

# Supporting Information

## Efficient Synthesis of SCF<sub>3</sub>-Containing 3-Alkenylquinoxalinones via Three-Component Radical Cascade Reaction

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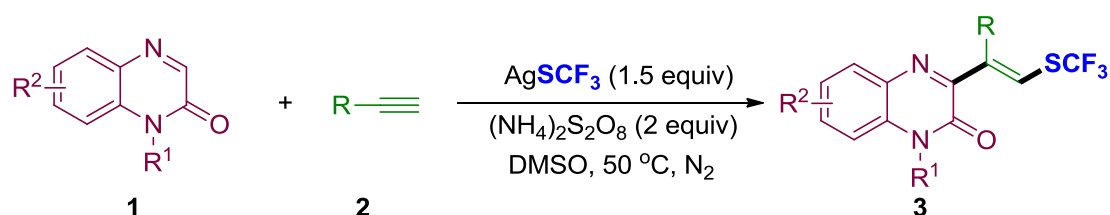
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## 1. General information

Unless otherwise noted, all solvents and reagents in this study were commercial and used without further purification.  $^1\text{H}$ ,  $^{13}\text{C}$  and  $^{19}\text{F}$  NMR spectra were recorded at 400, 100 and 376 MHz, respectively. Chemical shifts were quoted in ppm relative to  $\text{CDCl}_3$  ( $\delta_{\text{H}} = 7.26$ ,  $\delta_{\text{C}} = 77.0$  ppm). Data are reported as follows: s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet, dd = doublet of doublet, etc. Quinoxalin-2(1H)-ones were prepared according to the relevant literatures. The reactions were monitored by thin-layer chromatography (TLC) using GF254 silica gel-coated TLC plates. Mass spectra were performed on a spectrometer operating on ESI-TOF. Melting points were measured on a melting point apparatus and were uncorrected.

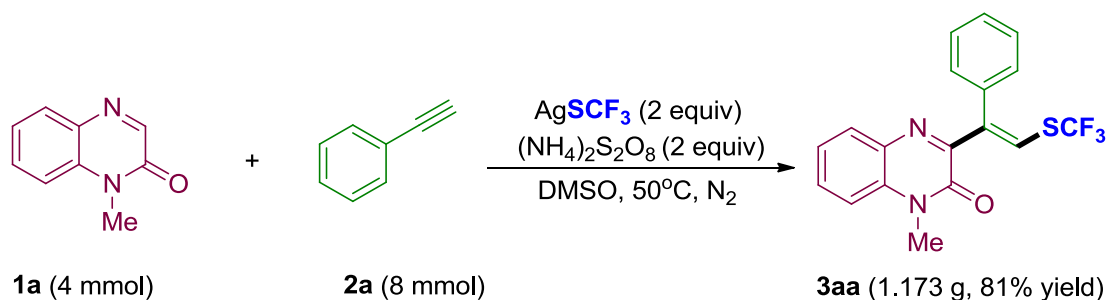
## 2. Experimental Section

### General procedure for the synthesis of $\text{SCF}_3$ -containing 3-alkenyl quinoxalin-2(1H)-ones **3**



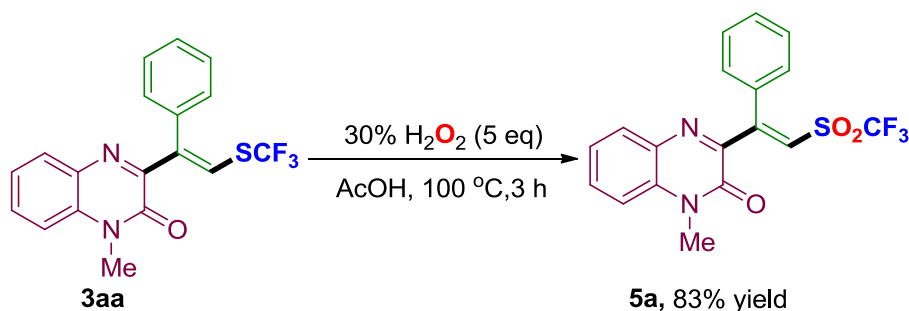
To an oven-dried reaction vessel equipped with a magnetic stir bar was added quinoxalin-2(1H)-one **1** (0.3 mmol), alkyne **2** (0.6 mmol, 2 eq),  $\text{AgSCF}_3$  (0.45 mmol, 1.5 eq) and  $(\text{NH}_4)_2\text{S}_2\text{O}_8$  (0.6 mmol, 2 eq) in DMSO (3 mL). The mixture was stirred at 50 °C using an oil bath under a  $\text{N}_2$  atmosphere for about 12 h. The reaction progress was monitored by thin layer chromatography (TLC). After completion, the reaction was allowed to cool to room temperature, then,  $\text{H}_2\text{O}$  (5 mL) was added to the mixture, which was further extracted with  $\text{CH}_2\text{Cl}_2$  for three times (10 mL  $\times$  3). The organic phase was then dried with anhydrous sodium sulfate, concentrated under vacuum. The residue was purified by flash column chromatography using a mixture of petroleum ether and ethyl acetate as eluent (PE/EA 6:1- 4:1) to obtain the desired products **3**.

### The Experimental Procedure for Gram-Scale Synthesis of **3aa**



To an oven-dried reaction vessel equipped with a magnetic stir bar was added quinoxalin-2(1*H*)-one **1a** (4 mmol, 0.640 g), phenylacetylene **2a** (8 mmol, 0.816 g), AgSCF<sub>3</sub> (6 mmol, 1.259 g) and (NH<sub>4</sub>)<sub>2</sub>S<sub>2</sub>O<sub>8</sub> (8 mmol, 1.826 g) in DMSO (40 mL). The mixture was stirred at 50 °C using an oil bath under a N<sub>2</sub> atmosphere for about 12 h. After completion, the reaction was allowed to cool to room temperature, then, H<sub>2</sub>O (30 mL) was added to the mixture, which was further extracted with CH<sub>2</sub>Cl<sub>2</sub> for three times (20 mL×3). The organic phase was then dried with anhydrous sodium sulfate, concentrated under vacuum. The residue was purified by flash column chromatography using a mixture of petroleum ether and ethyl acetate as eluent (PE/EA 6:1- 4:1) to obtain 1.173 g of **3aa**.

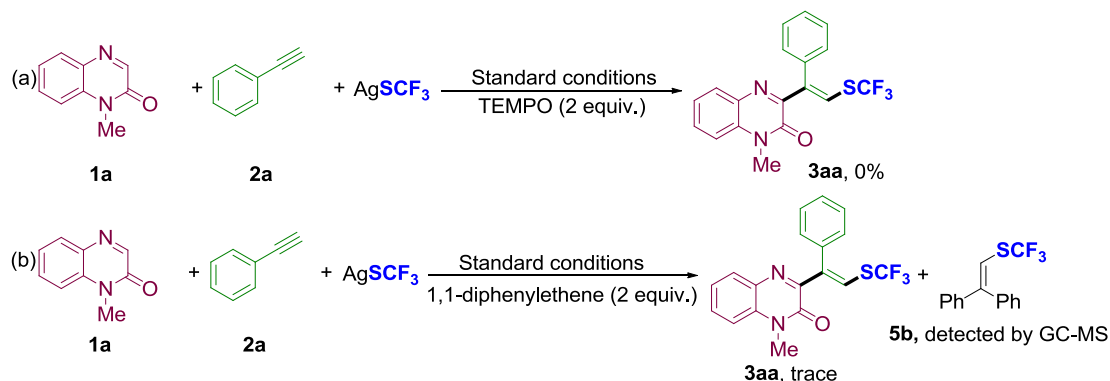
#### The Experimental Procedure for the synthesis of **5a** via the oxidation of **3aa**



To a solution of (*E*)-1-methyl-3-(1-phenyl-2-((trifluoromethyl)thio)vinyl)quinoxalin-2(1*H*)-one **3aa** (0.198 g, 0.5 mmol) in acetic acid (5 mL) was added 30% H<sub>2</sub>O<sub>2</sub> (0.283 g, 2.5 mmol) at room temperature. The reaction mixture was heated to 100 °C using an oil bath and stirred for about 3 h. After completion, the reaction was allowed to cool to room temperature, then saturated brine (10 mL) was added to the mixture, the organic layer was further washed with saturated brine (10 mL×2), which was further extracted with CH<sub>2</sub>Cl<sub>2</sub> for three times (10 mL×3). The organic phase was then dried with anhydrous sodium sulfate, concentrated under vacuum. The residue was purified by flash column chromatography using a mixture of petroleum ether and ethyl acetate as eluent

(PE/EA 4:1- 2:1) to obtain 0.1635 g of product **5a**.

### Radical Inhibition Experiment



An oven-dried reaction vessel charged with a stir bar was added quinoxalin-2(1*H*)-one **1a** (0.3 mmol), phenylacetylene **2a** (0.6 mmol, 2 eq), AgSCF<sub>3</sub> (0.45 mmol, 1.5 eq), (NH<sub>4</sub>)<sub>2</sub>S<sub>2</sub>O<sub>8</sub> (0.6 mmol, 2 eq) and radical inhibitor (TEMPO or 1,1-diphenylethene, 2 eq) in DMSO (3 mL). The reaction mixture was stirred at 50 °C using an oil bath under a N<sub>2</sub> atmosphere for 12 h, no **3aa** was observed by <sup>1</sup>H NMR, and the radical adduct **5b** was detected by GC-MS (MS: M<sup>+</sup> calcd for C<sub>15</sub>H<sub>11</sub>F<sub>3</sub>S 280.05, found 280.00). The MS spectra of compound **5b** are as following (Figure S1).

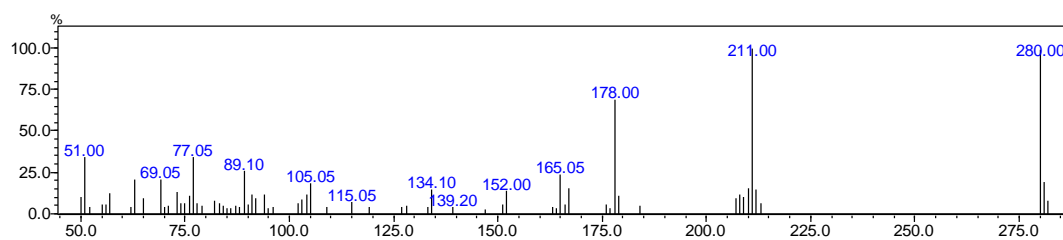
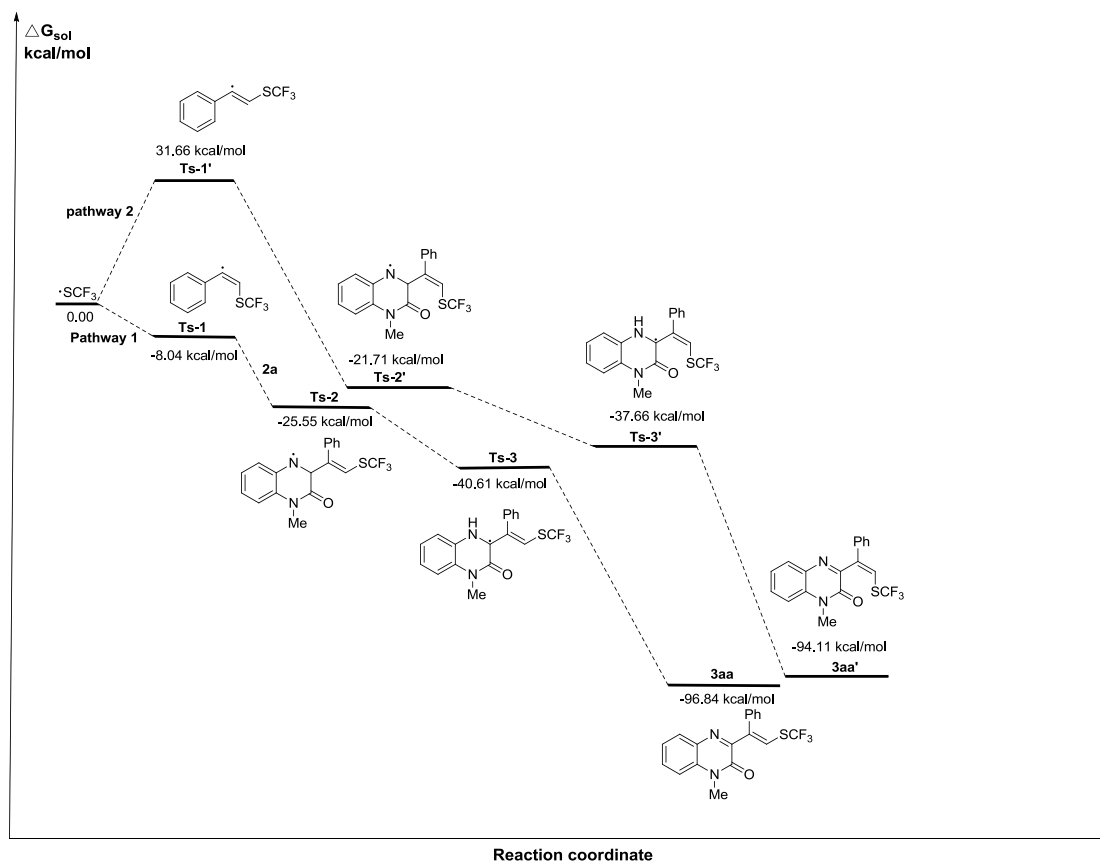


Figure S1. MS spectra of compound **5b**

### Density functional theory calculations

All data in this study were calculated with the Gaussian 16 software package<sup>[1]</sup> and were optimized at the M062X/6-31G(d) level of density functional theory (DFT).<sup>[2]</sup> Vibrational frequency analysis was computed to ensure the points that the minimum have no imaginary frequency and the transition states have only one imaginary frequency. In order to consider the solvent effects, the solvation corrected single-point energy calculations (based on the gas-phase optimized geometries) were calculated by using the M062X/6-311++G(d, p) method in conjunction with the SMD solvation model in solvent (Dimethyl sulfoxide). The single-point energy corrected relative free energies in kcal/mol are used for discussion throughout the text.



**Figure S2.** The free energy profiles for the two possible pathways. The free energies are reported in kcal/mol at the M062x/6-311++G(d, p) (DMSO) level of theory.

### Cartesian Coordinates for Optimized Structures

#### 1a

C 0	-2.540841	1.290389	0.203085
C 0	-2.537601	-0.101971	0.162461
C 0	-1.328283	-0.797227	0.092051
C 0	-0.108680	-0.108651	0.092051
C 0	-0.117376	1.305648	0.092051
C 0	-1.334344	1.989455	0.159823
N 0	1.094828	-0.832969	-0.058330
C 0	2.277853	-0.089720	0.369889
C 0	2.176321	1.397209	0.109148
N 0	1.067772	2.064719	0.011739
O 0	3.240636	-0.610404	0.880966
C 0	1.151548	-2.200952	-0.593406
H 0	-3.492785	1.837598	0.269144
H 0	-3.488464	-0.654521	0.185858
H 0	-1.333791	-1.895789	0.036078
H 0	-1.340943	3.089264	0.179236
H 0	3.116358	1.956530	-0.007008
H 0	2.208485	-2.549265	-0.611553
H 0	0.549684	-2.877234	0.054028

H 0 0.739621 -2.212110 -1.627312

**2a**

C	-4.34504789	0.11182108	0.00000000
C	-2.94988789	0.11182108	0.00000000
C	-2.25234989	1.31957208	0.00000000
C	-2.95000389	2.52808108	-0.00119900
C	-4.34482889	2.52800308	-0.00167800
C	-5.04242989	1.31979708	-0.00068200
H	-4.89480689	-0.84049592	0.00045000
H	-2.40037989	-0.84069192	0.00131500
H	-2.39980389	3.48022408	-0.00125800
H	-4.89495089	3.48028408	-0.00263100
H	-6.14203389	1.31998008	-0.00086200
C	-0.71235015	1.31968412	0.00088786
C	0.48264965	1.31977105	0.00157681
H	1.54364947	1.31984824	0.00218851

**Ts-1**

C	-0.91409965	-0.96432750	0.85936392
C	-0.94044765	0.09762950	1.67122692
C	-1.19498359	-0.79462465	-0.61731019
C	-1.16748888	-1.90251819	-1.46424963
C	-1.42637959	-1.74597719	-2.82591125
C	-1.71285834	-0.48160968	-3.34050480
C	-1.74044940	0.62625583	-2.49357108
C	-1.48146235	0.46974286	-1.13190375
S	0.01102835	1.58502450	1.25101792
C	-0.51179865	2.49271350	2.73323892
F	0.07033435	3.75714450	2.73323892
F	-1.89789365	2.62078650	2.73323892
F	-0.10901165	1.79669750	3.86945592
H	-1.53877765	0.06988950	2.59384992
H	-0.94165240	-2.89964973	-1.05838339
H	-1.40461463	-2.61965641	-3.49390052
H	-1.91703583	-0.35819814	-4.41432106
H	-1.96643481	1.62335974	-2.89942185
H	-1.50315368	1.34343723	-0.46393168

**Ts-2**

C	-4.03621800	-2.53602800	0.59536500
C	-3.24532800	-3.67278800	0.74063800
C	-1.85821000	-3.58061500	0.60952800
C	-1.24223600	-2.34898500	0.34976800
C	-2.05554400	-1.20723000	0.13361000

C	-3.44303500	-1.30920000	0.29759100
N	0.16497500	-2.31616900	0.19382300
C	0.71079600	-0.96032300	0.25704500
C	-0.12224400	0.00730100	-0.59506600
N	-1.51613500	0.08546300	-0.12965600
C	0.49084500	1.37080200	-0.51764400
C	1.80773697	1.52251484	-0.69185522
C	-0.27848353	2.43685941	-0.27428514
C	-0.72428510	3.23093400	-1.33078754
C	-1.52680987	4.34319426	-1.07684637
C	-1.88356735	4.66122219	0.23352801
C	-1.43785748	3.86711170	1.29001064
C	-0.63524141	2.75488793	1.03608995
O	1.68688400	-0.64437400	0.89477000
C	0.97791600	-3.49992600	-0.00704200
S	2.55106131	3.17565814	-0.59798534
C	4.23403207	2.57609293	-0.91791572
F	4.27465300	1.94527682	-2.15811171
F	5.11731650	3.65194956	-0.91617133
F	4.60068654	1.67166647	0.07467749
H	-5.12745900	-2.60539800	0.71528000
H	-3.71352300	-4.64397000	0.95880800
H	-1.24150100	-4.48576400	0.71137900
H	-4.07119500	-0.41257800	0.19042600
H	-0.12796300	-0.37096100	-1.64180100
H	2.44069345	0.64543030	-0.89207573
H	-0.44299807	2.98005069	-2.36419649
H	-1.87833504	4.96952121	-1.90999998
H	-2.51646161	5.53835152	0.43375114
H	-1.71927376	4.11791689	2.32340405
H	-0.28365694	2.12860826	1.86925287
H	0.32540400	-4.40154100	-0.01637400
H	1.51405900	-3.42056200	-0.97916400
H	1.71792200	-3.58626800	0.81982300

**Ts-3**

C	-4.56021700	0.08401500	-0.43457800
C	-4.56021700	-1.25298500	-0.43457800
C	-3.40234200	-1.92148600	-0.43457800
C	-2.24446600	-1.25298700	-0.43457800
C	-2.24446500	0.08401300	-0.43457800
C	-3.40234000	0.75251400	-0.43457800
N	-1.07970500	-1.92546200	-0.44622600
C	0.09254300	-1.35323800	-0.03082900

C	-0.22251100	0.03824200	0.47285700
N	-1.14811700	0.71698900	-0.44554200
C	1.04603300	0.82752900	0.56682400
C	1.76863087	0.80019312	1.69140139
C	1.45639666	1.55979353	-0.47382957
C	2.22017454	0.97208220	-1.48215967
C	2.64838262	1.73609951	-2.56777743
C	2.31269174	3.08770653	-2.64504971
C	1.54884683	3.67539375	-1.63678966
C	1.12070579	2.91140055	-0.55110185
O	1.18492500	-1.86806800	-0.06107500
C	-1.06518200	-3.29822200	-0.91293700
S	2.38210037	2.34811912	2.41376199
C	3.20150120	1.52183257	3.80662087
F	2.25773853	0.81930305	4.55054813
F	3.81328973	2.47496571	4.61589074
F	4.16143581	0.63795357	3.32190751
H	-5.51284400	0.63401500	-0.43457800
H	-5.51284600	-1.80298500	-0.43457800
H	-3.40234200	-3.02148600	-0.43457800
H	-3.40234000	1.85251400	-0.43457800
H	-0.93703200	1.57597500	-1.01130300
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H	3.25081040	1.27268070	-3.36296506
H	2.65037903	3.69018220	-3.50119842
H	1.28407968	4.74131058	-1.69778838
H	0.51834211	3.37484286	0.24412117
H	-2.09444700	-3.60077900	-1.20931800
H	-0.38658200	-3.38383600	-1.79096900
H	-0.70354700	-3.96343500	-0.09716600

### 3aa

C	-4.77427300	0.13687300	0.26046000
C	-4.77103400	-1.25548700	0.21983500
C	-3.56171600	-1.95074400	0.14942500
C	-2.34211300	-1.26216800	0.14942500
C	-2.35080800	0.15213000	0.14942500
C	-3.56777600	0.83593800	0.21719700
N	-1.13860500	-1.98648700	-0.00095600
C	0.04442000	-1.24323800	0.42726300
C	-0.05711100	0.24369100	0.16652200
N	-1.16566000	0.91120100	0.06911300
C	1.08546100	0.92351900	0.02534000



C	2.05827518	0.79174767	0.93299590
C	1.25521881	1.73511822	-1.02349617
C	1.33495400	3.11444666	-0.83222829
C	1.51193896	3.96114972	-1.92649692
C	1.60929377	3.42847210	-3.21190615
C	1.52965680	2.04916094	-3.40317095
C	1.35257362	1.20244060	-2.30890540
O	1.00720300	-1.76392300	0.93834000
C	-1.08188600	-3.35447000	-0.53603200
S	3.03089220	2.23875006	1.43740067
C	4.05976121	1.30024286	2.60138432
F	4.74285363	0.29989553	1.91556018
F	4.97604794	2.15701399	3.20473123
F	3.24986692	0.72432215	3.57608934
H	-5.72621700	0.68408200	0.32651800
H	-5.72189800	-1.80803700	0.24323300
H	-3.56722500	-3.04930500	0.09345200
H	-3.57437400	1.93574700	0.23661000
H	2.26918053	-0.19363763	1.37405757
H	1.25826957	3.53450560	0.18151232
H	1.57473200	5.04895711	-1.77572209
H	1.74888410	4.09621390	-4.07482977
H	1.60649362	1.62910123	-4.41689958
H	1.28970568	0.11463963	-2.45969453
H	-0.02494900	-3.70278300	-0.55417900
H	-1.68375100	-4.03075100	0.11140200
H	-1.49381200	-3.36562700	-1.56993800

**Ts-1'**

C	-1.44181300	-1.90029400	0.89325500
C	-1.41441700	-3.00814400	0.04625600
C	-0.65560800	-2.97295700	-1.12362600
C	0.07563500	-1.82991200	-1.44647900
C	0.04816900	-0.72204100	-0.59954900
C	-0.71057100	-0.75724900	0.57040100
C	0.74906300	0.37363200	-0.90909100
C	0.72271500	1.43558900	-0.09722800
S	1.67419100	2.92298400	-0.51743700
C	1.15136400	3.83067300	0.96478400
F	1.73349700	5.09510400	0.96478400
F	-0.23473100	3.95874700	0.96478400
F	1.55415100	3.13465700	2.10100000
H	-2.04013000	-1.92804800	1.81588600
H	-1.99118600	-3.90954400	0.30084400

H	-0.63389100	-3.84665700	-1.79158900
H	0.67401000	-1.80218900	-2.36907300
H	-0.73222400	0.11642700	1.23839900
H	0.12438500	1.40785000	0.82539400

**Ts-2'**

C	-4.03621800	-2.53602800	0.59536500
C	-3.24532800	-3.67278800	0.74063800
C	-1.85821000	-3.58061500	0.60952800
C	-1.24223600	-2.34898500	0.34976800
C	-2.05554400	-1.20723000	0.13361000
C	-3.44303500	-1.30920000	0.29759100
N	0.16497500	-2.31616900	0.19382300
C	0.71079600	-0.96032300	0.25704500
C	-0.12224400	0.00730100	-0.59506600
N	-1.51613500	0.08546300	-0.12965600
C	0.49084500	1.37080200	-0.51764400
C	1.80773697	1.52251484	-0.69185522
C	-0.27848353	2.43685941	-0.27428514
C	-0.72428510	3.23093400	-1.33078754
C	-1.52680987	4.34319426	-1.07684637
C	-1.88356735	4.66122219	0.23352801
C	-1.43785748	3.86711170	1.29001064
C	-0.63524141	2.75488793	1.03608995
O	1.68688400	-0.64437400	0.89477000
C	0.97791600	-3.49992600	-0.00704200
S	2.85211444	0.07532390	-1.02221787
C	4.38269594	1.04510725	-1.12740817
F	4.59821801	1.70543374	0.07890202
F	5.45328155	0.19434652	-1.38762833
F	4.27051068	1.97884876	-2.15366606
H	-5.12745900	-2.60539800	0.71528000
H	-3.71352300	-4.64397000	0.95880800
H	-1.24150100	-4.48576400	0.71137900
H	-4.07119500	-0.41257800	0.19042600
H	-0.12796300	-0.37096100	-1.64180100
H	2.25823706	2.52441939	-0.63496589
H	-0.44299807	2.98005069	-2.36419649
H	-1.87833504	4.96952121	-1.90999998
H	-2.51646161	5.53835152	0.43375114
H	-1.71927376	4.11791689	2.32340405
H	-0.28365694	2.12860826	1.86925287
H	0.32540400	-4.40154100	-0.01637400
H	1.51405900	-3.42056200	-0.97916400

H	1.71792200	-3.58626800	0.81982300
<b>Ts-3'</b>			
C	-4.56021700	0.08401500	-0.43457800
C	-4.56021700	-1.25298500	-0.43457800
C	-3.40234200	-1.92148600	-0.43457800
C	-2.24446600	-1.25298700	-0.43457800
C	-2.24446500	0.08401300	-0.43457800
C	-3.40234000	0.75251400	-0.43457800
N	-1.07970500	-1.92546200	-0.44622600
C	0.09254300	-1.35323800	-0.03082900
C	-0.22251100	0.03824200	0.47285700
N	-1.14811700	0.71698900	-0.44554200
C	1.04603300	0.82752900	0.56682400
C	1.76863087	0.80019312	1.69140139
C	1.45639666	1.55979353	-0.47382957
C	2.22017454	0.97208220	-1.48215967
C	2.64838262	1.73609951	-2.56777743
C	2.31269174	3.08770653	-2.64504971
C	1.54884683	3.67539375	-1.63678966
C	1.12070579	2.91140055	-0.55110185
O	1.18492500	-1.86806800	-0.06107500
C	-1.06518200	-3.29822200	-0.91293700
S	1.21155549	-0.19386720	3.10410648
C	2.62347114	0.26656907	4.14752187
F	3.80608212	-0.13444569	3.53247561
F	2.50905775	-0.36050186	5.38500210
F	2.63812398	1.64709950	4.32524244
H	-5.51284400	0.63401500	-0.43457800
H	-5.51284600	-1.80298500	-0.43457800
H	-3.40234200	-3.02148600	-0.43457800
H	-3.40234000	1.85251400	-0.43457800
H	-0.93703200	1.57597500	-1.01130300
H	2.70076093	1.38016394	1.76044908
H	2.48481961	-0.09386955	-1.42124478
H	3.25081040	1.27268070	-3.36296506
H	2.65037903	3.69018220	-3.50119842
H	1.28407968	4.74131058	-1.69778838
H	0.51834211	3.37484286	0.24412117
H	-2.09444700	-3.60077900	-1.20931800
H	-0.38658200	-3.38383600	-1.79096900
H	-0.70354700	-3.96343500	-0.09716600

**3aa'**

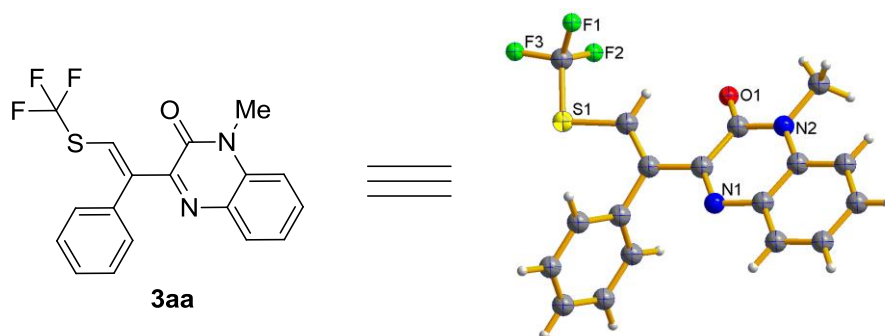
C	-4.77427300	0.13687300	0.26046000
C	-4.77103400	-1.25548700	0.21983500
C	-3.56171600	-1.95074400	0.14942500
C	-2.34211300	-1.26216800	0.14942500
C	-2.35080800	0.15213000	0.14942500
C	-3.56777600	0.83593800	0.21719700
N	-1.13860500	-1.98648700	-0.00095600
C	0.04442000	-1.24323800	0.42726300
C	-0.05711100	0.24369100	0.16652200
N	-1.16566000	0.91120100	0.06911300
C	1.08546100	0.92351900	0.02534000
C	2.05827518	0.79174767	0.93299590
C	1.25521881	1.73511822	-1.02349617
C	1.33495400	3.11444666	-0.83222829
C	1.51193896	3.96114972	-1.92649692
C	1.60929377	3.42847210	-3.21190615
C	1.52965680	2.04916094	-3.40317095
C	1.35257362	1.20244060	-2.30890540
O	1.00720300	-1.76392300	0.93834000
C	-1.08188600	-3.35447000	-0.53603200
S	1.82782536	-0.31001073	2.35680954
C	3.46567222	0.04163482	3.05539970
F	3.57059713	1.40184666	3.33194861
F	3.63355518	-0.68449957	4.23107389
F	4.44851424	-0.32257056	2.13940881
H	-5.72621700	0.68408200	0.32651800
H	-5.72189800	-1.80803700	0.24323300
H	-3.56722500	-3.04930500	0.09345200
H	-3.57437400	1.93574700	0.23661000
H	2.99831205	1.35106797	0.81684026
H	1.25826957	3.53450560	0.18151232
H	1.57473200	5.04895711	-1.77572209
H	1.74888410	4.09621390	-4.07482977
H	1.60649362	1.62910123	-4.41689958
H	1.28970568	0.11463963	-2.45969453
H	-0.02494900	-3.70278300	-0.55417900
H	-1.68375100	-4.03075100	0.11140200
H	-1.49381200	-3.36562700	-1.56993800

### Crystal data of **3aa**

The crystal was obtained by slow evaporation of **3aa** in a mixture of petroleum ether/ethyl acetate.

CCDC 2325553 (**3aa**) contains the supplementary crystallographic data for this paper. These data can

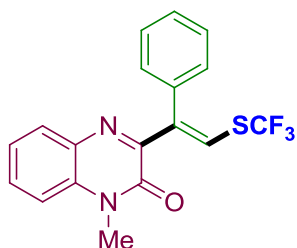
be obtained free of charge from the Cambridge Crystallographic Data Centre via [www.ccdc.cam.ac.uk/data\\_request/cif](http://www.ccdc.cam.ac.uk/data_request/cif).



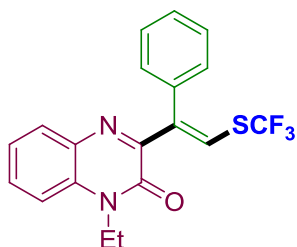
**Table S1 Crystal data and structure refinement of 3aa**

Identification code	11
Empirical formula	C <sub>18</sub> H <sub>13</sub> F <sub>3</sub> N <sub>2</sub> OS
Formula weight	362.36
Temperature/K	296.15
Crystal system	triclinic
Space group	P-1
a/Å	4.7880(12)
b/Å	10.509(3)
c/Å	16.019(4)
α/°	90.169(3)
β/°	91.422(3)
γ/°	90.026(3)
Volume/Å <sup>3</sup>	805.8(4)
Z	2
ρ <sub>calc</sub> /cm <sup>3</sup>	1.493
μ/mm <sup>-1</sup>	0.242
F(000)	372.0
Crystal size/mm <sup>3</sup>	0.46 × 0.42 × 0.23
Radiation	MoKα (λ = 0.71073)
2θ range for data collection/°	2.544 to 55.2
Index ranges	-6 ≤ h ≤ 6, -13 ≤ k ≤ 13, -20 ≤ l ≤ 20
Reflections collected	9105
Independent reflections	3587 [R <sub>int</sub> = 0.0200, R <sub>sigma</sub> = 0.0234]
Data/restraints/parameters	3587/0/227
Goodness-of-fit on F <sup>2</sup>	1.051
Final R indexes [I ≥ 2σ (I)]	R <sub>1</sub> = 0.0449, wR <sub>2</sub> = 0.1232
Final R indexes [all data]	R <sub>1</sub> = 0.0582, wR <sub>2</sub> = 0.1340
Largest diff. peak/hole / e Å <sup>-3</sup>	0.23/-0.27

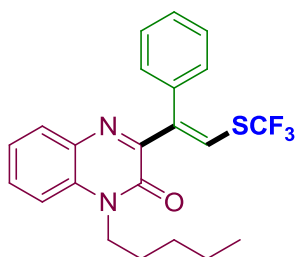
### 3. Characterization data of products



**(E)-1-methyl-3-(1-phenyl-2-((trifluoromethyl)thio)vinyl)quinoxalin-2(1H)-one (3aa):** White solid (91.2 mg, 84%), mp: 78–79 °C.  $^1\text{H}$  NMR (400 MHz, Chloroform-*d*)  $\delta$  8.39 (s, 1H), 7.59 (d,  $J = 8.0$  Hz, 1H), 7.42 (t,  $J = 7.7$  Hz, 1H), 7.37 – 7.27 (m, 3H), 7.17 (q,  $J = 7.2$  Hz, 4H), 3.61 (s, 3H);  $^{13}\text{C}\{^1\text{H}\}$  NMR (100 MHz, Chloroform-*d*)  $\delta$  154.4, 151.3, 139.7, 137.1, 132.8, 132.6, 130.9, 130.6, 129.3 (q,  $J_{\text{C-F}} = 306.6$  Hz), 129.0, 128.4, 128.2, 127.1 (q,  $J_{\text{C-F}} = 3.4$  Hz), 123.7, 113.4, 29.2;  $^{19}\text{F}$  NMR (376 MHz, Chloroform-*d*)  $\delta$  -42.20; HRMS (ESI):  $m/z$   $[\text{M}+\text{H}]^+$  calcd for  $\text{C}_{18}\text{H}_{14}\text{F}_3\text{N}_2\text{OS}$ : 363.0773; found: 363.0776.

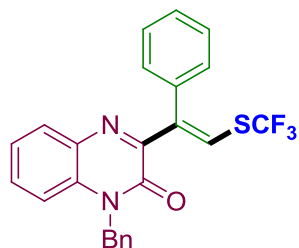


**(E)-1-ethyl-3-(1-phenyl-2-((trifluoromethyl)thio)vinyl)quinoxalin-2(1H)-one (3ba):** White solid (88.0 mg, 78%), mp: 66–67 °C.  $^1\text{H}$  NMR (400 MHz, Chloroform-*d*)  $\delta$  8.45 (s, 1H), 7.59 (d,  $J = 8.0$  Hz, 1H), 7.42 (t,  $J = 7.8$  Hz, 1H), 7.37 – 7.27 (m, 3H), 7.23 – 7.12 (m, 4H), 4.24 (q,  $J = 7.1$  Hz, 2H), 1.28 (t,  $J = 7.1$  Hz, 3H);  $^{13}\text{C}\{^1\text{H}\}$  NMR (100 MHz, Chloroform-*d*)  $\delta$  153.9, 151.1, 139.7, 137.1, 132.9, 131.7, 129.3 (q,  $J_{\text{C-F}} = 306.6$  Hz), 130.9, 130.6, 129.1, 128.4, 128.2, 127.3 (q,  $J_{\text{C-F}} = 3.5$  Hz), 123.5, 37.6, 12.4;  $^{19}\text{F}$  NMR (376 MHz, Chloroform-*d*)  $\delta$  -42.17; HRMS (ESI):  $m/z$   $[\text{M}+\text{H}]^+$  calcd for  $\text{C}_{19}\text{H}_{16}\text{F}_3\text{N}_2\text{OS}$ : 377.0930; found: 377.0932.

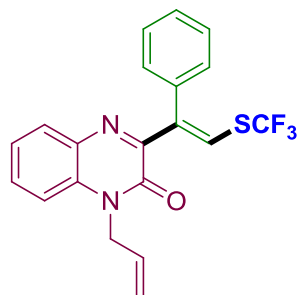


**(E)-1-pentyl-3-(1-phenyl-2-((trifluoromethyl)thio)vinyl)quinoxalin-2(1H)-one (3ca):** Yellow oil (96.6 mg, 77%).  $^1\text{H}$  NMR (400 MHz, Chloroform-*d*)  $\delta$  8.52 (s, 1H), 7.71 (d,  $J = 7.9$  Hz, 1H), 7.54 (t,  $J = 7.8$  Hz, 1H), 7.48 – 7.38 (m, 3H), 7.29 (d,  $J = 7.4$  Hz, 4H), 4.31 – 4.21 (m, 2H), 1.81 – 1.72 (m, 2H), 1.48 – 1.37 (m, 4H), 0.94 (t,  $J = 6.8$  Hz, 3H);  $^{13}\text{C}\{^1\text{H}\}$  NMR (100 MHz, Chloroform-*d*)  $\delta$  154.0, 151.3, 139.8, 137.1, 132.9, 132.0, 131.0, 130.6, 129.3 (q,  $J_{\text{C-F}} = 306.6$  Hz), 129.0, 128.4, 128.2, 127.0 (q,  $J_{\text{C-F}} = 3.3$  Hz),

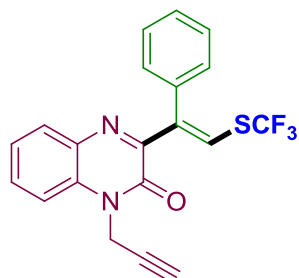
113.4, 42.6, 29.1, 26.9, 22.4, 14.0;  $^{19}\text{F}$  NMR (376 MHz, Chloroform-*d*)  $\delta$  -42.13; HRMS (ESI):  $m/z$   $[\text{M}+\text{H}]^+$  calcd for  $\text{C}_{22}\text{H}_{22}\text{F}_3\text{N}_2\text{OS}$ : 419.1399; found: 419.1402.



**(E)-1-benzyl-3-(1-phenyl-2-((trifluoromethyl)thio)vinyl)quinoxalin-2(1H)-one (3da):** White solid (94.6 mg, 72%), mp: 97–98 °C.  $^1\text{H}$  NMR (400 MHz, Chloroform-*d*)  $\delta$  8.60 (s, 1H), 7.68 (d,  $J = 7.9$  Hz, 1H), 7.47–7.36 (m, 4H), 7.34–7.27 (m, 4H), 7.25–7.16 (m, 5H), 5.52 (s, 2H);  $^{13}\text{C}\{^1\text{H}\}$  NMR (100 MHz, Chloroform-*d*)  $\delta$  154.5, 151.2, 139.6, 137.1, 135.0, 132.2, 130.8, 130.6, 129.3 (q,  $J_{\text{C-F}} = 306.6$  Hz), 129.1, 128.9, 128.5, 128.3, 127.8 (q,  $J_{\text{C-F}} = 3.3$  Hz), 127.7, 126.7, 123.8, 114.3, 46.0;  $^{19}\text{F}$  NMR (376 MHz, Chloroform-*d*)  $\delta$  -42.10; HRMS (ESI):  $m/z$   $[\text{M}+\text{H}]^+$  calcd for  $\text{C}_{24}\text{H}_{18}\text{F}_3\text{N}_2\text{OS}$ : 439.1086; found: 439.1092.

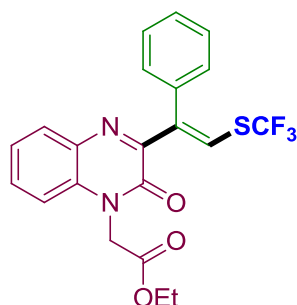


**(E)-1-allyl-3-(1-phenyl-2-((trifluoromethyl)thio)vinyl)quinoxalin-2(1H)-one (3ea):** White solid (86.2 mg, 74%), mp: 113–114 °C.  $^1\text{H}$  NMR (400 MHz, Chloroform-*d*)  $\delta$  8.46 (s, 1H), 7.58 (d,  $J = 8.2$  Hz, 1H), 7.42–7.27 (m, 4H), 7.24–7.10 (m, 4H), 5.94–5.76 (m, 1H), 5.17 (d,  $J = 10.4$  Hz, 1H), 5.05 (d,  $J = 17.3$  Hz, 1H), 4.82 (d,  $J = 4.6$  Hz, 2H);  $^{13}\text{C}\{^1\text{H}\}$  NMR (100 MHz, Chloroform-*d*)  $\delta$  154.0, 151.1, 139.6, 137.1, 132.8, 132.0, 130.8, 130.6, 130.5, 129.3 (q,  $J_{\text{C-F}} = 306.6$  Hz), 129.1, 128.5, 128.2, 127.6 (q,  $J_{\text{C-F}} = 3.5$  Hz), 123.7, 118.1, 114.0, 44.7;  $^{19}\text{F}$  NMR (376 MHz, Chloroform-*d*)  $\delta$  -42.14; HRMS (ESI):  $m/z$   $[\text{M}+\text{H}]^+$  calcd for  $\text{C}_{20}\text{H}_{16}\text{F}_3\text{N}_2\text{OS}$ : 389.0930; found: 389.0935.



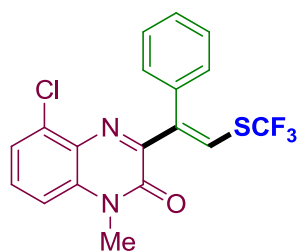
**(E)-3-(1-phenyl-2-((trifluoromethyl)thio)vinyl)-1-(prop-2-yn-1-yl)quinoxalin-2(1H)-one (3fa):** White solid (86.9 mg, 75%), mp: 134–135 °C.  $^1\text{H}$  NMR (400 MHz, Chloroform-*d*)  $\delta$  8.49 (s, 1H), 7.61 (d,  $J = 8.0$  Hz, 1H), 7.48 (t,  $J = 7.8$  Hz, 1H), 7.38–7.29 (m, 4H), 7.25–7.15 (m, 3H), 4.99 (d,  $J = 2.1$  Hz, 2H), 2.21 (s, 1H);  $^{13}\text{C}\{^1\text{H}\}$  NMR (100 MHz, Chloroform-*d*)  $\delta$  153.4, 150.9, 139.4, 136.9, 132.8, 131.3,

130.9, 130.7, 129.3 (q,  $J_{C-F} = 306.6$  Hz), 129.1, 128.5, 128.3, 128.0 (q,  $J_{C-F} = 3.5$  Hz), 124.1, 113.9, 76.7, 73.3, 31.7;  $^{19}\text{F}$  NMR (376 MHz, Chloroform-*d*)  $\delta$  -42.16; HRMS (ESI):  $m/z$   $[\text{M}+\text{H}]^+$  calcd for  $\text{C}_{20}\text{H}_{14}\text{F}_3\text{N}_2\text{OS}$ : 387.0773; found: 387.0771.



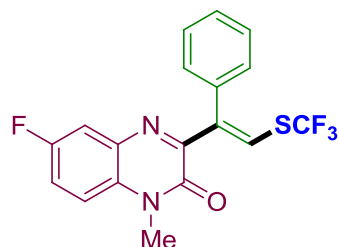
**(E)-ethyl 2-(2-oxo-3-(1-phenyl-2-((trifluoromethyl)thio)vinyl)quinoxalin-1(2H)-yl)acetate (3ga):**

White solid (93.8 mg, 72%), mp: 105–106 °C.  $^1\text{H}$  NMR (400 MHz, Chloroform-*d*)  $\delta$  8.56 (s, 1H), 7.72 (d,  $J = 8.0$  Hz, 1H), 7.54–7.40 (m, 4H), 7.33–7.27 (m, 3H), 7.06 (d,  $J = 8.4$  Hz, 1H), 5.06 (s, 2H), 4.27 (q,  $J = 7.1$  Hz, 2H), 1.29 (t,  $J = 7.1$  Hz, 3H);  $^{13}\text{C}\{^1\text{H}\}$  NMR (100 MHz, Chloroform-*d*)  $\delta$  167.0, 154.0, 150.8, 139.4, 136.9, 132.7, 131.9, 131.0, 130.8, 129.3 (q,  $J_{C-F} = 306.6$  Hz), 129.1, 128.5, 128.3, 127.9 (q,  $J_{C-F} = 3.5$  Hz), 124.0, 112.9, 43.6, 14.1;  $^{19}\text{F}$  NMR (376 MHz, Chloroform-*d*)  $\delta$  -42.17; HRMS (ESI):  $m/z$   $[\text{M}+\text{H}]^+$  calcd for  $\text{C}_{21}\text{H}_{18}\text{F}_3\text{N}_2\text{OS}$ : 435.0985; found: 435.0992.



**(E)-5-chloro-1-methyl-3-(1-phenyl-2-((trifluoromethyl)thio)vinyl)quinoxalin-2(1H)-one (3ha):**

White solid (95.0 mg, 80%), mp: 116–117 °C.  $^1\text{H}$  NMR (400 MHz, Chloroform-*d*)  $\delta$  8.74 (s, 1H), 7.51–7.30 (m, 7H), 7.19 (d,  $J = 8.2$  Hz, 1H), 3.73 (s, 3H);  $^{13}\text{C}\{^1\text{H}\}$  NMR (100 MHz, Chloroform-*d*)  $\delta$  154.1, 150.4, 139.5, 136.7, 135.5, 134.1, 130.4, 129.3 (q,  $J_{C-F} = 306.7$  Hz), 129.2, 128.9 (q,  $J_{C-F} = 3.5$  Hz), 128.3, 128.3, 124.6, 112.2, 29.7;  $^{19}\text{F}$  NMR (376 MHz, Chloroform-*d*)  $\delta$  -42.22; HRMS (ESI):  $m/z$   $[\text{M}+\text{H}]^+$  calcd for  $\text{C}_{18}\text{H}_{13}\text{ClF}_3\text{N}_2\text{OS}$ : 397.0384; found: 397.0385.

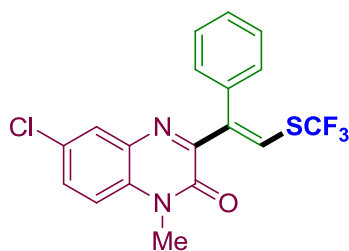


**(E)-6-fluoro-1-methyl-3-(1-phenyl-2-((trifluoromethyl)thio)vinyl)quinoxalin-2(1H)-one (3ia):**

White solid (88.9 mg, 78%), mp: 108–109 °C.  $^1\text{H}$  NMR (400 MHz, Chloroform-*d*)  $\delta$  8.60 (s, 1H), 7.44–7.38 (m, 4H), 7.25–7.15 (m, 4H), 3.68 (s, 3H);  $^{13}\text{C}\{^1\text{H}\}$  NMR (100 MHz, Chloroform-*d*)  $\delta$  158.7 (d,  $J_{C-F} = 242.6$  Hz), 154.1, 152.1, 139.4, 136.9, 133.2 (d,  $J_{C-F} = 11.5$  Hz), 129.4 (d,  $J_{C-F} = 19.0$  Hz), 129.2 (q,  $J_{C-F}$

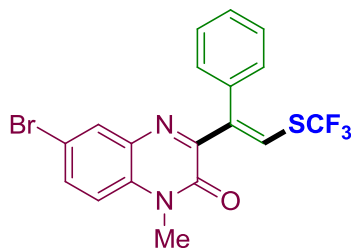


= 306.7 Hz), 129.1, 128.7 (q,  $J_{C-F}$  = 3.4 Hz), 128.5, 128.3, 118.4 (d,  $J_{C-F}$  = 22.3 Hz), 115.8 (d,  $J_{C-F}$  = 22.2 Hz), 114.5 (d,  $J_{C-F}$  = 8.7 Hz), 29.5;  $^{19}\text{F}$  NMR (376 MHz, Chloroform-*d*)  $\delta$  -118.78, -42.20; HRMS (ESI):  $m/z$   $[\text{M}+\text{H}]^+$  calcd for  $\text{C}_{18}\text{H}_{13}\text{F}_4\text{N}_2\text{OS}$ : 381.0679; found: 381.0684.



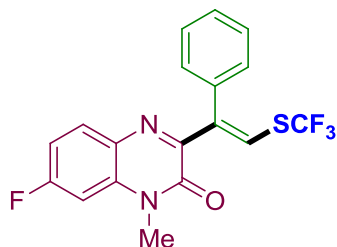
**(E)-6-chloro-1-methyl-3-(1-phenyl-2-((trifluoromethyl)thio)vinyl)quinoxalin-2(1H)-one (3ja):**

White solid (90.3 mg, 76%), mp: 115–116 °C.  $^1\text{H}$  NMR (400 MHz, Chloroform-*d*)  $\delta$  8.58 (s, 1H), 7.59 (s, 1H), 7.44 – 7.28 (m, 4H), 7.21 – 7.10 (m, 3H), 3.63 (s, 3H);  $^{13}\text{C}\{^1\text{H}\}$  NMR (100 MHz, Chloroform-*d*)  $\delta$  154.1, 151.9, 139.3, 136.8, 133.1, 131.4, 130.5, 129.8, 129.2 (q,  $J_{C-F}$  = 306.7 Hz), 129.1, 129.1, 128.9 (q,  $J_{C-F}$  = 3.5 Hz), 128.5, 128.3, 114.6, 29.4;  $^{19}\text{F}$  NMR (376 MHz, Chloroform-*d*)  $\delta$  -42.20; HRMS (ESI):  $m/z$   $[\text{M}+\text{H}]^+$  calcd for  $\text{C}_{18}\text{H}_{13}\text{ClF}_3\text{N}_2\text{OS}$ : 397.0384; found: 397.0381.



**(E)-6-bromo-1-methyl-3-(1-phenyl-2-((trifluoromethyl)thio)vinyl)quinoxalin-2(1H)-one (3ka):**

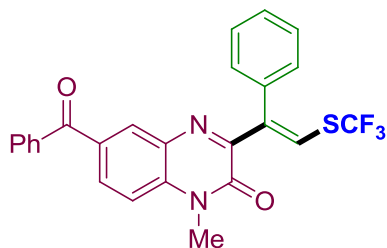
White solid (99.0 mg, 75%), mp: 112–113 °C.  $^1\text{H}$  NMR (400 MHz, Chloroform-*d*)  $\delta$  8.71 (s, 1H), 7.86 (d,  $J$  = 1.9 Hz, 1H), 7.63 (dd,  $J$  = 8.9, 1.9 Hz, 1H), 7.53 – 7.43 (m, 3H), 7.27 (d,  $J$  = 7.0 Hz, 2H), 7.19 (d,  $J$  = 8.9 Hz, 1H), 3.74 (s, 3H);  $^{13}\text{C}\{^1\text{H}\}$  NMR (100 MHz, Chloroform-*d*)  $\delta$  154.1, 151.8, 139.3, 136.8, 133.4, 133.2, 132.9, 131.8, 129.2 (q,  $J_{C-F}$  = 306.9 Hz), 129.1, 129.0 (q,  $J_{C-F}$  = 3.5 Hz), 128.5, 128.3, 116.4, 114.9, 29.4;  $^{19}\text{F}$  NMR (376 MHz, Chloroform-*d*)  $\delta$  -42.20; HRMS (ESI):  $m/z$   $[\text{M}+\text{H}]^+$  calcd for  $\text{C}_{18}\text{H}_{13}\text{BrF}_3\text{N}_2\text{OS}$ : 440.9879; found: 440.9883.



**(E)-7-fluoro-1-methyl-3-(1-phenyl-2-((trifluoromethyl)thio)vinyl)quinoxalin-2(1H)-one (3la):**

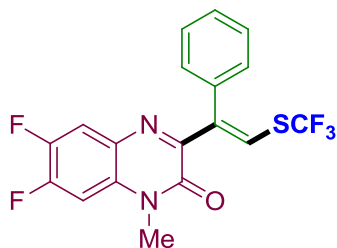
White solid (88.9 mg, 78%), mp: 106–107 °C.  $^1\text{H}$  NMR (400 MHz, Chloroform-*d*)  $\delta$  8.40 (s, 1H), 7.63 – 7.57 (m, 1H), 7.39 – 7.32 (m, 3H), 7.21 – 7.15 (m, 2H), 6.97 – 6.87 (m, 2H), 3.60 (s, 3H);  $^{13}\text{C}\{^1\text{H}\}$  NMR (100 MHz, Chloroform-*d*)  $\delta$  163.6 (d,  $J_{C-F}$  = 250.4 Hz), 154.3, 150.1, 139.5, 137.0, 134.3 (d,  $J_{C-F}$  = 11.6 Hz), 132.8 (d,  $J_{C-F}$  = 10.5 Hz), 129.4 (d,  $J_{C-F}$  = 2.5 Hz), 129.3 (q,  $J_{C-F}$  = 306.7 Hz), 129.0, 128.5, 128.3, 127.3 (q,  $J_{C-F}$  = 3.4 Hz), 111.8 (d,  $J_{C-F}$  = 23.4 Hz), 100.4 (d,  $J_{C-F}$  = 27.7 Hz), 29.5;  $^{19}\text{F}$  NMR (376 MHz,

Chloroform-*d*)  $\delta$  -106.11, -42.24; HRMS (ESI):  $m/z$   $[M+H]^+$  calcd for  $C_{18}H_{13}F_4N_2OS$ : 381.0679; found: 381.0685.



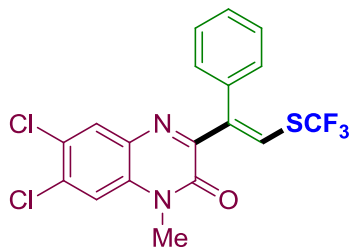
**(E)-6-benzoyl-1-methyl-3-(1-phenyl-2-((trifluoromethyl)thio)vinyl)quinoxalin-2(1H)-one (3ma):**

White solid (106.3 mg, 76%), mp: 94–95 °C.  $^1H$  NMR (400 MHz, Chloroform-*d*)  $\delta$  8.63 (s, 1H), 7.77 – 7.69 (m, 3H), 7.56 (t,  $J$  = 7.5 Hz, 2H), 7.44 (t,  $J$  = 7.6 Hz, 2H), 7.41 – 7.33 (m, 3H), 7.24 – 7.16 (m, 3H), 3.69 (s, 3H);  $^{13}C\{^1H\}$  NMR (100 MHz, Chloroform-*d*)  $\delta$  195.5, 152.8, 139.3, 138.7, 137.0, 136.8, 134.8, 133.0, 132.7, 130.4, 130.1, 129.6 (q,  $J_{C-F}$  = 3.5 Hz), 129.2 (q,  $J_{C-F}$  = 306.6 Hz), 129.1, 128.6, 128.5, 128.4, 125.1, 115.3, 29.5;  $^{19}F$  NMR (376 MHz, Chloroform-*d*)  $\delta$  -42.18; HRMS (ESI):  $m/z$   $[M+H]^+$  calcd for  $C_{25}H_{18}F_3N_2O_2S$ : 467.1036; found: 467.1042.



**(E)-6,7-difluoro-1-methyl-3-(1-phenyl-2-((trifluoromethyl)thio)vinyl)quinoxalin-2(1H)-one (3na):**

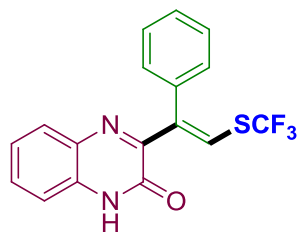
White solid (88.4 mg, 74%), mp: 97–98 °C.  $^1H$  NMR (400 MHz, Chloroform-*d*)  $\delta$  8.54 (s, 1H), 7.44 – 7.32 (m, 4H), 7.18 – 7.12 (m, 2H), 7.04 – 6.98 (m, 1H), 3.60 (s, 3H);  $^{13}C\{^1H\}$  NMR (100 MHz, Chloroform-*d*)  $\delta$  154.0, 151.7 (dd,  $J_{C-F}$  = 253.1 Hz, 14.4 Hz), 151.1 (d,  $J_{C-F}$  = 3.6 Hz), 146.8 (dd,  $J_{C-F}$  = 246.1 Hz, 13.9 Hz), 139.1, 136.8, 130.0 (dd,  $J_{C-F}$  = 8.9 Hz, 1.5 Hz), 129.2 (q,  $J_{C-F}$  = 306.7 Hz), 129.1, 128.9 (dd,  $J_{C-F}$  = 9.5 Hz, 2.8 Hz), 128.7 (q,  $J_{C-F}$  = 3.4 Hz), 128.6, 128.4, 118.0 (dd,  $J_{C-F}$  = 17.7 Hz, 2.1 Hz), 102.0 (d,  $J_{C-F}$  = 23.1 Hz), 29.8;  $^{19}F$  NMR (376 MHz, Chloroform-*d*)  $\delta$  -129.60 (d,  $J$  = 22.3 Hz), -141.72 (d,  $J$  = 22.3 Hz), -42.24; HRMS (ESI):  $m/z$   $[M+H]^+$  calcd for  $C_{18}H_{12}F_5N_2O_2S$ : 399.0585; found: 399.0579.



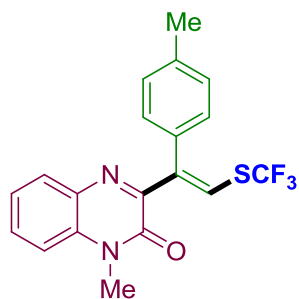
**(E)-6,7-dichloro-1-methyl-3-(1-phenyl-2-((trifluoromethyl)thio)vinyl)quinoxalin-2(1H)-one (3oa):**

White solid (95.5 mg, 74%), mp: 98–99 °C.  $^1H$  NMR (400 MHz, Chloroform-*d*)  $\delta$  8.70 (s, 1H), 7.75 (s, 1H), 7.48 – 7.42 (m, 3H), 7.38 (s, 1H), 7.23 (d,  $J$  = 6.9 Hz, 2H), 3.68 (s, 3H);  $^{13}C\{^1H\}$  NMR (100 MHz, Chloroform-*d*)  $\delta$  153.8, 151.7, 139.0, 136.7, 134.6, 132.0, 131.6, 131.2, 129.7 (q,  $J_{C-F}$  = 3.5 Hz), 129.3 (q,

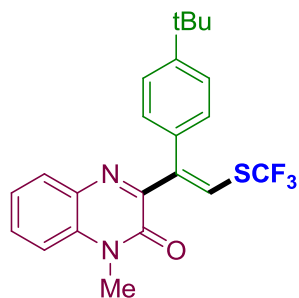
$J_{\text{C-F}} = 306.6$  Hz), 129.1, 128.6, 128.4, 128.1, 127.6, 29.5;  $^{19}\text{F}$  NMR (376 MHz, Chloroform-*d*)  $\delta$  -42.19; HRMS (ESI):  $m/z$   $[\text{M}+\text{H}]^+$  calcd for  $\text{C}_{18}\text{H}_{12}\text{Cl}_2\text{F}_3\text{N}_2\text{OS}$ : 430.9994; found: 430.9991.



