

Supporting information

Design, synthesis, insecticidal activity and 3D-QSR study for novel trifluoromethyl pyridine derivatives containing an 1,3,4-oxadiazole moiety

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1. Superimposition of compounds for the 3D-QSAR study

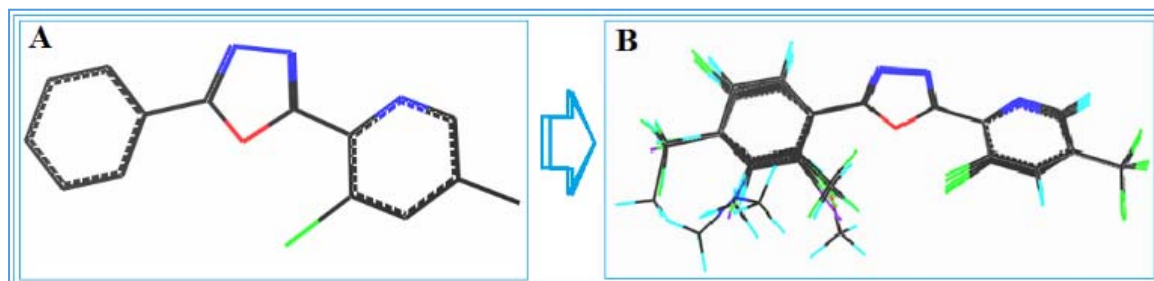


Fig. S1 Superimposition of compounds for the 3D-QSAR study. (A). Common substructure; (B) result of superimposition

2. The Tables for the results of 3D-QSAR study

Table S1. Statistical parameters of CoMFA and CoMSIA models

Statistical parameter	CoMFA	CoMSIA
q^2 ^a	0.742	0.614
ONC ^b	5	6
r^2 ^c	0.975	0.92
Standard Error of Estimate	0.044	0.084
F values	92.362	32.793
Fraction of field contributions ^d		
Steric	0.586	0.511
Electrostatic	0.414	0.489
Hydrophobic	-	0
Hydrogen-bond Donor	-	0
Hydrogen-bond Acceptor	-	0

^a Cross-validated correlation; ^b Optimum number of components;

^c Non-cross-validated correlation; ^d Field contributions.

Table S2. Results of experimental pLC₅₀ and predicted pLC₅₀

Compounds	Experimental PLC ₅₀	CoMFA		CoMSIA	
		Predc. ^a	Res. ^b	Predc. ^a	Res ^b
E1	3.058	3.014	0.046	3.054	0.004
E2	3.16	3.173	-0.033	3.153	0.007
E3	3.632	3.664	0.003	3.654	-0.022
E4	3.240	3.279	-0.033	3.224	0.016
E5	3.896	3.843	0.047	3.923	-0.027
E6	3.573	3.565	0.011	3.586	-0.013
E7*	3.615	3.493	0.122	3.809	-0.194
E8*	3.731	3.729	0.022	3.79	-0.059
E9*	3.82	3.847	0.047	3.861	-0.041
E10	3.603	3.635	-0.125	3.737	-0.134
E11	3.808	3.921	-0.114	3.745	0.063
E12	3.836	3.803	0.092	3.811	0.025
E13	3.975	4.003	-0.028	4.043	-0.068
E14	3.788	3.684	0.113	3.748	0.04
E15	3.863	3.901	0.099	3.787	0.076
E16*	3.768	3.797	-0.029	3.79	-0.022
E17	3.765	3.725	-0.16	3.748	0.017
E18	4.009	4.011	-0.002	4.010	-0.001
E19	3.824	3.854	0.028	3.856	-0.032
E20	3.683	3.691	0.027	3.654	0.029
E21	3.835	3.824	0.031	3.79	0.045
E22*	3.634	3.683	-0.019	3.765	-0.131
E23	3.742	3.772	0.03	3.744	-0.002
E24	3.659	3.679	-0.07	3.755	-0.096
E25	3.646	3.674	-0.178	3.765	-0.119
E26*	3.806	3.904	0.002	3.805	0.001
E27 [#]	4.106	4.055	0.051	3.855	0.251
E28 [#]	3.442	3.406	-0.184	3.47	-0.028

