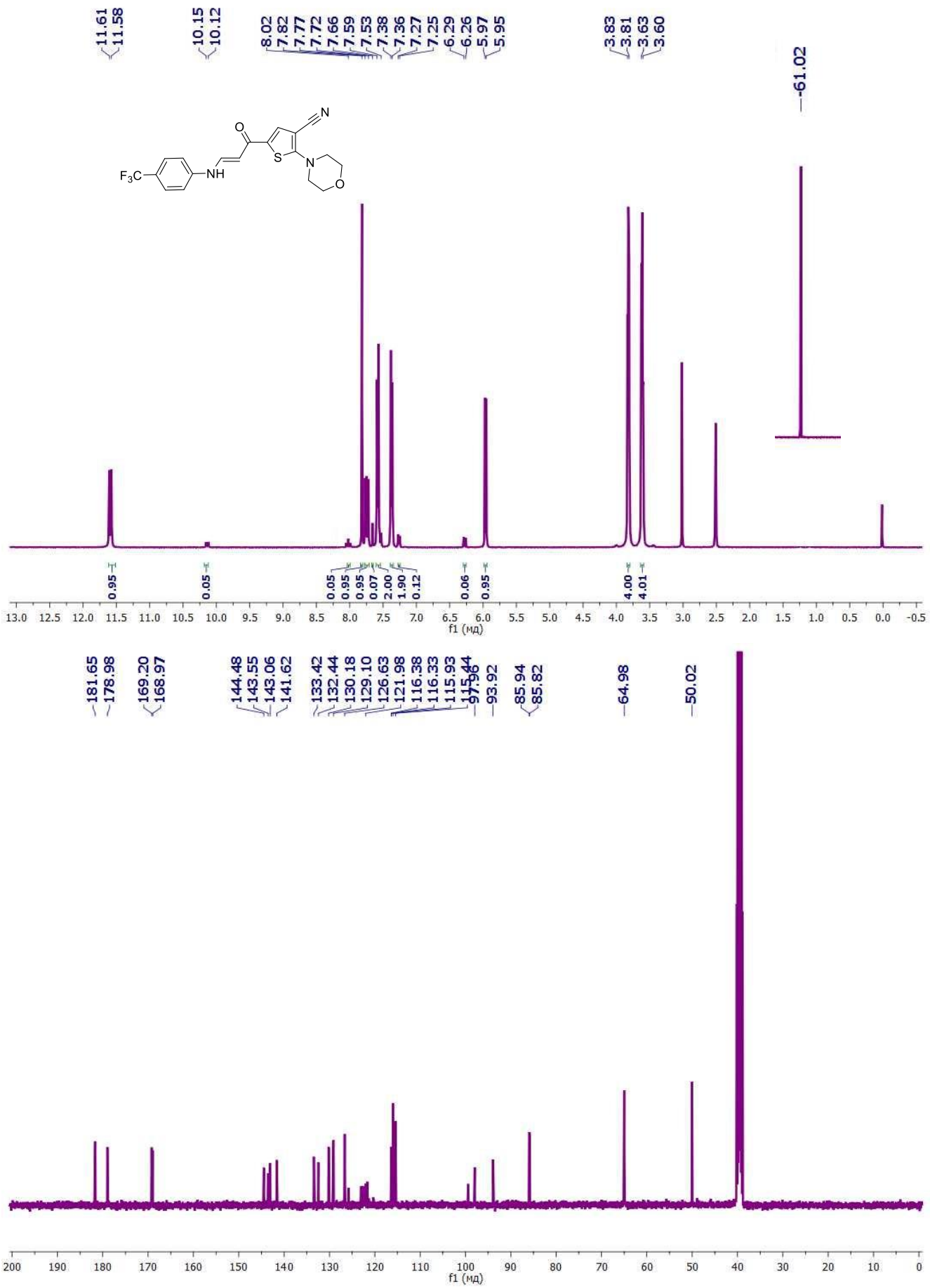


Fig. S11. ^{1}H NMR (400 MHz, DMSO-d_6, TMS) and ^{13}C NMR (100 MHz, DMSO-d_6) spectra of 2-morpholino-5-(3-((4-(trifluoromethyl)phenyl)amino)acryloyl)thiophene-3-carbonitrile **2d.**

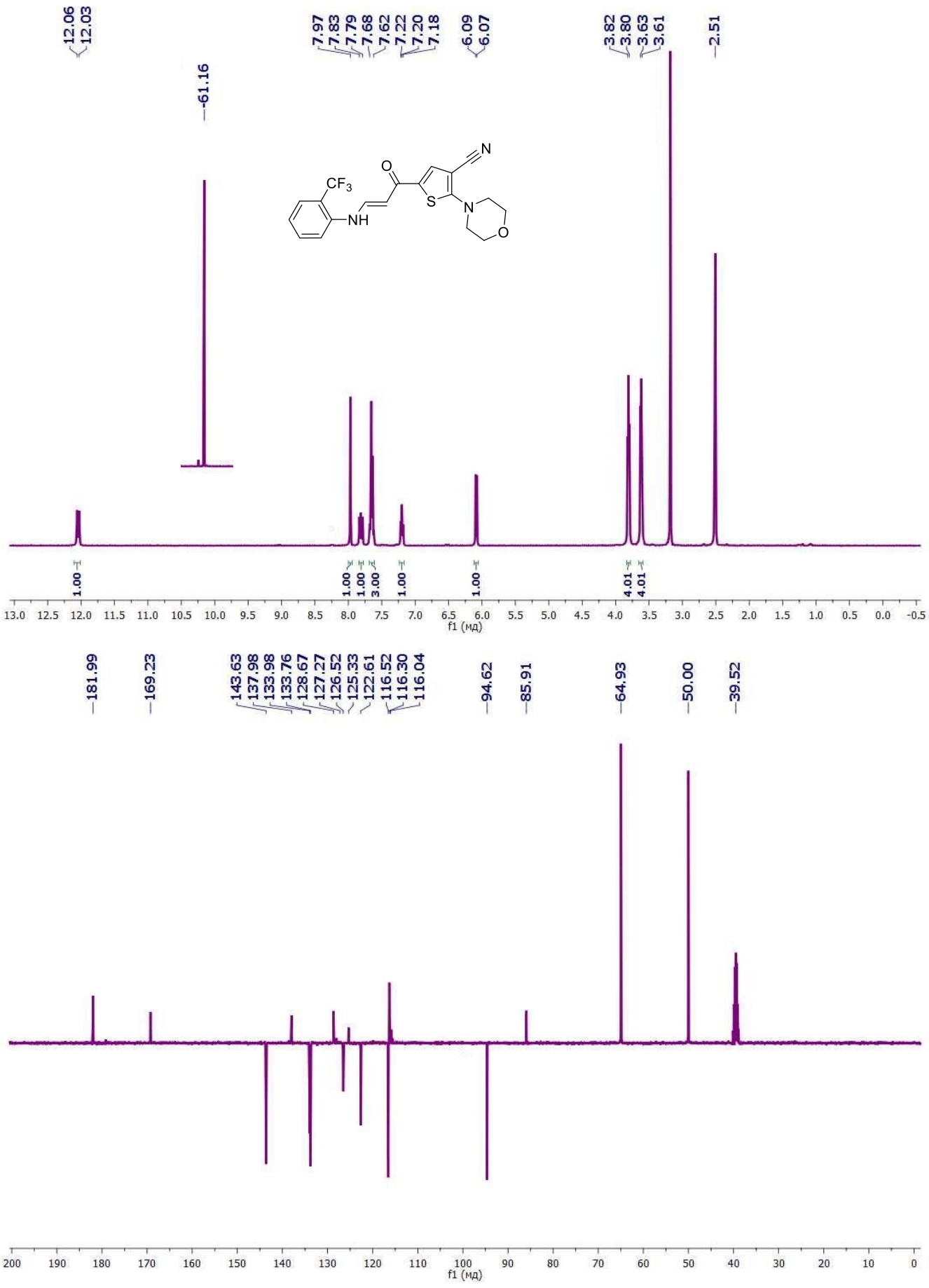


Fig. S12. ^{1}H NMR (400 MHz, DMSO-d_6, TMS) and ^{13}C NMR (100 MHz, DMSO-d_6) spectra of 2-morpholino-5-(3-((2-(trifluoromethyl)phenyl)amino)acryloyl)thiophene-3-carbonitrile **2e.**

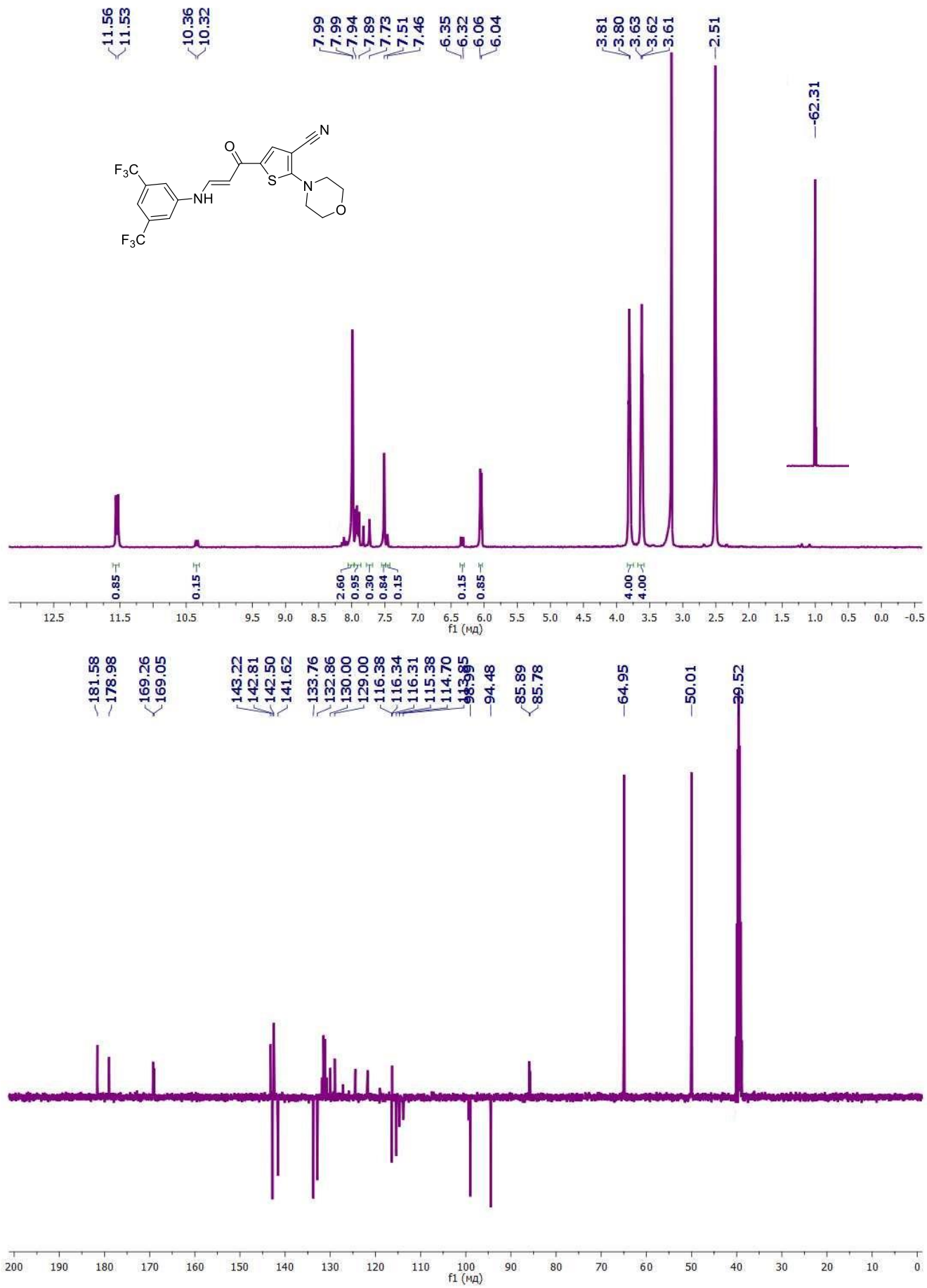


Fig. S13. ^{1}H NMR (400 MHz, DMSO-d_6, TMS) and ^{13}C NMR (100 MHz, DMSO-d_6) spectra of 5-(3-((3,5-bis(trifluoromethyl)phenyl)amino)acryloyl)-2-morpholinothiophene-3-carbonitrile **2f**.

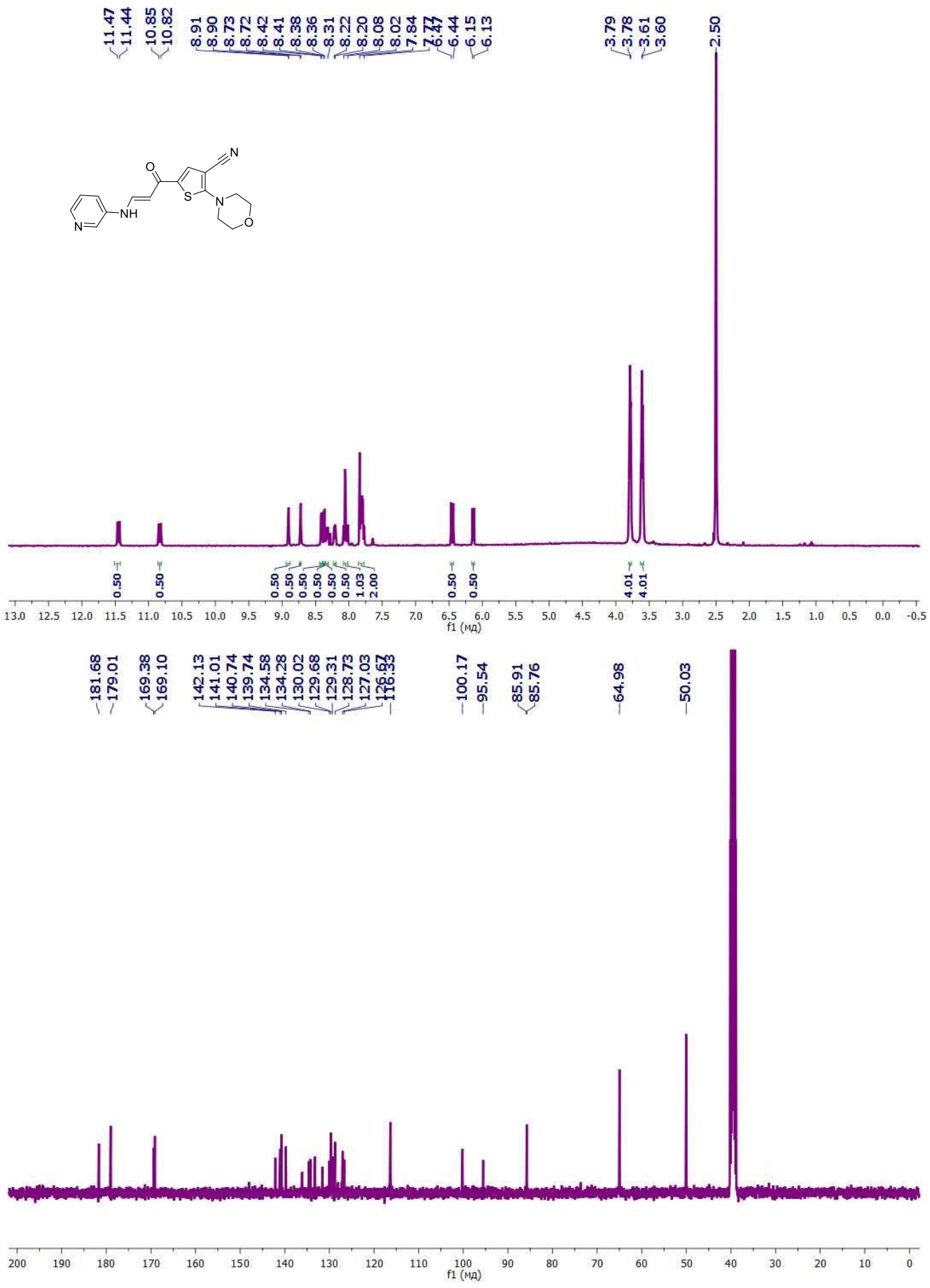


Fig. S14. ^{1}H NMR (400 MHz, DMSO-d_6, TMS) and ^{13}C NMR (100 MHz, DMSO-d_6) spectra of 2-morpholino-5-(3-(pyridin-3-ylamino)acryloyl)thiophene-3-carbonitrile **2g.**

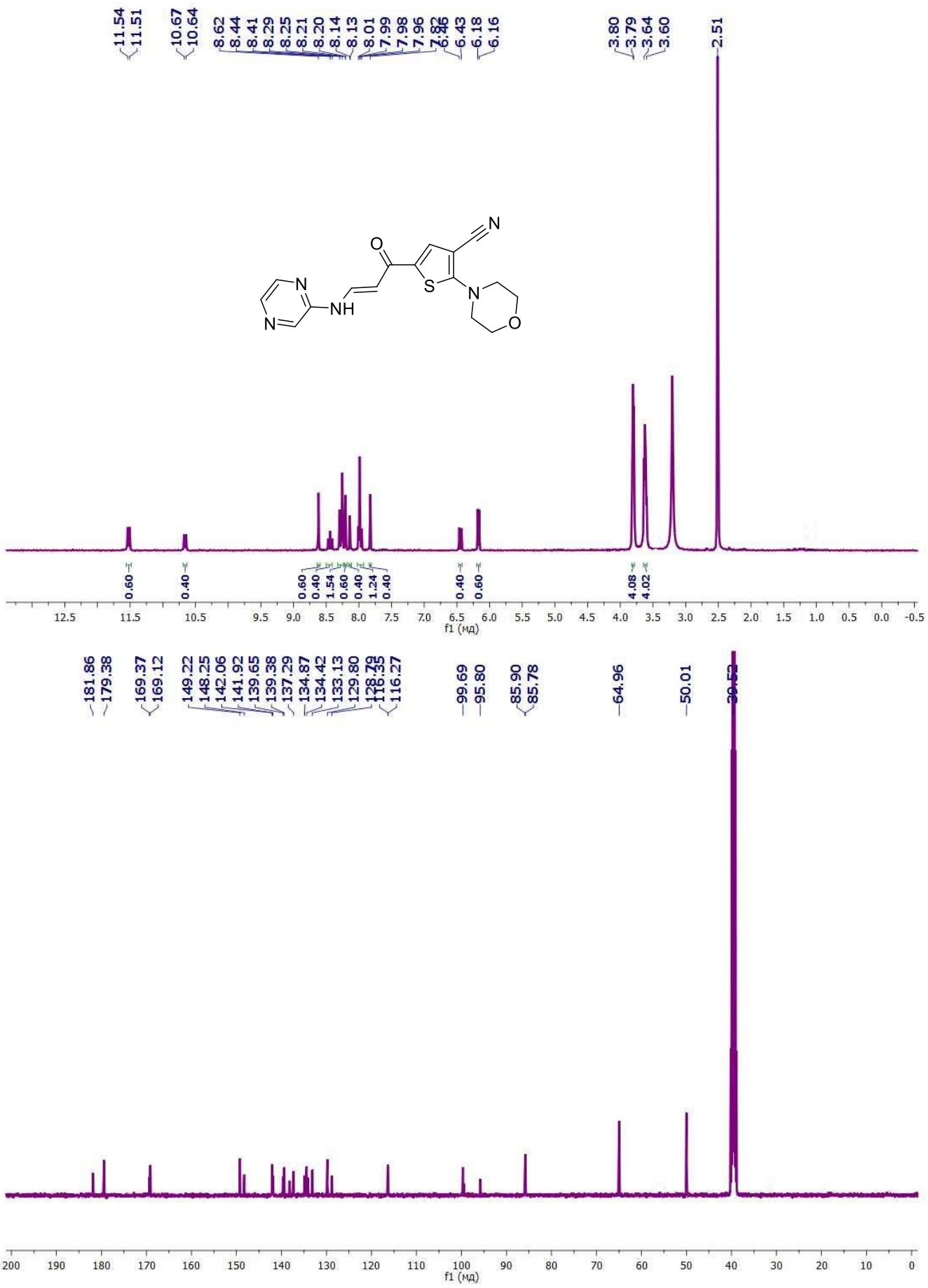


Fig. S15. ^{1}H NMR (400 MHz, DMSO-d_6, TMS) and ^{13}C NMR (100 MHz, DMSO-d_6) spectra of 2-morpholino-5-(3-(pyrazin-2-ylamino)acryloyl)thiophene-3-carbonitrile **2h.**

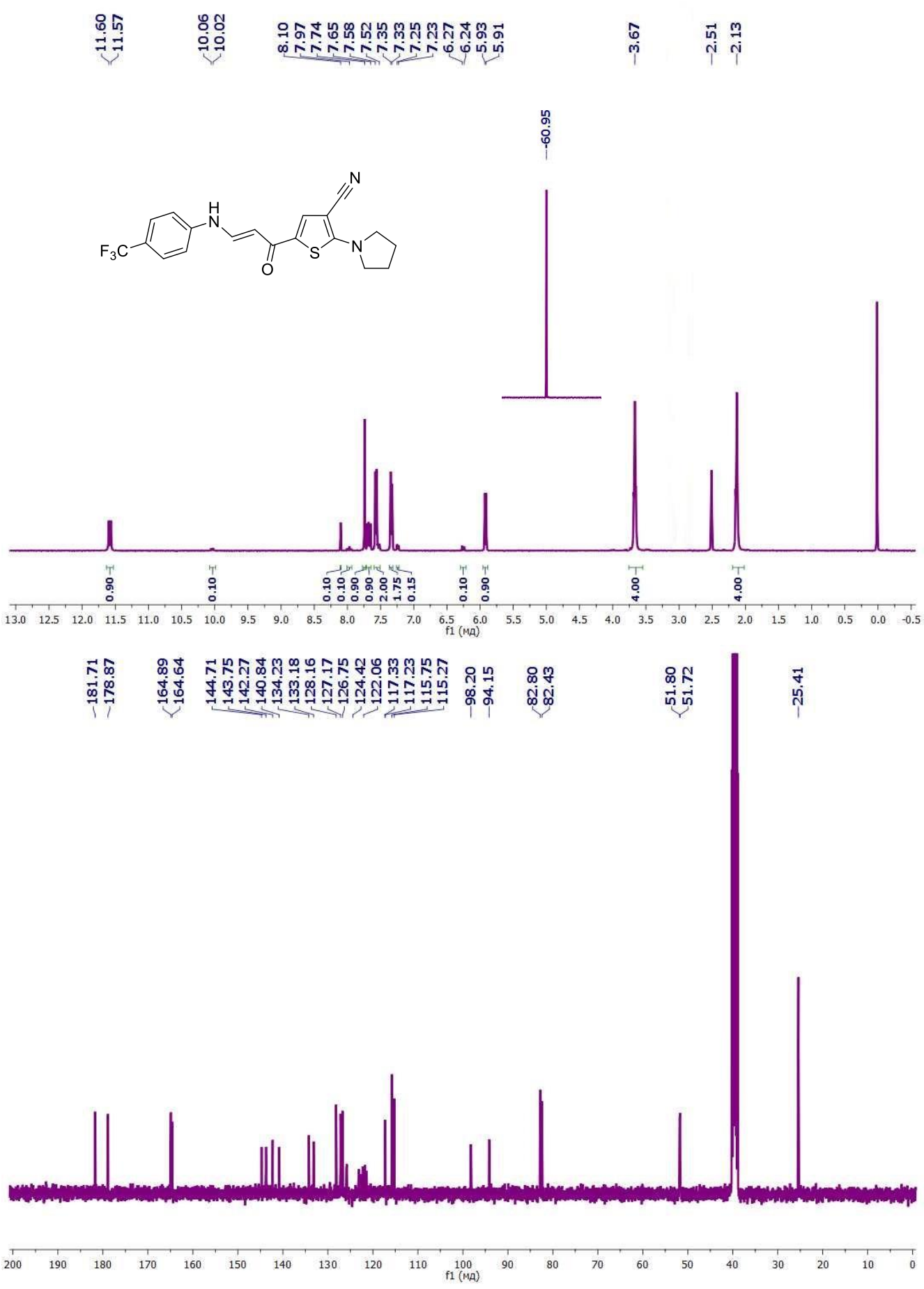


Fig. S16. ^{1}H NMR (400 MHz, DMSO-d_6, TMS) and ^{13}C NMR (100 MHz, DMSO-d_6) spectra of 2-(pyrrolidin-1-yl)-5-(3-((4-trifluoromethyl-phenyl)amino)acryloyl)thiophene-3-carbonitrile **2i.**

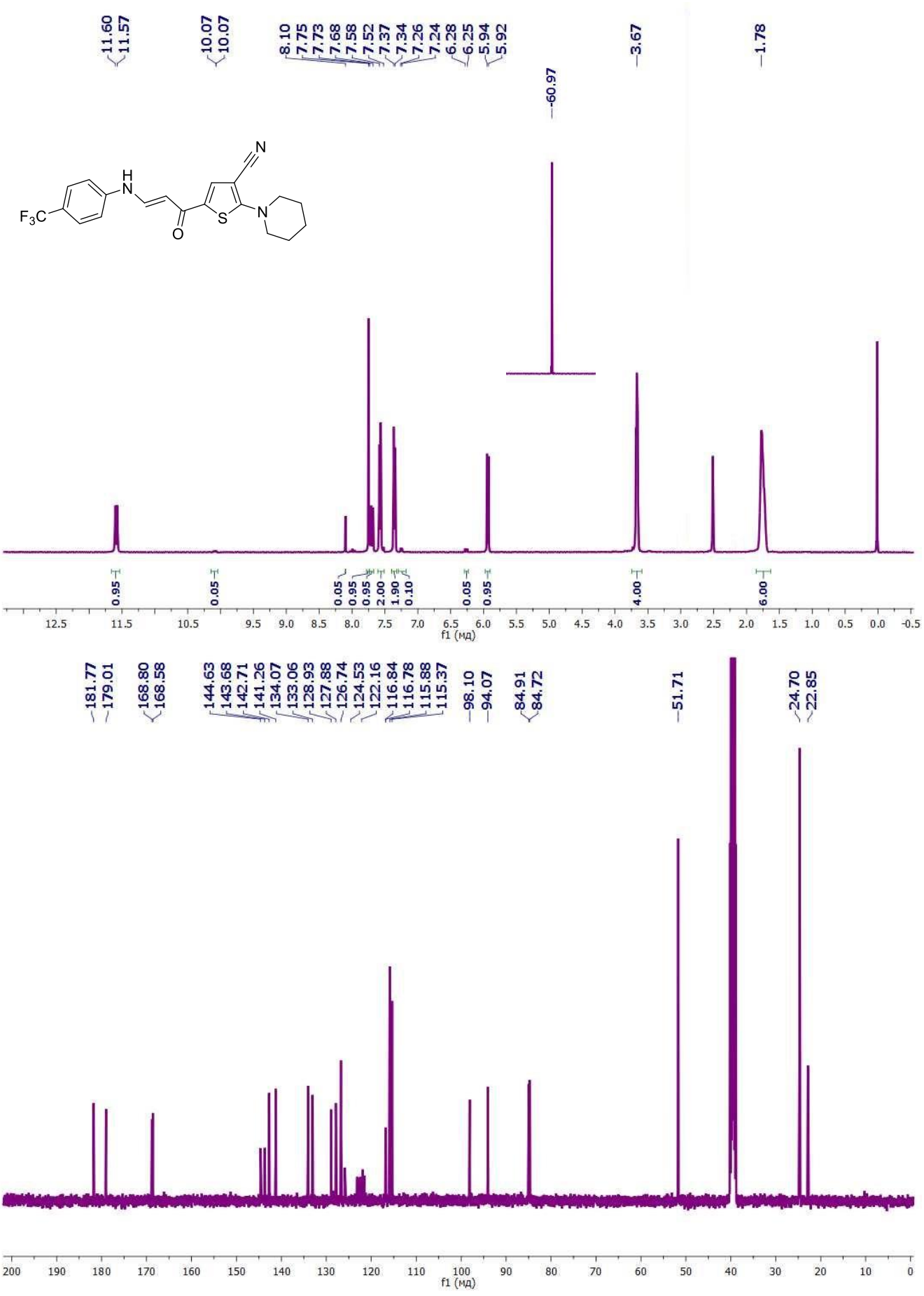


Fig. S17. ^{1}H NMR (400 MHz, DMSO-d_6, TMS) and ^{13}C NMR (100 MHz, DMSO-d_6) spectra of 2-(piperidin-1-yl)-5-(3-((4-trifluoromethylphenyl)amino)acryloyl)thiophene-3-carbonitrile **2j.**

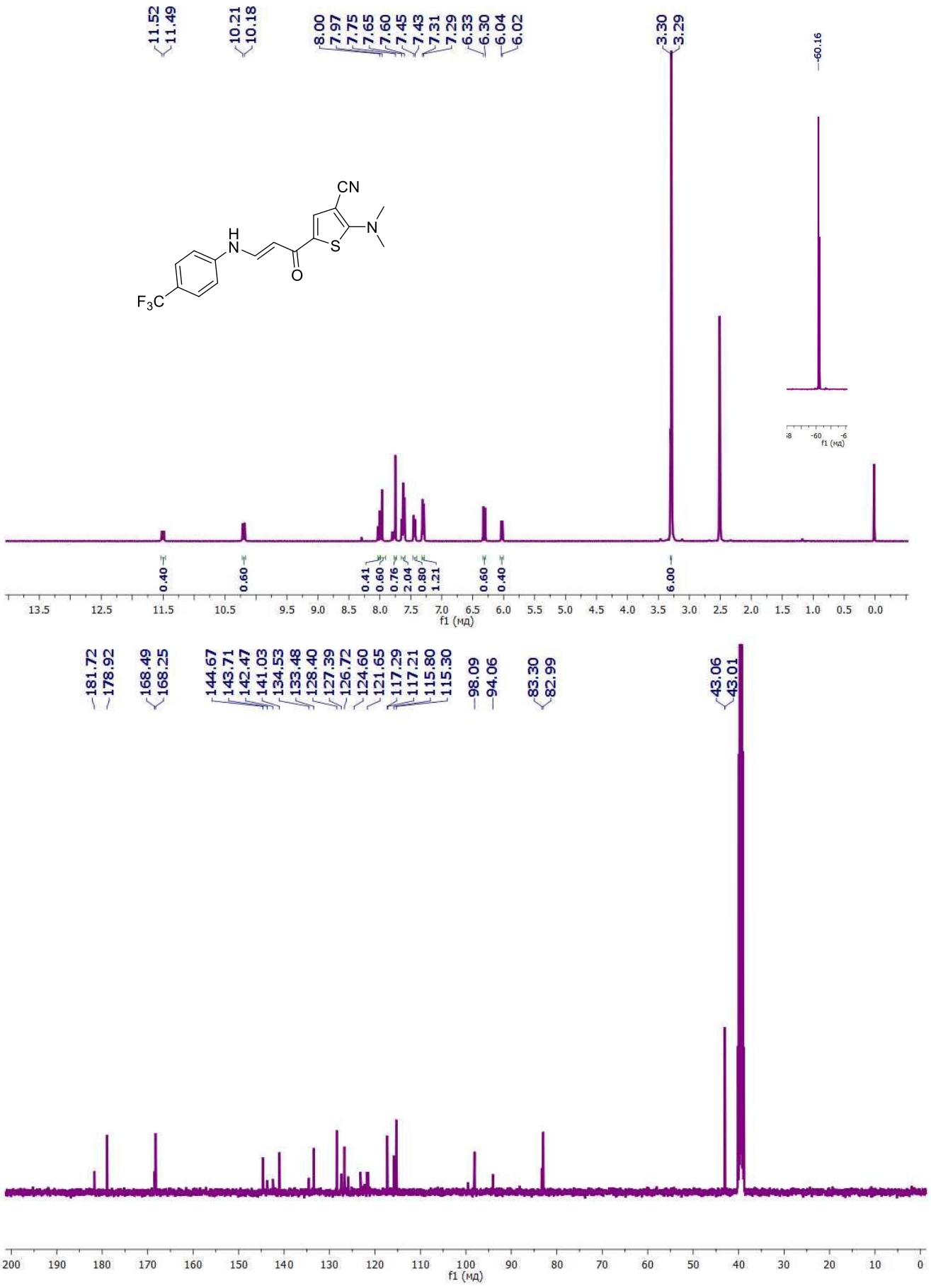


Fig. S18. ^{1}H NMR (400 MHz, DMSO-d_6, TMS) and ^{13}C NMR (100 MHz, DMSO-d_6) spectra of 2-(dimethylamino)-5-(3-((4-(trifluoromethyl)phenyl)amino)acryloyl)thiophene-3-carbonitrile **2k.**

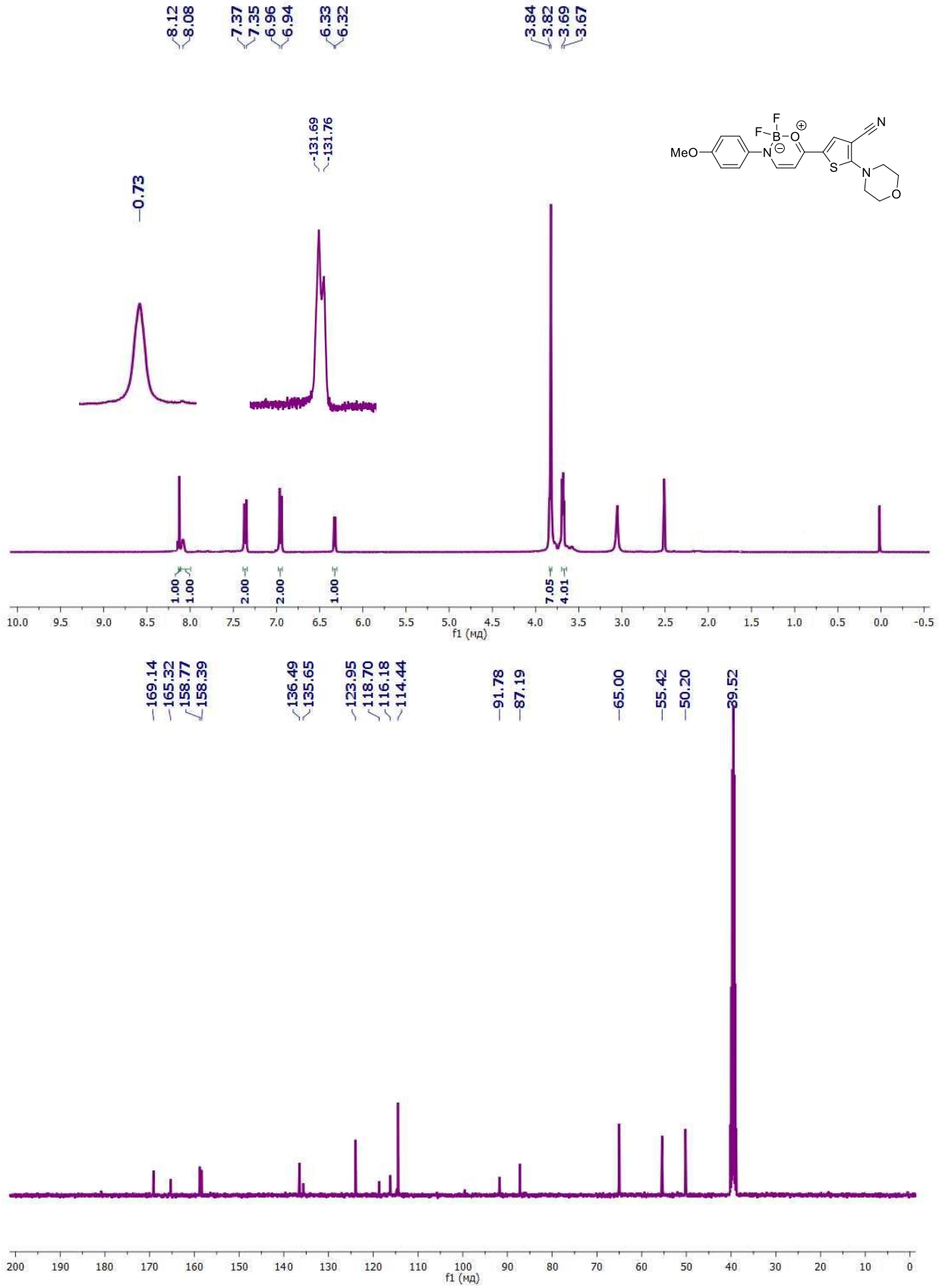


Fig. S19. ^{1}H NMR (400 MHz, DMSO-d_6, TMS), ^{13}C NMR APT (100 MHz, DMSO-d_6), ^{19}F NMR (376.5 MHz, $CDCl_3$) and ^{11}B NMR (128.4 MHz, $CDCl_3$) spectra 5-(2,2-difluoro-3-(4-methoxyphenyl)-2,3-dihydro-1λ^3,3,2λ^4-oxazaborinin-6-yl)-2-morpholinothiophene-3-carbonitrile **1a.**

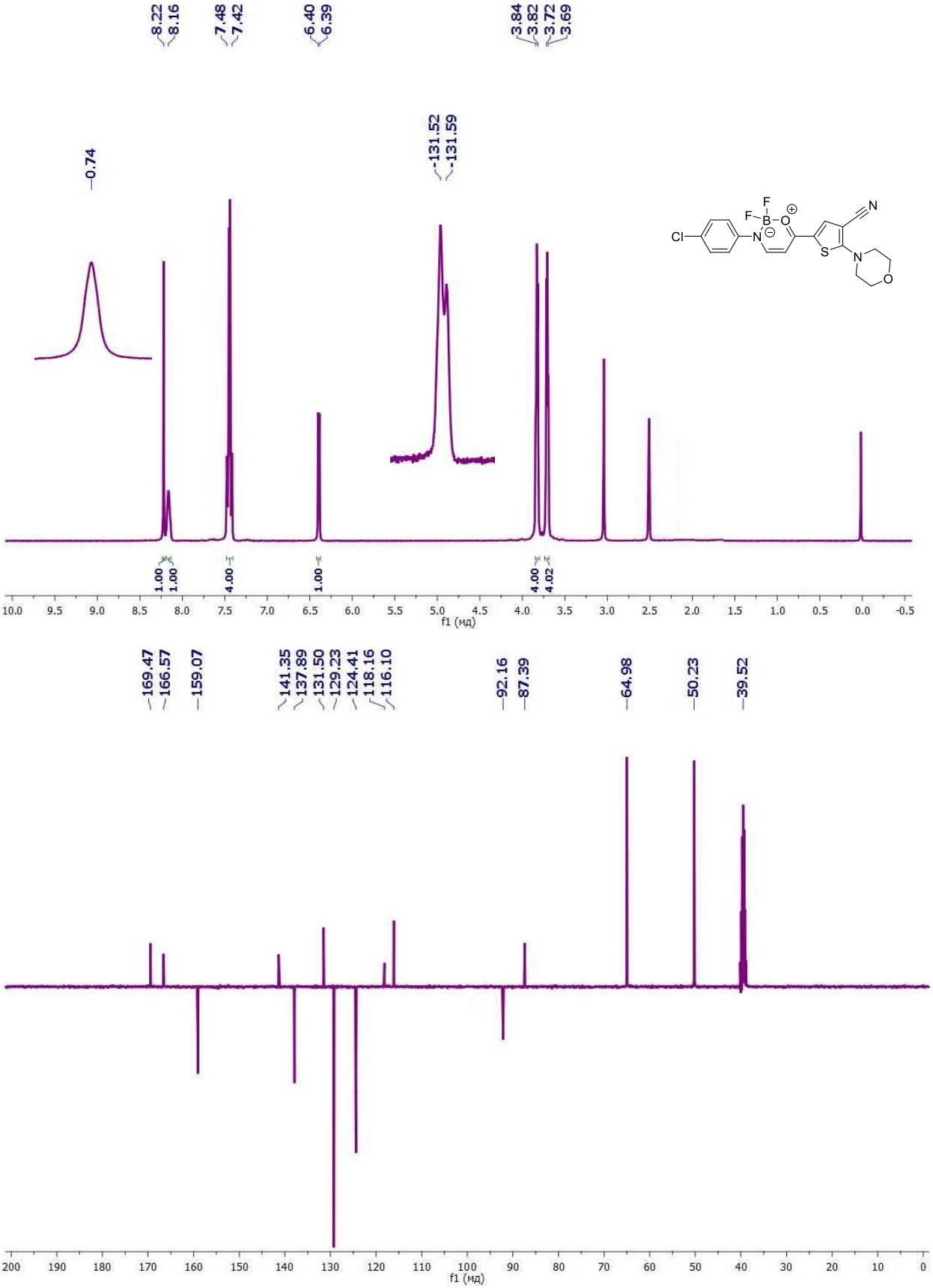


Fig. S20. ^{1}H NMR (400 MHz, DMSO-d_6, TMS), ^{13}C NMR APT (100 MHz, DMSO-d_6), ^{19}F NMR (376.5 MHz, $CDCl_3$) and ^{11}B NMR (128.4 MHz, $CDCl_3$) spectra **5**-(3-(4-chlorophenyl)-2,2-difluoro-2,3-dihydro-1λ^3,3,2λ^4-oxazaborinin-6-yl)-2-morpholinothiophene-3-carbonitrile **1b.**

