

Supporting Information

Catalytic Enantioselective Synthesis of Key Propargylic Alcohol Intermediates of the Anti-HIV Drug Efavirenz

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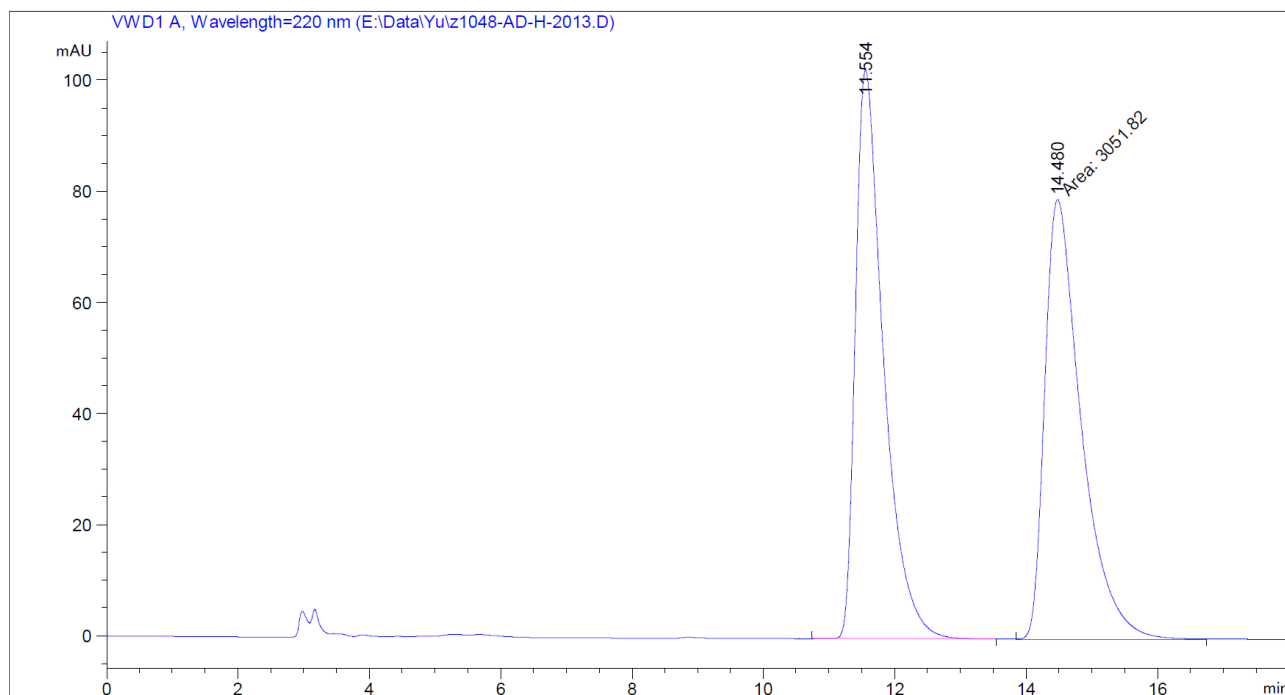
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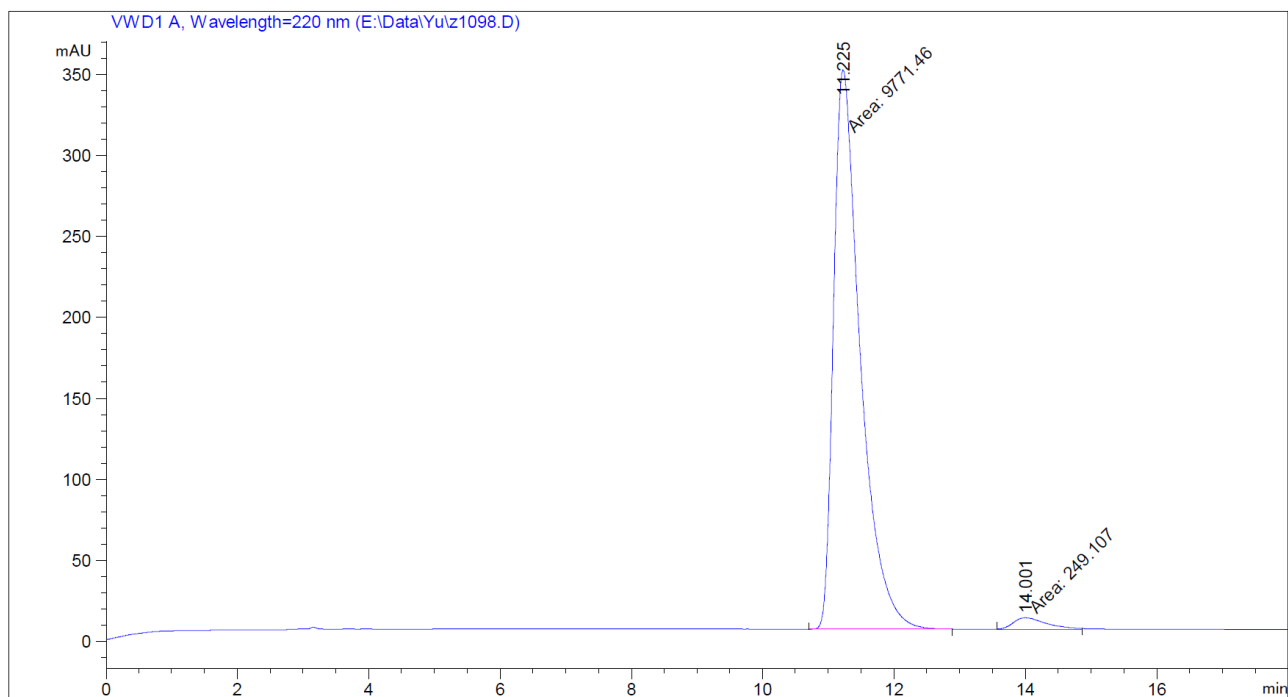
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1. Enantioselectivities as Determined by HPLC on Chiral Stationary Phase

