

Supporting Information for

One-pot Relay Reduction-Isomerization of β -Trifluoromethylated- α,β -Unsaturated Ketones to chiral β -Trifluoromethylated Saturated Ketones Over Combined Catalysts in Aqueous Medium

Xuelin Xia, Meng Wu, Ronghua Jin, Tanyu Cheng, Guohua Liu*

Key Laboratory of Resource Chemistry of Ministry of Education, Shanghai Key Laboratory of Rare Earth Functional Materials, Shanghai Normal University, No.100 Guilin Rd, Shanghai 200241, P. R. China

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Experimental

1. General

All experiments, which are sensitive to moisture or air, were carried out under an Ar atmosphere using the standard Schlenk techniques. (*R,R*)-1,2-diphenylenediamine, $[\text{RuCl}_2(p\text{-Cymene})]_2$, 1,2-bis(triethoxysilyl)ethane, surfactant P123 $(\text{CH}_2\text{-CH}_2\text{O})_{20}(\text{CH}_2(\text{CH}_3)\text{CH}_2\text{O})_{70}(\text{CH}_2\text{CH}_2\text{O})_{20}$ and tetraethoxysilane (TEOS) were purchased from Sigma-Aldrich Company Ltd. Compounds (*R,R*)-4-(trimethoxysilyl)ethylphenylsulfonyl-1,2-diphenylethylenediamine was synthesized according to the reported literatures [*J. Mater. Chem.* **2010**, *20*, 1970]

2. Preparation of ArDPEN-PMO (2). In a typical synthesis, 2.0 g of structure-directing agent, pluronic P123, was fully dissolved in a mixture of 80 mL hydrochloric acid (0.2 N) and 6.0 g KCl and the mixture was stirred at room temperature for 1.0 h. Then, 3.36 mL (9.10 mmol) of 1,2-bis(triethoxysilyl)ethane was added as the silica precursor at 40 °C. After pre-hydrolysis period of 40 min., 0.24 g (0.48 mmol) of (*R,R*)-DPEN-SO₂Ph(CH₂)₂Si(OMe)₃ was added. The reaction mixture was stirred at 40 °C for 24 h and aged at 100 °C for 24 h. The resulting solid was filtered and rinsed with excess ethanol before being dried overnight on a filter. The surfactant template was removed by refluxing in acidic ethanol (400 mL per gram) for 24 h. The solid was filtered and rinsed with ethanol again, and dried at 60 °C under reduced pressure overnight to afford **2** (1.36 g) in the form of a white powder. IR (KBr) cm⁻¹: 3443.5 (s), 2978.5 (w), 2928.8 (w), 1627.2 (m), 1460.2 (w), 1416.5 (w), 1382.7 (w), 1273.4 (m), 1164.1 (s), 1096.5 (s), 1028.9 (s), 919.7 (m), 766.7 (m), 699.1 (m), 438.8 (m); ¹³C CP MAS NMR (161.9 MHz): 150.0, 137.5, 128.7 (C_{of} Ph and Ar), 76.1–69.2 (C_{of} -NCHPh-), 59.4 (O-CH₂CH₃), 28.8 (C_{of} -CH₂Ar), 16.3 (O-CH₂CH₃), 5.2 (C_{of} -CH₂Si) ppm; ²⁹Si MAS/NMR (79.4 MHz): T¹ (δ = -49.1 ppm), T² (δ = -57.6 ppm), T³ (δ = -65.0 ppm).

3. General procedure for the reuse experiments using 4,4,4-trifluoro-1,3-diphenylbut-2-enone as a substrate.

The catalyst **3** (291.0 mg, 0.030 mmol of Ru based on ICP analysis), 4,4,4-trifluoro-1,3-diphenylbut-2-enone (1.50 mmol), HCO₂Na (2.04 g, 30.0 mmol), 20.0 mL of water were added sequentially to a 50.0 mL round-bottom flask. The mixture was then stirred at room temperature (20 °C) for 17 h. After completion of the reaction, the catalyst was separated by centrifugation (10,000 rpm). The collected solids were transferred to a fresh 50.0 mL round-bottom flask and 4,4,4-trifluoro-1,3-diphenylbut-2-enone (1.50 mmol), HCO₂Na (2.04 g, 30.0 mmol) and 20.0 mL of water were added again for next recycle. The aqueous solution was extracted with ethyl ether (3 × 3.0 mL). The combined ethyl ether extracts were washed with NaHCO₃ and brine, and then dehydrated with Na₂SO₄. After evaporation of ethyl ether, the residue was purified by silica gel flash column chromatography to afford the desired products.

Figure S1. FT-IR spectra of **2** and catalyst **3**.

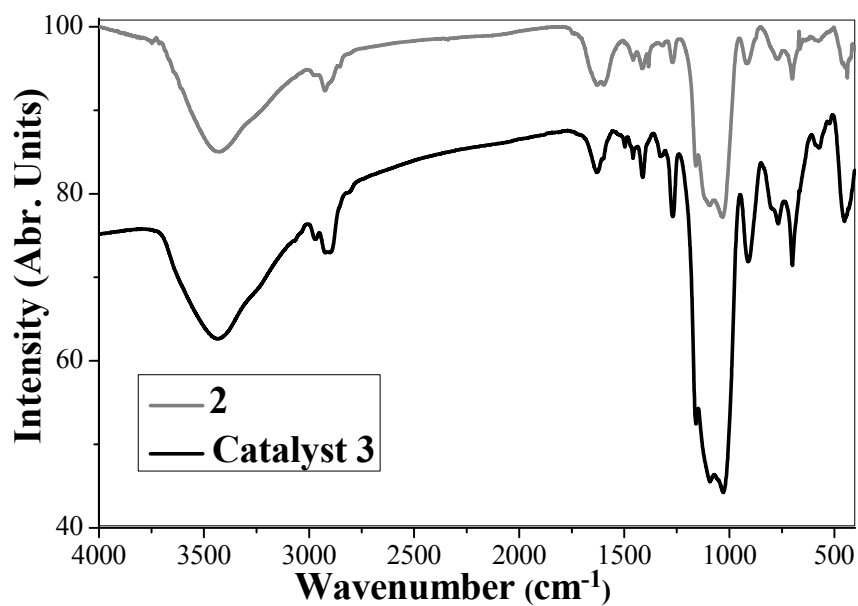


Figure S2. XPS spectrum of [RuCl₂(*p*-cymene)]₂.

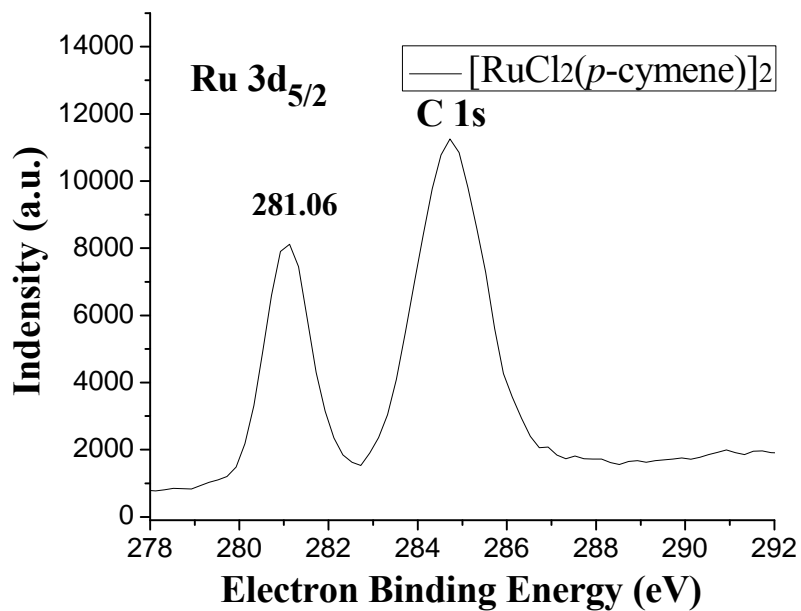
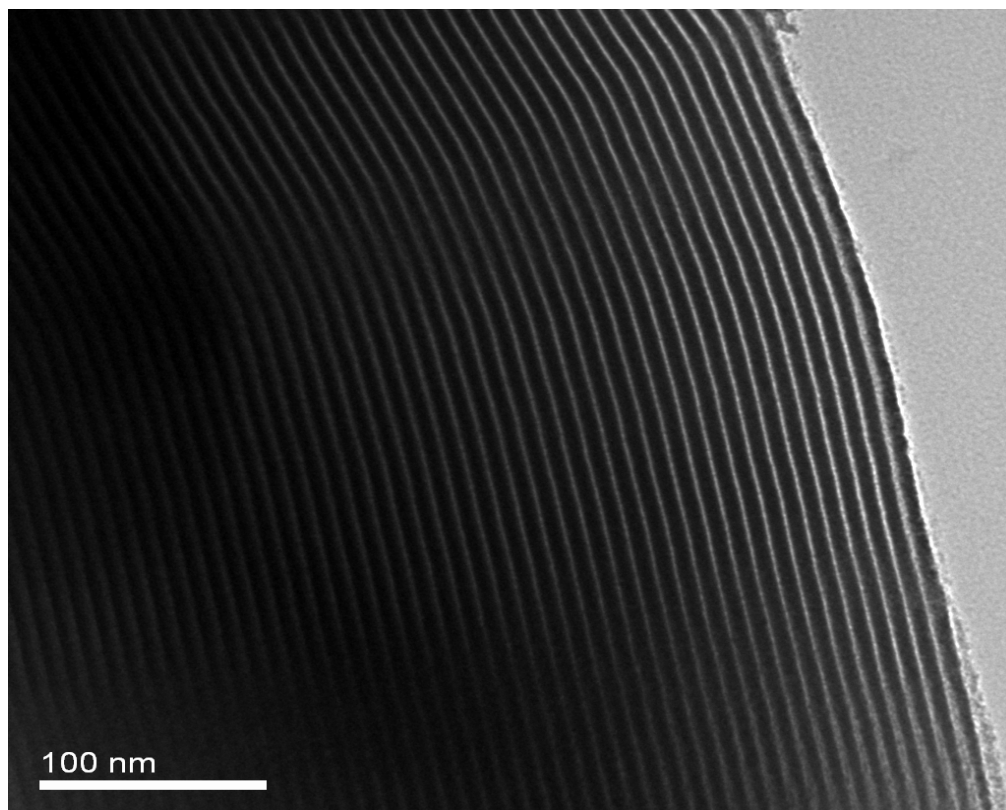


Figure S3. TEM images of catalyst **3** viewed along [100] (a) and [001] (b) directions.

(a) [100] direction.



(b) [001] direction.

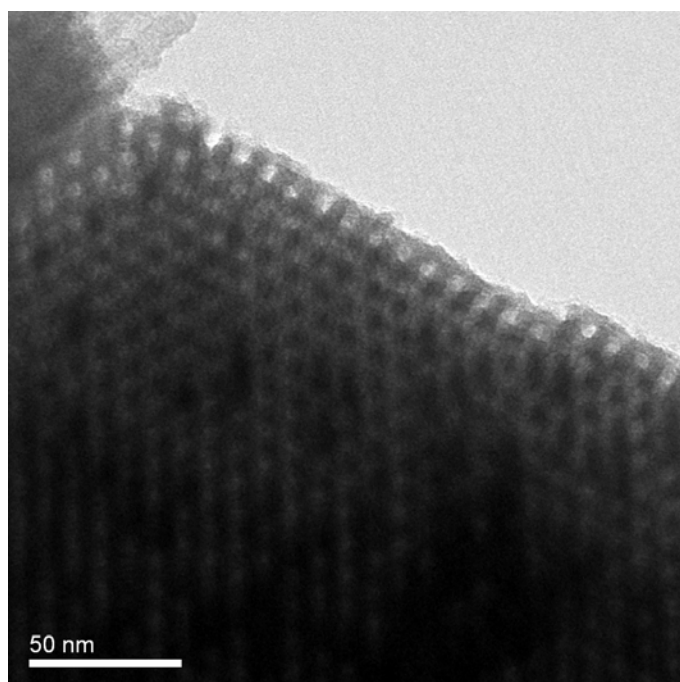
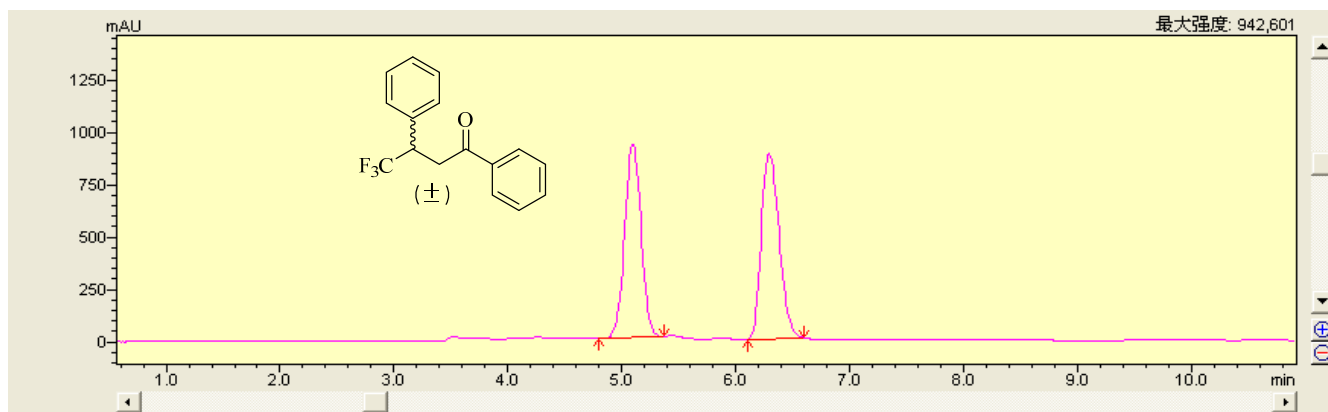


Figure S4. One-pot enantioselective reduction-isomerization of β -trifluoromethylated- α,β -unsaturated ketones to chiral β -trifluoromethylated saturated ketones. [The products were analyzed by a HPLC with a UV-Vis detector using a Daicel OD-H or OJ-H chiralcel column ($\Phi 0.46 \times 25$ cm)].

Translation of Chinese to English is as follows:

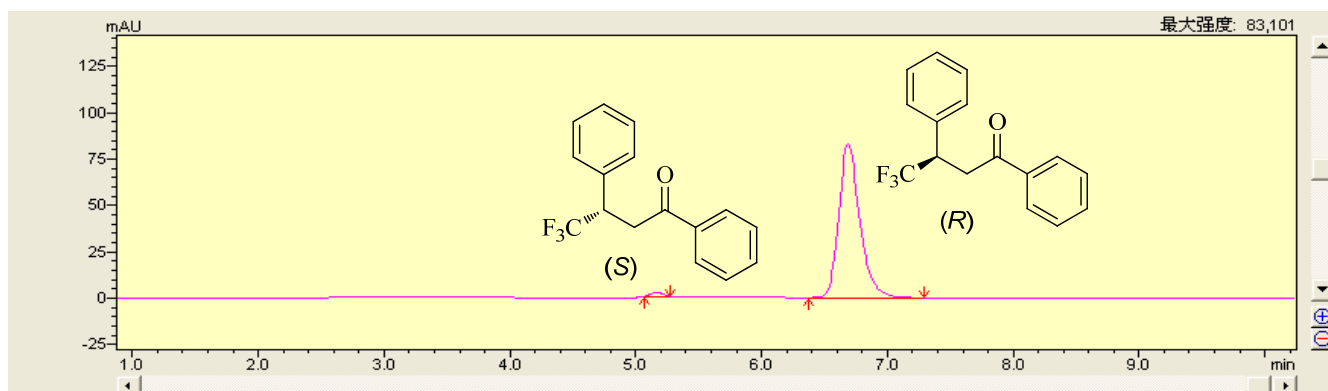
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2	19.395	9109.7	3.5589	1042.4	5.9606

6a: (*R*)-4,4,4-trifluoro-1,3-diphenylbutan-1-one (HPLC: Chiralcel OD-H, detected at 254 nm, eluent: n-hexane/2-propanol = 95/5, flow rate = 1.0 mL/min, 25 °C).



化合物表视图

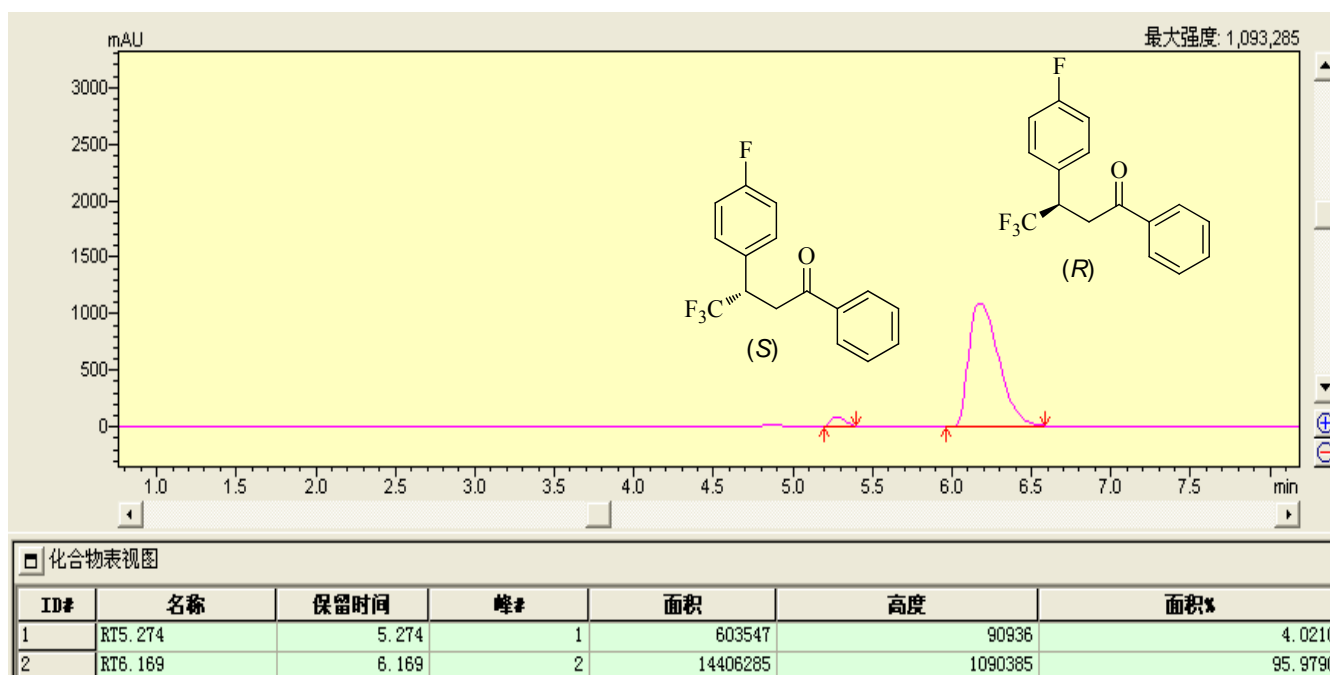
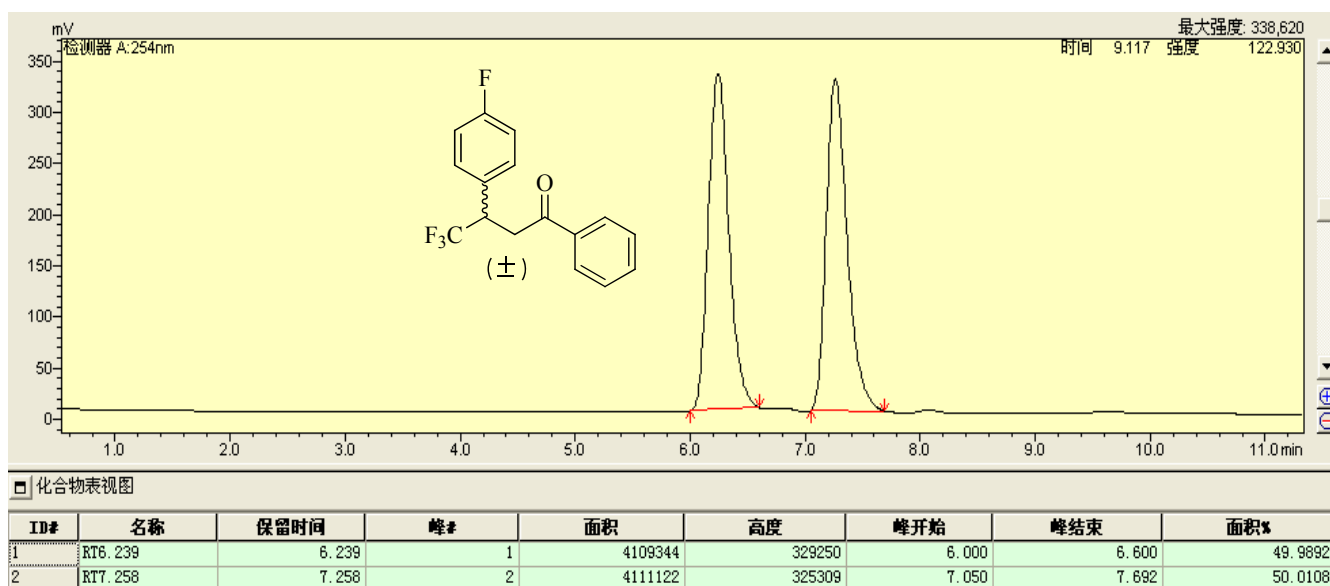
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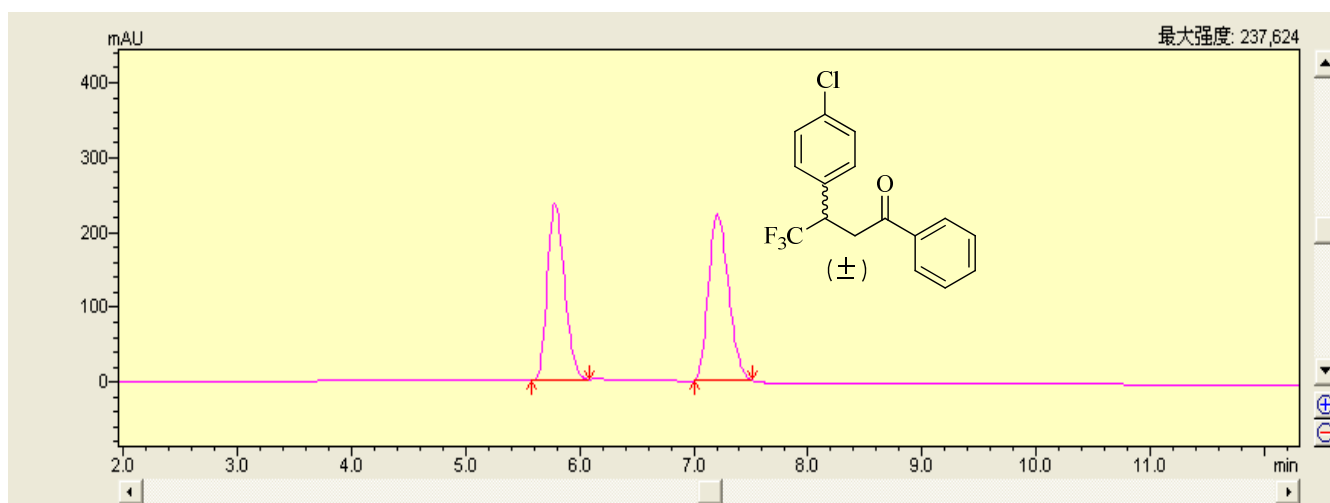
化合物表视图

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2	RT6.683	6.683	2	961425	82845	98.5763

6b: (R)-4,4,4-trifluoro-3-(4-fluorophenyl)-1-phenylbutan-1-one (HPLC: Chiracel OD-H, detected at 254 nm, eluent: n-hexane/2-propanol = 95/5, flow rate = 1.0 mL/min, 25 °C).

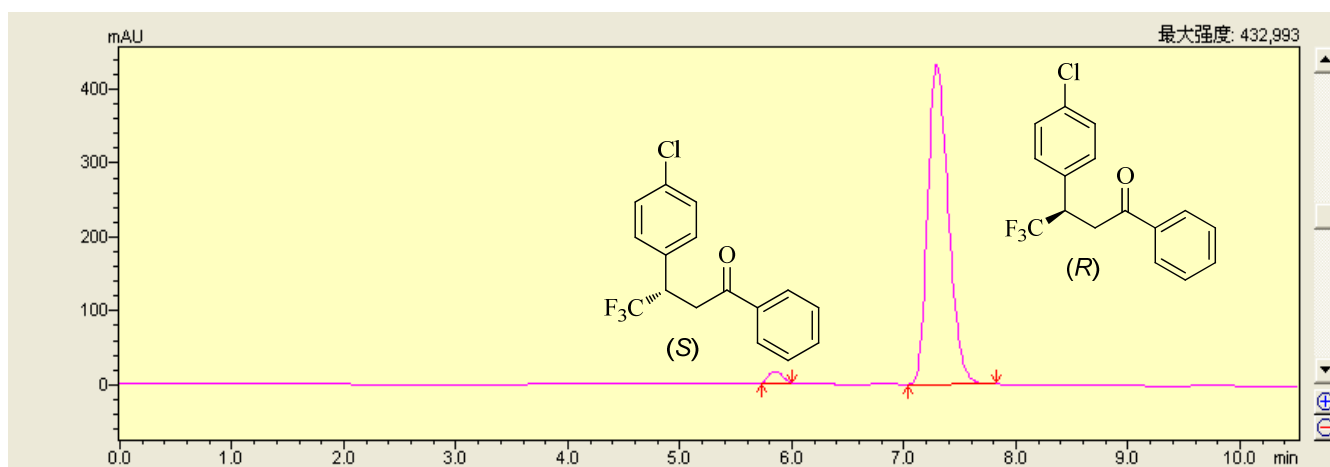


6c: (*R*)-3-(4-chlorophenyl)-4,4,4-trifluoro-1-phenylbutan-1-one (HPLC: Chiralcel OD-H, detected at 254 nm, eluent: n-hexane/2-propanol = 95/5, flow rate = 1.0 mL/min, 25 °C).



化合物表视图

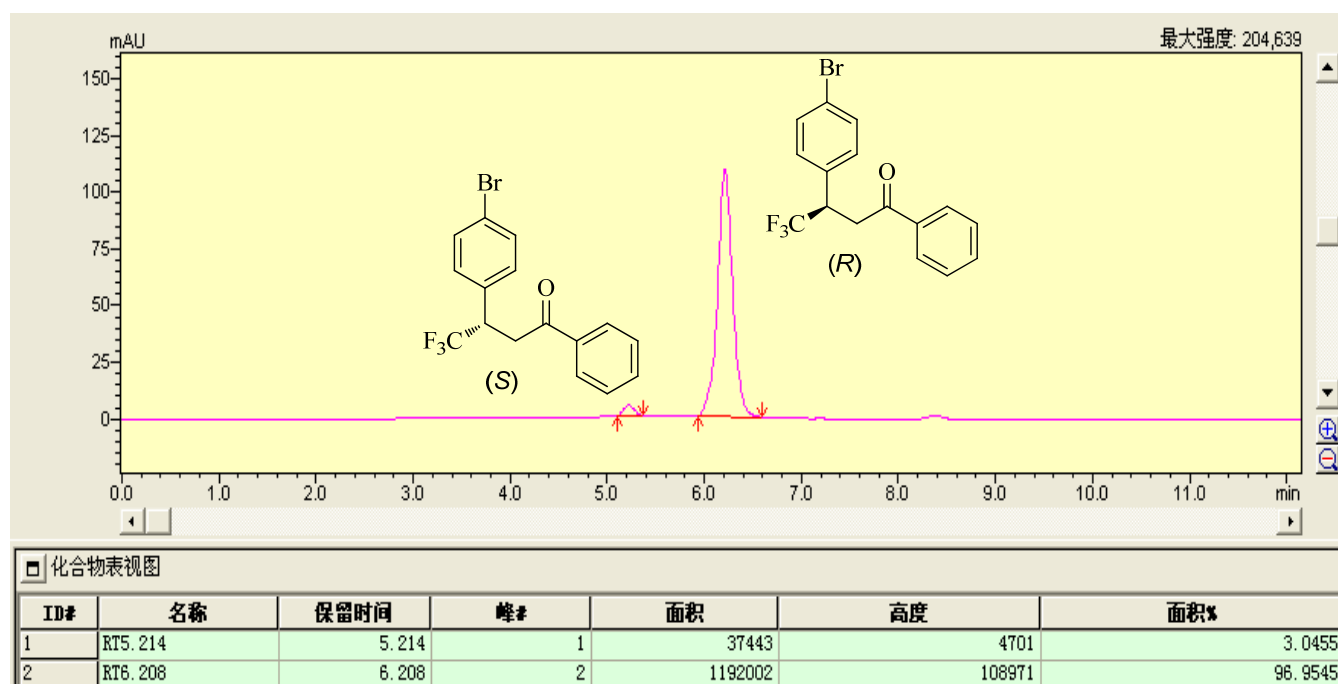
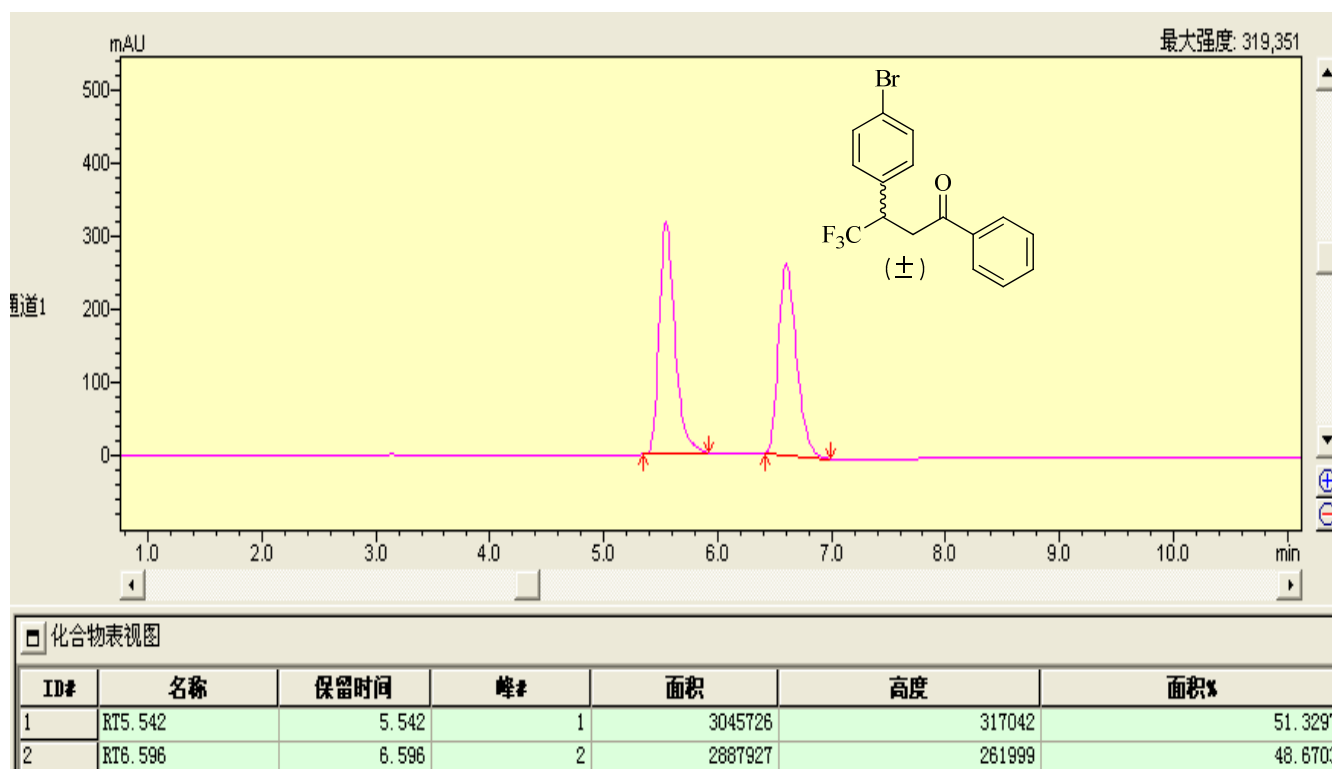
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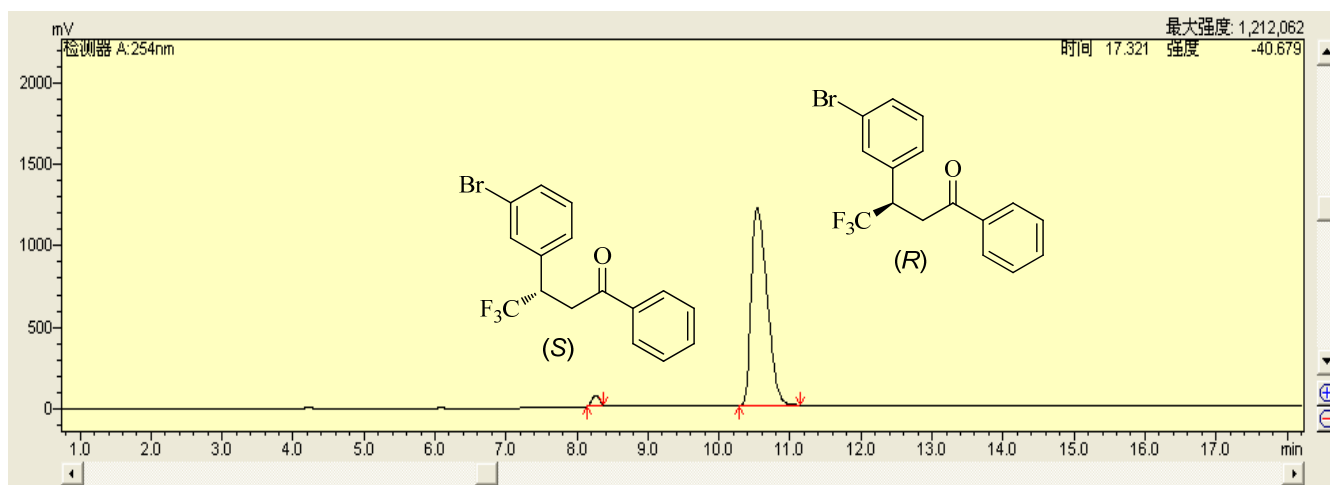
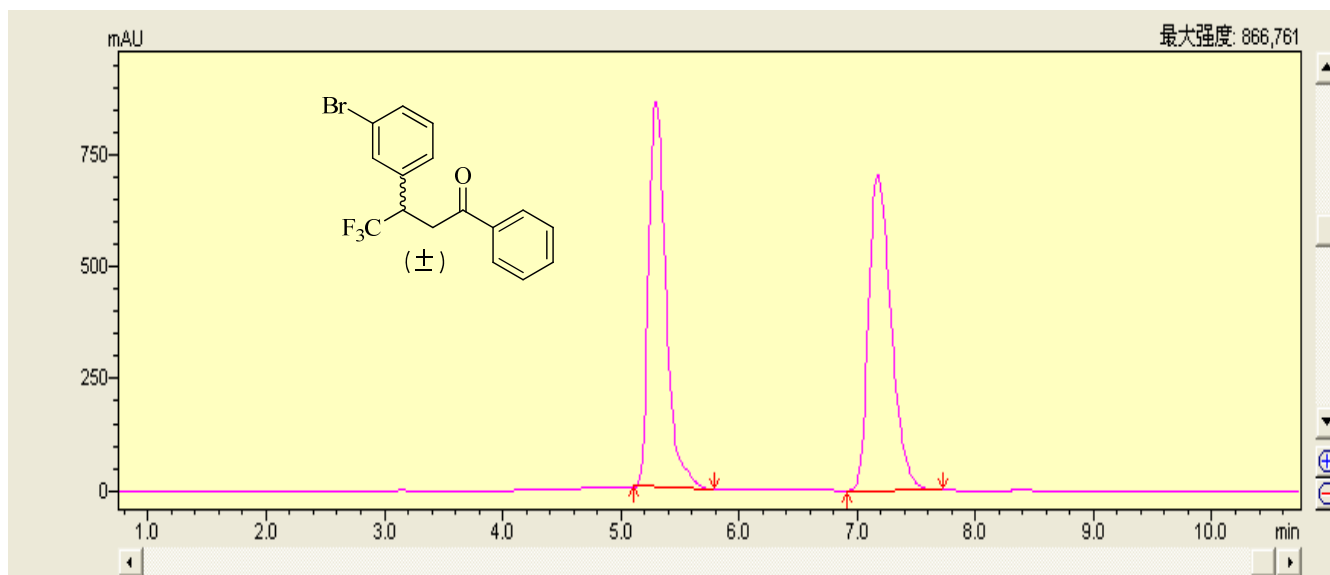
化合物表视图

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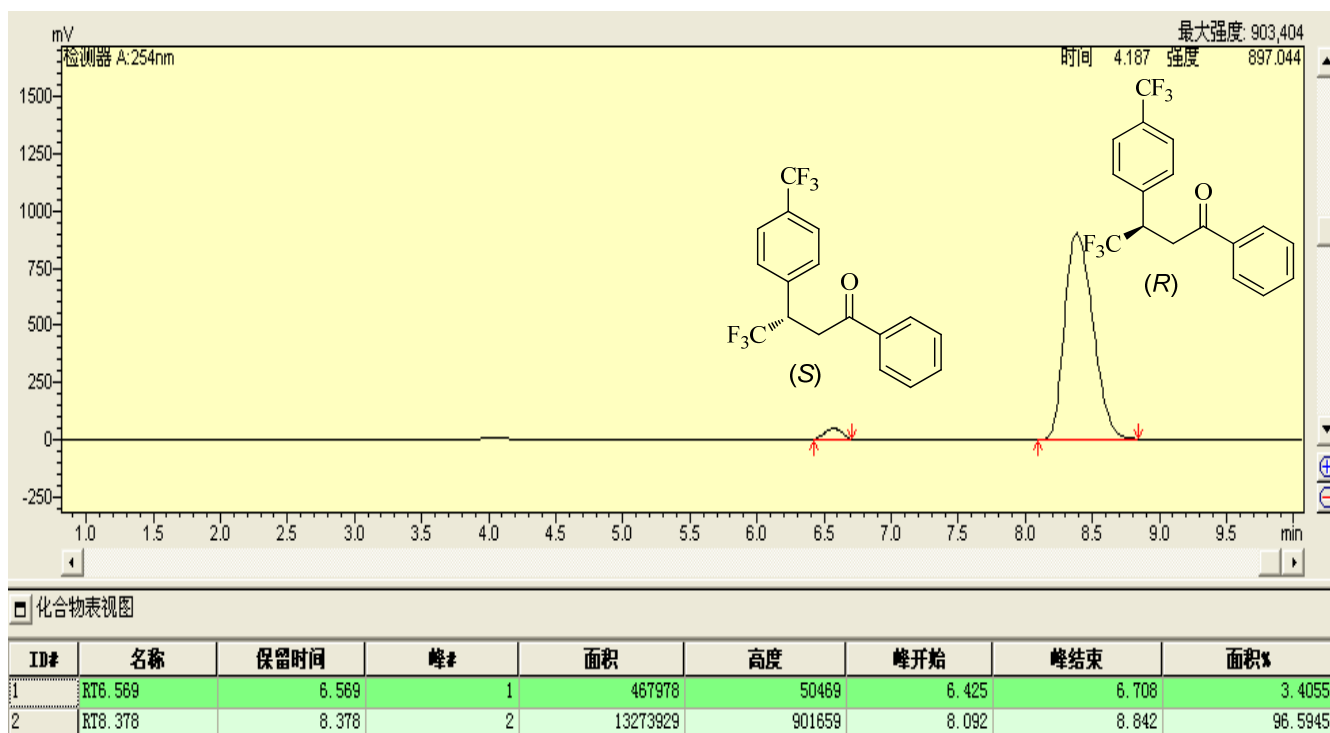
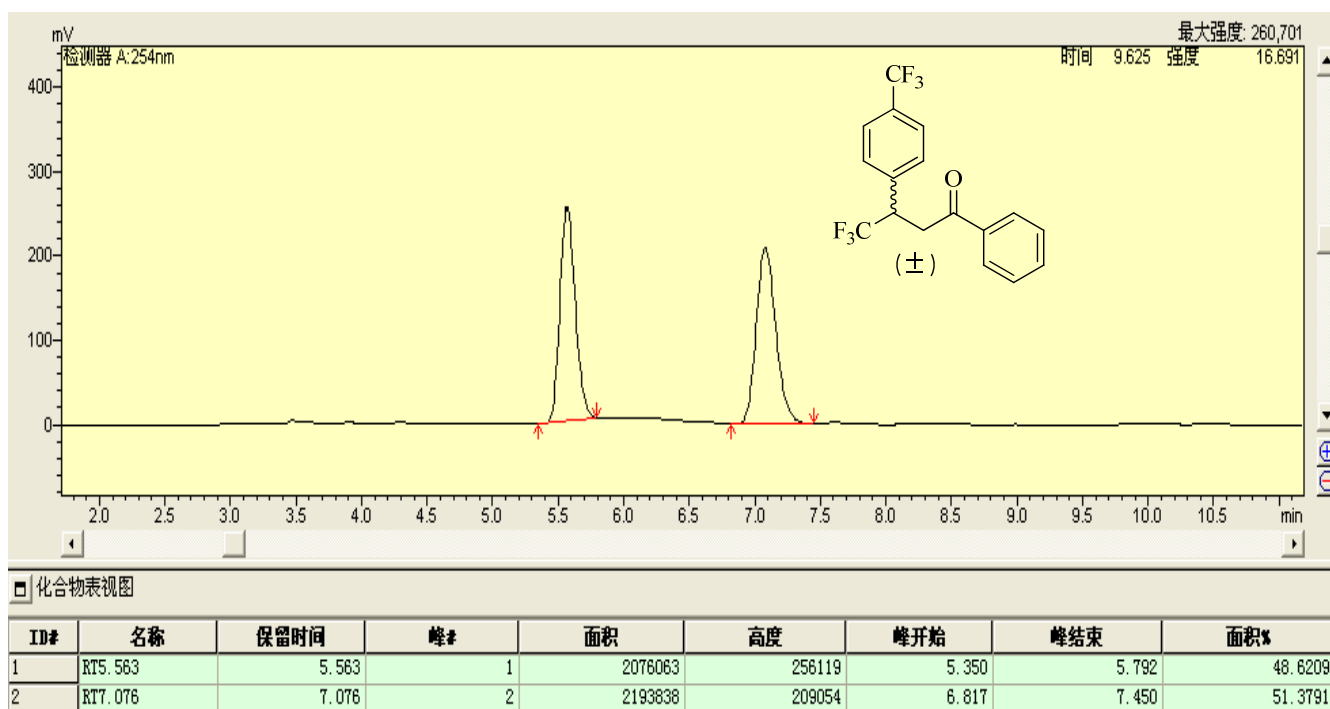
6d: (*R*)-3-(4-bromophenyl)-4,4,4-trifluoro-1-phenylbutan-1-one (HPLC: Chiralcel OD-H, detected at 254 nm, eluent: n-hexane/2-propanol = 95/5, flow rate = 1.0 mL/min, 25 °C).



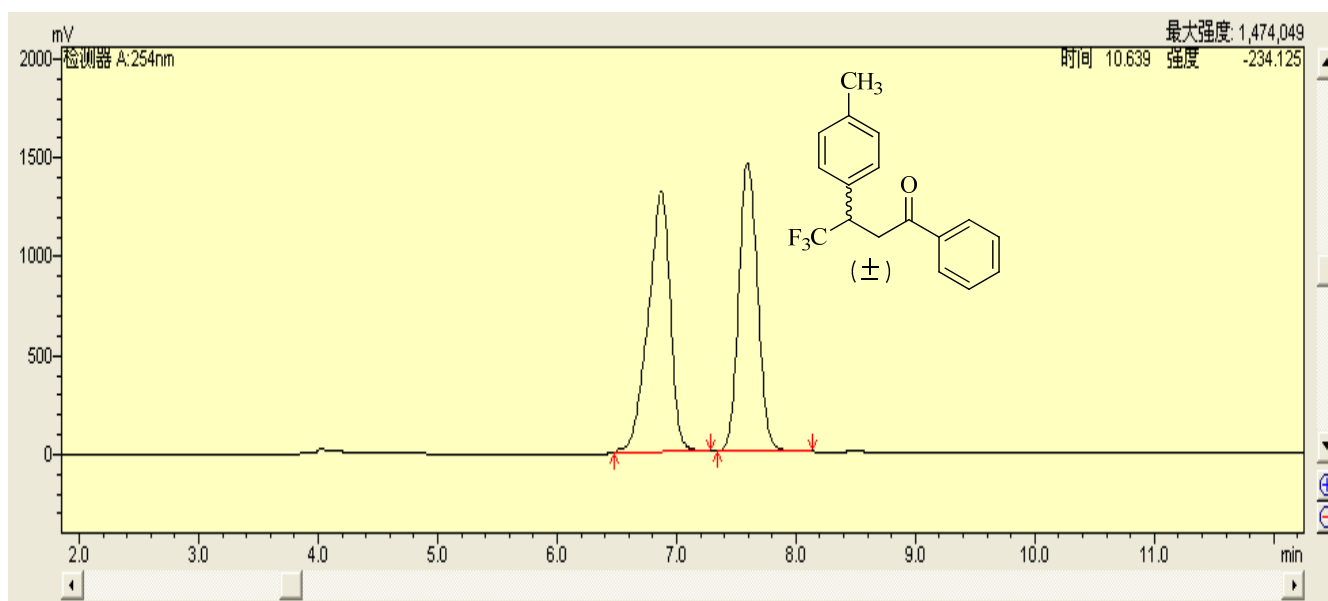
6e: (R)-3-(3-bromophenyl)-4,4,4-trifluoro-1-phenylbutan-1-one (4e): (HPLC: Chiralcel OD-H, detected at 254 nm, eluent: n-hexane/2-propanol = 95/5, flow rate = 1.0 mL/min, 25 °C).



6f: (R)-4,4,4-trifluoro-1-phenyl-3-(4-(trifluoromethyl)phenyl)butan-1-one (HPLC: Chiracel OD-H, detected at 254 nm, eluent: n-hexane/2-propanol = 95/5, flow rate = 1.0 mL/min, 25 °C).

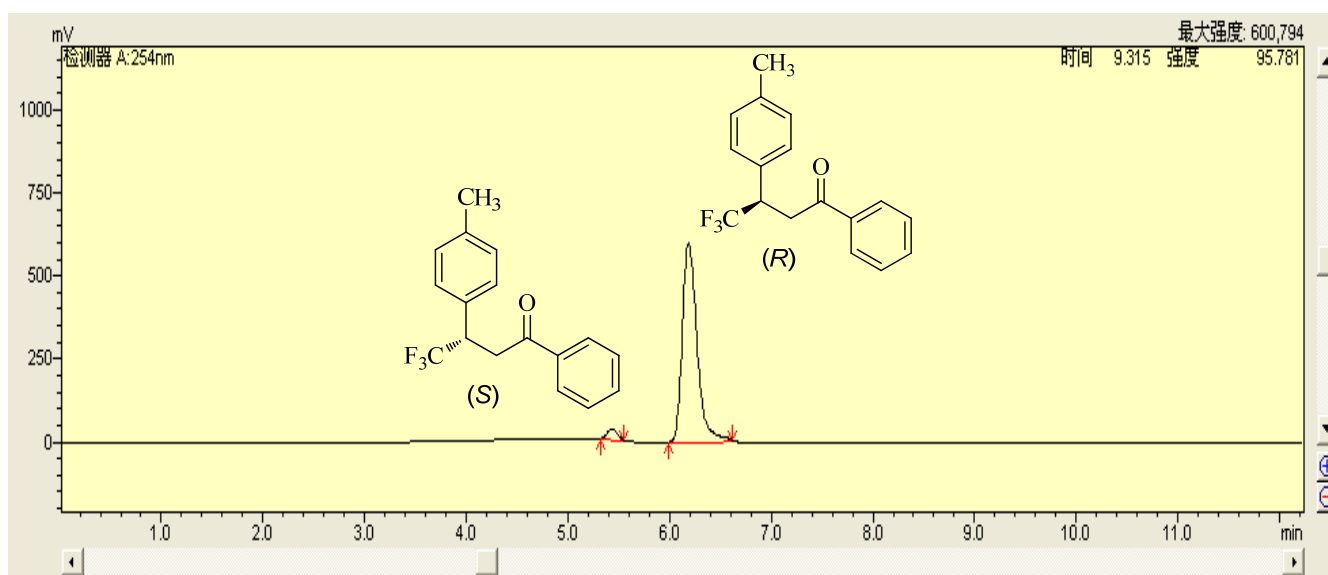


6g: (R)-4,4,4-trifluoro-1-phenyl-3-(p-tolyl)butan-1-one (HPLC: Chiralcel OD-H, detected at 254 nm, eluent: n-hexane/2-propanol = 95/5, flow rate = 1.0 mL/min, 25 °C).



化合物表视图

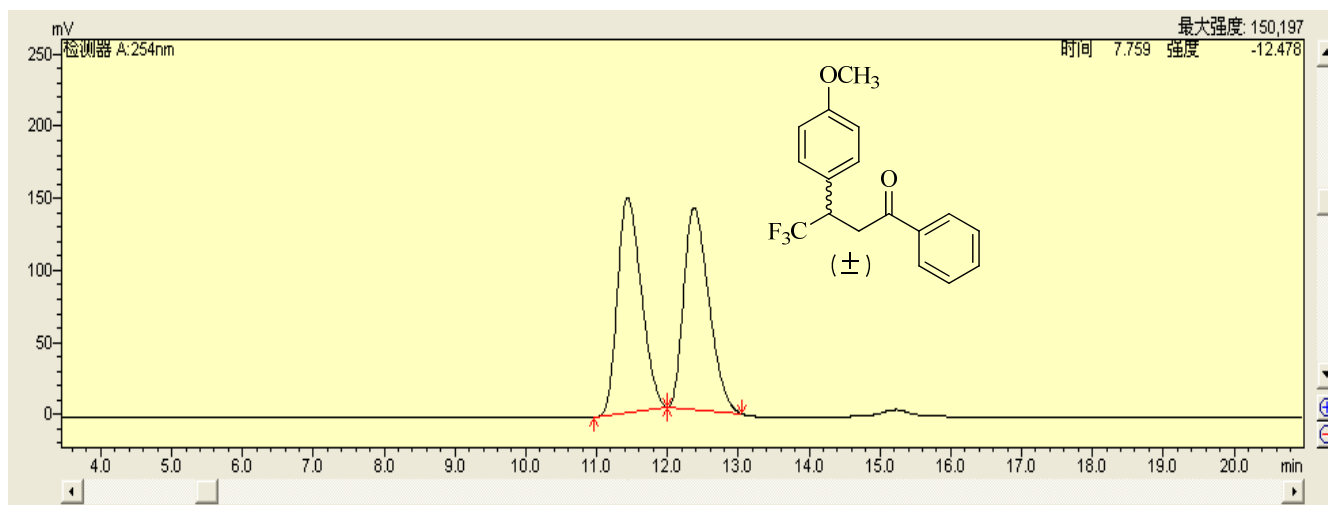
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2	RT7.591	7.591	2	16026354	1456893	7.342	8.133	48.4323



化合物表视图

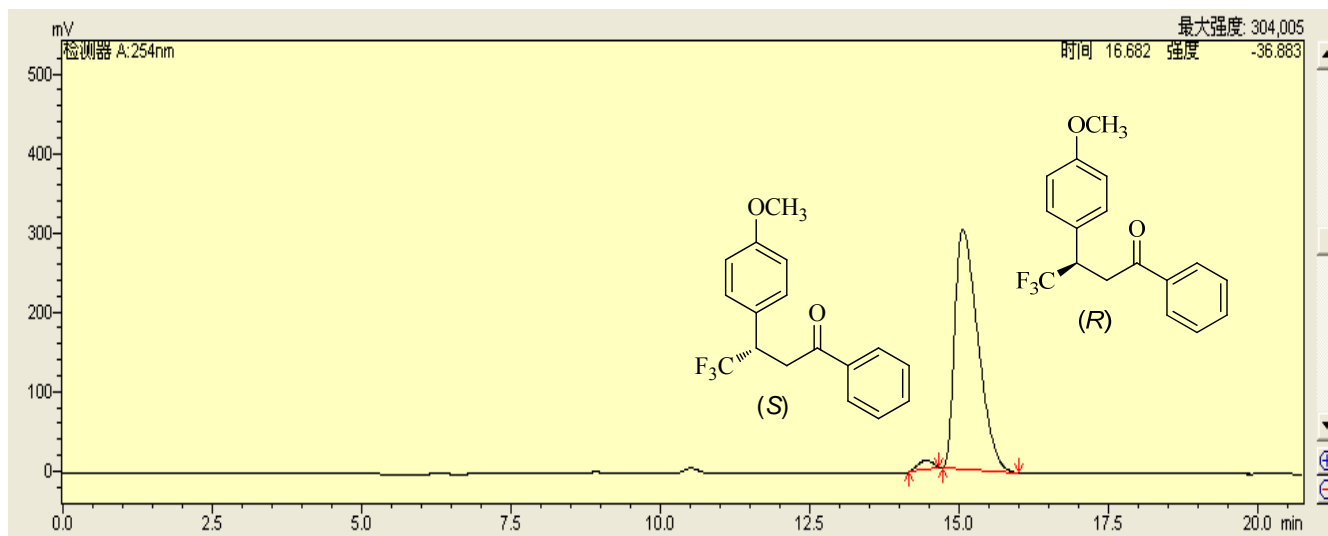
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2	RT6.183	6.183	2	6189997	601280	5.983	7.083	96.6872

6h: (R)-4,4,4-trifluoro-3-(4-methoxyphenyl)-1-phenylbutan-1-one (HPLC: Chiracel OD-H, detected at 254 nm, eluent: n-hexane/2-propanol = 95/5, flow rate = 1.0 mL/min, 25 °C).