**(E)-3-(1-phenyl-2-((trifluoromethyl)thio)vinyl)quinoxalin-2(1H)-one (3pa):** White solid (76.2 mg, 73%), mp: 234–235 °C.  $^1\text{H}$  NMR (400 MHz, DMSO-*d*<sub>6</sub>)  $\delta$  12.65 (s, 1H), 8.68 (s, 1H), 7.54 – 7.41 (m, 5H), 7.33 (d,  $J = 8.1$  Hz, 1H), 7.27 – 7.20 (m, 3H);  $^{13}\text{C}\{^1\text{H}\}$  NMR (100 MHz, DMSO-*d*<sub>6</sub>)  $\delta$  155.2, 152.0, 141.1, 137.3, 132.1, 132.0, 131.3, 129.8 (q,  $J_{\text{C-F}} = 306.2$  Hz), 129.5, 129.4, 129.0, 128.9, 125.4 (q,  $J_{\text{C-F}} = 2.9$  Hz), 124.1, 115.7;  $^{19}\text{F}$  NMR (376 MHz, DMSO-*d*<sub>6</sub>)  $\delta$  -41.66; HRMS (ESI):  $m/z$   $[\text{M}+\text{H}]^+$  calcd for  $\text{C}_{17}\text{H}_{12}\text{F}_3\text{N}_2\text{OS}$ : 349.0617; found: 349.0624.

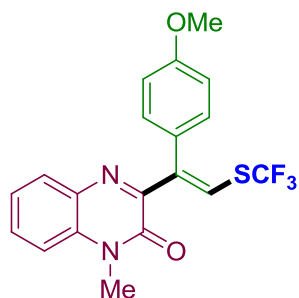


**(E)-1-methyl-3-(1-(p-tolyl)-2-((trifluoromethyl)thio)vinyl)quinoxalin-2(1H)-one (3ab):** White solid (88.0 mg, 78%), mp: 88–89 °C.  $^1\text{H}$  NMR (400 MHz, Chloroform-*d*)  $\delta$  8.29 (s, 1H), 7.66 (d,  $J = 8.2$  Hz, 1H), 7.46 (t,  $J = 7.8$  Hz, 1H), 7.25 – 7.19 (m, 2H), 7.16 (d,  $J = 7.8$  Hz, 2H), 7.09 (d,  $J = 7.7$  Hz, 2H), 3.64 (s, 3H), 2.32 (s, 3H);  $^{13}\text{C}\{^1\text{H}\}$  NMR (100 MHz, Chloroform-*d*)  $\delta$  154.4, 151.7, 139.7, 138.1, 134.0, 132.9, 132.7, 130.7, 130.6, 129.4 (q,  $J_{\text{C-F}} = 306.5$  Hz), 129.2, 128.8, 126.4 (q,  $J_{\text{C-F}} = 3.6$  Hz), 123.7, 113.5, 29.2, 21.4;  $^{19}\text{F}$  NMR (376 MHz, Chloroform-*d*)  $\delta$  -42.24; HRMS (ESI):  $m/z$   $[\text{M}+\text{H}]^+$  calcd for  $\text{C}_{19}\text{H}_{16}\text{F}_3\text{N}_2\text{OS}$ : 377.0930; found: 377.0932.



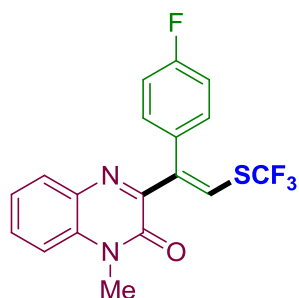
**(E)-3-(1-(4-(tert-butyl)phenyl)-2-((trifluoromethyl)thio)vinyl)-1-methylquinoxalin-2(1H)-one (3ac):** Yellow oil (90.3 mg, 72%).  $^1\text{H}$  NMR (400 MHz, Chloroform-*d*)  $\delta$  8.36 (s, 1H), 7.72 (d,  $J = 8.1$  Hz, 1H), 7.51 (t,  $J = 7.7$  Hz, 1H), 7.42 (d,  $J = 8.0$  Hz, 2H), 7.32 – 7.26 (m, 2H), 7.19 (d,  $J = 8.0$  Hz, 2H), 3.70 (s, 3H), 1.34 (s, 9H);  $^{13}\text{C}\{^1\text{H}\}$  NMR (100 MHz, Chloroform-*d*)  $\delta$  154.4, 151.7, 151.1, 139.6, 133.9, 132.8, 132.6, 130.7, 130.6, 129.4 (q,  $J_{\text{C-F}} = 306.6$  Hz), 128.6, 126.4 (q,  $J_{\text{C-F}} = 3.5$  Hz), 125.3, 123.7, 113.4, 34.7,

31.3, 29.2;  $^{19}\text{F}$  NMR (376 MHz, Chloroform-*d*)  $\delta$  -42.28; HRMS (ESI):  $m/z$   $[\text{M}+\text{H}]^+$  calcd for  $\text{C}_{22}\text{H}_{22}\text{F}_3\text{N}_2\text{OS}$ : 419.1399; found: 419.1403.



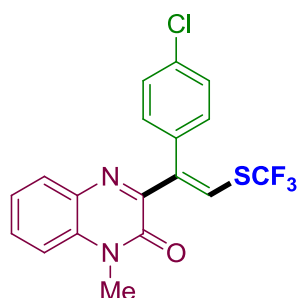
**(E)-3-(1-(4-methoxyphenyl)-2-((trifluoromethyl)thio)vinyl)-1-methylquinoxalin-2(1H)-one (3ad):**

White solid (90.6 mg, 77%), mp: 137–138 °C.  $^1\text{H}$  NMR (400 MHz, Chloroform-*d*)  $\delta$  8.36 (s, 1H), 7.74 (d,  $J = 8.3$  Hz, 1H), 7.55 (t,  $J = 7.8$  Hz, 1H), 7.31 (t,  $J = 7.1$  Hz, 2H), 7.22 (d,  $J = 8.4$  Hz, 2H), 6.96 (d,  $J = 8.4$  Hz, 2H), 3.85 (s, 3H), 3.72 (s, 3H);  $^{13}\text{C}\{^1\text{H}\}$  NMR (100 MHz, Chloroform-*d*)  $\delta$  159.4, 154.4, 151.7, 139.4, 132.9, 132.6, 130.7, 130.6, 130.3, 129.4 (q,  $J_{\text{C-F}} = 306.7$  Hz), 129.3, 126.4 (q,  $J_{\text{C-F}} = 3.4$  Hz), 123.7, 113.9, 113.5, 55.2, 29.2;  $^{19}\text{F}$  NMR (376 MHz, Chloroform-*d*)  $\delta$  -42.24; HRMS (ESI):  $m/z$   $[\text{M}+\text{H}]^+$  calcd for  $\text{C}_{19}\text{H}_{16}\text{F}_3\text{N}_2\text{O}_2\text{S}$ : 393.0879; found: 393.0874.



**(E)-3-(1-(4-fluorophenyl)-2-((trifluoromethyl)thio)vinyl)-1-methylquinoxalin-2(1H)-one (3ae):**

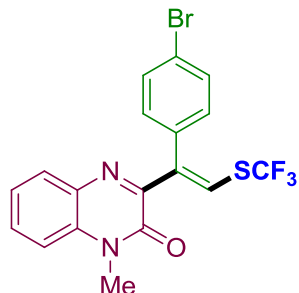
White solid (84.4 mg, 74%), mp: 82–83 °C.  $^1\text{H}$  NMR (400 MHz, Chloroform-*d*)  $\delta$  8.47 (s, 1H), 7.61 (d,  $J = 8.3$  Hz, 1H), 7.47 (t,  $J = 7.8$  Hz, 1H), 7.27 – 7.14 (m, 4H), 7.04 (t,  $J = 8.5$  Hz, 2H), 3.65 (s, 3H);  $^{13}\text{C}\{^1\text{H}\}$  NMR (100 MHz, Chloroform-*d*)  $\delta$  162.5 (d,  $J_{\text{C-F}} = 246.1$  Hz), 154.4, 150.9, 138.8, 132.9 (d,  $J_{\text{C-F}} = 3.4$  Hz), 132.7 (d,  $J_{\text{C-F}} = 20.9$  Hz), 132.6, 131.0 (d,  $J_{\text{C-F}} = 8.2$  Hz), 130.7 (d,  $J_{\text{C-F}} = 7.9$  Hz), 129.4 (q,  $J_{\text{C-F}} = 306.6$  Hz), 127.7 (q,  $J_{\text{C-F}} = 3.4$  Hz), 123.8, 115.5 (d,  $J_{\text{C-F}} = 21.5$  Hz), 113.5, 29.2;  $^{19}\text{F}$  NMR (376 MHz, Chloroform-*d*)  $\delta$  -113.13, -42.12; HRMS (ESI):  $m/z$   $[\text{M}+\text{H}]^+$  calcd for  $\text{C}_{18}\text{H}_{13}\text{F}_4\text{N}_2\text{OS}$ : 381.0679; found: 381.0684.



**(E)-3-(1-(4-chlorophenyl)-2-((trifluoromethyl)thio)vinyl)-1-methylquinoxalin-2(1H)-one (3af):**

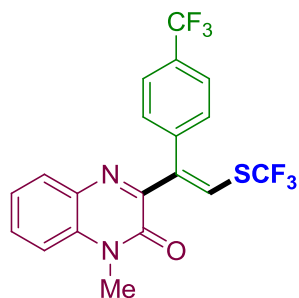
White solid (89.1 mg, 75%), mp: 107–108 °C.  $^1\text{H}$  NMR (400 MHz, Chloroform-*d*)  $\delta$  8.57 (s, 1H), 7.70 (d,

$J = 8.3$  Hz, 1H), 7.56 (t,  $J = 7.8$  Hz, 1H), 7.41 (d,  $J = 8.3$  Hz, 2H), 7.33 – 7.28 (m, 2H), 7.21 (d,  $J = 8.3$  Hz, 2H), 3.73 (s, 3H);  $^{13}\text{C}\{^1\text{H}\}$  NMR (100 MHz, )  $\delta$  154.3, 150.7, 138.6, 135.4, 134.2, 132.8, 132.6, 130.8, 130.7, 130.6, 129.4 (q,  $J_{\text{C-F}} = 306.6$  Hz), 128.8, 127.8 (q,  $J_{\text{C-F}} = 3.5$  Hz), 123.9, 113.5, 29.3;  $^{19}\text{F}$  NMR (376 MHz, Chloroform-*d*)  $\delta$  -42.09; HRMS (ESI):  $m/z$   $[\text{M}+\text{H}]^+$  calcd for  $\text{C}_{18}\text{H}_{13}\text{ClF}_3\text{N}_2\text{OS}$ : 397.0384; found: 397.0383.



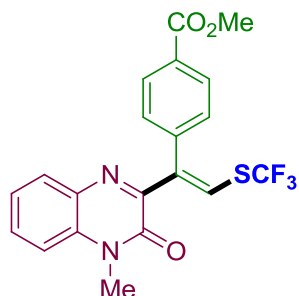
**(E)-3-(1-(4-bromophenyl)-2-((trifluoromethyl)thio)vinyl)-1-methylquinoxalin-2(1H)-one (3ag):**

White solid (96.4 mg, 73%), mp: 112–113 °C.  $^1\text{H}$  NMR (400 MHz, Chloroform-*d*)  $\delta$  8.57 (s, 1H), 7.71 (d,  $J = 8.1$  Hz, 1H), 7.59 – 7.53 (m, 3H), 7.35 – 7.28 (m, 2H), 7.15 (d,  $J = 8.1$  Hz, 2H), 3.73 (s, 3H);  $^{13}\text{C}\{^1\text{H}\}$  NMR (100 MHz, Chloroform-*d*)  $\delta$  154.3, 150.7, 138.6, 135.9, 132.8, 132.6, 131.7, 130.9, 130.7, 129.4 (q,  $J_{\text{C-F}} = 306.6$  Hz), 128.0, 127.7 (q,  $J_{\text{C-F}} = 3.5$  Hz), 123.9, 122.4, 113.5, 29.3;  $^{19}\text{F}$  NMR (376 MHz, Chloroform-*d*)  $\delta$  -42.09; HRMS (ESI):  $m/z$   $[\text{M}+\text{H}]^+$  calcd for  $\text{C}_{18}\text{H}_{13}\text{BrF}_3\text{N}_2\text{OS}$ : 440.9879; found: 440.9882.



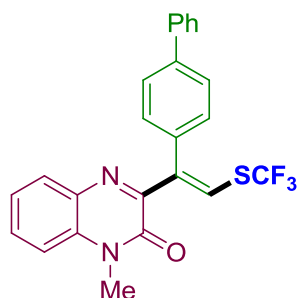
**(E)-1-methyl-3-(1-(4-(trifluoromethyl)phenyl)-2-((trifluoromethyl)thio)vinyl)quinoxalin-2(1H)-one (3ah):**

White solid (86.4 mg, 67%), mp: 127–128 °C.  $^1\text{H}$  NMR (400 MHz, Chloroform-*d*)  $\delta$  8.69 (s, 1H), 7.73 – 7.66 (m, 3H), 7.57 (t,  $J = 7.8$  Hz, 1H), 7.40 (d,  $J = 7.8$  Hz, 2H), 7.31 (t,  $J = 7.6$  Hz, 2H), 3.75 (s, 3H);  $^{13}\text{C}\{^1\text{H}\}$  NMR (100 MHz, Chloroform-*d*)  $\delta$  154.3, 150.4, 140.7, 138.5, 132.8, 132.5, 131.0, 130.7, 129.6, 129.4 (q,  $J_{\text{C-F}} = 306.8$  Hz), 128.3 (q,  $J_{\text{C-F}} = 3.2$  Hz), 125.5 (q,  $J_{\text{C-F}} = 3.6$  Hz), 123.9, 121.4 (q,  $J_{\text{C-F}} = 270.5$  Hz), 113.5, 29.3;  $^{19}\text{F}$  NMR (376 MHz, Chloroform-*d*)  $\delta$  -42.06, -62.57; HRMS (ESI):  $m/z$   $[\text{M}+\text{H}]^+$  calcd for  $\text{C}_{19}\text{H}_{13}\text{F}_6\text{N}_2\text{OS}$ : 431.0647; found: 431.0653.



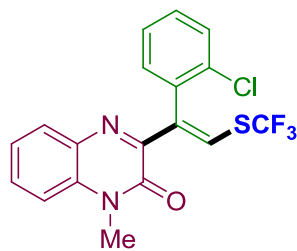
**(E)-3-(1-(4-carbomethoxy)-2-((trifluoromethyl)thio)vinyl)-1-methylquinoxalin-2(1H)-one (3ai):**

White solid (93.3 mg, 74%), mp: 133–134 °C. <sup>1</sup>H NMR (400 MHz, Chloroform-*d*) δ 8.61 (s, 1H), 8.09 (d, *J* = 8.0 Hz, 2H), 7.65 (d, *J* = 7.9 Hz, 1H), 7.54 (t, *J* = 7.8 Hz, 1H), 7.35 – 7.28 (m, 4H), 3.92 (s, 3H), 3.71 (s, 3H); <sup>13</sup>C{<sup>1</sup>H} NMR (100 MHz, Chloroform-*d*) δ 166.7, 154.3, 150.5, 141.8, 138.9, 132.8, 132.5, 130.9, 130.7, 129.8, 129.8, 129.4 (q, *J*<sub>C-F</sub> = 306.5 Hz), 129.2, 127.9 (q, *J*<sub>C-F</sub> = 3.4 Hz), 123.9, 113.5, 52.1, 29.2; <sup>19</sup>F NMR (376 MHz, Chloroform-*d*) δ -42.09; HRMS (ESI): *m/z* [M+H]<sup>+</sup> calcd for C<sub>20</sub>H<sub>16</sub>F<sub>3</sub>N<sub>2</sub>O<sub>3</sub>S: 421.0828; found: 421.0833.



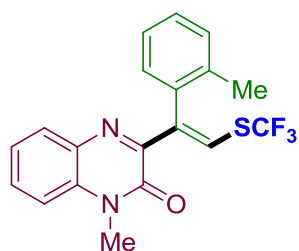
**(E)-3-(1-([1,1'-biphenyl]-4-yl)-2-((trifluoromethyl)thio)vinyl)-1-methylquinoxalin-2(1H)-one (3aj):**

White solid (94.6 mg, 72%), mp: 125–126 °C. <sup>1</sup>H NMR (400 MHz, Chloroform-*d*) δ 8.48 (s, 1H), 7.76 (d, *J* = 8.3 Hz, 1H), 7.72 – 7.64 (m, 4H), 7.56 (t, *J* = 7.8 Hz, 1H), 7.47 (t, *J* = 7.5 Hz, 2H), 7.40 – 7.31 (m, 5H), 3.74 (s, 3H); <sup>13</sup>C{<sup>1</sup>H} NMR (100 MHz, Chloroform-*d*) δ 154.4, 151.5, 140.9, 140.6, 139.4, 135.9, 132.9, 132.7, 130.8, 130.7, 129.5, 129.3 (q, *J*<sub>C-F</sub> = 306.6 Hz), 128.8, 127.4, 127.2, 127.1, 126.9 (q, *J*<sub>C-F</sub> = 3.4 Hz), 123.8, 113.5, 29.3; <sup>19</sup>F NMR (376 MHz, Chloroform-*d*) δ -42.16; HRMS (ESI): *m/z* [M+H]<sup>+</sup> calcd for C<sub>24</sub>H<sub>18</sub>F<sub>3</sub>N<sub>2</sub>OS: 439.1086; found: 439.1089.

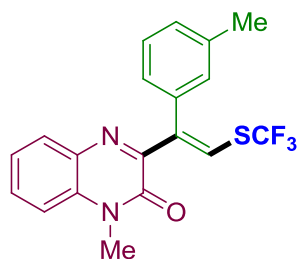


**(E)-3-(1-(2-chlorophenyl)-2-((trifluoromethyl)thio)vinyl)-1-methylquinoxalin-2(1H)-one (3ak):**

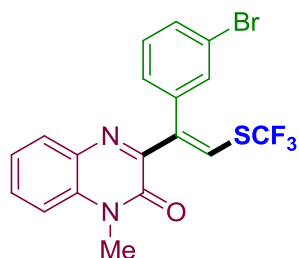
White solid (74.8 mg, 63%), mp: 68–69 °C. <sup>1</sup>H NMR (400 MHz, Chloroform-*d*) δ 8.86 (s, 1H), 7.54 (d, *J* = 8.0 Hz, 1H), 7.47 – 7.38 (m, 2H), 7.31 – 7.27 (m, 2H), 7.23 – 7.16 (m, 3H), 3.67 (s, 3H); <sup>13</sup>C{<sup>1</sup>H} NMR (100 MHz, Chloroform-*d*) δ 154.3, 149.2, 137.5, 136.2, 133.4, 132.7, 132.6, 131.0, 130.8, 130.6, 130.0 (q, *J*<sub>C-F</sub> = 3.4 Hz), 129.7, 129.7, 129.2 (q, *J*<sub>C-F</sub> = 306.7 Hz), 127.0, 123.7, 113.4, 29.2; <sup>19</sup>F NMR (376 MHz, Chloroform-*d*) δ -41.78; HRMS (ESI): *m/z* [M+H]<sup>+</sup> calcd for C<sub>18</sub>H<sub>13</sub>ClF<sub>3</sub>N<sub>2</sub>OS: 397.0384; found: 397.0389.



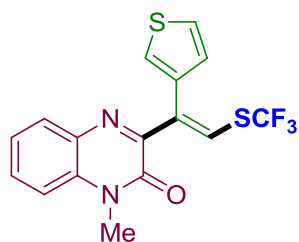
**(E)-1-methyl-3-(1-(o-tolyl)-2-((trifluoromethyl)thio)vinyl)quinoxalin-2(1H)-one (3al):** White solid (75.6 mg, 67%), mp: 61–62 °C.  $^1\text{H}$  NMR (400 MHz, Chloroform-*d*)  $\delta$  8.81 (s, 1H), 7.54 (d,  $J$  = 8.0 Hz, 1H), 7.43 (t,  $J$  = 7.8 Hz, 1H), 7.25 – 7.14 (m, 5H), 7.03 (d,  $J$  = 7.4 Hz, 1H), 3.67 (s, 3H), 2.08 (s, 3H);  $^{13}\text{C}\{^1\text{H}\}$  NMR (100 MHz, Chloroform-*d*)  $\delta$  154.5, 149.6, 139.3, 137.0, 136.4, 132.8, 132.5, 130.8, 130.5, 130.2, 129.4 (q,  $J_{\text{C-F}}$  = 3.4 Hz), 129.3 (q,  $J_{\text{C-F}}$  = 306.5 Hz), 129.2, 128.4, 126.0, 123.7, 113.4, 29.2, 19.4;  $^{19}\text{F}$  NMR (376 MHz, Chloroform-*d*)  $\delta$  -41.96; HRMS (ESI):  $m/z$   $[\text{M}+\text{H}]^+$  calcd for  $\text{C}_{19}\text{H}_{16}\text{F}_3\text{N}_2\text{OS}$ : 377.0930; found: 377.0931.



**(E)-1-methyl-3-(1-(m-tolyl)-2-((trifluoromethyl)thio)vinyl)quinoxalin-2(1H)-one (3am):** White solid (80.1 mg, 71%), mp: 84–85 °C.  $^1\text{H}$  NMR (400 MHz, Chloroform-*d*)  $\delta$  8.40 (s, 1H), 7.75 (d,  $J$  = 8.0 Hz, 1H), 7.55 (t,  $J$  = 7.7 Hz, 1H), 7.36 – 7.28 (m, 3H), 7.21 (d,  $J$  = 7.6 Hz, 1H), 7.11 – 7.07 (m, 2H), 3.73 (s, 3H), 2.39 (s, 3H);  $^{13}\text{C}\{^1\text{H}\}$  NMR (100 MHz, Chloroform-*d*)  $\delta$  154.4, 151.6, 139.8, 138.1, 136.9, 132.9, 132.7, 130.7, 130.6, 129.5, 129.4 (q,  $J_{\text{C-F}}$  = 306.6 Hz), 129.1, 128.3, 126.6 (q,  $J_{\text{C-F}}$  = 3.4 Hz), 126.0, 123.7, 113.4, 29.2, 21.5;  $^{19}\text{F}$  NMR (376 MHz, Chloroform-*d*)  $\delta$  -42.24; HRMS (ESI):  $m/z$   $[\text{M}+\text{H}]^+$  calcd for  $\text{C}_{19}\text{H}_{16}\text{F}_3\text{N}_2\text{OS}$ : 377.0930; found: 377.0933.

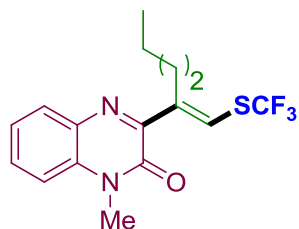


**(E)-3-(1-(3-bromophenyl)-2-((trifluoromethyl)thio)vinyl)-1-methylquinoxalin-2(1H)-one (3an):** White solid (89.8 mg, 68%), mp: 86–87 °C.  $^1\text{H}$  NMR (400 MHz, Chloroform-*d*)  $\delta$  8.62 (s, 1H), 7.70 (d,  $J$  = 8.1 Hz, 1H), 7.59 – 7.51 (m, 2H), 7.42 (s, 1H), 7.36 – 7.28 (m, 3H), 7.22 (d,  $J$  = 7.6 Hz, 1H), 3.73 (s, 3H);  $^{13}\text{C}\{^1\text{H}\}$  NMR (100 MHz, Chloroform-*d*)  $\delta$  154.3, 150.5, 139.0, 138.3, 132.7, 132.5, 132.0, 131.3, 130.9, 130.8, 130.0, 129.1 (q,  $J_{\text{C-F}}$  = 306.7 Hz), 128.2 (q,  $J_{\text{C-F}}$  = 3.4 Hz), 127.9, 123.9, 122.4, 113.5, 29.3;  $^{19}\text{F}$  NMR (376 MHz, Chloroform-*d*)  $\delta$  -42.05; HRMS (ESI):  $m/z$   $[\text{M}+\text{H}]^+$  calcd for  $\text{C}_{18}\text{H}_{13}\text{BrF}_3\text{N}_2\text{OS}$ : 440.9879; found: 440.9886.

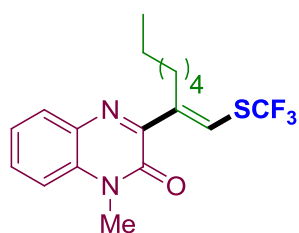


**(E)-1-methyl-3-(1-(thiophen-3-yl)-2-((trifluoromethyl)thio)vinyl)quinoxalin-2(1H)-one (3ao):**

White solid (86.1 mg, 78%), mp: 83–84 °C.  $^1\text{H}$  NMR (400 MHz, Chloroform-*d*)  $\delta$  8.43 (s, 1H), 7.75 (d,  $J = 8.1$  Hz, 1H), 7.56 (t,  $J = 7.8$  Hz, 1H), 7.43 – 7.28 (m, 4H), 7.08 (d,  $J = 4.9$  Hz, 1H), 3.73 (s, 3H);  $^{13}\text{C}\{^1\text{H}\}$  NMR (100 MHz, Chloroform-*d*)  $\delta$  154.2, 151.1, 136.8, 134.5, 132.8, 132.5, 130.7, 130.6, 129.3 (q,  $J_{\text{C-F}} = 306.8$  Hz), 128.4, 127.3 (q,  $J_{\text{C-F}} = 3.4$  Hz), 125.4, 125.0, 123.8, 113.5, 29.2;  $^{19}\text{F}$  NMR (376 MHz, Chloroform-*d*)  $\delta$  -42.30; HRMS (ESI):  $m/z$   $[\text{M}+\text{H}]^+$  calcd for  $\text{C}_{16}\text{H}_{12}\text{F}_3\text{N}_2\text{OS}_2$ : 369.0338; found: 369.0334.

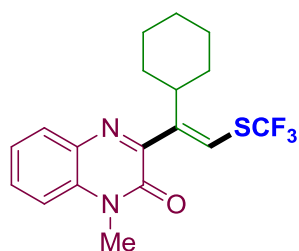


**(E)-1-methyl-3-(1-((trifluoromethyl)thio)hex-1-en-2-yl)quinoxalin-2(1H)-one (3ap):** White solid (79.0 mg, 77%), mp: 87–88 °C.  $^1\text{H}$  NMR (400 MHz, Chloroform-*d*)  $\delta$  8.49 (s, 1H), 7.84 (d,  $J = 8.0$  Hz, 1H), 7.55 (t,  $J = 7.8$  Hz, 1H), 7.35 (t,  $J = 7.6$  Hz, 1H), 7.29 (d,  $J = 8.4$  Hz, 1H), 3.71 (s, 3H), 2.80 – 2.66 (m, 2H), 1.52 – 1.36 (m, 4H), 0.94 (t,  $J = 7.2$  Hz, 3H);  $^{13}\text{C}\{^1\text{H}\}$  NMR (100 MHz, Chloroform-*d*)  $\delta$  154.5, 149.9, 140.0, 132.7, 132.5, 131.0, 130.4, 129.4 (q,  $J_{\text{C-F}} = 305.8$  Hz), 127.9, 124.8 (q,  $J_{\text{C-F}} = 3.4$  Hz), 123.7, 30.5, 30.1, 29.2, 22.7, 13.9;  $^{19}\text{F}$  NMR (376 MHz, Chloroform-*d*)  $\delta$  -41.81; HRMS (ESI):  $m/z$   $[\text{M}+\text{H}]^+$  calcd for  $\text{C}_{16}\text{H}_{18}\text{F}_3\text{N}_2\text{OS}$ : 343.1086; found: 343.1088.

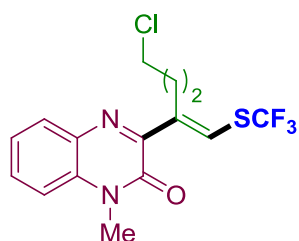


**(E)-1-methyl-3-(1-((trifluoromethyl)thio)oct-1-en-2-yl)quinoxalin-2(1H)-one (3aq):** White solid (78.8 mg, 71%), mp: 76–77 °C.  $^1\text{H}$  NMR (400 MHz, Chloroform-*d*)  $\delta$  8.48 (s, 1H), 7.85 (d,  $J = 8.0$  Hz, 1H), 7.56 (t,  $J = 7.8$  Hz, 1H), 7.41 – 7.28 (m, 2H), 3.73 (s, 3H), 2.85 – 2.64 (m, 2H), 1.54 – 1.46 (m, 2H), 1.43 – 1.27 (m, 6H), 0.89 (t,  $J = 6.4$  Hz, 3H);  $^{13}\text{C}\{^1\text{H}\}$  NMR (100 MHz, Chloroform-*d*)  $\delta$  154.5, 150.0, 140.1, 132.7, 132.6, 130.5, 130.4, 129.4 (q,  $J_{\text{C-F}} = 305.6$  Hz), 124.9 (q,  $J_{\text{C-F}} = 3.4$  Hz), 123.7, 113.5, 31.5, 30.9, 29.2, 29.2, 27.8, 22.5, 14.1;  $^{19}\text{F}$  NMR (376 MHz, Chloroform-*d*)  $\delta$  -41.81; HRMS (ESI):  $m/z$   $[\text{M}+\text{H}]^+$  calcd for  $\text{C}_{18}\text{H}_{22}\text{F}_3\text{N}_2\text{OS}$ : 371.1399; found: 371.1404.

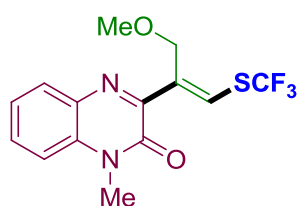




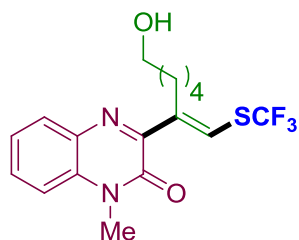
**(E)-3-(1-cyclohexyl-2-((trifluoromethyl)thio)vinyl)-1-methylquinoxalin-2(1H)-one (3ar):** White solid (67.4 mg, 61%), mp: 92–93 °C.  $^1\text{H}$  NMR (400 MHz, Chloroform-*d*)  $\delta$  7.87 (d,  $J$  = 8.0 Hz, 1H), 7.57 (t,  $J$  = 7.8 Hz, 1H), 7.36 (t,  $J$  = 7.6 Hz, 1H), 7.30 (d,  $J$  = 8.4 Hz, 1H), 7.26 (s, 1H), 3.71 (s, 3H), 2.75 – 2.66 (m, 1H), 1.90 – 1.73 (m, 6H), 1.37 – 1.20 (m, 4H);  $^{13}\text{C}\{^1\text{H}\}$  NMR (100 MHz, Chloroform-*d*)  $\delta$  154.4, 154.3, 144.7, 133.0, 132.3, 130.5, 130.4, 129.4 (q,  $J_{\text{C-F}}$  = 306.0 Hz), 123.7, 119.8 (q,  $J_{\text{C-F}}$  = 3.4 Hz), 113.5, 43.3, 30.1, 29.3, 26.7, 25.9;  $^{19}\text{F}$  NMR (376 MHz, Chloroform-*d*)  $\delta$  -42.14; HRMS (ESI):  $m/z$   $[\text{M}+\text{H}]^+$  calcd for  $\text{C}_{18}\text{H}_{20}\text{F}_3\text{N}_2\text{OS}$ : 369.1243; found: 369.1246.



**(E)-3-(5-chloro-1-((trifluoromethyl)thio)pent-1-en-2-yl)-1-methylquinoxalin-2(1H)-one (3as):** Yellow oil (79.7 mg, 73%).  $^1\text{H}$  NMR (400 MHz, Chloroform-*d*)  $\delta$  8.67 (s, 1H), 7.85 (d,  $J$  = 8.0 Hz, 1H), 7.57 (t,  $J$  = 7.8 Hz, 1H), 7.41 – 7.29 (m, 2H), 3.73 (s, 3H), 3.61 (t,  $J$  = 6.6 Hz, 2H), 2.95 – 2.83 (m, 2H), 2.08 – 1.99 (m, 2H);  $^{13}\text{C}\{^1\text{H}\}$  NMR (100 MHz, Chloroform-*d*)  $\delta$  154.5, 149.3, 137.9, 132.7, 132.5, 130.7, 130.5, 129.3 (q,  $J_{\text{C-F}}$  = 305.9 Hz), 126.6 (q,  $J_{\text{C-F}}$  = 3.4 Hz), 123.9, 113.5, 44.8, 30.9, 29.3, 28.4;  $^{19}\text{F}$  NMR (376 MHz, Chloroform-*d*)  $\delta$  -41.71; HRMS (ESI):  $m/z$   $[\text{M}+\text{H}]^+$  calcd for  $\text{C}_{15}\text{H}_{17}\text{ClF}_3\text{N}_2\text{OS}$ : 365.0697; found: 365.0692.

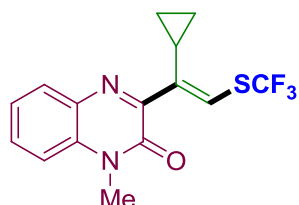


**(E)-3-(3-methoxy-1-((trifluoromethyl)thio)prop-1-en-2-yl)-1-methylquinoxalin-2(1H)-one (3at):** White solid (67.3 mg, 68%), mp: 108–109 °C.  $^1\text{H}$  NMR (400 MHz, Chloroform-*d*)  $\delta$  8.73 (s, 1H), 7.83 (d,  $J$  = 8.0 Hz, 1H), 7.55 (t,  $J$  = 7.8 Hz, 1H), 7.35 (t,  $J$  = 7.6 Hz, 1H), 7.30 (d,  $J$  = 8.4 Hz, 1H), 4.71 (s, 2H), 3.72 (s, 3H), 3.40 (s, 3H);  $^{13}\text{C}\{^1\text{H}\}$  NMR (100 MHz, Chloroform-*d*)  $\delta$  154.2, 149.6, 134.3, 132.7, 132.4, 130.5, 130.4, 129.4 (q,  $J_{\text{C-F}}$  = 306.6 Hz), 128.9 (q,  $J_{\text{C-F}}$  = 3.4 Hz), 123.8, 113.5, 70.1, 58.2, 29.2;  $^{19}\text{F}$  NMR (376 MHz, Chloroform-*d*)  $\delta$  -44.04; HRMS (ESI):  $m/z$   $[\text{M}+\text{H}]^+$  calcd for  $\text{C}_{14}\text{H}_{14}\text{F}_3\text{N}_2\text{O}_2\text{S}$ : 331.0723; found: 331.0727.



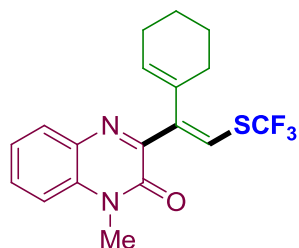
**(E)-3-(4-hydroxy-1-((trifluoromethyl)thio)but-1-en-2-yl)-1-methylquinoxalin-2(1H)-one (3au):**

White solid (82.6 mg, 74%), mp: 123–124 °C. <sup>1</sup>H NMR (400 MHz, Chloroform-*d*) δ 8.50 (s, 1H), 7.84 (d, *J* = 8.0 Hz, 1H), 7.56 (t, *J* = 7.8 Hz, 1H), 7.36 (t, *J* = 7.6 Hz, 1H), 7.30 (d, *J* = 8.4 Hz, 1H), 3.72 (s, 3H), 3.65 (t, *J* = 6.5 Hz, 2H), 2.85 – 2.64 (m, 2H), 1.66 – 1.45 (m, 6H); <sup>13</sup>C{<sup>1</sup>H} NMR (100 MHz, Chloroform-*d*) δ 154.5, 149.8, 139.7, 132.7, 132.5, 130.5, 130.4, 129.4 (q, *J*<sub>C-F</sub> = 305.7 Hz), 125.1 (q, *J*<sub>C-F</sub> = 3.4 Hz), 123.8, 113.5, 62.8, 32.4, 30.7, 29.2, 27.6, 25.6; <sup>19</sup>F NMR (376 MHz, Chloroform-*d*) δ -41.77; HRMS (ESI): *m/z* [M+H]<sup>+</sup> calcd for C<sub>17</sub>H<sub>20</sub>F<sub>3</sub>N<sub>2</sub>OS: 373.1192; found: 373.1188.



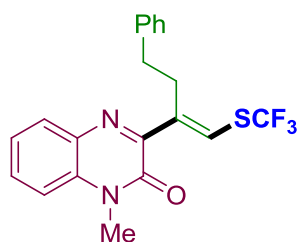
**(E)-3-(1-cyclopropyl-2-((trifluoromethyl)thio)vinyl)-1-methylquinoxalin-2(1H)-one (3av):**

White solid (62.6 mg, 64%), mp: 81–82 °C. <sup>1</sup>H NMR (400 MHz, Chloroform-*d*) δ 7.86 (d, *J* = 7.9 Hz, 1H), 7.69 (s, 1H), 7.56 (t, *J* = 7.7 Hz, 1H), 7.39 – 7.28 (m, 2H), 3.72 (s, 3H), 2.01 – 1.91 (m, 1H), 0.96 – 0.87 (m, 2H), 0.57 – 0.49 (m, 2H); <sup>13</sup>C{<sup>1</sup>H} NMR (100 MHz, Chloroform-*d*) δ 154.1, 153.6, 139.2, 133.0, 132.6, 130.4, 130.4, 129.5 (q, *J*<sub>C-F</sub> = 305.8 Hz), 125.8 (q, *J*<sub>C-F</sub> = 3.2 Hz), 123.8, 113.6, 29.2, 12.9, 7.2; <sup>19</sup>F NMR (376 MHz, Chloroform-*d*) δ -42.01; HRMS (ESI): *m/z* [M+H]<sup>+</sup> calcd for C<sub>15</sub>H<sub>14</sub>F<sub>3</sub>N<sub>2</sub>OS: 327.0773; found: 327.0779.



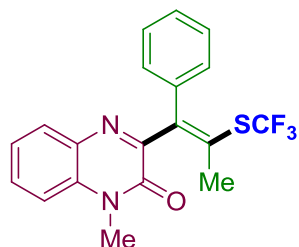
**(E)-3-(1-(cyclohex-1-en-1-yl)-2-((trifluoromethyl)thio)vinyl)-1-methylquinoxalin-2(1H)-one (3aw):**

White solid (79.1 mg, 72%), mp: 102–103 °C. <sup>1</sup>H NMR (400 MHz, Chloroform-*d*) δ 8.39 (s, 1H), 7.83 (d, *J* = 7.9 Hz, 1H), 7.54 (t, *J* = 7.7 Hz, 1H), 7.37 – 7.27 (m, 2H), 5.72 (s, 1H), 3.72 (s, 3H), 2.26 – 2.11 (m, 4H), 1.80 – 1.68 (m, 4H); <sup>13</sup>C{<sup>1</sup>H} NMR (100 MHz, Chloroform-*d*) δ 154.4, 149.8, 141.7, 137.2, 132.7, 132.6, 130.6, 130.4, 129.6 (q, *J*<sub>C-F</sub> = 306.9 Hz), 129.3, 126.2 (q, *J*<sub>C-F</sub> = 3.4 Hz), 123.7, 113.4, 29.2, 27.6, 22.7, 22.0; <sup>19</sup>F NMR (376 MHz, Chloroform-*d*) δ -42.65; HRMS (ESI): *m/z* [M+H]<sup>+</sup> calcd for C<sub>18</sub>H<sub>18</sub>F<sub>3</sub>N<sub>2</sub>OS: 367.1086; found: 367.1094.



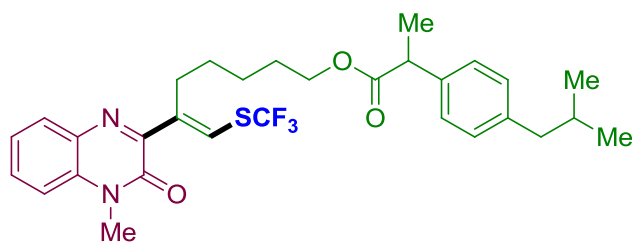
**(E)-1-methyl-3-(4-phenyl-1-((trifluoromethyl)thio)but-1-en-2-yl)quinoxalin-2(1H)-one (3ax):**

White solid (91.3 mg, 78%), mp: 100–101 °C. <sup>1</sup>H NMR (400 MHz, Chloroform-*d*) δ 8.67 (s, 1H), 7.90 (d, *J* = 8.0 Hz, 1H), 7.58 (t, *J* = 7.8 Hz, 1H), 7.39 (t, *J* = 7.6 Hz, 1H), 7.35 – 7.27 (m, 5H), 7.23 – 7.17 (m, 1H), 3.74 (s, 3H), 3.08 – 3.01 (m, 2H), 2.88 – 2.80 (m, 2H); <sup>13</sup>C{<sup>1</sup>H} NMR (100 MHz, Chloroform-*d*) δ 154.4, 149.3, 141.6, 138.7, 132.7, 132.5, 130.5, 130.5, 129.4 (q, *J*<sub>C-F</sub> = 305.7 Hz), 128.5, 128.3, 126.1 (q, *J*<sub>C-F</sub> = 3.4 Hz), 126.0, 123.8, 113.5, 34.1, 33.3, 29.2; <sup>19</sup>F NMR (376 MHz, Chloroform-*d*) δ -41.71; HRMS (ESI): *m/z* [M+H]<sup>+</sup> calcd for C<sub>20</sub>H<sub>18</sub>F<sub>3</sub>N<sub>2</sub>OS: 391.1086; found: 391.1089.



**(E)-1-methyl-3-(1-phenyl-2-((trifluoromethyl)thio)prop-1-en-1-yl)quinoxalin-2(1H)-one (3ay):**

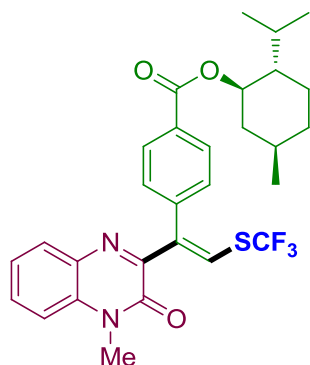
White solid (69.9 mg, 62%), mp: 126–127 °C. <sup>1</sup>H NMR (400 MHz, Chloroform-*d*) δ 7.95 (d, *J* = 8.0 Hz, 1H), 7.59 (t, *J* = 7.8 Hz, 1H), 7.45 (d, *J* = 7.3 Hz, 2H), 7.42 – 7.29 (m, 5H), 3.66 (s, 3H), 2.26 (s, 3H); <sup>13</sup>C{<sup>1</sup>H} NMR (100 MHz, Chloroform-*d*) δ 156.8, 153.5, 144.5, 137.5, 133.4, 132.7, 130.9, 130.5, 129.3, 129.2 (q, *J*<sub>C-F</sub> = 307.7 Hz), 128.2, 128.1, 127.5, 123.9, 113.7, 29.2, 22.3; <sup>19</sup>F NMR (376 MHz, Chloroform-*d*) δ -37.82; HRMS (ESI): *m/z* [M+H]<sup>+</sup> calcd for C<sub>19</sub>H<sub>16</sub>F<sub>3</sub>N<sub>2</sub>OS: 377.0930; found: 377.0934.



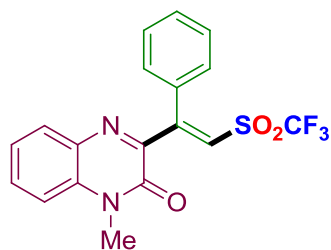
**(E)-6-(4-methyl-3-oxo-3,4-dihydroquinoxalin-2-yl)-7-((trifluoromethyl)thio)hept-6-en-1-yl**

**2-(4-isobutylphenyl)propanoate (4aa):** White solid (124.4 mg, 74%), mp: 96–97 °C. <sup>1</sup>H NMR (400 MHz, Chloroform-*d*) δ 8.52 (s, 1H), 7.80 (d, *J* = 7.9 Hz, 1H), 7.53 (t, *J* = 7.7 Hz, 1H), 7.39 – 7.25 (m, 2H), 7.17 (d, *J* = 7.2 Hz, 2H), 7.05 (d, *J* = 7.2 Hz, 2H), 4.04 (d, *J* = 6.0 Hz, 2H), 3.73 – 3.60 (m, 4H), 2.73 – 2.60 (m, 2H), 2.40 (d, *J* = 6.8 Hz, 2H), 1.84 – 1.75 (m, 1H), 1.66 – 1.55 (m, 2H), 1.52 – 1.41 (m, 5H), 1.37 – 1.30 (m, 2H), 0.85 (d, *J* = 6.1 Hz, 6H); <sup>13</sup>C{<sup>1</sup>H} NMR (100 MHz, Chloroform-*d*) δ 174.7, 154.4, 149.6, 140.4, 139.5, 137.8, 132.7, 132.5, 130.5, 130.4, 129.4 (q, *J*<sub>C-F</sub> = 305.8 Hz), 129.2, 127.1, 125.2 (q, *J*<sub>C-F</sub> = 3.3 Hz), 123.7, 113.5, 64.5, 45.1, 45.0, 30.5, 30.1, 29.2, 28.2, 27.3, 25.6, 22.3, 18.4; <sup>19</sup>F NMR (376 MHz,

Chloroform-*d*)  $\delta$  -41.73; HRMS (ESI):  $m/z$   $[M+H]^+$  calcd for  $C_{30}H_{36}F_3N_2O_3S$ : 561.2393; found: 561.2398.



**2-isopropyl-5-methylcyclohexyl-((E)-1-(4-methyl-3-oxo-3,4-dihydroquinoxalin-2-yl)-2-((trifluoromethyl)thio)vinyl)benzoate (4ab)**: White solid (102.9 mg, 63%), mp: 134–135 °C.  $^1H$  NMR (400 MHz, Chloroform-*d*)  $\delta$  8.58 (s, 1H), 8.12 (d,  $J = 7.9$  Hz, 2H), 7.70 (d,  $J = 8.2$  Hz, 1H), 7.56 (t,  $J = 7.7$  Hz, 1H), 7.37 – 7.27 (m, 4H), 4.97 (t,  $J = 10.5$  Hz, 1H), 3.73 (s, 3H), 2.15 (d,  $J = 11.7$  Hz, 1H), 2.08 – 1.97 (m, 1H), 1.74 (d,  $J = 11.4$  Hz, 2H), 1.57 (t,  $J = 10.0$  Hz, 2H), 1.15 (d,  $J = 11.8$  Hz, 2H), 1.01 – 0.87 (m, 7H), 0.82 (d,  $J = 6.8$  Hz, 3H);  $^{13}C\{^1H\}$  NMR (100 MHz, Chloroform-*d*)  $\delta$  165.7, 150.7, 141.6, 139.0, 132.8, 132.6, 130.9, 130.7, 130.5, 129.9, 129.8, 129.4 (q,  $J_{C-F} = 305.9$  Hz), 129.1, 127.7 (q,  $J_{C-F} = 3.5$  Hz), 123.9, 113.5, 74.9, 47.2, 41.0, 34.3, 31.4, 29.3, 26.3, 23.5, 22.0, 20.8, 16.4;  $^{19}F$  NMR (376 MHz, Chloroform-*d*)  $\delta$  -42.09; HRMS (ESI):  $m/z$   $[M+H]^+$  calcd for  $C_{29}H_{32}F_3N_2O_3S$ : 545.2080; found: 545.2086.



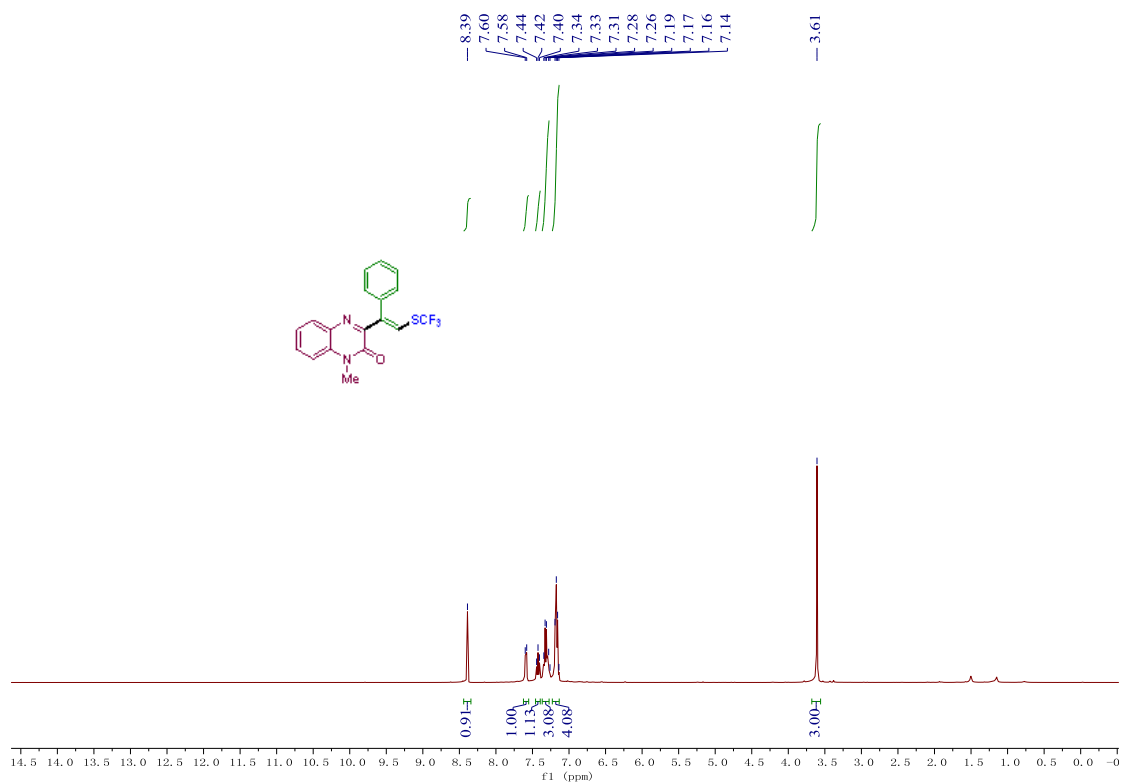
**(E)-1-methyl-3-(1-phenyl-2-((trifluoromethyl)sulfonyl)vinyl)quinoxalin-2(1H)-one (5a)**: White solid (98.1 mg, 83%), mp: 122–123 °C.  $^1H$  NMR (400 MHz, Chloroform-*d*)  $\delta$  8.03 (s, 1H), 7.82 (d,  $J = 7.8$  Hz, 1H), 7.65 (t,  $J = 7.7$  Hz, 1H), 7.49 – 7.41 (m, 3H), 7.40 – 7.29 (m, 4H), 3.72 (s, 3H);  $^{13}C\{^1H\}$  NMR (100 MHz, Chloroform-*d*)  $\delta$  154.7, 153.8, 151.6, 134.6, 133.5, 132.6 (q,  $J_{C-F} = 2.7$  Hz), 132.5, 132.4, 131.4, 129.5, 129.3, 128.3, 125.6 (q,  $J_{C-F} = 332.9$  Hz), 124.1, 113.7, 29.3;  $^{19}F$  NMR (376 MHz, Chloroform-*d*)  $\delta$  -72.01; HRMS (ESI):  $m/z$   $[M+H]^+$  calcd for  $C_{18}H_{14}F_3N_2O_3S$ : 395.0672; found: 395.0675.

## 4. References

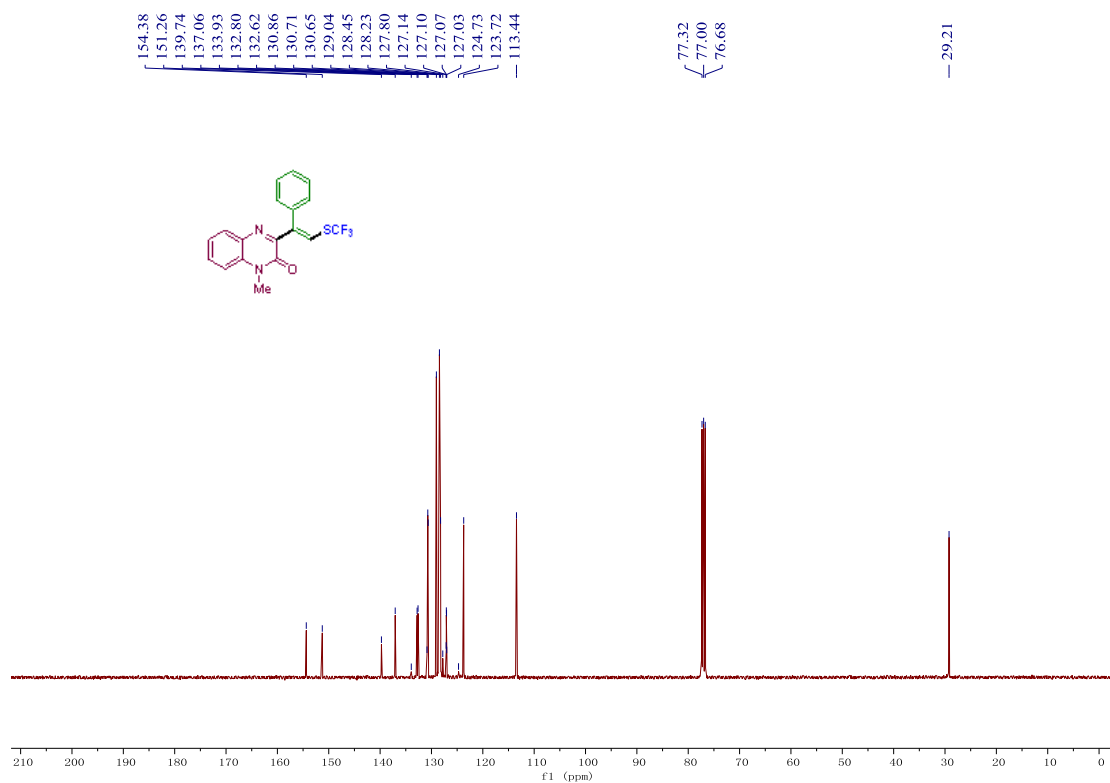
- [1] Frisch, M. J.; Trucks, G.W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Petersson, G. A.; Nakatsuji, H.; Li, X.; Caricato, M.; Marenich, A. V.; Bloino, J.; Janesko, B. G.; Gomperts, R.; Mennucci, B.; Hratchian, H. P.; Ortiz, J. V.; Izmaylov, A. F.; Sonnenberg, J. L.; Williams-Young, D.; Ding, F.; Lipparini, F.; Egidi, F.; Goings, J.; Peng, B.;

- Petrone, A.; Henderson, T.; Ranasinghe, D.; Zakrzewski, V. G.; Gao, J.; Rega, N.; Zheng, G.; Liang, W.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Throssell, K.; Montgomery, J. A. Jr.; Peralta, J. E.; Ogliaro, F.; Bearpark, M. J.; Heyd, J. J.; Brothers, E. N.; Kudin, K. N.; Staroverov, V. N.; Keith, T. A.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A. P.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Millam, J. M.; Klene, M.; Adamo, C.; Cammi, R.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Farkas, O.; Foresman, J. B.; Fox, D. J. Gaussian Inc Wallingford CT, **2016**.
- [2] Marenich, A. V.; Cramer, C. J.; Truhlar, D. G. Universal Solvation Model Based on Solute Electron Density and on a Continuum Model of the Solvent Defined by the Bulk Dielectric Constant and Atomic Surface Tensions. *J. Phys. Chem. B.* **2009**, *113*, 6378–6396.