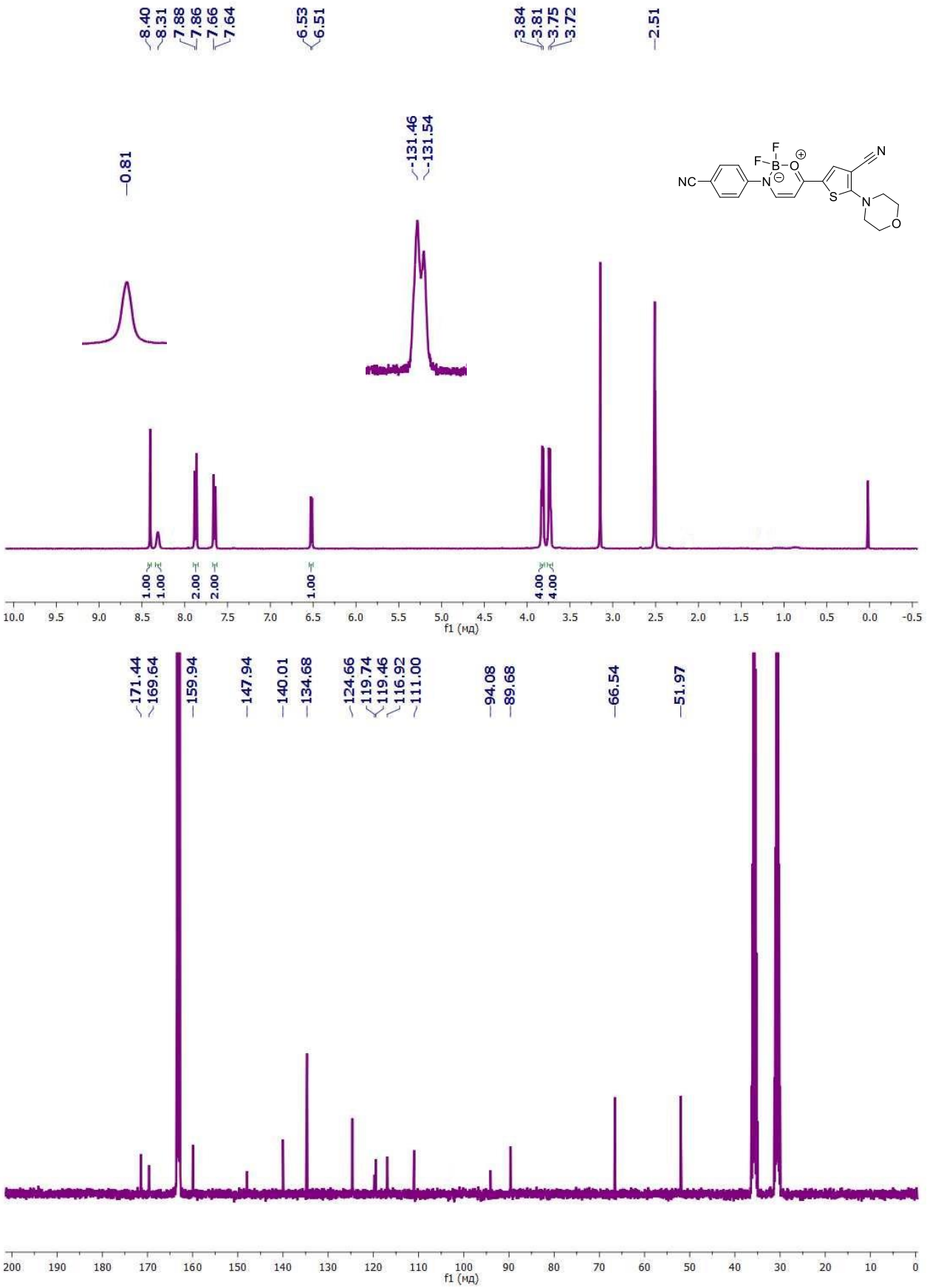


Fig. S21. ^{1}H NMR (400 MHz, DMSO-d_6, TMS), ^{13}C NMR APT (100 MHz, DMSO-d_6), ^{19}F NMR (376.5 MHz, $CDCl_3$) and ^{11}B NMR (128.4 MHz, $CDCl_3$) spectra 5-(3-(4-cyanophenyl)-2,2-difluoro-2,3-dihydro-1λ^3,3,2λ^4-oxazaborinin-6-yl)-2-morpholinothiophene-3-carbonitrile **1c.**

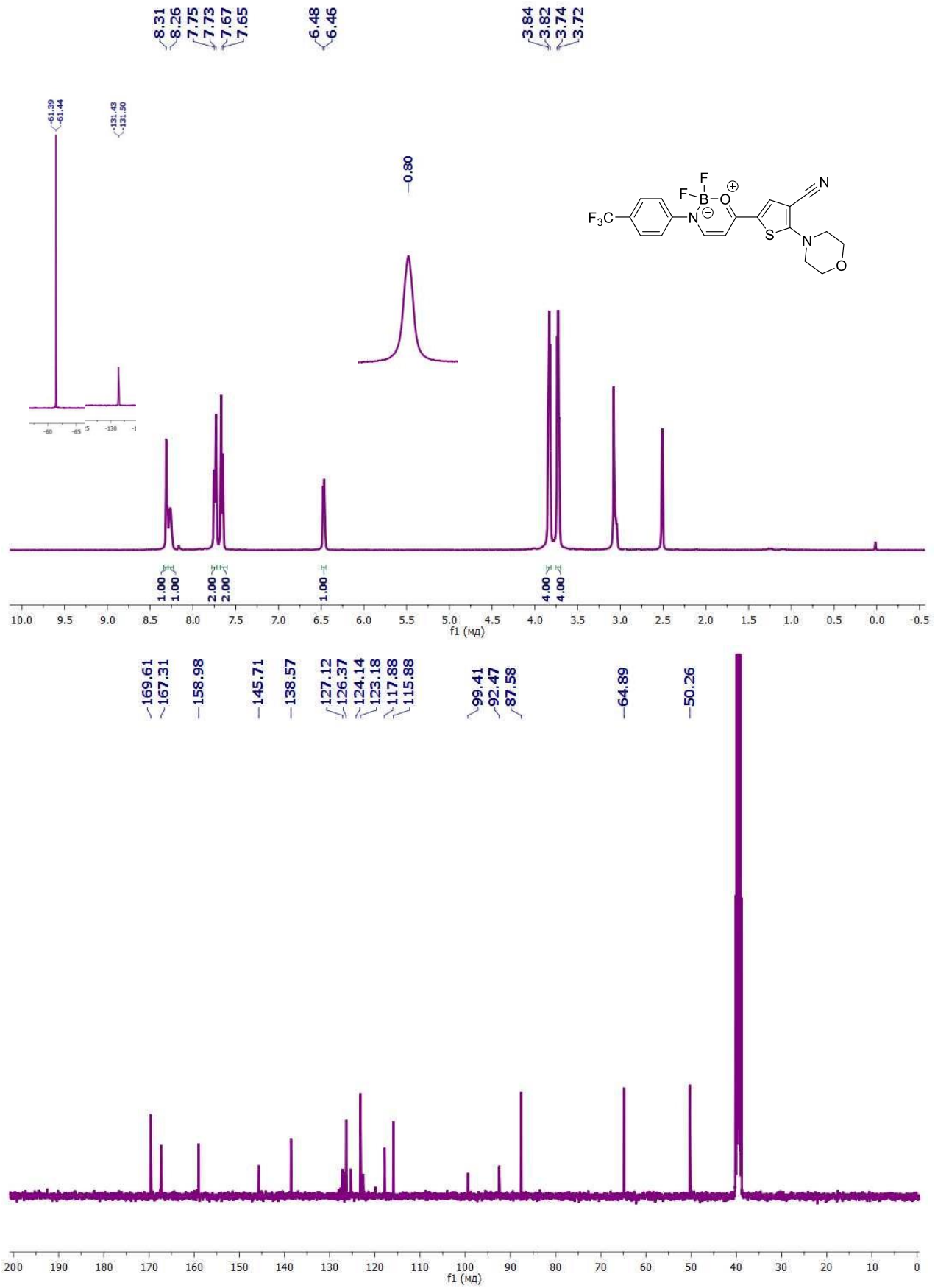


Fig. S22. ^{1}H NMR (400 MHz, DMSO-d_6, TMS), ^{13}C NMR APT (100 MHz, DMSO-d_6), ^{19}F NMR (376.5 MHz, $CDCl_3$) and ^{11}B NMR (128.4 MHz, $CDCl_3$) spectra 5-(2,2-difluoro-3-(4-(trifluoromethyl)phenyl)-2,3-dihydro-1λ^3,3,2λ^4-oxazaborinin-6-yl)-2-morpholinothiophene-3-carbonitrile **1d.**

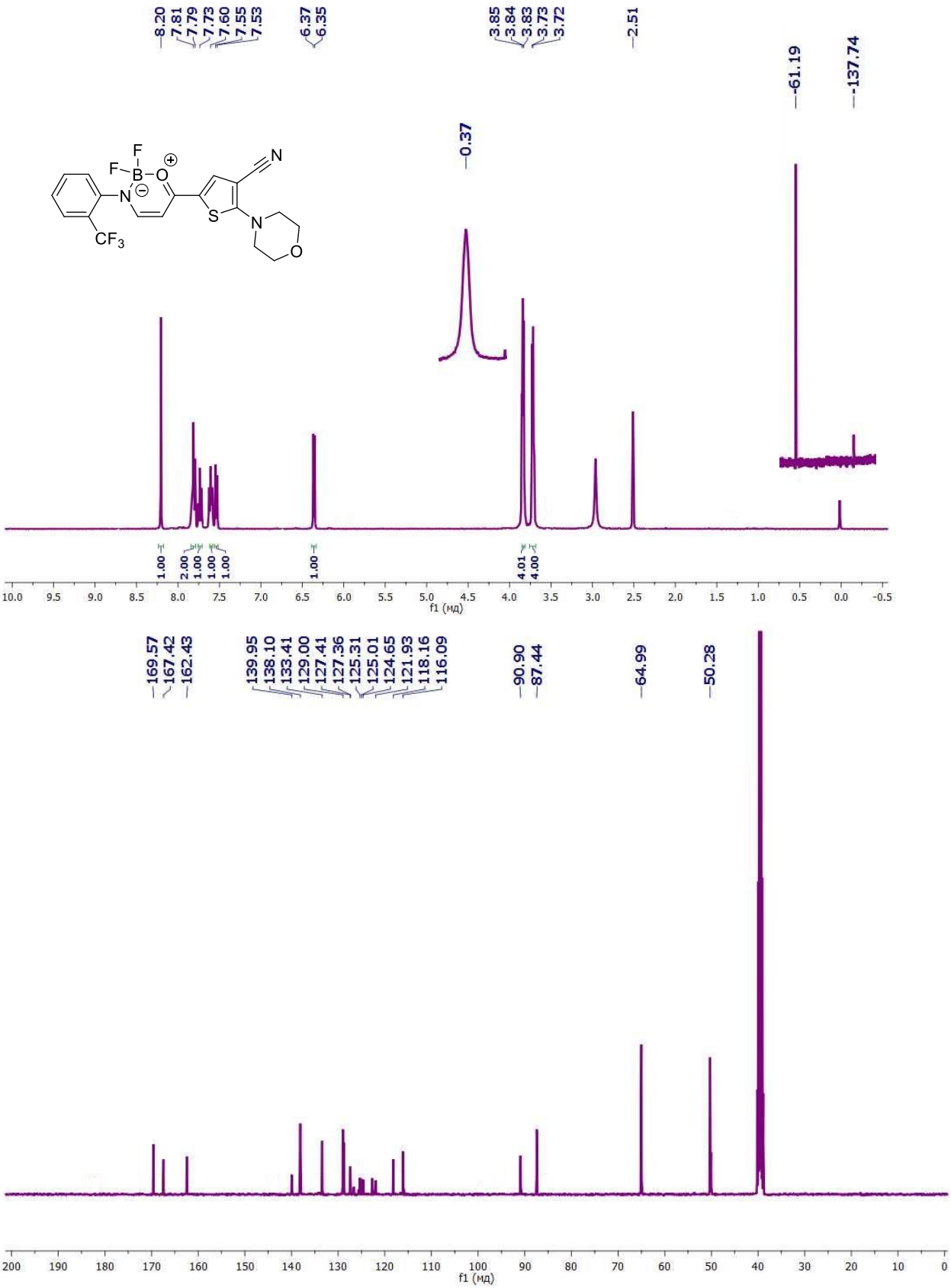


Fig. S23. ^{1}H NMR (400 MHz, DMSO-d_6, TMS), ^{13}C NMR APT (100 MHz, DMSO-d_6), ^{19}F NMR (376.5 MHz, $CDCl_3$) and ^{11}B NMR (128.4 MHz, $CDCl_3$) spectra 5-(2,2-difluoro-3-(2-(trifluoromethyl)phenyl)-2,3-dihydro-1λ^3,3,2λ^4-oxazaborinin-6-yl)-2-morpholinothiophene-3-carbonitrile **1e.**

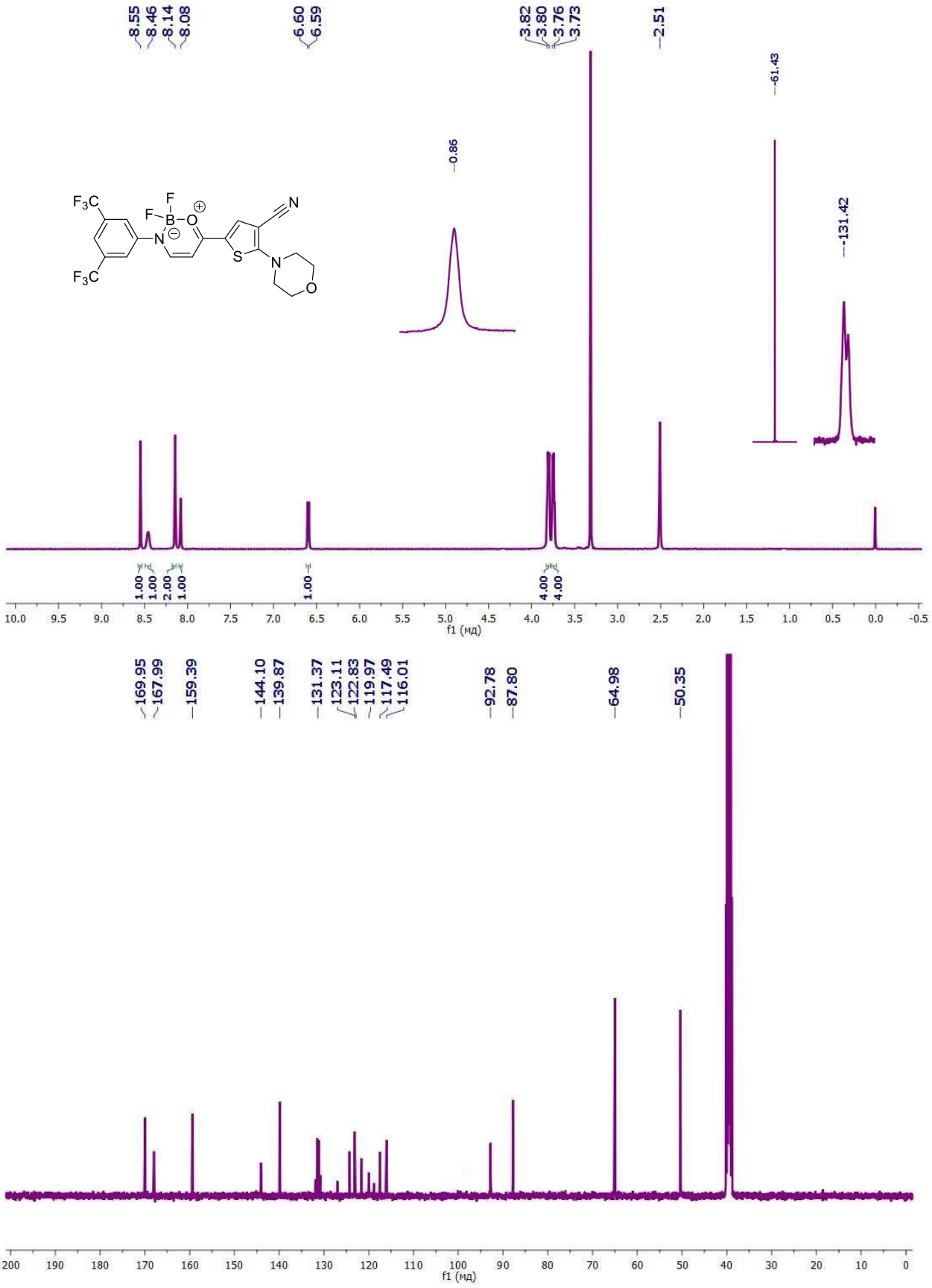


Fig. S24. ^{1}H NMR (400 MHz, DMSO-d_6, TMS), ^{13}C NMR APT (100 MHz, DMSO-d_6), ^{19}F NMR (376.5 MHz, $CDCl_3$) and ^{11}B NMR (128.4 MHz, $CDCl_3$) spectra 5-(3-(3,5-bis(trifluoromethyl)phenyl)-2,2-difluoro-2,3-dihydro-1λ^3,3,2λ^4-oxazaborinin-6-yl)-2-morpholinothiophene-3-carbonitrile **1f.**

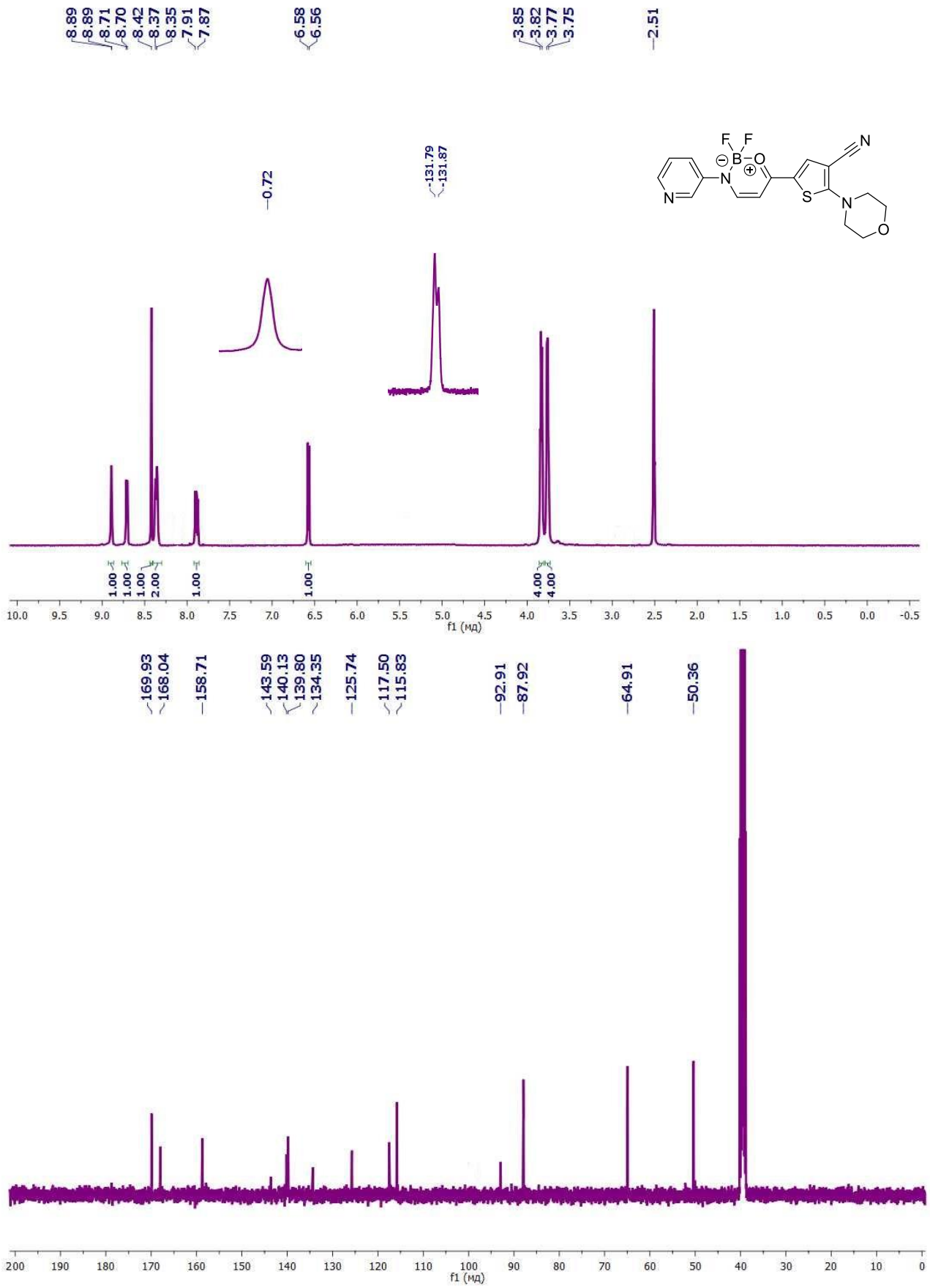


Fig. S25. ^{1}H NMR (400 MHz, DMSO-d_6, TMS), ^{13}C NMR APT (100 MHz, DMSO-d_6), ^{19}F NMR (376.5 MHz, $CDCl_3$) and ^{11}B NMR (128.4 MHz, $CDCl_3$) spectra 5-(2,2-difluoro-3-(pyridin-3-yl)-2,3-dihydro-1λ^3,3,2λ^4-oxazaborinin-6-yl)-2-morpholinothiophene-3-carbonitrile **1g.**

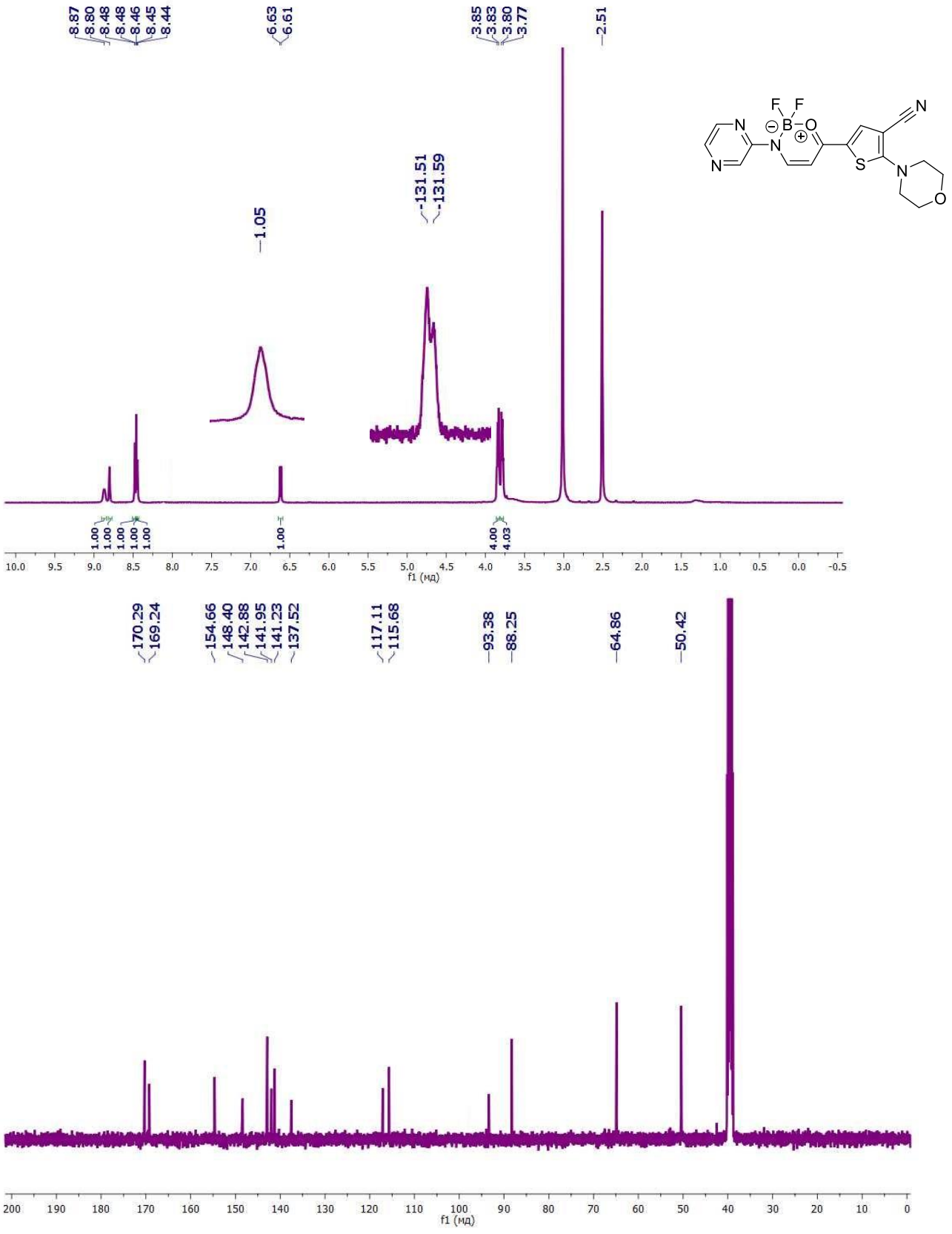


Fig. S26. ^{1}H NMR (400 MHz, DMSO-d_6, TMS), ^{13}C NMR APT (100 MHz, DMSO-d_6), ^{19}F NMR (376.5 MHz, $CDCl_3$) and ^{11}B NMR (128.4 MHz, $CDCl_3$) spectra 5-(2,2-difluoro-3-(pyrazin-2-yl)-2,3-dihydro-1λ^3,3,2λ^4-oxazaborinin-6-yl)-2-morpholinothiophene-3-carbonitrile **1h.**

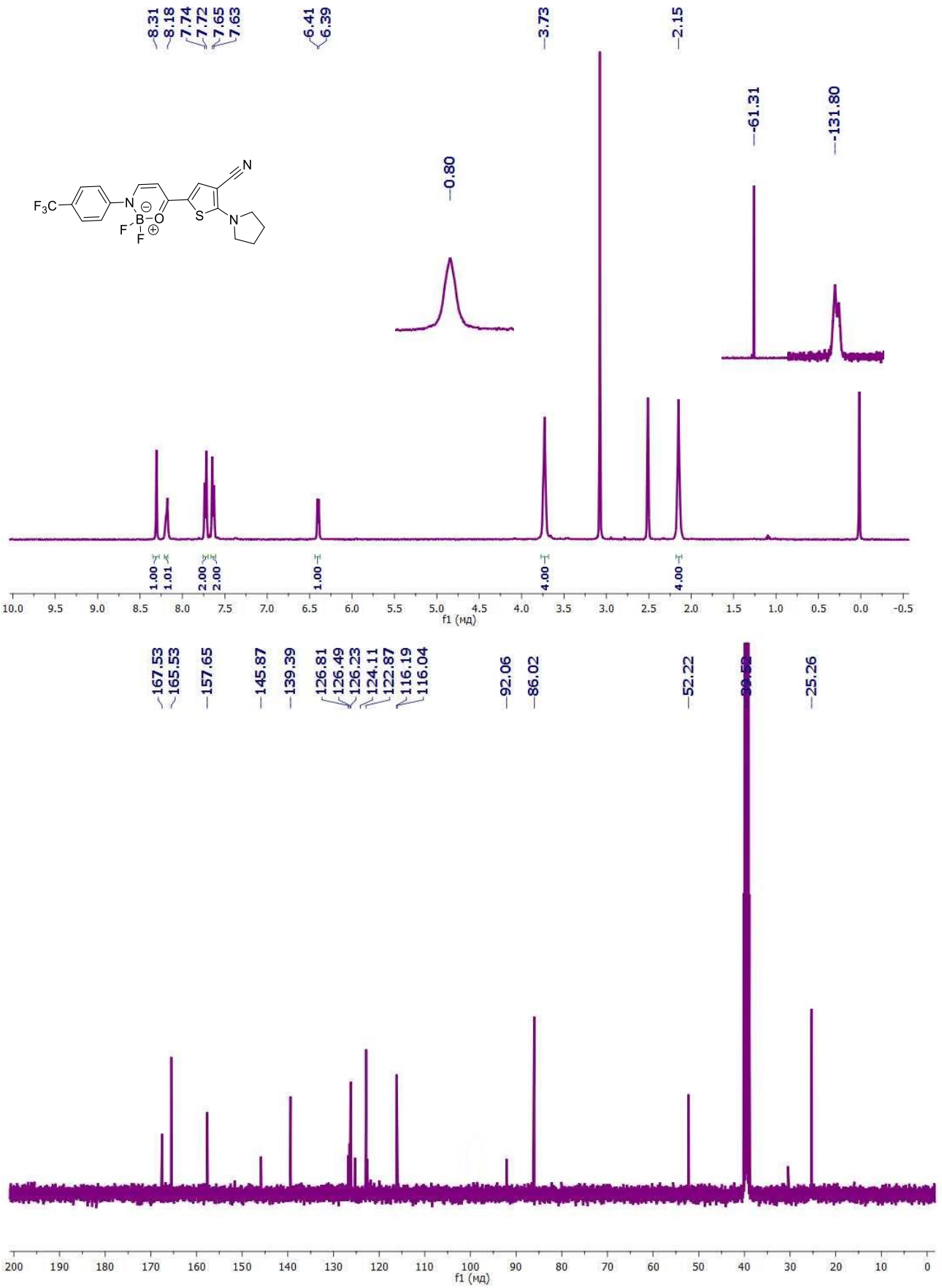


Fig. S27. ^{1}H NMR (400 MHz, DMSO-d_6, TMS), ^{13}C NMR APT (100 MHz, DMSO-d_6), ^{19}F NMR (376.5 MHz, $CDCl_3$) and ^{11}B NMR (128.4 MHz, $CDCl_3$) spectra 5-(2,2-difluoro-3-(4-(trifluoromethyl)phenyl)-2,3-dihydro-1λ^3,3,2λ^4-oxazaborinin-6-yl)-2-(pyrrolidin-1-yl)thiophene-3-carbonitrile **1i.**

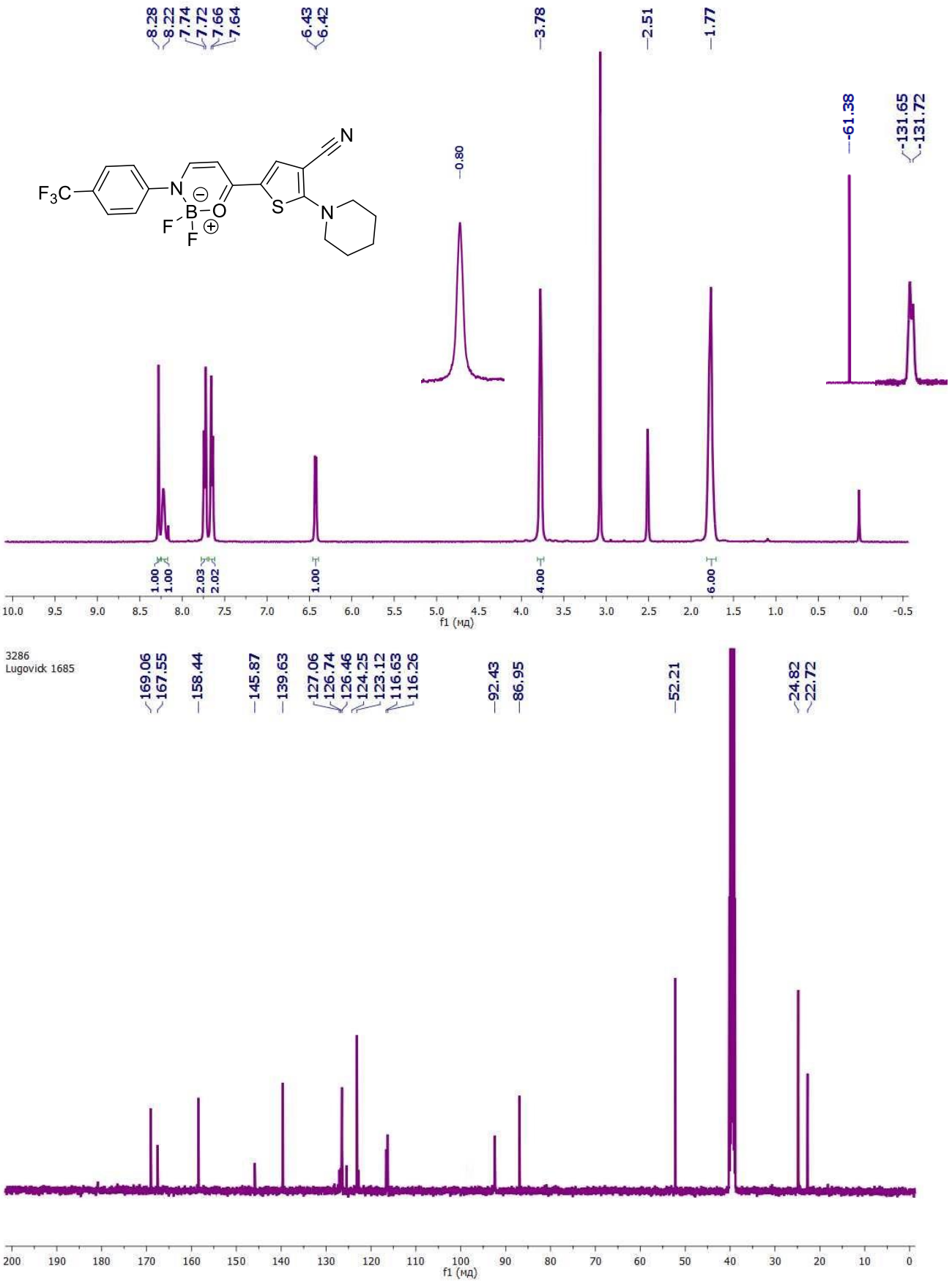


Fig. S28. ^{1}H NMR (400 MHz, DMSO-d_6, TMS), ^{13}C NMR APT (100 MHz, DMSO-d_6), ^{19}F NMR (376.5 MHz, $CDCl_3$) and ^{11}B NMR (128.4 MHz, $CDCl_3$) spectra 5-(2,2-difluoro-3-(4-(trifluoromethyl)phenyl)-2,3-dihydro-1λ^3,3,2λ^4-oxazaborinin-6-yl)-2-(piperidin-1-yl)thiophene-3-carbonitrile **1j.**

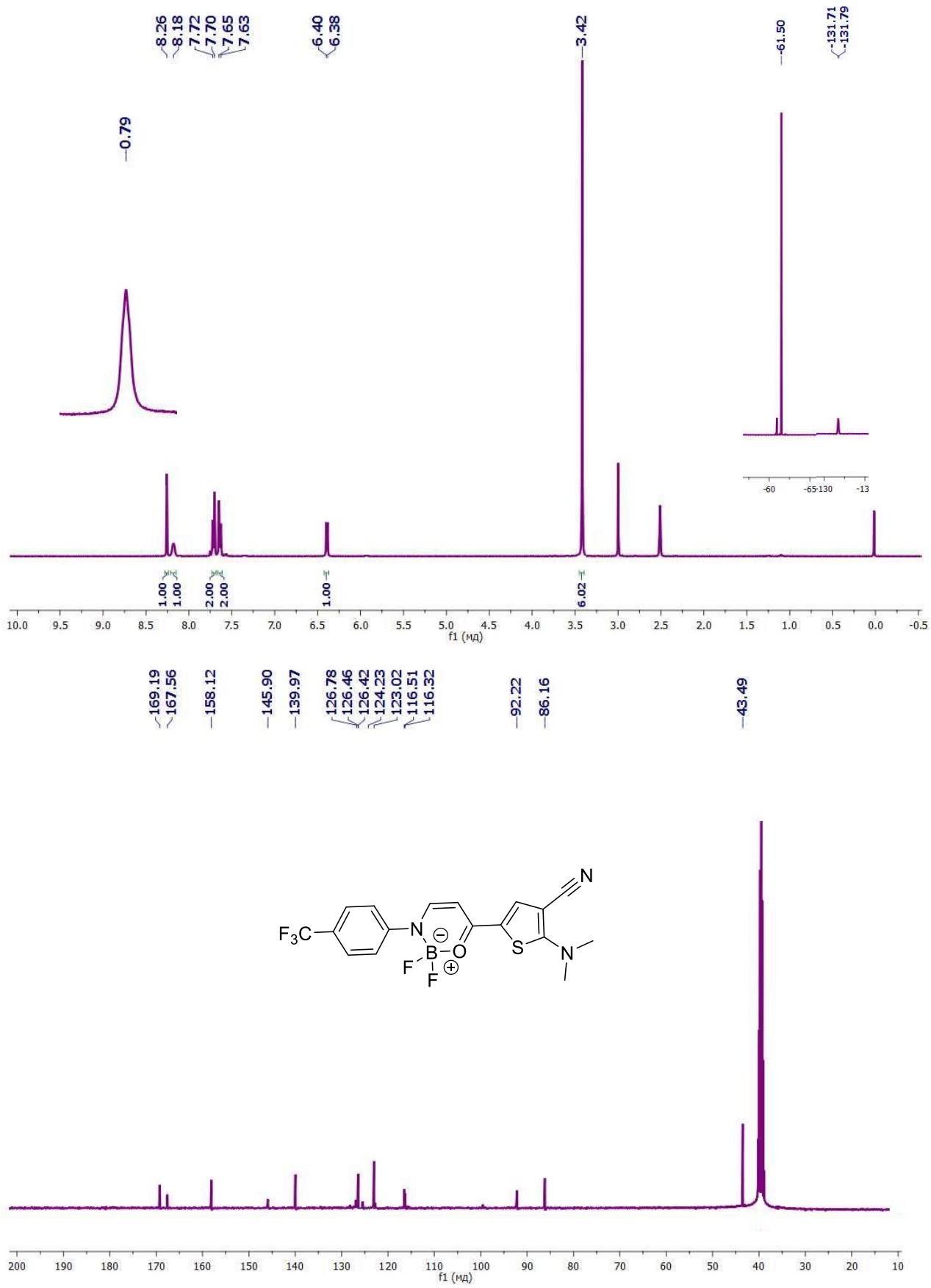


Fig. 29. ^{1}H NMR (400 MHz, DMSO-d_6, TMS), ^{13}C NMR APT (100 MHz, DMSO-d_6), ^{19}F NMR (376.5 MHz, $CDCl_3$) and ^{11}B NMR (128.4 MHz, $CDCl_3$) spectra 5-(2,2-difluoro-3-(4-(trifluoromethyl)phenyl)-2,3-dihydro-1λ^{3},3,2λ^{4}l4-oxazaborinin-6-yl)-2-(dimethylamino)thiophene-3-carbonitrile **1k.**

3. XRD crystal structures of complex 1j

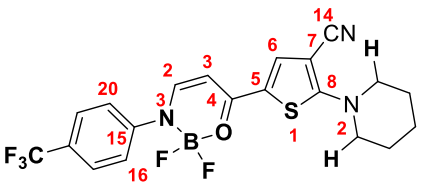
XRD data were obtained on an "Xcalibur 3" (*Oxford-Diffraction Ltd, UK*) diffractometer using a standard procedure (MoK-irradiation, graphite monochromator, ω-scanning with step 1°, T= 295(2) K The single crystal (red prism, 0.41×0.33×0.22) of compound $C_{20}H_{17}BF_5N_3OS$ was used for X-ray analysis. The analysis was performed at 295(2) K on standard procedure using graphite monochromated MoK-irradiation (λ= 0.71073 Å) and ω-scanning with step 1°. An empirical absorption correction was applied (μ = 0.224 mm^{-1}).

The crystal is monoclinic, space group $P2_1/c$ with a = 17.347(2), b = 8.8962(15), c = 14.148(2) Å, β = 112.523(14)°, V = 2016.8(5) $Å^3$, Z = 4. On the angles 2.77 < θ < 28.29° 19162 reflections measured, 4817 (R_{int} = 0.0611), 2140 reflections with I>2σ(I). Completeness to θ = 28.29° is 96.2 % %. The structure was solved by ShelXS program and refined with the ShelXL[5] refinement package using Least Squares minimisation. All non-hydrogen atoms were refined anisotropically, the positions of the hydrogen atoms at C-H bonds were calculated as a riding model in isotropic approximation with distance C_{sp2}-H= 0.93 Å.

Goodness to fit at F^2 1.000; final R values [I>2σ(I)]: R_1 = 0.0500, wR_2 = 0.0888; R value (all reflections): R_1 = 0.2070, wR_2 = 0.1009. Largest difference peak and hole were 0.245 and -0.235 ēÅ^{-3}.

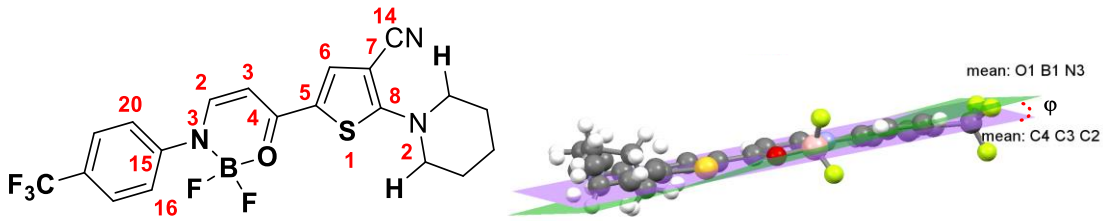
CCDC 1827433 for **1j** can be obtained free of charge from the Cambridge Crystallographic Data Centre via link www.ccdc.cam.ac.uk/data_request/cif.

Table S1. Selected bonds length [Å] for BF_2AATs **1g** and **1h** (XRD data).



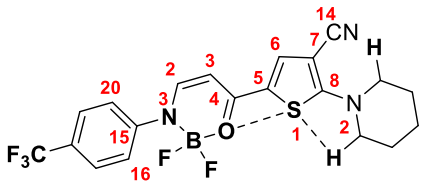
Bond	C15-N3	C8-N2	C7-C14	C2-C3	N3-C2	N3-B1	B1-O1	C4-O1	C16···F4	C16H···F5
Length	1.414	1.340	1.404	1.359	1.307	1.567	1.459	1.297	2.380	2.569

Table S2. Selected bond (ϕ [°]) and torsion (*ϑ* [°]*)* angles for **BF_2 EAT 1j** (XRD data).



Angle	C16H15N9B1	C15N3B1O1	N3B1O1C4	B1O1C4C5	O1C4C5S1	C4C5S1C8	C5S1C8N2	ϕ
°	-11.9	-174.3	-8.3	-173.9	-2.6	0.5	-179.3	5.9

Table S3 Selected noncovalent interactions for for BF_2 AAT **1j** (XRD data).



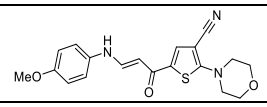
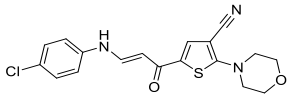
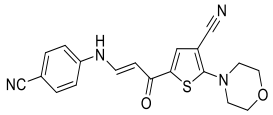
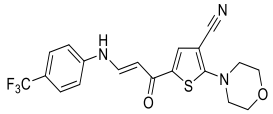
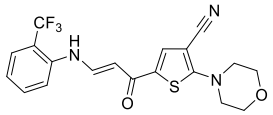
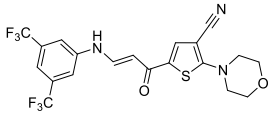
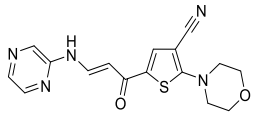
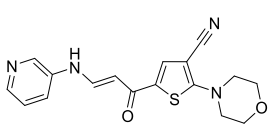
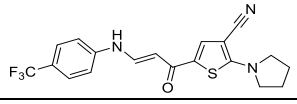
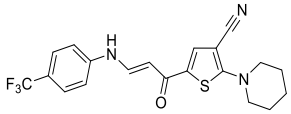
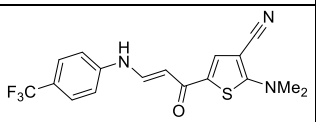
Bond	C16H…F4	C16H…F5	S1…O	S1….H
Length, [Å]	2.380	2.569	2.854	2.414

4. Photophysical investigations

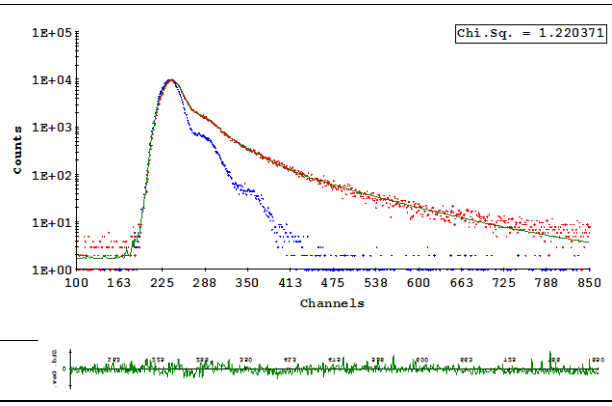
UV-Vis absorption spectra were recorded on a Perkin-Elmer Lambda 35 UV-Vis spectrophotometer (Shelton, CT USA). Fluorescence of the sample solutions was measured using a Hitachi F-7000 spectrophotometer (Tokyo, Japan). The absorption and emission spectra were recorded in Toluene, Dioxane, CH_2Cl_2, $CHCl_3$, THF, EtOH, EtOAc, Acetone, MeCN, DMF, DMSO using 10.00 mm quartz cells. The excitation wavelength was at the absorption maxima. Atmospheric oxygen contained in solutions was not removed. Concentration of the compounds in the solution was 5.0×10^{-5} M and 5.0×10^{-6} M for absorption and fluorescence measurements, respectively. The relative fluorescence quantum yields (Φ_F) were determined using quinine sulfate (5×10^{-5} M) in 0.1 M H_2SO_4 as a standard ($\Phi_F = 0.546$).