*Sample of the test set; [#] Compounds Predicted by the 3D-QSAR models

3. The ^1H , ^{13}C , ^{19}F NMR and HR-MS spectra of the title compounds

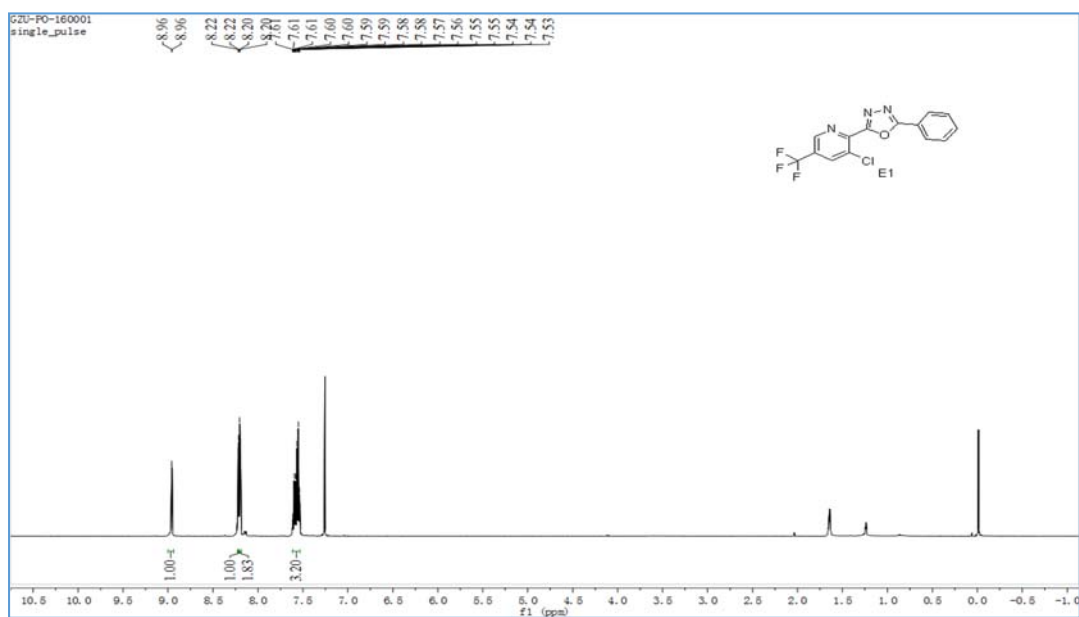


Fig. S2 ^1H NMR spectra of compound E1

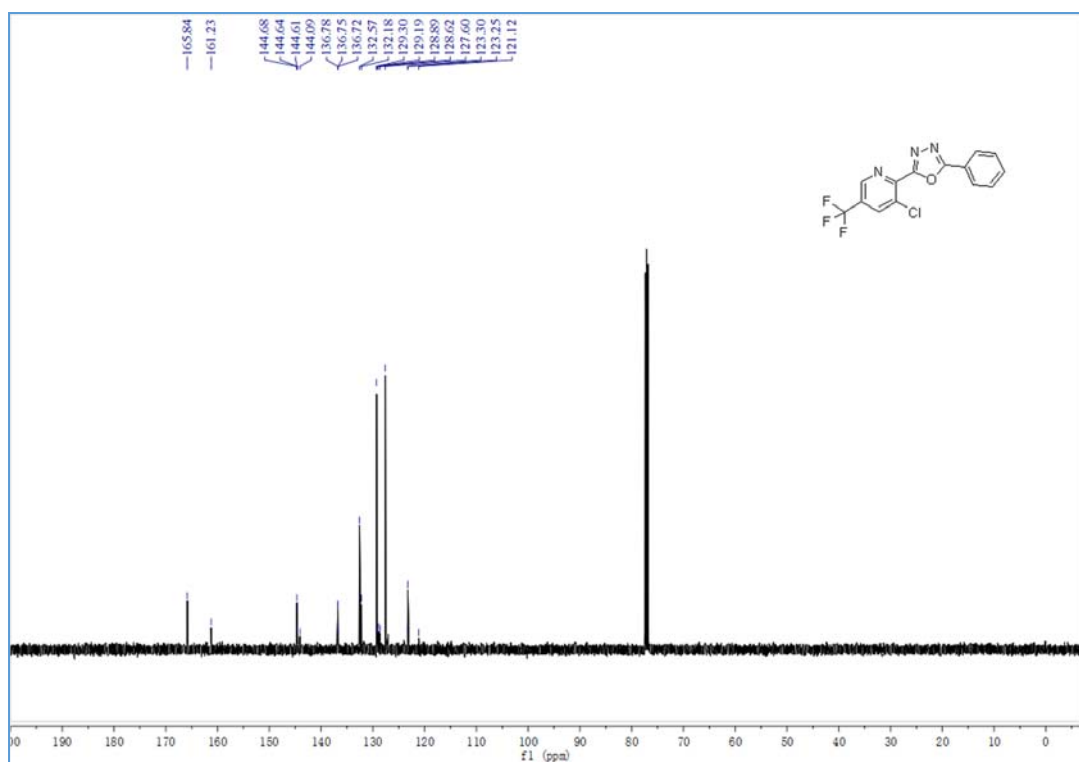


Fig. S3 ^{13}C NMR spectra of compound E1

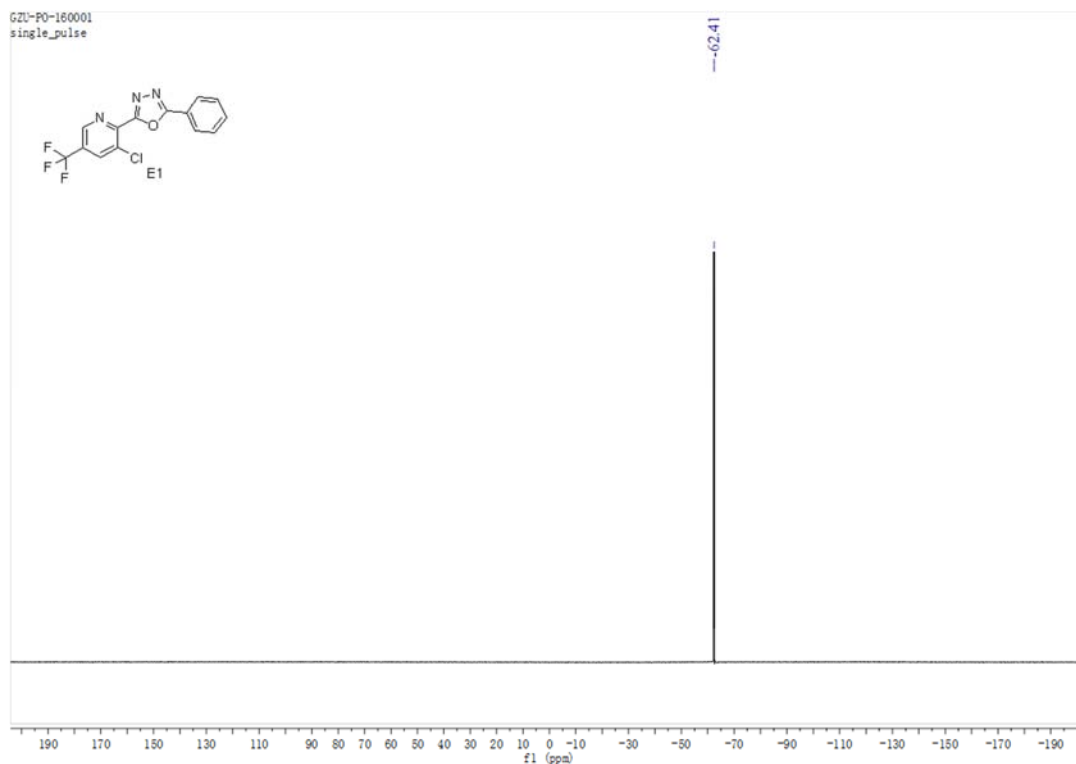


Fig. S4 ^{19}F NMR spectra of compound **E1**

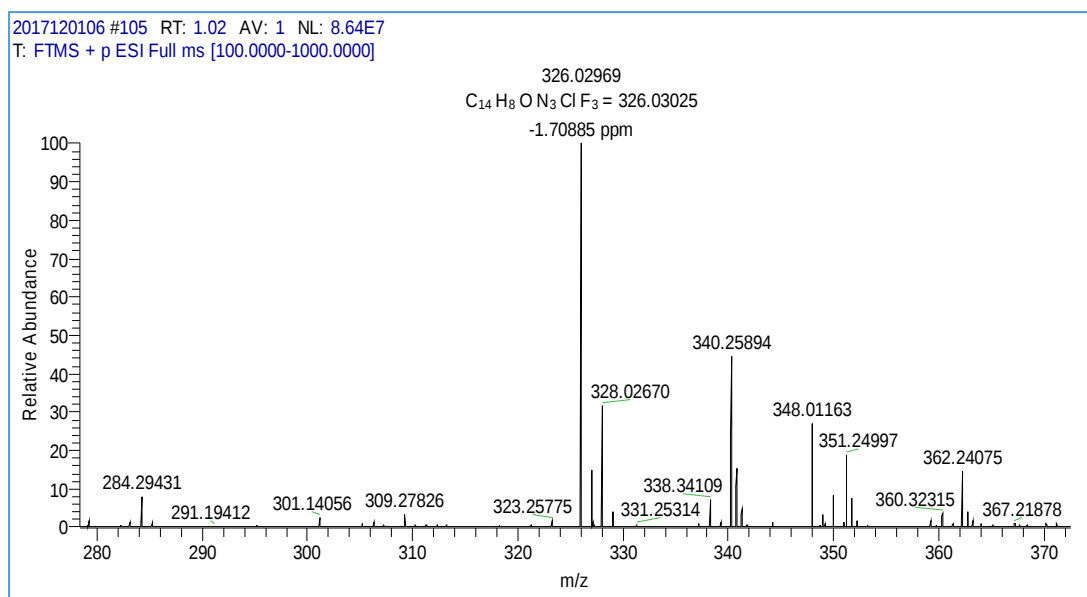


Fig. S5 HR-MS spectra of compound **E1**

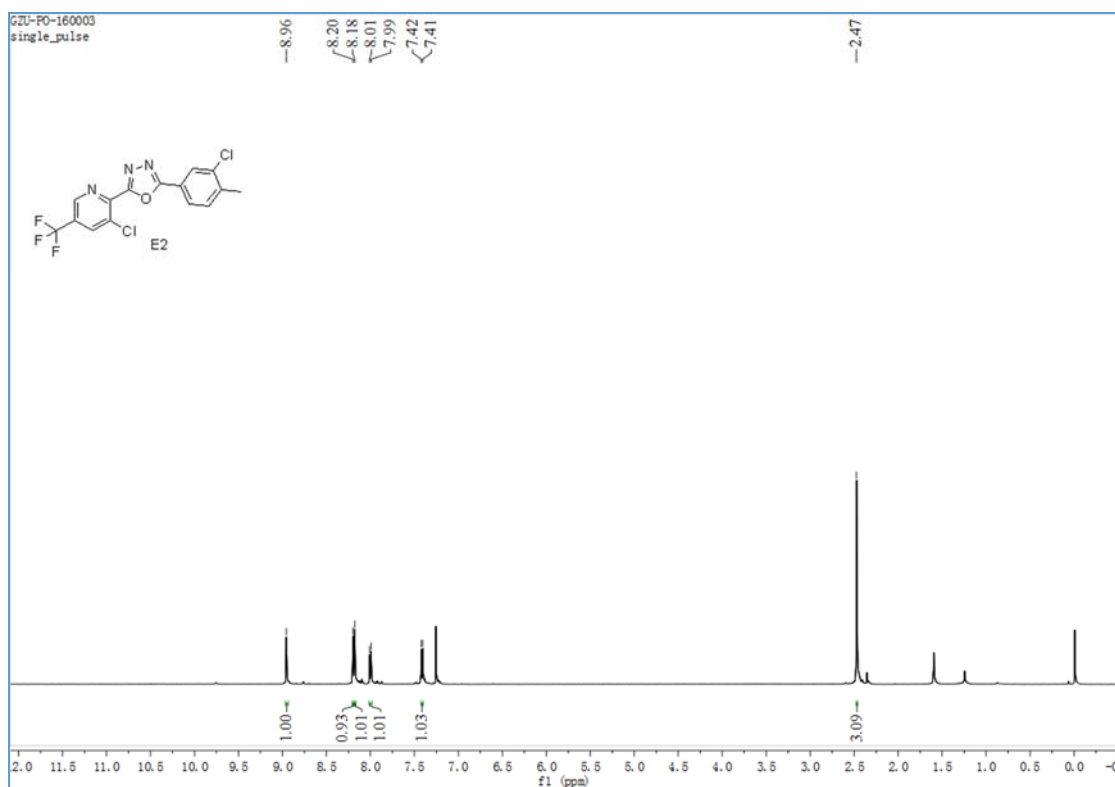


Fig. S6 ^1H NMR spectra of compound E2

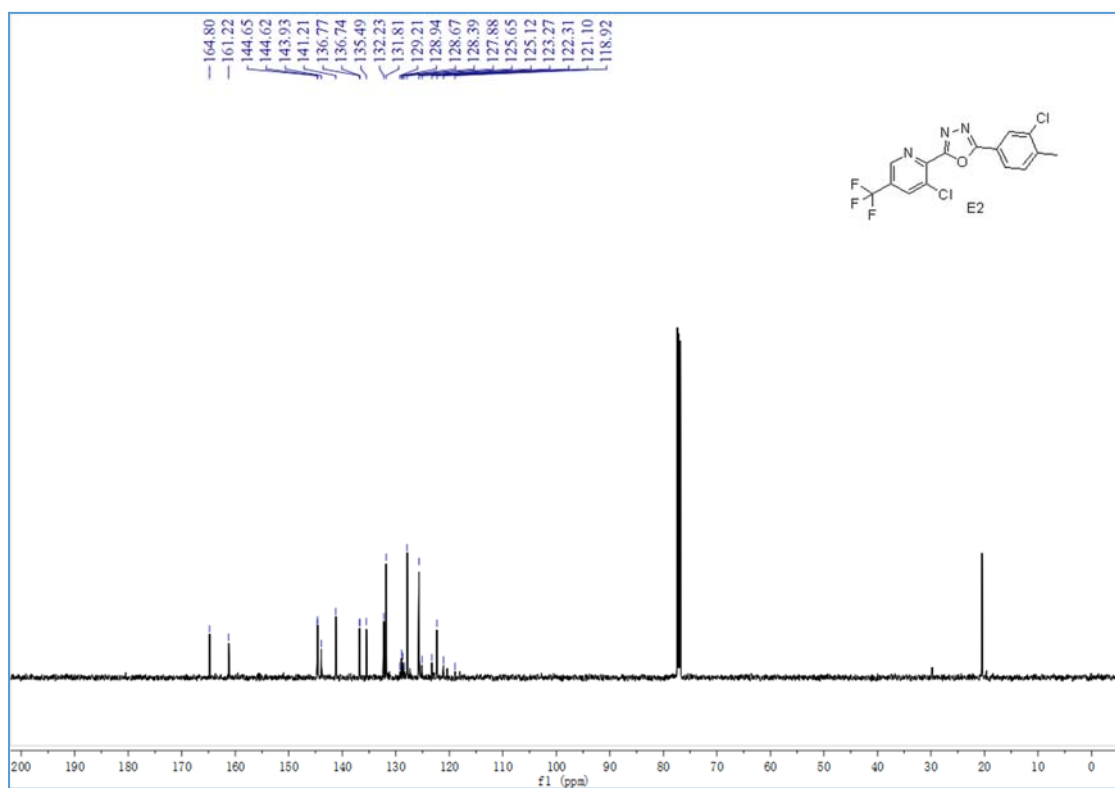


Fig. S7 ^{13}C NMR spectra of compound E2

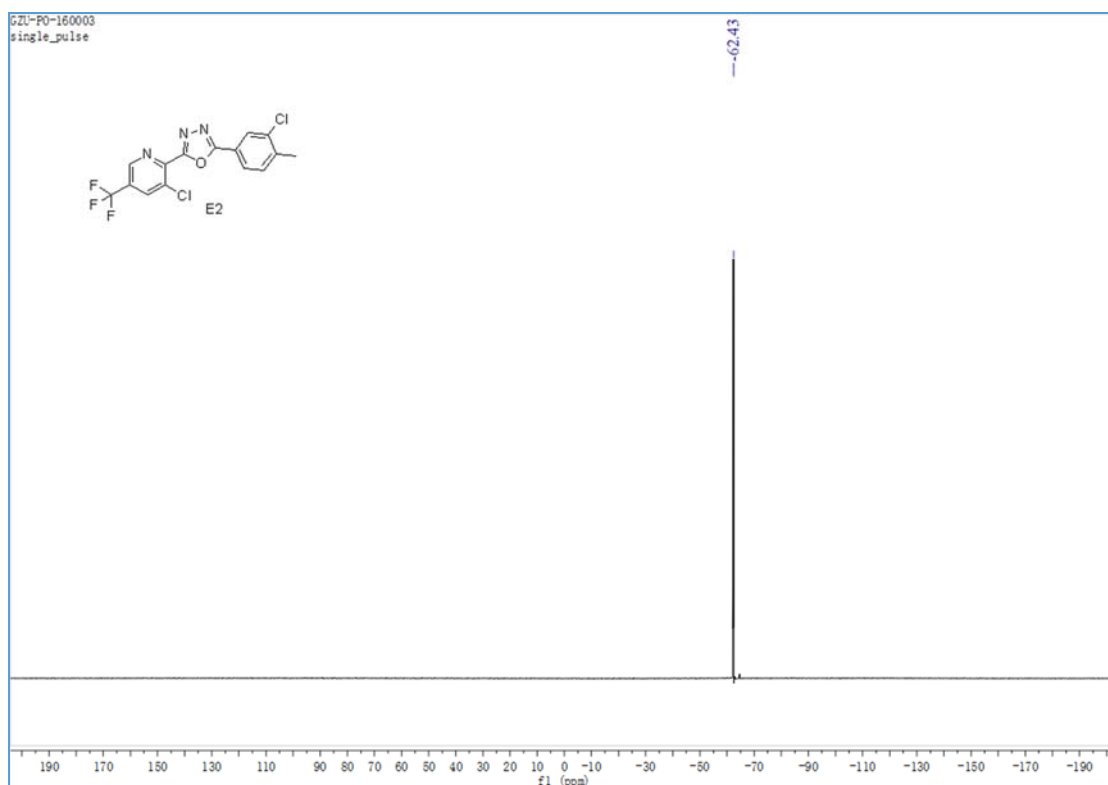


Fig. S8 ^{19}F NMR spectra of compound E2

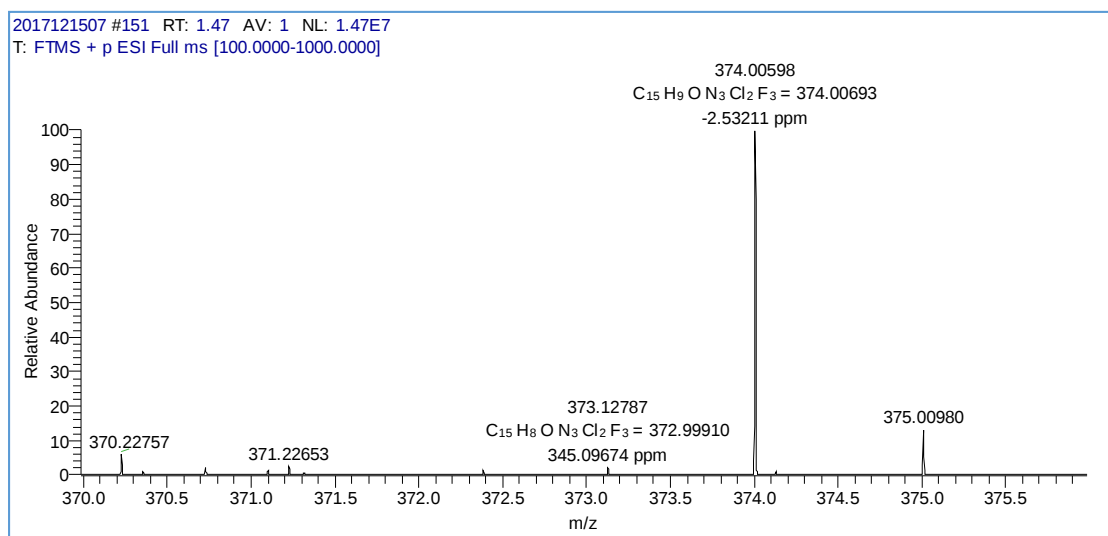


Fig. S9 HR-MS spectra of compound E2

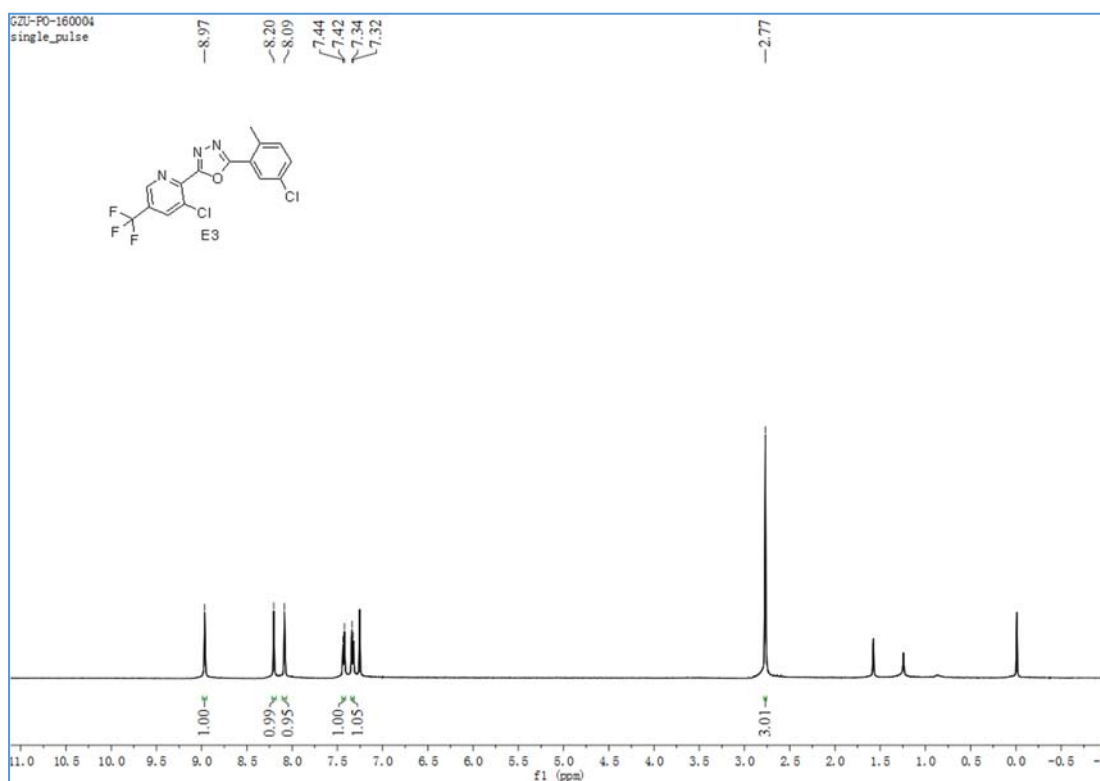


Fig. S10 ^1H NMR spectra of compound **E3**

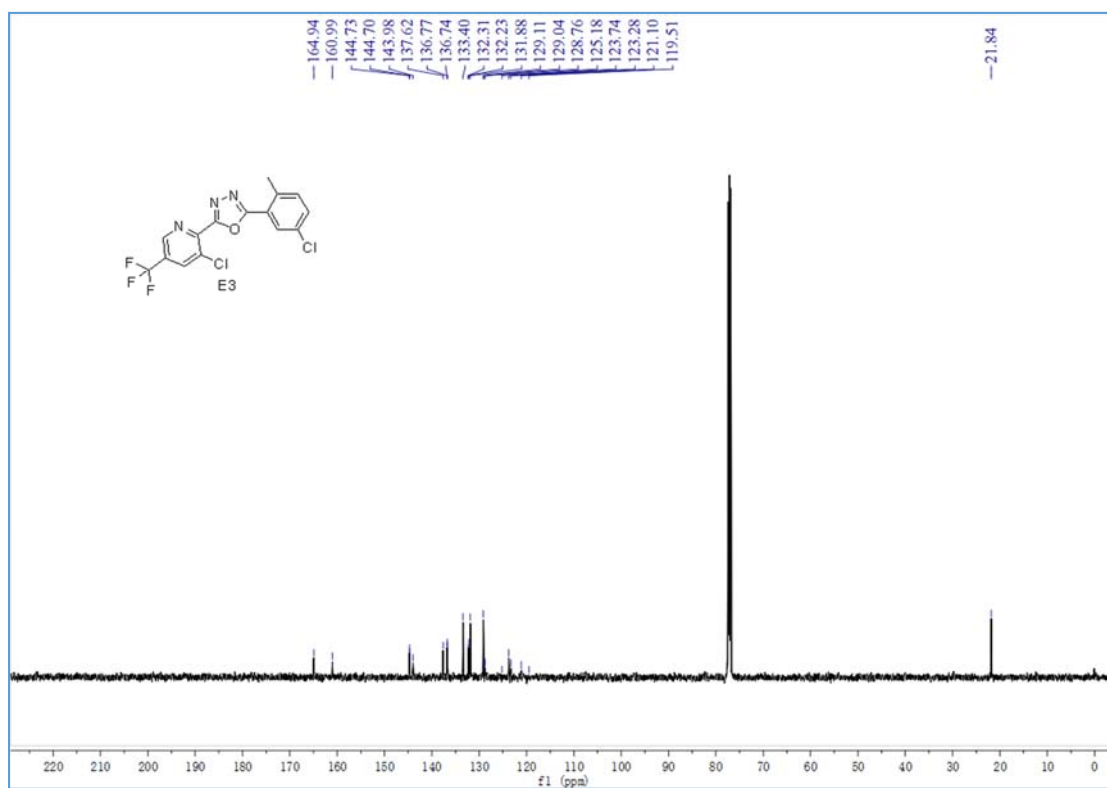


Fig. S11 ^{13}C NMR spectra of compound **E3**

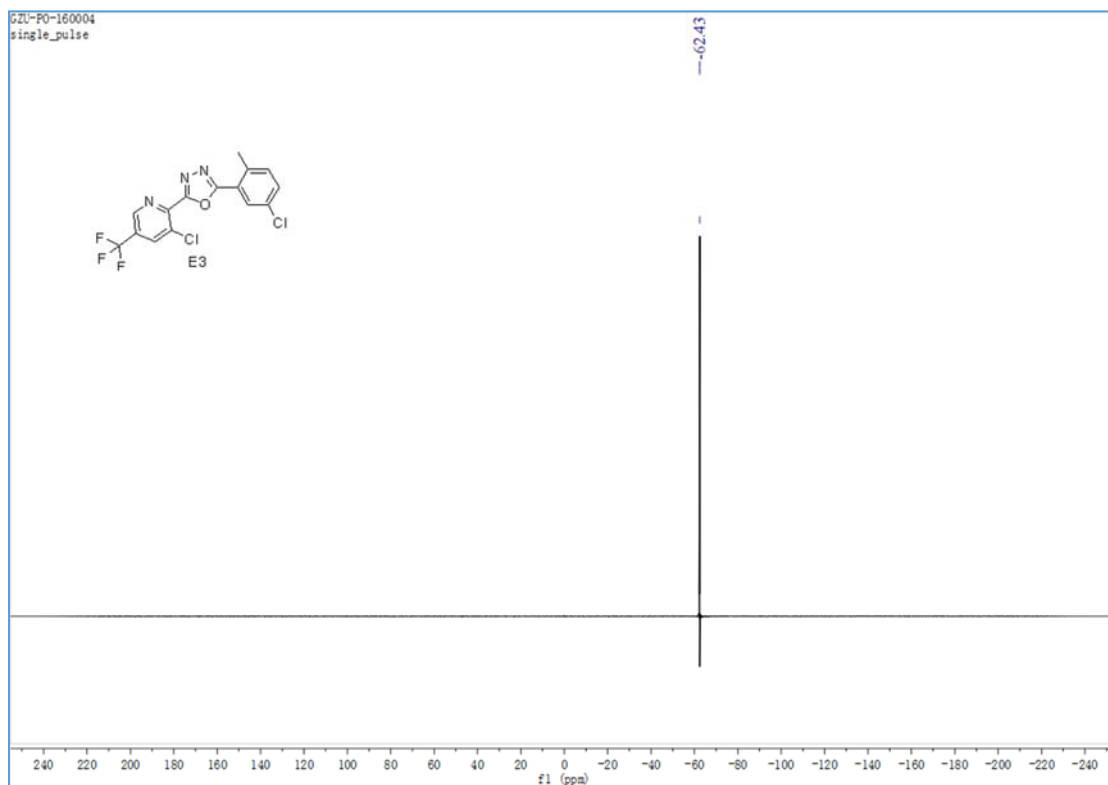


Fig. S12 ^{19}F NMR spectra of compound **E3**

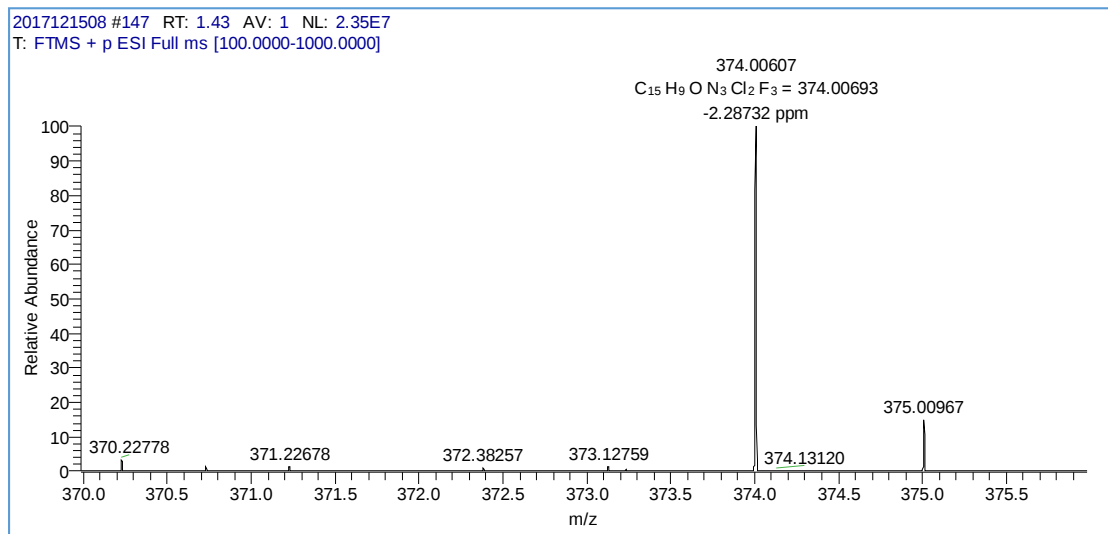


Fig. S13 HR-MS spectra of compound **E3**

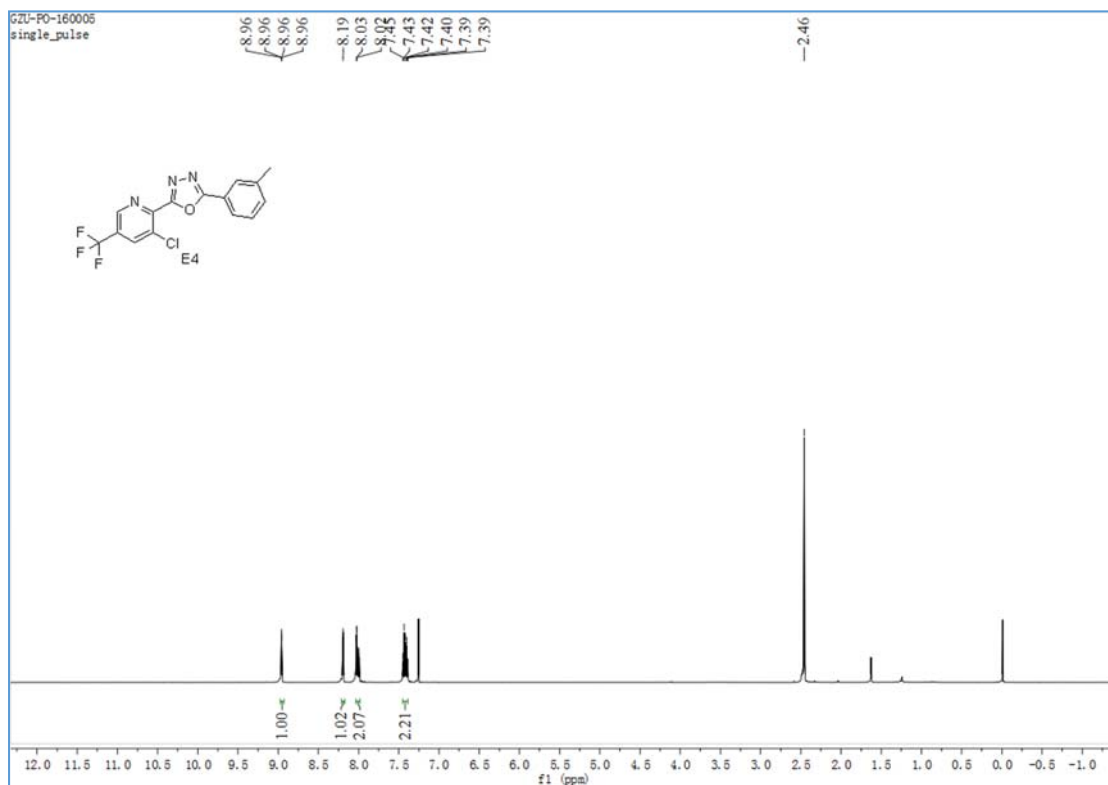


Fig. S14 ^1H NMR spectra of compound E4

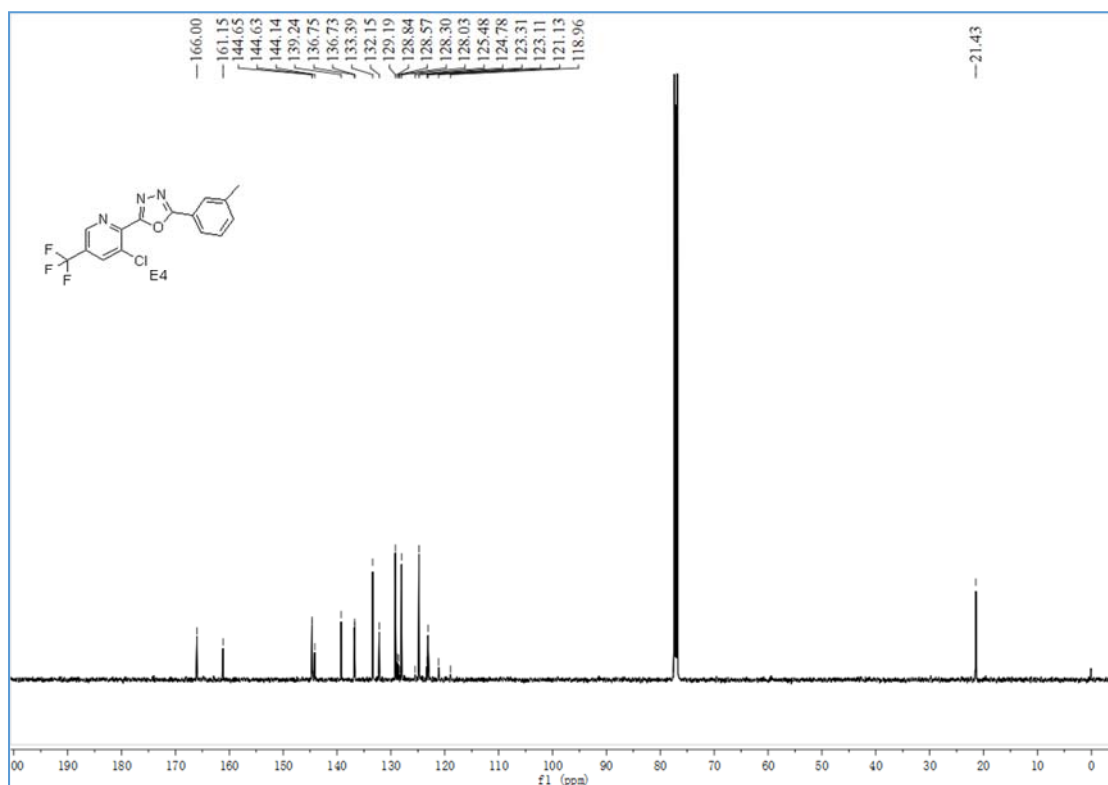


Fig. S15 ^{13}C NMR spectra of compound E4

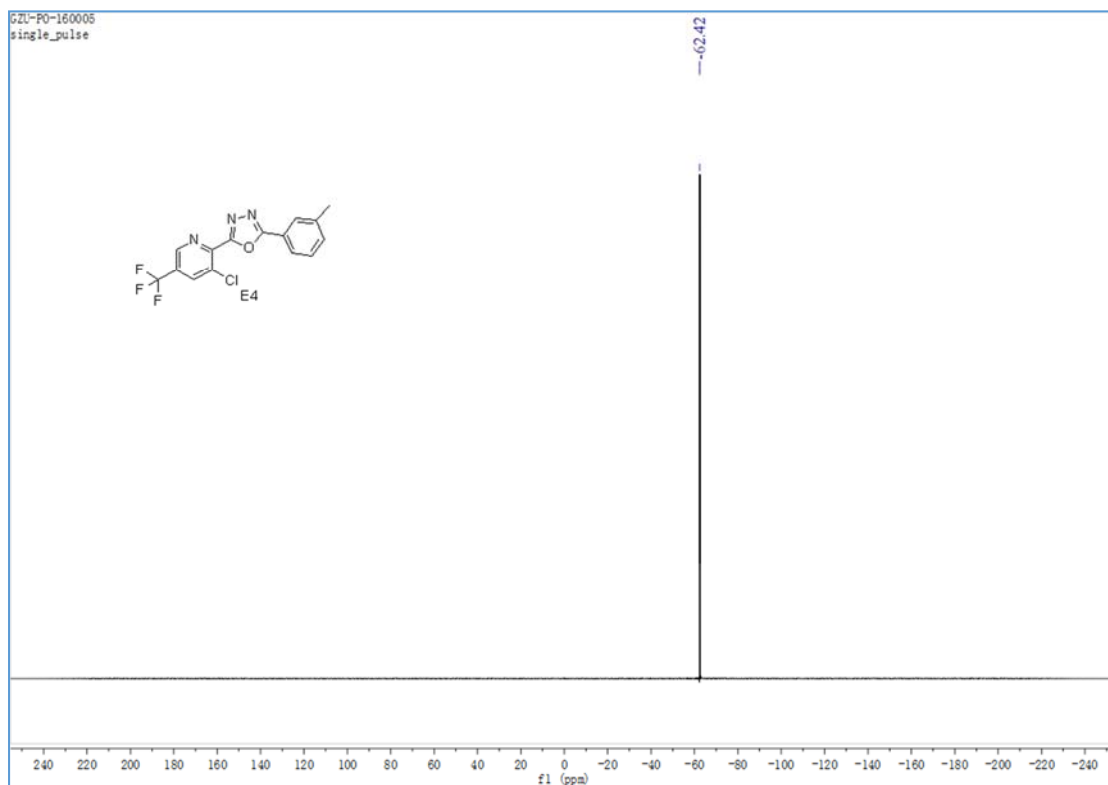


Fig. S16 ^{19}F NMR spectra of compound E4

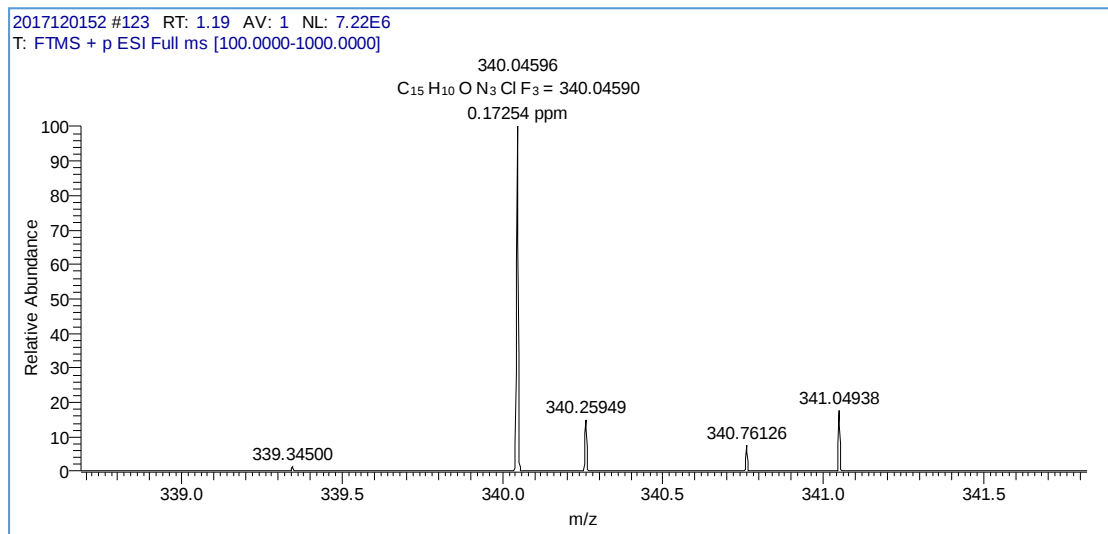


