Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Supporting Information

Transition-metal-free decarboxylative C3-difluoroarylmethylation of quinoxalin-2(1*H*)-ones with α,α-difluoroarylacetic acids

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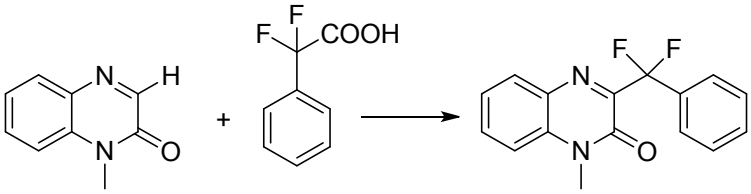
Contents

1. Screening the reaction conditions



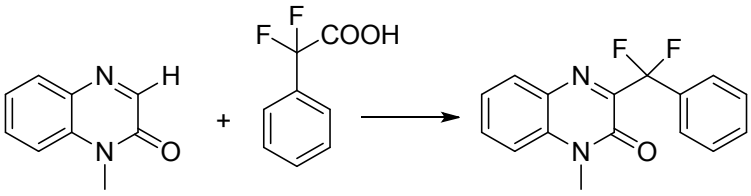
1a **2a** **3aa**

Table S1 Screening the leading amount of $(NH_4)_2S_2O_8$[a]

Entry	The leading amount of $(NH_4)_2S_2O_8$ (eq)	Yields (%)[b]
1	1.0	10
2	2.0	20
3	2.5	42
4	3.0	60
5	4.0	57

[a)] Reaction conditions: 1-methylquinoxalin-2(1*H*)-one **1a** (0.2 mmol, 32.0 mg), α,α-difluorophenylacetic acid **2a** (0.24 mmol, 41.3 mg), and $(NH_4)_2S_2O_8$ in DMSO (2.0 mL) at 60 °C for 3 h under N_2 atmosphere.

[b)] Isolated yield.



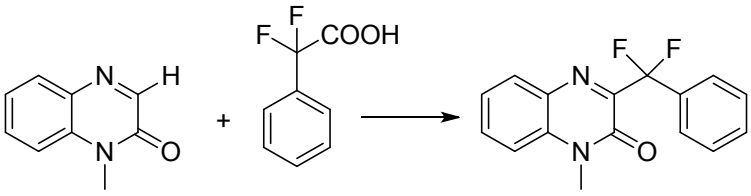
1a **2a** **3aa**

Table S2 Screening the reaction temperature[a]

Entry	The reaction temperature	Yields (%)[b]
1	20	0
2	50	21
3	60	60
4	70	58
5	80	50
6	90	46

a) Reaction conditions: 1-methylquinoxalin-2(1*H*)-one **1a** (0.2 mmol, 32.0 mg), 2,2-difluoro-2-phenylacetic acid **2a** (0.24 mmol, 41.3 mg), and $(NH_4)_2S_2O_8$ (0.6 mmol, 136.8 mg) in DMSO (2.0 mL) for 3 h under N_2 atmosphere.

b) Isolated yield.



1a **2a** **3aa**

Table S3 Screening the molar ratio of **1a** with **2a**[a]

Entry	The molar ratio of **1a** and **2a**	Yields (%)[b]
1	1:1	37
2	1:1.2	60
3	1:1.5	56
4	1:2	50
5	1:2.5	42

[a)] Reaction conditions: 1-methylquinoxalin-2(1*H*)-one **1a** (0.2 mmol, 32.0 mg), 2,2-difluoro-2-phenylacetic acid **2a**, and $(NH_4)_2S_2O_8$ (0.6 mmol, 136.8 mg) in DMSO (2.0 mL) at 60 °C for 3 h under N_2 atmosphere.

[b)] Isolated yield.