Absolute quantum yield for solid state and time-resolution study were recorded on Horiba FlouroMax 4 Spectrofluorometer (Kyoto, Japan) with Quanta-ϕ integrating sphere using FluorEssence 3.5 Software.

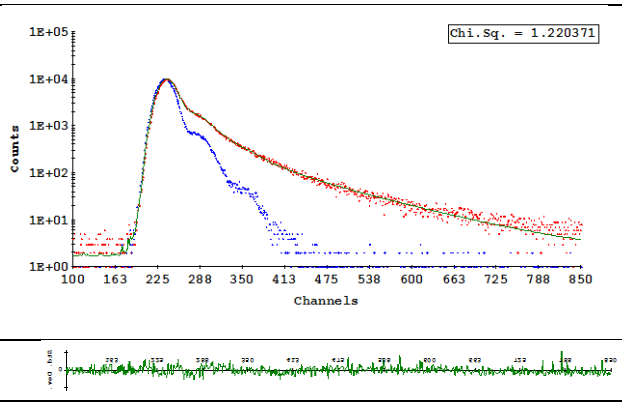
Table S4. Photophysical properties of 1,3-thiazoles **3a-i** and **4a-d** in 1,4-dioxane

Entry	Compound		UV-Vis		FL		SS, nm/cm^{-1}
			λ_{abs}, nm	ε_{max}, M^{-1}.cm^{-1}	λ_{em}, nm	Φ_F [a]	
1		**2a**	408 296 252	39437 6793 12433	464	0.82	56/2958
2		**2b**	405 293 255	44841 6740 11415	437	0.35	32/1808
3		**2c**	411 281	59277 11098	441	0.56	30/1655
4		**2d**	406 291	53046 6502	440	0.51	34/1903
5		**2e**	401 296 256	50741 7741 10352	433	0.30	32/1843
6		**2f**	402 295 259	51706 7091 9468	438 512 (sh)	0.39	36/2045
7		**2g**	404 293 252	44325 7403 10557	444 519	0.33	40/2230
8		**2h**	399 270	39146 30913	427	0.47	28/1643
9		**2i**	413 289 257	52325 8235 8362	444 518 (sh)	0.55	31/1691
10		**2j**	410 294 259	53060 7278 9348	443	0.54	33/1817
11		**2k**	397 290 258	52896 7764 9217	435	0.37	38/2200

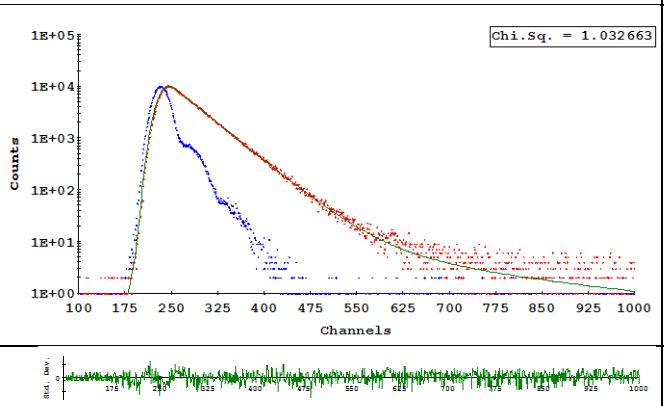
1a



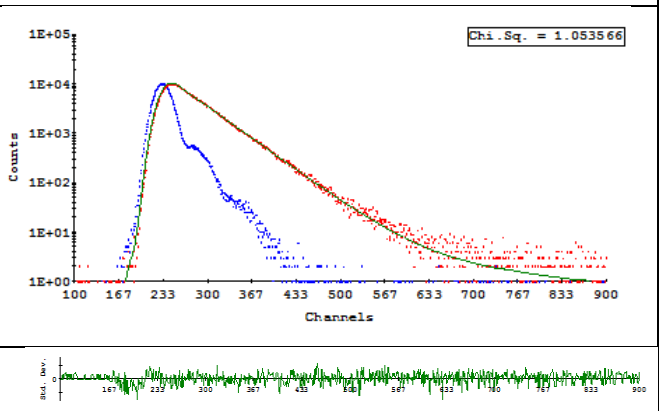
1b



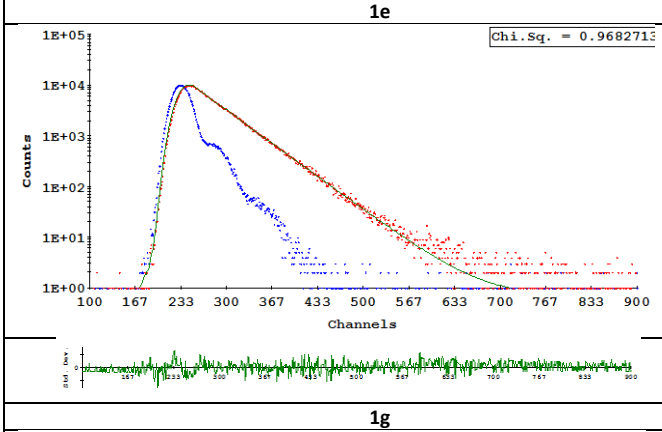
1c



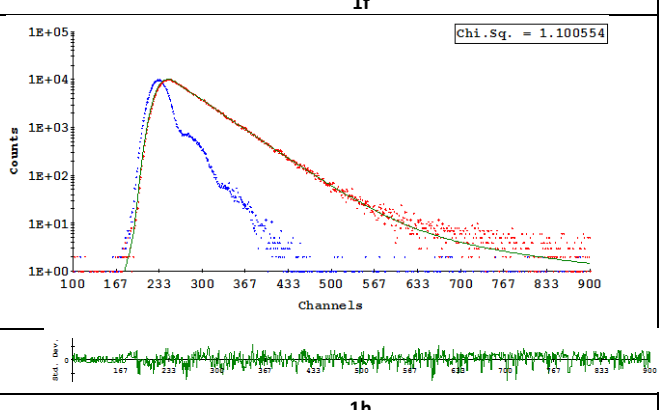
1d



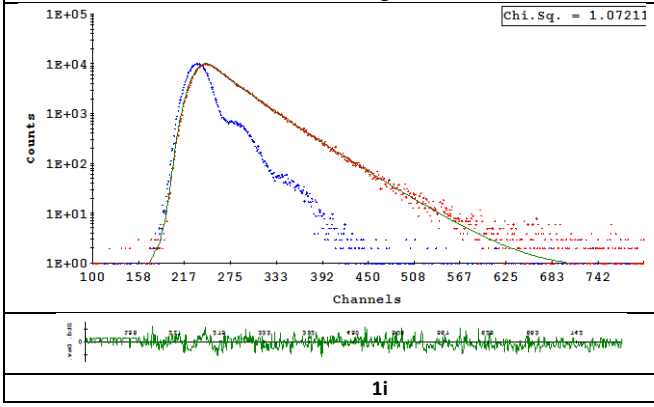
1e



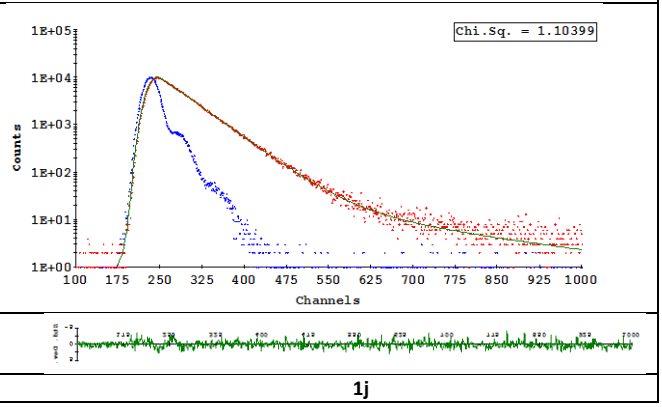
1f



1g



1h



1i

1j

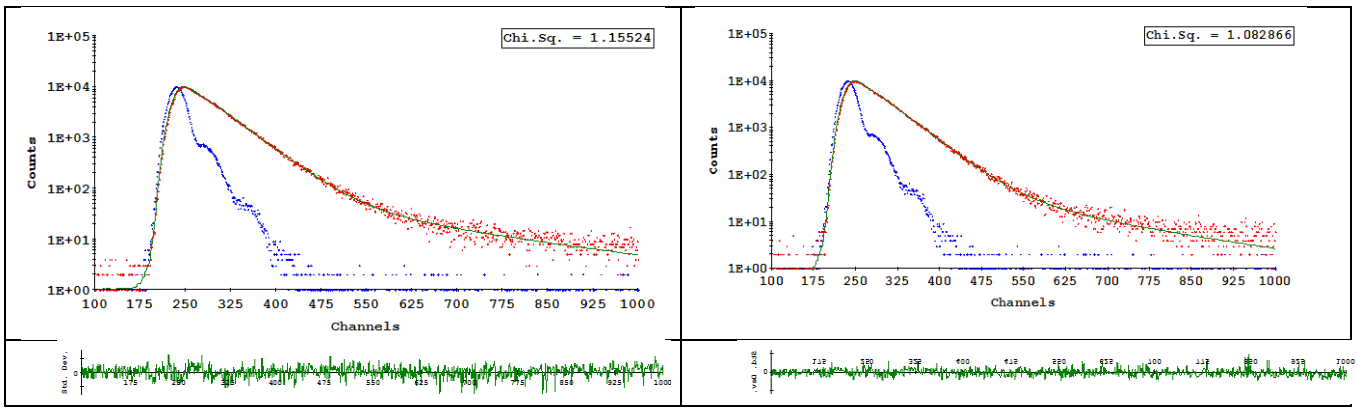
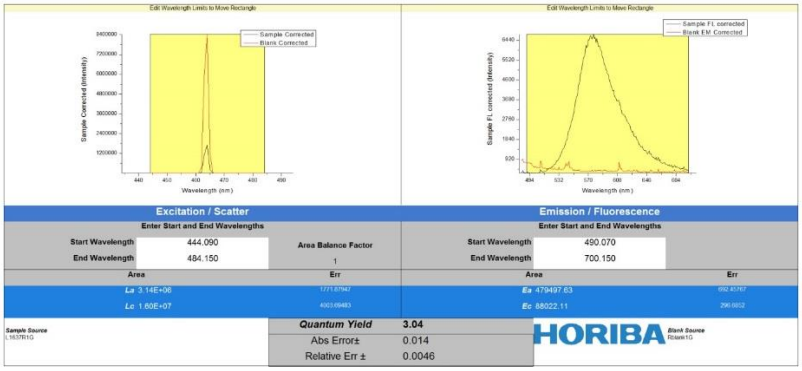


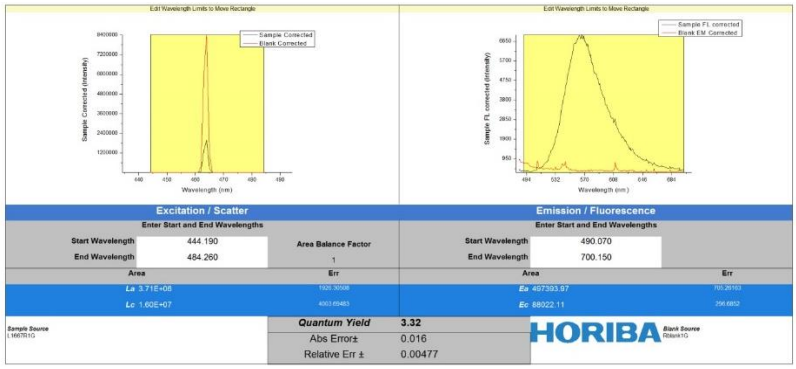
Fig. S30. Fluorescence decay curves of BF_2AATs **1a-j** in 1,4-dioxane solution.

Quantum yield for solid samples

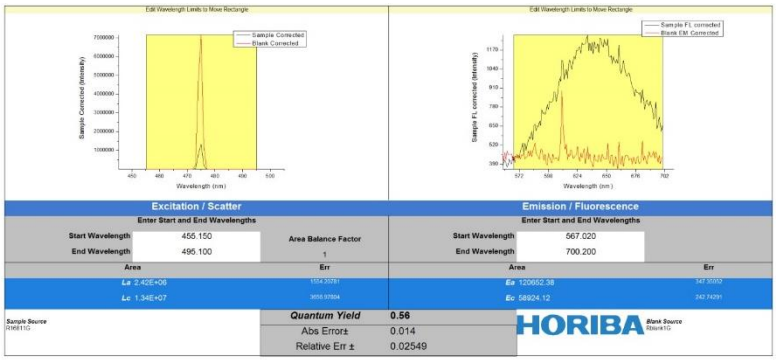
1d



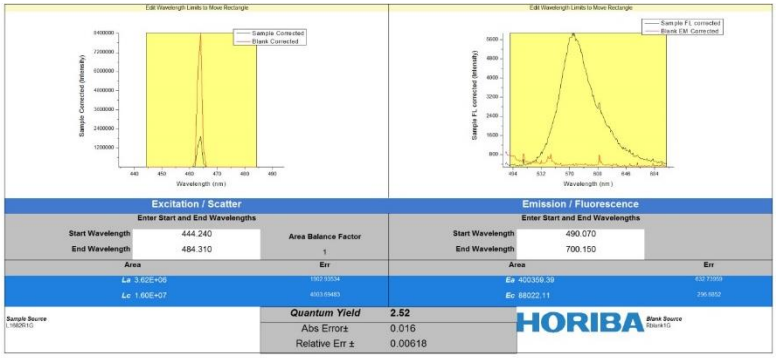
1f



1i



1j



1k

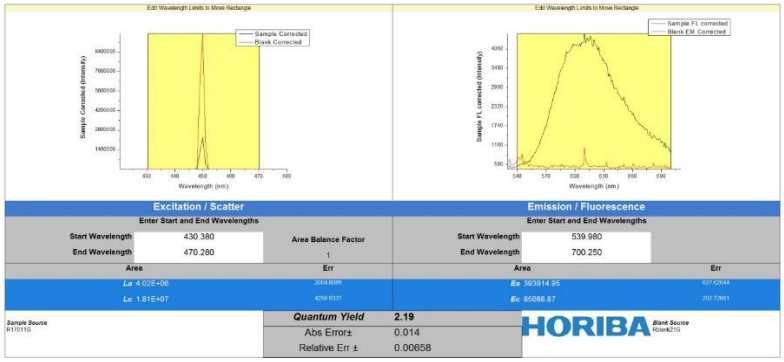


Fig. S31. Experimental data for the detection of absolute quantum yields for compounds **1d**, **f**, **i**, **j**, **k** in solid state

5. Quantum Mechanical Calculations

The ground state molecular geometry of the compounds under investigation was fully optimized at density functional theory (DFT) level, both in vacuo and in solvents (1,4-dioxane; for molecule **1a** additional solvents were used, viz., DCM, EtOH, Acetone, MeCN, and DMSO) the same solvents used for optimisations). We compared the results obtained by employing different functionals and different basis sets with the experimental data. In particular, we chose hybrid (viz. B3LYP[6], and M06−2X[7]), long-range corrected (viz. CAM−B3LYP[8] and ωB97X[9]), coupled with the 6−311++G** basis set. The D3 version of Grimme's semi-empirical dispersion with Becke-Johnson damping GD3B[10] was also included in the case of the B3LYP, CAM-B3LYP, and ωB97X functionals. Solvent effects were taken into account via the implicit polarizable continuum model in its integral equation formalism (IEF−PCM).[11] For geometry optimizations and frequency calculations, the PCM molecular cavity was built according to the universal force field (UFF)[12] radii within the value used in the last implementation of the PCM (based on a continuum surface charge formalism). For topological analysis and the evaluation of energetics, SMD parameterization was employed.[13] The standard values for dielectric constants and refractive indexes were always assumed. The vibrational frequencies and thermochemicals were computed in harmonic approximation at T = 298.15 K and p = 1 atm, and no imaginary frequencies were found.

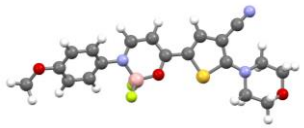
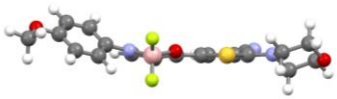
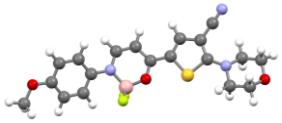
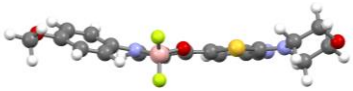
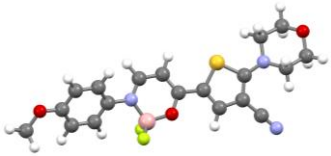
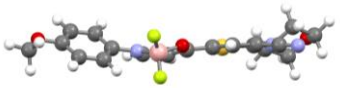
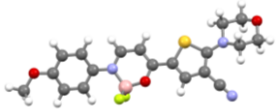
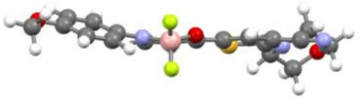
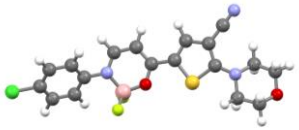
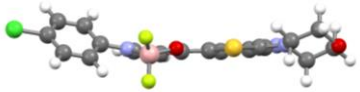
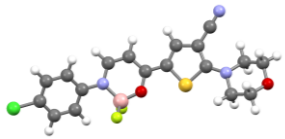
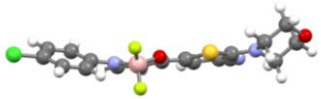
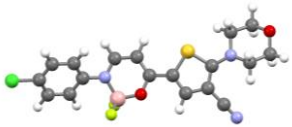
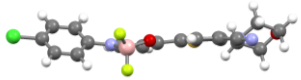
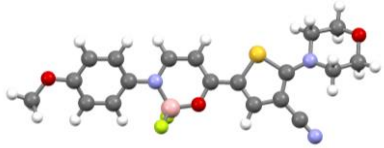
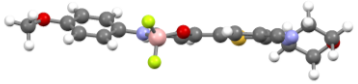
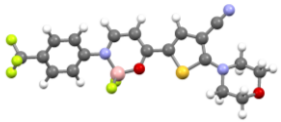
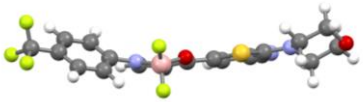
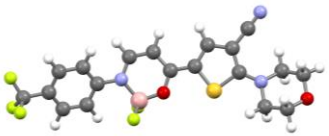
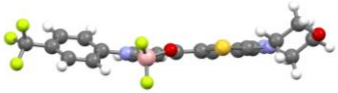
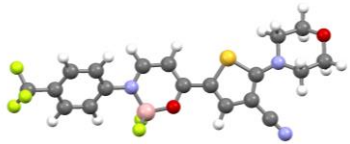
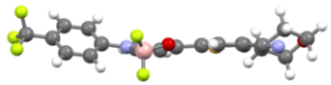
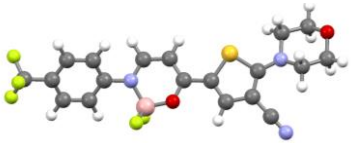
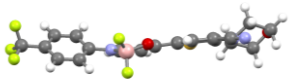
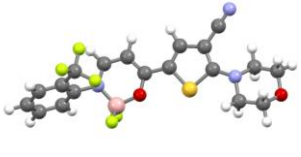
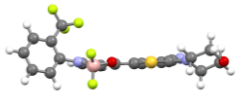
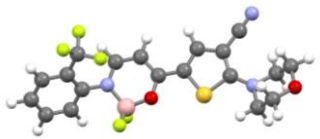
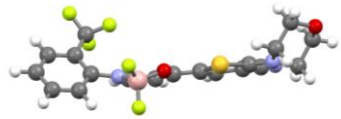
The UV-vis absorption spectra for the equilibrium geometries were calculated at time dependent density functional theory (TD-DFT) level, accounting for $S_0 \rightarrow S_n$ (n = 1 to 5); the energy of the first 5 triplet states was also computed. The nature of the vertical excited electronic state was analysed both in vacuo and in the solvated phase (dioxane, DCM, EtOH, Acetone, MeCN and DMSO). This investigation was performed by employing the long-range corrected functional wB97X-D coupled with the 6−31++G** basis set. In the case of the solvated phase, state-specific (SS)[14] treatment of the solvent effects was considered, both within the non-equilibrium (neq) and equilibrium (eq) solvation regimes[15] of all non-dark electronic transitions were also simulated, including the Duschinsky and Herzberg–Teller effects. The first singlet excited state $S(\pi,\pi^*)$ state geometry was optimized using analytical gradients and the first transitions $S_1 \rightarrow S_0$ of the emission. In this case, SS (both eq and neq) treatment of the solvent effects was considered, and the electronic emission band was simulated by accounting for the vibronic progressions, as was done for the absorption. Solvent effects were taken into account via UFF parameterization of IEF-PCM.

The atomic charge population analysis, electric multiple moments, electronic density, and electrostatic potential were also computed using Mulliken's and the CHelpG procedure[16] for both the ground and the S_1 excited (vertical and relaxed) states.

To investigate the presence and nature of possible intramolecular H-bonding interactions the non-covalent interaction (NCI) index combined with the second derivative of the reduced density gradient along the second main axis of variation were employed.[17] This procedure was applied both to the ground and first singlet excited states.

The integration grid for the electronic density for topological and RDG analysis was set to 150 radial shells and 974 angular points. For the rest of the calculations, the integration grid was set as 99 radial shells and 590 angular points. The convergence criteria of the self-consistent field was set to 10-12 for the RMS change in the density matrix and 10-10 for the maximum change in the density matrix. The Convergence criteria for optimizations were set to 2×10^{-6} a.u. for maximum force, 1×10^{-6} a.u. for RMS force, 6×10^{-6} a.u. for maximum displacement and 4×10^{-6} a.u. for RMS displacement.

All calculations were performed using the GAUSSIAN G09.D01 software package.[18] The location of BCPs and subsequent calculation of SF values were performed using a modified version of the PROAIMV program.[19]

Compd	*GS*		*ES*	
1a/A				
1a/B				
2a/A				
2a/B				
1d/A				
1d/B				
1e/A				

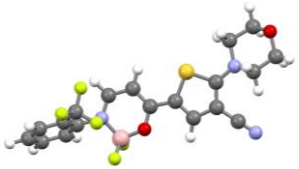
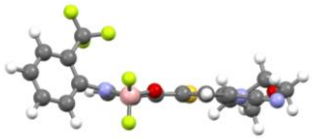
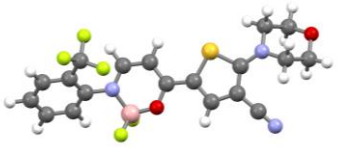
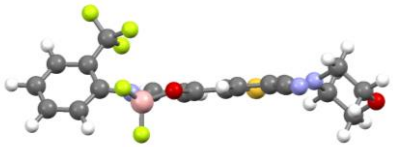
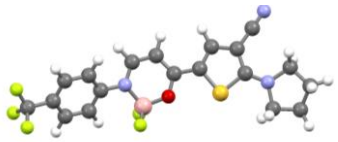
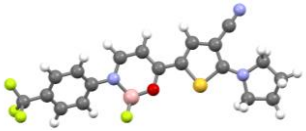
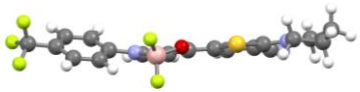
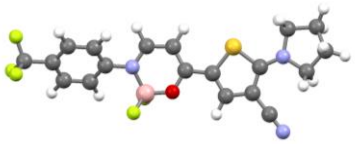
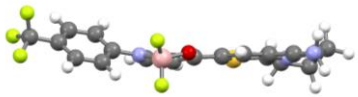
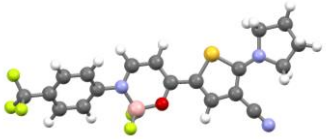
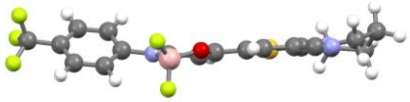
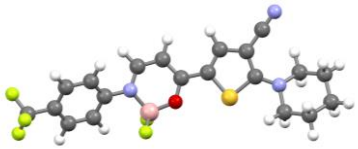
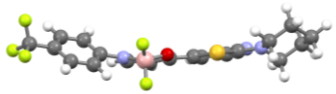
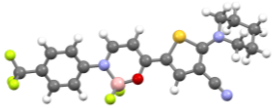
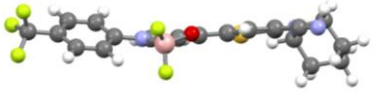
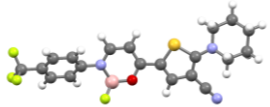
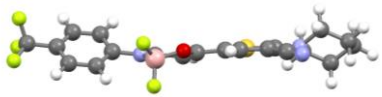
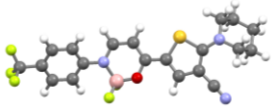
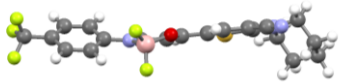
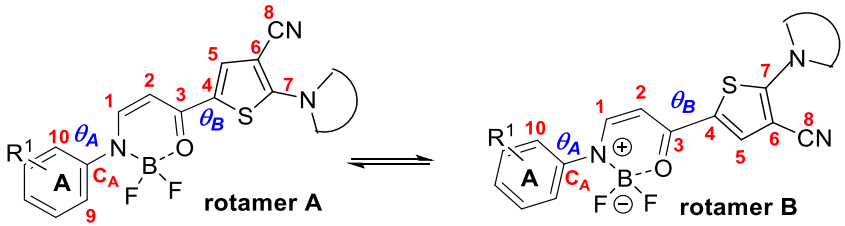
1e/B				
1i/A				
1i/B				
1j/A				
1j/B				

Fig. S32. Optimized geometries of the investigated molecules **1a-e**, **i**, **j** in their ground (*GS*) and exciting (*ES*) state, in 1,4-dioxane, depicted from two orthogonal viewpoints. Level of theory: DFT /IEF-PCM(UFF). Legend of colours: white (H), grey (C), lilac (N), yellow (S), red (O), and green (Cl).

Table S5. Differences in thermochemicals (kJ mol^{-1}) for rotamers A and B computed between as $\Delta X \equiv X(B) - X(A)$, at T = 298.15 K and p = 1.00 atm.

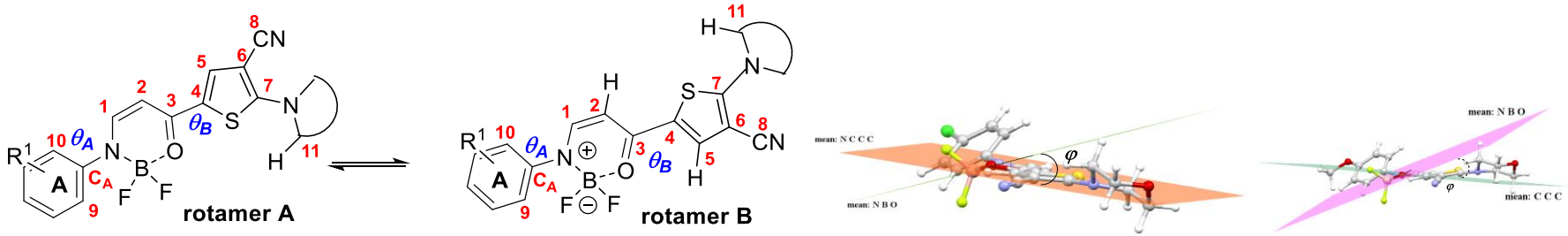
Thermochemicals	ACE	CHL	DMF	DMSO	EtOH	MeCN	THF	TOL
ΔE	4.2	3.8	4.3	4.2	3.5	4.2	4.3	3.9
Δ(E+ZPE)	3.7	3.8	3.8	3.9	3.6	3.9	3.5	2.9
ΔH	4.0	3.8	4.1	4.1	3.6	4.1	4.1	3.3
ΔG	1.4	3.7	0.3	1.9	3.9	1.3	-4.0	0.5

Table S6. Selected bonds lengths (in Å) for the GS (S_0) optimized geometries of compounds **1a-e**, **i**, **j** in 1,4-dioxane



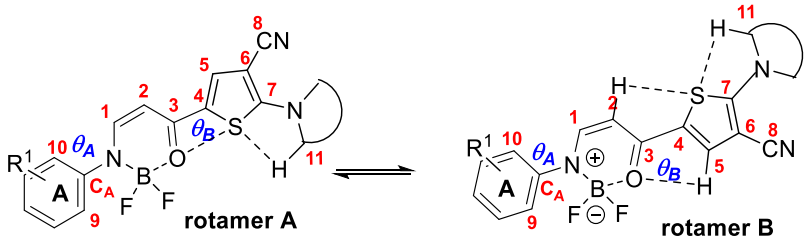
Entry	Comp	C_A-N	N-C_1	C_1-C_2	C_2-C_3	C_3-O	N-B	O-B	C_3-C_4	C_4-C_5	C_5-C_6	C_6-C_7	C_4-S	C_7-S	C_7-N	C_6-C_8
1	**1a/A**	1.426	1.313	1.400	1.382	1.305	1.568	1.483	1.446	1.365	1.417	1.400	1.744	1.739	1.359	1.421
2	**1a/B**	1.426	1.311	1.402	1.382	1.304	1.571	1.480	1.448	1.364	1.418	1.397	1.745	1.742	1.359	1.421
3	**1b/A**	1.423	1.317	1.395	1.387	1.303	1.567	1.484	1.443	1.366	1.415	1.403	1.745	1.740	1.356	1.421
4	**1b/B**	1.423	1.314	1.398	1.386	1.303	1.571	1.480	1.445	1.365	1.417	1.399	1.745	1.743	1.356	1.421
5	**1c/A**	1.418	1.321	1.391	1.391	1.302	1.567	1.485	1.440	1.367	1.414	1.405	1.746	1.740	1.354	1.421
6	**1c/B**	1.419	1.318	1.394	1.390	1.301	1.571	1.481	1.442	1.366	1.415	1.400	1.746	1.743	1.355	1.421
7	**1d/A**	1.421	1.320	1.393	1.389	1.302	1.567	1.485	1.441	1.366	1.414	1.404	1.745	1.740	1.354	1.421
8	**1d/B**	1.421	1.317	1.395	1.388	1.302	1.571	1.481	1.443	1.366	1.416	1.400	1.746	1.742	1.355	1.421
9	**1e/A**	1.429	1.316	1.395	1.388	1.303	1.564	1.485	1.444	1.366	1.415	1.402	1.745	1.739	1.356	1.421
10	**1e/B**	1.429	1.314	1.397	1.387	1.302	1.568	1.481	1.446	1.365	1.417	1.399	1.745	1.742	1.357	1.421
11	**1i/A**	1.419	1.323	1.389	1.394	1.303	1.565	1.485	1.434	1.369	1.411	1.412	1.754	1.742	1.329	1.420
12	**1i/B**	1.420	1.320	1.392	1.392	1.303	1.569	1.480	1.436	1.367	1.413	1.409	1.754	1.744	1.330	1.421
13	**1j/A**	1.420	1.321	1.391	1.391	1.302	1.566	1.485	1.438	1.367	1.412	1.408	1.748	1.743	1.347	1.420
14	**1j/B**	1.420	1.318	1.394	1.390	1.302	1.570	1.481	1.441	1.367	1.414	1.403	1.747	1.745	1.349	1.421

Table S7. Selected bond (φ (°)) and torsional (ϑ (°)) angles for the GS (S_{1v}) optimised geometries compounds **1a-e**, **i**, **j** in 1,4-dioxane of BF_2AATs **1a-e**, **i**, **j** in 1,4-dioxane



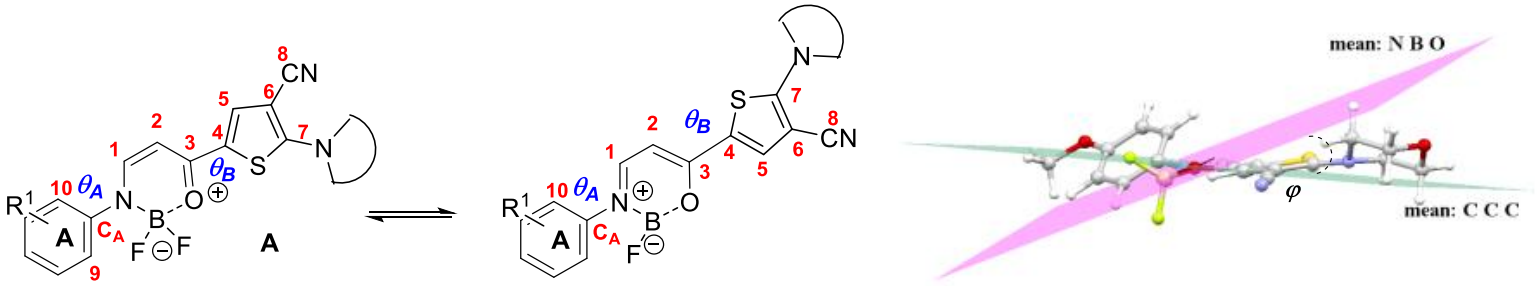
Entry	Comp	ϑ_A	C_ANBO	$NBOC_3$	$NC_1C_2C_3$	BOC_3C_2	BOC_3C_4	ϑ_B	$C_3C_4SC_7$	NBF_1	OBF_2	NBO	φ
1	**1a/A**	-40.17	-158.6	-28.3	-7.8	14.5	-167.4	8.8	-178.4	110.5	108.9	108.2	28.4
2	**1a/B**	-39.2	-158.0	-29.3	-7.7	16.0	-166.1	-170.9	-177.0	110.3	109.2	108.3	28.5
3	**1b/A**	-40.2	-158.7	-28.8	-7.8	15.2	-166.9	3.2	-178.3	110.4	108.9	108.0	28.4
4	**1b/B**	-40.6	-157.9	-30.4	-8.0	16.9	-165.2	-174.2	-176.3	110.2	109.2	108.0	29.2
5	**1c/A**	-38.0	-158.9	-28.8	-7.7	15.0	-167.1	3.2	-178.2	110.4	108.9	107.9	28.5
6	**1c/B**	-38.0	-158.4	-29.5	-7.8	16.0	-166.2	-172.6	-177.1	110.1	109.2	108.0	28.8
7	**1d/A**	-38.8	-158.9	-28.8	-7.7	15.0	-167.1	3.5	-178.2	110.4	108.9	108.1	28.6
8	**1d/B**	-39.4	-158.3	-30.0	-7.9	16.5	-165.7	-174.2	-176.6	110.1	109.0	108.0	29.0
9	**1e/A**	-72.0	-160.4	-26.7	-7.6	13.3	-168.6	4.4	-178.1	110.3	108.9	107.7	27.3
10	**1e/B**	-72.2	-157.9	-29.6	-8.4	14.9	-167.4	-172.7	-177.4	110.2	109.9	107.6	30.2
11	**1i/A**	-38.3	-158.8	-28.5	-7.4	14.7	-167.5	3.2	-178.9	110.4	108.9	108.1	28.2
12	**1i/B**	-38.4	-158.8	-29.8	-7.6	16.2	-165.9	-175.0	-178.7	110.2	109.2	108.2	28.7
13	**1j/A**	-37.8	-159.0	-28.3	-7.5	14.5	-167.5	5.1	-177.6	110.4	108.9	108.1	28.2
14	**1j/B**	-38.8	-158.4	-30.0	-7.7	16.4	-172.9	-176.3	-176.2	110.1	109.2	108.1	29.0

Table S8. Nonbonded intramolecular interactions for the GS (S_0) optimized geometries of compounds **1a-e**, **i**, **j** in 1,4-dioxane



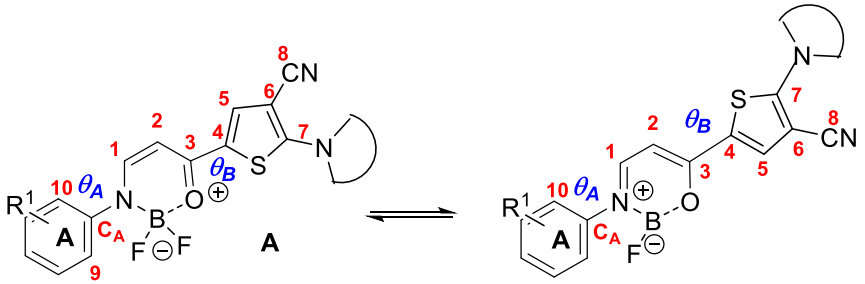
Entry	Comp	$C_9H\cdots F_1$	$C_9H\cdots F_2$	S···O	S···H-C_2	O···H-C_5	S···$C_{11}H$
1	**1a/A**	2.441	2.744	2.878	-	-	2.636
2	**1a/B**	2.443	2.717	-	2.801	2.591	2.659
3	**1b/A**	2.426	2.736	2.867			2.615
4	**1b/B**	2.438	2.733		2.793	2.585	2.652
5	**1c/A**	2.417	2.667	2.869			2.606
6	**1c/B**	2.422	2.667		2.795	2.588	2.638
7	**1d/A**	2.421	2.690	2.868			2.609
8	**1d/B**	2.428	2.701		2.791	2.586	2.606
9	**1e/A**	2.578	3.499	2.866			2.632
10	**1e/B**	2.616	3.465		2.782	2.588	2.650
11	**1i/A**	2.421	2.684	2.867			2.804
12	**1i/B**	2.417	2.672		2.782	2.586	2.813
13	**1j/A**	2.420	2.675	2.877			2.564
14	**1j/B**	2.431	2.685		2.788	2.594	2.590

Table S9. Selected bonds lengths (in Å) for the excited state (S_0) optimized geometries compounds **1a-e**, **i**, **j** in 1,4-dioxane



Entry	Comp	C_A-N	N-C_1	C_1-C_2	C_2-C_3	C_3-O	N-B	O-B	C_3-C_4	C_4-C_5	C_5-C_6	C_6-C_7	C_4-S	C_7-S	C_7-N	C_6-C_8
1	**1a/A**	1.378	1.366	1.375	1.417	1.324	1.579	1.470	1.406	1.393	1.406	1.411	1.756	1.750	1.349	1.419
2	**1a/B**	1.373	1.370	1.374	1.417	1.322	1.580	1.466	1.410	1.389	1.406	1.407	1.761	1.748	1.352	1.420
3	**1b/A**	1.387	1.356	1.380	1.416	1.324	1.583	1.470	1.405	1.399	1.402	1.416	1.754	1.755	1.342	1.419
4	**1b/B**	1.383	1.359	1.379	1.416	1.323	1.584	1.467	1.409	1.396	1.401	1.416	1.761	1.752	1.344	1.420
5	**1c/A**	1.386	1.355	1.381	1.414	1.324	1.587	1.469	1.406	1.400	1.401	1.418	1.753	1.757	1.339	1.419
6	**1c/B**	1.383	1.356	1.381	1.414	1.322	1.589	1.466	1.411	1.397	1.400	1.417	1.760	1.754	1.341	1.420
7	**1d/A**	1.390	1.353	1.381	1.415	1.324	1.584	1.470	1.405	1.401	1.401	1.418	1.753	1.757	1.339	1.419
8	**1d/B**	1.383	1.356	1.381	1.414	1.322	1.589	1.466	1.411	1.397	1.400	1.417	1.760	1.754	1.341	1.420
9	**1e/A**	1.402	1.346	1.382	1.416	1.326	1.577	1.471	1.404	1.406	1.400	1.418	1.753	1.762	1.338	1.419
10	**1e/B**	1.400	1.346	1.382	1.415	1.325	1.578	1.469	1.409	1.405	1.397	1.418	1.760	1.761	1.338	1.420
11	**1i/A**	1.390	1.352	1.382	1.414	1.326	1.585	1.469	1.407	1.402	1.402	1.419	1.756	1.753	1.328	1.418
12	**1i/B**	1.388	1.355	1.382	1.413	1.324	1.585	1.466	1.411	1.398	1.401	1.419	1.763	1.751	1.329	1.419
13	**1j/A**	1.391	1.352	1.382	1.414	1.325	1.583	1.469	1.406	1.401	1.403	1.420	1.751	1.761	1.336	1.419
14	**1j/B**	1.390	1.353	1.382	1.412	1.324	1.584	1.467	1.411	1.399	1.401	1.419	1.759	1.759	1.336	1.420

Table S10. Selected bond (ϕ (°)) and torsional (ϑ (°)) angles for the ES (S_{1v}) geometries of compounds **1a-e**, **i**, **j** in 1,4-dioxane