Fig. S17 HR-MS spectra of compound E4

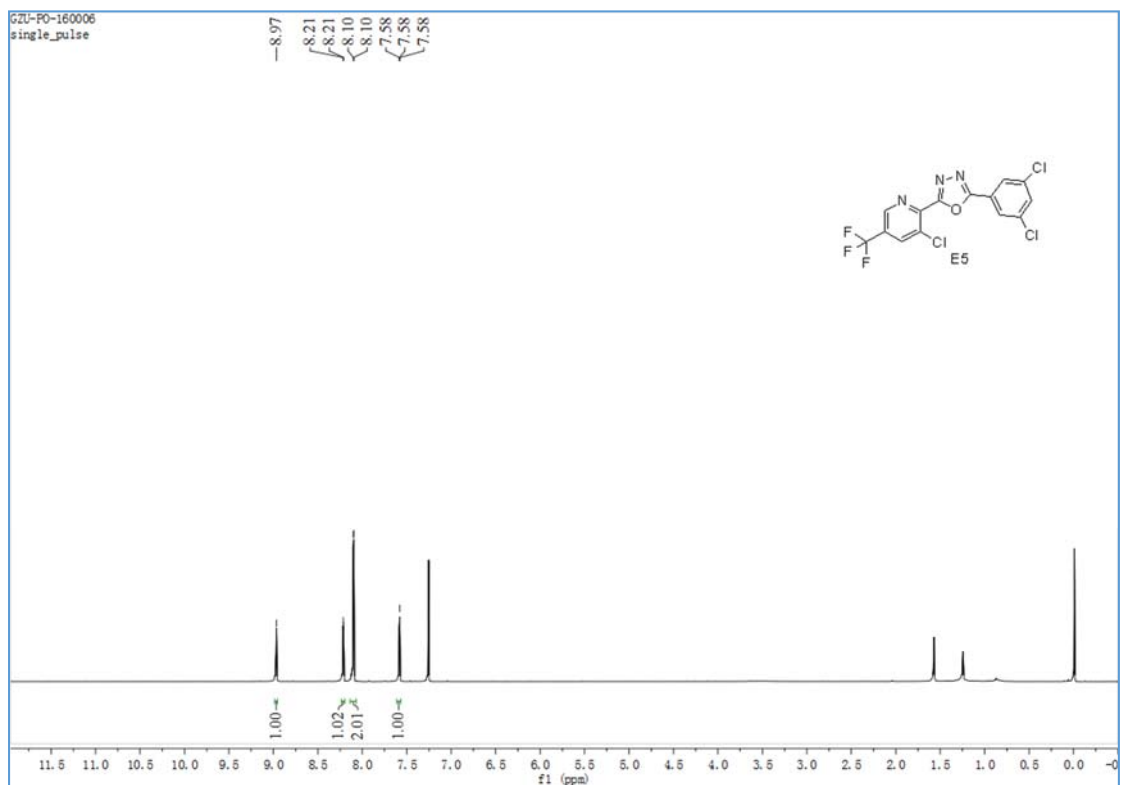


Fig. S18 ^1H NMR spectra of compound E5

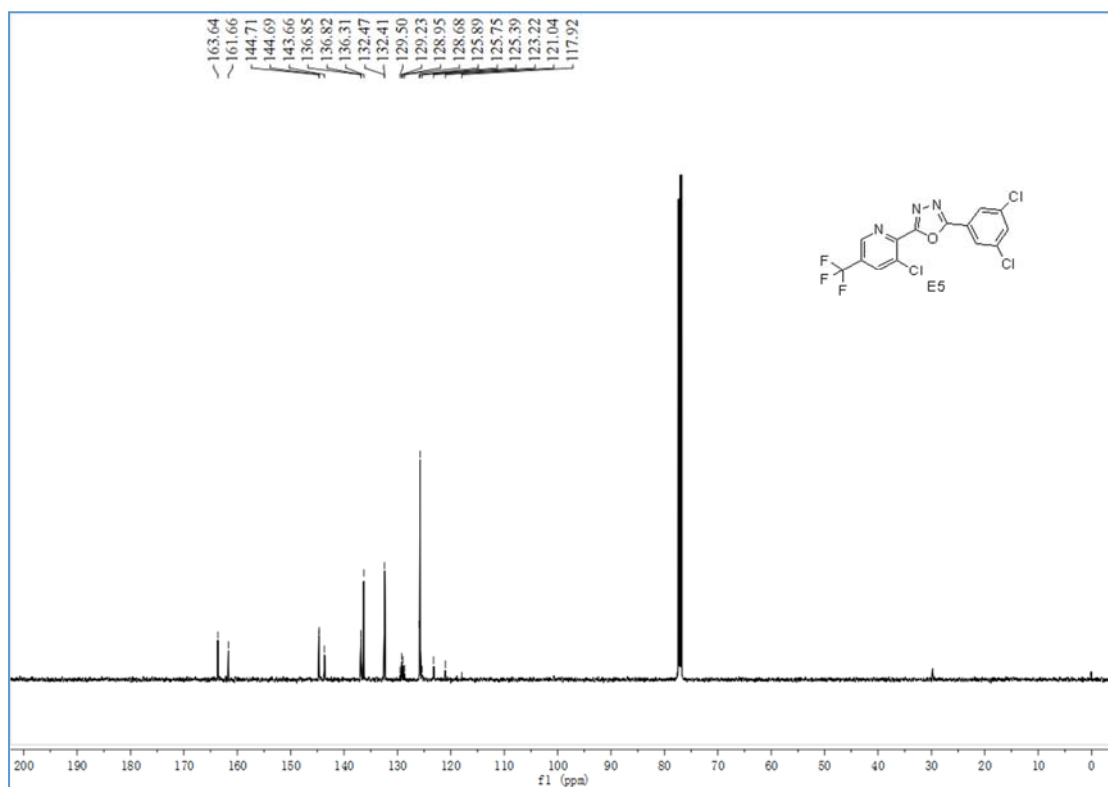


Fig. S19 ^{13}C NMR spectra of compound E5

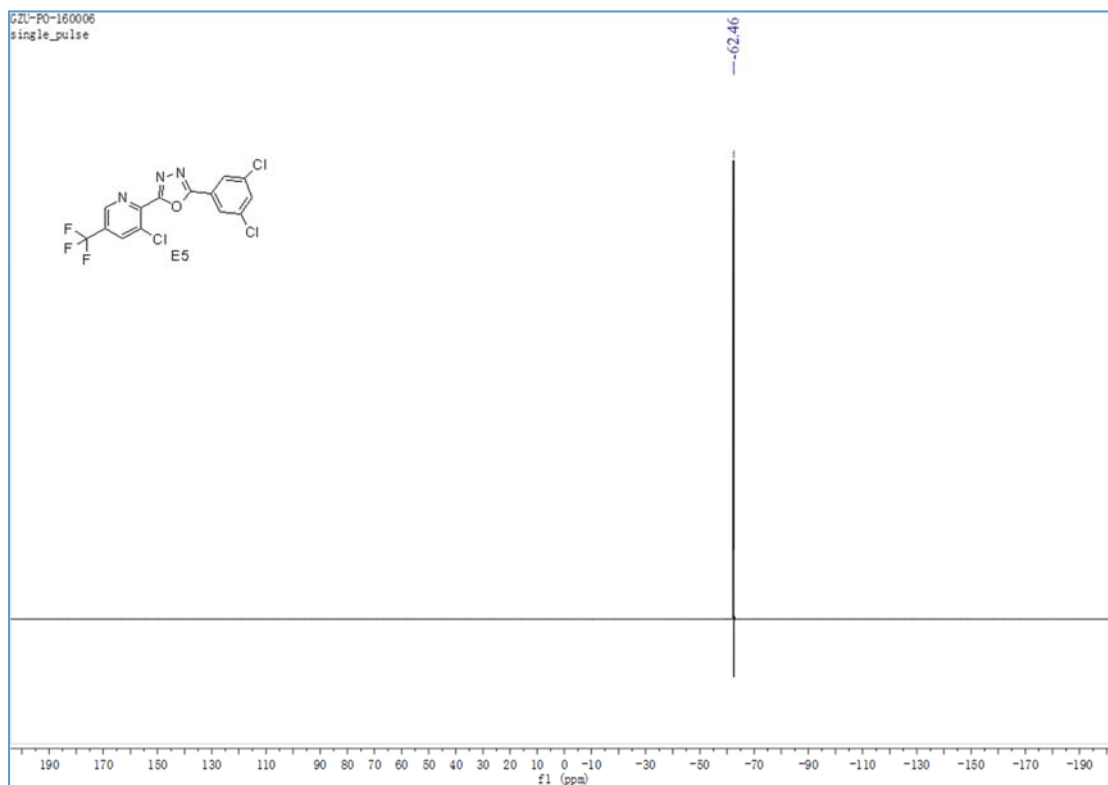


Fig. S20 ^{19}F NMR spectra of compound **E5**

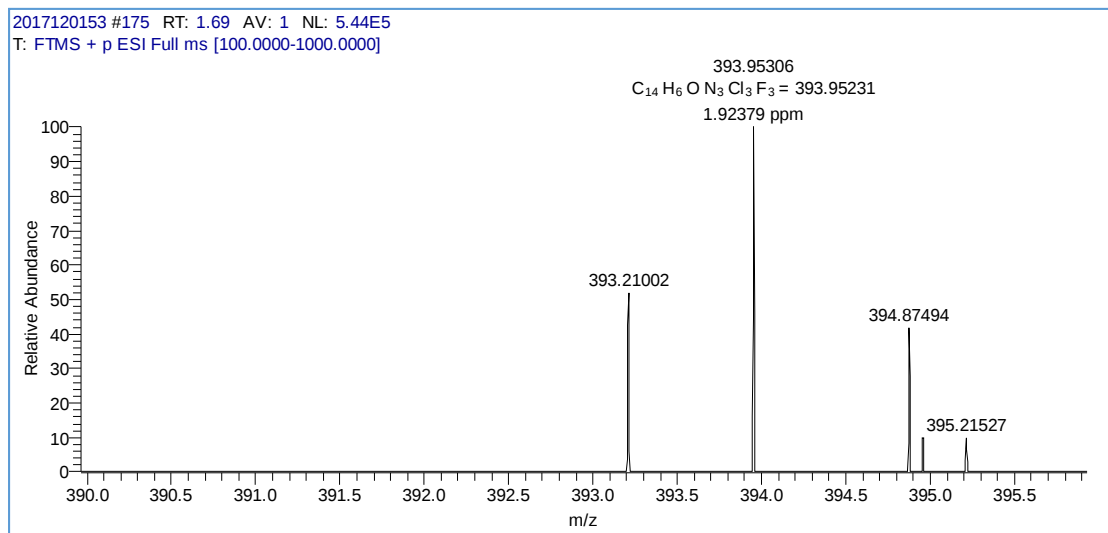


Fig. S21 HR-MS spectra of compound **E5**

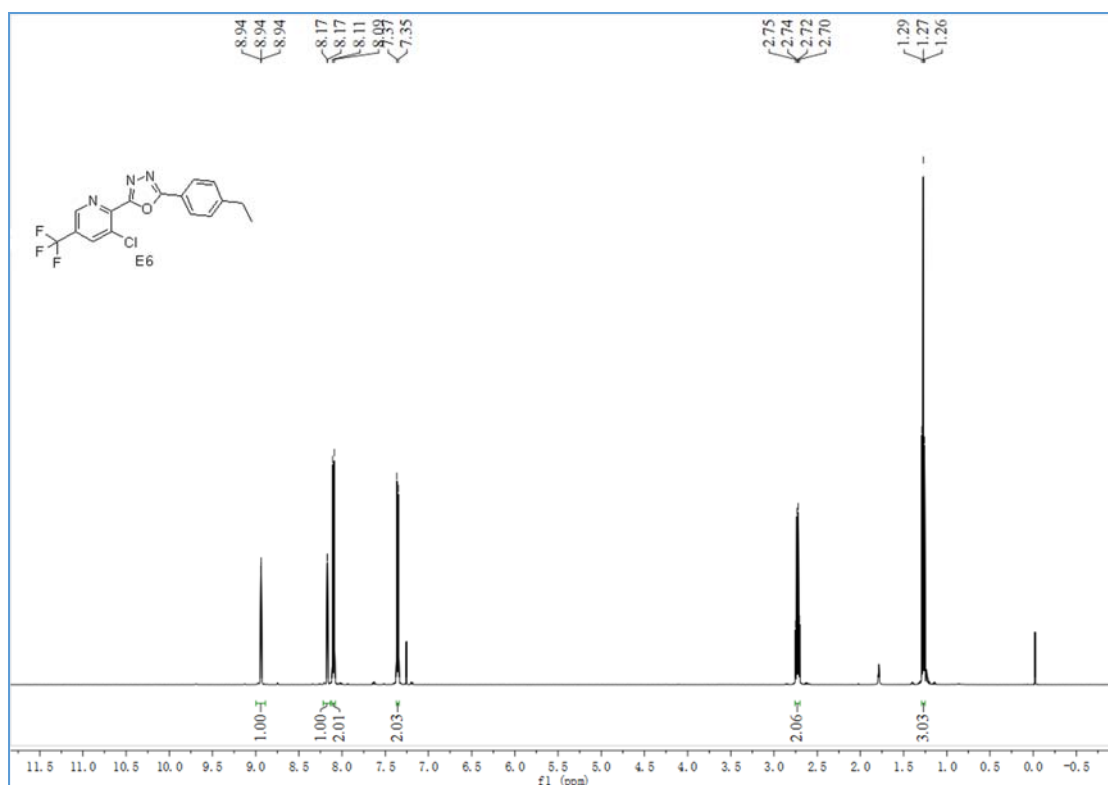


Fig. S22 ¹H NMR spectra of compound E6

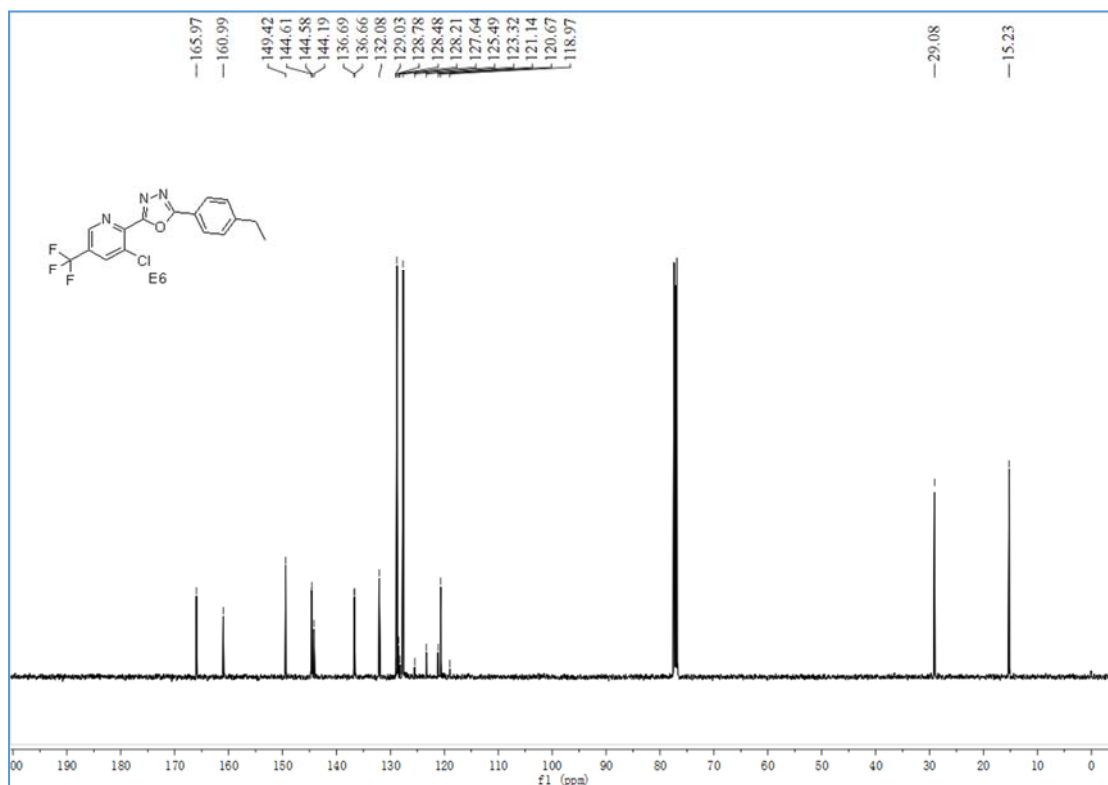


Fig. S23 ¹³C NMR spectra of compound E6

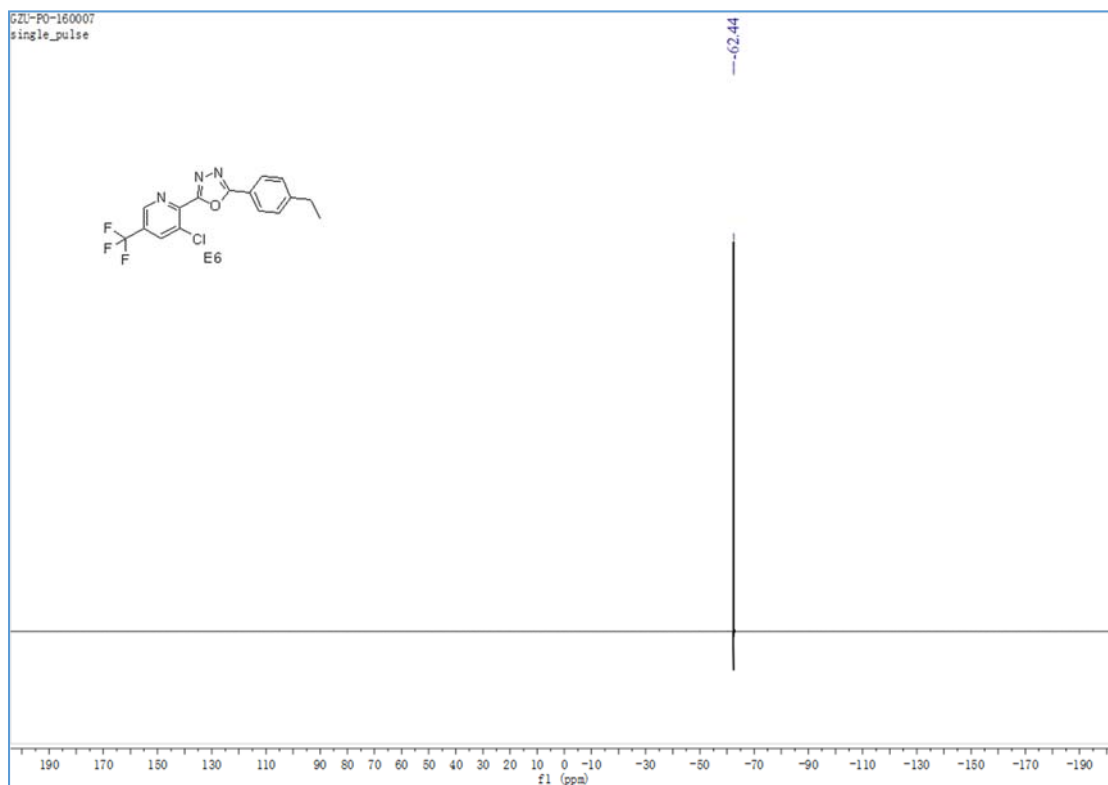


Fig. S24 ^{19}F NMR spectra of compound **E6**

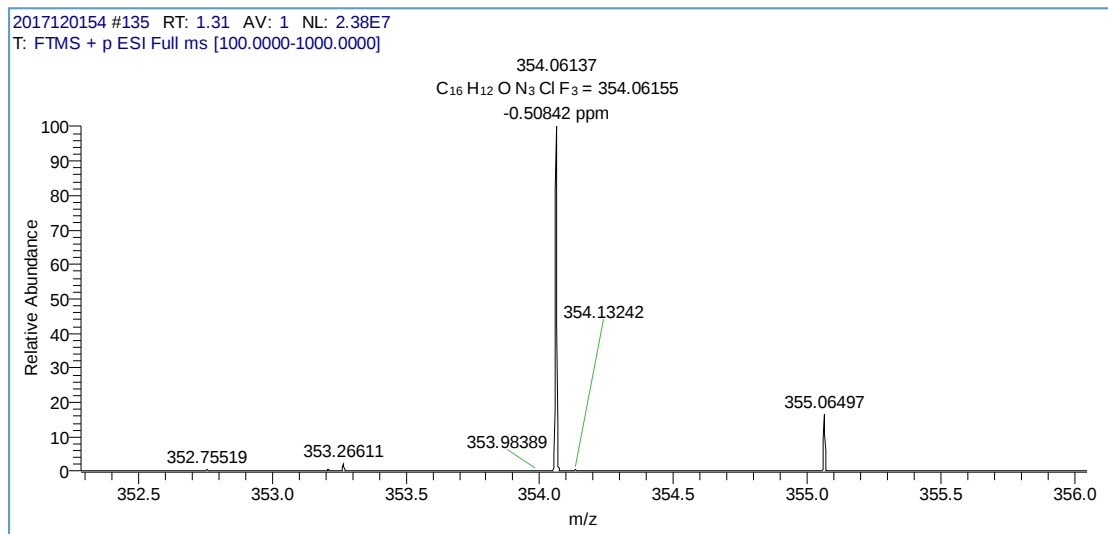


Fig. S25 HR-MS spectra of compound **E6**

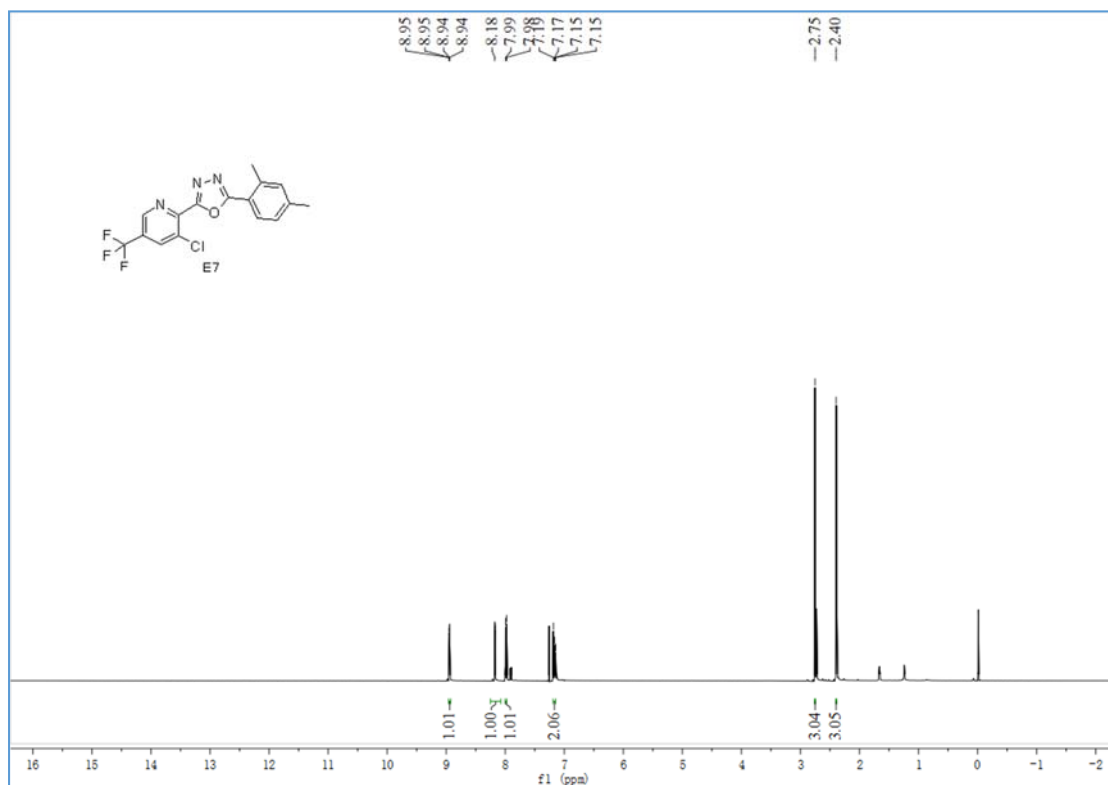


Fig. S26 ¹H NMR spectra of compound E7

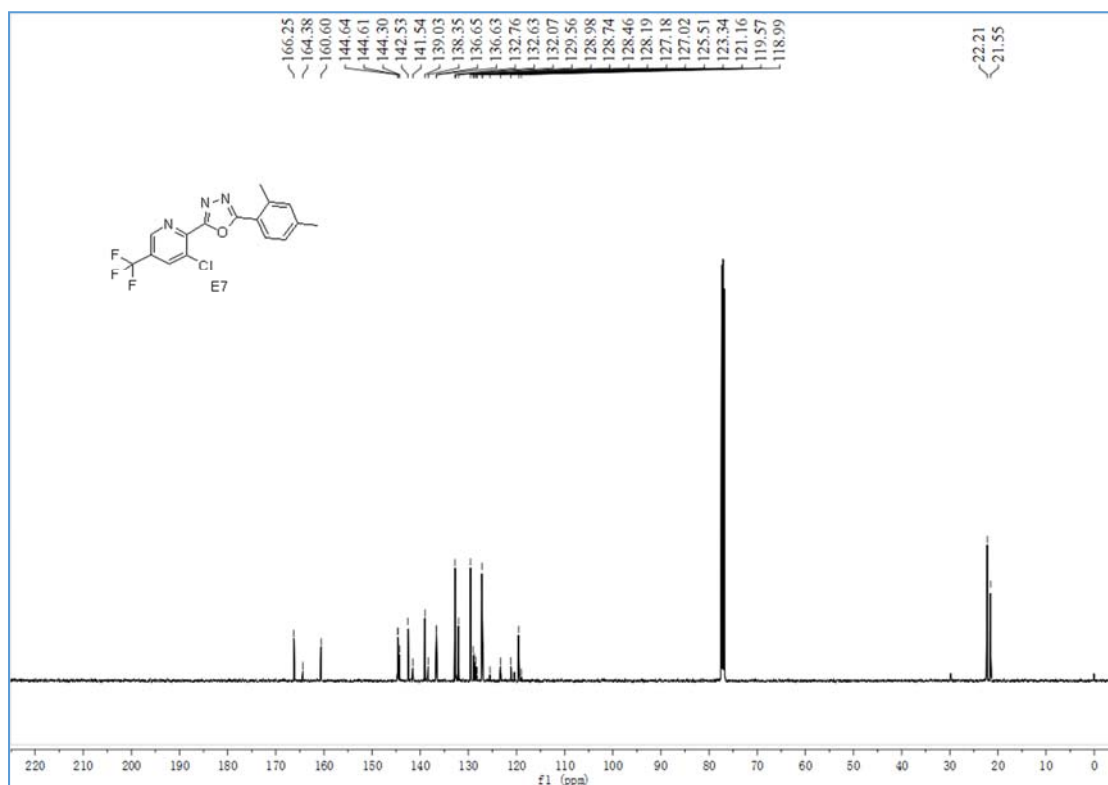


Fig. S27 ¹³C NMR spectra of compound E7

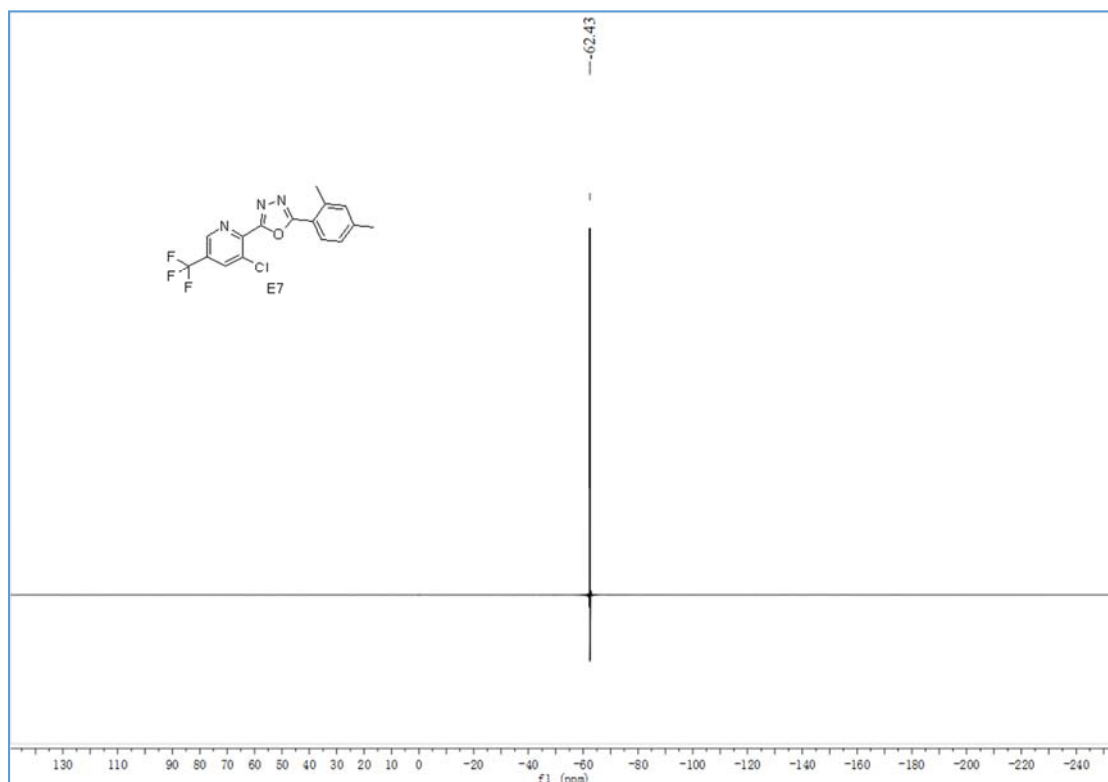


Fig. S28 ^{19}F NMR spectra of compound E7

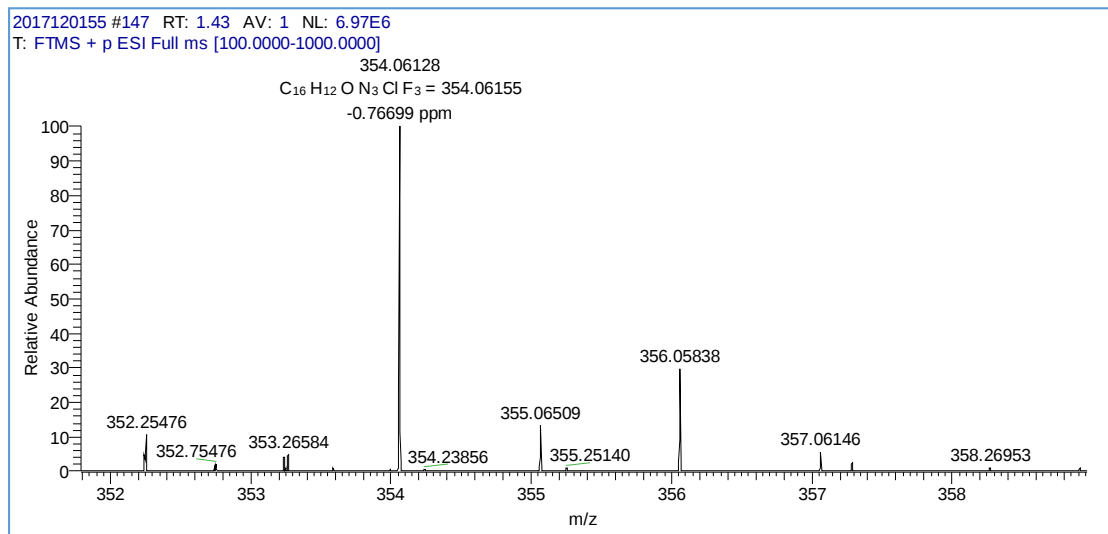


Fig. S29 HR-MS spectra of compound E7

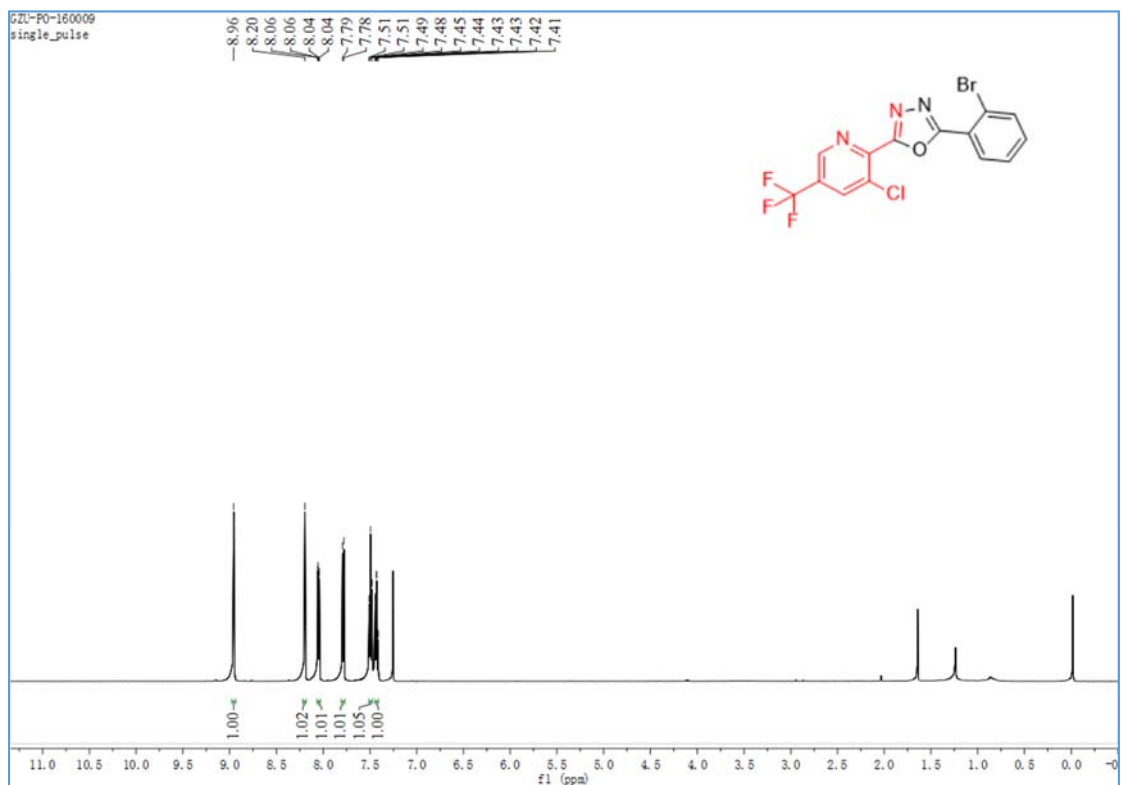


Fig. S30 ^1H NMR spectra of compound **E8**

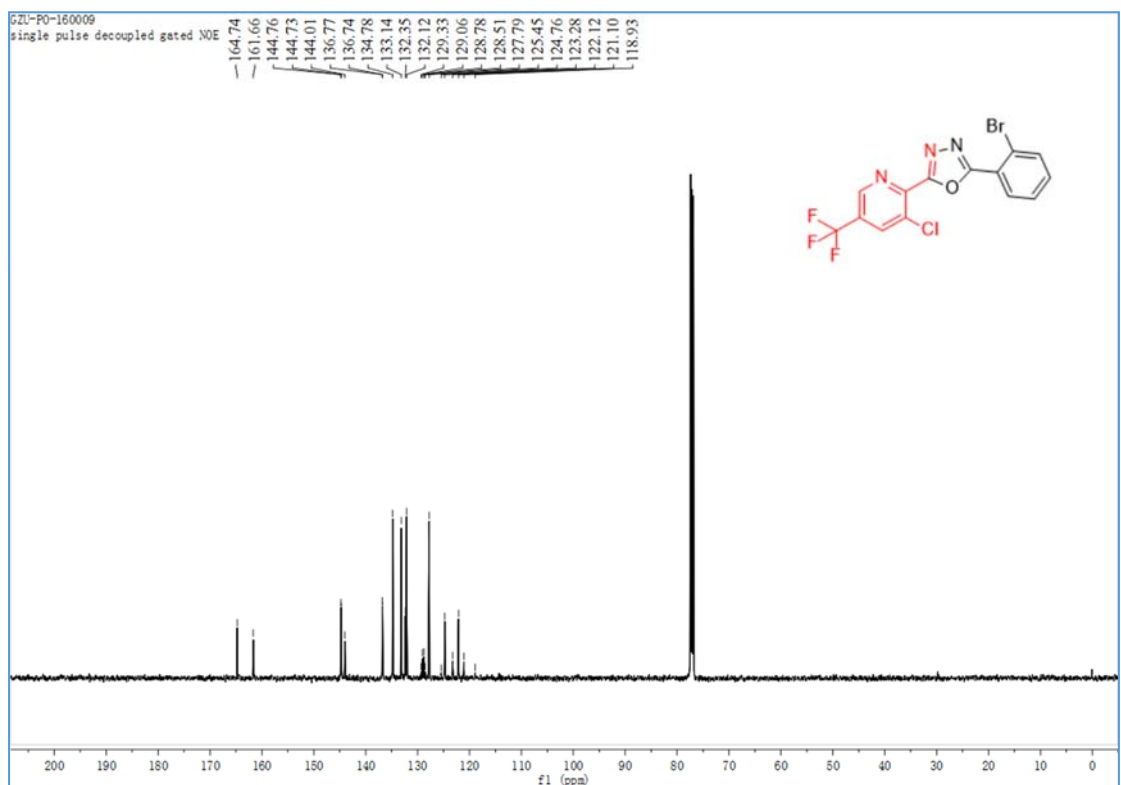


Fig. S31 ^{13}C NMR spectra of compound **E8**

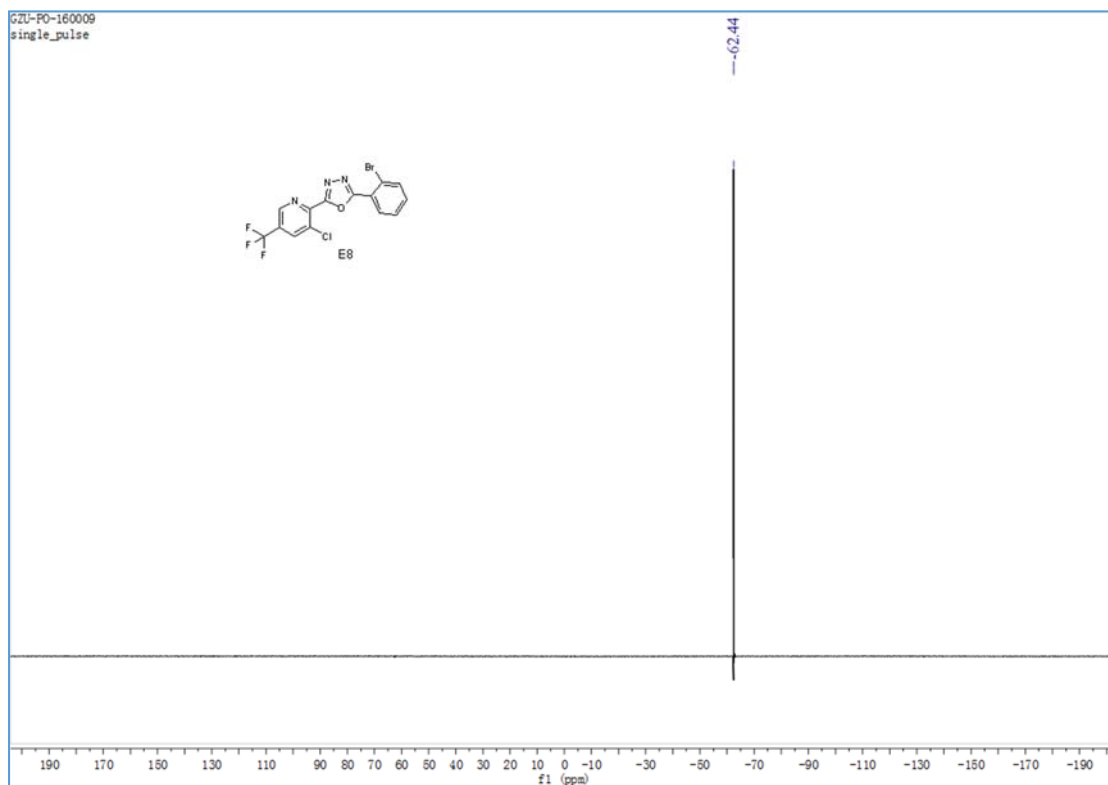


Fig. S32 ^{19}F NMR spectra of compound **E8**

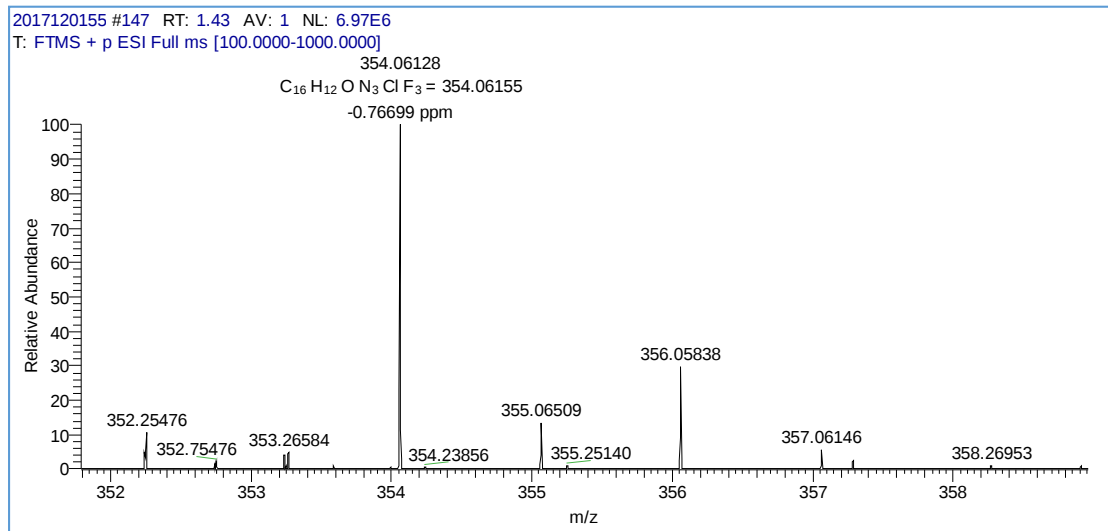


Fig. S33 HR-MS spectra of compound **E8**

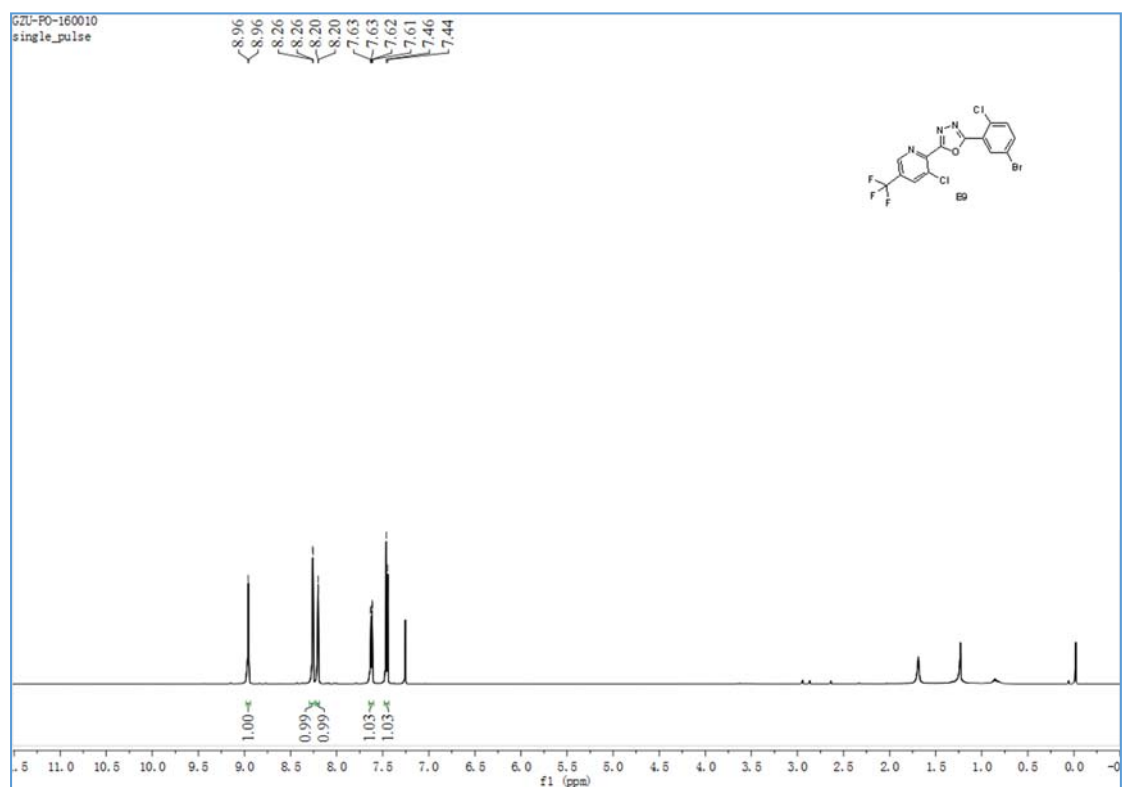


Fig. S34 ^1H NMR spectra of compound **E9**