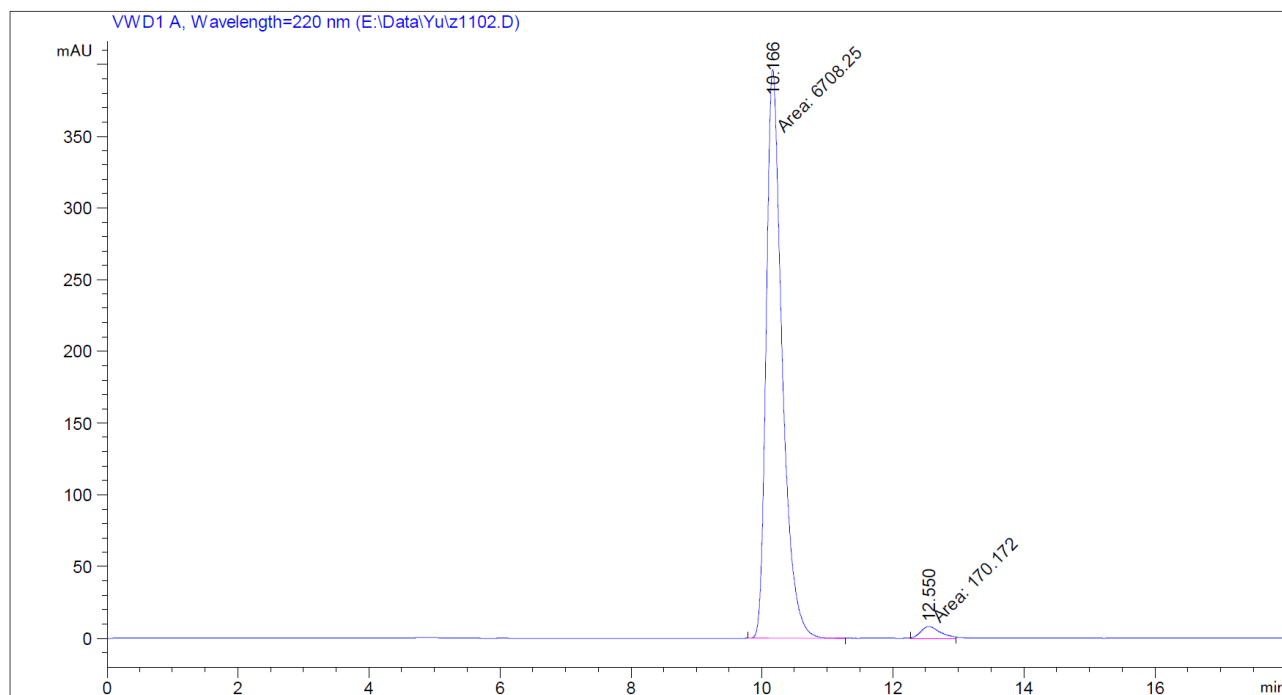
The enantiomeric excess of the compounds **2b** and **2c** from catalytic reactions were determined on a Daicel Chiralpak AD-H, or OD-H (250×4.6 mm) HPLC column on an Agilent 1200 Series HPLC System using hexane/isopropanol as a mobile phase. The column temperature was 25 °C and UV-absorption was measured at 220 nm.



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	11.554	BB	0.4432	3046.60596	102.37451	49.9572
2	14.480	MM	0.6424	3051.82495	79.18198	50.0428