化合物表视图

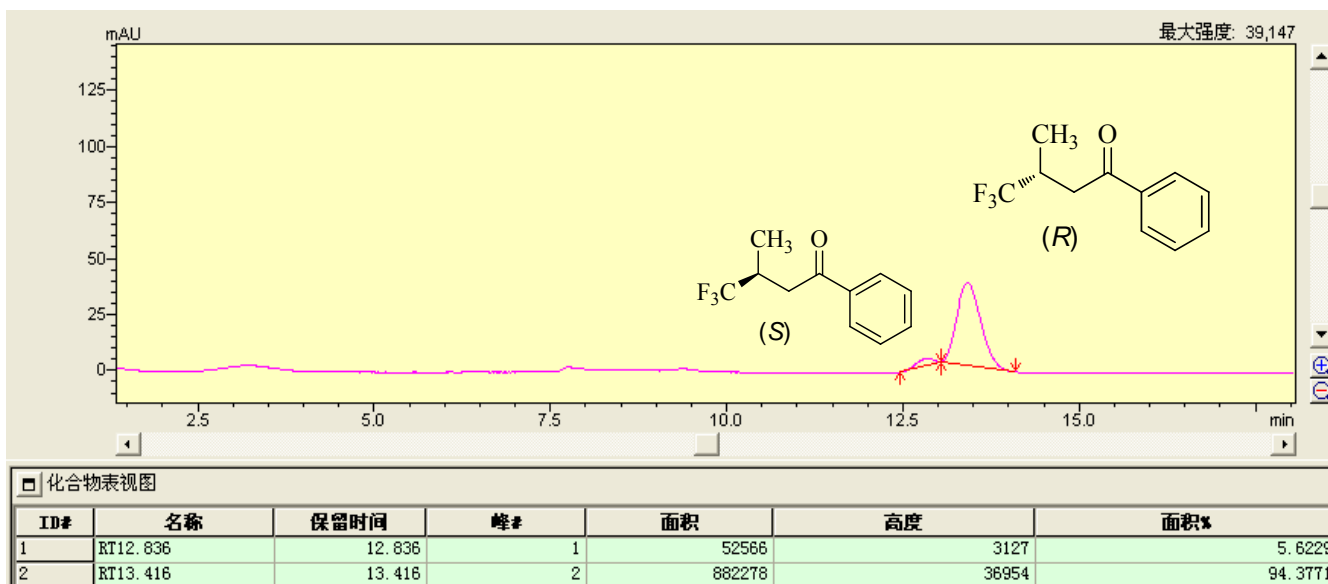
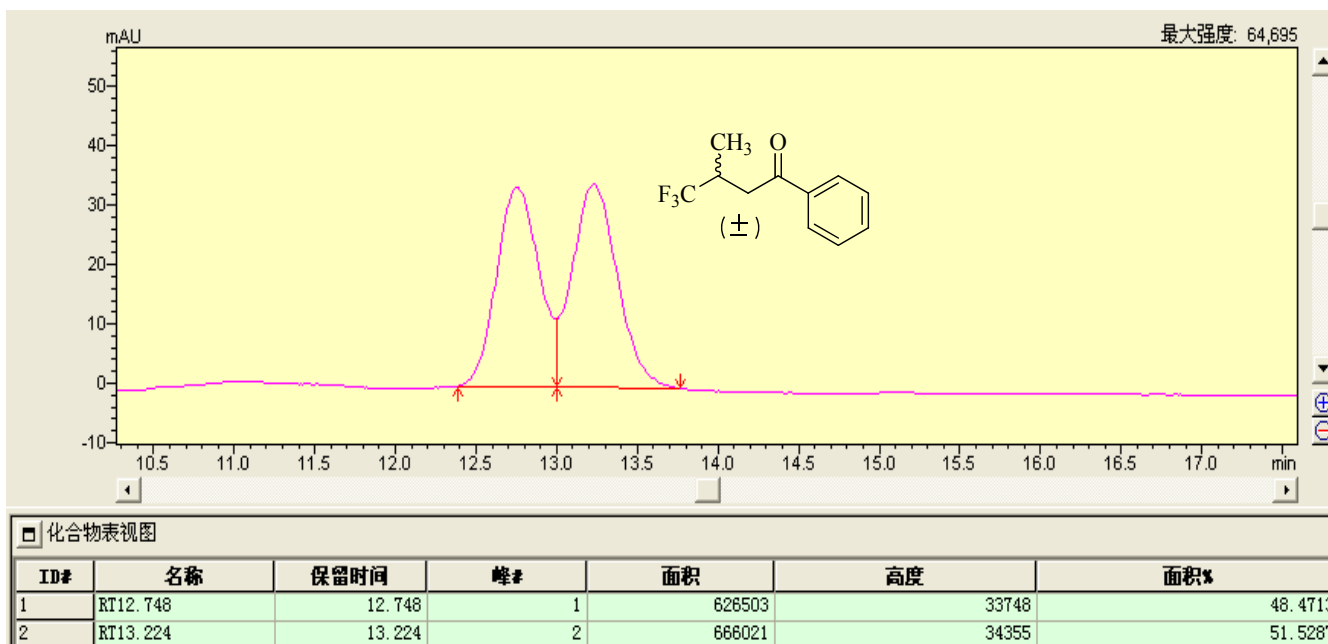
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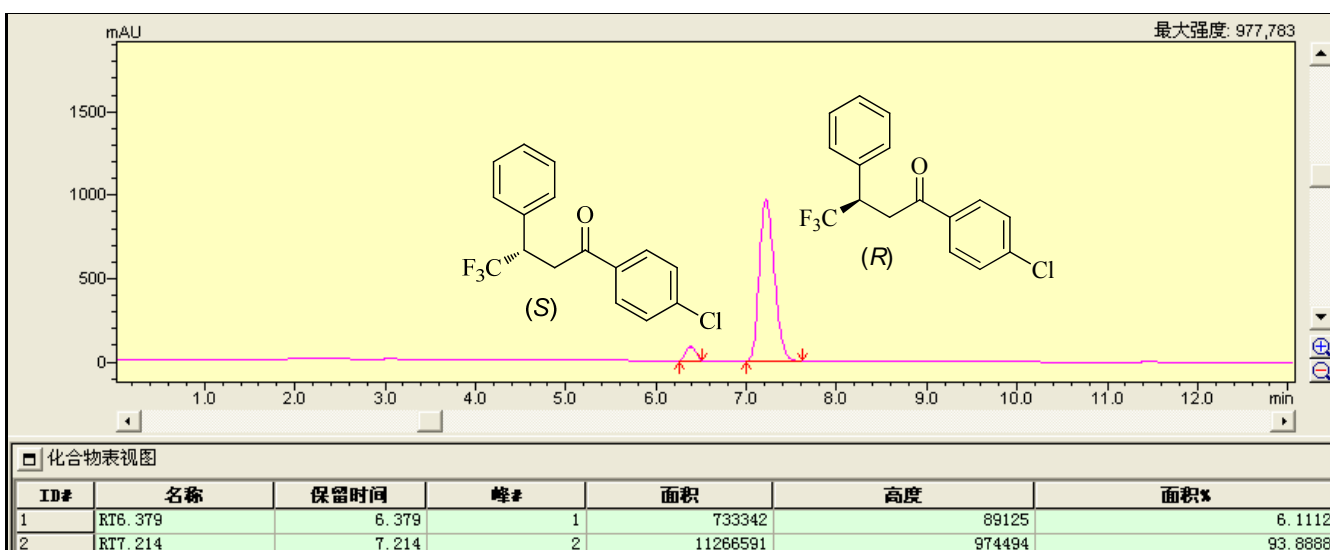
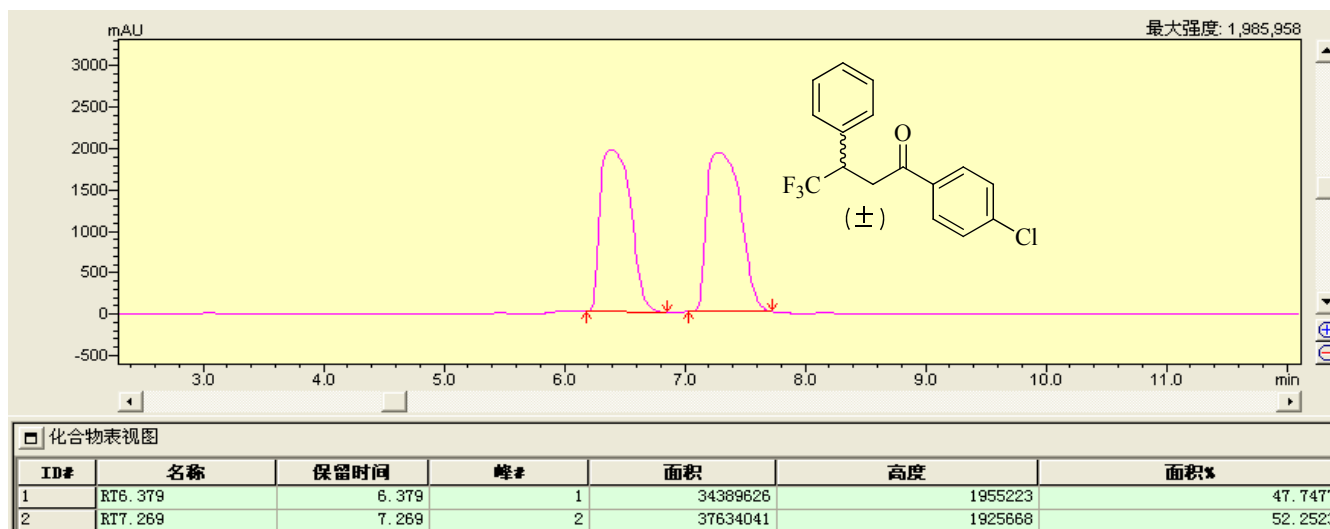
化合物表视图

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2	RT15.062	15.062	2	8156293	301374	14.733	16.008	97.6780

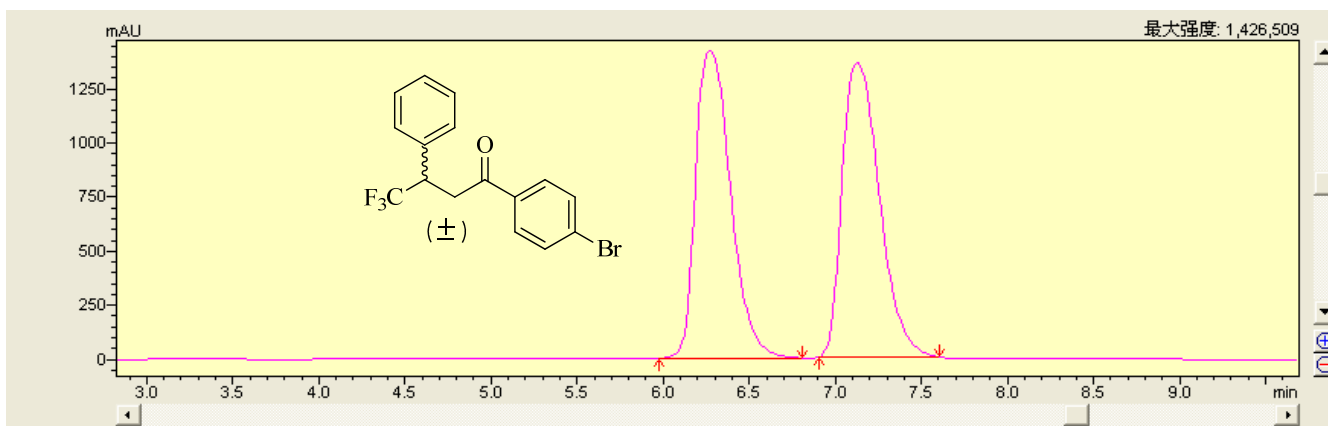
6i: (*R*)-4,4,4-trifluoro-3-methyl-1-phenylbutan-1-one (HPLC: Chiracel OJ-H, detected at 254 nm, eluent: n-hexane/2-propanol = 99/1, flow rate = 0.5 mL/min, 25 °C).



6j: (R)-1-(4-chlorophenyl)-4,4,4-trifluoro-3-phenylbutan-1-one (HPLC: Chiracel OD-H, detected at 254 nm, eluent: n-hexane/2-propanol = 95/5, flow rate = 1.0 mL/min, 25 °C)

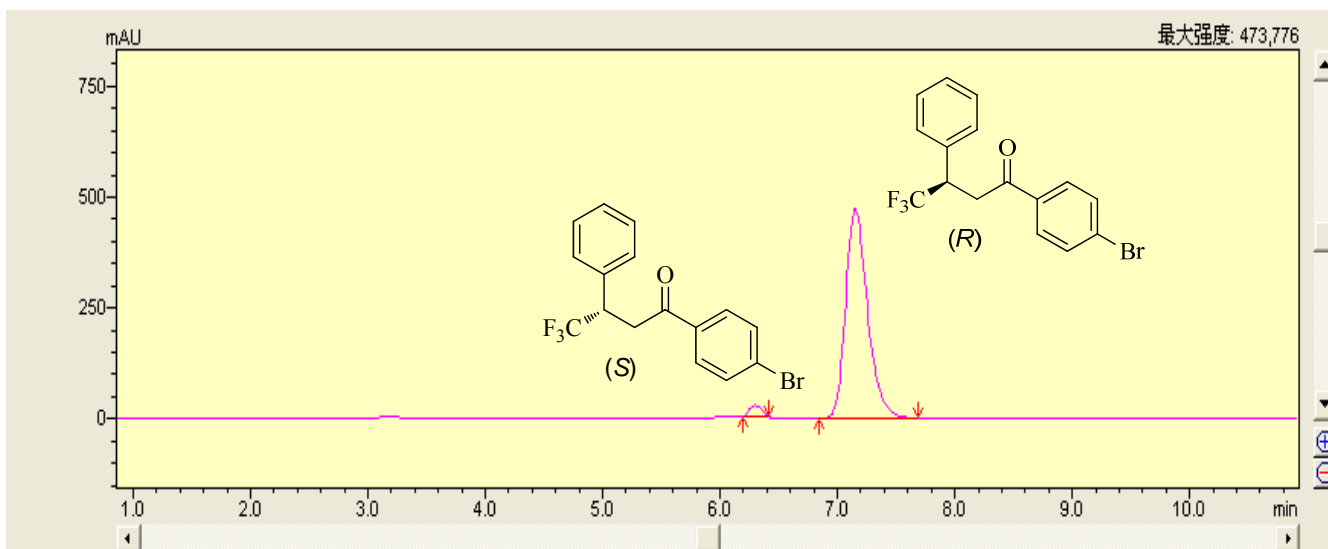


6k: (R)-1-(4-bromophenyl)-4,4,4-trifluoro-3-phenylbutan-1-one (HPLC: Chiracel OD-H, detected at 254 nm, eluent: n-hexane/2-propanol = 95/5, flow rate = 1.0 mL/min, 25 °C).



化合物表视图

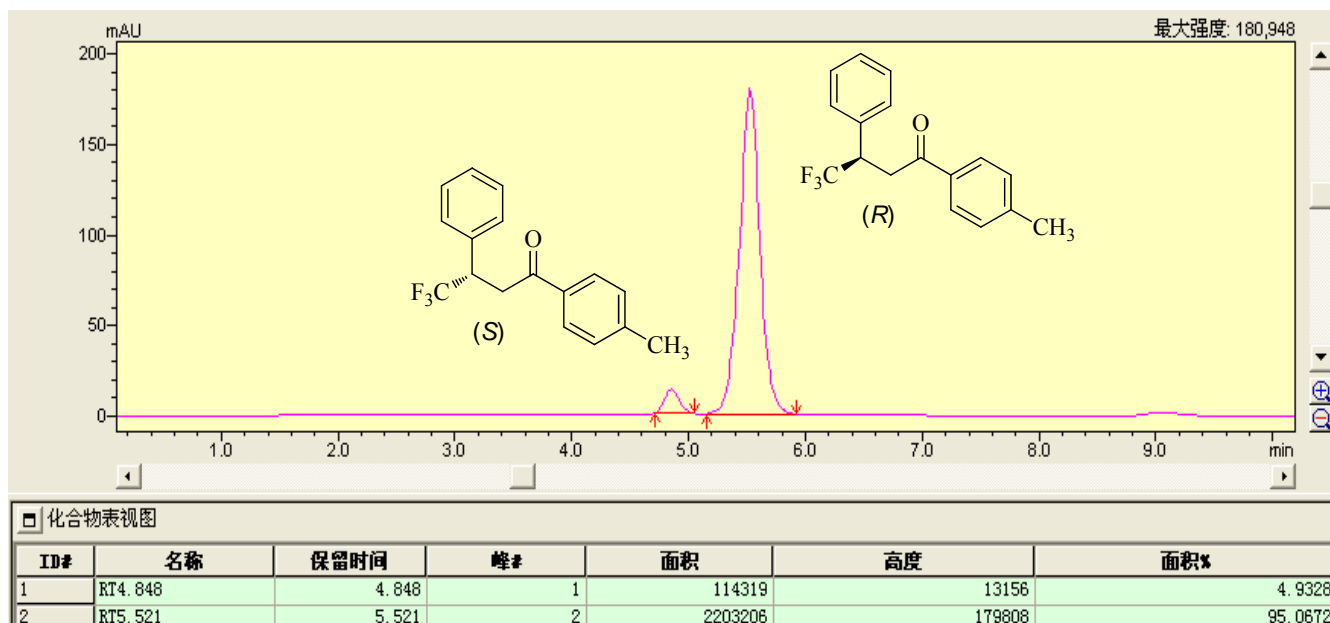
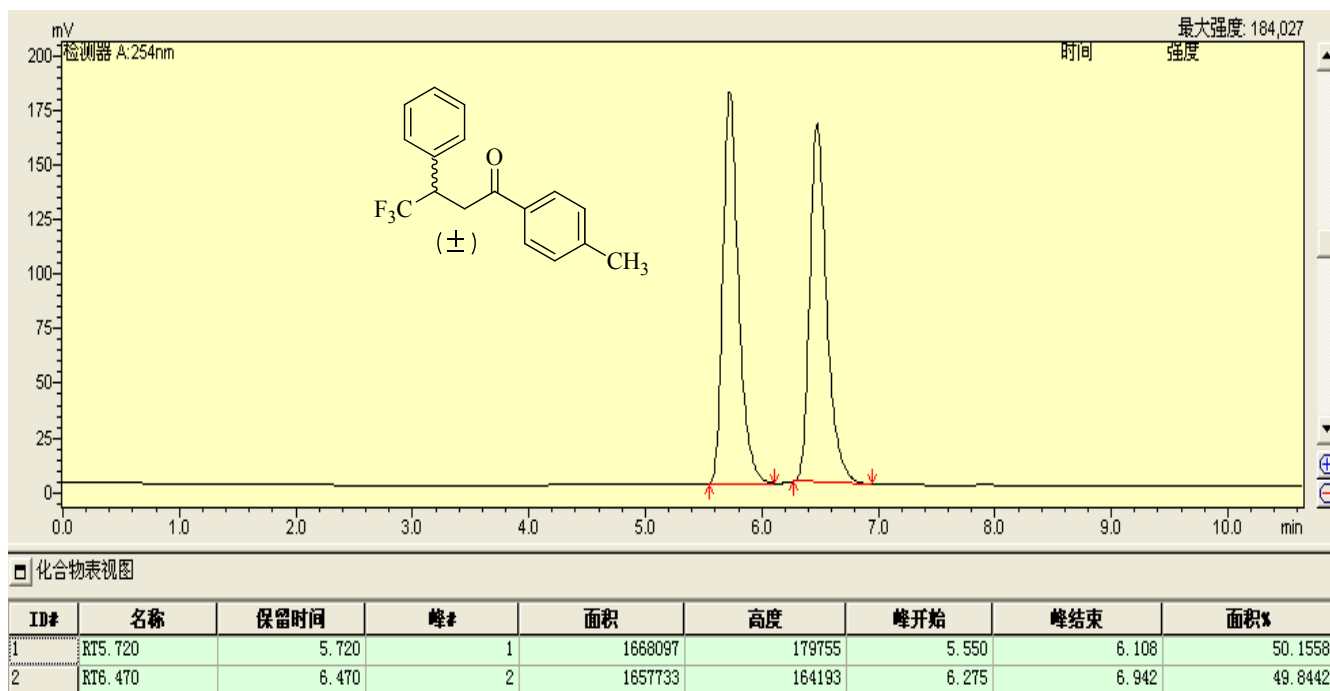
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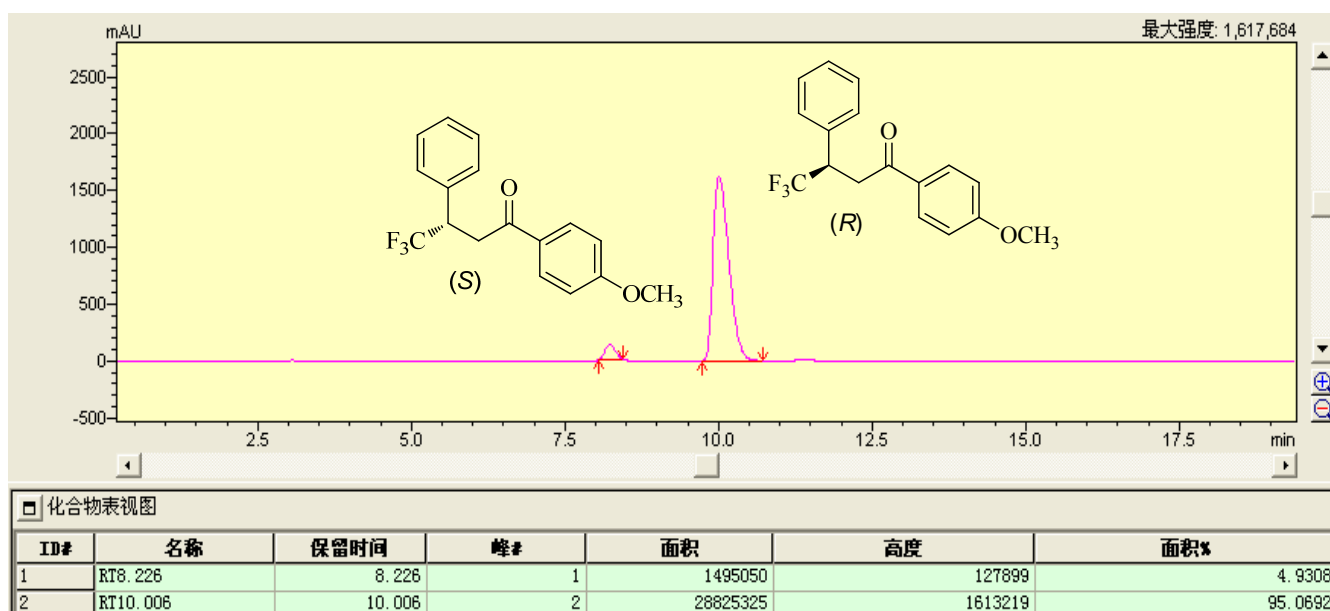
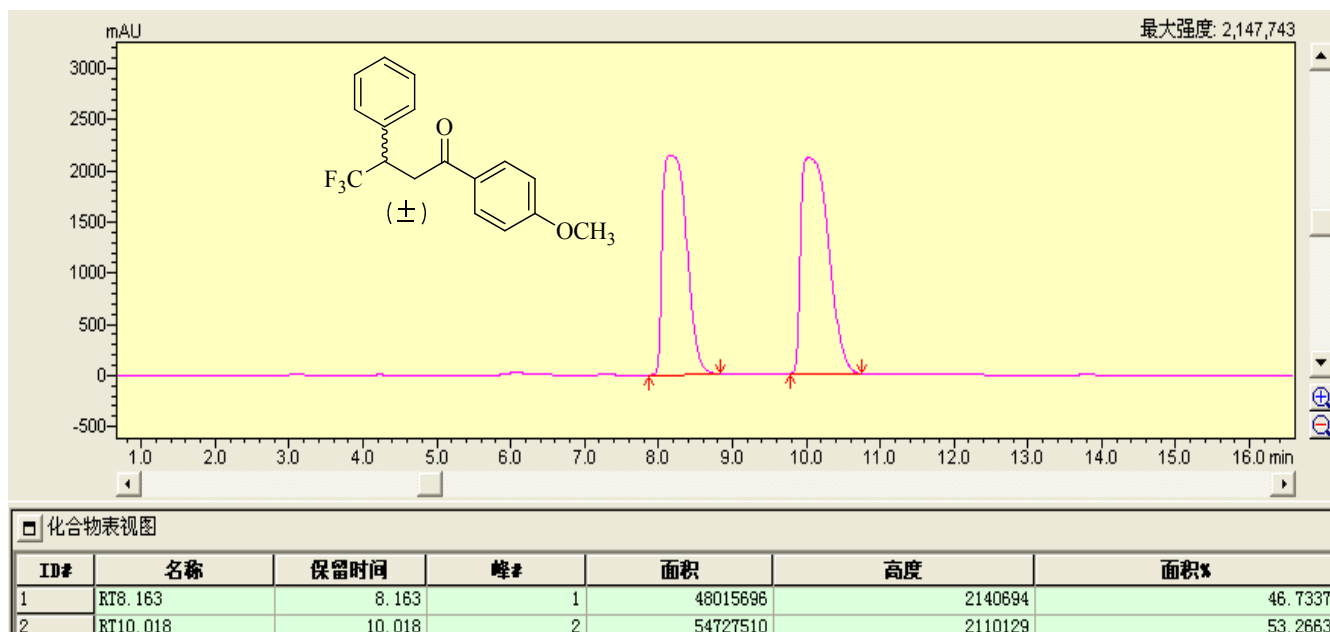
化合物表视图

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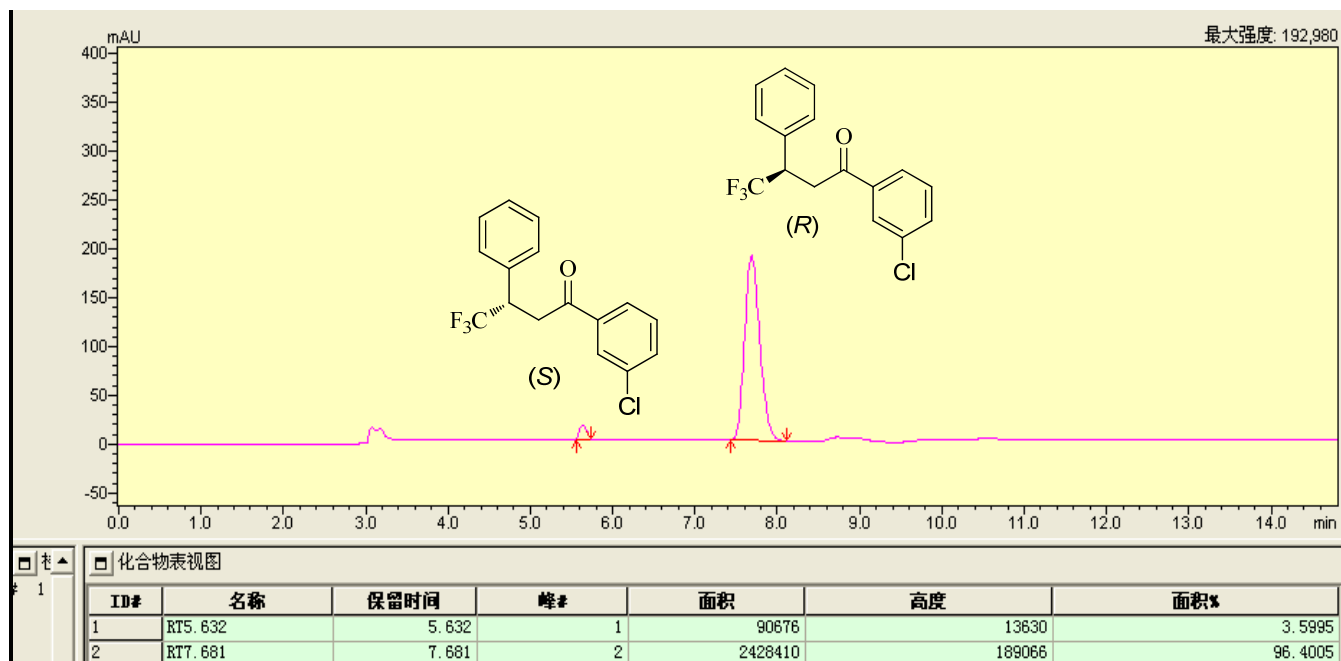
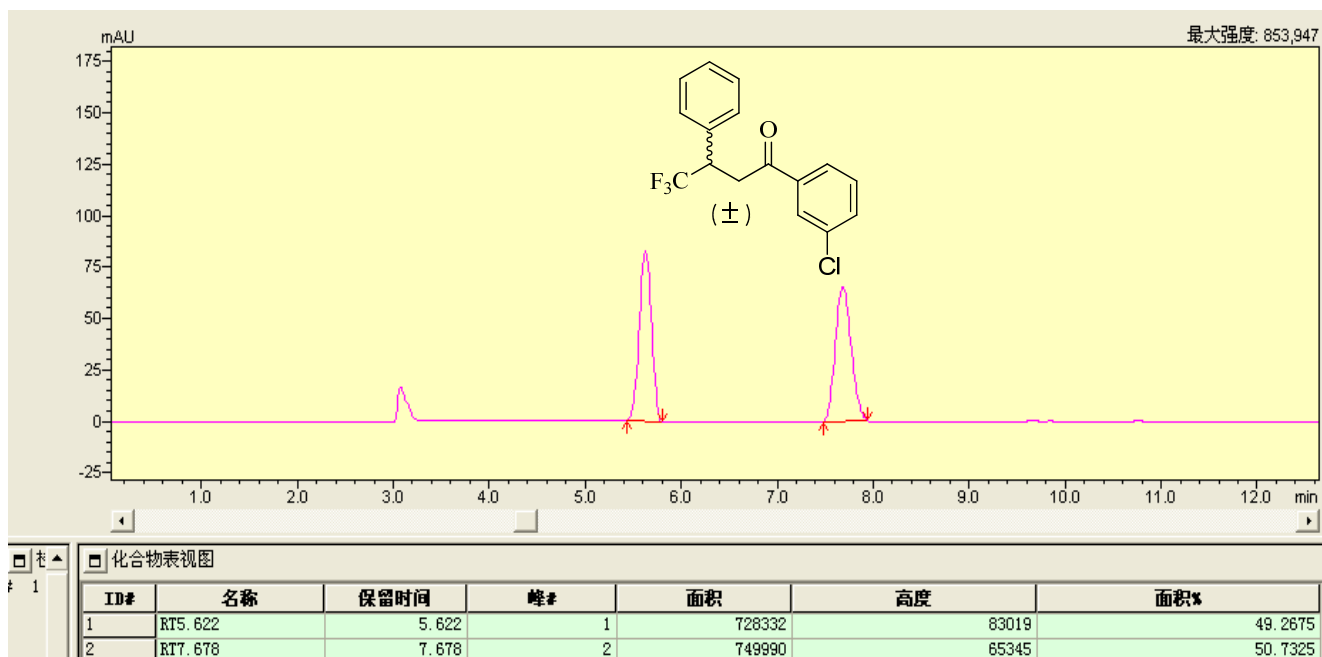
6L: (R)-4,4,4-trifluoro-3-phenyl-1-(p-tolyl)butan-1-one (HPLC: Chiracel OD-H, detected at 254 nm, eluent: n-hexane/2-propanol = 95/5, flow rate = 1.0 mL/min, 25 °C).



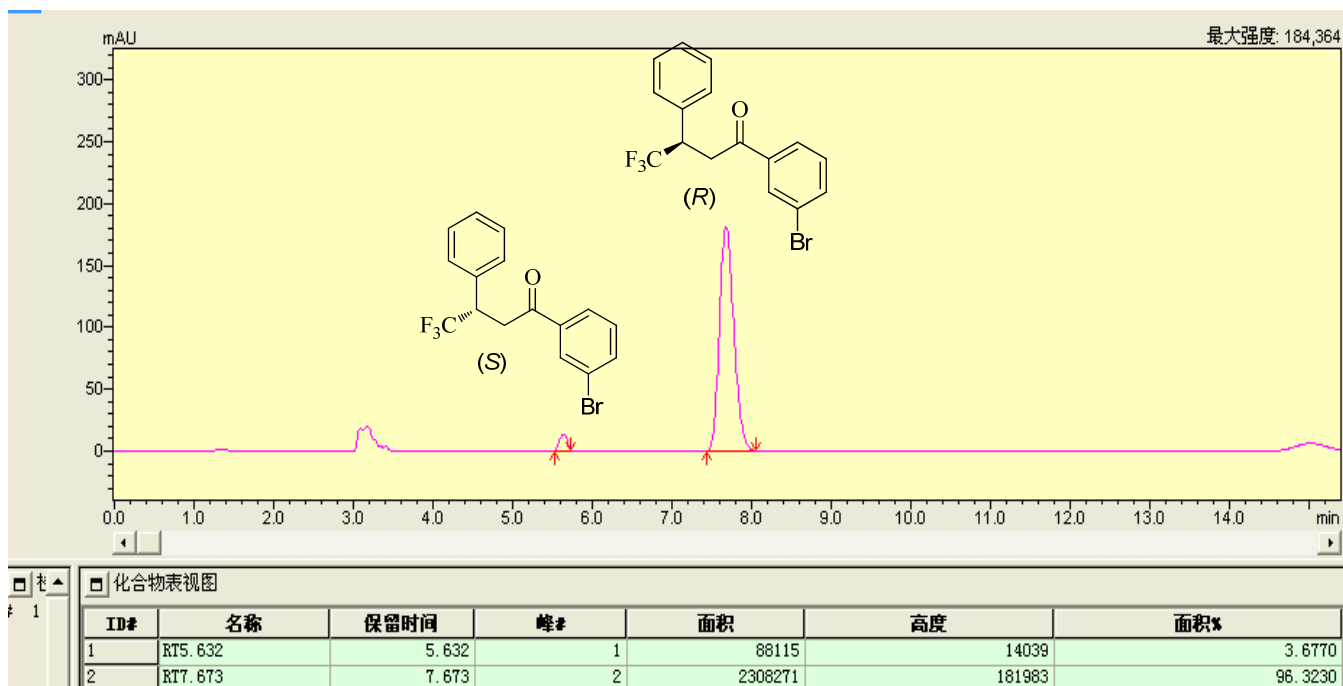
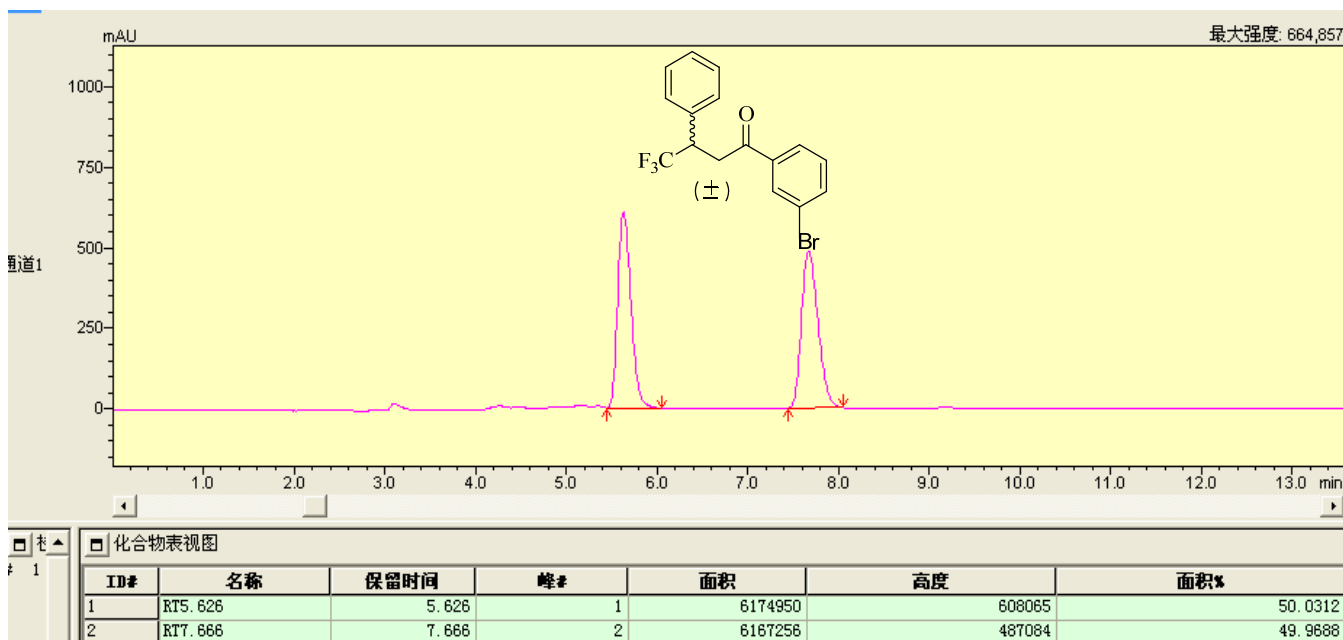
6m: (R)-4,4,4-trifluoro-1-(4-methoxyphenyl)-3-phenylbutan-1-one (4m): (HPLC: Chiracel OD-H, detected at 254 nm, eluent: n-hexane/2-propanol = 95/5, flow rate = 1.0 mL/min, 25 °C).



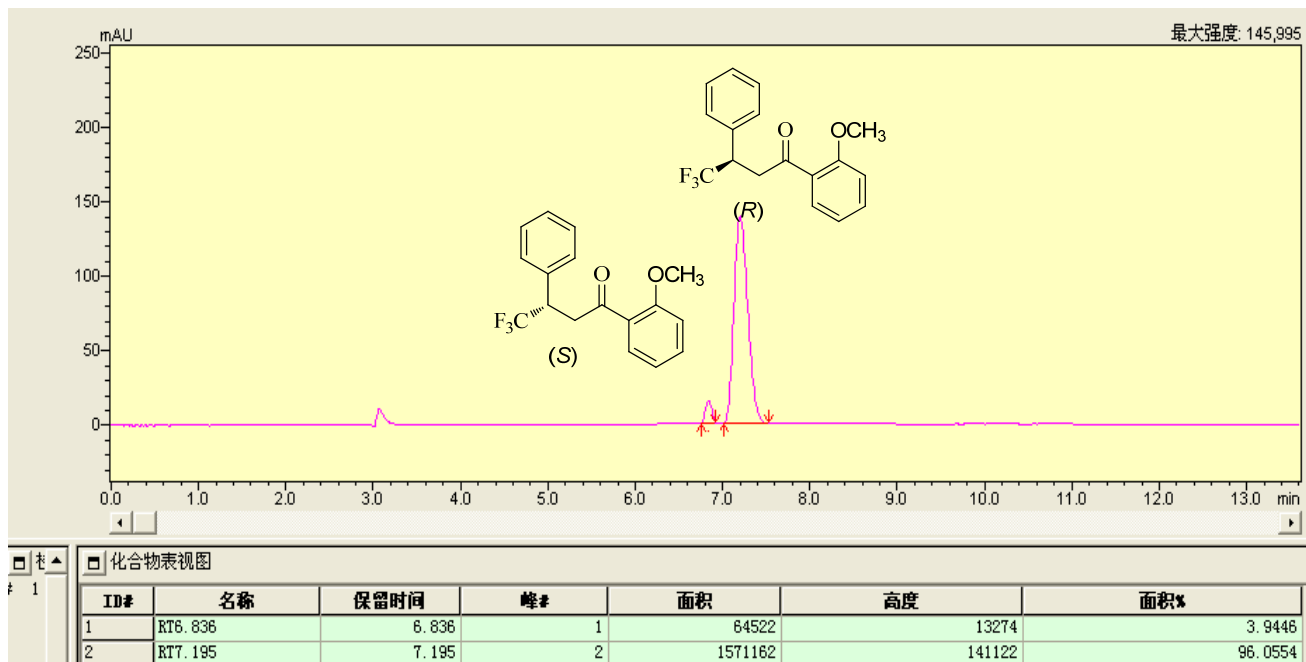
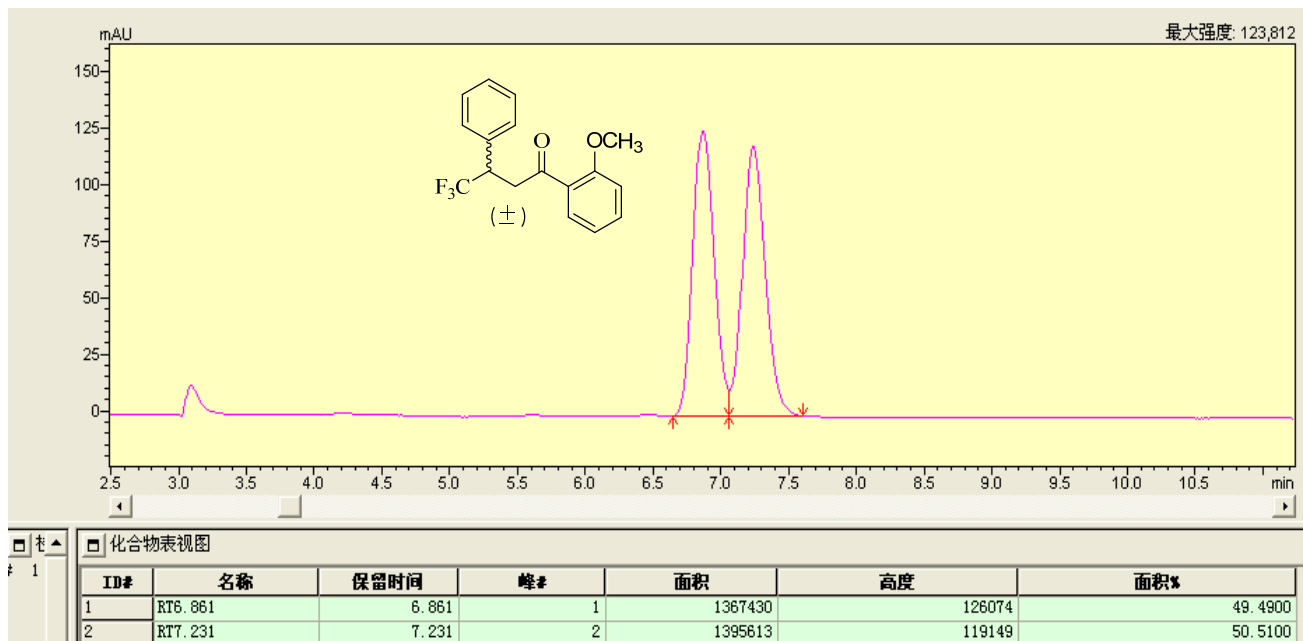
6n: (R)-1-(3-chlorophenyl)-4,4,4-trifluoro-3-phenylbutan-1-one (HPLC: Chiracel OD-H, detected at 254 nm, eluent: n-hexane/2-propanol = 97/3, flow rate = 1.0 mL/min, 25 °C)



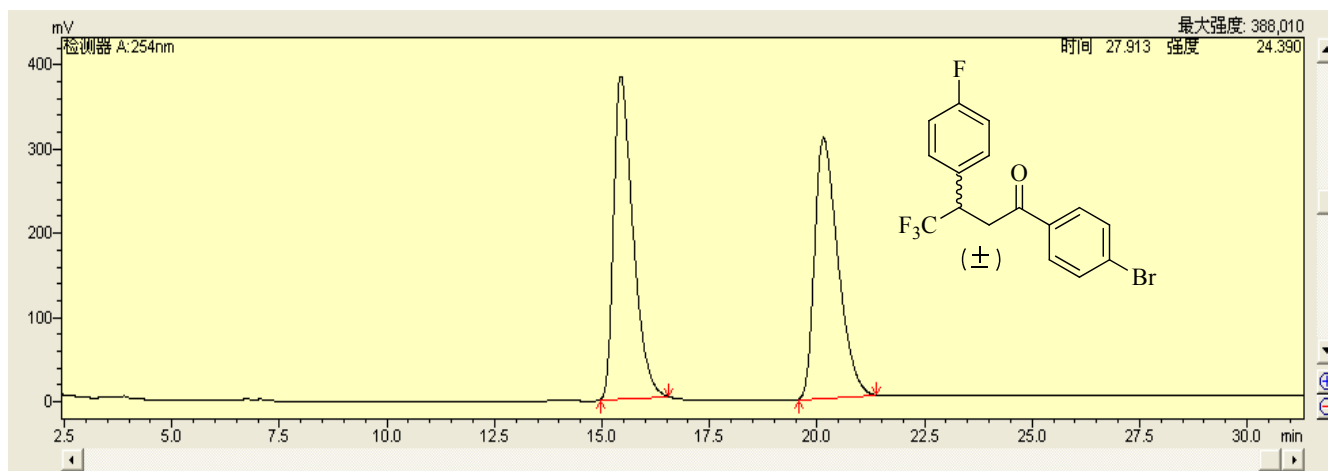
60: (R)-1-(3-bromophenyl)-4,4,4-trifluoro-3-phenylbutan-1-one (HPLC: Chiracel OD-H, detected at 254 nm, eluent: n-hexane/2-propanol = 97/3, flow rate = 1.0 mL/min, 25 °C).



6p: (R)-4,4,4-trifluoro-1-(2-methoxyphenyl)-3-phenylbutan-1-one (HPLC: Chiracel OD-H, detected at 254 nm, eluent: n-hexane/2-propanol = 97/3, flow rate = 1.0 mL/min, 25 °C).

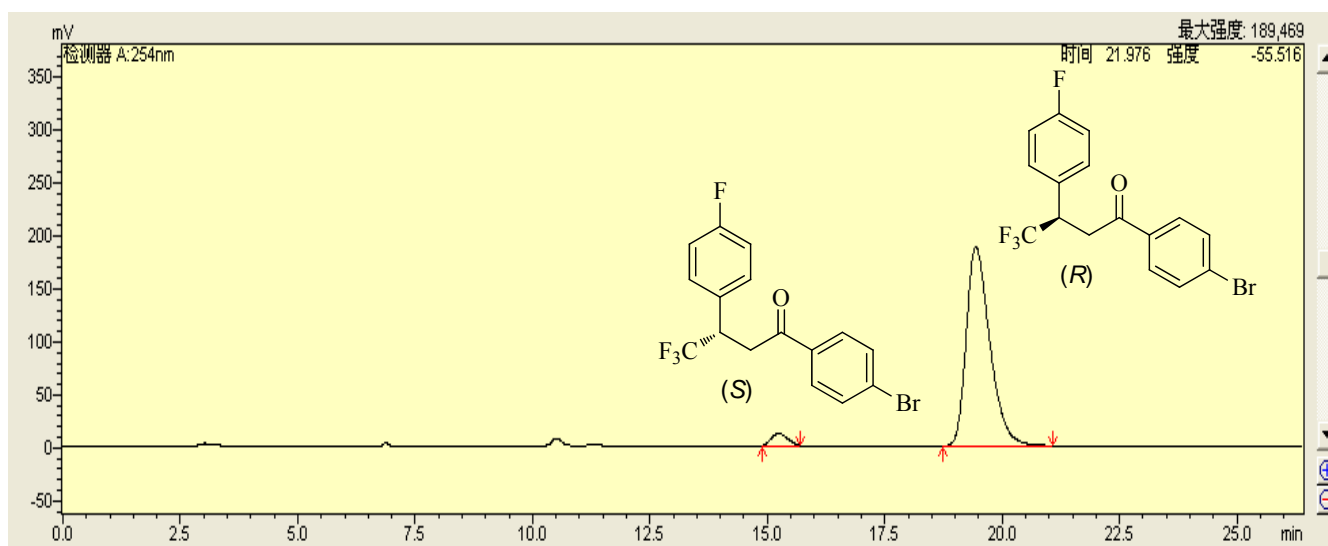


6q: (R)-1-(4-bromophenyl)-4,4,4-trifluoro-3-(4-fluorophenyl)butan-1-one (HPLC: Chiralcel OJ-H, detected at 254 nm, eluent: n-hexane/2-propanol = 95/5, flow rate = 1.5 mL/min, 25 °C).



化合物表视图

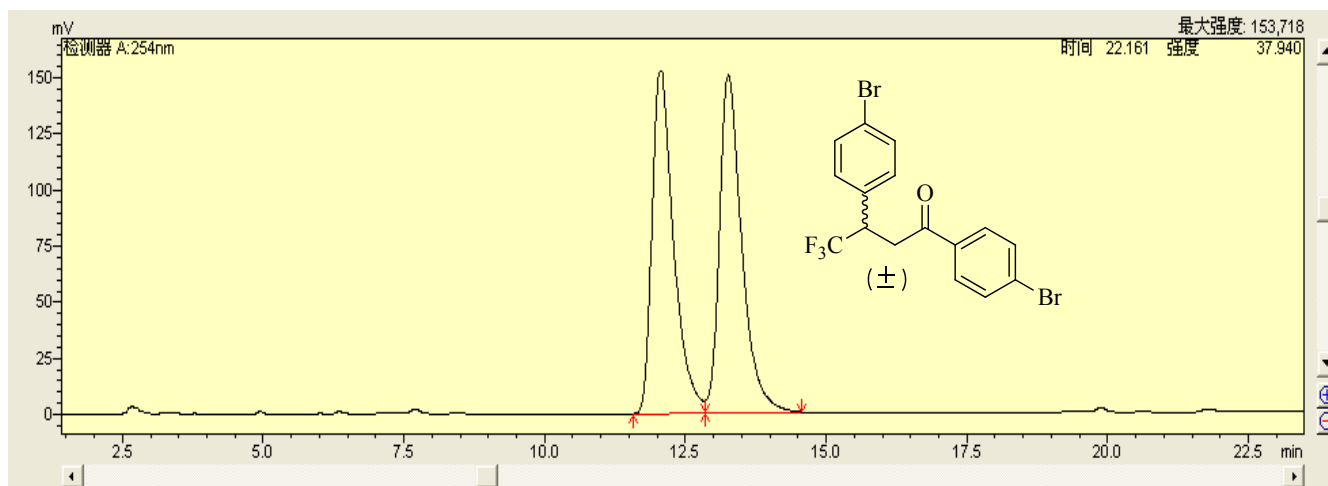
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化合物表视图

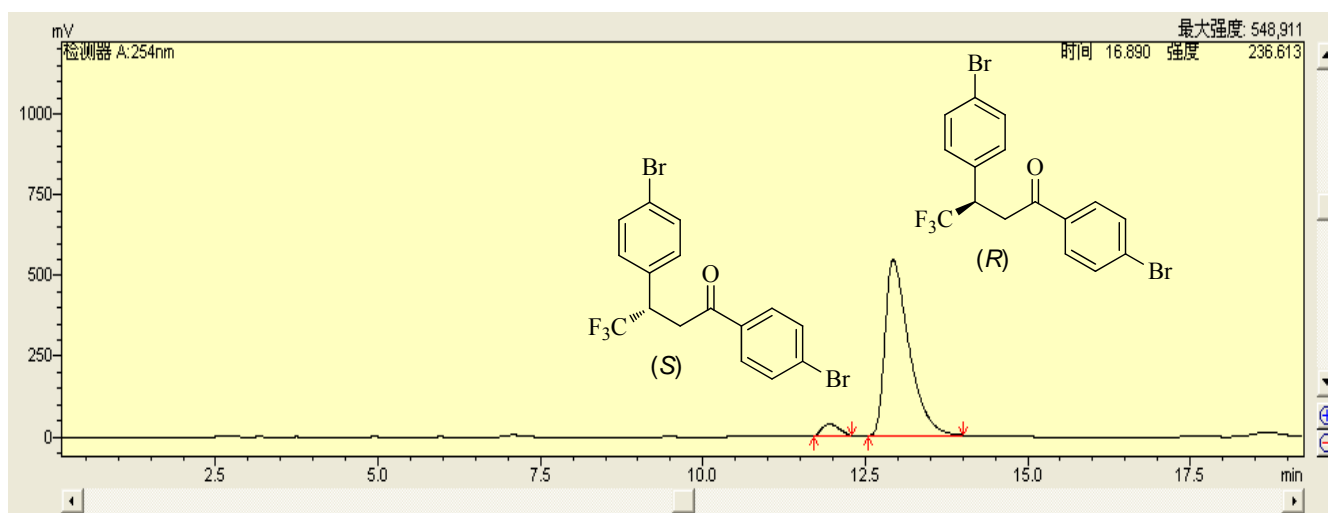
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2	RT19.438	19.438	2	6608002	187855	18.750	21.083	95.6958

6r: (R)-1,3-bis(4-bromophenyl)-4,4,4-trifluorobutan-1-one (4o): (HPLC: Chiracel OJ-H, detected at 254 nm, eluent: n-hexane/2-propanol = 95/5, flow rate = 1.5 mL/min, 25 °C).



