Chemistry of Heterocyclic Compounds **2023**, *59*(4/5), 304–308

The nitration and bromination of 2-(pentafluorosulfanyl)-1,3-benzothiazole and 2-(trifluoromethyl)-1,3-benzothiazole

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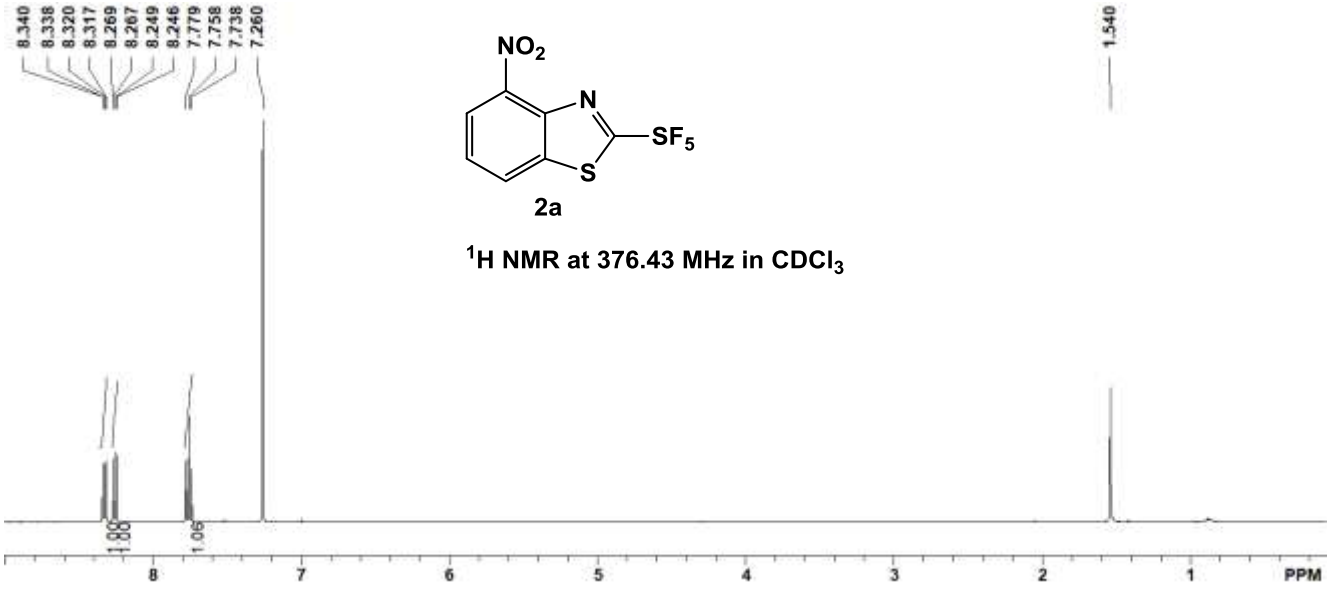
SUPPLEMENTARY INFORMATION

General Information

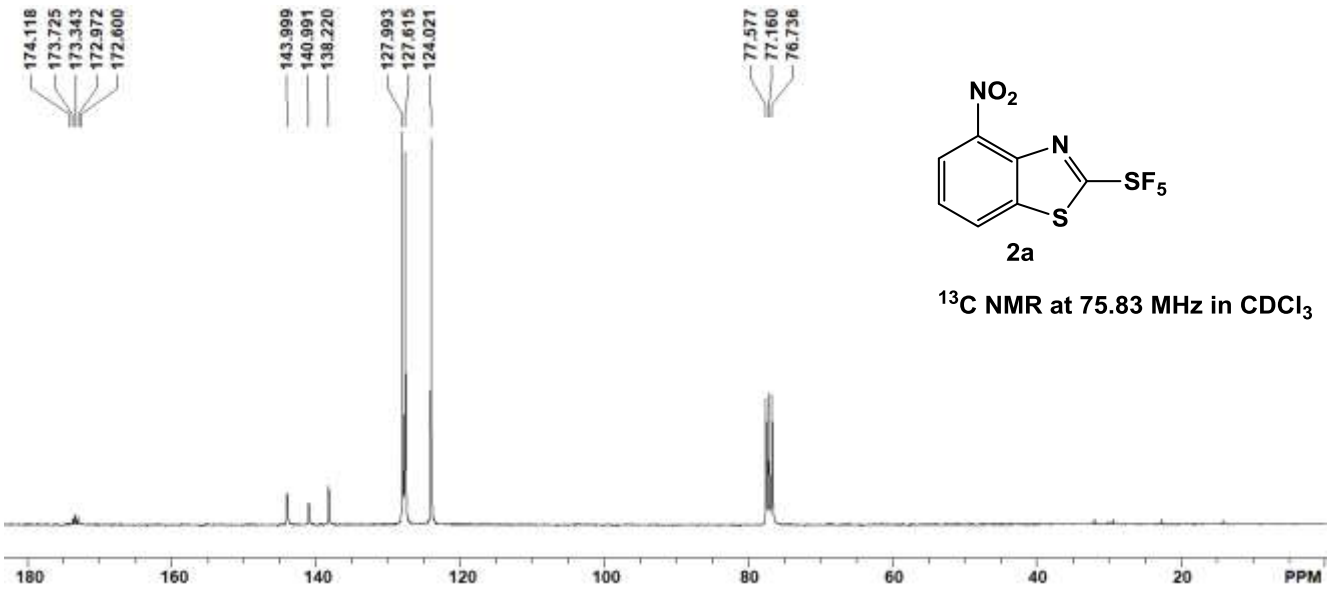
^{1}H, ^{13}C, ^{19}F, NMR spectra were acquired on a Varian VXR-300, Varian VXR-400, and Bruker Avance-500 spectrometers in $CDCl_3$, using the residual solvent signals as internal standards (7.26 ppm for ^{1}H nuclei and 77.16 ppm for ^{13}C nuclei; C_6F_6: –162.9 ppm relative to $CFCl_3$ for ^{19}F nuclei. GC/MS spectra were recorded on a Hewlett-Packard 5890/5972 system with 70 eV in the EI ionization mode. LC/MS spectra were registered on an Agilent 1100 Series system equipped with an Agilent LC/MSD SL Diode Array Mass Selective Detector, electrospray ionization. Elemental analysis was performed in the analytical laboratory of the Institute of Organic Chemistry of the National Academy of Sciences of Ukraine. Elemental analysis data were obtained by the express gravimetric method (C, H), Schöniger ignition method (S), and Pregl–Dumas method (N). Melting points were determined on a Thyle apparatus.

