

Supporting Information

Enzymatic Reduction of Halogenated Aryl Ketones in Aqueous Micellar Solution with Enhanced Catalytic Performance

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Chemicals and materials

All chemicals and reagents were purchased from J & K, Acros, Aldrich, and Aladdin, and chemicals were obtained from authentic suppliers of at least of reagent grade and used without further purification. Nicotinamide adenine dinucleotide (NADH) was purchased from Aladdin (Shanghai, China).

Preparation of DL- α -Tocopherol Succinate

Vitamin E (4.3 g) and succinic anhydride (1.5 g) were dissolved in toluene (20 mL), followed by the addition of triethylamine (0.35 mL), and the reaction was carried out at 60 °C for 5 h. Water was added to the reacted mixture, and extraction was carried out using dichloromethane. The organic layer after the extraction was cleaned using hydrochloric acid (1 M, 50 mL) and water (30 mL) for 3-4 times, dried with anhydrous sodium sulfate, and concentrated in vacuum to obtain a yellow liquid. The yellow liquid was purified using column chromatography with 10% ethyl acetate/hexane and 35% ethyl acetate/hexane to obtain DL- α -vitamin E succinate and a white solid.

Preparation of TPGS-750-M

DL- α -Vitamin E Succinate (2.97 g), Polyethylene Glycol Monomethyl Ether-750 (4.00 g), p-Toluene Sulfonic Acid (0.15 g), and Toluene (20 mL) were added to a 50 mL single-necked flask and refluxed for 5 h at 130 °C using a Dean-Stark refluxer. The mixture was cooled to room temperature, then saturated aqueous phase was added and extracted with dichloromethane using sodium bicarbonate solution. The extracted organic layer was washed 3-4 times with saturated sodium bicarbonate (50 mL) and brine (30 mL), dried with anhydrous sodium sulfate and concentrated in vacuum to

obtain a yellow liquid.

Preparation of substrate solubilization

Surfactant, excess substrate and appropriate amount of water were added to the centrifuge tube and shaken in a water bath shaker for 24 h. Undissolved substrates were removed with a filter membrane, and the substrate dissolved in water was diluted 10-100 times with ethanol, and the solubility of the substrate dissolved in water was determined by UV-visible spectrometry (double-beam mode, wavelengths of 200-600 nm, and a scanning speed of 600 nm/min). A calibration curve was established by determining the solubility of different concentrations of the substrate in ethanol.

Table S1 The productive reaction of 9a with or without micelles.

Substrate concentration	Conversion ^a	
	buffer only ^b	6 wt% TPGS-750-M in buffer ^c
0.5 M	58%	70%

^a Reaction conditions: 2 mL PBS buffer (1 M, pH = 7), LfSDR1 (4.5 U), GDH (9 U), NADH (2 mM), n(substrate)/n(glucose) = 5/6, 30 °C, 24 h.

^b Reaction conditions: 2 mL PBS buffer (1 M, pH = 7), LfSDR1 (4.5 U), GDH (9 U), NADH (2 mM), TPGS-750-M (6 wt%) n(substrate)/n(glucose) = 5/6, 30 °C, 24 h.

^c The conversion and ee value were determined by GC.

Table S2. Effect of various surfactants on the enzyme activity of LfSDR1

Time (h)	Enzyme activity of LfSDR1 (U/mg)							
	PBS	TPGS-750- M	Tween- 60	Solutol HS-15	Tween-40	Brij- 30	Triton X- 100	Trilaurin
0	0.456	0.453	0.371	0.384	0.421	0.430	0.449	0.446
4	0.437	0.430	0.336	0.382	0.420	0.396	0.396	0.411
8	0.418	0.385	0.324	0.377	0.381	0.372	0.376	0.385
12	0.369	0.366	0.323	0.343	0.362	0.351	0.334	0.208
24	0.361	0.356	0.312	0.304	0.348	0.327	0.208	0.182

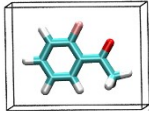
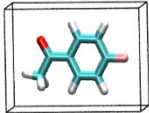
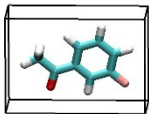
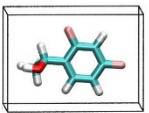
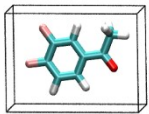
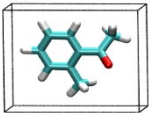
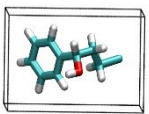
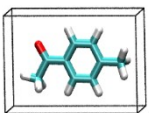
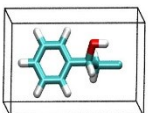
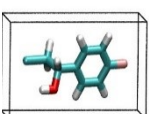
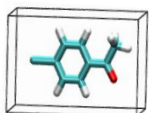
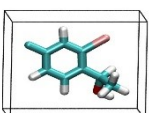
Table S3. Effect of various surfactants on the enzyme activity of GDH

Time (h)	Enzyme activity of GDH (U/mg)							
	PBS	TPGS-750- M	Tween-60	Solutol HS- 15	Tween-40	Brij-30	Triton X- 100	Trilaurin
0	4.86	4.55	3.54	3.49	3.92	3.66	3.50	3.94
4	4.10	3.85	3.31	3.36	3.56	2.42	3.23	3.65
8	3.95	3.78	2.98	3.27	3.46	2.22	3.22	3.37
12	3.72	3.49	2.77	3.15	3.17	2.12	2.50	3.24
24	2.68	3.39	2.27	3.07	2.62	1.89	2.33	2.49

Table S4. The relative activity of LfSDR1 and GDH treated by TPGS-750-M.

Time (h)	LfSDR1 enzyme activity (U/mg)		GDH enzyme activity (U/mg)	
	Pure PBS	With TPGS-750-M	Pure PBS	With TPGS-750-M
0	0.456	0.453	4.86	4.55
4	0.437	0.430	4.10	3.85
8	0.418	0.385	3.95	3.78
12	0.369	0.366	3.72	3.49
24	0.361	0.356	2.68	3.39

Table S5. Molecular van der Waals volumes based on the Marching Tetrahedron algorithm calculation

Name	Molecular volume
2-Fluoroacetophenone (1a)	 V=292.90 Å ³
4-Fluoroacetophenone (2a)	 V=287.64 Å ³
3-Fluoroacetophenone (3a)	 V=291.56 Å ³
2',4'-Difluoroacetophenone (4a)	 V=446.71 Å ³
3',4'-Difluoroacetophenone (5a)	 V=290.89 Å ³
2'-Chloroacetophenone (6a)	 V=391.24 Å ³
3-Chloropropiophenone (7a)	 V=515.62 Å ³
4'-Chloroacetophenone (8a)	 V=305.91 Å ³
2-Chloroacetophenone (9a)	 V=378.75 Å ³
2-Chloro-4'-fluoroacetophenone (10a)	 V=395.67 Å ³
4'-Bromoacetophenone (11a)	 V=313.06 Å ³
2'-Bromo-4'-Fluoroacetophenone (12a)	 V=373.67 Å ³

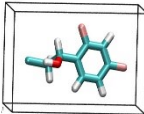
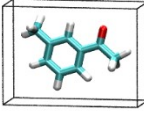
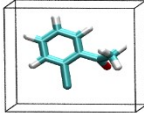
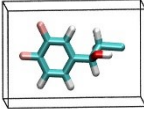
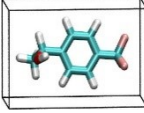
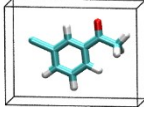
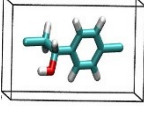
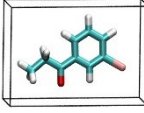
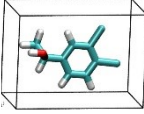
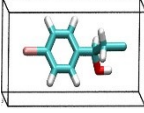
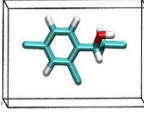
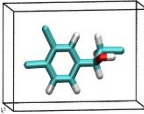
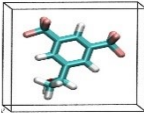
Name	Molecular volume	
2-Chloro-2',4'-difluoroacetophenone (13a)		V=497.57 Å ³
3'-Chloroacetophenone (14a)		V=336.88 Å ³
2'-Bromoacetophenone (15a)		V=442.27 Å ³
2-Chloro-1-(3,4-difluoro-phenyl)-ethanone (16a)		V=481.14 Å ³
4'-(Trifluoromethyl)acetophenone (17a)		V=480.15 Å ³
3'-Bromoacetophenone (18a)		V=357.69 Å ³
2,4'-Dichloroacetophenone (19a)		V=417.88 Å ³
3'-Bromopropiophenone (20a)		V=396.86 Å ³
3',4'-Dichloroacetophenone (21a)		V=500.68 Å ³
1-(4-bromophenyl)-2-chloroethan-1-one (22a)		V=425.47 Å ³
2,2',4'-Trichloroacetophenone (23a)		V=513.15 Å ³
2,3',4'-Trichloroacetophenone (24a)		V=545.76 Å ³
3',5'-Bis(trifluoromethyl)acetophenone (25a)		V=586.62 Å ³

Table S6. Solubilization in pure buffer and 2 wt% TPGS-750-M solution

Substrate	Solubilization (ppm)		Relative Increase
	Buffer only	2 wt% TPGS-750-M	
1a	6300	7755	1455
20a	2600	6000	3400
24a	1410	12320	10890

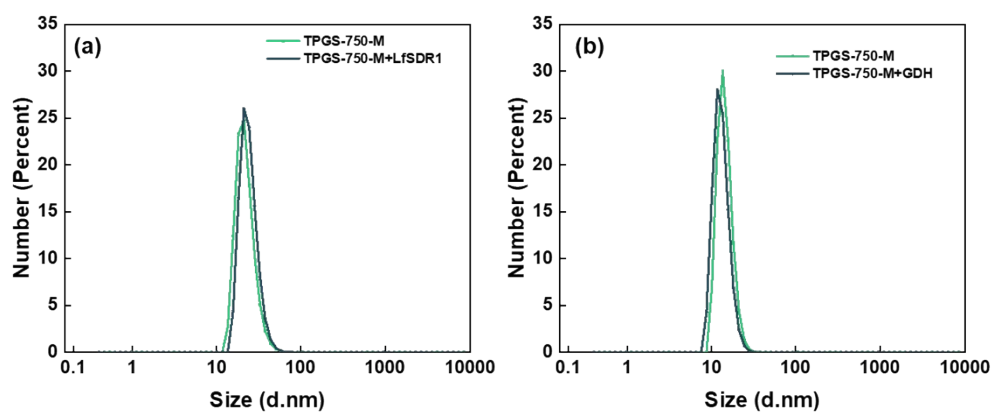


Fig S1. DLS spectra of the micellar solution involving (a) LfSDR1 and (b) GDH.

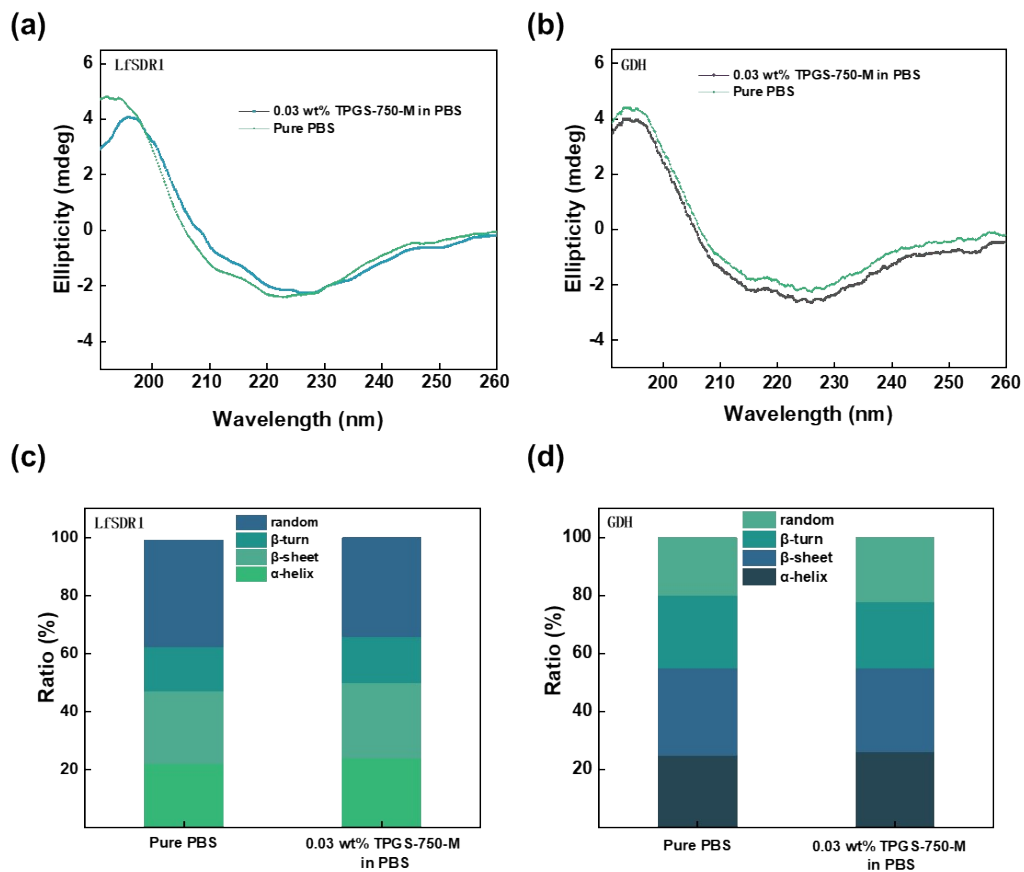


Fig S2. CD spectra of (a) LfSDR1 and (b) GDH with or without TPGS-750-M and (c-d) the corresponding domains distribution.

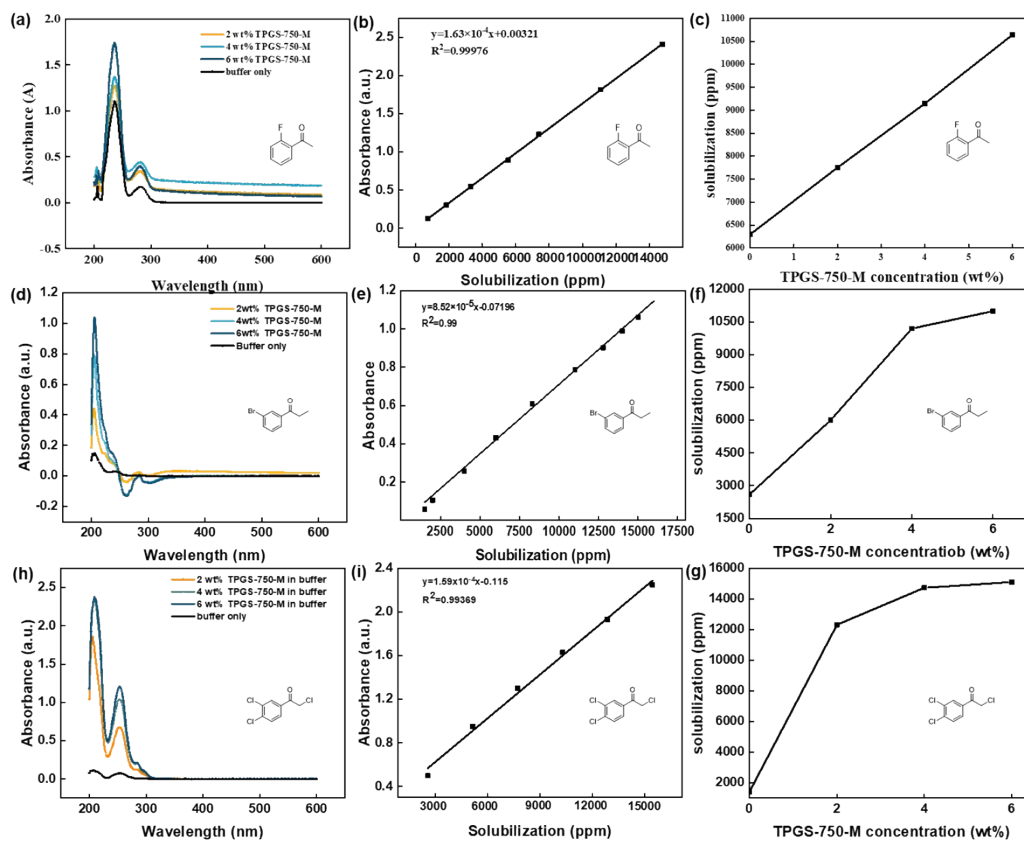
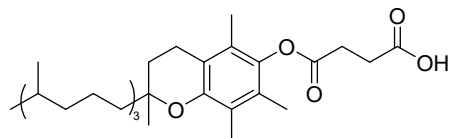


Fig S3. Solubilization of (a) **1a**; (d) **20a**; (g) **24a** in TPGS-750-M; Solubilization calibration curve of (b) **1a**; (e) **20a**; (h) **24a** in TPGS-750-M; MAC of (c) **1a**; (f) **20a**; (i) **24a** in TPGS-750-M solution with various concentrations.

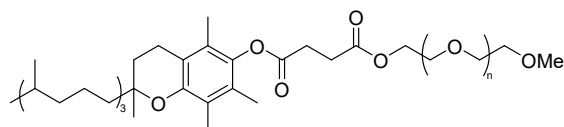
¹H and ¹³C NMR spectra of TPGS-750-M in CDCl₃

DL- α -Tocopherol Succinate



¹H NMR (400 MHz, Chloroform-*d*) δ 2.01 (s, 3H), 1.89 – 1.75 (m, 2H), 1.76 (s, 1H), 1.62 – 1.51 (m, 3H), 2.98 (t, 2H), 2.87 (t, 2H), 2.62 (t, 2H), 2.13 (s, 3H), 2.06 (s, 3H), 1.27 (s, 21H), 0.92 – 0.87 (m, 12H). **¹³C NMR** (101 MHz, Chloroform-*d*) δ 176.78, 171.18, 149.52, 140.46, 127.79, 124.99, 123.13, 117.47, 75.13, 39.44, 37.52, 37.6, 37.5, 37.4, 33, 32.86, 31.4, 29.78, 28.81, 28.06, 24.89, 24.53, 24.1, 22.80, 22.71, 21.12, 20.67, 19.83, 19.76, 12.98, 12.12, 11.90.

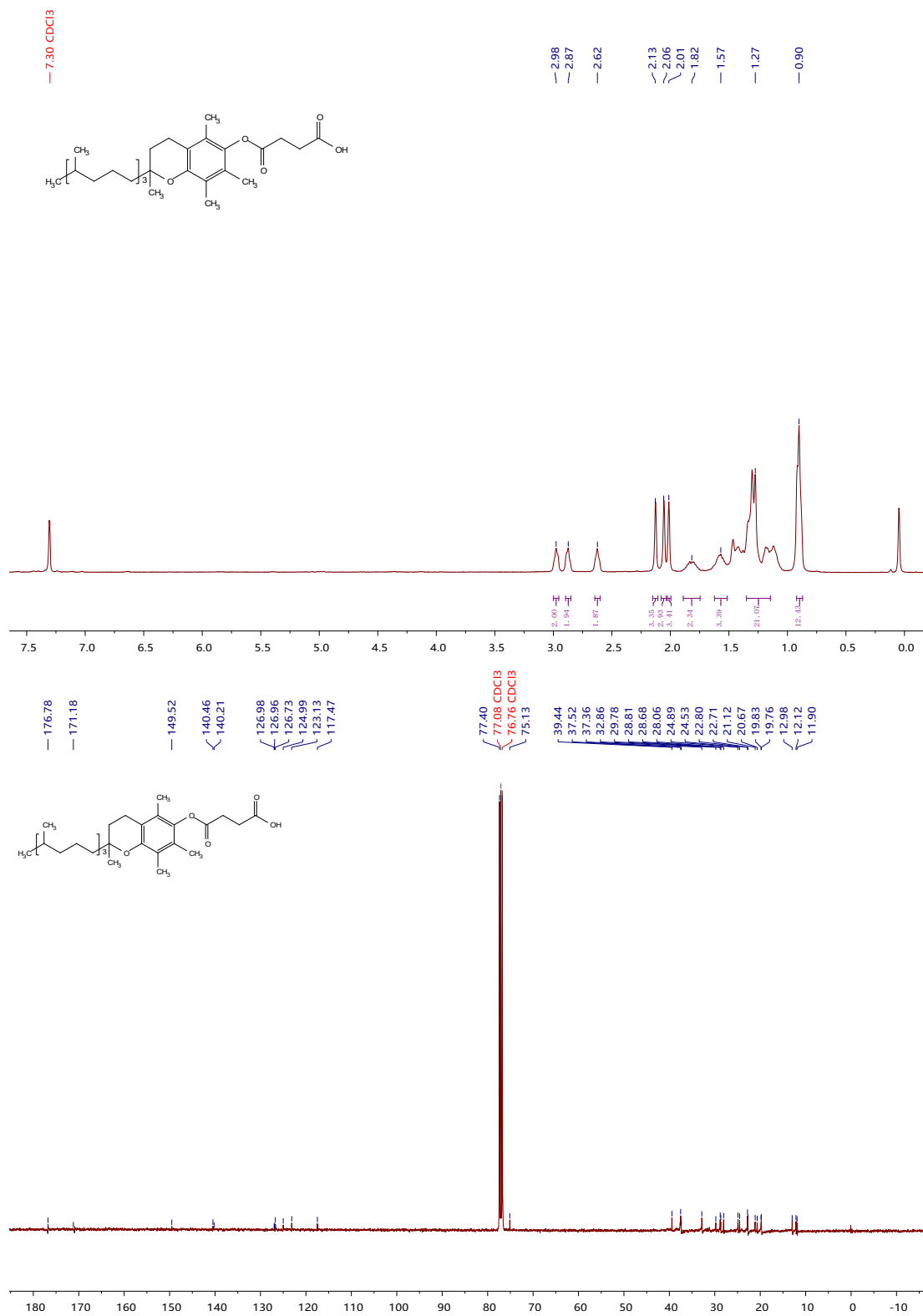
TPGS-750-M



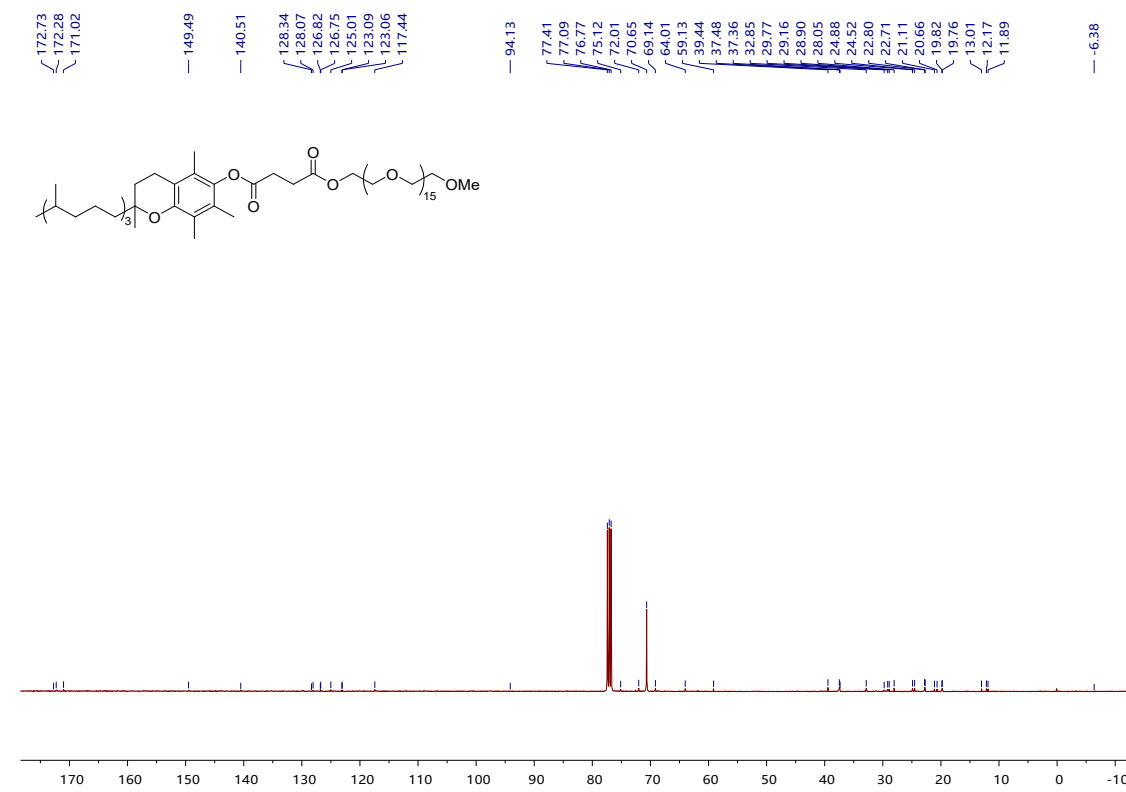
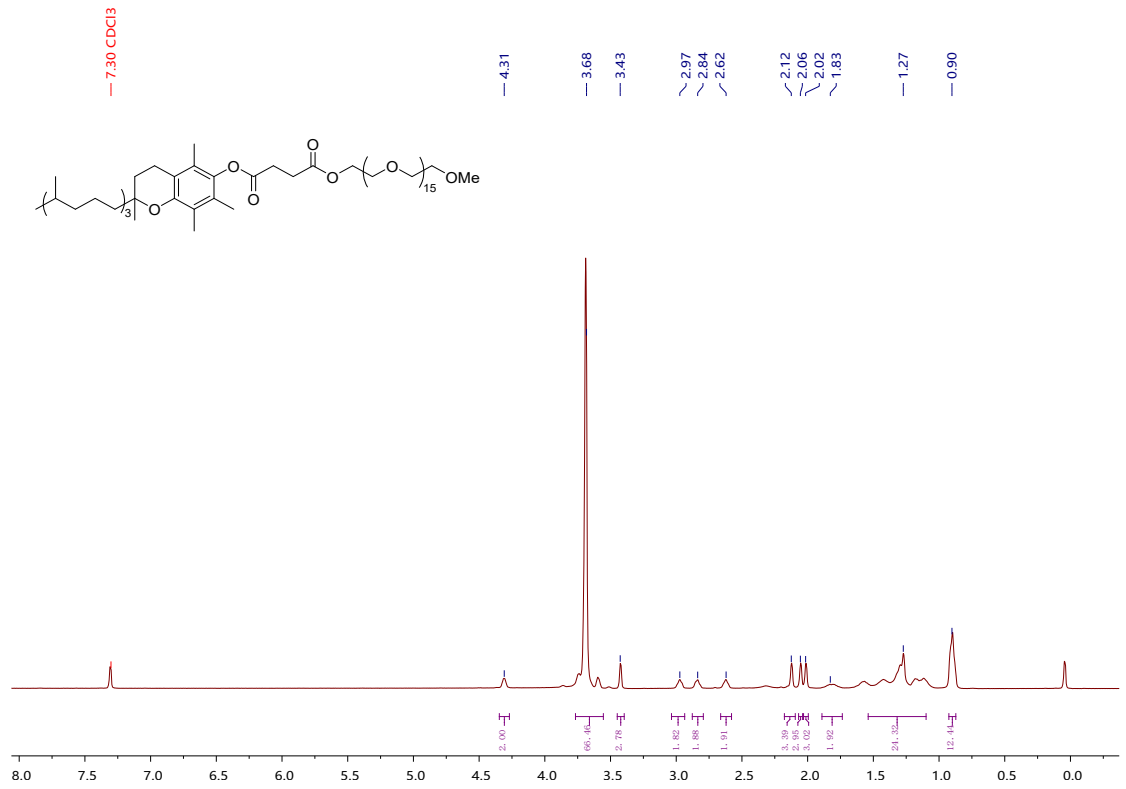
¹H NMR (400 MHz, Chloroform-*d*) δ 4.35 – 4.27 (m, 2H), 3.77 – 3.55 (m, 66H), 3.43 (s, 3H), 2.97 (t, 2H), 2.84 (t, 2H), 2.62 (t, 2H), 2.12 (s, 3H), 2.06 (s, 3H), 2.02 (s, 3H), 1.89 – 1.74 (m, 2H), 1.54 – 1.10 (m, 24H), 0.93 – 0.87 (m, 12H). **¹³C NMR** (101 MHz, Chloroform-*d*) δ 172.73, 171.02, 149.49, 140.51, 126.82, 125.01, 123.06, 117.44, 94.13, 75.12, 72.01, 70.65, 69.14, 64.01, 59.13, 39.44, 37.48, 37.32, 37.28, 32.85, 32.71, 31.05, 29.77, 28.90, 28.05, 24.88, 24.52, 22.80, 22.71, 21.11, 20.66, 19.82, 19.76, 13.01, 12.17, 11.89.

NMR spectra of TPGS-750-M

DL- α -Tocopherol Succinate

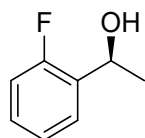


TPGS-750-M



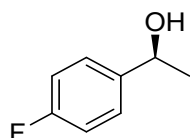
¹H and ¹³C NMR spectra of the products recorded in CDCl₃

(S)-1-(2-fluorophenyl)ethan-1-ol **1b**



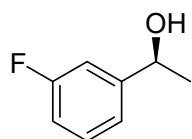
¹H NMR (400 MHz, Chloroform-*d*) δ 7.52 (s, 1H), 7.28 (d, $J = 7.3$ Hz, 1H), 7.18 (t, $J = 7.6$ Hz, 1H), 7.05 (t, $J = 9.6$ Hz, 1H), 5.23 (d, $J = 5.9$ Hz, 1H), 2.00 (d, $J = 4.0$ Hz, 1H), 1.55 (d, $J = 6.2$ Hz, 3H). **¹³C NMR** (101 MHz, Chloroform-*d*) δ 161.01, 158.57, 132.77, 132.63, 128.87, 128.79, 126.71, 126.66, 124.39, 124.36, 115.46, 115.24, 64.62, 64.58, 24.06.

(S)-1-(4-fluorophenyl)ethan-1-ol **2b**



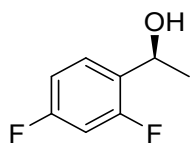
¹H NMR (400 MHz, Chloroform-*d*) δ 7.38 (s, 2H), 7.07 (s, 2H), 4.92 (d, $J = 6.0$ Hz, 1H), 1.97 (s, 1H), 1.52 (s, 3H). **¹³C NMR** (101 MHz, Chloroform-*d*) δ 163.39, 160.95, 141.60, 141.56, 127.15, 127.07, 115.42, 115.21, 69.82, 25.34.

(S)-1-(3-fluorophenyl)ethan-1-ol **3b**



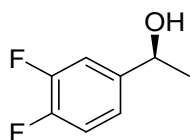
¹H NMR (400 MHz, Chloroform-*d*) δ 7.34 (d, $J = 5.7$ Hz, 1H), 7.17 (s, 1H), 7.12 (s, 1H), 6.99 (s, 1H), 4.93 (d, $J = 5.8$ Hz, 1H), 1.97 (s, 1H), 1.53 (s, 3H). **¹³C NMR** (101 MHz, Chloroform-*d*) δ 164.43, 161.98, 148.75, 148.68, 130.24, 130.16, 121.15, 121.12, 114.53, 114.32, 112.62, 112.40, 70.00, 25.42.

(R)-1-(2,4-difluorophenyl)ethanol **4b**



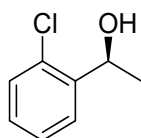
$^1\text{H NMR}$ (400 MHz, Chloroform-*d*) δ 7.52 – 7.40 (m, 1H), 6.96 – 6.84 (m, 1H), 6.78 (t, $J = 11.0$ Hz, 1H), 5.15 (q, $J = 6.5$ Hz, 1H), 2.38 (d, $J = 12.7$ Hz, 1H), 1.28 (s, 1H), 0.87 (s, 2H). $^{13}\text{C NMR}$ (101 MHz, Chloroform-*d*) δ 163.40, 128.54, 127.64, 127.59, 127.55, 127.49, 111.41, 111.37, 111.19, 111.16, 103.89, 103.64, 103.38, 64.01, 63.98, 24.06.

(R)-1-(3,4-difluorophenyl)ethan-1-ol **5b**



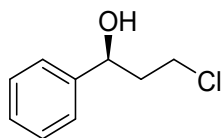
$^1\text{H NMR}$ (400 MHz, Chloroform-*d*) δ 7.34 – 7.20 (m, 1H), 7.13 (d, $J = 12.1$ Hz, 2H), 4.91 (s, 1H), 2.03 (s, 1H), 1.51 (s, 3H). $^{13}\text{C NMR}$ (101 MHz, Chloroform-*d*) δ 142.92, 121.29, 117.27, 114.55, 69.38, 25.38.

(S)-1-(2-chlorophenyl)ethan-1-ol **6b**



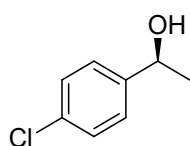
$^1\text{H NMR}$ (400 MHz, Chloroform-*d*) δ 7.63 (d, $J = 7.7$ Hz, 1H), 7.33 (s, 2H), 7.24 (d, $J = 7.0$ Hz, 1H), 5.33 (d, $J = 6.3$ Hz, 1H), 2.03 (d, $J = 3.9$ Hz, 1H), 1.53 (d, $J = 5.8$ Hz, 3H). $^{13}\text{C NMR}$ (101 MHz, Chloroform-*d*) δ 143.12, 131.72, 129.48, 128.48, 127.29, 126.48, 67.04, 23.57.

(S)-3-chloro-1-phenyl-1-propanol 7b



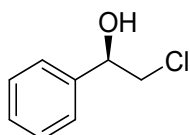
¹H NMR (400 MHz, Chloroform-*d*) δ 7.42 – 7.33 (m, 2H), 3.83 – 3.51 (m, 1H), 2.33 – 2.07 (m, 2H), 1.31 (d, $J = 11.2$ Hz, 3H), 0.88 (d, $J = 9.3$ Hz, 3H). **¹³C NMR** (101 MHz, Chloroform-*d*) δ 143.73, 128.70, 127.96, 125.81, 71.35, 41.74, 41.46, 37.13, 29.74.

(S)-1-(4-chlorophenyl)ethan-1-ol 8b



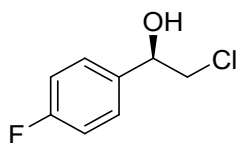
¹H NMR (400 MHz, Chloroform-*d*) δ 7.33 (s, 4H), 4.89 (d, $J = 6.4$ Hz, 1H), 2.03 (s, 1H), 1.49 (d, $J = 5.6$ Hz, 3H). **¹³C NMR** (101 MHz, Chloroform-*d*) δ 144.32, 133.12, 128.67, 126.87, 69.79, 25.33.

