Optimization and Gram-scale Preparation of S-Trifluoromethyl- Sulfoximines and Sulfilimino iminiums, Powerful Reagents for the Late Stage Introduction of the CF_3 Group

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Supporting Information

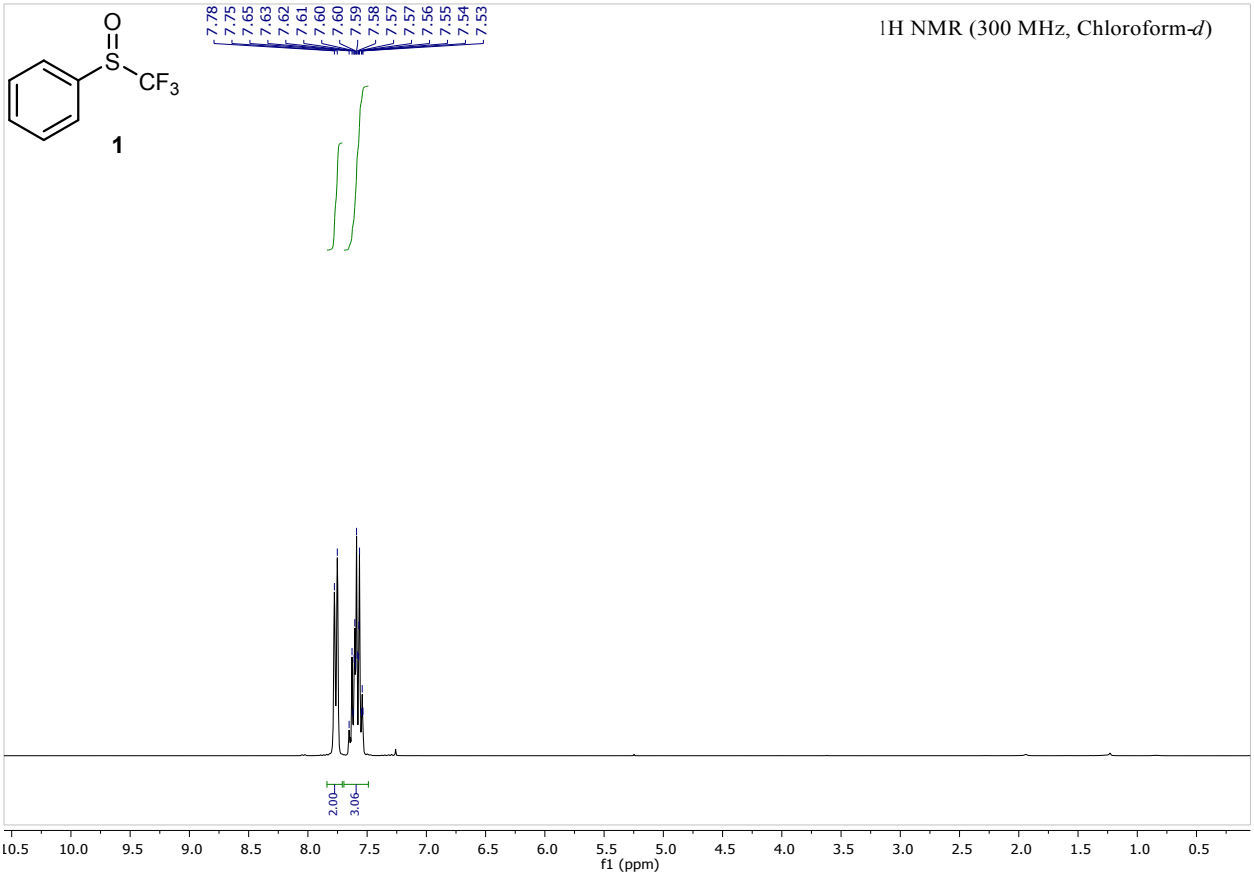
General information