^{1}H NMR, ^{19}F NMR, ^{13}C NMR, and MS data



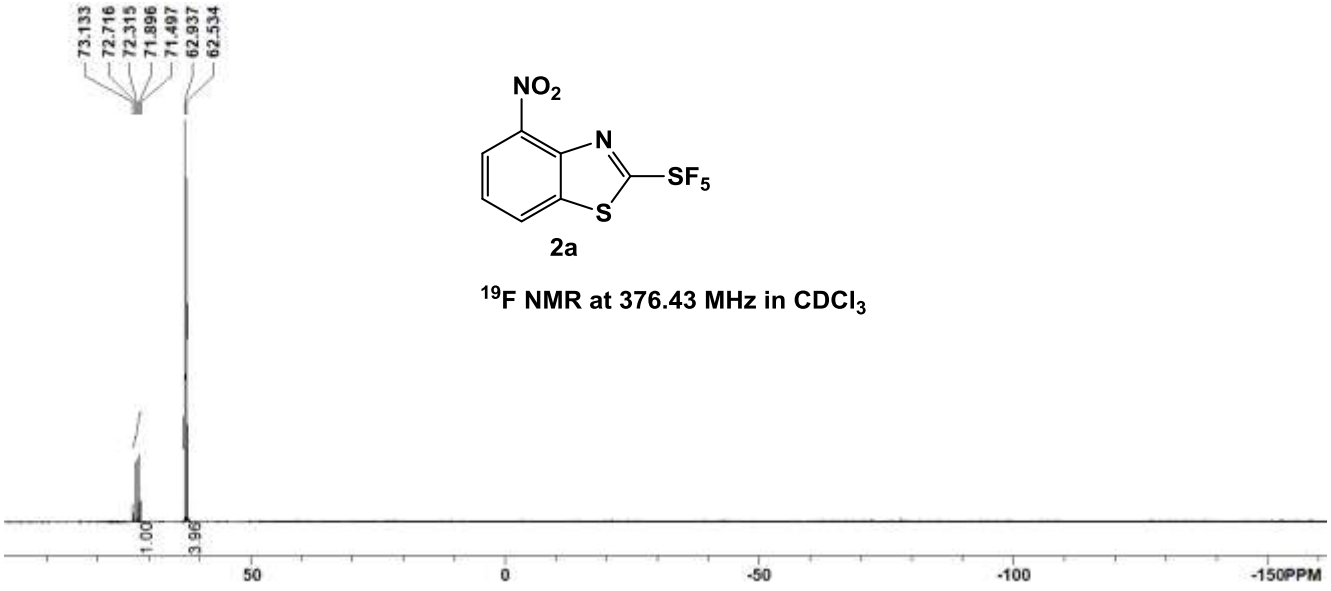
2a

^{1}H NMR at 376.43 MHz in $CDCl_3$



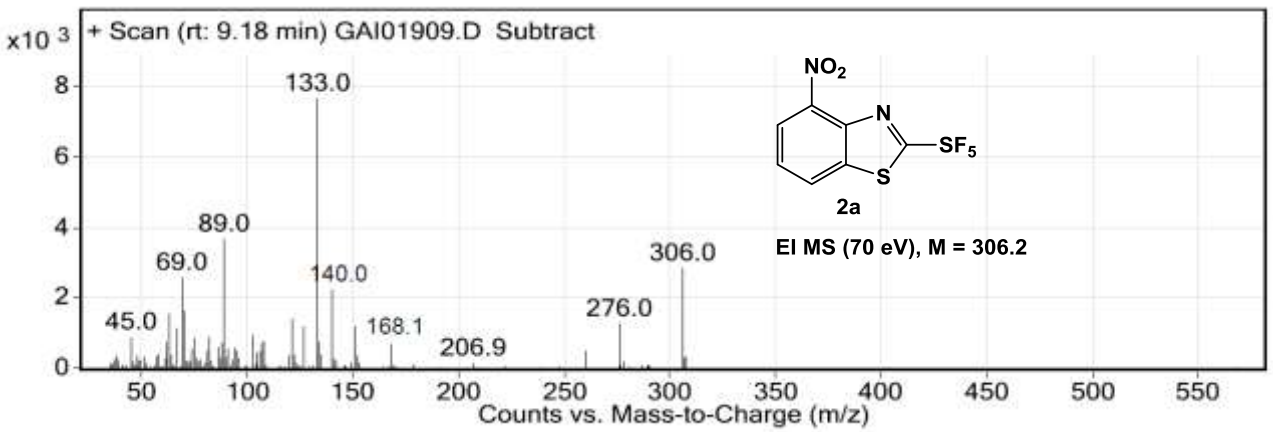
2a

