Supporting Information *for*

An Integrated Immobilization Strategy Manipulates Dual Active Centers to Boost Enantioselective Tandem Reaction

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CONTENTS

Experimental

1. General: All experiments, which are sensitive to moisture or air, were carried out under an Ar atmosphere using the standard Schlenk techniques. Tetraethoxysilane (TEOS), 1,4−bis(triethyoxysilyl)ethane, cetyltrimethylammonium bromide (CTAB), fluorocarbon surfactant (FC−4: $[C_3F_7O(CF(CF_3)CF_2O)_2CF(CF_3)CONH(CH_2)_3N^+(C_2H_5)_2CH_3]I^-$), 4−(2−(trimethoxysilyl)ethyl)benzene−1−sulfonyl chloride, 4−(methylphenylsulfonyl)−1,2−diphenylethylenediamine [(S,S)−TsDPEN], 1,3–bis(2,6–diisopropylphenyl)–2,3–dihydro–1*H*–imidazolium chloride, $PdCl_2$, 3-Chloropyridine, $AgBF_4$, $(MesityleneRuCl_2)_2$ were purchased from Sigma−Aldrich Company Ltd and used as received. Compound of (S,S)−4−(trimethoxysilyl)ethyl)phenylsulfonyl−1,2−diphenylethylenediamine [*J. Mater. Chem.* **2010,** *20*, 1970−1975.] and $IPrPdBF_4$ complex [*Chem. Eur. J.* **2006,** *12*, 4743−4748.] were synthesized according to the reported literature.

2. Characterization: Ru and Pd loading amounts in the catalysts were analyzed using an inductively coupled plasma optical emission spectrometer (ICP, Varian VISTA−MPX). Fourier transform infrared (FT−IR) spectra were collected on a Nicolet Magna 550 spectrometer using KBr method. Scanning electron microscopy (SEM) images were obtained using a JEOL JSM−6380LV microscope operating at 20 kV. Transmission electron microscopy (TEM) images were performed on a JEOL JEM2010 electron microscope at an acceleration voltage of 220 kV. X−ray photoelectron spectroscopy (XPS) measurements were performed on a Perkin−Elmer PHI 5000C ESCA system. A 200 μm diameter spot size was scanned using a monochromatized Aluminum *Kα* X−ray source (1486.6.6 eV) at 40 W and 15 kV with 58.7 eV pass energies. All the binding energies were calibrated by using the contaminant carbon (C_{1s} = 284.6 eV) as a reference. Nitrogen adsorption isotherms were measured at 77 K with a Quantachrome Nova 4000 analyzer. The samples were measured after being outgassed at 423 K overnight. Pore size distributions were calculated by using the BJH model. The specific surface areas (S_{BET}) of samples were determined from the linear parts of BET plots (p/p_0 = 0.05−1.00). Solid state NMR experiments were explored on a Bruker AVANCE spectrometer at a magnetic field strength of 9.4 T with ^1H frequency of 400.1 MHz, ^{13}C frequency of 100.5 MHz, ^{29}Si frequency of 79.4 MHz and ^{19}F frequency of 169.3 MHz with 4 mm rotor at two spinning frequency of 5.5 kHz and 8.0 kHz, TPPM decoupling is applied in the during acquisition period. ^1H cross polarization in all solid state NMR experiments was employed using a contact time of 2 ms and the pulse lengths of 4μs.

3. Preparation of Me/Shell@ArDPEN (4). For a typical synthetic route, *(The first step in synthesis of silicate core (**1**) and protection with trimethysilyl groups),* to a solution of 0.10 g (0.27 mmol) of cetyltrimethylammonium bromide (CTAB) in 45.0 mL of aqueous sodium hydroxide (0.35 mL, 2.0 N) was added 0.43 g of (2.07 mmol) of tetraethoxysilane (TEOS) and 0.40 mL of ethyl acetate, and the mixture was stirred at 80 ℃ for 2 h. After cooling the above mixture down to 38 ℃, an aqueous solution (80.0 mL of water, 50.0 mL of ethanol, 0.30 g (0.82 mmol) of CTAB and 1.0 mL (25 wt%) of $NH_3 \cdot H_2O$) was added, and the mixture was stirred 38 ℃ for another 0.5 h. Subsequently, 0.5 mL, 0.47 g (2.26 mmol) of TEOS was added and the mixture was stirred at 38 ℃ for another 2 h. For coating of above SiO_2, to this solution was added an solution (0.04 g (0.044 mmol) of FC–4 (FC–4: $[C_3F_7O(CF(CF_3)CF_2O)_2CF(CF_3)CONH(CH_2)_3N^+(C_2H_5)_2CH_3]I^-$), 0.08 g (0.22 mmol) of CTAB and 0.20

mL (25 wt%) of $NH_3 \cdot H_2O$ in 3.0 mL of water), and the mixture was stirred at 38 ℃ for 0.5 h. Then, 0.89 g (2.50 mmol) of 1,2–bis(triethoxysilyl)ethane and 0.125 g (0.25 mmol) of (*S*,*S*)–4–(trimethoxysilyl)ethyl)phenylsulfonyl–1,2–diphenylethylenediamine (**2**) in 2 mL of ethanol (2 min later) were added subsequently, and the mixture was stirred under vigorous stirring for another 1.5 h. Finally, after cooling the above mixture down to room temperature, the resulting solid was collected by filtration. For protection with trimethysilyl groups, the collected solids (1.0 g) were suspended in 25.0 mL of dry toluene and $[(CH_3)_3Si)_2N]$ (10.0 mL, 0.050 mol) was added, and mixture was stirred overnight at room temperature. The solids were filtered and washed with excess ethanol, and dried at ambient temperature under vacuum overnight to afford Me/Shell@ArDPEN@SiO_2 (**3**) as a white powder. *(The second step for the synthesis of Me/Shell@ArDPEN (4) via the selective etching)* The collected solids were suspended in an alkaline solution (0.35 mL of NaOH (2.0 N) and 1.20 mL (25 wt%) of $NH_3 \cdot H_2O$ in the mixed 125.0 mL of water and 50.0 mL of ethanol), and the mixture was stirred vigorously at 100 ℃ for 12 h. After cooling the above mixture down to room temperature, the solids were filtered and washed with excess ethanol. To remove the surfactant, the collected solids were dispersed in 120.0 mL of solution (80 mg (1.0 mmol) of ammonium nitrate in 120.0 mL (95%) of ethanol), and the mixture was stirred at 60 ℃ for 8 h. After being filtered, the solids were filtered and washed with excess water and ethanol, and dried at 60 ℃ under *vacuum* overnight to afford Me/Shell@ArDPEN **(4)** as a white powder. ^{13}C CP/MAS NMR (161.9 MHz): 153.5−121.5 (*C* of Ph and Ar groups), 71.9−57.3 (*C*H of −NCHPh, and *C* of –N*C*H_2 and –N*C*H_3 in CTAB molecule), 35.7−24.9 (*C*H_2 of −*C*H_2Ar, and *C* of CH_3*C*H_2− in CTAB molecule), 21.1−11.2 (*C* of *C*H_3CH_2− in CTAB molecule), 5.5 (*C*H_2 of −*C*H_2Si) ppm. ^{29}Si MAS/NMR (79.4 MHz): T^2 (δ = −59.2 ppm), T^3 (δ = −65.8 ppm), Q^2 (δ = −92.5 ppm), Q^3 (δ = −102.5 ppm), Q^4 (δ = −112.8 ppm).

4. Catalyst 5 preparation. For a typical synthetic route, to a suspension of **4** (0.50 g) in a mixed solution (2.0 mL of 3-chloropyridine in 10.0 mL of dry CH_2Cl_2) was added $PdCl_2$ (17.7 mg, 0.10 mmol), 1,3–bis(2,6–diisopropylphenyl)–2,3–dihydro–1*H*–imidazolium chloride (46.8 mg, 0.11 mmol), K_2CO_3 (138.6 mg, 1.0 mmol) at room temperature. The resulting mixture was heated with vigorous stirring for 16 h at 80 ℃. After cooling to RT, 19.4 mg of $AgBF_4$ (0.10 mmol) was added to a suspension, and the reaction mixture was stirred at 25 ℃ for 10 h. The solids was filtered and rinsed with excess dry CH_2Cl_2. The collected solids was suspended in 20.0 mL of dry CH_2Cl_2 again and 50.0 mg of $(MesityleneRuCl_2)_2$ (0.086 mmol) was added (*For the preparion of Me@MesityleneRuArDPEN@HSMSNs (**5''**): 50.0 mg of $(MesityleneRuCl_2)_2$ (0.086 mmol) was added to a suspension of **4** (0.50 g) in 20.0 mL of dry CH_2Cl_2, and the resulting mixture was stirred at 25 ℃ for 12 h.*). The resulting mixture was stirred at 25 ℃ for another 12 h. The solid was filtered and rinsed with excess dry CH_2Cl_2. After Soxhlet extraction for 4.0 h in CH_2Cl_2, the solids were collected and dried at 60 ℃ under *vacuum* overnight to afford catalyst **5** as a light–yellow powder. ICP analysis showed that the Pd and Ru loadings were 9.57 mg (0.090 mmol of Pd) and 15.46 mg (0.15 mmol of Ru) per gram of catalyst, respectively. ^{13}C CP/MAS NMR (161.9 MHz): 158.3−121.3 (*C* of carbene, and *C* of Ph, Ar and –CH=CH– groups), 106.1−94.6 (*C* of mesitylene), 71.9−57.9 (*C*H of −NCHPh, and *C* of –N*C*H_2 and –N*C*H_3 in CTAB molecule), 36.6−11.6 (*C*H of −*C*$H(CH_3)_2$, *C*H_2 of −*C*H_2Ar, and *C* of *C*H_3*C*H_2− in CTAB molecule), 19.5 (*C*H_3 of mesitylene), 5.5 (*C*H_2 of −*C*H_2Si) ppm. ^{29}Si MAS/NMR (79.4 MHz): T^2 (δ = −59.7 ppm), T^3 (δ = −66.4 ppm), Q^2 (δ = −92.8 ppm), Q^3 (δ = −102.7 ppm), Q^4 (δ = −111.9 ppm).

5. General procedure for asymmetric reaction. For a typical catalytic procedure. Catalyst **5** (13.35 mg, 2.0 μmol of Ru and 1.20 μmol of Pd, based on ICP analysis), Cs_2CO_3 (0.12 mmol), HCO_2Na (1.0 mmol), haloacetophenones (0.10 mmol) and arylboronic acids (0.12 mmol), and 2.0 mL of $H_2O/^iPrOH$ (v/v = 1:3) were added sequentially to a 10.0 mL round–bottom flask. The mixture was then stirred at 80 ℃ for 0.5–1.5 h. During this period, the reaction was monitored constantly by TLC. After reaction was finished, the catalyst was collected *via* centrifugation (10 000 rpm), where parts of them for the further recycling experiment. The aqueous solution was extracted with ethyl ether (3 × 3.0 mL). The combined ethyl ether extracts were washed with brine twice and then dehydrated with Na_2SO_4. After evaporation of ethyl ether, the residue was purified by silica gel flash column chromatography to afford the desired products. The *ee* values were determined by a HPLC analysis using a UV–Vis detector and a Daicel chiralcel column (Φ 0.46 × 25 cm).

Figure S1. FT−IR spectrum of **4** and catalyst **5.**

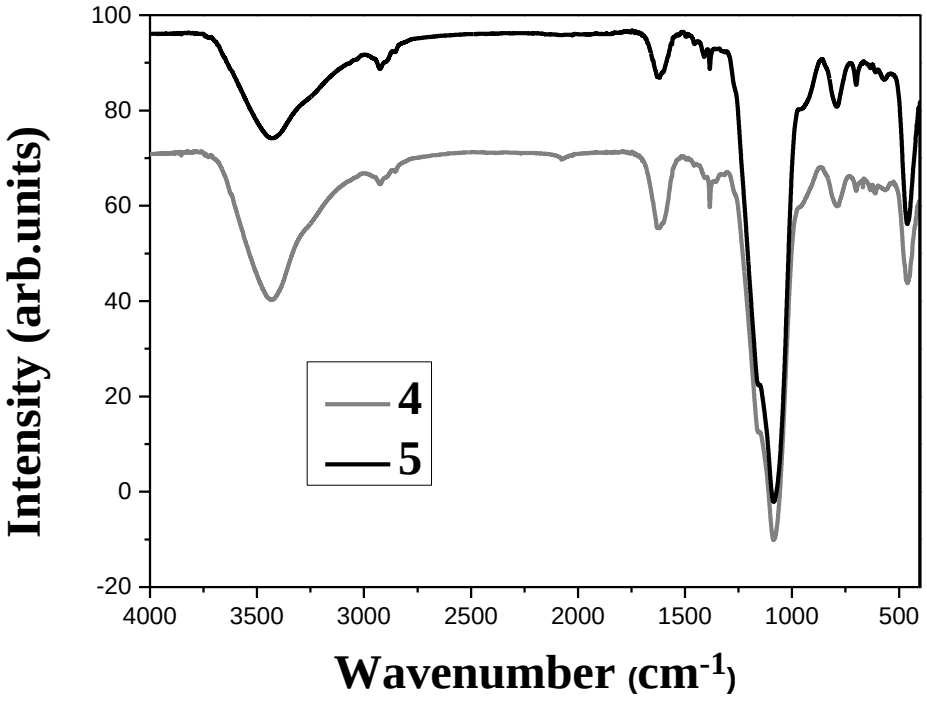
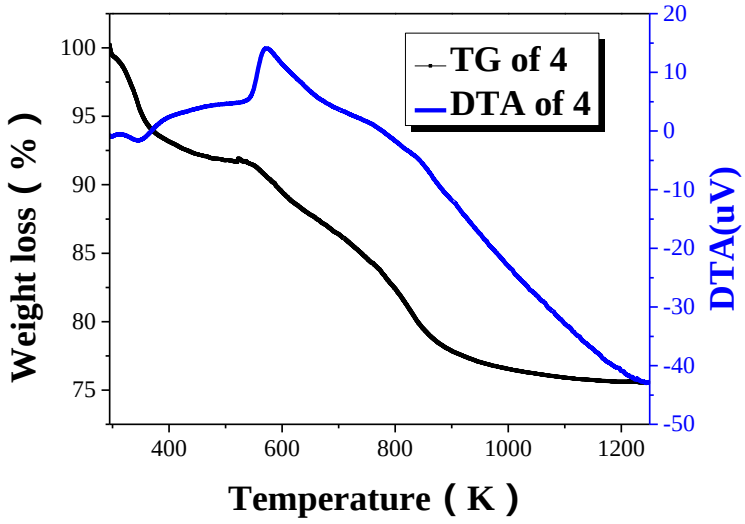
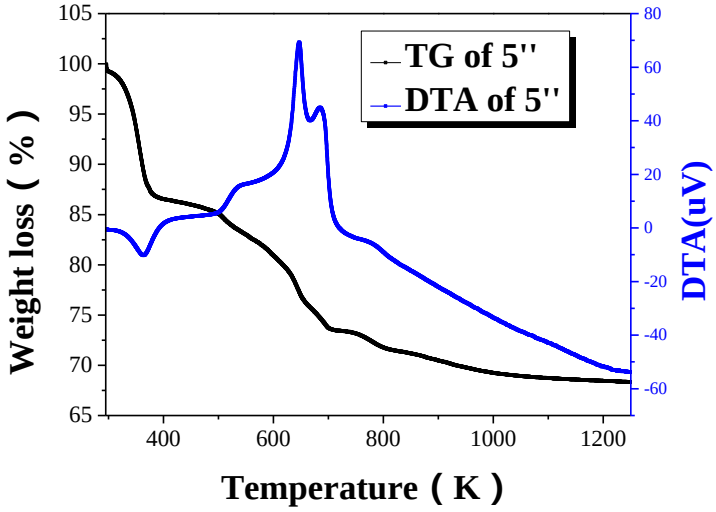
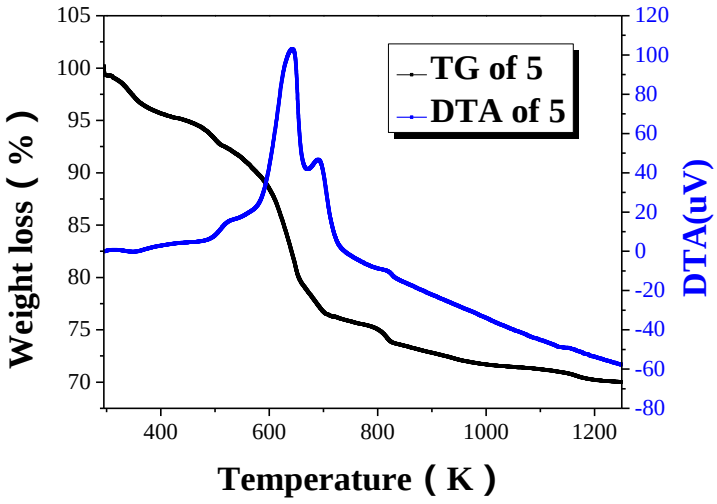


Figure S2. TG/DTA curves of **4**, Me@MesityleneRuArDPEN@HSMSNs (**5''**) and catalyst **5.**







Explanation: The TG/DTA curves of **4** was treated in the air as shown above. An endothermic peak around 345 K with weight loss of (92.36) 7.64% could be attributed to the release of physical adsorption water while the comprehensive endothermic peaks between 440 K and 1200 K with weight loss of (92.36-75.60) 16.1% could be assigned to the oxidation of organic molecules (including alkyl-linked ArDPEN moiety, alkyl fragments and part of the residual surfactant). Apparently, totally weight loss of the oxidation of organic molecules was 16.76% per 92.36% the extracted samples when eliminated the part of water, meaning the 18.14% weight loss of the oxidation of organic molecules per 100% materials.

For the Me@MesityleneRuArDPEN@HSMSNs (**5''**), an endothermic peak around 352 K with weight loss of (100-86.11) 13.89% could be attributed to the release of physical adsorption water. In addition, the weight loss of (86.11-68.45) 17.66% between 440 K and 1200 K could be assigned to the oxidation of the organic moieties (including alkyl-linked MesityleneRuArDPEN complexes, alkyl-linked ArDPEN moiety, alkyl fragments and part of the residual surfactant). Because the totally weight loss of organic moieties was 17.66% per 86.11% the extracted catalyst when eliminated the part of water, meaning the whole weight loss 20.50% of the oxidation of the organic molecules per 100% materials.

As compared the weight loss of **4** with **5''**, the weight loss of the MesityleneCl moieties was 2.36% (20.50-18.14) per 100% materials. This finding means that the mole amounts of MesityleneRuTsDPEN in **5''** is 0.01517 mol% (Mr = 155.5), demonstrating the 15.4582 mg (0.1517 mmol of Ru) of the Pd loading per gram of **5''**.

For catalyst **5**, it was found easily that a similar endothermic peak around 349 K with weight loss of (100-95.08) 4.92% were strongly similar to that of parent **5''** due to the release of physical adsorption water. It was worth mentioning that the all exothermic peaks were combined into one complicated exothermic peak between 440 K and 1200 K with weight loss of (95.08-70.21) 24.87% could be assigned to the oxidation of organic molecules (including alkyl-linked MesityleneRuArDPEN complexes, alkyl-linked ArDPEN moiety, hydrogen−bonding $IPrPdBF_4$ complexes, alkyl fragments and part of the residual surfactant). Because the totally weight loss of organic moieties was 24.87% per 95.08% the extracted catalyst when eliminated the part of water, meaning the whole weight loss 26.15% of the oxidation of the organic molecules per 100% materials.

As compared the weight loss of the **5''** with catalyst **5**, the true weight loss of IPr(Cl)(3−chloropyridine)BF_4 moieties (Mr = 624.2) was 5.65% (26.15−20.50) per 100% materials. This finding means that the mole amounts of $IPrPdBF_4$ is 0.009033 mol%, demonstrating the 9.5659 mg (0.09033 mmol of Pd) of the Pd loading per gram of catalyst **5**.

Figure S3. Solid−state ^{13}C CP/MAS NMR spectra of of **4** and catalyst **5.**

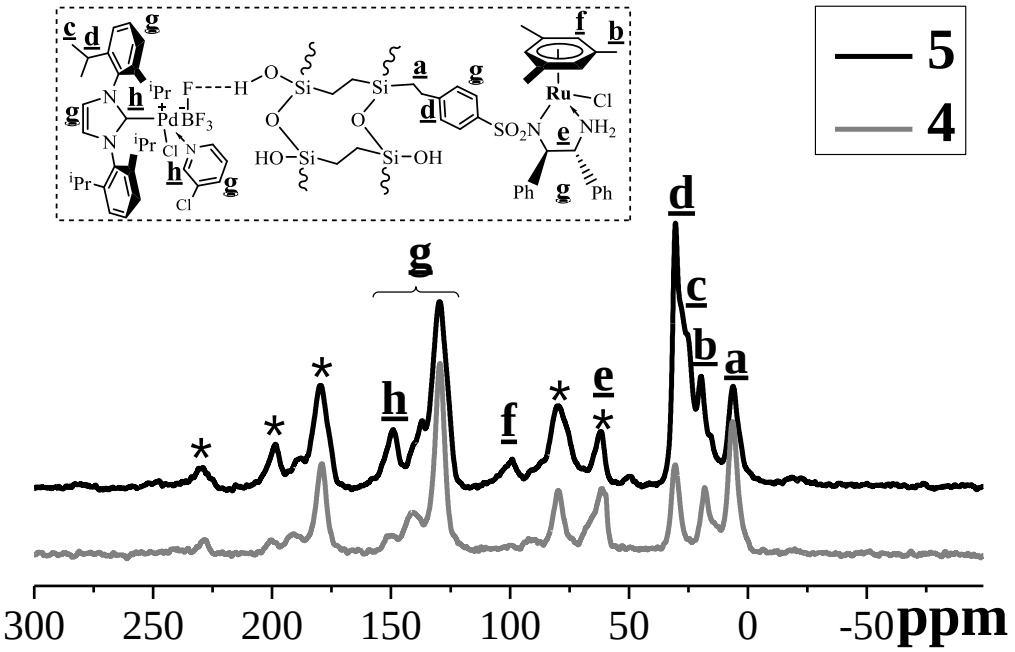
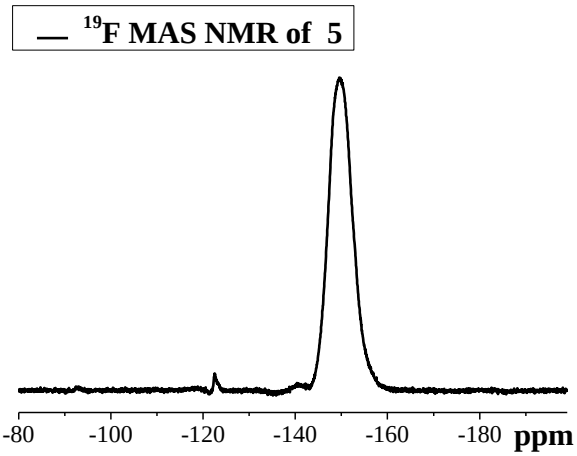


Figure S4. (a) Solid−state ^{19}F NMR spectrum of catalyst **5** and (b) liquid−state ^{19}F NMR of $IPrPdBF_4$ in $CDCl_3$.