化合物视图

ID#	名称	保留时间	峰#	面积	高度	峰开始	峰结束	面积%
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化合物视图

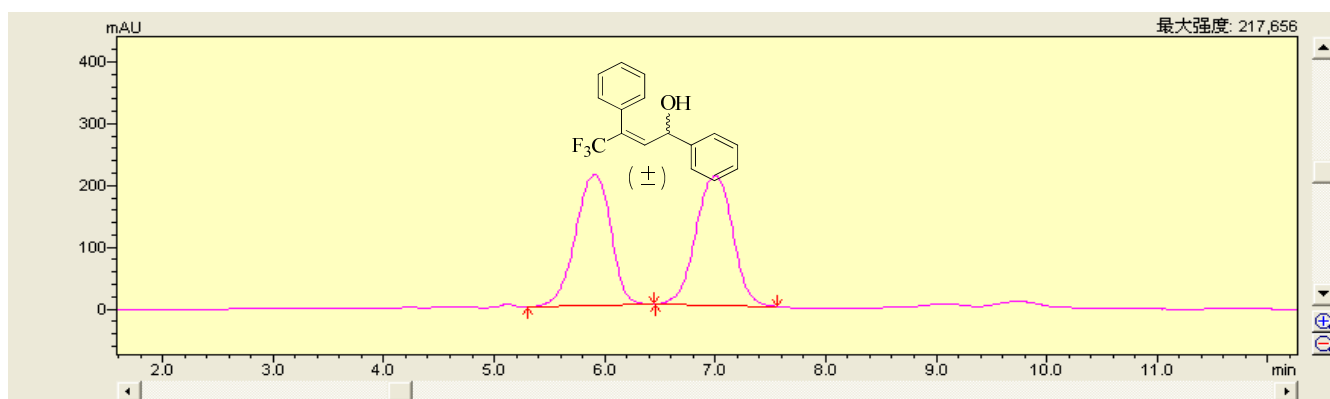
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2	RT12.928	12.928	2	14266521	545199	12.542	14.325	95.0430

Figure S5. Enantioselectivereductions of β -trifluoromethylated- α,β -unsaturated ketones to chiral β -trifluoromethylated alcohols. [The products were analyzed by a HPLC with a UV-Vis detector using a Daicel OD-H or AD-H chiralcel column ($\Phi 0.46 \times 25$ cm). Please see literatures (Catal. Sci. Technol. 2015, 5, 1750; Angew. Chem. Int. Ed. 2012, 51, 6467).

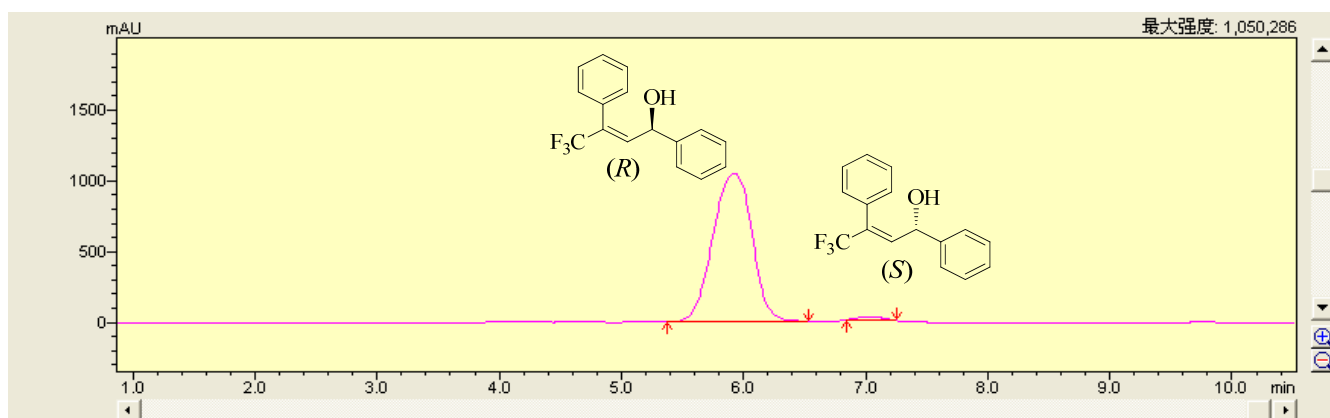
Translation of Chinese to English is as follows:

Peak	RetTime [min]	Area	Area%	Height	Height%
峰号	保留时间	面积	面积%	峰高	峰高%
1	18.474	235819.9	92.0500	13827.2	79.0685
2	19.395	9109.7	3.5589	1042.4	5.9806

5a: (*R,E*)-4,4,4-trifluoro-1,3-diphenylbut-2-en-1-ol (HPLC: Chiralcel OD-H, detected at 254 nm, eluent: n-hexane/2-propanol = 95/5, flow rate = 1.0 mL/min, 25 °C).

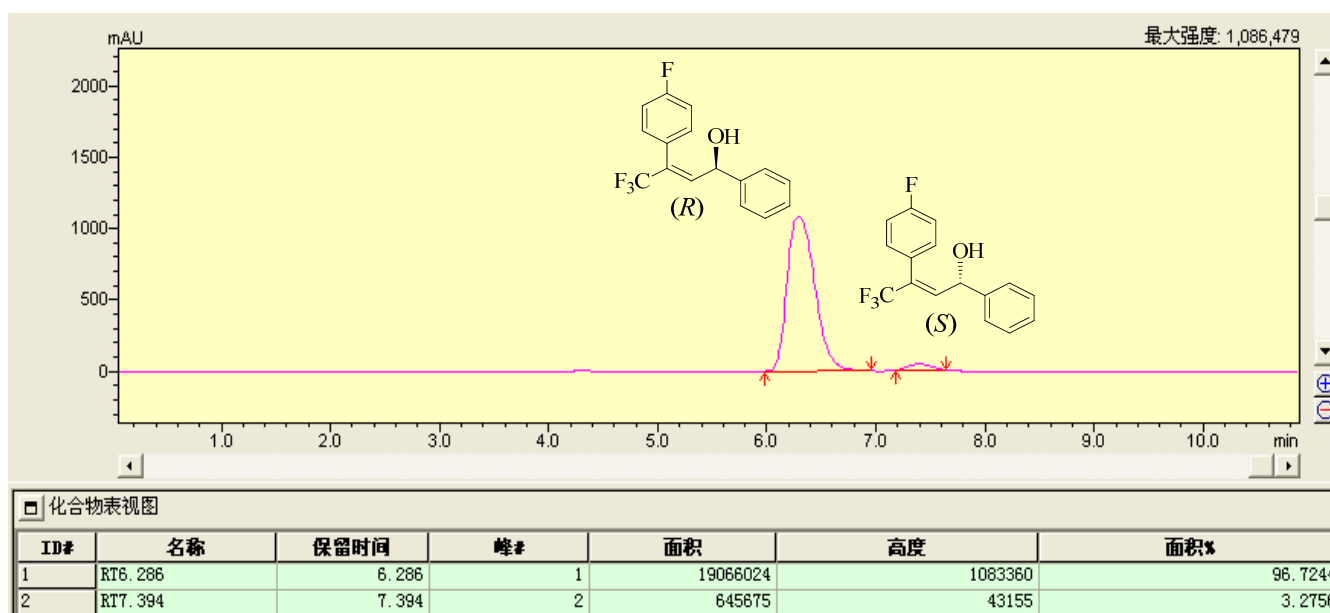
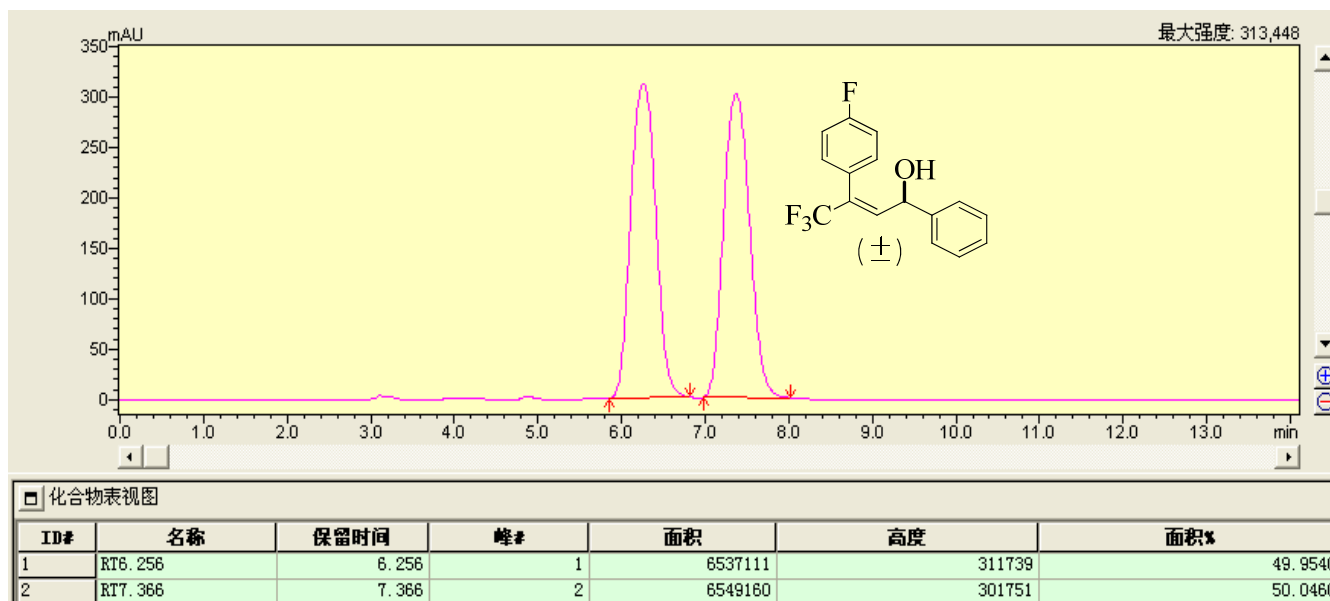


ID#	名称	保留时间	峰#	面积	高度	面积%
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2	RT6.995	6.995	2	4848753	209191	50.7772

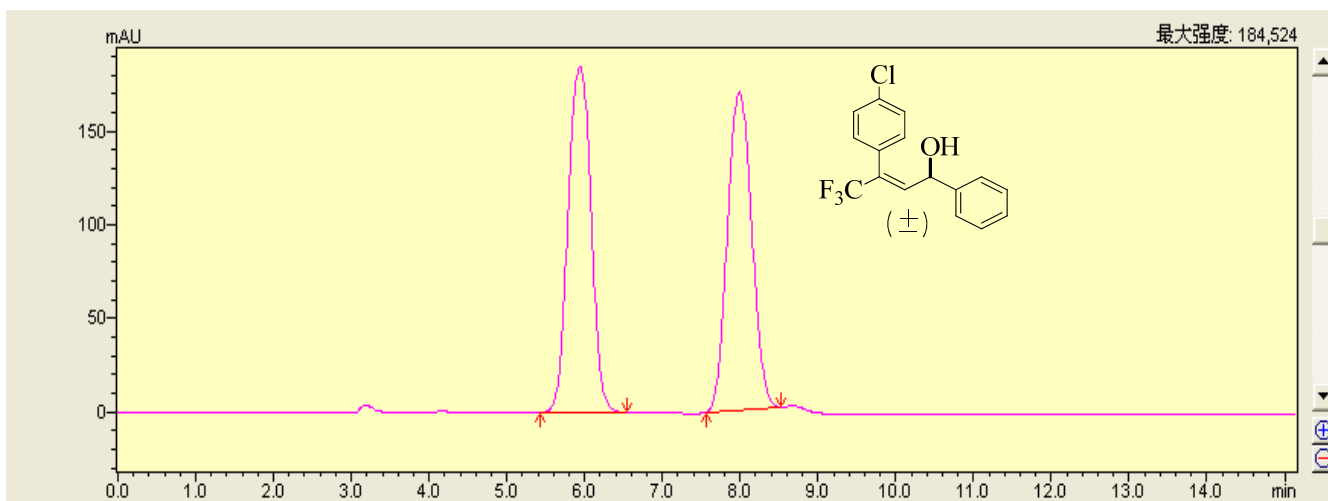


ID#	名称	保留时间	峰#	面积	高度	面积%
1	RT5.917	5.917	1	23384182	1045374	98.5174
2	RT7.027	7.027	2	351920	23303	1.4826

5b: (*R,E*)-4,4,4-trifluoro-3-(4-fluorophenyl)-1-phenylbut-2-en-1-ol (HPLC: Chiralcel OD-H, detected at 254 nm, eluent: n-hexane/2-propanol = 95/5, flow rate = 1.0 mL/min, 25 °C).

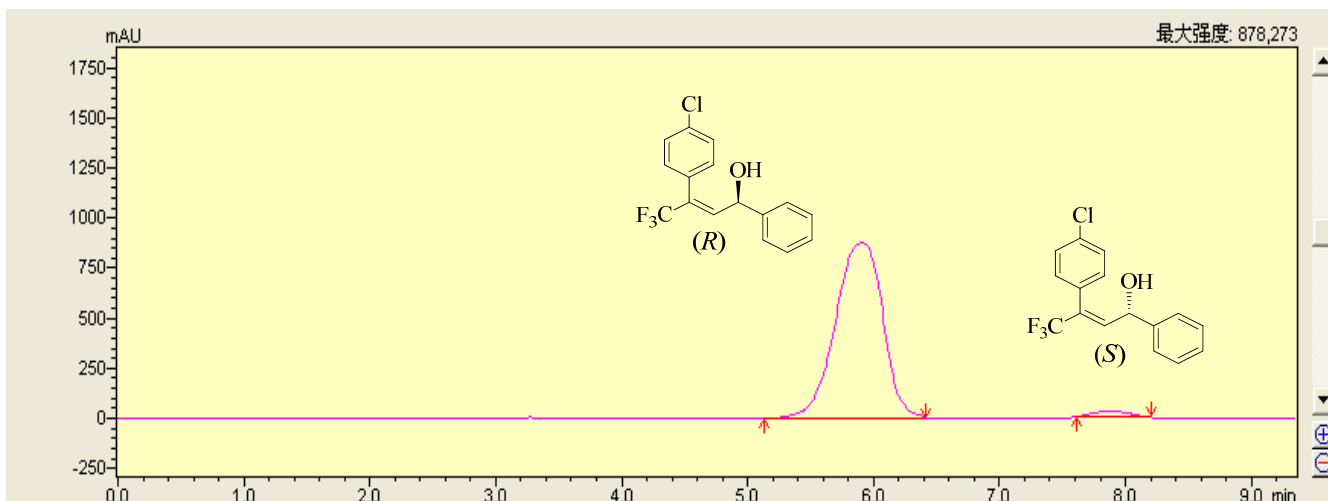


5c: (R,E)-3-(4-chlorophenyl)-4,4,4-trifluoro-1-phenylbut-2-en-1-ol (HPLC: Chiralcel OD-H, detected at 254 nm, eluent: n-hexane/2-propanol = 95/5, flow rate = 1.0 mL/min, 25 °C).



化合物表视图

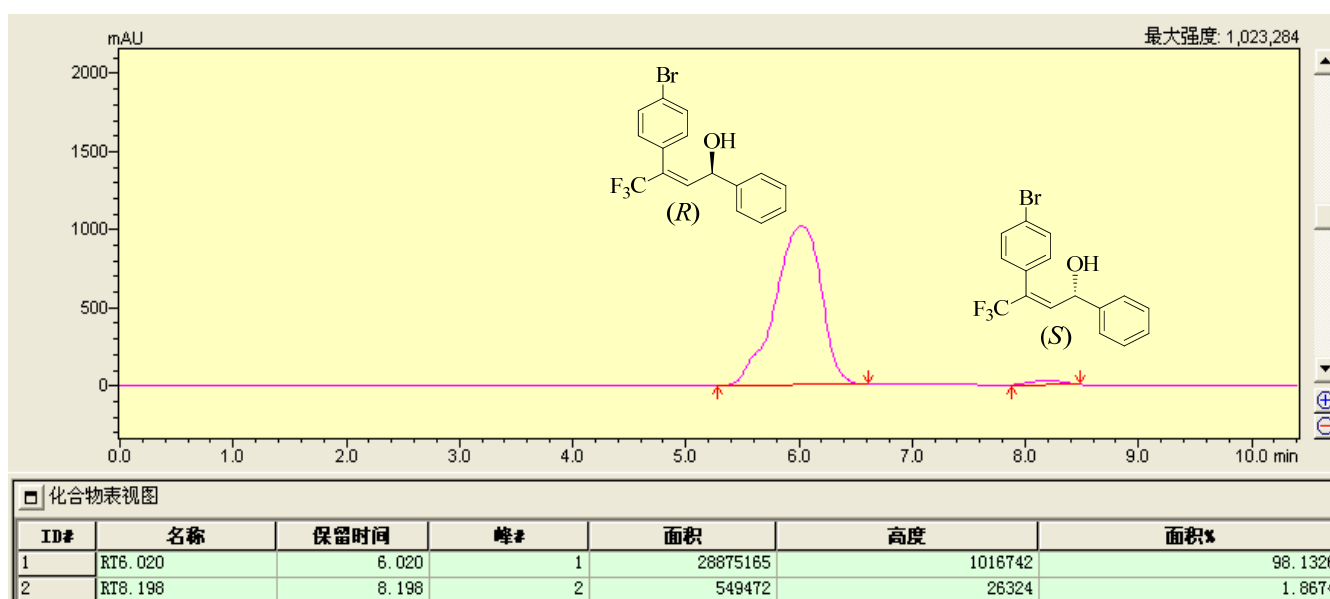
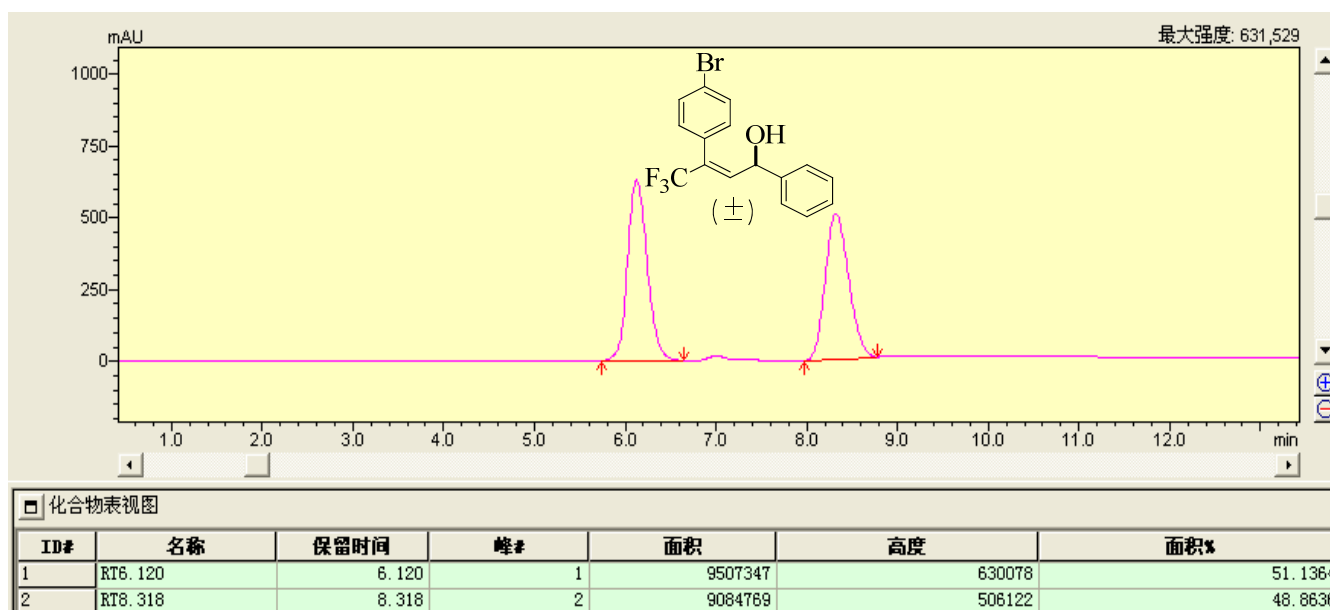
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2	RT7.985	7.985	2	3703022	170076	49.2094



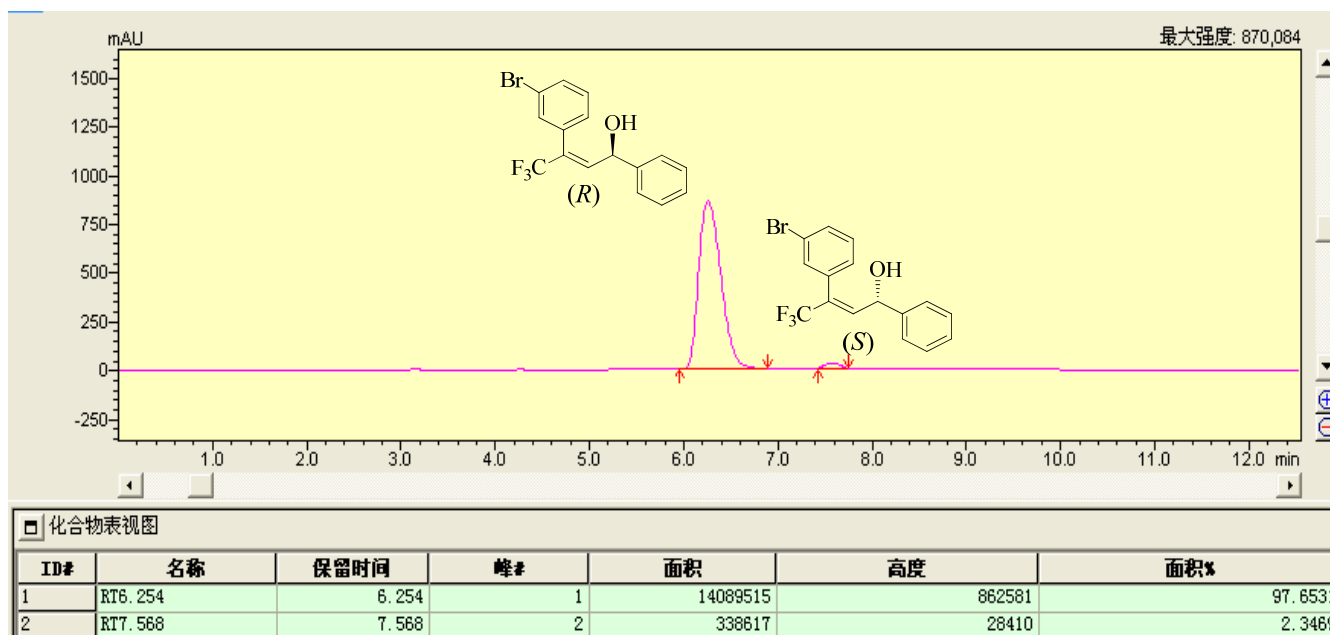
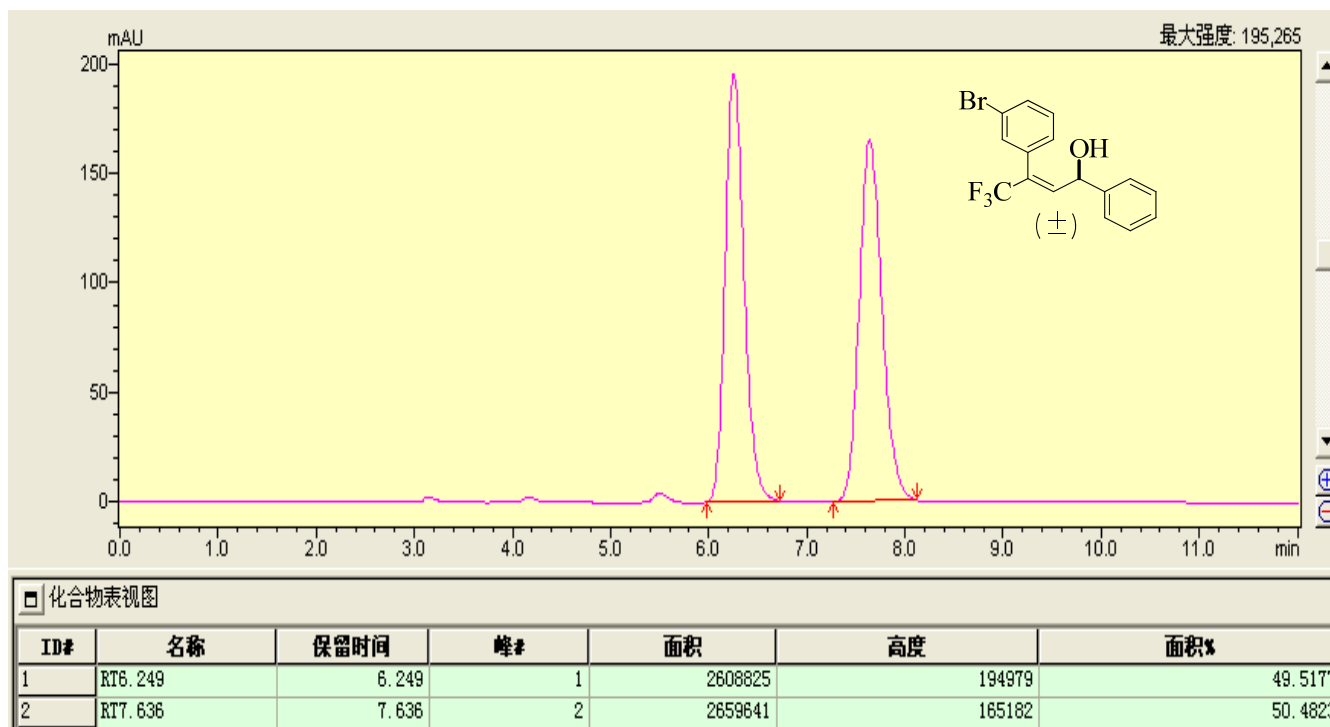
化合物表视图

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2	RT7.880	7.880	2	582729	28561	2.4776

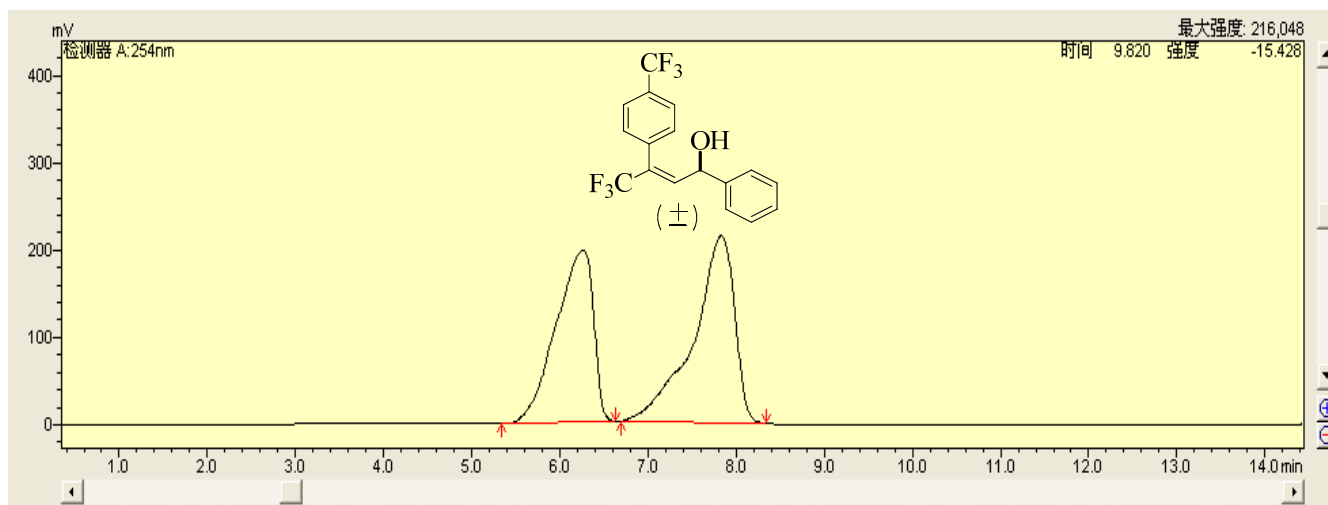
5d: (*R,E*)-3-(4-bromophenyl)-4,4,4-trifluoro-1-phenylbut-2-en-1-ol (HPLC: Chiracel OD-H, detected at 254 nm, eluent: n-hexane/2-propanol = 95/5, flow rate = 1.0 mL/min, 25 °C).



5e: (*R,E*)-3-(3-bromophenyl)-4,4,4-trifluoro-1-phenylbut-2-en-1-ol (HPLC: Chiracel OD-H, detected at 254 nm, eluent: n-hexane/2-propanol = 95/5, flow rate = 1.0 mL/min, 25 °C).

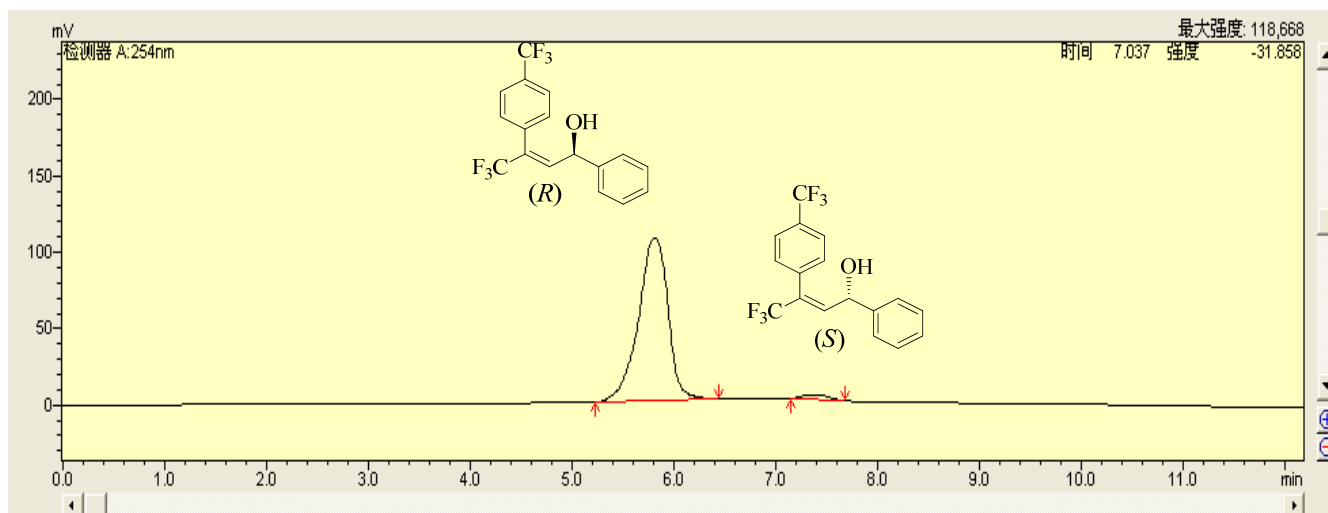


5f: (R,E)-4,4,4-trifluoro-1-phenyl-3-(4-(trifluoromethyl)phenyl)but-2-en-1-ol (HPLC: Chiracel OD-H, detected at 254 nm, eluent: n-hexane/2-propanol = 97/3, flow rate = 1.0 mL/min, 25 °C).



化合物表视图

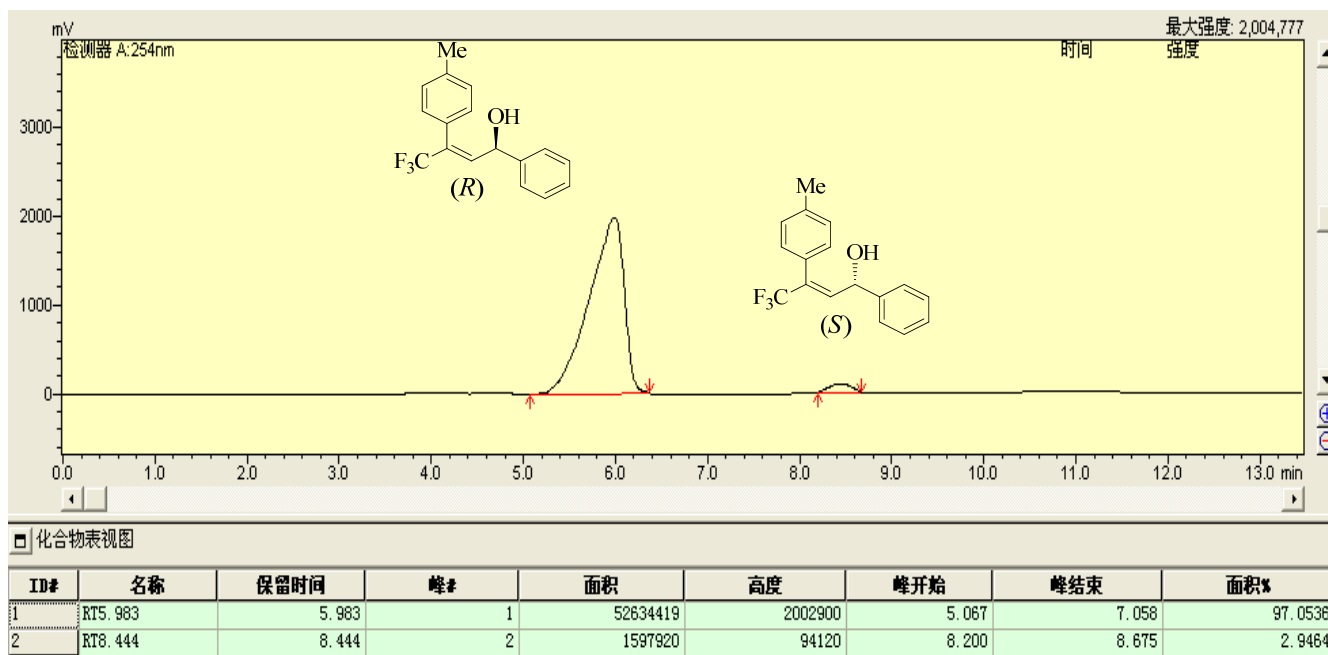
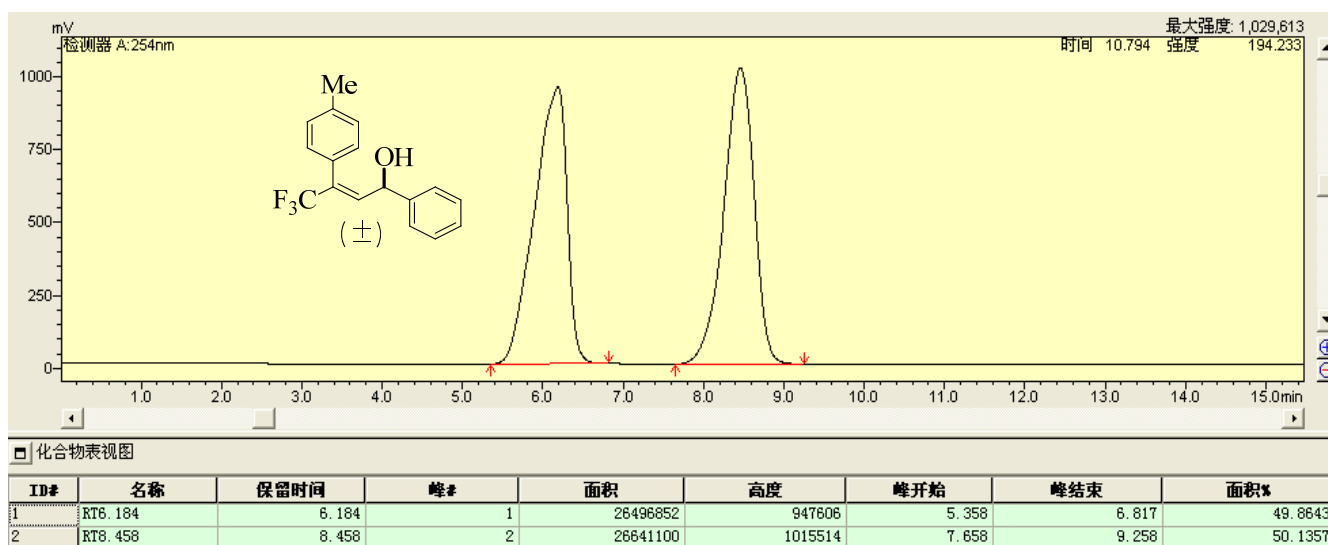
ID#	名称	保留时间	峰#	面积	高度	峰开始	峰结束	面积%
1	RT6.261	6.261	1	5842032	197596	5.333	6.625	45.7465
2	RT7.826	7.826	2	6928428	213650	6.700	8.342	54.2535



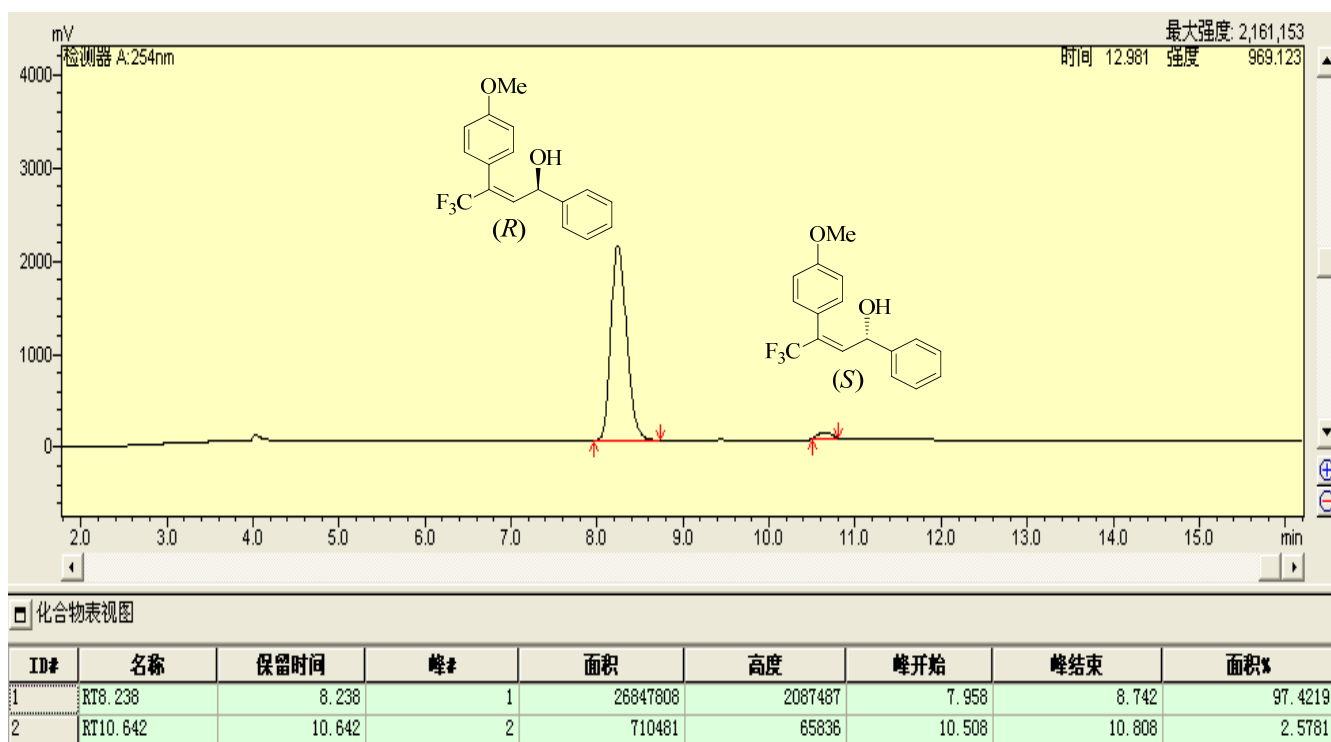
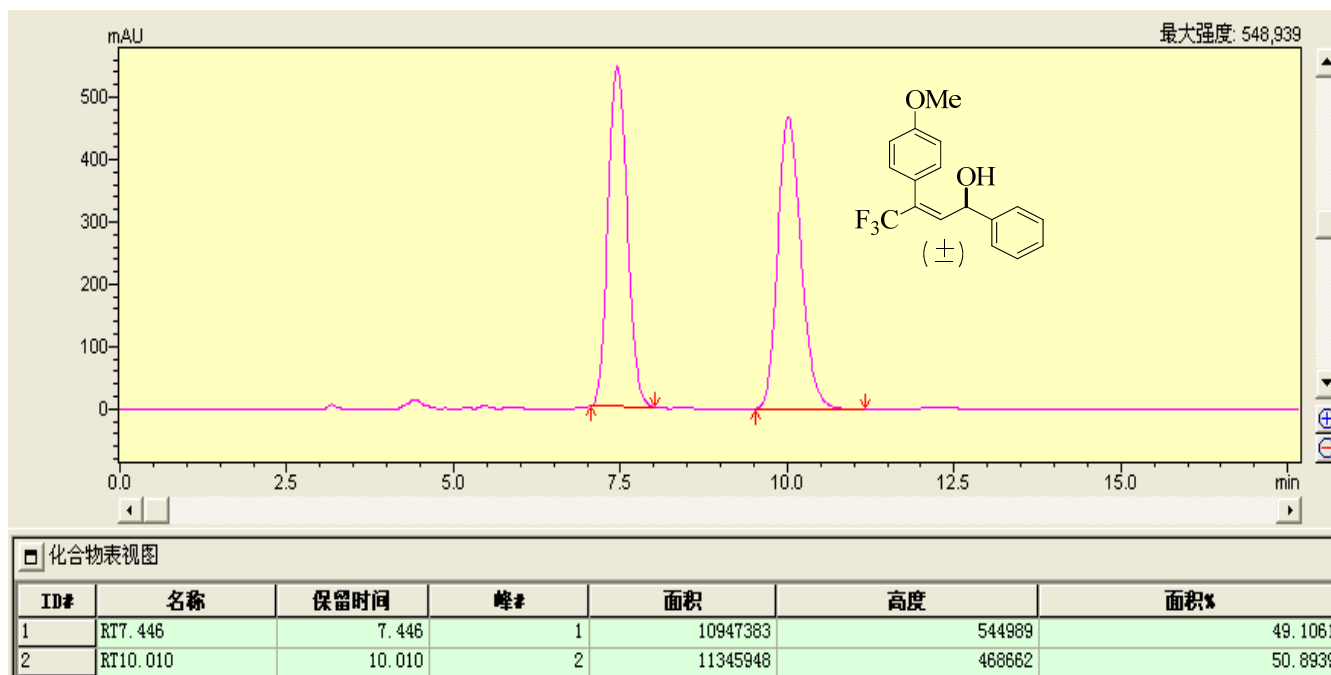
化合物表视图

ID#	名称	保留时间	峰#	面积	高度	峰开始	峰结束	面积%
1	RT5.802	5.802	1	2168805	106949	5.225	6.433	97.6351
2	RT7.353	7.353	2	52532	2984	7.150	7.675	2.3649

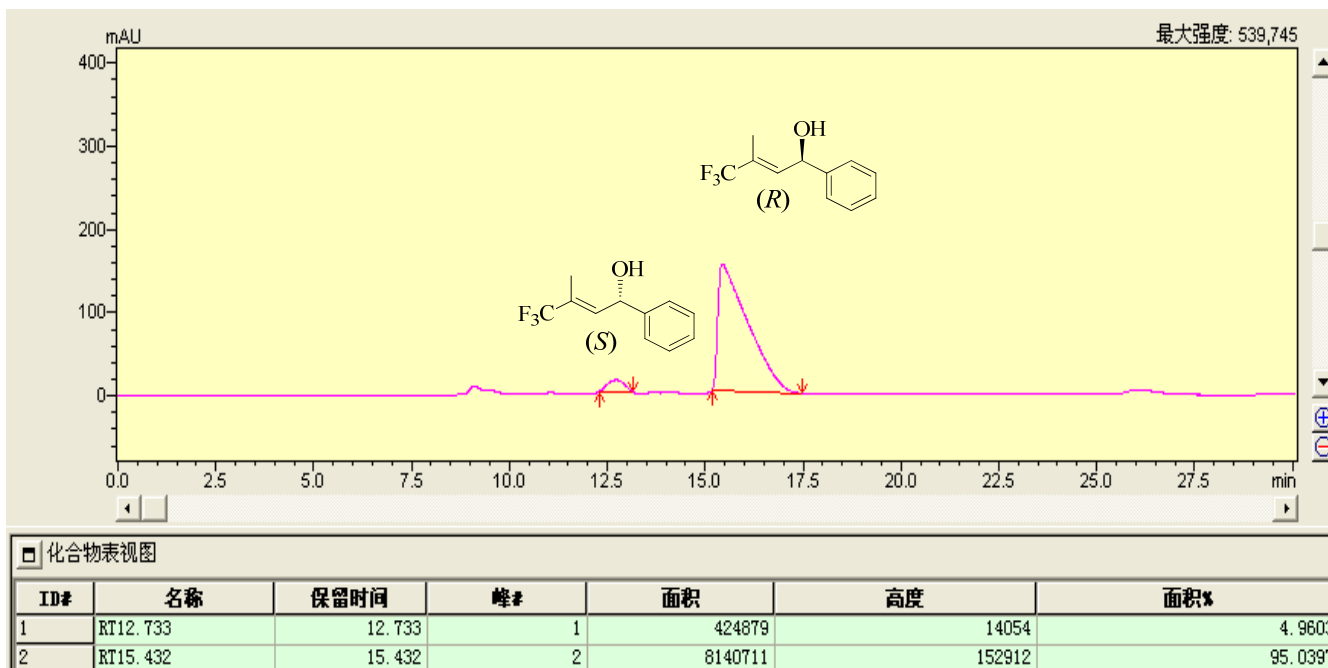
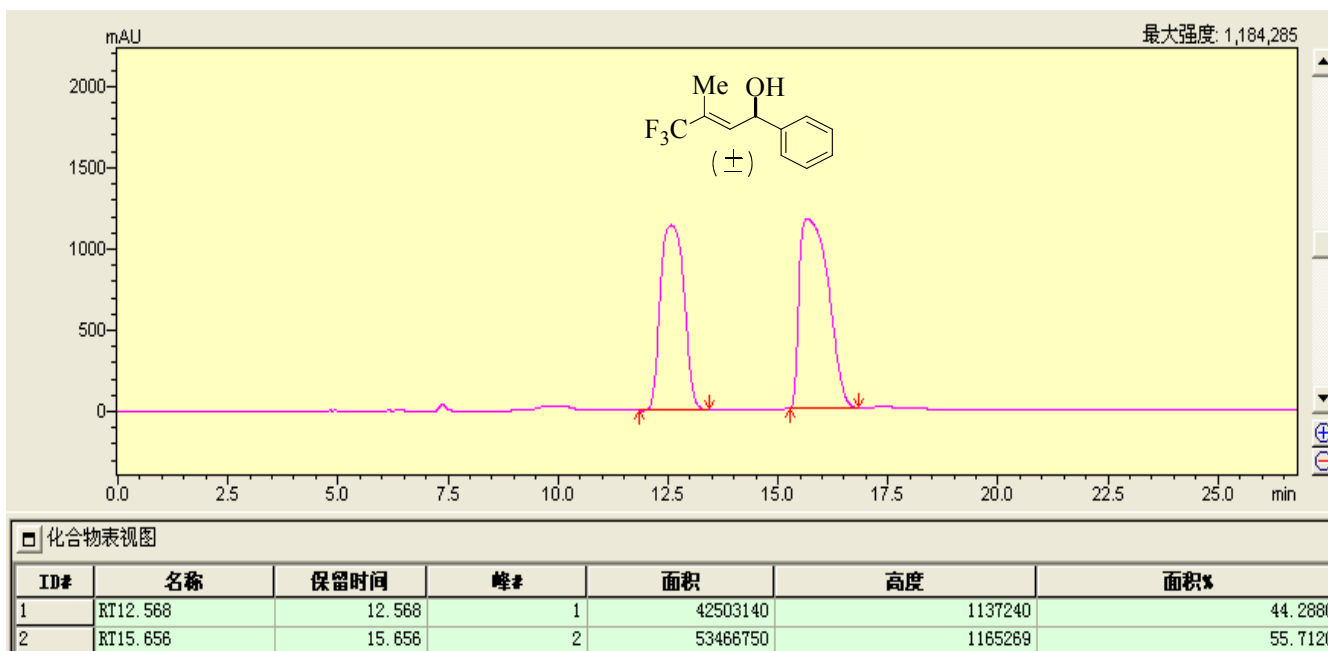
5g: (*R,E*)-4,4,4-trifluoro-1-phenyl-3-(*p*-tolyl)but-2-en-1-ol (HPLC: Chiracel OD-H, detected at 254 nm, eluent: n-hexane/2-propanol = 95/5, flow rate = 1.0 mL/min, 25 °C).



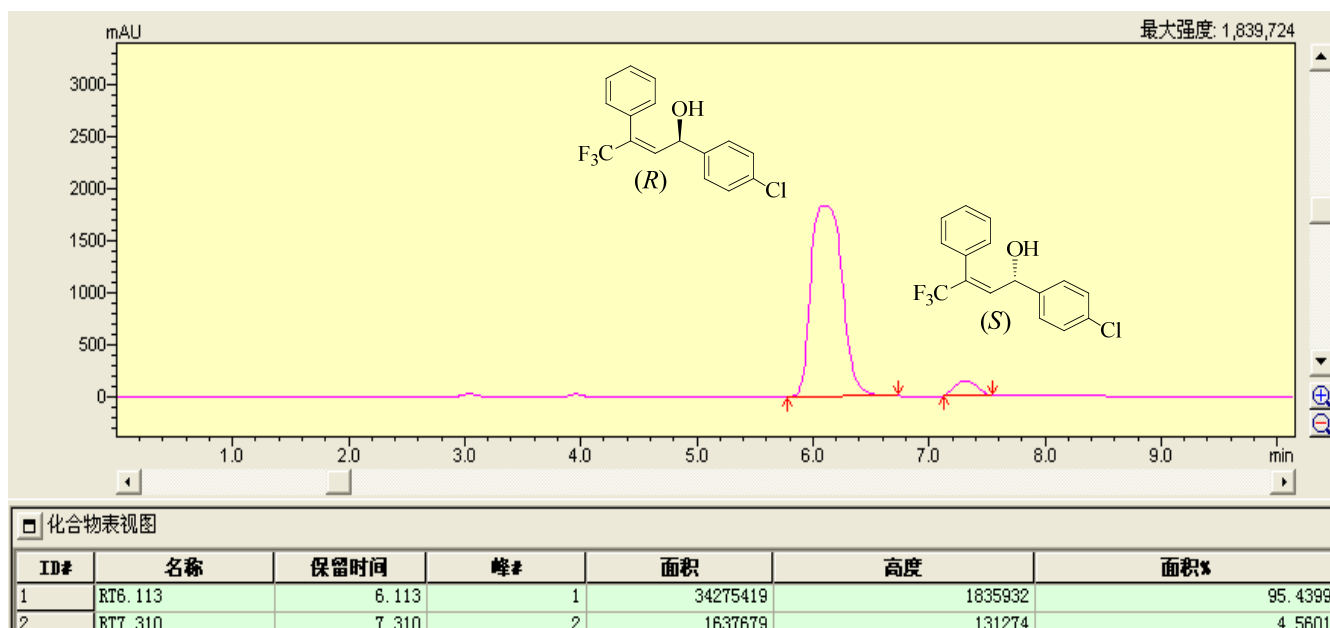
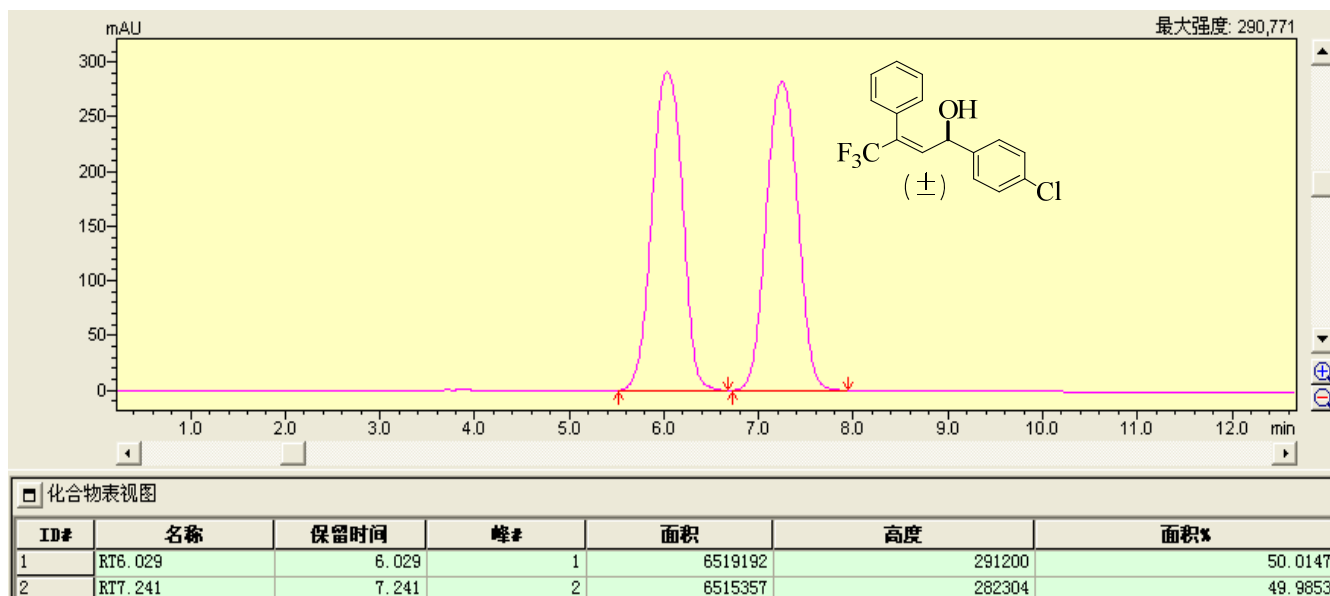
5h: (R,E)-4,4,4-trifluoro-3-(4-methoxyphenyl)-1-phenylbut-2-en-1-ol: (HPLC: ChiralcelOD-H, detected at 254 nm, eluent: n-hexane/2-propanol = 95/5, flow rate = 1.0 mL/min, 25 °C).