(R)-2-chloro-1-phenylethanol 9b



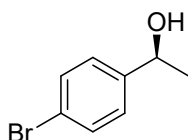
¹H NMR (400 MHz, Chloroform-*d*) δ 7.41 (d, $J = 4.4$ Hz, 4H), 4.91 (dd, $J = 8.7, 3.5$ Hz, 1H), 3.76 (dd, $J = 11.2, 3.5$ Hz, 1H), 3.73 – 3.62 (m, 1H), 1.31 (s, 1H), 0.96 – 0.84 (m, 1H). **¹³C NMR** (101 MHz, Chloroform-*d*) δ 140.01, 128.72, 128.50, 126.13, 74.10, 50.86.

(R)-2-chloro-1-(4-fluorophenyl)ethanol 10b



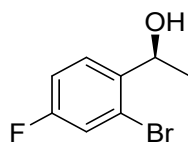
$^1\text{H NMR}$ (400 MHz, Chloroform-*d*) δ 7.37 (dd, $J = 8.6, 5.4$ Hz, 2H), 7.08 (t, $J = 8.7$ Hz, 2H), 4.89 (dd, $J = 8.7, 3.5$ Hz, 1H), 3.72 (dd, $J = 11.3, 3.6$ Hz, 1H), 2.94 (s, 0H), 1.29 (s, 1H). $^{13}\text{C NMR}$ (101 MHz, Chloroform-*d*) δ 163.91, 161.46, 135.75, 135.72, 127.89, 127.81, 115.71, 115.50, 73.44, 50.76, 29.73.

(R)-1-(4-bromophenyl)ethan-1-ol 11b



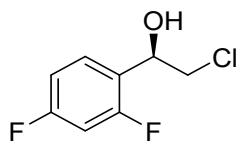
$^1\text{H NMR}$ (400 MHz, Chloroform-*d*) δ 7.47 (d, $J = 8.4$ Hz, 2H), 7.23 (d, $J = 8.5$ Hz, 2H), 4.83 (q, $J = 6.5$ Hz, 1H), 2.40 (s, 1H), 1.46 (d, $J = 6.5$ Hz, 3H). $^{13}\text{C NMR}$ (101 MHz, Chloroform-*d*) δ 144.80, 131.55, 127.19, 121.14, 69.73, 25.23.

(R)-1-(2-bromo-4-fluorophenyl)ethanol 12b



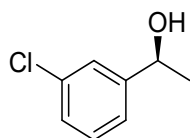
$^1\text{H NMR}$ (400 MHz, Chloroform-*d*) δ 7.58 (dd, $J = 8.7, 6.1$ Hz, 1H), 7.27 (dd, $J = 8.2, 2.6$ Hz, 1H), 7.08 (td, $J = 8.3, 2.6$ Hz, 1H), 5.21 (q, $J = 6.4$ Hz, 1H), 1.48 (s, 2H), 1.29 (d, $J = 11.7$ Hz, 1H), 0.87 (d, $J = 6.7$ Hz, 1H). $^{13}\text{C NMR}$ (101 MHz, Chloroform-*d*) δ 162.68, 160.20, 140.61, 140.58, 127.77, 127.69, 121.50, 121.41, 119.81, 119.57, 115.07, 114.86, 68.67, 29.73, 23.78.

(*S*)-2-chloro-1-(2,4-difluorophenyl)ethanol **13b**



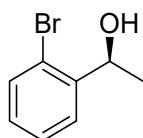
$^1\text{H NMR}$ (400 MHz, Chloroform-*d*) δ 7.58 – 7.50 (m, 1H), 6.96 – 6.80 (m, 2H), 5.19 (dd, $J = 8.3, 3.3$ Hz, 1H), 3.82 (dd, $J = 11.2, 3.3$ Hz, 1H), 3.63 (dd, $J = 11.2, 8.3$ Hz, 1H), 1.28 (s, 1H), 0.86 (d, $J = 5.4$ Hz, 1H). $^{13}\text{C NMR}$ (101 MHz, Chloroform-*d*) δ 164.09, 128.70, 128.64, 128.61, 128.55, 111.77, 111.73, 111.56, 111.52, 104.14, 103.88, 103.63, 67.84, 49.56, 29.73.

(*S*)-1-(3-chlorophenyl)ethan-1-ol **14b**



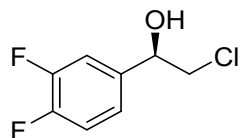
$^1\text{H NMR}$ (400 MHz, Chloroform-*d*) δ 7.41 (s, 1H), 7.29 (s, 3H), 4.90 (s, 1H), 2.08 (s, 1H), 1.51 (d, $J = 3.3$ Hz, 3H). $^{13}\text{C NMR}$ (101 MHz, Chloroform-*d*) δ 147.92, 134.42, 129.86, 127.59, 125.70, 123.61, 69.85, 25.29.

(*R*)-1-(2-bromophenyl)ethan-1-ol **15b**



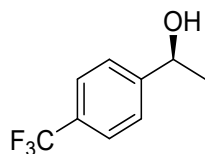
$^1\text{H NMR}$ (400 MHz, Chloroform-*d*) δ 7.63 (d, $J = 7.6$ Hz, 1H), 7.55 (d, $J = 7.9$ Hz, 1H), 7.39 (t, $J = 7.7$ Hz, 1H), 7.18 (d, $J = 8.0$ Hz, 1H), 5.28 (d, $J = 3.9$ Hz, 1H), 1.95 (s, 1H), 1.53 (dd, $J = 6.1, 2.6$ Hz, 3H). $^{13}\text{C NMR}$ (101 MHz, Chloroform-*d*) δ 144.66, 132.74, 128.86, 127.93, 126.73, 121.80, 69.27, 23.63.

(*S*)-2-chloro-1-(3,4-difluorophenyl)ethan-1-ol **16b**



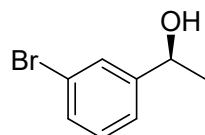
$^1\text{H NMR}$ (400 MHz, Chloroform-*d*) δ 7.31 – 7.10 (m, 3H), 4.88 (dd, $J = 8.5, 3.5$ Hz, 1H), 3.73 (dd, $J = 11.3, 3.5$ Hz, 1H), 3.60 (dd, $J = 11.3, 8.5$ Hz, 1H), 1.29 (d, $J = 11.1$ Hz, 1H), 0.87 (d, $J = 2.7$ Hz, 1H). $^{13}\text{C NMR}$ (101 MHz, Chloroform-*d*) δ 151.74, 151.61, 151.48, 151.36, 149.27, 149.01, 148.89, 136.97, 122.21, 122.18, 122.15, 122.11, 117.55, 117.38, 115.34, 115.16, 72.89, 50.50, 29.72.

(*S*)-1-[4-(trifluoromethyl)phenyl]ethan-1-ol **17b**



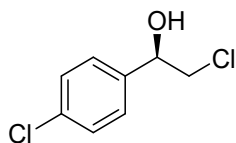
$^1\text{H NMR}$ (400 MHz, Chloroform-*d*) δ 7.61 (d, $J = 8.1$ Hz, 2H), 7.48 (d, $J = 8.1$ Hz, 2H), 4.95 (q, $J = 6.5$ Hz, 1H), 1.50 (d, $J = 6.5$ Hz, 3H), 1.29 (s, 1H). $^{13}\text{C NMR}$ (101 MHz, Chloroform-*d*) δ 149.70, 125.66, 125.49, 125.46, 125.42, 69.80, 29.73, 25.32.

(*R*)-1-(3-bromophenyl)ethan-1-ol **18b**



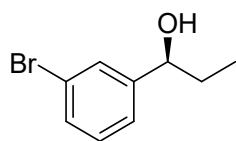
$^1\text{H NMR}$ (400 MHz, Chloroform-*d*) δ 7.57 (s, 1H), 7.43 (s, 1H), 7.32 (s, 1H), 7.25 (s, 1H), 4.90 (d, $J = 6.5$ Hz, 1H), 1.93 (s, 1H), 1.51 (s, 3H). $^{13}\text{C NMR}$ (101 MHz, Chloroform-*d*) δ 148.18, 130.55, 130.17, 128.64, 124.09, 122.68, 69.83, 25.33.

(*S*)-2-chloro-1-(4-chlorophenyl)ethanol **19b**



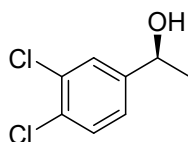
$^1\text{H NMR}$ (400 MHz, Chloroform-*d*) δ 7.35 (d, $J = 6.3$ Hz, 2H), 4.89 (dd, $J = 8.6, 3.5$ Hz, 1H), 3.74 – 3.60 (m, 2H), 2.90 (s, 1H), 1.29 (s, 1H), 0.88 (d, $J = 2.8$ Hz, 1H). $^{13}\text{C NMR}$ (101 MHz, Chloroform-*d*) δ 138.40, 134.24, 128.87, 127.49, 73.38, 50.65, 29.74.

(*R*)-1-(3-bromophenyl)propanol **20b**



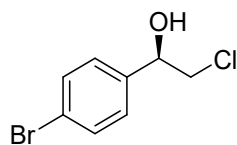
$^1\text{H NMR}$ (400 MHz, Chloroform-*d*) δ 7.53 (s, 1H), 7.42 (dt, $J = 7.6, 1.7$ Hz, 1H), 7.33 – 7.17 (m, 2H), 4.60 (t, $J = 6.5$ Hz, 1H), 1.84 – 1.73 (m, 1H), 1.28 (s, 2H), 0.94 (t, $J = 7.4$ Hz, 1H), 0.87 (t, $J = 3.5$ Hz, 2H). $^{13}\text{C NMR}$ (101 MHz, Chloroform-*d*) δ 146.95, 130.53, 130.00, 129.10, 124.62, 122.58, 75.30, 37.12, 31.97, 29.73, 29.39, 22.72, 14.16, 10.00.

(*R*)-1-(3,4-dichlorophenyl)ethan-1-ol **21b**



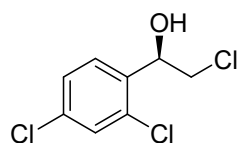
$^1\text{H NMR}$ (400 MHz, Chloroform-*d*) δ 7.53 (s, 1H), 7.46 (d, $J = 8.3$ Hz, 1H), 7.26 (s, 1H), 4.92 (s, 1H), 1.92 (s, 1H), 1.53 (s, 3H). $^{13}\text{C NMR}$ (101 MHz, Chloroform-*d*) δ 146.06, 132.58, 131.24, 130.51, 127.56, 124.85, 69.31, 25.37.

(*S*)-1-(4-bromophenyl)-2-chloroethanol **22b**



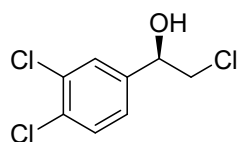
$^1\text{H NMR}$ (400 MHz, Chloroform-*d*) δ 7.53 (d, $J = 8.5$ Hz, 2H), 7.30 (d, $J = 8.8$ Hz, 2H), 4.90 (dd, $J = 8.6, 3.5$ Hz, 1H), 4.14 (q, $J = 7.1$ Hz, 1H), 3.74 (dd, $J = 11.3, 3.5$ Hz, 1H), 3.63 (dd, $J = 11.2, 8.7$ Hz, 1H). $^{13}\text{C NMR}$ (101 MHz, Chloroform-*d*) δ 138.87, 131.83, 127.79, 122.40, 73.41, 50.66, 37.12, 32.80, 31.95, 29.73, 29.39.

(*R*)-2-chloro-1-(2,4-dichlorophenyl)ethan-1-ol **23b**



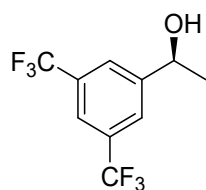
$^1\text{H NMR}$ (400 MHz, Chloroform-*d*) δ 7.59 (d, $J = 8.4$ Hz, 1H), 7.40 (d, $J = 2.1$ Hz, 1H), 7.33 (dd, $J = 8.4, 2.1$ Hz, 1H), 5.28 (dt, $J = 8.4, 3.2$ Hz, 1H), 3.89 (dd, $J = 11.3, 2.8$ Hz, 1H), 3.54 (dd, $J = 11.3, 8.5$ Hz, 1H), 2.87 (d, $J = 3.6$ Hz, 1H). $^{13}\text{C NMR}$ (101 MHz, Chloroform-*d*) δ 135.89, 134.65, 132.49, 129.33, 128.56, 127.61, 70.31, 49.18.

(*S*)-2-chloro-1-(3,4-dichlorophenyl)ethan-1-ol **24b**



$^1\text{H NMR}$ (400 MHz, Chloroform-*d*) δ 7.59 – 7.44 (m, 2H), 7.25 (d, $J = 10.5$ Hz, 2H), 4.90 (dd, $J = 8.5, 3.5$ Hz, 1H), 3.75 (dd, $J = 11.3, 3.5$ Hz, 1H), 3.62 (dd, $J = 11.3, 8.5$ Hz, 1H). $^{13}\text{C NMR}$ (101 MHz, Chloroform-*d*) δ 140.07, 132.92, 130.65, 128.88, 128.83, 128.20, 126.85, 125.42, 72.79, 50.48.

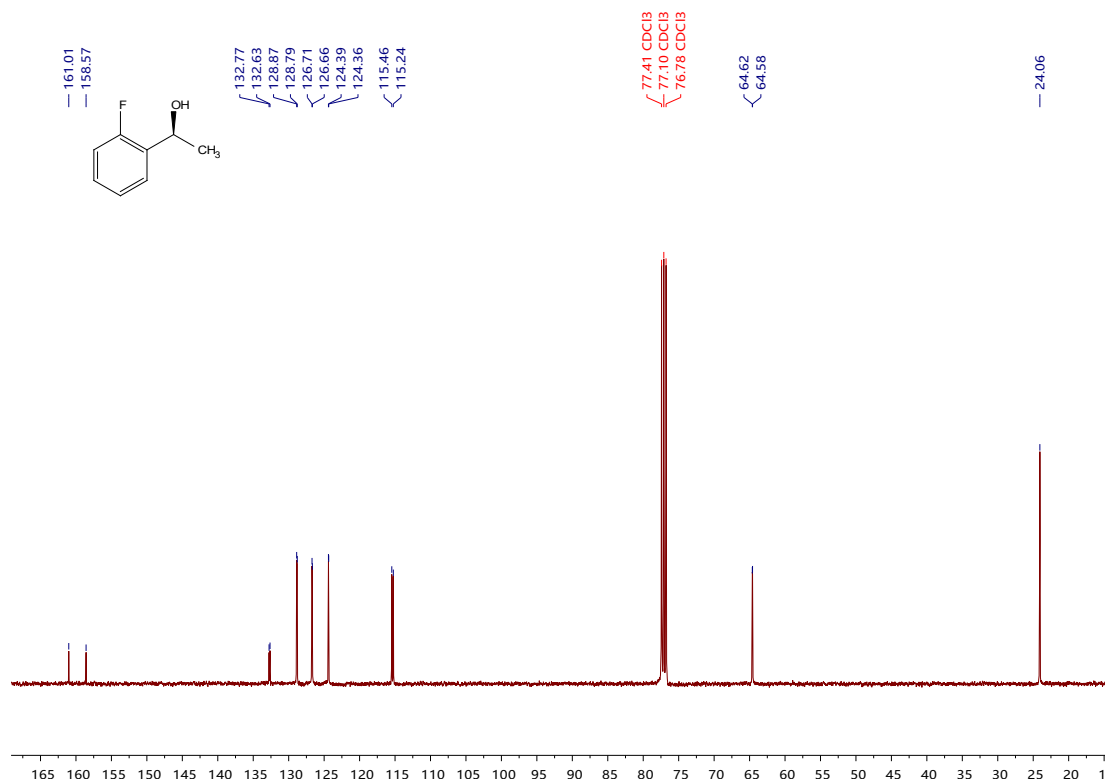
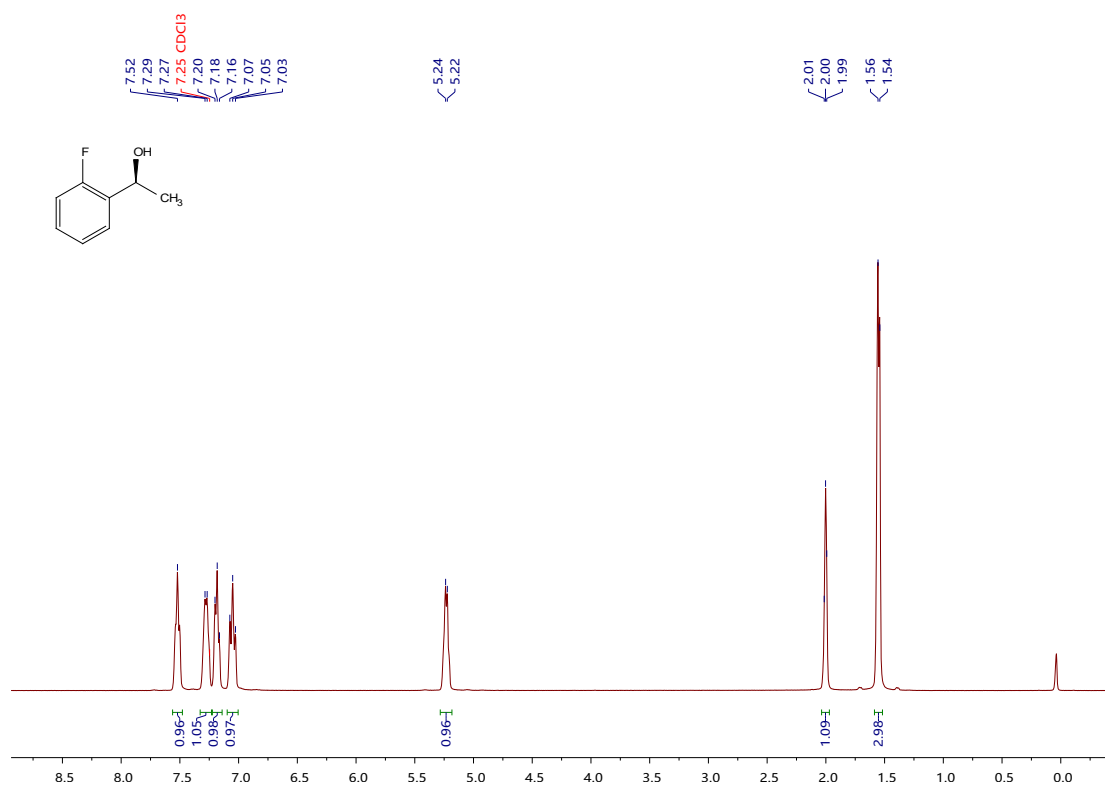
(*S*)-1-[3,5-bis(trifluoromethyl)phenyl]ethanol **25b**



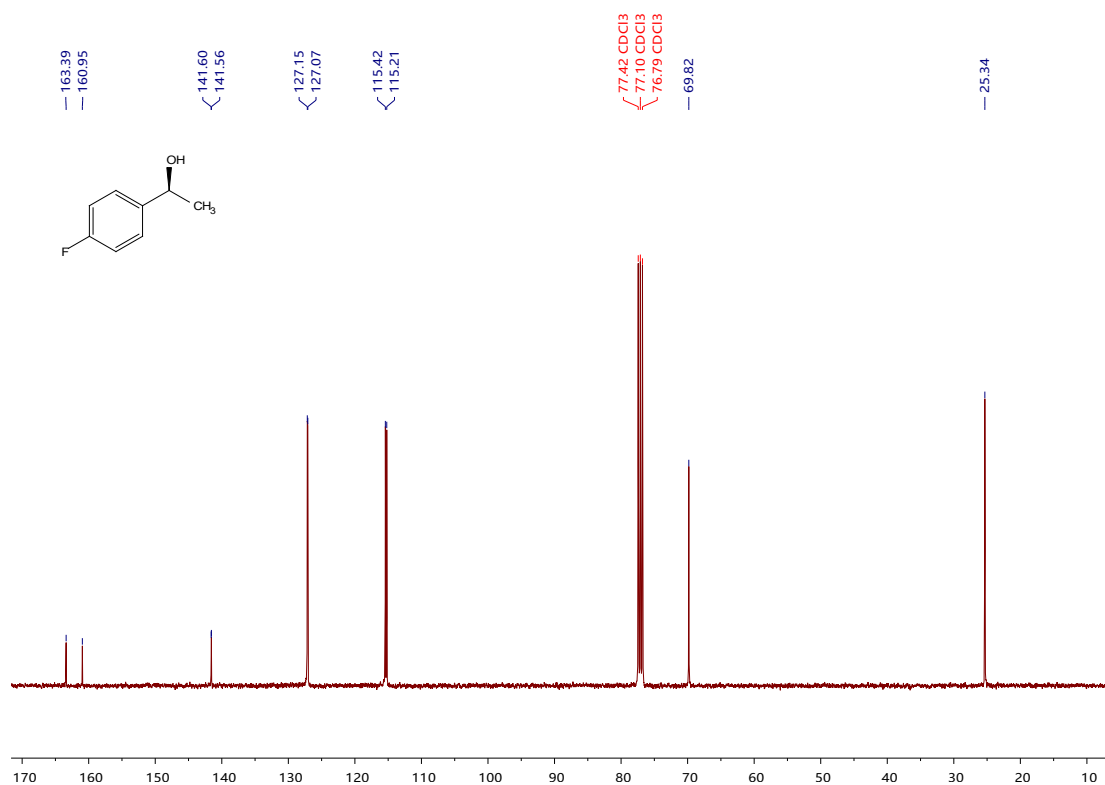
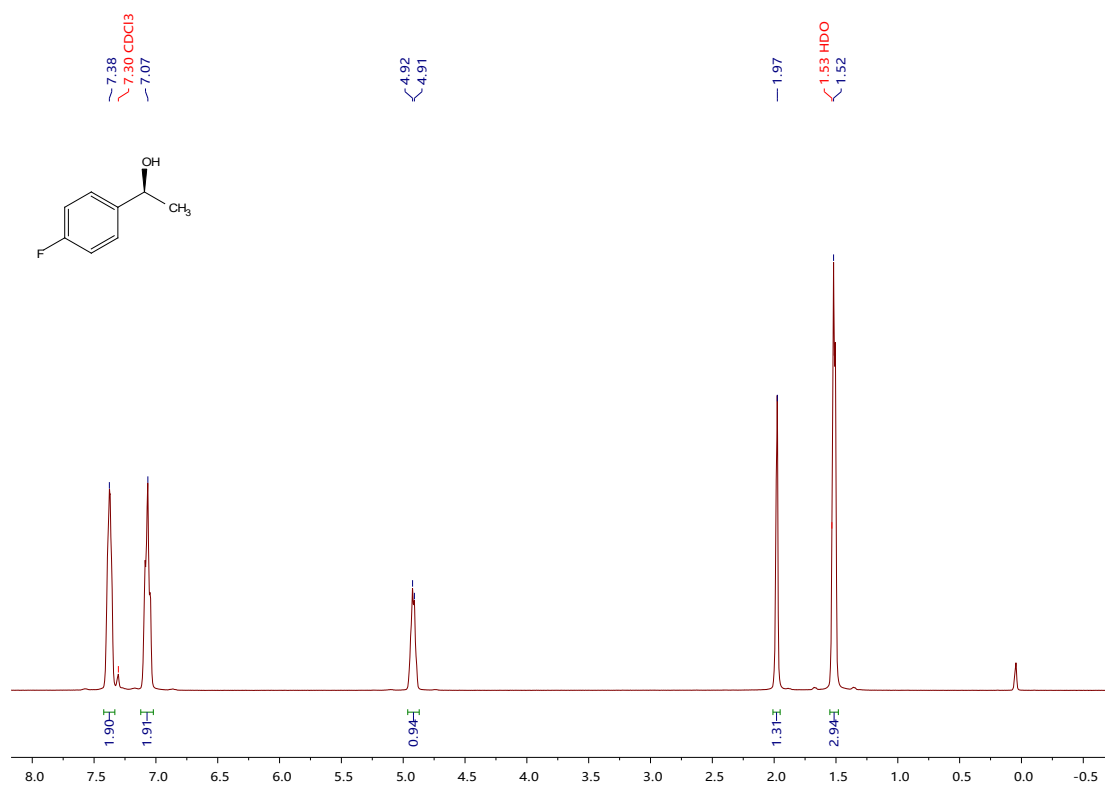
¹H NMR (400 MHz, Chloroform-*d*) δ 1.30 (d, $J = 10.9$ Hz, 4H), 0.87 (s, 4H). **¹³C NMR** (101 MHz, Chloroform-*d*) δ 148.24, 125.69, 125.65, 121.33, 69.29, 30.06, 29.76, 29.73, 29.69, 25.63, 22.72, 14.15.

NMR spectra of compounds

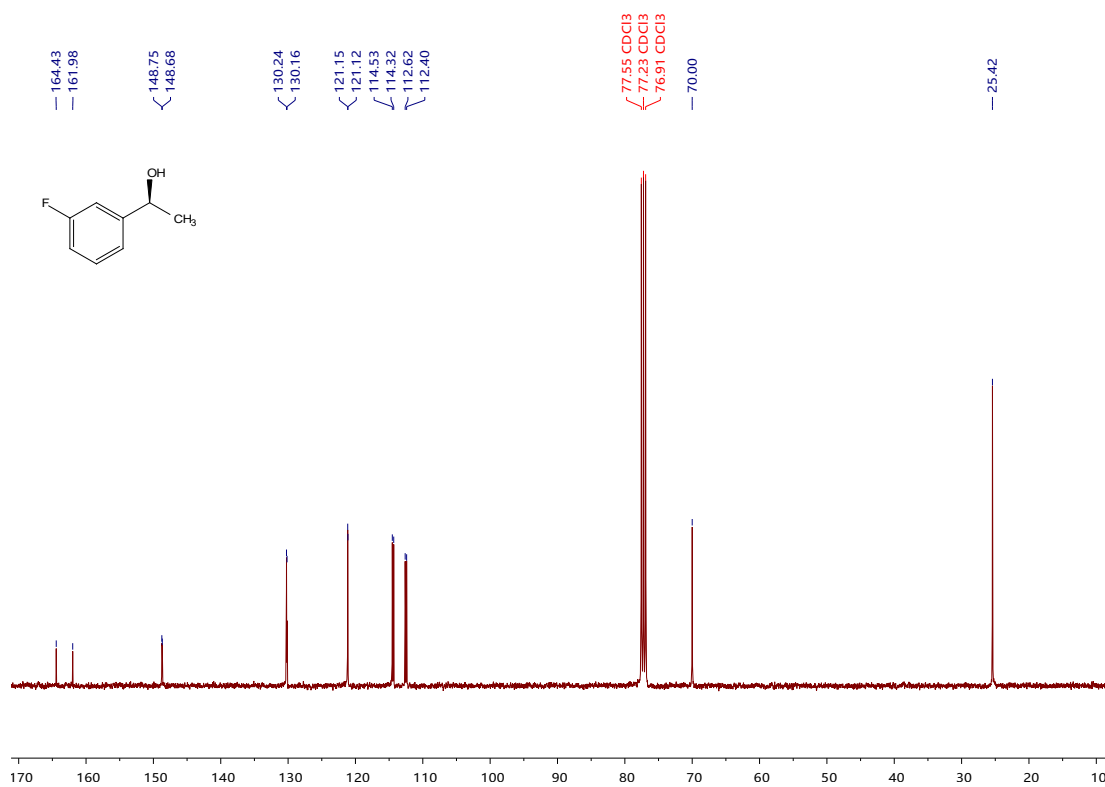
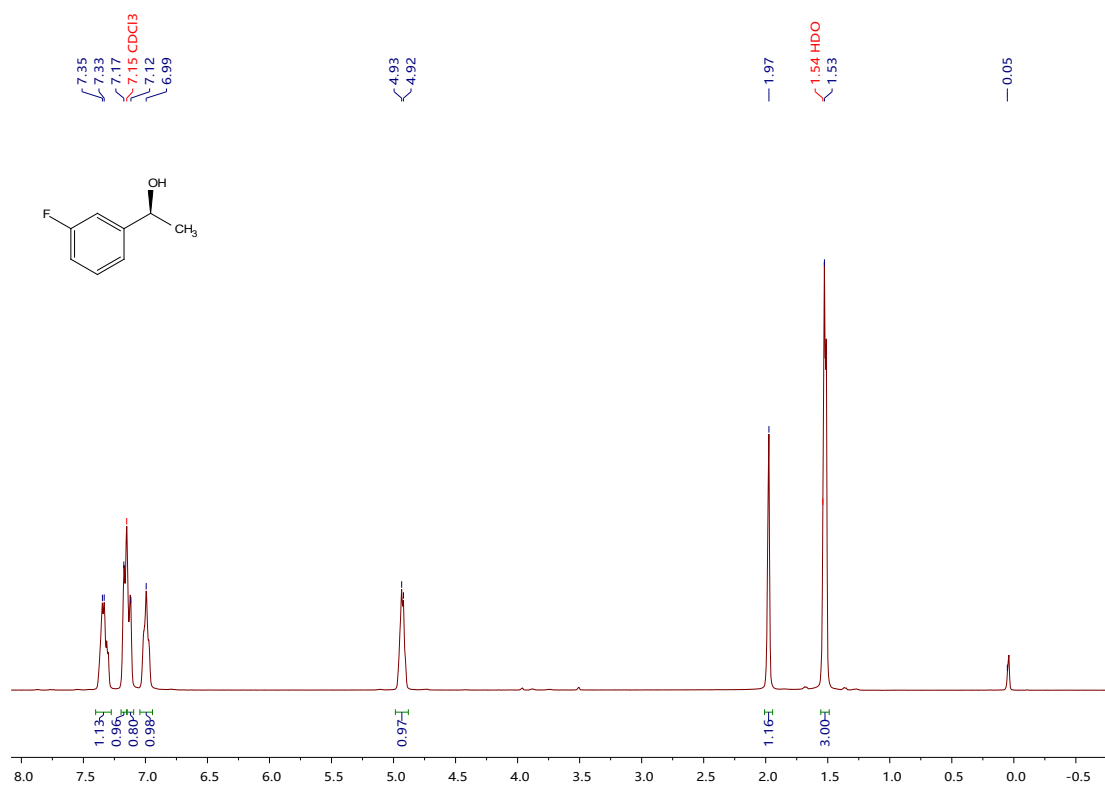
(S)-1-(2-fluorophenyl)ethan-1-ol **1b**



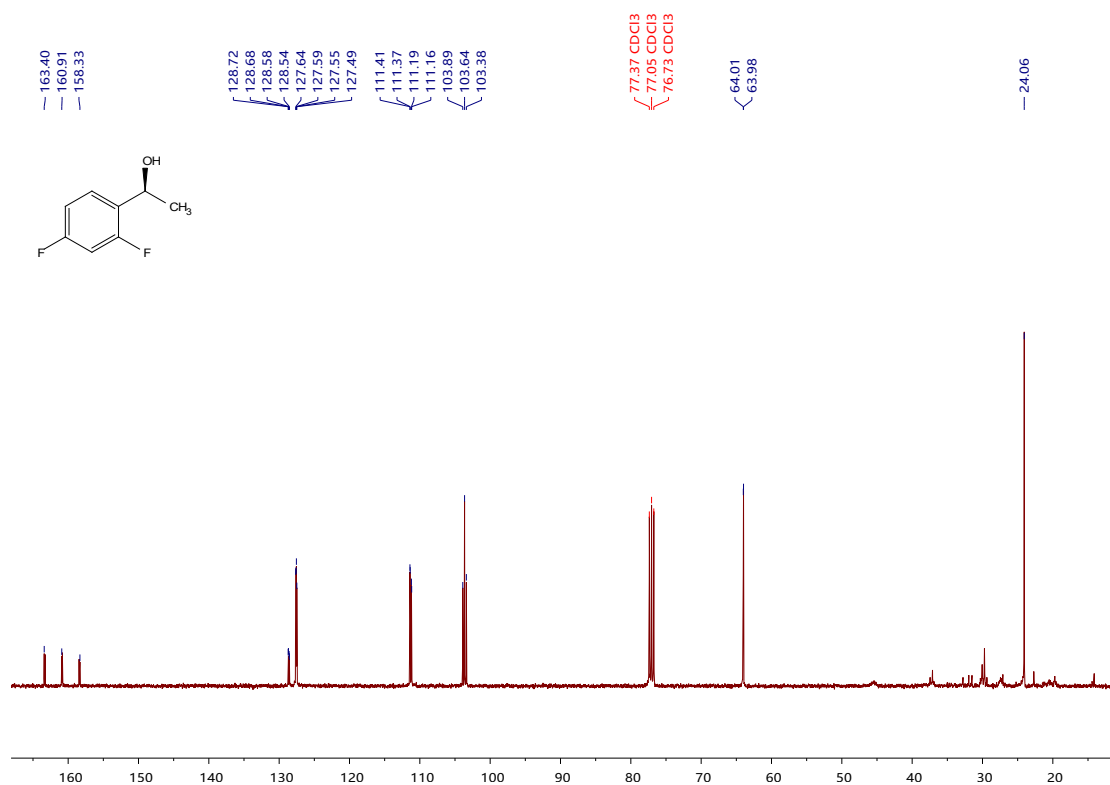
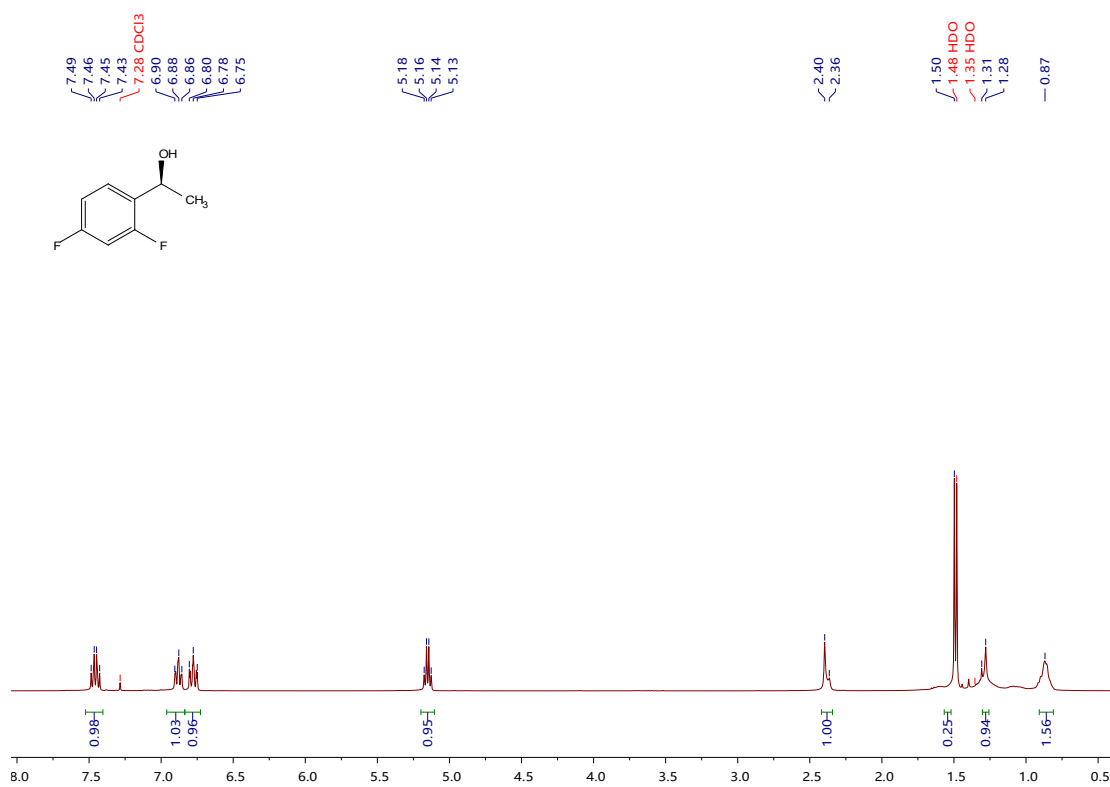
(S)-1-(4-fluorophenyl)ethan-1-ol **2b**



