

Supporting information

(Imidazol-2-ylidene)→S Coordination Interaction and its Modulation Upon S-Oxidation

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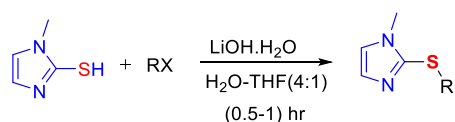
1. General Information

The reagents and chemicals required for the study were procured without further purification unless otherwise mentioned. The progress of the reaction was monitored by Thin Layer Chromatography (TLC) performed on silica gel aluminium plates using UV light. ^1H NMR and ^{13}C NMR spectra were recorded at 600 MHz and 151 MHz respectively, with TMS as an internal standard using Jeol 600 (Model no. JNM-ECZ600R/S1). ^{19}F NMR was recorded at 202.4 MHz with TMS as an internal standard. The ^1H NMR and ^{13}C NMR spectra were recorded using $\text{DMSO-}d_6$ at 2.50 ppm (^1H NMR) and 39.51 ppm (^{13}C NMR) and CDCl_3 at 7.25 ppm (^1H NMR) and 77.31 ppm (^{13}C NMR) and for a few compounds CD_3OD $\delta = 3.34, 4.87$ ppm (^1H NMR) and 49.3 (^{13}C NMR) and $(\text{CD}_3)_2\text{CO}$ $\delta = 2.06, 3.08$ ppm (^1H NMR) and 20.7, 206.07 (^{13}C NMR) respectively. Chemical shift (δ) is reported in parts per million (ppm). Coupling constants (J) were reported in Hertz (Hz). The abbreviations used to characterize the signals are as follows: s = singlet, m = multiplet, d = doublet, br. s. = broad singlet, dd = doublet of doublet, t = triplet, =quartet, m=multiplet, quin=quintuplet, sext=sextet, sep=septet, br=broad, dd=double-doublet, ddd=double-double-doublet, td=triple-doublet. High resolution mass spectrums were recorded using ESI-TOF method (Model no. Agilent 6546). IR spectrums were recorded using IR spectrophotometer.

2. Experimental Section

Experimental procedures for the compounds (1a-8a)

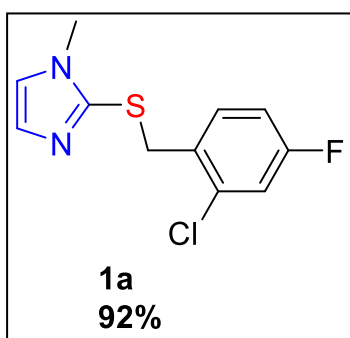
Preparation of the compound **1a**: 2-Chloro-4-Fluoro benzyl bromide (266 mgs, 1.2 mmol, 1 equiv.) was added to the magnetically stirred mixture of 1-methyl-1H-imidazole-2-thiol (114 mgs, 1 mmol, 1 equiv) and base $\text{LiOH}\cdot\text{H}_2\text{O}$ (21 mgs, 1 mmol, 0.5 equiv) in a biphasic solvent media of (THF/ H_2O), and reaction was continued for at the room temperature for 0.5 hr. Reaction progress was monitored through thin layer chromatography (TLC). Upon of the reaction completion, the product was diluted with EtOAc and thoroughly washed with water (3*10 ml). The organic layer was separated through work-up and dried over (Na_2SO_4). Without any additional purification, the volatile components were extracted in vacuo, yielding a pure product in the form of greyish liquid.



Scheme S1: Synthesis of sulfide derivatives (**1a-8a**)

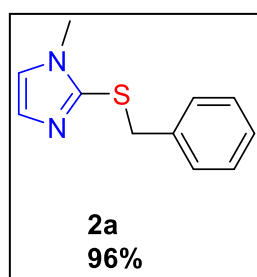
Characterization data of 1a-8a

2-((2-chloro-4-fluorobenzyl)thio)-1-methyl-1H-imidazole (1a)



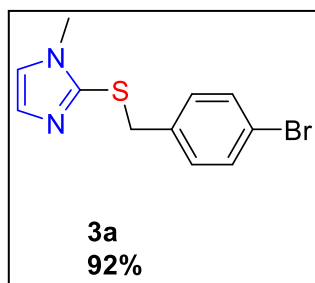
The title compound was isolated by (EtOAc/H₂O) work up; Yield: 92 % (235 mgs), Yellowish liquid, ¹H NMR (600MHz, CDCl₃) δ 7.15 – 7.08 (m, 2H), 6.99 (dd, *J* = 8.6, 6.1 Hz, 1H), 6.88 (s, 1H), 6.80 (td, *J* = 8.3, 2.6 Hz, 1H), 4.23 (s, 1H), 3.32 (s, 2H); ¹³C{¹H} NMR (151 MHz, CDCl₃): 165.34 (d, ¹*J*_{C-F} = 250.1 Hz), 139.99, 134.64 (d, ³*J*_{C-F} = 10.3 Hz), 131.65 (d, ³*J*_{C-F} = 9.0 Hz), 129.86, 122.64, 116.98 (d, ²*J*_{C-F} = 24.7 Hz), 113.96 (d, ²*J*_{C-F} = 20.9 Hz), 36.97, 33.11.

2-(benzylthio)-1-methyl-1H-imidazole (2a)



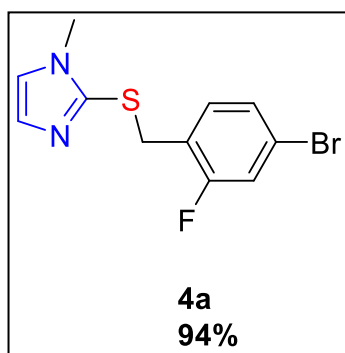
The title compound was isolated by (EtOAc/H₂O) work up; Yield: 96 % (195 mgs), Yellowish liquid, ¹H NMR (600MHz, CDCl₃) δ 7.22-7.20 (m, 3H), 7.11-7.09 (m, 3H), 6.83 (s, 1H), 4.13 (s, 2H), 3.21 (s, 3H); ¹³C{¹H} NMR (151 MHz, CDCl₃): δ 140.58, 137.99, 129.86, 128.85, 128.59, 127.45, 122.51, 40.23, 33.13.

2-((4-bromobenzyl)thio)-1-methyl-1H-imidazole (3a)



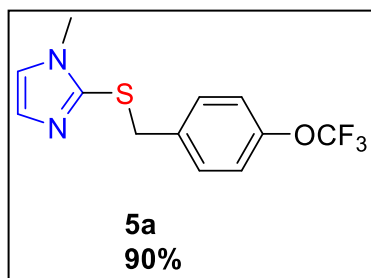
The title compound was isolated by (EtOAc/H₂O) work up; Yield: 92 % (258 mg), Yellowish liquid, ¹H NMR (600MHz, CDCl₃) δ 7.36 (d, *J* = 8.4 Hz, 2H), 7.11 (s, 1H), 7.01 (d, *J* = 8.4 Hz, 2H), 6.87 (s, 1H), 4.11 (s, 2H), 3.30 (s, 3H); ¹³C{¹H} NMR (151 MHz, CDCl₃): δ 140.25, 137.22, 131.73, 130.58, 129.97, 122.67, 121.44, 39.39, 33.28.

2-((4-bromo-2-fluorobenzyl)thio)-1-methyl-1H-imidazole (4a)



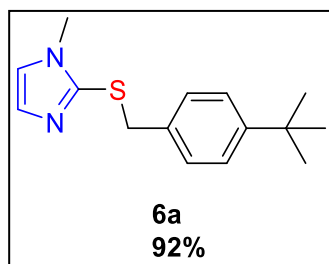
The title compound was isolated by (EtOAc/H₂O) work up; Yield: 94% (281 mg), Yellowish liquid, ¹H NMR (600MHz, CDCl₃): δ 7.21 (dd, *J* = 9.3, 1.8 Hz, 1H), 7.16 – 7.09 (m, 2H), 6.94 – 6.88 (t, 2H), 4.14 (s, 2H), 3.36 (s, 3H); ¹³C{¹H} NMR (151 MHz, CDCl₃): δ 160.50 (d, ¹*J*_{C-F} = 252.6 Hz), 140.00, 131.89, 129.97, 127.43, 124.62 (d, ²*J*_{C-F} = 14.9 Hz), 122.80, 121.69 (d, ³*J*_{C-F} = 9.5 Hz), 119.19 (d, ²*J*_{C-F} = 24.8 Hz), 33.26, 32.58.

1-methyl-2-((4-(trifluoromethoxy)benzyl)thio)-1H-imidazole (5a)



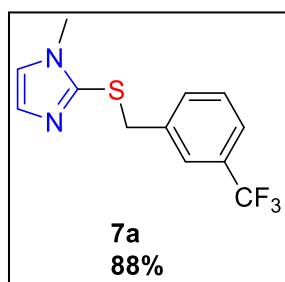
The title compound was isolated by (EtOAc/H₂O) work up; Yield: 90% (259 mgs), Yellowish liquid, NMR (600MHz, CDCl₃) δ 7.19 – 7.15 (m, 2H), 7.13 (s, 1H), 7.10 (d, J = 8.2 Hz, 2H), 6.88 (s, 1H), 4.18 (s, 2H), 3.29 (s, 3H); ¹³C{¹H} NMR (151 MHz, CDCl₃): δ 148.47, 140.08, 136.80, 130.17, 129.72, 122.56, 121.03, 39.08, 33.08.

2-((4-(tert-butyl)benzyl)thio)-1-methyl-1H-imidazole (6a)



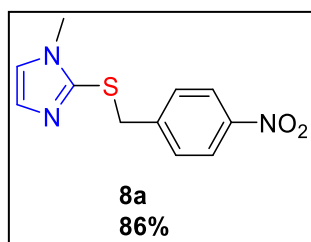
The title compound was isolated by (EtOAc/H₂O) work-up; Yield: 92 % (239 mgs), Yellowish liquid, ¹H NMR (600MHz, CDCl₃) δ 7.27 (d, J = 8.2 Hz, 2H), 7.11 (s, 1H), 7.08 – 7.05 (m, 2H), 6.87 (s, 1H), 4.15 (s, 2H), 3.25 (s, 3H); ¹³C{¹H} NMR (151 MHz, CDCl₃): δ 149.48, 139.80, 133.58, 128.65, 127.44, 124.40, 121.32, 38.64, 33.48, 31.98, 30.30.

1-methyl-2-((3-(trifluoromethyl)benzyl)thio)-1H-imidazole (7a)



The title compound was isolated by (EtOAc/H₂O) work up; Yield: 88% (239 mgs), Yellowish liquid, ¹H NMR (600MHz, CDCl₃) δ 7.49 (t, J = 2.0 Hz, 3H), 7.47 (s, 1H), 7.45 – 7.40 (m, 2H), 4.34 (s, 2H), 3.69 (s, 3H); ¹³C{¹H} NMR (151 MHz, CDCl₃): δ 142.36, 138.65 (q, J = 2.6 Hz), 131.68 (d, J = 32.2 Hz), 130.26, 129.66 (d, J = 18 Hz), 128.82, 127.22 (t, J = 5 Hz), 125.40, 123.89 (t, J = 7 Hz), 122.88, 36.67, 33.47.

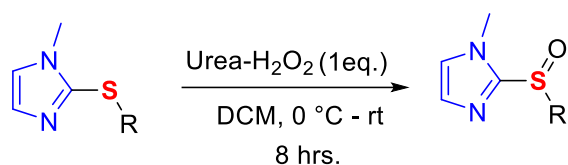
1-methyl-2-((4-nitrobenzyl)thio)-1H-imidazole- (8a)



The title compound was isolated by (EtOAc/H₂O) work up; Yield: 86% (215 mgs), Brownish liquid, ¹H NMR (600 MHz, CDCl₃) δ 8.10 (d, J = 8.7 Hz, 2H), 7.34 (d, J = 8.7 Hz, 2H), 7.11 (s, 1H), 6.89 (s, 1H), 4.26 (s, 2H), 3.35 (s, 3H); ¹³C{¹H} NMR (151 MHz, CDCl₃): δ 147.20, 145.89, 139.59, 129.96, 129.68, 123.80, 122.83, 38.80, 33.25.

Experimental procedures for the compounds (1b-8b)

2-((2-chloro-4-fluorobenzyl)thio)-1-methyl-1H-imidazole (**1a**) (256mgs, 1mmol, 1 equiv.) was added in ice cooled Dichloromethane (DCM). The reaction mixture was stirred for 10 minutes, and after that urea-H₂O₂ (118 mgs, 1.25 mmol, 1.25 equiv) was added dropwise. The reaction was continued for 8 hr. at room temperature. Reaction progress was monitored by TLC. Upon completion, the reaction was quenched with saturated aqueous solution of Sodium Bicarbonate (NaHCO₃) and extracted with DCM (3*10 ml). The combined organic layer was dried over (Na₂SO₄), concentrated and purified by column chromatography to provide the pure product as white solid.



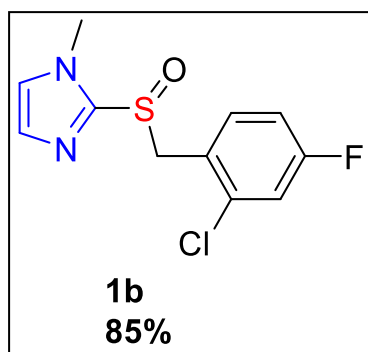
Scheme S2: Synthesis of sulfide derivatives (**1b-8b**)

Table S1. Screening of oxidation process

S.NO.	Oxidising agents	Solvent	(equiv.)	Temp.	Time (h)	Isolated yield (%)
1	Urea-H ₂ O ₂	DCM	1	0 °C - rt	8 hrs.	85 %
2	Urea-H ₂ O ₂	DCE	1	0 °C - rt	8 hrs.	82 %
3	Urea-H ₂ O ₂	DCM	1	Rt	14 hrs.	65 %
4	Urea-H ₂ O ₂	DCM	1	60 °C	8 hrs.	60%
5	Urea-H ₂ O ₂	DCM	1.5	Rt	8 hrs.	54%
6	H ₂ O ₂ (30 %)	DCM	1	0 °C - rt	8 hrs.	75 %
7	TBHP	DCM	1	0 °C - rt	8hrs	60 %
8	mCPBA	DCM	1	0 °C - rt	8 hrs.	72 %
9	mCPBA	CAN	1	rt	8 hrs.	55 %
10	NBS	β-CD/H ₂ O	1	0 °C - rt	12 hrs.	No product formed
11	NFSI	CAN	1	0 °C - rt	8 hrs.	62%

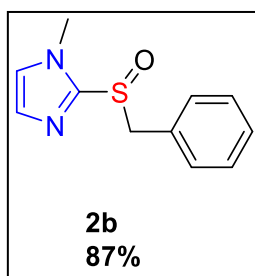
Characterization data of 1b-8b

2-((2-chloro-4-fluorobenzyl)sulfinyl)-1-methyl-1H-imidazole (1b)



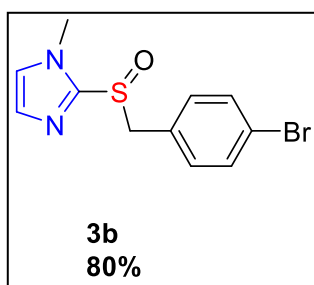
The title compound was isolated by flash chromatography; Yield: 85 % (218 mgs), Yellowish liquid, ¹H NMR (600MHz, CDCl₃) δ 7.24 – 7.20 (m, 2H), 7.17 (dd, *J* = 8.4, 2.6 Hz, 1H), 6.98 (s, 1H), 6.93 (td, *J* = 8.3, 2.6 Hz, 1H), 4.85 (d, *J* = 12.8 Hz, 1H), 4.64 (d, *J* = 12.8 Hz, 1H), 3.68 (s, 3H); ¹³C{¹H} NMR (151 MHz, CDCl₃): δ ¹³C NMR (151 MHz,) δ 161.59 (d, ¹*J*_{C-F} = 252.0 Hz), 143.20, 134.95 (d, ³*J*_{C-F} = 10.3 Hz), 133.24 (d, ³*J*_{C-F} = 8.8 Hz), 129.03, 123.97, 122.65, 116.14 (d, ²*J*_{C-F} = 24.9 Hz), 113.47 (d, ²*J*_{C-F} = 21.2 Hz), 55.38, 32.32.

2-(benzylsulfinyl)-1-methyl-1H-imidazole (2b)



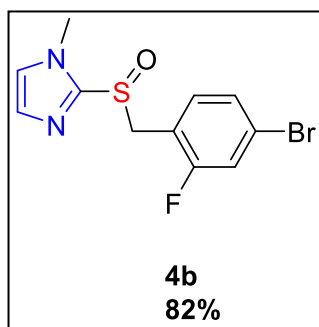
The title compound was isolated by flash chromatography; Yield: 87 % (294 mg), Yellowish liquid; ^1H NMR (600MHz, CDCl_3) δ 7.35 – 7.27 (m, 3H), 7.21 (s, 1H), 7.06 (d, $J = 7.2$ Hz, 2H), 6.85 (s, 1H), 4.59 (d, $J = 12.7$ Hz, 1H), 4.40 (d, $J = 12.7$ Hz, 1H), 3.33 (s, 3H); $^{13}\text{C}\{^1\text{H}\}$ NMR (151 MHz, CDCl_3): δ 143.32, 130.54, 129.84, 129.03, 128.62, 128.57, 124.60, 60.32, 32.91.

2-((4-bromobenzyl)sulfinyl)-1-methyl-1H-imidazole (3b)



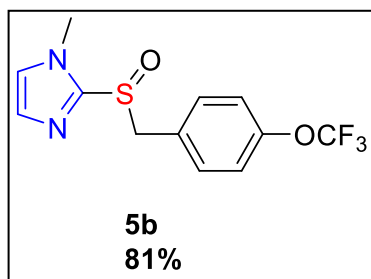
The title compound was isolated by flash chromatography; Yield: 80 % (328 mg), White solid, m.p. 160-163 °C; ^1H NMR (600MHz, CDCl_3) δ 7.43 (d, $J = 8.3$ Hz, 2H), 7.22 (s, 1H), 6.98 (d, $J = 8.3$ Hz, 2H), 6.90 (s, 1H), 4.57 (d, $J = 12.8$ Hz, 1H), 4.37 (d, $J = 12.8$ Hz, 1H), 3.47 (s, 3H); $^{13}\text{C}\{^1\text{H}\}$ NMR (151 MHz, CDCl_3): δ 143.05, 132.16, 131.76, 129.84, 128.21, 124.85, 122.91, 59.33, 33.12.

2-((4-bromo-2-fluorobenzyl)sulfinyl)-1-methyl-1H-imidazole (4b)



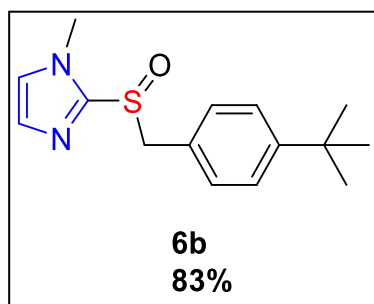
The title compound was isolated by flash chromatography; Yield: 82% (246 mg), White solid, 128-130 °C; ^1H NMR (600MHz, CDCl_3) δ 7.30 – 7.27 (m, 1H), 7.25 (dd, $J = 8.2, 1.7$ Hz, 1H), 7.23 (d, $J = 1.1$ Hz, 1H), 7.05 (t, $J = 7.9$ Hz, 1H), 6.98 (s, 1H), 4.69 (d, $J = 12.2$ Hz, 1H), 4.53 (d, $J = 12.2$ Hz, 1H), 3.69 (s, 3H); $^{13}\text{C}\{^1\text{H}\}$ NMR (151 MHz, CDCl_3): δ 161.12 (d, $^1J_{\text{C-F}} = 253.7$ Hz), 143.58, 133.64, 129.87 (d, $^3J_{\text{C-F}} = 4.8$ Hz), 127.69, 125.00, 119.24 (d, $^3J_{\text{C-F}} = 5.7$ Hz), 119.08, 116.05 (d, $^2J_{\text{C-F}} = 15.2$ Hz), 52.38, 33.29.

1-methyl-2-((4-(trifluoromethoxy)benzyl)sulfinyl)-1H-imidazole (5b)



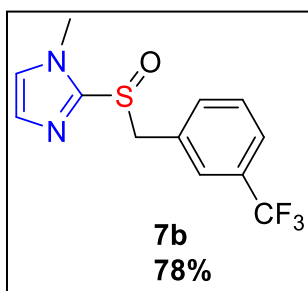
The title compound was isolated by flash chromatography; Yield: 81% (274 mg), Yellowish liquid, NMR (600MHz, CDCl_3) δ 7.21 (s, 1H), 7.16-7.13 (m, 4H), 6.88 (s, 1H), 4.58 (d, $J = 12.9$ Hz, 1H), 4.41 (d, $J = 12.9$ Hz, 1H), 3.44 (s, 3H); $^{13}\text{C}\{^1\text{H}\}$ NMR (151 MHz, CDCl_3): δ 149.60, 143.03, 132.15, 129.95, 128.16, 125.00, 121.17, 119.63, 59.27, 33.14.

2-((4-(tert-butyl)benzyl)sulfinyl)-1-methyl-1H-imidazole (6b)



The title compound was isolated by flash chromatography; Yield: 83 % (310 mg), White solid, m.p. 120-122 °C; ^1H NMR (600MHz, CDCl_3) δ 7.31 (d, $J = 8.2$ Hz, 2H), 7.21 (s, 1H), 7.01 (d, $J = 8.2$ Hz, 2H), 6.86 (s, 1H), 4.55 (d, $J = 12.8$ Hz, 1H), 4.37 (d, $J = 12.8$ Hz, 1H), 3.33 (s, 3H), 1.30 (s, 9H); $^{13}\text{C}\{^1\text{H}\}$ NMR (151 MHz, CDCl_3): δ 150.82, 142.58, 129.22, 128.75, 124.99, 124.54, 123.54, 58.96, 33.61, 31.83, 30.25.

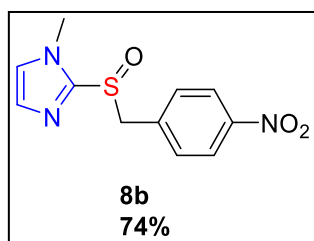
1-methyl-2-((3-(trifluoromethyl)benzyl)sulfinyl)-1H-imidazole (7b)



The title compound was isolated by flash chromatography; Yield: 78% (263 mg), Yellowish liquid, ^1H NMR (600MHz, CDCl_3) δ 7.61 (d, $J = 7.9$ Hz, 1H), 7.45 (t, $J = 7.7$ Hz, 1H), 7.38 (d, $J = 7.7$ Hz, 1H), 7.24 (d, $J = 9.9$ Hz, 2H), 6.88 (s, 1H), 4.63 (d, $J = 12.9$ Hz, 1H), 4.46 (d, $J = 12.9$ Hz, 1H), 3.40 (s, 3H); $^{13}\text{C}\{^1\text{H}\}$ NMR (151 MHz, CDCl_3): δ 142.58, 134.19, 131.08 (q, $J = 32.4$ Hz), 130.35, 129.86, 129.04, 127.10, 125.30, 124.99, 124.62, 122.82, 59.59,

33.01.

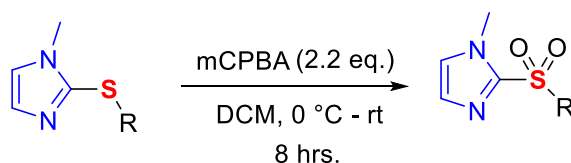
1-methyl-2-((4-nitrobenzyl)sulfinyl)-1H-imidazole (8b)



The title compound was isolated by flash chromatography; Yield: 74% (321 mg), White solid, m.p. 115-117 °C; ^1H NMR (600MHz, CDCl_3) δ 8.17 (d, $J = 8.7$ Hz, 2H), 7.35 (d, $J = 8.7$ Hz, 2H), 7.22 (s, 1H), 6.93 (s, 1H), 4.71 (d, $J = 12.8$ Hz, 1H), 4.57 (d, $J = 12.8$ Hz, 1H), 3.56 (s, 3H); $^{13}\text{C}\{^1\text{H}\}$ NMR (151 MHz, CDCl_3): δ 147.96, 142.68, 136.84, 131.56, 129.91, 125.24, 123.61, 58.94, 33.35.

Experimental procedures for the compounds (1c-8c)

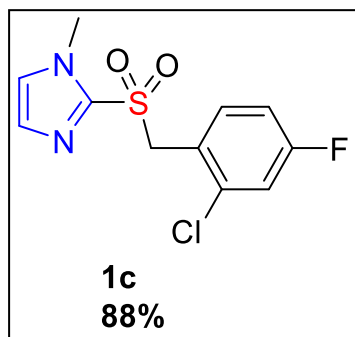
2-((2-chloro-4-fluorobenzyl)thio)-1-methyl-1H-imidazole (**1a**) (256 mgs, 1 mmol, 1 equiv) was added in ice cooled Dichloromethane (DCM). To the solution of the reaction mixture mCPBA (459.2 mgs, 2.8 mmol, 2.8 equiv.) was added. The reaction was continued for 8 hr. at room temperature. Progression of the reaction was monitored by TLC. Upon completion the reaction was quenched with saturated aqueous solution of Sodium Bicarbonate (NaHCO₃) and extracted with DCM (3*10 ml). The combined organic layer was dried over (Na₂SO₄), concentrated to provide pure product as white solid without any further purification.



Scheme S3: Synthesis of sulfide derivatives (**1c-8c**)

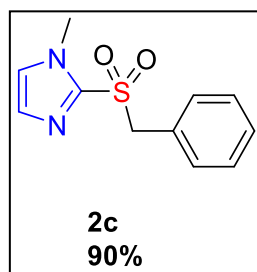
Characterization data of 1c-8c

2-((2-chloro-4-fluorobenzyl)sulfonyl)-1-methyl-1H-imidazole (**1c**)



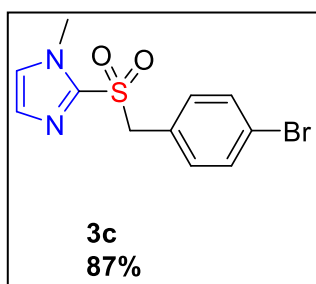
The title compound was isolated by (DCM/H₂O) work up; Yield: 88 % (253 mgs), white solid, m.p. 124-126 °C; ¹H NMR (600MHz, CDCl₃) δ 7.26 – 7.23 (m, 1H), 7.21 (s, 1H), 7.16 (dd, *J* = 8.3, 2.6 Hz, 1H), 7.01 – 6.95 (m, 2H), 4.81 (s, 2H), 3.59 (s, 3H); ¹³C{¹H} NMR (151 MHz, CDCl₃): δ 162.82 (d, ¹*J*_{C-F} = 253.3 Hz), 140.68, 136.70 (d, ³*J*_{C-F} = 10.4 Hz), 134.26 (d, ³*J*_{C-F} = 9.8 Hz), 129.92 (d, ²*J*_{C-F} = 14.4 Hz), 126.16 (d, ²*J*_{C-F} = 25.9 Hz), 121.85, 121.84, 117.50 (d, ²*J*_{C-F} = 19.2 Hz), 114.68 (d, ³*J*_{C-F} = 10.5 Hz), 57.96, 34.88.

2-(benzylsulfonyl)-1-methyl-1H-imidazole (**2c**)



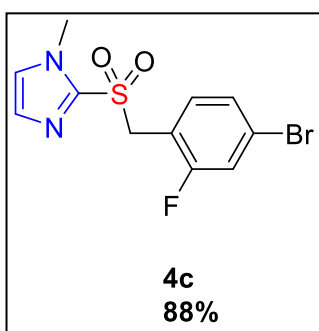
The title compound was isolated by (DCM/H₂O) work up; Yield: 90 % (212.4 mgs), White solid, m.p. 105-108 °C; ¹H NMR (600MHz, CDCl₃) δ 7.37 – 7.34 (m, 1H), 7.30-7.28 (m, 2H); 7.22 (s, 1H), 7.06 (d, *J* = 8.2 Hz, 2H), 6.84 (s, 1H), 4.57 (s, 2H), 3.26 (s, 3H); ¹³C{¹H} NMR (151 MHz, CDCl₃): 140.55, 130.98, 129.73, 129.14, 128.70, 127.32, 125.62, 62.29, 34.52.

2-((4-bromobenzyl)sulfonyl)-1-methyl-1H-imidazole (3c)



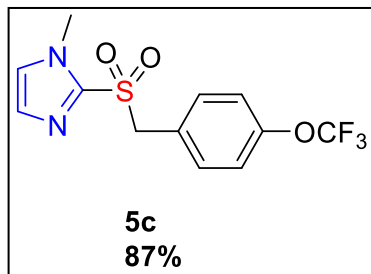
The title compound was isolated by (DCM/H₂O) work up; Yield: 87 % (272 mgs), white solid, m.p. 145-147 °C; ¹H NMR (600MHz, CDCl₃) δ 7.44 (d, *J* = 8.4 Hz, 2H), 7.22 (s, 1H), 6.99 (d, *J* = 8.4 Hz, 2H), 6.89 (s, 1H), 4.56 (s, 2H), 3.44 (s, 3H); ¹³C{¹H} NMR (151 MHz, CDCl₃): 140.52, 132.64, 132.52, 131.91, 129.77, 129.66, 126.33, 125.75, 125.66, 123.61, 61.33, 34.76.

2-((4-bromo-2-fluorobenzyl)sulfonyl)-1-methyl-1H-imidazole (4c)



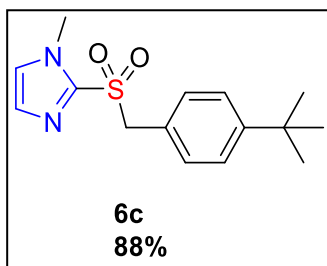
The title compound was isolated by (DCM/H₂O) work up; Yield: 88% (292 mgs), White solid, m.p. 115-120 °C; ¹H NMR (600MHz, CDCl₃) δ 7.21 (d, *J* = 1.9 Hz, 1H), 7.20 – 7.17 (m, 1H), 7.16 (s, 1H), 6.96 (t, *J* = 7.8 Hz, 1H), 6.90 (d, *J* = 1.1 Hz, 1H), 4.61 (s, 2H), 3.55 (s, 3H); ¹³C{¹H} NMR (151 MHz, CDCl₃): 161.34 (d, ¹*J*_{C-F} = 255.6 Hz), 140.68, 133.61, 129.79, 127.85, 125.97, 124.04 (d, ³*J*_{C-F} = 9.5 Hz), 119.55 (d, ²*J*_{C-F} = 24.7 Hz), 114.17 (d, ²*J*_{C-F} = 14.9 Hz), 54.60, 34.93.

1-methyl-2-((4-(trifluoromethoxy)benzyl)sulfonyl)-1H-imidazole (5c)



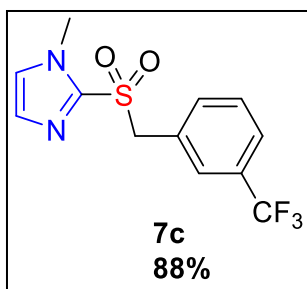
The title compound was isolated by (DCM/H₂O) work up; Yield: 87% (278 mgs), White solid, m.p. 97-100 °C; NMR (500MHz, CDCl₃) δ 7.23 (s, 1H), 7.16 (s, 4H), 6.89 (s, 1H), 4.62 (s, 2H), 3.41 (s, 3H); ¹³C{¹H} NMR (151 MHz, CDCl₃): δ 149.94, 140.57, 132.69, 132.19, 129.87, 126.18, 125.85, 121.22, 61.27, 34.76.

2-((4-(tert-butyl)benzyl)sulfonyl)-1-methyl-1H-imidazole (6c)



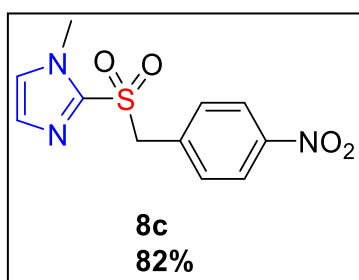
The title compound was isolated by (DCM/H₂O) work-up Yield: 88 % (256 mg), white solid, m.p. 128-130 °C; ¹H NMR (600MHz, CDCl₃) δ 7.31 (d, *J* = 8.3 Hz, 2H), 7.22 (s, 1H), 6.99 (d, *J* = 8.3 Hz, 2H), 6.85 (s, 1H), 4.53 (s, 2H), 3.23 (s, 3H), 1.29 (s, 9H); ¹³C{¹H} NMR (151 MHz, CDCl₃): 152.65, 140.82, 130.81, 129.81, 125.73, 124.24, 62.00, 34.80, 34.49, 31.35.

1-methyl-2-((3-(trifluoromethyl)benzyl)sulfonyl)-1H-imidazole (7c)



The title compound was isolated by (DCM/H₂O) work up; Yield: 88% (267 mgs), white solid, m.p. 110-112 °C; ¹H NMR (600MHz, CDCl₃) δ 7.63 (d, *J* = 7.7 Hz, 1H), 7.47 (t, *J* = 7.7 Hz, 1H), 7.41 (d, *J* = 7.7 Hz, 1H), 7.24 (s, 2H), 6.87 (s, 1H), 4.66 (s, 2H), 3.38 (s, 3H); ¹³C{¹H} NMR (151 MHz, CDCl₃): δ 139.20, 133.53, 130.17 (q, *J* = 32.7 Hz), 128.83, 128.28, 127.55, 126.54, 124.79, 123.41, 121.60, 60.50, 33.6.

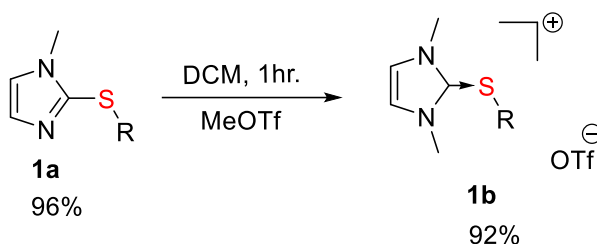
1-methyl-2-((4-nitrobenzyl)sulfonyl)-1H-imidazole (8c)



The title compound was isolated by (DCM/H₂O) work up; Yield: 82% (230 mgs), White solid, m.p. 155-160 °C; ¹H NMR (600MHz, CDCl₃) δ 8.18 (d, *J* = 6.9 Hz, 2H), 7.40 (d, *J* = 8.7 Hz, 2H), 7.23 (s, 1H), 6.93 (s, 1H), 4.78 (s, 2H), 3.57 (s, 3H); ¹³C{¹H} NMR (151 MHz, CDCl₃): 147.23, 139.49, 133.41, 131.10, 128.69, 124.87, 122.71, 59.91, 33.93.

Experimental procedures for the compounds (1d-8d)

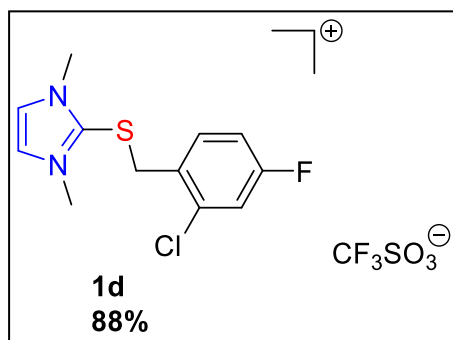
The neutral sulfide (**1a**) (256 mgs, 1 mmol, 1 equiv) was dissolved in ice cooled DCM. The reaction was stirred continuously for 10 mins, and then MeOTf (137 μ l, 1.25 mmol, 1.25 equiv.) was added. The reaction was continued at room temperature for 1 hr. Progression of the reaction was monitored by TLC. The product was washed thoroughly with diethyl ether to give the desired product as white powder.



Scheme S4. Synthetic reaction scheme for the *N*-methylation of sulfides

Characterization data of 1d-8d

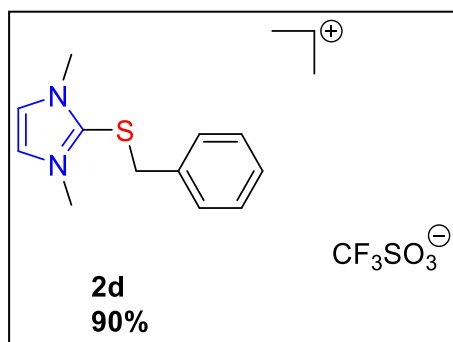
1,3-dimethyl-2-((2-chloro-4-fluorobenzyl)thio)-1H-imidazol-3-ium Triflate (**1d**)



The title compound was isolated by successive Diethyl ether wash; Yield: 88 % (368 mgs), white solid, m.p. 115-117 °C; ^1H NMR (600MHz, $\text{DMSO-}d_6$) δ 7.90 (s, 2H), 7.53 (dd, $J = 8.8, 2.7$ Hz, 1H), 7.34 (dd, $J = 8.6, 6.1$ Hz, 1H), 7.22 (td, $J = 8.5, 2.6$ Hz, 1H), 4.34 (s, 2H), 3.64 (s, 6H); $^{13}\text{C}\{^1\text{H}\}$ NMR (151 MHz, $\text{DMSO-}d_6$): δ 161.74 (d, $^1J_{\text{C-F}} = 249.6$ Hz), 138.33, 133.83 (d, $^3J_{\text{C-F}} = 10.6$ Hz), 132.78 (d, $^3J_{\text{C-F}} = 9.0$ Hz), 130.57, 125.38, 117.21 (d, $^2J_{\text{C-F}} = 25.3$ Hz), 115.24 (d, $^2J_{\text{C-F}} = 21.3$ Hz), 40.05, 35.83;

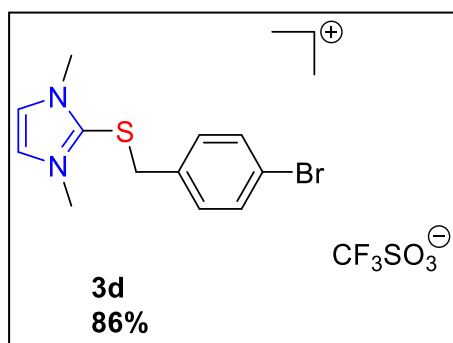
^{19}F -NMR (600 MHz, $\text{DMSO-}d_6$) $\delta = -110.32$; HRMS (ESI-TOF) m/z Calcd for $\text{C}_{12}\text{H}_{13}\text{ClFN}_2\text{S}^+$ [M^+] 271.0467 found 271.0478.

1,3-dimethyl-2-(benzylthio)-1H-imidazol-3-ium Triflate (**2d**)



The title compound was isolated by successive Diethyl ether wash; Yield: 90 % (331.2 mg), white solid, m.p. 110-112 °C; ^1H NMR (600MHz, $\text{DMSO-}d_6$): δ 7.86 (s, 2H), 7.31 (d, $J = 6.4$ Hz, 3H), 7.13 (d, $J = 5.8$ Hz, 2H), 4.27 (s, 2H), 3.59 (s, 6H); $^{13}\text{C}\{^1\text{H}\}$ NMR (151 MHz, $\text{DMSO-}d_6$): 138.90, 136.52, 128.91, 128.86, 128.14, 125.11, 38.82, 35.78; HRMS (ESI-TOF) m/z Calcd for $\text{C}_{12}\text{H}_{15}\text{N}_2\text{S}^+$ [M^+] 219.0950 found 219.0959.

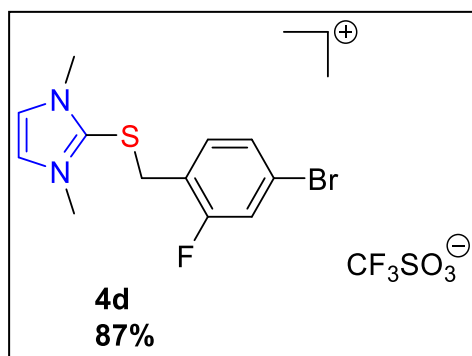
1,3-dimethyl-2-((4-bromobenzyl)thio)-1H-imidazol-3-ium Triflate (3d)



The title compound was isolated by successive Diethyl ether wash; Yield: 86 % (382 mg), white solid, m.p. 140-142 °C; ¹H NMR (600MHz, DMSO-*d*₆) δ 7.89 (s, 2H), 7.53 (d, *J* = 7.8 Hz, 2H), 7.13 (d, *J* = 7.8 Hz, 2H), 4.25 (s, 2H), 3.63 (s, 6H); ¹³C{¹H} NMR (151 MHz, DMSO-*d*₆): δ 138.74, 136.10, 131.84, 131.09, 125.21, 121.36, 37.97, 35.89; HRMS (ESI-TOF) m/z Calcd for C₁₂H₁₄⁷⁹BrN₂S⁺ [M⁺] 297.0056 found 297.0065; m/z Calcd for C₁₂H₁₄⁸¹BrN₂S⁺ [M⁺] 299.0030 found

299.0044

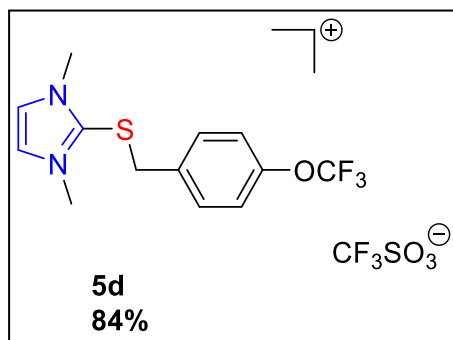
1,3-dimethyl-2-((2-fluoro-4-bromobenzyl)thio)-1H-imidazol-3-ium Triflate (4d)



The title compound was isolated by successive Diethyl ether wash; Yield: 87 % (403.68 mgs), white solid, m.p. 125-127 °C; ¹H NMR (600MHz, DMSO-*d*₆) δ 7.91 (d, *J* = 8.1 Hz, 1H), 7.76 (d, *J* = 7.9 Hz, 1H), 7.44-7.42 (m, 1H), 7.39 (d, *J* = 8.5 Hz, 2H), 7.36 (d, *J* = 6.4 Hz, 2H), 7.32-7.29 (m, 1H), 4.60 (s, 2H), 1.32 (s, 9H); ¹³C{¹H} NMR (151 MHz, DMSO-*d*₆): δ 166.85, 153.33, 150.92, 135.43, 133.09, 128.97, 126.18, 125.82, 124.37, 121.66, 121.13, 37.52, 34.70, 31.43;

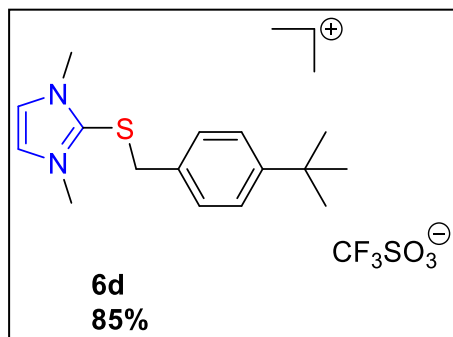
¹⁹F-NMR (600 MHz, DMSO-*d*₆) δ = -115.57; HRMS (ESI-TOF) m/z Calcd for C₁₂H₁₃⁷⁹BrFN₂S⁺ [M⁺] 314.9961 found 314.9973; m/z Calcd for C₁₂H₁₃⁸¹BrFN₂S⁺ [M⁺] 316.9940 found 316.9952.

1,3-dimethyl-2-((4-(trifluoromethoxy)benzyl)thio)-1H-imidazol-3-ium Triflate (5d)



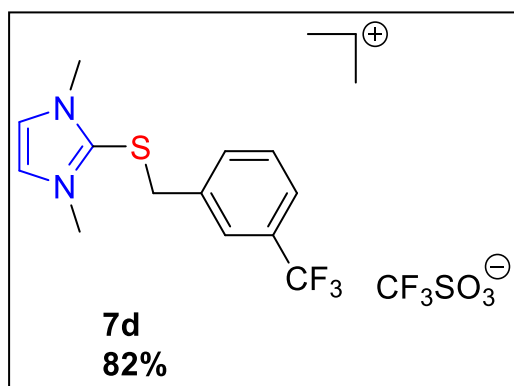
The title compound was isolated by successive Diethyl ether wash; Yield: 84 % (379.70 mgs), white solid, m.p. 85-87 °C; ¹H NMR (600MHz, DMSO-*d*₆) δ 7.88 (s, 2H), 7.32 (s, 4H), 4.30 (s, 2H), 3.62 (s, 6H); ¹³C{¹H} NMR (151 MHz, DMSO-*d*₆): δ 147.99, 138.73, 136.22, 130.92, 125.22, 121.49, 37.77, 35.83; ¹⁹F-NMR (600 MHz, DMSO-*d*₆) δ = -56.79; HRMS (ESI-TOF) m/z Calcd for C₁₃H₁₄F₃N₂OS⁺ [M⁺] 303.0773 found 303.0786.

1,3-dimethyl-2-((4-(tert-butyl)benzyl)thio)-1H-imidazol-3-ium Triflate (6d)



The title compound was isolated by successive Diethyl ether wash; Yield: 85 % (360 mgs), white solid, m.p. 130-132 °C; ¹H NMR (600MHz, DMSO-*d*₆) δ 7.87 (s, 2H), 7.31 (d, *J* = 8.1 Hz, 2H), 7.04 (d, *J* = 8.1 Hz, 2H), 4.23 (s, 2H), 3.57 (s, 6H), 1.26 (s, 9H); ¹³C{¹H} NMR (151 MHz, DMSO-*d*₆): 150.97, 138.96, 133.38, 128.58, 125.58, 125.08, 38.70, 35.71, 34.33, 31.04; HRMS (ESI-TOF) *m/z* Calcd for C₁₆H₂₃N₂S⁺ [M⁺] 275.1576 found 275.1589.

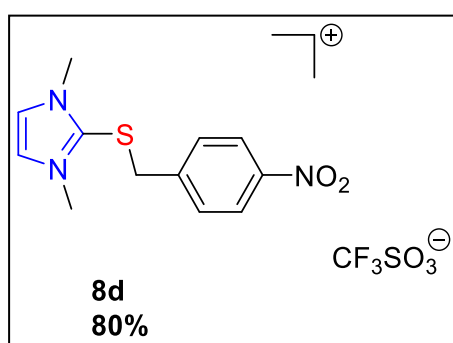
1,3-dimethyl-2-((3-(trifluoromethyl)benzyl)thio)-1H-imidazol-3-ium Triflate (7d)



The title compound was isolated by successive Diethyl ether wash; Yield: 82 % (357 mgs), white solid, m.p. 90-93 °C; ¹H NMR (600MHz, DMSO-*d*₆) δ 7.90 (s, 2H), 7.70 (d, *J* = 7.1 Hz, 1H), 7.60 – 7.55 (m, 2H), 7.48 (s, 1H), 4.36 (s, 2H), 3.60 (s, 6H); ¹³C{¹H} NMR (151 MHz, DMSO-*d*₆): δ 138.64, 138.29, 133.18, 130.15, 129.64, 129.42, 125.49, 125.24, 124.72, 37.88, 35.83; ¹⁹F-NMR (600 MHz, DMSO-*d*₆) δ = -62.61; HRMS (ESI-TOF) *m/z* Calcd for C₁₃H₁₄F₃N₂S⁺ [M⁺] 287.0824 found

287.0768.

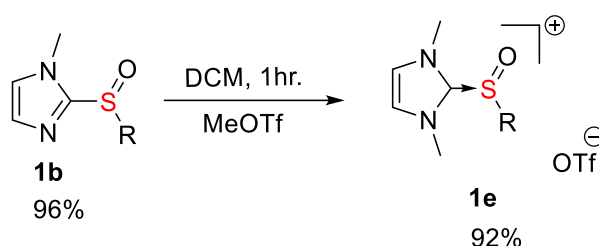
1,3-dimethyl-2-((4-nitrobenzyl)thio)-1H-imidazol-3-ium Triflate (8d)



The title compound was isolated by successive Diethyl ether wash; Yield: 80 % (330 mgs), white solid, m.p. 130-132 °C; ¹H NMR (600MHz, DMSO-*d*₆) δ 8.19 (d, *J* = 8.5 Hz, 2H), 7.88 (s, 2H), 7.47 (d, *J* = 8.5 Hz, 2H), 4.40 (s, 2H), 3.63 (s, 6H); ¹³C{¹H} NMR (151 MHz, DMSO-*d*₆): δ 147.06, 144.59, 138.41, 130.20, 125.34, 124.07, 37.64, 35.98; HRMS (ESI-TOF) *m/z* Calcd for C₁₂H₁₄N₃O₂S⁺ [M⁺] 264.0801 found 264.0812.

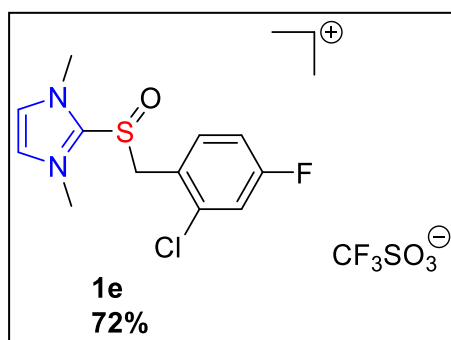
Experimental procedures for the compounds (1e-8e)

The neutral sulfoxide (**1b**) (272 mgs, 1 mmol, 1 equiv.) was dissolved in ice cooled DCM. The reaction was stirred continuously for 10 mins, and then MeOTf (137 μ l, 1.25 mmol, 1.25 equiv.) was added. The reaction was continued at room temperature for 1 hr. Progression of the reaction was monitored by TLC. The product was washed thoroughly with diethyl ether to give the desired product as white powder.



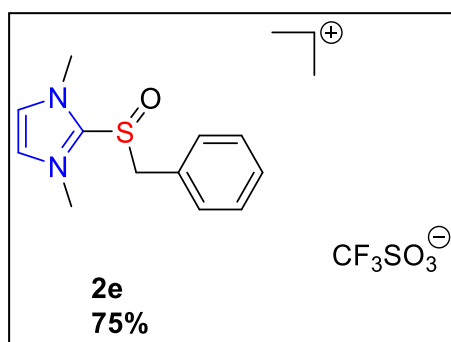
Scheme S5. Synthetic reaction scheme for the *N*-methylation of sulfoxides

1,3-dimethyl-2-((2-chloro-4-fluorobenzyl)sulfinyl)-1H-imidazol-3-ium Triflate (**1e**)



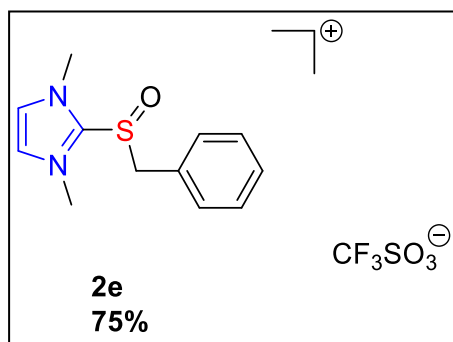
The title compound was isolated by successive Diethyl ether wash; Yield: 72 % (314 mgs), white solid, m.p. 135-137 °C; ^1H NMR (600MHz, CD_3OD) δ 7.76 (s, 2H), 7.55 (dd, $J = 8.6, 5.9$ Hz, 1H), 7.40 (dd, $J = 8.5, 2.6$ Hz, 1H), 7.23 (td, $J = 8.3, 2.7$ Hz, 1H), 5.02 (d, $J = 13.6$ Hz, 1H), 4.96 (d, $J = 13.6$ Hz, 1H), 3.74 (s, 6H); $^{13}\text{C}\{^1\text{H}\}$ NMR (151 MHz, CD_3OD): δ 164.82 (d, $^1J_{\text{C-F}} = 253.2$ Hz), 141.80, 136.82 (d, $^3J_{\text{C-F}} = 11.0$ Hz), 136.56 (d, $^3J_{\text{C-F}} = 9.0$ Hz), 127.96, 123.14, 118.87 (d, $^2J_{\text{C-F}} = 25.2$ Hz), 116.43 (d, $^2J_{\text{C-F}} = 21.2$ Hz), 56.76, 36.24; ^{19}F -NMR (600 MHz, $\text{DMSO-}d_6$) $\delta = -103.61$; HRMS (ESI-TOF) m/z Calcd for $\text{C}_{12}\text{H}_{13}\text{ClFN}_2\text{OS}^+$ [M^+] 287.0416 found 287.0458.

1,3-dimethyl-2-(benzylsulfinyl)-1H-imidazol-3-ium Triflate (**2e**)



The title compound was isolated by successive Diethyl ether wash; Yield: 75 % (288 mgs), white solid, m.p. 125-127 °C; ^1H NMR (600MHz, $\text{DMSO-}d_6$) δ 7.85 (s, 2H), 7.41 (dt, $J = 35.0, 7.6$ Hz, 3H), 7.21 (s, 2H), 4.91 (s, 2H), 3.56 (s, 6H); $^{13}\text{C}\{^1\text{H}\}$ NMR (151 MHz, $\text{DMSO-}d_6$): δ 140.21, 130.68, 129.20, 129.00, 127.88, 126.04, 58.14, 35.22; HRMS (ESI-TOF) m/z Calcd for [M^+] $\text{C}_{12}\text{H}_{15}\text{N}_2\text{OS}^+$ [M^+] 235.0900 found 235.0916.

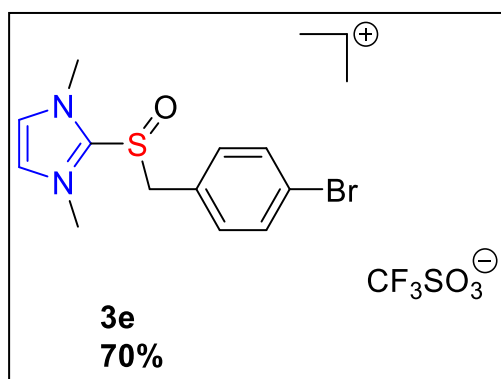
1,3-dimethyl-2-(benzylsulfinyl)-1H-imidazol-3-ium Triflate (2e)



The title compound was isolated by successive Diethyl ether wash; Yield: 75 % (288 mgs), white solid, m.p. 125-127 °C; ¹H NMR (600MHz, (CD₃)₂CO); δ 7.88 (s, 2H), 7.49 (t, *J* = 7.3 Hz, 1H), 7.43 (t, *J* = 7.5 Hz, 2H), 7.35 (d, *J* = 1.2 Hz, 2H), 5.02 (d, *J* = 13.2 Hz, 1H), 4.99 (d, *J* = 13.2 Hz, 1H), 3.80 (s, 6H); ¹³C{¹H} NMR (151 MHz, (CD₃)₂CO); δ 141.77, 131.75, 130.38, 130.13, 128.73, 127.45, 60.15, 36.24; HRMS (ESI-TOF) m/z Calcd for [M⁺] C₁₂H₁₅N₂OS⁺ [M⁺] 235.0900 found

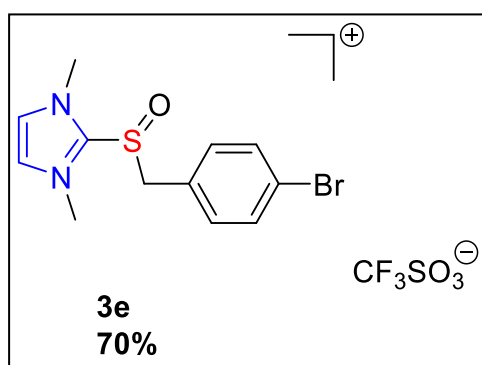
235.0916.

1,3-dimethyl-2-((4-bromobenzyl)sulfinyl)-1H-imidazol-3-ium Triflate (3e)



The title compound was isolated by successive Diethyl ether wash; Yield: 70 % (323 mgs), white solid, m.p. 140-142 °C; ¹H NMR (600MHz, DMSO-*d*₆); δ 7.87 (s, 2H), 7.61 (d, *J* = 8.0 Hz, 2H), 7.19 (d, *J* = 8.1 Hz, 2H), 4.87 (s, 2H), 3.60 (s, 6H); ¹³C{¹H} NMR (151 MHz, (DMSO-*d*₆); δ 140.04, 132.81, 131.96, 127.50, 126.14, 122.78, 57.31, 35.34; HRMS (ESI-TOF) m/z Calcd for C₁₂H₁₄⁷⁹BrN₂OS⁺ [M⁺] 313.0005 found 313.0014; m/z Calcd for C₁₂H₁₄⁸¹BrN₂OS⁺ [M⁺] 314.9982 found 314.9993.

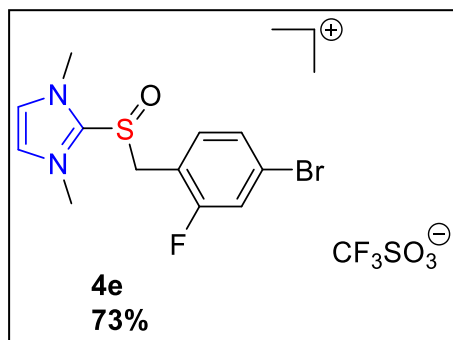
1,3-dimethyl-2-((4-bromobenzyl)sulfinyl)-1H-imidazol-3-ium Triflate (3e)



The title compound was isolated by successive Diethyl ether wash; Yield: 70 % (323 mgs), white solid, m.p. 140-142 °C; ¹H NMR (600MHz, (CD₃)₂CO); δ 7.91 (s, 2H), 7.63 (d, *J* = 8.4 Hz, 2H), 7.35 (d, *J* = 8.4 Hz, 2H), 5.02 (d, *J* = 13.2 Hz, 1H), 4.99 (d, *J* = 13.2 Hz, 1H), 3.88 (s, 6H); ¹³C{¹H} NMR (151 MHz, (CD₃)₂CO); δ 133.55, 132.95, 128.12, 127.36, 124.01, 59.04, 36.16; HRMS (ESI-TOF) m/z Calcd for C₁₂H₁₄⁷⁹BrN₂OS⁺ [M⁺] 313.0005 found 313.0014; m/z

Calcd for C₁₂H₁₄⁸¹BrN₂OS⁺ [M⁺] 314.9982 found 314.9993.

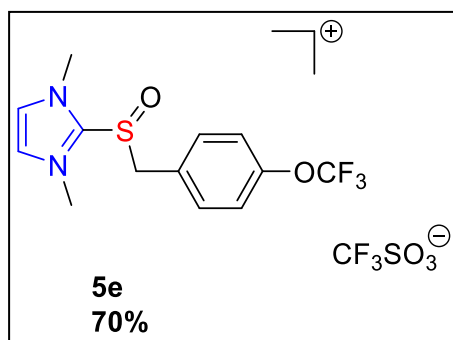
1,3-dimethyl-2-((2-fluoro-4-bromobenzyl)sulfinyl)-1H-imidazol-3-ium Triflate (4e)



The title compound was isolated by successive Diethyl ether wash; Yield: 73 % (349 mgs), white solid, m.p. 130-132 °C; ¹H NMR (600MHz, DMSO-*d*₆) δ 7.91 (s, 2H), 7.66 (d, *J* = 9.2 Hz, 1H), 7.54 (d, *J* = 7.9 Hz, 1H), 7.36 (t, *J* = 7.9 Hz, 1H), 4.99 (d, *J* = 13.4 Hz, 1H), 4.91 (d, *J* = 13.4 Hz, 1H), 3.67 (s, 6H); ¹³C{¹H} NMR (151 MHz, DMSO-*d*₆): 160.74 (d, ¹*J*_{C-F} = 252.6 Hz), 139.94, 134.58, 128.44, 126.32, 123.42 (d, ³*J*_{C-F} = 9.3 Hz), 119.32 (d, ²*J*_{C-F} = 24.8 Hz), 115.11 (d, ²*J*_{C-F} = 15.0 Hz),

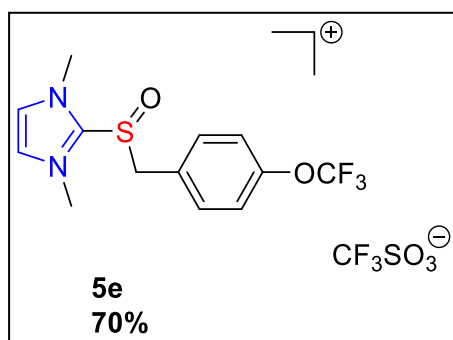
51.39, 35.37; ¹⁹F-NMR (600 MHz, DMSO-*d*₆) δ = -110.46; HRMS (ESI-TOF) m/z Calcd for C₁₂H₁₃⁷⁹BrFN₂OS⁺ [M⁺] 330.9911 found 330.9923; m/z Calcd for C₁₂H₁₃⁸¹BrFN₂OS⁺ [M⁺] 332.9892 found 332.9902.

1,3-dimethyl-2-((4-(trifluoromethoxy)benzyl)sulfinyl)-1H-imidazol-3-ium Triflate (5e)



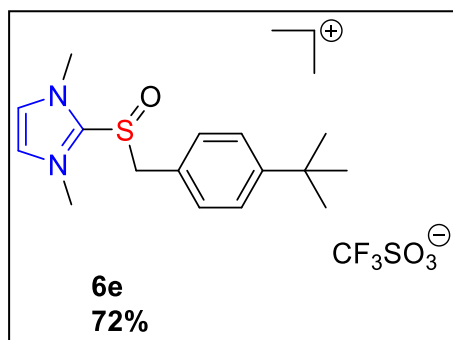
The title compound was isolated by successive Diethyl ether wash; Yield: 70 % (327 mgs), white solid, m.p. 137-139 °C; ¹H NMR (600MHz, DMSO-*d*₆) δ 7.88 (s, 2H), 7.45 – 7.36 (m, 4H), 4.93 (s, 2H), 3.61 (s, 6H); ¹³C{¹H} NMR (151 MHz, DMSO-*d*₆): δ 148.94, 140.02, 132.78, 127.68, 126.16, 121.54, 57.07, 35.28; ¹⁹F-NMR (600 MHz, DMSO-*d*₆) δ = -52.39; HRMS (ESI-TOF) m/z Calcd for C₁₃H₁₄F₃N₂O₂S⁺ [M]⁺ 319.0723; found: 319.0744.

1,3-dimethyl-2-((4-(trifluoromethoxy)benzyl)sulfinyl)-1H-imidazol-3-ium Triflate (5e)



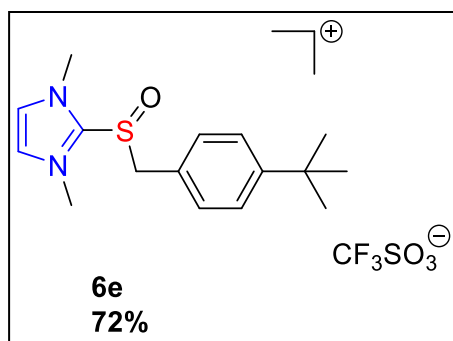
The title compound was isolated by successive Diethyl ether wash; Yield: 70 % (327 mgs), white solid, m.p. 137-139 °C; ¹H NMR (600MHz, CD₃OD) δ 7.73 (s, 2H), 7.34 (s, 4H), 4.88 (d, *J* = 13.3 Hz, 1H), 4.83 (d, *J* = 13.3 Hz, 1H), 3.68 (s, 6H); ¹³C{¹H} NMR (151 MHz, CD₃OD): δ 151.52, 142.06, 133.87, 128.32, 127.71, 122.91, 59.37, 36.23; ¹⁹F-NMR (600 MHz, DMSO-*d*₆) δ = -52.39; HRMS (ESI-TOF) m/z Calcd for C₁₃H₁₄F₃N₂O₂S⁺ [M]⁺ 319.0723; found: 319.0744.

1,3-dimethyl-2-((4-(tert-butyl)benzyl)sulfinyl)-1H-imidazol-3-ium Triflate (6e)



The title compound was isolated by successive Diethyl ether wash; Yield: 72 % (316 mgs), yellow solid, m.p. 135-137 °C; ¹H NMR (600MHz, DMSO-*d*₆) δ 7.86 (s, 2H), 7.39 (d, *J* = 8.1 Hz, 2H), 7.12 (d, *J* = 8.0 Hz, 2H), 4.87 (s, 2H), 3.53 (s, 6H), 1.27 (s, 9H); ¹³C{¹H} NMR (151 MHz, DMSO-*d*₆): 152.15, 140.31, 130.41, 126.01, 125.74, 124.79, 57.89, 35.14, 34.47, 30.99; HRMS (ESI-TOF) *m/z* Calcd for C₁₆H₂₃N₂OS⁺ [M⁺] 291.1526 found 291.1545.

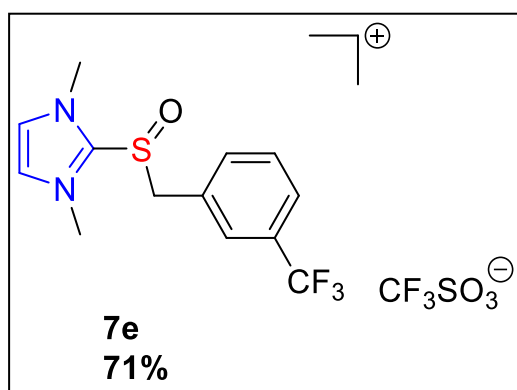
1,3-dimethyl-2-((4-(tert-butyl)benzyl)sulfinyl)-1H-imidazol-3-ium Triflate (6e)



The title compound was isolated by successive Diethyl ether wash; Yield: 72 % (316 mgs), yellow solid, m.p. 135-137 °C; ¹H NMR (600MHz, (CD₃)₂CO) δ 7.89 (s, 2H), 7.47 (d, *J* = 8.3 Hz, 2H), 7.26 (d, *J* = 8.3 Hz, 2H), 4.99 (d, *J* = 13.2 Hz, 1H), 4.96 (d, *J* = 13.2 Hz, 1H), 3.77 (s, 6H), 1.32 (s, 9H); ¹³C{¹H} NMR (151 MHz, (CD₃)₂CO): 153.80, 141.87, 131.49, 127.38, 127.00, 125.54, 59.87, 36.17, 35.31, 31.45; HRMS (ESI-TOF) *m/z* Calcd for C₁₆H₂₃N₂OS⁺ [M⁺] 291.1526 found

291.1545.

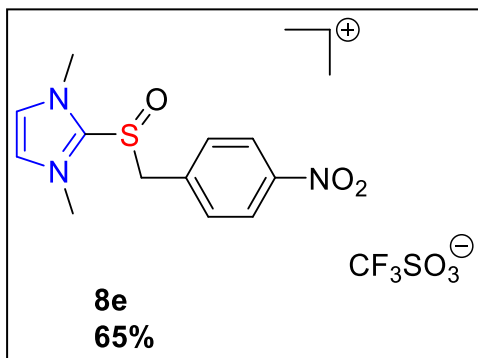
1,3-dimethyl-2-((3-(trifluoromethyl)benzyl)sulfinyl)-1H-imidazol-3-ium Triflate (7e)



The title compound was isolated by successive Diethyl ether wash; Yield: 71 % (320 mgs), white solid, m.p. 145-147 °C; ¹H NMR (600MHz, DMSO-*d*₆) δ 7.89 (s, 2H), 7.83 (d, *J* = 7.6 Hz, 1H), 7.67 (t, *J* = 7.7 Hz, 1H), 7.62 (d, *J* = 7.8 Hz, 1H), 7.59 (s, 1H), 5.00 (d, *J* = 12.9 Hz, 1H), 4.96 (d, *J* = 12.9 Hz, 1H), 3.58 (s, 6H); ¹³C{¹H} NMR (151 MHz, DMSO-*d*₆): 139.92, 135.13, 130.05, 129.75, 127.28, 126.16, 125.78, 122.92, 57.26, 35.30; ¹⁹F-NMR (600 MHz, DMSO-*d*₆) δ = -56.76; HRMS (ESI-TOF) *m/z* Calcd for C₁₃H₁₄F₃N₂OS⁺ [M⁺]

303.0773 found 303.0785.

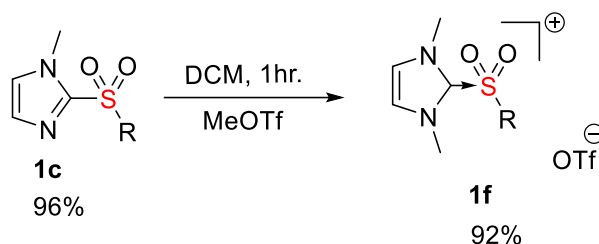
1,3-dimethyl-2-((4-nitrobenzyl)sulfinyl)-1H-imidazol-3-ium Triflate (8e)



The title compound was isolated by successive Diethyl ether wash; Yield: 65 % (278 mgs), white solid, m.p. 150-152 °C; ^1H NMR (600MHz, $\text{DMSO-}d_6$) δ 8.26 (d, $J = 8.4$ Hz, 2H), 7.88 (s, 2H), 7.55 (d, $J = 8.4$ Hz, 2H), 5.06 (d, $J = 12.8$ Hz, 1H), 5.02 (d, $J = 12.8$ Hz, 1H), 3.63 (s, 6H); $^{13}\text{C}\{^1\text{H}\}$ NMR (151 MHz, $\text{DMSO-}d_6$): δ 147.89, 139.75, 135.91, 132.06, 126.28, 123.93, 57.26, 35.48; HRMS (ESI-TOF) m/z Calcd for $[\text{M}^+]$ $\text{C}_{12}\text{H}_{14}\text{N}_3\text{O}_3\text{S}^+$ 280.0750 found 280.0768.

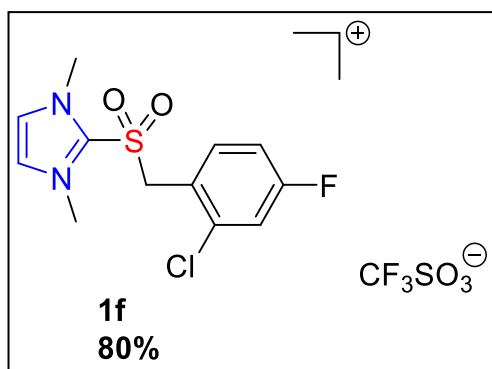
Experimental procedures for the compounds (1f-8f)

The neutral sulfone (**1c**) (288 mgs, 1 mmol, 1 equiv.) was dissolved in ice cooled DCM. The reaction was stirred continuously for 10 mins, and then MeOTf (137 μ l, 1.25 mmol, 1.25 equiv.) was added. The reaction was continued at room temperature for 1 hr. Progression of the reaction was monitored by TLC. The product was washed thoroughly with diethyl ether to give the desired product as white powder.



Scheme S6. Synthetic reaction scheme for the *N*-methylation of sulfones

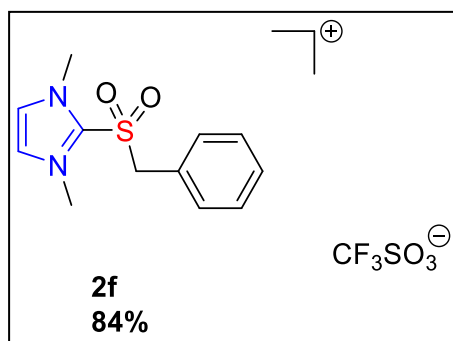
1,3-dimethyl-2-((2-chloro-4-fluorobenzyl)sulfonyl)-1H-imidazol-3-ium Triflate (1f)



The title compound was isolated by successive Diethyl ether wash; Yield: 80 % (360 mgs), white solid, m.p. 142-144 °C; ^1H NMR (600MHz, CD_3OD) δ 7.93 (s, 2H), 7.65 (dd, $J = 8.7, 5.8$ Hz, 1H), 7.39 (dd, $J = 8.5, 2.6$ Hz, 1H), 7.28 (td, $J = 8.3, 2.6$ Hz, 1H), 5.28 (s, 2H), 3.92 (s, 6H); $^{13}\text{C}\{^1\text{H}\}$ NMR (151 MHz, CD_3OD): δ 165.05 (d, $^1J_{\text{C-F}} = 254.0$ Hz), 137.63 (d, $^3J_{\text{C-F}} = 10.7$ Hz), 137.38, 137.13 (d, $^3J_{\text{C-F}} = 9.2$ Hz), 128.92, 122.88, 121.48, 120.77, 118.81 (d, $^2J_{\text{C-F}} = 25.6$ Hz), 116.84 (d, $^2J_{\text{C-F}} = 20.9$ Hz), 60.02, 38.98; ^{19}F -NMR

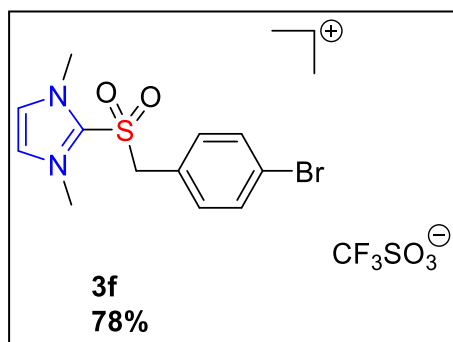
(600 MHz, $\text{DMSO-}d_6$) $\delta = -107.77$; HRMS (ESI-TOF) m/z Calcd for $\text{C}_{12}\text{H}_{13}\text{ClFN}_2\text{O}_2\text{S}^+ [\text{M}^+]$ 303.0365 found 303.0384.

1,3-dimethyl-2-(benzylsulfonyl)-1H-imidazol-3-ium Triflate (2f)



The title compound was isolated by successive Diethyl ether wash; Yield: 84 % (336 mgs), white solid, m.p. 132-134 °C; ^1H NMR (600MHz, CD_3OD) δ 7.85 (s, 2H), 7.53 – 7.49 (m, 1H), 7.45 – 7.42 (m, 2H), 7.25 (d, $J = 7.5$ Hz, 2H), 5.08 (s, 2H), 3.80 (s, 6H); $^{13}\text{C}\{^1\text{H}\}$ NMR (151 MHz, CD_3OD): δ 137.50, 132.54, 131.44, 130.61, 128.36, 126.98, 122.89, 63.71, 38.87; HRMS (ESI-TOF) m/z Calcd for $\text{C}_{12}\text{H}_{15}\text{N}_2\text{O}_2\text{S}^+ [\text{M}^+]$ 251.0849 found 251.0864.

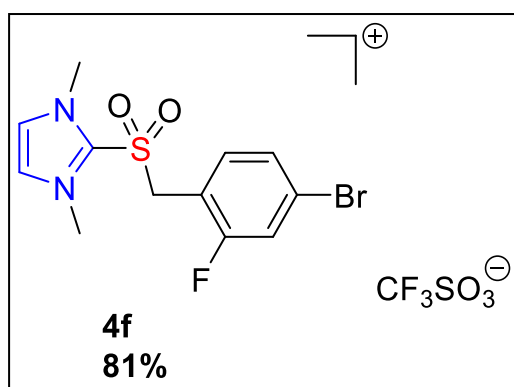
1,3-dimethyl-2-((4-bromobenzyl)sulfonyl)-1H-imidazol-3-ium Triflate (3f)



The title compound was isolated by successive Diethyl ether wash; Yield: 78 % (372 mg), white solid, m.p. 152-154 °C; ^1H NMR (600MHz, $\text{DMSO-}d_6$) δ 8.08 (s, 2H), 7.68 (d, $J = 7.9$ Hz, 2H), 7.26 (d, $J = 7.9$ Hz, 2H), 5.30 (s, 2H), 3.82 (s, 6H); $^{13}\text{C}\{^1\text{H}\}$ NMR (151 MHz, $\text{DMSO-}d_6$): δ 134.90, 133.55, 132.19, 127.30, 124.93, 123.61, 60.90, 38.04; HRMS (ESI-TOF) m/z Calcd for $\text{C}_{12}\text{H}_{14}^{79}\text{BrN}_2\text{O}_2\text{S}^+ [\text{M}^+]$ 328.9954 found 328.9971; m/z Calcd for $\text{C}_{12}\text{H}_{14}^{81}\text{BrN}_2\text{O}_2\text{S}^+ [\text{M}^+]$ 330.9936 found

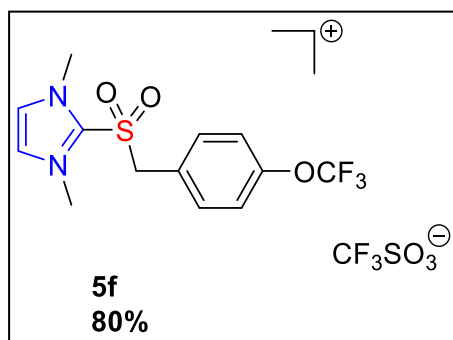
330.9950.

1,3-dimethyl-2-((2-fluoro-4-bromobenzyl)sulfonyl)-1H-imidazol-3-ium Triflate (4f)



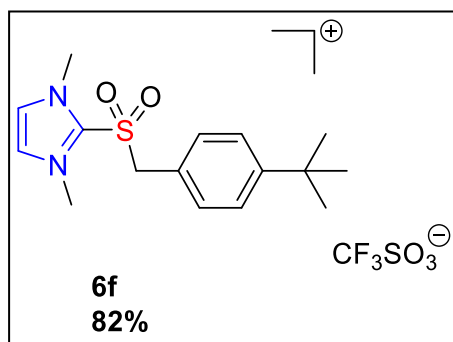
The title compound was isolated by successive Diethyl ether wash; Yield: 81 % (400 mgs), white solid, m.p. 136-198 °C; ^1H NMR (600MHz, $\text{DMSO-}d_6$) δ 8.12 (s, 2H), 7.74 (d, $J = 8.3$ Hz, 1H), 7.58 (d, $J = 6.8$ Hz, 1H), 7.37 (t, $J = 8.0$ Hz, 1H), 5.40 (s, 2H), 3.89 (s, 6H); $^{13}\text{C}\{^1\text{H}\}$ NMR (151 MHz, $\text{DMSO-}d_6$): δ 160.98 (d, $^1J_{\text{C-F}} = 254.6$ Hz), 134.96 (d, $^2J_{\text{C-F}} = 18.5$ Hz), 128.69, 127.49, 124.41, 119.57 (d, $^2J_{\text{C-F}} = 32.6$ Hz), 112.47 (d, $^3J_{\text{C-F}} = 14.9$ Hz), 55.35, 38.08; ^{19}F -NMR (600 MHz, $\text{DMSO-}d_6$) $\delta = -114.79$; HRMS (ESI-TOF) m/z Calcd for $\text{C}_{12}\text{H}_{13}^{79}\text{BrFN}_2\text{O}_2\text{S}^+ [\text{M}^+]$ 346.9860 found 346.9881; m/z Calcd for $\text{C}_{12}\text{H}_{13}^{81}\text{BrFN}_2\text{O}_2\text{S}^+ [\text{M}^+]$ 348.9850 found 348.9861.

1,3-dimethyl-2-((4-(trifluoromethoxy)benzyl)sulfonyl)-1H-imidazol-3-ium Triflate (5f)



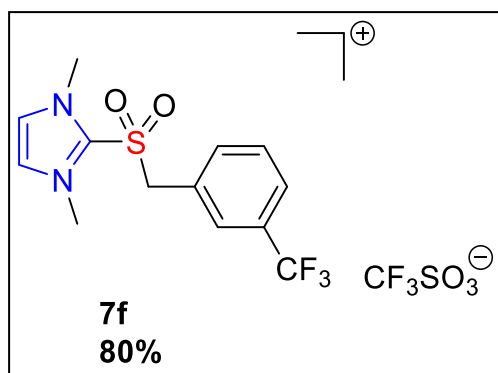
The title compound was isolated by successive Diethyl ether wash; Yield: 80 % (387 mgs), white solid, m.p. 178-180 °C; ^1H NMR (600MHz, $\text{DMSO-}d_6$) δ 8.12 – 8.04 (m, 2H), 7.50 – 7.44 (m, 4H), 5.36 (s, 2H), 3.82 (s, 6H); $^{13}\text{C}\{^1\text{H}\}$ NMR (151 MHz, $\text{DMSO-}d_6$): 149.37, 134.90, 133.65, 127.34, 125.00, 121.67, 60.69, 38.00; ^{19}F -NMR (600 MHz, $\text{DMSO-}d_6$) $\delta = -52.19$; HRMS (ESI-TOF) m/z Calcd for $\text{C}_{13}\text{H}_{14}\text{F}_3\text{N}_2\text{O}_3\text{S}^+ [\text{M}^+]$ 335.0672 found 335.0689.

1,3-dimethyl-2-((4-(tert-butyl)benzyl)sulfonyl)-1H-imidazol-3-ium Triflate (6f)



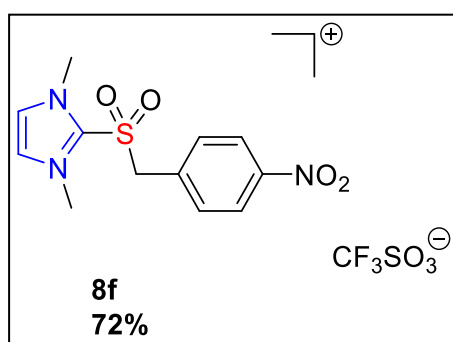
The title compound was isolated by successive Diethyl ether wash; Yield: 82 % (374 mgs), white solid, m.p. 172-174 °C; ^1H NMR (600MHz, DMSO- d_6) δ 8.05 (s, 2H), 7.44 (d, J = 8.0 Hz, 2H), 7.16 (d, J = 8.0 Hz, 2H), 5.26 (s, 2H), 3.73 (s, 6H); $^{13}\text{C}\{^1\text{H}\}$ NMR (151 MHz, DMSO- d_6): δ 152.78, 135.02, 131.14, 127.09, 125.86, 122.49, 61.41, 37.78, 34.51, 30.93; HRMS (ESI-TOF) m/z Calcd for $\text{C}_{16}\text{H}_{23}\text{N}_2\text{O}_2\text{S}^+$ [M^+] 307.1475 found 307.1496.

1,3-dimethyl-2-((3-(trifluoromethyl)benzyl)sulfonyl)-1H-imidazol-3-ium Triflate (7f)



The title compound was isolated by successive Diethyl ether wash; Yield: 80 % (375 mgs), white solid, m.p. 152-154 °C; ^1H NMR (600MHz, DMSO- d_6) δ 8.10 (s, 2H), 7.90 (d, J = 7.0 Hz, 1H), 7.74 – 7.70 (m, 2H), 7.67 (s, 1H), 5.41 (s, 2H), 3.82 (s, 6H); $^{13}\text{C}\{^1\text{H}\}$ NMR (151 MHz, DMSO- d_6): δ 135.86, 134.81, 130.38, 129.84, 129.62, 127.99, 127.34, 127.06, 126.53, 60.88, 38.05; ^{19}F -NMR (600 MHz, DMSO- d_6) δ = -56.76; HRMS (ESI-TOF) m/z Calcd for $\text{C}_{13}\text{H}_{14}\text{F}_3\text{N}_2\text{O}_2\text{S}^+$ [M^+] 319.0723 found 319.0507.

1,3-dimethyl-2-((4-nitrobenzyl)sulfonyl)-1H-imidazol-3-ium Triflate (8f)



The title compound was isolated by successive Diethyl ether wash; Yield: 72 % (320 mgs), white solid, m.p. 184-186 °C; ^1H NMR (600MHz, DMSO- d_6) δ 8.32 (d, J = 8.4 Hz, 2H), 8.09 (s, 2H), 7.63 (d, J = 8.3 Hz, 2H), 5.50 (s, 2H), 3.86 (s, 6H); $^{13}\text{C}\{^1\text{H}\}$ NMR (151 MHz, DMSO- d_6): δ 148.34, 134.82, 132.93, 132.72, 127.46, 124.15, 60.83, 38.20; HRMS (ESI-TOF) m/z Calcd for $\text{C}_{12}\text{H}_{14}\text{N}_3\text{O}_4\text{S}^+$ [M^+] 296.0700 found 296.0718.