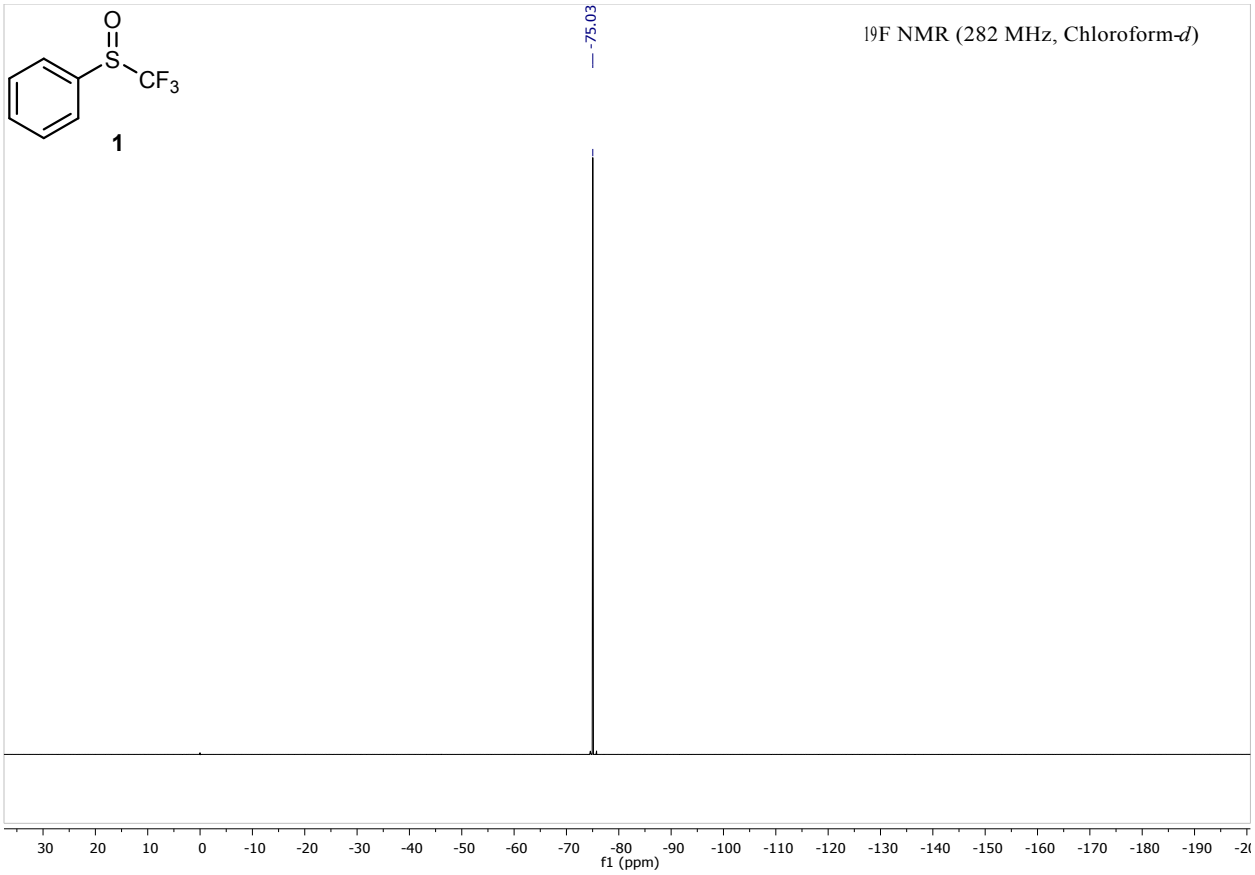
Commercial starting materials and solvents were used without further purification. Nuclear magnetic resonance (^{1}H NMR, ^{19}F NMR and ^{13}C NMR) spectra were recorded on a Brucker AC-300 spectrometer in $CDCl_3$. Reported coupling constants and