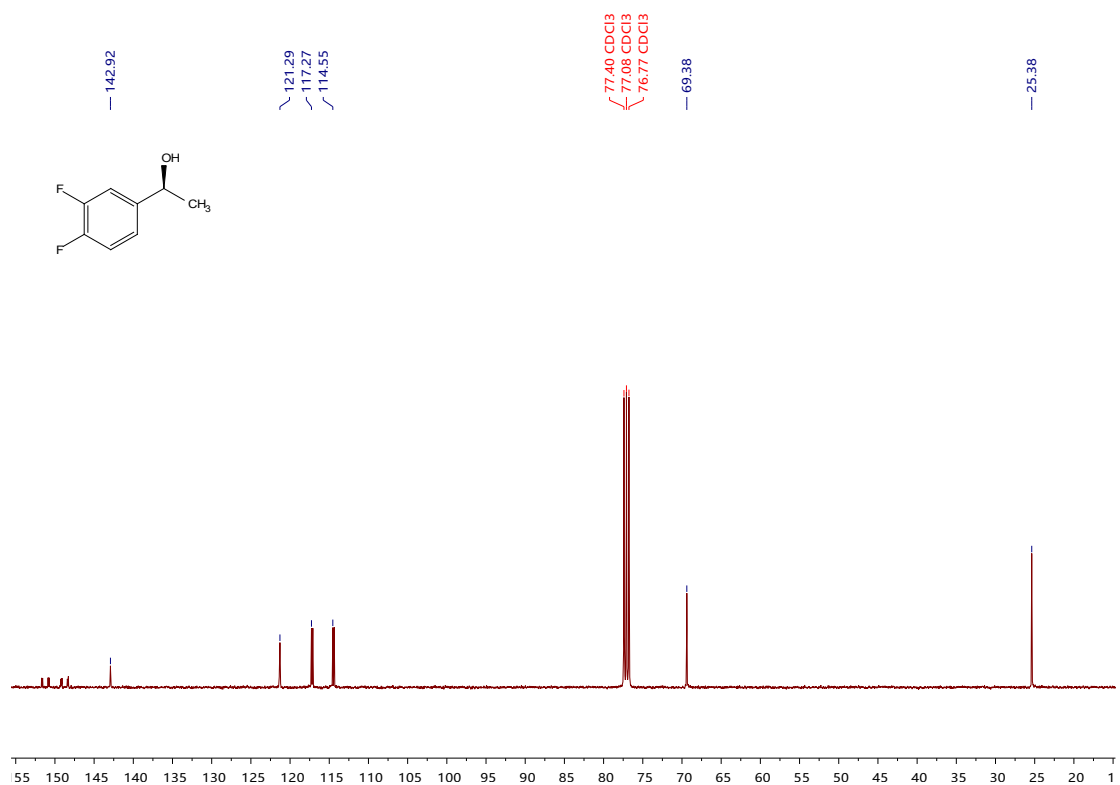
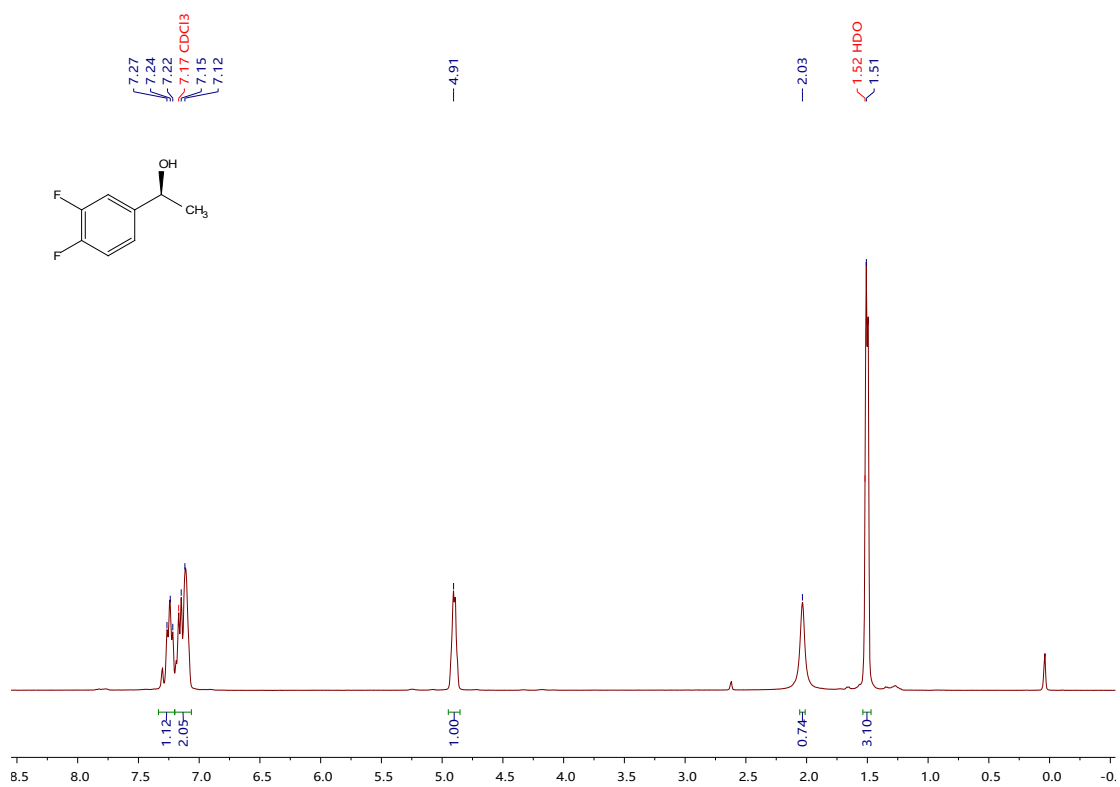
(S)-1-(3-fluorophenyl)ethan-1-ol **3b**



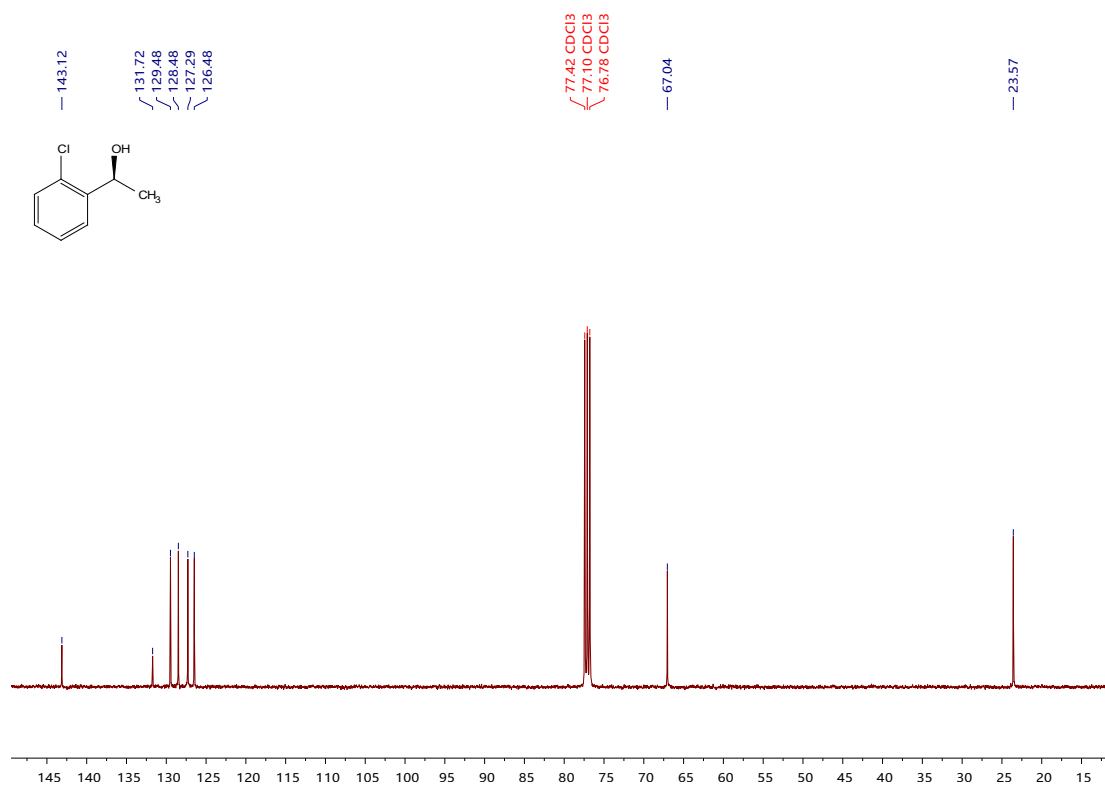
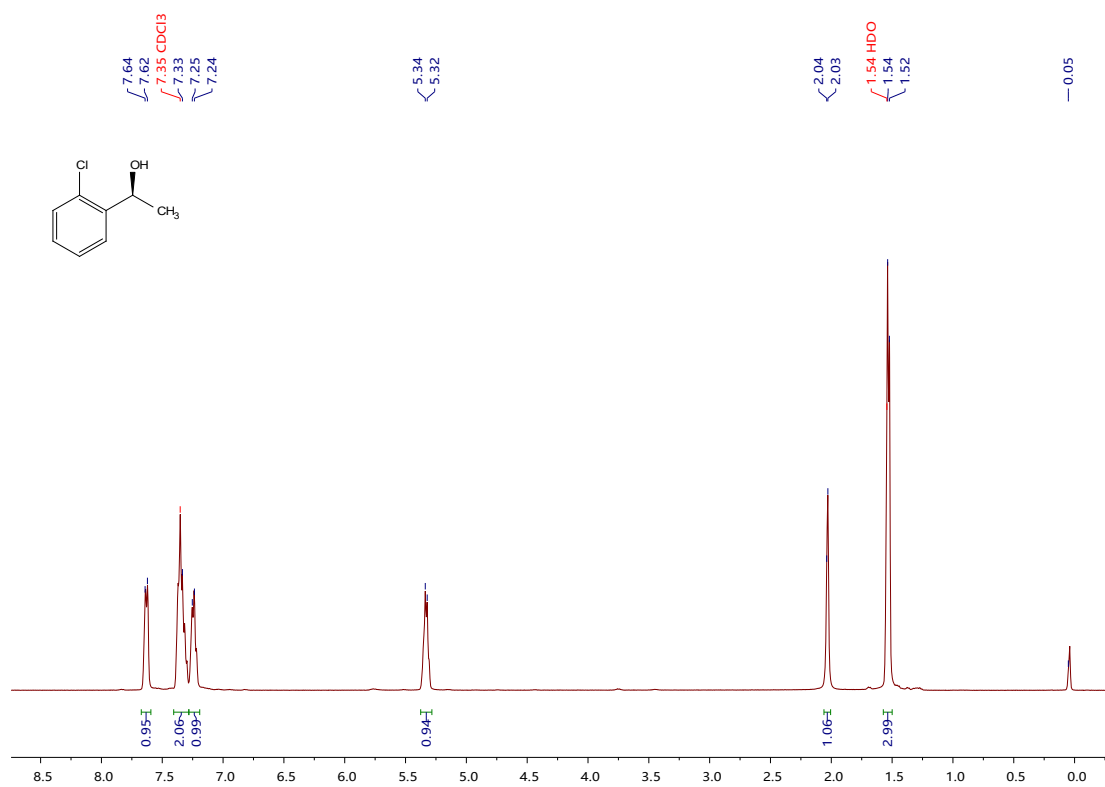
(R)-1-(2,4-difluorophenyl)ethanol 4b



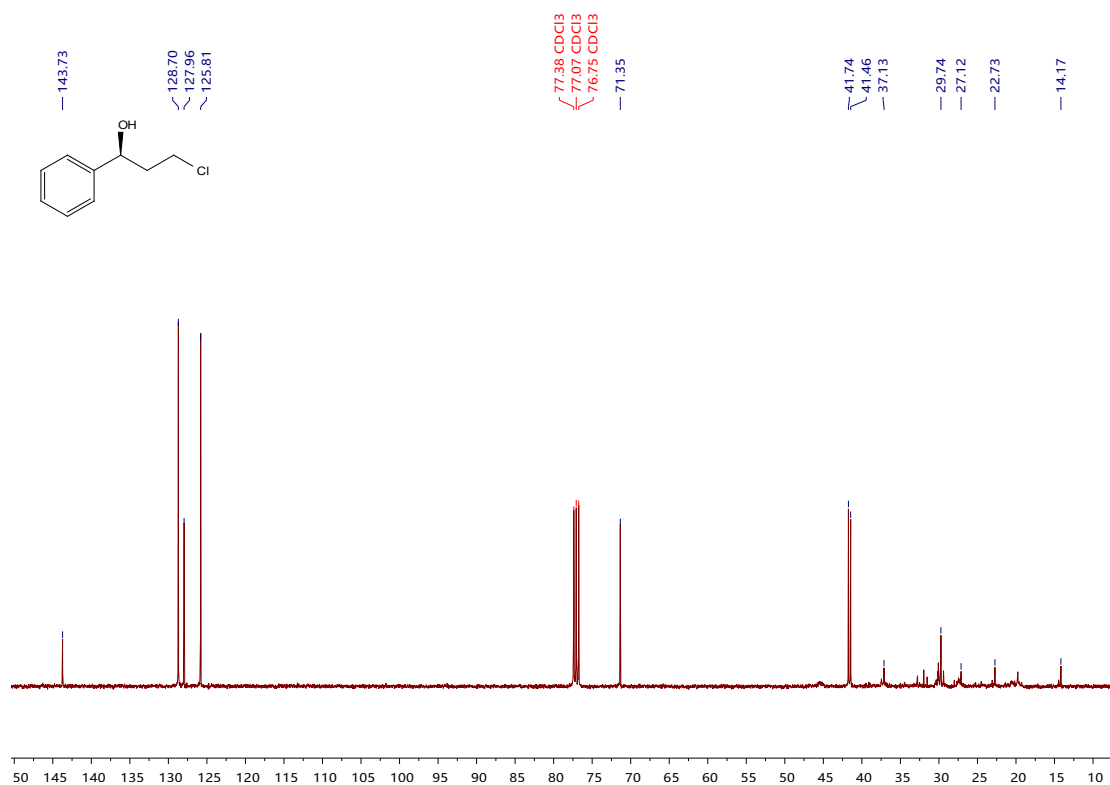
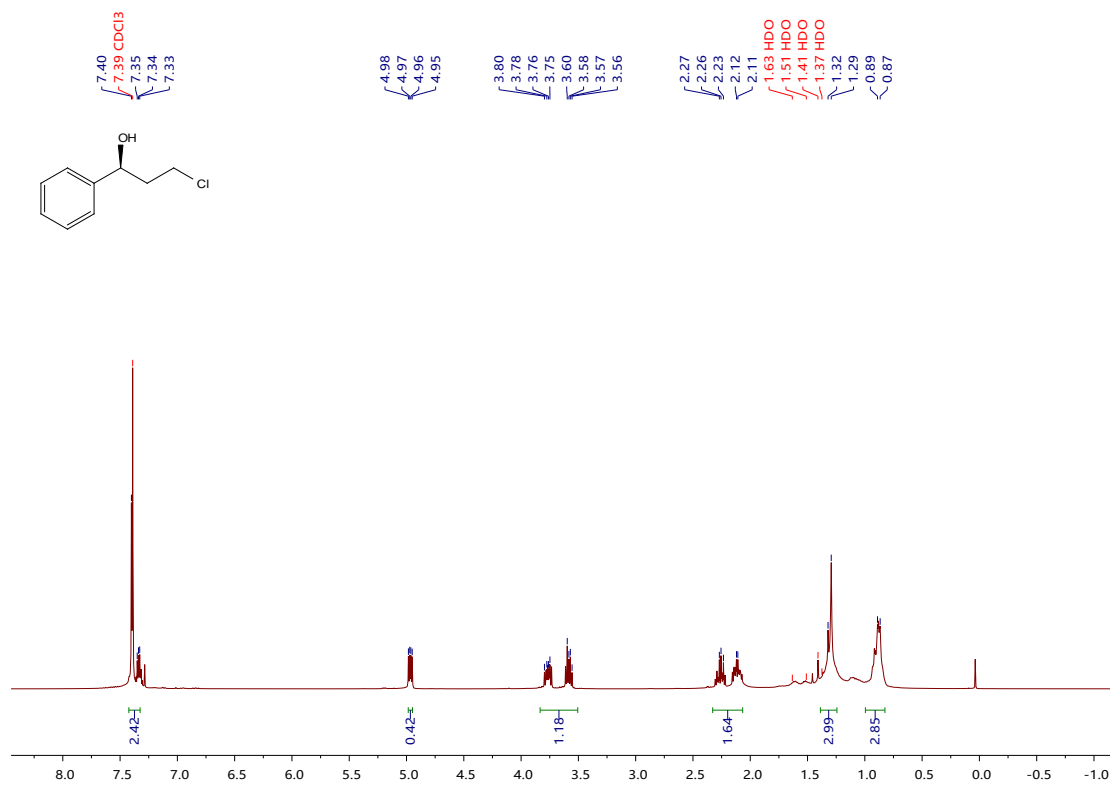
(R)-1-(3,4-difluorophenyl)ethan-1-ol 5b



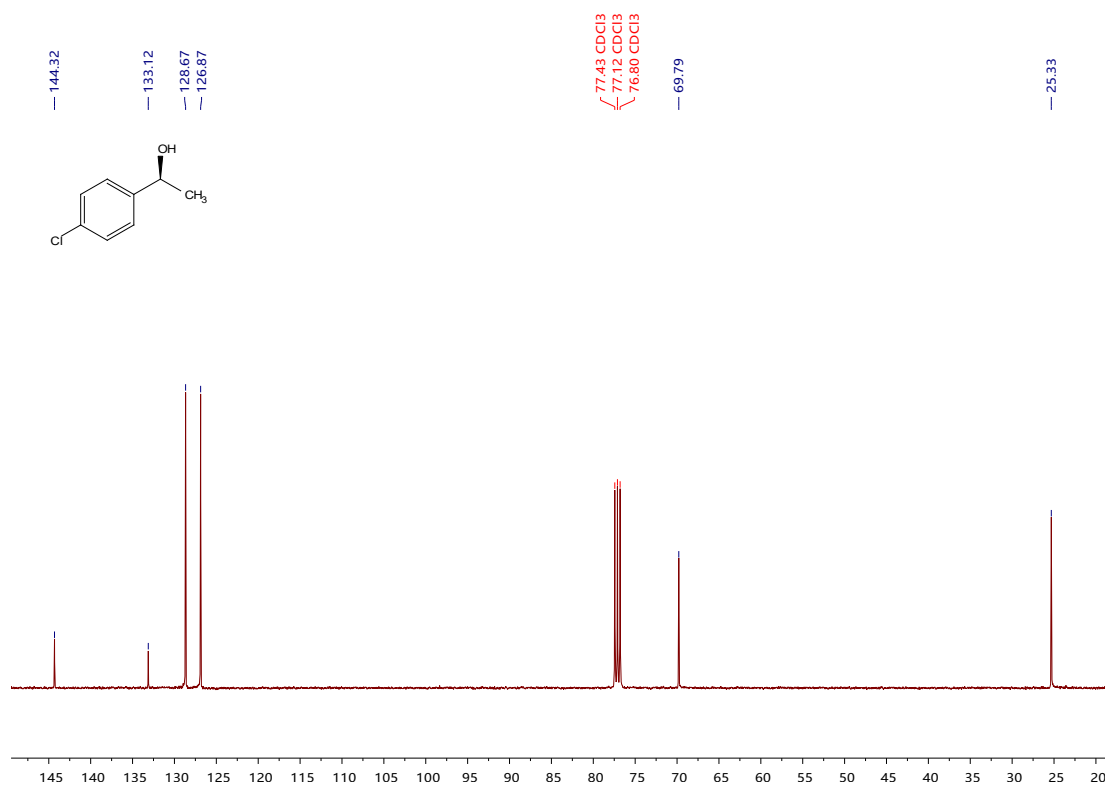
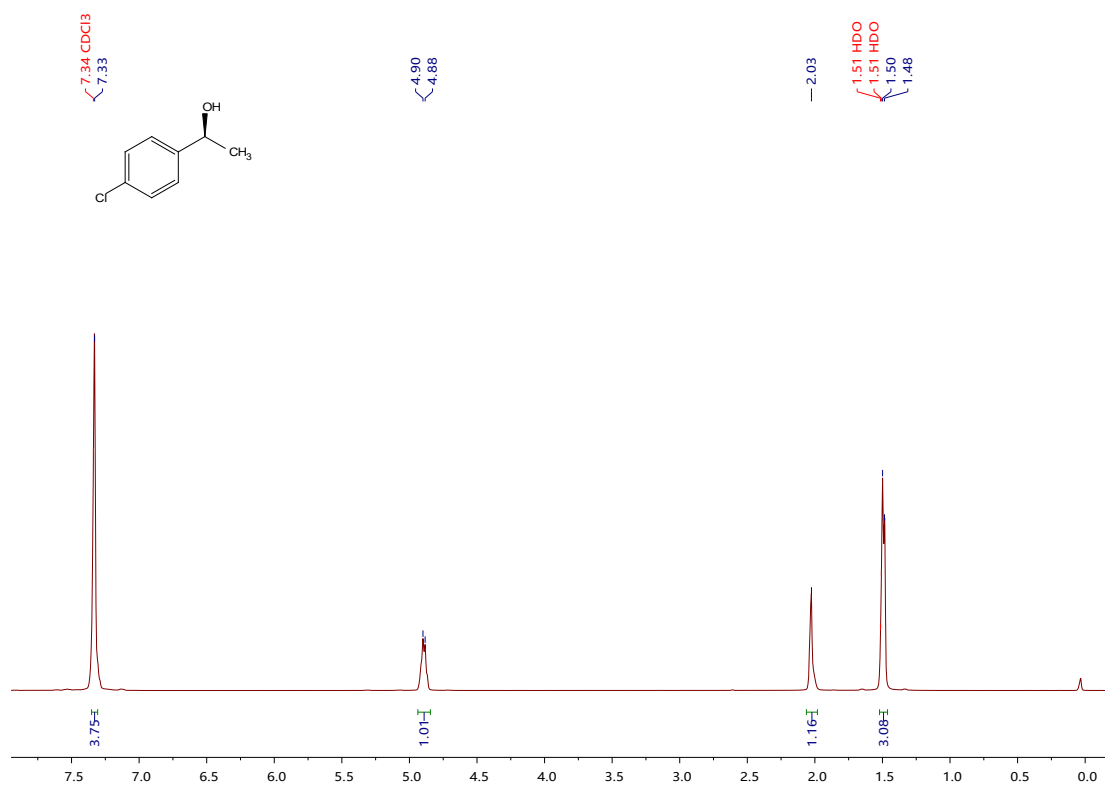
(S)-1-(2-chlorophenyl)ethan-1-ol **6b**



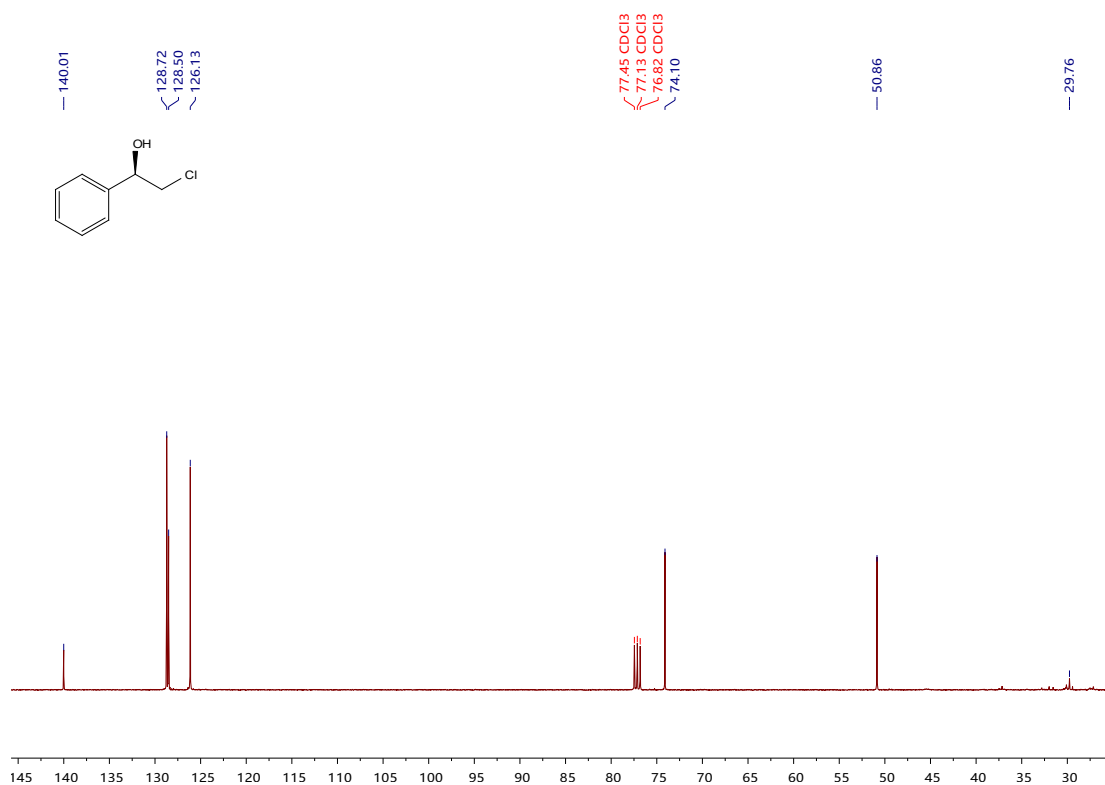
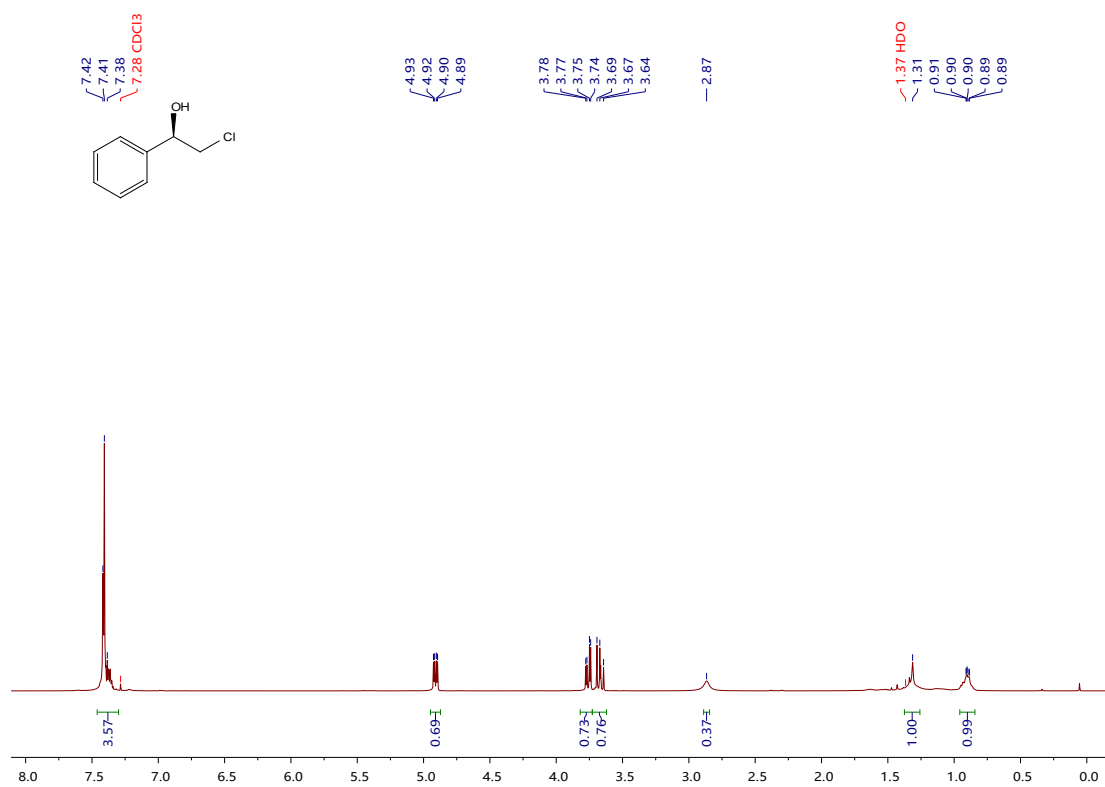
(S)-3-chloro-1-phenyl-1-propanol **7b**



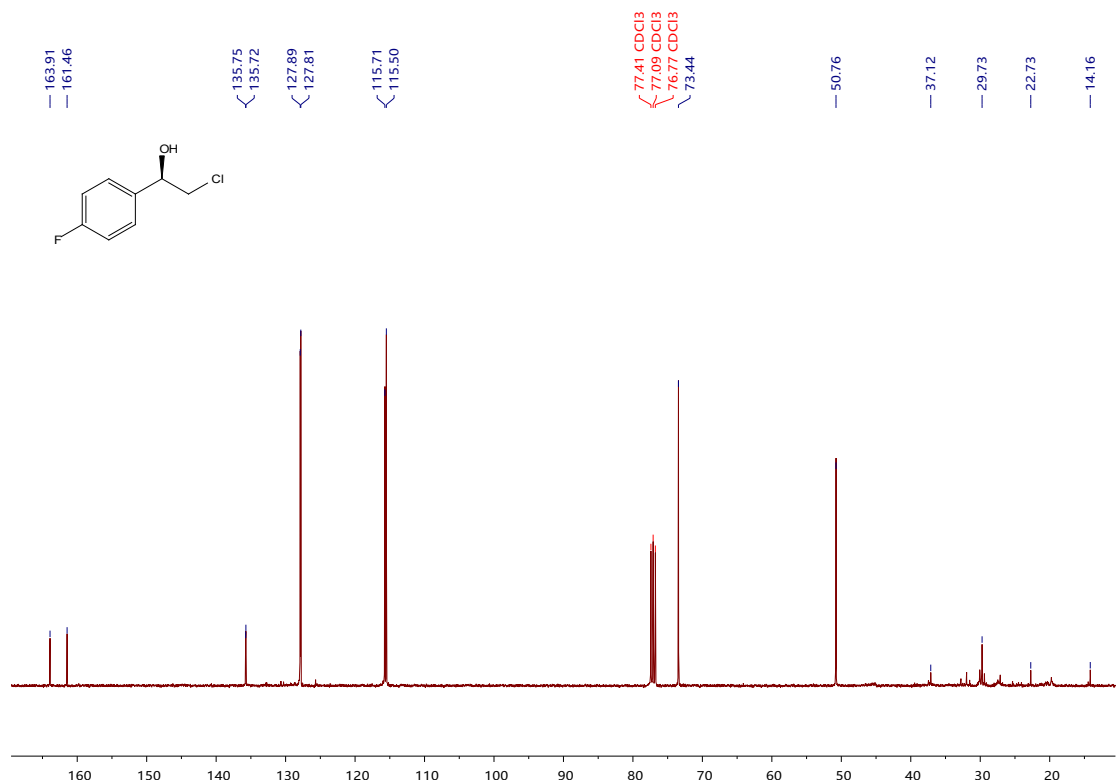
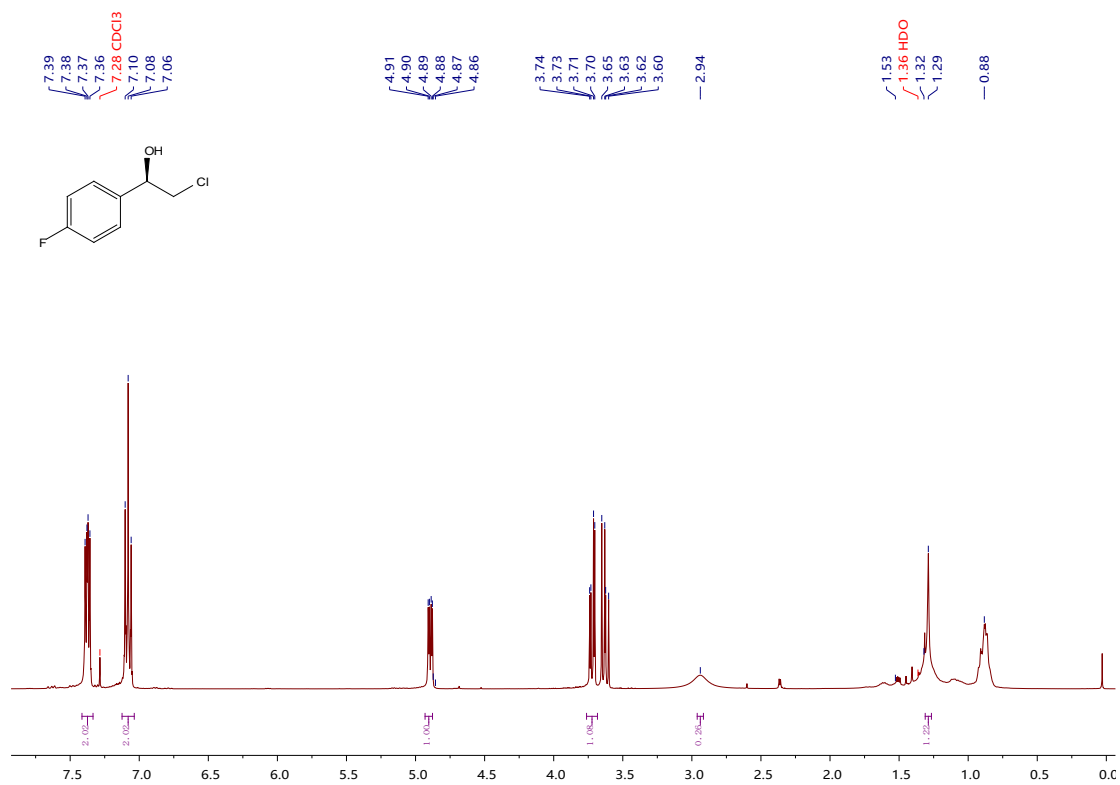
(S)-1-(4-chlorophenyl)ethan-1-ol **8b**