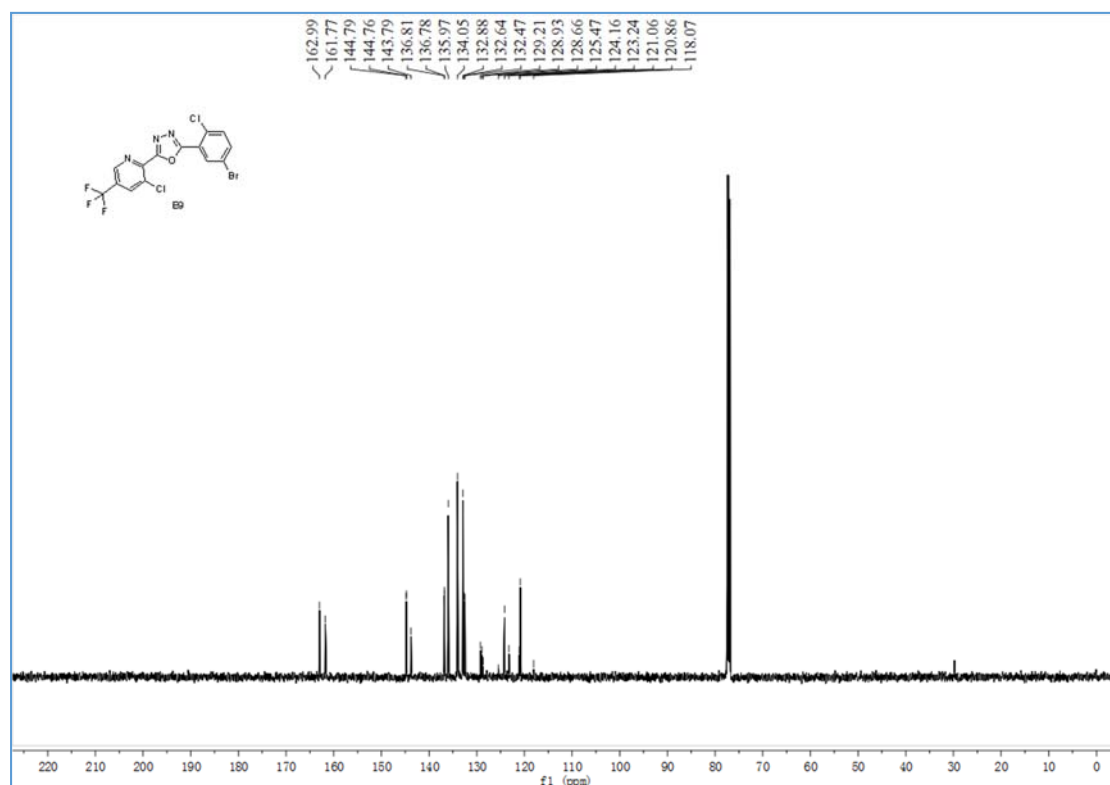


Fig. S35 ^{13}C NMR spectra of compound **E9**

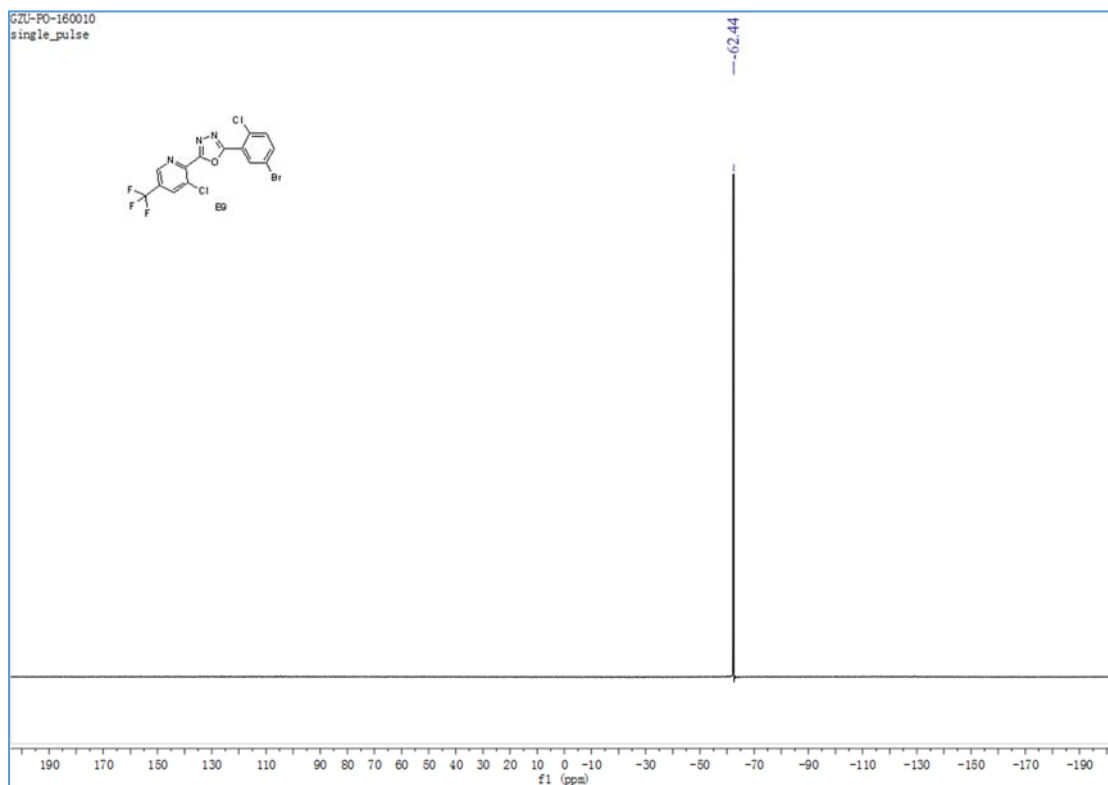


Fig. S36 ^{19}F NMR spectra of compound **E9**

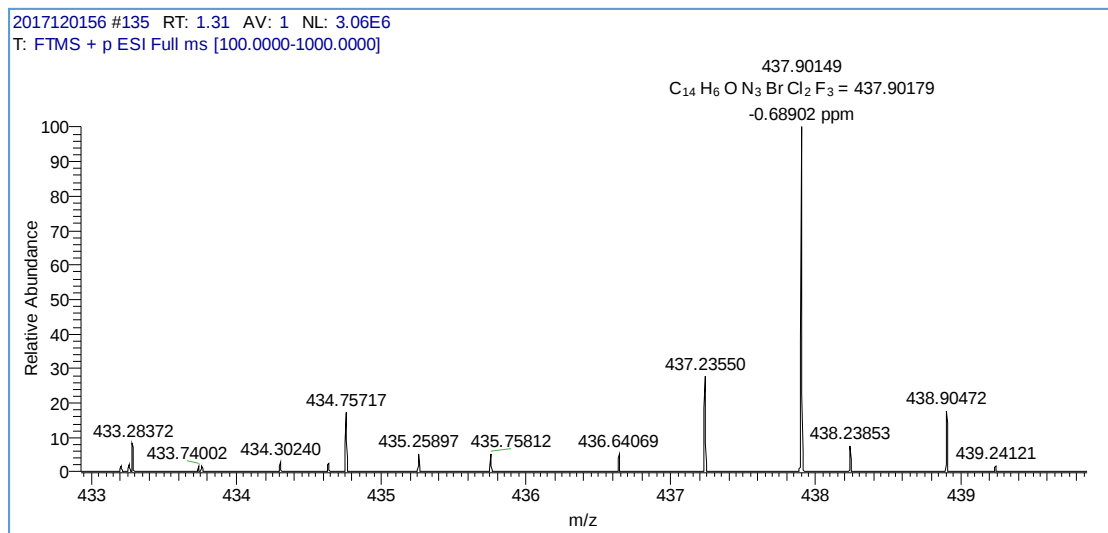


Fig. S37 HR-MS spectra of compound **E9**

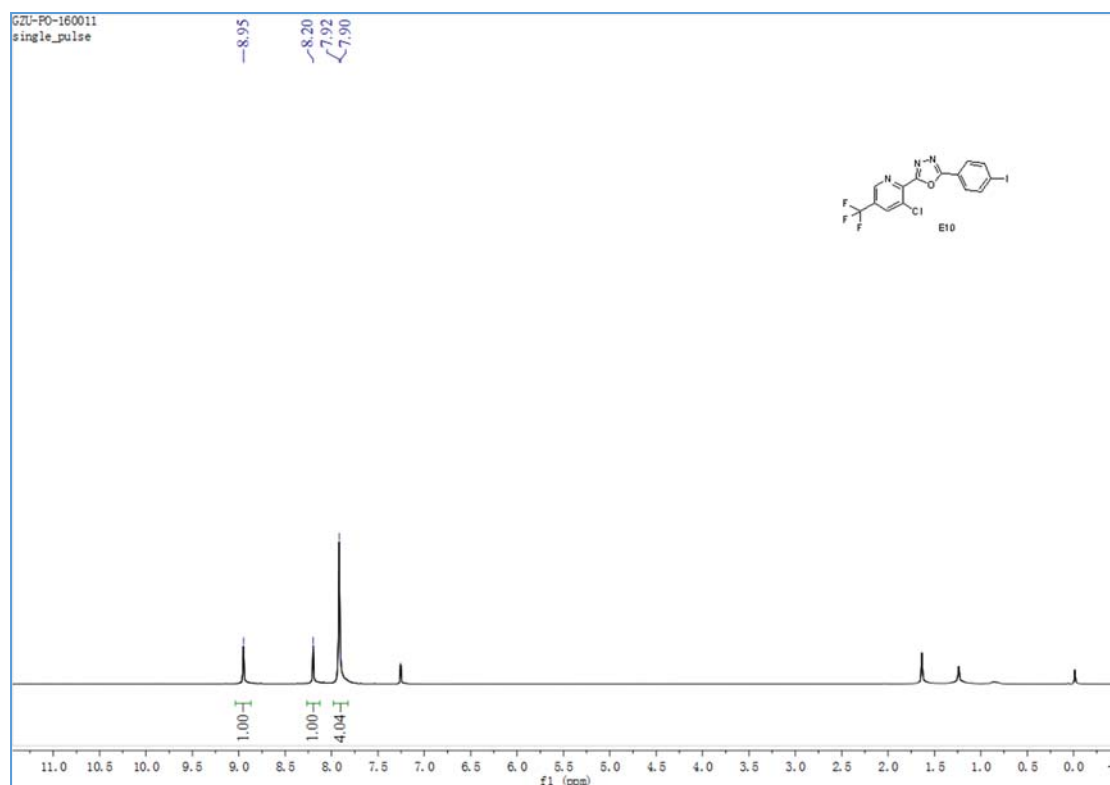


Fig. S38 ^1H NMR spectra of compound **E10**

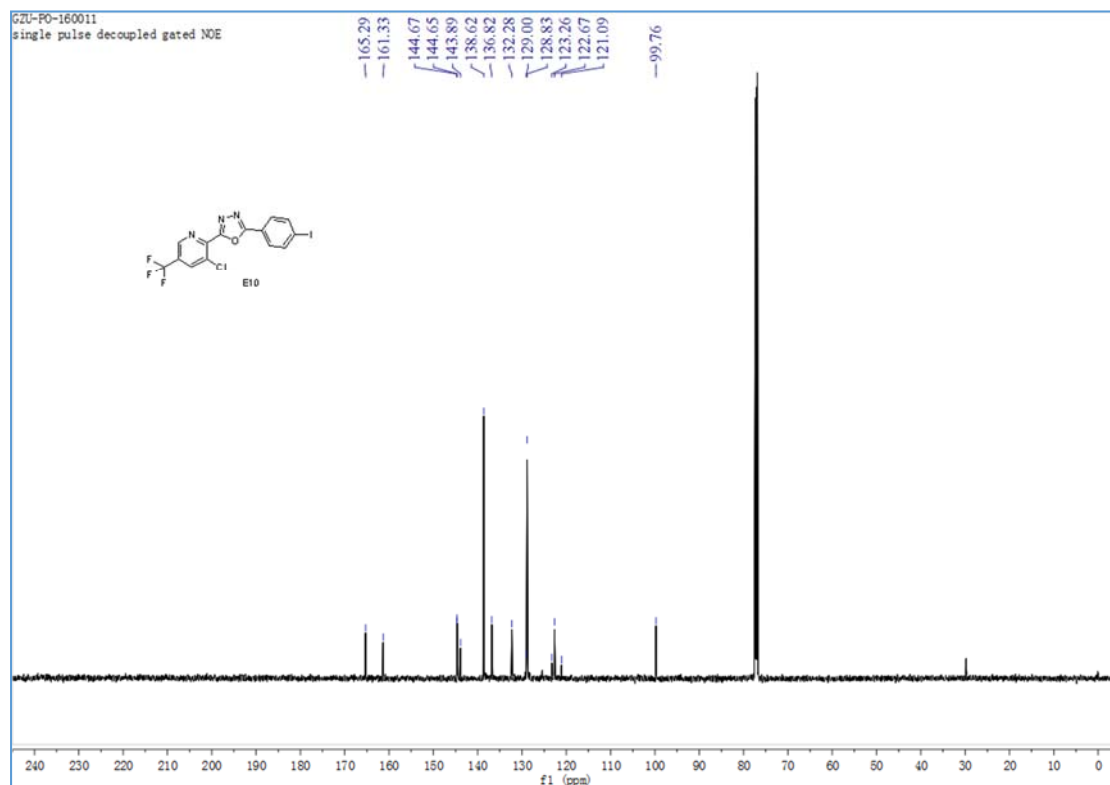


Fig. S39 ^{13}C NMR spectra of compound **E10**

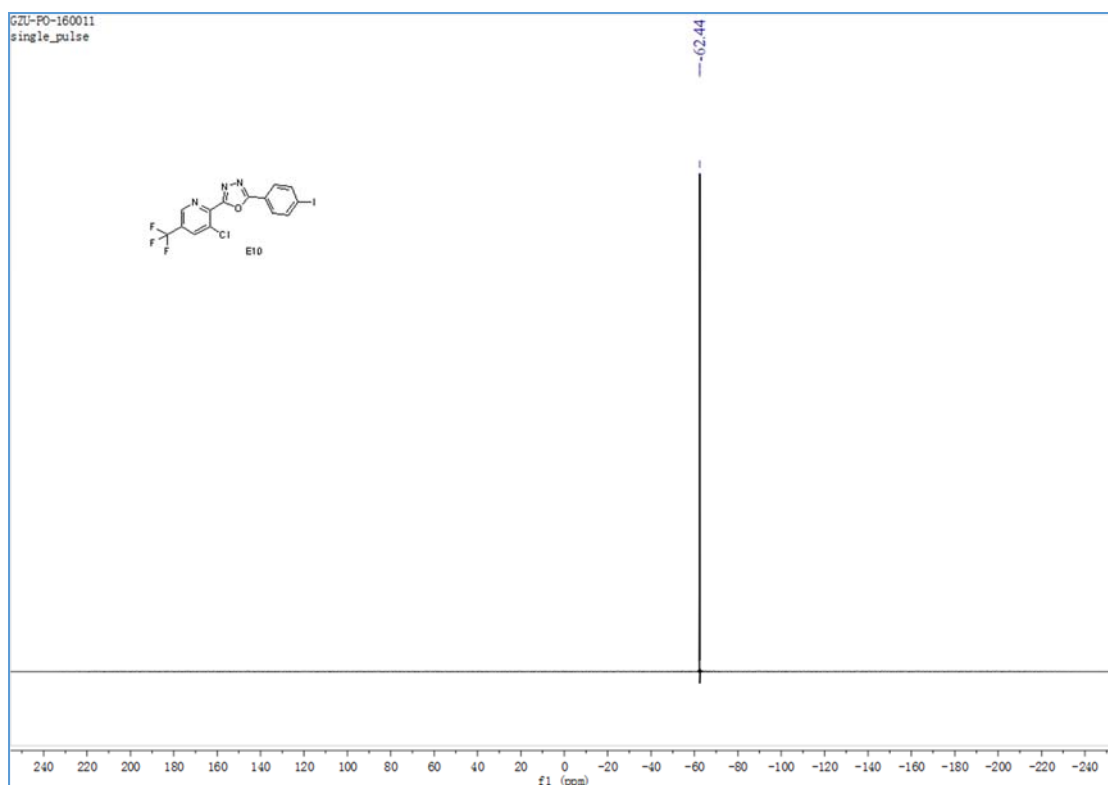


Fig. S40 ^{19}F NMR spectra of compound **E10**

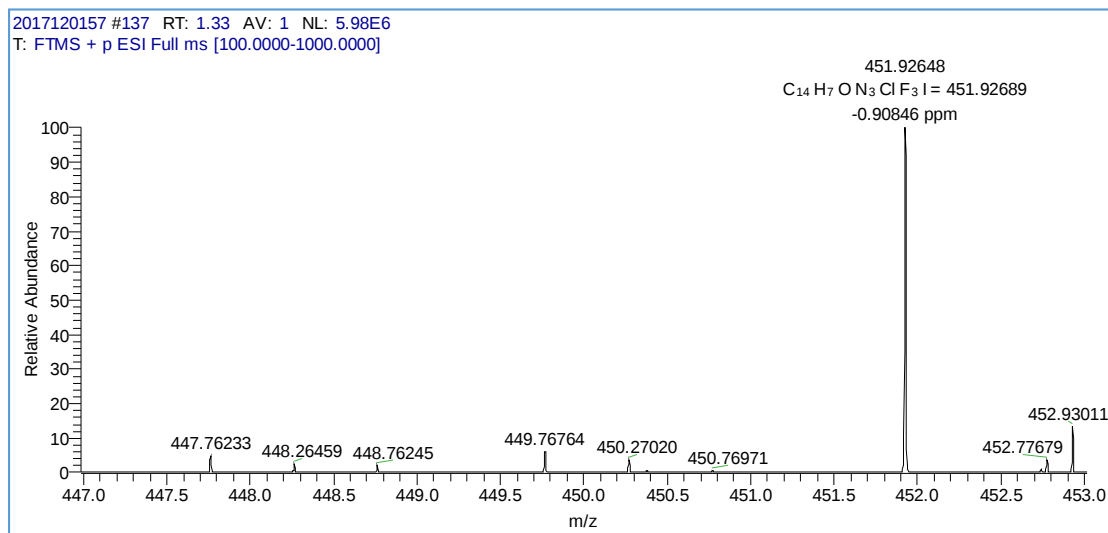


Fig. S41 HR-MS spectra of compound **E10**

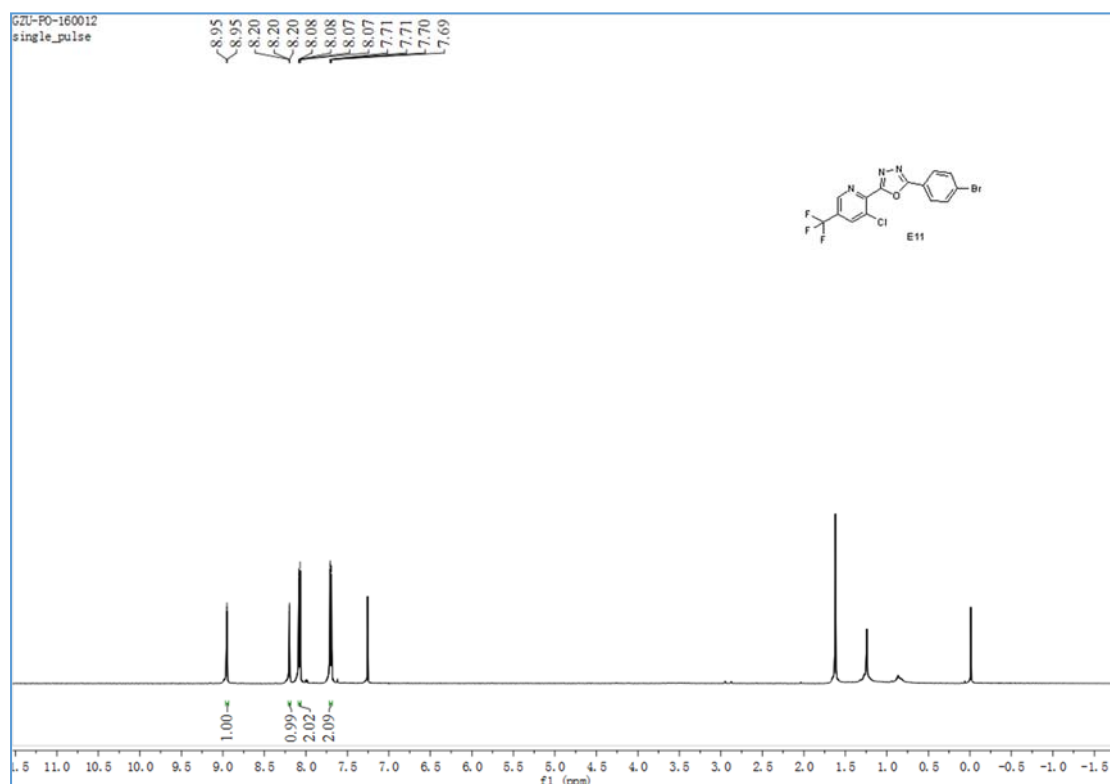


Fig. S42 ^1H NMR spectra of compound **E11**

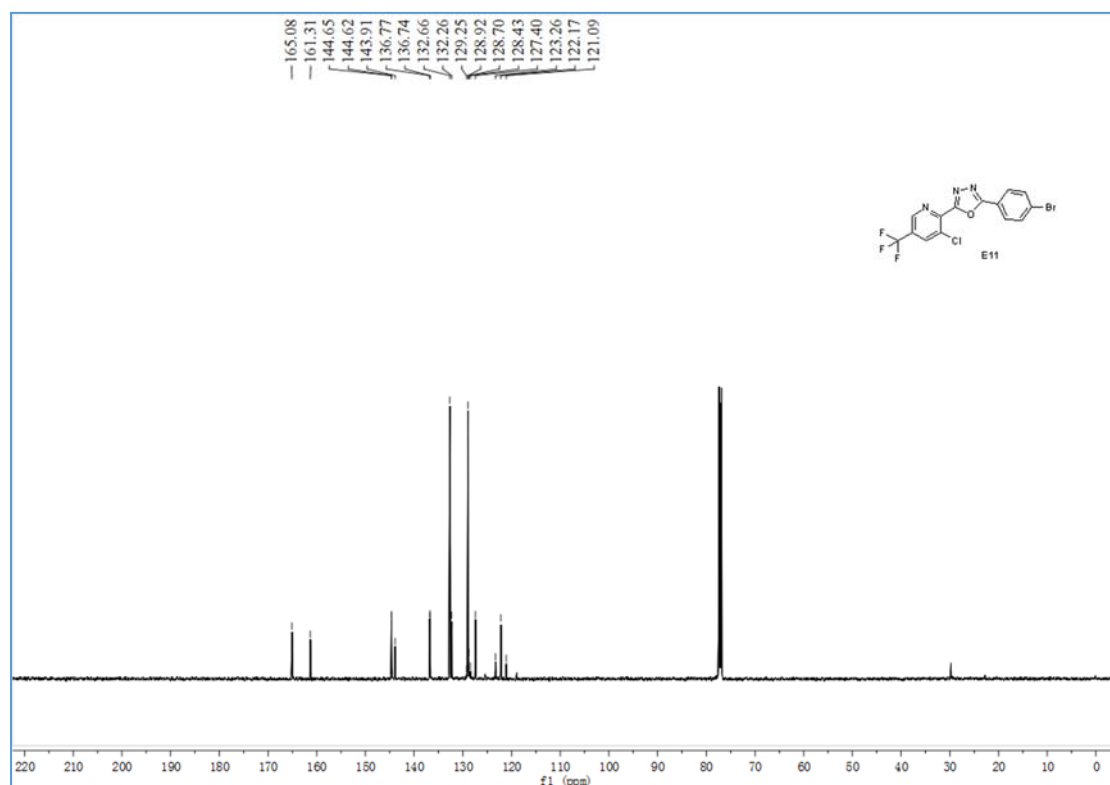


Fig. S43 ^{13}C NMR spectra of compound **E11**

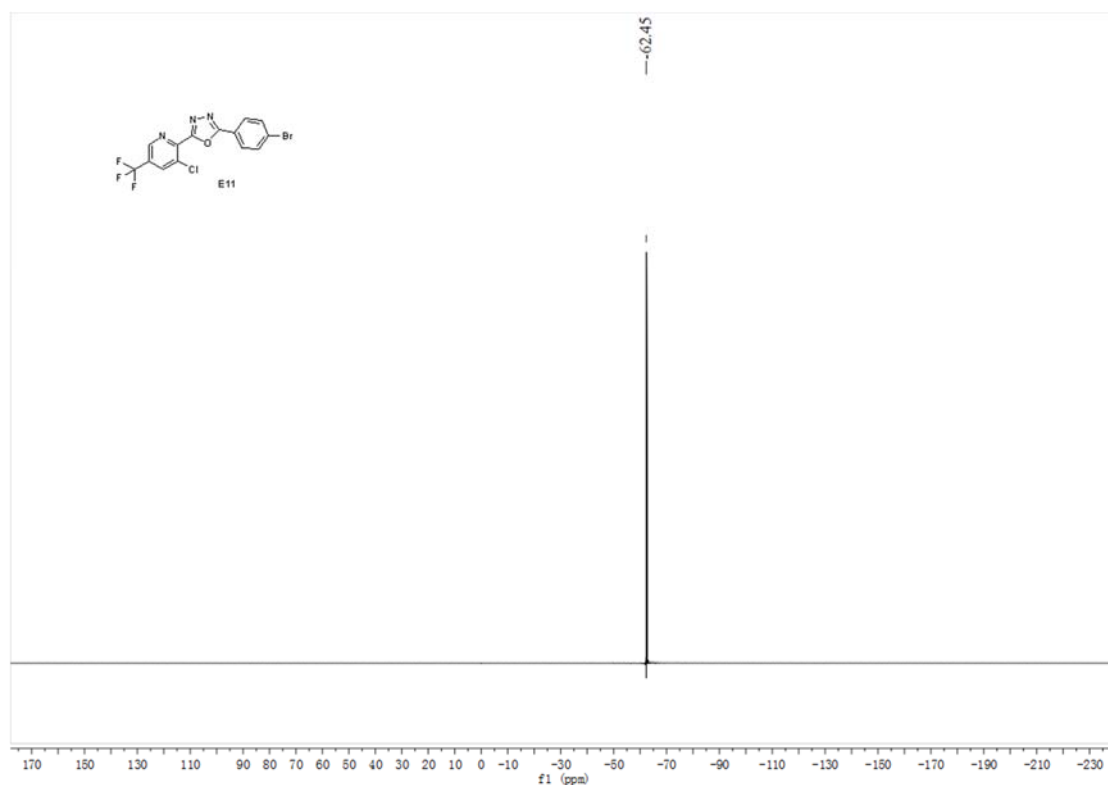


Fig. S44 ¹⁹F NMR spectra of compound **E11**

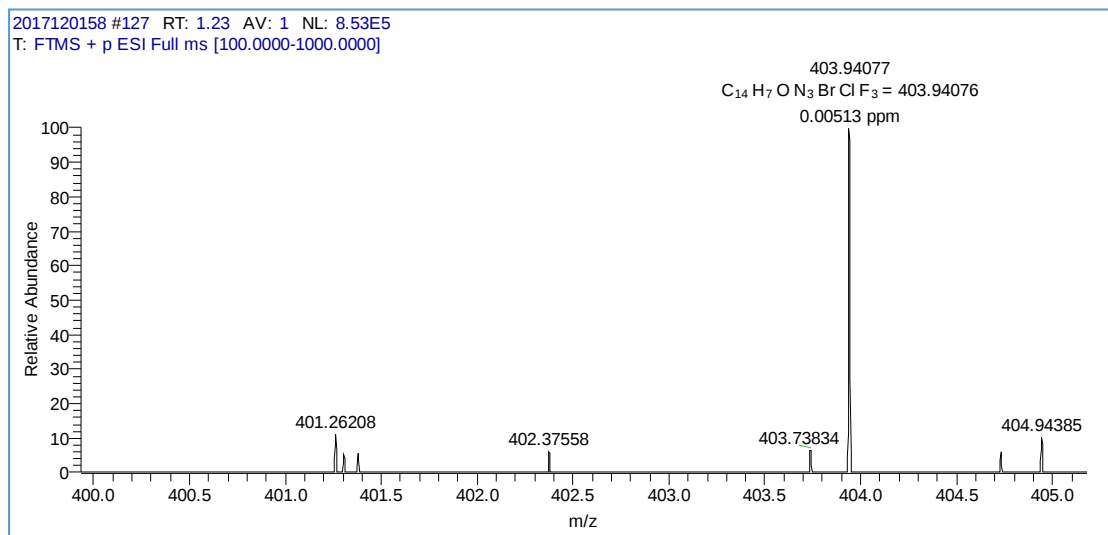


Fig. S45 HR-MS spectra of compound **E11**

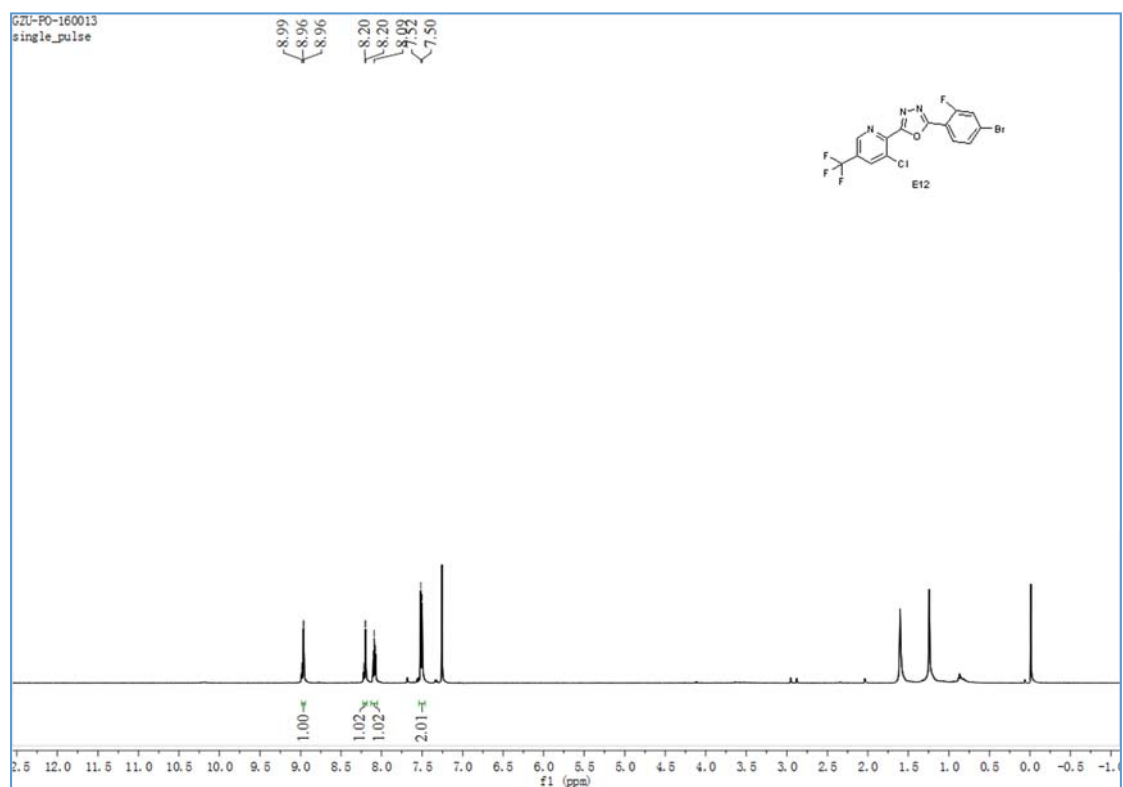


Fig. S46 ^1H NMR spectra of compound E12

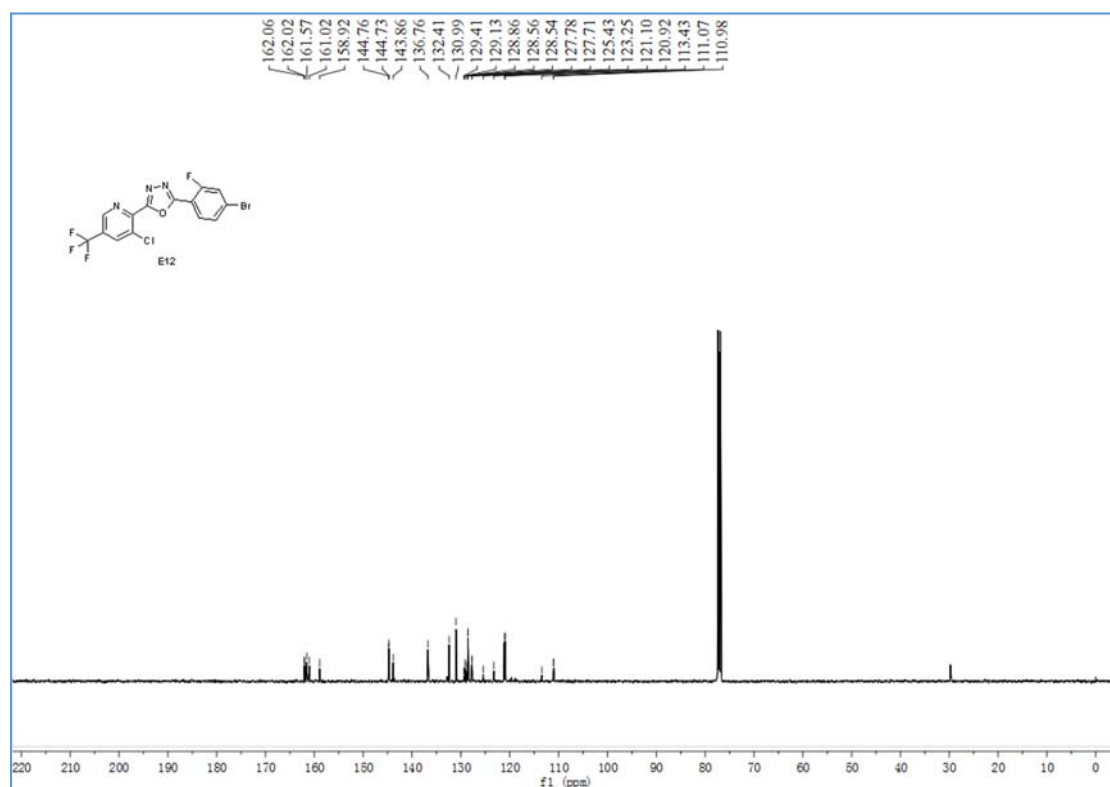


Fig. S47 ^{13}C NMR spectra of compound E12

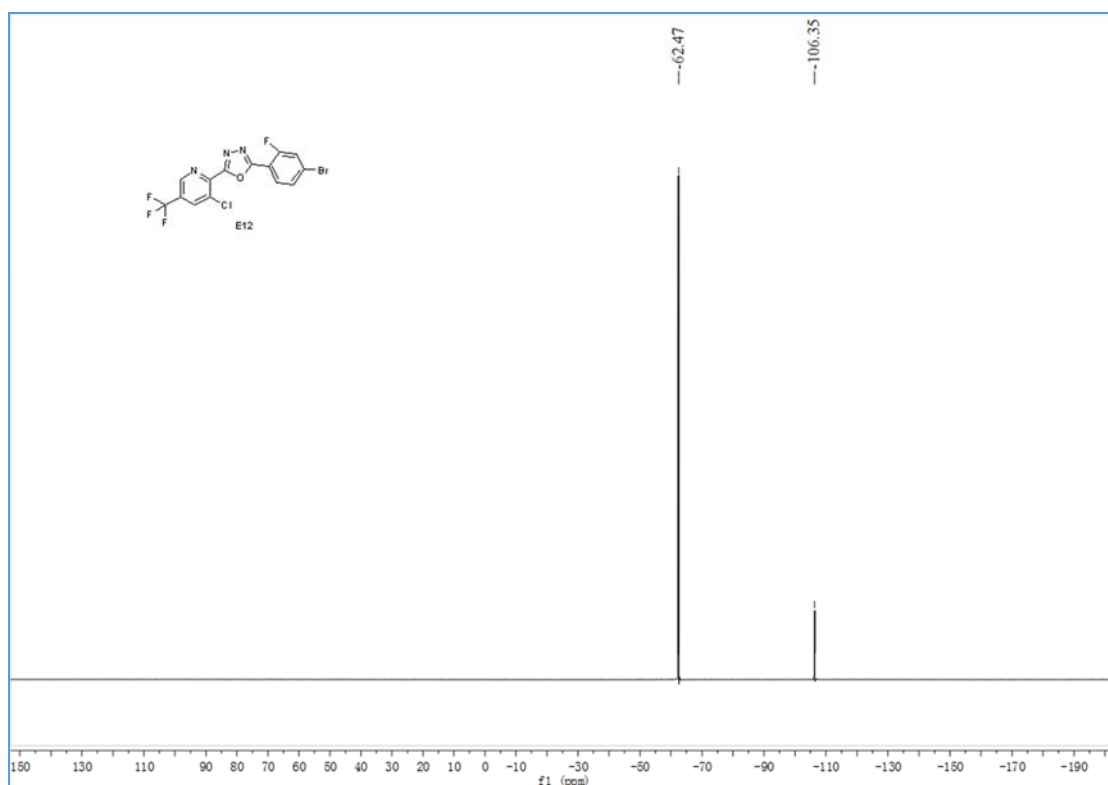


Fig. S48 ¹⁹F NMR spectra of compound E12

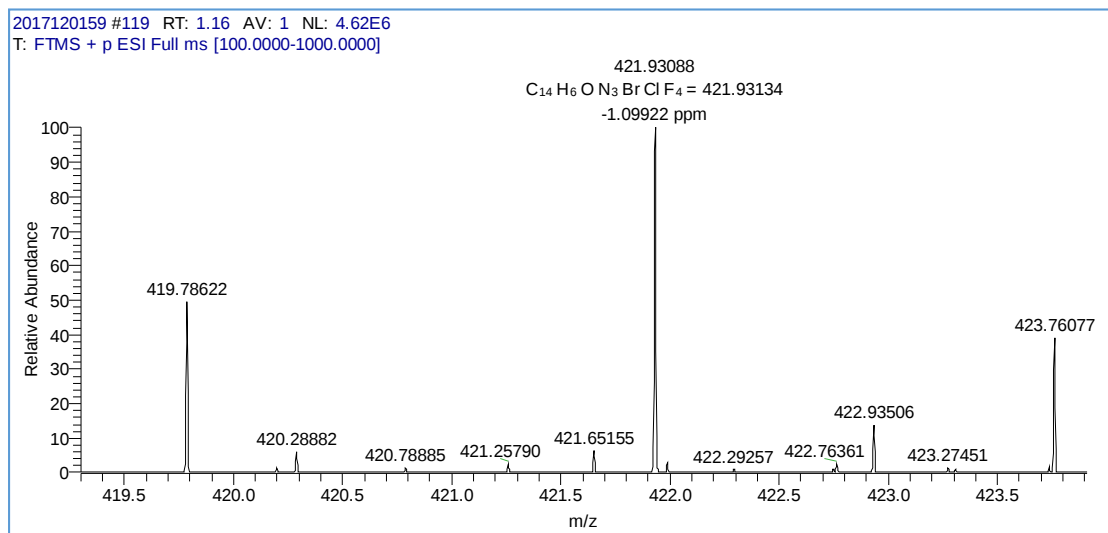


Fig. S49 HR-MS spectra of compound E12

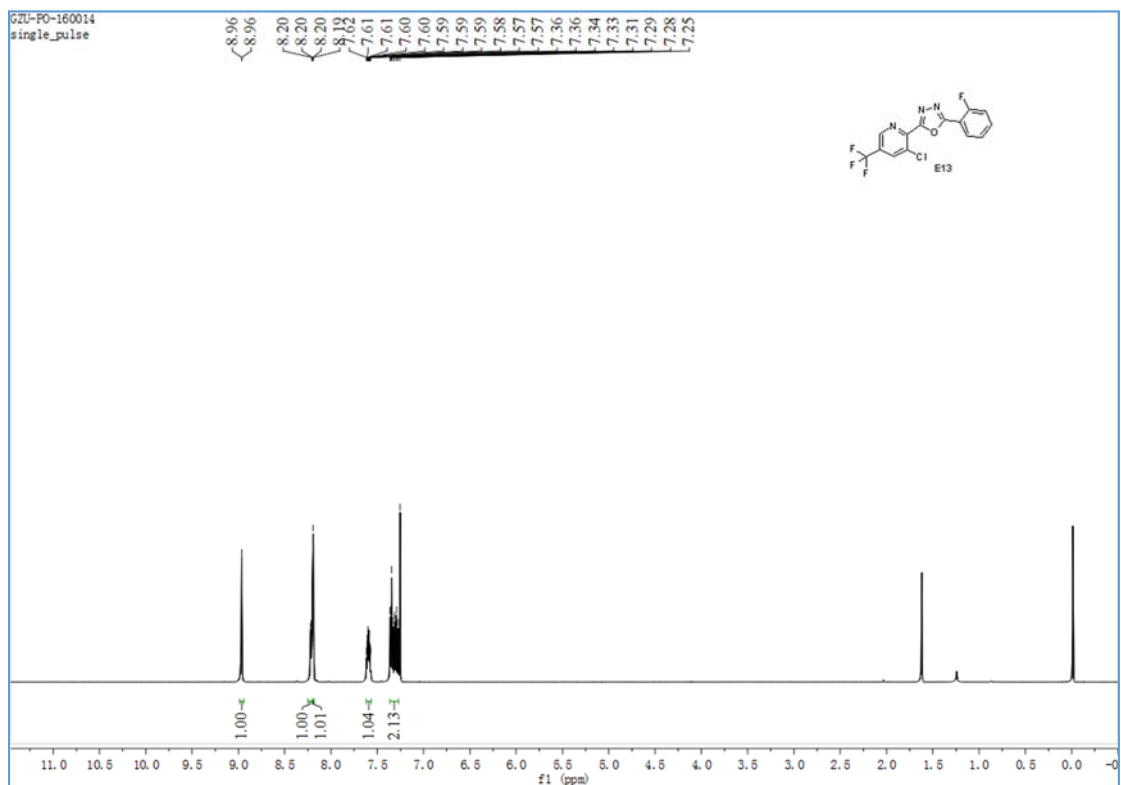


Fig. S50 ^1H NMR spectra of compound E13

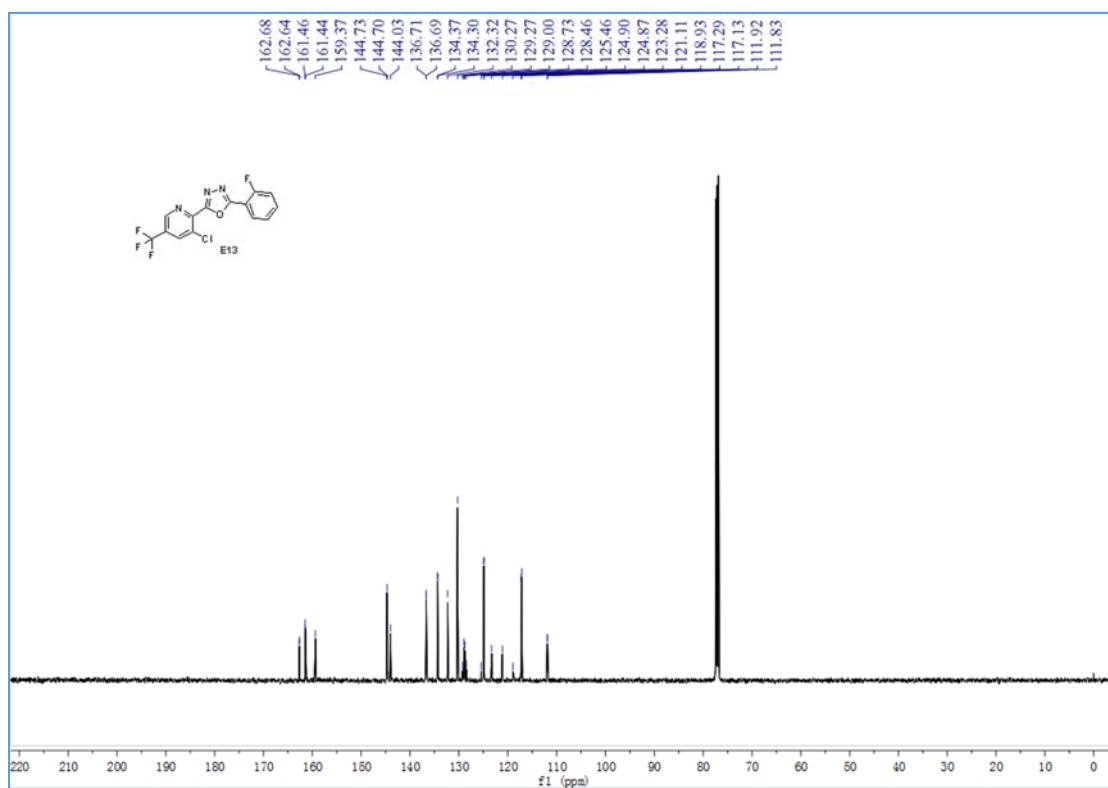


Fig. S51 ^{13}C NMR spectra of compound E13