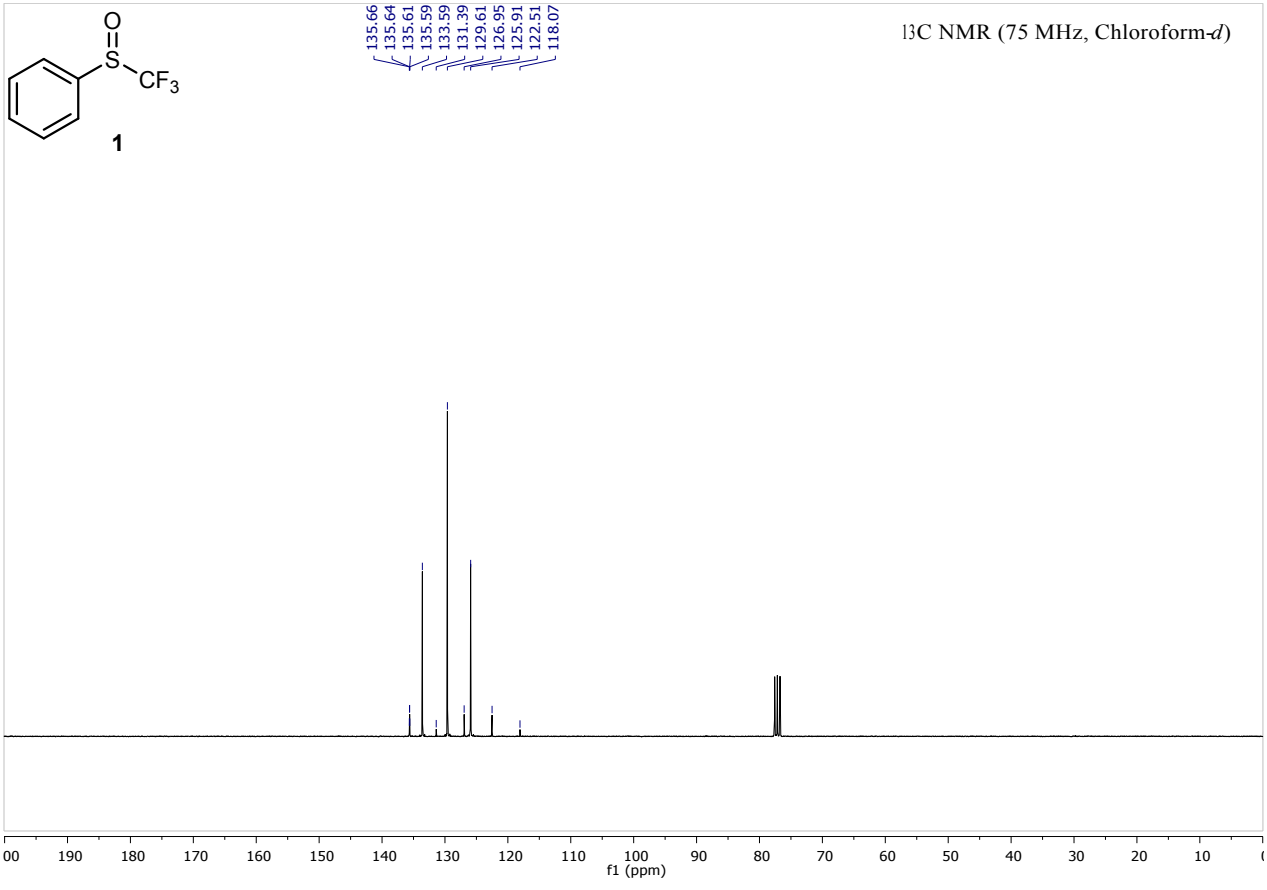
chemicals shifts were based on a first order analysis. Internal references were the residual peak of $CHCl_3$ (7.26 ppm) for ^{1}H (300 MHz) NMR spectra, central peak of $CDCl_3$ (77.16 ppm) for ^{13}C (75 MHz) NMR spectra, and $CFCl_3$ (0.00 ppm) as internal reference for ^{19}F (282 MHz) NMR spectra. Multiplicities are indicated as follows: s (singlet), d (doublet), t (triplet), q (quartet), m (multiplet), br (broad).