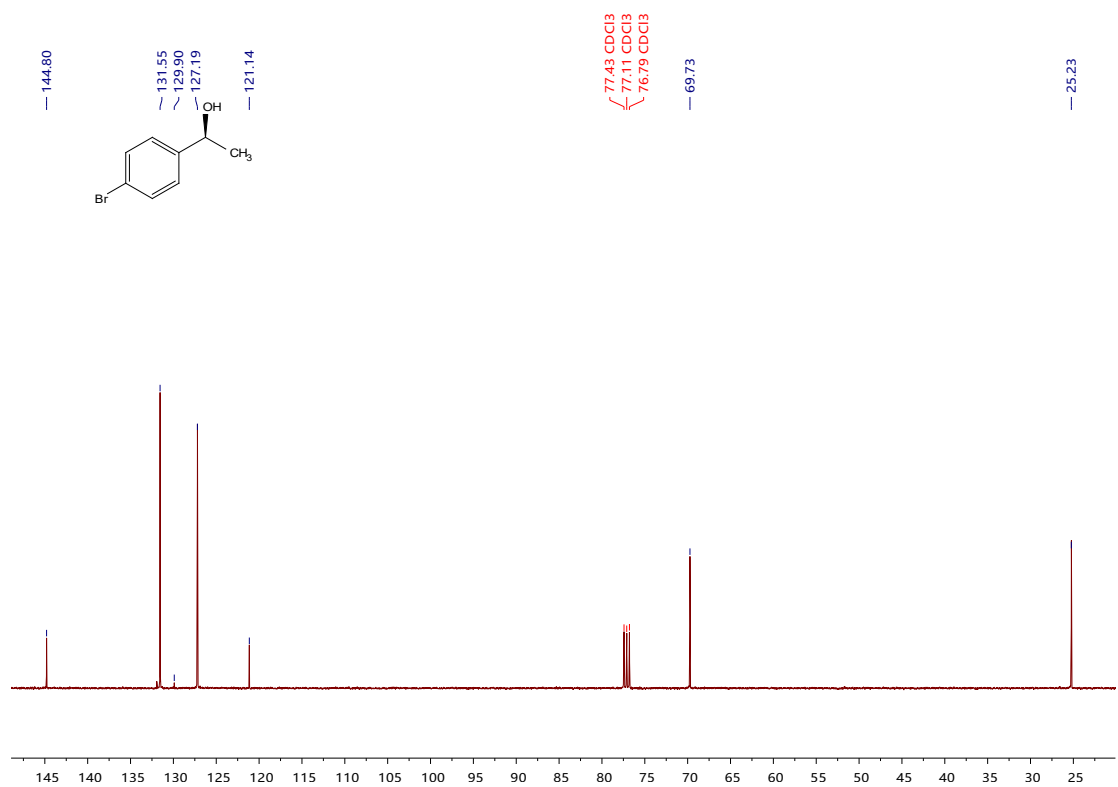
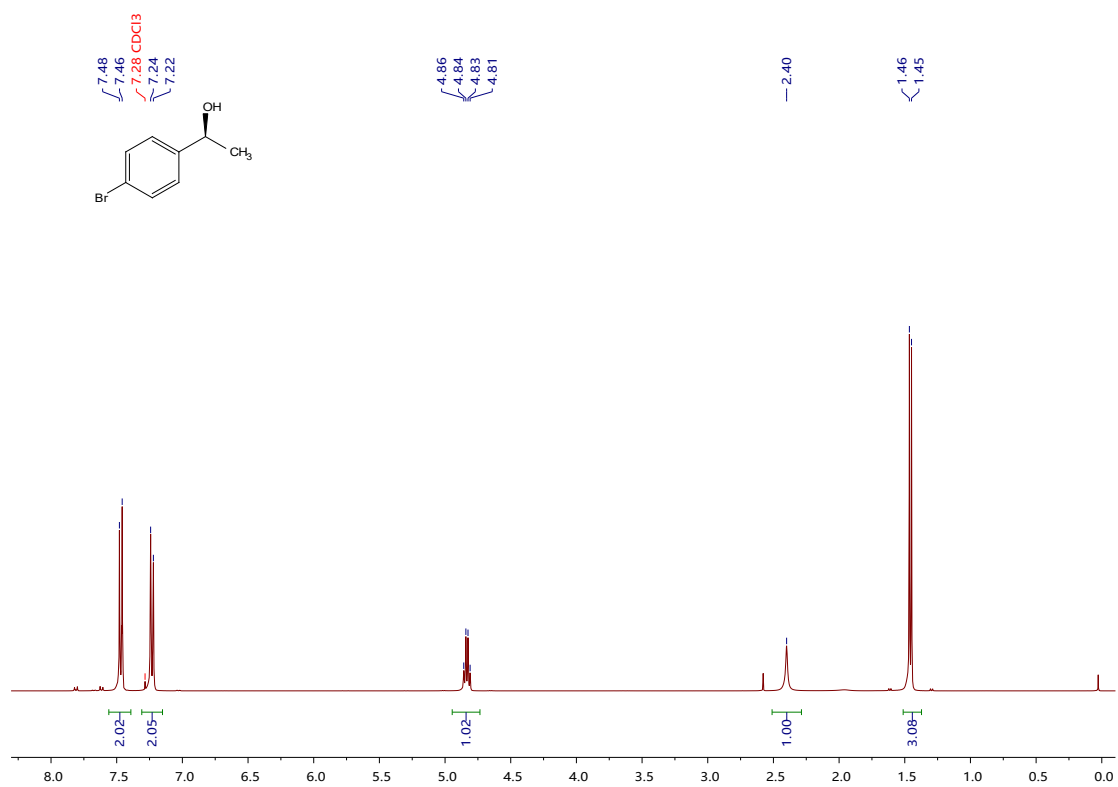
(R)-2-chloro-1-phenylethanol 9b



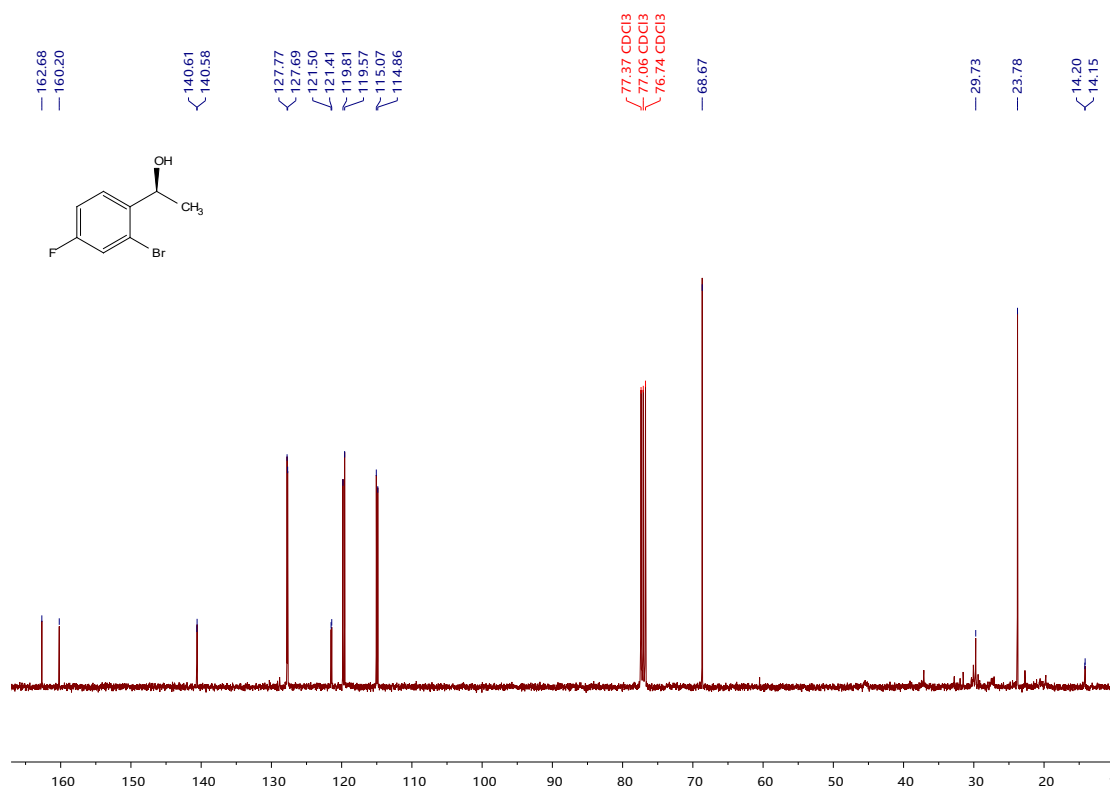
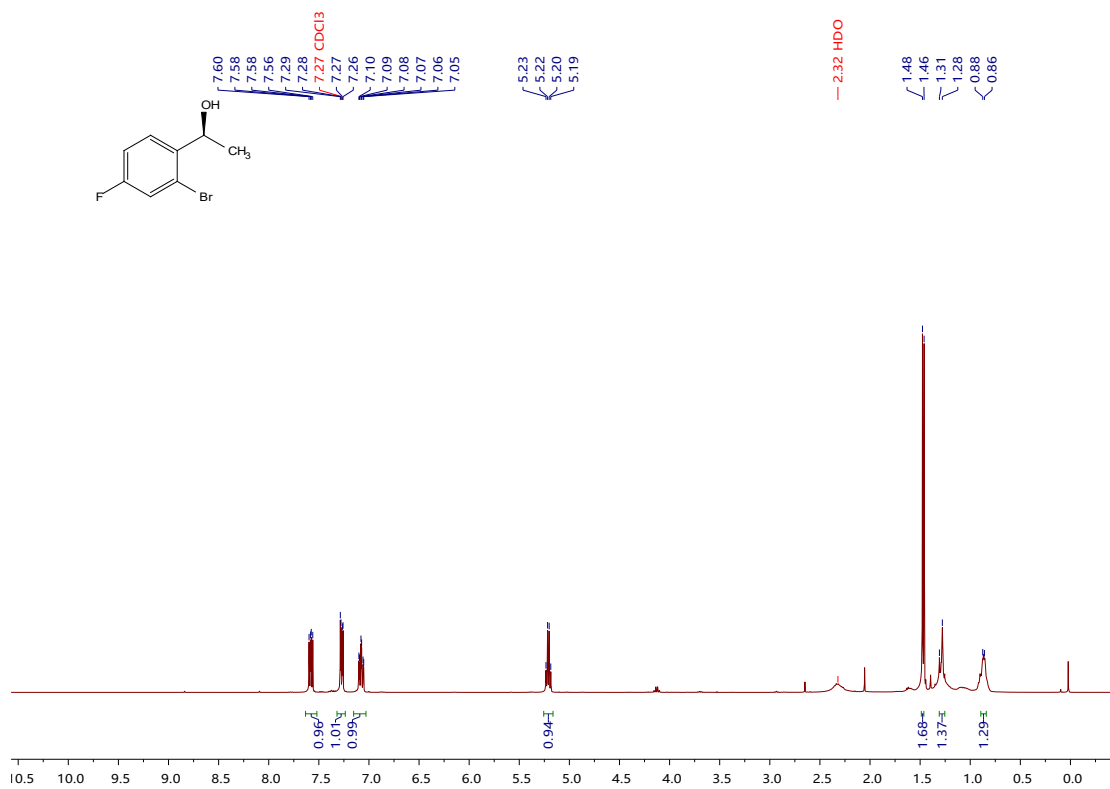
(R)-2-chloro-1-(4-fluorophenyl)ethanol 10b



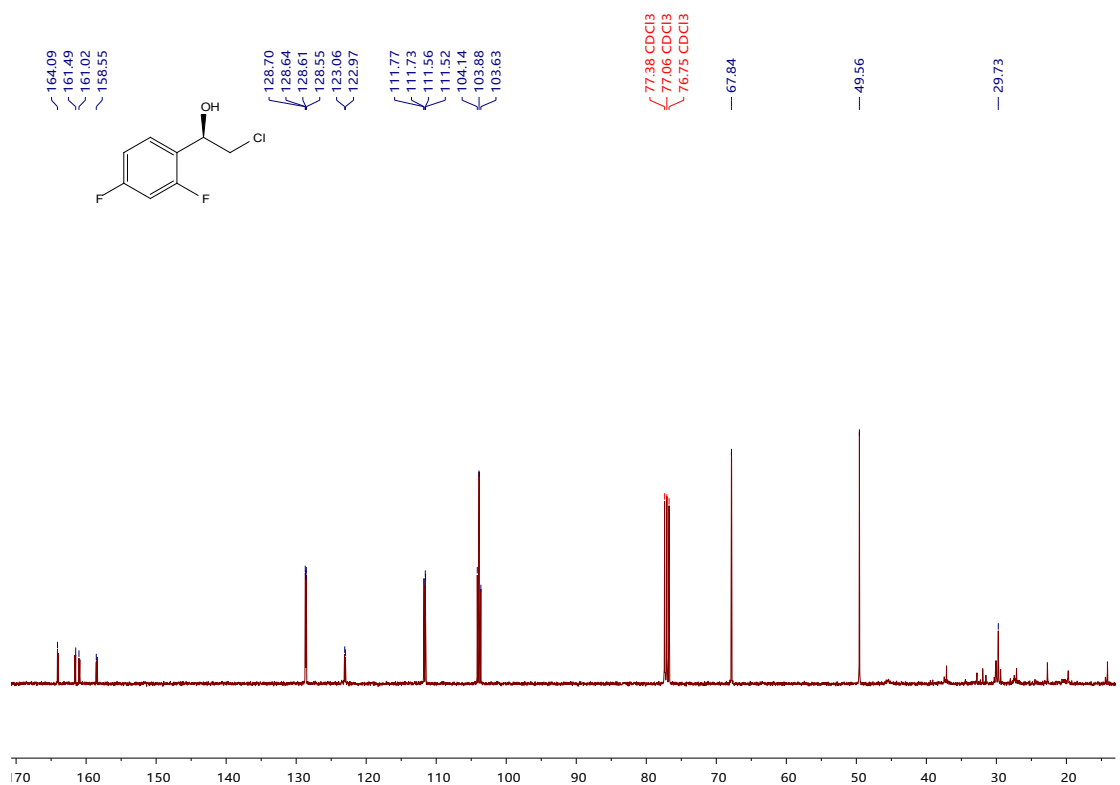
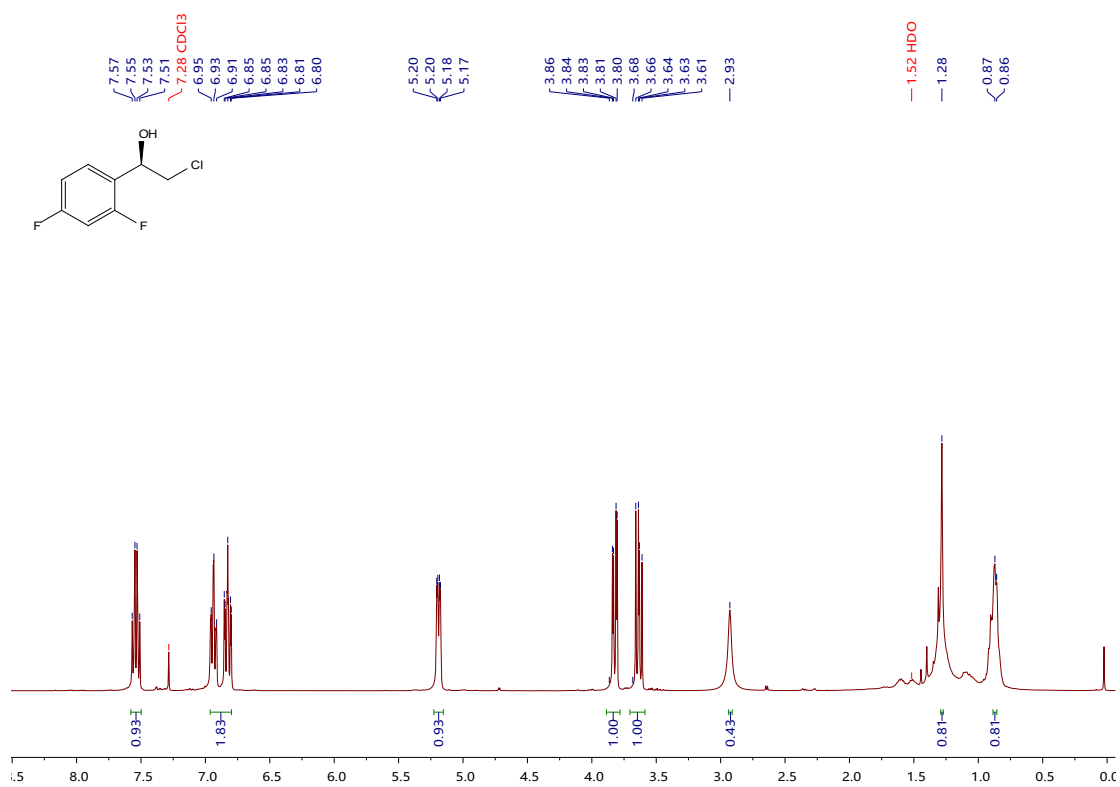
(R)-1-(4-bromophenyl)ethan-1-ol 11b



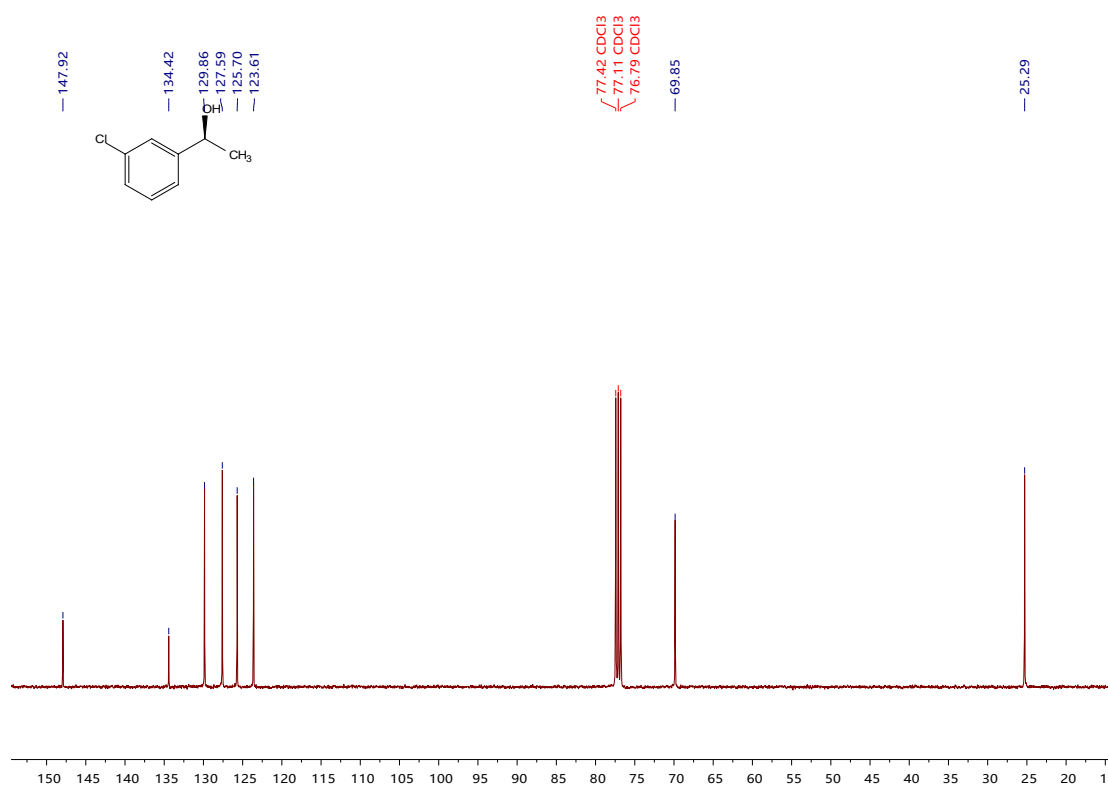
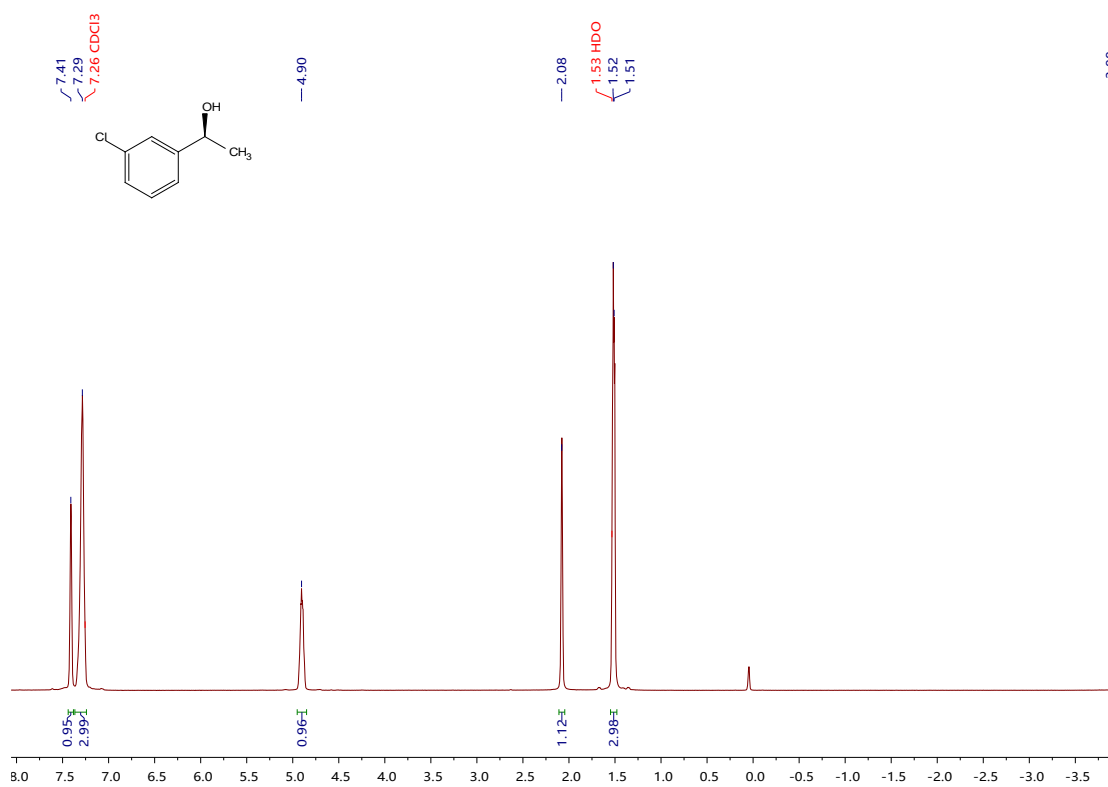
(R)-1-(2-bromo-4-fluorophenyl)ethanol 12b



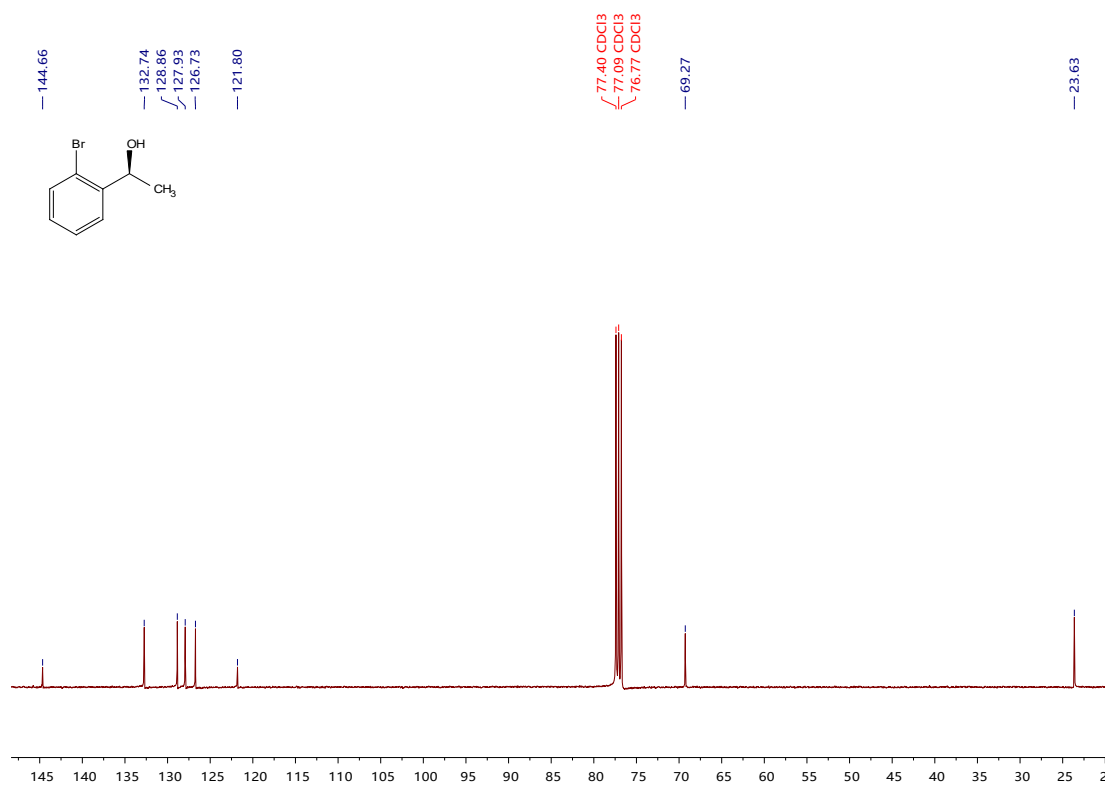
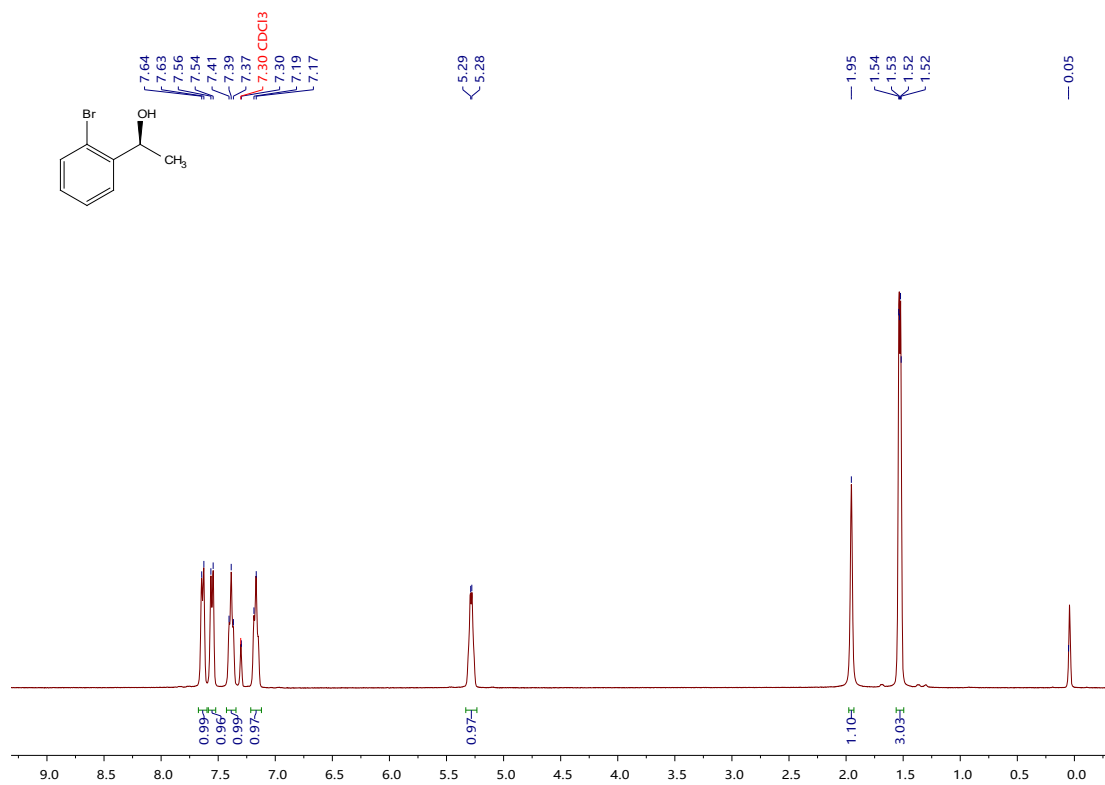
(S)-2-chloro-1-(2,4-difluorophenyl)ethanol **13b**



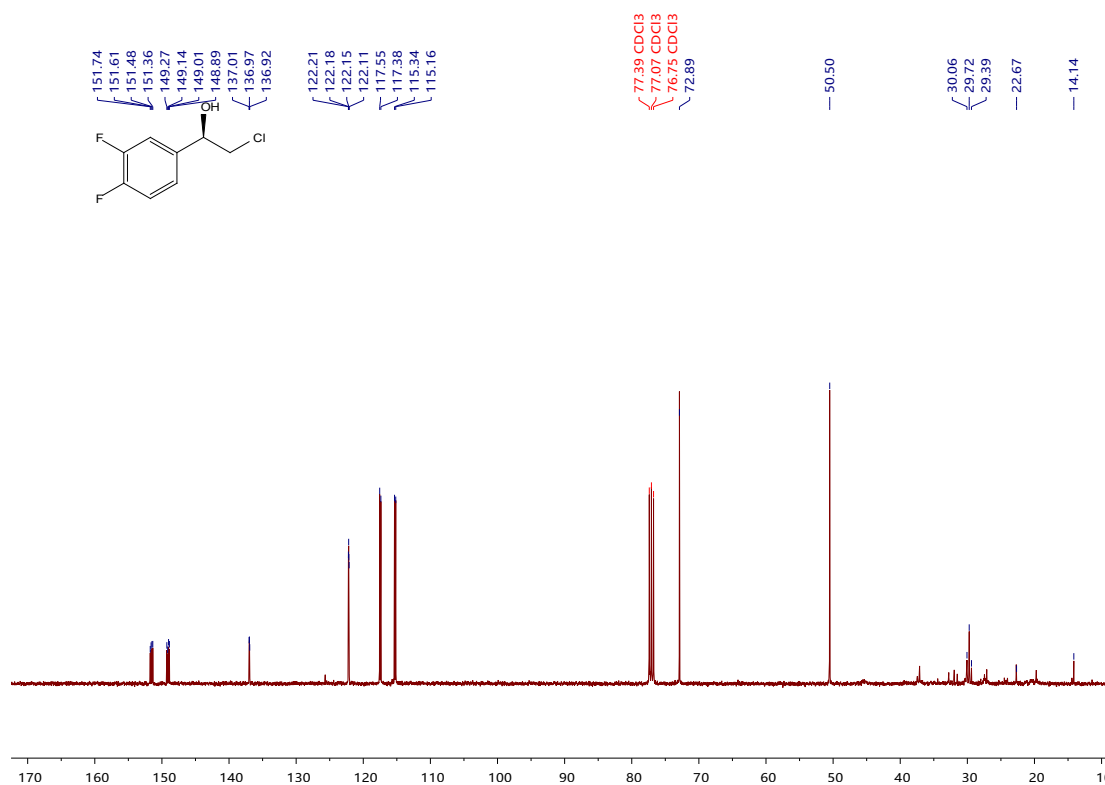
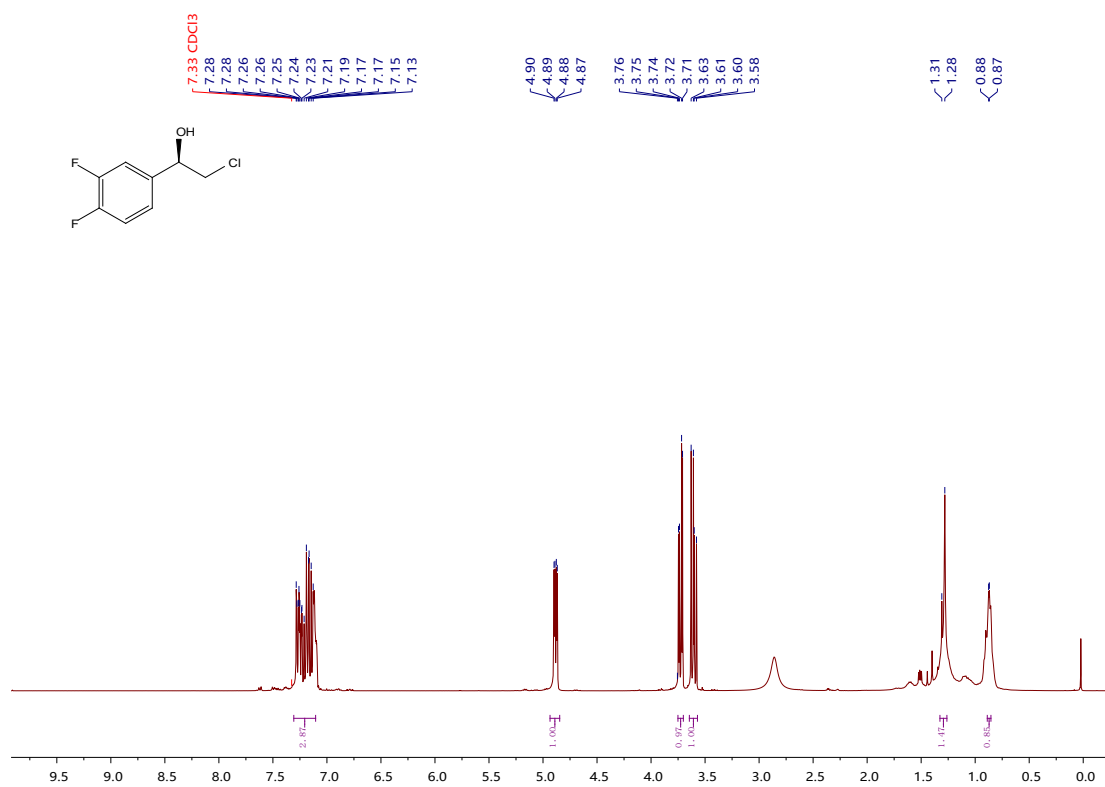
(S)-1-(3-chlorophenyl)ethan-1-ol **14b**