2. Copies of spectra of products

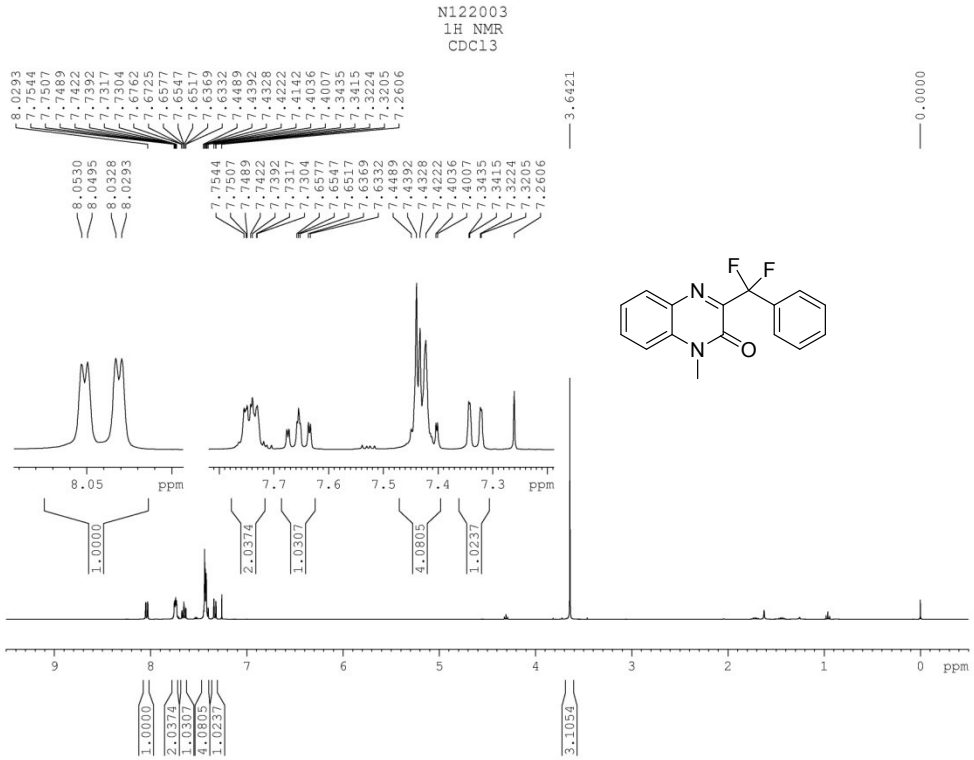


Fig. S1 ^{1}H NMR spectrum of compound **3aa**

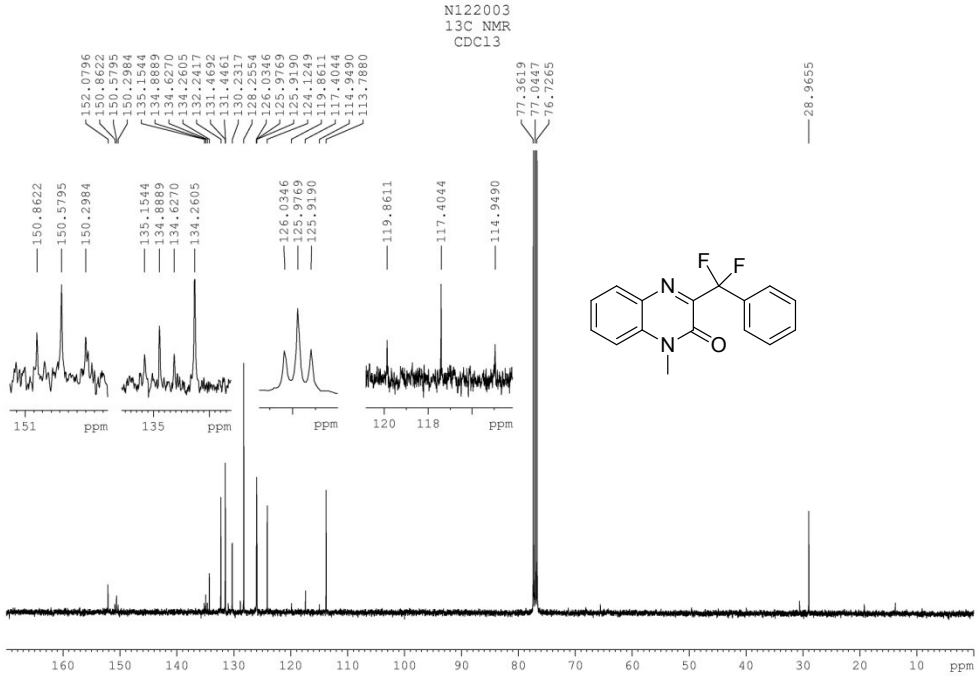


Fig. S2 ^{13}C NMR spectrum of compound **3aa**

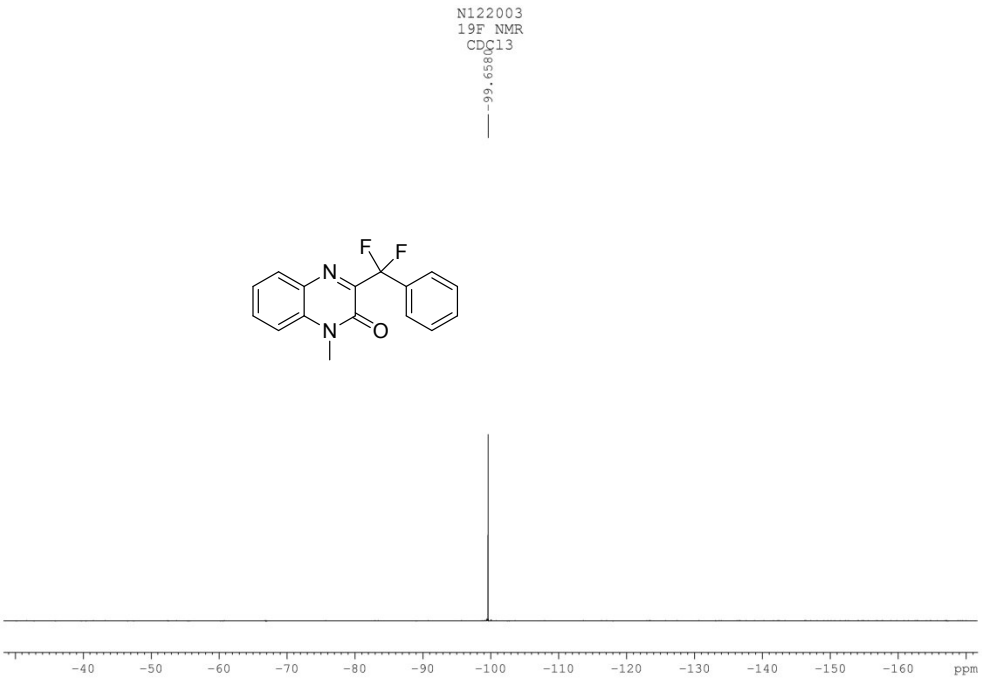


Fig. S3 ^{19}F NMR spectrum of compound **3aa**

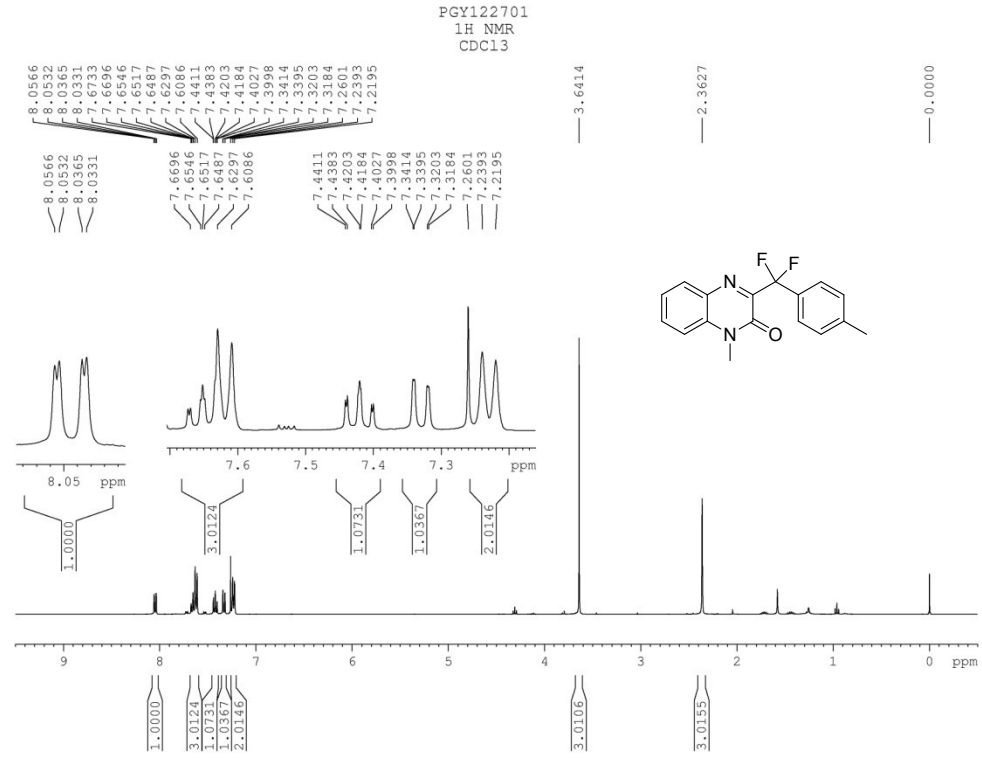


Fig. S4 ^{1}H NMR spectrum of compound **3ab**

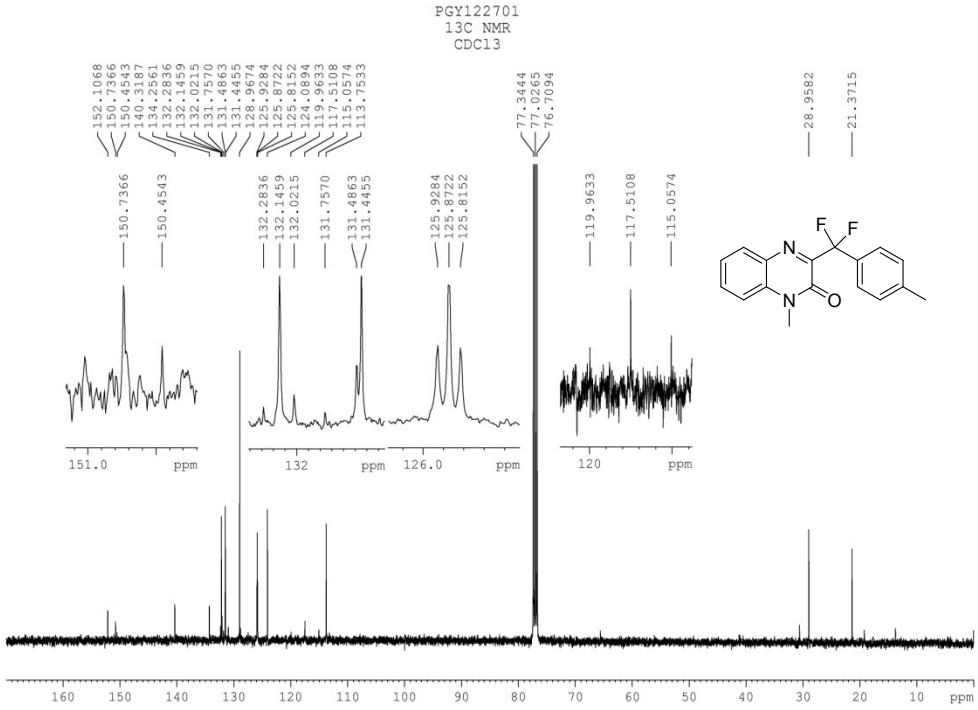


Fig. S5 ^{13}C NMR spectrum of compound **3ab**

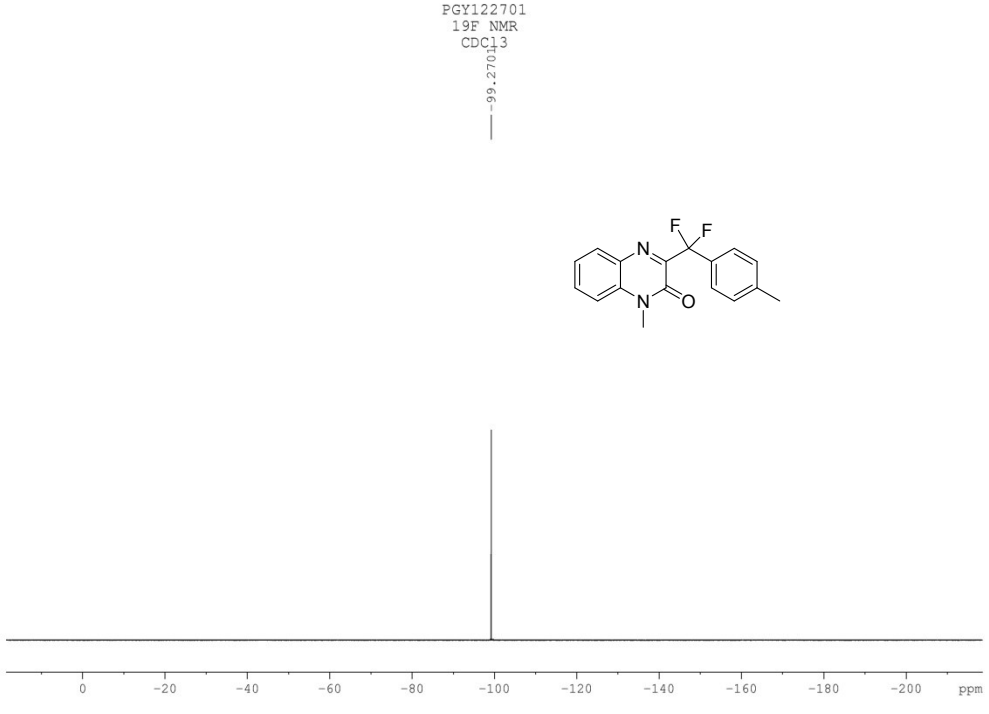


Fig. S6 ^{19}F NMR spectrum of compound **3ab**

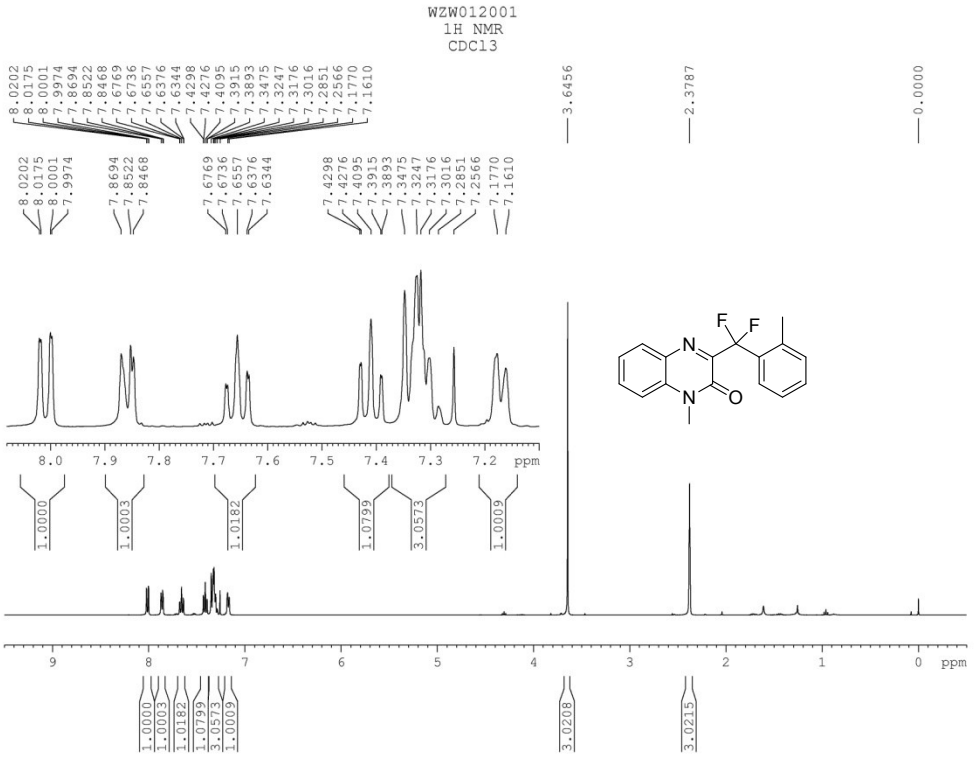


Fig. S7 ^{1}H NMR spectrum of compound **3ac**

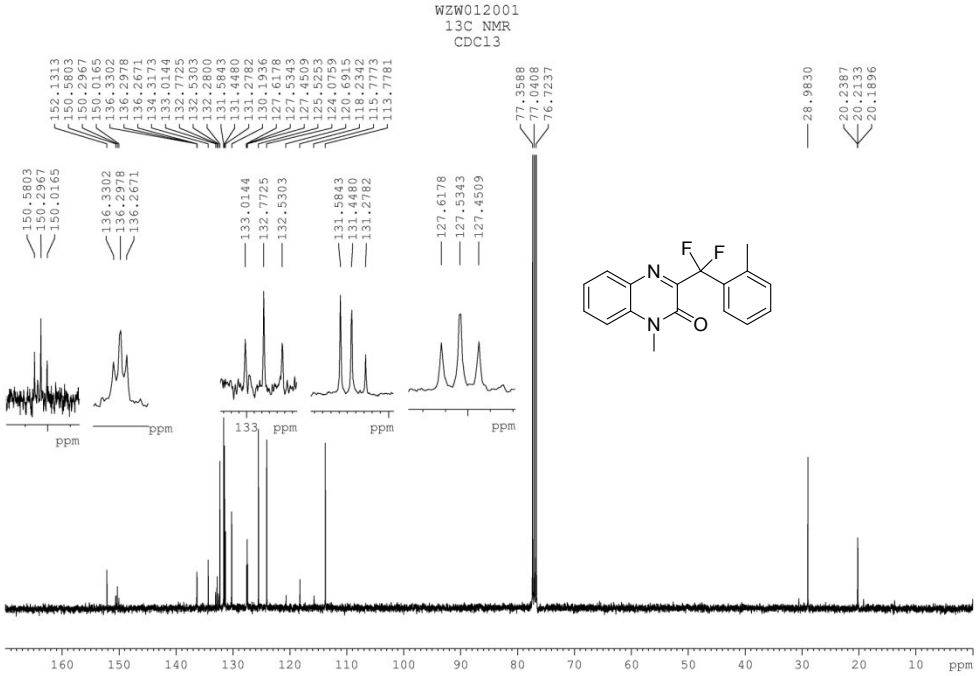


Fig. S8 ^{13}C NMR spectrum of compound **3ac**

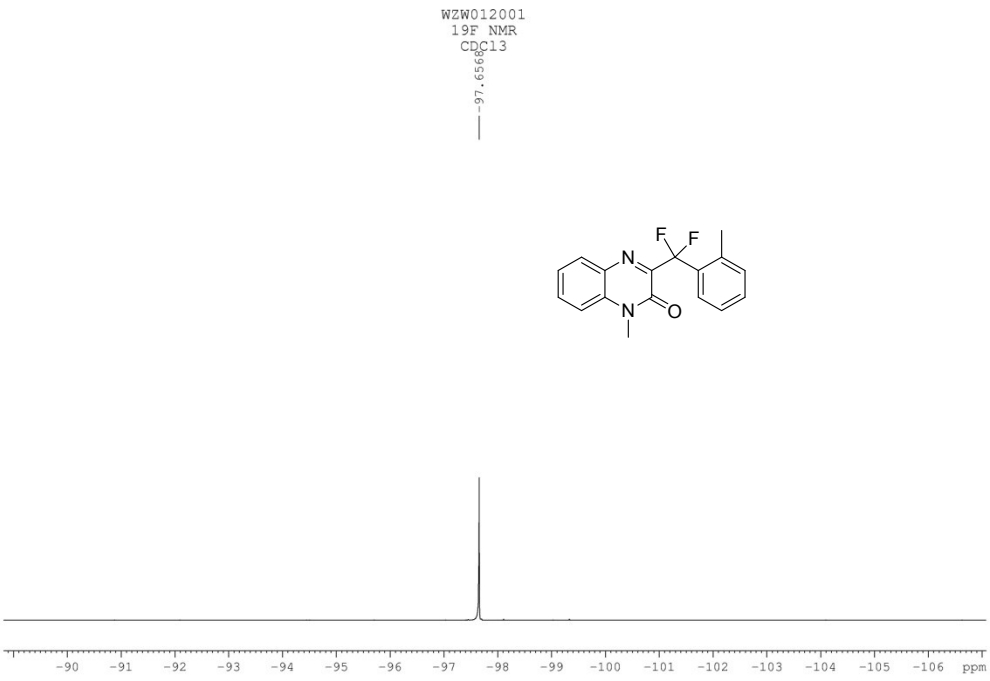


Fig. S9 ^{19}F NMR spectrum of compound **3ac**

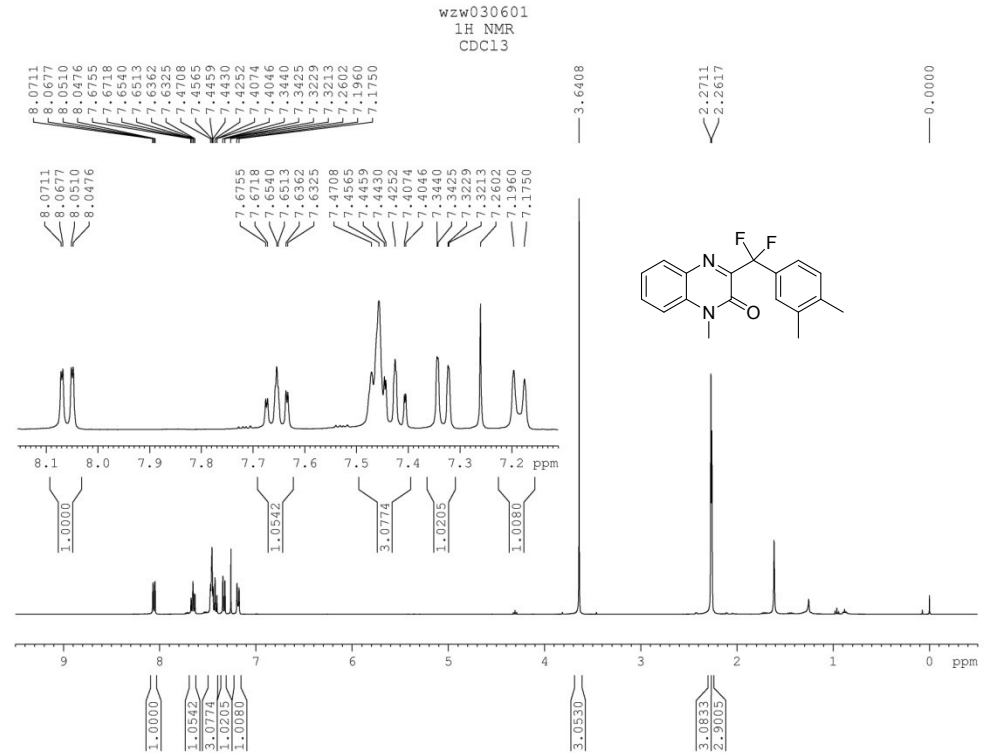


Fig. S10 ^{1}H NMR spectrum of compound **3ad**

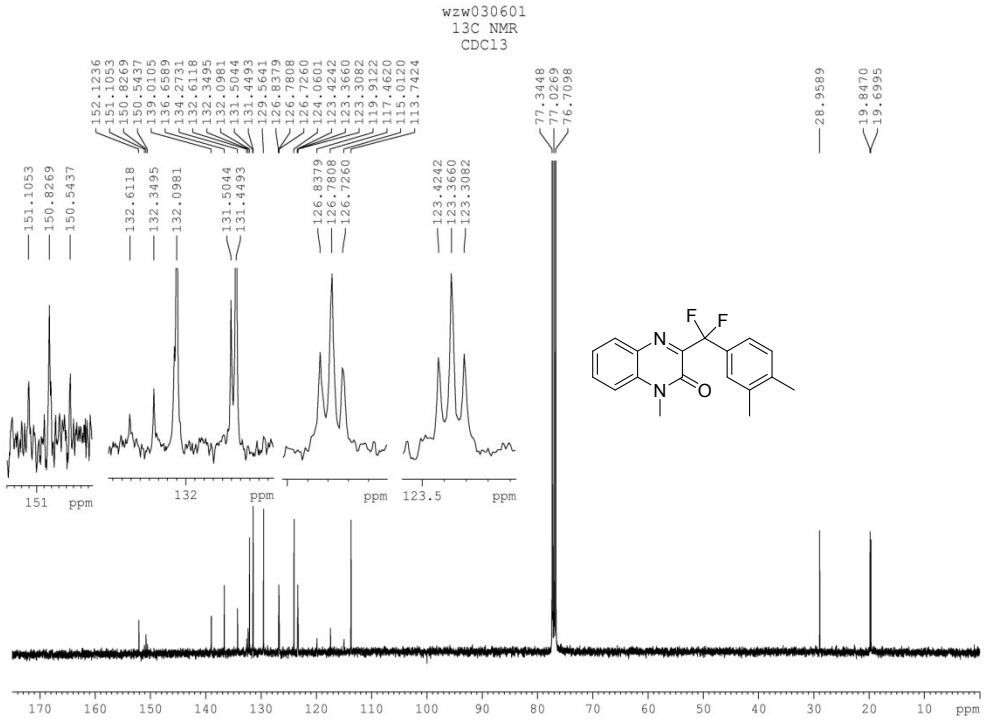


Fig. S11 ^{13}C NMR spectrum of compound **3ad**

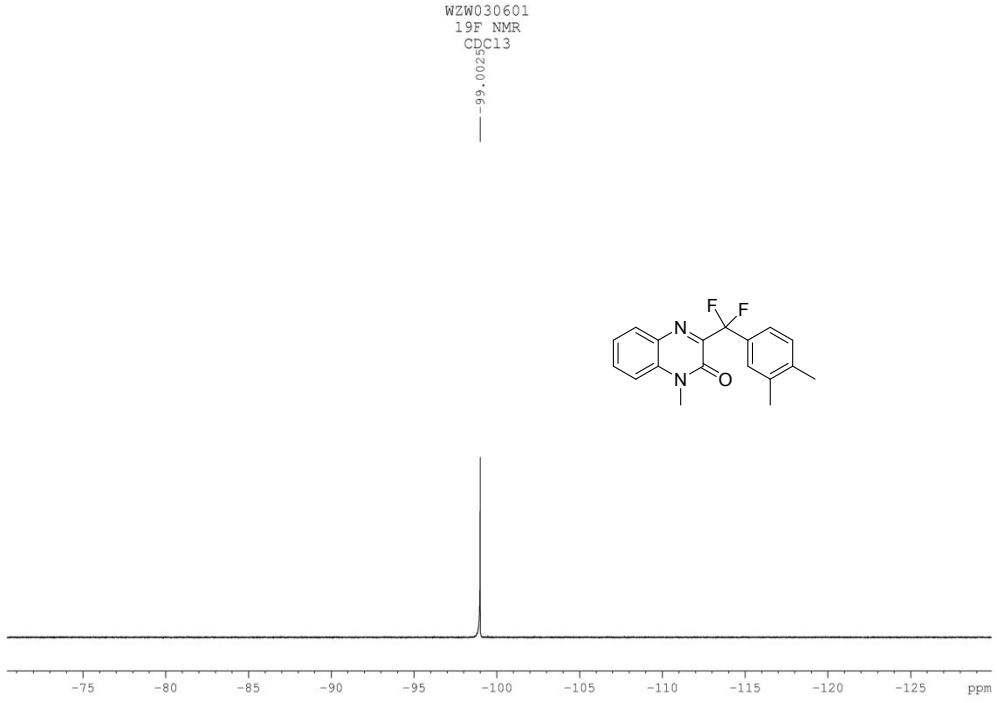


Fig. S12 ^{19}F NMR spectrum of compound **3ad**

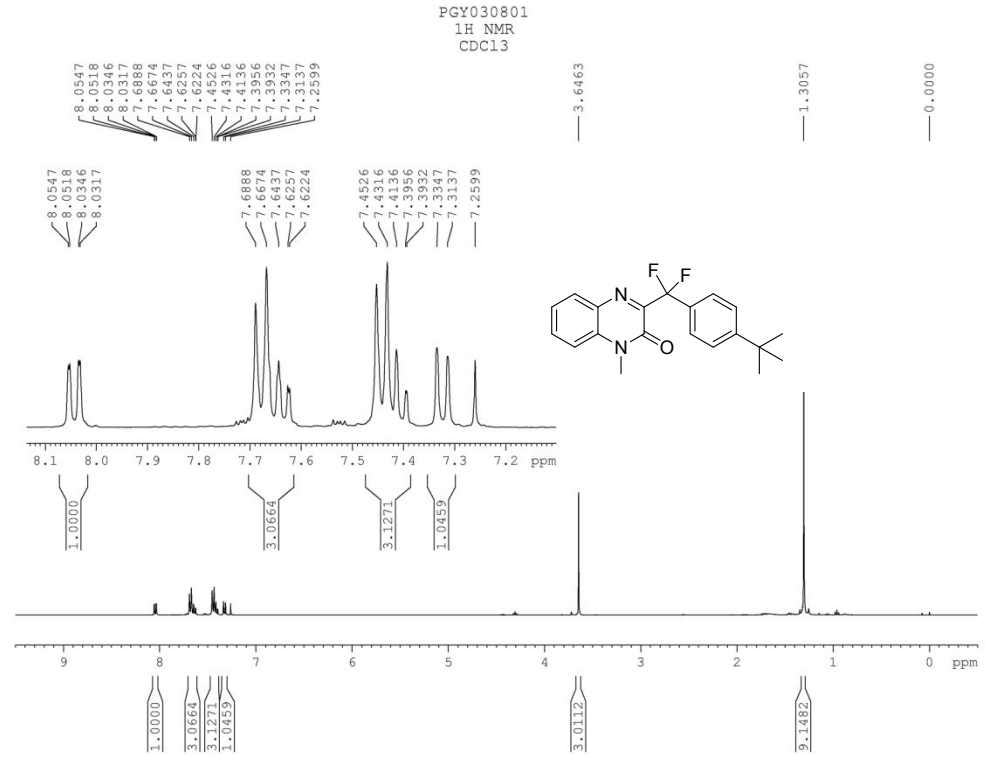


Fig. S13 ^{1}H NMR spectrum of compound **3ae**