(a) Solid−state ^{19}F NMR spectrum of catalyst **5**.



(b) liquid−state ^{19}F NMR of $IPrPdBF_4$ in $CDCl_3$

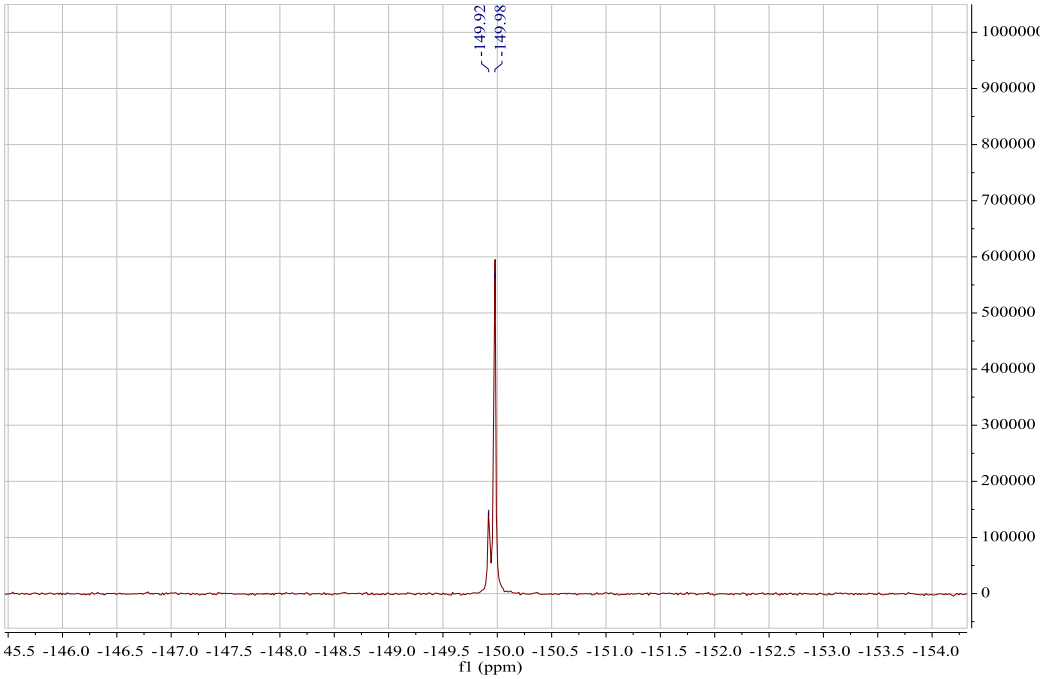


Figure S5. Solid−state ^{29}Si MAS NMR spectra of **4** and catalyst **5.**

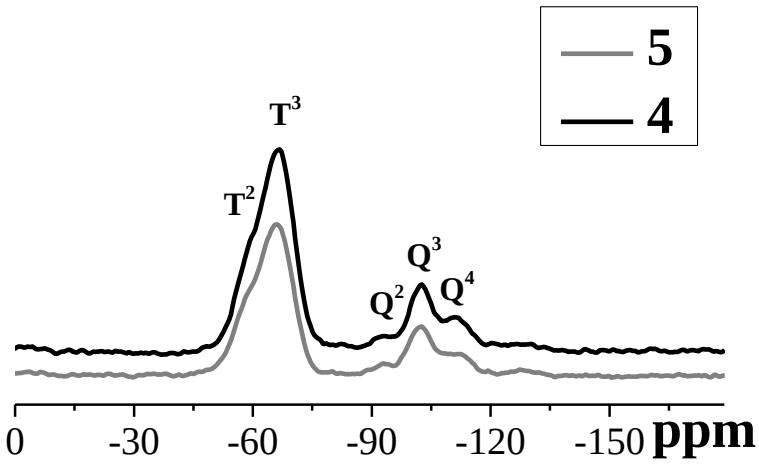


Figure S6. TEM image with a chemical mapping of **5** showing the distribution of Si (white), Pd (green) and Ru (red).

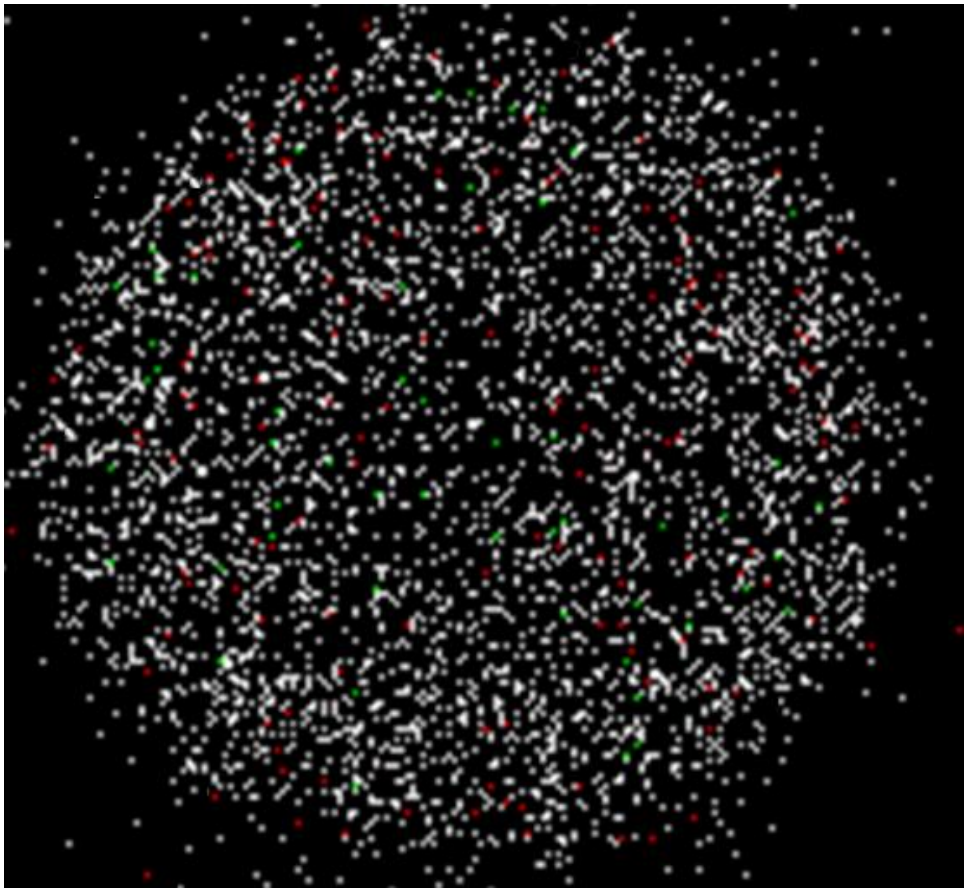


Figure S7. Small−angle powder XRD patterns **4** and catalyst **5**.

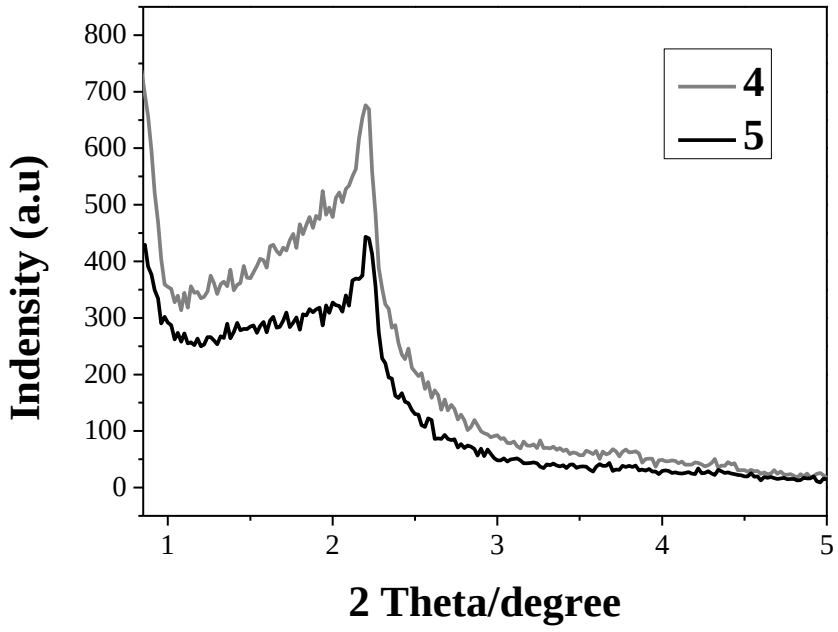


Figure S8. Nitrogen adsorption−desorption isotherms of **4** and catalyst **5**.

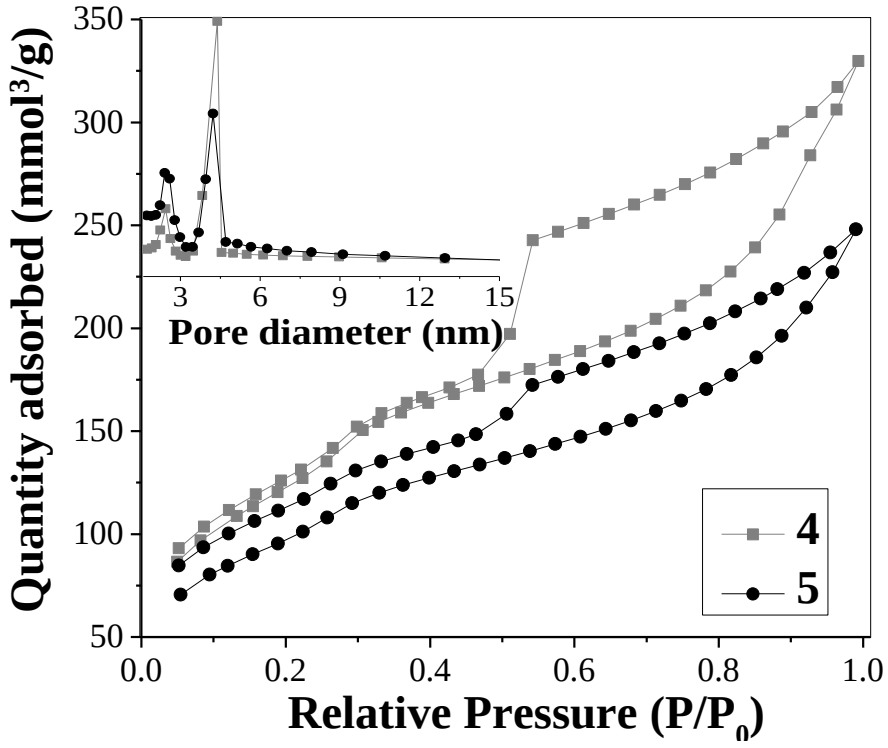
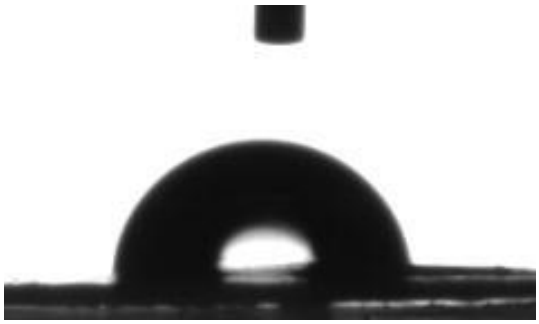


Figure S9. Water contact angle of catalyst **5** and its analogue **5'**.

(a) The water contact angle of 91.7 °for catalyst **5**.



(b) The water contact angle of 50.4 °for its analogue **5'.**

Figure S10. Time course in the transformation of 4–chloracetophenone (**6a**) and phenylboronic acid (1 equivalent of 4–chloroacetophenone, 1.1 equivalent of phenylboronic acid and 5 ((1.2 mol % of Pd and 2.0 mol% of Ru) at 80 ℃).

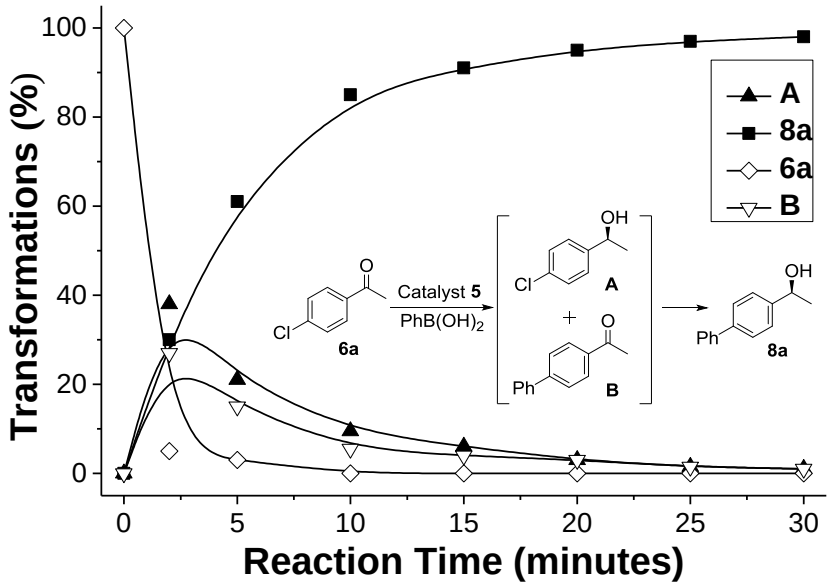
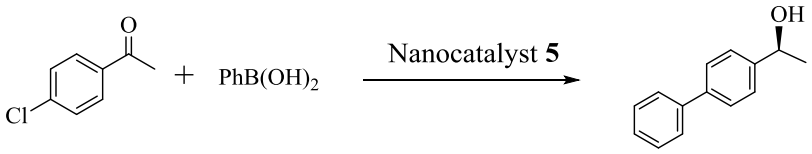


Table S1. Optimizing reaction conditions for the Suzuki coupling–ATH of enantioselective tandem reactions of 4−chloroacetophenone and phenylboronic acid.[a]

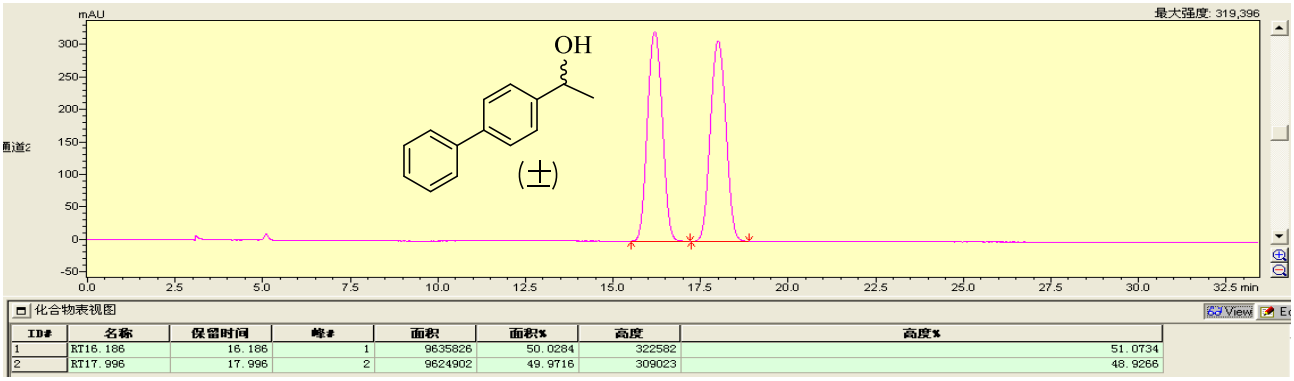


Entry	H-resource, Solvent	ºC	Yield (%)	ee(%)
1	HCO_2Na, H_2O/ ^{i}PrOH (1:3)	40	56	94
2	HCO_2Na, H_2O/ ^{i}PrOH (1:3)	50	63	94
3	HCO_2Na, H_2O/ ^{i}PrOH (1:3)	60	83	93
4	HCO_2Na, H_2O/ ^{i}PrOH (1:3)	70	91	95
5	HCO_2Na, H_2O/ ^{i}PrOH (1:3)	80	97	96
6	HCO_2Na, H_2O/ EtOH (1:3)	80	91	90
7	HCO_2Na, H_2O/ MeOH (1:3)	80	92	92
8	HCO_2Na, H_2O/ ^{i}PrOH (1:1)	80	92	93
9	HCO_2Na, H_2O/ ^{i}PrOH (1:5)	80	93	95
10	HCOOH	80	81	74
11	^{i}PrOH	80	89	88
12	HCOOH−NEt_3	80	93	84

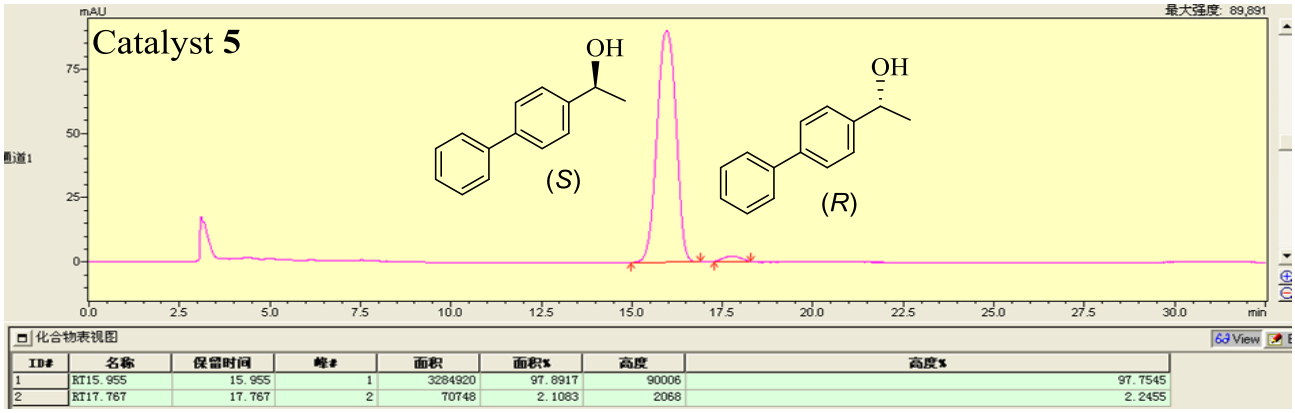
[a] Reaction conditions: catalyst **5** (13.35 mg, 2.0 μmol of Ru and 1.20 μmol of Pd, based on ICP analysis), Cs_2CO_3 (0.12 mmol), HCO_2Na (1.0 mmol), 4−chloroacetophenone (0.10 mmol) and phenylboronic acid (0.12 mmol), and 2.0 mL of H_2O/^{i}PrOH (v/v = 1:3), reaction time (0.5–1.5 h).

Figure S10. HPLC analyses for chiral products **(**Suzuki coupling–ATH of enantioselective tandem reactions of chloracetophenones and arylboronic acids).

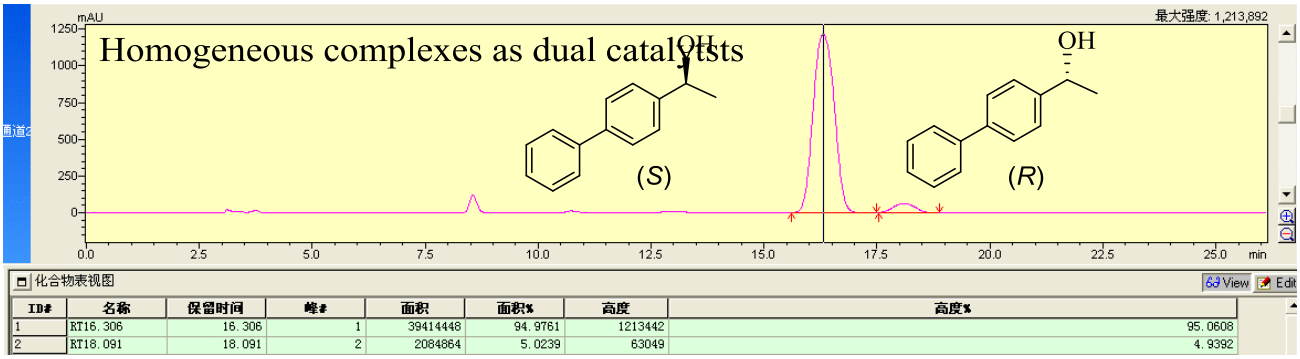
(*S*)−4−phenylacetophenol (8a): (HPLC: Chiracel AD−H, detected at 254 nm, eluent: n−hexane/2−propanol = 97/3, flow rate = 1.0 mL/min, 25 ℃). [Literature (*Chem. Eur. J.* **2010,** 16, 6748): HPLC: Chiracel AD−H, eluent: n−hexane/2−propanol = 95/5, flow rate = 0.7 mL/min, detected at 254 nm, Retention time: 10.98 min (S), 12.16 min (R).]