NMR Spectra of the compounds 1, 4 and 5

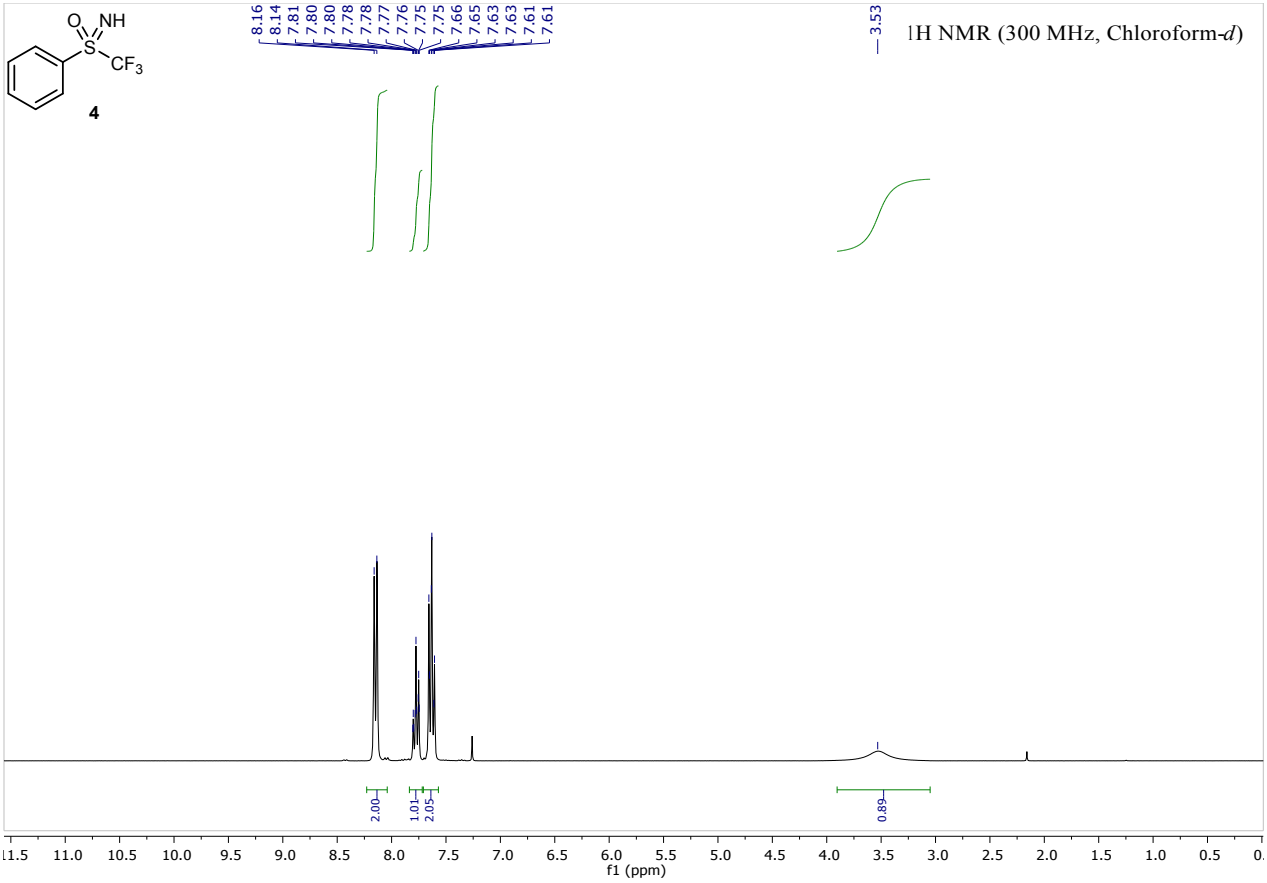
1) NMR spectra of 1