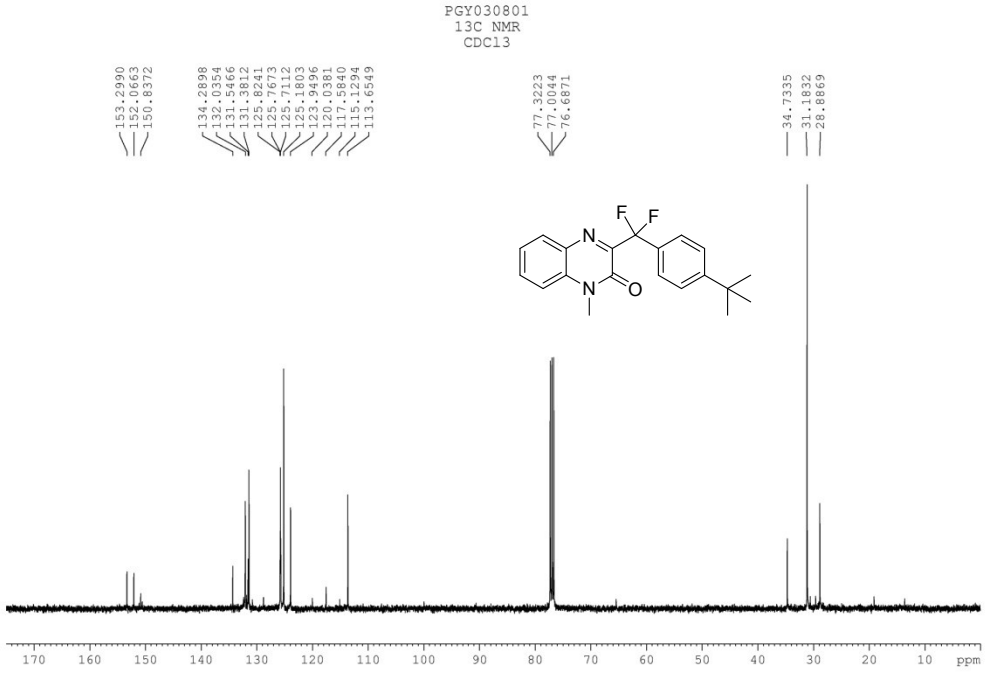


Fig. S14 ^{13}C NMR spectrum of compound **3ae**

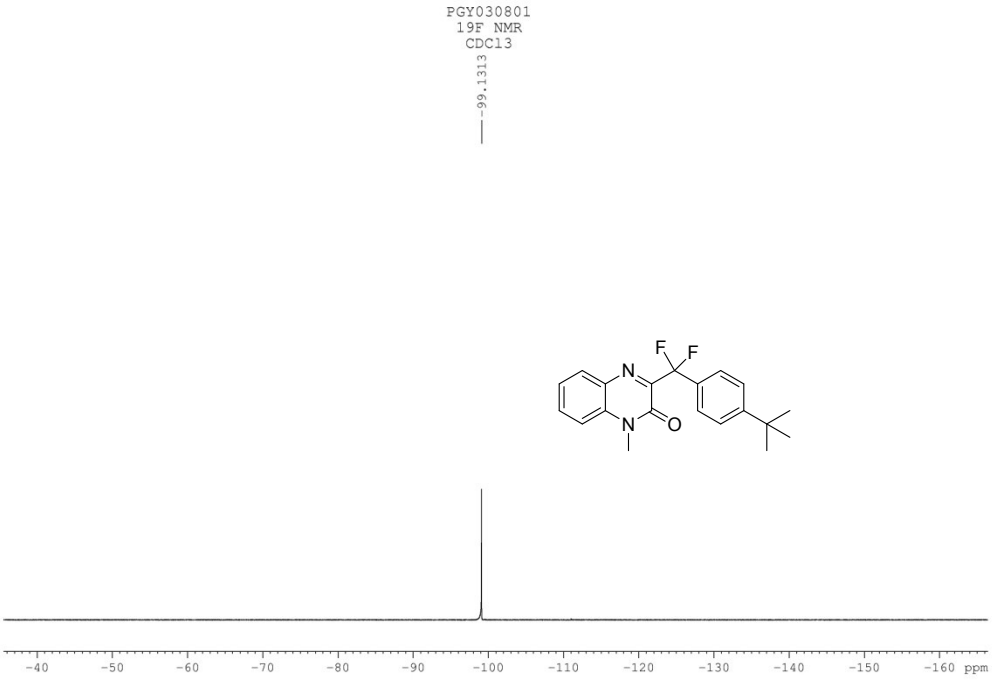


Fig. S15 ^{19}F NMR spectrum of compound **3ae**

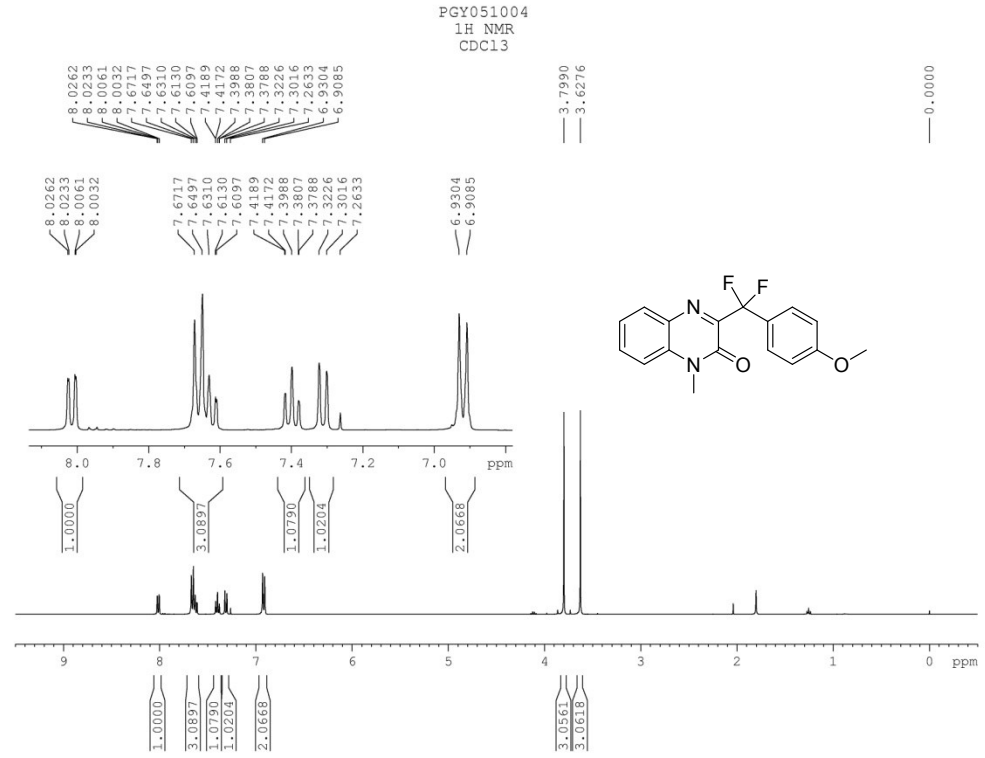


Fig. S16 ^{1}H NMR spectrum of compound **3af**

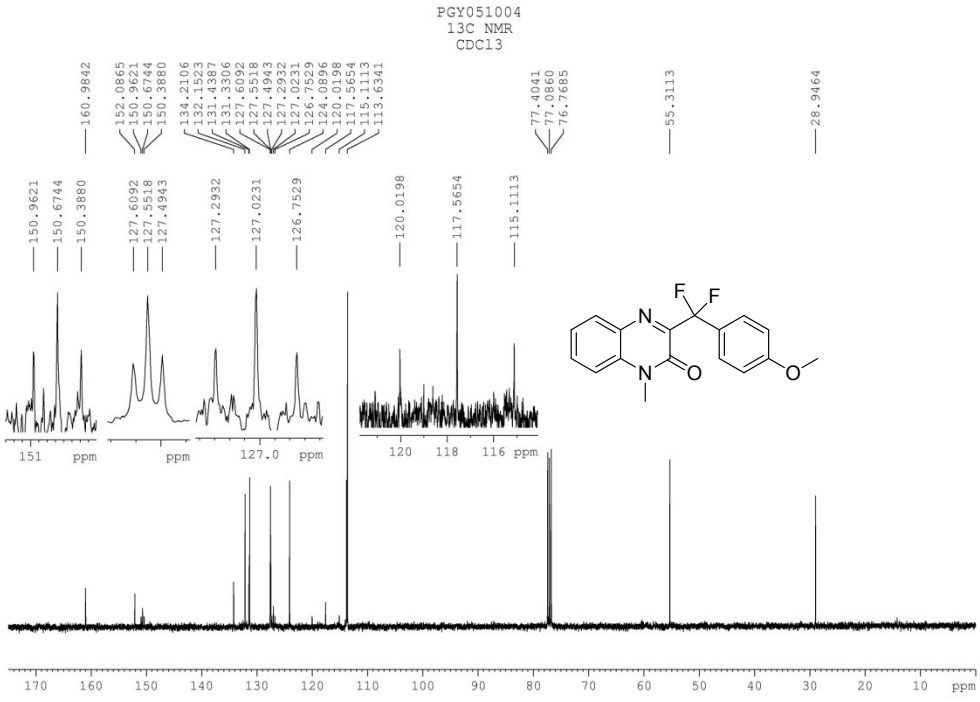


Fig. S17 ^{13}C NMR spectrum of compound **3af**

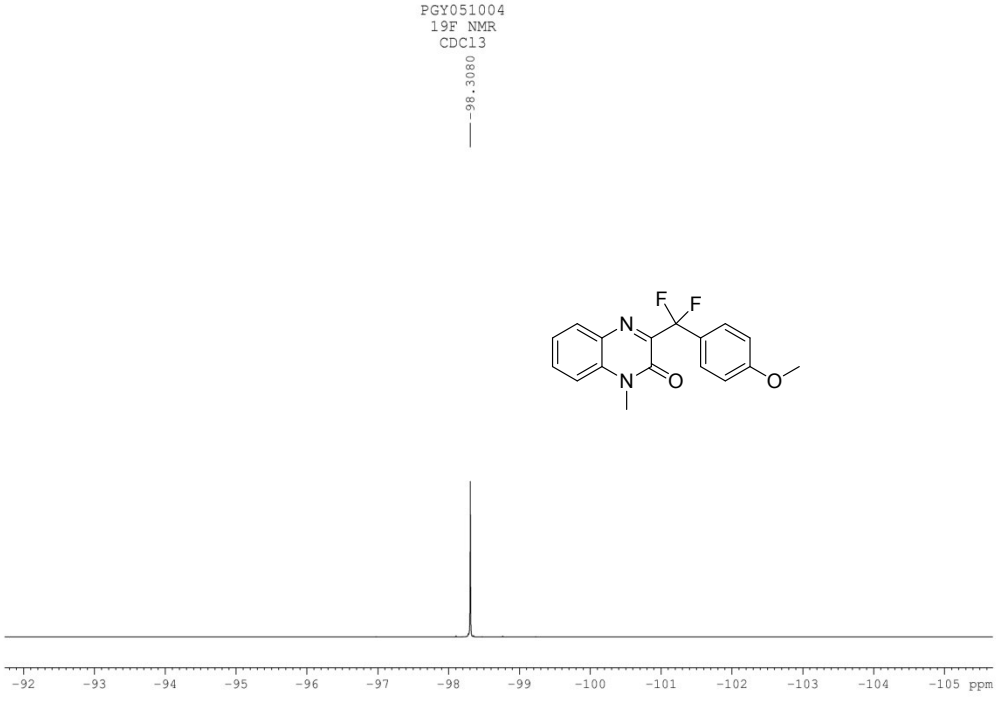


Fig. S18 ^{19}F NMR spectrum of compound **3af**

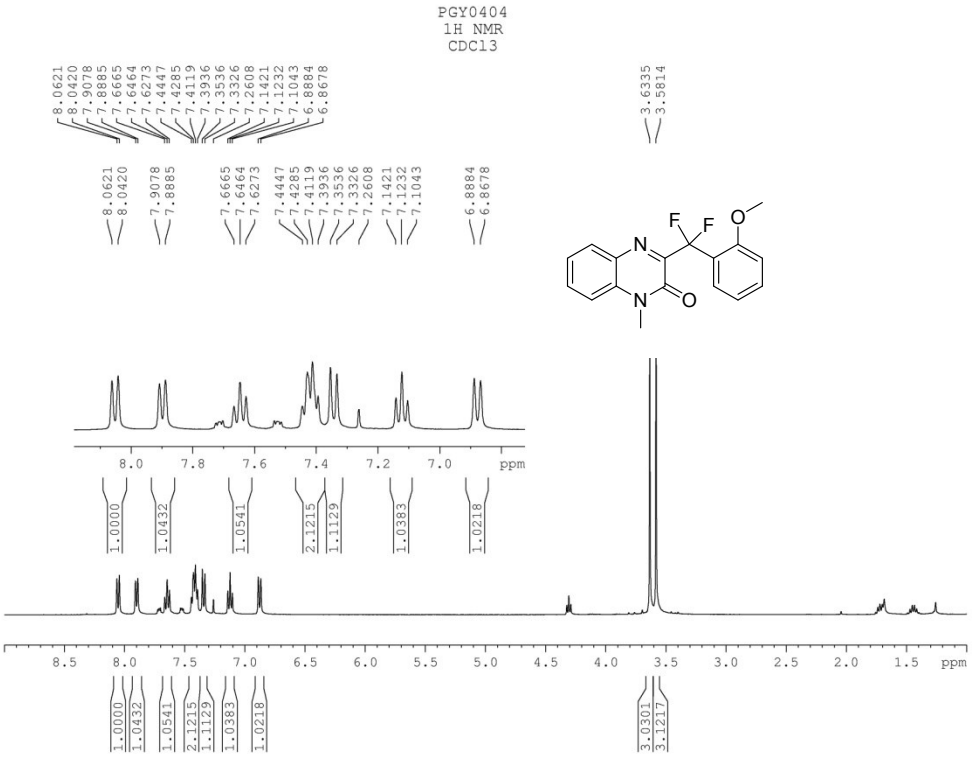


Fig. S19 ^{1}H NMR spectrum of compound **3ag**

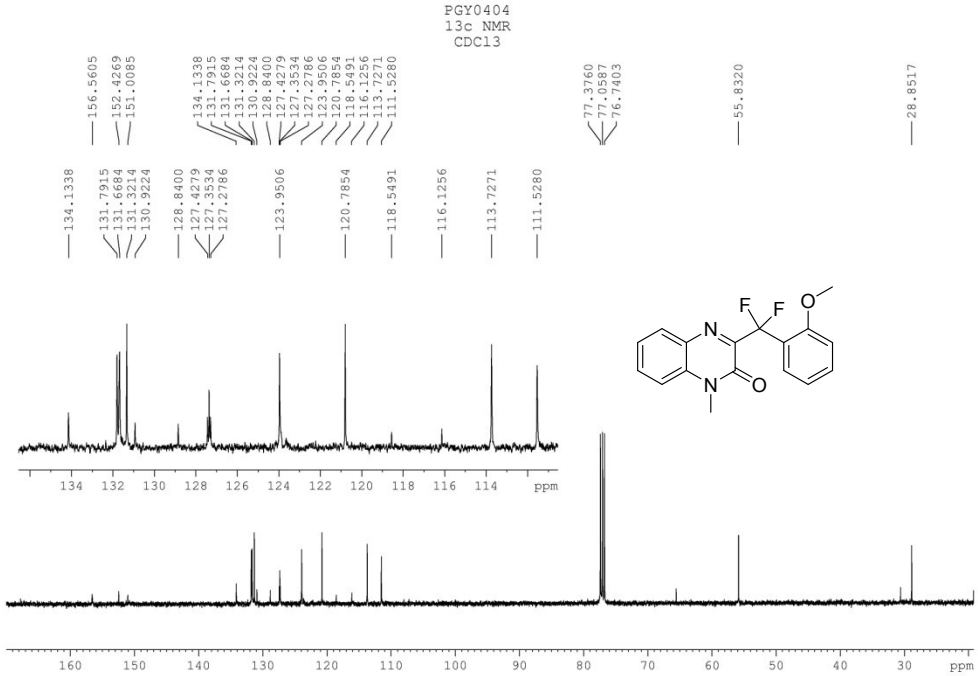


Fig. S20 ^{13}C NMR spectrum of compound **3ag**

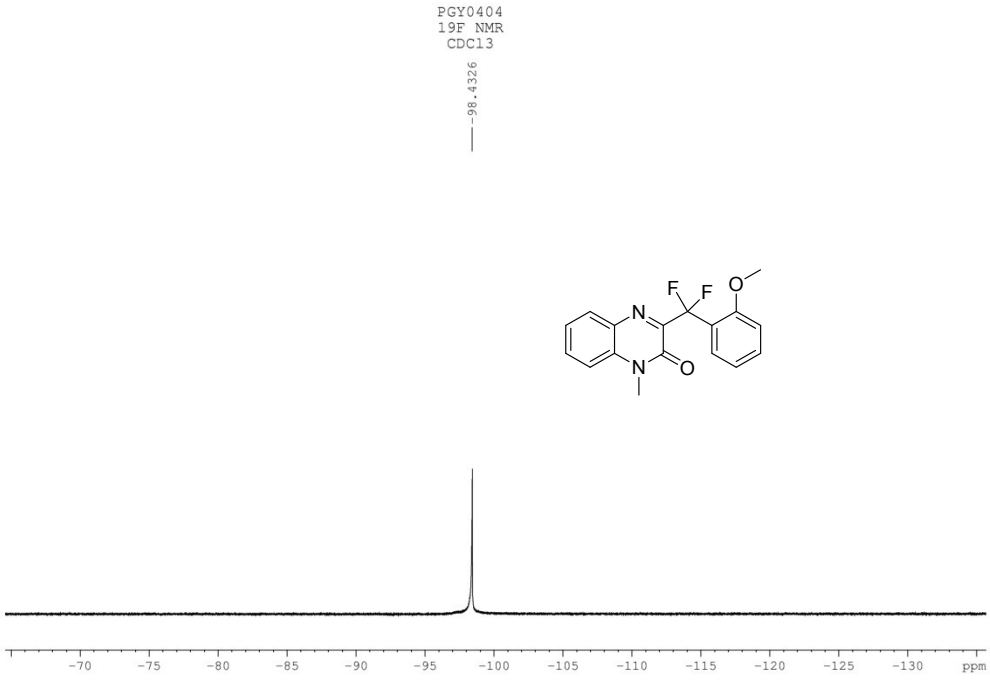


Fig. S21 ^{19}F NMR spectrum of compound **3ag**

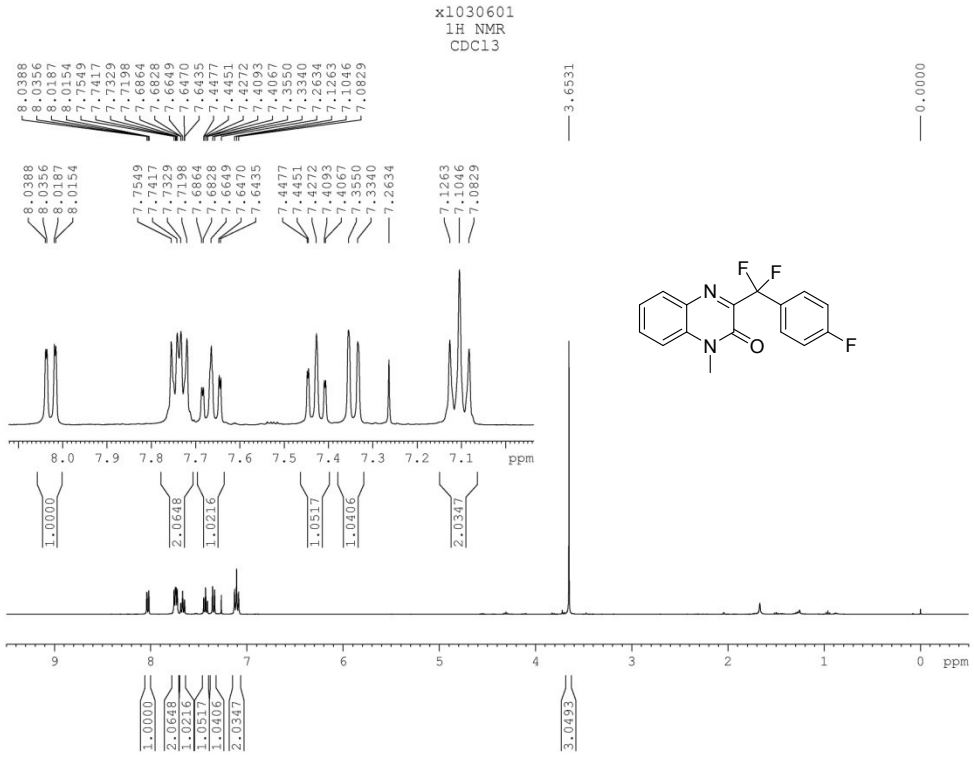


Fig. S22 ^{1}H NMR spectrum of compound **3ah**

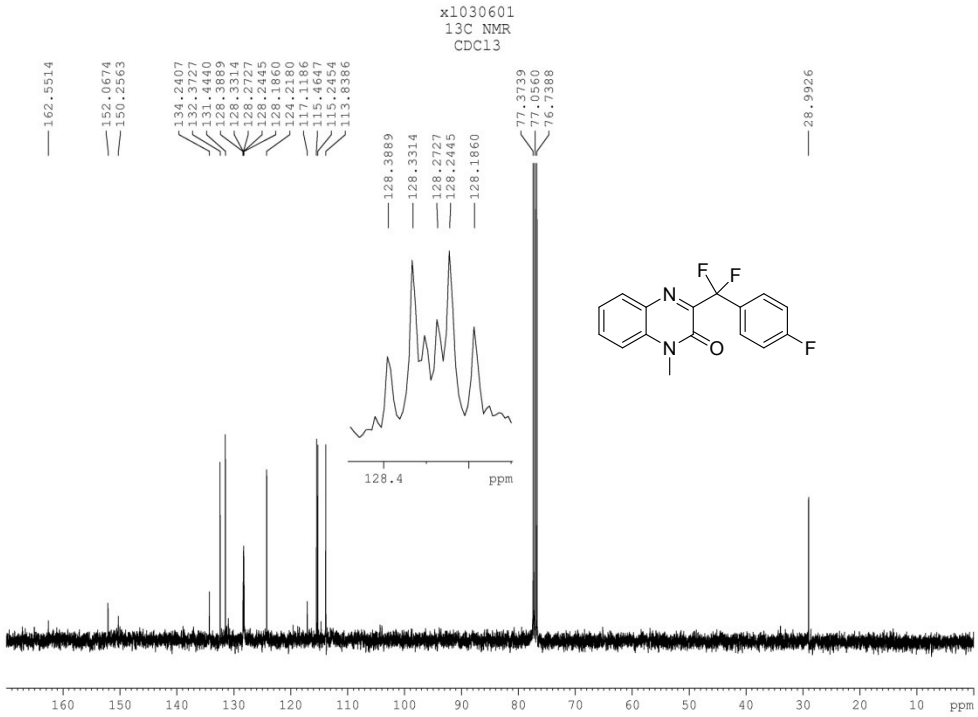


Fig. S23 ^{13}C NMR spectrum of compound **3ah**

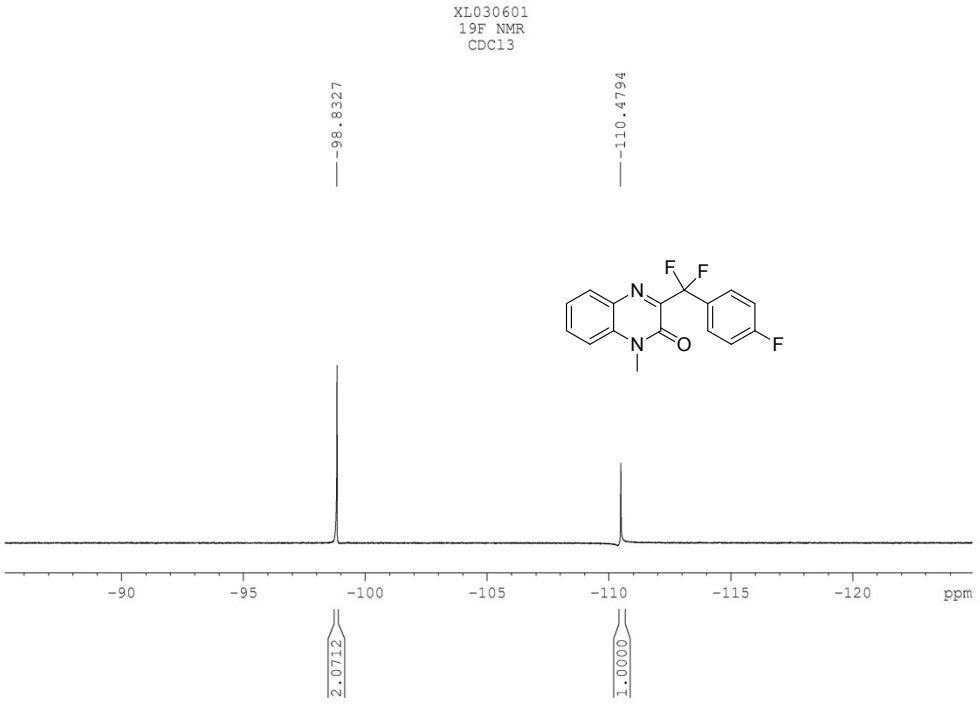


Fig. S24 ^{19}F NMR spectrum of compound **3ah**

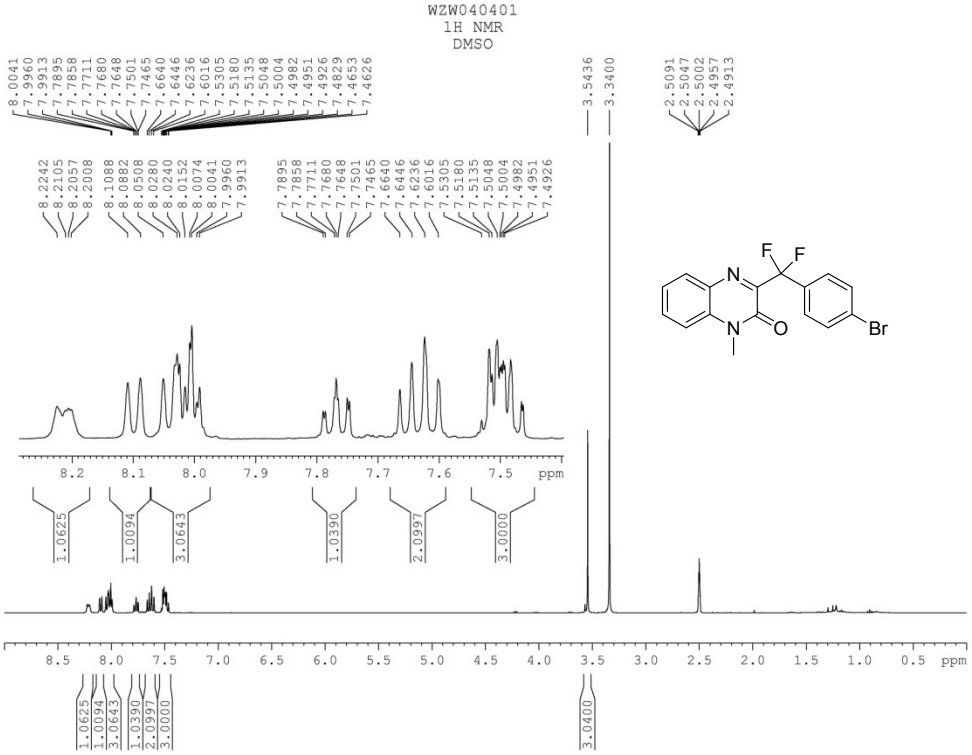


Fig. S25 ^{1}H NMR spectrum of compound **3ai**

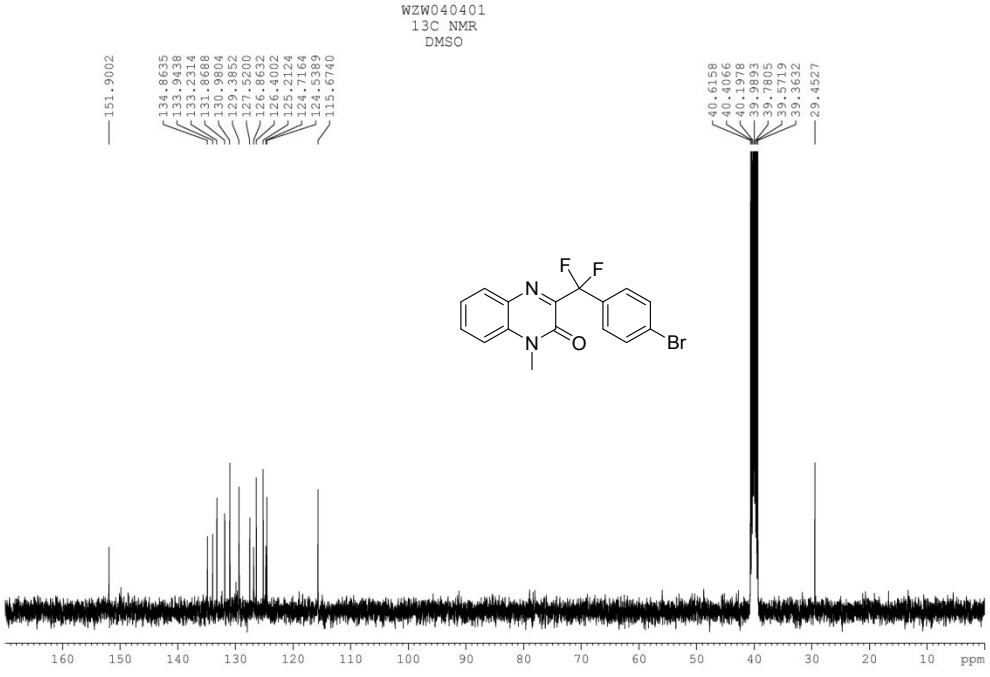


Fig. S26 ^{13}C NMR spectrum of compound **3ai**

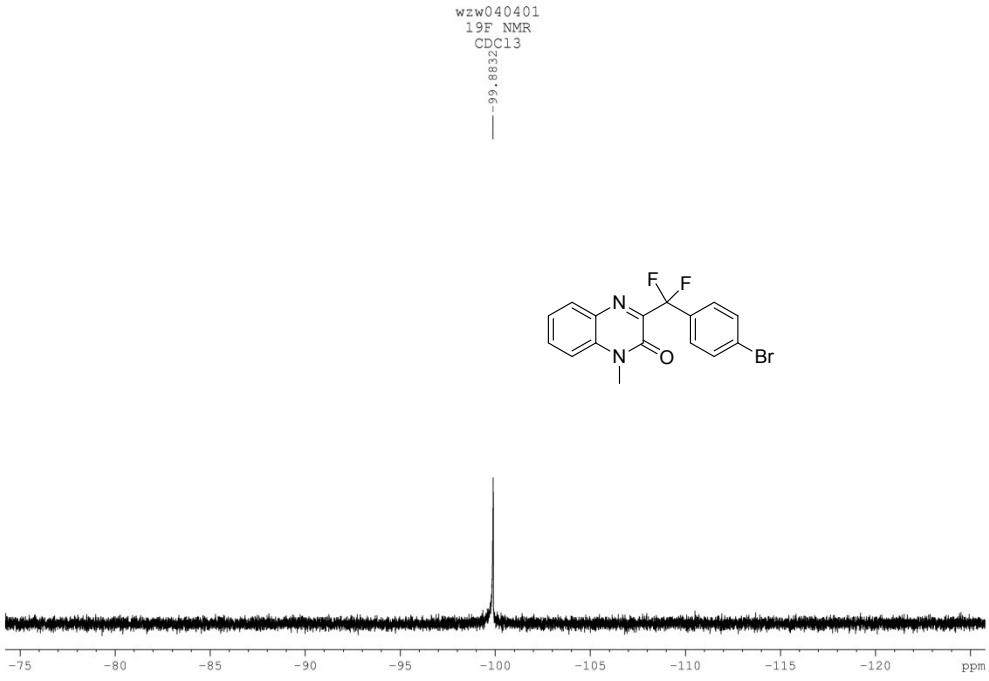


