

Supporting Information

Enantioselective Construction of Tertiary α -alkyl Fluoride via BTM Catalysed Fluorination of α -Alkynyl Substituted Acetic Acids

Shiru Yuan, Wen-Hua Zheng*

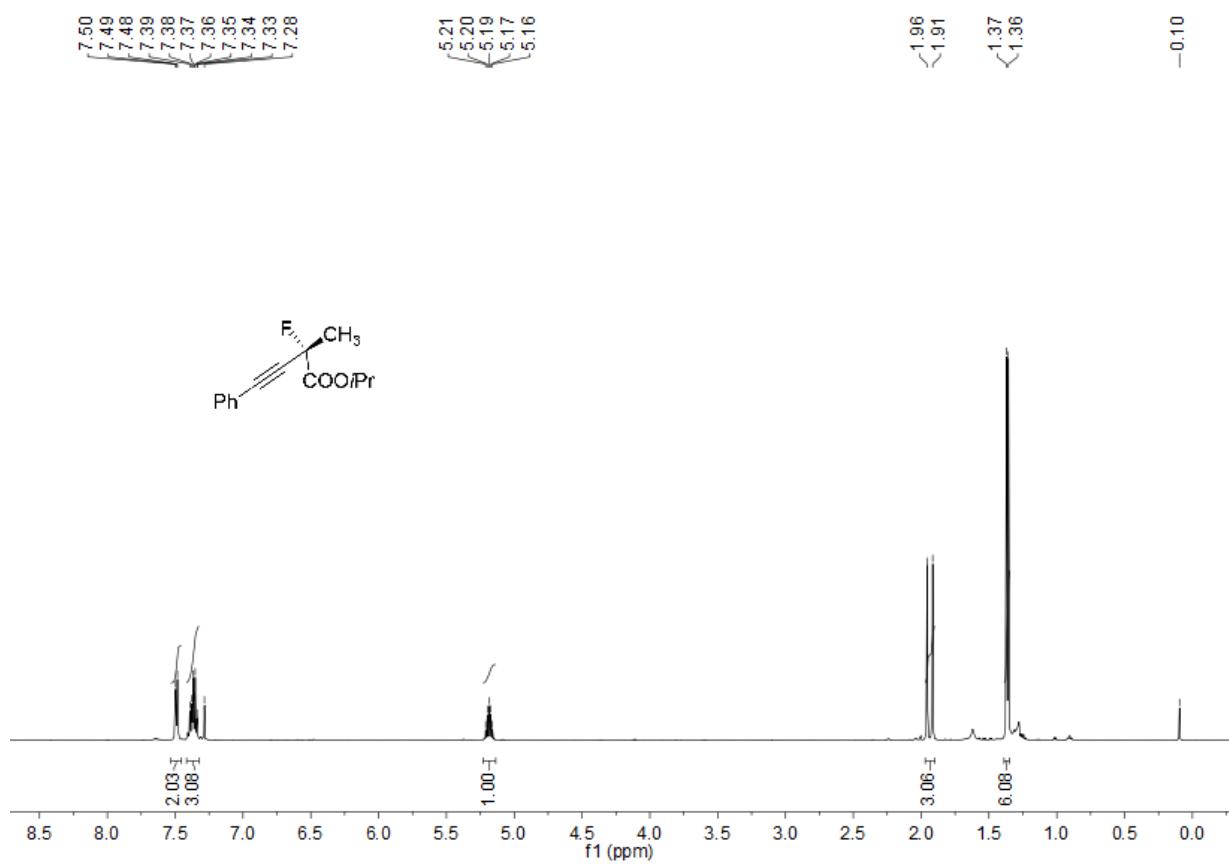
wzheng@nju.edu.cn

State Key Laboratory of Coordination Chemistry, Jiangsu Key Laboratory of Advanced Organic Materials, School of Chemistry and Chemical Engineering, Nanjing University, 163 Xianlin Avenue, Nanjing 210023, Jiangsu, China

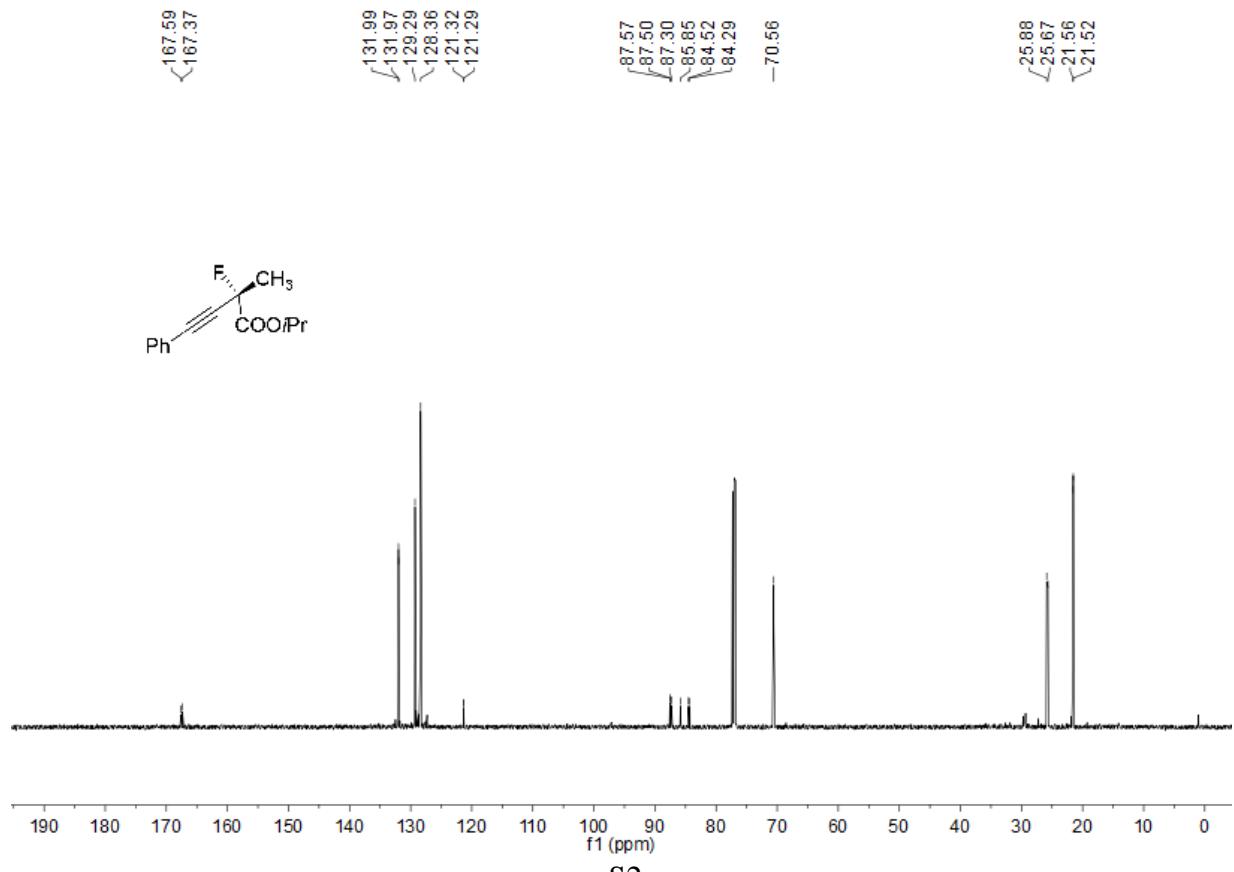
Table of Contents

NMR and HPLC Spectra for Products.....	S2-S69
-----------------------------------------------	---------------

^1H NMR of 2b (500 MHz, CDCl_3)

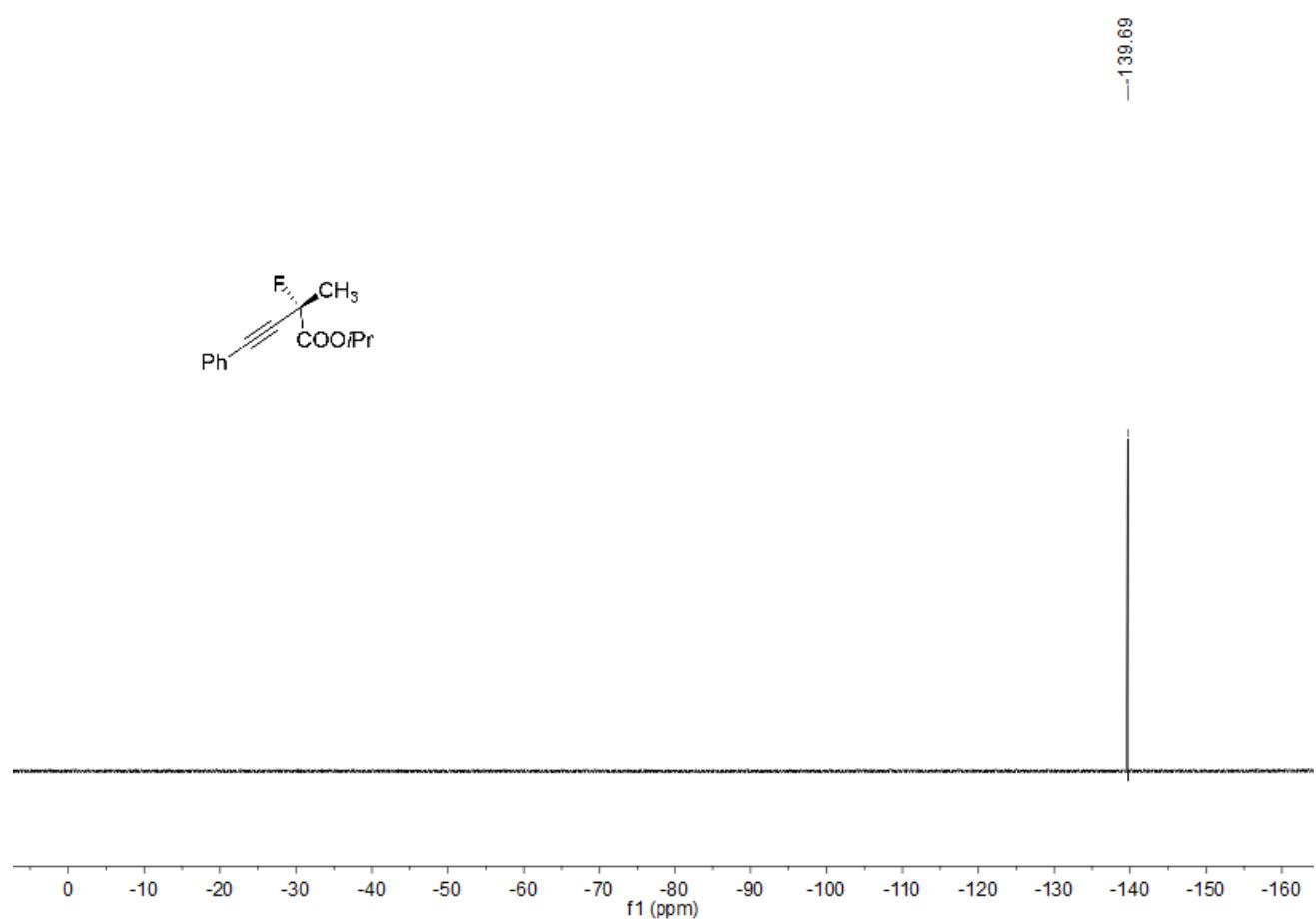


$^{13}\text{C}\{^1\text{H}\}$ NMR of 2b (125 MHz, CDCl_3)

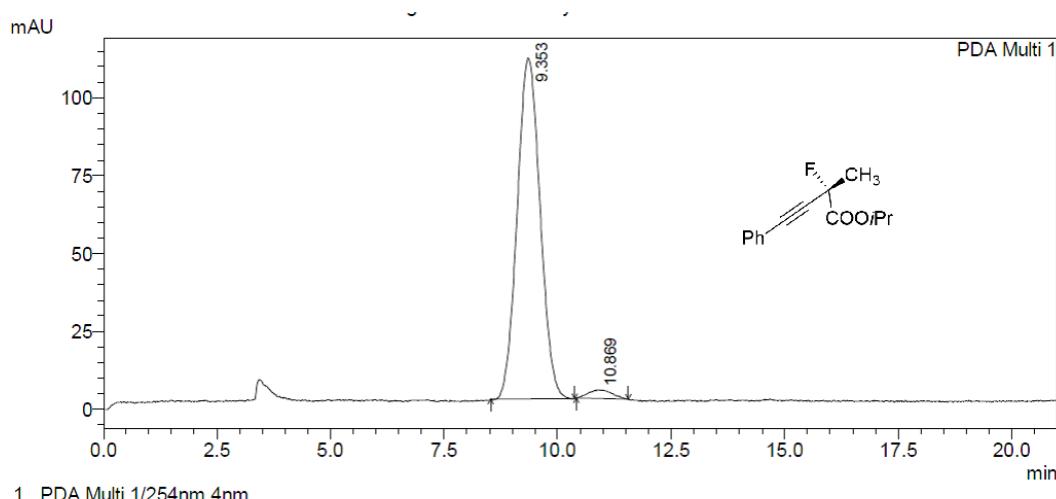
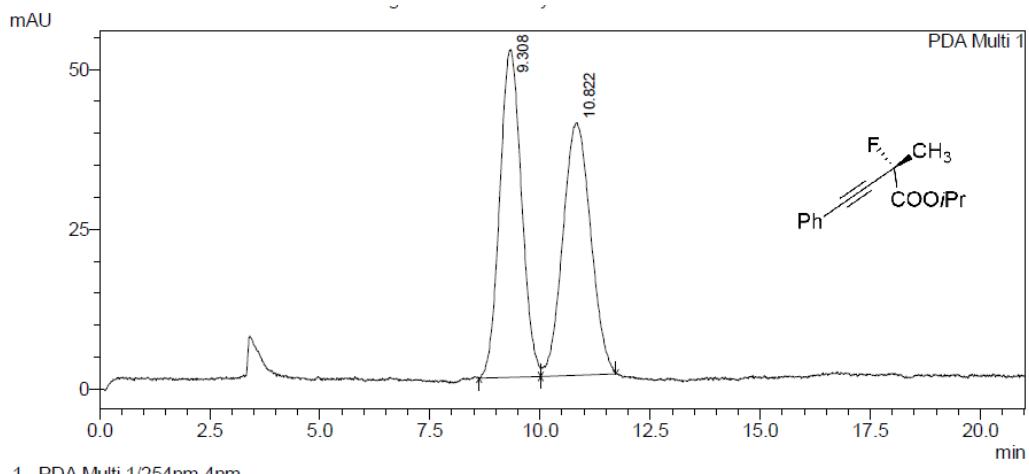


S2

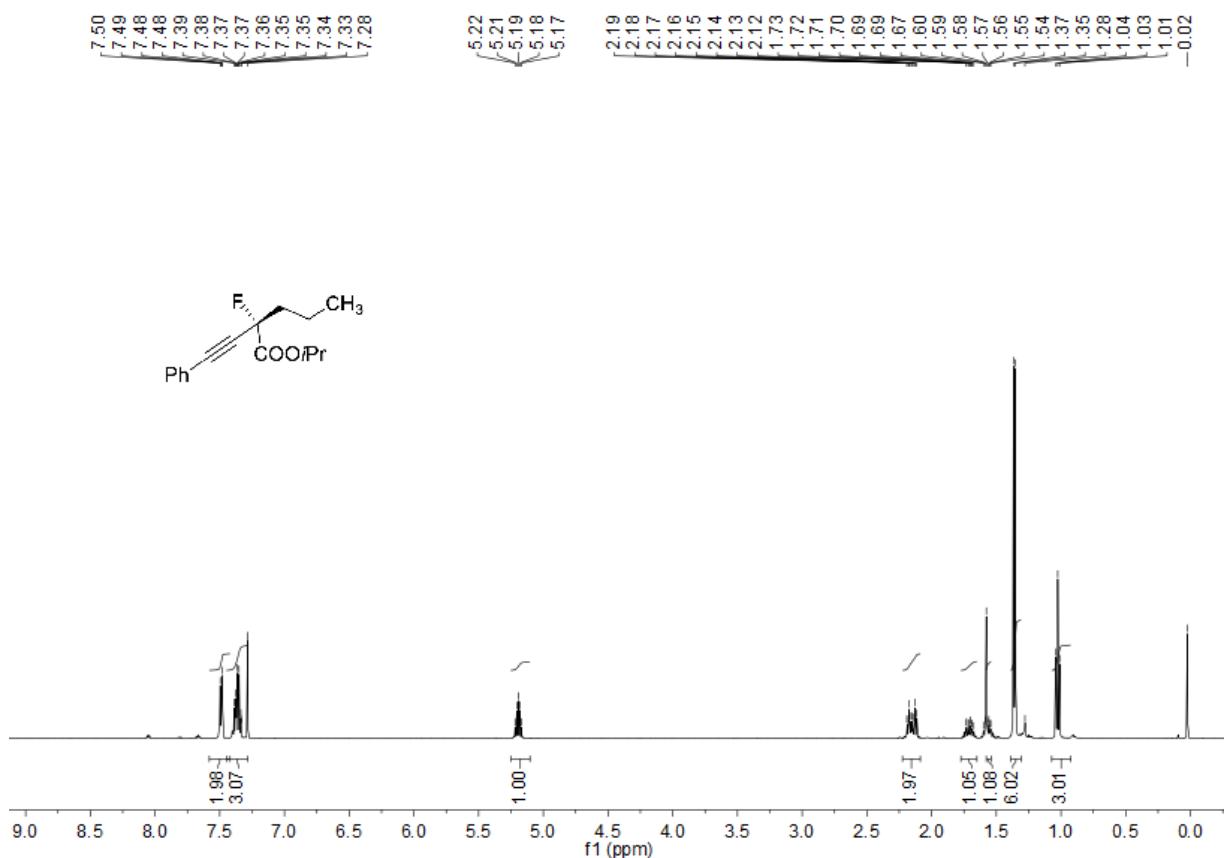
^{19}F NMR of 2b (470 MHz, CDCl_3)



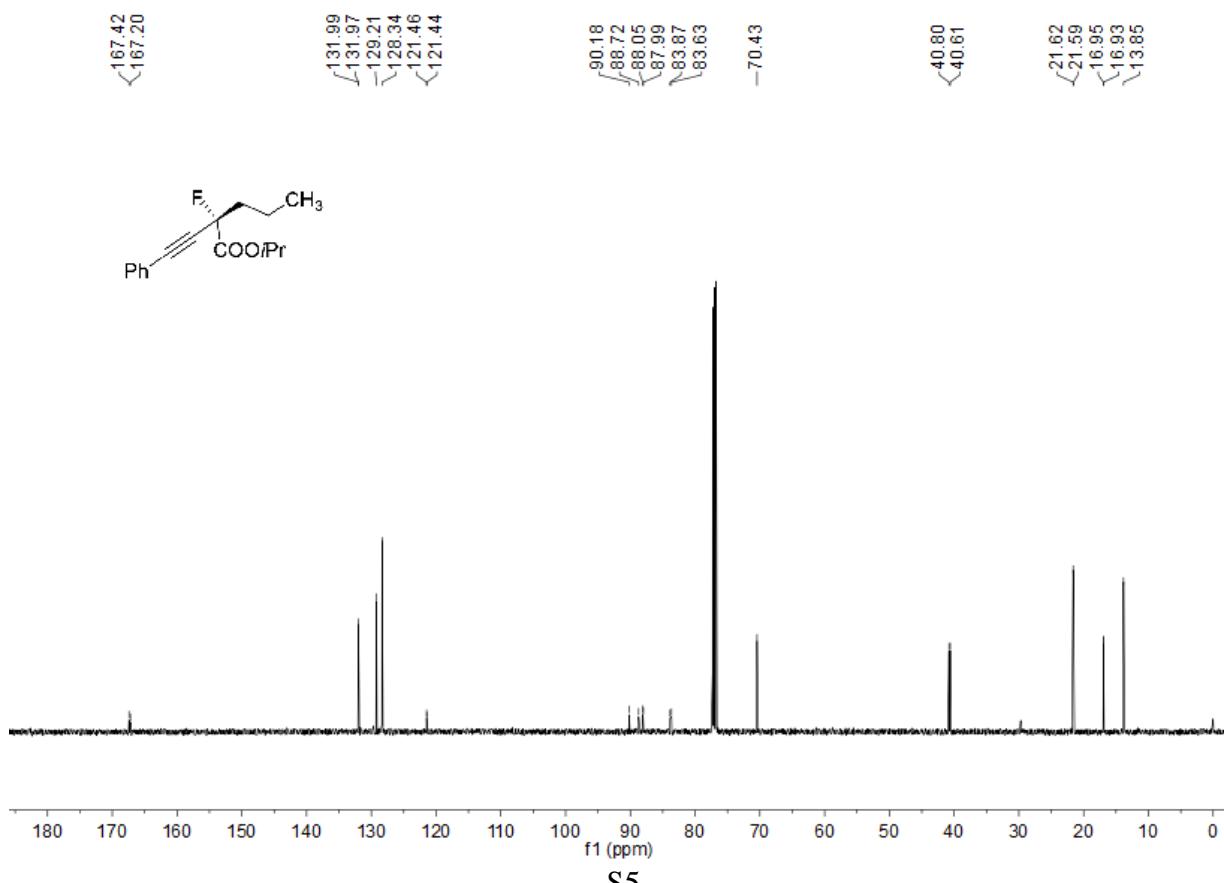
HPLC of 2b



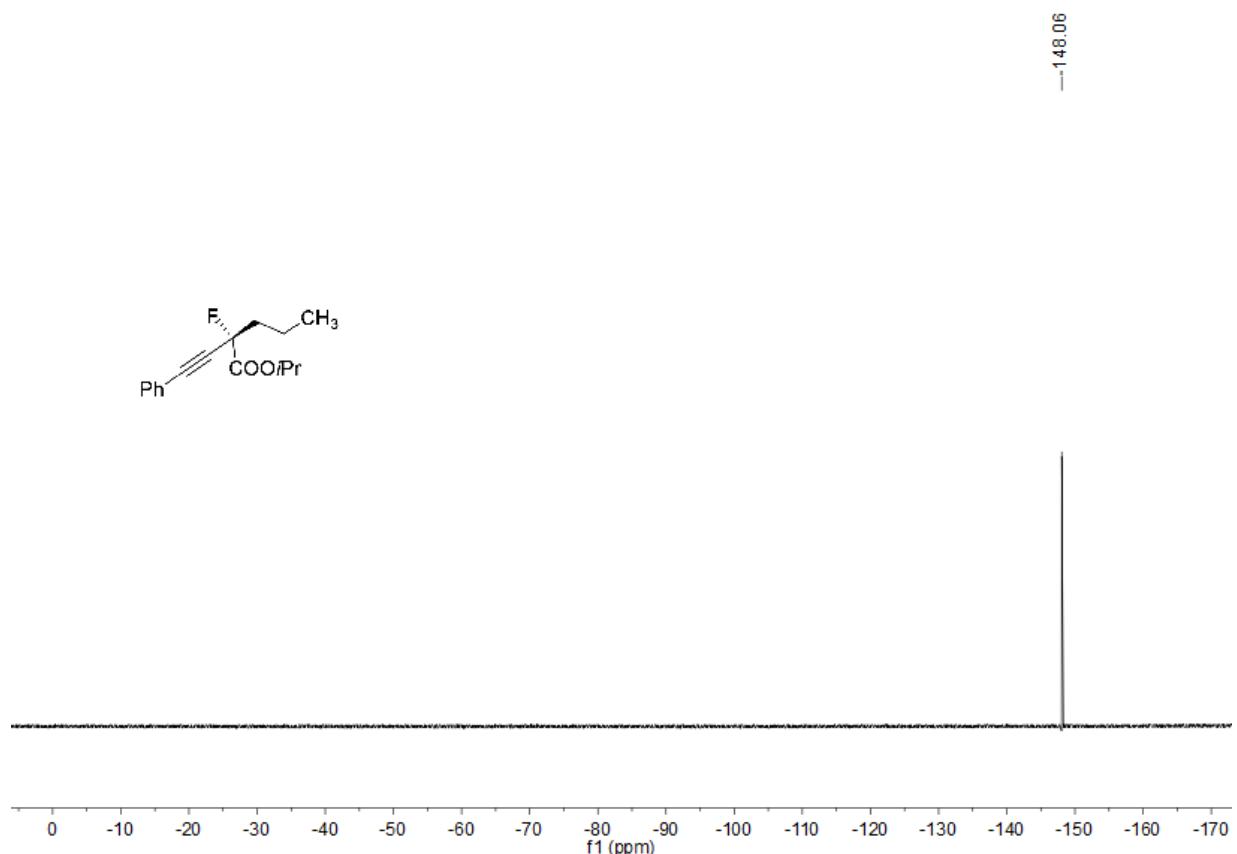
^1H NMR of 2c (500 MHz, CDCl_3)



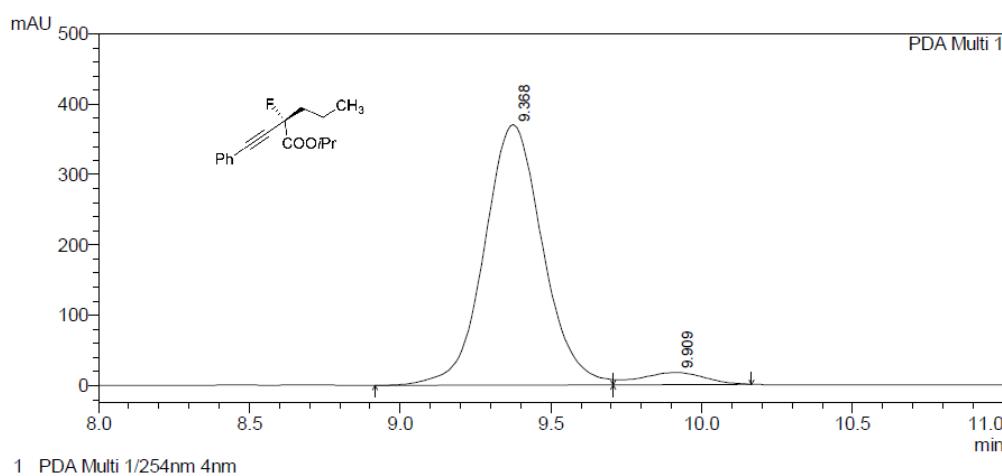
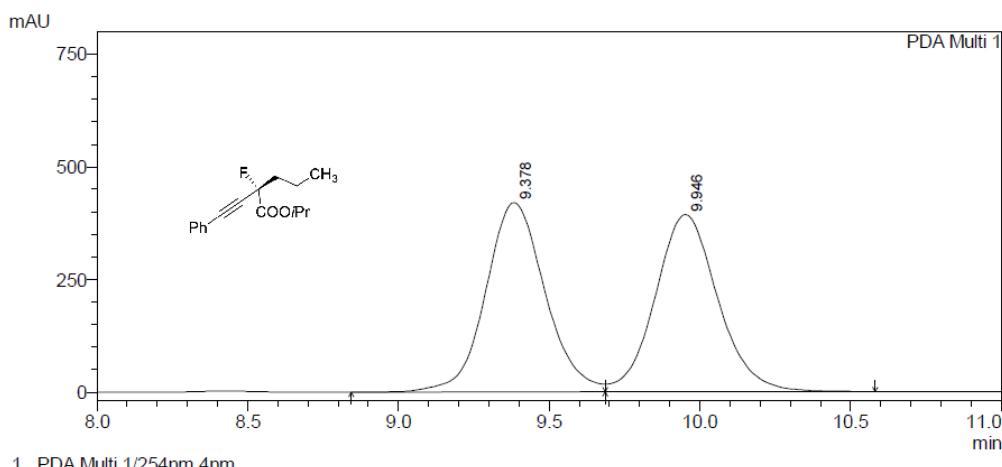
$^{13}\text{C}\{\text{H}\}$ NMR of 2c (125 MHz, CDCl_3)



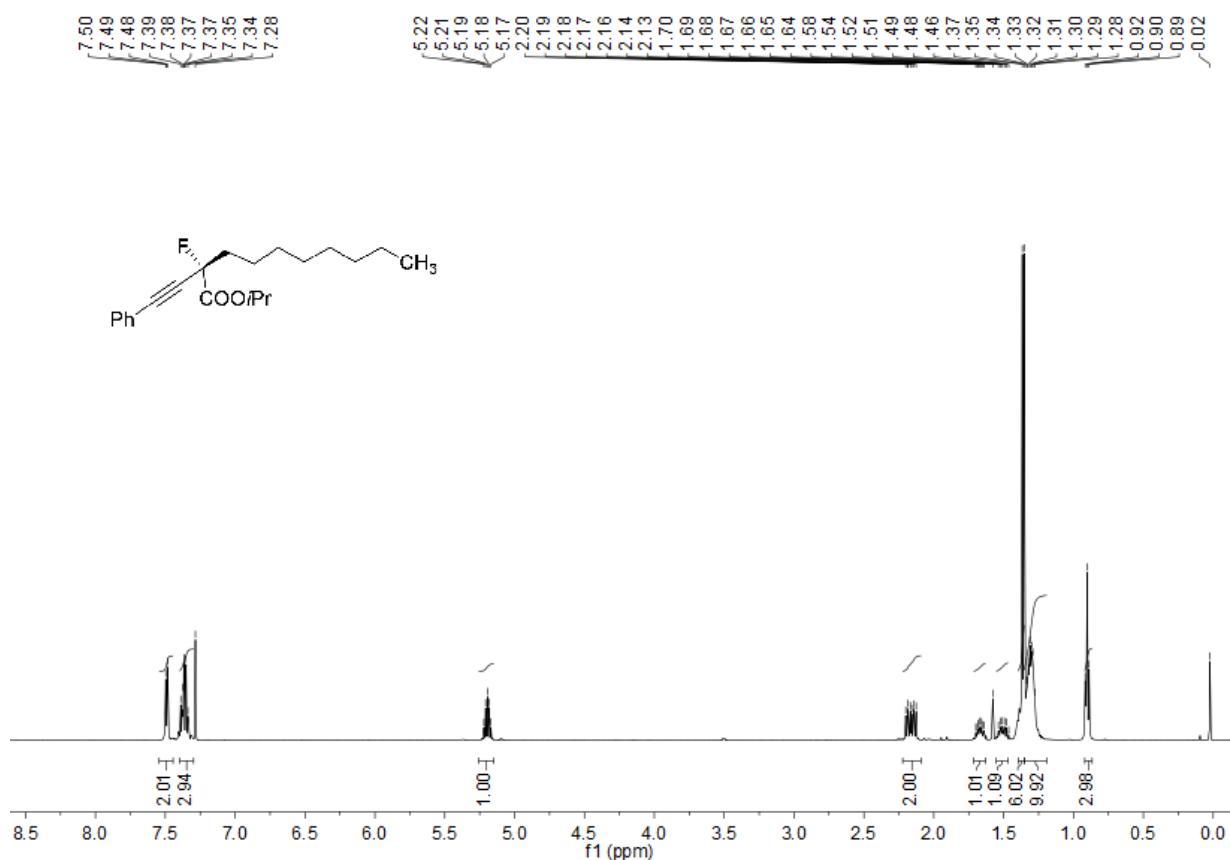
^{19}F NMR of 2c (470 MHz, CDCl_3)



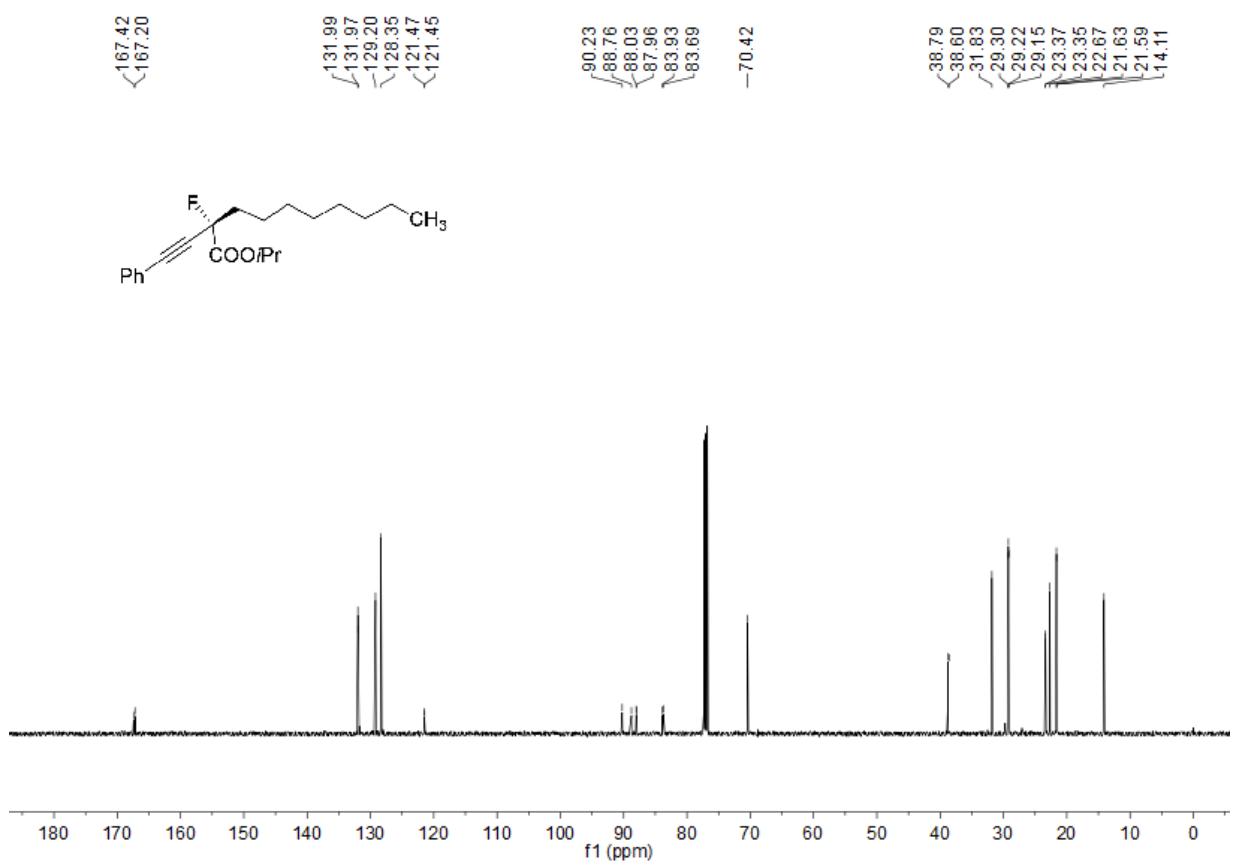
HPLC of 2c



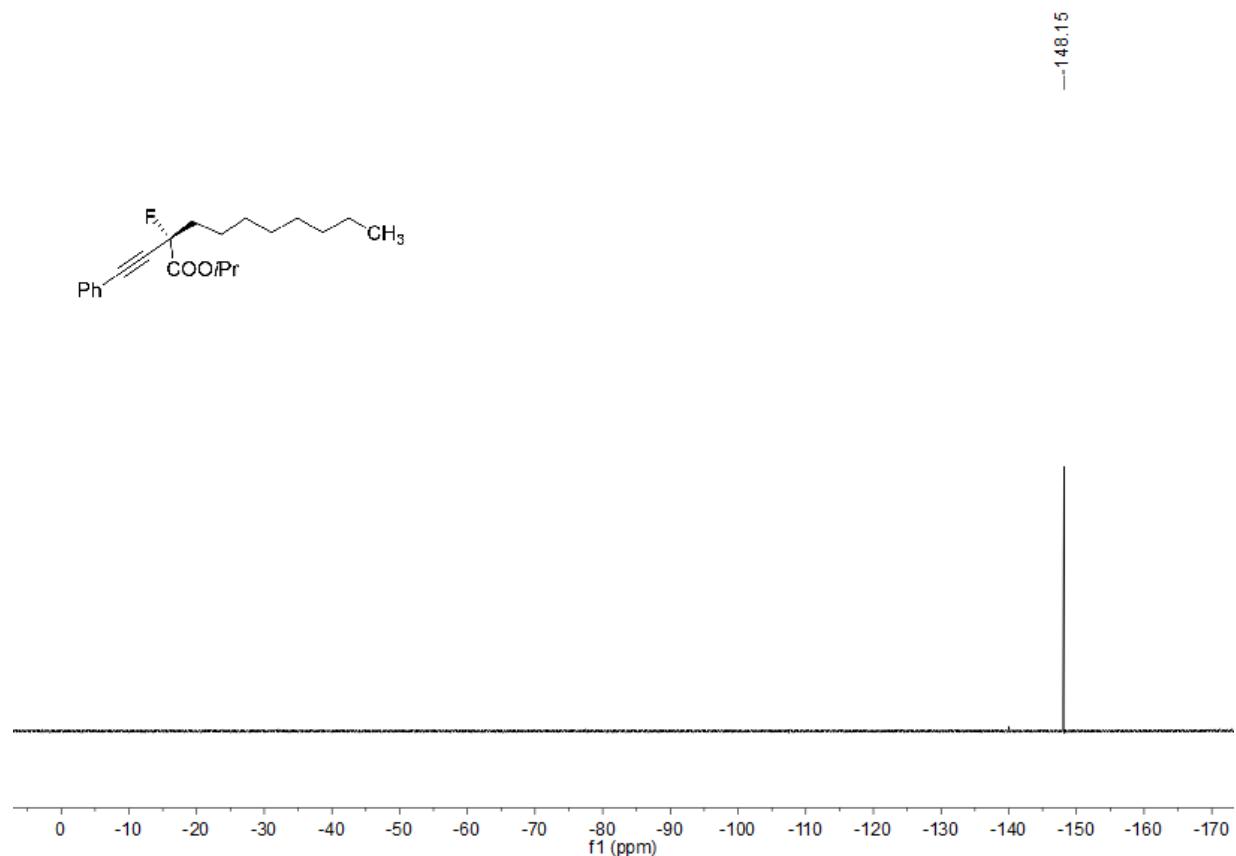
^1H NMR of 2d (500 MHz, CDCl_3)



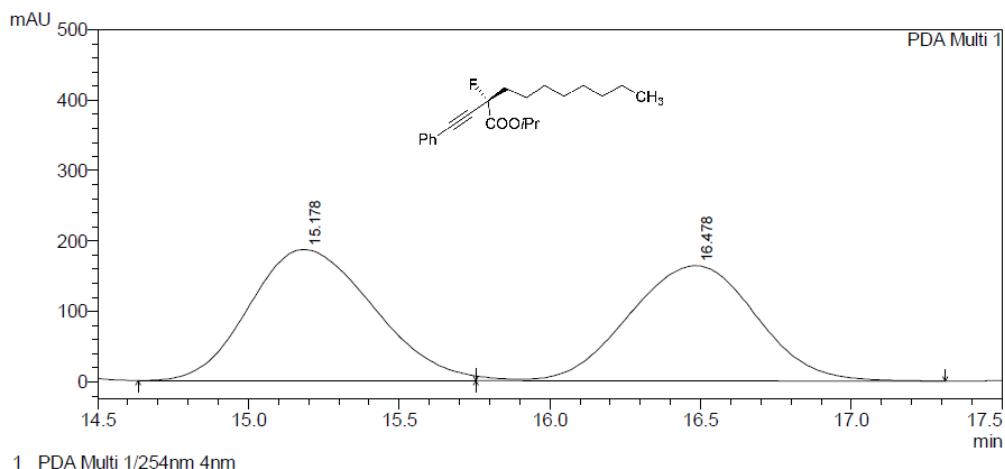
$^{13}\text{C}\{^1\text{H}\}$ NMR of 2d (125 MHz, CDCl_3)