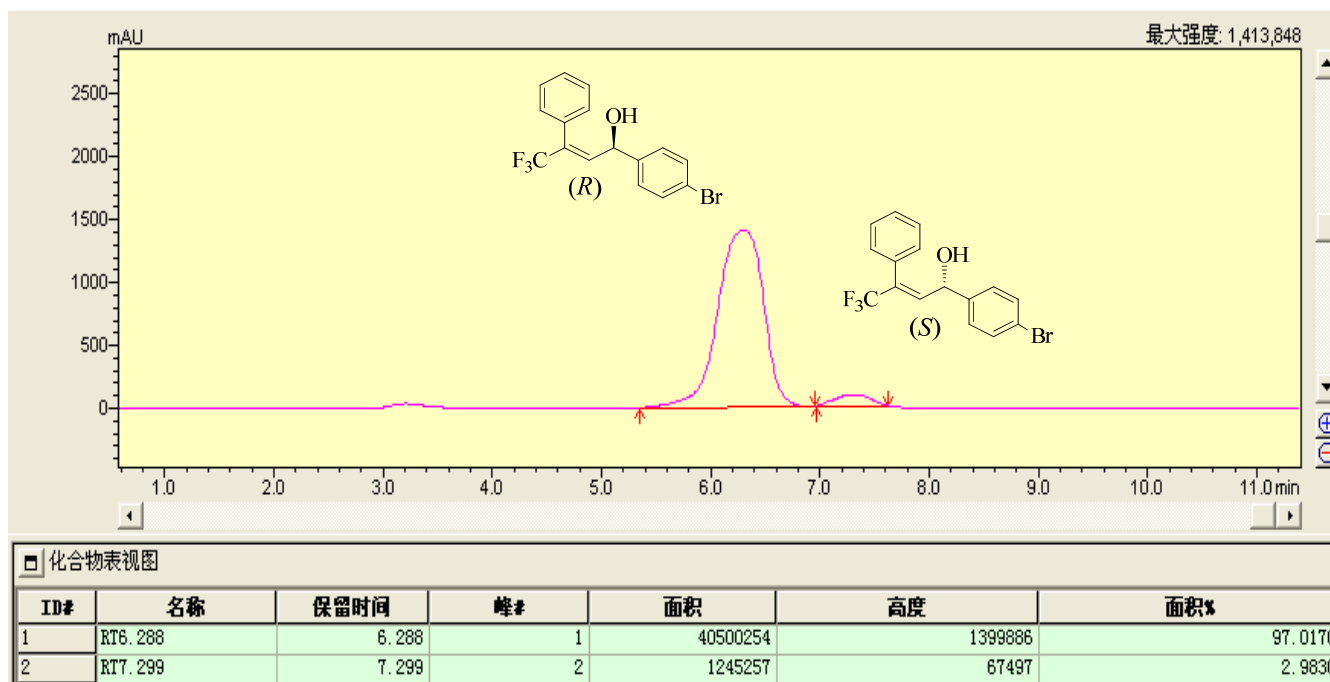
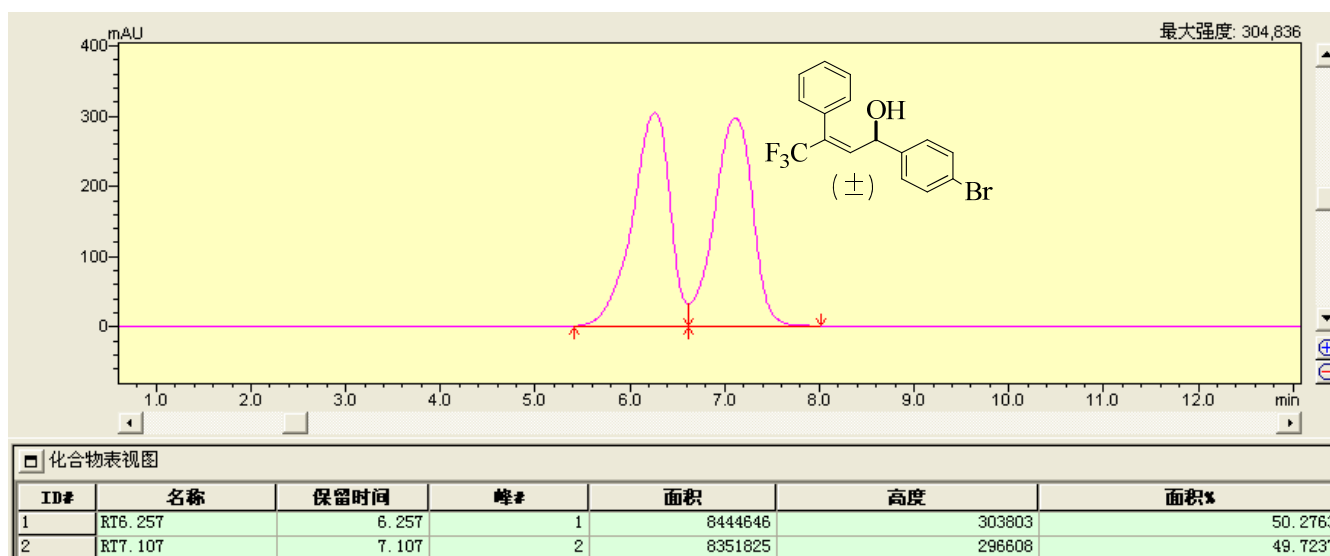
5i: (R,E)-4,4,4-trifluoro-3-methyl-1-phenylbut-2-en-1-ol: (HPLC: Chiralcel OD-H, detected at 254 nm, eluent: n-hexane/2-propanol = 95/5, flow rate = 1.0 mL/min, 25 °C).



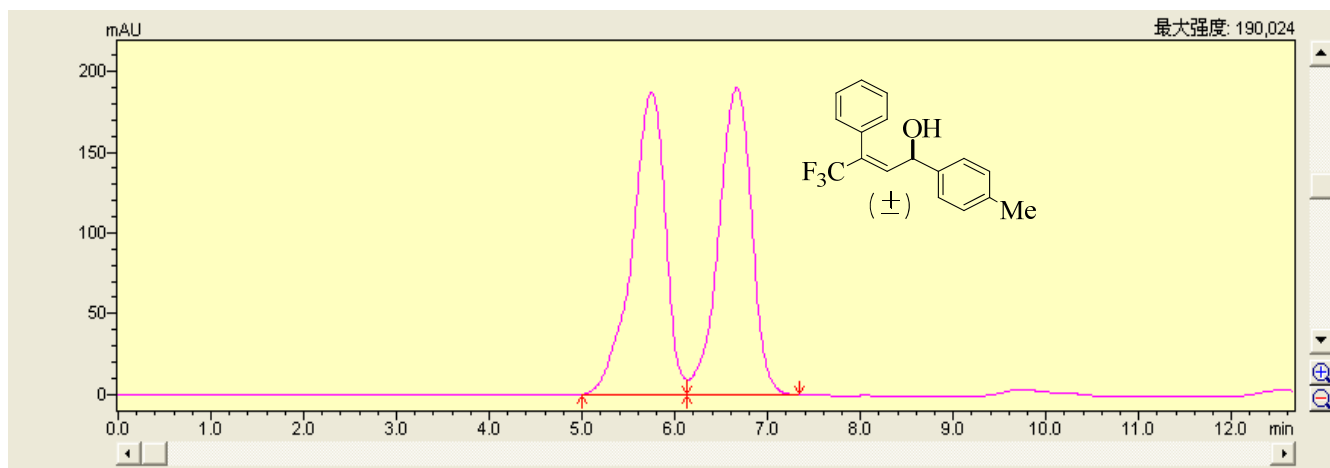
5j: (R,E)-1-(4-chlorophenyl)-4,4,4-trifluoro-3-phenylbut-2-en-1-ol: (HPLC: Chiracel OD-H, detected at 254 nm, eluent: n-hexane/2-propanol = 95/5, flow rate = 1.0 mL/min, 25 °C).



5k: (R,E)-1-(4-bromophenyl)-4,4,4-trifluoro-3-phenylbut-2-en-1-ol: (HPLC: Chiracel OD-H, detected at 254 nm, eluent: n-hexane/2-propanol = 95/5, flow rate = 1.0 mL/min, 25 °C).

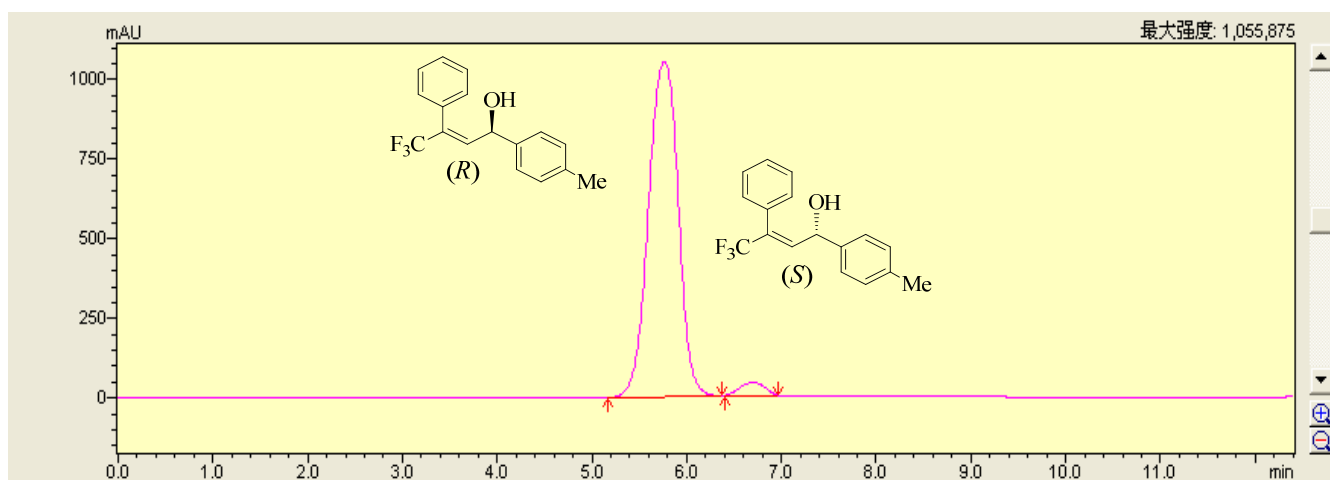


5L: (R,E)-4,4,4-trifluoro-3-phenyl-1-(p-tolyl)but-2-en-1-ol: (HPLC: Chiracel OD-H, detected at 254 nm, eluent: n-hexane/2-propanol = 95/5, flow rate = 1.0 mL/min, 25 °C).



化合物表视图

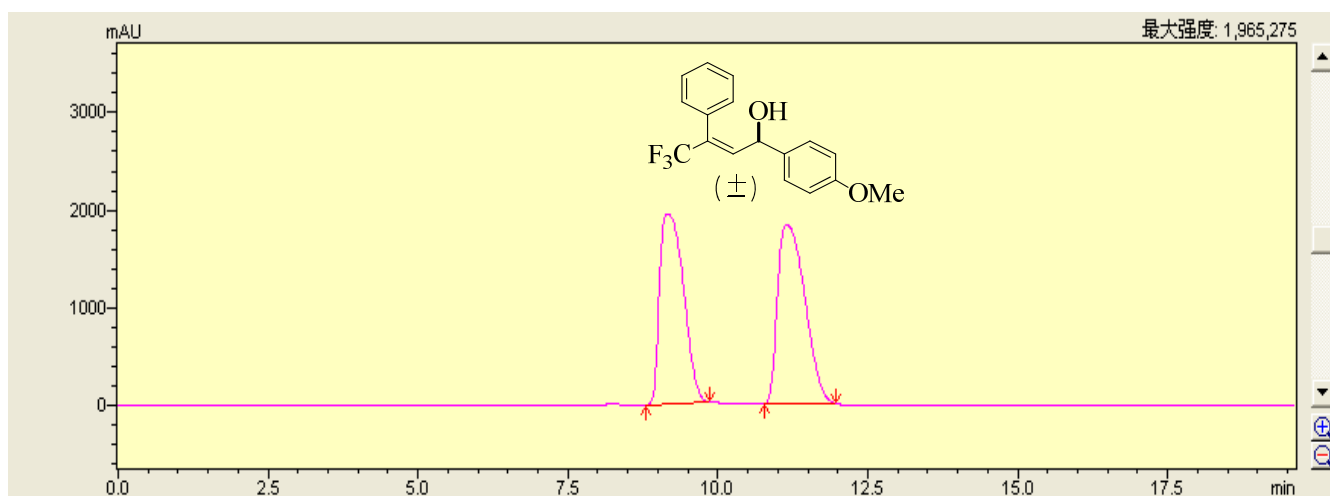
ID#	名称	保留时间	峰#	面积	高度	面积%
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2	RT6.662	6.662	2	4725292	190637	50.1981



化合物表视图

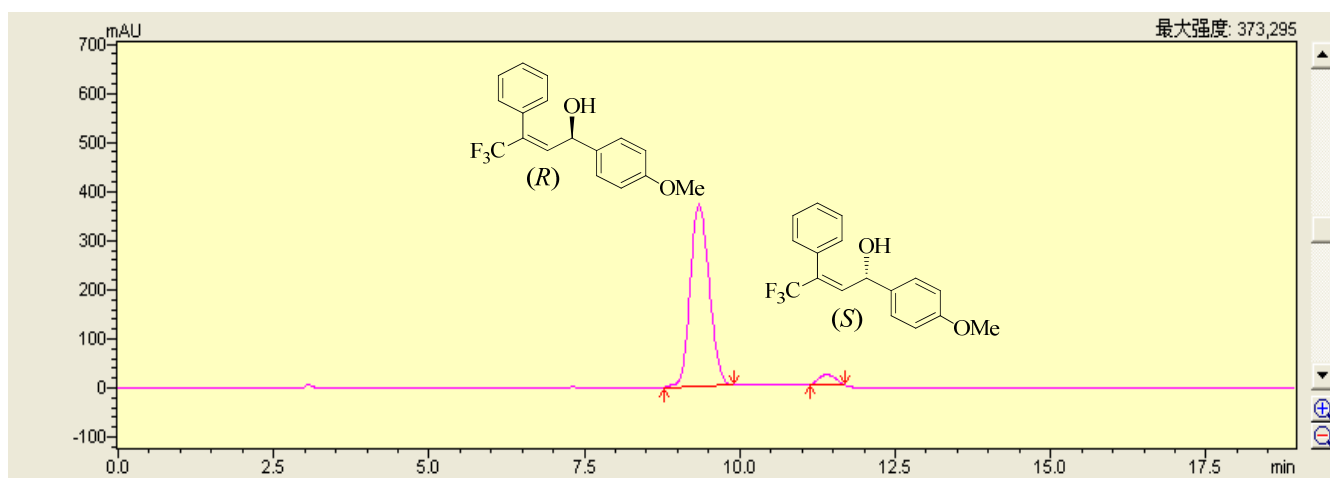
ID#	名称	保留时间	峰#	面积	高度	面积%
1	RT5.759	5.759	1	22945012	1051230	97.0651
2	RT6.695	6.695	2	693778	38988	2.9349

5m: (R,E)-4,4,4-trifluoro-1-(4-methoxyphenyl)-3-phenylbut-2-en-1-ol: (HPLC: Chiracel OD-H, detected at 254 nm, eluent: n-hexane/2-propanol = 95/5, flow rate = 1.0 mL/min, 25 °C).



化合物表视图

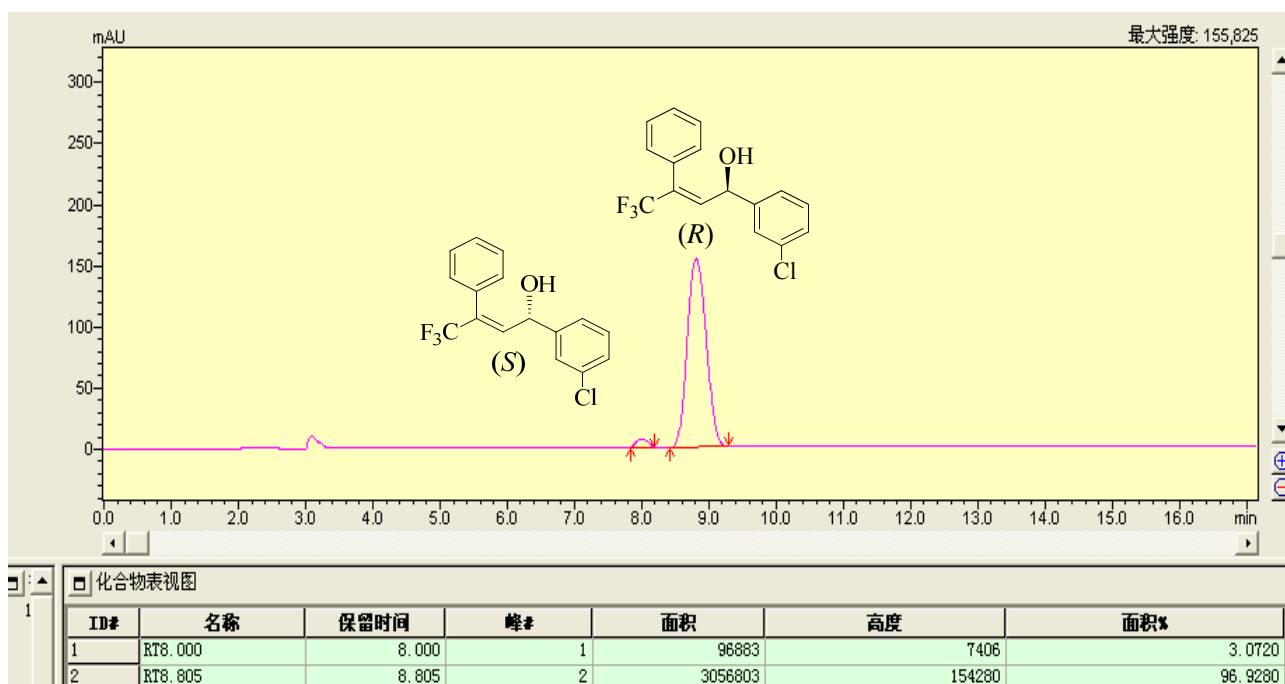
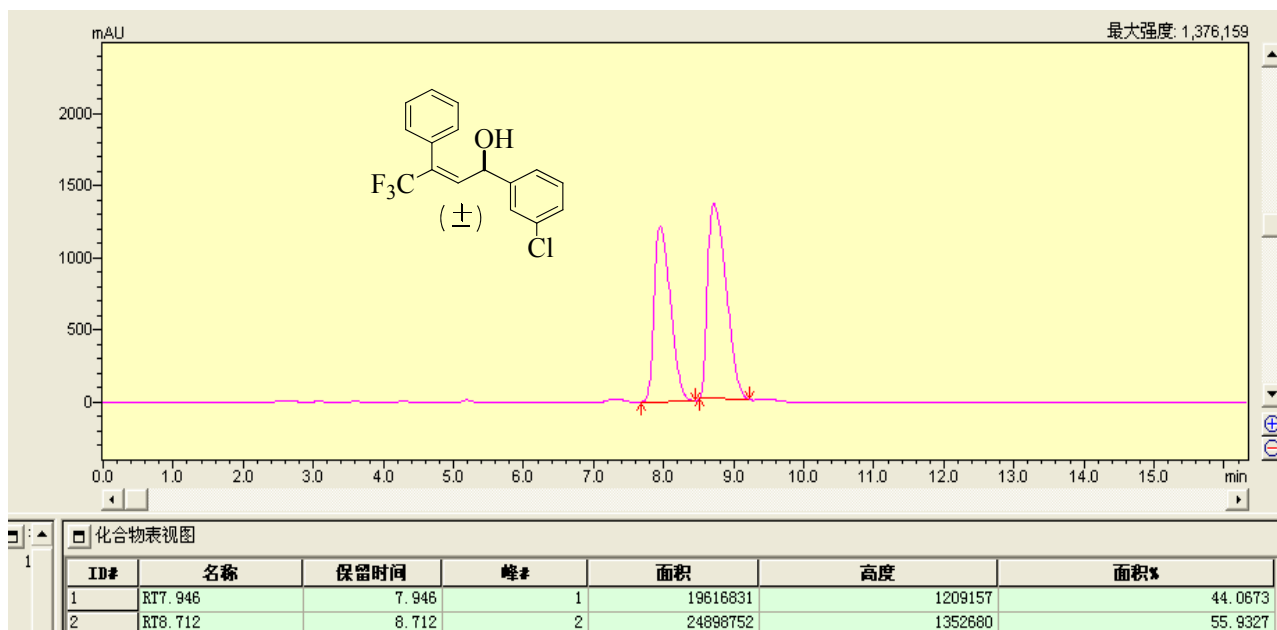
ID#	名称	保留时间	峰#	面积	高度	面积%
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2	RT11.144	11.144	2	58107807	1834026	51.7379



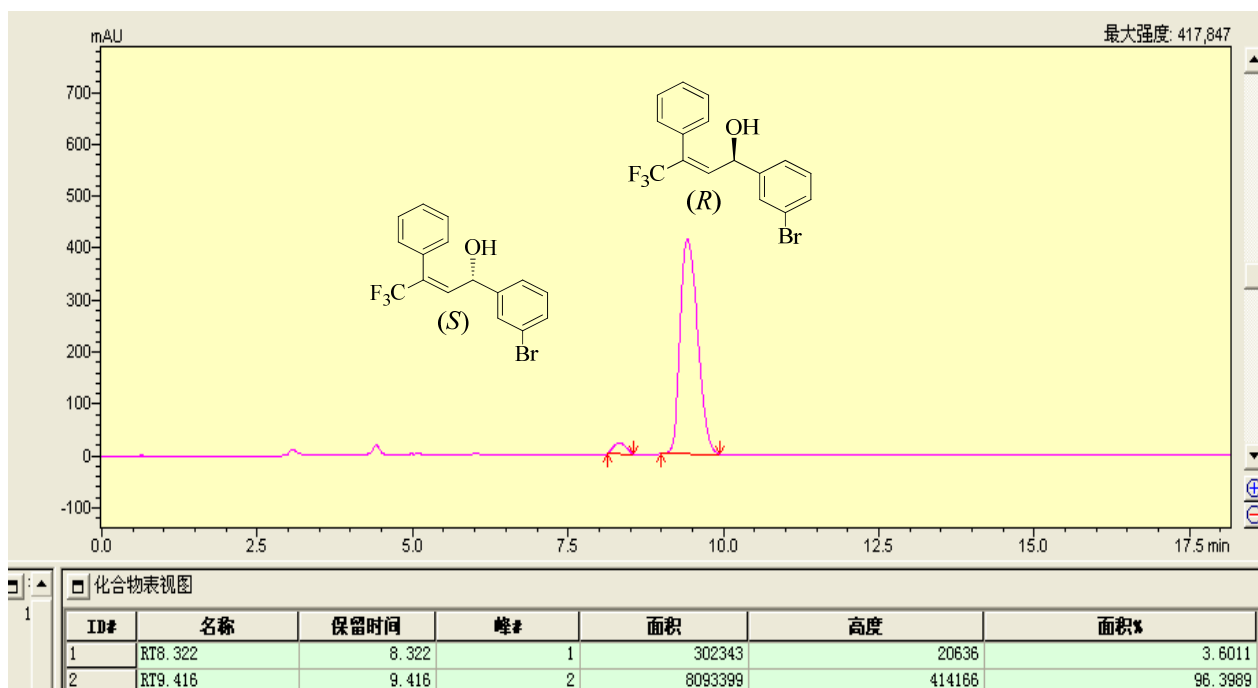
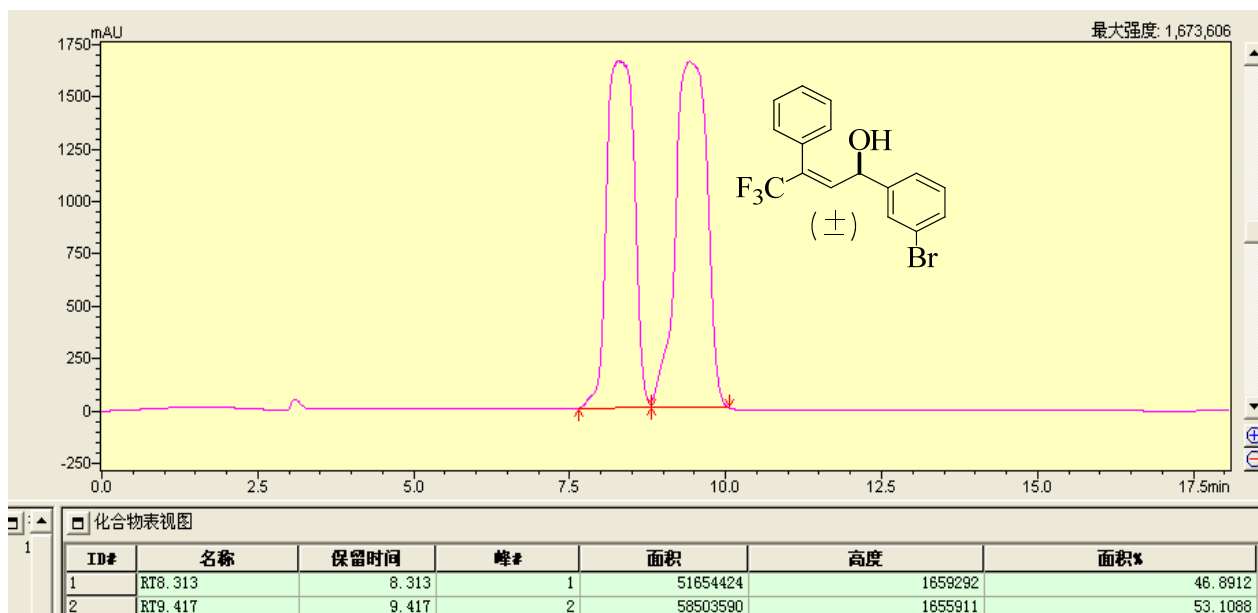
化合物表视图

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2	RT11.397	11.397	2	417688	21536	5.0319

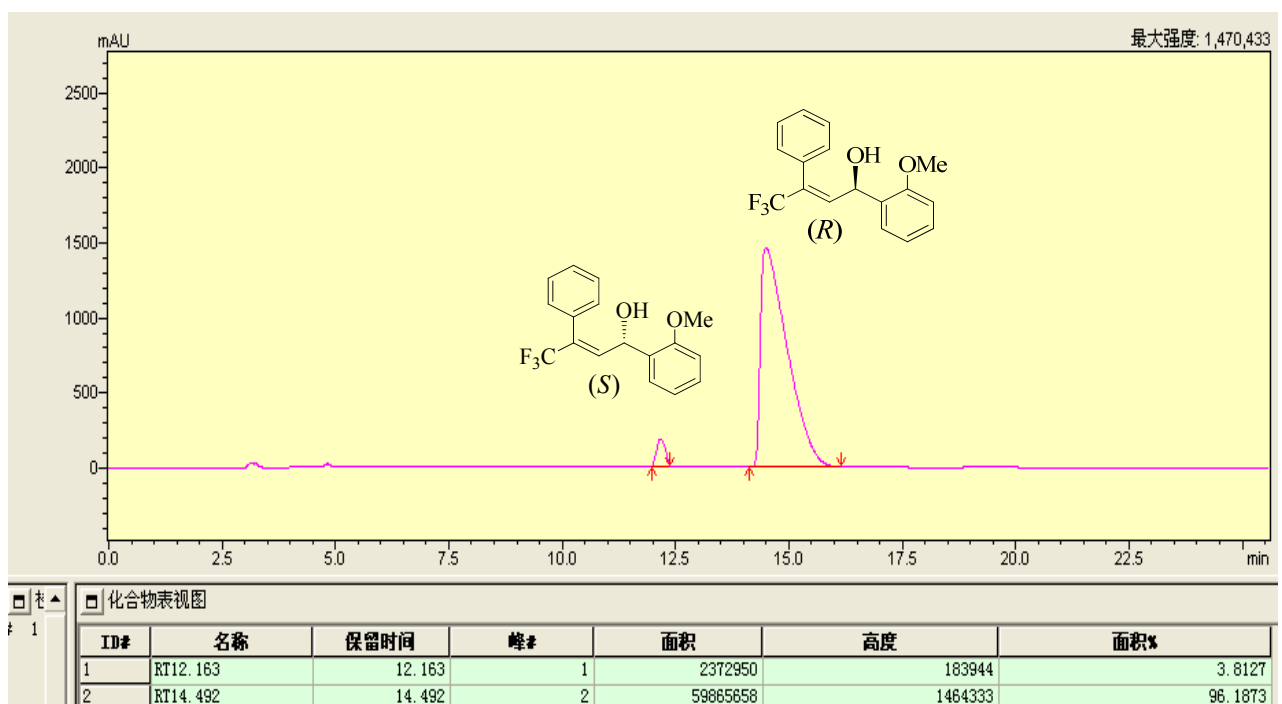
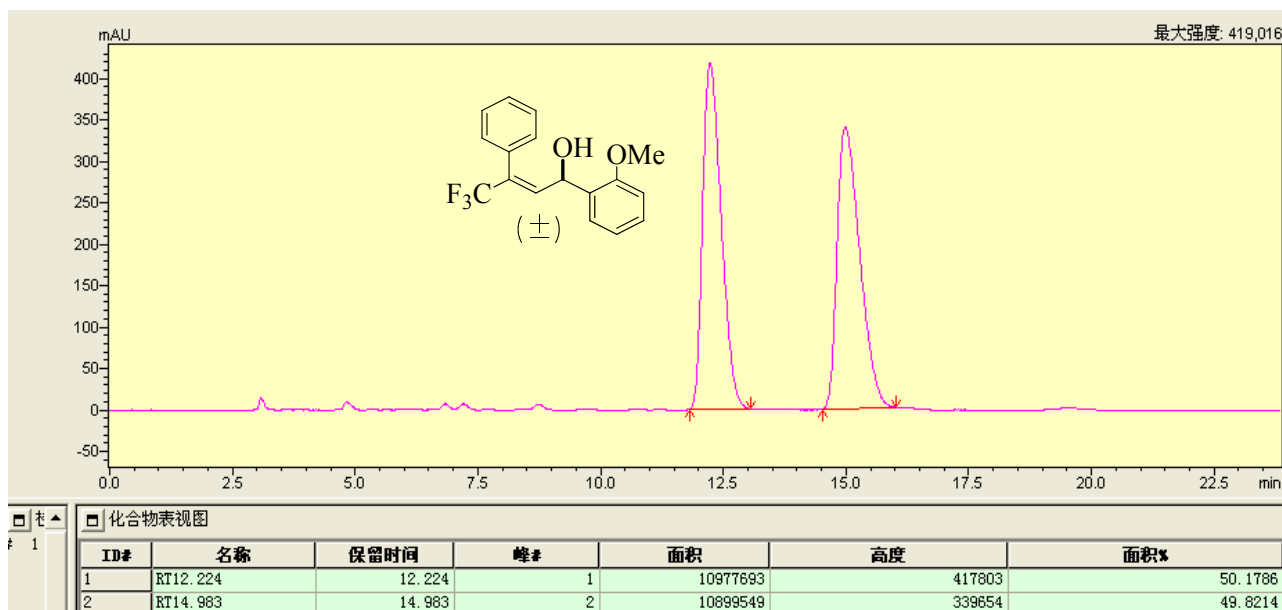
5n: (R,E)-1-(3-chlorophenyl)-4,4,4-trifluoro-3-phenylbut-2-en-1-ol (HPLC: Chiracel AD-H, detected at 254 nm, eluent: n-hexane/2-propanol = 95/5, flow rate = 1.0 mL/min, 25 °C).



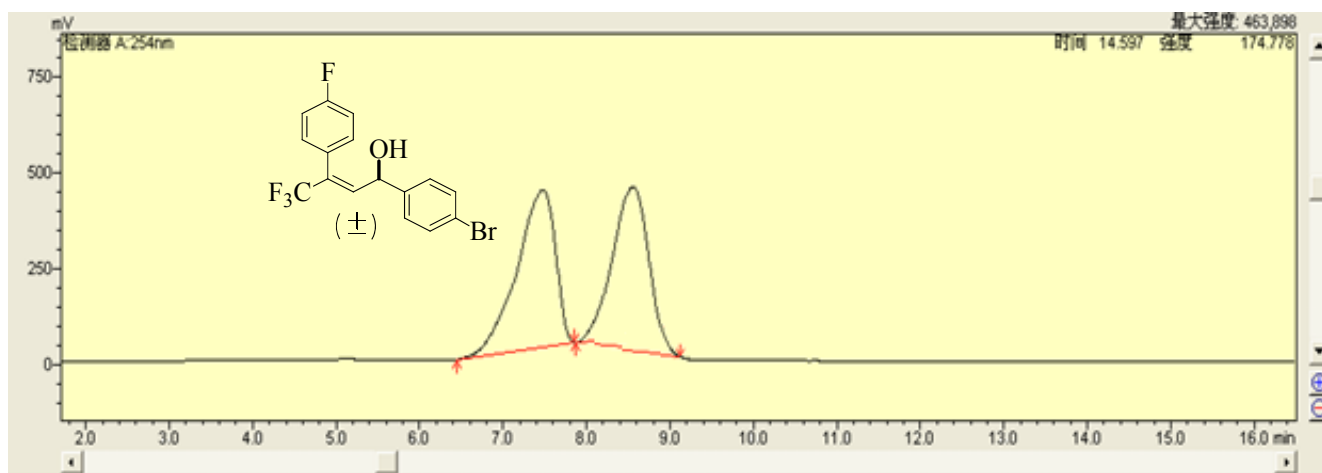
5o: (*R,E*)-1-(3-bromophenyl)-4,4,4-trifluoro-3-phenylbut-2-en-1-ol (HPLC: Chiralcel AD-H, detected at 254 nm, eluent: n-hexane/2-propanol = 95/5, flow rate = 1.0 mL/min, 25 °C).



5p: (*R,E*)-4,4,4-trifluoro-1-(2-methoxyphenyl)-3-phenylbut-2-en-1-ol (HPLC: Chiracel OD-H, detected at 254 nm, eluent: n-hexane/2-propanol = 97/3, flow rate = 1.0 mL/min, 25 °C).

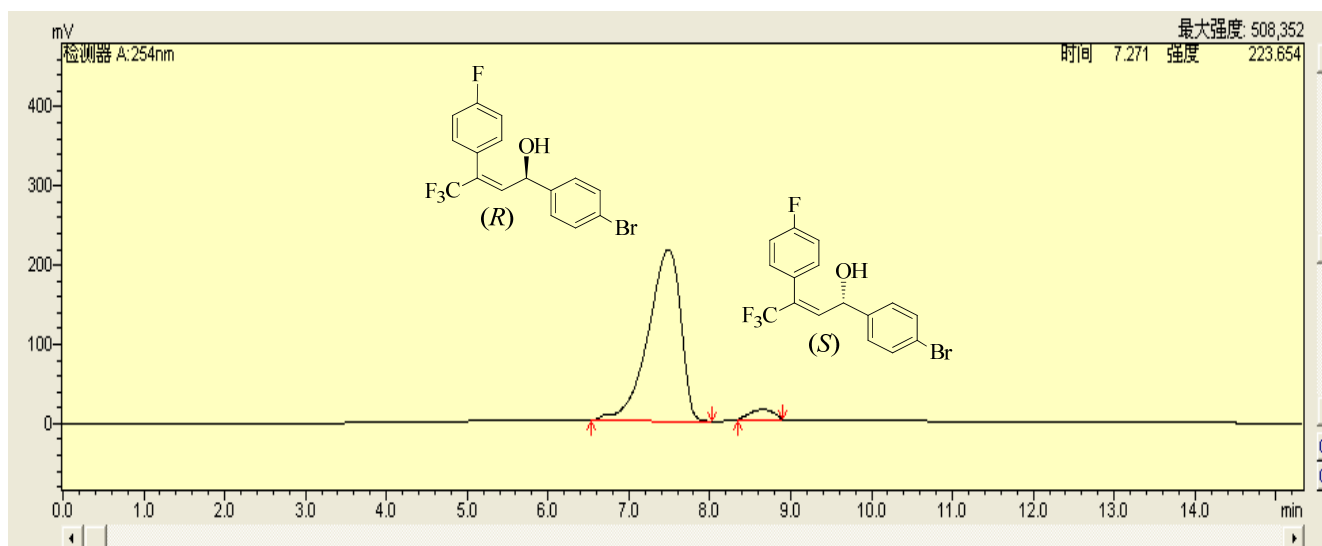


5q: (R,E)-1-(4-bromophenyl)-4,4,4-trifluoro-3-(4-fluorophenyl)but-2-en-1-ol: (HPLC: Chiracel OD-H, detected at 254 nm, eluent: n-hexane/2-propanol = 95/5, flow rate = 1.0 mL/min, 25 °C).



化合物表视图

ID#	名称	保留时间	峰#	面积	高度	峰开始	峰结束	面积%
1	RT7.471	7.471	1	13250338	411542	6.450	7.858	53.6715
2	RT8.548	8.548	2	11437513	396518	7.875	8.983	46.3285



化合物表视图

ID#	名称	保留时间	峰#	面积	高度	峰开始	峰结束	面积%
1	RT7.481	7.481	1	6043868	216566	6.533	8.033	95.7932
2	RT8.648	8.648	2	265422	12728	8.342	8.908	4.2068

5r: (*R,E*)-1,3-bis(4-bromophenyl)-4,4-trifluorobut-2-en-1-ol: (HPLC: Chiracel OD-H, detected at 254 nm, eluent: n-hexane/2-propanol = 95/5, flow rate = 1.0 mL/min, 25 °C).

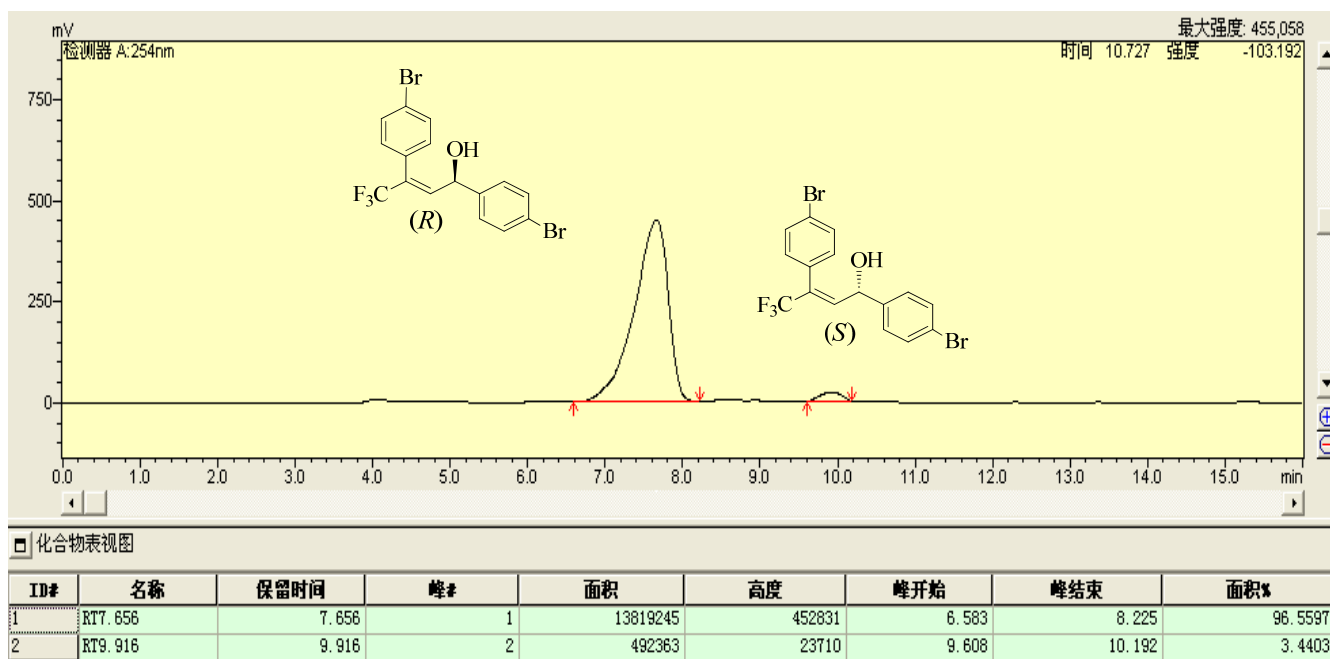
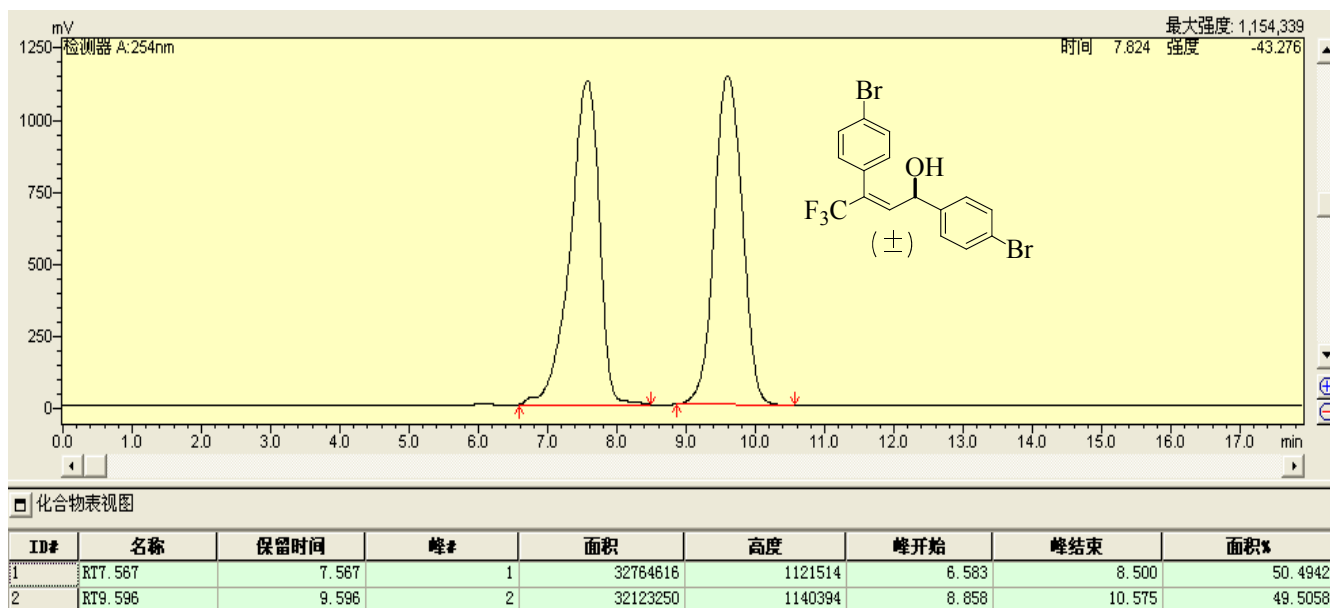
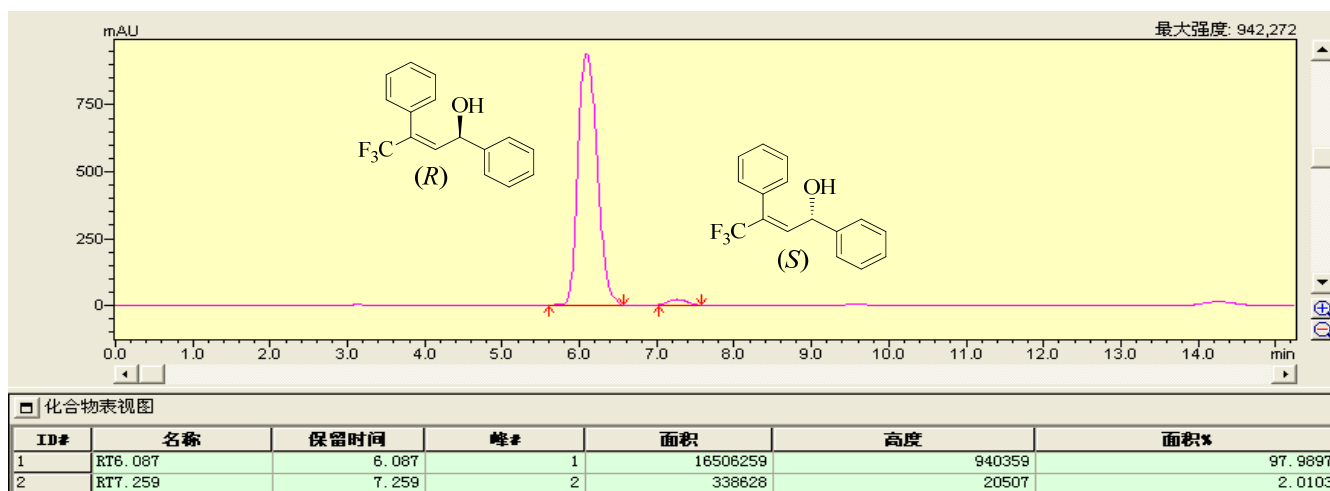
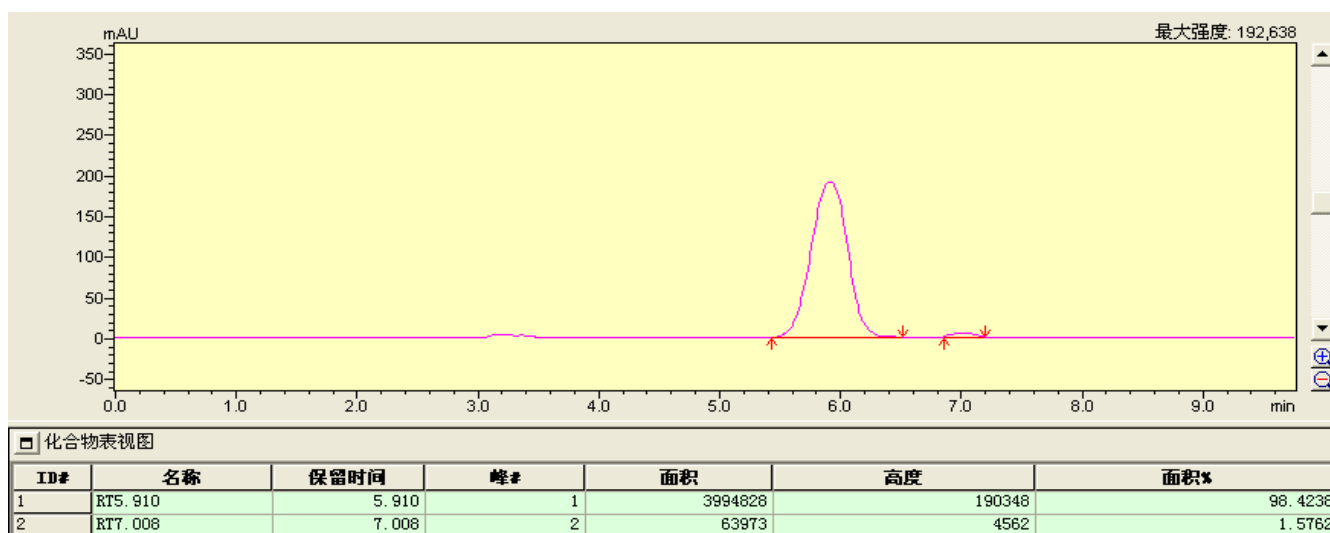


Figure S6. Reusability of catalyst **3** for enantioselective reduction of 4,4,4-trifluoro-1,3-diphenylbut-2-enone to (*R*)-4,4,4-trifluoro-1,3-diphenylbut-2-enol.

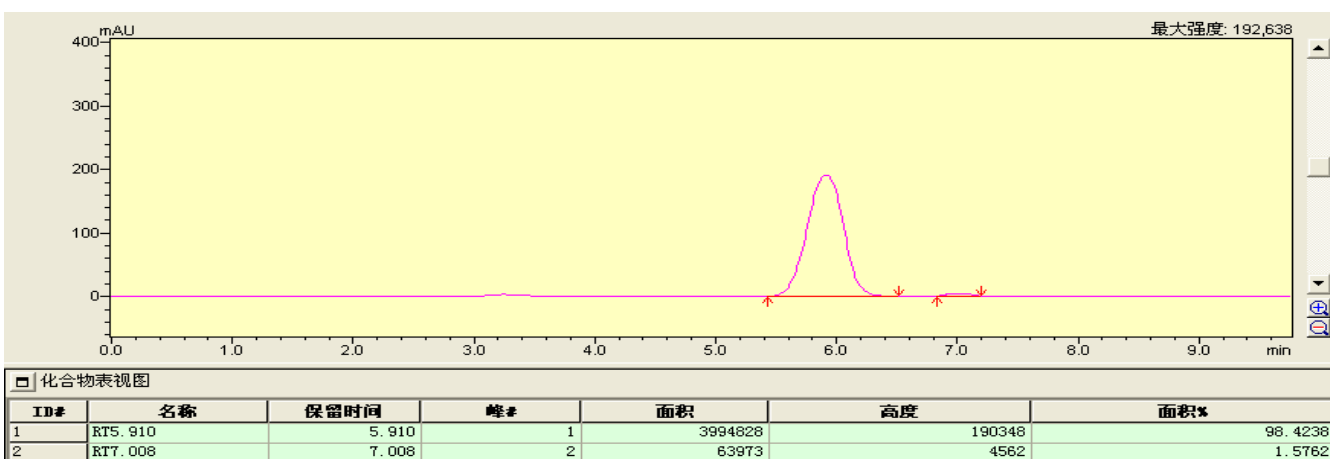
Recycle 2.