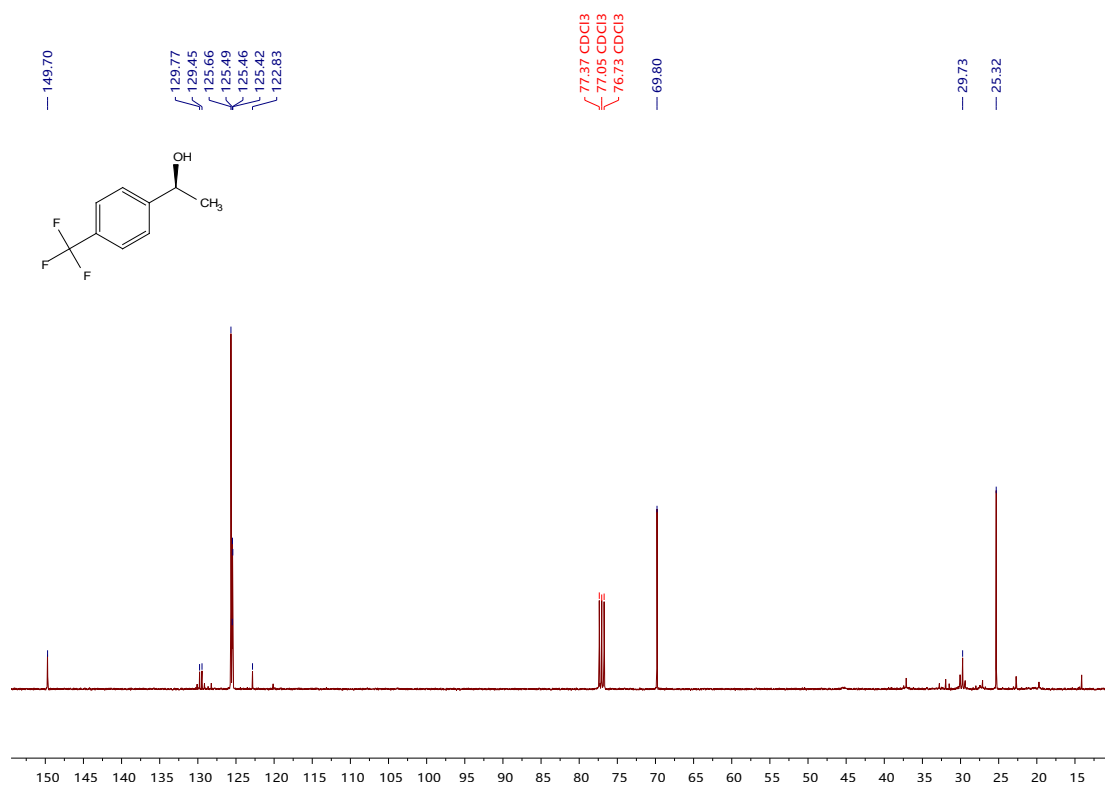
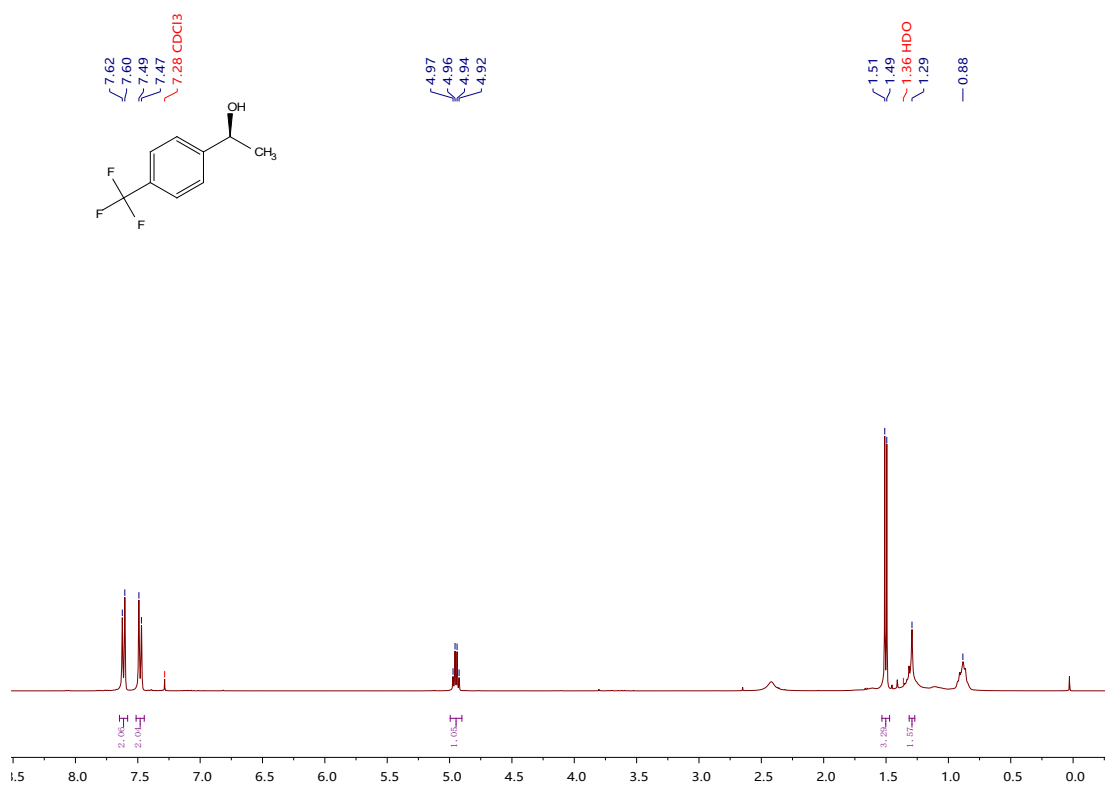
(R)-1-(2-bromophenyl)ethan-1-ol **15b**



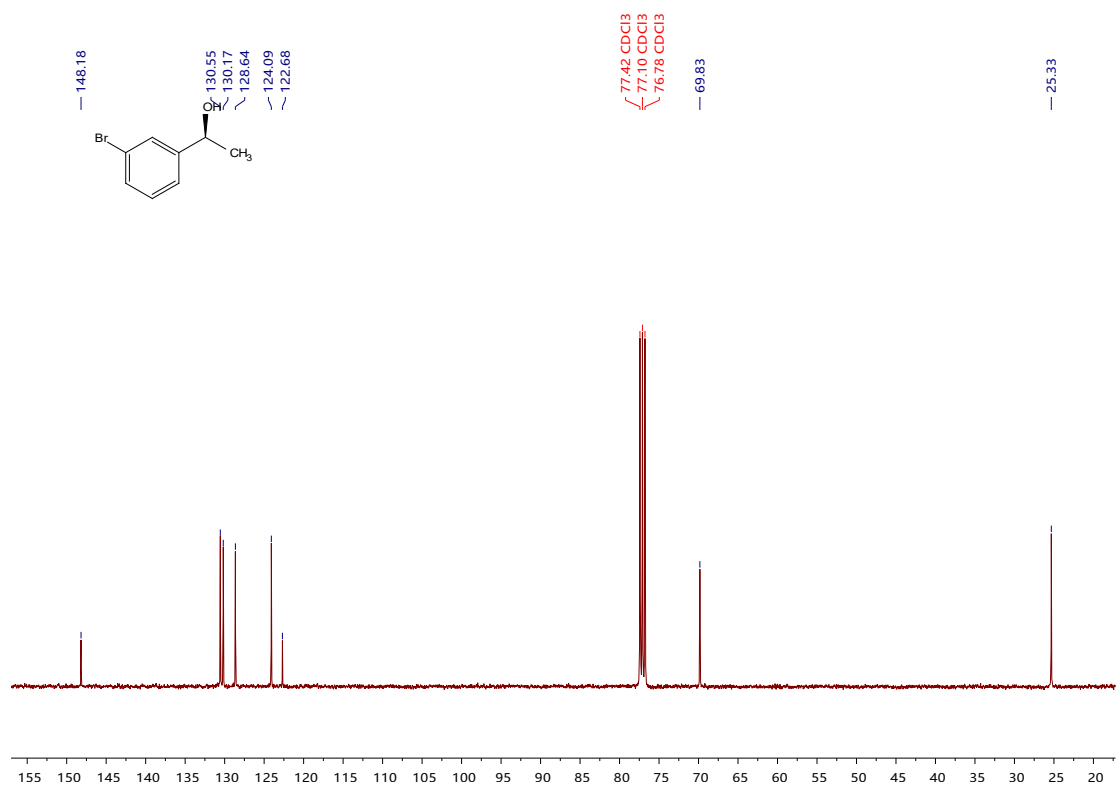
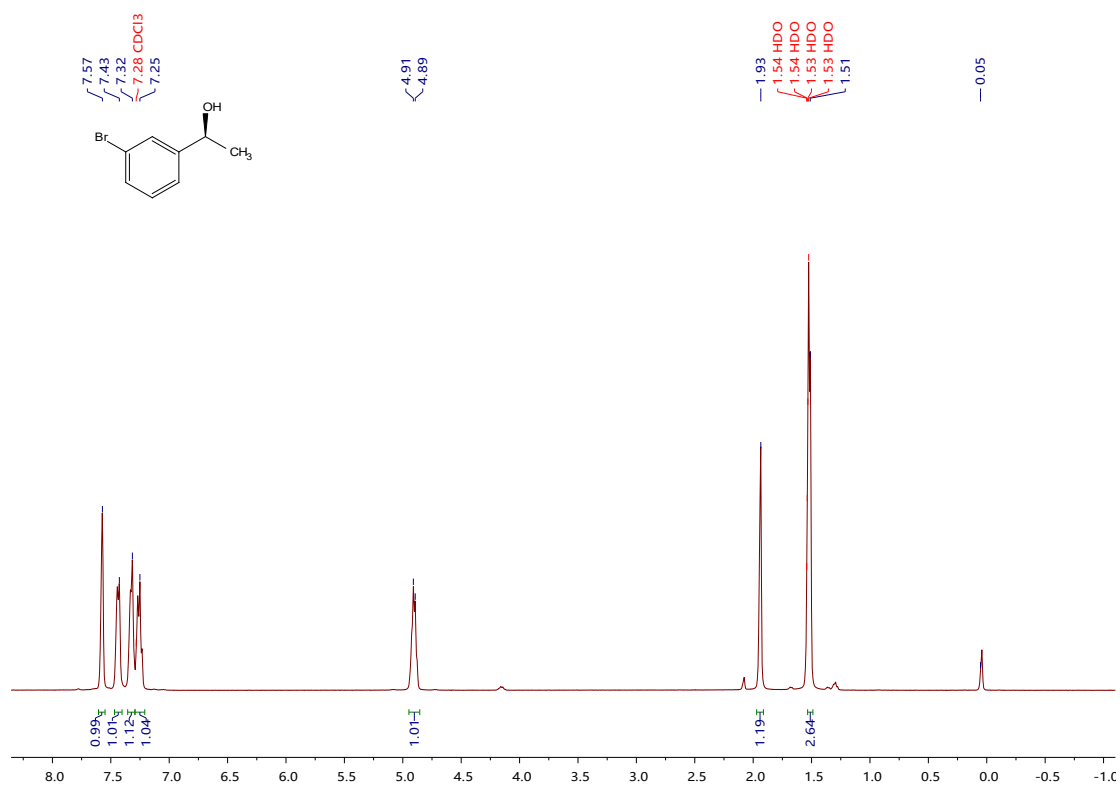
(S)-2-chloro-1-(3,4-difluorophenyl)-1-ethanol **16b**



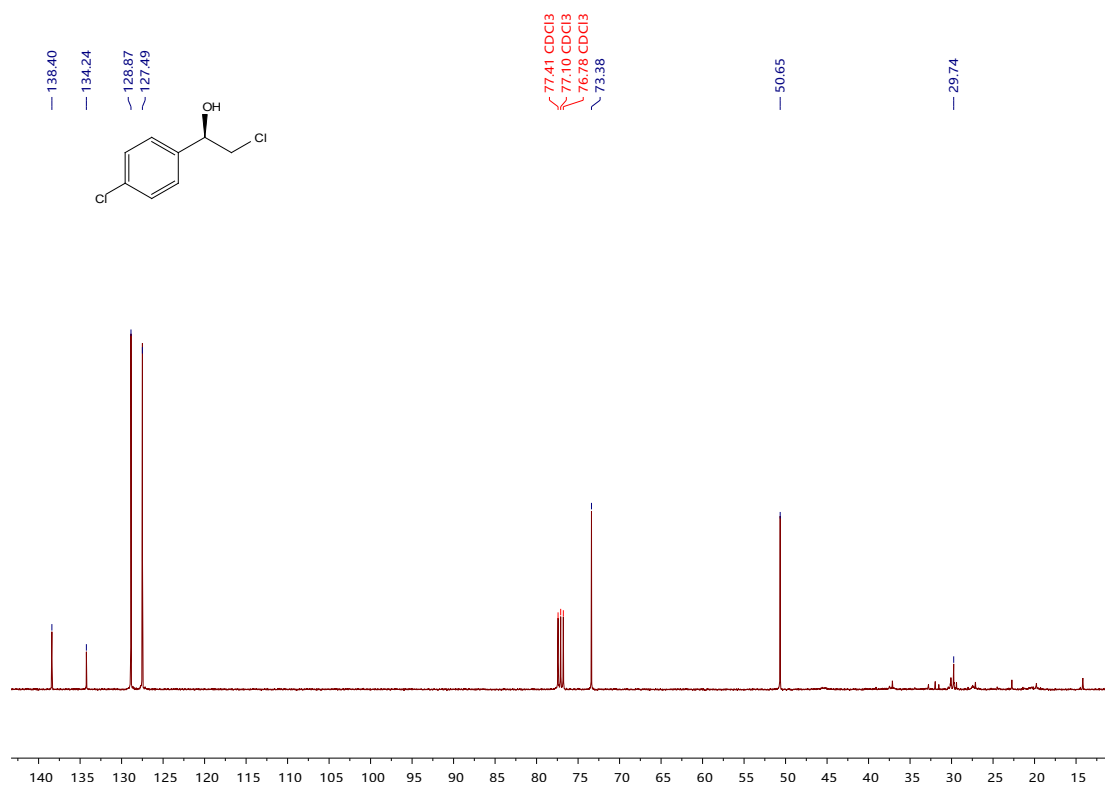
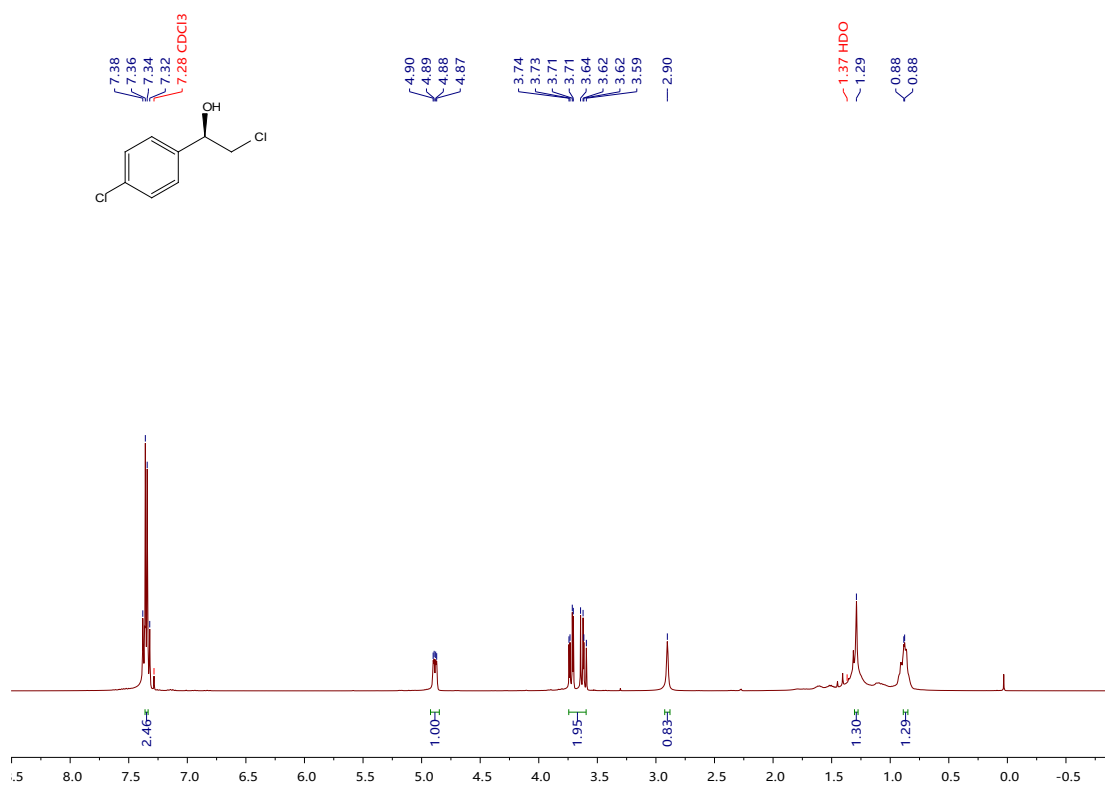
(S)-1-[4-(Trifluoromethyl)phenyl]ethan-1-ol **17b**



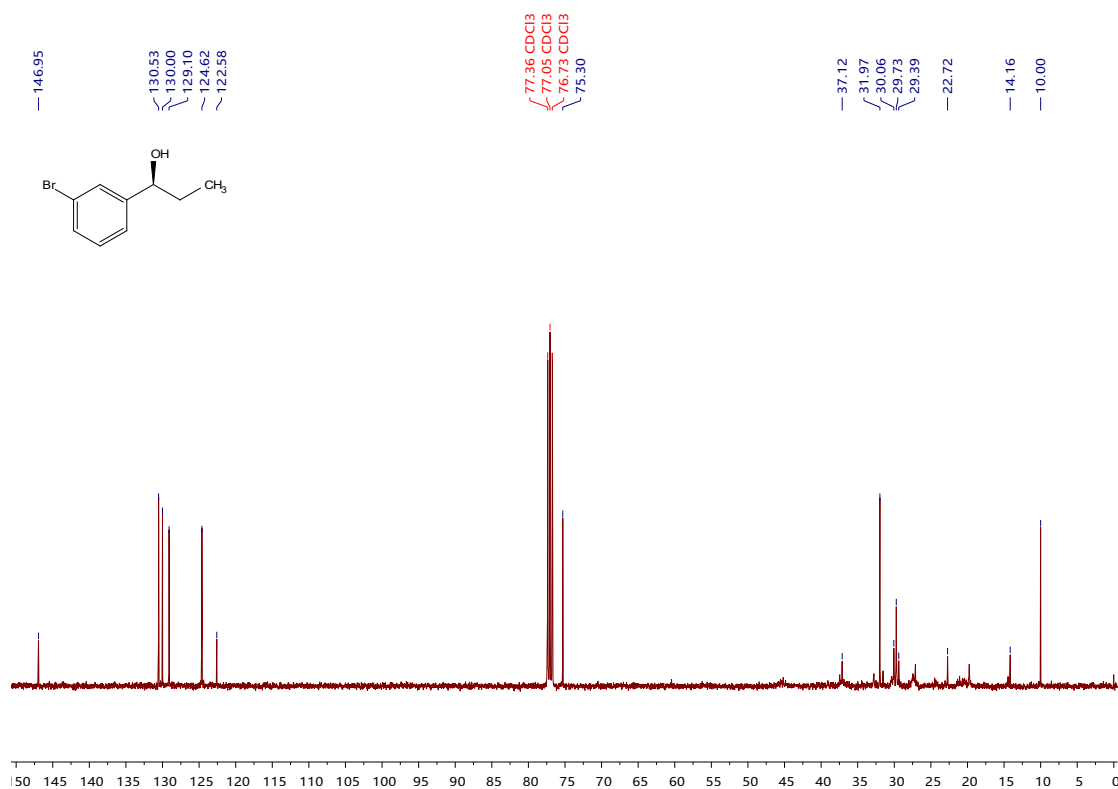
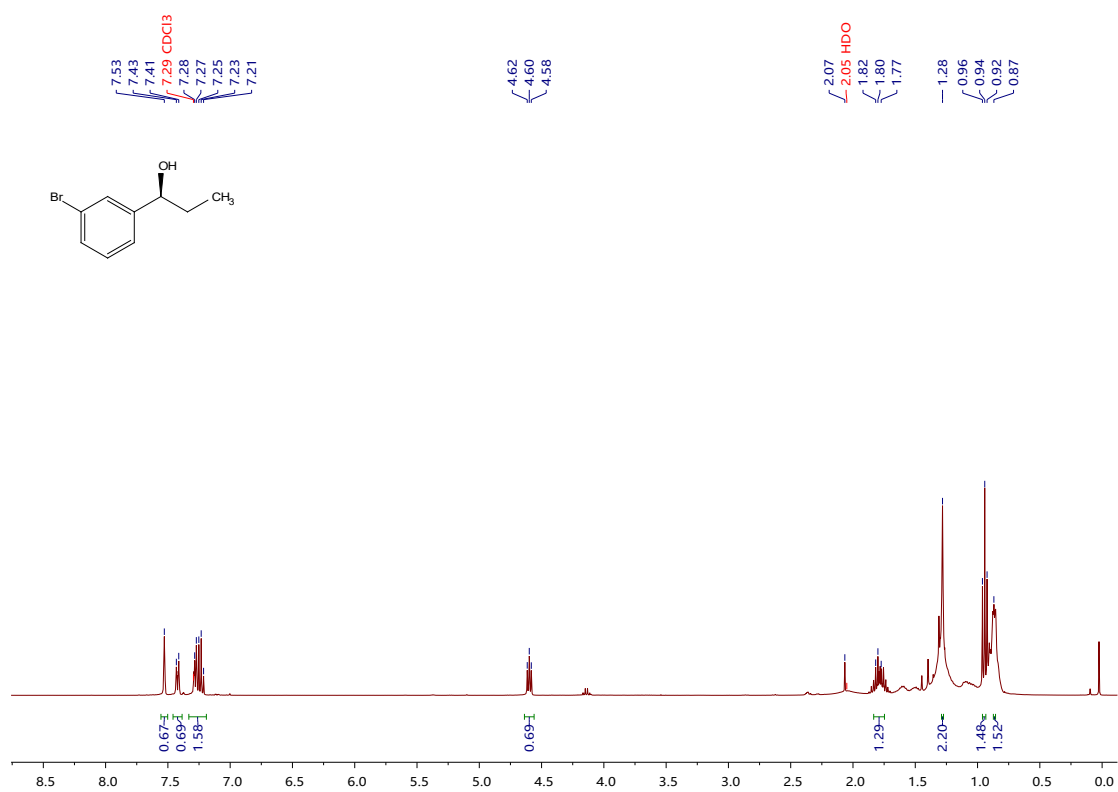
(R)-1-(3-bromophenyl)ethan-1-ol 18b



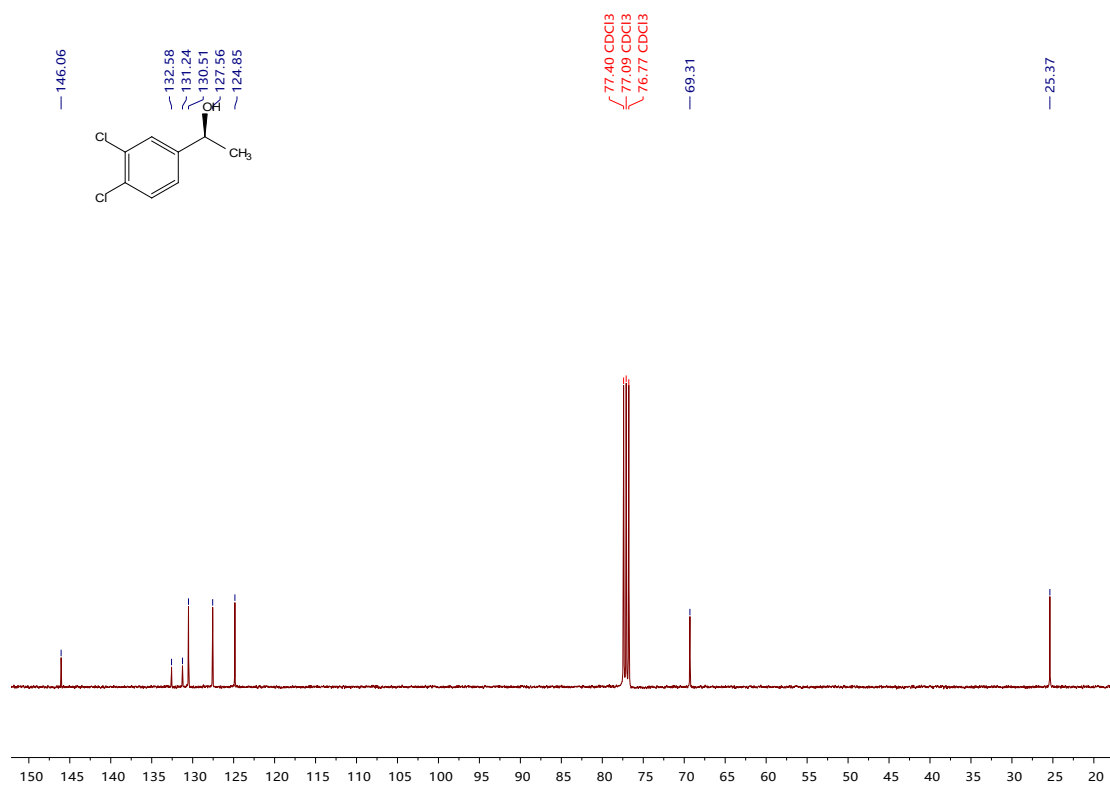
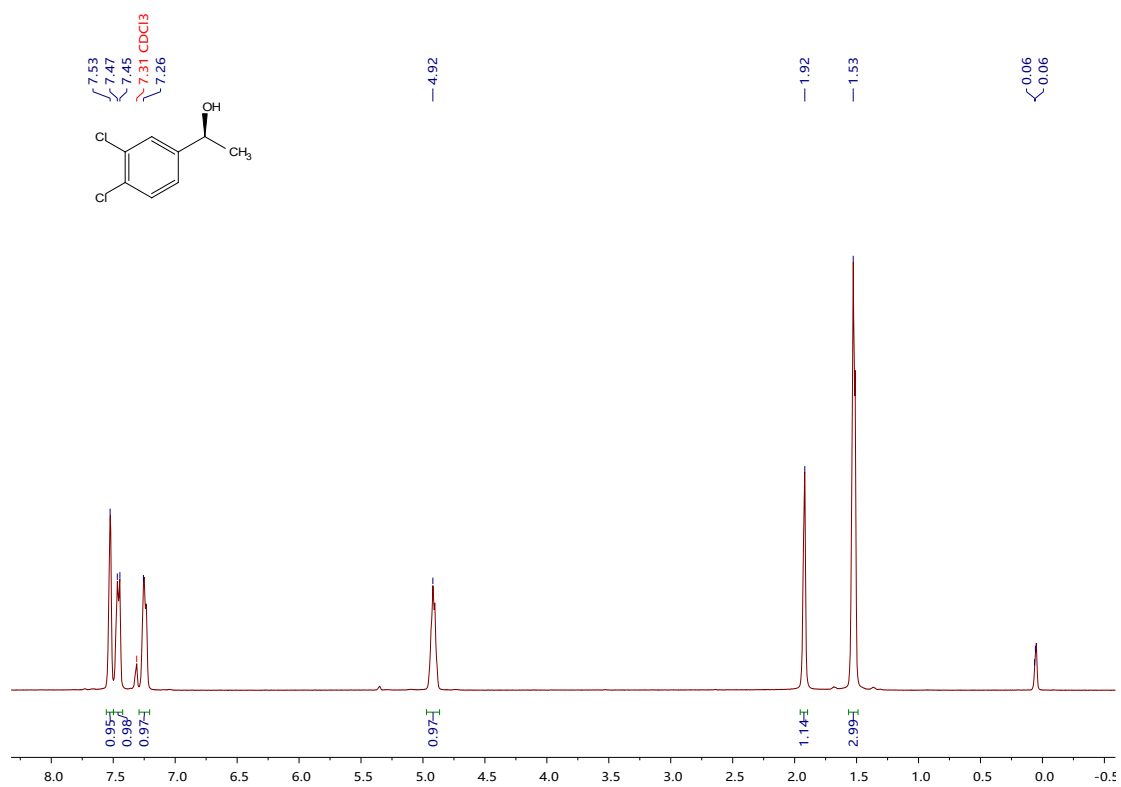
(S)-2-chloro-1-(4-chlorophenyl)ethanol **19b**



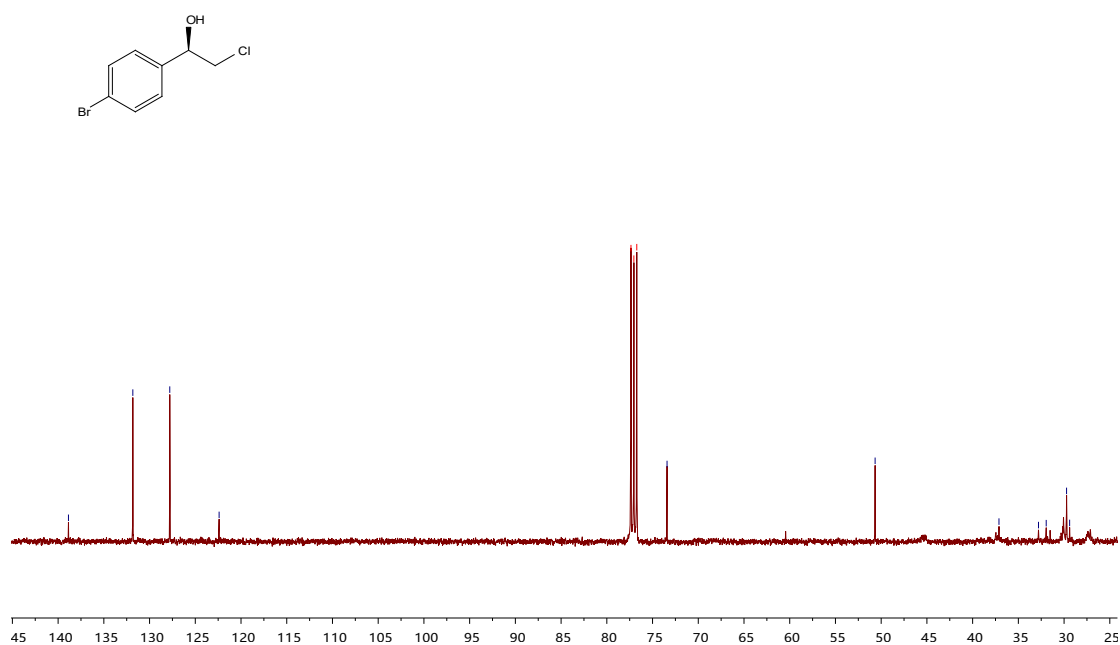
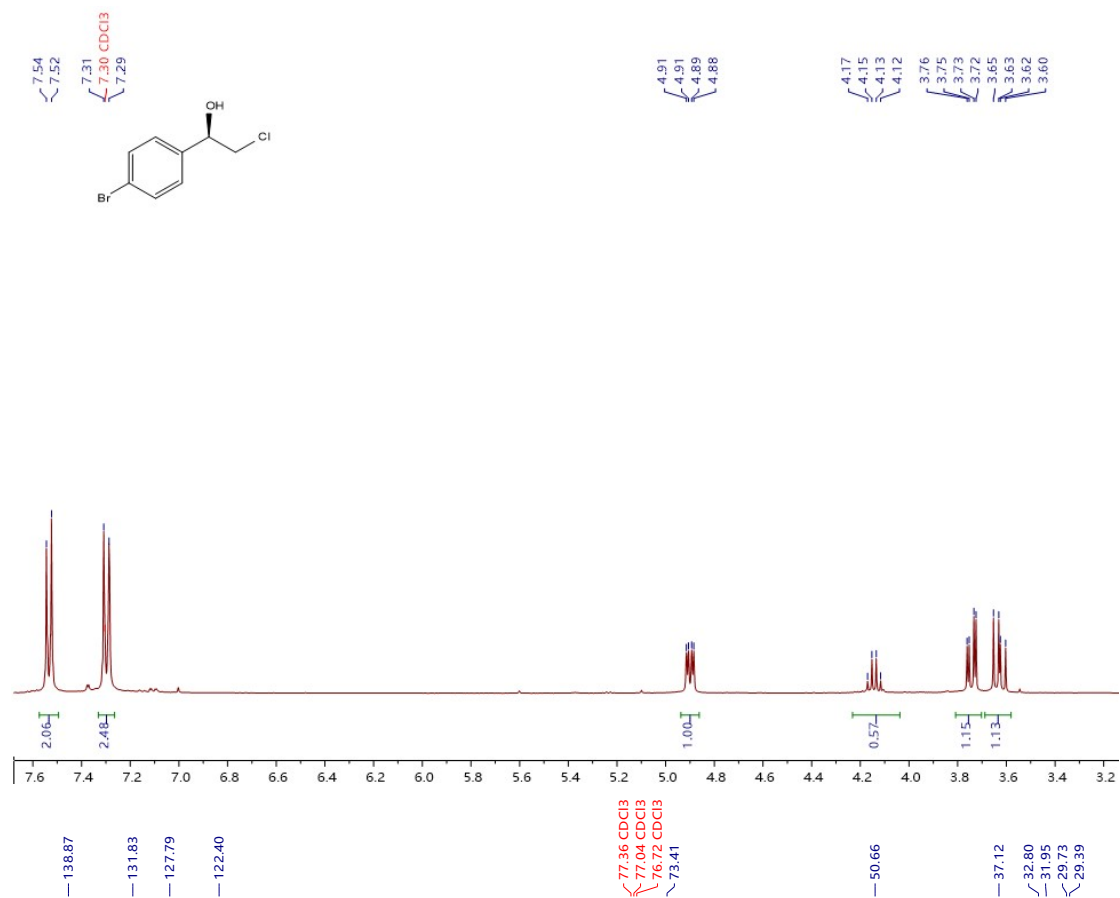
(R)-1-(3-bromophenyl)propanol **20b**