¹⁹FNMR of 2d (470 MHz, CDCl₃)

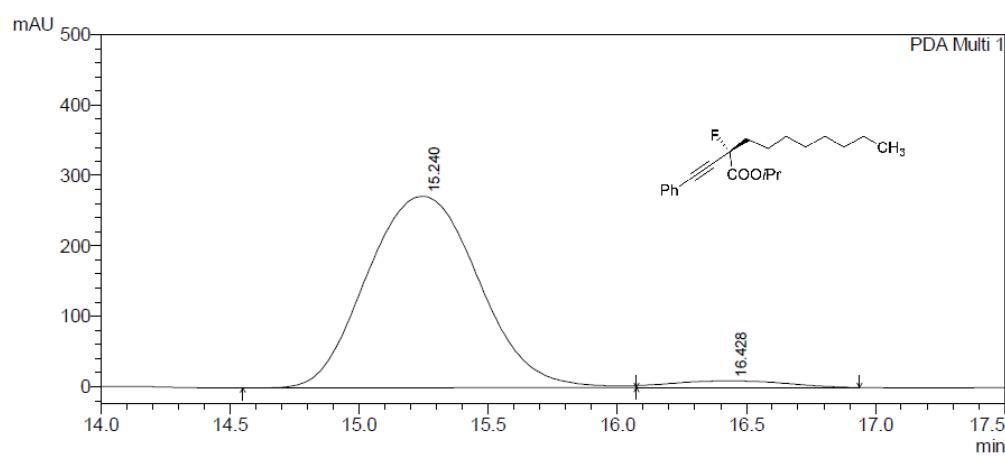


HPLC of 2d



PeakTable

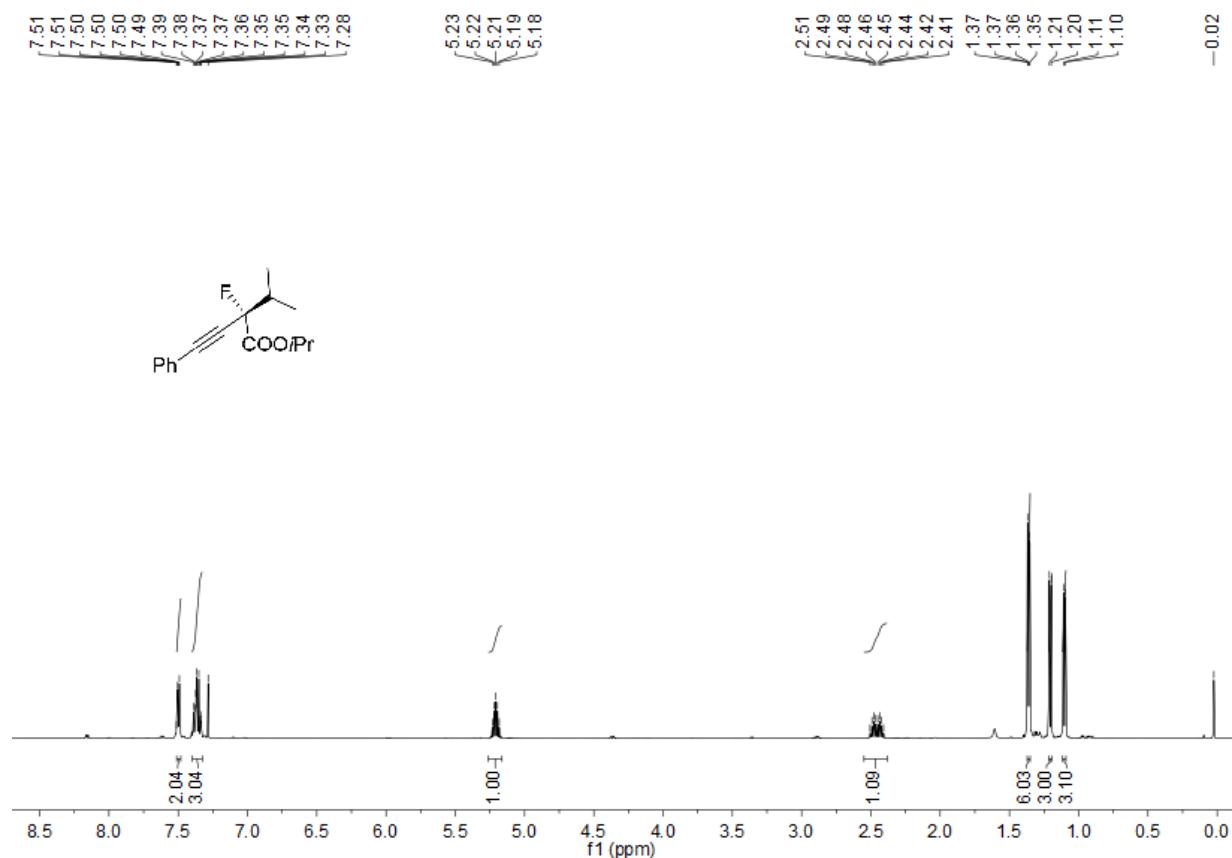
Peak#	Ret. Time	Area	Height	Area %	Height %
1	15.178	5315607	186247	52.419	53.231
2	16.478	4824970	163639	47.581	46.769
Total		10140578	349886	100.000	100.000



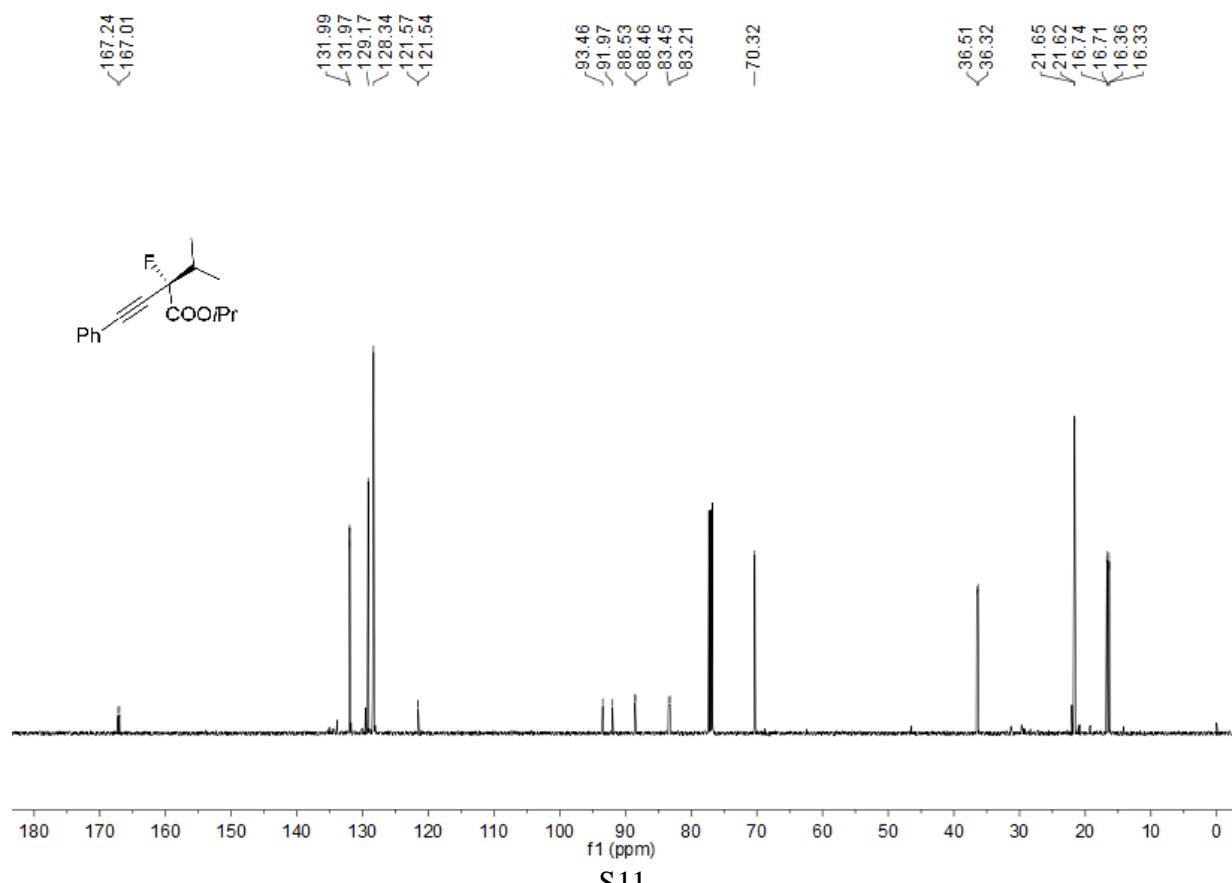
PeakTable

Peak#	Ret. Time	Area	Height	Area %	Height %
1	15.240	8186230	272274	96.513	96.568
2	16.428	295757	9676	3.487	3.432
Total		8481987	281949	100.000	100.000

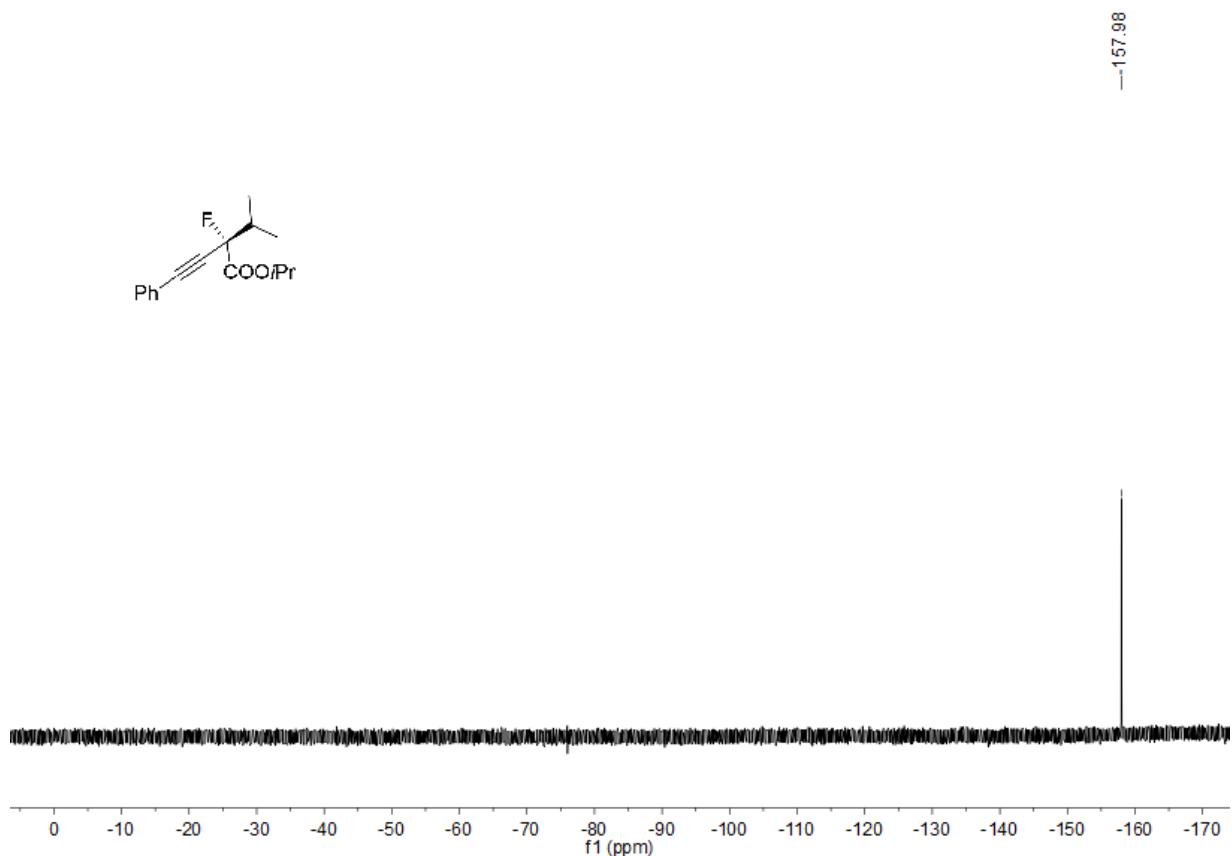
^1H NMR of 2e (500 MHz, CDCl_3)



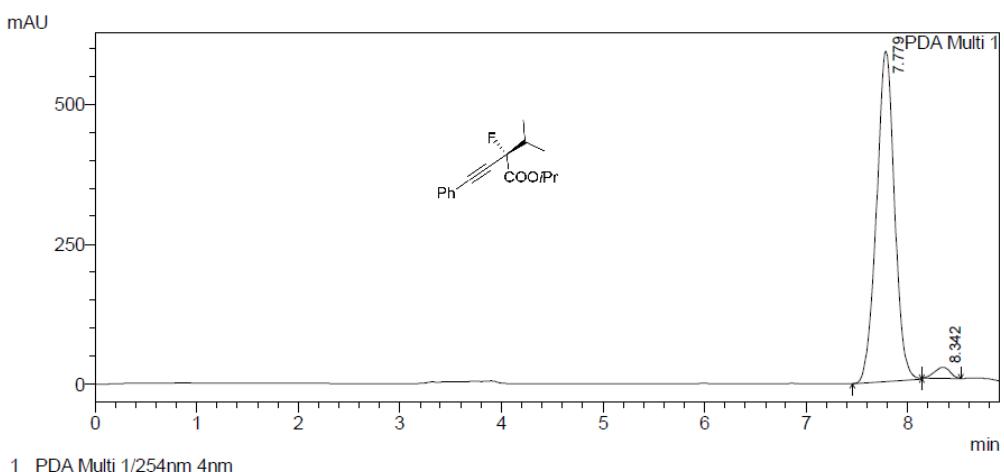
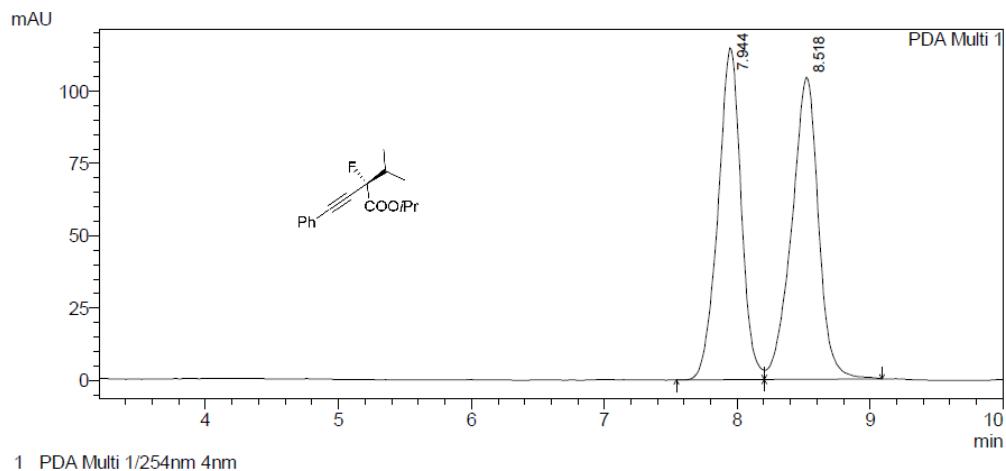
$^{13}\text{C}\{^1\text{H}\}$ NMR of 2e (125 MHz, CDCl_3)



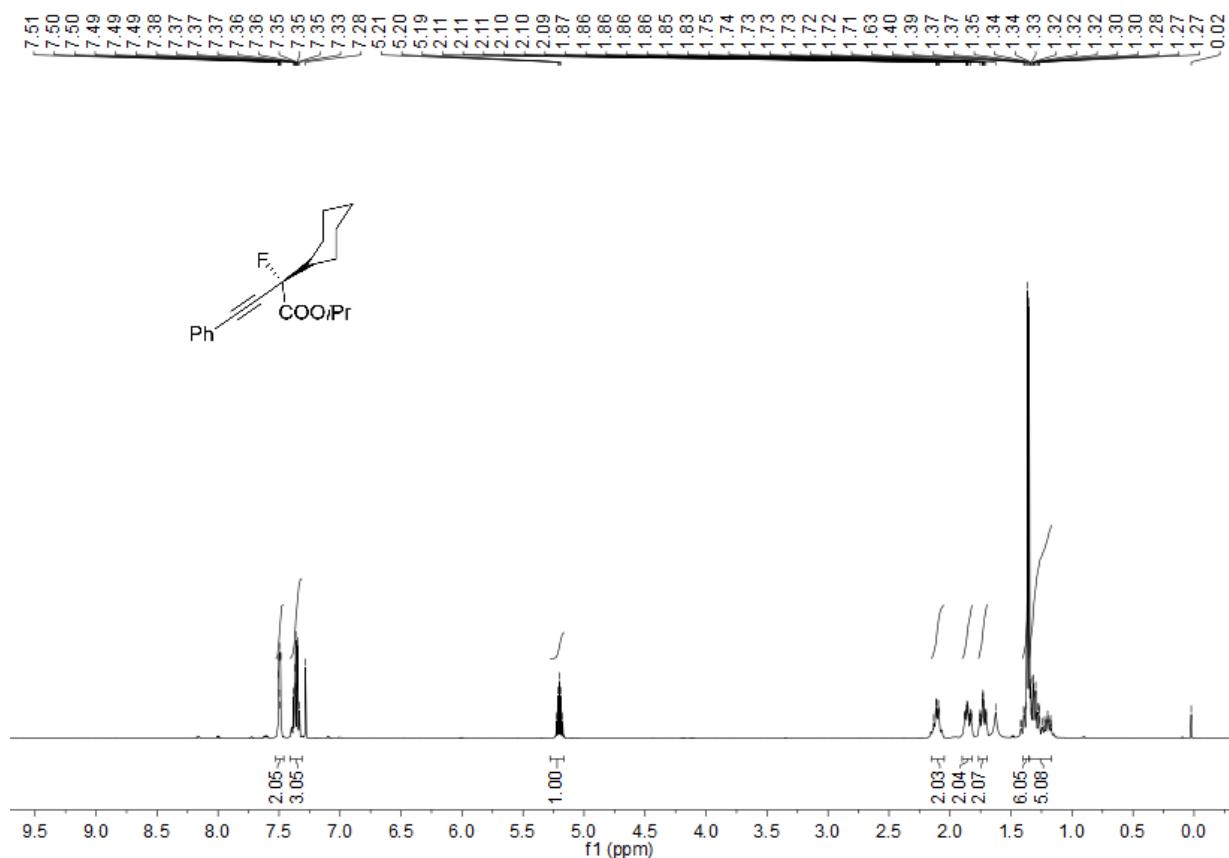
^{19}F NMR of 2e (470 MHz, CDCl_3)



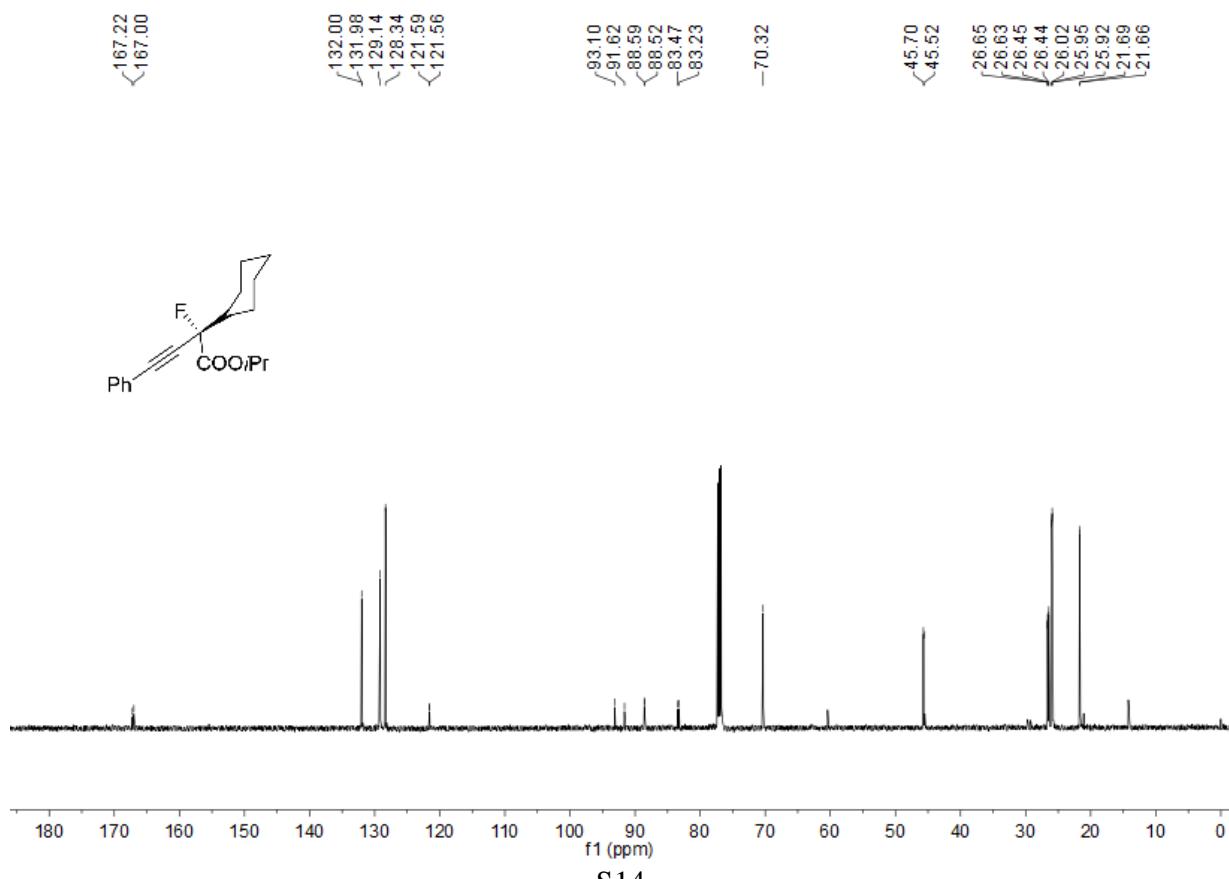
HPLC of 2e



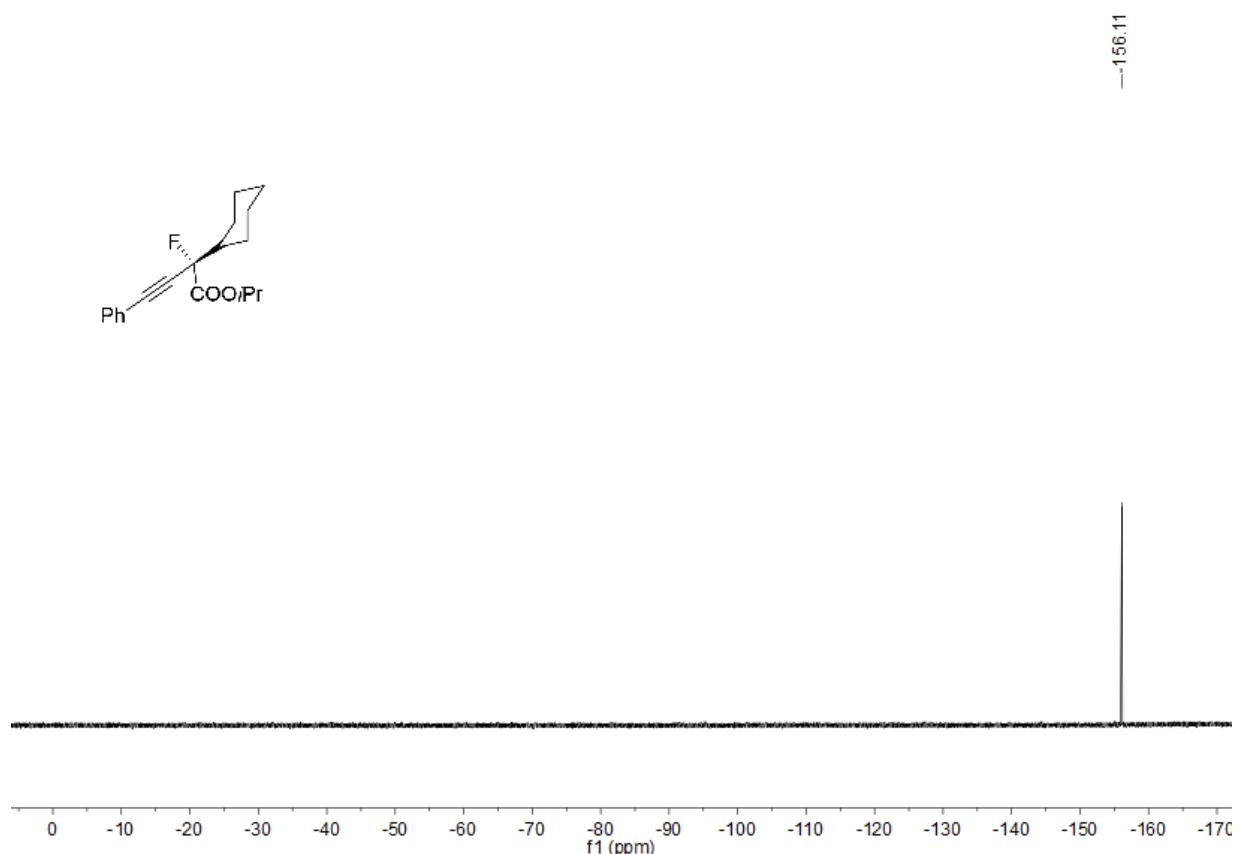
^1H NMR of 2f (500 MHz, CDCl_3)



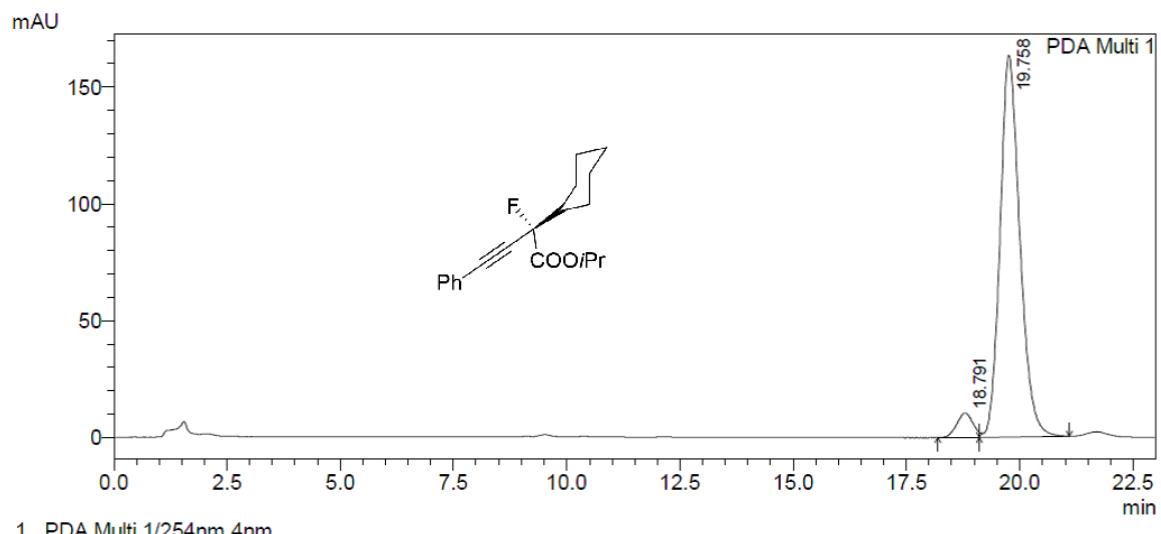
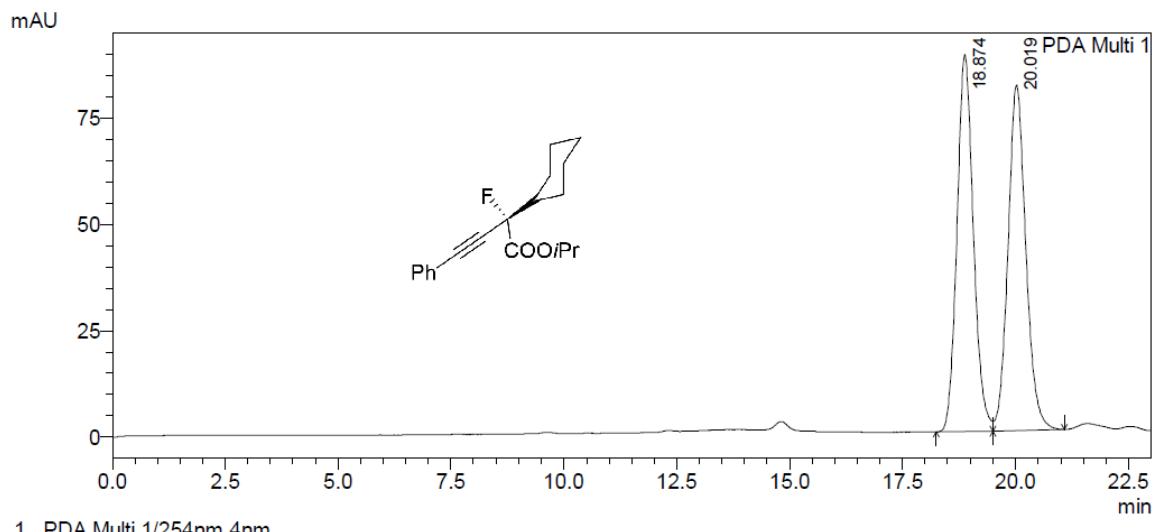
$^{13}\text{C}\{^1\text{H}\}$ NMR of 2f (125 MHz, CDCl_3)



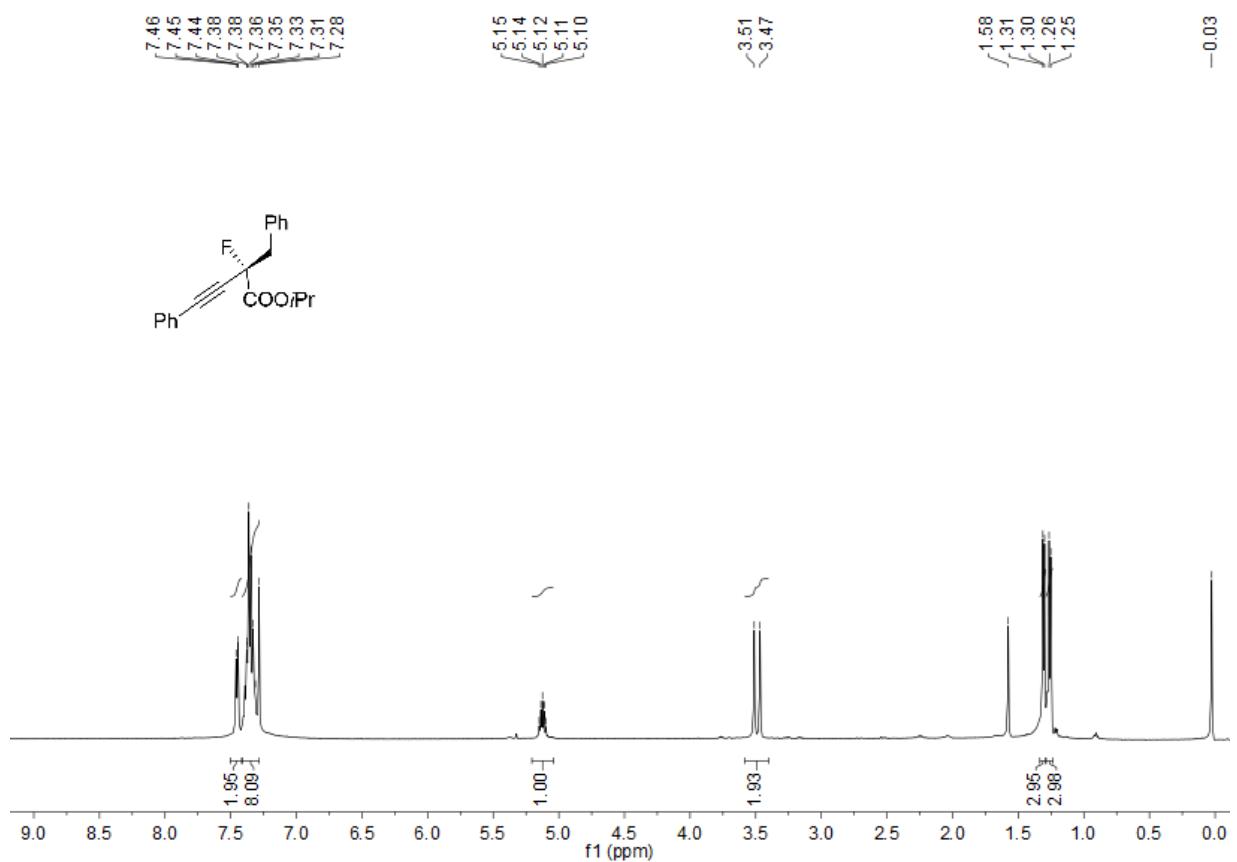
^{19}F NMR of 2f (470 MHz, CDCl_3)



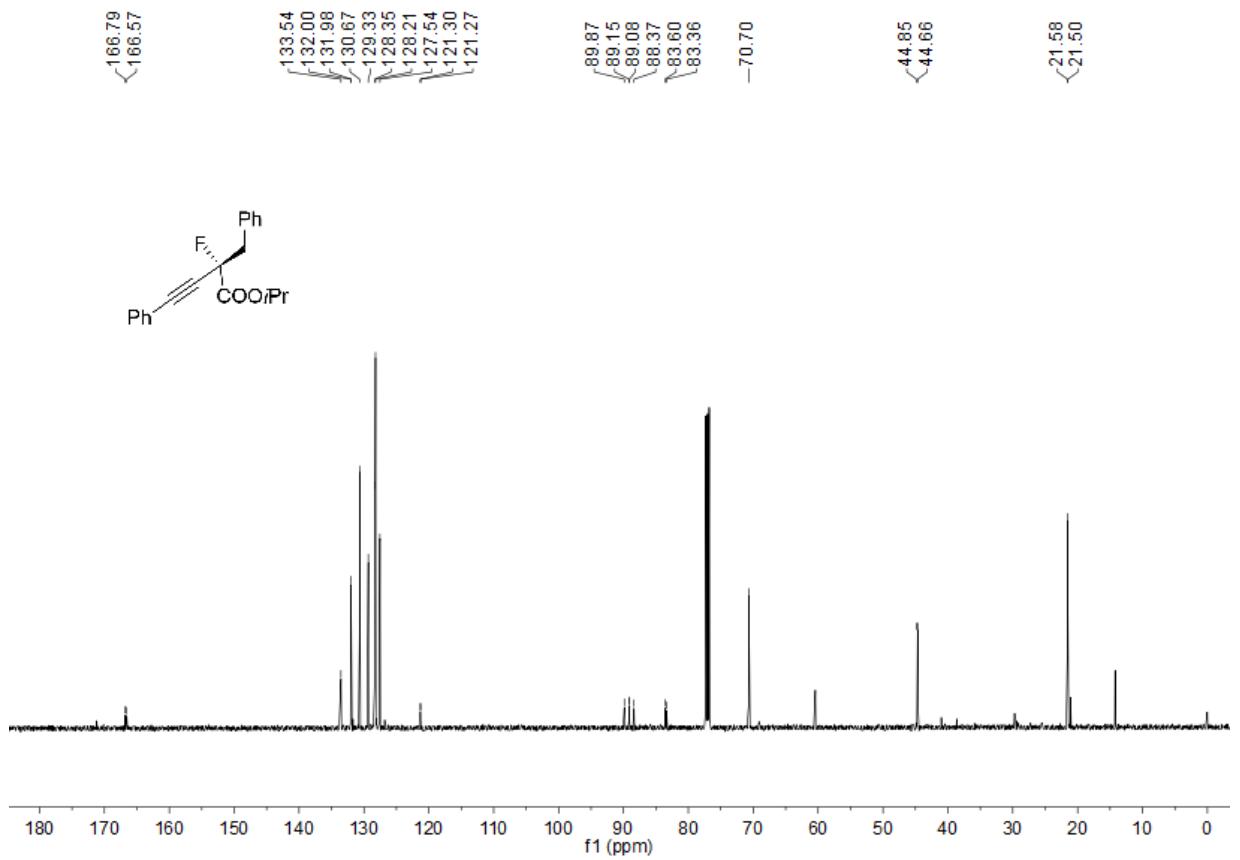
HPLC of 2f



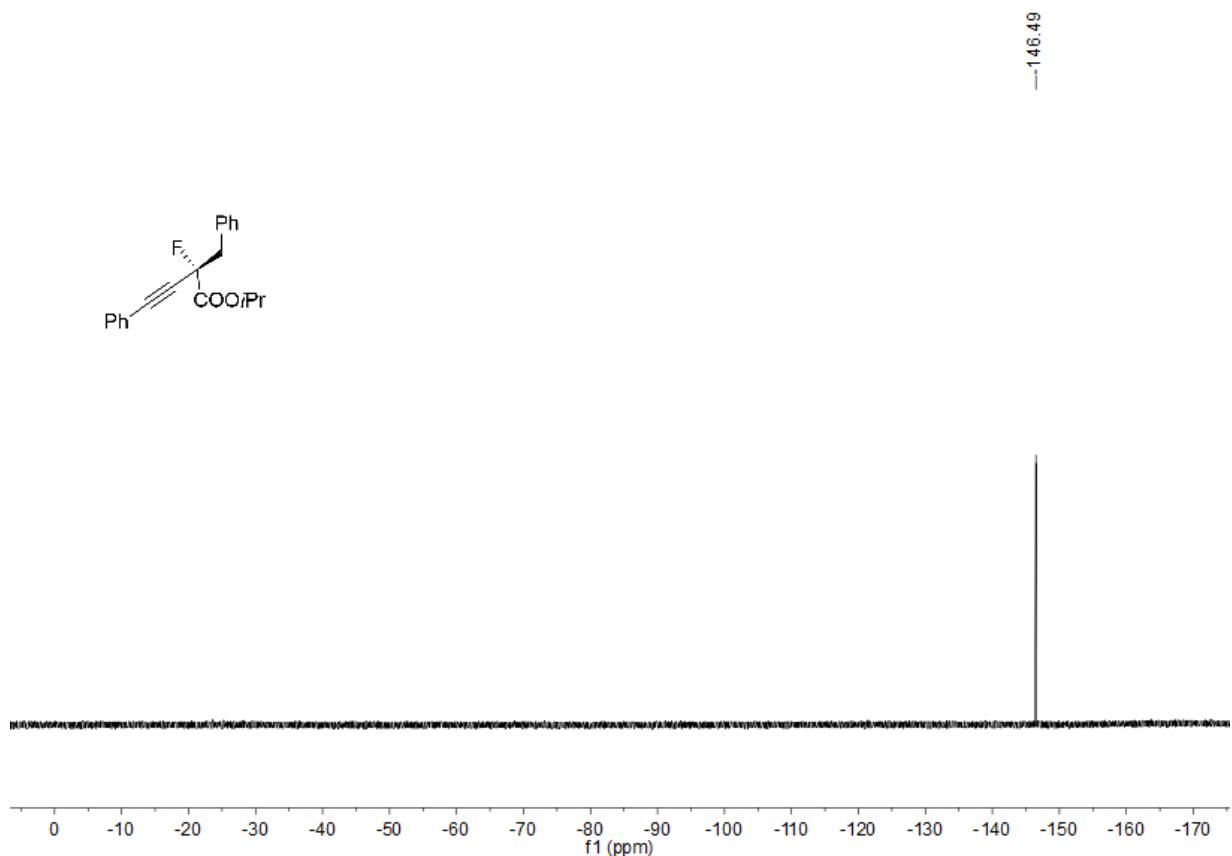
^1H NMR of 2g (500 MHz, CDCl_3)