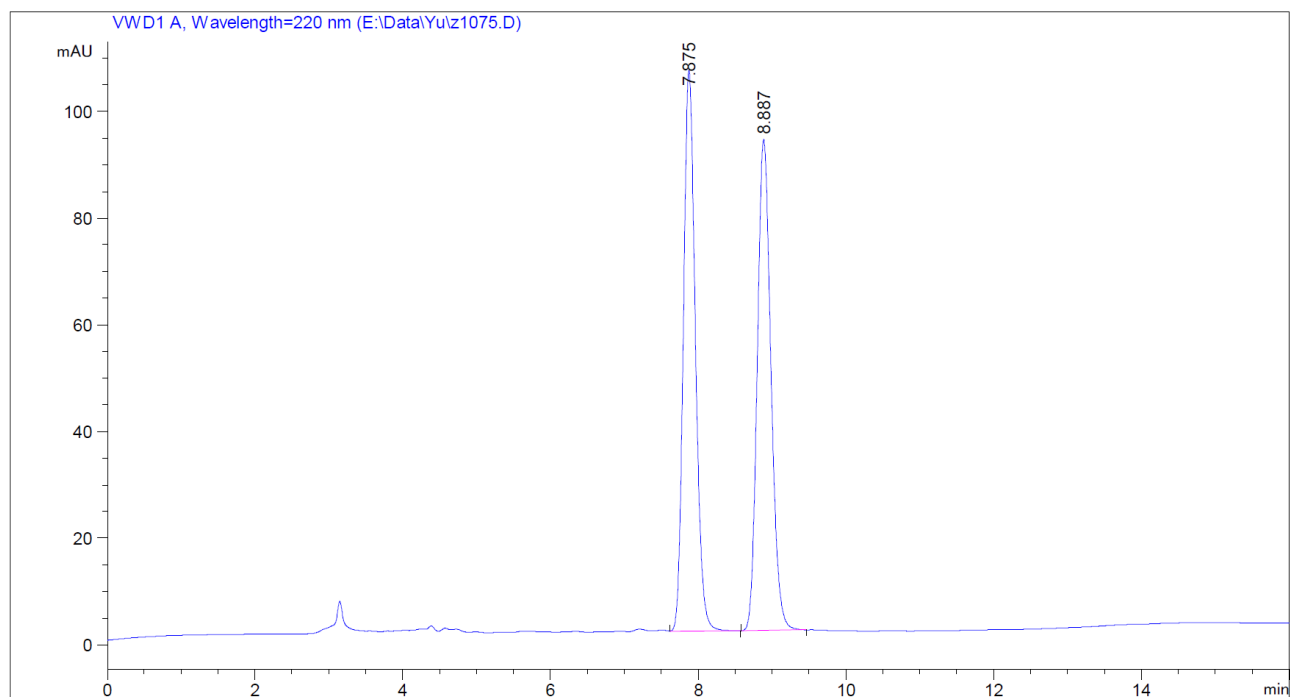


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	11.225	MM	0.4713	9771.46191	345.55936	97.5140
2	14.001	MM	0.5840	249.10698	7.10932	2.4860

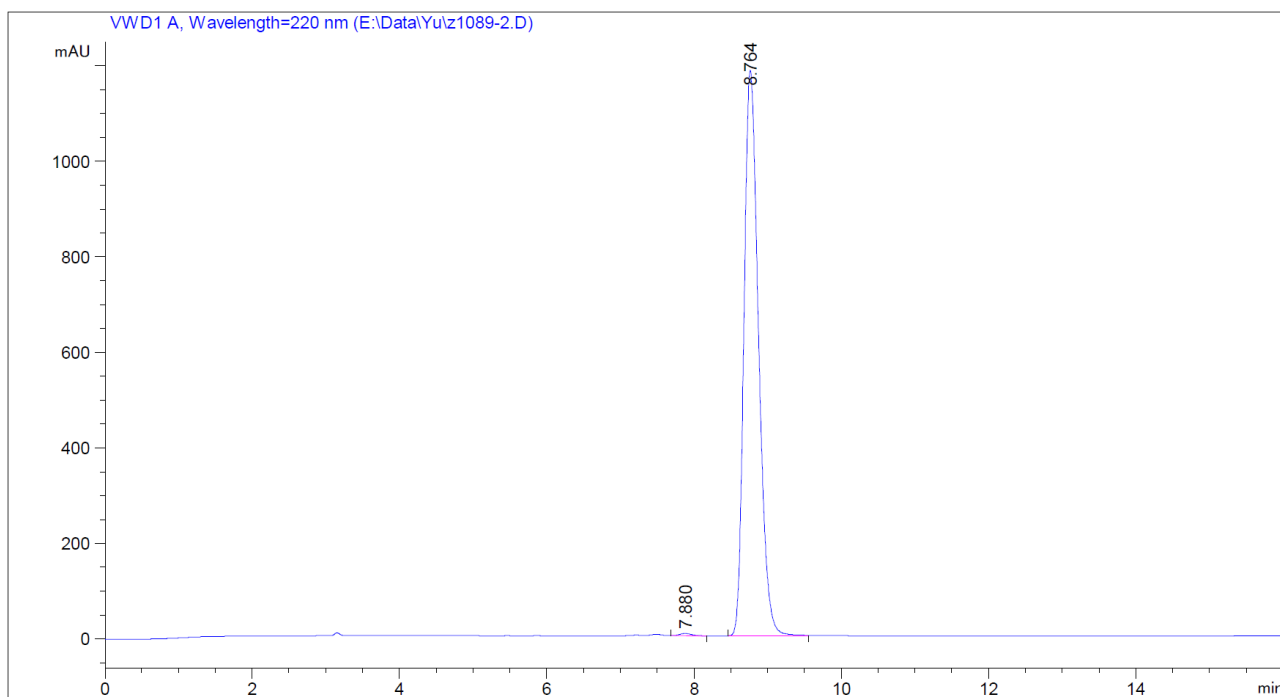


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	10.166	MM	0.2822	6708.25244	396.23730	97.5260
2	12.550	MM	0.3446	170.17244	8.23030	2.4740