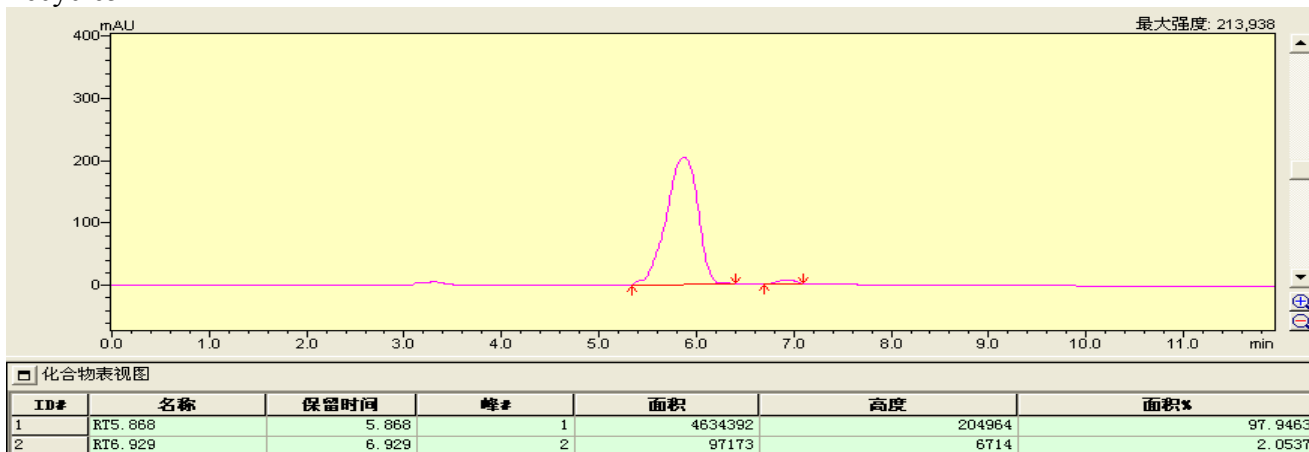
Recycle3



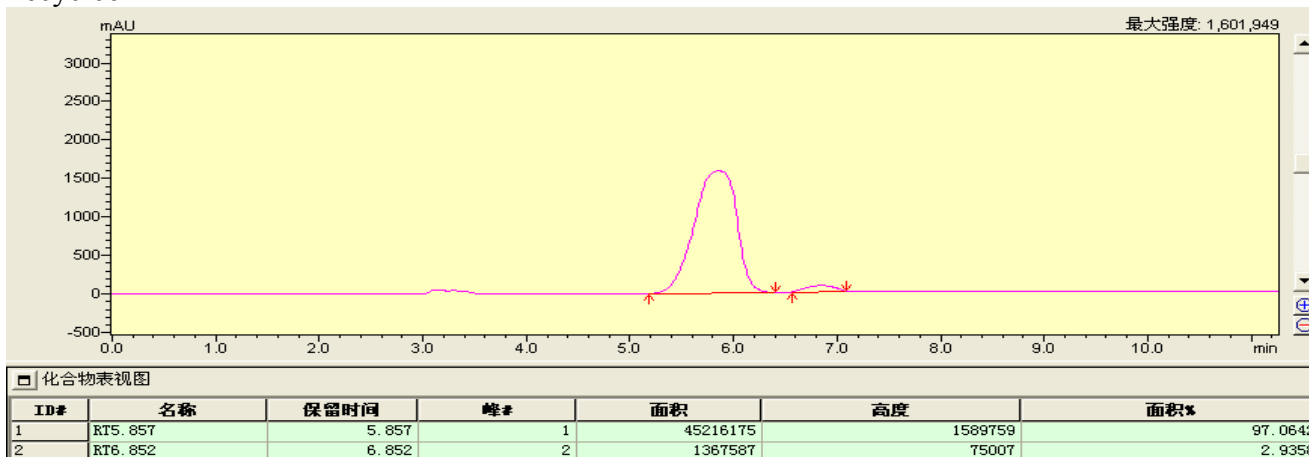
Recycle4



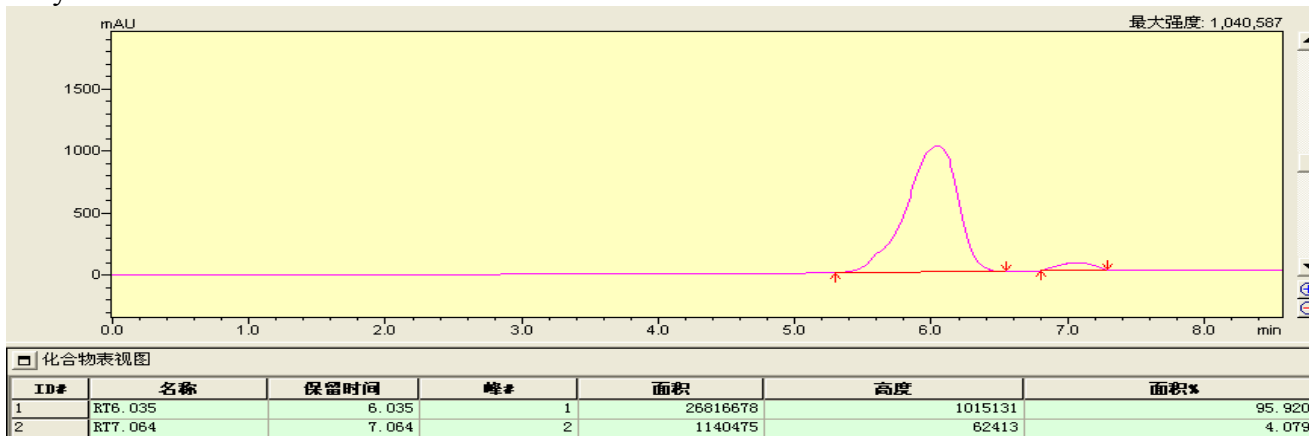
Recycle5



Recycle6



Recycle7



Recycle8

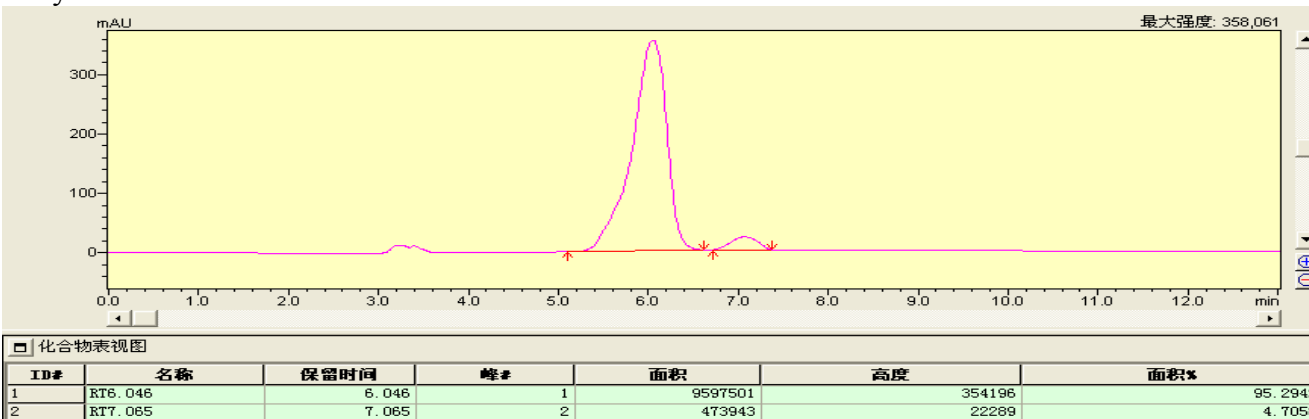
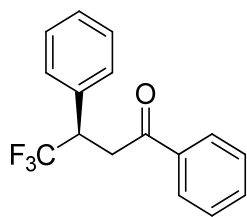
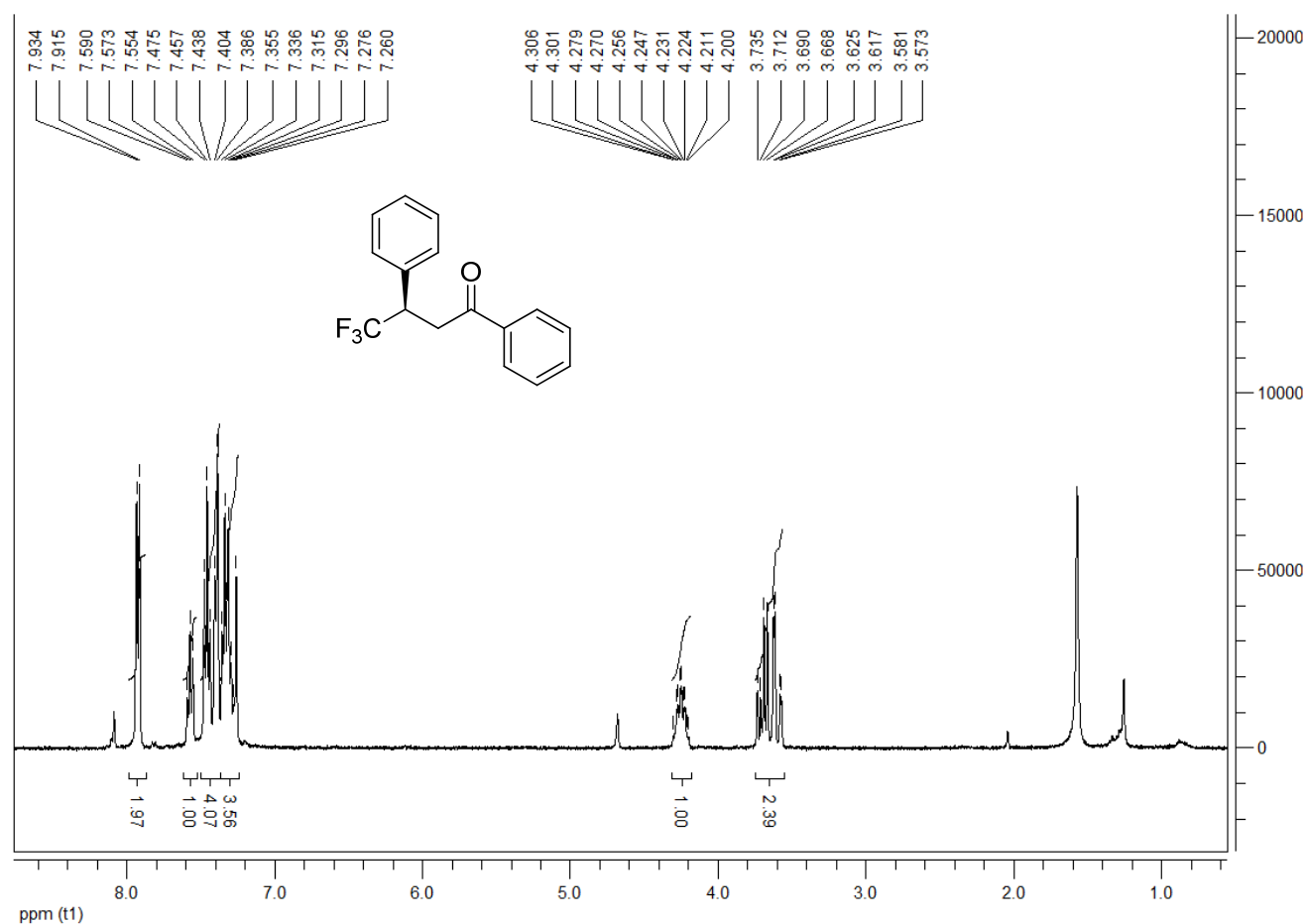


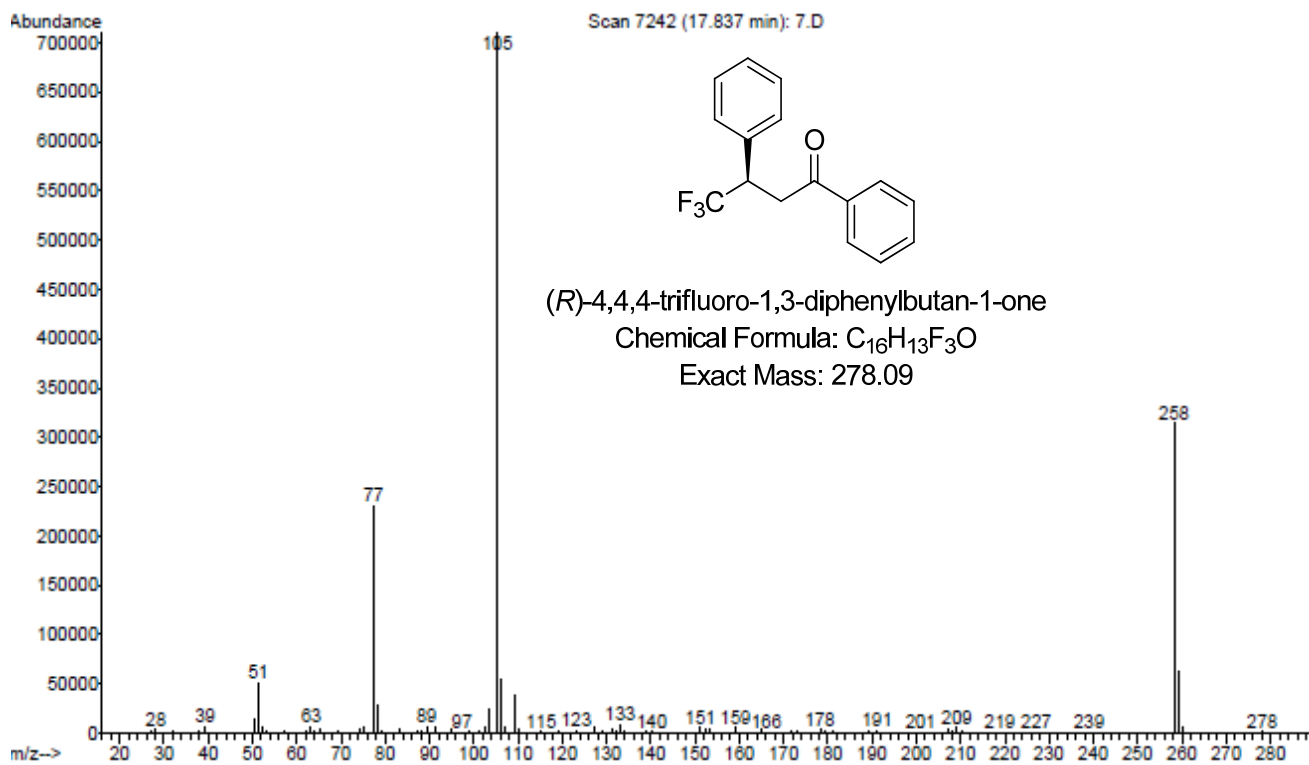
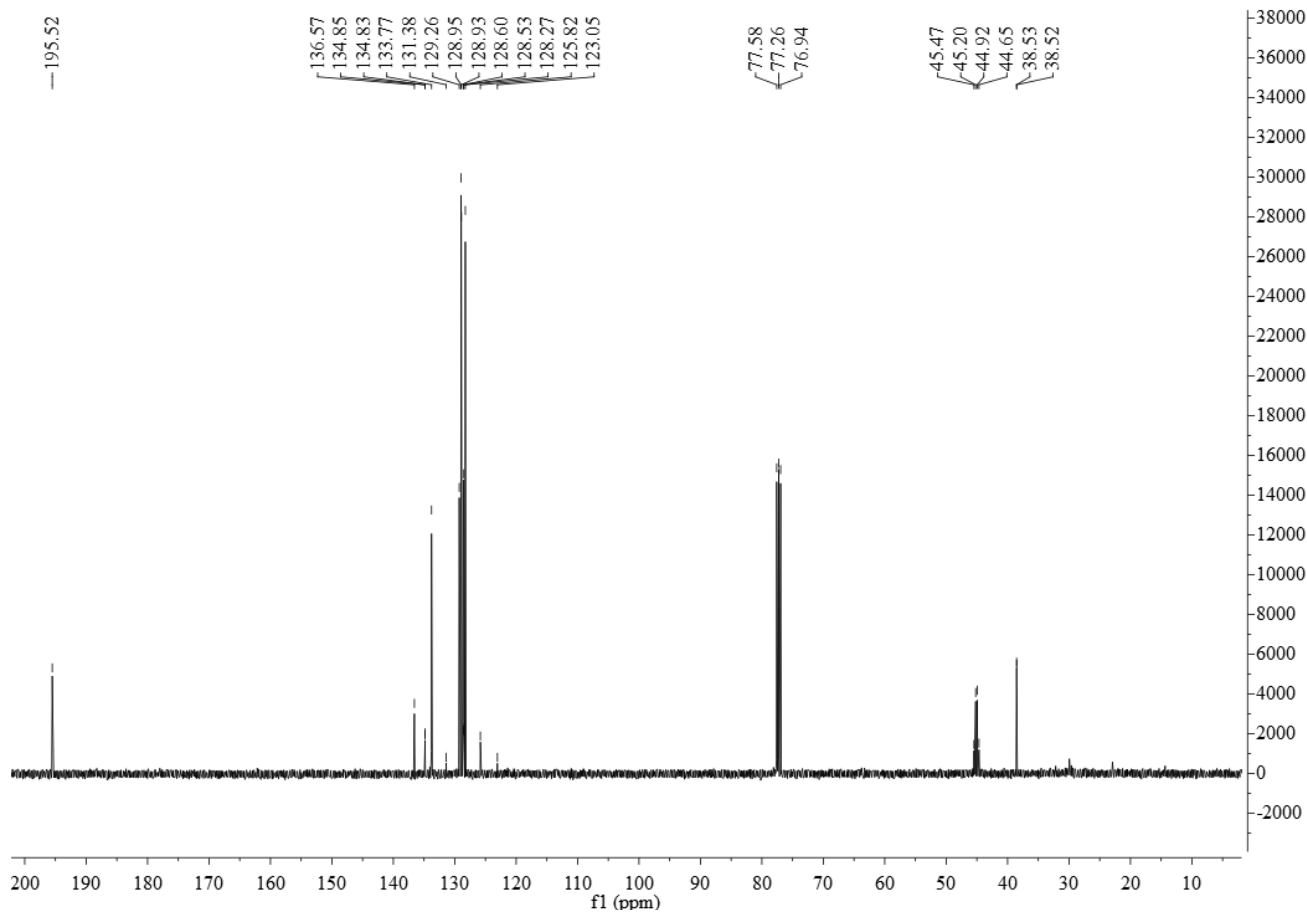
Figure S7. $^1\text{H-NMR}$, $^{13}\text{C-NMR}$ and GC-MS of all chiral products.

6a: (R)-4,4,4-Trifluoro-1,3-diphenylbutan-1-one

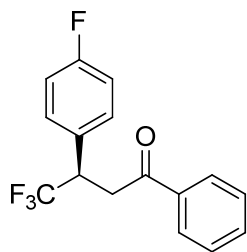


Yield: 96% (97% ee, 100% es); $^1\text{H NMR}$ (400 MHz, CDCl_3): δ 3.52 (dd, 1H, $J = 18$ Hz, $J = 4.5$ Hz), 3.64 (dd, 1H, $J = 18$ Hz, $J = 4.5$ Hz), 4.18-4.29 (m, 1H), 7.21-7.96 (m, 10H); $^{13}\text{C NMR}$ (100 MHz, CDCl_3): δ 38.5 (q, $J = 2$ Hz), 44.9 (q, $J = 27.7$ Hz), 127.2 (q, $J = 280$ Hz), 128.3, 128.5, 128.9, 129.0, 129.2, 133.8, 134.8 (q, $J = 2$ Hz), 136.5, 195.5; GC/MS (m/z): 278.09; HPLC (OD-H, elute: *n*-hexanes/*i*-PrOH = 95/5, detector: 254 nm, flow rate: 1.0 mL/min, 25 °C) $t_1 = 5.1$ min, $t_2 = 6.6$ min.

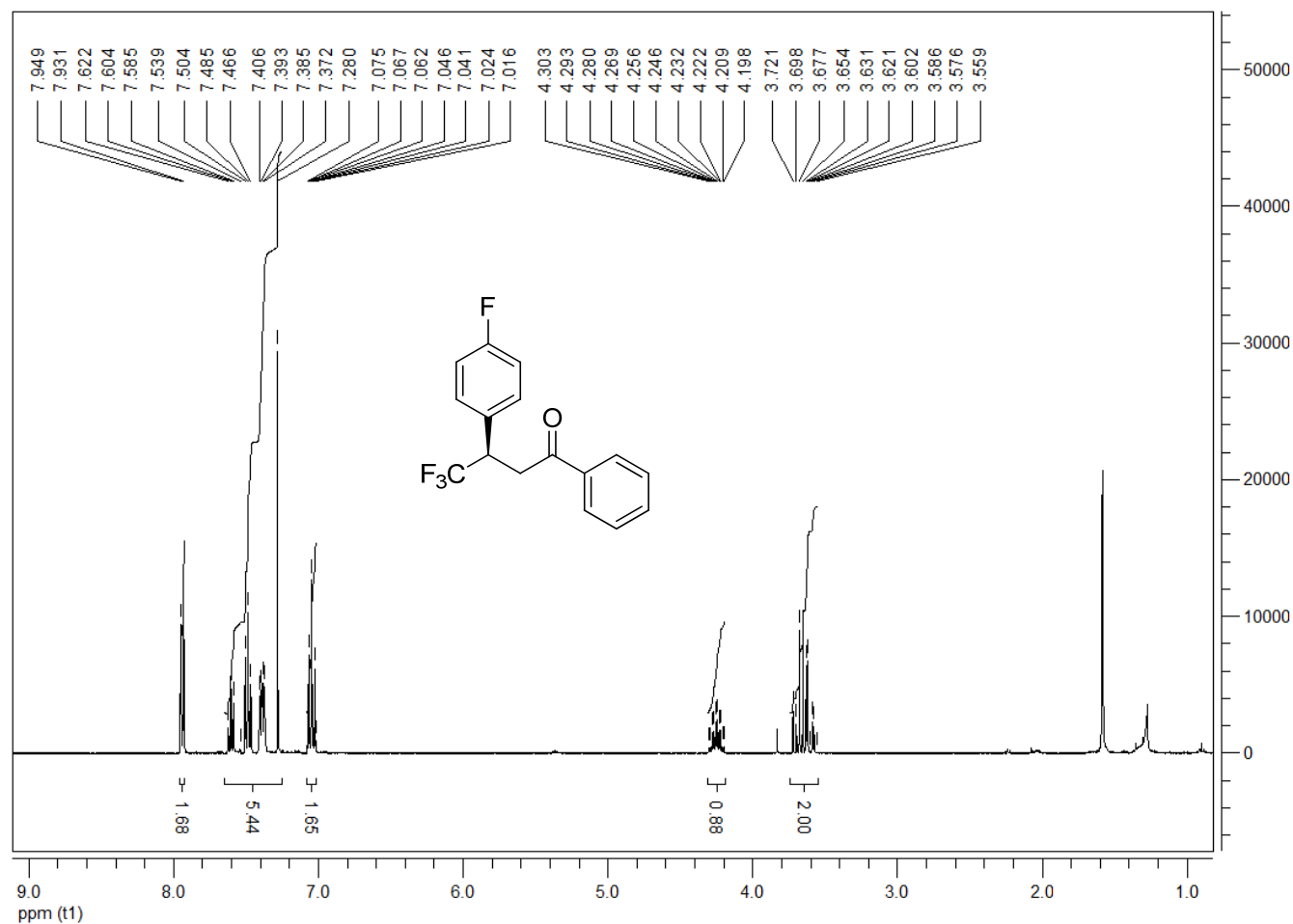


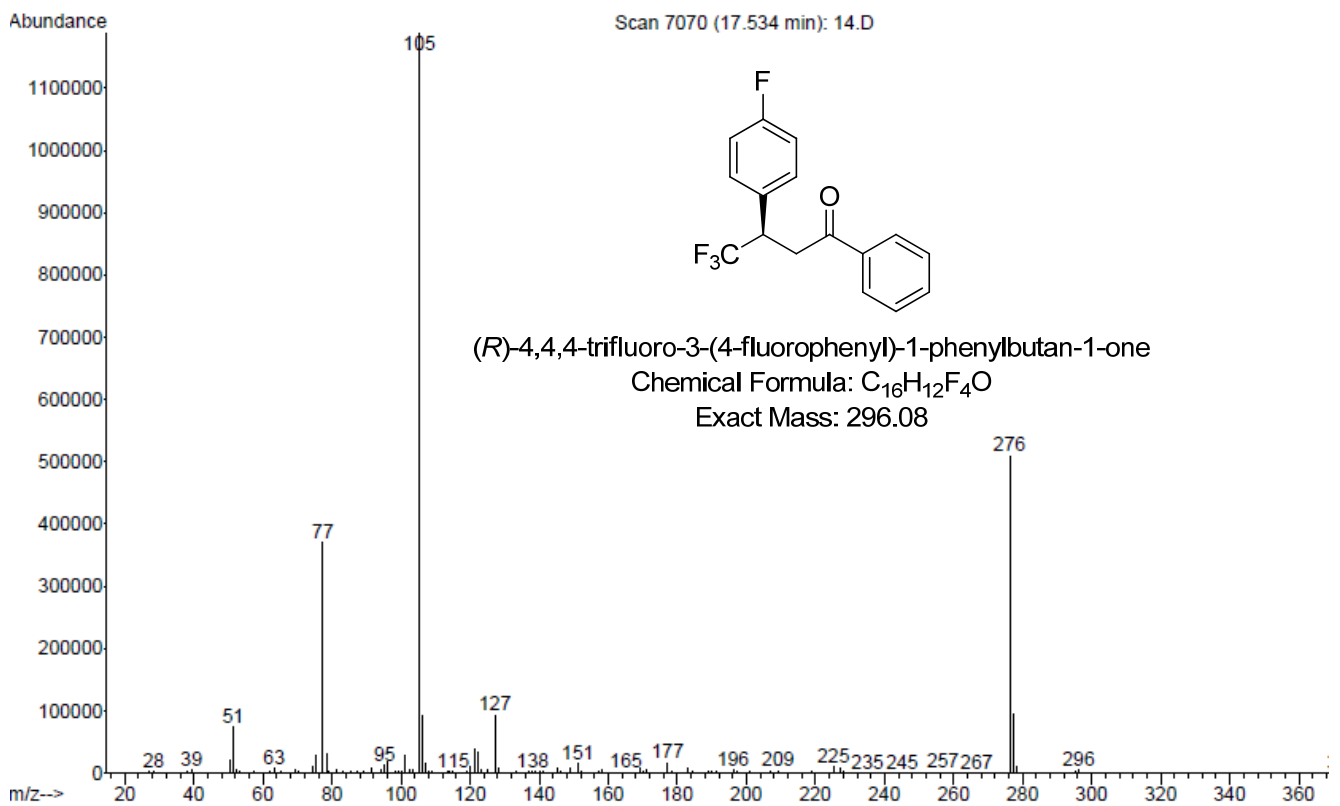
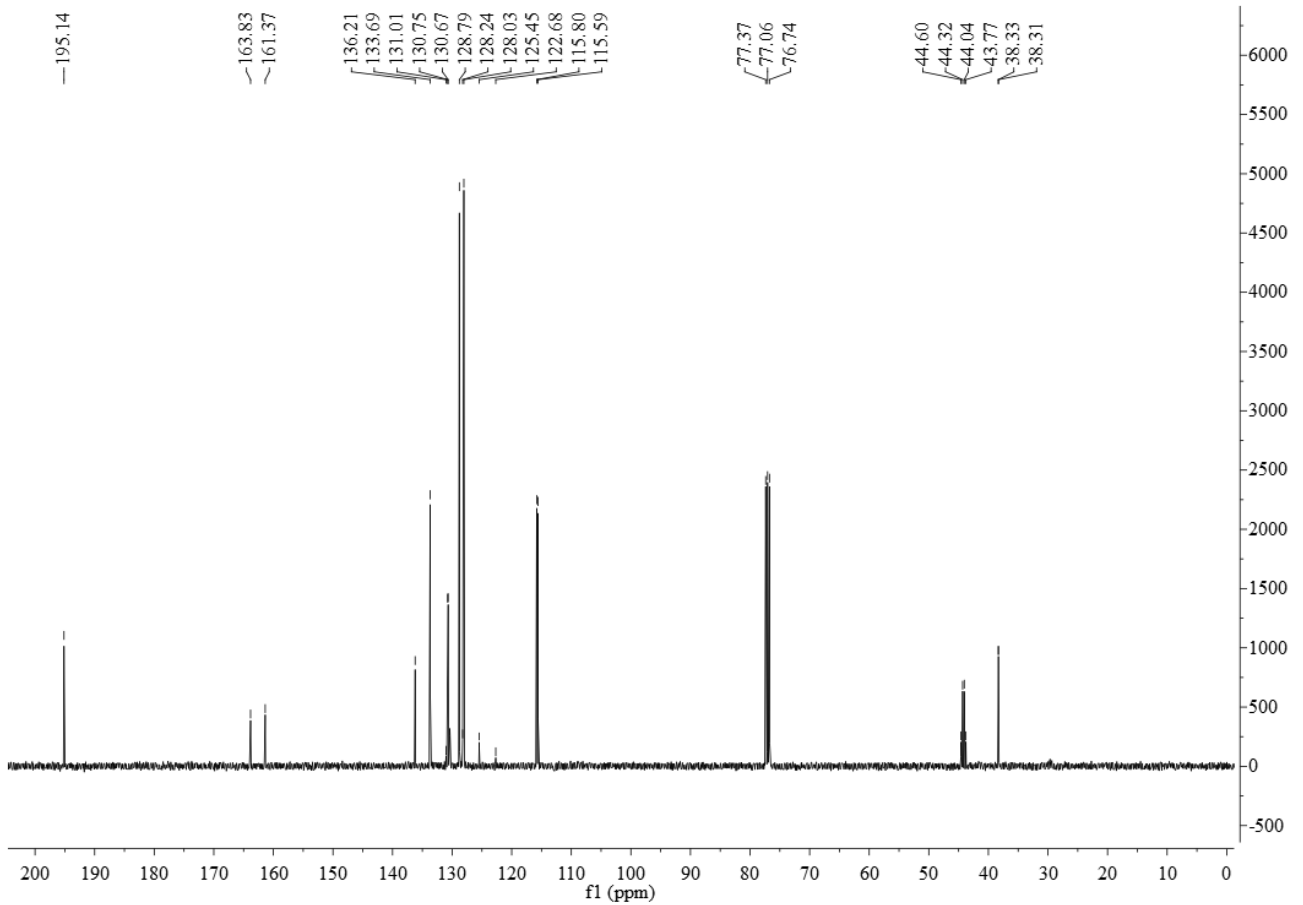


6b: (R)-4,4,4-Trifluoro-3-(4-fluorophenyl)-1-phenylbutan-1-one

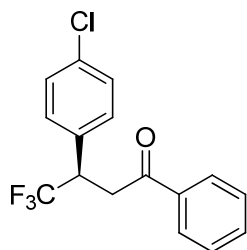


Yield: 96% (92% ee, 98% es); ^1H NMR (400 MHz, CDCl_3): δ 3.51 (dd, $J = 3.99$, 17.76 Hz, 1H), 3.59 (dd, $J = 9.40$, 17.76 Hz, 1H), 4.22–4.30 (m, 1H), 7.04–7.13 (m, 2H), 7.24–7.65 (m, 5H), 7.83–7.85 (m, 2H); ^{13}C NMR (100 MHz, CDCl_3): δ 38.3 (q, $J = 2$ Hz), 44.2 (q, $J = 28$ Hz), 115.7 (d, $J = 21$ Hz), 126.3 (q, $J = 278.4$ Hz), 128.0, 128.8, 130.6, 130.7, 133.7, 136.2, 162.6 (d, $J = 246.1$ Hz), 195.1; GC/MS (m/z): 296.08; HPLC (OD-H, elute: *n*-hexanes/*i*-PrOH = 95/5, detector: 254 nm, flow rate: 1.0 mL/min, 25 °C) $t_1 = 5.2$ min, $t_2 = 6.1$ min.

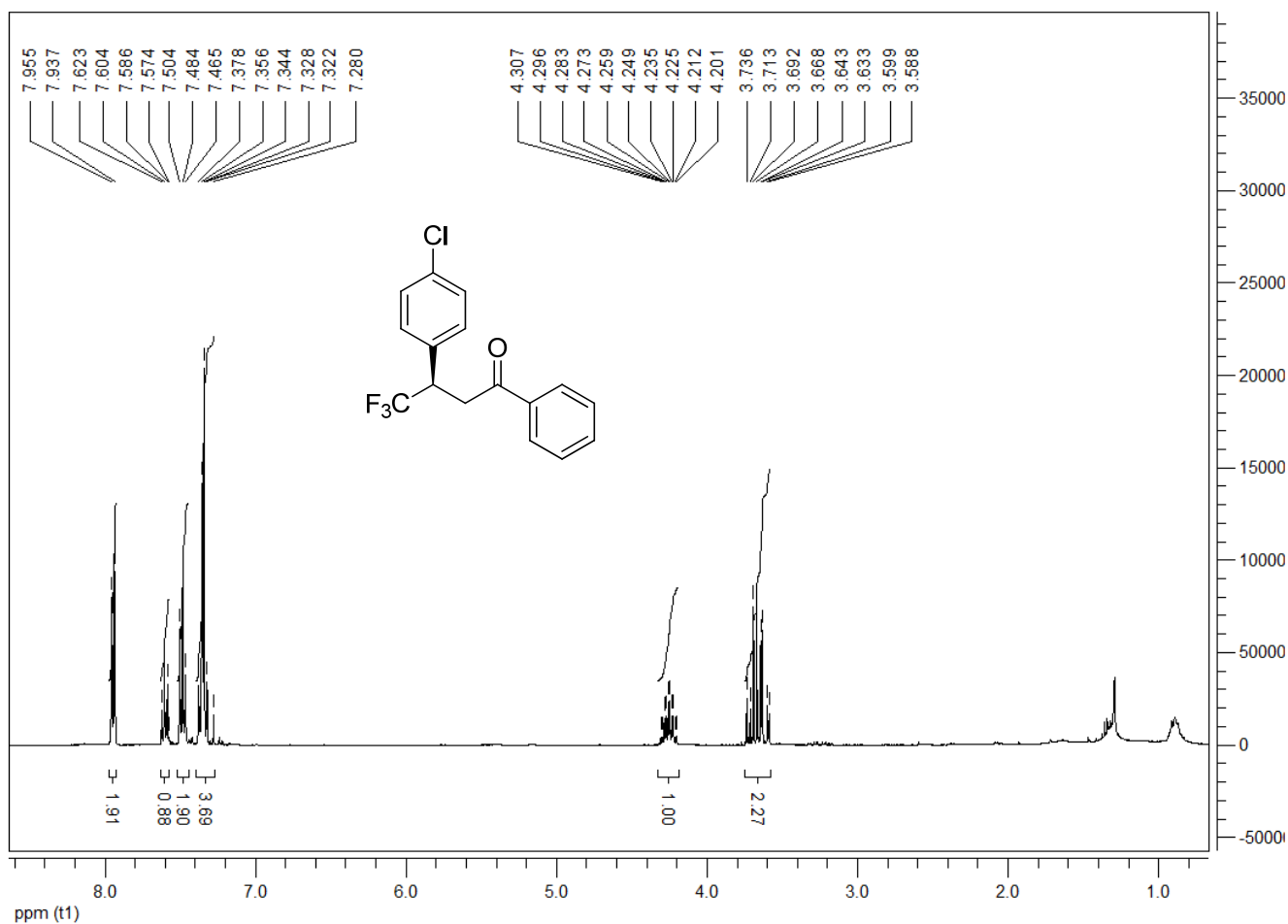


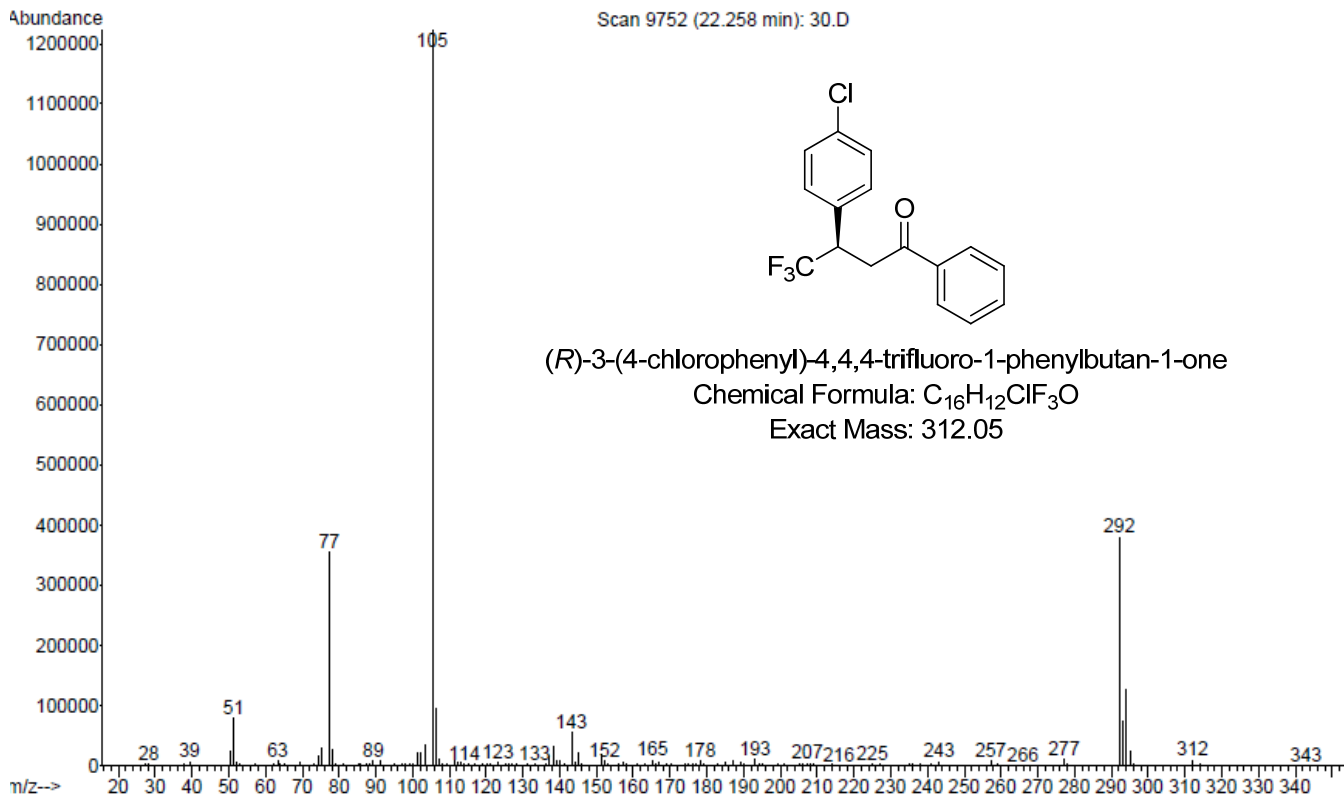
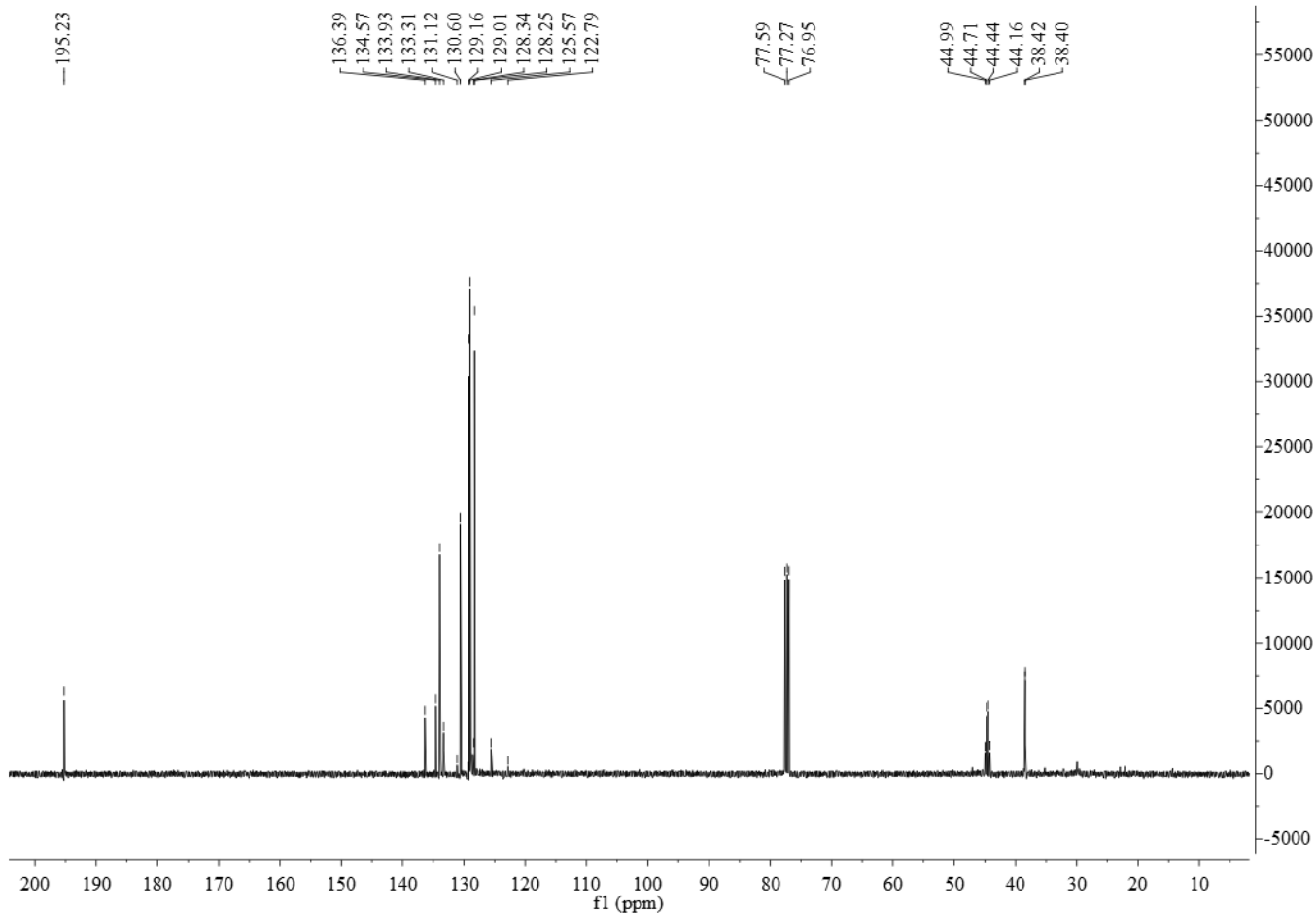


6c: (R)-3-(4-Chlorophenyl)-4,4,4-trifluoro-1-phenylbutan-1-one

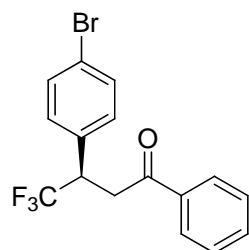


Yield: 97% (95% ee, 100% es); ^1H NMR (400 MHz, CDCl_3): δ 3.60 (dd, 1H, $J = 17.9$ Hz, $J = 4.3$ Hz), 3.68 (dd, 1H, $J = 17.8$ Hz, $J = 9.1$ Hz), 4.21–4.33 (m, 1H), 7.30–7.36 (m, 4H), 7.46 (t, 2H, $J = 7.8$ Hz), 7.61 (t, 1H, $J = 7.4$ Hz), 7.92 (d, 2H, $J = 7.3$ Hz); ^{13}C NMR (100 MHz, CDCl_3): δ 38.2 (q, $J = 2$ Hz), 44.6 (q, $J = 27$ Hz), 126.9 (q, $J = 277.7$ Hz), 128.3, 129.0, 129.2, 130.6, 133.3 (q, $J = 1.5$ Hz), 133.9, 134.6, 136.4, 195.2; GC/MS (m/z): 312.05; HPLC (OD-H, elute: *n*-hexanes/*i*-PrOH = 95/5, detector: 254 nm, flow rate: 1.0 mL/min, 25 °C) $t_1 = 5.8$ min, $t_2 = 7.2$ min.

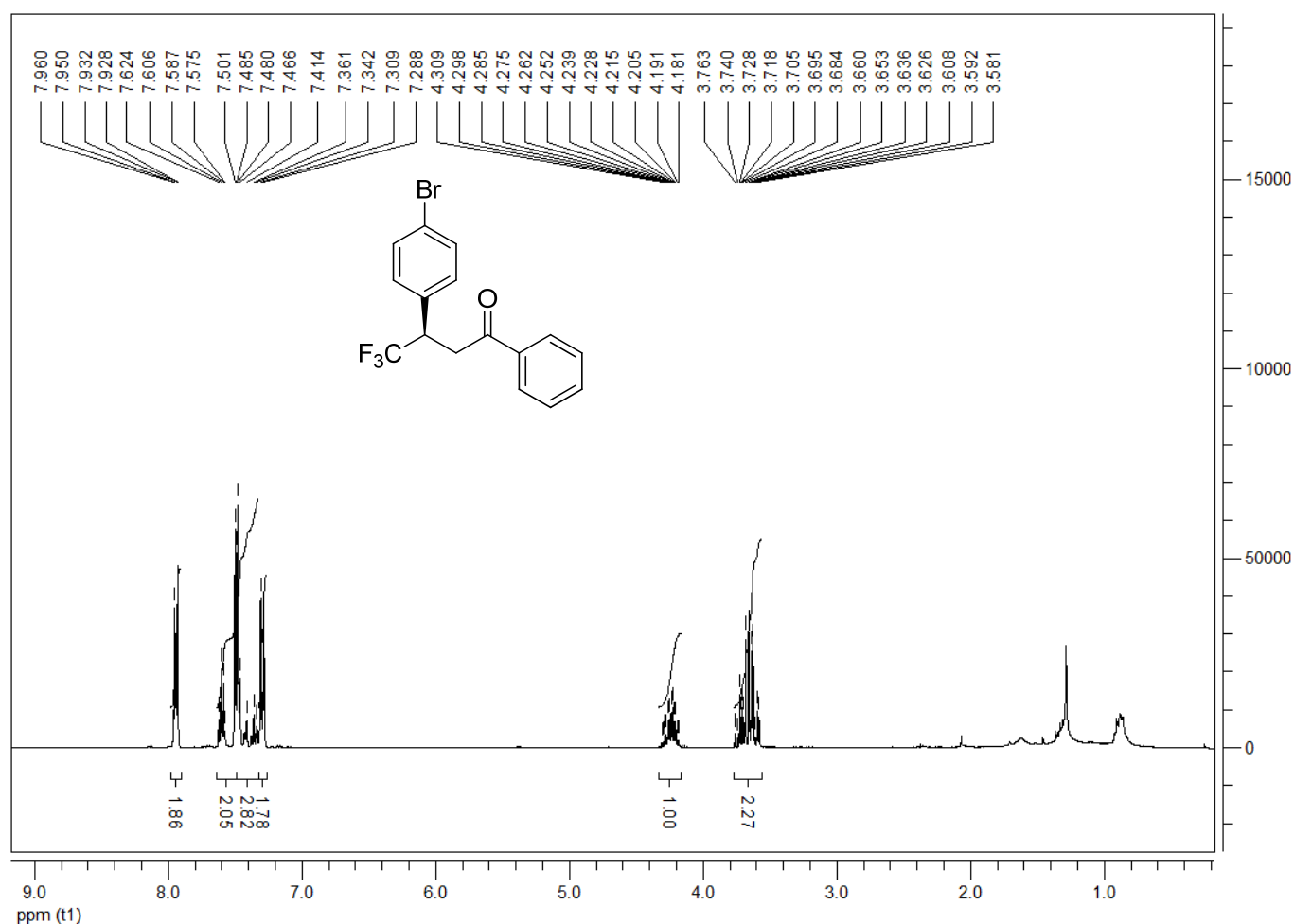


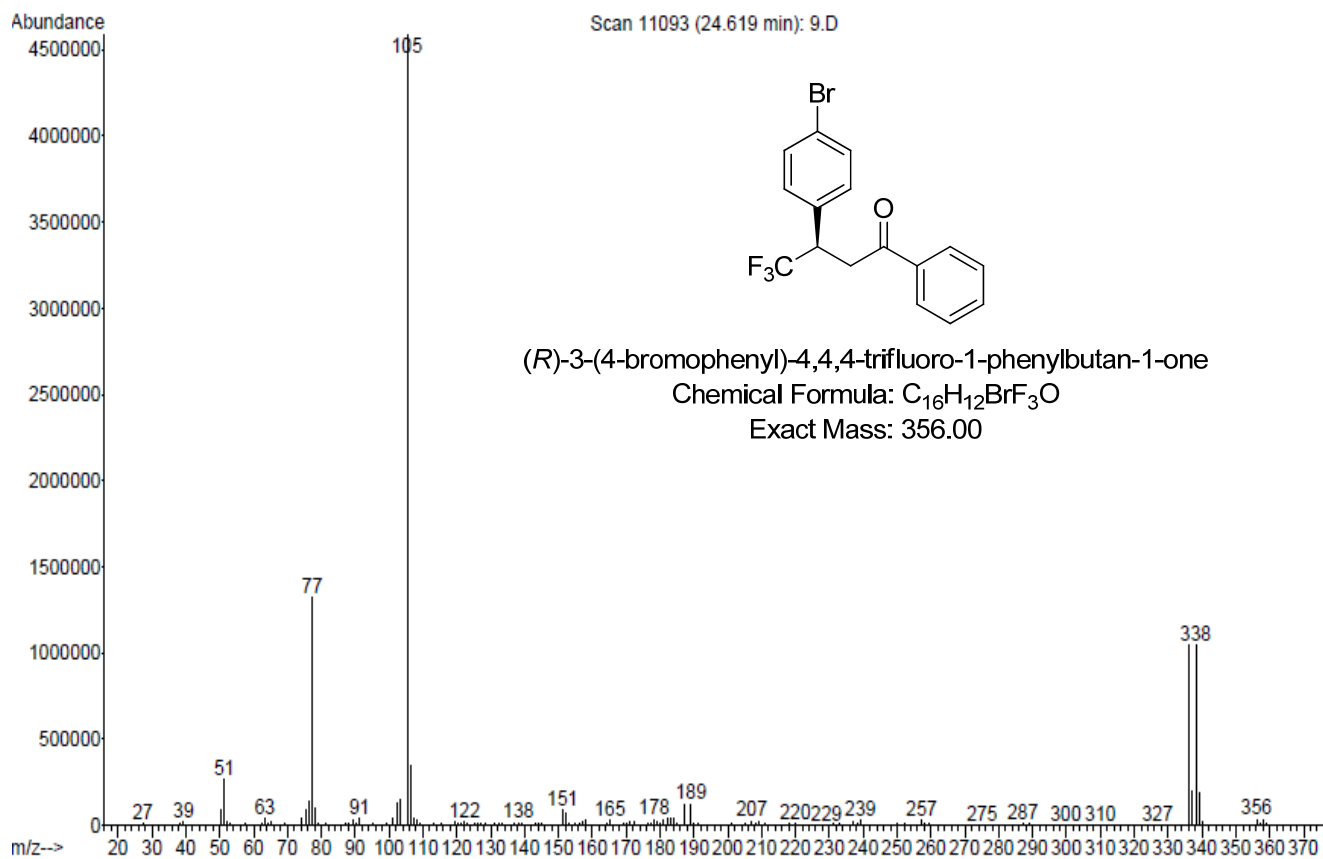
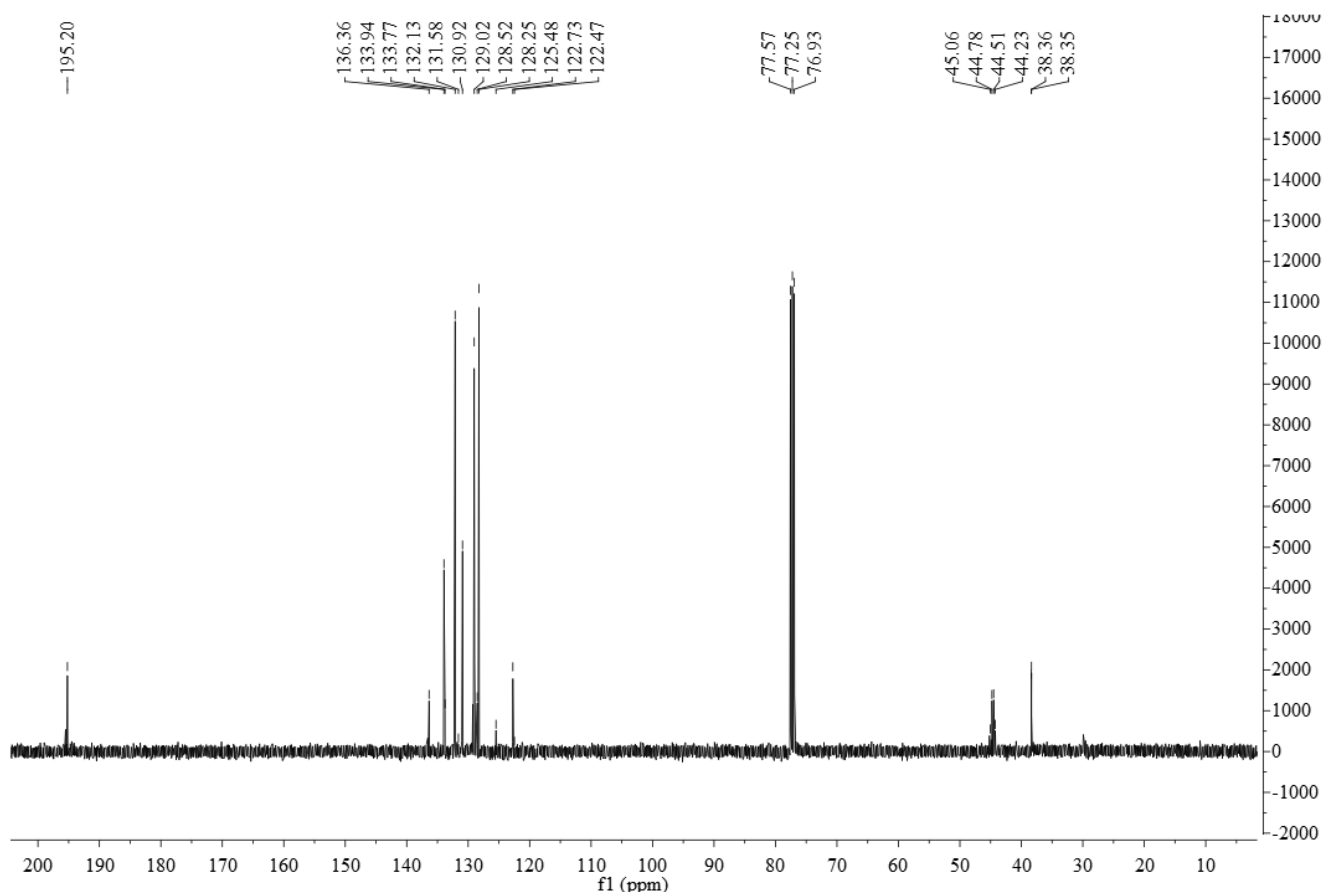


6d: (R)-3-(4-Bromoophenyl)-4,4,4-trifluoro-1-phenylbutan-1-one

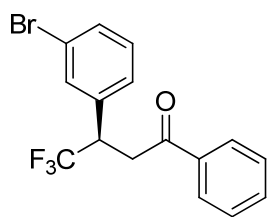


Yield: 95% (94% ee, 98% es); ^1H NMR (400 MHz, CDCl_3): δ 3.58 (dd, 1H, $J = 3$ Hz, $J = 18$ Hz), 3.67 (dd, 1H, $J = 9$ Hz, $J = 18$ Hz), 4.21 (m, 1H), 7.25-7.28 (m, 2H), 7.43-7.48 (m, 3H), 7.56-7.60 (m, 2H), 7.90-7.93 (m, 2H); ^{13}C NMR (100 MHz, CDCl_3): δ 38.2 (q, $J = 2$ Hz), 44.6 (q, $J = 27$ Hz), 122.7, 126.9 (q, $J = 279$ Hz), 128.3, 129.0, 130.9, 132.1, 133.8, 133.9, 136.4, 195.2; GC/MS (m/z): 356.00; HPLC (OD-H, elute: n -hexanes/ i -PrOH = 95/5, detector: 254 nm, flow rate: 1.0 mL/min, 25 °C) $t_1 = 5.2$ min, $t_2 = 6.2$ min.