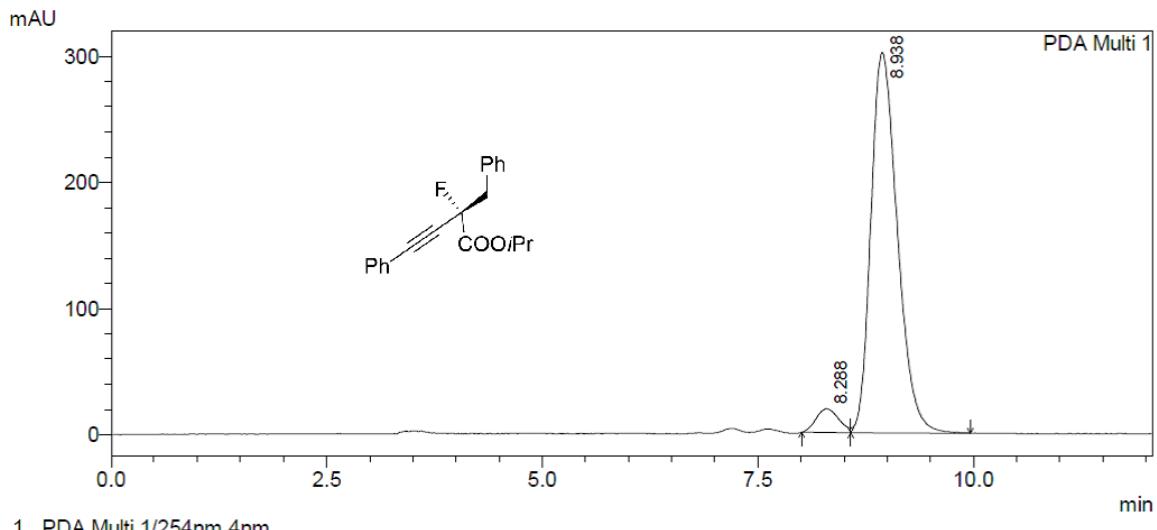
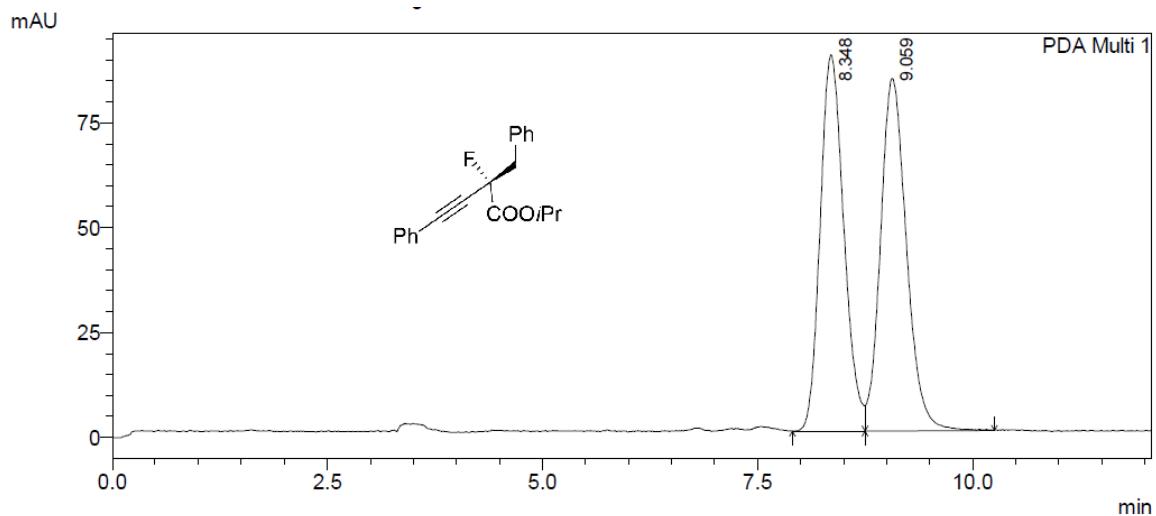
$^{13}\text{C}\{^1\text{H}\}$ NMR of 2g (125 MHz, CDCl_3)



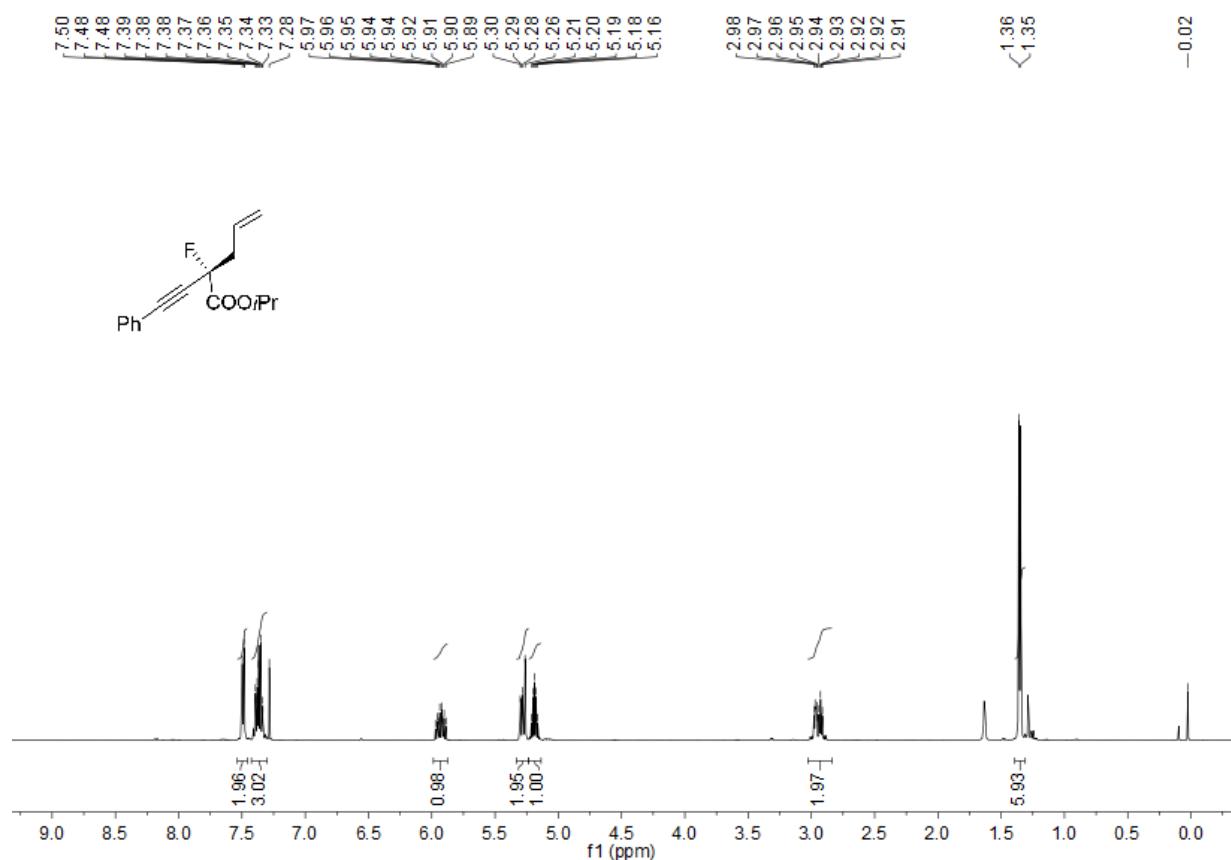
^{19}F NMR of 2g (470 MHz, CDCl_3)



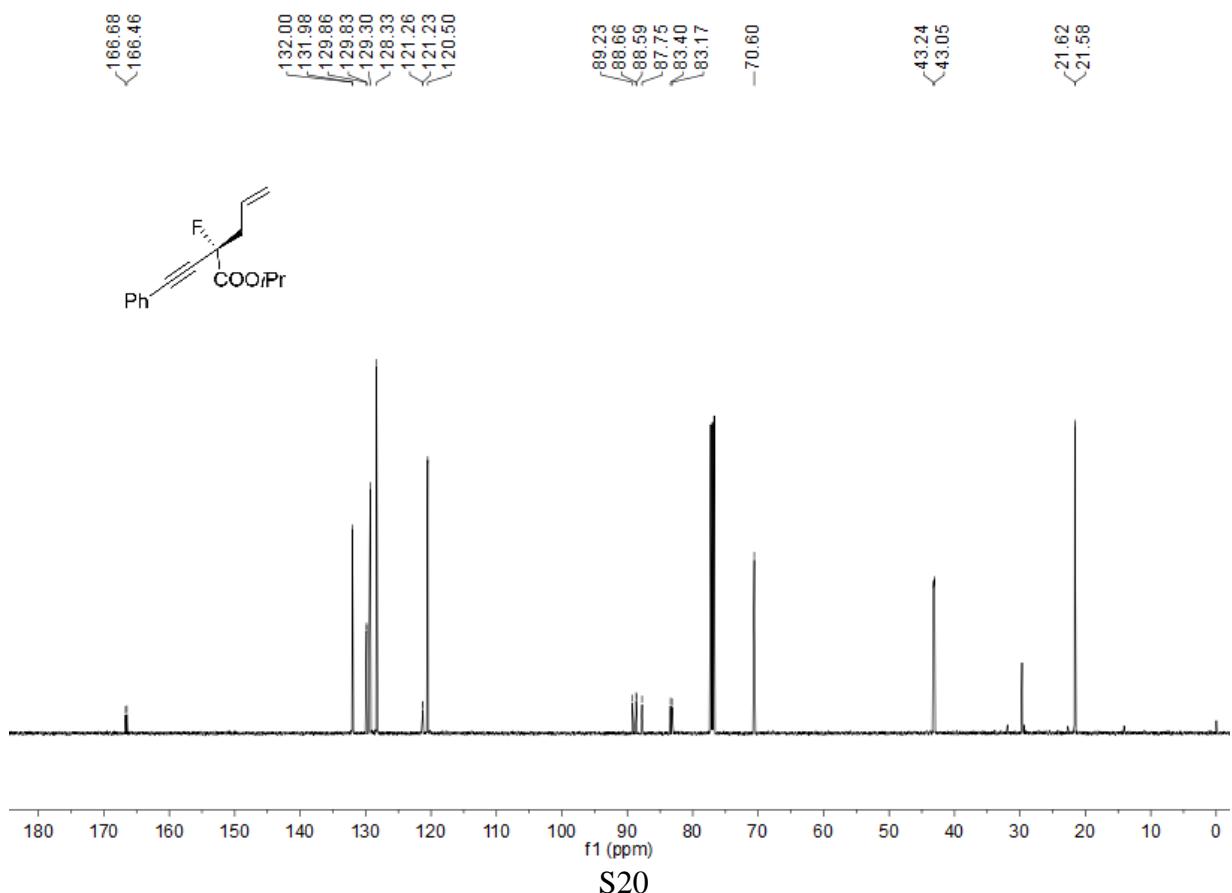
HPLC of 2g



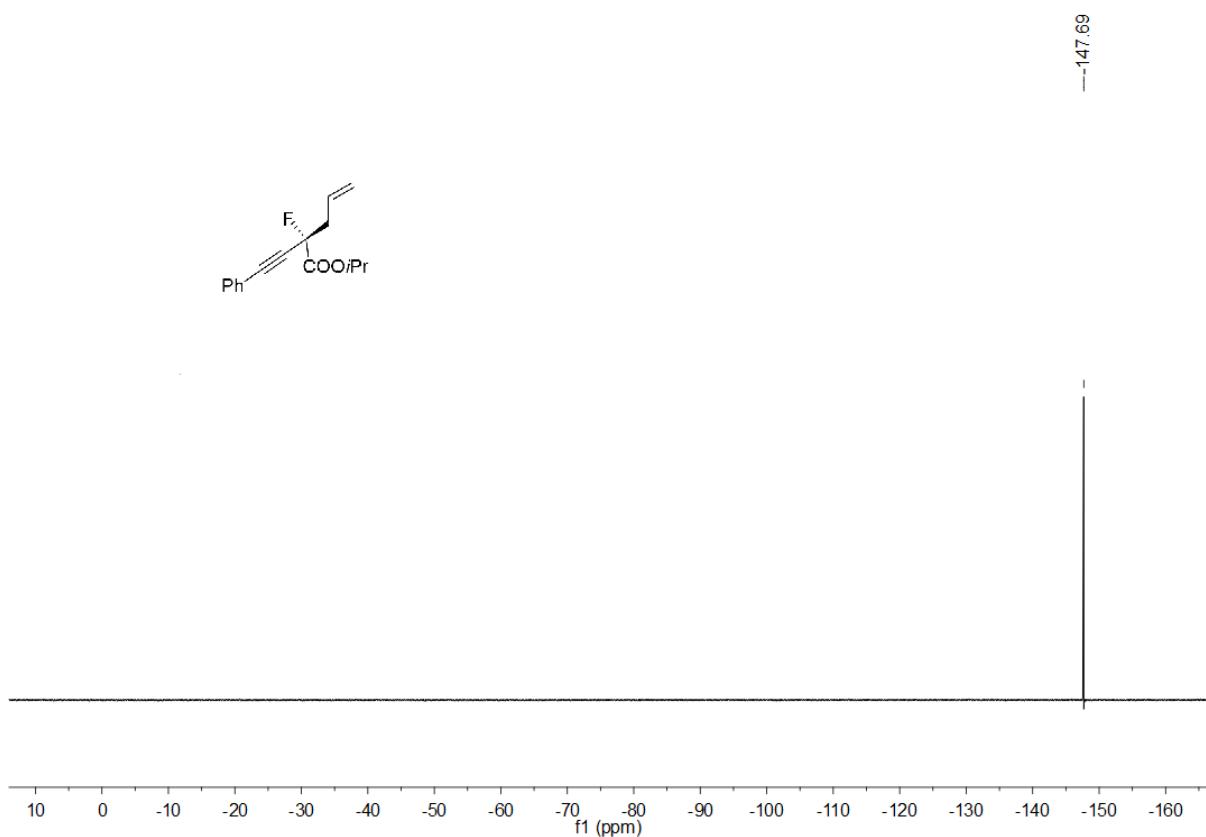
^1H NMR of 2h (500 MHz, CDCl_3)



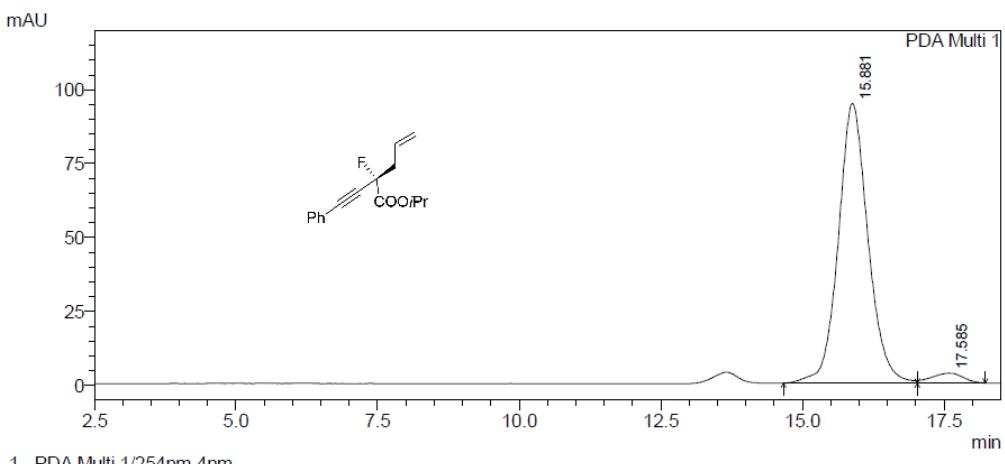
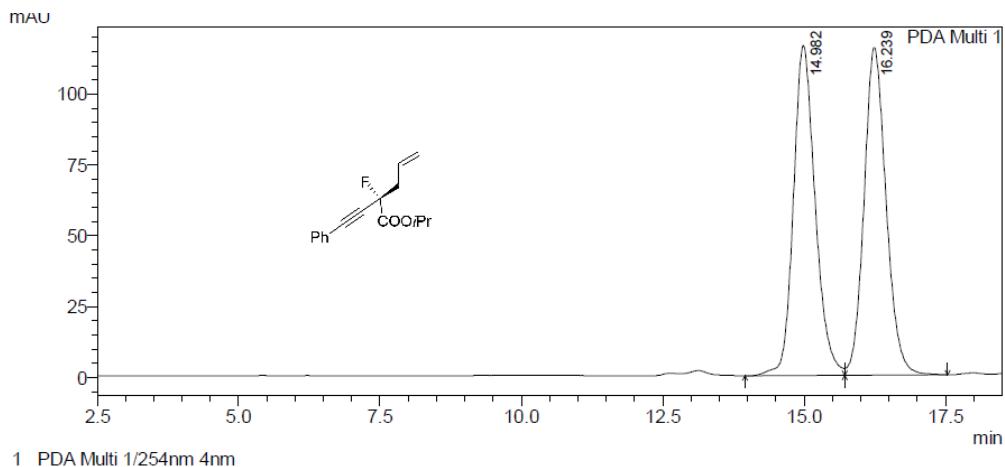
$^{13}\text{C}\{^1\text{H}\}$ NMR of 2h (125 MHz, CDCl_3)



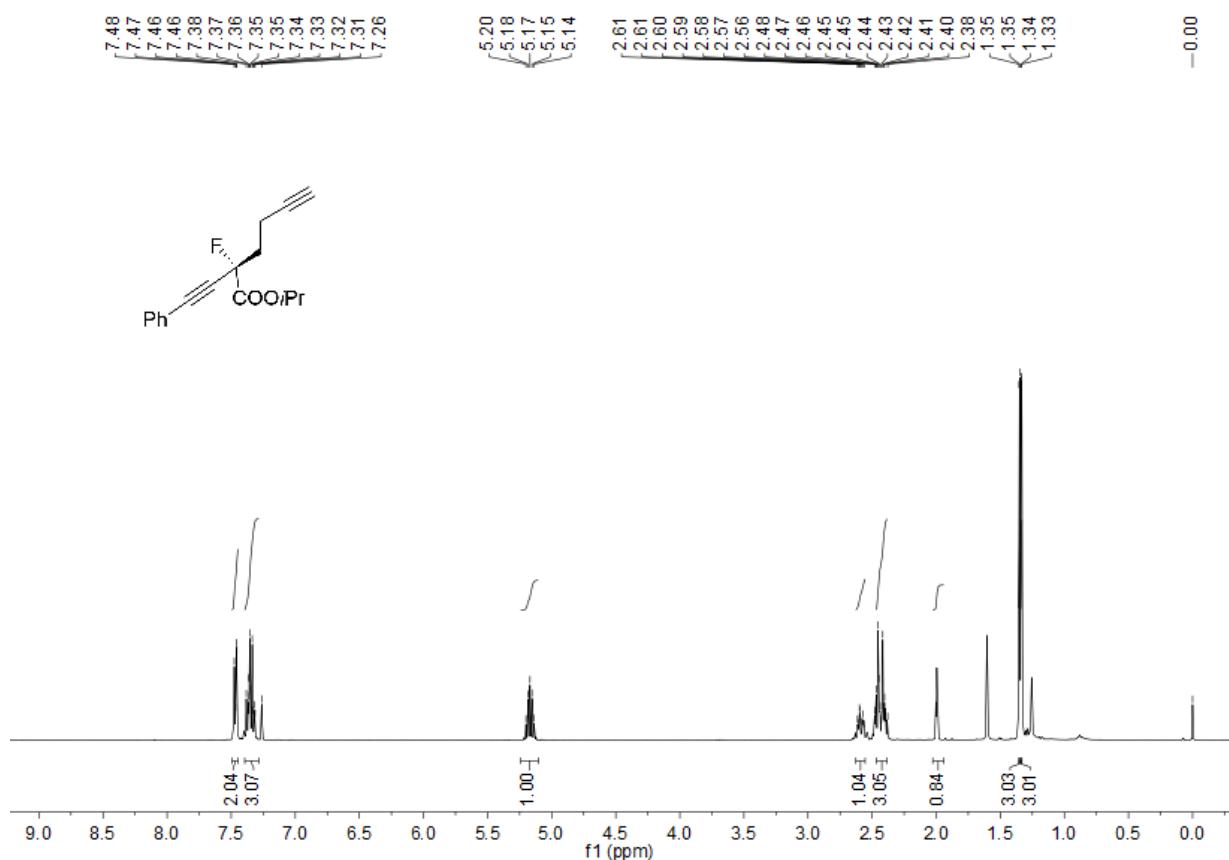
^{19}F NMR of 2h (470 MHz, CDCl_3)



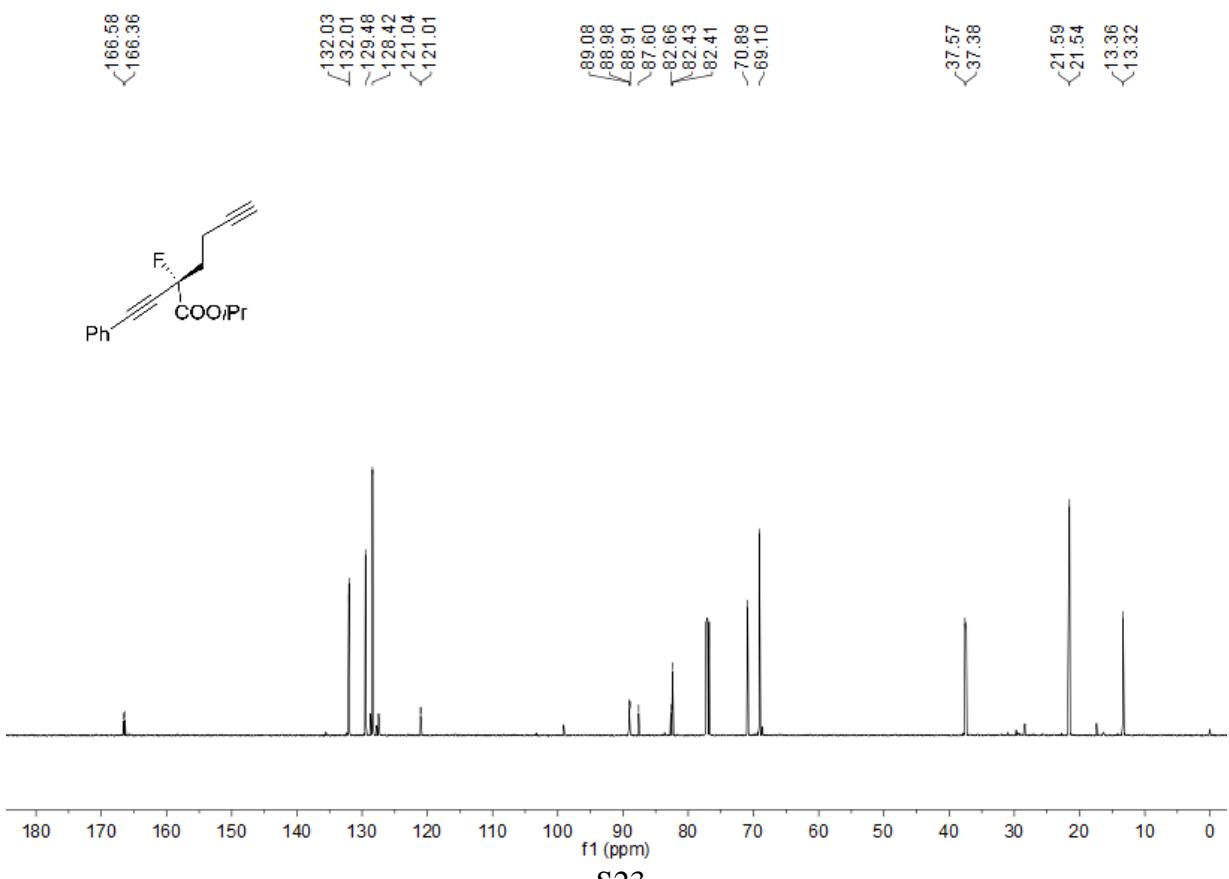
HPLC of 2h



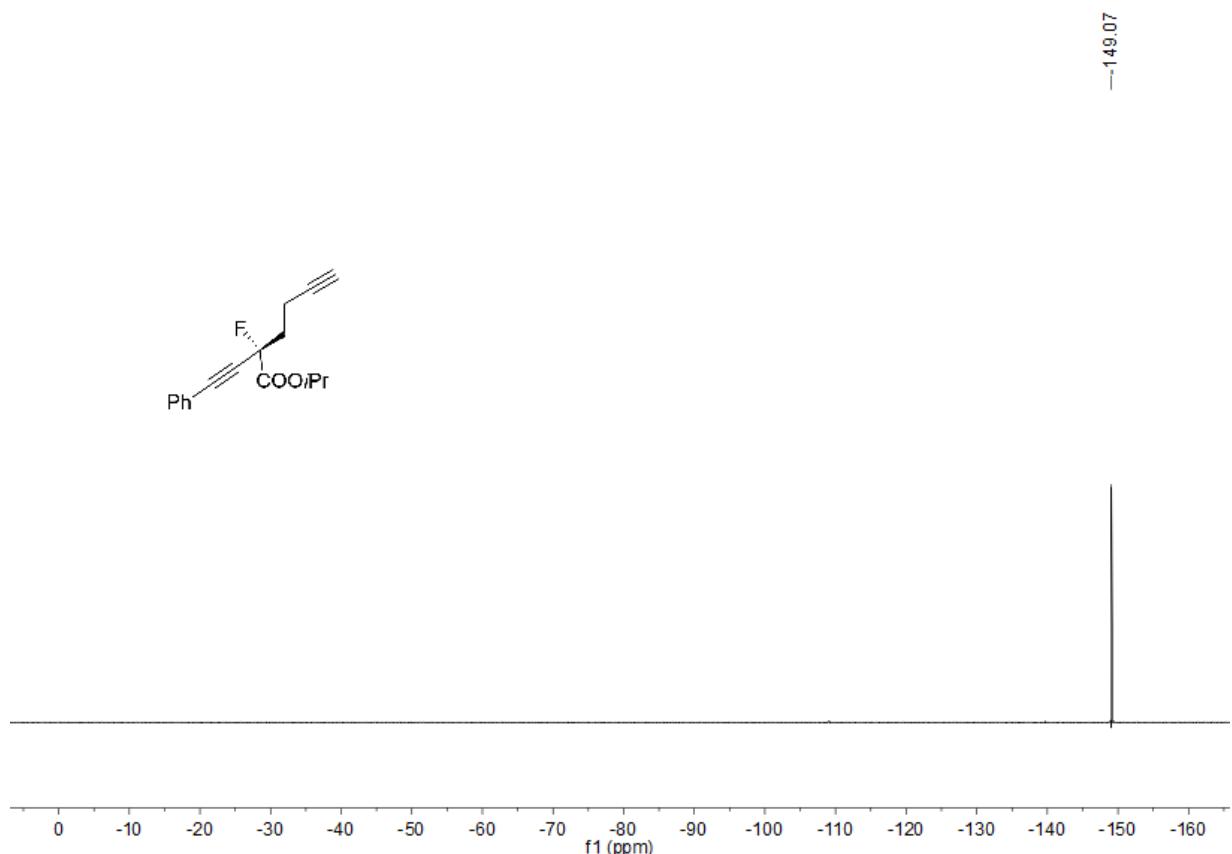
^1H NMR of 2i (500 MHz, CDCl_3)



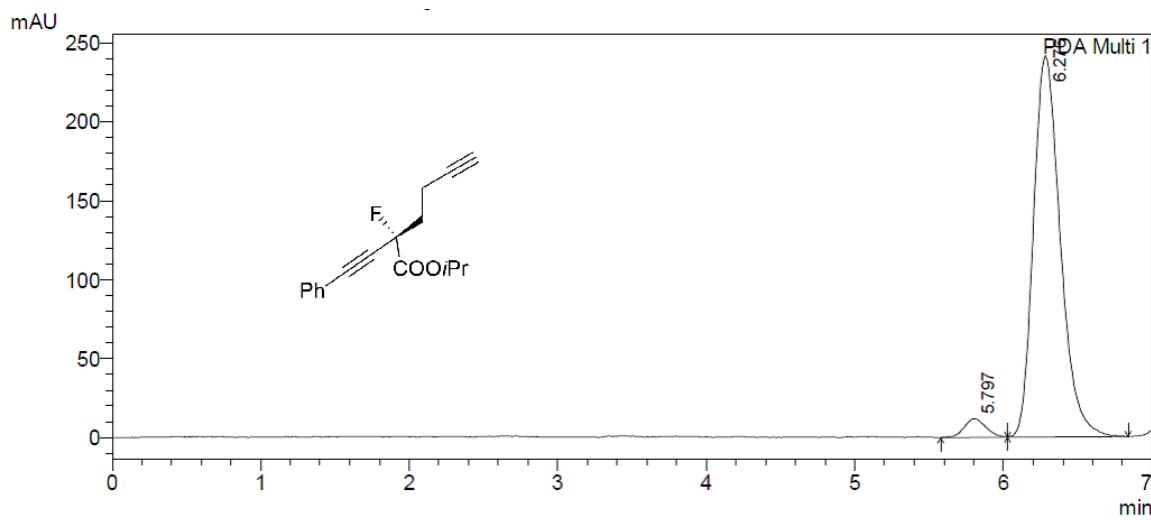
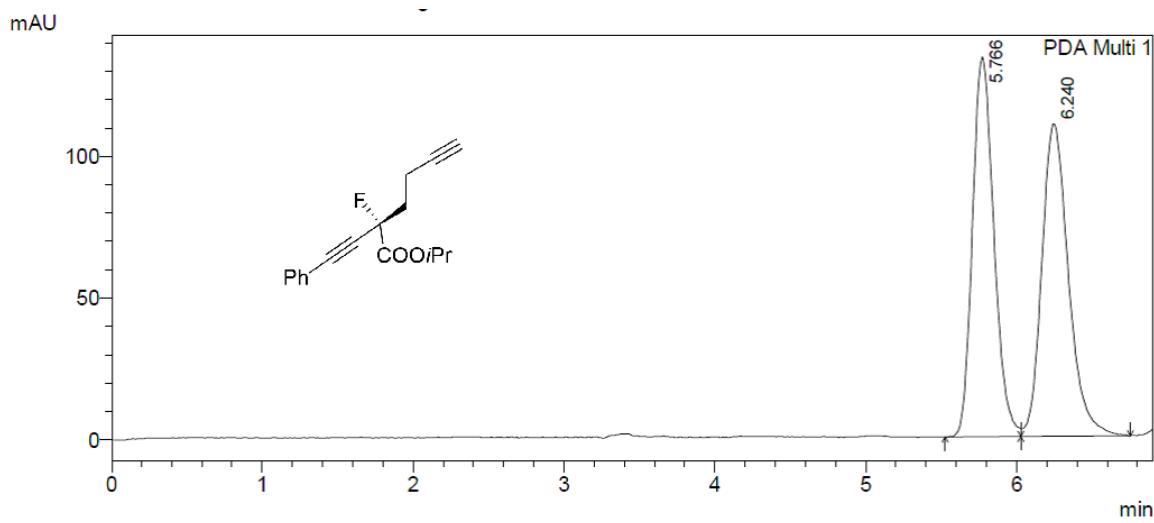
$^{13}\text{C}\{^1\text{H}\}$ NMR of 2i (125 MHz, CDCl_3)



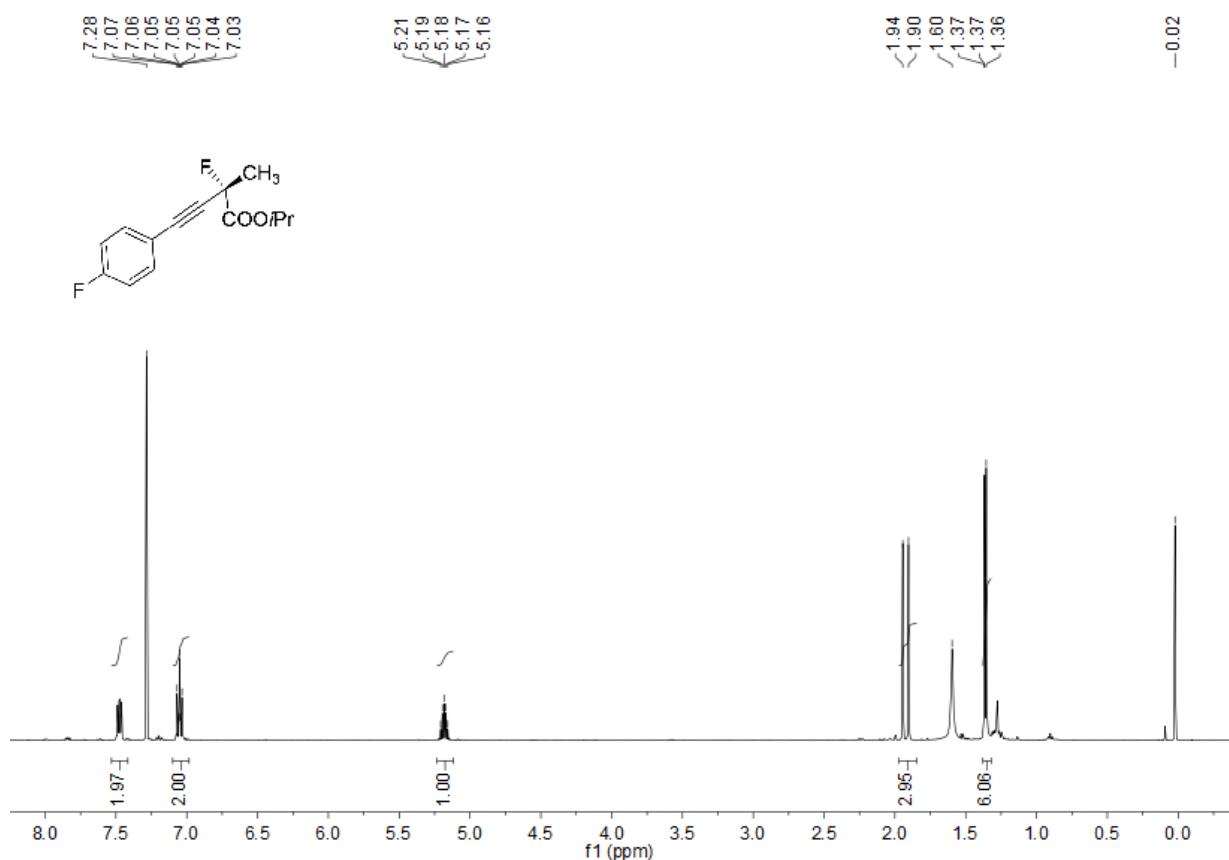
^{19}F NMR of 2i (470 MHz, CDCl_3)