Entry	Comp	ϑ_A	C_ANBO	$NBOC_3$	$NC_1C_2C_3$	BOC_3C_2	BOC_3C_4	ϑ_B	$C_3C_4SC_7$	NBF_1	OBF_2	NBO	φ
1	**1a/A**	-24.1	-158.3	-28.8	-3.7	16.4	-165.4	1.6	-179.7	110.0	110.0	110.0	25.8
2	**1a/B**	-23.0	-159.2	-29.2	-4.1	17.4	-164.0	-178.0	-178.6	109.9	107.6	110.1	25.5
3	**1b/A**	-27.1	-157.3	-30.8	-4.3	18.4	-163.9	1.8	-179.5	110.0	110.0	109.6	27.0
4	**1b/B**	-26.1	-156.9	-33.0	-4.9	19.2	-162.9	-178.1	-179.8	109.9	110.2	109.6	28.3
5	**1c/A**	-26.9	-157.5	-31.2	-4.4	19.2	-163.2	1.9	-179.2	109.9	110.2	109.4	27.1
6	**1c/B**	-26.4	-157.2	-32.5	-5.2	20.0	-162.3	-178.6	-179.8	109.8	107.9	109.4	28.2
7	**1d/A**	-28.2	-157.4	-31.5	-4.5	19.3	-163.1	1.9	-179.0	110.0	110.0	109.4	27.3
8	**1d/B**	-26.4	-157.2	-32.5	-5.2	20.0	-162.3	-178.6	-179.8	110.4	109.0	109.4	28.3
9	**1e/A**	-48.3	-154.3	-35.5	-5.6	20.4	-162.5	1.3	-179.6	110.0	109.7	108.7	32.5
10	**1e/B**	-47.8	-153.8	-36.7	-6.5	20.8	-161.4	-178.9	-178.7	110.0	110.0	108.7	33.9
11	**1i/A**	-28.2	-157.4	-31.6	-4.5	19.6	-162.5	2.9	-179.9	109.9	110.1	109.5	27.2
12	**1i/B**	-27.6	-156.5	-33.1	-5.0	20.5	-161.7	-178.8	-180.0	109.9	110.3	109.5	26.6
13	**1j/A**	-28.9	-156.1	-32.3	-4.7	19.2	-163.7	1.4	-179.8	110.0	110.1	109.3	28.6
14	**1j/B**	-28.4	-156.7	-33.0	-5.4	20.5	-161.9	-179.3	-179.5	109.9	110.2	109.4	28.7

Table S11. Nonbonded intramolecular interactions for the ES (S_0) optimized geometries of compounds **1a-e**, **i**, **j** in 1,4-dioxane

Entry	Comp	$C_9H\cdots F_1$	$C_9H\cdots F_2$	S···O	S···H-C_2	O···H-C_5	S···$C_{11}H$
1	**1a/A**	2.392	2.507	2.863	-	-	2.566
2	**1a/B**	2.378	2.491	-	2.756	2.610	2.605
3	**1b/A**	2.440	2.5016	2.858			2.535
4	**1b/B**	2.409	2.526		2.753	2.609	2.577
5	**1c/A**	2.435	2.495	2.854			2.522
6	**1c/B**	2.411	2.507		2.759	2.602	2.554
7	**1d/A**	2.458	2.491	2.853			2.526
8	**1d/B**	2.411	2.507		2.759	2.602	2.554
9	**1e/A**	2.404	2.762	2.849			2.510
10	**1e/B**	2.414	2.735		2.750	2.606	2.558
11	**1i/A**	2.464	2.493	2.858			2.770
12	**1i/B**	2.437	2.518		2.758	2.601	2.803
13	**1j/A**	2.462	2.523	2.850			2.462
14	**1j/B**	2.461	2.510		2.757	2.603	2.482

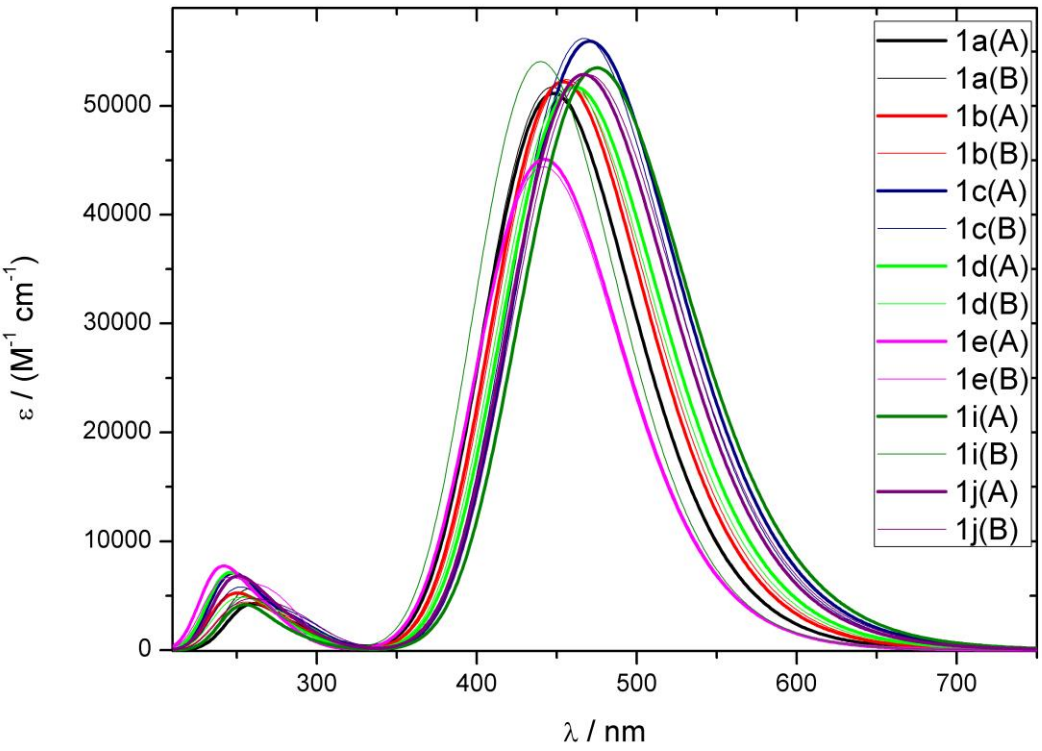
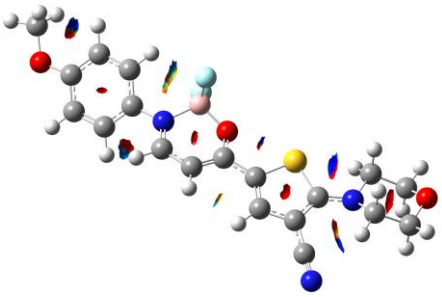
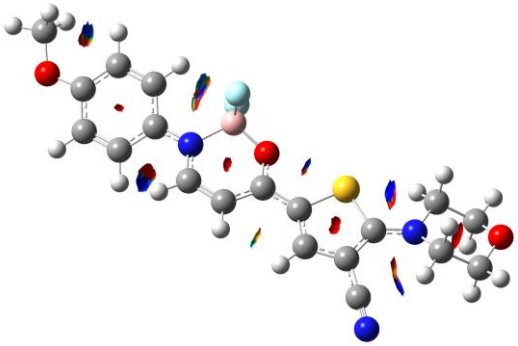
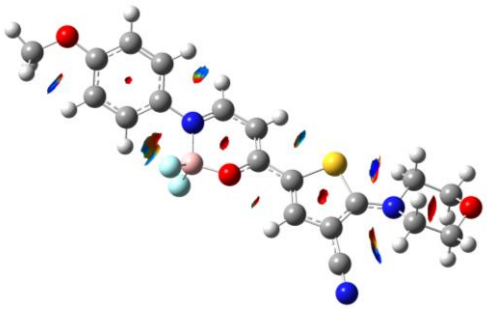
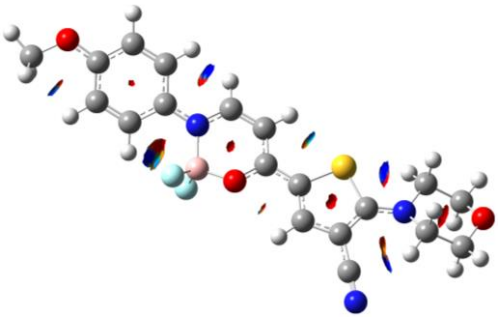
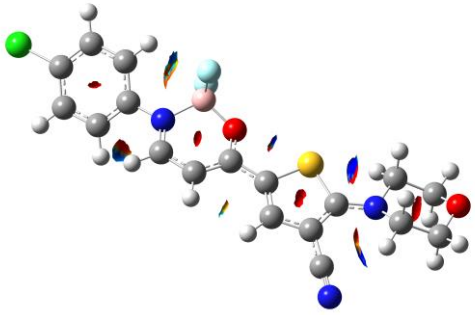
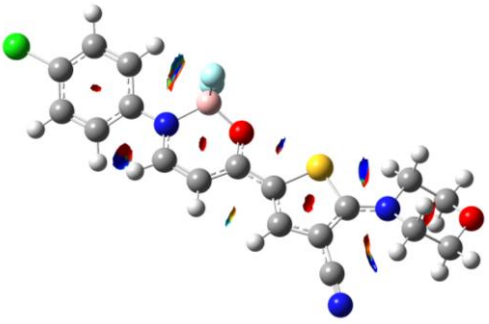
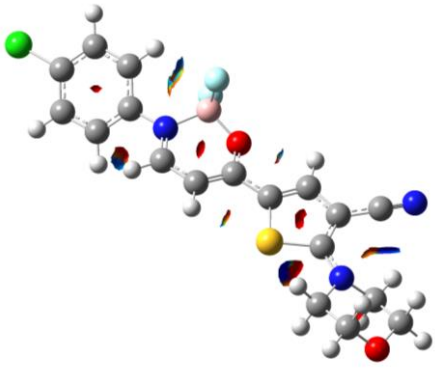
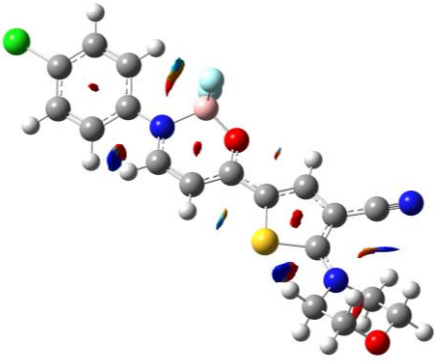
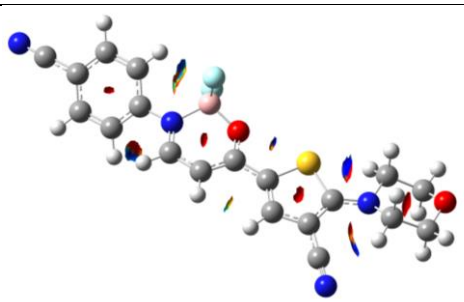
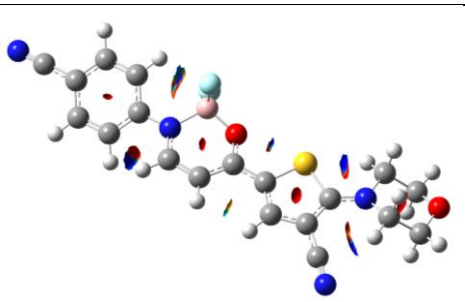
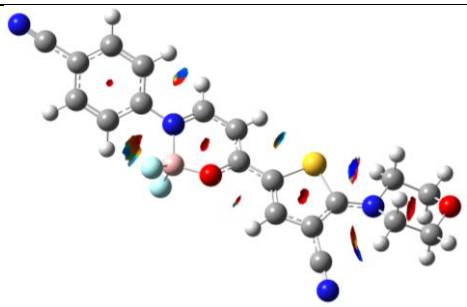
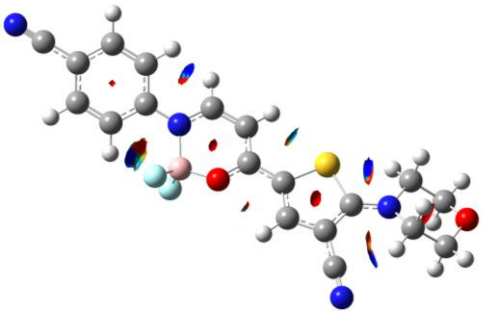
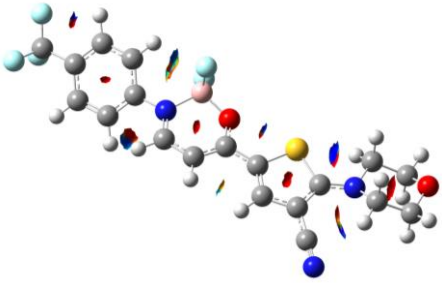
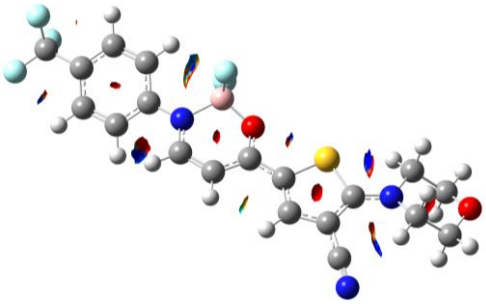
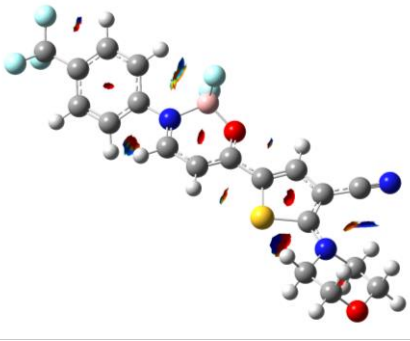
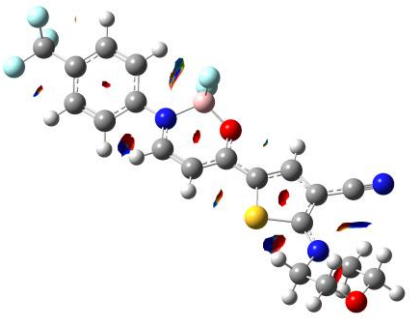
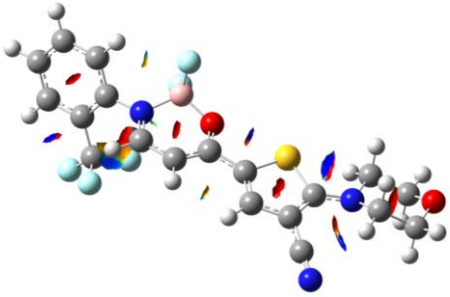
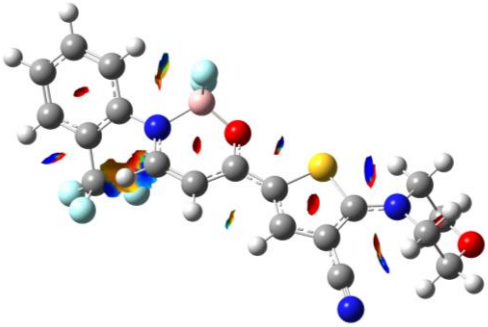


Fig. S33. Absorption ($S_0 \rightarrow S_1$) vibronic spectra of compounds **1a-e**, **i, j** in the solvated phase (1,4-dioxane).

Entry	Compd/ Rotamer	S_0	S_{1r}
1	**1a/A**		
2	**1a/B**		
3	**1b/A**		
4	**1b/B**		

5	**1c/A**		
6	**1c/B**		
7	**1d/A**		
8	**1d/B**		
9	**1e/A**		

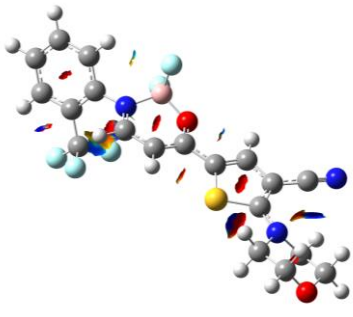
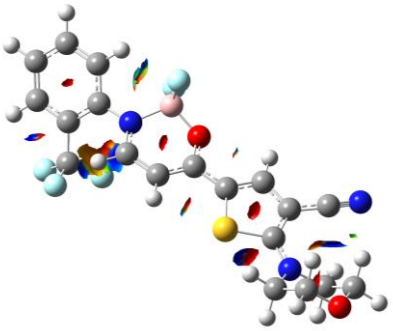
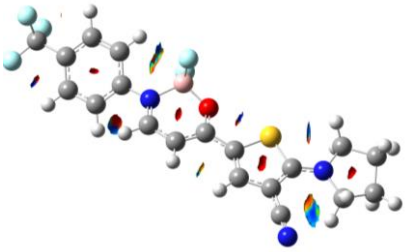
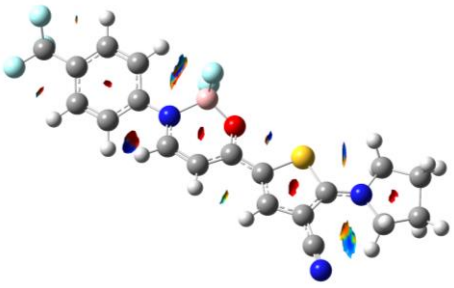
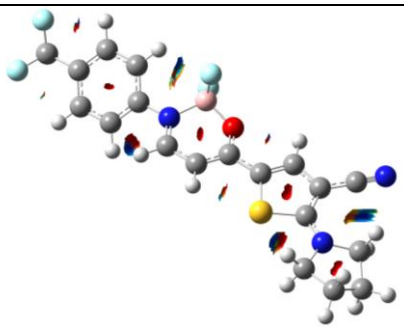
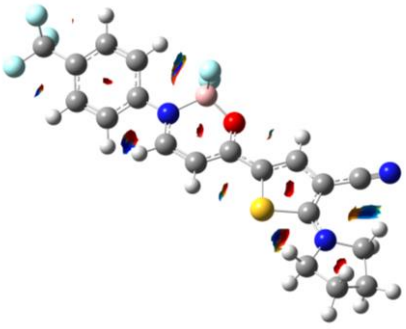
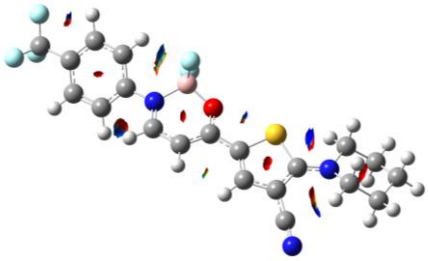
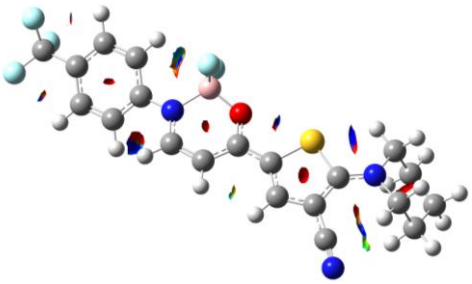
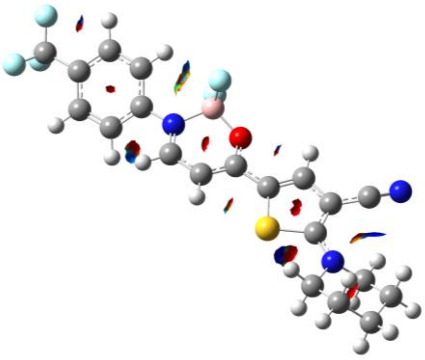
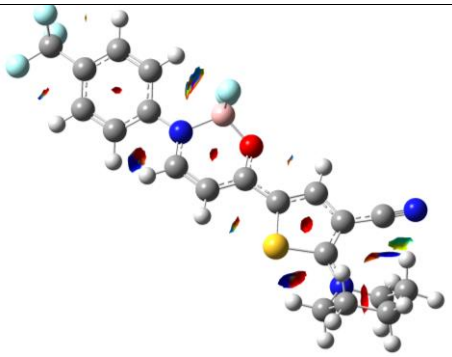
10	**1e/B**		
11	**1i/A**		
12	**1i/B**		
13	**1j/A**		
14	**1j/B**		

Fig. S34. Plots of the NCI isosurfaces (s = 0.5 a.u. and a blue-green-red colour scale from -0.012 a.u. < sign(λ_2) ρ(r) < +0.012 a.u.) compounds' **1a-e, i, j** in GS and ES

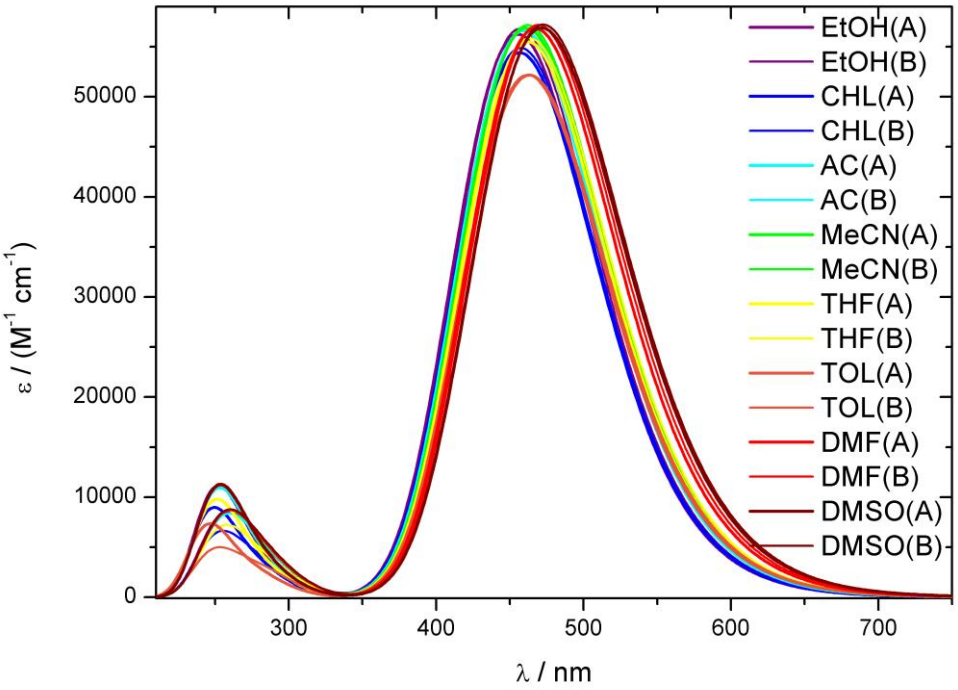


Fig. S35. Absorption ($S_0 \rightarrow S_1$) vibronic spectra of compound **1d** (rotamers A and B) in the EtOH, Chloroform (CHL), Acetone (AC), MeCN, THF, Toluene (TOL), DMF and DMSO.

Table S12. Calculated absorption[a] and emission properties[b'] for BF_2AAT **1d** in different solvent.

Solvent	Rotamer	c_{HL}	λ_{abs}, nm	f_{01}	$\mu(S_0)$, D	$\mu(S_{1v})$, D	$\vartheta(S_0\text{-}S_{1v})$/degs	c_{LH}	λ_{em}, nm	f_{10}	$\mu(S_{1r})$, D	$\theta(S_0\text{-}S_{1r})$/degs
Toluene	A	0.67560	463.3	1.2880	5.7	8.9	11.7	-0.68545	519.3	1.3584	9.8	12.7
	B	0.67182	462.1	1.2887	11.5	13.8	14.7	0.68390	519.9	1.3948	14.9	15.6
$CHCl_3$	A	0.67548	456.8	1.3433	6.2	9.9	13.9	-0.68550	516.2	1.4315	11.1	15.6
	B	0.67151	457.4	1.3549	12.7	15.3	15.8	0.68334	514.6	1.4725	14.8	15.2
THF	A	0.67560	462.1	1.3703	6.6	10.6	13.3	-0.68554	524.6	1.4607	11.7	14.5
	B	0.67120	463.6	1.3790	13.4	16.1	16.3	-0.68338	523.0	1.5018	17.7	18.3
EtOH	A	0.67542	455.5	1.3888	6.8	11.1	17.5	-0.68528	520.2	1.4923	12.7	21.2
	B	0.67096	457.1	1.4026	14.0	16.9	17.7	0.68343	520.1	1.5390	18.8	20.4
Acetone	A	0.67570	459.4	1.3975	7.1	11.3	14.1	-0.68526	529.4	1.4888	12.7	16.2
	B	0.67100	460.6	1.4054	14.2	17.0	16.9	0.68343	528.1	1.5357	18.7	18.8
DMF	A	0.67573	467.3	1.4034	7.2	11.5	14.4	-0.68532	531.6	1.4978	12.8	16.4
	B	0.67094	469.3	1.4118	14.4	17.3	17.1	0.68344	532.5	1.5441	19.0	18.9
MeCN	A	0.67570	461.1	1.4042	7.2	11.5	14.5	-0.68532	524.5	1.4973	12.8	16.6
	B	0.67100	462.1	1.4114	14.4	17.3	17.1	0.68344	525.4	1.5437	19.0	19.1
DMSO	A	0.67575	471.7	1.4045	7.2	11.5	14.4	-0.68534	532.1	1.5001	12.9	16.4
	B	0.67087	472.6	1.4127	14.7	17.5	16.9	0.68344	533.1	1.5462	19.1	19.4

[a]Transition coefficient ($c_{H\text{-}L}$), absorption wavelength (λ_a), oscillator strength (f_{01}), modulus of electric dipole moments of ground state (μ_0) and of vertical FC excited state (μ_{1v}), angles formed by the dipole moment vectors ($\vartheta_{0,1v}$).

[b]Transition coefficient ($c_{L\text{-}H}$), emission wavelength (λ_e) and oscillator strength (f_{10}), modulus of electric dipole moments of relaxed excited state ($\mu_{1r,}$), and angles formed by dipole moment vectors ($\vartheta_{0,1r}$).

Table S13. Spectral overlap (J_{DA}), Förster radius (R_{DA}), rate constant of EET (k_{EET}) for solution complexes **1a-e, i, j** in 1,4-dioxane.

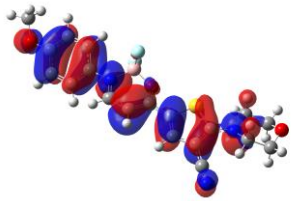
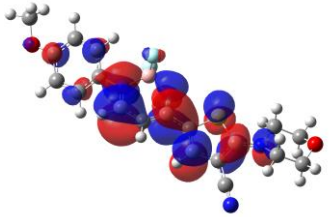
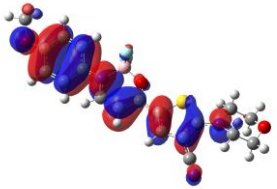
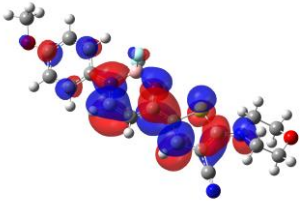
Entry	Compd	τ_f, ns	Φ_f, %	J_{DA}, $cm^3 M^{-1}$	R_{DA}, Å	k_{EET}, Hz	ratio
1	**1a**	0.99	0.96	3.67×10^{-10}	9.941	3.73×10^{18}	0.00
2	**1b**	1.21	0.15	1.30×10^{-8}	9.833	1.78×10^{19}	0.02
3	**1c**	2.21	0.35	1.99×10^{-7}	9.871	3.47×10^{20}	0.31
4	**1d**	2.35	0.42	6.20×10^{-8}	9.993	1.13×10^{20}	0.10
5	**1e**	2.05	0.42	5.27×10^{-7}	9.979	1.11×10^{21}	1.00
6	**1i**	2.73	0.28	1.04×10^{-7}	9.912	1.16×10^{20}	0.10
7	**1j**	2.54	0.30	7.22×10^{-8}	10.045	8.29×10^{19}	0.07

Table S14. Spectral overlap (J_{DA}), Förster radius (R_{DA}), rate constant of EET (k_{EET}) for solution complex **1d** in in different solvents

Entry	Solvent	n^2	τ_f, ns	Φ_f	J_{DA}, $cm^3 M^{-1}$)	R_{DA}, Å	k_{EET}, Hz	ratio
1	Dioxane	2.023222	2.35	0.42	1.57×10^{-15}	9.993	1.1×10^{13}	1.00
2	Acetone	1.846337		0.29	1.14×10^{-15}	9.994		
3	$CHCl_3$	2.090627	2.32	0.28	1.52×10^{-15}	9.995	7.17×10^{12}	0.62
4	EtOAc			0.31	1.41×10^{-15}			
5	EtOH	1.852593	2.16	0.28	1.09×10^{-15}	9.992	6.99×10^{12}	0.60
6	*i*-PrOH			0.29	1.38×10^{-15}			
7	MeCN	1.806874		0.25	$1.43E\times10^{-15}$	9.994		
8	THF	1.974025		0.33	1.46×10^{-15}	9.994		
9	Toluene	2.238315	2.33	0.30	1.83×10^{-15}	9.993	8.01×10^{12}	0.69
10	DMSO	2.007889	1.96	0.14	1.82×10^{-15}	9.994	5.49×10^{12}	0.47
11	DMF	2.04633	1.91	0.21	1.63×10^{-15}	9.995	7.27×10^{12}	0.62

Table S15. Quantum yield of BF_2AAT **1d** in different solvents and calculated (TD-DFT) $\Delta E_{(S1\text{-}T2)}$

Entry	Solvent	$\Delta E(S_1\text{-}T_1)$ / eV	QY
1	Dioxane	0.1654	0.42
2	THF	0.1437	0.33
3	Tol	0.1385	0.30
4	Ac	0.1376	0.29
5	EtOH	0.1365	0.28
6	$CHCl_3$	0.1351	0.28
7	MeCN	0.1314	0.25
8	DMF	0.1238	0.21
9	DMSO	0.1135	0.14

GS		ES	
HOMO	LUMO	HOMO	LUMO
1a/A			
			
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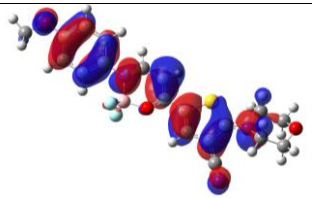	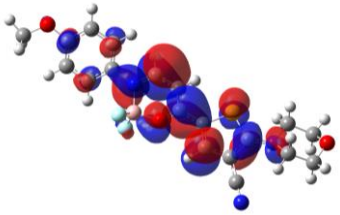	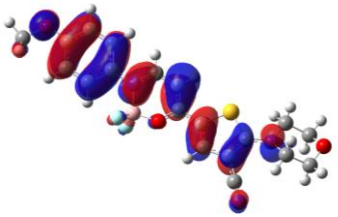	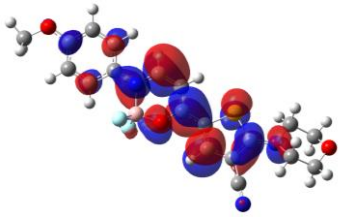
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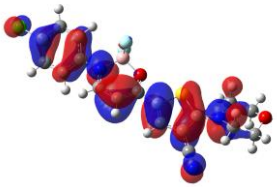	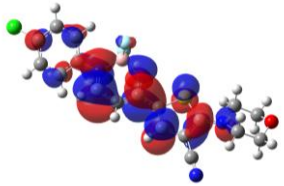		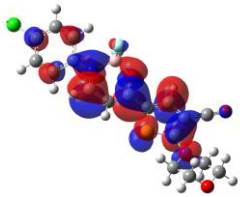
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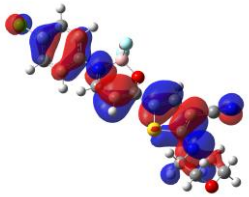	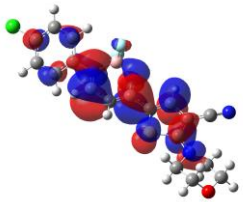	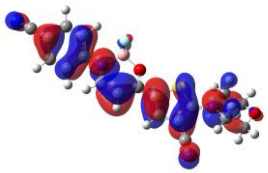	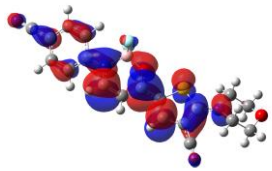
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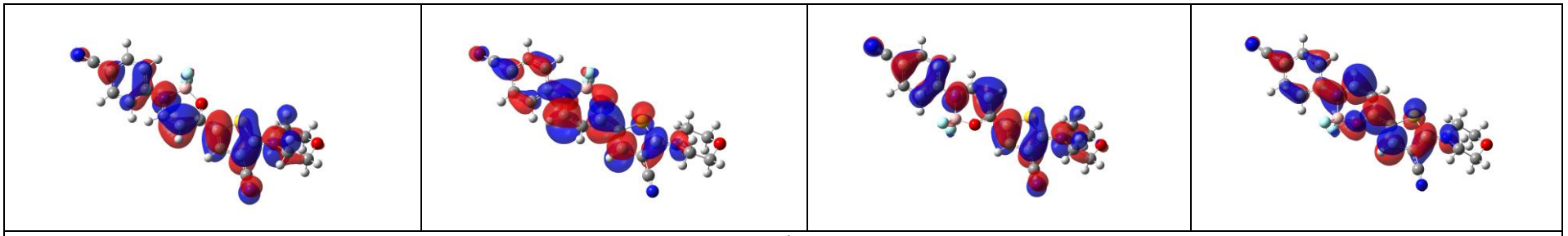

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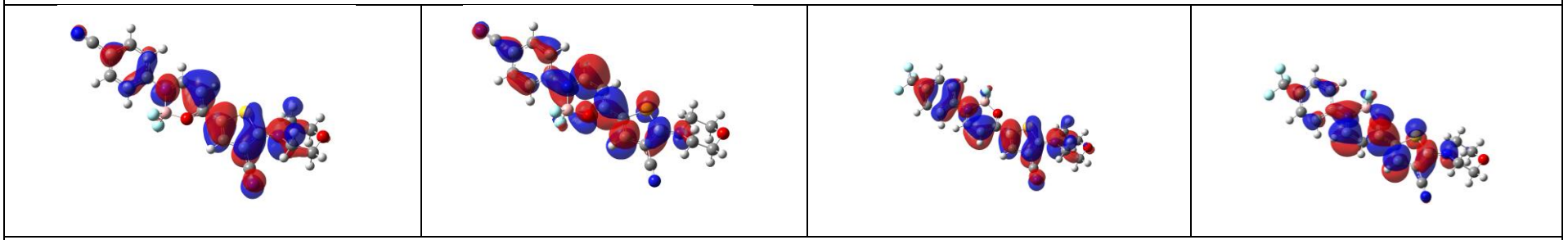

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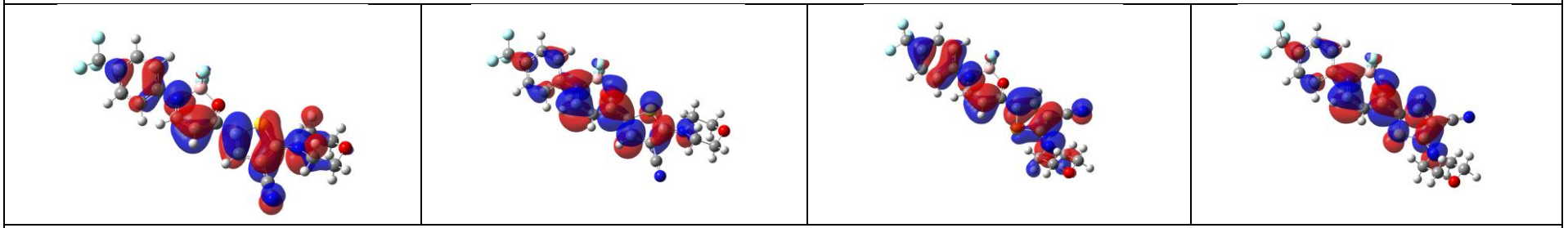

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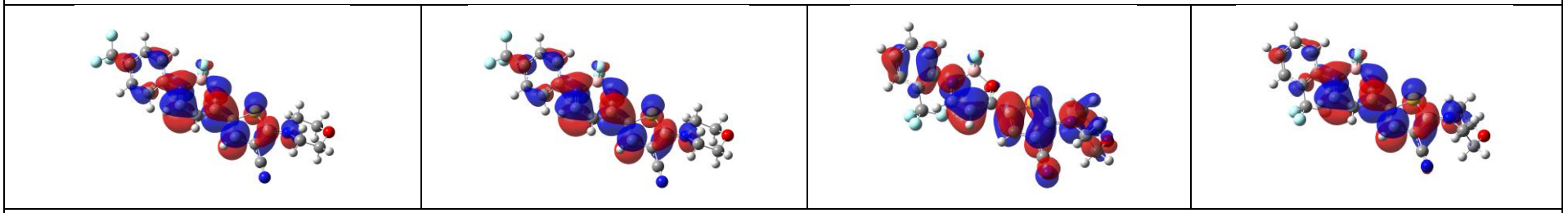

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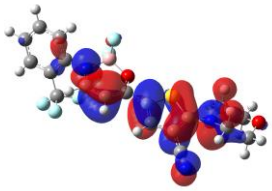	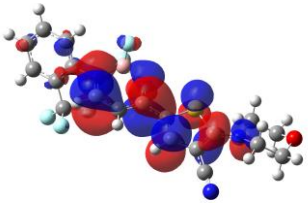	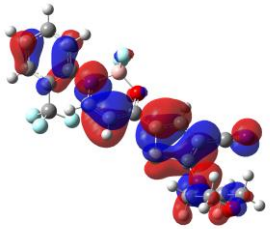	
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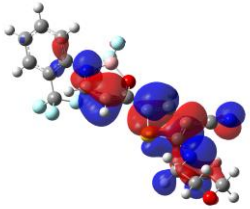	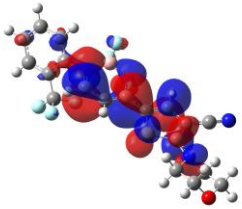	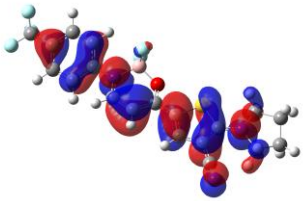	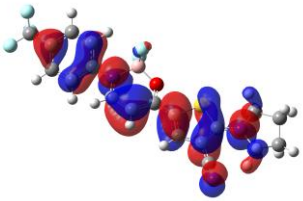
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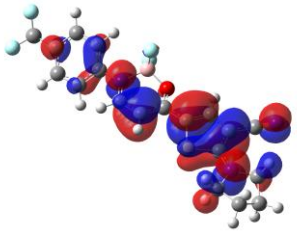	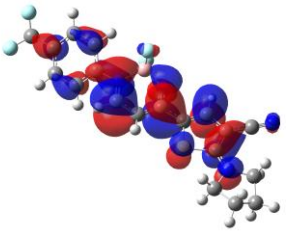	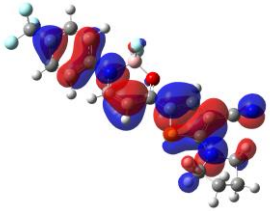	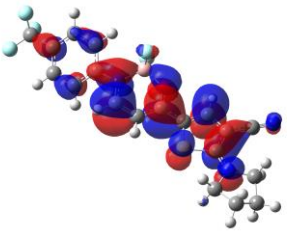
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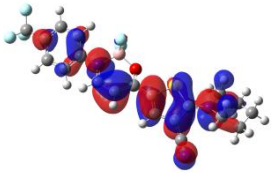	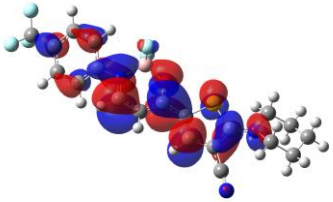	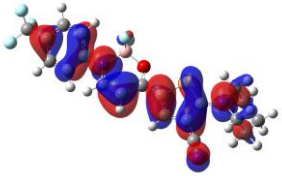	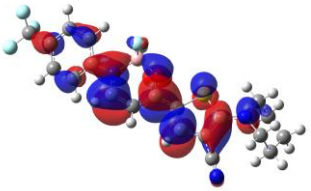
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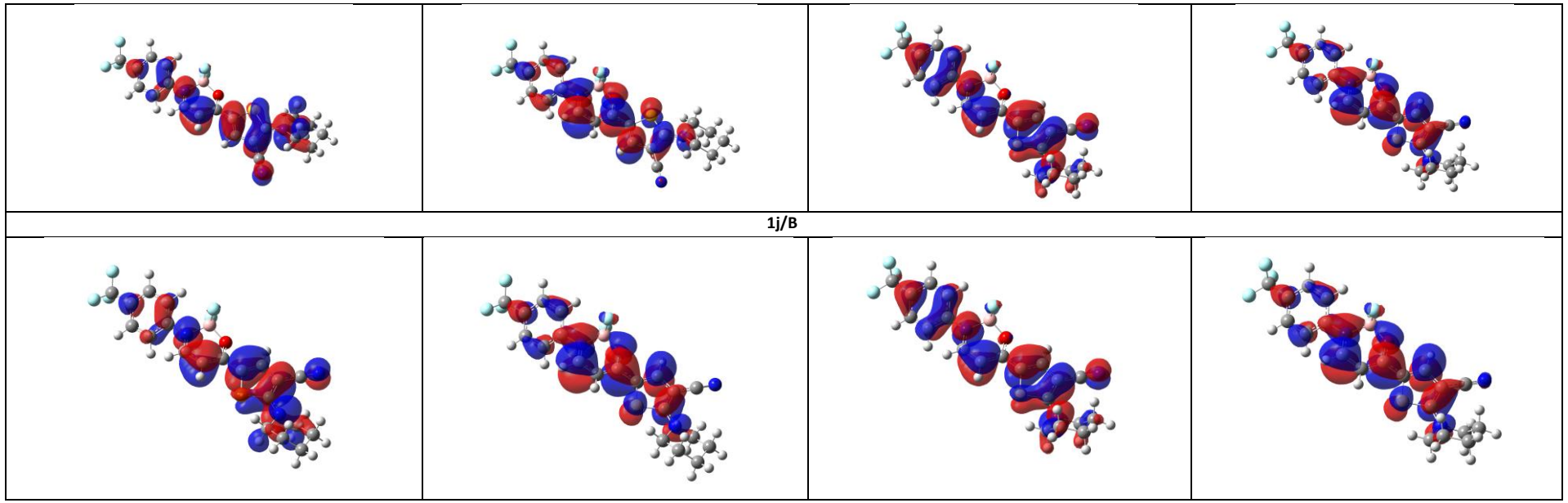
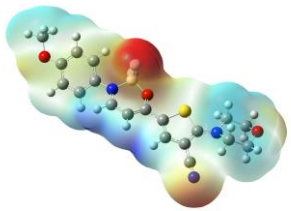
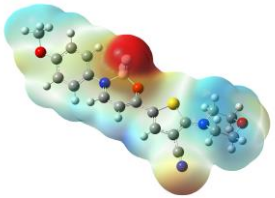
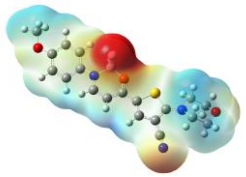
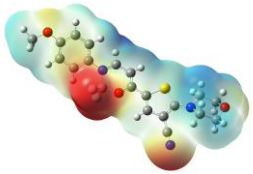
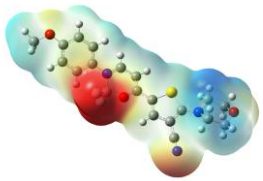
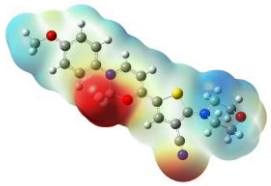
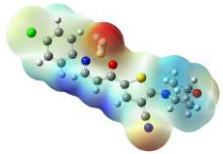
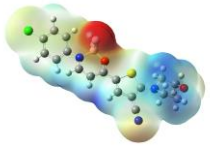
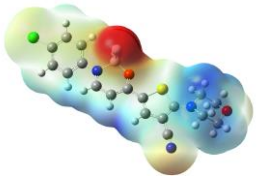
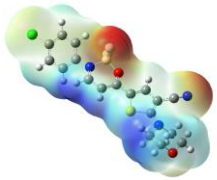
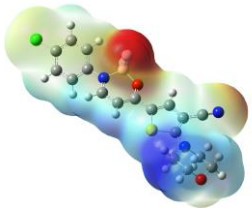
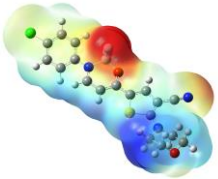
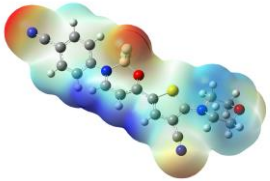
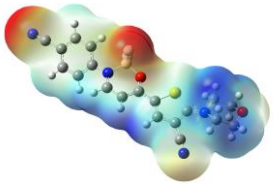
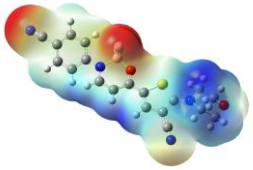
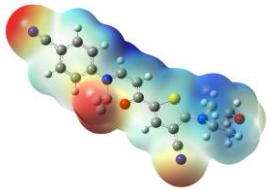
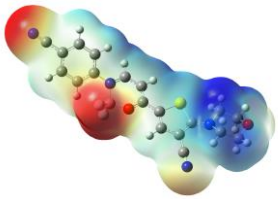
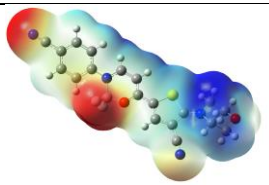
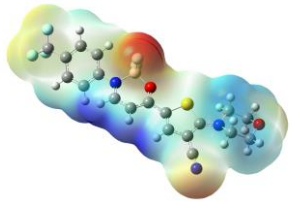
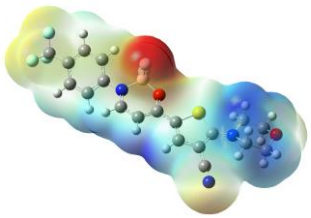
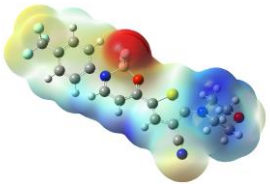
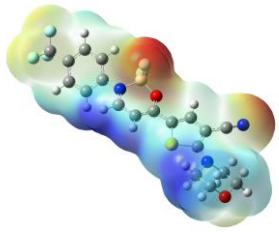
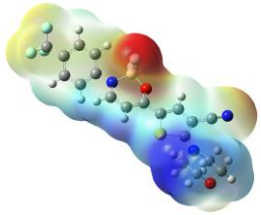
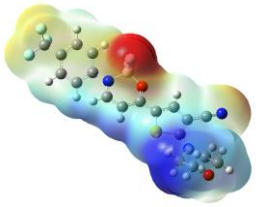
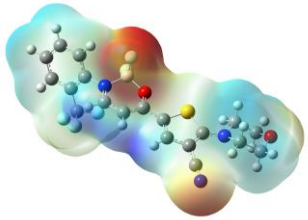
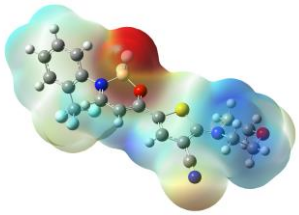
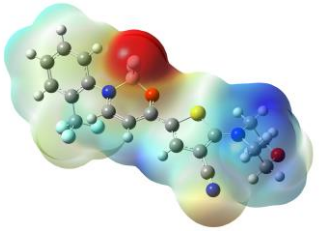
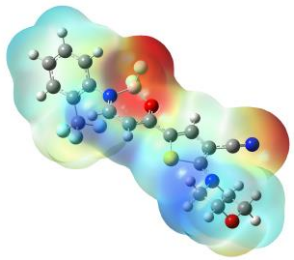
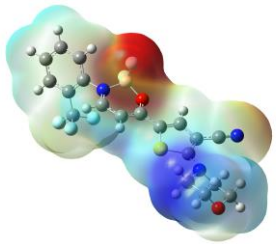
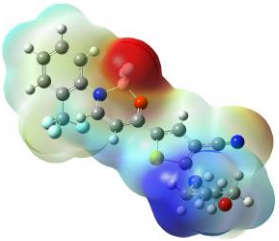


Fig. S36. Frontier molecular orbitals (FMOs) HOMO and LUMO in the ground and excited states for BF_2ATAs **1a-e**, **i**, **j** (|Isovalue(MO)| = 0.02 a.u.; |Isovalue(ρ)| = 0.0004 a.u.)