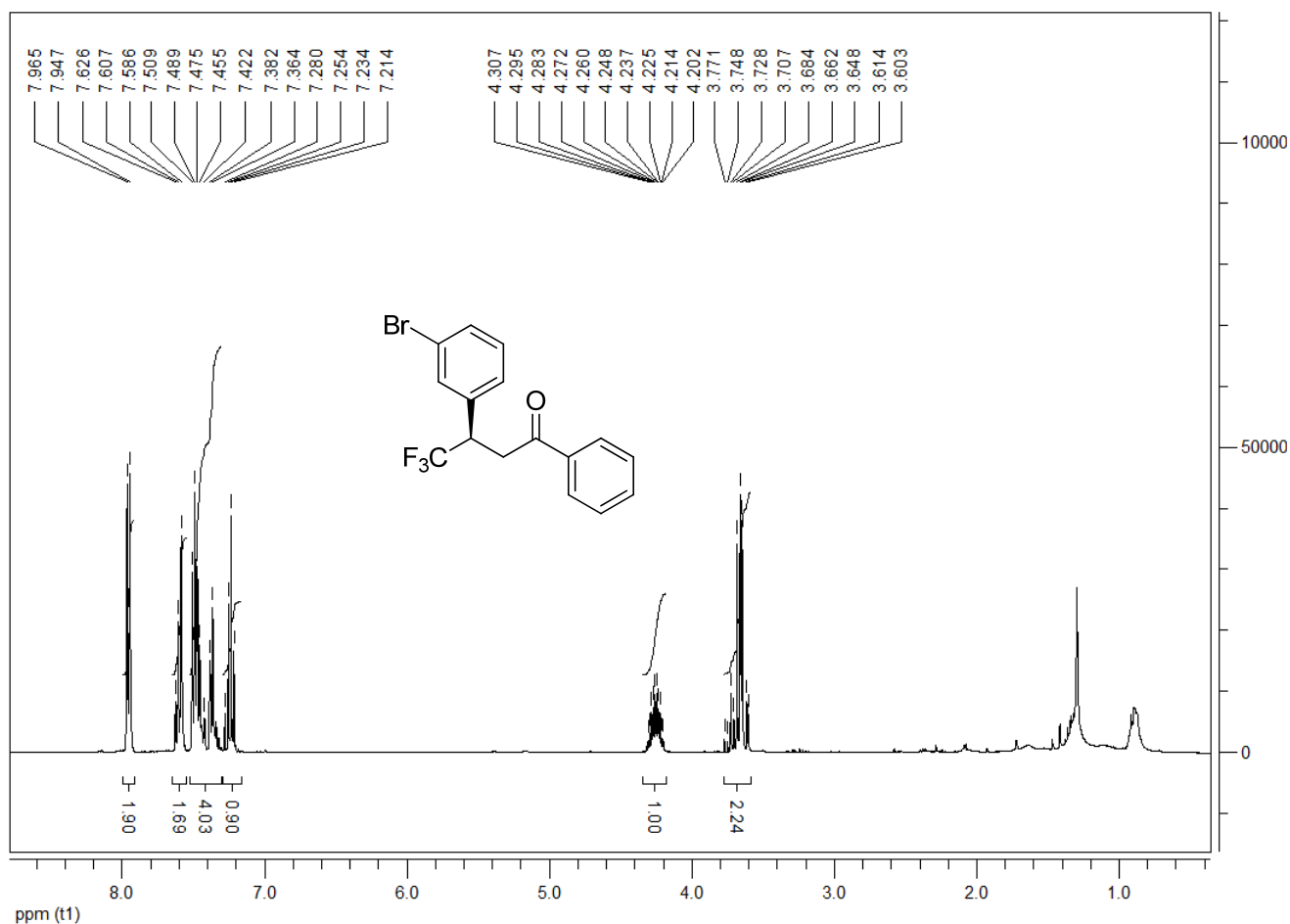


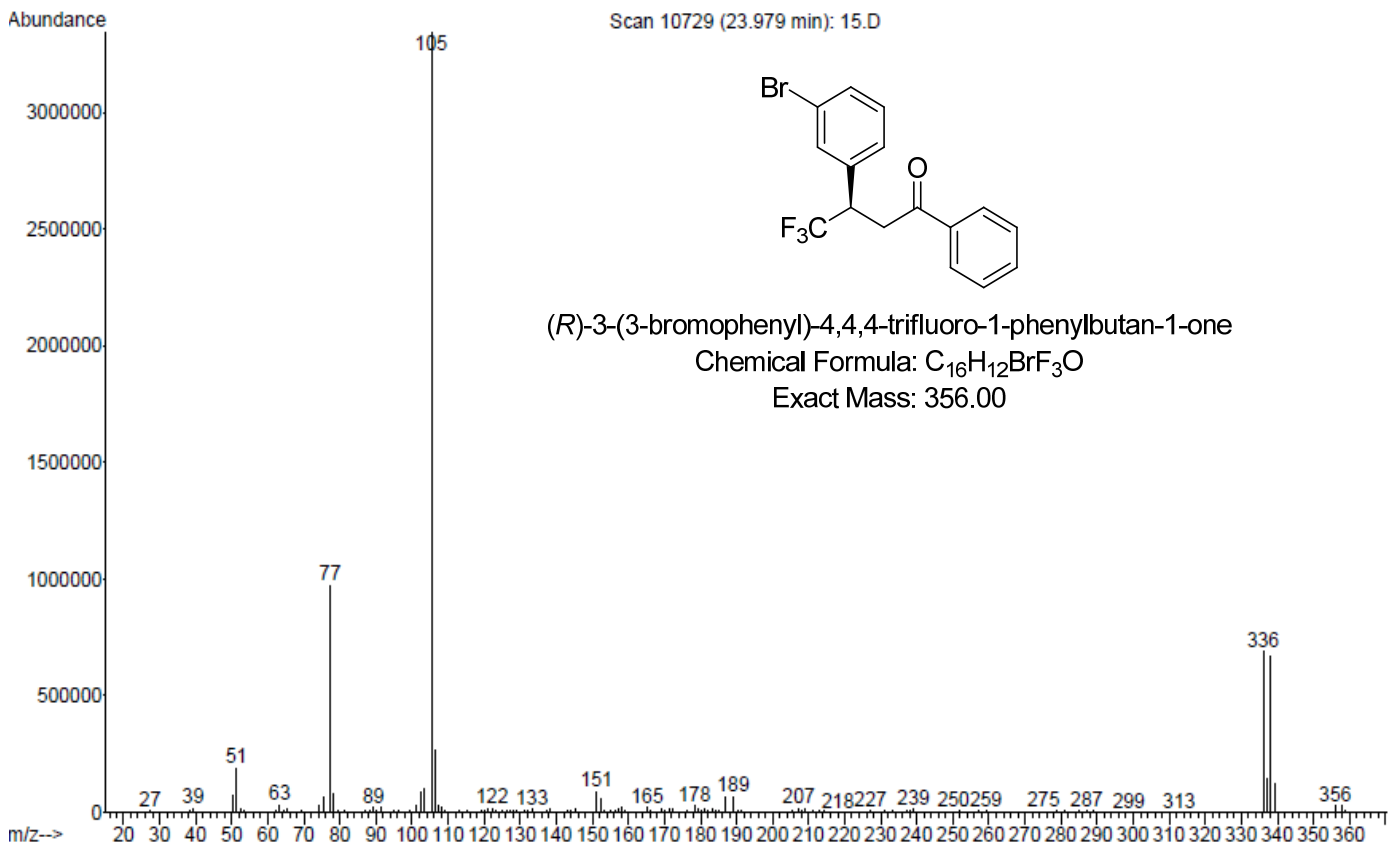
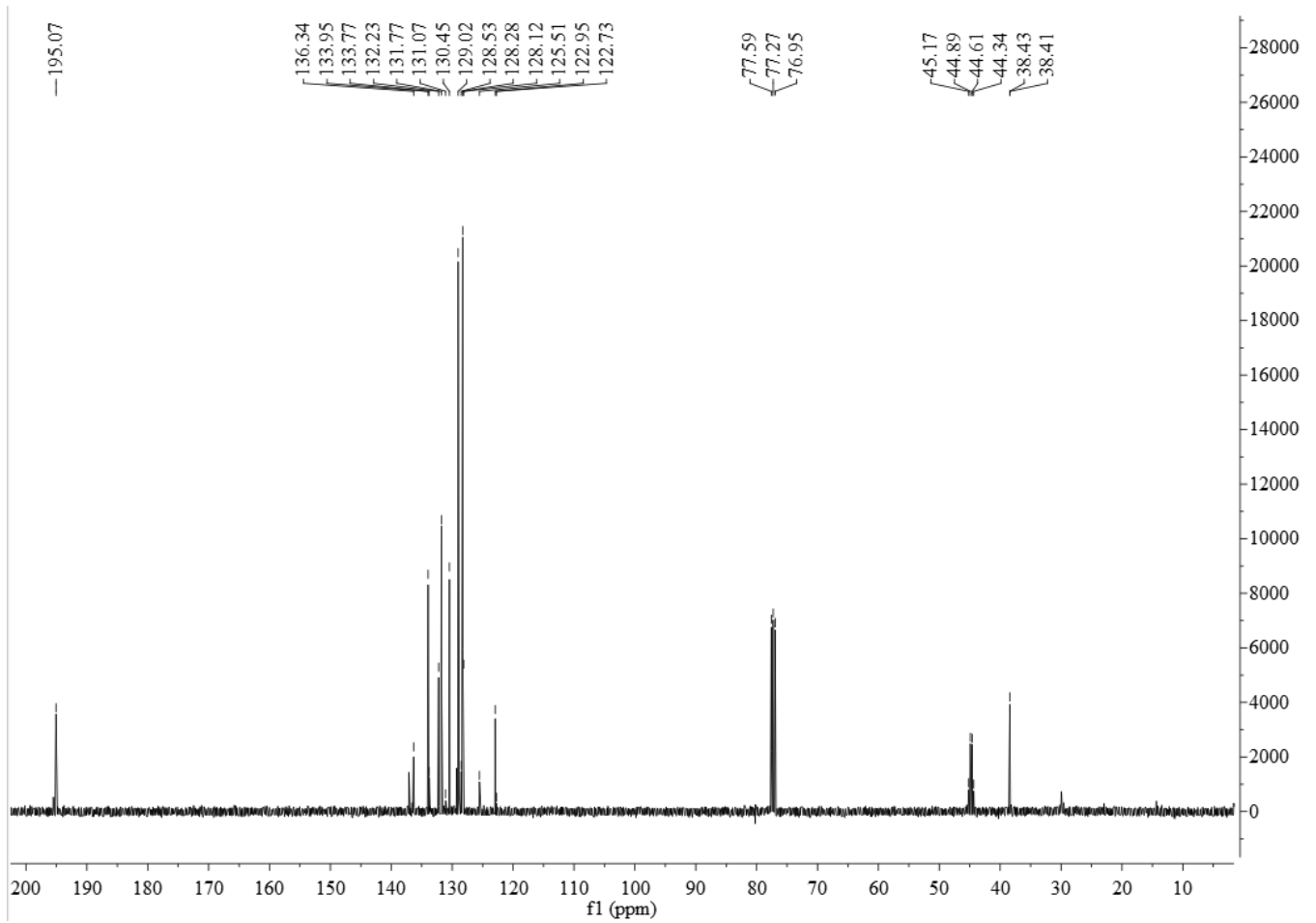
6e: (R)-3-(3-Bromoephnyl)-4,4,4-trifluoro-1-phenylbutan-1-one.



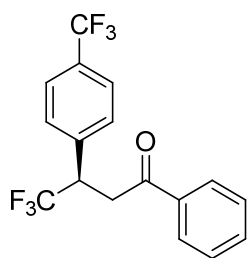
Yield: 94% (95% ee, 100% es); ^1H NMR (400 MHz, CDCl_3): δ 3.58 (dd, 1H, $J = 3$ Hz, $J = 18$ Hz), 3.67 (dd, 1H, $J = 9$ Hz, $J = 18$ Hz), 4.20 (m, 1H), 7.21-7.28 (m, 1H), 7.33-7.41 (m, 1H), 7.42-7.53 (m, 3H), 7.56-7.65 (m, 2H), 7.90-7.98 (m, 2H); ^{13}C NMR (100 MHz, CDCl_3): δ 38.4 (q, $J = 2$ Hz), 44.7 (q, $J = 27$ Hz), 122.9, 127.0 (q, $J = 278$ Hz), 128.1, 128.3, 129.0, 130.4, 131.7, 132.2, 133.8, 133.9, 136.3,

195.1; GC/MS (m/z): 356.00; HPLC (OD-H, elute: *n*-hexanes/*i*-PrOH = 95/5, detector: 254 nm, flow rate: 1.0 mL/min, 25 °C) $t_1 = 8.2$ min, $t_2 = 10.5$ min.

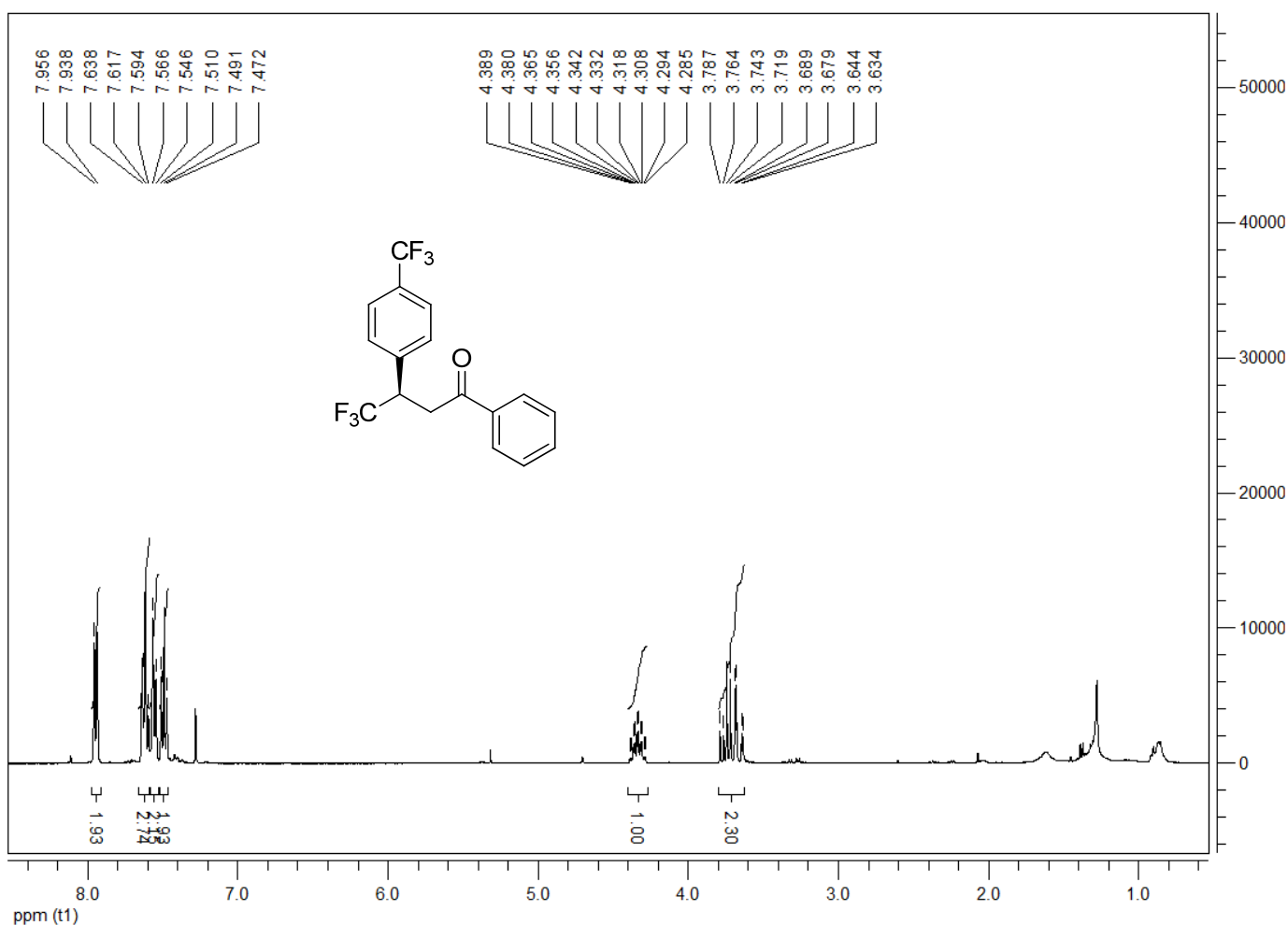


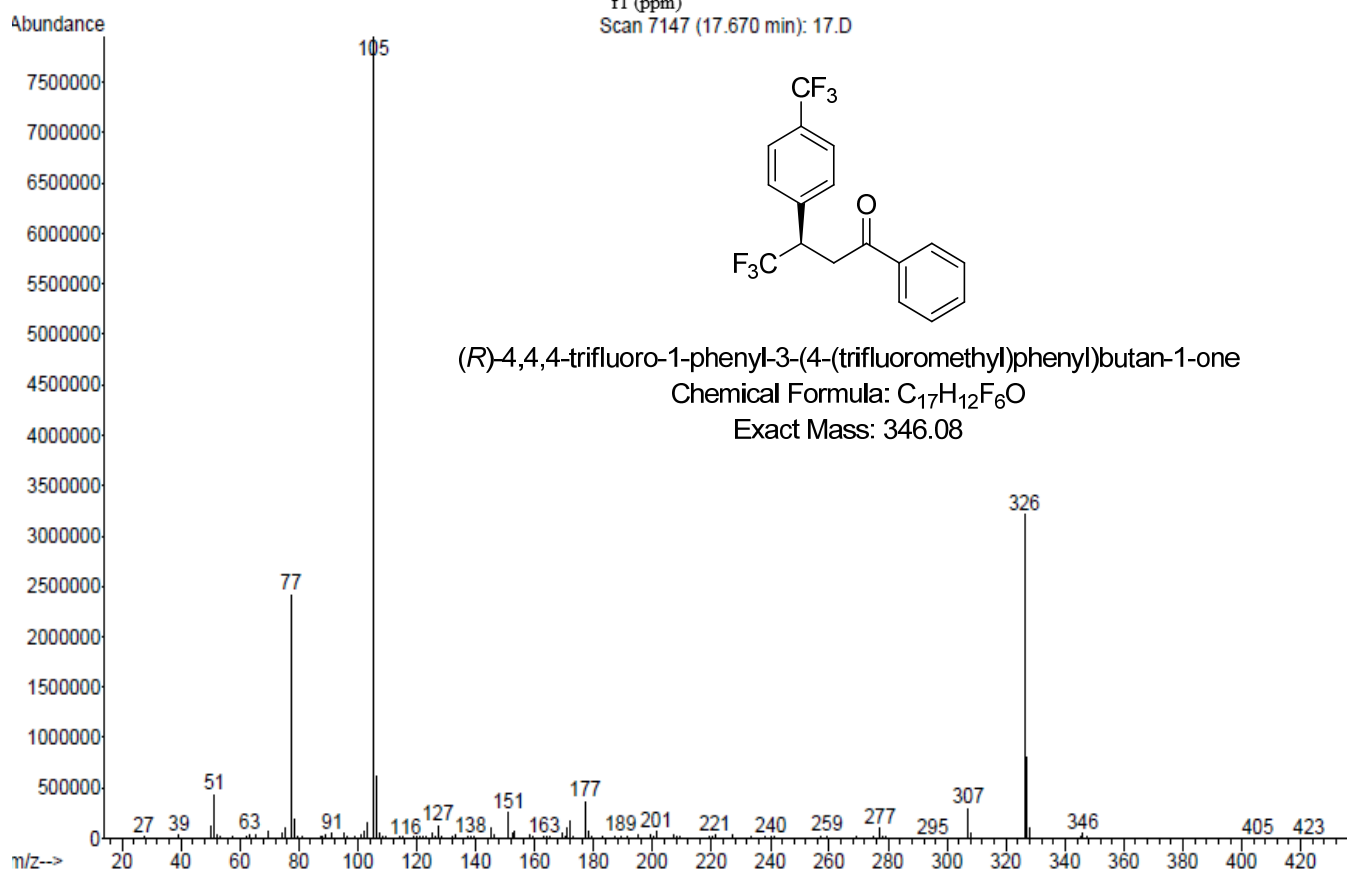
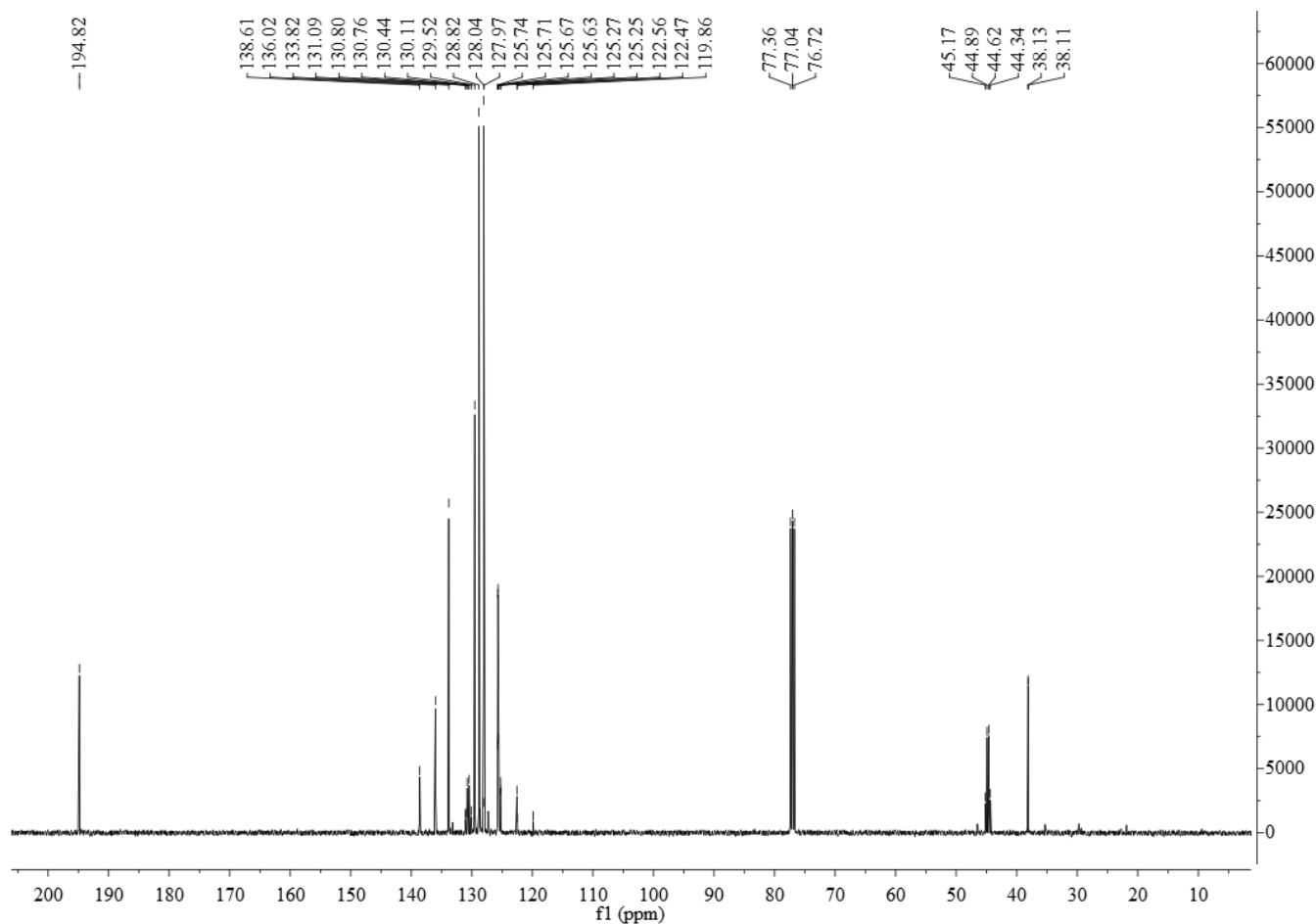


6f: (R)-4,4,4-Trifluoro-1-phenyl-3-(4'-(trifluoromethyl)phenyl)butan-1-one

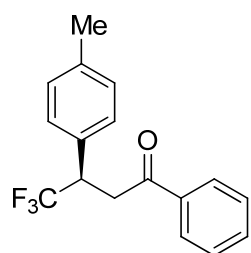


Yield: 97% (93% ee, 98% es); ^1H NMR (400 MHz, CDCl_3): δ 3.64 (dd, 1H, $J = 3$ Hz, $J = 18$ Hz), 3.74 (dd, 1H, $J = 9$ Hz, $J = 18$ Hz), 4.32 (m, 1H), 7.45-7.62 (m, 7H), 7.91-7.94 (m, 2H); ^{13}C NMR (100 MHz, CDCl_3): δ 38.1 (q, $J = 1.5$ Hz), 44.7 (q, $J = 28$ Hz), 123.9 (q, $J = 271$ Hz), 125.7 (q, $J = 4$ Hz), 126.6 (q, $J = 278$ Hz), 128.0, 128.8, 129.5, 130.6 (q, $J = 32$ Hz), 133.8, 136.0, 138.6, 194.8; GC/MS (m/z): 346.08; HPLC (OD-H, elute: *n*-hexanes/*i*-PrOH = 95/5, detector: 254 nm, flow rate: 1.0 mL/min, 25 $^\circ\text{C}$) $t_1 = 6.5$ min, $t_2 = 8.3$ min

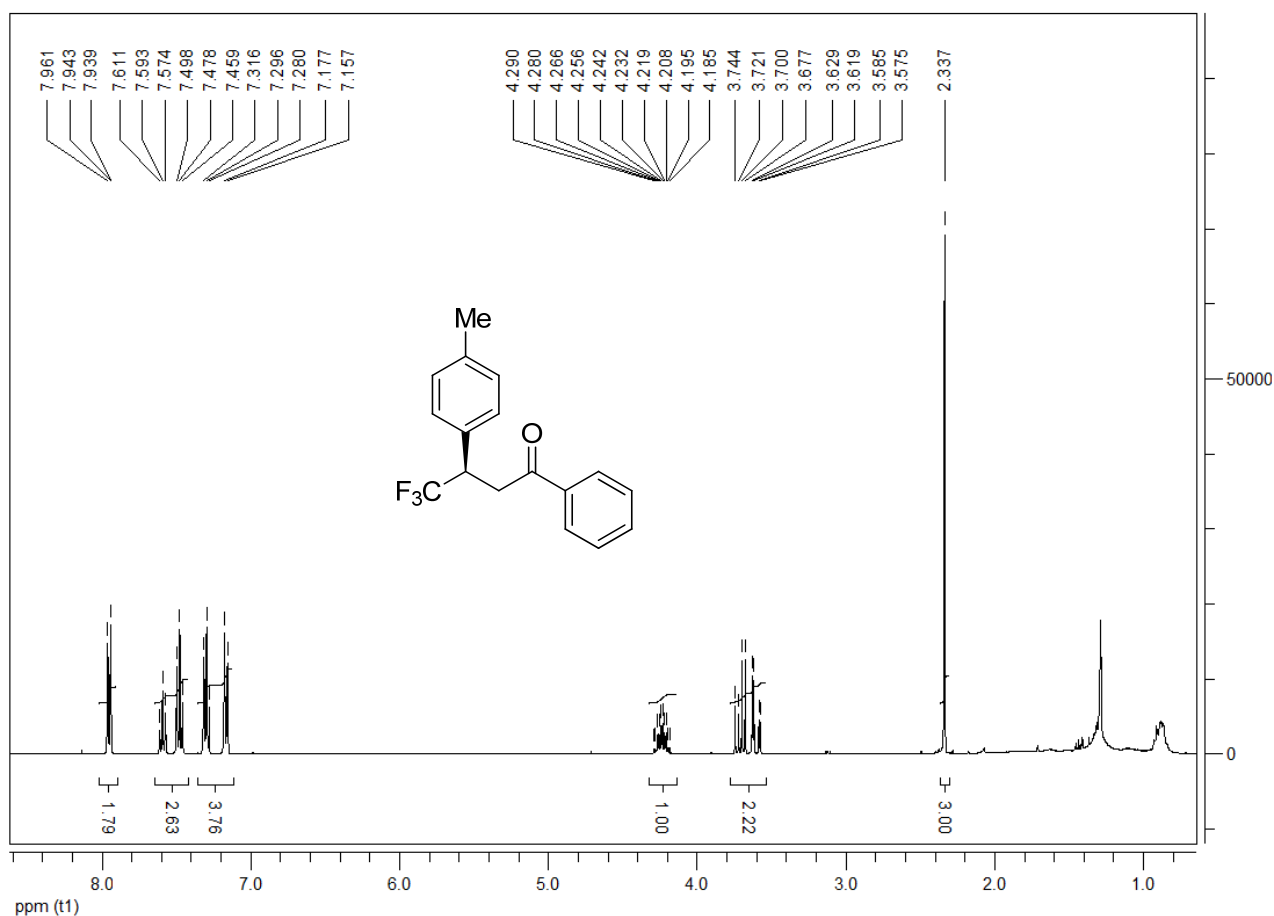


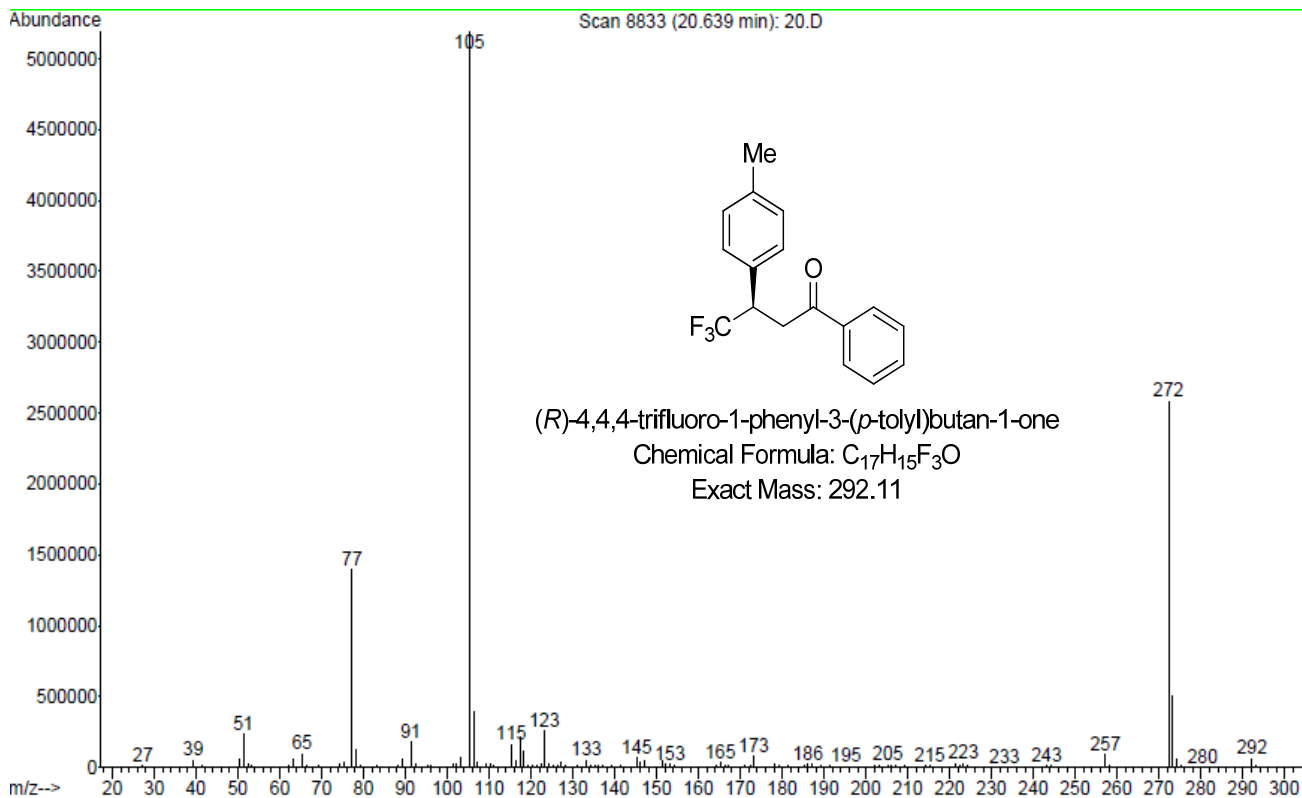
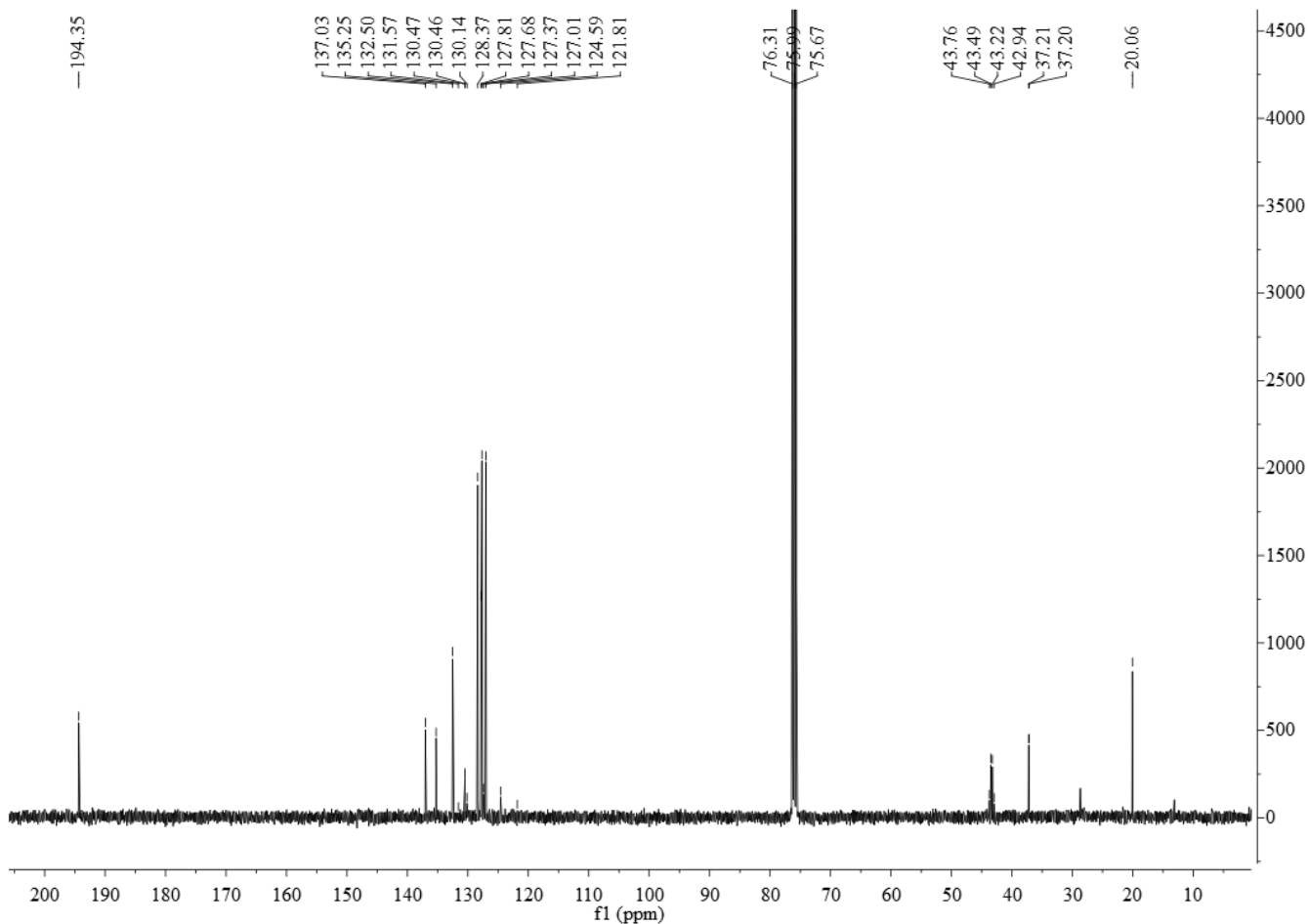


6g: (R)-4,4,4-trifluoro-1-phenyl-3-*p*-tolylbutan-1-one

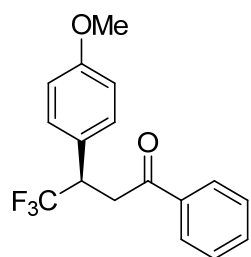


Yield: 96% (93% ee, 99% es); ^1H NMR (400 MHz, CDCl_3): δ 2.32 (s, 3H), 3.59 (dd, 1H, $J = 17.7$ Hz, $J = 3.9$ Hz), 3.73 (dd, 1H, $J = 17.8$ Hz, $J = 9.2$ Hz), 4.19–4.25 (m, 1H), 7.16 (d, 2H, $J = 7.7$ Hz), 7.30 (d, 2H, $J = 7.7$ Hz), 7.46 (t, 2H, $J = 7.6$ Hz), 7.58 (t, 1H, $J = 7.2$ Hz), 7.94 (d, 2H, $J = 7.6$ Hz); ^{13}C NMR (100 MHz, CDCl_3): δ 20.0, 37.2 (q, $J = 1.5$ Hz), 43.3 (q, $J = 27$ Hz), 125.9 (q, $J = 277$ Hz), 127.0, 127.6, 127.8, 128.3, 130.4 (q, $J = 2$ Hz), 131.5, 132.5, 135.2, 137.0, 194.3; GC/MS (m/z): 292.11; HPLC (OD-H, elute: *n*-hexanes/*i*-PrOH = 95/5, detector: 254 nm, flow rate: 1.0 mL/min, 25 °C) $t_1 = 5.4$ min, $t_2 = 6.1$ min.

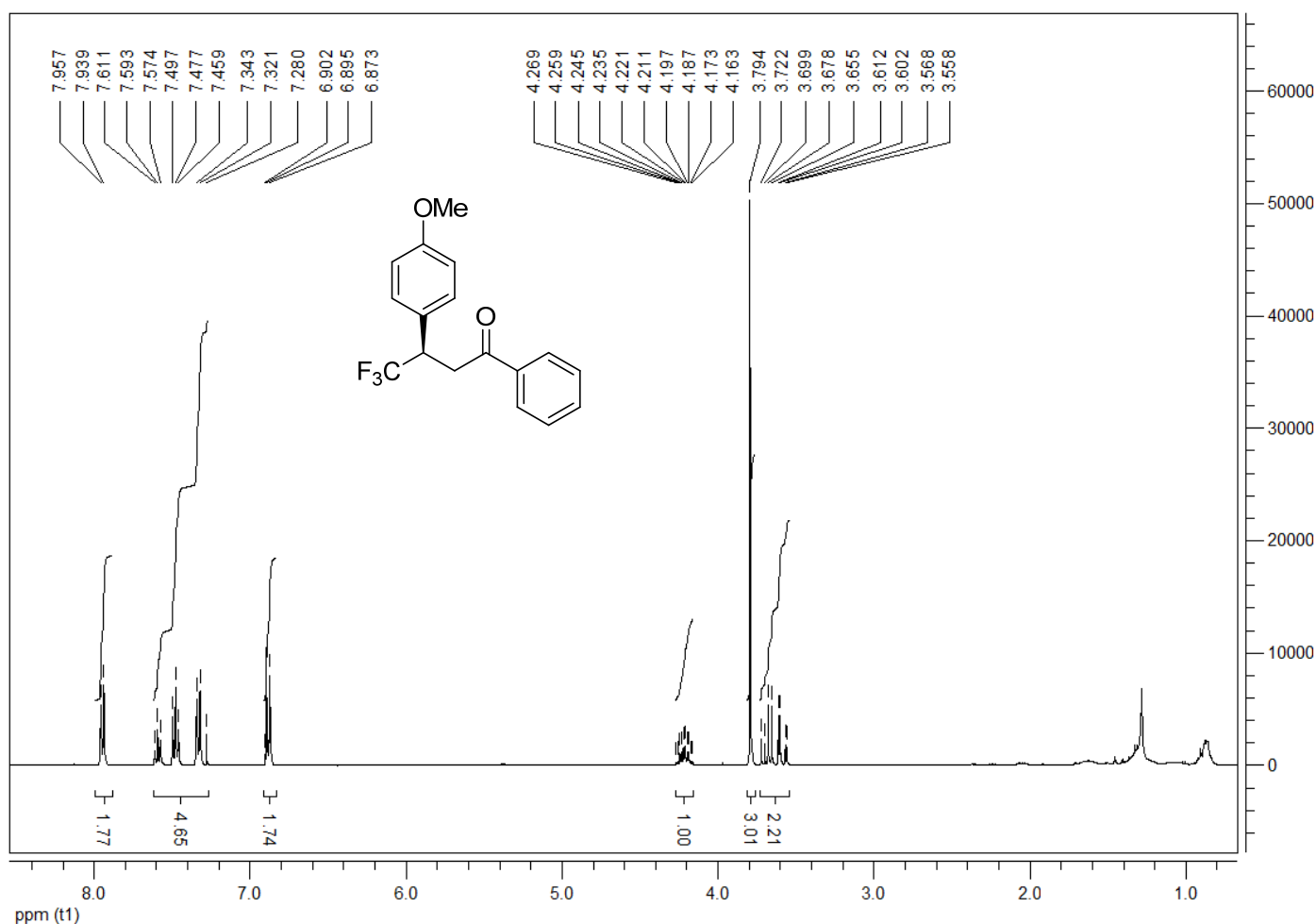


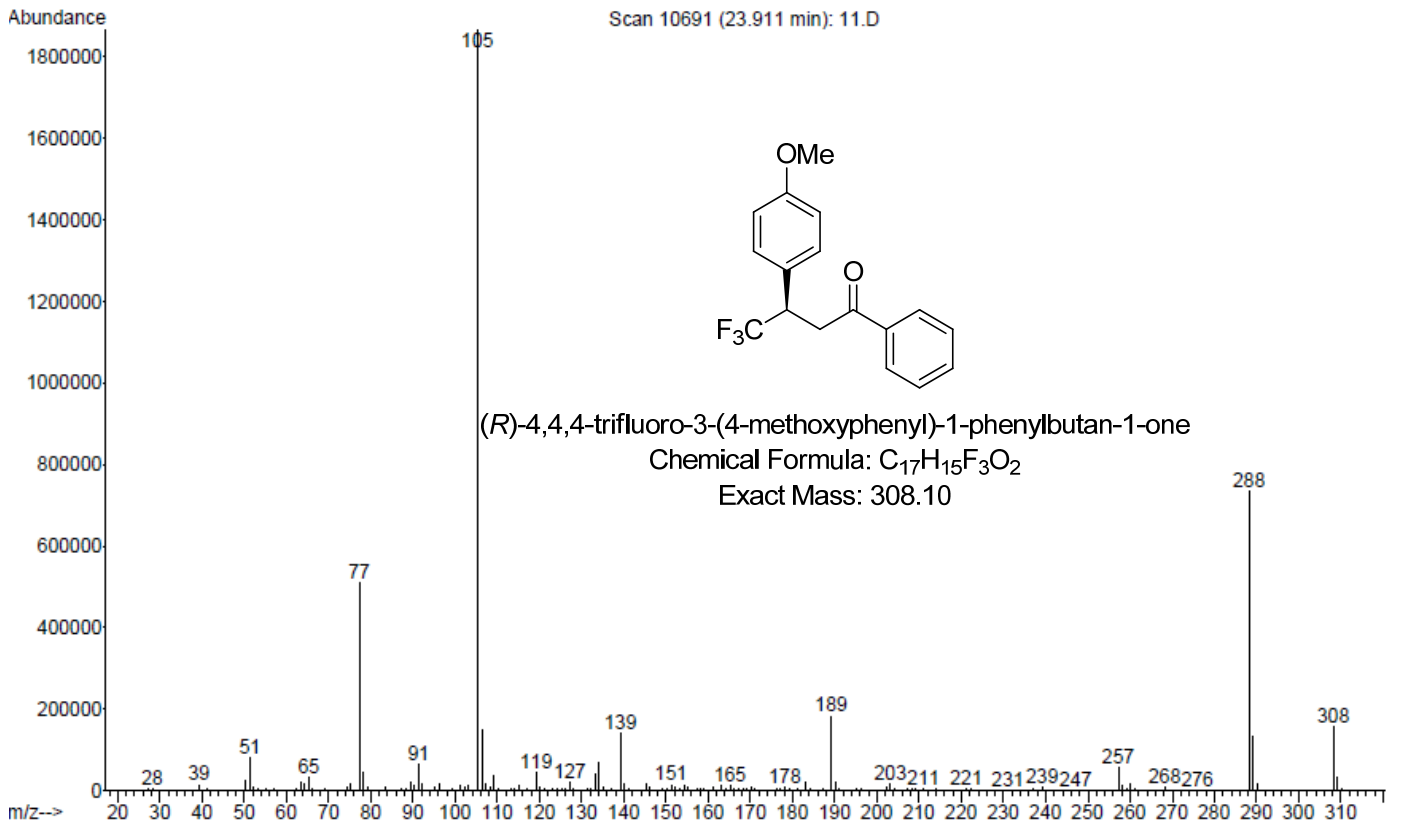
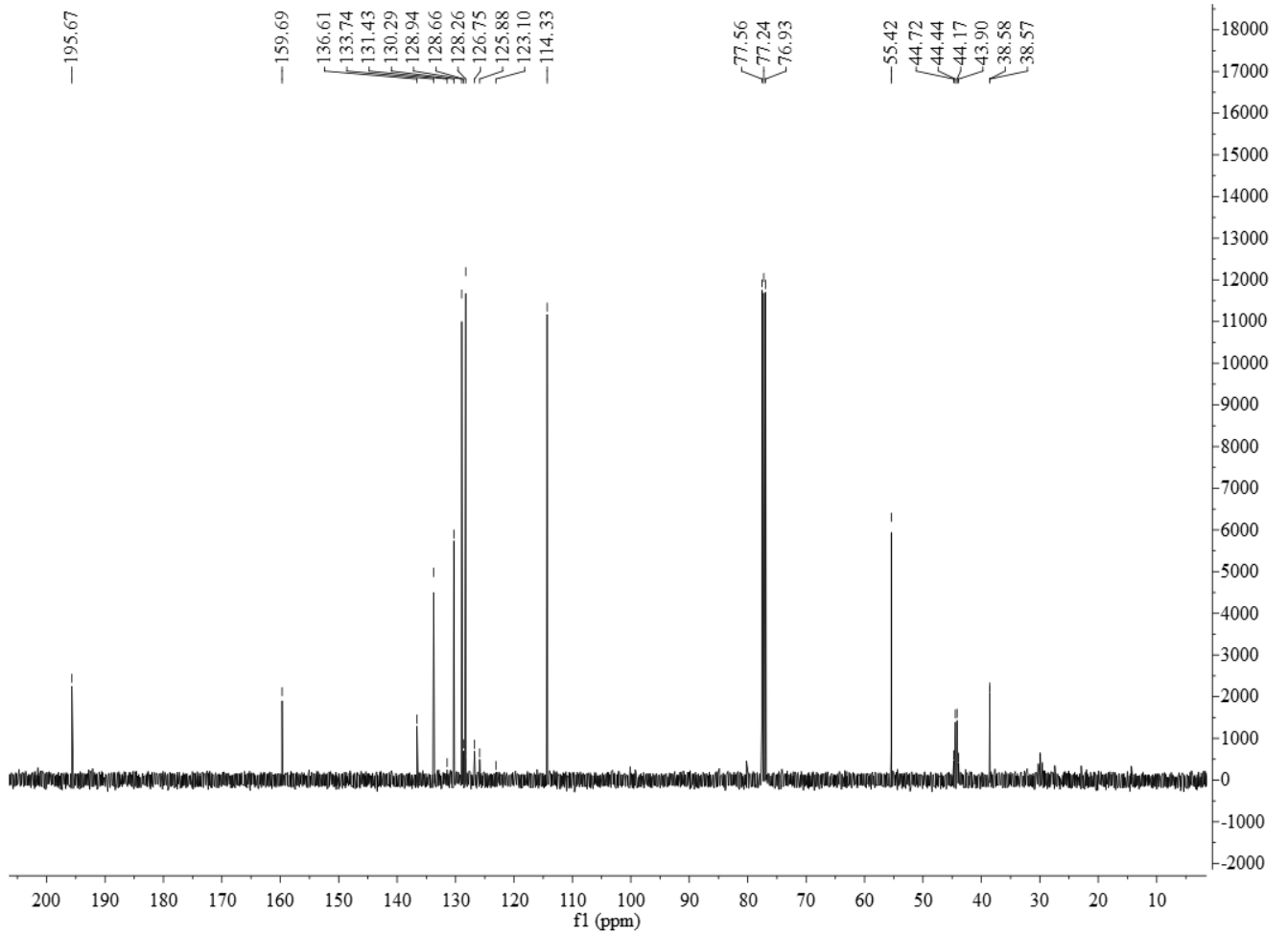


6h: (R)-4,4,4-Trifluoro-3-(4-methoxyphenyl)-1-phenylbutan-1-one

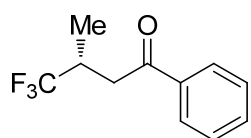


Yield: 92% (93% ee, 95% es); ^1H NMR (400 MHz, CDCl_3): δ 3.56 (dd, 1H, $J = 4$ Hz, $J = 18$ Hz), 3.68 (dd, 1H, $J = 9$ Hz, $J = 18$ Hz), 3.77 (s, 3H), 4.12-4.27 (m, 1H), 6.85-6.89 (m, 2H), 7.30-7.33 (m, 2H), 7.43-7.48 (m, 2H), 7.54-7.60 (m, 1H), 7.91-7.95 (m, 2H); ^{13}C NMR (100 MHz, CDCl_3): δ 38.6 (q, $J = 2$ Hz), 44.3 (q, $J = 27$ Hz), 55.4, 114.3, 126.7 (q, $J = 2$ Hz), 127.3 (q, $J = 277$ Hz), 128.3, 128.9, 130.3, 133.7, 136.6, 159.7, 195.7; GC/MS (m/z): 308.10; HPLC (OD-H, elute: *n*-hexanes/*i*-PrOH = 95/5, detector: 254 nm, flow rate: 1.0 mL/min, 25 °C) $t_1 = 14.4$ min, $t_2 = 15.0$ min.