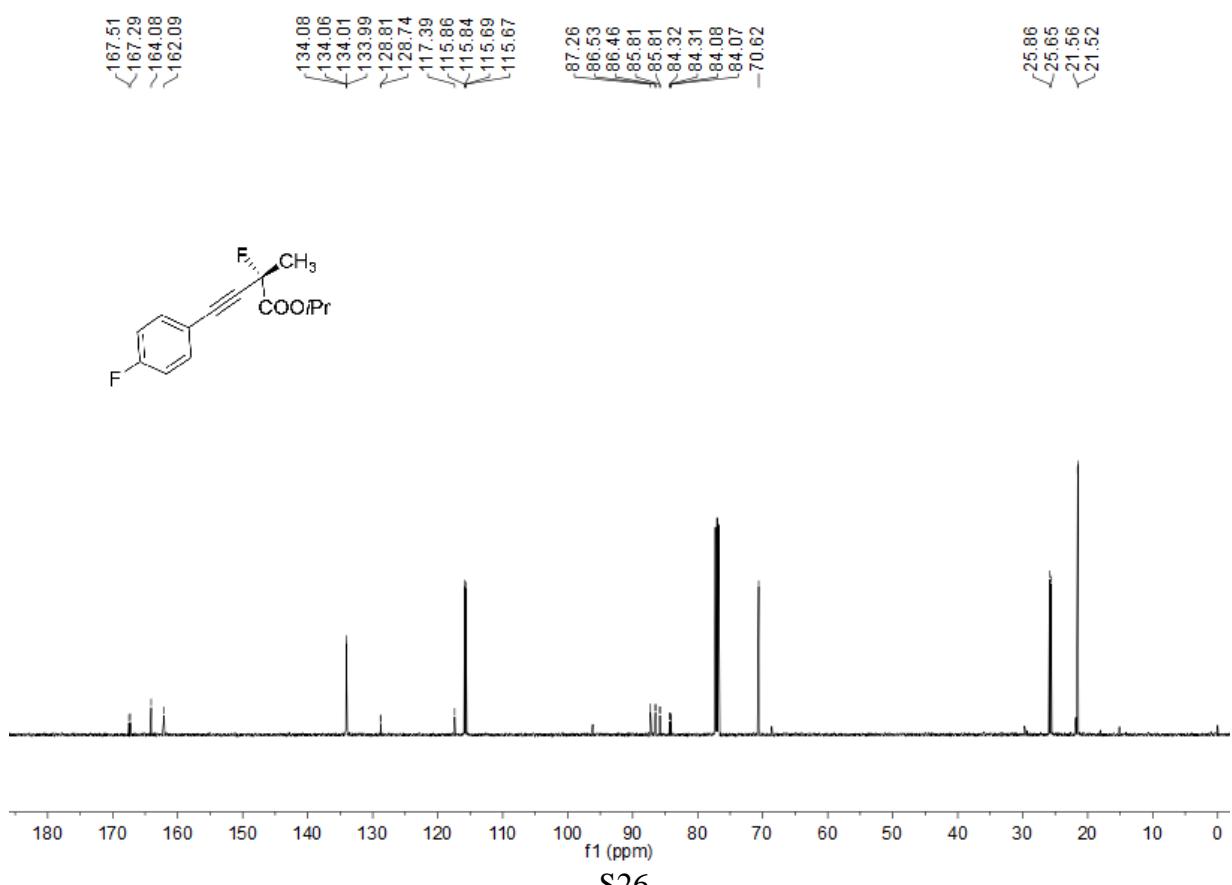
HPLC of 2i



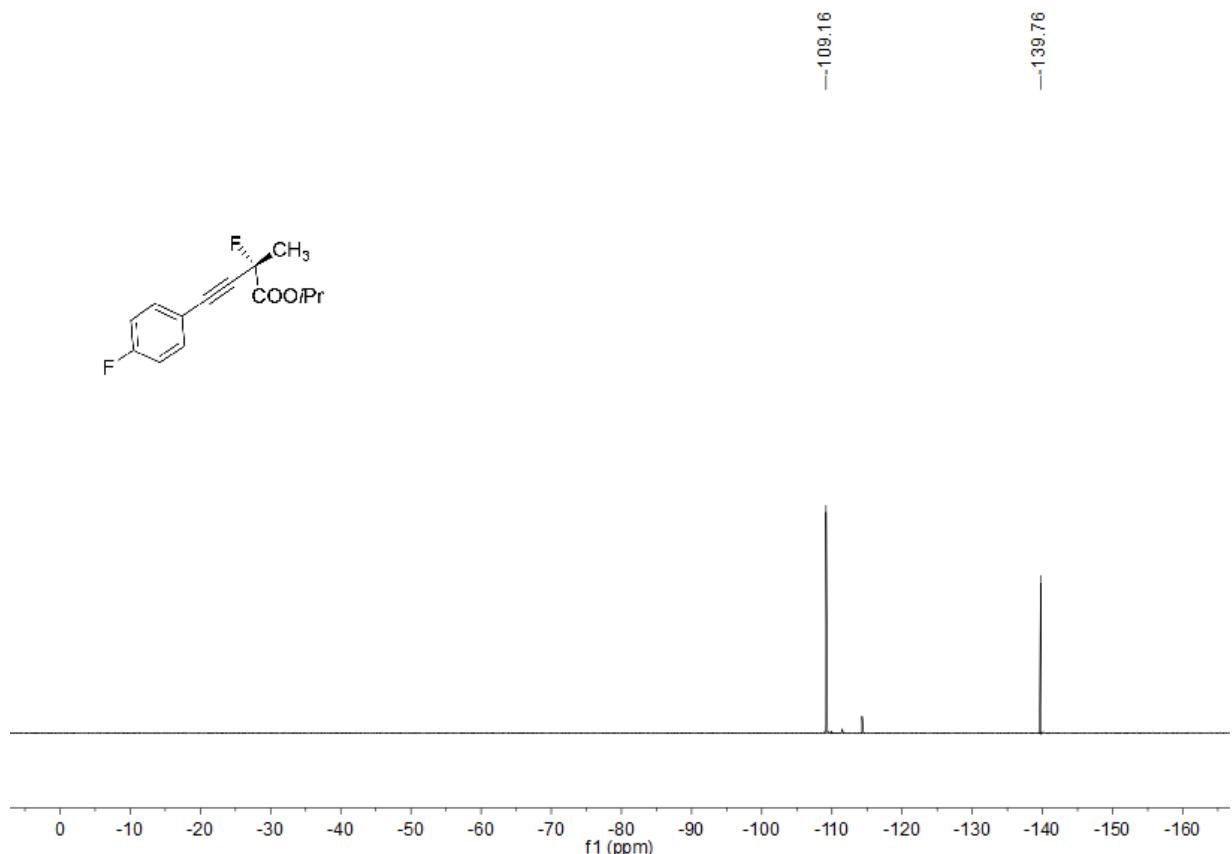
^1H NMR of 2j (500 MHz, CDCl_3)



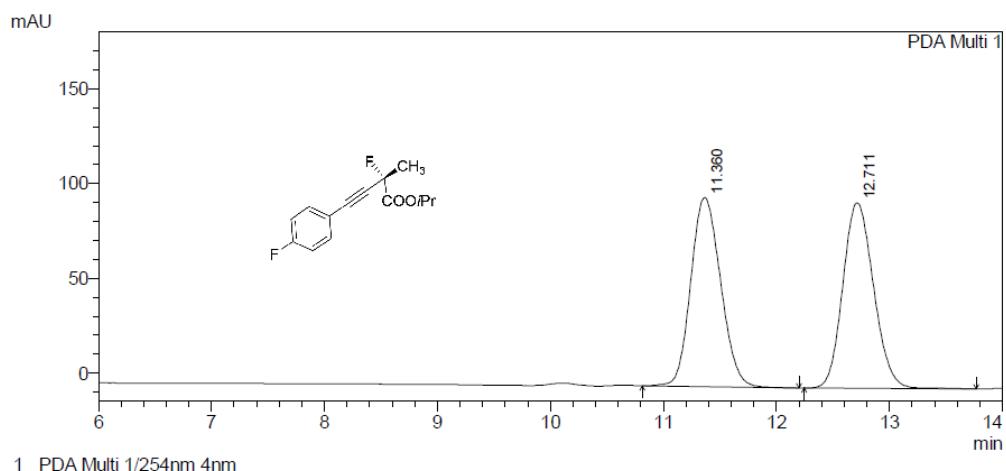
$^{13}\text{C}\{^1\text{H}\}$ NMR of 2j (125 MHz, CDCl_3)



¹⁹FNMR of 2j (470 MHz, CDCl₃)



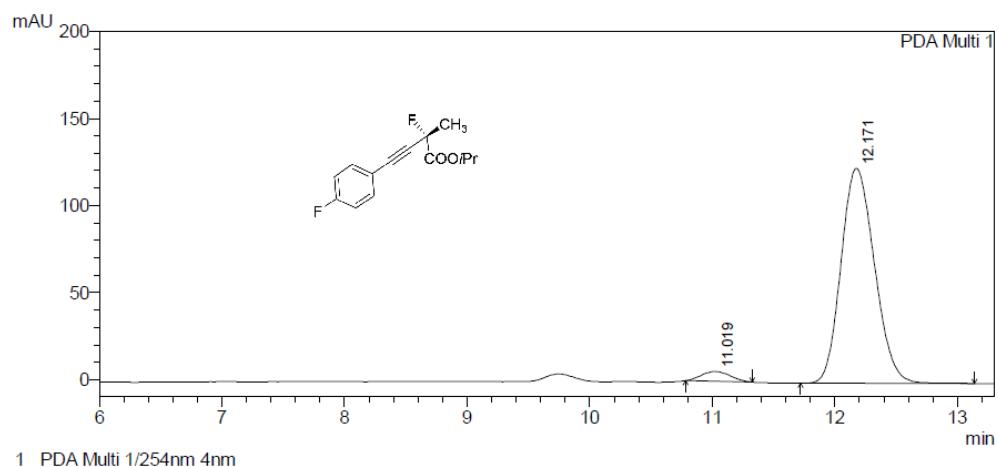
HPLC of 2j



PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	11.360	1842619	99876	49.785	50.488
2	12.711	1858549	97944	50.215	49.512
Total		3701168	197820	100.000	100.000

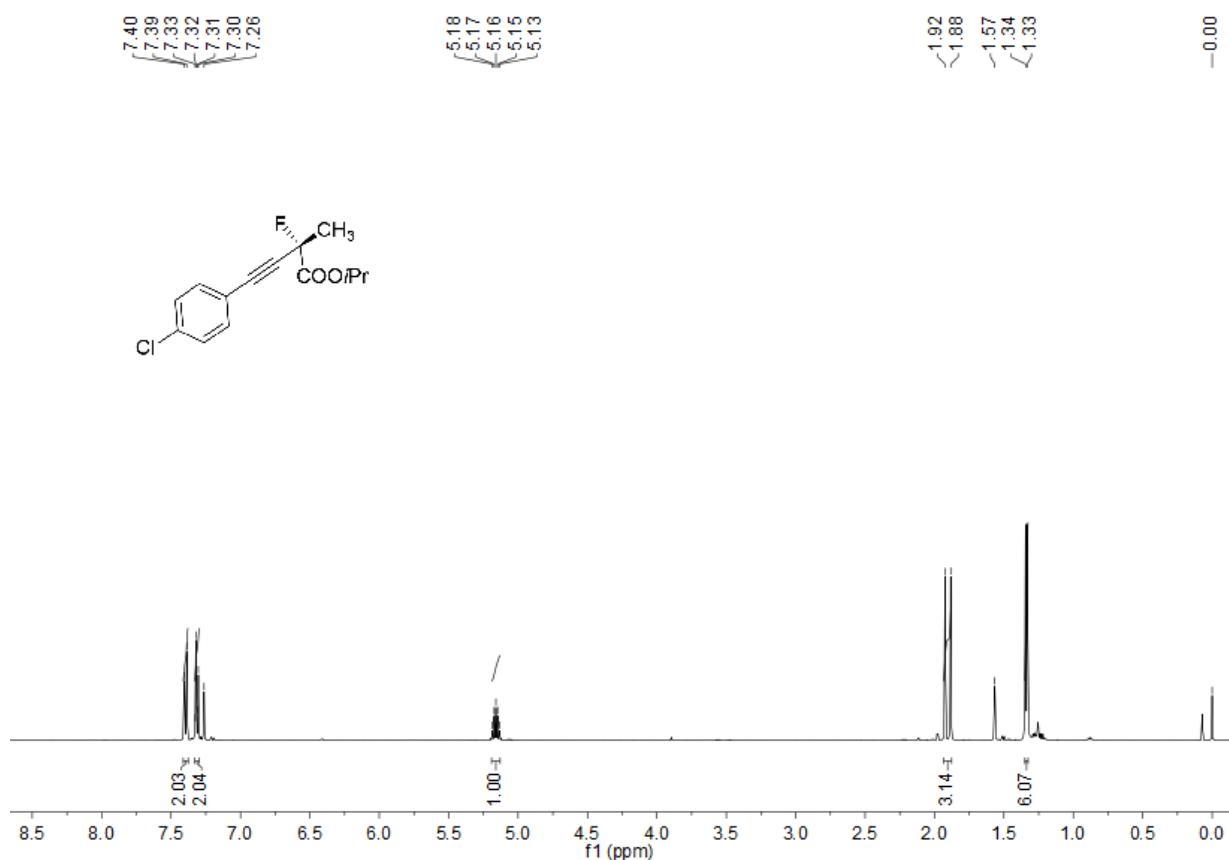


PeakTable

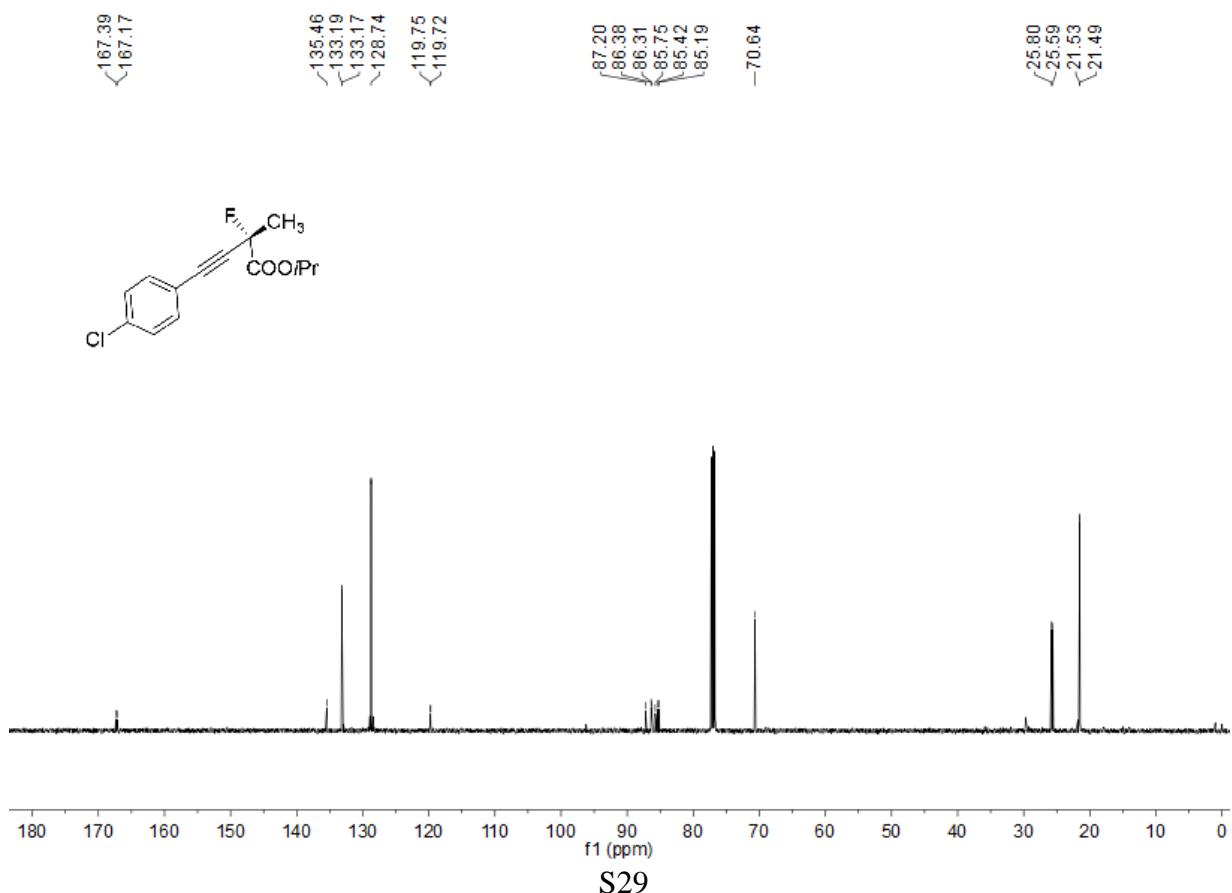
PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	11.019	92001	5581	3.778	4.327
2	12.171	2343234	123393	96.222	95.673
Total		2435235	128974	100.000	100.000

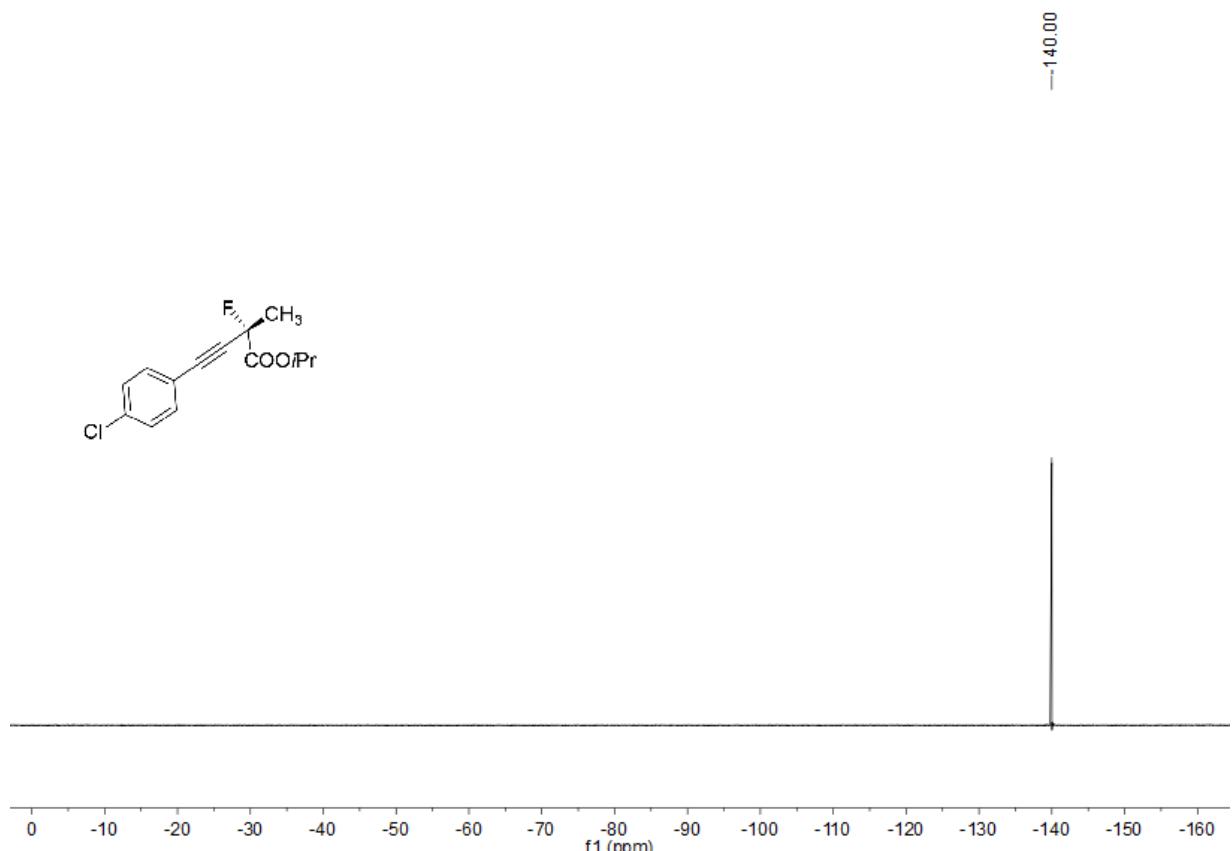
^1H NMR of 2k (500 MHz, CDCl_3)



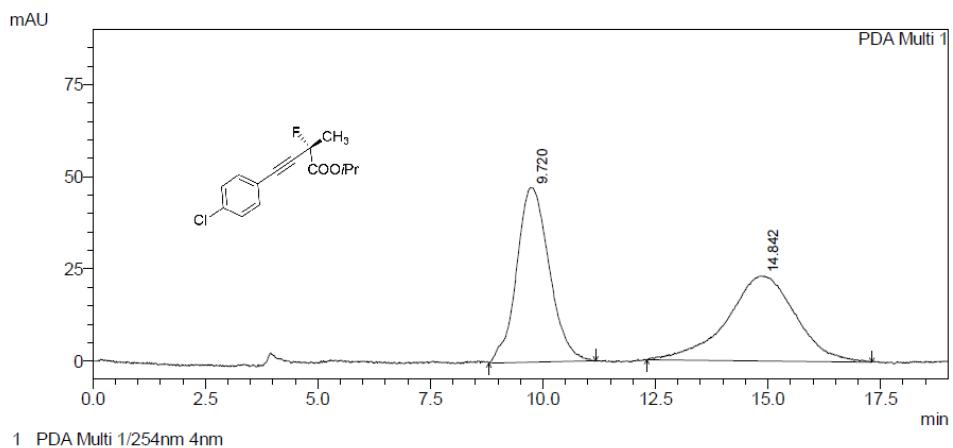
$^{13}\text{C}\{\text{H}\}$ NMR of 2k (125 MHz, CDCl_3)



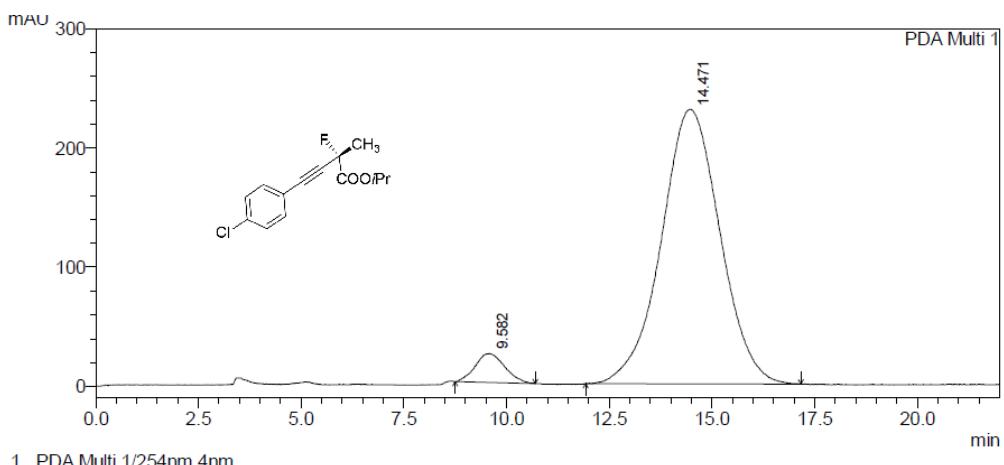
¹⁹FNMR of 2k (470 MHz, CDCl₃)



HPLC of 2k

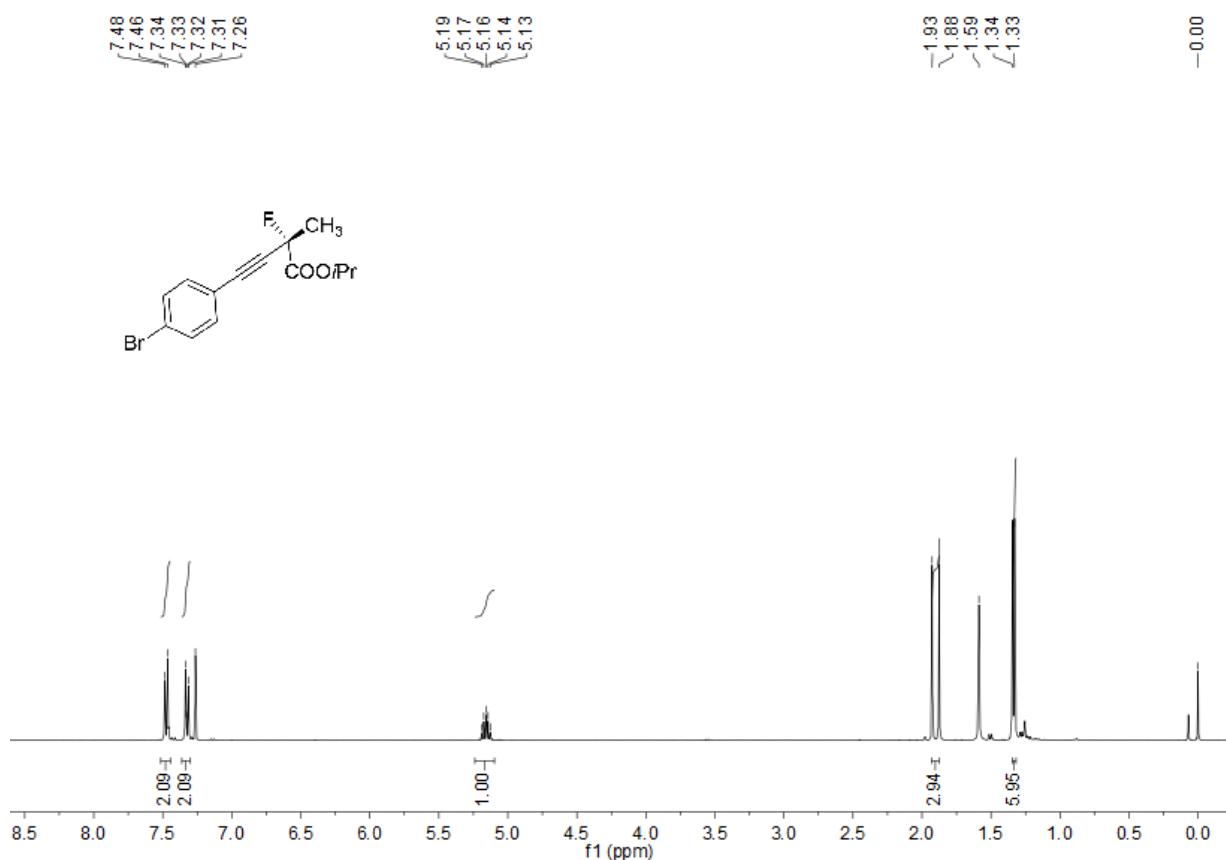


PDA Ch1 254nm 4nm					
Peak#	Ret. Time	Area	Height	Area %	Height %
1	9.720	2380113	47414	49.461	67.240
2	14.842	2431952	23101	50.539	32.760
Total		4812065	70515	100.000	100.000

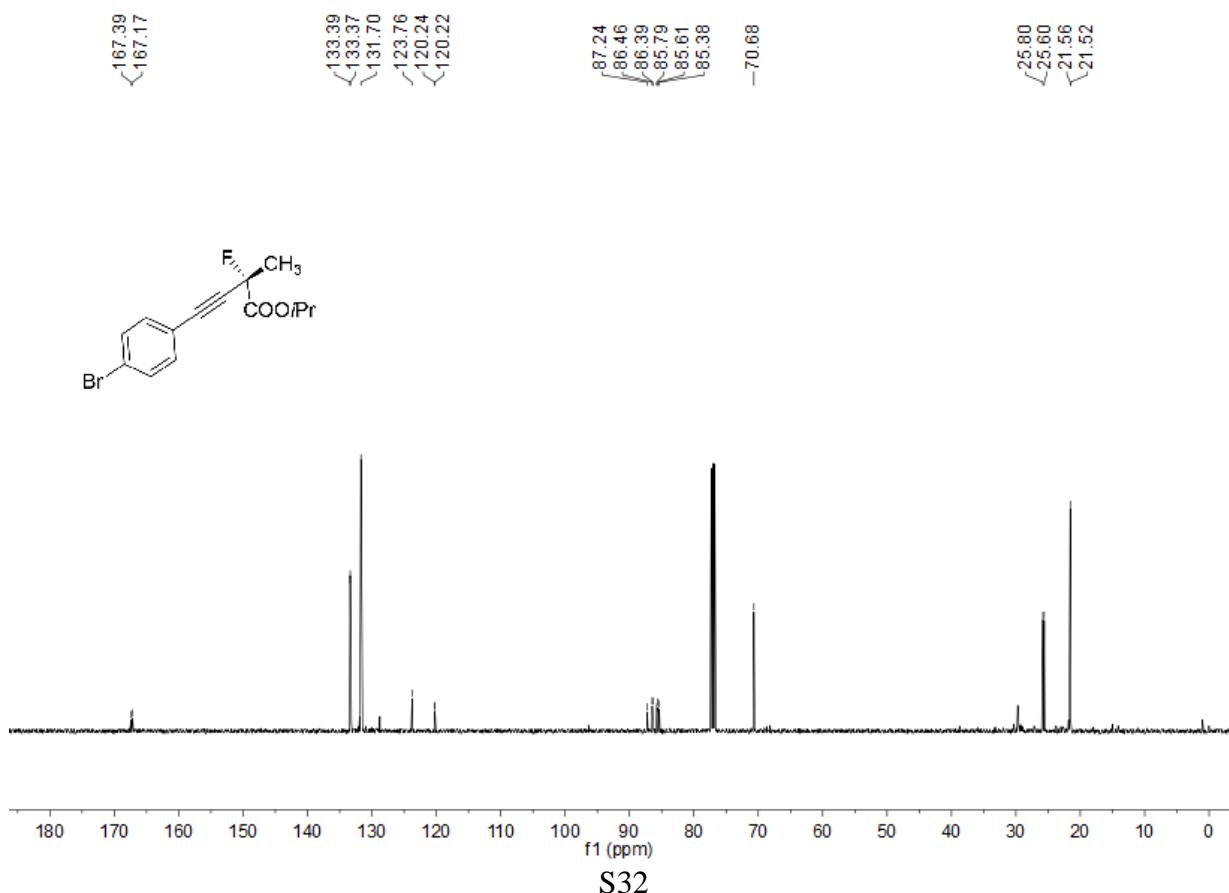


PDA Ch1 254nm 4nm					
Peak#	Ret. Time	Area	Height	Area %	Height %
1	9.582	1209045	24342	5.002	9.544
2	14.471	22961176	230722	94.998	90.456
Total		24170220	255064	100.000	100.000

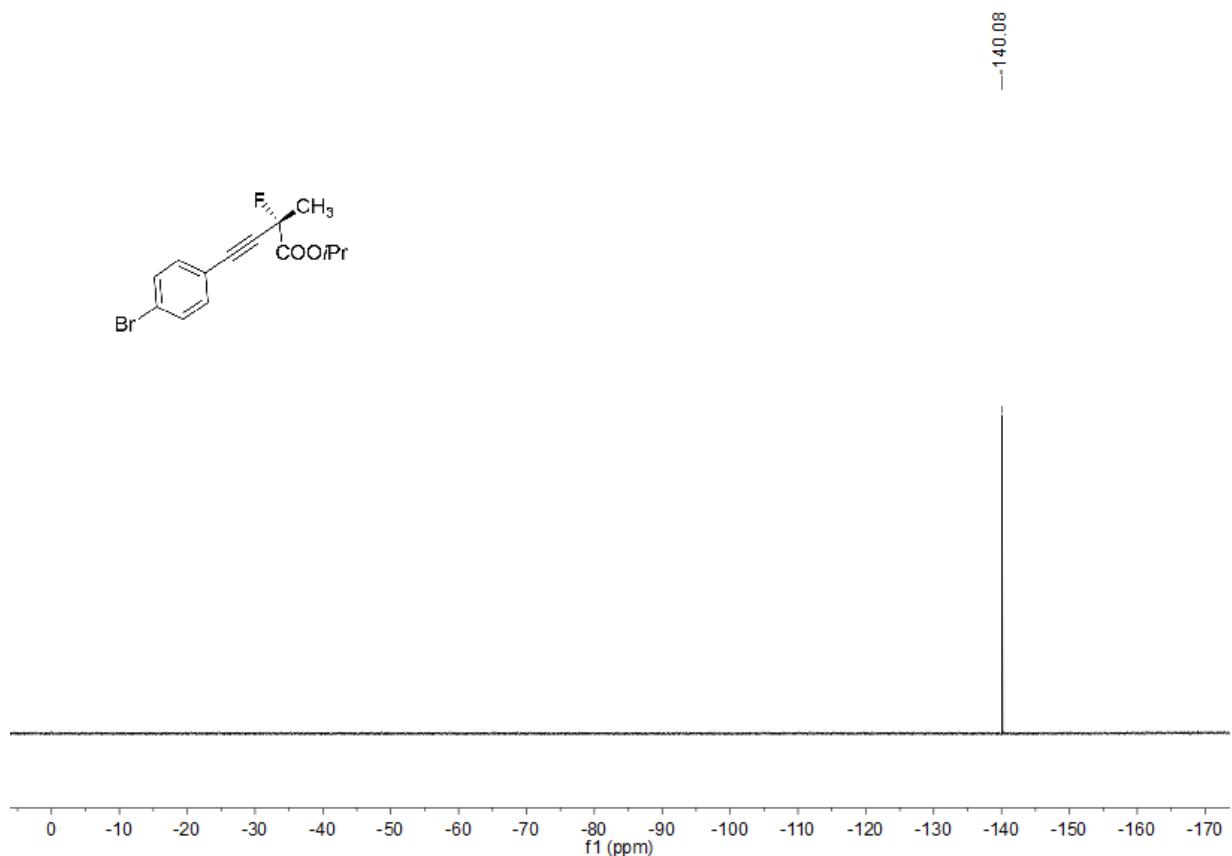
^1H NMR of 2l (500 MHz, CDCl_3)



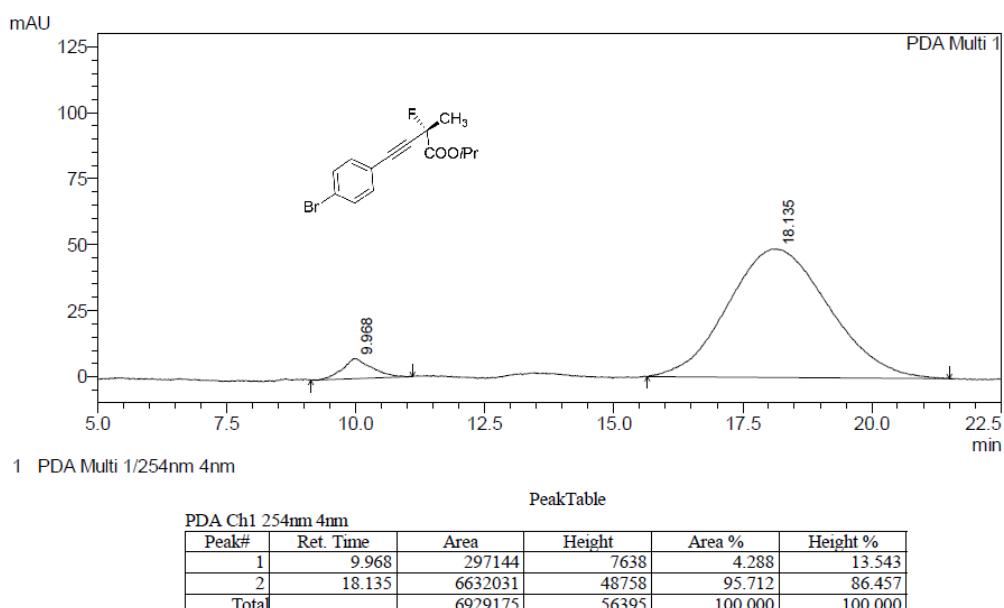
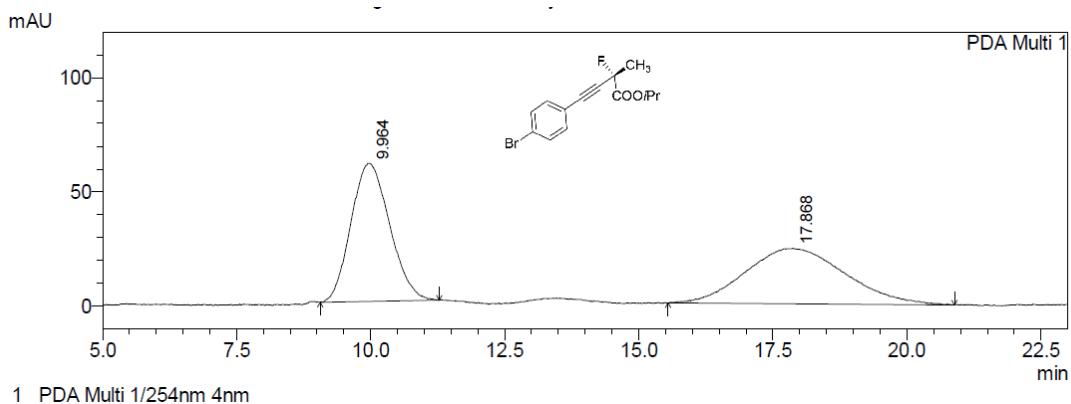
$^{13}\text{C}\{\text{H}\}$ NMR of 2l (125 MHz, CDCl_3)



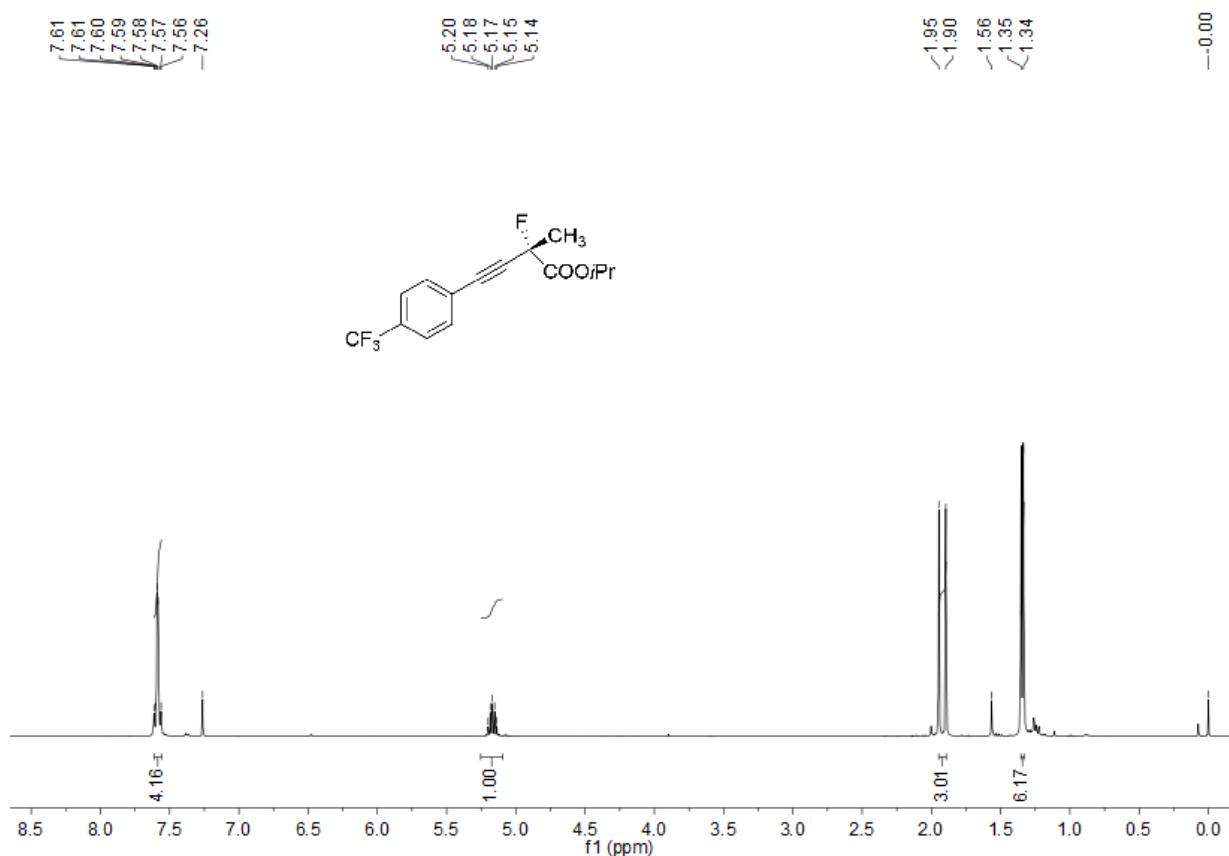
^{19}F NMR of 2l (470 MHz, CDCl_3)