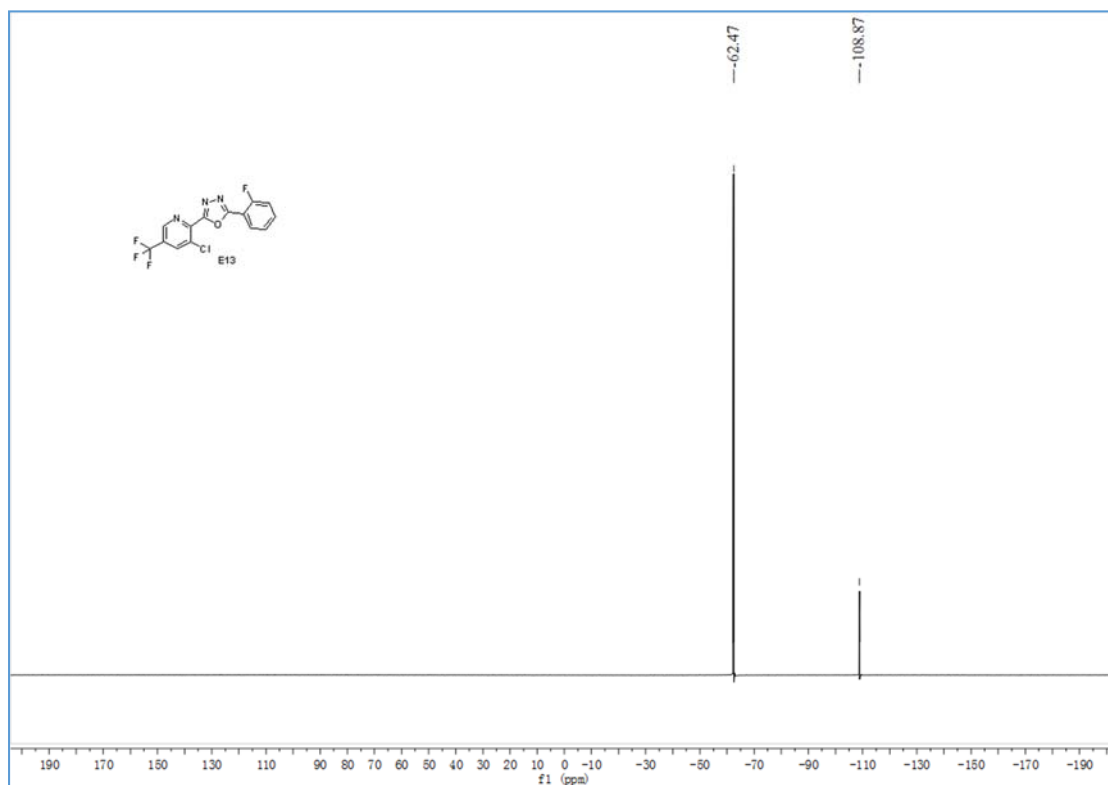


Fig. S52 ¹⁹F NMR spectra of compound **E13**

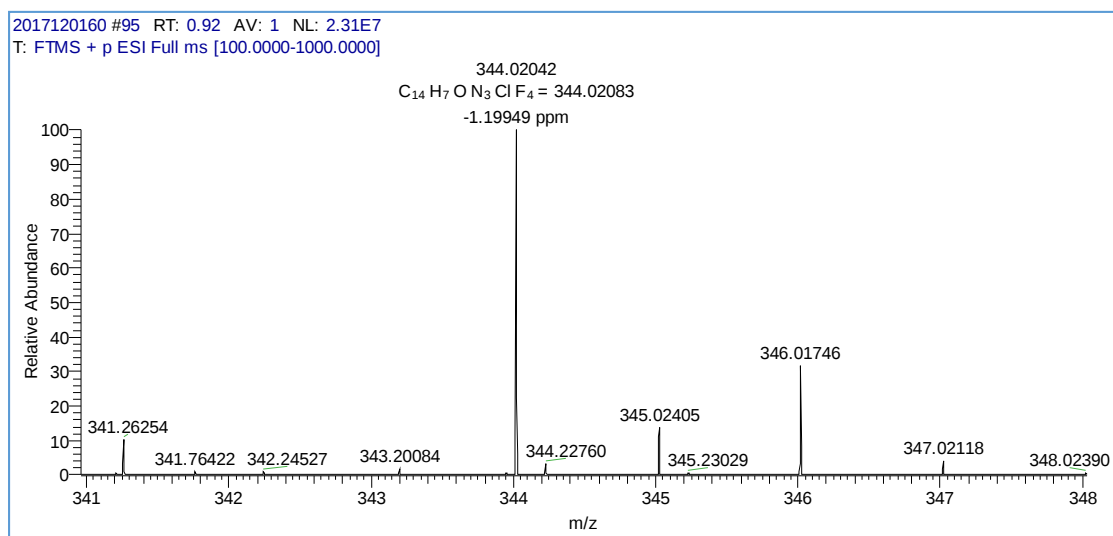


Fig. S53 HR-MS spectra of compound **E13**

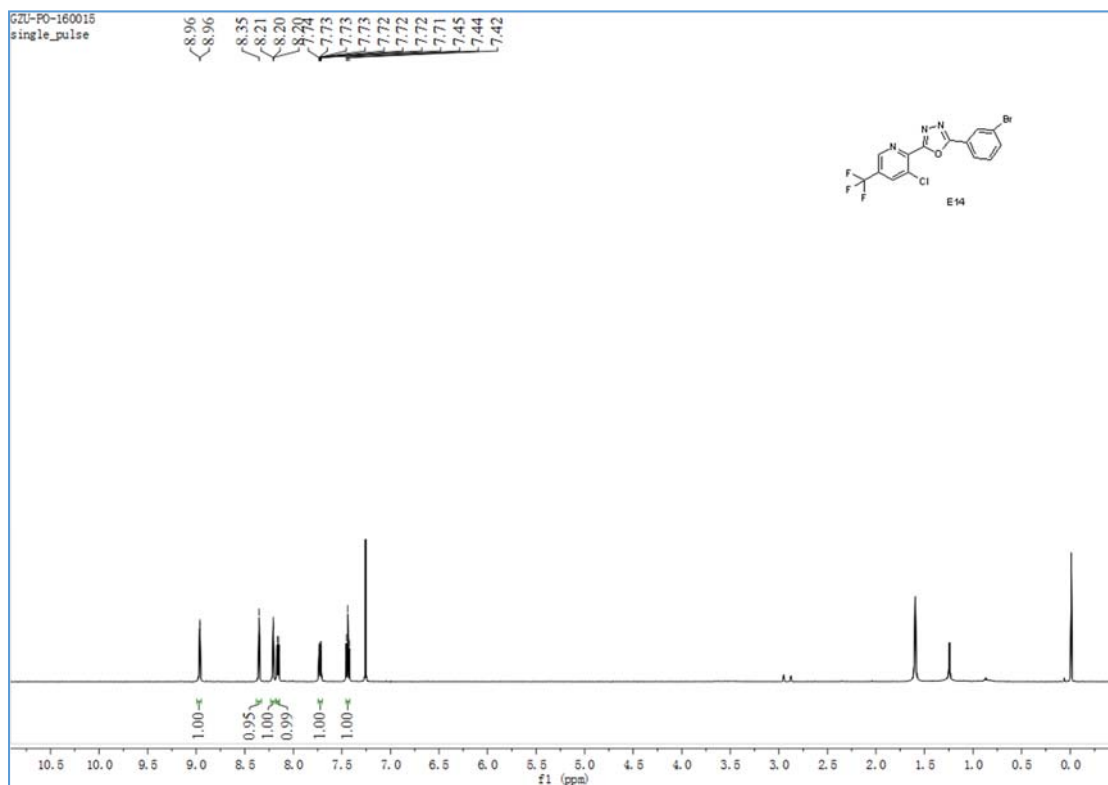


Fig. S54 ^1H NMR spectra of compound E14

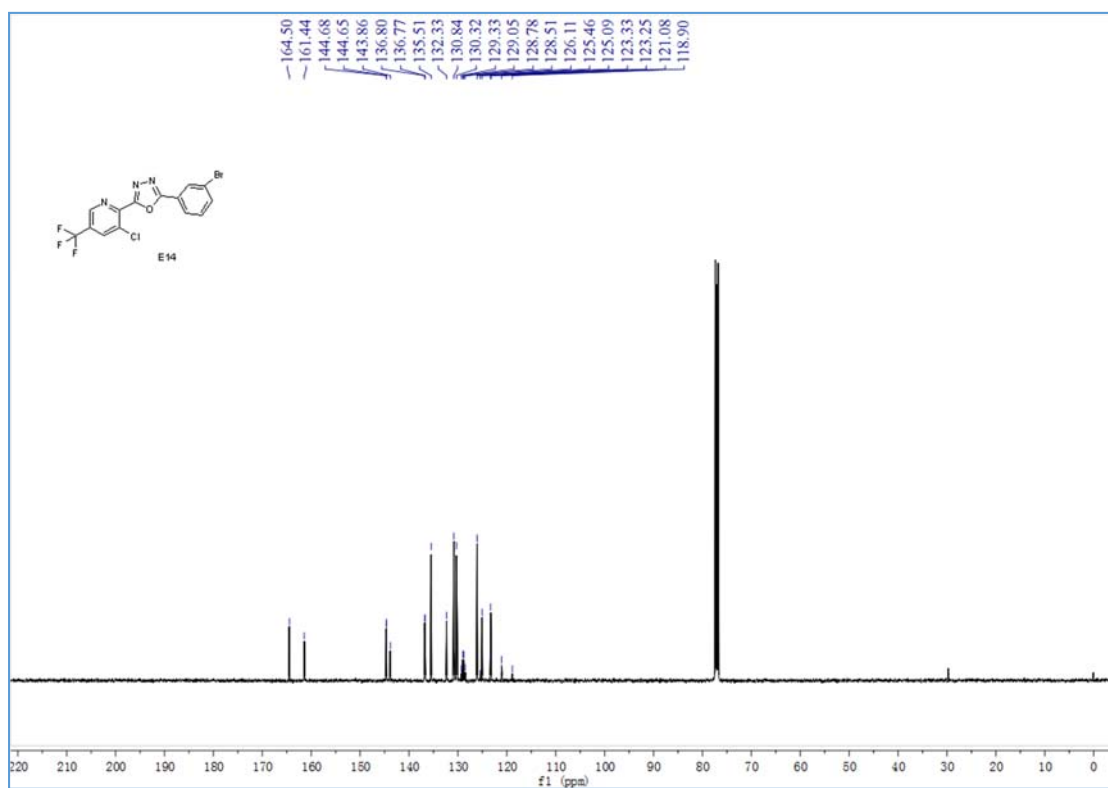


Fig. S55 ^{13}C NMR spectra of compound E14

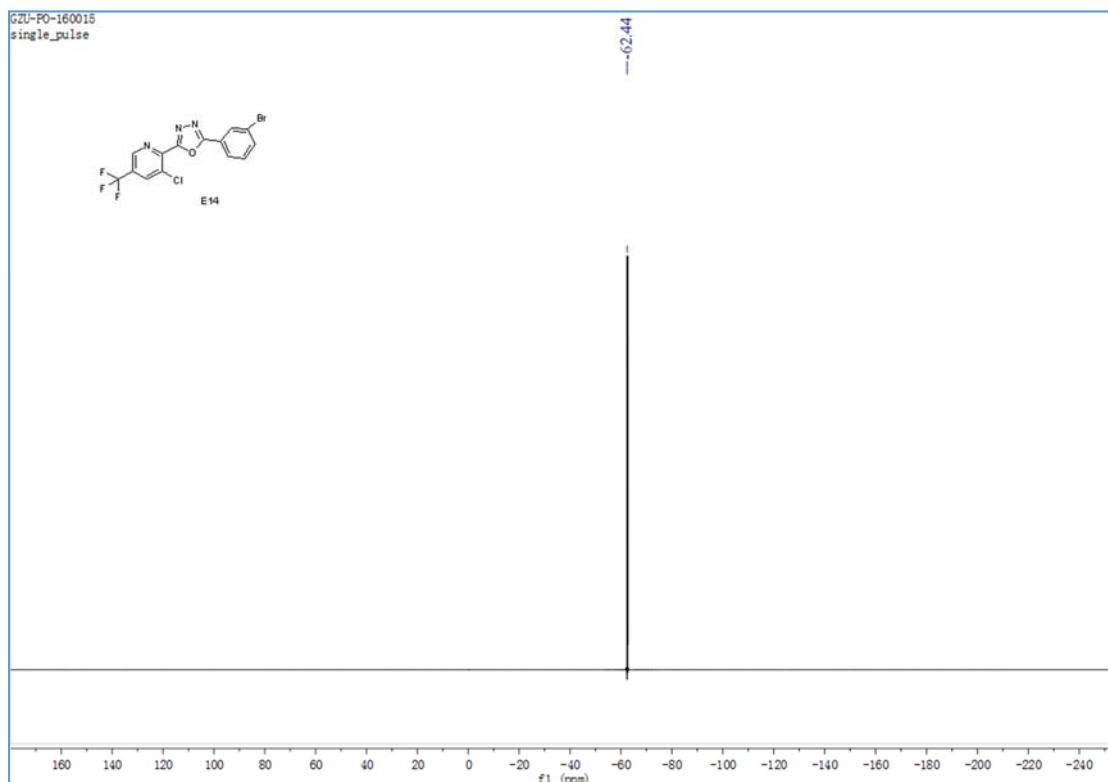


Fig. S56 ¹⁹F NMR spectra of compound **E14**

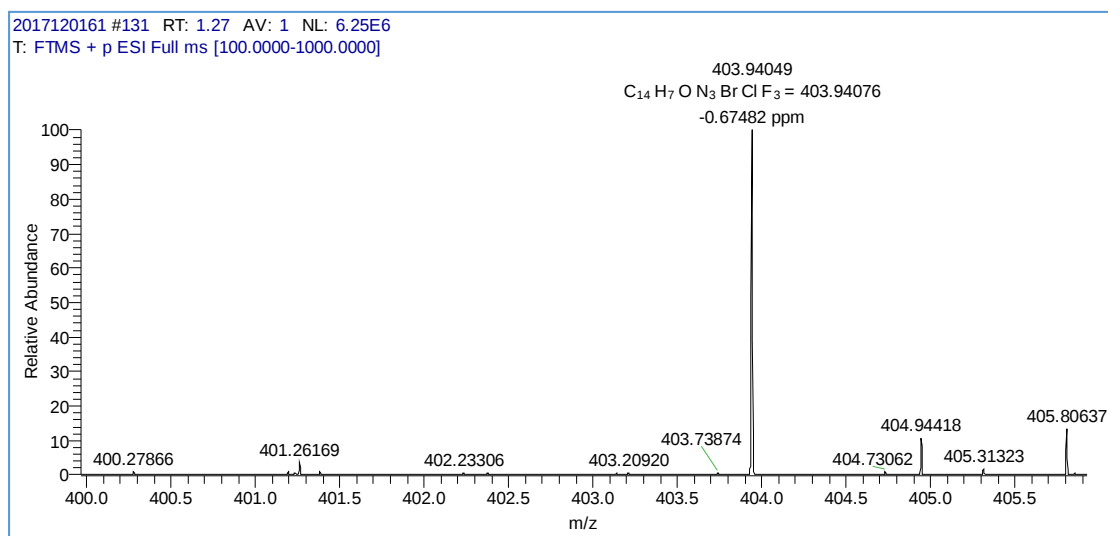


Fig. S57 HR-MS spectra of compound **E14**

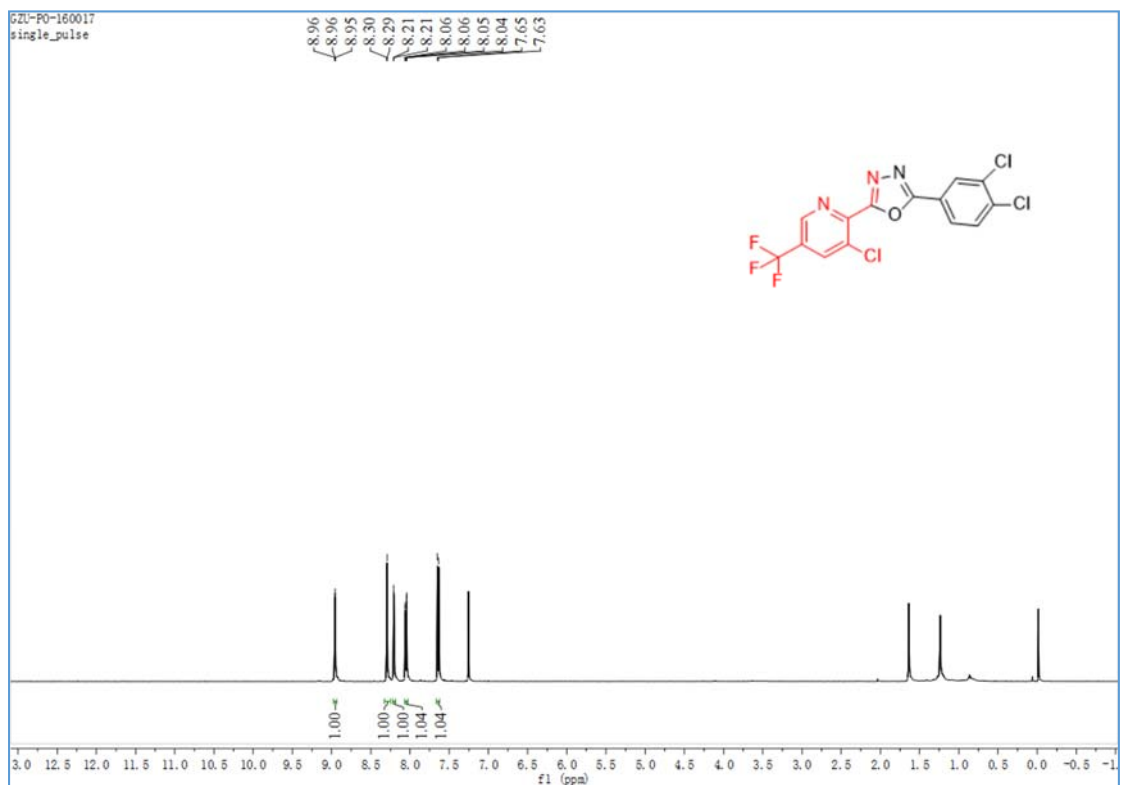


Fig. S58 ^1H NMR spectra of compound E15

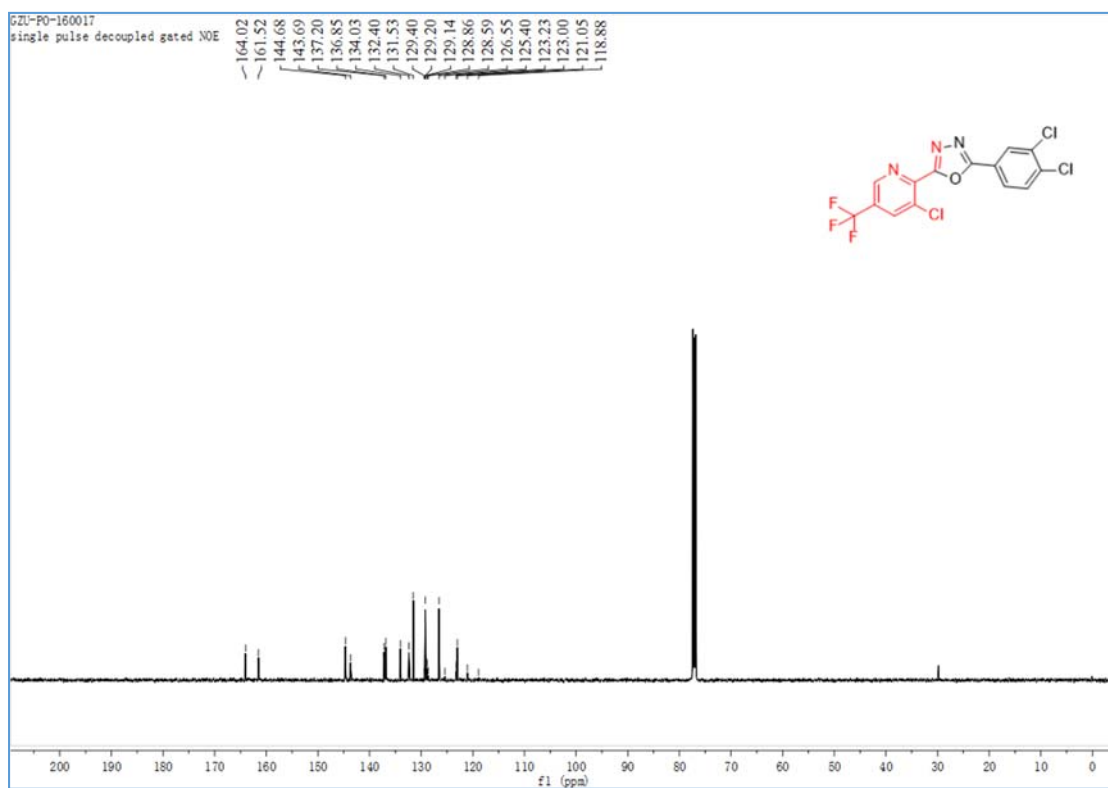


Fig. S59 ^{13}C NMR spectra of compound E15

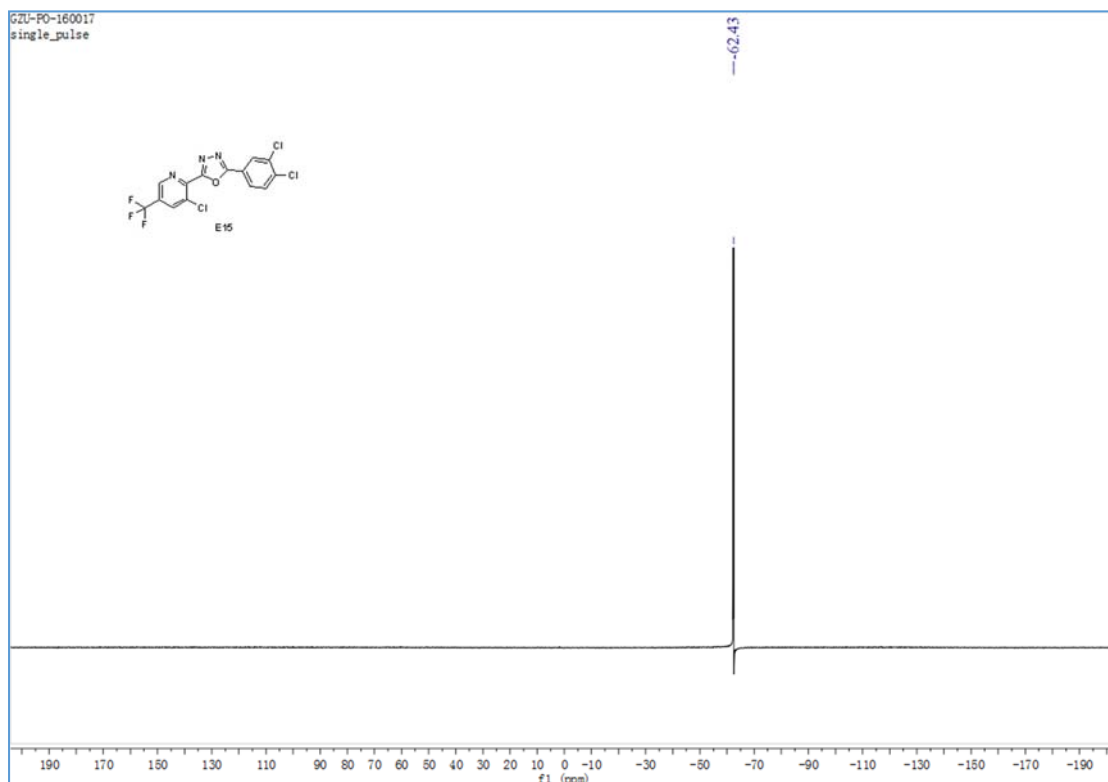


Fig. S60 ^{19}F NMR spectra of compound **E15**

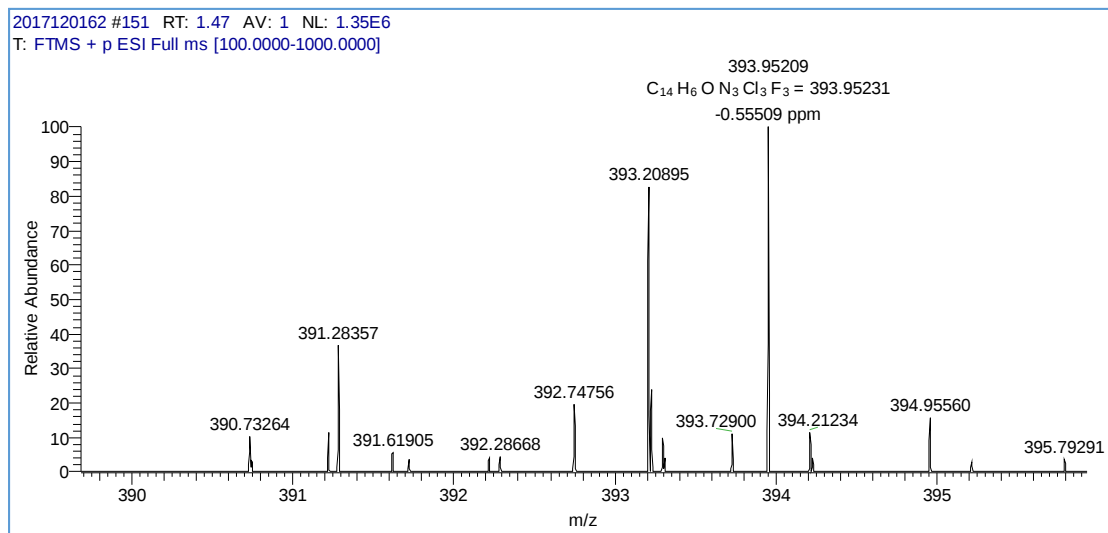


Fig. S61 HR-MS spectra of compound **E15**

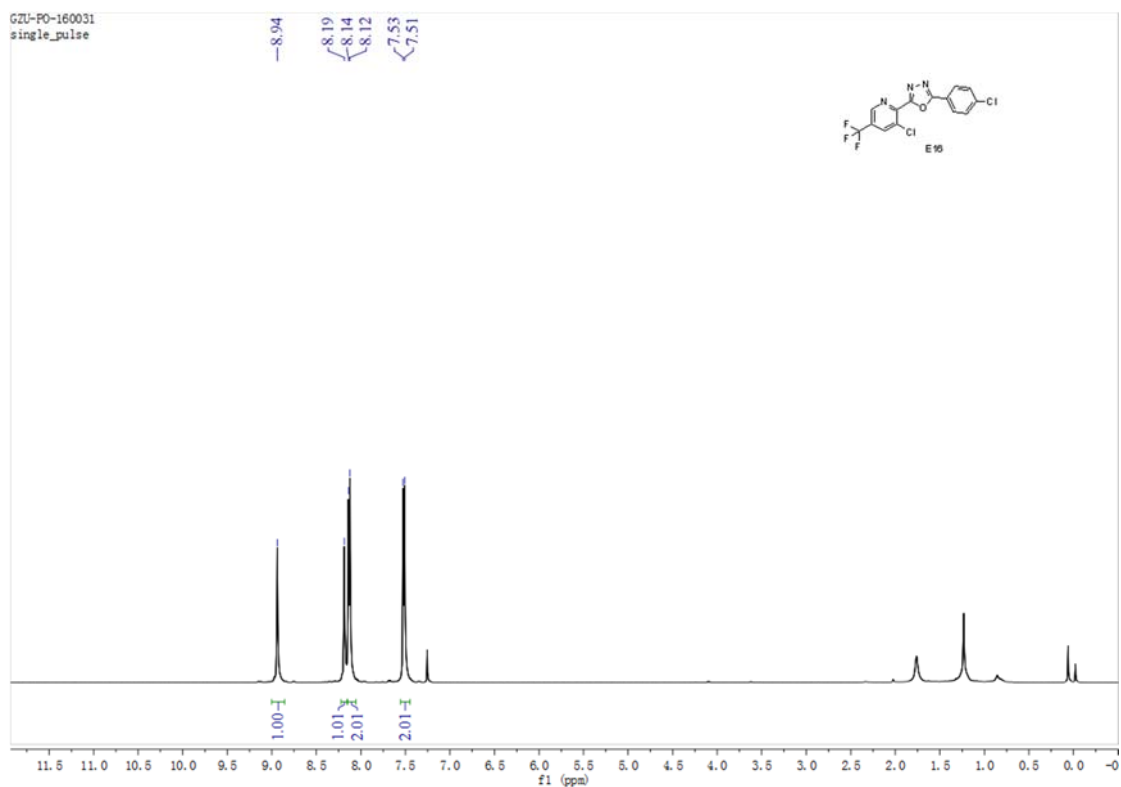


Fig. S62 ^1H NMR spectra of compound E16

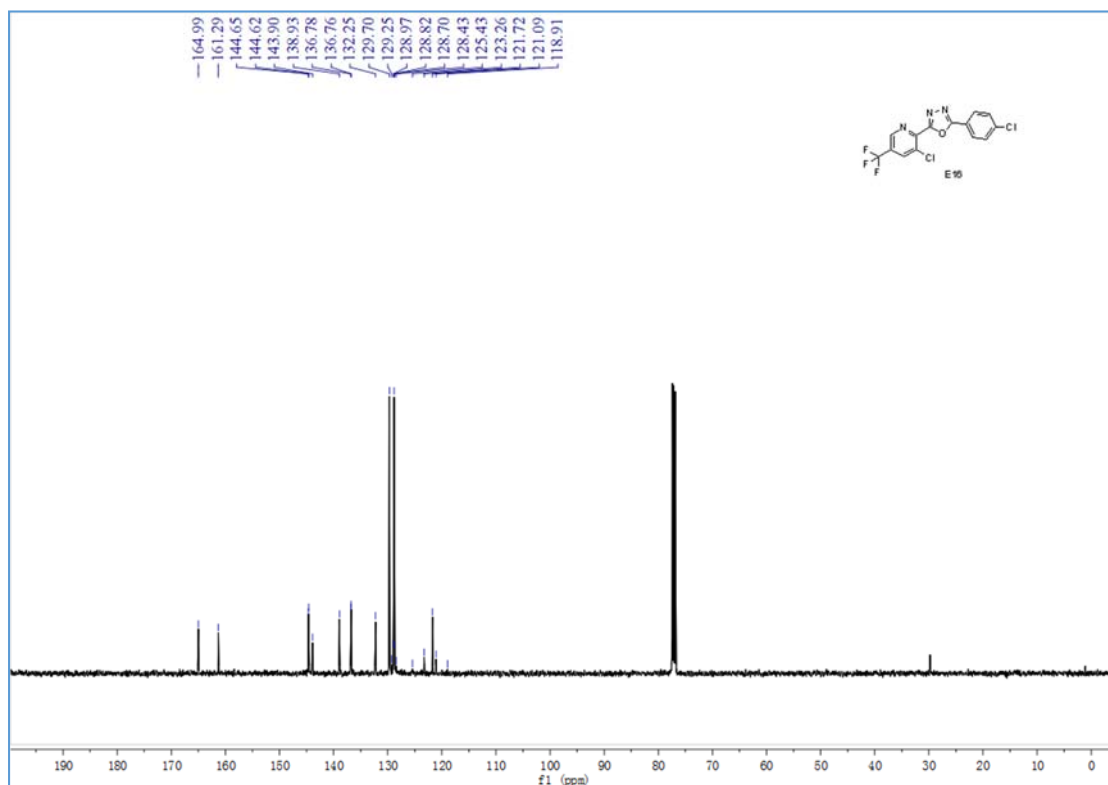


Fig. S63 ^{13}C NMR spectra of compound E16

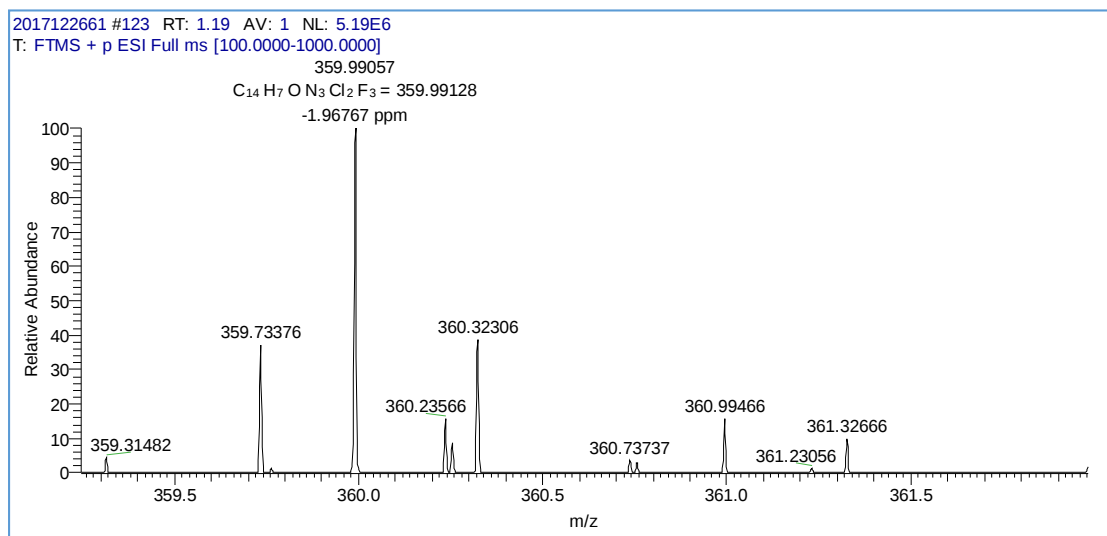


Fig. S64 HR-MS spectra of compound **E16**

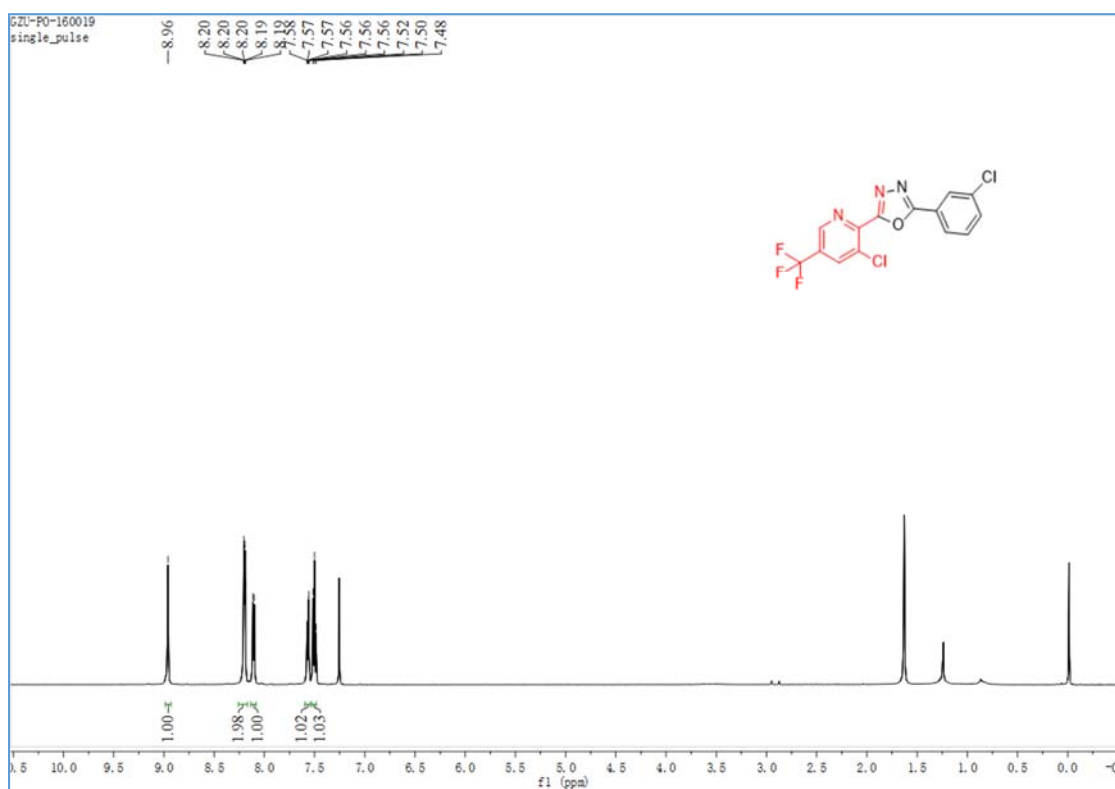


Fig. S65 ¹H NMR spectra of compound **E17**

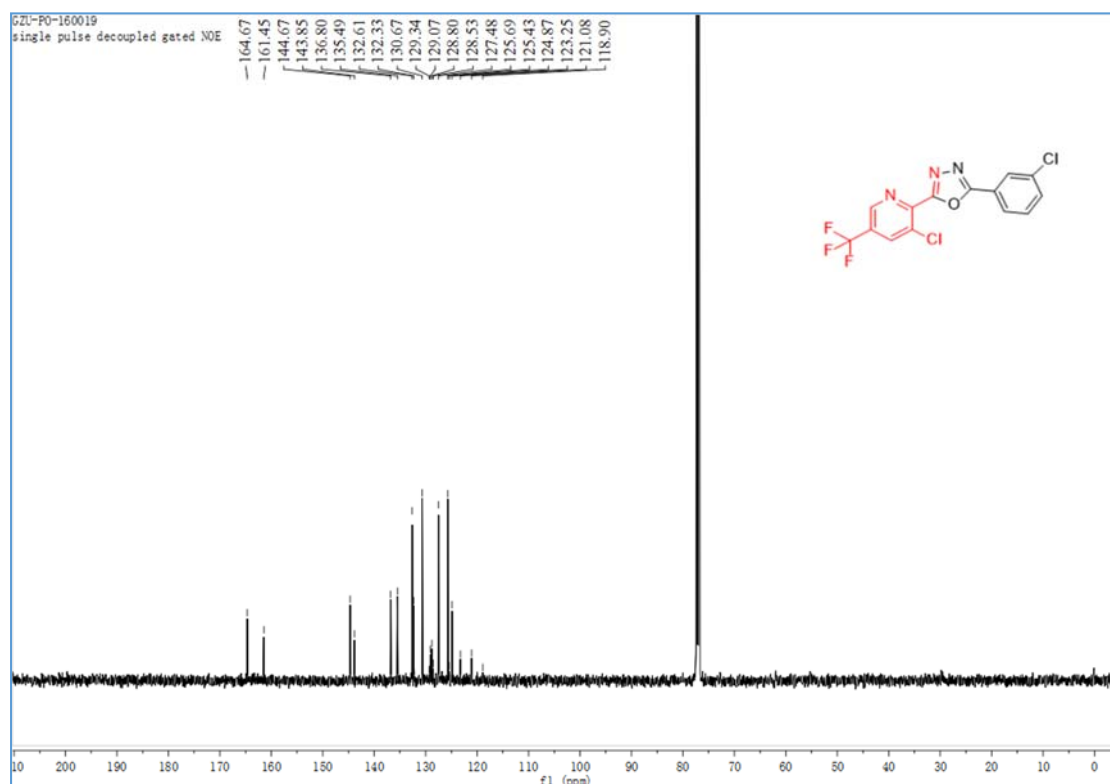


Fig. S66 ^{13}C NMR spectra of compound E17

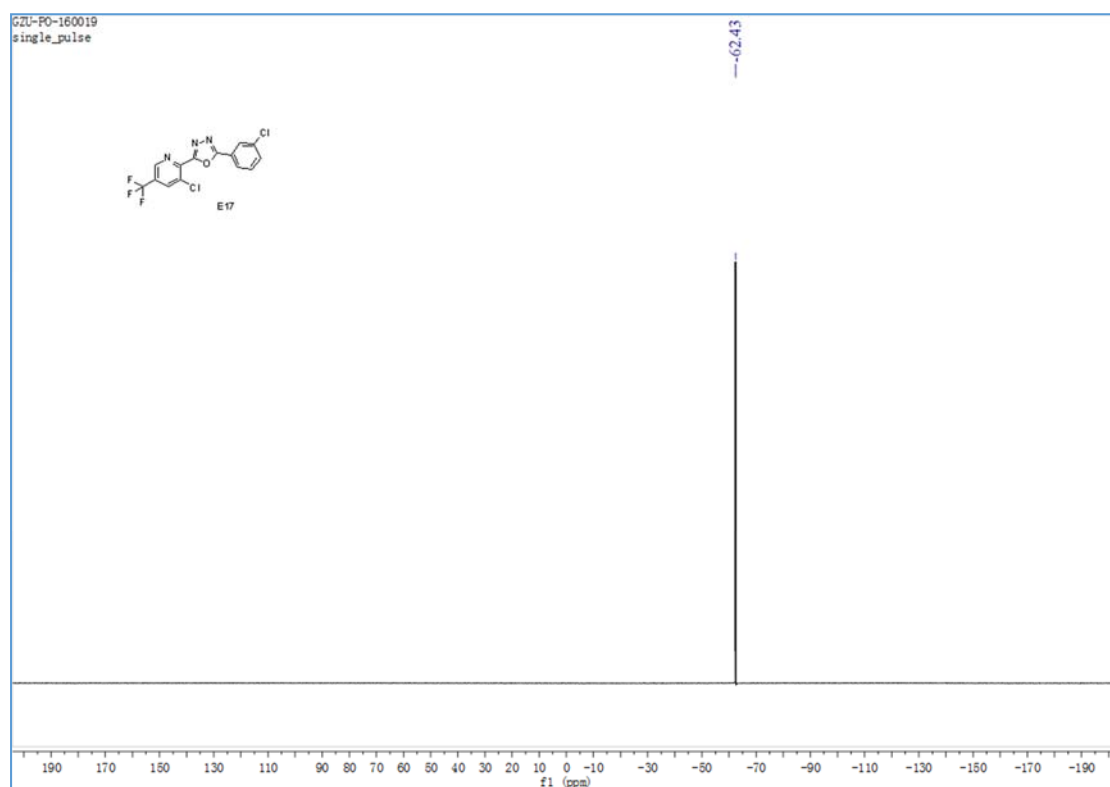


Fig. S67 ^{19}F NMR spectra of compound E17

2017120164 #123 RT: 1.19 AV: 1 NL: 6.66E6
T: FTMS + p ESI Full ms [100.0000-1000.0000]