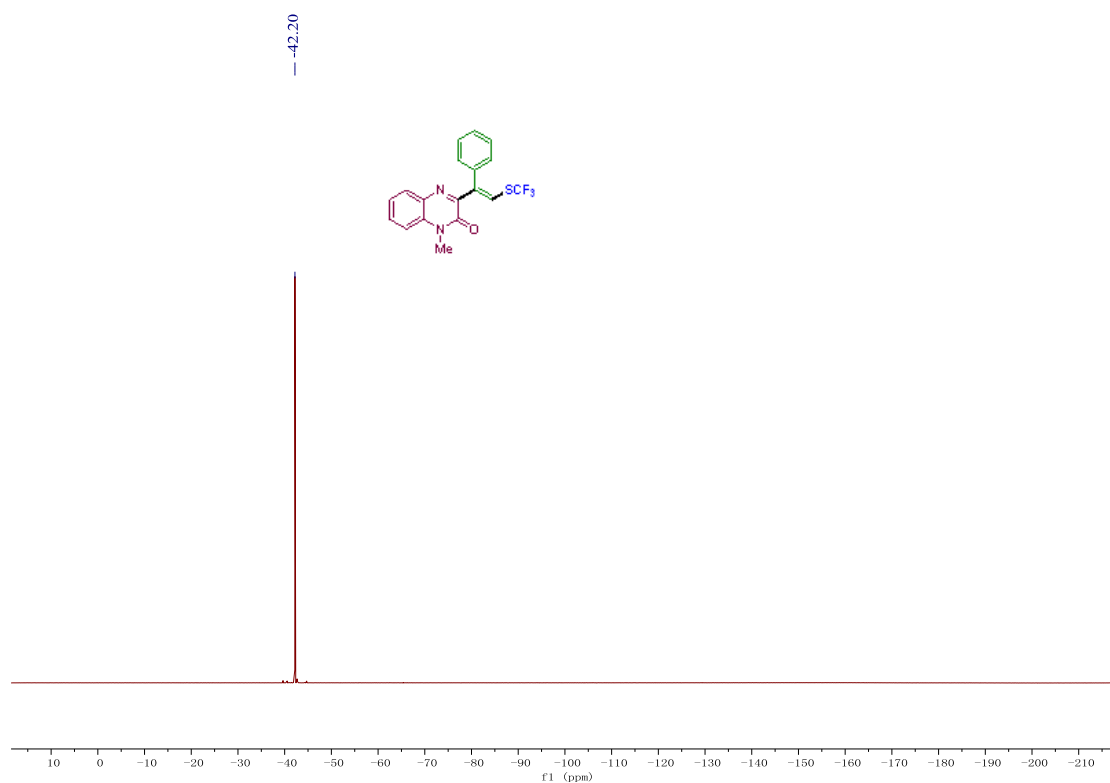
## 5. $^1\text{H}$ , $^{13}\text{C}$ and $^{19}\text{F}$ NMR spectra of products



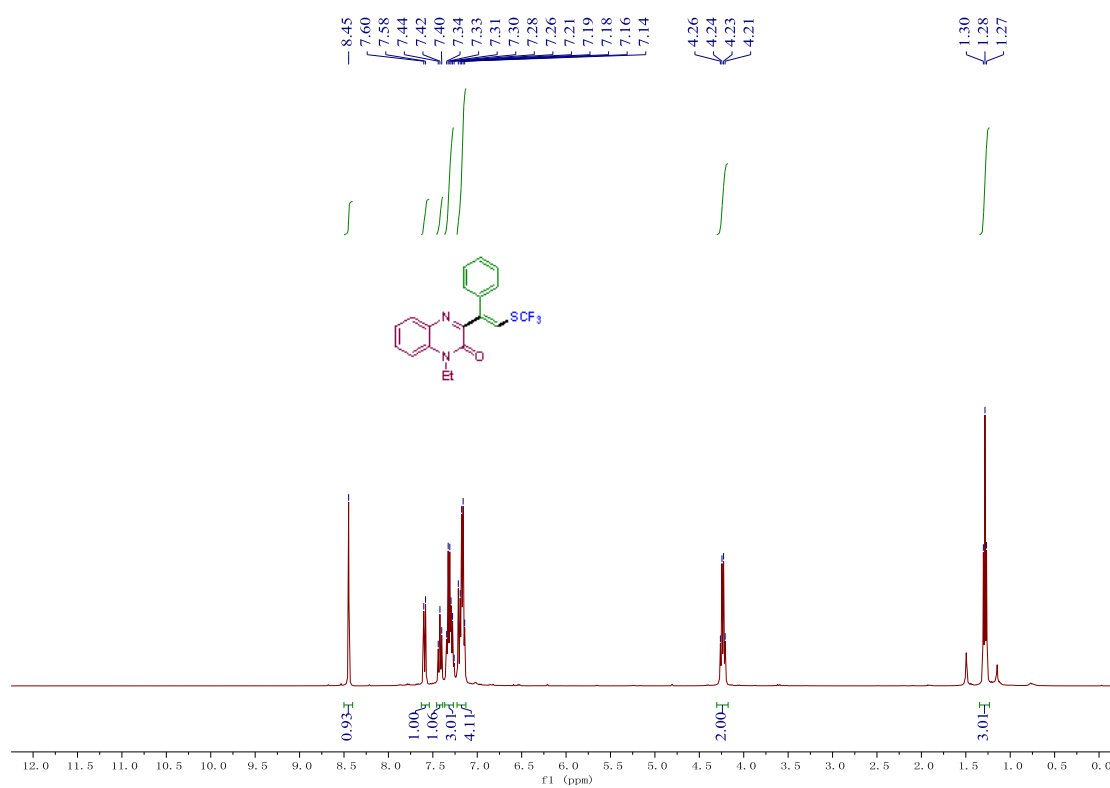
$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ) spectra of **3aa**



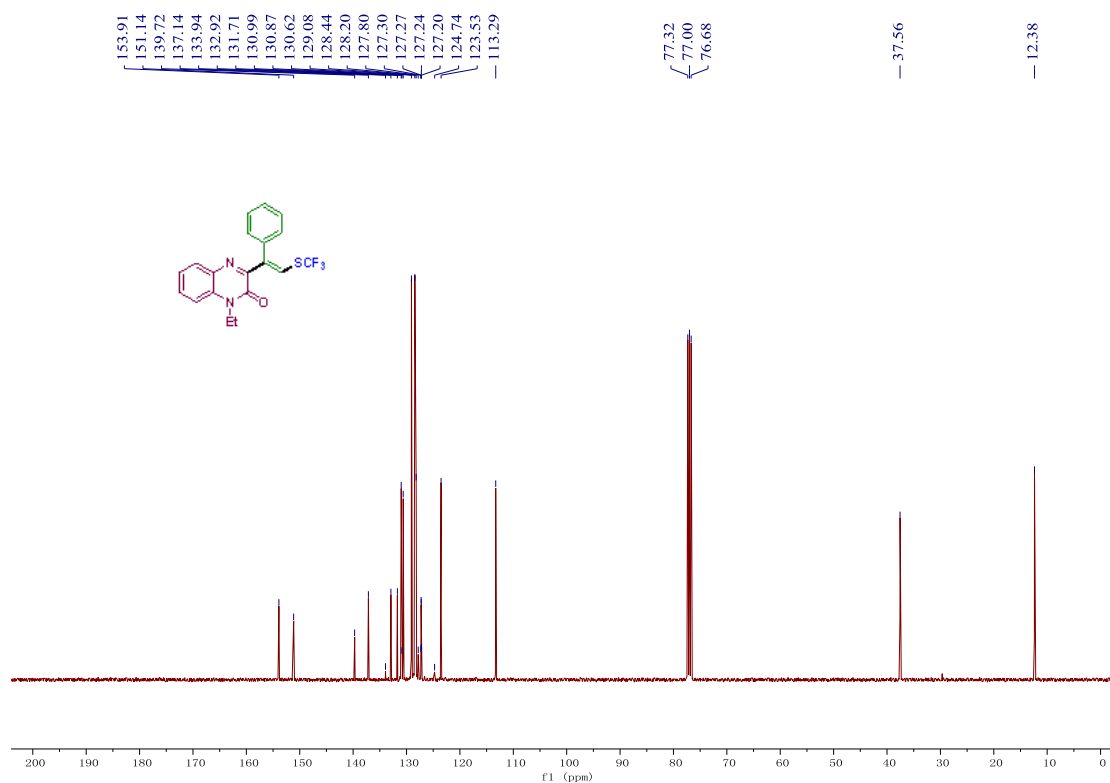
$^{13}\text{C}\{^1\text{H}\}$  NMR (100 MHz,  $\text{CDCl}_3$ ) spectra of **3aa**



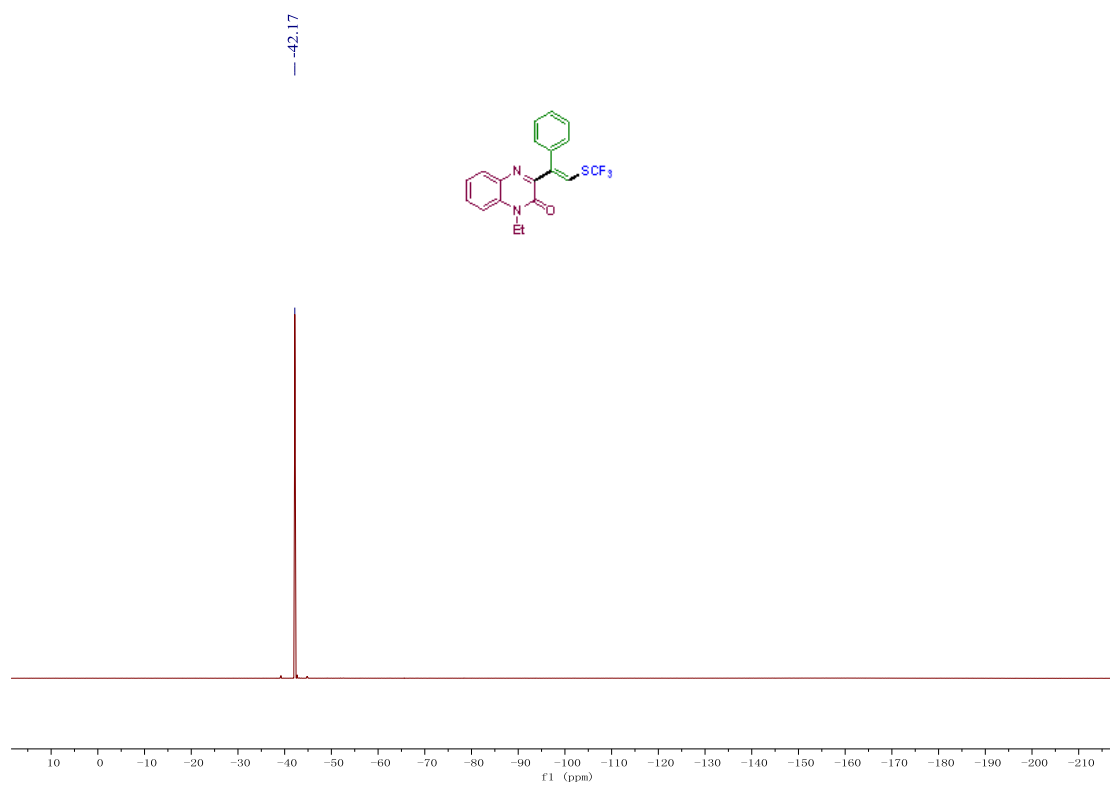
$^{19}\text{F}$  NMR (376 MHz,  $\text{CDCl}_3$ ) spectra of **3aa**



$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ) spectra of **3ba**

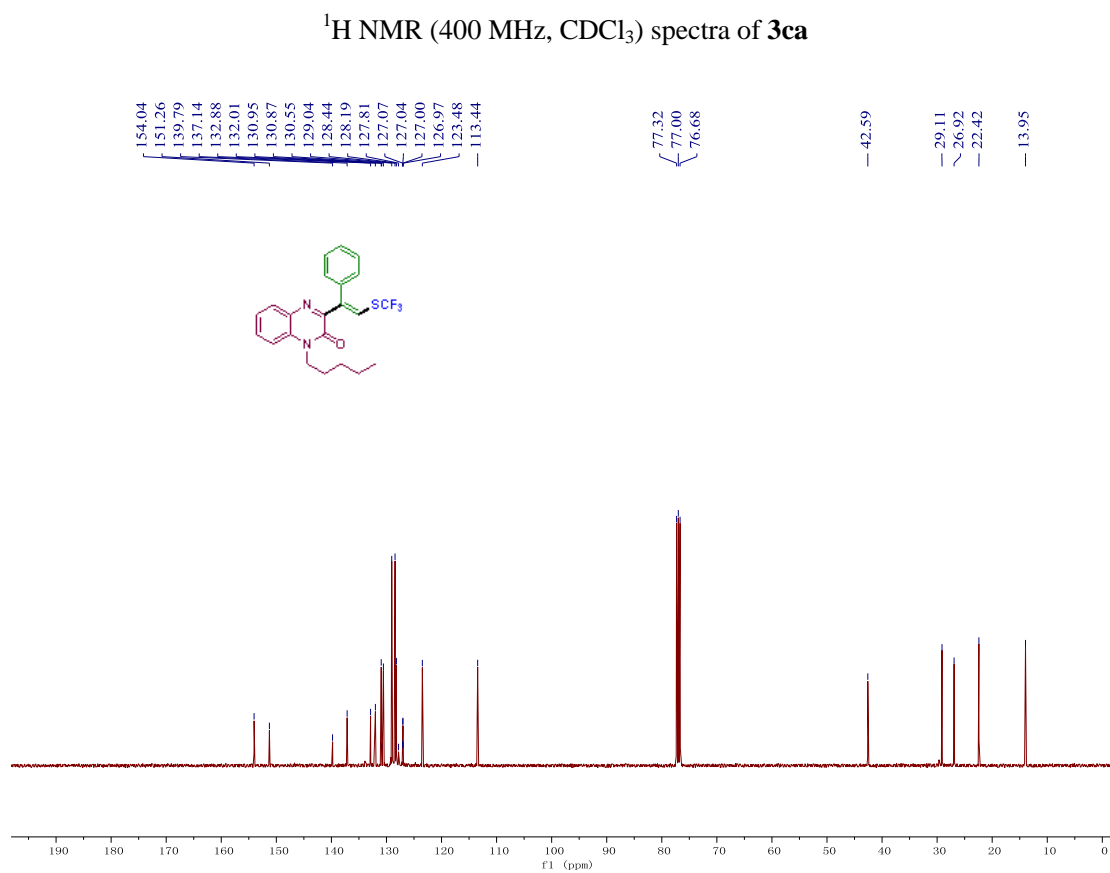
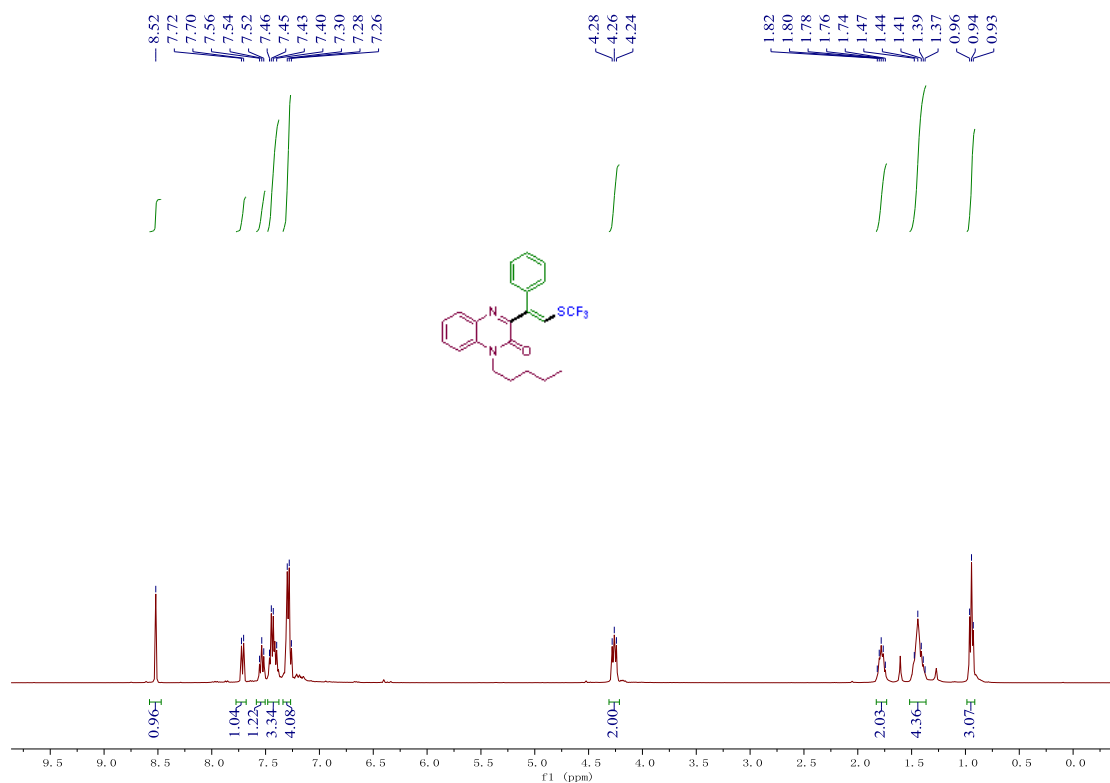


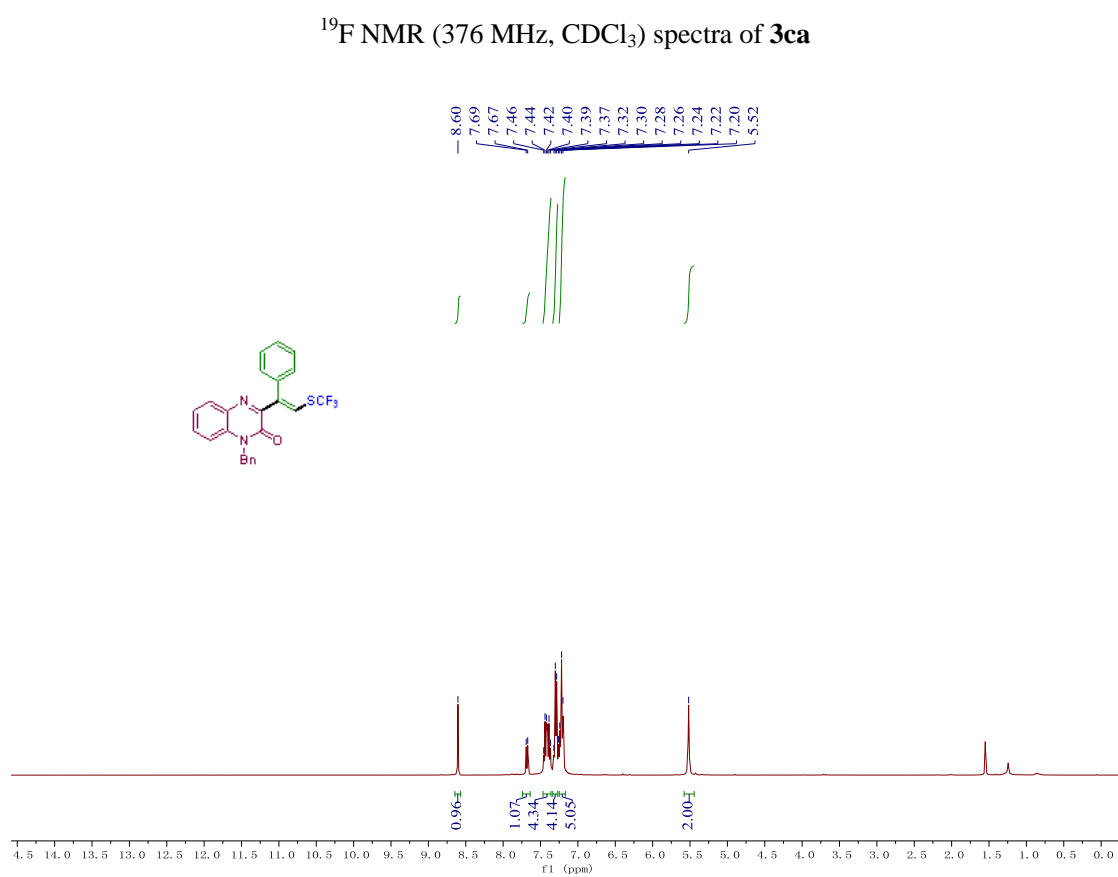
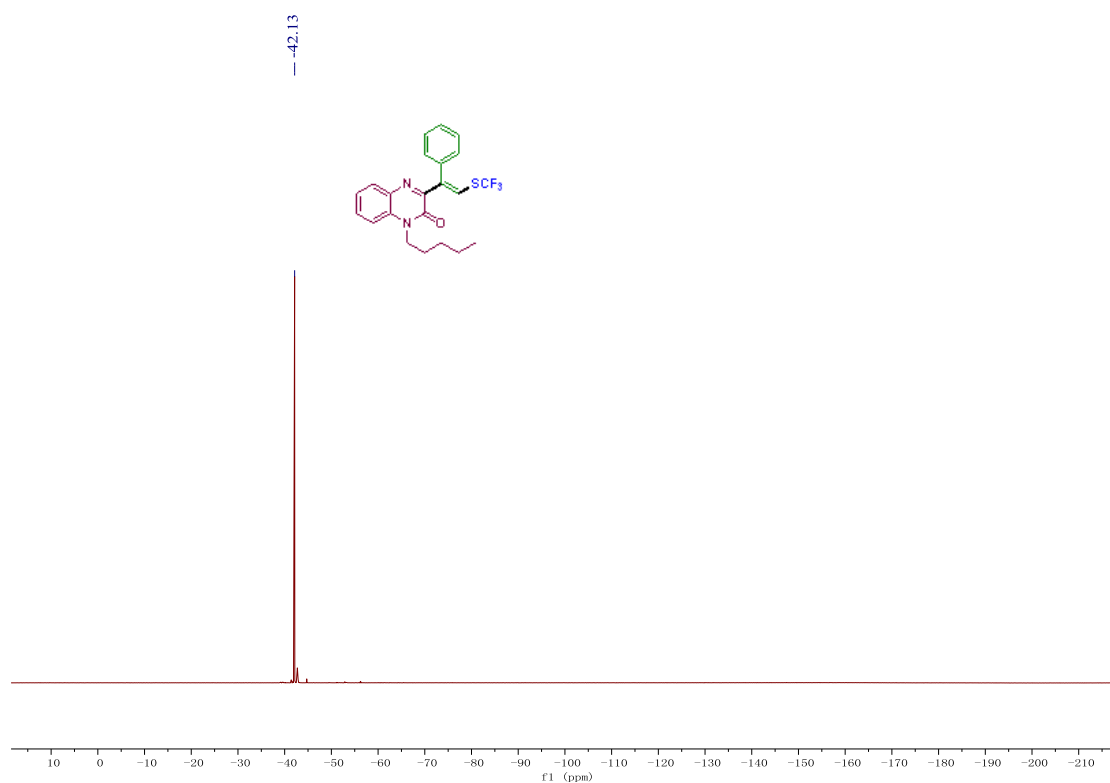
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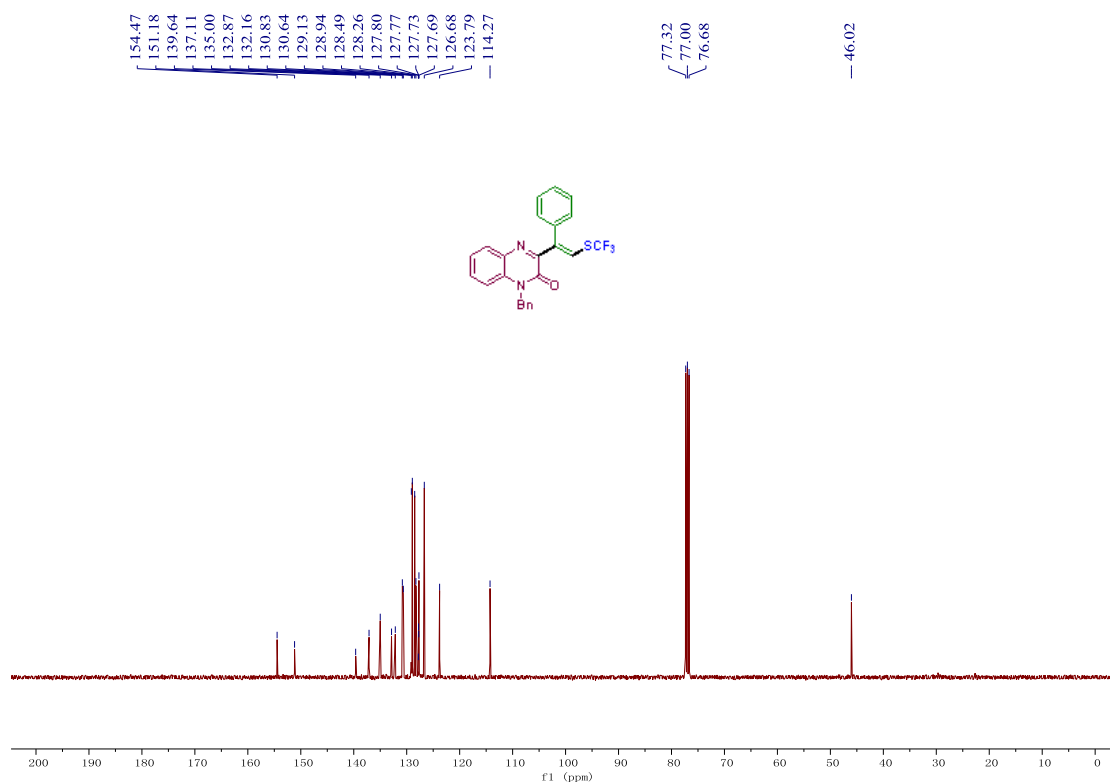


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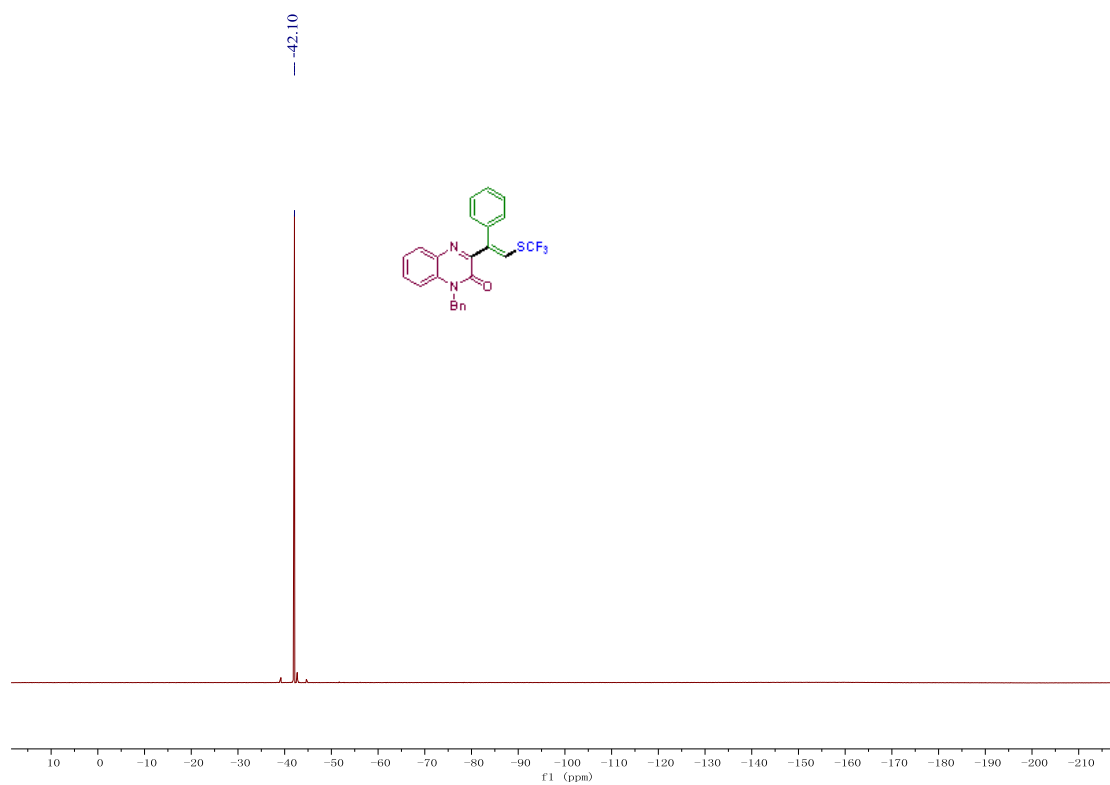




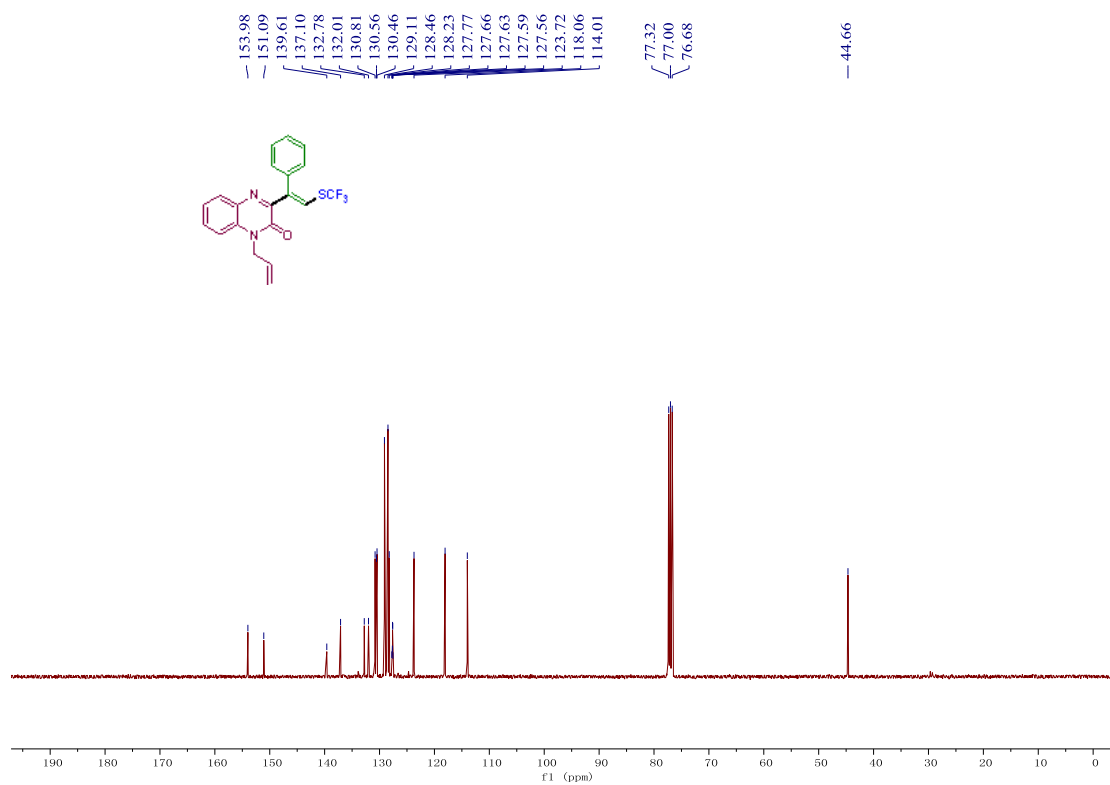
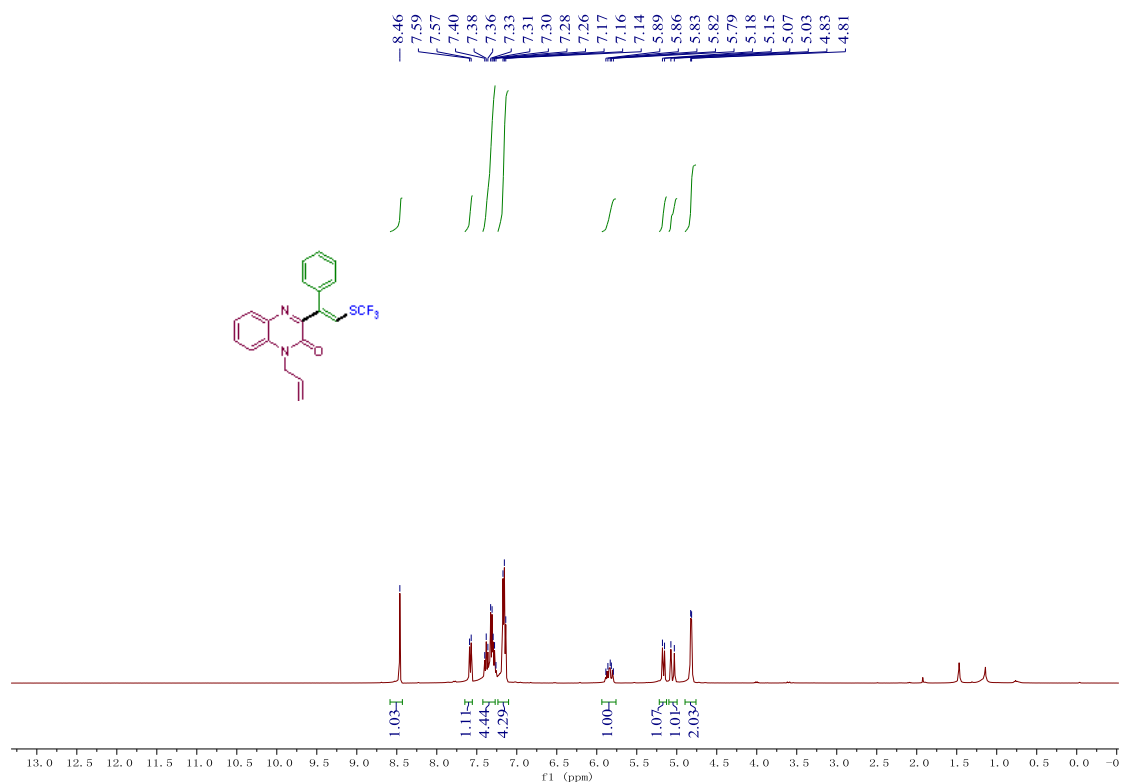


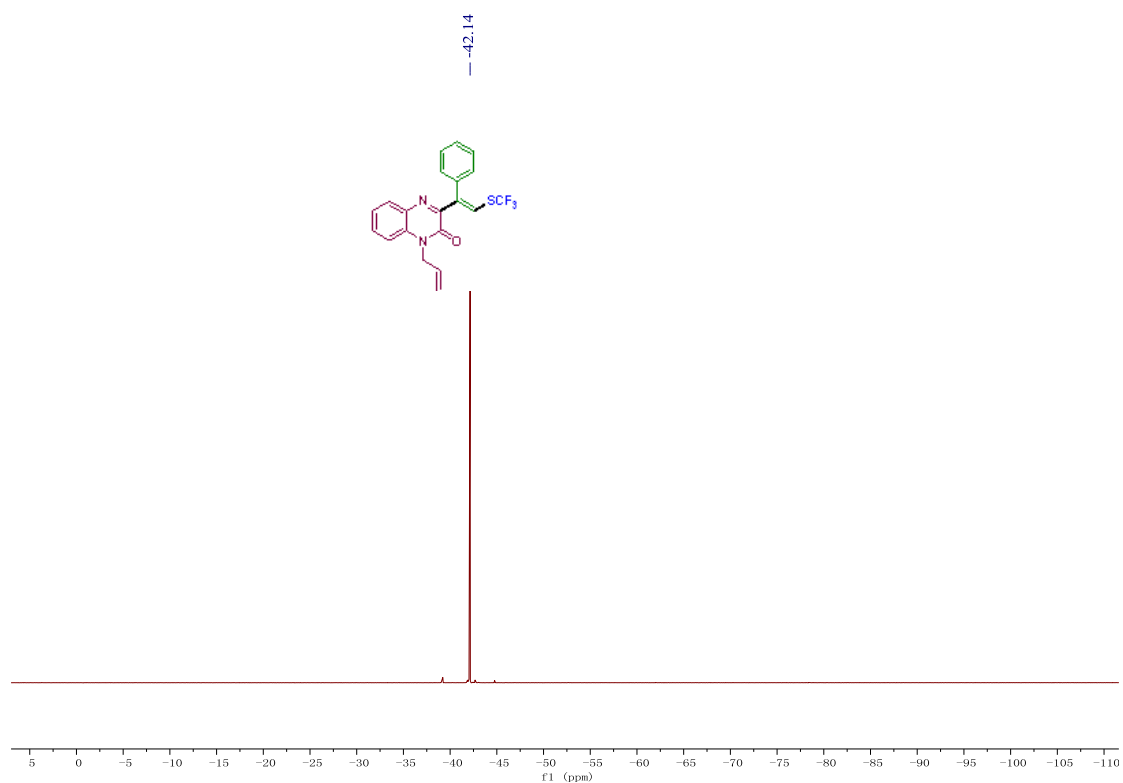


$^{13}\text{C}\{^1\text{H}\}$  NMR (100 MHz,  $\text{CDCl}_3$ ) spectra of **3da**

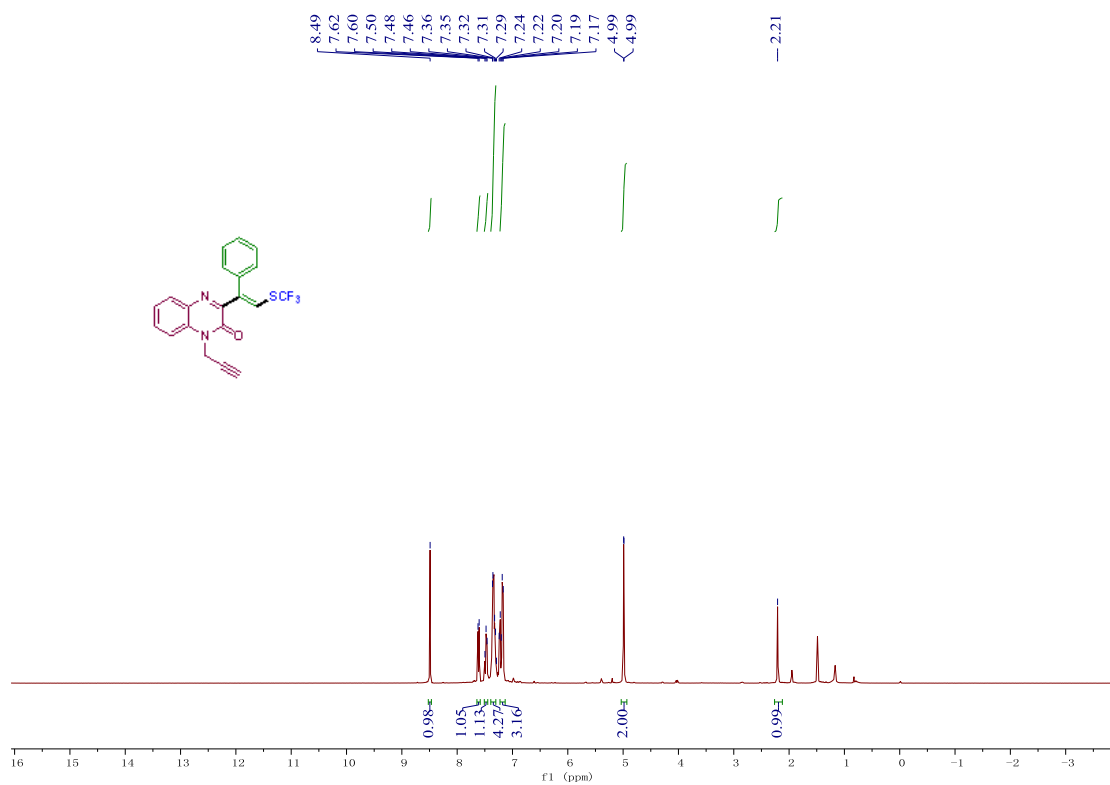


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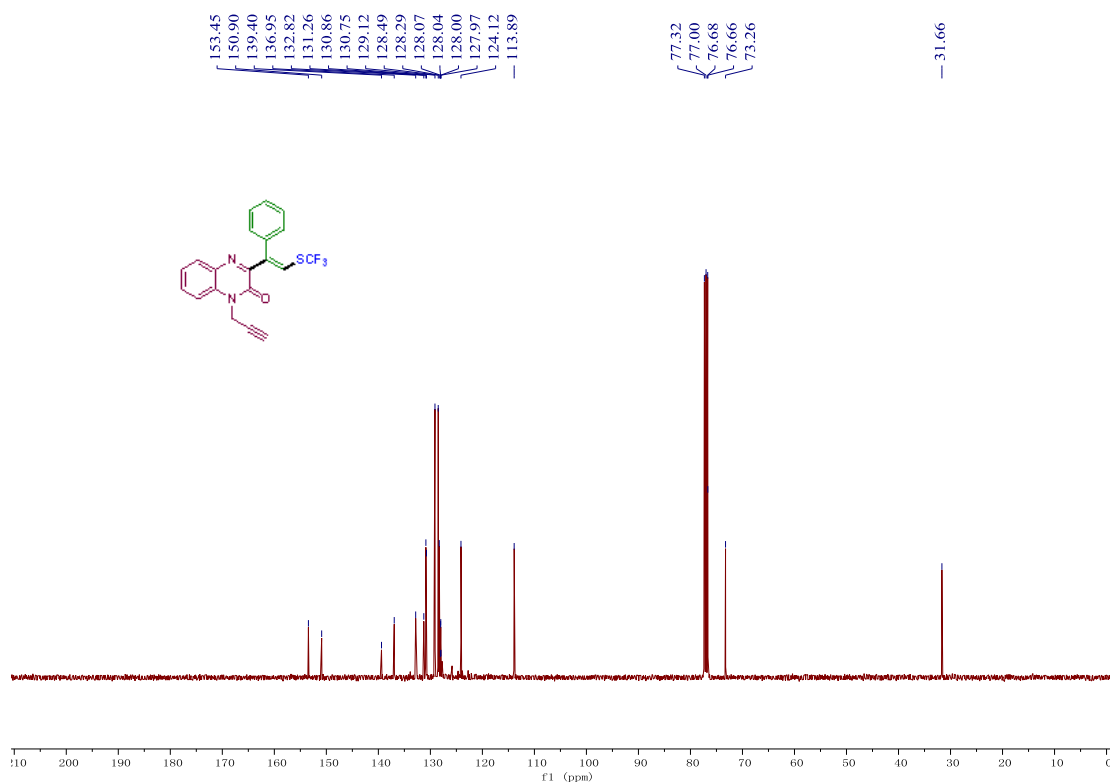




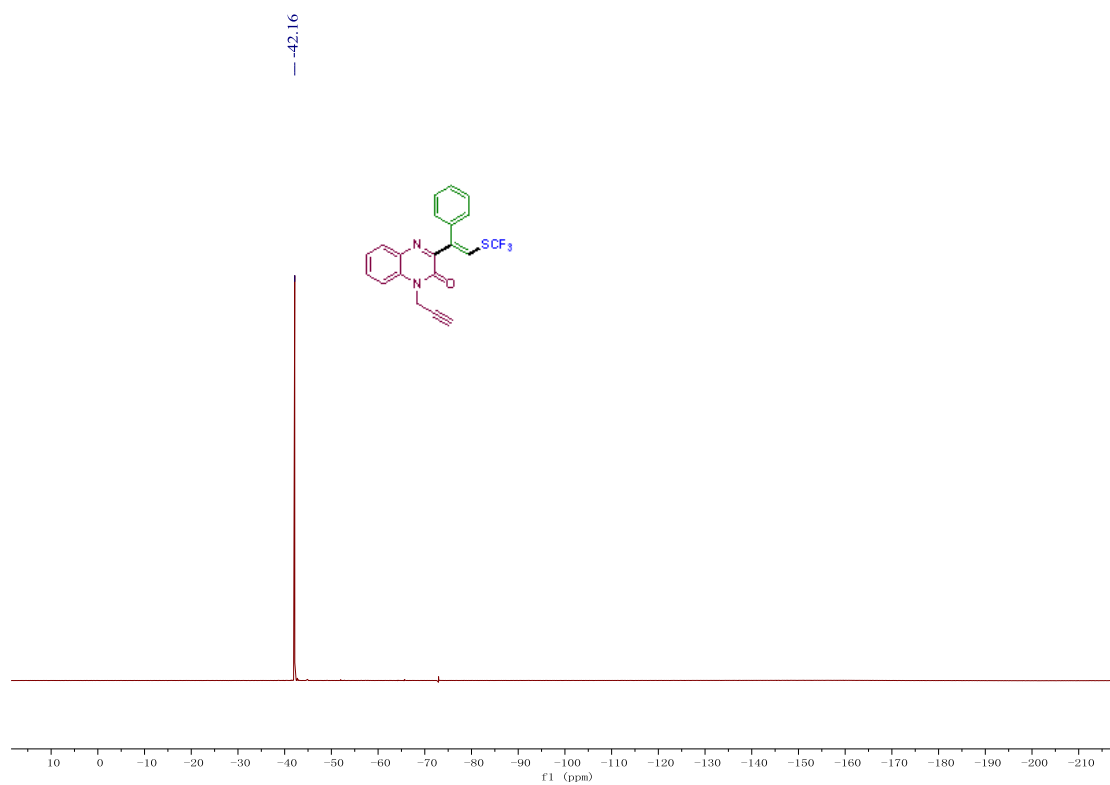
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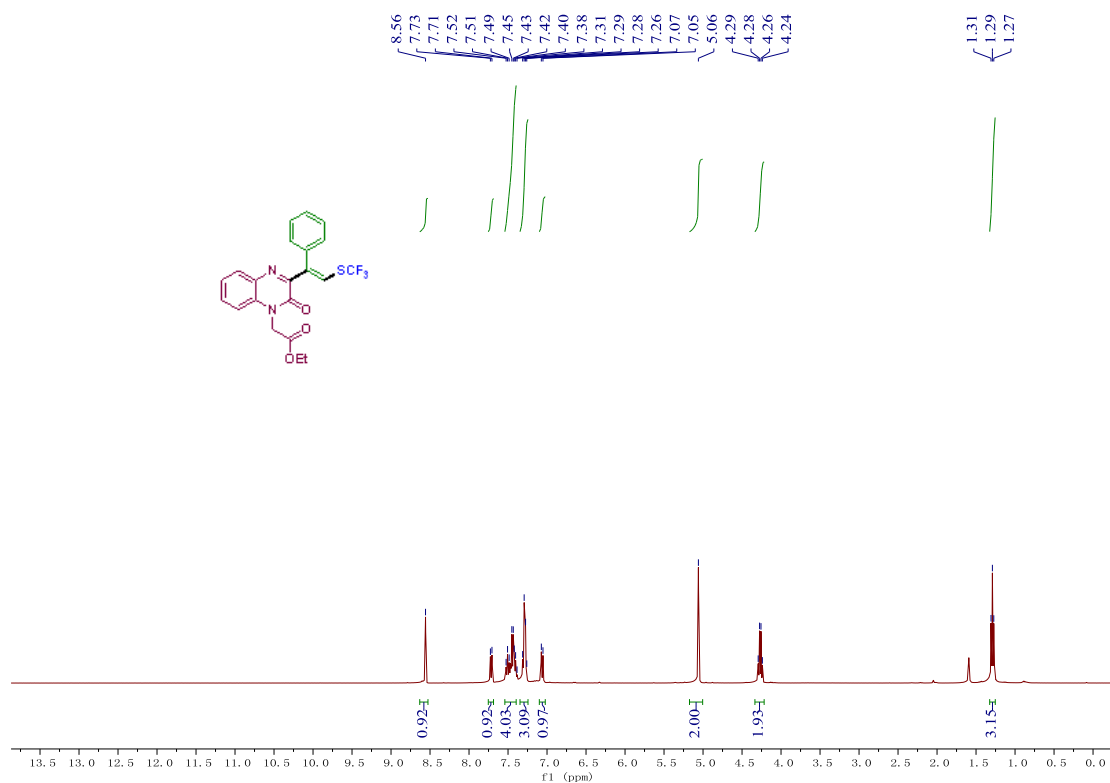
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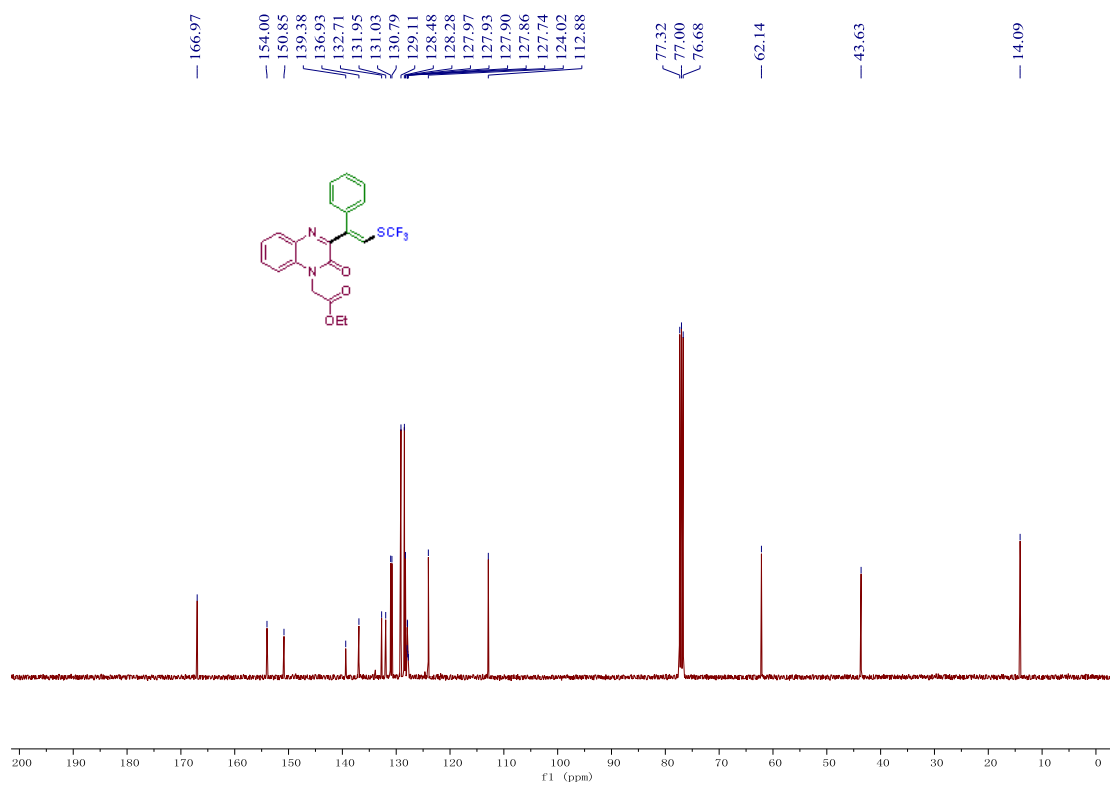
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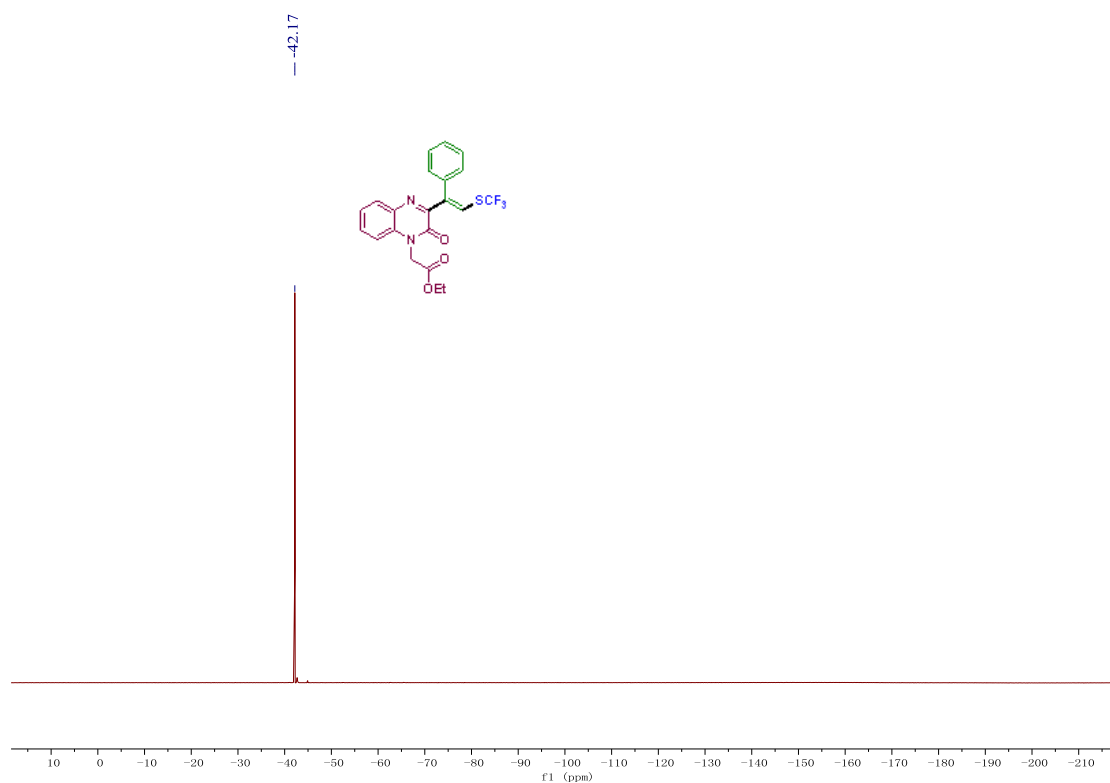
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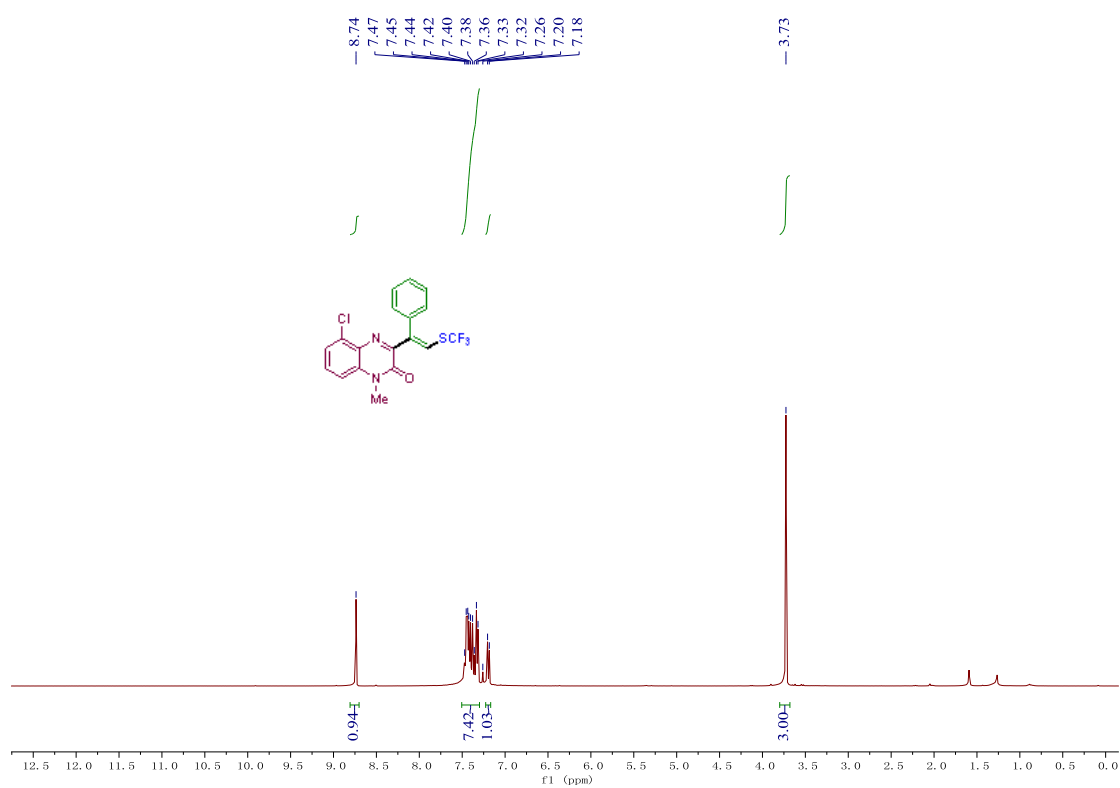
<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) spectra of **3ga**



<sup>13</sup>C{<sup>1</sup>H} NMR (100 MHz, CDCl<sub>3</sub>) spectra of **3ga**

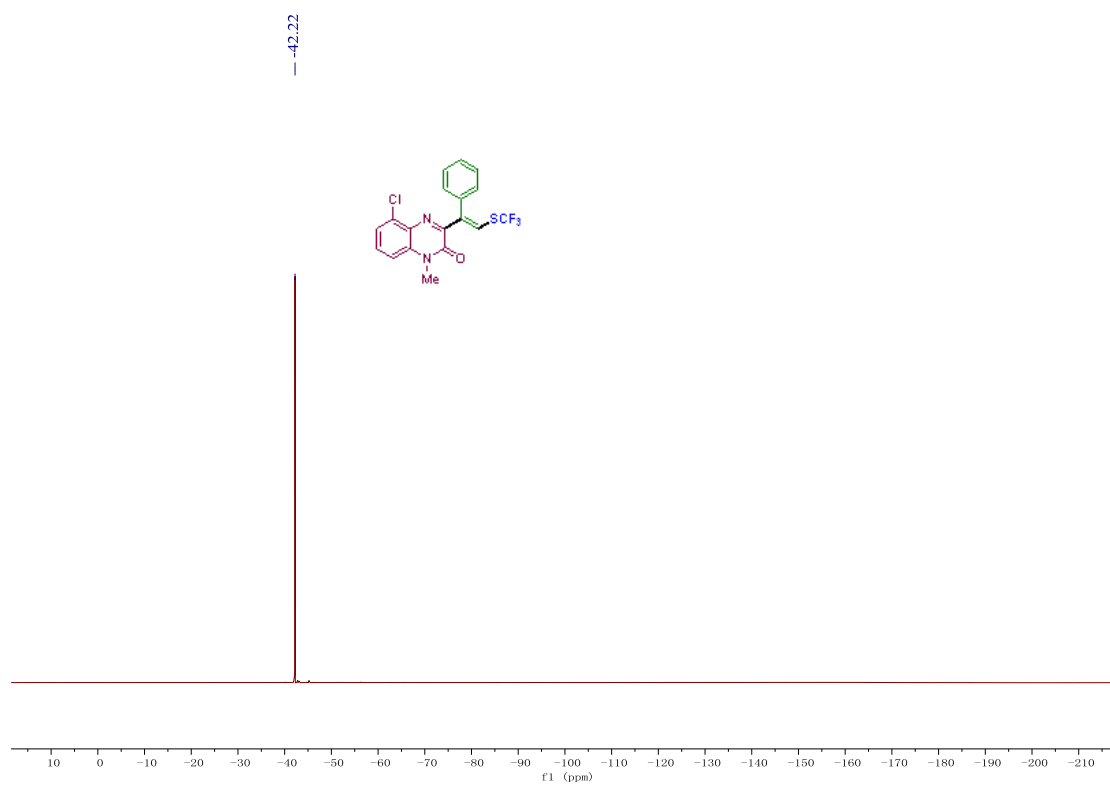
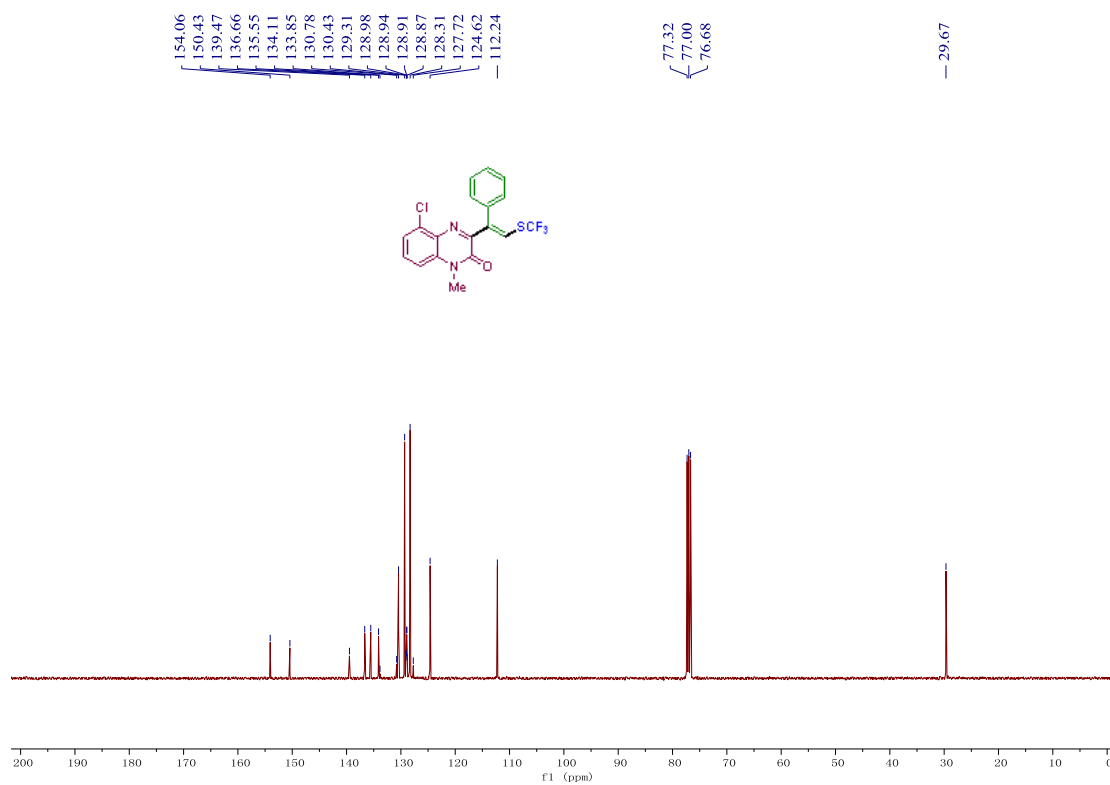