^{13}C NMR at 75.83 MHz in $CDCl_3$



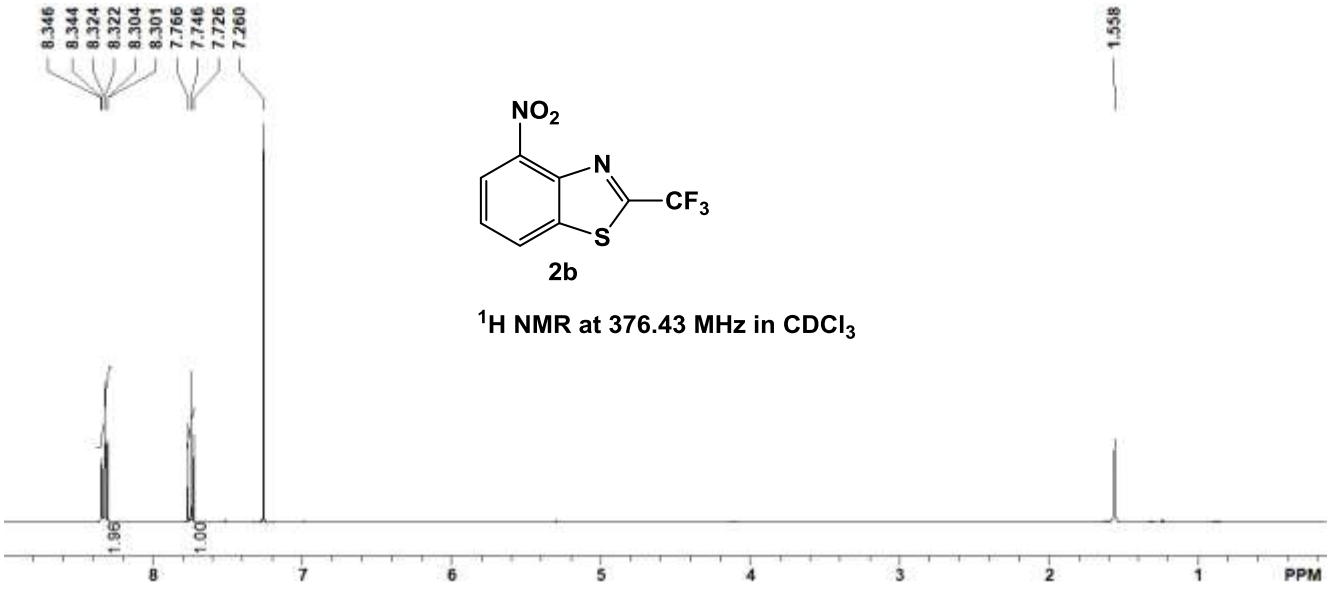
2a

^{19}F NMR at 376.43 MHz in $CDCl_3$



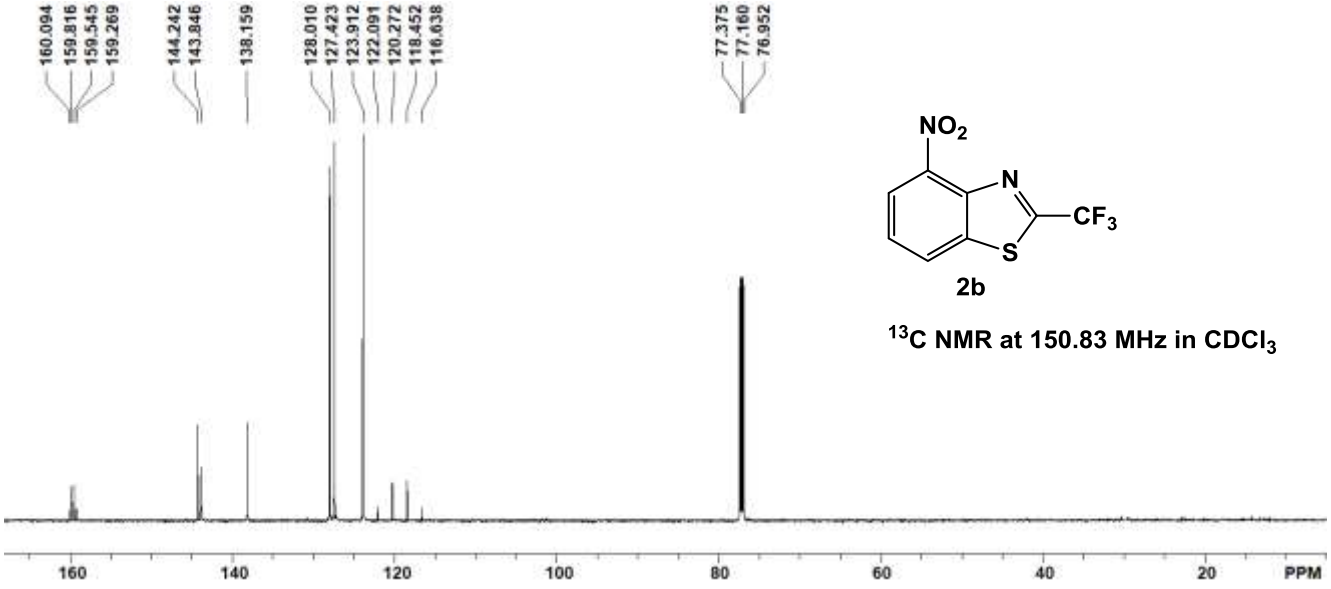
2a

EI MS (70 eV), M = 306.2