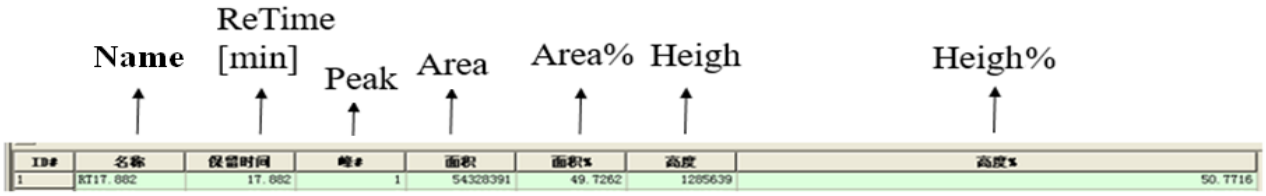
ID#	名称	保留时间	峰#	面积	面积%	高度	高度%
1	RT16.186	16.186	1	9635826	50.0284	322582	51.0734
2	RT17.996	17.996	2	9624902	49.9716	309023	48.9266



ID#	名称	保留时间	峰#	面积	面积%	高度	高度%
1	RT15.955	15.955	1	3284920	97.8917	90006	97.7545
2	RT17.767	17.767	2	70748	2.1083	2068	2.2455

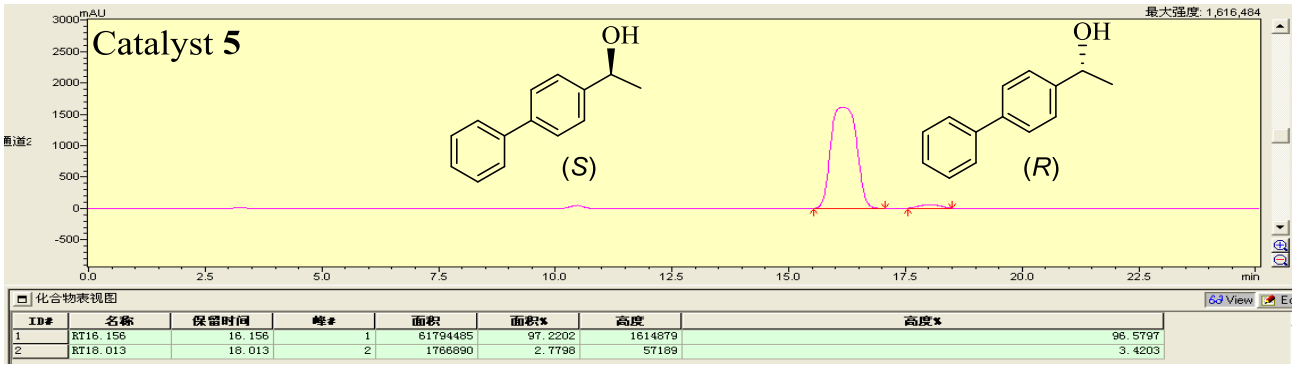


ID#	名称	保留时间	峰#	面积	面积%	高度	高度%
1	RT16.306	16.306	1	39414448	94.9761	1213442	95.0608
2	RT18.091	18.091	2	2084864	5.0239	63049	4.9392

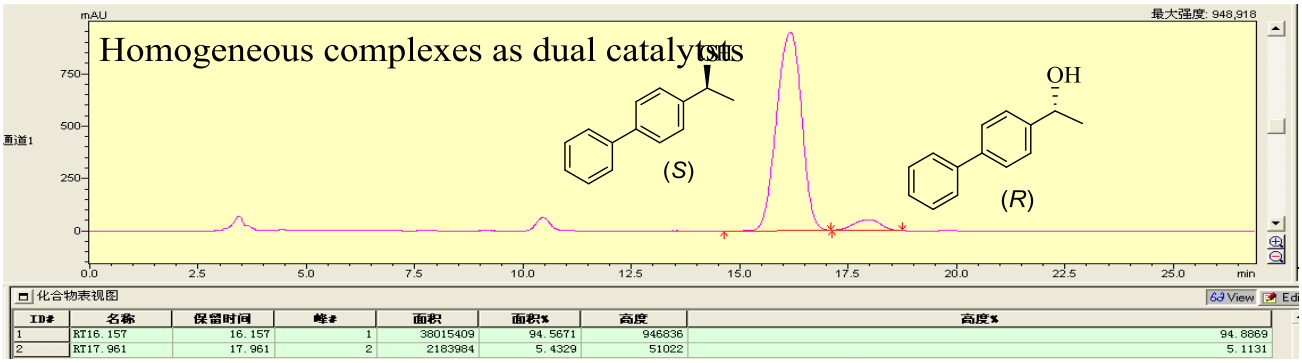


ID#	名称	保留时间	峰#	面积	面积%	高度	高度%
1	RT17.882	17.882	1	54328391	49.7262	1285639	50.7716

(*S*)−4−phenylacetophenol (8a). Data were obtained using bromoacetophenone and phenylboronic acid as substrate.

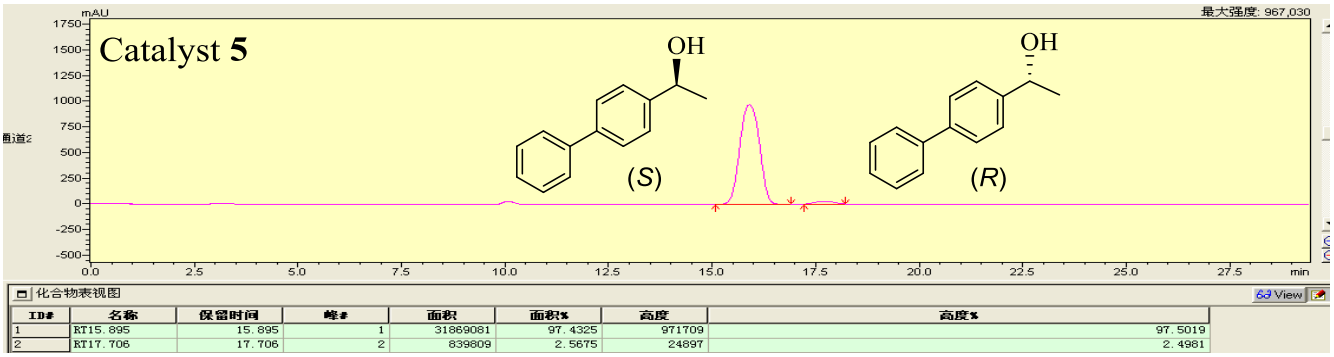


ID#	名称	保留时间	峰#	面积	面积%	高度	高度%
1	RT16.156	16.156	1	81794485	97.2202	1614879	96.5797
2	RT18.013	18.013	2	1766890	2.7798	57189	3.4203

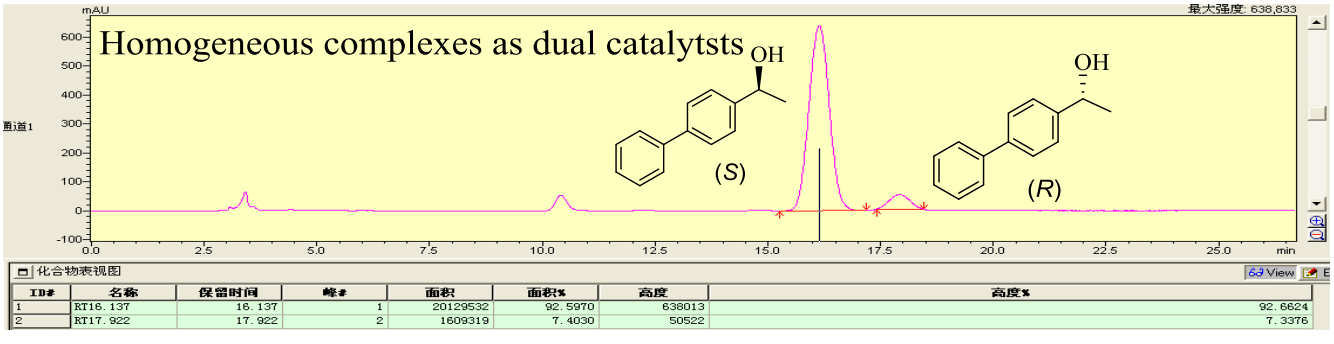


ID#	名称	保留时间	峰#	面积	面积%	高度	高度%
1	RT16.157	16.157	1	38015409	94.5671	946836	94.8869
2	RT17.961	17.961	2	2183984	5.4329	51022	5.1131

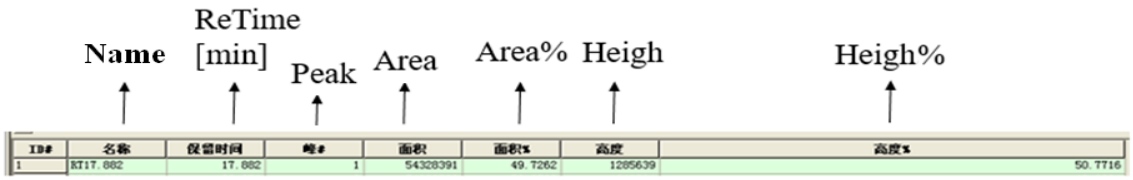
(*S*)−4−phenylacetophenol (8a). Data were obtained using iodooacetophenone and phenylboronic acid as substrate.



ID#	名称	保留时间	峰#	面积	面积%	高度	高度%
1	RT15.895	15.895	1	31869081	97.4325	971709	97.5019
2	RT17.706	17.706	2	839809	2.5675	24897	2.4981

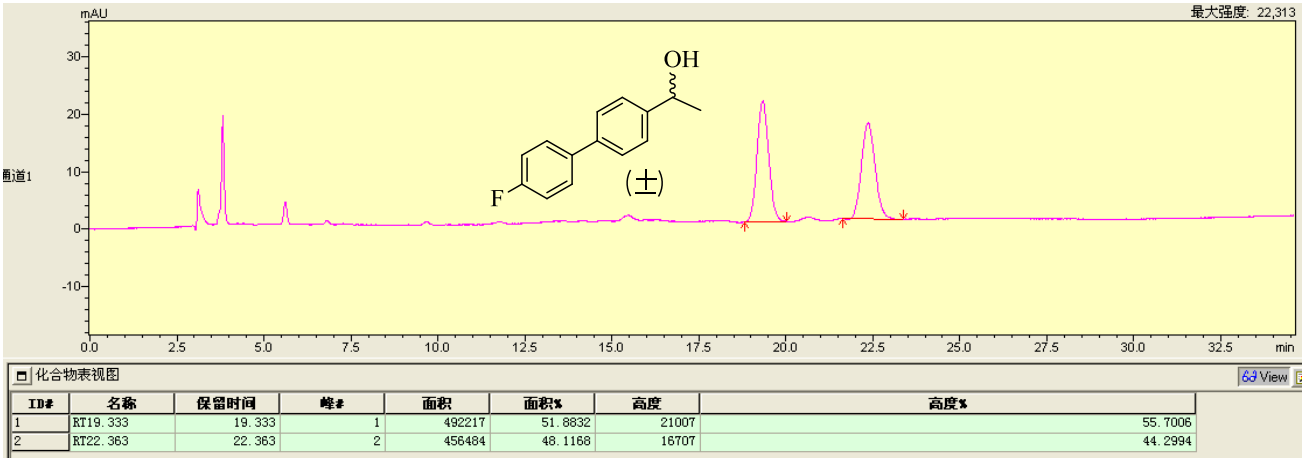


ID#	名称	保留时间	峰#	面积	面积%	高度	高度%
1	RT16.137	16.137	1	20129532	92.5970	638013	92.6624
2	RT17.922	17.922	2	1609319	7.4030	50522	7.3376

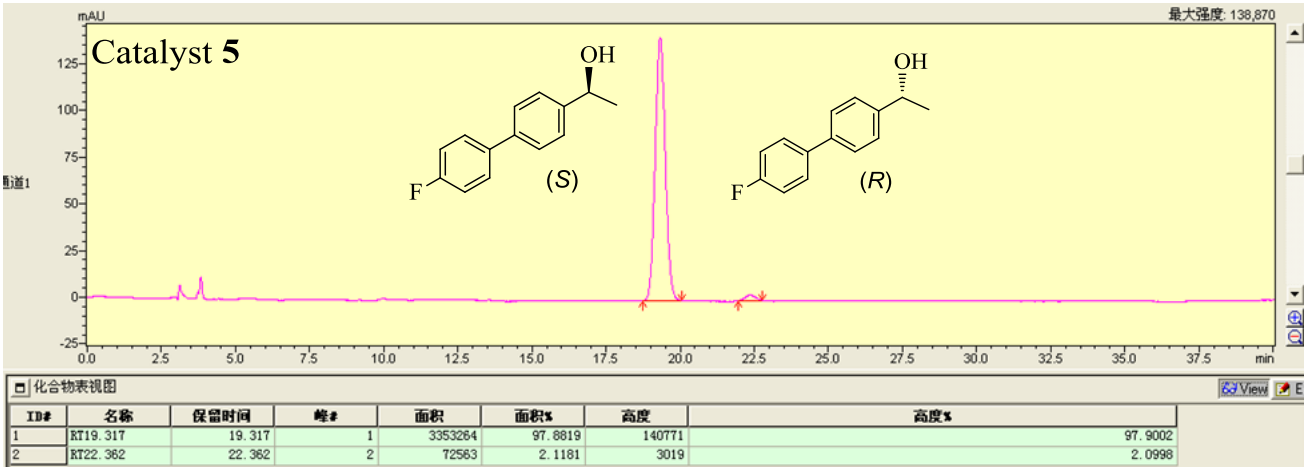


ID#	名称	保留时间	峰#	面积	面积%	高度	高度%
1	RT17.882	17.882	1	54328391	49.7262	1285639	50.7716

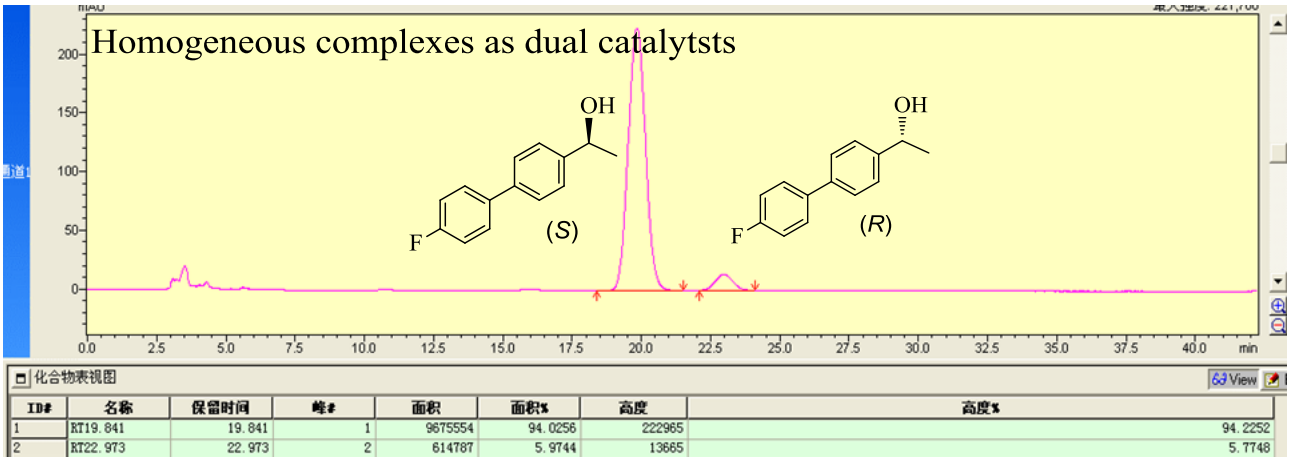
(*S*)−1−(4−(4−floro)phenyl)ethanol (8b): (HPLC: Chiracel AD−H, detected at 254 nm, eluent: n−hexane/2−propanol = 97/3, flow rate = 1.0 mL/min, 25 ℃).



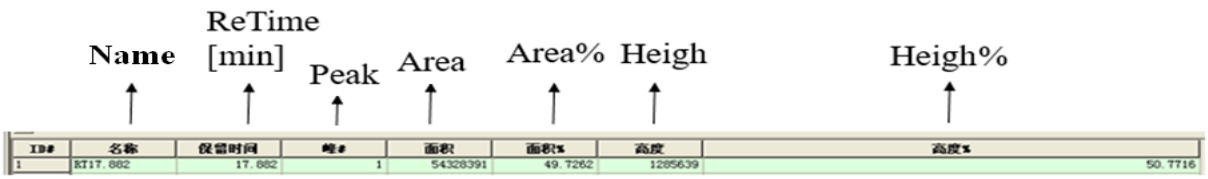
ID#	名称	保留时间	峰#	面积	面积%	高度	高度%
1	RT19.333	19.333	1	492217	51.8832	21007	55.7006
2	RT22.363	22.363	2	456484	48.1168	16707	44.2994



ID#	名称	保留时间	峰#	面积	面积%	高度	高度%
1	RT19.317	19.317	1	3353264	97.8819	140771	97.9002
2	RT22.362	22.362	2	72563	2.1181	3019	2.0998

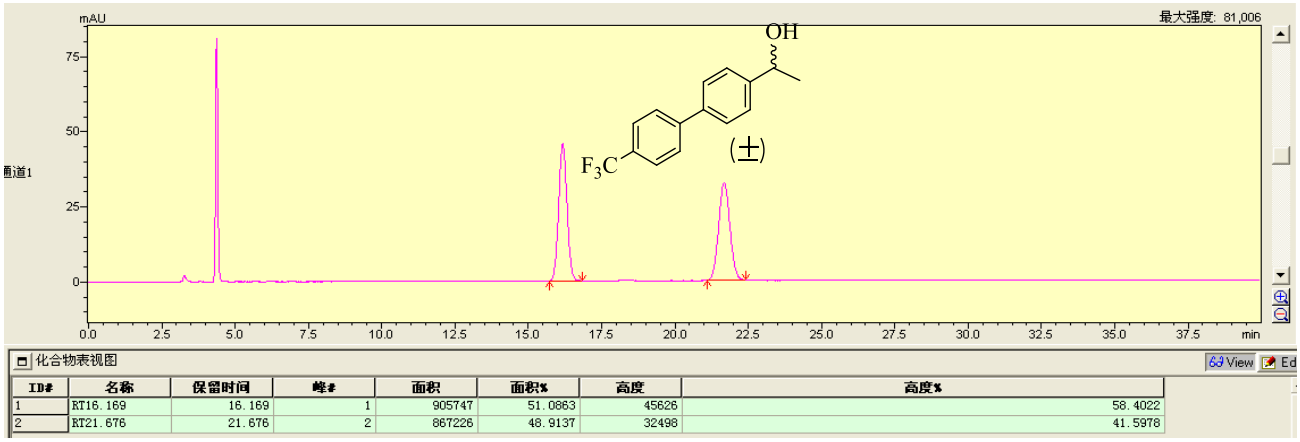


ID#	名称	保留时间	峰#	面积	面积%	高度	高度%
1	RT19.841	19.841	1	9675554	94.0256	222965	94.2252
2	RT22.973	22.973	2	614787	5.9744	13665	5.7748

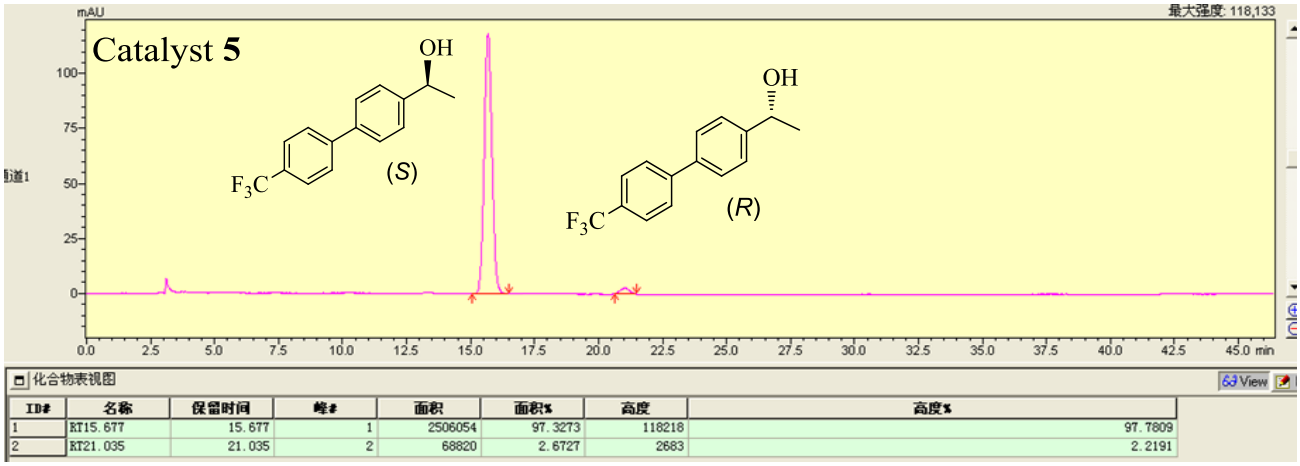


ID#	名称	保留时间	峰#	面积	面积%	高度	高度%
1	RT17.882	17.882	1	54328391	49.7262	1285639	50.7716

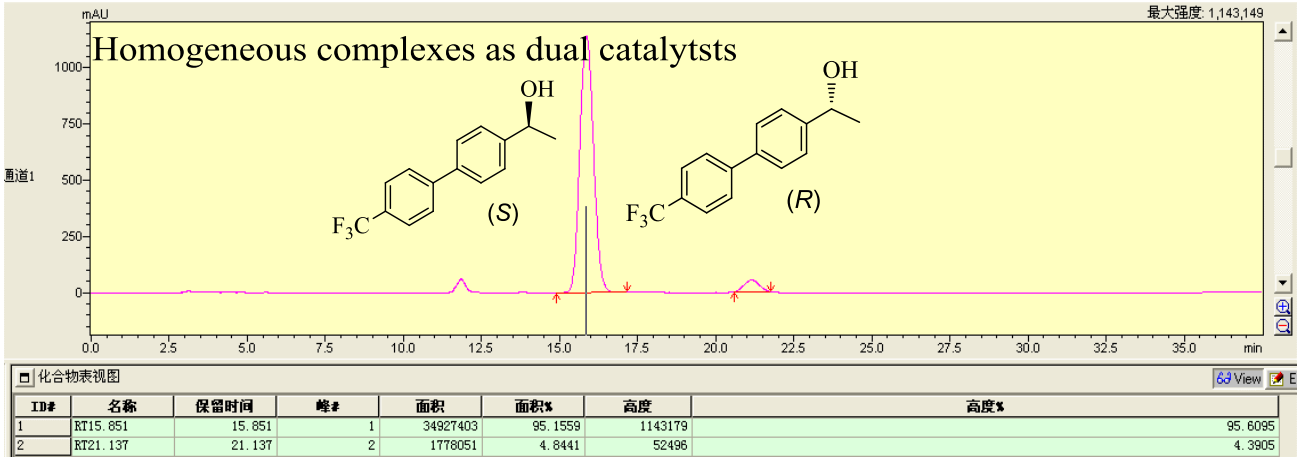
(*S*)−1−(4−(4−trifluoromethyl)phenyl)ethanol (8c): (HPLC: Chiracel AD−H, detected at 254 nm, eluent: n−hexane/2−propanol = 97/3, flow rate = 1.0 mL/min, 25 ℃).