3. Spectra

2-((2-chloro-4-fluorobenzyl)thio)-1-methyl-1H-imidazole (**1a**)

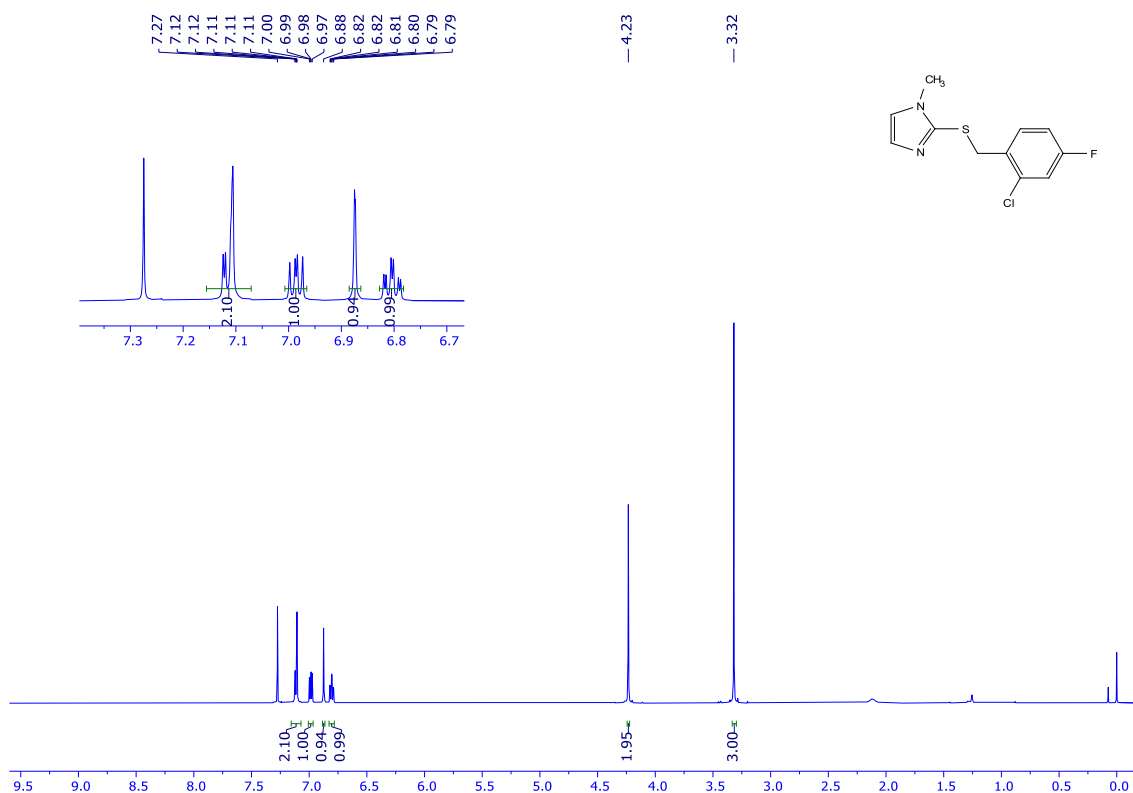


Fig. S1. ^1H NMR spectrum of compound **1a** (CDCl_3 , 600 MHz)

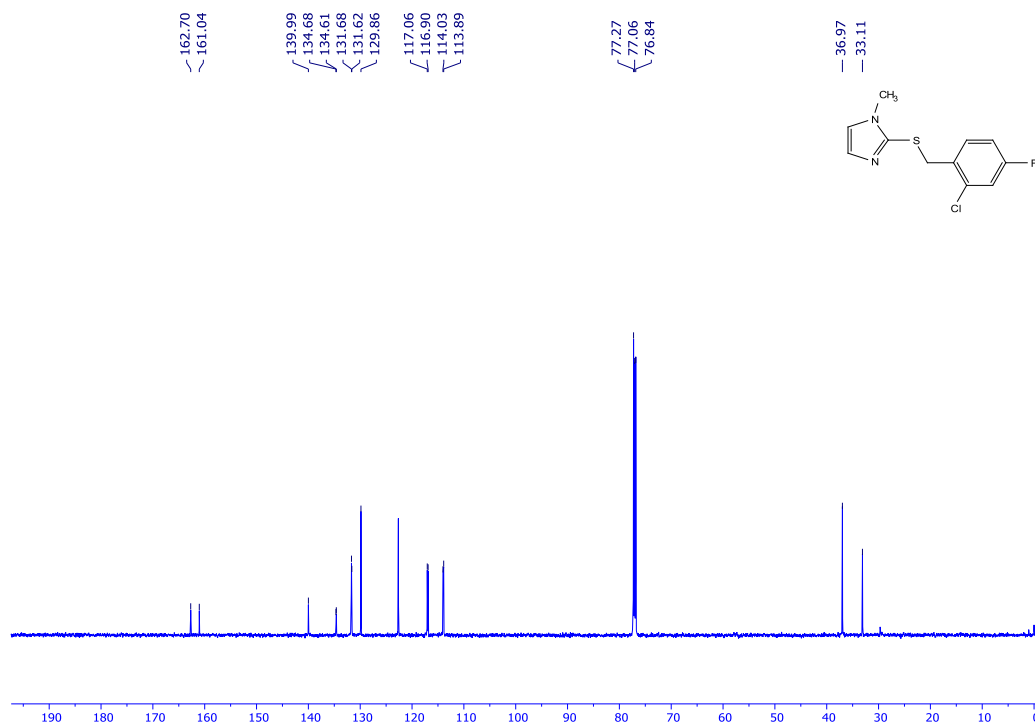


Fig. S2. ^{13}C NMR spectrum of compound **1a** (CDCl_3 , 600 MHz)

2-(benzylthio)-1-methyl-1H-imidazole (2a)

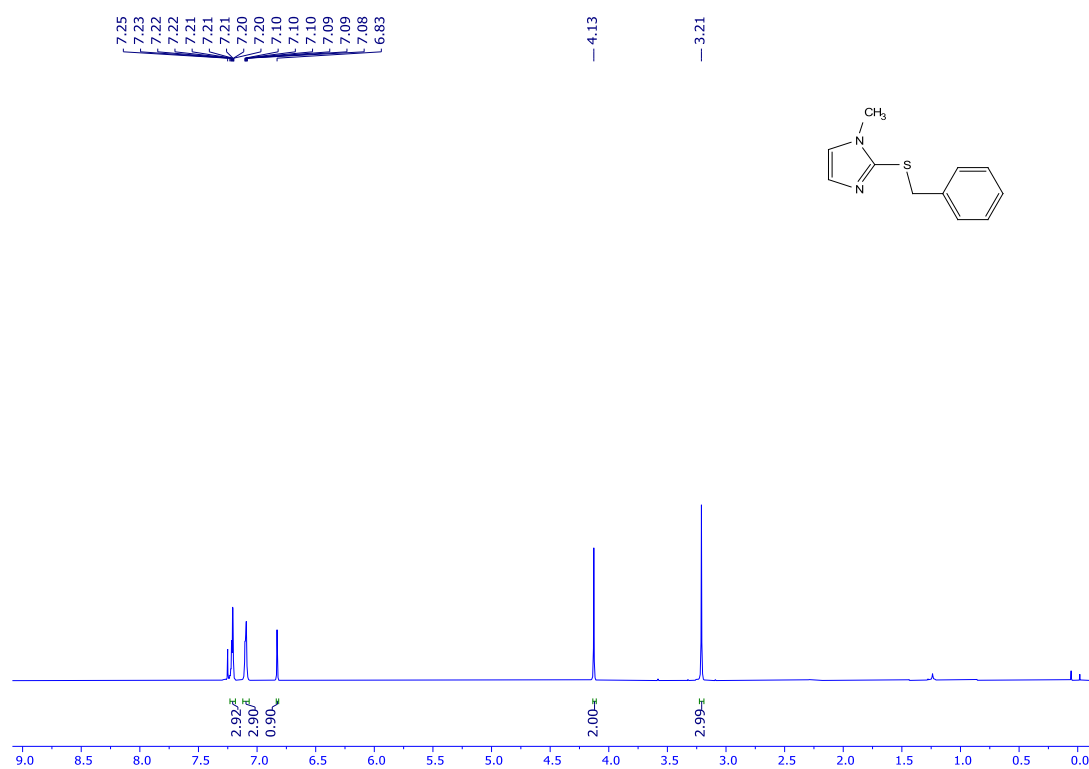


Fig. S3. ^1H NMR spectrum of compound **2a** (CDCl_3 , 600 MHz)

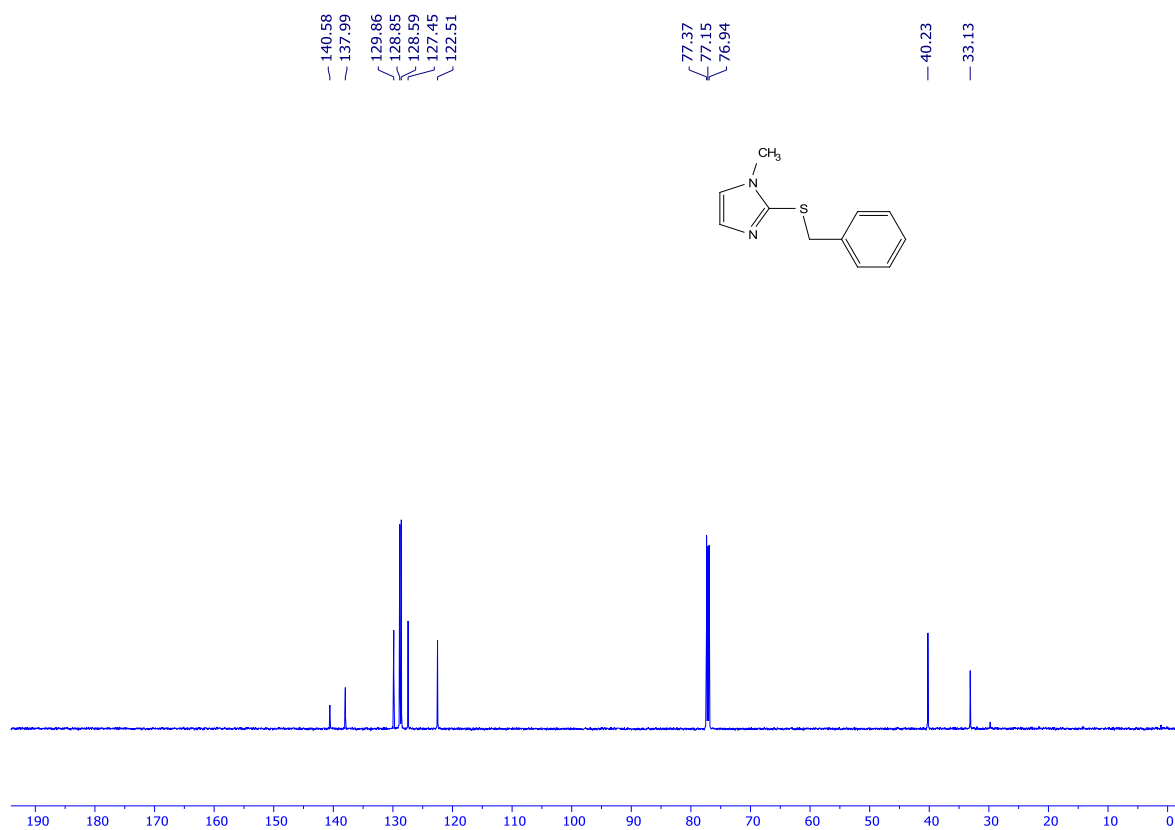


Fig. S4. ^{13}C NMR spectrum of compound **2a** (CDCl_3 , 600 MHz)

2-((4-bromobenzyl)thio)-1-methyl-1H-imidazole (3a)

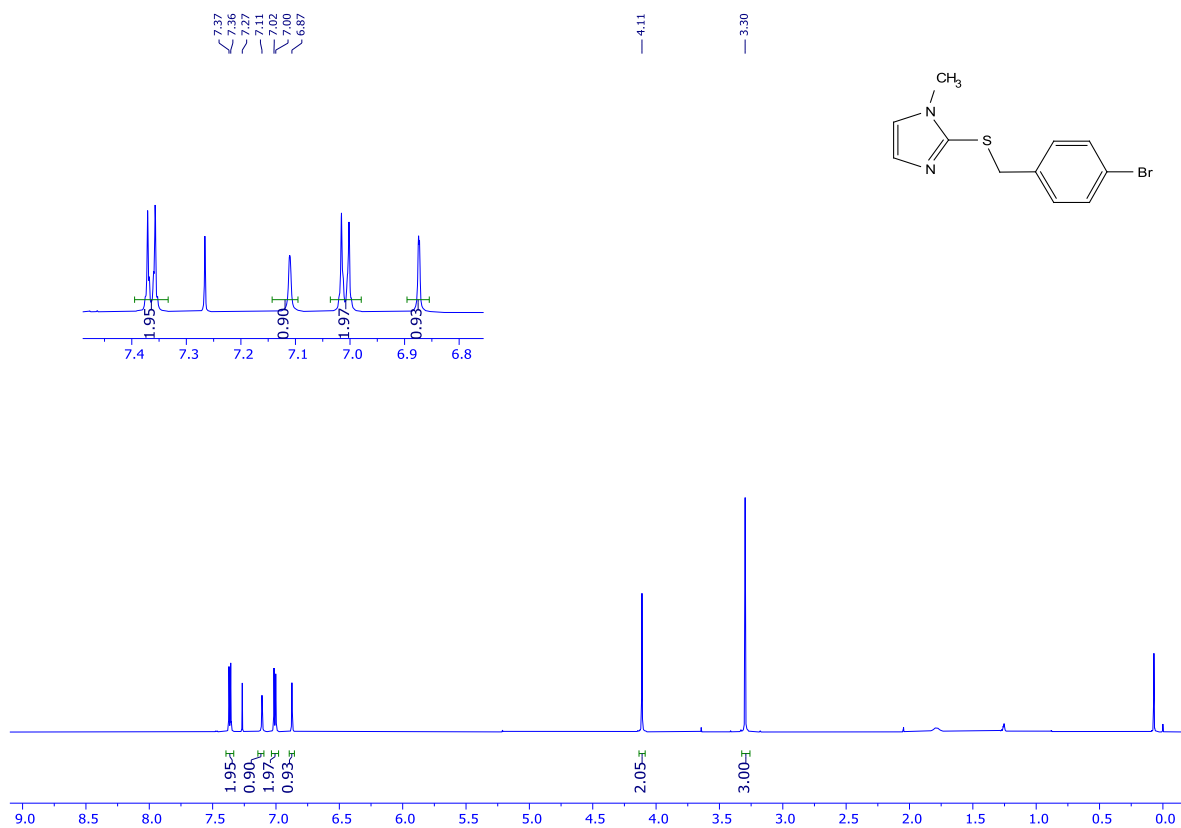


Fig. S5. ¹H NMR spectrum of compound **3a** (CDCl₃, 600 MHz)

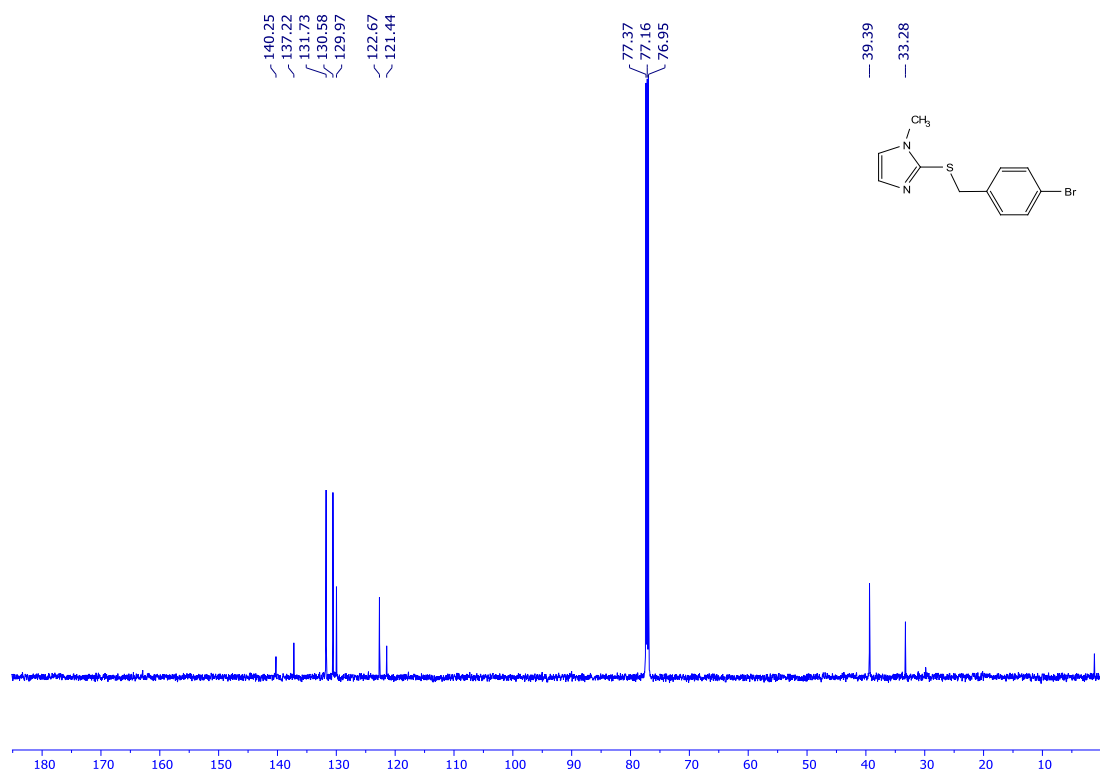


Fig. S6. ¹³C NMR spectrum of compound **3a** (CDCl₃, 600 MHz)

2-((4-bromo-2-fluorobenzyl)thio)-1-methyl-1H-imidazole (4a)

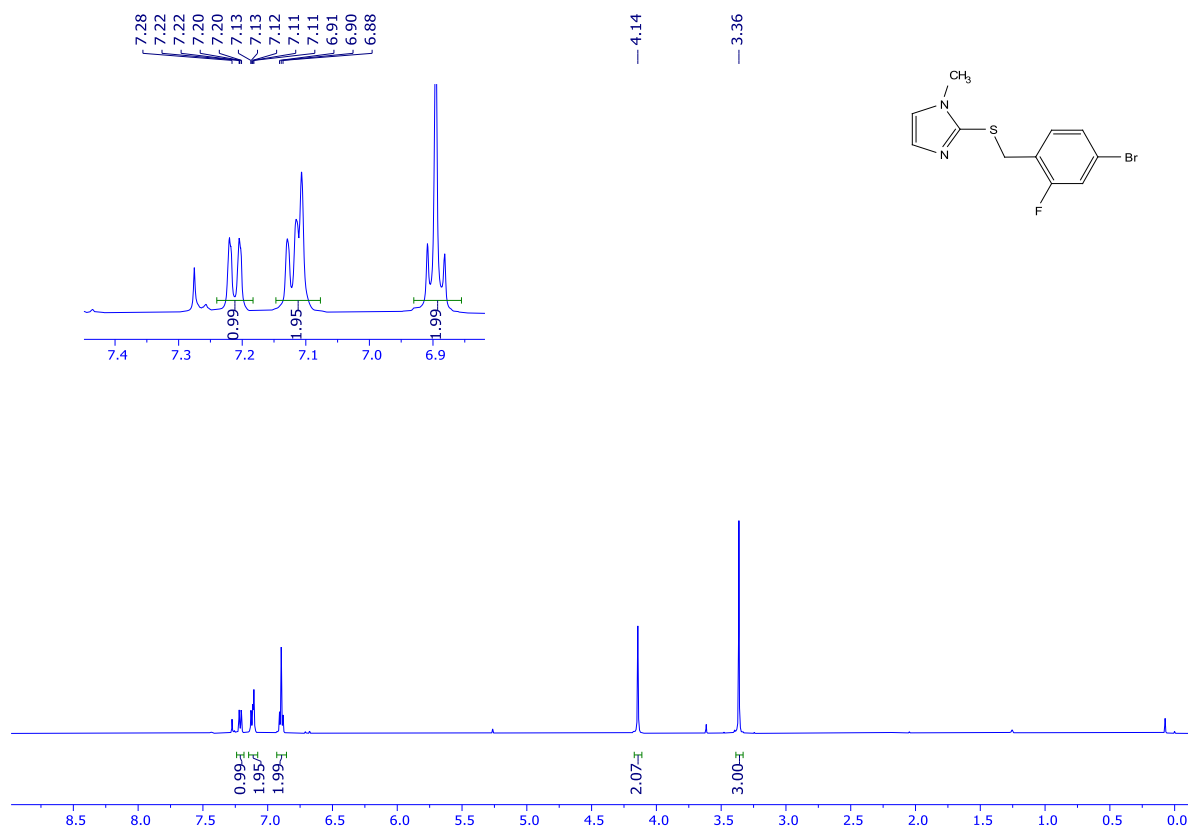


Fig. S7. ¹H NMR spectrum of compound **4a** (CDCl₃, 600 MHz)

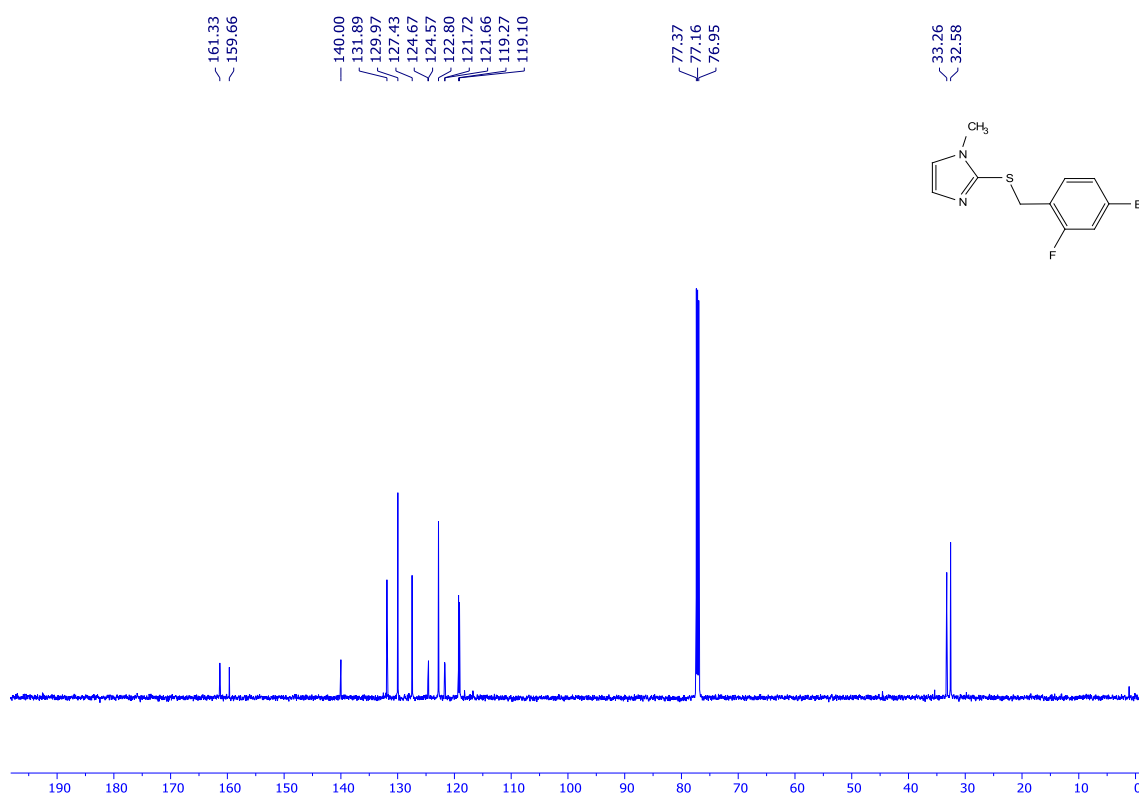


Fig. S8. ¹³C NMR spectrum of compound **4a** (CDCl₃, 600 MHz)

1-methyl-2-((4-(trifluoromethoxy)benzyl)thio)-1H-imidazole (5a)

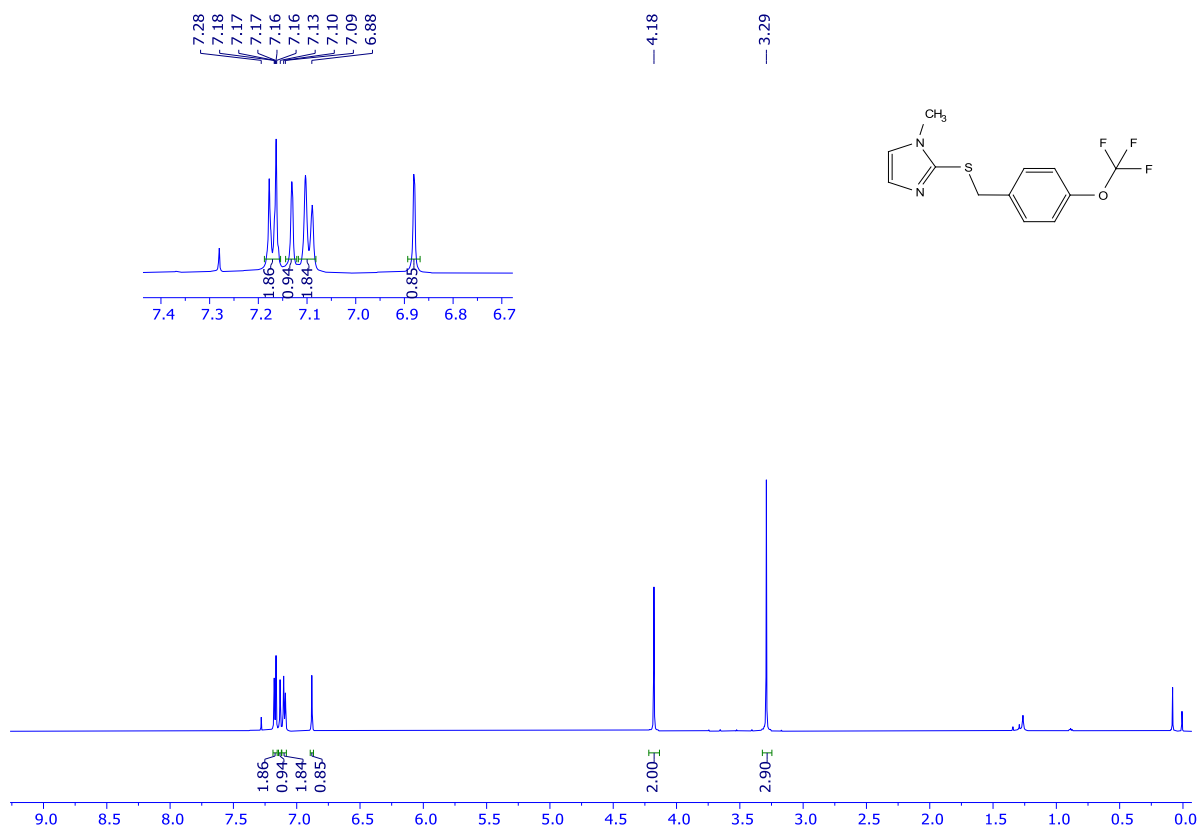


Fig. S9. ¹H NMR spectrum of compound 5a (CDCl₃, 600 MHz)

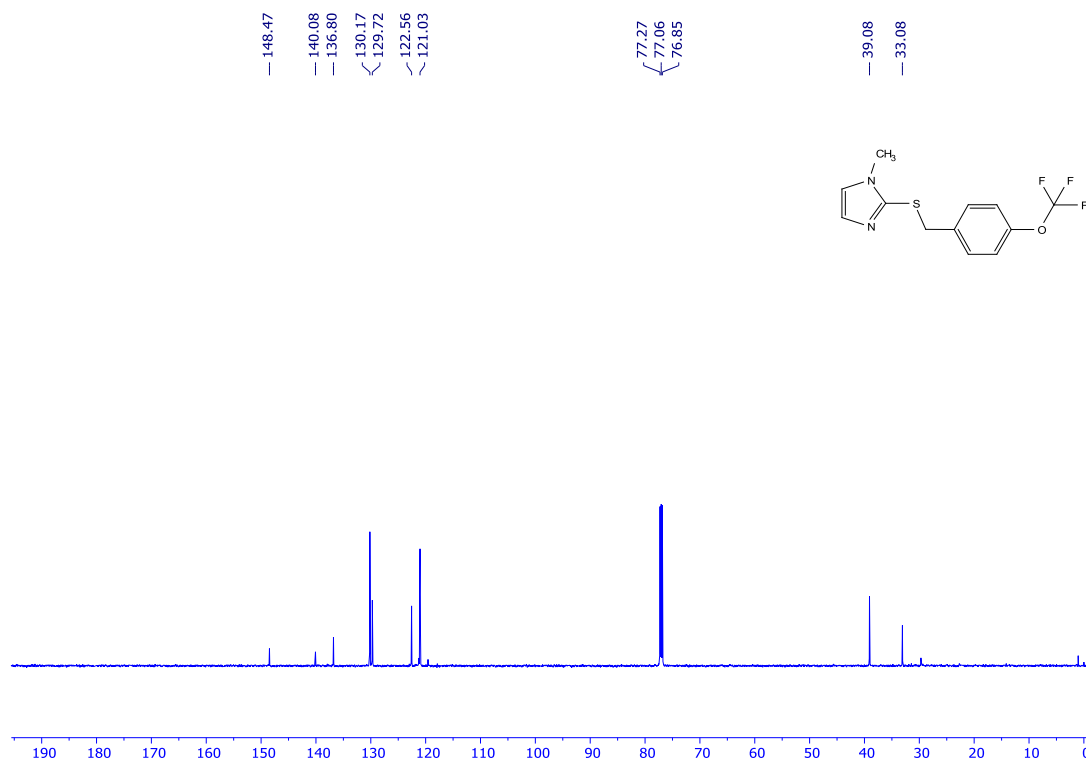


Fig. S10. ¹³C NMR spectrum of compound 5a (CDCl₃, 600 MHz)

2-((4-(tert-butyl)benzyl)thio)-1-methyl-1H-imidazole (6a)

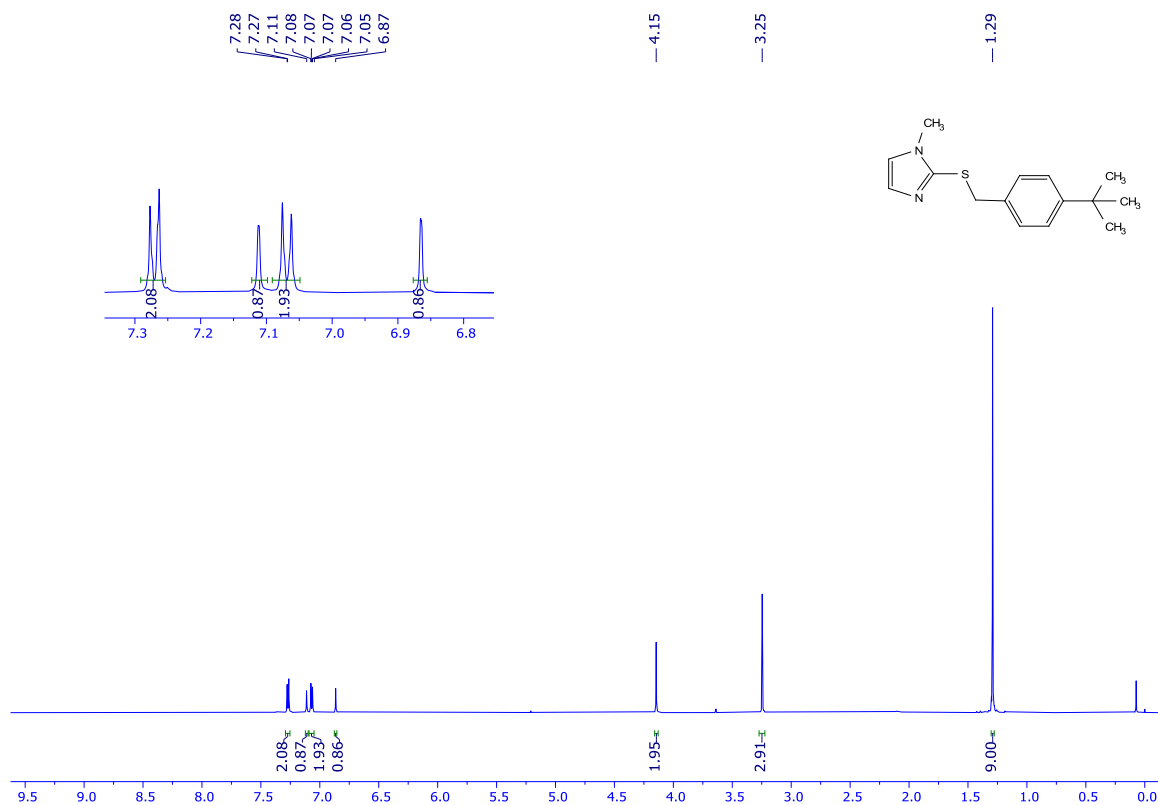


Fig. S11. ¹H NMR spectrum of compound **6a** (CDCl₃, 600 MHz)

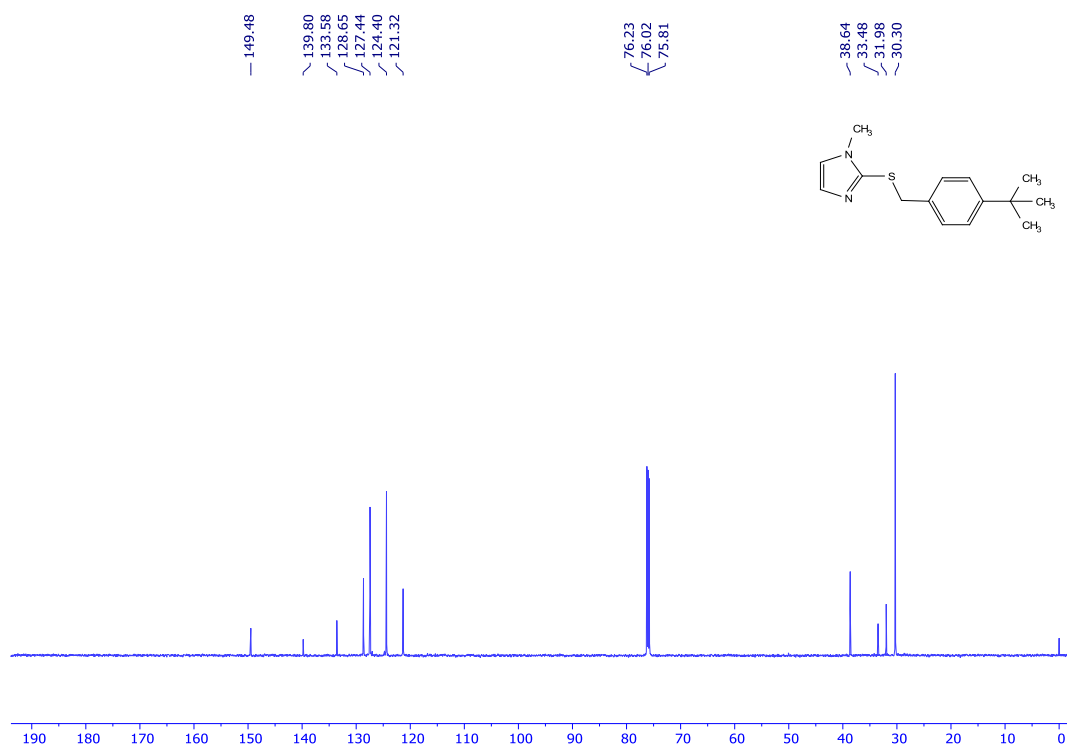


Fig. S12. ¹³C NMR spectrum of compound **6a** (CDCl₃, 600 MHz)

1-methyl-2-((4-nitrobenzyl)thio)-1H-imidazole (**8a**)

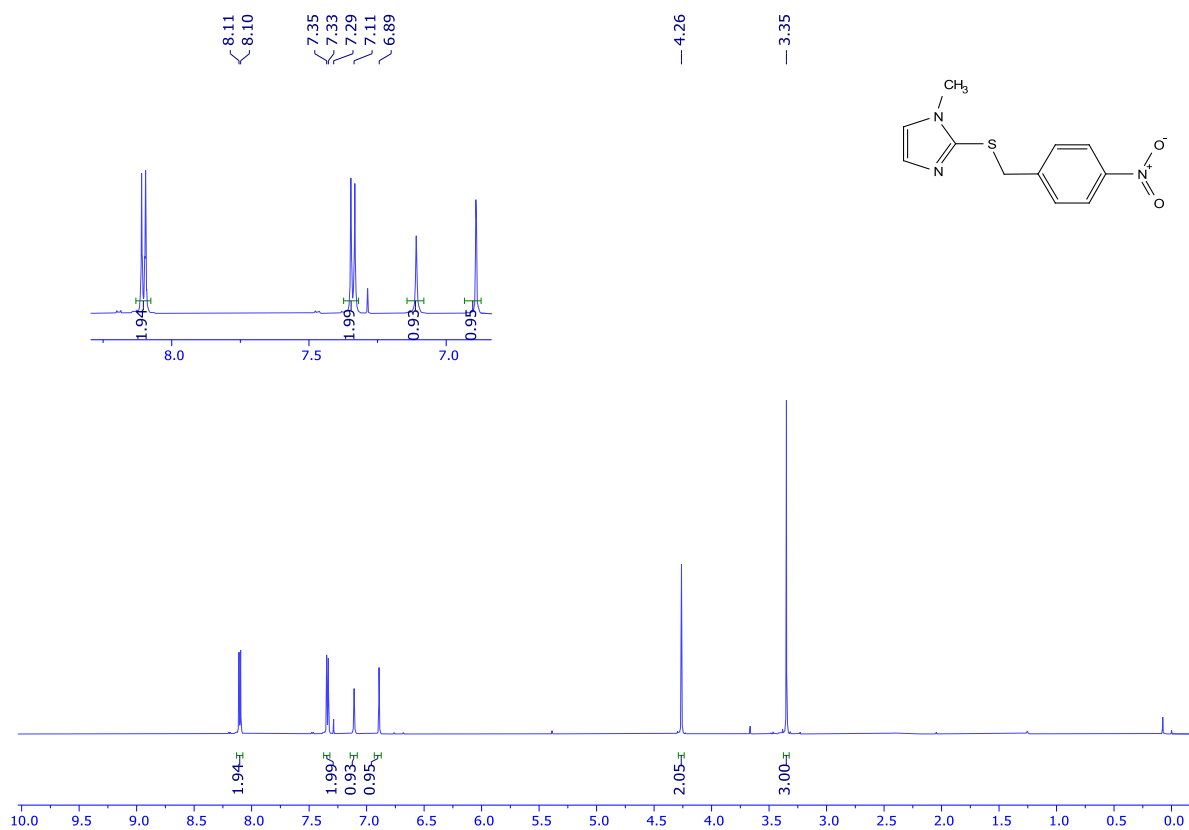


Fig. S13. ¹H NMR spectrum of compound **8a** (CDCl₃, 600 MHz)

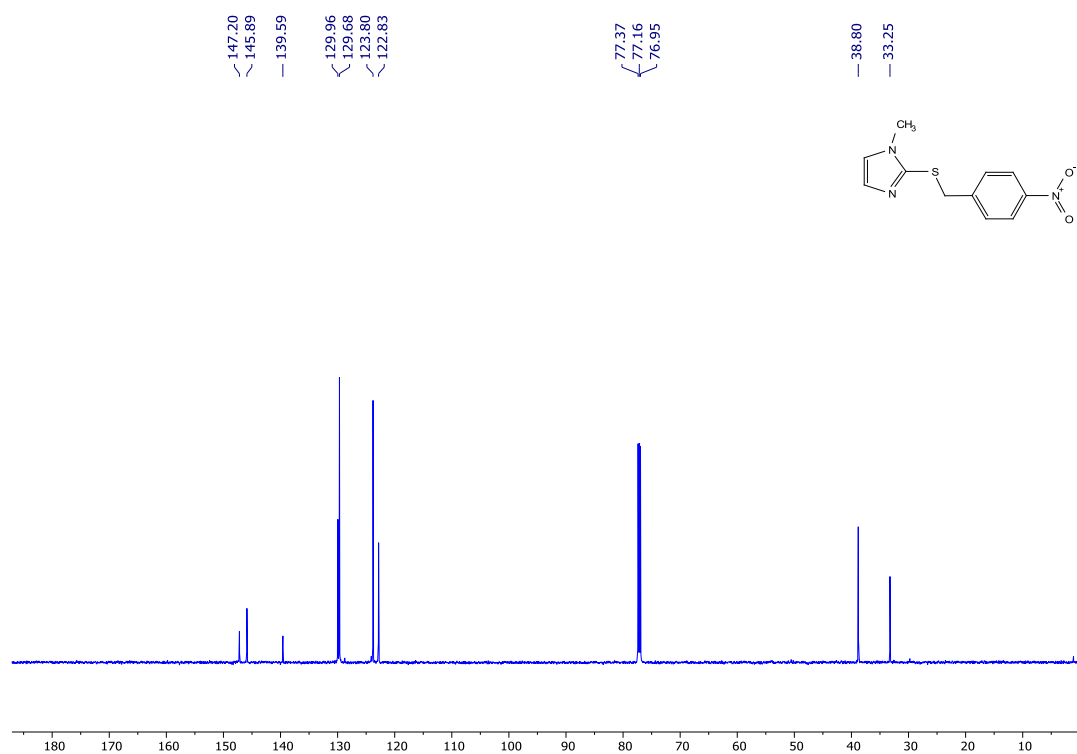


Fig. S14. ¹³C NMR spectrum of compound **8a** (CDCl₃, 600 MHz)

2-((2-chloro-4-fluorobenzyl)sulfinyl)-1-methyl-1H-imidazole (**1b**)

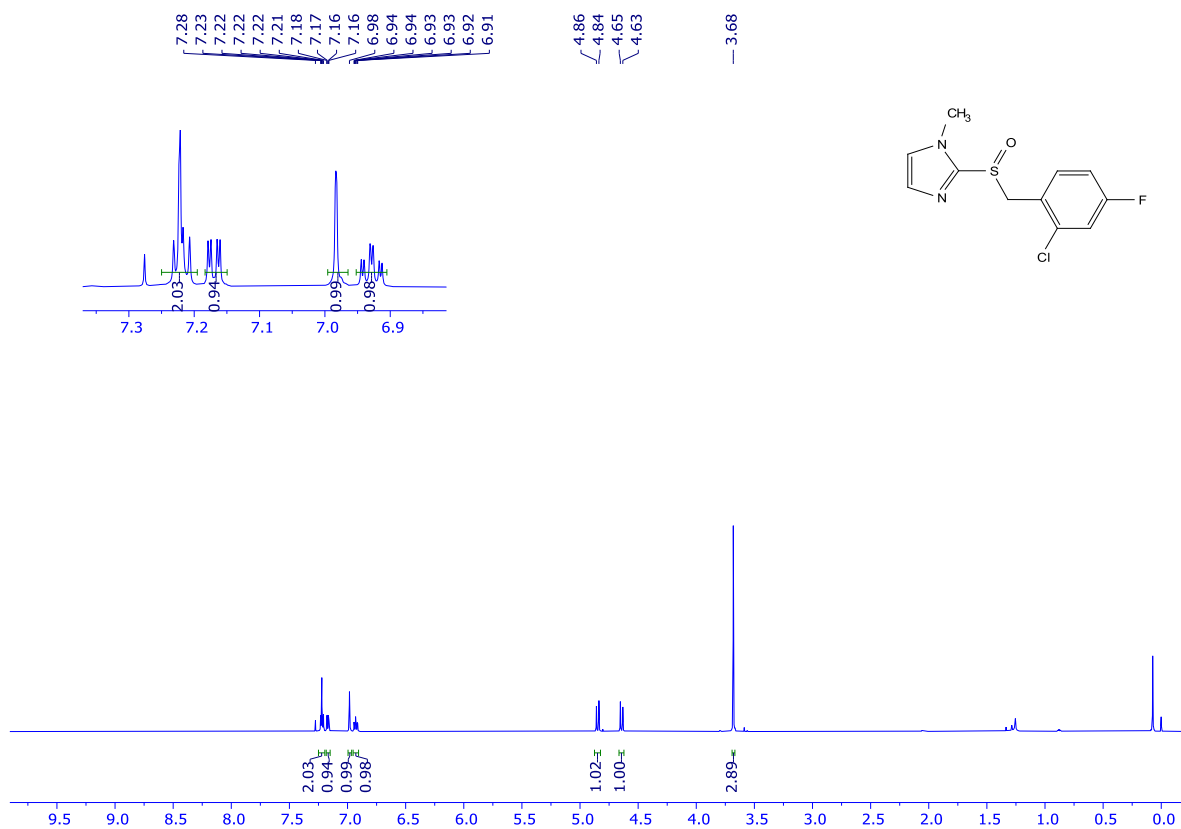


Fig. S15. ¹H NMR spectrum of compound **1b** (CDCl₃, 600 MHz)

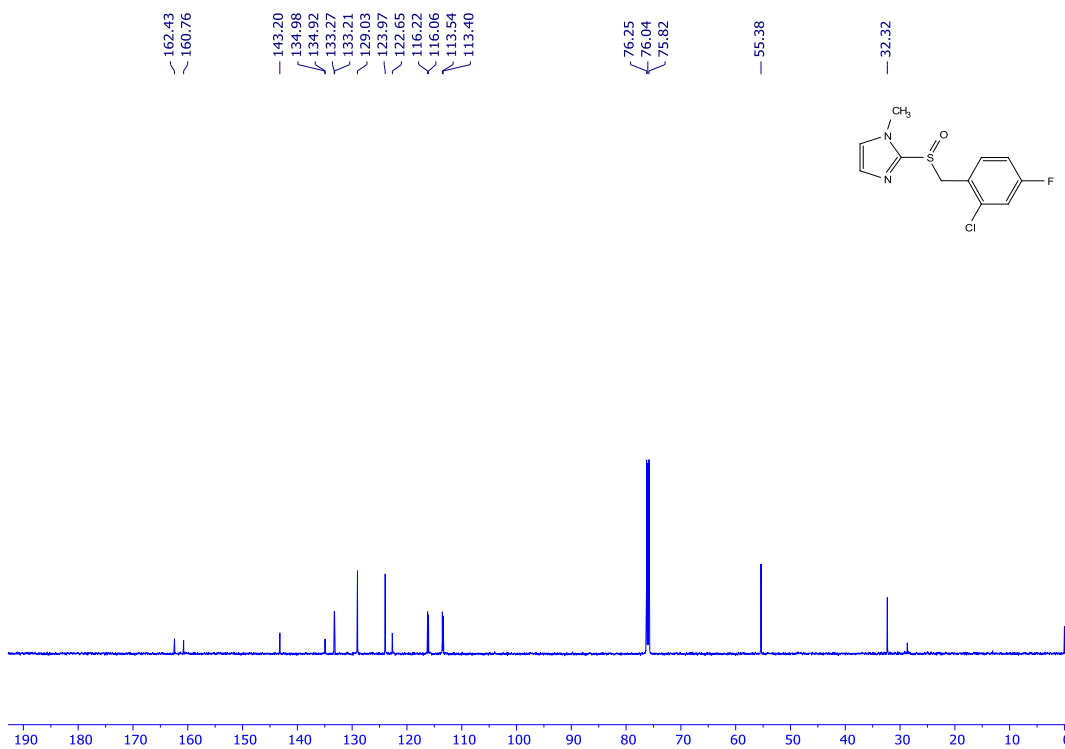


Fig. S16. ¹³C NMR spectrum of compound **1b** (CDCl₃, 600 MHz)

2-(benzylsulfinyl)-1-methyl-1H-imidazole (2b)

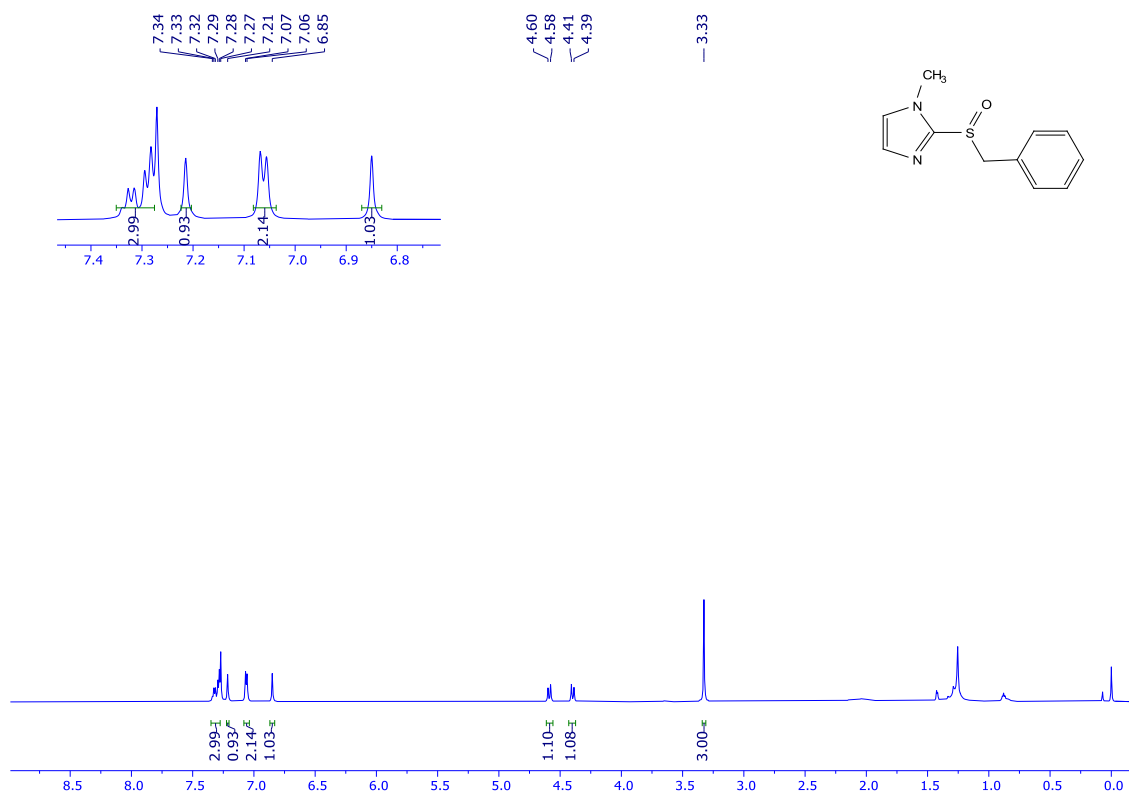


Fig. S17. ¹H NMR spectrum of compound **2b** (CDCl₃, 600 MHz)

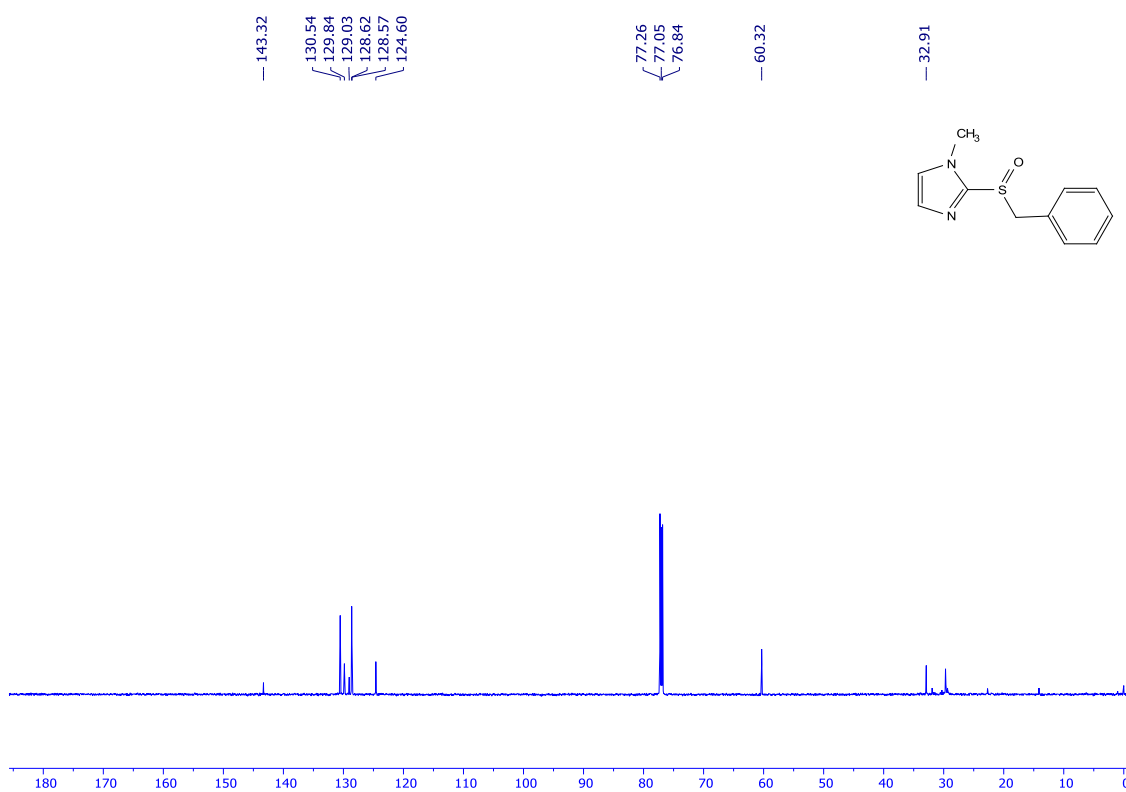


Fig. S18. ¹³C NMR spectrum of compound **2b** (CDCl₃, 600 MHz)

2-((4-bromobenzyl)sulfinyl)-1-methyl-1H-imidazole (3b)

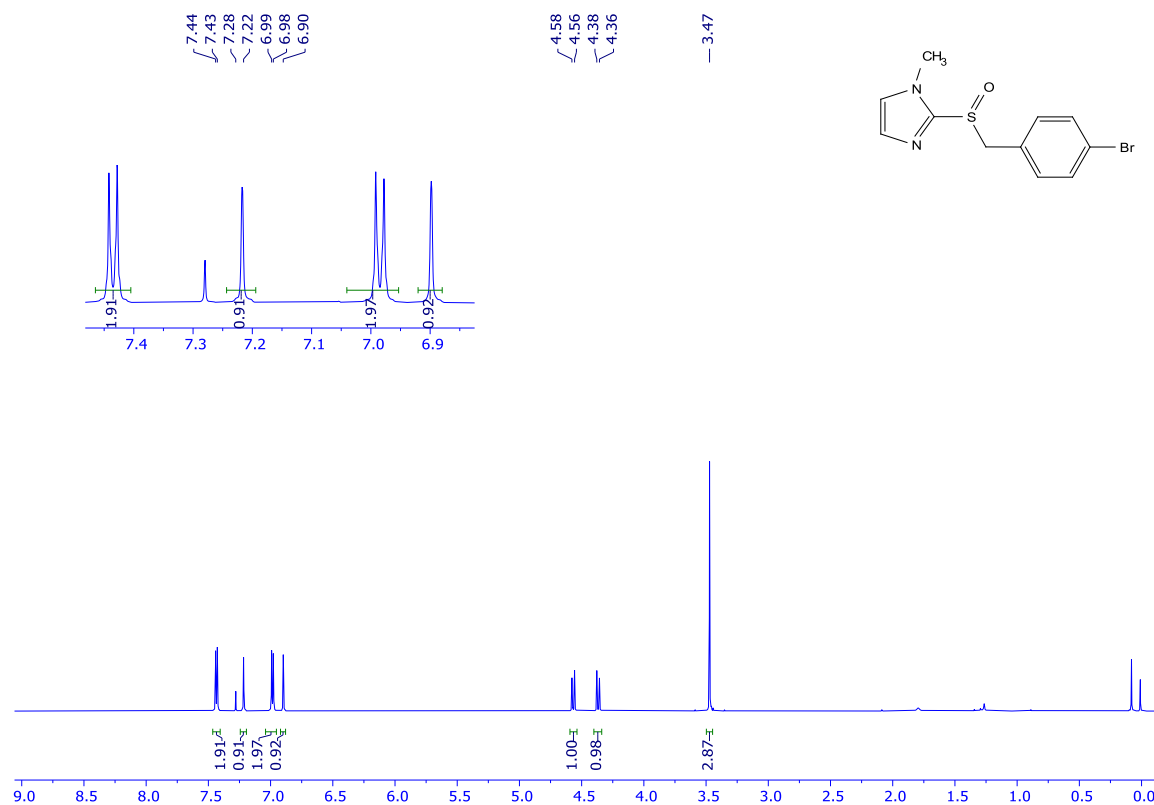


Fig. S19. ¹H NMR spectrum of compound **3b** (CDCl₃, 600 MHz)

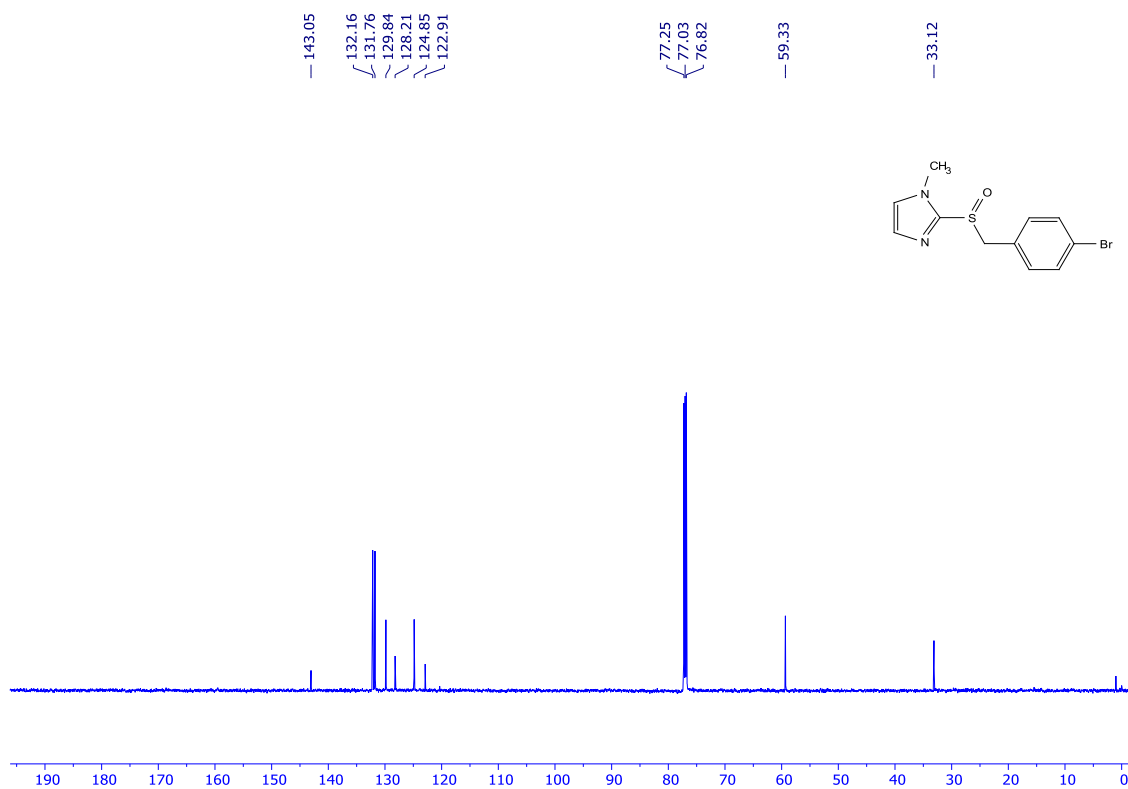


Fig. S20. ¹³C NMR spectrum of compound **3b** (CDCl₃, 600 MHz)

2-((4-bromo-2-fluorobenzyl)sulfinyl)-1-methyl-1H-imidazole (4b)

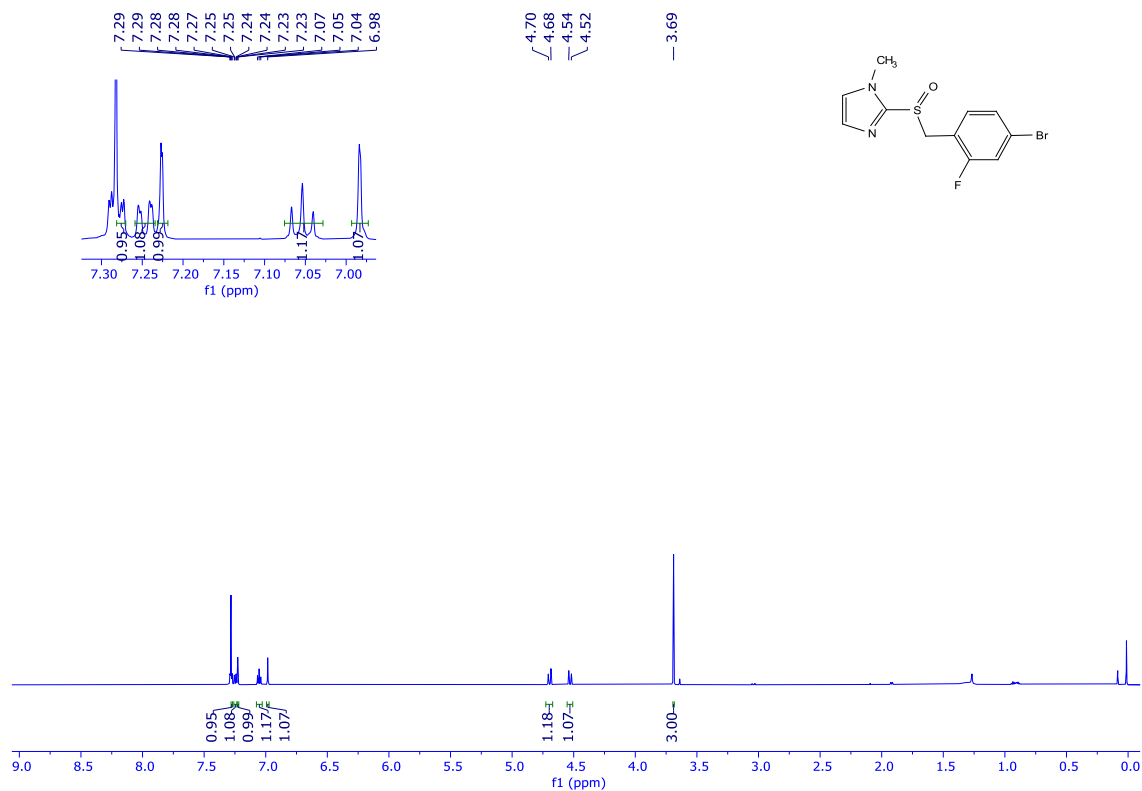


Fig. S21. ¹H NMR spectrum of compound **4b** (CDCl₃, 600 MHz)

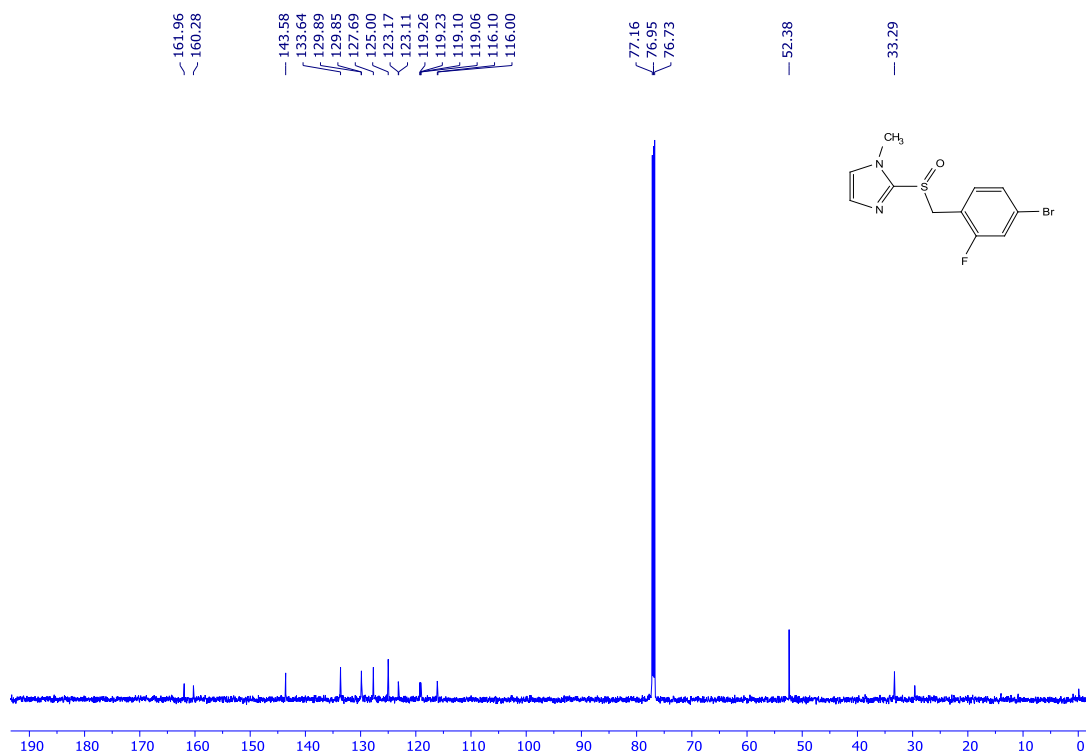


Fig. S22. ¹³C NMR spectrum of compound **4b** (CDCl₃, 600 MHz)

1-methyl-2-((4-(trifluoromethoxy)benzyl)sulfinyl)-1H-imidazole (5b)

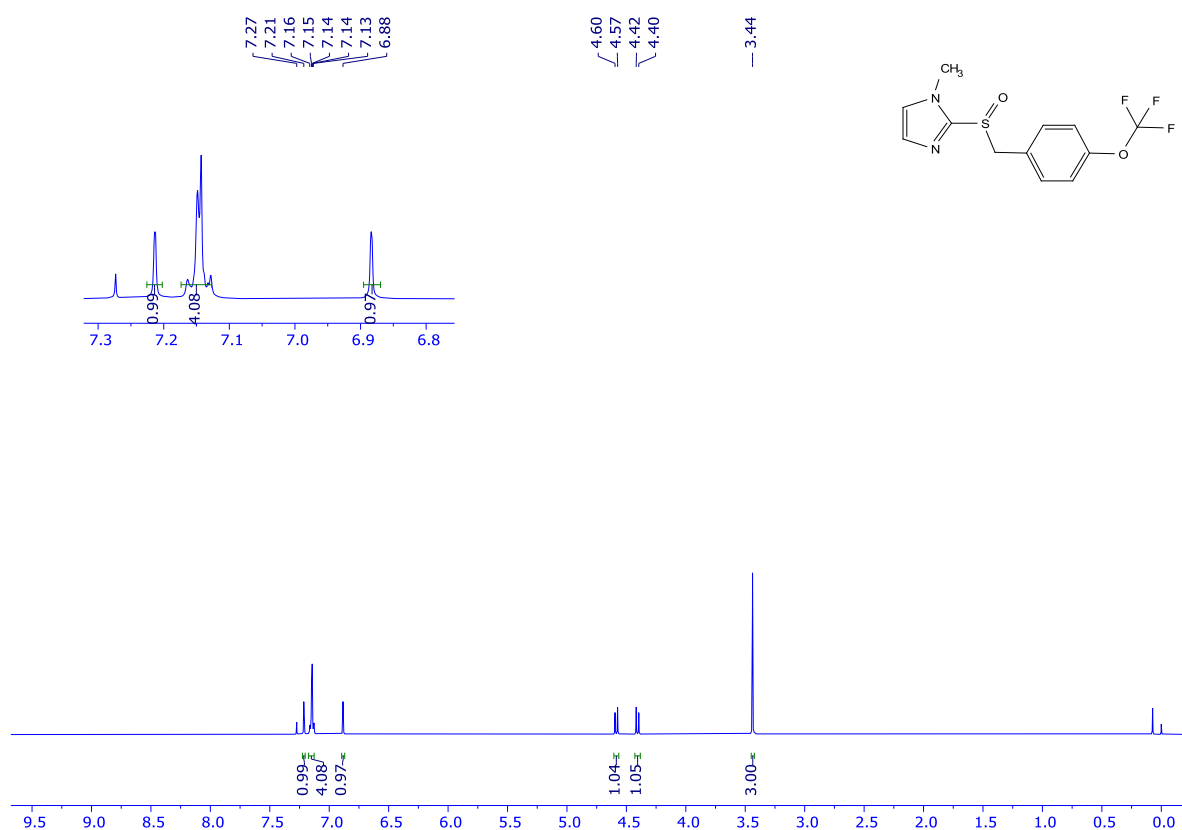


Fig. S23. ¹H NMR spectrum of compound **5b** (CDCl₃, 600 MHz)

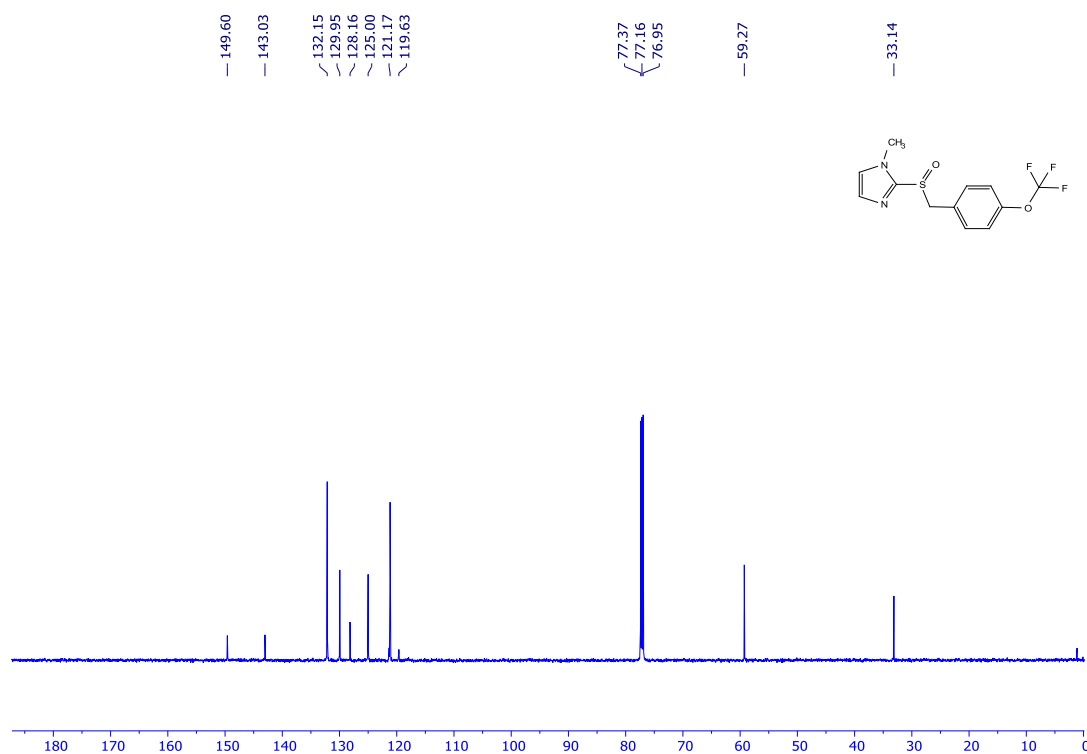


Fig. S24. ¹³C NMR spectrum of compound **5b** (CDCl₃, 600 MHz)

2-((4-(tert-butyl)benzyl)sulfinyl)-1-methyl-1H-imidazole (**6b**)

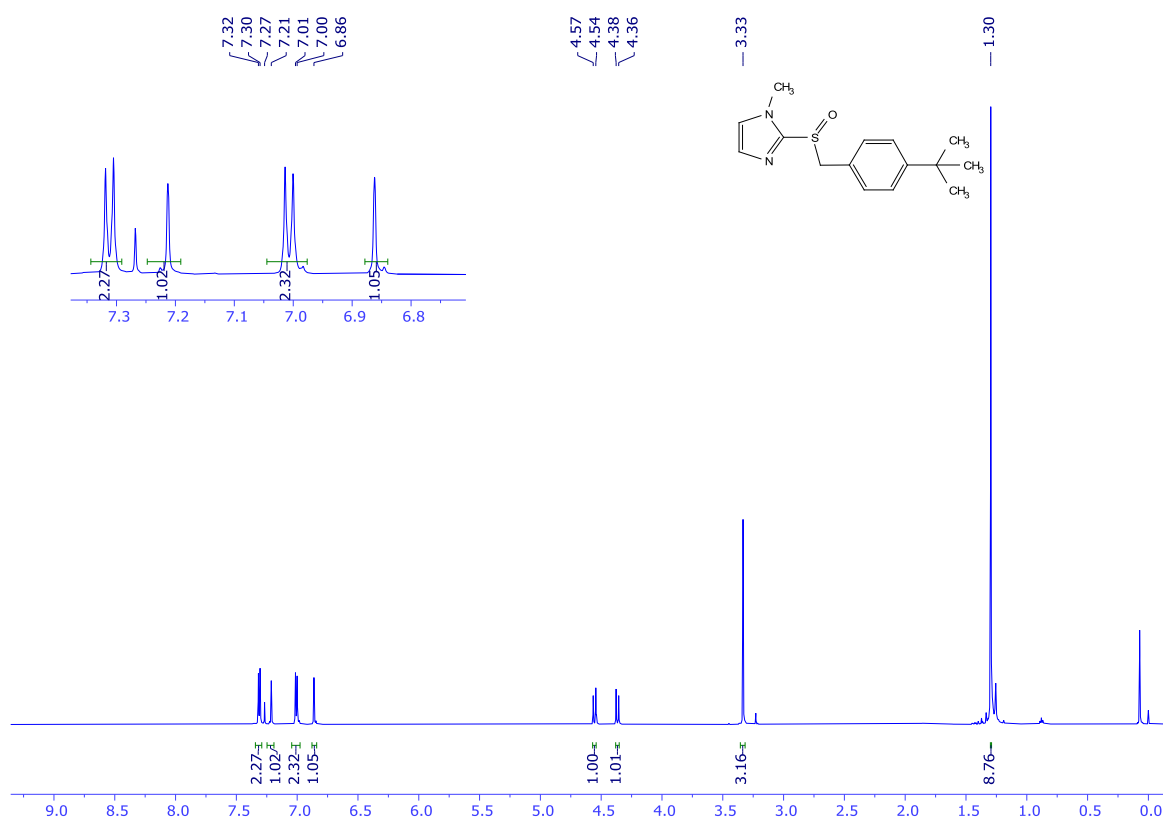


Fig. S25. ¹H NMR spectrum of compound **6b** (CDCl₃, 600 MHz)

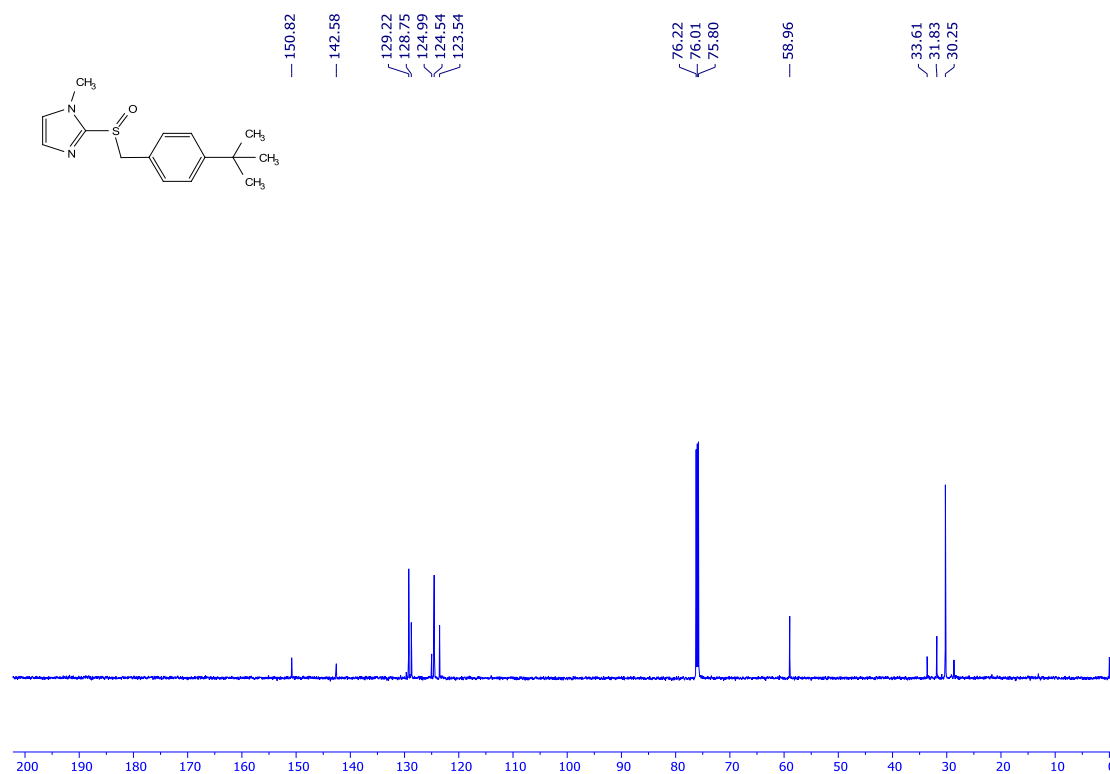


Fig. S26. ¹³C NMR spectrum of compound **6b** (CDCl₃, 600 MHz)

1-methyl-2-((3-(trifluoromethyl)benzyl)sulfinyl)-1H-imidazole (7b)

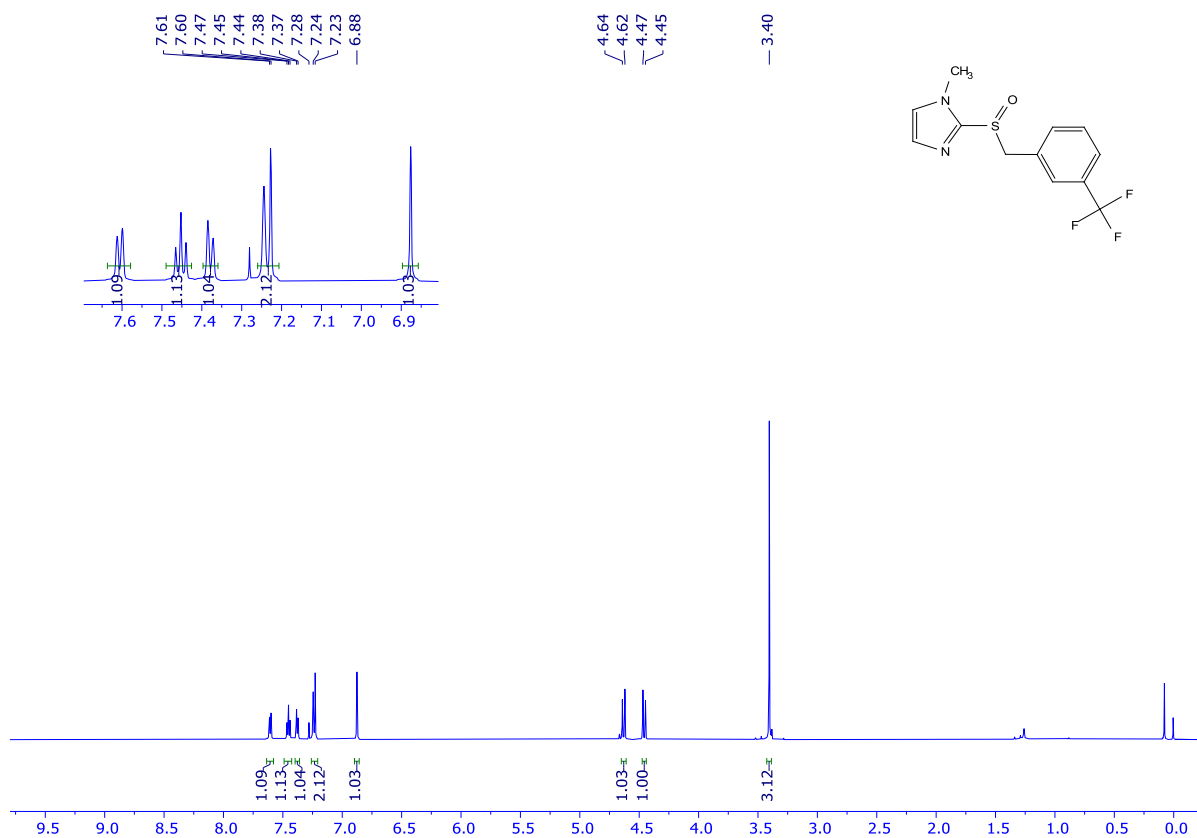


Fig. S27. ¹H NMR spectrum of compound **7b** (CDCl₃, 600 MHz)

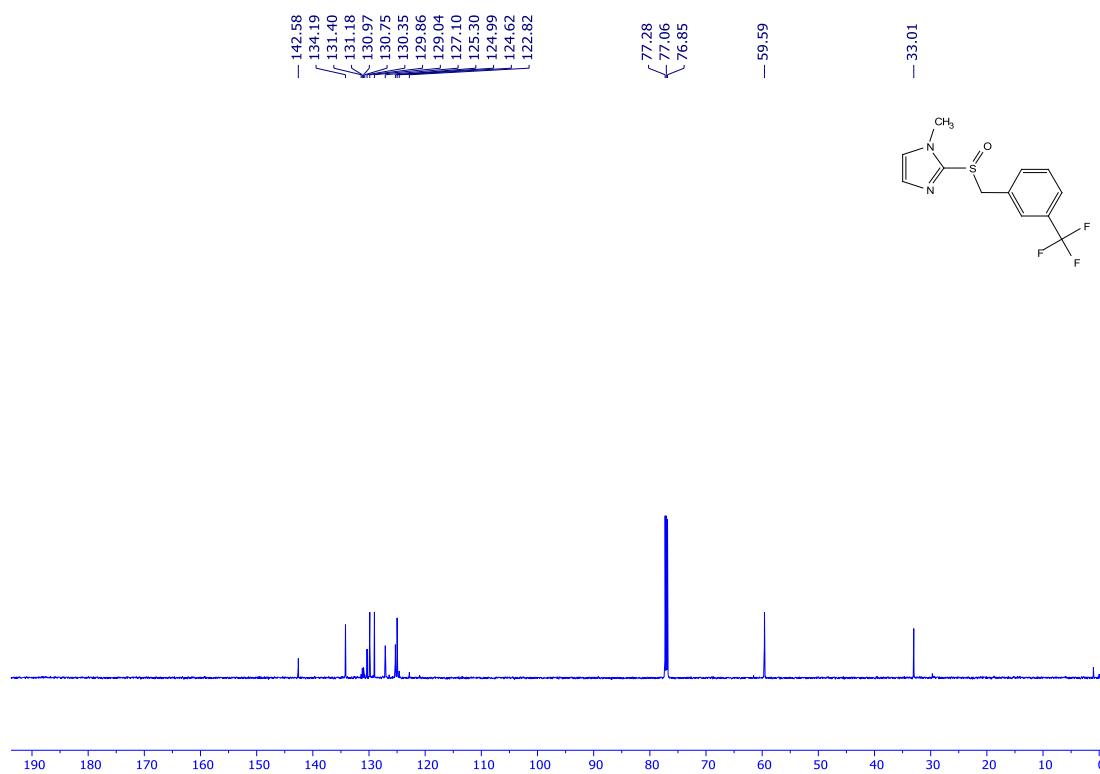


Fig. S28. ¹³C NMR spectrum of compound **7b** (CDCl₃, 600 MHz)

1-methyl-2-((4-nitrobenzyl)sulfinyl)-1H-imidazole (8b)

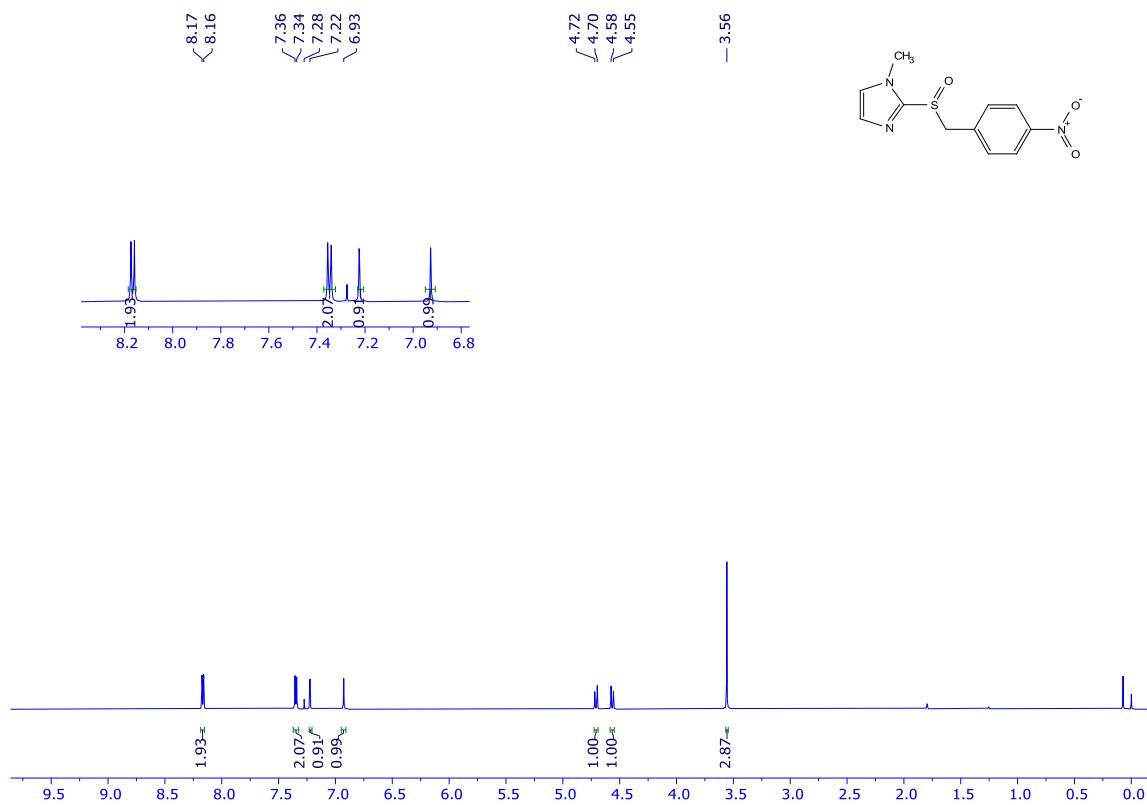


Fig. S29. ¹H NMR spectrum of compound **8b** (CDCl₃, 600 MHz)

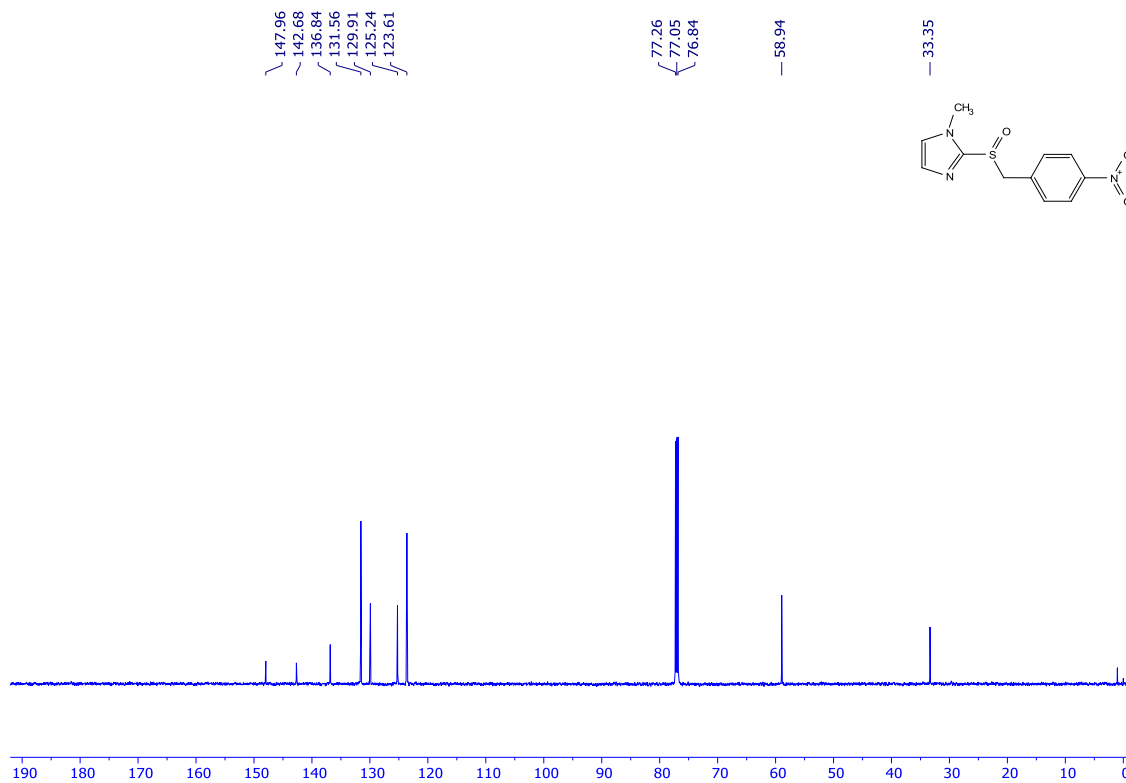


Fig. S30. ¹³C NMR spectrum of compound **8b** (CDCl₃, 600 MHz)

2-((2-chloro-4-fluorobenzyl)sulfonyl)-1-methyl-1H-imidazole (1c)

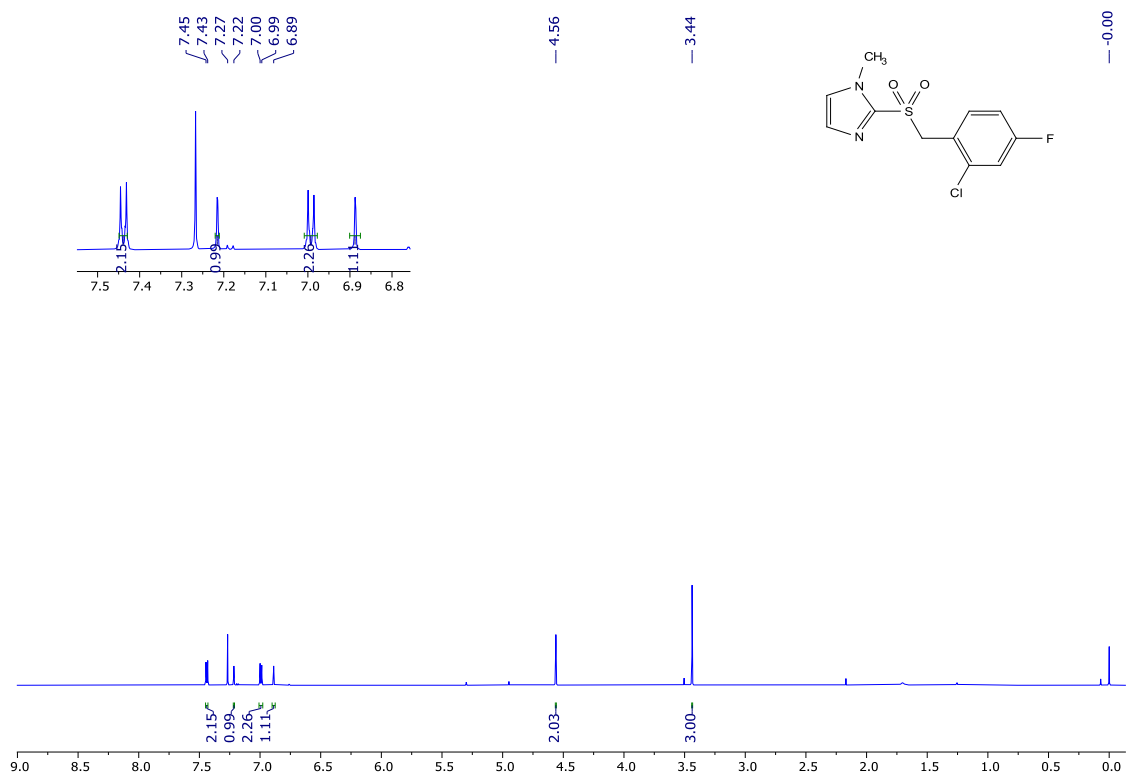


Fig. S31. ¹H NMR spectrum of compound **1c** (CDCl₃, 600 MHz)

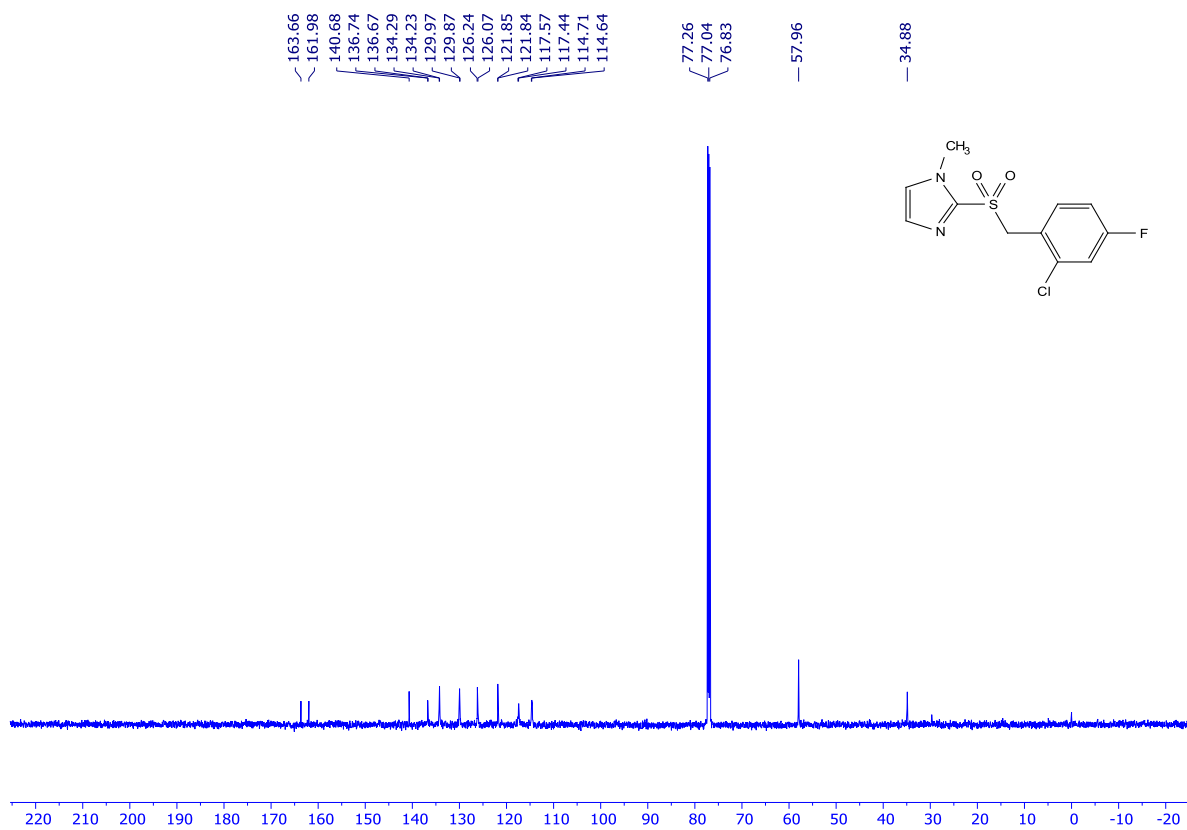


Fig. S32. ¹³C NMR spectrum of compound **1c** (CDCl₃, 600 MHz)

2-(benzylsulfonyl)-1-methyl-1H-imidazole (2c)

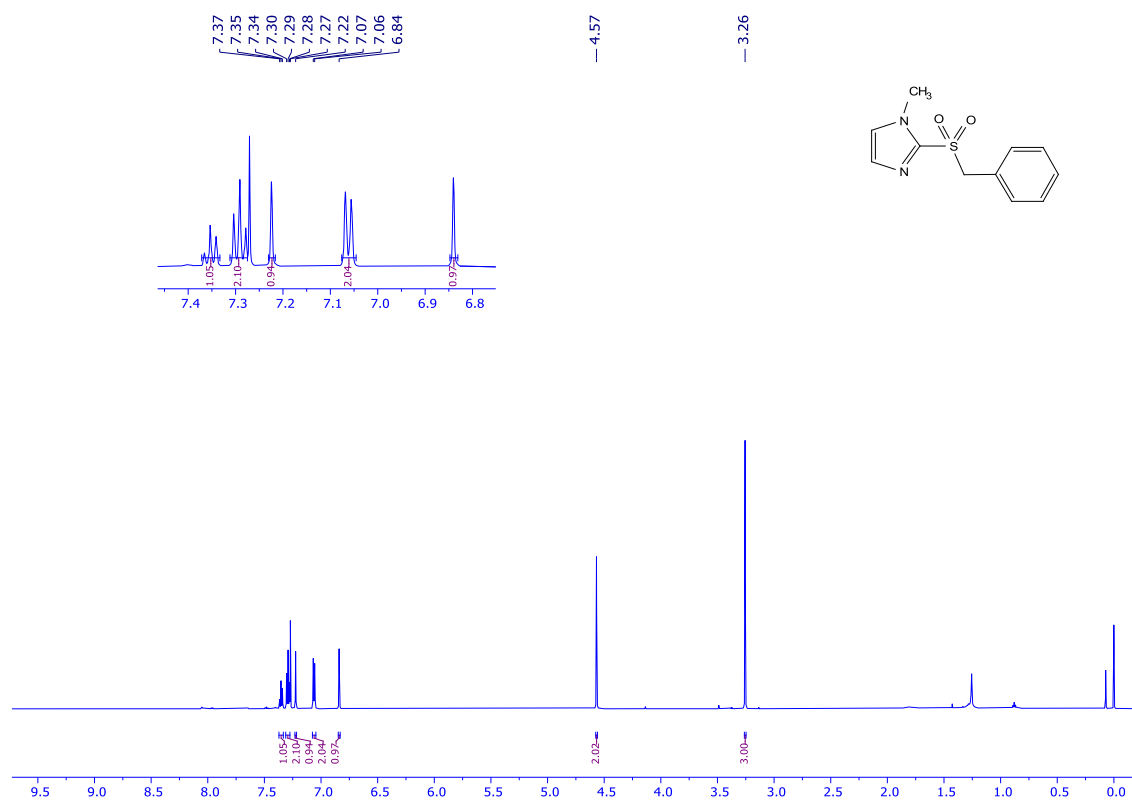


Fig. S33. ¹H NMR spectrum of compound 1c (CDCl₃, 600 MHz)