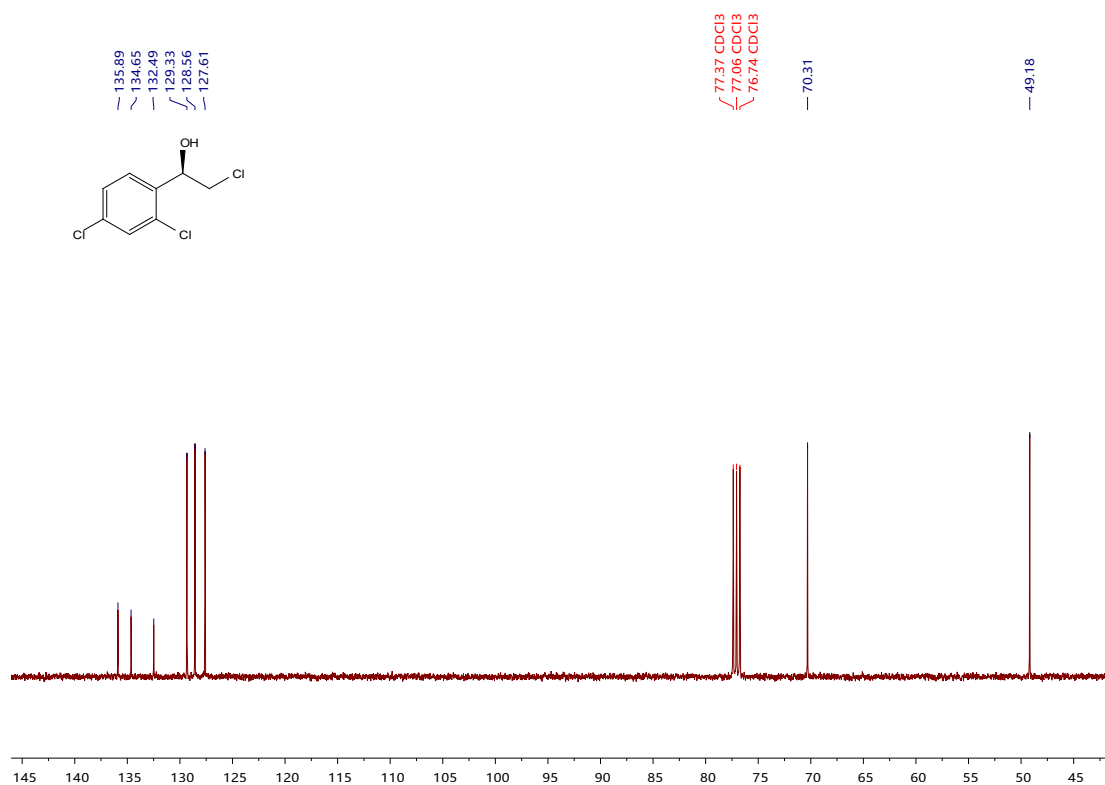
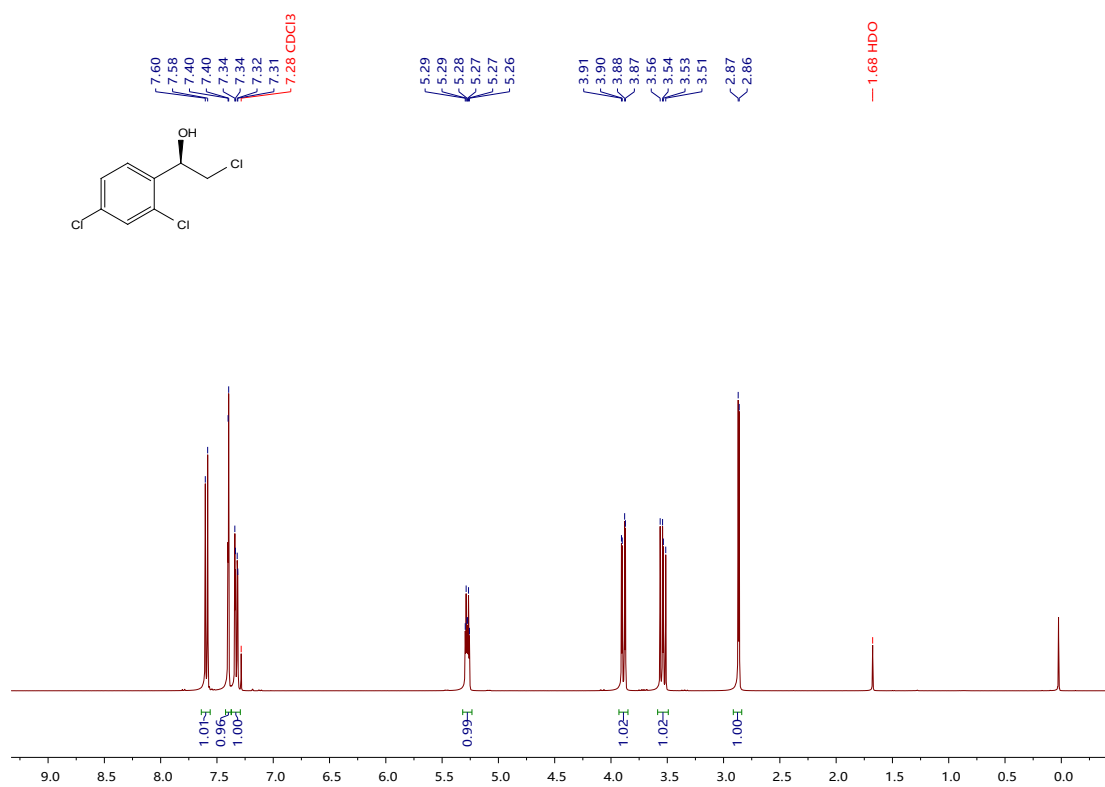
(R)-1-(3,4-dichlorophenyl)ethan-1-ol 21b



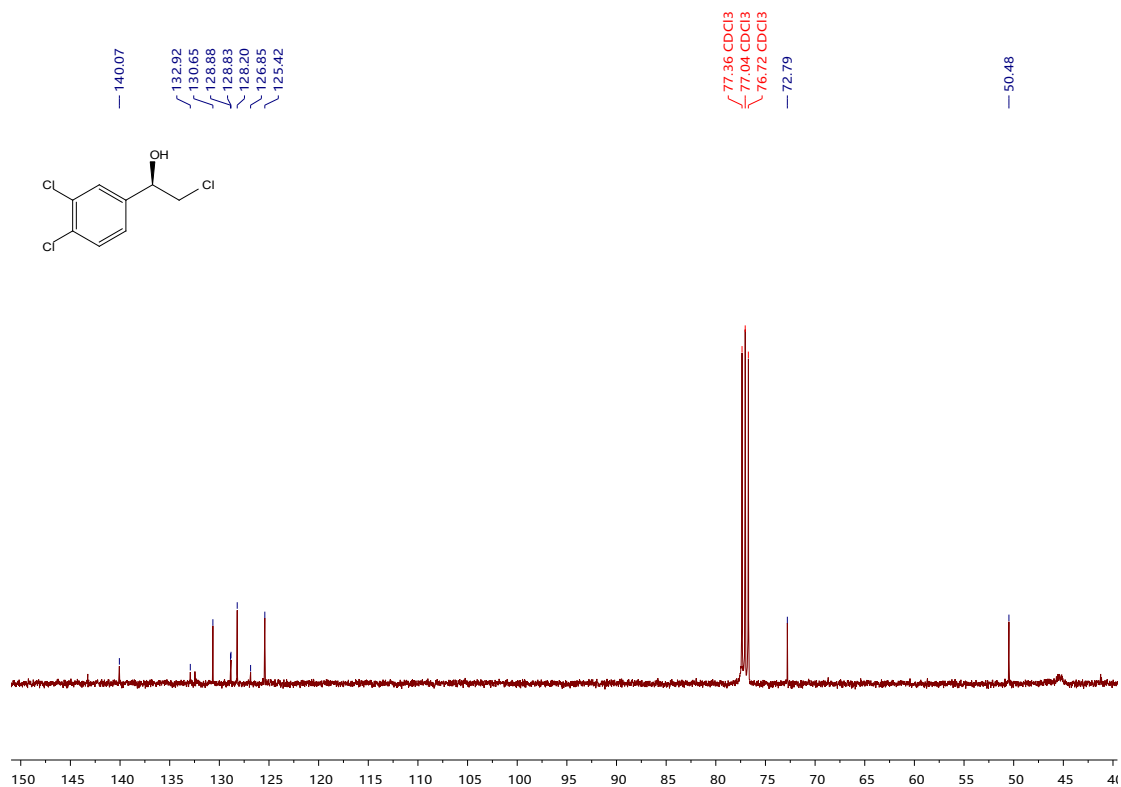
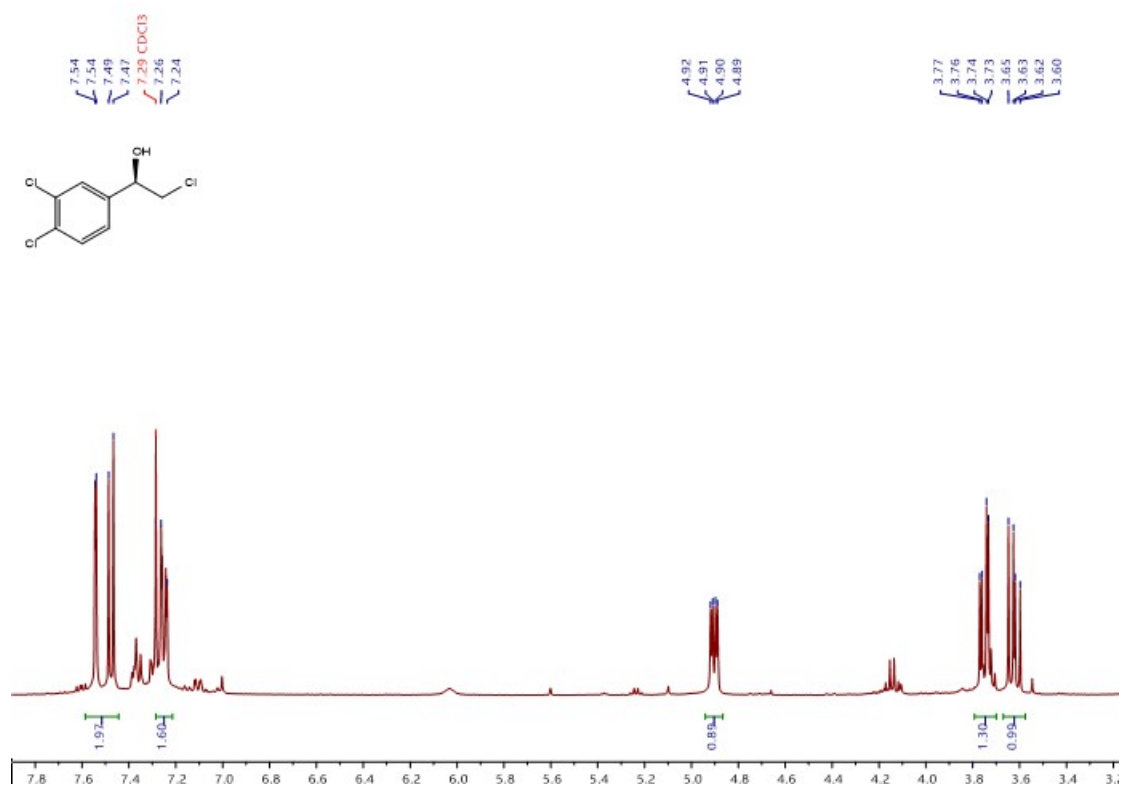
(S)-1-(4-bromophenyl)-2-chloroethanol **22b**



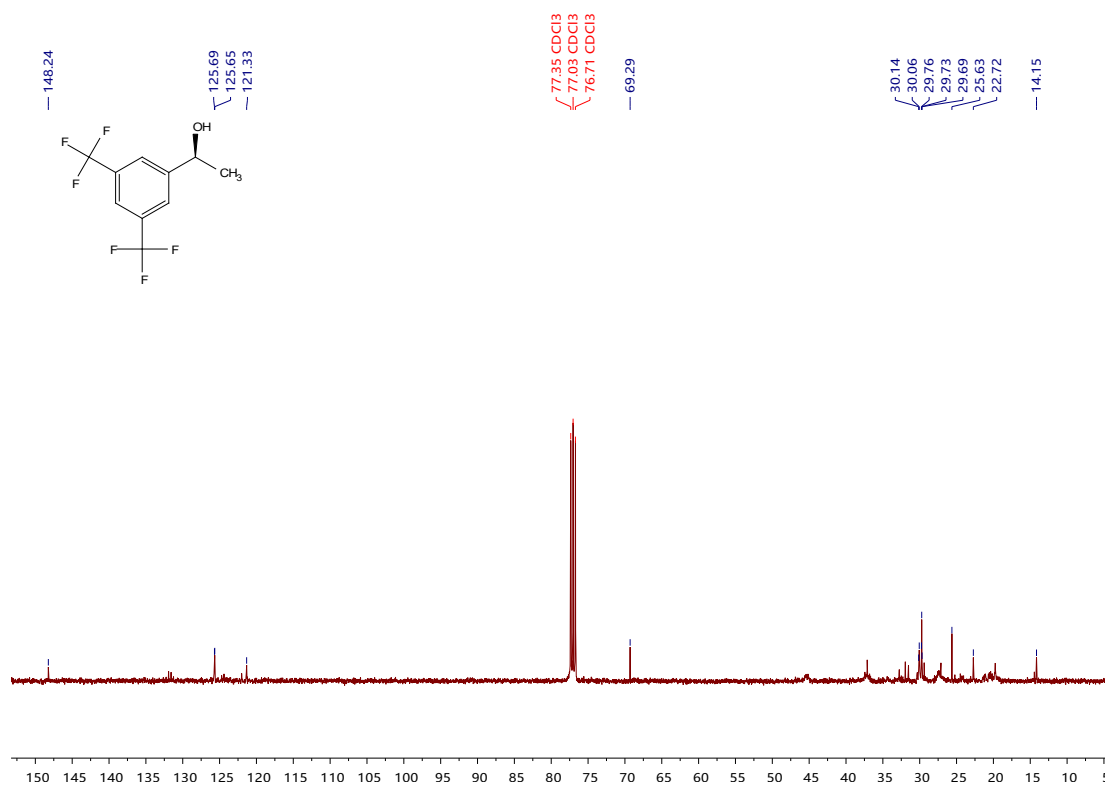
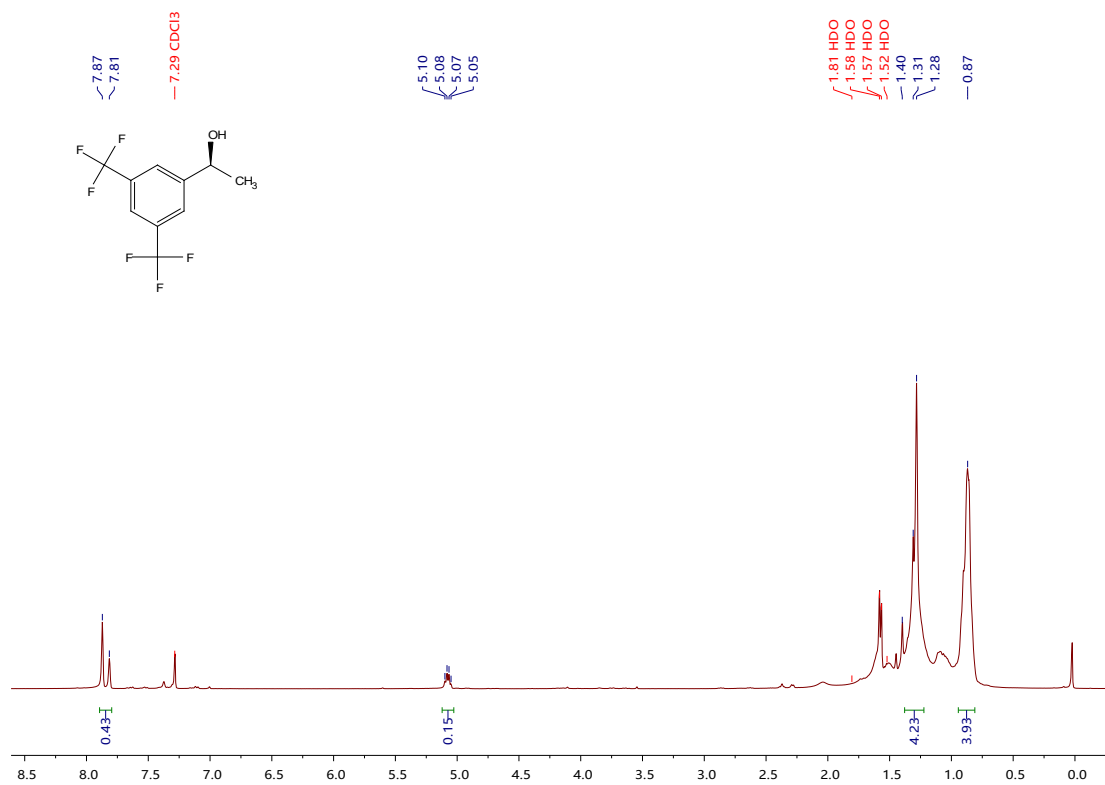
(R)-2-chloro-1-(2,4-dichlorophenyl)ethan-1-ol 23b



(S)-2-chloro-1-(3,4-dichlorophenyl)ethan-1-ol **24b**

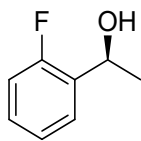


(S)-1-[3,5-bis(trifluoromethyl)phenyl]ethanol **25b**

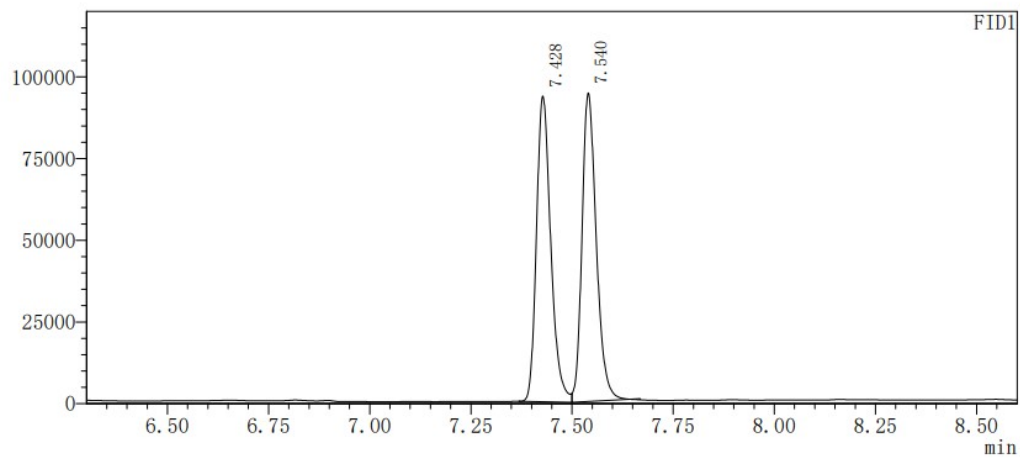


GC traces for productions

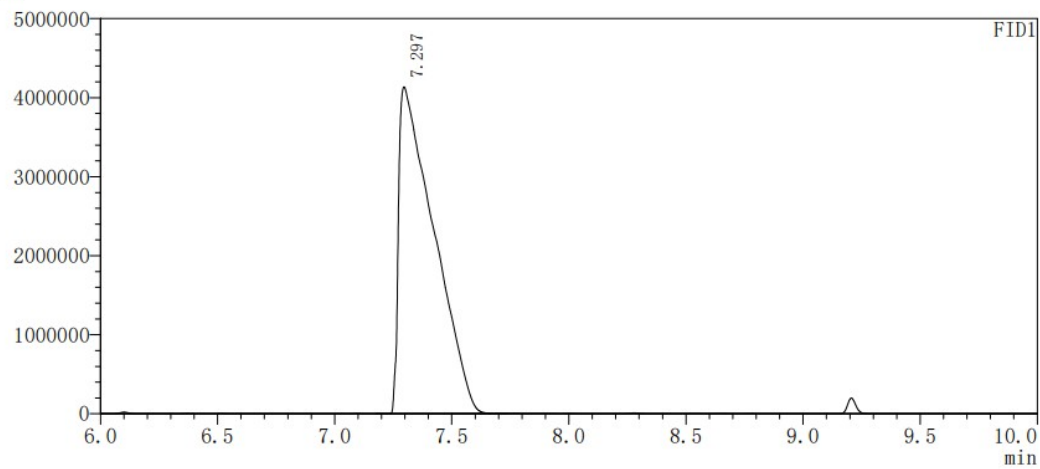
(*S*)-1-(2-fluorophenyl)ethan-1-ol **1b**



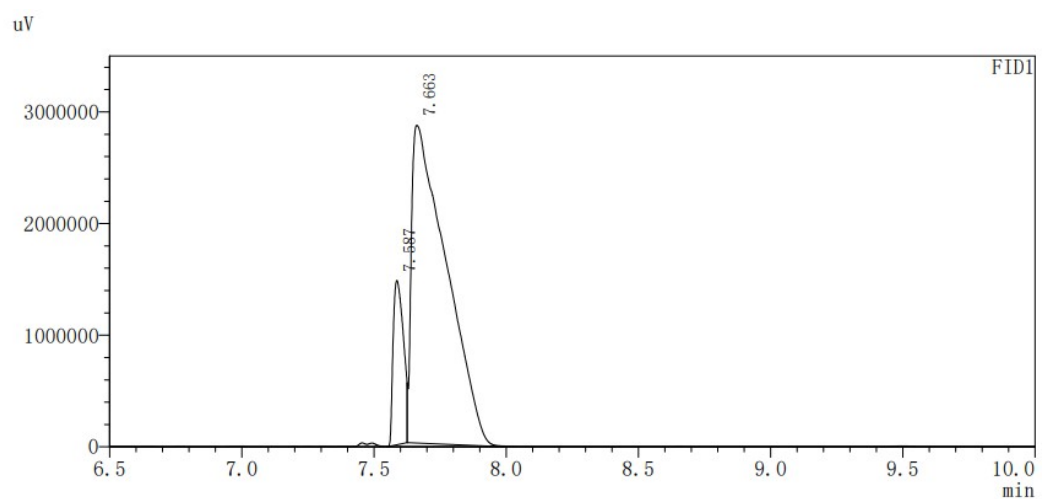
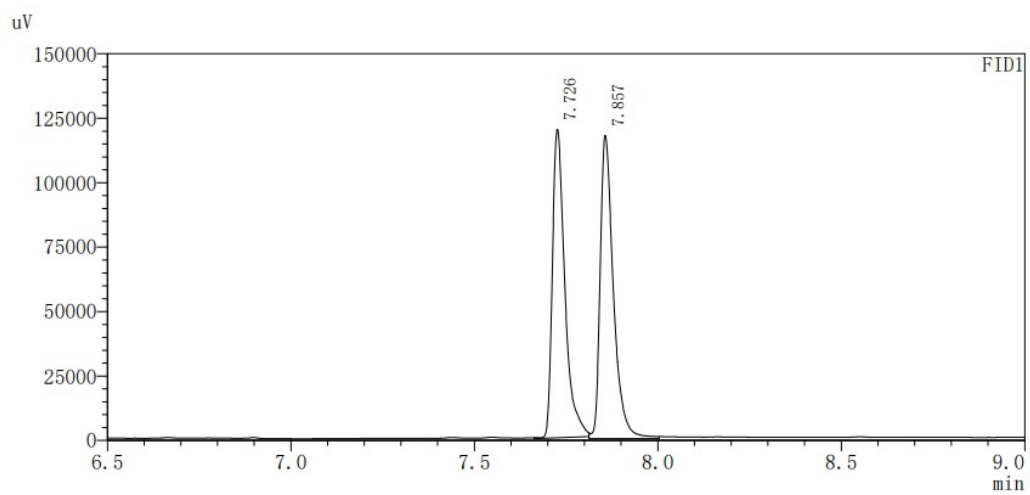
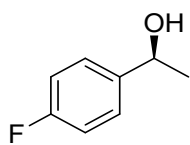
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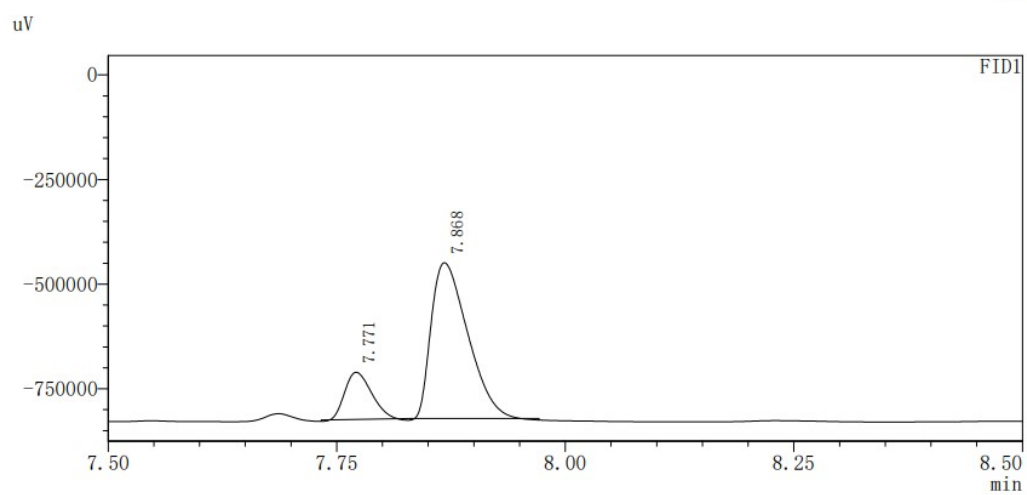
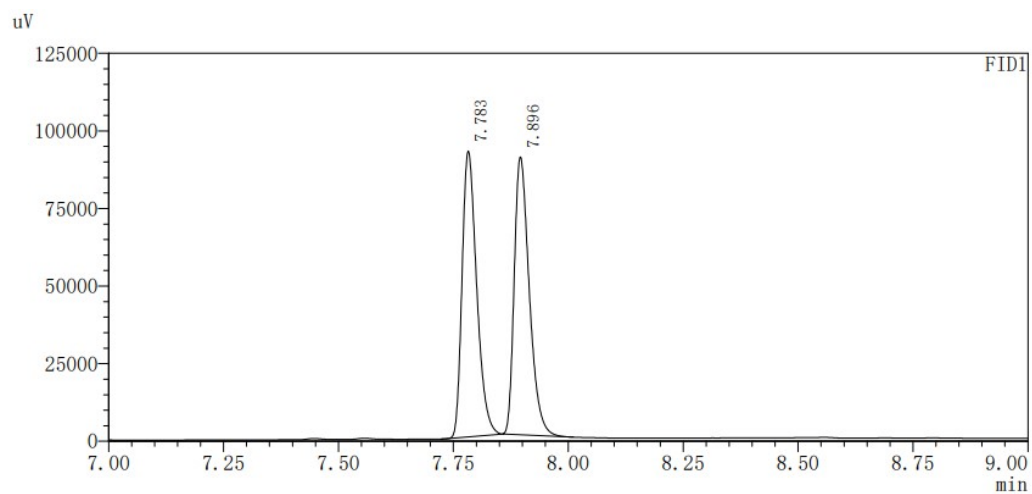
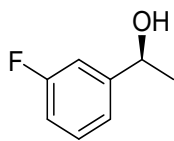
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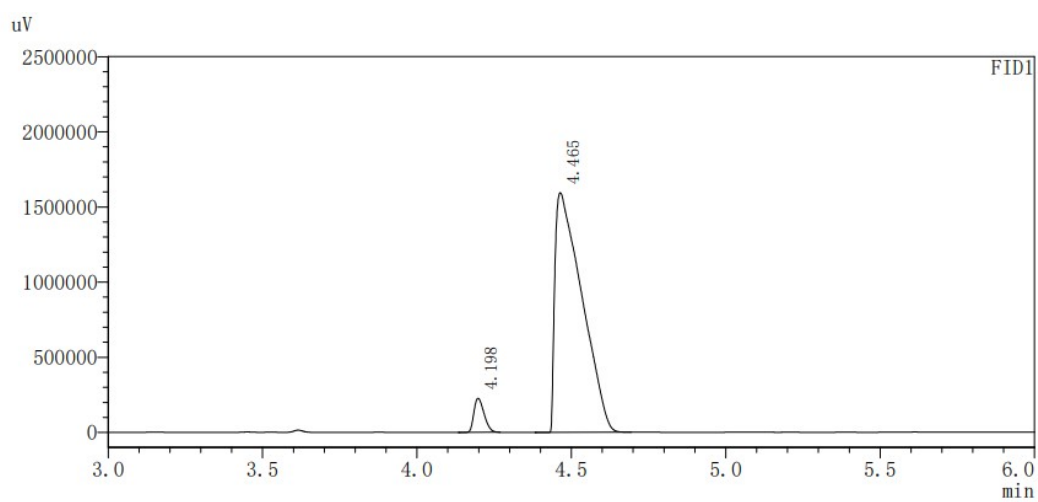
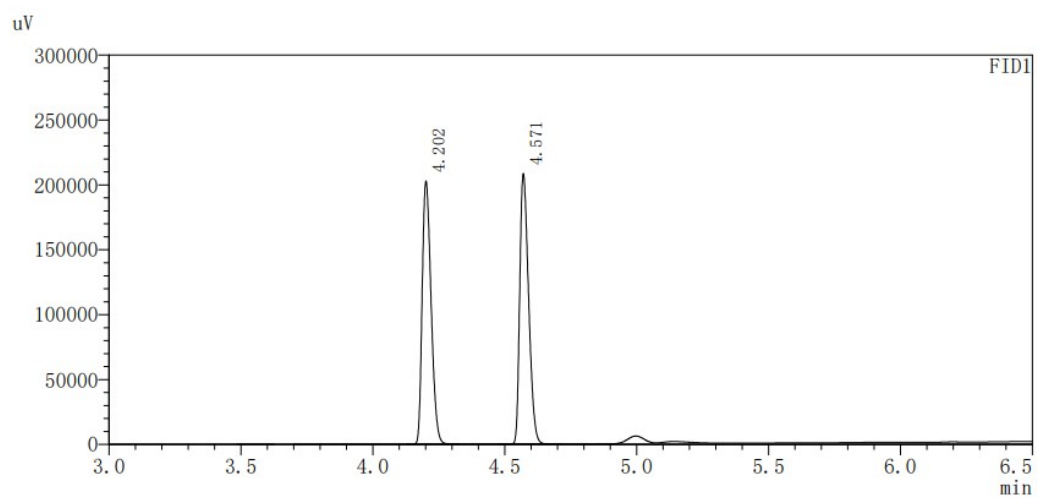
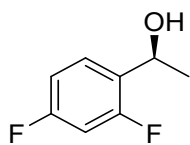
(S)-1-(4-fluorophenyl)ethan-1-ol **2b**



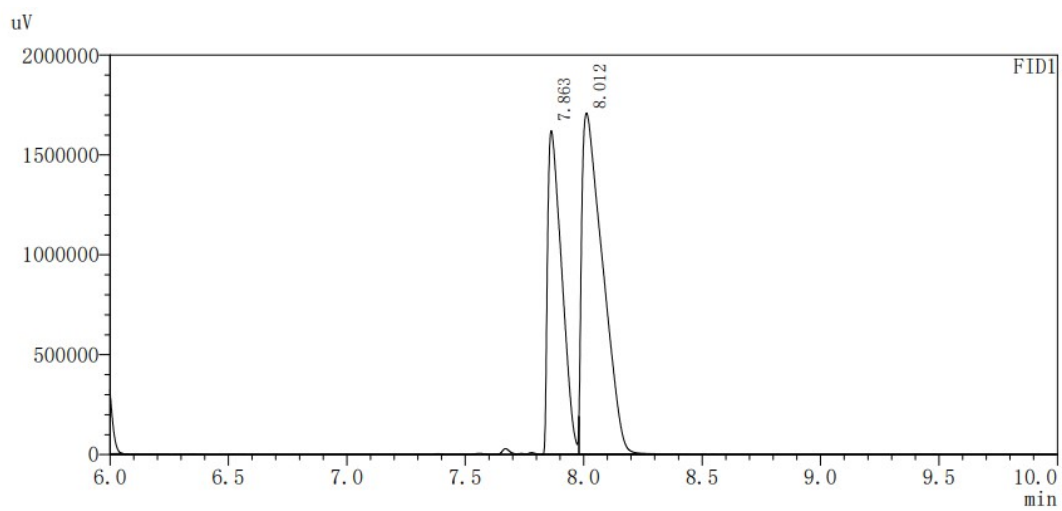
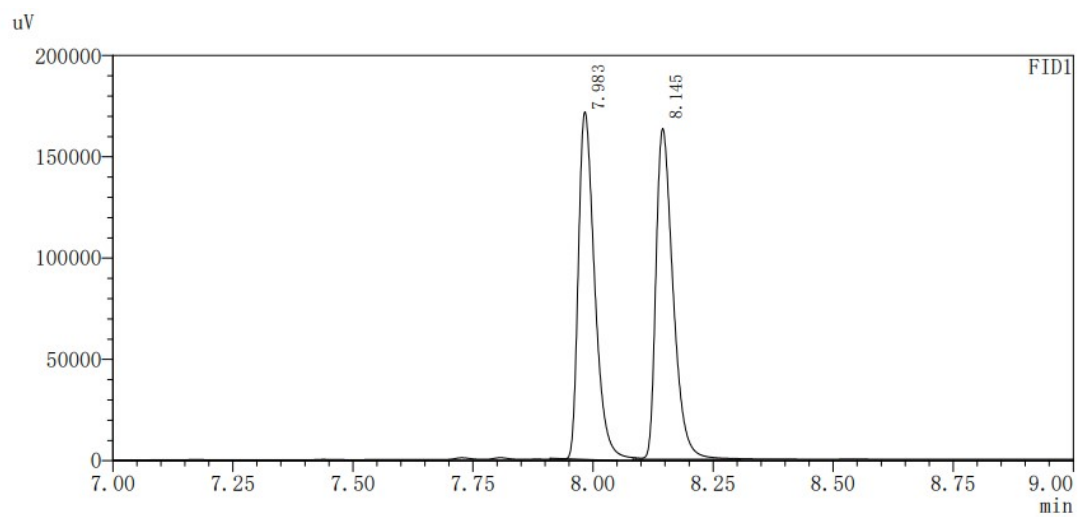
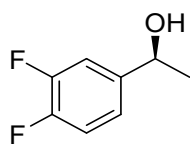
(S)-1-(3-fluorophenyl)ethan-1-ol **3b**