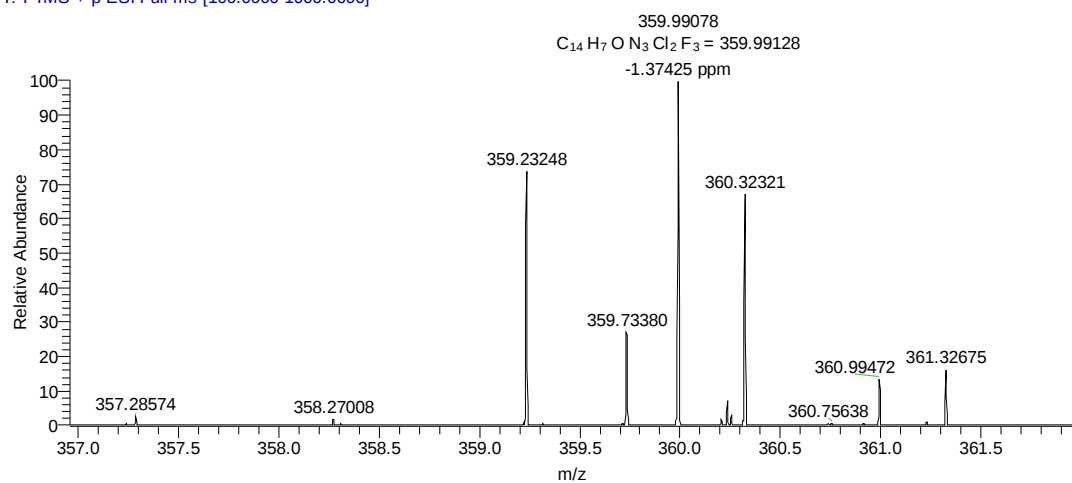


Fig. S68 HR-MS spectra of compound E17

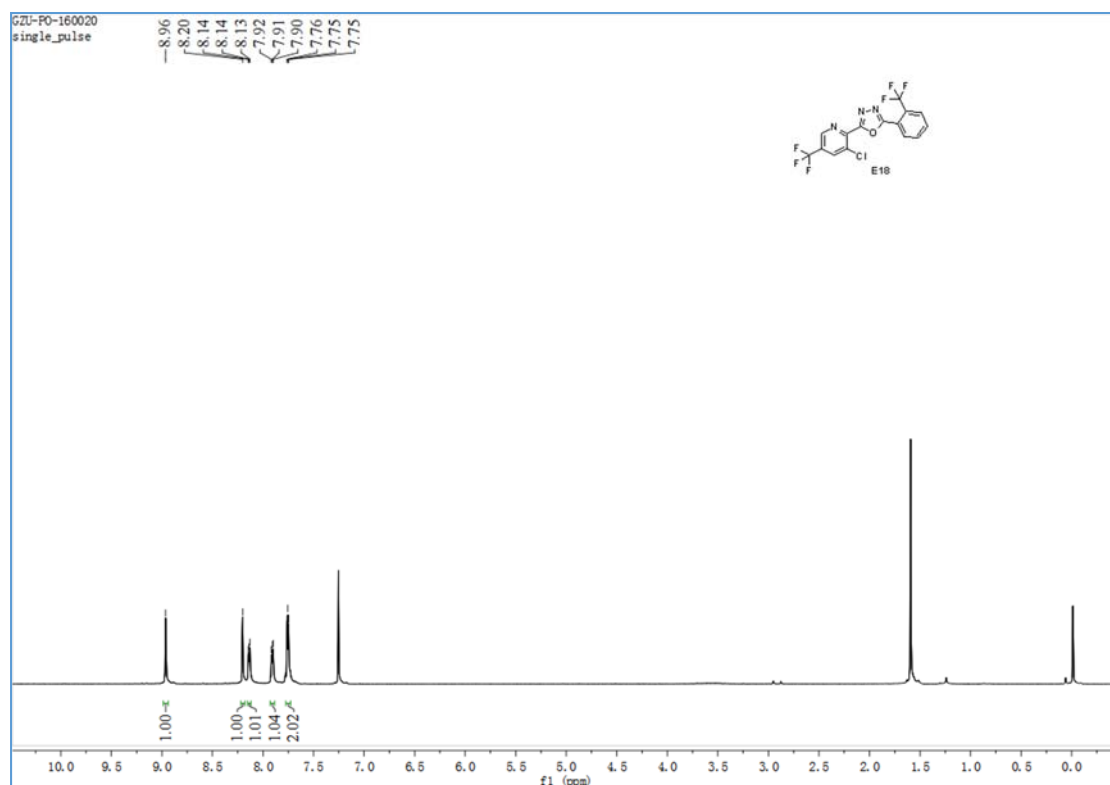


Fig. S69 ^1H NMR spectra of compound E18

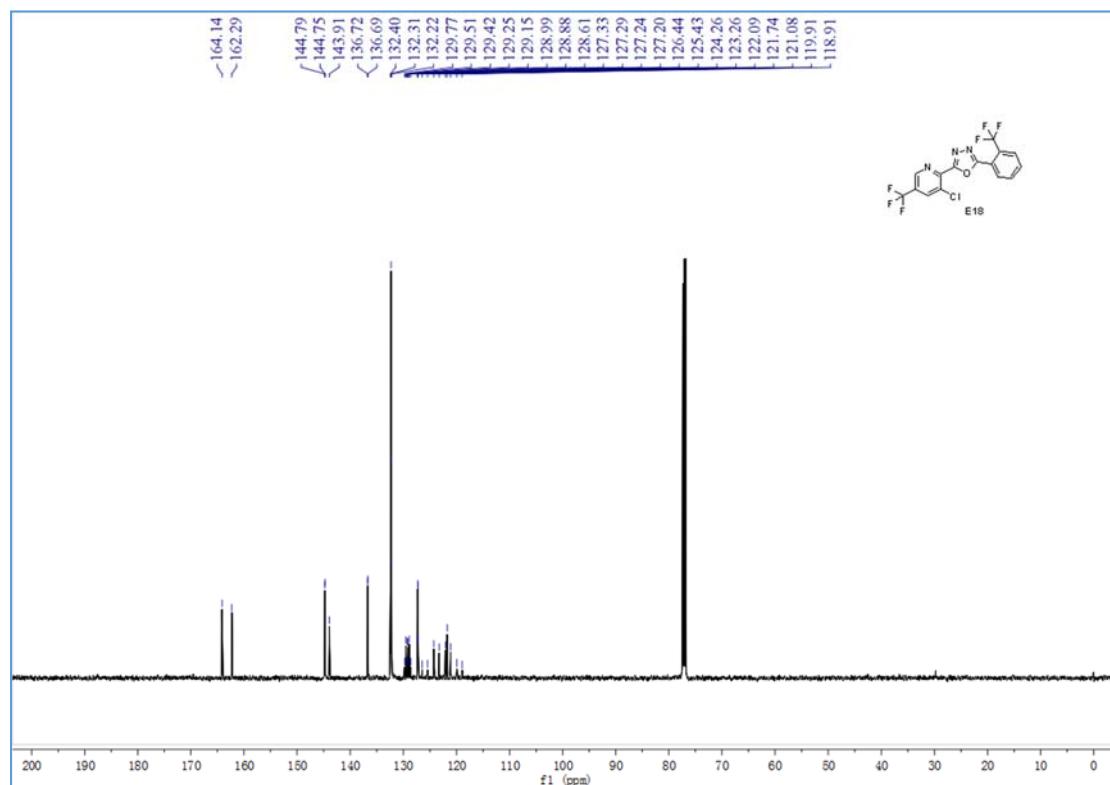


Fig. S70 ^{13}C NMR spectra of compound E18

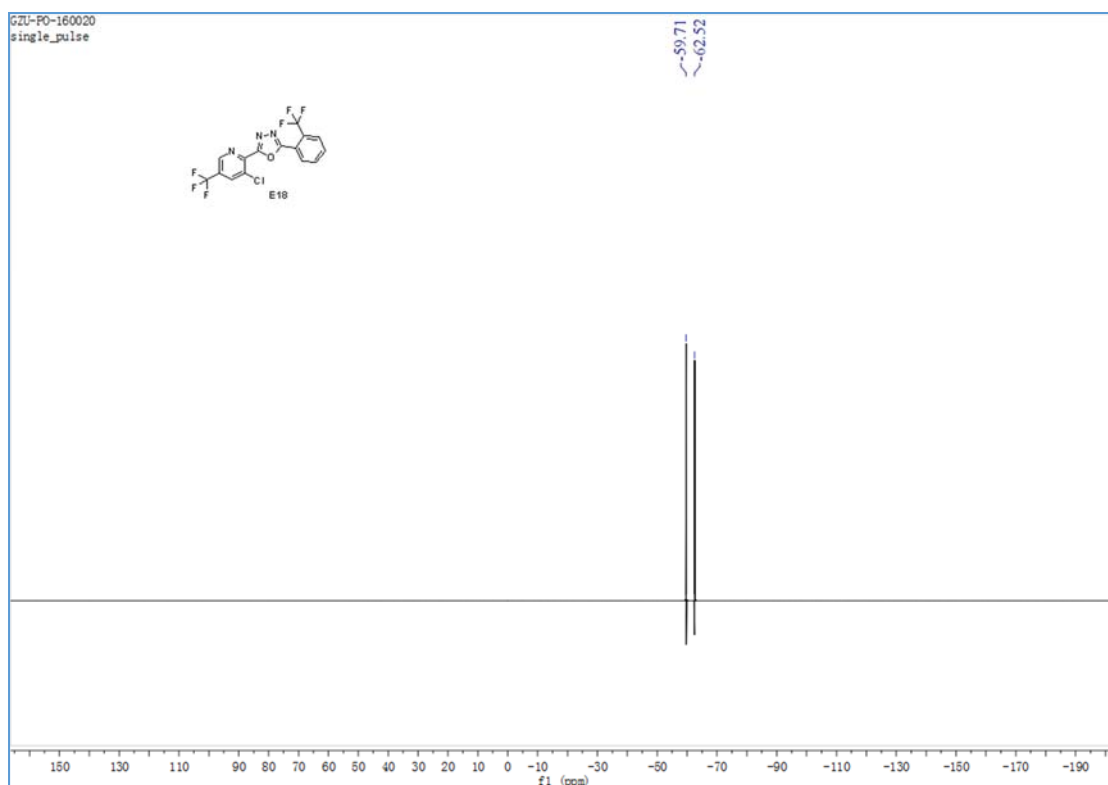


Fig. S71 ^{19}F NMR spectra of compound **E18**

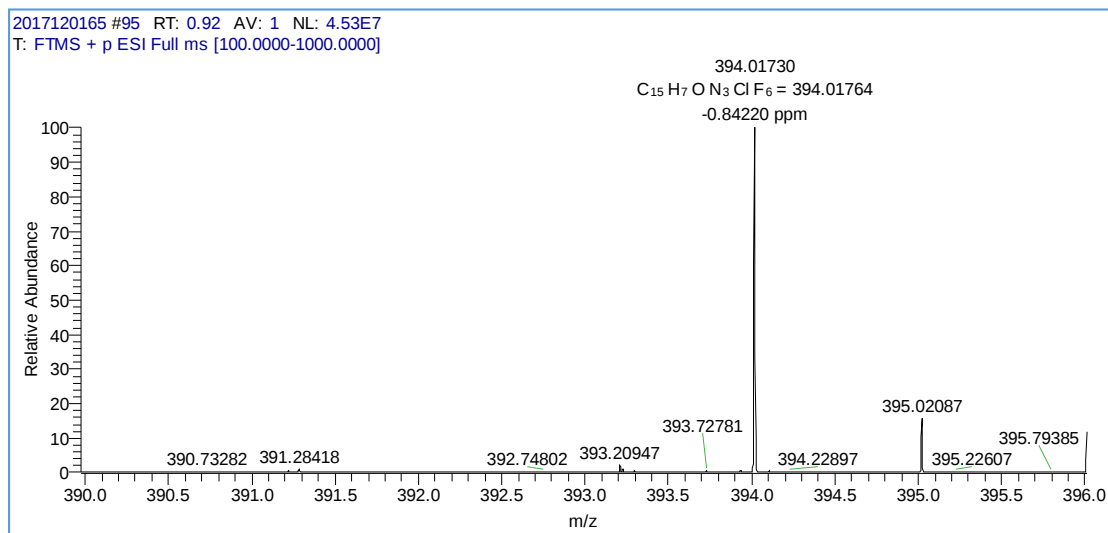


Fig. S72 HR-MS spectra of compound **E18**

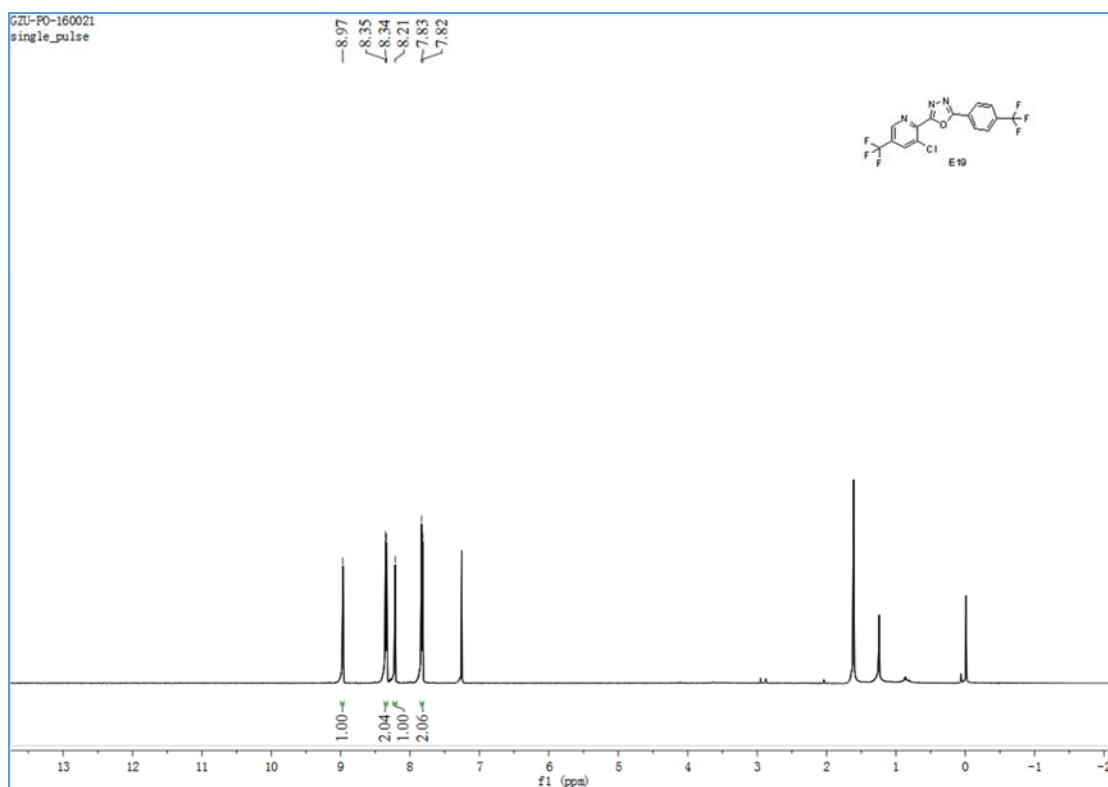


Fig. S73 ^1H NMR spectra of compound E19

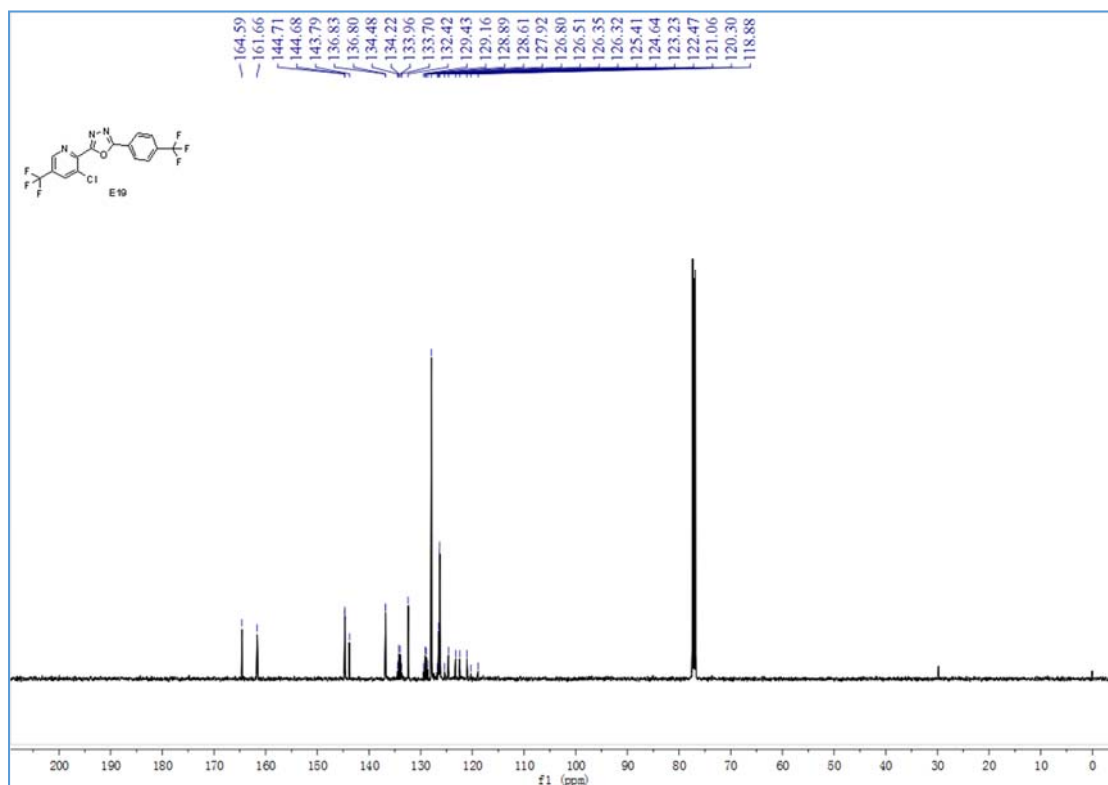


Fig. S74 ^{13}C NMR spectra of compound E19

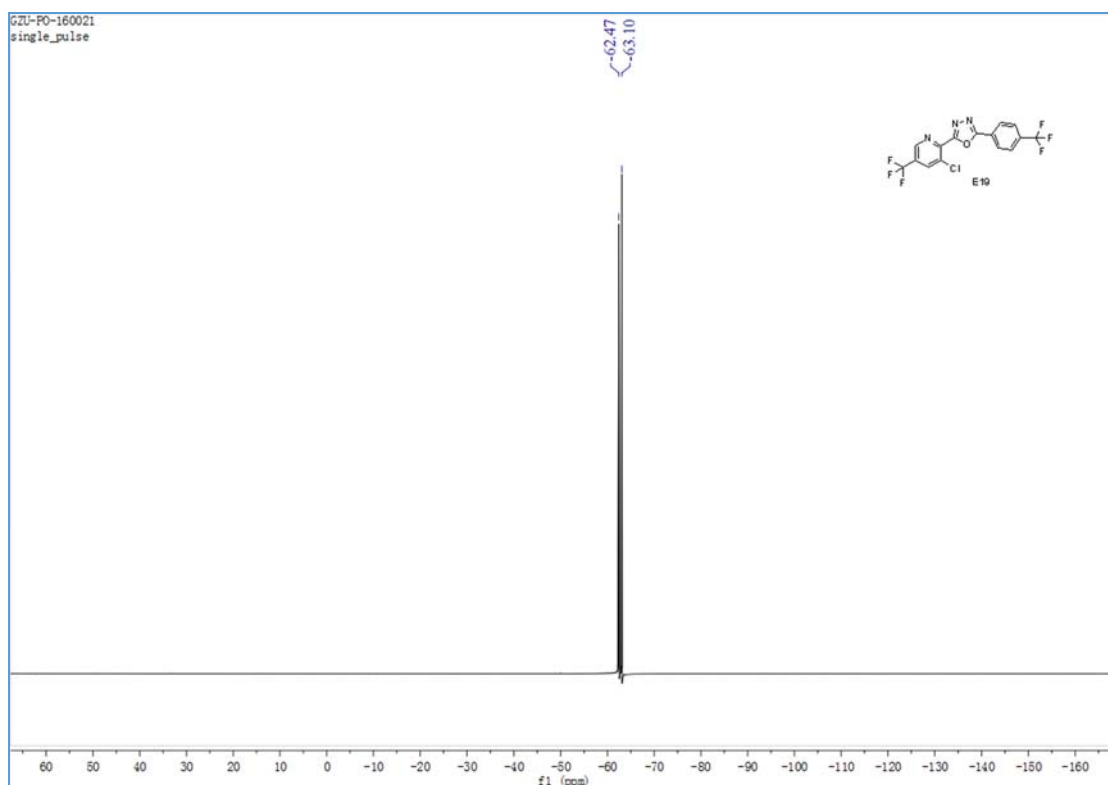


Fig. S75 ^{19}F NMR spectra of compound **E19**

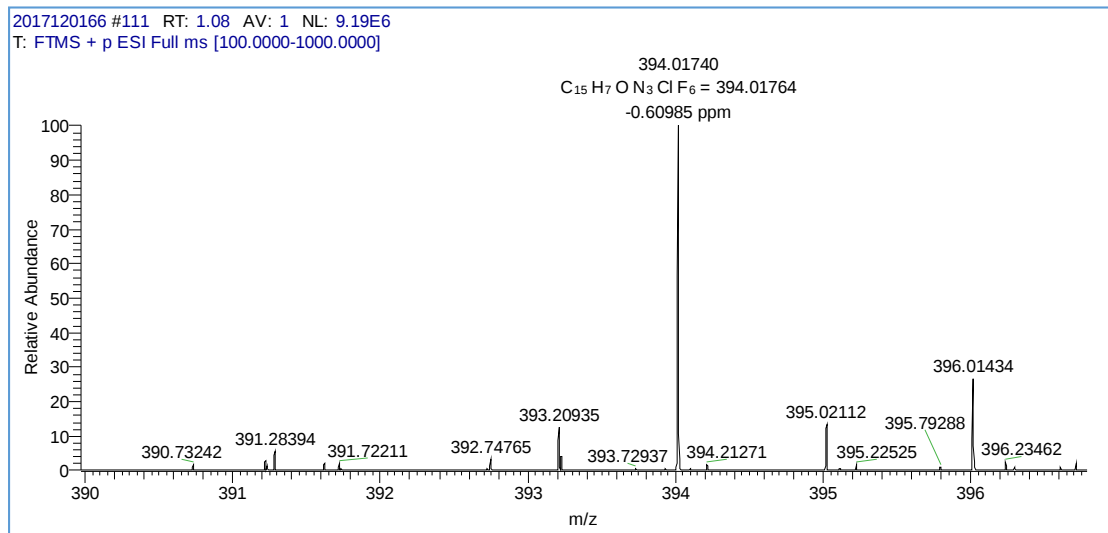


Fig. S76 HR-MS spectra of compound **E19**

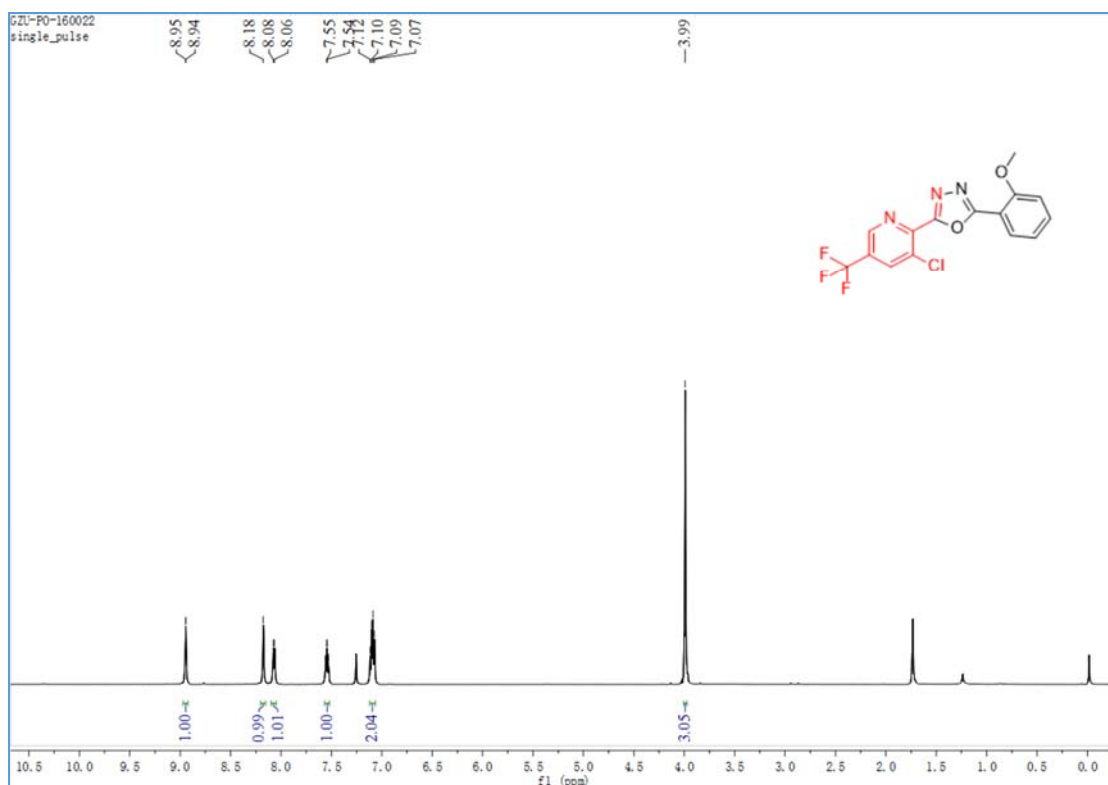


Fig. S77 ^1H NMR spectra of compound E20

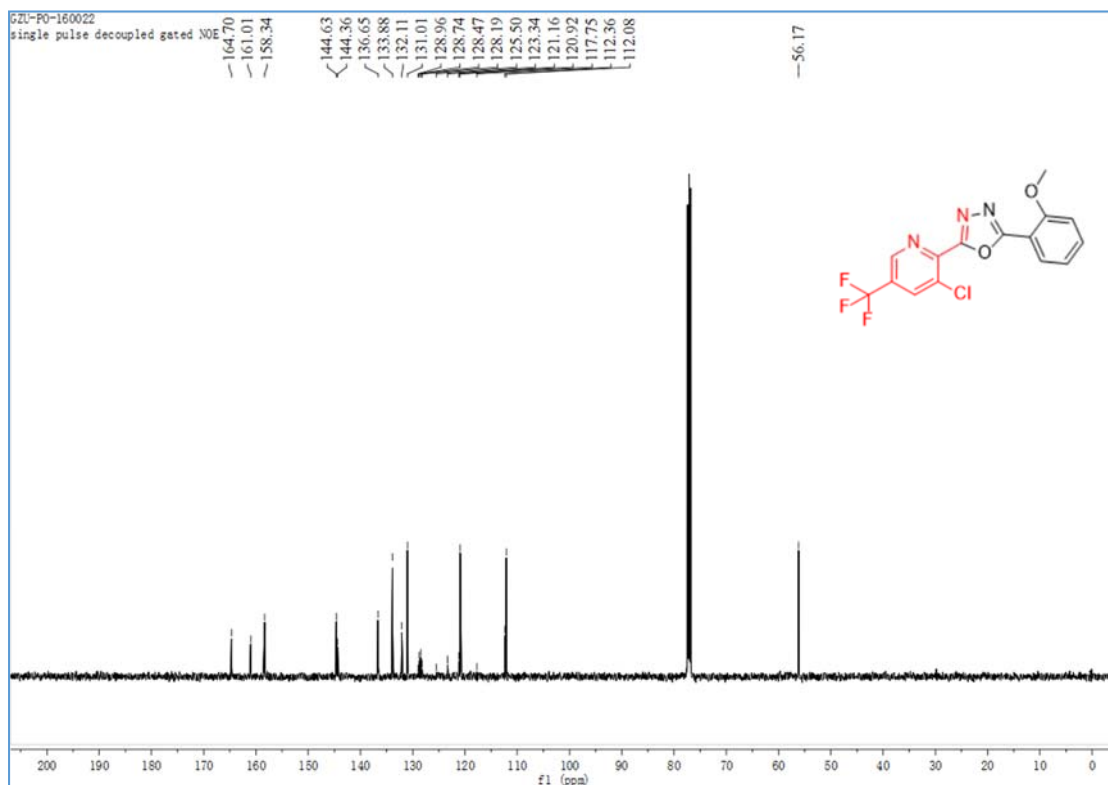


Fig. S78 ^{13}C NMR spectra of compound E20

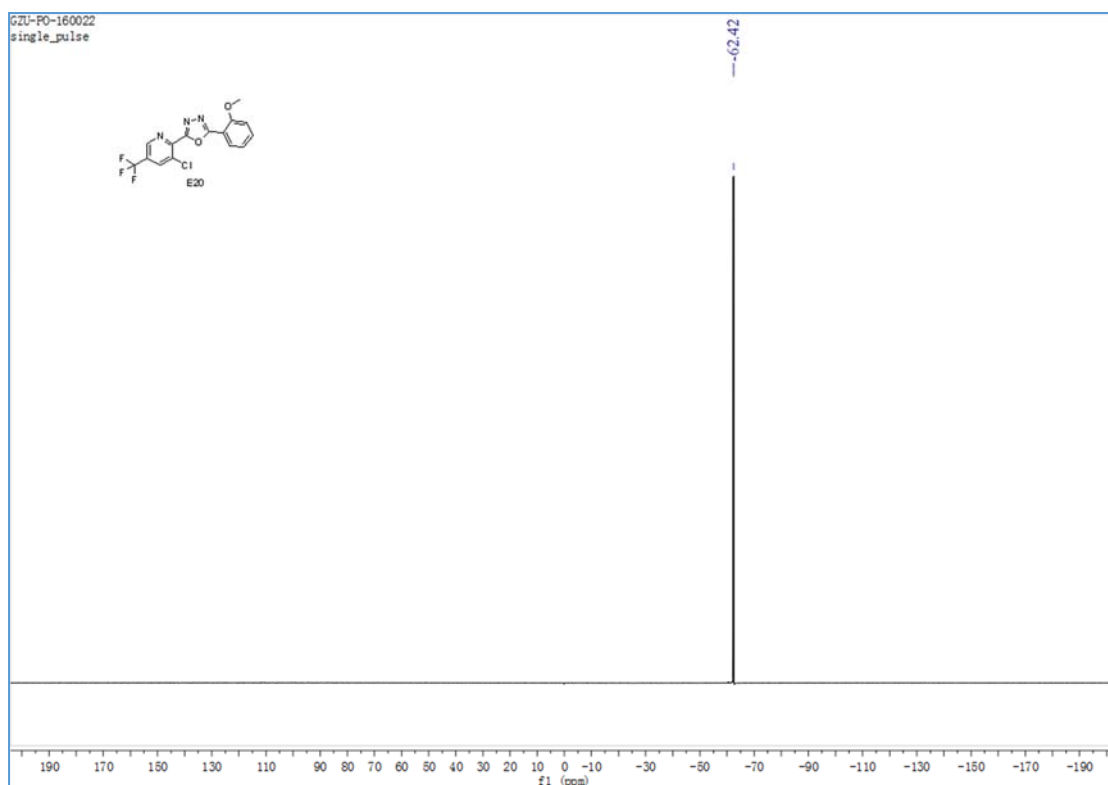


Fig. S79 ^{19}F NMR spectra of compound E20

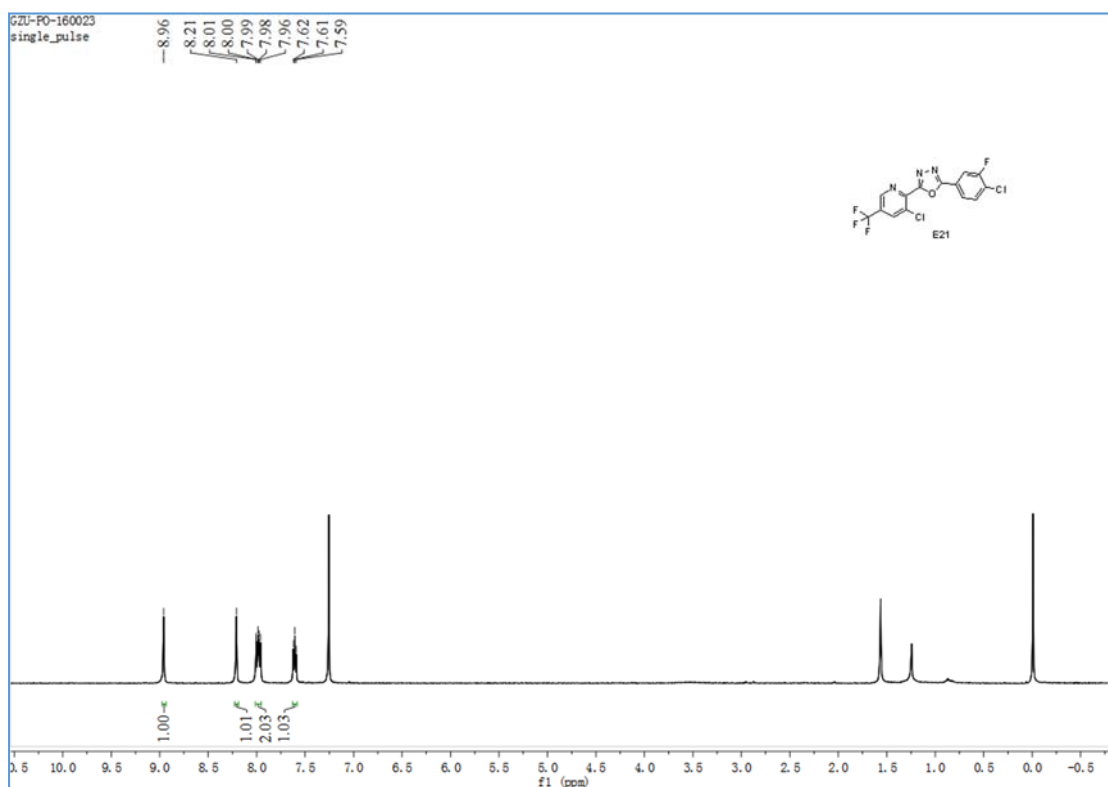


Fig. S80 ^1H NMR spectra of compound E21

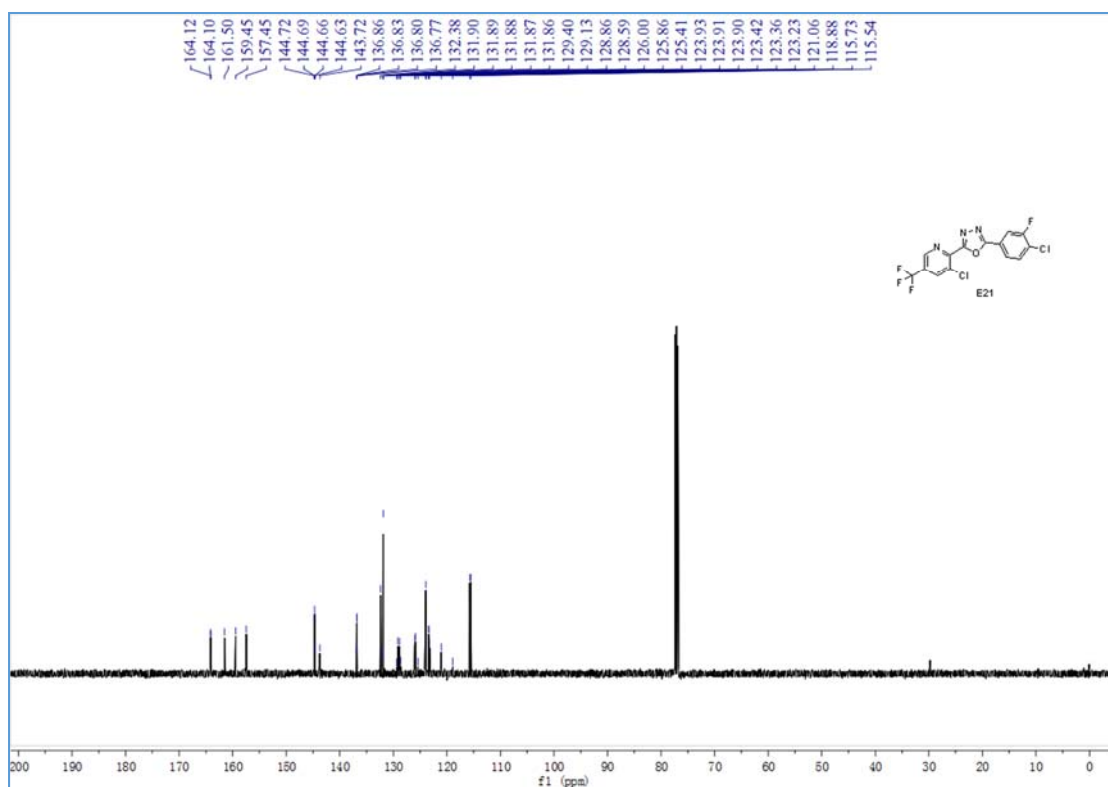


Fig. S81 ¹³C NMR spectra of compound E21

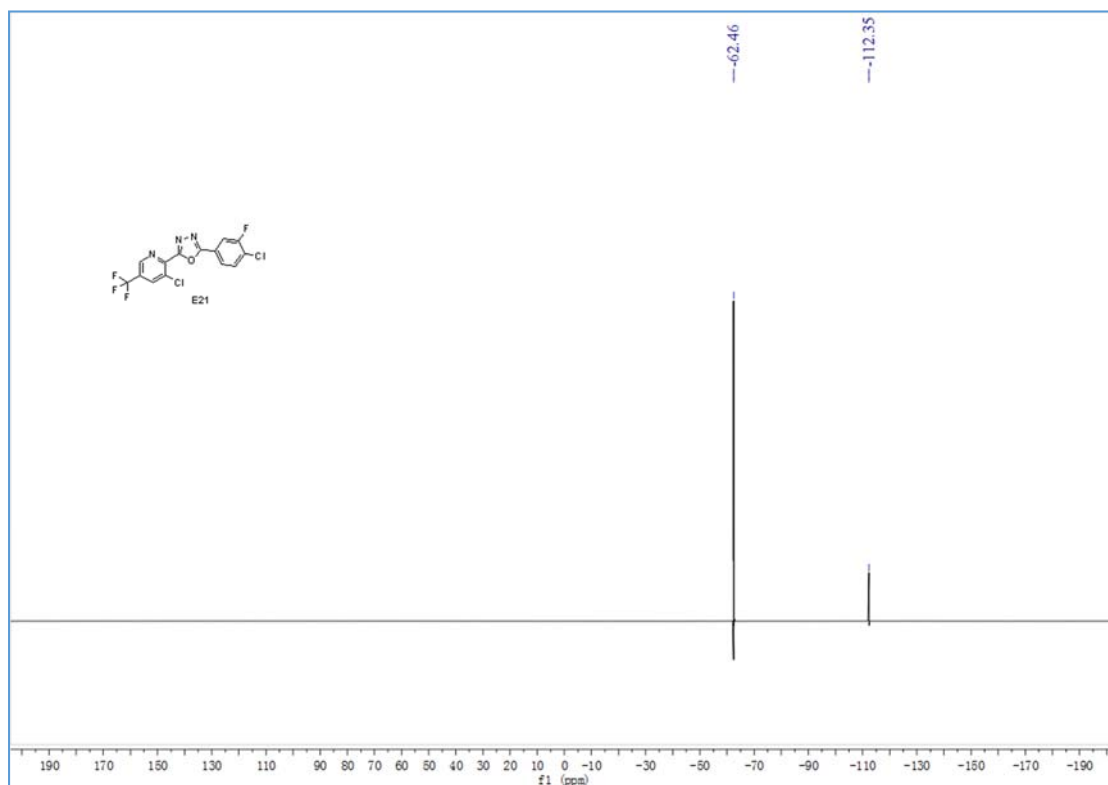


Fig. S82 ¹⁹F NMR spectra of compound E21