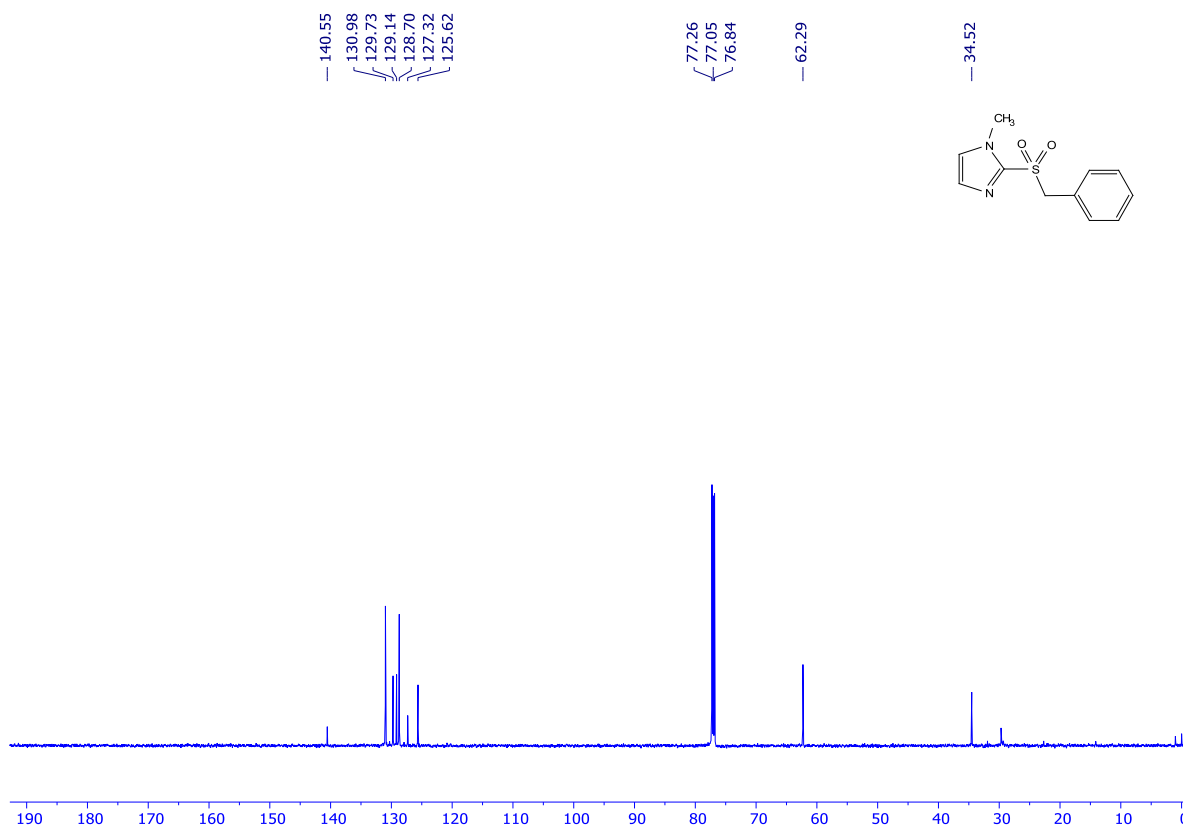


Fig. S34. ¹³C NMR spectrum of compound 1c (CDCl₃, 600 MHz)

2-((4-bromobenzyl)sulfonyl)-1-methyl-1H-imidazole (3c)

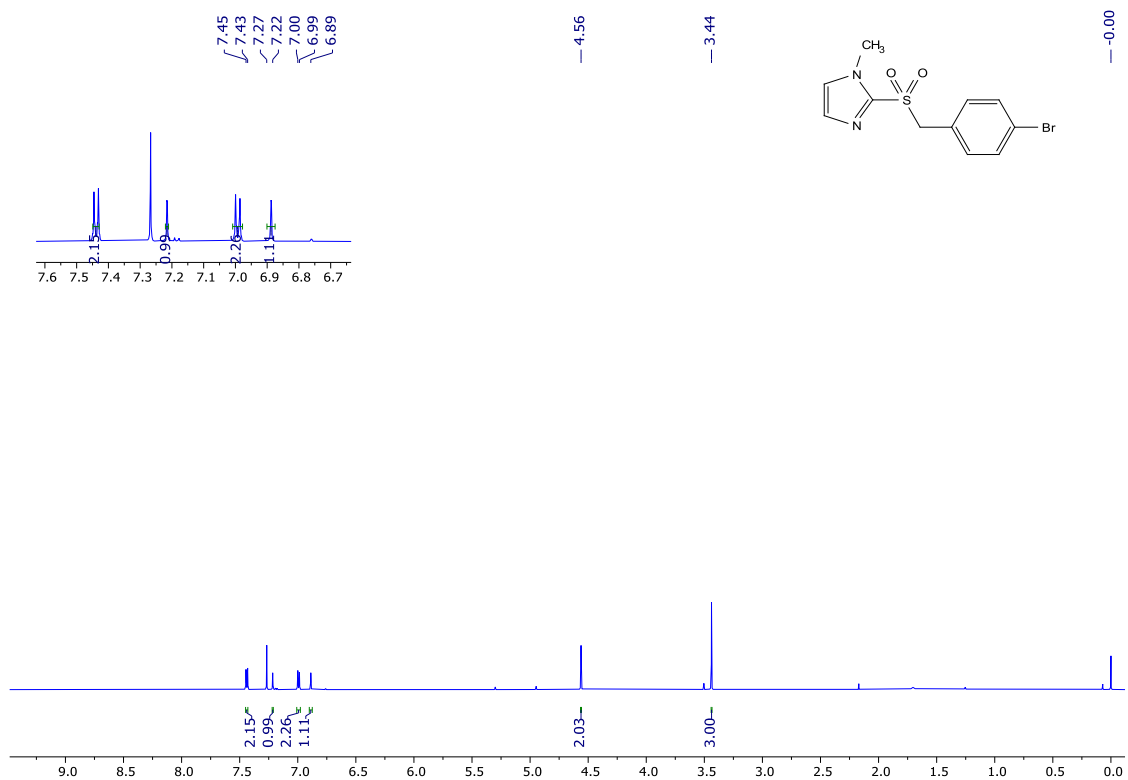


Fig. S35. ¹H NMR spectrum of compound **3c** (CDCl₃, 600 MHz)

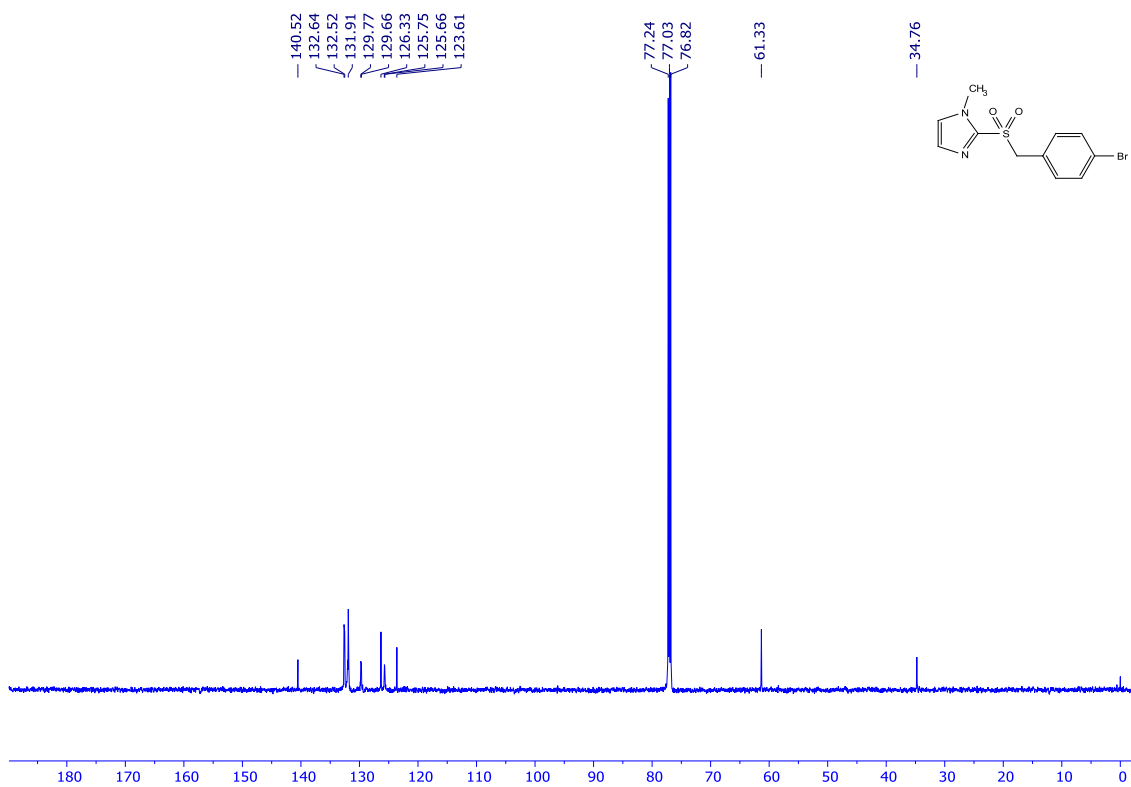


Fig. S36. ¹³C NMR spectrum of compound **3c** (CDCl₃, 600 MHz)

2-((4-bromo-2-fluorobenzyl)sulfonyl)-1-methyl-1H-imidazole (4c)

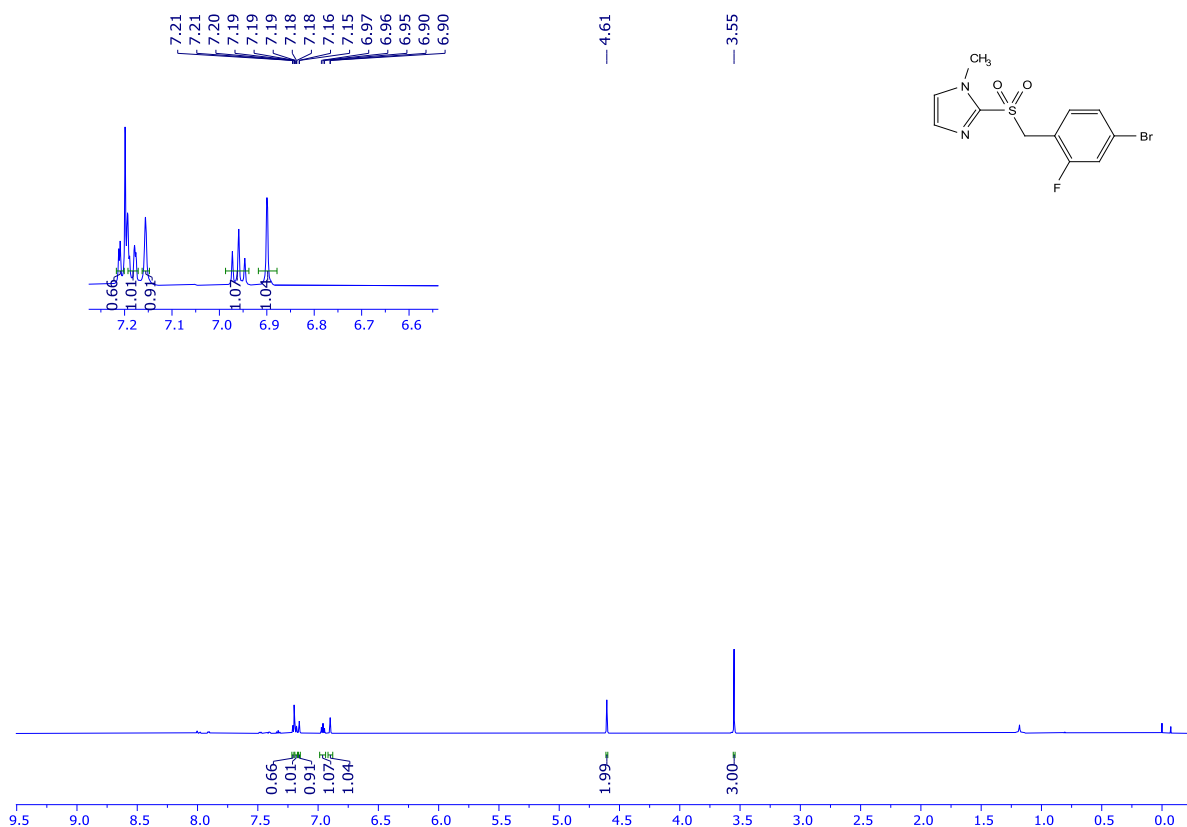


Fig. S37. ^1H NMR spectrum of compound **4c** (CDCl_3 , 600 MHz)

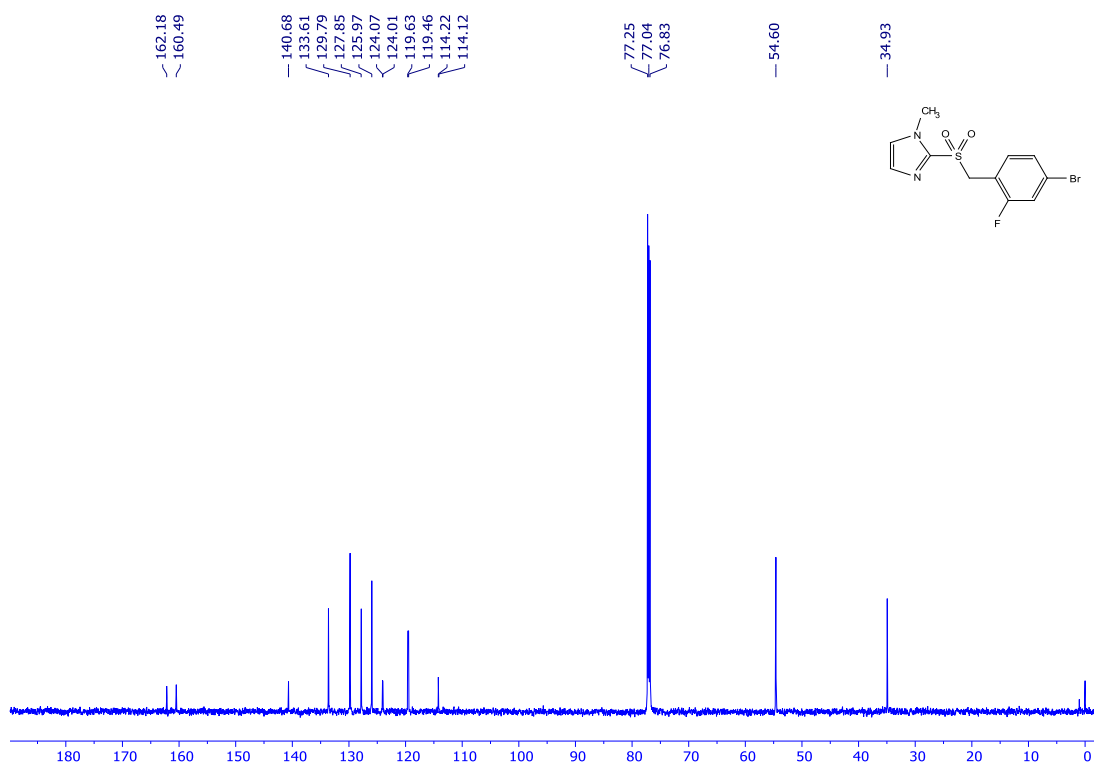


Fig. S38. ^{13}C NMR spectrum of compound **4c** (CDCl_3 , 600 MHz)

1-methyl-2-((4-(trifluoromethoxy)benzyl)sulfonyl)-1H-imidazole (5c)

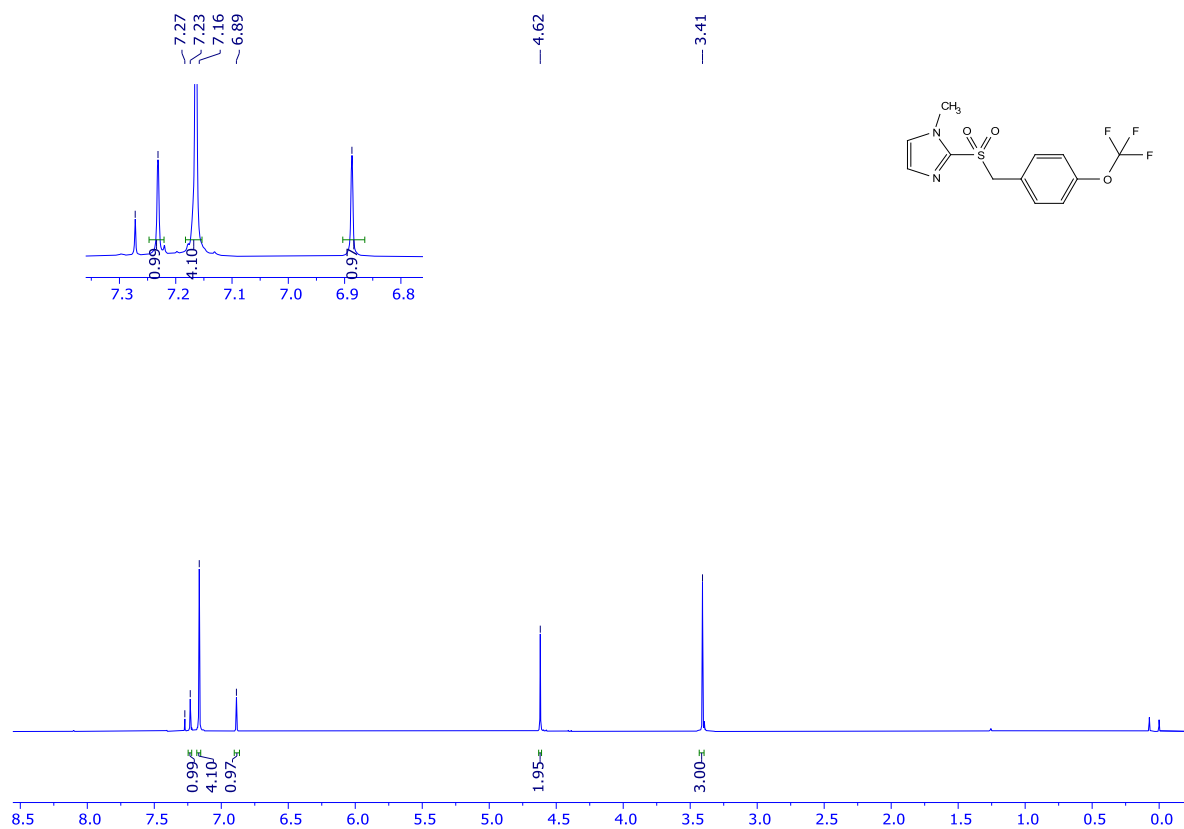


Fig. S39. ^1H NMR spectrum of compound **5c** (CDCl_3 , 600 MHz)

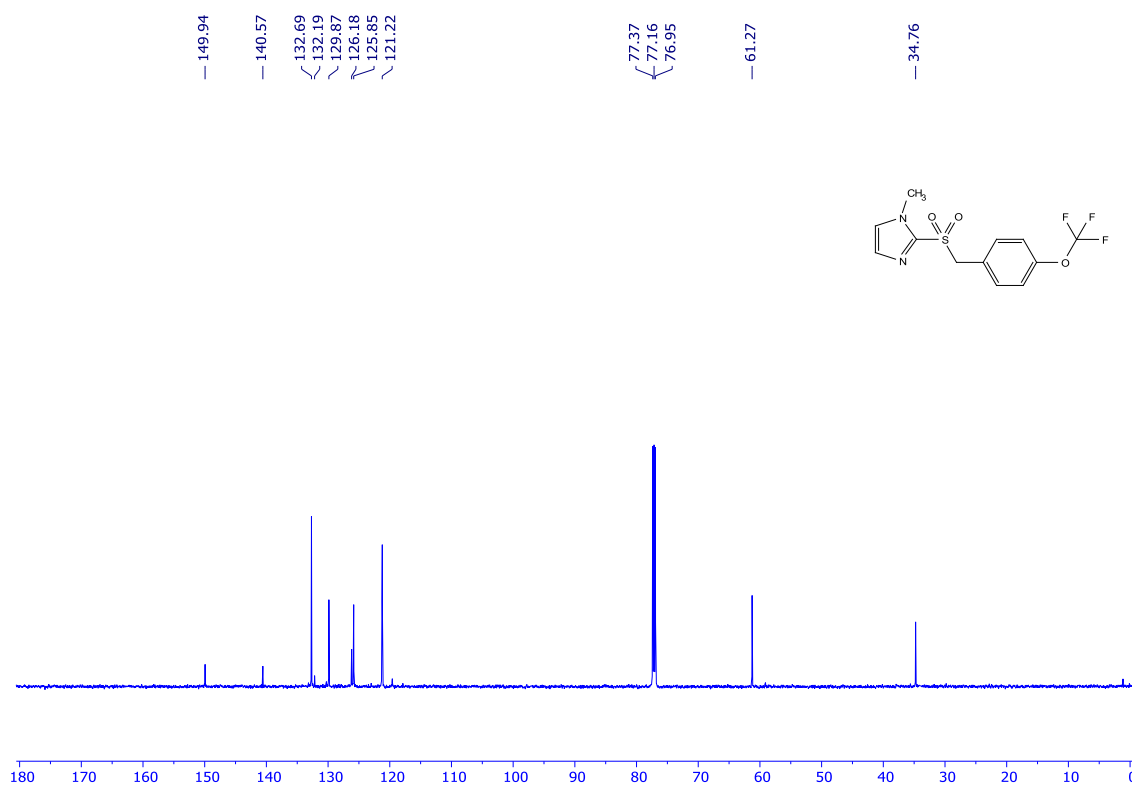


Fig. S40. ^{13}C NMR spectrum of compound **5c** (CDCl_3 , 600 MHz)

2-((4-(tert-butyl)benzyl)sulfinyl)-1-methyl-1H-imidazole (6c)

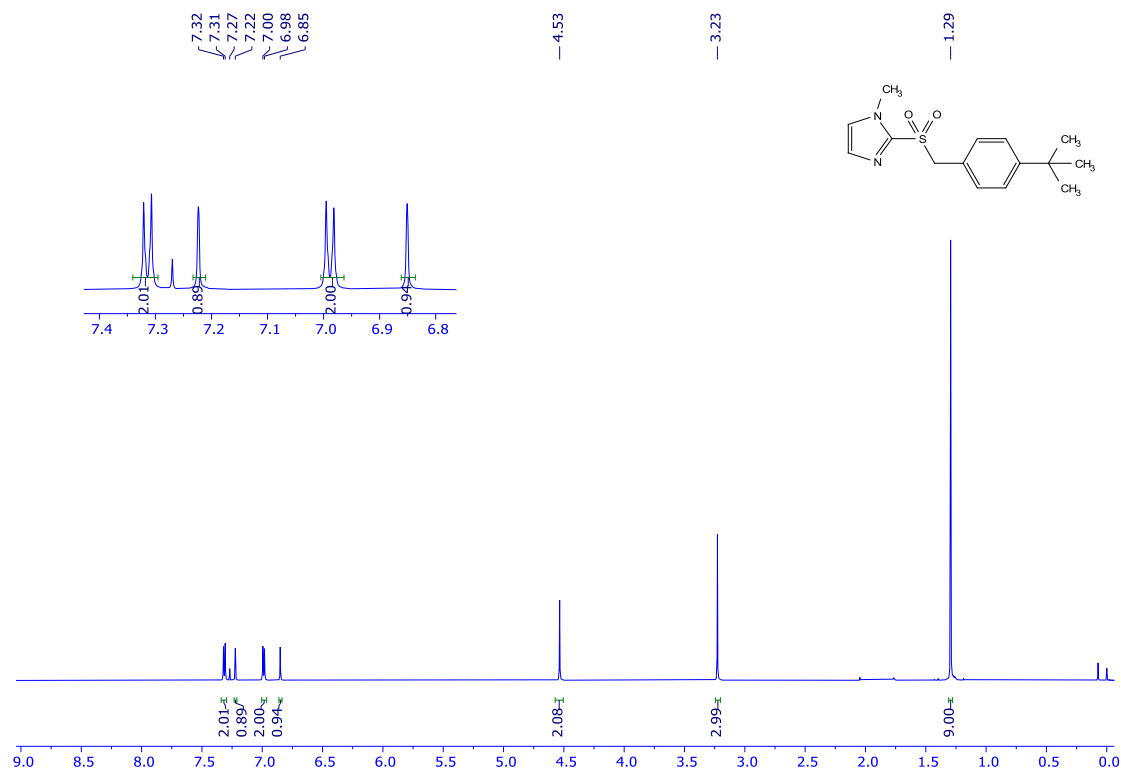


Fig. S41. ¹H NMR spectrum of compound **6c** (CDCl₃, 600 MHz)

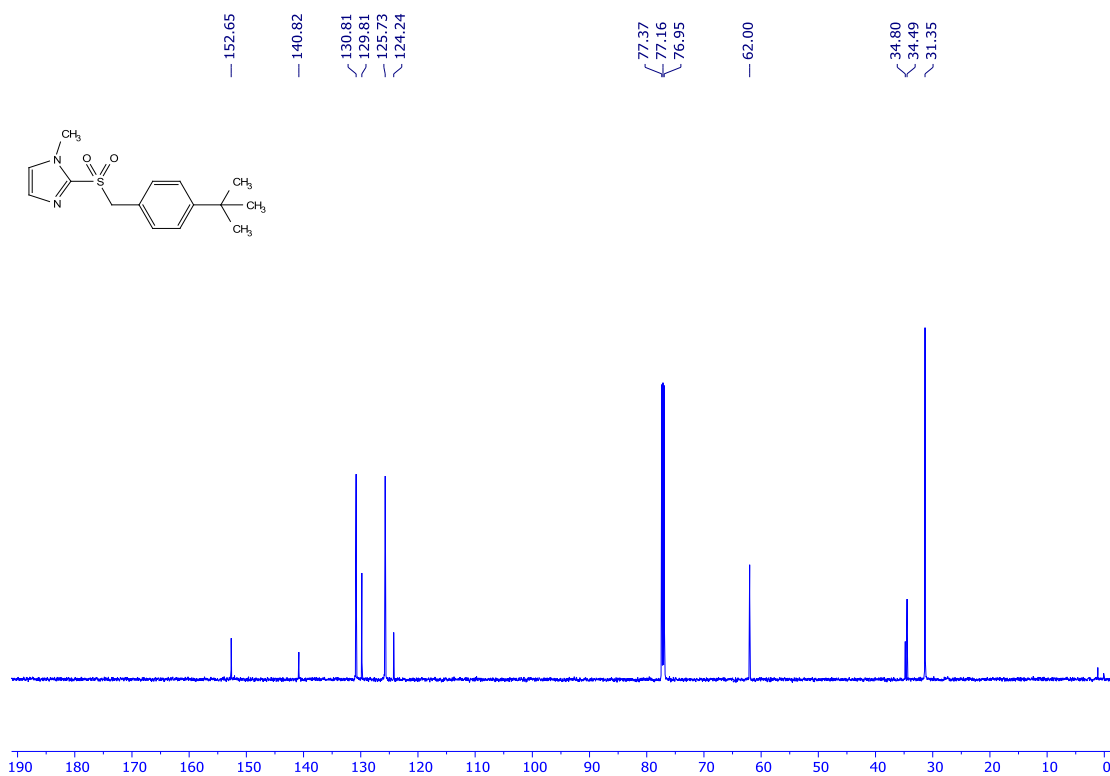


Fig. S42. ¹³C NMR spectrum of compound **6c** (CDCl₃, 600 MHz)

1-methyl-2-((3-(trifluoromethyl)benzyl)sulfonyl)-1H-imidazole (7c)

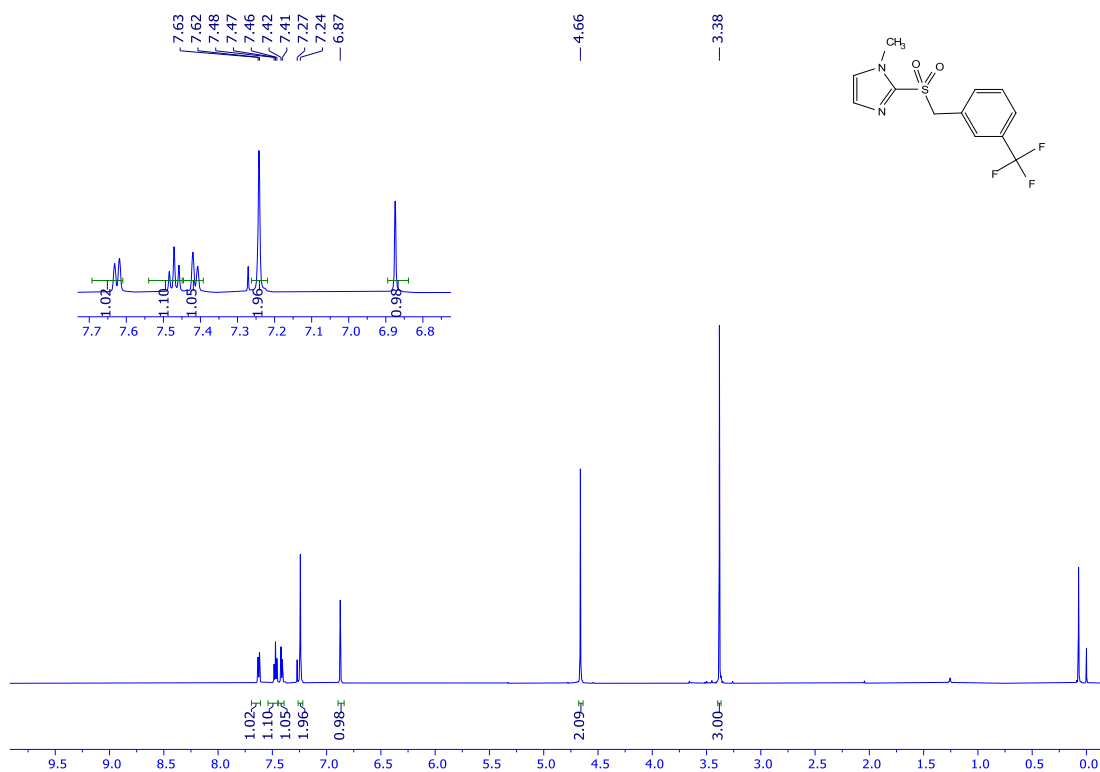


Fig. S43. ¹H NMR spectrum of compound **7c** (CDCl₃, 600 MHz)

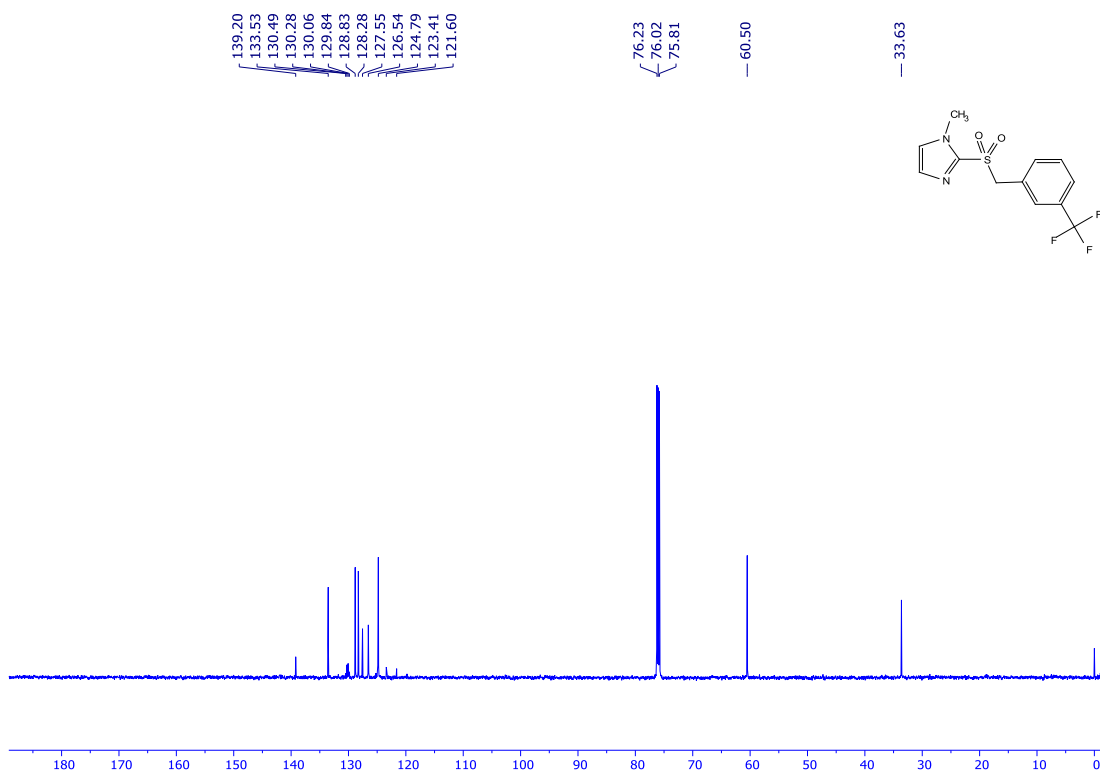


Fig. S44. ¹³C NMR spectrum of compound **7c** (CDCl₃, 600 MHz)

1-methyl-2-((4-nitrobenzyl)sulfonyl)-1H-imidazole (8c)

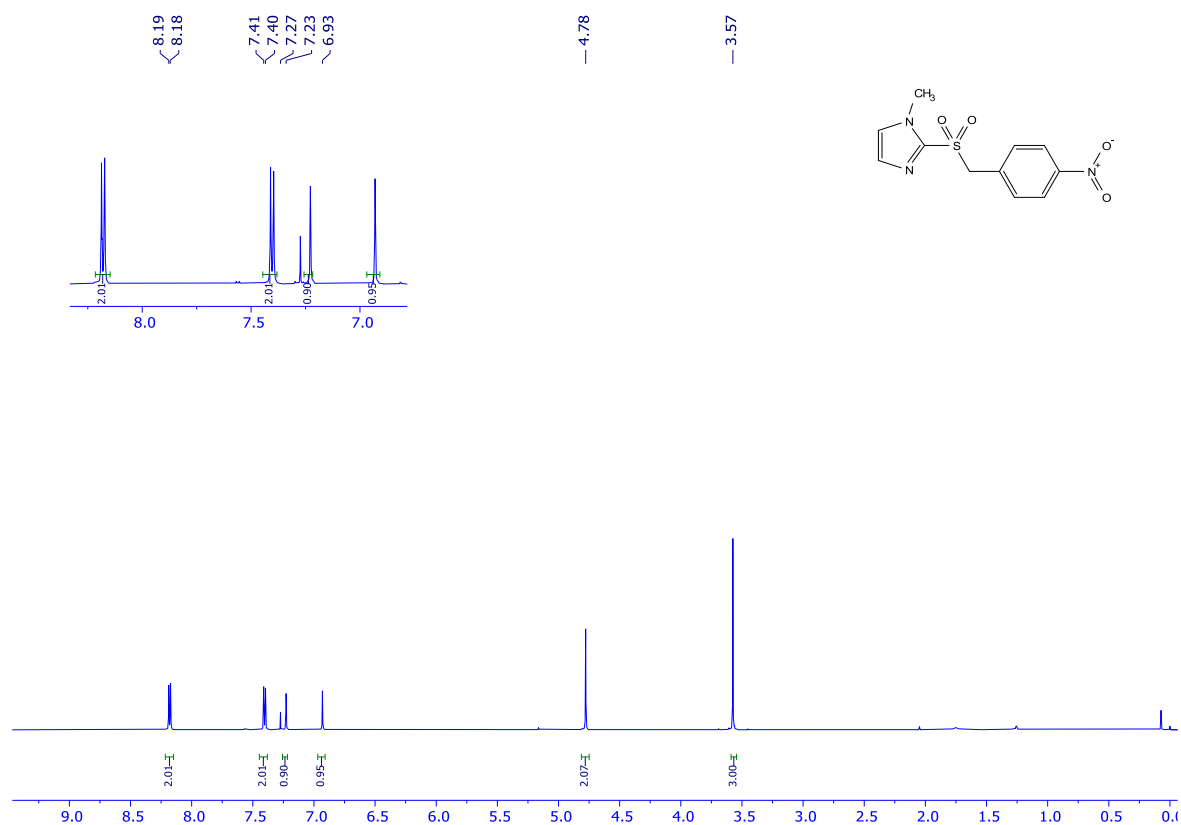


Fig. S45. ^1H NMR spectrum of compound **8c** (CDCl_3 , 600 MHz)

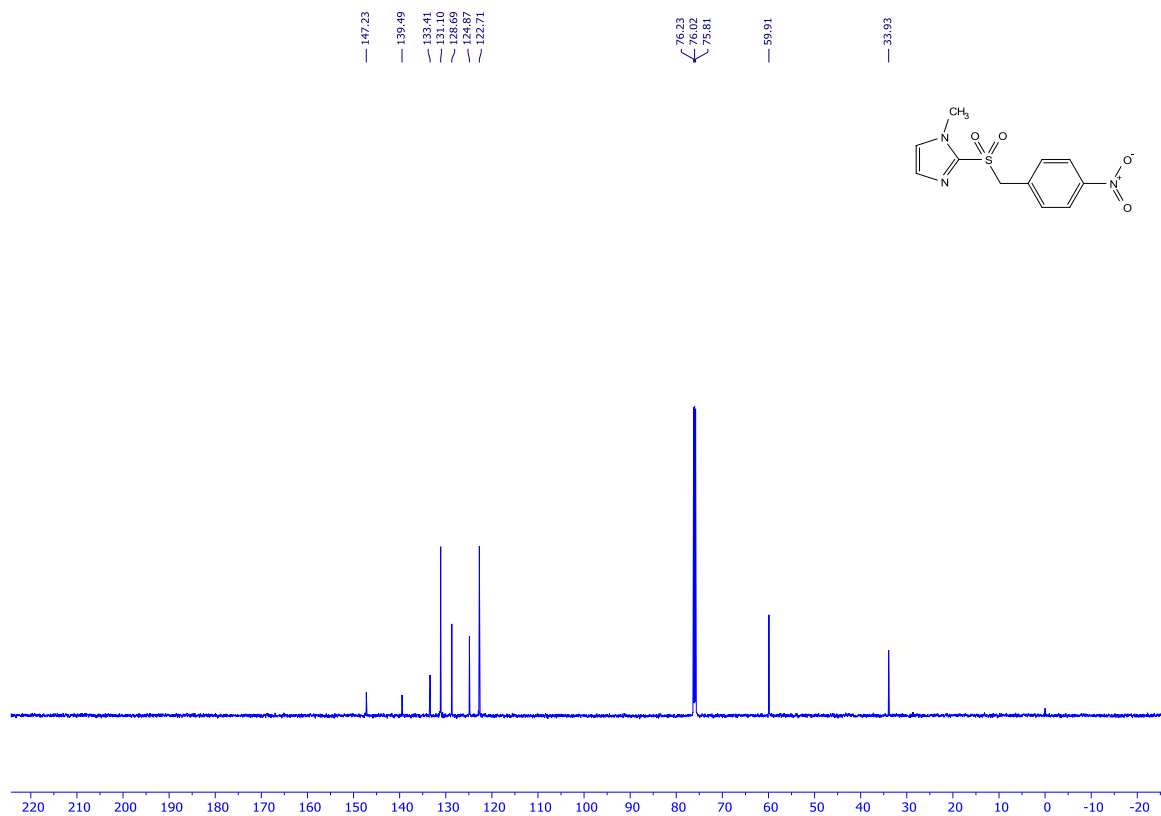


Fig. S46. ^{13}C NMR spectrum of compound **8c** (CDCl_3 , 600 MHz)

1,3-dimethyl-2-((2-chloro-4-fluorobenzyl)thio)-1H-imidazol-3-ium Triflate (1d)

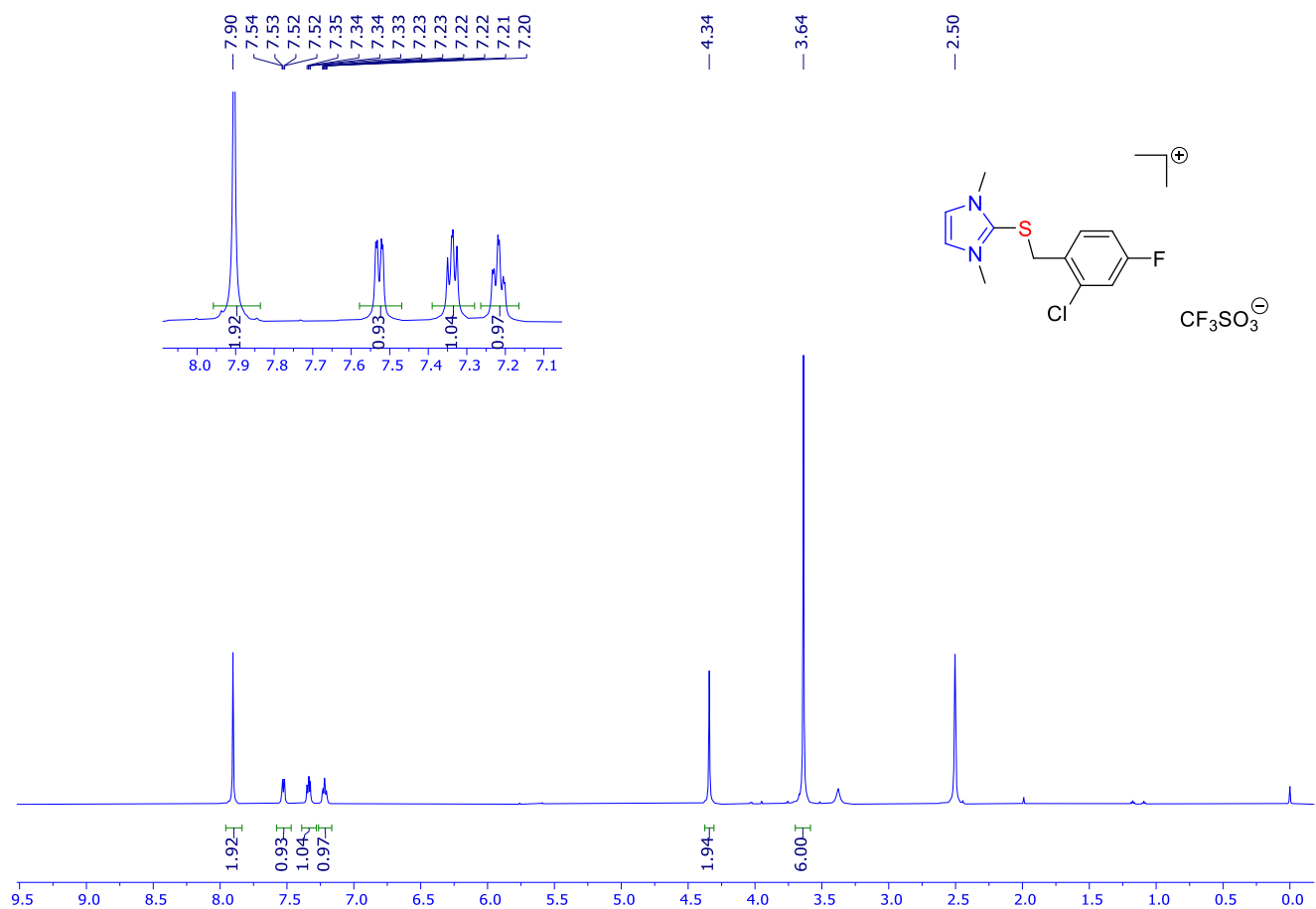


Fig. S47. ¹H NMR spectrum of compound **1d** (DMSO-*d*₆, 600 MHz)

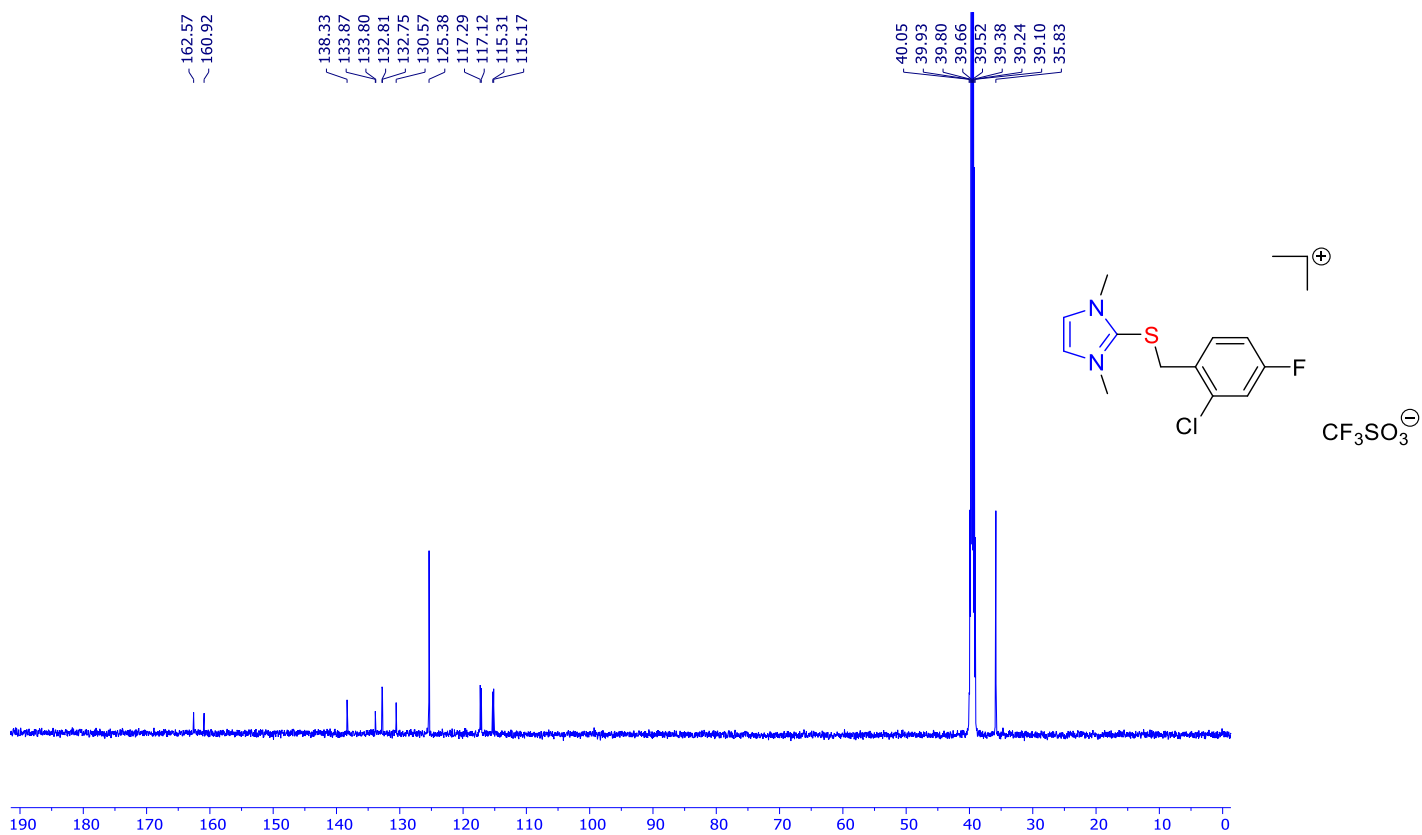


Fig. S48. ^{13}C NMR spectrum of compound **1d** (DMSO- d_6 , 600 MHz)

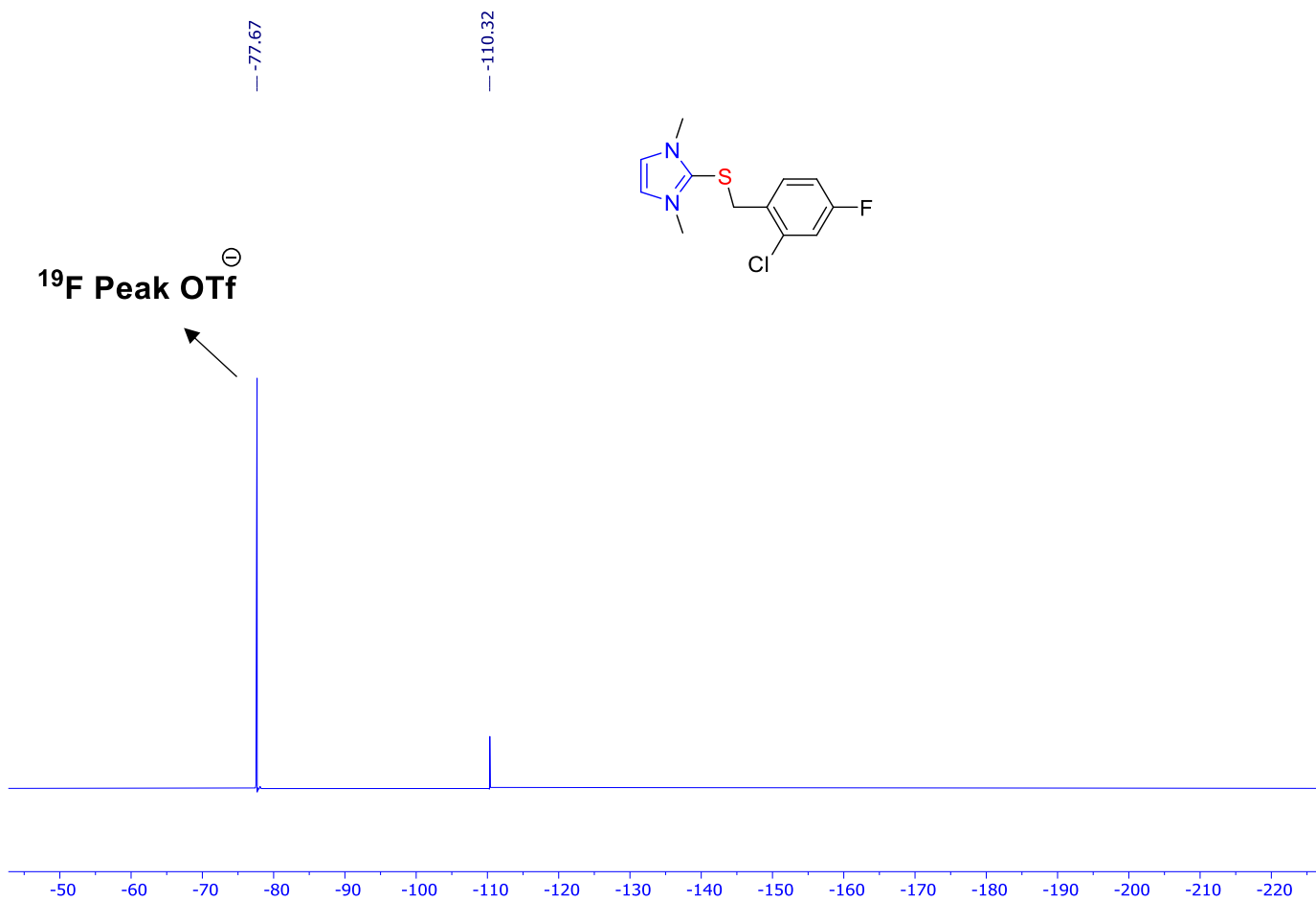


Fig. S49. ^{19}F NMR spectrum of compound **1d** ($\text{DMSO}-d_6$, 600 MHz)

1,3-dimethyl-2-(benzylthio)-1H-imidazol-3-ium Triflate (2d)

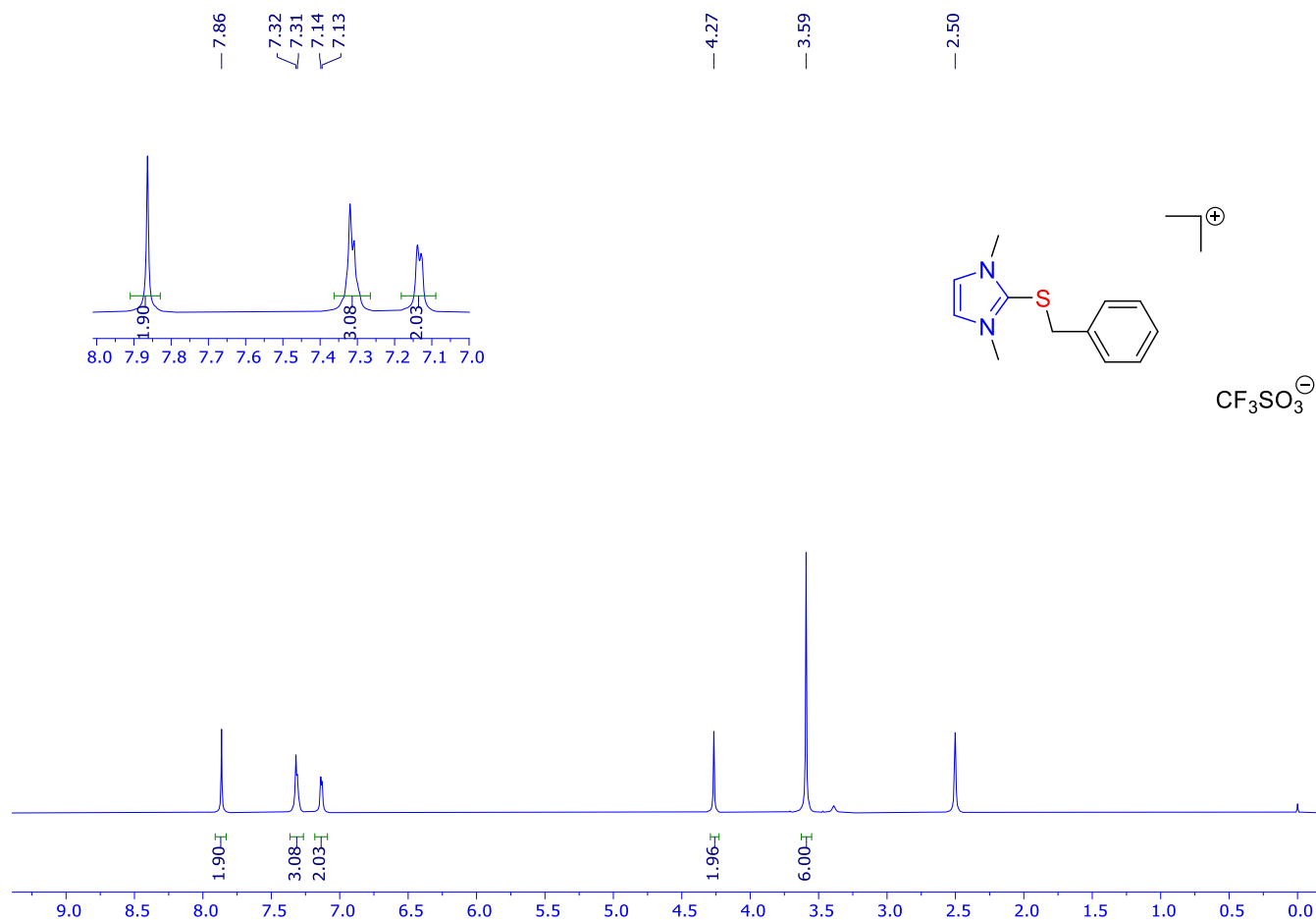


Fig. S50. ¹H NMR spectrum of compound 2d (DMSO-*d*₆, 600 MHz)

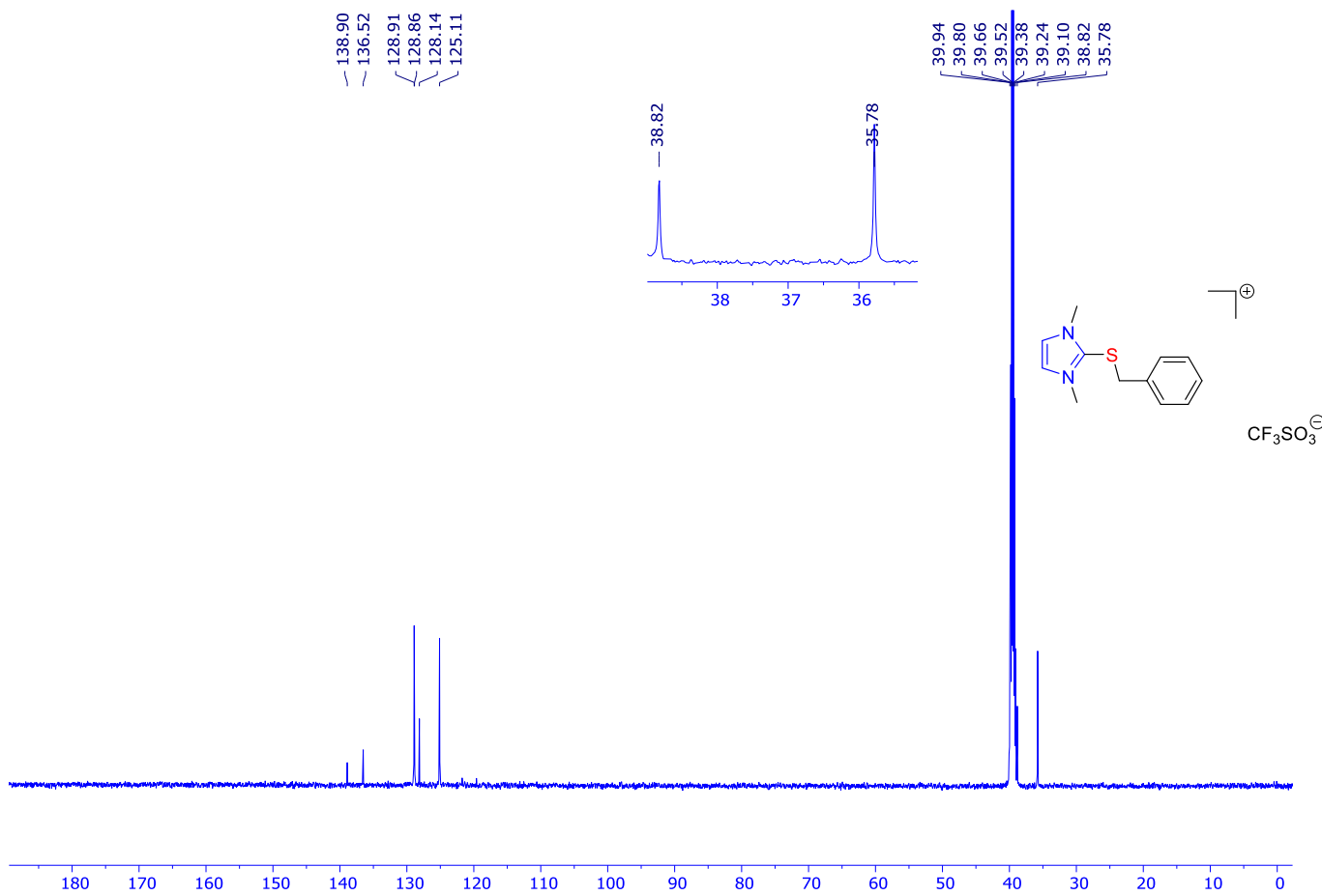


Fig. S51. ^{13}C NMR spectrum of compound **2d** ($\text{DMSO}-d_6$, 600 MHz)

1,3-dimethyl-2-((4-bromobenzyl)thio)-1H-imidazol-3-ium Triflate (3d)

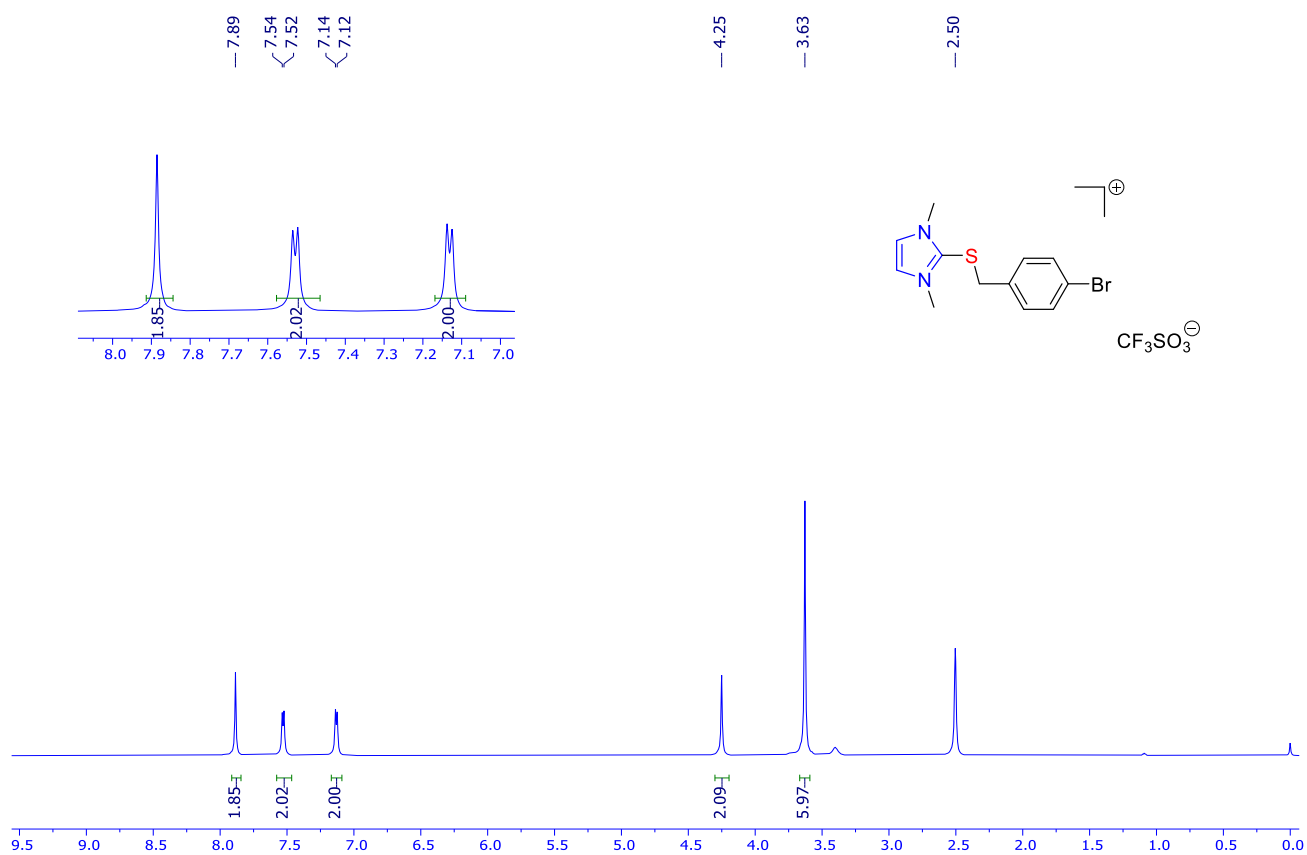


Fig. S52. ^1H NMR spectrum of compound **3d** ($\text{DMSO-}d_6$, 600 MHz)

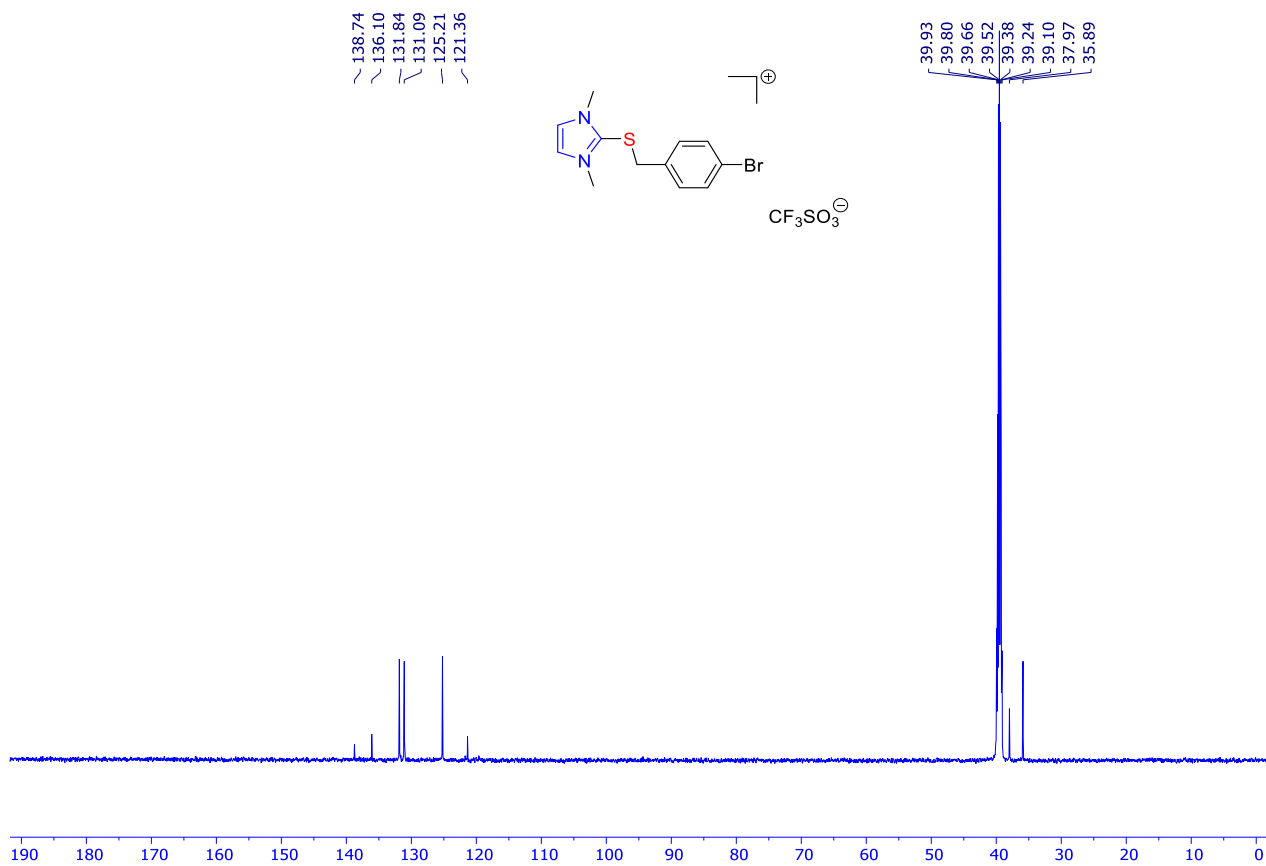


Fig. S53. ^{13}C NMR spectrum of compound **3d** (DMSO- d_6 , 600 MHz)

1,3-dimethyl-2-((2-fluoro-4-bromobenzyl)thio)-1H-imidazol-3-ium Triflate (4d)

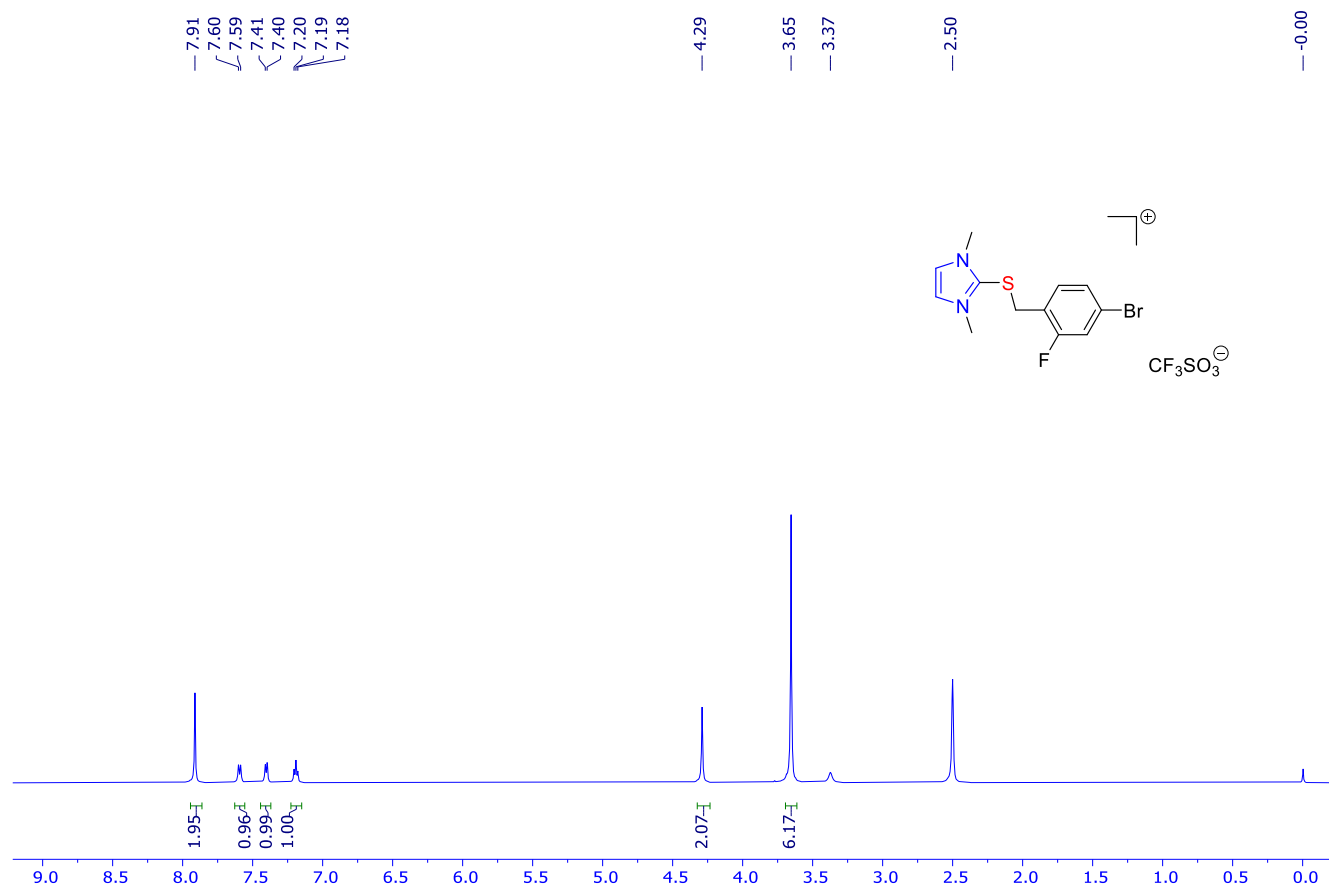


Fig. S54. ¹H NMR spectrum of compound **4d** (DMSO-*d*₆, 600 MHz)

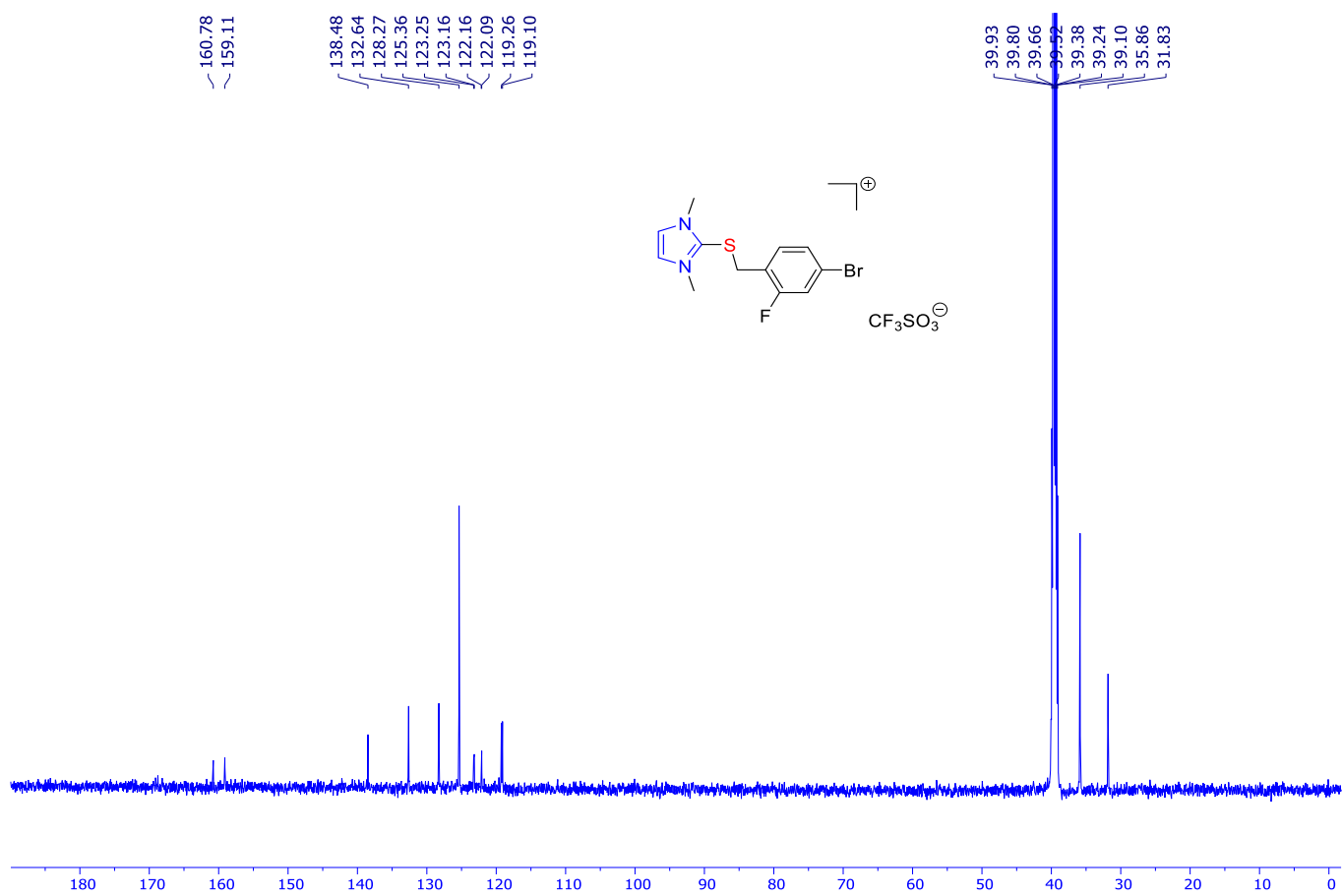


Fig. S55. ^{13}C NMR spectrum of compound **4d** (DMSO- d_6 , 600 MHz)

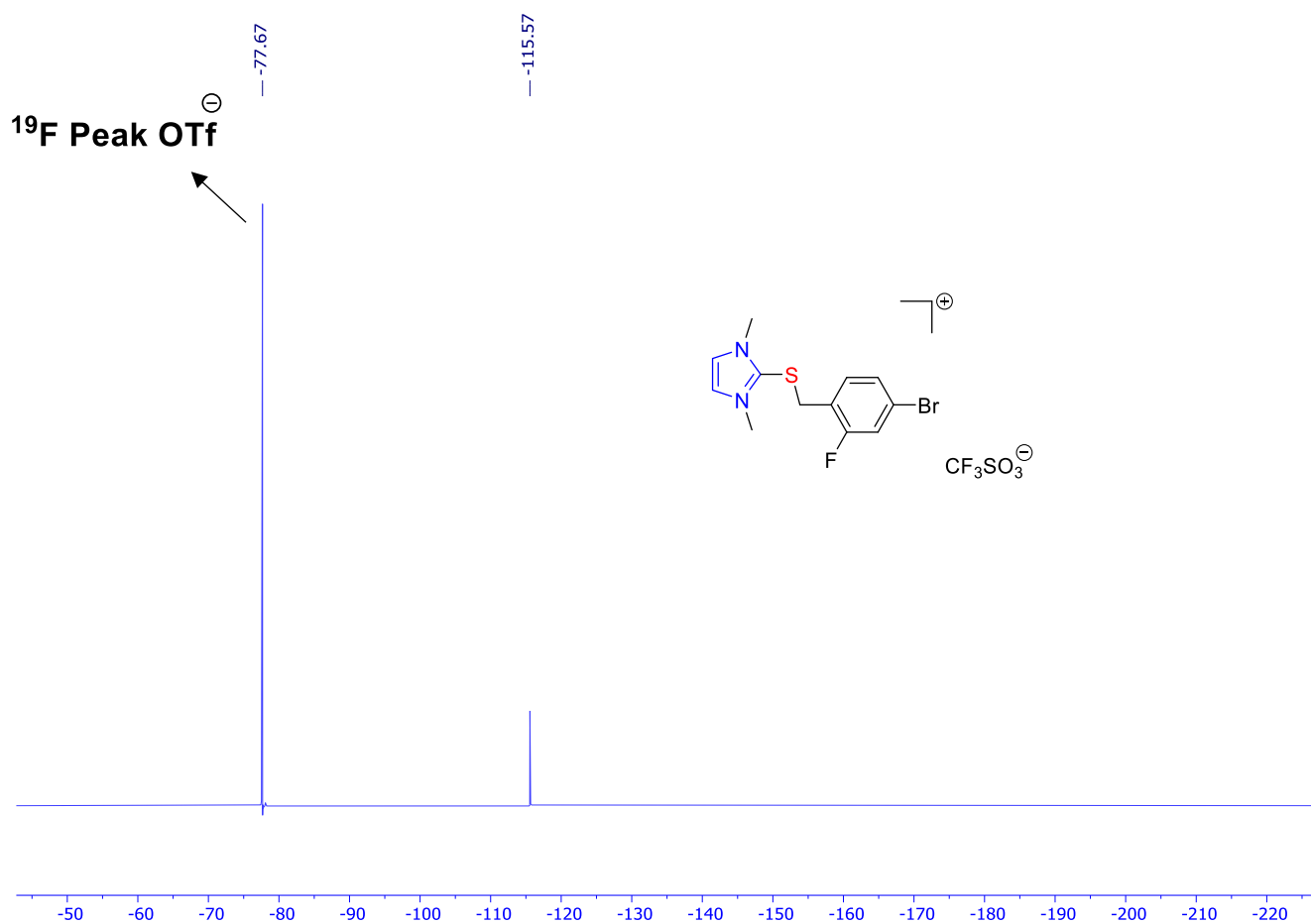


Fig. S56. ^{19}F NMR spectrum of compound **4d** (DMSO- d_6 , 600 MHz)

1,3-dimethyl-2-((4-(trifluoromethoxy)benzyl)thio)-1H-imidazol-3-iumTriflate (5d)

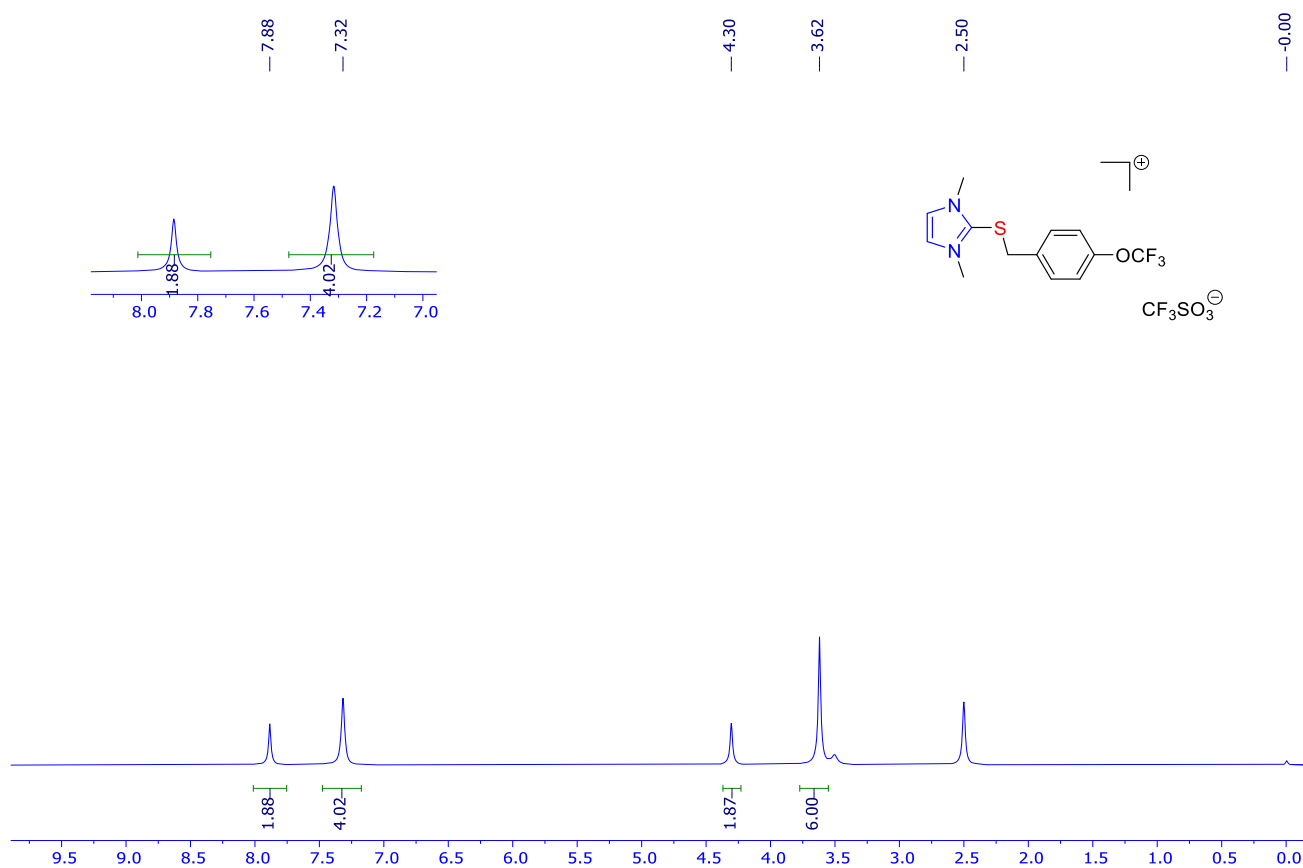


Fig. S57. ¹H NMR spectrum of compound **5d** (DMSO-*d*₆, 600 MHz)

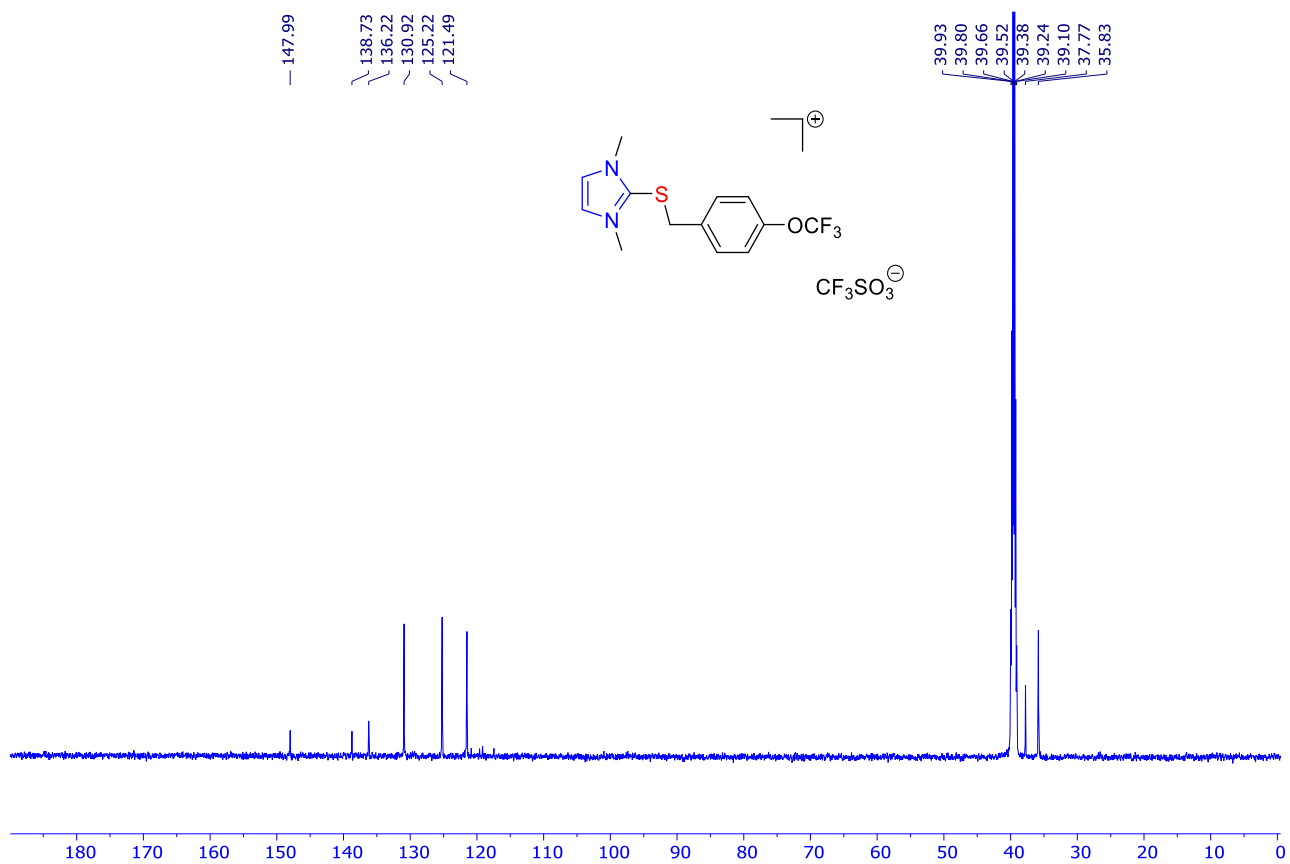


Fig. S58. ^{13}C NMR spectrum of compound **5d** ($\text{DMSO}-d_6$, 600 MHz)

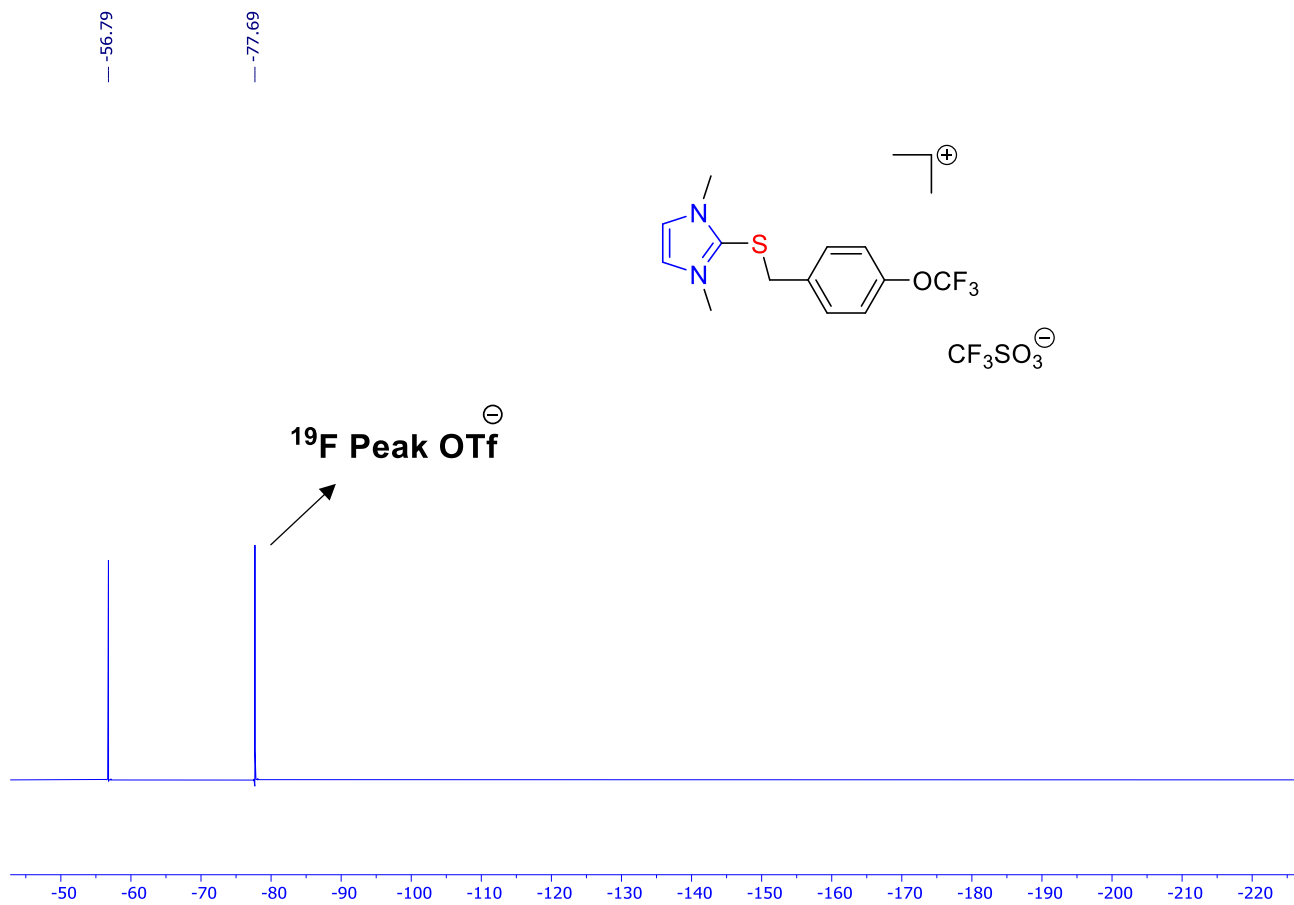


Fig. S59. ^{19}F NMR spectrum of compound **5d** ($\text{DMSO}-d_6$, 600 MHz)

1,3-dimethyl-2-((4-(tert-butyl)benzyl)thio)-1H-imidazol-3-ium Triflate (6d)