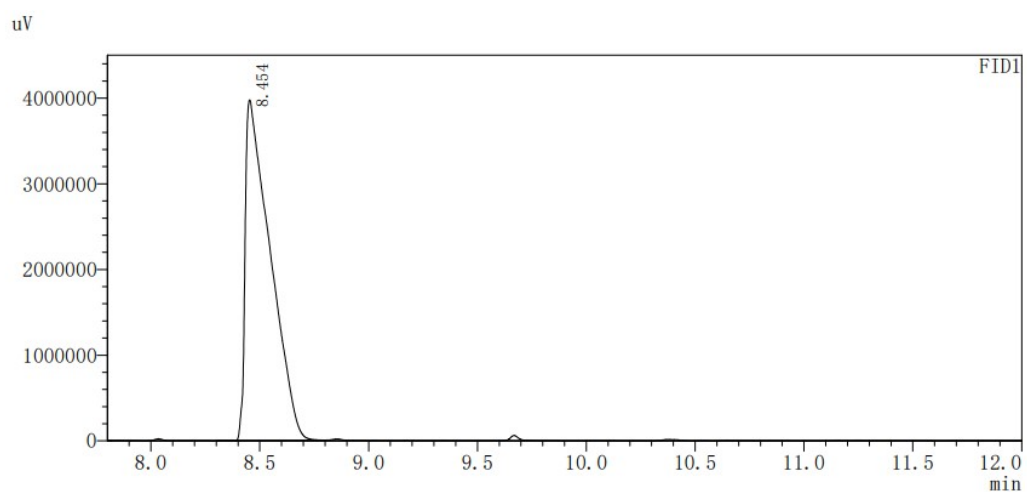
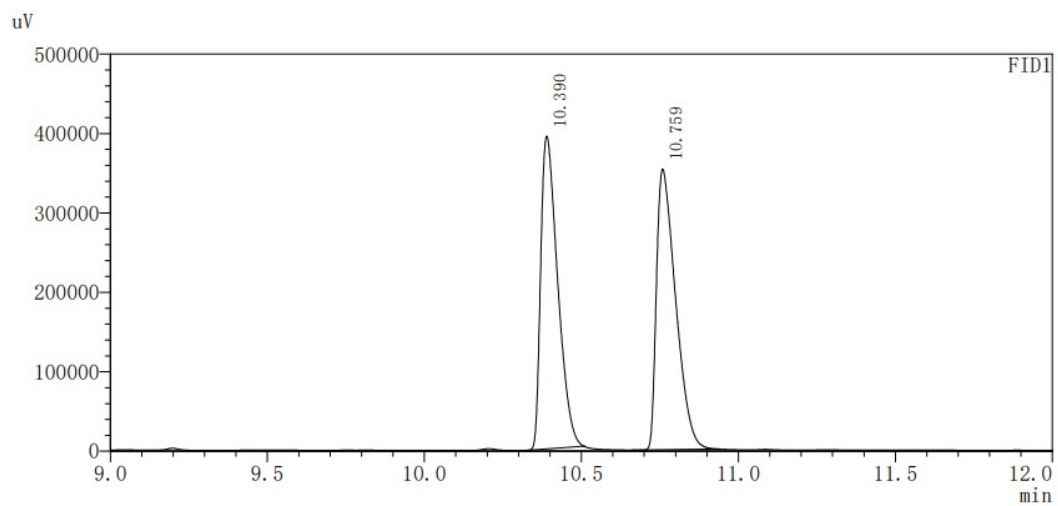
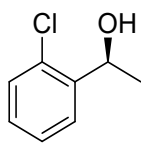
(R)-1-(2,4-difluorophenyl)ethanol **4b**



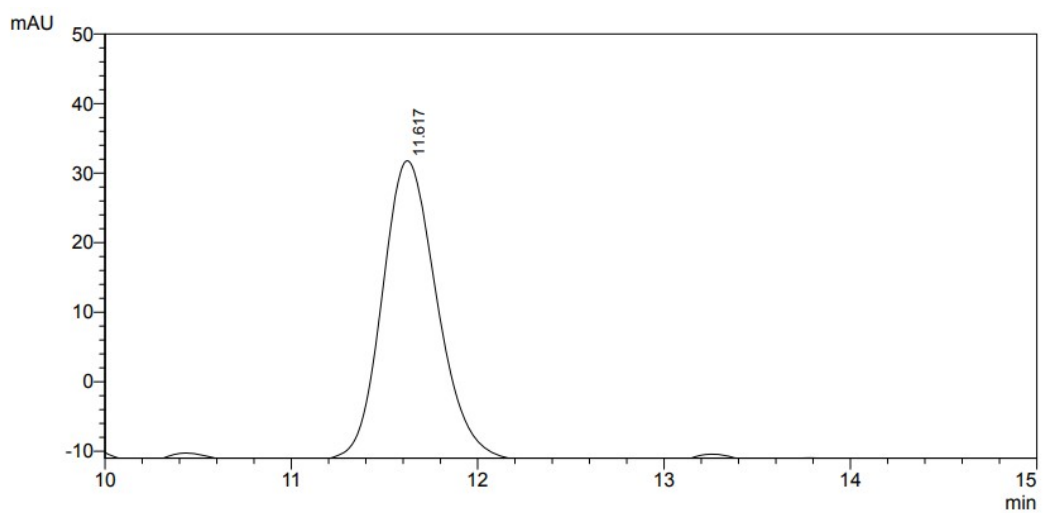
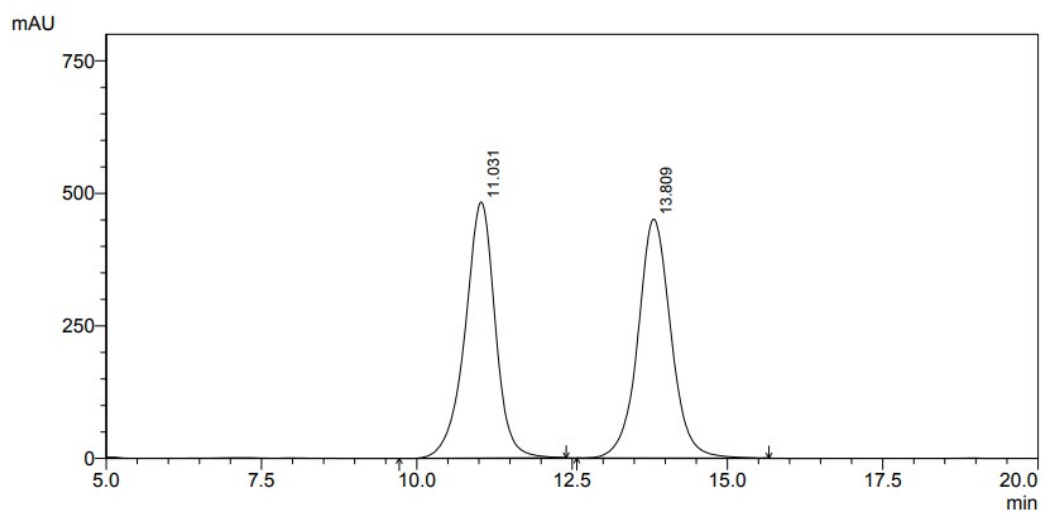
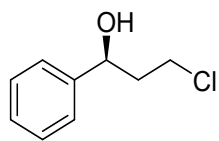
(R)-1-(3,4-difluorophenyl)ethan-1-ol **5b**



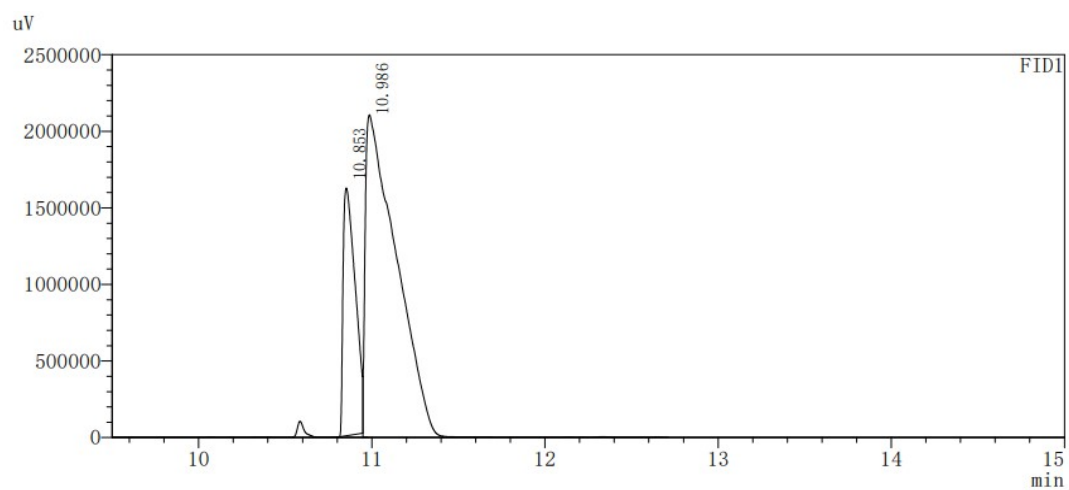
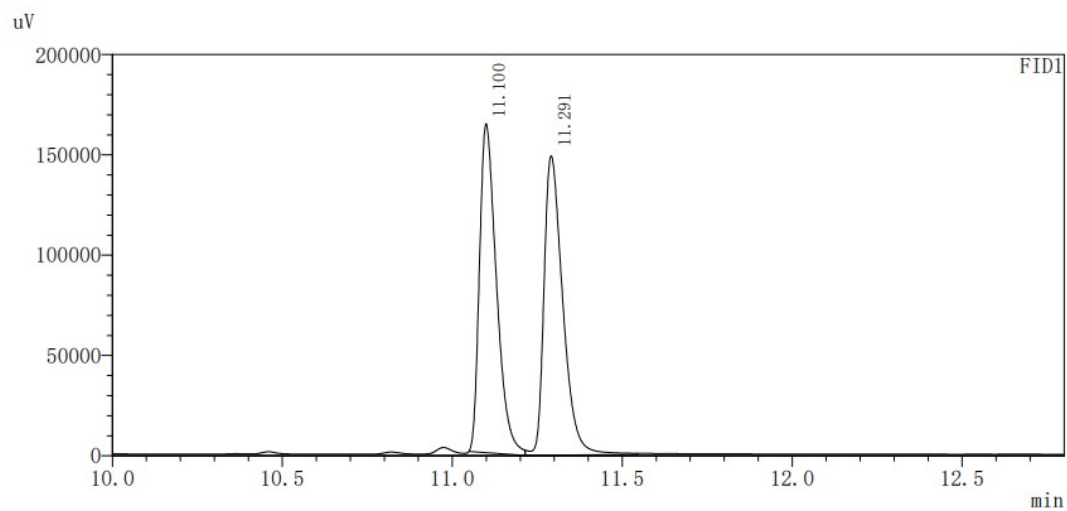
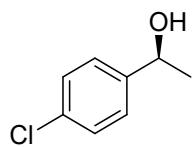
(S)-1-(2-chlorophenyl)ethan-1-ol **6b**



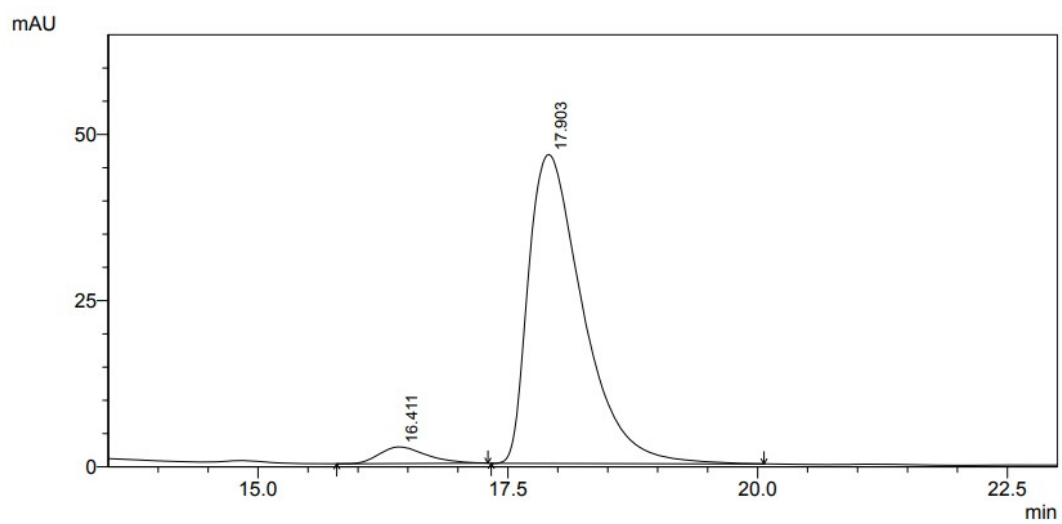
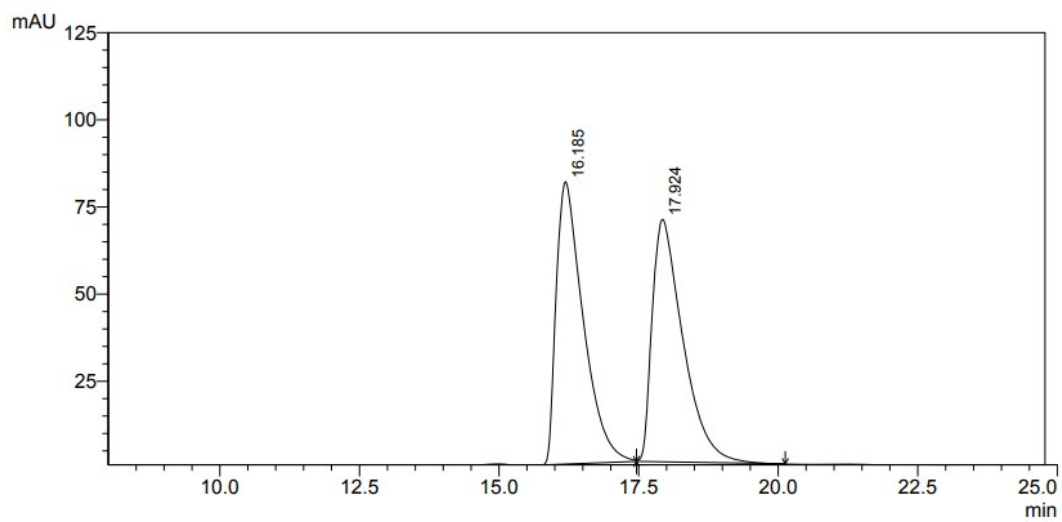
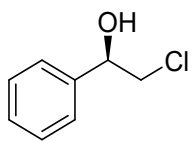
(*S*)-3-chloro-1-phenyl-1-propanol **7b**



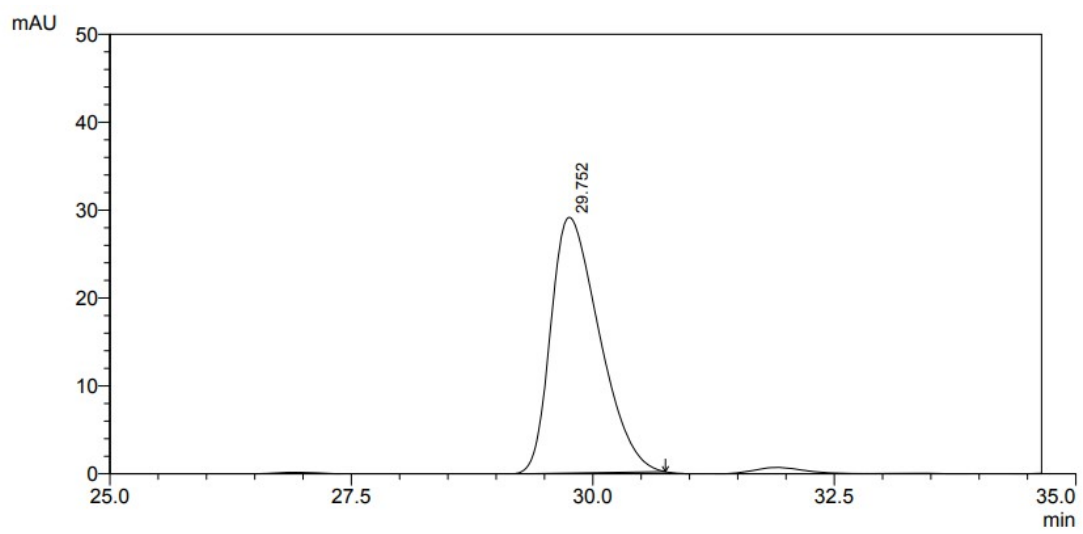
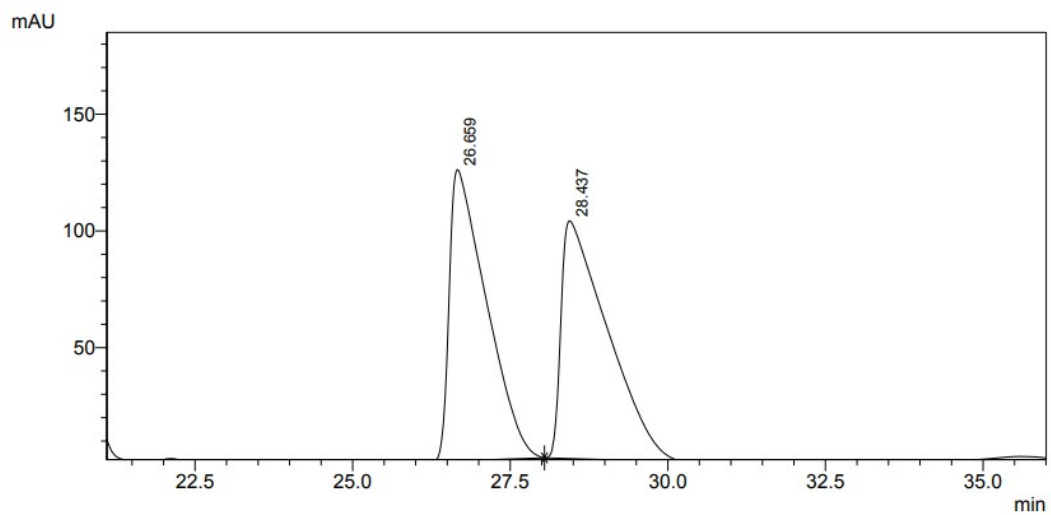
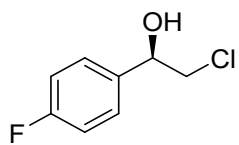
(S)-1-(4-chlorophenyl)ethan-1-ol **8b**



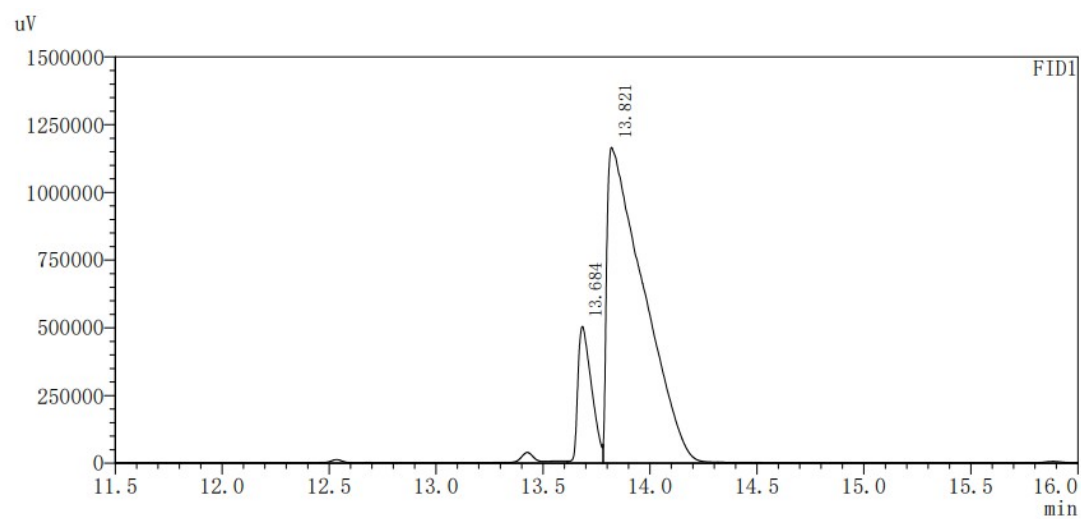
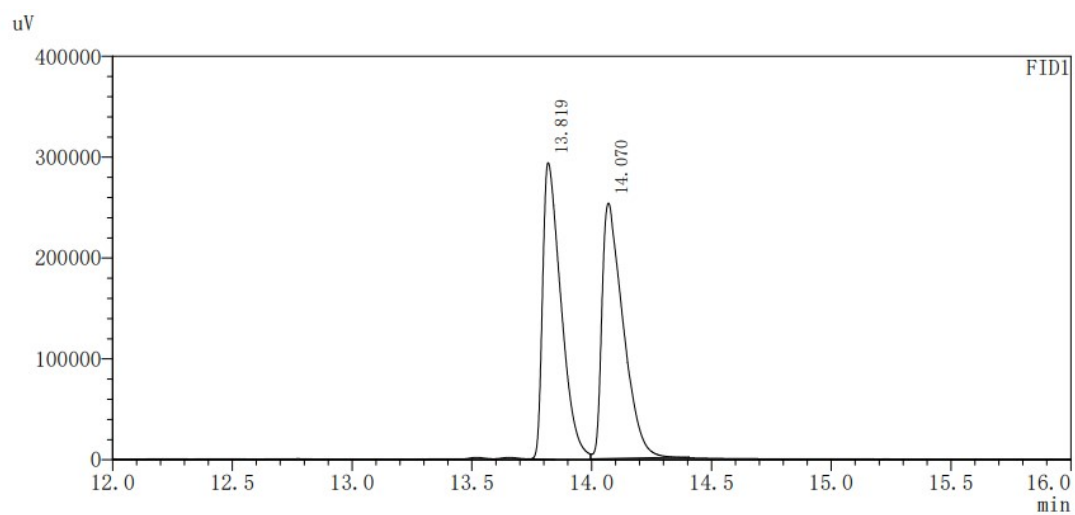
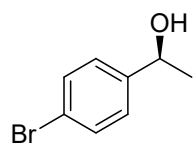
(R)-2-chloro-1-phenylethanol **9b**



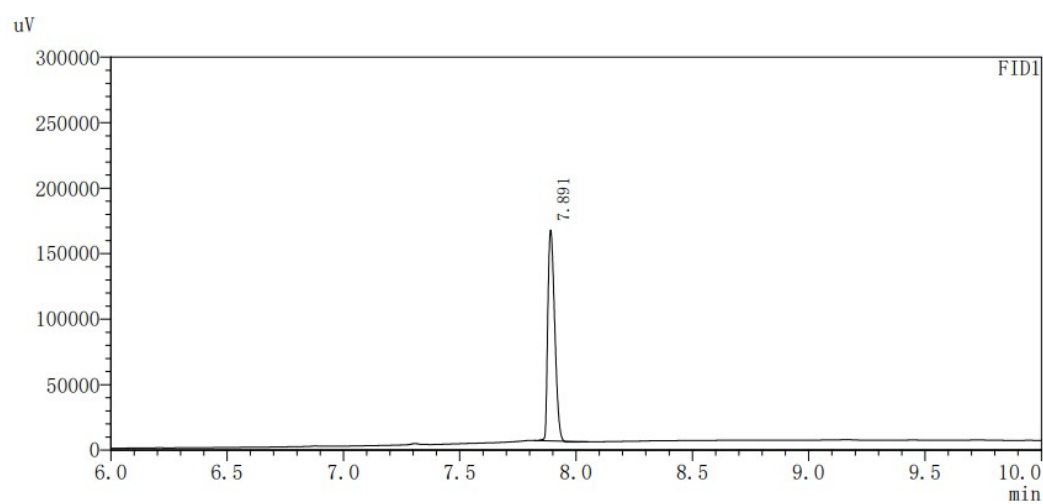
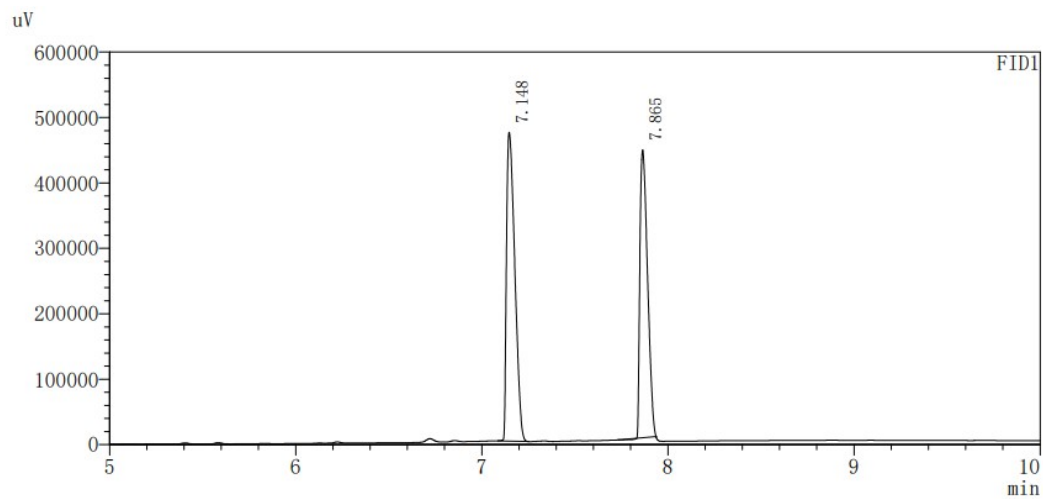
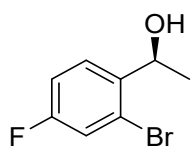
(R)-2-chloro-1-(4-fluorophenyl)ethanol **10b**



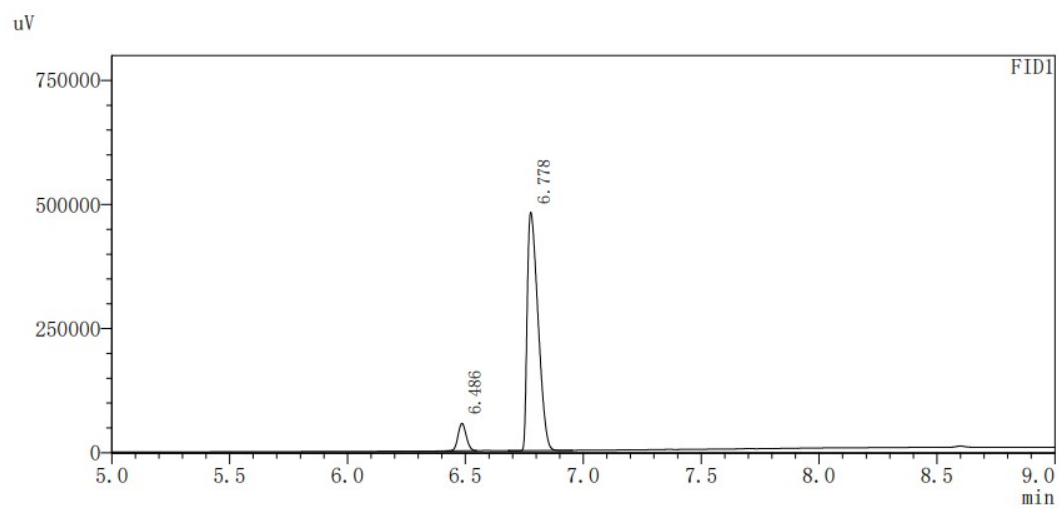
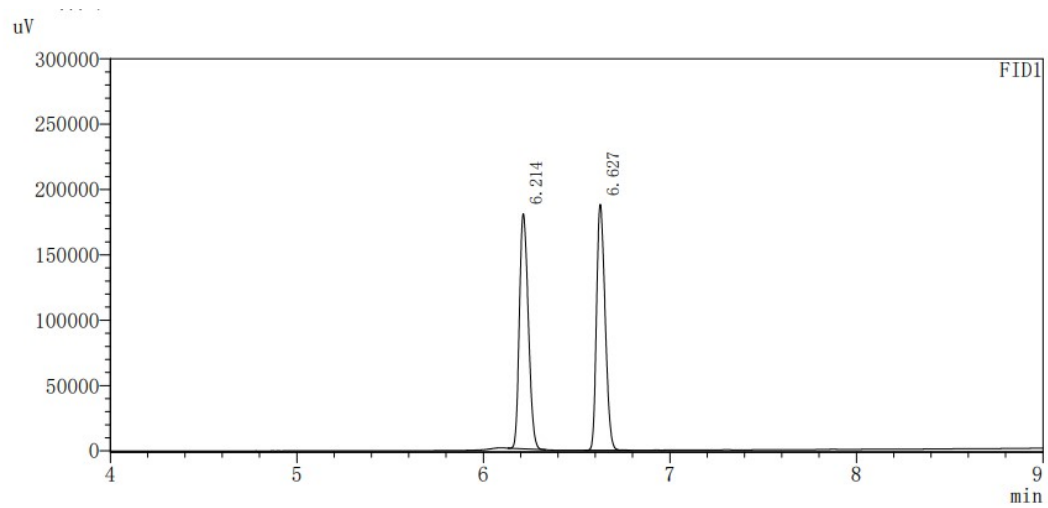
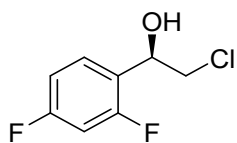
(*R*)-1-(4-bromophenyl)ethan-1-ol **11b**



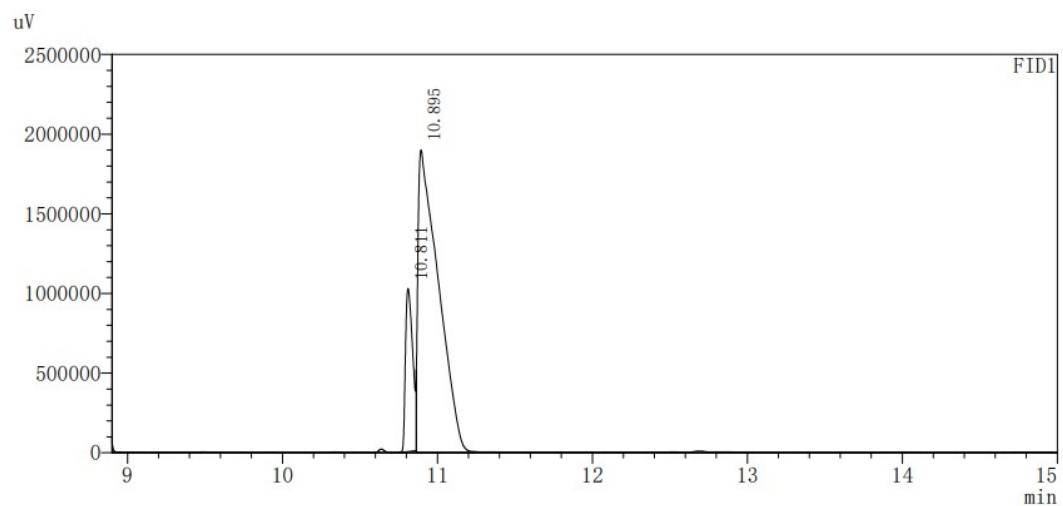
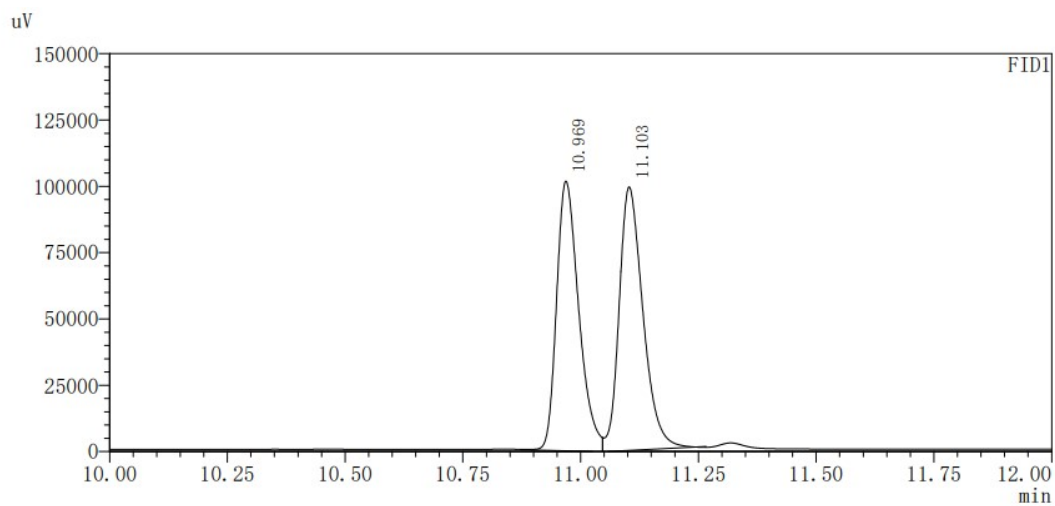
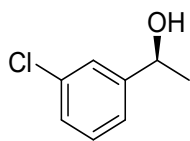
(R)-1-(2-bromo-4-fluorophenyl)ethanol **12b**



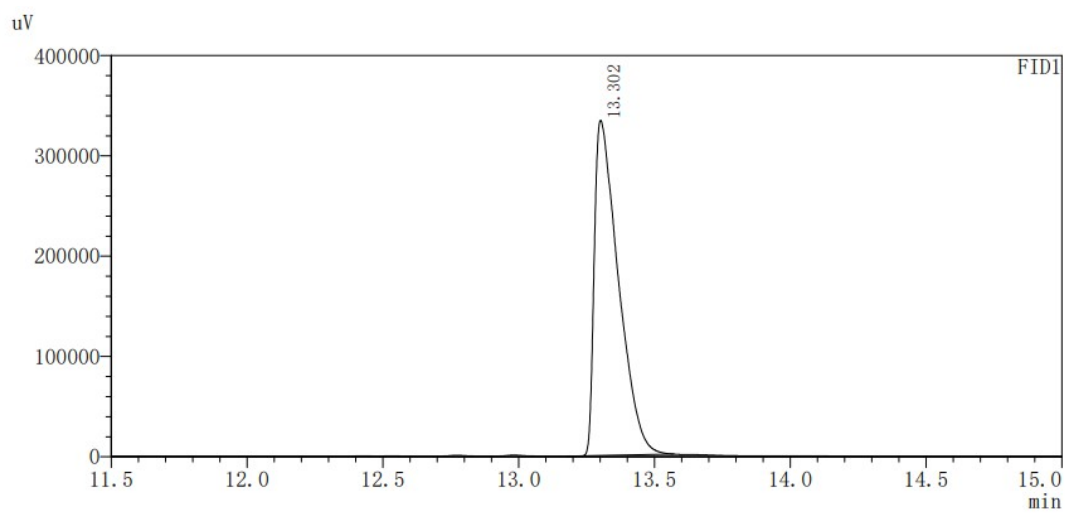
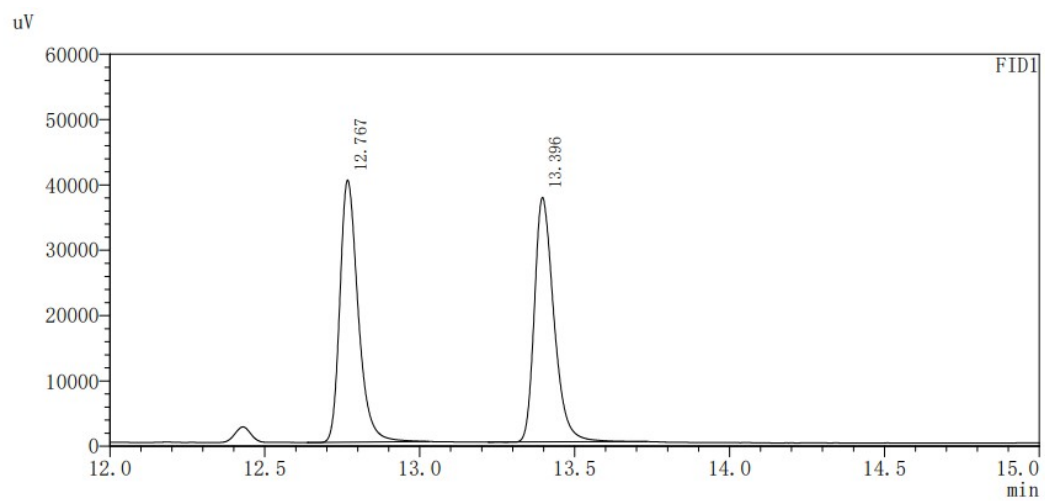
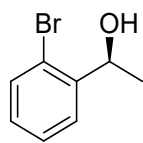
(S)-2-chloro-1-(2,4-difluorophenyl)ethanol **13b**