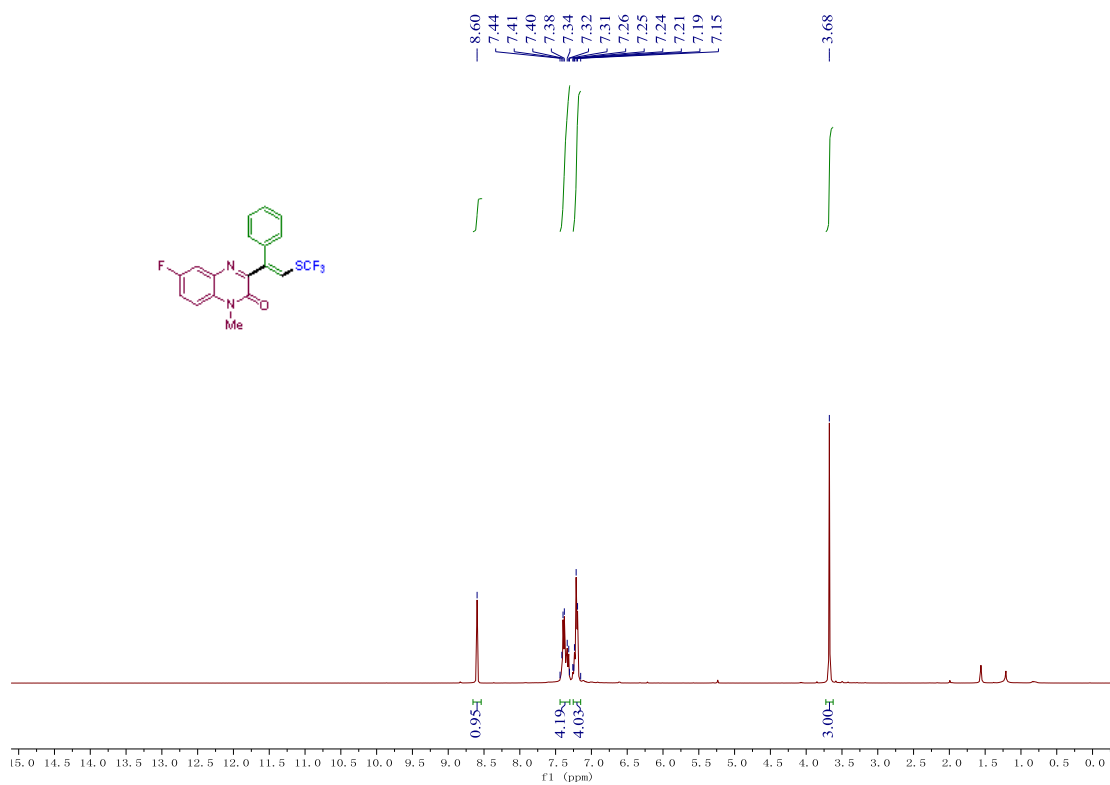
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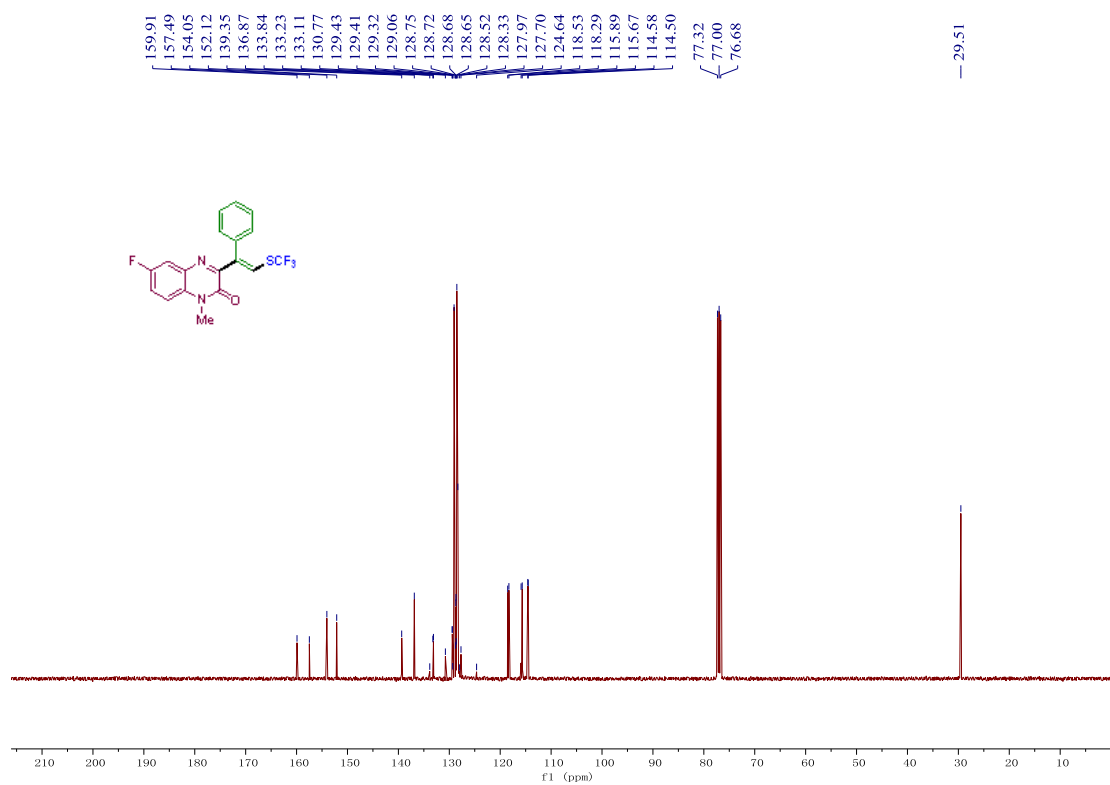
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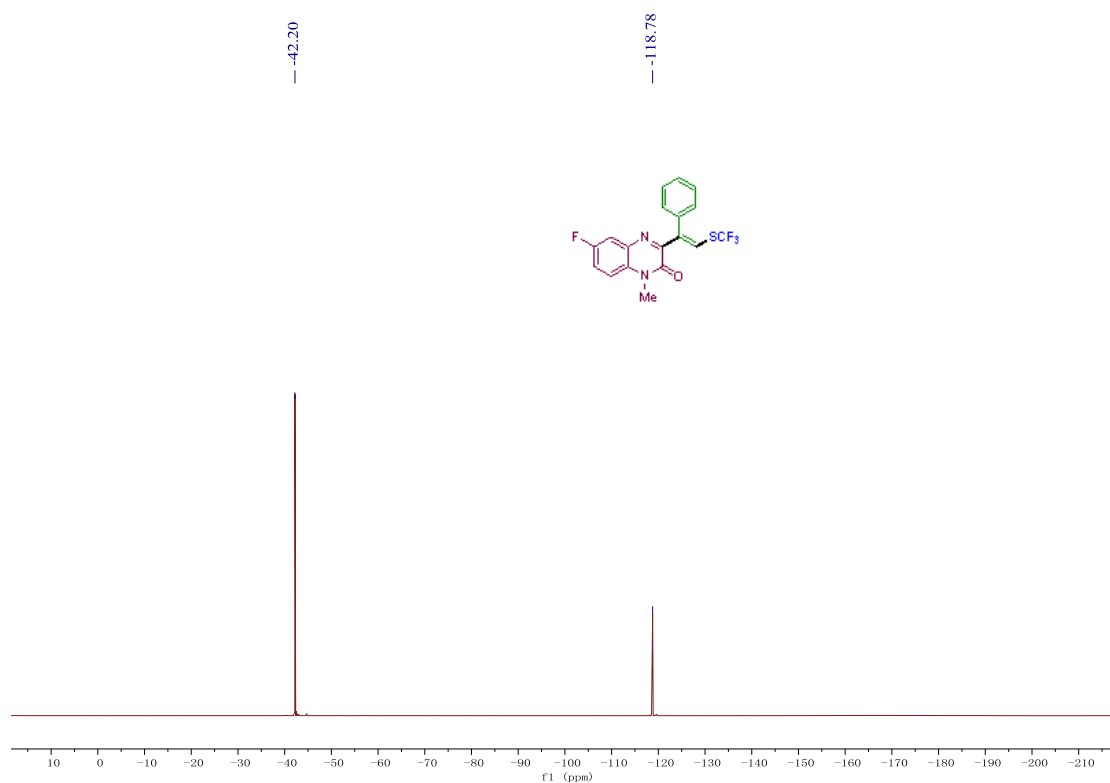




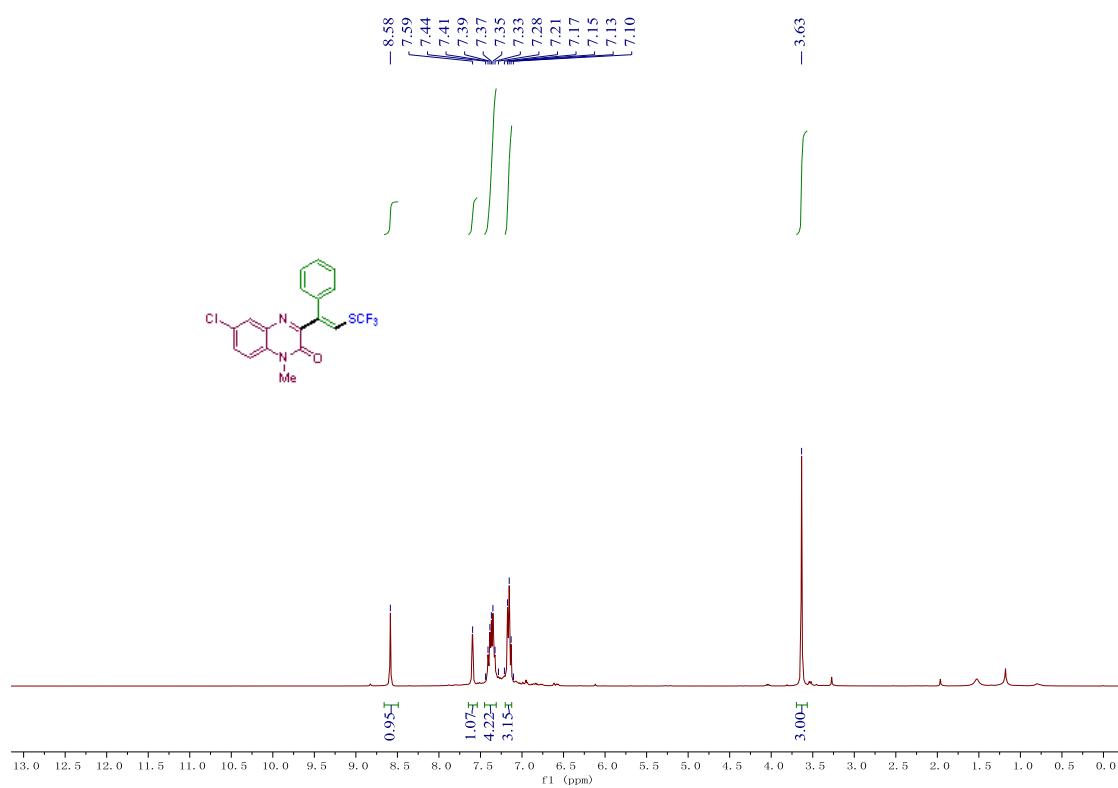
$^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ ) spectra of **3ia**



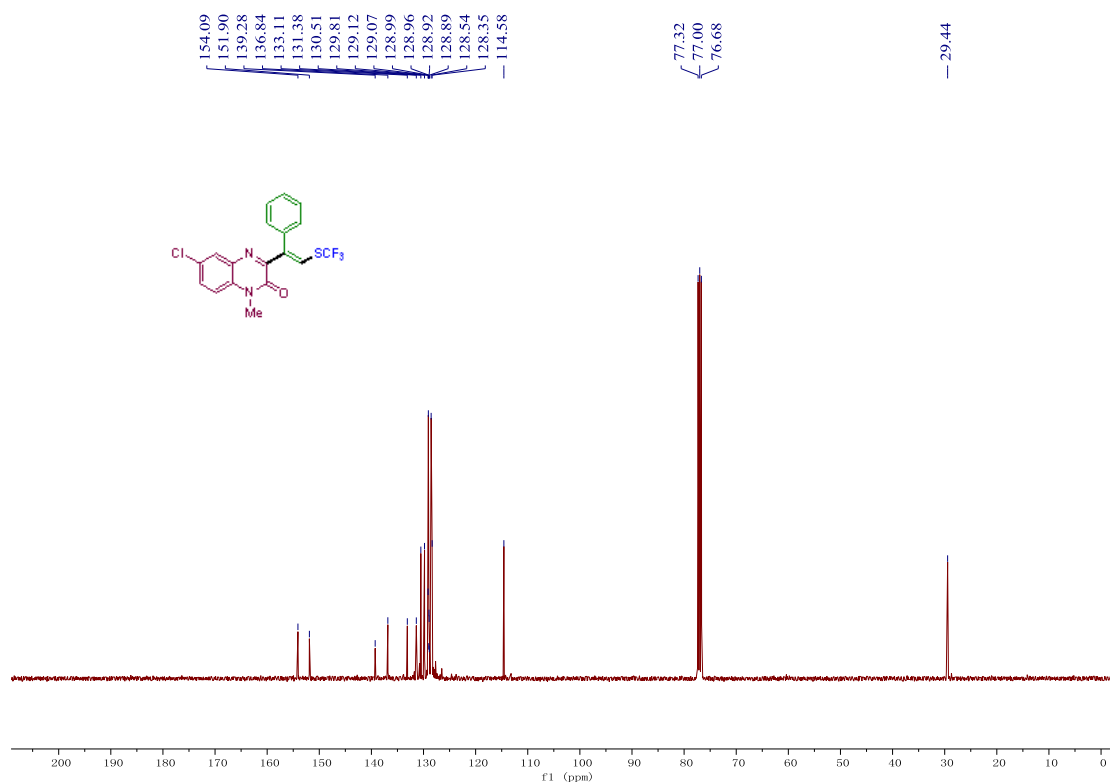
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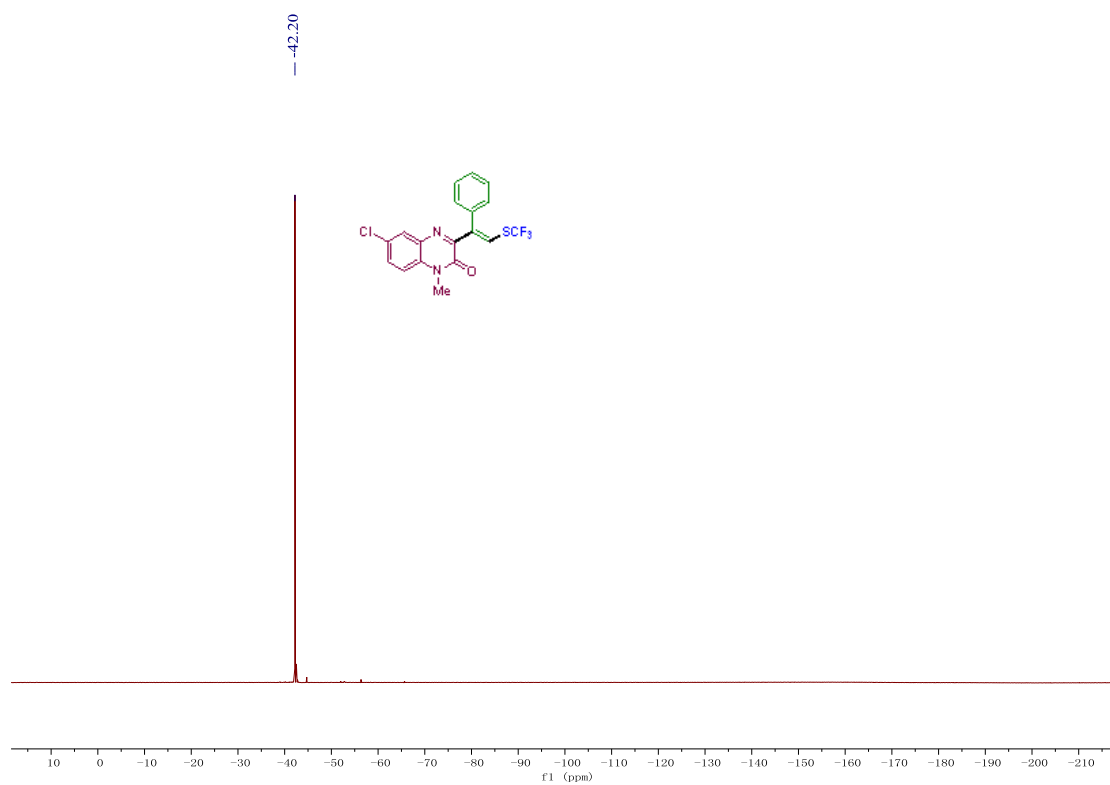
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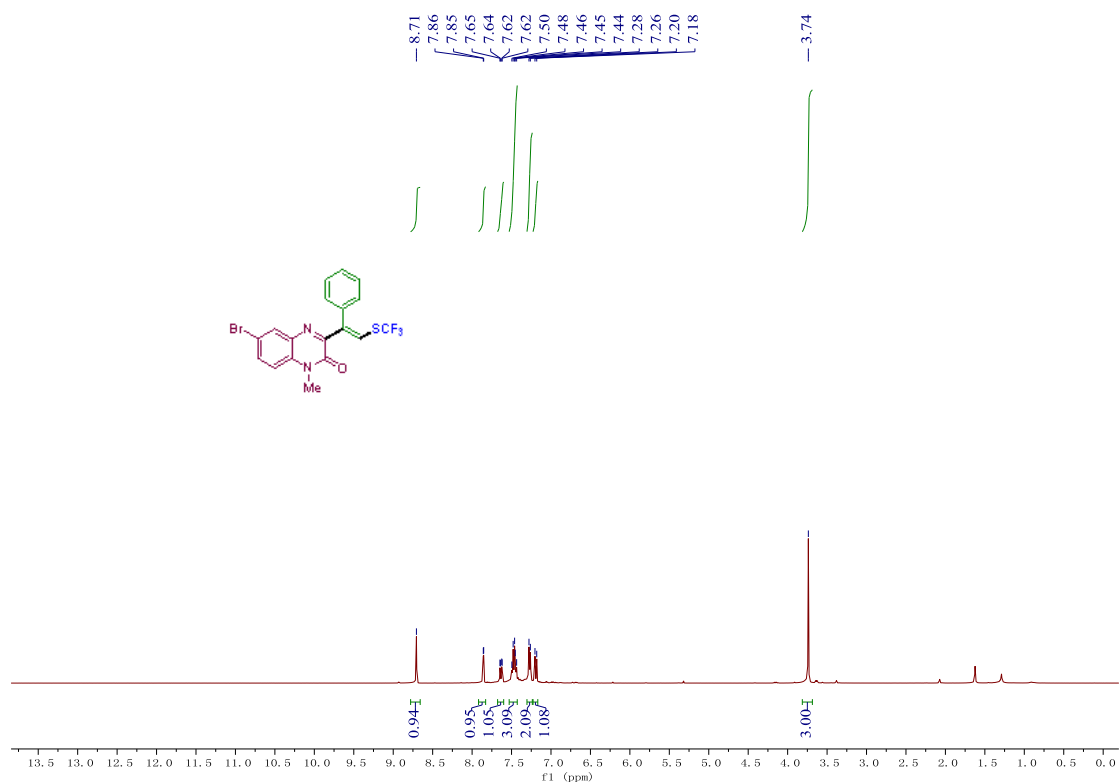
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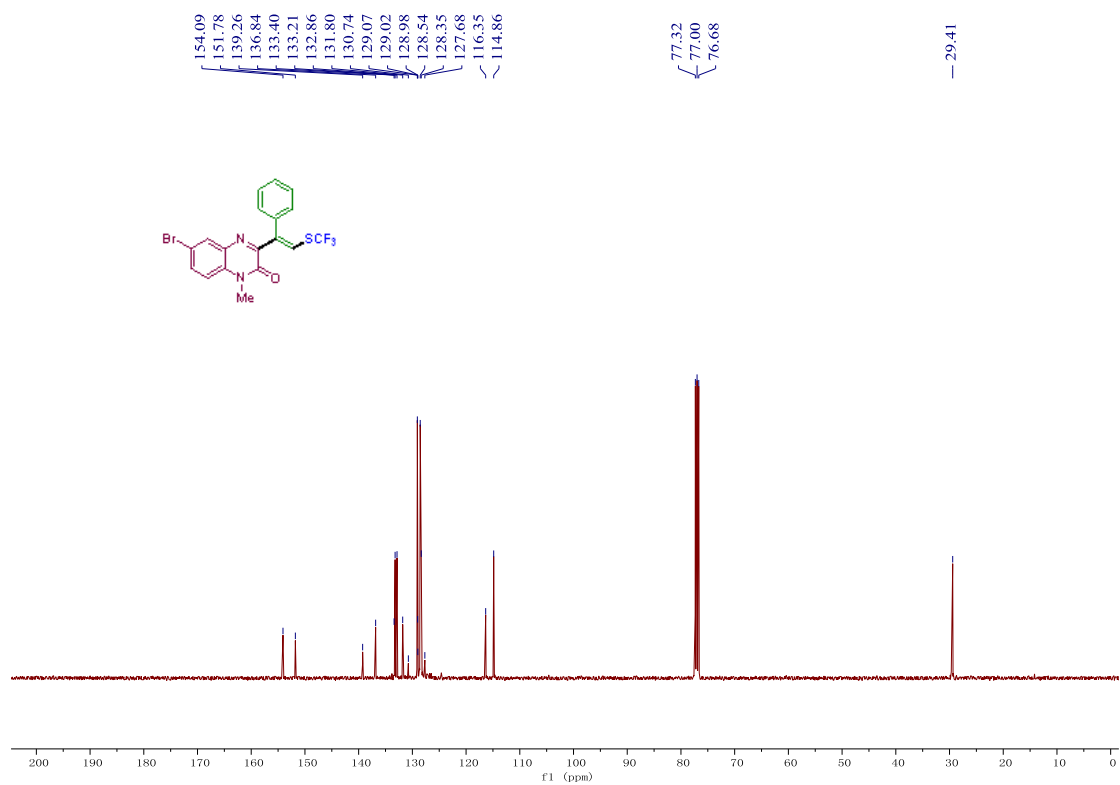
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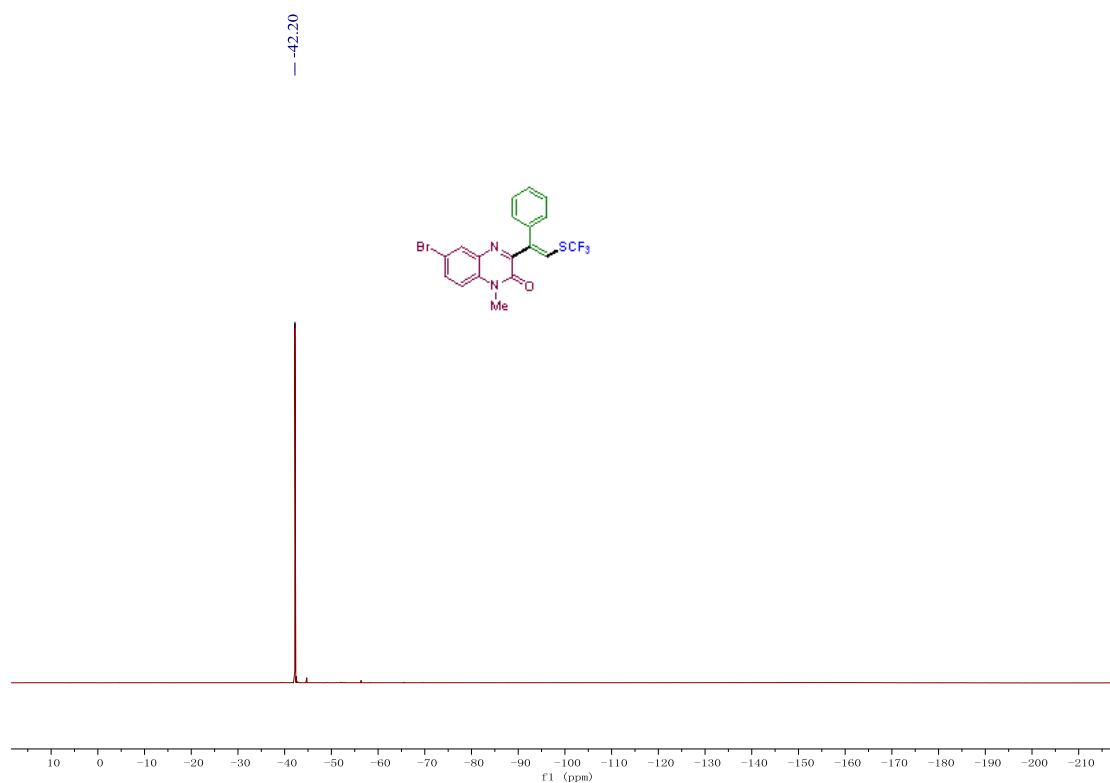
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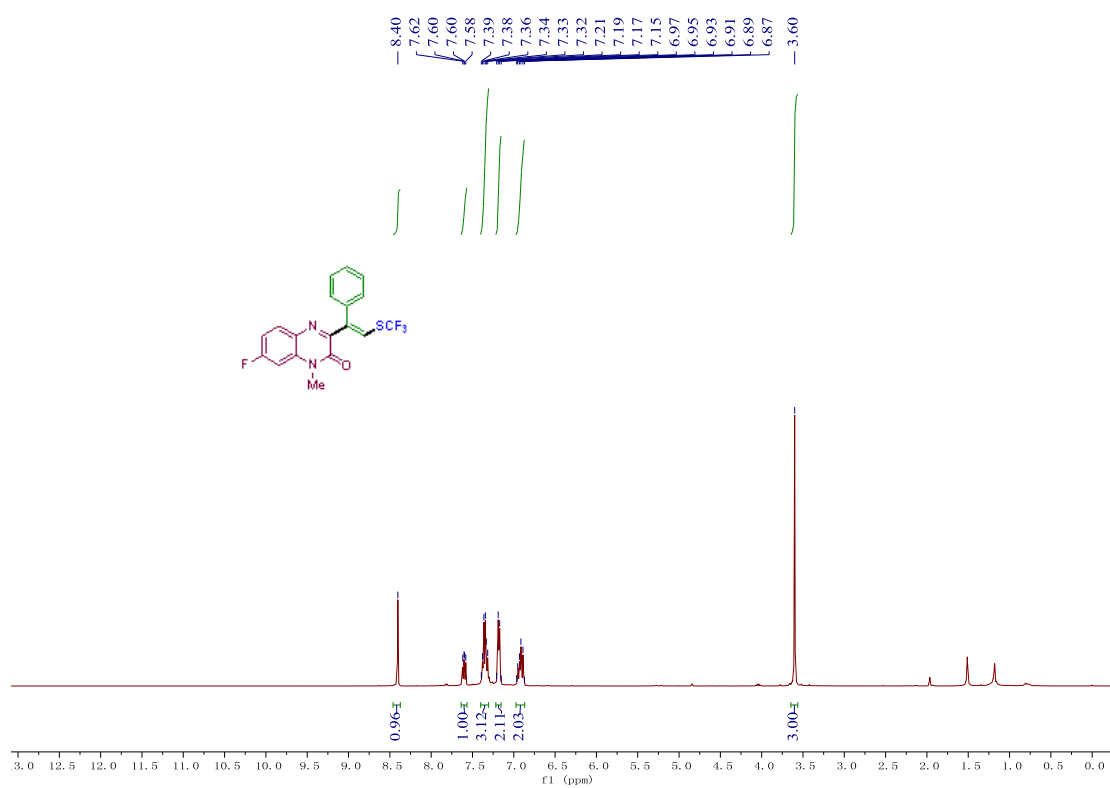
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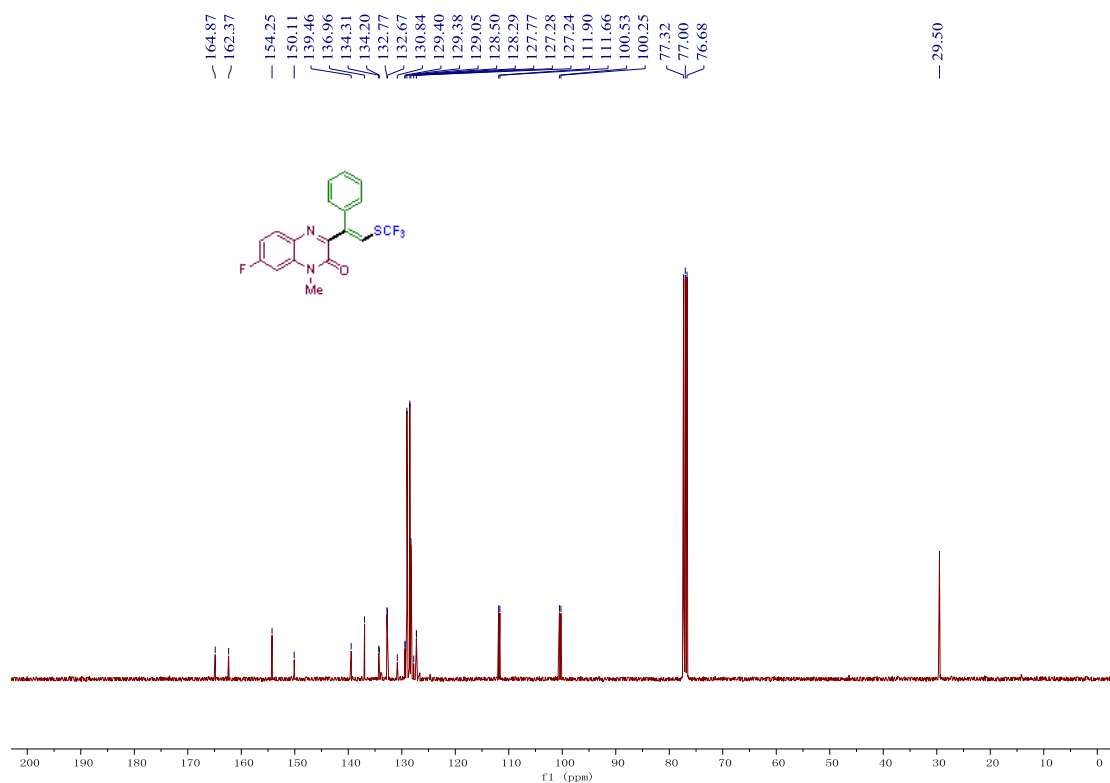
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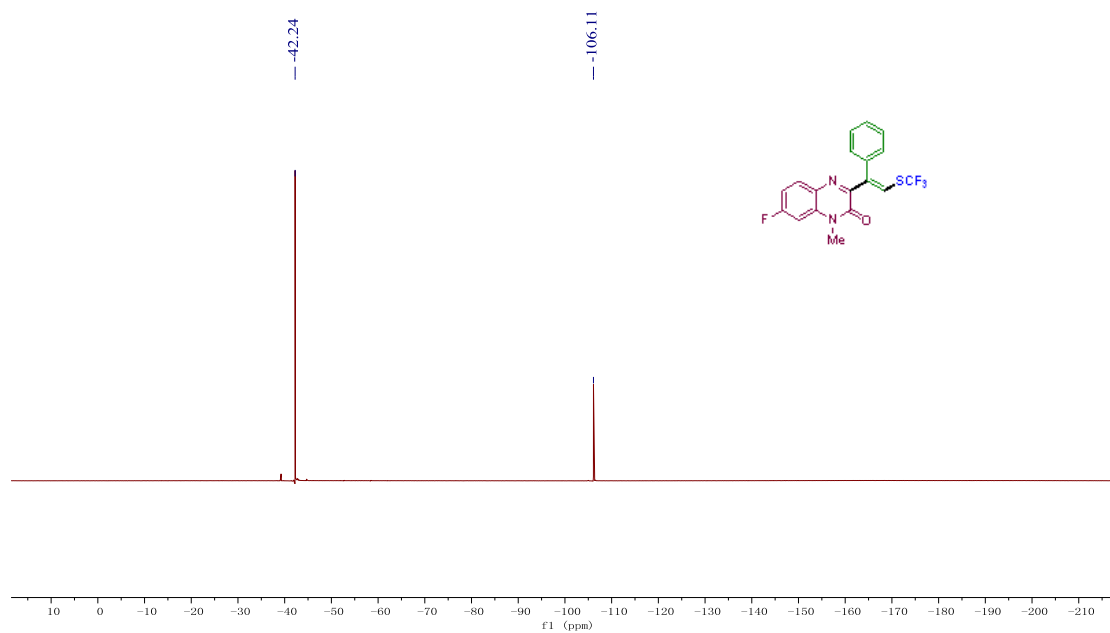
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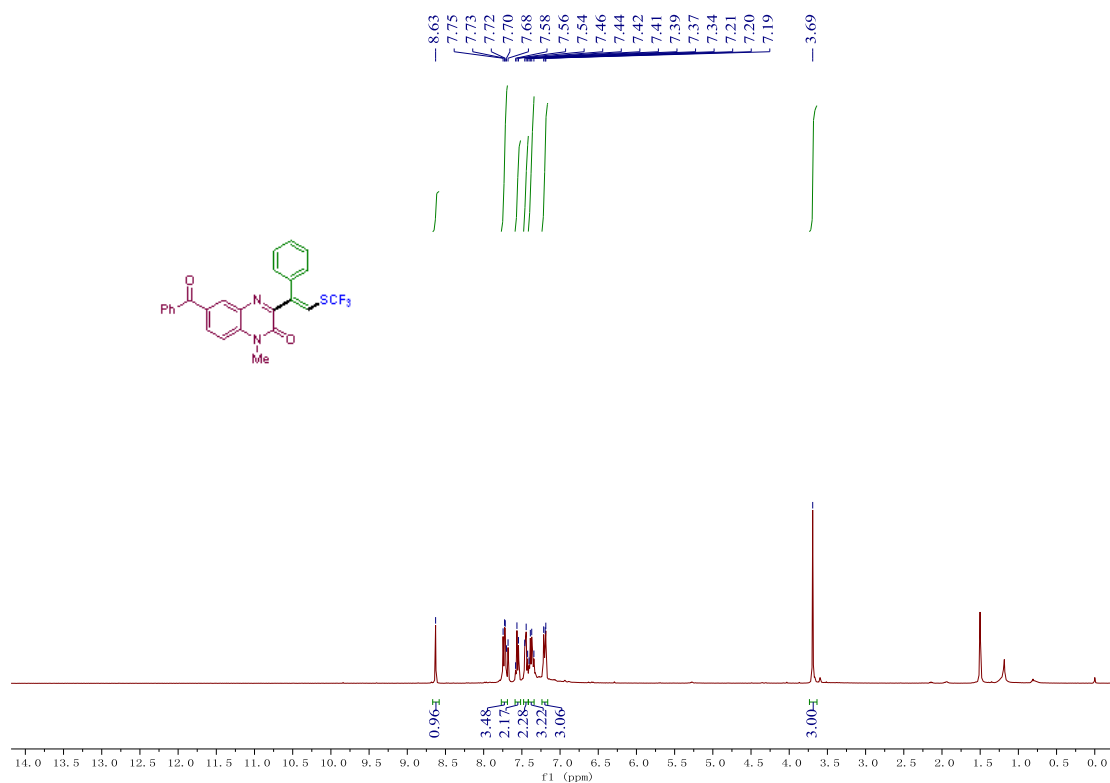
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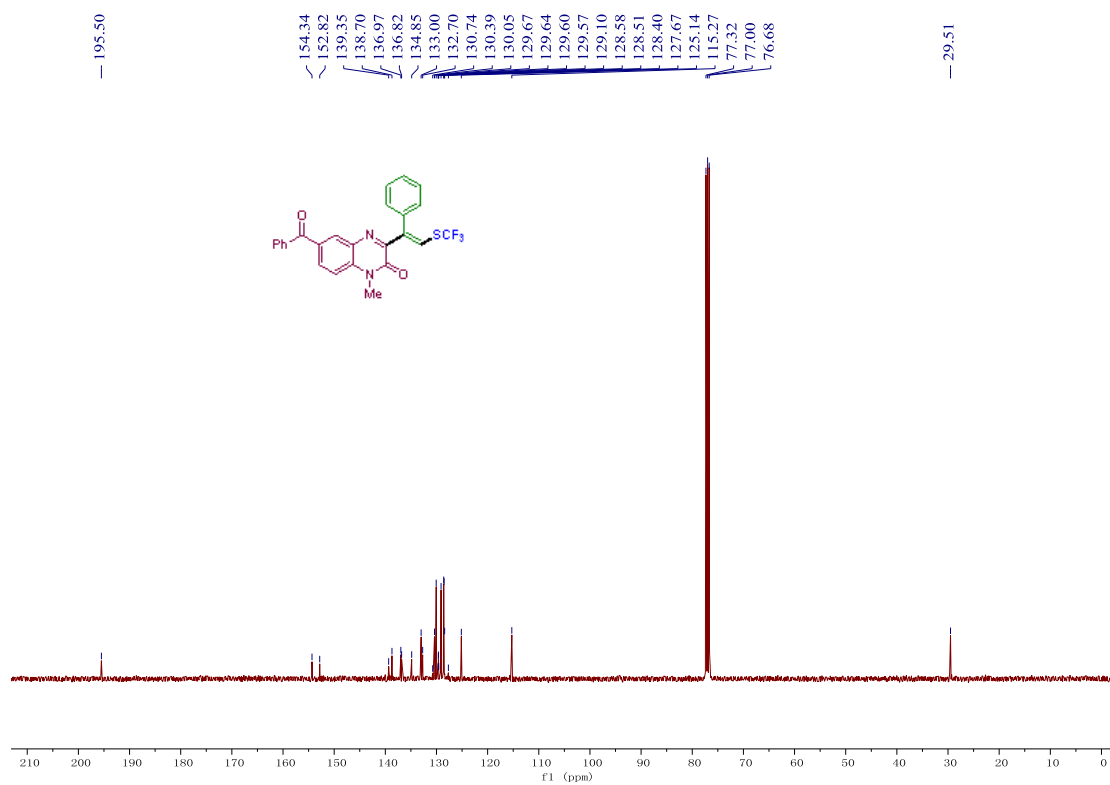
$^{13}\text{C}\{^1\text{H}\}$  NMR (100 MHz,  $\text{CDCl}_3$ ) spectra of **3la**



$^{19}\text{F}$  NMR (376 MHz,  $\text{CDCl}_3$ ) spectra of **3la**

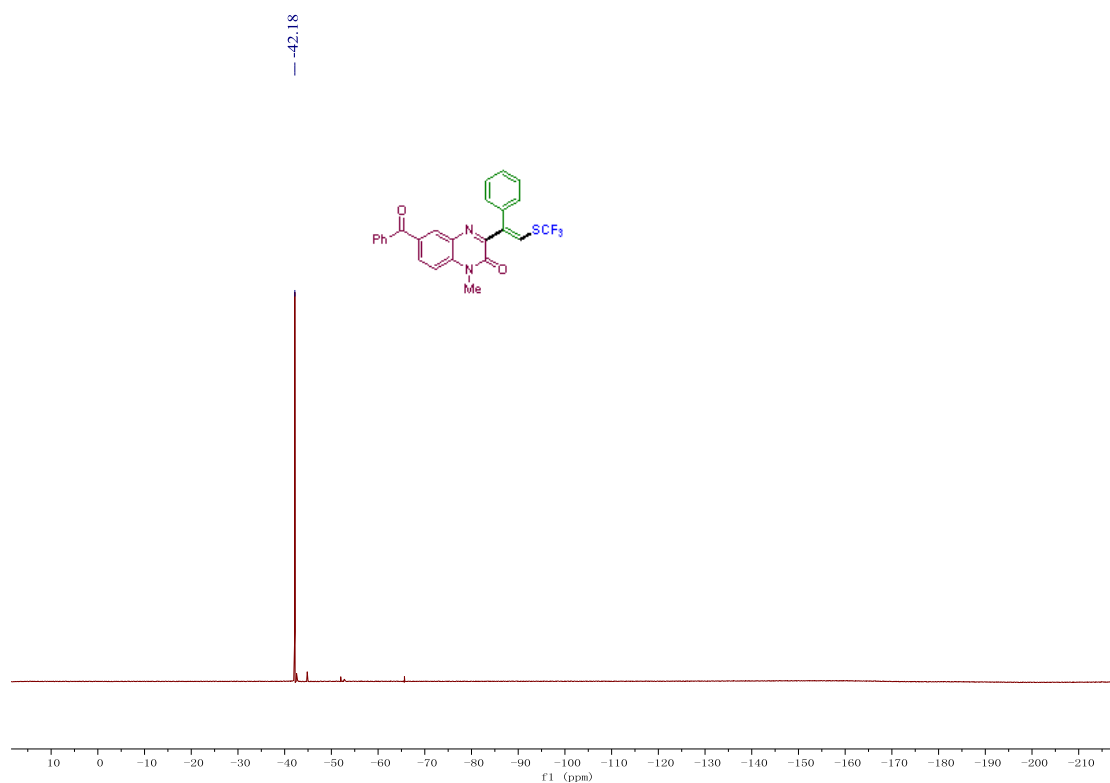


$^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ ) spectra of **3ma**

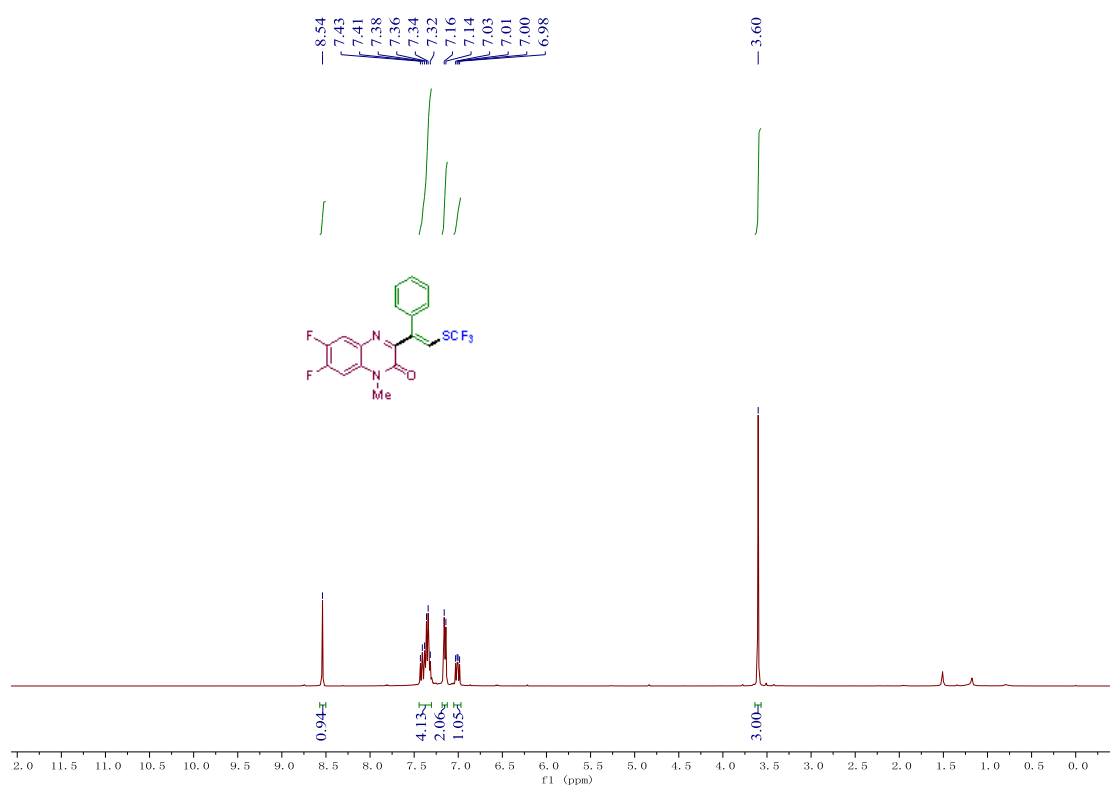


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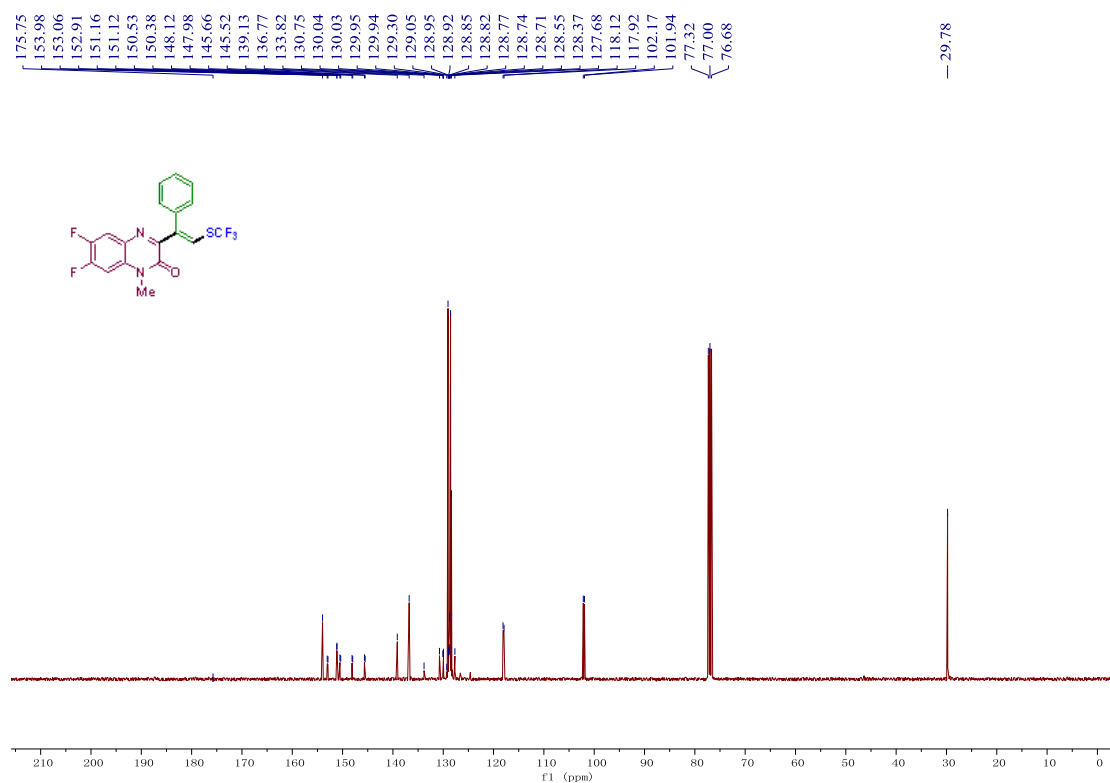




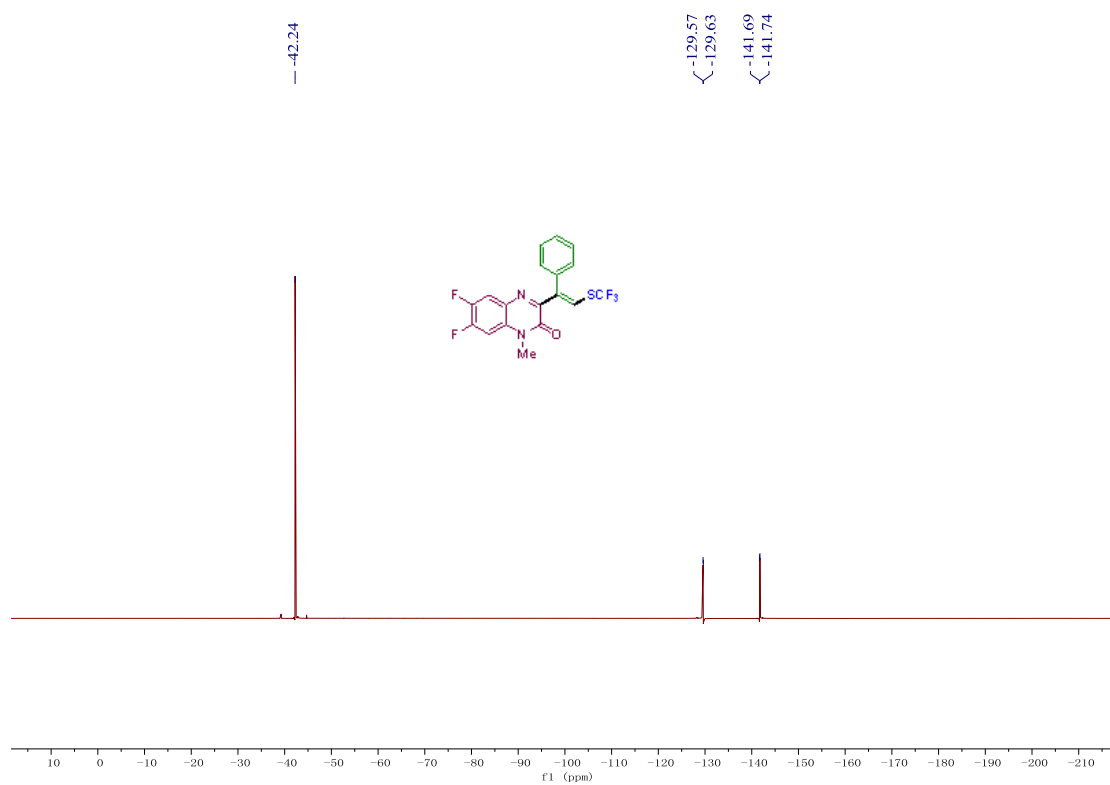
<sup>19</sup>F NMR (376 MHz, CDCl<sub>3</sub>) spectra of **3a**