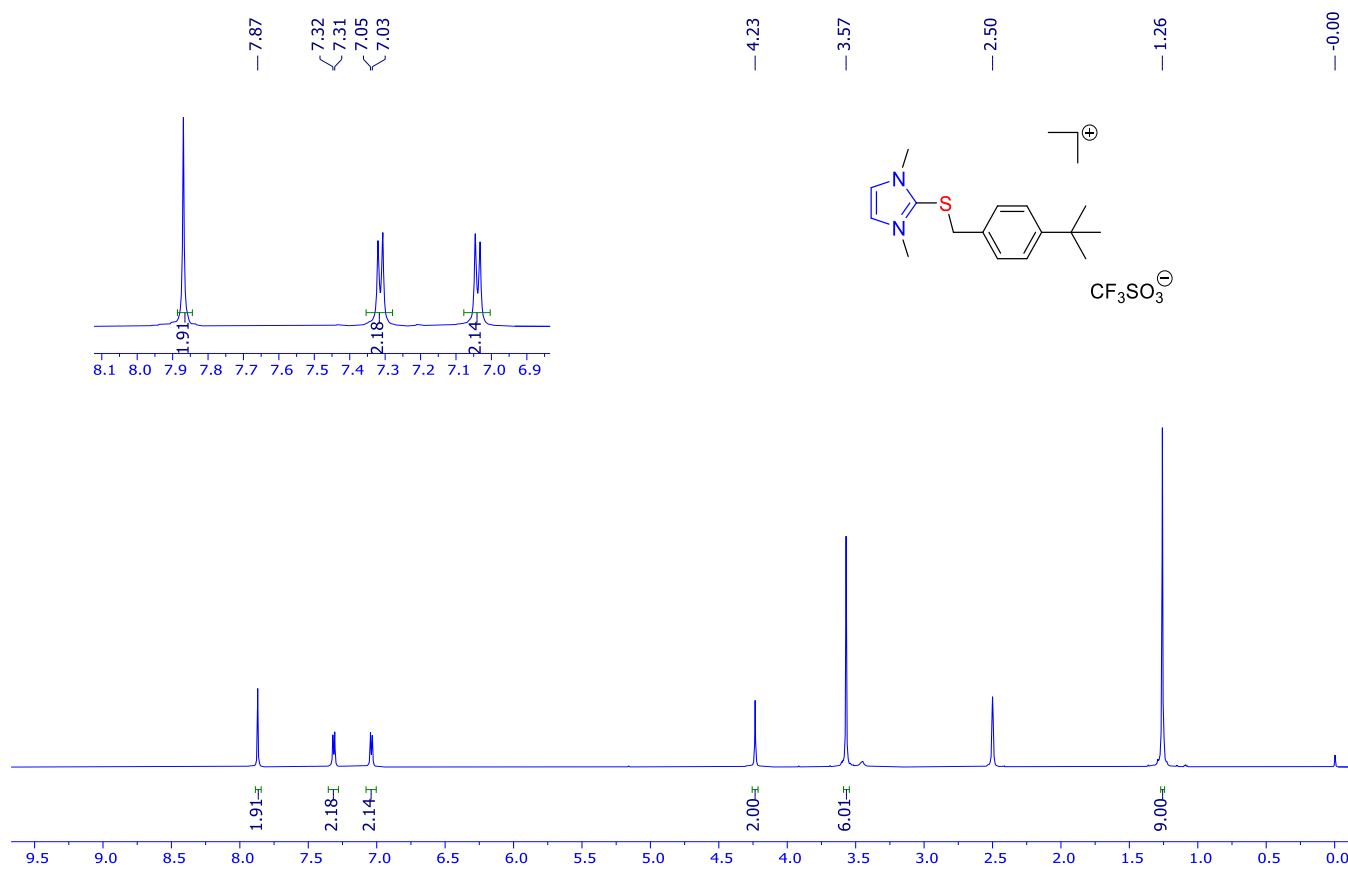


Fig. S60. ¹H NMR spectrum of compound **6d** (DMSO-*d*₆, 600 MHz)

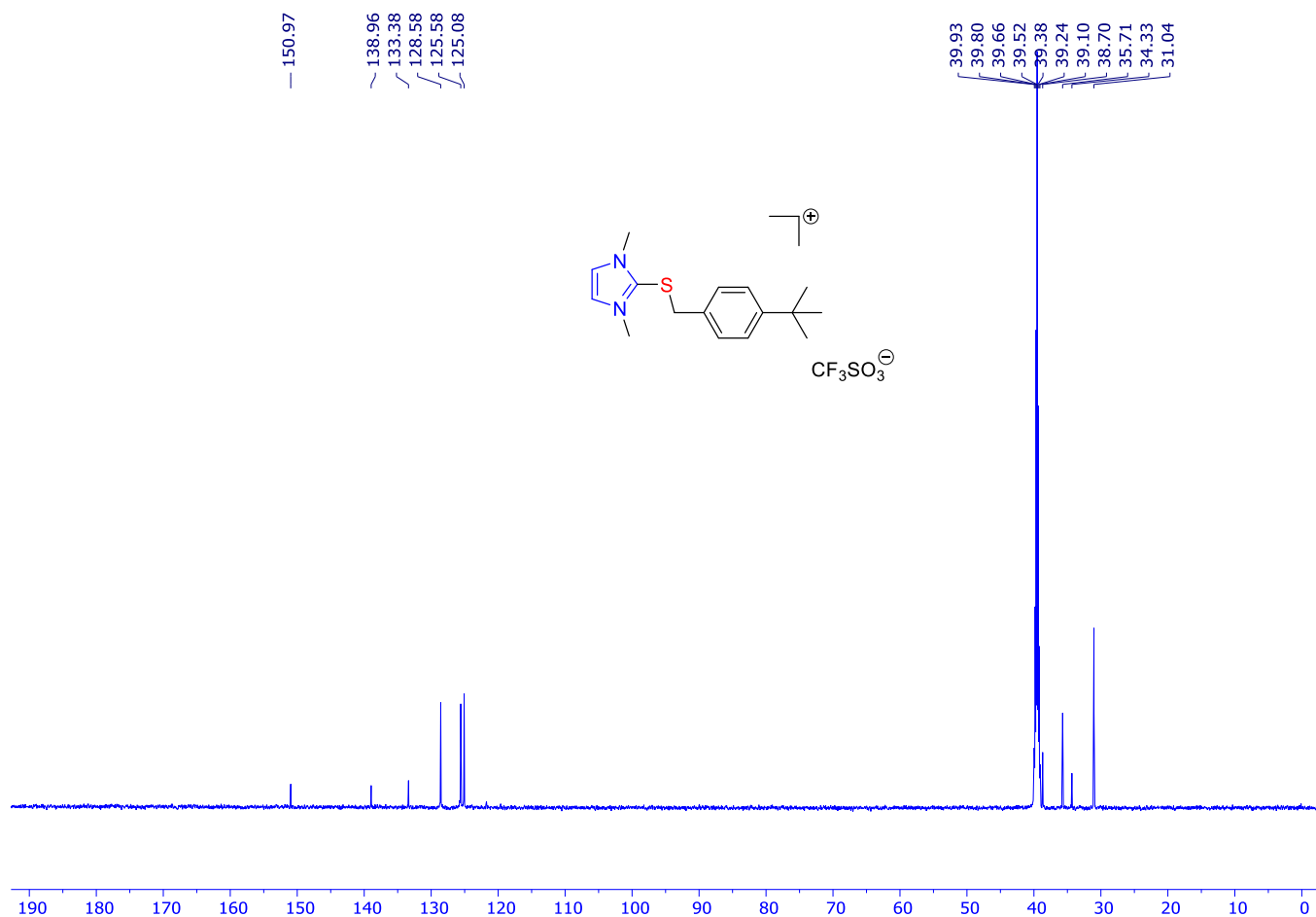


Fig. S61. ^{13}C NMR spectrum of compound **6d** ($\text{DMSO-}d_6$, 600 MHz)

1,3-dimethyl-2-((3-(trifluoromethyl)benzyl)thio)-1H-imidazol-3-ium Triflate (7d)

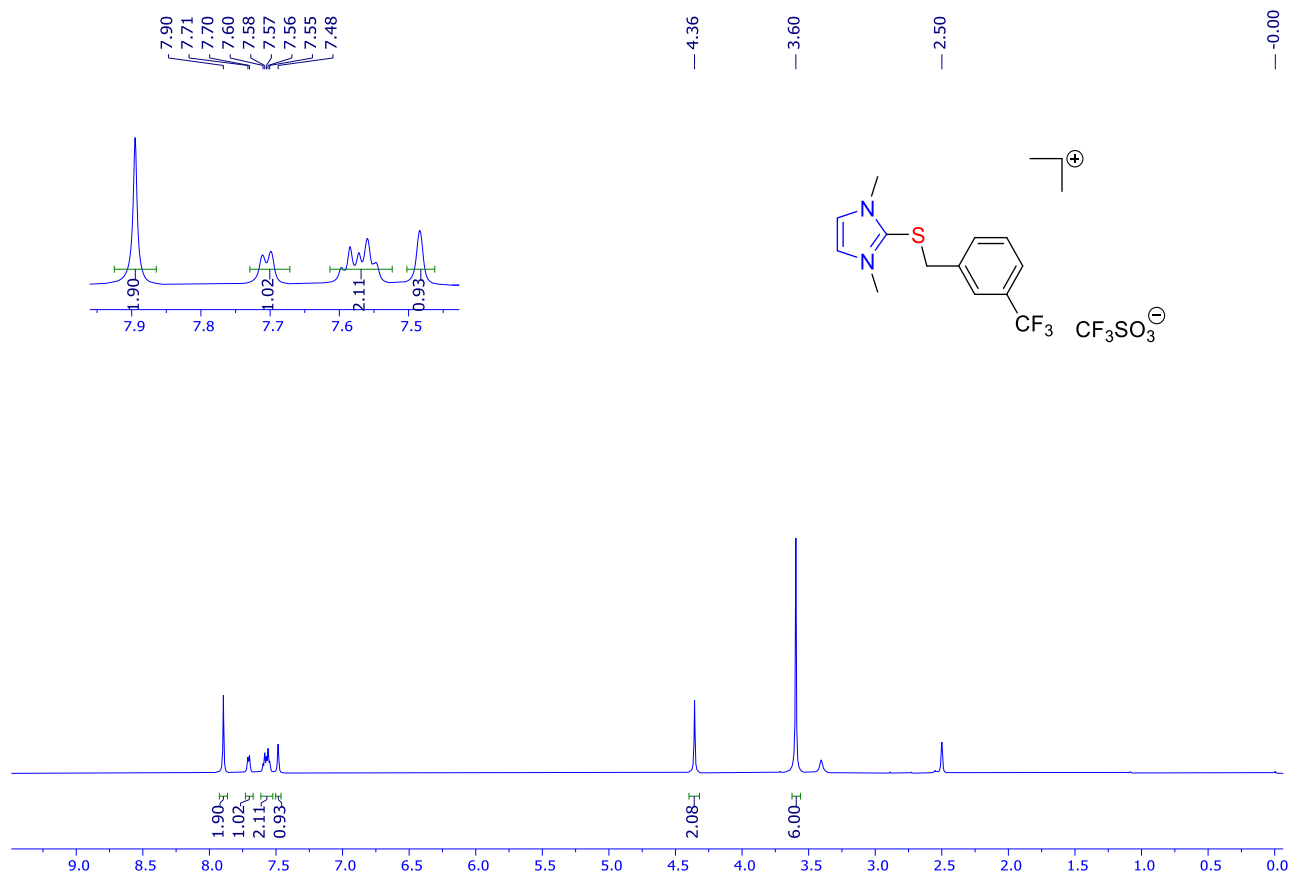


Fig. S62. ^1H NMR spectrum of compound **7d** ($\text{DMSO-}d_6$, 600 MHz)

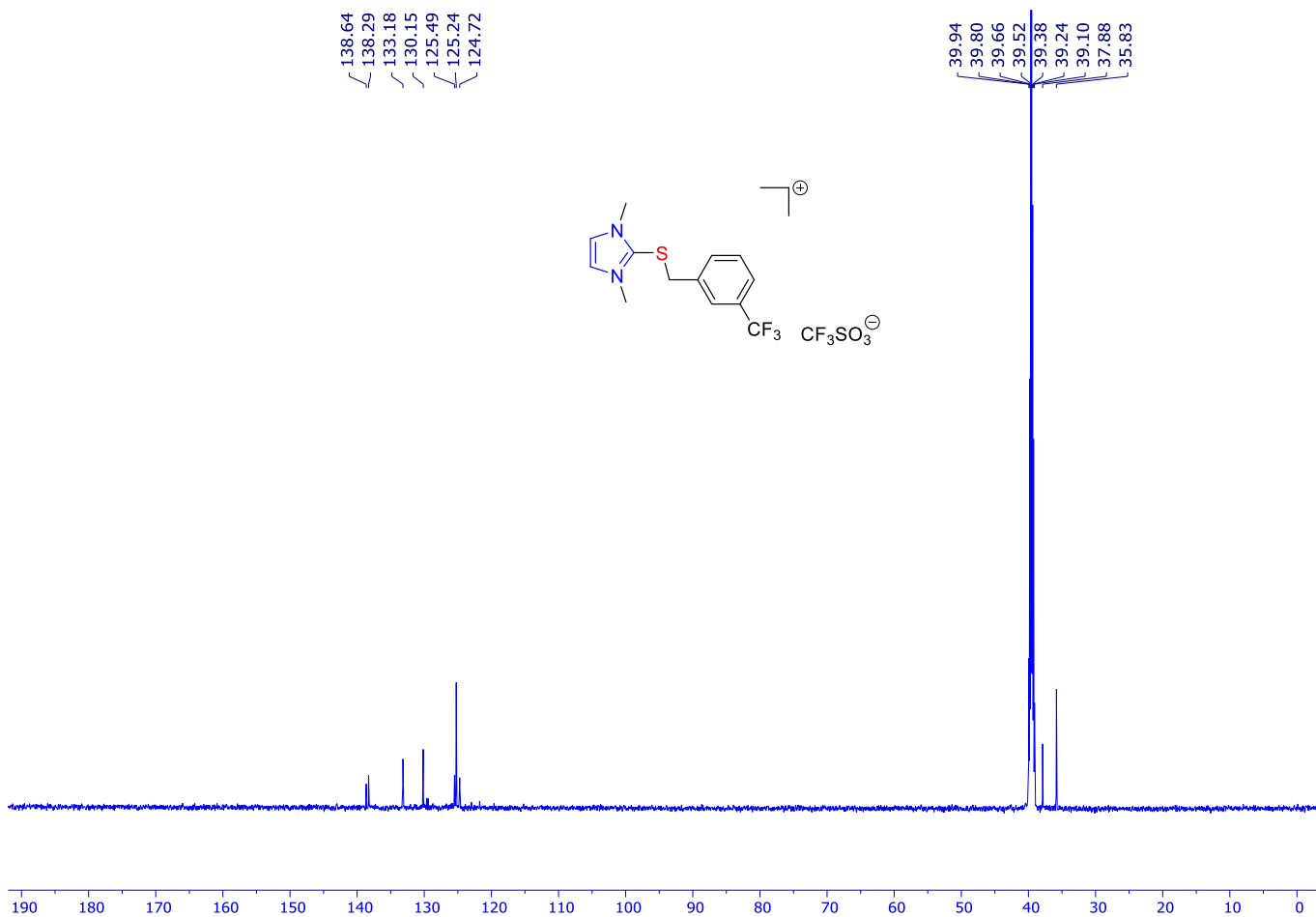


Fig. S63. ^{13}C NMR spectrum of compound **7d** ($\text{DMSO}-d_6$, 600 MHz)

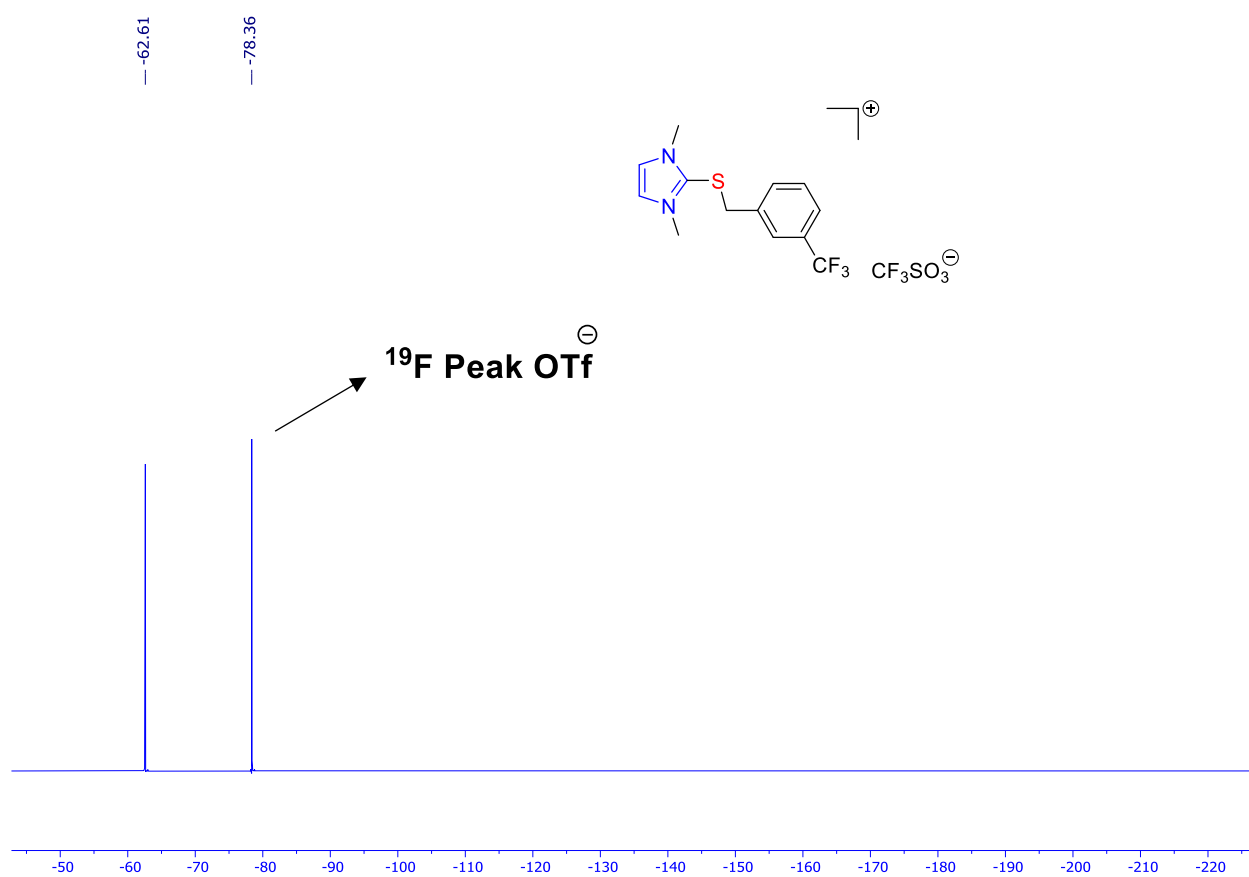


Fig. S64. ^{19}F NMR spectrum of compound **7d** (DMSO- d_6 , 600 MHz)

1,3-dimethyl-2-((4-nitrobenzyl)thio)-1H-imidazol-3-ium Triflate (8d)

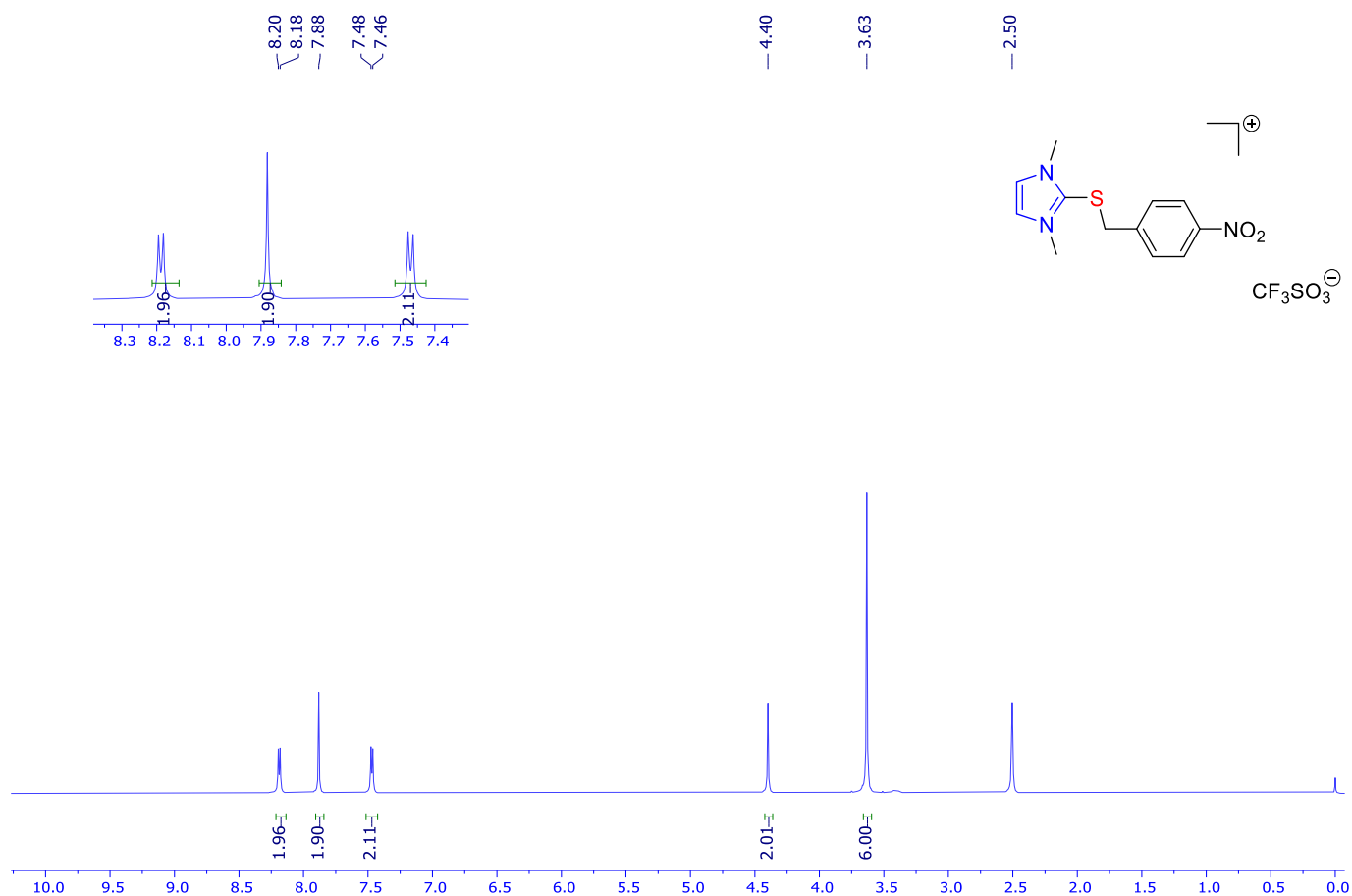


Fig. S65. ¹H NMR spectrum of compound **8d** (DMSO-*d*₆, 600 MHz)

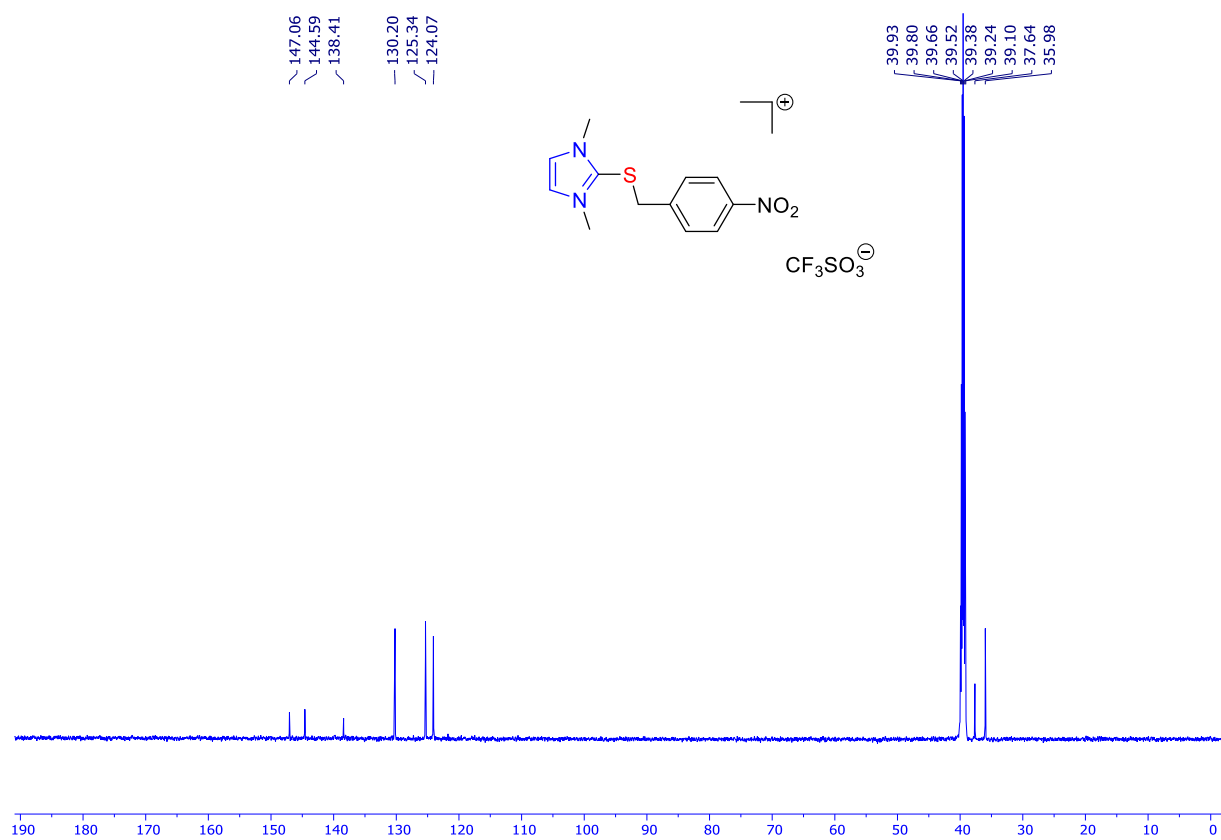


Fig. S66. ^{13}C NMR spectrum of compound **8d** (DMSO- d_6 , 600 MHz)

1,3-dimethyl-2-((2-chloro-4-fluorobenzyl)sulfinyl)-1H-imidazol-3-ium Triflate (1e)

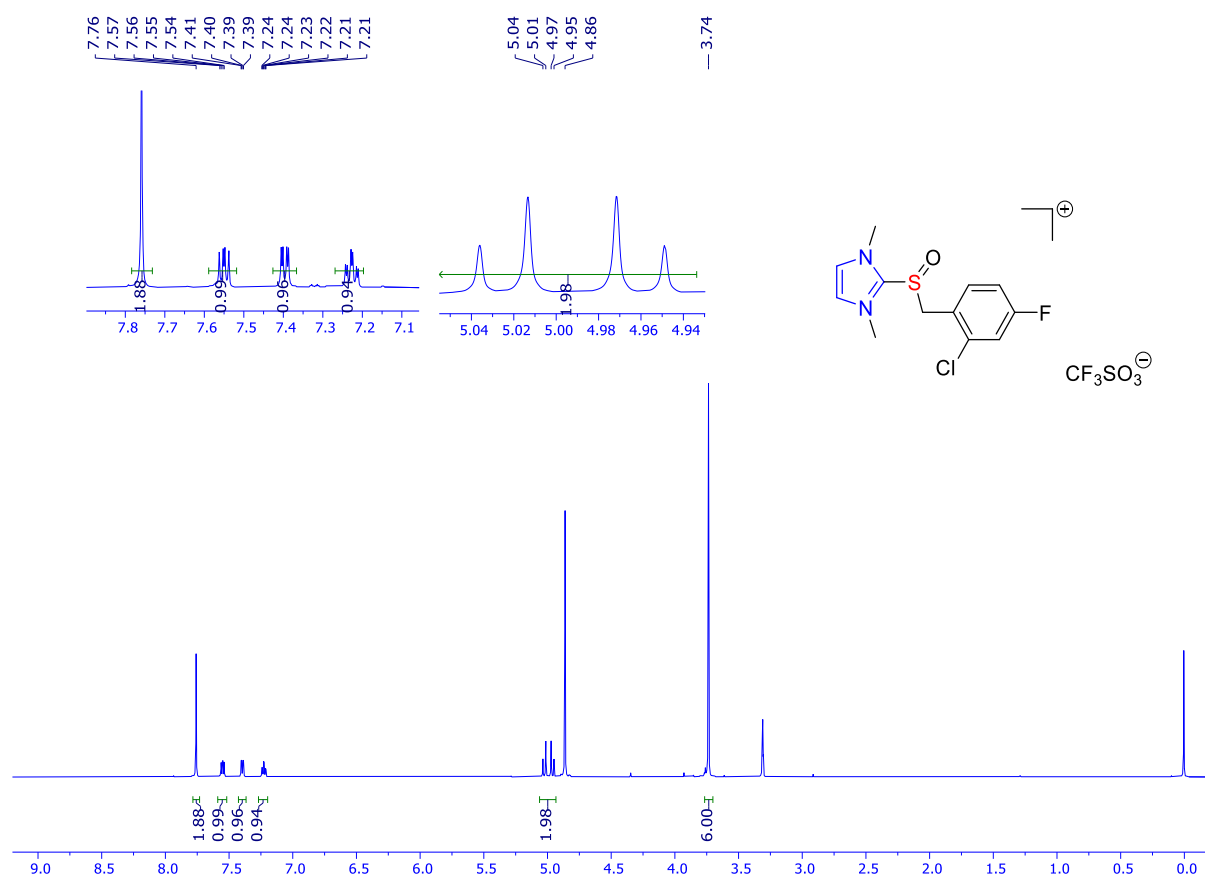


Fig. S67. ¹H NMR spectrum of compound **1e** (CD₃OD, 600 MHz)

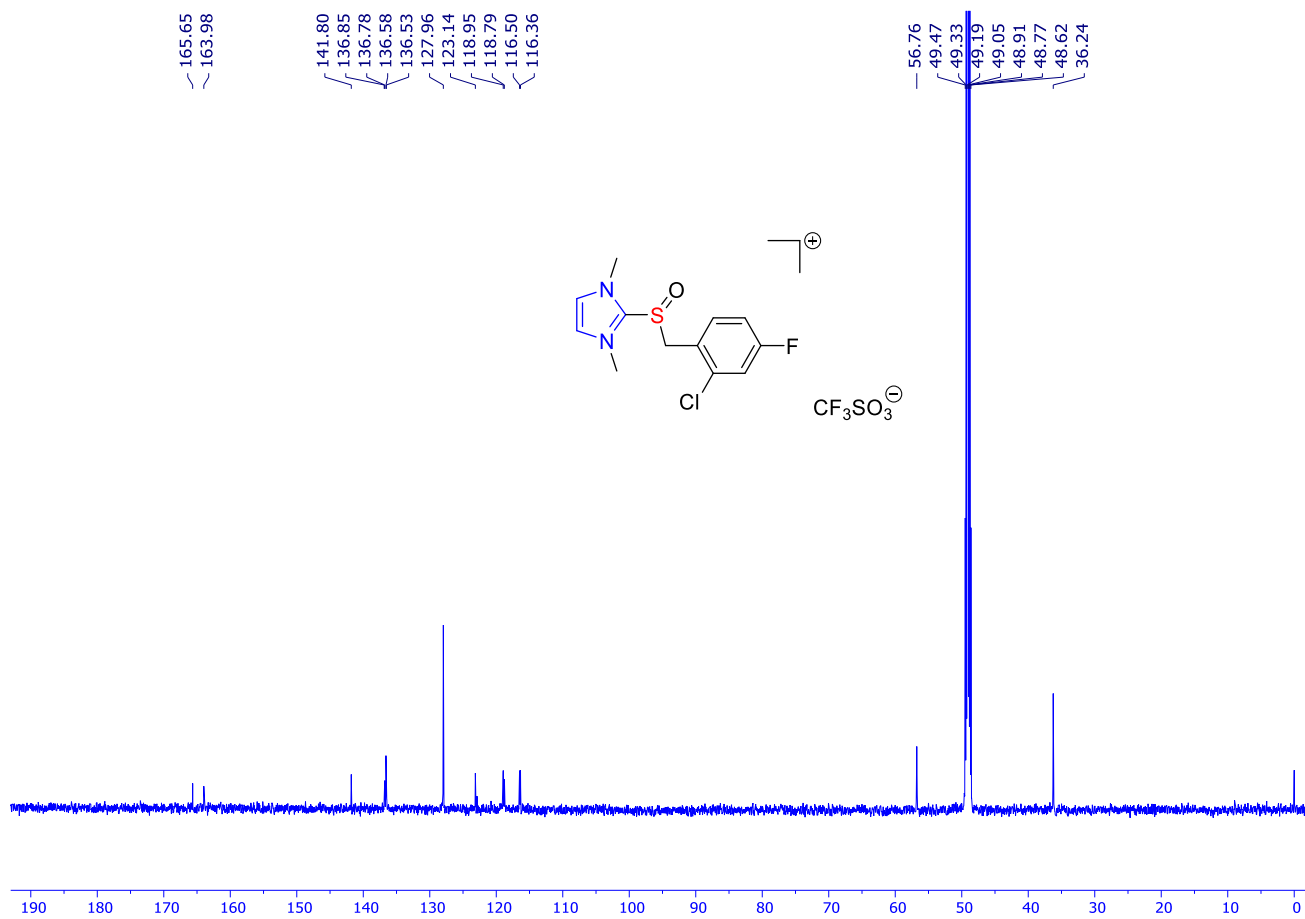


Fig. S68. ^{13}C NMR spectrum of compound **1e** (CD_3OD , 600 MHz)

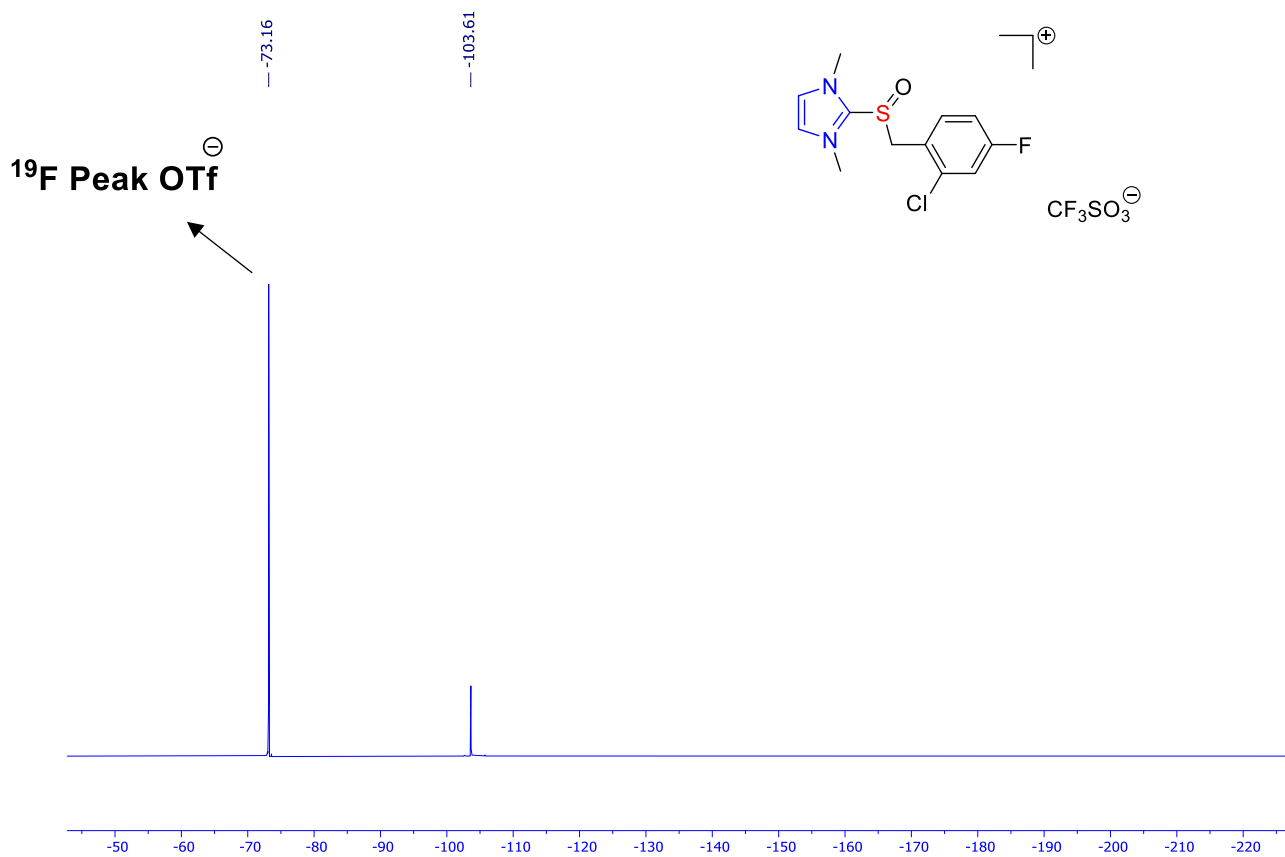


Fig. S69. ^{19}F NMR spectrum of compound **1e** (CD_3OD , 600 MHz)

1,3-dimethyl-2-(benzylsulfinyl)-1H-imidazol-3-ium Triflate (2e)

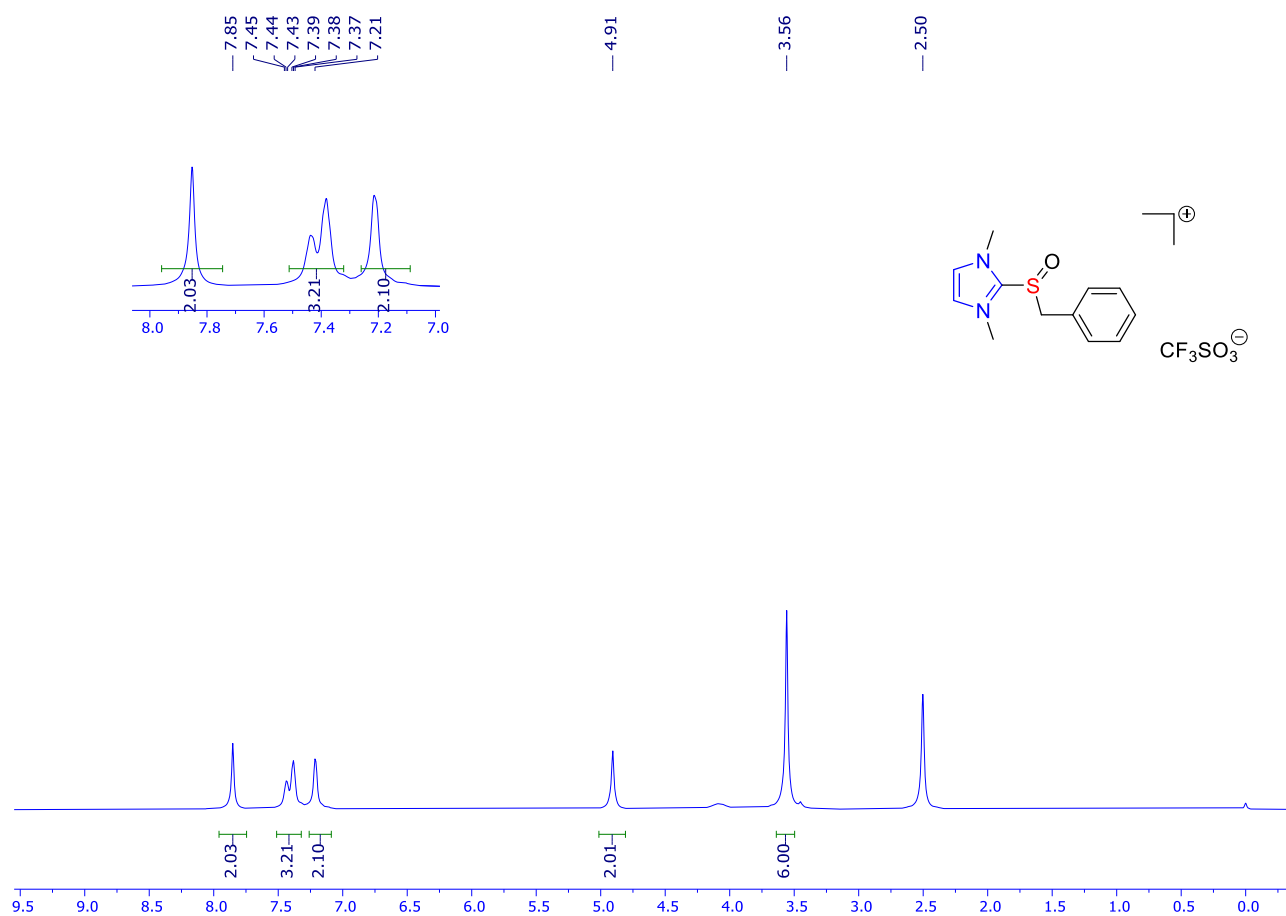


Fig. S70. ¹H NMR spectrum of compound **2e** (DMSO-*d*₆, 600 MHz)

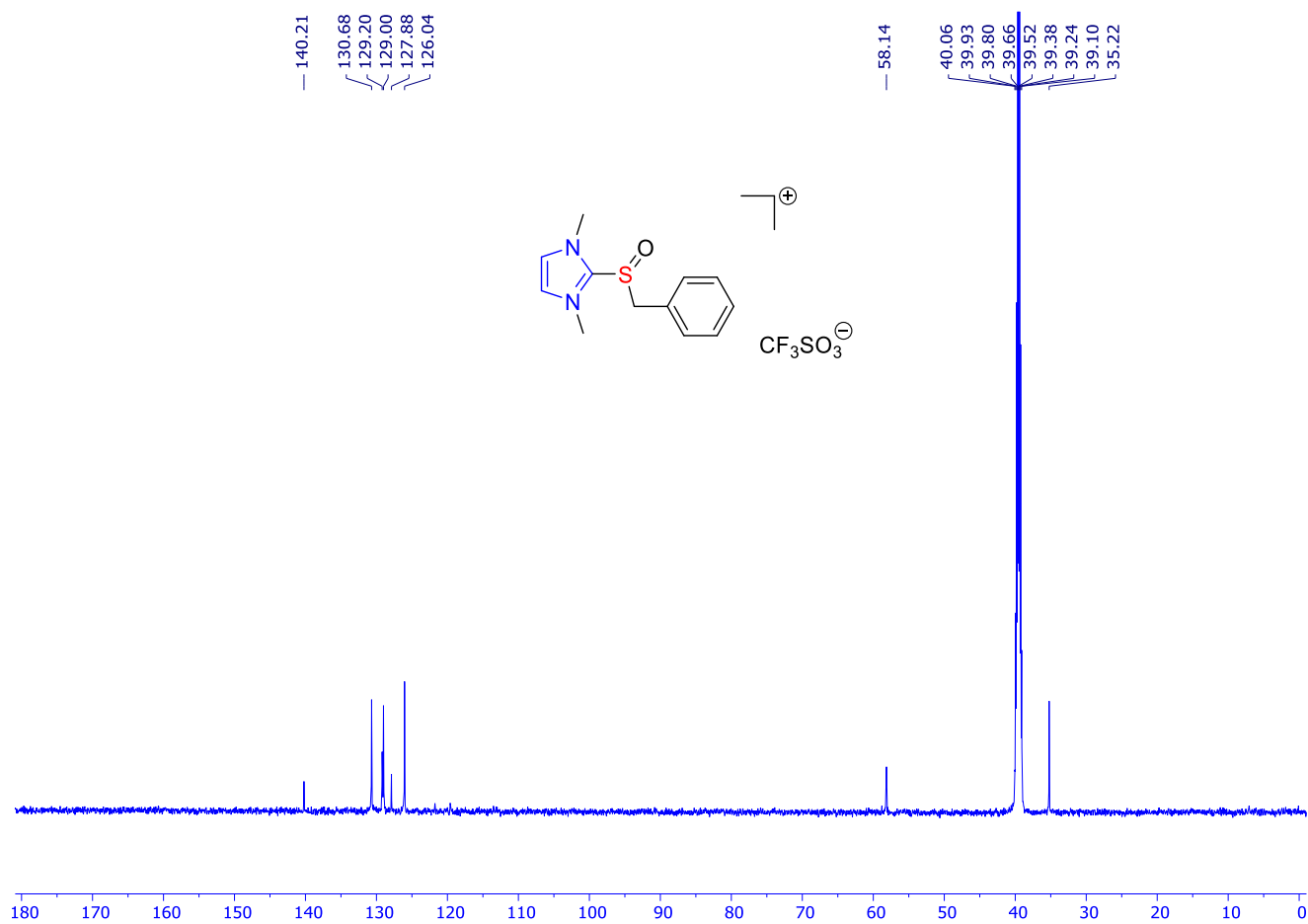


Fig. S71. ^{13}C NMR spectrum of compound **2e** ($\text{DMSO-}d_6$, 600 MHz)

1,3-dimethyl-2-(benzylsulfinyl)-1H-imidazol-3-ium Triflate (2e)

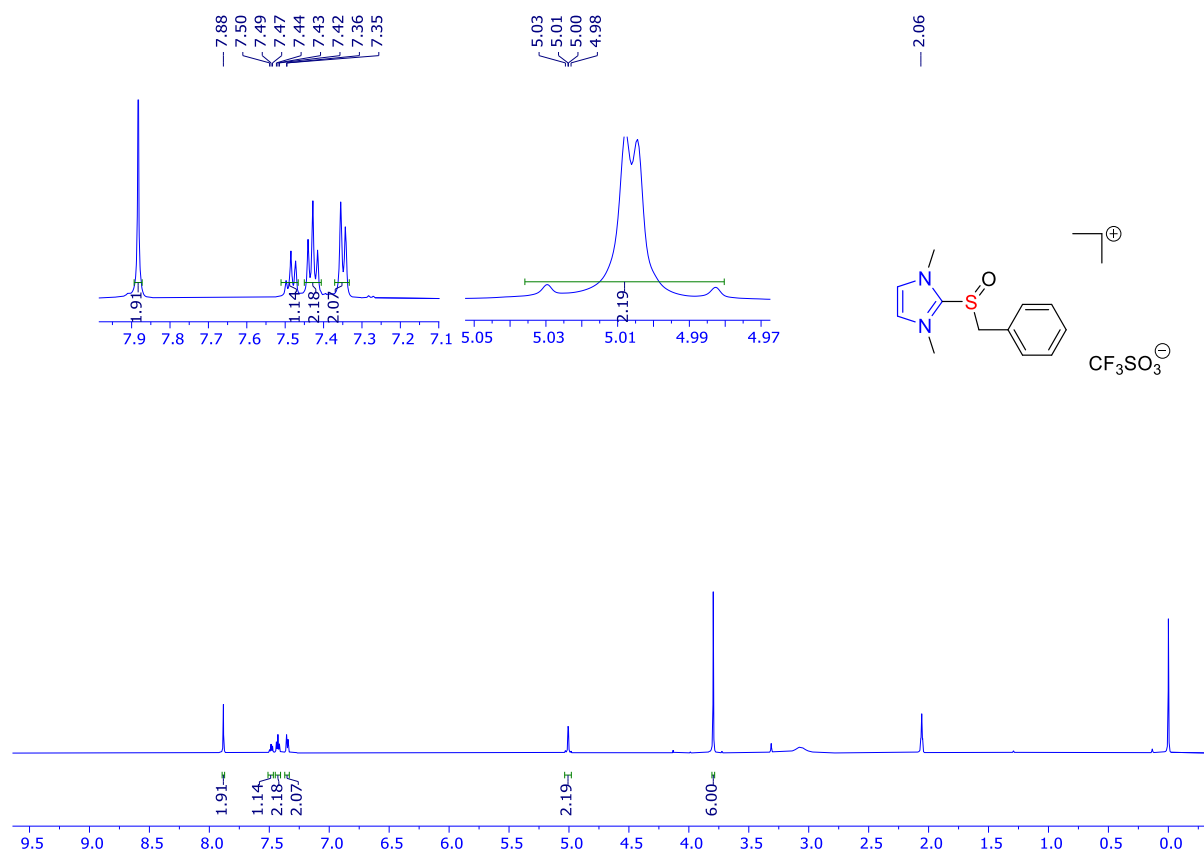


Fig. S72. ¹H NMR spectrum of compound **2e** ((CD₃)₂CO, 600 MHz)

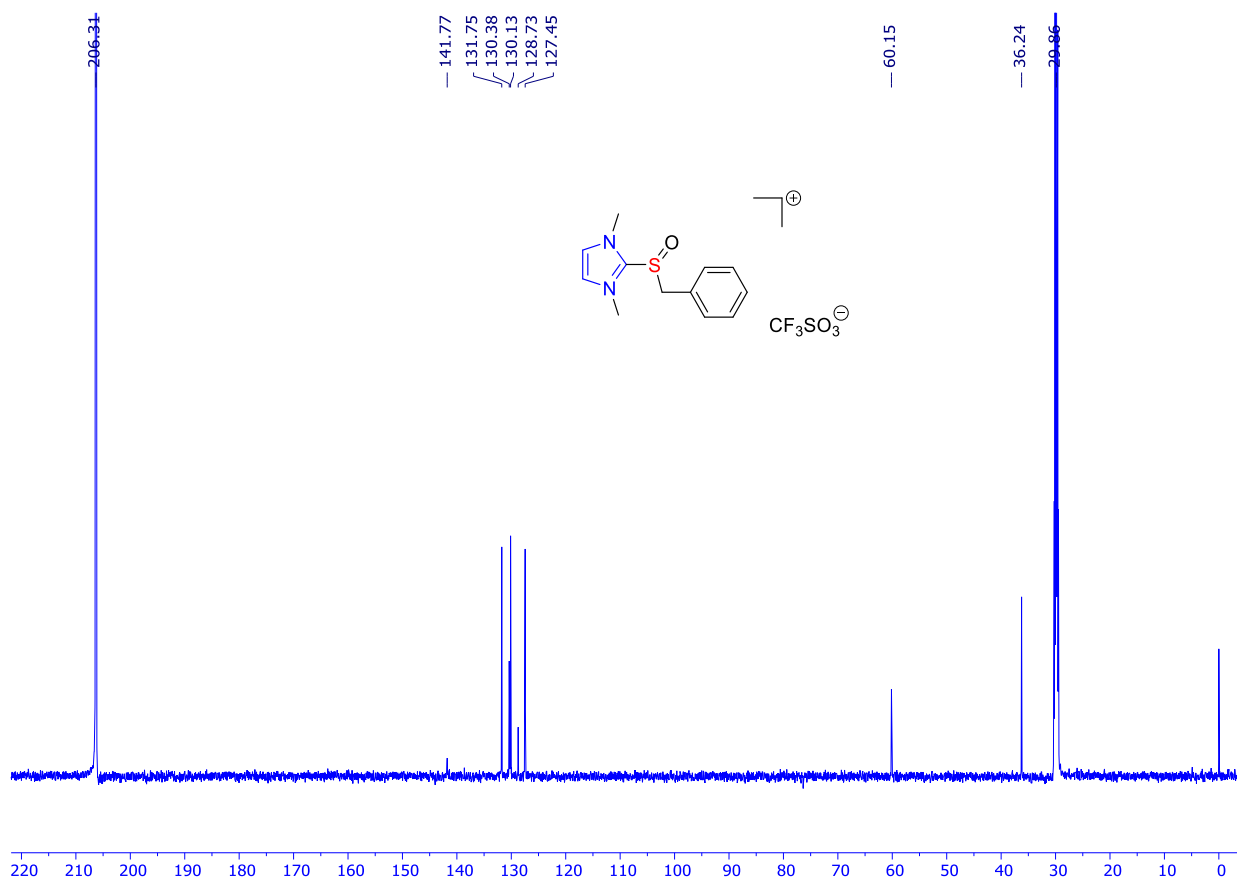


Fig. S73. ¹³C NMR spectrum of compound **2e** ((CD₃)₂CO, 600 MHz)

1,3-dimethyl-2-((4-bromobenzyl)sulfinyl)-1H-imidazol-3-ium Triflate (3e)

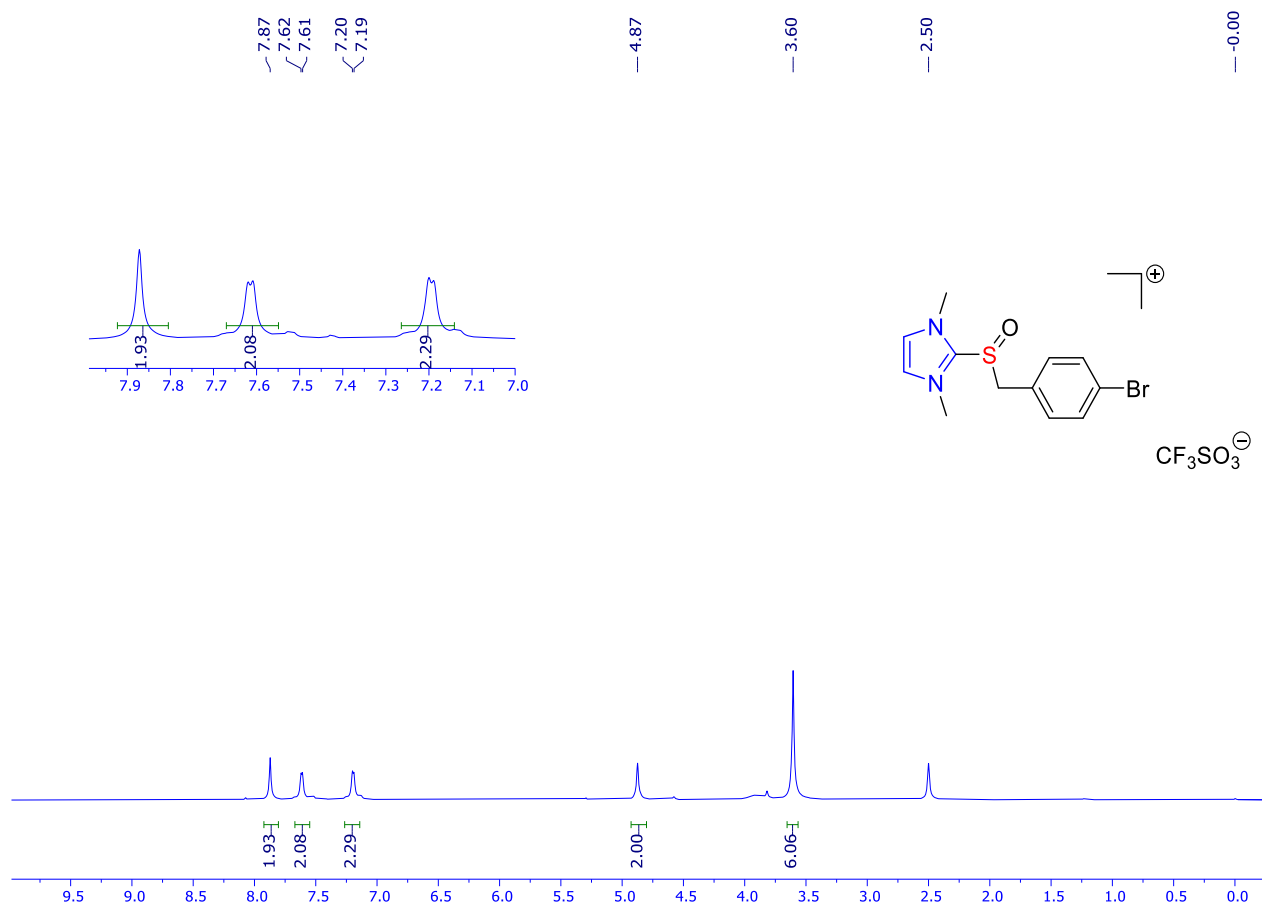


Fig. S74. ¹H NMR spectrum of compound 3e (DMSO-*d*₆, 600 MHz)

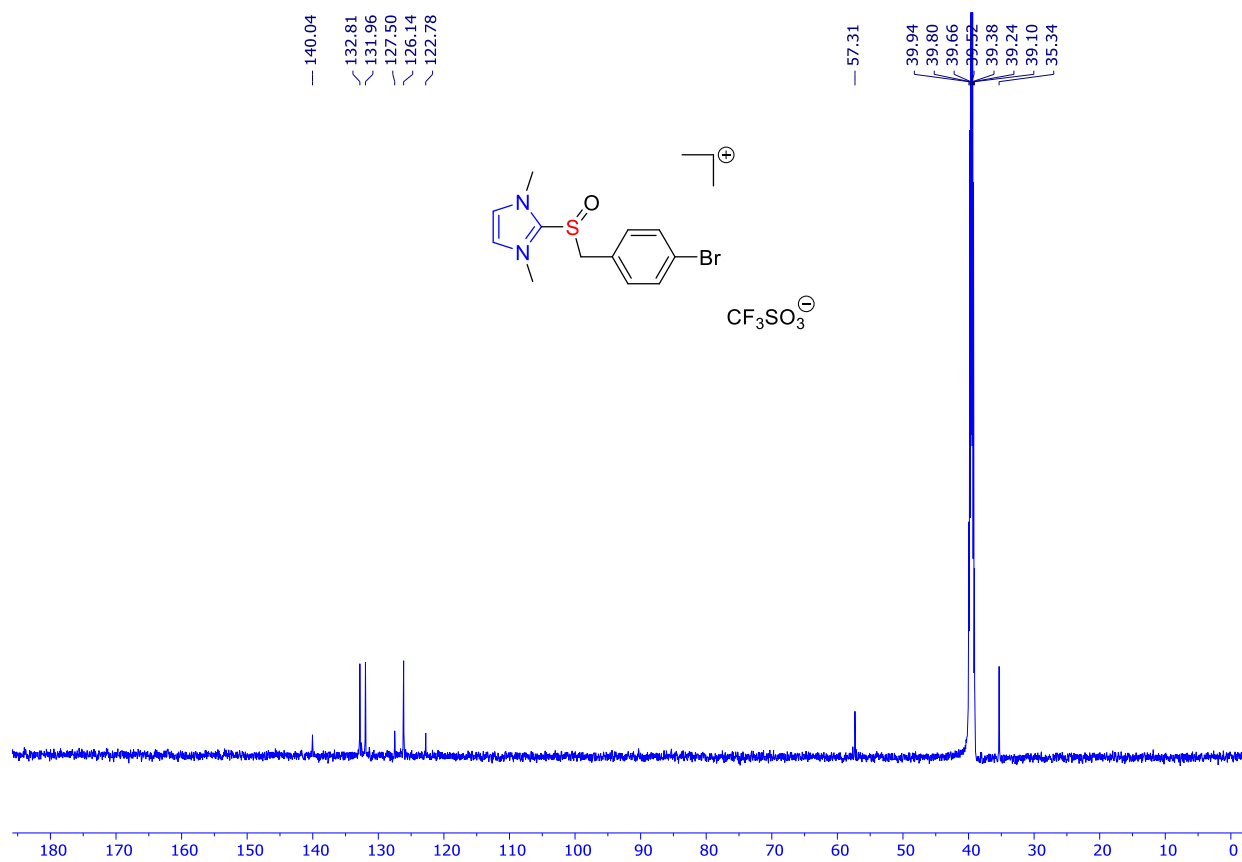


Fig. S75. ^{13}C NMR spectrum of compound **3e** (DMSO- d_6 , 600 MHz)

1,3-dimethyl-2-((4-bromobenzyl)sulfinyl)-1H-imidazol-3-ium Triflate (3e)

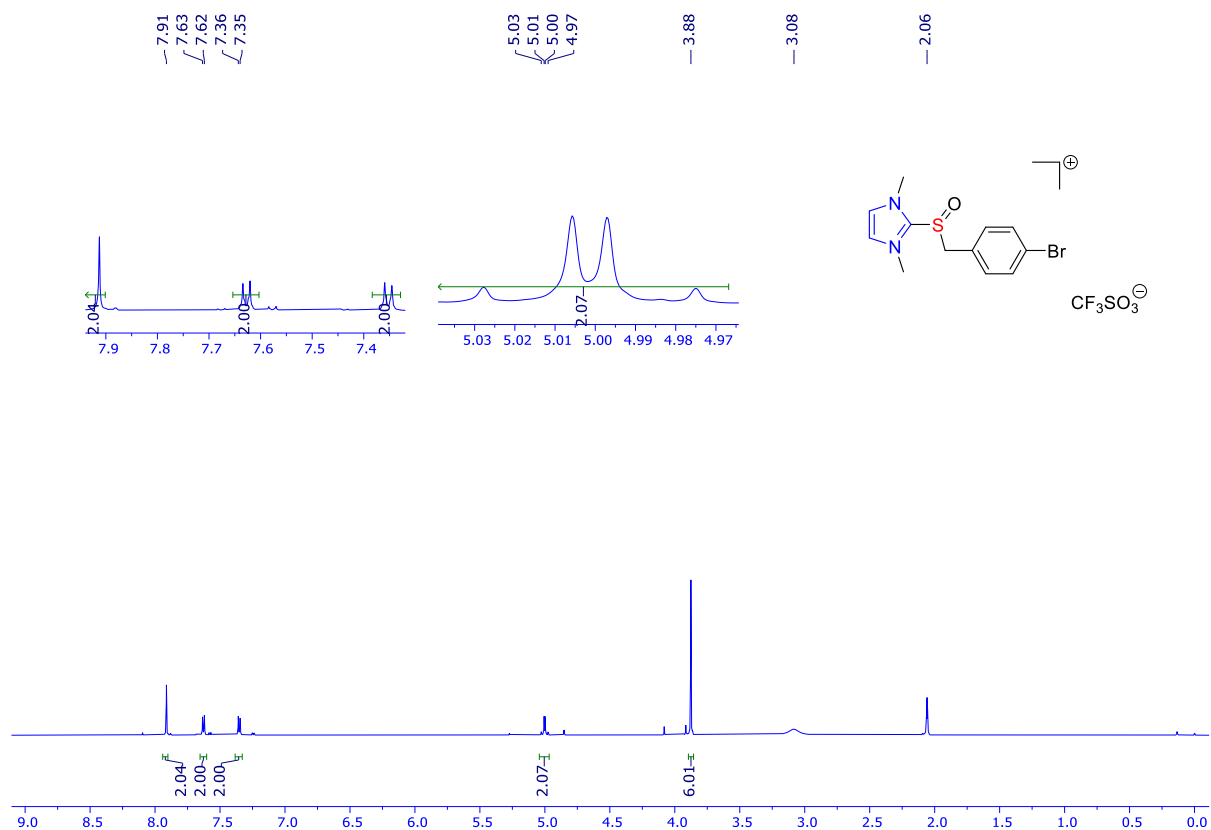


Fig. S76. ¹H NMR spectrum of compound **3e** ((CD₃)₂CO, 600 MHz)

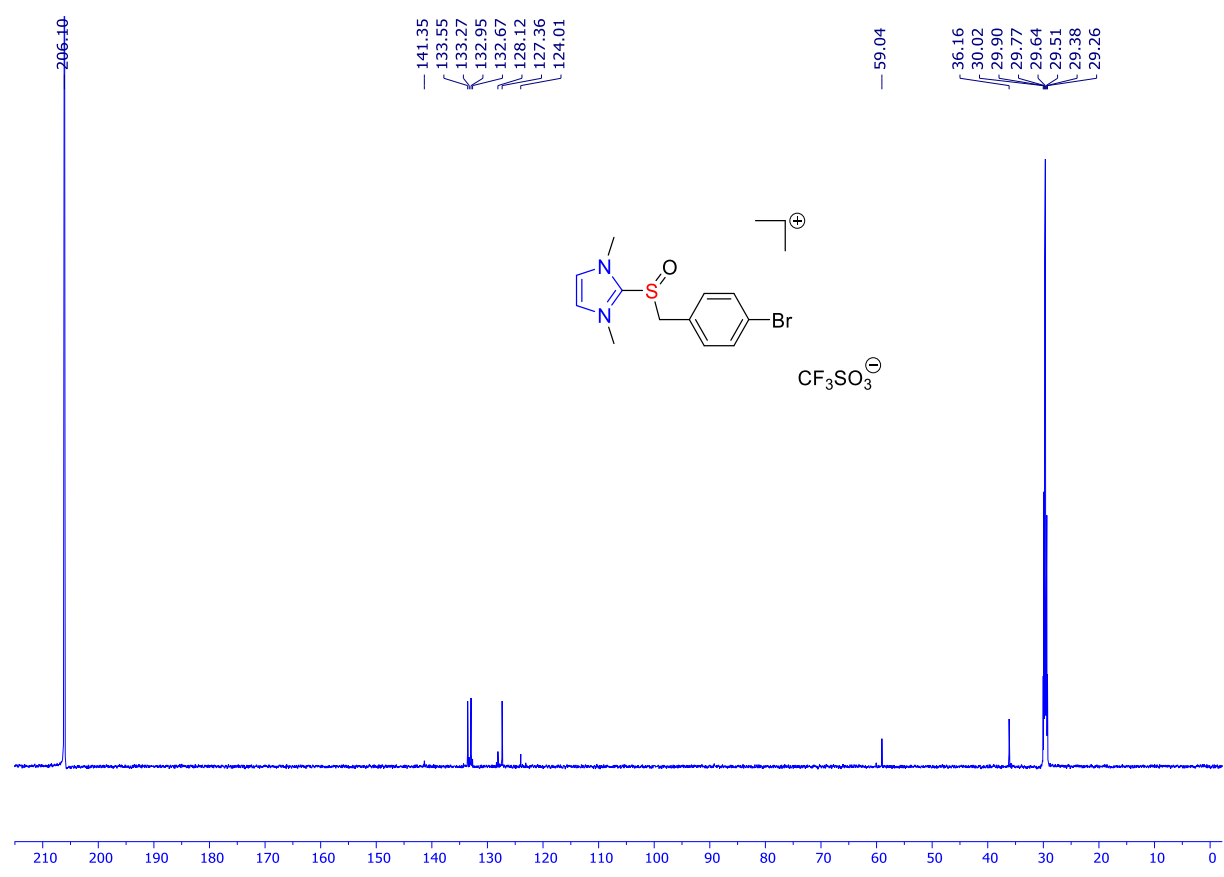


Fig. S77. ¹³C NMR spectrum of compound **3e** ((CD₃)₂CO, 600 MHz)

1,3-dimethyl-2-((2-fluoro-4-bromobenzyl)sulfinyl)-1H-imidazol-3-iumTriflate (4e)

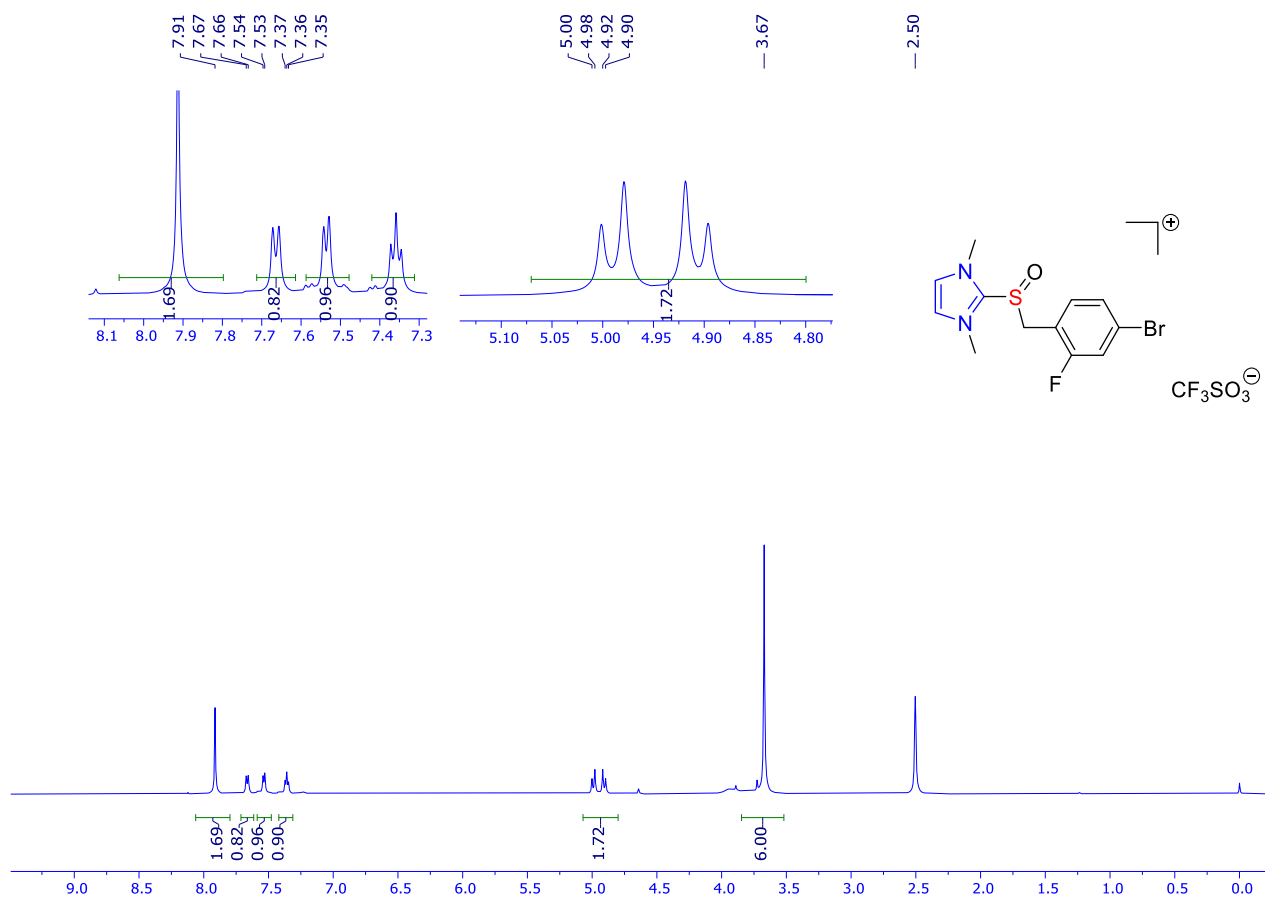


Fig. S78. ^1H NMR spectrum of compound **4e** ($\text{DMSO-}d_6$, 600 MHz)

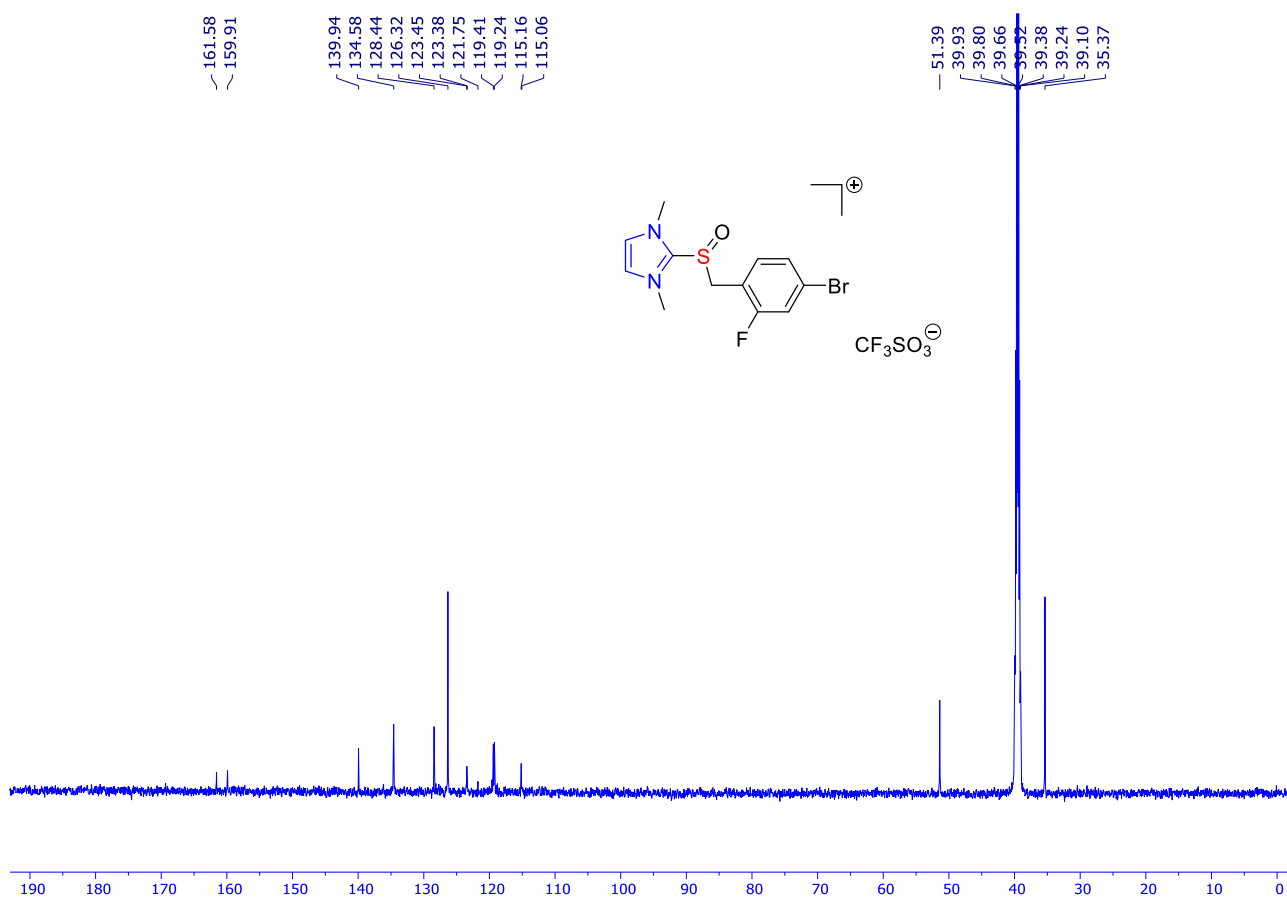


Fig. S79. ^{13}C NMR spectrum of compound **4e** ($\text{DMSO-}d_6$, 600 MHz)

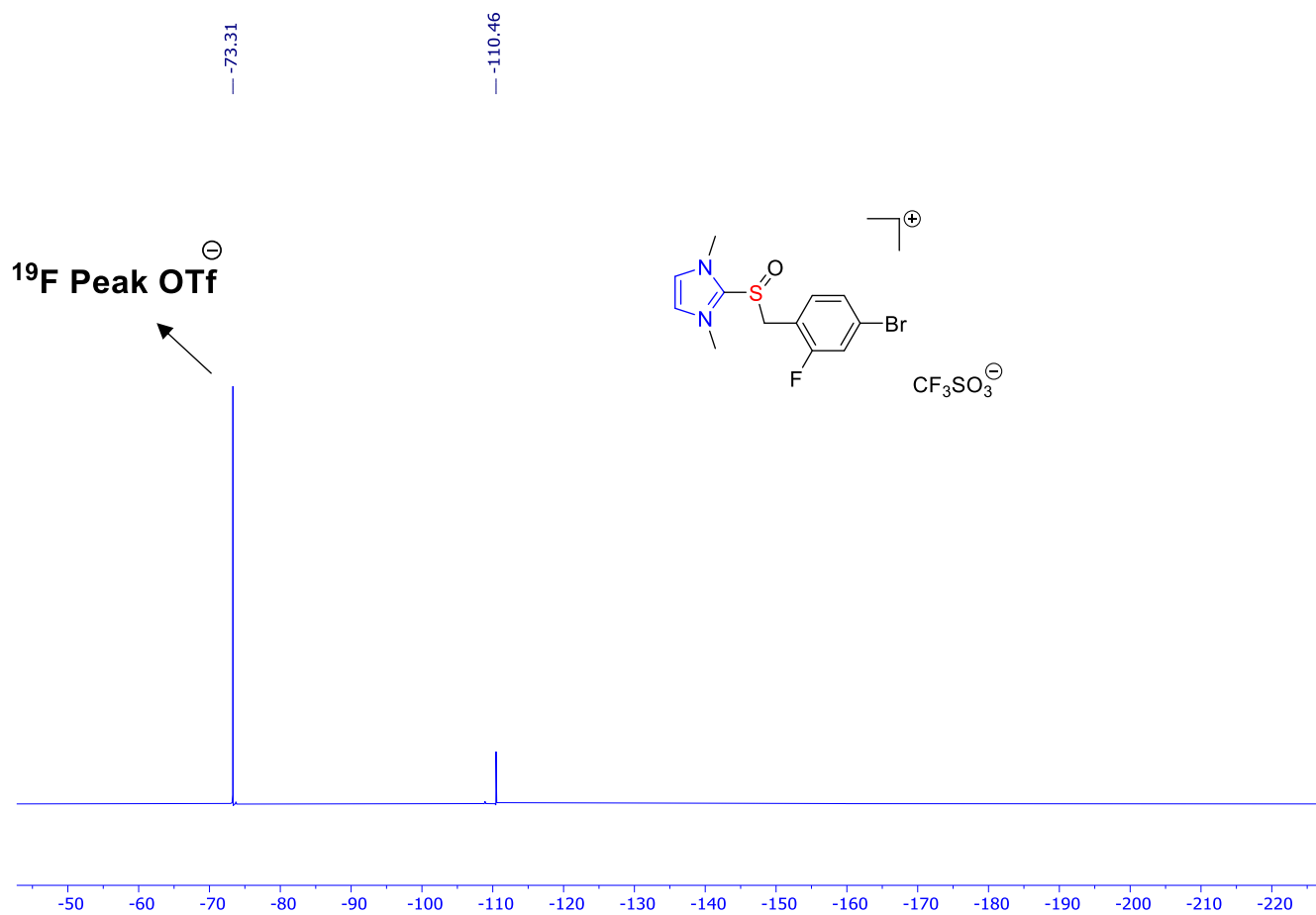


Fig. S80. ^{19}F NMR spectrum of compound **4e** ($\text{DMSO-}d_6$, 600 MHz)

1,3-dimethyl-2-((4-(trifluoromethoxy)benzyl)sulfinyl)-1H-imidazol-3-iumTriflate (5e)

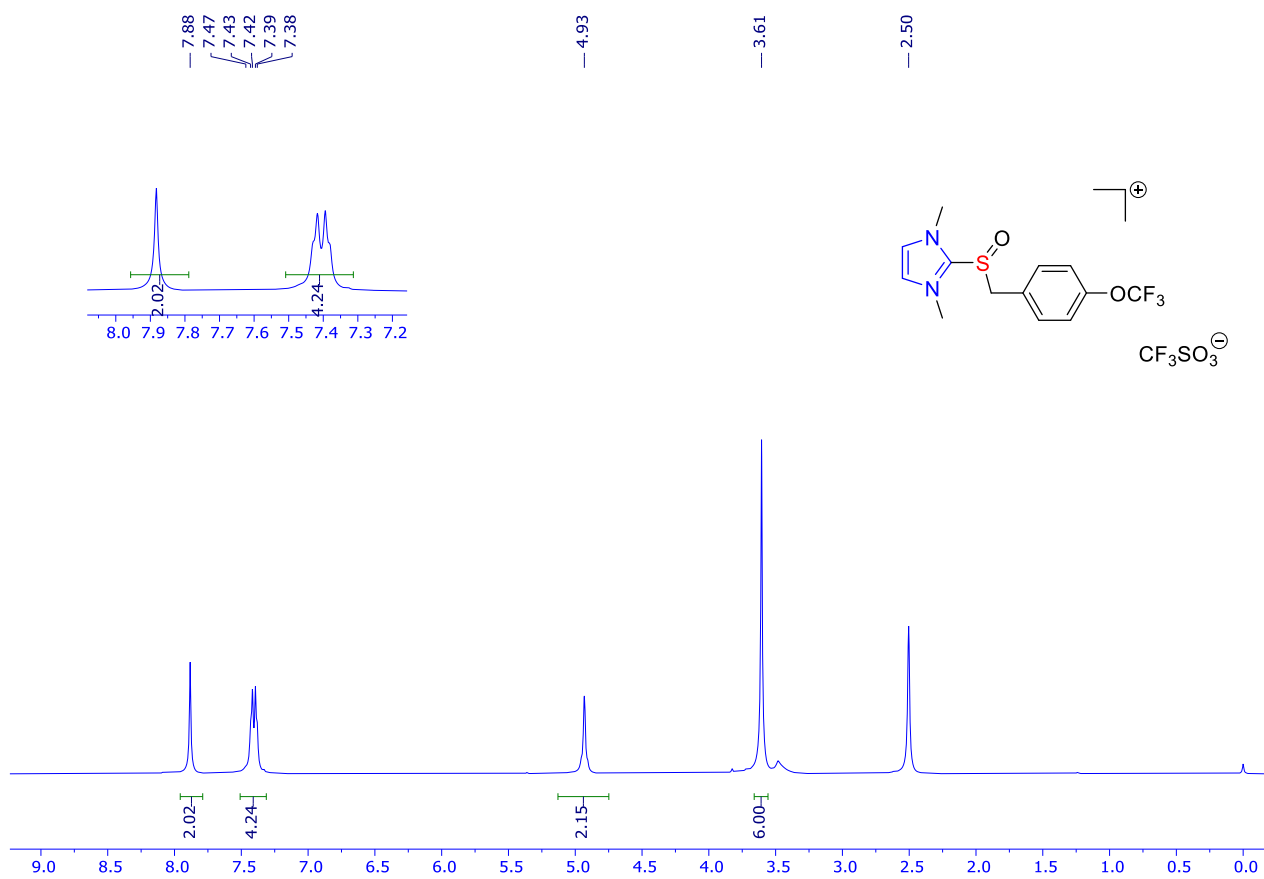


Fig. S81. ¹H NMR spectrum of compound **5e** (DMSO-*d*₆, 600 MHz)

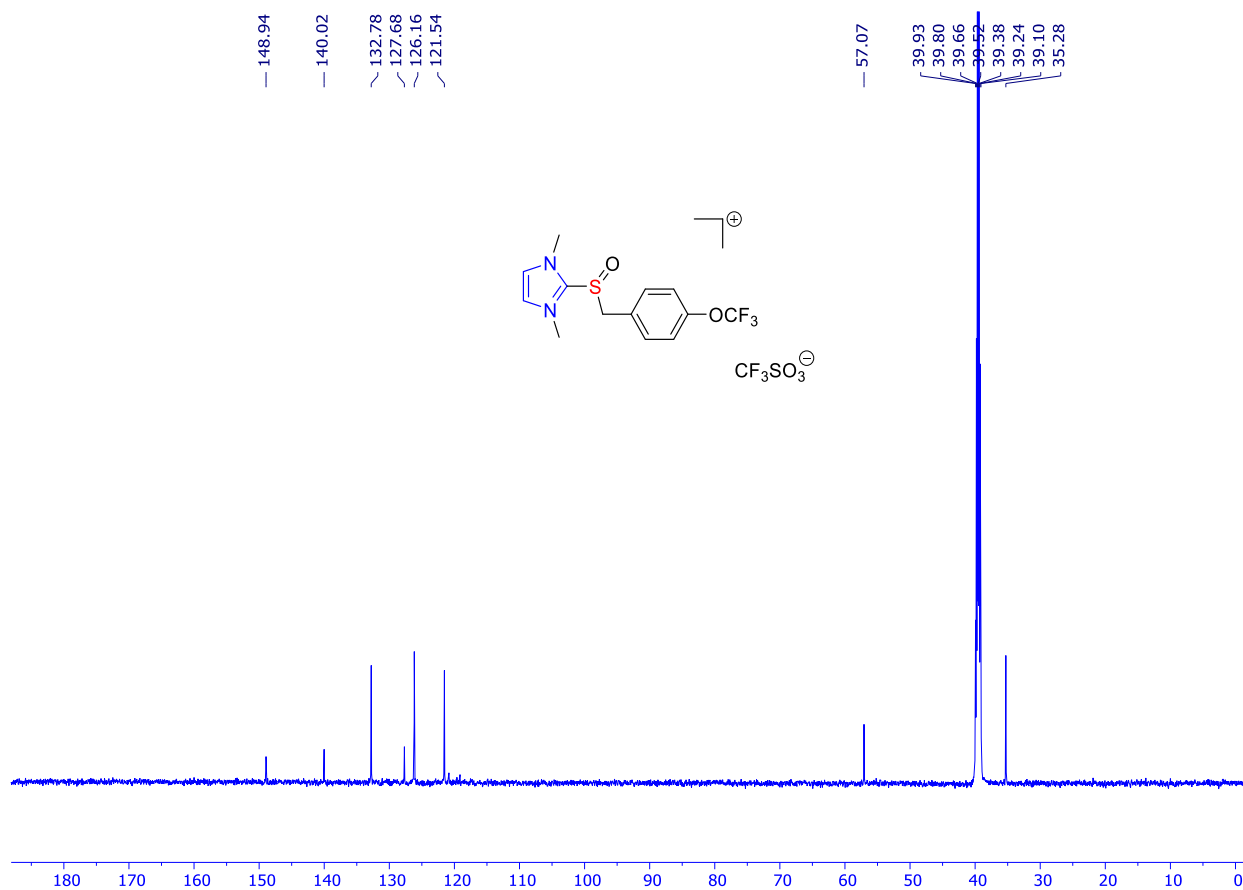


Fig. S82. ¹³C NMR spectrum of compound **5e** (DMSO-*d*₆, 600 MHz)

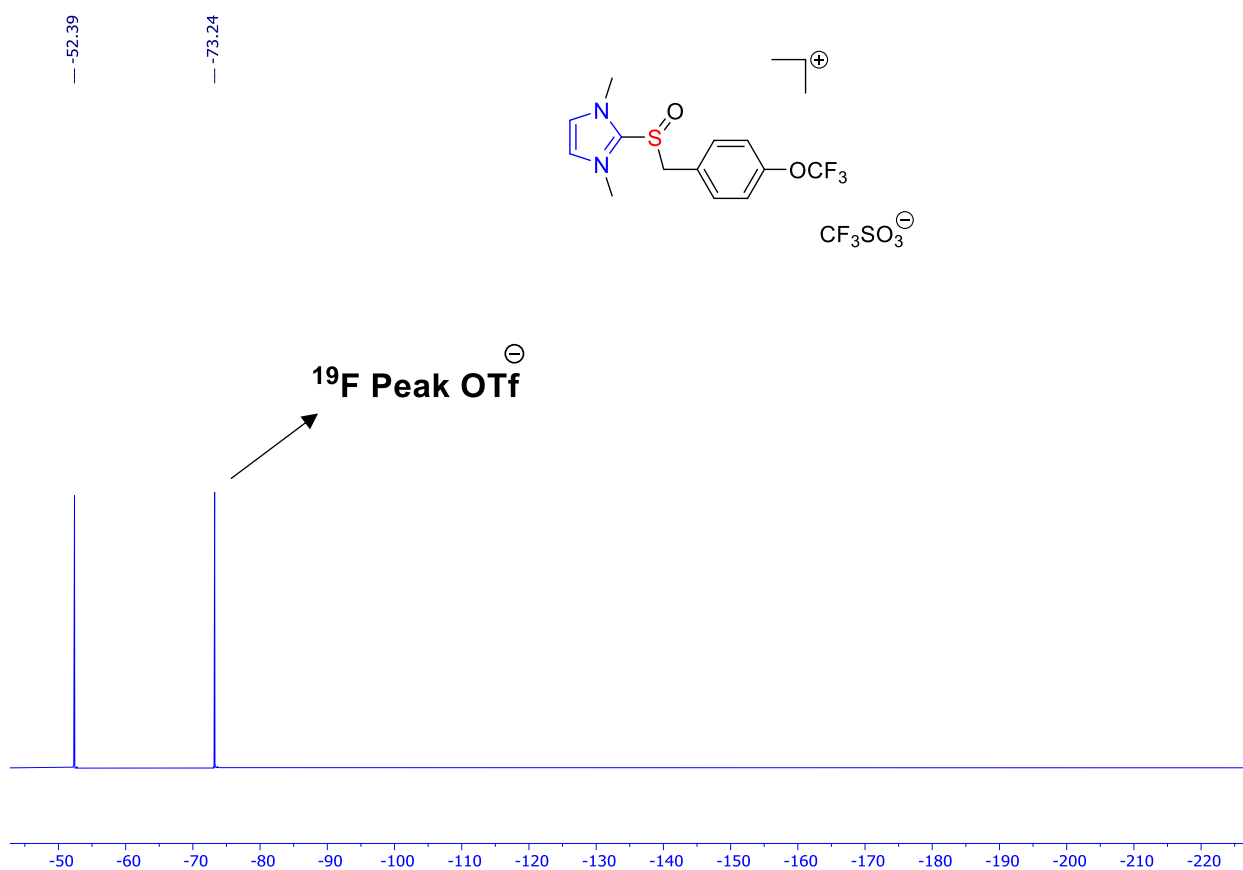


Fig. S83. ^{19}F NMR spectrum of compound **5e** ($\text{DMSO-}d_6$, 600 MHz)

1,3-dimethyl-2-((4-(trifluoromethoxy)benzyl)sulfinyl)-1H-imidazol-3-iumTriflate (5e)

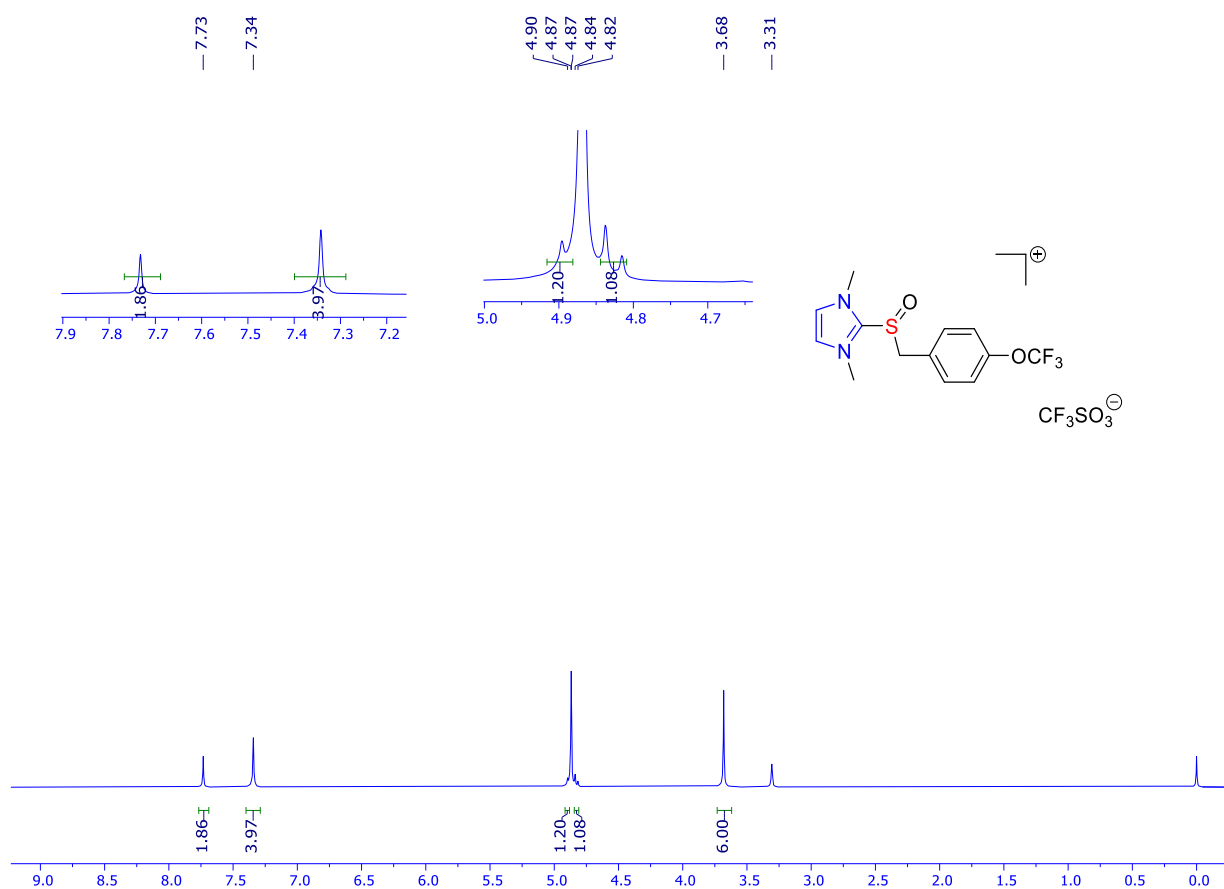


Fig. S84. ^1H NMR spectrum of compound **5e** (CD_3OD , 600 MHz)