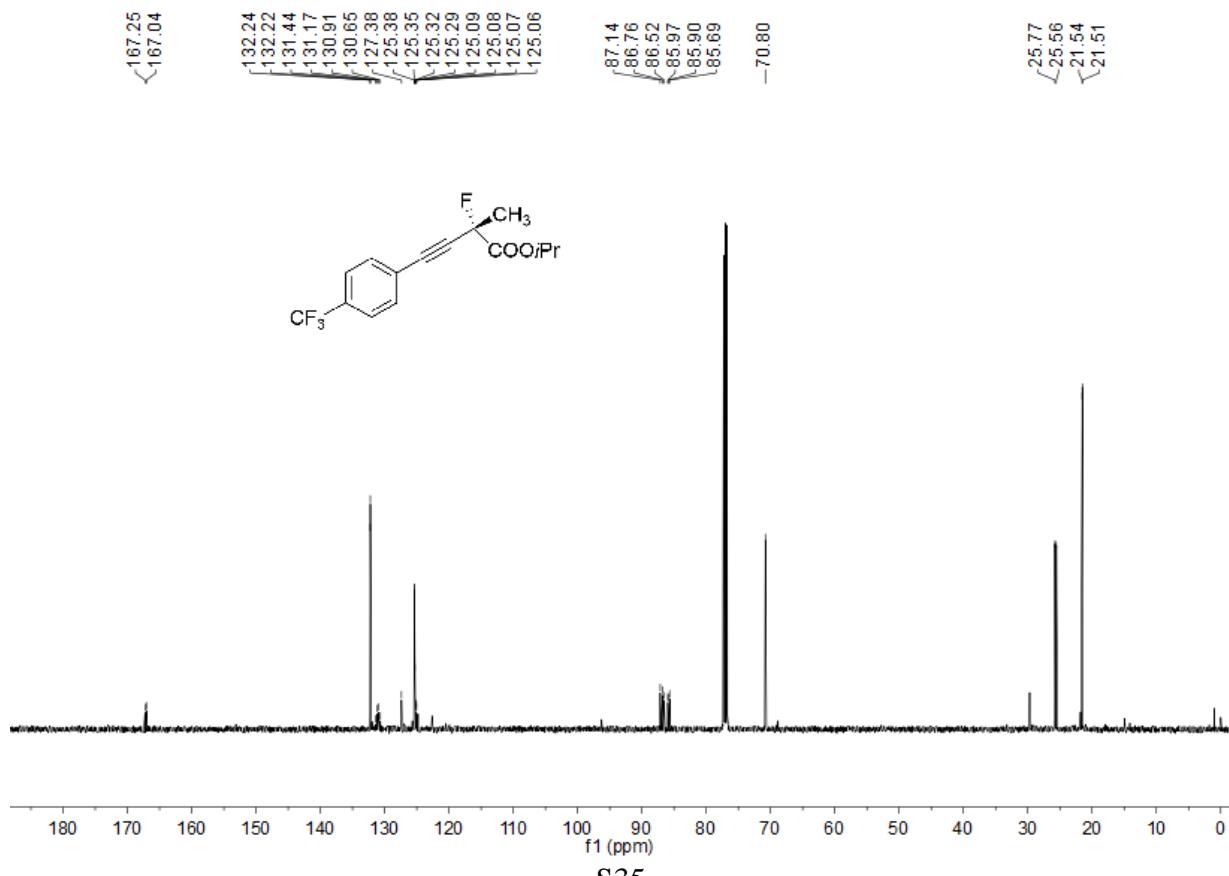
HPLC of 2l



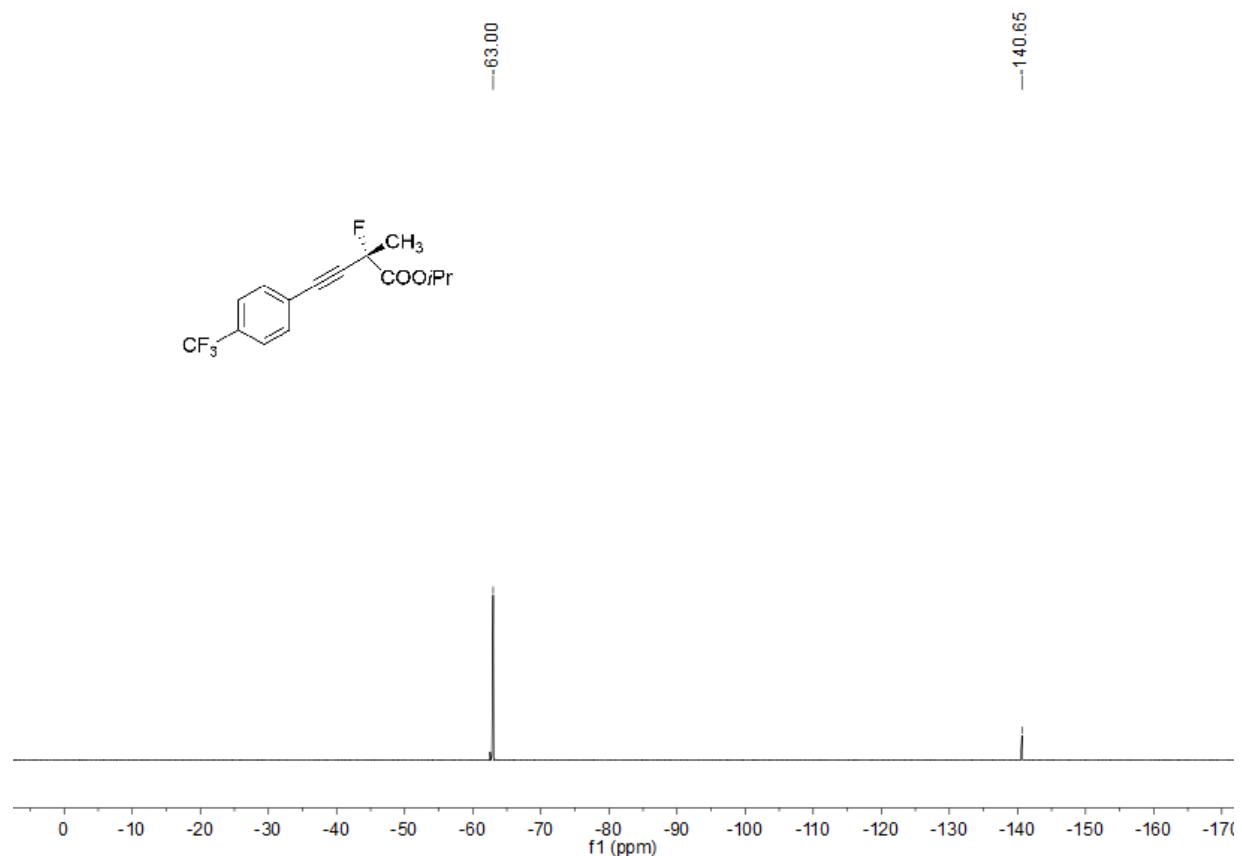
^1H NMR of 2m (500 MHz, CDCl_3)



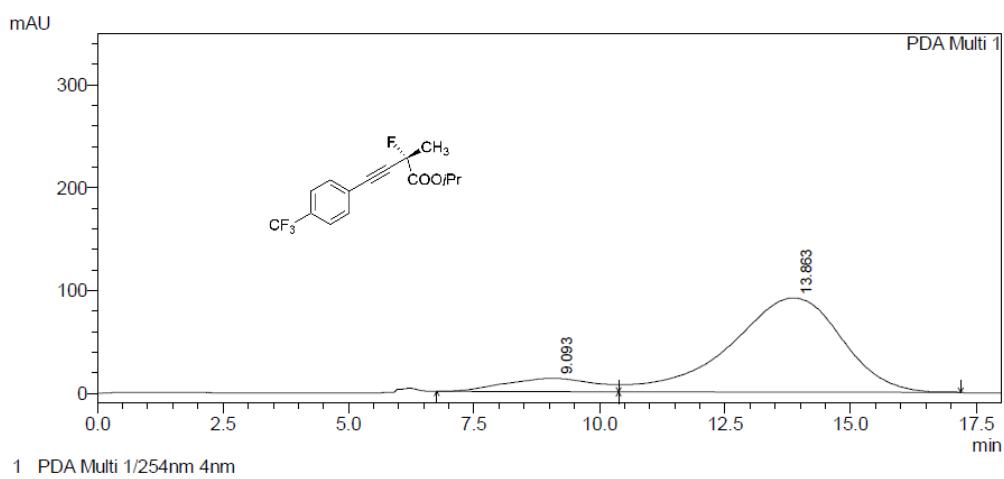
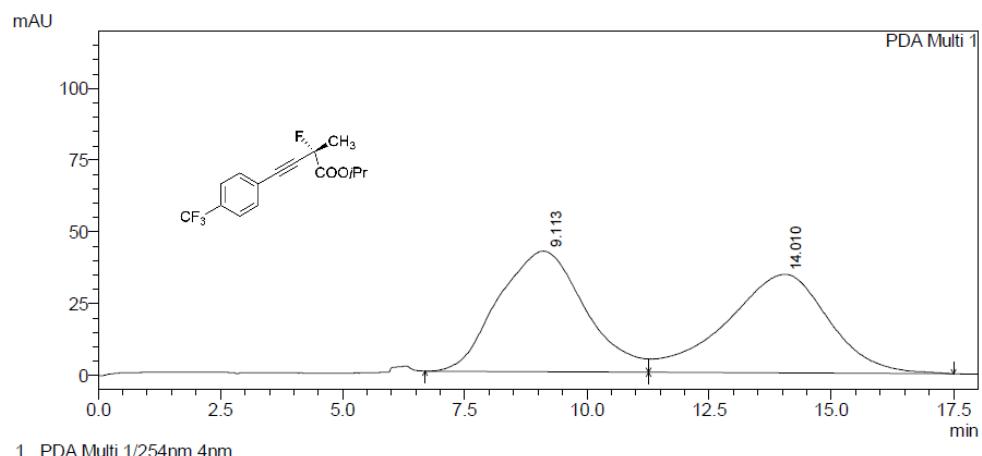
$^{13}\text{C}\{^1\text{H}\}$ NMR of 2m (125 MHz, CDCl_3)



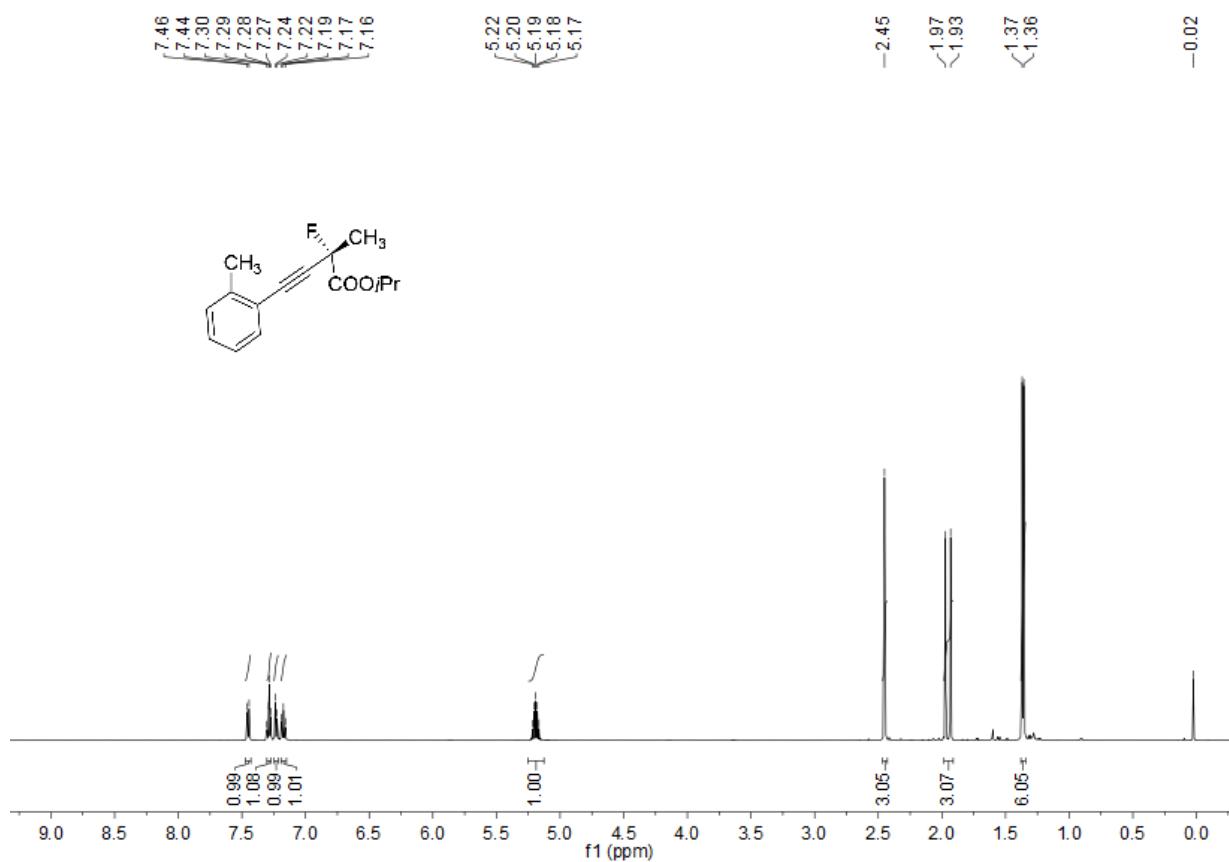
¹⁹FNMR of 2m (470 MHz, CDCl₃)



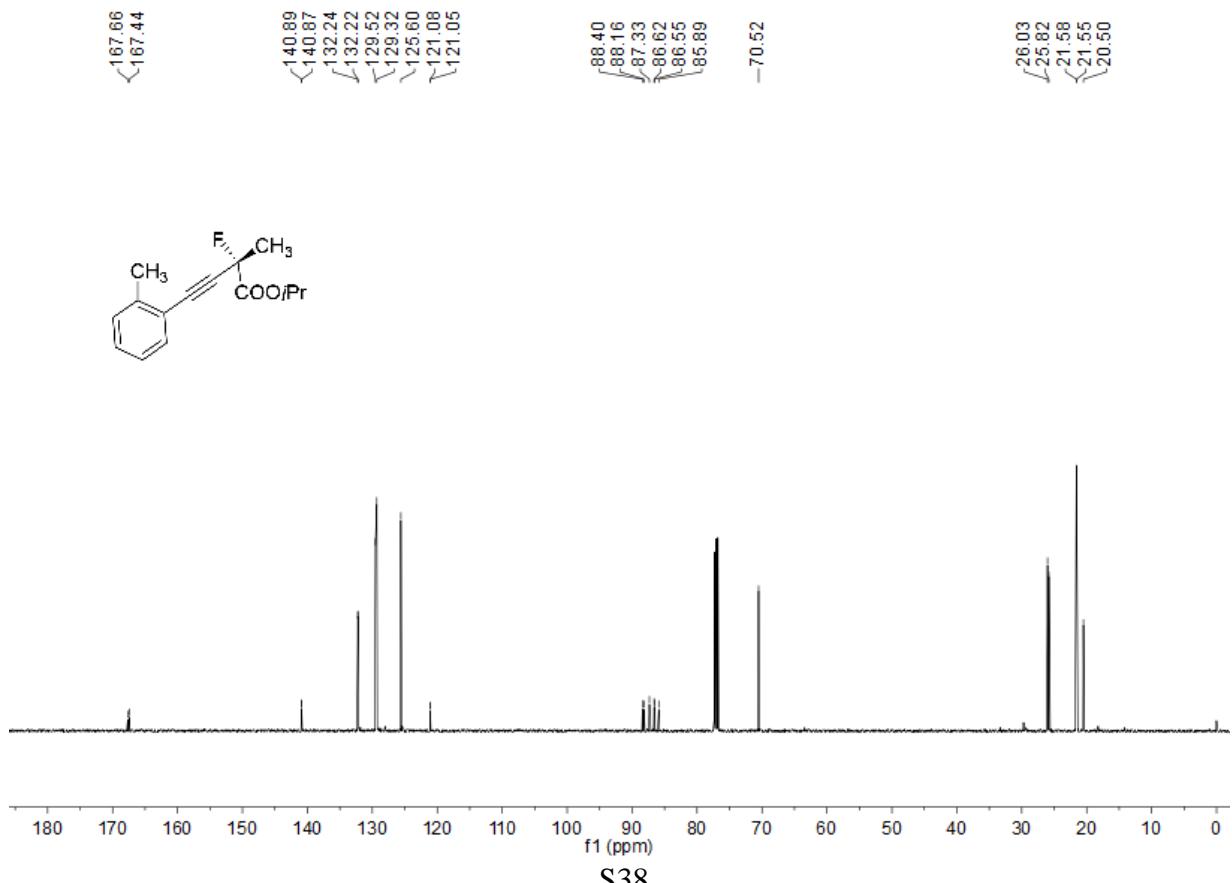
HPLC of 2m



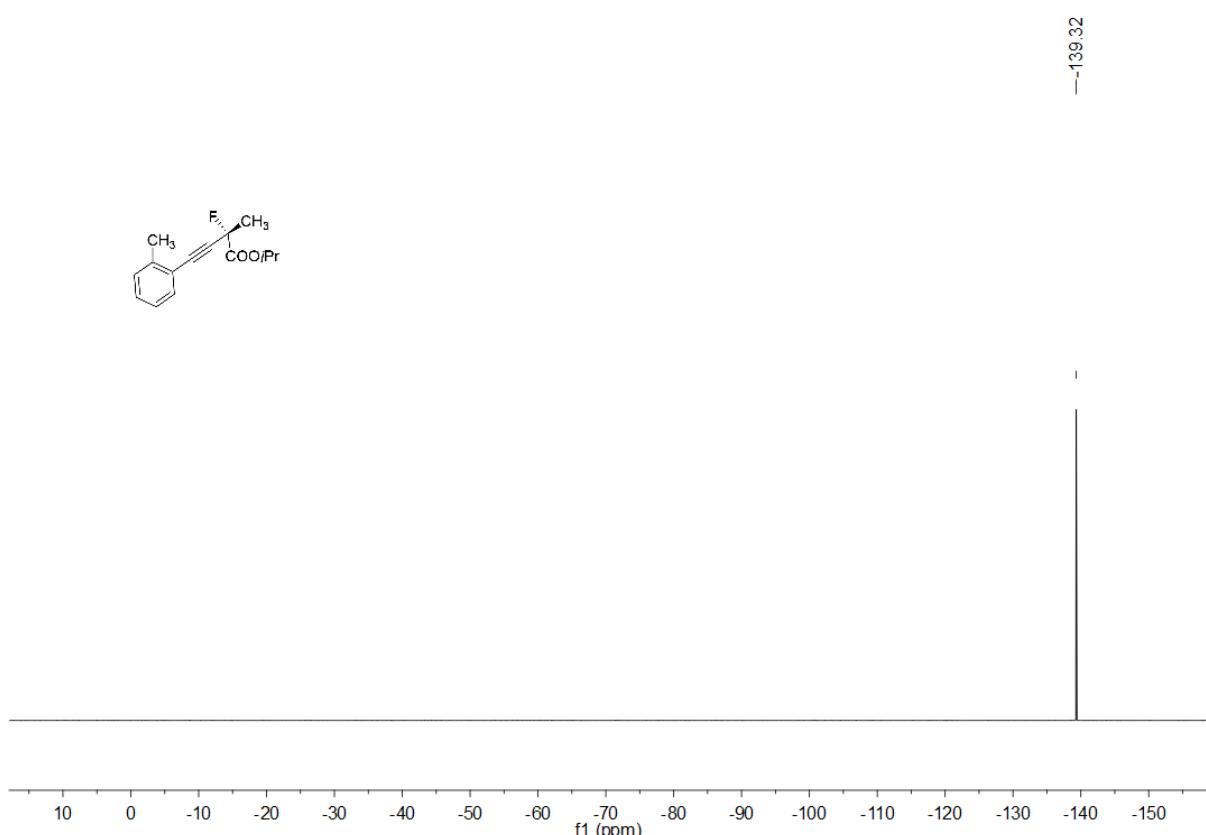
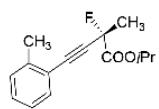
^1H NMR of 2n (500 MHz, CDCl_3)



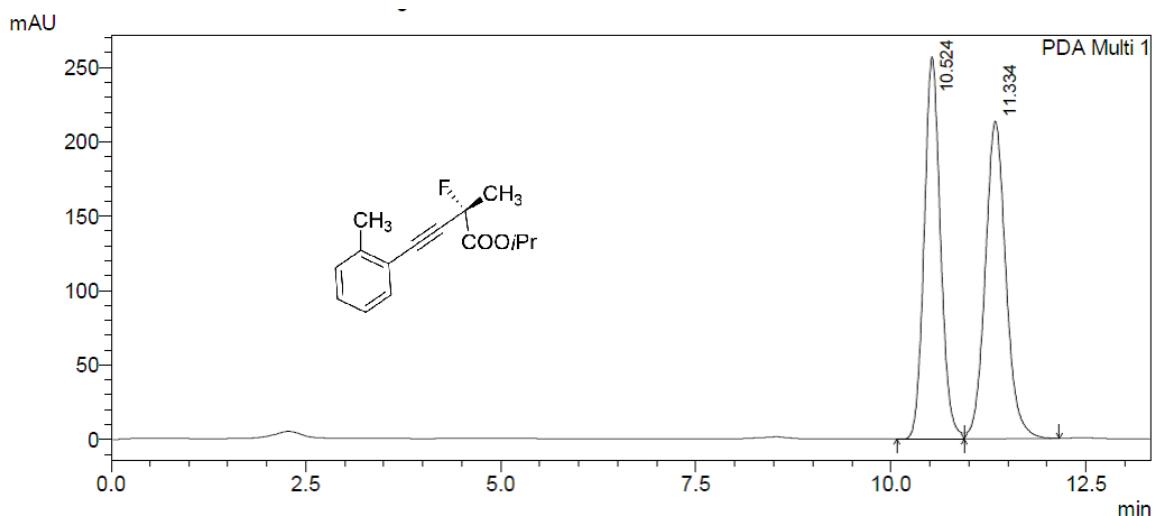
$^{13}\text{C}\{^1\text{H}\}$ NMR of 2n (125 MHz, CDCl_3)



¹⁹FNMR of 2n (470 MHz, CDCl₃)



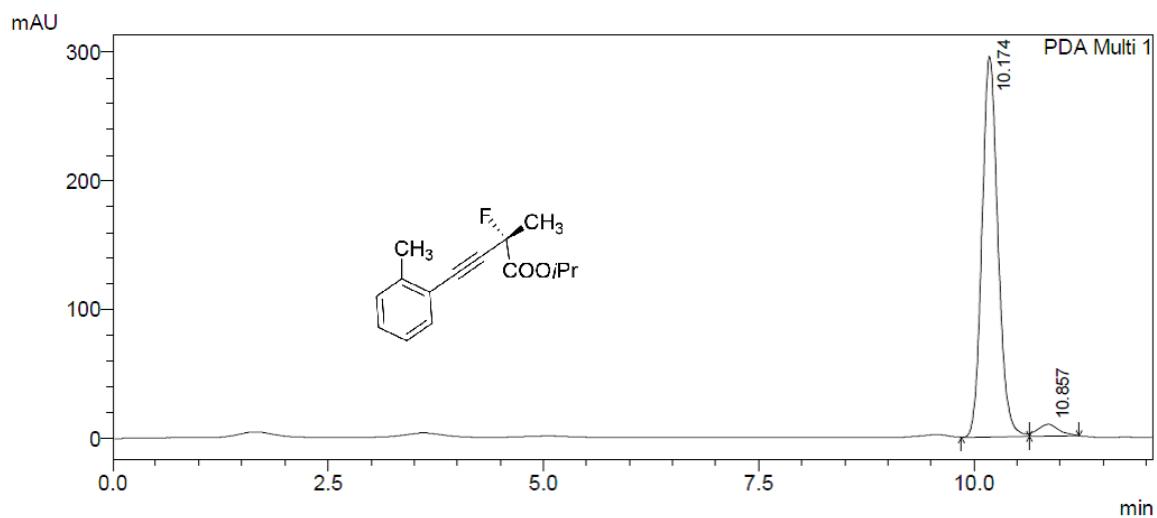
HPLC of 2n



PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	10.524	3741680	256812	48.725	54.612
2	11.334	3937566	213434	51.275	45.388
Total		7679246	470246	100.000	100.000

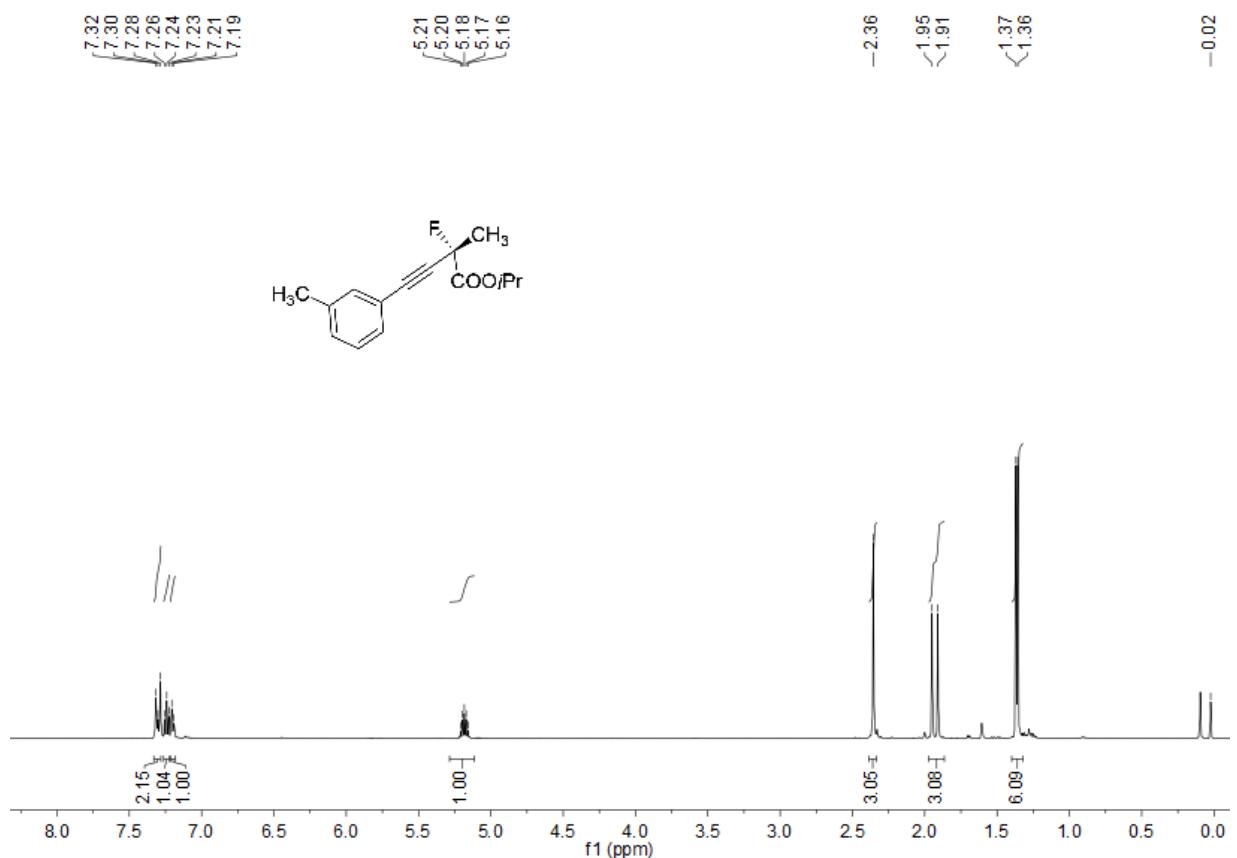


PeakTable

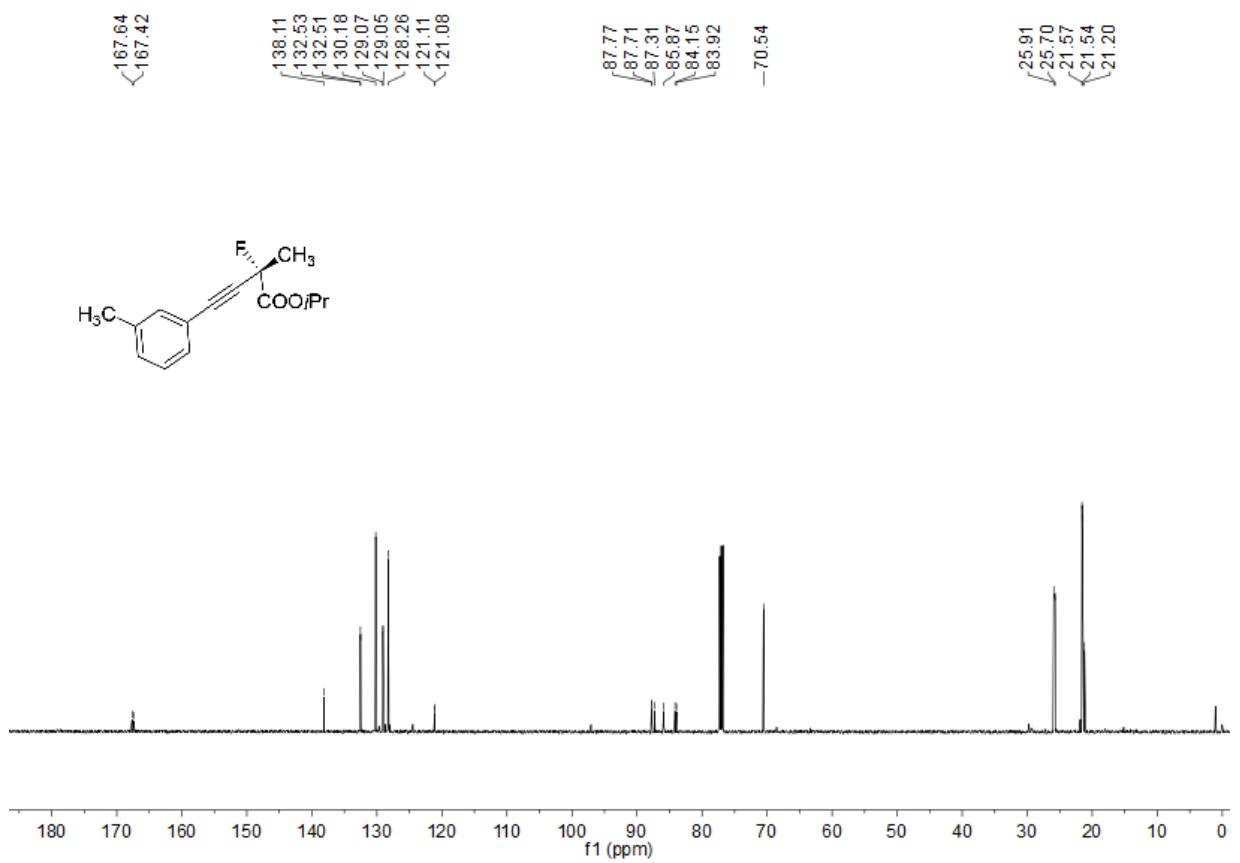
PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	10.174	3810563	295456	96.057	96.971
2	10.857	156432	9227	3.943	3.029
Total		3966995	304683	100.000	100.000

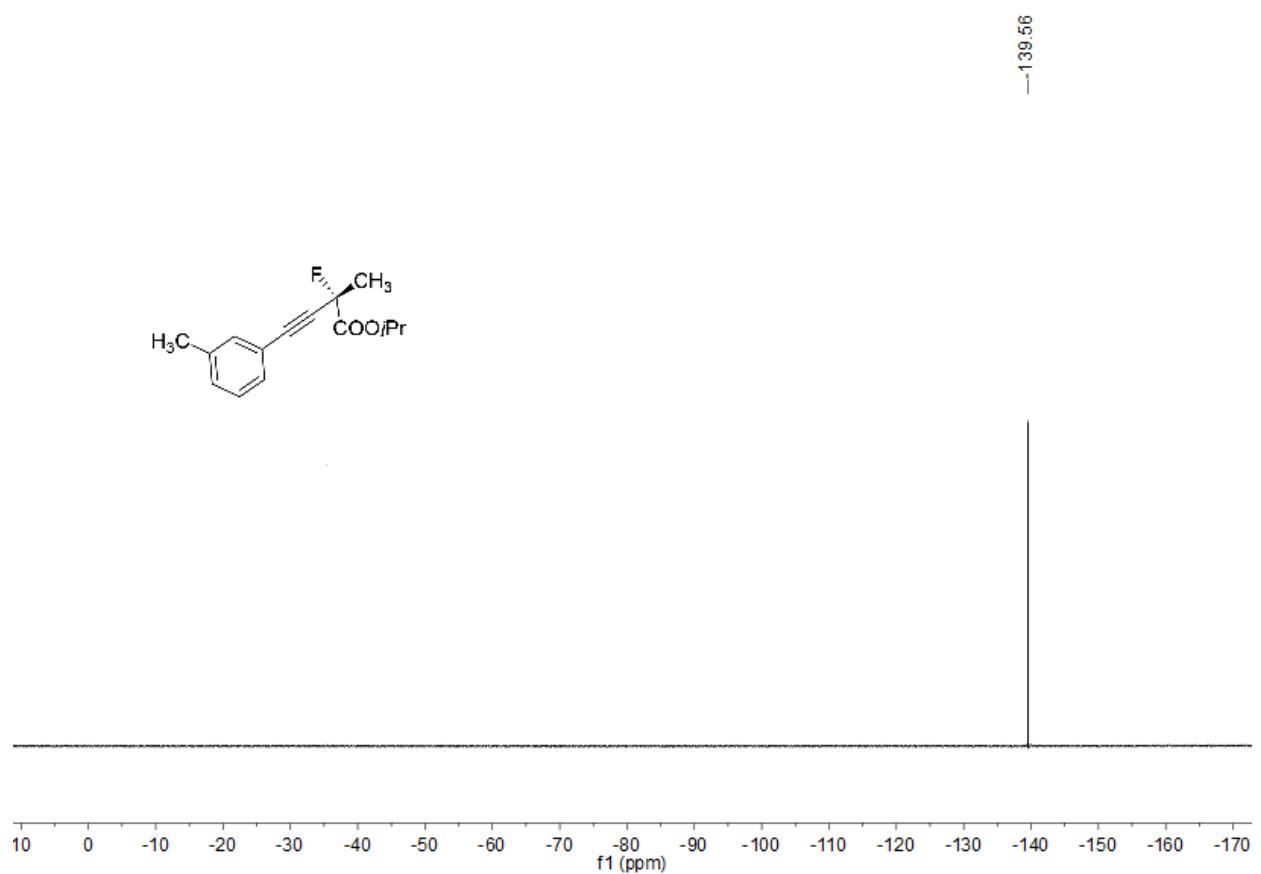
^1H NMR of 2o (500 MHz, CDCl_3)



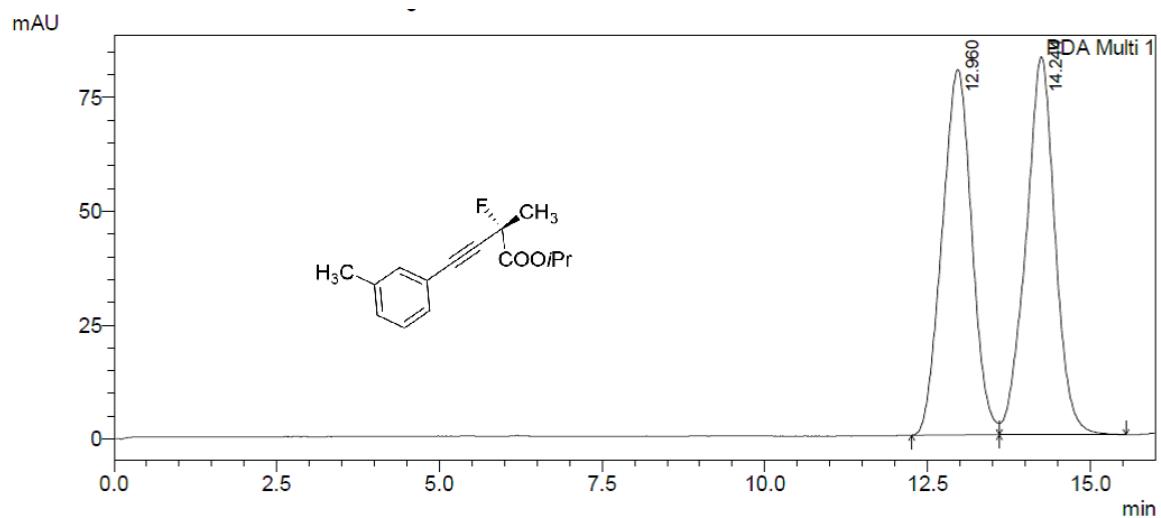
$^{13}\text{C}\{^1\text{H}\}$ NMR of 2o (125 MHz, CDCl_3)



¹⁹FNMR of 2o (470 MHz, CDCl₃)



HPLC of 2o

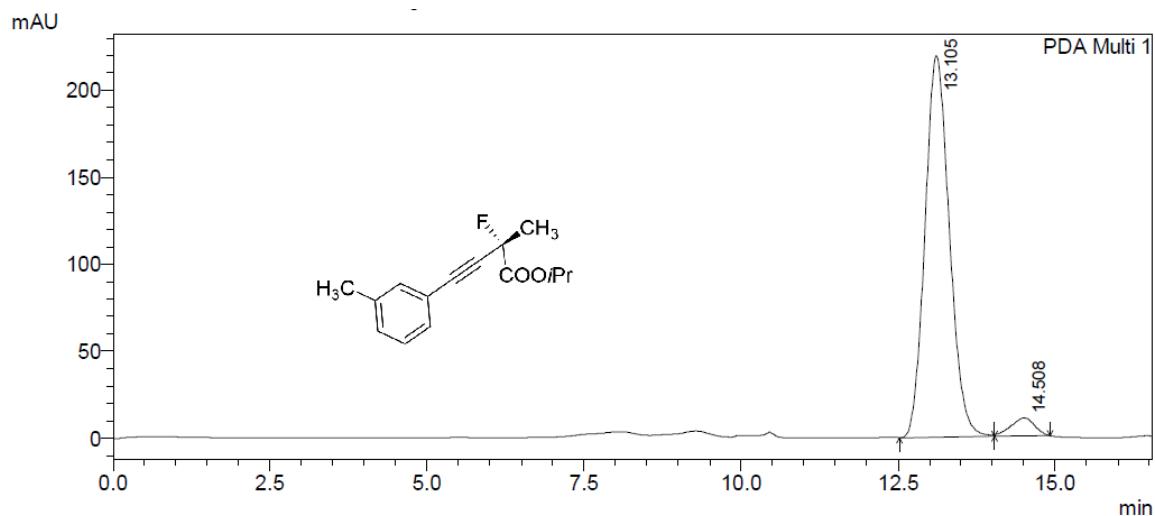


1 PDA Multi 1/254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	12.960	2548824	80221	49.659	49.162
2	14.244	2583795	82955	50.341	50.838
Total		5132619	163176	100.000	100.000