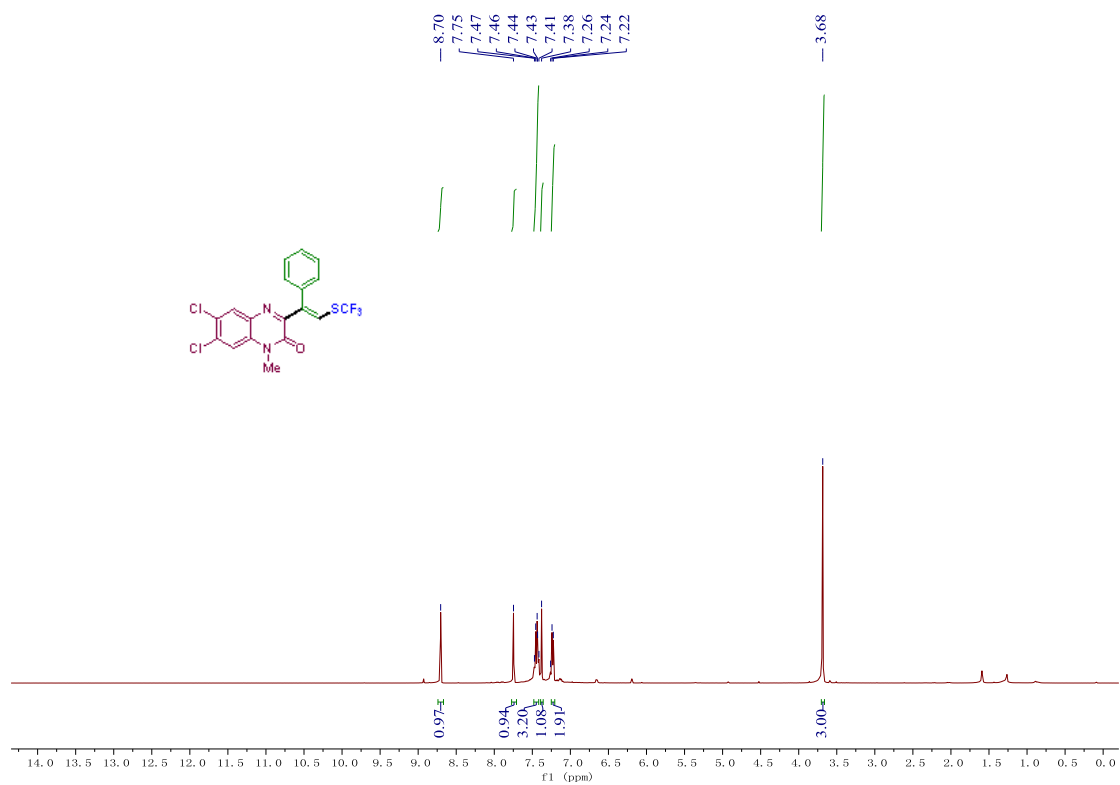
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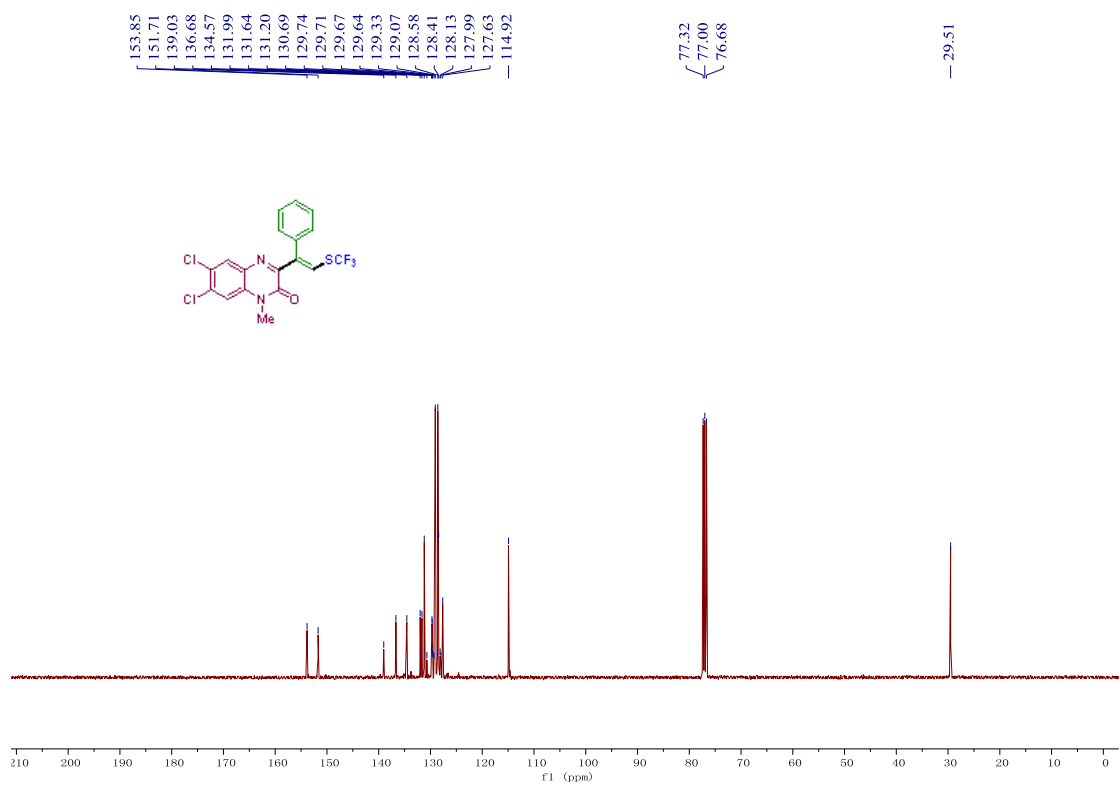
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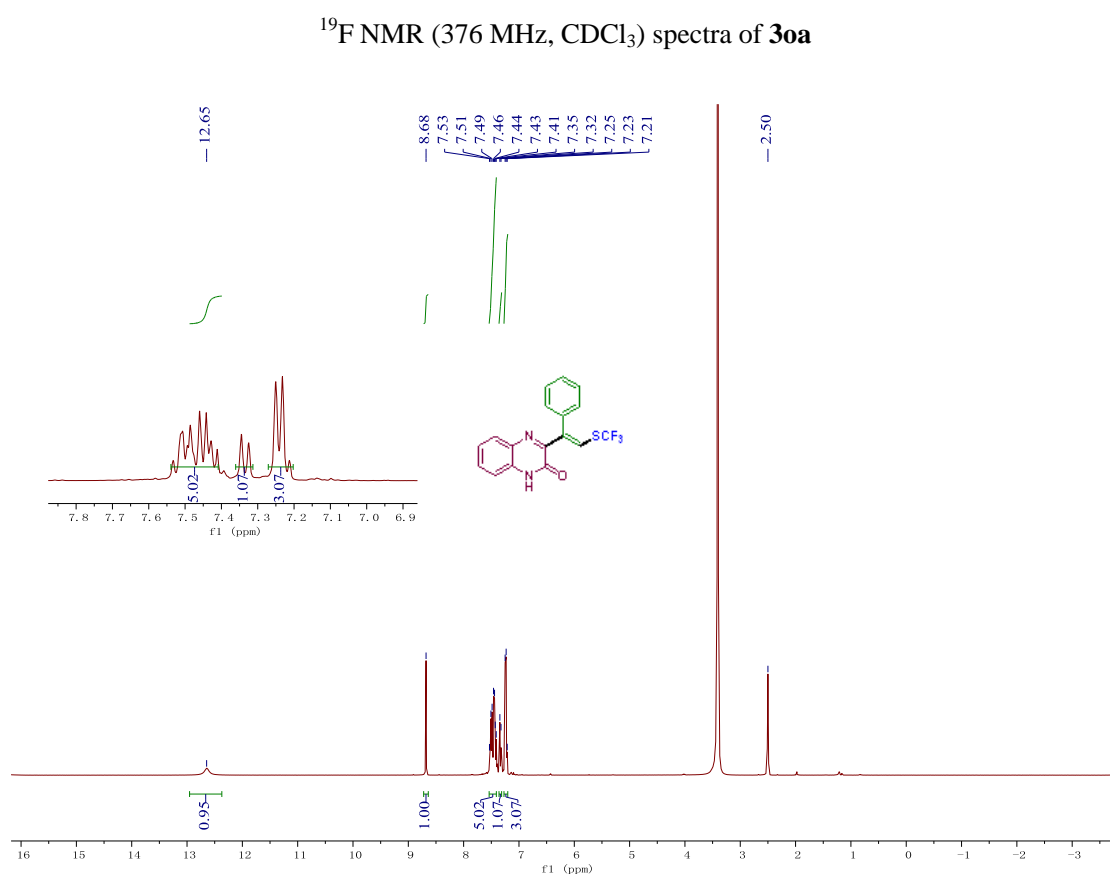
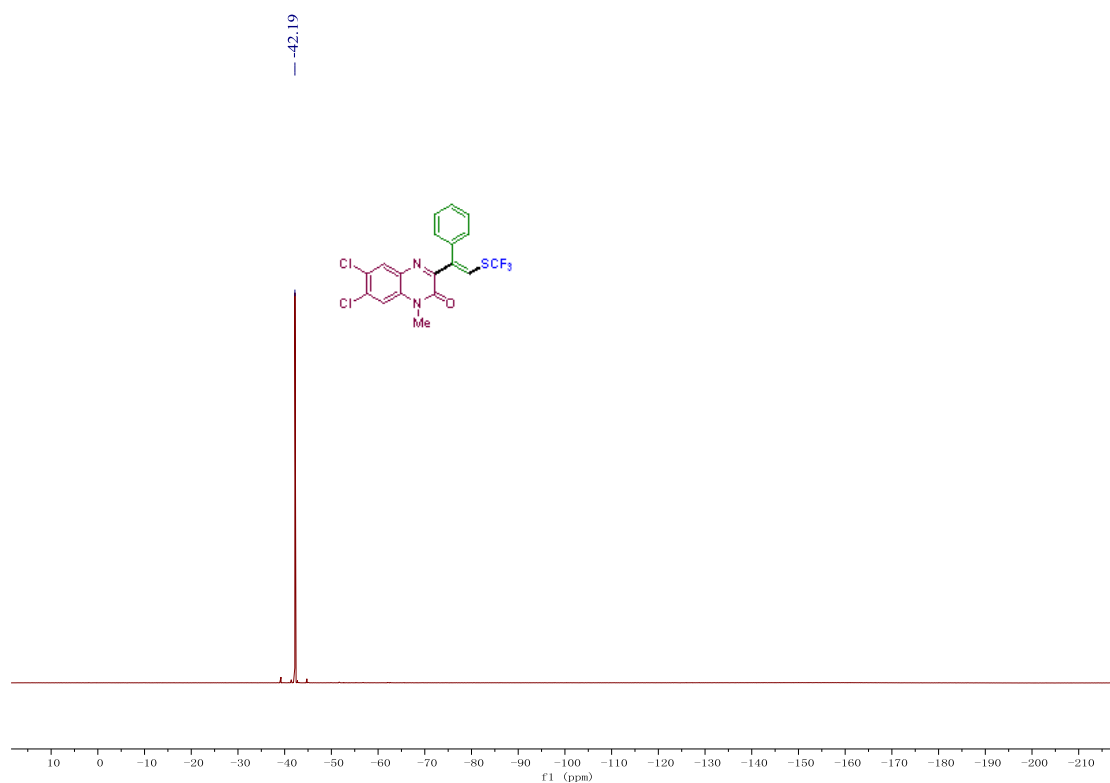
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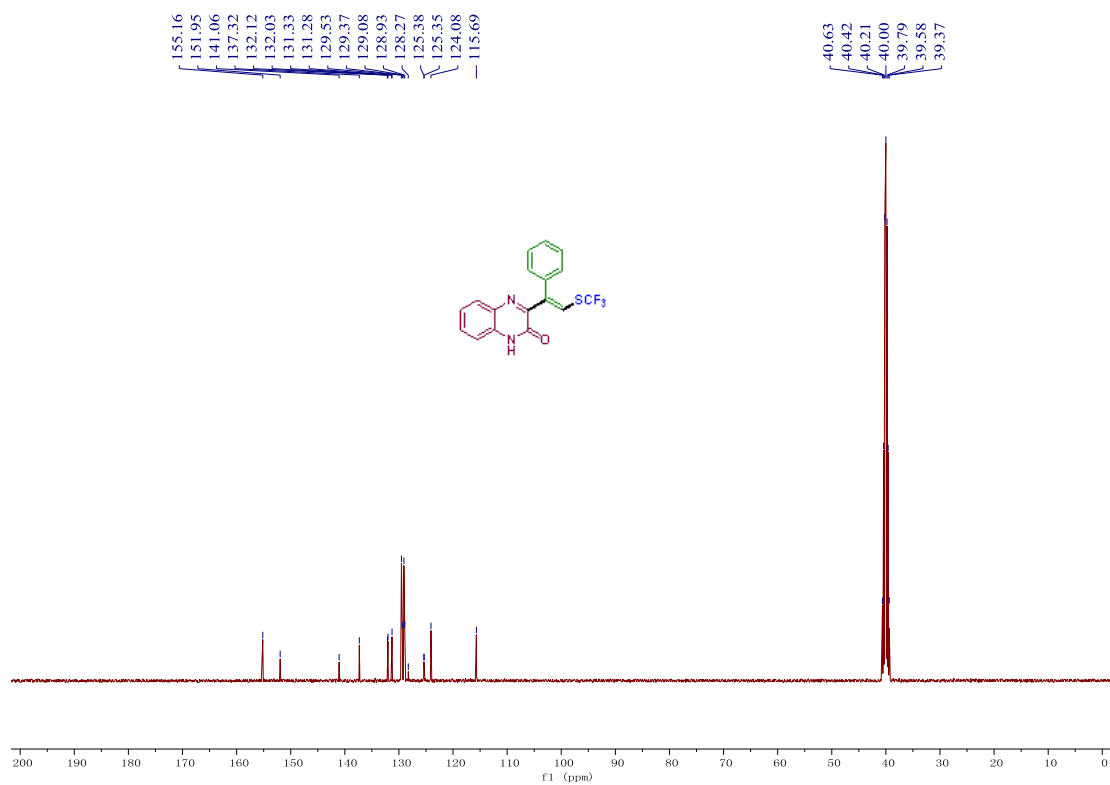
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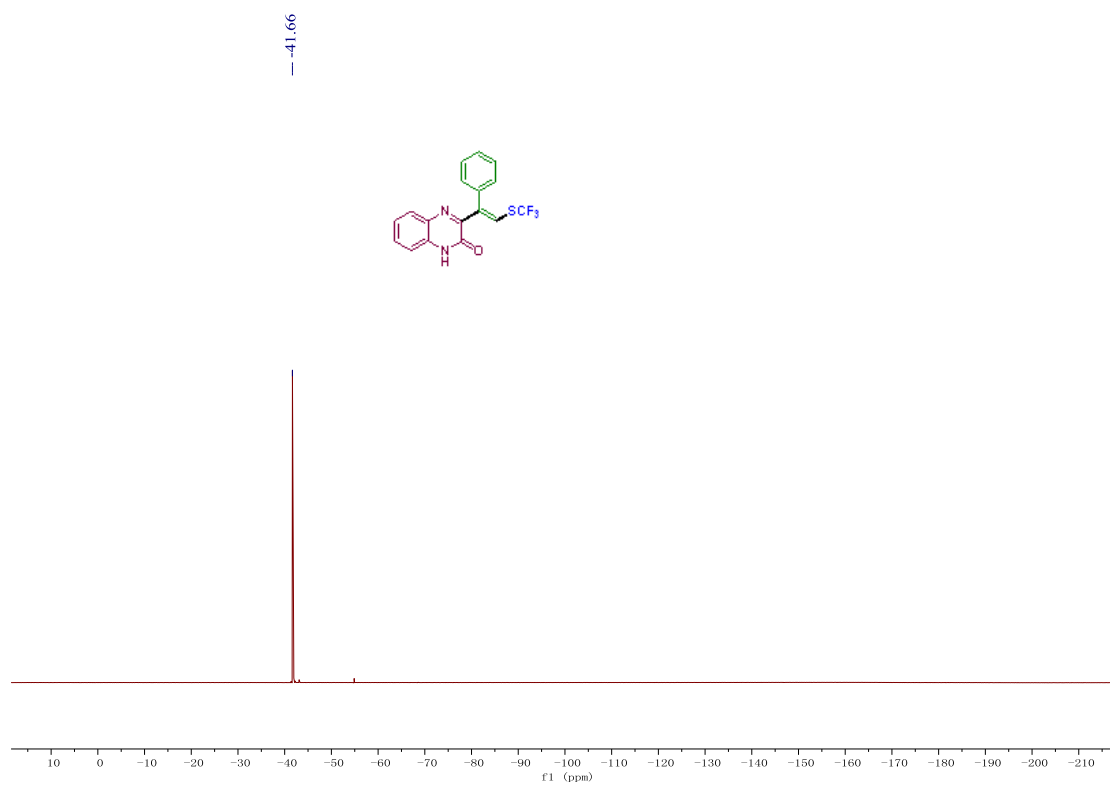
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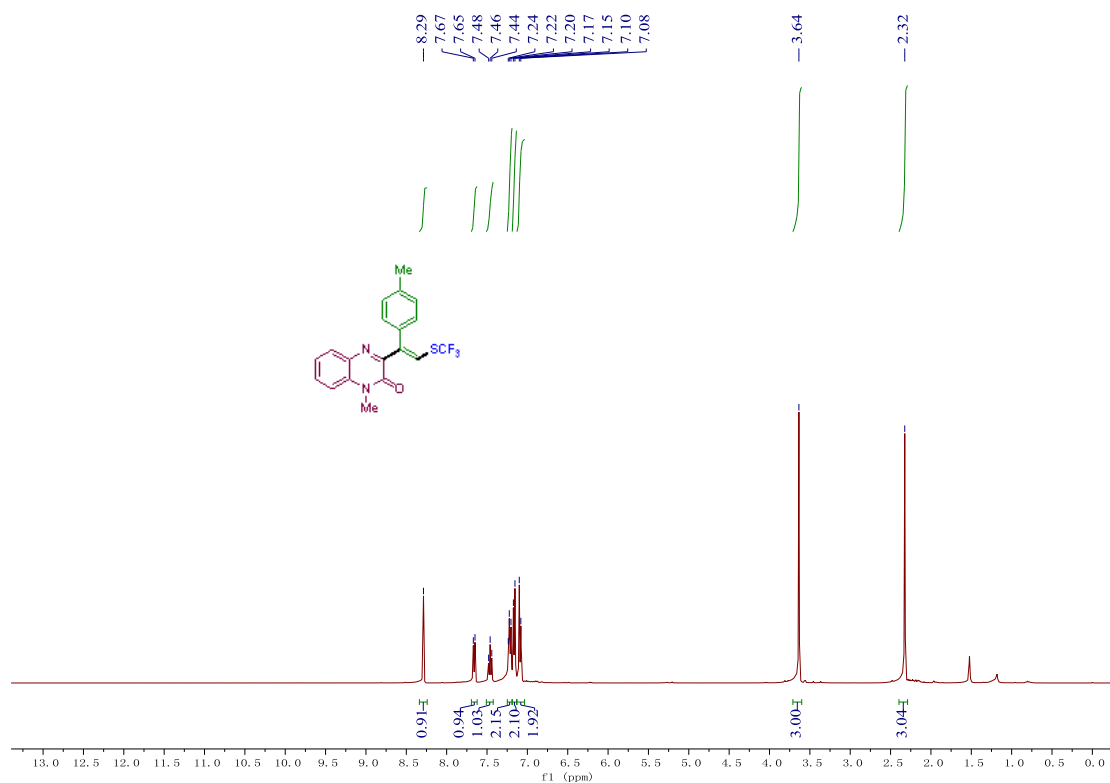
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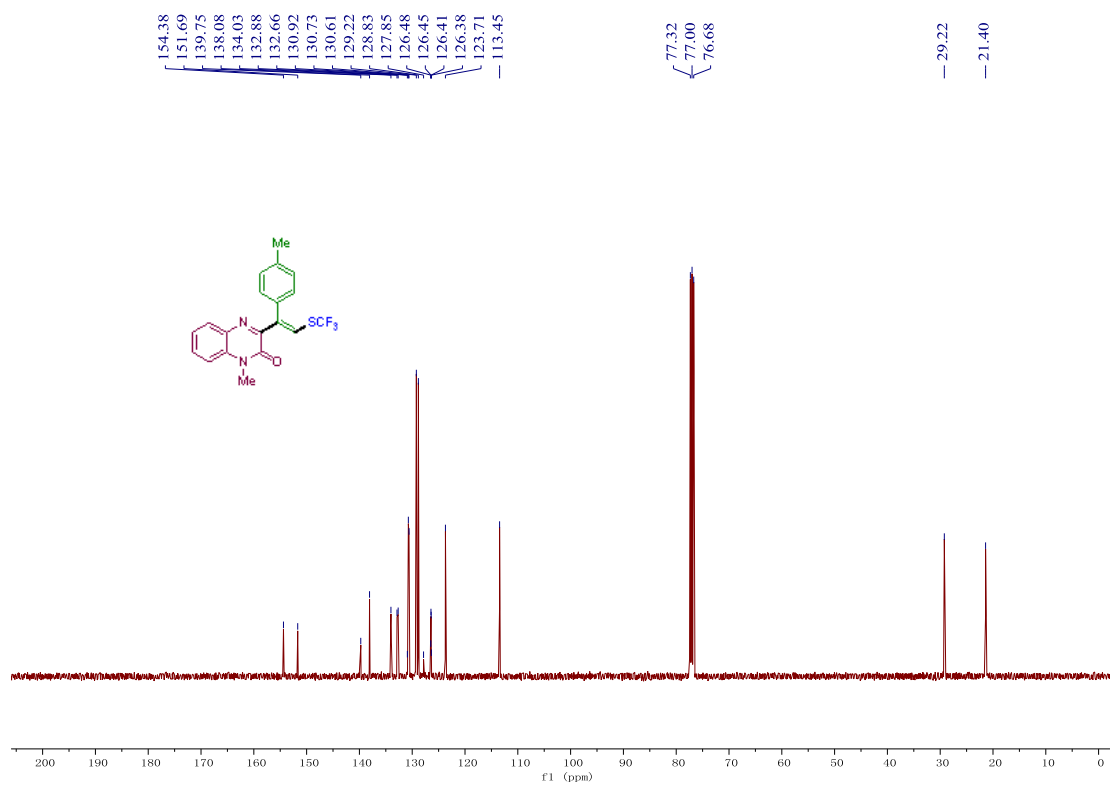
<sup>13</sup>C{<sup>1</sup>H} NMR (100 MHz, DMSO-*d*<sub>6</sub>) spectra of **3pa**



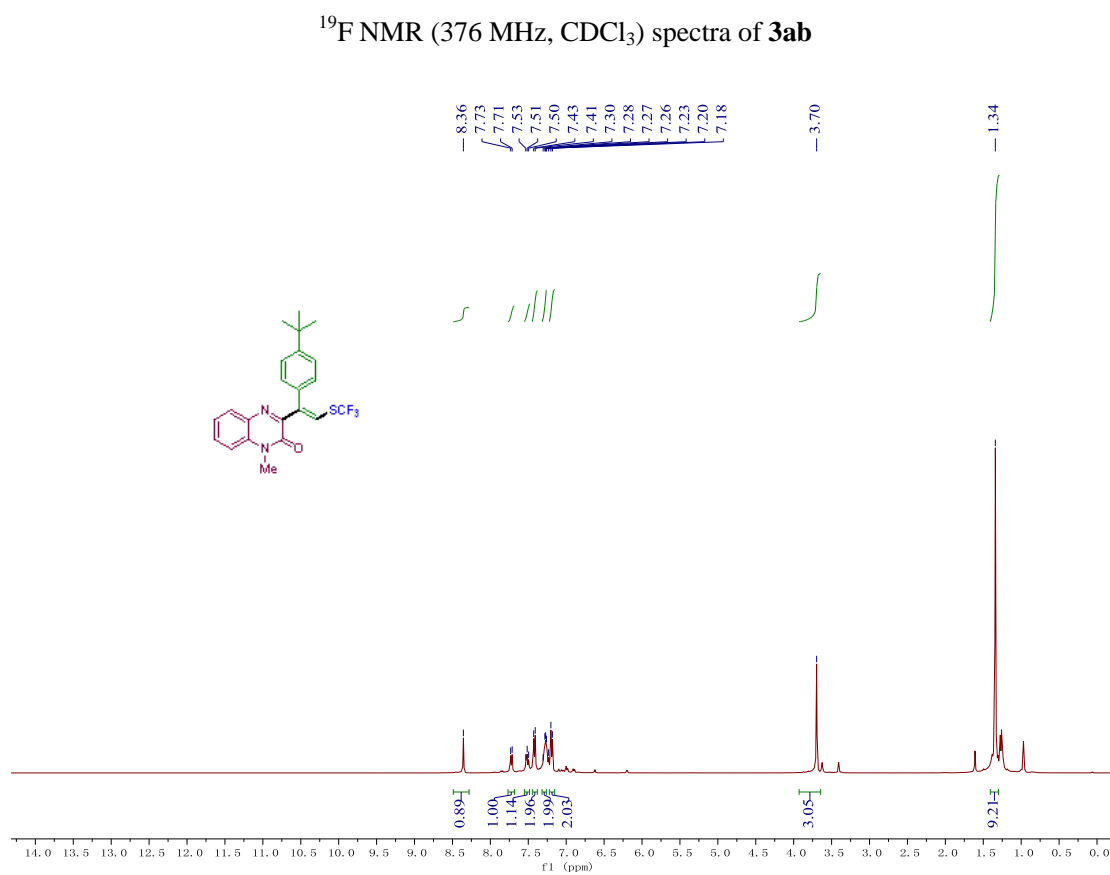
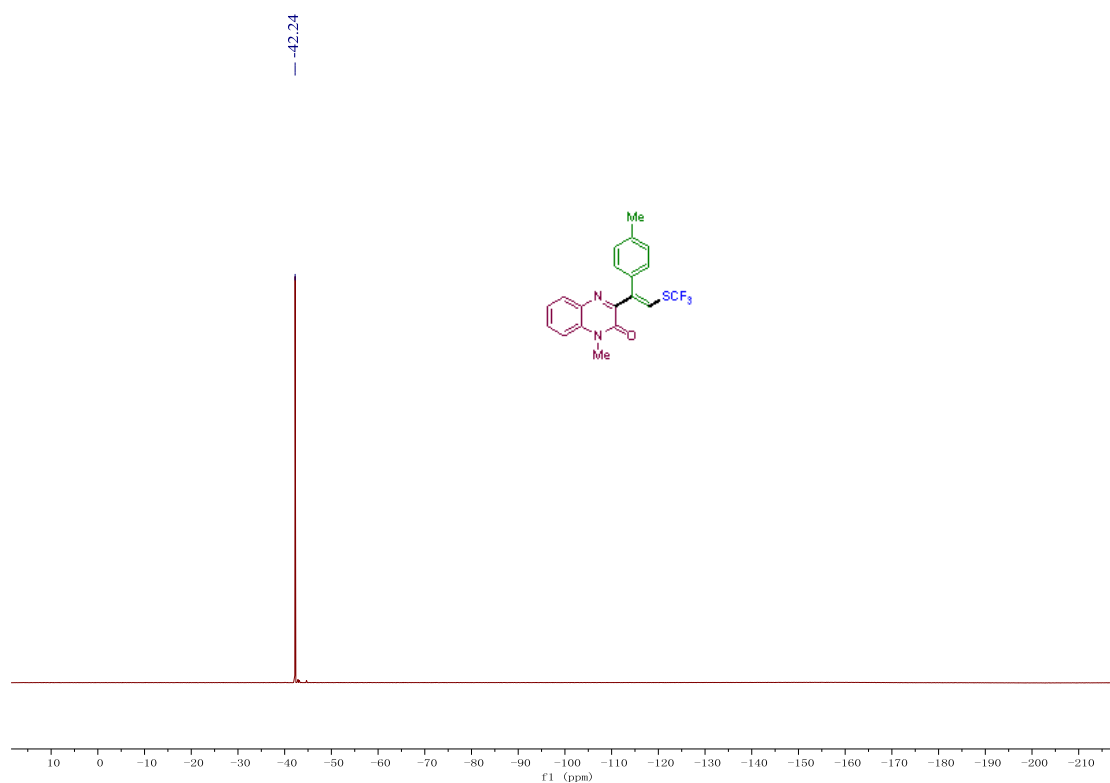
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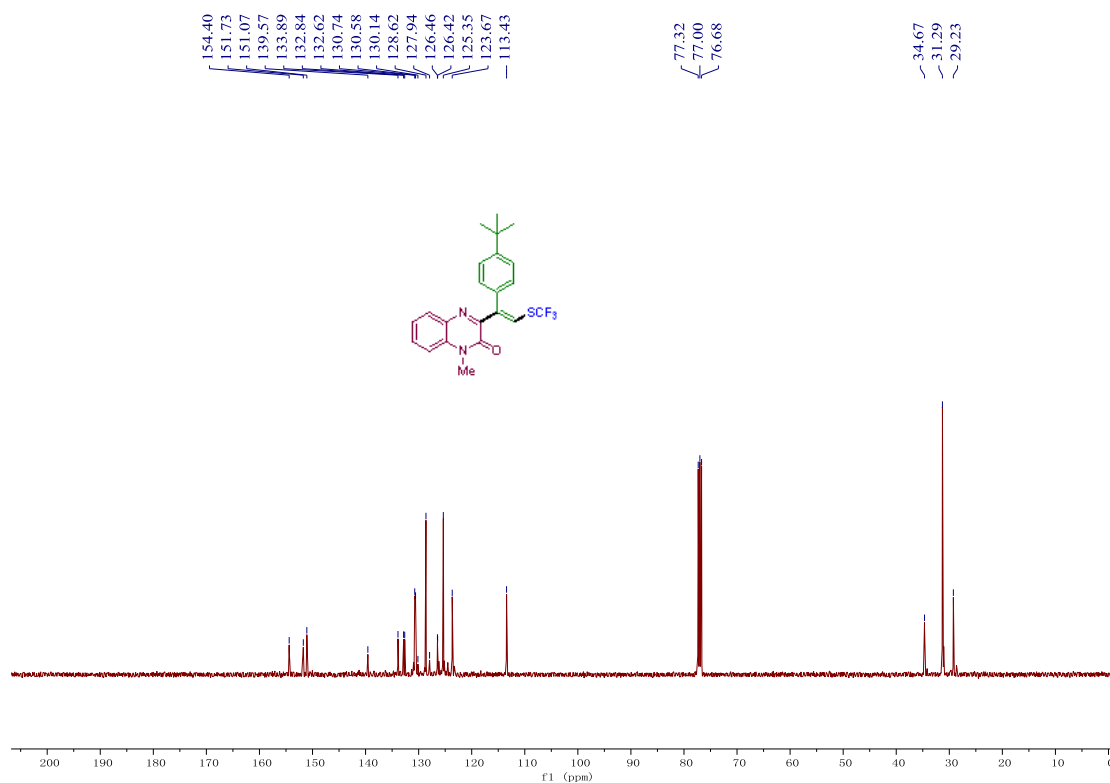


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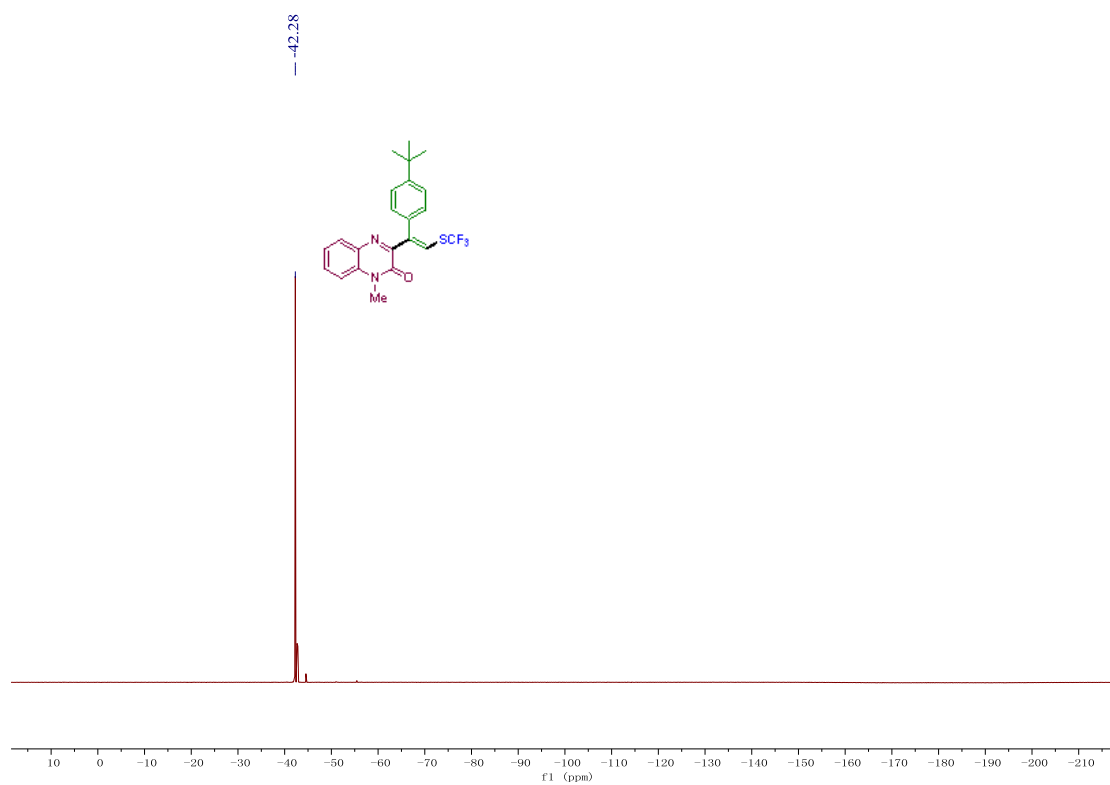


$^{13}\text{C}\{^1\text{H}\}$  NMR (100 MHz,  $\text{CDCl}_3$ ) spectra of **3ab**



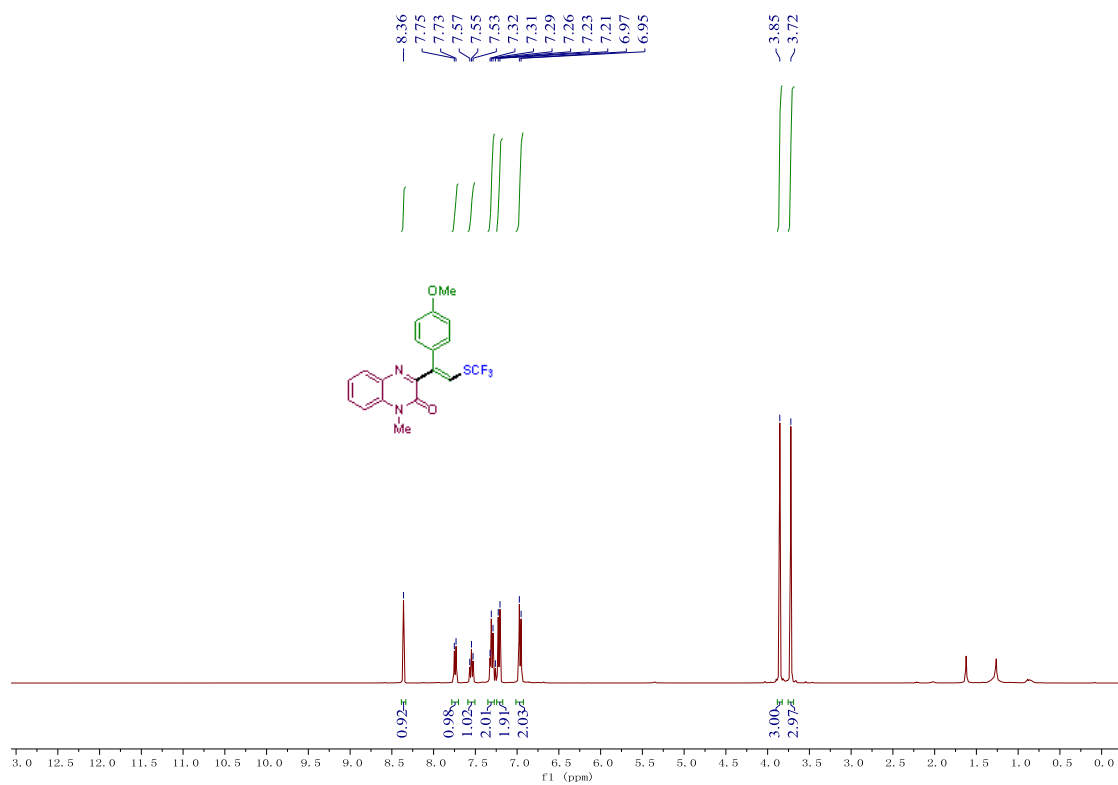


$^{13}\text{C}\{^1\text{H}\}$  NMR (100 MHz,  $\text{CDCl}_3$ ) spectra of **3ac**

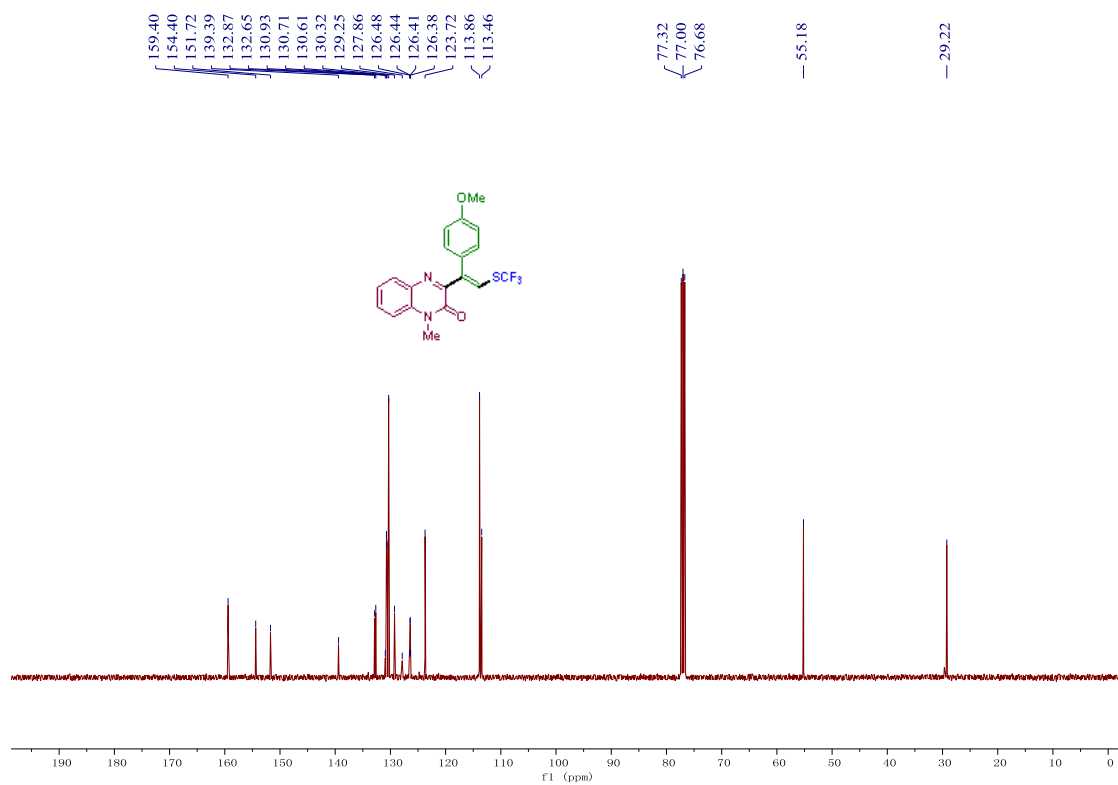


$^{19}\text{F}$  NMR (376 MHz,  $\text{CDCl}_3$ ) spectra of **3ac**

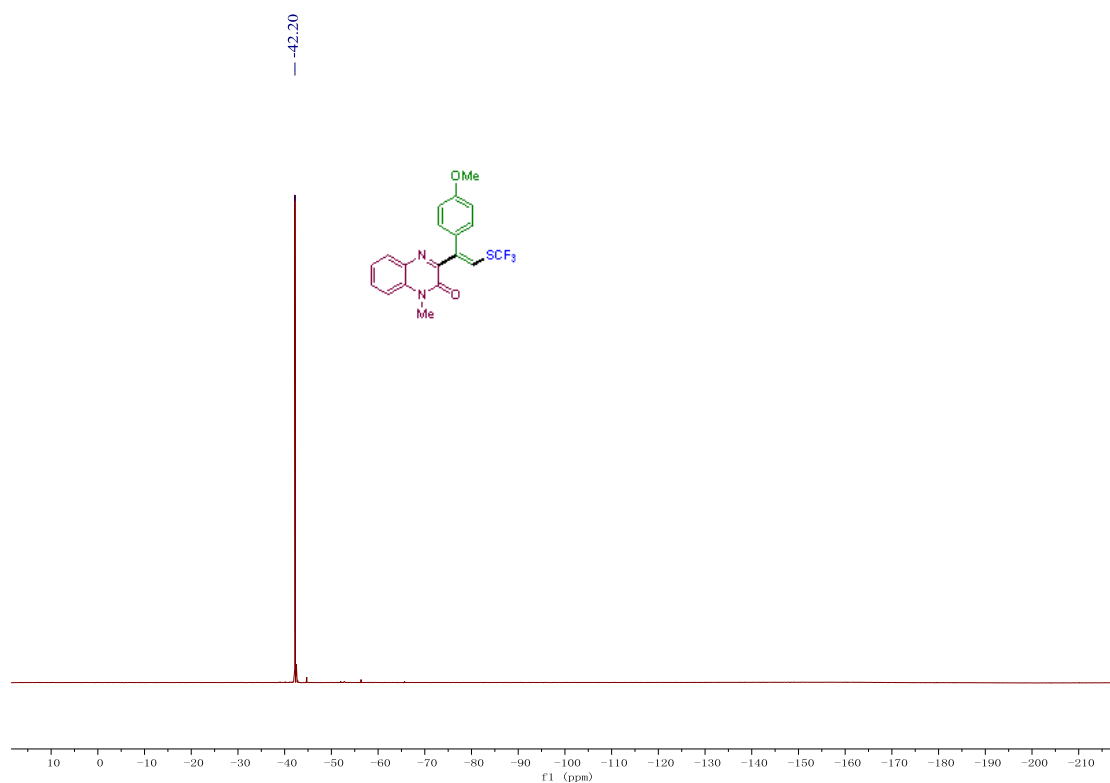




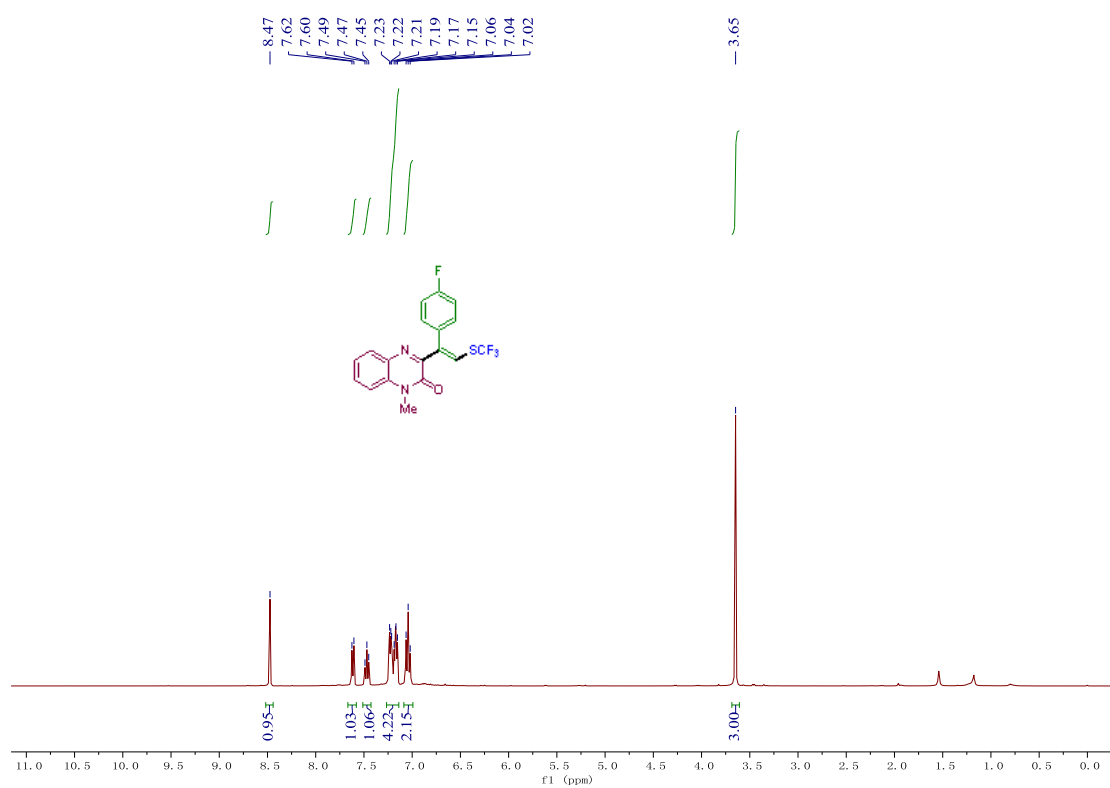
$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ) spectra of **3ad**



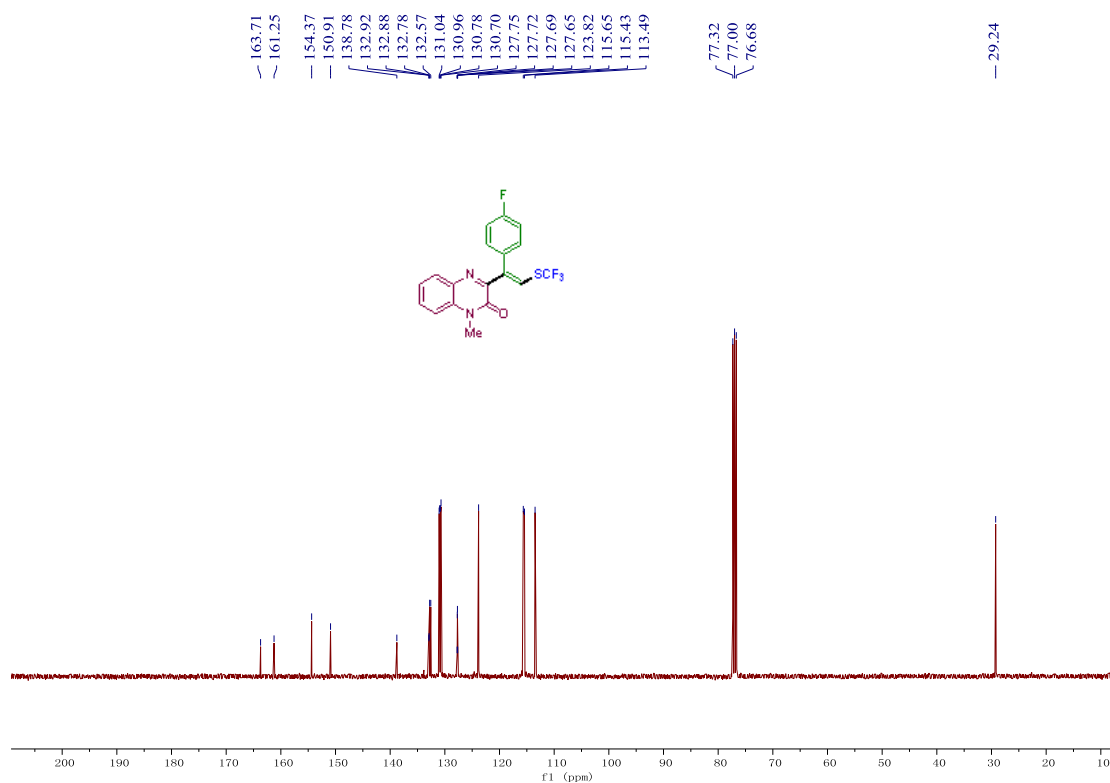
$^{13}\text{C}\{^1\text{H}\}$  NMR (100 MHz,  $\text{CDCl}_3$ ) spectra of **3ad**



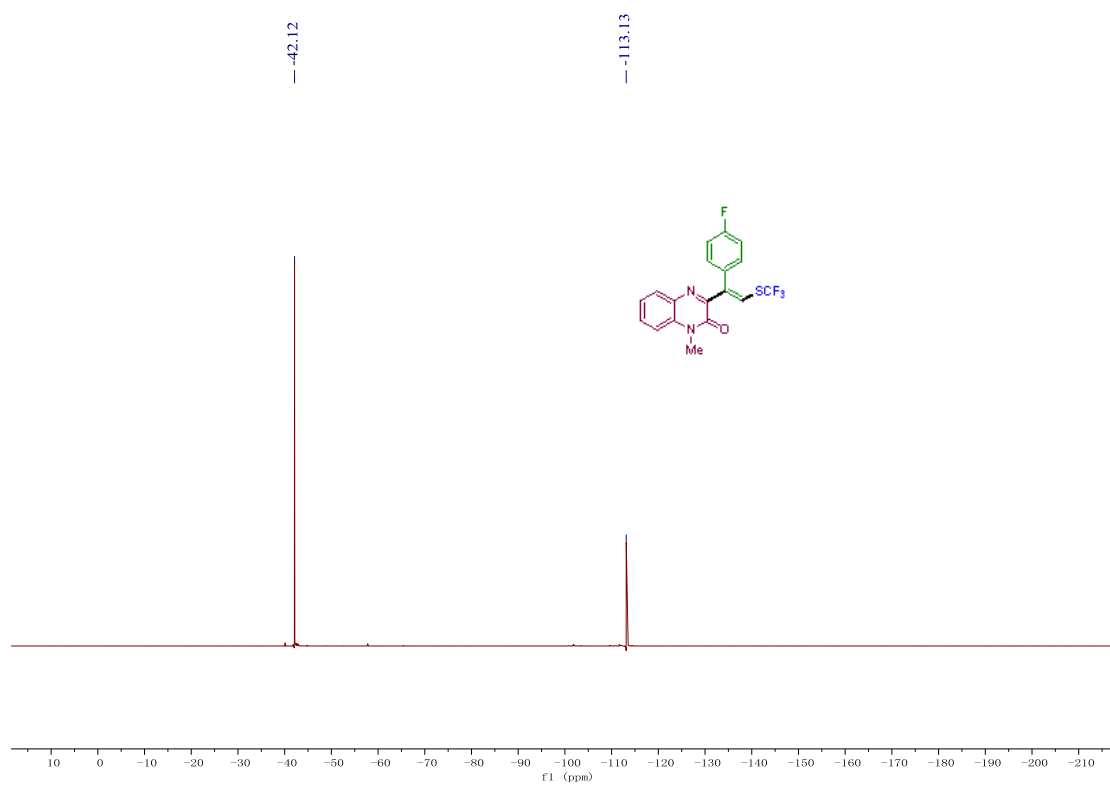
$^{19}\text{F}$  NMR (376 MHz,  $\text{CDCl}_3$ ) spectra of **3ad**



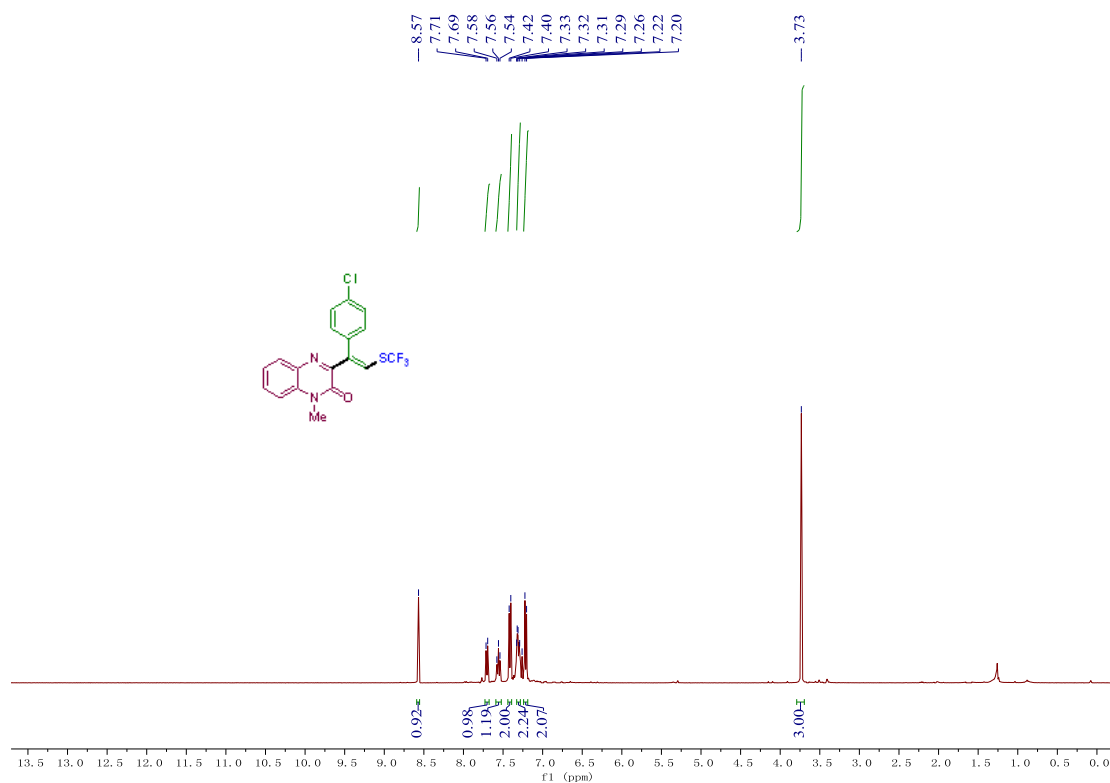
$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ) spectra of **3ae**



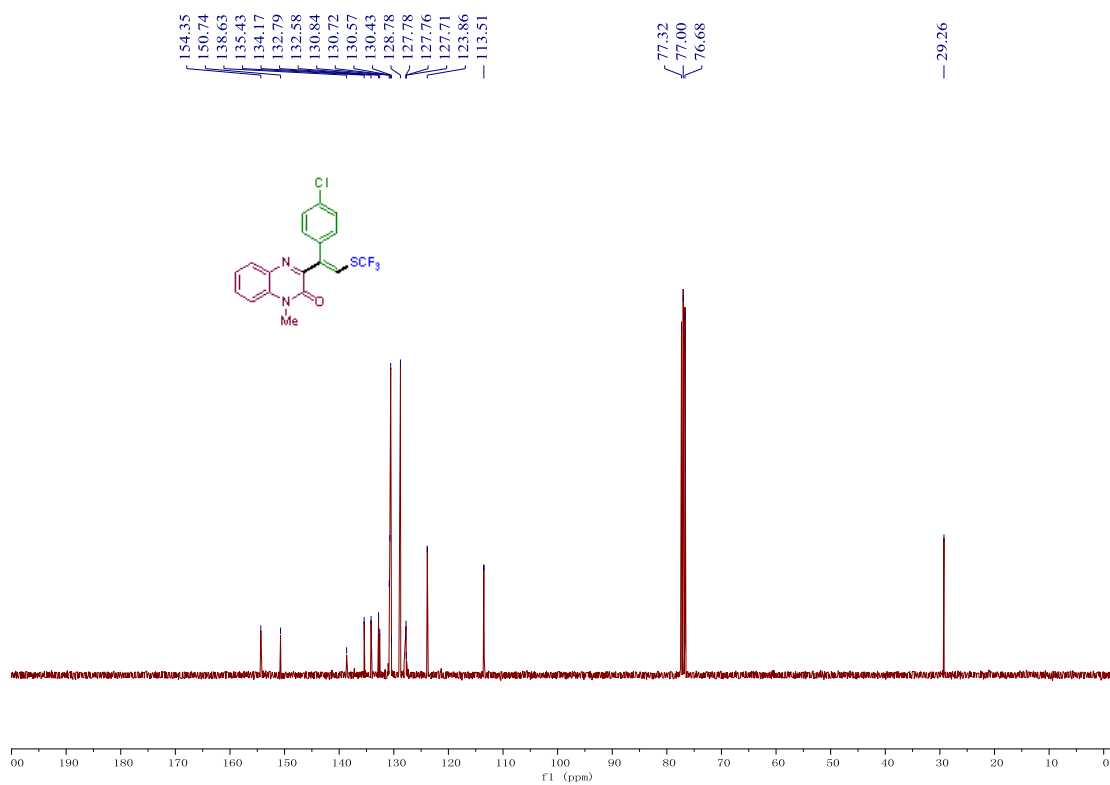
$^{13}\text{C}\{^1\text{H}\}$  NMR (100 MHz,  $\text{CDCl}_3$ ) spectra of **3ae**



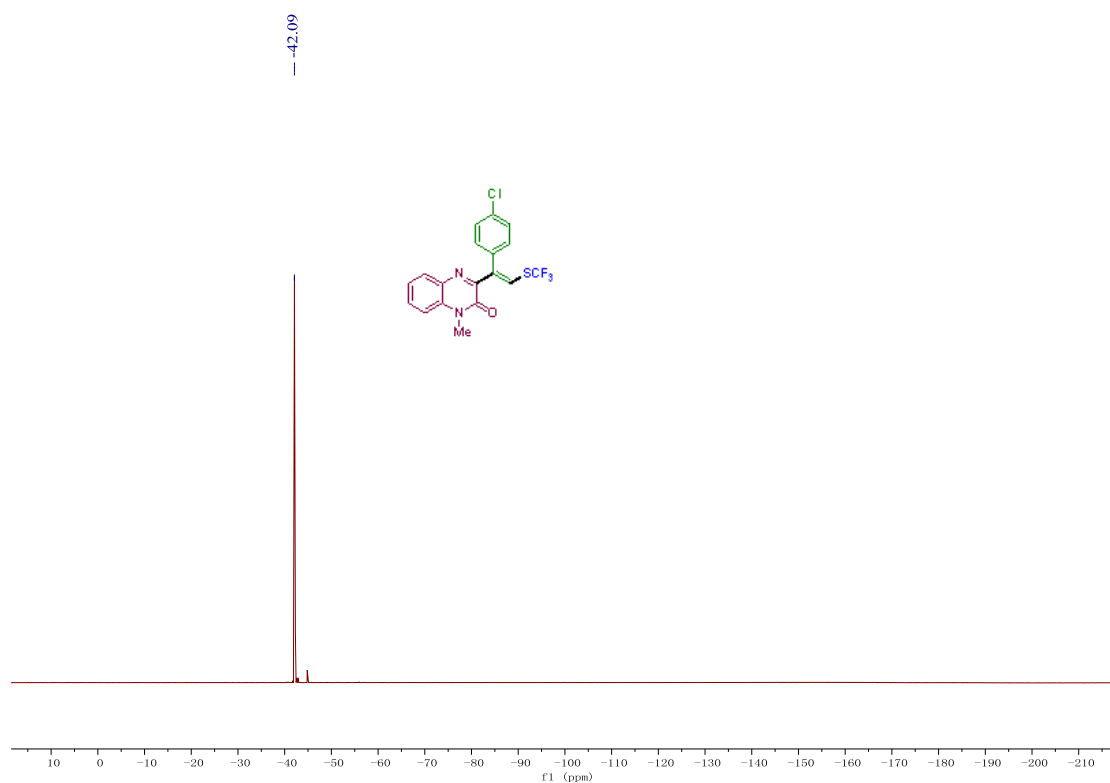
$^{19}\text{F}$  NMR (376 MHz,  $\text{CDCl}_3$ ) spectra of **3ae**



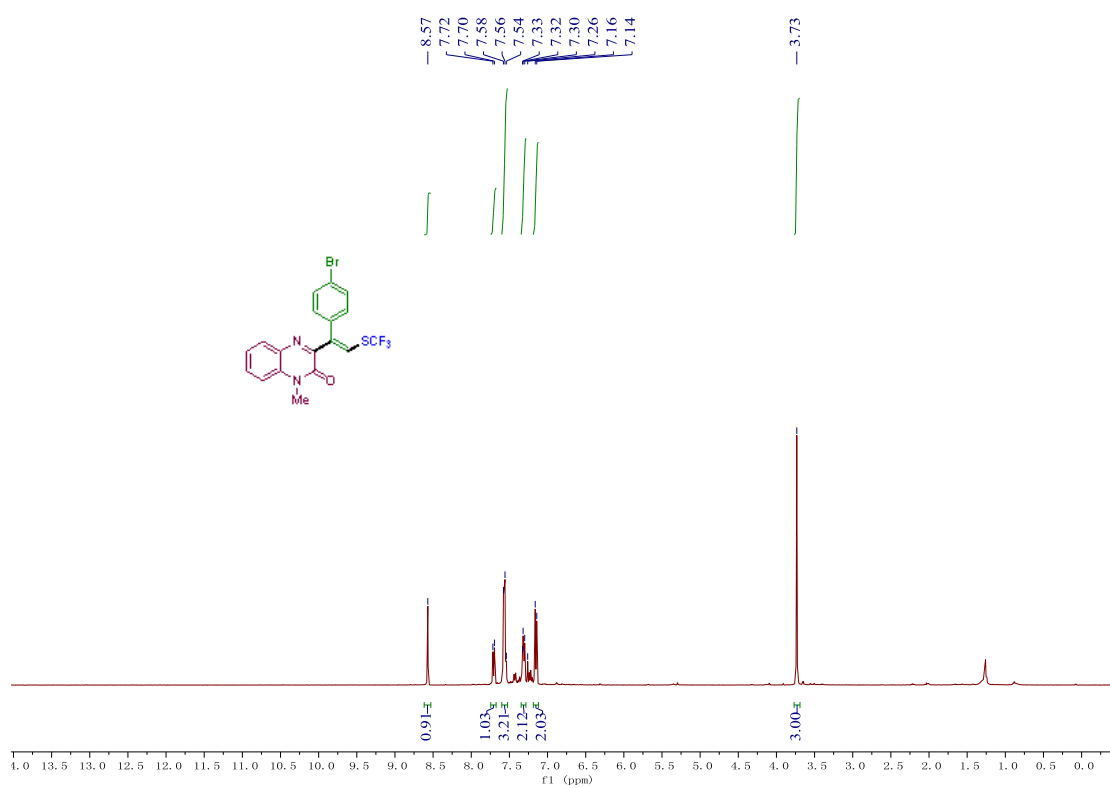
$^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ ) spectra of **3af**



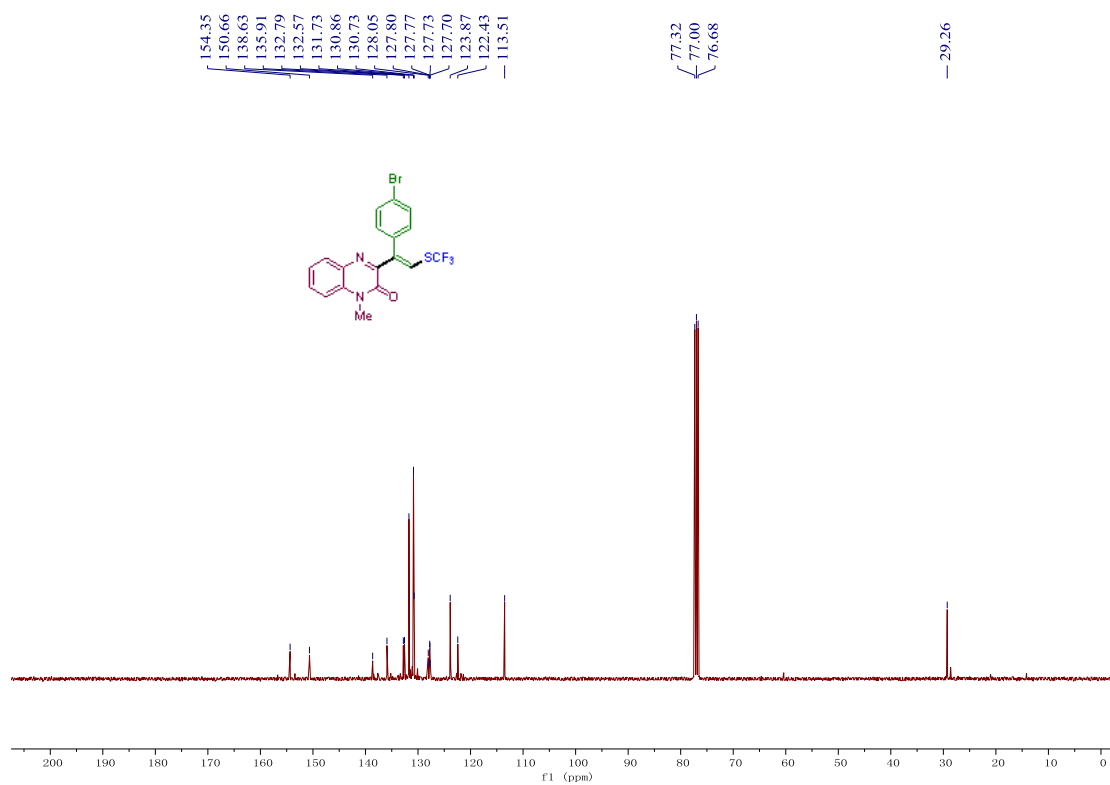
$^{13}\text{C}\{^1\text{H}\}$  NMR (100 MHz,  $\text{CDCl}_3$ ) spectra of **3af**



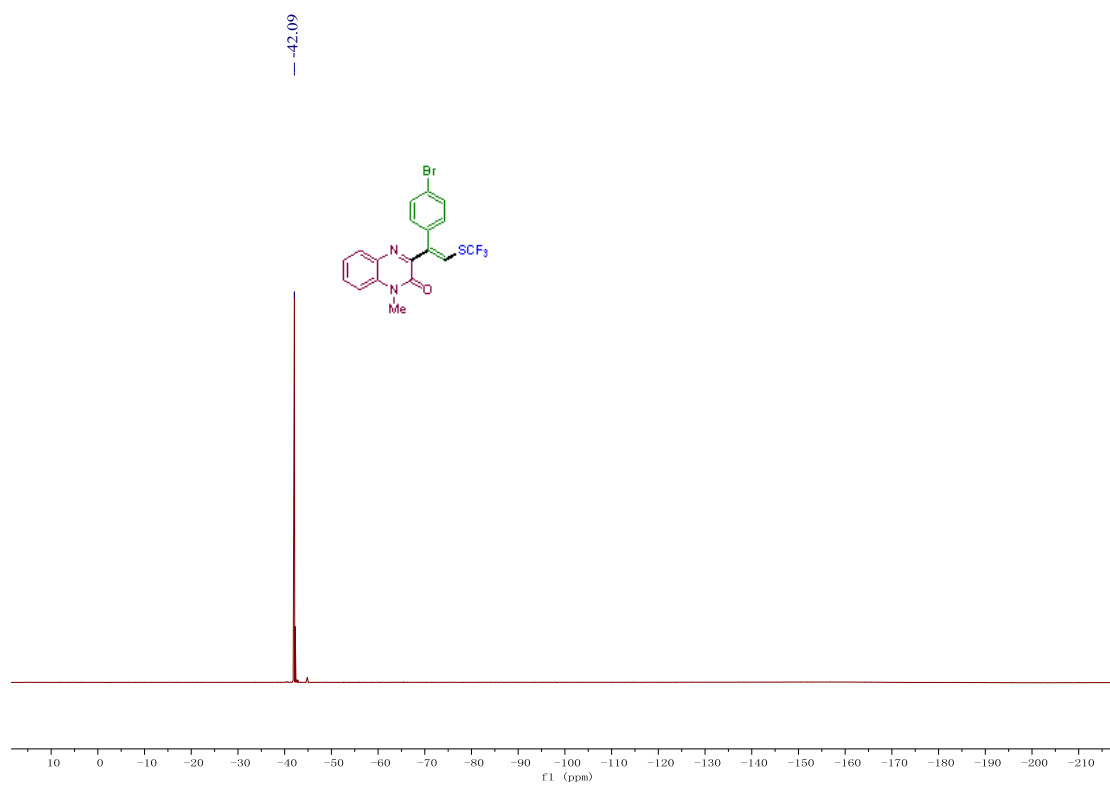
$^{19}\text{F}$  NMR (376 MHz,  $\text{CDCl}_3$ ) spectra of **3af**



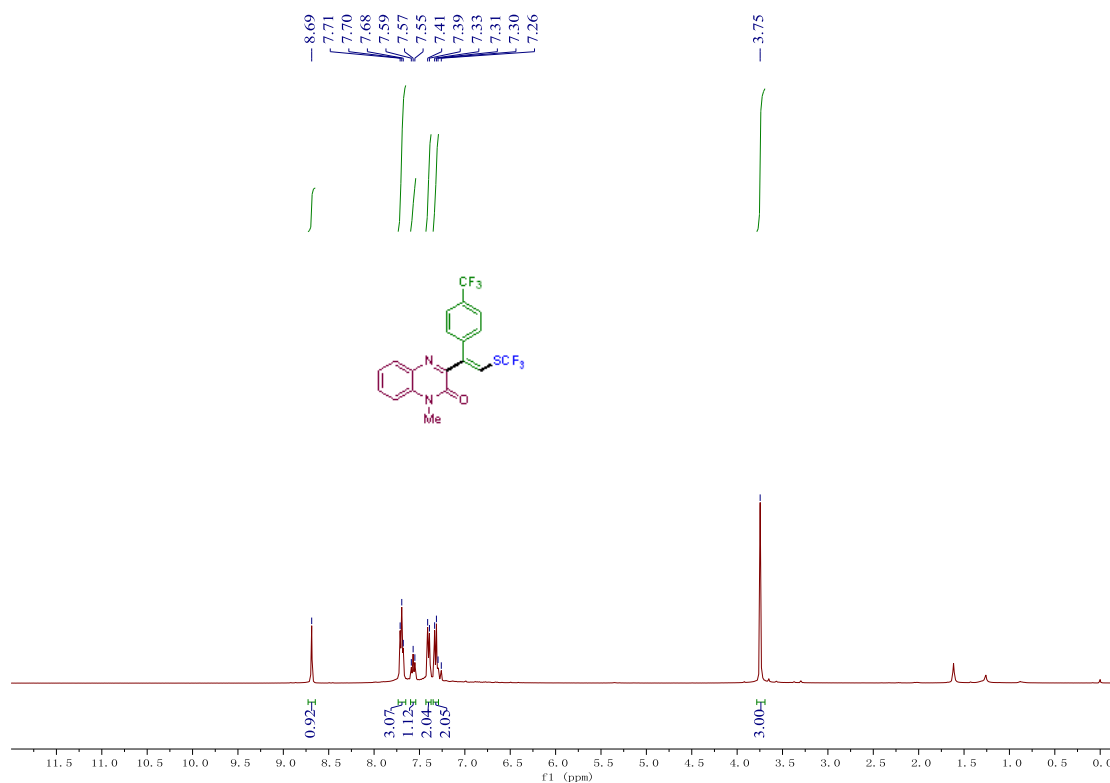
$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ) spectra of **3ag**