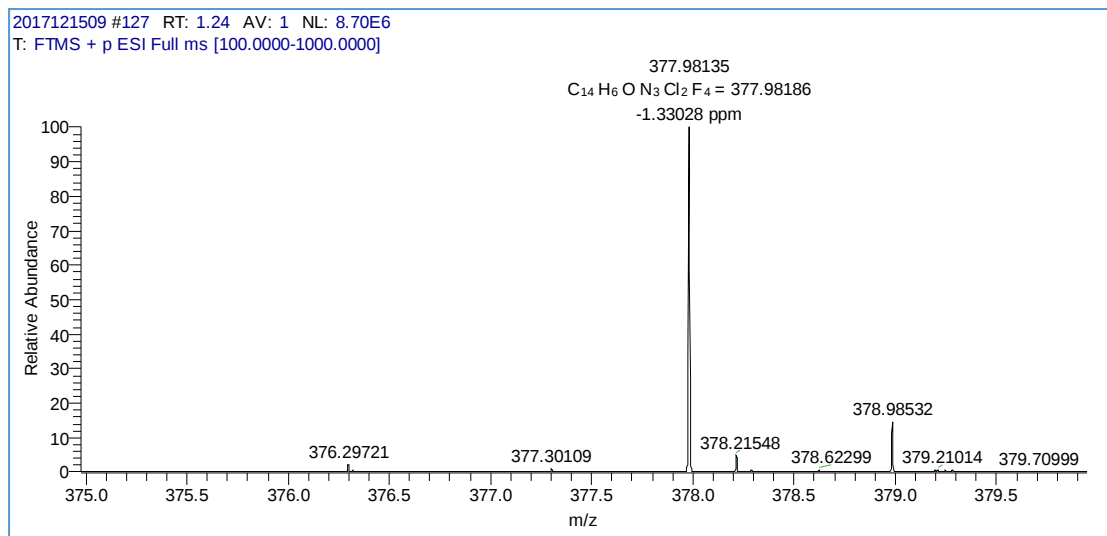


Fig. S83 HR-MS spectra of compound **E21**

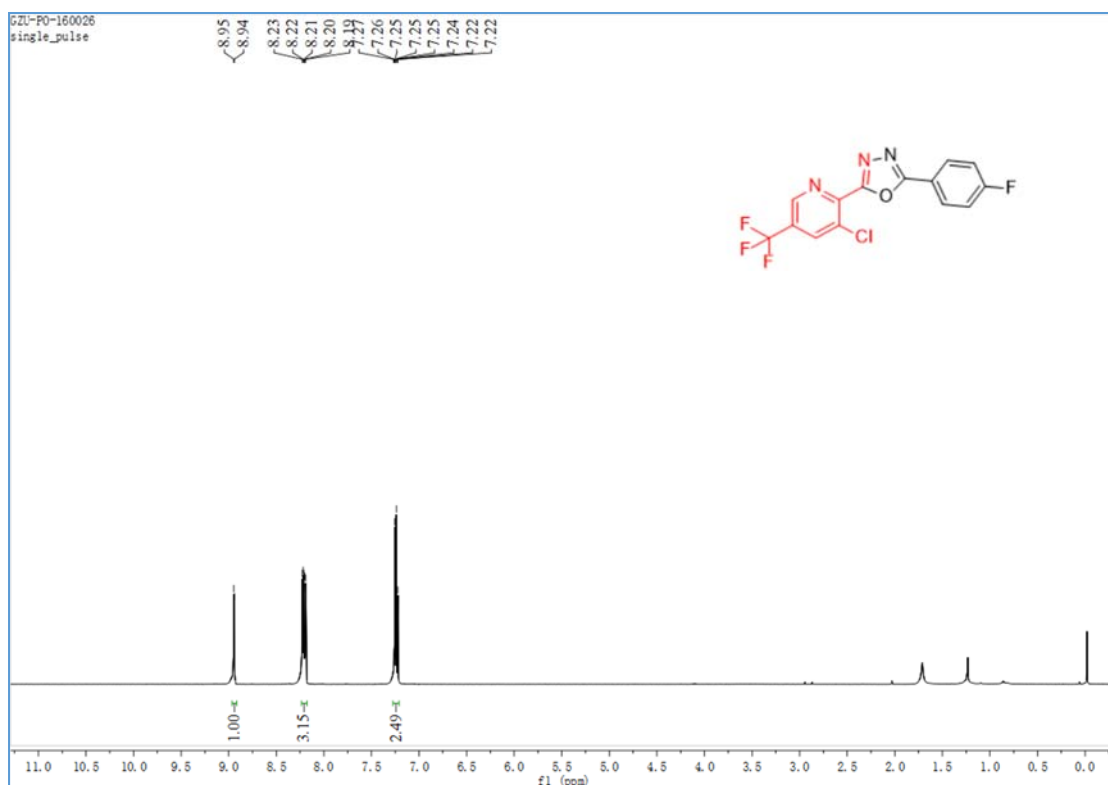


Fig. S84 ^1H NMR spectra of compound E22

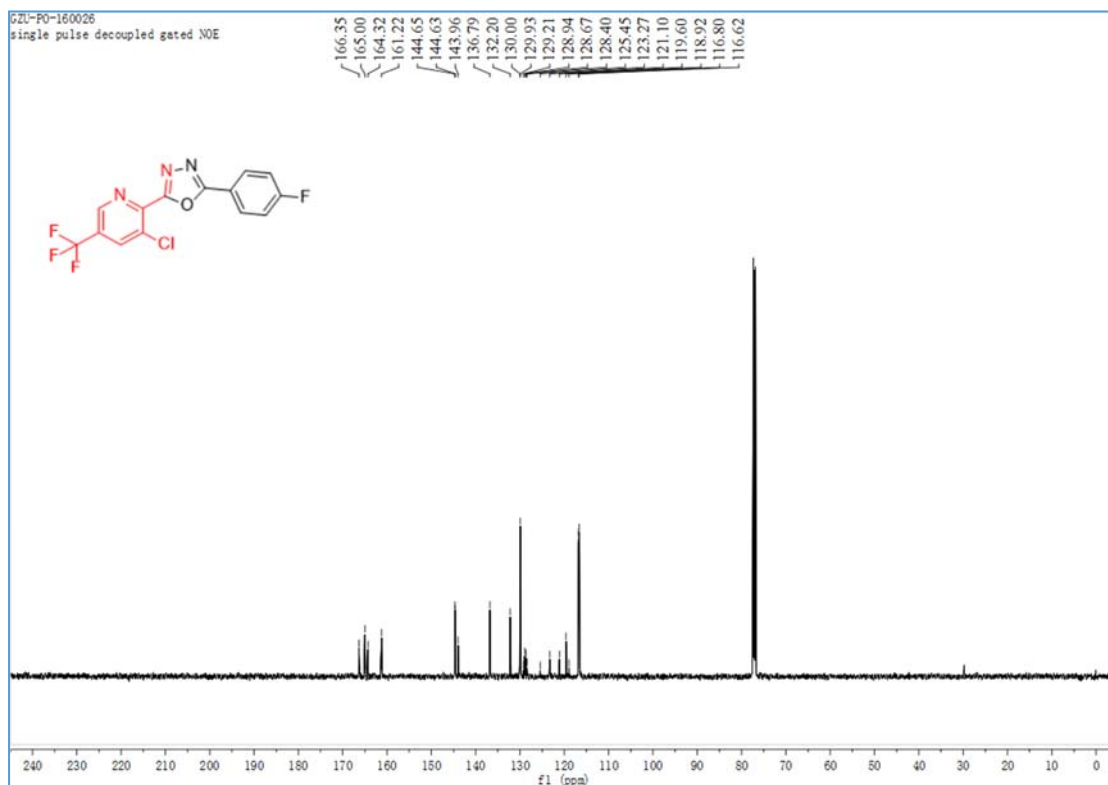


Fig. S85 ^{13}C NMR spectra of compound E22

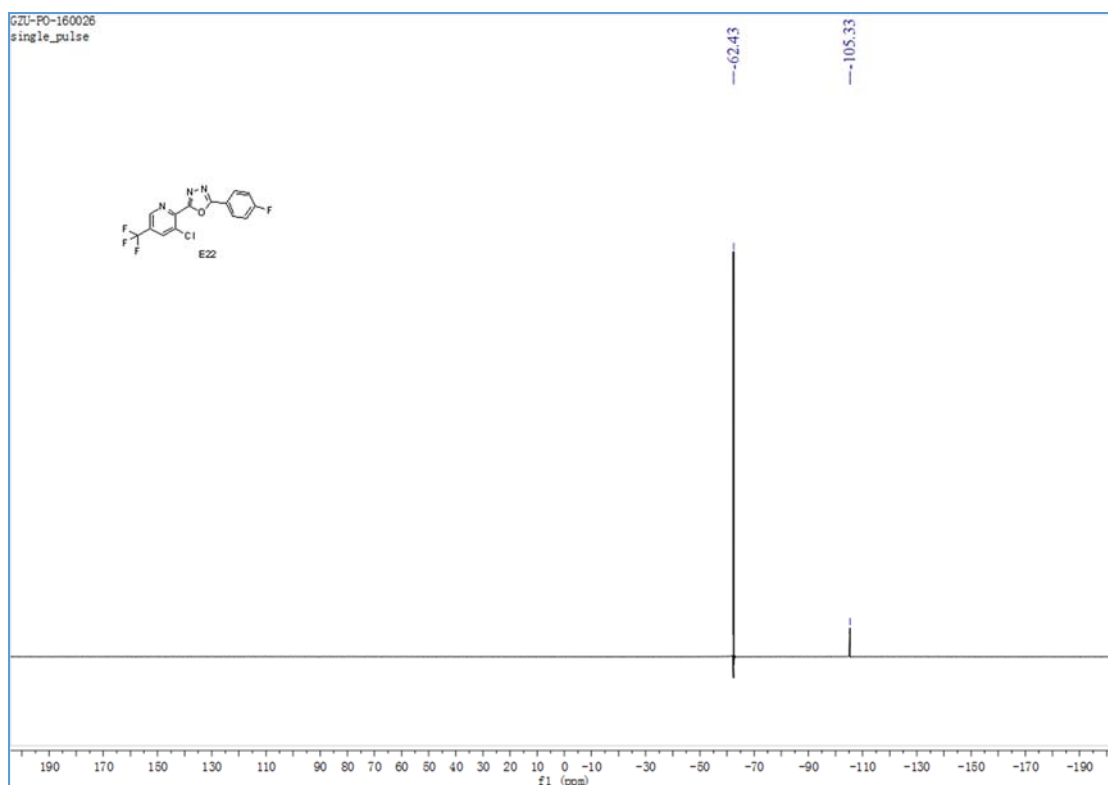


Fig. S86 ^{19}F NMR spectra of compound E22

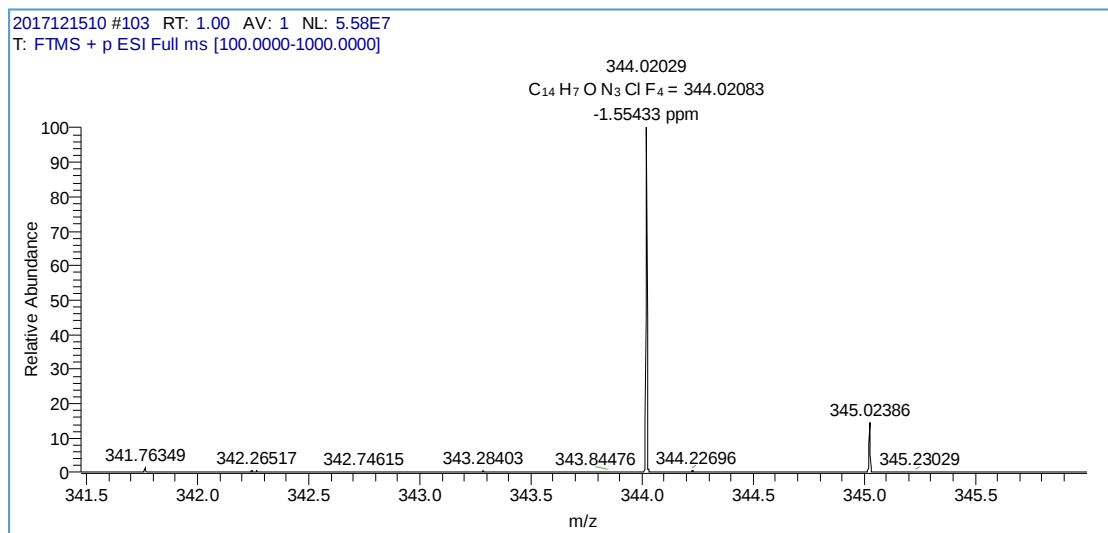


Fig. S87 HR-MS spectra of compound E22

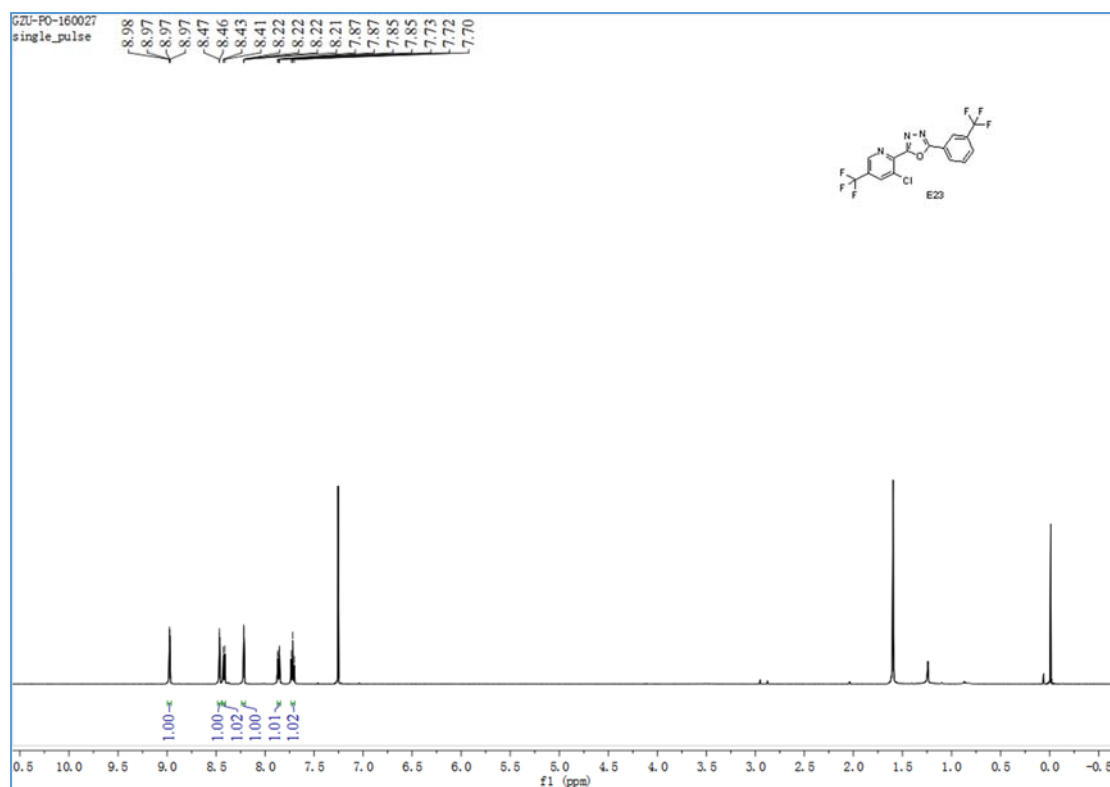


Fig. S88 ^1H NMR spectra of compound E23

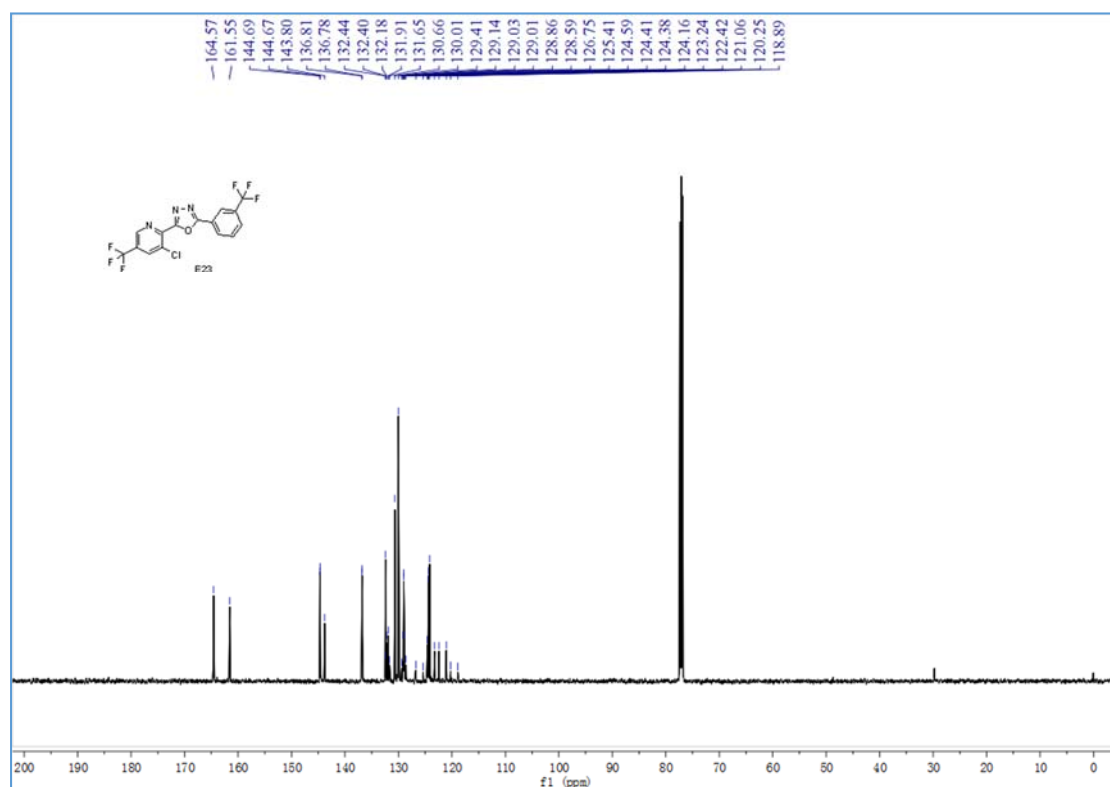


Fig. S89 ^{13}C NMR spectra of compound E23

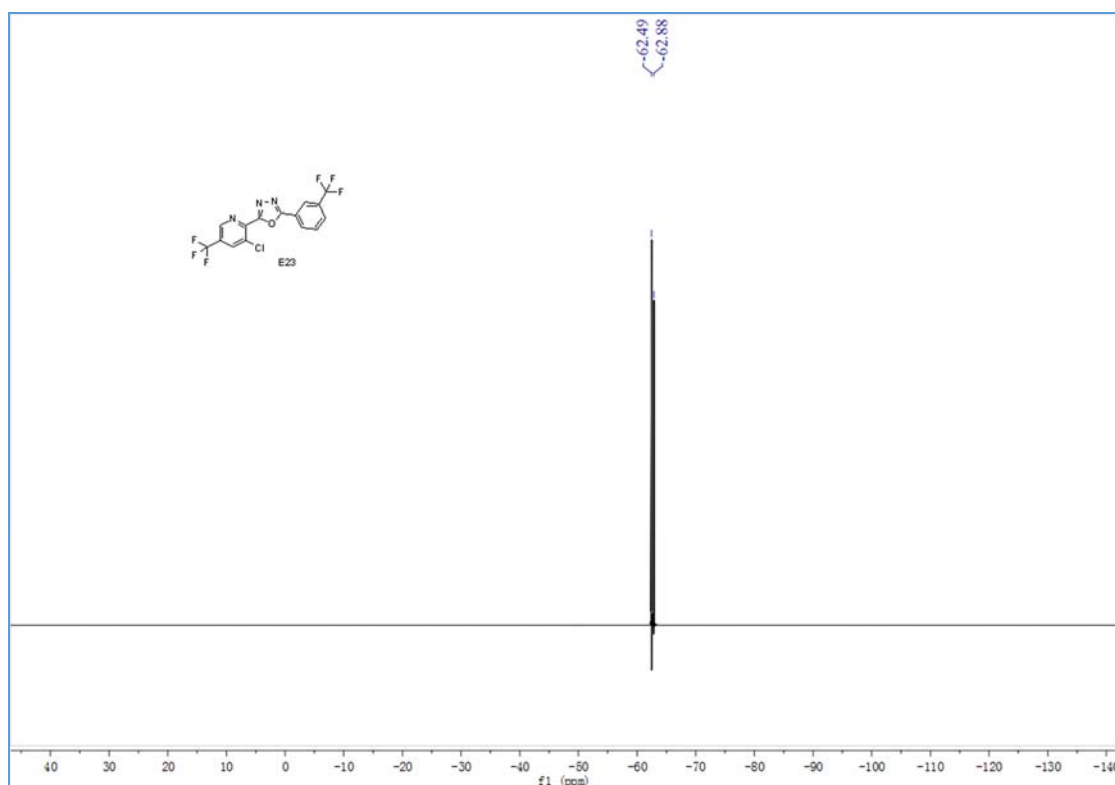


Fig. S90 ^{19}F NMR spectra of compound **E23**

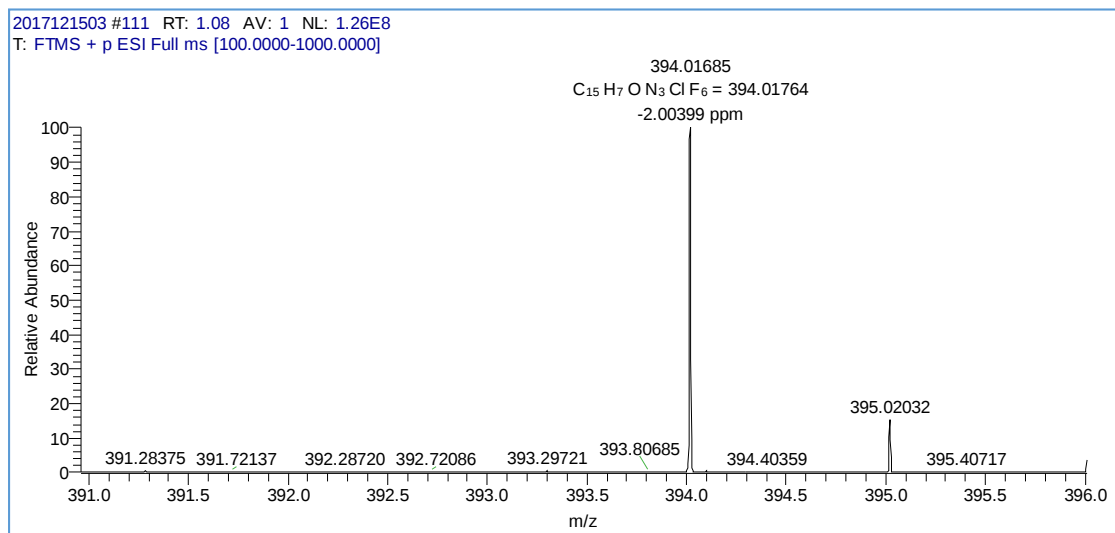


Fig. S91 HR-MS spectra of compound **E23**

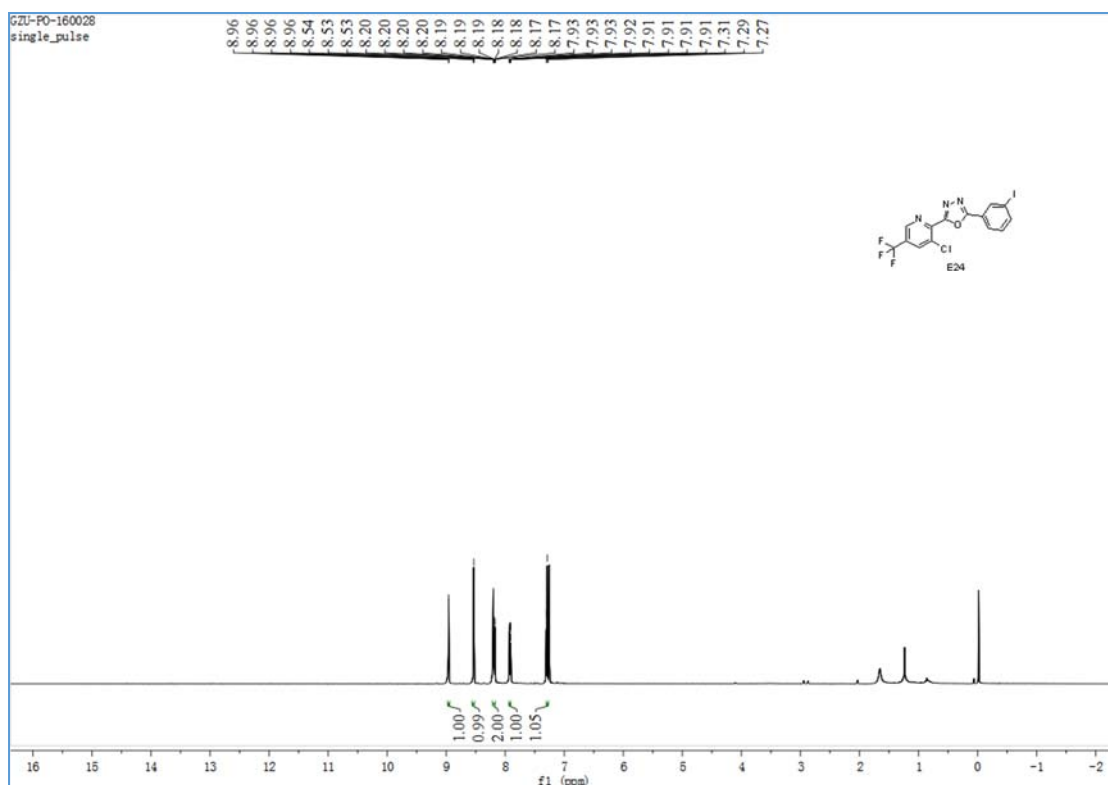


Fig. S92 ^1H NMR spectra of compound E24

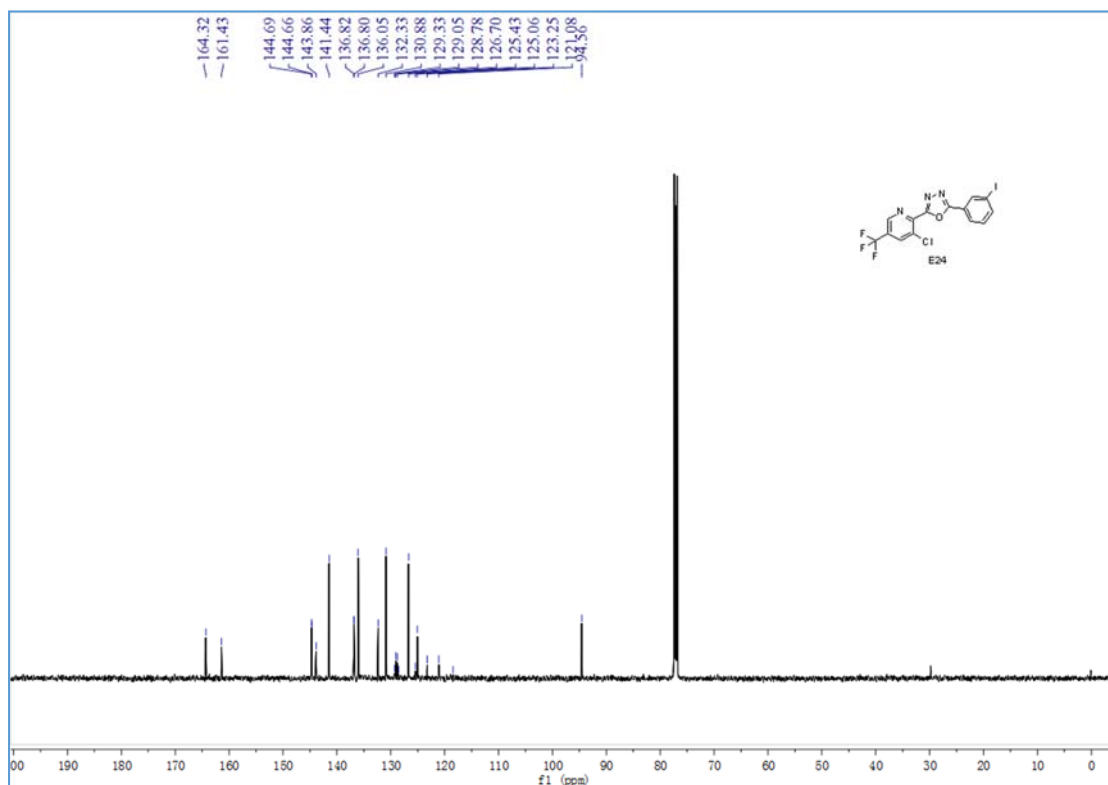


Fig. S93 ^{13}C NMR spectra of compound E24

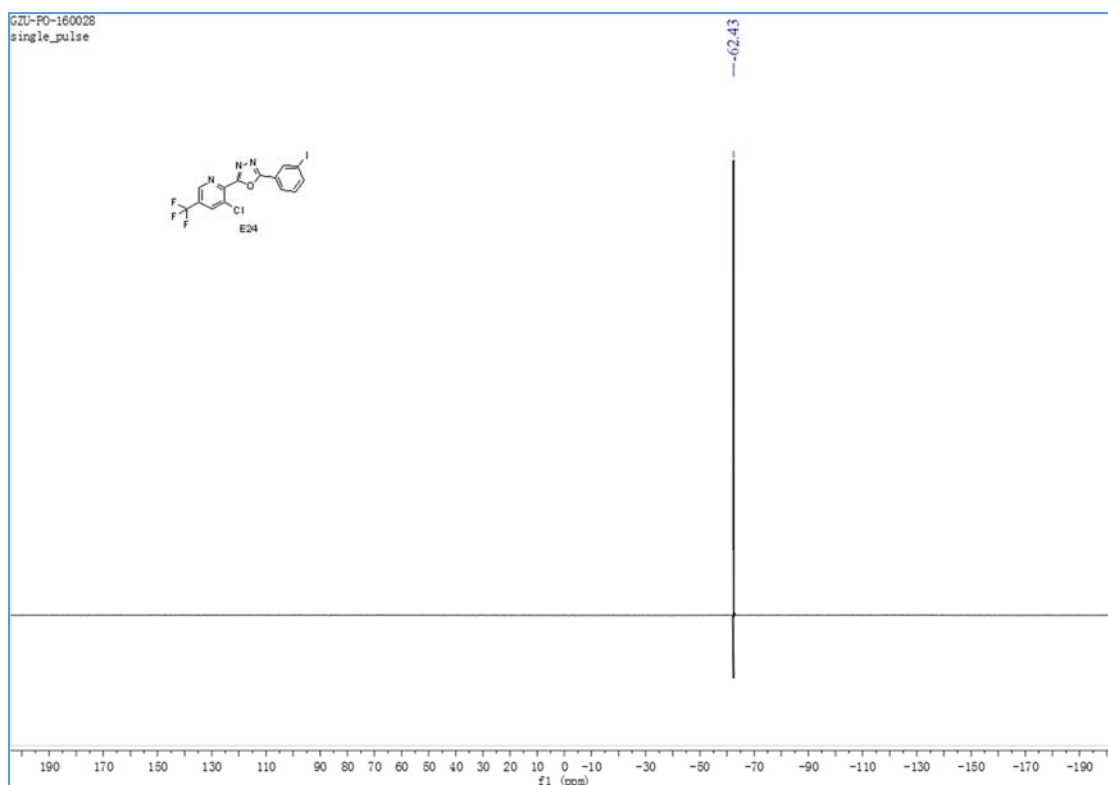


Fig. S94 ^{19}F NMR spectra of compound E24

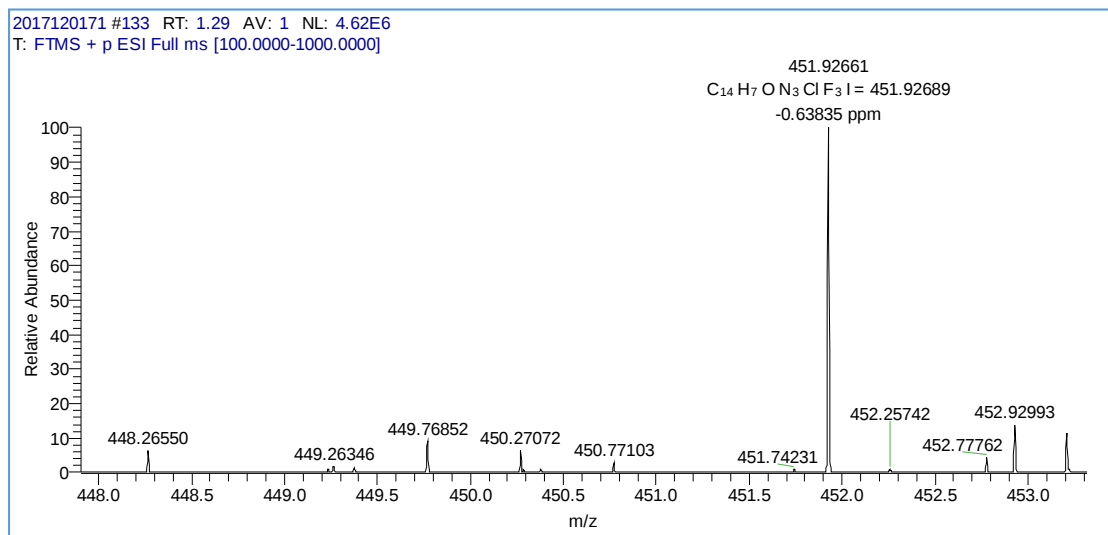


Fig. S95 HR-MS spectra of compound E24

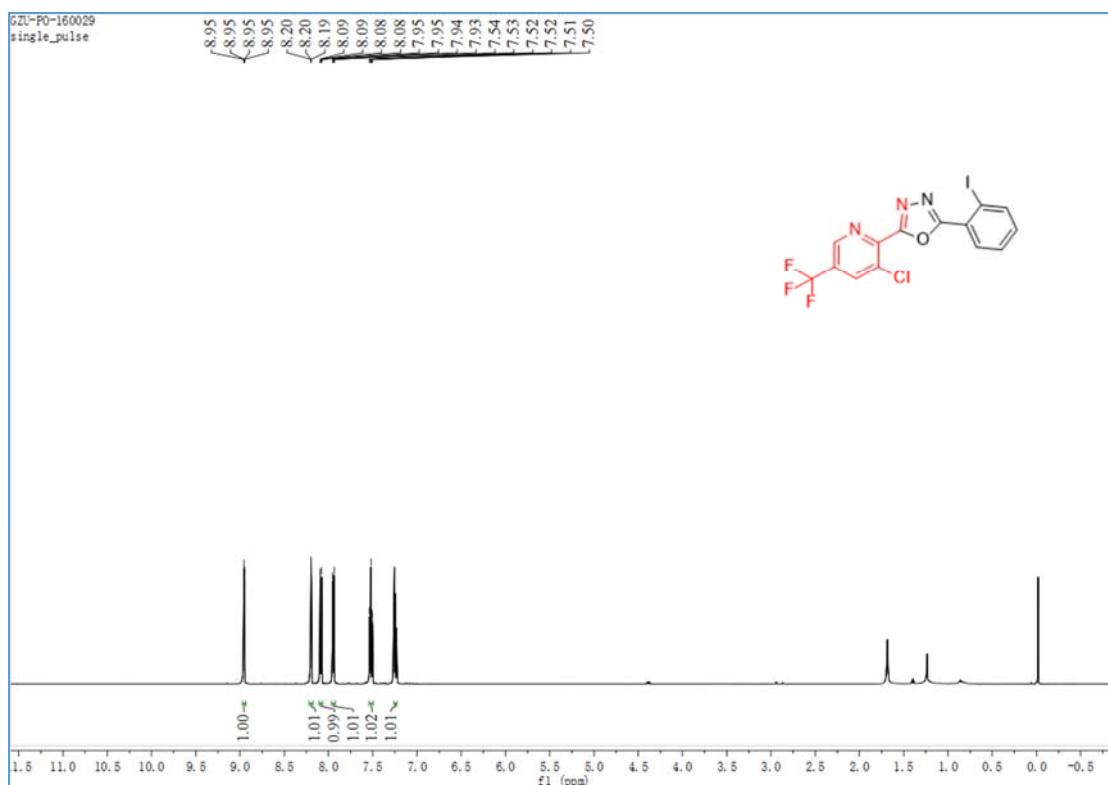


Fig. S96 ^1H NMR spectra of compound E25

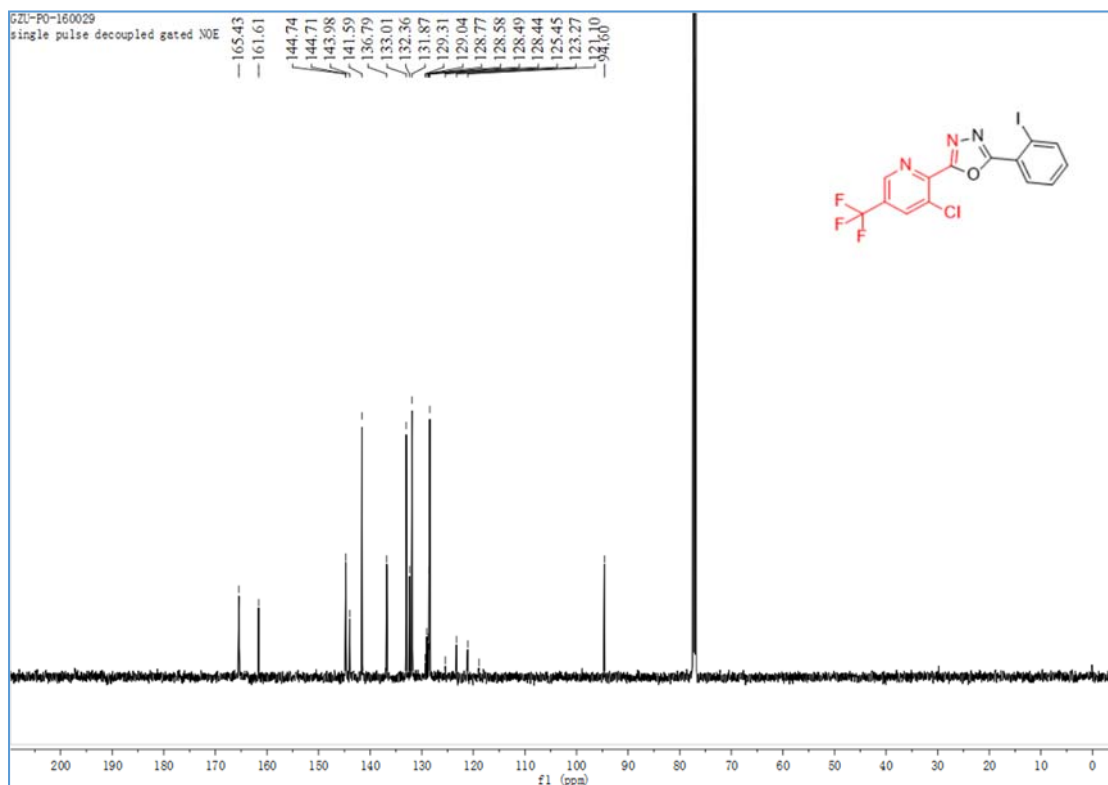


Fig. S97 ^{13}C NMR spectra of compound E25