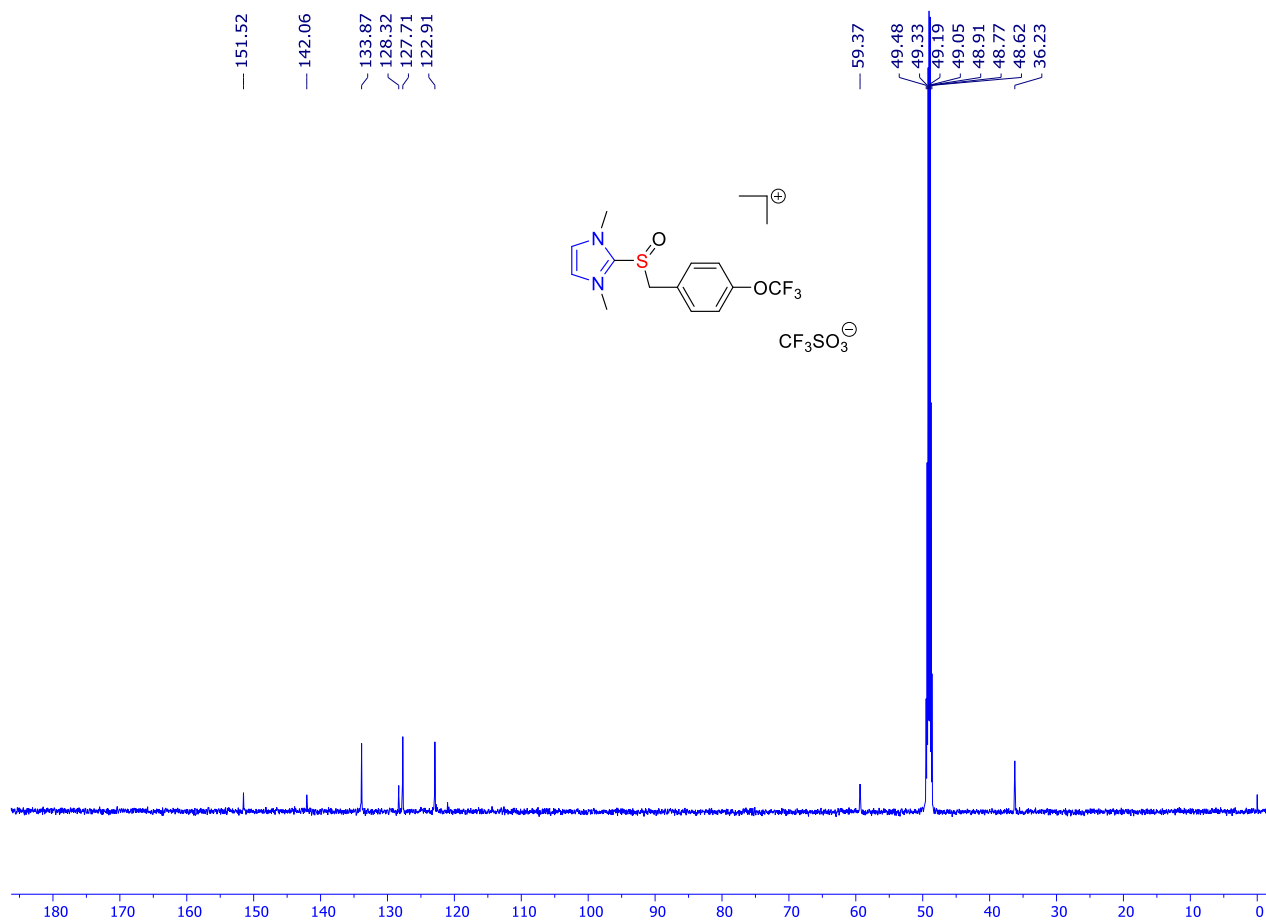


Fig. S85. ^{13}C NMR spectrum of compound **5e** (CD_3OD , 600 MHz)

1,3-dimethyl-2-((4-(tert-butyl)benzyl)sulfinyl)-1H-imidazol-3-ium Triflate (6e)

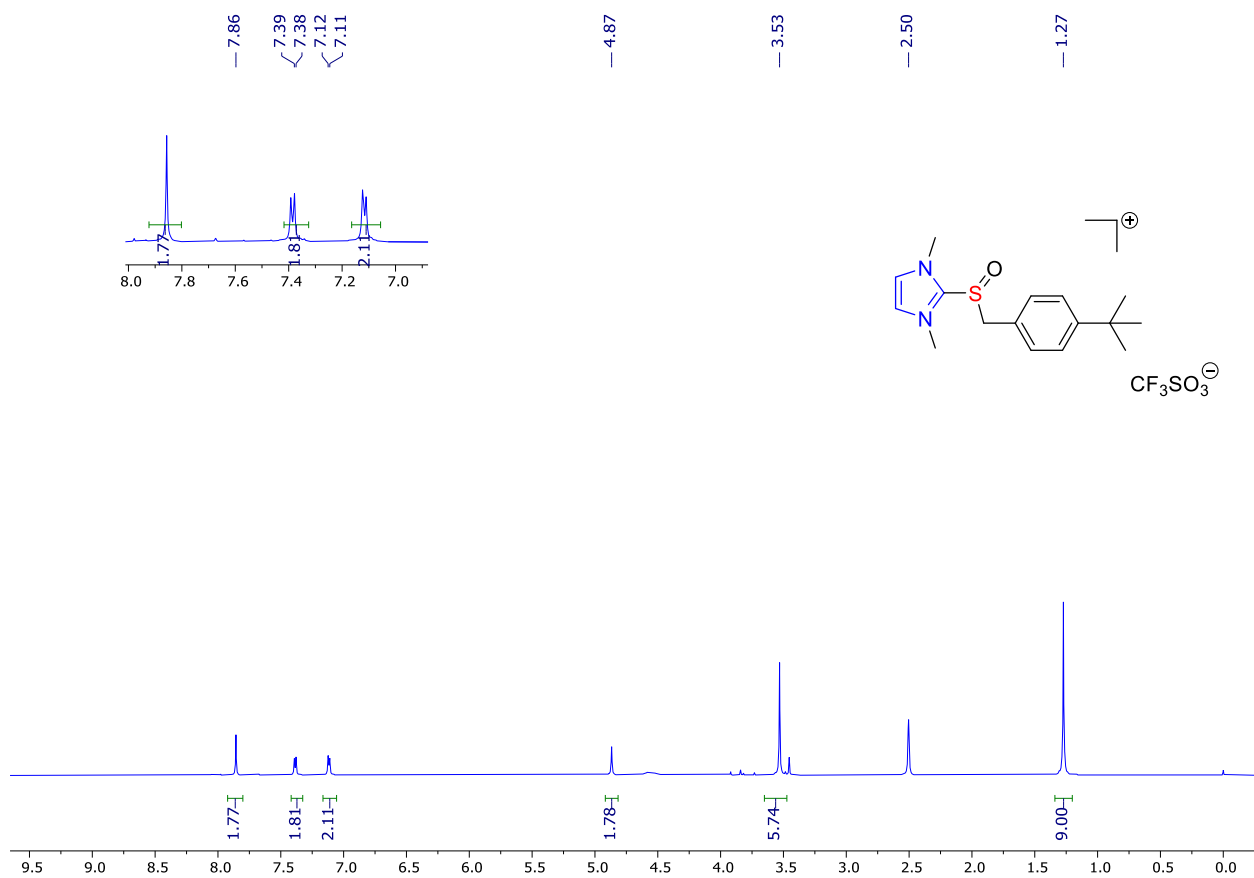


Fig. S86. ¹H NMR spectrum of compound **6e** (DMSO-*d*₆, 600 MHz)

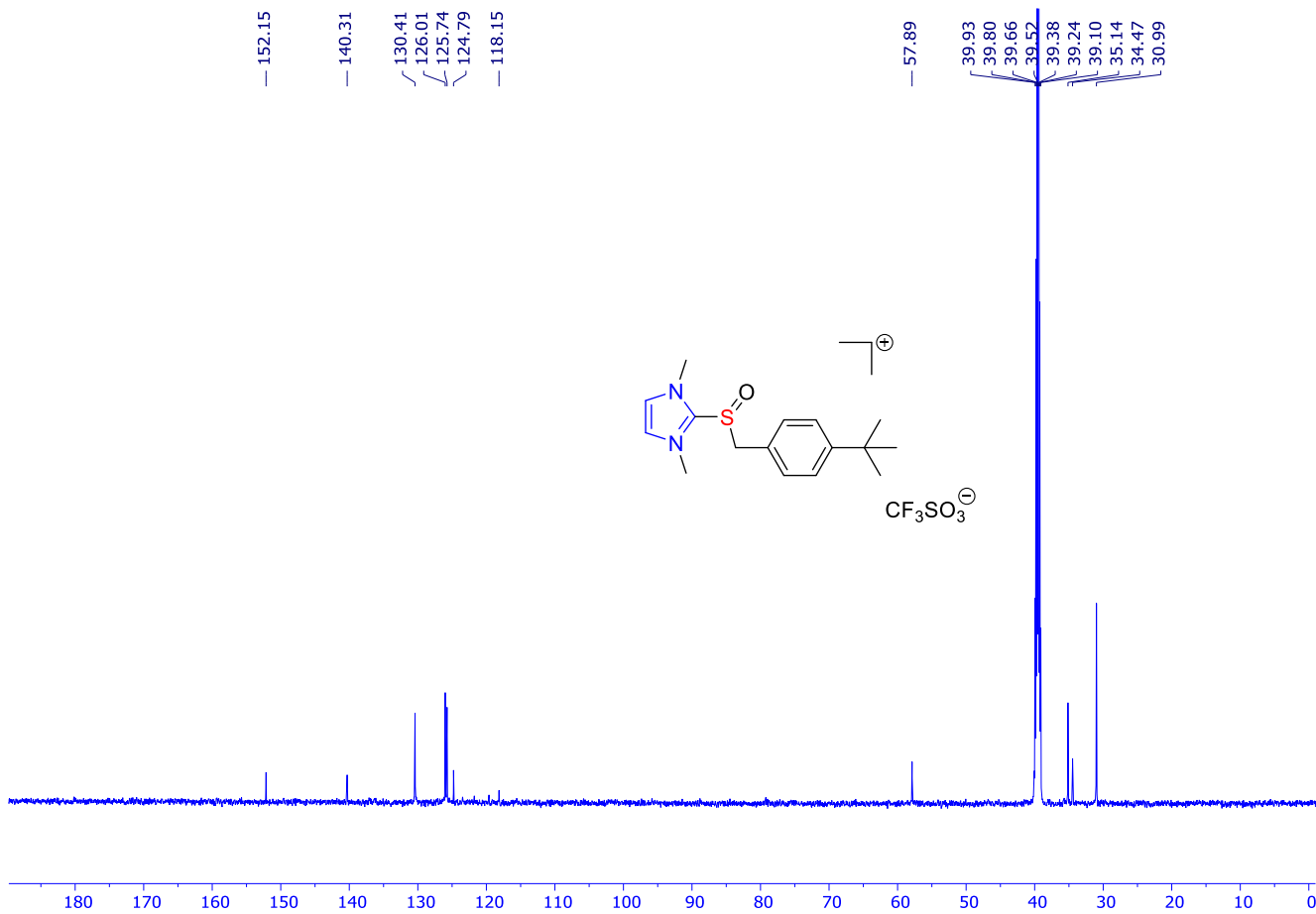


Fig. S87. ^{13}C NMR spectrum of compound **6e** (DMSO- d_6 , 600 MHz)

1,3-dimethyl-2-((4-(tert-butyl)benzyl)sulfinyl)-1H-imidazol-3-ium Triflate (6e)

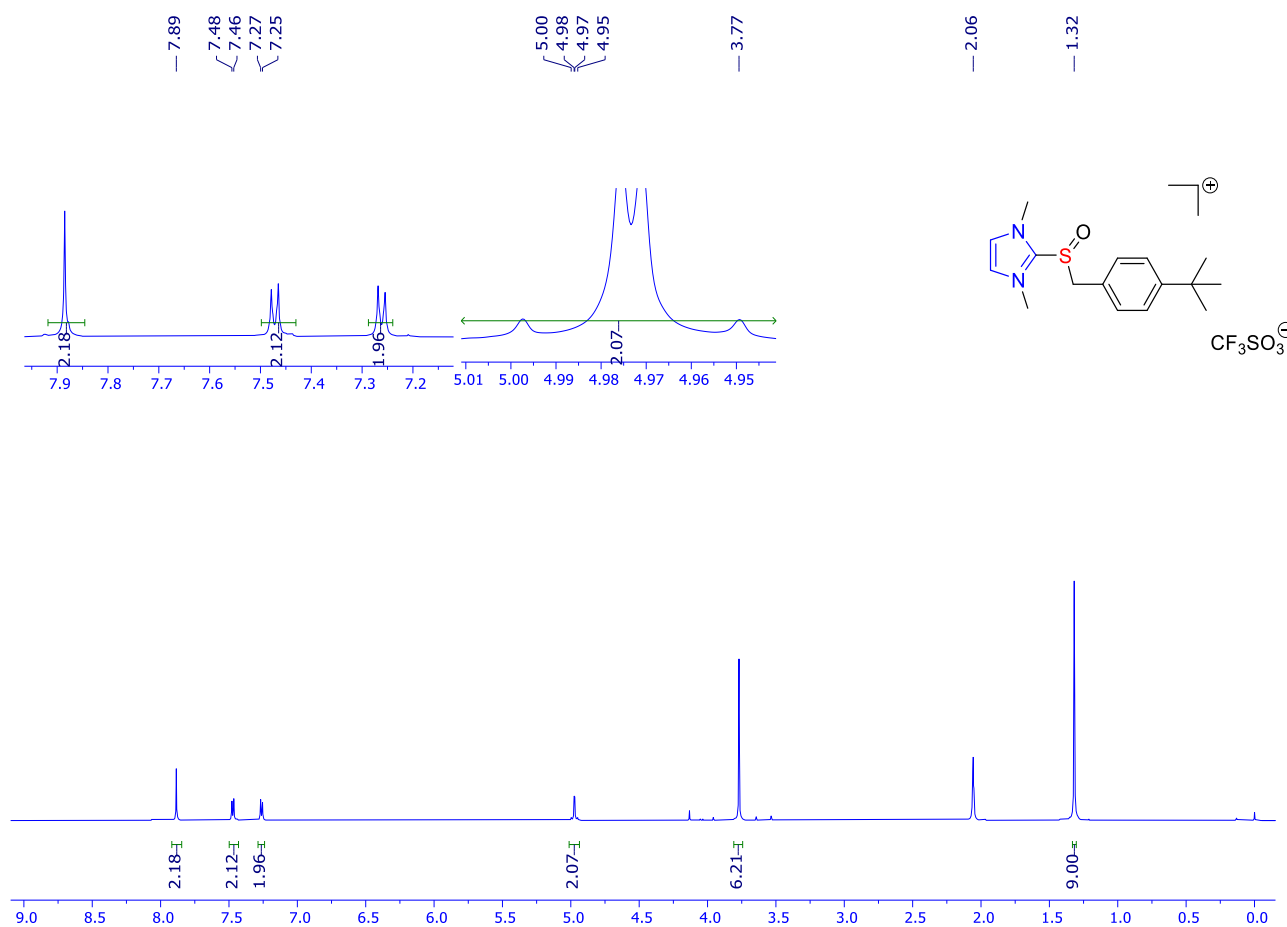


Fig. S88. ¹H NMR spectrum of compound **6e** ((CD₃)₂CO, 600 MHz)

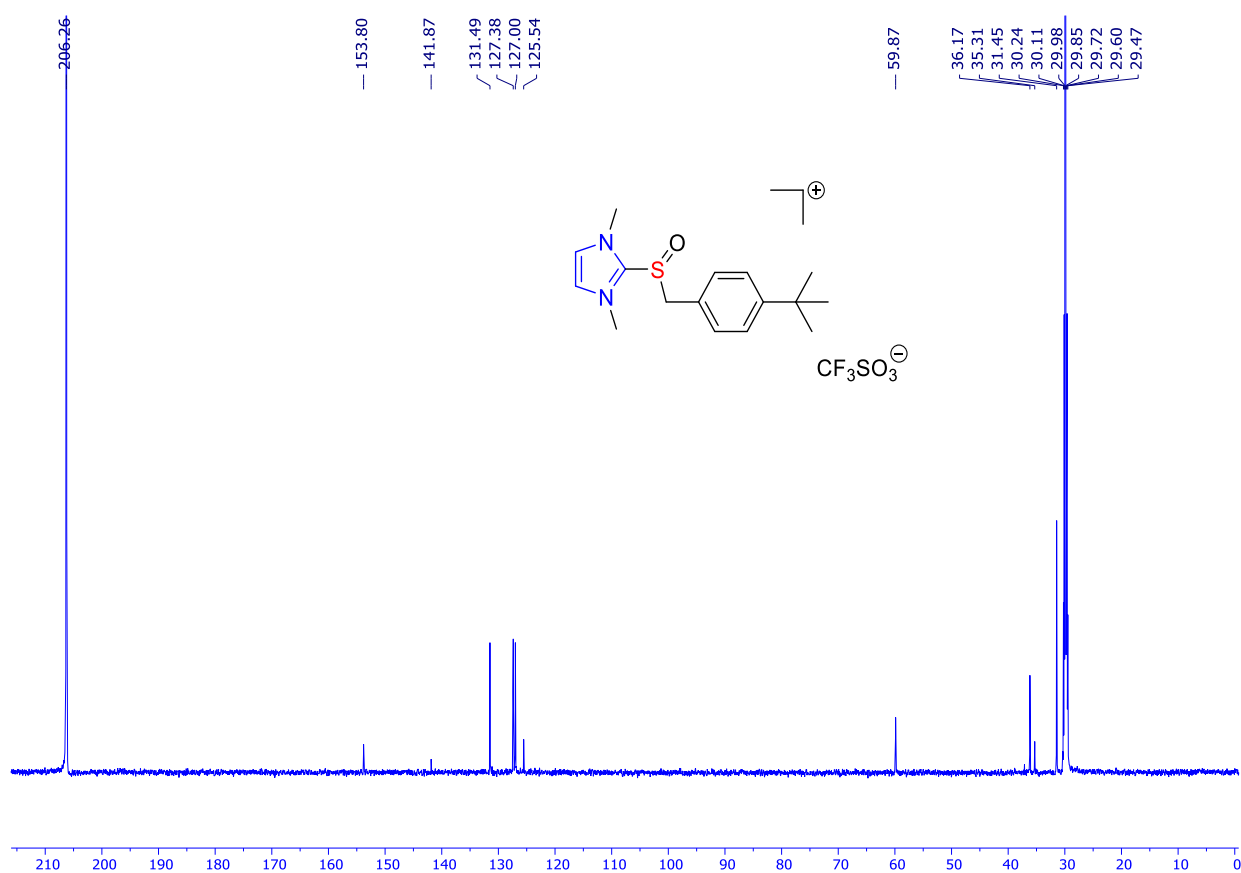


Fig. S89. ^{13}C NMR spectrum of compound **6e** ($(\text{CD}_3)_2\text{CO}$, 600 MHz)

1,3-dimethyl-2-((3-(trifluoromethyl)benzyl)sulfinyl)-1H-imidazol-3-ium Triflate (7e)

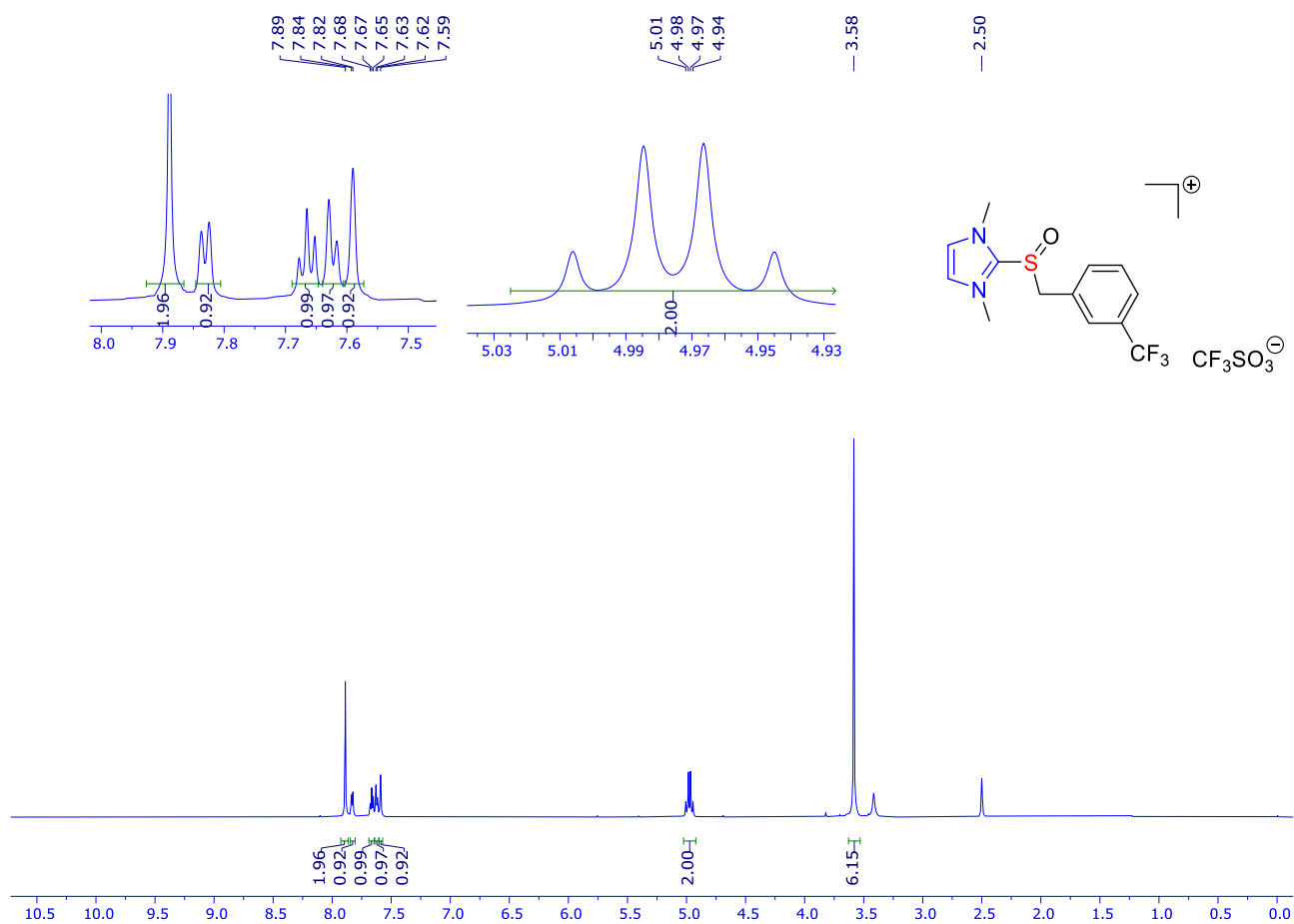


Fig. S90. ¹H NMR spectrum of compound 7e (DMSO-*d*₆, 600 MHz)

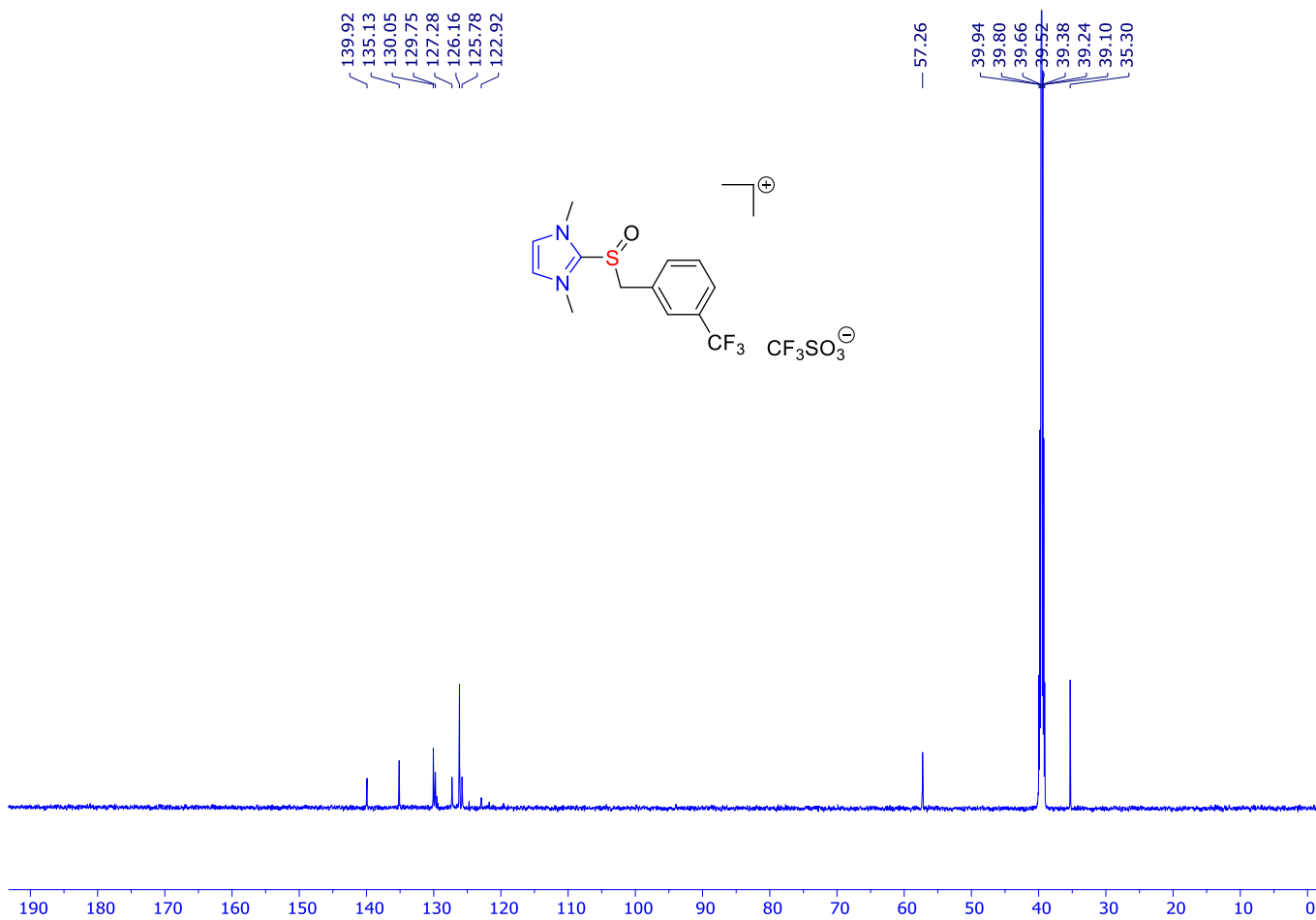


Fig. S91. ^{13}C NMR spectrum of compound **7e** (DMSO- d_6 , 600 MHz)

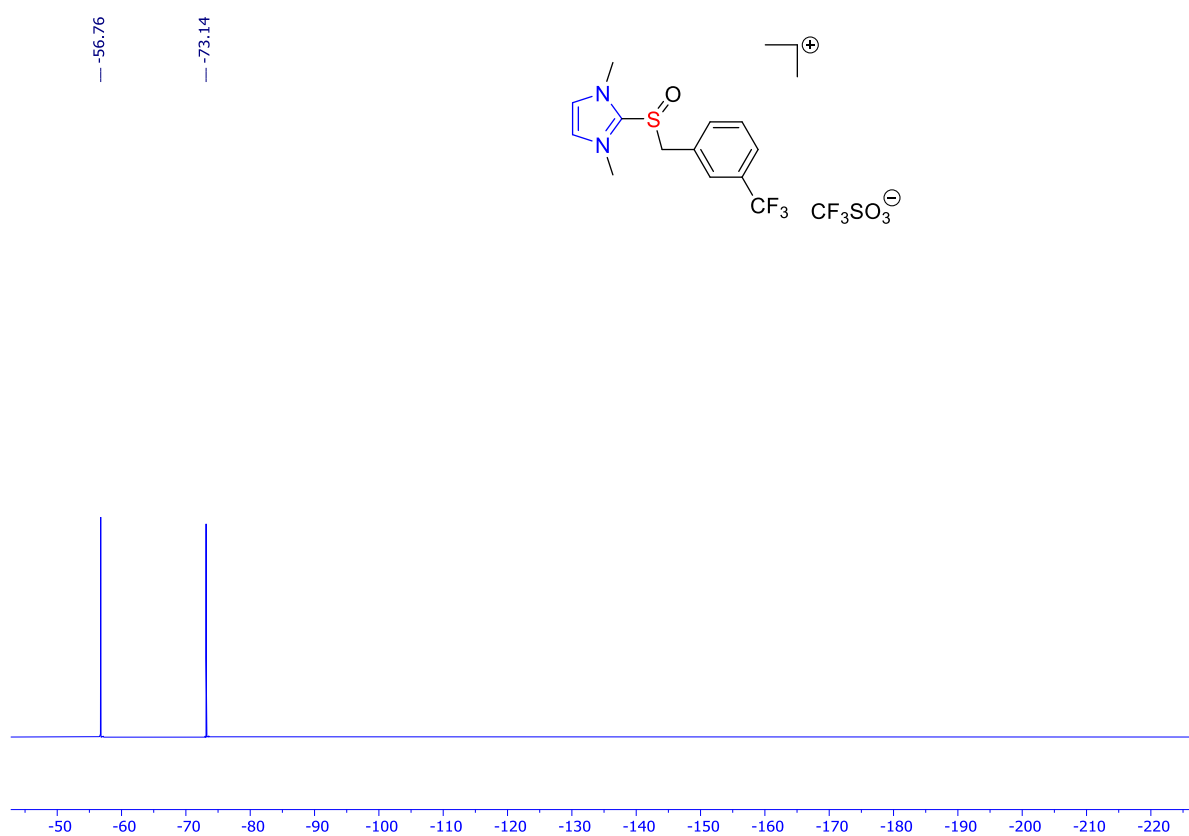


Fig. S92. ^{19}F NMR spectrum of compound **7e** ($\text{DMSO-}d_6$, 600 MHz)

1,3-dimethyl-2-((4-nitrobenzyl)sulfinyl)-1H-imidazol-3-ium Triflate (8e)

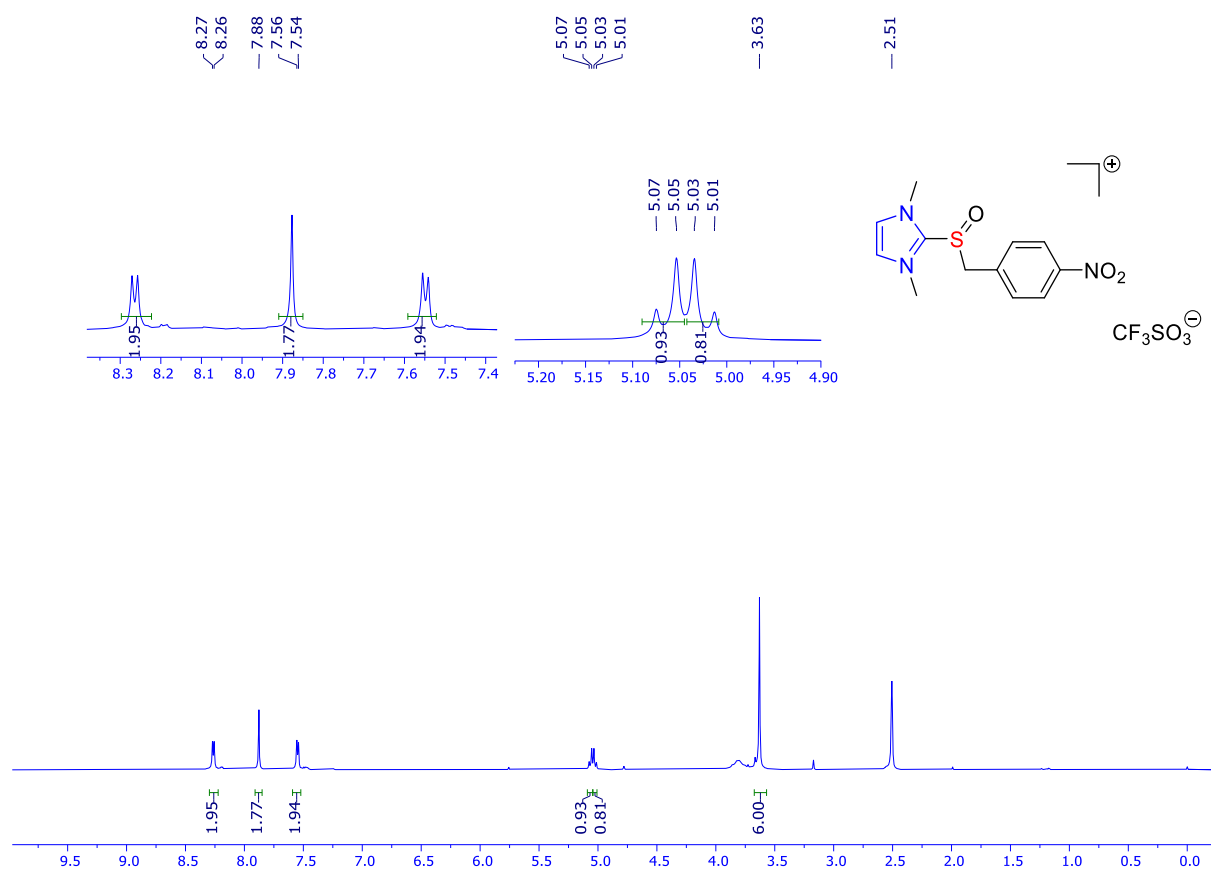


Fig. S93. ¹H NMR spectrum of compound **8e** (DMSO-*d*₆, 600 MHz)

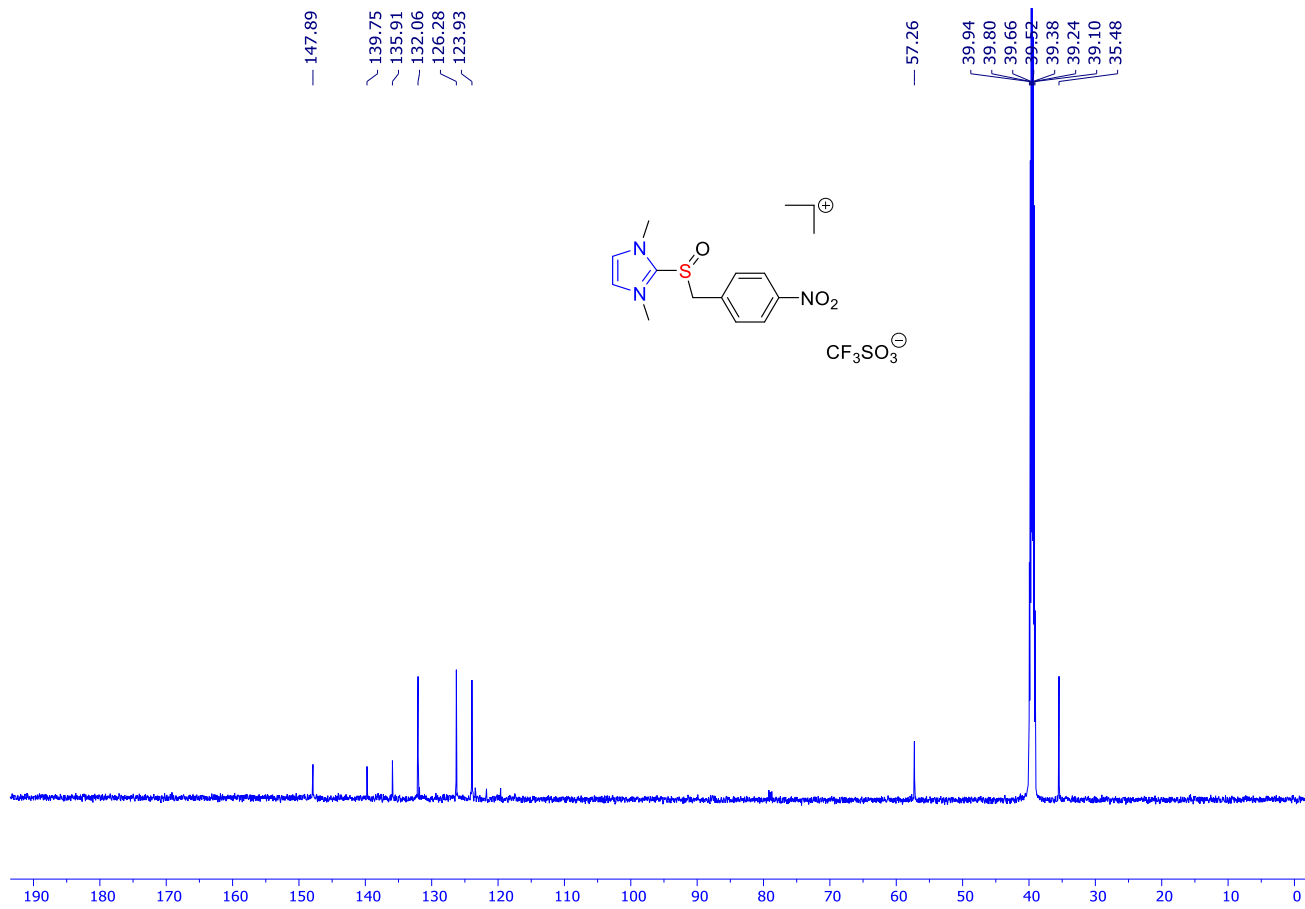


Fig. S94. ^{13}C NMR spectrum of compound **8e** ($\text{DMSO-}d_6$, 600 MHz)

1,3-dimethyl-2-((2-chloro-4-fluorobenzyl)sulfonyl)-1H-imidazol-3-iumTriflate (1f)

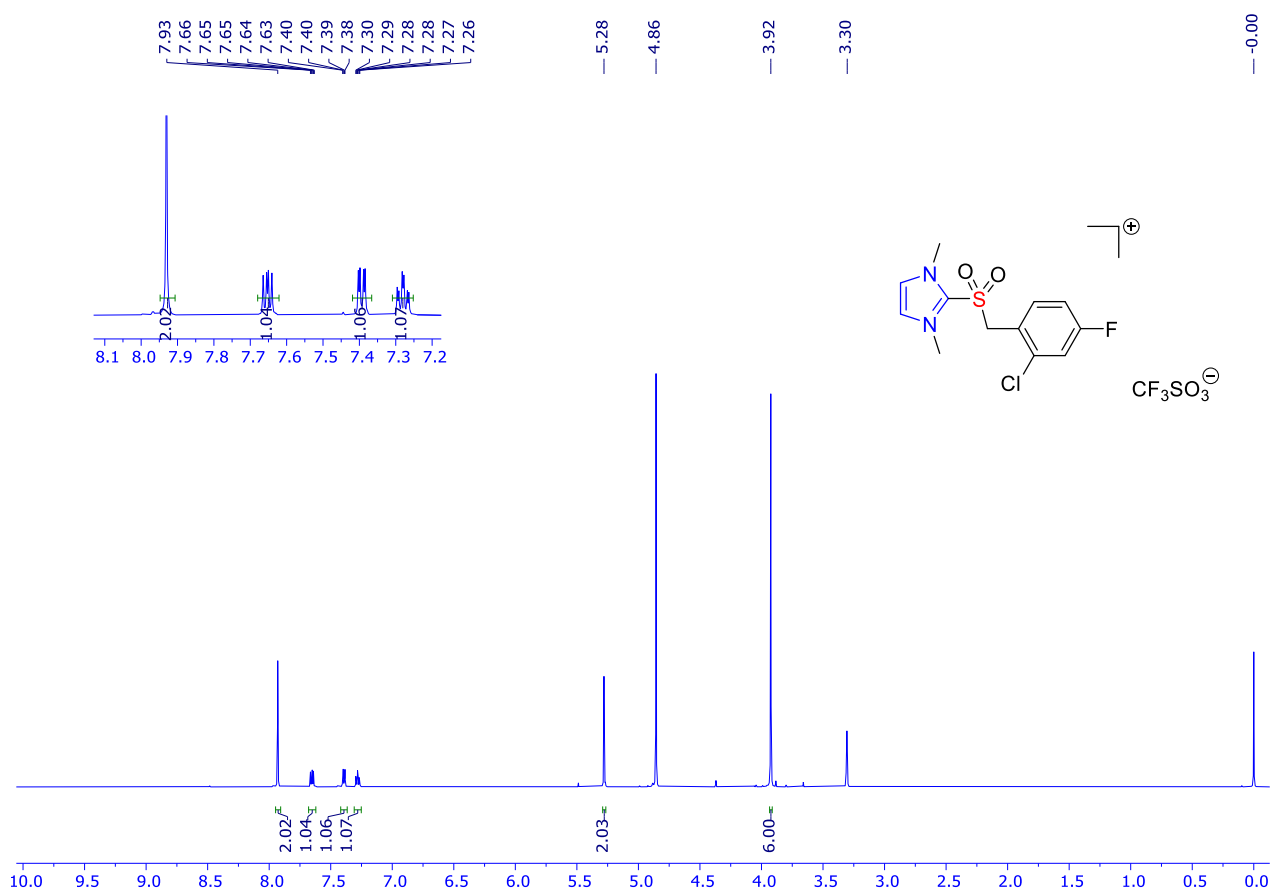


Fig. S95. ¹H NMR spectrum of compound **1f** (CD₃OD, 600 MHz)

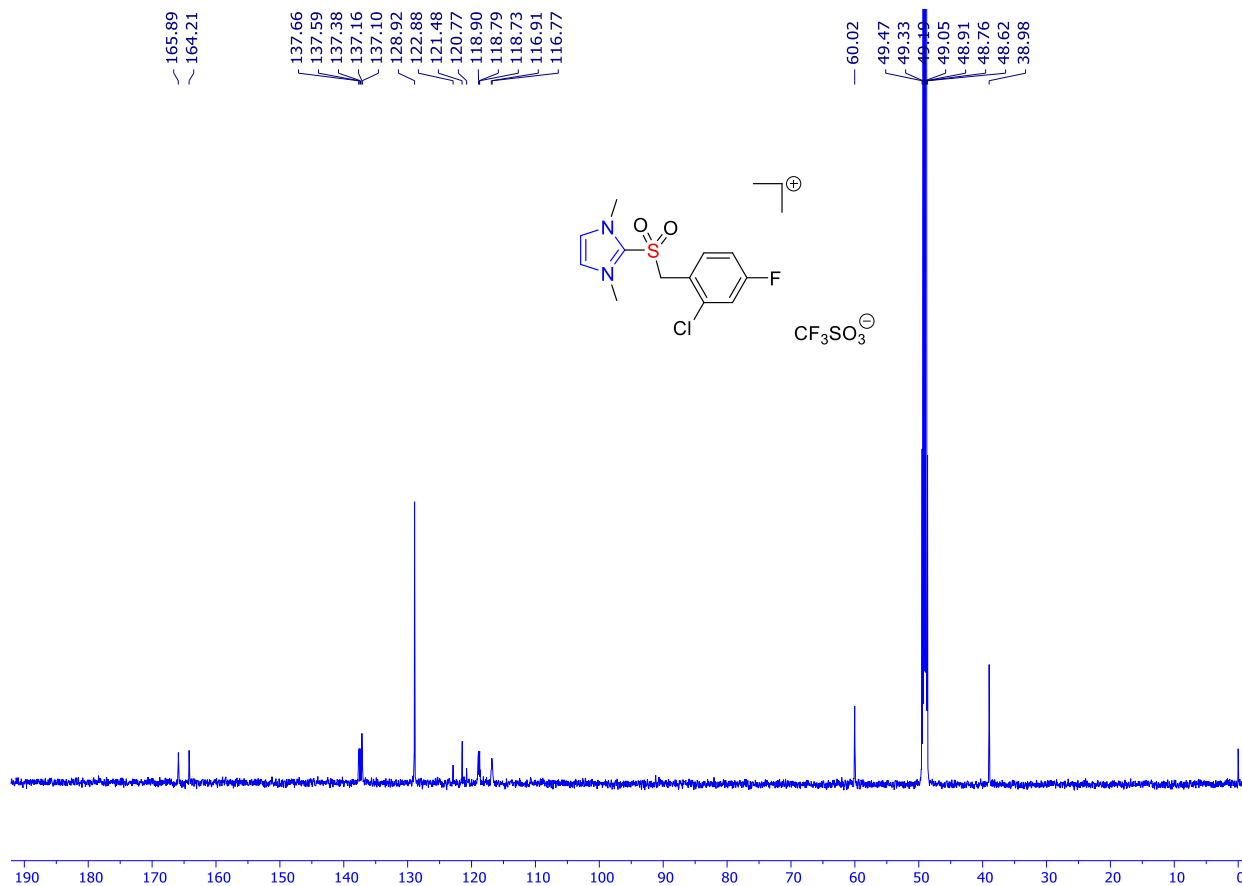


Fig. S96. ^{13}C NMR spectrum of compound **1f** (CD_3OD , 600 MHz)

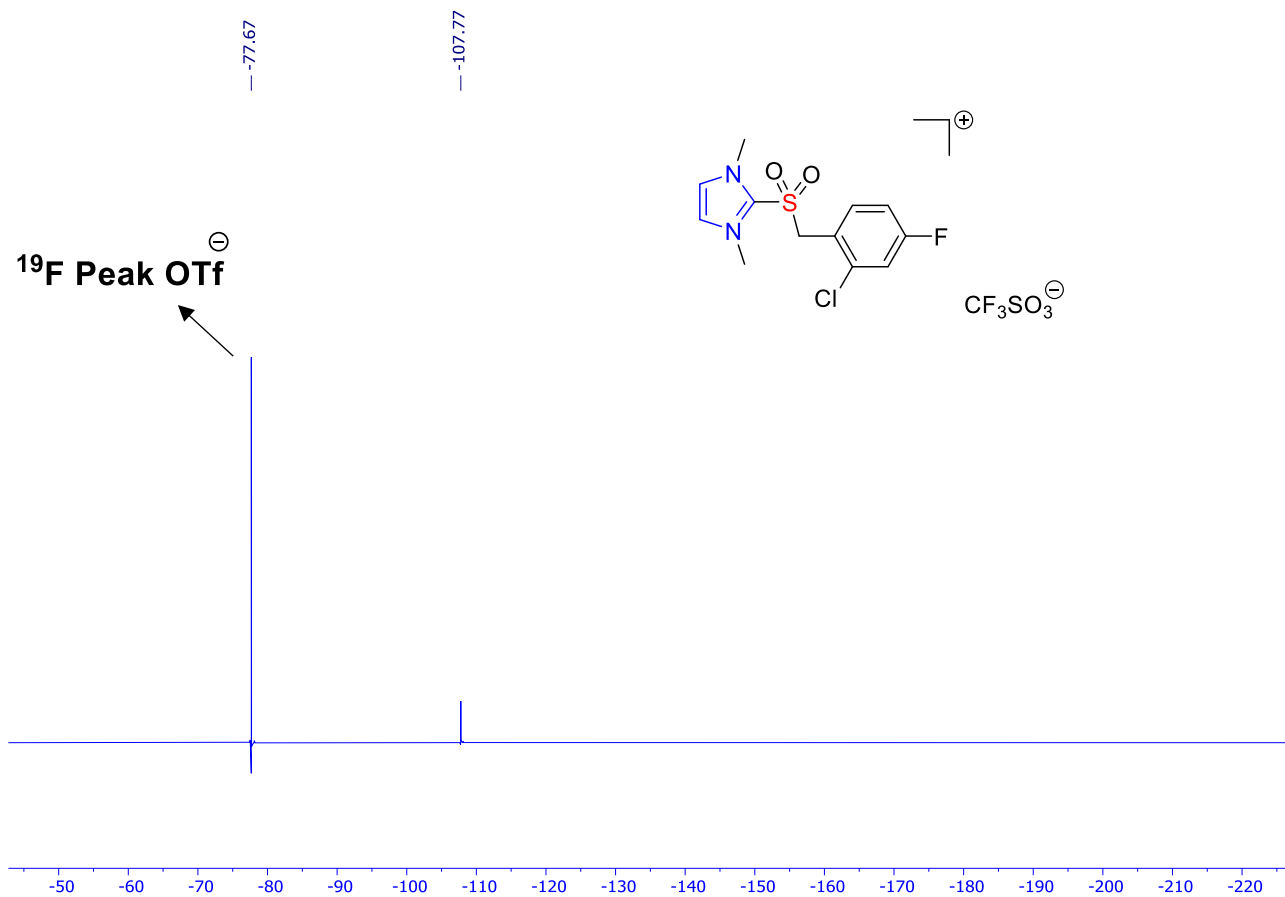


Fig. S97. ^{19}F NMR spectrum of compound **1f** (CD_3OD , 600 MHz)

1,3-dimethyl-2-(benzylsulfonyl)-1H-imidazol-3-ium Triflate (2f)

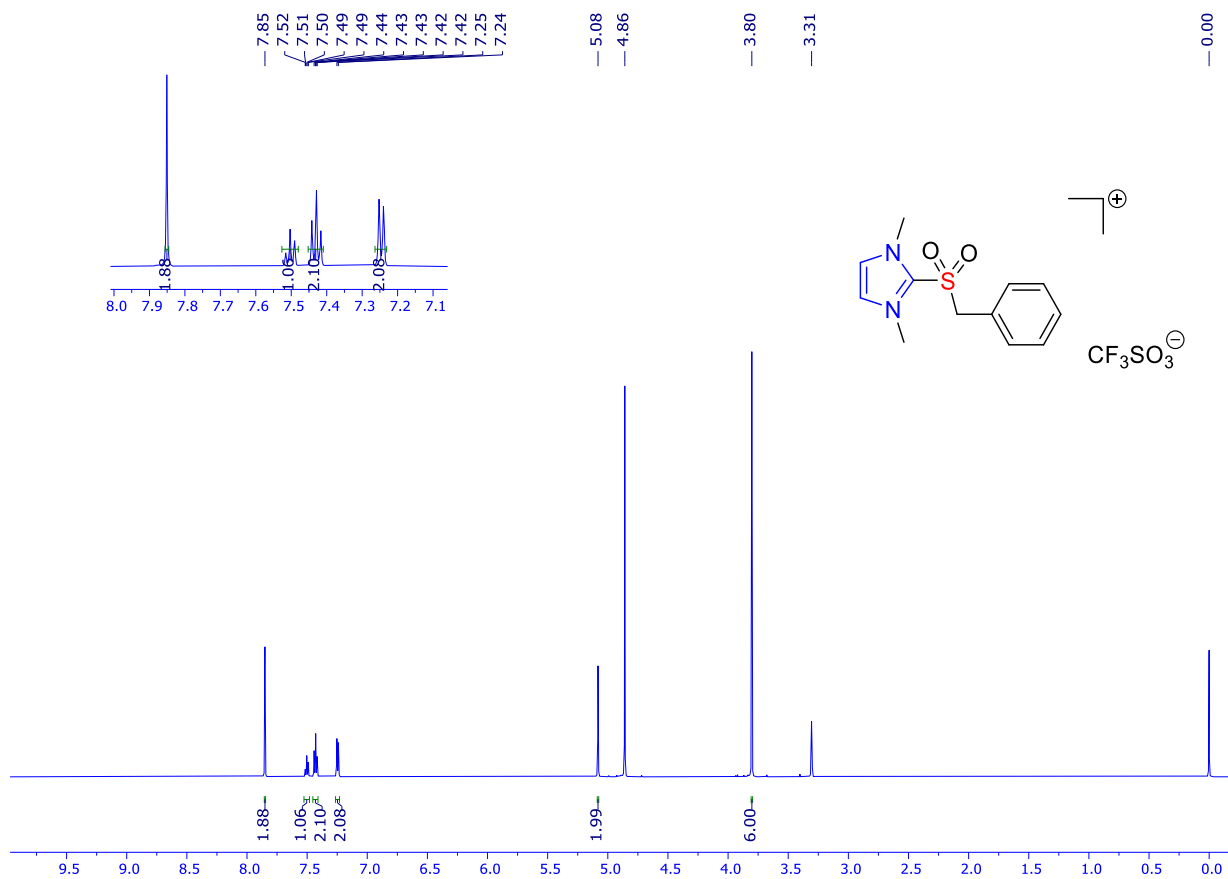


Fig. S98. ¹H NMR spectrum of compound **2f** (CD₃OD, 600 MHz)

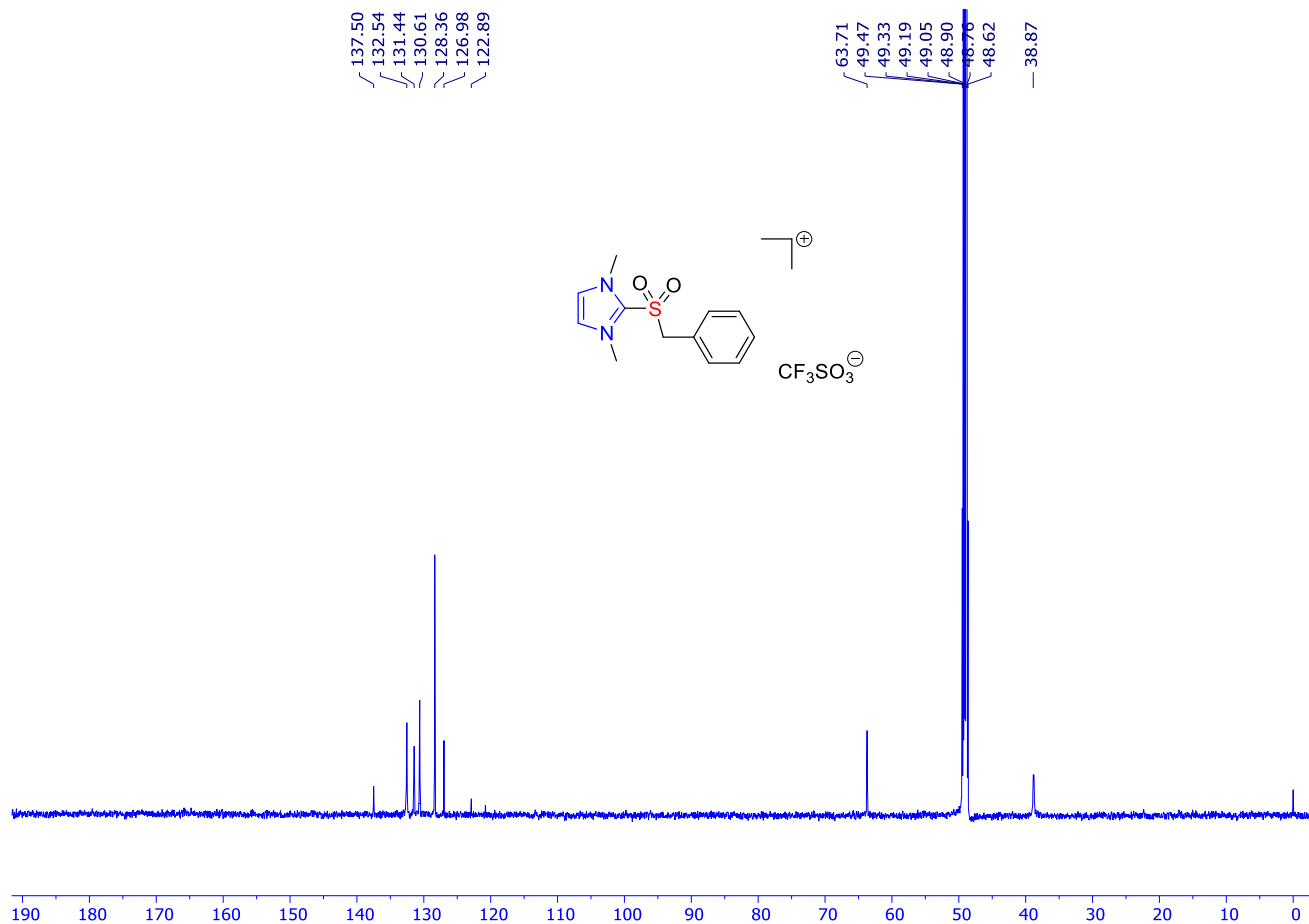


Fig. S99. ^{13}C NMR spectrum of compound **2f** (CD_3OD , 600 MHz)

1,3-dimethyl-2-((4-bromobenzyl)sulfonyl)-1H-imidazol-3-ium Triflate (3f)

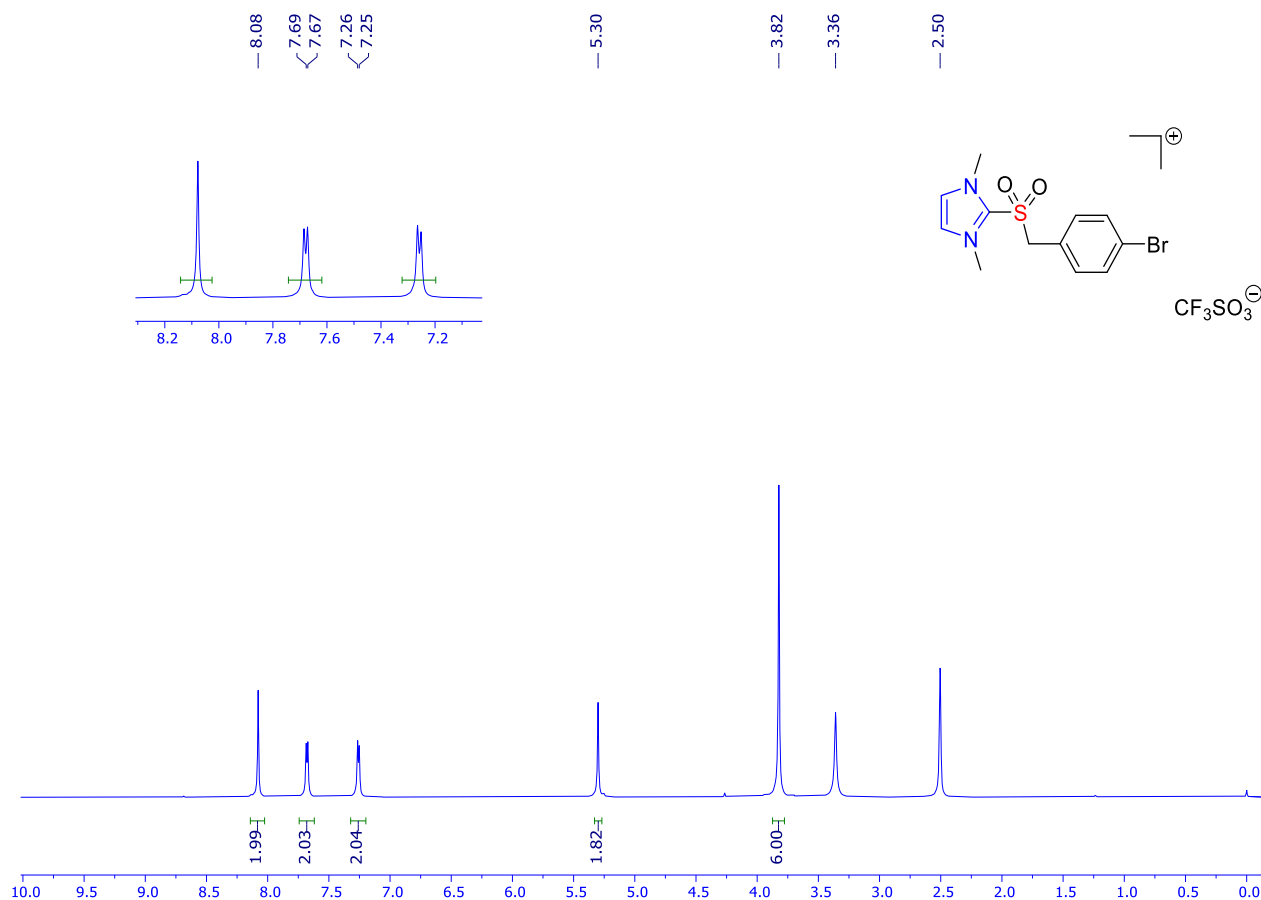


Fig. S100. ^1H NMR spectrum of compound **3f** ($\text{DMSO-}d_6$, 600 MHz)

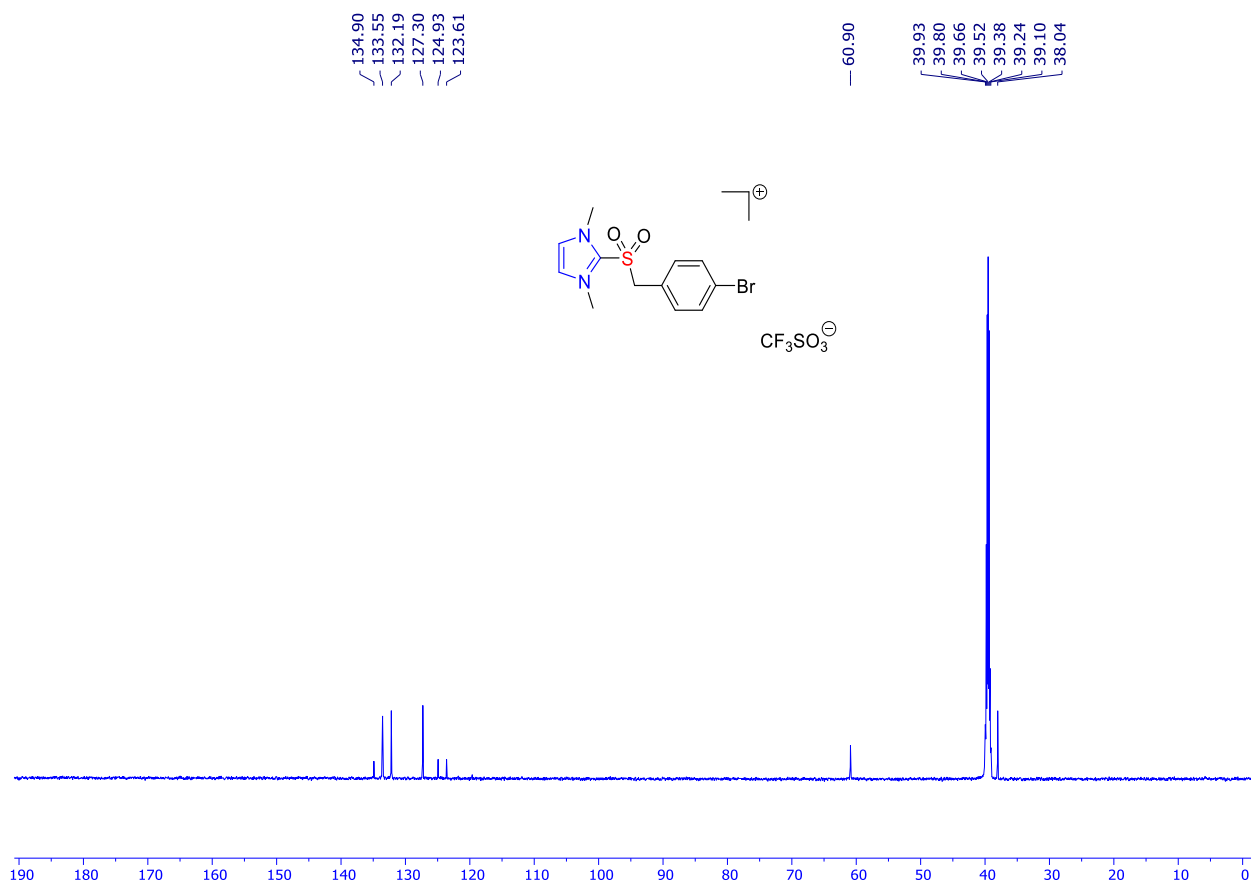


Fig. S101. ¹³C NMR spectrum of compound **3f** (DMSO-*d*₆, 600 MHz)

1,3-dimethyl-2-((2-fluoro-4-bromobenzyl)sulfonyl)-1H-imidazol-3-ium Triflate (4f)

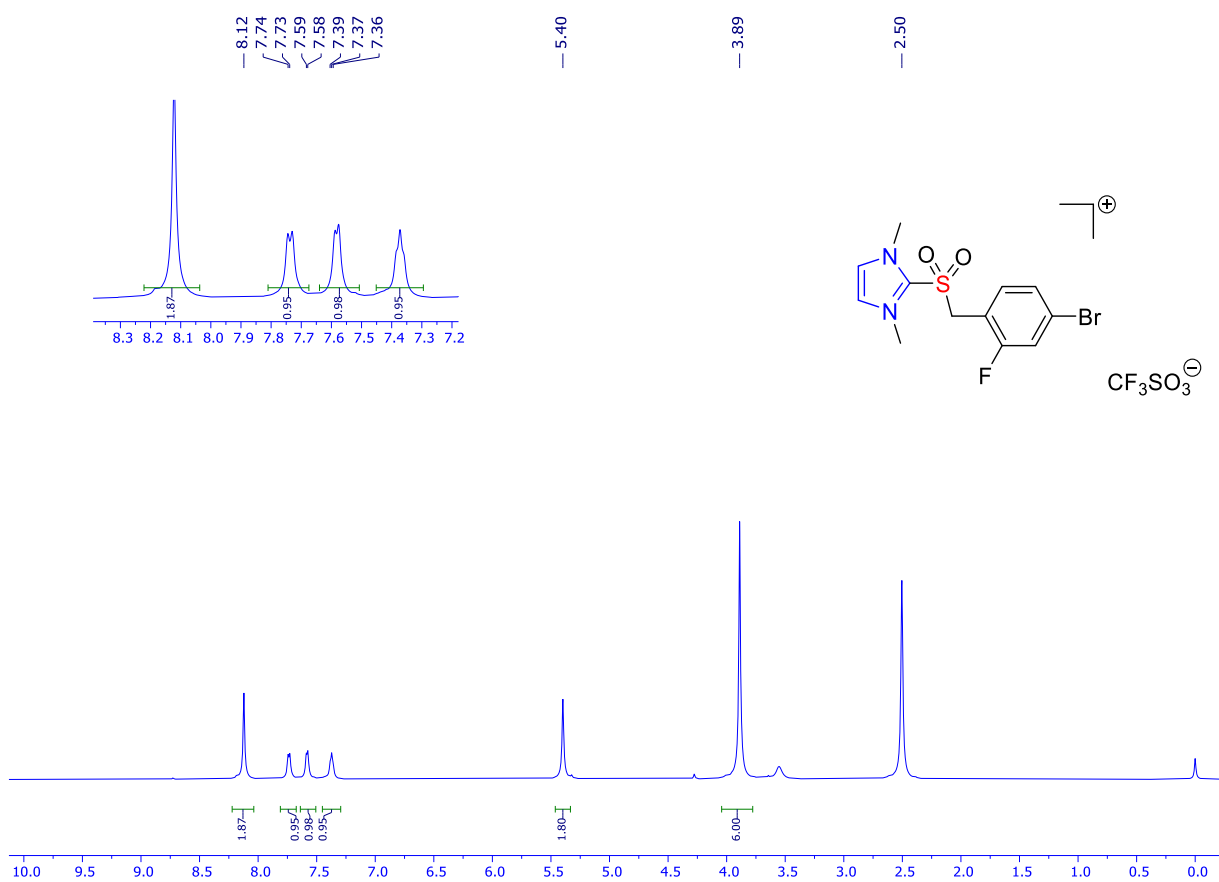


Fig. S102. ¹H NMR spectrum of compound **4f** (DMSO-*d*₆, 600 MHz)

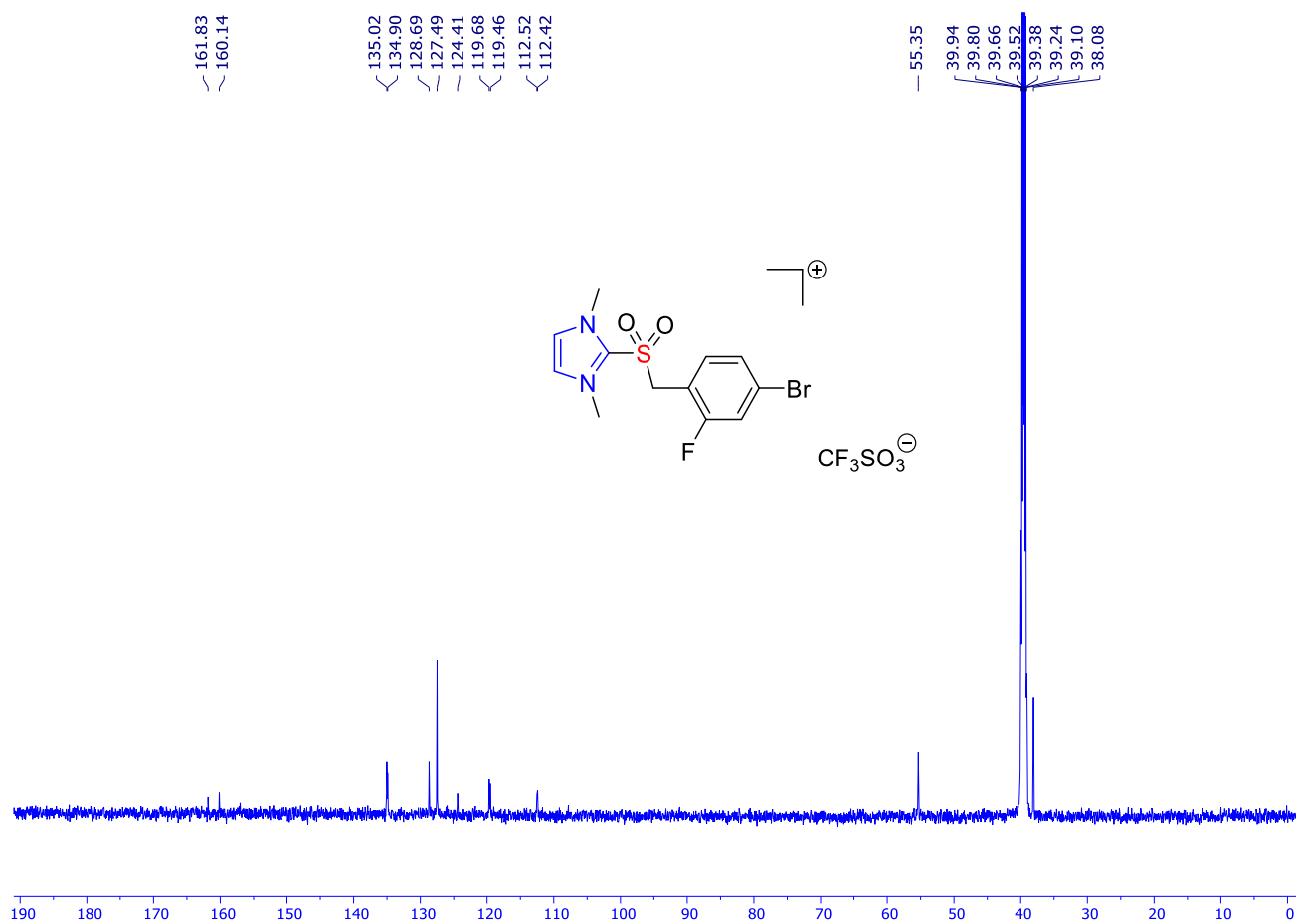


Fig. S103. ¹³C NMR spectrum of compound **4f** (DMSO-*d*₆, 600 MHz)

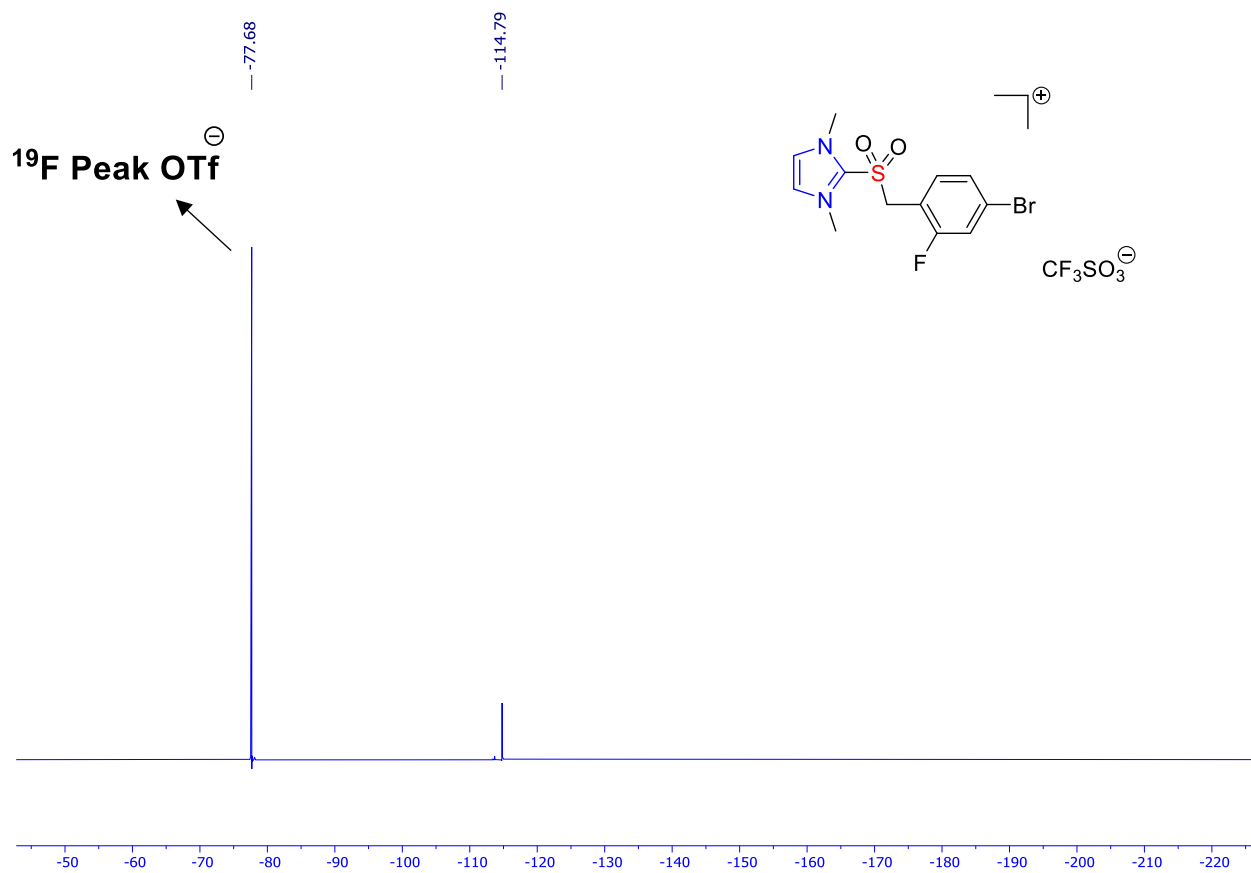


Fig. S104. ^{19}F NMR spectrum of compound **4f** ($\text{DMSO}-d_6$, 600 MHz)

1,3-dimethyl-2-((4-(trifluoromethoxy)benzyl)sulfonyl)-1H-imidazol-3-ium Triflate (5f)

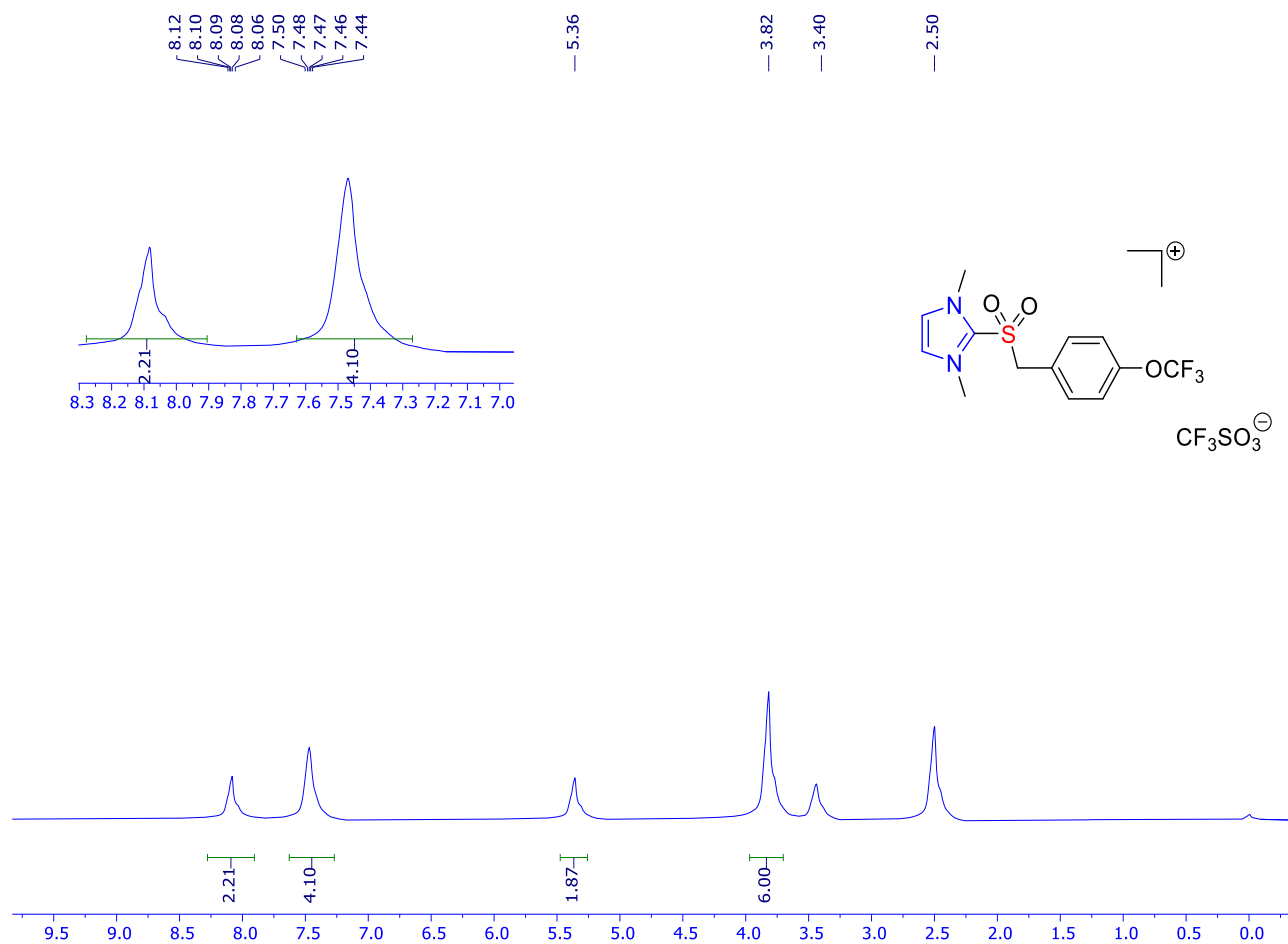


Fig. S105. ^1H NMR spectrum of compound **5f** ($\text{DMSO-}d_6$, 600 MHz)

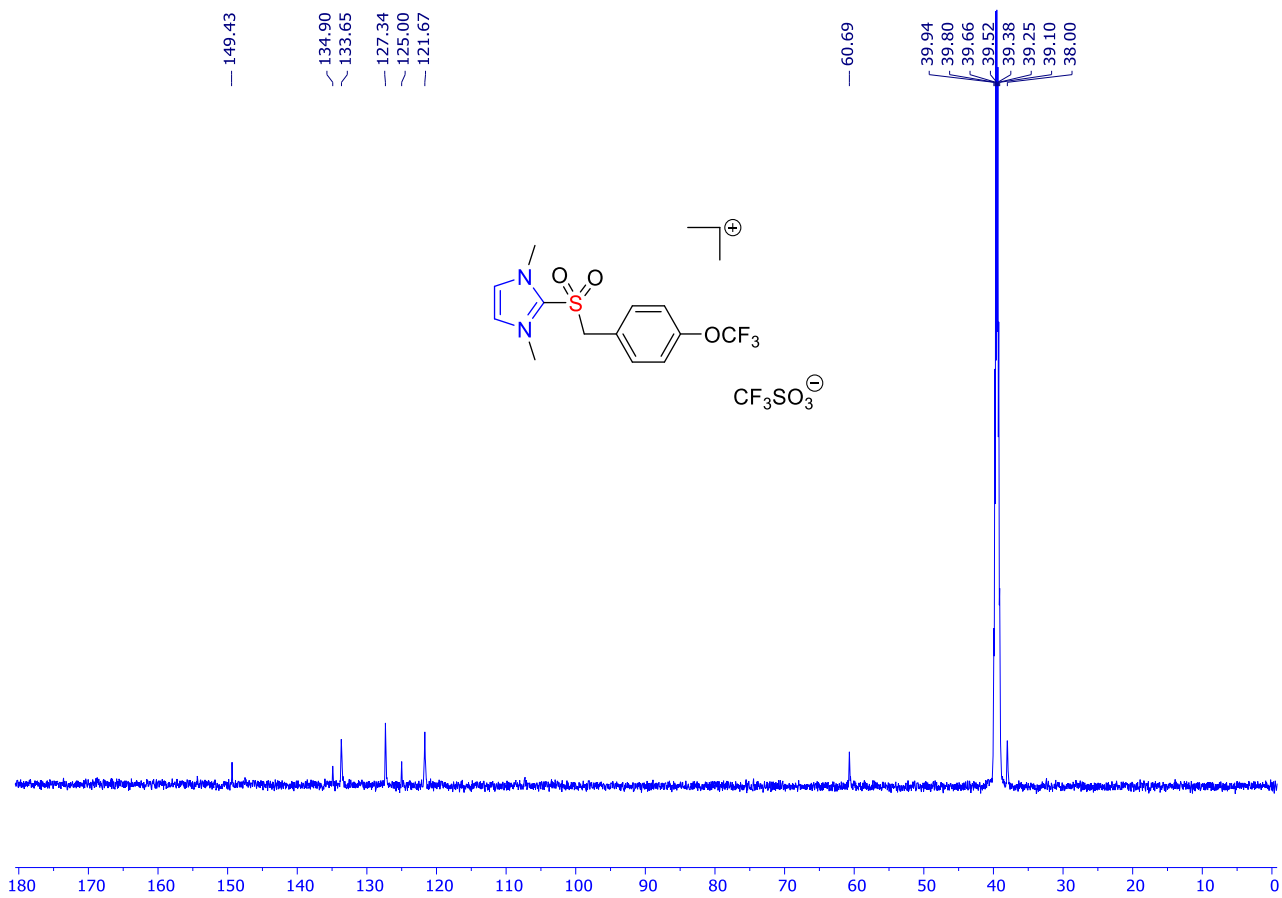


Fig. S106. ^{13}C NMR spectrum of compound **5f** (DMSO- d_6 , 600 MHz)

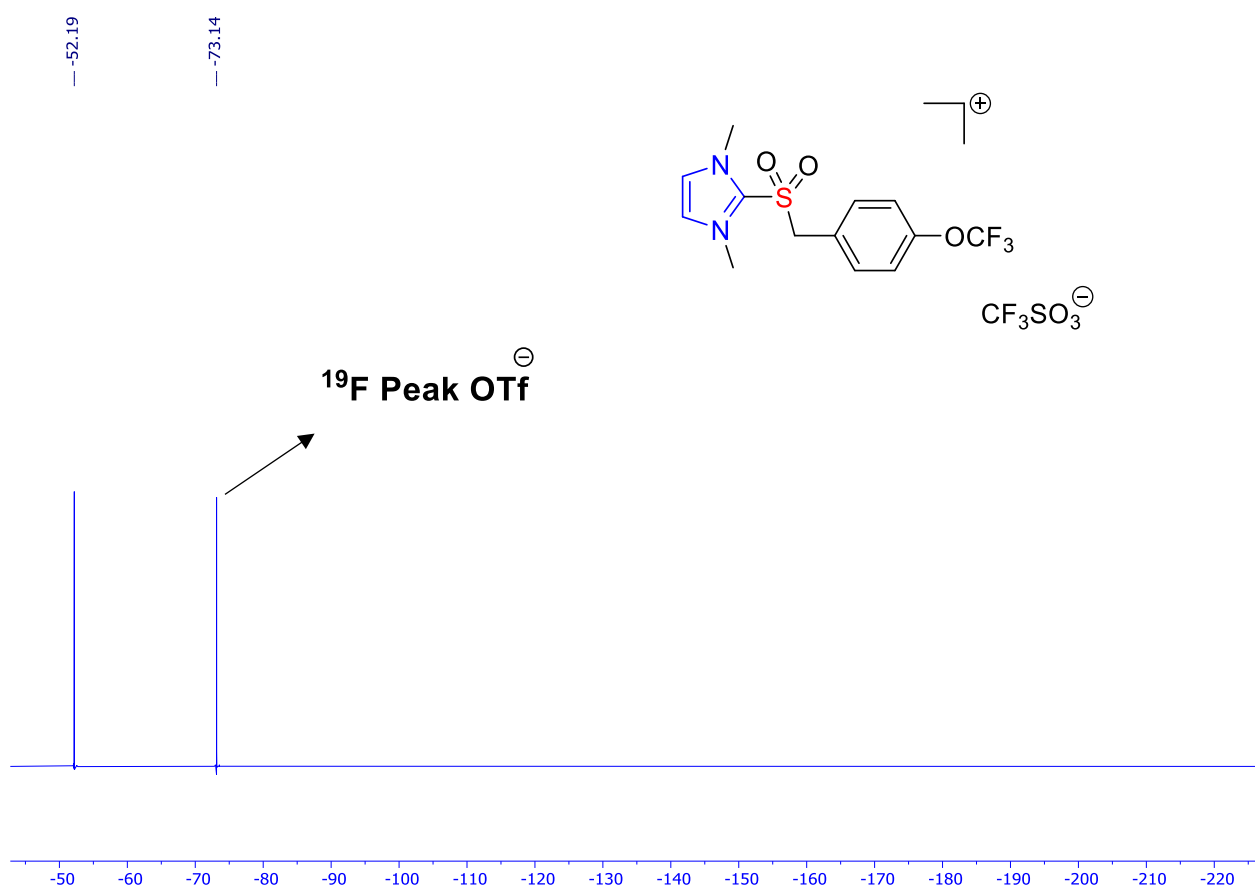


Fig. S107. ^{19}F NMR spectrum of compound **5f** ($\text{DMSO}-d_6$, 600 MHz)

1,3-dimethyl-2-((4-(tert-butyl)benzyl)sulfonyl)-1H-imidazol-3-ium Triflate (6f)

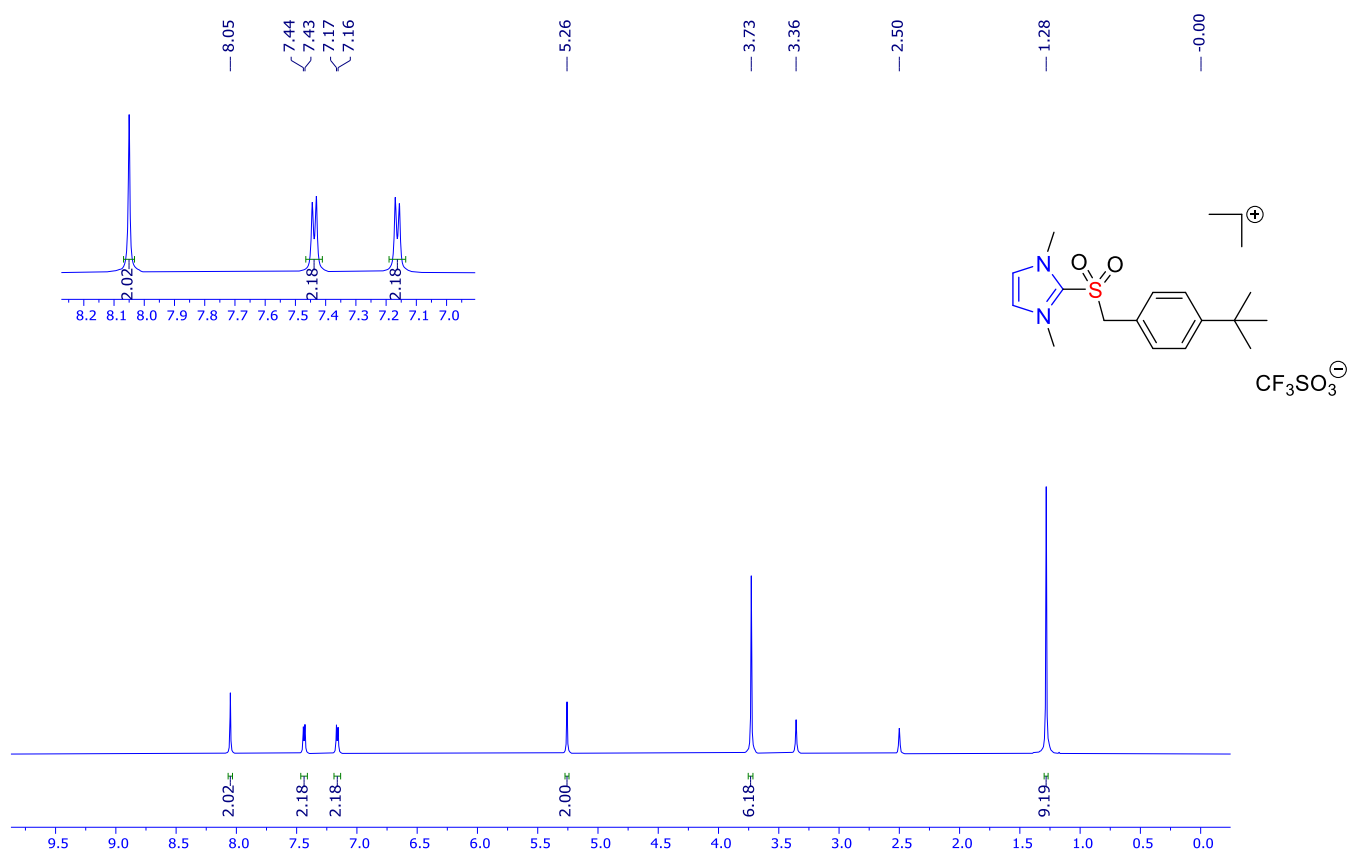


Fig. S108. ¹H NMR spectrum of compound **6f** (DMSO-*d*₆, 600 MHz)