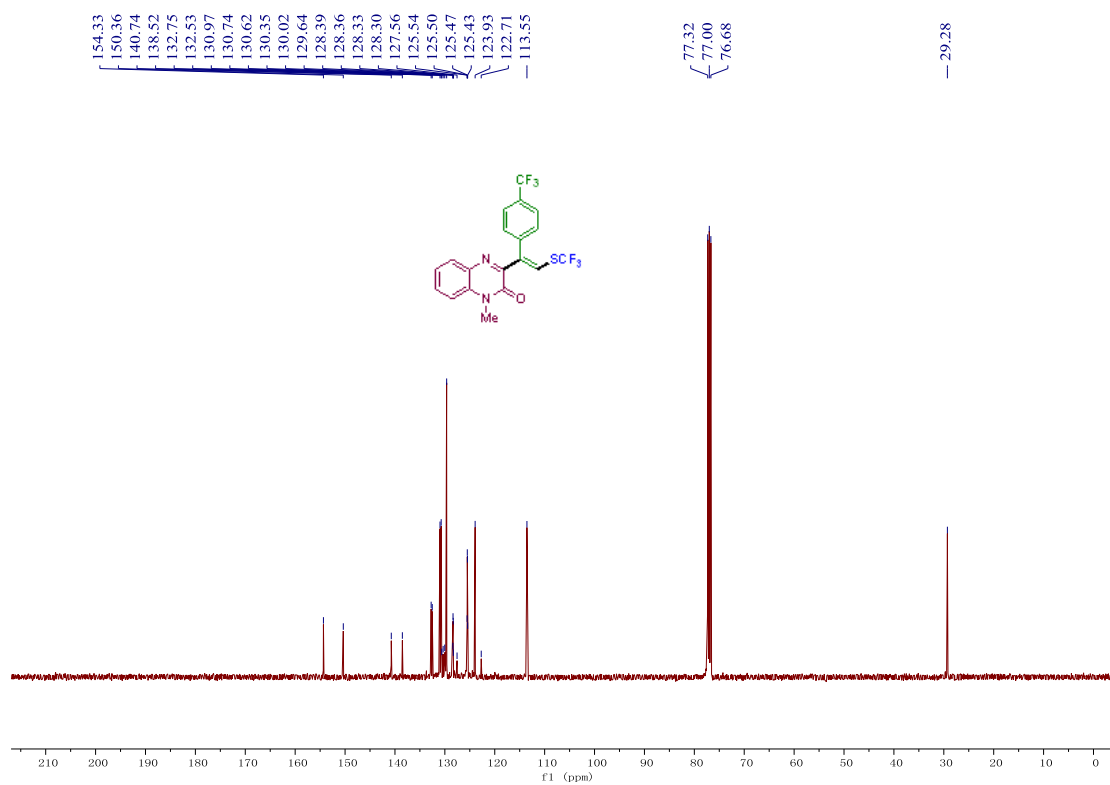
$^{13}\text{C}\{^1\text{H}\}$  NMR (100 MHz,  $\text{CDCl}_3$ ) spectra of **3ag**



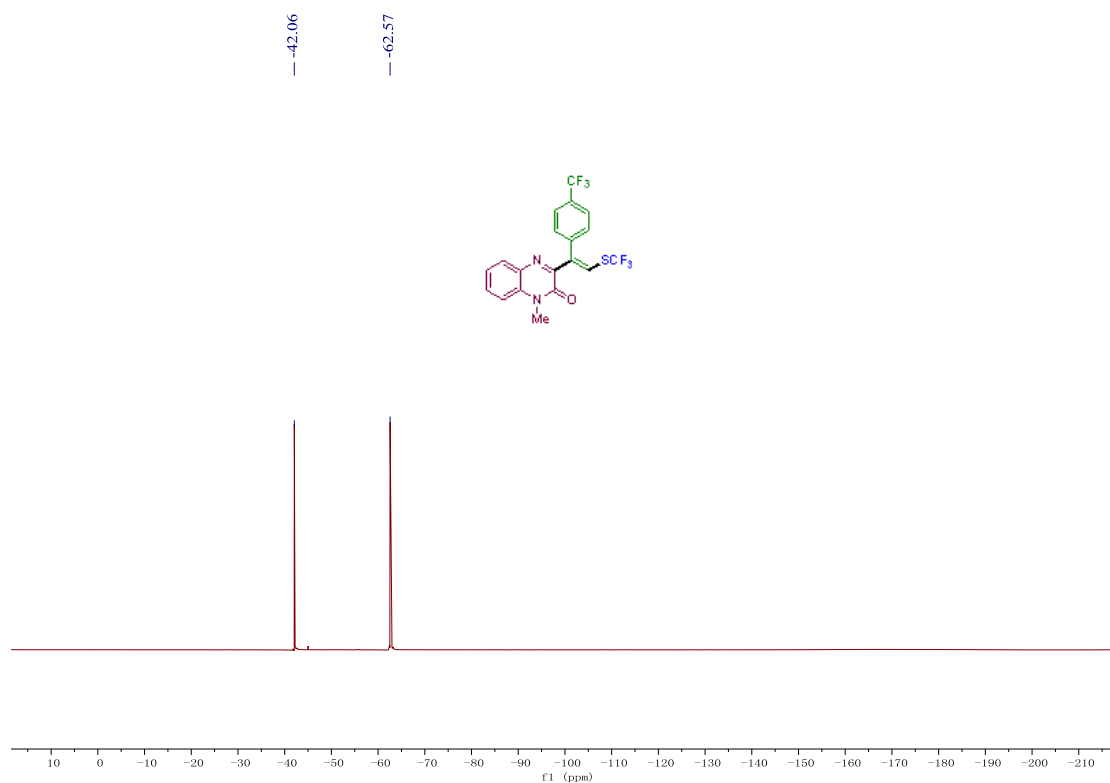
$^{19}\text{F}$  NMR (376 MHz,  $\text{CDCl}_3$ ) spectra of **3ag**



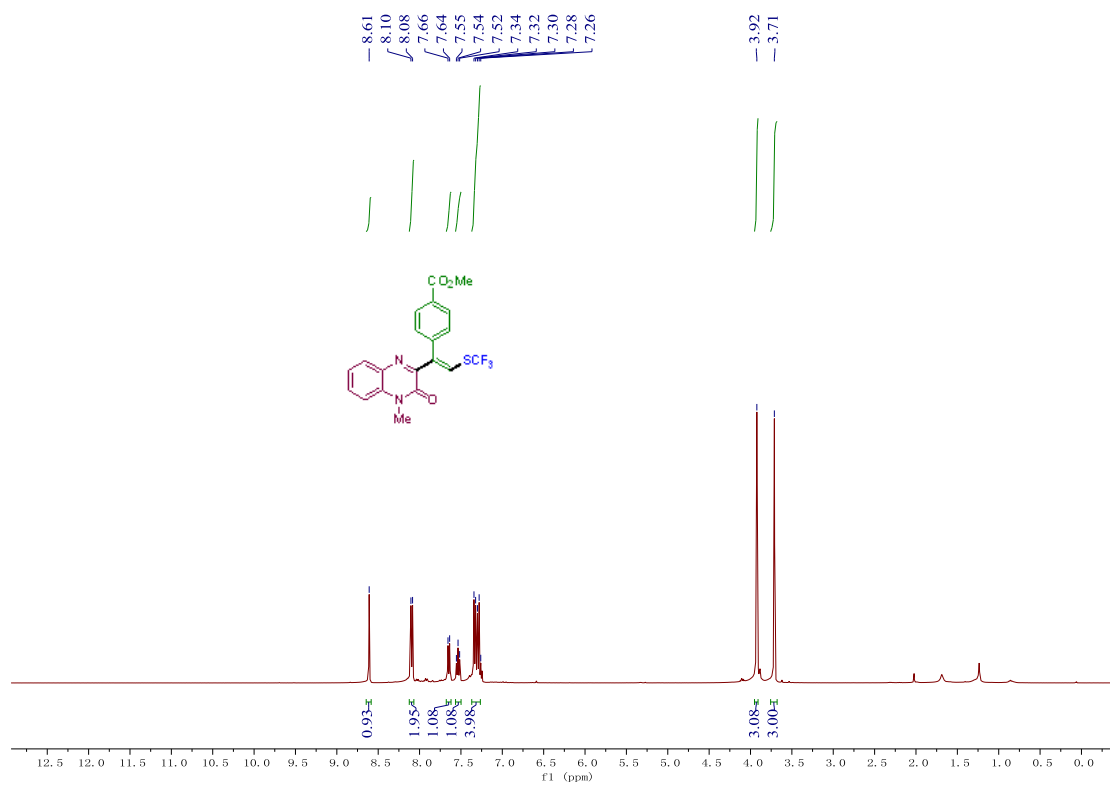
$^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ ) spectra of **3ah**



$^{13}\text{C}\{^1\text{H}\}$  NMR (100 MHz,  $\text{CDCl}_3$ ) spectra of **3ah**

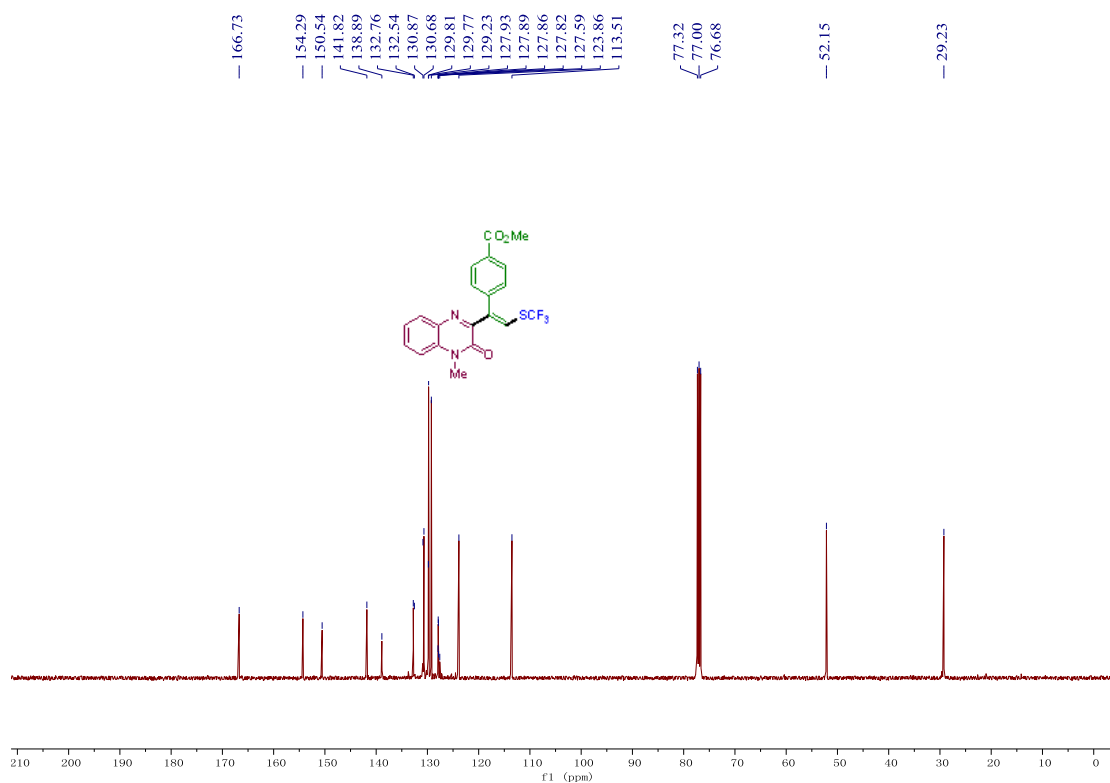


$^{19}\text{F}$  NMR (376 MHz,  $\text{CDCl}_3$ ) spectra of **3ah**

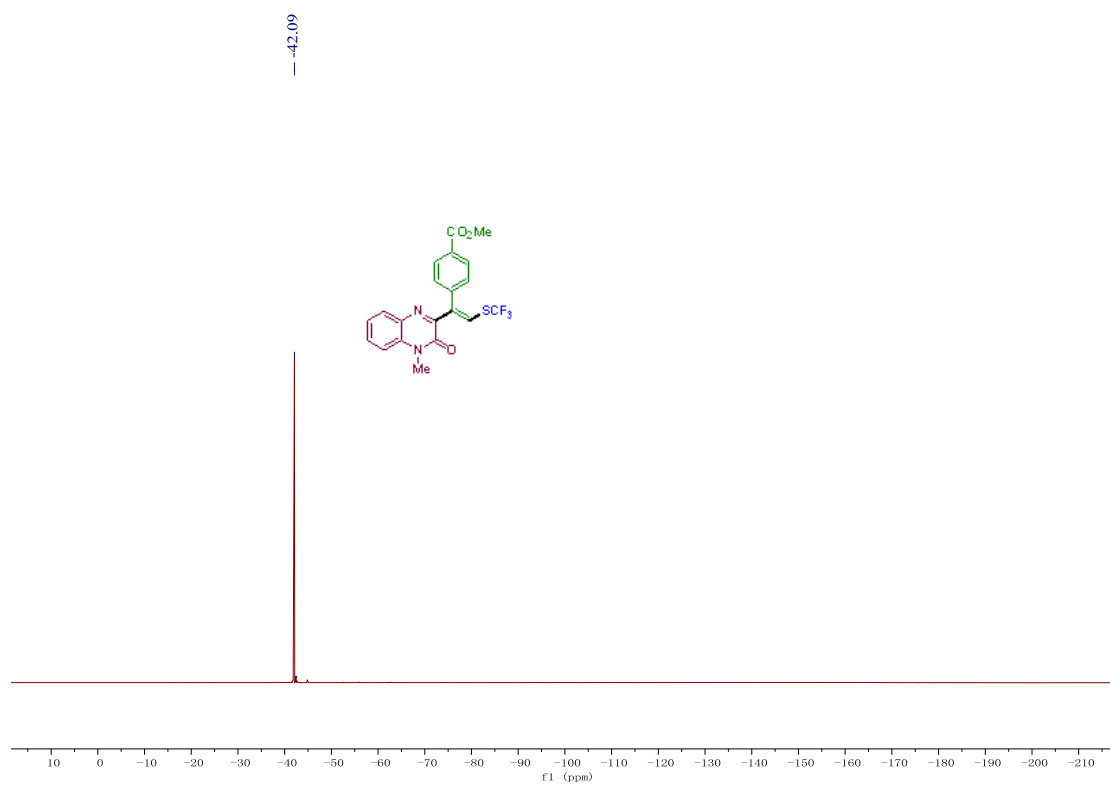


$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ) spectra of **3ai**

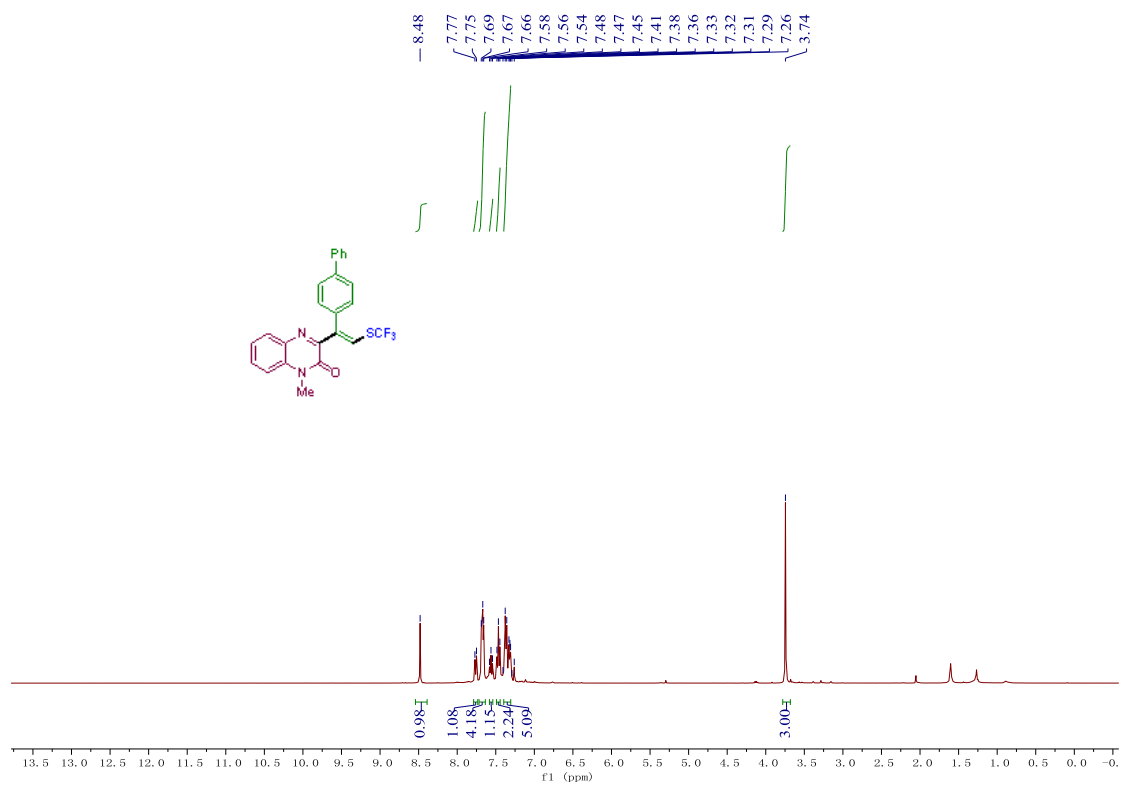




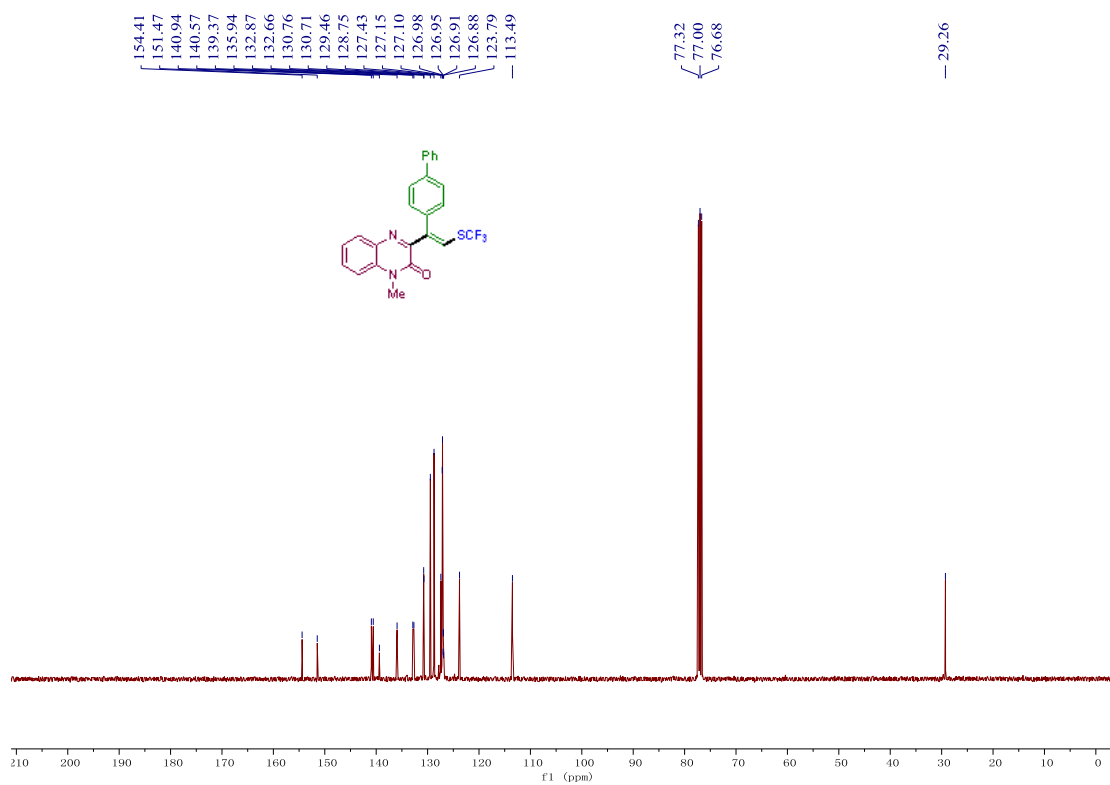
<sup>13</sup>C{<sup>1</sup>H} NMR (100 MHz, CDCl<sub>3</sub>) spectra of **3ai**



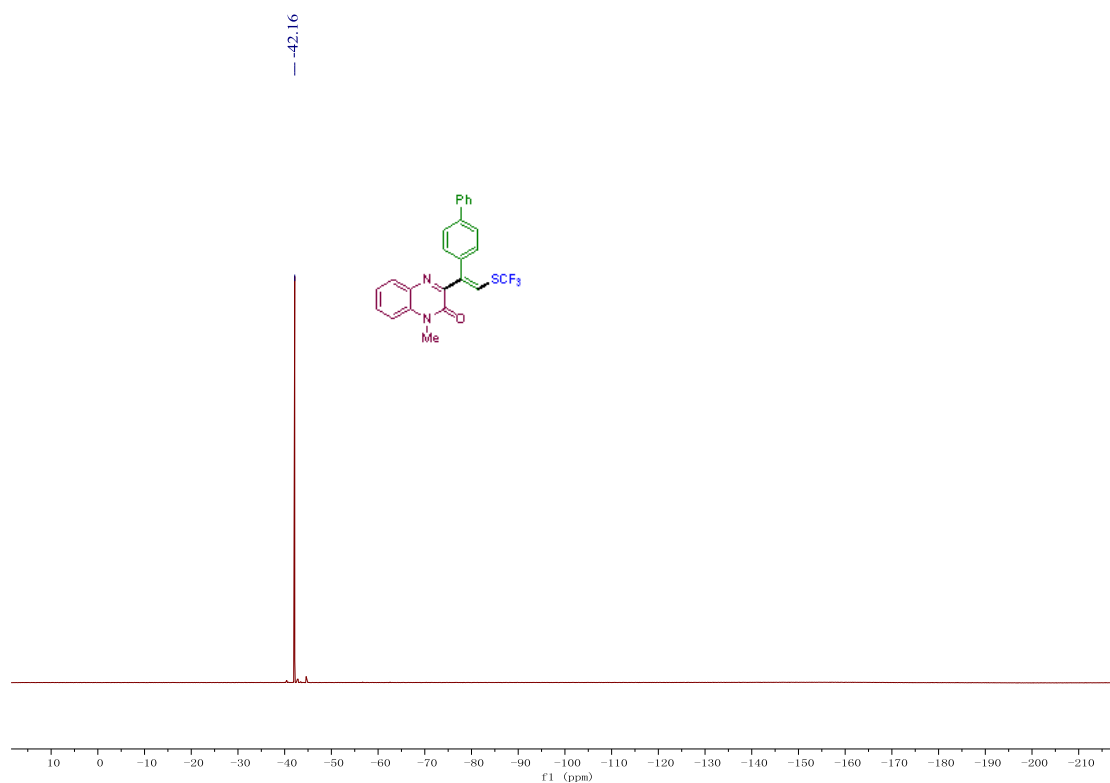
<sup>19</sup>F NMR (376 MHz, CDCl<sub>3</sub>) spectra of **3ai**



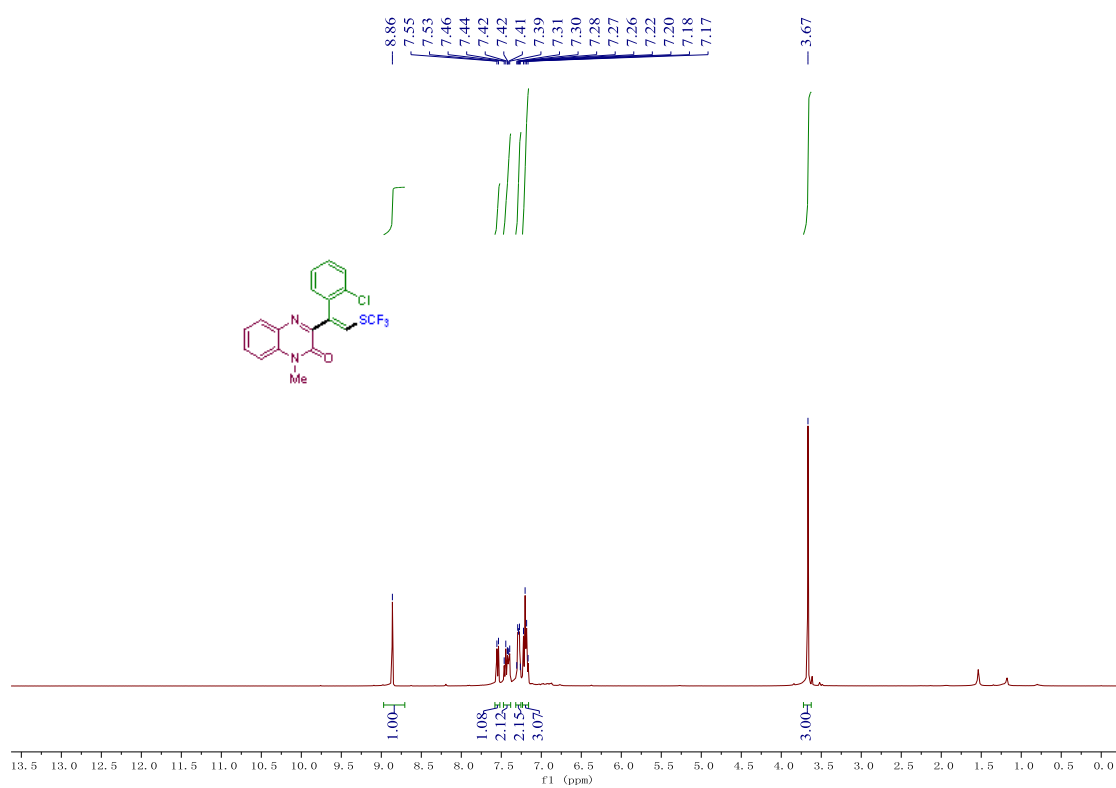
$^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ ) spectra of **3aj**



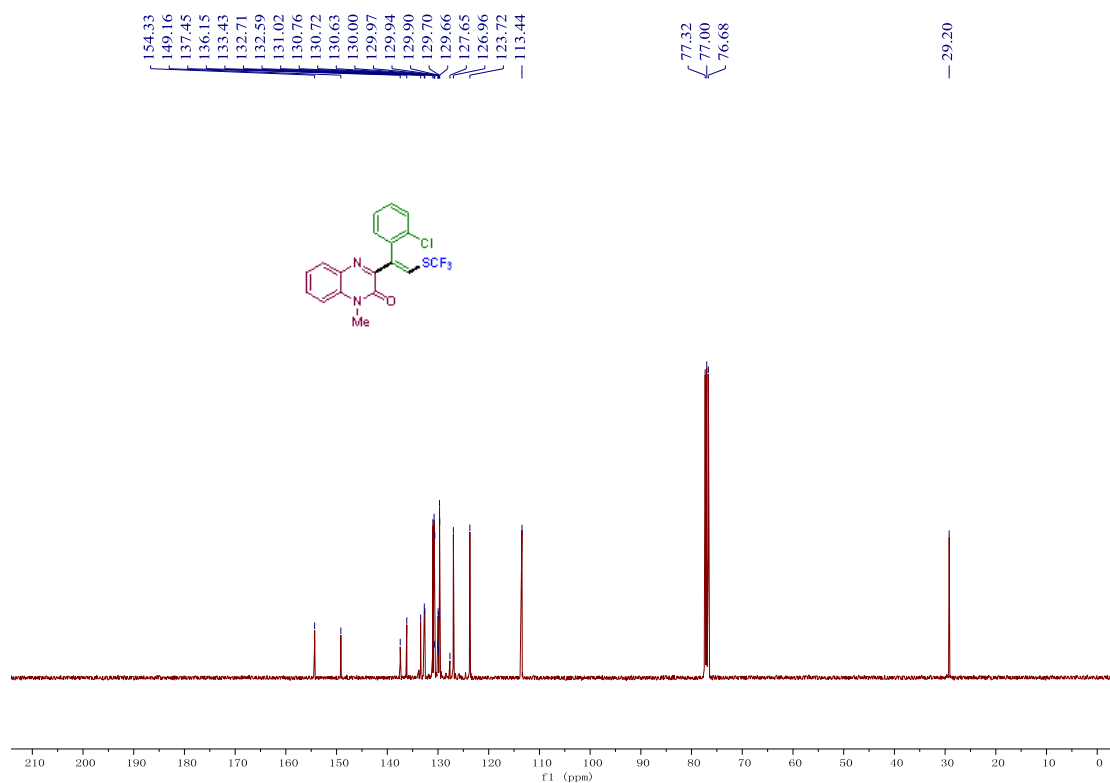
$^{13}\text{C}\{^1\text{H}\}$  NMR (100 MHz,  $\text{CDCl}_3$ ) spectra of **3aj**



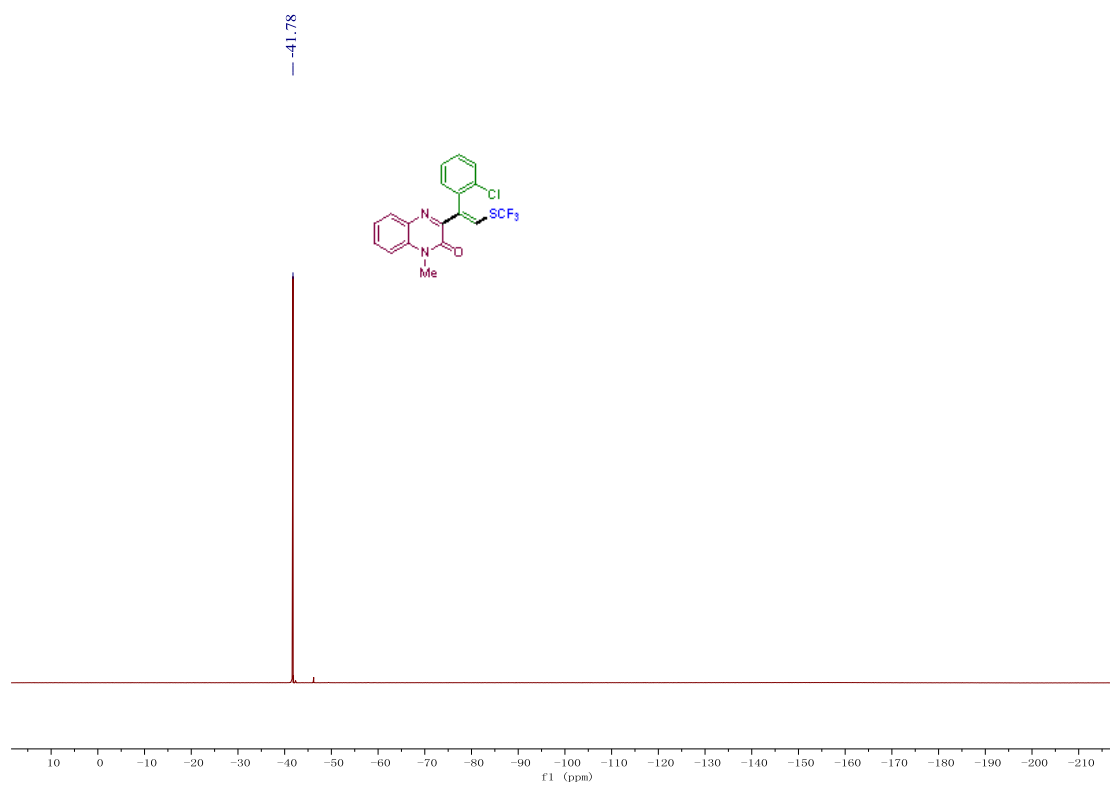
<sup>19</sup>F NMR (376 MHz, CDCl<sub>3</sub>) spectra of **3aj**



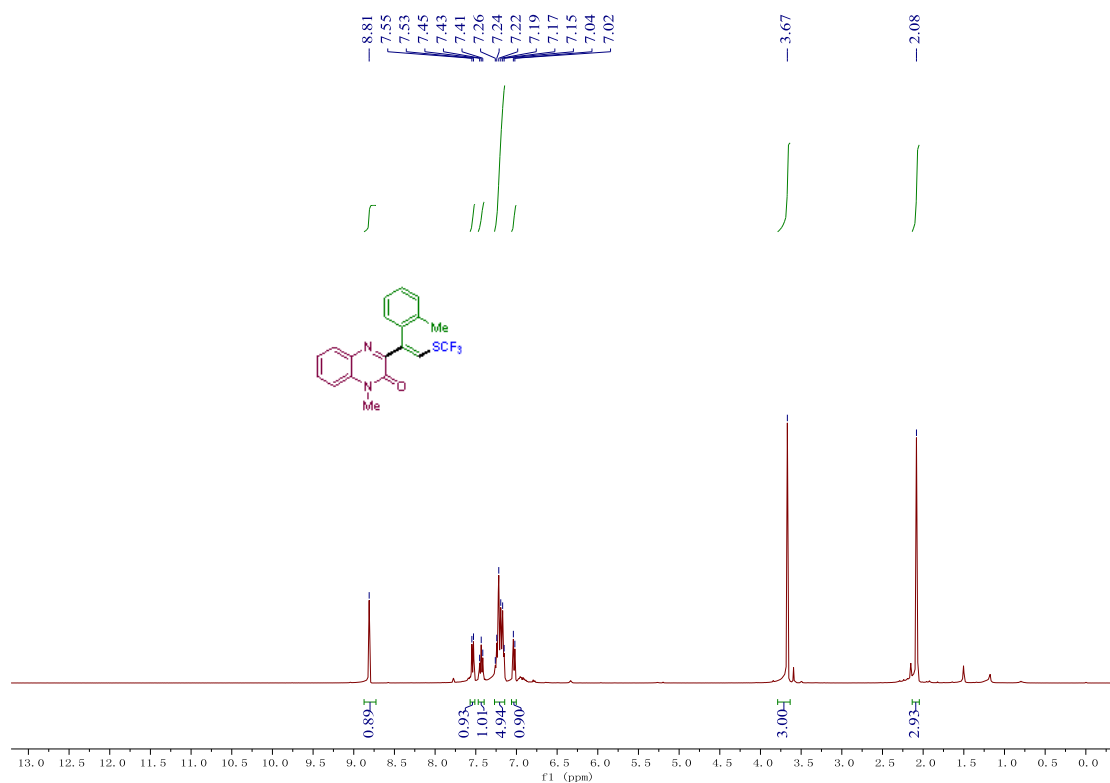
<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) spectra of **3ak**



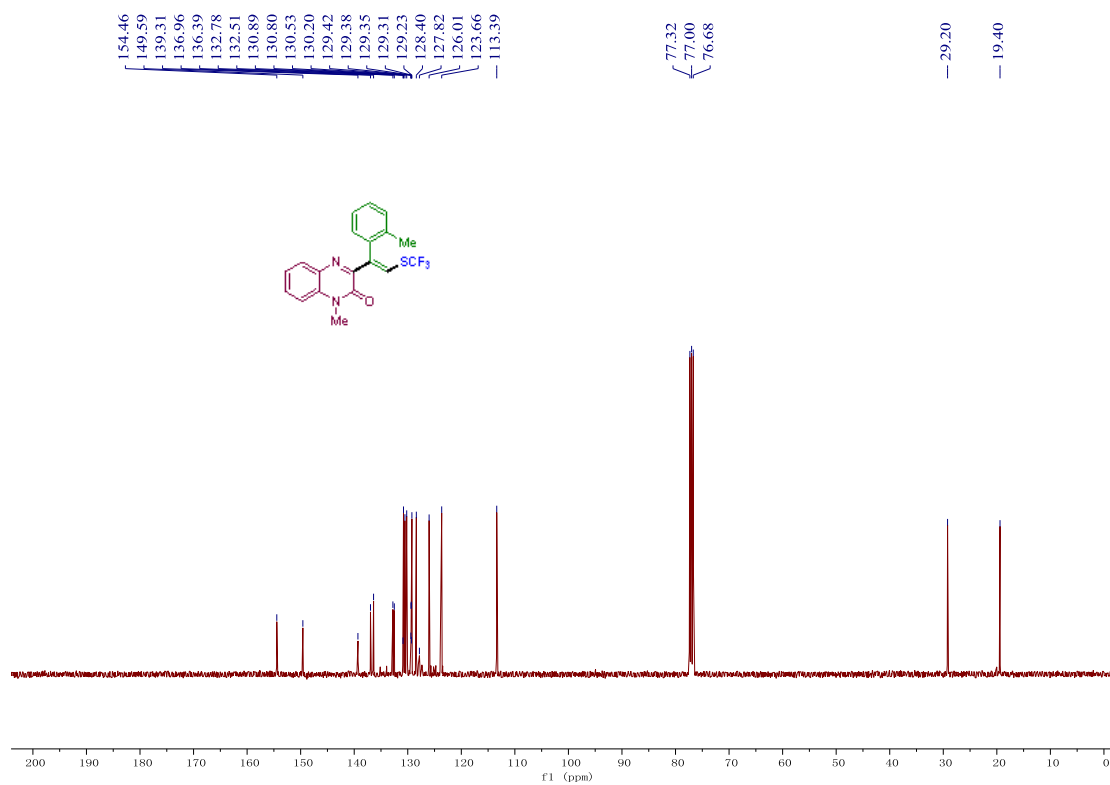
$^{13}\text{C}\{^1\text{H}\}$  NMR (100 MHz,  $\text{CDCl}_3$ ) spectra of **3ak**



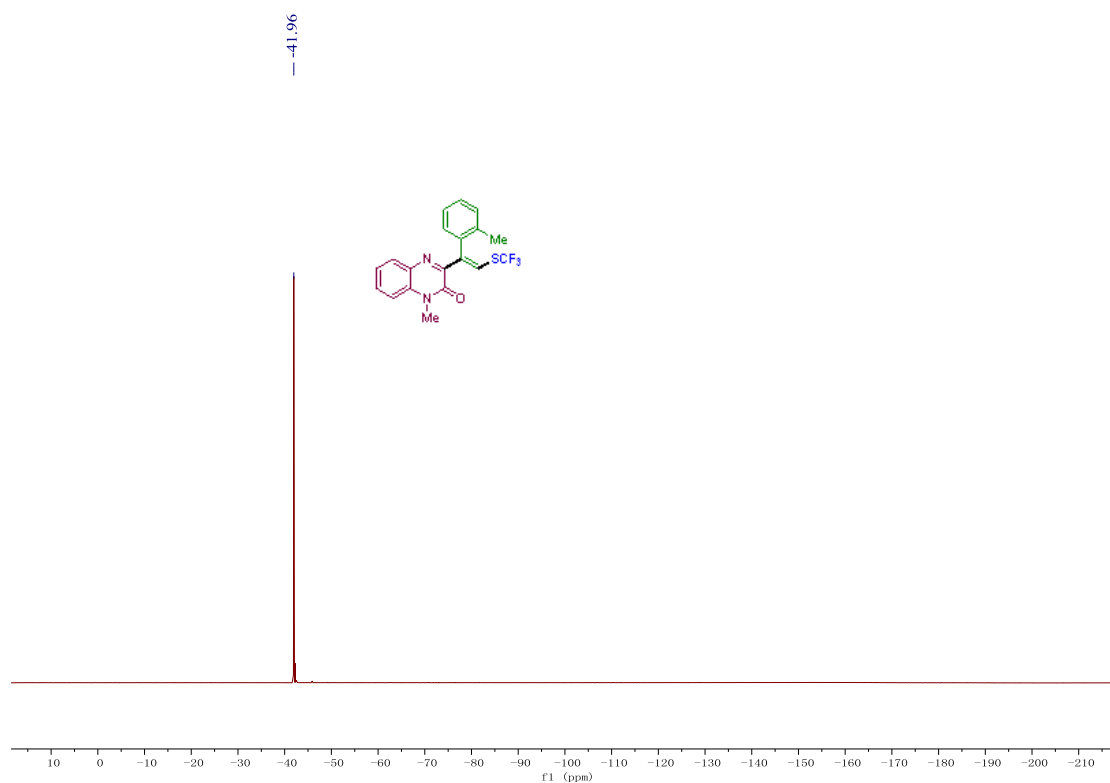
$^{19}\text{F}$  NMR (376 MHz,  $\text{CDCl}_3$ ) spectra of **3ak**



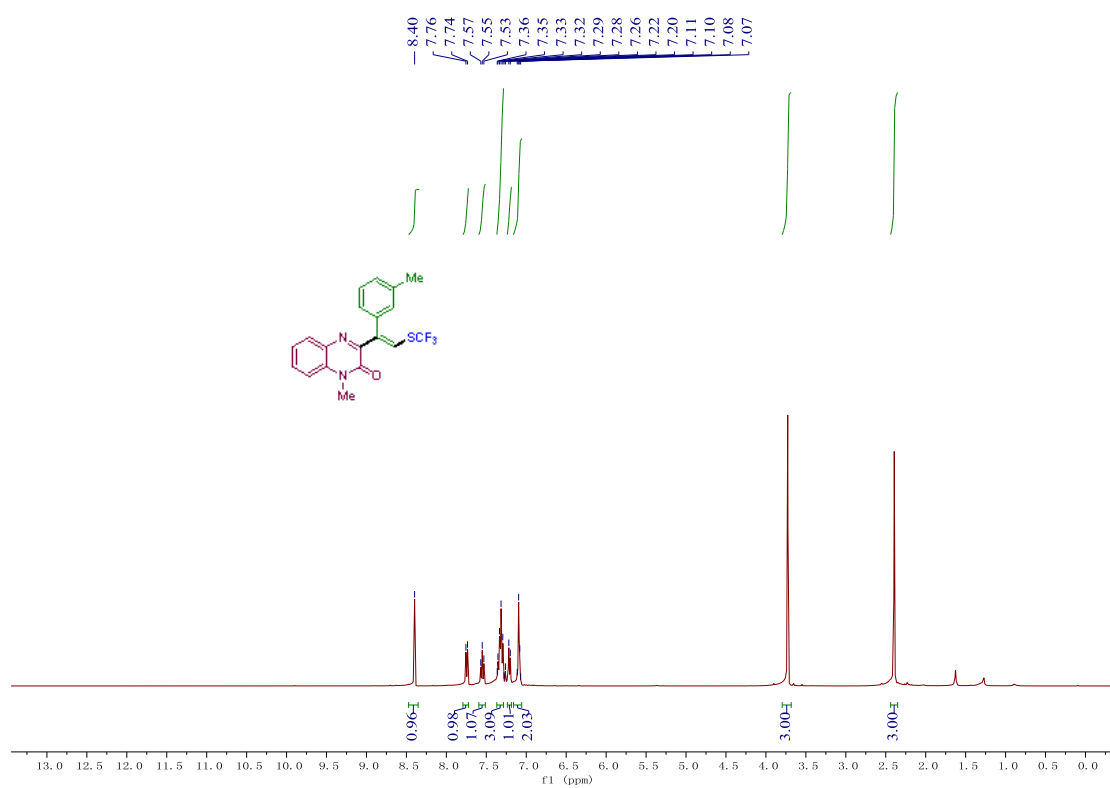
$^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ ) spectra of **3al**



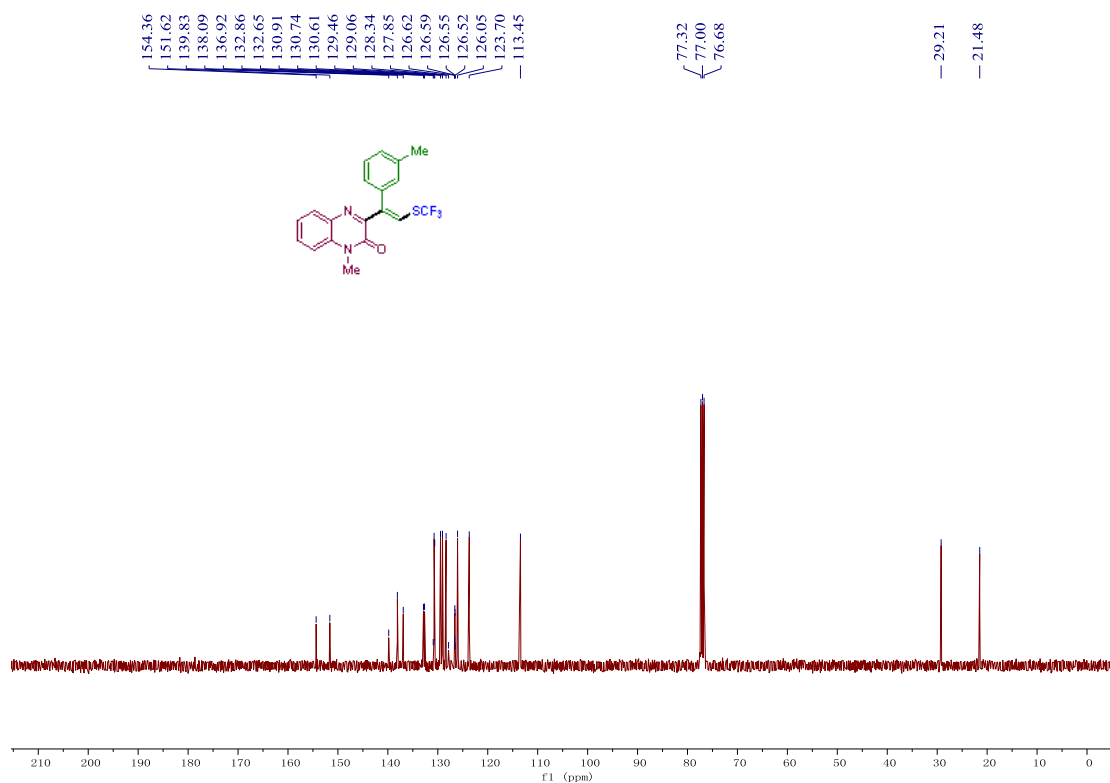
$^{13}\text{C}\{^1\text{H}\}$  NMR (100 MHz,  $\text{CDCl}_3$ ) spectra of **3al**



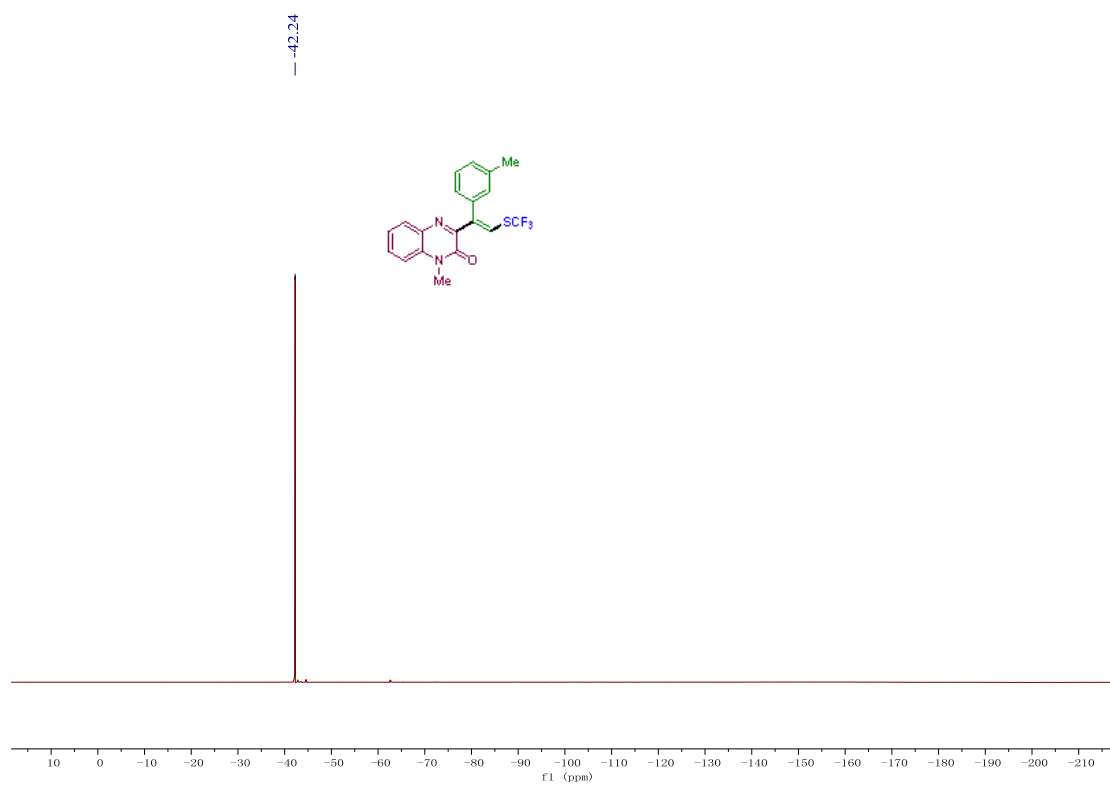
$^{19}\text{F}$  NMR (376 MHz,  $\text{CDCl}_3$ ) spectra of **3aI**



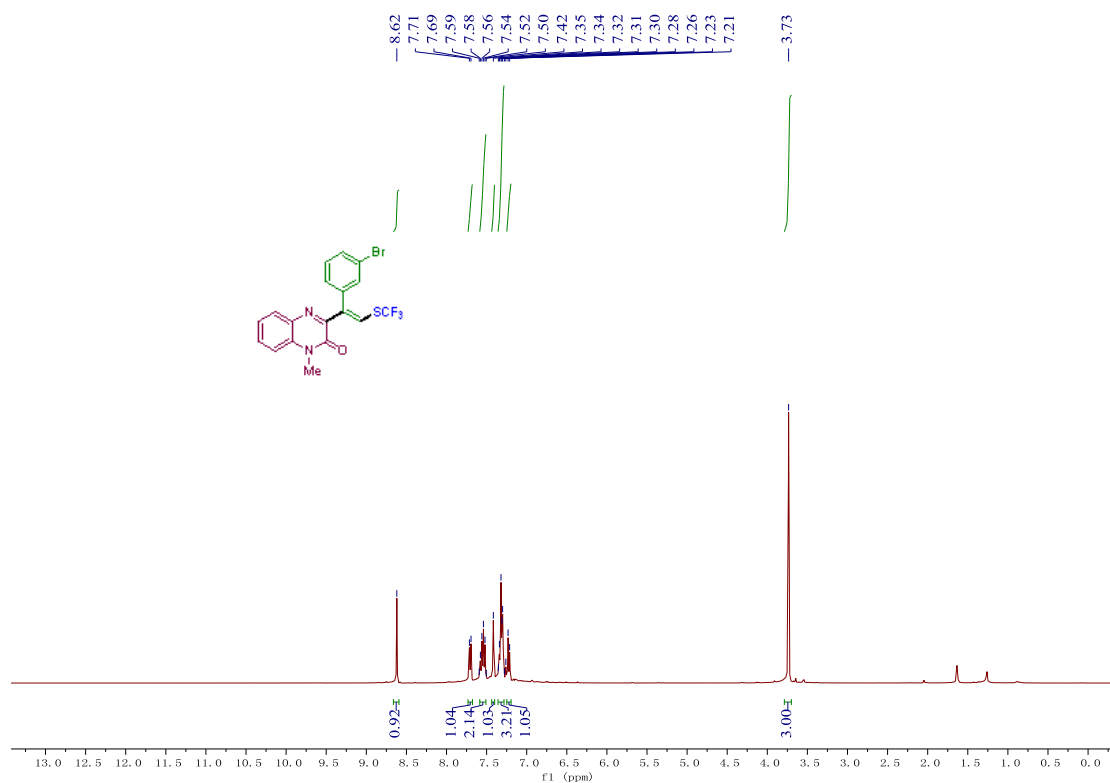
$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ) spectra of **3aI**



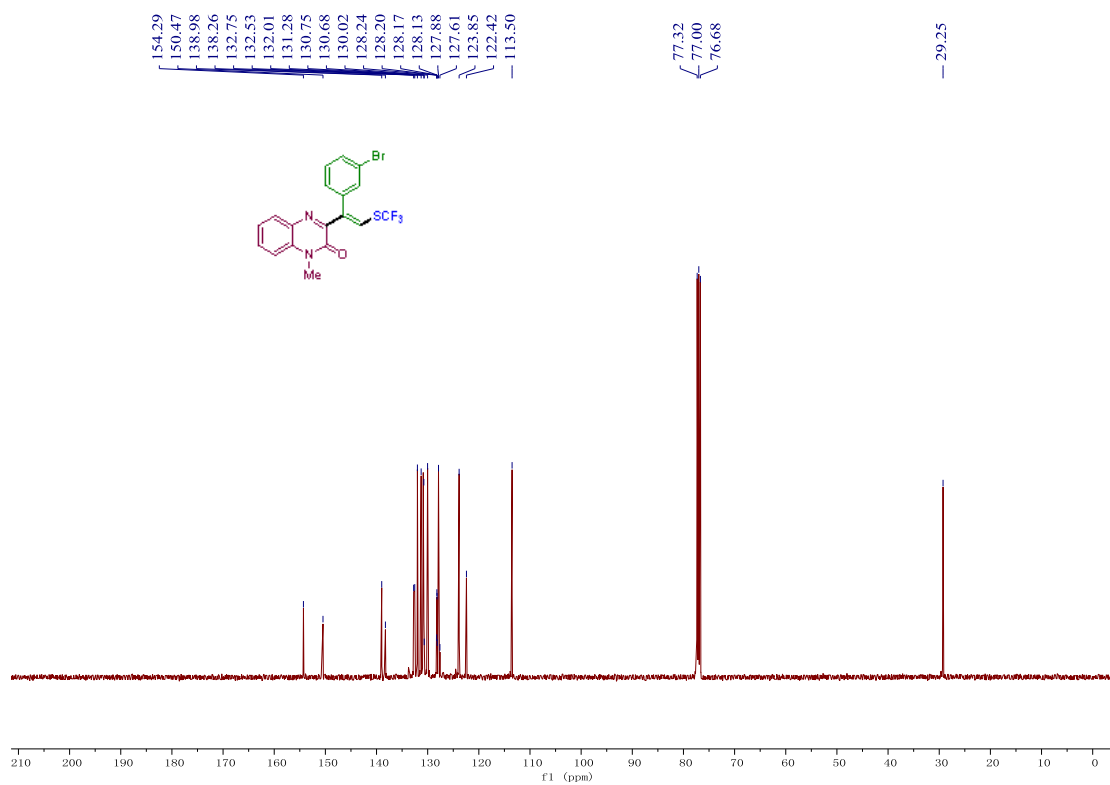
$^{13}\text{C}\{^1\text{H}\}$  NMR (100 MHz,  $\text{CDCl}_3$ ) spectra of **3am**



$^{19}\text{F}$  NMR (376 MHz,  $\text{CDCl}_3$ ) spectra of **3am**

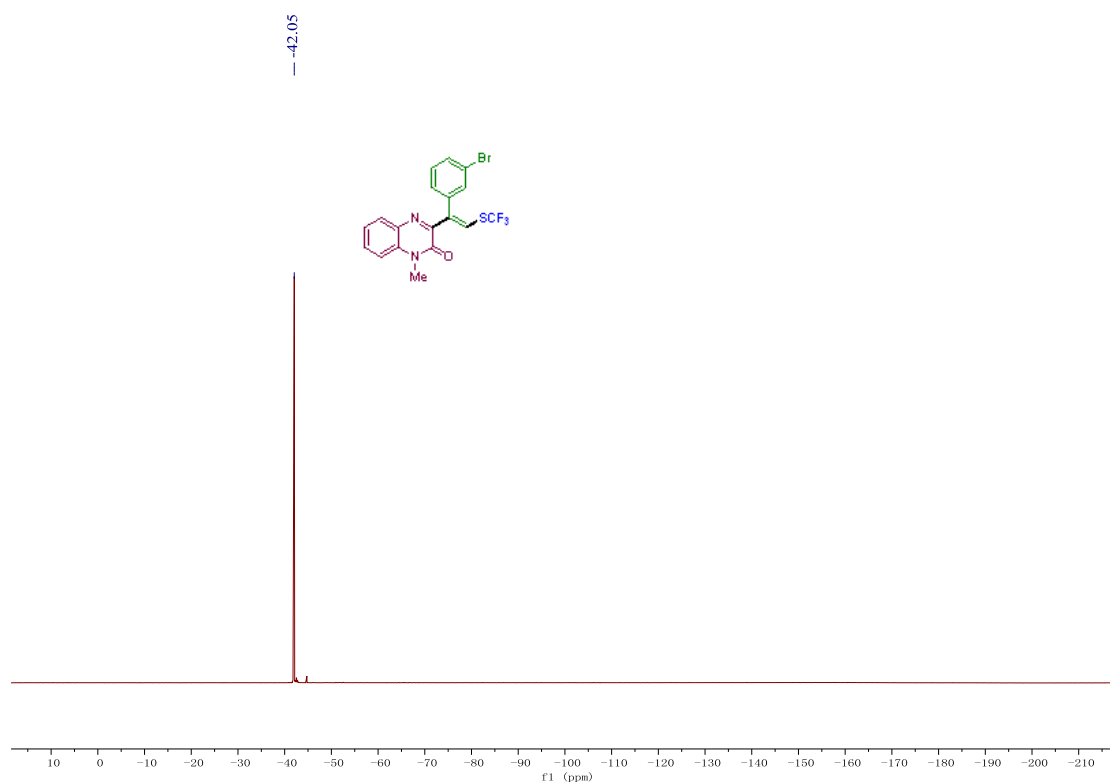


$^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ ) spectra of **3an**

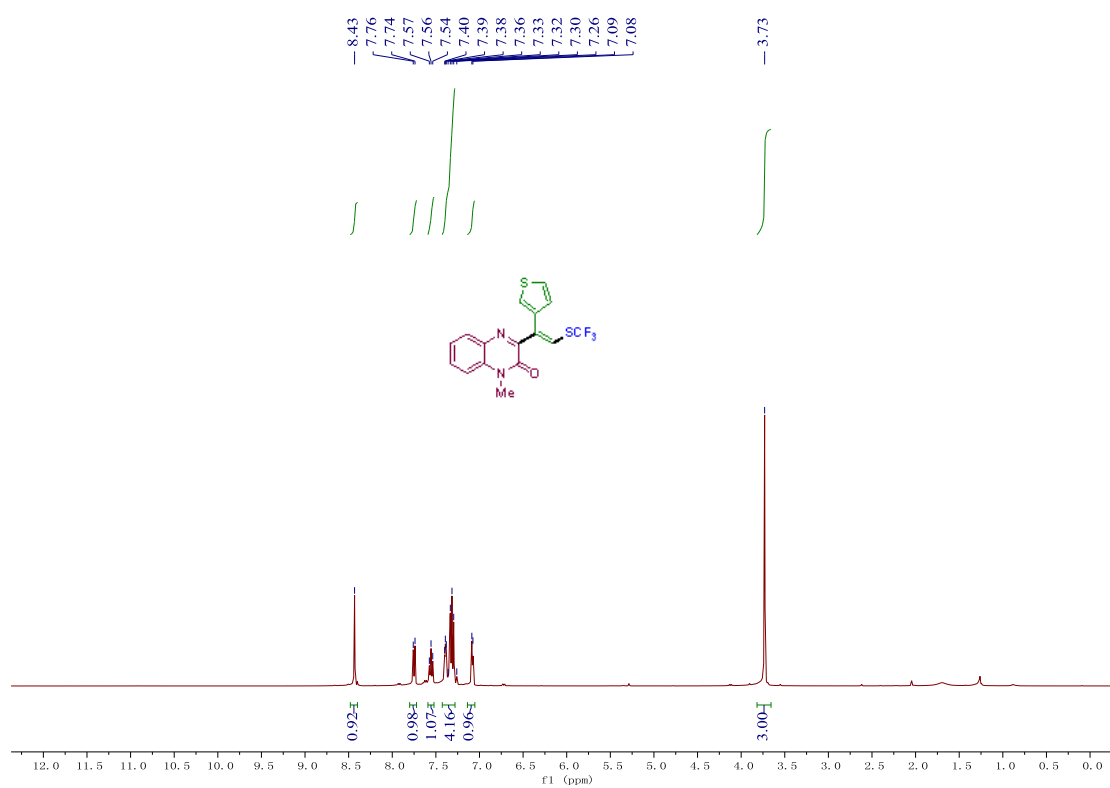


$^{13}\text{C}\{^1\text{H}\}$  NMR (100 MHz,  $\text{CDCl}_3$ ) spectra of **3an**