Fig. S27 ^{19}F NMR spectrum of compound **3ai**

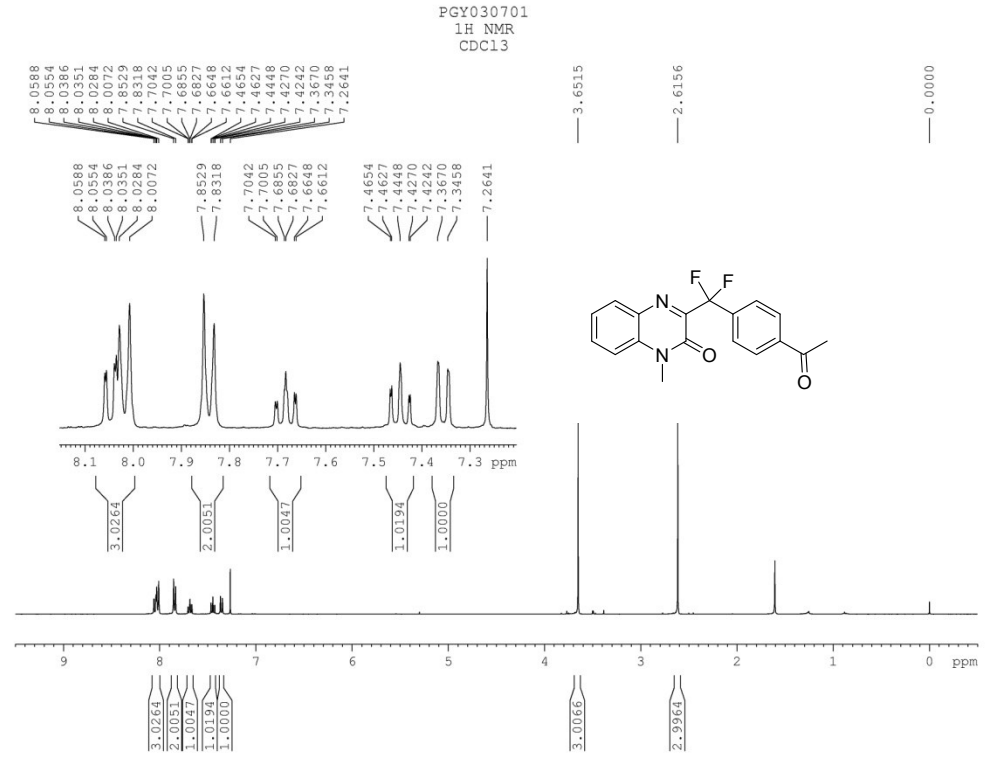


Fig. S28 ^{1}H NMR spectrum of compound **3aj**

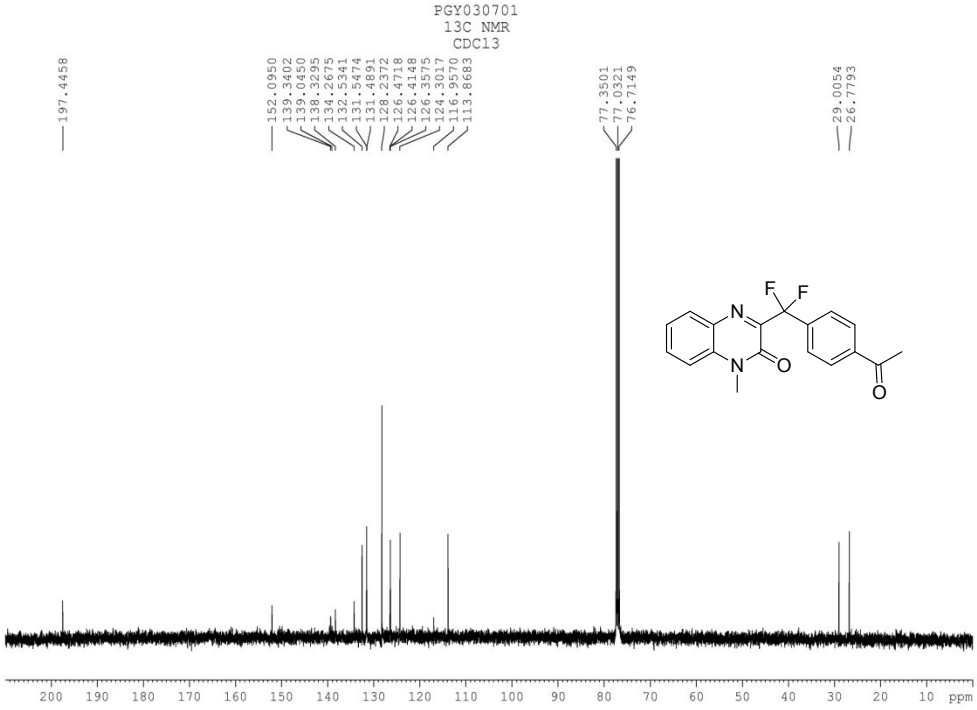


Fig. S29[13]C NMR spectrum of compound **3aj**

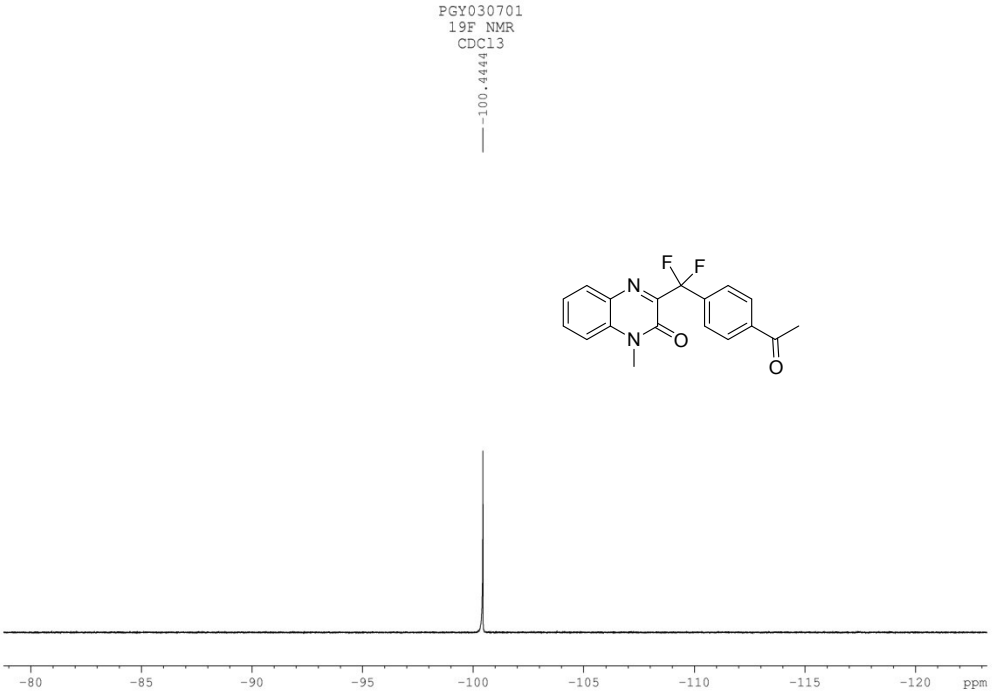


Fig. S30 [19]F NMR spectrum of compound **3aj**

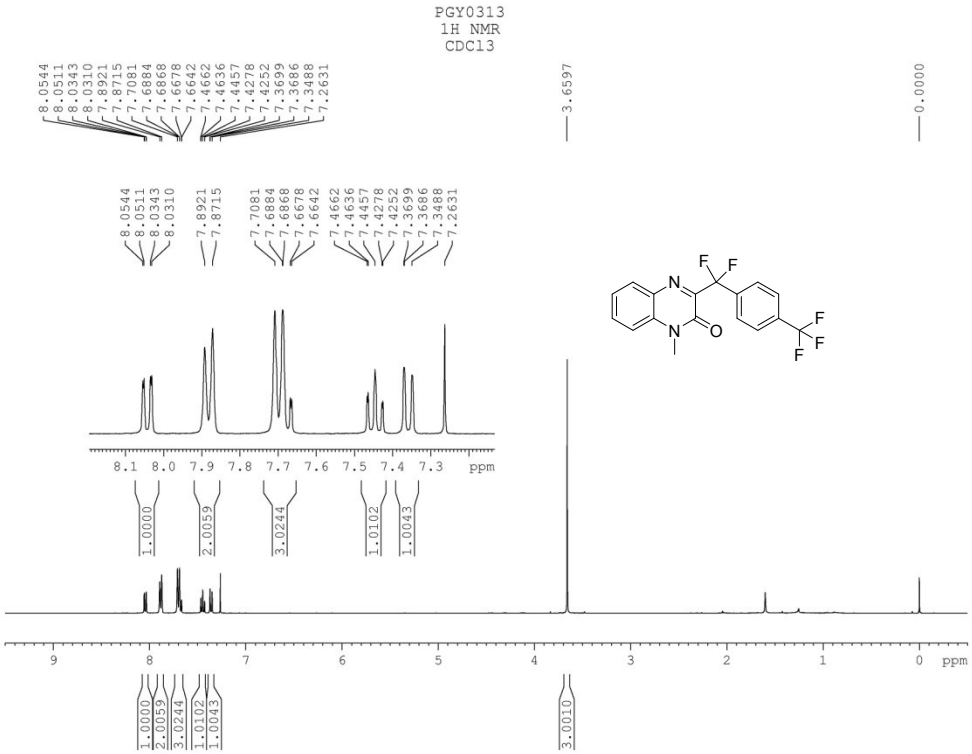


Fig. S31 ^{1}H NMR spectrum of compound **3ak**

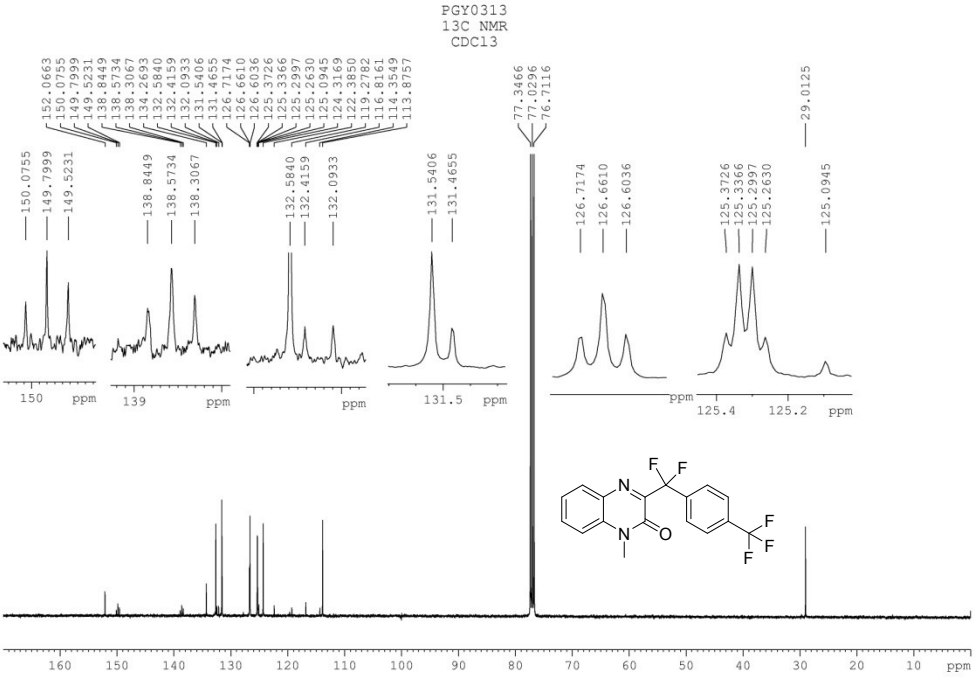


Fig. S32 ^{13}C NMR spectrum of compound **3ak**

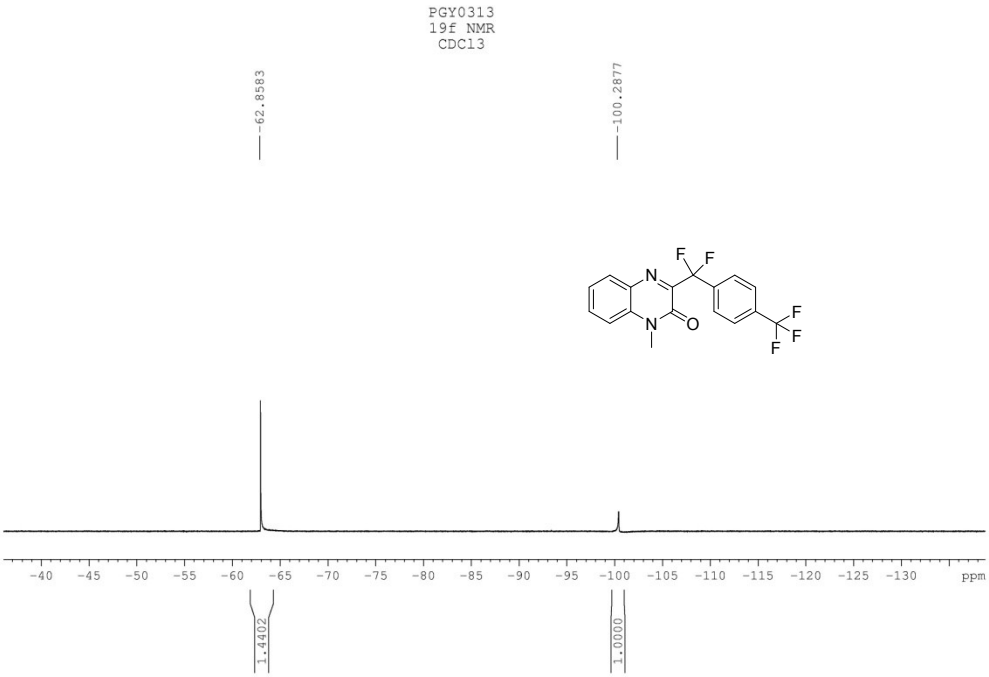


Fig. S33 ^{19}F NMR spectrum of compound **3ak**

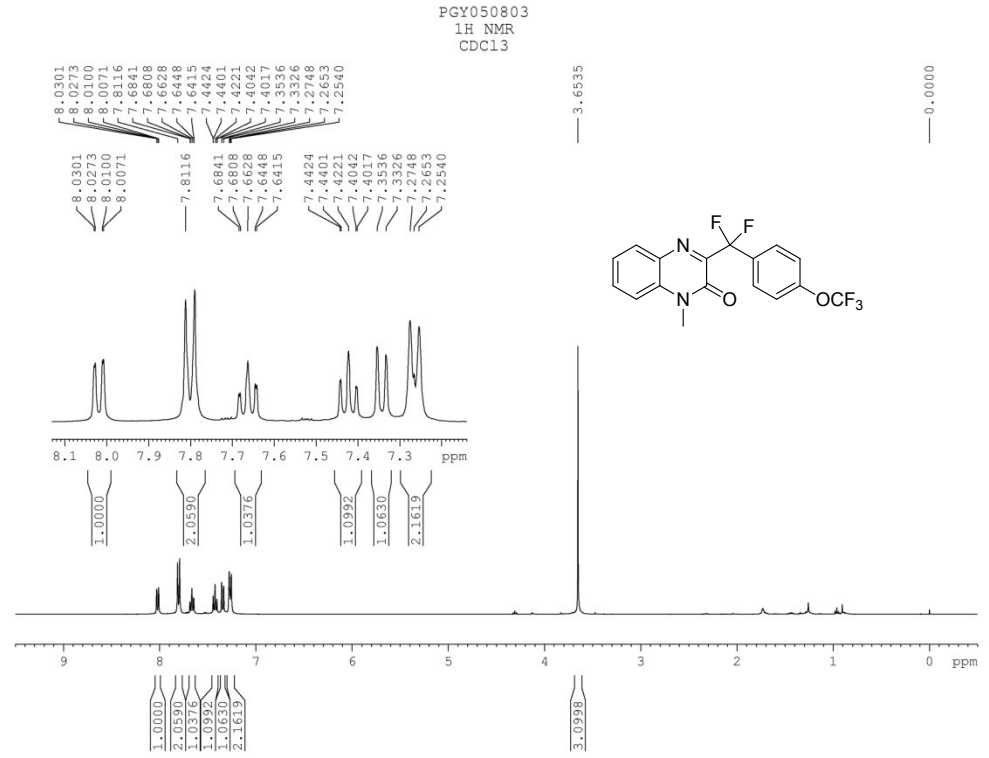


Fig. S34 ^{1}H NMR spectrum of compound **3al**

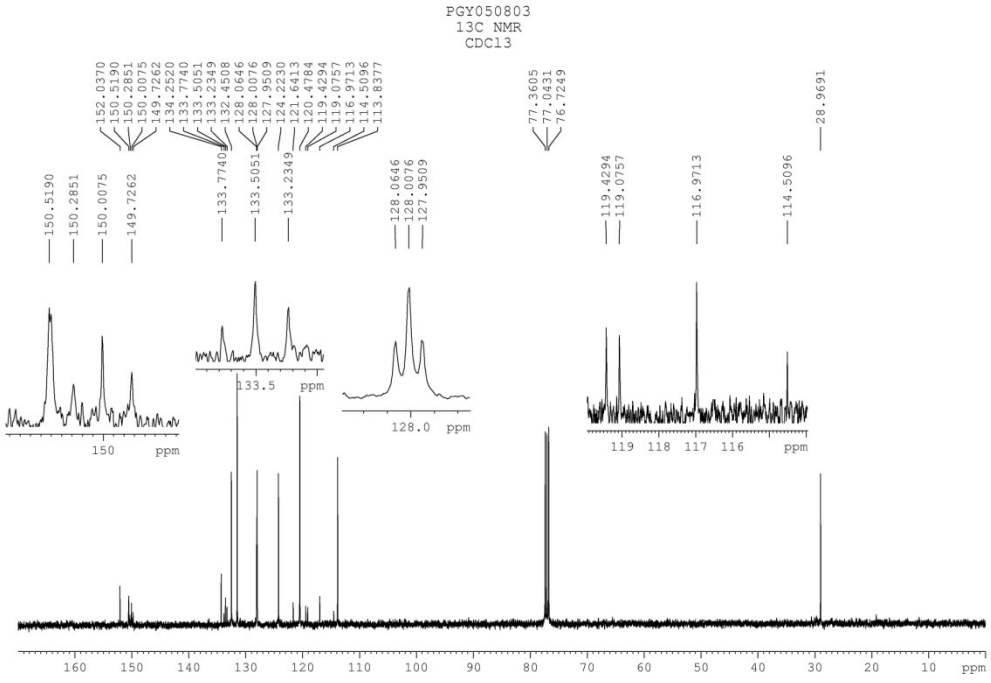


Fig. S35 ^{13}C NMR spectrum of compound **3al**

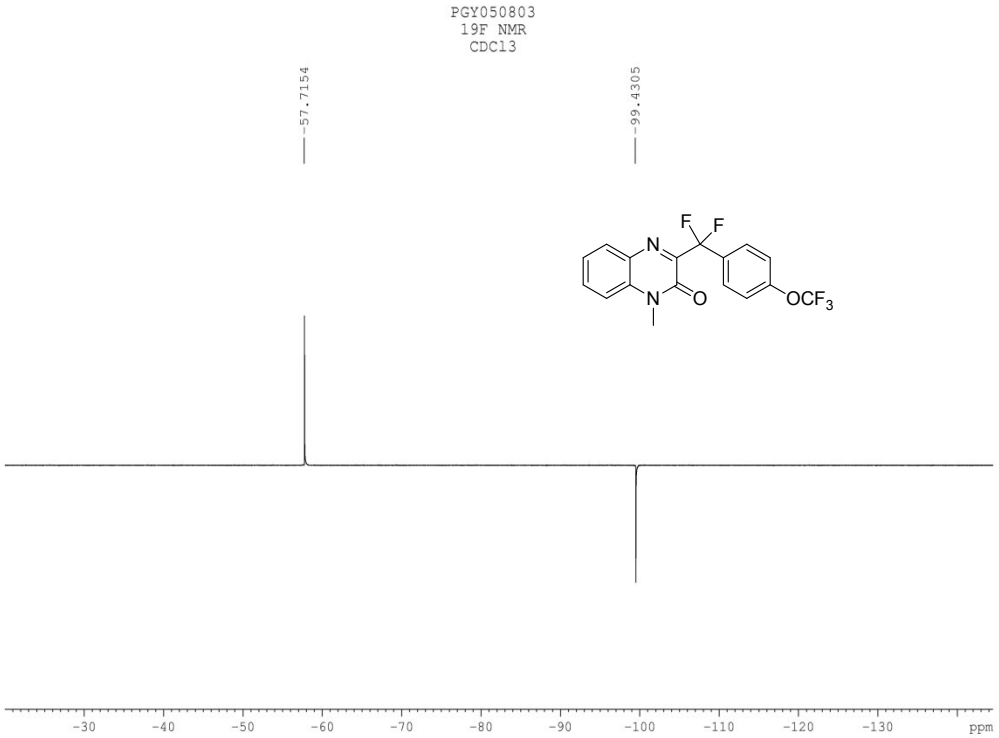


Fig. S36 ^{19}F NMR spectrum of compound **3al**

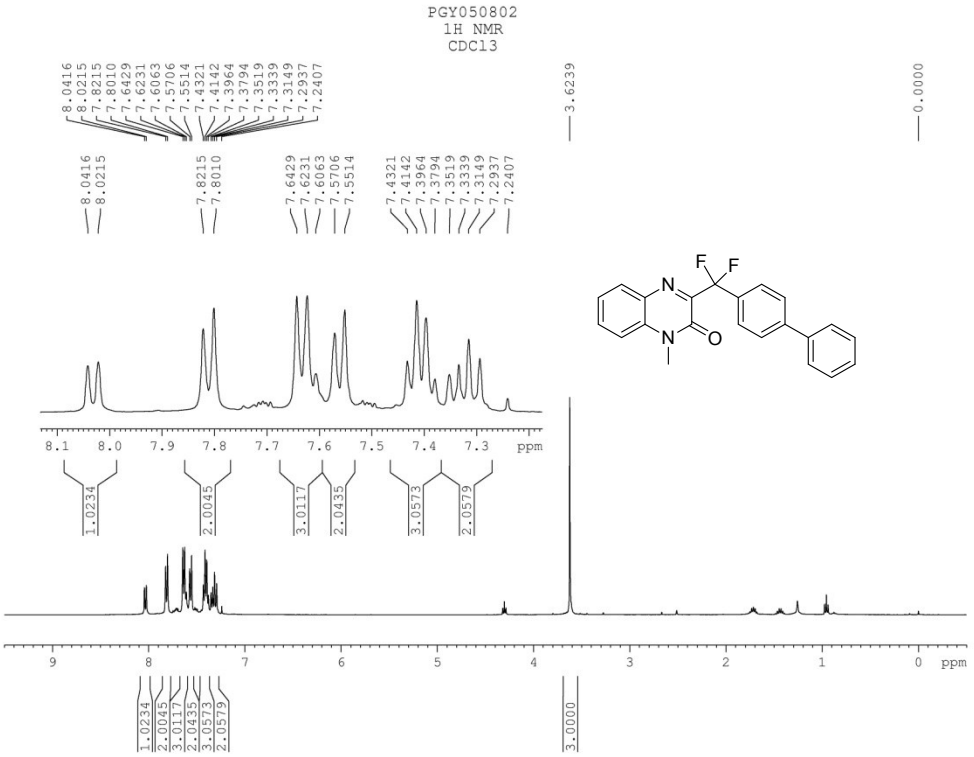


Fig. S37 ^{1}H NMR spectrum of compound **3am**

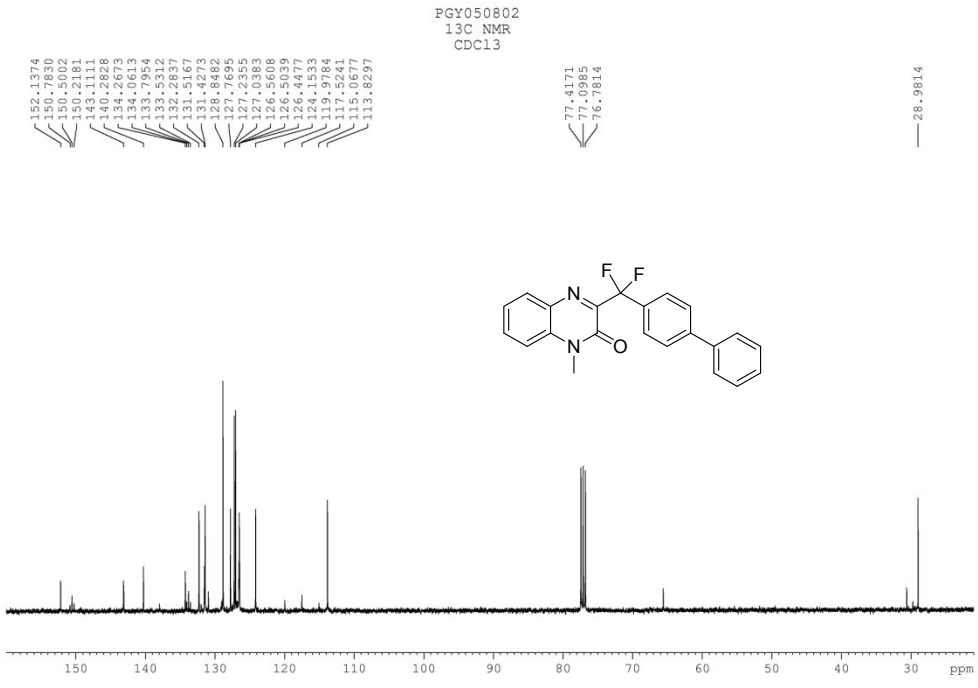


Fig. S38 ^{13}C NMR spectrum of compound **3am**

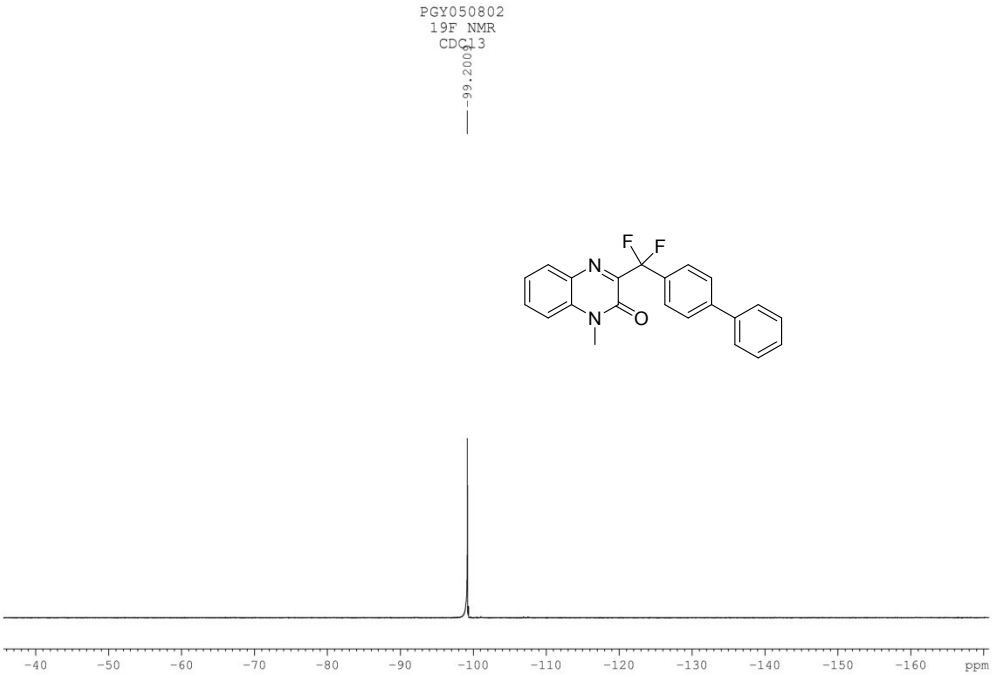


Fig. S39 ^{19}F NMR spectrum of compound **3am**

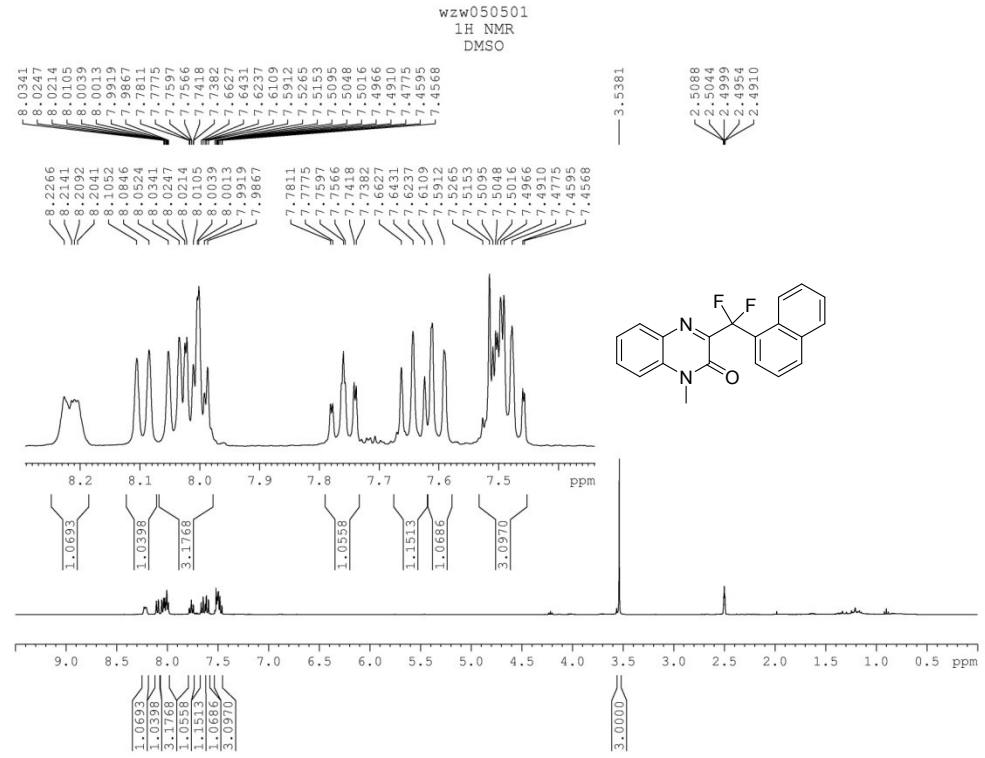


Fig. S40 ^{1}H NMR spectrum of compound **3an**