Entry	Compd/Rotamer	S_0	S_{1v}	S_{1r}
1	**1a/A**			
2	**1a/B**			
3	**1b/A**			
4	**1b/B**			
5	**1c/A**			
	1c/B			

6	**1d/A**			
7	**1d/B**			
8	**1e/A**			
9	**1e/B**			

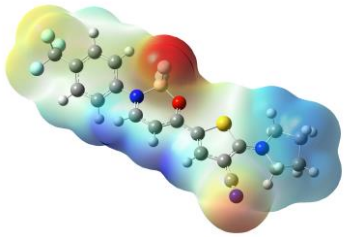
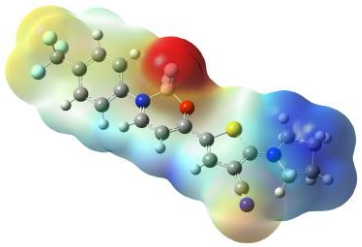
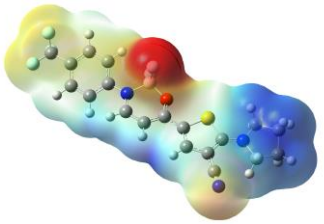
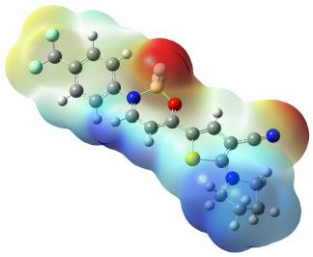
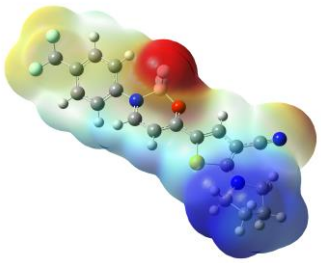
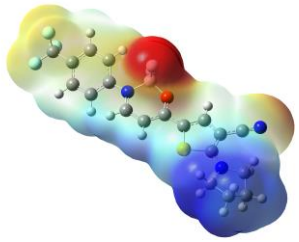
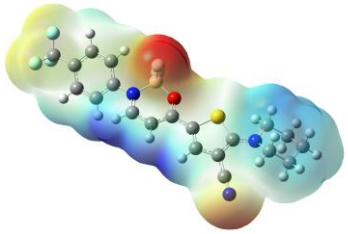
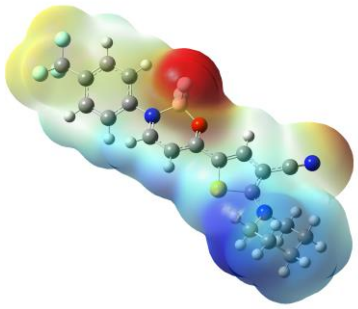
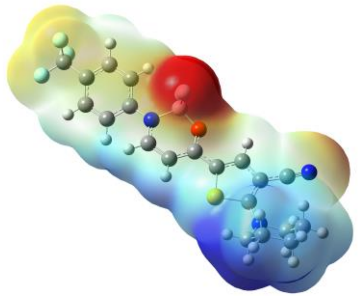
10	**1i/A**			
11	**1i/B**			
12	**1j/A**			

Fig. S37. Plot of MEPs of complexes **1a-e**, **i**, **j** calculated at (TD-)DFT ω-B97X-D / 6−311++G** // IEF-PCM(UFF) level of theory, for GS and ESs in dioxane. Legend of map colours: red (negative potential), blue (positive potential). Legend of elements: hydrogen (white), carbon (grey), nitrogen (blue), oxygen (red), sulfur (yellow), chlorine (green).

6. Biological investigations

Cell cultivation

HeLa, human fibroblasts (FH), and rhabdomyosarcoma (RD) cell culture was obtained from the cell culture bank of the Institute of Cytology RAS (Russia, St. Petersburg). The cell culture was maintained in culture flasks (Eppendorf) in DMEM medium (Sigma-Aldrich, USA) supplemented with 10% fetal bovine serum (Biolot, Russia) and 0.5% gentamicin (Biolot, Russia)

Staining protocol

The cells were diluted to a concentration of 10^3 cells/mL, transferred to glass-bottomed bottles (Nest Biotechnology Co., China) and subjected to confocal microscopy. The dye solution in DMSO (10^{-3} mmol/L) was added at 10 µL/mL nutrient medium. Additional staining of the cell nucleus was performed using a nuclear dye Hoechst 33258 (incubation for 30 min at a dye concentration of 0.1 µg/mL in the medium). After staining, the preparations were washed twice with phosphate buffer (Biolot) and the medium in which subsequent microscopic studies were conducted.

Microscopic examination

Microscopic examination was performed using the equipment of the Shared Research Center of Scientific Equipment SRC IIP UrB RAS. After staining and washing, preparations of living cells were examined using a confocal laser scanning microscope LSM-710 (Carl Zeiss) with a multichannel QUASAR detector (34 channels). Lasers at wavelengths of 405 and 488 nm were used. Images were obtained using an immersion lens (40×, 1.3 Oil) with a resolution of 1024×1024 pixels and an image size of 212×212 microns. To obtain an informative fluorescent image using special software ZEN (Carl Zeiss), a special lambda mode (λ-mode) was used, which allowed determination of the emission range with the maximum contrast for this preparation.

Bleaching of the dye was investigated using standard functions of the microscope software. Laser action was conducted at 100% power of the 405-nm laser for 30 s, after which the image was taken.

Flow cytometry

Cells were cultured in a 12-well plate to an 80% monolayer. The dye solution in DMSO (10^{-3} mmol/L) was added at 10 µL/mL nutrient medium. The cells were incubated at 37 °C in an incubator for 30 min and then cleaved with trypsin–versene solution, centrifuged, and examined using a Beckman Coulter FC500 flow cytometer.

MTT test

Cells were crossed into a 96-well plate (Eppendorf) and cultured for a day to a concentration of about 105 cells/mL, with subsequently addition of a substance in DMSO solution. DMSO was used as the control. After incubating for 72 h, the medium was changed to fresh DMEM and methylthiazolyldiphenyl-tetrazolium bromide (MTT) was added at a concentration of 1 mg/mL. The cells were incubated with the dye for 4 h and the color intensity was determined using a flatbed photometer at a wavelength of 540 nm.

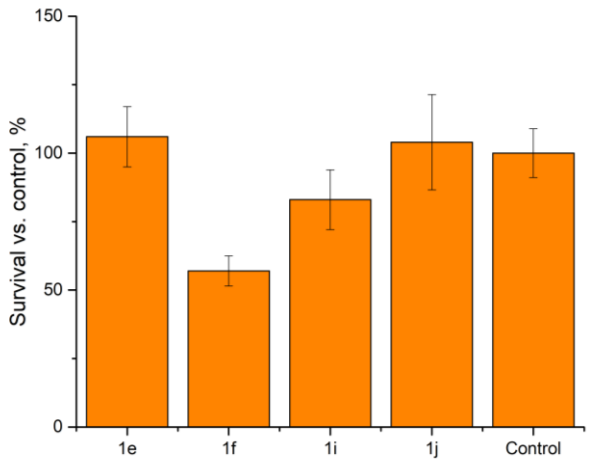


Fig. S38. Viability of HeLa cells in the presence complexes **1e–f**, **i**, **j**. determined by MTT assay. All values are normalized to the DMSO negative control, which was set to 100 %.

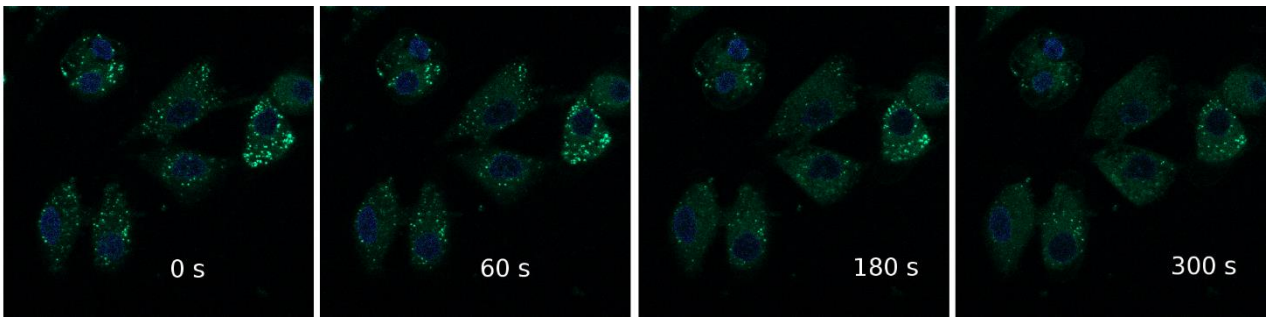


Fig. S39. A series of images in the process of photo bleaching of HeLa cell culture stained with Hoechst 33258 (blue) and substance **1f** (green). The image was obtained by excitation with 405 wavelength laser for Hoechst 33258 dye and 488 for substance **1f**. Photo bleaching was carried out with a maximum laser power of 405 wavelength. Time is given directly for bleaching process.

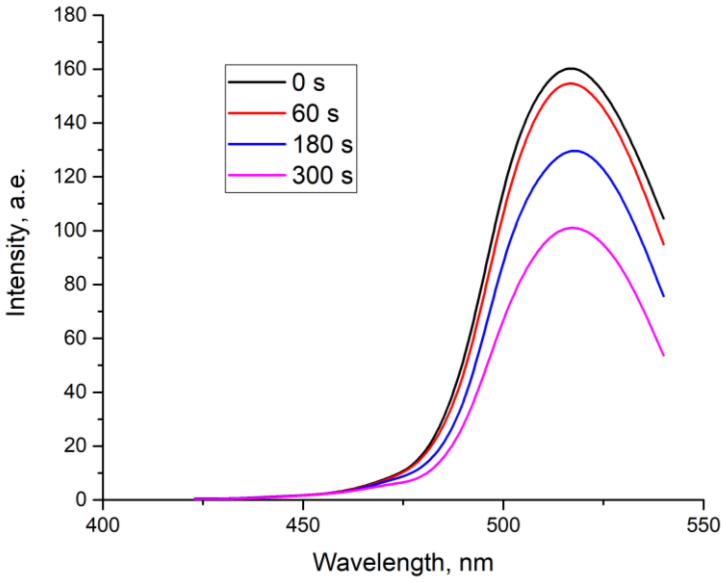


Fig. S40. Fluorescence spectra of the dye **1f**, taken in the process of photobleaching. The spectra were recorded with excitation at 488 nm, using the lambda-mode of a confocal microscope, at a bright point in the cell.

6. Reference

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Cartesian coordinates (Å) of the optimized structure for compounds 1a-e, i, j

Ground state optimized geometries (S_0) (in dioxane)

Optimised Geometries (GS and ES in dioxane)

*** molecule **1a** rotamer A S_0 - dioxane

47

6	0.84322251	0.90380359	0.09945700
6	1.00582904	-0.28705357	0.74591339
16	2.36358817	1.52265059	-0.49044496
6	2.35032736	-0.73370831	0.76994065
1	0.19393763	-0.86429896	1.16798856
6	3.22934527	0.14577656	0.12562979
6	2.70970882	-2.00983244	1.28070296
7	2.98391650	-3.05263447	1.68716147
6	5.25862442	1.03850549	-0.86167231
6	5.40864319	-0.44822245	1.06682017
6	6.61127354	0.49987486	-1.30102075
1	5.39013765	1.96650184	-0.28727004
1	4.66238006	1.25140069	-1.75094144
6	6.75090043	-0.91428140	0.53253248
1	5.55418274	0.37528167	1.77841259
1	4.92360851	-1.27400242	1.58055748
1	7.16104912	1.27705075	-1.83203679
1	6.46293342	-0.35539980	-1.97378863
1	7.40472434	-1.17952062	1.36328551
1	6.60960383	-1.79658039	-0.10583239
7	4.57241533	0.03464581	-0.04599392
8	7.39759749	0.11105335	-0.19558917
6	-0.37057547	1.64793670	-0.15260459
6	-1.59554072	1.30898239	0.39124723
6	-2.73374459	1.99545617	-0.04788691
1	-1.69485397	0.48673368	1.08186746
1	-3.71727933	1.65397699	0.26312585
8	-0.23793393	2.65491829	-0.97183418
5	-1.28257769	3.69347561	-1.14574123
7	-2.67528433	3.04258548	-0.83820967
6	-3.86890001	3.63413278	-1.34699709
6	-3.96640922	5.01728582	-1.43878566
6	-4.93583426	2.83842864	-1.77070117
6	-5.12745195	5.61117991	-1.92169626
1	-3.13644324	5.63677356	-1.12139322
6	-6.09627499	3.42358182	-2.24262092
1	-4.84536534	1.75801464	-1.75929350
6	-6.20225528	4.81500599	-2.31828553
1	-5.17731767	6.68989622	-1.97947180
1	-6.92862389	2.81873730	-2.58105381
8	-7.37410642	5.29692477	-2.79617920
6	-7.50828486	6.70185980	-2.91490952
1	-8.50460735	6.87625019	-3.31594833
1	-7.42067040	7.19291008	-1.94112146
1	-6.76509005	7.11355258	-3.60432987

9	-1.24161217	4.15468166	-2.44210638
9	-1.05682350	4.72004787	-0.23138098

*** molecule **1a** rotamer B S_0 - dioxane

47

6	0.89153270	1.00790445	0.02323586
6	0.99527655	-0.22448168	0.59840628
16	2.45457127	1.61723584	-0.45681291
6	2.32512150	-0.71620505	0.63950260
1	0.13877899	-0.78289922	0.95157209
6	3.25538666	0.17028629	0.09159440
6	2.64081841	-2.03317514	1.06997274
7	2.89484167	-3.10588145	1.40442560
6	5.34842634	1.04608739	-0.77257736
6	5.37394849	-0.51657780	1.10033393
6	6.70455114	0.48670700	-1.17533020
1	5.48117039	1.94567066	-0.15430610
1	4.79689309	1.31123621	-1.67657370
6	6.72351801	-1.00255171	0.60483921
1	5.51248676	0.27740430	1.84616164
1	4.84255893	-1.34438104	1.56272003
1	7.29931974	1.26782888	-1.64903763
1	6.56321257	-0.33584448	-1.88905551
1	7.33314616	-1.31996440	1.45073392
1	6.58458942	-1.85466634	-0.07368886
7	4.60130053	0.03023928	-0.02976179
8	7.42964079	0.03118967	-0.05382797
6	-0.33691587	1.73577484	-0.21440241
6	-0.41109574	2.89974075	-0.95616241
6	-1.62671923	3.59742772	-0.99309952
1	0.45766706	3.31713911	-1.44188603
1	-1.66719164	4.57955776	-1.45618860
8	-1.38740921	1.22866849	0.36928202
5	-2.76773539	1.63167112	0.02060085
7	-2.73448385	3.12088576	-0.47843672
6	-3.91730586	3.91580396	-0.43599093
6	-5.15165560	3.32268469	-0.67274968
6	-3.85282423	5.27958837	-0.14185264
6	-6.31565045	4.08271446	-0.64278546
1	-5.20570374	2.26325128	-0.89156992
6	-5.00601266	6.04205038	-0.11961775
1	-2.90186651	5.73911930	0.10257381
6	-6.24642293	5.44956831	-0.37183765
1	-7.26263073	3.59637235	-0.83289539
1	-4.97164132	7.09856845	0.11662360
8	-7.32006522	6.27275827	-0.31977386
6	-8.60033055	5.69814126	-0.51360030
1	-9.31458287	6.51267966	-0.41189553
1	-8.69244222	5.26210813	-1.51284823
1	-8.81086193	4.93692048	0.24347594
9	-3.56189023	1.51954611	1.13927256
9	-3.23149791	0.82916265	-1.01952647

*** molecule **1b** rotamer A S_0 - dioxane

43

6	0.83453606	0.90616063	0.14382056
6	1.01328327	-0.26783345	0.81814356
16	2.34423194	1.51713838	-0.48291912
6	2.35793781	-0.70913167	0.83342031
1	0.21364147	-0.83344329	1.27769980
6	3.22442927	0.15574335	0.14846399
6	2.72198973	-1.96850102	1.38130701
7	2.99446127	-2.99912523	1.81864689
6	5.23203442	1.04953518	-0.88093430
6	5.42475599	-0.46068895	1.02978098
6	6.57094670	0.50860600	-1.35806084
1	5.38031338	1.97418213	-0.30576259
1	4.61547281	1.26843960	-1.75473601
6	6.75068691	-0.92479366	0.45434808
1	5.59236889	0.34989881	1.75082899
1	4.94985630	-1.29303898	1.54163429
1	7.10951956	1.28854694	-1.89636843
1	6.40259169	-0.34013053	-2.03448532
1	7.42365982	-1.20368065	1.26494518
1	6.59007852	-1.79829644	-0.19151676
7	4.56108263	0.04602418	-0.05116766
8	7.38284641	0.10704877	-0.27653114
6	-0.38245202	1.63953095	-0.10730607
6	-1.62451258	1.24529055	0.36664131
6	-2.75427462	1.93764271	-0.07075015
1	-1.73753795	0.37227151	0.98932724
1	-3.74204609	1.56256282	0.18233388
8	-0.24225823	2.69424068	-0.86028116
5	-1.29659734	3.72845916	-1.00585409
7	-2.68639802	3.03716698	-0.79226304
6	-3.86852969	3.64268960	-1.30306749
6	-3.97656956	5.03330728	-1.30562584
6	-4.90365654	2.86207376	-1.81390091
6	-5.12639264	5.63753468	-1.79101935
1	-3.16672223	5.63811936	-0.91681352
6	-6.06057623	3.46280632	-2.29316669
1	-4.79807297	1.78491842	-1.86994749
6	-6.16092708	4.84608523	-2.27371875
1	-5.22038676	6.71593390	-1.79045376
1	-6.86620747	2.86225789	-2.69597434
17	-7.60964792	5.60754415	-2.88073654
9	-1.21987548	4.27130173	-2.26792455
9	-1.12009849	4.69489584	-0.01963186

*** molecule **1b** rotamer B S_0 - dioxane

43

6	0.72051245	0.77057376	0.13809992
6	1.98624391	1.08622699	-0.26424385
16	0.70552032	-0.68967591	1.09412452
6	2.96923541	0.18137115	0.20681631
1	2.21445706	1.96519430	-0.85202807
6	2.43696732	-0.85214835	0.98448127
6	4.36078486	0.39873124	0.01736751
7	5.48891098	0.58276069	-0.12558945
6	2.31964699	-2.75441727	2.49112202

6	4.15090485	-2.59747434	0.88445017
6	3.27968299	-3.49006380	3.41443307
1	1.73260777	-3.47666847	1.90611142
1	1.64337577	-2.15075772	3.09934737
6	5.02064755	-3.33303391	1.88729210
1	3.69031501	-3.31379577	0.19154274
1	4.76450780	-1.90320940	0.31644791
1	2.72904970	-4.21033642	4.01976346
1	3.77124140	-2.76832697	4.08047169
1	5.75666115	-3.94095533	1.36148162
1	5.54536786	-2.60900541	2.52435363
7	3.07785901	-1.87947732	1.59546883
8	4.24900133	-4.21031083	2.68526781
6	-0.47152110	1.54381105	-0.12479368
6	-1.71538713	1.24741698	0.40967848
6	-2.82493072	1.97603206	-0.02934740
1	-1.85564608	0.42357333	1.09274427
1	-3.82240392	1.66939570	0.27392492
8	-0.30483518	2.53672833	-0.95210151
5	-1.29703694	3.62469141	-1.10386215
7	-2.72058411	3.02897277	-0.80908699
6	-3.88322820	3.67453212	-1.31635372
6	-3.91509503	5.06714561	-1.38276993
6	-4.97325488	2.92901956	-1.75988906
6	-5.04529287	5.71076277	-1.86349503
1	-3.06162391	5.64302928	-1.04694527
6	-6.11007772	3.56973163	-2.23548654
1	-4.92669736	1.84633156	-1.76597299
6	-6.13503551	4.95595086	-2.27892298
1	-5.08087283	6.79160478	-1.91159047
1	-6.95862342	2.99669979	-2.58696261
17	-7.55836527	5.76747224	-2.88080334
9	-1.24251147	4.10785550	-2.39068162
9	-1.03053266	4.62069342	-0.16872164

*** molecule **1c** rotamer A S_0 - dioxane

44

6	0.83313818	0.91485179	0.13783338
6	1.01016916	-0.26295144	0.80833576
16	2.34624520	1.53198891	-0.47595889
6	2.35381336	-0.70155371	0.83145030
1	0.20857070	-0.83283928	1.25920655
6	3.22460081	0.16912315	0.15548981
6	2.71332828	-1.96358612	1.37648660
7	2.98032462	-2.99664893	1.81124635
6	5.23912428	1.07316029	-0.85325392
6	5.42171634	-0.47004999	1.03400856
6	6.57262091	0.52714080	-1.34032057
1	5.39526263	1.98806029	-0.26517409
1	4.62392334	1.30925227	-1.72347441
6	6.74161237	-0.93759491	0.44756381
1	5.59914400	0.32728653	1.76710748
1	4.93958203	-1.30537864	1.53373326
1	7.11762237	1.31071477	-1.86669781
1	6.39537345	-0.30868164	-2.03037754
1	7.41321398	-1.23696776	1.25192536

1	6.57116054	-1.79853506	-0.21247922
7	4.56050056	0.06438035	-0.03565471
8	7.38192744	0.10041448	-0.26684650
6	-0.38223658	1.64366275	-0.11751785
6	-1.62926530	1.24069046	0.34743172
6	-2.75655661	1.92561095	-0.09375600
1	-1.74129552	0.36623357	0.96826951
1	-3.74289637	1.54703861	0.15865005
8	-0.24427092	2.70209609	-0.86279998
5	-1.30357330	3.73170013	-1.01394052
7	-2.69116081	3.03020210	-0.81592135
6	-3.86981709	3.62893130	-1.32966720
6	-3.96163438	5.02218503	-1.37274992
6	-4.91968143	2.84069059	-1.80468969
6	-5.10950066	5.62097625	-1.86065396
1	-3.14030786	5.62761557	-1.01110669
6	-6.07322086	3.43857673	-2.28515708
1	-4.82321964	1.76202808	-1.83128971
6	-6.17102272	4.83073337	-2.31083970
1	-5.19066642	6.70030598	-1.88981749
1	-6.88907860	2.83240953	-2.65867986
9	-1.21880596	4.27717166	-2.27407416
9	-1.14050740	4.69511378	-0.02406655
6	-7.36296804	5.45268701	-2.81253809
7	-8.31990341	5.95192222	-3.21046463

*** molecule **1c** rotamer B S_0 - dioxane

44

6	0.87710905	1.00546035	0.06720021
6	1.00365331	-0.20989102	0.67812903
16	2.42546516	1.61054186	-0.46555569
6	2.33460210	-0.68985189	0.70843771
1	0.15939367	-0.76415941	1.06608966
6	3.24853436	0.18695079	0.11088965
6	2.66090313	-1.99125299	1.17744939
7	2.91715051	-3.05198580	1.54618802
6	5.31391383	1.06156266	-0.81760378
6	5.39753306	-0.49237650	1.06604411
6	6.65578701	0.49561715	-1.25794998
1	5.46546415	1.96790719	-0.21433968
1	4.73430316	1.31600443	-1.70694962
6	6.73019448	-0.98127356	0.52895674
1	5.56020429	0.30242381	1.80552863
1	4.88025836	-1.31850632	1.54629211
1	7.23538320	1.27185179	-1.75768035
1	6.49011232	-0.33298119	-1.95933010
1	7.36576760	-1.29530681	1.35670517
1	6.56989713	-1.83652232	-0.14078223
7	4.58876797	0.05660182	-0.03792400
8	7.41494253	0.04904699	-0.15631524
6	-0.35883353	1.71266087	-0.16324507
6	-0.45212965	2.87842849	-0.91358437
6	-1.66622770	3.56207894	-0.94116873
1	0.40866568	3.30071437	-1.40913394
1	-1.72082970	4.53761767	-1.41628551
8	-1.39918083	1.20139671	0.42797990

5	-2.78869417	1.58744626	0.09013425
7	-2.77126750	3.07688198	-0.41032532
6	-3.95587163	3.85657649	-0.36811039
6	-5.18804248	3.23039448	-0.56879836
6	-3.89595244	5.22761006	-0.11388835
6	-6.35125485	3.97916301	-0.54412308
1	-5.22701982	2.16499341	-0.75678469
6	-5.05908079	5.97999649	-0.09671979
1	-2.94664752	5.70175337	0.10422676
6	-6.28869803	5.35673468	-0.31577026
1	-7.30954963	3.50191464	-0.70629446
1	-5.02021138	7.04318675	0.10482647
9	-3.57047687	1.47615892	1.21642616
9	-3.25085165	0.77700558	-0.94122193
6	-7.49440386	6.13465424	-0.29549490
7	-8.45930419	6.76072106	-0.28151274

*** molecule **1d** rotamer A S_0 - dioxane

46

6	0.83754909	0.90749993	0.13689631
6	1.01622880	-0.26427252	0.81647032
16	2.34909519	1.52053946	-0.48416341
6	2.36094759	-0.70174943	0.84088193
1	0.21562884	-0.83105782	1.27296049
6	3.22958676	0.16377894	0.15709266
6	2.72313590	-1.95904275	1.39491664
7	2.99282108	-2.98835400	1.83693914
6	5.24127591	1.06273101	-0.86076350
6	5.42764815	-0.45929579	1.04257406
6	6.57894035	0.51956368	-1.33918240
1	5.39127967	1.98436643	-0.28151220
1	4.62663967	1.28694057	-1.73455119
6	6.75203891	-0.92488574	0.46474196
1	5.59806765	0.34632579	1.76834756
1	4.94934101	-1.29272166	1.54924347
1	7.12059687	1.30070736	-1.87260522
1	6.40836919	-0.32470140	-2.02060666
1	7.42332914	-1.21140937	1.27404672
1	6.58858502	-1.79381182	-0.18655451
7	4.56622513	0.05828448	-0.03508751
8	7.38822386	0.10916955	-0.25921103
6	-0.37932736	1.63443807	-0.12334934
6	-1.62360536	1.23904331	0.35094157
6	-2.75279768	1.92052626	-0.09599581
1	-1.73461561	0.37243181	0.98284998
1	-3.73903148	1.54495143	0.16170254
8	-0.24211052	2.68344948	-0.88284910
5	-1.30090247	3.71243251	-1.04151445
7	-2.68809943	3.01468123	-0.83075975
6	-3.87032279	3.60955778	-1.34735287
6	-3.96971389	4.99936891	-1.39058226
6	-4.91553568	2.81459455	-1.82285505
6	-5.12365472	5.59209128	-1.88278658
1	-3.15254104	5.60964133	-1.02754880
6	-6.07026430	3.40961098	-2.30397733
1	-4.81290099	1.73632043	-1.84671154

6	-6.17251151	4.79737603	-2.32878866
1	-5.20603400	6.67122093	-1.90969848
1	-6.88296772	2.79617189	-2.67614418
6	-7.42602387	5.40936043	-2.87649585
9	-7.58015482	5.14975737	-4.18787458
9	-7.45454286	6.74023244	-2.73671881
9	-8.52460712	4.92557260	-2.26882126
9	-1.13354778	4.68613443	-0.06187220
9	-1.21930439	4.24501480	-2.30733977

*** molecule **1d** rotamer B S_0 - dioxane

46

6	0.72724301	0.77536357	0.13641494
6	1.99219939	1.09467611	-0.26744871
16	0.71899970	-0.67939546	1.10128161
6	2.97884923	0.19739974	0.20753118
1	2.21641978	1.97090537	-0.86091047
6	2.45097518	-0.83539010	0.99104899
6	4.36877416	0.42201606	0.01427521
7	5.49504541	0.61326134	-0.13320856
6	2.33653026	-2.73879570	2.49573543
6	4.18178966	-2.56495776	0.90512961
6	3.29435216	-3.46883142	3.42568997
1	1.75903291	-3.46432192	1.90550955
1	1.65164355	-2.14064564	3.09974511
6	5.04698000	-3.29661594	1.91479469
1	3.73426884	-3.28274991	0.20535390
1	4.79617347	-1.86437740	0.34596756
1	2.74361422	-4.19358270	4.02550841
1	3.77562959	-2.74494219	4.09685125
1	5.79206986	-3.89778132	1.39404887
1	5.56089487	-2.57079127	2.55855162
7	3.09457224	-1.85751981	1.60570877
8	4.27425938	-4.18119020	2.70327285
6	-0.46779077	1.53782952	-0.13581192
6	-1.71357556	1.23295931	0.39519097
6	-2.82603805	1.94486009	-0.05488970
1	-1.84896115	0.41289234	1.08380389
1	-3.82095099	1.63232716	0.25026869
8	-0.30700200	2.52707107	-0.96679763
5	-1.31122994	3.60219140	-1.13880403
7	-2.72950123	2.99261793	-0.84662377
6	-3.89600908	3.62072288	-1.36115163
6	-3.93053645	5.01030956	-1.46415160
6	-4.98834514	2.85600400	-1.77438037
6	-5.06906300	5.63508903	-1.95257074
1	-3.07550417	5.59549744	-1.15016573
6	-6.12684840	3.48346809	-2.25330922
1	-4.93548850	1.77418297	-1.75104947
6	-6.16543805	4.87216232	-2.33589430
1	-5.10202280	6.71473410	-2.02538074
1	-6.97655003	2.89350049	-2.57746943
6	-7.40117044	5.51999753	-2.88351837
9	-7.56585117	5.26076182	-4.19361271
9	-7.38804367	6.85163743	-2.74905230
9	-8.51215241	5.07226236	-2.27140097

9	-1.06168549	4.61219220	-0.21526276
9	-1.25338005	4.06824249	-2.43161367

*** molecule **1e** rotamer A S_0 - dioxane

46

6	0.84238189	0.97685485	0.28691014
6	1.05548780	-0.10322760	1.09492392
16	2.30631792	1.46278069	-0.52868838
6	2.39035634	-0.57261962	1.06429439
1	0.28462209	-0.58575673	1.68077494
6	3.21280123	0.17559663	0.21032365
6	2.78388475	-1.76269293	1.73326286
7	3.08732738	-2.73725575	2.26783155
6	5.14847675	0.85312583	-1.08897933
6	5.46620452	-0.34356445	1.01511525
6	6.43931969	0.21038024	-1.57316336
1	5.35484451	1.85083206	-0.67667225
1	4.46951574	0.95104217	-1.93813782
6	6.73303494	-0.93321918	0.42330560
1	5.70617745	0.56916429	1.57630883
1	5.01881280	-1.06549306	1.69290973
1	6.94849513	0.88547313	-2.26095176
1	6.20785937	-0.72508872	-2.09994041
1	7.46237050	-1.10536812	1.21464759
1	6.50480455	-1.89037306	-0.06424944
7	4.52959138	0.00584602	-0.06719321
8	7.32482792	-0.04591494	-0.50469491
6	-0.38158107	1.69895841	0.03141307
6	-1.57915346	1.41596856	0.67243489
6	-2.73644296	2.05573057	0.22907598
1	-1.64506258	0.64838256	1.42672653
1	-3.70512928	1.75021739	0.61385344
8	-0.29019175	2.62226178	-0.88288284
5	-1.34811738	3.63540906	-1.12390446
7	-2.71130675	3.01761914	-0.66896575
6	-3.92158267	3.58993941	-1.16829485
6	-4.24015959	4.89662612	-0.81770544
6	-4.75612928	2.87816568	-2.03691380
6	-5.40338634	5.48118711	-1.30392462
1	-3.56634390	5.44038200	-0.16679726
6	-5.92199102	3.46741006	-2.51447019
6	-6.24748705	4.76651720	-2.14466175
1	-5.64721375	6.49882411	-1.02359038
1	-6.56487366	2.91427646	-3.18699629
1	-7.15407812	5.22100344	-2.52442127
6	-4.39404800	1.48459280	-2.47554774
9	-4.50529784	0.59200026	-1.46676538
9	-3.13678905	1.39536654	-2.92257406
9	-5.19292350	1.04500504	-3.45549290
9	-1.38861282	3.94618924	-2.46221037
9	-1.08587900	4.75877019	-0.34375377

*** molecule 1e rotamer B S_0 - dioxane

46

6	0.72186359	0.78127183	0.17741651
6	1.93800791	0.96478022	-0.41411388
16	0.75825052	-0.55281836	1.30129401
6	2.92765705	0.05863410	0.04125777
1	2.12990705	1.74981605	-1.13327700
6	2.44906824	-0.84226563	0.99798202
6	4.29079587	0.16003788	-0.34747712
7	5.39746215	0.25295544	-0.65342400
6	2.41549539	-2.56718290	2.70552605
6	4.03893111	-2.69804566	0.88800702
6	3.43240691	-3.28574074	3.57966446
1	1.71449059	-3.29281413	2.26888345
1	1.86017588	-1.86065826	3.32515814
6	4.97574074	-3.40340491	1.85130876
1	3.45212895	-3.43770821	0.32758543
1	4.62406300	-2.10882902	0.18700506
1	2.91516690	-3.90247648	4.31485027
1	4.04866630	-2.54514115	4.10671026
1	5.59952860	-4.11109838	1.30549764
1	5.62231660	-2.66746921	2.34730056
7	3.10962308	-1.83758759	1.64280404
8	4.25472914	-4.14253635	2.81822788
6	-0.46202812	1.58080746	-0.04458934
6	-1.63609721	1.42639209	0.67800415
6	-2.77550659	2.11528551	0.25437301
1	-1.71334218	0.71167299	1.48301772
1	-3.74162182	1.89244659	0.69814089
8	-0.36197837	2.43827327	-1.01914748
5	-1.34661648	3.52409774	-1.23174332
7	-2.73136089	3.02053663	-0.69664861
6	-3.92429101	3.63440411	-1.18775987
6	-4.15482735	4.97480475	-0.90264544
6	-4.82637866	2.92554616	-1.98794066
6	-5.29919573	5.59855962	-1.38484270
1	-3.42826558	5.51304594	-0.30592583
6	-5.97271941	3.55460870	-2.46192668
6	-6.21087832	4.88900197	-2.15673848
1	-5.47526752	6.64266104	-1.15590718
1	-6.66848773	3.00343694	-3.08137647
1	-7.10250770	5.37436971	-2.53362448
6	-4.55862164	1.49040775	-2.35425150
9	-4.68816094	0.66564734	-1.29111346
9	-3.32311372	1.30206338	-2.83046059
9	-5.41205140	1.04296303	-3.28277015
9	-1.43361620	3.81225034	-2.57222522
9	-0.96906510	4.63898498	-0.48764397

*** molecule **1i** rotamer A S_0 - dioxane

45

6	0.82278601	0.87101178	0.11210266
6	1.00975277	-0.25948396	0.86034495
16	2.33250377	1.43975126	-0.57519159
6	2.35136568	-0.69496145	0.91234772
1	0.21506430	-0.77717603	1.38145716
6	3.21660410	0.13520259	0.16689197
6	2.75005323	-1.81067307	1.69575688

7	3.03931683	-2.71448933	2.35020709
6	-0.38321652	1.60537542	-0.14054085
6	-1.62755791	1.24529024	0.37326723
6	-2.75291996	1.92798580	-0.06934617
1	-1.73705668	0.40417216	1.03890804
1	-3.73845362	1.58082131	0.22790088
8	-0.25115382	2.62856870	-0.93688253
5	-1.30046432	3.66427225	-1.11212508
7	-2.69044446	2.99661619	-0.84639419
6	-3.87470213	3.58577610	-1.35952933
6	-3.95463261	4.97747961	-1.46068455
6	-4.94217492	2.79143163	-1.77487088
6	-5.10861638	5.56329665	-1.95029862
1	-3.11983336	5.58887325	-1.14247194
6	-6.10209705	3.38298979	-2.25827413
1	-4.85764980	1.71150941	-1.75248107
6	-6.18296418	4.76614087	-2.34044840
1	-5.17800909	6.64265178	-2.02122900
1	-6.93016629	2.76543613	-2.58272344
6	-7.40463173	5.43131011	-2.89644152
9	-7.18784585	5.93813563	-4.12436964
9	-7.80664628	6.46139230	-2.13231632
9	-8.44465043	4.59250164	-3.00349695
9	-1.09531270	4.67649358	-0.17823832
9	-1.23863001	4.14662724	-2.40068525
7	4.52766008	0.03224654	-0.02647419
6	5.35388723	-1.11015262	0.40245627
6	5.30215748	1.03414325	-0.77082401
6	6.65280986	-0.89964012	-0.37506642
1	5.51411303	-1.07007479	1.48368574
6	6.74705496	0.62287583	-0.50011818
1	5.05515537	0.97632839	-1.83773771
1	7.50692498	-1.34363986	0.13456795
1	7.08394708	1.05916377	0.44332637
1	5.06686680	2.03853389	-0.41040453
1	4.85776800	-2.04930168	0.15657808
1	6.56751589	-1.35281927	-1.36579682
1	7.41984758	0.94917548	-1.29197725

*** molecule **1i** rotamer B S_0 - dioxane

45

6	0.77074972	0.86946907	0.22519888
6	2.03785562	1.21114629	-0.15878961
16	0.77449854	-0.60135028	1.18127119
6	3.03679833	0.32313014	0.29935977
1	2.25059298	2.09448268	-0.74635454
6	2.50912316	-0.73888713	1.06050429
6	4.41946033	0.55113219	0.06588645
7	5.53548818	0.76354945	-0.12816826
6	-0.43095658	1.59777721	-0.07108969
6	-1.68719917	1.24252428	0.41292863
6	-2.80484566	1.92725069	-0.05480673
1	-1.81695222	0.40464801	1.08101962
1	-3.79743311	1.58171157	0.22019993
8	-0.28023269	2.61167917	-0.87592606
5	-1.31562174	3.65339277	-1.06086661