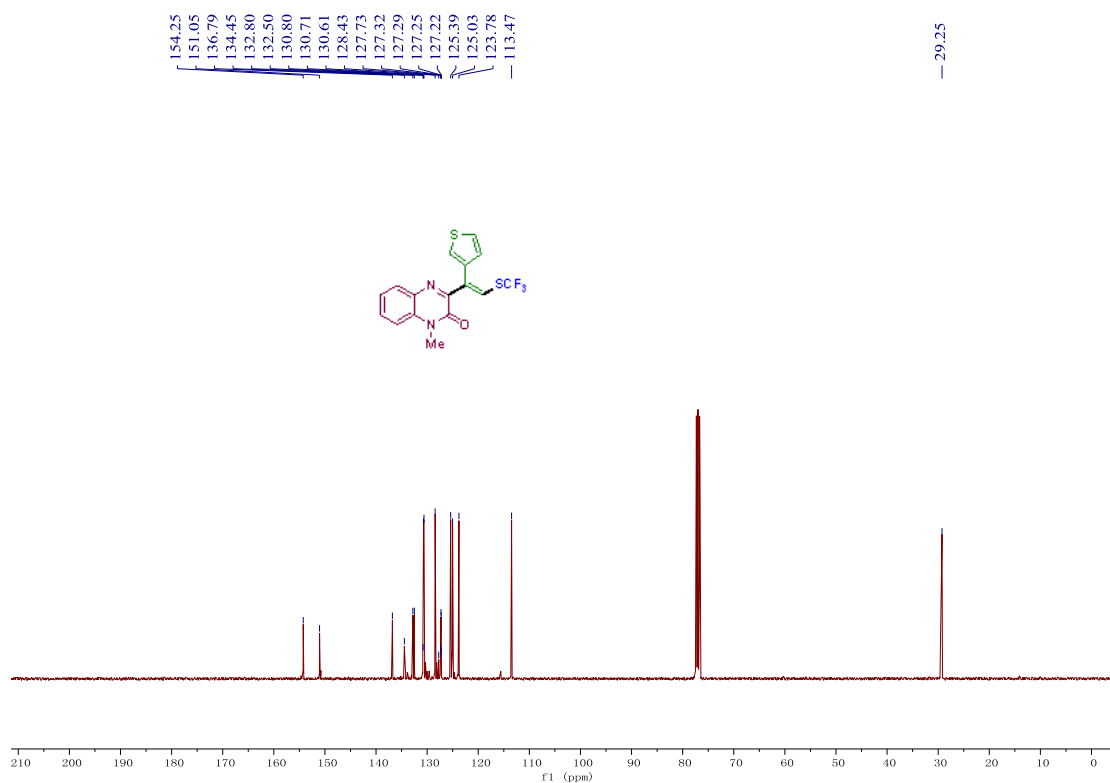




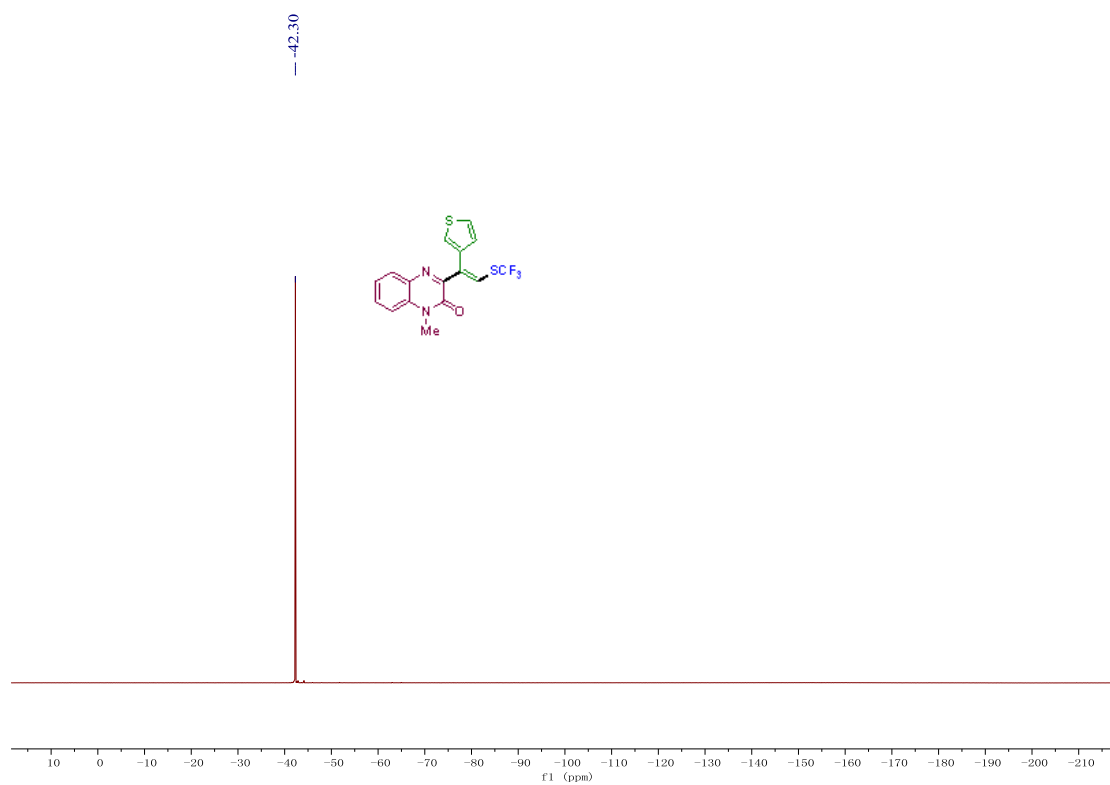
$^{19}\text{F}$  NMR (376 MHz,  $\text{CDCl}_3$ ) spectra of **3an**



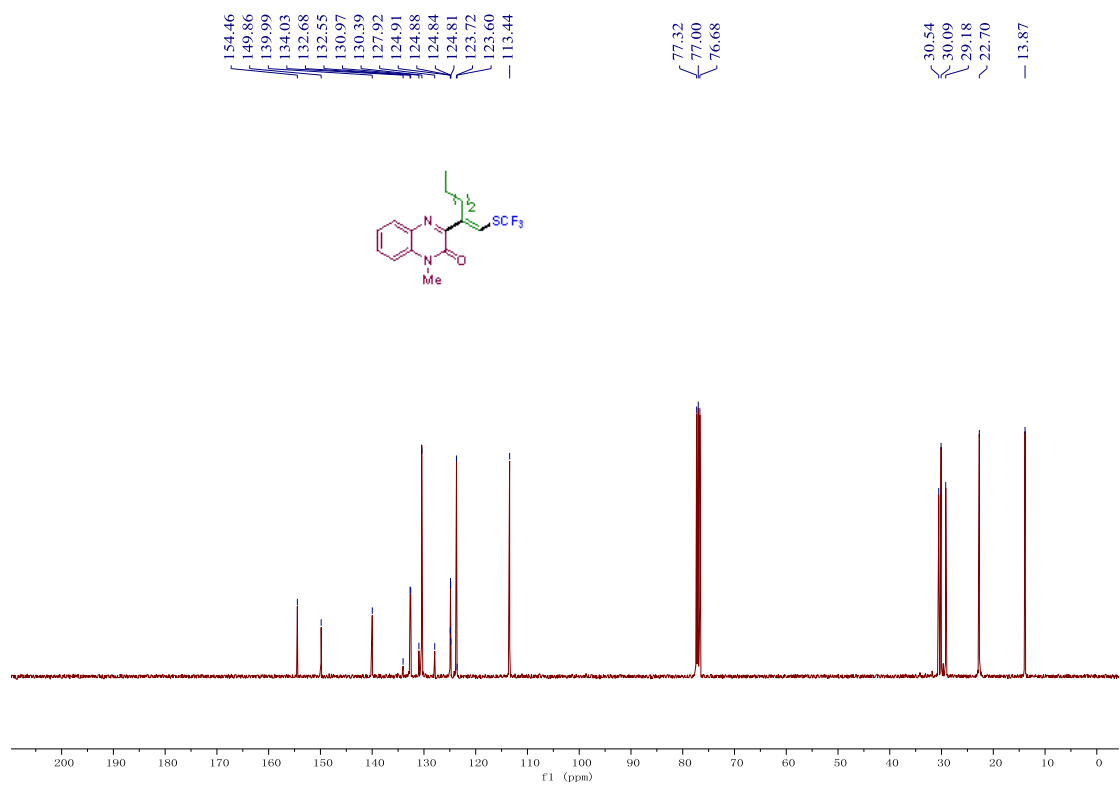
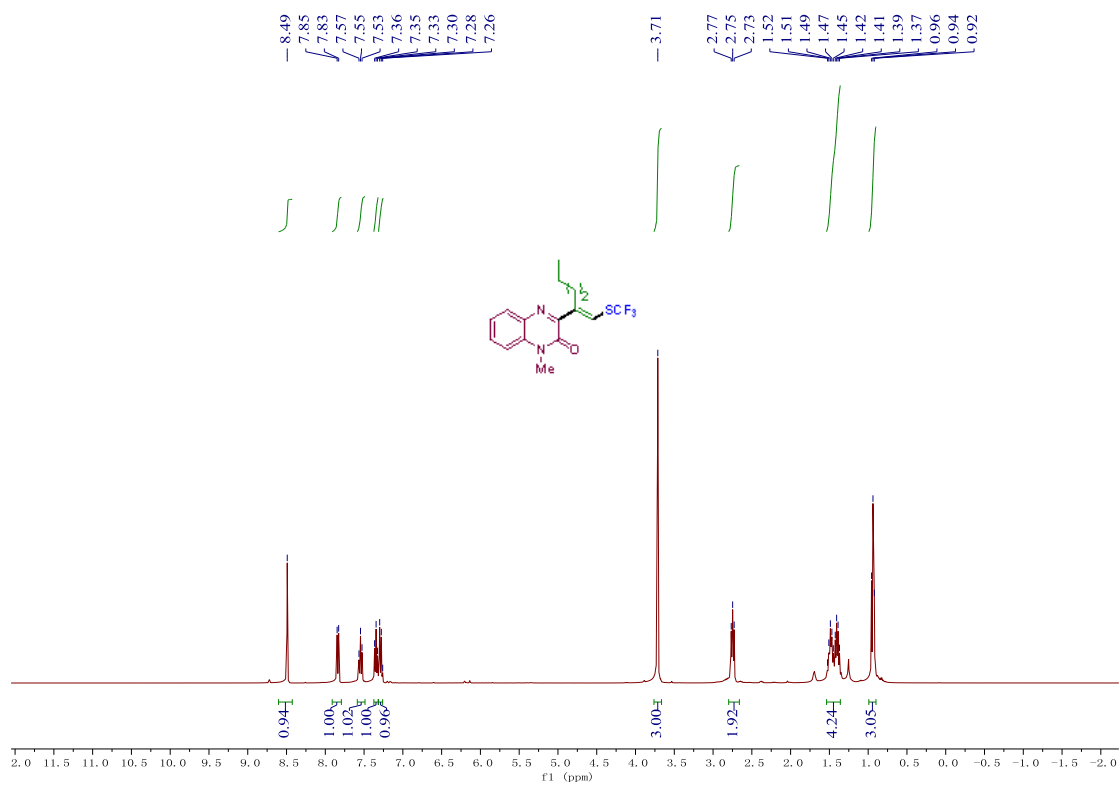
$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ) spectra of **3ao**

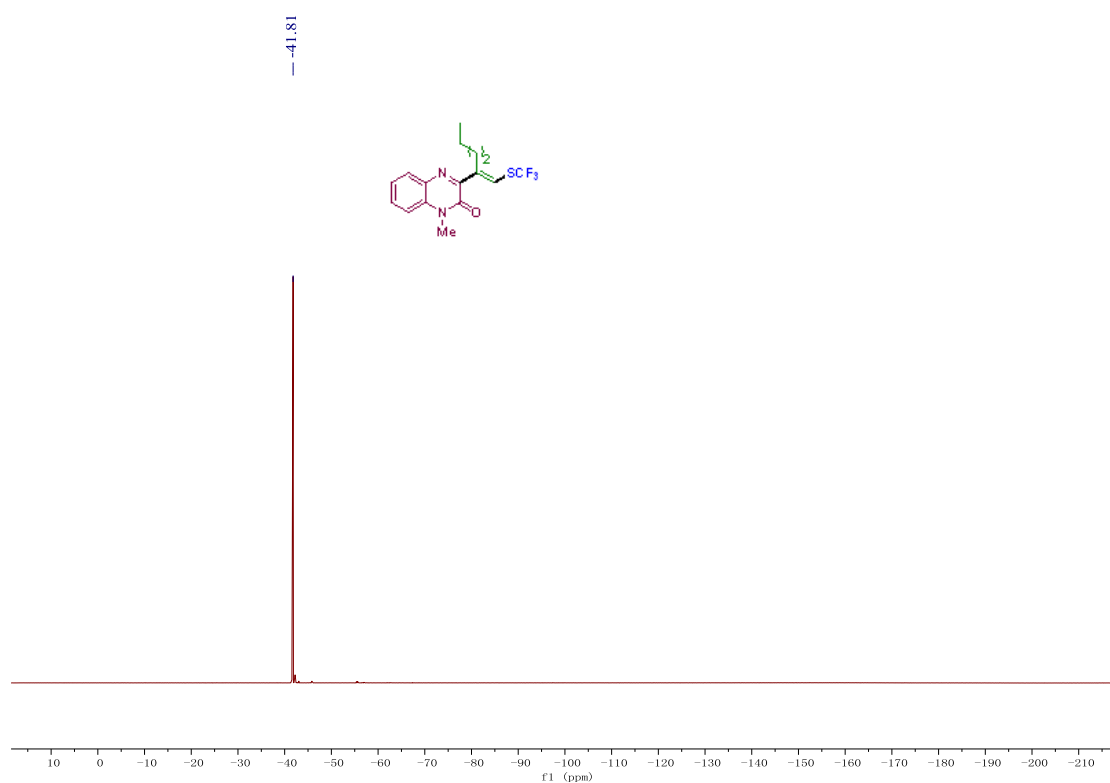


$^{13}\text{C}\{^1\text{H}\}$  NMR (100 MHz,  $\text{CDCl}_3$ ) spectra of **3ao**

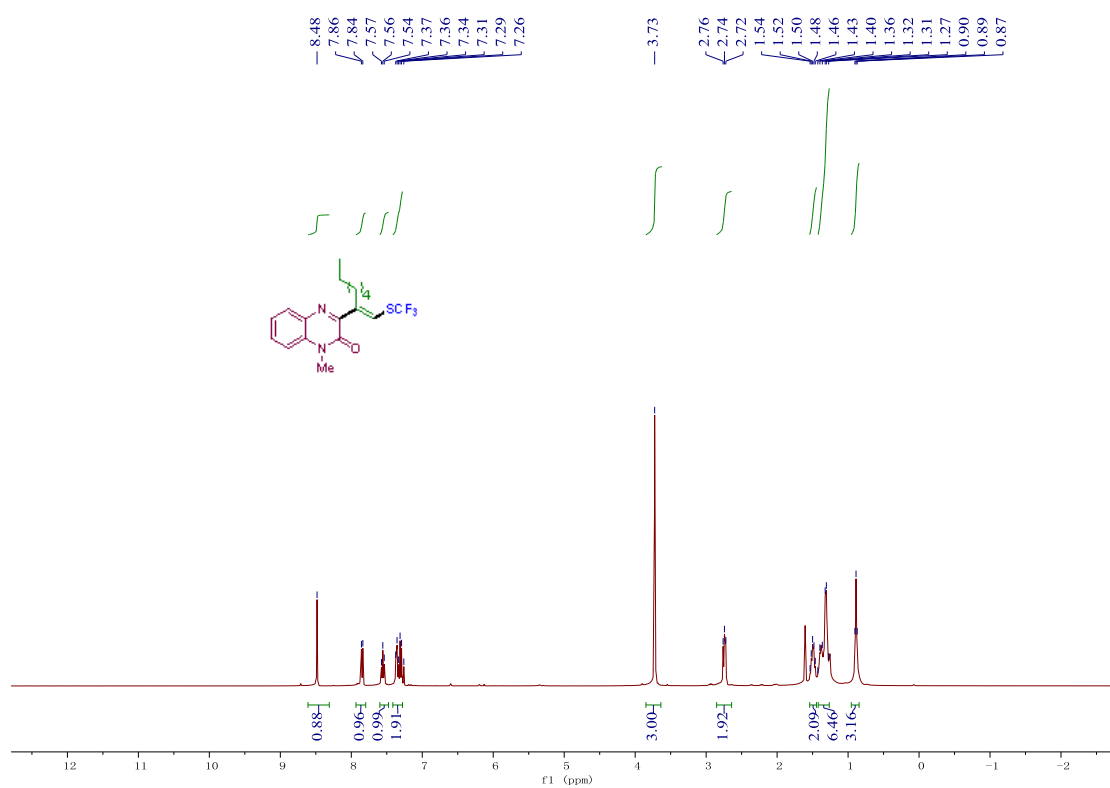


$^{19}\text{F}$  NMR (376 MHz,  $\text{CDCl}_3$ ) spectra of **3ao**

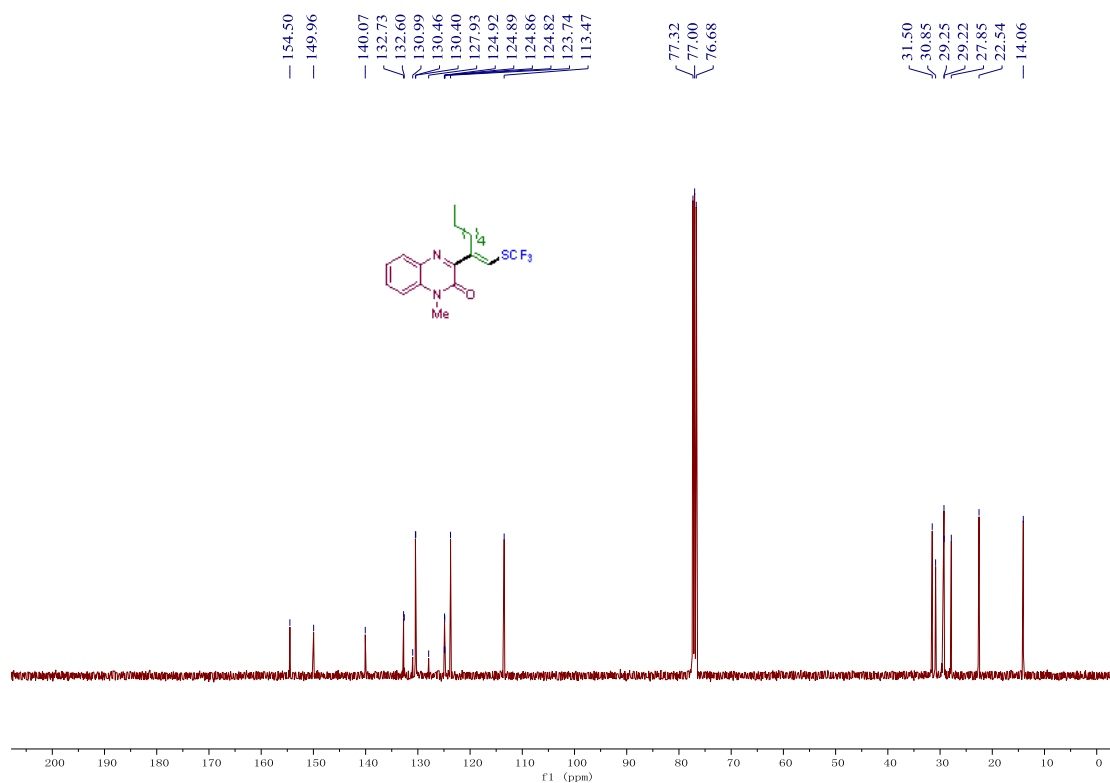




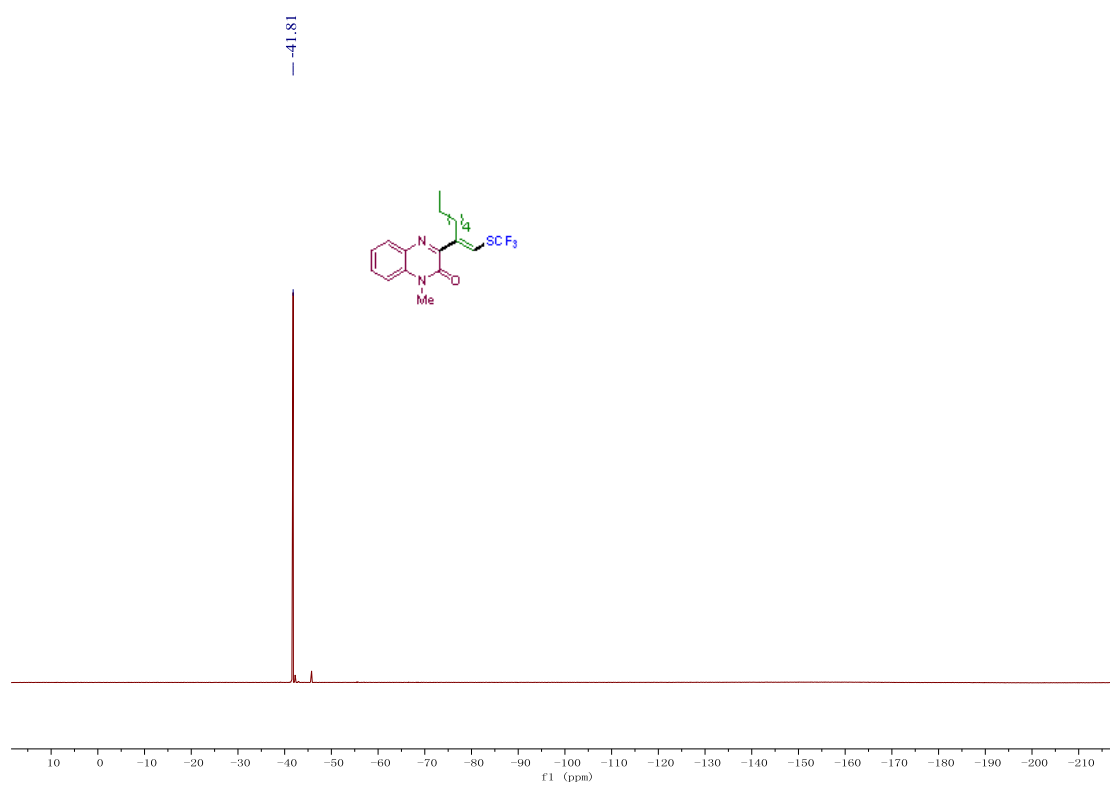
$^{19}\text{F}$  NMR (376 MHz,  $\text{CDCl}_3$ ) spectra of **3ap**



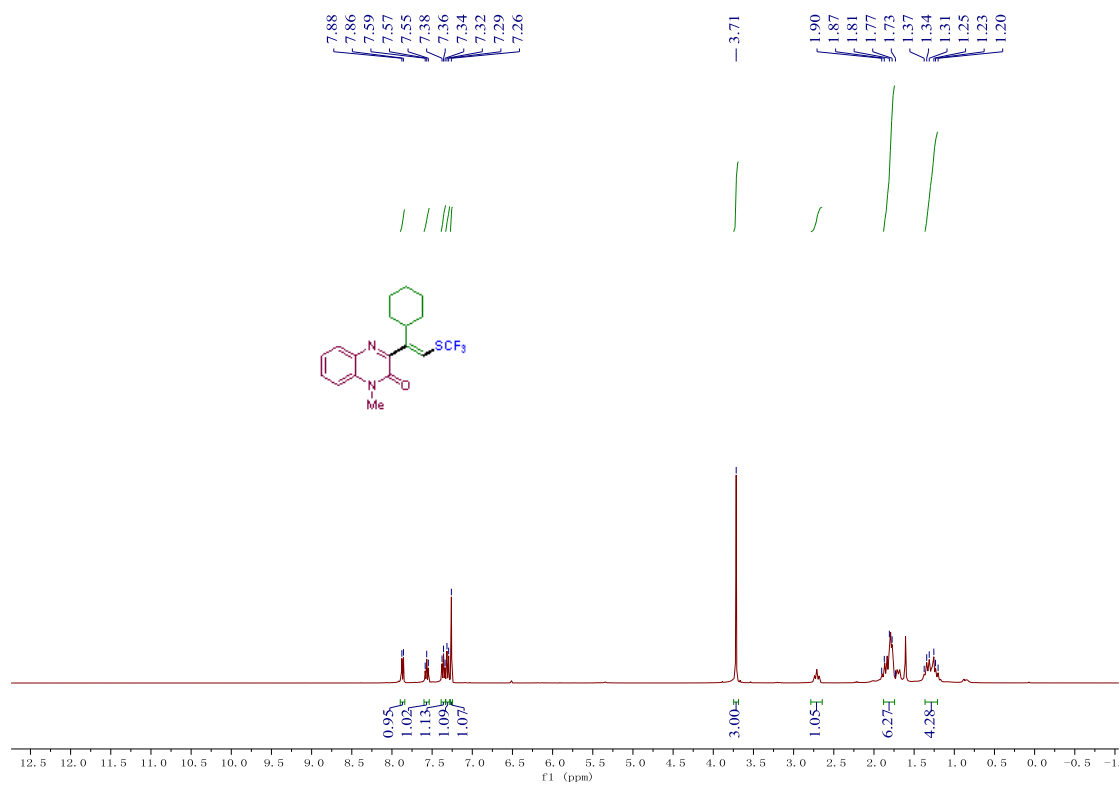
$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ) spectra of **3aq**



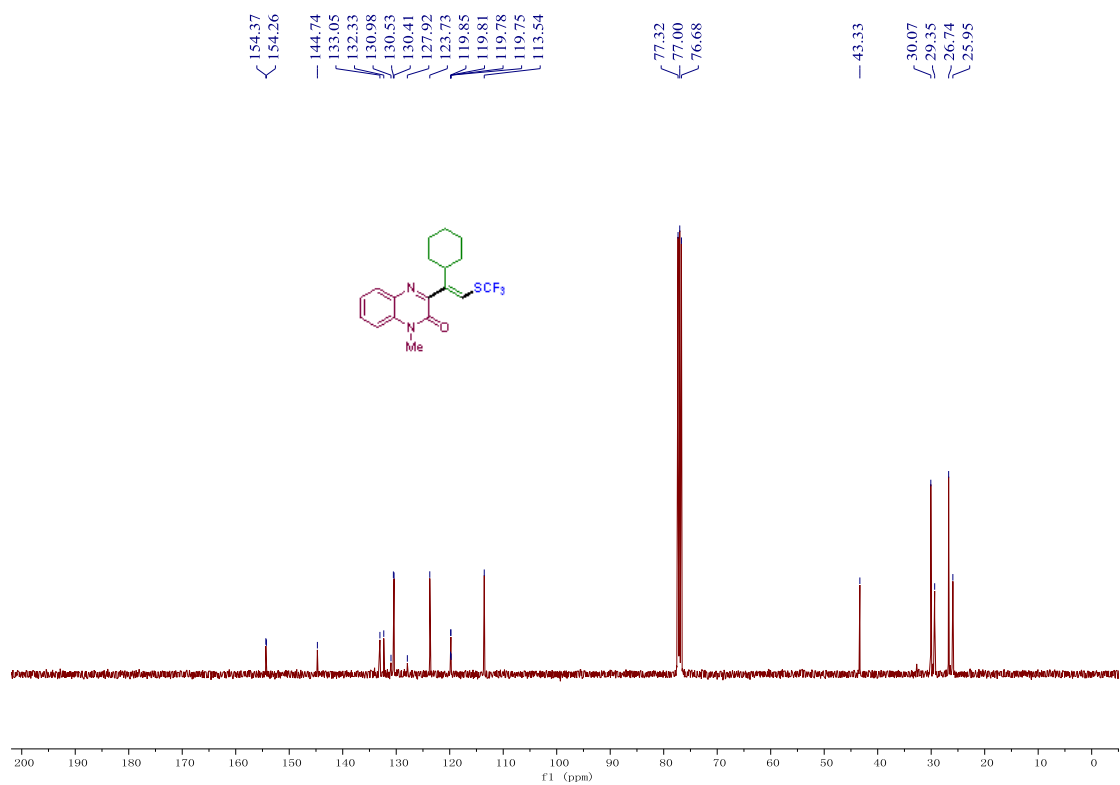
$^{13}\text{C}\{^1\text{H}\}$  NMR (100 MHz,  $\text{CDCl}_3$ ) spectra of **3aq**



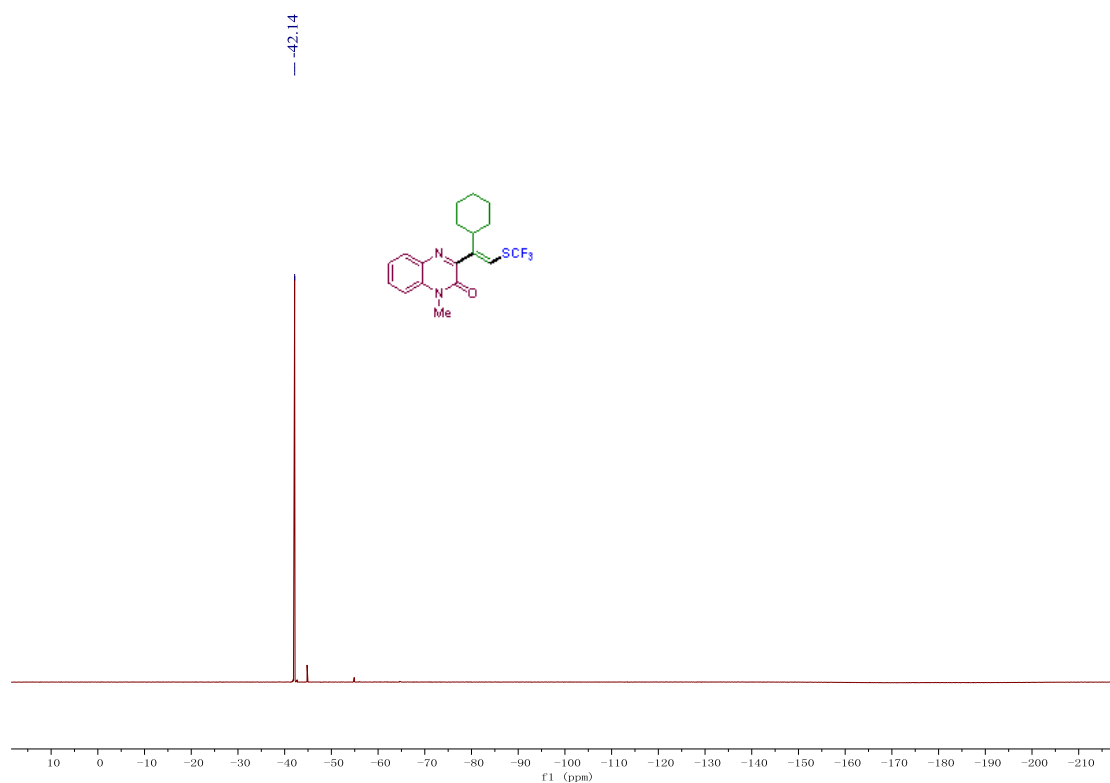
$^{19}\text{F}$  NMR (376 MHz,  $\text{CDCl}_3$ ) spectra of **3aq**



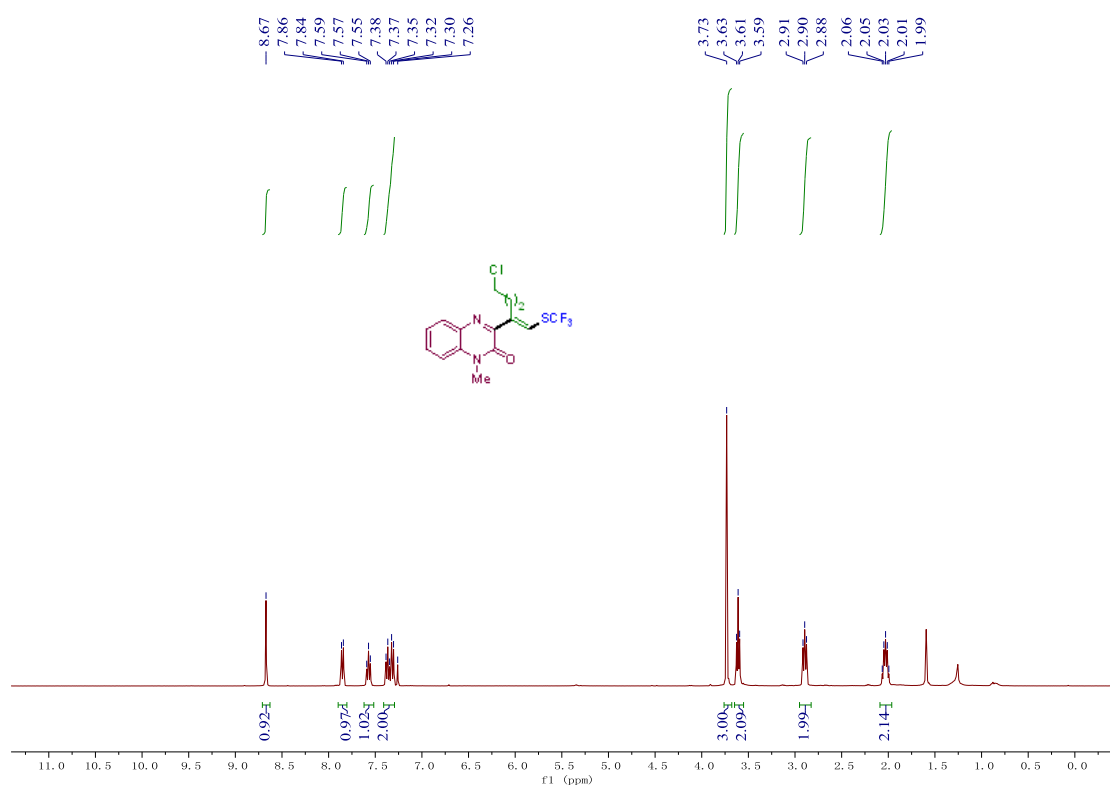
<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) spectra of **3ar**



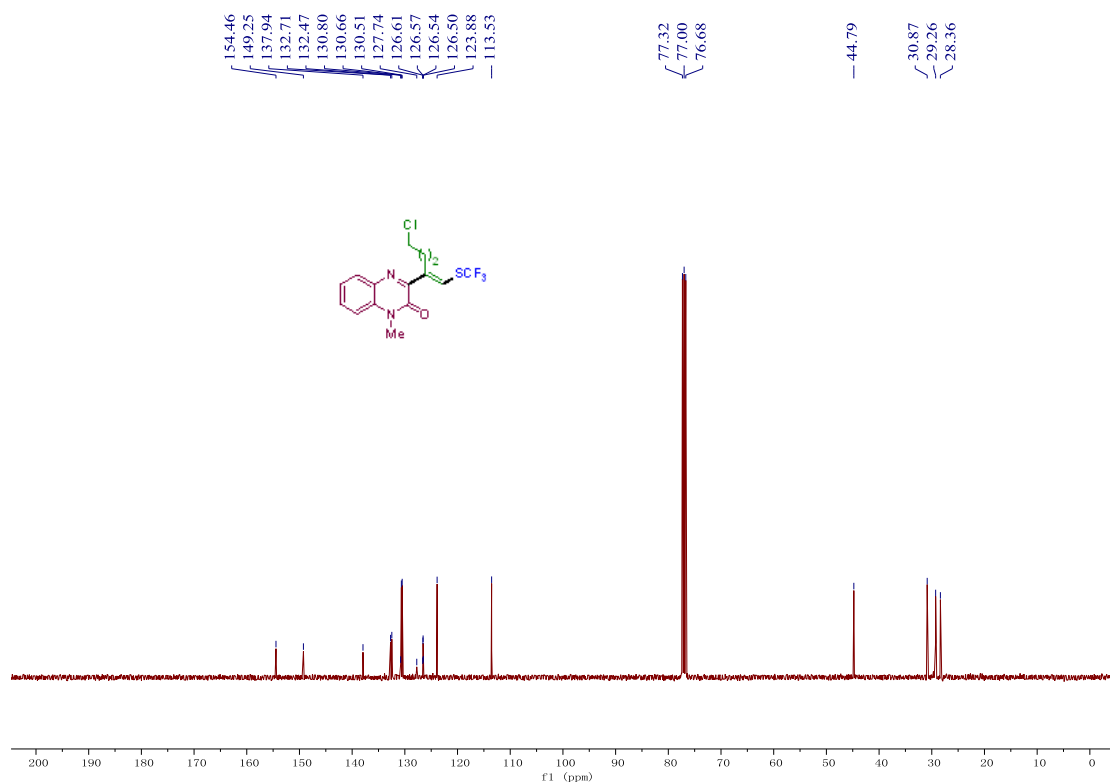
<sup>13</sup>C{<sup>1</sup>H} NMR (100 MHz, CDCl<sub>3</sub>) spectra of **3ar**



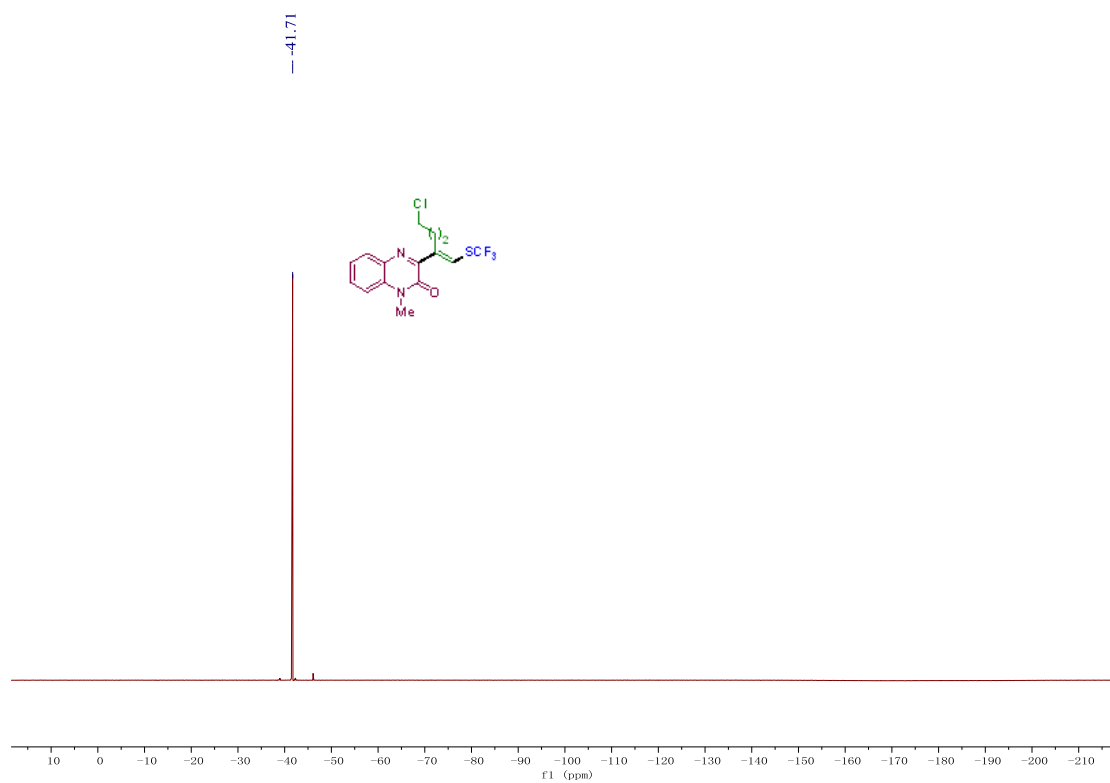
$^{19}\text{F}$  NMR (376 MHz,  $\text{CDCl}_3$ ) spectra of **3ar**



$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ) spectra of **3as**

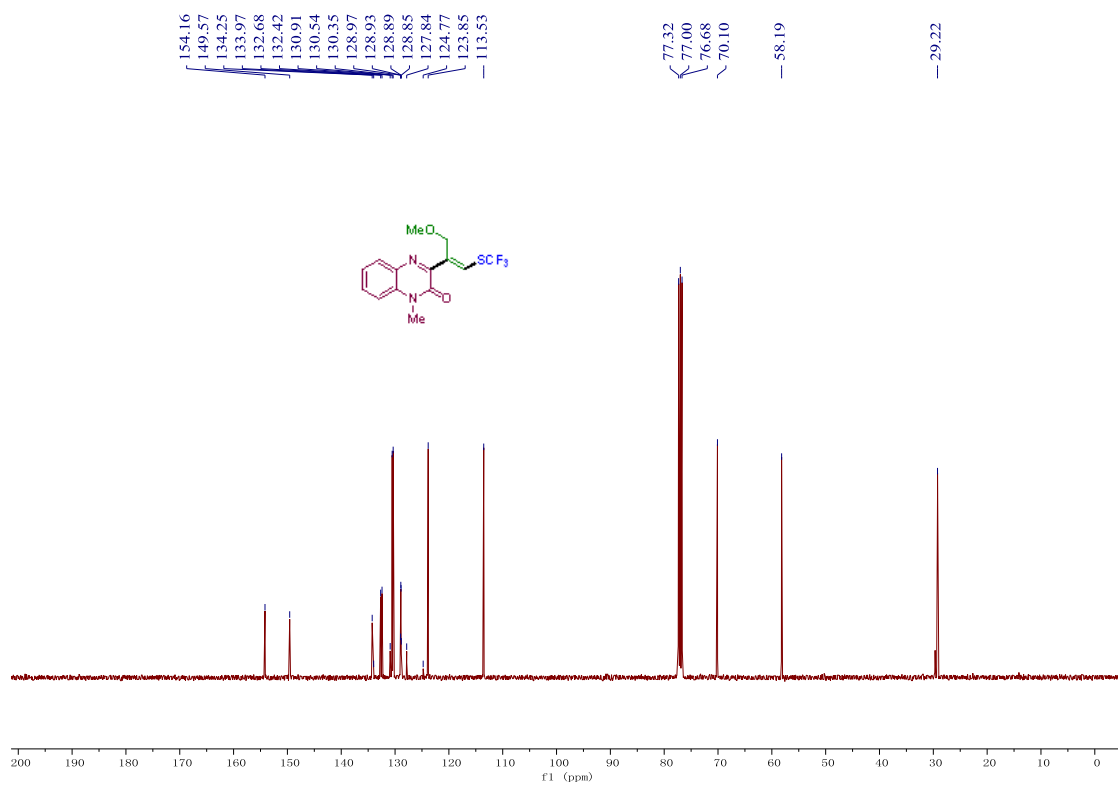
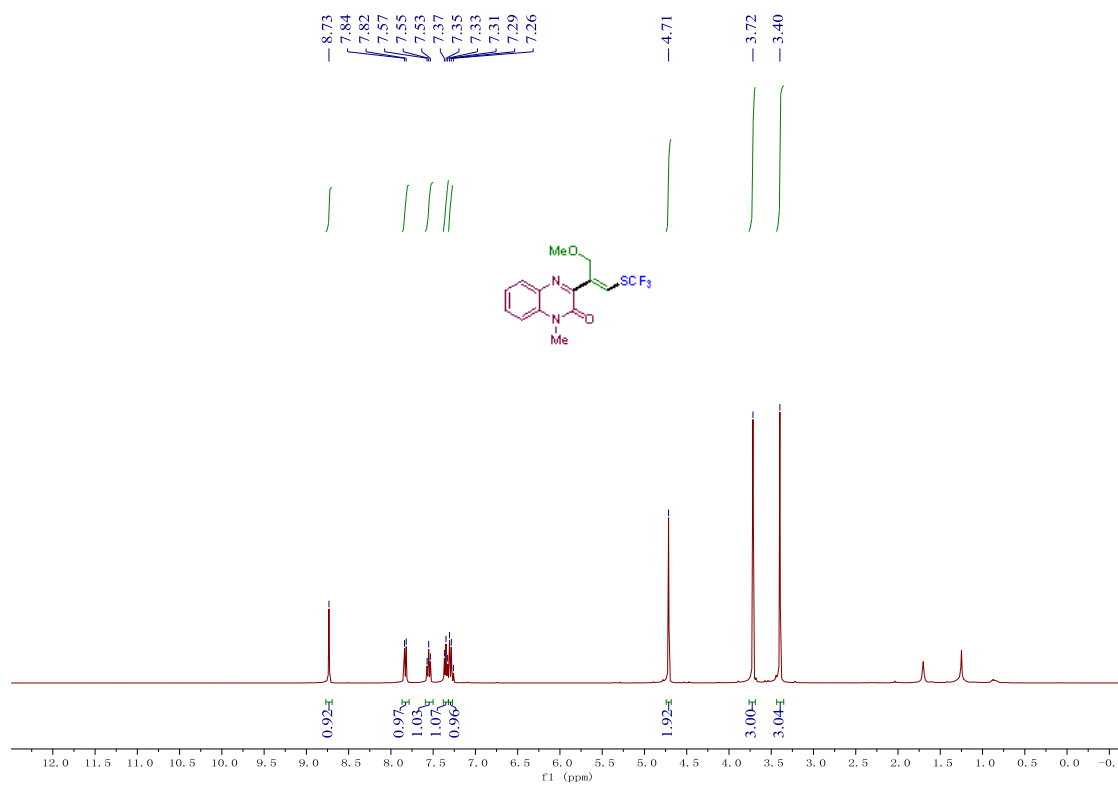


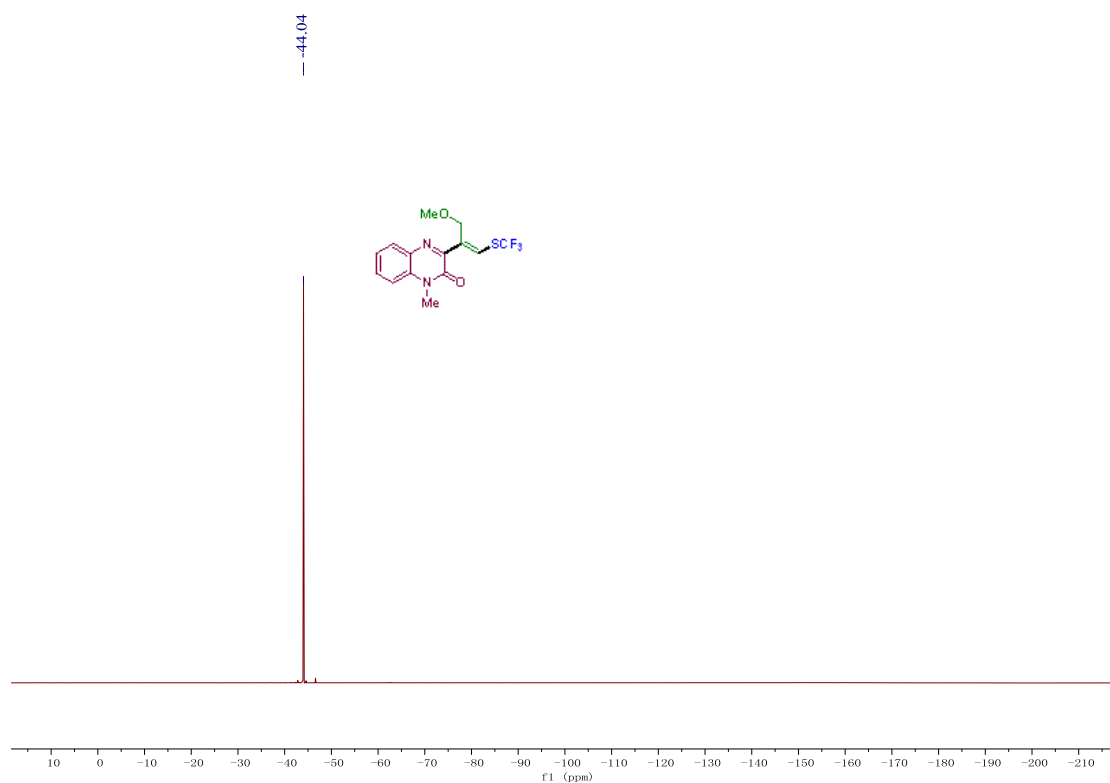
$^{13}\text{C}\{^1\text{H}\}$  NMR (100 MHz,  $\text{CDCl}_3$ ) spectra of **3as**



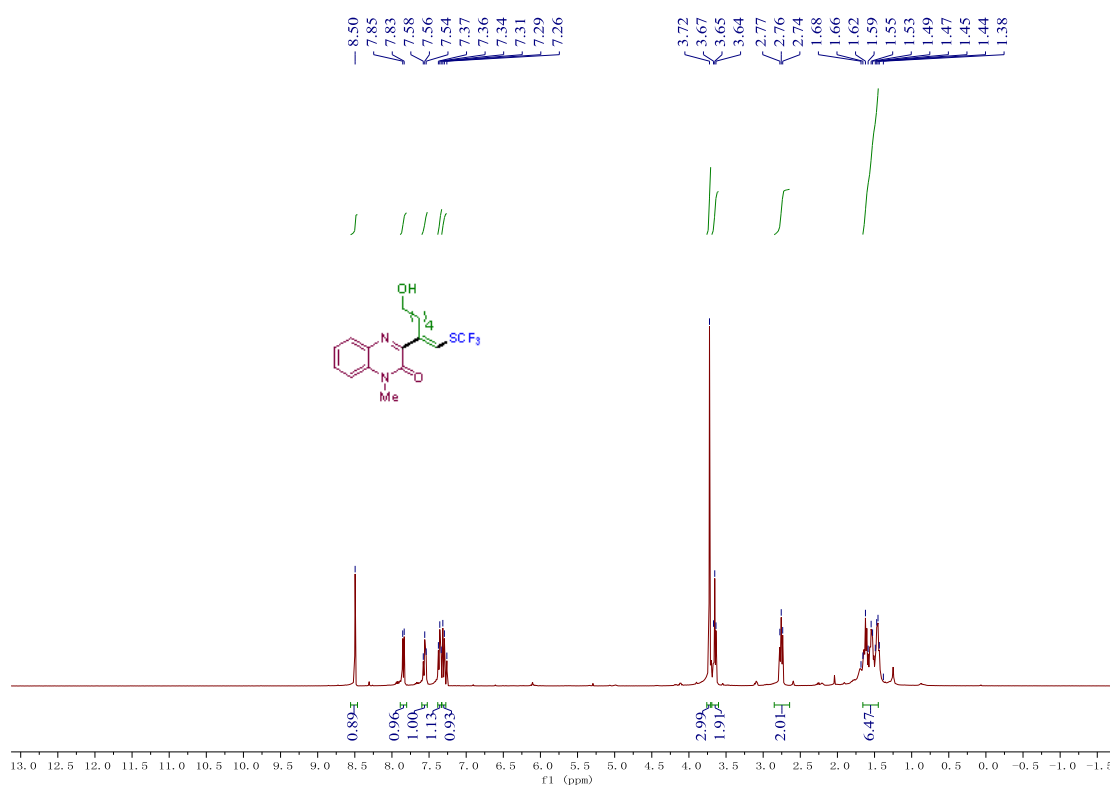
$^{19}\text{F}$  NMR (376 MHz,  $\text{CDCl}_3$ ) spectra of **3as**



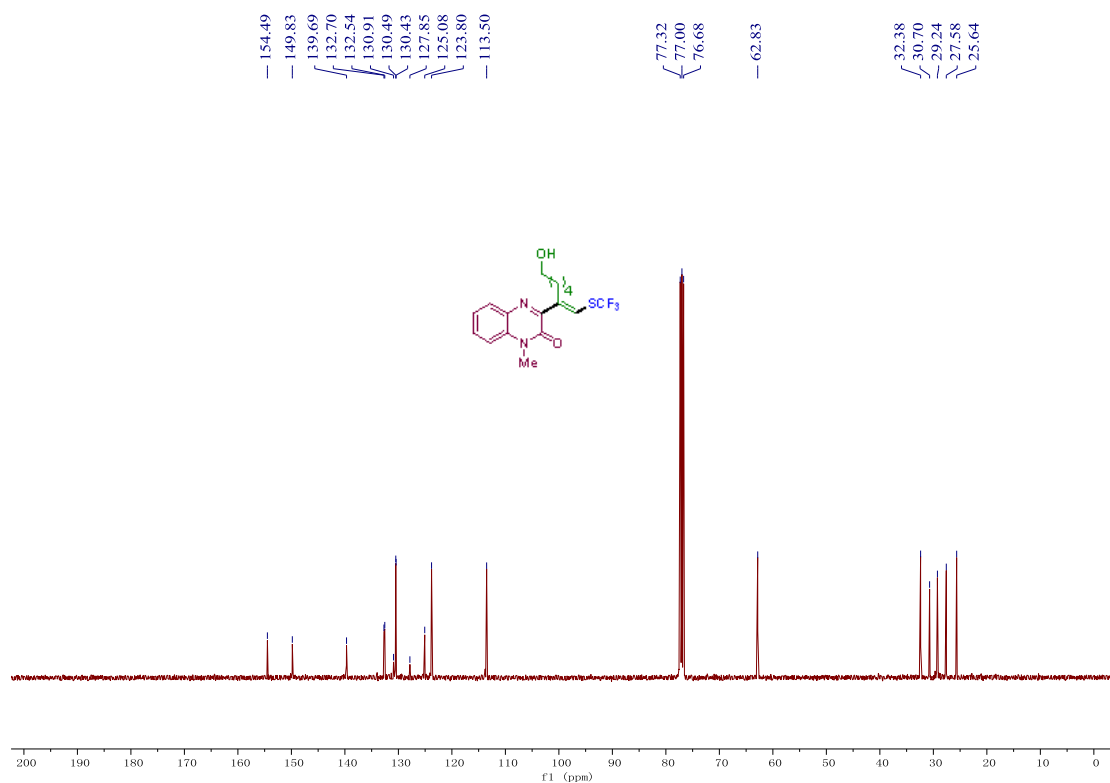




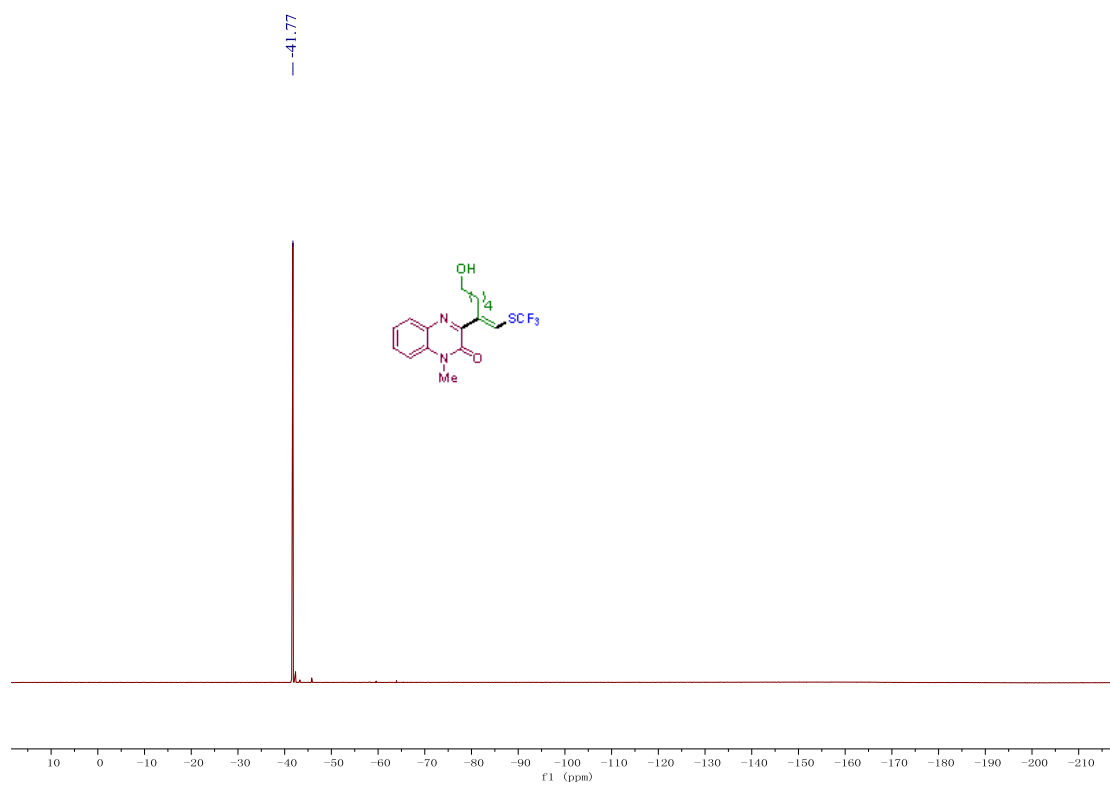
$^{19}\text{F}$  NMR (376 MHz,  $\text{CDCl}_3$ ) spectra of **3at**