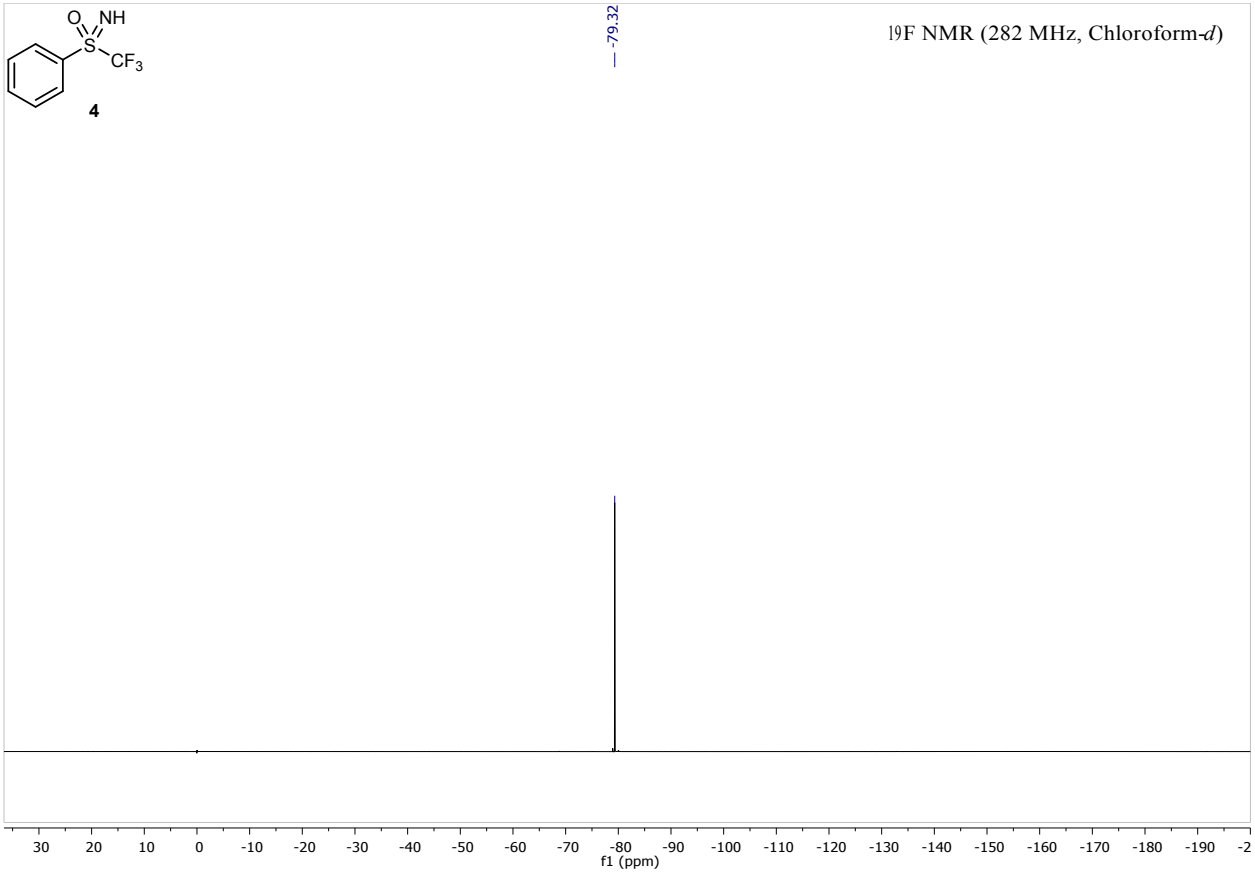




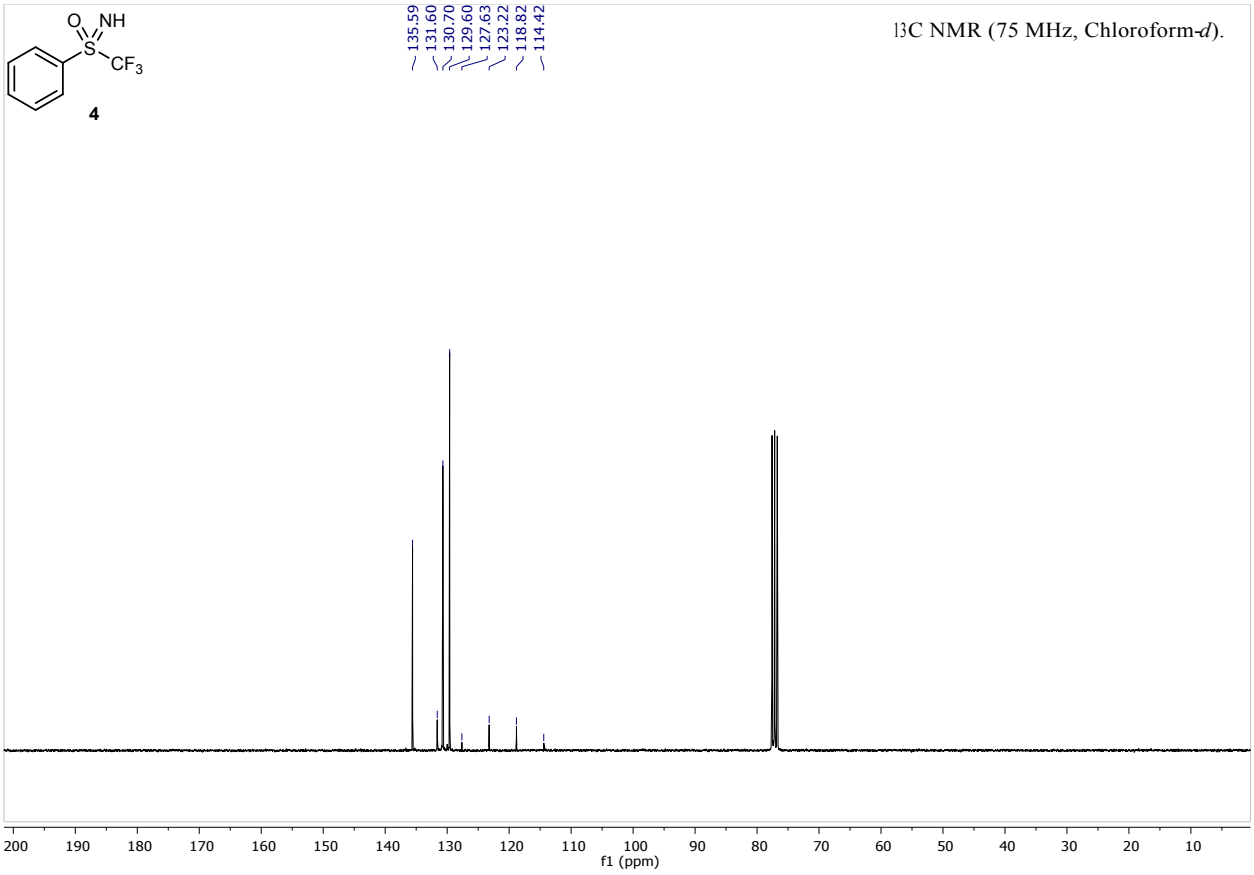