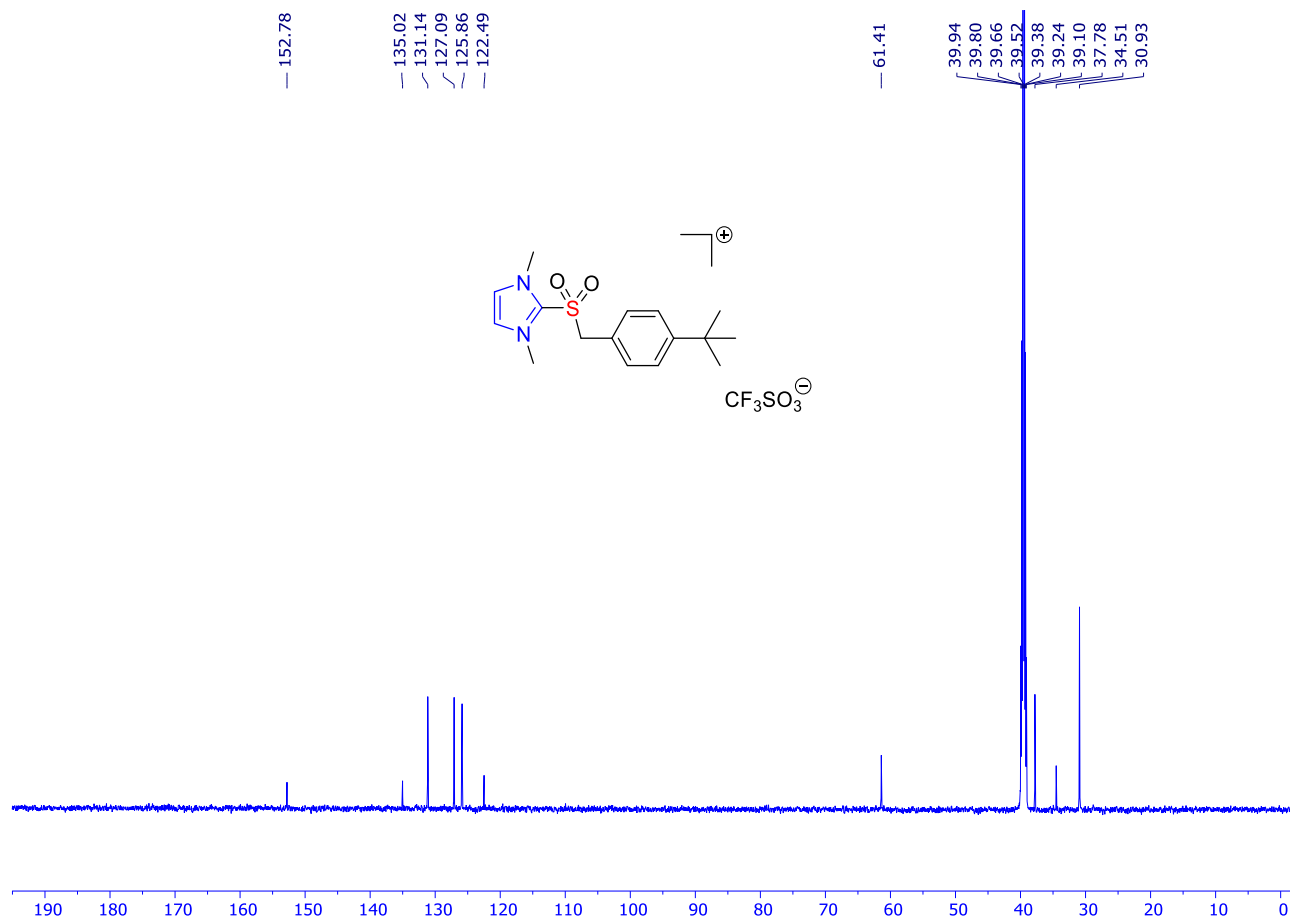


Fig. S109. ¹³C NMR spectrum of compound **6f** (DMSO-*d*₆, 600 MHz)

1,3-dimethyl-2-((3-(trifluoromethyl)benzyl)sulfonyl)-1H-imidazol-3-ium Triflate (7f)

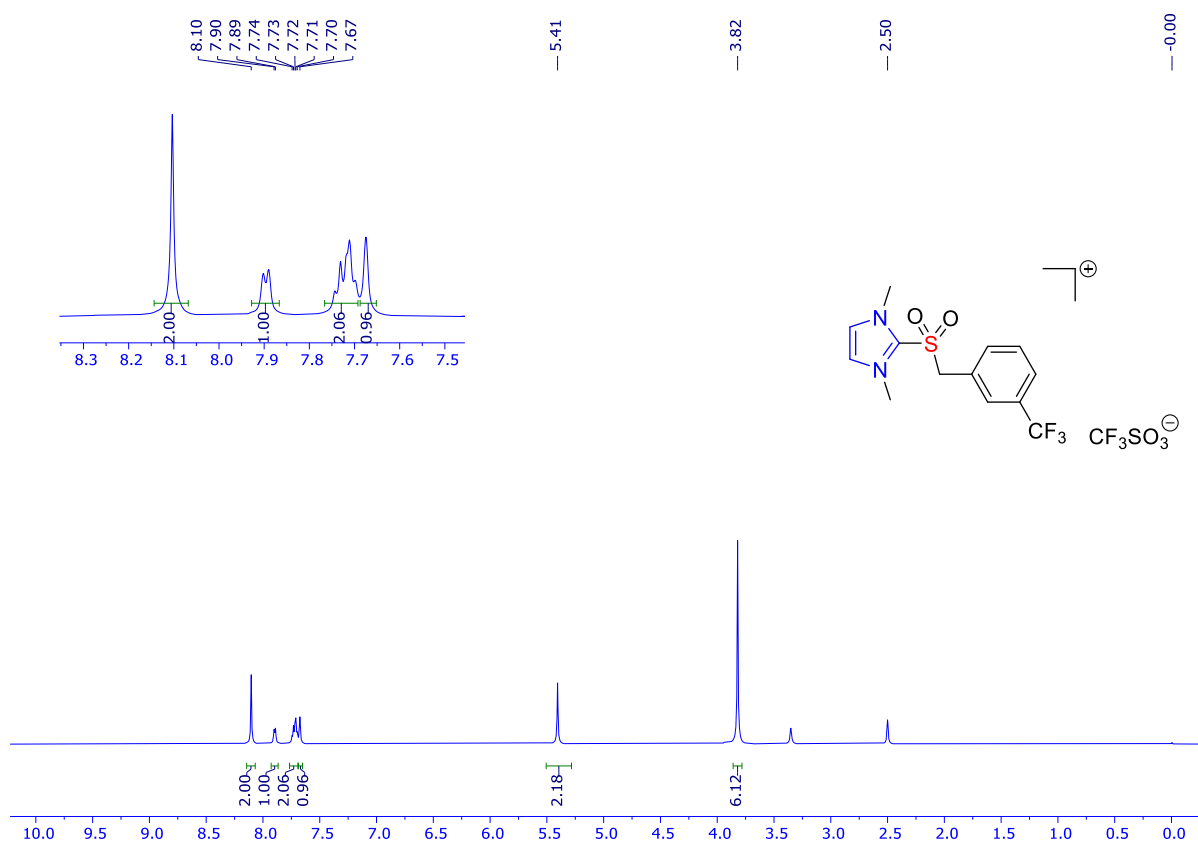


Fig. S110. ^1H NMR spectrum of compound **7f** ($\text{DMSO-}d_6$, 600 MHz)

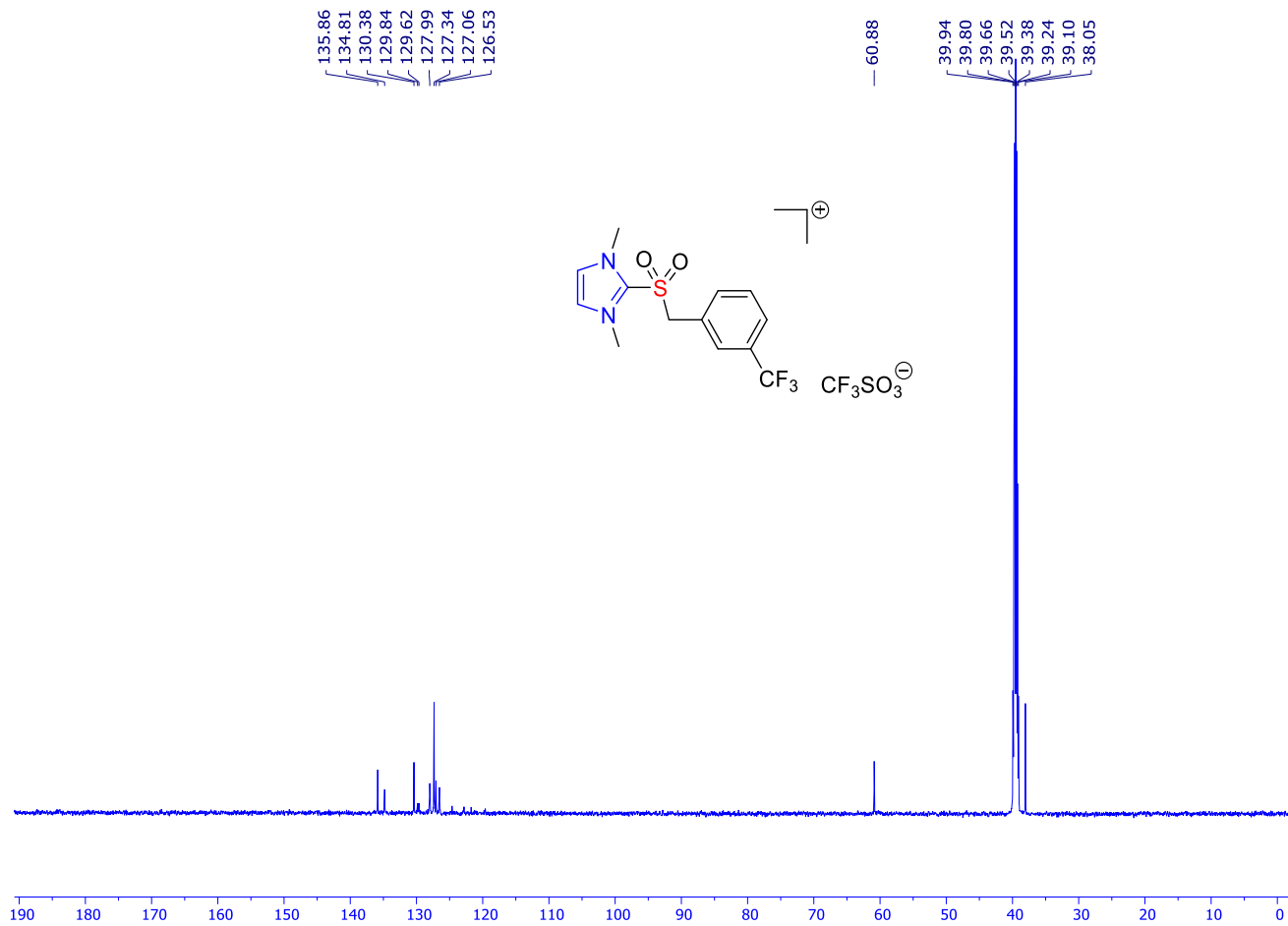


Fig. S111. ^{13}C NMR spectrum of compound **7f** ($\text{DMSO-}d_6$, 600 MHz)

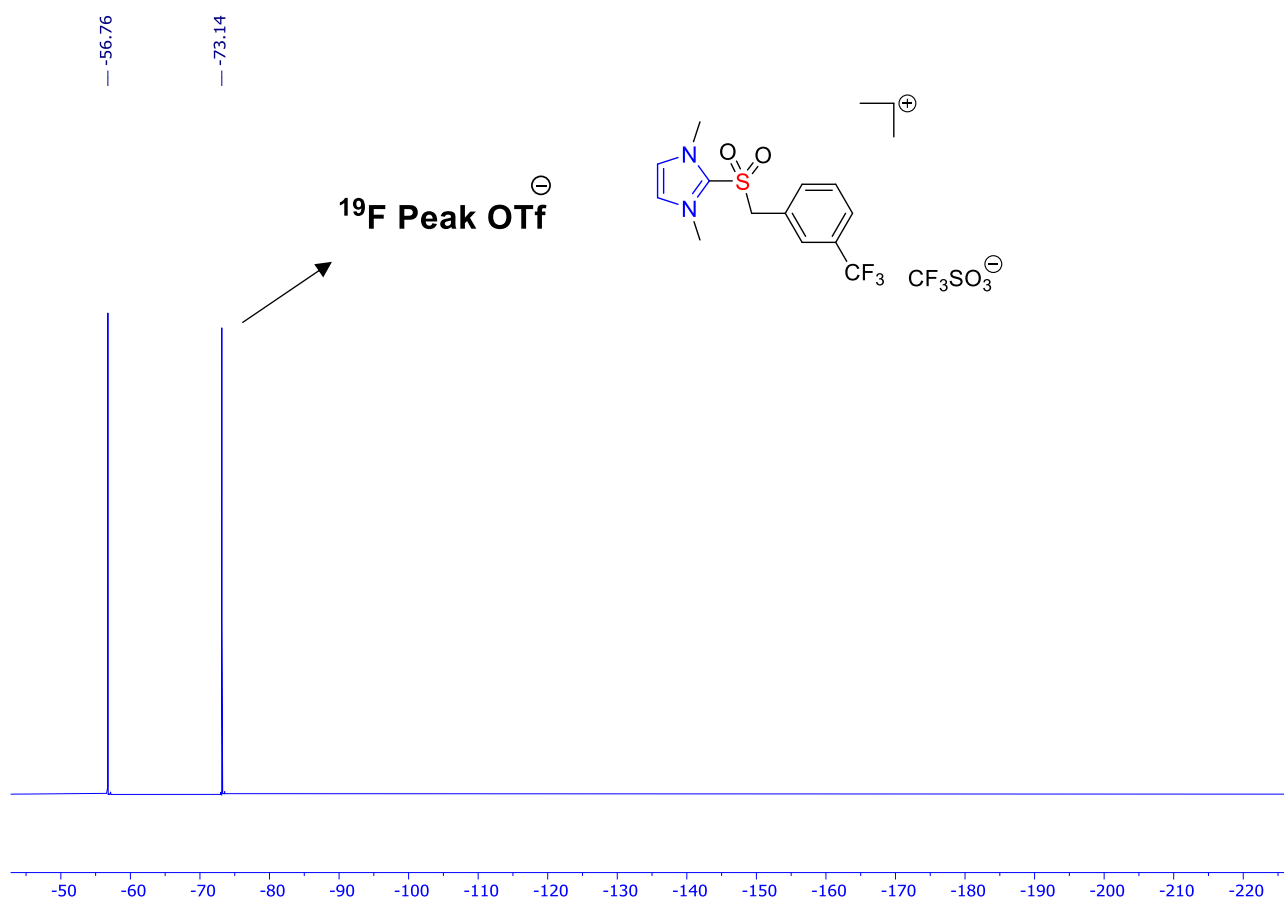


Fig. S112. ^{19}F NMR spectrum of compound **7f** ($\text{DMSO-}d_6$, 600 MHz)

1,3-dimethyl-2-((4-nitrobenzyl)sulfonyl)-1H-imidazol-3-ium Triflate (8f)

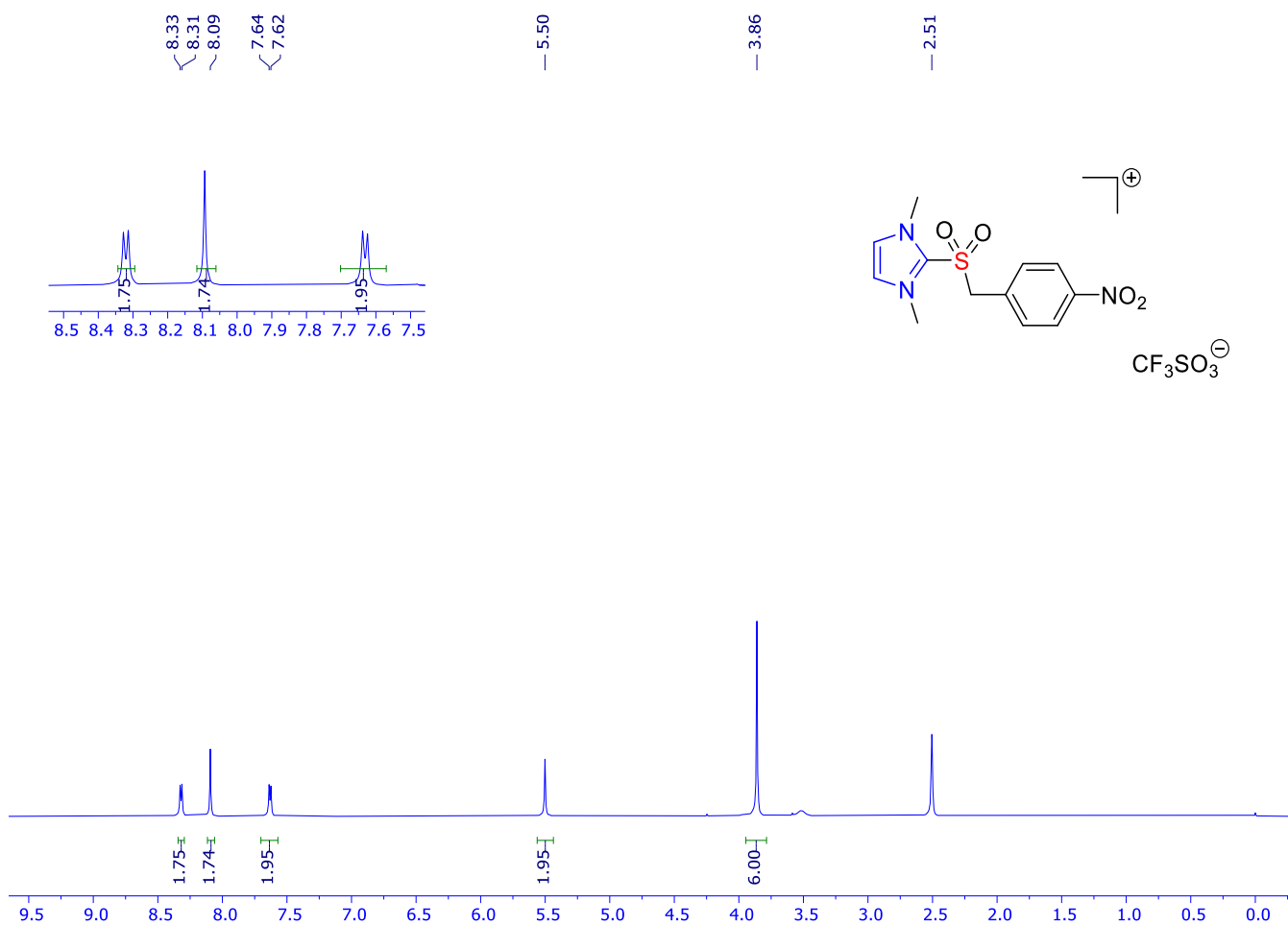


Fig. S113. ¹H NMR spectrum of compound **8f** (DMSO-*d*₆, 600 MHz)

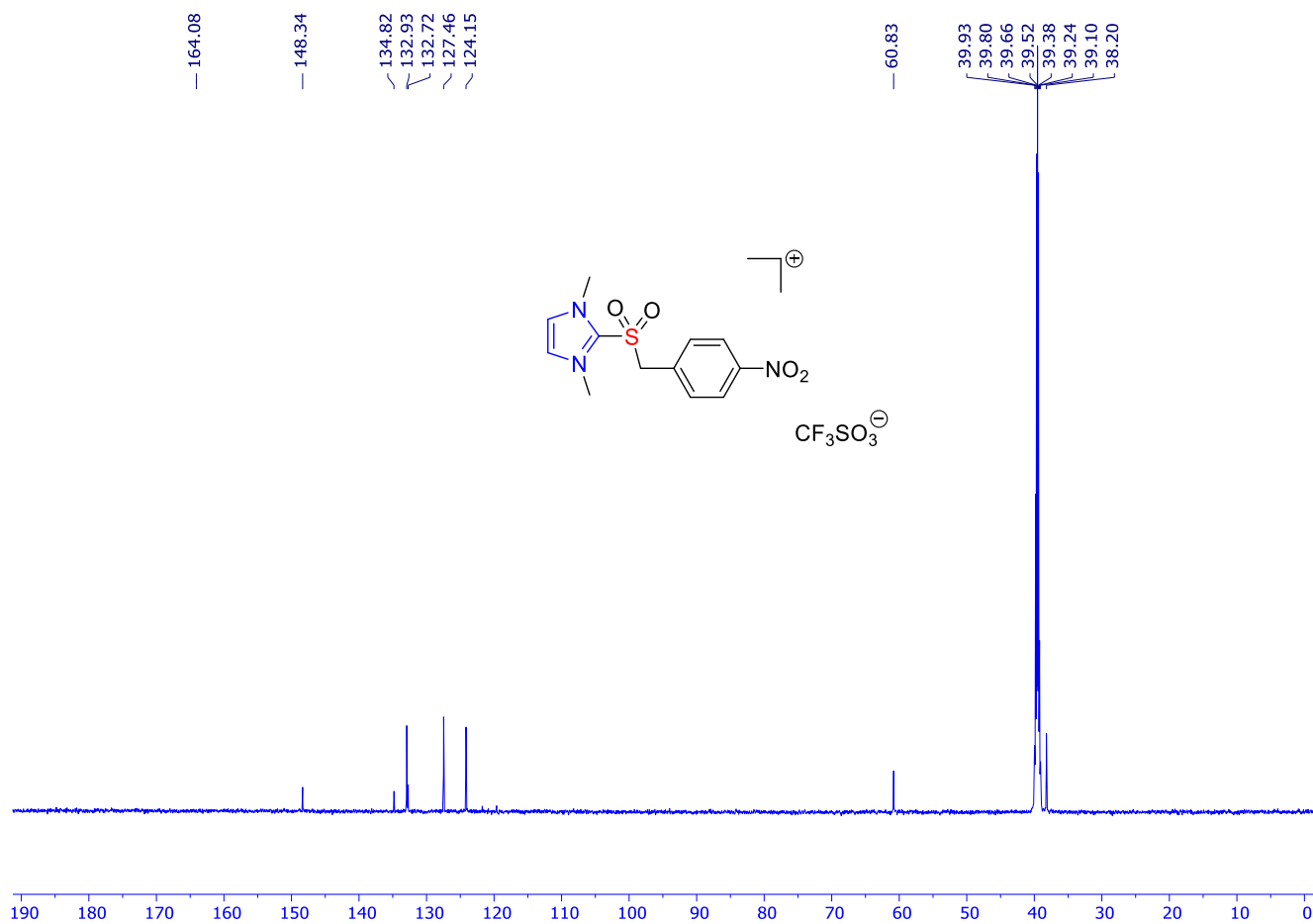


Fig. S114. ¹³C NMR spectrum of compound **8f** (DMSO-*d*₆, 600 MHz)

IR Data-

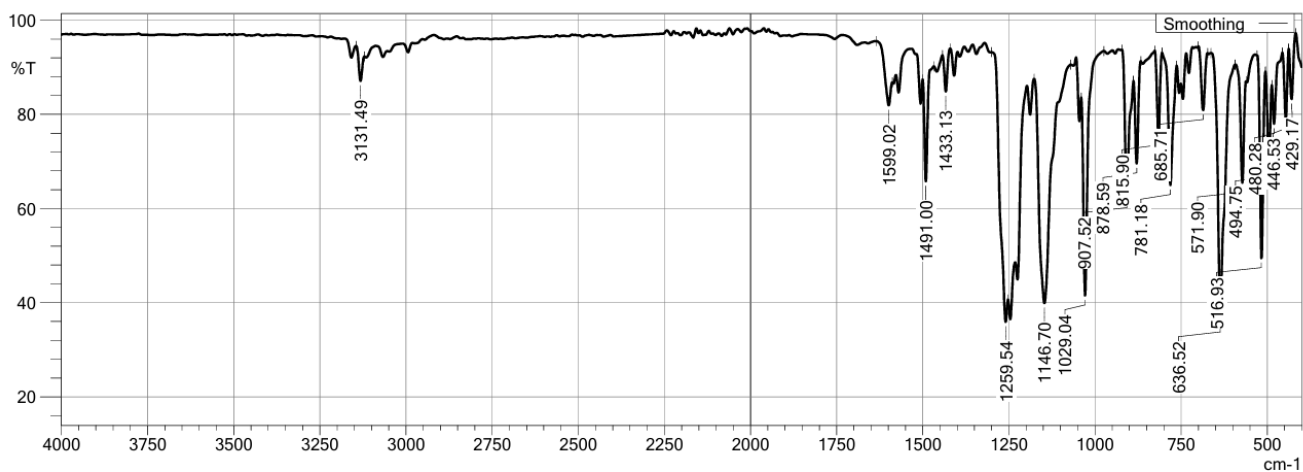


Fig. S115. IR data of compound 1d

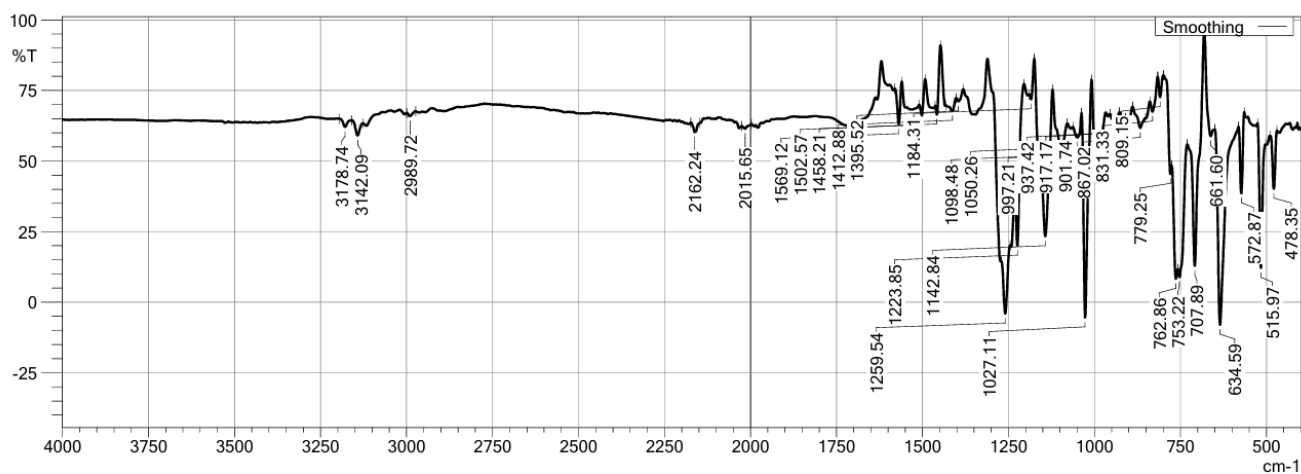


Fig. S116. IR data of compound 2d

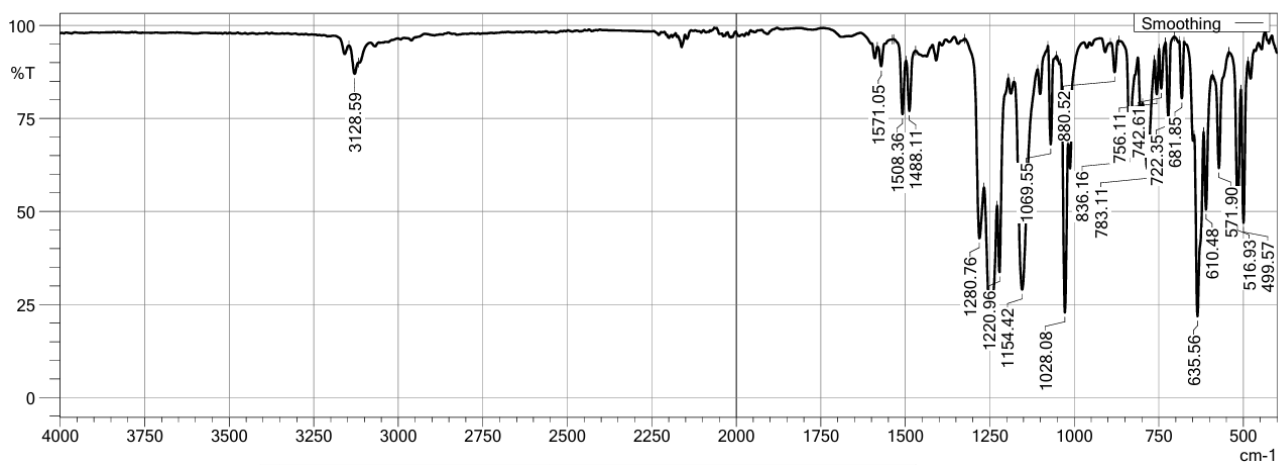


Fig. S117. IR data of compound 3d

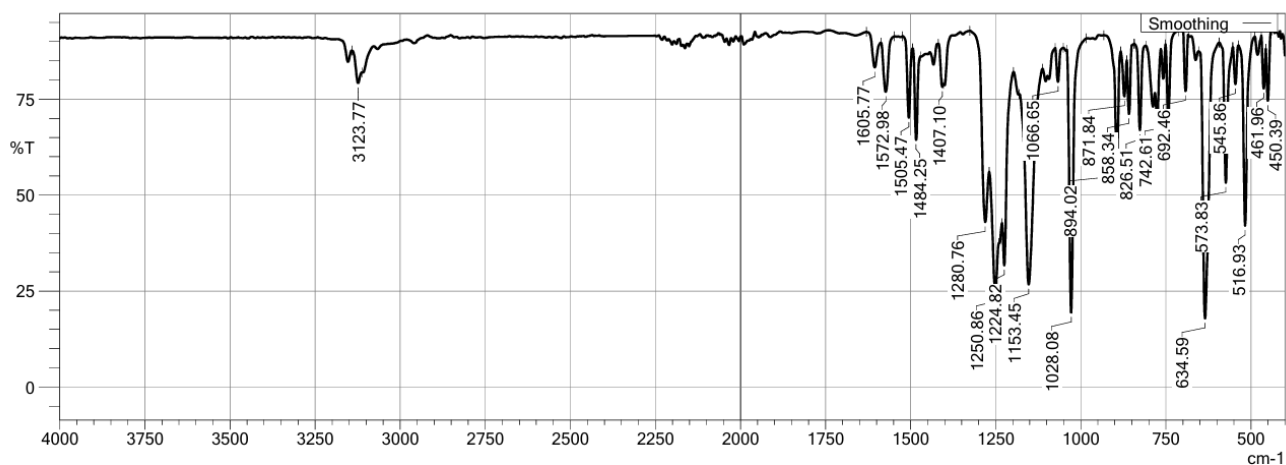


Fig. S118. IR data of compound **4d**

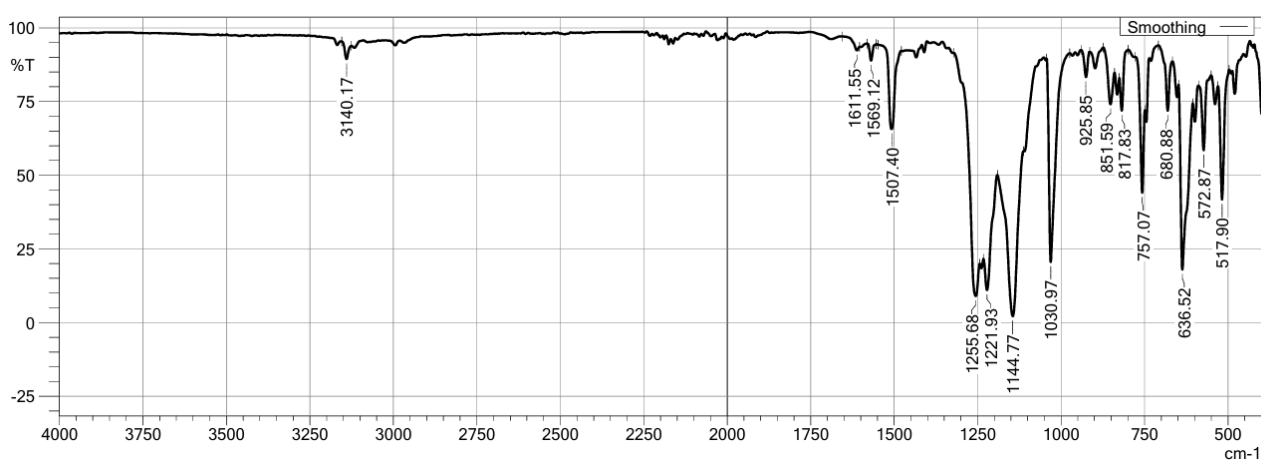


Fig. S119. IR data of compound **5d**

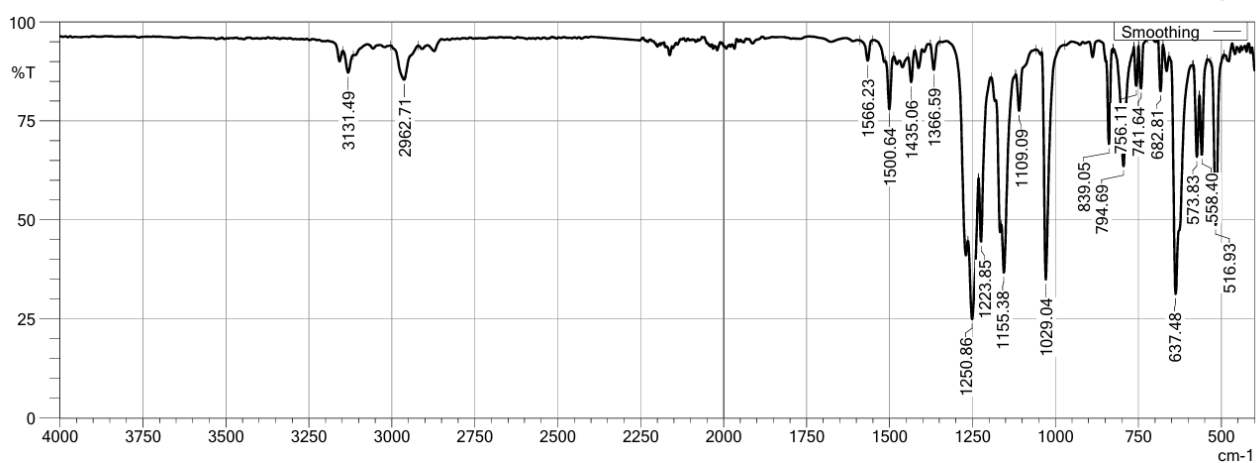


Fig. S120. IR data of compound **6d**

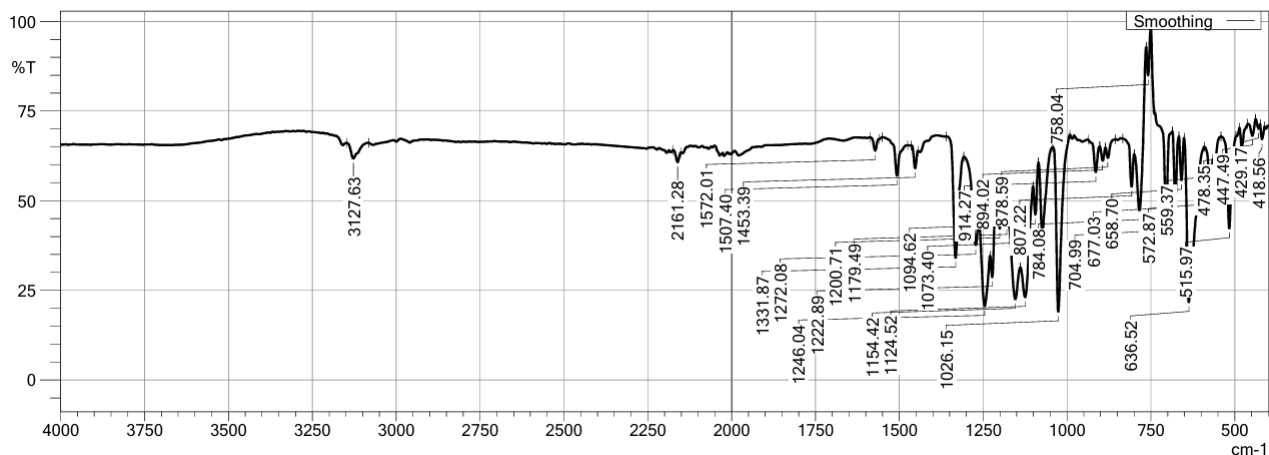


Fig. S121. IR data of compound 7d



Fig. S122. IR data of compound 8d



Fig. S123. IR data of compound 1e



Fig. S124. IR data of compound 2e

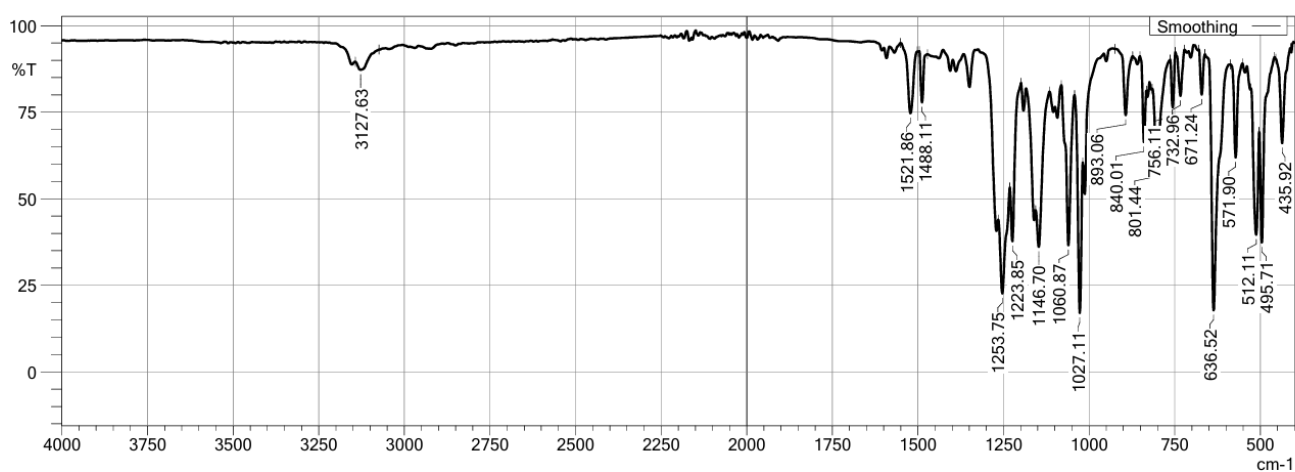


Fig. S125. IR data of compound 3e

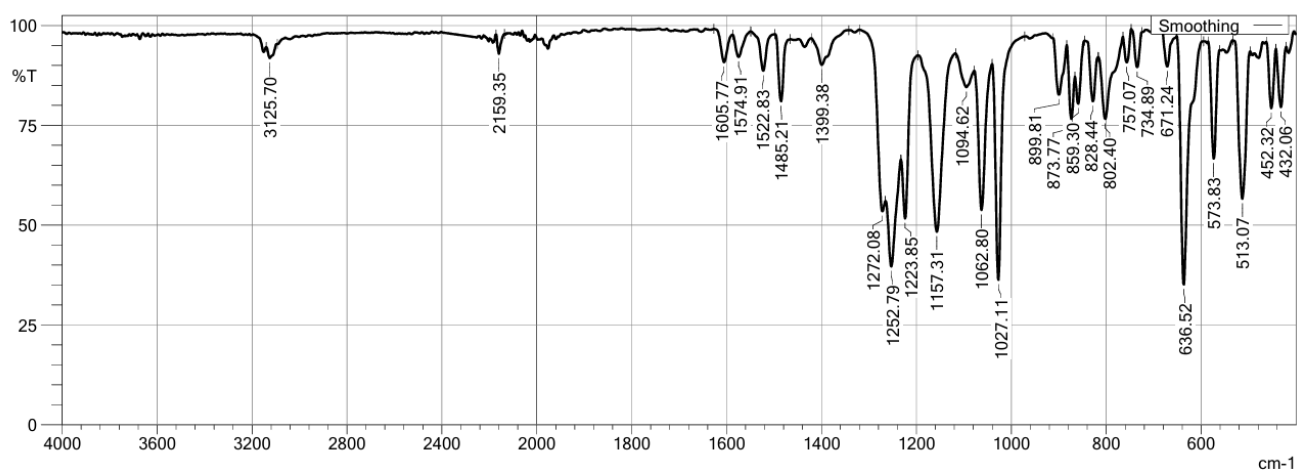


Fig. S126. IR data of compound 4e

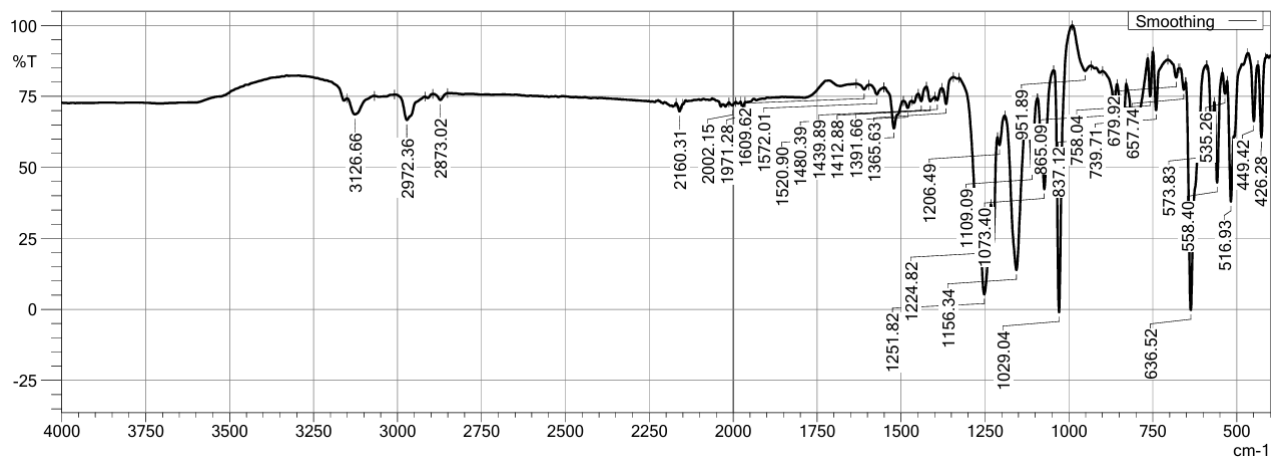


Fig. S127. IR data of compound 5e

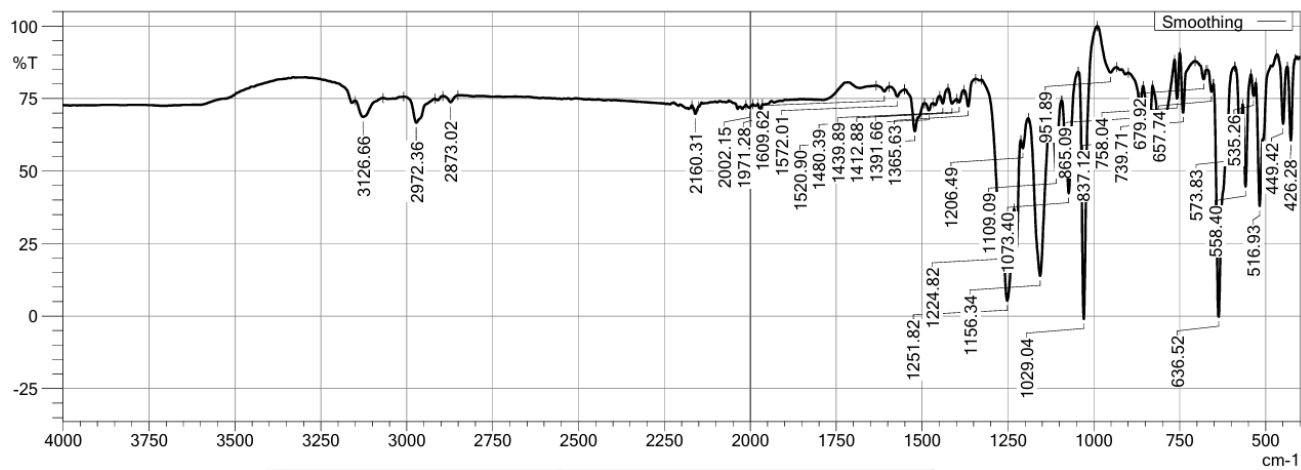


Fig. S128. IR data of compound 6e

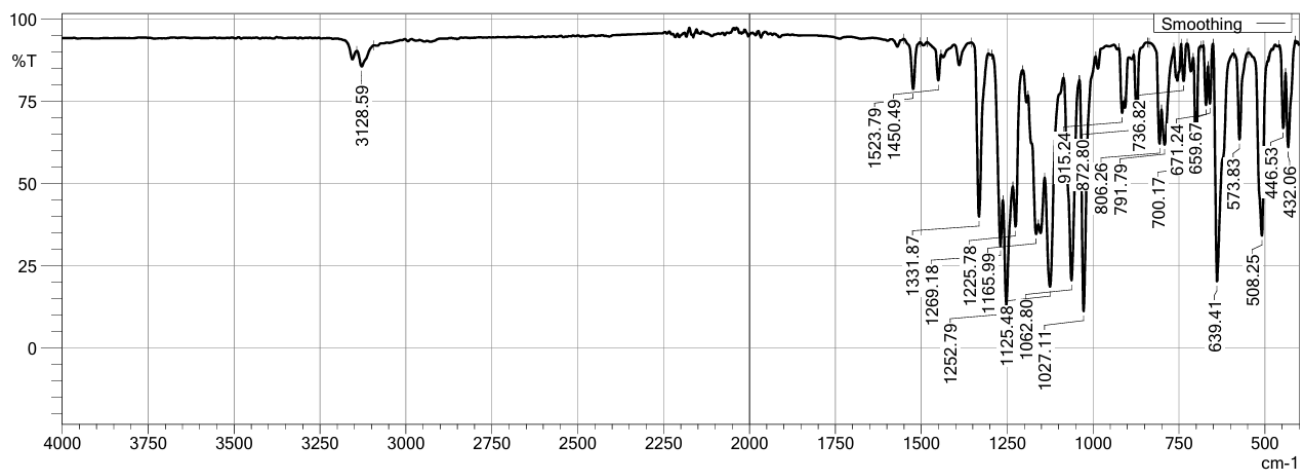


Fig. S129. IR data of compound 7e

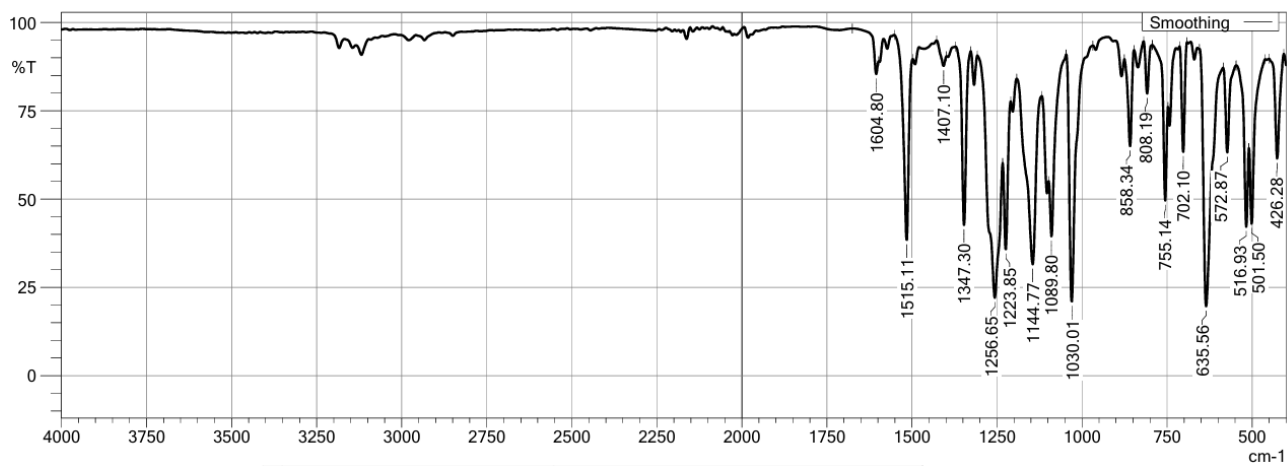


Fig. S130. IR data of compound **8e**

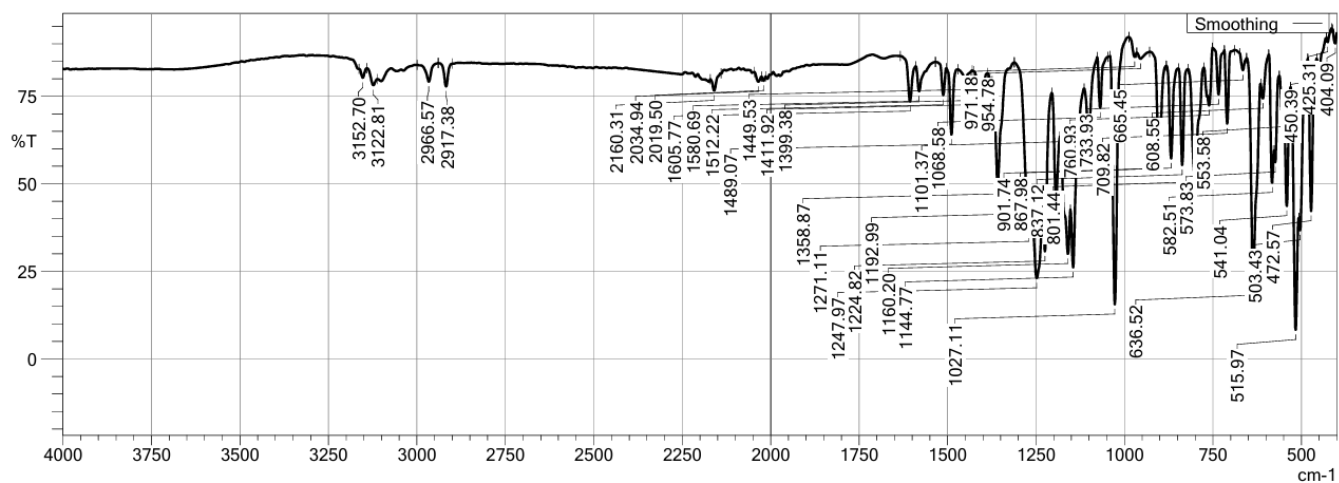


Fig. S131. IR data of compound **1f**

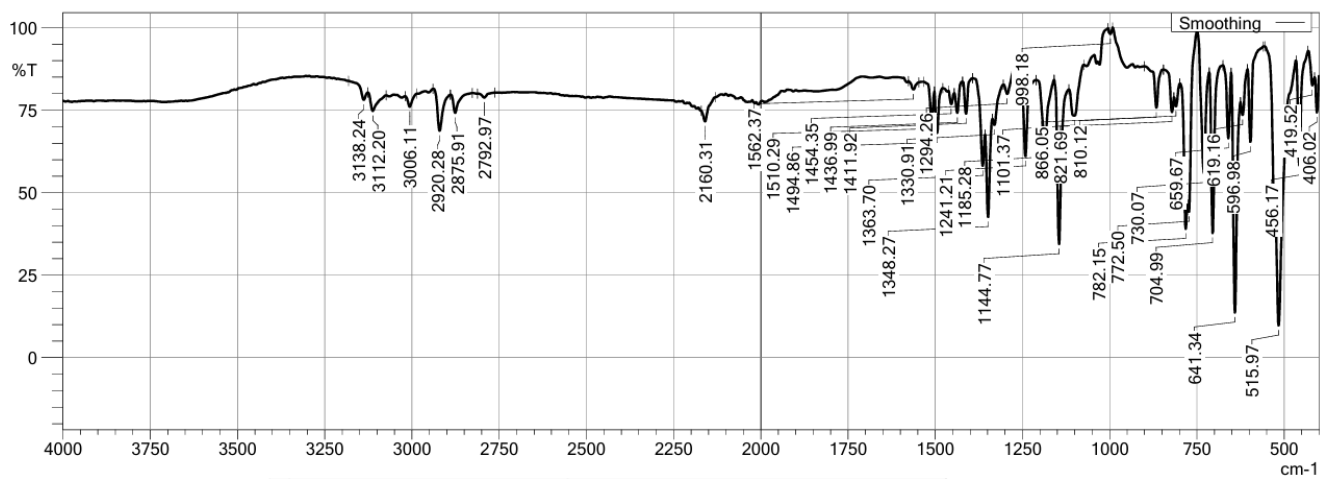


Fig. S132. IR data of compound **2f**

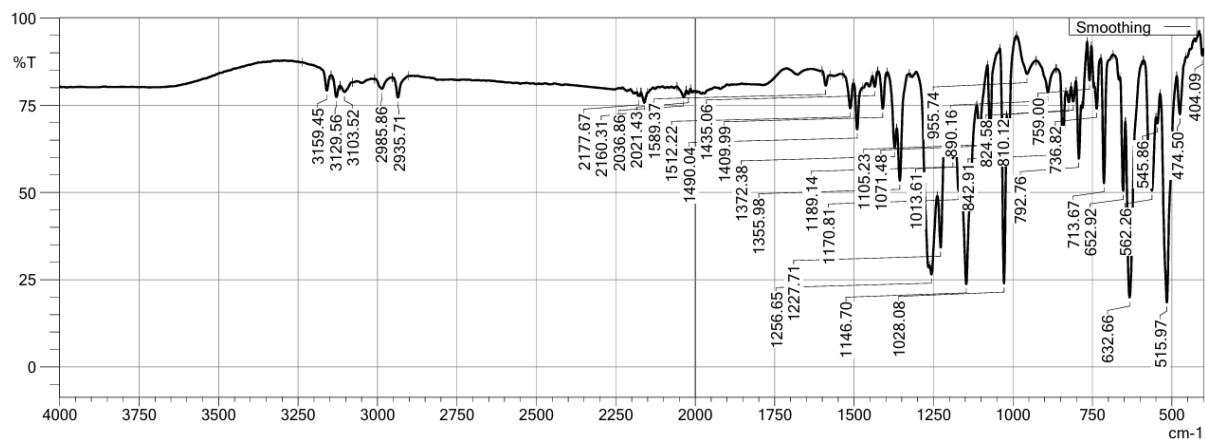


Fig. S133. IR data of compound 3f

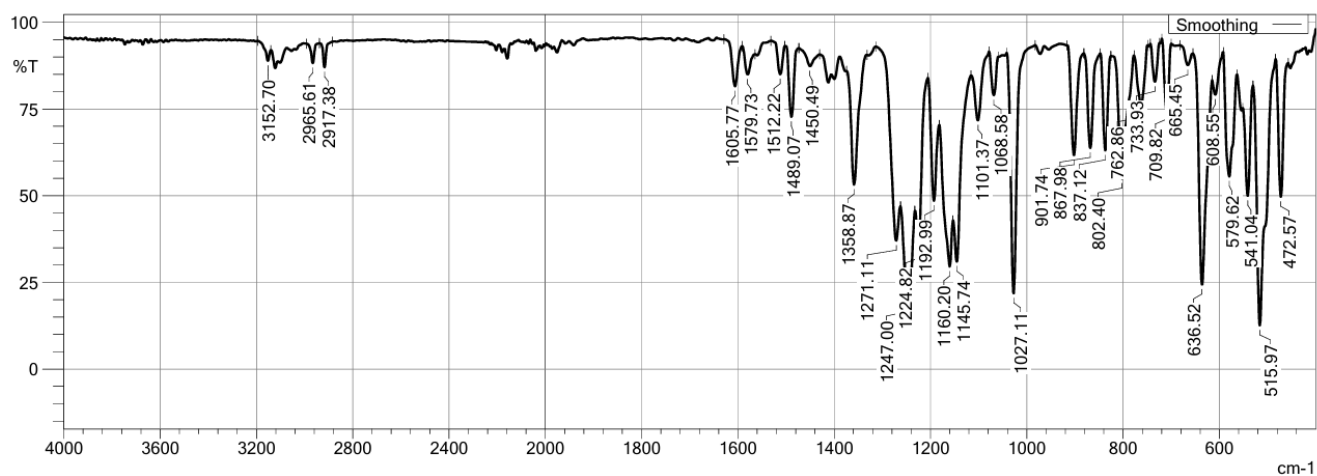


Fig. S134. IR data of compound 4f

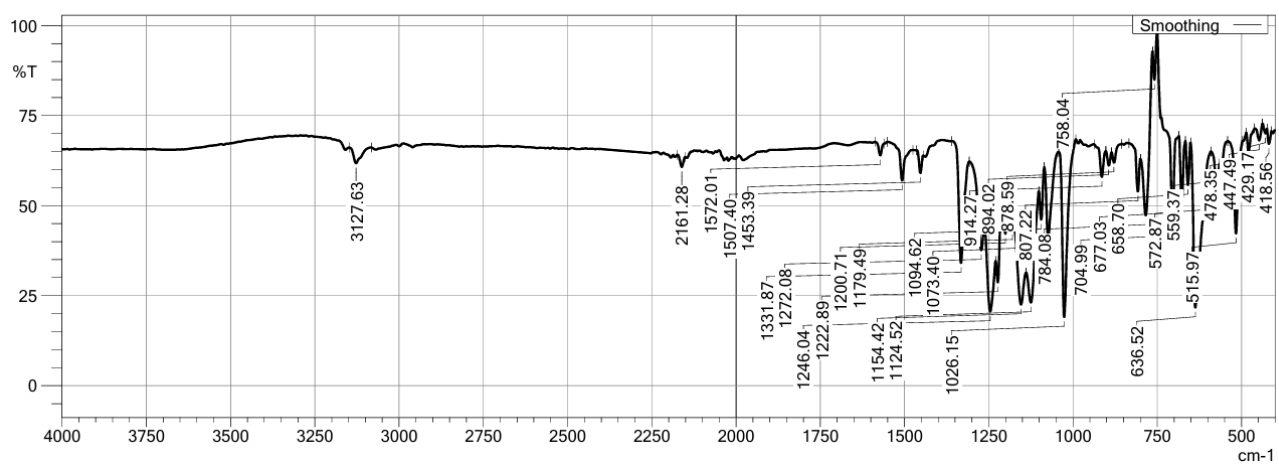


Fig. S135. IR data of compound 5f

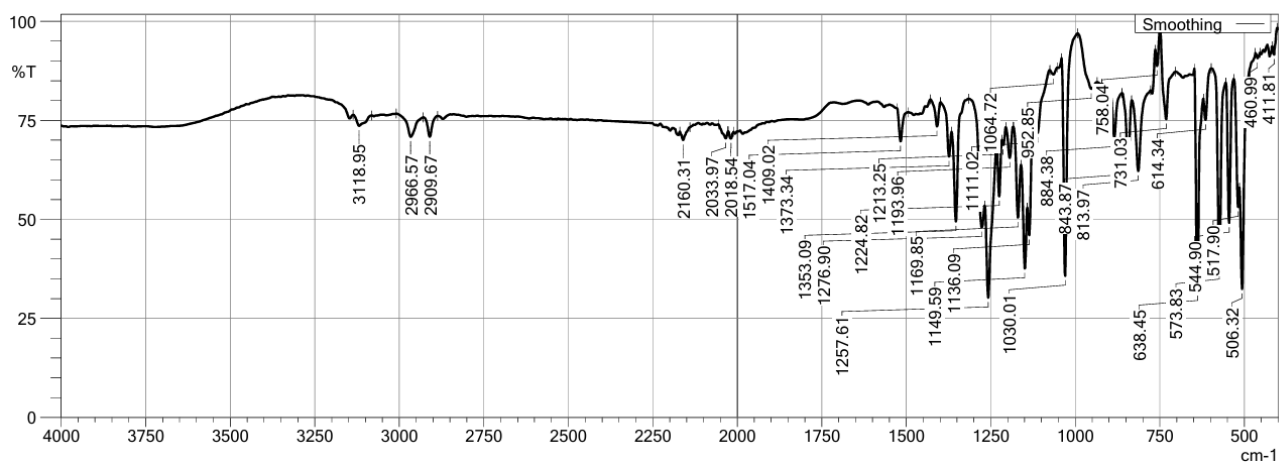


Fig. S136. IR data of compound 6f

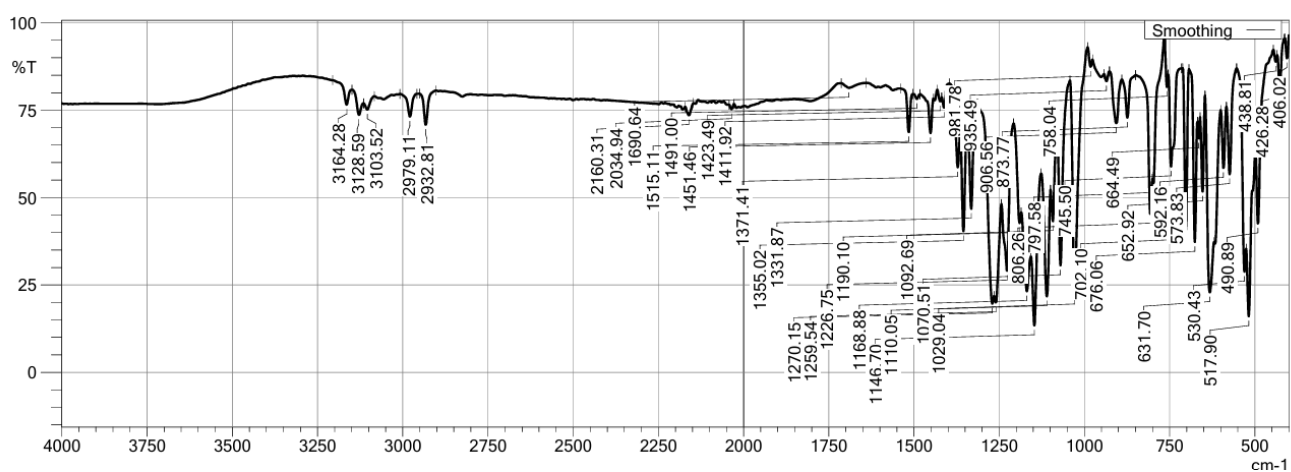


Fig. S137. IR data of compound 7f

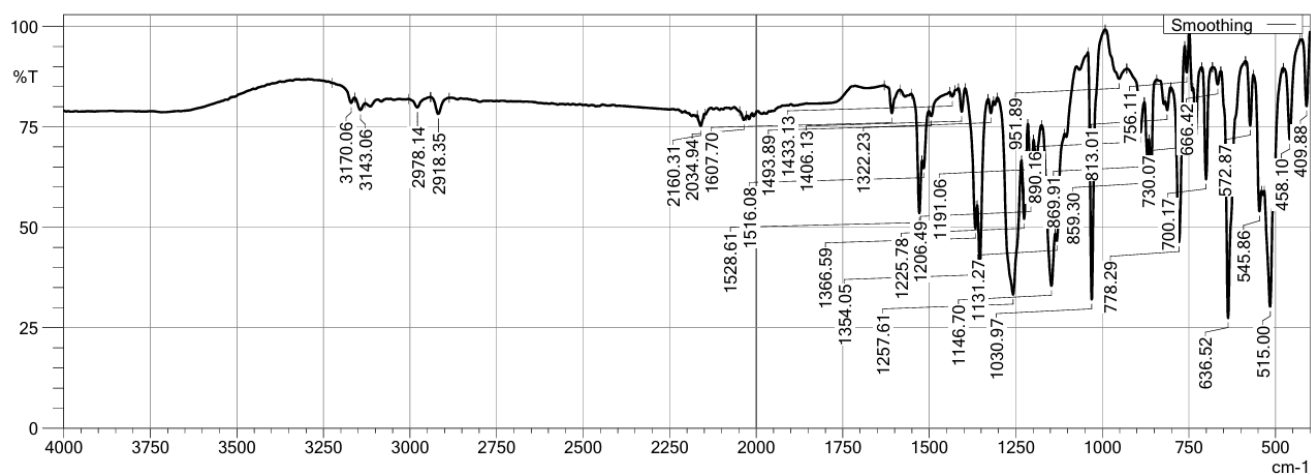
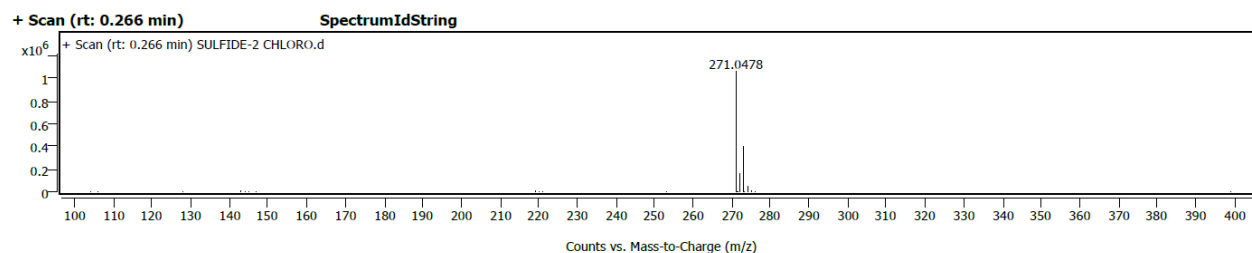


Fig. S138. IR data of compound 8f

HRMS DATAS OF THE COMPOUNDS (1d-8d)

(Compound 1d)

Peak Spec

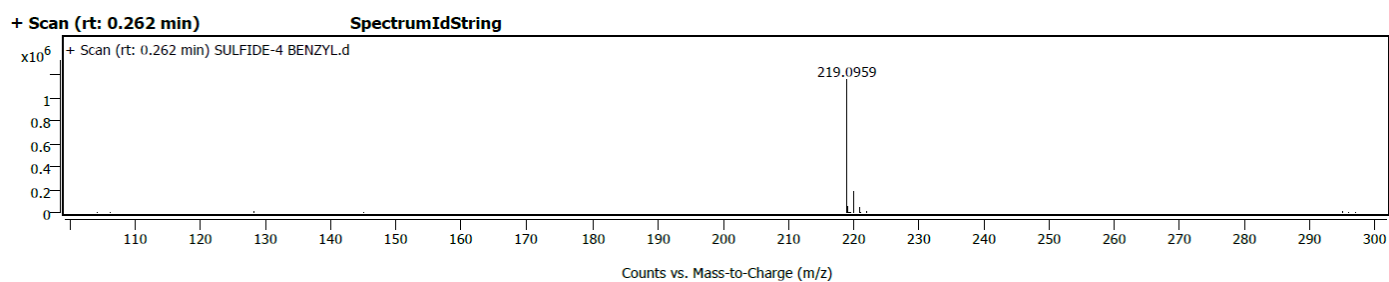


SpectrumIdString	m/z	Z	Abund	Abund %	m/z (Calc)	Diff (ppm)	Ion Species	Formula	Ion Type
	271.0478	1	1059720	100.00					
	271.0850		44763	4.22					
	271.1331		25904	2.44					
	272.0508	1	160251	15.12					
	272.0598		22309	2.11					
	273.0447	1	401807	37.92					
	273.0800		14144	1.33					
	274.0477	1	45160	4.26					

Fig. S139. HRMS spectrum of compound 1d

(Compound 2d)

Peak Spec

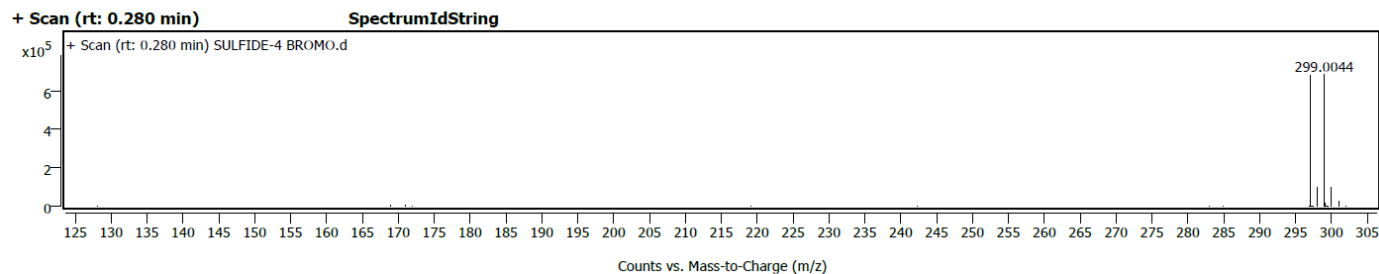


SpectrumIdString	m/z	Z	Abund	Abund %	m/z (Calc)	Diff (ppm)	Ion Species	Formula	Ion Type
	219.0959	1	1155276	100.00					
	219.1296		47360	4.10					
	219.1728		27160	2.35					
	220.0990	1	179415	15.53					
	221.0919		39266	3.40					
	221.1005	1	16401	1.42					

Fig. S140. HRMS spectrum of compound 2d

(Compound 3d)

Peak Spec

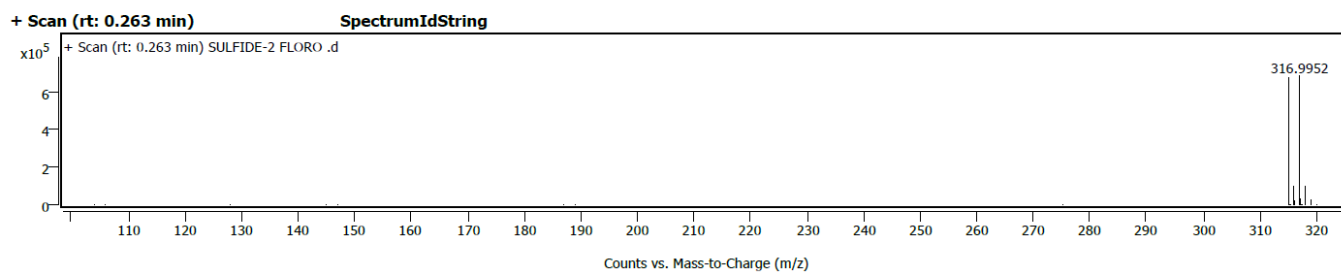


<i>SpectrumIdString</i>	<i>m/z</i>	<i>Z</i>	Abund	Abund %	<i>m/z (Calc)</i>	<i>Diff (ppm)</i>	<i>Ion Species</i>	<i>Formula</i>	<i>Ion Type</i>
	297.0065	1	678076	99.11					
	297.0450		29441	4.30					
	298.0096	1	96980	14.18					
	299.0044	1	684141	100.00					
	299.0428		30887	4.51					
	299.0940		16664	2.44					
	300.0074	1	97218	14.21					
	301.0018	1	22810	3.33					

Fig. S141. HRMS spectrum of compound **3d**

(Compound 4d)

Peak Spec

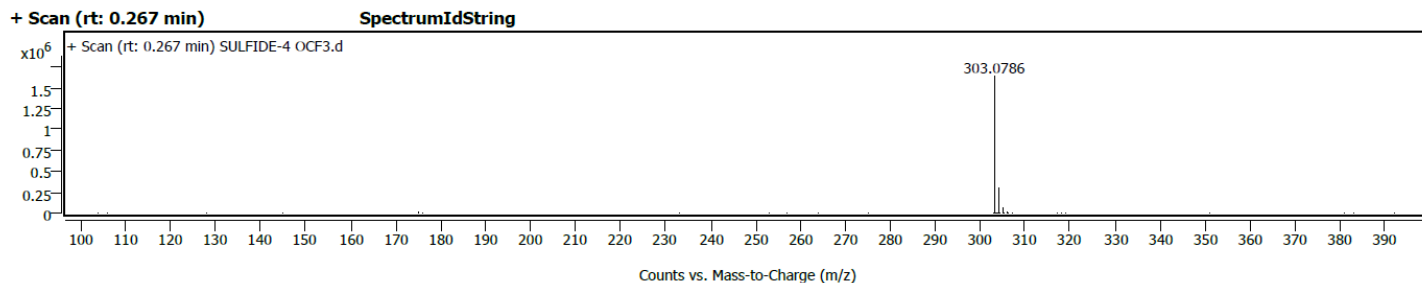


<i>SpectrumIdString</i>	<i>m/z</i>	<i>Z</i>	Abund	Abund %	<i>m/z (Calc)</i>	<i>Diff (ppm)</i>	<i>Ion Species</i>	<i>Formula</i>	<i>Ion Type</i>
	314.9973	1	671791	98.33					
	315.0367		28262	4.14					
	315.0890		17516	2.56					
	316.0003	1	96041	14.06					
	316.0115		18192	2.66					
	316.9952	1	683233	100.00					
	317.0347		30864	4.52					
	317.0872		19132	2.80					
	317.9984	1	95182	13.93					
	318.9927	1	22961	3.36					

Fig. S142. HRMS spectrum of compound **4d**

(Compound 5d)

Peak Spec

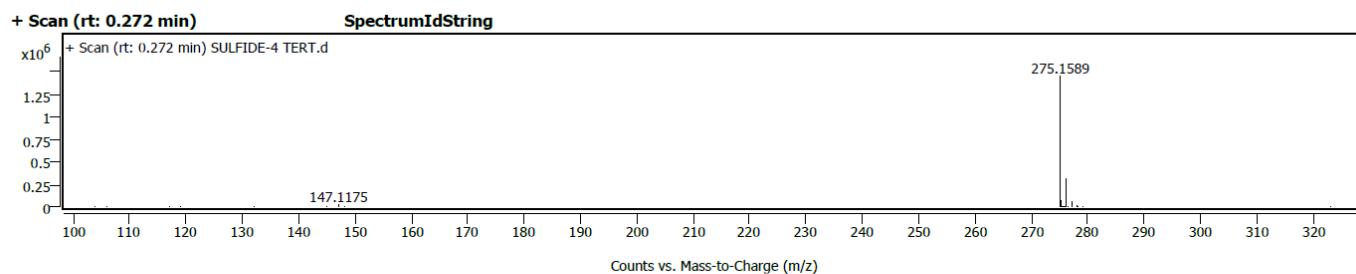


SpectrumIdString	m/z	Z	Abund	Abund %	m/z (Calc)	Diff (ppm)	Ion Species	Formula	Ion Type
	303.0786	1	1630154	100.00					
	303.0996	1	90715	5.56					
	303.1180		76652	4.70					
	303.1688		46090	2.83					
	304.0815	1	292996	17.97					
	304.0921	1	20264	1.24					
	305.0762	1	59830	3.67					

Fig. S143. HRMS spectrum of compound 5d

(Compound 6d)

Peak Spec

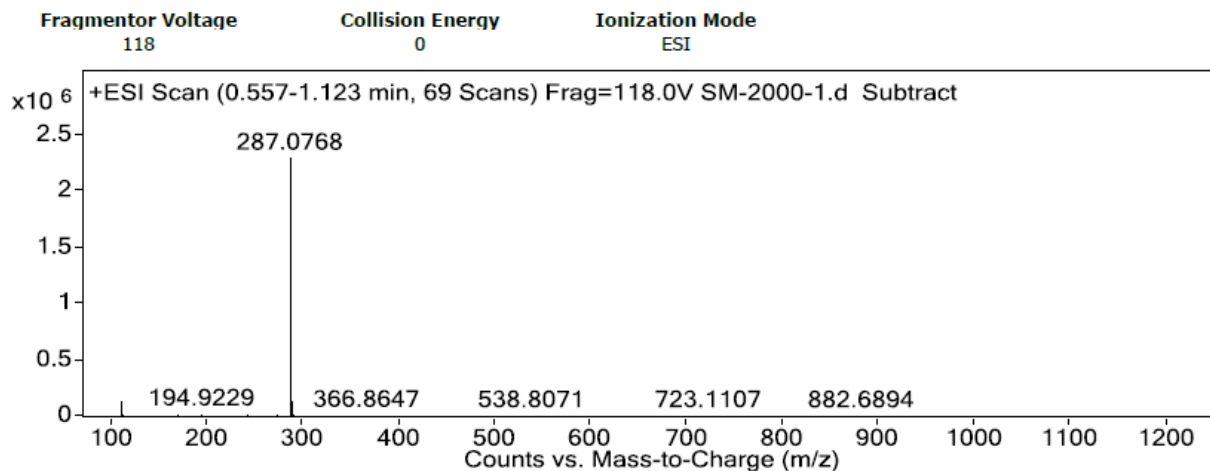


SpectrumIdString	m/z	Z	Abund	Abund %	m/z (Calc)	Diff (ppm)	Ion Species	Formula	Ion Type
	147.1175		21984	1.52					
	275.1589	1	1446506	100.00					
	275.1793	1	71361	4.93					
	275.1964		65994	4.56					
	275.2449		41352	2.86					
	276.1619	1	312441	21.60					
	276.1718	1	22725	1.57					
	277.1550		52456	3.63					
	277.1625	1	35961	2.49					

Fig. S144. HRMS spectrum of compound 6d

(Compound 7d)

User Spectra



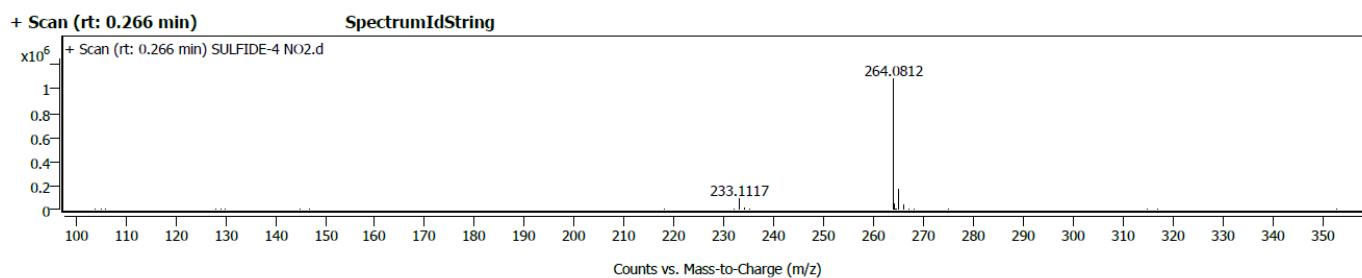
Peak List

m/z	z	Abund
111.0352	1	136191.94
113.0504	1	12543.04
169.0754	1	9813.88
194.9229	1	17520.89
273.0583	1	13568.95
287.0768	1	2296812.75

Fig. S145. HRMS spectrum of compound 7d

(Compound 8d)

Peak Spec



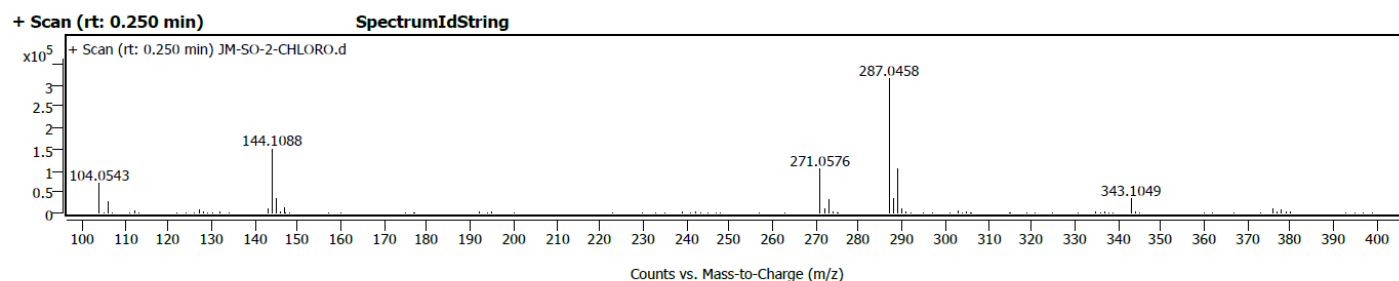
SpectrumIdString	m/z	Z	Abund	Abund %	m/z (Calc)	Diff (ppm)	Ion Species	Formula	Ion Type
	233.1117		89056	8.21					
	264.0812	1	1085375	100.00					
	264.1181		46757	4.31					
	264.1656		24965	2.30					
	265.0842	1	167222	15.41					
	265.0931		21625	1.99					
	266.0791	1	36637	3.38					

Fig. S146. HRMS spectrum of compound 8d

HRMS DATAS OF THE COMPOUNDS (1e-8e)

(Compound 1e)

Peak Spec

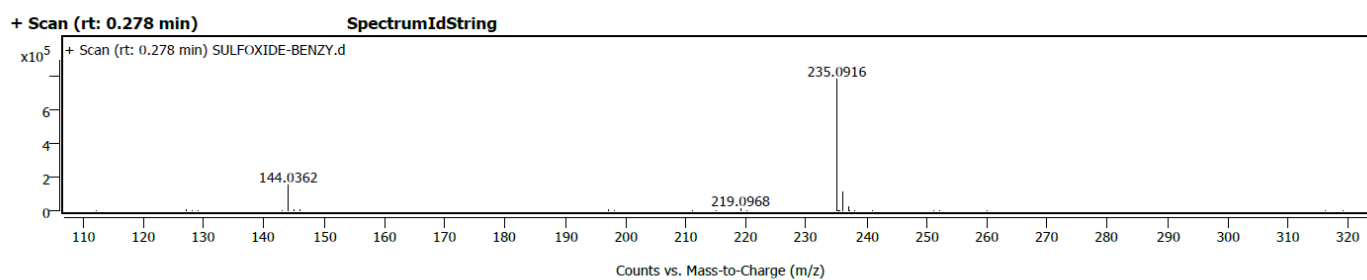


SpectrumIdString		Abund	Abund %	m/z (Calc)	Diff (ppm)	Ion Species	Formula	Ion Type
m/z	Z							
104.0543		69003	21.95					
106.0512		26920	8.56					
144.1088		150187	47.77					
145.0552		34238	10.89					
271.0576		103506	32.92					
273.0538		31716	10.09					
287.0458	1	314397	100.00					
288.0487	1	34011	10.82					
289.0419	1	104630	33.28					
343.1049		32492	10.33					

Fig. S147. HRMS spectrum of compound 1e

(Compound 2e)

Peak Spec

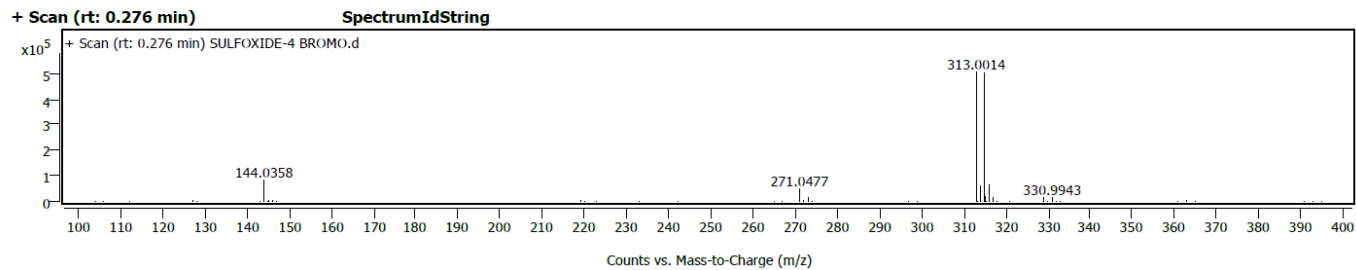


SpectrumIdString		Abund	Abund %	m/z (Calc)	Diff (ppm)	Ion Species	Formula	Ion Type
m/z	Z							
144.0362		154159	19.51					
144.0438		14706	1.86					
219.0968		10498	1.33					
235.0916	1	789985	100.00					
235.1259		30822	3.90					
236.0946	1	111757	14.15					
237.0877		25612	3.24					
237.0957	1	13033	1.65					

Fig. S148. HRMS spectrum of compound 2e

(Compound 3e)

Peak Spec

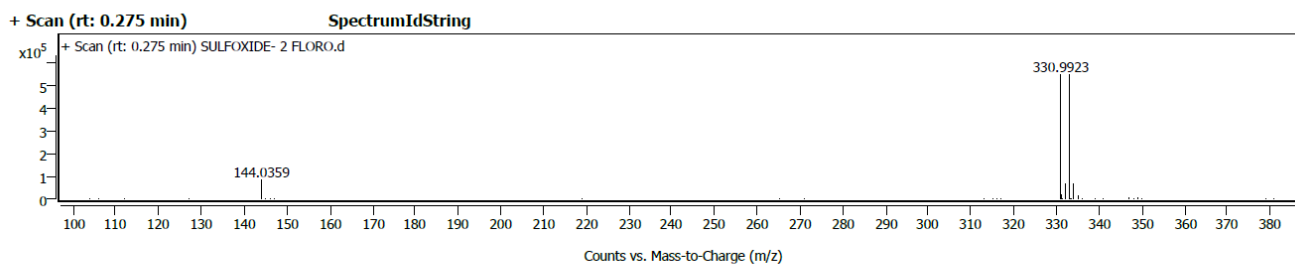


SpectrumIdString	m/z	Z	Abund	Abund %	m/z (Calc)	Diff (ppm)	Ion Species	Formula	Ion Type
	144.0358		82062	16.23					
	271.0477		47281	9.35					
	313.0014	1	505570	100.00					
	313.0402		19244	3.81					
	314.0047	1	58870	11.64					
	314.9993	1	504272	99.74					
	315.0381		18756	3.71					
	316.0024	1	62851	12.43					
	316.9972	1	13845	2.74					
	330.9943		14815	2.93					

Fig. S149. HRMS spectrum of compound 3e

(Compound 4e)

Peak Spec

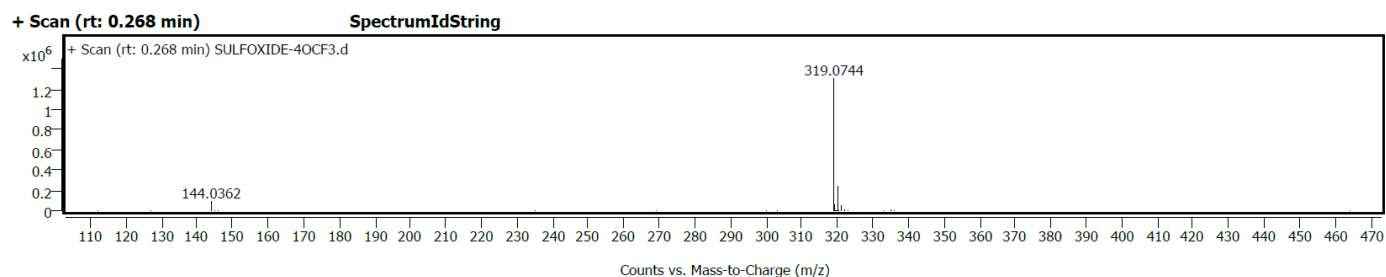


SpectrumIdString	m/z	Z	Abund	Abund %	m/z (Calc)	Diff (ppm)	Ion Species	Formula	Ion Type
	144.0359		84826	15.44					
	330.9923	1	549323	100.00					
	331.0323		20964	3.82					
	331.0863		13576	2.47					
	331.9954	1	68678	12.50					
	332.9902	1	548939	99.93					
	333.0301		22152	4.03					
	333.0847		12982	2.36					
	333.9933	1	69048	12.57					
	334.9881	1	15917	2.90					

Fig. S150. HRMS spectrum of compound 4e

(Compound 5e)

Peak Spec

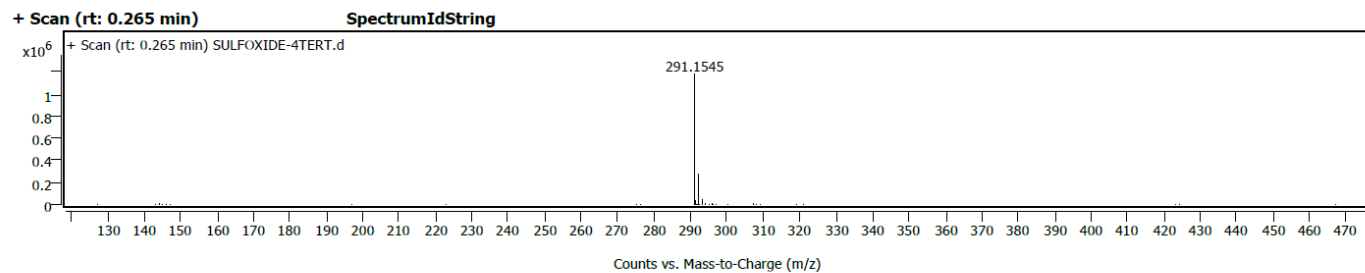


SpectrumIdString	m/z	Z	Abund	Abund %	m/z (Calc)	Diff (ppm)	Ion Species	Formula	Ion Type
	144.0362		94561	7.24					
	319.0744	1	1306992	100.00					
	319.0964	1	57612	4.41					
	319.1147		54508	4.17					
	319.1670		36223	2.77					
	320.0773	1	240371	18.39					
	320.0883	1	22806	1.74					
	321.0725	1	48561	3.72					

Fig. S151. HRMS spectrum of compound 5e

(Compound 6e)

Peak Spec

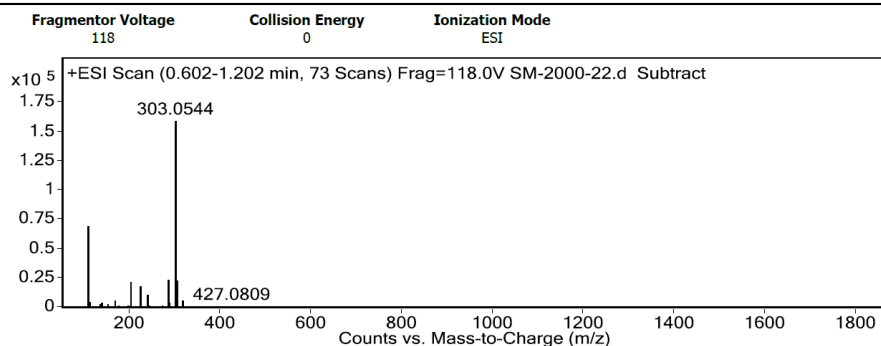


SpectrumIdString	m/z	Z	Abund	Abund %	m/z (Calc)	Diff (ppm)	Ion Species	Formula	Ion Type
	291.1545	1	1183333	100.00					
	291.1757		48804	4.12					
	291.1932		50444	4.26					
	291.2429		29913	2.53					
	292.1575	1	273633	23.12					
	293.1536	1	42725	3.61					

Fig. S152. HRMS spectrum of compound 6e

(Compound 7e)

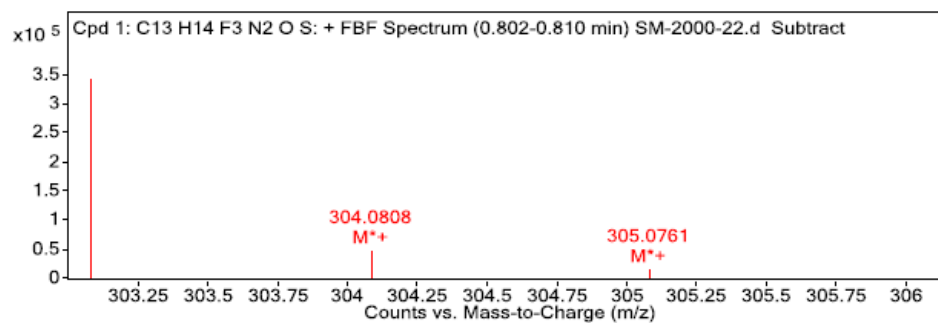
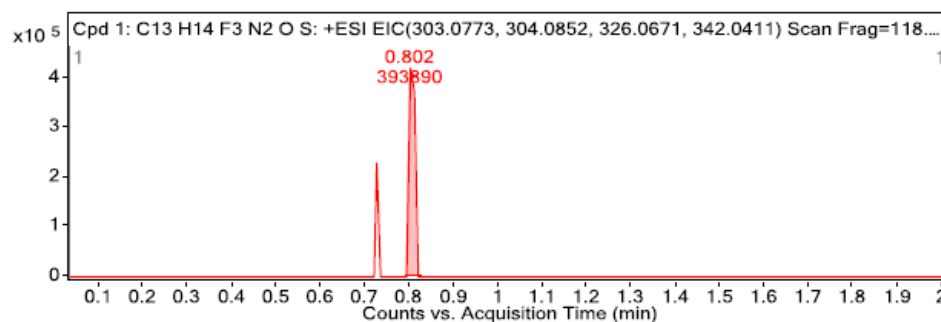
User Spectra