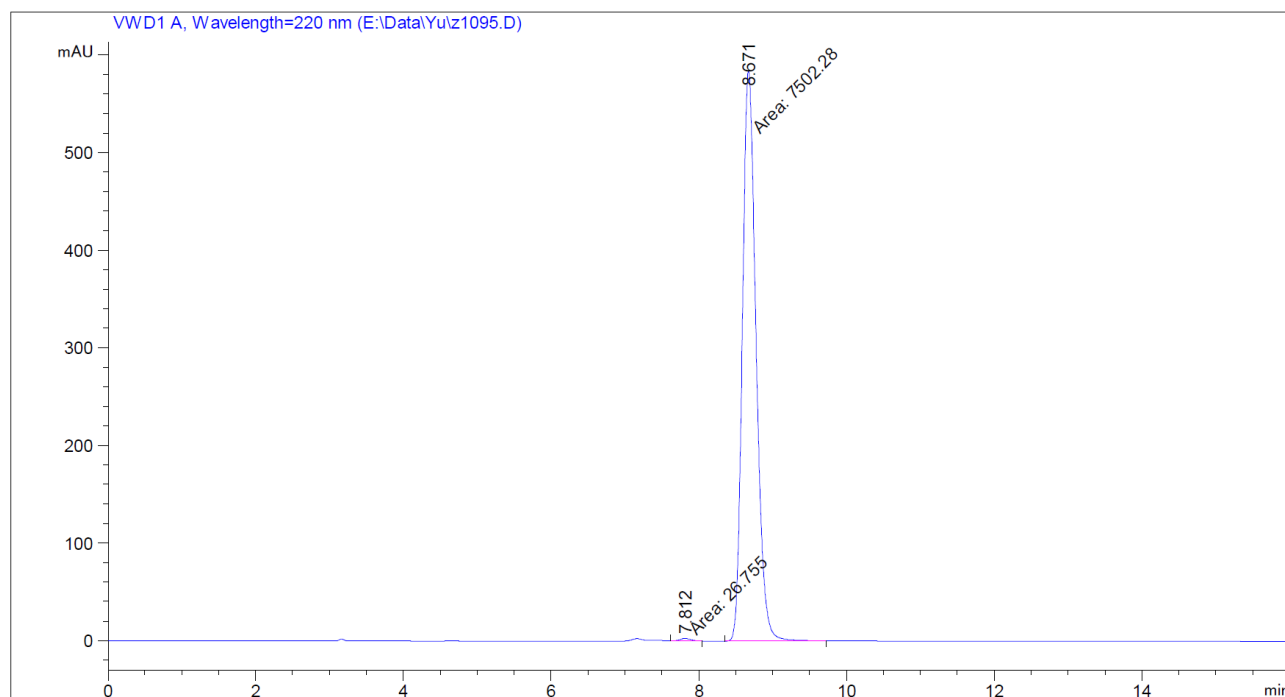
Figure S1. HPLC traces (Daicel Chiralpak AD-H column) of *rac*-**2b** (reference), (*S*)-**2b** (from catalytic reaction) and (*S*)-**2b** (from gram-scale reaction).



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	7.875	BB	0.1731	1180.99463	105.07318	49.9676
2	8.887	BB	0.1989	1182.52405	92.03837	50.0324



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	7.880	MM R	0.1885	54.65084	4.83102	0.3345
2	8.764	MM R	0.2151	1.62838e4	1184.01367	99.6655

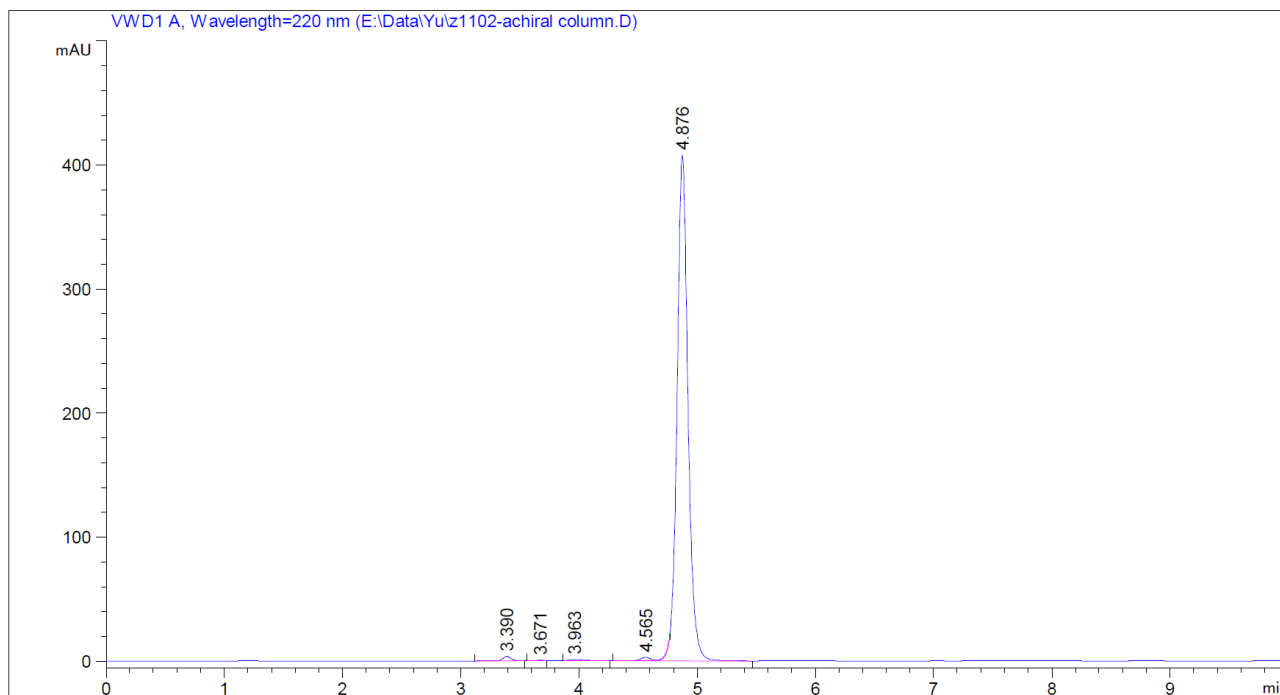


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	7.812	MM	0.1784	26.75496	2.49910	0.3554
2	8.671	MM	0.2140	7502.27881	584.16650	99.6446

Figure S2. HPLC traces (Daicel Chiralpak OD-H column) of *rac*-**2c** (reference), (*S*)-**2c** (from catalytic reaction) and (*S*)-**2c** (from gram-scale reaction).