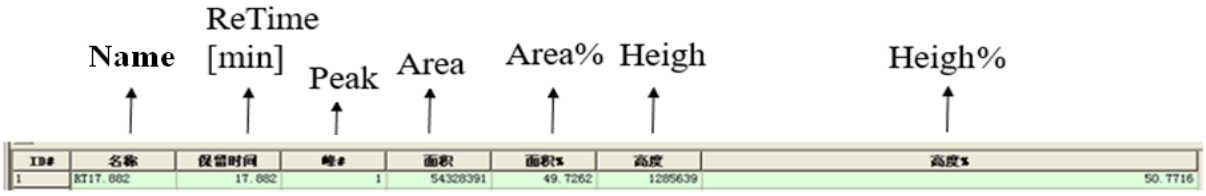
ID#	名称	保留时间	峰#	面积	面积%	高度	高度%
1	RT16.169	16.169	1	905747	51.0863	45626	58.4022
2	RT21.676	21.676	2	867226	48.9137	32498	41.5978



ID#	名称	保留时间	峰#	面积	面积%	高度	高度%
1	RT15.677	15.677	1	2506054	97.3273	118218	97.7809
2	RT21.035	21.035	2	68820	2.6727	2683	2.2191

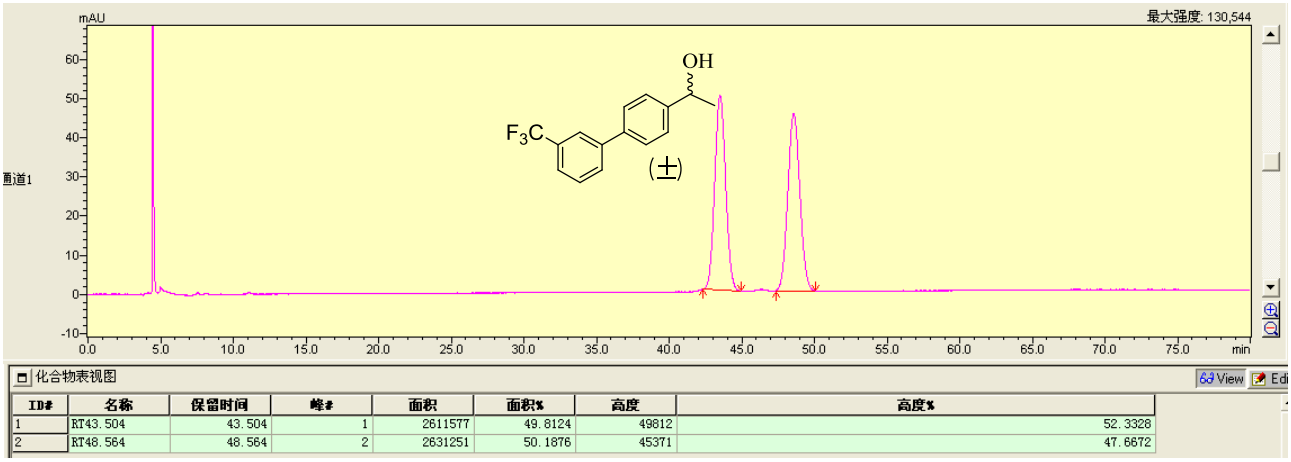


ID#	名称	保留时间	峰#	面积	面积%	高度	高度%
1	RT15.851	15.851	1	34927403	95.1559	1143179	95.6095
2	RT21.137	21.137	2	1778051	4.8441	52496	4.3905



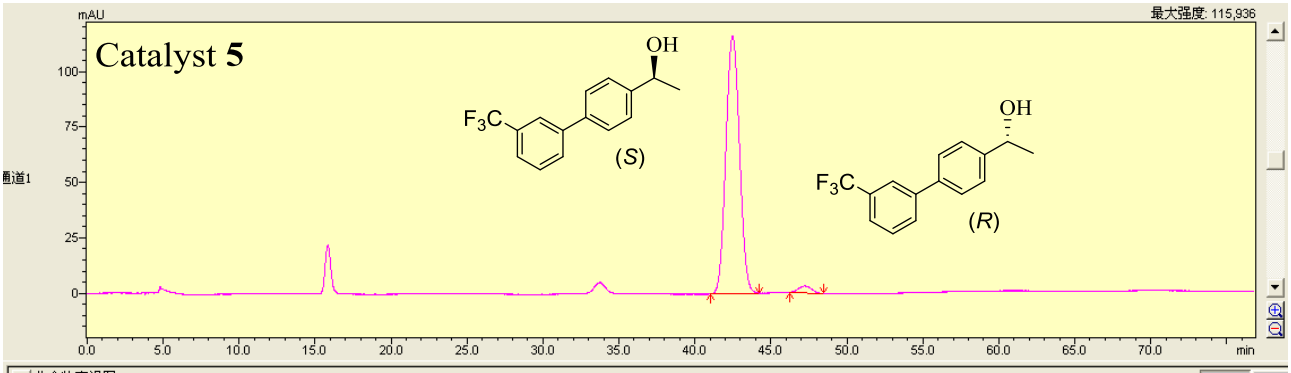
ID#	名称	保留时间	峰#	面积	面积%	高度	高度%
1	RT17.882	17.882	1	54328391	49.7262	1285639	50.7716

(*S*)−1−(4−(3−trifluouomethyl)phenyl)ethanol (8d): (HPLC: Chiracel AD−H, detected at 254 nm, eluent: n−hexane/2−propanol = 79/1, flow rate = 0.8 mL/min, 25 ℃).



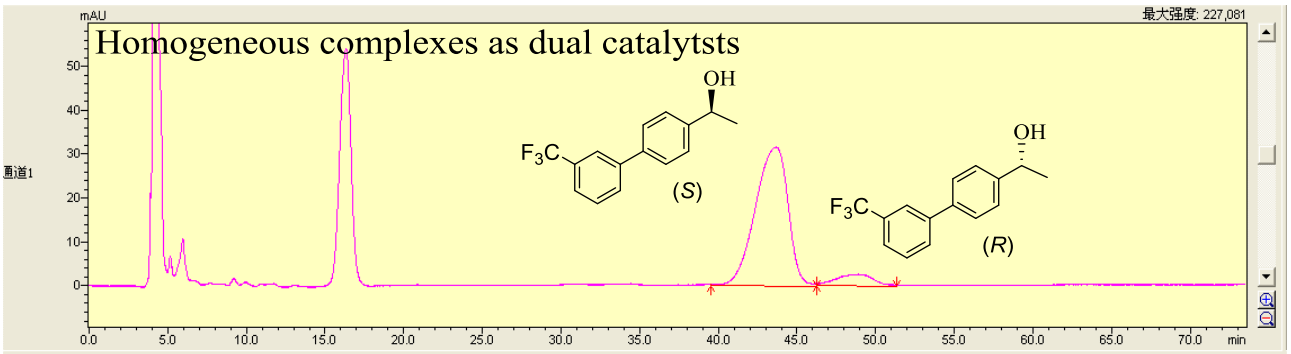
化合物表视图

ID#	名称	保留时间	峰#	面积	面积%	高度	高度%
1	RT43.504	43.504	1	2611577	49.8124	49812	52.3328
2	RT48.564	48.564	2	2631251	50.1876	45371	47.6672



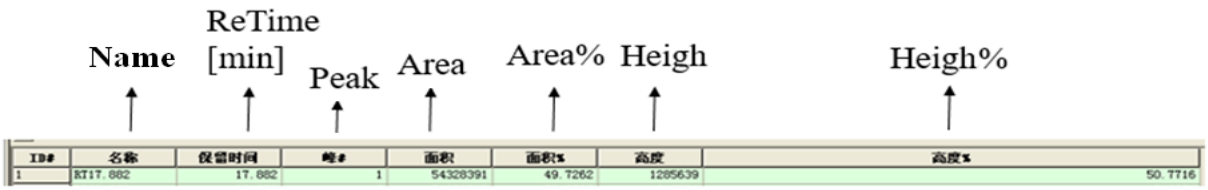
化合物表视图

ID#	名称	保留时间	峰#	面积	面积%	高度	高度%
1	RT42.478	42.478	1	7282560	97.4507	116122	97.3726
2	RT47.216	47.216	2	190513	2.5493	3133	2.6274



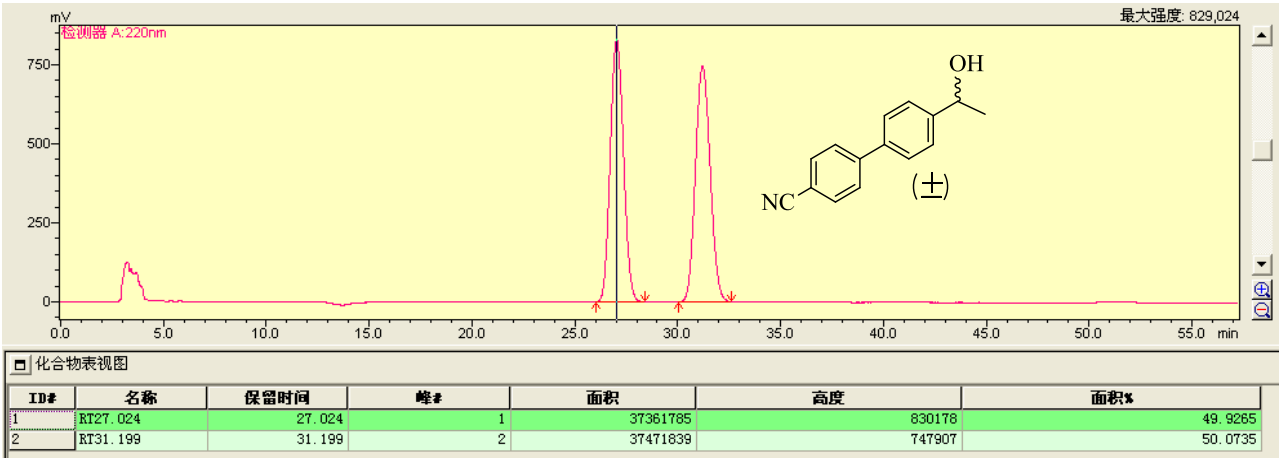
化合物表视图

ID#	名称	保留时间	峰#	面积	面积%	高度	高度%
1	RT43.651	43.651	1	4560326	91.5465	31594	92.3921
2	RT48.874	48.874	2	421103	8.4535	2602	7.6079



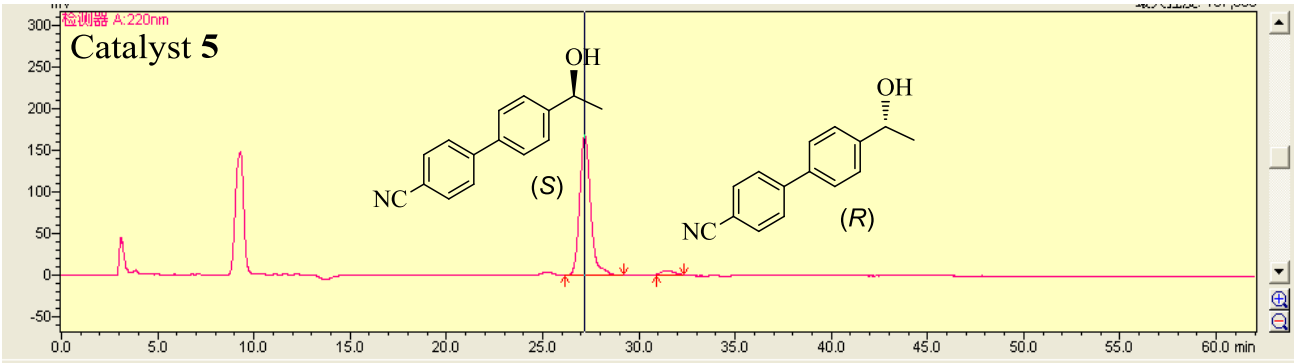
ID#	名称	保留时间	峰#	面积	面积%	高度	高度%
1	RT17.882	17.882	1	54328391	49.7262	1285639	50.7716

(*S*)−1−(4−(4−cyano)phenyl)ethanol (8e): (HPLC: Chiracel AD−H, detected at 254 nm, eluent: n−hexane/2−propanol = 90/10, flow rate = 1.0 mL/min, 25 ℃).



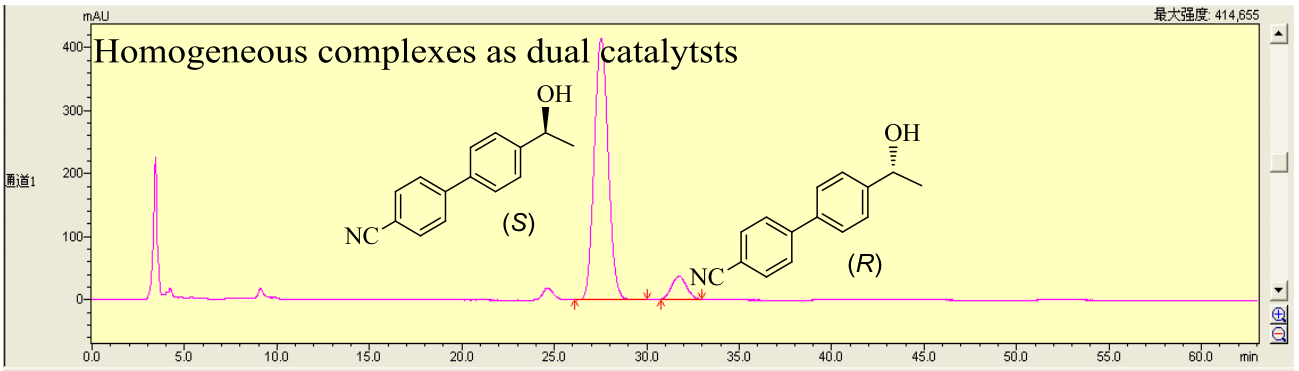
化合物表视图

ID#	名称	保留时间	峰#	面积	高度	面积%
1	RT27.024	27.024	1	37361785	830178	49.9265
2	RT31.199	31.199	2	37471839	747907	50.0735



化合物表视图

ID#	名称	保留时间	峰#	面积	高度	面积%
1	RT27.188	27.188	1	6691012	167689	96.5063
2	RT31.439	31.439	2	242226	5230	3.4937



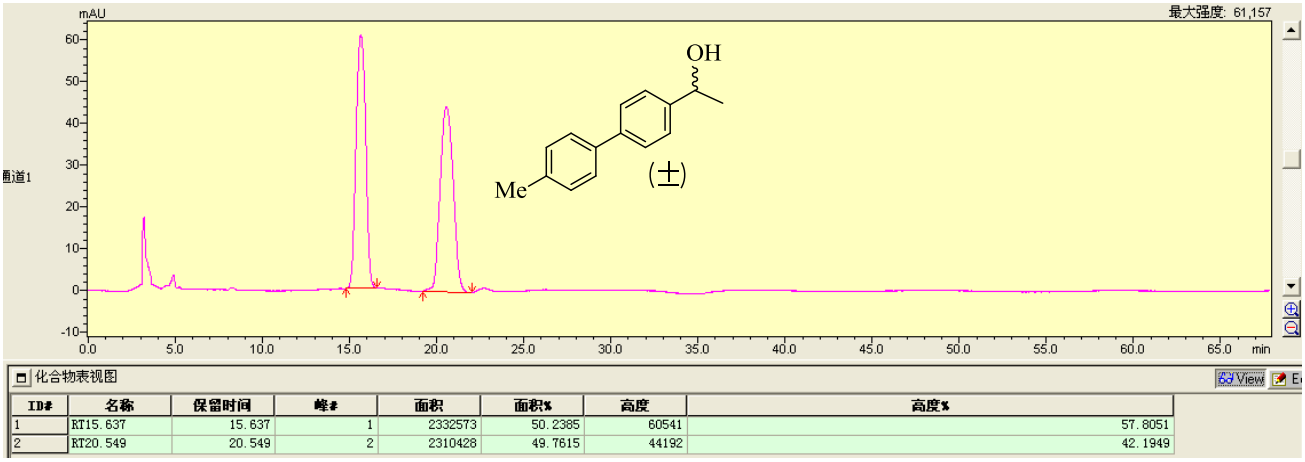
化合物表视图

ID#	名称	保留时间	峰#	面积	面积%	高度	高度%
1	RT27.532	27.532	1	21849759	91.3742	414869	91.8542
2	RT31.740	31.740	2	2062629	8.6258	36791	8.1458

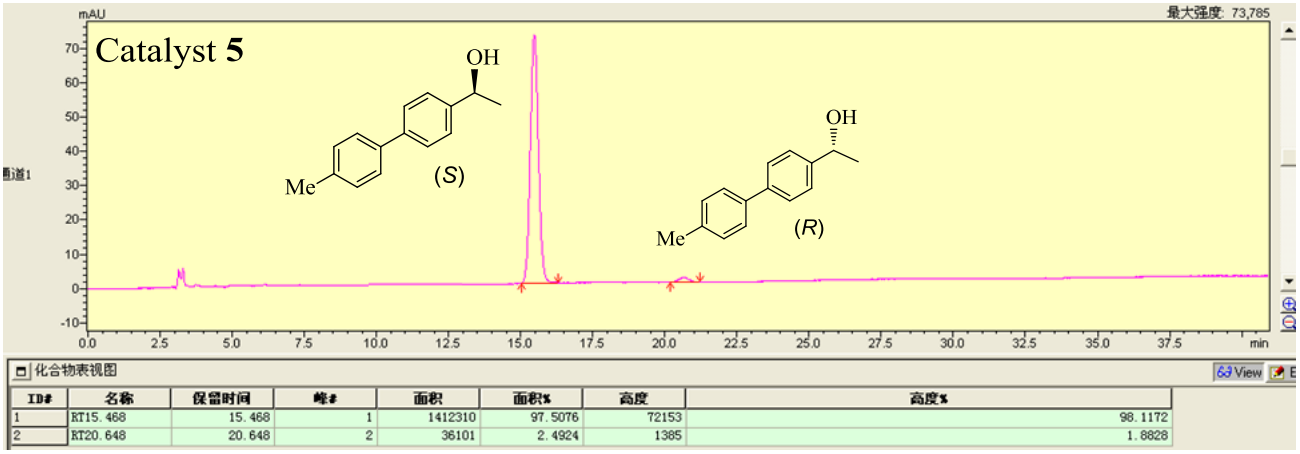
Name | RetTime [min] | Peak | Area | Heighth | Area ratio %

ID#	名称	保留时间	峰#	面积	高度	面积%
1	RT27.188	27.188	1	6691012	167689	96.5063
2	RT31.439	31.439	2	242226	5230	3.4937

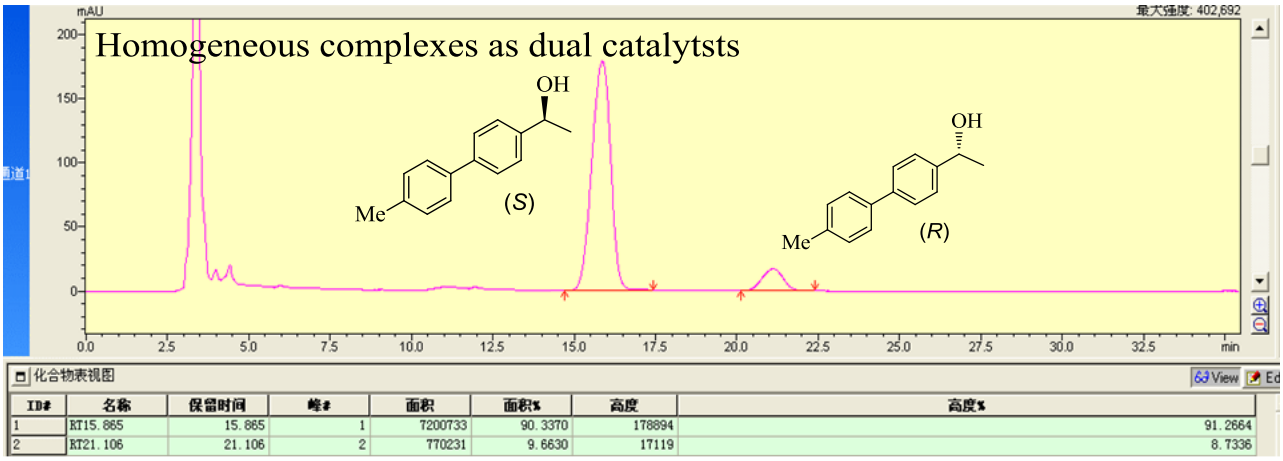
(*S*)−1−(4−(4−methyl)phenyl)ethanol (8f): (HPLC: Chiracel AD−H, detected at 254 nm, eluent: n−hexane/2−propanol = 97/3, flow rate = 1.0 mL/min, 25 ℃).