Peak List

<i>m/z</i>	<i>z</i>	Abund
108.9868	1	6364.35
110.9521	1	69461.4
203.0189	1	21658.67
225.0074	1	18221.76
242.2513	1	10799.57
287.0568	1	23602.17
303.0544	1	159331.55
304.0567	1	22652.58
305.0524	1	7896.24
319.0544	1	5993.04

Compounds



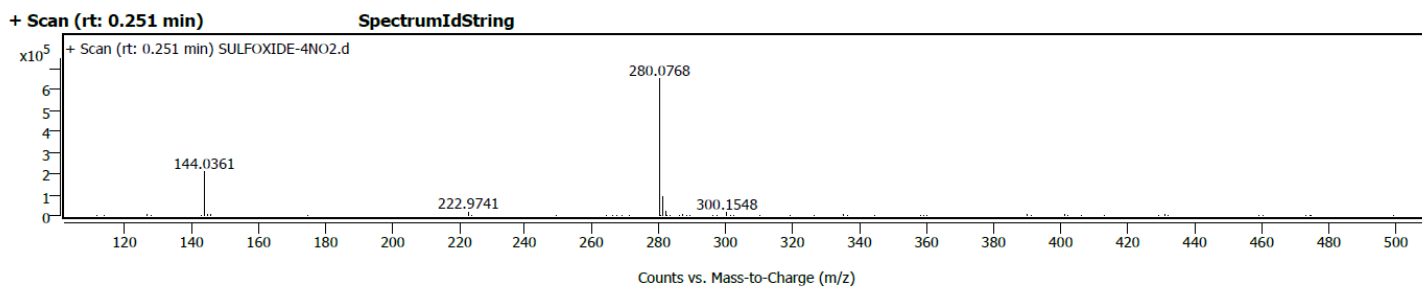
Peak List

<i>m/z</i>	<i>z</i>	Abund	Formula	Ion
303.0785	1	344159.31	C13H14F3N2O5	M*+
304.0808	1	49666.82	C13H14F3N2O5	M*+
305.0761	1	17474.68	C13H14F3N2O5	M*+
306.0796	1	2907.25	C13H14F3N2O5	M*+

Fig. S153. HRMS spectrum of compound 7e

(Compound 8e)

Peak Spec



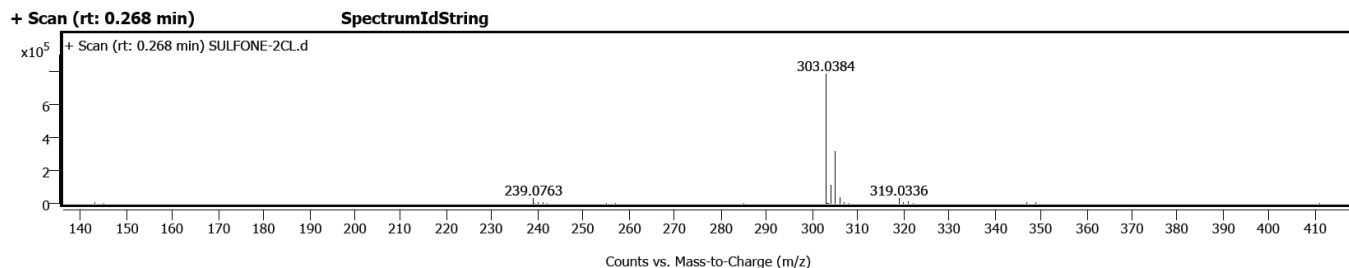
<i>SpectrumIdString</i>	m/z	Z	Abund	Abund %	m/z (Calc)	Diff (ppm)	Ion Species	Formula	Ion Type
	144.0361		208550	32.14					
	144.0439		18083	2.79					
	222.9741		15717	2.42					
	280.0768	1	648800	100.00					
	280.1140		25264	3.89					
	281.0800	1	87546	13.49					
	282.0753	1	20297	3.13					
	300.1548		13711	2.11					

Fig. S154. HRMS spectrum of compound 8e

HRMS DATAS OF THE COMPOUNDS (1f-8f)

(Compound 1f)

Peak Spec

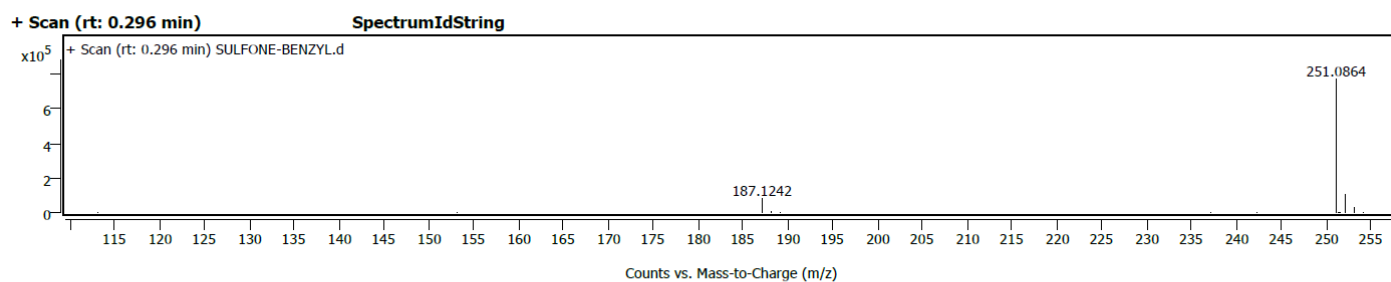


<i>SpectrumIdString</i>	m/z	Z	Abund	Abund %	m/z (Calc)	Diff (ppm)	Ion Species	Formula	Ion Type
	239.0763		27802	3.56					
	303.0384	1	780786	100.00					
	303.0772		32740	4.19					
	303.1287		18481	2.37					
	304.0415	1	110332	14.13					
	305.0354	1	313860	40.20					
	305.0447		25005	3.20					
	306.0386	1	33308	4.27					
	319.0336		27904	3.57					

Fig. S155. HRMS spectrum of compound 1f

(Compound 2f)

Peak Spec

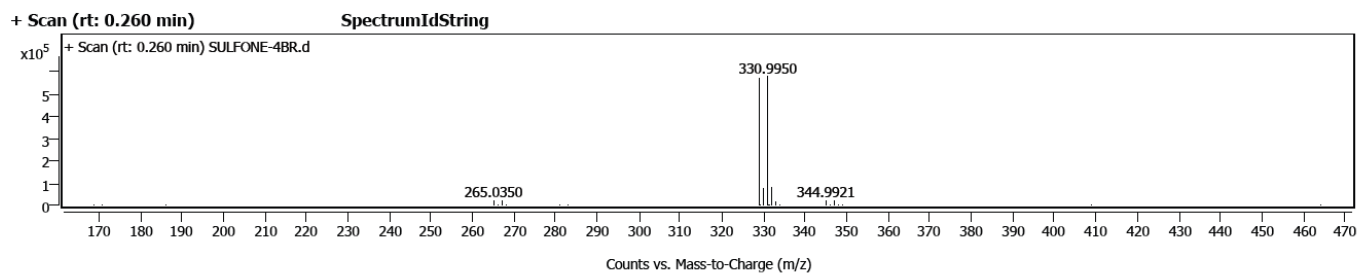


<i>SpectrumIdString</i>	m/z	Z	Abund	Abund %	m/z (Calc)	Diff (ppm)	Ion Species	Formula	Ion Type
	187.1242		80195	10.38					
	251.0864	1	772326	100.00					
	251.1219		30312	3.92					
	252.0895	1	104483	13.53					
	253.0841	1	25326	3.28					

Fig. S156. HRMS spectrum of compound 2f

(Compound 3f)

Peak Spec

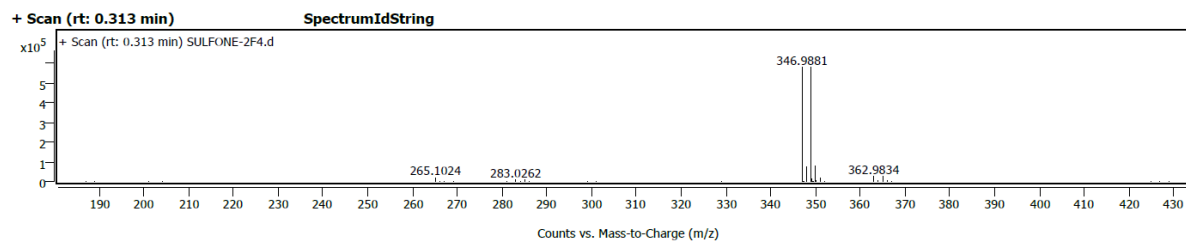


SpectrumIdString	m/z	Z	Abund	Abund %	m/z (Calc)	Diff (ppm)	Ion Species	Formula	Ion Type
	265.0350		21801	3.77					
	267.0332		21123	3.66					
	328.9971	1	570031	98.65					
	329.0371		23236	4.02					
	330.0002	1	78078	13.51					
	330.9950	1	577803	100.00					
	331.0350		23275	4.03					
	331.9980	1	78302	13.55					
	344.9921		21581	3.73					
	346.9901		21508	3.72					

Fig. S157. HRMS spectrum of compound 3f

(Compound 4f)

Peak Spec

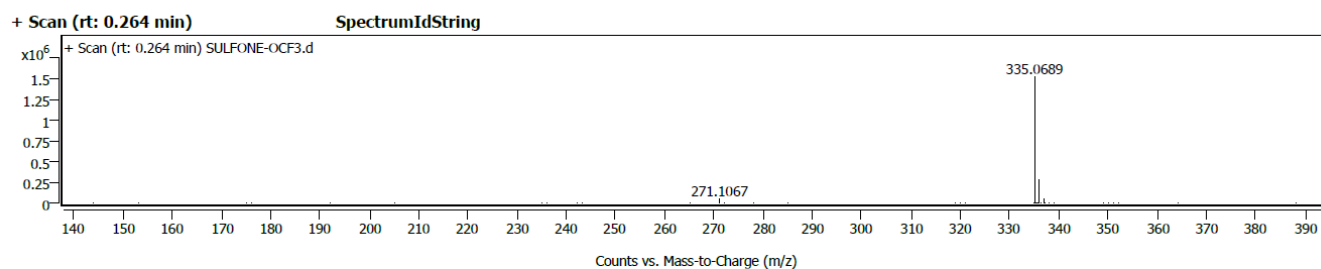


SpectrumIdString	m/z	Z	Abund	Abund %	m/z (Calc)	Diff (ppm)	Ion Species	Formula	Ion Type
	265.1024		17551	3.03					
	283.0262		6920	1.20					
	285.0243		6208	1.07					
	346.9881	1	578785	100.00					
	347.0288		22032	3.81					
	347.9913	1	74275	12.83					
	348.9861	1	578342	99.92					
	349.0270		23468	4.05					
	349.0828		13965	2.41					
	349.9892	1	78526	13.57					
	350.9845	1	17890	3.09					
	362.9834		24649	4.26					
	364.9812		24012	4.15					

Fig. S158. HRMS spectrum of compound 4f

(Compound 5f)

Peak Spec

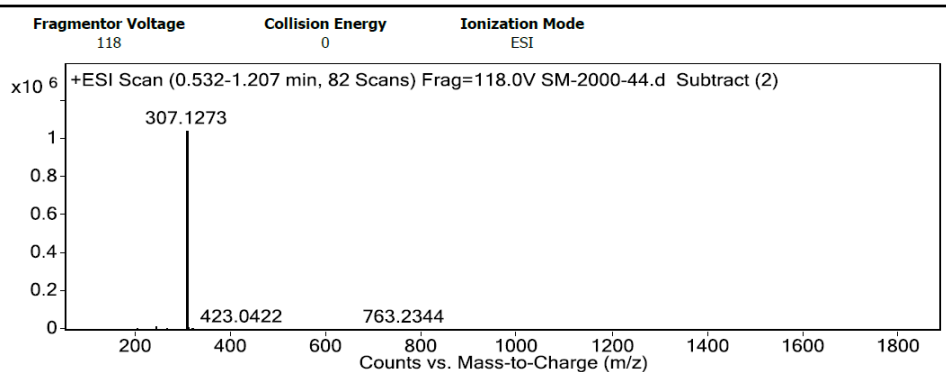


SpectrumIdString	m/z	Z	Abund	Abund %	m/z (Calc)	Diff (ppm)	Ion Species	Formula	Ion Type
	271.1067		54925	3.60					
	335.0689	1	1526019	100.00					
	335.0913		70300	4.61					
	335.1101		67737	4.44					
	335.1635		43074	2.82					
	336.0718	1	281132	18.42					
	337.0675	1	56532	3.70					

Fig. S159. HRMS spectrum of compound 5f

(Compound 6f)

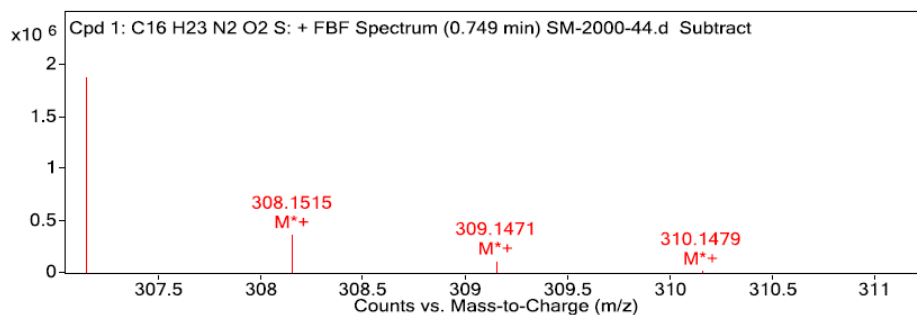
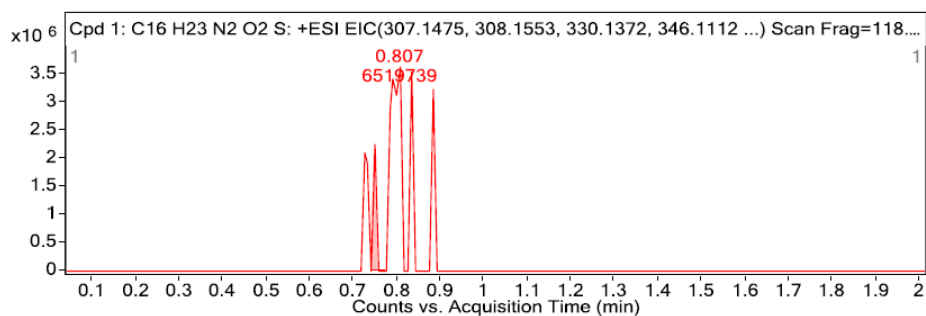
User Spectra



Peak List

m/z	z	Abund
203.0186	1	3802.13
243.1541	1	21019.6
244.1574	1	3665.28
265.0715	1	3292.87
307.1273	1	1045648.25
307.273		53974.18
308.1291	1	218458.7
309.1252	1	65153.61
310.1256	1	9611.72
319.0549	1	8144.65

Compounds



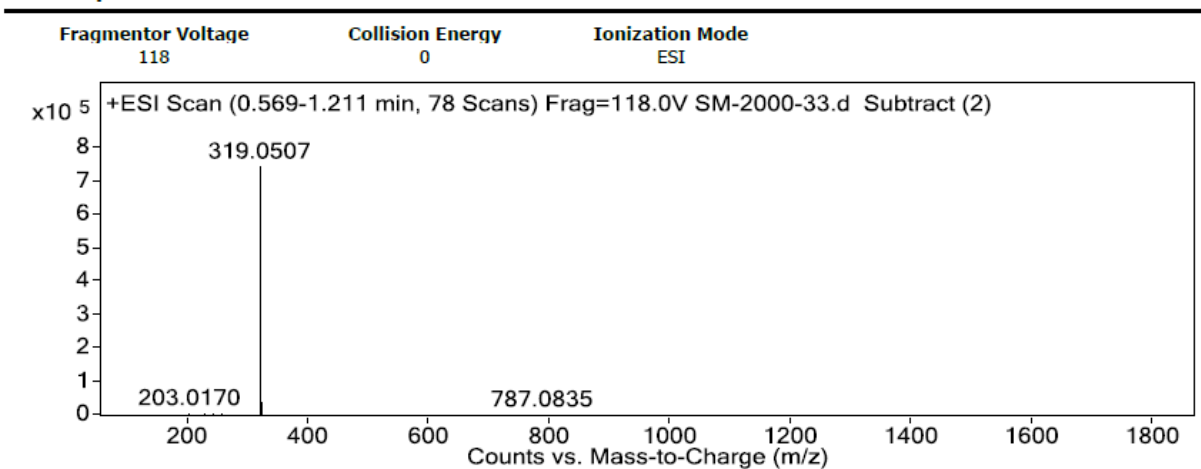
Peak List

m/z	z	Abund	Formula	Ion
307.1496	1	1882525.63	C ₁₆ H ₂₃ N ₂ O ₂ S	M*+
308.1515	1	368326.19	C ₁₆ H ₂₃ N ₂ O ₂ S	M*+
309.1471	1	115604.96	C ₁₆ H ₂₃ N ₂ O ₂ S	M*+
310.1479	1	18221.96	C ₁₆ H ₂₃ N ₂ O ₂ S	M*+
311.1446	1	2374.77	C ₁₆ H ₂₃ N ₂ O ₂ S	M*+

Fig. S160. HRMS spectrum of compound 6f

(Compound 7f)

User Spectra



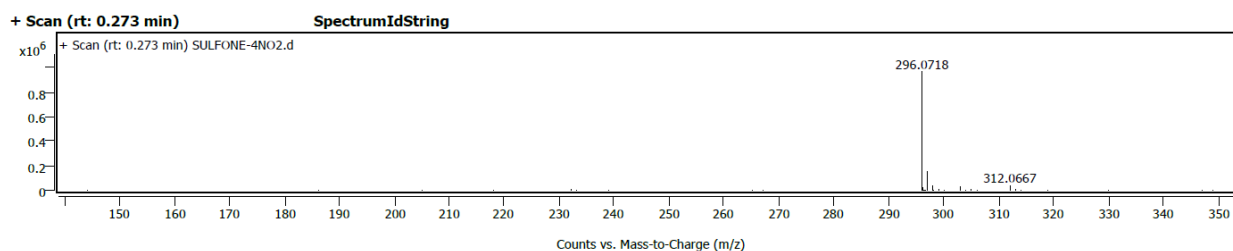
Peak List

m/z	z	Abund
203.017	1	4324.97
225.0069	1	2400.84
242.2499	1	2750.08
255.0785	1	3737.81
287.0538		2151.81
319.0507	1	743757.5

Fig. S161. HRMS spectrum of compound 7f

(Compound 8f)

Peak Spec



SpectrumIdString	m/z	Z	Abund	Abund %	m/z (Calc)	Diff (ppm)	Ion Species	Formula	Ion Type
	296.0718	1	964905	100.00					
	296.1106		40975	4.25					
	296.1610		22353	2.32					
	297.0749	1	153702	15.93					
	298.0705	1	34171	3.54					
	303.0385		26652	2.76					
	312.0667		36808	3.81					

Fig. S162. HRMS spectrum of compound 8f

X-ray Crystallography

On Hampton cryoloops, crystals were mounted. A HyPix3000 (CCD plate) detector with increasing ω (width of 0.3_ per frame) and a microfocus sealed X-ray tube Mo-K α ($\lambda = 0.71073 \text{ \AA}$) X-ray source was used with a SuperNova (Mo) X-ray diffractometer to collect all geometric and intensity data for the crystals at either 5 or 10 s/frame scan speed. CrysAlisPro software was used for both the data acquisition and extraction. Olex2¹ was used to solve the structure using the SIR2004² structure solution program utilizing direct methods. The ShelXL6³ refinement package then used least squares minimization to refine the structure. Anisotropic thermal parameters were used in the refinement of all nonhydrogen atoms. All the H-atoms were added with calculated positions. Details of crystallographic data and structural refinement parameters are summarized in Table S2, S4 and S6 for the compounds **1d**, **1e** and **1f** and geometrical parameters for are listed in Table S3, S5 and S7 for the compounds **1d**, **1e** and **1f**. CCDC number for **1d**, **1e** and **1f** is respectively 2339882, 2335137 and 2339878.

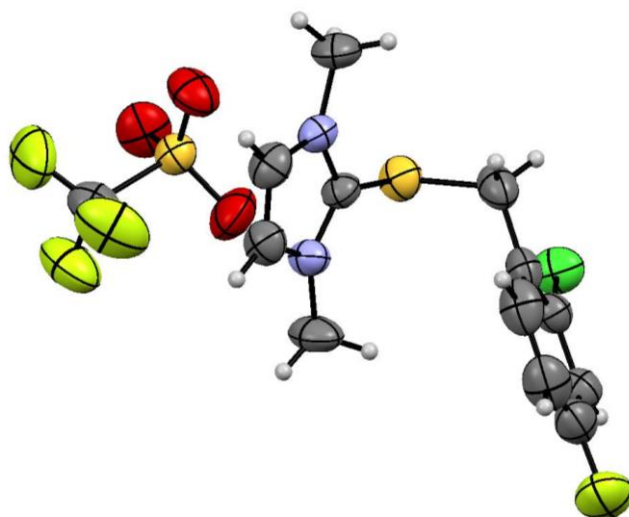


Fig. S163. ORTEP diagram for **1d** at 50% probability.

Table S2. List of crystallographic parameters for the crystal structure 1d.

CCDC number	2332405
Identification code	Ex-JMSO2A2_auto
Empirical formula	C ₁₃ H ₁₃ ClF ₄ N ₂ O ₃ S ₂
Formula weight	420.82
Temperature/K	293(2)
Crystal system	triclinic
Space group	P-1
a/Å	7.7328(7)
b/Å	7.9098(6)
c/Å	15.8738(9)
α/°	82.544(6)
β/°	81.102(6)
γ/°	67.567(9)
Volume/Å³	883.98(12)
Z	2
ρ_{calc}/cm³	1.581
μ/mm⁻¹	0.507
F(000)	428.0
Crystal size/mm³	0.008 × 0.005 × 0.004
Radiation	Mo Kα (λ = 0.71073)
2θ range for data collection/°	6.348 to 54.19
Index ranges	-9 ≤ h ≤ 9, -9 ≤ k ≤ 10, -19 ≤ l ≤ 17
Reflections collected	10987
Independent reflections	3596 [R _{int} = 0.0355, R _{sigma} = 0.0476]
Data/restraints/parameters	3596/0/228
Goodness-of-fit on F²	1.083
Final R indexes [I ≥ 2σ (I)]	R ₁ = 0.0482, wR ₂ = 0.1094
Final R indexes [all data]	R ₁ = 0.0780, wR ₂ = 0.1258

Table S3. Geometrical parameters of 1d.

Bond	Length	Bond	Length
S2 O1	1.427(2)	N2 C2	1.364(3)
S2 O2	1.421(2)	N2 C4	1.467(3)
S2 O3	1.418(2)	F2 C13	1.313(4)
S2 C13	1.815(3)	F3 C13	1.316(4)
S1 C1	1.733(3)	C8 C7	1.386(4)
S1 C6	1.844(3)	C8 C9	1.379(4)
C11 C8	1.733(3)	C7 C6	1.492(4)
F1 C10	1.362(4)	C7 C12	1.383(4)
F4 C13	1.321(3)	C3 C2	1.343(4)
N1 C1	1.340(3)	C9 C10	1.364(4)
N1 C3	1.367(3)	C10 C11	1.352(5)
N1 C5	1.455(3)	C12 C11	1.376(5)
N2 C1	1.335(3)		
Bond Angle	Angle	Bond Angle	Angle
O1 S2 C13	103.52(14)	C8 C7 C6	122.1(3)
O2 S2 O1	115.10(15)	C12 C7 C8	116.4(3)
O2 S2 C13	102.70(16)	C12 C7 C6	121.5(3)
O3 S2 O1	115.54(16)	C2 C3 N1	107.2(3)
O3 S2 O2	114.55(15)	C10 C9 C8	116.8(3)
O3 S2 C13	102.90(17)	C3 C2 N2	107.6(3)
C1 S1 C6	99.69(13)	F1 C10 C9	117.5(3)
C1 N1 C3	108.7(2)	C11 C10 F1	119.3(3)
C1 N1 C5	126.0(2)	C11 C10 C9	123.2(3)
C3 N1 C5	125.2(2)	C7 C6 S1	113.2(2)
C1 N2 C2	108.8(2)	C11 C12 C7	121.8(3)
C1 N2 C4	125.7(2)	F4 C13 S2	111.9(2)
C2 N2 C4	125.3(2)	F2 C13 S2	111.8(2)
N1 C1 S1	125.6(2)	F2 C13 F4	107.0(3)
N2 C1 S1	126.6(2)	F2 C13 F3	106.5(3)
N2 C1 N1	107.7(2)	F3 C13 S2	111.1(3)
C7 C8 C11	118.9(2)	F3 C13 F4	108.4(3)
C9 C8 C11	117.9(2)	C10 C11 C12	118.6(3)
C9 C8 C7	123.2(3)		

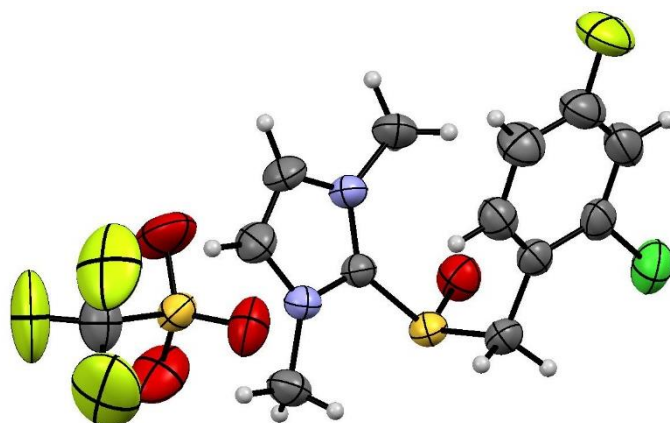


Fig. S164. ORTEP diagram for **1e** (2335137) at 50% probability.

Table S4. List of crystallographic parameters for the crystal structure **1e**.

Identification code	Ex-NipJmSO2Cl4F_autored
Empirical formula	C ₁₃ H ₁₃ ClF ₄ N ₂ O ₄ S ₂
Formula weight	436.82
Temperature/K	293(2)
Crystal system	monoclinic
Space group	P2 ₁ /n
a/Å	6.1258(3)
b/Å	25.4289(9)
c/Å	11.3897(4)
α/°	90
β/°	93.209(4)
γ/°	90
Volume/Å ³	1771.42(12)
Z	4
ρ _{calc} /cm ³	1.638
μ/mm ⁻¹	0.514
F(000)	888.0
Crystal size/mm ³	0.011 × 0.01 × 0.008
Radiation	Mo Kα (λ = 0.71073)
2θ range for data collection/°	6.408 to 54.13
Index ranges	-7 ≤ h ≤ 6, -32 ≤ k ≤ 31, -14 ≤ l ≤ 14
Reflections collected	16277
Independent reflections	3565 [R _{int} = 0.0562, R _{sigma} = 0.0393]
Data/restraints/parameters	3565/0/237
Goodness-of-fit on F ²	1.063
Final R indexes [I ≥ 2σ (I)]	R ₁ = 0.0576, wR ₂ = 0.1622
Final R indexes [all data]	R ₁ = 0.0749, wR ₂ = 0.1749

Table S5. Geometrical parameters of 1e.

Bond	Length	Bond	Length
S1 O1	1.474(3)	N2 C5	1.467(4)
S1 C1	1.790(3)	F1 C10	1.369(4)
S1 C6	1.831(3)	C7 C6	1.502(4)
S2 O2	1.417(3)	C7 C8	1.390(5)
S2 O4	1.427(3)	C7 C12	1.381(4)
S2 O3	1.396(3)	C8 C9	1.370(5)
S2 C13	1.797(4)	F4 C13	1.275(5)
C11 C12	1.739(4)	C12 C11	1.383(5)
N1 C1	1.336(3)	C3 C2	1.349(5)
N1 C4	1.467(4)	F2 C13	1.322(5)
N1 C3	1.367(4)	F3 C13	1.300(5)
N2 C1	1.336(4)	C11 C10	1.360(6)
N2 C2	1.374(4)	C9 C10	1.365(6)
Angle	Bond angle	Angle	Bond angle
O1 S1 C1	106.69(14)	C12 C7 C8	117.5(3)
O1 S1 C6	109.00(15)	C7 C6 S1	113.6(2)
C1 S1 C6	96.88(15)	C9 C8 C7	121.6(3)
O2 S2 O4	111.94(18)	C7 C12 C11	120.2(3)
O2 S2 C13	104.87(19)	C7 C12 C11	122.3(3)
O4 S2 C13	103.0(2)	C11 C12 C11	117.5(3)
O3 S2 O2	117.4(2)	C2 C3 N1	107.8(3)
O3 S2 O4	113.8(2)	C3 C2 N2	106.9(3)
O3 S2 C13	104.0(2)	C10 C11 C12	116.9(3)
C1 N1 C4	128.3(3)	C10 C9 C8	117.8(4)
C1 N1 C3	108.4(3)	C11 C10 F1	117.8(4)
C3 N1 C4	123.3(3)	C11 C10 C9	123.8(3)
C1 N2 C2	108.7(2)	C9 C10 F1	118.3(4)
C1 N2 C5	126.3(3)	F4 C13 S2	113.6(3)
C2 N2 C5	124.9(3)	F4 C13 F2	108.1(4)
N1 C1 S1	128.7(2)	F4 C13 F3	108.7(4)
N2 C1 S1	122.9(2)	F2 C13 S2	109.7(3)
N2 C1 N1	108.3(3)	F3 C13 S2	111.5(3)
C8 C7 C6	119.6(3)	F3 C13 F2	104.7(4)
C12 C7 C6	122.8(3)		

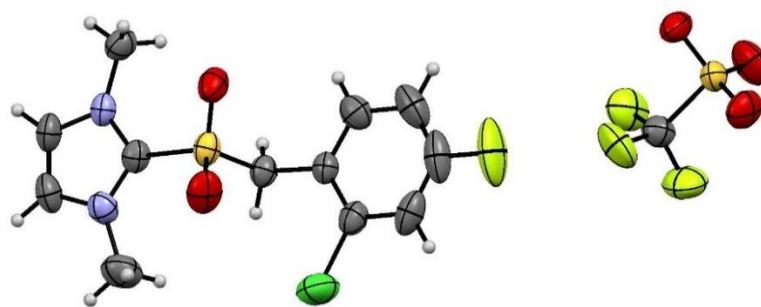


Fig. S165. ORTEP diagram for **1f** (2339878) at 50% probability.

Table S6. List of crystallographic parameters for the crystal structure **1f**.

CCDC number	2339878
Identification code	Ex-JMSO2
Empirical formula	C ₅₂ H ₅₂ Cl ₄ F ₁₆ N ₈ O ₂₀ S ₈
Formula weight	1811.29
Temperature/K	293(2)
Crystal system	Monoclinic
Space group	P2 ₁ /n
a/Å	7.7355(4)
b/Å	10.8997(5)
c/Å	21.2900(10)
α/°	90
β/°	92.262(4)
γ/°	90
Volume/Å³	1793.66(12)
Z	1
ρ_{calc}/cm³	1.677
μ/mm⁻¹	0.515
F(000)	920.0
Crystal size/mm³	0.011 × 0.008 × 0.006
Radiation	Mo Kα (λ = 0.71073)
2θ range for data collection/°	6.462 to 54.248
Index ranges	-9 ≤ h ≤ 9, -13 ≤ k ≤ 13, -27 ≤ l ≤ 26
Reflections collected	17191
Independent reflections	3648 [R _{int} = 0.0597, R _{sigma} = 0.0607]
Data/restraints/parameters	3648/0/246
Goodness-of-fit on F²	1.057
Final R indexes [I ≥ 2σ (I)]	R ₁ = 0.0505, wR ₂ = 0.1094
Final R indexes [all data]	R ₁ = 0.0903, wR ₂ = 0.1256

Table S7. Geometrical parameters of 1f.

Bond	Bond length	Bond	Bond length
S2 O3	1.429(2)	N2 C2	1.362(4)
S2 O5	1.432(2)	N1 C1	1.338(4)
S2 O4	1.423(2)	N1 C3	1.365(4)
S2 C13	1.812(3)	N1 C5	1.478(4)
S1 O2	1.424(2)	F1 C10	1.350(4)
S1 O1	1.423(2)	C7 C6	1.496(4)
S1 C1	1.782(3)	C7 C8	1.387(4)
S1 C6	1.772(3)	C7 C12	1.380(4)
C11 C8	1.725(3)	C3 C2	1.334(4)
F2 C13	1.315(3)	C8 C9	1.392(5)
F4 C13	1.312(4)	C12 C11	1.380(5)
F3 C13	1.316(4)	C9 C10	1.357(5)
N2 C1	1.346(4)	C10 C11	1.351(5)
N2 C4	1.470(4)		
Angle	Bond angle	Angle	Bond angle
O3 S2 O5	113.71(15)	N2 C1 S1	125.4(2)
O3 S2 C13	103.34(15)	N1 C1 S1	126.4(2)
O5 S2 C13	103.03(14)	N1 C1 N2	107.9(3)
O4 S2 O3	115.82(16)	C7 C6 S1	108.47(19)
O4 S2 O5	115.02(17)	F2 C13 S2	111.7(2)
O4 S2 C13	103.62(16)	F2 C13 F3	106.4(3)
O2 S1 C1	105.89(13)	F4 C13 S2	112.0(2)
O2 S1 C6	109.42(14)	F4 C13 F2	107.3(3)
O1 S1 O2	119.60(14)	F4 C13 F3	108.2(3)
O1 S1 C1	106.31(14)	F3 C13 S2	111.0(2)
O1 S1 C6	110.21(14)	C2 C3 N1	108.2(3)
C6 S1 C1	104.18(13)	C3 C2 N2	107.6(3)
C1 N2 C4	128.4(2)	C7 C8 C11	120.6(2)
C1 N2 C2	108.3(3)	C7 C8 C9	121.4(3)
C2 N2 C4	123.3(3)	C9 C8 C11	118.0(3)
C1 N1 C3	108.0(3)	C11 C12 C7	121.3(3)
C1 N1 C5	127.5(3)	C10 C9 C8	117.8(3)
C3 N1 C5	124.3(3)	F1 C10 C9	117.1(4)
C8 C7 C6	123.0(3)	F1 C10 C11	119.8(4)
C12 C7 C6	119.2(3)	C11 C10 C9	123.1(4)
C12 C7 C8	117.7(3)	C10 C11 C12	118.7(3)

References

1. O. V. Dolomanov, L. J. Bourhis, R. J. Gildea, J. A. Howard, H. Puschmann, *J. Appl. Crystallogr.*, 2009, 42, 339-341.
2. M. C. Burla, R. Caliandro, M. Camalli, B. Carrozzini, G. L. Cascarano, L. De Caro, C. Giacovazzo, G. Polidori, D. Siliqi and R. Spagna, *J. Appl. Crystallogr.*, 2007, 40, 609-613.
3. G. M. Sheldrick, *Acta Crystallogr. Sect. C: Struct. Chem.*, 2015, 71, 3-8.

4. Computational Details

Table S8. The geometrical data comparison between experimental and quantum chemical study.

Methodology	C ₁ →S Bond Length (Å)		
	1d	1e	1f
Experimental	1.732	1.790	1.782
M06-2x/6-311+G (2d,p)	1.743	1.821	1.809
M06-2x/def2tzvpp	1.738	1.812	1.803
B3LYP/6-311+G (2d,p)	1.747	1.844	1.853
M06-2x/6-311+G (2d,p)/SDD	1.759	1.933	2.011
B3LYP/6-311+G (2d,p)/SDD	1.763	2.015	2.153
MPW1PW91/6-311+G (2d,p)	1.736	1.820	1.810
CAM-B3LYP/6-311+G (2d,p)	1.744	1.827	1.814
HF/6-311+G (2d,p)	1.757	1.814	1.808

Table S9. List of absolute Gibbs free energy values of all optimized geometries associated with Table 1 of the main manuscript obtained at MPW1PW91/6-311++G(2d,p) level of quantum chemical level

Str.	E (a.u.)
1a	-1492.870411
1b	-1568.053685
1c	-1643.279358
1d	-1532.529003
1e	-1607.697595
1f	-1682.919423
1,3-dimethyl-imidazole-2-ylidene	-304.711360
frag-1 (1a, 1b and 1c)	-264.846013
frag-2 (1a and 1d)	-1227.683953
frag-2 (1b and 1e)	-1302.888703
frag-2 (1c and 1f)	-1378.092772

Table S10. List of absolute Gibbs free energy values of all optimized geometries associated with Table 1 of the main manuscript obtained at MPW1PW91/ 6-311++G(2d,p) level of quantum chemical chemistry.

Str.	E (a.u.)	Str.	E (a.u.)
1a	-1492.870411	1d	-1532.529003
2a	-933.969021	2d	-973.631687
3a	-3507.684727	3d	-3547.344148
4a	-3606.941311	4d	-3646.602089
5a	-1346.270926	5d	-1385.928898
6a	-1091.126247	6d	-1130.791406
7a	-1271.051632	7d	-1310.709825
8a	-1138.489577	8d	-1178.142522
1b	-1568.053685	1e	-1607.697595
2b	-1009.153730	2e	-1048.803932
3b	-3582.870088	3e	-3622.516492
4b	-3682.124915	4e	-3721.768998
5b	-1421.456259	5e	-1461.101011
6b	-1166.311318	6e	-1205.964001
7b	-1346.236097	7e	-1385.881962
8b	-1213.674366	8e	-1253.313922
1c	-1643.279358	1f	-1682.919423
2c	-1084.379803	2f	-1124.022422
3c	-3658.095655	3f	-3697.734946
4c	-3757.350755	4f	-3796.990704
5c	-1496.681926	5f	-1536.319903
6c	-1241.537488	6f	-1281.182451
7c	-1421.462460	7f	-1461.099396
8c	-1288.899593	8f	-1328.532407

Table S11. Comparison of NMR (Experimental vs. Theoretical)

Methodology	¹³ C NMR SHIFT OF (1a) (ppm)	¹³ C NMR SHIFT OF (1d) (ppm)	Difference in the ¹³ C NMR value (ppm)	¹³ C NMR (1b) (ppm)	¹³ C NMR SHIFT OF (1e) (ppm)	Difference in the ¹³ C NMR value (ppm)	¹³ C NMR SHIFT OF (1c) (ppm)	¹³ C NMR SHIFT OF (1f) (ppm)	Difference in the ¹³ C NMR value (ppm)
Experimental	139.99	138.33	-1.66	145.21	141.80	-3.41	140.68	137.66	-3.02
M06-2x/6-311+G (2d,p)	159.58	160.19	0.61	160.37	162.08	1.71	162.66	157.27	-5.39
M06-2x/def2tzvpp	161.01	162.35	1.34	161.60	163.29	1.69	163.49	158.40	-5.09
B3LYP/6-311+G (2d,p)	151.15	150.81	-0.34	150.93	152.31	1.38	154.18	150.03	-4.15
M06-2x/6-311+G (2d,p)/SDD	146.38	155.40	9.02	135.57	156.82	21.25	142.28	156.04	13.76
B3LYP/6-311+G (2d,p)/SDD	139.42	141.23	1.81	129.97	151.00	21.03	138.31	157.29	18.98
MPW1PW91/6-311+G (2d,p)	147.56	146.35	-1.21	145.38	147.05	1.67	149.97	144.84	-5.13
CAM-B3LYP/6-311+G (2d,p)	152.93	152.02	-0.91	150.45	152.41	1.96	154.54	149.75	-4.79
HF/6-311+G (2d,p)	153.46	154.28	0.82	150.28	154.49	4.21	151.15	149.22	-1.93

Table S12. Second order delocalisation energies ($E^{(2)}$) in **1e and **1f** at MPW1PW91/ 6-311++G(2d,p) levels**

Structure	$E^{(2)a}$	$E_1^a - E_1^b$	F_{ij}^b
1e (Sulfoxide)			
(LP-3 of O)			
$n_{O} \rightarrow \sigma^*_{C(1)-S}$	23.59	0.40	0.089
$n_{O} \rightarrow \sigma^*_{C(2)-S}$	8.00	0.41	0.052
(LP-2 of O)			
$n_{O} \rightarrow \sigma^*_{C(1)-S}$	3.95	0.41	0.036
$n_{O} \rightarrow \sigma^*_{C(2)-S}$	15.45	0.42	0.072
1f (Sulfone)			
(LP-3 of O₁)			
$n_{O(1)} \rightarrow \sigma^*_{C(1)-S}$	19.55	0.42	0.081
$n_{O(1)} \rightarrow \sigma^*_{O(2)-S}$	18.57	0.64	0.100
(LP-2 of O₁)			
$n_{O(1)} \rightarrow \sigma^*_{C(1)-S}$	7.57	0.42	0.051
$n_{O(1)} \rightarrow \sigma^*_{O(2)-S}$	7.14	0.64	0.061
$n_{O(1)} \rightarrow \sigma^*_{C(2)-S}$	19.57	0.45	0.084
(LP-3 of O₂)			
$n_{O(2)} \rightarrow \sigma^*_{C(1)-S}$	16.77	0.42	0.075
$n_{O(2)} \rightarrow \sigma^*_{O(1)-S}$	21.23	0.63	0.106
(LP-2 of O₂)			
$n_{O(2)} \rightarrow \sigma^*_{C(1)-S}$	10.33	0.42	0.059
$n_{O(2)} \rightarrow \sigma^*_{O(2)-S}$	4.87	0.63	0.050
$n_{O(2)} \rightarrow \sigma^*_{C(2)-S}$	20.66	0.45	0.086

Conformational Search For **1d**

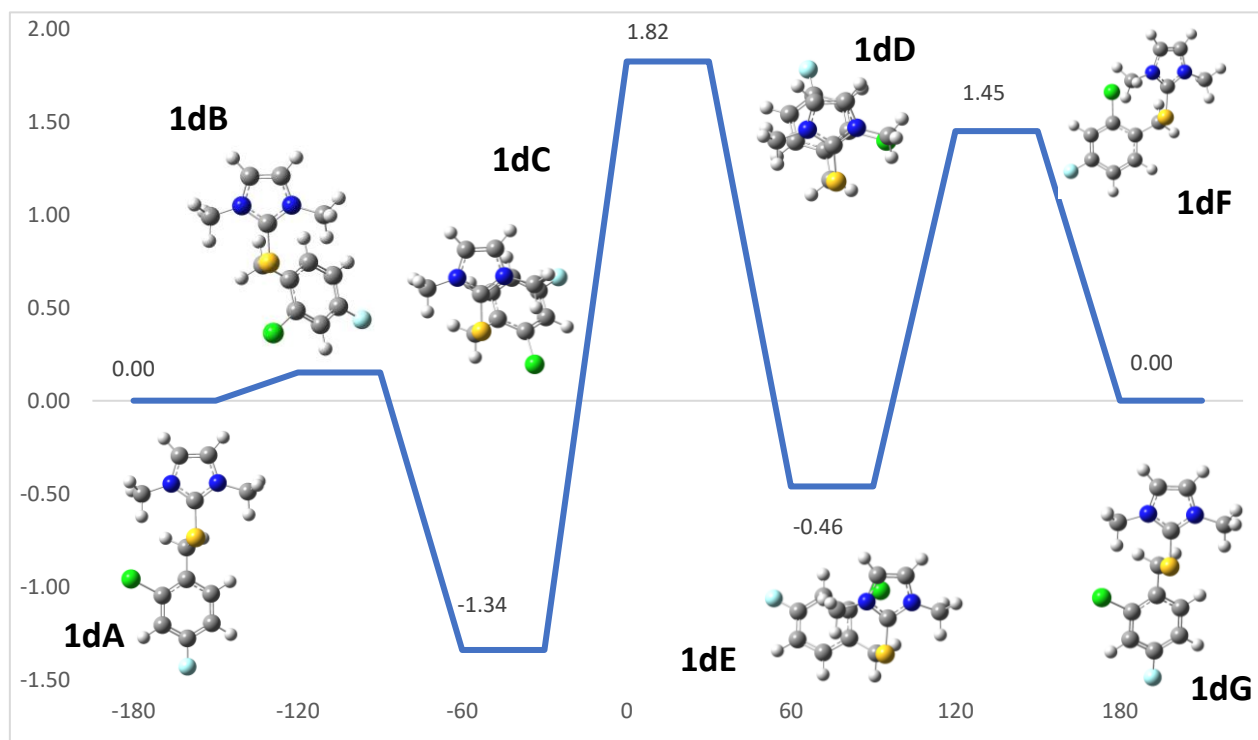


Fig. S166. Conformational analysis of **1d** around S-C₂ bond. Energy differences values are provided in kcal/mol.

Table S13. List of absolute energy values of all the conformers of cationic sulfide (**1d**) derivative obtained at MPW1PW91/ 6-311++G(2d,p) level of quantum chemical chemistry.

Conformer	Energy (a.u.)
1dA	-1532.716156
1dB	-1532.715914
1dC	-1532.718292
1dD	-1532.713248
1dE	-1532.716889
1dF	-1532.713846
1dG	-1532.716156

Conformational Search For **1e**

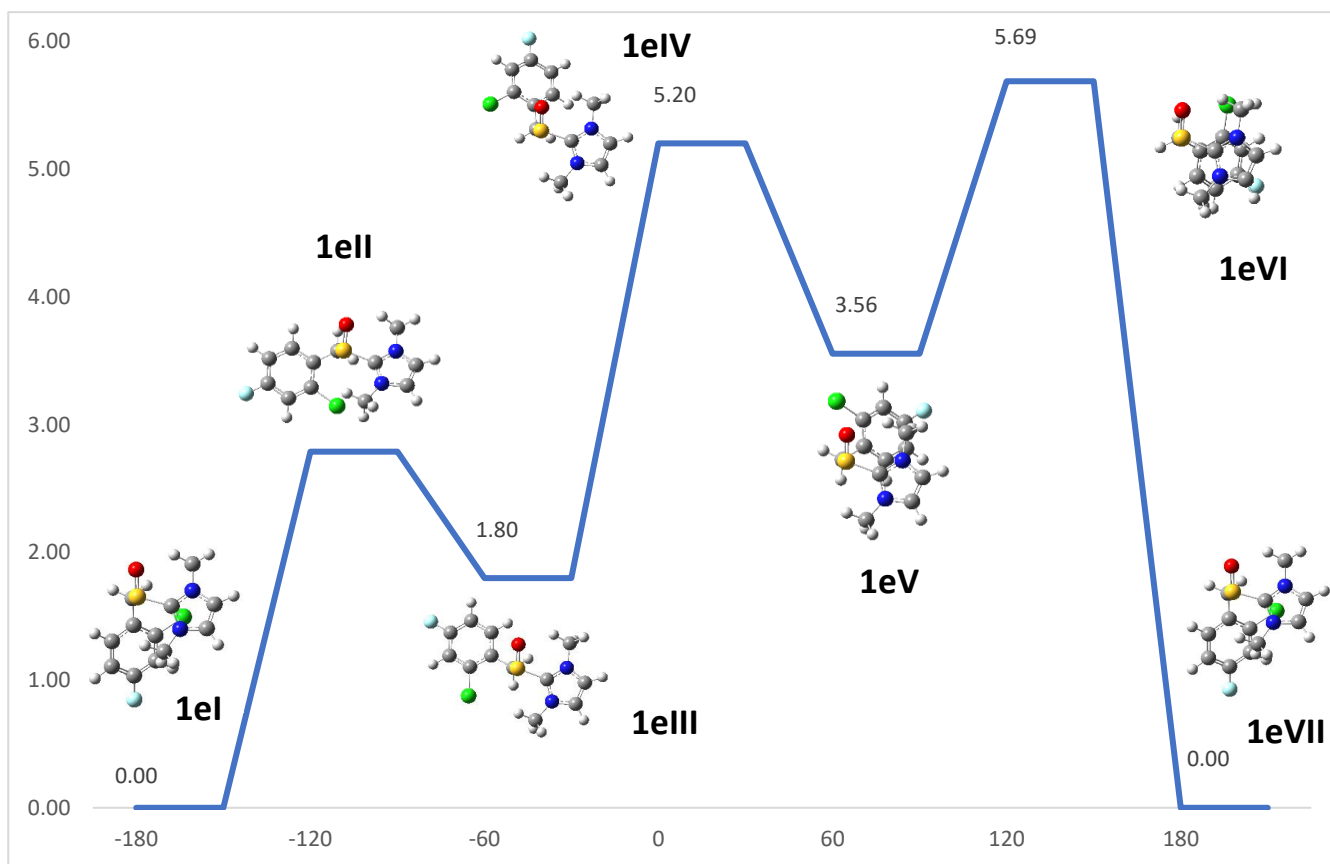


Fig. S167. Conformational analysis of **1e** around S-C₂ bond. Energy differences values are provided in kcal/mol.

Table S14. List of absolute energy values of all conformers of cationic sulfoxide (**1e**) derivative obtained at MPW1PW91/6-311++G(2d,p) level of quantum chemical chemistry.

Conformer	Energy (a.u.)
1eI	-1607.893972
1eII	-1607.889529
1eIII	-1607.891107
1eIV	-1607.885680
1eV	-1607.888306
1eVI	-1607.884904
1eVII	-1607.893972

Conformational Search For **1f**

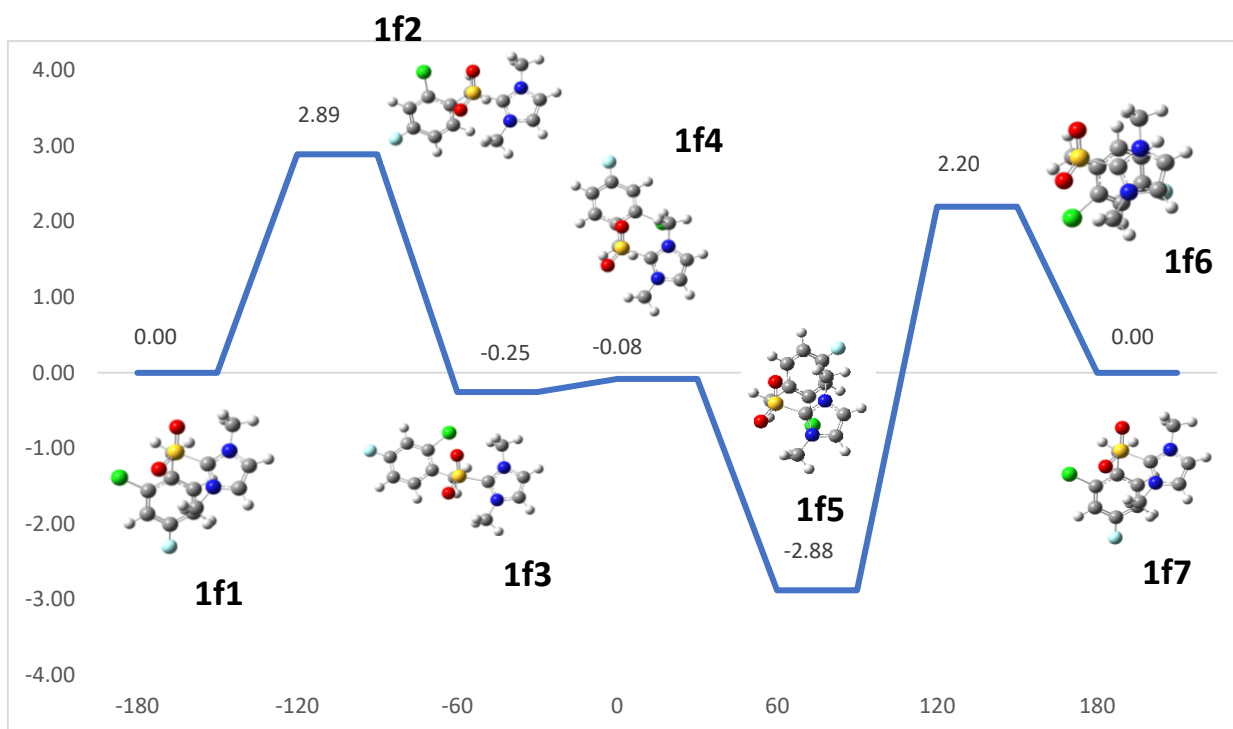


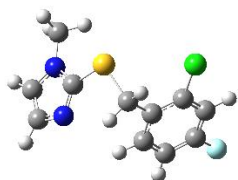
Fig. S168. Conformational analysis of **1f** around S-C₂ bond. Energy differences values are provided in kcal/mol.

Table S15. List of absolute energy values of all conformers of cationic sulfone (**1f**) derivative obtained at MPW1PW91/6-311++G(2d,p) level of quantum chemical chemistry.

Conformer	Energy (a.u.)
1f1	-1683.113673
1f2	-1683.109067
1f3	-1683.114078
1f4	-1683.113803
1f5	-1683.118262
1f6	-1683.110171
1f7	-1683.113673

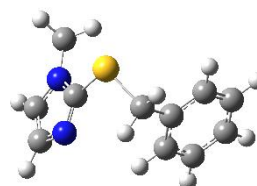
Cartesian Coordinates of All Optimized Geometries at MPW1PW91/6-311++G(2d,p) level

1a



H	4.12699400	1.46167200	1.68361300
H	3.75692200	0.08027800	2.73621000

2a



0 1

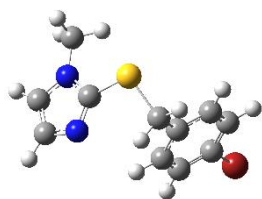
S	1.29592300	1.51598300	-0.29572500
Cl	-2.23617300	2.39786100	0.14559600
F	-3.94634300	-2.23720200	1.00580000
N	2.31195800	-0.89276400	-1.14762200
N	3.15141300	-0.16106300	0.76801000
C	2.27863300	0.06317500	-0.25026200
C	-2.11938900	0.67099100	-0.03810300
C	-1.07353500	0.11402900	-0.77229200
C	3.25417000	-1.77746800	-0.69596300
H	3.48842300	-2.67762900	-1.24083200
C	-3.09343400	-0.10696600	0.56368600
H	-3.90163700	0.33777300	1.12651900
C	3.79222900	-1.34217500	0.47695700
H	4.55078900	-1.74942000	1.12330500
C	-3.00751500	-1.47681100	0.42494800
C	-0.02087400	0.94250000	-1.43069900
H	-0.42949900	1.86307300	-1.84408600
H	0.47788600	0.38774500	-2.22226400
C	-1.03837100	-1.27489500	-0.88200700
H	-0.22399300	-1.72172800	-1.43818200
C	-1.99470900	-2.08195600	-0.28931800
H	-1.96279300	-3.15953700	-0.37635800
C	3.39153500	0.68749700	1.91024300
H	2.45814200	1.16250200	2.21051600

0 1

S	-0.78176100	-1.77091200	-0.24218300
N	-1.78679100	0.52705000	-1.34529100
N	-2.34240500	0.22398800	0.77865300
C	-1.66269300	-0.25627100	-0.29960500
C	2.61100700	-0.97653500	0.30456500
C	1.66188200	-0.43824600	-0.56161900
C	-2.58023000	1.55897000	-0.93208300
H	-2.84526500	2.36736100	-1.59442400
C	3.52176300	-0.15876300	0.95284200
H	4.25767400	-0.59300700	1.61896200
C	-2.94661600	1.38602700	0.37043100
H	-3.56661800	1.96607400	1.03258600
C	3.49446500	1.21409000	0.74571700
C	0.67638100	-1.31923300	-1.26015700
H	1.11289900	-2.28514600	-1.51688000
H	0.28767000	-0.86184700	-2.16774500
C	1.64449700	0.93847600	-0.76672600
H	0.90672000	1.36318000	-1.43677100
C	2.55437200	1.75923600	-0.11544200
H	2.52977900	2.82900000	-0.28530400

C	-2.43507100	-0.36822600	2.09158700
H	-1.54076200	-0.96060600	2.27678300
H	-3.31214800	-1.01252400	2.17570500
H	-2.49865800	0.42113000	2.83877500
H	2.63537000	-2.04801400	0.47189500
H	4.20734300	1.85457200	1.25075800

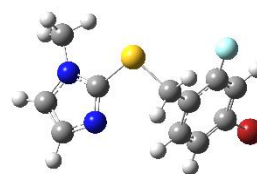
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0 1			
S	2.56934400	1.59838100	0.38626900
N	2.96398400	-0.47107100	-1.36913800
N	3.41641700	-0.96855100	0.74262100
C	2.98519400	-0.02329600	-0.13629500
C	-0.94168000	1.88399300	0.33287800
C	-0.04452400	1.33853500	-0.58170600
C	3.40337000	-1.76336400	-1.29081100
H	3.48075300	-2.38669200	-2.16698700
C	-2.16257400	1.28161800	0.58564100
H	-2.85492100	1.71555800	1.29419800
C	3.70051400	-2.08775000	-0.00061600
H	4.07737800	-2.98867200	0.45266200
C	-2.48814600	0.11465200	-0.08575600
C	1.27307900	1.99270300	-0.84796000
H	1.19791600	3.07935700	-0.79773500
H	1.67784900	1.71652700	-1.81941500
C	-0.39952800	0.16819000	-1.24533400
H	0.29217600	-0.26943400	-1.95451700
C	-1.61779000	-0.44868900	-1.00113400
H	-1.88586100	-1.35815600	-1.52151300
C	3.57551000	-0.82795800	2.17018500
H	2.84111800	-0.11561400	2.54307600

H	4.57589500	-0.47408800	2.42604700
H	3.40530100	-1.79170700	2.64679000
H	-0.68494800	2.79608200	0.86024500
Br	-4.15987200	-0.71976300	0.25279800

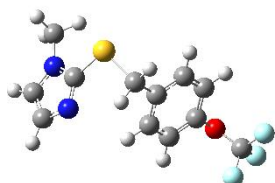
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0 1			
S	2.52462500	1.49268600	0.12934200
N	2.92407900	-0.83447000	-1.27521500
N	3.66069900	-0.88144600	0.81425200
C	3.03862200	-0.16026200	-0.15619800
C	-0.98735100	1.68065000	-0.02474100
C	-0.06046800	1.00769700	-0.80832400
C	3.50320700	-2.04914600	-1.02391700
H	3.54556200	-2.81943000	-1.77684200
C	-2.20784900	1.14794800	0.33407000
H	-2.89094200	1.72266900	0.94299600
C	3.97377500	-2.09685700	0.25335900
H	4.48779500	-2.86194000	0.80965100
C	-2.51238700	-0.12605400	-0.11294600
C	1.24455800	1.63265200	-1.17189600
H	1.14583400	2.70653100	-1.32258900
H	1.66350600	1.18275700	-2.06917000
C	-0.41189500	-0.26828000	-1.23877000
H	0.29625300	-0.82018100	-1.84410900
C	-1.62677500	-0.84278100	-0.89824900
H	-1.88058300	-1.83564300	-1.24203300
C	3.97005900	-0.45043600	2.15635500
H	3.18340700	0.21354200	2.51291700

H	4.92483300	0.07725100	2.19496600
H	4.01702500	-1.31983700	2.80934700
F	-0.68960700	2.91727500	0.40565200
Br	-4.18041800	-0.89210100	0.36110900

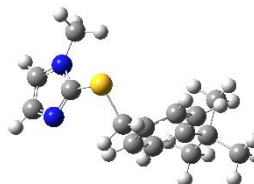
5a



O 1			
S	2.88133000	1.63287300	0.00122700
N	3.18644000	-0.76222300	-1.30072300
N	3.92160200	-0.75891600	0.79000800
C	3.32902500	-0.05005200	-0.20862900
C	-0.62153400	1.82086700	0.21977300
C	0.20822900	1.11066300	-0.64460900
C	3.71277500	-1.98872100	-1.00196500
H	3.72239900	-2.78903900	-1.72414200
C	-1.79022000	1.26137600	0.70614600
H	-2.43807400	1.80679700	1.37916500
C	4.18322100	-2.00604800	0.27697700
H	4.66722100	-2.76940700	0.86190100
C	-2.12752400	-0.02211200	0.31735300
C	1.47160900	1.71961100	-1.16462300
H	1.35534300	2.78893100	-1.34321100
H	1.80306300	1.24672800	-2.08673900
C	-0.15596700	-0.18063100	-1.01482300
H	0.49092700	-0.74325000	-1.67599500
C	-1.32285600	-0.75404600	-0.53295800
H	-1.60925000	-1.75957100	-0.81077400
C	4.24581100	-0.29482300	2.11757000
H	3.51050000	0.44635500	2.42755000
H	5.23974400	0.15518100	2.15023800

H	4.21184900	-1.13463900	2.80920200
H	-0.34908500	2.82581100	0.52167000
O	-3.27003800	-0.61949000	0.86120500
C	-4.41858300	-0.47016600	0.18157000
F	-4.36226700	-0.98655100	-1.05092000
F	-4.77730200	0.81176500	0.04672600
F	-5.36996800	-1.09982000	0.85376800

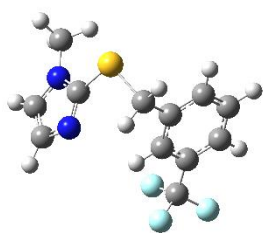
6a



O 1			
S	2.59221700	1.61107900	0.44243500
N	3.09927300	-0.37658500	-1.37250300
N	3.20343100	-1.03554800	0.74094300
C	2.97210700	-0.00501500	-0.11994100
C	-0.92637700	1.86249200	0.40126400
C	-0.02168700	1.38564200	-0.54505400
C	3.42679300	-1.70110200	-1.32594200
H	3.58674100	-2.27511000	-2.22452800
C	-2.13765600	1.23014100	0.60727600
H	-2.81500000	1.63737600	1.34881300
C	3.51075600	-2.12584400	-0.03206300
H	3.75585400	-3.07951700	0.40362200
C	-2.50265100	0.09187300	-0.11725200
C	1.29043200	2.06268100	-0.77157700
H	1.20982800	3.14484600	-0.66079200
H	1.70004200	1.84476400	-1.75582500
C	-0.37545800	0.25804100	-1.27287200
H	0.31340300	-0.13340200	-2.01210000
C	-1.59337000	-0.37627900	-1.05963900

H	-1.82508900	-1.25153500	-1.65154500
C	3.15589200	-1.00164000	2.18302200
H	2.47753800	-0.20976300	2.49529300
H	4.14320800	-0.81244600	2.60832700
H	2.78373700	-1.95533500	2.55398300
H	-0.67749400	2.74222900	0.98545000
C	-3.85187400	-0.57653300	0.14097400
C	-4.98039800	0.42540300	-0.14176700
H	-5.95298900	-0.03747200	0.04371000
H	-4.90580900	1.30932400	0.49341900
H	-4.95456300	0.75810200	-1.18137300
C	-4.06918100	-1.80307200	-0.74473000
H	-4.05858500	-1.54494100	-1.80572000
H	-3.31078000	-2.56932100	-0.57080200
H	-5.04233400	-2.24612000	-0.52323600
C	-3.92653500	-1.02458600	1.60760000
H	-3.81954700	-0.18324700	2.29394200
H	-4.88978000	-1.49976600	1.80999700
H	-3.13753300	-1.74421600	1.83553400

7a

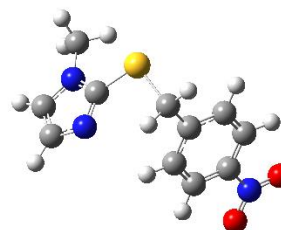


0 1

S	2.43285100	1.55228800	-0.34482000
N	1.98956300	-0.99579600	-1.25295100
N	2.98104100	-0.89550900	0.72645800
C	2.44333600	-0.20184800	-0.31292300
C	-0.87041700	2.63309900	0.24166900
C	-0.35305100	1.61982000	-0.56243300
C	2.24533200	-2.26344500	-0.80849900
H	1.96339400	-3.13012100	-1.38409200
C	-2.04306600	2.44527300	0.95260400

H	-2.43817200	3.24472200	1.56679800
C	2.86769700	-2.22569000	0.40338500
H	3.22960700	-3.00052500	1.05738500
C	-2.71890000	1.23658600	0.87544700
C	0.91391900	1.82297900	-1.33115000
H	1.01101700	2.85330900	-1.67419000
H	0.98091900	1.16045800	-2.19164200
C	-1.03565300	0.41195300	-0.64154200
H	-0.64162100	-0.38201200	-1.26299500
C	-2.21003900	0.22550600	0.07541700
C	3.58034300	-0.35457300	1.92269400
H	3.09974800	0.59161100	2.16712700
H	4.65068900	-0.18613300	1.79053400
H	3.42769300	-1.04978300	2.74626100
H	-0.34784800	3.58099800	0.30806500
H	-3.63893500	1.08423800	1.42349100
C	-2.90277600	-1.10184500	0.00769800
F	-2.84418900	-1.63911500	-1.21854200
F	-4.19846400	-1.01493000	0.34140200
F	-2.34809000	-1.99608000	0.84621100

8a

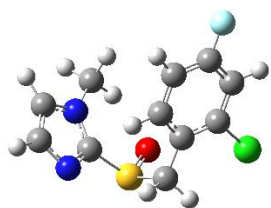


0 1

S	2.05927900	1.66568000	0.15598100
N	2.51779400	-0.61801700	-1.29312200
N	3.15895800	-0.73515600	0.82524400
C	2.58322700	0.01893500	-0.14892200
C	-1.44531900	1.77470600	0.11329200
C	-0.53249200	1.13174500	-0.72252700
C	3.08060900	-1.84217600	-1.05551000

H	3.15425800	-2.58844500	-1.82985100
C	-2.62792800	1.16133800	0.47806000
H	-3.34781200	1.64736800	1.12072400
C	3.49379800	-1.93213600	0.23983300
H	3.98115300	-2.71662400	0.79310000
C	-2.89040200	-0.11138100	-0.00213100
C	0.74654500	1.80228000	-1.11085900
H	0.61233200	2.87769100	-1.22873500
H	1.15822000	1.39564700	-2.03223300
C	-0.82773200	-0.14605600	-1.19337600
H	-0.11709300	-0.64892000	-1.83652900
C	-2.00708200	-0.77524600	-0.83443100
H	-2.25240400	-1.76588600	-1.18960700
C	3.40848100	-0.35204800	2.19448100
H	2.62303500	0.32505400	2.52752500
H	4.37463300	0.14494600	2.29860300
H	3.39514700	-1.24054300	2.82287200
H	-1.22597900	2.76935400	0.48361300
N	-4.14011100	-0.76951800	0.37978800
O	-4.89765600	-0.16018100	1.11140800
O	-4.34617700	-1.88625100	-0.05591000

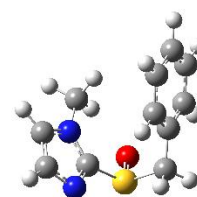
1b



0 1			
S	1.30105400	-1.80429800	-0.02547800
Cl	-2.63176700	-2.09617600	0.14774300
O	0.63775500	-1.89267900	1.30762800
N	2.35942700	0.68320600	0.83724700
N	2.92171600	-0.00317900	-1.19861100
F	-3.25966600	2.86349100	0.40074700
C	2.21858100	-0.26482500	-0.12288200

C	-0.88390500	-0.25414900	-0.85383400
C	0.01587500	-1.35244500	-1.28779500
H	0.60136400	-1.09631400	-2.17075200
H	-0.51270800	-2.28882400	-1.46056000
C	-0.53421800	1.07270800	-1.10999000
H	0.38151500	1.27081000	-1.65409300
C	-2.07748900	-0.48184800	-0.16638900
C	1.72404500	0.78369700	2.14111800
H	0.96316100	1.56417000	2.12259200
H	2.47929500	1.03149900	2.88599200
H	1.25765100	-0.16553800	2.38308200
C	3.21003100	1.61908700	0.31313600
H	3.49977000	2.49096300	0.87526900
C	3.54217700	1.18217200	-0.93871000
H	4.19803500	1.64898400	-1.65568200
C	-2.88410100	0.56206200	0.25831600
H	-3.80873300	0.37560700	0.78555800
C	-1.31864400	2.13438400	-0.69681300
H	-1.04547800	3.15981600	-0.90544900
C	-2.48297600	1.85289300	-0.01084400

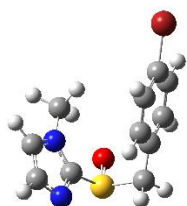
2b



0 1			
S	-1.04778000	1.79642300	-0.08957400
O	-0.45346000	2.10624600	1.24663100
N	-1.44414300	-0.85379000	0.82708300
N	-2.50811300	-0.25155100	-1.02829100
C	-1.67479000	0.12231300	-0.08657400
C	1.36279200	0.53791500	-0.78567500
C	0.35958900	1.52415600	-1.26501100

H	-0.12039400	1.23291900	-2.19979400
H	0.77452600	2.52774800	-1.37395700
C	1.33969100	-0.77698100	-1.24837300
H	0.59974500	-1.07133000	-1.98407200
C	2.31653800	0.90258700	0.16331200
C	-0.54269200	-0.84597800	1.96645800
H	0.40638700	-1.30914000	1.69515000
H	-1.00307100	-1.40422300	2.78037500
H	-0.36590600	0.18077800	2.27159400
C	-2.18271500	-1.92830500	0.41587300
H	-2.19187700	-2.84949800	0.97402100
C	-2.82489100	-1.54209700	-0.72828400
H	-3.50633700	-2.11537200	-1.33579900
C	3.22898700	-0.02819400	0.63589300
H	3.96613100	0.26841000	1.37213000
C	2.25345700	-1.70653200	-0.77706200
H	2.22952400	-2.72254900	-1.15218700
C	3.20021000	-1.33434100	0.16794100
H	2.33442200	1.91867700	0.53685800
H	3.91773700	-2.05902600	0.53328800

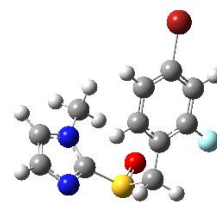
3b



O 1			
S	-2.85239600	1.34221900	0.16612100
O	-2.27036500	1.75633300	1.47894400
N	-2.06372600	-1.31048500	0.78176700
N	-3.42148000	-1.02794300	-0.95420800
C	-2.74127900	-0.43494000	-0.00237100
C	-0.24666500	1.25768300	-0.85573200
C	-1.60878300	1.77695200	-1.13962600

H	-2.03628000	1.38928400	-2.06447000
H	-1.64996400	2.86735000	-1.15471700
C	0.21141200	0.09258400	-1.46759400
H	-0.41999500	-0.42306400	-2.18191400
C	0.58028200	1.89933700	0.06414400
C	-1.16164500	-1.04326300	1.88920800
H	-0.12707400	-1.09942500	1.54973900
H	-1.32983500	-1.78669900	2.66704400
H	-1.35964800	-0.04844300	2.27561200
C	-2.33372500	-2.55020100	0.27141400
H	-1.92456200	-3.44150000	0.71680900
C	-3.16424400	-2.35672100	-0.79770600
H	-3.59945100	-3.09954100	-1.44642300
C	1.83592500	1.39548700	0.36484700
H	2.47243600	1.89997500	1.07895300
C	1.46519900	-0.42082900	-1.17760900
H	1.81596900	-1.32105000	-1.66369200
C	2.26674900	0.23745500	-0.25957500
Br	3.98575700	-0.45753300	0.14415800
H	0.23527700	2.79831500	0.55874200

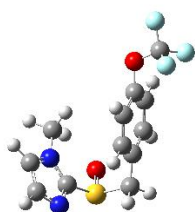
4b



O 1			
S	-2.75919100	1.31413300	0.18988100
O	-2.10786500	1.61529100	1.49759100
N	-2.35293800	-1.42949100	0.78726400
N	-3.42403200	-0.95107300	-1.09904900
C	-2.81484300	-0.46295400	-0.04524700
C	-0.18599500	1.07924700	-0.87644000
C	-1.52362800	1.65814200	-1.15273300
H	-1.98670100	1.25344600	-2.05244400

H	-1.50548600	2.74613700	-1.20608800
C	0.15681900	-0.21001900	-1.28068200
H	-0.56431200	-0.79060100	-1.84395700
C	0.77450300	1.79107500	-0.16922800
C	-1.59023800	-1.30393300	2.01868800
H	-0.54380300	-1.54718100	1.83325400
H	-1.99725400	-1.99221100	2.75820800
H	-1.66147200	-0.28293300	2.37873300
C	-2.69057300	-2.61807500	0.19862900
H	-2.44456600	-3.56095900	0.65750500
C	-3.34422400	-2.30446900	-0.96039800
H	-3.76862900	-2.97597600	-1.68911800
C	2.01604600	1.27383400	0.14492900
H	2.72436200	1.87562000	0.69611700
C	1.39095500	-0.76384300	-0.98496200
H	1.63888800	-1.76312100	-1.31418000
C	2.30779600	-0.01341700	-0.26685500
F	0.50923600	3.04669800	0.20405300
Br	3.99985400	-0.75487200	0.15299900

5b

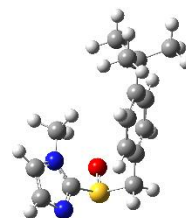


0 1

S	3.09909100	-1.42127100	-0.07140500
O	2.62766500	-1.90669800	1.26109800
N	2.58312500	1.21470900	0.83739900
N	3.68842300	0.99480800	-1.07740800
C	3.09188900	0.36765300	-0.09218500
C	0.41358500	-1.10027800	-0.79390500
C	1.70245300	-1.66875200	-1.26591500
H	2.05686700	-1.22524400	-2.19644600

H	1.66925700	-2.75395600	-1.37521600
C	-0.02490900	0.14007900	-1.25452800
H	0.56602500	0.68063500	-1.98441600
C	-0.35110700	-1.77535300	0.15604900
C	1.80847100	0.91253500	2.02900900
H	0.74701700	1.06612200	1.83275700
H	2.12830700	1.57289700	2.83377400
H	1.97601000	-0.12296600	2.30783000
C	2.87530900	2.47387100	0.39012600
H	2.59039600	3.34847400	0.95056100
C	3.54934800	2.31934900	-0.78958200
H	3.95225200	3.08530200	-1.43221700
C	-1.53313700	-1.23045100	0.63032800
H	-2.13032900	-1.74539000	1.37078700
C	-1.20587900	0.69363600	-0.78879900
H	-1.55370700	1.65448200	-1.14363000
C	-1.94813200	-0.00441200	0.14602800
H	-0.01137900	-2.73010800	0.53578900
O	-3.10415600	0.57994700	0.67157000
C	-4.26181800	0.31964800	0.03848900
F	-4.55551800	-0.98427700	0.01695300
F	-5.22539900	0.95512400	0.68510000
F	-4.25925200	0.73718900	-1.23194900

6b

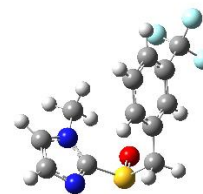


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S	2.82781100	-1.37992700	0.13083400
O	2.26088700	-1.79595800	1.45042000
N	2.06882400	1.27201300	0.76889100
N	3.48840100	1.00232100	-0.91884900

C	2.75980200	0.40094000	-0.00854100
C	0.20454500	-1.23385000	-0.86649000
C	1.55753300	-1.77251300	-1.16057100
H	1.98467500	-1.38475100	-2.08604900
H	1.57920800	-2.86355700	-1.18809100
C	-0.24575000	-0.06329700	-1.46577400
H	0.38967500	0.45355300	-2.17648400
C	-0.63679500	-1.86914100	0.04569200
C	1.11421100	0.99266400	1.82755200
H	0.09911000	1.01347500	1.43000700
H	1.22049300	1.75008400	2.60290900
H	1.31727700	0.00787700	2.23708600
C	2.38033200	2.51719500	0.29795900
H	1.97130000	3.40606700	0.74832200
C	3.24872100	2.33171700	-0.74227700
H	3.72313200	3.08052700	-1.35574500
C	-1.88418900	-1.34713400	0.33638100
H	-2.50935100	-1.87245300	1.04862000
C	-1.49955100	0.45401300	-1.17048000
H	-1.81016500	1.36232500	-1.66890000
C	-2.34941500	-0.17457500	-0.26356200
H	-0.30503200	-2.77586100	0.53619300
C	-3.74064400	0.35737700	0.07666800
C	-4.06838100	1.64653300	-0.67625200
H	-3.36816200	2.44895700	-0.43405000
H	-4.06021400	1.49903900	-1.75818600
H	-5.06773500	1.98737500	-0.39853300
C	-4.79211500	-0.69761500	-0.29660100
H	-4.63825900	-1.63190400	0.24518800
H	-5.79421600	-0.33371900	-0.05661300
H	-4.75808200	-0.92111000	-1.36475400
C	-3.82427500	0.64586600	1.58234100
H	-4.82026800	1.01296000	1.84190800
H	-3.63333300	-0.24769500	2.17826700
H	-3.09687700	1.40588300	1.87564100

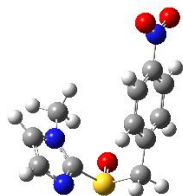
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S	-1.95401500	1.83061000	-0.12923400
O	-0.99423200	2.16904400	0.96435500
N	-2.29899400	-0.69103500	1.12000100
N	-3.68178600	-0.18028100	-0.54272500
C	-2.65472400	0.21212900	0.17223300
C	0.07979100	0.32975200	-1.32772700
C	-0.94281900	1.36889500	-1.61328100
H	-1.67462500	1.06061100	-2.35991900
H	-0.50426100	2.32269000	-1.91102300
C	-0.14827700	-1.00192200	-1.66722400
H	-1.06889100	-1.27340900	-2.17060700
C	1.26294600	0.66732400	-0.67428700
C	-1.19068100	-0.65071300	2.05954100
H	-0.36391700	-1.25648000	1.68789400
H	-1.52717500	-1.04456200	3.01742400
H	-0.85914500	0.37618800	2.17526700
C	-3.16738400	-1.73806800	0.97736600
H	-3.11574600	-2.60101700	1.61988600
C	-4.00574500	-1.40926400	-0.05172800
H	-4.82824800	-1.98101000	-0.44998300
C	2.19709800	-0.31259900	-0.37828600
C	0.79076700	-1.97760200	-1.37138200
H	0.60722400	-3.00691100	-1.65272800
C	1.96776300	-1.63764200	-0.72473400
H	1.45005300	1.69522700	-0.39501700
H	2.71005700	-2.39258600	-0.50043200
C	3.45070500	0.04395700	0.36291700
F	3.77189500	1.33511000	0.22903500

F	4.50166600	-0.67536100	-0.05860300
F	3.32883800	-0.19387500	1.68187500

8b

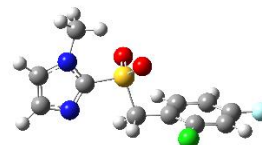


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S	-2.39976400	1.43817200	0.06477400
O	-1.80315300	1.89000400	1.35685200
N	-1.87318000	-1.22772500	0.88721400
N	-2.98090300	-0.94432500	-1.01775000
C	-2.38205700	-0.35083100	-0.01375000
C	0.19885900	1.15591300	-0.91723600
C	-1.12816900	1.72719200	-1.25653600
H	-1.56849000	1.30006600	-2.15713400
H	-1.11042300	2.81482300	-1.33993400
C	0.59548300	-0.07298100	-1.44671800
H	-0.05876900	-0.59611000	-2.13338000
C	1.04416200	1.81837800	-0.02643900
C	-1.11158700	-0.97037500	2.09825400
H	-0.06204900	-1.21599900	1.93580500
H	-1.50650000	-1.58735200	2.90428400
H	-1.20043300	0.07962800	2.35713000
C	-2.16937400	-2.47158700	0.40002100
H	-1.88202100	-3.36440300	0.92958500
C	-2.84510700	-2.27796200	-0.77255400
H	-3.24811000	-3.02200300	-1.44029000
C	2.26494800	1.27174600	0.32533500
H	2.93340400	1.77064300	1.01217300
C	1.81370100	-0.62971500	-1.10501600
H	2.14048500	-1.57605000	-1.51145200
C	2.63116900	0.05366500	-0.22043500
H	0.73741400	2.76472200	0.39884500

N	3.92269800	-0.53053400	0.14763700
O	4.62589700	0.09605300	0.91661300
O	4.21091000	-1.60871900	-0.33612400

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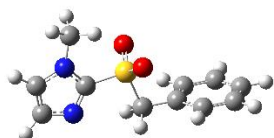


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S	1.00004900	-0.50980800	0.28666200
Cl	-1.73463100	2.48438500	0.39977200
O	0.89537800	-1.94899700	0.18437000
O	0.78139900	0.11407900	1.57278600
N	2.82121900	0.51412900	-1.46667300
N	3.73551700	-0.19910300	0.42897500
F	-5.41681000	-0.90223100	0.25692200
C	-1.49689500	-0.03636100	-0.62171400
C	2.60320700	-0.02392900	-0.29397300
C	-0.06883200	0.24469000	-0.95613600
H	0.16902200	1.30513800	-0.96249400
H	0.23499300	-0.19673800	-1.90338100
C	4.75130700	0.26273900	-0.36018700
H	5.77547100	0.24358500	-0.02789600
C	4.17127700	0.70068600	-1.51856500
H	4.64879800	1.14309900	-2.37730600
C	-2.32352300	0.90167900	-0.00343100
C	-2.04663200	-1.28074000	-0.92706400
H	-1.41456200	-2.02482000	-1.39436500
C	-3.64711000	0.61971000	0.29234200
H	-4.28400800	1.35367500	0.76466400
C	-4.13884400	-0.62726400	-0.02940300
C	-3.36201500	-1.59203400	-0.63780300
H	-3.78389700	-2.55900500	-0.87464700

C	3.86905500	-0.81303000	1.73685500
H	3.03996000	-0.50418700	2.36902000
H	4.80408900	-0.48152600	2.18242300
H	3.87202900	-1.89947600	1.65007000

2c

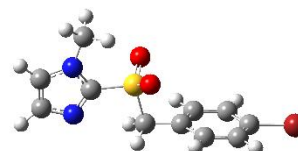


O 1

S	-0.42180300	-0.42070400	0.06879100
O	-0.24769300	-0.94185100	1.40627900
O	-0.28439600	-1.32290800	-1.05519300
N	-2.24684900	1.60765400	-0.11472100
N	-3.17292900	-0.40859900	0.00001500
C	2.08090400	0.58314700	-0.09812200
C	-2.03139800	0.32006200	-0.02695700
C	0.64847300	1.00940100	-0.16861200
H	0.37374800	1.42416400	-1.13675800
H	0.37170400	1.71560100	0.61188200
C	-4.19247700	0.49924500	-0.07029100
H	-5.22385700	0.18947600	-0.06734100
C	-3.60540900	1.73193400	-0.14350900
H	-4.08390000	2.69441400	-0.22057500
C	2.75295300	0.18147400	-1.24864700
C	2.75349800	0.57387700	1.12020900
H	2.23184700	0.87203400	2.02158800
C	4.08024100	-0.21127500	-1.18382100
H	4.59465900	-0.51910300	-2.08584000
C	4.74689000	-0.21115600	0.03273000
C	4.08064400	0.18095400	1.18469800
H	4.59547800	0.18015000	2.13757200
C	-3.30139500	-1.84651900	0.14155100

H	-2.52758600	-2.33948200	-0.44261400
H	-4.27761700	-2.14715000	-0.23193200
H	-3.20397100	-2.13795200	1.18705000
H	2.23104900	0.17338300	-2.19794100
H	5.78491000	-0.51645800	0.08313600

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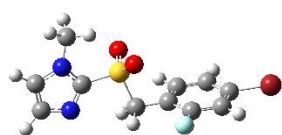


O 1

S	1.81269500	0.37645200	0.06056500
O	1.58067100	0.88668600	1.39315600
O	1.62587700	1.26205300	-1.06930000
N	3.76657900	-1.52718000	-0.07739000
N	4.55985200	0.54646200	0.01246700
C	-0.61236800	-0.79043100	-0.13020300
C	3.46820500	-0.25489800	-0.01154400
C	0.84399900	-1.12425300	-0.18538700
H	1.15435500	-1.52192600	-1.14980400
H	1.15766300	-1.81011600	0.59912200
C	5.63604500	-0.29483400	-0.03570600
H	6.64531100	0.08072600	-0.02961900
C	5.13036500	-1.56397200	-0.09407200
H	5.67053500	-2.49456100	-0.15253000
C	-1.29993900	-0.43420300	-1.28588800
C	-1.29823700	-0.81648200	1.07988800
H	-0.77300000	-1.07633300	1.99071000
C	-2.64921200	-0.12405800	-1.24248100
H	-3.17928900	0.14833400	-2.14469000
C	-3.31104800	-0.16629000	-0.02753100
C	-2.64734700	-0.50857700	1.13804300

H	-3.17609400	-0.53402300	2.08088000
C	4.59475500	1.99177500	0.13306600
H	3.79333500	2.42521300	-0.46092700
H	5.55104600	2.34928000	-0.24173100
H	4.47488700	2.29148000	1.17389900
Br	-5.16041100	0.24872700	0.04095000
H	-0.77620700	-0.39431700	-2.23311500

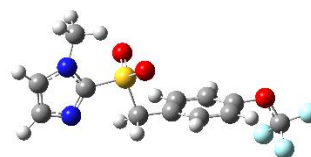
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S	1.85616200	-0.46129800	0.09472600
O	1.65361000	-1.69471400	-0.63258500
O	1.63672900	-0.45007800	1.52415300
N	3.79885500	1.08299500	-1.03351700
N	4.60002500	-0.44628200	0.36581800
C	-0.56896300	0.54567200	-0.51179800
C	3.50679800	0.10722900	-0.21199400
C	0.88331900	0.84365500	-0.68404200
H	1.18139600	1.77352800	-0.20636500
H	1.19279300	0.85728700	-1.72728700
C	5.66972800	0.23640800	-0.14154200
H	6.67863300	0.00018700	0.15171200
C	5.15905300	1.17443800	-0.99566100
H	5.69318000	1.90926100	-1.57524300
C	-1.31878000	1.18766600	0.46347300
C	-1.23023800	-0.38314900	-1.31088200
H	-0.66988200	-0.91156400	-2.07161200
C	-2.66482300	0.94936800	0.65504900
H	-3.20119000	1.48377700	1.42586100
C	-3.28127200	0.01874800	-0.16092500
C	-2.57745800	-0.65377700	-1.14610500

H	-3.07339800	-1.37906800	-1.77523300
C	4.64940900	-1.57529200	1.27598600
H	3.81743400	-1.51552300	1.97354700
H	5.58540000	-1.53573600	1.82830700
H	4.59165900	-2.51333200	0.72400900
F	-0.72651400	2.09694100	1.24654000
Br	-5.12661400	-0.33328500	0.07628100

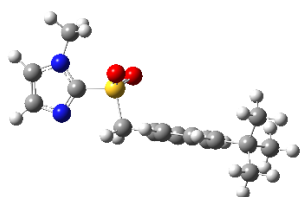
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S	2.15861000	-0.43160500	-0.07819700
O	1.99173400	-0.93998700	-1.42119000
O	2.03044300	-1.34655100	1.03626900
N	3.93475400	1.63256100	0.12266200
N	4.90886100	-0.36156900	0.01142000
C	-0.36089700	0.51472200	0.08987200
C	3.75078400	0.34041500	0.03069400
C	1.05957000	0.97558000	0.17155900
H	1.31950100	1.38586300	1.14548800
H	1.32213100	1.69721600	-0.59941000
C	5.90583800	0.57002300	0.09129800
H	6.94424700	0.28475000	0.09565600
C	5.28955200	1.78866900	0.16237800
H	5.74469800	2.76189200	0.24517300
C	-1.02539700	0.07607800	1.23111200
C	-1.02655400	0.49674600	-1.13200700
H	-0.51126800	0.81544300	-2.02934800
C	-2.33844900	-0.35728300	1.16119100
H	-2.86304700	-0.70339100	2.04132100
C	-2.98044500	-0.34881800	-0.06244300

C	-2.33956200	0.06567100	-1.21444700
H	-2.86503600	0.04438400	-2.15946800
C	5.07251800	-1.79590700	-0.13245700
H	4.30619400	-2.30872900	0.44441900
H	6.05248900	-2.07420600	0.24822400
H	4.99094500	-2.08669900	-1.17947800
H	-0.50935000	0.06584400	2.18294100
O	-4.28241200	-0.84736000	-0.15066300
C	-5.28568800	0.03265800	0.00899000
F	-5.26568900	0.62620800	1.20744500
F	-6.42518900	-0.62934800	-0.10995800
F	-5.26693500	1.00827500	-0.90556600

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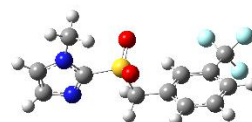


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S	-1.78220100	0.36794500	-0.06688800
O	-1.56470400	0.87049800	-1.40520100
O	-1.59639200	1.26607400	1.05384500
N	-3.74028900	-1.53464500	0.10251900
N	-4.52910900	0.53897300	-0.01243000
C	0.64755600	-0.79736600	0.12264400
C	-3.43865300	-0.26415900	0.01883900
C	-0.80915800	-1.12747300	0.18713800
H	-1.11744900	-1.51547500	1.15645300
H	-1.12771100	-1.81947100	-0.59018300
C	-5.60742100	-0.29893100	0.04994000
H	-6.61580100	0.07898800	0.04184200
C	-5.10427800	-1.56809900	0.12355600
H	-5.64630900	-2.49668800	0.19584400
C	1.34306100	-0.41551900	1.26625400

C	1.33668500	-0.85108800	-1.08062200
H	0.81330400	-1.13268700	-1.98667900
C	2.68942000	-0.10956000	1.20096500
H	3.19758100	0.18094200	2.11256700
C	3.39649500	-0.16548800	-0.00199500
C	2.68810600	-0.54290200	-1.13895900
H	3.18633100	-0.60072700	-2.09696300
C	-4.56114100	1.98238000	-0.15193600
H	-3.75645400	2.42141800	0.43346200
H	-5.51545000	2.34708100	0.22122700
H	-4.44364000	2.26823000	-1.19695300
H	0.82312400	-0.35319600	2.21488200
C	4.88404700	0.18002600	-0.02837500
C	5.48166400	0.05990400	-1.43001800
H	6.54258800	0.31580800	-1.39743400
H	5.40025000	-0.95643000	-1.82129700
H	5.00076900	0.73972400	-2.13643900
C	5.07836700	1.62445200	0.45472000
H	4.71010100	1.76477300	1.47198200
H	6.13946200	1.88584800	0.44491900
H	4.54832800	2.32659300	-0.19176500
C	5.64515200	-0.77502000	0.90218800
H	5.52729300	-1.81132400	0.57898500
H	6.71157300	-0.53622800	0.89779600
H	5.29247200	-0.70412200	1.93214900