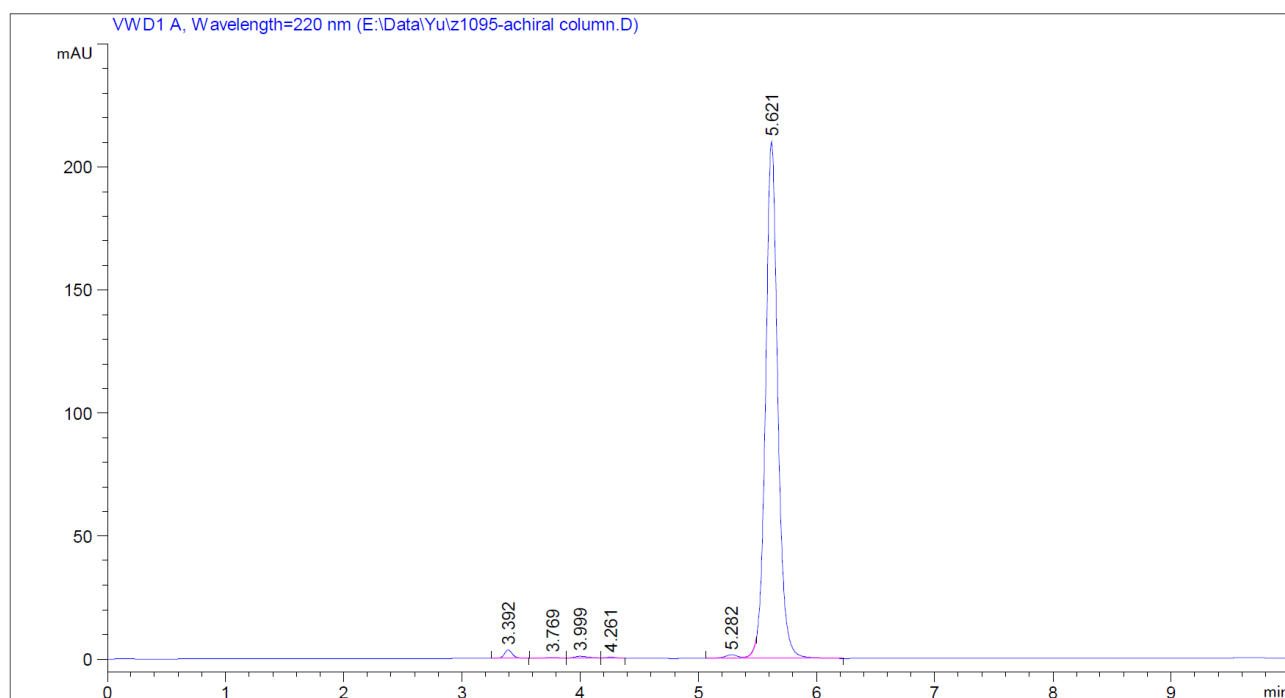
2. Product Purities as Determined by HPLC Analysis

The degree of purities of the compounds **2b** and **2c** were determined by a Purospher® STAR Si column (4.6×250 mm, 5 µm, Merck) with an Agilent 1200 HPLC system using hexane/isopropanol as a mobile phase. The column temperature was 25 °C and UV-absorption was measured at 220 nm.



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	3.390	BB	0.0726	17.18505	3.54130	0.6416
2	3.671	BB	0.0717	6.78882e-1	1.47467e-1	0.0253
3	3.963	BB	0.1246	8.48316	9.74286e-1	0.3167
4	4.565	BV E	0.1076	21.15614	2.84873	0.7899
5	4.876	VB R	0.0972	2630.93726	408.03421	98.2265