6i: (R)-4,4,4-Trifluoro-3-methyl-1-phenylbutan-1-one



Yield: 97% (88% ee, 98% es); ^1H NMR (400 MHz, CDCl_3): δ 1.19 (d, $J = 6\text{ Hz}$, 3H),

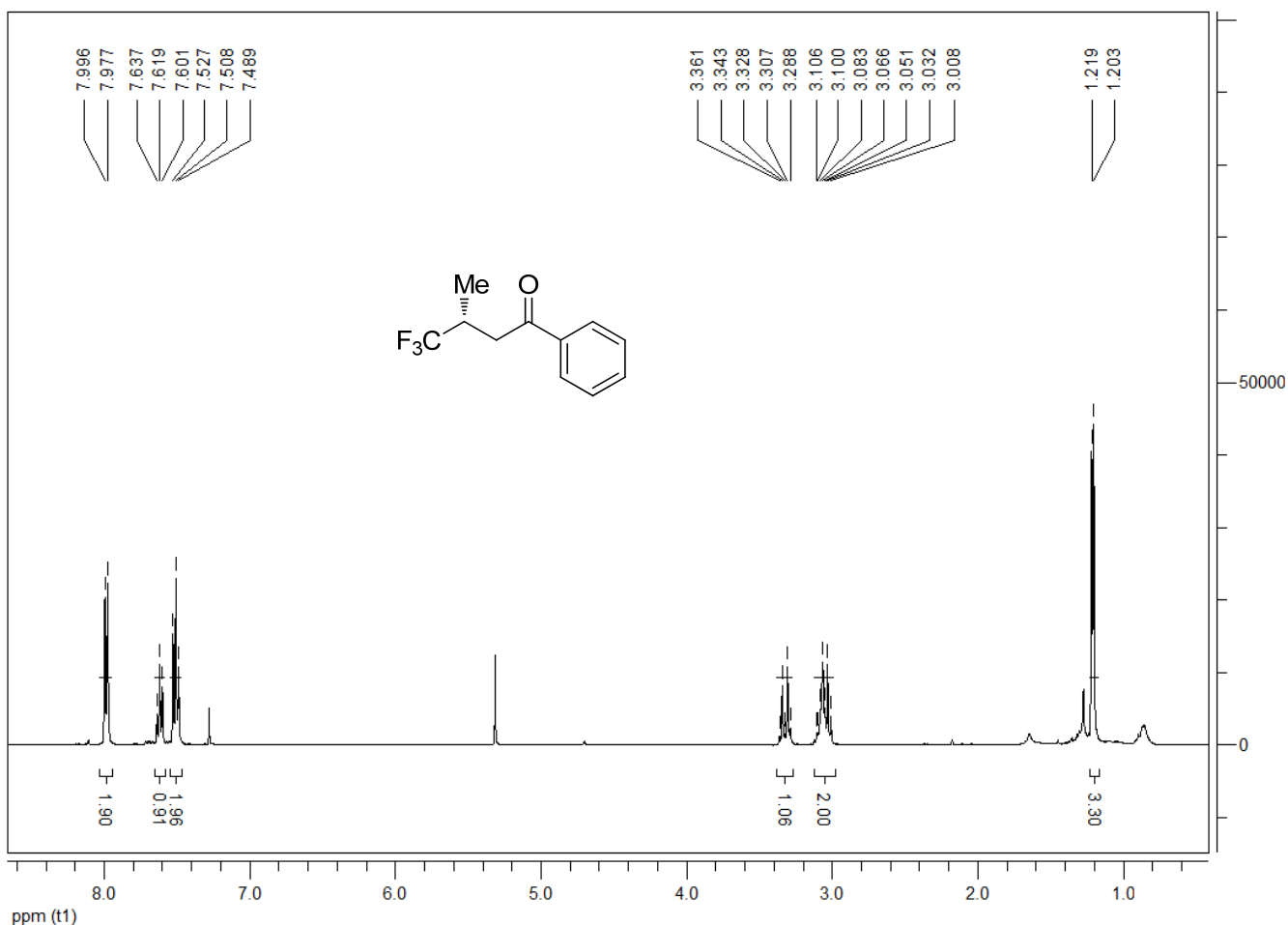
2.98-3.06 (m, 2H), 3.26-3.35 (m, 1H), 7.49 (t, $J = 7\text{ Hz}$, 2H), 7.60 (t, $J = 7\text{ Hz}$, 1H),

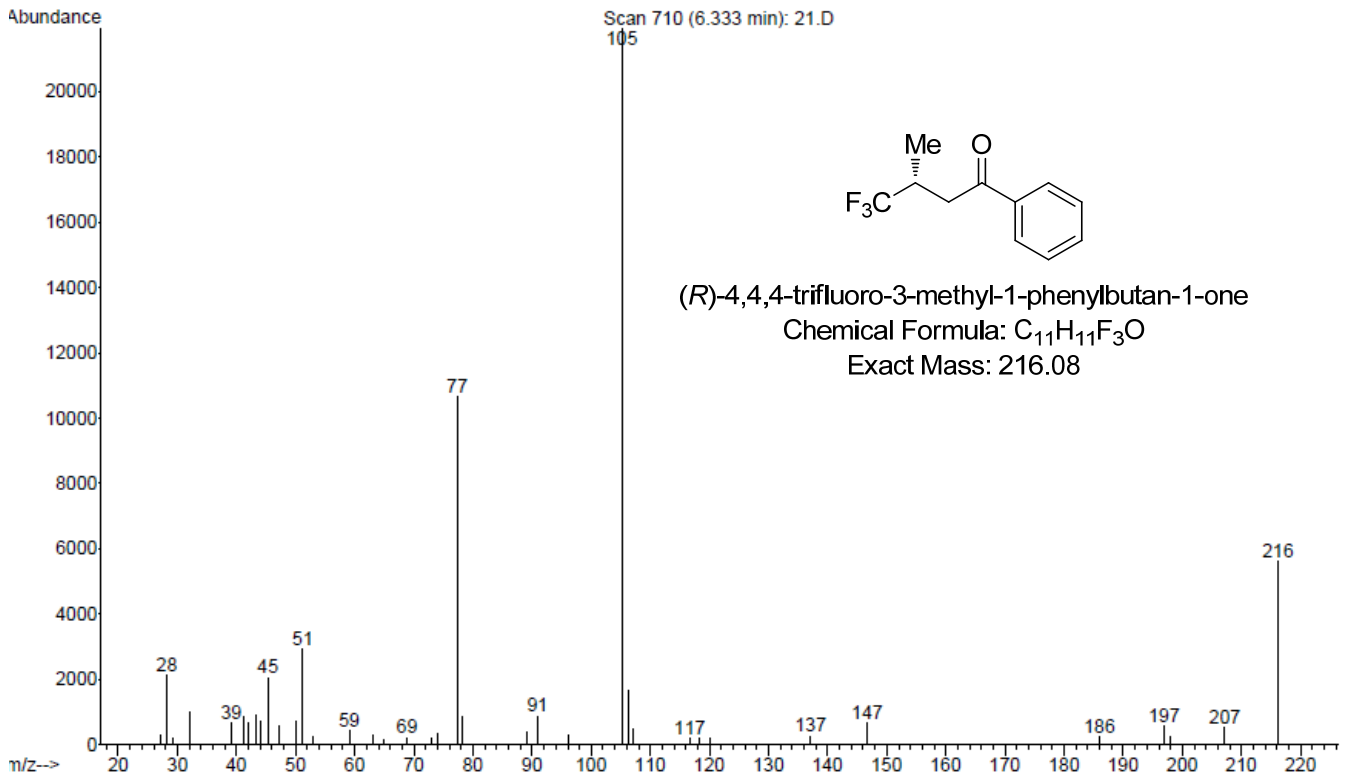
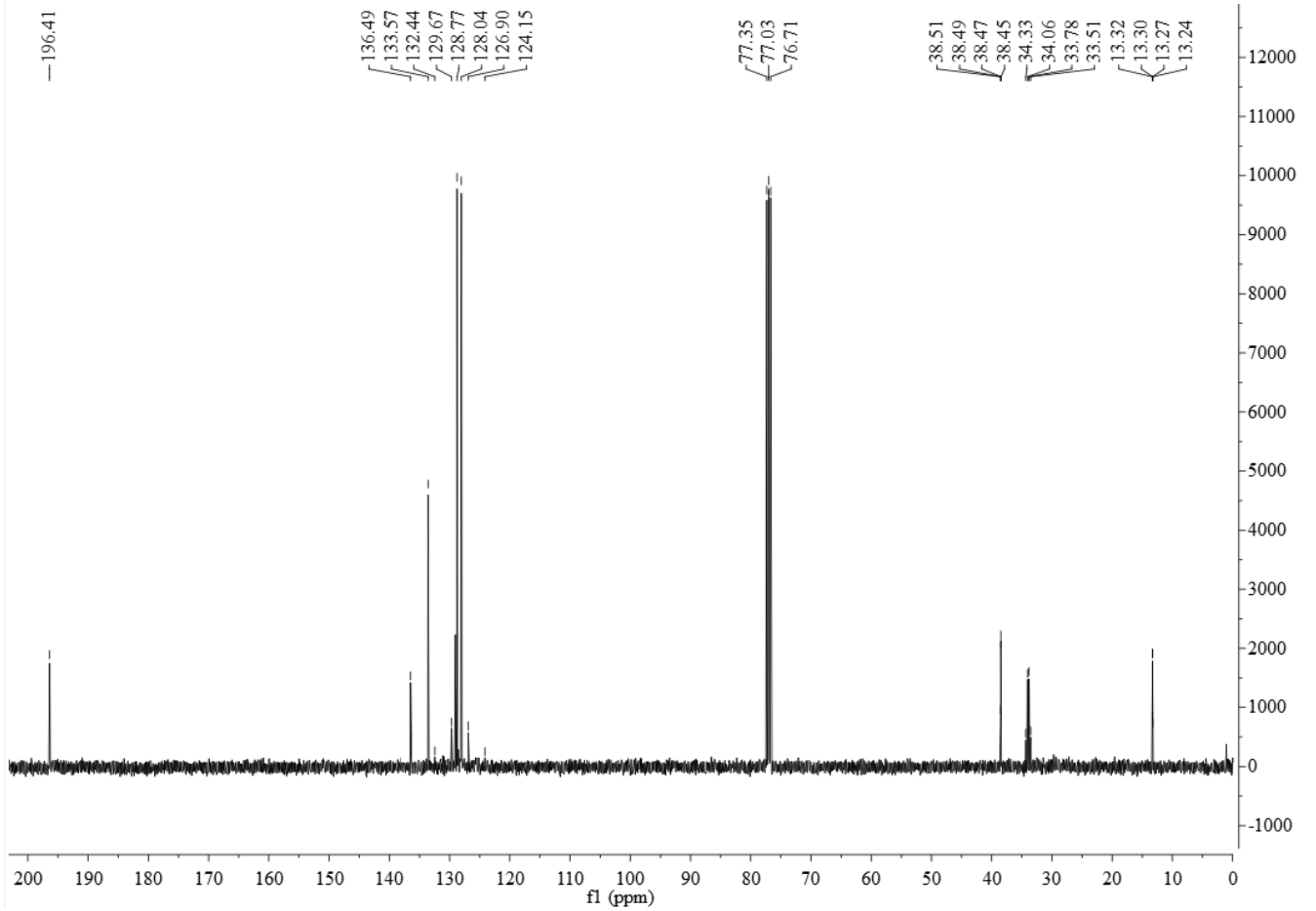
7.97 (d, $J = 7\text{ Hz}$, 2H); ^{13}C NMR (100 MHz, CDCl_3): δ 13.3 (q, $J = 2\text{ Hz}$), 33.9 (q, J

$= 27\text{ Hz}$), 38.5 (q, $J = 2\text{ Hz}$), 128.0, 128.3 (q, $J = 276\text{ Hz}$), 128.8, 133.6, 136.5, 196.4; GC/MS (m/z):

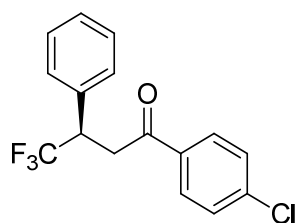
216.08; HPLC (OJ-H, elute: *n*-hexanes/*i*-PrOH = 99/1, detector: 254 nm, flow rate: 0.5 mL/min, 25 °C)

$t_1 = 12.8\text{ min}$, $t_2 = 13.4\text{ min}$.

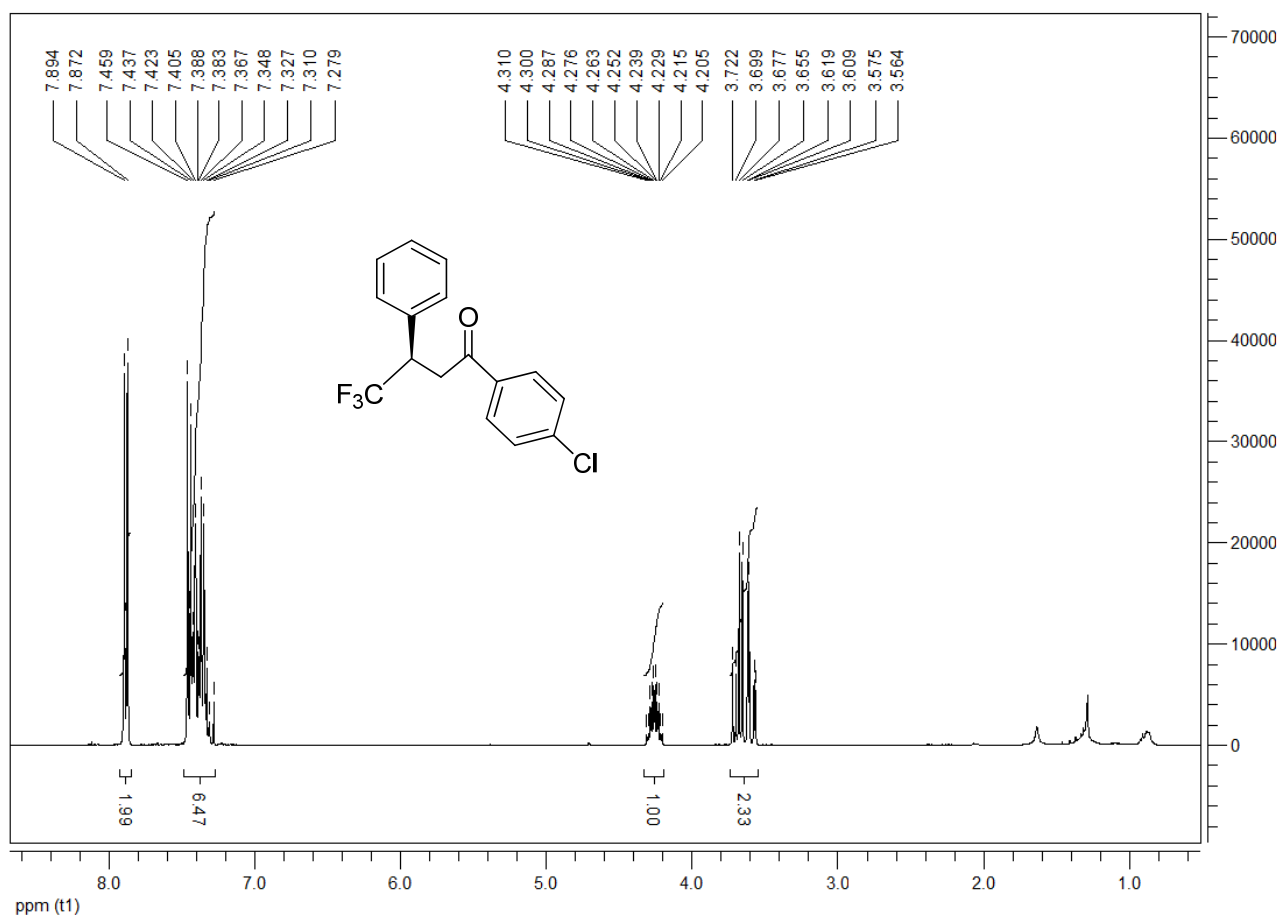


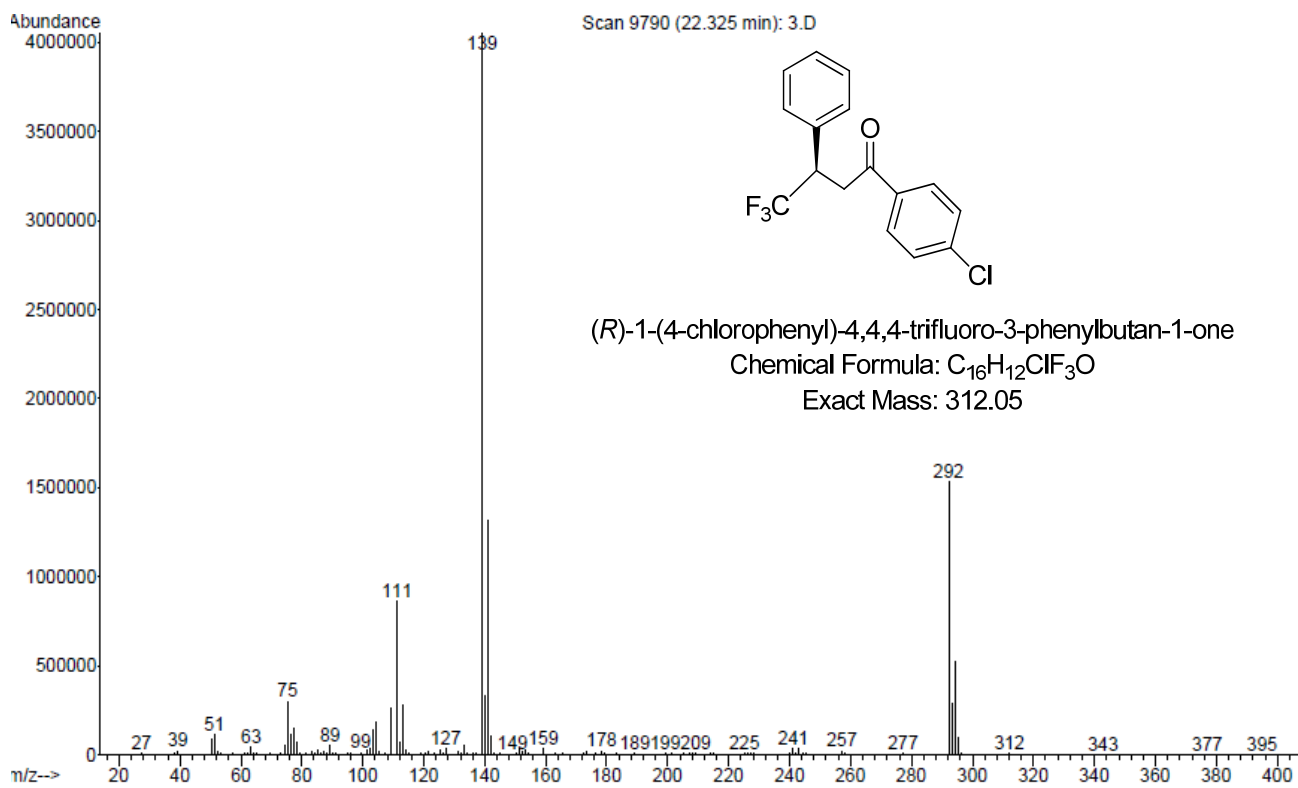
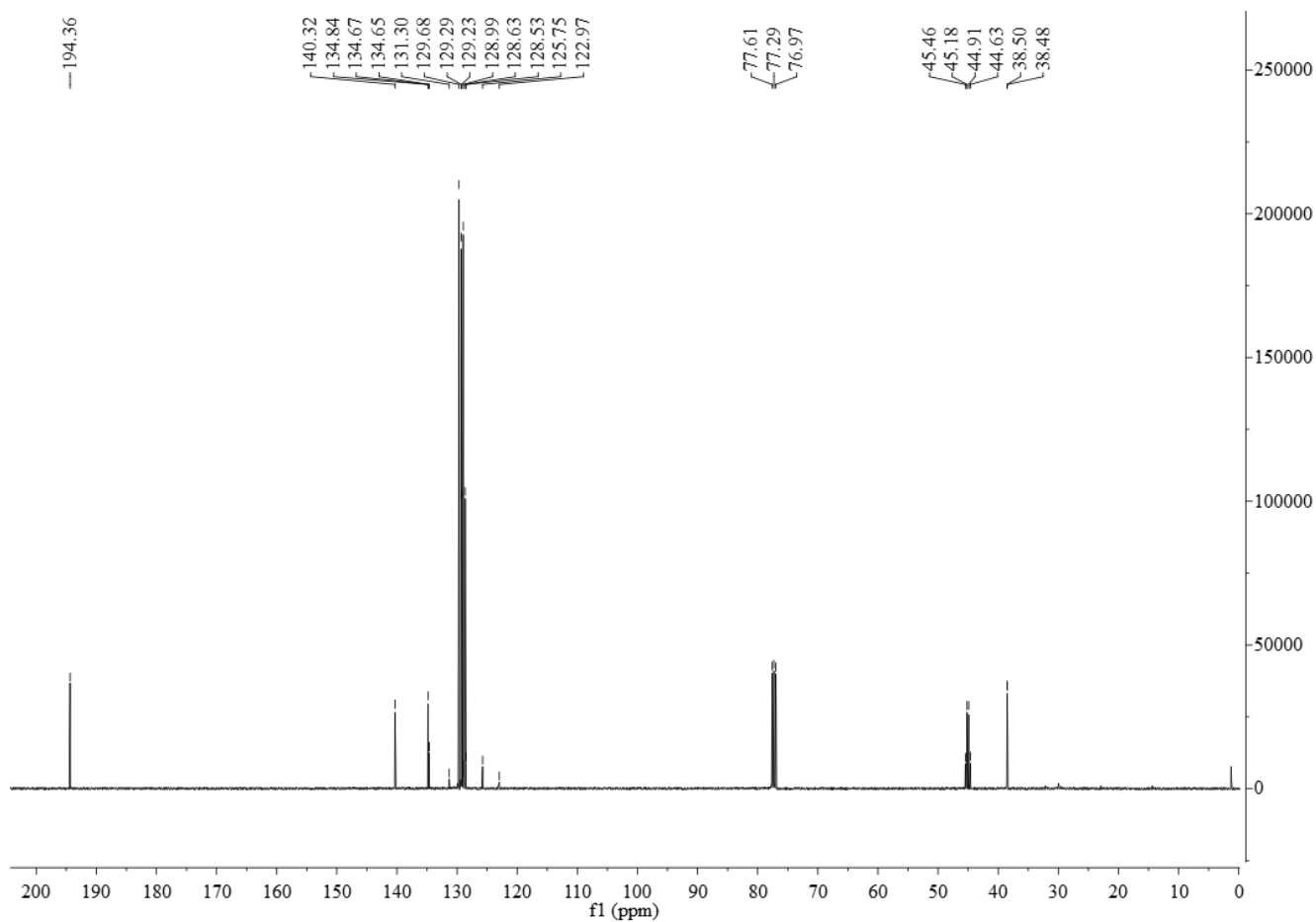


6j: (R)-1-(4-Chlorophenyl)-4,4,4-trifluoro-3-phenyl-1-butanone

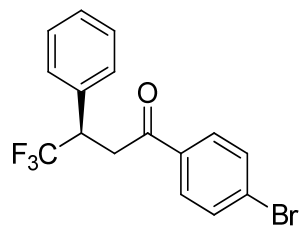


Yield: 96% (88% ee, 97% es); ¹H NMR (400 MHz, CDCl₃): δ3.53 (dd, 1H, *J* = 17.8 Hz, *J* = 4.4 Hz), 3.64 (dd, 1H, *J* = 17.8 Hz, *J* = 8.8 Hz), 4.12–4.26 (m, 1H), 7.28–7.40 (m, 7H), 7.82 (d, 2H, *J* = 8.6 Hz); ¹³C NMR (100 MHz, CDCl₃): δ38.5 (q, *J* = 2 Hz) 45.0 (q, *J* = 27 Hz), 127.0 (q, *J* = 277.8 Hz), 128.6, 129.0, 129.2, 129.3, 129.7, 134.6 (q, *J* = 2 Hz), 134.8, 140.3, 194.3; GC/MS (*m/z*): 312.05; HPLC (OD-H, elute: *n*-hexanes/*i*-PrOH = 95/5, detector: 254 nm, flow rate: 1.0 mL/min, 25 °C) *t*₁ = 6.3 min, *t*₂ = 7.2 min.

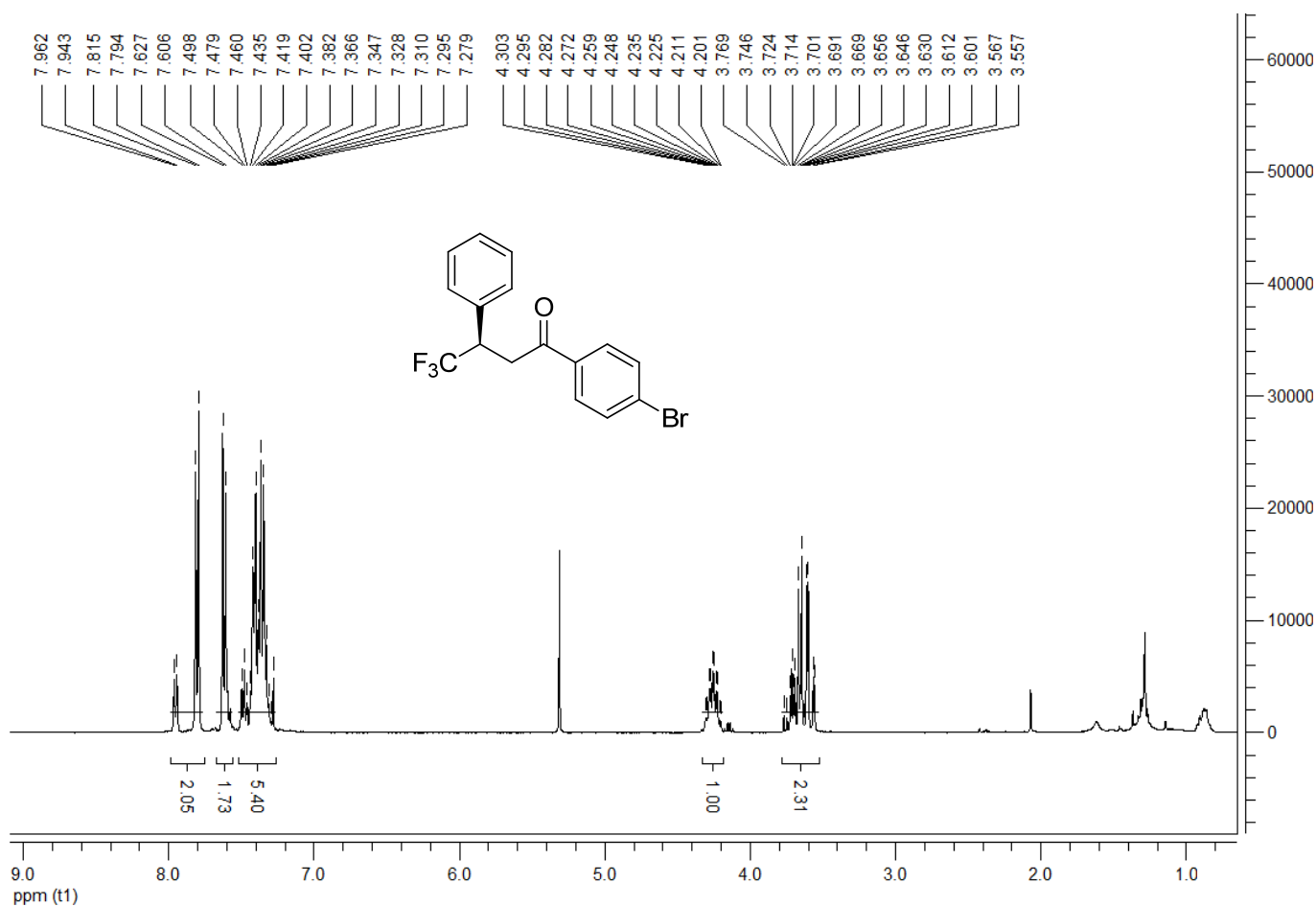


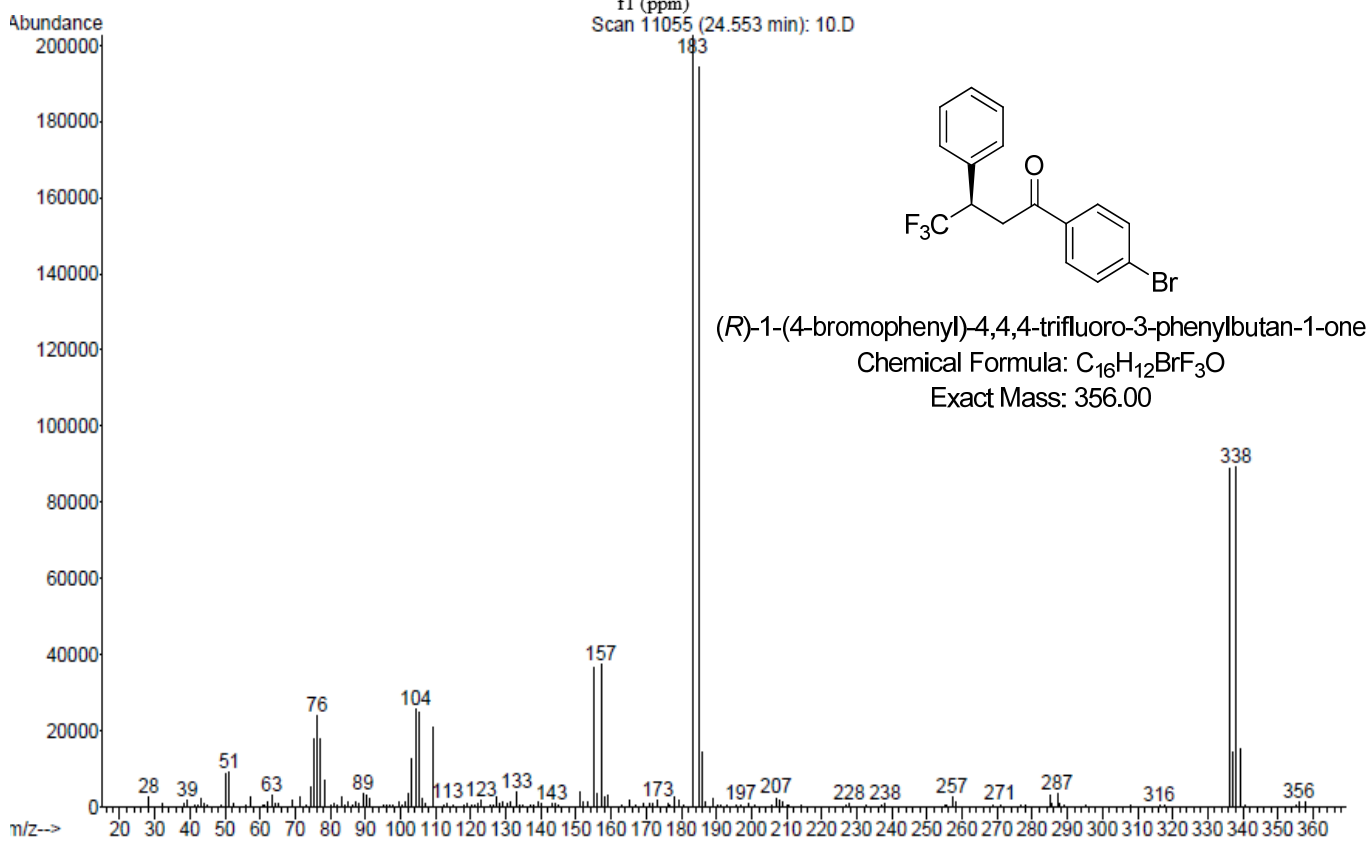
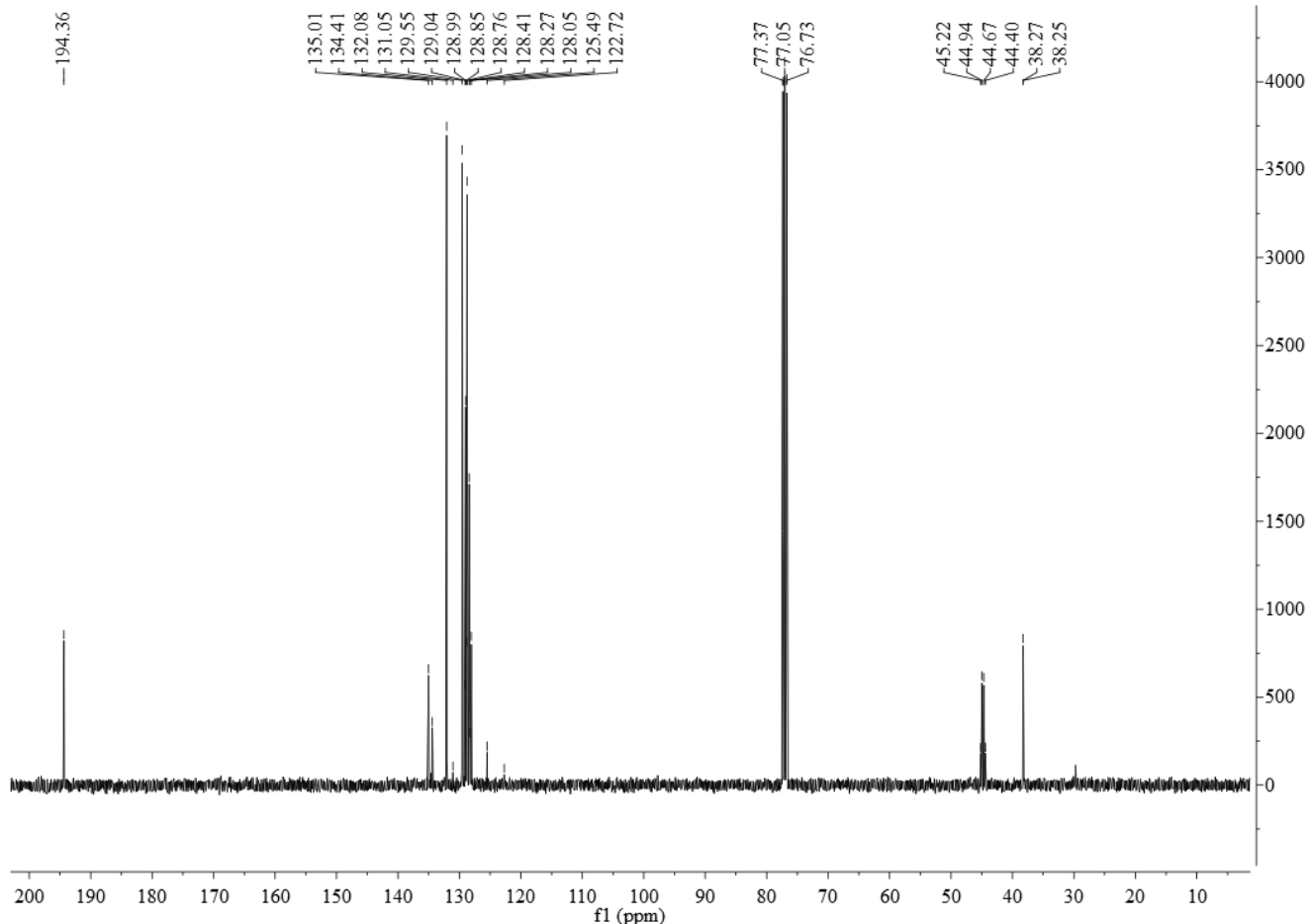


6k: (R)-1-(4-Bromophenyl)-4,4,4-trifluoro-3-phenylbutan-1-one

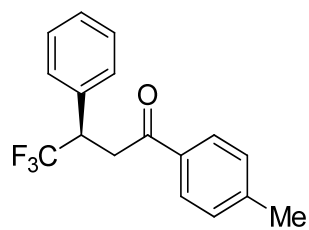


Yield: 95% (94% ee, 100% es); ^1H NMR (400 MHz, CDCl_3): δ 3.57 (dd, 1H, $J = 17.7$ Hz, $J = 4.4$ Hz), 3.66 (dd, 1H, $J = 17.7$ Hz, $J = 8.8$ Hz), 4.16–4.30 (m, 1H), 7.30–7.40 (m, 5H), 7.60 (d, 2H, $J = 8.5$ Hz), 7.78 (d, 2H, $J = 8.5$ Hz); ^{13}C NMR (100 MHz, CDCl_3): δ 38.3 (q, $J = 2$ Hz), 44.8 (q, $J = 27$ Hz), 126.9 (q, $J = 277.7$ Hz), 128.4, 128.8, 129.0, 129.1, 129.6, 132.1, 134.4 (q, $J = 2$ Hz), 135.0, 194.4; GC/MS (m/z): 356.00; HPLC (OD-H, elute: *n*-hexanes/*i*-PrOH = 95/5, detector: 254 nm, flow rate: 1.0 mL/min, 25 °C) $t_1 = 6.2$ min, $t_2 = 7.1$ min.

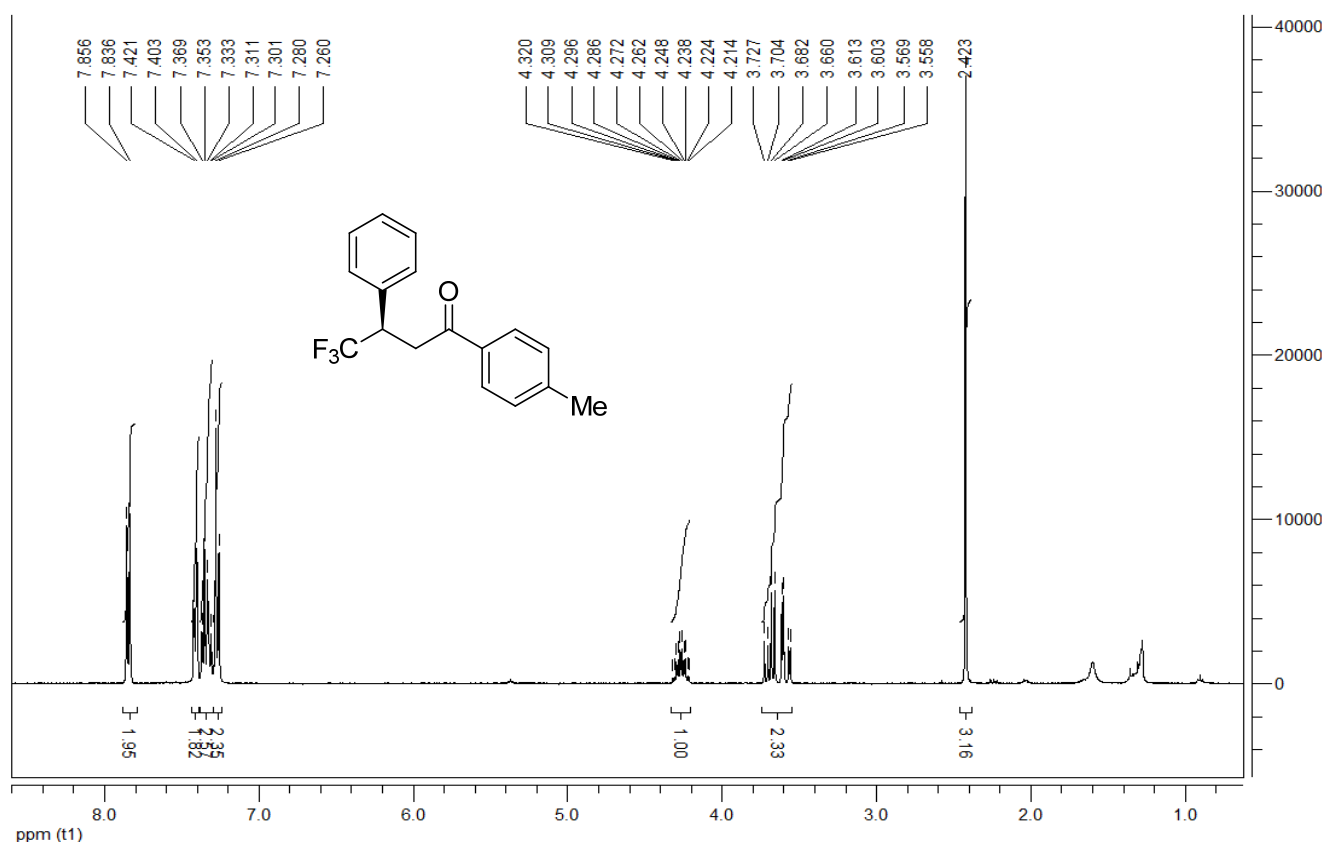


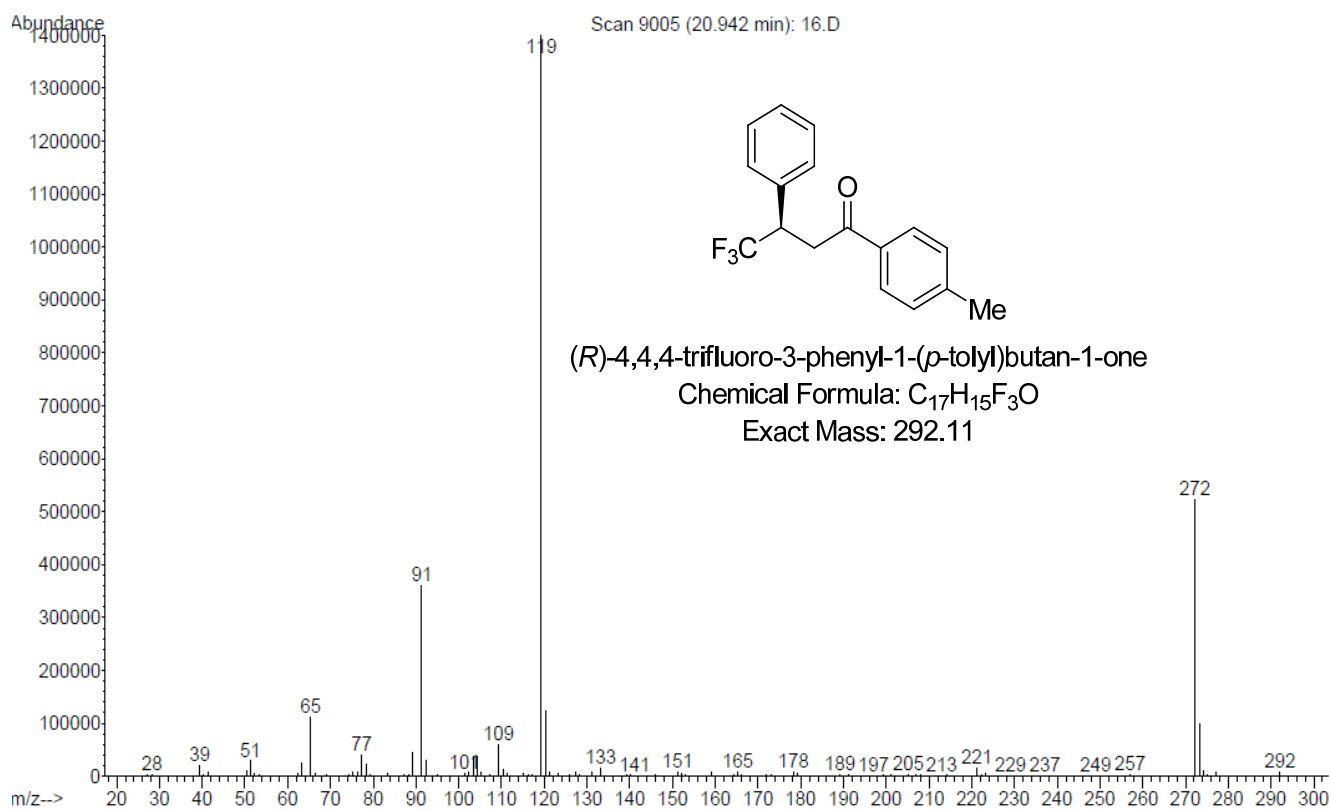
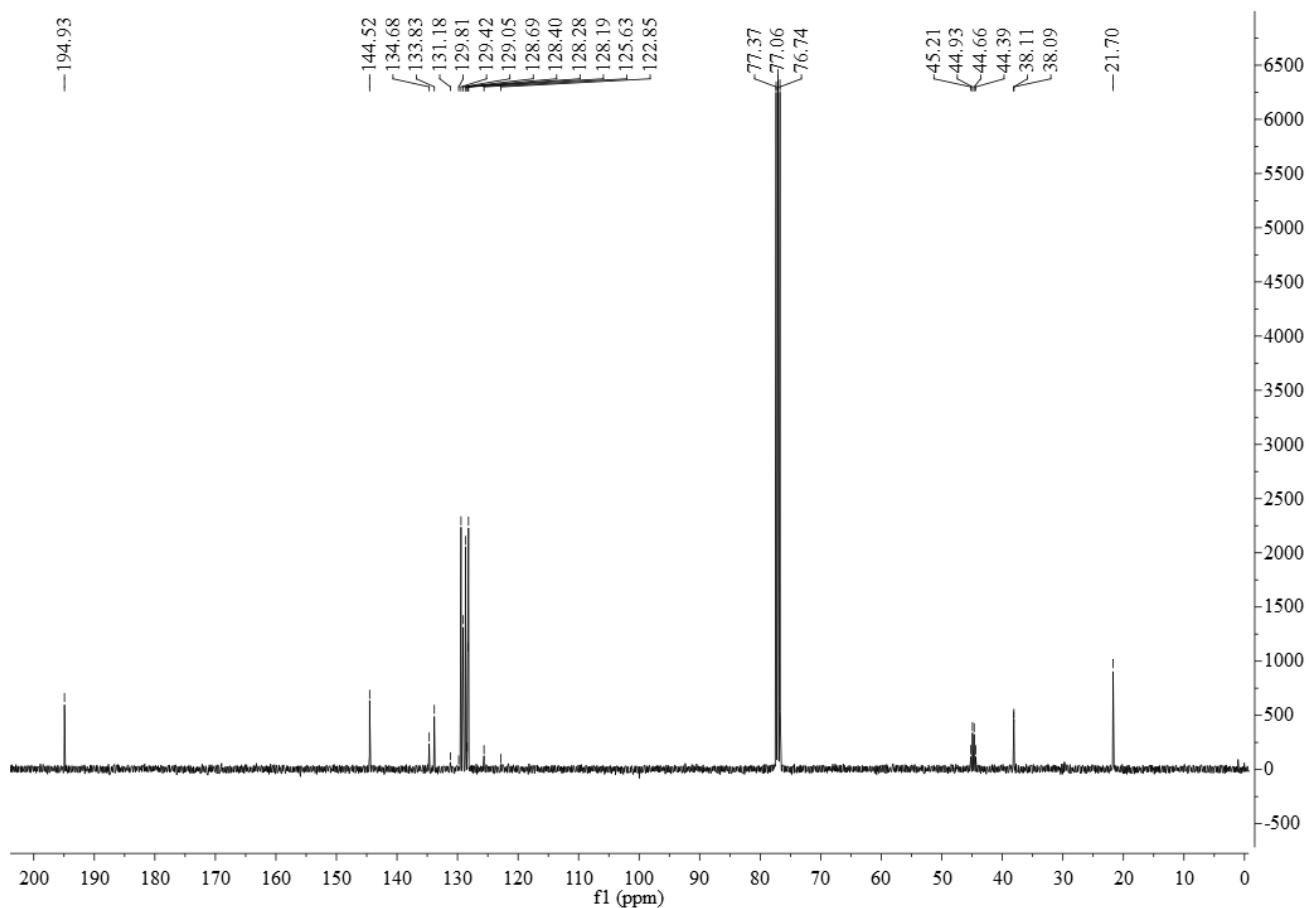


6l: (R)-4,4,4-Trifluoro-1-(4-methylphenyl)-3-phenyl-1-butanone

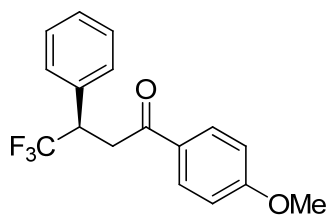


Yield: 95% (90% ee, 95% es); ^1H NMR (400 MHz, CDCl_3): δ 2.40, (s, 3H), 3.53-3.60 (m, 1H), 3.68 (ddd, $J = 1.9, 8.9, 17.8$ Hz, 1H), 4.21-4.28 (m, 1H), 7.24-7.38 (m, 7H), 7.81-7.84 (m, 2H); ^{13}C NMR (100 MHz, CDCl_3): δ 21.7, 38.1 (q, $J = 2$ Hz), 44.8 (q, $J = 27.7$ Hz), 127.0 (q, $J = 279.2$ Hz), 128.2, 128.3, 128.7, 129.0, 129.4, 129.8, 133.8, 134.6, 144.5, 194.9; GC/MS (m/z): 292.11; HPLC (OD-H, elute: n -hexanes/ i -PrOH = 95/5, detector: 254 nm, flow rate: 1.0 mL/min, 25 $^\circ\text{C}$) $t_1 = 4.8$ min, $t_2 = 5.5$ min.

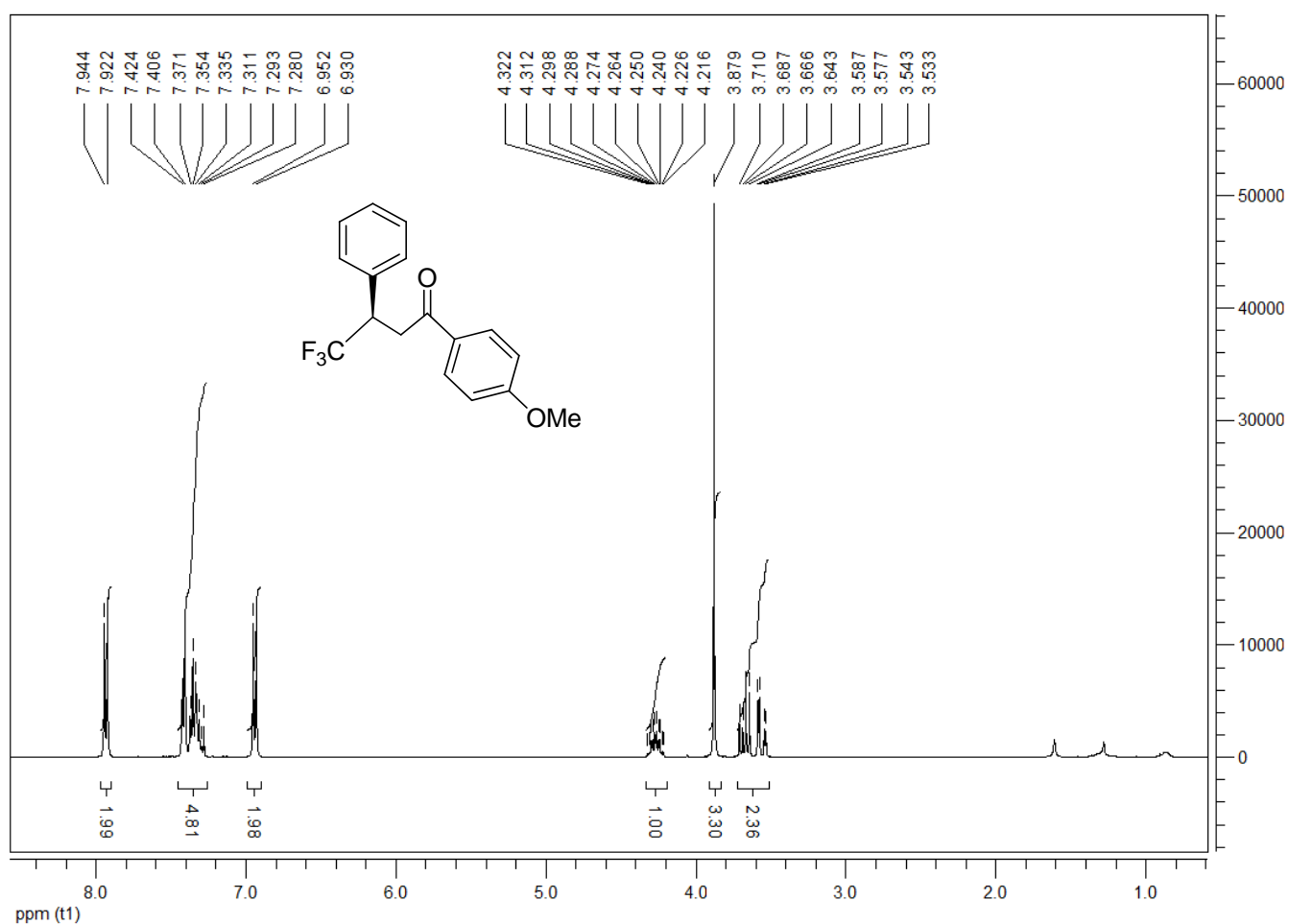


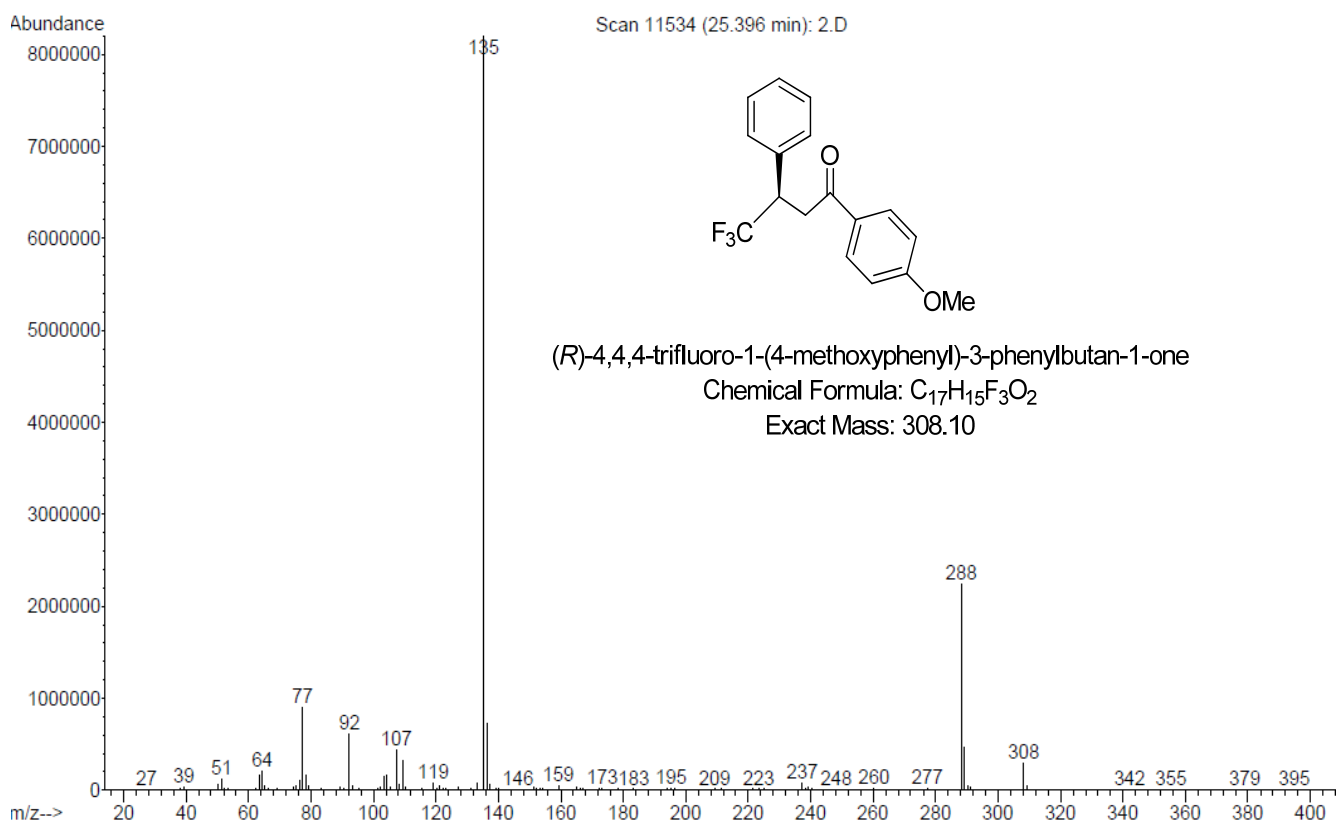
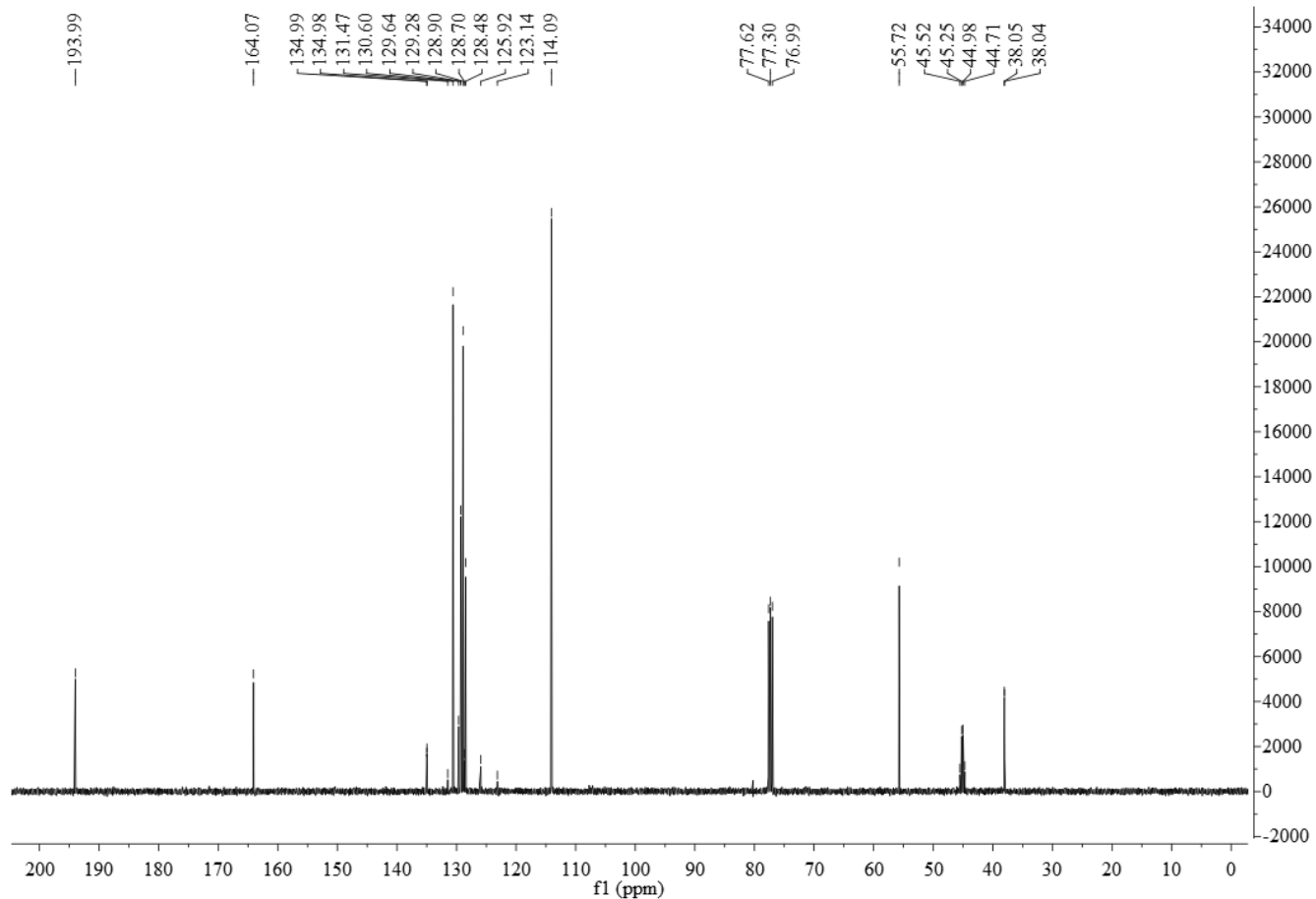


6m: (R)-4,4,4-Trifluoro-1-(4-methoxyphenyl)-3-phenyl-1-butanone

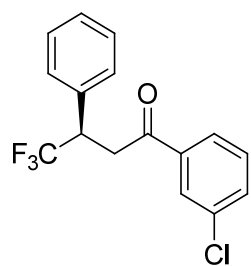


Yield: 92% (90% ee, 100% es); ^1H NMR (400 MHz, CDCl_3): δ 3.53 (dd, $J = 3.9, 17.4$ Hz, 1H), 3.65 (dd, $J = 9.0, 17.4$ Hz, 1H), 3.85(s, 3H), 4.18-4.31 (m, 1H), 6.92 (d, $J = 8.4$ Hz, 2H), 7.29-7.40 (m, 5H), 7.91 (d, $J = 8.7$ Hz, 2H); ^{13}C NMR (100 MHz, CDCl_3): δ 38.0 (q, $J = 1.5$ Hz), 45.1 (q, $J = 27.7$ Hz), 55.7, 114.0, 127.3 (q, $J = 278.2$ Hz), 128.4, 128.9, 129.2, 129.6, 130.6, 135.0, 164.0, 194.0; GC/MS (m/z): 308.10; HPLC (OD-H, elute: *n*-hexanes/*i*-PrOH = 95/5, detector: 254 nm, flow rate: 1.0 mL/min, 25 °C) $t_1 = 8.2$ min, $t_2 = 10.0$ min.