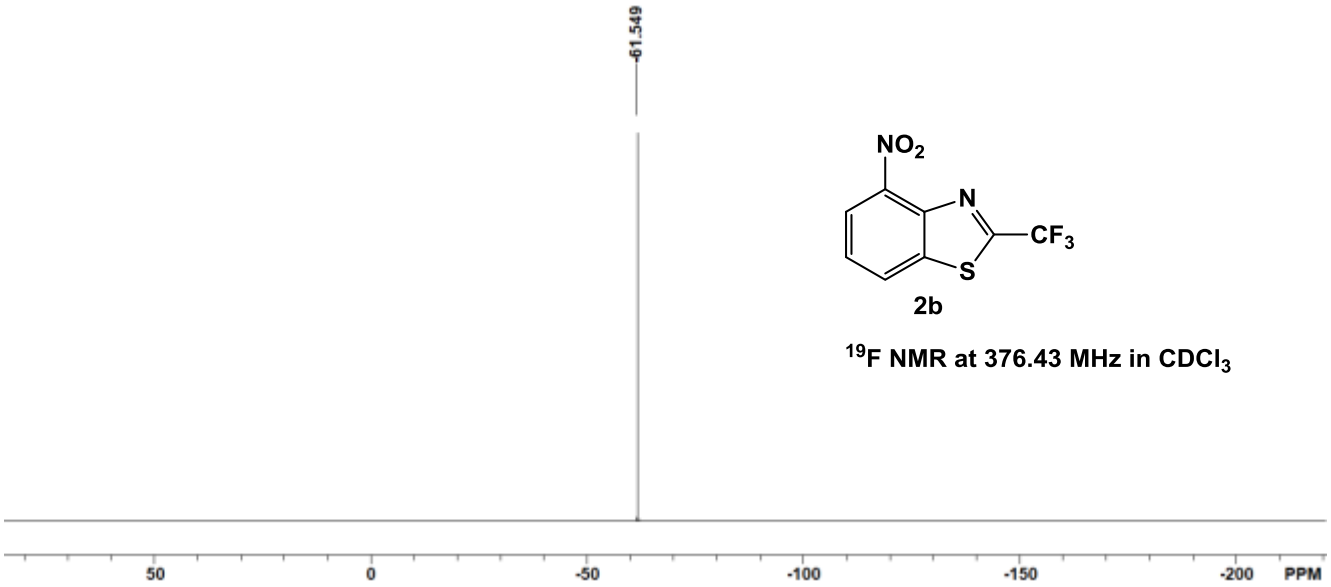
2b

^{1}H NMR at 376.43 MHz in $CDCl_3$



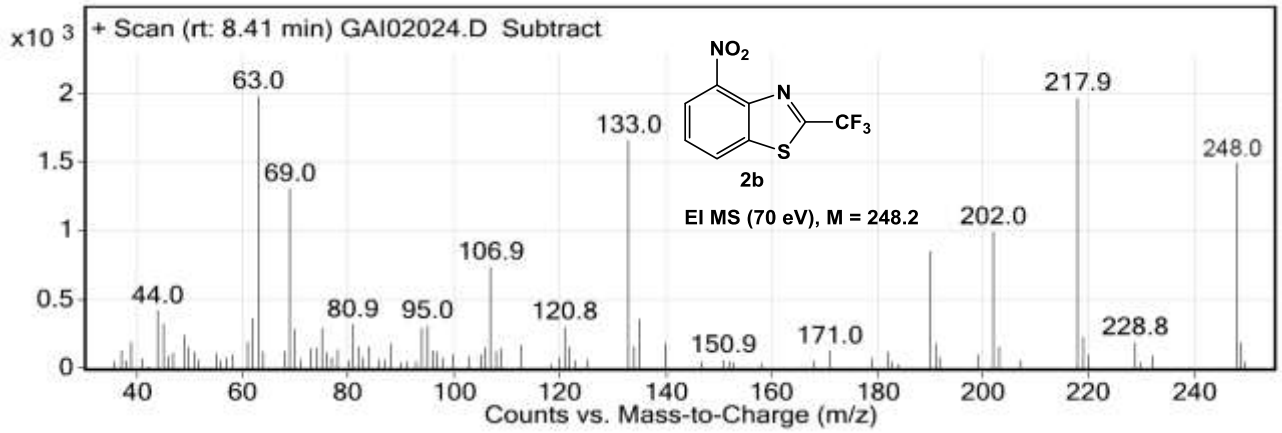
2b

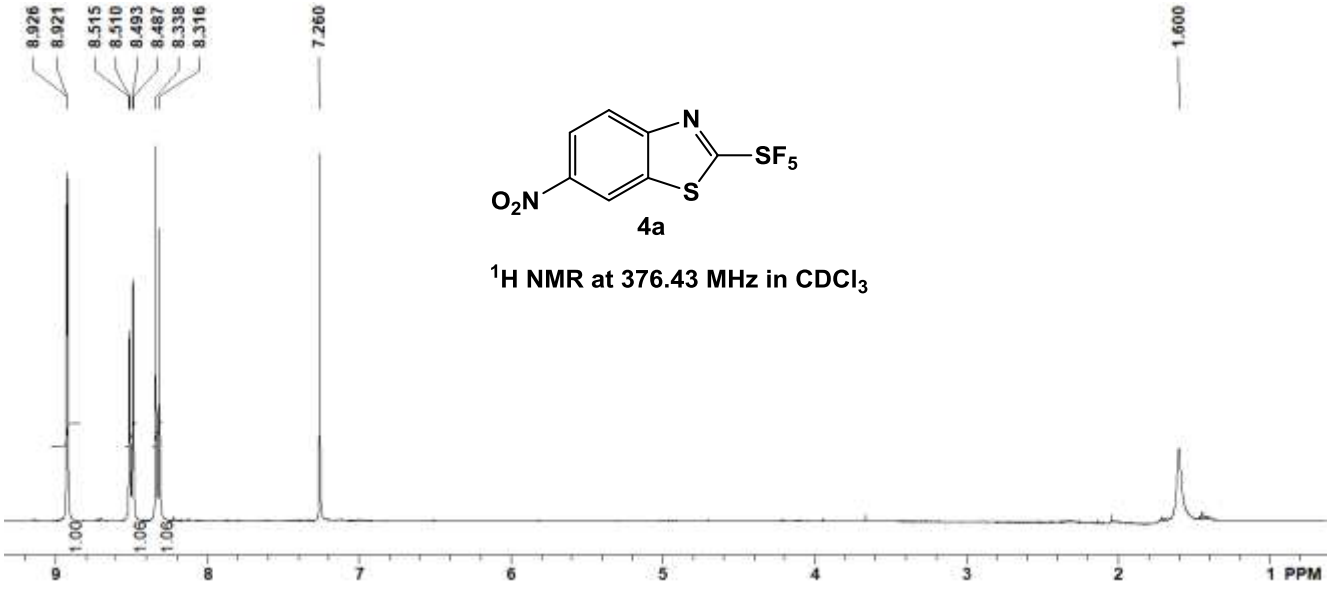