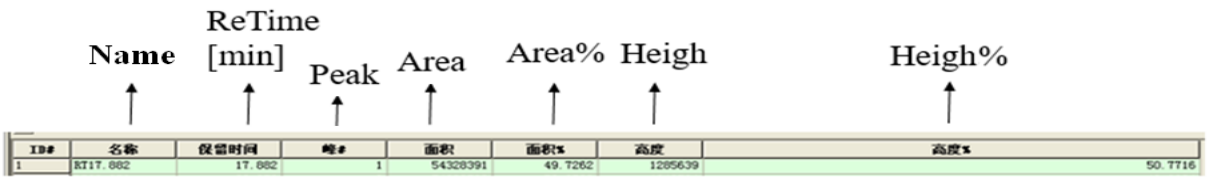
ID#	名称	保留时间	峰#	面积	面积%	高度	高度%
1	RT15.637	15.637	1	2332573	50.2385	60541	57.8051
2	RT20.549	20.549	2	2310428	49.7615	44192	42.1949



ID#	名称	保留时间	峰#	面积	面积%	高度	高度%
1	RT15.468	15.468	1	1412310	97.5076	72153	98.1172
2	RT20.648	20.648	2	36101	2.4924	1385	1.8828

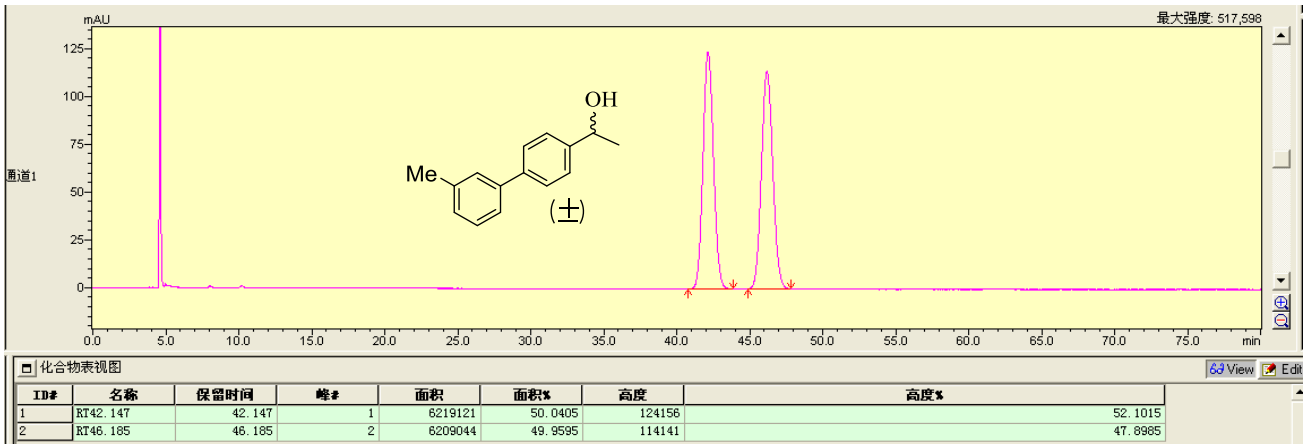


ID#	名称	保留时间	峰#	面积	面积%	高度	高度%
1	RT15.865	15.865	1	7200733	90.3370	178894	91.2664
2	RT21.106	21.106	2	770231	9.6630	17119	8.7336



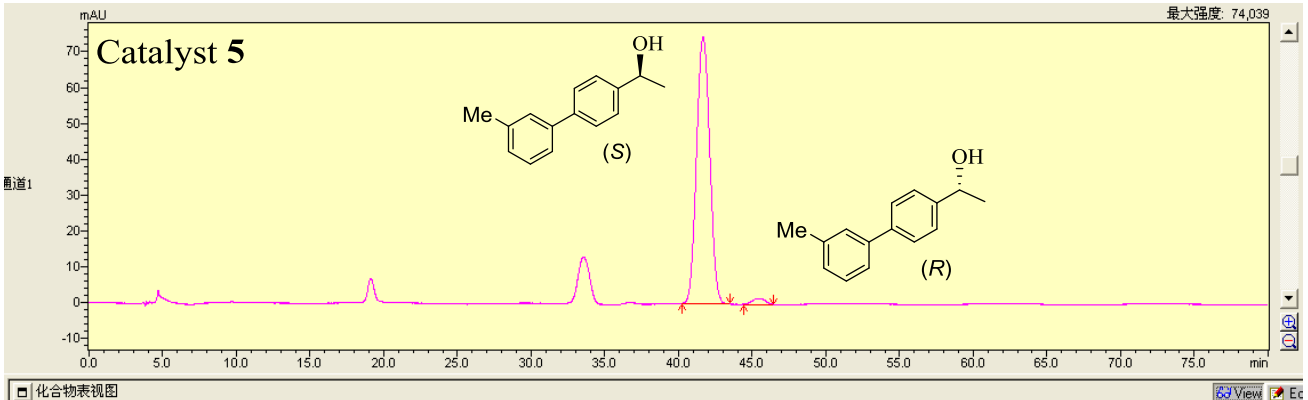
ID#	名称	保留时间	峰#	面积	面积%	高度	高度%
1	RT17.882	17.882	1	54328391	49.7262	1285639	50.7716

(*S*)−1−(4−(3−methyl)phenyl)ethanol (8g): (HPLC: Chiracel AD−H, detected at 254 nm, eluent: n−hexane/2−propanol = 79/1, flow rate = 0.8 mL/min, 25 ℃).



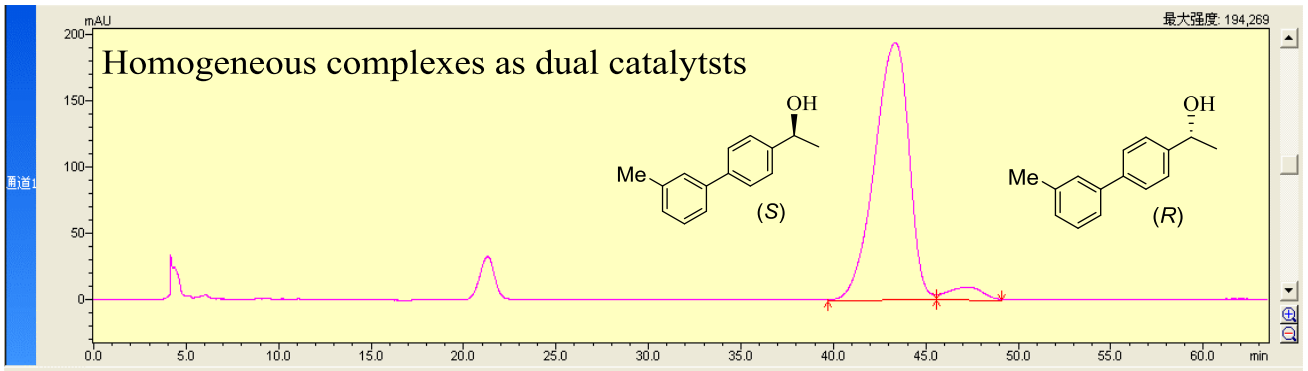
化合物表视图

ID#	名称	保留时间	峰#	面积	面积%	高度	高度%
1	RT42.147	42.147	1	6219121	50.0405	124156	52.1015
2	RT46.185	46.185	2	6209044	49.9595	114141	47.8985



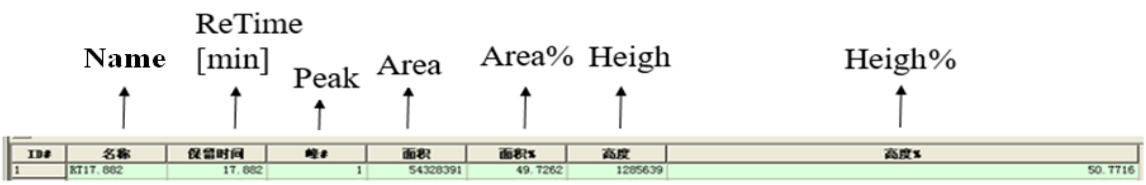
化合物表视图

ID#	名称	保留时间	峰#	面积	面积%	高度	高度%
1	RT41.663	41.663	1	4642164	97.8979	74291	97.8239
2	RT45.521	45.521	2	99680	2.1021	1653	2.1761



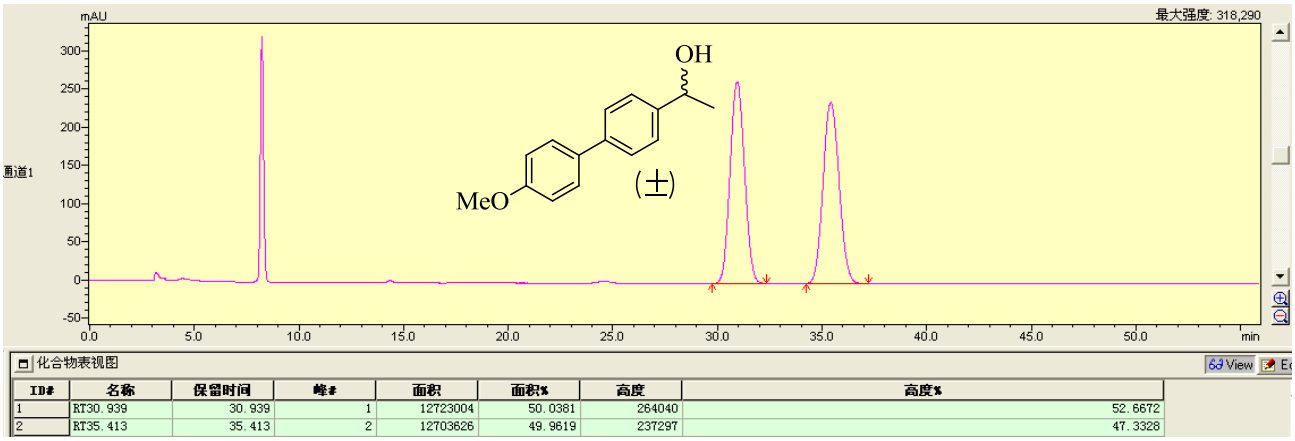
化合物表视图

ID#	名称	保留时间	峰#	面积	面积%	高度	高度%
1	RT43.343	43.343	1	25090640	95.2790	194324	95.3138
2	RT47.306	47.306	2	1243216	4.7210	9554	4.6862



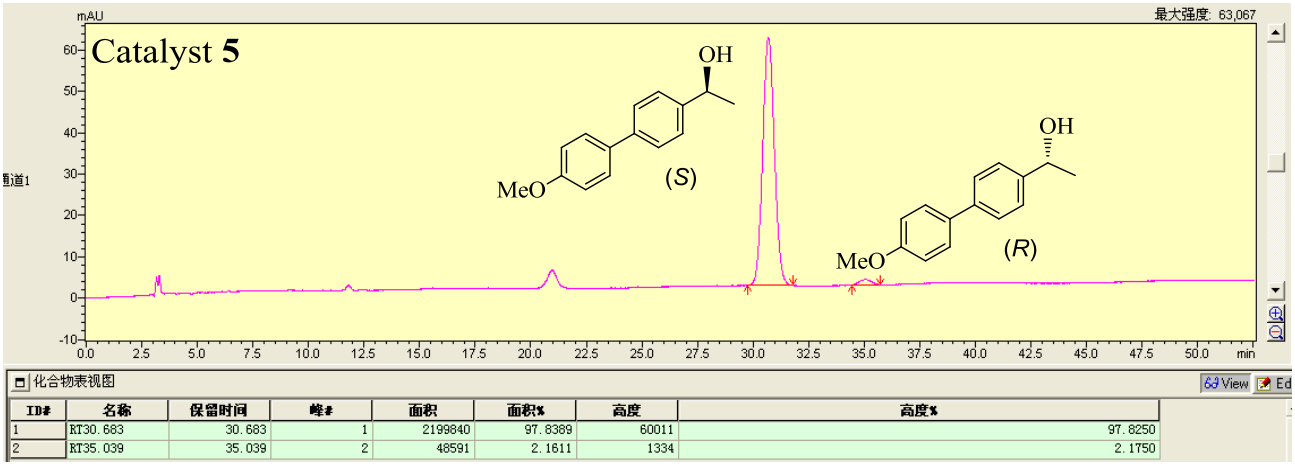
ID#	名称	保留时间	峰#	面积	面积%	高度	高度%
1	RT17.882	17.882	1	54328391	49.7262	1285639	50.7716

(*S*)−1−(4−(4−methoxy)phenyl)ethanol (8h): (HPLC: Chiracel AD−H, detected at 254 nm, eluent: n−hexane/2−propanol = 97/3, flow rate = 1.0 mL/min, 25 ℃).



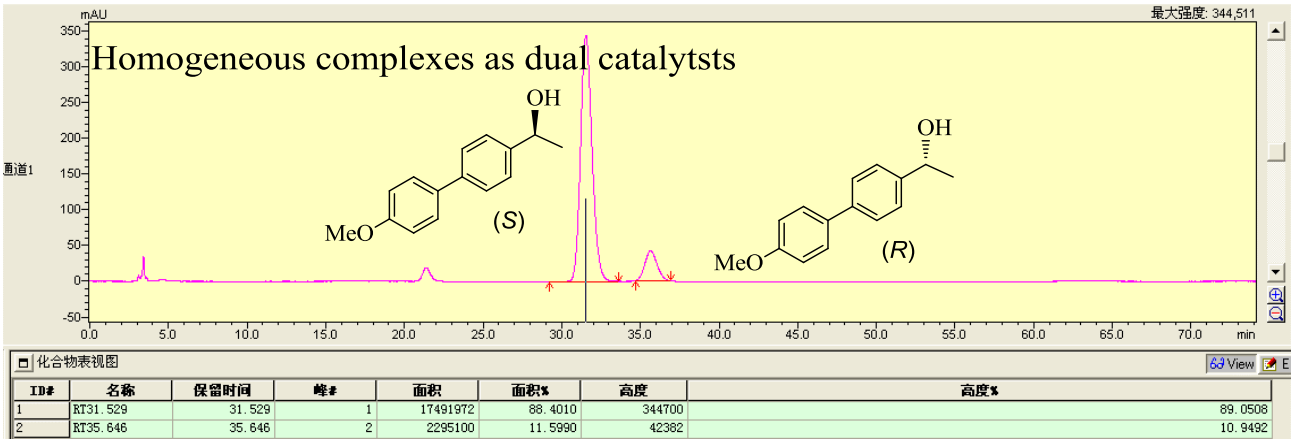
化合物表视图

ID#	名称	保留时间	峰#	面积	面积%	高度	高度%
1	RT30.939	30.939	1	12723004	50.0381	264040	52.6672
2	RT35.413	35.413	2	12703626	49.9619	237297	47.3328



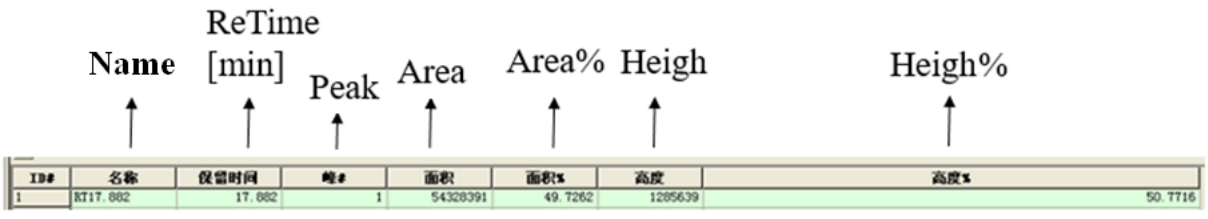
化合物表视图

ID#	名称	保留时间	峰#	面积	面积%	高度	高度%
1	RT30.683	30.683	1	2199840	97.8389	60011	97.8250
2	RT35.039	35.039	2	48591	2.1611	1334	2.1750



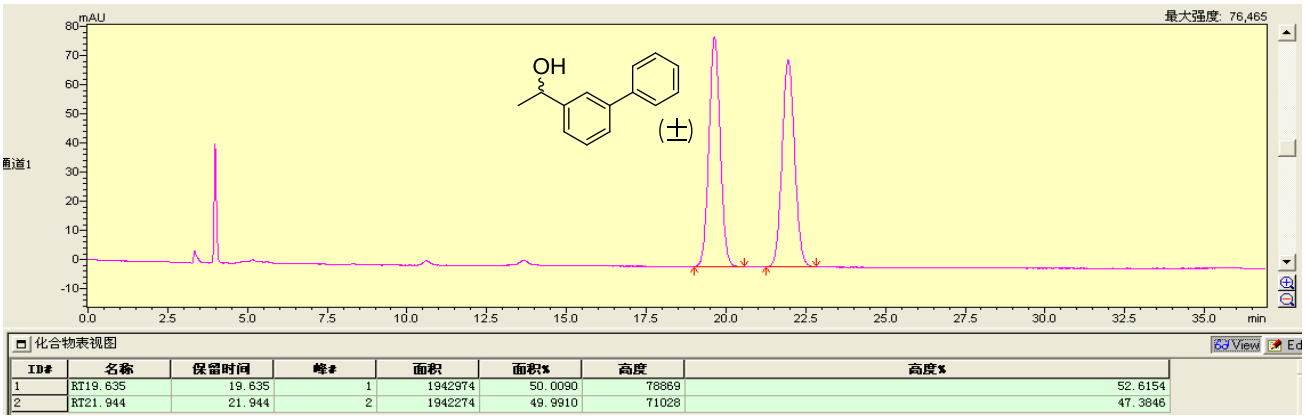
化合物表视图

ID#	名称	保留时间	峰#	面积	面积%	高度	高度%
1	RT31.529	31.529	1	17491972	88.4010	344700	89.0508
2	RT35.646	35.646	2	2295100	11.5990	42382	10.9492



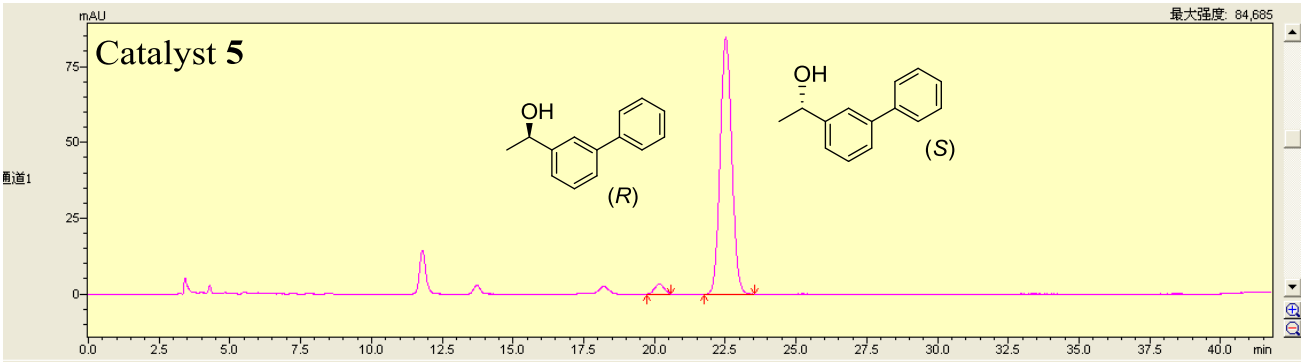
ID#	名称	保留时间	峰#	面积	面积%	高度	高度%
1	RT17.882	17.882	1	54328391	49.7262	1285639	50.7716

(*S*)−3−phenylacetophenol (8i): (HPLC: Chiracel AD−H, detected at 254 nm, eluent: n−hexane/2−propanol = 97/3, flow rate = 1.0 mL/min, 25 ℃).



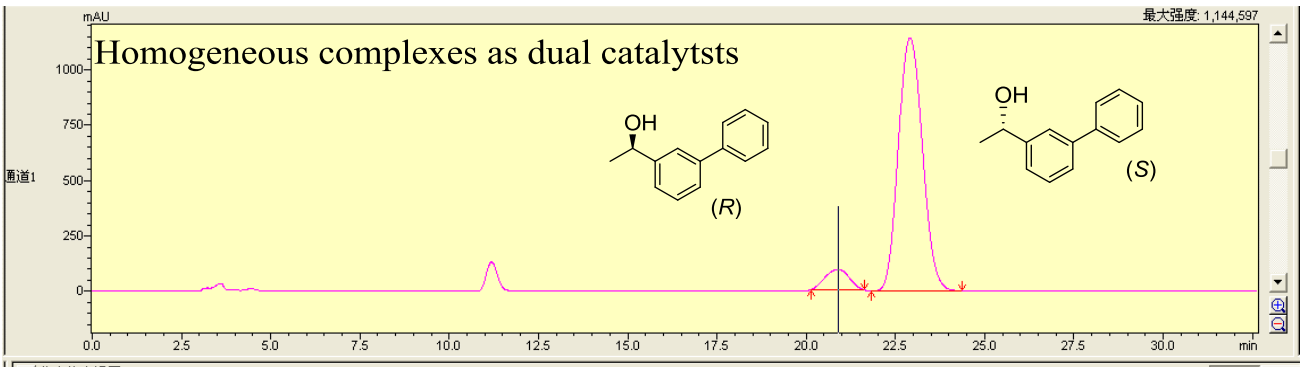
化合物表视图

ID#	名称	保留时间	峰#	面积	面积%	高度	高度%
1	RT19.635	19.635	1	1942974	50.0090	78869	52.6154
2	RT21.944	21.944	2	1942274	49.9910	71028	47.3846



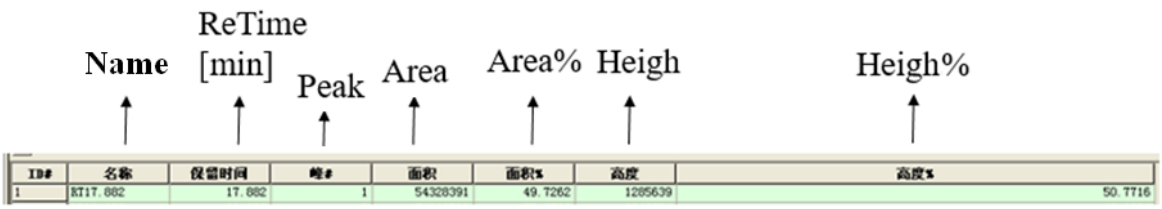
化合物表视图

ID#	名称	保留时间	峰#	面积	面积%	高度	高度%
1	RT20.164	20.164	1	77769	3.1007	3338	3.7878
2	RT22.514	22.514	2	2430331	96.8993	84778	96.2122



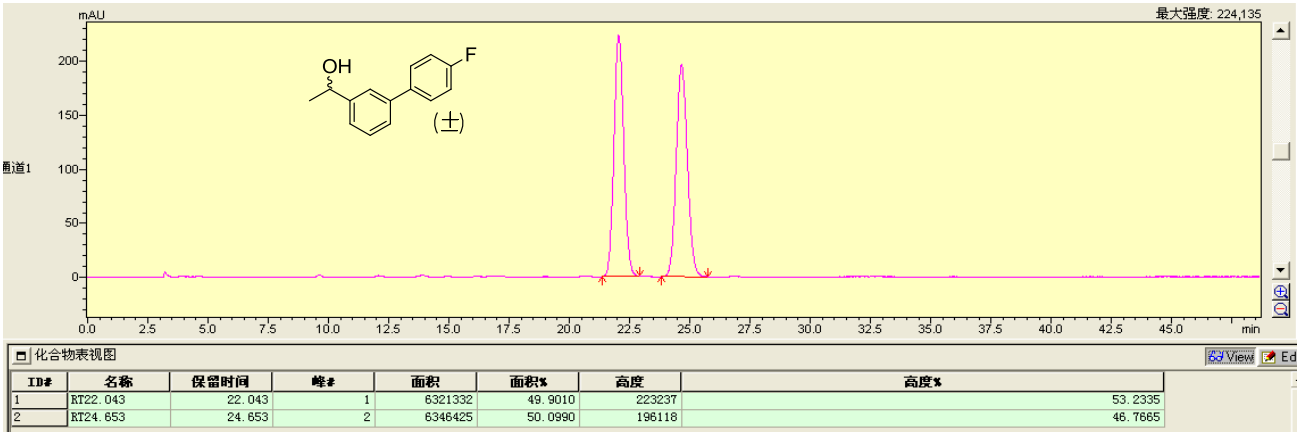
化合物表视图

ID#	名称	保留时间	峰#	面积	面积%	高度	高度%
1	RT20.889	20.889	1	4312410	7.4502	92676	7.5001
2	RT22.900	22.900	2	53570420	92.5498	1142977	92.4999



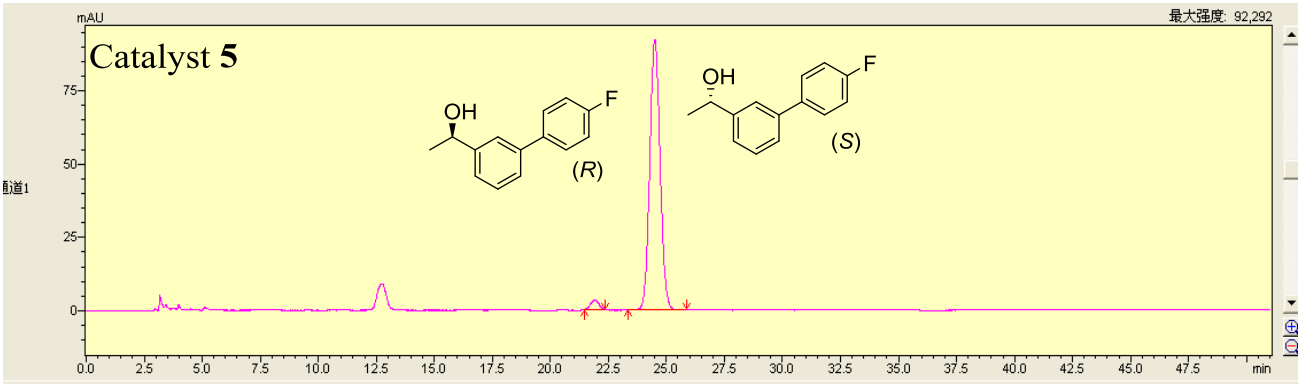
ID#	名称	保留时间	峰#	面积	面积%	高度	高度%
1	RT17.882	17.882	1	54328391	49.7262	1285639	50.7716

(*S*)−1−(3−(4−fluoro)phenyl)ethanol (8j): (HPLC: Chiracel AD−H, detected at 254 nm, eluent: n−hexane/2−propanol = 97/3, flow rate = 1.0 mL/min, 25 ℃).