2) NMR spectra of 4



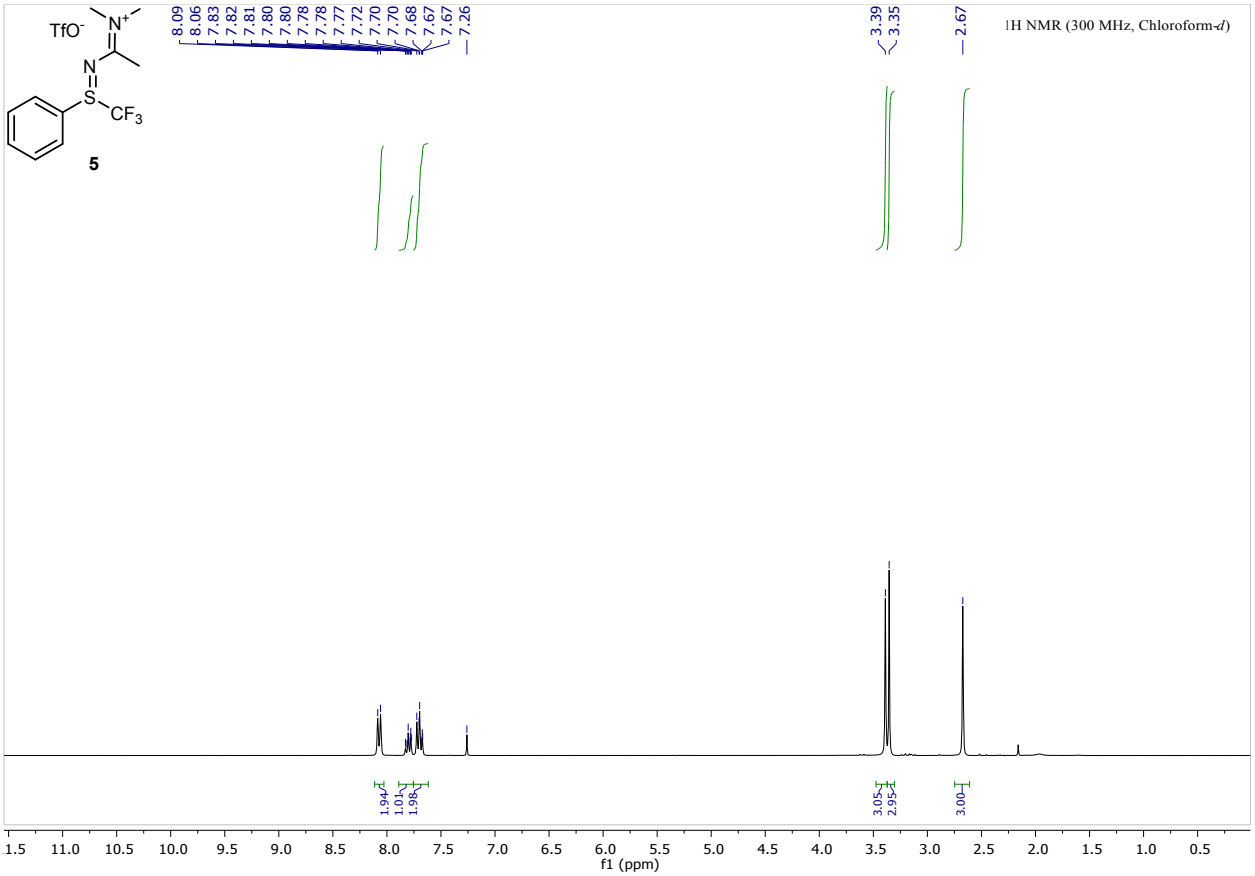
^{1}H NMR (300 MHz, Chloroform-*d*)