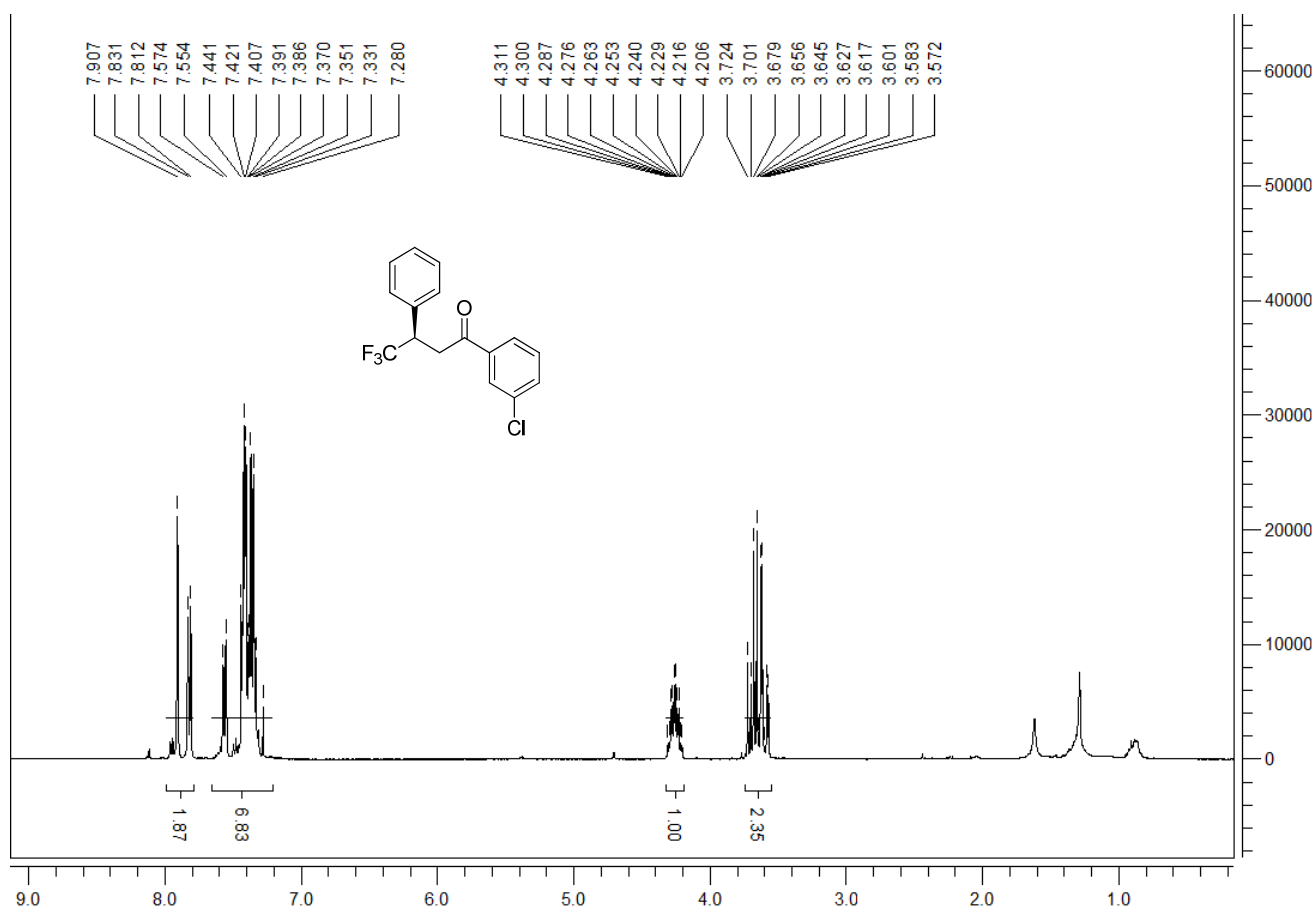


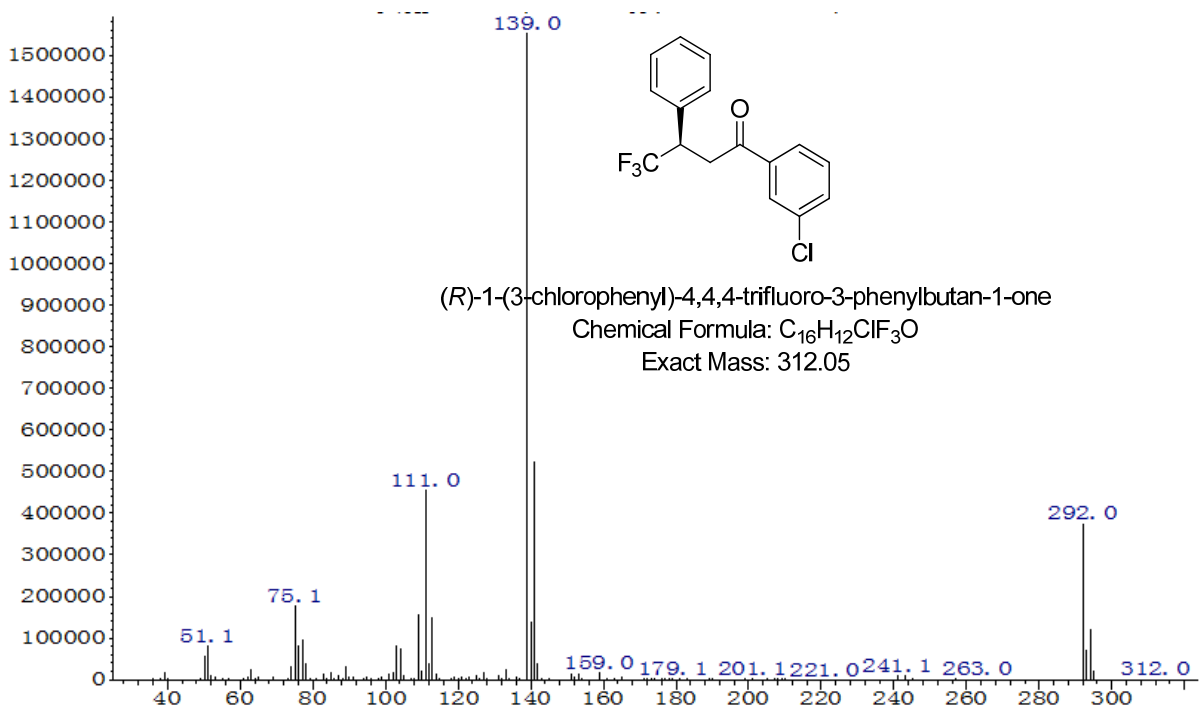
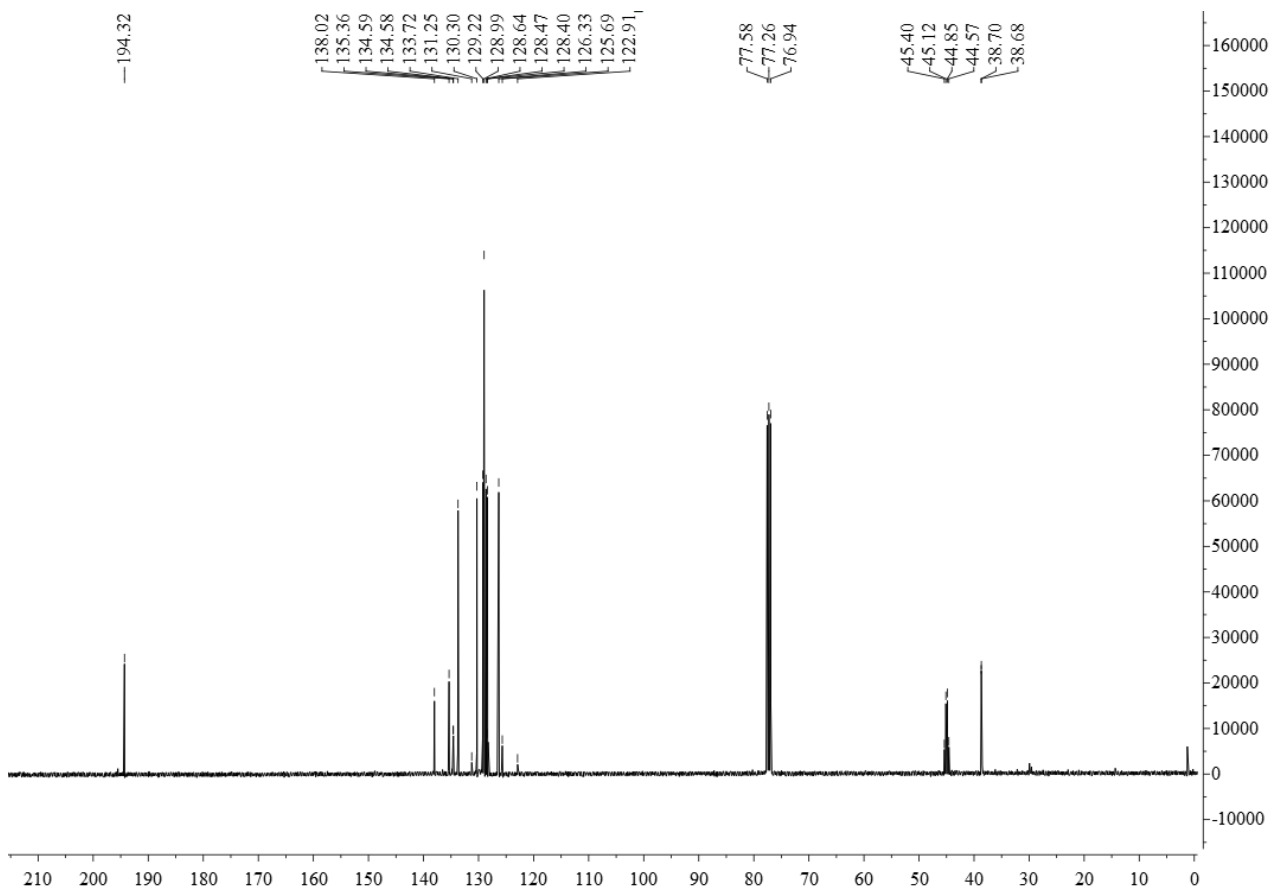
6n: (R)-1-(3-Chlorophenyl)-4,4,4-trifluoro-3-phenyl-1-butanone



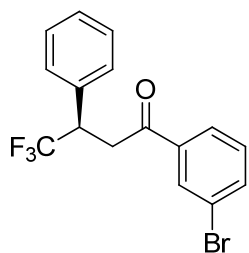
Yield: 95% (93% ee, 99% es); ^1H NMR (400 MHz, CDCl_3): δ 3.58 (dd, 1H, $J = 17.8$ Hz, $J = 4.4$ Hz), 3.68 (dd, 1H, $J = 17.8$ Hz, $J = 8.8$ Hz), 4.21–4.32 (m, 1H), 7.28–7.58 (m, 7H), 7.85 (d, 2H, $J = 8.6$ Hz); ^{13}C NMR (100 MHz, CDCl_3): δ 38.7 (q, $J = 2$ Hz), 45.0 (q, $J = 27$ Hz), 126.3, 127.0 (q, $J = 277.8$ Hz), 128.4, 128.6, 129.2, 130.3, 133.7, 134.6 (q, $J = 2$ Hz), 135.4, 138.0, 194.3; GC/MS (m/z): 312;

HPLC (OD-H, elute: Hexanes/*i*-PrOH = 97/3, detector: 254 nm, flow rate: 1.0 mL/min, 25 °C), $t_1 = 5.6$ min, $t_2 = 7.6$ min



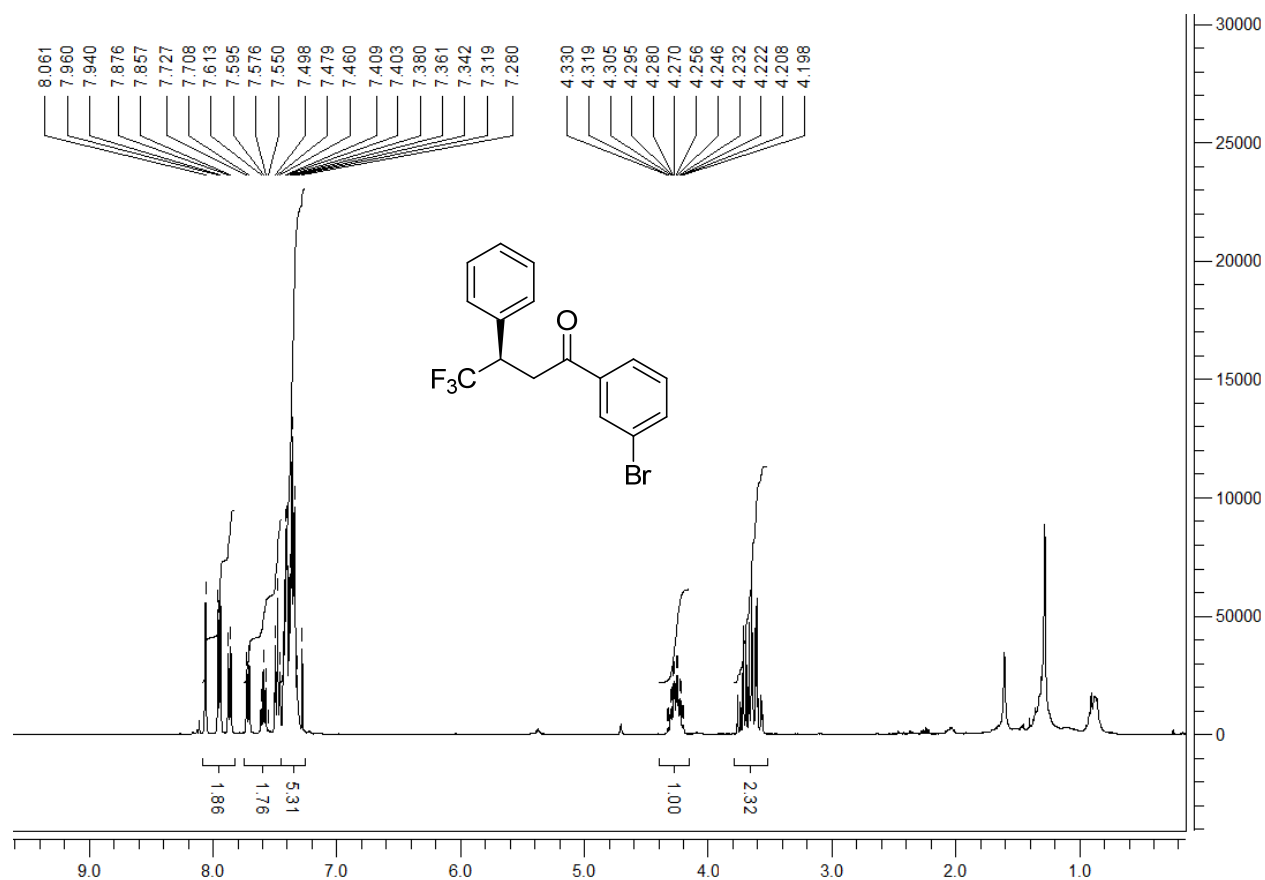


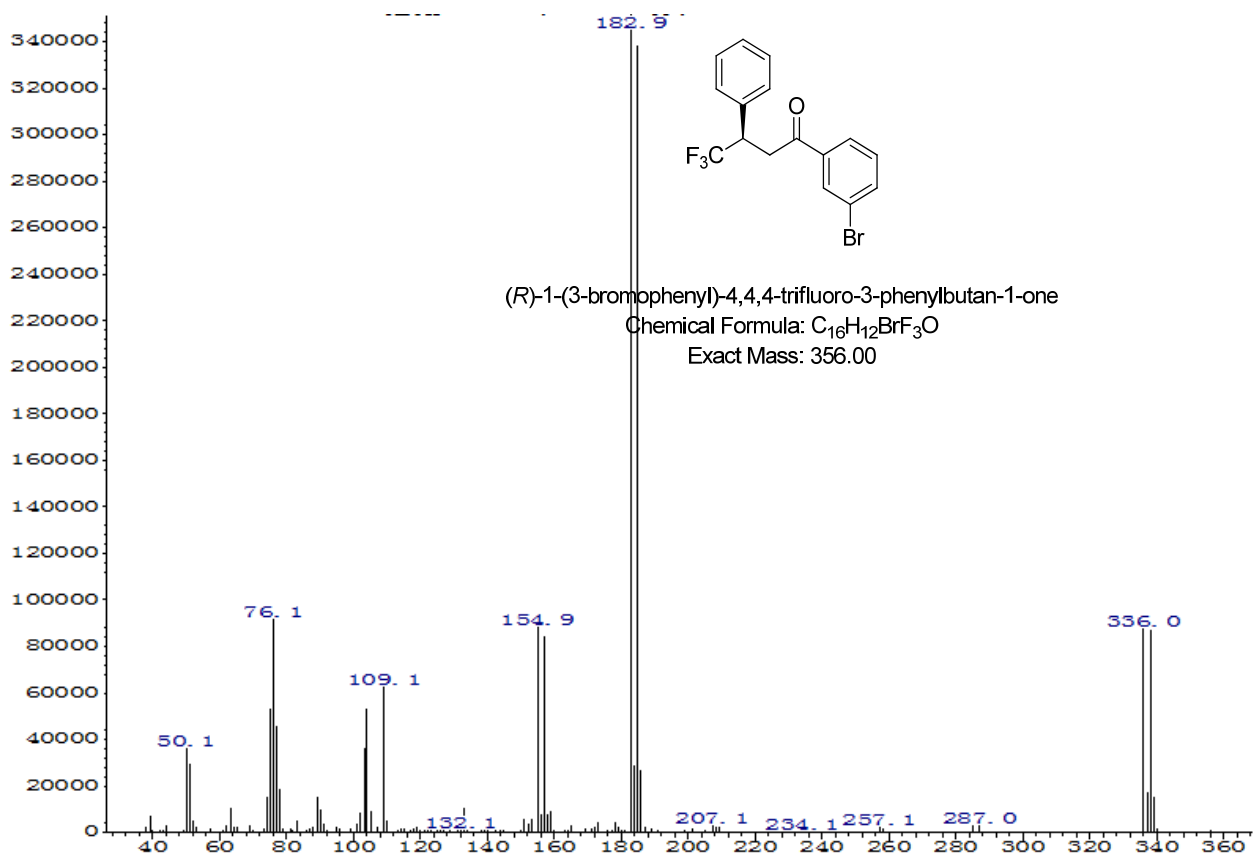
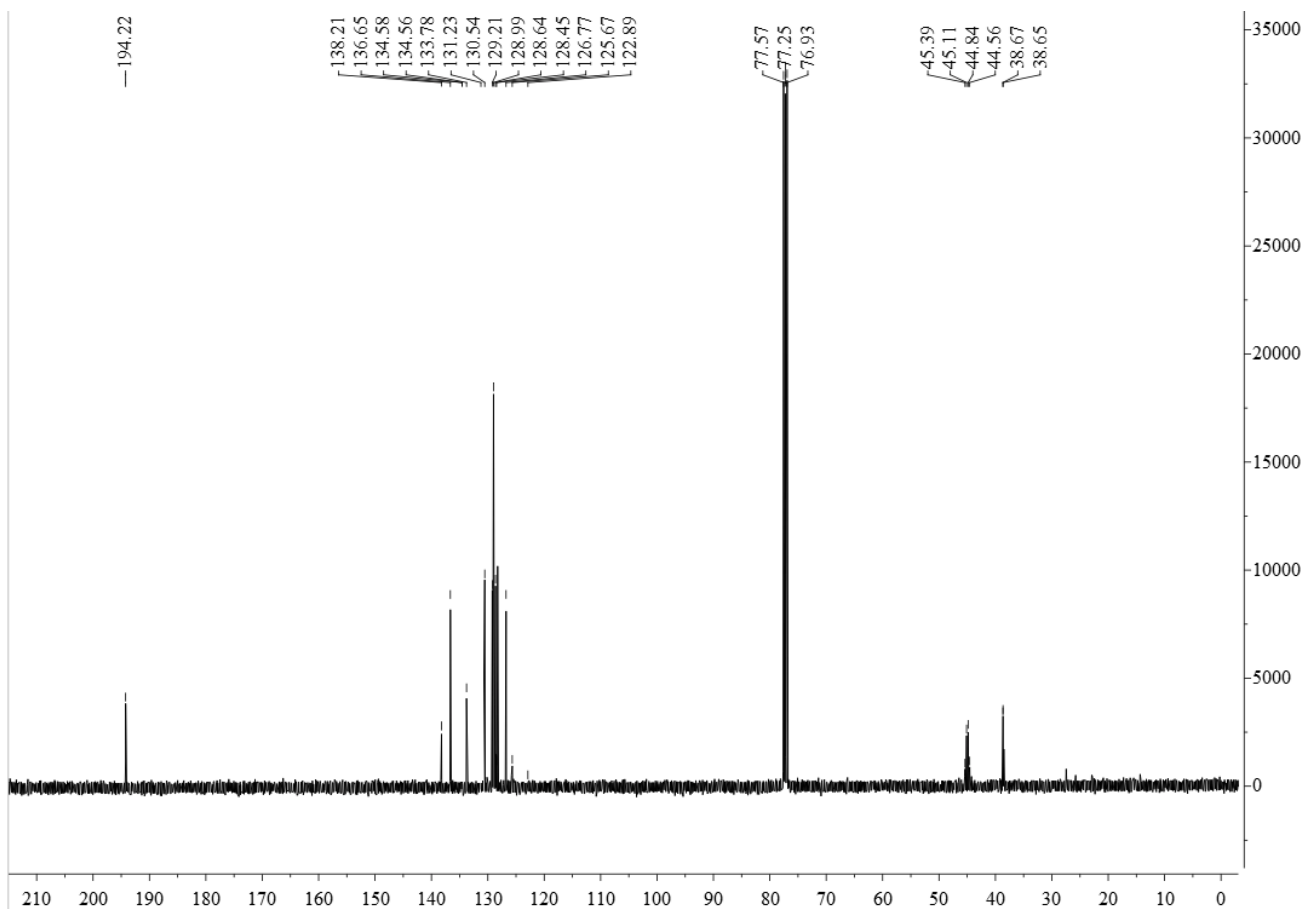
60: (R)-1-(3-Bromophenyl)-4,4,4-trifluoro-3-phenylbutan-1-one



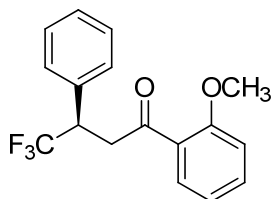
Yield: 96% (93% ee, 100% es); ^1H NMR (400 MHz, CDCl_3): δ 3.57 (dd, 1H, $J = 17.7$ Hz, $J = 4.4$ Hz), 3.66 (dd, 1H, $J = 17.7$ Hz, $J = 8.8$ Hz), 7.27–7.42 (m, 5H), 4.18–4.33 (m, 1H), 7.62 (d, 2H, $J = 8.5$ Hz), 7.88 (d, 2H, $J = 8.5$ Hz); ^{13}C NMR (100MHz, CDCl_3): δ 38.6 (q, $J = 2$ Hz), 45.0 (q, $J = 27$ Hz), 126.7, 127.0 (q, $J = 277.9$ Hz), 128.6, 128.9, 129.2, 130.5, 133.7, 134.6 (q, $J = 2$ Hz), 136.6, 138.2,

194.2; GC/MS (m/z): 356; HPLC (OD-H, elute: Hexanes/i-PrOH = 97/3, detector: 254 nm, flow rate: 1.0 mL/min, 25 °C), $t_1 = 5.6$ min, $t_2 = 7.6$ min.

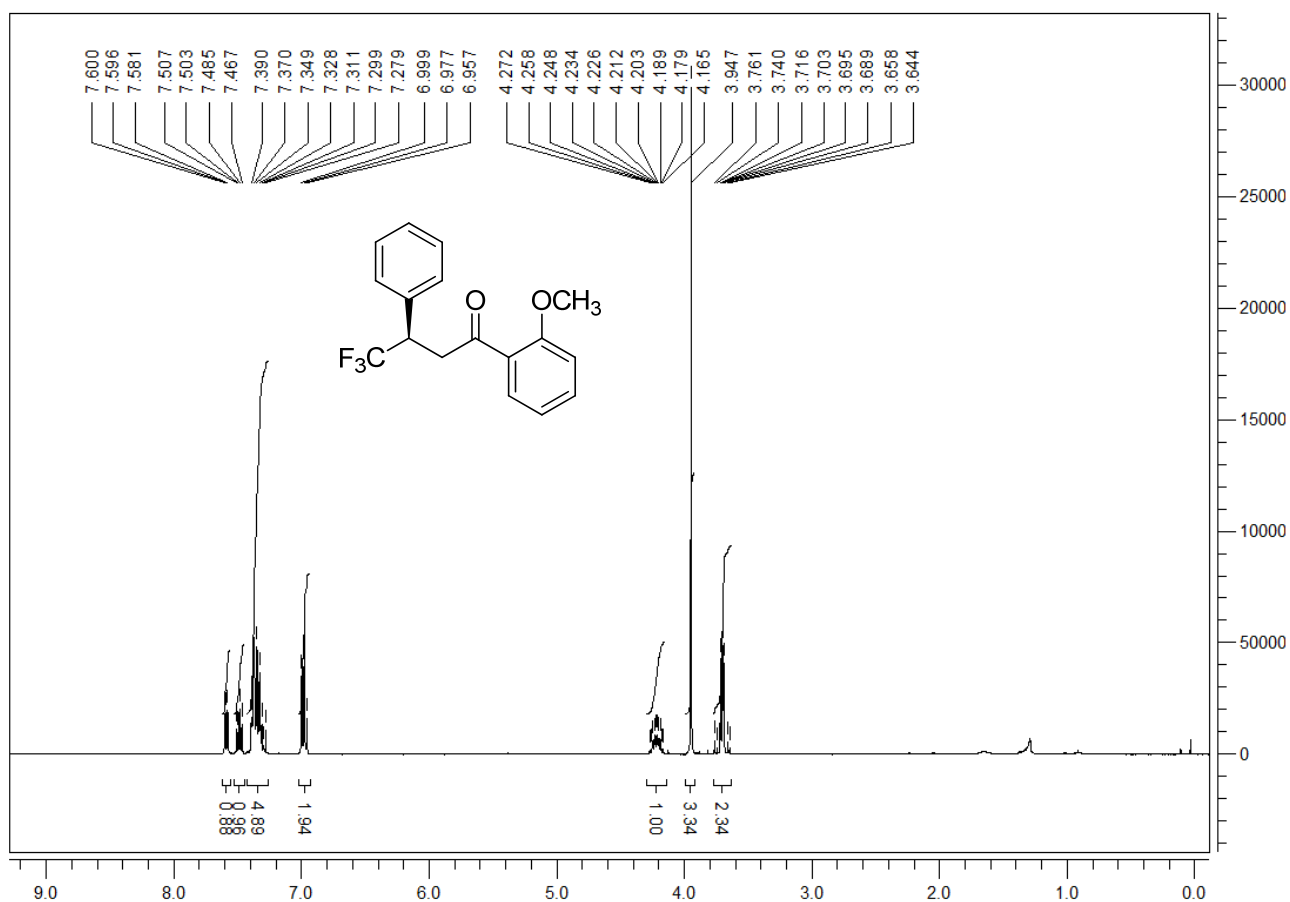


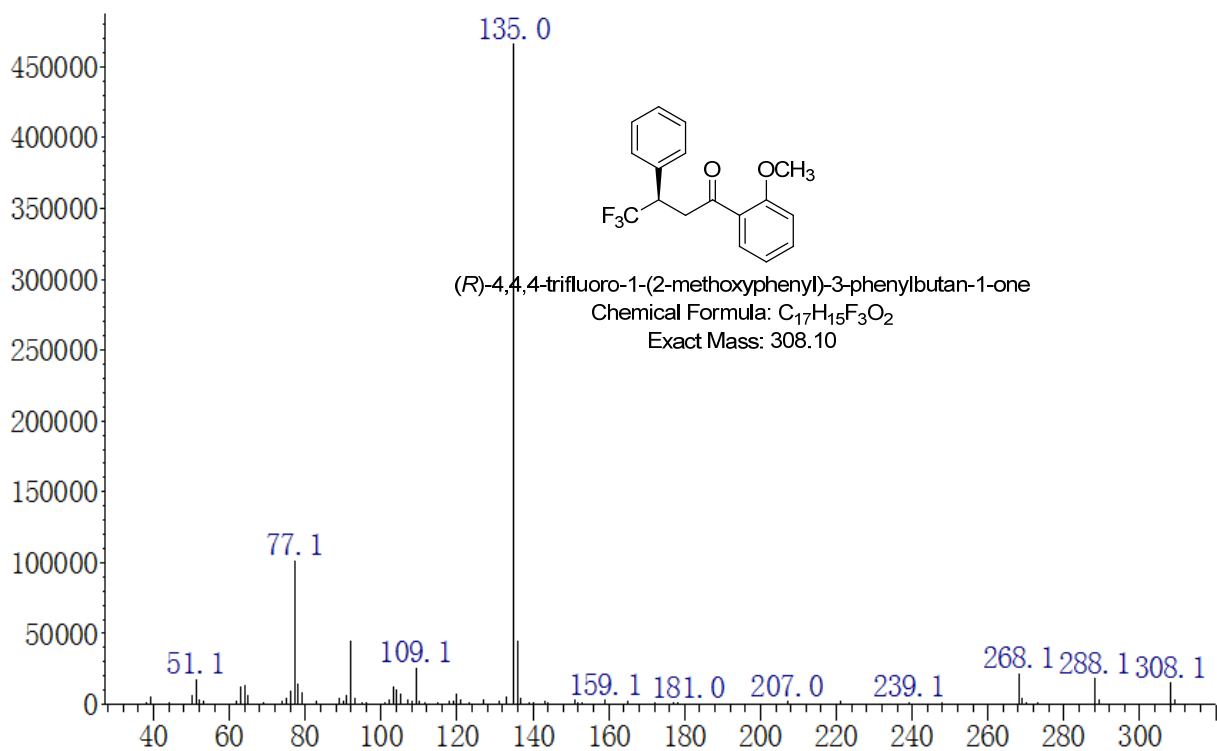
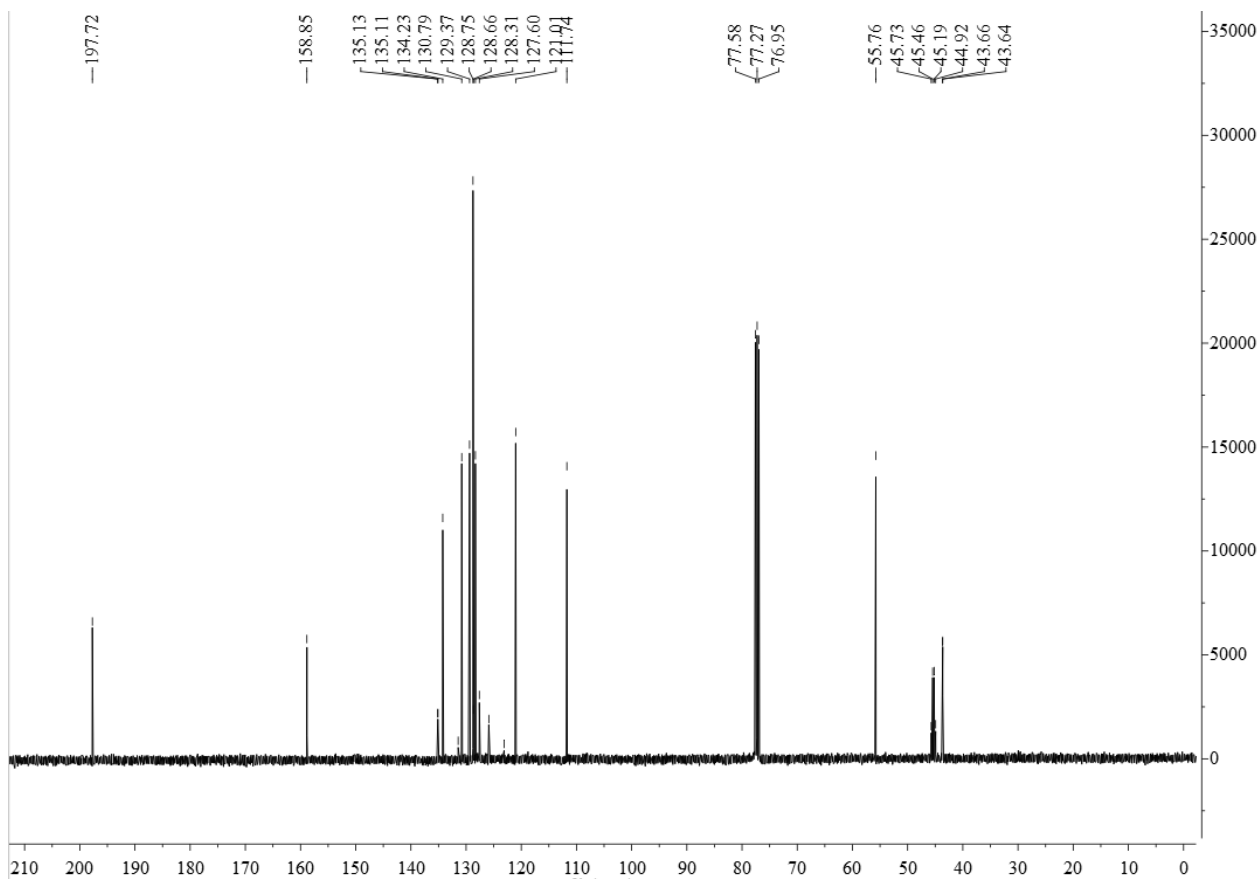


6p: (R)-4,4,4-Trifluoro-1-(2-methoxyphenyl)-3-phenyl-1-butanone

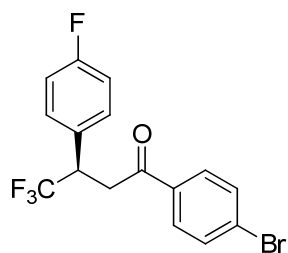


Yield: 95% (92% ee, 100% es); ^1H NMR (400 MHz, CDCl_3): δ 3.63 (dd, 1H, $J = 13.2$ Hz, $J = 1.0$ Hz), 3.74 (dd, 1H, $J = 17.9$ Hz, $J = 3.2$ Hz), 3.95 (s, 3H), 4.16–4.28 (m, 1H), 6.94–7.10 (m, 2H), 7.57–7.61 (m, 1H), 7.28–7.40 (m, 5H), 7.45–7.51 (m, 1H); ^{13}C NMR (100 MHz, CDCl_3): δ 43.6 (q, $J = 2$ Hz), 45.3 (q, $J = 27$ Hz), 55.7, 111.7, 121.0, 127.2 (q, $J = 277.9$ Hz), 127.6, 128.3, 128.7, 129.4, 130.8, 134.2, 135.1 (q, $J = 1.5$ Hz), 158.8, 197.7; GC/MS (m/z): 308; HPLC (OD-H, elute: Hexanes/*i*-PrOH = 97/3, detector: 254 nm, flow rate: 1.0 mL/min, 25 °C), $t_1 = 6.8$ min, $t_2 = 7.2$ min

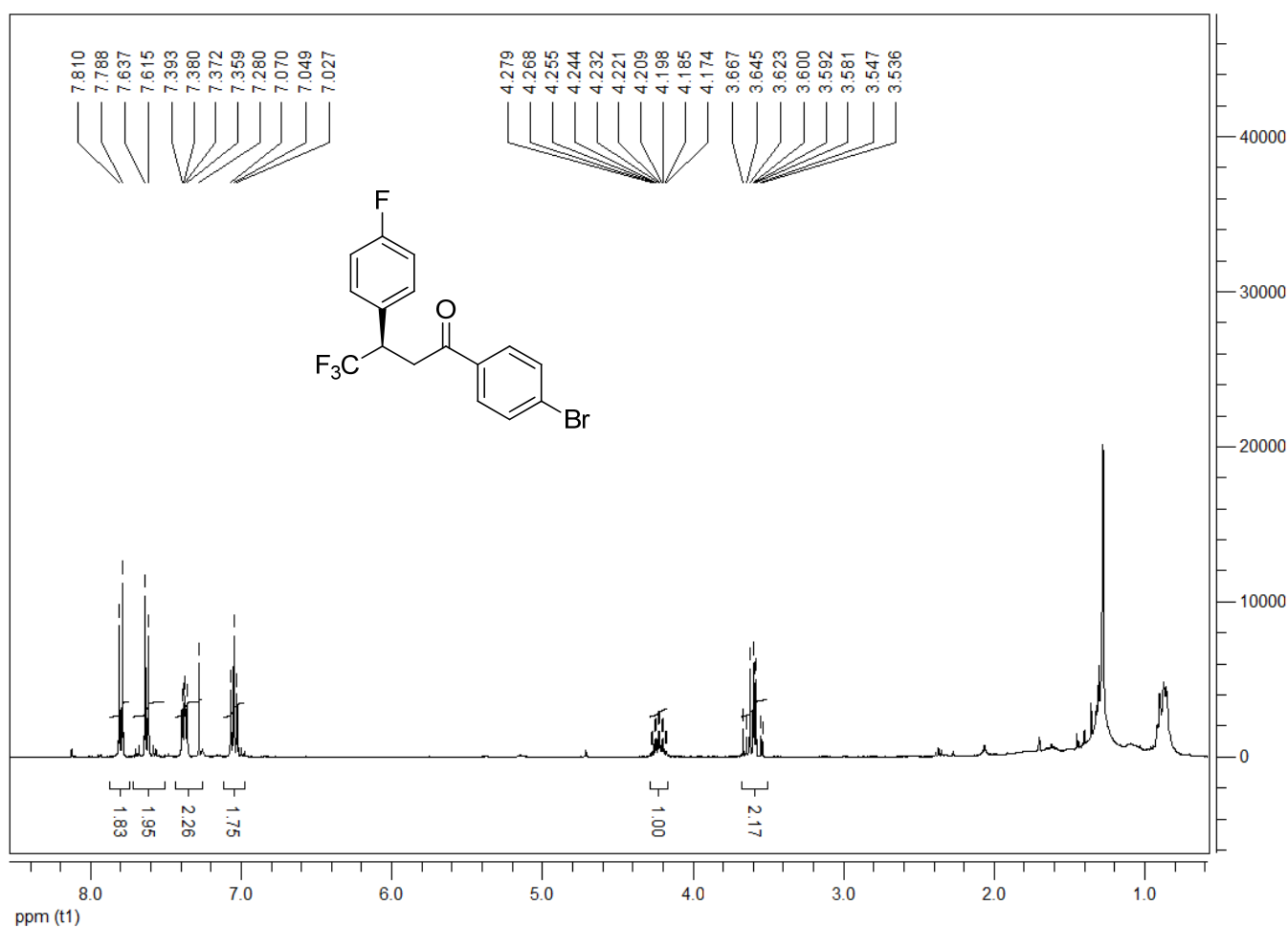


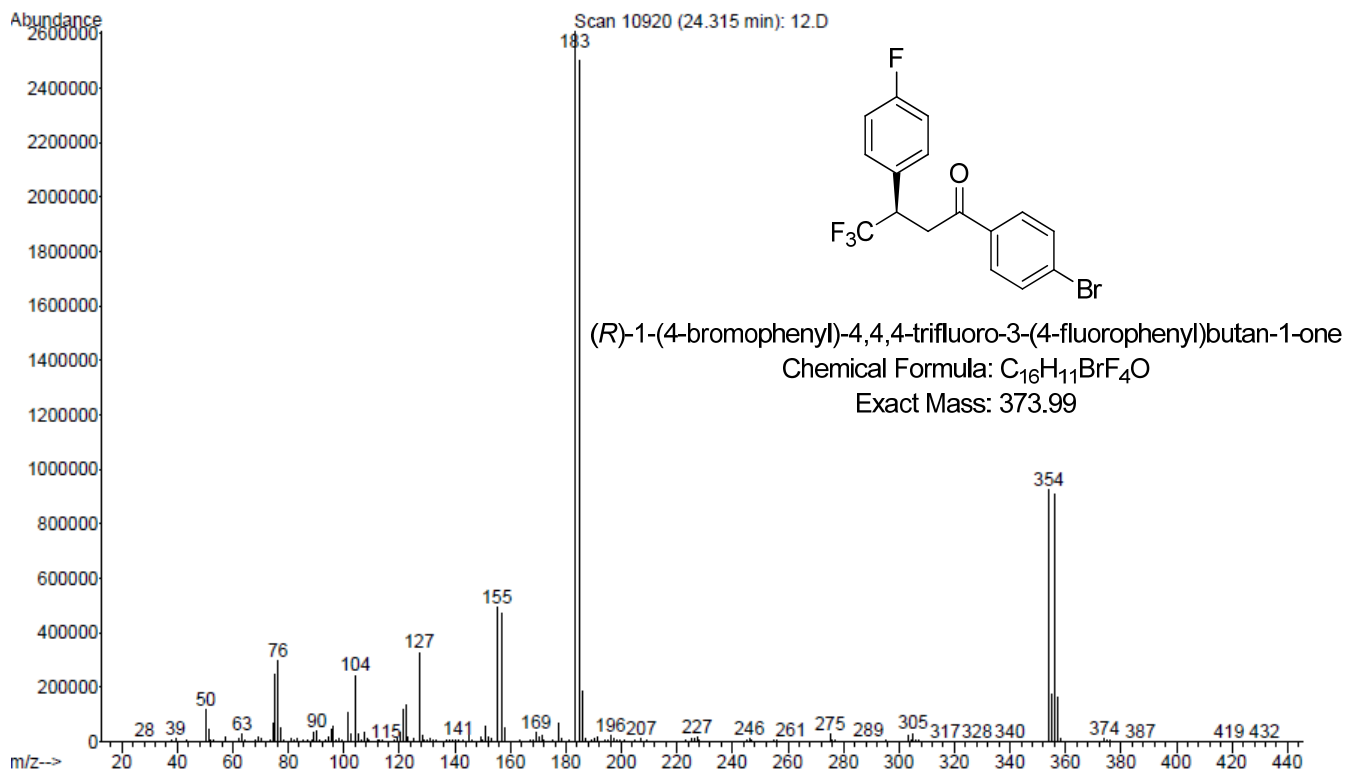
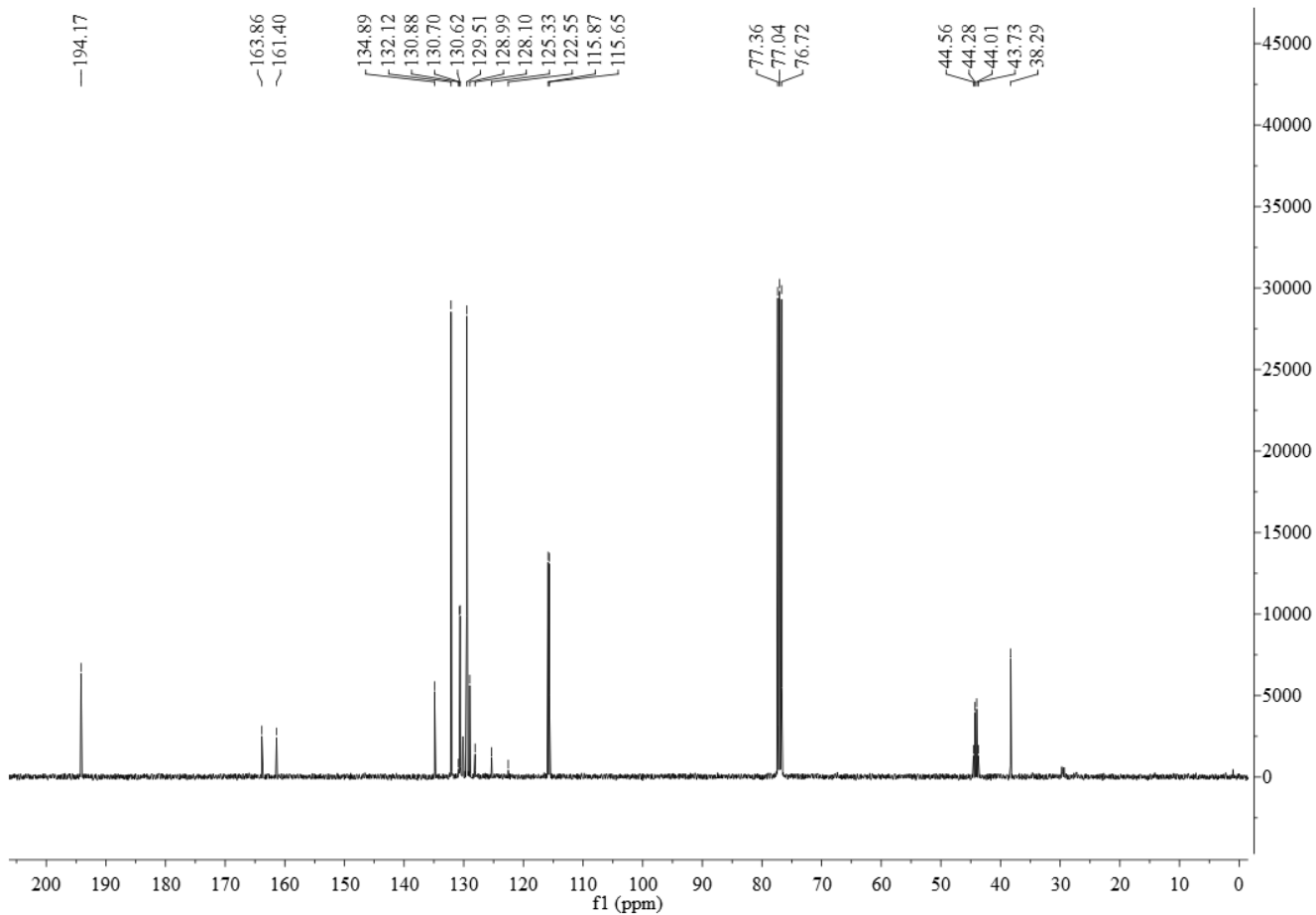


6q: (R)-1-(4-bromophenyl)-4,4,4-trifluoro-3-(4-fluorophenyl)butan-1-one

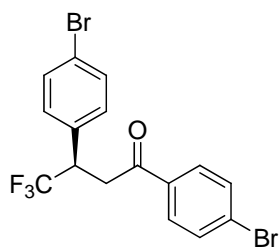


Yield: 95% (91% ee, 100% es); ^1H NMR (400 MHz, CDCl_3): δ 3.52–3.67 (m, 2H), 4.21 (dd, $J = 9.4, 4.4$ Hz, 1H), 7.02–7.07 (m, 2H), 7.28–7.39 (m, 2H), 7.61–7.63 (m, 2H), 7.78–7.81 (m, 2H); ^{13}C NMR (100 MHz, CDCl_3): δ 38.3 (q, $J = 2$ Hz), 44.2 (q, $J = 28$ Hz), 115.7 (d, $J = 22$ Hz), 126.7 (q, $J = 278$ Hz), 129.0, 129.5, 130.6, 130.7, 132.1, 134.9, 162.6 (d, $J = 246$ Hz), 194.2; GC/MS (m/z): 373.99; HPLC (OJ-H, elute: *n*-hexanes/*i*-PrOH = 95/5, detector: 254 nm, flow rate: 1.5 mL/min, 25 °C) $t_1 = 15.2$ min, $t_2 = 19.4$ min.





6r: (R)-4,4,4-Trifluoro-1,3-bis(4-bromophenyl)butan-1-one



Yield: 94% (90% ee, 97% es); ^1H NMR (400 MHz, CDCl_3): δ 3.51–3.65 (m, 2H), 4.18 (dd, $J = 9.4, 4.4$ Hz, 1H), 7.23–7.29 (m, 2H), 7.44–7.49 (m, 2H), 7.57–7.62 (m, 2H), 7.74–7.79 (m, 2H); ^{13}C NMR (100 MHz, CDCl_3): $\delta = 38.1$ (q, $J = 1.5$ Hz), 44.4 (q, $J = 27$ Hz), 122.6, 126.5 (q, $J = 279$ Hz), 129.1, 129.5 (d, $J = 2$ Hz), 130.6, 131.9, 132.1, 133.4 (d, $J = 1.7$ Hz), 134.8, 194.0; GC/MS (m/z): 433.91; HPLC (OJ-H, elute: *n*-hexanes/*i*-PrOH = 95/5, detector: 254 nm, flow rate: 1.5 mL/min, 25 °C) $t_1 = 11.9$ min, $t_2 = 12.9$ min.