7	-2.72013585	2.99433098	-0.82671236
6	-3.89012156	3.59716460	-1.35862753
6	-3.95488824	4.98762116	-1.45511689
6	-4.95918176	2.81284656	-1.79486012
6	-5.09721925	5.58947418	-1.95960008
1	-3.11917723	5.58973983	-1.12209231
6	-6.10400663	3.41840093	-2.28963192
1	-4.88484472	1.73214272	-1.77721054
6	-6.17208885	4.80528585	-2.36466698
1	-5.15287921	6.66888250	-2.02630389
1	-6.93562798	2.81262583	-2.62995730
6	-7.39428288	5.44294232	-2.95182032
9	-7.37128141	5.43492439	-4.29795240
9	-7.53291312	6.72251512	-2.57840889
9	-8.51870463	4.80145947	-2.59156444
9	-1.13037385	4.65688788	-0.11301788
9	-1.23055827	4.14698153	-2.34347385
7	3.12773396	-1.76313661	1.64052428
6	4.55364022	-2.09311849	1.46297820
6	2.42353468	-2.75311805	2.46539067
6	4.63594848	-3.52595252	1.98786370
1	4.83347822	-2.00811935	0.41286805
6	3.56170529	-3.56590545	3.07721491
1	1.80485375	-2.25112811	3.21350726
1	4.38502962	-4.22657595	1.18774232
1	3.24895524	-4.57639130	3.33701015
1	1.77759273	-3.37159963	1.83021886
1	5.17173731	-1.40665382	2.04845205
1	5.63216416	-3.76639157	2.35662013
1	3.92294565	-3.07094137	3.98180866

*** molecule **1j** rotamer A S_0 - dioxane

48

6	0.86055628	0.98444396	0.16100630
6	1.04440625	-0.22336432	0.77534704
16	2.37884553	1.66478485	-0.37380692
6	2.39450415	-0.63601435	0.81660771
1	0.23996897	-0.83532405	1.16148354
6	3.27006527	0.28799394	0.21593745
6	2.77022012	-1.92811075	1.27137204
7	3.05820630	-2.98599256	1.62674129
6	5.31668942	1.17301440	-0.77770351
6	5.45379331	-0.37387143	1.12732606
6	6.54116155	0.51538455	-1.40971778
1	5.61157616	2.04392235	-0.17477982
1	4.64406303	1.51424958	-1.56487512
6	6.65733697	-1.07793005	0.51831420
1	5.78738305	0.44875674	1.77591161
1	4.87016706	-1.05792480	1.73500074
1	7.07584877	1.27014645	-1.99104292
1	6.19879086	-0.25602491	-2.10682787
1	7.27658746	-1.47328928	1.32668111
1	6.30592449	-1.92733436	-0.07585934
7	4.60700959	0.21369778	0.07388609
6	-0.36475772	1.68958931	-0.10412685
6	-1.60988891	1.25395077	0.33814681

6	-2.74545689	1.91836569	-0.11199010
1	-1.70989590	0.37237336	0.95102673
1	-3.72663151	1.51614528	0.12358637
8	-0.24071425	2.76113527	-0.83384990
5	-1.32269039	3.76497414	-0.99460000
7	-2.69544611	3.03077354	-0.82312462
6	-3.88260118	3.60606271	-1.34799932
6	-4.01026583	4.99415440	-1.38053810
6	-4.90662563	2.79529538	-1.84371412
6	-5.16965624	5.56821947	-1.88191399
1	-3.20993173	5.61751538	-1.00260795
6	-6.06730271	3.37145587	-2.33305338
1	-4.78264924	1.71954378	-1.87718650
6	-6.19722397	4.75711137	-2.34755061
1	-5.27303507	6.64572391	-1.90092605
1	-6.86283232	2.74498275	-2.72045250
6	-7.45767119	5.34806739	-2.90161522
9	-7.61119311	5.06909762	-4.20917790
9	-7.50084447	6.68032277	-2.77958768
9	-8.55076138	4.86082870	-2.28609323
9	-1.19685732	4.72717518	0.00340014
9	-1.22963469	4.32268047	-2.24966400
6	7.45241625	-0.11086223	-0.35673127
1	8.28635433	-0.62576698	-0.83834624
1	7.88093056	0.67810017	0.27239700

*** molecule **1j** rotamer B S_0 - dioxane

48

6	0.68705023	0.72302689	0.10323501
6	1.96392733	1.05150924	-0.25689085
16	0.65006025	-0.76709020	1.01492215
6	2.93554578	0.13641869	0.21039217
1	2.20520438	1.95049459	-0.80823885
6	2.38642909	-0.92698254	0.94257114
6	4.33143108	0.37217787	0.08855306
7	5.46346613	0.57025504	0.00672429
6	2.27954548	-2.84266519	2.44451808
6	4.13417963	-2.64326583	0.84192693
6	3.22821692	-3.43875931	3.48084758
1	1.78359829	-3.64035126	1.87162698
1	1.51298022	-2.25509077	2.95088718
6	5.11597483	-3.21534425	1.85358790
1	3.70742180	-3.45214481	0.23143242
1	4.63064796	-1.94828871	0.17174016
1	2.66007095	-4.11996655	4.11861656
1	3.60239976	-2.62790916	4.11367996
1	5.90817913	-3.73760704	1.31230360
1	5.57949280	-2.38978866	2.40272178
7	3.01394150	-1.96899001	1.52551737
6	-0.49584638	1.50168865	-0.16281267
6	-1.74940401	1.19919169	0.35579291
6	-2.85146854	1.92902339	-0.08554498
1	-1.89493234	0.37052159	1.03177170
1	-3.85024464	1.62290433	0.21314651
8	-0.32279659	2.50563516	-0.97405687
5	-1.31755664	3.59151396	-1.13217554

7	-2.74230706	2.99000496	-0.86016937
6	-3.90076503	3.63659638	-1.36769621
6	-3.91918247	5.02756181	-1.45887976
6	-5.00382685	2.88967703	-1.78610839
6	-5.05071423	5.67055125	-1.93991804
1	-3.05677843	5.59980309	-1.14129903
6	-6.13534704	3.53512911	-2.25733252
1	-4.96525711	1.80717652	-1.77275812
6	-6.15731264	4.92488126	-2.32782806
1	-5.07024351	6.75112533	-2.00325172
1	-6.99247958	2.95797661	-2.58513428
6	-7.38666051	5.59203942	-2.86580003
9	-7.56738742	5.33330997	-4.17401379
9	-7.35085660	6.92354501	-2.73386221
9	-8.49995647	5.16383571	-2.24343209
9	-1.06441853	4.58344361	-0.18935910
9	-1.24702293	4.08119307	-2.41628307
6	4.40097218	-4.15816036	2.81922690
1	5.09381235	-4.52750516	3.57814488
1	4.03138257	-5.03097803	2.26819549

*** molecule **1a** rotamer A S_{1r} - dioxane

47

6	0.82827932	0.90368932	0.07081338
6	1.02237531	-0.30305646	0.74001428
16	2.35534052	1.56753172	-0.48563961
6	2.37131237	-0.69428683	0.80131059
1	0.22190883	-0.90080042	1.15200883
6	3.25001008	0.22070244	0.18458001
6	2.75038268	-1.95343199	1.33436264
7	3.02721987	-2.99077094	1.75830529
6	5.30266941	1.14903052	-0.75653218
6	5.45155505	-0.43861860	1.08579958
6	6.57469090	0.52312198	-1.31550323
1	5.55097349	2.03118148	-0.15107691
1	4.66998820	1.46046200	-1.58866994
6	6.71148463	-0.99232769	0.44051399
1	5.71714771	0.33663221	1.81693998
1	4.93019133	-1.23711655	1.60548508
1	7.15601093	1.28234817	-1.83914412
1	6.30924825	-0.27353683	-2.02492802
1	7.39455842	-1.34594465	1.21283660
1	6.45282810	-1.83360355	-0.21753228
7	4.59257948	0.17086306	0.06491113
8	7.39331057	0.00544427	-0.29089966
6	-0.35298426	1.61266466	-0.20743117
6	-1.63453510	1.15917982	0.19414612
6	-2.77232848	1.84035348	-0.16807696
1	-1.72786965	0.26509291	0.79382267
1	-3.74395878	1.48562121	0.14836534
8	-0.22684372	2.72939811	-0.90769584
5	-1.30419026	3.72413271	-1.00634230
7	-2.70782664	3.01568538	-0.86186638
6	-3.85970072	3.60011080	-1.34078311
6	-3.90798679	4.99005810	-1.58363504
6	-5.02951778	2.84398257	-1.59789047

6	-5.05966357	5.59623188	-2.04077576
1	-3.03592789	5.59576451	-1.38274077
6	-6.17445507	3.44875766	-2.05803062
1	-5.01849591	1.76755421	-1.48371914
6	-6.20878606	4.83261738	-2.28122589
1	-5.05736470	6.66628636	-2.19912952
1	-7.06186288	2.86621028	-2.27407911
8	-7.37555785	5.32937739	-2.72729933
6	-7.46946925	6.72048673	-2.98913139
1	-8.48463124	6.88870670	-3.34172423
1	-7.29780523	7.30429908	-2.07966408
1	-6.75879856	7.02373690	-3.76396229
9	-1.20273499	4.32980750	-2.25343062
9	-1.17668126	4.67071024	0.02184541

*** molecule **1a** rotamer B S_{1r} - dioxane

47

6	0.88790714	1.05655736	0.10738840
6	1.01057229	-0.21260186	0.65871789
16	2.46643529	1.68657169	-0.35191029
6	2.33439455	-0.68594012	0.68854293
1	0.15604513	-0.78209005	0.99433020
6	3.27317027	0.22826272	0.17533675
6	2.64861668	-2.01024682	1.09180298
7	2.88648547	-3.09442869	1.40709724
6	5.38203839	1.10256891	-0.68360359
6	5.41767280	-0.58287033	1.07681494
6	6.65255114	0.46516629	-1.23269912
1	5.63894578	1.94560063	-0.02677612
1	4.78603005	1.47460944	-1.51852104
6	6.68128572	-1.14232670	0.44517560
1	5.68046993	0.14162490	1.85957380
1	4.85212148	-1.39137781	1.53154748
1	7.27543930	1.23001843	-1.69721230
1	6.38676649	-0.28558207	-1.99035356
1	7.32666602	-1.55757181	1.21916515
1	6.42013232	-1.93888976	-0.26524561
7	4.61474628	0.10701961	0.05981081
8	7.41849484	-0.12973901	-0.20962954
6	-0.30810568	1.77723868	-0.08875790
6	-0.36271262	3.06523319	-0.67588960
6	-1.54911456	3.75028725	-0.78684428
1	0.53967465	3.52740609	-1.05364468
1	-1.57347285	4.72795396	-1.24800012
8	-1.41573817	1.19684868	0.34127588
5	-2.75099301	1.63564838	-0.07681224
7	-2.73656939	3.18050692	-0.40917275
6	-3.89095235	3.92417389	-0.41322529
6	-5.15077963	3.28879303	-0.51666340
6	-3.87211330	5.34008211	-0.32372738
6	-6.31944248	4.01828945	-0.54273161
1	-5.19698477	2.21289988	-0.60461689
6	-5.03859636	6.06415183	-0.34374673
1	-2.93596295	5.86501453	-0.18437481
6	-6.27827536	5.41688152	-0.45858614
1	-7.25996850	3.49250231	-0.63806946

1	-5.02422045	7.14356887	-0.25375199
8	-7.35854592	6.21354569	-0.47477700
6	-8.64509115	5.62168080	-0.57135396
1	-9.35299323	6.44728434	-0.55757463
1	-8.75166004	5.06464572	-1.50702785
1	-8.83755785	4.96052382	0.27877231
9	-3.62456219	1.38724177	0.97684233
9	-3.14842789	0.94032757	-1.22965926

*** molecule **1b** rotamer A S_{1r} - dioxane

43

6	0.83774337	0.92408171	0.07753378
6	1.03381847	-0.28506374	0.75416592
16	2.36003550	1.59843205	-0.47553974
6	2.38192657	-0.66283335	0.83054274
1	0.23329202	-0.88629549	1.16037885
6	3.26218766	0.26297753	0.21994777
6	2.76349901	-1.91811895	1.37078590
7	3.03843344	-2.95355439	1.80017962
6	5.32806302	1.19124764	-0.70923206
6	5.46996469	-0.43669069	1.09665511
6	6.52980420	0.49791063	-1.34349887
1	5.66066632	2.03640293	-0.09360679
1	4.67802477	1.56542799	-1.50025770
6	6.65927259	-1.05786770	0.38003383
1	5.82097806	0.31720971	1.81297910
1	4.92674847	-1.20179551	1.64239699
1	7.13098986	1.23089509	-1.88180004
1	6.17902229	-0.26470345	-2.05308843
1	7.35669925	-1.46498646	1.11196011
1	6.31587535	-1.87095379	-0.27448281
7	4.60066004	0.23880710	0.12858249
8	7.36254390	-0.09013649	-0.37028344
6	-0.34473918	1.62810417	-0.20355228
6	-1.62390162	1.16282512	0.18826391
6	-2.76517631	1.84615308	-0.17783472
1	-1.71880752	0.26069549	0.77524889
1	-3.73904891	1.47274780	0.11144354
8	-0.22235546	2.74455040	-0.90532625
5	-1.29767366	3.74440714	-0.97317232
7	-2.70113054	3.02417063	-0.84641294
6	-3.86012160	3.61733092	-1.32516795
6	-3.92354936	5.01575880	-1.48541220
6	-4.99433190	2.85066042	-1.65538187
6	-5.07964628	5.61933866	-1.93729041
1	-3.06853406	5.62474584	-1.22797626
6	-6.15053881	3.45730532	-2.11104994
1	-4.95838209	1.76971698	-1.60504284
6	-6.19079584	4.83966510	-2.24573819
1	-5.12397570	6.69585375	-2.04396067
1	-7.01203383	2.85827502	-2.37828736
17	-7.64958459	5.60660481	-2.81634730
9	-1.20326953	4.38697276	-2.19833341
9	-1.17566700	4.65301905	0.08740256

*** molecule **1b** rotamer B S_{1r} - dioxane

43

6	0.70026847	0.76002239	0.11614237
6	2.00629434	1.06569120	-0.27147585
16	0.65711870	-0.73774978	1.04178535
6	2.95231045	0.13416646	0.17560566
1	2.24788499	1.95616086	-0.83321179
6	2.39243307	-0.93880032	0.90713550
6	4.34595268	0.34031744	0.00081835
7	5.47566229	0.53207351	-0.13310088
6	2.28572600	-2.89174523	2.37668408
6	4.19446695	-2.63207087	0.88318114
6	3.26014122	-3.42040950	3.42490796
1	1.84305166	-3.72726859	1.81858755
1	1.49064776	-2.34029064	2.87982863
6	5.07962764	-3.16622684	1.99797601
1	3.86811625	-3.45891938	0.23894985
1	4.75016814	-1.92294114	0.27708591
1	2.75916586	-4.16066776	4.04915711
1	3.59862708	-2.58980186	4.06004225
1	5.91278842	-3.72382951	1.57069551
1	5.47728078	-2.33059479	2.59015751
7	2.99534573	-2.00840376	1.45422253
8	4.36600644	-4.05869648	2.82908070
6	-0.45543138	1.51339609	-0.16891029
6	-1.75552602	1.14120378	0.25094970
6	-2.86133789	1.87465453	-0.12616402
1	-1.89980062	0.26900245	0.87446710
1	-3.85090509	1.56652989	0.18452317
8	-0.28051984	2.59711680	-0.90683983
5	-1.28951227	3.66000095	-0.97905061
7	-2.73582844	3.03103146	-0.82846367
6	-3.85998637	3.67682145	-1.31143205
6	-3.83756787	5.07061511	-1.52861521
6	-5.04918253	2.97286317	-1.59234190
6	-4.95997244	5.72852730	-1.98720494
1	-2.94116178	5.63307308	-1.30977840
6	-6.17067188	3.63429480	-2.05615217
1	-5.08288290	1.89491767	-1.49781797
6	-6.12440297	5.01033358	-2.24742413
1	-4.93747589	6.80054300	-2.13713364
1	-7.07356876	3.08257579	-2.28597529
17	-7.54018809	5.84601036	-2.82680287
9	-1.16834698	4.27696850	-2.21521631
9	-1.10486979	4.57615660	0.06627063

*** molecule **1c** rotamer A S_{1r} - dioxane

44

6	0.83861845	0.92138131	0.06567771
6	1.03629683	-0.28297948	0.75143508
16	2.35844242	1.60378312	-0.47936974
6	2.38513144	-0.65030092	0.84427874
1	0.23594272	-0.88700064	1.15378569
6	3.26525033	0.27996550	0.23581038
6	2.76857236	-1.89909258	1.39786593

7	3.04310288	-2.92995249	1.83817012
6	5.33624928	1.21450893	-0.68070991
6	5.47302328	-0.42484369	1.11447668
6	6.51318143	0.49889472	-1.33808459
1	5.69637450	2.04542777	-0.06213553
1	4.68308436	1.61031383	-1.45817766
6	6.63785913	-1.06822470	0.37631224
1	5.85140685	0.32238527	1.82327377
1	4.92315263	-1.17742374	1.67047747
1	7.12088644	1.22233552	-1.88187321
1	6.13482585	-0.25172863	-2.04621327
1	7.33817022	-1.49212184	1.09576495
1	6.26742115	-1.87177553	-0.27512055
7	4.60219505	0.27111337	0.16247191
8	7.34800058	-0.11150168	-0.38105075
6	-0.34703816	1.61905371	-0.22704178
6	-1.62479891	1.15113332	0.15703436
6	-2.76687629	1.83172901	-0.21610663
1	-1.72218759	0.24795322	0.74197026
1	-3.74081247	1.45237521	0.06476188
8	-0.22329596	2.73142980	-0.93415550
5	-1.29541451	3.73317678	-1.00413915
7	-2.70287546	3.00991351	-0.88152489
6	-3.85945471	3.60391667	-1.36149812
6	-3.91884140	5.00374222	-1.51959948
6	-4.99358263	2.83462899	-1.69257122
6	-5.07364122	5.60587327	-1.96770845
1	-3.06238299	5.60978866	-1.26127447
6	-6.14610753	3.44221206	-2.14519615
1	-4.95560183	1.75401756	-1.64315574
6	-6.20028092	4.83351512	-2.28151555
1	-5.11412888	6.68323600	-2.07090359
1	-7.00626194	2.84027046	-2.41180331
9	-1.20029598	4.37457764	-2.22799542
9	-1.18117478	4.63731583	0.05866857
6	-7.39672646	5.46107875	-2.74557580
7	-8.36402291	5.96606665	-3.11896488

*** molecule **1c** rotamer B S_{1r} - dioxane

44

6	0.89230059	1.07510566	0.13433547
6	1.04261240	-0.16747620	0.75582337
16	2.44763841	1.70410955	-0.39613593
6	2.36923214	-0.61123809	0.79933542
1	0.20059134	-0.72893524	1.13351826
6	3.29169726	0.29736554	0.22452778
6	2.70606543	-1.90631338	1.27300091
7	2.95524942	-2.96929088	1.64542331
6	5.38843773	1.14639826	-0.70725824
6	5.46884855	-0.51385375	1.07731915
6	6.56002174	0.41241450	-1.35348564
1	5.75751482	1.97089557	-0.08415106
1	4.74952864	1.55273434	-1.49188889
6	6.63068952	-1.17054980	0.34795487
1	5.85061843	0.21333073	1.80537633
1	4.89380513	-1.26445792	1.61064386

1	7.18872090	1.12706212	-1.88505793
1	6.17679916	-0.32680604	-2.07083413
1	7.31286244	-1.61563768	1.07193161
1	6.25469682	-1.95936801	-0.31783275
7	4.62617142	0.21458659	0.12207596
8	7.36964794	-0.21885133	-0.38913280
6	-0.32056039	1.76792760	-0.06182076
6	-0.40635566	3.03645606	-0.67949883
6	-1.61333574	3.70075596	-0.77402294
1	0.47844343	3.51093744	-1.08222585
1	-1.65827654	4.68412062	-1.22321520
8	-1.40775196	1.18556974	0.41495354
5	-2.75201843	1.56923517	-0.02741624
7	-2.77190700	3.11946233	-0.37467724
6	-3.94950444	3.84506533	-0.36281686
6	-5.18708072	3.18230152	-0.50718777
6	-3.94506023	5.24847718	-0.21495482
6	-6.36305793	3.89803050	-0.52531831
1	-5.20870844	2.10909208	-0.63080500
6	-5.12633093	5.95930313	-0.22769892
1	-3.01774730	5.77746950	-0.03692261
6	-6.34648935	5.29336319	-0.38944412
1	-7.30614607	3.38089420	-0.65250246
1	-5.11247106	7.03436034	-0.09590740
9	-3.63302279	1.30867788	1.00934038
9	-3.10285449	0.86739855	-1.18726653
6	-7.56772720	6.03364208	-0.40789894
7	-8.55230922	6.63418452	-0.42357057

*** molecule **1d** rotamer A S_{1r} - dioxane

46

6	0.84539426	0.92244594	0.07307348
6	1.04905924	-0.26576025	0.78780664
16	2.36039521	1.59022868	-0.50409369
6	2.39890447	-0.62959463	0.87760233
1	0.25215564	-0.85951031	1.21154127
6	3.27353734	0.28543512	0.23919052
6	2.79022445	-1.86411006	1.45723166
7	3.07330606	-2.88338583	1.91861791
6	5.33821237	1.18909049	-0.72296904
6	5.48873529	-0.38663661	1.12610988
6	6.50681257	0.44811369	-1.36718906
1	5.70705245	2.03870688	-0.13567039
1	4.67843092	1.56105511	-1.50656324
6	6.64485559	-1.05900004	0.40005959
1	5.87585271	0.38520421	1.80321321
1	4.94270950	-1.11677960	1.71489799
1	7.11117329	1.15064268	-1.94133442
1	6.11951808	-0.32525399	-2.04536375
1	7.35156930	-1.45880859	1.12702099
1	6.26603338	-1.88419408	-0.21870150
7	4.61037080	0.27615759	0.15796021
8	7.34960304	-0.13156430	-0.39795722
6	-0.34159588	1.61278138	-0.22567598
6	-1.61649854	1.15389935	0.18307105
6	-2.76145613	1.82632077	-0.19784141

1	-1.70811156	0.26586927	0.79162278
1	-3.73413518	1.45394894	0.09761365
8	-0.22485175	2.70726196	-0.96197315
5	-1.29968781	3.70682692	-1.04273450
7	-2.70192985	2.98626546	-0.89128989
6	-3.86653558	3.57006462	-1.37699245
6	-3.93502932	4.96640650	-1.54427735
6	-4.99205846	2.79261970	-1.70236183
6	-5.09579013	5.55487649	-2.00055289
1	-3.08257950	5.57973452	-1.28894339
6	-6.15058871	3.39244142	-2.16225628
1	-4.94756502	1.71258346	-1.64258308
6	-6.21153831	4.77426402	-2.30570318
1	-5.13959290	6.63200955	-2.10862258
1	-7.00479712	2.77890210	-2.41988984
6	-7.44503244	5.43280916	-2.84543448
9	-7.31943026	5.74254599	-4.15407686
9	-7.72215132	6.58662945	-2.21005282
9	-8.53379236	4.65264185	-2.73928908
9	-1.17216776	4.63395009	0.00014588
9	-1.21655360	4.32445021	-2.28005466

*** molecule **1d** rotamer B S_{1r} - dioxane

46

6	0.68906464	0.71691592	0.08398201
6	1.99179456	1.01872281	-0.32747579
16	0.65954888	-0.75435177	1.05055949
6	2.94424051	0.10093082	0.12841019
1	2.22263007	1.89657335	-0.91295805
6	2.39503433	-0.95865179	0.89186703
6	4.33499811	0.30769569	-0.06731947
7	5.46189342	0.50181550	-0.21945249
6	2.32201703	-2.87487927	2.41549666
6	4.22233081	-2.63041971	0.91013224
6	3.31360910	-3.30618417	3.49316371
1	1.91689264	-3.75574229	1.90165325
1	1.50304839	-2.32920514	2.88479557
6	5.12631419	-3.06594975	2.05330372
1	3.92223490	-3.50608155	0.32060112
1	4.74993145	-1.94164027	0.25769184
1	2.83897426	-4.02880788	4.15732546
1	3.61802298	-2.42881665	4.08079504
1	5.97947721	-3.61662489	1.65788911
1	5.49280630	-2.18339402	2.59531197
7	3.00206172	-2.01810284	1.44627569
8	4.44389956	-3.93433318	2.93425929
6	-0.47233293	1.45880183	-0.21127478
6	-1.76649913	1.09194918	0.22690337
6	-2.87702568	1.81717104	-0.15928050
1	-1.90579292	0.23122746	0.86717759
1	-3.86537679	1.50716812	0.15459514
8	-0.30571761	2.52396965	-0.97751457
5	-1.31380235	3.58809243	-1.05322750
7	-2.75817337	2.95874839	-0.87800861
6	-3.89048653	3.59864498	-1.36264413
6	-3.87803600	4.99290754	-1.56606136

6	-5.06664919	2.88283762	-1.65283580
6	-5.00732141	5.63784001	-2.02344927
1	-2.98759778	5.56067521	-1.33695980
6	-6.19266992	3.53933954	-2.11540774
1	-5.08676480	1.80402543	-1.56467213
6	-6.17217966	4.91811389	-2.29515830
1	-4.98814140	6.71260162	-2.15931770
1	-7.08554509	2.97225077	-2.34683122
6	-7.37073958	5.63922936	-2.83353912
9	-7.22437902	5.95593873	-4.13803363
9	-7.59518969	6.79895786	-2.18738970
9	-8.49600749	4.91136837	-2.73905984
9	-1.11861767	4.51489684	-0.01997840
9	-1.20860083	4.18902202	-2.29713531

*** molecule **1e** rotamer A S_{1r} - dioxane

51

6	0.80782414	0.82349309	-0.00480277
6	1.00453020	-0.40283821	0.60755913
16	2.33899020	1.53255714	-0.48646452
6	2.36297566	-0.78040446	0.68072049
1	0.20444084	-1.03278930	0.96993984
6	3.23626272	0.16850631	0.12964735
6	2.75843805	-2.05526469	1.16170006
7	3.05862570	-3.10330727	1.54162056
6	5.28685127	1.16509835	-0.72479050
6	5.40371141	-0.39709434	1.13718329
6	6.65178029	0.65221355	-1.16276179
1	5.40581304	2.06974105	-0.11092312
1	4.70624669	1.41899745	-1.61337405
6	6.75937616	-0.84060743	0.61450126
1	5.53366972	0.39497391	1.88792319
1	4.90967367	-1.24218335	1.60958936
1	7.21122542	1.45703028	-1.64029949
1	6.52067844	-0.16664530	-1.88448848
1	7.39869177	-1.13197179	1.44804806
1	6.63391067	-1.70257249	-0.05573912
7	4.59131652	0.12887145	0.03375428
8	7.41852273	0.20889469	-0.06472119
6	-0.38220788	1.53023417	-0.28560309
6	-1.66377357	1.06471973	0.08244653
6	-2.79705927	1.74727282	-0.27594908
1	-1.76005390	0.15733766	0.66168526
1	-3.76944424	1.39570590	0.04007999
8	-0.24600285	2.66987411	-0.94580905
5	-1.32953508	3.65454170	-1.07109597
7	-2.72847144	2.94572070	-0.95264058
6	-3.86970361	3.52762328	-1.43080544
6	-3.90968423	4.91861421	-1.71939596
6	-5.06104726	2.78972902	-1.65459375
6	-5.04833031	5.52025524	-2.17910349
1	-3.02723334	5.51847207	-1.54946255
6	-6.20282658	3.39088638	-2.12186306
1	-5.06970640	1.71768055	-1.50743748
6	-6.24314986	4.78138558	-2.39642888
1	-5.02517151	6.58507388	-2.36501593

1	-7.07355600	2.77407059	-2.29678296
9	-1.21907788	4.61552241	-0.05185678
9	-1.20354737	4.25537073	-2.32314158
7	-7.37347061	5.38305457	-2.84943671
6	-7.37764132	6.80285731	-3.15739890
1	-6.63883482	7.04467696	-3.92813652
1	-8.36018479	7.08328630	-3.52992780
1	-7.16513654	7.40482610	-2.26779512
6	-8.58644817	4.61063539	-3.04997141
1	-8.44861148	3.84031799	-3.81656135
1	-8.90604827	4.12688889	-2.12139371
1	-9.38290967	5.27555587	-3.37586240

*** molecule 1e rotamer B S_{1r} - dioxane

51

6	0.71863318	0.81053766	0.16628890
6	2.01331556	1.20335941	-0.11276332
16	0.71184927	-0.72899027	1.01466802
6	2.99099807	0.30717951	0.37416421
1	2.24161362	2.12863569	-0.62163352
6	2.45510214	-0.81079495	1.02095016
6	4.38102057	0.58680084	0.30649196
7	5.50927895	0.82529354	0.26157661
6	2.34710942	-2.81676765	2.39571612
6	4.24065546	-2.48598995	0.90400550
6	3.29020901	-3.56163289	3.33089139
1	1.82548519	-3.53387325	1.74409044
1	1.60673389	-2.28297637	2.99468249
6	5.09753138	-3.24126213	1.90497114
1	3.85519984	-3.17904774	0.14291104
1	4.84841872	-1.73257998	0.40877962
1	2.74461035	-4.34400245	3.85933591
1	3.70579667	-2.85867416	4.06676373
1	5.88019027	-3.79076530	1.38172707
1	5.56569715	-2.53167809	2.60136137
7	3.10489421	-1.86087862	1.59429538
8	4.33446287	-4.19154784	2.62207107
6	-0.46856889	1.51458388	-0.15227337
6	-1.76319470	1.07663722	0.19918712
6	-2.88242630	1.76251820	-0.19852245
1	-1.88701083	0.18543877	0.80014654
1	-3.86458798	1.43158975	0.10886331
8	-0.30673661	2.63001709	-0.84334807
5	-1.36959249	3.62790037	-1.00698017
7	-2.78362031	2.94618039	-0.89973038
6	-3.90667060	3.53592271	-1.40608355
6	-3.91510917	4.91962886	-1.73566017
6	-5.11133072	2.81541979	-1.62320863
6	-5.03357580	5.52872255	-2.23117220
1	-3.02300164	5.50623300	-1.57064277
6	-6.23285377	3.42448125	-2.12644115
1	-5.14486436	1.74925408	-1.44178275
6	-6.23997089	4.80647115	-2.44589407
1	-4.98625770	6.58667760	-2.44875737
1	-7.11420373	2.82089124	-2.29402372
9	-1.26411449	4.60915142	-0.00591922

9	-1.21335912	4.20133926	-2.26897663
7	-7.34937343	5.41550201	-2.93653802
6	-7.31974269	6.82466083	-3.29060132
1	-6.56429738	7.02576153	-4.05673530
1	-8.29052822	7.11198478	-3.68765681
1	-7.10878104	7.45064044	-2.41755514
6	-8.57441056	4.66136232	-3.13548501
1	-8.43759767	3.86387367	-3.87381009
1	-8.92115707	4.21519106	-2.19798469
1	-9.35043858	5.33117024	-3.49832193

*** molecule 25A S1r - dioxane

46

6	0.92954407	1.09486346	0.29776769
6	1.17592042	-0.06485093	1.05322134
16	2.41165500	1.77024361	-0.34913941
6	2.53422312	-0.39921282	1.11504972
1	0.40175090	-0.65921331	1.51583108
6	3.37282221	0.50906169	0.41970467
6	2.96404098	-1.60694602	1.72430296
7	3.27478859	-2.60624140	2.21085583
6	5.40146426	1.23375023	-0.76576548
6	5.62724568	-0.26788628	1.11221649
6	6.09748104	0.17876939	-1.62940595
1	6.14005306	1.91512650	-0.33375139
1	4.70348345	1.81053237	-1.37096528
6	6.31445403	-1.27545647	0.19422608
1	6.37671192	0.40940523	1.53462897
1	5.11407815	-0.76044247	1.93198687
1	6.69442688	0.66531133	-2.40117360
1	5.33760916	-0.45368725	-2.11036996
1	7.07120386	-1.83201354	0.74676878
1	5.57234123	-1.98183719	-0.20313041
7	4.70668549	0.54906619	0.32438684
8	6.97860429	-0.60957906	-0.86070986
6	-0.27991804	1.74168122	-0.00258053
6	-1.53454331	1.25809452	0.44181787
6	-2.70230423	1.86340237	0.01620335
1	-1.59340029	0.39505960	1.08867803
1	-3.66573698	1.44992423	0.28615009
8	-0.20436549	2.81088312	-0.78312094
5	-1.31536962	3.77217894	-0.85209479
7	-2.67576723	2.98307465	-0.72992560
6	-3.85266872	3.51095457	-1.27917329
6	-4.08617940	4.88426114	-1.11614345
6	-4.80436960	2.74569993	-1.98720749
6	-5.24845351	5.47046556	-1.57927279
1	-3.34597095	5.47139257	-0.58835244
6	-5.97496291	3.35306728	-2.43747698
6	-6.20953358	4.70262442	-2.22861154
1	-5.40848327	6.53102628	-1.42404366
1	-6.69897499	2.76307143	-2.98442645
1	-7.12631447	5.15313248	-2.58869196
6	-4.59959157	1.29822900	-2.35938170
9	-4.98919345	0.44735199	-1.37729480
9	-3.32386712	1.00103672	-2.64306484

9	-5.32125532	0.95950423	-3.44067799
9	-1.25840124	4.43076694	-2.06732953
9	-1.22722857	4.67567845	0.22105384

*** molecule 25B S1r - dioxane

46

6	0.65859330	0.62164381	0.12946384
6	1.94979687	0.84918323	-0.37417950
16	0.61575692	-0.81658763	1.14315372
6	2.87881613	-0.10798009	0.04140114
1	2.18479468	1.70176525	-0.99384966
6	2.32640295	-1.12401103	0.86246598
6	4.26474764	0.01810598	-0.24093201
7	5.39023195	0.14505654	-0.45955937
6	2.38338291	-2.91747275	2.54472133
6	4.12719160	-2.83571199	0.86185959
6	3.48769513	-2.95258365	3.60387540
1	2.09723788	-3.93656965	2.26422077
1	1.51090960	-2.39956555	2.94179028
6	5.16656413	-2.87302714	1.97669512
1	3.88020460	-3.85996478	0.55988774
1	4.50036102	-2.30499048	-0.00862616
1	3.16079618	-3.54527898	4.45871770
1	3.69984589	-1.92751514	3.93942903
1	6.05082980	-3.41680237	1.64528058
1	5.45867232	-1.84930084	2.24788651
7	2.89645587	-2.22580805	1.36408775
8	4.65813557	-3.55788069	3.10414058
6	-0.48417387	1.40653149	-0.12149451
6	-1.76724468	1.10245571	0.39111831
6	-2.86734718	1.84615001	0.00671334
1	-1.90976342	0.26951843	1.06609171
1	-3.86150602	1.56195724	0.32658365
8	-0.31091370	2.44803880	-0.92121573
5	-1.28298397	3.54892934	-0.93914602
7	-2.73083568	2.94815550	-0.75470773
6	-3.85150240	3.62162877	-1.25634624
6	-3.89013799	5.01644110	-1.10858842
6	-4.93322300	2.98357193	-1.90256578
6	-4.98536972	5.74861443	-1.52408922
1	-3.05203641	5.50453757	-0.62864157
6	-6.03314491	3.73849822	-2.30516166
6	-6.07339592	5.10982381	-2.11006683
1	-4.99327158	6.82286316	-1.38116456
1	-6.85726850	3.24590918	-2.80475629
1	-6.93881912	5.67568506	-2.43244173
6	-4.94522337	1.51792718	-2.25970579
9	-5.39808335	0.73765080	-1.24585202
9	-3.73777843	1.04575018	-2.59881669
9	-5.75919326	1.26951918	-3.29919112
9	-1.19422476	4.20200871	-2.15550426
9	-1.02950579	4.42711679	0.12946045

*** molecule **1i** rotamer A S_{1r} - dioxane

45

6	0.80927843	0.82487561	0.02002064
6	0.99504058	-0.34378263	0.77122769
16	2.33080728	1.42788728	-0.61518153
6	2.33570190	-0.74772174	0.84386978
1	0.19335417	-0.88132714	1.25661133
6	3.21347980	0.10976874	0.13084541
6	2.73076993	-1.88397152	1.59536265
7	3.00529577	-2.81160318	2.22517298
6	-0.36533946	1.53949888	-0.27635575
6	-1.63757399	1.14762161	0.19942330
6	-2.77275559	1.84533903	-0.16760252
1	-1.73727432	0.29052263	0.84963649
1	-3.74570915	1.52048432	0.17838075
8	-0.23883720	2.59314303	-1.07094157
5	-1.27788471	3.62762531	-1.15537435
7	-2.69946546	2.97029047	-0.91482110
6	-3.86118198	3.57558980	-1.38100734
6	-3.88812258	4.96407407	-1.60973119
6	-5.02605916	2.82643285	-1.62666300
6	-5.04508610	5.57439280	-2.04879430
1	-3.00607565	5.55731324	-1.41488119
6	-6.17979611	3.44723024	-2.06846850
1	-5.01743614	1.74931545	-1.51816555
6	-6.19871709	4.82320901	-2.27353380
1	-5.05500532	6.64629966	-2.20498242
1	-7.06501239	2.85452211	-2.26365393
6	-7.43205924	5.49054460	-2.80153102
9	-7.41145049	5.59780460	-4.14840064
9	-7.57935052	6.73970728	-2.32516519
9	-8.55283787	4.81497389	-2.49168706
9	-1.07485964	4.59751845	-0.16353687
9	-1.22403801	4.18576503	-2.42292558
7	4.52973669	0.02918640	-0.02999108
6	5.37344429	-1.07683782	0.44801270
6	5.31206770	1.04832269	-0.74304182
6	6.70990689	-0.82830982	-0.24794538
1	5.46469345	-1.02429959	1.53767228
6	6.75487831	0.69315460	-0.39863922
1	5.12150973	0.96904428	-1.82017063
1	7.54425360	-1.22770831	0.32780393
1	7.03869467	1.16214969	0.54705119
1	5.02305679	2.04863588	-0.41188651
1	4.92668580	-2.03645787	0.18545714
1	6.71304391	-1.30712165	-1.23074228
1	7.44955341	1.02806607	-1.16836687

*** molecule **1i** rotamer B S_{1r} - dioxane

45

6	0.76216625	0.85574660	0.18569614
6	2.06103909	1.20482667	-0.19740662
16	0.76596416	-0.61228673	1.16117723
6	3.04065036	0.32469842	0.28045529
1	2.26863646	2.08205719	-0.79245853
6	2.50819191	-0.74522800	1.04512270
6	4.42315538	0.54130976	0.04509038

7	5.53847941	0.75548728	-0.15896662
6	-0.42090383	1.55312490	-0.13834956
6	-1.70988646	1.13720669	0.26276828
6	-2.83653095	1.82584639	-0.14580555
1	-1.83504001	0.26427997	0.88947108
1	-3.82075910	1.47999364	0.14253857
8	-0.27281813	2.62639342	-0.89989840
5	-1.31456128	3.65421073	-0.99322278
7	-2.74017821	2.97455176	-0.85716907
6	-3.88139254	3.57605955	-1.36888337
6	-3.91283727	4.97050392	-1.56923414
6	-5.02509841	2.82136861	-1.68926789
6	-5.05215120	5.57755548	-2.05302382
1	-3.04840202	5.56811660	-1.31764539
6	-6.16146060	3.44004414	-2.17798352
1	-5.01027364	1.74229755	-1.60359503
6	-6.18483948	4.81928965	-2.35448640
1	-5.06638093	6.65274805	-2.18614024
1	-7.02825057	2.84291121	-2.43217045
6	-7.39365586	5.49820010	-2.92257014
9	-7.23616474	5.79962937	-4.22986455
9	-7.66176947	6.66083583	-2.29848146
9	-8.49988530	4.74017845	-2.83514648
9	-1.17810762	4.58198620	0.04989387
9	-1.19993343	4.26849208	-2.23064261
7	3.12794861	-1.76729087	1.62705655
6	4.55745657	-2.08304237	1.48036195
6	2.43185493	-2.74824120	2.46956172
6	4.66353279	-3.49799393	2.04431177
1	4.85568949	-2.01636943	0.43357975
6	3.56913593	-3.53671101	3.11218011
1	1.79568116	-2.23902480	3.19813522
1	4.45387369	-4.22891886	1.25884666
1	3.26258898	-4.54836292	3.37657977
1	1.80022460	-3.38896997	1.84145310
1	5.15376161	-1.36899838	2.05726705
1	5.65790026	-3.70011412	2.44126437
1	3.90570910	-3.03154792	4.02114990

*** molecule **1j** rotamer A S_{1r} - dioxane

48

6	0.96016109	1.09898361	0.33017671
6	1.18742555	-0.12533550	0.97239255
16	2.46524933	1.88136659	-0.10569075
6	2.54860169	-0.43116203	1.11643694
1	0.40102457	-0.78714216	1.30519009
6	3.40949677	0.57203879	0.59743571
6	2.94894375	-1.68201700	1.65355291
7	3.21626000	-2.72038973	2.08128352
6	5.46980123	1.53852879	-0.31099897
6	5.61972025	-0.34892963	1.20967306
6	6.03492327	0.70575155	-1.46526733
1	6.27781292	2.01001662	0.25685223
1	4.81789903	2.33124860	-0.67426636
6	6.18484906	-1.26046876	0.11980544
1	6.43078910	0.19945678	1.70029798

1	5.09122758	-0.90094004	1.98022983
1	6.60351998	1.36226920	-2.12880325
1	5.19756039	0.30173160	-2.04451512
1	6.85929822	-1.98724182	0.57884962
1	5.36147293	-1.82332149	-0.33289590
7	4.74258834	0.65752039	0.60812828
6	-0.24444735	1.73908977	-0.01245309
6	-1.51331734	1.18007790	0.26302412
6	-2.66514574	1.80037018	-0.18198167
1	-1.59517629	0.25329448	0.81241464
1	-3.63215624	1.34888735	0.00156532
8	-0.14188992	2.88442961	-0.67145454
5	-1.27167254	3.81768733	-0.78009271
7	-2.62627558	2.99863132	-0.80694917
6	-3.78052130	3.52615256	-1.37711757
6	-3.94516939	4.92025892	-1.47051174
6	-4.80016660	2.68941024	-1.86371927
6	-5.09766791	5.44917100	-2.01450979
1	-3.17617517	5.57843328	-1.09175005
6	-5.95094806	3.22908565	-2.40876492
1	-4.67361183	1.61413581	-1.86037036
6	-6.10938842	4.60927795	-2.47988593
1	-5.21697128	6.52463446	-2.06559818
1	-6.72245204	2.57115721	-2.78940530
6	-7.33058992	5.19833331	-3.11797147
9	-7.13352917	5.47539955	-4.42576662
9	-7.70048623	6.35455316	-2.53854622
9	-8.38915331	4.37120491	-3.06012217
9	-1.30139561	4.67067891	0.33205516
9	-1.12376576	4.53157160	-1.95875637
6	6.91463103	-0.43151943	-0.94029139
1	7.23237488	-1.07105065	-1.76692158
1	7.82468005	-0.00709153	-0.49927687