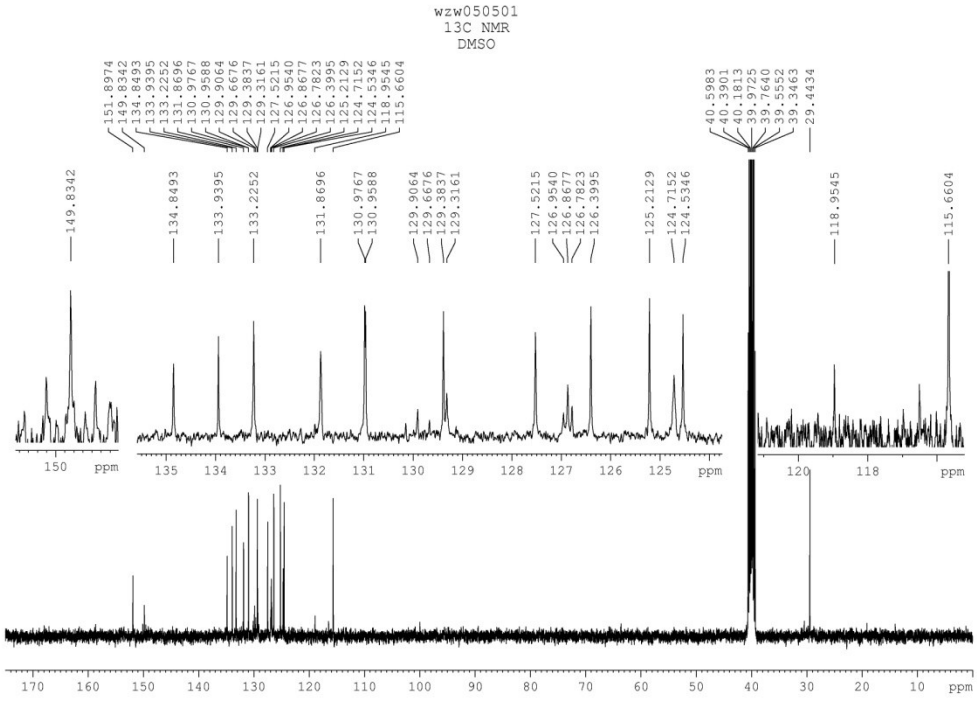


Fig. S41 ^{13}C NMR spectrum of compound **3an**

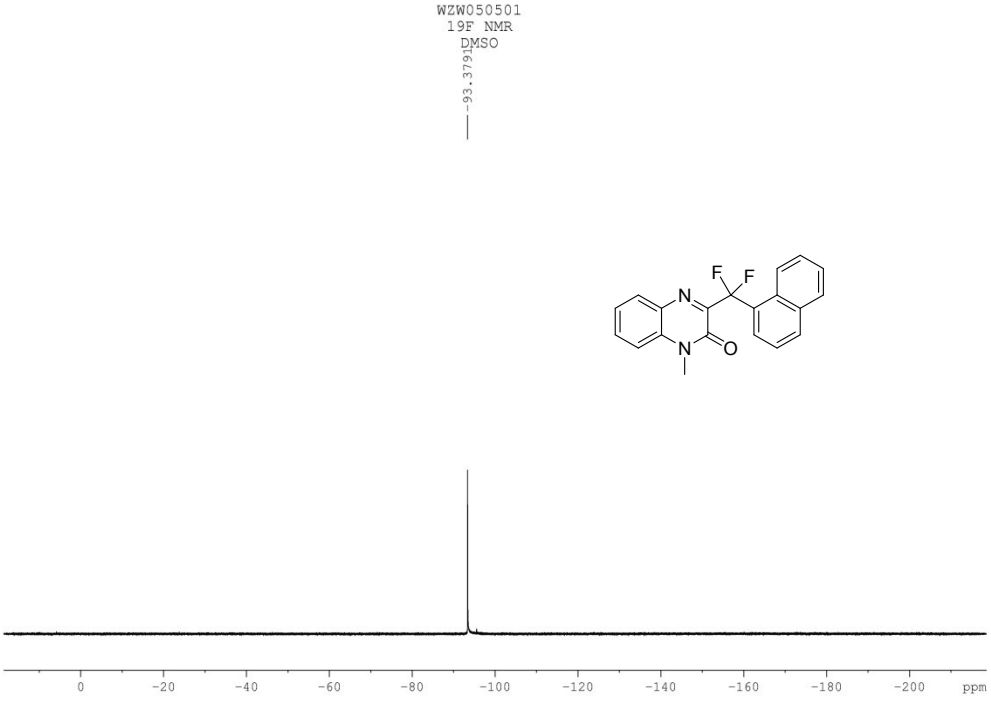


Fig. S42 ^{19}F NMR spectrum of compound **3an**

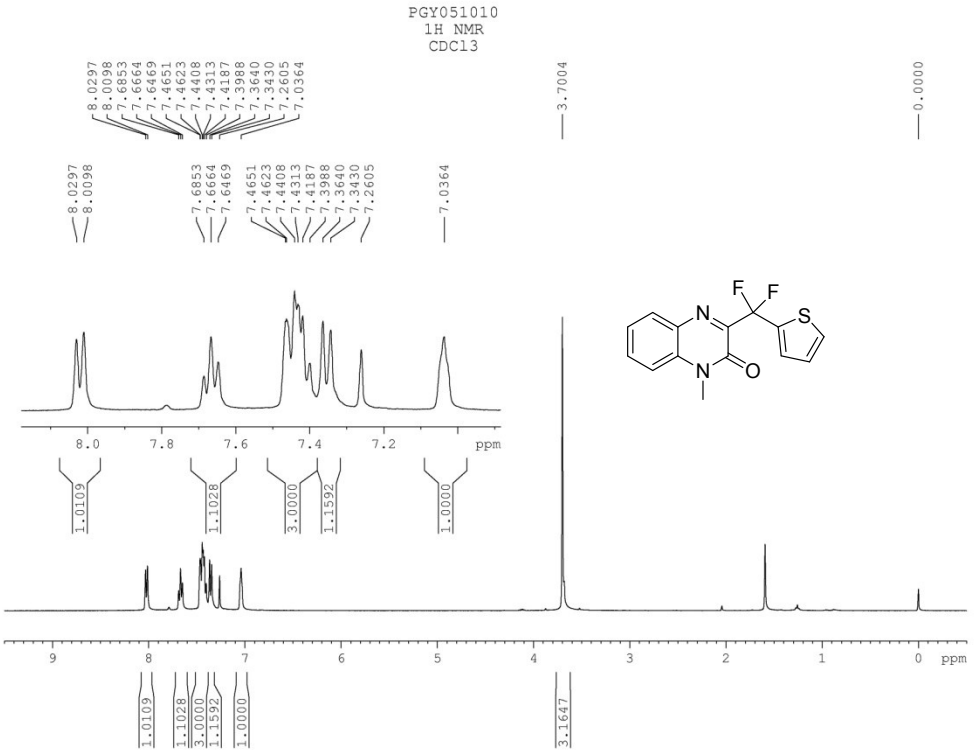


Fig. S43 ^{1}H NMR spectrum of compound **3ao**

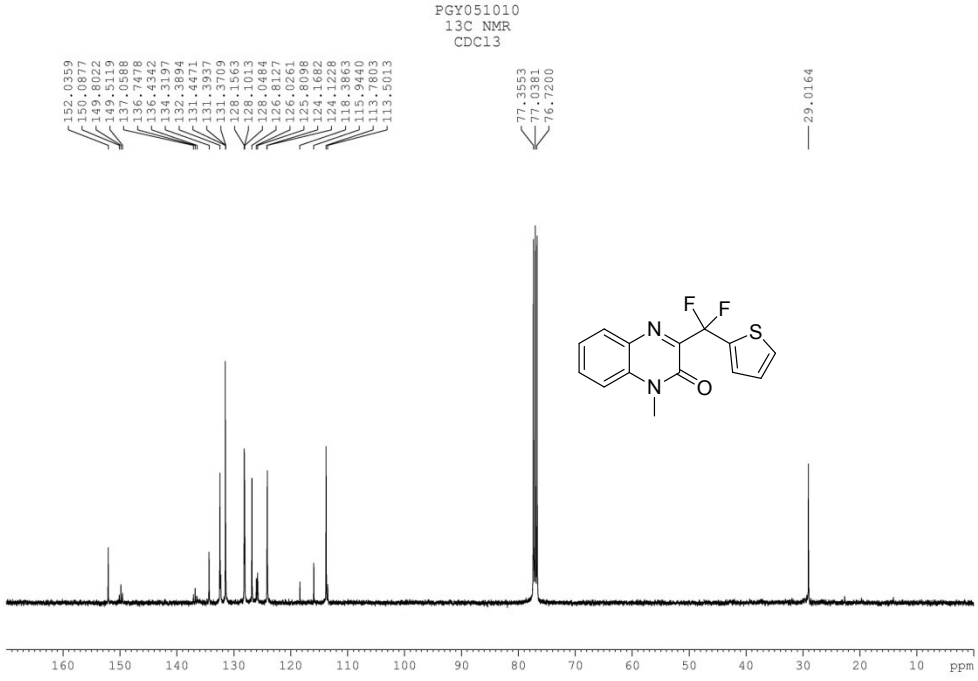


Fig. S44 ^{13}C NMR spectrum of compound **3ao**

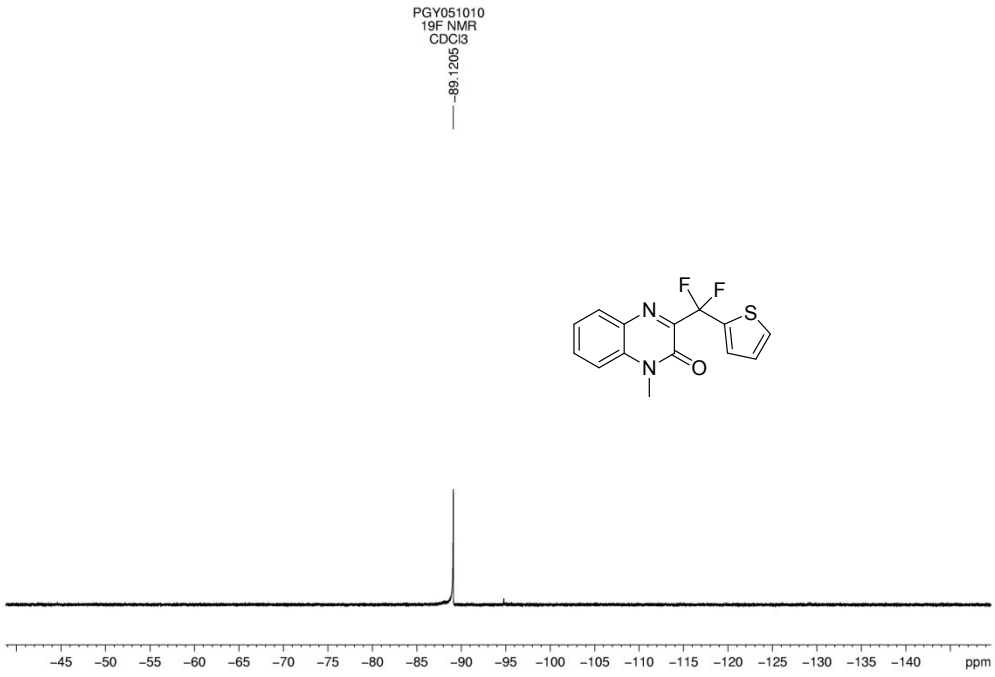


Fig. S45 ^{19}F NMR spectrum of compound **3ao**

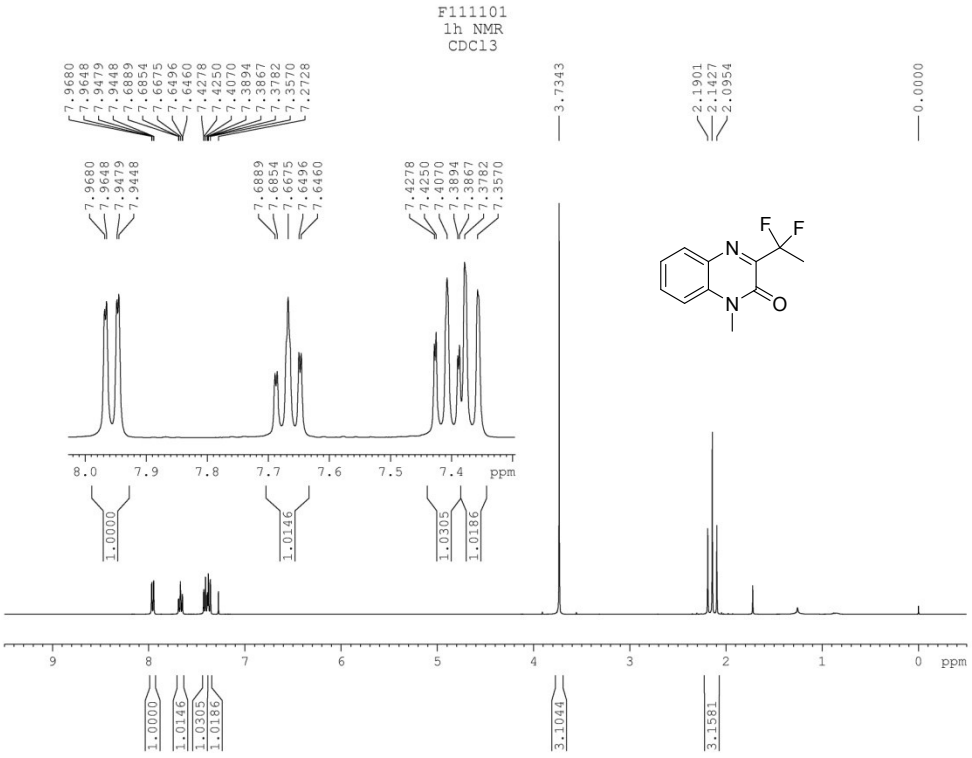


Fig. S46 ^{1}H NMR spectrum of compound **3ap**

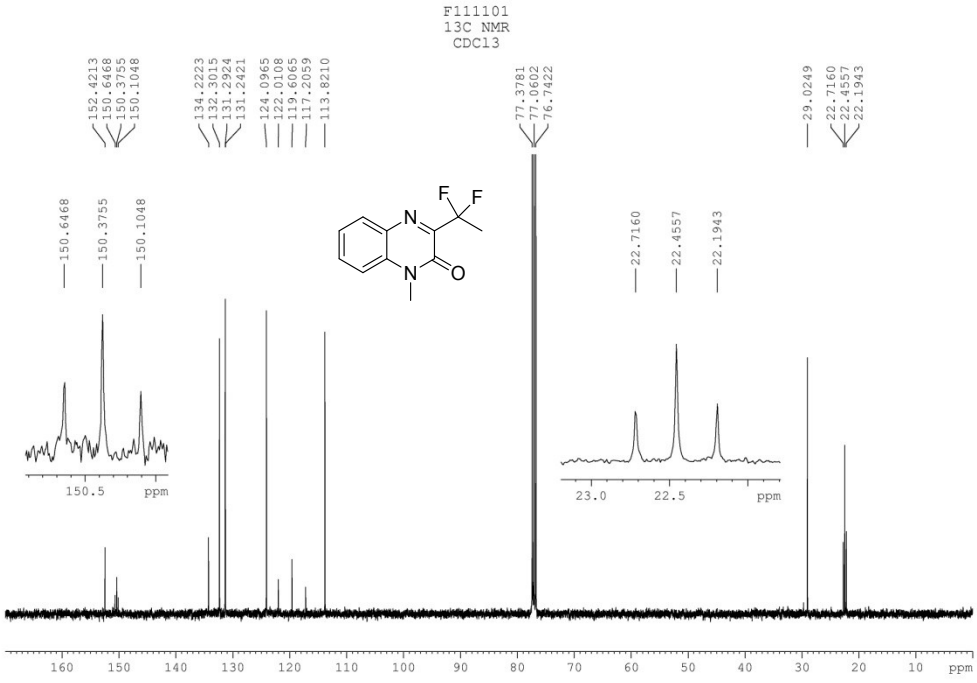


Fig. S47 ^{13}C NMR spectrum of compound **3ap**

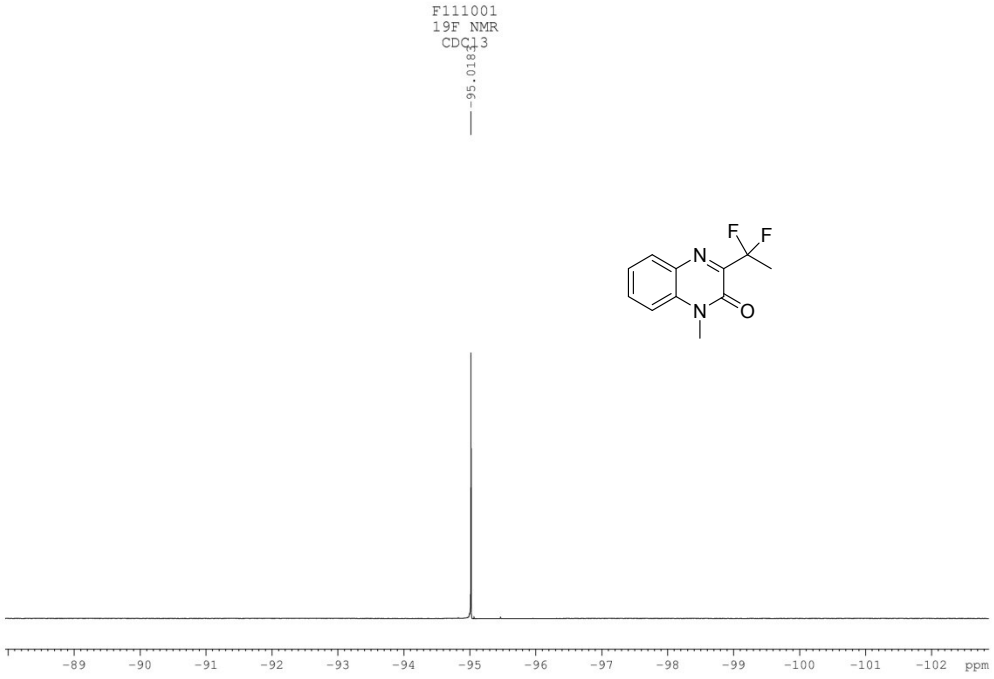


Fig. S48 ^{19}F NMR spectrum of compound **3ap**

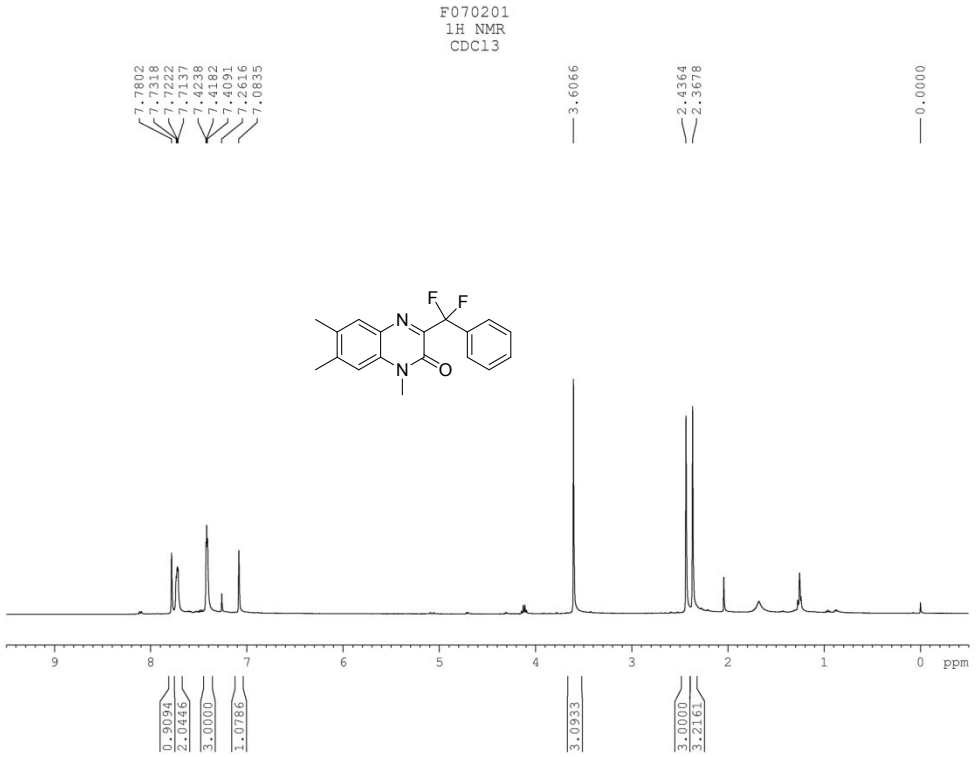


Fig. S49 ^{1}H NMR spectrum of compound **3ba**

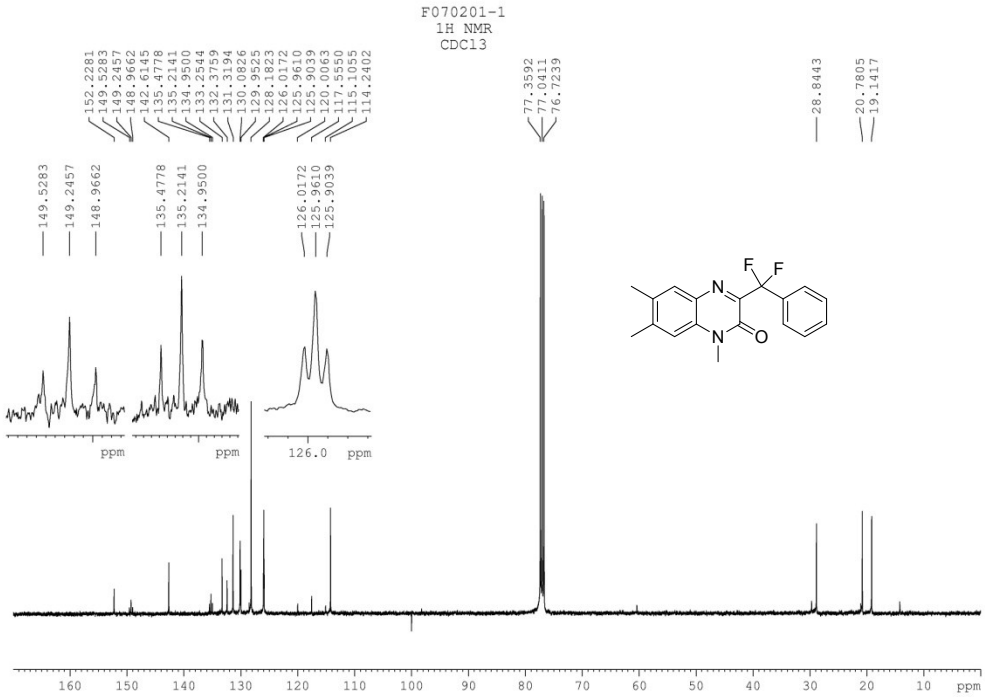


Fig. S50 ^{13}C NMR spectrum of compound **3ba**

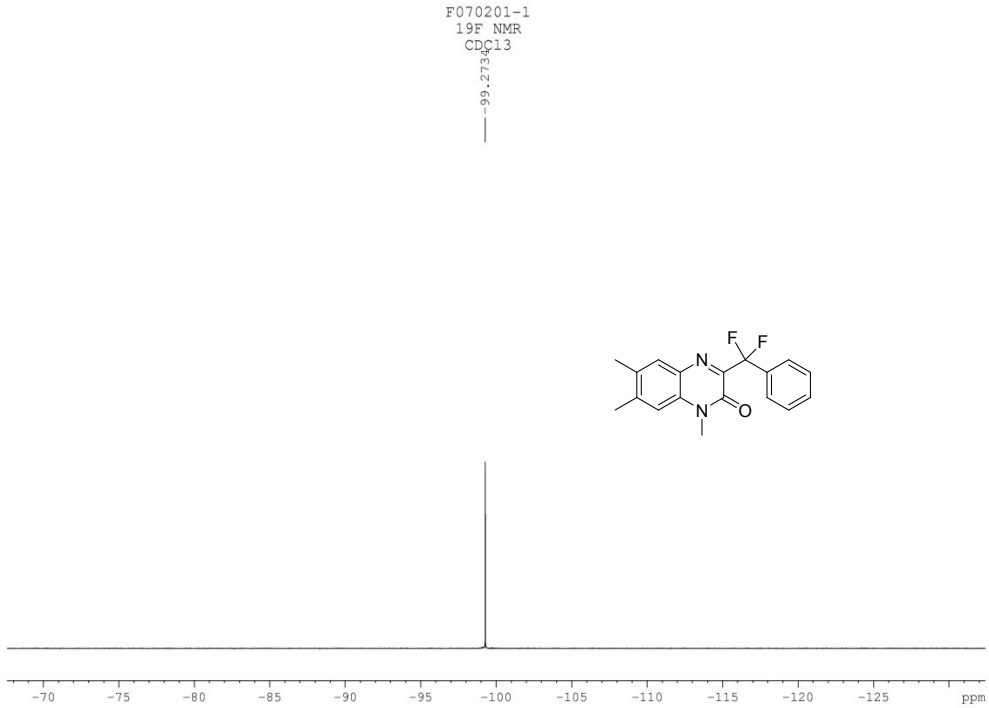


Fig. S51 ^{19}F NMR spectrum of compound **3ba**

Fig. S52 ^{1}H NMR spectrum of compound **3ca**

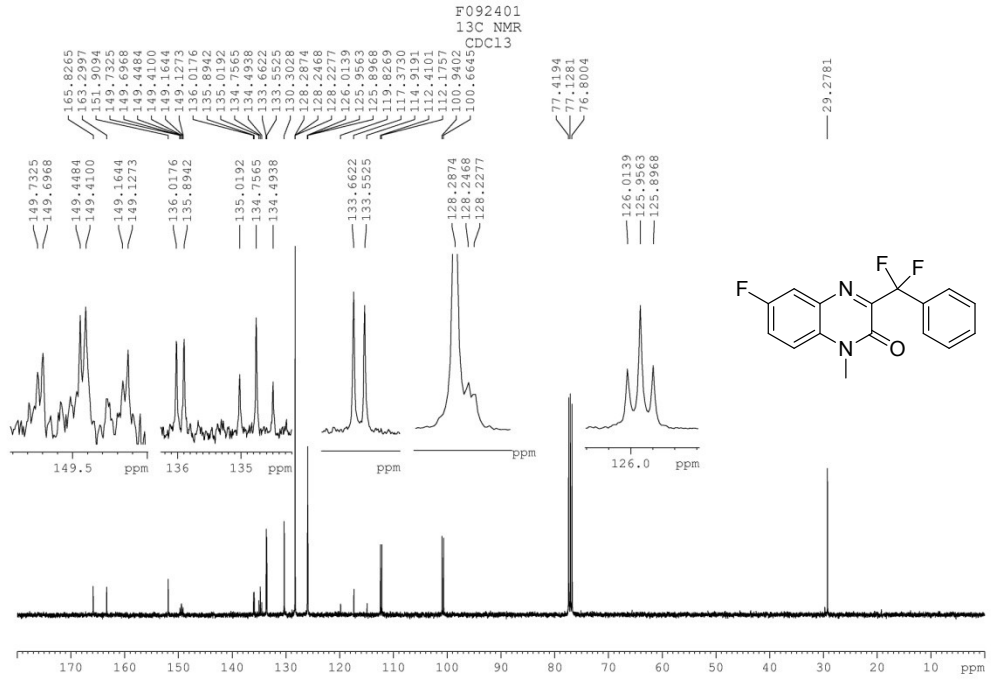


Fig. S53 ^{13}C NMR spectrum of compound **3ca**

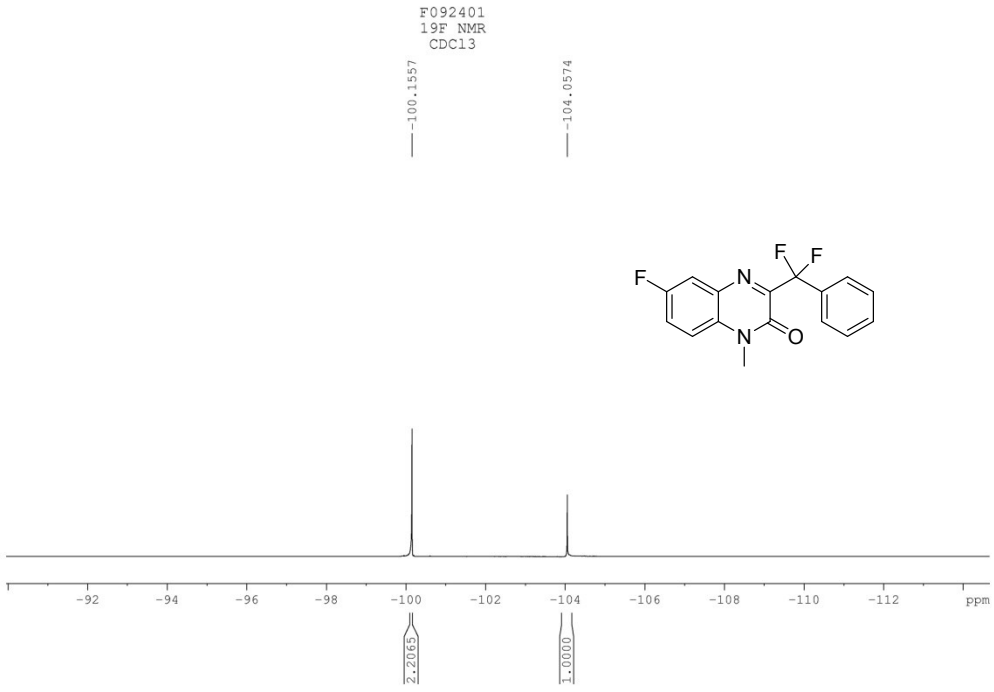


Fig. S54 ^{19}F NMR spectrum of compound **3ca**