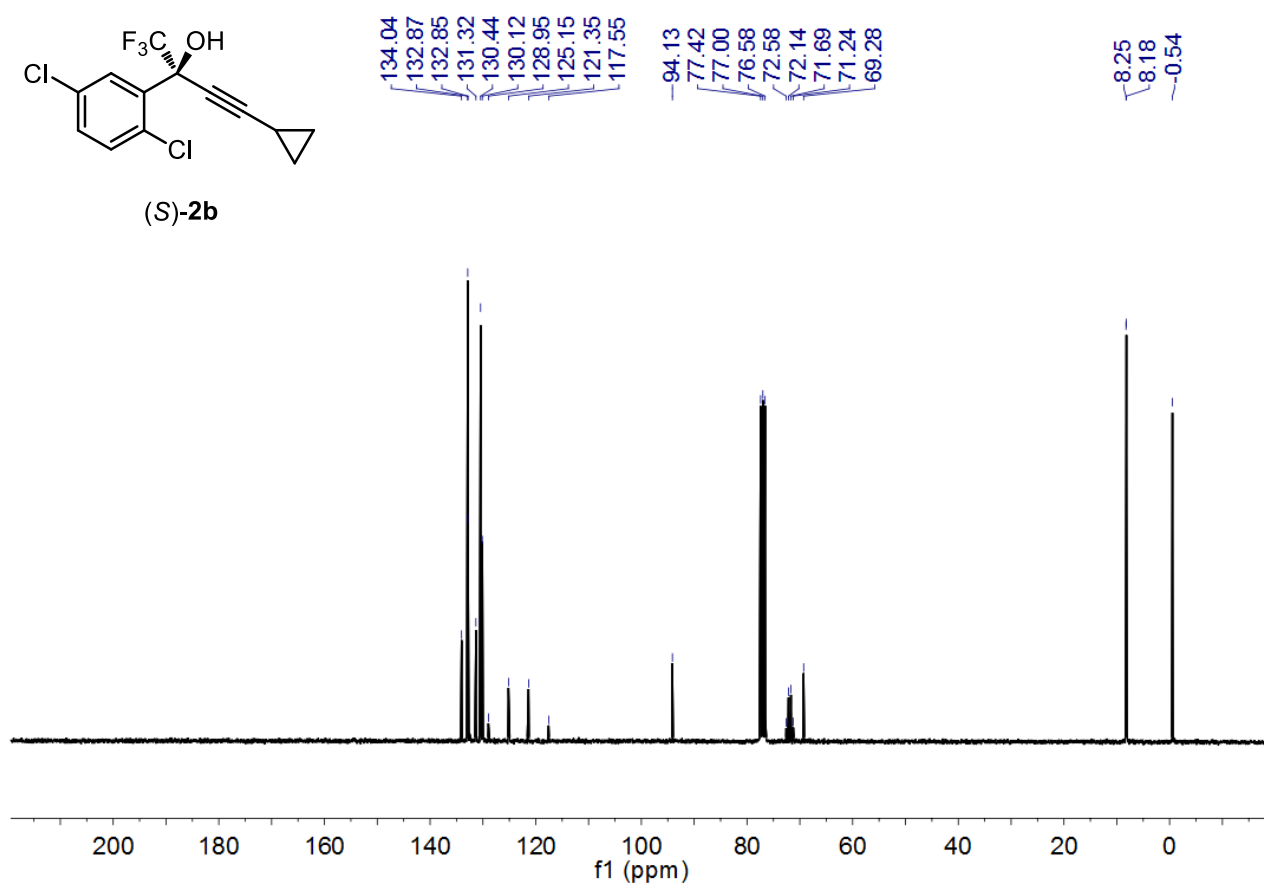
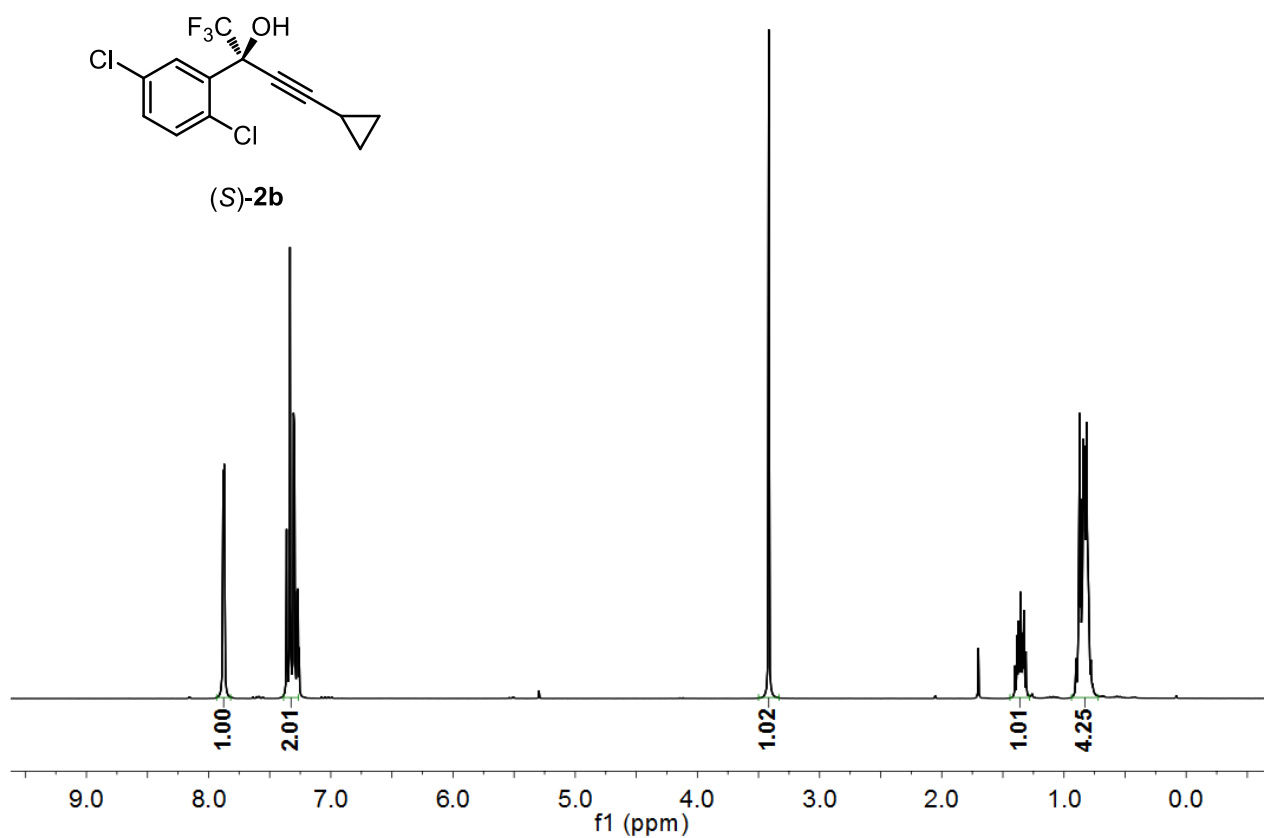
Figure S3. HPLC trace of (*S*)-**2b** from gram-scale reaction.