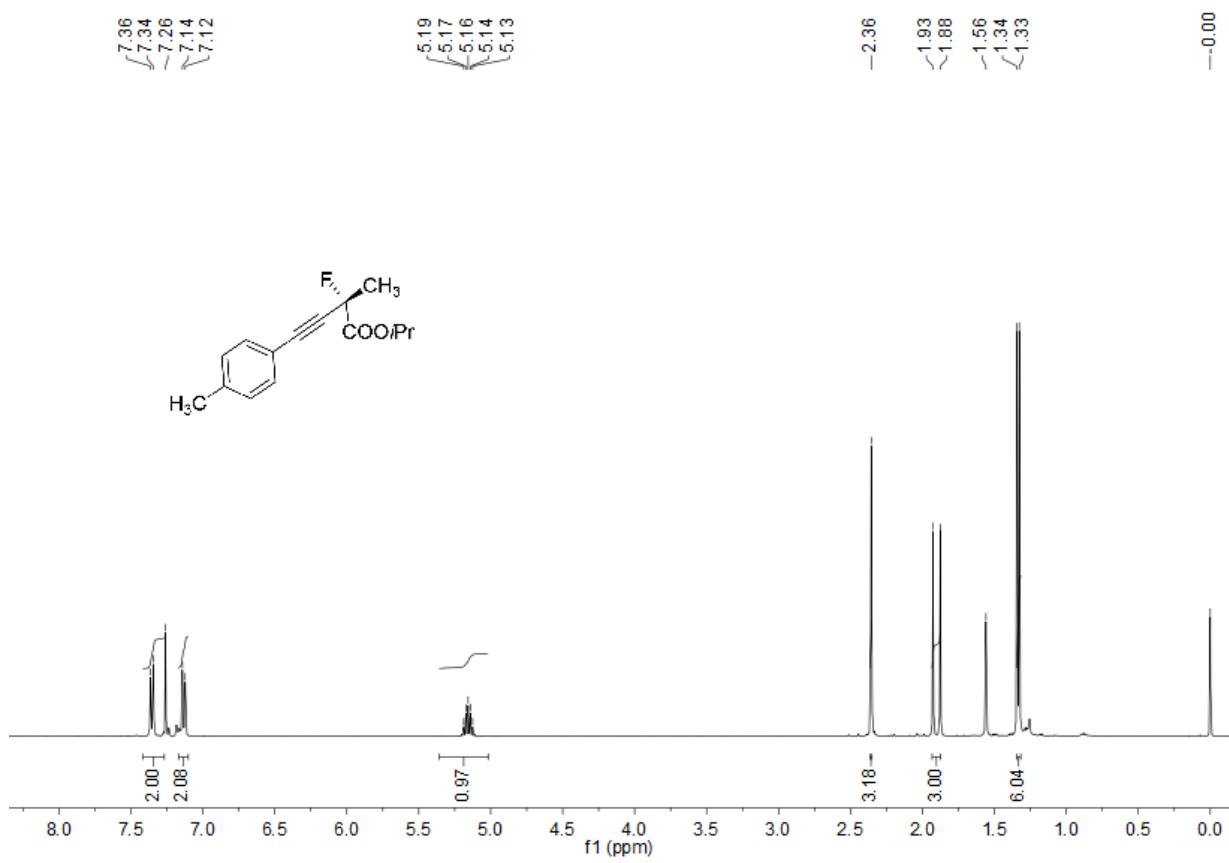
1 PDA Multi 1/254nm 4nm

PeakTable

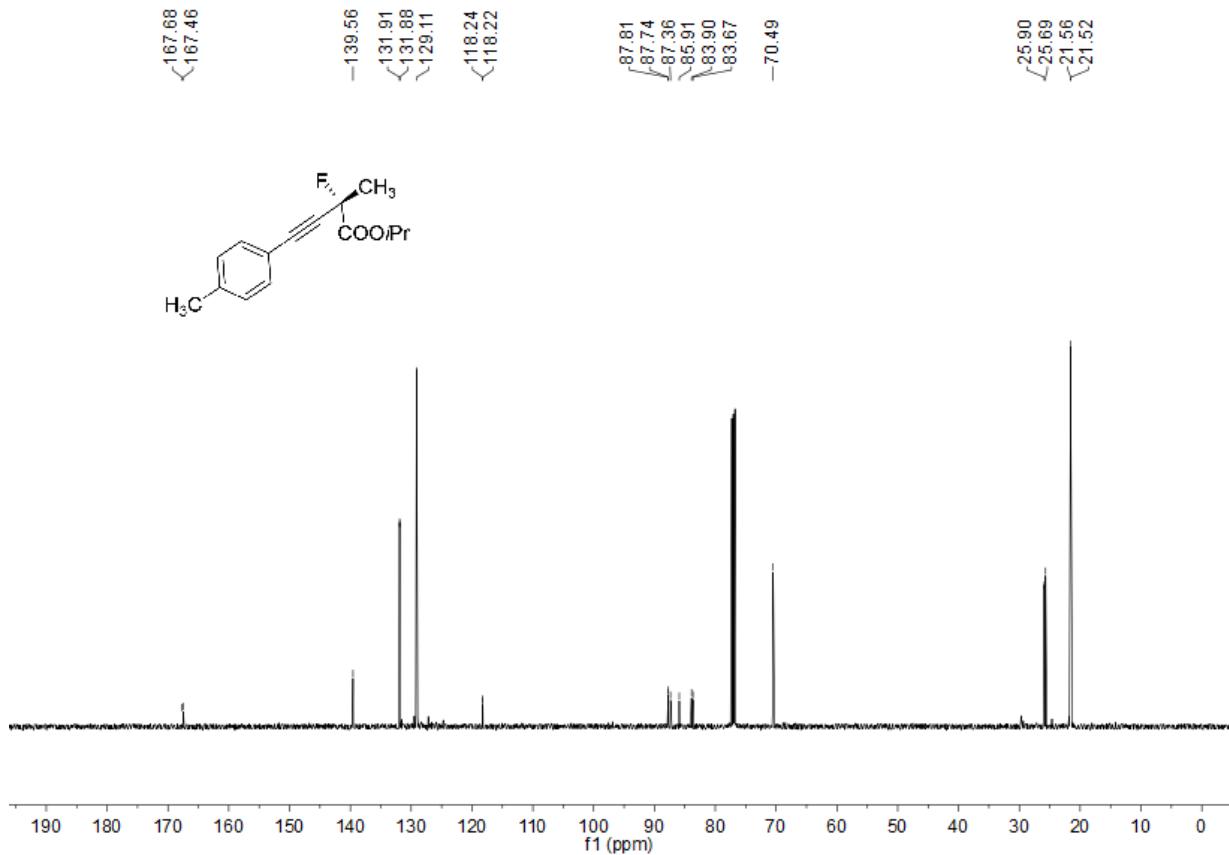
PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	13.105	5931842	219218	95.547	95.472
2	14.508	276433	10396	4.453	4.528
Total		6208275	229615	100.000	100.000

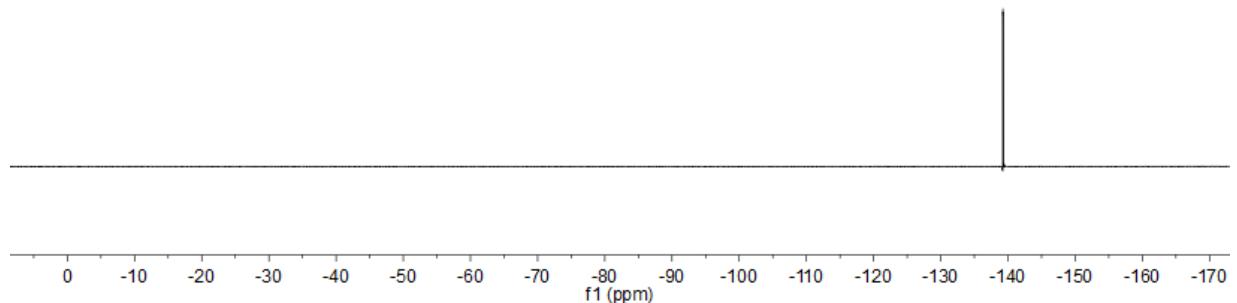
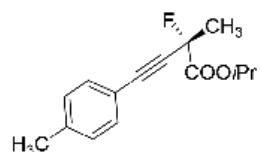
^1H NMR of 2p (500 MHz, CDCl_3)



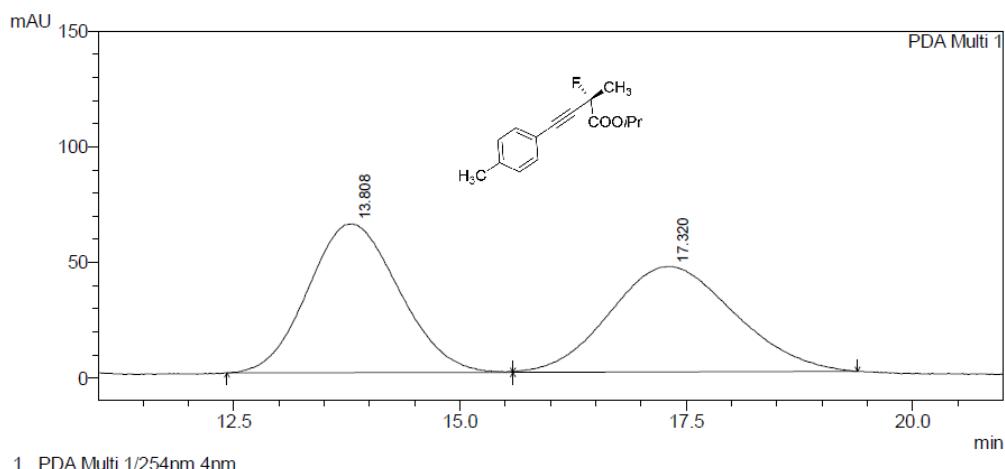
$^{13}\text{C}\{^1\text{H}\}$ NMR of 2p (125 MHz, CDCl_3)



¹⁹CNMR of 2p (470 MHz, CDCl₃)



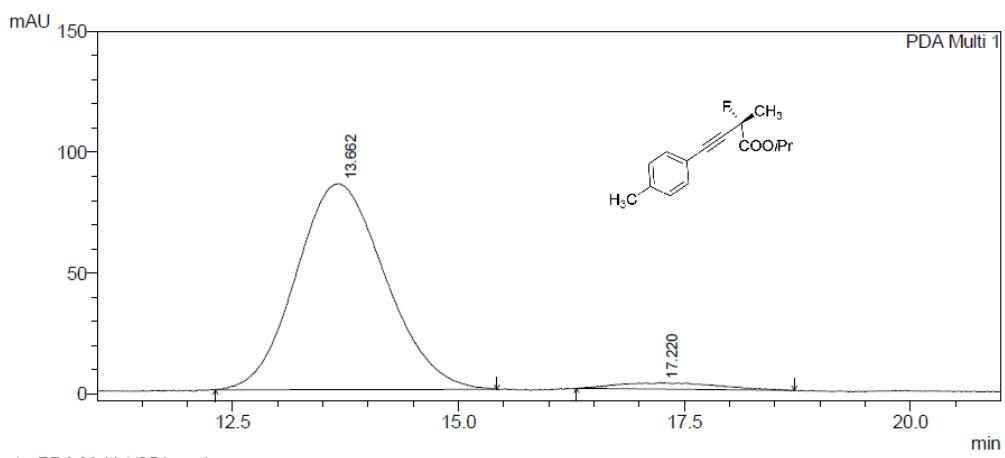
HPLC of 2p



PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	13.808	4505611	64419	50.662	58.514
2	17.320	4387844	45673	49.338	41.486
Total		8893454	110093	100.000	100.000

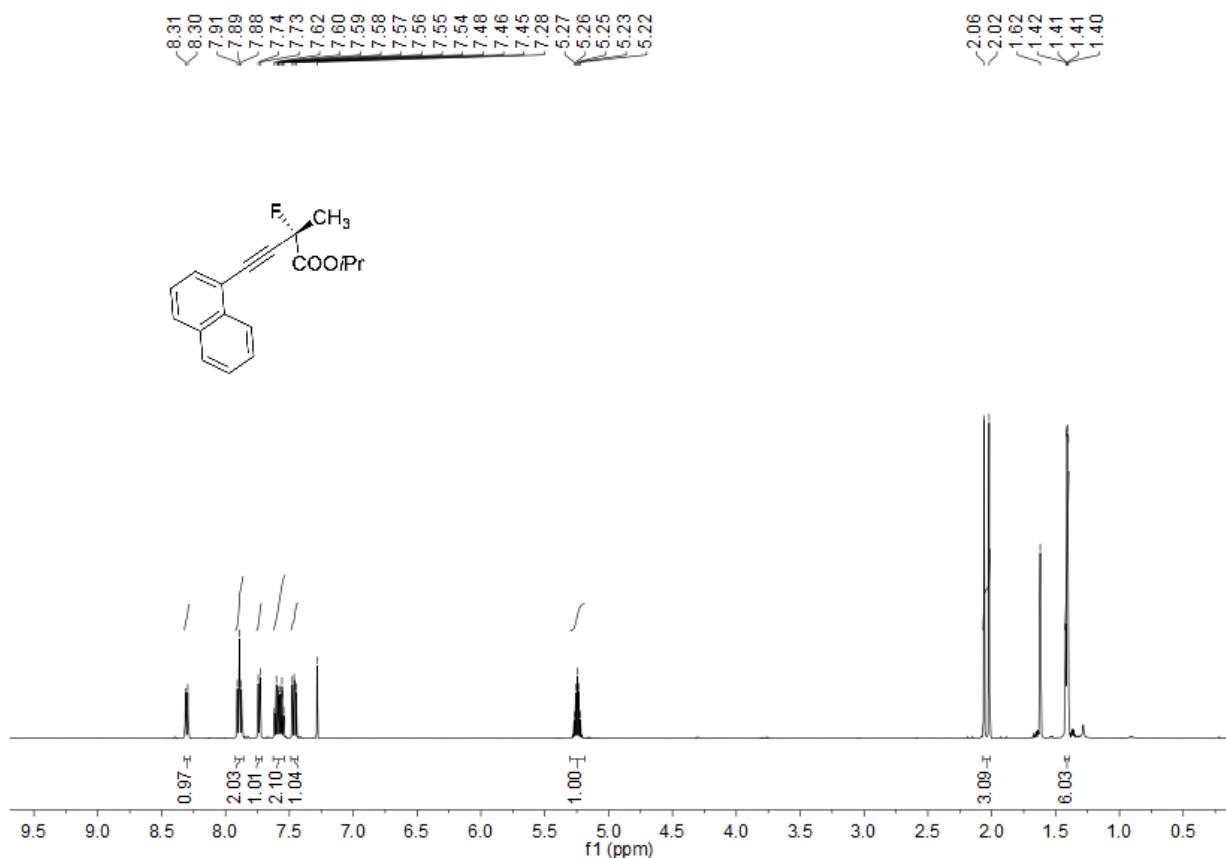


PeakTable

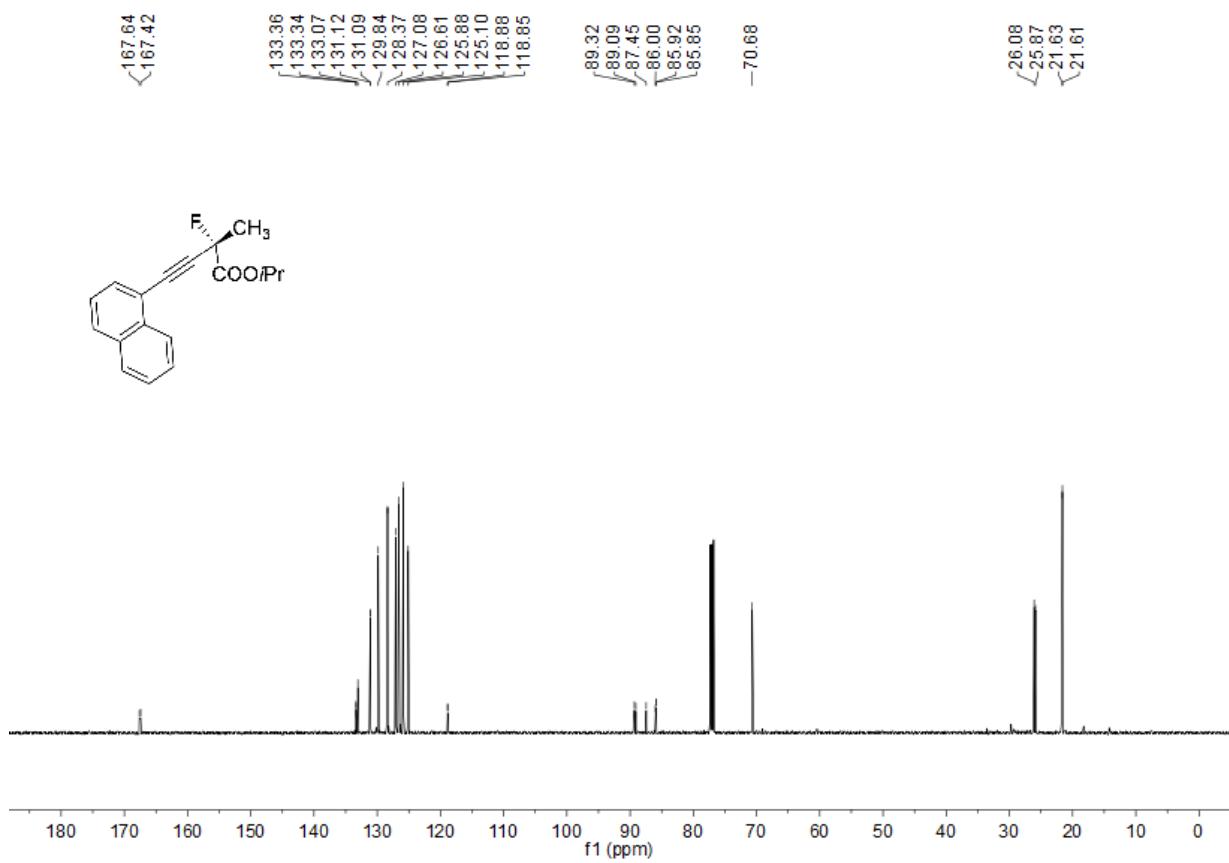
PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	13.662	5864121	85198	96.582	96.971
2	17.220	207502	2661	3.418	3.029
Total		6071622	87859	100.000	100.000

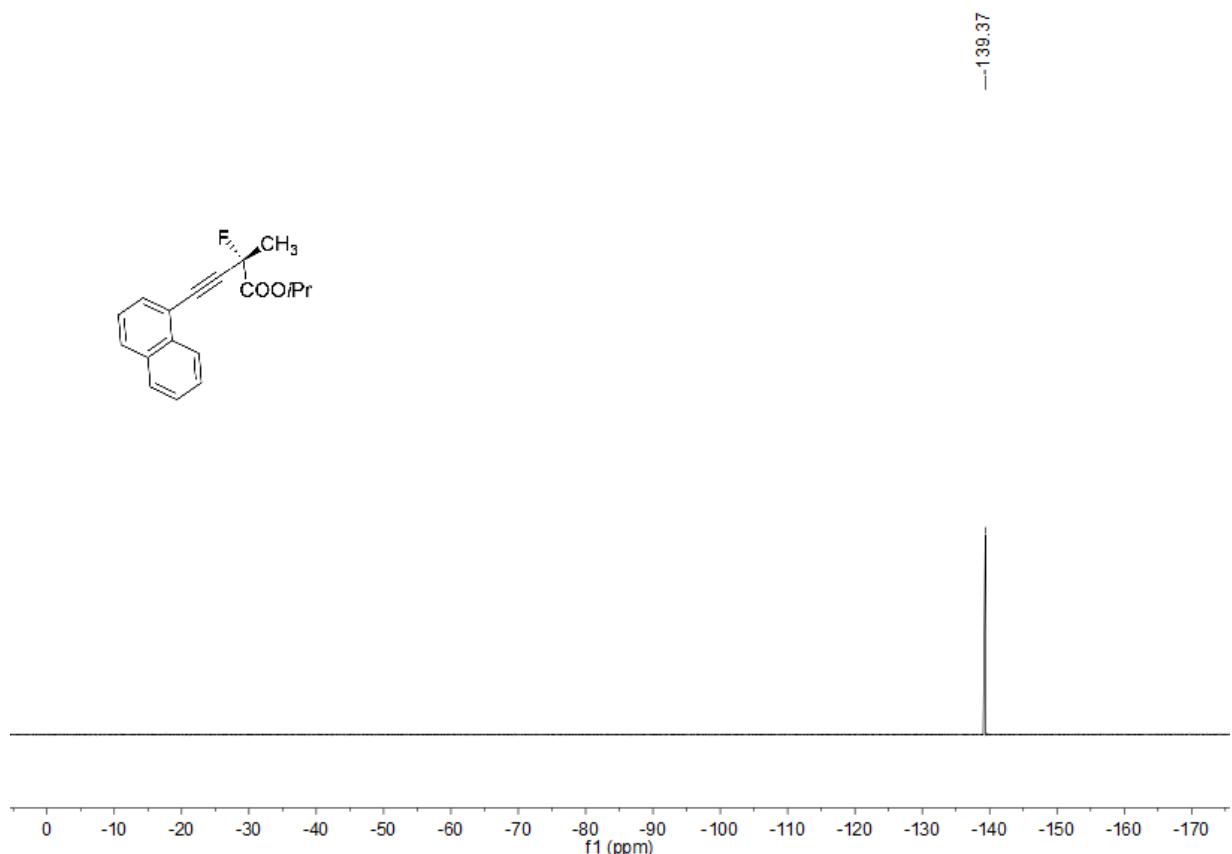
^1H NMR of 2q (500 MHz, CDCl_3)



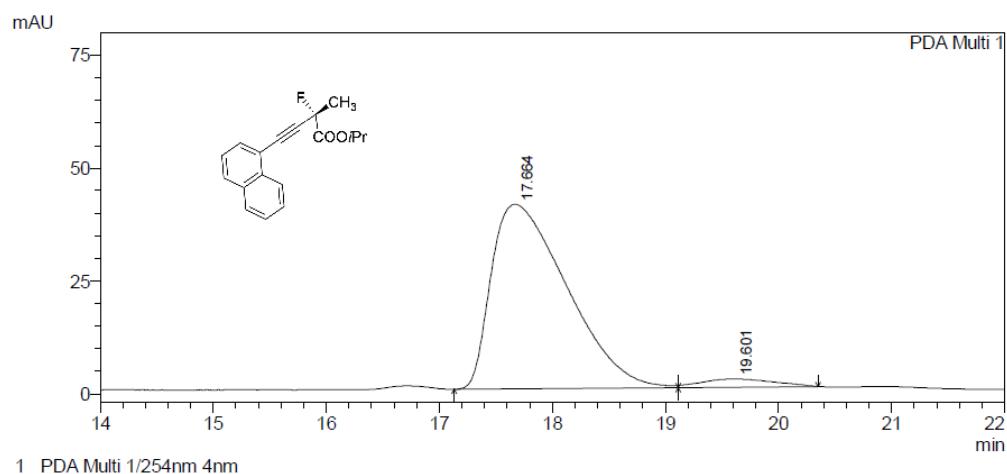
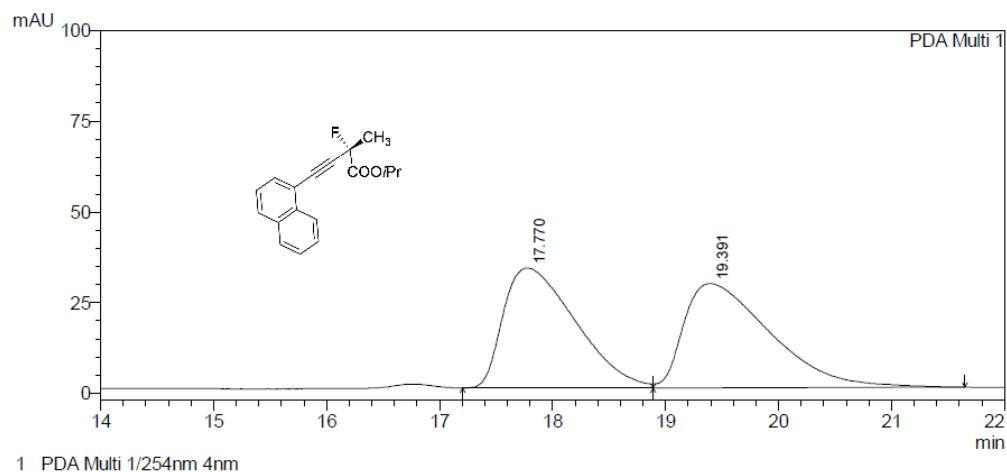
$^{13}\text{C}\{\text{H}\}$ NMR of 2q (125 MHz, CDCl_3)



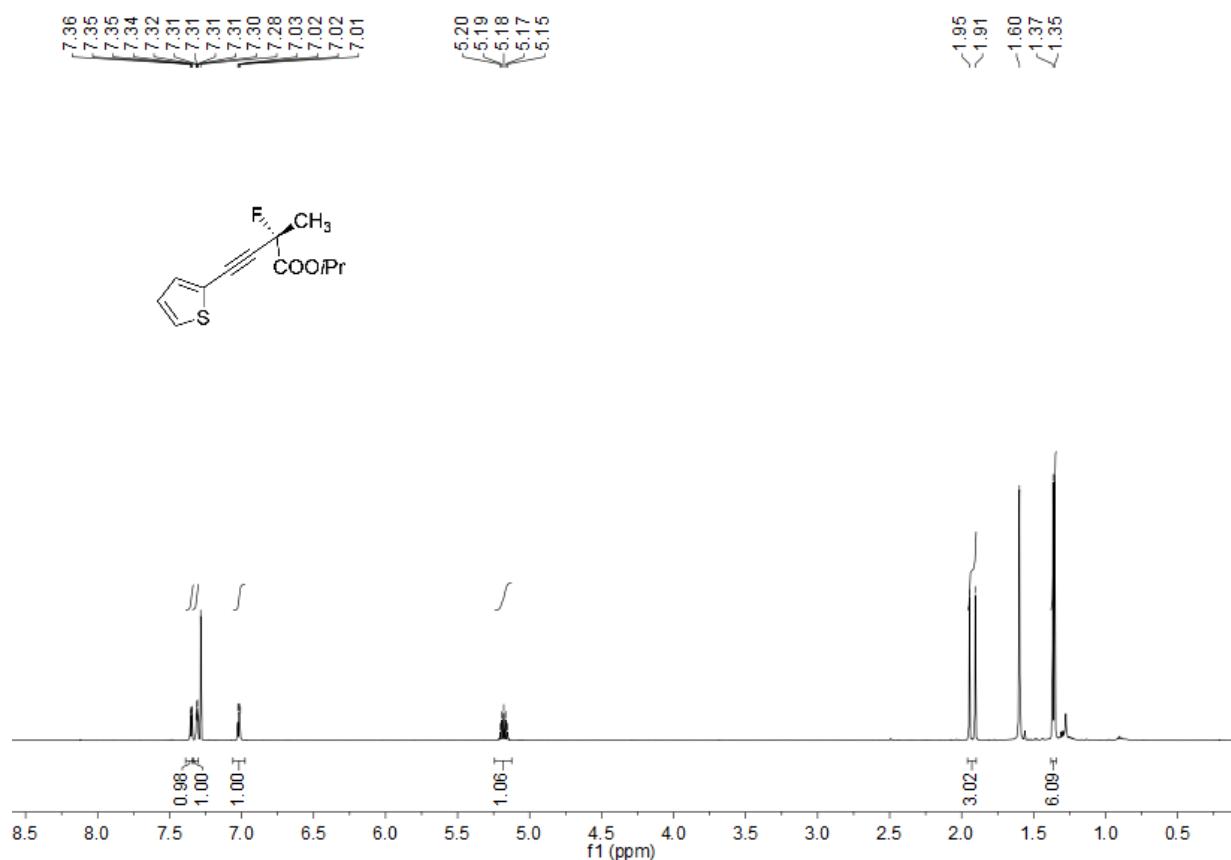
^{19}F NMR of 2q (470 MHz, CDCl_3)



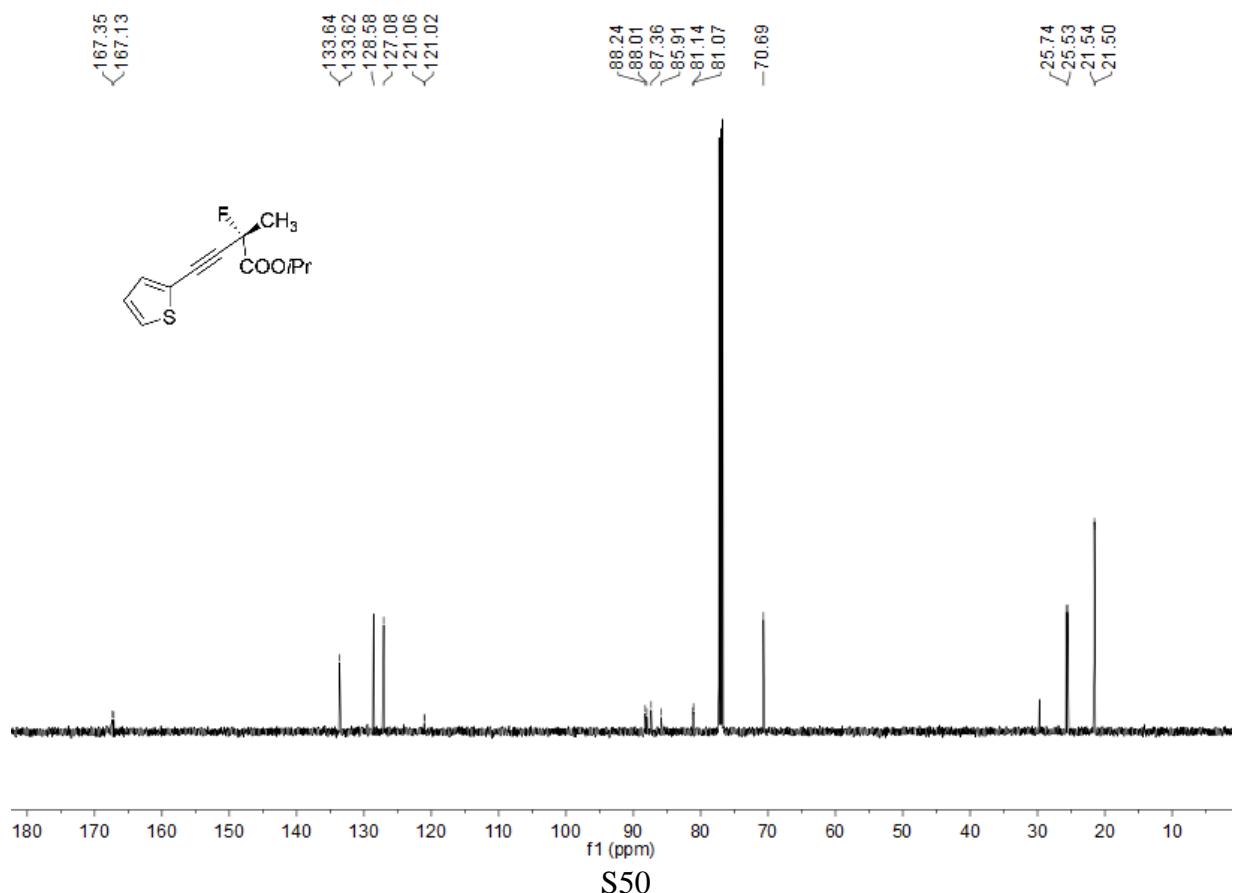
HPLC of 2q



^1H NMR of 2r (500 MHz, CDCl_3)

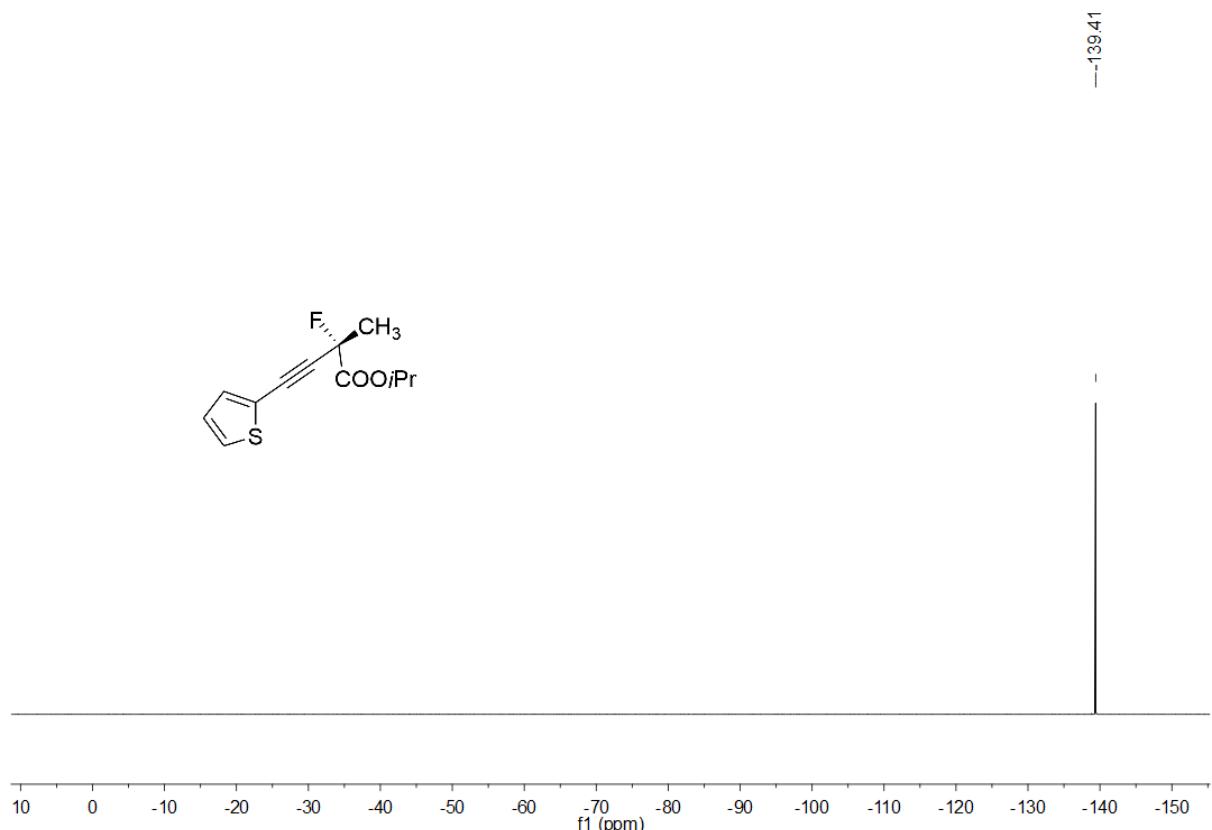


$^{13}\text{C}\{^1\text{H}\}$ NMR of 2r (125 MHz, CDCl_3)

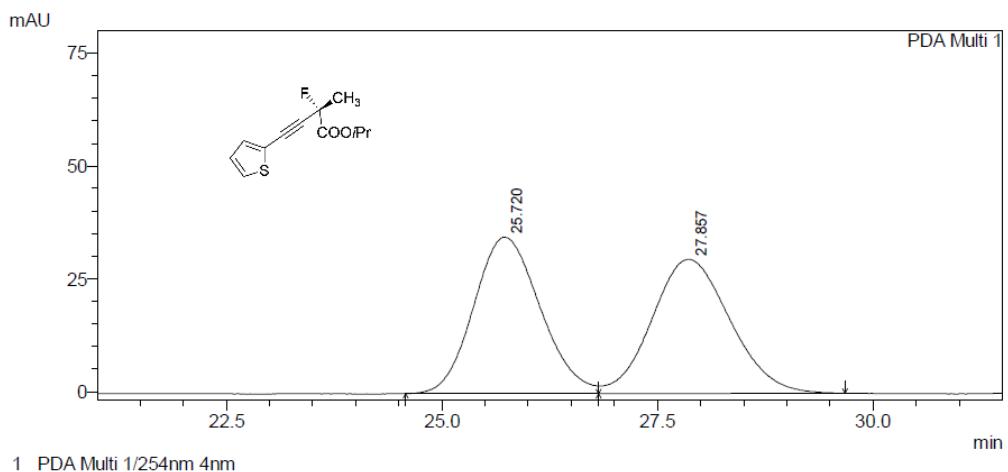


S50

^{19}F NMR of 2r (470 MHz, CDCl_3)