Fig. S55 ^{1}H NMR spectrum of compound **3da**

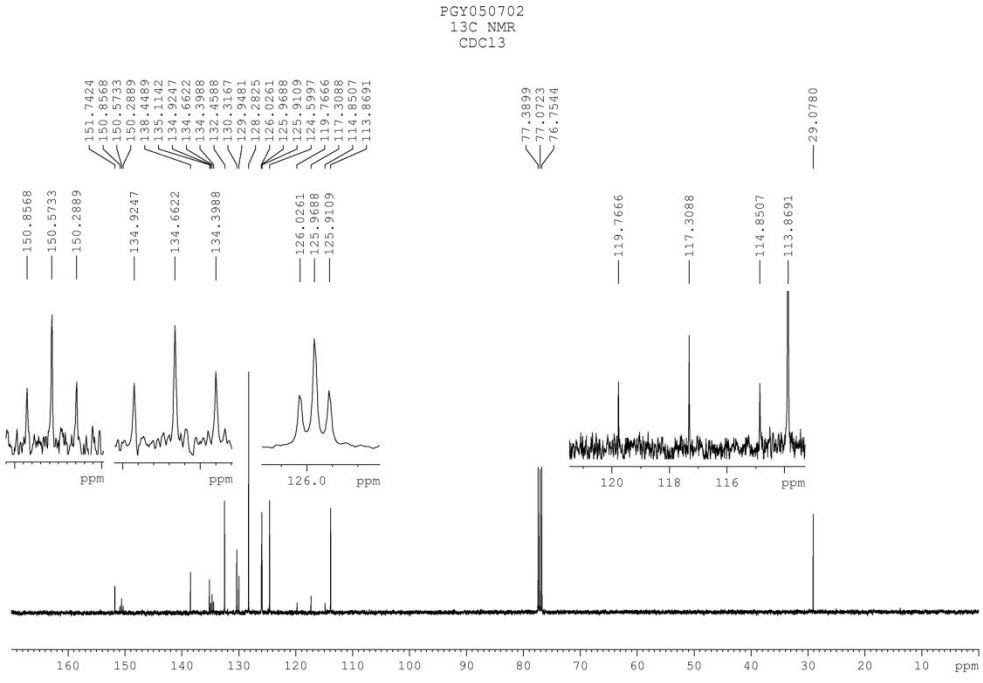


Fig. S56 ^{13}C NMR spectrum of compound **3da**

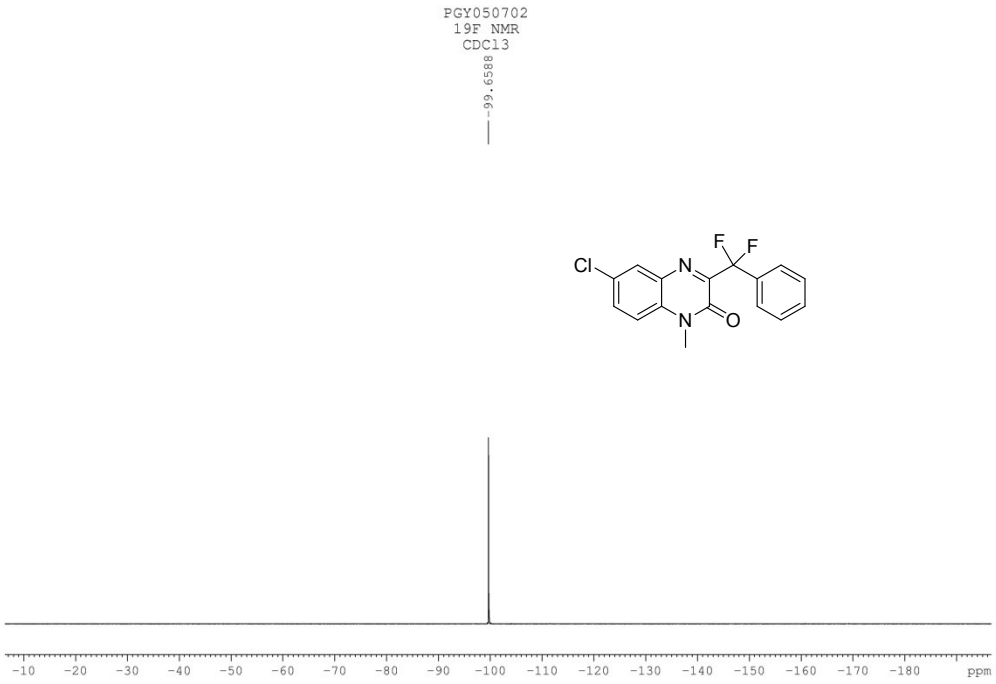


Fig. S57 ^{19}F NMR spectrum of compound **3da**

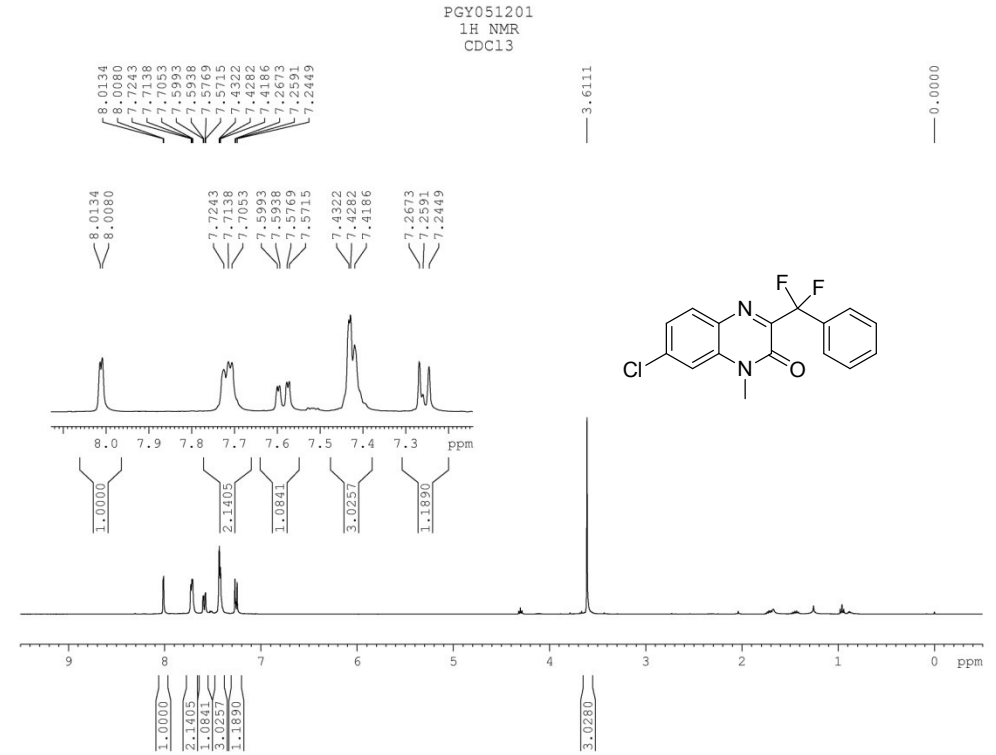


Fig. S58 ^{1}H NMR spectrum of compound **3ea**

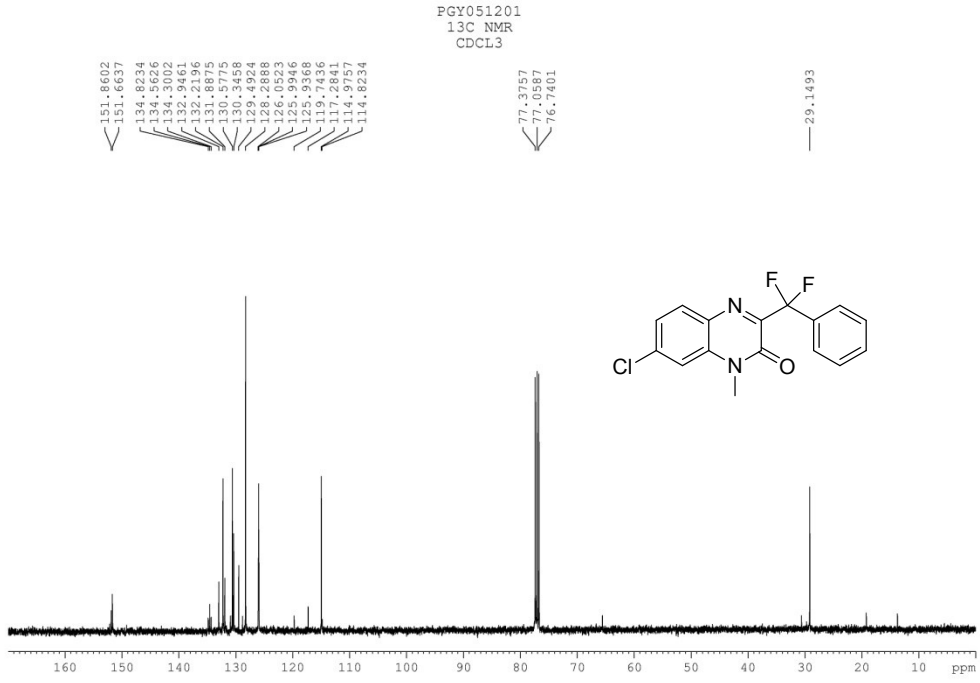


Fig. S59 ^{13}C NMR spectrum of compound **3ea**

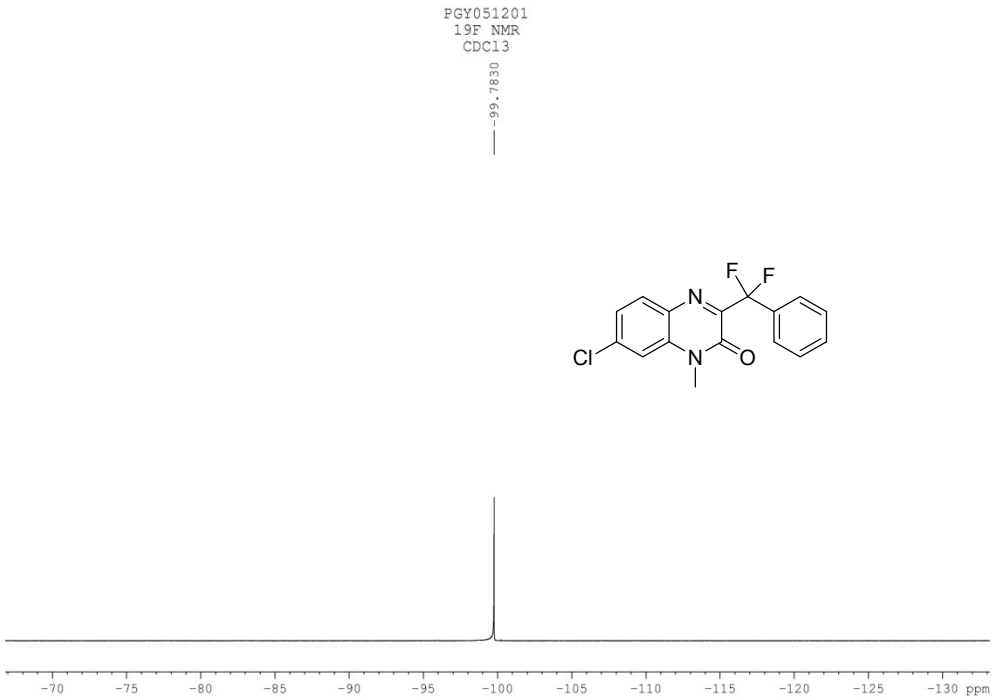


Fig. S60 ^{19}F NMR spectrum of compound **3ea**

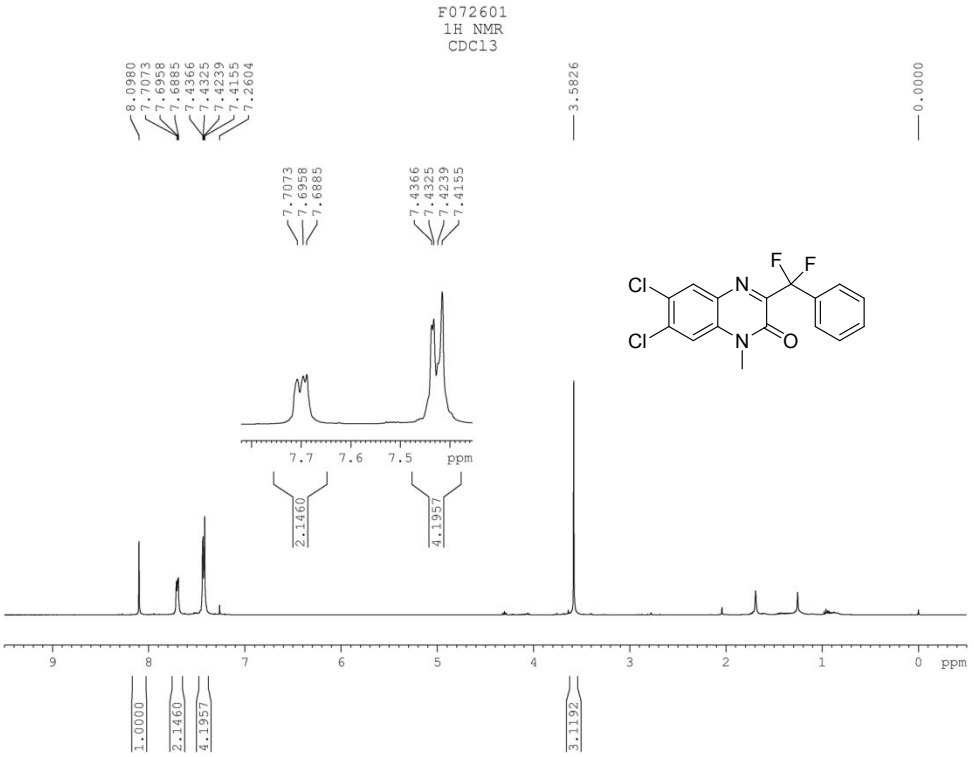


Fig. S61 ^{1}H NMR spectrum of compound **3fa**

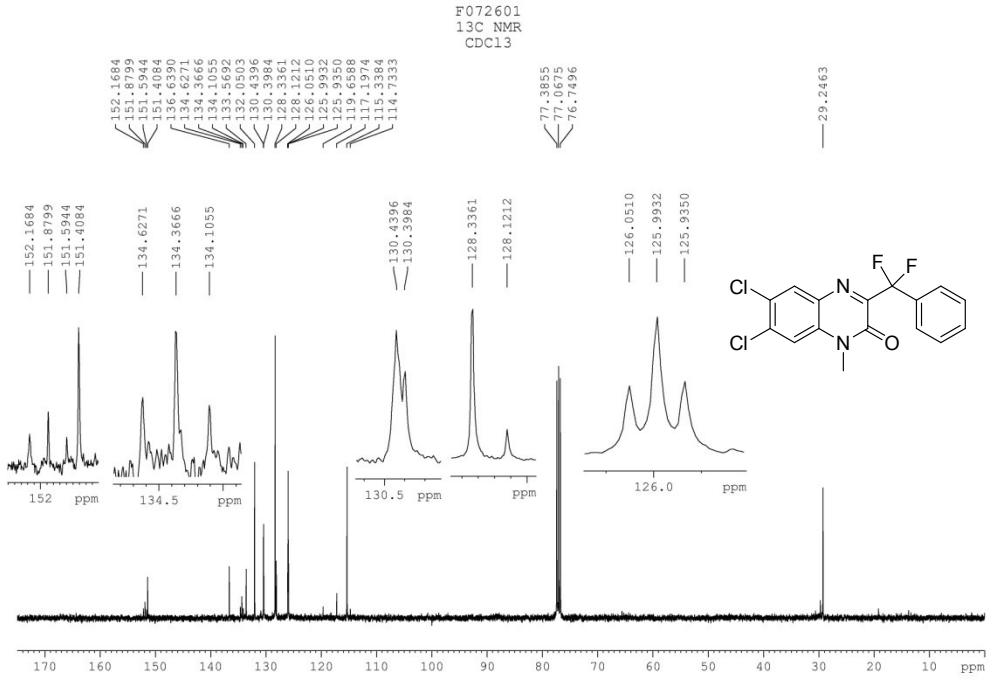


Fig. S62 ^{13}C NMR spectrum of compound **3fa**

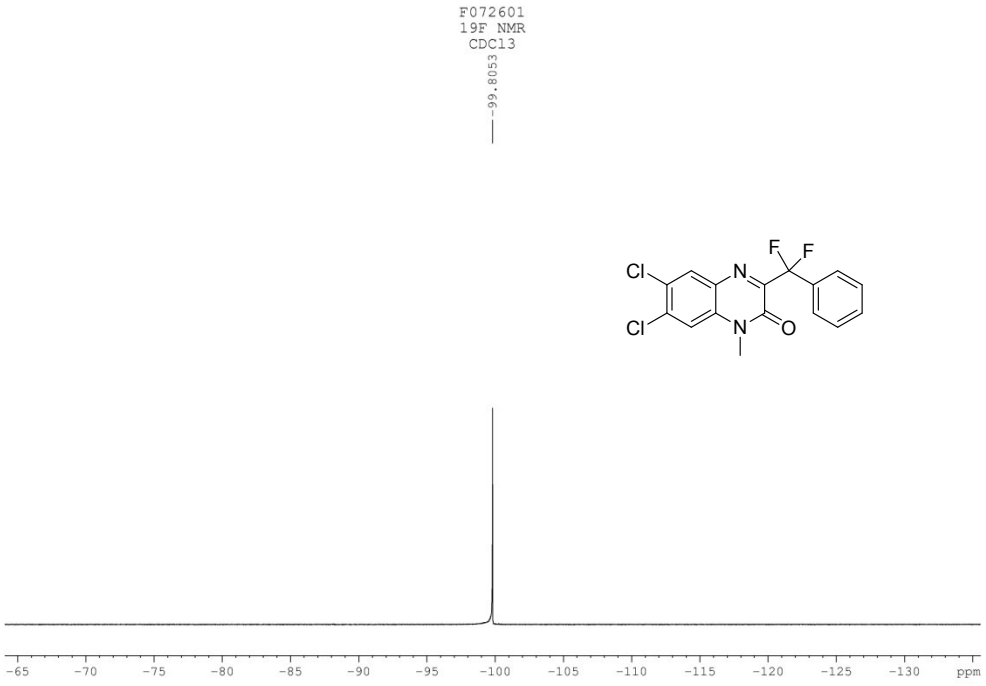


Fig. S63 ^{19}F NMR spectrum of compound **3fa**

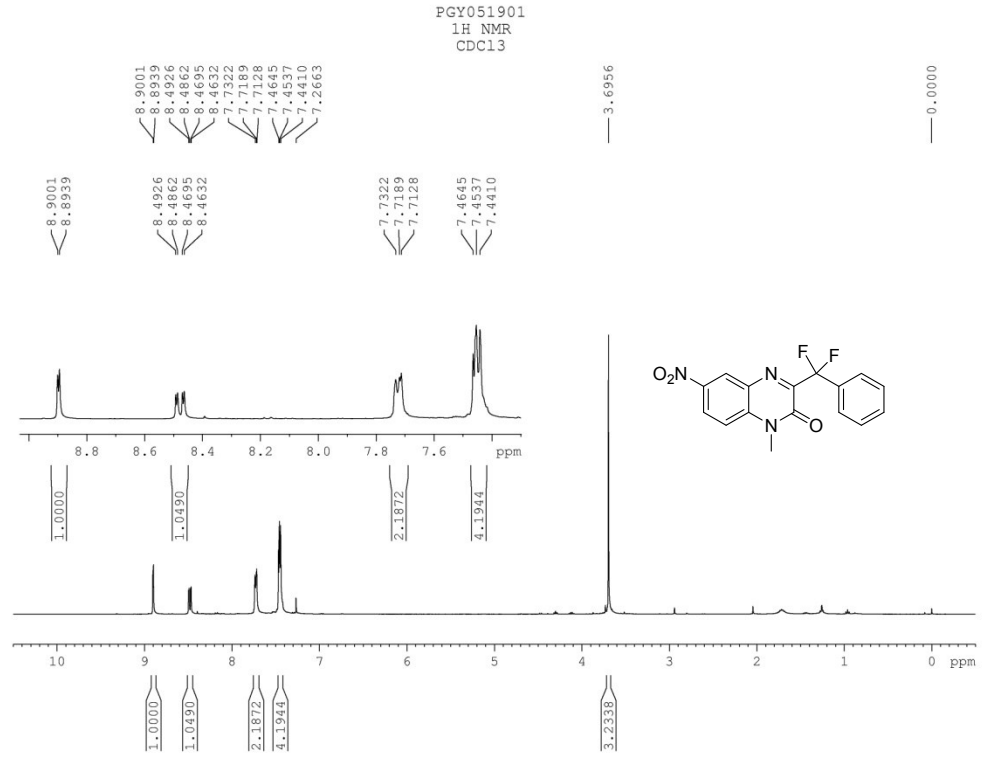


Fig. S64 ^{1}H NMR spectrum of compound **3ga**

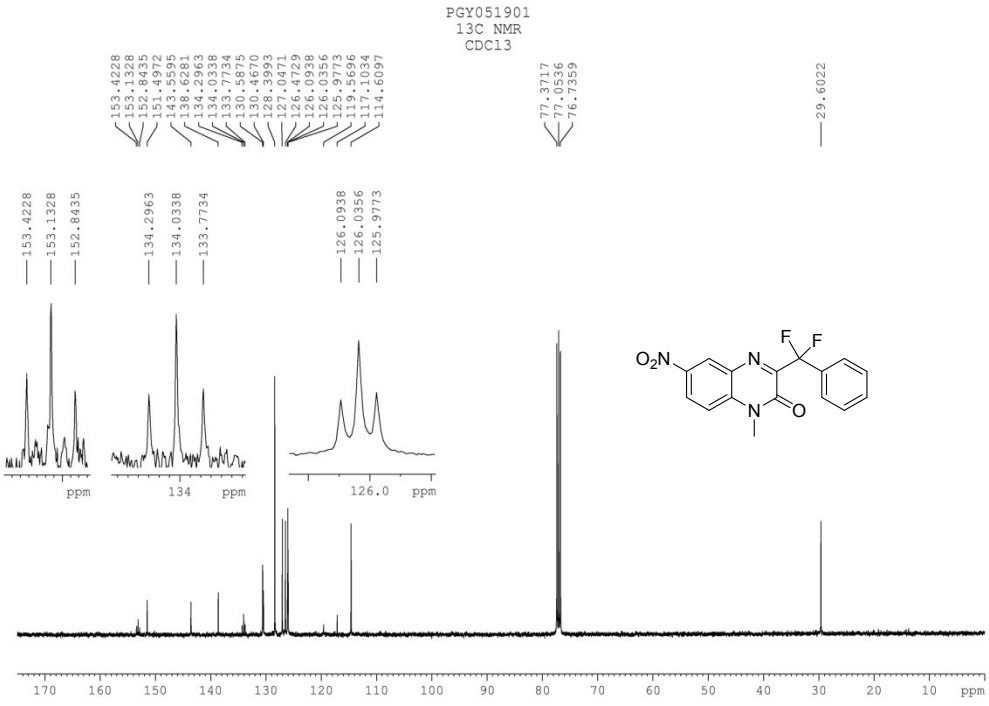


Fig. S65 ^{13}C NMR spectrum of compound **3ga**

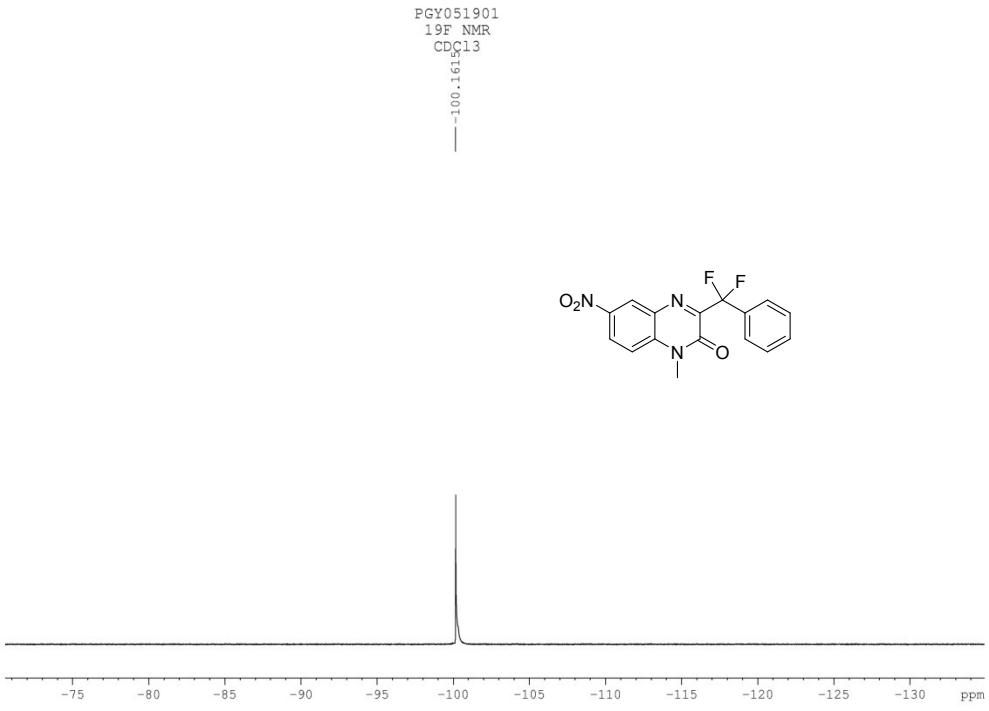


Fig. S66 ^{19}F NMR spectrum of compound **3ga**

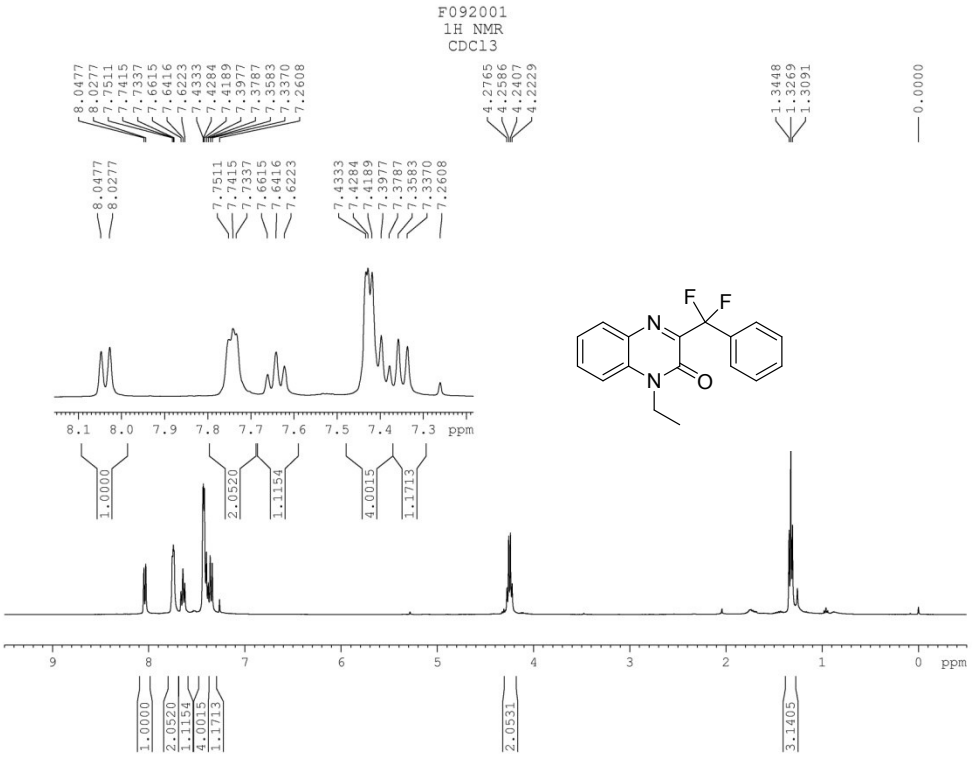


Fig. S67 ^{1}H NMR spectrum of compound **3ha**

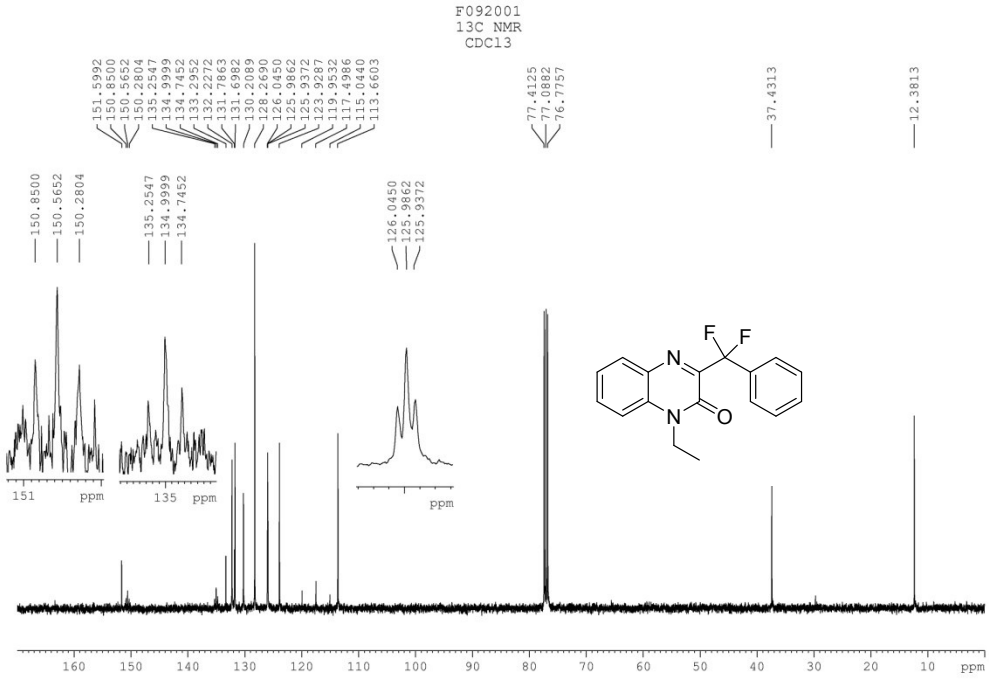


Fig. S68 ^{13}C NMR spectrum of compound **3ha**