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	3.392	BB	0.0696	15.75715	3.43263	1.0119
2	3.769	BV	0.1273	1.69205	1.96817e-1	0.1087
3	3.999	VV	0.1275	7.12608	8.11219e-1	0.4576
4	4.261	VB	0.0906	2.75583	4.62217e-1	0.1770
5	5.282	BV E	0.1150	10.98457	1.42391	0.7054
6	5.621	VB R	0.1094	1518.85229	210.00136	97.5394

Figure S4. HPLC trace of (*S*)-**2c** from gram-scale reaction.

4. NMR Spectra



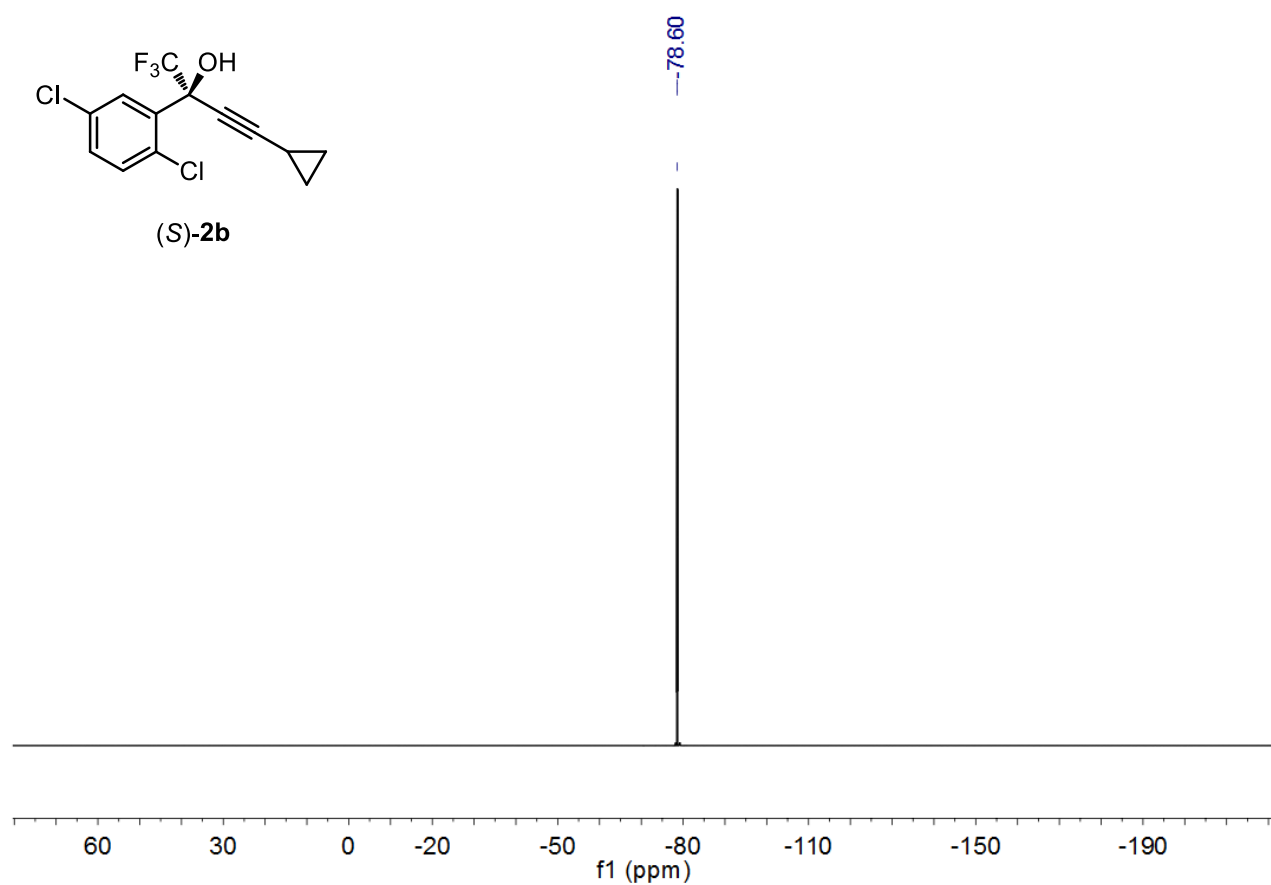
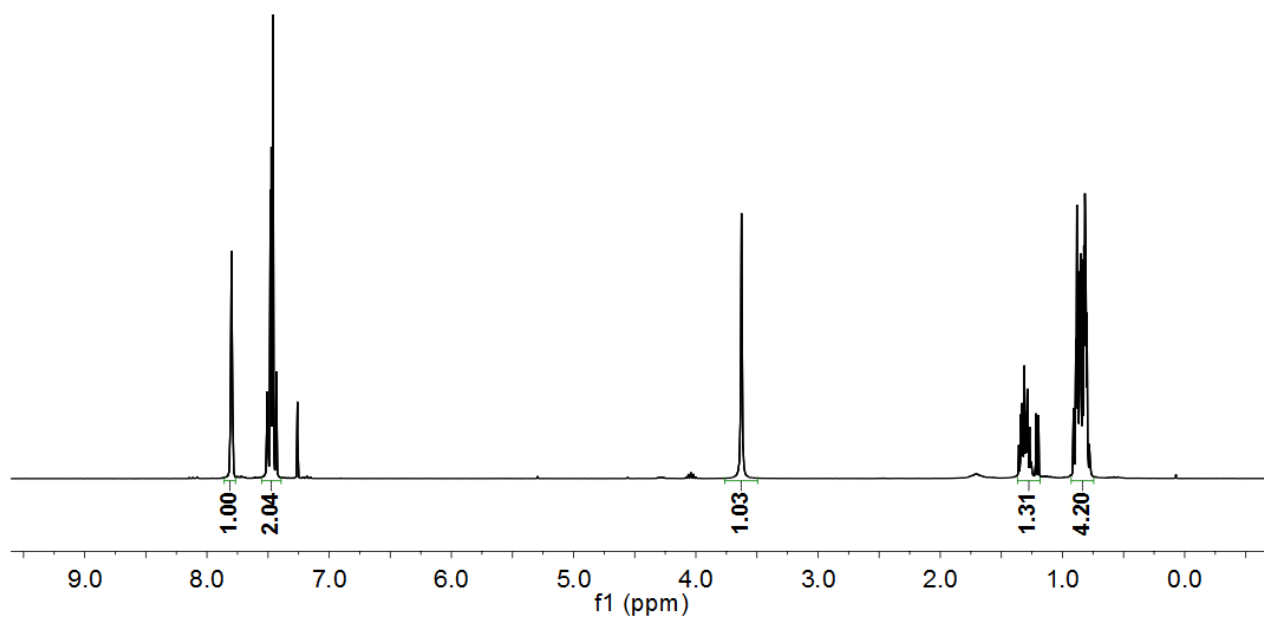
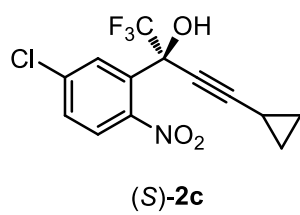