*** molecule **1j** rotamer B S_{1r} - dioxane

48

6	0.62702470	0.45613856	-0.07000786
6	1.94166975	0.75261099	-0.44579618
16	0.54756290	-1.07935663	0.78347999
6	2.86706946	-0.22464398	-0.05783664
1	2.20231763	1.66691362	-0.95839842
6	2.28070501	-1.32956422	0.61319831
6	4.25982312	-0.02645213	-0.24867545
7	5.38398142	0.18271892	-0.40329780
6	2.21037106	-3.27172351	2.10865513
6	4.22046104	-2.84888764	0.80592754
6	2.97025750	-3.04966142	3.41966755
1	2.26708261	-4.32128585	1.80283309
1	1.15761304	-3.01334764	2.21401651
6	5.05816274	-2.61063219	2.06185248
1	4.20886396	-3.91623289	0.55838980
1	4.60861096	-2.32056470	-0.05946204
1	2.52569969	-3.67828044	4.19557853
1	2.83636871	-2.00653882	3.72633869
1	6.08373042	-2.93552251	1.87114668
1	5.09205476	-1.53551948	2.26646433

7	2.82795763	-2.46722147	1.05099659
6	-0.51159754	1.25260228	-0.31497142
6	-1.82073983	0.88390220	0.06560600
6	-2.90363890	1.67358392	-0.27119618
1	-1.99588369	-0.02938583	0.61824040
1	-3.90679156	1.36285936	-0.00853020
8	-0.30199793	2.37675791	-0.98226390
5	-1.27830594	3.47200220	-0.97338328
7	-2.74094562	2.87230596	-0.87718059
6	-3.84813301	3.58725137	-1.31744963
6	-3.79952223	4.99332333	-1.37589342
6	-5.03222080	2.93416692	-1.70371276
6	-4.90346028	5.70988952	-1.78780048
1	-2.90169283	5.51193340	-1.07101662
6	-6.13295325	3.66200585	-2.11839923
1	-5.07776145	1.85267792	-1.72676038
6	-6.07787826	5.05109969	-2.15472212
1	-4.85680279	6.79205919	-1.81226242
1	-7.03312662	3.14368442	-2.42434051
6	-7.24804286	5.84921145	-2.64339080
9	-7.08927880	6.24681394	-3.92457711
9	-7.43395877	6.97038310	-1.92173560
9	-8.39903765	5.15649156	-2.59817891
9	-1.07327889	4.29531585	0.14365427
9	-1.13585190	4.18317850	-2.15461183
6	4.45840783	-3.36514543	3.25088786
1	4.99929457	-3.11730212	4.16692405
1	4.58097604	-4.44328959	3.09123110

Optimised Geometries of compound **1d** (GS and ES in different solvents)

*** molecule **1d** S_0 acetone

```
   46

   6      0.84811036      0.96497399      0.19728164
   6      1.02159711     -0.21996537      0.85680057
  16      2.36595750      1.57973079     -0.41831839
   6      2.36271098     -0.66574650      0.87449245
   1      0.21593466     -0.78903620      1.30277171
   6      3.24394103      0.20624257      0.20188990
   6      2.69160252     -1.93829380      1.40974468
   7      2.91273946     -2.98554184      1.83868487
   6      5.27301511      1.14136713     -0.76143081
   6      5.43985240     -0.55659971      0.99109135
   6      6.55933614      0.57175851     -1.33986745
   1      5.49050126      1.99535212     -0.10716617
   1      4.64984960      1.47356559     -1.59312486
   6      6.70731668     -1.04649614      0.31557126
   1      5.68699886      0.17328367      1.77148677
   1      4.93463612     -1.40169716      1.44741156
   1      7.12342088      1.37155187     -1.81941458
   1      6.31573316     -0.19344369     -2.08823453
   1      7.38417343     -1.45170123      1.06745525
   1      6.46253458     -1.83426145     -0.40886052
   7      4.56999410      0.10608343      0.00442773
   8      7.38313047      0.01381665     -0.33493030
   6     -0.36658430      1.68870897     -0.05418347
   6     -1.61103892      1.29657402      0.42398536
   6     -2.74122715      1.96508217     -0.03286076
   1     -1.72050319      0.43145129      1.05926872
   1     -3.72478447      1.58401902      0.22488858
   8     -0.23474163      2.74285499     -0.81885272
   5     -1.30390274      3.74427851     -1.00127030
   7     -2.68004256      3.05569920     -0.78271265
   6     -3.86450678      3.62278579     -1.32609402
   6     -3.98345262      5.01027734     -1.40736575
   6     -4.89311001      2.80035258     -1.79345775
   6     -5.13708484      5.57588730     -1.93326937
   1     -3.18497540      5.64604284     -1.04593960
   6     -6.04802918      3.36728796     -2.30796170
   1     -4.78156823      1.72269367     -1.77759004
   6     -6.16728107      4.75339482     -2.37381035
   1     -5.23078951      6.65331623     -1.98781029
   1     -6.84664390      2.73057727     -2.67261611
   6     -7.41903630      5.33274015     -2.95570165
   9     -7.55503563      5.03570875     -4.26385033
   9     -7.47031233      6.66776440     -2.85798219
   9     -8.52469168      4.85516632     -2.35261890
   9     -1.13284365      4.76579220     -0.05753813
   9     -1.21046383      4.25918622     -2.28608763
```

*** molecule **1d** S_0 chloroform

```
   46

   6      0.83477136      0.90675185      0.14613553
```

6	1.01494410	-0.26443603	0.82694686
16	2.34581872	1.51919234	-0.48147870
6	2.35991817	-0.70129594	0.84868921
1	0.21466845	-0.82956095	1.28675965
6	3.23027928	0.16376870	0.16109505
6	2.71396996	-1.96027678	1.40210466
7	2.96791707	-2.99424104	1.84375886
6	5.24092291	1.08329546	-0.84092000
6	5.42849727	-0.48581541	1.02644434
6	6.57637580	0.54941342	-1.33482214
1	5.39319079	1.99036193	-0.24045291
1	4.62802595	1.32691084	-1.71055009
6	6.74778718	-0.94390129	0.43262964
1	5.60526943	0.30247231	1.76883672
1	4.94969111	-1.32892086	1.51545826
1	7.11749479	1.34446191	-1.84746782
1	6.40607600	-0.27751155	-2.03637376
1	7.41800514	-1.25598299	1.23341303
1	6.57886033	-1.79164792	-0.24416267
7	4.56344454	0.06307361	-0.03372491
8	7.38709359	0.10873705	-0.26456751
6	-0.38141572	1.63227873	-0.10955820
6	-1.62559117	1.24391757	0.36992923
6	-2.75283686	1.93052984	-0.07201977
1	-1.73833023	0.37754442	1.00242772
1	-3.73905438	1.55982101	0.19154423
8	-0.24467675	2.68265973	-0.87305773
5	-1.30079495	3.70440006	-1.04353324
7	-2.68652935	3.02499779	-0.81079506
6	-3.86937767	3.61595870	-1.33254390
6	-3.97032141	5.00553893	-1.38959236
6	-4.91222351	2.81484902	-1.80420468
6	-5.12196152	5.59329352	-1.89456705
1	-3.15752535	5.62251049	-1.02779296
6	-6.06486828	3.40415972	-2.29786960
1	-4.81056293	1.73618598	-1.81237484
6	-6.16735431	4.79217831	-2.33811226
1	-5.20369165	6.67229558	-1.93205771
1	-6.87497032	2.78521635	-2.66720207
6	-7.41801065	5.39750433	-2.89769811
9	-7.57043643	5.12186475	-4.20743666
9	-7.44867095	6.73077885	-2.77707926
9	-8.52150863	4.92383058	-2.28867718
9	-1.11192817	4.71066550	-0.09390978
9	-1.21994438	4.21475684	-2.32523904

*** molecule **1d** S_0 DMF

46

6	0.84754702	0.96370195	0.19606272
6	1.02263227	-0.21964518	0.85832600
16	2.36503062	1.57950642	-0.42024311
6	2.36435902	-0.66272228	0.87832779
1	0.21755871	-0.78907229	1.30500236
6	3.24491367	0.20881994	0.20384417
6	2.69557250	-1.93301181	1.41683802
7	2.91942757	-2.97868576	1.84818374

6	5.27188101	1.13908960	-0.76839835
6	5.44330020	-0.54621730	0.99551891
6	6.55286451	0.56101191	-1.34954704
1	5.49481548	1.99665001	-0.12077117
1	4.64575890	1.46742251	-1.59932162
6	6.70733530	-1.04297642	0.31844012
1	5.69377894	0.18938840	1.76936684
1	4.93877944	-1.38713910	1.46034265
1	7.11538374	1.35494759	-1.84033957
1	6.30165938	-0.20996005	-2.08953351
1	7.38684286	-1.44270076	1.07102685
1	6.45814263	-1.83732166	-0.39735586
7	4.57053969	0.11064052	0.00770521
8	7.38197443	0.01000780	-0.34529286
6	-0.36758272	1.68599370	-0.05533524
6	-1.61219862	1.29138562	0.42035182
6	-2.74276698	1.95880192	-0.03688291
1	-1.72145758	0.42395981	1.05253602
1	-3.72618616	1.57440900	0.21627817
8	-0.23640736	2.74228522	-0.81824600
5	-1.30626078	3.74380326	-0.99186361
7	-2.68142862	3.05277751	-0.78217291
6	-3.86512065	3.62103130	-1.32567351
6	-3.98623051	5.00887058	-1.39805821
6	-4.89082093	2.79985858	-1.80144154
6	-5.13864424	5.57618771	-1.92458975
1	-3.19072205	5.64398286	-1.02895806
6	-6.04458445	3.36840808	-2.31668542
1	-4.77822554	1.72225033	-1.79097636
6	-6.16550632	4.75470526	-2.37464740
1	-5.23378783	6.65382244	-1.97221829
1	-6.84087688	2.73267902	-2.68806985
6	-7.41515373	5.33559094	-2.95896188
9	-7.54532502	5.04442328	-4.26915609
9	-7.46807053	6.67017120	-2.85572478
9	-8.52331249	4.85479222	-2.36313436
9	-1.13782117	4.75679411	-0.03727786
9	-1.21117039	4.27386735	-2.27094322

*** molecule 1d S_0 DMSO

46

6	0.84845132	0.96685621	0.19620110
6	1.02250757	-0.21726554	0.85733387
16	2.36652919	1.58191881	-0.41952171
6	2.36375407	-0.66137303	0.87725673
1	0.21681264	-0.78641215	1.30320642
6	3.24516713	0.21003597	0.20371581
6	2.69340367	-1.93231833	1.41486151
7	2.91545290	-2.97871767	1.84536992
6	5.27330355	1.13967093	-0.76645429
6	5.44263513	-0.54861011	0.99436620
6	6.55281075	0.56036261	-1.34928316
1	5.49780951	1.99550768	-0.11716629
1	4.64762359	1.47079605	-1.59657874
6	6.70528490	-1.04657767	0.31579392
1	5.69465240	0.18568281	1.76890519

1	4.93704582	-1.38924149	1.45856243
1	7.11620883	1.35416667	-1.83922442
1	6.29956452	-0.20895561	-2.09028952
1	7.38426873	-1.44911151	1.06732217
1	6.45406749	-1.83905755	-0.40131841
7	4.57053777	0.11100064	0.00791073
8	7.38179303	0.00617062	-0.34653076
6	-0.36635200	1.68970979	-0.05416464
6	-1.61037077	1.29604817	0.42378708
6	-2.74149470	1.96211895	-0.03375324
1	-1.71877894	0.42952159	1.05734640
1	-3.72466813	1.57758042	0.22011497
8	-0.23586923	2.74517205	-0.81866603
5	-1.30615671	3.74631337	-0.99090016
7	-2.68071113	3.05510356	-0.78057508
6	-3.86471715	3.62185793	-1.32465009
6	-3.98784184	5.00951243	-1.39642691
6	-4.88879314	2.79924166	-1.80121958
6	-5.14060750	5.57530727	-1.92370123
1	-3.19377265	5.64578396	-1.02620059
6	-6.04286791	3.36625528	-2.31731637
1	-4.77462302	1.72180960	-1.79050026
6	-6.16559797	4.75234943	-2.37522479
1	-5.23734682	6.65280652	-1.97095089
1	-6.83789348	2.72945018	-2.68952987
6	-7.41507467	5.33124856	-2.96153956
9	-7.54321165	5.03846401	-4.27158135
9	-7.46956349	6.66586317	-2.85991156
9	-8.52350246	4.84996554	-2.36668996
9	-1.13733467	4.75921992	-0.03604440
9	-1.21209818	4.27735361	-2.26980958

*** molecule **1d** S_0 EtOH

46

6	0.84307289	0.93081073	0.14832451
6	1.00987632	-0.25268711	0.81132072
16	2.36138036	1.53077214	-0.47770543
6	2.34872915	-0.70706830	0.82358303
1	0.20148497	-0.81379968	1.26241606
6	3.23190318	0.15707958	0.14785076
6	2.67302769	-1.97987006	1.36065413
7	2.88793121	-3.02838003	1.78944217
6	5.25603323	1.11146904	-0.78503269
6	5.40906071	-0.57050733	0.98877529
6	6.60227049	0.61337941	-1.28186285
1	5.39088263	1.98449248	-0.13302841
1	4.66476370	1.40002346	-1.65600242
6	6.73910349	-0.98993553	0.39386732
1	5.56713604	0.16293527	1.78883606
1	4.92571366	-1.44807128	1.40716688
1	7.14933722	1.44196053	-1.73084379
1	6.45659357	-0.17043290	-2.03536488
1	7.39061923	-1.35517823	1.18738213
1	6.58864455	-1.78854682	-0.34324719
7	4.56202705	0.04897638	-0.04722982
8	7.39415487	0.10847346	-0.22012948

6	-0.36736413	1.66621258	-0.09507913
6	-1.60275001	1.31324700	0.42917401
6	-2.73343742	1.99249793	-0.01305557
1	-1.70912114	0.47237406	1.09693288
1	-3.71594624	1.64077479	0.28776216
8	-0.23699384	2.69495588	-0.89606281
5	-1.29339454	3.70517704	-1.09653575
7	-2.67401306	3.05819345	-0.79653312
6	-3.86483601	3.63077188	-1.32195795
6	-3.96975559	5.01760847	-1.42468761
6	-4.91173178	2.81180096	-1.75158267
6	-5.12875737	5.58689418	-1.93437401
1	-3.15684525	5.65092645	-1.09203290
6	-6.07146511	3.38257547	-2.25095976
1	-4.81097875	1.73334418	-1.71806257
6	-6.17716112	4.76844577	-2.33805842
1	-5.21168271	6.66435930	-2.00486731
1	-6.88418869	2.74808090	-2.58707916
6	-7.43195446	5.35266219	-2.90870828
9	-7.56764211	5.07767720	-4.22192268
9	-7.48763341	6.68587834	-2.78898160
9	-8.53507636	4.86137994	-2.31298692
9	-1.06524050	4.77493529	-0.22120798
9	-1.23534022	4.14591677	-2.41197394

*** molecule **1d** S_0 MeCN

46

6	0.84689196	0.96428751	0.20082767
6	1.02119400	-0.22130265	0.85915242
16	2.36447342	1.58091175	-0.41429860
6	2.36261102	-0.66601941	0.87653439
1	0.21555387	-0.79117099	1.30423634
6	3.24379281	0.20753080	0.20499858
6	2.69130653	-1.93880791	1.41094670
7	2.91149557	-2.98654464	1.83933264
6	5.27298247	1.14785397	-0.75374454
6	5.44086424	-0.56059964	0.98764046
6	6.55550982	0.57843201	-1.34059102
1	5.49512314	1.99586765	-0.09357168
1	4.64851947	1.48797666	-1.58112410
6	6.70386433	-1.05152911	0.30471239
1	5.69382223	0.16567176	1.76938410
1	4.93475374	-1.40569513	1.44273507
1	7.12056544	1.37999233	-1.81572706
1	6.30724579	-0.18086099	-2.09321795
1	7.38188643	-1.46326315	1.05188631
1	6.45366743	-1.83352909	-0.42386756
7	4.56931994	0.10938769	0.00743032
8	7.38100387	0.01057741	-0.34211465
6	-0.36765379	1.68768789	-0.04996594
6	-1.61206814	1.29760259	0.42982923
6	-2.74184244	1.96684001	-0.02654643
1	-1.72149509	0.43303763	1.06589059
1	-3.72554668	1.58690689	0.23209621
8	-0.23574878	2.74133824	-0.81630157
5	-1.30380740	3.74229335	-0.99979187

7	-2.68009652	3.05717403	-0.77750662
6	-3.86414931	3.62329063	-1.32280281
6	-3.98233276	5.01070080	-1.40830056
6	-4.89279628	2.79992860	-1.78861008
6	-5.13494850	5.57552841	-1.93744370
1	-3.18412295	5.64723221	-1.04762524
6	-6.04674392	3.36605119	-2.30629215
1	-4.78241550	1.72226016	-1.76844620
6	-6.16494571	4.75207370	-2.37680831
1	-5.22800154	6.65282605	-1.99533901
1	-6.84544521	2.72875373	-2.66967229
6	-7.41525681	5.33012999	-2.96277411
9	-7.54765182	5.03160549	-4.27113994
9	-7.46759607	6.66531875	-2.86707055
9	-8.52258450	4.85289596	-2.36250134
9	-1.12814672	4.76848957	-0.06098503
9	-1.21061473	4.25345259	-2.28712147

*** molecule **1d** S_0 THF

46

6	0.84422451	0.94796142	0.18182294
6	1.02099647	-0.23047597	0.85133901
16	2.35898217	1.56158272	-0.43921351
6	2.36379202	-0.67228553	0.87142079
1	0.21815253	-0.79803381	1.30383841
6	3.23976162	0.19586202	0.19069877
6	2.70421815	-1.93858118	1.41545487
7	2.94110012	-2.97947525	1.85075472
6	5.26047614	1.11679634	-0.79912821
6	5.43950833	-0.52288280	1.00740815
6	6.55986145	0.54906003	-1.34919884
1	5.46062488	1.99546597	-0.17189984
1	4.63666800	1.41248973	-1.64416438
6	6.72282505	-1.00981316	0.35952022
1	5.66618728	0.23303863	1.76934011
1	4.94343715	-1.36329609	1.48278686
1	7.11556906	1.34001852	-1.85247754
1	6.33327077	-0.24497343	-2.07273794
1	7.40118457	-1.37626981	1.12981218
1	6.50023305	-1.82726691	-0.33890206
7	4.56832578	0.09455721	-0.00745735
8	7.38412951	0.03984688	-0.32091942
6	-0.37174923	1.67143903	-0.07230939
6	-1.61684451	1.27382804	0.39922241
6	-2.74658811	1.94623862	-0.05537850
1	-1.72720910	0.40468675	1.02853946
1	-3.73107976	1.56306850	0.19595348
8	-0.23823112	2.72748638	-0.83078368
5	-1.30488378	3.73748713	-0.99917438
7	-2.68376227	3.04223628	-0.79440635
6	-3.86660024	3.61824469	-1.33163826
6	-3.98191942	5.00667515	-1.39505018
6	-4.89676373	2.80435894	-1.80982049
6	-5.13442996	5.58107006	-1.91324111
1	-3.18043093	5.63455673	-1.02676484
6	-6.05052700	3.38020356	-2.31661989

1	-4.78563725	1.72656726	-1.81061433
6	-6.16680724	4.76706435	-2.36391979
1	-5.22636235	6.65914638	-1.95487917
1	-6.85067586	2.75092011	-2.69038466
6	-7.41802700	5.35682691	-2.93736963
9	-7.55829547	5.07106918	-4.24683136
9	-7.46251951	6.69079164	-2.82708515
9	-8.52295630	4.87801146	-2.33442706
9	-1.13981952	4.73493662	-0.03275941
9	-1.21097261	4.27234598	-2.27202459

*** molecule **1d** S_0 Toluene

46

6	0.83702288	0.91368576	0.15206161
6	1.01705473	-0.26052265	0.82719068
16	2.34799134	1.52981997	-0.46861268
6	2.36203112	-0.69780757	0.84852813
1	0.21706050	-0.82932603	1.28236643
6	3.23036560	0.17057615	0.16630160
6	2.72327291	-1.95755244	1.39777677
7	2.99166716	-2.98881236	1.83626626
6	5.24201089	1.07540776	-0.84996413
6	5.43219902	-0.47011446	1.03477537
6	6.57131184	0.52639102	-1.34590731
1	5.40417413	1.98886666	-0.26129409
1	4.62239298	1.31420145	-1.71624225
6	6.74690409	-0.94168114	0.43971584
1	5.61704404	0.32673225	1.76651699
1	4.95071689	-1.30406729	1.53705527
1	7.11584460	1.30930857	-1.87375264
1	6.38744976	-0.30777280	-2.03618434
1	7.42266270	-1.24370915	1.23962676
1	6.56941140	-1.80114154	-0.22044498
7	4.56583308	0.06716653	-0.02927994
8	7.38547028	0.09540878	-0.27764297
6	-0.38027916	1.64006026	-0.10656556
6	-1.62583064	1.24109292	0.36207729
6	-2.75410360	1.92371958	-0.08509507
1	-1.73795199	0.37100588	0.98902475
1	-3.74050365	1.54594942	0.16831697
8	-0.24243758	2.69372103	-0.85969385
5	-1.30240682	3.71980354	-1.02297907
7	-2.68900012	3.02075884	-0.81648256
6	-3.87039220	3.61222270	-1.33948982
6	-3.97167435	5.00181950	-1.38987483
6	-4.91215062	2.81352311	-1.81711597
6	-5.12346394	5.59058747	-1.89244507
1	-3.15730086	5.61498830	-1.02544567
6	-6.06486585	3.40445201	-2.30820746
1	-4.80821077	1.73528159	-1.83491993
6	-6.16869397	4.79213100	-2.34057949
1	-5.20718811	6.66944882	-1.92559010
1	-6.87462530	2.78812710	-2.68215808
6	-7.42067781	5.39951673	-2.89696161
9	-7.57471573	5.12418335	-4.20533742
9	-7.44758614	6.73211290	-2.77364582

9	-8.52091325	4.92504940	-2.28437769
9	-1.13871062	4.69671222	-0.04516784
9	-1.21577254	4.25126014	-2.28981143

*** molecule 1d rotamer B S_0 Acetone

46

6	0.72698896	0.76571984	0.12514584
6	1.99282656	1.08294018	-0.28032334
16	0.71758760	-0.69715578	1.08321556
6	2.97954211	0.18088222	0.18248724
1	2.22469711	1.96058583	-0.86945459
6	2.45102808	-0.86288598	0.96463319
6	4.35990529	0.43651662	-0.02534629
7	5.47364914	0.68195515	-0.19458179
6	2.30240838	-2.82700524	2.39058552
6	4.25806679	-2.52126375	0.95442037
6	3.22317976	-3.52288194	3.38112010
1	1.81081734	-3.56405981	1.74234622
1	1.54605677	-2.28161858	2.95723138
6	5.07975911	-3.22240224	2.02022551
1	3.90729127	-3.24743360	0.21096509
1	4.87804953	-1.78118950	0.45778884
1	2.66285054	-4.28667452	3.92010214
1	3.61045970	-2.78886205	4.09951756
1	5.89757442	-3.76559606	1.54715992
1	5.49567545	-2.48391873	2.71795479
7	3.07601804	-1.88996121	1.56856875
8	4.29905713	-4.16803196	2.72866813
6	-0.46519239	1.52720726	-0.13924615
6	-1.70601438	1.24164207	0.41140899
6	-2.81918331	1.95729945	-0.02776177
1	-1.84295888	0.43176323	1.11240651
1	-3.80914309	1.65615224	0.30169047
8	-0.31157387	2.51129364	-0.98848465
5	-1.31548630	3.57185182	-1.16966586
7	-2.72622455	2.99824353	-0.83588199
6	-3.89711585	3.62753260	-1.34255484
6	-3.91346689	5.01374097	-1.49484732
6	-5.01161571	2.86650463	-1.70364144
6	-5.04892103	5.64118018	-1.98935243
1	-3.04866775	5.60197710	-1.21524200
6	-6.14721134	3.49577605	-2.18789999
1	-4.98368483	1.78609109	-1.62977389
6	-6.16223304	4.88154056	-2.32812943
1	-5.06167520	6.71810903	-2.10126181
1	-7.01263434	2.90633041	-2.47058446
6	-7.39967922	5.52863328	-2.86882701
9	-7.68744006	5.10804156	-4.11632293
9	-7.30783790	6.86387999	-2.92409107
9	-8.48563800	5.24453674	-2.12370641
9	-1.02569732	4.63004348	-0.29795069
9	-1.26701555	4.00821714	-2.48550571

*** molecule **1d** rotamer B S_0 $CHCl_3$

46

6	0.71964593	0.75163998	0.11979948
6	1.98348957	1.07887703	-0.28259545
16	0.72045023	-0.70022991	1.09131912
6	2.97626006	0.19029817	0.19479727
1	2.20447135	1.95540634	-0.87750036
6	2.45481490	-0.84676431	0.98364481
6	4.35963899	0.44112059	-0.00601843
7	5.47800363	0.66864591	-0.16570795
6	2.32699120	-2.77712401	2.45226951
6	4.23619416	-2.52674329	0.94547770
6	3.26210199	-3.49996198	3.40958422
1	1.79243106	-3.50395410	1.82556530
1	1.60540440	-2.20835709	3.04138339
6	5.07505894	-3.25311316	1.98045930
1	3.84102130	-3.24214654	0.21331266
1	4.85834986	-1.80163780	0.42879499
1	2.70205065	-4.24906726	3.96929518
1	3.69815734	-2.77904295	4.11336418
1	5.85894508	-3.82155649	1.48047468
1	5.53716133	-2.52808682	2.66283787
7	3.09623036	-1.86169152	1.60395523
8	4.29195787	-4.17509376	2.71640380
6	-0.47668660	1.50625989	-0.15576912
6	-1.72308432	1.20623607	0.37491069
6	-2.83246290	1.92886765	-0.06421278
1	-1.86310179	0.38666408	1.06364206
1	-3.82572688	1.62480141	0.25326565
8	-0.31651761	2.49711239	-0.99095410
5	-1.31779317	3.56541639	-1.17116897
7	-2.73427113	2.97972672	-0.85575441
6	-3.90118381	3.61965805	-1.35749043
6	-3.91533887	5.00811311	-1.48485002
6	-5.01406885	2.86656993	-1.73799771
6	-5.05019664	5.64416283	-1.96890400
1	-3.04823887	5.58767091	-1.19470752
6	-6.14884026	3.50455297	-2.21215469
1	-4.98273367	1.78496313	-1.68982052
6	-6.16440933	4.89258959	-2.32231445
1	-5.06400816	6.72283902	-2.06120302
1	-7.01293825	2.92155649	-2.51082566
6	-7.39842983	5.55074298	-2.85936274
9	-7.62447138	5.22577141	-4.14673832
9	-7.34052437	6.88726575	-2.80241593
9	-8.50140128	5.17749258	-2.18328801
9	-1.04338221	4.60332758	-0.27780399
9	-1.26184176	4.01146890	-2.47779425

*** molecule **1d** rotamer B S_0 DMF

46

6	0.73040798	0.77031402	0.12478778
6	1.99692168	1.08510862	-0.28037068
16	0.71761946	-0.69434547	1.08043317
6	2.98168799	0.18018084	0.18050969
1	2.23114669	1.96287968	-0.86825742
6	2.45078866	-0.86416352	0.96125798

6	4.36190977	0.43459037	-0.02799660
7	5.47542352	0.68047764	-0.19837993
6	2.29655803	-2.83278898	2.38066746
6	4.25963531	-2.52103025	0.95611552
6	3.21384204	-3.52598413	3.37617761
1	1.81043985	-3.57040535	1.72919866
1	1.53585475	-2.28997856	2.94386200
6	5.07714355	-3.21922137	2.02691770
1	3.91517778	-3.24834716	0.21092917
1	4.88040350	-1.77952622	0.46274577
1	2.65225589	-4.29129715	3.91163610
1	3.59361017	-2.79090252	4.09751544
1	5.89971129	-3.75921812	1.55848163
1	5.48713500	-2.47916910	2.72656923
7	3.07202332	-1.89359068	1.56274625
8	4.29615896	-4.16765466	2.73102904
6	-0.46058239	1.53362264	-0.13773644
6	-1.69986376	1.25089883	0.41760621
6	-2.81438088	1.96350157	-0.02260063
1	-1.83544466	0.44347482	1.12171936
1	-3.80359160	1.66237920	0.30894004
8	-0.30855392	2.51531636	-0.99066793
5	-1.31351408	3.57436892	-1.17136484
7	-2.72294797	3.00164424	-0.83479818
6	-3.89483736	3.62797949	-1.34260591
6	-3.91280787	5.01379172	-1.49837217
6	-5.00900085	2.86488260	-1.70030182
6	-5.04951383	5.63920248	-1.99239404
1	-3.04873014	5.60403793	-1.22073000
6	-6.14590131	3.49215144	-2.18404589
1	-4.98055461	1.78466794	-1.62345962
6	-6.16248461	4.87753394	-2.32757499
1	-5.06330231	6.71589839	-2.10638658
1	-7.01125721	2.90106086	-2.46347547
6	-7.40182577	5.52216806	-2.86628983
9	-7.69555155	5.09495918	-4.11022138
9	-7.30973257	6.85709742	-2.92953369
9	-8.48479179	5.24308988	-2.11488121
9	-1.02223180	4.63509356	-0.30210628
9	-1.26727400	4.01049748	-2.48809001

*** molecule 1d rotamer B S_0 DMSO

46

6	0.73228763	0.79037516	0.15153725
6	1.99446420	1.09280429	-0.27586501
16	0.72321786	-0.66846052	1.11586616
6	2.97904746	0.18237293	0.17418763
1	2.22616464	1.96453473	-0.87359394
6	2.45232854	-0.85363126	0.96842659
6	4.35764529	0.42364616	-0.05863975
7	5.47013202	0.65960550	-0.24856701
6	2.30311917	-2.81683163	2.39409807
6	4.24143398	-2.52887597	0.93106839
6	3.22989568	-3.52712266	3.36800241
1	1.79312159	-3.54534060	1.75055213
1	1.56222769	-2.26497970	2.97468518

6	5.06920107	-3.24442457	1.98217254
1	3.87162905	-3.24690834	0.18908599
1	4.86407083	-1.79433155	0.42966401
1	2.66761636	-4.28506133	3.91304368
1	3.63672410	-2.80082510	4.08344788
1	5.87368023	-3.79466987	1.49462692
1	5.50449661	-2.51396180	2.67653135
7	3.07531204	-1.88622214	1.56329095
8	4.28815609	-4.18376537	2.69826356
6	-0.45840081	1.55684847	-0.10286537
6	-1.69181615	1.28401743	0.47018510
6	-2.81117929	1.98674278	0.02661489
1	-1.82050901	0.48674951	1.18708462
1	-3.79744634	1.68833143	0.36913142
8	-0.31357776	2.52784790	-0.96925826
5	-1.32170722	3.58303916	-1.15462546
7	-2.72750002	3.01110314	-0.80380470
6	-3.90318765	3.62104208	-1.32173457
6	-3.92528851	5.00580013	-1.50781423
6	-5.01447461	2.84907348	-1.65808445
6	-5.06370861	5.61370737	-2.01065113
1	-3.06232951	5.60431141	-1.24474724
6	-6.15826453	3.46182642	-2.15281723
1	-4.98378518	1.77086119	-1.55723935
6	-6.17930873	4.84031614	-2.32454725
1	-5.08397247	6.68850168	-2.15016995
1	-7.02003589	2.85995873	-2.41396428
6	-7.38321197	5.51277315	-2.90680193
9	-7.21392713	5.81845225	-4.20995060
9	-7.66656006	6.67257647	-2.28818072
9	-8.48657327	4.75421647	-2.83613763
9	-1.02800755	4.65352503	-0.29816704
9	-1.28402153	4.00569881	-2.47613533

*** molecule **1d** rotamer B S_0 EtOH

46

6	0.72713386	0.76761674	0.13581557
6	1.99220248	1.09350982	-0.26497424
16	0.72332556	-0.69147476	1.09800884
6	2.98194494	0.19850567	0.20512935
1	2.21992063	1.97231849	-0.85438980
6	2.45704458	-0.84435155	0.98811563
6	4.36186176	0.45842395	0.00082994
7	5.47464669	0.70922565	-0.16633048
6	2.31195146	-2.80341936	2.41526984
6	4.24862255	-2.51010807	0.95371294
6	3.23007130	-3.53585648	3.37906347
1	1.79753203	-3.51990542	1.76129241
1	1.57394677	-2.25566177	3.00379738
6	5.07393939	-3.24938911	1.98869336
1	3.87065733	-3.21216776	0.20037727
1	4.87866050	-1.77394822	0.46313787
1	2.66257118	-4.29883284	3.91144884
1	3.64940458	-2.82740627	4.10407651
1	5.86991371	-3.80253550	1.49063822
1	5.51720252	-2.53742182	2.69605757

7	3.09157211	-1.86408513	1.60132664
8	4.28310657	-4.19328157	2.69458597
6	-0.46782740	1.52219086	-0.13592685
6	-1.70876087	1.23867730	0.41151447
6	-2.82131033	1.95411946	-0.03170861
1	-1.84830654	0.43157676	1.11530189
1	-3.81133306	1.65435496	0.29922399
8	-0.31312594	2.50361342	-0.99130226
5	-1.31793923	3.56134149	-1.18443192
7	-2.72762763	2.99312693	-0.84133813
6	-3.89821397	3.62374528	-1.34809778
6	-3.91311377	5.00984726	-1.49915234
6	-5.01281185	2.86386434	-1.71018132
6	-5.04806494	5.63899150	-1.99245735
1	-3.04835857	5.59778422	-1.21863071
6	-6.14797754	3.49481233	-2.19318495
1	-4.98570307	1.78322346	-1.63793400
6	-6.16195490	4.88068280	-2.33179665
1	-5.05925492	6.71615155	-2.10280830
1	-7.01378472	2.90592089	-2.47608694
6	-7.39966620	5.52969025	-2.86938549
9	-7.69482181	5.10479993	-4.11364937
9	-7.30351363	6.86437551	-2.93082132
9	-8.48293068	5.25264894	-2.11764094
9	-1.02339086	4.63234775	-0.33035744
9	-1.27026181	3.97760503	-2.50762650

*** molecule **1d** rotamer B S_0 MeCN

46

6	0.72862158	0.76629689	0.12443177
6	1.99410026	1.08437177	-0.28161087
16	0.72040494	-0.69512368	1.08456609
6	2.98170884	0.18359021	0.18196595
1	2.22452755	1.96184980	-0.87171966
6	2.45395541	-0.85985076	0.96589126
6	4.36122447	0.44090562	-0.02866227
7	5.47387886	0.68938289	-0.20112815
6	2.30016201	-2.82658358	2.38574650
6	4.26379742	-2.51429259	0.96062001
6	3.21496721	-3.53032218	3.37585174
1	1.80925739	-3.55828206	1.73104972
1	1.54310823	-2.28296886	2.95312129
6	5.07885475	-3.22298077	2.02640792
1	3.91694361	-3.23515867	0.21029751
1	4.88741264	-1.77139271	0.47298392
1	2.65038559	-4.29663380	3.90656656
1	3.60077921	-2.80199742	4.10062560
1	5.89882730	-3.76355930	1.55420551
1	5.49059132	-2.48991012	2.73216248
7	3.07826636	-1.88602418	1.57146035
8	4.29310678	-4.17296803	2.72374211
6	-0.46398972	1.52621226	-0.14068239
6	-1.70378989	1.24277466	0.41285412
6	-2.81745014	1.95820116	-0.02543616
1	-1.83979605	0.43489660	1.11633694
1	-3.80678603	1.65869065	0.30709896

8	-0.31150948	2.50811223	-0.99367603
5	-1.31544813	3.56731762	-1.17589508
7	-2.72536019	2.99722533	-0.83663997
6	-3.89690776	3.62647540	-1.34216136
6	-3.91140989	5.01223439	-1.49960604
6	-5.01388043	2.86598456	-1.69694291
6	-5.04708562	5.63993238	-1.99341425
1	-3.04508518	5.60025654	-1.22437976
6	-6.14974695	3.49554805	-2.18034798
1	-4.98827127	1.78588753	-1.61823771
6	-6.16268342	4.88084091	-2.32599430
1	-5.05829424	6.71644302	-2.10924860
1	-7.01711737	2.90656748	-2.45787331
6	-7.40012357	5.52811976	-2.86628228
9	-7.68893133	5.10704287	-4.11354676
9	-7.30776985	6.86337367	-2.92271945
9	-8.48604875	5.24530824	-2.12066446
9	-1.02139680	4.62997924	-0.30986603
9	-1.26882126	3.99947385	-2.49404626

*** molecule **1d** rotamer B S_0 THF

46

6	0.72172644	0.75301730	0.11316230
6	1.98704769	1.07339817	-0.29064605
16	0.71597546	-0.70322893	1.07990664
6	2.97592792	0.17819634	0.18128112
1	2.21496119	1.94920717	-0.88378075
6	2.44998006	-0.86059901	0.96807428
6	4.35841357	0.43007064	-0.02072882
7	5.47533743	0.66413840	-0.18265830
6	2.31489517	-2.80194188	2.42543043
6	4.24570495	-2.52983856	0.94967906
6	3.24733405	-3.49890600	3.40462960
1	1.80400260	-3.54179466	1.79497104
1	1.57409910	-2.24234102	2.99892496
6	5.07970918	-3.23094498	2.00610783
1	3.87478532	-3.25891035	0.21861908
1	4.86325951	-1.79943207	0.43552171
1	2.69074741	-4.25227117	3.96197908
1	3.65558058	-2.76271814	4.10934068
1	5.88260242	-3.78808118	1.52383254
1	5.51750394	-2.49070255	2.68855998
7	3.08255218	-1.88074337	1.58153056
8	4.30218710	-4.16073307	2.73732134
6	-0.47196159	1.51251048	-0.15603882
6	-1.71548718	1.21919632	0.38515292
6	-2.82691170	1.93879425	-0.05293172
1	-1.85382169	0.40324219	1.07862040
1	-3.81877062	1.63531205	0.26903947
8	-0.31530792	2.50020067	-0.99740691
5	-1.31666374	3.56764168	-1.17158791
7	-2.73086824	2.98656605	-0.84990813
6	-3.89932413	3.62311036	-1.35226996
6	-3.91506267	5.01116588	-1.48473084
6	-5.01233220	2.86741893	-1.72745440
6	-5.05080500	5.64490315	-1.96976150

1	-3.04927796	5.59377978	-1.19667788
6	-6.14801400	3.50296375	-2.20294456
1	-4.98156222	1.78608488	-1.67243805
6	-6.16443367	4.89059815	-2.31925932
1	-5.06498949	6.72331036	-2.06544650
1	-7.01208230	2.91766633	-2.49733521
6	-7.39883883	5.54567346	-2.85790963
9	-7.62582502	5.21594642	-4.14444633
9	-7.34246746	6.88272901	-2.80692167
9	-8.50213398	5.17517019	-2.18049470
9	-1.03430620	4.60885126	-0.28144031
9	-1.26590720	4.01757018	-2.47926248

*** molecule **1d** rotamer B S_0 Toluene

46

6	0.72401168	0.76860999	0.13354537
6	1.98821546	1.08944699	-0.27173359
16	0.71920213	-0.68523123	1.10039738
6	2.97714812	0.19420778	0.20273063
1	2.21041900	1.96557645	-0.86624288
6	2.45177474	-0.83937260	0.98832239
6	4.36581626	0.42323732	0.00546725
7	5.49098546	0.61824802	-0.14601087
6	2.33603347	-2.74758282	2.48772947
6	4.19442665	-2.55929610	0.91307511
6	3.29071388	-3.47212851	3.42547585
1	1.76910137	-3.47636472	1.89148874
1	1.64217077	-2.15483565	3.08665978
6	5.05559975	-3.28606458	1.93005937
1	3.75843963	-3.27984759	0.20898841
1	4.80909699	-1.85385469	0.36070245
1	2.73936594	-4.20162121	4.01896581
1	3.76131839	-2.74591820	4.10166877
1	5.80925214	-3.88143036	1.41497350
1	5.55861523	-2.55767744	2.57947519
7	3.09517070	-1.86041164	1.60377523
8	4.28160129	-4.17659707	2.71032348
6	-0.47177730	1.52919068	-0.13964800
6	-1.71954078	1.22052695	0.38449854
6	-2.82994951	1.93847121	-0.06094741
1	-1.85738918	0.39581016	1.06707358
1	-3.82539779	1.62640639	0.24260946
8	-0.30897766	2.52399033	-0.96393257
5	-1.31265686	3.59810904	-1.13855455
7	-2.73157349	2.99124657	-0.84649382
6	-3.89753812	3.62304957	-1.35871709
6	-3.92917726	5.01277526	-1.46258577
6	-4.99183713	2.86047318	-1.77187164
6	-5.06628755	5.63966922	-1.95261435
1	-3.07283565	5.59645265	-1.14943496
6	-6.12873259	3.48976838	-2.25208922
1	-4.94140927	1.77864037	-1.74743158
6	-6.16402367	4.87879125	-2.33607209
1	-5.09691785	6.71928110	-2.02685490
1	-6.97950987	2.90133036	-2.57662850
6	-7.40121748	5.52794746	-2.87891815

9	-7.60041478	5.22521759	-4.17482572
9	-7.36481031	6.86303114	-2.79193889
9	-8.50541811	5.12057684	-2.22647850
9	-1.06185201	4.61132197	-0.21792895
9	-1.25205646	4.06207712	-2.43284742