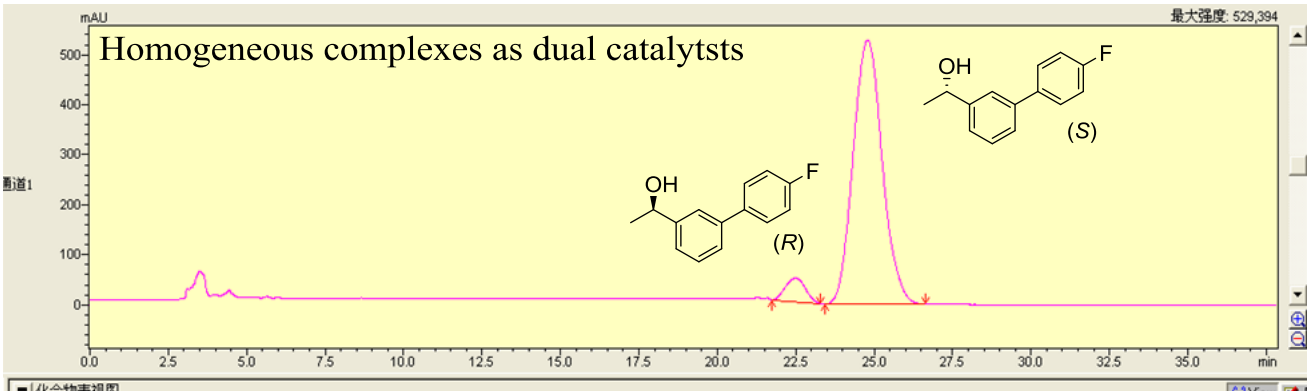
化合物表视图

ID#	名称	保留时间	峰#	面积	面积%	高度	高度%
1	RT22.043	22.043	1	6321332	49.9010	223237	53.2335
2	RT24.653	24.653	2	6346425	50.0990	196118	46.7665



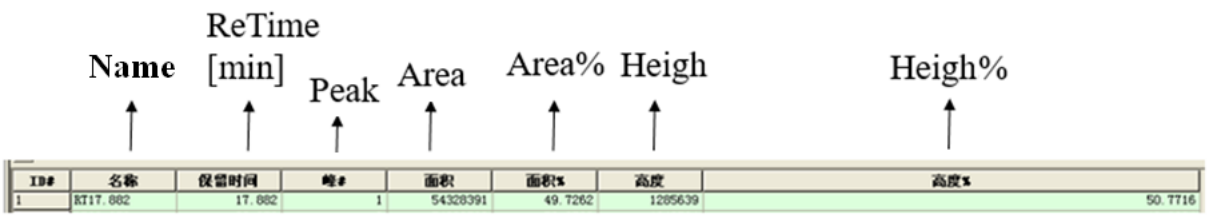
化合物表视图

ID#	名称	保留时间	峰#	面积	面积%	高度	高度%
1	RT21.898	21.898	1	84139	2.8604	3270	3.4310
2	RT24.497	24.497	2	2857382	97.1396	92037	96.5690



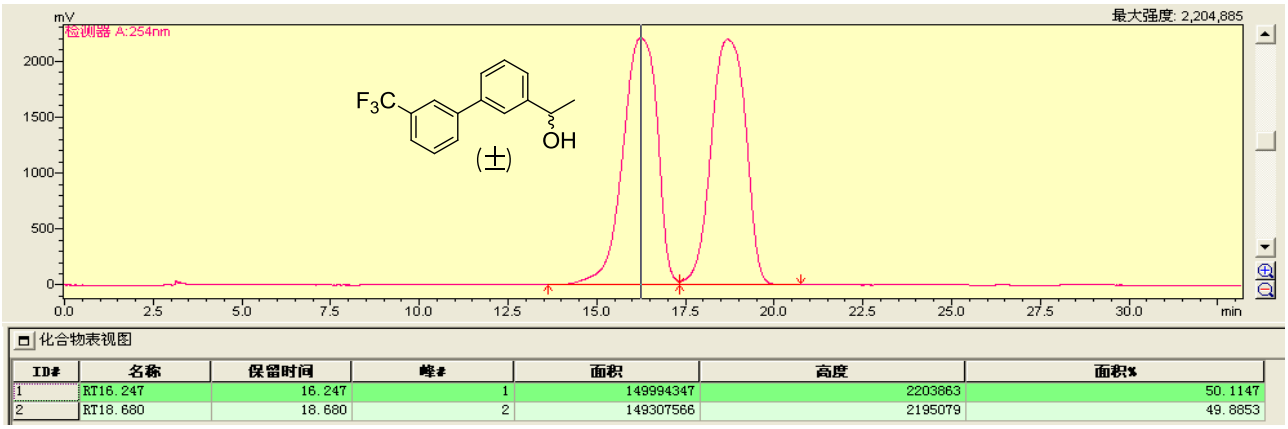
化合物表视图

ID#	名称	保留时间	峰#	面积	面积%	高度	高度%
1	RT22.500	22.500	1	2069826	5.7287	46868	8.1530
2	RT24.791	24.791	2	34060746	94.2713	527988	91.8470

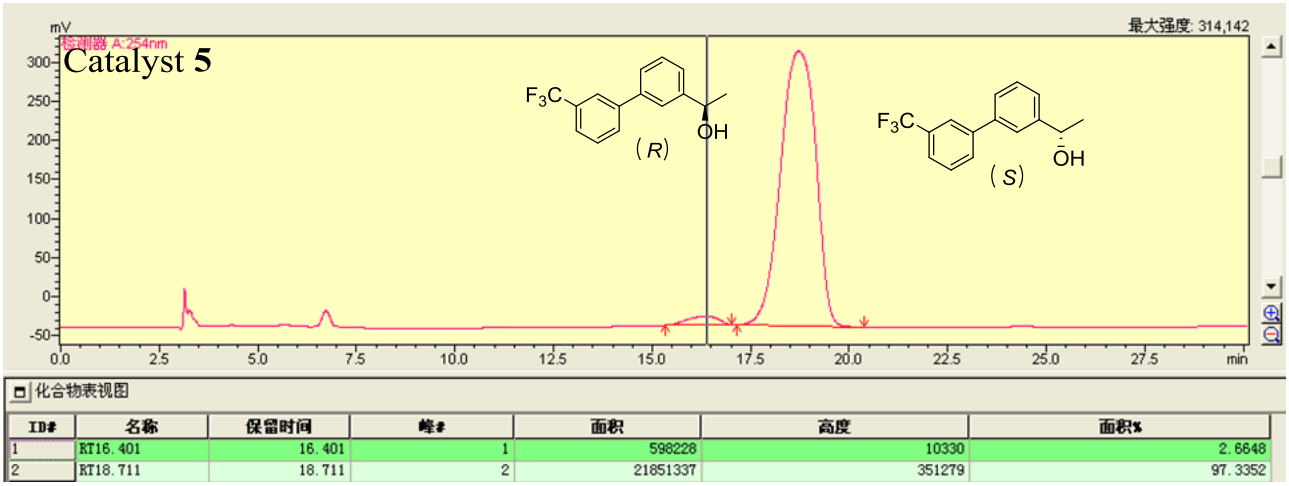


ID#	名称	保留时间	峰#	面积	面积%	高度	高度%
1	RT17.882	17.882	1	54328391	49.7262	1285639	50.7716

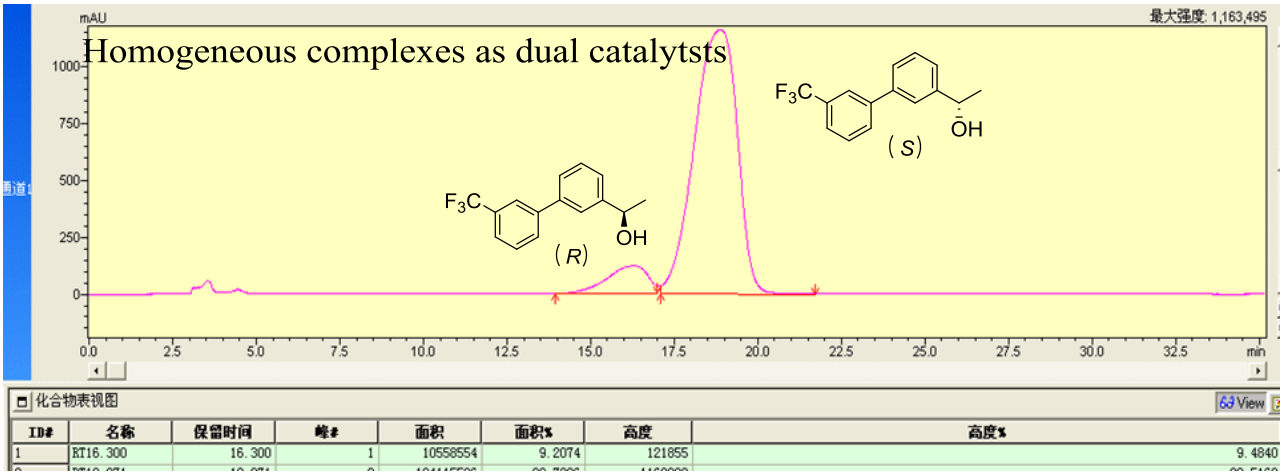
(*S*)−1−(3−(3−trifluouomethyl)phenyl)ethanol (8k): (HPLC: Chiracel AD−H, detected at 254 nm, eluent: n−hexane/2−propanol = 97/3, flow rate = 1.0 mL/min, 25 ℃).



ID#	名称	保留时间	峰#	面积	高度	面积%
1	RT16.247	16.247	1	149994347	2203863	50.1147
2	RT18.680	18.680	2	149307566	2195079	49.8853



ID#	名称	保留时间	峰#	面积	高度	面积%
1	RT16.401	16.401	1	598228	10330	2.6648
2	RT18.711	18.711	2	21851337	351279	97.3352

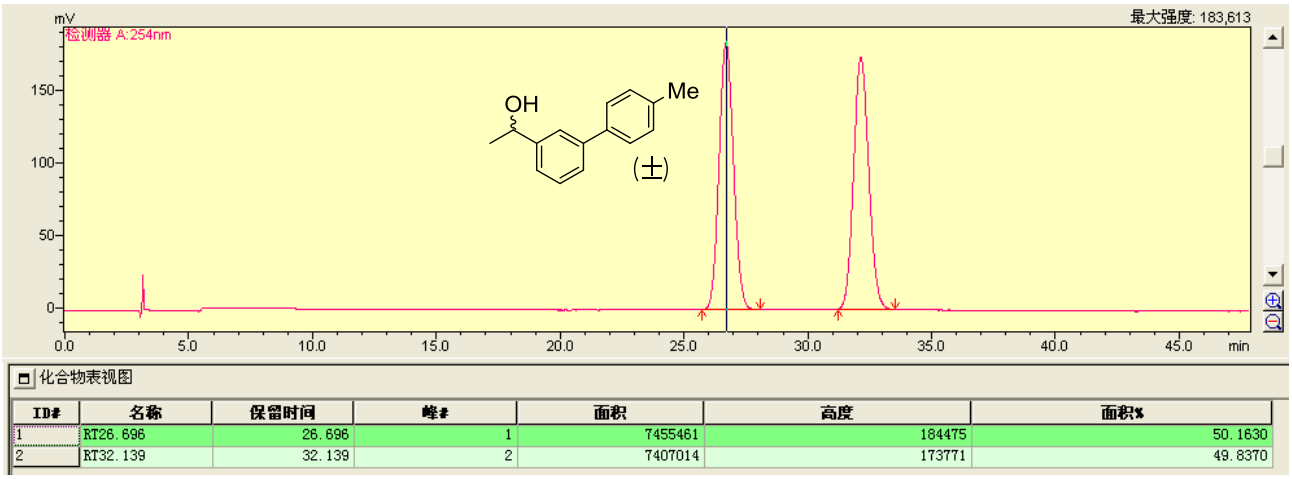


ID#	名称	保留时间	峰#	面积	面积%	高度	高度%
1	RT16.300	16.300	1	10558554	9.2074	121855	9.4840

Name RetTime [min] Peak Area Heighth Area ratio %

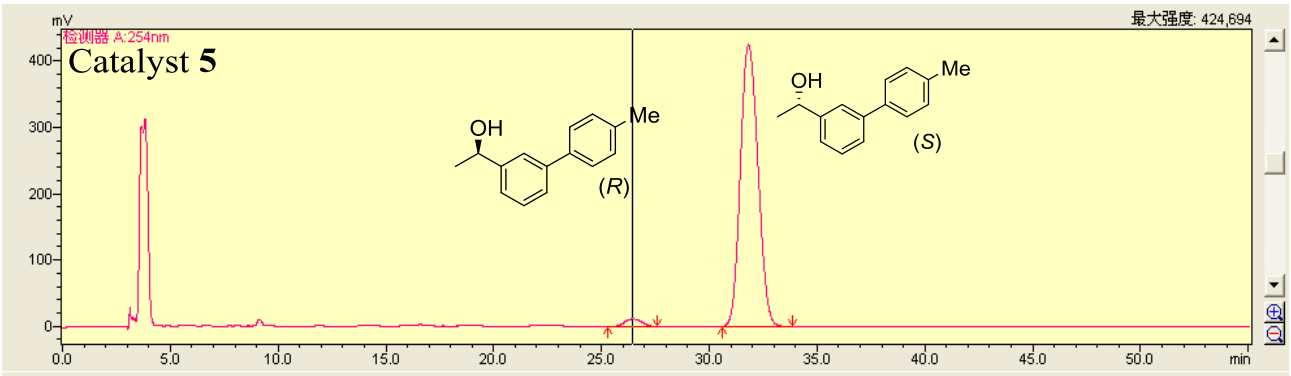
ID#	名称	保留时间	峰#	面积	高度	面积%
1	RT27.188	27.188	1	6691012	167689	96.5063
2	RT31.439	31.439	2	242226	5230	3.4937

(*S*)−1−(3−(4−methyl)phenyl)ethanol (8l): (HPLC: Chiracel AD−H, detected at 254 nm, eluent: n−hexane/2−propanol = 97/3, flow rate = 1.0 mL/min, 25 ℃).



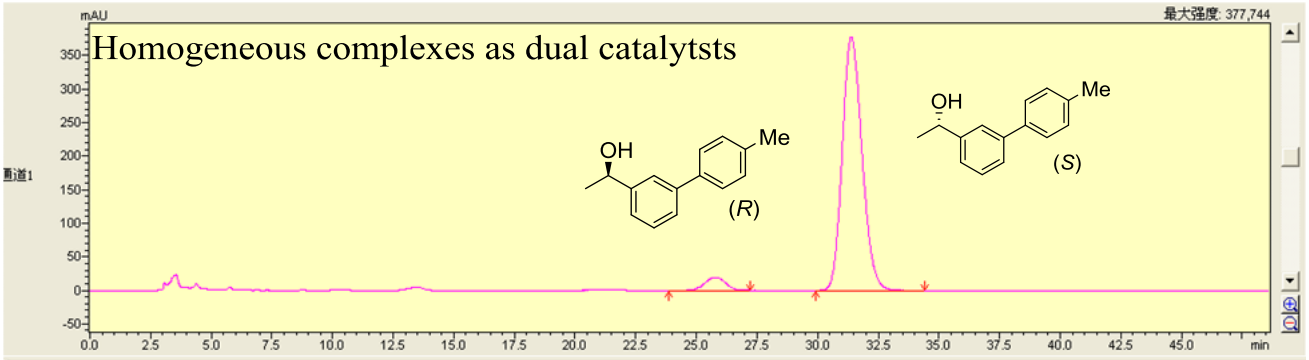
化合物表视图

ID#	名称	保留时间	峰#	面积	高度	面积%
1	RT26.696	26.696	1	7455461	184475	50.1630
2	RT32.139	32.139	2	7407014	173771	49.8370



化合物表视图

ID#	名称	保留时间	峰#	面积	高度	面积%
1	RT26.451	26.451	1	654614	11486	2.6465
2	RT31.818	31.818	2	24080451	424948	97.3535



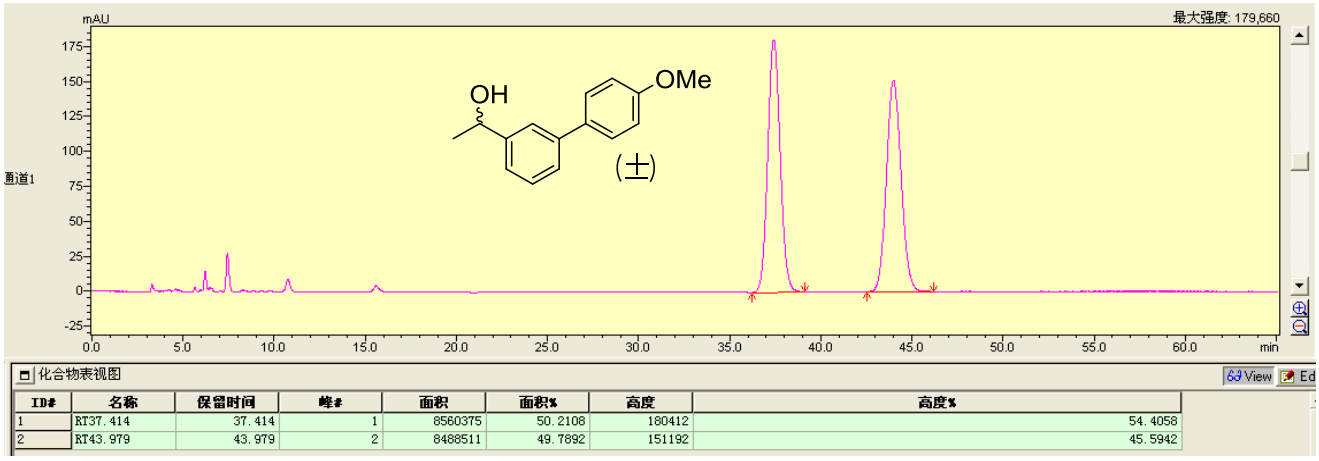
化合物表视图

ID#	名称	保留时间	峰#	面积	面积%	高度	高度%
1	RT25.787	25.787	1	1148457	5.0953	19521	4.9119
2	RT31.386	31.386	2	21390924	94.9047	377907	95.0881

Name | RetTime [min] | Peak | Area | Heighth | Area ratio %

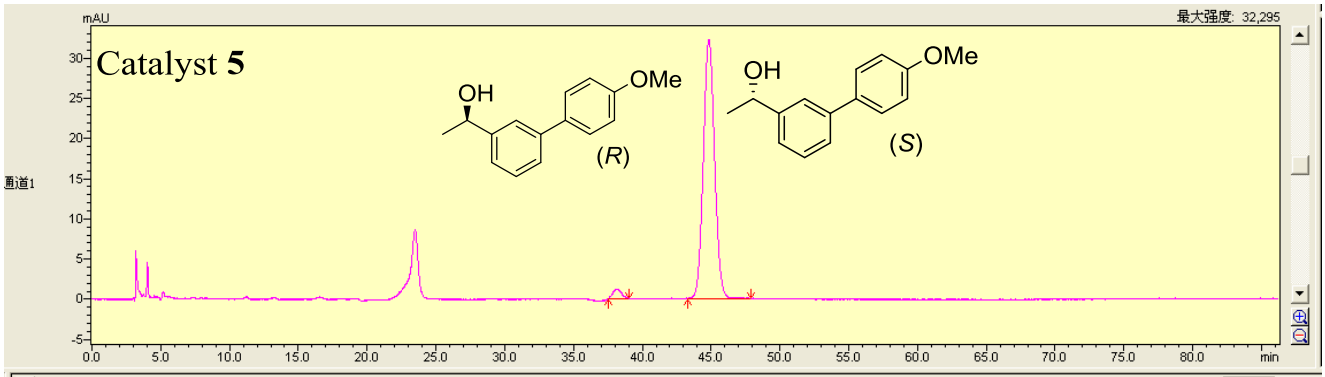
ID#	名称	保留时间	峰#	面积	高度	面积%
1	RT27.188	27.188	1	6691012	167689	96.5063
2	RT31.439	31.439	2	242226	5230	3.4937

(*S*)−1−(3−(4−methoxy)phenyl)ethanol (8m): (HPLC: Chiracel AD−H, detected at 254 nm, eluent: n−hexane/2−propanol = 97/3, flow rate = 1.0 mL/min, 25 ℃).