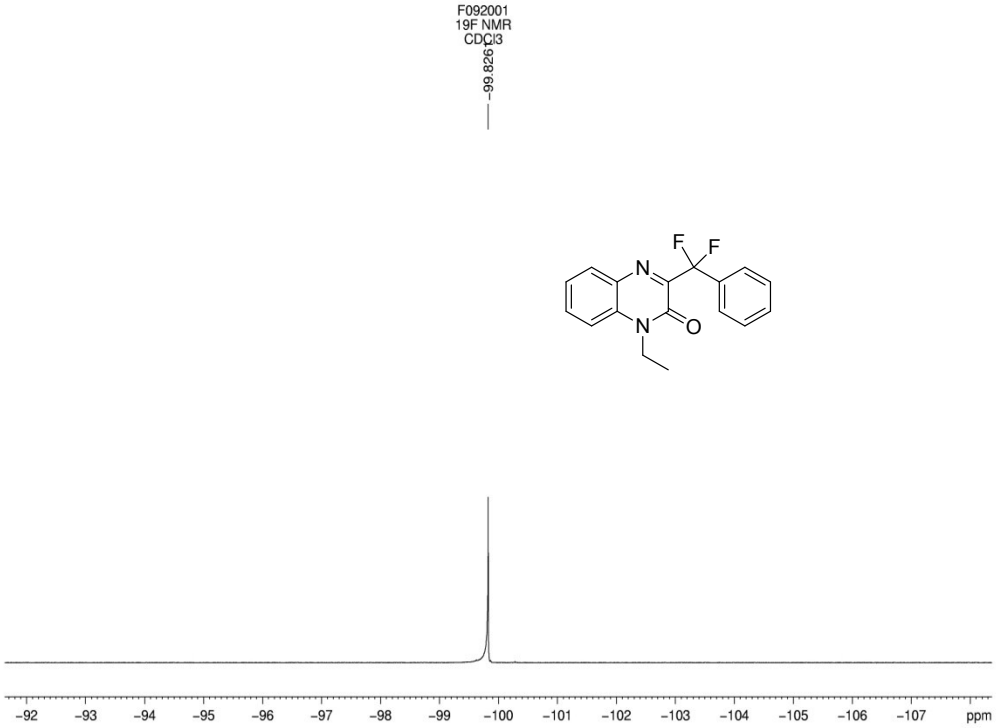


Fig. S69 ^{19}F NMR spectrum of compound **3ha**

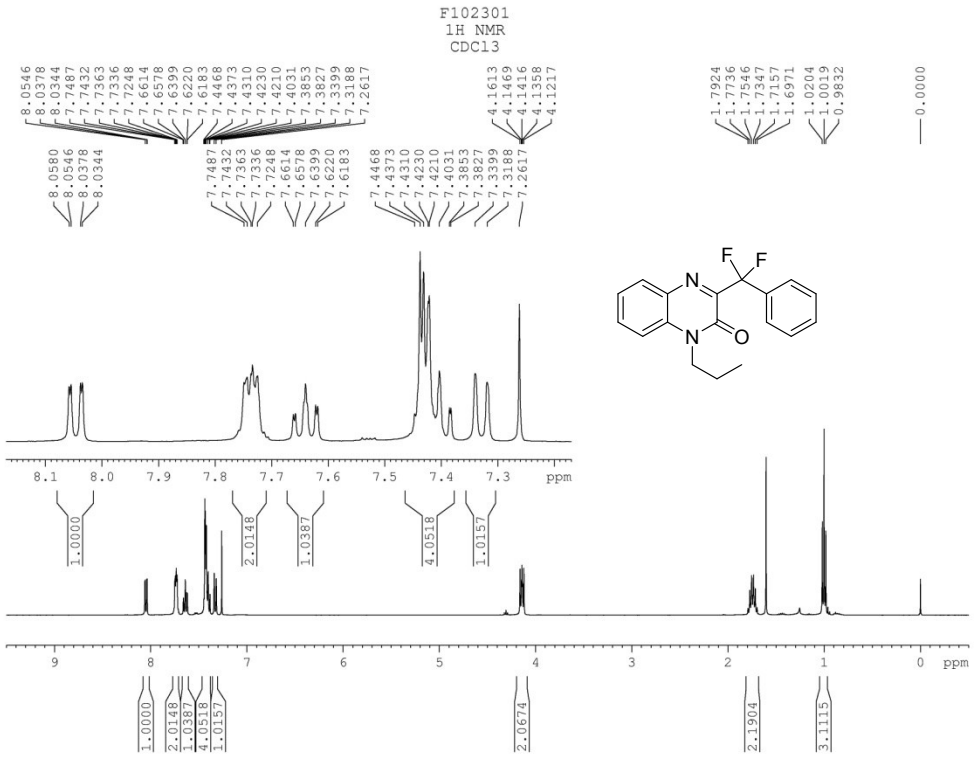


Fig. S70 ^{1}H NMR spectrum of compound **3ia**

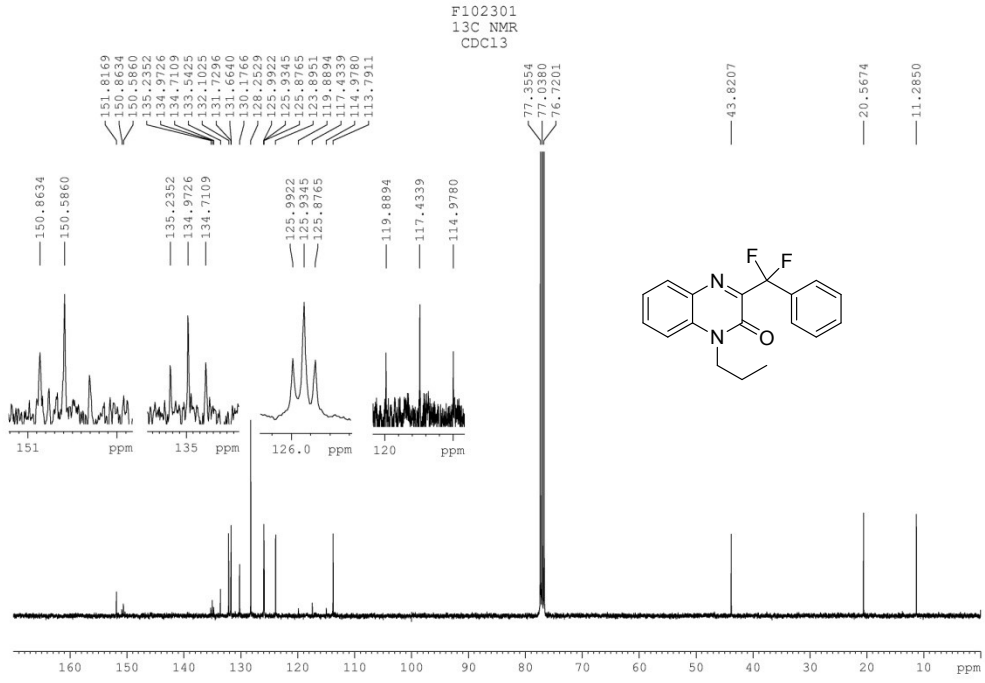


Fig. S71 ^{13}C NMR spectrum of compound **3ia**

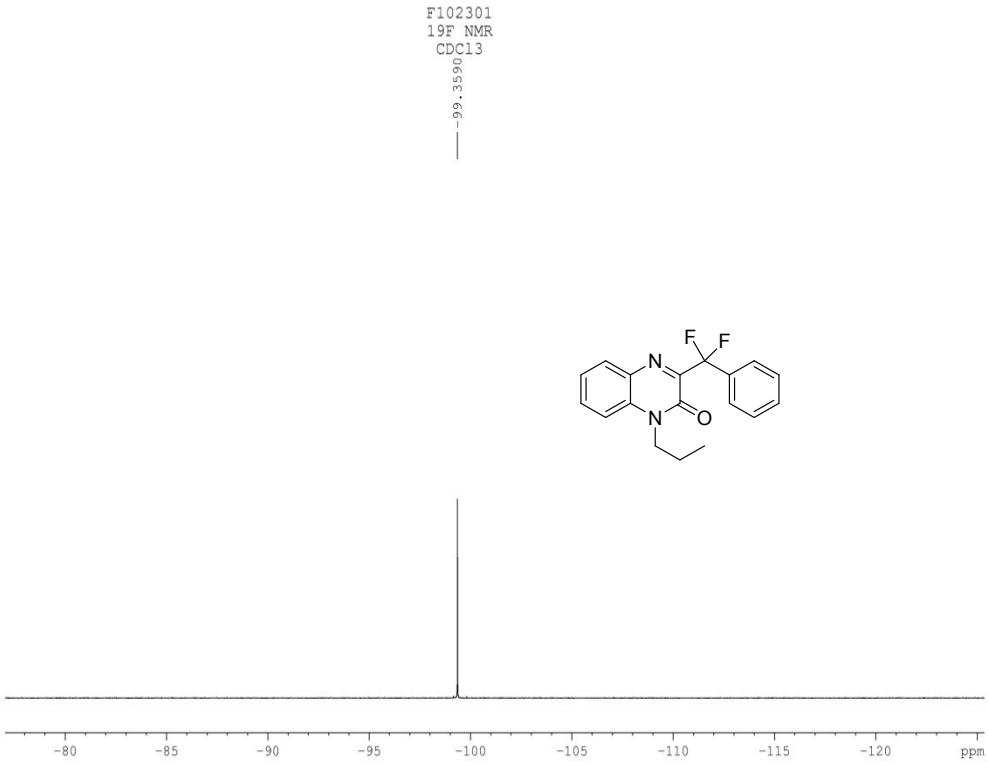


Fig. S72 ^{19}F NMR spectrum of compound **3ia**

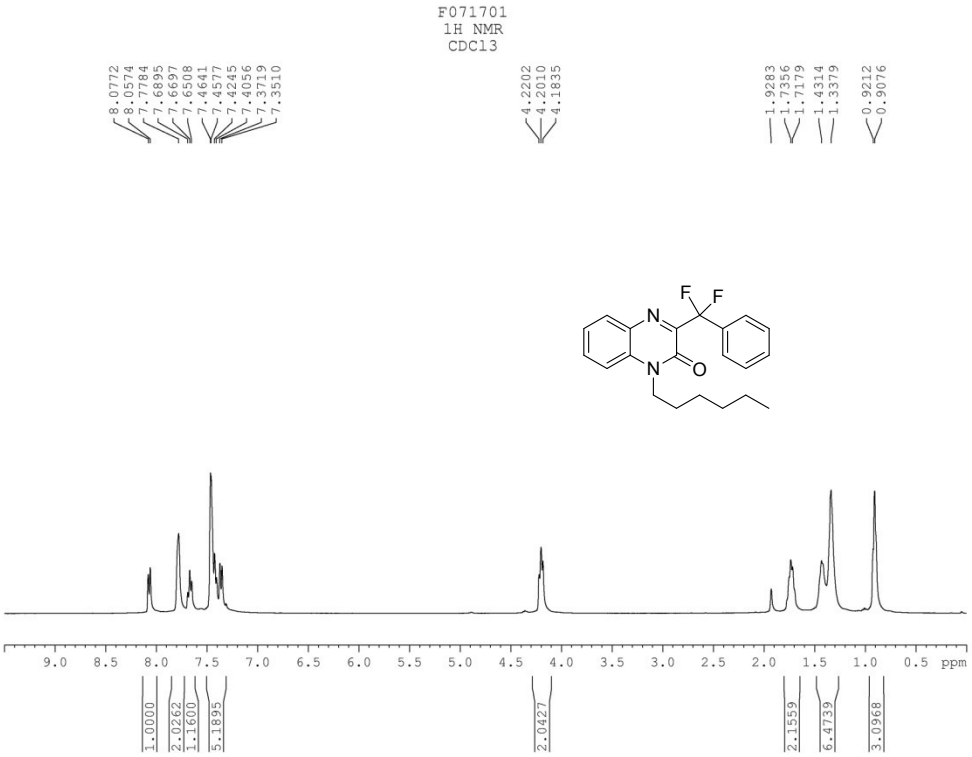


Fig. S73 ^{1}H NMR spectrum of compound **3ja**

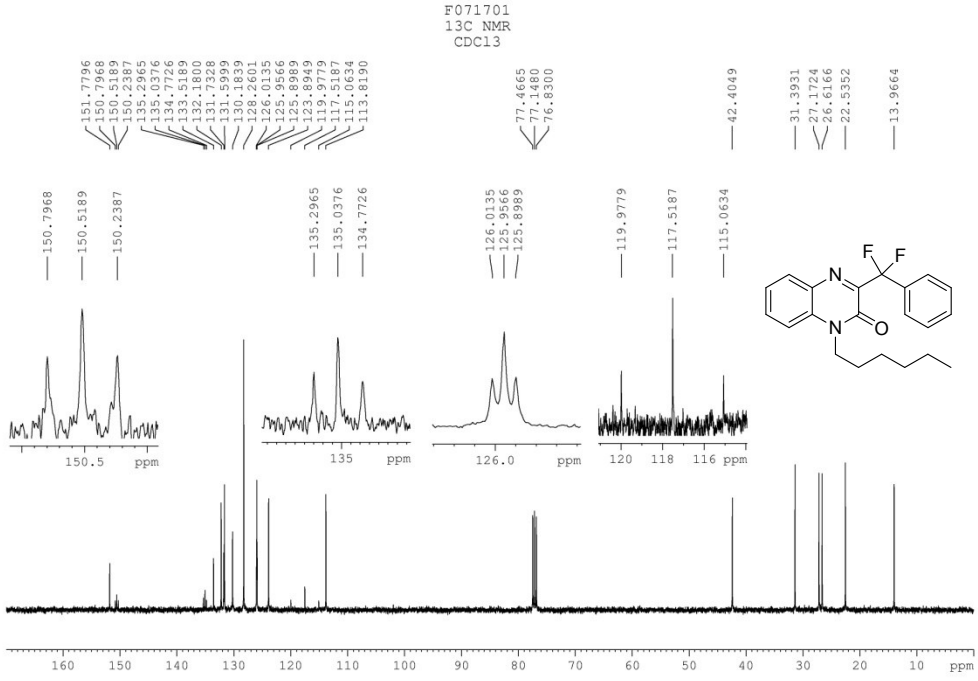


Fig. S74 ^{13}C NMR spectrum of compound **3ja**

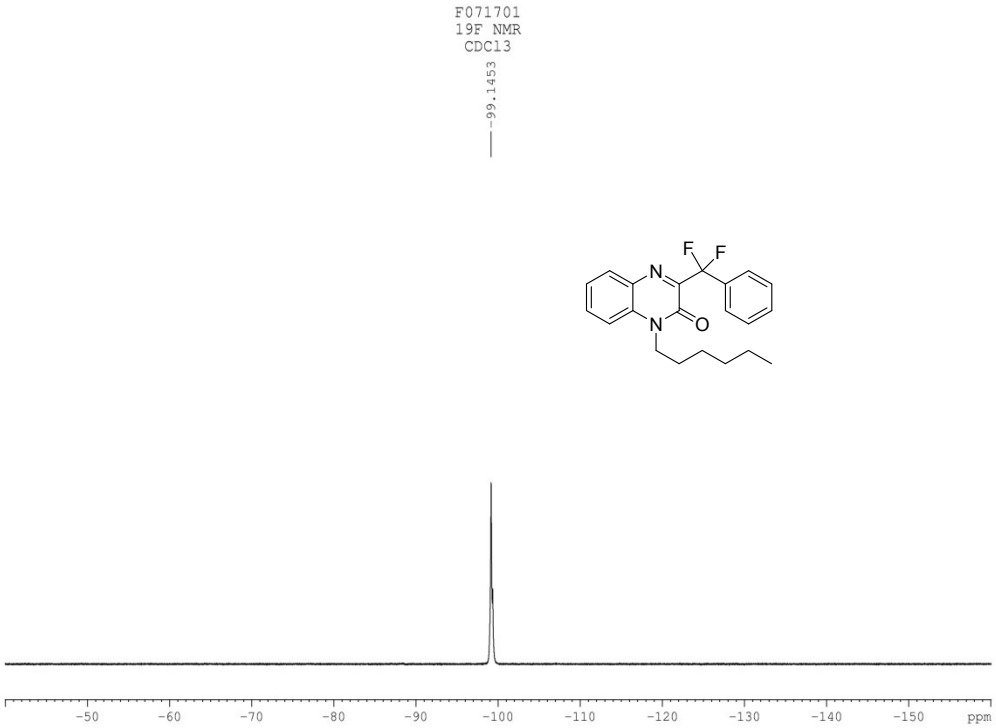


Fig. S75 ^{19}F NMR spectrum of compound **3ja**

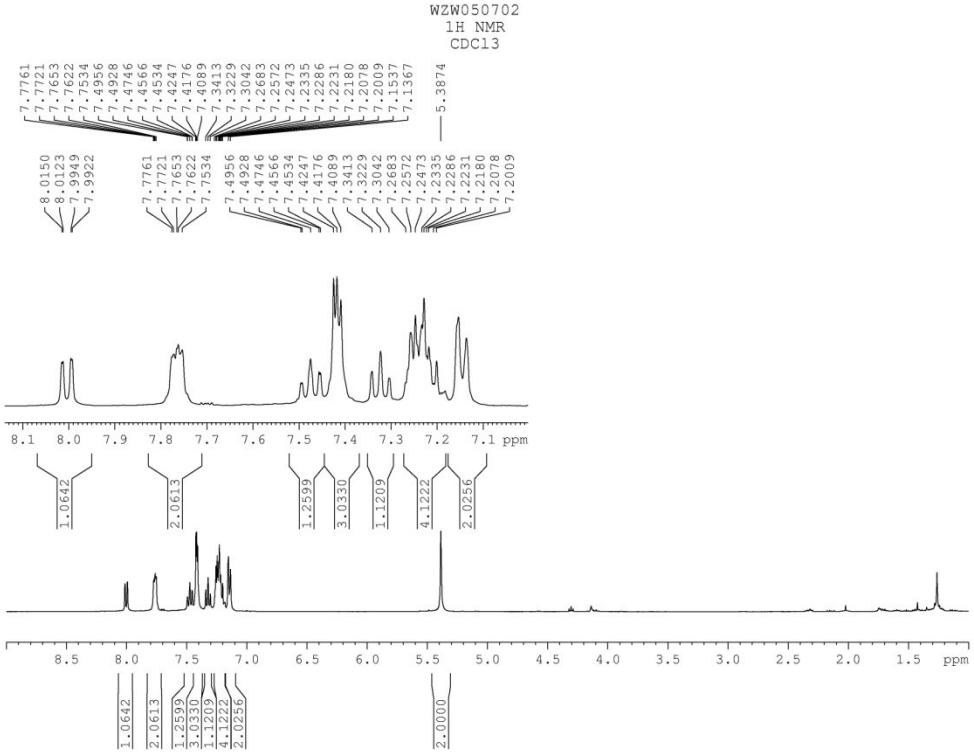


Fig. S76 ^{1}H NMR spectrum of compound **3ka**

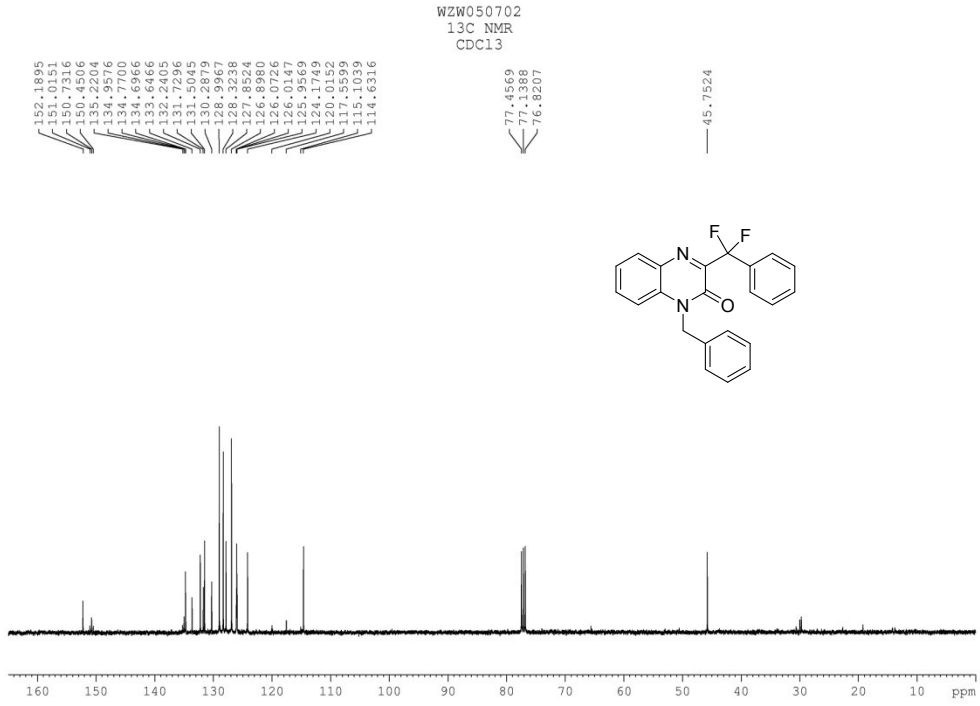


Fig. S77 ^{13}C NMR spectrum of compound **3ka**

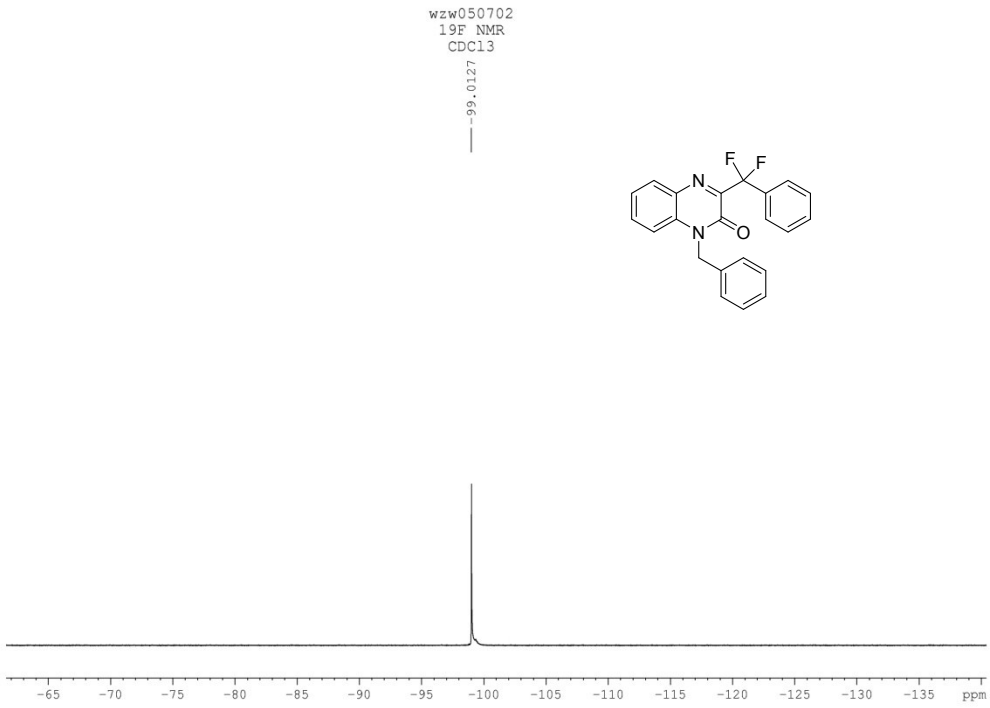


Fig. S78 ^{19}F NMR spectrum of compound **3ka**

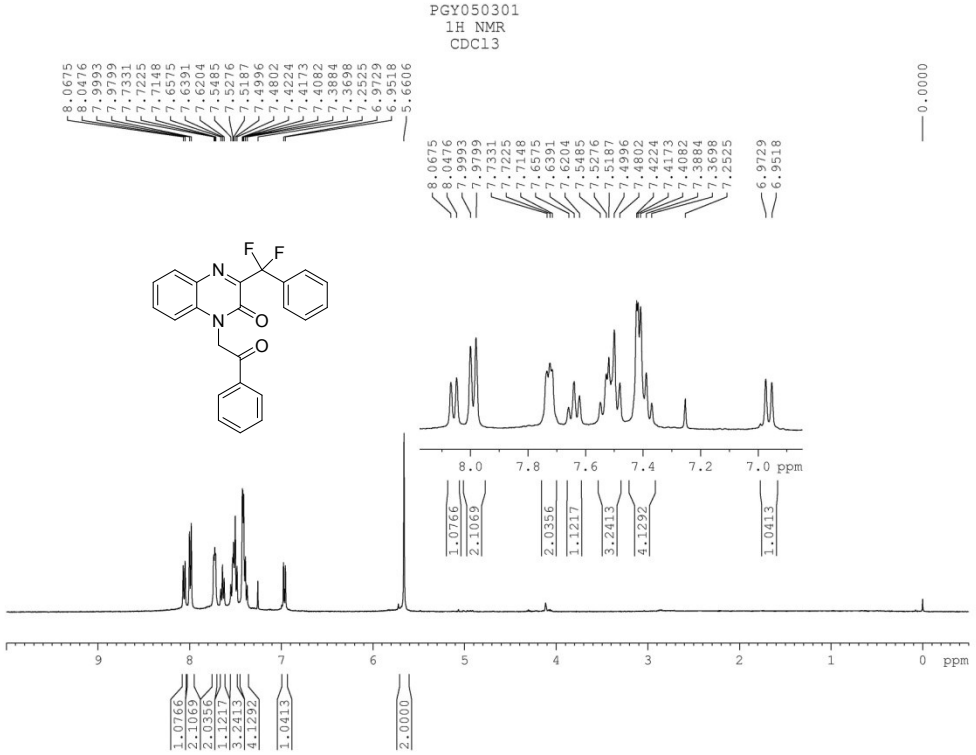


Fig. S79 ^{1}H NMR spectrum of compound **3la**

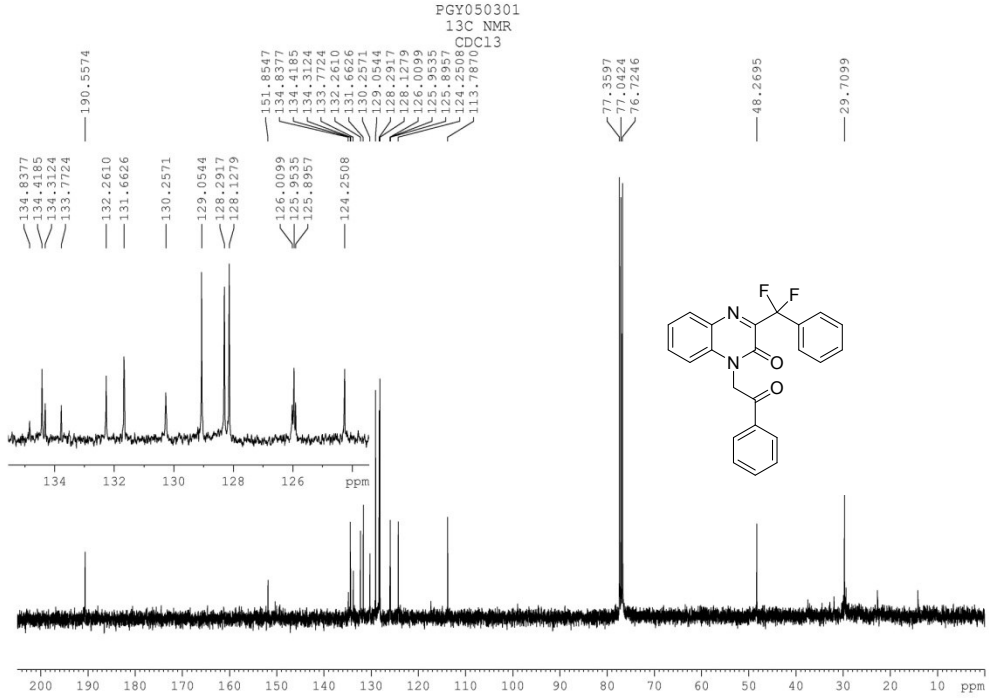


Fig. S80 ^{13}C NMR spectrum of compound **3la**

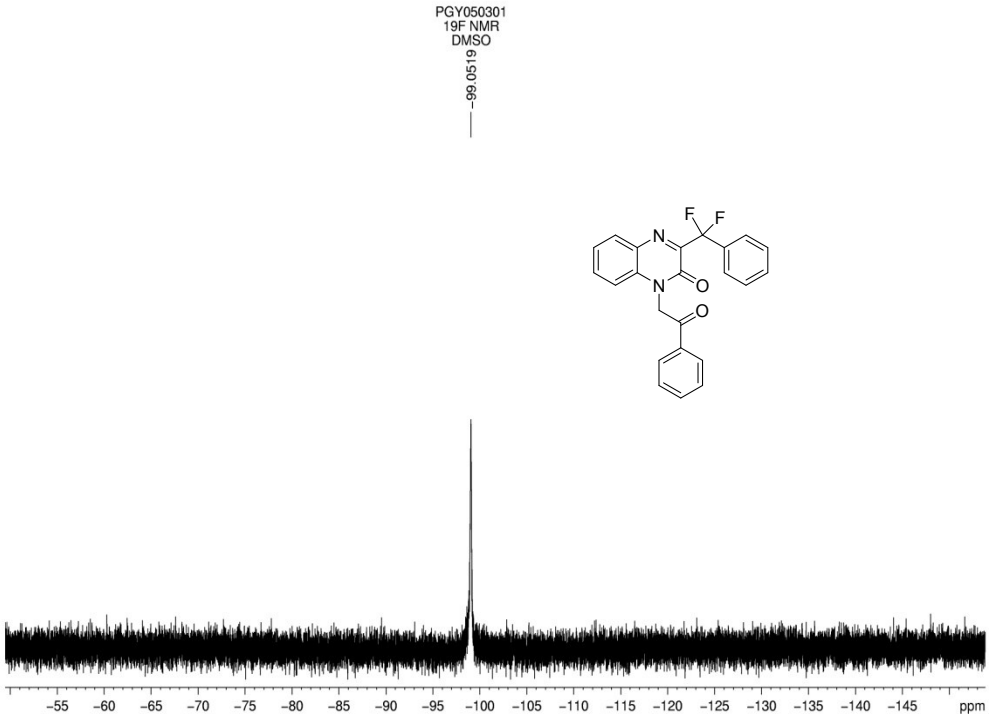


Fig. S81 ^{19}F NMR spectrum of compound **3la**

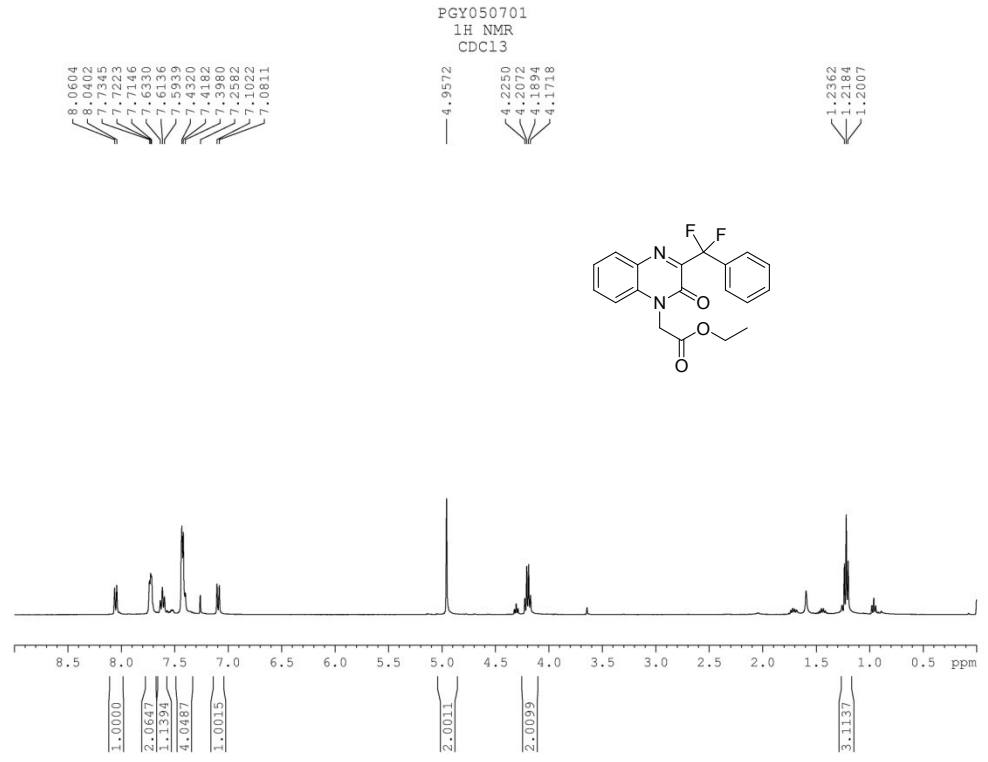