*** molecule **1d** rotamer A S_{1r} acetone

46

6	0.88043612	0.97379571	0.14042650
6	1.09516836	-0.20431574	0.87561137
16	2.39152000	1.66273207	-0.41648644
6	2.44665641	-0.54189132	0.99648959
1	0.30079790	-0.80390831	1.29558841
6	3.32189684	0.38330032	0.35987490
6	2.83062717	-1.75623529	1.61979577
7	3.08625076	-2.76367567	2.12223724
6	5.39326837	1.29333797	-0.59760821
6	5.55005325	-0.40564320	1.12082624
6	6.33218823	0.44157270	-1.45107797
1	5.96574734	2.00564321	0.00407138
1	4.71521744	1.84500173	-1.24640116
6	6.48161771	-1.19561489	0.20835545
1	6.13512298	0.28014745	1.74254800
1	4.99812932	-1.07082618	1.77566926
1	6.95379970	1.09171726	-2.06648953
1	5.73868601	-0.21121104	-2.10554336
1	7.21374848	-1.73376216	0.80979846
1	5.90144609	-1.91855863	-0.38064917
7	4.65007207	0.41443841	0.30761360
8	7.20000396	-0.32943327	-0.64735393
6	-0.31499419	1.63026084	-0.18962660
6	-1.58835337	1.14471718	0.17828611
6	-2.73706232	1.80127586	-0.22196406
1	-1.68208580	0.24407579	0.76771559
1	-3.70885554	1.39979166	0.03478977
8	-0.20740796	2.73442473	-0.93280109
5	-1.29414895	3.70866292	-1.00280675
7	-2.68328915	2.97817089	-0.88925608
6	-3.84900264	3.55238400	-1.39083148
6	-3.94629375	4.95120833	-1.51515023
6	-4.94386752	2.76085378	-1.77508270
6	-5.10494143	5.52845822	-1.99102989
1	-3.11905231	5.57744520	-1.21219345
6	-6.10268877	3.34862717	-2.25343735
1	-4.87874656	1.68092159	-1.74257379
6	-6.19121151	4.73181345	-2.35817134
1	-5.16911617	6.60768450	-2.06590217
1	-6.93197221	2.72175395	-2.55565252
6	-7.42324548	5.38891843	-2.89814995
9	-7.21755739	5.92447196	-4.12294672
9	-7.84070401	6.40545866	-2.11523122
9	-8.45680425	4.54083293	-3.01980668
9	-1.18617693	4.63396180	0.05781231
9	-1.19444000	4.36980037	-2.22695508

*** molecule **1d** rotamer A S_{1r} $CHCl_3$

46

6	0.84811280	0.91348789	0.06803918
6	1.05509311	-0.26230916	0.80556158
16	2.36194375	1.57719357	-0.51443065
6	2.40476702	-0.61699682	0.91067438
1	0.25871677	-0.85032105	1.23808836
6	3.28128253	0.29165970	0.25852364
6	2.78885152	-1.83589522	1.52591687
7	3.05423870	-2.84504950	2.01937620
6	5.34378789	1.21930775	-0.68497418
6	5.49892697	-0.40670101	1.11890377
6	6.48838832	0.47720835	-1.36931131
1	5.73499659	2.04325591	-0.07747465
1	4.68017967	1.62591030	-1.44718064
6	6.63194309	-1.07815626	0.35568015
1	5.90804731	0.34291954	1.80678217
1	4.95344656	-1.14278499	1.69986491
1	7.09191257	1.18676166	-1.93519374
1	6.07781708	-0.27205555	-2.06000230
1	7.34195685	-1.50777087	1.06193125
1	6.23058911	-1.88016996	-0.27850695
7	4.61390151	0.29493518	0.18446877
8	7.33919153	-0.14096581	-0.42959485
6	-0.34076259	1.59273377	-0.24307757
6	-1.61444435	1.13946397	0.16852892
6	-2.75958479	1.81347592	-0.21137509
1	-1.70870997	0.25333431	0.77943972
1	-3.73170208	1.44151799	0.08555248
8	-0.22718621	2.68111237	-0.99890450
5	-1.29731860	3.67908361	-1.07168509
7	-2.69979347	2.97329415	-0.90612917
6	-3.86585102	3.56260926	-1.38515399
6	-3.93047768	4.95917400	-1.55045526
6	-4.99542745	2.78994219	-1.70556169
6	-5.09036886	5.55302934	-2.00245392
1	-3.07587608	5.57049245	-1.29746196
6	-6.15397005	3.39459103	-2.16047951
1	-4.95687810	1.70993143	-1.64382511
6	-6.21014494	4.77651714	-2.30412373
1	-5.12933867	6.63054315	-2.10924466
1	-7.01078561	2.78298455	-2.41377975
6	-7.44170614	5.44199790	-2.83696911
9	-7.30926895	5.78452994	-4.13811757
9	-7.72868602	6.58145187	-2.17809393
9	-8.52976406	4.65792175	-2.75780461
9	-1.15168389	4.61992780	-0.03620533
9	-1.21792526	4.29946185	-2.31343053

*** molecule **1d** rotamer A S_{1r} dioxane

46

6	0.84539426	0.92244594	0.07307348
6	1.04905924	-0.26576025	0.78780664
16	2.36039521	1.59022868	-0.50409369
6	2.39890447	-0.62959463	0.87760233

1	0.25215564	-0.85951031	1.21154127
6	3.27353734	0.28543512	0.23919052
6	2.79022445	-1.86411006	1.45723166
7	3.07330606	-2.88338583	1.91861791
6	5.33821237	1.18909049	-0.72296904
6	5.48873529	-0.38663661	1.12610988
6	6.50681257	0.44811369	-1.36718906
1	5.70705245	2.03870688	-0.13567039
1	4.67843092	1.56105511	-1.50656324
6	6.64485559	-1.05900004	0.40005959
1	5.87585271	0.38520421	1.80321321
1	4.94270950	-1.11677960	1.71489799
1	7.11117329	1.15064268	-1.94133442
1	6.11951808	-0.32525399	-2.04536375
1	7.35156930	-1.45880859	1.12702099
1	6.26603338	-1.88419408	-0.21870150
7	4.61037080	0.27615759	0.15796021
8	7.34960304	-0.13156430	-0.39795722
6	-0.34159588	1.61278138	-0.22567598
6	-1.61649854	1.15389935	0.18307105
6	-2.76145613	1.82632077	-0.19784141
1	-1.70811156	0.26586927	0.79162278
1	-3.73413518	1.45394894	0.09761365
8	-0.22485175	2.70726196	-0.96197315
5	-1.29968781	3.70682692	-1.04273450
7	-2.70192985	2.98626546	-0.89128989
6	-3.86653558	3.57006462	-1.37699245
6	-3.93502932	4.96640650	-1.54427735
6	-4.99205846	2.79261970	-1.70236183
6	-5.09579013	5.55487649	-2.00055289
1	-3.08257950	5.57973452	-1.28894339
6	-6.15058871	3.39244142	-2.16225628
1	-4.94756502	1.71258346	-1.64258308
6	-6.21153831	4.77426402	-2.30570318
1	-5.13959290	6.63200955	-2.10862258
1	-7.00479712	2.77890210	-2.41988984
6	-7.44503244	5.43280916	-2.84543448
9	-7.31943026	5.74254599	-4.15407686
9	-7.72215132	6.58662945	-2.21005282
9	-8.53379236	4.65264185	-2.73928908
9	-1.17216776	4.63395009	0.00014588
9	-1.21655360	4.32445021	-2.28005466

*** molecule **1d** rotamer A S_{1r} DMF

46

6	0.87819824	0.96969241	0.13911374
6	1.09226423	-0.20635669	0.87819182
16	2.38959182	1.65443590	-0.42174289
6	2.44315692	-0.54547808	0.99880402
1	0.29746733	-0.80288860	1.30171735
6	3.31945096	0.37615313	0.35748453
6	2.82476098	-1.75700713	1.62886937
7	3.07697729	-2.76211362	2.13770159
6	5.38957620	1.29255429	-0.59540161
6	5.54759618	-0.41513743	1.11512940
6	6.34090664	0.45291809	-1.44668797

1	5.95208844	2.00703490	0.01314248
1	4.71159661	1.84119374	-1.24675787
6	6.49163889	-1.19168387	0.20411370
1	6.12242612	0.27018341	1.74682764
1	4.99630311	-1.09040194	1.75997575
1	6.96078669	1.11176220	-2.05450804
1	5.75747370	-0.20152420	-2.10837250
1	7.22309592	-1.72807527	0.80792030
1	5.92132902	-1.91514473	-0.39369283
7	4.64705009	0.40446656	0.30164316
8	7.20982368	-0.31500454	-0.64104133
6	-0.31676151	1.62641043	-0.19148110
6	-1.59025847	1.14428934	0.17965023
6	-2.73862360	1.80182543	-0.22012831
1	-1.68474538	0.24522483	0.77136216
1	-3.71053208	1.40240331	0.03921905
8	-0.20886920	2.72848247	-0.93912500
5	-1.29395143	3.70364317	-1.00932258
7	-2.68402362	2.97725023	-0.89035117
6	-3.84973440	3.55254171	-1.39098376
6	-3.94456384	4.95122693	-1.51897993
6	-4.94698418	2.76220873	-1.77081276
6	-5.10281372	5.52957595	-1.99459597
1	-3.11578741	5.57689406	-1.21906396
6	-6.10548415	3.35101818	-2.24879470
1	-4.88442891	1.68226100	-1.73484395
6	-6.19130962	4.73406195	-2.35764672
1	-5.16481020	6.60873523	-2.07233074
1	-6.93655472	2.72480384	-2.54741694
6	-7.42285452	5.39223420	-2.89717247
9	-7.21736393	5.92700328	-4.12253699
9	-7.83864455	6.40999731	-2.11473282
9	-8.45765406	4.54562586	-3.01773412
9	-1.18109056	4.63353000	0.04772000
9	-1.19527874	4.36175936	-2.23599629

*** molecule **1d** rotamer A S_{1r} DMSO

46

6	0.87768335	0.96876969	0.13857907
6	1.09165651	-0.20637214	0.87923446
16	2.38907012	1.65194767	-0.42410771
6	2.44239027	-0.54596623	0.99958821
1	0.29680440	-0.80179459	1.30421862
6	3.31887319	0.37429971	0.35631638
6	2.82346207	-1.75647511	1.63190119
7	3.07489160	-2.76073282	2.14280184
6	5.38851160	1.29171474	-0.59628759
6	5.54708647	-0.41701326	1.11344388
6	6.34349881	0.45493891	-1.44616507
1	5.94805352	2.00744316	0.01355489
1	4.71046920	1.83878007	-1.24888723
6	6.49478707	-1.19035536	0.20355872
1	6.11889503	0.26871746	1.74743996
1	4.99604041	-1.09467087	1.75595233
1	6.96280143	1.11580122	-2.05237006
1	5.76305128	-0.20059994	-2.10935031

1	7.22610217	-1.72564994	0.80850515
1	5.92742006	-1.91451699	-0.39615851
7	4.64631437	0.40170409	0.29919651
8	7.21279517	-0.31129897	-0.63928413
6	-0.31718033	1.62552633	-0.19211375
6	-1.59064600	1.14462940	0.18051275
6	-2.73897523	1.80236571	-0.21907482
1	-1.68523763	0.24627818	0.77328963
1	-3.71087154	1.40373120	0.04148096
8	-0.20932788	2.72666172	-0.94150444
5	-1.29388703	3.70216102	-1.01188888
7	-2.68424691	2.97707376	-0.89064746
6	-3.85006910	3.55255433	-1.39088410
6	-3.94415586	4.95115406	-1.52042651
6	-4.94815732	2.76248697	-1.76881803
6	-5.10241093	5.52969952	-1.99581636
1	-3.11482336	5.57672583	-1.22185798
6	-6.10668438	3.35147690	-2.24654788
1	-4.88637331	1.68254769	-1.73149077
6	-6.19169894	4.73443805	-2.35706165
1	-5.16375472	6.60881196	-2.07475041
1	-6.93839197	2.72539341	-2.54365760
6	-7.42326093	5.39280719	-2.89624107
9	-7.21807599	5.92739894	-4.12177924
9	-7.83853528	6.41085870	-2.11383609
9	-8.45835114	4.54652345	-3.01632507
9	-1.17927371	4.63377688	0.04368608
9	-1.19583222	4.35883356	-2.23959688

*** molecule **1d** rotamer A S_{1r} EtOH

46

6	0.87973605	0.97242997	0.13993035
6	1.09427941	-0.20483888	0.87668185
16	2.39089954	1.65982681	-0.41852860
6	2.44555960	-0.54290269	0.99749945
1	0.29977601	-0.80329924	1.29802381
6	3.32115027	0.38096185	0.35906063
6	2.82872269	-1.75615930	1.62336326
7	3.08314457	-2.76271041	2.12820458
6	5.39205613	1.29305340	-0.59705813
6	5.54933256	-0.40870488	1.11885445
6	6.33502764	0.44523865	-1.44983962
1	5.96128114	2.00609391	0.00685537
1	4.71400717	1.84370255	-1.24668688
6	6.48498979	-1.19430248	0.20684396
1	6.13103541	0.27701375	1.74379537
1	4.99765689	-1.07719125	1.77048698
1	6.95602759	1.09824288	-2.06282090
1	5.74480690	-0.20814823	-2.10661467
1	7.21693185	-1.73180858	0.80908144
1	5.90804837	-1.91747682	-0.38499618
7	4.64910409	0.41115242	0.30554272
8	7.20327718	-0.32470098	-0.64549224
6	-0.31555481	1.62889535	-0.19036832
6	-1.58894037	1.14458123	0.17876736
6	-2.73755435	1.80145001	-0.22130222

1	-1.68291430	0.24453099	0.76906078
1	-3.70937032	1.40069015	0.03642967
8	-0.20791973	2.73225400	-0.93527869
5	-1.29407154	3.70679450	-1.00531251
7	-2.68353106	2.97779991	-0.88968994
6	-3.84928003	3.55238180	-1.39087587
6	-3.94570313	4.95115396	-1.51653992
6	-4.94501761	2.76126498	-1.77345965
6	-5.10423611	5.52878425	-1.99227679
1	-3.11789817	5.57720151	-1.21473420
6	-6.10375438	3.34939365	-2.25163108
1	-4.88081962	1.68132671	-1.73967643
6	-6.19132079	4.73252761	-2.35787394
1	-5.16763530	6.60798645	-2.06819488
1	-6.93369124	2.72273894	-2.55249184
6	-7.42321166	5.39000002	-2.89762722
9	-7.21764370	5.92534426	-4.12260951
9	-7.84008773	6.40693459	-2.11482400
9	-8.45719669	4.54242559	-3.01890947
9	-1.18425519	4.63382785	0.05397036
9	-1.19480658	4.36682455	-2.23040768

*** molecule **1d** rotamer A S_{1r} MeCN

46

6	0.87849281	0.97017868	0.13912559
6	1.09269096	-0.20576588	0.87831741
16	2.38979393	1.65498469	-0.42192860
6	2.44363186	-0.54474912	0.99888471
1	0.29797005	-0.80235347	1.30190602
6	3.31978193	0.37690312	0.35746055
6	2.82548816	-1.75629139	1.62878075
7	3.07802388	-2.76141790	2.13741222
6	5.38990810	1.29232038	-0.59645955
6	5.54799364	-0.41384387	1.11551646
6	6.34012340	0.45126796	-1.44763125
1	5.95330555	2.00690154	0.01113674
1	4.71185927	1.84090173	-1.24779779
6	6.49092604	-1.19193859	0.20466220
1	6.12372229	0.27184280	1.74599710
1	4.99671193	-1.08795978	1.76158373
1	6.96008378	1.10910698	-2.05645913
1	5.75578504	-0.20335763	-2.10834235
1	7.22250345	-1.72816348	0.80847208
1	5.91975456	-1.91565942	-0.39201227
7	4.64740789	0.40540489	0.30174636
8	7.20904251	-0.31652697	-0.64186840
6	-0.31654065	1.62678712	-0.19145066
6	-1.58997543	1.14456765	0.17981071
6	-2.73841710	1.80196466	-0.21996684
1	-1.68433619	0.24555306	0.77161830
1	-3.71028069	1.40249237	0.03948076
8	-0.20878054	2.72878305	-0.93914991
5	-1.29395277	3.70389213	-1.00937261
7	-2.68396178	2.97732198	-0.89029445
6	-3.84975725	3.55246529	-1.39089152
6	-3.94473931	4.95113467	-1.51892714

6	-4.94694319	2.76199961	-1.77062550
6	-5.10309516	5.52933899	-1.99445507
1	-3.11599425	5.57688782	-1.21910369
6	-6.10554680	3.35066714	-2.24852744
1	-4.88424378	1.68205856	-1.73466134
6	-6.19153611	4.73369829	-2.35739029
1	-5.16522192	6.60848874	-2.07221768
1	-6.93657309	2.72436317	-2.54708554
6	-7.42321426	5.39172989	-2.89679804
9	-7.21787109	5.92661550	-4.12212403
9	-7.83910674	6.40935933	-2.11424597
9	-8.45788801	4.54496298	-3.01735554
9	-1.18116275	4.63376988	0.04763542
9	-1.19542569	4.36189810	-2.23607348

*** molecule **1d** rotamer A S1r THF

46

6	0.85003403	0.91591320	0.07776382
6	1.05778652	-0.25627983	0.82202008
16	2.36366040	1.57759067	-0.50638620
6	2.40700727	-0.60956906	0.93054990
1	0.26139162	-0.84150575	1.25825510
6	3.28472286	0.29621703	0.27309307
6	2.78669602	-1.82221591	1.56024434
7	3.04351485	-2.82691927	2.06729109
6	5.34575209	1.23517981	-0.66243287
6	5.50453985	-0.42616282	1.10807027
6	6.47482562	0.49545454	-1.37429685
1	5.75135610	2.04176149	-0.04174727
1	4.67912880	1.66459223	-1.40906216
6	6.62239366	-1.09384446	0.31913502
1	5.92796474	0.30670964	1.80476164
1	4.95958088	-1.16827369	1.68136074
1	7.07790367	1.21061692	-1.93339857
1	6.04930926	-0.23656361	-2.07409217
1	7.33510174	-1.54365095	1.00986969
1	6.20643255	-1.87944304	-0.32582911
7	4.61545263	0.30149682	0.19755174
8	7.33058108	-0.14870205	-0.45609262
6	-0.33938849	1.59109984	-0.23810738
6	-1.61297112	1.13886049	0.17245983
6	-2.75819882	1.81181683	-0.20967843
1	-1.70837984	0.25346357	0.78425901
1	-3.73024946	1.43894853	0.08597753
8	-0.22662714	2.67779597	-1.00045651
5	-1.29645839	3.67331472	-1.07365542
7	-2.69825606	2.97130146	-0.90573496
6	-3.86435373	3.56041906	-1.38608586
6	-3.92882524	4.95672913	-1.55338582
6	-4.99370319	2.78760362	-1.70630648
6	-5.08777099	5.55036980	-2.00835143
1	-3.07485751	5.56879305	-1.29998682
6	-6.15160918	3.39183641	-2.16386293
1	-4.95643671	1.70779254	-1.64151393
6	-6.20720795	4.77346488	-2.31055907
1	-5.12592972	6.62776814	-2.11682891

1	-7.00800034	2.77946103	-2.41666791
6	-7.43724613	5.43867525	-2.84628160
9	-7.29991067	5.78689192	-4.14596231
9	-7.72930346	6.57585884	-2.18495149
9	-8.52488944	4.65341506	-2.77530016
9	-1.14789280	4.62073591	-0.04172137
9	-1.21623359	4.29376738	-2.31759525

*** molecule 1dA S_{1r} Toluene

46

6	0.84566026	0.92104557	0.07168099
6	1.04975086	-0.26565993	0.78919254
16	2.36050689	1.58841704	-0.50608981
6	2.39962197	-0.62828417	0.88098310
1	0.25292679	-0.85884266	1.21385621
6	3.27444850	0.28608933	0.24103905
6	2.79015066	-1.86106797	1.46467384
7	3.07121966	-2.87930884	1.92961599
6	5.33902731	1.19248077	-0.71881378
6	5.48983550	-0.38824046	1.12588941
6	6.50507179	0.45102224	-1.36707441
1	5.71029397	2.03946112	-0.12943297
1	4.67894022	1.56808421	-1.50033089
6	6.64350460	-1.06088905	0.39611734
1	5.87933877	0.38145404	1.80393472
1	4.94377811	-1.11874285	1.71410422
1	7.10943103	1.15411570	-1.94047575
1	6.11525837	-0.31992484	-2.04647757
1	7.35049793	-1.46378980	1.12107237
1	6.26224442	-1.88376169	-0.22416451
7	4.61082069	0.27857030	0.16106363
8	7.34864364	-0.13265485	-0.40072969
6	-0.34156318	1.61008191	-0.22856196
6	-1.61626777	1.15202075	0.18079331
6	-2.76125419	1.82476147	-0.19980792
1	-1.70817555	0.26428426	0.78972777
1	-3.73385285	1.45257895	0.09604529
8	-0.22519961	2.70371440	-0.96733829
5	-1.29933623	3.70326794	-1.04693624
7	-2.70170220	2.98462833	-0.89345163
6	-3.86652952	3.56920133	-1.37812746
6	-3.93449191	4.96557366	-1.54507783
6	-4.99264982	2.79241827	-1.70272795
6	-5.09522079	5.55479812	-2.00051902
1	-3.08167597	5.57858060	-1.29019787
6	-6.15125362	3.39292437	-2.16170356
1	-4.94889151	1.71237267	-1.64284846
6	-6.21158229	4.77477799	-2.30502580
1	-5.13838873	6.63198680	-2.10836440
1	-7.00586828	2.77969170	-2.41869407
6	-7.44493316	5.43425265	-2.84360926
9	-7.31895549	5.74768488	-4.15149678
9	-7.72285242	6.58651858	-2.20548520
9	-8.53370267	4.65374008	-2.74016926
9	-1.16931537	4.63198193	-0.00494058
9	-1.21687244	4.32117045	-2.28478587

*** molecule **1d** rotamer B S_{1r} acetone

46

6	0.68916757	0.61690586	-0.02017289
6	1.99820812	0.92981858	-0.41695903
16	0.65609083	-0.87118722	0.91373224
6	2.95120352	0.00669366	0.02140014
1	2.23455253	1.81732248	-0.98509301
6	2.39642597	-1.07441509	0.76484321
6	4.33234256	0.23653837	-0.20405190
7	5.44322972	0.48087860	-0.40022538
6	2.29375665	-3.04825544	2.22293764
6	4.34175579	-2.59731218	1.00388189
6	3.14360226	-3.20414200	3.48286878
1	2.15945656	-4.01645713	1.73077354
1	1.31698268	-2.65330639	2.49694620
6	5.11185533	-2.76531865	2.30790358
1	4.26039974	-3.56270270	0.49328214
1	4.85481888	-1.90589804	0.34465705
1	2.68722113	-3.94614828	4.13762336
1	3.19296532	-2.24237831	4.01090275
1	6.09318740	-3.19046862	2.09983628
1	5.23995594	-1.78859527	2.79350785
7	2.97849801	-2.14625829	1.29428303
8	4.44346098	-3.66010641	3.17459192
6	-0.47052666	1.36164391	-0.30366311
6	-1.76524582	0.99384917	0.11805268
6	-2.86914955	1.74703195	-0.23318671
1	-1.91671953	0.10823778	0.72037224
1	-3.85872185	1.43135987	0.06928775
8	-0.29998783	2.45272481	-1.05279041
5	-1.29666336	3.51779304	-1.07890965
7	-2.74158217	2.91711114	-0.90613299
6	-3.87238922	3.59405545	-1.35019700
6	-3.84572767	4.99307772	-1.49613795
6	-5.06169574	2.90534331	-1.65487091
6	-4.97175631	5.67418659	-1.91586354
1	-2.94794226	5.54315395	-1.25281522
6	-6.18354532	3.59515845	-2.07299804
1	-5.09874851	1.82480829	-1.60523799
6	-6.14783133	4.98201856	-2.19884472
1	-4.93664682	6.75252099	-2.00804341
1	-7.08702541	3.04684584	-2.31168477
6	-7.35806939	5.70774699	-2.69849584
9	-7.46834189	5.64506603	-4.04617588
9	-7.34785511	7.01314029	-2.38015866
9	-8.50187410	5.19233551	-2.20751079
9	-1.06518034	4.43048672	-0.02608844
9	-1.18873298	4.17034298	-2.30817176

*** molecule **1d** rotamer B S_{1r} Chloroform

46

6	0.67328172	0.62924992	0.01475027
6	1.97915740	0.93178321	-0.39353851

16	0.63763344	-0.85413777	0.95872099
6	2.92934643	0.00448880	0.04552958
1	2.21517765	1.81711717	-0.96529147
6	2.37466212	-1.06738935	0.79535648
6	4.31580945	0.22181995	-0.16308910
7	5.43535752	0.44124579	-0.33624886
6	2.30843405	-2.99891041	2.31275161
6	4.28251404	-2.64996437	0.94524289
6	3.23973883	-3.16430205	3.51320492
1	2.10042484	-3.97229871	1.85652343
1	1.37063154	-2.55539111	2.64434198
6	5.13628448	-2.82491544	2.19469005
1	4.13104997	-3.62177390	0.46214832
1	4.77050858	-1.98967418	0.23625356
1	2.80586047	-3.87563341	4.21595420
1	3.36179805	-2.19466328	4.01527376
1	6.08351230	-3.29405914	1.93044816
1	5.33712428	-1.84500904	2.64863224
7	2.96092287	-2.14346633	1.32161107
8	4.49531230	-3.67553780	3.12404324
6	-0.48451167	1.38076534	-0.26592712
6	-1.78011203	1.01465190	0.15919163
6	-2.88385185	1.76162997	-0.20522427
1	-1.92996515	0.13565072	0.77155924
1	-3.87491832	1.44938862	0.09687302
8	-0.31070884	2.46565038	-1.01322305
5	-1.30828440	3.53528712	-1.05162409
7	-2.75516951	2.92413363	-0.88893921
6	-3.88357181	3.59015552	-1.35186950
6	-3.86162444	4.99041051	-1.50366855
6	-5.06319194	2.89398579	-1.67029409
6	-4.98448416	5.66021002	-1.94148301
1	-2.96894779	5.54442709	-1.25064871
6	-6.18395628	3.57490923	-2.11172942
1	-5.09286873	1.81314589	-1.61862923
6	-6.15326190	4.95866860	-2.24318156
1	-4.95620623	6.73905782	-2.03811302
1	-7.07944791	3.02119743	-2.36440839
6	-7.34529315	5.70913042	-2.75190155
9	-7.18308321	6.10854417	-4.03298216
9	-7.58271201	6.82811858	-2.03918448
9	-8.47161618	4.97776800	-2.71901872
9	-1.09326487	4.44097744	0.00398704
9	-1.19631161	4.17880413	-2.27966533

*** molecule **1d** rotamer B S_{1r} dioxane

46

6	0.72724301	0.77536357	0.13641494
6	1.99219939	1.09467611	-0.26744871
16	0.71899970	-0.67939546	1.10128161
6	2.97884923	0.19739974	0.20753118
1	2.21641978	1.97090537	-0.86091047
6	2.45097518	-0.83539010	0.99104899
6	4.36877416	0.42201606	0.01427521
7	5.49504541	0.61326134	-0.13320856
6	2.33653026	-2.73879570	2.49573543

6	4.18178966	-2.56495776	0.90512961
6	3.29435216	-3.46883142	3.42568997
1	1.75903291	-3.46432192	1.90550955
1	1.65164355	-2.14064564	3.09974511
6	5.04698000	-3.29661594	1.91479469
1	3.73426884	-3.28274991	0.20535390
1	4.79617347	-1.86437740	0.34596756
1	2.74361422	-4.19358270	4.02550841
1	3.77562959	-2.74494219	4.09685125
1	5.79206986	-3.89778132	1.39404887
1	5.56089487	-2.57079127	2.55855162
7	3.09457224	-1.85751981	1.60570877
8	4.27425938	-4.18119020	2.70327285
6	-0.46779077	1.53782952	-0.13581192
6	-1.71357556	1.23295931	0.39519097
6	-2.82603805	1.94486009	-0.05488970
1	-1.84896115	0.41289234	1.08380389
1	-3.82095099	1.63232716	0.25026869
8	-0.30700200	2.52707107	-0.96679763
5	-1.31122994	3.60219140	-1.13880403
7	-2.72950123	2.99261793	-0.84662377
6	-3.89600908	3.62072288	-1.36115163
6	-3.93053645	5.01030956	-1.46415160
6	-4.98834514	2.85600400	-1.77438037
6	-5.06906300	5.63508903	-1.95257074
1	-3.07550417	5.59549744	-1.15016573
6	-6.12684840	3.48346809	-2.25330922
1	-4.93548850	1.77418297	-1.75104947
6	-6.16543805	4.87216232	-2.33589430
1	-5.10202280	6.71473410	-2.02538074
1	-6.97655003	2.89350049	-2.57746943
6	-7.40117044	5.51999753	-2.88351837
9	-7.56585117	5.26076182	-4.19361271
9	-7.38804367	6.85163743	-2.74905230
9	-8.51215241	5.07226236	-2.27140097
9	-1.06168549	4.61219220	-0.21526276
9	-1.25338005	4.06824249	-2.43161367

*** molecule **1d** rotamer B S_{1r} DMF

46

6	0.69091064	0.61291539	-0.02769315
6	2.00004252	0.92648650	-0.42465501
16	0.65890135	-0.87416202	0.90733626
6	2.95383652	0.00488262	0.01463705
1	2.23595960	1.81317463	-0.99423469
6	2.39966355	-1.07595428	0.76002770
6	4.33392772	0.23600805	-0.21524709
7	5.44326290	0.48325230	-0.41680539
6	2.29307384	-3.05319719	2.21300676
6	4.35025024	-2.58913617	1.01490960
6	3.13112026	-3.20667888	3.48098047
1	2.16929285	-4.02086977	1.71718516
1	1.31134968	-2.66484996	2.47831269
6	5.10829673	-2.75510462	2.32631118
1	4.27890003	-3.55394572	0.50193641
1	4.86647200	-1.89406525	0.36215160

1	2.67193358	-3.95222436	4.12965909
1	3.17018935	-2.24566883	4.01107429
1	6.09393317	-3.17431674	2.12671336
1	5.22607502	-1.77862934	2.81492677
7	2.98176781	-2.14562355	1.29233463
8	4.43660260	-3.65522132	3.18492549
6	-0.46915967	1.35658176	-0.31143920
6	-1.76339776	0.98968119	0.11178504
6	-2.86741153	1.74375906	-0.23716382
1	-1.91474811	0.10400108	0.71403069
1	-3.85650227	1.42849797	0.06713891
8	-0.29953808	2.44750519	-1.06253669
5	-1.29570408	3.51222643	-1.08719671
7	-2.74034331	2.91408838	-0.91020334
6	-3.87169871	3.59274219	-1.35072371
6	-3.84340227	4.99163768	-1.49766462
6	-5.06323593	2.90587614	-1.65076820
6	-4.96974343	5.67444414	-1.91395539
1	-2.94415556	5.54075122	-1.25762706
6	-6.18547412	3.59732014	-2.06526795
1	-5.10230492	1.82550589	-1.59986689
6	-6.14795965	4.98404766	-2.19227624
1	-4.93302994	6.75266408	-2.00687750
1	-7.09066885	3.05014151	-2.30003718
6	-7.35882188	5.71139545	-2.68774329
9	-7.47556113	5.64641972	-4.03494166
9	-7.34441525	7.01749044	-2.37220394
9	-8.50162052	5.19963536	-2.19064709
9	-1.06010067	4.42757259	-0.03655767
9	-1.18958604	4.16419013	-2.31784544

*** molecule **1d** rotamer B S_{1r} DMSO

46

6	0.69131005	0.61201104	-0.02937972
6	2.00045618	0.92550122	-0.42663001
16	0.65950332	-0.87459483	0.90627461
6	2.95438586	0.00425375	0.01297114
1	2.23630511	1.81183570	-0.99678713
6	2.40032058	-1.07628944	0.75914190
6	4.33422893	0.23548142	-0.21813986
7	5.44320019	0.48324587	-0.42113356
6	2.29276162	-3.05399871	2.21133266
6	4.35187792	-2.58749874	1.01758093
6	3.12833315	-3.20711974	3.48094739
1	2.17100633	-4.02152573	1.71475675
1	1.31009663	-2.66686497	2.47484827
6	5.10738159	-2.75318863	2.33049895
1	4.28247498	-3.55214732	0.50408618
1	4.86885485	-1.89171364	0.36621288
1	2.66844597	-3.95332611	4.12835208
1	3.16543590	-2.24628542	4.01145593
1	6.09383342	-3.17130201	2.13263107
1	5.22315338	-1.77680461	2.81975111
7	2.98238227	-2.14537695	1.29228741
8	4.43489650	-3.65433612	3.18742248
6	-0.46880960	1.35546074	-0.31322592

6	-1.76290766	0.98902246	0.11064370
6	-2.86692608	1.74331419	-0.23781761
1	-1.91422978	0.10351613	0.71315060
1	-3.85588345	1.42832437	0.06715573
8	-0.29941265	2.44613343	-1.06512982
5	-1.29537766	3.51083055	-1.08961890
7	-2.73996695	2.91349738	-0.91124357
6	-3.87145707	3.59253059	-1.35095811
6	-3.84267026	4.99134775	-1.49858147
6	-5.06362960	2.90612146	-1.64950286
6	-4.96908400	5.67453013	-1.91410094
1	-2.94300090	5.54023516	-1.25962472
6	-6.18596139	3.59792518	-2.06318451
1	-5.10327411	1.82581253	-1.59793944
6	-6.14791335	4.98457527	-2.19091449
1	-4.93190526	6.75269059	-2.00754233
1	-7.09164661	3.05102227	-2.29669995
6	-7.35891274	5.71228198	-2.68544331
9	-7.47719528	5.64665187	-4.03251997
9	-7.34348046	7.01857446	-2.37069390
9	-8.50147341	5.20146587	-2.18684774
9	-1.05855582	4.42713314	-0.03982180
9	-1.18979240	4.16229339	-2.32081587

*** molecule **1d** rotamer B S_{1r} EtOH

46

6	0.68983418	0.61529240	-0.02316295
6	1.99889241	0.92835853	-0.42014777
16	0.65717938	-0.87231095	0.91133272
6	2.95219202	0.00582410	0.01859164
1	2.23506779	1.81547379	-0.98895689
6	2.39765963	-1.07507851	0.76294735
6	4.33291088	0.23608732	-0.20875512
7	5.44318310	0.48150827	-0.40717034
6	2.29342493	-3.05014417	2.21919340
6	4.34504963	-2.59418925	1.00828211
6	3.13866845	-3.20499790	3.48229240
1	2.16321885	-4.01818402	1.72566260
1	1.31470561	-2.65774794	2.48978470
6	5.11044254	-2.76130073	2.31521664
1	4.26760337	-3.55939479	0.49680907
1	4.85936828	-1.90139587	0.35153626
1	2.68117154	-3.94833326	4.13473118
1	3.18401769	-2.24348375	4.01107553
1	6.09346744	-3.18415304	2.11048650
1	5.23452077	-1.78463167	2.80193861
7	2.97972991	-2.14604935	1.29357942
8	4.44073776	-3.65809950	3.17881955
6	-0.46999297	1.35964321	-0.30673432
6	-1.76451439	0.99228211	0.11567672
6	-2.86845107	1.74583370	-0.23466295
1	-1.91594089	0.10669335	0.71803982
1	-3.85783333	1.43038576	0.06860075
8	-0.29981084	2.45059524	-1.05672300
5	-1.29623682	3.51557828	-1.08227117
7	-2.74106636	2.91595550	-0.90773623

6	-3.87208455	3.59357312	-1.35041590
6	-3.84475596	4.99253904	-1.49680607
6	-5.06228698	2.90559310	-1.65322054
6	-4.97090447	5.67431655	-1.91518941
1	-2.94637959	5.54222894	-1.25481091
6	-6.18428543	3.59605010	-2.06993360
1	-5.10014570	1.82512397	-1.60304747
6	-6.14784011	4.98285259	-2.19629263
1	-4.93514805	6.75260206	-2.00770503
1	-7.08845477	3.04819024	-2.30704809
6	-7.35831848	5.70921932	-2.69431467
9	-7.47112811	5.64561568	-4.04180808
9	-7.34644475	7.01489425	-2.37709294
9	-8.50173816	5.19525796	-2.20092205
9	-1.06305033	4.42934282	-0.03035454
9	-1.18905577	4.16783032	-2.31210998

*** molecule **1d** rotamer B S_{1r} MeCN

46

6	0.69078978	0.61312165	-0.02724340
6	1.99989887	0.92644898	-0.42442160
16	0.65869030	-0.87383339	0.90800791
6	2.95360892	0.00474149	0.01486297
1	2.23585950	1.81305380	-0.99411288
6	2.39938557	-1.07592036	0.76041071
6	4.33375442	0.23561901	-0.21497905
7	5.44317781	0.48255803	-0.41640943
6	2.29298316	-3.05270847	2.21402807
6	4.34953101	-2.58984761	1.01435040
6	3.13188422	-3.20630447	3.48142865
1	2.16836493	-4.02045503	1.71855437
1	1.31164526	-2.66379196	2.47994654
6	5.10844354	-2.75590119	2.32523432
1	4.27739322	-3.55473413	0.50161829
1	4.86557801	-1.89512678	0.36107411
1	2.67283998	-3.95149842	4.13061559
1	3.17177862	-2.24519451	4.01128911
1	6.09374081	-3.17562640	2.12504208
1	5.22703995	-1.77937465	2.81355411
7	2.98144572	-2.14567616	1.29267248
8	4.43693167	-3.65551303	3.18451803
6	-0.46922472	1.35690312	-0.31096957
6	-1.76347047	0.99014332	0.11239401
6	-2.86745801	1.74418720	-0.23671095
1	-1.91483060	0.10460004	0.71483834
1	-3.85656636	1.42904018	0.06766219
8	-0.29954799	2.44767967	-1.06218547
5	-1.29566439	3.51249115	-1.08702146
7	-2.74034490	2.91435511	-0.90999815
6	-3.87166743	3.59289769	-1.35074880
6	-3.84339480	4.99177093	-1.49790117
6	-5.06314430	2.90593910	-1.65081941
6	-4.96971432	5.67446615	-1.91442146
1	-2.94418170	5.54093574	-1.25785327
6	-6.18535744	3.59727606	-2.06556123
1	-5.10215684	1.82557135	-1.59977561

6	-6.14787461	4.98398360	-2.19277347
1	-4.93303755	6.75267318	-2.00750981
1	-7.09050713	3.05004017	-2.30036827
6	-7.35869133	5.71122427	-2.68852489
9	-7.47506461	5.64629340	-4.03574836
9	-7.34449711	7.01730274	-2.37291523
9	-8.50155638	5.19931306	-2.19174091
9	-1.06011091	4.42787228	-0.03645782
9	-1.18952299	4.16425106	-2.31772637

*** molecule **1d** rotamer B S_{1r} THF

46

6	0.68195737	0.63210991	0.01081297
6	1.99139920	0.94372373	-0.38257667
16	0.64330167	-0.86161176	0.93737829
6	2.94065149	0.01425966	0.05216027
1	2.23014719	1.83560815	-0.94282018
6	2.38235418	-1.06952447	0.78481576
6	4.32635589	0.23941820	-0.15132044
7	5.44374784	0.47169100	-0.32246528
6	2.29820484	-3.02977178	2.26316057
6	4.30427763	-2.63173515	0.95816962
6	3.19597771	-3.19145576	3.48926952
1	2.12386399	-4.00061206	1.78859412
1	1.34190305	-2.60962366	2.57098802
6	5.12419414	-2.80391205	2.23066166
1	4.18232799	-3.60088781	0.46222809
1	4.80152610	-1.95742031	0.26932424
1	2.75369372	-3.91836539	4.17035114
1	3.28544557	-2.22573593	4.00521735
1	6.08724146	-3.25250622	1.98899471
1	5.29287619	-1.82535970	2.70018003
7	2.96399338	-2.15070222	1.30090192
8	4.47227174	-3.67582479	3.13255513
6	-0.47604065	1.38092552	-0.27243887
6	-1.77285796	1.00969701	0.14259117
6	-2.87609389	1.75935716	-0.21802081
1	-1.92513876	0.12451637	0.74535430
1	-3.86751688	1.44202399	0.07717225
8	-0.30157169	2.47304817	-1.01356349
5	-1.30078385	3.53871969	-1.04715662
7	-2.74646110	2.92837601	-0.89089590
6	-3.87502132	3.59883715	-1.34876086
6	-3.85401959	4.99812840	-1.49312879
6	-5.05623802	2.90340222	-1.66926700
6	-4.97863663	5.67273738	-1.92622100
1	-2.96161213	5.55193543	-1.23864823
6	-6.17646250	3.58700634	-2.10142319
1	-5.08634078	1.82241392	-1.62258013
6	-6.14702089	4.97408927	-2.22500633
1	-4.94913290	6.75134695	-2.01721624
1	-7.07375624	3.03448583	-2.35327113
6	-7.35424852	5.69413873	-2.74105092
9	-7.43540761	5.64667811	-4.09079961
9	-7.36298725	6.99526474	-2.40624081
9	-8.50213694	5.16114281	-2.27961146

9	-1.08591637	4.44292034	0.01275989
9	-1.18513157	4.19229372	-2.27195279

*** molecule **1d** rotamer B S_{1r} Toluene

46

6	0.68738609	0.70729758	0.07411820
6	1.99062229	1.01036053	-0.33558968
16	0.65764265	-0.76523544	1.03843703
6	2.94328571	0.09272077	0.11995401
1	2.22181172	1.88911752	-0.91954170
6	2.39373943	-0.96855822	0.88172658
6	4.33353075	0.30257848	-0.07538833
7	5.45954874	0.50137092	-0.22828862
6	2.31942907	-2.88795492	2.40267229
6	4.23225176	-2.62917405	0.91679605
6	3.30452699	-3.29686154	3.49510493
1	1.93394273	-3.77783936	1.88977608
1	1.48674711	-2.35180160	2.85830549
6	5.13010026	-3.04265778	2.07314186
1	3.94892763	-3.51398044	0.33293019
1	4.75713008	-1.94007872	0.26266595
1	2.83236768	-4.02110787	4.15921861
1	3.58963250	-2.41080653	4.07931234
1	5.99485811	-3.58470502	1.69130120
1	5.47857387	-2.15070764	2.61158900
7	2.99891042	-2.02843206	1.43524518
8	4.45007828	-3.91316393	2.95396652
6	-0.47394286	1.44934270	-0.22050172
6	-1.76815874	1.08229715	0.21623438
6	-2.87808267	1.81014186	-0.16702355
1	-1.90848580	0.21935562	0.85327892
1	-3.86664524	1.49972454	0.14567980
8	-0.30686438	2.51647629	-0.98515312
5	-1.31356299	3.58146352	-1.05591955
7	-2.75829036	2.95438300	-0.88136515
6	-3.89034705	3.59769920	-1.36263808
6	-3.87673959	4.99279735	-1.55959168
6	-5.06722274	2.88434944	-1.65554191
6	-5.00557447	5.64097073	-2.01362645
1	-2.98582352	5.55885362	-1.32812224
6	-6.19290789	3.54402855	-2.11455950
1	-5.08847137	1.80520187	-1.57195211
6	-6.17122047	4.92357608	-2.28810884
1	-4.98529966	6.71633205	-2.14453009
1	-7.08635134	2.97866798	-2.34800383
6	-7.36919788	5.64826586	-2.82258910
9	-7.22306618	5.97161682	-4.12566091
9	-7.59278373	6.80511435	-2.17075271
9	-8.49521298	4.92106438	-2.73168281
9	-1.11529393	4.50572235	-0.02007278
9	-1.20831971	4.18742095	-2.29804585