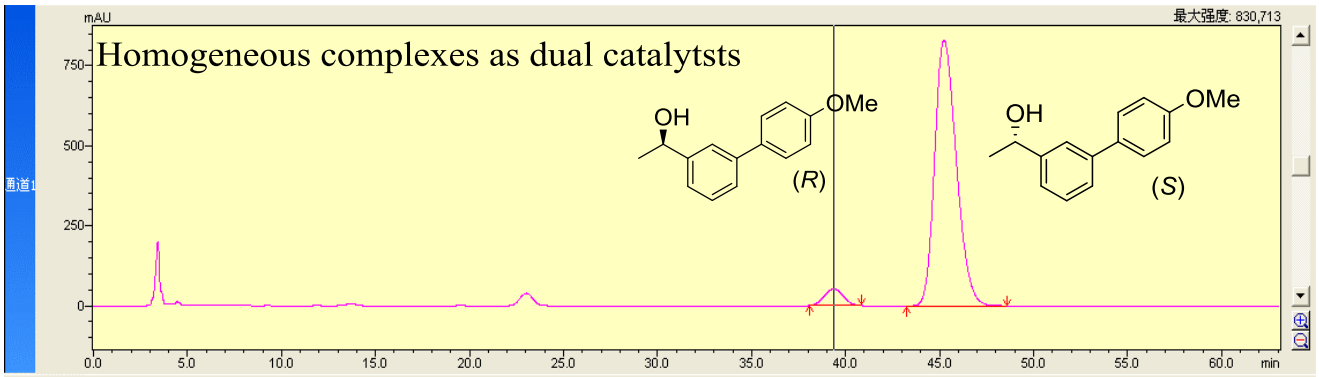
化合物表视图

ID#	名称	保留时间	峰#	面积	面积%	高度	高度%
1	RT37.414	37.414	1	8560375	50.2108	180412	54.4058
2	RT43.979	43.979	2	8488511	49.7892	151192	45.5942



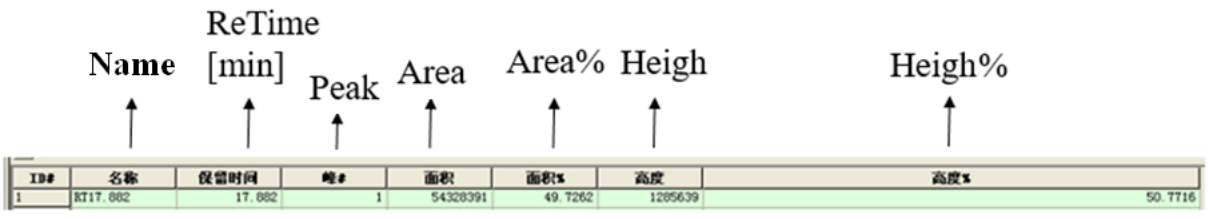
化合物表视图

ID#	名称	保留时间	峰#	面积	面积%	高度	高度%
1	RT38.149	38.149	1	47494	2.5252	1131	3.3909
2	RT44.827	44.827	2	1833329	97.4748	32210	96.6091



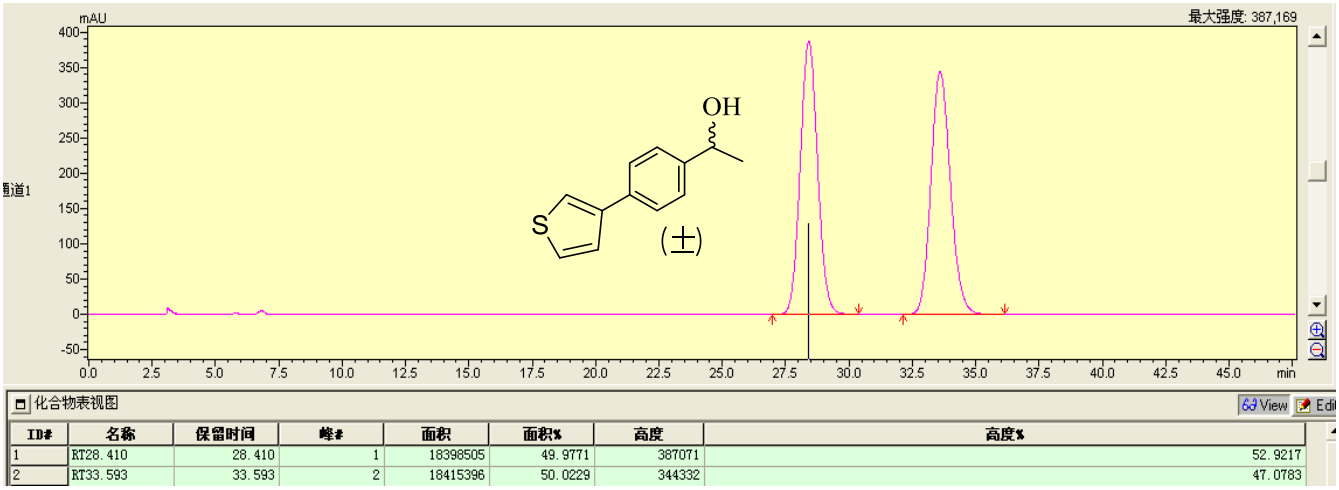
化合物表视图

ID#	名称	保留时间	峰#	面积	面积%	高度	高度%
1	RT39.374	39.374	1	3667757	5.2051	52269	5.9185
2	RT45.227	45.227	2	66796465	94.7949	830881	94.0815



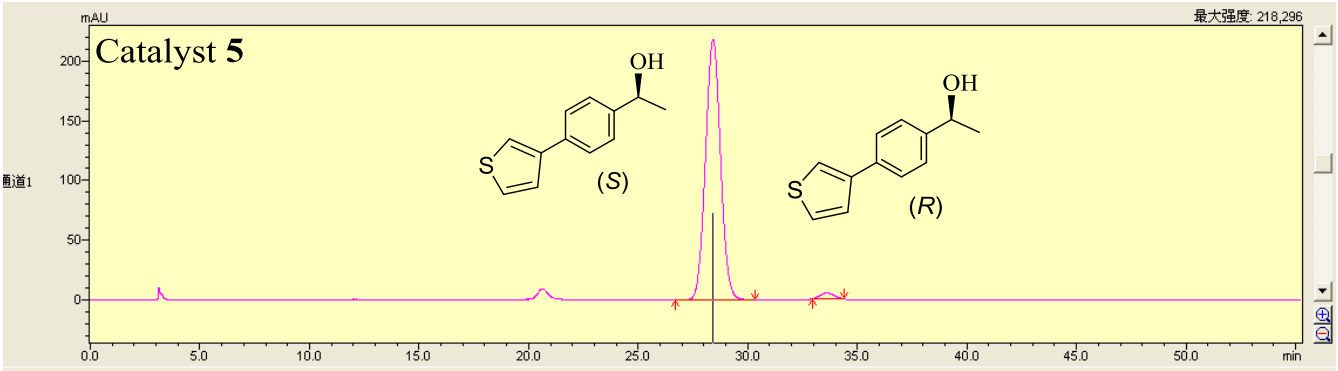
ID#	名称	保留时间	峰#	面积	面积%	高度	高度%
1	RT17.882	17.882	1	54328391	49.7262	1285639	50.7716

(*S*)−1−(4−(thiophen−3−yl)phenyl)ethanol (8n): (HPLC: Chiracel AD−H, detected at 254 nm, eluent: n−hexane/2−propanol = 97/3, flow rate = 1.0 mL/min, 25 ℃).



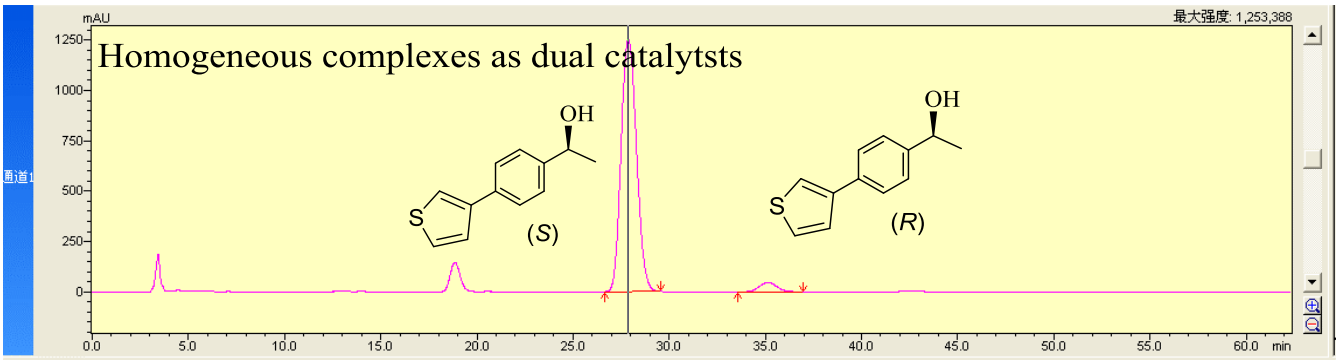
化合物表视图

ID#	名称	保留时间	峰#	面积	面积%	高度	高度%
1	RT28.410	28.410	1	18398505	49.9771	387071	52.9217
2	RT33.593	33.593	2	18415396	50.0229	344332	47.0783



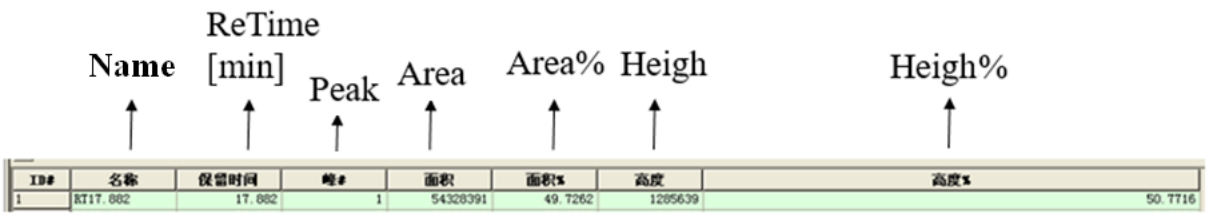
化合物表视图

ID#	名称	保留时间	峰#	面积	面积%	高度	高度%
1	RT28.411	28.411	1	10406591	97.9253	218269	97.7837
2	RT33.608	33.608	2	220477	2.0747	4947	2.2163



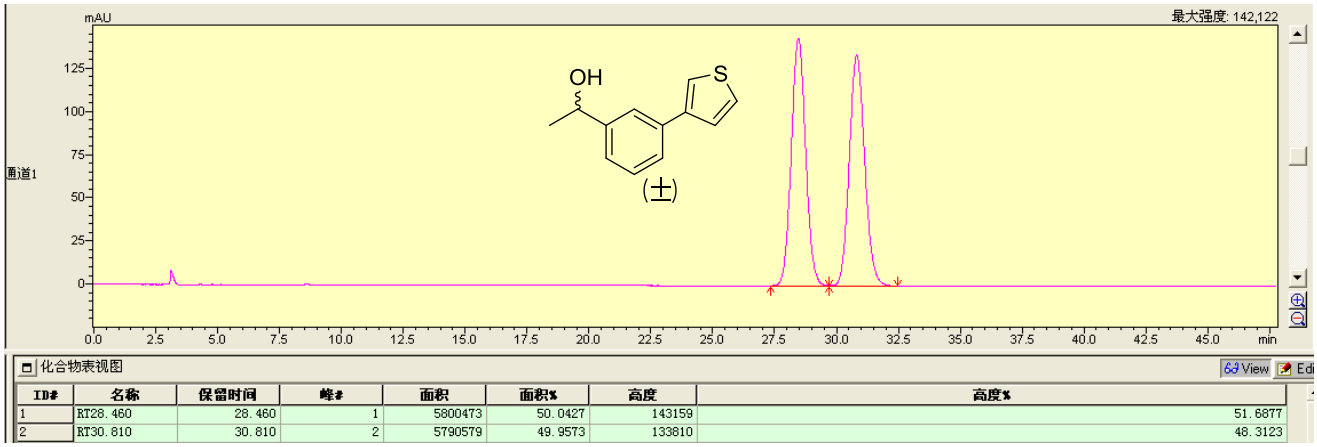
化合物表视图

ID#	名称	保留时间	峰#	面积	面积%	高度	高度%
1	RT27.876	27.876	1	69936671	96.0144	1252319	96.5256
2	RT35.126	35.126	2	2903139	3.9856	45077	3.4744



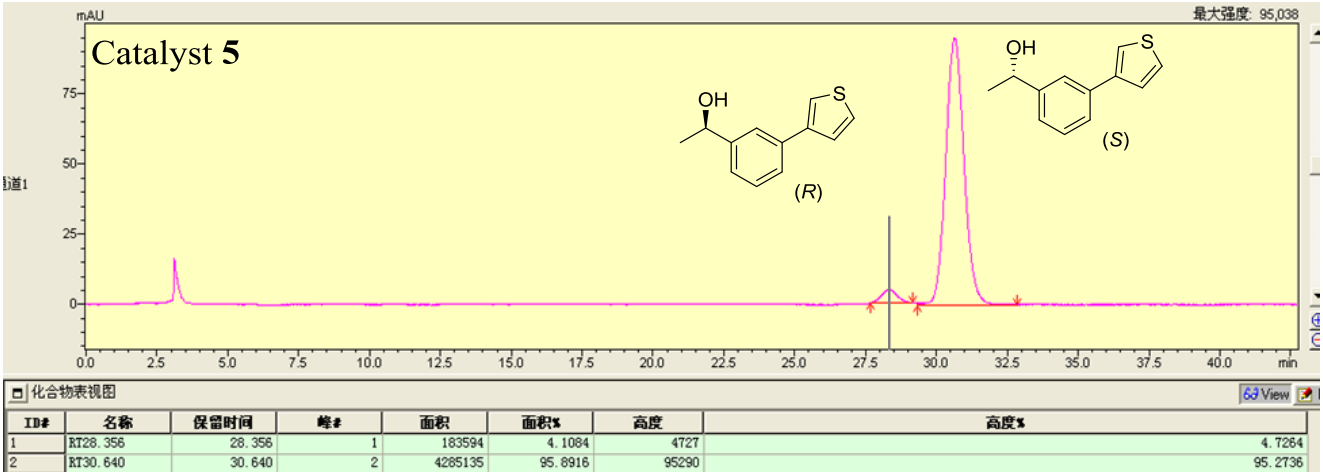
ID#	名称	保留时间	峰#	面积	面积%	高度	高度%
1	RT17.882	17.882	1	54328391	49.7262	1285639	50.7716

(*S*)−1−(3−(thiophen−3−yl)phenyl)ethanol (8o): (HPLC: Chiracel AD−H, detected at 254 nm, eluent: n−hexane/2−propanol = 97/3, flow rate = 1.0 mL/min, 25 ℃).



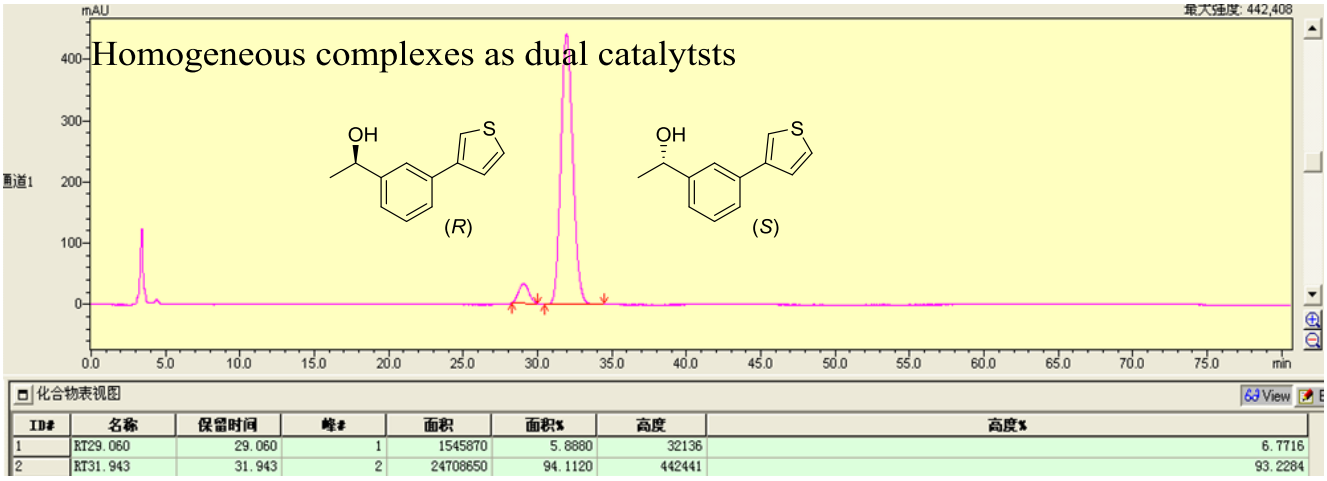
化合物表视图

ID#	名称	保留时间	峰#	面积	面积%	高度	高度%
1	RT28.460	28.460	1	5800473	50.0427	143159	51.6877
2	RT30.810	30.810	2	5790579	49.9573	133810	48.3123



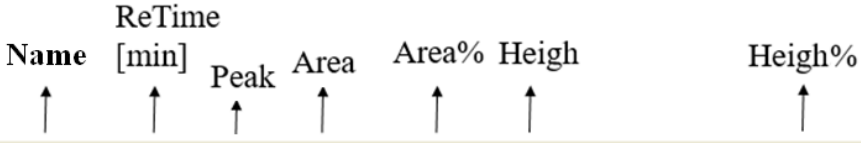
化合物表视图

ID#	名称	保留时间	峰#	面积	面积%	高度	高度%
1	RT28.356	28.356	1	183594	4.1084	4727	4.7264
2	RT30.640	30.640	2	4285135	95.8916	95290	95.2736



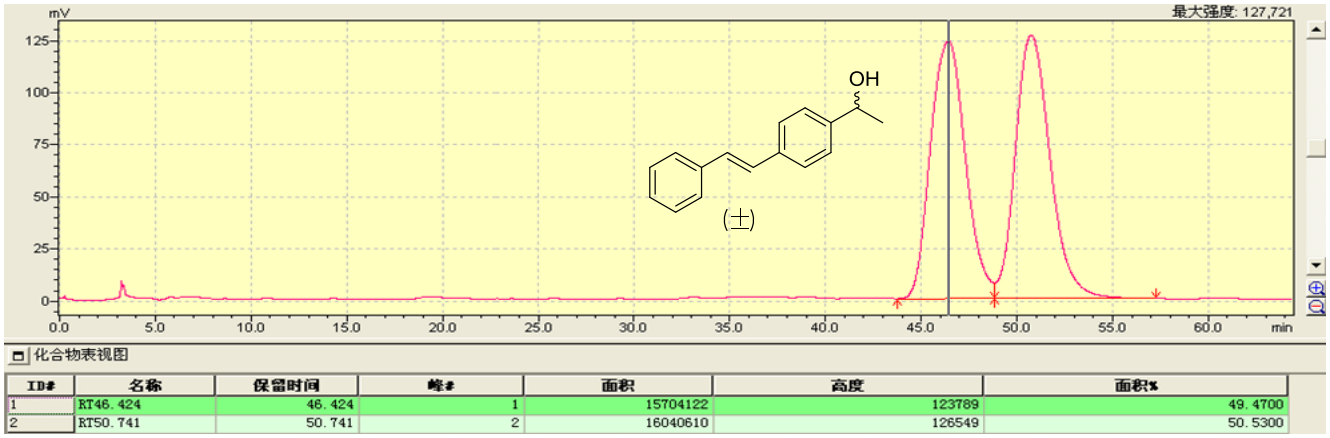
化合物表视图

ID#	名称	保留时间	峰#	面积	面积%	高度	高度%
1	RT29.060	29.060	1	1545870	5.8880	32136	6.7716
2	RT31.943	31.943	2	24708650	94.1120	442441	93.2284



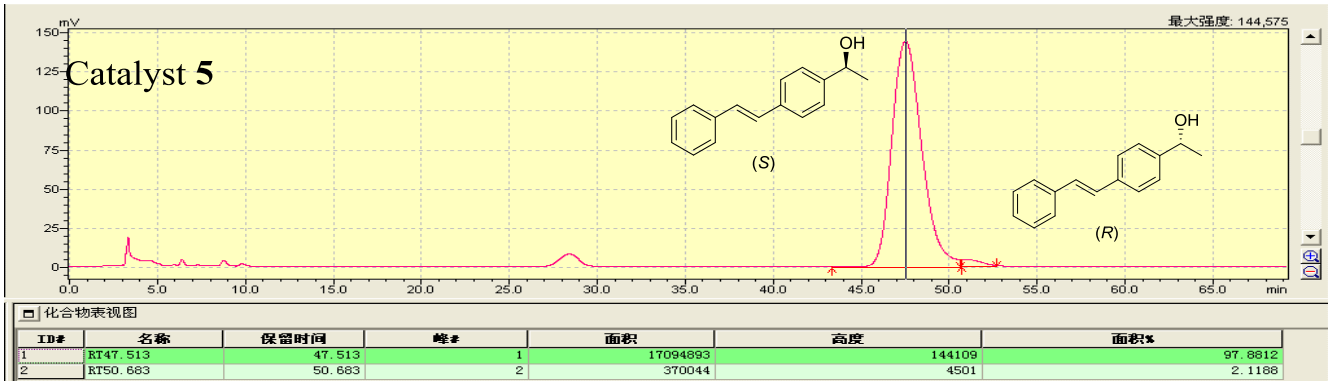
ID#	名称	保留时间	峰#	面积	面积%	高度	高度%
1	RT17.882	17.882	1	54328391	49.7262	1285639	50.7716

(*S*,*E*)−1−(4−styrylphenyl)ethanol (8p): (HPLC: Chiracel AD−H, detected at 254 nm, eluent: n−hexane/2−propanol = 98.5/1.5, flow rate = 1.0 mL/min, 25 ℃).