Fig. S82 ^{1}H NMR spectrum of compound **3ma**

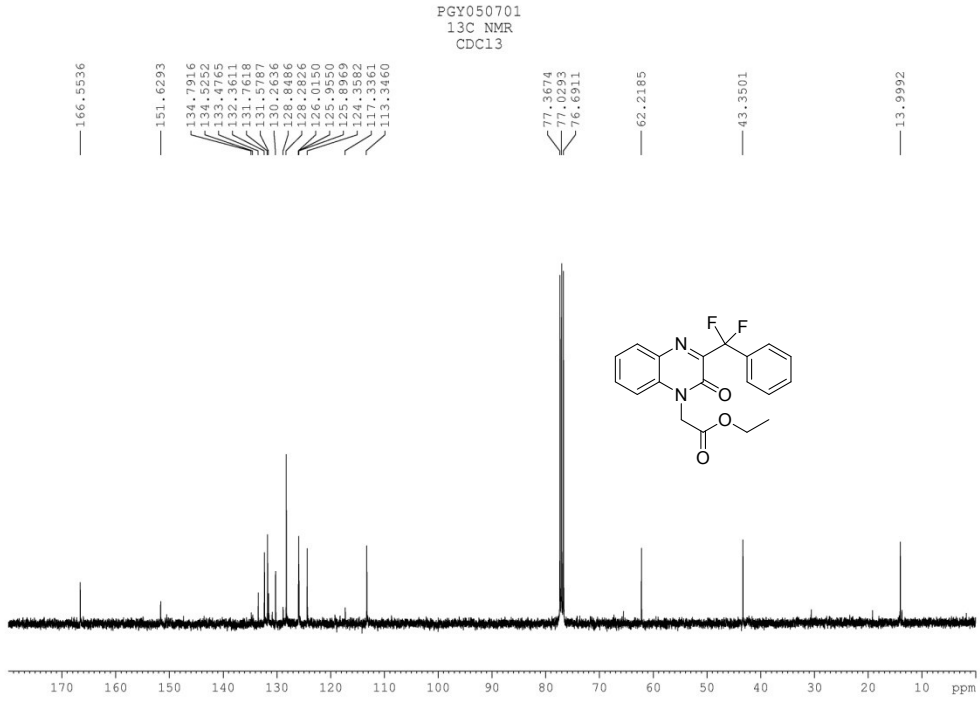


Fig. S83 ^{13}C NMR spectrum of compound **3ma**

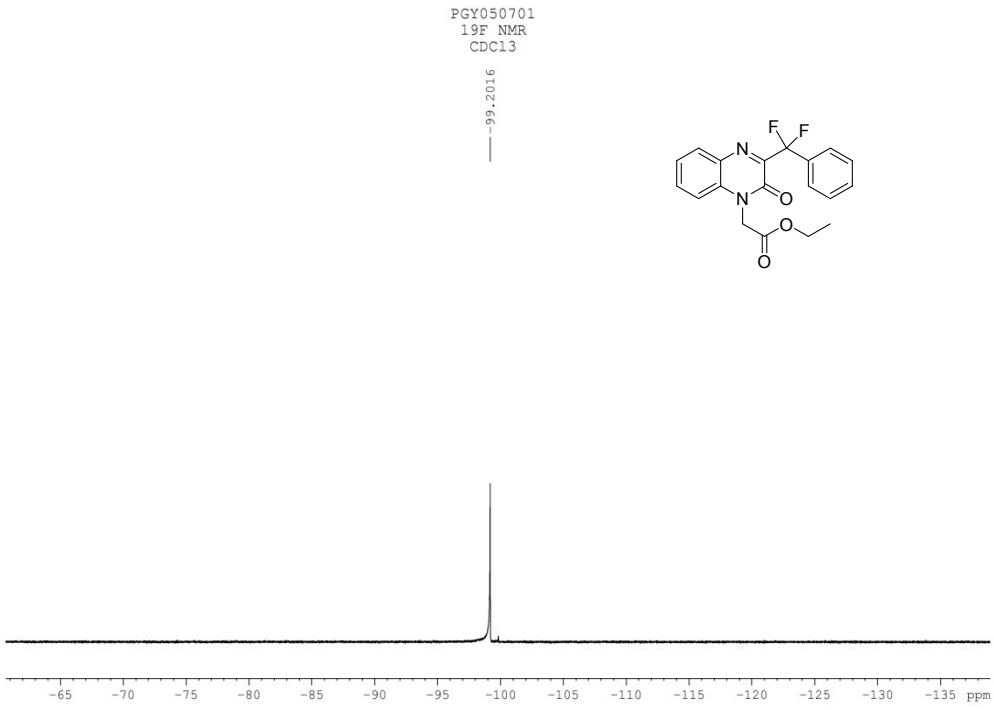


Fig. S84 ^{19}F NMR spectrum of compound **3ma**

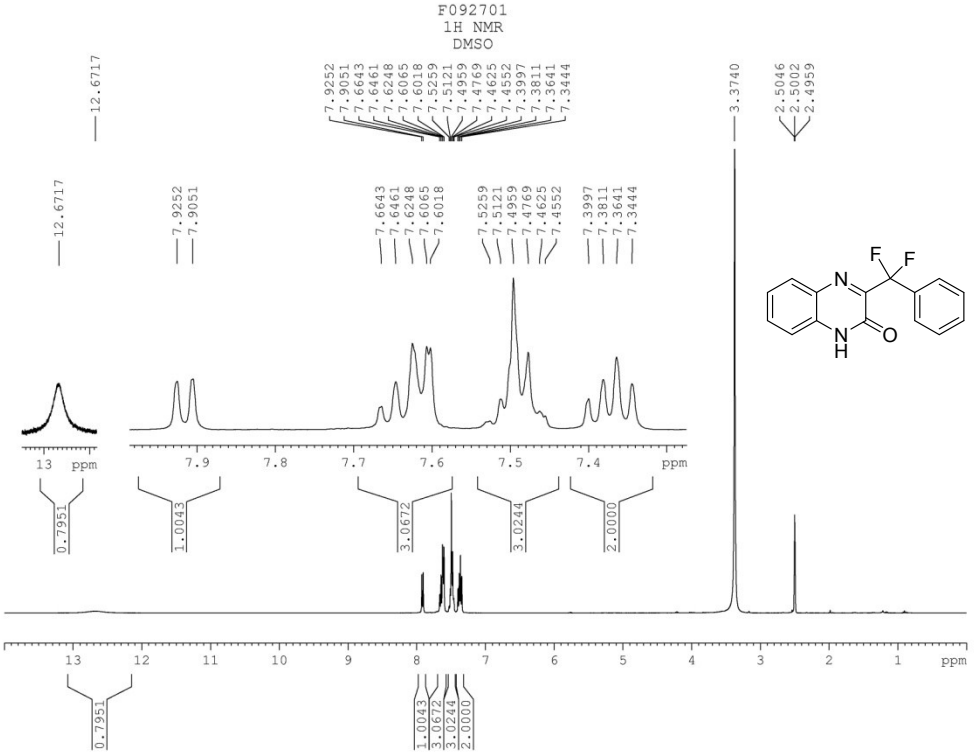


Fig. S85 ^{1}H NMR spectrum of compound **3na**

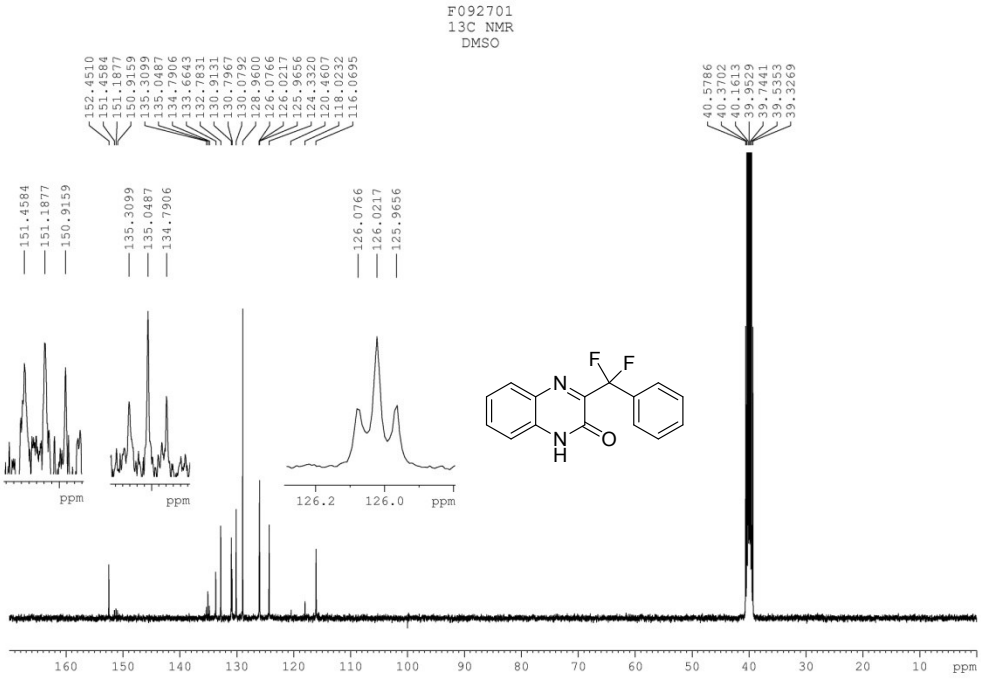


Fig. S86 ^{13}C NMR spectrum of compound **3na**

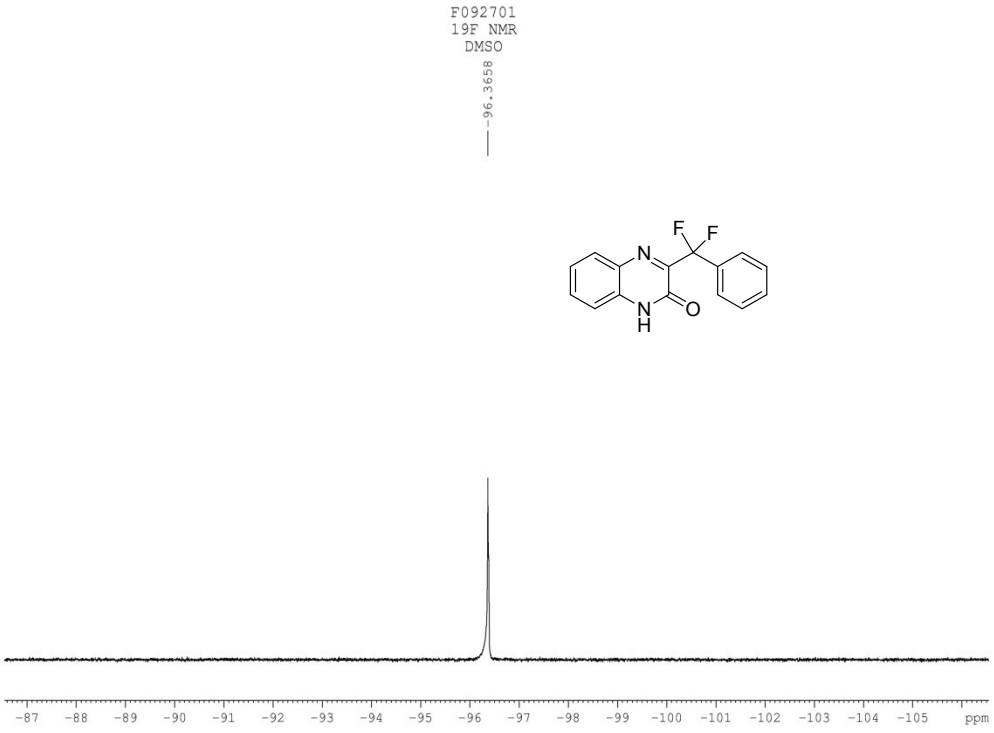


Fig. S87 ^{19}F NMR spectrum of compound **3na**

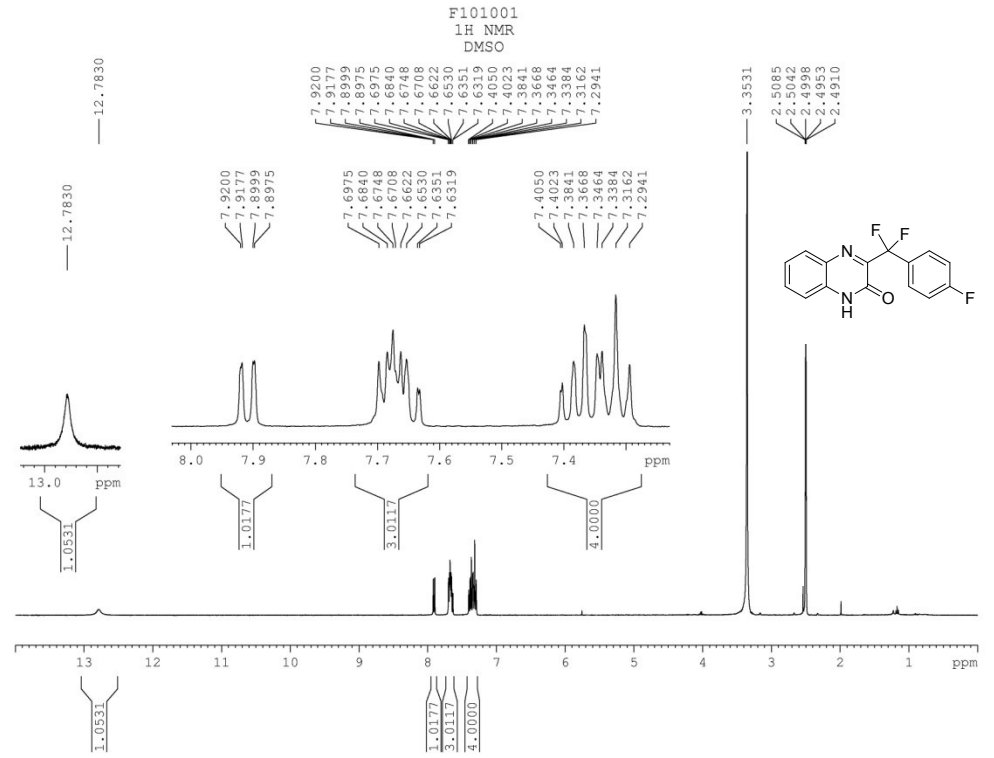


Fig. S88 ^{1}H NMR spectrum of compound **3nh**

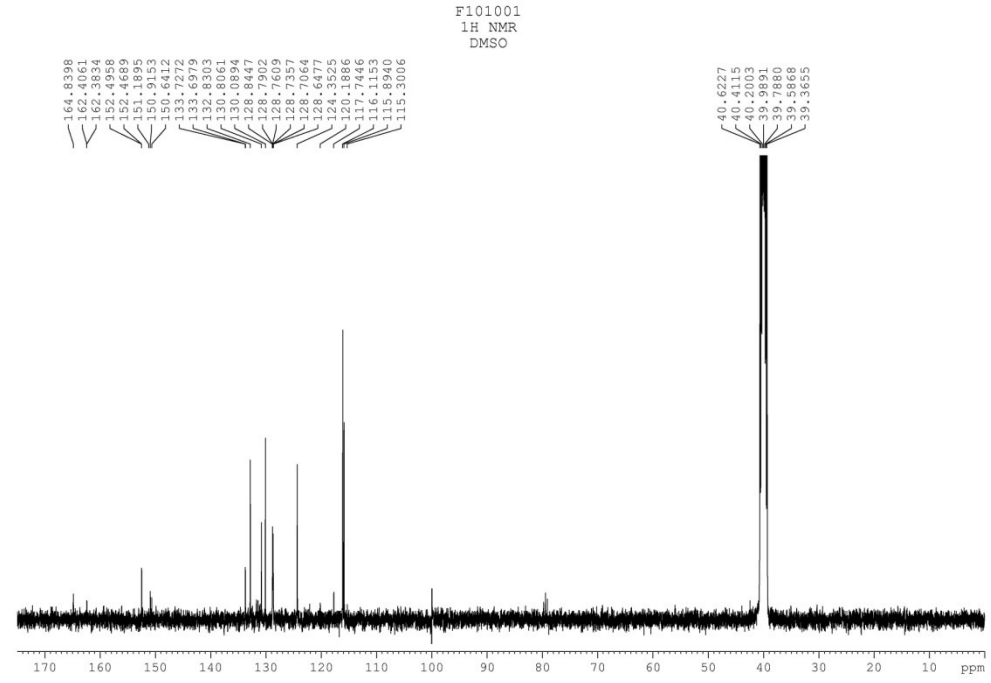


Fig. S89 ^{13}C NMR spectrum of compound **3nh**

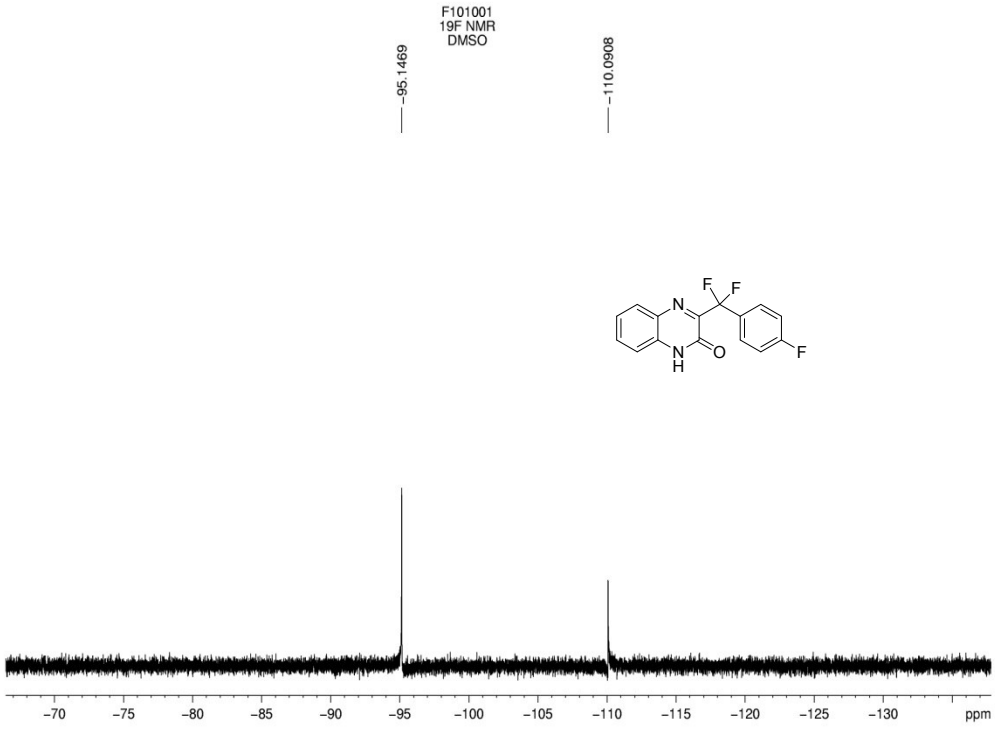


Fig. S90 ^{19}F NMR spectrum of compound **3nh**

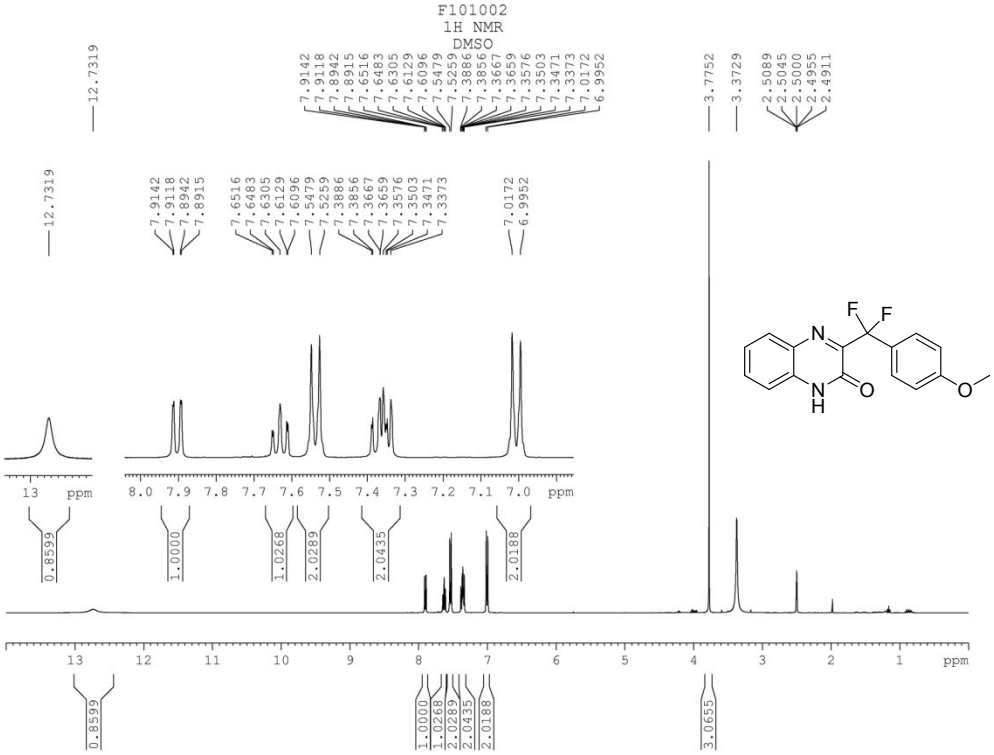


Fig. S91 ^{1}H NMR spectrum of compound **3nf**

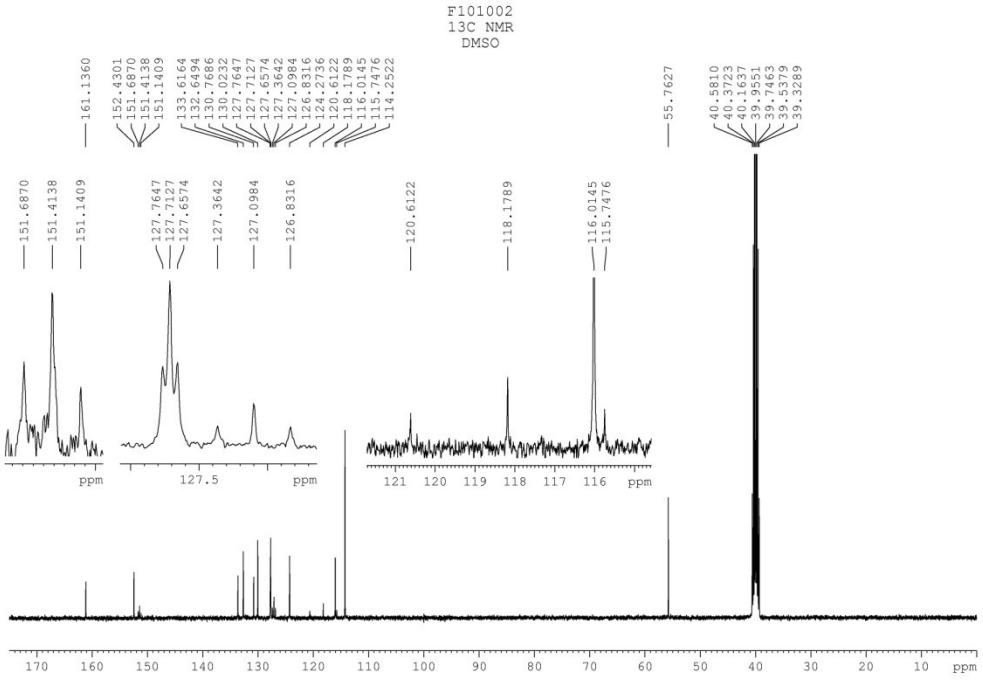


Fig. S92 ^{13}C NMR spectrum of compound **3nf**

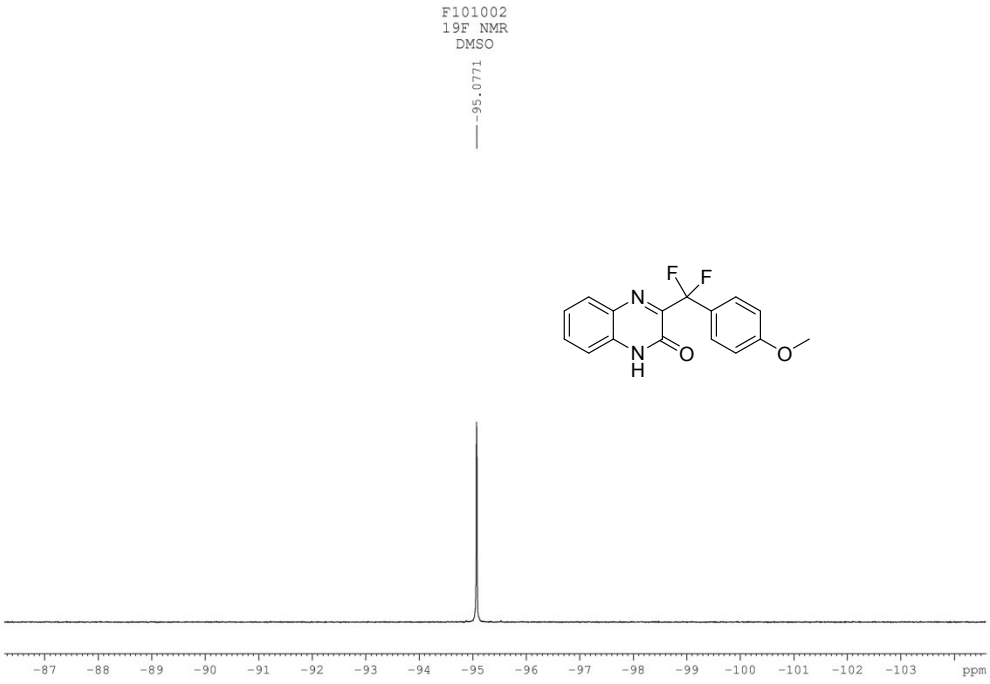


Fig. S93 ^{19}F NMR spectrum of compound **3nf**

3. HR MS of the adduct of TEMPO and α,α-difluorophenylmethyl radical

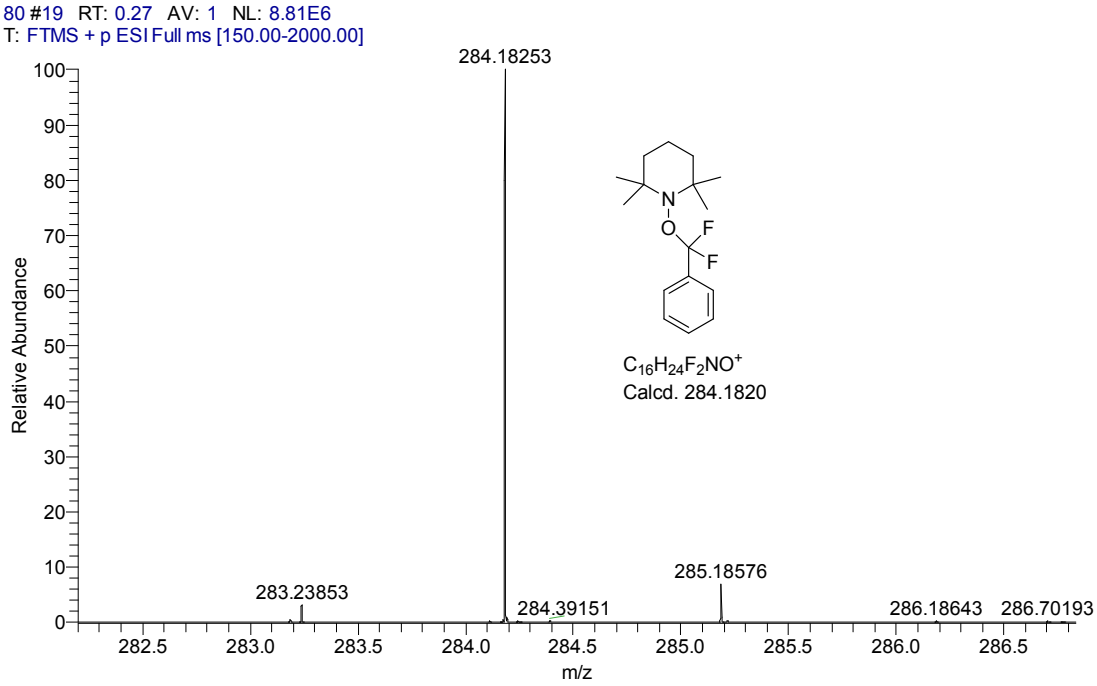


Fig. S94 HR MS of the adduct of TEMPO and α,α-difluorobenzyl radical