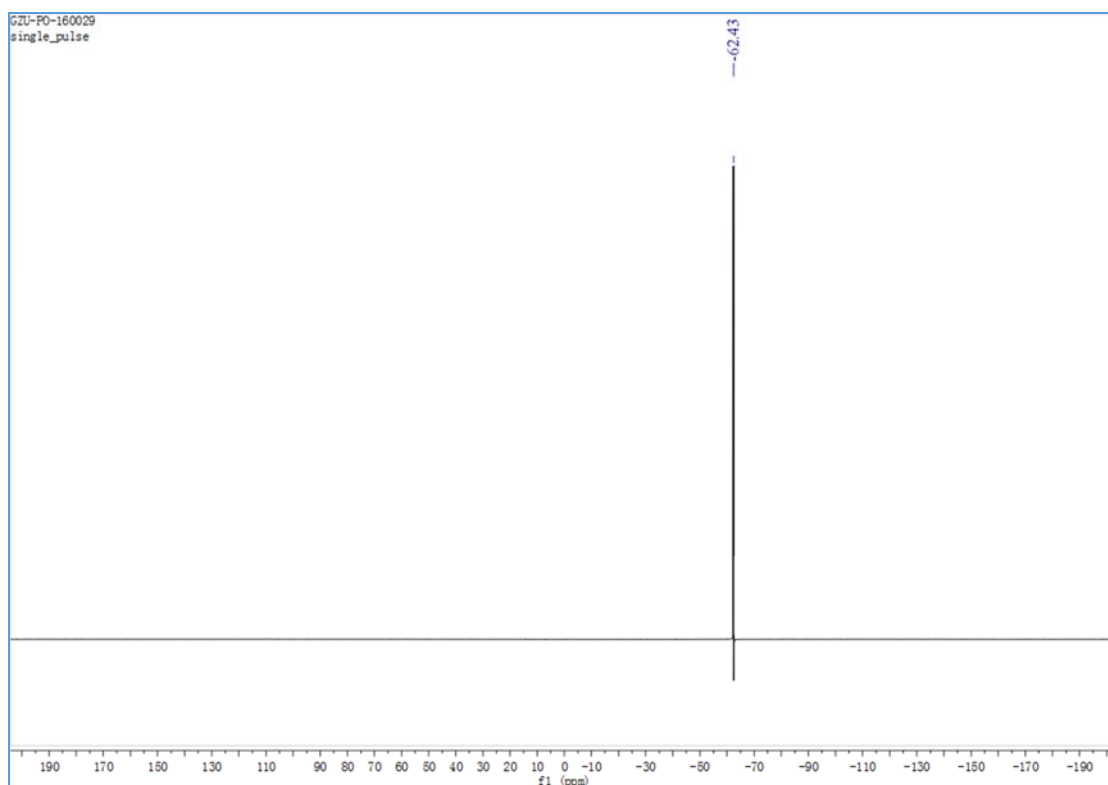


Fig. S98 ^{19}F NMR spectra of compound **E25**

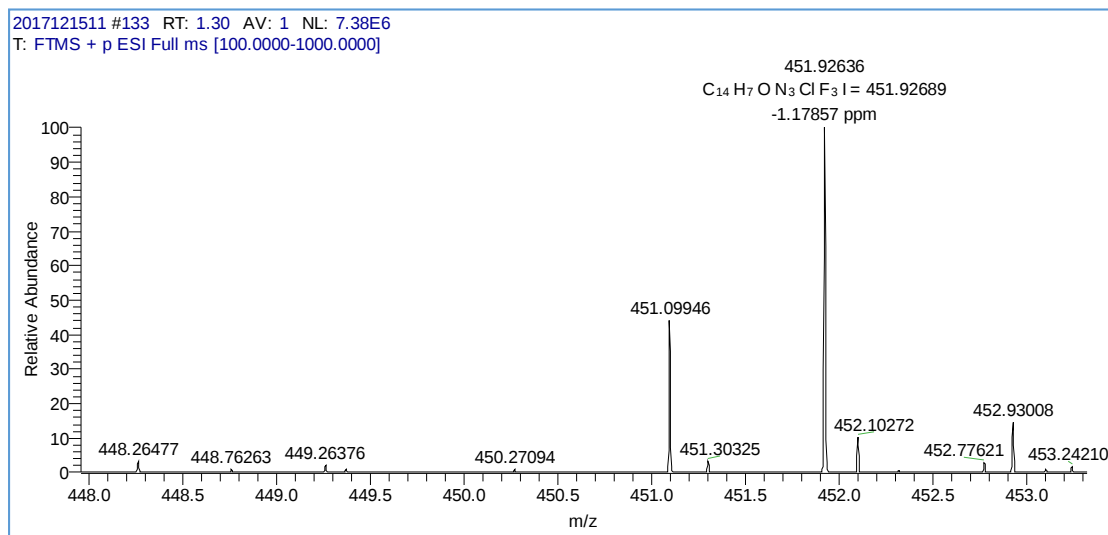


Fig. S99 HR-MS spectra of compound **E25**

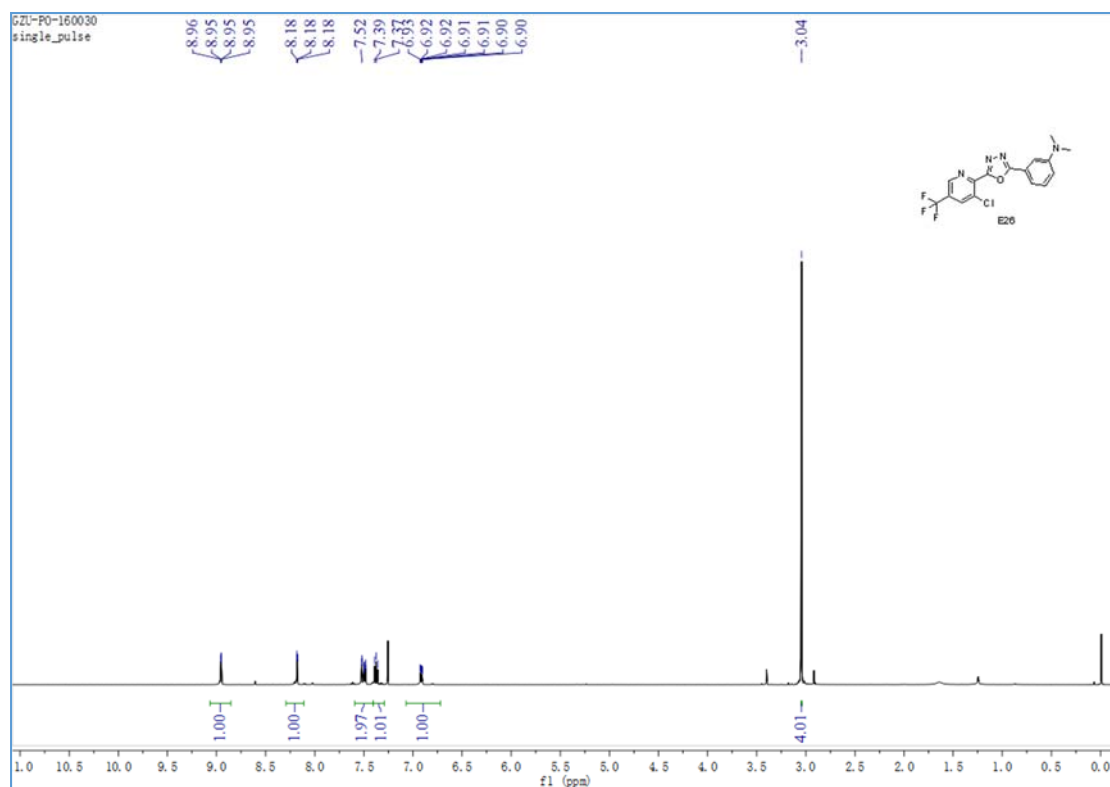


Fig. S100 ^1H NMR spectra of compound **E26**

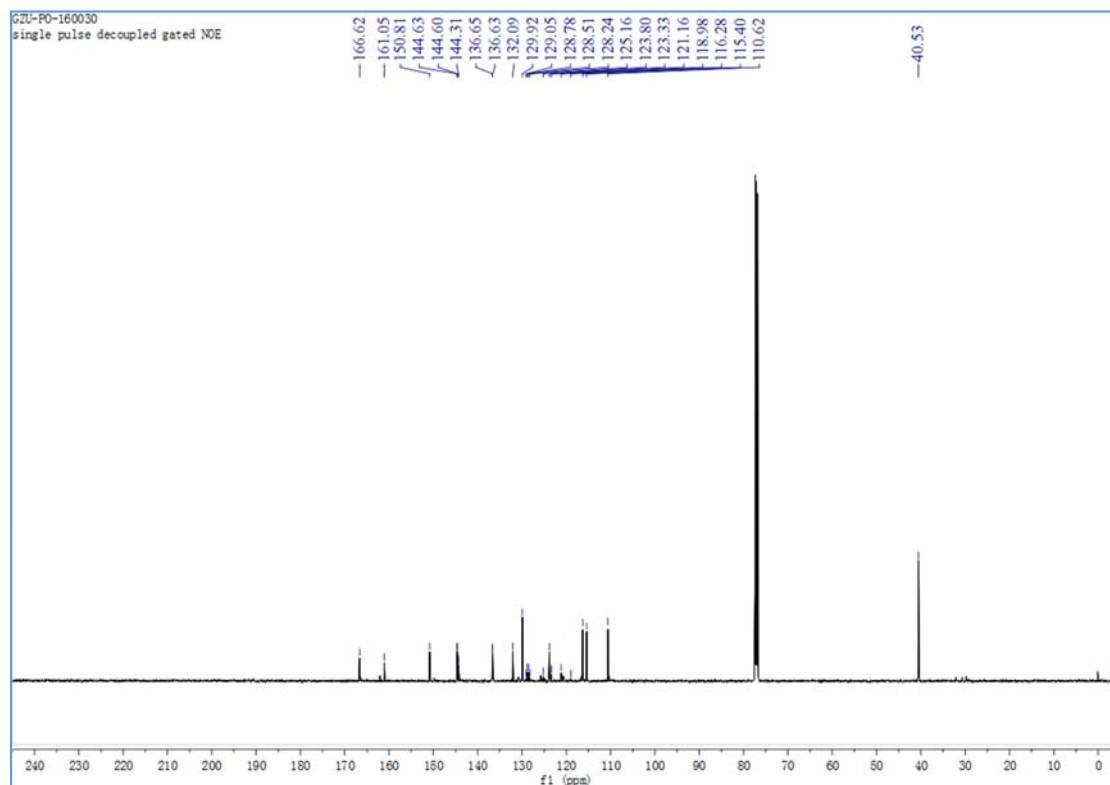


Fig. S101 ^{13}C NMR spectra of compound **E26**

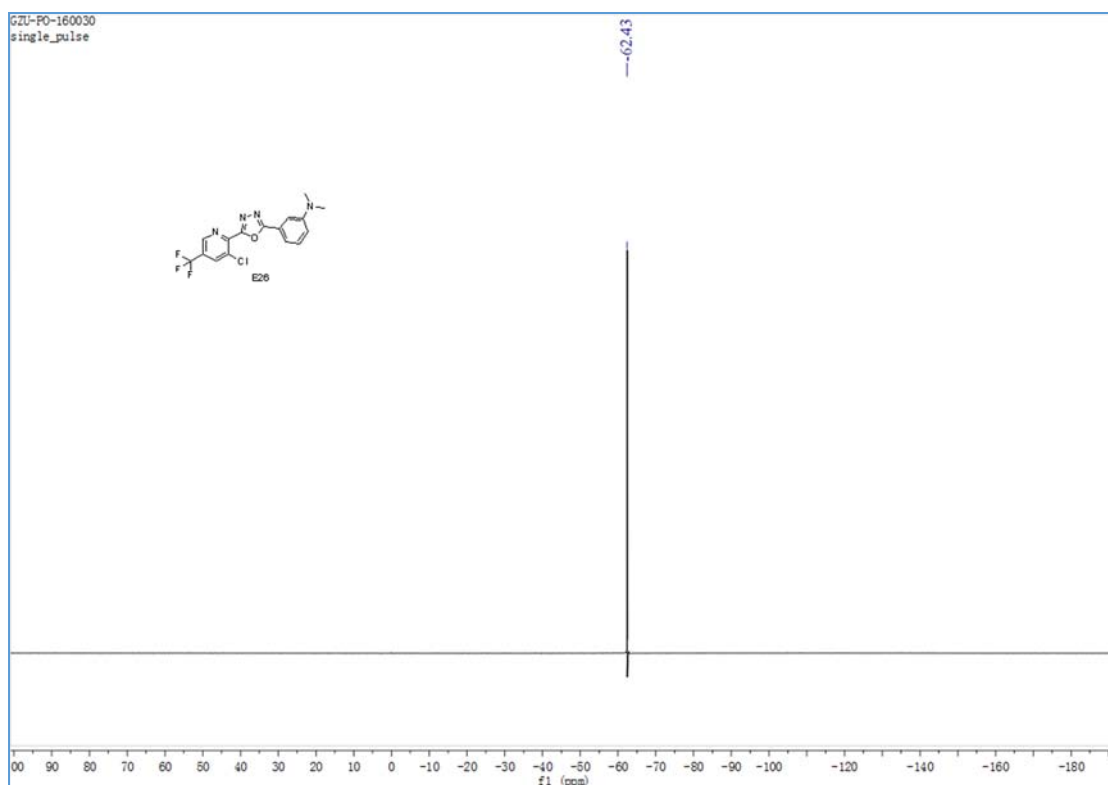


Fig. S102 ^{19}F NMR spectra of compound **E26**

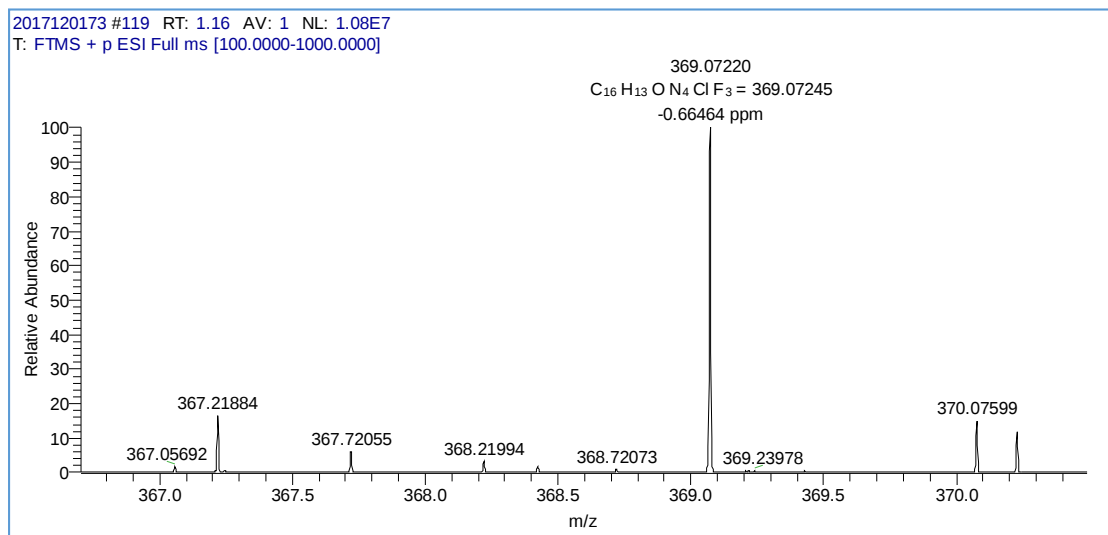


Fig. S103 HR-MS spectra of compound **E26**

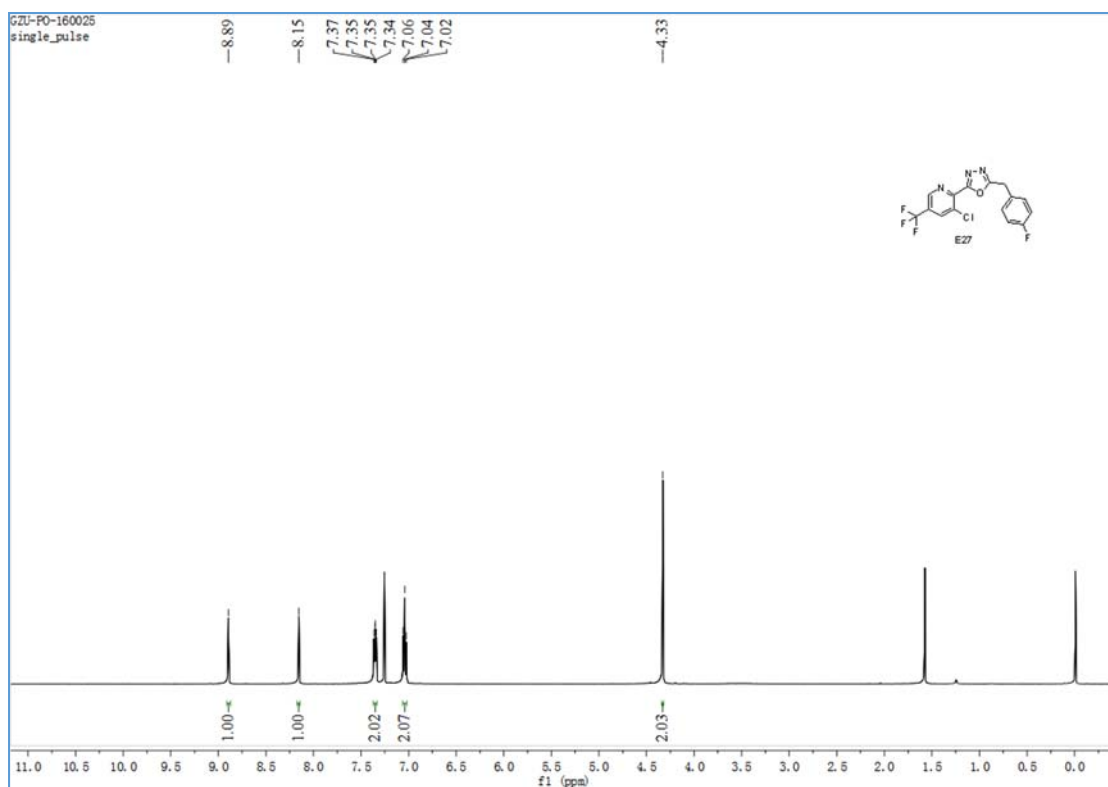


Fig. S104 ^1H NMR spectra of compound **E27**

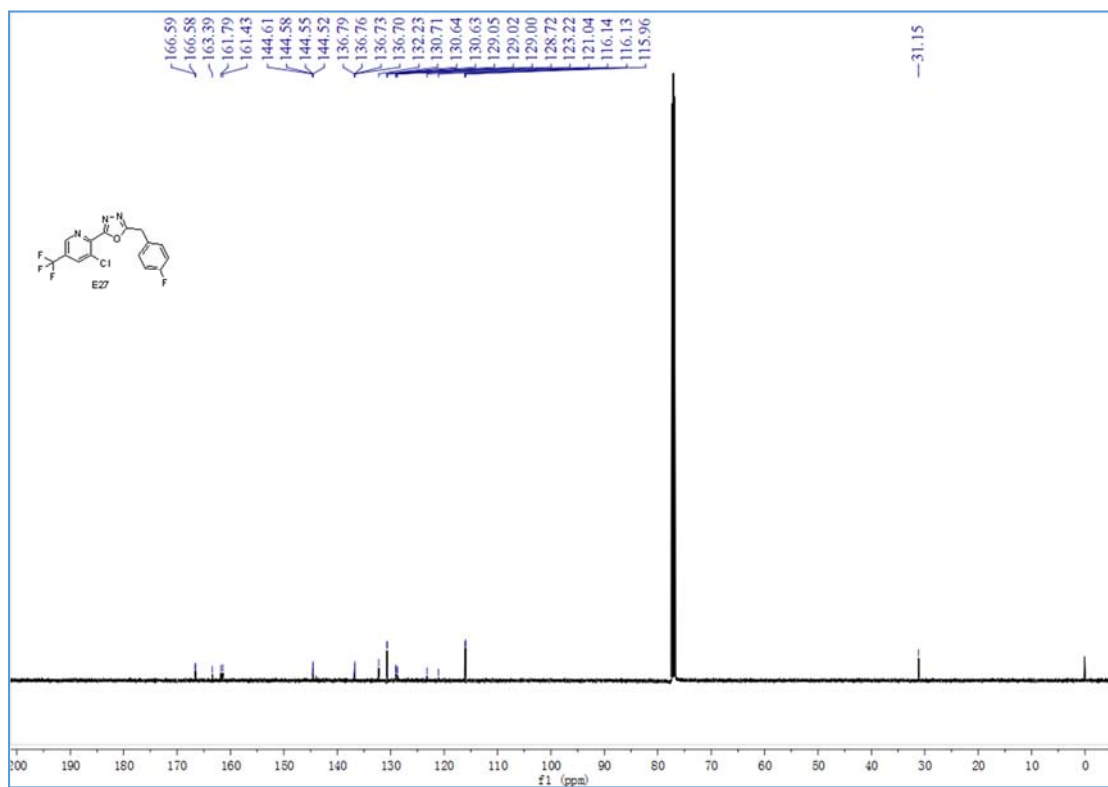


Fig. S105 ^{13}C NMR spectra of compound **E27**

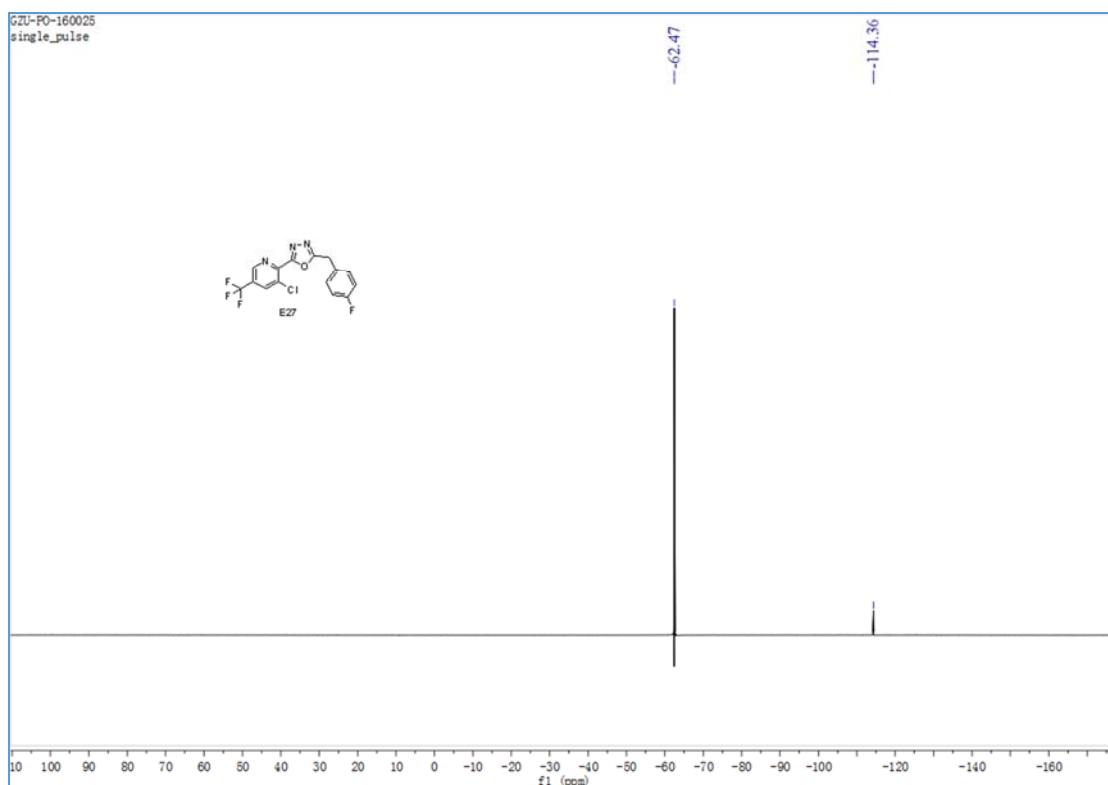


Fig. S106 ^{19}F NMR spectra of compound **E27**

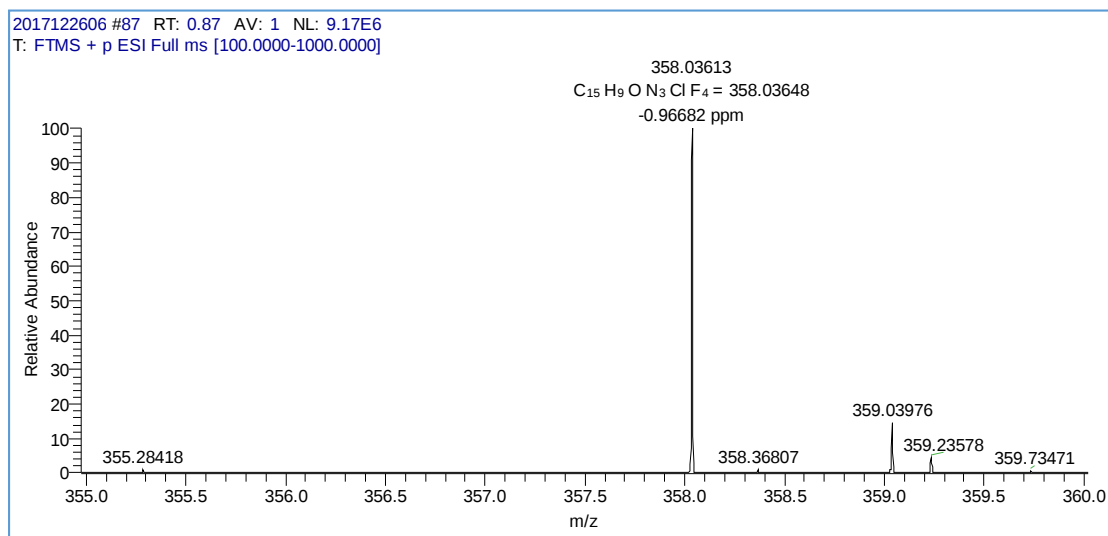


Fig. S107 HR-MS spectra of compound **E27**

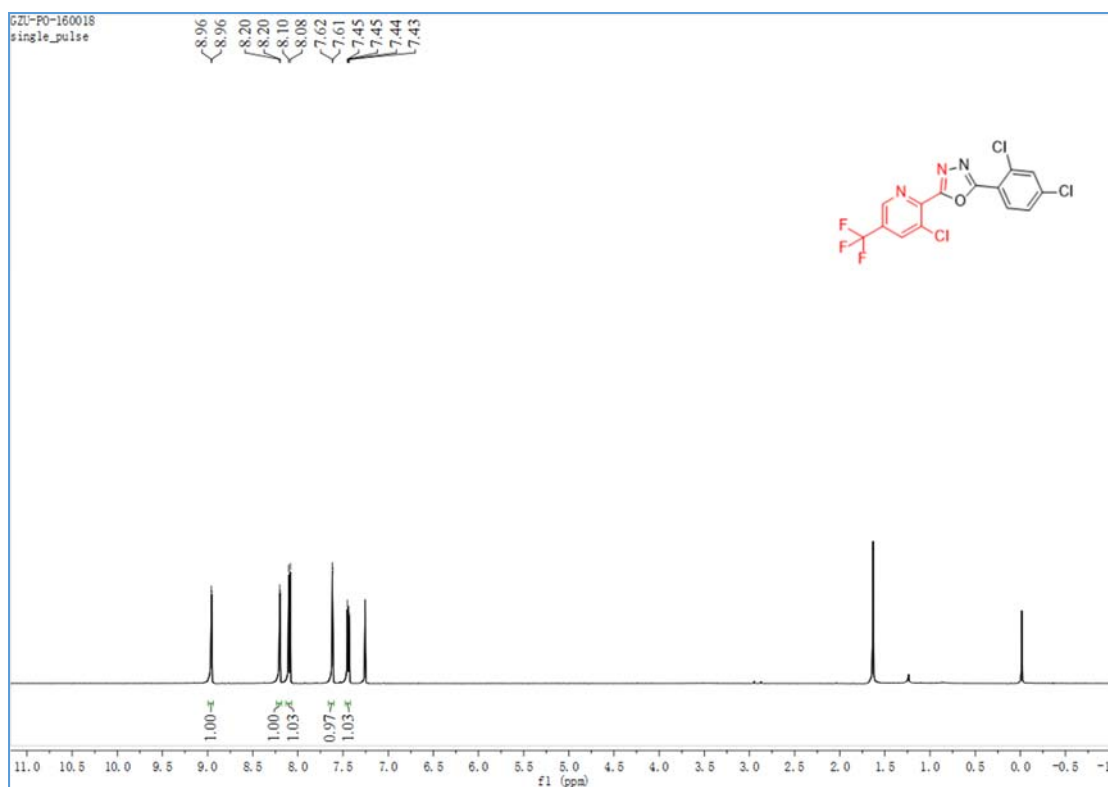


Fig. S108 ^1H NMR spectra of compound **E28**

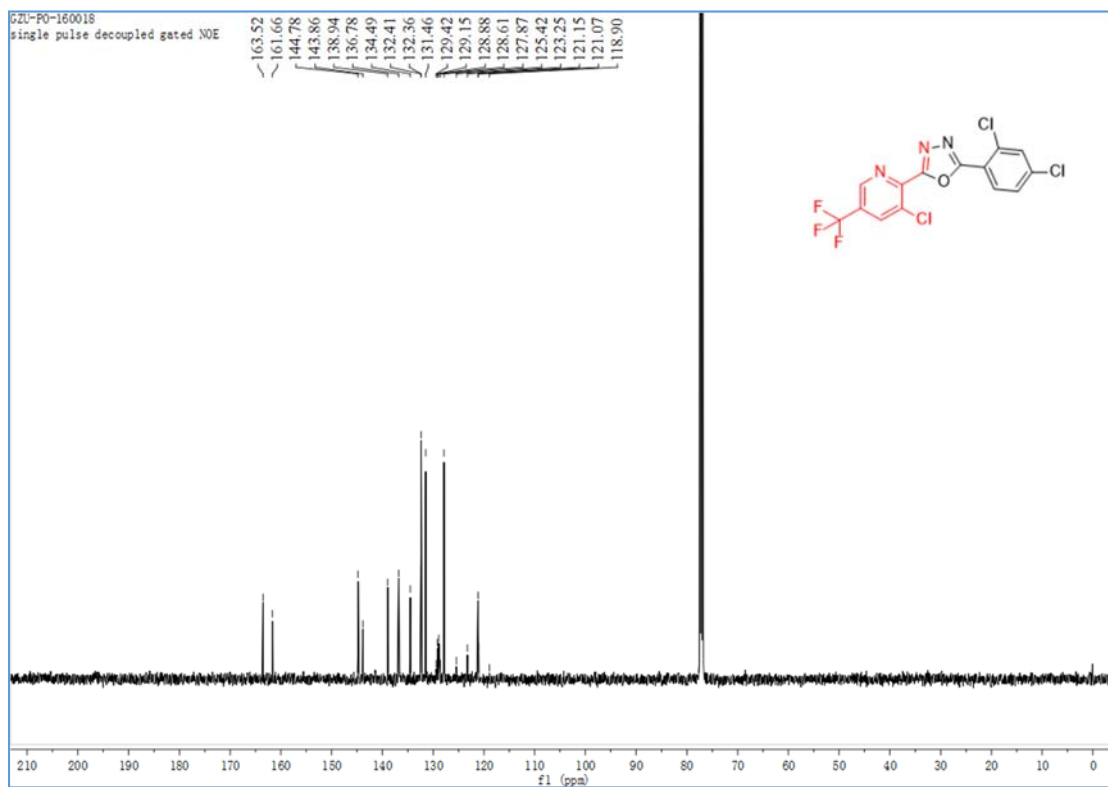


Fig. S109 ^{13}C NMR spectra of compound **E28**

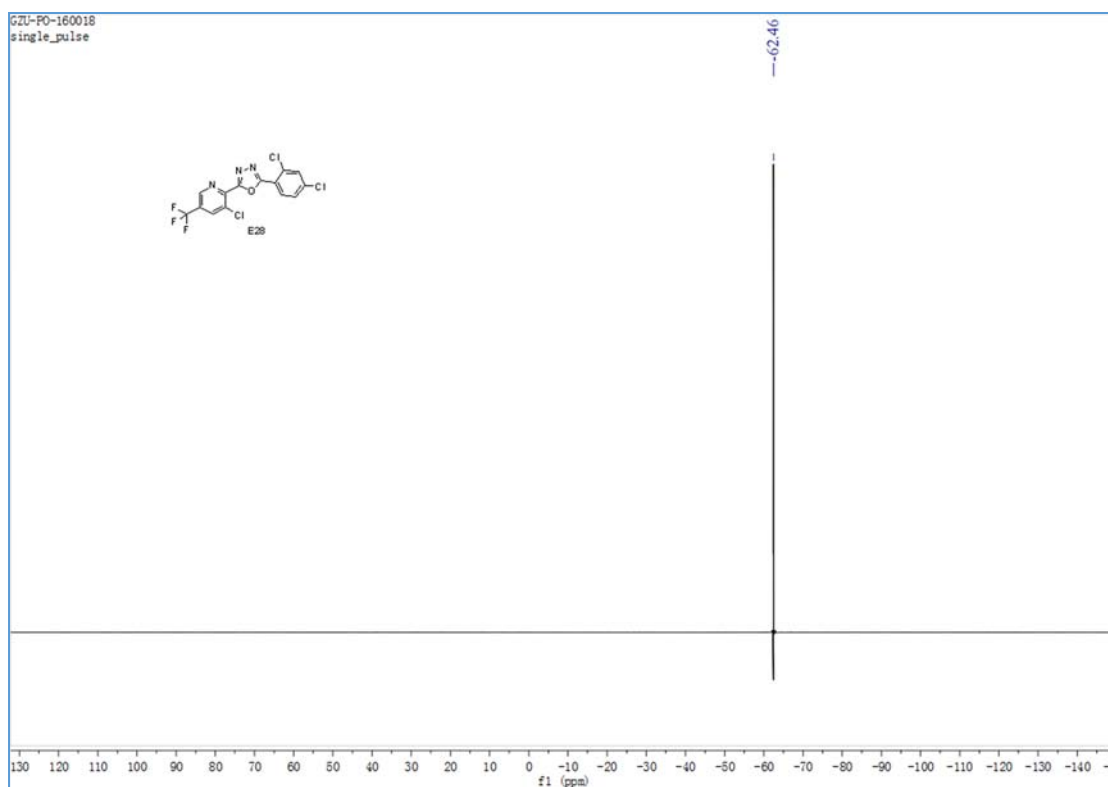


Fig. S110 ^{19}F NMR spectra of compound **E28**

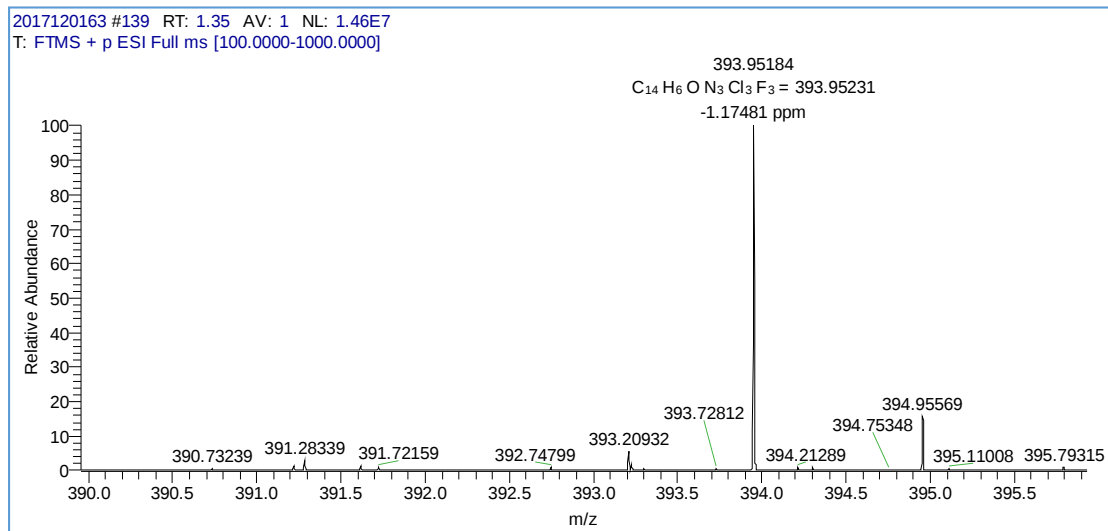


Fig. S111 HR-MS spectra of compound **E28**