^{13}C NMR at 150.83 MHz in $CDCl_3$



2b

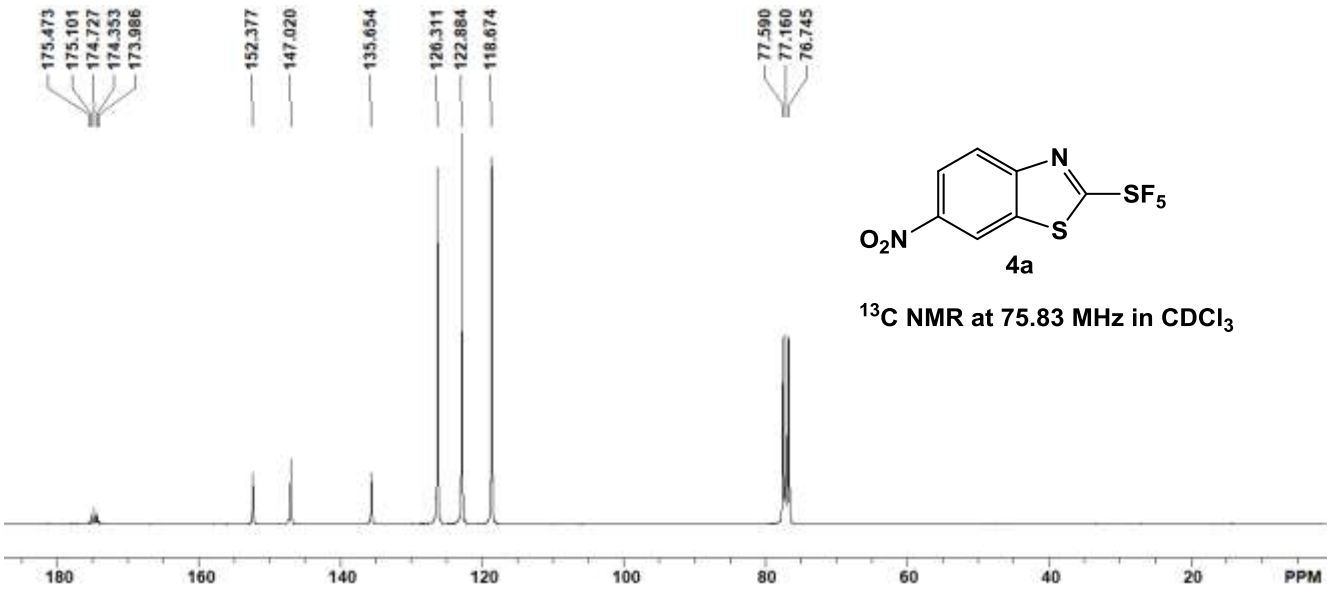
^{19}F NMR at 376.43 MHz in $CDCl_3$





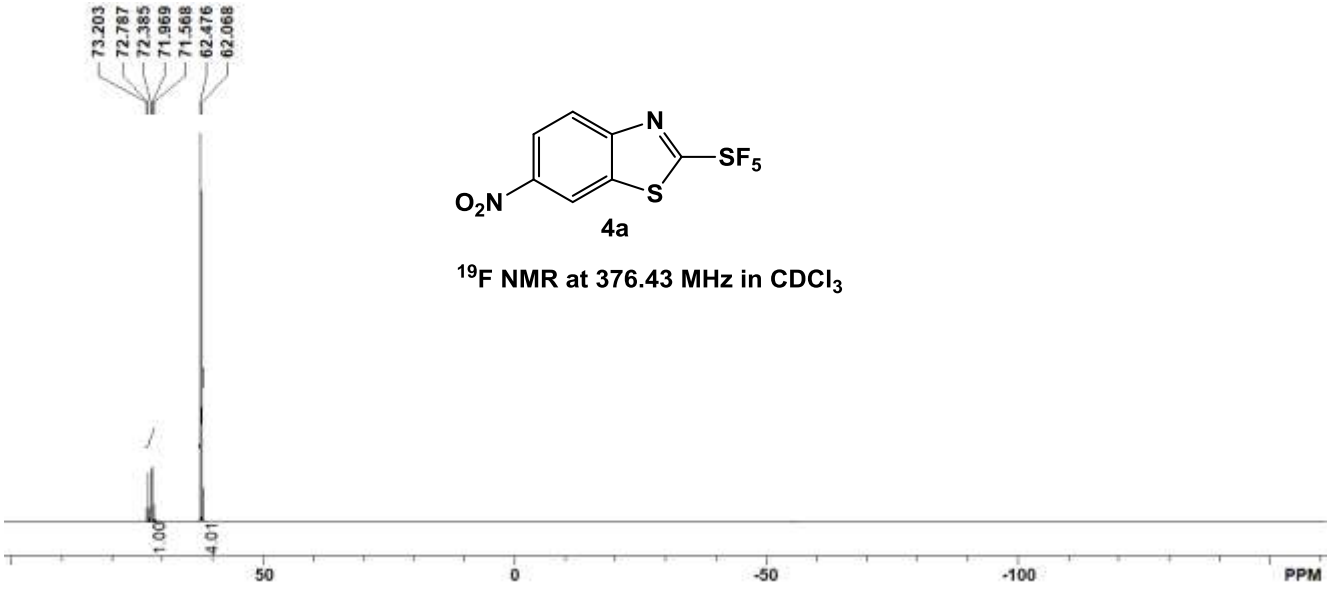
4a