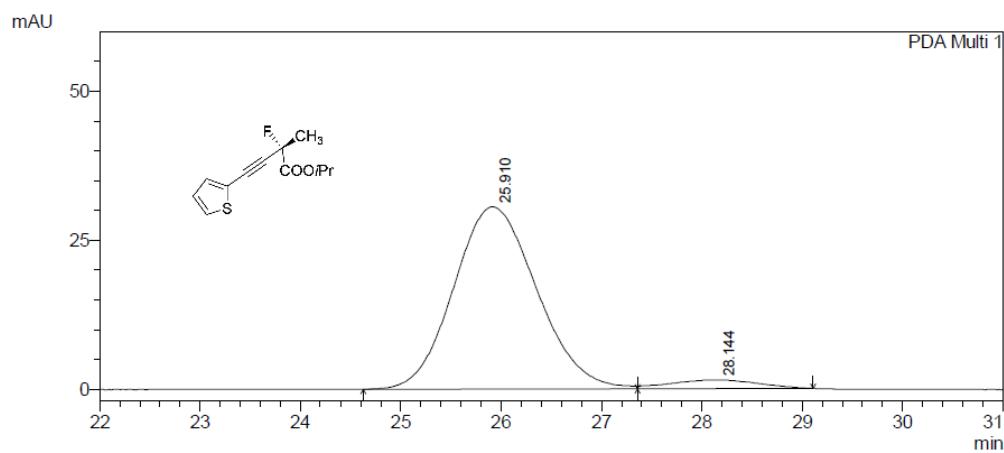


HPLC of 2r



PeakTable

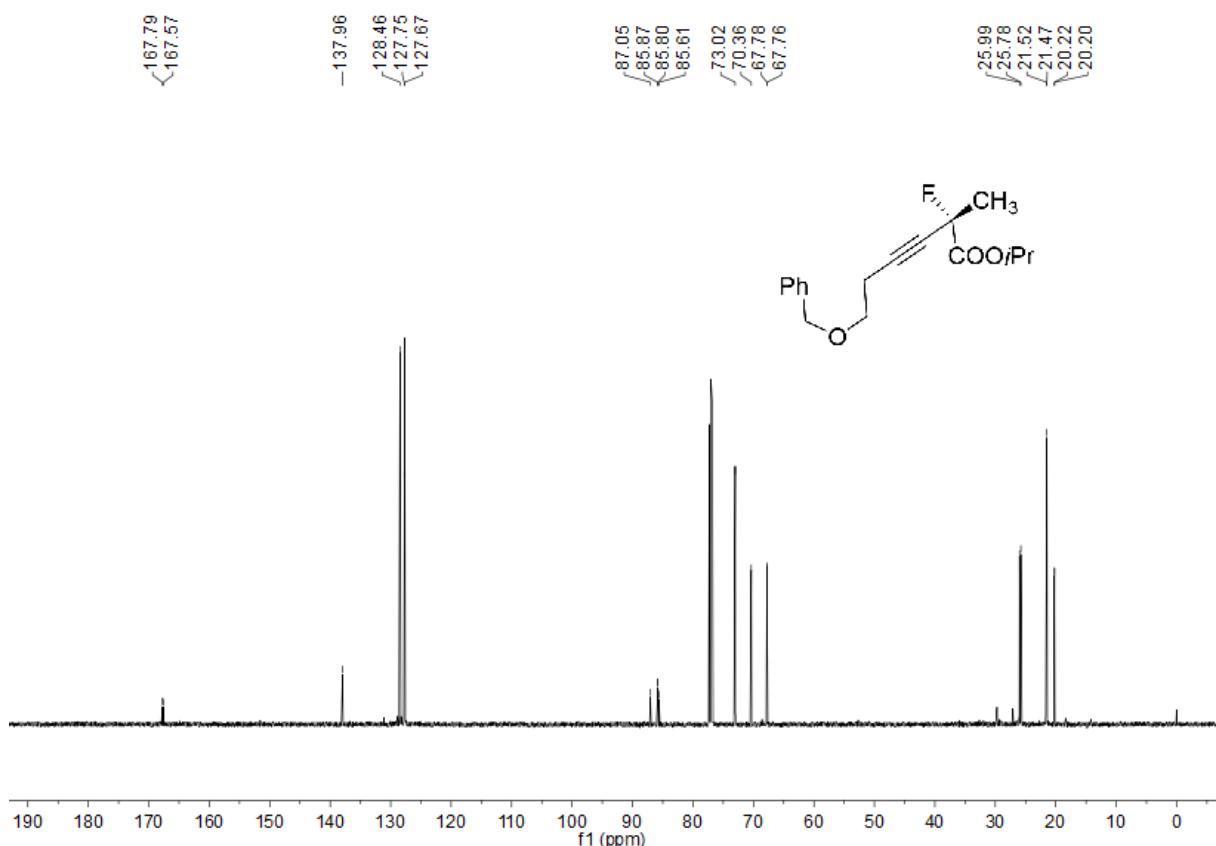
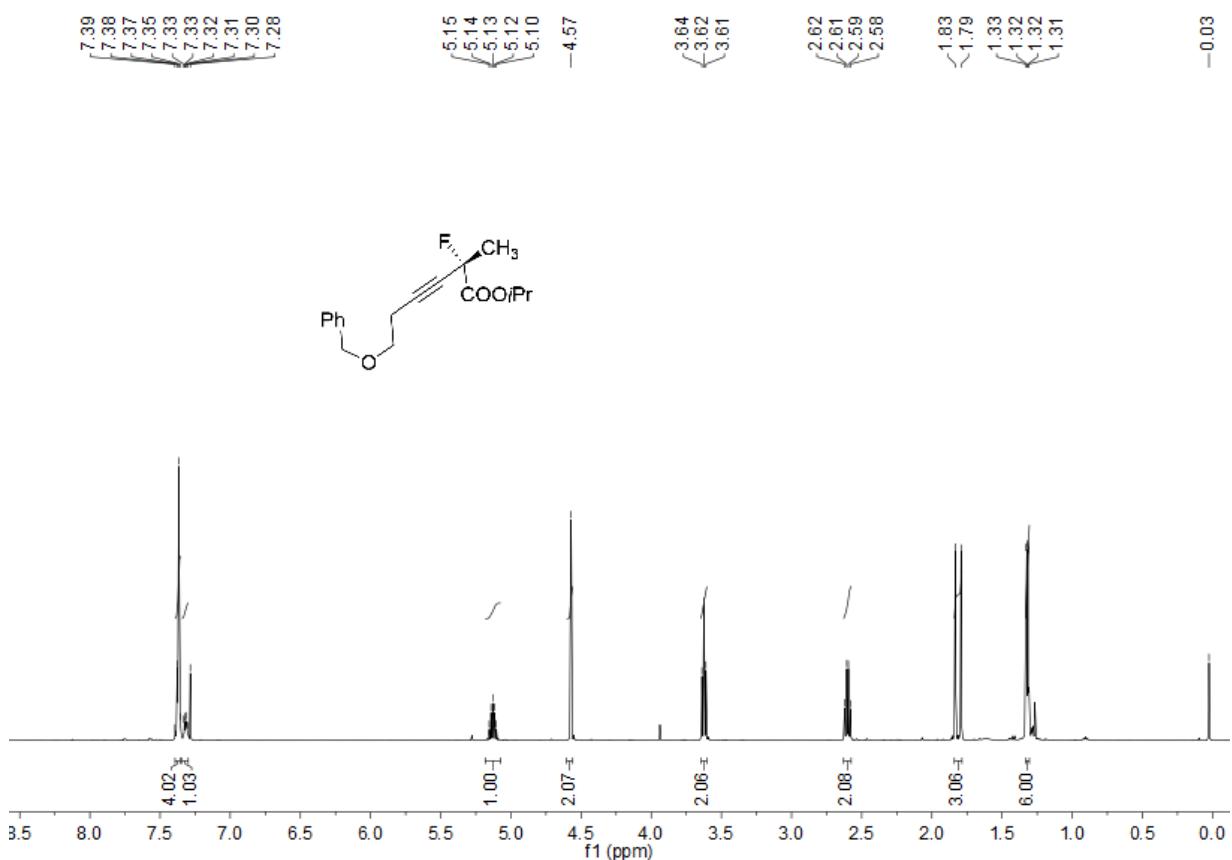
PDA Ch1 254nm 4nm					
Peak#	Ret. Time	Area	Height	Area %	Height %
1	25.720	1861672	34665	49.859	53.832
2	27.857	1872166	29730	50.141	46.168
Total		3733838	64396	100.000	100.000



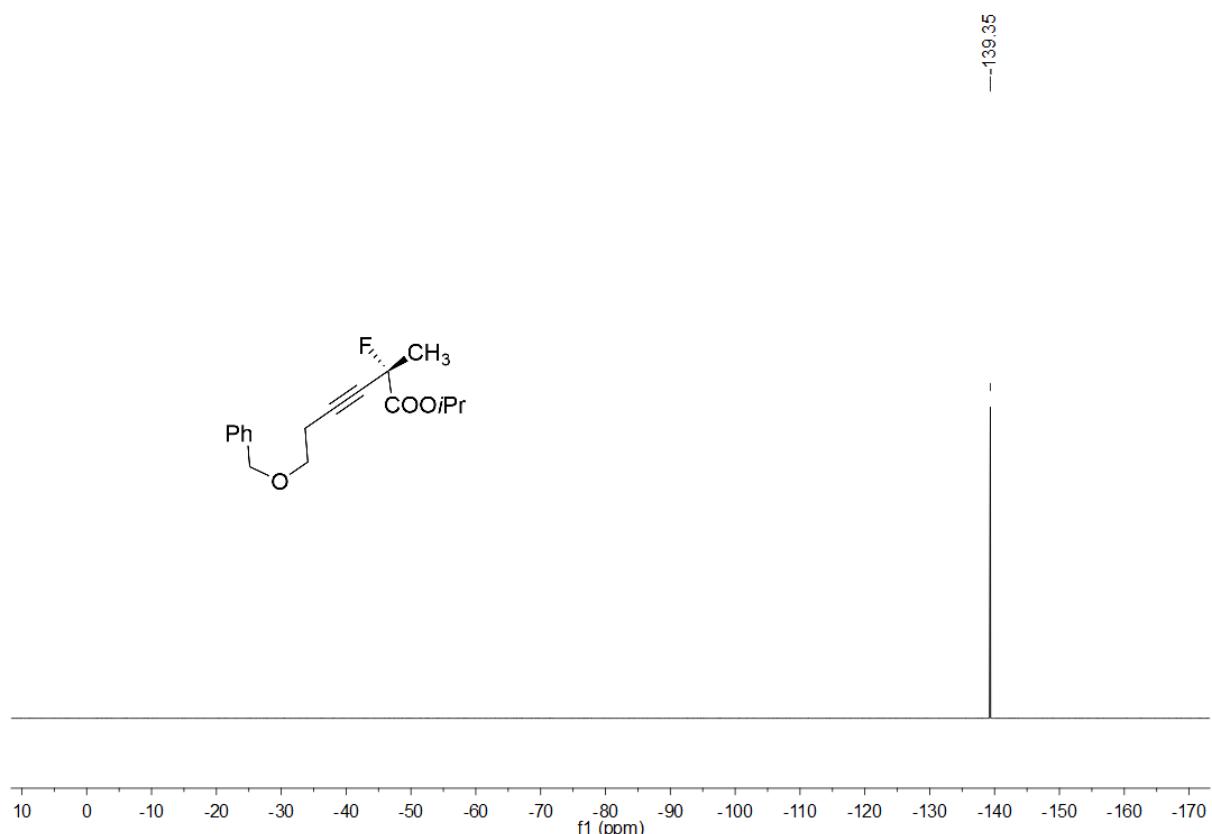
PeakTable

PDA Ch1 254nm 4nm					
Peak#	Ret. Time	Area	Height	Area %	Height %
1	25.910	1759606	30552	95.225	95.434
2	28.144	88240	1462	4.775	4.566
Total		1847846	32013	100.000	100.000

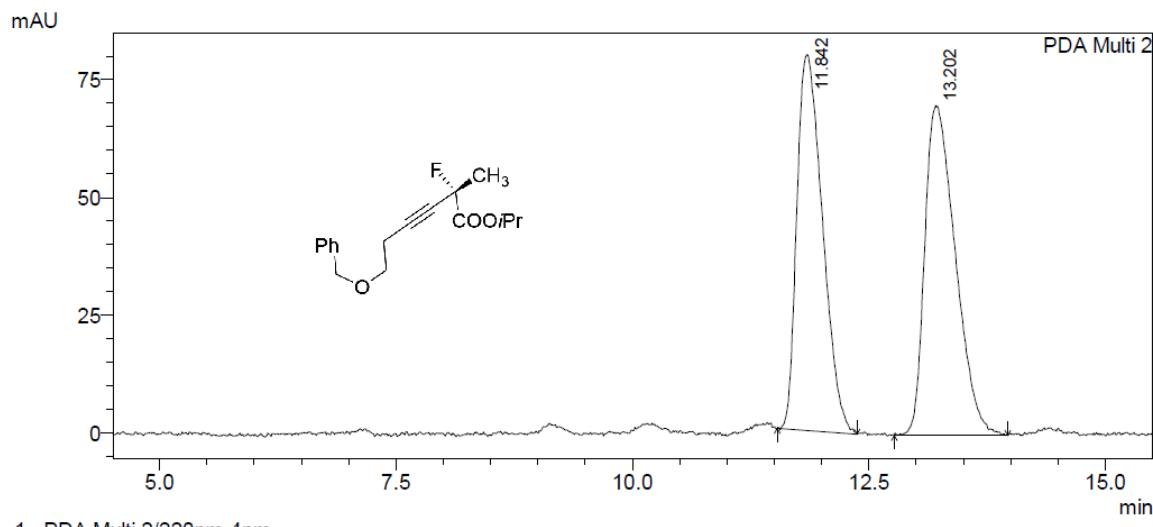
¹H NMR of 2s (500 MHz, CDCl₃)



^{19}F NMR of 2s (470 MHz, CDCl_3)



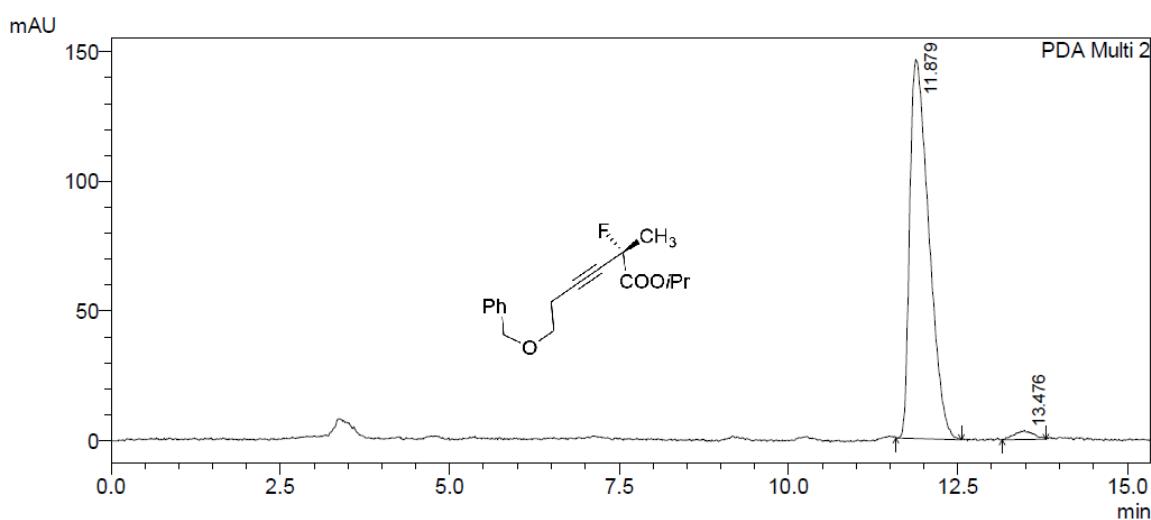
HPLC of 2s



PeakTable

PDA Ch2 220nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	11.842	1507141	79742	48.844	53.267
2	13.202	1578479	69960	51.156	46.733
Total		3085620	149702	100.000	100.000

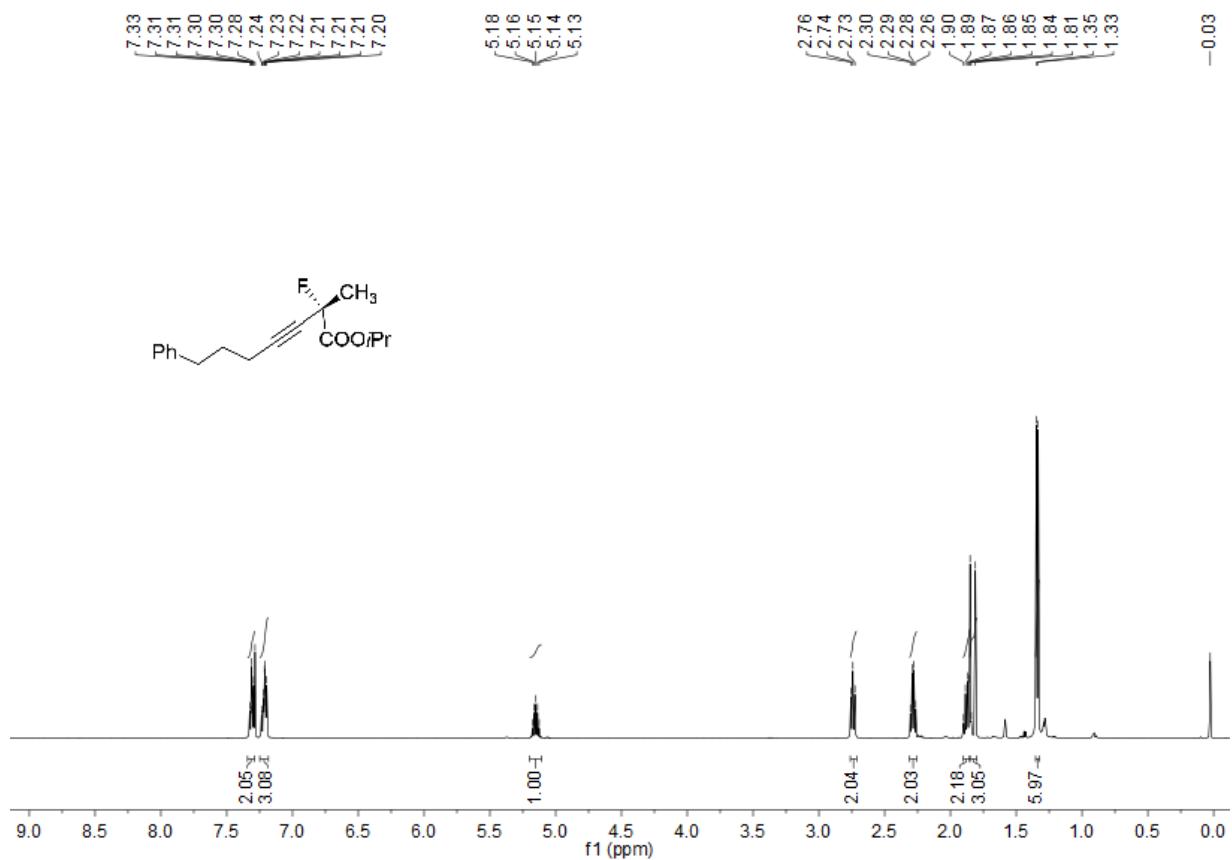


PeakTable

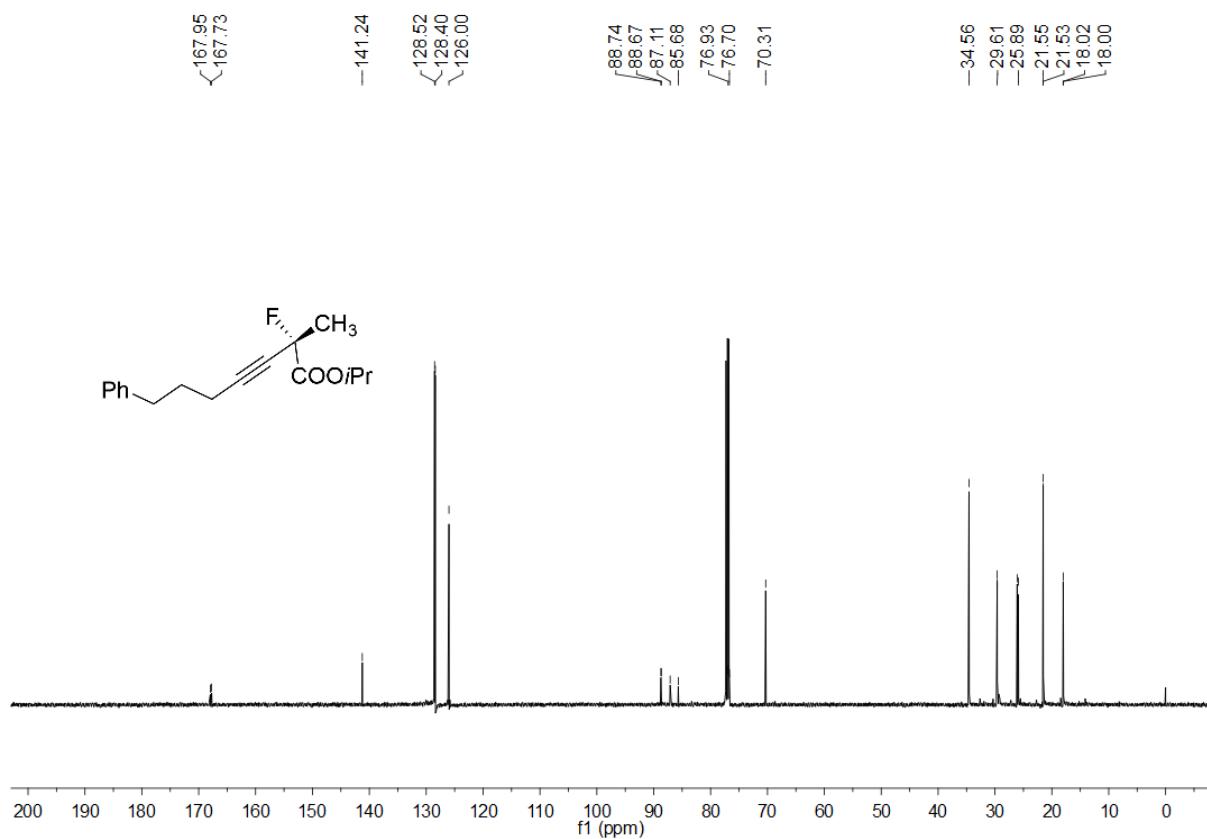
PDA Ch2 220nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	11.879	2859055	146087	97.598	97.589
2	13.476	70361	3610	2.402	2.411
Total		2929416	149697	100.000	100.000

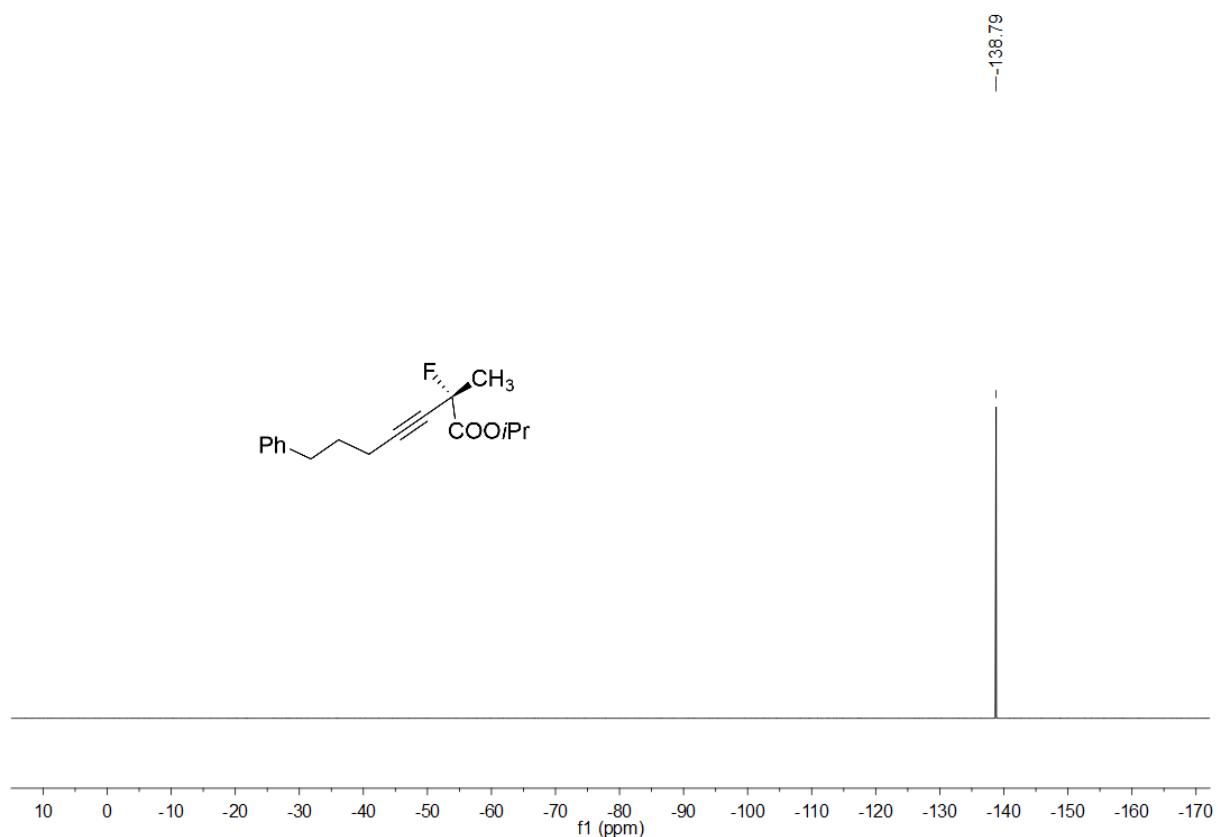
^1H NMR of 2t (500 MHz, CDCl_3)



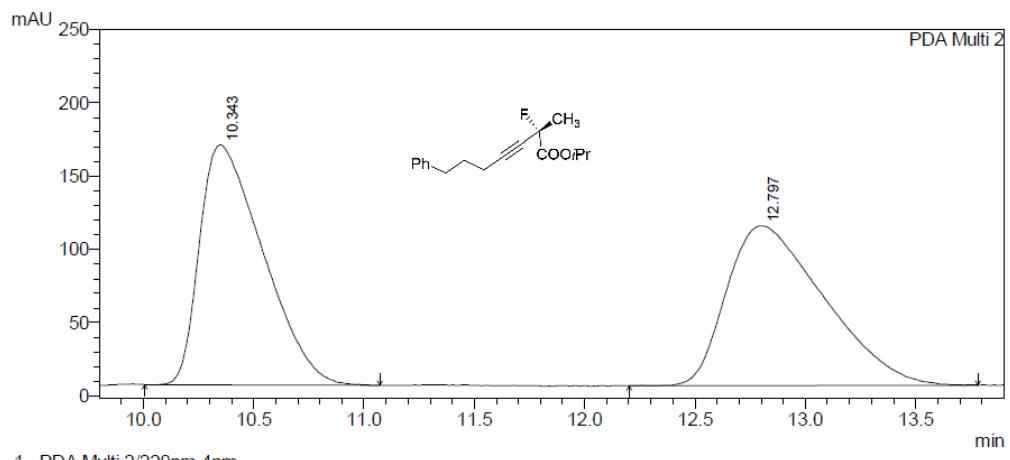
$^{13}\text{C}\{^1\text{H}\}$ NMR of 2t (125 MHz, CDCl_3)



^{19}F NMR of 2t (470 MHz, CDCl_3)



HPLC of 2t

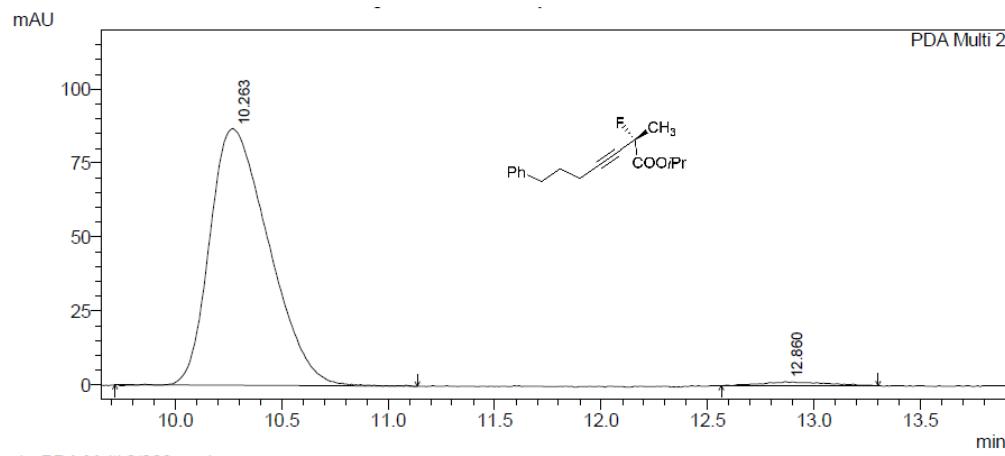


1 PDA Multi 2/220nm 4nm

PeakTable

PDA Ch2 220nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	10.343	3282240	163799	49.385	60.037
2	12.797	3363950	109031	50.615	39.963
Total		6646190	272830	100.000	100.000



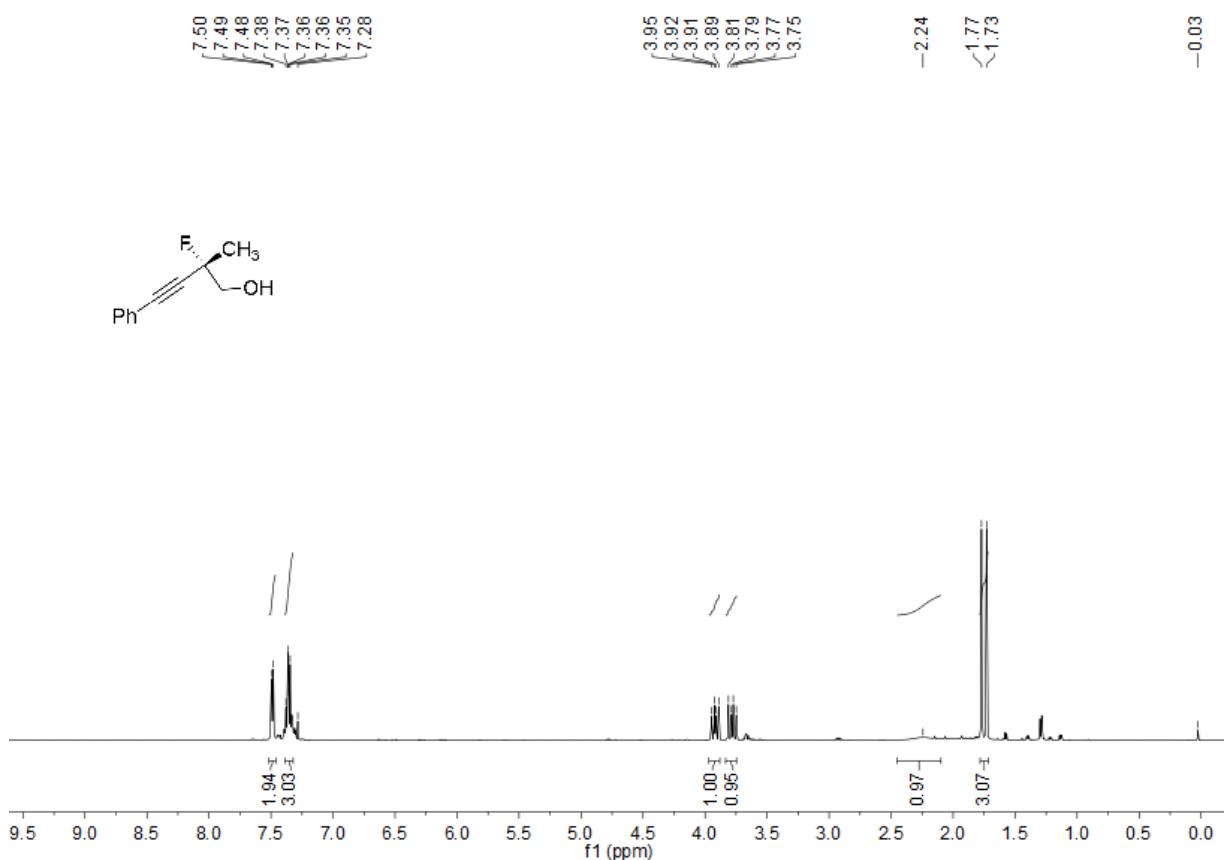
1 PDA Multi 2/220nm 4nm

PeakTable

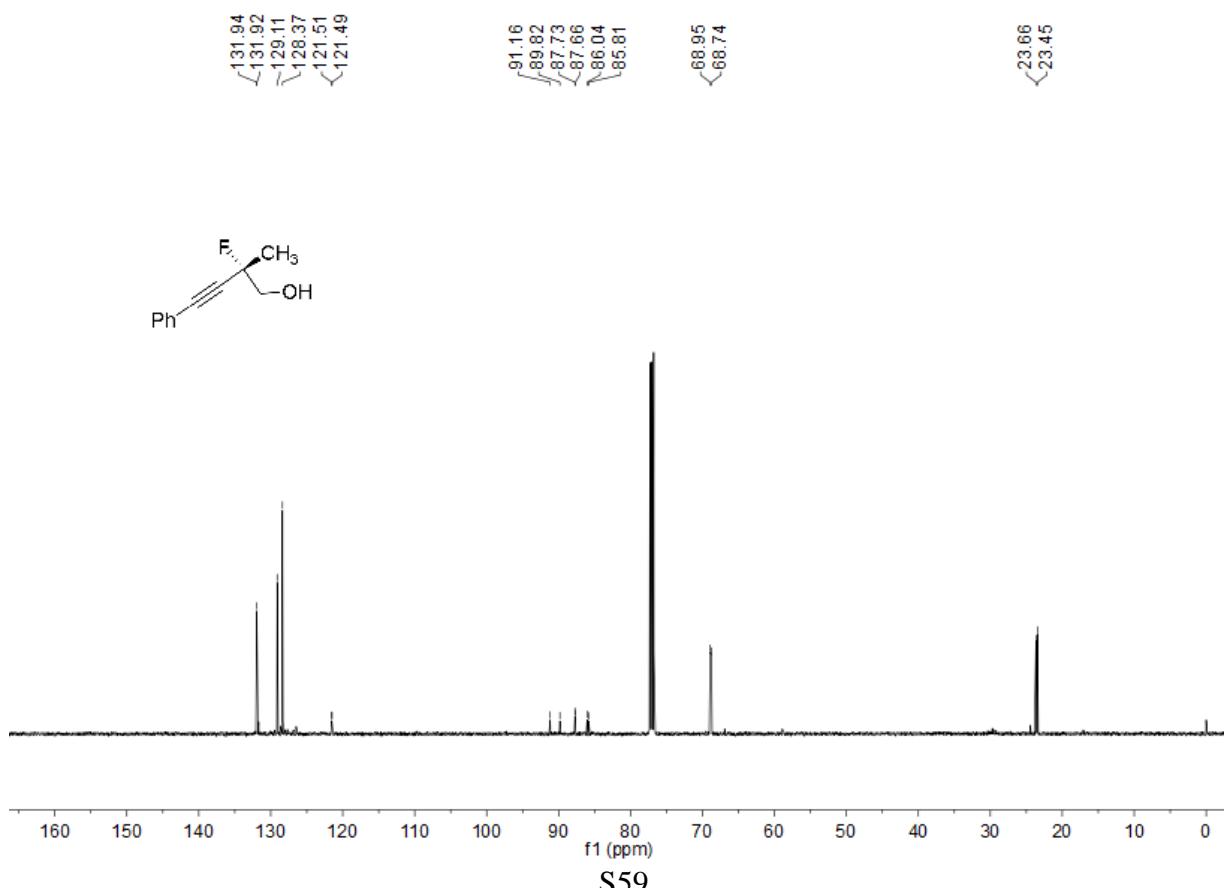
PDA Ch2 220nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	10.263	1673479	86843	98.466	98.497
2	12.860	26075	1325	1.534	1.503
Total		1699554	88168	100.000	100.000

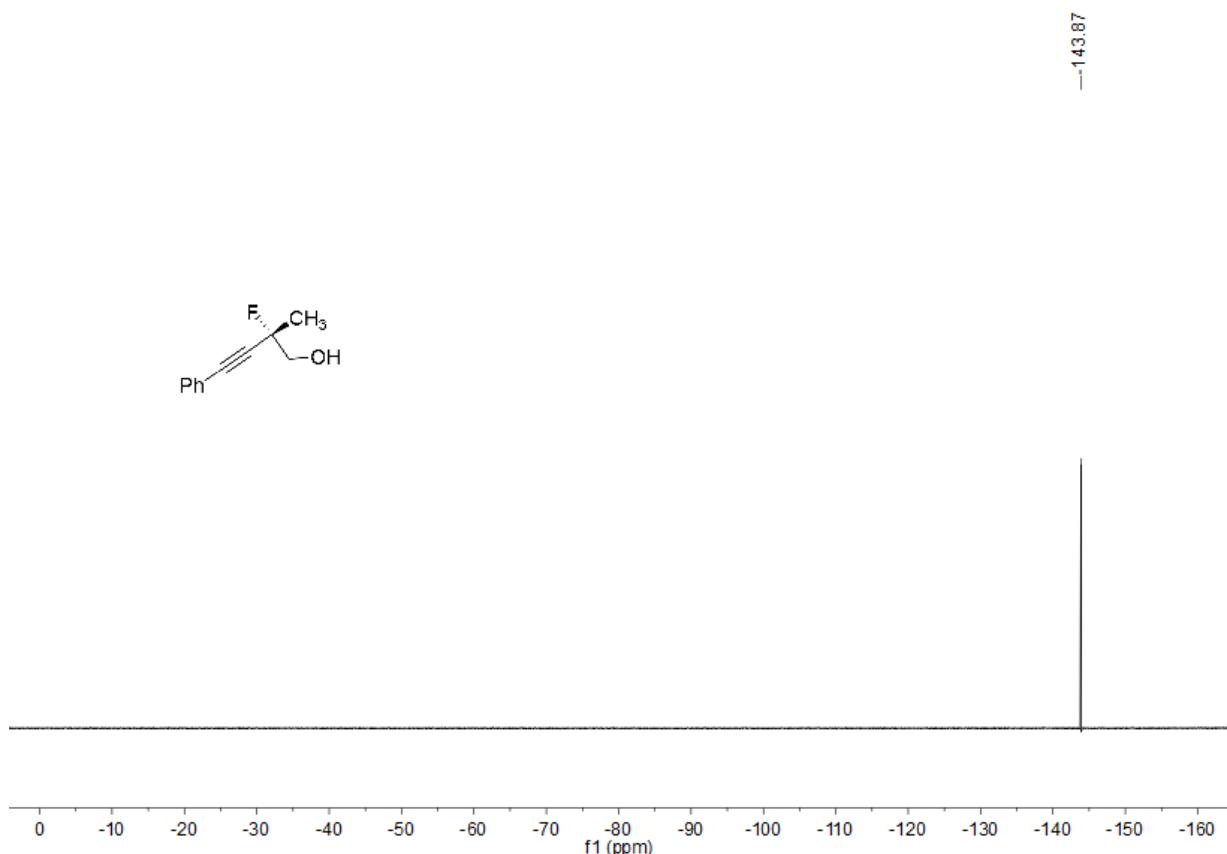
^1H NMR of 3 (500 MHz, CDCl_3)



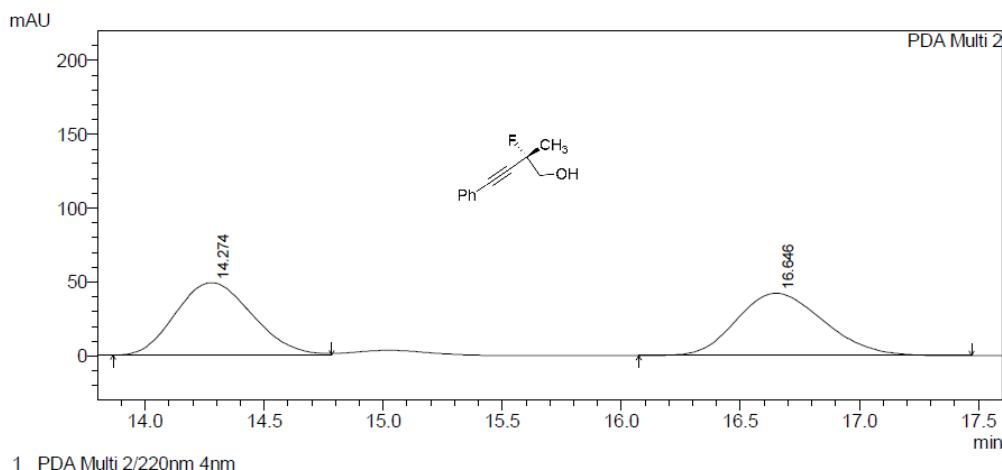
$^{13}\text{C}\{^1\text{H}\}$ NMR of 3 (125 MHz, CDCl_3)



^{19}F NMR of 3 (470 MHz, CDCl_3)