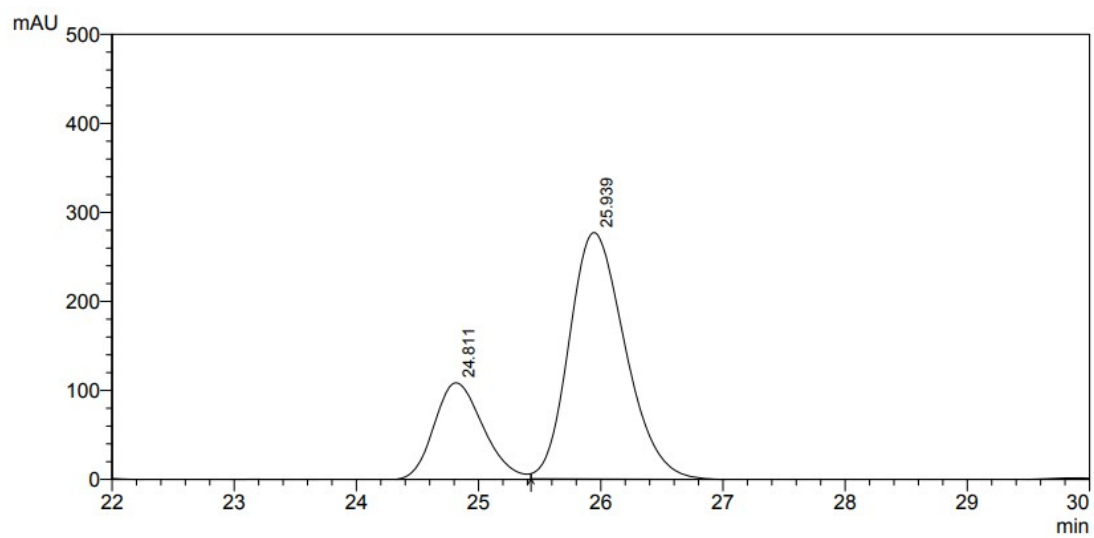
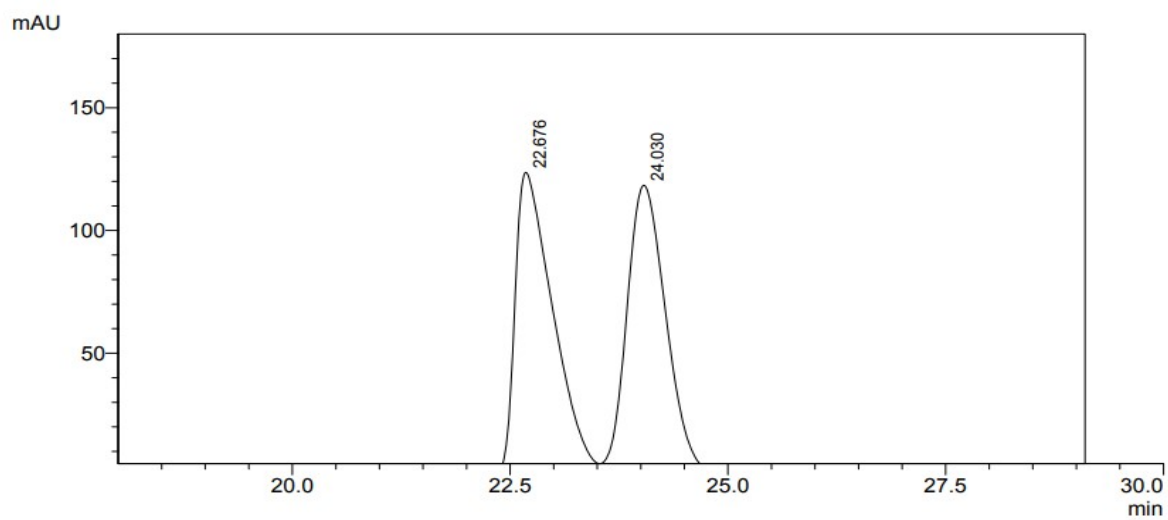
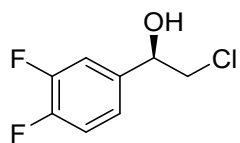
(S)-1-(3-chlorophenyl)ethan-1-ol **14b**



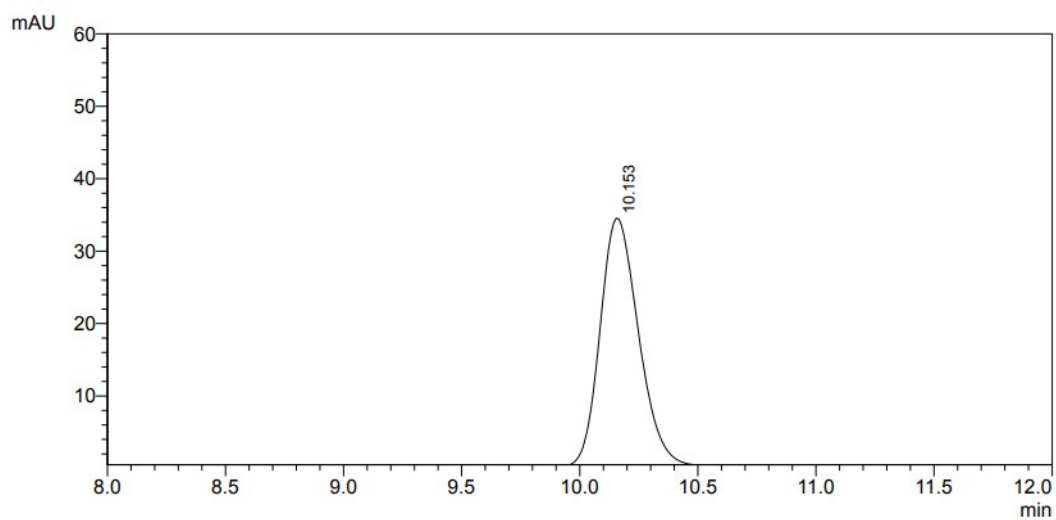
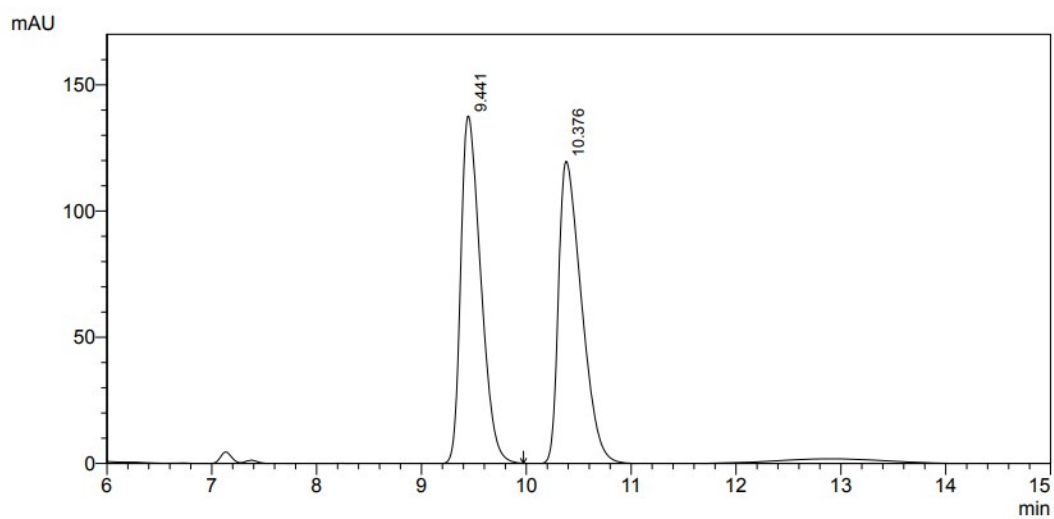
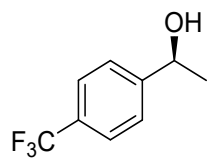
(R)-1-(2-bromophenyl)ethan-1-ol **15b**



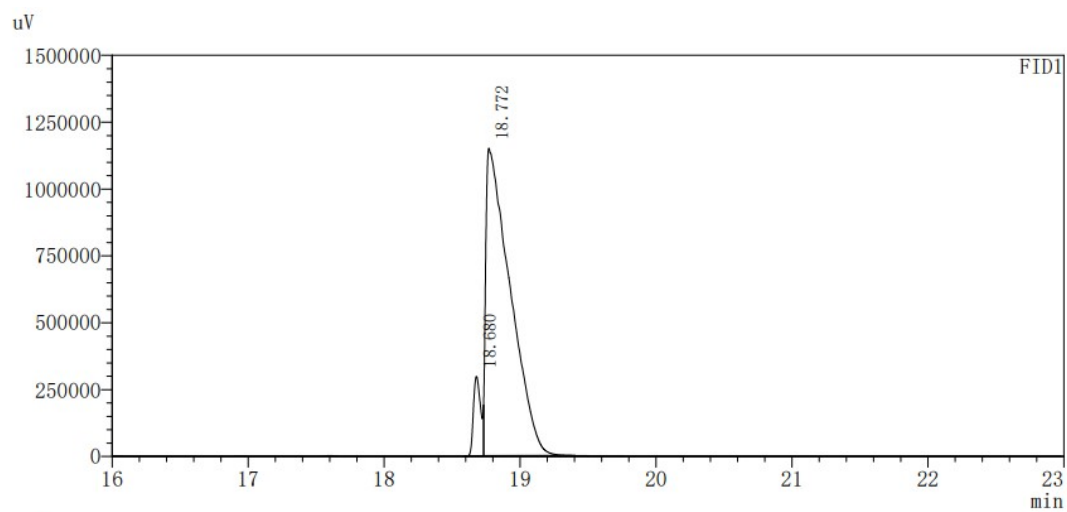
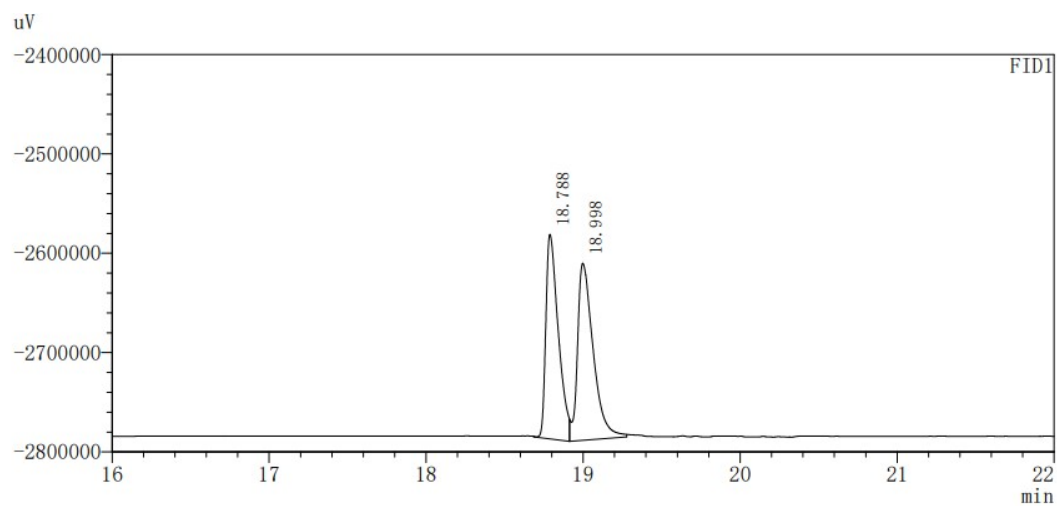
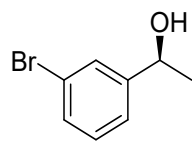
(S)-2-chloro-1-(3,4-difluorophenyl)-1-ethanol **16b**



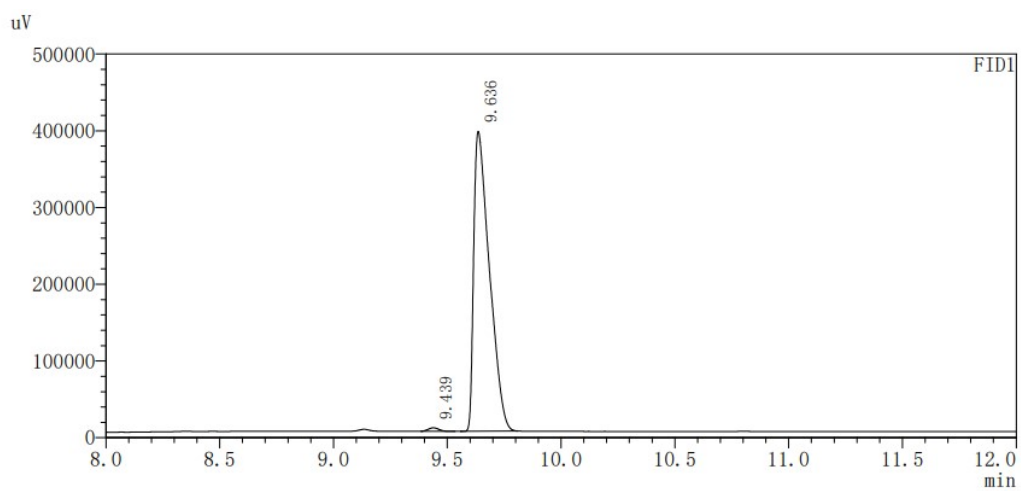
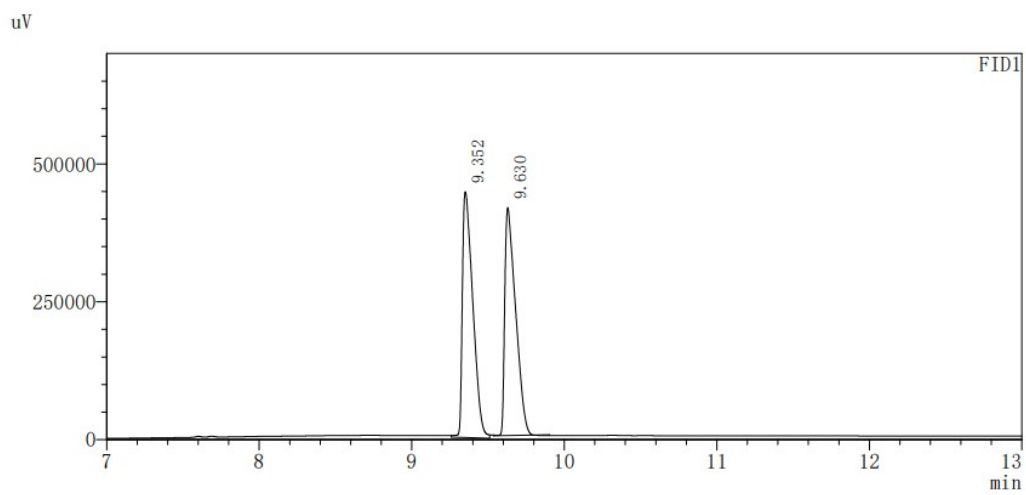
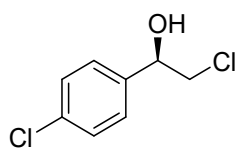
(S)-1-[4-(trifluoromethyl)phenyl]ethan-1-ol **17b**



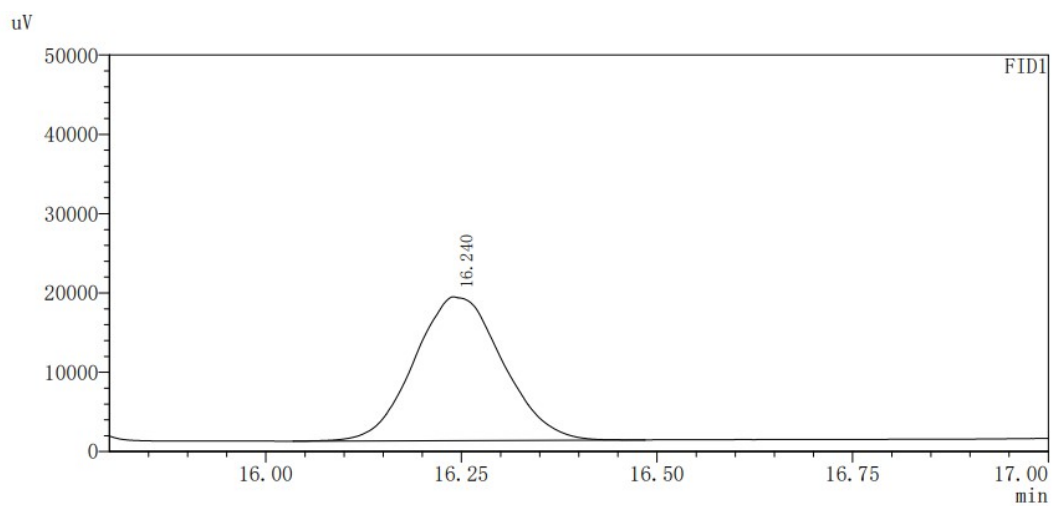
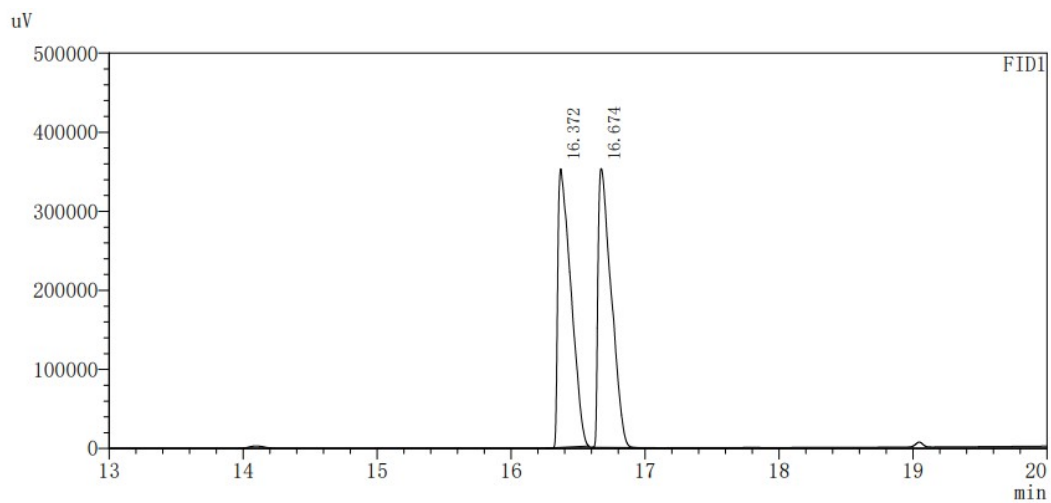
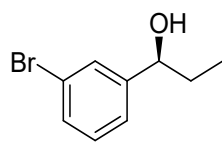
(R)-1-(3-bromophenyl)ethan-1-ol **18b**



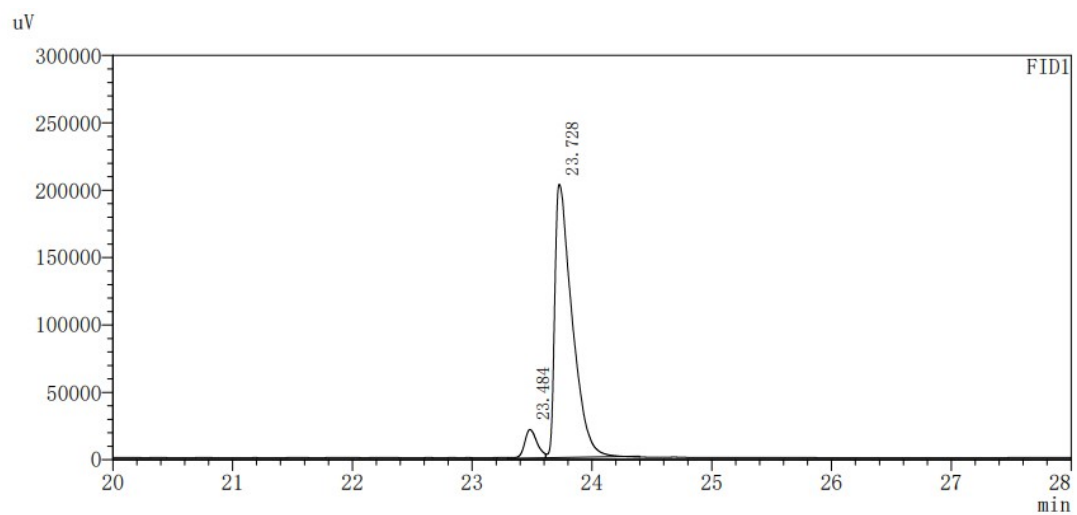
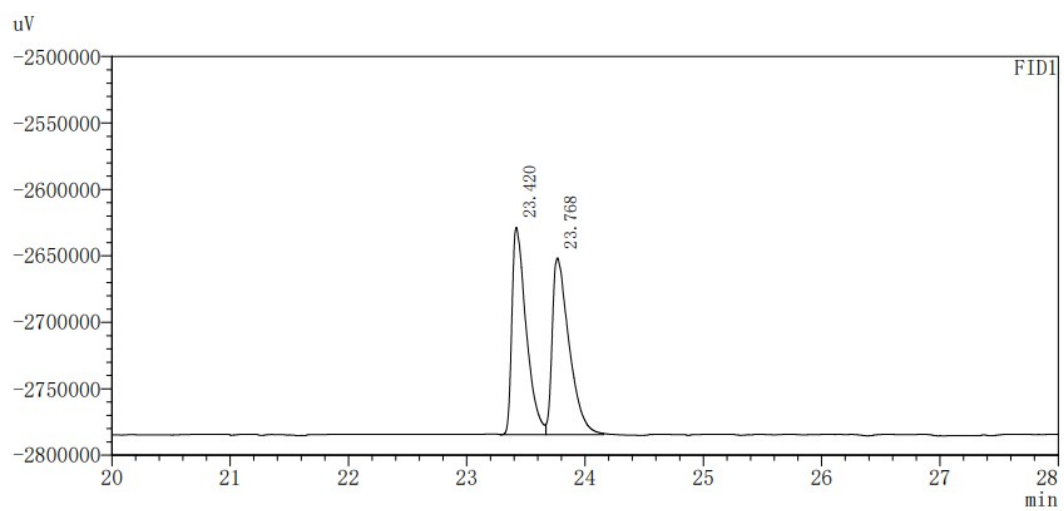
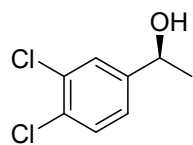
(S)-2-chloro-1-(4-Chlorophenyl)ethanol **19b**



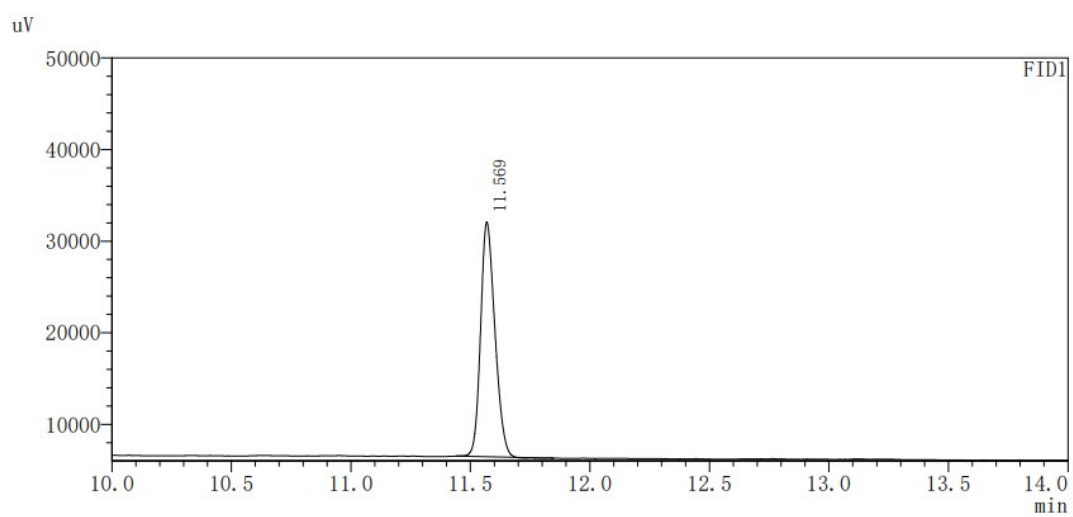
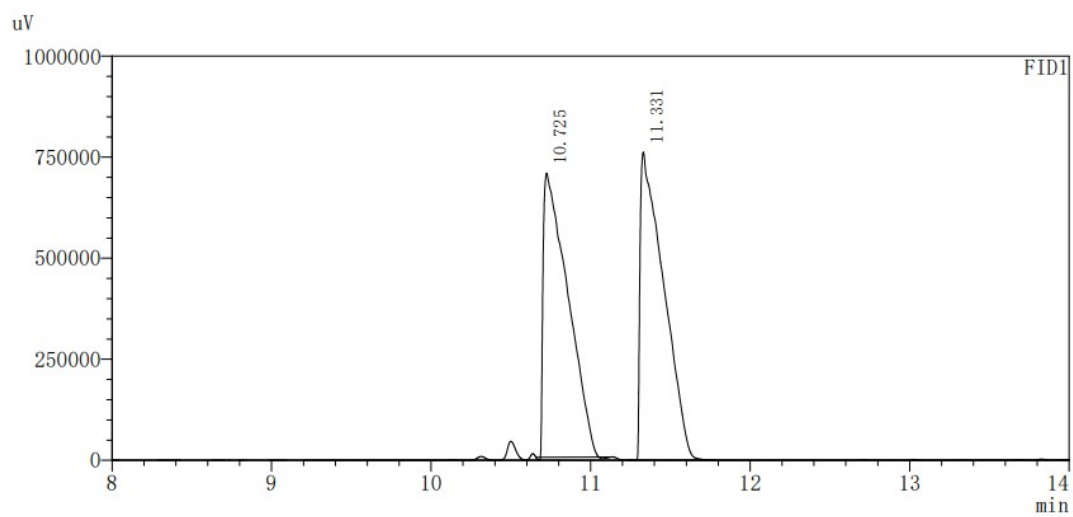
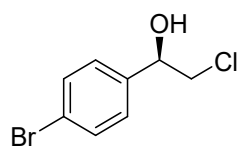
(R)-1-(3-bromophenyl)propanol 20b



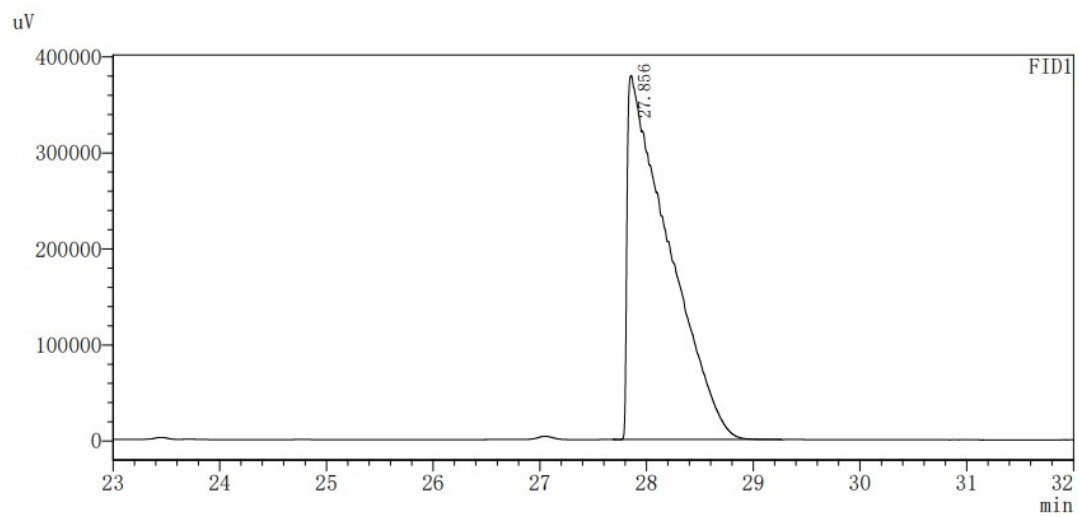
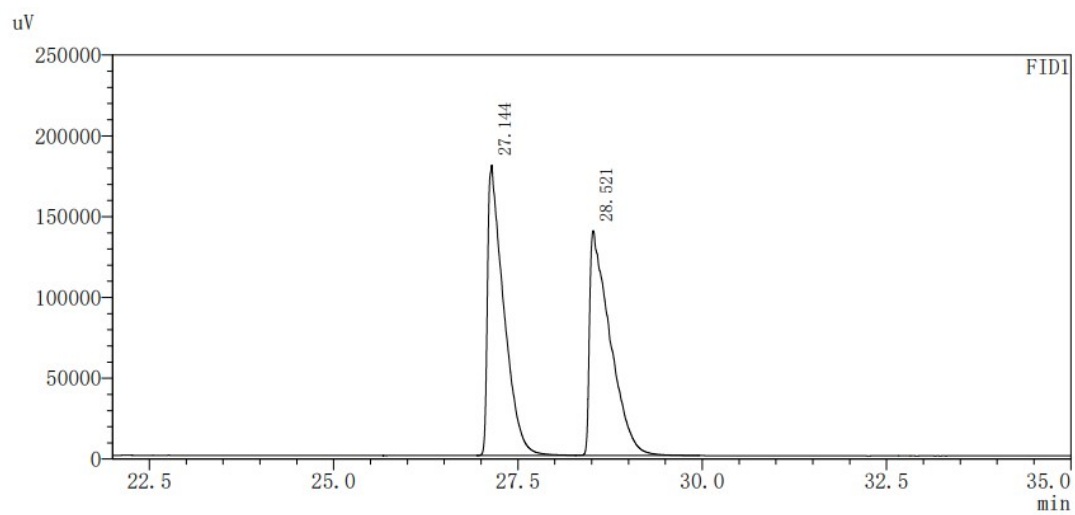
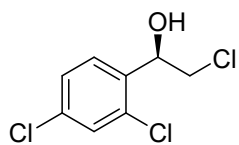
(R)-1-(3,4-dichlorophenyl)ethan-1-ol **21b**



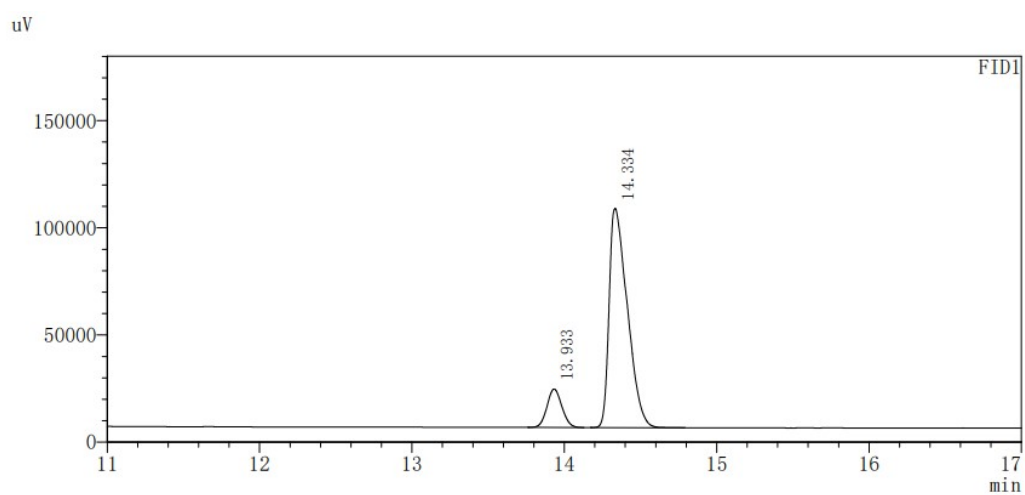
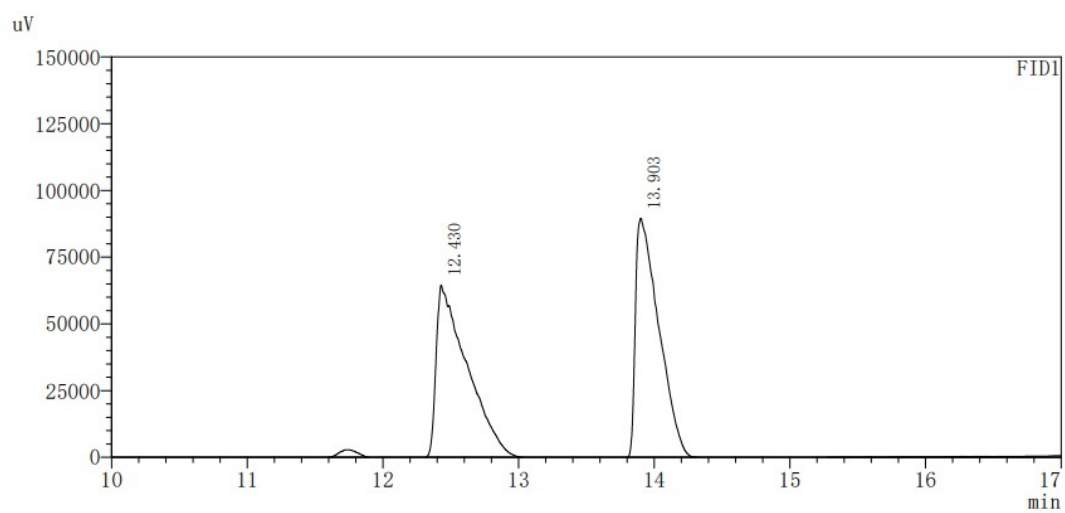
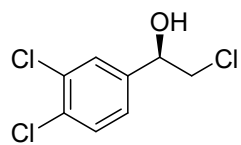
(S)-1-(4-bromophenyl)-2-chloroethanol **22b**



(R)-2-chloro-1-(2,4-dichlorophenyl)ethan-1-ol **23b**



(S)-2-chloro-1-(3,4-dichlorophenyl)ethan-1-ol **24b**



(S)-1-[3,5-bis(trifluoromethyl)phenyl]ethanol **25b**