^{1}H NMR at 376.43 MHz in $CDCl_3$



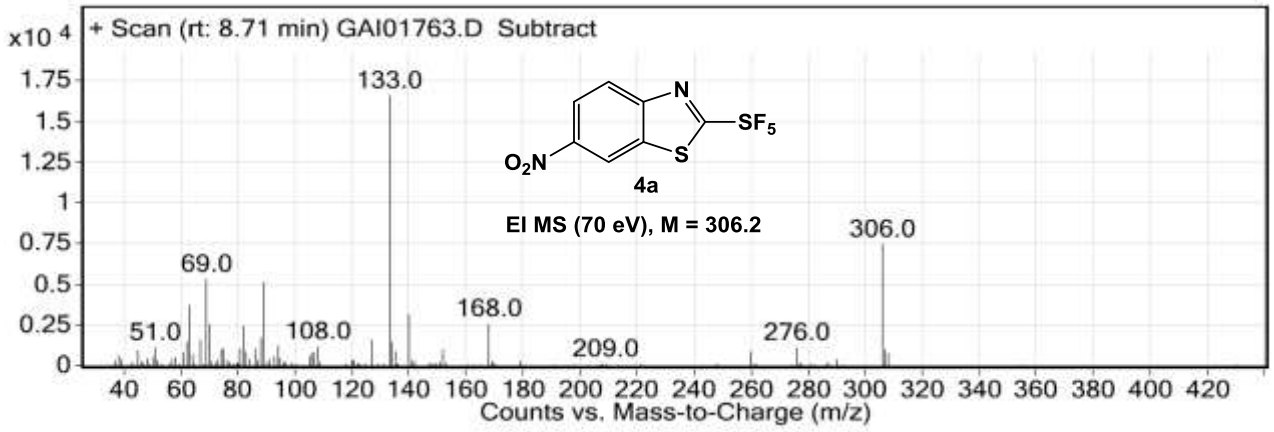
4a

^{13}C NMR at 75.83 MHz in $CDCl_3$



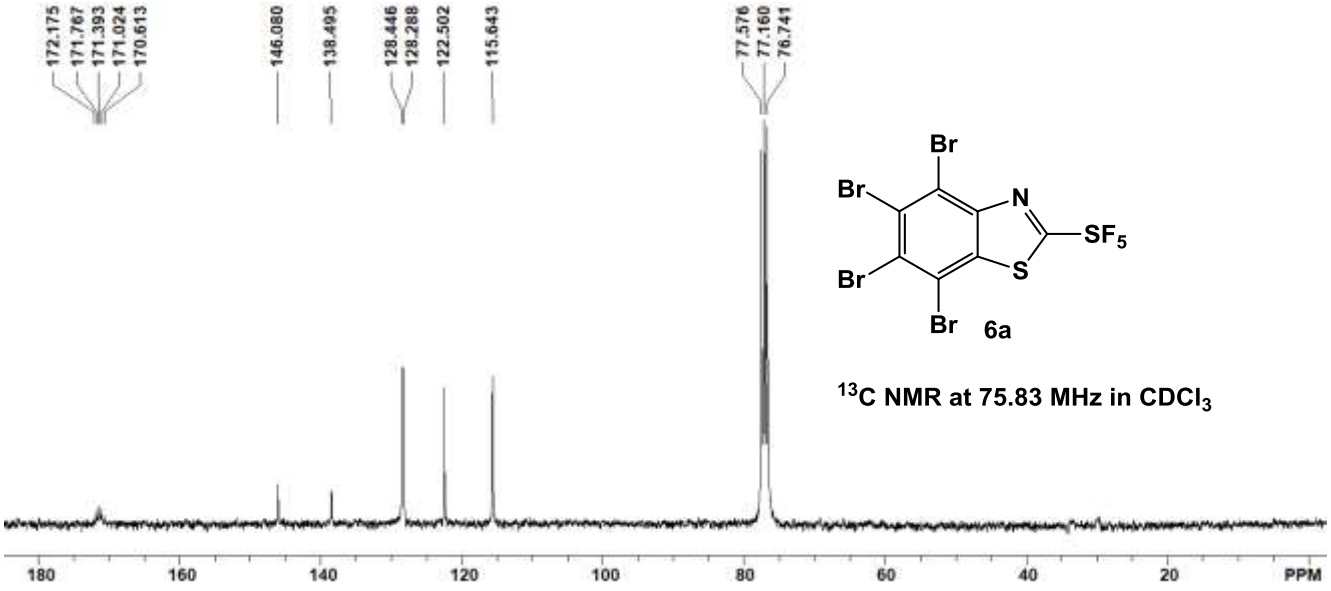
4a

^{19}F NMR at 376.43 MHz in $CDCl_3$