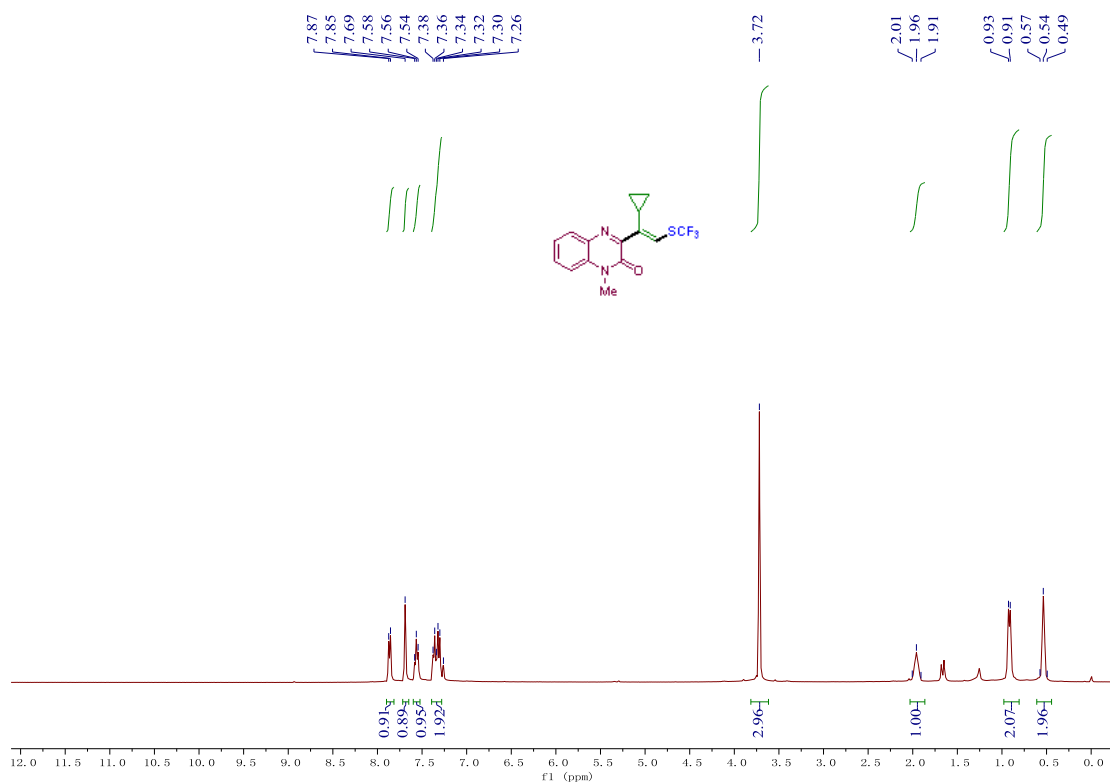
$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ) spectra of **3au**



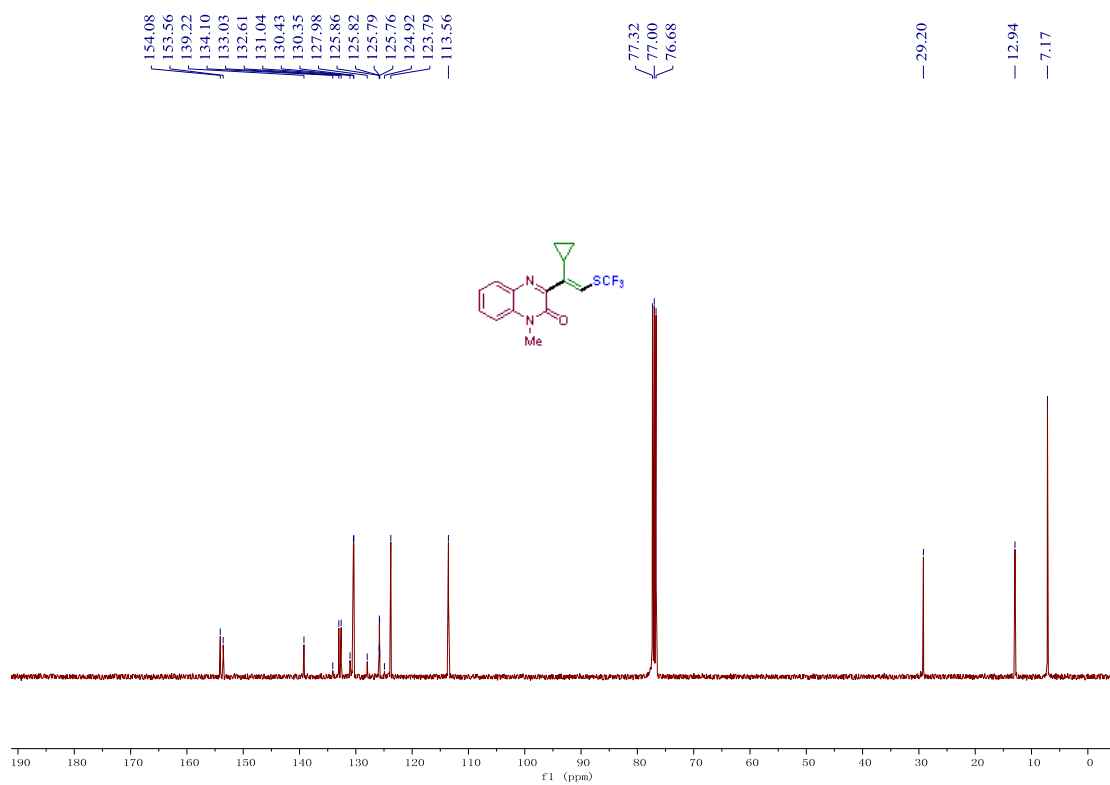
$^{13}\text{C}\{^1\text{H}\}$  NMR (100 MHz,  $\text{CDCl}_3$ ) spectra of **3au**



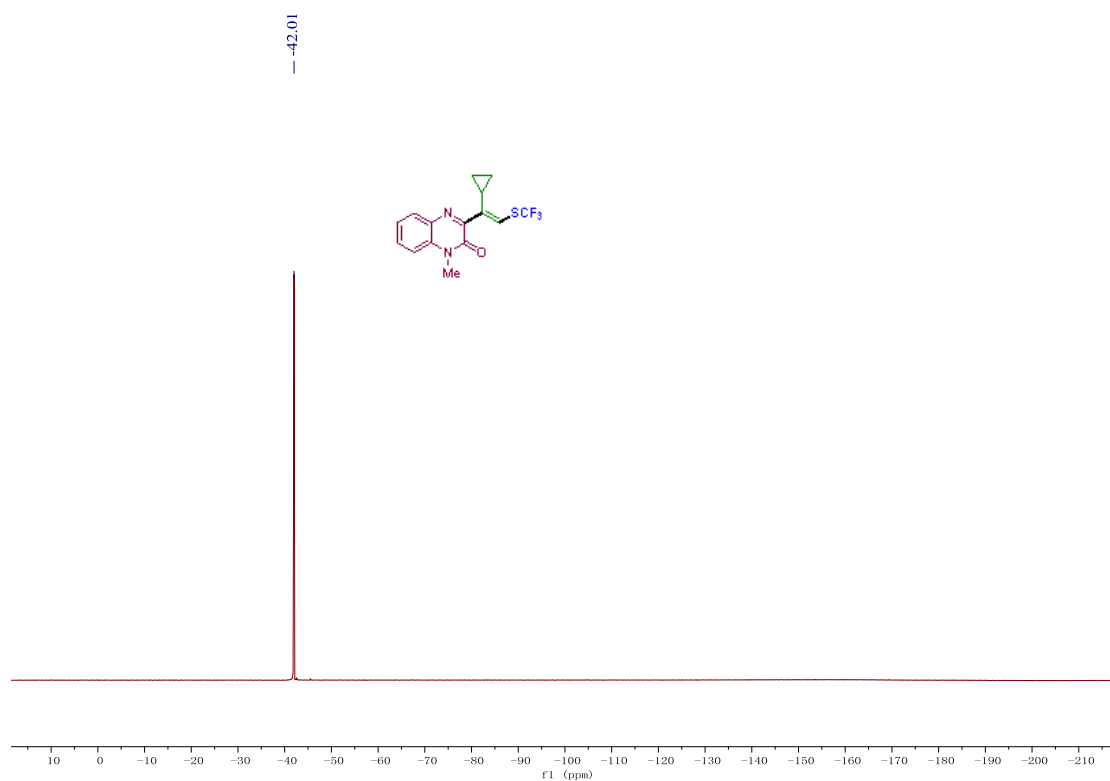
$^{19}\text{F}$  NMR (376 MHz,  $\text{CDCl}_3$ ) spectra of **3au**



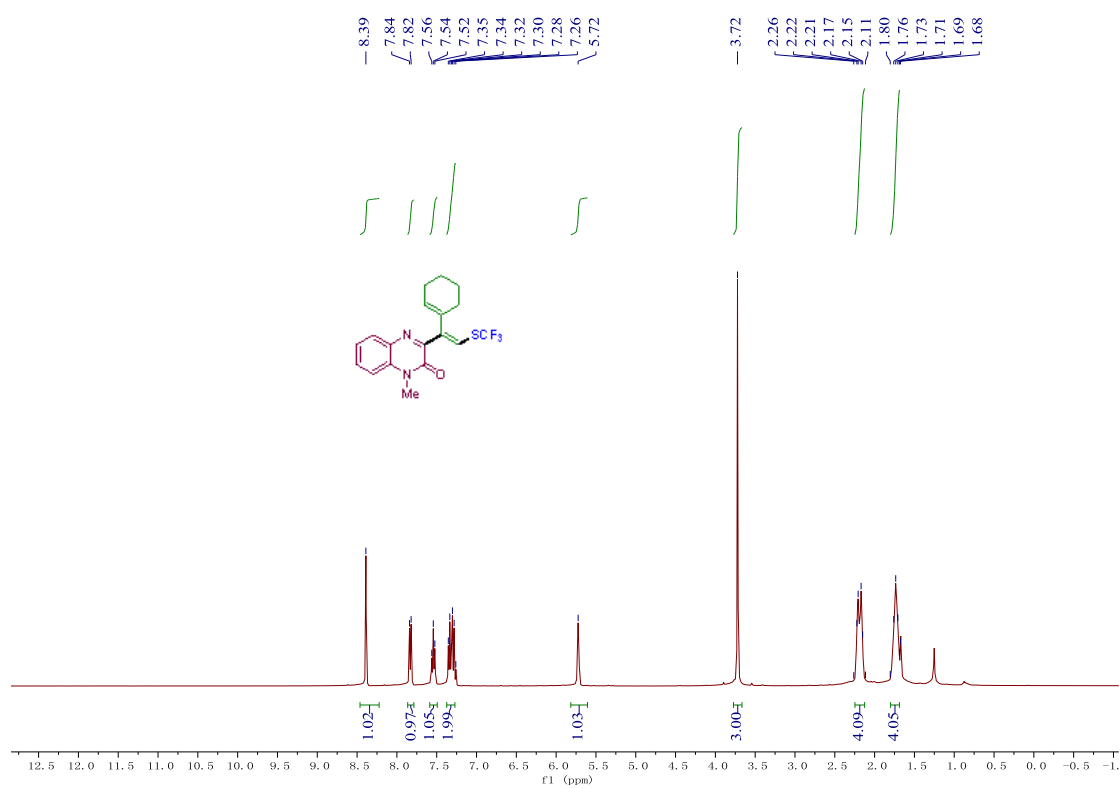
$^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ ) spectra of **3av**



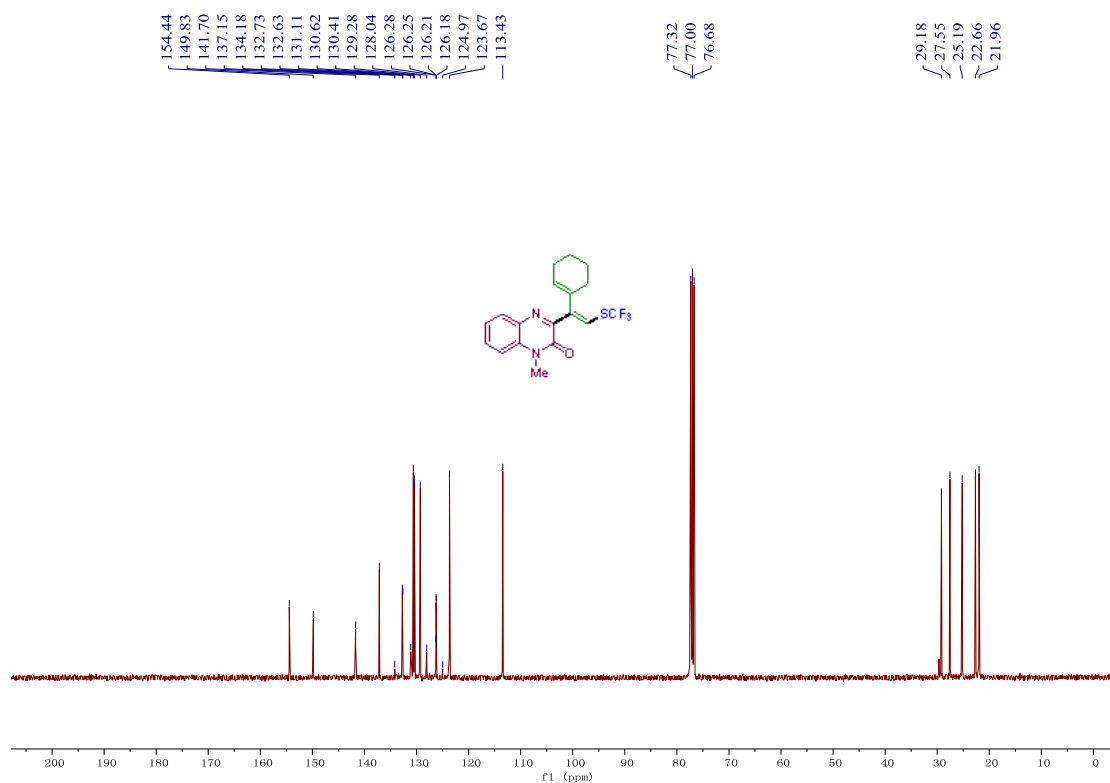
$^{13}\text{C}\{^1\text{H}\}$  NMR (100 MHz,  $\text{CDCl}_3$ ) spectra of **3av**



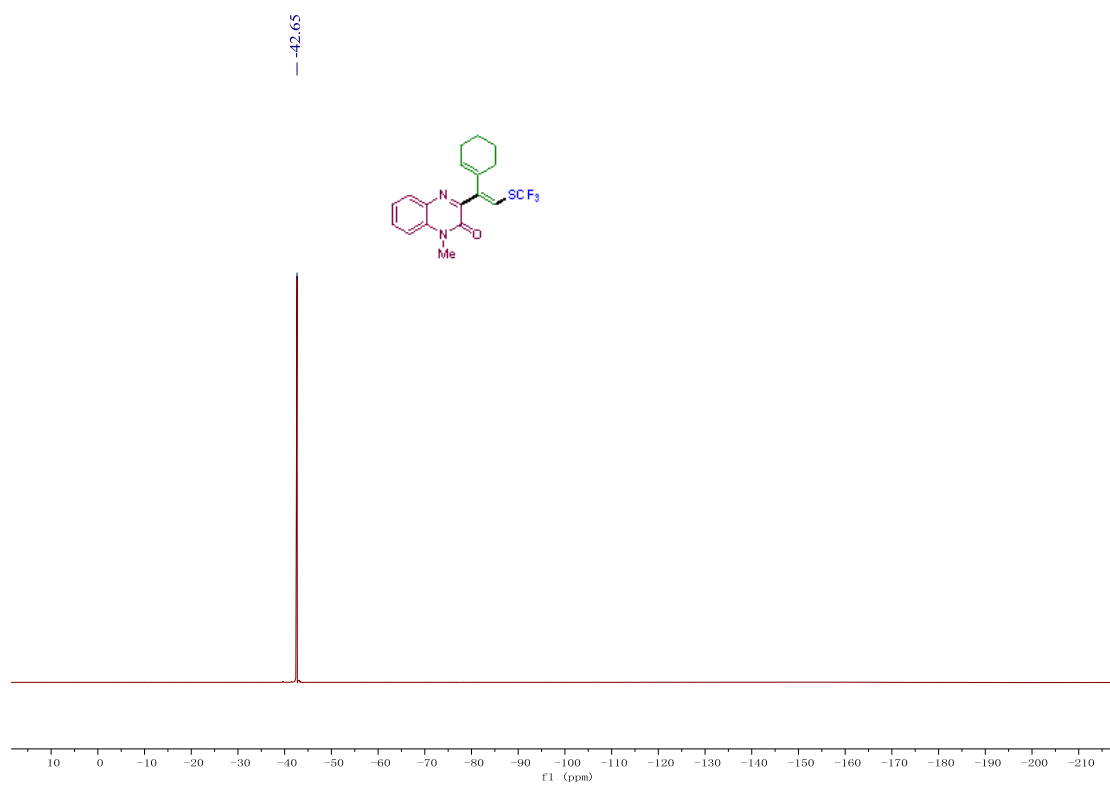
$^{19}\text{F}$  NMR (376 MHz,  $\text{CDCl}_3$ ) spectra of **3av**



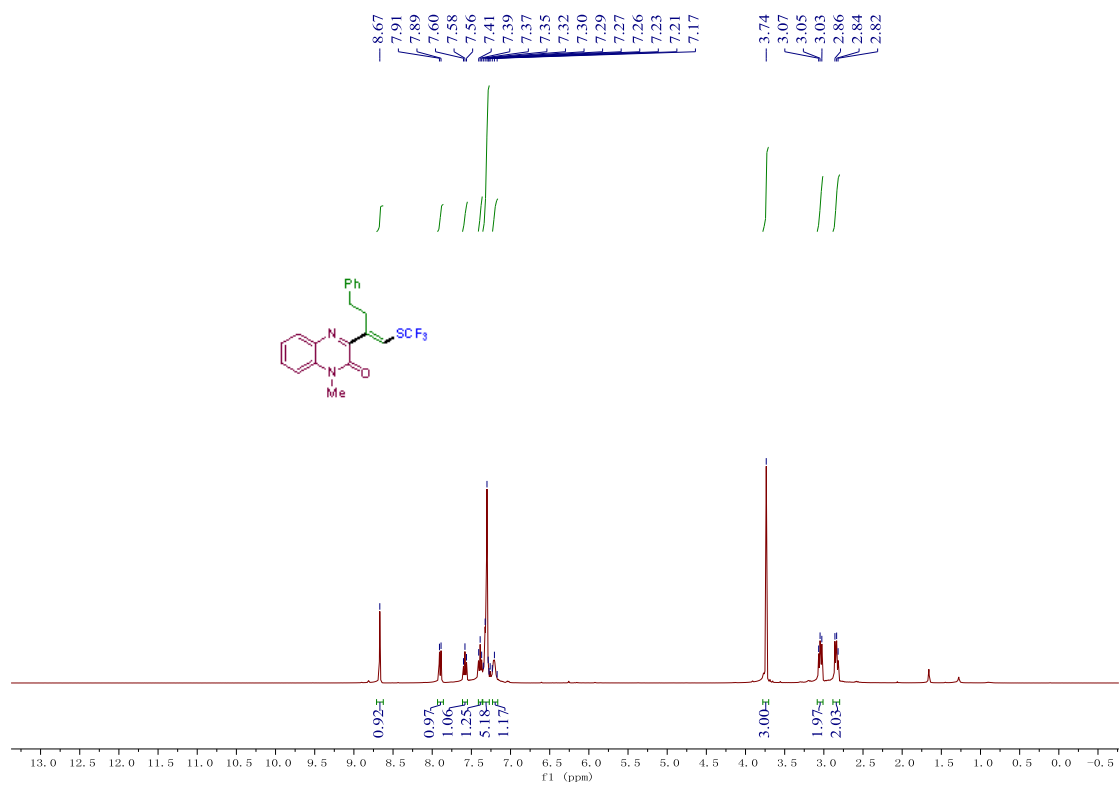
$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ) spectra of **3aw**



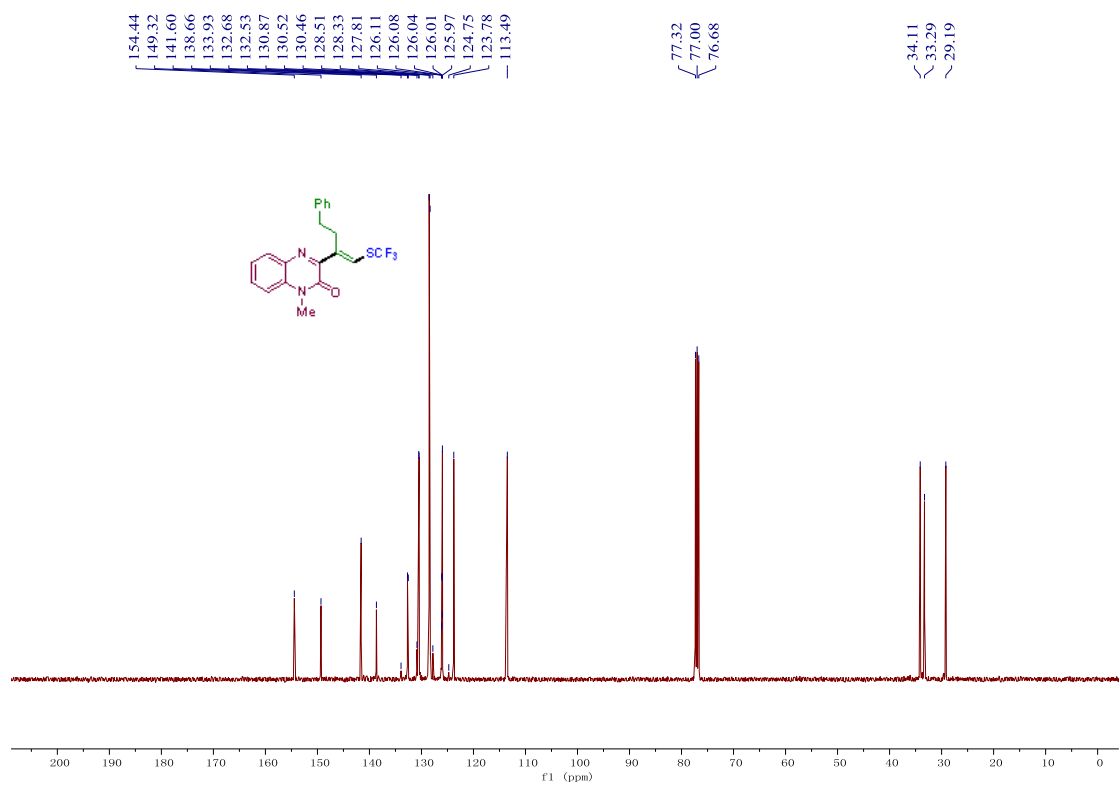
$^{13}\text{C}\{^1\text{H}\}$  NMR (100 MHz,  $\text{CDCl}_3$ ) spectra of **3aw**



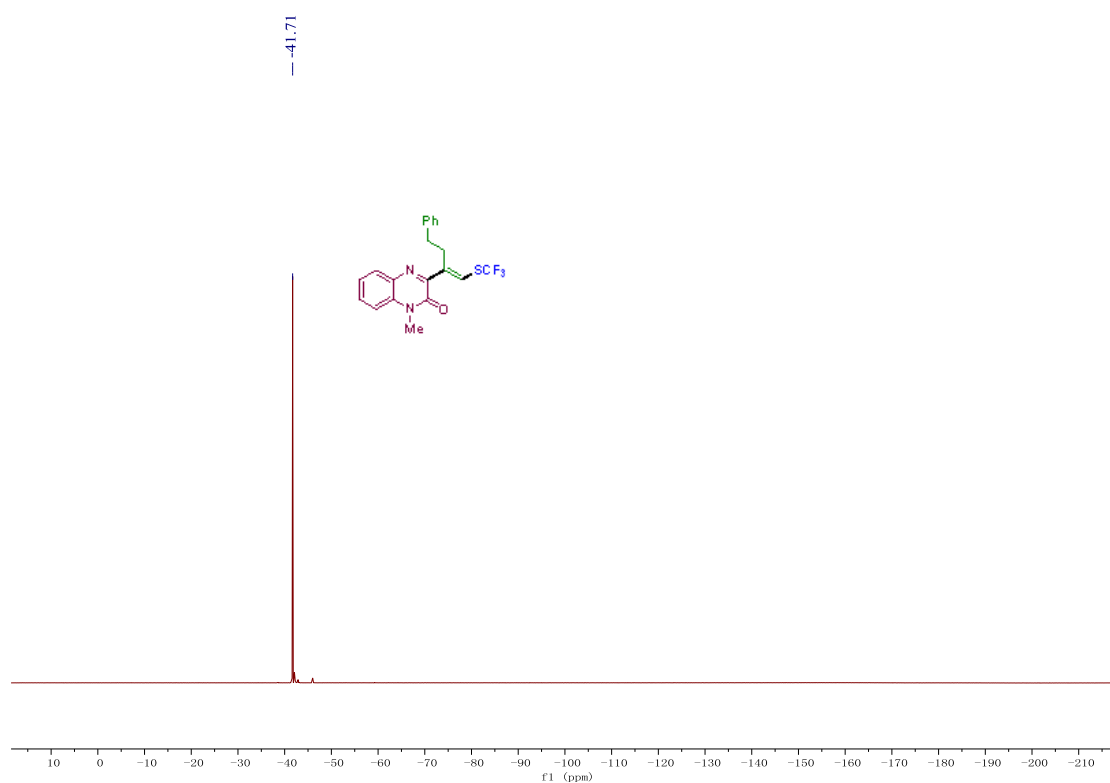
$^{19}\text{F}$  NMR (376 MHz,  $\text{CDCl}_3$ ) spectra of **3aw**



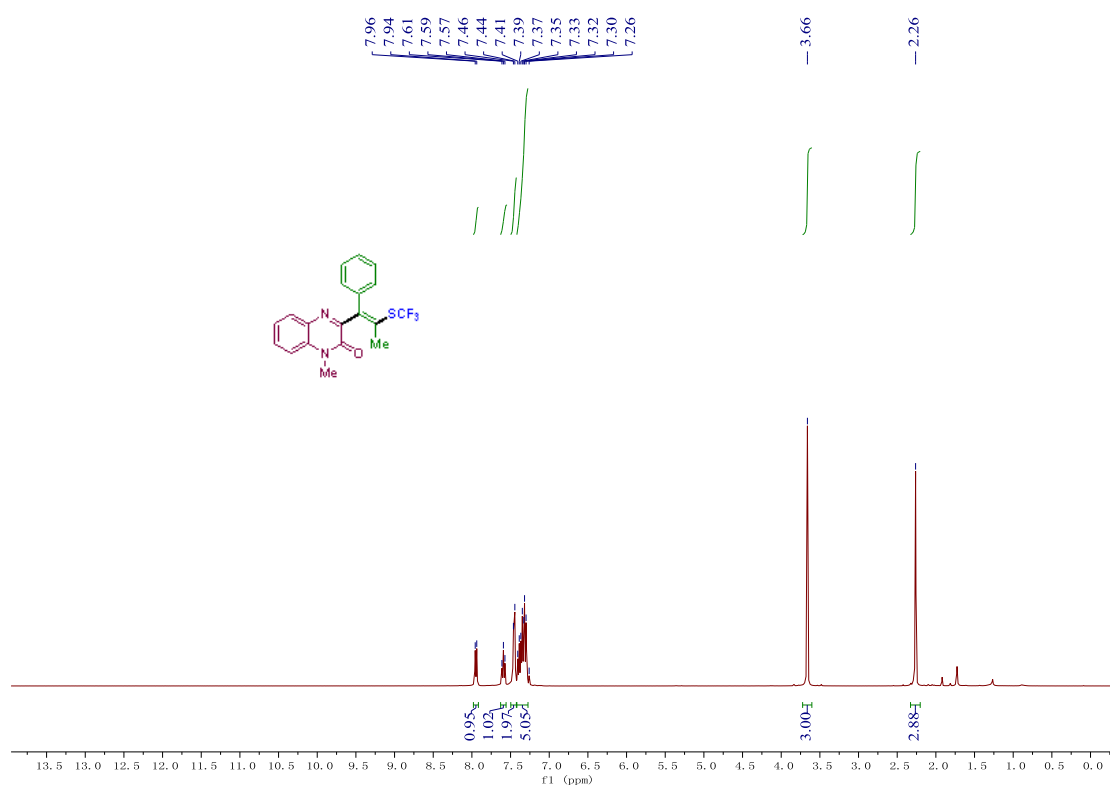
$^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ ) spectra of **3ax**



$^{13}\text{C}\{^1\text{H}\}$  NMR (100 MHz,  $\text{CDCl}_3$ ) spectra of **3ax**

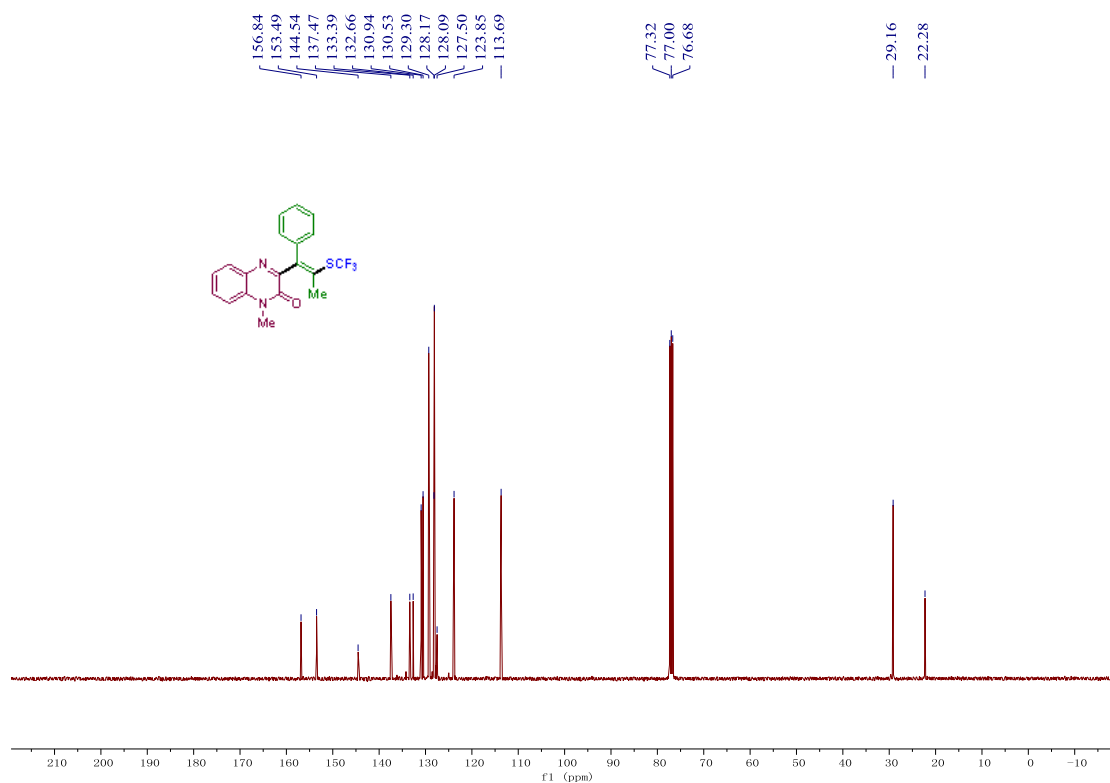


$^{19}\text{F}$  NMR (376 MHz,  $\text{CDCl}_3$ ) spectra of **3ax**

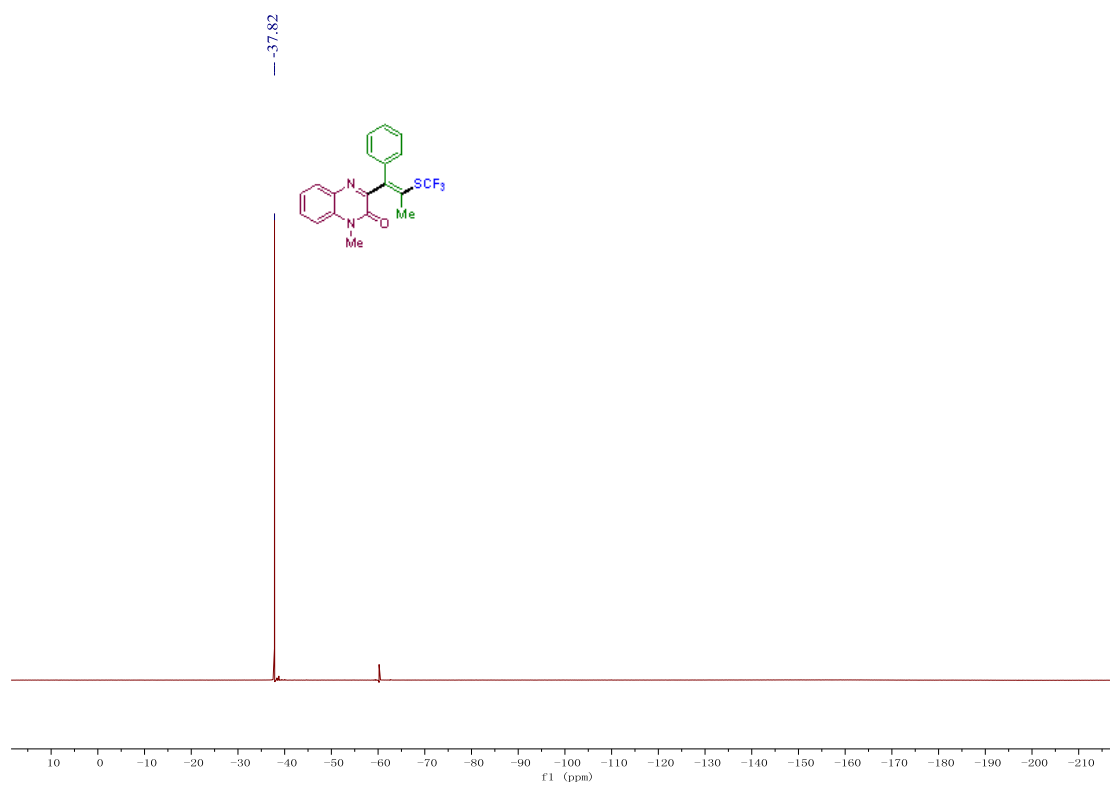


$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ) spectra of **3ay**

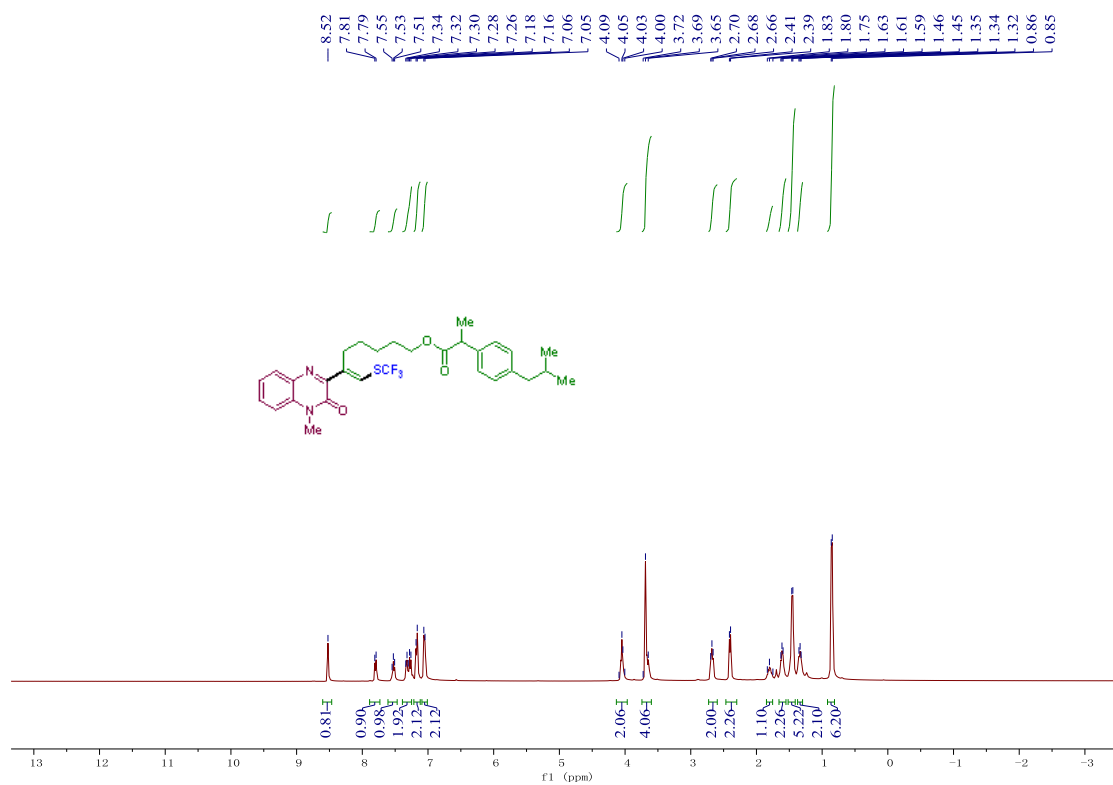




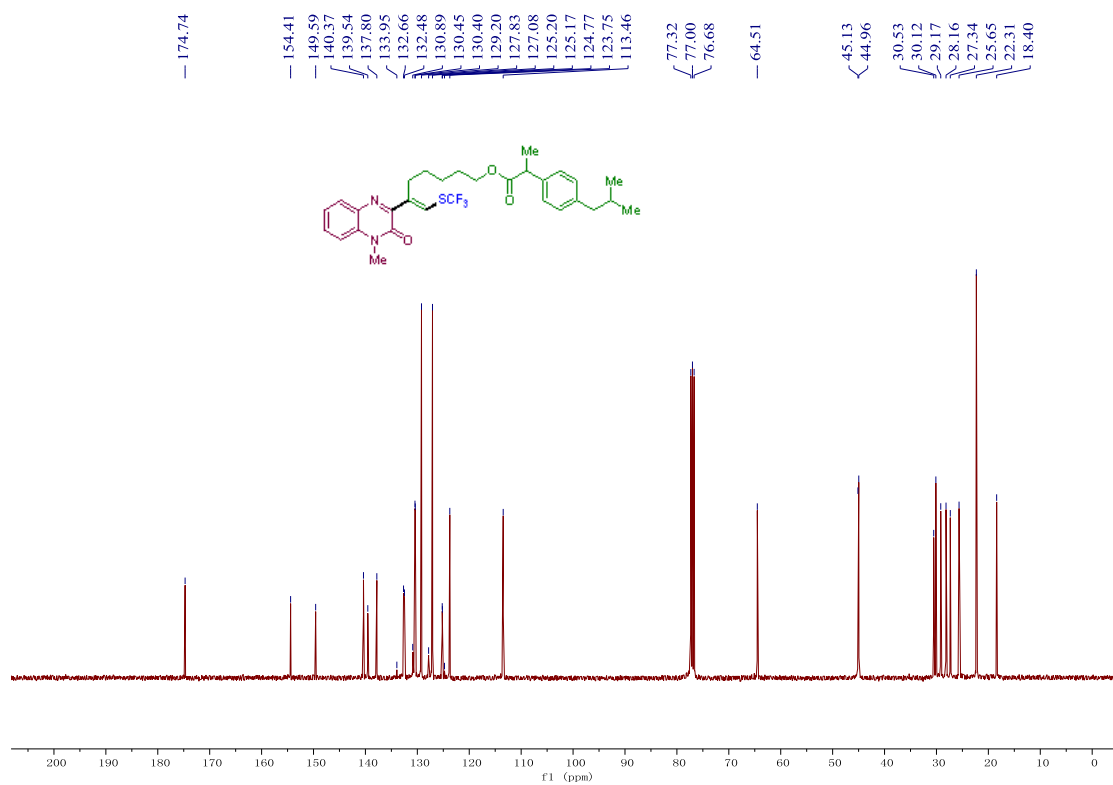
$^{13}\text{C}\{^1\text{H}\}$  NMR (100 MHz,  $\text{CDCl}_3$ ) spectra of **3ay**



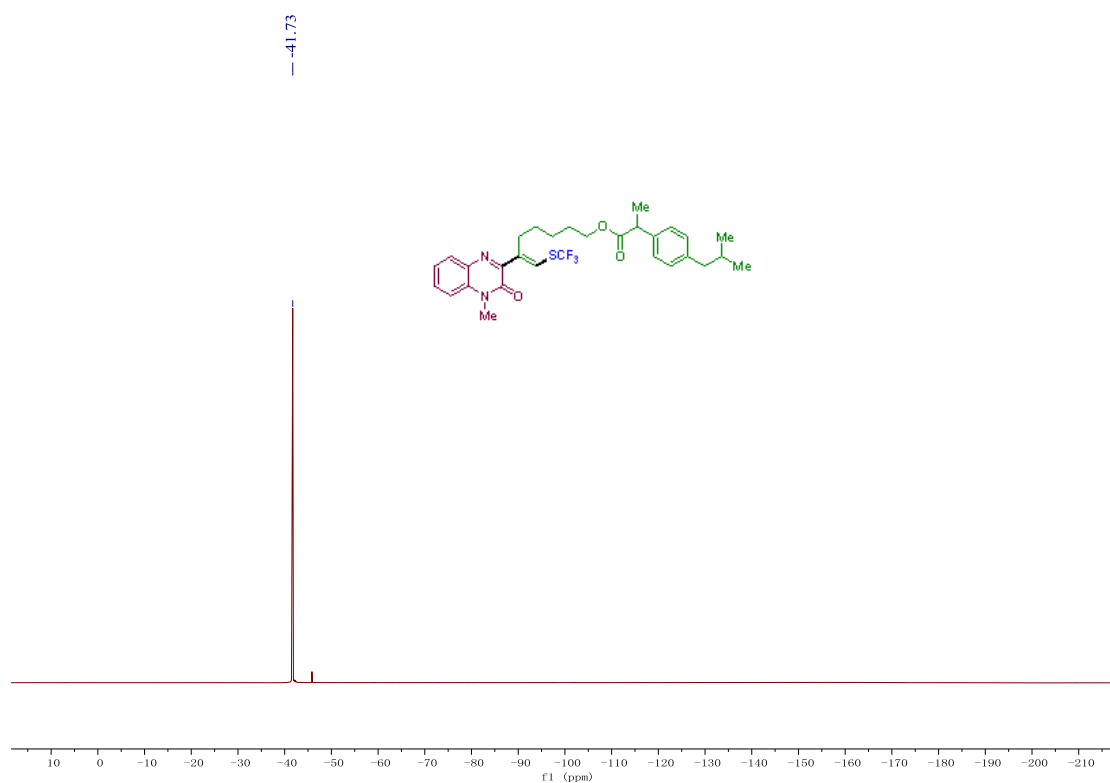
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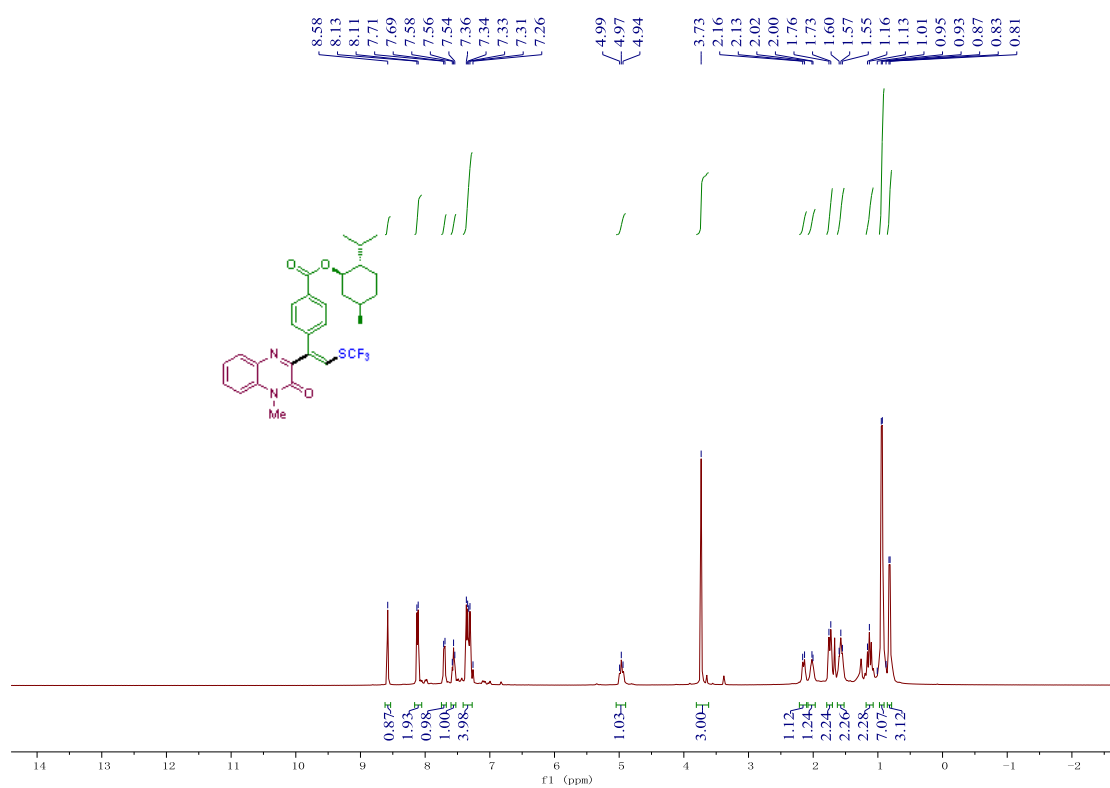
<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) spectra of 4aa



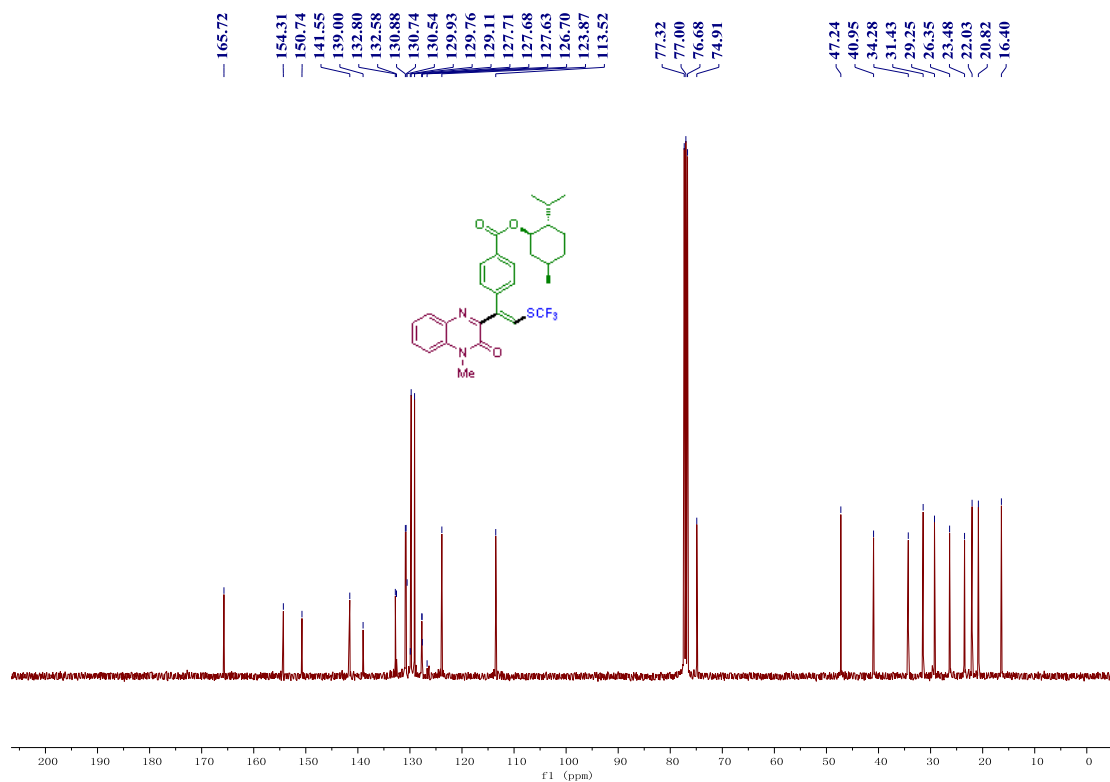
<sup>13</sup>C{<sup>1</sup>H} NMR (100 MHz, CDCl<sub>3</sub>) spectra of 4aa



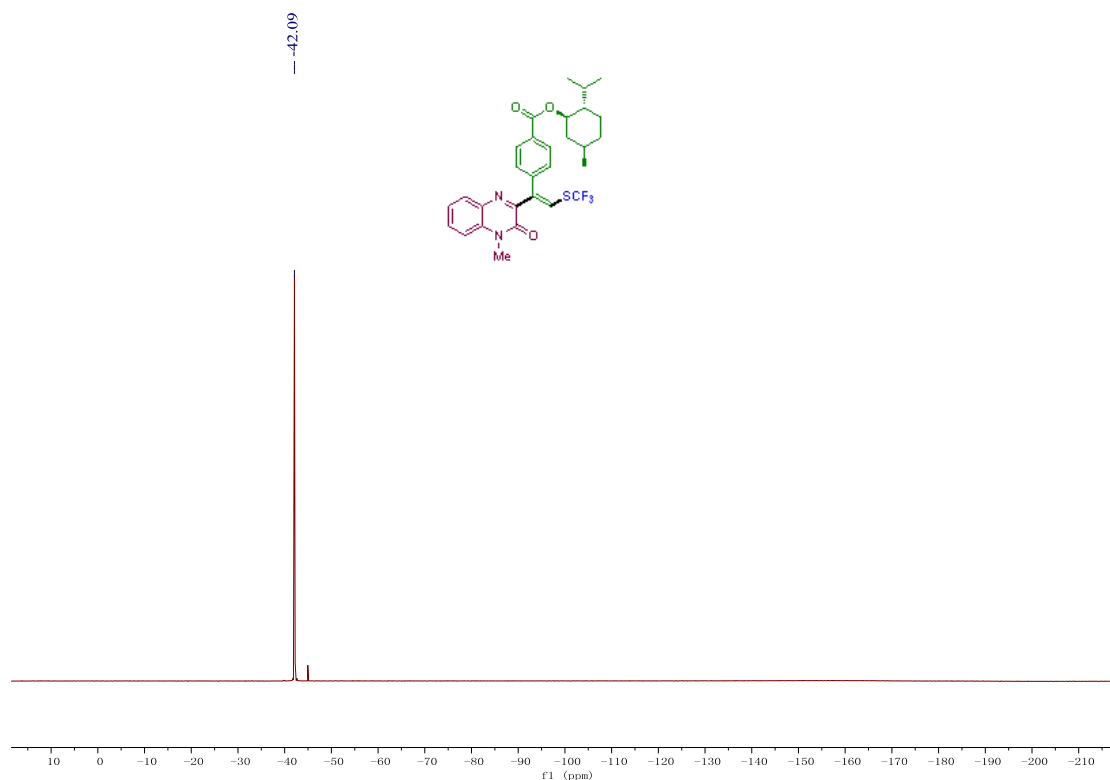
$^{19}\text{F}$  NMR (376 MHz,  $\text{CDCl}_3$ ) spectra of **4aa**



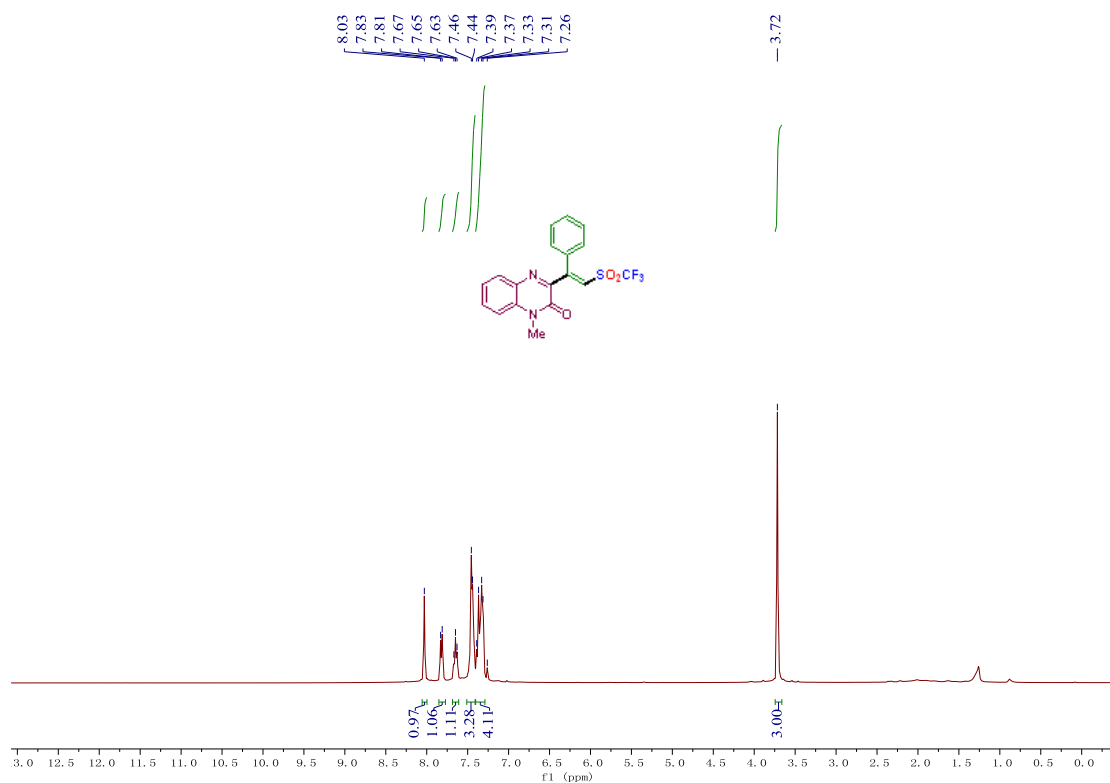
$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ) spectra of **4ab**



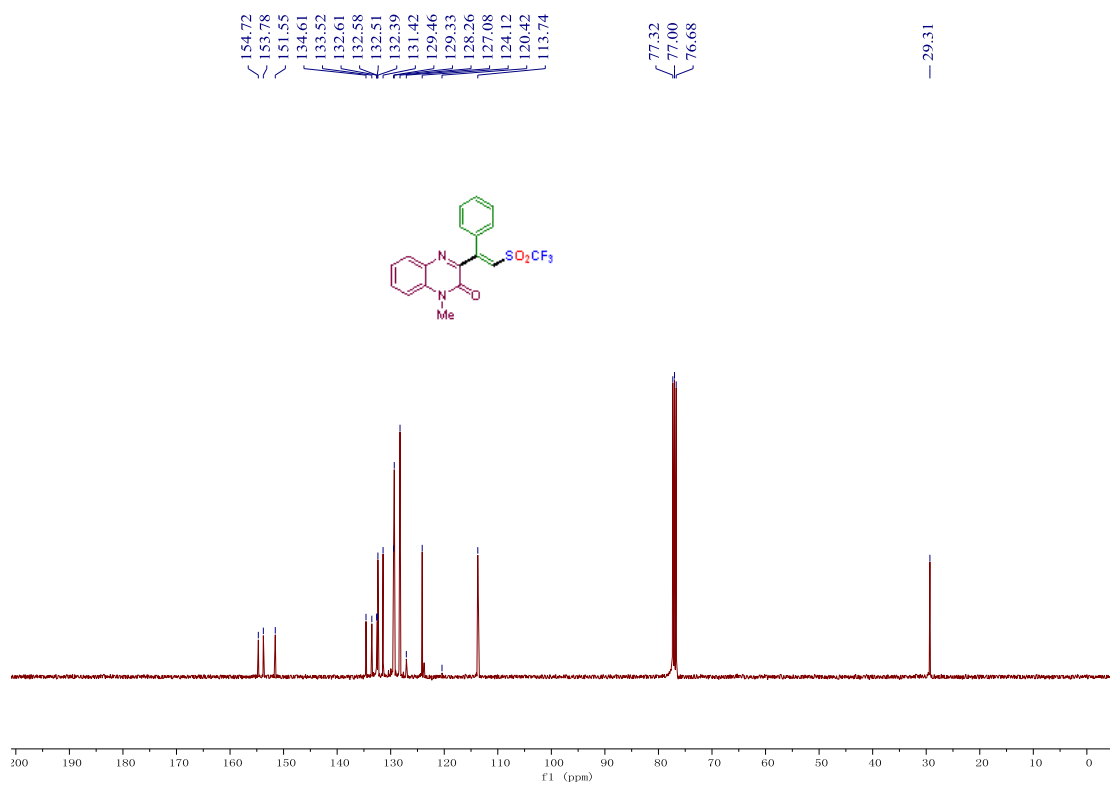
$^{13}\text{C}\{^1\text{H}\}$  NMR (100 MHz,  $\text{CDCl}_3$ ) spectra of **4ab**



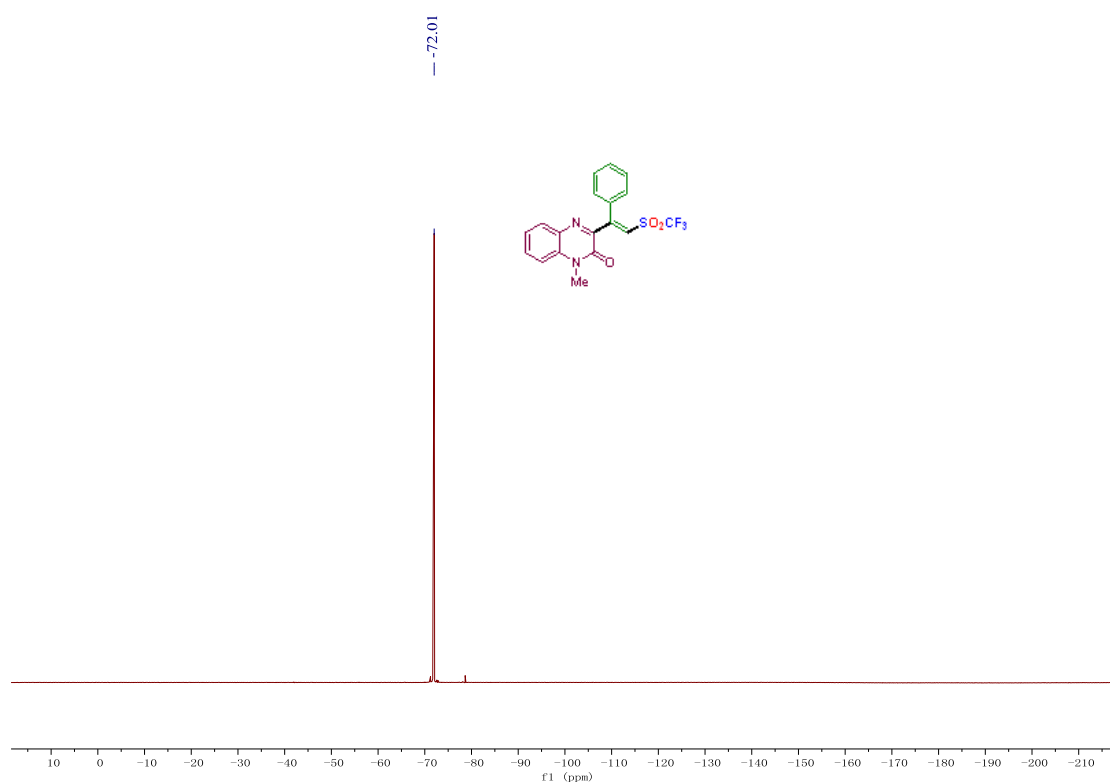
$^{19}\text{F}$  NMR (376 MHz,  $\text{CDCl}_3$ ) spectra of **4ab**



$^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ ) spectra of **5a**



$^{13}\text{C}\{^1\text{H}\}$  NMR (100 MHz,  $\text{CDCl}_3$ ) spectra of **5a**



$^{19}\text{F}$  NMR (376 MHz, CDCl<sub>3</sub>) spectra of **5a**