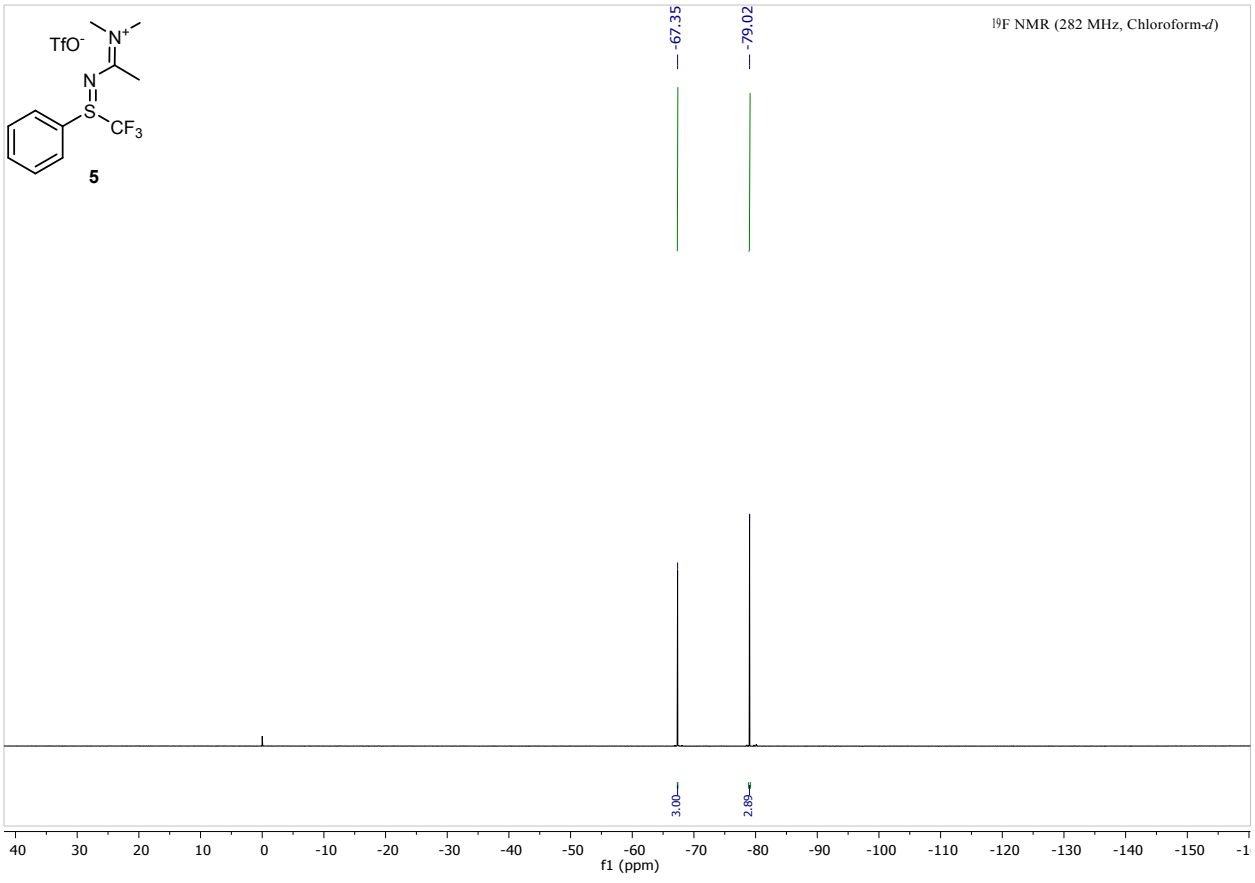


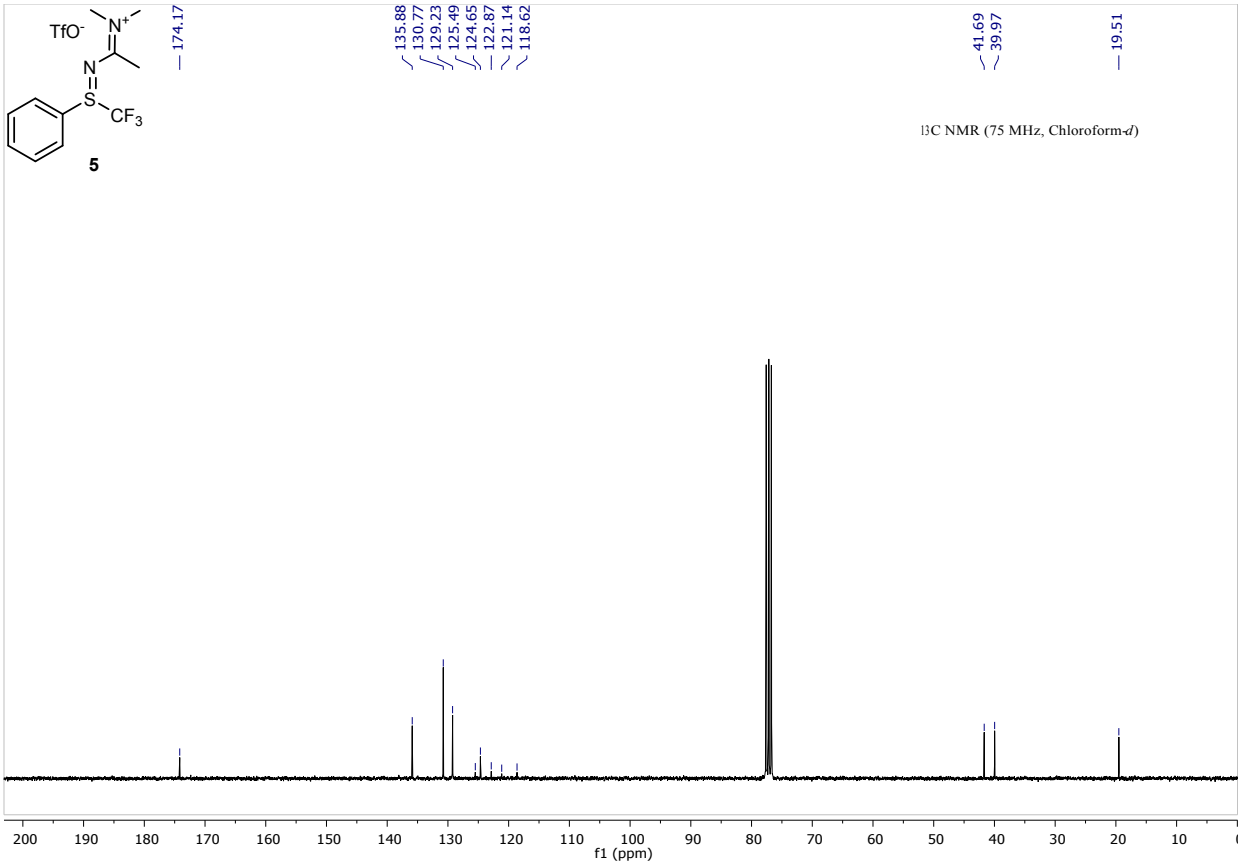
^{19}F NMR (282 MHz, Chloroform-*d*)



3) NMR spectra of 5


TfO-
N+
N
S
CF3
5
8.09
8.06
7.83
7.82
7.81
7.80
7.80
7.78
7.78
7.77
7.72
7.70
7.70
7.68
7.67
7.67
7.26
3.39
3.35
2.67
1H NMR (300 MHz, Chloroform-d)
1.94
1.01
1.98
3.05
2.95
3.00
f1 (ppm)


TfO-
N+
N
S
CF3
5
-67.35
-79.02
19F NMR (282 MHz, Chloroform-d)
3.00
2.89
f1 (ppm)


TfO-
N+
N
S
CF3
5
174.17
135.88
130.77
129.23
125.49
124.65
122.87
121.14
118.62
41.69
39.97
19.51
13C NMR (75 MHz, Chloroform-d)
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)