Figure S5. ^1H NMR, ^{13}C NMR and ^{19}F NMR spectra of **2b** (CDCl_3).



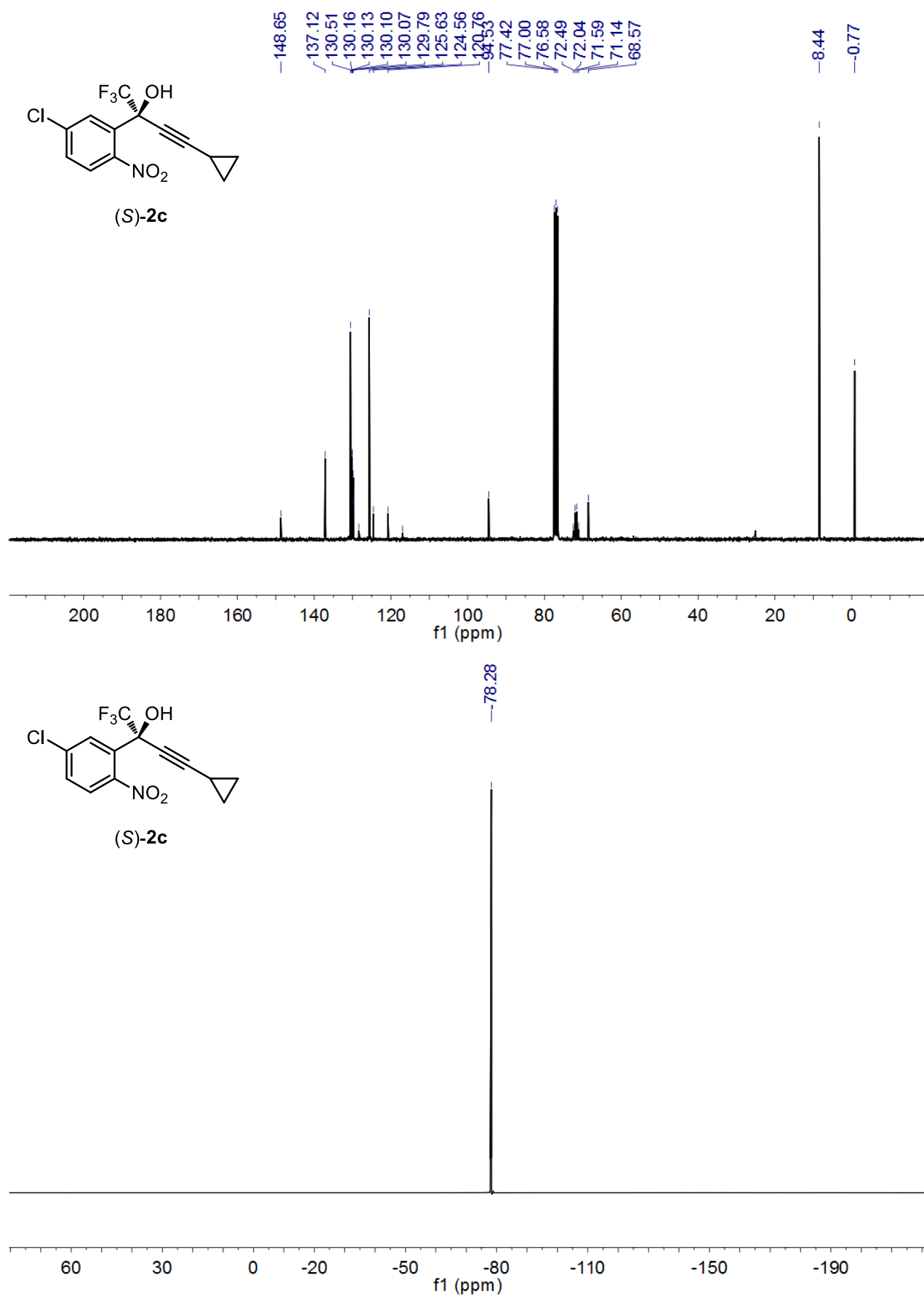


Figure S6. ¹H NMR, ¹³C NMR and ¹⁹F NMR spectra of **2c** (CDCl₃).