7c

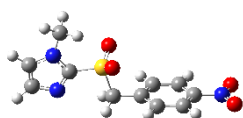


0 1

S	1.54781400	0.22948800	0.40572600
O	1.06488400	-0.92812800	1.12397800
O	1.69011400	1.48303900	1.11532400

N	3.32781500	-0.30686900	-1.59491400
N	4.22626700	-0.39460800	0.43567500
C	-0.85865800	0.82364500	-0.65216400
C	3.11739400	-0.17622000	-0.31026900
C	0.53870800	0.48716600	-1.06611100
H	1.02312800	1.28759300	-1.62205600
H	0.60596100	-0.43551400	-1.63892900
C	5.21727900	-0.69423500	-0.45666600
H	6.21990400	-0.91527500	-0.13177100
C	4.64862500	-0.63291200	-1.69882900
H	5.11655400	-0.79983800	-2.65502800
C	-1.22409700	2.14230000	-0.40650900
C	-1.80249700	-0.18567300	-0.49024900
H	-1.52728800	-1.21767100	-0.66180100
C	-2.51756700	2.45200500	-0.01481000
H	-2.79249900	3.48179600	0.17408800
C	-3.45679300	1.44762500	0.13766700
C	-3.09324000	0.12843600	-0.10167500
C	4.33619800	-0.37786400	1.88220400
H	3.76133700	0.45482000	2.28167900
H	5.38246400	-0.24999500	2.14964600
H	3.96155300	-1.30970400	2.30468800
H	-0.48892000	2.92998300	-0.51622900
H	-4.46789000	1.68394900	0.44381700
C	-4.13107700	-0.94362600	0.04288000
F	-3.60883400	-2.17293900	-0.01675200
F	-4.78850100	-0.84441300	1.20841600
F	-5.06083500	-0.86429100	-0.92636200

8c

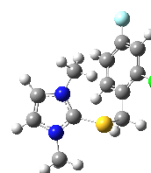


O 1

S	1.38085800	0.37621300	0.11129500
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O	1.14589900	0.71227700	1.49685200
O	1.19749800	1.39658500	-0.89823500
N	3.30713100	-1.51886100	-0.25872200
N	4.12959900	0.51942900	0.07050700
C	-1.05120200	-0.73568500	-0.22103100
C	3.02738000	-0.25922900	-0.04219100
C	0.40125100	-1.07534500	-0.32343100
H	0.70407800	-1.34813800	-1.33242000
H	0.70813200	-1.85891500	0.36629900
C	5.19331500	-0.32502900	-0.08175100
H	6.20780200	0.03337200	-0.03641800
C	4.66995900	-1.57180200	-0.28666700
H	5.19687700	-2.49614100	-0.45706800
C	-1.73185900	-0.22503400	-1.32384600
C	-1.73058800	-0.91215500	0.98196400
H	-1.20224400	-1.29332200	1.84640900
C	-3.07480000	0.09197300	-1.23683700
H	-3.62209400	0.48581100	-2.08095000
C	-3.72520900	-0.10378000	-0.03149700
C	-3.07353400	-0.59950800	1.08374200
H	-3.61980600	-0.73219000	2.00632100
C	4.18542000	1.94010100	0.36063300
H	3.39121900	2.45251900	-0.17755300
H	5.14710100	2.32509300	0.02972900
H	4.06964400	2.11648600	1.42972200
H	-1.20451800	-0.07120300	-2.25662100
N	-5.15077300	0.22366100	0.06676000
O	-5.69772100	0.65775200	-0.92833100
O	-5.69722800	0.03970800	1.13689800

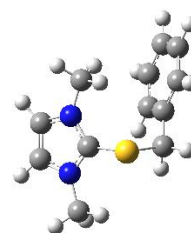
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1 1

S	1.31890400	1.68821600	0.17830600
Cl	-2.18007000	2.32880800	0.67245900
F	-3.93793100	-2.29895700	-0.08923100
N	3.15552000	-0.30603400	-0.32924800
N	1.66667400	-0.87031200	1.13846300
C	2.04887100	0.11871700	0.31059600
C	-2.06857600	0.75751500	-0.04877600
C	-0.99078900	0.44328500	-0.88087400
C	3.46178700	-1.56914500	0.09277500
H	4.31367600	-2.10948700	-0.28213500
C	-3.06834300	-0.15928200	0.22303000
H	-3.90561900	0.09258000	0.85893900
C	2.52901800	-1.92218100	1.01086800
H	2.41731800	-2.82809900	1.58086600
C	-2.98108200	-1.41423800	-0.34995300
C	0.08665700	1.41993900	-1.19072800
H	-0.29562700	2.43213400	-1.32774600
H	0.63972100	1.13922200	-2.08421300
C	3.93123100	0.45179100	-1.30075400
H	3.84824300	-0.01373600	-2.28137800
H	4.97339300	0.47061300	-0.98901500
H	3.54497800	1.46640100	-1.33654800
C	-0.95695900	-0.83283200	-1.44086300
H	-0.14770800	-1.08961300	-2.11512300
C	-1.93986800	-1.77304000	-1.18493200
H	-1.92059300	-2.75742400	-1.63242000
C	0.52189000	-0.84764800	2.03969100
H	0.18268300	0.17846700	2.14667500
H	0.83134800	-1.23645000	3.00724900
H	-0.28008000	-1.45804900	1.62824700

2d

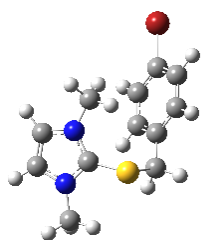


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S	0.85474600	-1.62000900	-0.88207100
N	2.53980900	0.12551200	0.42418700
N	1.06312100	1.12819500	-0.80207100
C	1.48394300	-0.07955800	-0.38692000
C	-2.57612700	-0.94958100	-0.50664200
C	-1.54376900	-0.91042600	0.42893000
C	2.77497300	1.46765400	0.52435000
H	3.57733200	1.86748000	1.11973400
C	-3.57490600	0.00953300	-0.48912200
H	-4.37888200	-0.03673200	-1.21289500
C	1.84947800	2.09460700	-0.24249900
H	1.69466000	3.14195600	-0.43469600
C	-3.55357000	1.02120800	0.46338600
C	-0.45553600	-1.92825400	0.40525500
H	-0.81432600	-2.91372700	0.10390000
H	0.04430400	-2.02872000	1.36662700
C	3.33038300	-0.90324900	1.08434100
H	3.18330200	-0.84477700	2.16145600
H	4.38154800	-0.75346500	0.84713000
H	3.01042500	-1.87444400	0.71795900
C	-1.53727300	0.09803100	1.38901900
H	-0.75945700	0.11872200	2.14520700
C	-2.53651600	1.06129000	1.40608200
H	-2.53011400	1.83265300	2.16612900
C	-0.05763400	1.39316200	-1.69475700
H	-0.29050900	0.48424900	-2.24076300
H	0.23066500	2.17886400	-2.38929300
H	-0.92525200	1.69928300	-1.11241700
H	-4.33939000	1.76583500	0.48093500

H -2.60143200 -1.73949000 -1.24922200

3d



1 1

S 2.56488100 1.51126200 0.75232000
N 3.57189600 -0.73806200 -0.48067800
N 1.94922600 -1.17341000 0.88589200
C 2.67874500 -0.17536400 0.35627600
C -0.92613500 1.88847200 0.54350400
C -0.00476900 1.48293600 -0.42020500
C 3.39440700 -2.09274200 -0.48199300
H 4.00246600 -2.75128200 -1.07763500
C -2.16497800 1.28007500 0.64225000
H -2.87827100 1.60687500 1.38669000
C 2.37806500 -2.36444600 0.37295700
H 1.93518500 -3.30334900 0.65638300
C -2.49087200 0.25119600 -0.23143100
C 1.33808300 2.12008700 -0.51145400
H 1.31027000 3.18523900 -0.27627000
H 1.79065000 2.00236800 -1.49398000
C 4.58684200 -0.03726300 -1.25424100
H 4.35769600 -0.11346800 -2.31581200
H 5.55899200 -0.48286000 -1.05428400
H 4.59615700 1.00538600 -0.94988400
C -0.35950000 0.46208200 -1.29740600
H 0.32707900 0.15508000 -2.07913400
C -1.59688500 -0.15785100 -1.20855900
H -1.87007500 -0.94139500 -1.90233700
C 0.86387900 -1.03577400 1.84834800
H 0.92829900 -0.05455000 2.30815200

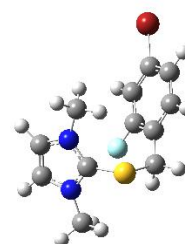
H 0.97171100 -1.80763200 2.60697900

H -0.09267100 -1.13741900 1.33853100

H -0.67809100 2.69376900 1.22592700

Br -4.17504700 -0.58814500 -0.09700600

4d

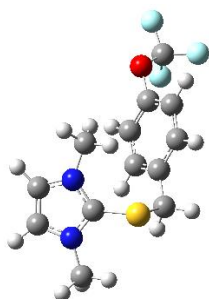


1 1

S -2.54436500 1.53802100 -0.85649400
N -3.45951500 -0.70373100 0.46107400
N -2.03969900 -1.15728800 -1.10976100
C -2.66552600 -0.15069600 -0.47347400
C 1.03804100 1.96828200 -0.55724000
C 0.03947800 1.48354200 0.28585500
C -3.32098100 -2.06133600 0.42128400
H -3.85890100 -2.71328600 1.08733100
C 2.27792000 1.36037000 -0.63707900
H 3.04202300 1.75683600 -1.29081700
C -2.43602800 -2.34612600 -0.56535500
H -2.06580300 -3.29183400 -0.92106200
C 2.53735800 0.24153800 0.14292600
C -1.29553300 2.12941100 0.39132600
H -1.24532800 3.19241900 0.15401400
H -1.73580600 2.02056800 1.37891900
C -4.30950100 0.01659000 1.39668700
H -3.82126100 0.07600800 2.36826800
H -5.25551400 -0.51119600 1.49087700
H -4.48765800 1.01570900 1.00844800
C 0.35108000 0.36429600 1.04471600
C 1.57485000 -0.26858600 0.99977200
H 1.76521900 -1.12742500 1.62816800

C	-1.09340700	-1.03207800	-2.20999800
H	-1.00942500	0.01635900	-2.47802100
H	-1.45810500	-1.60238500	-3.06205100
H	-0.12221100	-1.40879800	-1.89520400
H	0.84148900	2.84854000	-1.15854000
Br	4.22138400	-0.59696300	0.04754100
F	-0.59103500	-0.13224700	1.87043500

5d

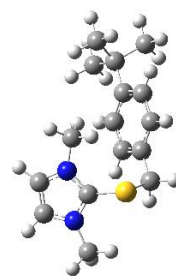


1 1

S	-2.84483600	-1.59733600	0.57962800
N	-3.91879300	0.64968800	-0.60023600
N	-2.47010900	1.11069700	0.94220600
C	-3.06181700	0.09964900	0.28154800
C	0.66230600	-1.73033000	0.68168300
C	-0.18880600	-1.31163000	-0.33966500
C	-3.85623900	2.01067000	-0.49775500
H	-4.46029700	2.66101400	-1.10637500
C	1.84541300	-1.05978200	0.93505800
H	2.51426900	-1.37962300	1.72279200
C	-2.94891700	2.29860700	0.46747300
H	-2.61482600	3.24641500	0.85233300
C	2.17953100	0.03757900	0.15701100
C	-1.47205700	-2.02283700	-0.60279100
H	-1.38858900	-3.09947200	-0.44594000
H	-1.84082400	-1.85714500	-1.61302500
C	-4.79655100	-0.07057100	-1.51176100
H	-4.47375200	0.09210900	-2.53870000
H	-5.81533900	0.28917200	-1.38449700
H	-4.75291700	-1.12898400	-1.27155400

C	0.17336900	-0.21136300	-1.11180200
C	1.35541500	0.47054500	-0.86663000
H	1.64861900	1.32180200	-1.46628500
C	-1.47074300	0.98854800	1.99551300
H	-1.48587700	-0.02886300	2.37369800
H	-1.71928300	1.68380200	2.79413900
H	-0.48481100	1.21300200	1.59223400
H	0.40120000	-2.59218000	1.28516700
H	-0.46171000	0.10950800	-1.93021000
O	3.32526900	0.75682700	0.45625900
C	4.46728700	0.38959500	-0.17998700
F	4.79845600	-0.87464600	0.08130000
F	5.42674600	1.18351200	0.24214700
F	4.35730000	0.50417900	-1.50445200

6d

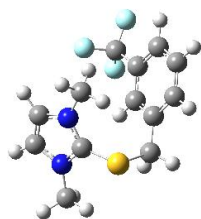


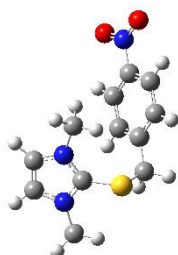
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S	-2.54694900	-1.54174300	0.72757900
N	-3.56789500	0.72120800	-0.46729900
N	-1.92754400	1.13964400	0.88286900
C	-2.66608600	0.14855300	0.35366400
C	0.96100400	-1.87047500	0.51562200
C	0.02825700	-1.46589600	-0.43852800
C	-3.38729100	2.07556000	-0.45810900
H	-4.00146000	2.74099300	-1.03951300
C	2.19029400	-1.24737200	0.60644100
H	2.89394500	-1.59827800	1.35101400
C	-2.35922200	2.33641700	0.38591500
H	-1.90985100	3.27131500	0.67179800
C	2.54827400	-0.19505900	-0.24471600
C	-1.30393600	-2.12072300	-0.53876500

H	-1.26353200	-3.18747400	-0.31262800	S	2.45524900	1.58646200	-0.02681600
H	-1.75851700	-1.99809700	-1.51984300	N	2.73277600	-1.13145400	-0.39700000
C	-4.59169900	0.02933500	-1.23639900	N	1.54415800	-0.62811000	1.34195400
H	-4.38153700	0.12838100	-2.29999100	C	2.21813300	-0.10245400	0.30341100
H	-5.56355600	0.46321000	-1.01055100	C	-0.94126100	2.70599800	0.07909500
H	-4.58750300	-1.01931000	-0.95325100	C	-0.28897900	1.70575200	-0.64083800
C	0.37350300	-0.42881800	-1.29528600	C	2.36933200	-2.30605000	0.19894800
C	1.61063200	0.19648000	-1.19720500	H	2.66675400	-3.26413000	-0.19073100
H	1.84470100	0.98980900	-1.89378200	C	-2.19067000	2.47466200	0.62802800
C	-0.82705300	0.98756100	1.82548400	H	-2.69722600	3.26323500	1.16930000
H	-0.91575900	0.02091400	2.31162000	C	1.62633000	-1.99032500	1.28785900
H	-0.89325300	1.78191300	2.56540700	H	1.15263100	-2.62275700	2.01838000
H	0.12138500	1.03915000	1.29290300	C	-2.80123700	1.23572500	0.48310500
H	0.72528600	-2.68708900	1.18959100	C	1.06731500	1.93148800	-1.21698200
H	-0.31838500	-0.11379600	-2.07002000	H	1.24596900	2.97978900	-1.45955800
C	3.92595400	0.45022700	-0.12225700	H	1.24403300	1.34133500	-2.11409200
C	4.09817300	1.02003900	1.29335800	C	3.55750900	-1.03145900	-1.59257400
H	4.00433500	0.24978900	2.06026000	H	2.99197200	-1.36505200	-2.46120800
H	5.08819600	1.46810300	1.39713700	H	4.44027500	-1.65464200	-1.46774400
H	3.35734400	1.79628000	1.49893700	H	3.85971800	0.00411300	-1.72070000
C	5.00156300	-0.61674500	-0.37655900	C	-0.91355700	0.47613200	-0.80336400
H	4.90403900	-1.04241300	-1.37690700	C	-2.15681300	0.23965600	-0.23287500
H	5.99487100	-0.17135300	-0.29392300	C	0.83080000	0.10952100	2.37594500
H	4.94495300	-1.43403900	0.34376200	H	1.02391800	1.16924200	2.24291600
C	4.12438700	1.58486600	-1.12655100	H	1.19008500	-0.21206600	3.35138500
H	4.05767600	1.23441500	-2.15850800	H	-0.23612400	-0.08439200	2.28534300
H	3.39810200	2.38883200	-0.98594400	H	-0.47207400	3.67568400	0.20099300
H	5.11725000	2.01695800	-0.99448900	H	-0.44252600	-0.30254000	-1.39258300
				H	-3.77706200	1.05047800	0.91175400
				C	-2.75627700	-1.13091500	-0.36158200
				F	-2.58547700	-1.63481200	-1.58815100
				F	-4.05503300	-1.14880500	-0.08335000
				F	-2.15244800	-1.98873100	0.49282100

7d

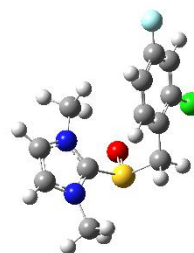


8d

I 1

S	-2.08563400	-1.58337700	0.70924900
N	-3.25073800	0.62650100	-0.45599600
N	-1.68792300	1.13522000	0.95471500
C	-2.32579100	0.10424900	0.37214900
C	1.39941700	-1.78631000	0.45650400
C	0.45725500	-1.37728000	-0.48676200
C	-3.18401700	1.98984600	-0.40023500
H	-3.83441300	2.62121400	-0.98053300
C	2.61304400	-1.13314000	0.56829800
H	3.36152400	-1.43904700	1.28589300
C	-2.20625800	2.30777100	0.48356200
H	-1.84696900	3.26721900	0.81323900
C	2.87064400	-0.06290800	-0.27137800
C	-0.85921200	-2.07088800	-0.59670200
H	-0.77487300	-3.14409400	-0.41800800
H	-1.32567400	-1.92666400	-1.56909000
C	-4.19507000	-0.12161700	-1.27424100
H	-3.93429100	-0.01834800	-2.32626400
H	-5.19714400	0.26586700	-1.10399600
H	-4.15616700	-1.16709900	-0.98200100
C	0.75562600	-0.31020100	-1.33109100
C	1.96559100	0.35652300	-1.22799000
H	2.22184000	1.18151700	-1.87793600
C	-0.61256500	1.04775500	1.93432200
H	-0.55545800	0.02723400	2.29964100
H	-0.83303400	1.72281600	2.75826000
H	0.33051000	1.32279100	1.46571200
H	1.18633100	-2.62716800	1.10622000

H	0.04741800	-0.00756700	-2.09410100
N	4.15303500	0.64929400	-0.14632900
O	4.93698500	0.23463300	0.67985600
O	4.32650900	1.60479700	-0.87365200

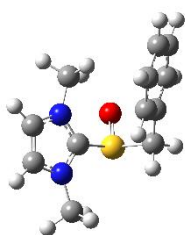
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I 1

S	1.28524200	-1.67033500	0.09807300
Cl	-2.52930800	-2.26889000	0.28494500
O	0.62152000	-1.92018200	1.39215900
N	1.69169700	0.97127600	1.06910000
N	3.10688800	0.36834200	-0.45765800
F	-3.79801900	2.55916300	0.00721100
C	1.99618000	0.00228200	0.19970300
C	-1.01740100	-0.32189100	-0.87806100
C	0.01194500	-1.33908600	-1.21000000
H	0.59423300	-1.07620500	-2.09592900
H	-0.40711600	-2.33602500	-1.35824600
C	-0.84384900	1.00050200	-1.28925000
H	0.03093700	1.25898400	-1.87580700
C	-2.18795200	-0.64050400	-0.18110800
C	0.55826500	1.01687600	1.99560500
H	-0.26928300	1.54066500	1.52056500
H	0.87716400	1.55031100	2.88748700
H	0.26487600	0.00237000	2.24677200
C	2.61277500	1.97672800	0.94302700
H	2.56804600	2.86657900	1.54677100
C	3.49566400	1.60388300	-0.01431100
H	4.36372200	2.10641300	-0.40437100
C	3.79761900	-0.40508500	-1.48237100

H	3.62975000	-1.46570900	-1.30838800
H	4.86265100	-0.19909400	-1.41371900
H	3.43640100	-0.12984100	-2.47219800
C	-3.12870500	0.33037300	0.12247200
H	-4.03594100	0.08195500	0.65529900
C	-1.76797000	1.98727100	-1.00125800
H	-1.64159000	3.00753600	-1.33695900
C	-2.89649800	1.62868600	-0.28557800

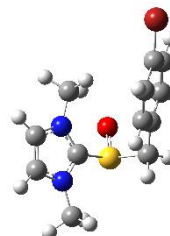
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S	0.85261000	-1.71504800	0.31228200
O	0.18350400	-1.87475000	1.62051200
N	1.01720400	1.05521400	0.94147600
N	2.50419100	0.38074900	-0.48367400
C	1.41974900	0.00936100	0.21356900
C	-1.53051200	-0.65931200	-0.76079700
C	-0.44334000	-1.64236600	-1.00839200
H	0.10194800	-1.46739200	-1.93846700
H	-0.79411900	-2.67717200	-1.00835500
C	-1.53839000	0.56465600	-1.42879500
H	-0.77308200	0.78472600	-2.16587500
C	-2.54639100	-0.94746000	0.14915100
C	-0.13287400	1.12419000	1.84522800
H	-1.00390100	1.46682500	1.28922800
H	0.10971500	1.82676000	2.63847200
H	-0.31938100	0.13739600	2.25692300
C	1.84785000	2.11235800	0.68345600
H	1.71460900	3.06807700	1.15987400
C	2.77534000	1.69437600	-0.21107700
H	3.60099700	2.21552200	-0.66357800

C	3.27331300	-0.45694400	-1.39542800
H	3.20012600	-1.49550500	-1.08035100
H	4.31443500	-0.14719500	-1.35639400
H	2.89928900	-0.35109200	-2.41270300
C	-3.54628700	-0.01886200	0.39377400
H	-4.33579000	-0.25299900	1.09660500
C	-2.54091000	1.49044000	-1.18516500
H	-2.55117600	2.42994600	-1.72351800
C	-3.54354000	1.20115800	-0.26832200
H	-2.55479800	-1.90001000	0.66407700
H	-4.33246900	1.91957000	-0.08437500

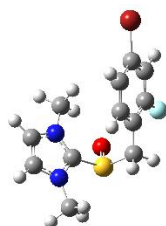
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1 1			
S	-2.52465900	1.49149100	0.34387800
O	-1.92019300	1.84084100	1.64666900
N	-1.77884500	-1.19322000	0.92576400
N	-3.41604300	-1.01300200	-0.48307200
C	-2.50396700	-0.32199400	0.21757300
C	0.05804300	1.29389900	-0.76556800
C	-1.29381700	1.86605300	-0.99088000
H	-1.76172400	1.53299400	-1.91970100
H	-1.30416800	2.95852500	-0.97666800
C	0.46826200	0.15405000	-1.45503900
H	-0.18124200	-0.29659500	-2.19795800
C	0.93155800	1.88010800	0.14897700
C	-0.66327500	-0.90250600	1.82885200
H	0.27021900	-0.95217400	1.27119800
H	-0.67006600	-1.65035800	2.61774000
H	-0.79540700	0.09018600	2.24713000
C	-2.22559400	-2.45792600	0.65143200

H	-1.78680100	-3.32673100	1.11068300
C	-3.24584700	-2.34787200	-0.23295300
H	-3.86263100	-3.10073800	-0.69220100
C	-4.42335500	-0.45476200	-1.37681300
H	-4.68917700	0.54549100	-1.04196200
H	-5.30696700	-1.08669400	-1.34114900
H	-4.04413900	-0.41585400	-2.39692300
C	2.18166100	1.33129000	0.38261100
H	2.85712300	1.79325000	1.08969100
C	1.71738800	-0.40077800	-1.23154600
H	2.03772500	-1.27410600	-1.78338100
C	2.56562000	0.18928000	-0.30472400
H	0.63570000	2.77303200	0.68514900
Br	4.26633700	-0.56315100	0.00921600

4e

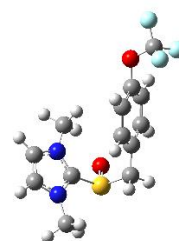


1 1

S	-2.51683800	1.42021400	0.25774000
O	-1.90867100	1.78754400	1.55110400
N	-1.90742300	-1.26404400	0.97721100
N	-3.51060000	-1.08175300	-0.47012700
C	-2.57757900	-0.39830200	0.20975700
C	0.06017800	1.07538700	-0.84830700
C	-1.27199600	1.67866200	-1.09420700
H	-1.75080100	1.30395800	-2.00110700
H	-1.23924900	2.76872100	-1.14455400
C	0.41806700	-0.16503300	-1.37513800
H	-0.28053000	-0.69217600	-2.01588000
C	1.01427400	1.74001400	-0.08470200
C	-0.79516700	-0.97959900	1.88707500
H	0.14475200	-1.11983900	1.35611600
H	-0.86147600	-1.67306300	2.72157900

H	-0.87794800	0.04388400	2.23889100
C	-2.41067600	-2.51916200	0.76132100
H	-2.02271900	-3.38208000	1.27435500
C	-3.40980500	-2.40807900	-0.14664700
H	-4.05550100	-3.15412100	-0.57642700
C	-4.47670300	-0.52340200	-1.40832500
H	-4.69525100	0.50580100	-1.13191100
H	-5.39205300	-1.10684500	-1.35219600
H	-4.08334400	-0.55957100	-2.42318900
C	2.25904900	1.20708400	0.18431600
H	2.96410000	1.76858500	0.78128900
C	1.65704100	-0.72861200	-1.12826000
H	1.92417400	-1.68359300	-1.55865400
C	2.56753100	-0.03818200	-0.33759500
Br	4.25525600	-0.79512900	0.01573000
F	0.72794600	2.95133400	0.38701500

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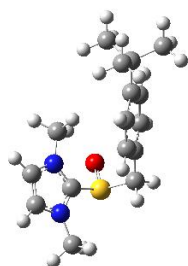


1 1

S	-2.77946000	1.55104300	0.12526100
O	-2.28169200	1.98518600	1.44733900
N	-2.27970700	-1.10630500	1.01590600
N	-3.75051200	-0.96413600	-0.56977000
C	-2.86839600	-0.26484000	0.16027100
C	-0.11654800	1.11487000	-0.68664800
C	-1.40453000	1.72856400	-1.10325400
H	-1.79692200	1.32925300	-2.04079100
H	-1.34908700	2.81602200	-1.19327100
C	0.29193500	-0.10352300	-1.22717700
H	-0.30941300	-0.59088200	-1.98684300
C	0.69034400	1.74454100	0.25994800
C	-1.24410400	-0.79734100	2.00414400

H	-0.26442800	-0.94649500	1.55388100
H	-1.37655300	-1.47106100	2.84684700
H	-1.35459100	0.23412900	2.32316600
C	-2.78210500	-2.36278100	0.80798500
H	-2.45264700	-3.20858400	1.38626100
C	-3.69815800	-2.27698000	-0.18635800
H	-4.31569100	-3.03230900	-0.64058100
C	-4.62285200	-0.43481800	-1.61113600
H	-4.85148300	0.60676100	-1.39635400
H	-5.54693000	-1.00704300	-1.61314900
H	-4.14189600	-0.51600300	-2.58480600
C	1.87945800	1.16317400	0.66701000
H	2.51343300	1.64214300	1.40097400
C	1.48097500	-0.69071000	-0.82899200
H	1.81466600	-1.62890100	-1.25154400
C	2.26299500	-0.04837300	0.11749100
O	3.41595300	-0.66579900	0.57290200
C	4.56794200	-0.38841000	-0.09146100
F	4.86012300	0.91103100	-0.05981300
F	5.53264800	-1.06321400	0.49347600
F	4.49949200	-0.74780800	-1.37443800
H	0.38824000	2.69393900	0.68318200

6e



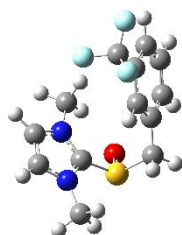
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S	2.50744200	-1.51620100	0.30530000
O	1.92129200	-1.88481300	1.61173500
N	1.76976000	1.15720600	0.93549000
N	3.40471800	1.00074100	-0.47828100
C	2.49347900	0.29835900	0.21184000
C	-0.08383800	-1.26519700	-0.78190100

C	1.25823400	-1.85340200	-1.02141600
H	1.72686100	-1.51316900	-1.94771000
H	1.25401800	-2.94614700	-1.02305900
C	-0.48112400	-0.10566400	-1.43891400
H	0.17669900	0.35863000	-2.16700000
C	-0.97296900	-1.85799000	0.11393100
C	0.65051600	0.84876700	1.82755000
H	-0.27812300	0.88457000	1.26020900
H	0.64144300	1.59426400	2.61872300
H	0.79257500	-0.14394100	2.24292700
C	2.21650100	2.42627100	0.68237600
H	1.77878200	3.28711200	1.15706700
C	3.23545600	2.33134100	-0.20516200
H	3.85194900	3.09159900	-0.65228000
C	4.40773900	0.45664300	-1.38477700
H	4.67190500	-0.55001600	-1.06834900
H	5.29285600	1.08600300	-1.34126000
H	4.02471400	0.43579800	-2.40400000
C	-2.21484200	-1.29504400	0.34219000
H	-2.88303600	-1.78724500	1.03763200
C	-1.73064400	0.45119800	-1.20520400
H	-2.00961400	1.34162200	-1.75163200
C	-2.62788900	-0.12821600	-0.30851500
H	-0.69191100	-2.76643900	0.63253000
C	-4.01918600	0.44134500	-0.04513600
C	-5.07077100	-0.60603400	-0.44196500
H	-4.96770800	-1.52706400	0.13331500
H	-6.07325700	-0.21350700	-0.26112100
H	-4.99290300	-0.85963100	-1.50076000
C	-4.16179500	0.76605500	1.44904100
H	-5.16096000	1.15614900	1.65178800
H	-4.01937500	-0.11510600	2.07621700
H	-3.43856000	1.52403700	1.75894900
C	-4.28325500	1.71705600	-0.84410200
H	-3.57832300	2.51281900	-0.59202500
H	-4.23820900	1.54245500	-1.92103600

H -5.28426100 2.08636800 -0.61729400

7e



1 1

S -2.51496700 1.22618200 -0.32995500
O -2.39159700 2.12168800 0.83880000
N -1.34691000 -0.78623000 1.31367700
N -2.47292200 -1.55823400 -0.36972500
C -2.01914900 -0.43783500 0.21212700
C 0.23948300 1.52697900 -0.81256500
C -1.09317800 1.56011400 -1.47036800
H -1.19653400 0.84107800 -2.28560100
H -1.35767800 2.54909400 -1.85103000
C 1.02462700 0.38210400 -0.88950600
H 0.69590900 -0.46982400 -1.47388100
C 0.70596300 2.62643900 -0.09266100
C -0.66835700 0.09514000 2.26619600
H 0.38228100 0.17279600 1.99333700
H -0.76606000 -0.34489800 3.25544800
H -1.13587900 1.07398100 2.23995500
C -1.35489000 -2.15138500 1.41671400
H -0.86478800 -2.66197200 2.22749600
C -2.05441300 -2.63612200 0.36300400
H -2.29072400 -3.64760400 0.08153600
C -3.26971900 -1.63853300 -1.58791900
H -3.86431500 -0.73355300 -1.69214600
H -3.93727700 -2.49273600 -1.50971200
H -2.62304800 -1.76061000 -2.45566500
C 1.93734400 2.57422300 0.53991600
H 2.29951800 3.43599700 1.08529800
C 2.24991000 0.33009800 -0.24239100
C 2.71196400 1.42476100 0.47394000

H 0.10607300 3.52593300 -0.03367700

H 3.67581100 1.38299900 0.96356900

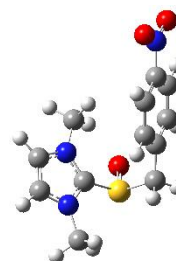
C 3.03451700 -0.94988900 -0.28813400

F 2.98351500 -1.51961900 -1.49651600

F 2.51903300 -1.84708900 0.58196400

F 4.31113800 -0.77645000 0.03523800

8e

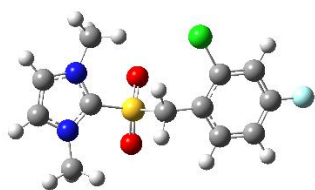


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S 2.07706500 -1.56075800 0.27069800
O 1.44398500 -1.93730700 1.55096700
N 1.51038200 1.13479700 0.99566500
N 3.12566900 0.92021200 -0.43389900
C 2.17101900 0.25591000 0.23512700
C -0.48707000 -1.17598600 -0.82781300
C 0.83879900 -1.79821700 -1.08542800
H 1.32296300 -1.43491100 -1.99403500
H 0.79272500 -2.88861200 -1.13529500
C -0.83856300 0.01607200 -1.46174900
H -0.16478900 0.46990600 -2.17974400
C -1.38339500 -1.77525900 0.05671000
C 0.38409100 0.87241200 1.89423900
H -0.54755000 1.03039500 1.35432200
H 0.45430900 1.56537500 2.72877100
H 0.44283800 -0.15184500 2.24813300
C 2.04144600 2.37914500 0.78644700
H 1.66510200 3.24984800 1.29516900
C 3.04796800 2.24783900 -0.11088800
H 3.71256700 2.98105400 -0.53400600
C 4.09096500 0.34484600 -1.36324900
H 4.29092500 -0.68746600 -1.08456300

H	5.01492400	0.91363200	-1.29910700
H	3.70718900	0.38735600	-2.38150300
C	-2.60883800	-1.18560600	0.31708200
H	-3.32233600	-1.63328900	0.99470900
C	-2.06061000	0.61388000	-1.21007300
H	-2.36194500	1.52958500	-1.69925700
C	-2.92182000	0.00390200	-0.31486800
H	-1.12416000	-2.70665300	0.54303600
N	-4.21889800	0.64286800	-0.03283100
O	-4.96786700	0.06259300	0.72226000
O	-4.43609400	1.70833500	-0.57117300

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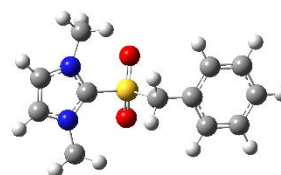


1 1

S	0.79793500	-0.56916800	0.57850400
Cl	-1.65427600	2.37272500	-0.53419900
O	0.87727100	-1.97680800	0.85391300
O	0.43349200	0.38857500	1.58113600
N	3.44332500	-0.92129000	-0.33564900
N	2.98194300	1.14362000	0.15519600
F	-5.60585600	-0.54653800	0.39175200
C	-1.63349600	-0.35879900	-0.57068400
C	2.47543800	-0.09552300	0.08749200
C	-0.18257200	-0.31340800	-0.91786600
H	0.11402100	0.65147700	-1.32855100
H	0.11114000	-1.11563600	-1.59463300
C	3.36964100	-2.37173100	-0.53078100
H	3.24037100	-2.86621400	0.42747000
H	4.30021300	-2.68381700	-0.99582000
H	2.53606500	-2.62160200	-1.17985700
C	4.29014800	1.09967600	-0.22854300
H	4.90927400	1.97964000	-0.25117400
C	4.57877500	-0.19107900	-0.53494000

H	5.49552200	-0.64148400	-0.87370500
C	-2.37946700	0.80261000	-0.36251300
C	-2.28051100	-1.58723700	-0.44002900
H	-1.71770500	-2.49925500	-0.59606400
C	-3.72243300	0.74921800	-0.04175400
H	-4.30262100	1.64829300	0.10985800
C	-4.31679700	-0.49205000	0.08117600
C	-3.61971400	-1.66947400	-0.11412400
H	-4.12488800	-2.62010200	-0.01412800
C	2.30954700	2.36393600	0.60975900
H	1.31313000	2.42723200	0.18385600
H	2.90716400	3.20825300	0.27803500
H	2.23239700	2.35513800	1.69389800

2f

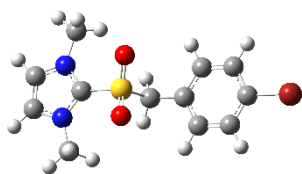


1 1

S	0.22775600	0.00012600	0.59608700
O	0.07145900	-1.25758200	1.26979300
O	0.07159100	1.25806000	1.26938200
N	2.71220700	-1.08553000	-0.17457500
N	2.71231100	1.08537900	-0.17475100
C	-2.19142600	-0.00007700	-0.59507900
C	1.95301200	-0.00002900	0.03316300
C	-0.73129900	-0.00003200	-0.92973500
H	-0.42497800	0.89296200	-1.47605000
H	-0.42480400	-0.89300500	-1.47598400
C	2.32810100	-2.49193300	-0.03057800
H	2.13508800	-2.71540500	1.01451600
H	3.15257800	-3.09344900	-0.40216300
H	1.43545500	-2.69952500	-0.61290700
C	3.96894200	0.67845900	-0.51741100
H	4.75873500	1.37811100	-0.72886300
C	3.96883900	-0.67878600	-0.51746200

H	4.75853700	-1.37855200	-0.72888300
C	-2.87094500	1.20422900	-0.43531300
C	-2.87093100	-1.20432700	-0.43499600
H	-2.34636400	-2.14498000	-0.55348400
C	-4.22115300	1.20233600	-0.12832600
H	-4.74772600	2.14074300	-0.01141300
C	-4.89626100	0.00001800	0.02602500
C	-4.22114000	-1.20234000	-0.12802600
H	-4.74773000	-2.14070800	-0.01088800
C	2.32850400	2.49182200	-0.03044600
H	1.43434900	2.69914000	-0.61051100
H	3.15201100	3.09322200	-0.40437600
H	2.13814500	2.71575700	1.01505300
H	-5.95248500	0.00002800	0.26364500
H	-2.34638600	2.14484300	-0.55409300

3f

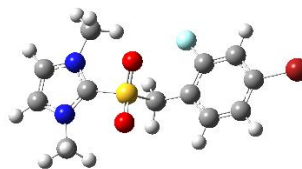


1 1

S	1.58100100	-0.00002300	0.55634300
O	1.39520300	-1.25806600	1.22188800
O	1.39514700	1.25804000	1.22182100
N	4.09429200	-1.08560100	-0.11085600
N	4.09419000	1.08565900	-0.11099200
C	-0.79022200	-0.00008300	-0.72287200
C	3.32701800	-0.00000100	0.06544300
C	0.67927200	-0.00005500	-1.00609300
H	1.00501400	0.89276900	-1.54116300
H	1.00511100	-0.89280800	-1.54122100
C	3.70563100	-2.49234100	0.01794800
H	3.46701900	-2.71468000	1.05382000
H	4.54643100	-3.09334500	-0.31593500
H	2.84007800	-2.70186300	-0.60330600
C	5.36368000	0.67875800	-0.40161900

H	6.16157900	1.37840100	-0.58024400
C	5.36372500	-0.67861000	-0.40162700
H	6.16168200	-1.37820200	-0.58019300
C	-1.47887200	1.20155300	-0.58432800
C	-1.47891300	-1.20166400	-0.58422800
H	-0.95664300	-2.14562600	-0.68331100
C	-2.83723700	1.20658800	-0.32305400
H	-3.37211100	2.14079400	-0.22277300
C	-3.50833900	0.00000300	-0.19326000
C	-2.83727800	-1.20662000	-0.32296600
H	-3.37221300	-2.14078400	-0.22262700
C	3.70548600	2.49235100	0.01807100
H	2.83861800	2.70148100	-0.60145100
H	4.54547500	3.09343800	-0.31771400
H	3.46892300	2.71500500	1.05435800
H	-0.95656700	2.14547300	-0.68351500
Br	-5.36012300	0.00002400	0.15767300

4f

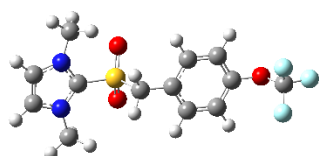


1 1

S	-1.64501100	-0.48833400	0.54826200
O	-1.22450300	0.51532800	1.48205600
O	-1.73072000	-1.87834100	0.89862100
N	-3.79805700	1.24922700	0.08996100
N	-4.34421600	-0.83338500	-0.19910400
C	0.73675700	-0.27710400	-0.70551000
C	-3.33259100	-0.00778100	0.10401800
C	-0.72382800	-0.31900200	-1.00000300
H	-1.01027700	-1.17889800	-1.60456200
H	-1.07083300	0.60171100	-1.46941000
C	-3.06601400	2.47930100	0.40525800
H	-2.91552700	2.54856500	1.47936300

H	-3.66329300	3.31425900	0.05024900
H	-2.09967100	2.48356700	-0.08941600
C	-5.46667200	-0.08465200	-0.40416600
H	-6.41257000	-0.53103900	-0.65726800
C	-5.12502800	1.21704000	-0.22445000
H	-5.71854900	2.11218200	-0.29247600
C	1.50421600	-1.43156200	-0.57218900
C	1.37920900	0.94343800	-0.54822300
C	2.85756700	-1.36113000	-0.29982200
H	3.44451600	-2.26316200	-0.20203900
C	3.45764300	-0.11764200	-0.15650100
C	2.72519500	1.05239100	-0.28277700
H	3.17994900	2.02725600	-0.17879500
C	-4.32315300	-2.29705300	-0.27238300
H	-3.52902600	-2.62851000	-0.93407800
H	-5.28414600	-2.61538200	-0.66578200
H	-4.16299700	-2.71314200	0.71798500
H	1.03476900	-2.40121200	-0.68556500
Br	5.30051900	-0.00947600	0.20980500
F	0.65639800	2.06717400	-0.68050000

5f

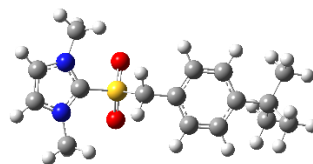


1 1

S	1.92836000	0.00036700	0.63406700
O	1.80368600	-1.25740600	1.31390000
O	1.80421200	1.25879300	1.31275000
N	4.36788400	-1.08620500	-0.26285400
N	4.36841600	1.08527400	-0.26326600
C	-0.55208600	0.00029700	-0.42081200
C	3.62027400	-0.00024500	-0.01751800
C	0.88655100	-0.00010500	-0.83760900
H	1.16055300	0.89222100	-1.40154300
H	1.16033600	-0.89297100	-1.40079700

C	3.99223500	-2.49297800	-0.09932000
H	3.84915300	-2.71542700	0.95398500
H	4.79891000	-3.09410800	-0.50861200
H	3.07364600	-2.70218700	-0.63922400
C	5.60572500	0.67790000	-0.66866600
H	6.38419500	1.37723400	-0.91967900
C	5.60539000	-0.67959000	-0.66843800
H	6.38352100	-1.37940600	-0.91915500
C	-1.22135300	1.20401900	-0.21886700
C	-1.22188700	-1.20294200	-0.21787600
C	-2.54969900	1.20884300	0.16620300
H	-3.08400700	2.13514000	0.32656100
C	-3.20074600	0.00120400	0.34892700
C	-2.55022600	-1.20688800	0.16722900
H	-3.08487300	-2.13284200	0.32840000
C	3.99380900	2.49227200	-0.09938000
H	3.07285600	2.70123200	-0.63526100
H	4.79880900	3.09285900	-0.51276700
H	3.85544200	2.71571100	0.95437300
H	-0.70653900	2.14599600	-0.36263700
H	-0.70746700	-2.14526500	-0.36080000
O	-4.51093400	0.00193900	0.79792600
C	-5.48477600	-0.00041200	-0.14426700
F	-5.41665800	-1.07591500	-0.93193400
F	-6.64205500	0.00115800	0.48037800
F	-5.41655100	1.07115600	-0.93725900

6f



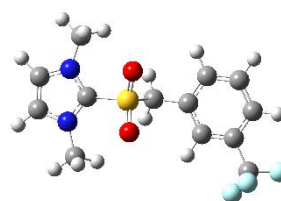
1 1

S	1.54841800	0.00451300	0.55709300
O	1.36187500	-1.25376400	1.22276900
O	1.37528400	1.26130600	1.22908200

N	4.05621100	-1.09216200	-0.12156400
N	4.06708200	1.07827100	-0.11757200
C	-0.82134400	0.01926500	-0.72531000
C	3.29548100	-0.00342000	0.06155700
C	0.64773100	0.01326900	-1.00510800
H	0.98053700	0.90679300	-1.53511100
H	0.97287500	-0.87972500	-1.54091700
C	3.65964500	-2.49649500	0.00595300
H	3.43015200	-2.72123800	1.04337200
H	4.49273900	-3.10193300	-0.33918000
H	2.78573300	-2.69757700	-0.60625500
C	5.33336800	0.66576900	-0.41625800
H	6.13349400	1.36190300	-0.59824500
C	5.32656700	-0.69124900	-0.41873500
H	6.11968400	-1.39468400	-0.60331300
C	-1.51009100	1.21751800	-0.59176100
C	-1.51945900	-1.17736400	-0.58303800
H	-1.00193000	-2.12490800	-0.67825900
C	-2.87121800	1.21925900	-0.33171000
H	-3.37604000	2.17063800	-0.24091900
C	-3.58622000	0.03205900	-0.19007800
C	-2.87544100	-1.16435800	-0.32386800
H	-3.39176500	-2.11072100	-0.22554900
C	3.68449000	2.48602500	0.01500400
H	2.81200100	2.69771600	-0.59563300
H	4.52318800	3.08438700	-0.32888300
H	3.45814600	2.70950200	1.05339900
H	-0.98670400	2.16119700	-0.69385600
C	-5.08446800	-0.00130700	0.09507600
C	-5.32760200	-0.74300900	1.41793400
H	-6.39743300	-0.77795200	1.63303400
H	-4.96416200	-1.77109300	1.38354100
H	-4.83168100	-0.23785800	2.24900400
C	-5.68284100	1.40019400	0.21034900
H	-5.57047400	1.97063400	-0.71413100
H	-6.75130800	1.32195500	0.41627500

H	-5.23462600	1.97041500	1.02681400
C	-5.79782600	-0.74144700	-1.04618700
H	-5.44809800	-1.76979600	-1.14841800
H	-6.87184900	-0.77550800	-0.85291700
H	-5.64212500	-0.23572100	-2.00112500

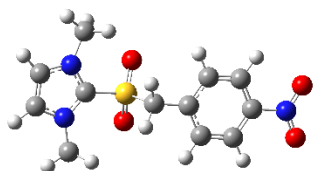
7f



1 1			
S	-1.32997600	0.26369700	0.57908400
O	-1.52666900	1.52575600	1.23353300
O	-0.81788200	-0.88851500	1.26352200
N	-4.02719200	0.58825100	-0.16701500
N	-3.40169600	-1.49153200	-0.16397700
C	1.00229800	0.87740000	-0.62173100
C	-2.98494100	-0.23189600	0.03169400
C	-0.41373700	0.51542900	-0.95303500
H	-0.48609500	-0.42046200	-1.50825800
H	-0.93610300	1.30738900	-1.49058700
C	-4.06450900	2.04653900	-0.02916700
H	-3.93802900	2.32072500	1.01408500
H	-5.03000300	2.38261500	-0.39589400
H	-3.27380800	2.50044500	-0.61873800
C	-4.72585000	-1.46519800	-0.49059500
H	-5.28332100	-2.36369700	-0.69073700
C	-5.11696000	-0.16514200	-0.49230800
H	-6.07750400	0.27612500	-0.69415800
C	1.95726800	-0.12375700	-0.48683200
C	1.36508700	2.20804800	-0.43888700
H	0.62479700	2.99248700	-0.53935700
C	3.26576400	0.20940600	-0.18400900
C	3.62933700	1.53709200	-0.00615700
C	2.67626300	2.53431200	-0.13472600

H	2.95790200	3.57055600	-0.00196800
C	-2.62803600	-2.72803300	-0.02231800
H	-1.71896300	-2.67328300	-0.61363500
H	-3.24825800	-3.54243200	-0.38518000
H	-2.36962400	-2.88269300	1.02112900
H	4.65671700	1.78908600	0.22215400
H	1.68996700	-1.16307600	-0.62648400
C	4.29438500	-0.87379100	-0.00996900
F	4.45657800	-1.18310600	1.28302600
F	3.93916400	-1.99821600	-0.64443700
F	5.48562900	-0.49982800	-0.48180800

8f

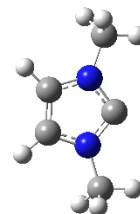


1 1

S	1.16249100	-0.00015700	0.56001200
O	0.97690200	-1.25884300	1.22295500
O	0.97681100	1.25802500	1.22388500
N	3.66908000	-1.08604100	-0.12053800
N	3.66888200	1.08617800	-0.12075800
C	-1.21995600	0.00026000	-0.70047600
C	2.90194800	0.00001300	0.05564000
C	0.25048600	0.00039200	-0.99503700
H	0.56825000	0.89340100	-1.53403200
H	0.56829400	-0.89221700	-1.53466500
C	3.28231600	-2.49354300	0.00978000
H	3.05289900	-2.71727800	1.04749400
H	4.12079600	-3.09344500	-0.33173600
H	2.41212400	-2.70316600	-0.60485400
C	4.93747700	0.67905800	-0.41242100
H	5.73544200	1.37852800	-0.59187500
C	4.93760700	-0.67874900	-0.41227000
H	5.73571200	-1.37811300	-0.59152200
C	-1.90159600	1.20598700	-0.55850200

C	-1.90158400	-1.20559600	-0.55959000
H	-1.37564000	-2.14631300	-0.66369900
C	-3.25775800	1.21148100	-0.28762900
H	-3.81369900	2.13169100	-0.17798500
C	-3.91059800	0.00000500	-0.15763300
C	-3.25775600	-1.21134300	-0.28873900
H	-3.81369100	-2.13166300	-0.17999300
C	3.28163400	2.49360100	0.00890800
H	2.41417800	2.70371800	-0.60949000
H	4.12159000	3.09370200	-0.32859600
H	3.04777400	2.71664000	1.04575100
H	-1.37566500	2.14679900	-0.66180700
N	-5.35604800	-0.00012300	0.12801000
O	-5.89716700	-1.07977900	0.23468000
O	-5.89716400	1.07943700	0.23568400

1,3-dimethyl-imidazol-2-ylidene-singlet

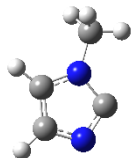


0 1

C	0.00000900	-1.20612300	0.67459700
C	0.00000900	-1.20612300	-0.67459700
C	-0.00001200	0.97237600	0.00000000
N	-0.00000200	0.11981700	1.05648900
C	-0.00000200	0.56984900	2.42760000
H	0.88883600	0.21525000	2.95256200
H	-0.00003600	1.65634100	2.41613700
H	-0.88880700	0.21519300	2.95257800
N	-0.00000200	0.11981700	-1.05648900
C	-0.00000200	0.56984900	-2.42760000
H	-0.00003600	1.65634100	-2.41613700
H	0.88883600	0.21525000	-2.95256200

H	-0.88880700	0.21519300	-2.95257800
H	0.00001600	-2.02498400	1.37405700
H	0.00001600	-2.02498400	-1.37405700

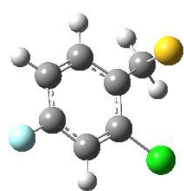
frag-1 (1a, 1b and 1c)



-1 1

C	0.21374800	1.08191900	0.00007500
C	1.48239000	0.57244600	0.00021200
C	0.16031700	-1.20101400	-0.00010300
N	-0.59693800	-0.03124700	-0.00004000
C	-2.02529400	-0.01251000	-0.00006700
H	-2.43277900	0.48914500	-0.88768700
H	-2.35529900	-1.05209300	-0.00065600
H	-2.43286700	0.48812900	0.88809300
N	1.45180400	-0.79713200	-0.00008000
H	-0.16120800	2.09539300	-0.00002400
H	2.41112600	1.13303000	0.00039600

frag-2 (1a and 1d)

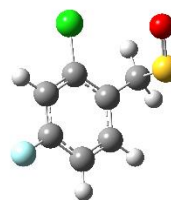


1 1

S	1.93990000	-1.09688600	-0.79195700
C	1.86067800	-0.82725000	0.95812100
H	2.36404100	0.05618500	1.33181900
C	0.52014400	-0.56287800	0.30164700
C	-0.46828300	-1.61888200	0.35069600
C	0.04822100	0.80060200	0.08651300
C	-1.78807100	-1.36858600	0.16417000
H	-0.11009200	-2.62559200	0.52572700

C	-1.28427800	1.04504700	-0.08850200
C	-2.16815600	-0.03559700	-0.05118900
H	-2.54119200	-2.14456600	0.17806700
H	-1.66673000	2.04264500	-0.25642500
H	1.91082000	-1.70485100	1.59145500
Cl	1.14973600	2.08078700	0.06018700
F	-3.42914200	0.21758100	-0.22791700

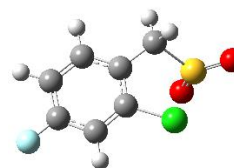
frag-2 (1b and 1e)



1 1

S	-1.91071800	-1.09145100	-0.57739700
C	-1.55338800	-0.79846600	1.16627800
H	-1.64080500	-1.70346200	1.76054300
C	-0.17568200	-0.52449500	0.64955500
C	0.24368400	0.78507400	0.25555300
C	0.77195300	-1.58474400	0.57601000
C	1.53547600	1.00592600	-0.16684900
C	2.05280400	-1.36743500	0.16155600
H	0.46535500	-2.57967000	0.87631100
C	2.41281600	-0.06670700	-0.20615600
H	1.87339100	1.99190300	-0.45544100
H	2.78665000	-2.16047100	0.11298500
H	-2.11230800	0.04527300	1.55830200
O	-2.61501100	0.03561500	-1.16061800
Cl	-0.84364400	2.09085900	0.32524800
F	3.63725200	0.14946600	-0.60825800

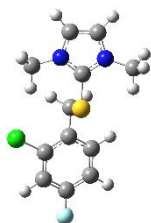
frag-2 (1c and 1f)



1 1

S	-2.23330700	0.29683000	0.27913000
C	-1.06264300	1.19625400	-0.80592500
H	-1.27520100	2.25178500	-0.61721600
C	0.31670000	0.78270600	-0.46466000
C	0.60384100	-0.56674800	-0.27690000
C	1.35575600	1.69542300	-0.30738800
C	1.85399500	-1.04278500	0.03750400
C	2.63577100	1.25860400	-0.02283500
H	1.16701400	2.75479000	-0.42840400
C	2.86415200	-0.09768800	0.14097000
H	2.06120700	-2.09123400	0.20067300
H	3.45782600	1.95346100	0.08356000
H	-1.42129500	0.90279400	-1.79536900
O	-3.47514000	-0.01920100	-0.32162200
Cl	-0.76233400	-1.66245800	-0.36710000
F	4.08159900	-0.51642100	0.42198300
O	-1.95445500	0.39846300	1.66274000

Conformer A (1d)

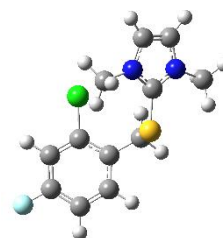


1 1

S	0.86877200	-0.36844100	0.77325200
Cl	-1.59213900	2.32832600	0.08223600
F	-5.51557100	-0.76956600	0.32664500
N	3.13003600	0.97147400	-0.06777400
N	3.42243100	-1.16637600	0.11027000
C	2.51068300	-0.18421100	0.23580500
C	-2.30284600	0.75143900	-0.08730600
C	-1.52746700	-0.33112700	-0.50646100
C	4.43216300	0.71254700	-0.39478600
H	5.11837300	1.49091100	-0.68011200
C	-3.64955100	0.61659100	0.19412700

H	-4.24772300	1.45916600	0.51093400
C	4.61742700	-0.62419800	-0.27599500
H	5.49676900	-1.22486800	-0.43102200
C	-4.22217700	-0.63319700	0.05764500
C	-0.07907700	-0.19177700	-0.82439700
H	0.15429700	0.78237000	-1.24700800
H	0.25452300	-0.98298200	-1.49138200
C	2.52622300	2.29584000	-0.03894900
H	2.36090300	2.65133300	-1.05479800
H	3.19344200	2.97673200	0.48475700
H	1.57886400	2.23360100	0.49063900
C	-2.15478800	-1.57058000	-0.62572300
H	-1.57351800	-2.42452300	-0.95312300
C	-3.49808900	-1.73771400	-0.35012800
H	-3.98674700	-2.69703600	-0.45007000
C	3.20479900	-2.58273600	0.36852000
H	2.14837400	-2.74075900	0.56446700
H	3.78452900	-2.88801400	1.23781700
H	3.51299800	-3.15726400	-0.50253300

Conformer B (1d)

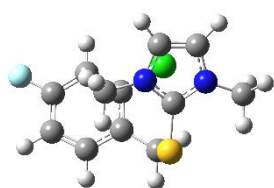


1 1

S	0.92535100	-1.10620600	1.10527100
Cl	-0.56585600	1.48508100	-1.20661800
F	-5.29584100	0.67787500	0.22982300
N	2.56902200	1.05373600	0.73535600
N	3.18313600	-0.66874200	-0.42540600
C	2.24515700	-0.21408500	0.42642500
C	-1.81472300	0.45595000	-0.56063600
C	-1.52232400	-0.86342000	-0.21517200
C	3.71390600	1.39897200	0.07073200
H	4.16492800	2.37049700	0.17292300

C	-3.08134200	0.98823600	-0.41960800
H	-3.30286600	2.00830800	-0.69989300
C	4.09149900	0.32668800	-0.66512500
H	4.92595400	0.19390800	-1.33136100
C	-4.07544100	0.17307700	0.08915900
C	-0.16552400	-1.44883300	-0.38101800
H	0.35272600	-1.05441000	-1.25114100
H	-0.21342400	-2.53308900	-0.45063800
C	1.84593700	1.92656000	1.64908200
H	1.84236600	2.93355300	1.23957100
H	2.32934000	1.92357300	2.62493100
H	0.82592100	1.56633000	1.74321700
C	-2.56262500	-1.64243100	0.28929700
H	-2.36549400	-2.67396000	0.55685300
C	-3.84074900	-1.14004200	0.44806800
H	-4.64776300	-1.74682000	0.83505500
C	3.24817900	-2.01026900	-0.98254900
H	2.73216600	-2.69149100	-0.30998600
H	4.29178000	-2.30394700	-1.06400100
H	2.78404800	-2.03778300	-1.96736500

Conformer C (1d)

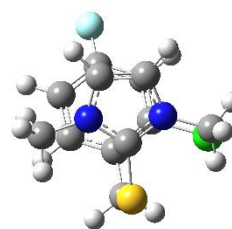


1 1

S	1.38122300	-1.93997800	0.37911400
Cl	-0.09670600	1.06135300	-1.94928900
F	-4.46747300	1.13475700	0.48485500
N	1.34484500	0.58515100	1.48591700
N	2.81826000	0.36193900	-0.08521500
C	1.83625000	-0.27655900	0.57705400
C	-1.30248700	0.28392600	-0.96029800
C	-1.14084400	-1.03860100	-0.54785100

C	2.00809400	1.77420600	1.37981800
H	1.78142000	2.61605100	2.01054800
C	-2.42027400	1.02762700	-0.62032200
H	-2.54505400	2.04667000	-0.95881100
C	2.92951800	1.63446300	0.39493300
H	3.65059900	2.33354500	0.00852100
C	-3.39342000	0.42660500	0.15349100
C	0.04627000	-1.85677300	-0.91626800
H	0.50591400	-1.53753800	-1.84736200
H	-0.21359400	-2.91205500	-1.00657800
C	0.28210900	0.31888200	2.44526300
H	-0.62070700	0.84920300	2.14773200
H	0.60476600	0.65122600	3.42956700
H	0.08902400	-0.74923300	2.46245900
C	-2.16007000	-1.59759500	0.22546400
H	-2.06619200	-2.62846100	0.54694500
C	-3.28616600	-0.88316100	0.58508000
H	-4.07773700	-1.32437100	1.17533400
C	3.61299000	-0.18452600	-1.17440300
H	3.54558800	-1.26835700	-1.14758500
H	4.64840700	0.12044500	-1.04266100
H	3.23570700	0.18610800	-2.12639200

Conformer D (1d)

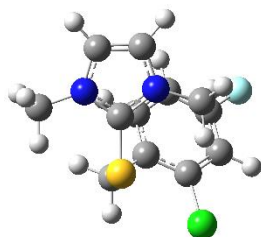


1 1

S	1.86252600	-0.41484700	1.61003600
Cl	-0.66181300	-2.59839300	-0.22696000
F	-3.99904000	0.95893200	-1.35007100
N	1.57333400	1.65954100	-0.19018800
N	2.10473100	-0.22366200	-1.11747700
C	1.80072400	0.35569400	0.05998200
C	-1.39566100	-1.05223400	0.06568000

C	-0.98754400	-0.27590000	1.15283200
C	1.71130700	1.89230300	-1.52892900
H	1.56399600	2.86703800	-1.96046400
C	-2.40799400	-0.64603300	-0.78555700
H	-2.72674300	-1.25991100	-1.61630900
C	2.05104800	0.71517000	-2.10785100
H	2.26273100	0.47692800	-3.13569200
C	-3.02784700	0.56278200	-0.53517800
C	0.06605700	-0.71623900	2.10237400
H	0.03806200	-1.79061700	2.27153300
H	-0.02982000	-0.19964500	3.05421500
C	1.29468000	2.69074800	0.79661600
H	0.25877700	3.01213500	0.71471000
H	1.96071500	3.53312100	0.62139700
H	1.48134700	2.28147400	1.78562200
C	-1.66389000	0.92531800	1.37058400
H	-1.40193600	1.52165800	2.23696400
C	-2.68090300	1.35886100	0.54026100
H	-3.21557300	2.28092400	0.72421100
C	2.51600800	-1.60534100	-1.32605000
H	2.39281000	-2.14948300	-0.39551100
H	3.56157800	-1.62475000	-1.62918800
H	1.89344800	-2.05096100	-2.09802100

Conformer E (1d)

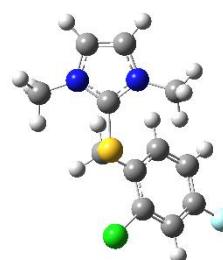


1 1

S	1.34450900	-1.71847400	-0.12907700
Cl	-2.18330400	-2.31521100	-0.66420900
F	-3.86947900	2.34027200	0.08893400
N	3.11012700	0.35087500	0.32461700
N	1.62619300	0.81115800	-1.18356800
C	2.02606800	-0.13250300	-0.31246000

C	-2.04986700	-0.74626100	0.05858800
C	-0.97102300	-0.44940900	0.89583100
C	3.38403700	1.60533000	-0.14274300
H	4.21362900	2.18597300	0.22177000
C	-3.03366100	0.18639900	-0.21789900
H	-3.87247200	-0.05249100	-0.85680000
C	2.45430700	1.89323200	-1.08629800
H	2.32316800	2.77234400	-1.69294900
C	-2.92821900	1.44033300	0.35423900
C	0.08616700	-1.44483000	1.21553200
H	-0.31257000	-2.45287600	1.33449800
H	0.62481200	-1.17971500	2.12253300
C	3.89452100	-0.34435700	1.33508900
H	3.78081300	0.15383700	2.29640100
H	4.94158900	-0.33995200	1.03969500
H	3.54125400	-1.36931700	1.40292200
C	-0.91862100	0.82680400	1.45429700
H	-0.10872900	1.07069700	2.13254700
C	-1.88438800	1.78297400	1.19274300
H	-1.85052000	2.76749400	1.63904500
C	0.49550400	0.71915400	-2.09780500
H	0.17862900	-0.31789100	-2.15738100
H	0.81061000	1.06532700	-3.07968500
H	-0.32406100	1.33286900	-1.72825400

Conformer F (1d)

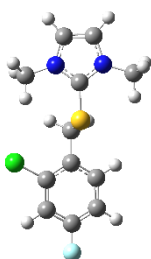


1 1

S	0.99324500	-0.90144800	-0.66707100
Cl	-2.03682200	-2.32669700	-0.76881800
F	-5.00463300	1.63065800	0.06192100
N	3.40613300	-0.37387200	0.56477600
N	2.73921000	1.22056500	-0.74019500

C	2.40191900	0.01570000	-0.24371000
C	-2.34990800	-0.76432700	-0.08105500
C	-1.35042700	-0.12783000	0.65572500
C	4.37111700	0.59554600	0.58386700
H	5.26701600	0.50271900	1.17274400
C	-3.58629900	-0.18394200	-0.28964800
H	-4.35713800	-0.68324700	-0.85962200
C	3.95836400	1.58842900	-0.24006400
H	4.43256500	2.51634900	-0.50853200
C	-3.81829700	1.06444700	0.25624700
C	-0.03283800	-0.77357700	0.90058400
H	-0.13705000	-1.80163200	1.24217800
H	0.55169000	-0.21168200	1.62468700
C	3.47252800	-1.63284500	1.29115200
H	3.14389100	-1.49428700	2.32016800
H	4.49968500	-1.98911200	1.28061800
H	2.83098700	-2.35512500	0.79237400
C	-1.63477300	1.13027300	1.18217600
H	-0.88068300	1.63990900	1.77088600
C	-2.86305000	1.73756000	0.99368500
H	-3.09025300	2.70859000	1.41175000
C	1.96272800	2.00779000	-1.68831500
H	0.95905500	1.59648600	-1.74253900
H	2.42862200	1.96336500	-2.67140500
H	1.92357200	3.03857400	-1.34348900

Conformer G (1d)

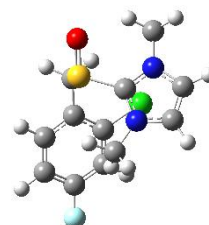


1 1

S	0.86882200	0.36853800	-0.77324600
Cl	-1.59234000	-2.32840500	-0.08235300
F	-5.51551900	0.76980400	-0.32667900
N	3.13000300	-0.97148100	0.06784700

N	3.42252100	1.16634300	-0.11032600
C	2.51070400	0.18421900	-0.23580800
C	-2.30292600	-0.75146800	0.08725600
C	-1.52746700	0.33101400	0.50651000
C	4.43214200	-0.71260600	0.39484000
H	5.11832700	-1.49097600	0.68021400
C	-3.64960400	-0.61648800	-0.19418800
H	-4.24784400	-1.45898800	-0.51107300
C	4.61747700	0.62412500	0.27597900
H	5.49686200	1.22474400	0.43097100
C	-4.22215000	0.63333800	-0.05761100
C	-0.07908100	0.19161300	0.82441800
H	0.15440100	-0.78260100	1.24680900
H	0.25454300	0.98272700	1.49148900
C	2.52613500	-2.29582300	0.03902600
H	2.36097500	-2.65138900	1.05487700
H	3.19323000	-2.97670100	-0.48485800
H	1.57869000	-2.23349800	-0.49039900
C	-2.15470500	1.57049400	0.62587700
H	-1.57338200	2.42437400	0.95335100
C	-3.49799900	1.73775900	0.35027400
H	-3.98657700	2.69711300	0.45031000
C	3.20496800	2.58270000	-0.36861700
H	2.14859600	2.74070500	-0.56486800
H	3.78498100	2.88800900	-1.23771200
H	3.51286800	3.15722400	0.50255500

Conformer I (1e)

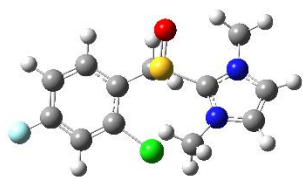


1 1

S	1.28228900	1.72846200	0.44126700
Cl	-0.35521000	-1.28299400	-1.90650300

O	2.50921900	2.41233200	-0.02147300
N	2.62677000	-0.69858500	-0.12881100
N	1.20636100	-0.85743700	1.49982800
F	-4.69796900	-0.80850700	0.52850500
C	1.67797400	-0.04232600	0.54728400
C	-1.17183900	0.96816600	-0.59028400
C	0.09690000	1.64651500	-0.97594400
H	-0.05315500	2.70773000	-1.18321700
H	0.61184300	1.19390400	-1.81977900
C	-2.12457700	1.65973300	0.16179500
H	-1.92904400	2.69016300	0.43556100
C	-1.46831000	-0.34857600	-0.94814100
C	3.38803700	-0.20540300	-1.27516300
H	2.84817800	-0.43697400	-2.19230600
H	4.35216800	-0.70679300	-1.28238700
H	3.52676100	0.86756500	-1.17537400
C	2.73721000	-1.96022600	0.38689700
H	3.44038600	-2.67557400	-0.00313100
C	1.84564100	-2.06284700	1.40278000
H	1.62369200	-2.88414000	2.06163600
C	0.16416500	-0.54497600	2.47138800
H	0.20432400	0.51346800	2.71606900
H	0.34678300	-1.12888400	3.36968600
H	-0.81364100	-0.78900900	2.06000500
C	-2.65613800	-0.95666900	-0.57986900
H	-2.88798200	-1.96944100	-0.87856300
C	-3.31600400	1.07858200	0.55129300
H	-4.05493500	1.62182100	1.12438700
C	-3.55929000	-0.22835100	0.17059900

Conformer II (1e)

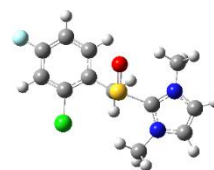


1 1

S	0.83308800	0.96735900	0.89582400
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Cl	-0.85055000	-1.90065500	-0.86787900
O	1.34969900	2.33019700	1.17113300
N	3.20022400	0.50804700	-0.59280500
N	2.62332400	-1.17157200	0.64700700
F	-5.49174800	-0.42601800	0.31503800
C	2.24976200	0.04252500	0.22530900
C	-1.60766200	0.67027800	-0.40026000
C	-0.20381100	1.08231300	-0.66382000
H	-0.12333200	2.14525800	-0.89170600
H	0.26498100	0.49177400	-1.44795800
C	-2.57359300	1.62151200	-0.07259600
H	-2.28735500	2.66502500	-0.01681800
C	-2.01173200	-0.66256000	-0.46580900
C	3.20734100	1.80783100	-1.26136300
H	2.70111800	1.73142000	-2.22237600
H	4.24129300	2.10264900	-1.41929400
H	2.71365600	2.53501400	-0.62113600
C	4.18287700	-0.43743600	-0.70700300
H	5.05616100	-0.28284900	-1.31690400
C	3.82084800	-1.49071800	0.06522700
H	4.31703700	-2.42723200	0.25206300
C	1.90491100	-2.03516400	1.57861700
H	1.15361800	-1.45217400	2.10323700
H	2.61604400	-2.43926200	2.29525100
H	1.42018700	-2.84228100	1.03381600
C	-3.31657200	-1.04893300	-0.23130300
H	-3.62382500	-2.08323700	-0.29364100
C	-3.88738300	1.26910800	0.17279800
H	-4.63759000	2.00723100	0.42099000
C	-4.23477700	-0.06553600	0.08710200

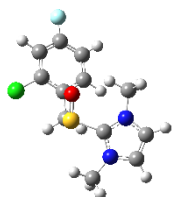
Conformer III (1e)



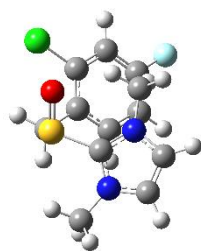
1 1

S	0.81631400	0.04710100	0.81437500	I 1			
Cl	-1.71810700	-2.45367700	-0.12659000	S	1.00236300	-1.09067300	0.53516700
O	0.56684000	1.34648400	1.47481600	Cl	-2.20195400	-2.45644400	0.34137000
N	3.24439500	1.16084700	-0.16999900	O	0.27622600	-0.51422300	1.68541400
N	3.26583600	-0.99928300	-0.00716100	N	2.46915500	1.35401900	0.51060600
F	-5.52721000	0.77890000	0.22511200	N	3.48765200	-0.30220300	-0.44467600
C	2.49767400	0.09089000	0.12273200	F	-4.81842000	1.80390400	0.03508200
C	-1.54004500	0.23315100	-0.53038500	C	2.34081000	0.07691800	0.13735800
C	-0.09138500	0.04965400	-0.80889700	C	-1.29987700	-0.14014400	-0.74721500
H	0.30916200	0.87564800	-1.39473500	C	-0.03210800	-0.84224100	-1.04514900
H	0.14287300	-0.90251200	-1.28574000	H	0.58002000	-0.30646900	-1.76751500
C	-2.10871100	1.50503500	-0.56858100	H	-0.18778400	-1.86643700	-1.38141400
H	-1.48193900	2.35577800	-0.80436300	C	-1.47879000	1.19384800	-1.10997700
C	-2.37046000	-0.84344200	-0.21108700	H	-0.68039800	1.71085200	-1.63025400
C	2.81893100	2.56082200	-0.16635600	C	-2.35973700	-0.79211500	-0.11136700
H	2.57088500	2.86643700	-1.18173000	C	1.47478000	2.19352600	1.18263900
H	3.64190500	3.16594500	0.20568600	H	1.09148200	2.92597400	0.47496300
H	1.95660300	2.66605000	0.48612500	H	1.96093000	2.70168200	2.01243600
C	4.50420700	0.73782900	-0.50520600	H	0.67154300	1.56489100	1.55351300
H	5.28350500	1.42914000	-0.77592900	C	3.71565900	1.79429100	0.14559000
C	4.51699700	-0.61291100	-0.40932900	H	4.04573900	2.79828900	0.34946900
H	5.30693700	-1.32217400	-0.58584600	C	4.35082500	0.76205700	-0.45690000
C	2.85119600	-2.37956800	0.21926400	H	5.33735000	0.69521100	-0.88172300
H	2.00493300	-2.39388100	0.90220700	C	3.78144300	-1.62230600	-0.99021700
H	3.68021700	-2.92299500	0.66546700	H	3.21967600	-2.37325100	-0.43883600
H	2.57079500	-2.84544800	-0.72402000	H	4.84421600	-1.81712500	-0.87267400
C	-3.71756900	-0.67371000	0.04214200	H	3.51695700	-1.66269100	-2.04578300
H	-4.35897100	-1.51016500	0.28086500	C	-3.55163900	-0.14648500	0.15669700
C	-3.45182100	1.70692800	-0.31738000	H	-4.37088500	-0.65385100	0.64619800
H	-3.89660100	2.69177500	-0.35164300	C	-2.65970500	1.86493900	-0.85696000
C	-4.23317100	0.60738400	-0.01670400	H	-2.80886600	2.89435300	-1.15243900
				C	-3.67603500	1.17684900	-0.21991200

Conformer IV (1e)



Conformer V (1e)



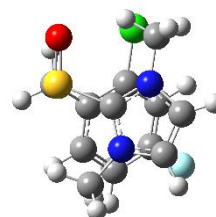
I 1

S	1.36550800	-1.69754300	-0.04799200
Cl	-2.50522000	-2.24469700	0.29840700
O	0.78762100	-2.14689800	1.23373600
N	1.57814700	0.86419300	1.16219300
N	3.01809400	0.51624900	-0.41937700
F	-3.70398200	2.60252700	0.03561300
C	1.94410400	0.00780400	0.20344000
C	-0.99100700	-0.32592400	-0.90790000
C	0.00990100	-1.36312200	-1.26794200
H	0.54366500	-1.12055200	-2.19003800
H	-0.42262200	-2.35961300	-1.37546900
C	-0.80221400	0.99447100	-1.31863500
H	0.06493200	1.23940800	-1.92205800
C	-2.15281900	-0.62407500	-0.18725100
C	0.44972000	0.73413200	2.08542400
H	-0.41949200	1.23011700	1.65712600
H	0.72726700	1.20931200	3.02291600
H	0.24219300	-0.31980200	2.24522500
C	2.42022500	1.94276400	1.13043800
H	2.31597500	2.76550100	1.81644900
C	3.31846500	1.72955000	0.13866000
H	4.14264800	2.33055200	-0.20444200
C	3.75401000	-0.10172100	-1.51577900
H	3.66251400	-1.18342200	-1.44681900
H	4.80221600	0.17215100	-1.42810900
H	3.36590400	0.24277100	-2.47318200
C	-3.07204600	0.36182700	0.13413700
H	-3.97345800	0.12790300	0.68323800
C	-1.70180900	1.99718900	-1.00882100

H -1.56203600 3.01630900 -1.34262000

C -2.82451700 1.65697900 -0.27533300

Conformer VI (1e)

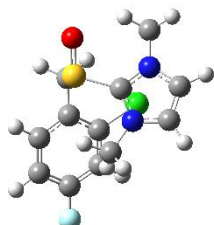


I 1

S	1.88726300	-0.28739000	-1.45606600
Cl	-0.58490900	-2.49815500	0.66782700
O	2.71547200	-1.46436000	-1.11861700
N	1.86289600	0.22002200	1.34952400
N	1.26044500	1.90963000	0.13520200
F	-4.35293000	0.78113100	0.95887100
C	1.57946700	0.60743500	0.10104600
C	-1.01788100	-0.46480900	-1.08752500
C	0.15587400	-0.91487100	-1.87662400
H	0.06059800	-0.64021200	-2.92670900
H	0.33718100	-1.98854200	-1.80414900
C	-1.79860700	0.59787100	-1.54904600
H	-1.53192700	1.07298400	-2.48642200
C	-1.43981600	-1.10878300	0.07926400
C	2.33637000	-1.08501500	1.81984000
H	1.58034200	-1.51803400	2.46996500
H	3.26156800	-0.92882600	2.37104500
H	2.51835000	-1.72984000	0.96827900
C	1.68901000	1.28945100	2.18884200
H	1.85789900	1.21004600	3.24883800
C	1.30756500	2.34421900	1.43250100
H	1.07472200	3.35867000	1.70586800
C	0.94580300	2.75784400	-1.00648900
H	1.39679600	2.33785800	-1.90317500
H	1.36829200	3.74426800	-0.83091900
H	-0.13215500	2.83189300	-1.13148300
C	-2.56177800	-0.69626900	0.77594800

H	-2.88973300	-1.20965600	1.66901600
C	-2.92289000	1.03533000	-0.87389800
H	-3.53319900	1.84753900	-1.24499900
C	-3.27849500	0.38024200	0.29028400

Conformer VII (1e)

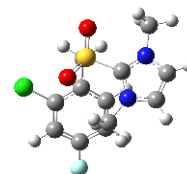


1 1

S	1.28228500	-1.72845100	-0.44117400
Cl	-0.35539300	1.28292900	1.90669000
O	2.50918200	-2.41231800	0.02169400
N	2.62686500	0.69855500	0.12879800
N	1.20659000	0.85735100	-1.49996400
F	-4.69803900	0.80849900	-0.52859100
C	1.67800000	0.04232100	-0.54721900
C	-1.17189400	-0.96810400	0.59022900
C	0.09683700	-1.64643700	0.97593700
H	-0.05319800	-2.70763400	1.18337400
H	0.61180100	-1.19377000	1.81972800
C	-2.12449900	-1.65961400	-0.16207500
H	-1.92889800	-2.69000000	-0.43596300
C	-1.46845900	0.34857200	0.94823200
C	3.38776500	0.20554500	1.27547000
H	2.84781400	0.43766300	2.19241600
H	4.35209000	0.70657200	1.28266200
H	3.52619700	-0.86750400	1.17608700
C	2.73749400	1.96010300	-0.38709800
H	3.44076300	2.67540800	0.00283700
C	1.84603600	2.06267400	-1.40308300
H	1.62424200	2.88389600	-2.06208300
C	0.16429300	0.54493300	-2.47141000
H	0.20427500	-0.51355200	-2.71596100
H	0.34693800	1.12870000	-3.36979400

H	-0.81344600	0.78915200	-2.05998000
C	-2.65630300	0.95664800	0.57997400
H	-2.88823500	1.96935400	0.87881700
C	-3.31590300	-1.07845200	-0.55163000
H	-4.05472400	-1.62161400	-1.12493800
C	-3.55933400	0.22838600	-0.17069700

Conformer 1 (1f)



1 1

S	-1.15885500	-1.35433500	0.19726400
Cl	2.52267900	-2.32244900	0.40813800
O	-0.52661900	-1.43108700	1.48098500
O	-2.16637700	-2.28642500	-0.22384400
N	-1.69774000	1.28536500	1.01873100
N	-3.08616200	0.57588700	-0.49393400
F	4.23617100	2.34818200	-0.09993600
C	1.19362700	-0.29620400	-0.83294300
C	-1.98925100	0.25726400	0.20965700
C	0.07068900	-1.23187500	-1.11648000
H	0.38992100	-2.27332500	-1.21302200
H	-0.48822900	-0.96544600	-2.01415300
C	-0.60560700	1.38593700	1.99145100
H	-0.79539800	0.71580200	2.82491400
H	-0.57119100	2.41648900	2.33284500
H	0.33495600	1.12305300	1.51702700
C	-3.49009200	1.82538800	-0.12532900
H	-4.35693200	2.29636200	-0.55534700
C	-2.62165400	2.26835200	0.82011800
H	-2.59300700	3.19710700	1.36289400
C	2.33849200	-0.69323800	-0.13404000
C	1.13237400	1.01848000	-1.29552100
H	0.27595500	1.33159100	-1.88253200
C	3.36836500	0.19774900	0.11674100

H	4.25649800	-0.11015800	0.65071100
C	3.24893800	1.49483600	-0.34325500
C	2.14694200	1.92731400	-1.05778500
H	2.10717800	2.94190300	-1.42977100
C	-3.80235900	-0.25350500	-1.46614800
H	-3.11323900	-0.64534400	-2.20830900
H	-4.53932100	0.37845000	-1.95323600
H	-4.28810800	-1.08077700	-0.95666900

Conformer 2 (1f)



1 1			
S	-0.88447100	-0.63646600	0.51133400
Cl	2.16887600	-2.38930200	0.33187700
O	-0.34760700	0.15333900	1.58172300
O	-1.28188000	-2.00534500	0.68039000
N	-2.75873700	1.47020000	0.39503400
N	-3.46997500	-0.34183300	-0.56702100
F	5.28420000	1.52006600	0.02536900
C	1.53344800	0.04273900	-0.68604200
C	-2.42708200	0.21377000	0.06609200
C	0.17153100	-0.48080400	-0.97944300
H	0.17571600	-1.49325600	-1.38447400
H	-0.36712600	0.18124800	-1.65876800
C	-1.96098500	2.45262400	1.13512000
H	-1.91329900	2.17136300	2.18357400
H	-2.44954500	3.41636500	1.02332400
H	-0.95402700	2.49847700	0.73394800
C	-4.47612300	0.57739800	-0.63785900
H	-5.42073600	0.35664200	-1.10374000
C	-4.03213000	1.70945600	-0.03519100
H	-4.52015600	2.65536400	0.12330600
C	2.52127800	-0.75244900	-0.10174700
C	1.86309600	1.35405700	-1.02273200
H	1.11888700	1.98201300	-1.49936400

C	3.79099300	-0.26277100	0.14075700
H	4.55527500	-0.87998700	0.59146200
C	4.06635200	1.04551200	-0.20686500
C	3.12329000	1.87039600	-0.79090700
H	3.38536800	2.88398800	-1.06095000
C	-3.57722600	-1.70730900	-1.08703300
H	-2.76288600	-1.91097200	-1.77701100
H	-4.52345500	-1.78151900	-1.61488900
H	-3.54293600	-2.41694600	-0.26587800

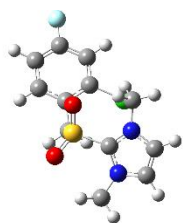
Conformer 3 (1f)



1 1			
S	-0.79672700	0.50283100	0.59431700
Cl	1.71576600	-2.39787100	-0.47689300
O	-0.82449300	1.90526700	0.90277500
O	-0.47991400	-0.49393900	1.57489400
N	-3.42490800	0.97555900	-0.31943500
N	-3.03392400	-1.11917000	0.10051500
F	5.60444800	0.63081300	0.36048700
C	1.63072700	0.33096700	-0.56583800
C	-2.48687800	0.10435500	0.07874600
C	0.17878100	0.24263900	-0.90215400
H	-0.09773300	-0.73629700	-1.29255800
H	-0.13700800	1.02530100	-1.59231300
C	-3.30306500	2.42888600	-0.46187500
H	-3.16682400	2.88449700	0.51455000
H	-4.21892200	2.78731200	-0.92270500
H	-2.45578900	2.67470800	-1.09450800
C	-4.33784200	-1.01908600	-0.28746200
H	-4.98511100	-1.87698100	-0.34419900
C	-4.58252400	0.29038000	-0.54937800
H	-5.48222900	0.78222000	-0.87597700
C	2.40524200	-0.80894100	-0.34163400
C	2.24907500	1.57660400	-0.46355300

H	1.66347400	2.47190000	-0.63132400
C	3.74911100	-0.71728900	-0.03290000
H	4.35160000	-1.59934500	0.13118700
C	4.31467300	0.53974500	0.06152800
C	3.58839700	1.69655400	-0.15037900
H	4.07168000	2.66050900	-0.07228800
C	-2.40400400	-2.37571200	0.51528100
H	-1.40995700	-2.45965500	0.08743200
H	-3.02930300	-3.18815300	0.15616100
H	-2.32736700	-2.40479300	1.59905700

Conformer 4 (1f)



1 1			
S	-0.89523500	1.26647600	0.55818100
Cl	0.73978600	-1.81730800	-1.14136500
O	-1.60626800	2.51458800	0.49745700
O	-0.24047300	0.80645400	1.74808700
N	-3.17243000	0.13364400	-0.63936000
N	-2.30118400	-1.15649100	0.87522900
F	5.36892500	-0.63232900	0.36148500
C	1.59951000	0.69481600	-0.53230800
C	-2.15972700	0.01002800	0.23144500
C	0.24347500	1.20094700	-0.87003800
H	-0.25547500	0.60883900	-1.63737300
H	0.26408400	2.24443500	-1.18607600
C	-3.43031400	1.24780600	-1.55230700
H	-3.36770800	2.18570300	-1.00976200
H	-4.42847800	1.11695600	-1.95951000
H	-2.70808400	1.23691200	-2.36681500
C	-3.41720000	-1.78010200	0.39803000
H	-3.73968300	-2.73571800	0.77293000
C	-3.96064500	-0.97615100	-0.55059700

H	-4.84019900	-1.10347800	-1.15736700
C	1.93476100	-0.65453300	-0.62760200
C	2.59063300	1.58143600	-0.11516800
H	2.35577600	2.63597500	-0.03387800
C	3.20198000	-1.11765900	-0.33385100
H	3.45997200	-2.16360300	-0.42027300
C	4.14862900	-0.19684700	0.07544800
C	3.86675500	1.15098700	0.19194100
H	4.63750400	1.83816500	0.51258400
C	-1.46222800	-1.72032300	1.93740800
H	-0.42888700	-1.76051600	1.60877400
H	-1.82768100	-2.72399300	2.13436300
H	-1.53861500	-1.10891500	2.83148500

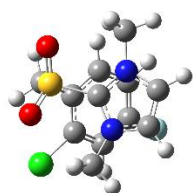
Conformer 5 (1f)



1 1			
S	-1.38176600	1.55046800	-0.18781200
Cl	0.44393300	-1.63373800	-1.80226700
O	-2.58963400	1.80856500	-0.91944600
O	-0.96006200	2.38139900	0.90455800
N	-2.47219100	-1.01976400	0.08460300
N	-1.09192000	-0.52651700	1.68838400
F	4.68640400	-0.78621600	0.70911800
C	1.21656300	0.78868600	-0.80481800
C	-1.62079900	-0.08763600	0.53719400
C	-0.02478200	1.39590000	-1.36411600
H	-0.42916300	0.85520700	-2.21792100
H	0.11832600	2.44086700	-1.65202300
C	-3.28614700	-0.98156700	-1.13187000
H	-4.02236000	-0.18713200	-1.05891800
H	-3.77624800	-1.94631400	-1.22445600
H	-2.65080300	-0.81395600	-1.99711400

C	-1.60938900	-1.75727200	1.96013600
H	-1.33195300	-2.31215200	2.83933400
C	-2.47119200	-2.06600100	0.95643300
H	-3.07846700	-2.94049700	0.80044300
C	1.52191600	-0.56555000	-0.94846700
C	2.13893000	1.59212800	-0.13092900
H	1.92790100	2.64840900	-0.01731200
C	2.69042300	-1.10805100	-0.44338600
H	2.92925300	-2.15440500	-0.57223700
C	3.56535200	-0.27055000	0.22166200
C	3.31220300	1.07888500	0.38820400
H	4.02983300	1.70486600	0.90082600
C	-0.14189900	0.16237800	2.56494500
H	0.71608200	0.49611200	1.98893000
H	0.17590000	-0.54990400	3.32079300
H	-0.62527500	1.01706400	3.02938500

Conformer 6 (1f)



1 1

S	-1.70195000	-1.00324500	-0.80665400
Cl	1.74155700	-2.48225700	0.54471700
O	-1.96836100	-2.14823500	0.01631900
O	-2.63294900	-0.53046100	-1.79446600
N	-1.36072100	0.26734200	1.68657000
N	-1.88369400	1.65454900	0.10006500
F	4.16822200	1.88857400	0.36484000
C	1.05254500	-0.37711000	-1.04485400
C	-1.58330300	0.37490000	0.36909200
C	-0.06622000	-1.18851800	-1.60463100
H	0.10838500	-2.26184100	-1.52815100
H	-0.27690700	-0.92462400	-2.64016800
C	-1.07798800	-0.94233200	2.46402900
H	-1.98802000	-1.52736100	2.56824500

H	-0.71940900	-0.62353600	3.43864200
H	-0.31944200	-1.53947000	1.97017000
C	-1.83579900	2.36570100	1.26267600
H	-2.04035300	3.42163800	1.29550600
C	-1.50954200	1.49834400	2.25403400
H	-1.37749000	1.65959600	3.30971600
C	1.92448300	-0.86989000	-0.06941200
C	1.30267700	0.90161100	-1.54586900
H	0.68386900	1.27995200	-2.35121300
C	2.97822600	-0.11214000	0.41189700
H	3.65846000	-0.50354800	1.15542800
C	3.16150700	1.15855000	-0.09764900
C	2.34412200	1.68245200	-1.08202800
H	2.54473600	2.66613700	-1.48414100
C	-2.27778200	2.24263800	-1.18087400
H	-1.61645900	1.90501500	-1.97080600
H	-2.20607000	3.32188200	-1.07994400
H	-3.29672000	1.95037900	-1.42029800

Conformer 7 (1f)



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S	-1.15888600	-1.35444000	0.19729500
Cl	2.52245200	-2.32245800	0.40796600
O	-0.52669700	-1.43137200	1.48102100
O	-2.16635100	-2.28649200	-0.22403000
N	-1.69801700	1.28513400	1.01918400
N	-3.08585300	0.57603000	-0.49419700
F	4.23639900	2.34803800	-0.09991700
C	1.19352100	-0.29596800	-0.83290100
C	-1.98931400	0.25716500	0.20986200
C	0.07056100	-1.23162000	-1.11650000
H	0.38988200	-2.27300200	-1.21336100
H	-0.48857000	-0.96492900	-2.01395900

C	-0.60617300	1.38551100	1.99225100
H	-0.79468600	0.71303400	2.82408700
H	-0.57381900	2.41531300	2.33609300
H	0.33495600	1.12563900	1.51723900
C	-3.48971400	1.82558400	-0.12567700
H	-4.35629200	2.29672100	-0.55604100
C	-2.62166500	2.26830900	0.82023400
H	-2.59317200	3.19695400	1.36320600
C	2.33840600	-0.69317600	-0.13412300
C	1.13234600	1.01876000	-1.29532400
H	0.27588400	1.33204400	-1.88218100
C	3.36840800	0.19766100	0.11665800
H	4.25654200	-0.11038300	0.65054600
C	3.24906500	1.49479700	-0.34321700
C	2.14703400	1.92745600	-1.05758200
H	2.10733400	2.94209200	-1.42944500
C	-3.80169000	-0.25313300	-1.46687200
H	-3.11257200	-0.64326600	-2.20996600
H	-4.53970500	0.37849900	-1.95277200
H	-4.28612300	-1.08155600	-0.95803100