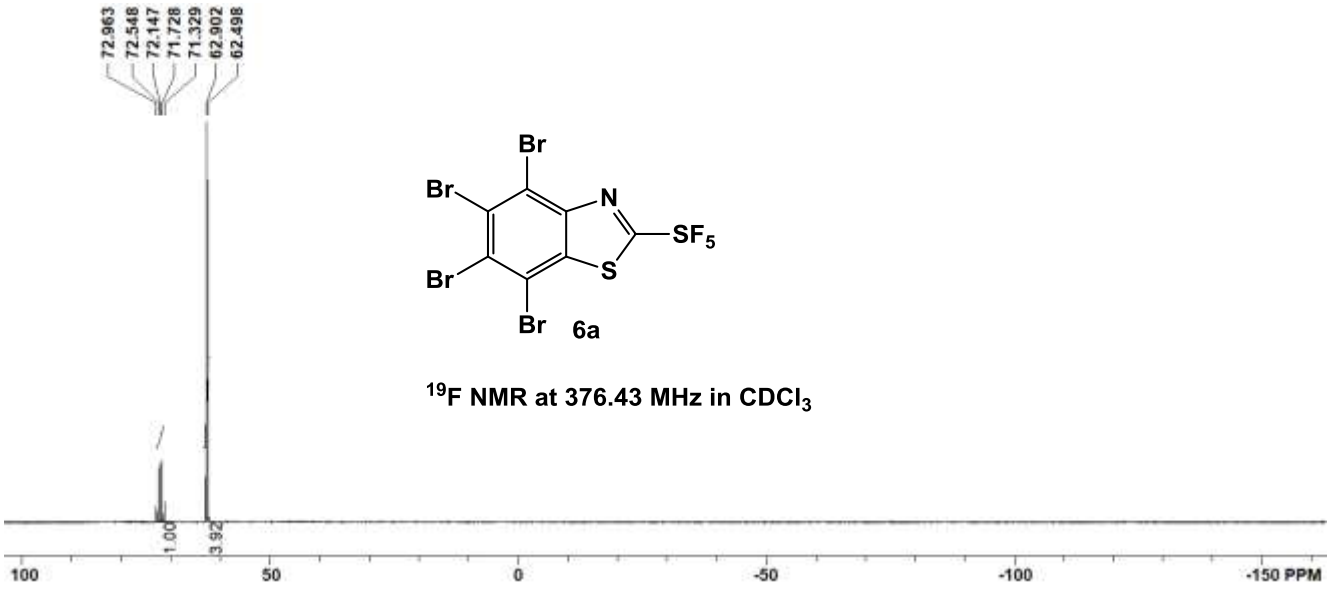


4a

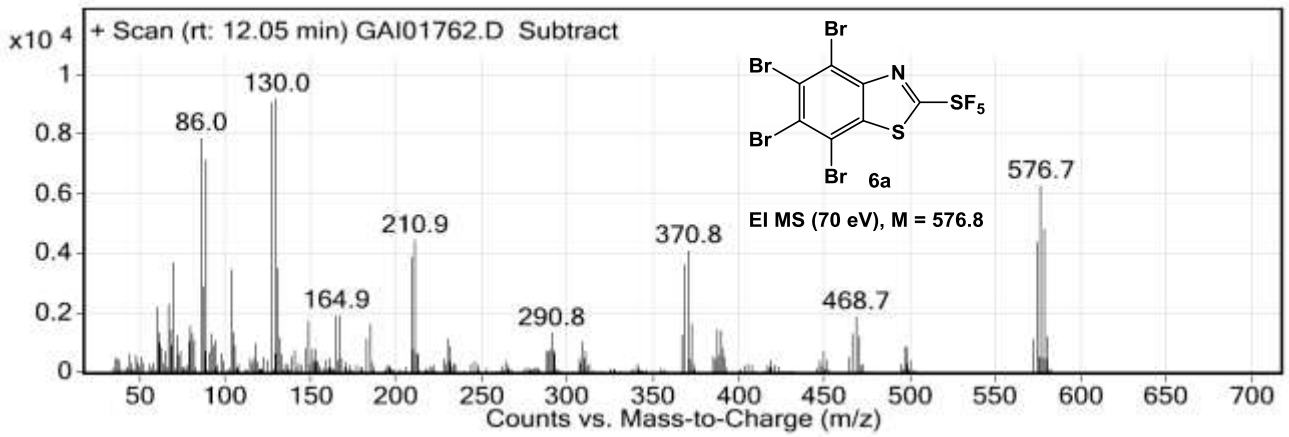
EI MS (70 eV), M = 306.2

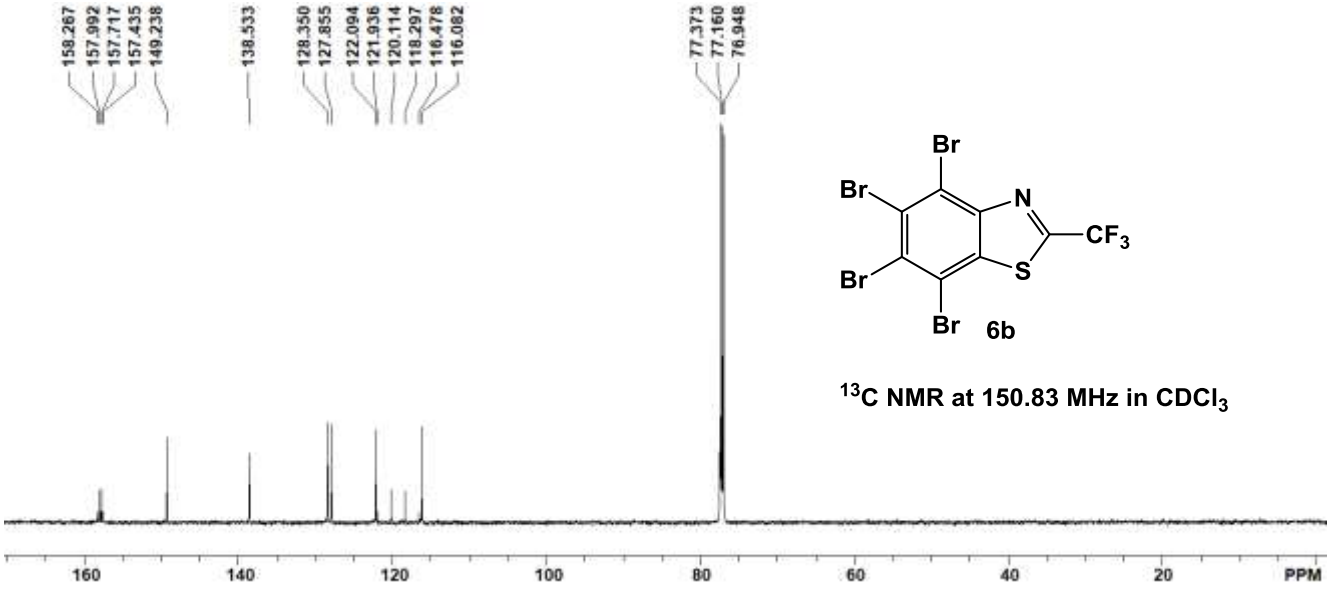


^{13}C NMR at 75.83 MHz in $CDCl_3$