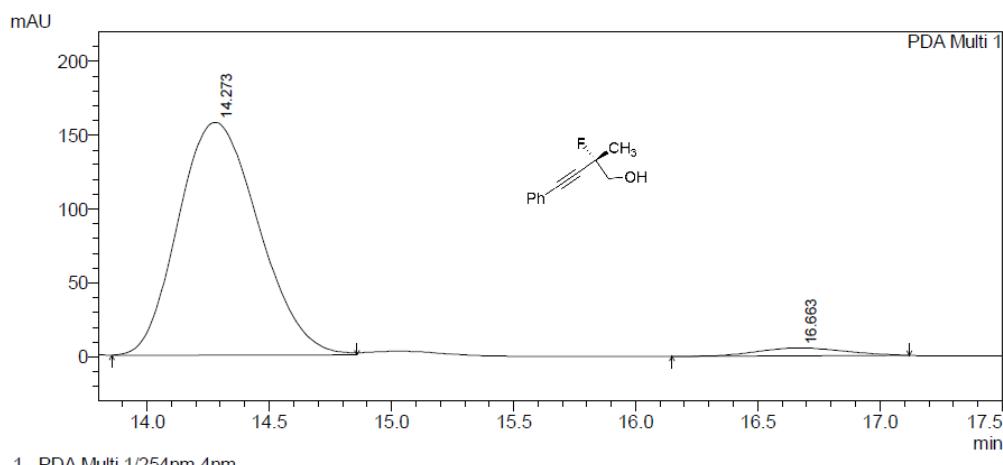


HPLC of 3



PeakTable

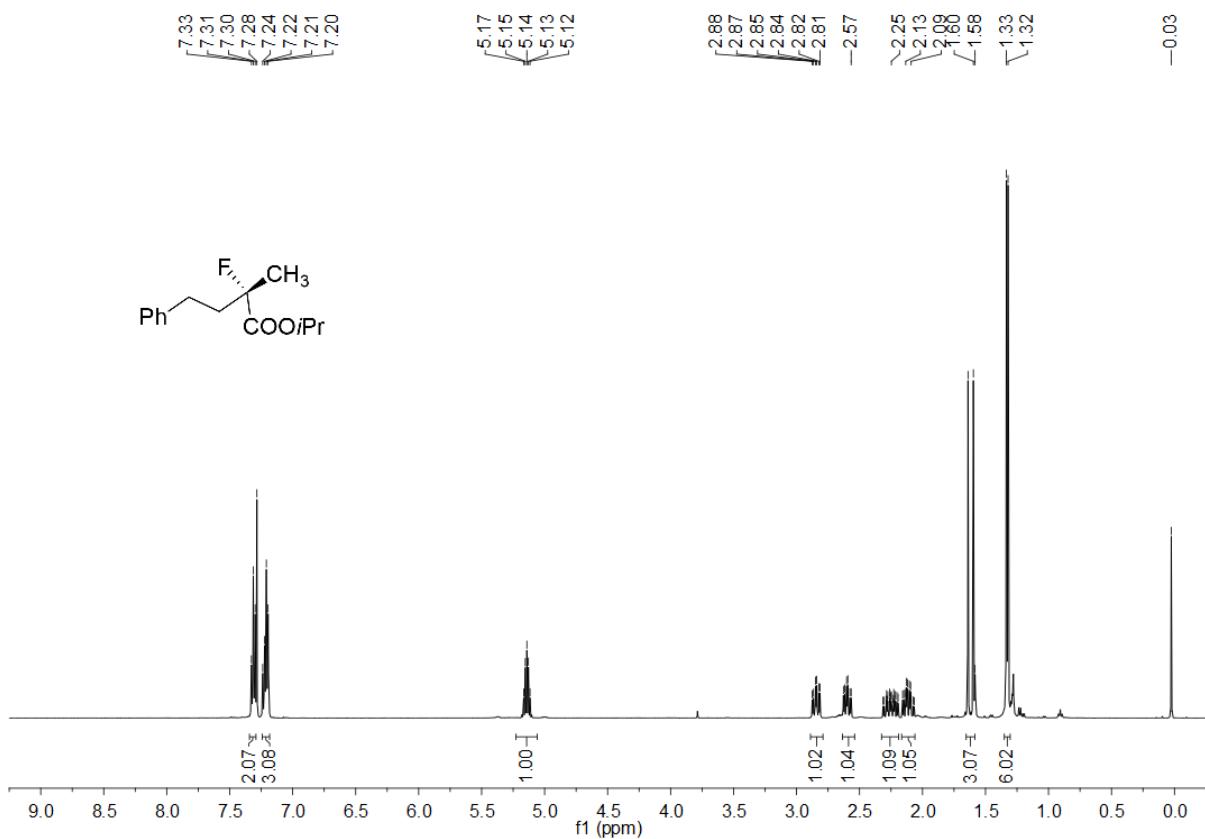
Peak#	Ret. Time	Area	Height	Area %	Height %
1	14.274	1099500	48960	50.556	53.780
2	16.646	1075312	42078	49.444	46.220
Total		2174812	91038	100.000	100.000



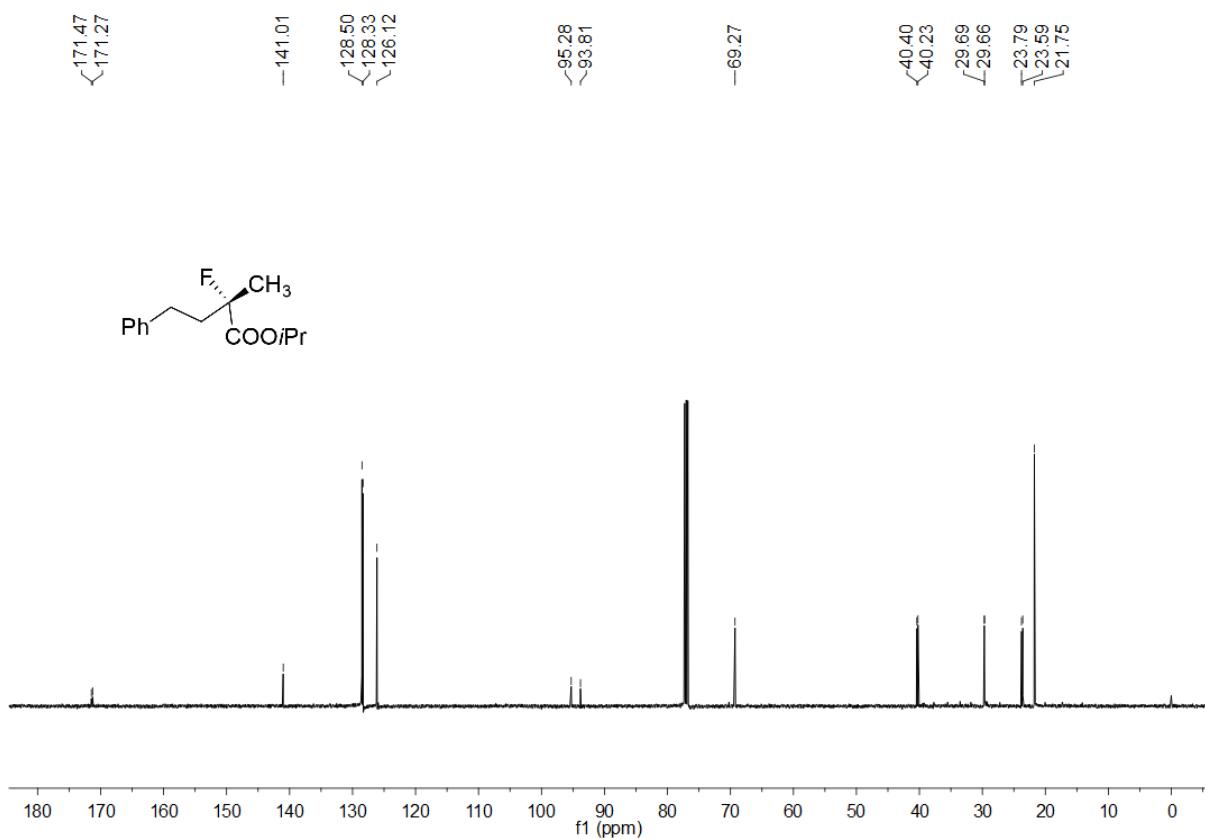
PeakTable

Peak#	Ret. Time	Area	Height	Area %	Height %
1	14.273	3602701	157411	96.480	96.741
2	16.663	131436	5303	3.520	3.259
Total		3734137	162714	100.000	100.000

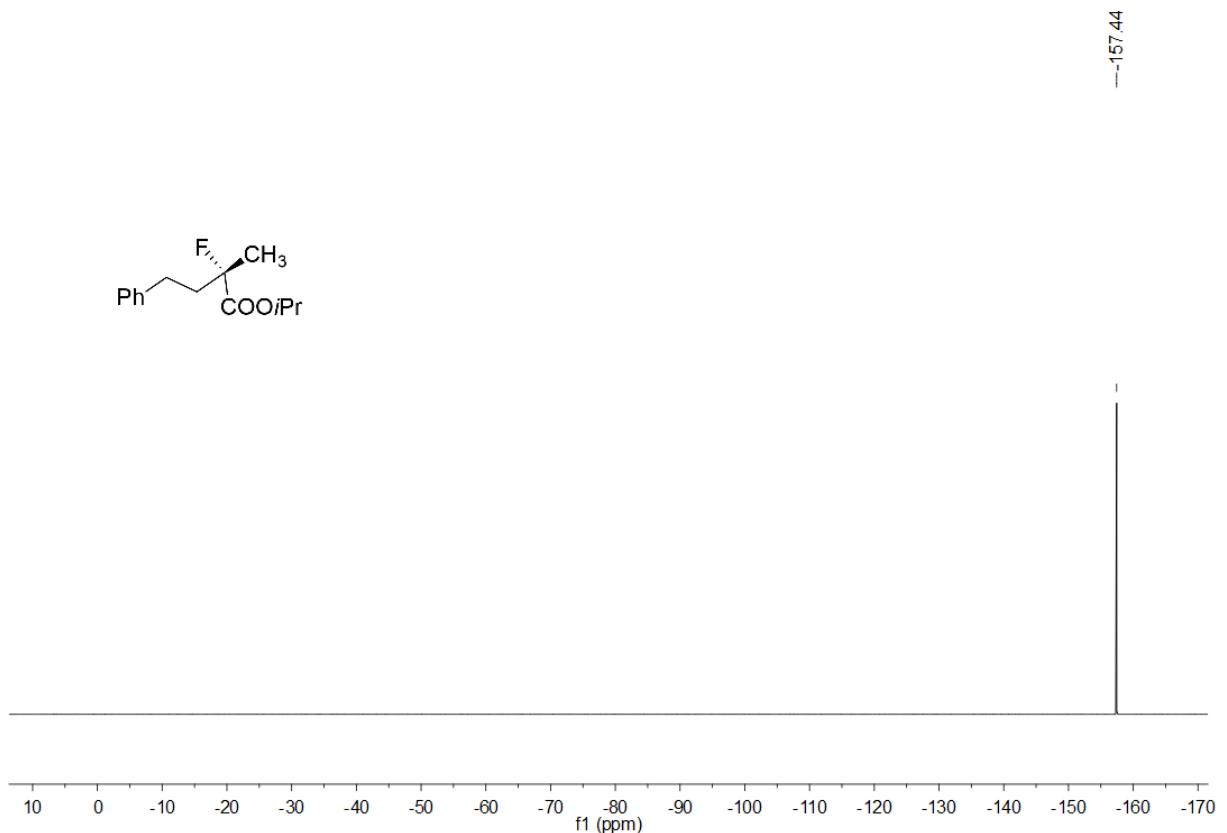
^1H NMR of 4 (500 MHz, CDCl_3)



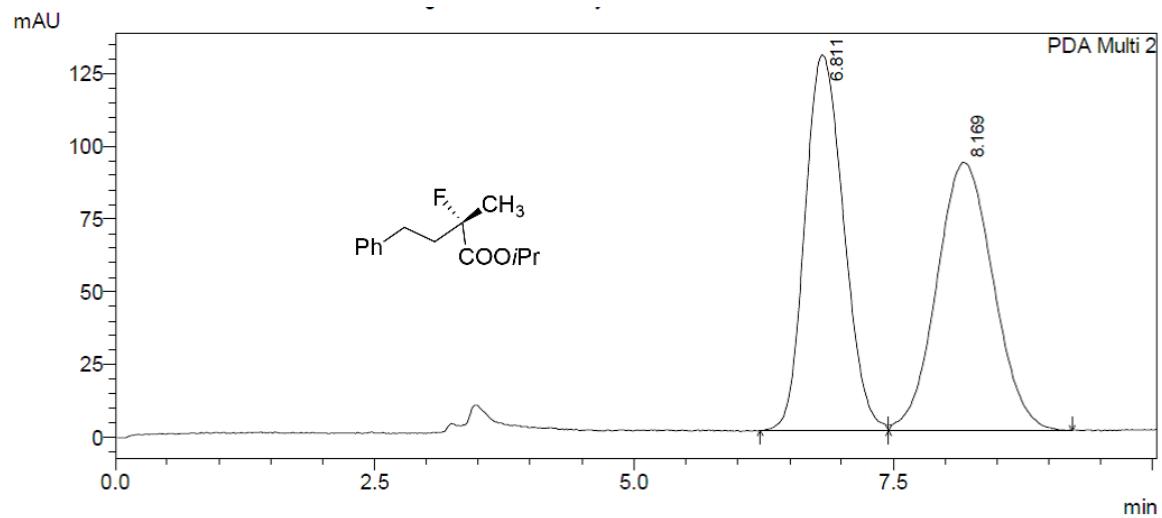
$^{13}\text{C}\{^1\text{H}\}$ NMR of 4 (125 MHz, CDCl_3)



^{19}F NMR of 4 (470 MHz, CDCl_3)



HPLC of 4

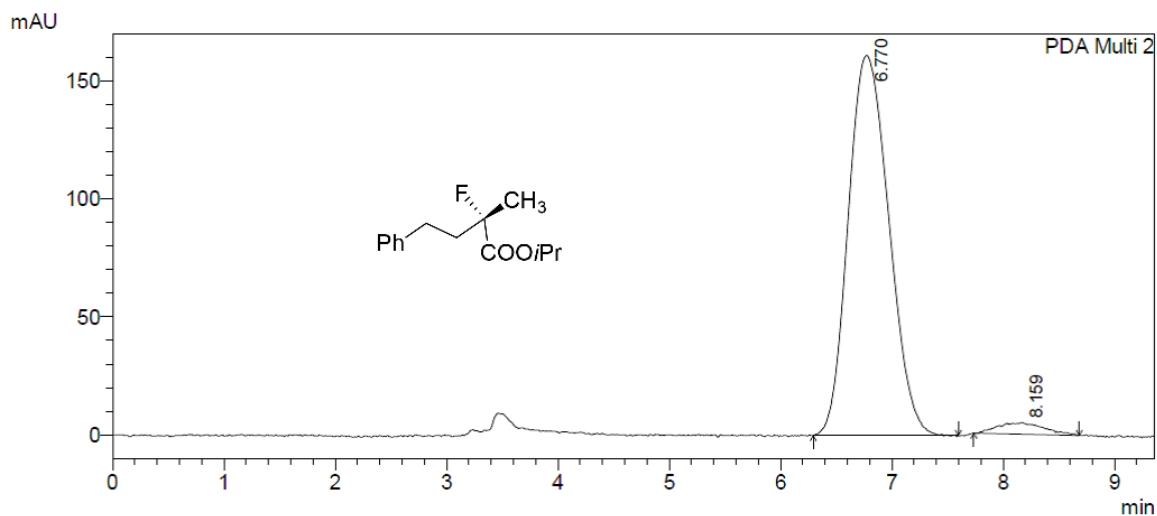


1 PDA Multi 2/220nm 4nm

PeakTable

PDA Ch2 220nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	6.811	3353454	129053	49.037	58.315
2	8.169	3485127	92252	50.963	41.685
Total		6838581	221305	100.000	100.000



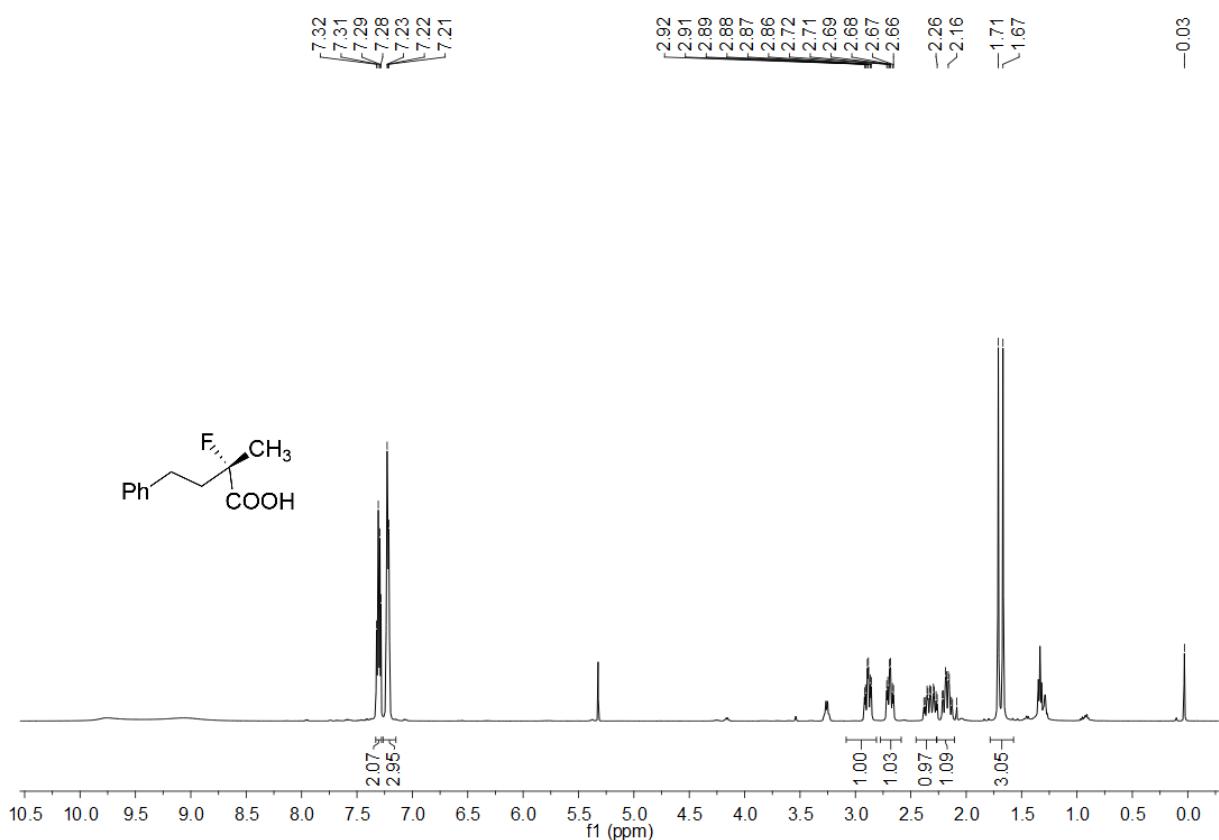
1 PDA Multi 2/220nm 4nm

PeakTable

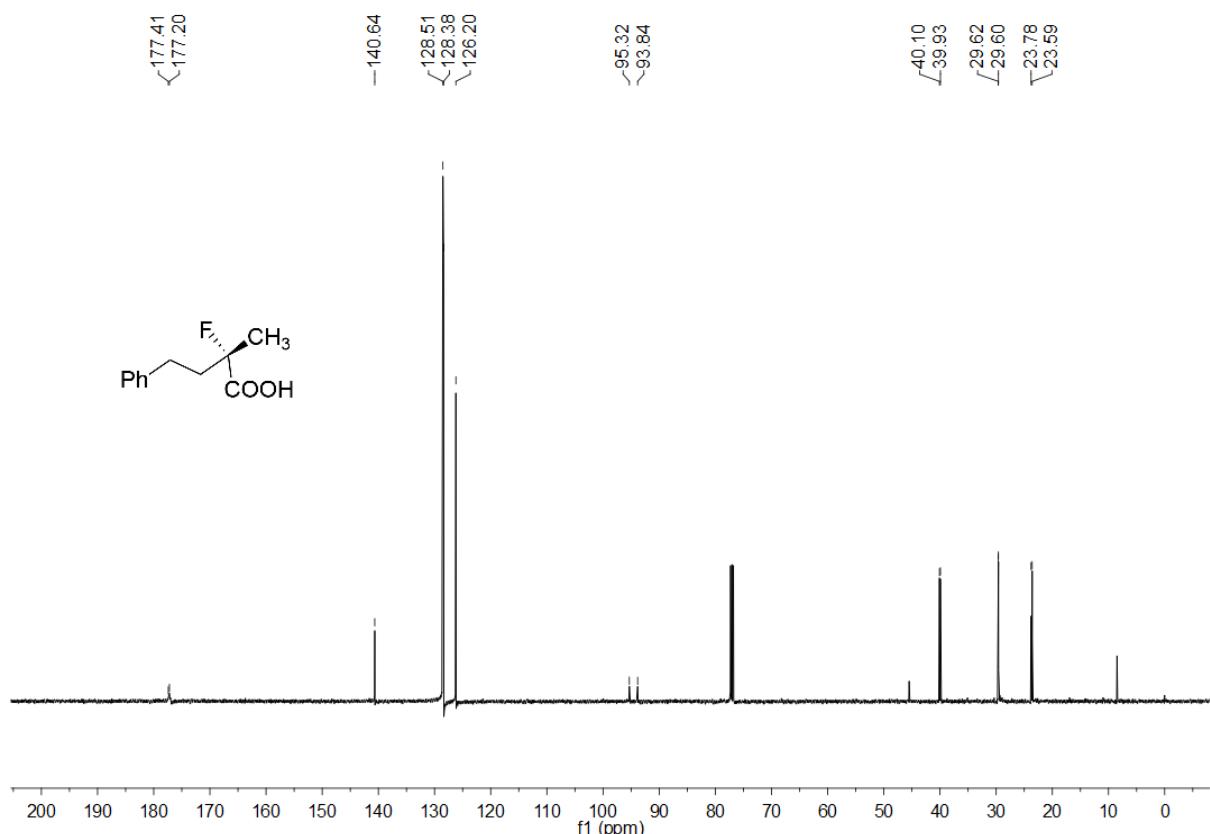
PDA Ch2 220nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	6.770	4099950	160798	96.590	96.961
2	8.159	144744	5040	3.410	3.039
Total		4244694	165838	100.000	100.000

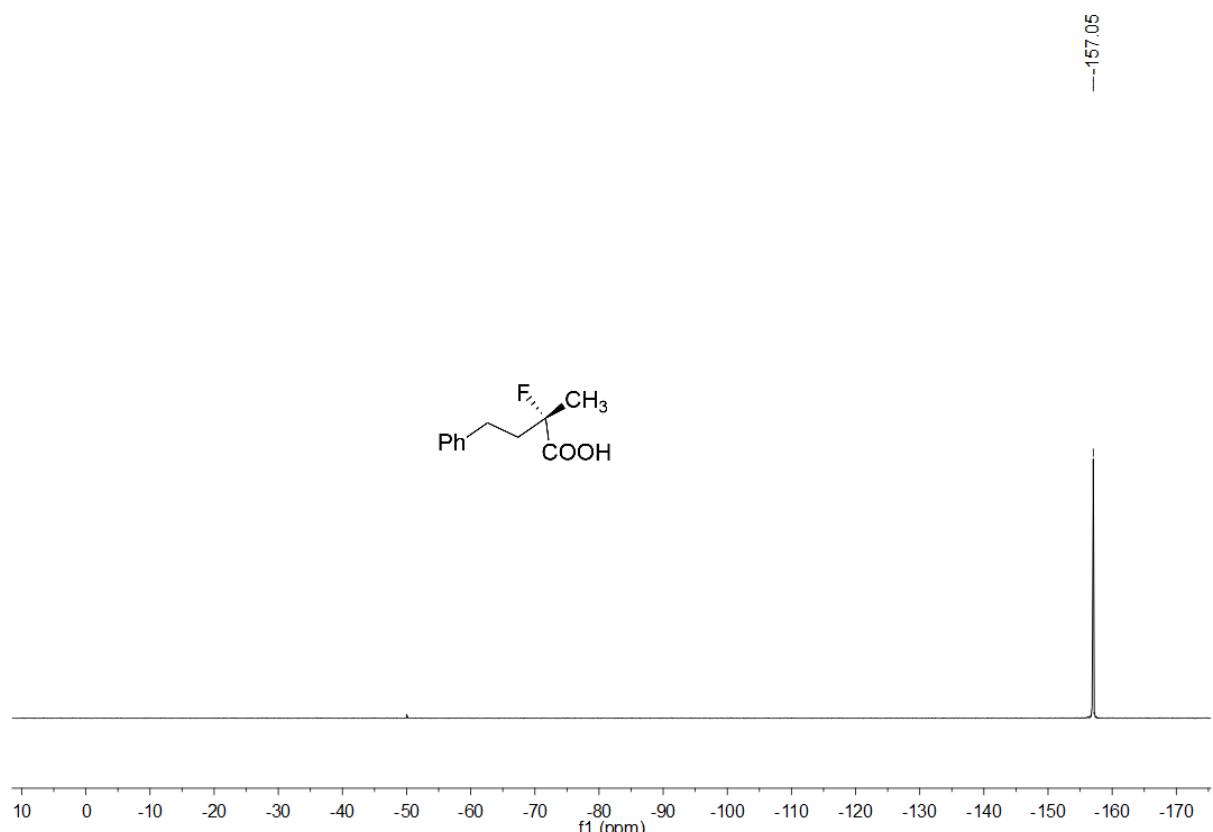
^1H NMR of 5 (500 MHz, CDCl_3)



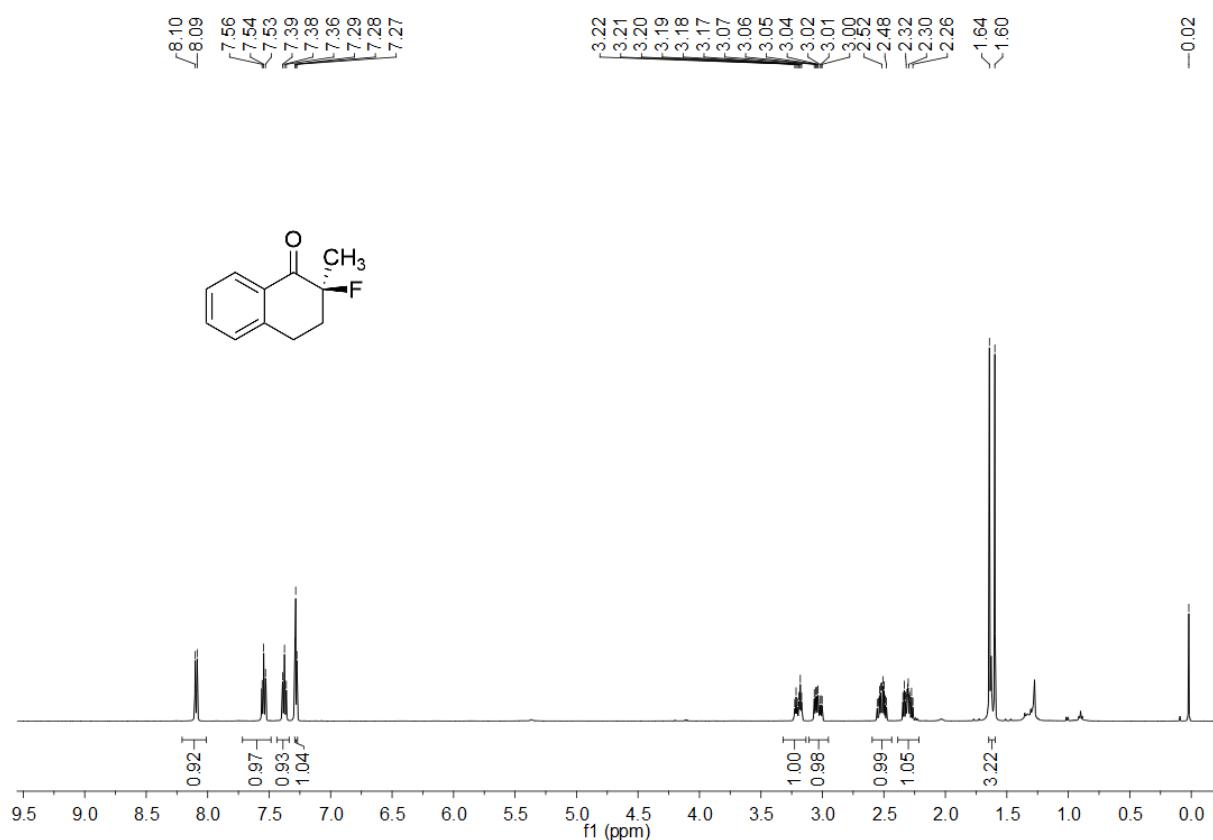
$^{13}\text{C}\{^1\text{H}\}$ NMR of 5 (125 MHz, CDCl_3)



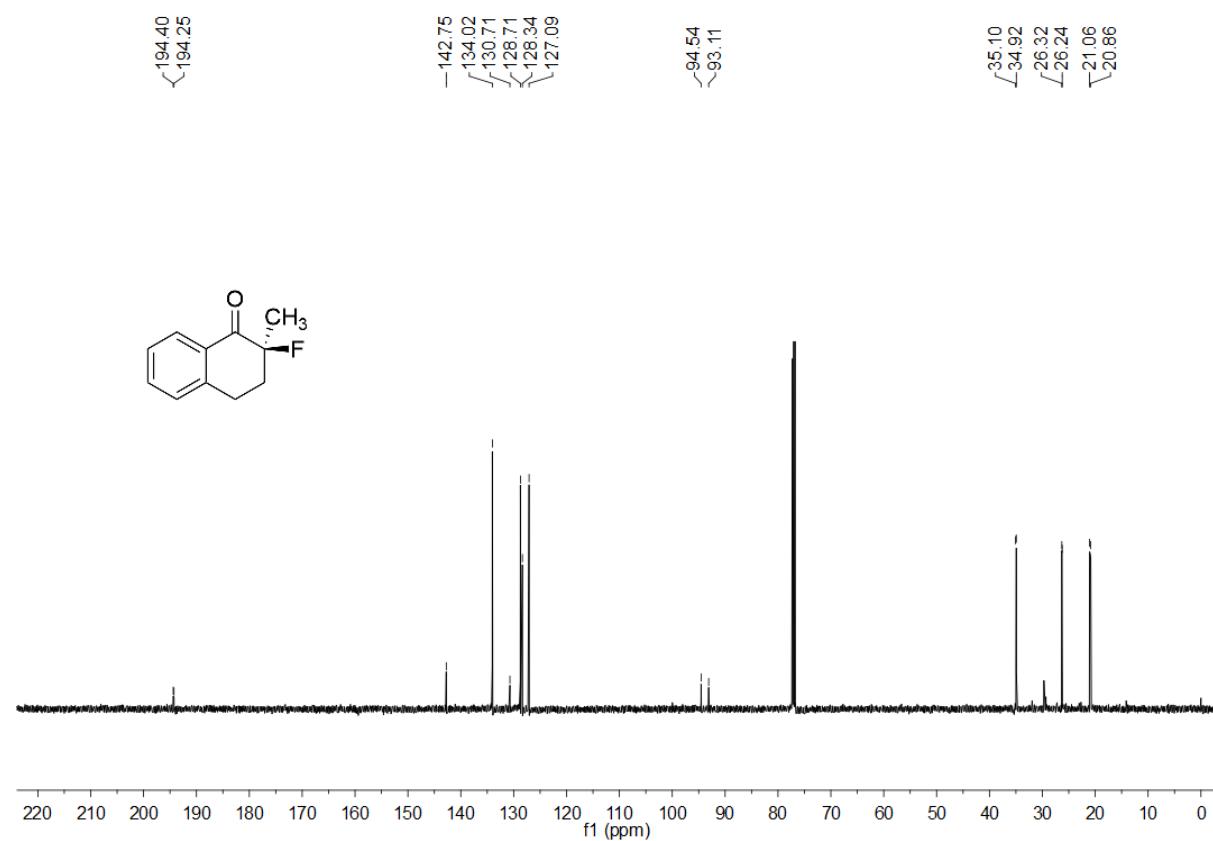
^{19}F NMR of 5 (470 MHz, CDCl_3)



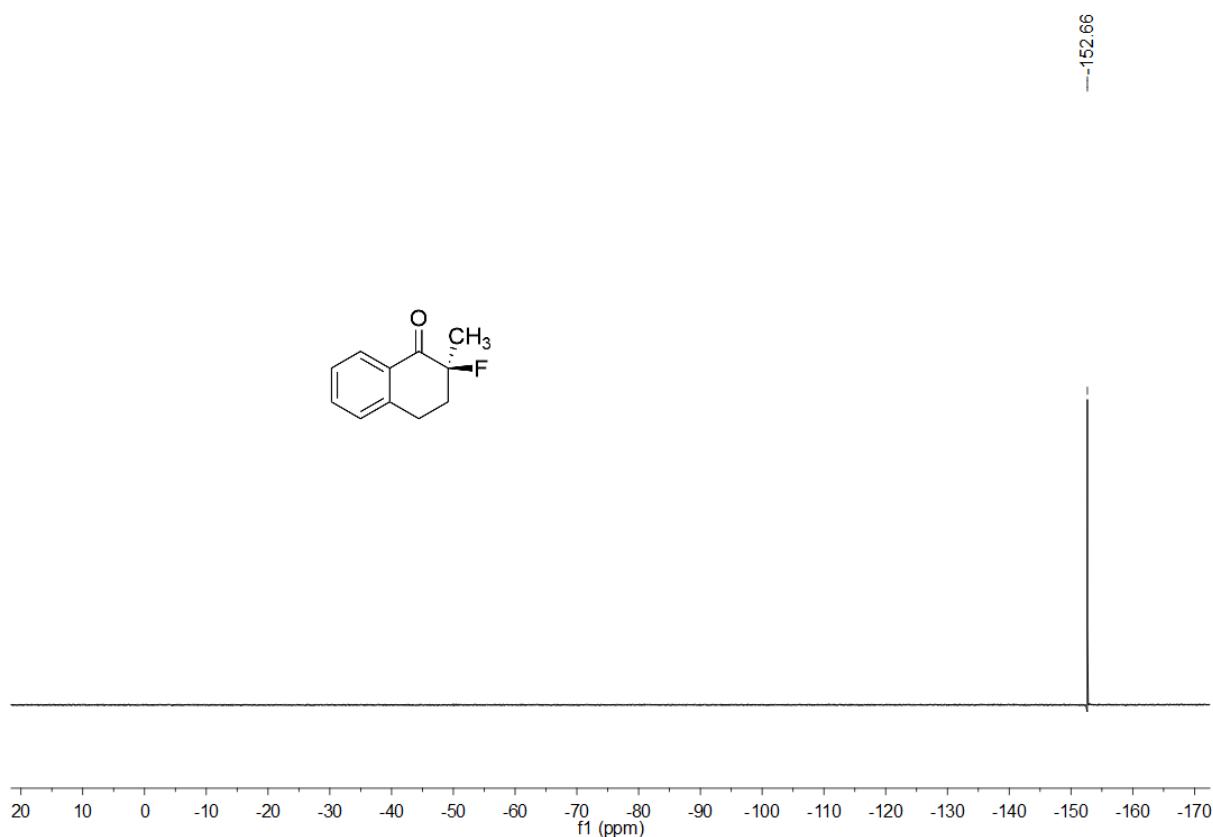
^1H NMR of 6 (500 MHz, CDCl_3)



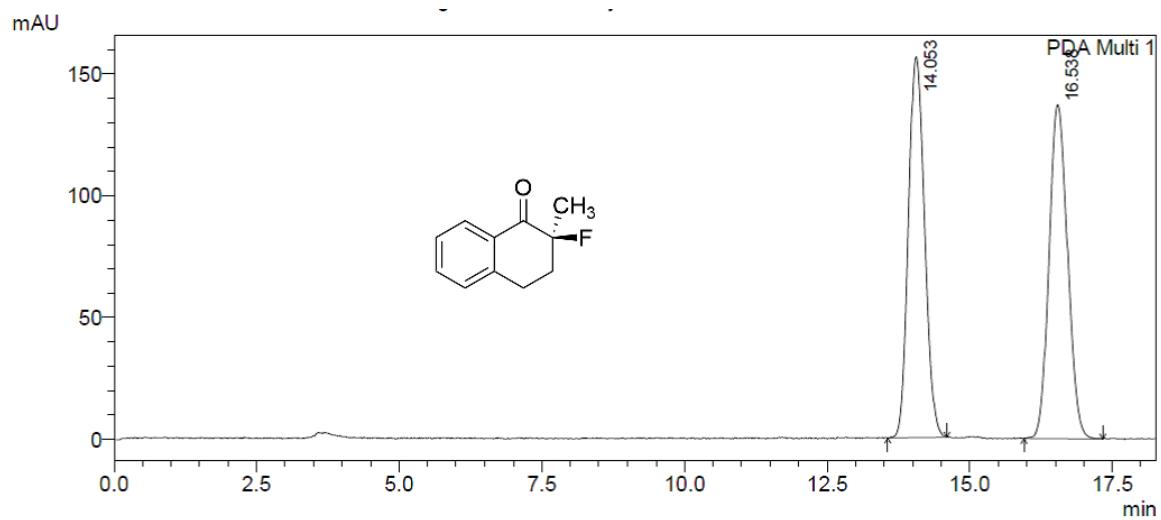
$^{13}\text{C}\{^1\text{H}\}$ NMR of 6 (125 MHz, CDCl_3)



¹⁹FNMR of 6 (470 MHz, CDCl₃)



HPLC of 6

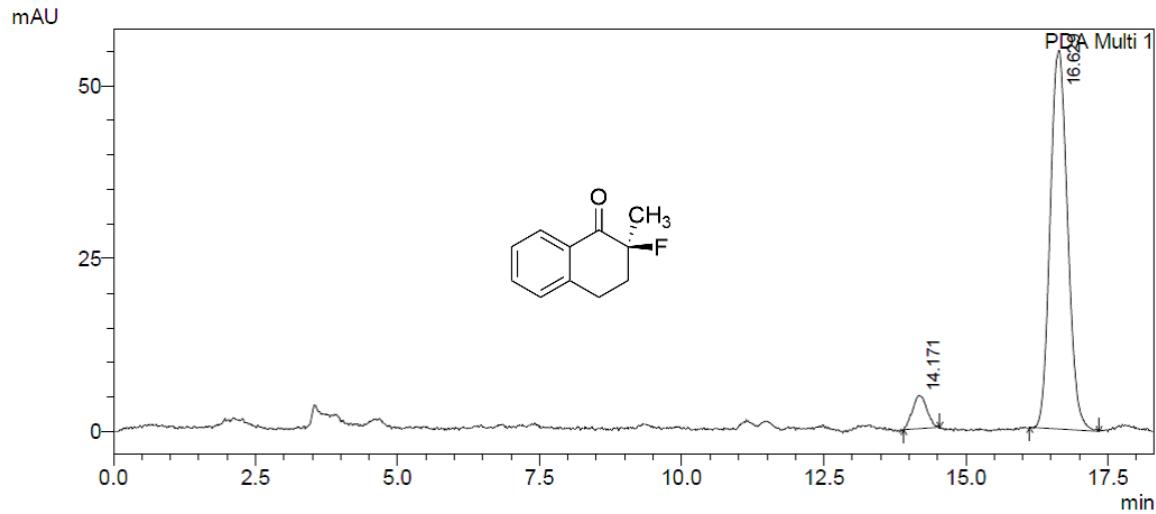


1 PDA Multi 1/254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	14.053	3087616	156311	49.878	53.291
2	16.538	3102663	137003	50.122	46.709
Total		6190279	293315	100.000	100.000



1 PDA Multi 1/254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	14.171	86135	4849	6.921	8.143
2	16.629	1158454	54697	93.079	91.857
Total		1244589	59546	100.000	100.000