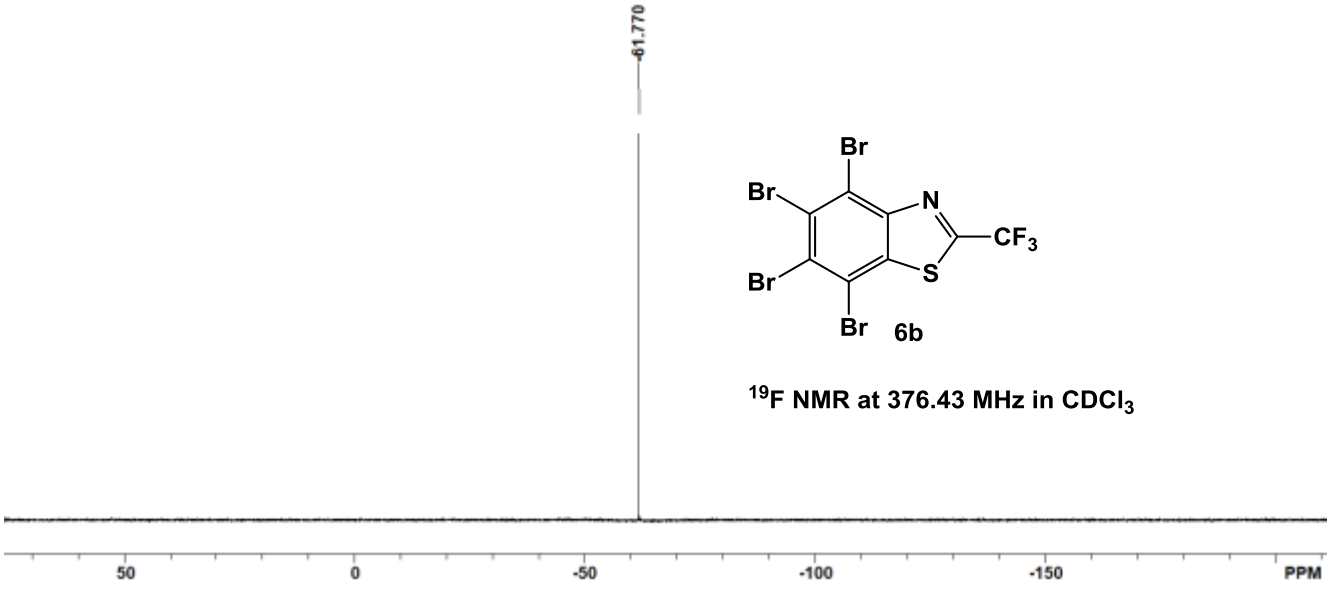
^{19}F NMR at 376.43 MHz in $CDCl_3$





6b

^{13}C NMR at 150.83 MHz in $CDCl_3$



6b

^{19}F NMR at 376.43 MHz in $CDCl_3$