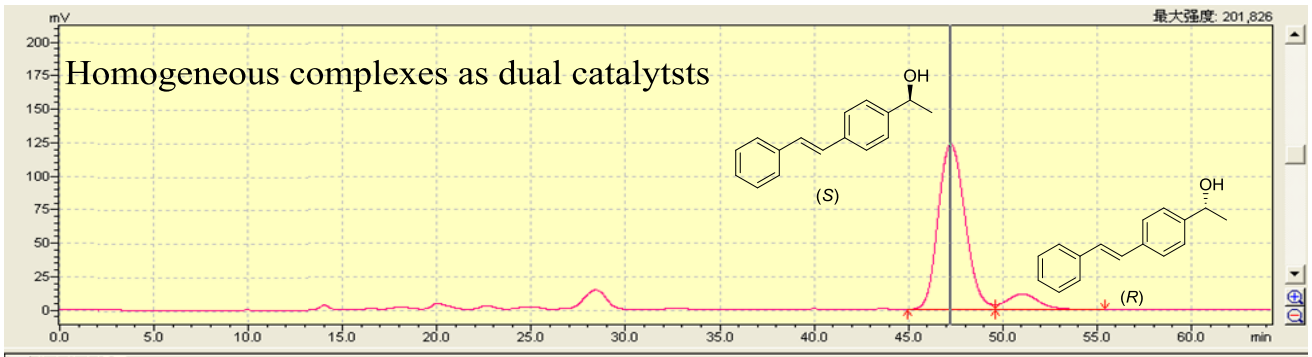
化合物表视图

ID#	名称	保留时间	峰#	面积	高度	面积%
1	RT46.424	46.424	1	15704122	123789	49.4700
2	RT50.741	50.741	2	16040610	126549	50.5300



化合物表视图

ID#	名称	保留时间	峰#	面积	高度	面积%
1	RT47.513	47.513	1	17094893	144109	97.8812
2	RT50.683	50.683	2	370044	4501	2.1188



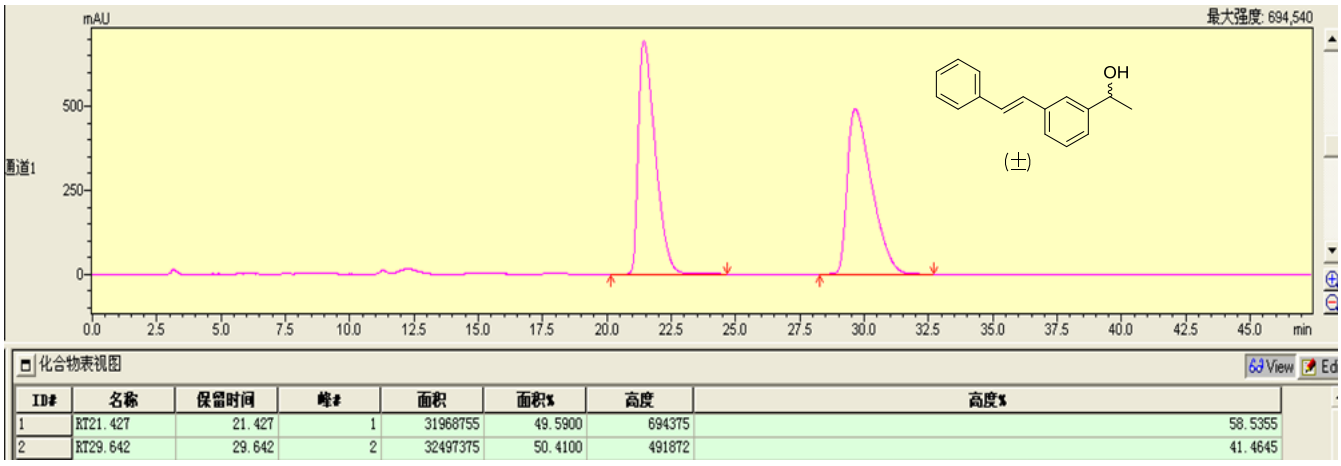
化合物表视图

ID#	名称	保留时间	峰#	面积	高度	面积%
1	RT47.245	47.245	1	12261794	123462	89.8300
2	RT51.046	51.046	2	1388207	11592	10.1700

Name RetTime [min] Peak Area Heighth Area ratio %

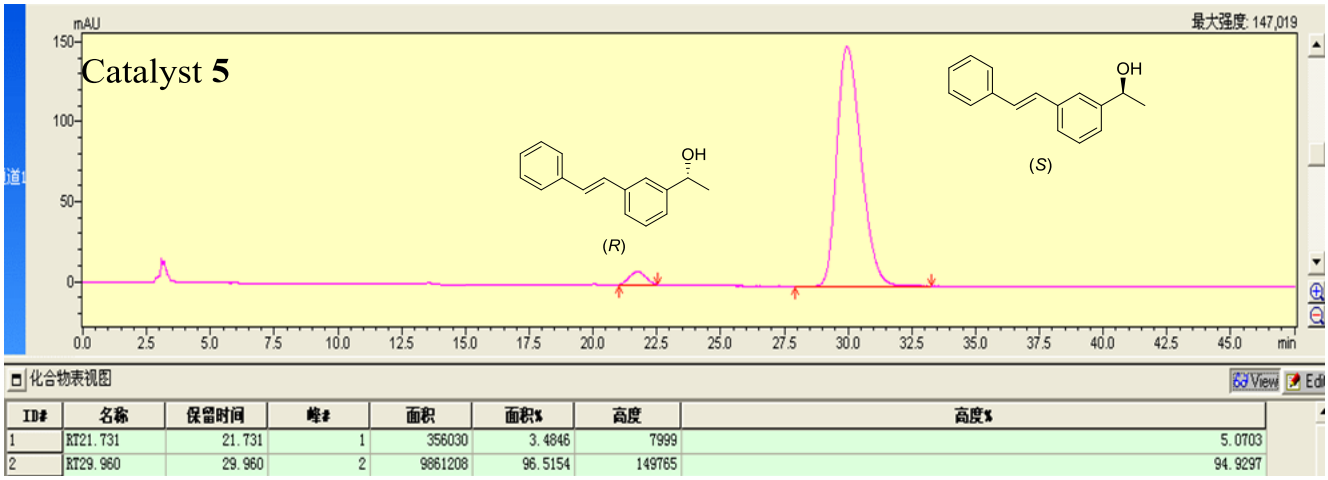
ID#	名称	保留时间	峰#	面积	高度	面积%
1	RT27.188	27.188	1	6691012	167689	96.5063
2	RT31.439	31.439	2	242226	5230	3.4937

(*S*,*E*)−1−(3−styrylphenyl)ethanol (8q): (HPLC: Chiracel OD−H, detected at 254 nm, eluent: n−hexane/2−propanol = 97/3, flow rate = 1.0 mL/min, 25 ℃).



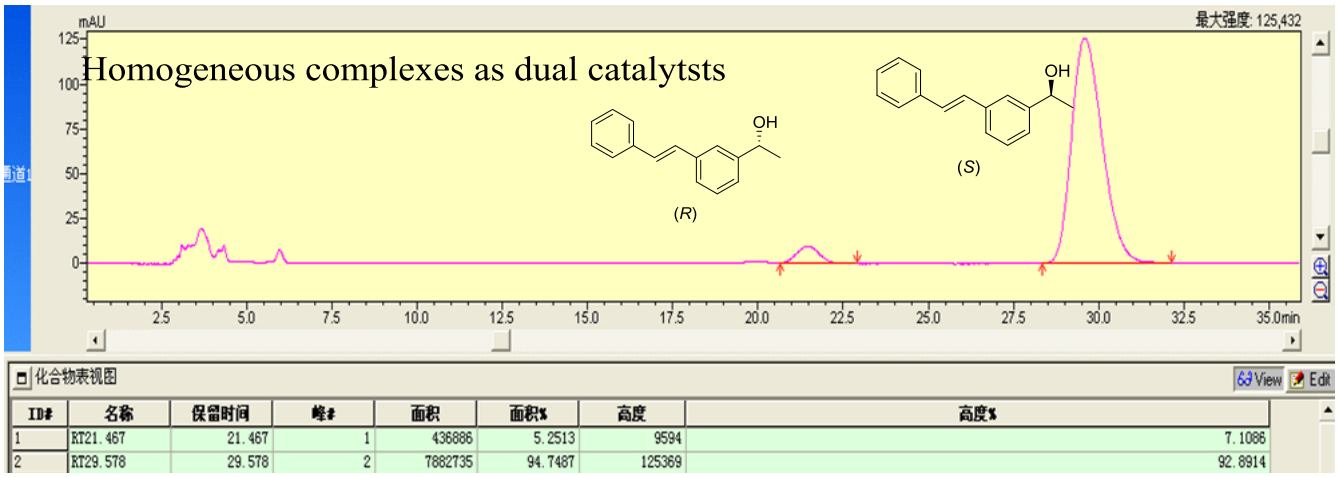
化合物表视图

ID#	名称	保留时间	峰#	面积	面积%	高度	高度%
1	RT21.427	21.427	1	31968755	49.5900	694375	58.5355
2	RT29.642	29.642	2	32497375	50.4100	491872	41.4645



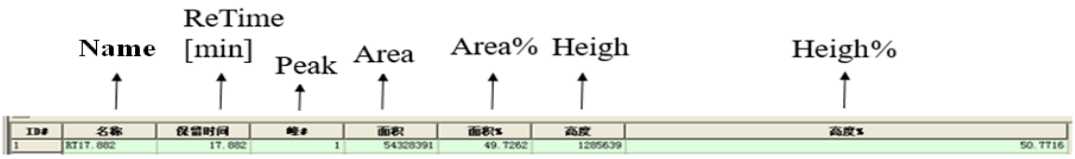
化合物表视图

ID#	名称	保留时间	峰#	面积	面积%	高度	高度%
1	RT21.731	21.731	1	356030	3.4846	7999	5.0703
2	RT29.960	29.960	2	9861208	96.5154	149765	94.9297

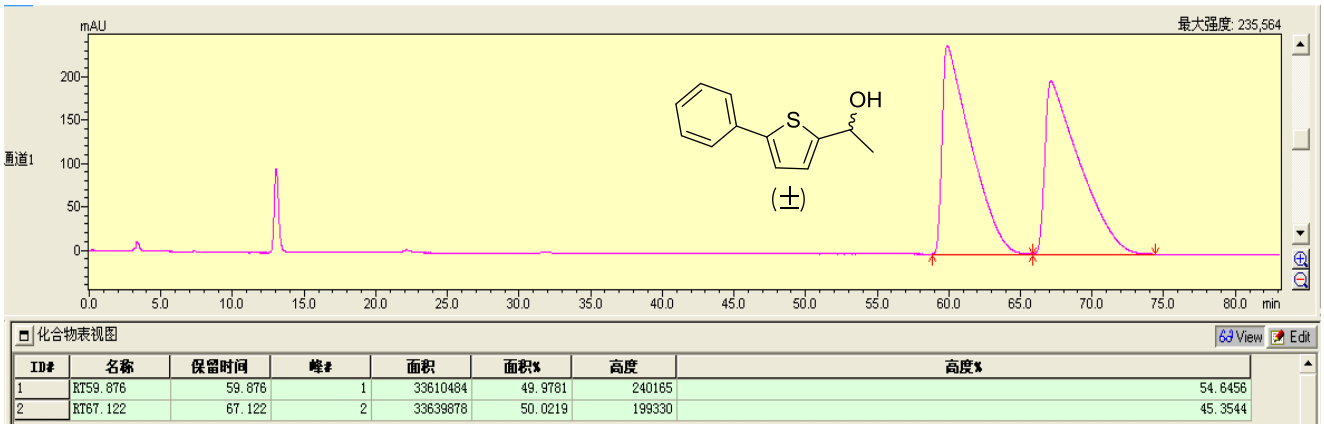


化合物表视图

ID#	名称	保留时间	峰#	面积	面积%	高度	高度%
1	RT21.467	21.467	1	436886	5.2513	9594	7.1086
2	RT29.578	29.578	2	7882735	94.7487	125369	92.8914

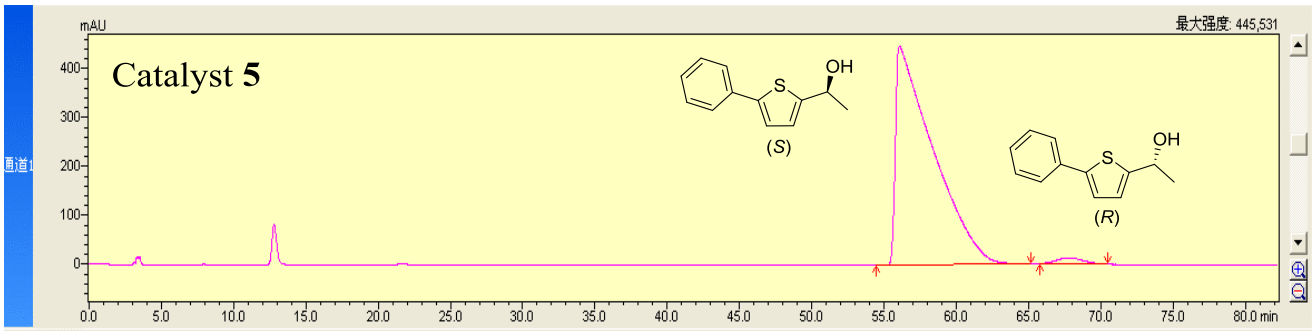


(*S*)−1−(5−phenylthiophen−2−yl)ethanol (8r): (HPLC: Chiracel OB−H, detected at 254 nm, eluent: n−hexane/2−propanol = 98/2, flow rate = 1.0 mL/min, 25 ℃).



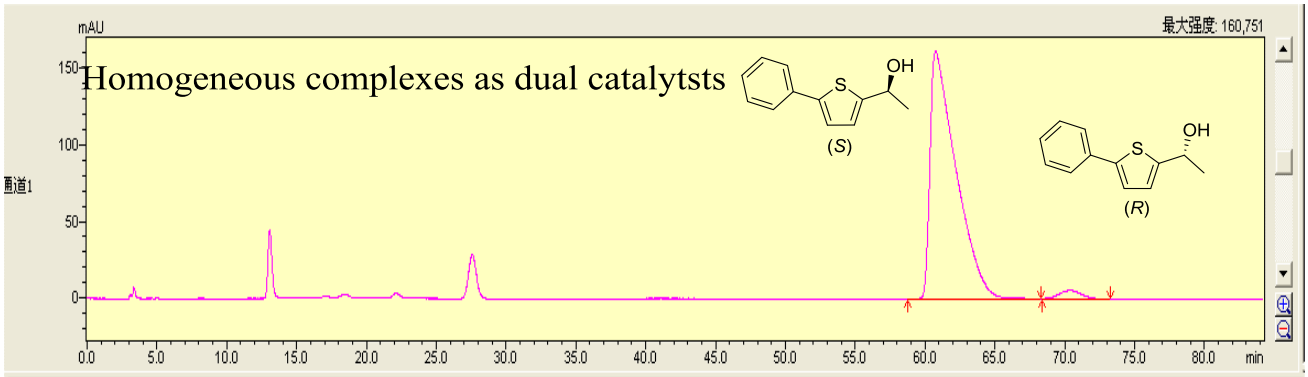
化合物表视图

ID#	名称	保留时间	峰#	面积	面积%	高度	高度%
1	RT59.876	59.876	1	33610484	49.9781	240165	54.6456
2	RT67.122	67.122	2	33639878	50.0219	199330	45.3544



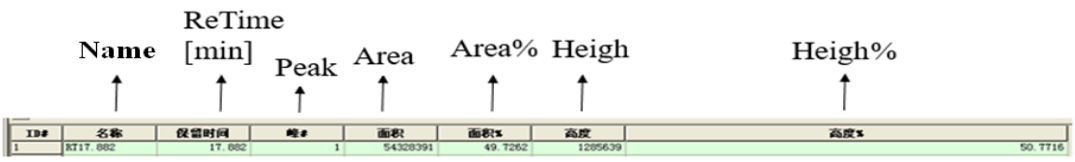
化合物表视图

ID#	名称	保留时间	峰#	面积	面积%	高度	高度%
1	RT56.067	56.067	1	80516696	98.0656	446437	97.3453
2	RT67.728	67.728	2	1588205	1.9344	12175	2.6547



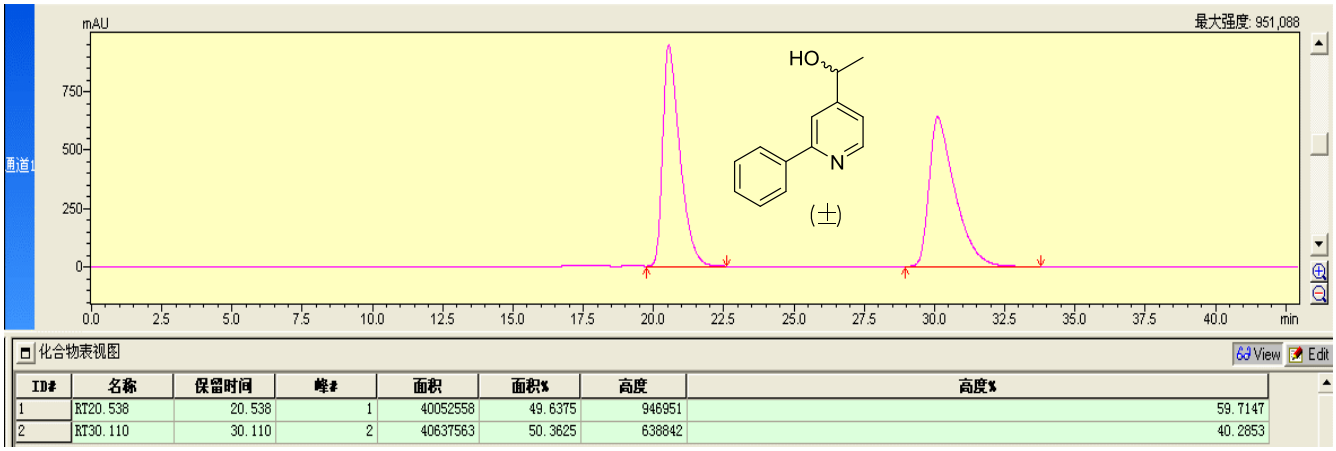
化合物表视图

ID#	名称	保留时间	峰#	面积	面积%	高度	高度%
1	RT60.752	60.752	1	20720954	97.1347	161141	96.6429
2	RT70.368	70.368	2	611228	2.8653	5598	3.3571



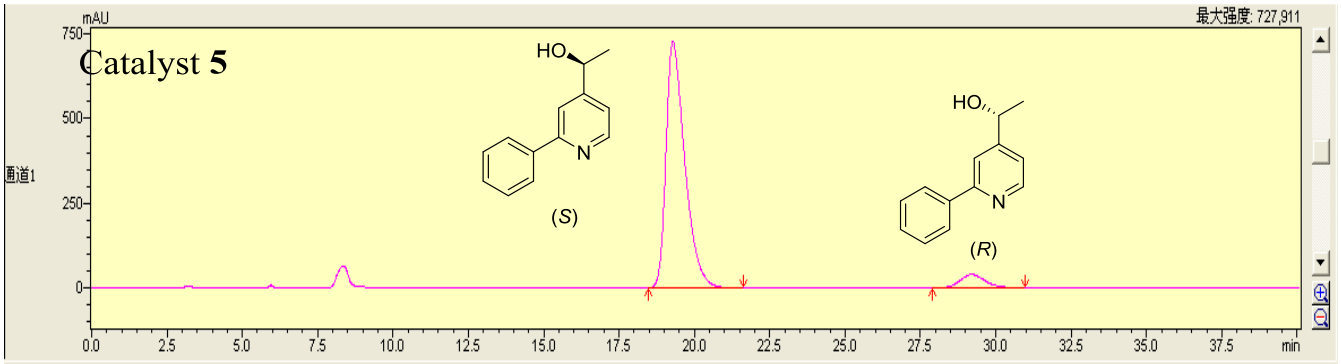
ID#	名称	保留时间	峰#	面积	面积%	高度	高度%
1	RT17.882	17.882	1	54328391	49.7262	1285639	50.7716

(*S*)−1−(2−phenylpyridin−4−yl)ethanol (8s): (HPLC: Chiracel OJ−H, detected at 254 nm, eluent: n−hexane/2−propanol = 90/10, flow rate = 1.0 mL/min, 25 ℃).



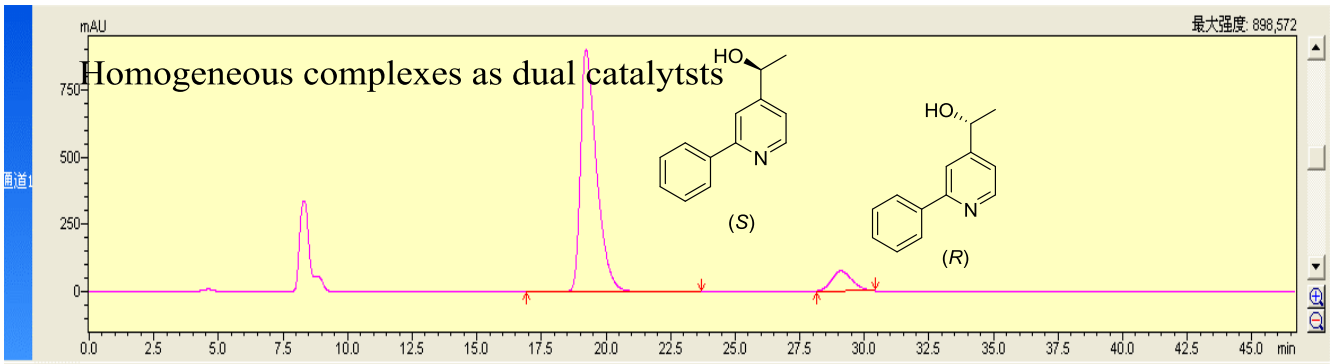
化合物表视图

ID#	名称	保留时间	峰#	面积	面积%	高度	高度%
1	RT20.538	20.538	1	40052558	49.6375	946951	59.7147
2	RT30.110	30.110	2	40637563	50.3625	638842	40.2853



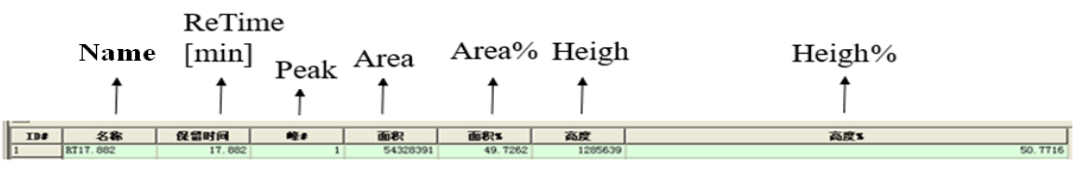
化合物表视图

ID#	名称	保留时间	峰#	面积	面积%	高度	高度%
1	RT19.282	19.282	1	31500227	93.0507	727229	94.7788
2	RT29.191	29.191	2	2352534	6.9493	40062	5.2212



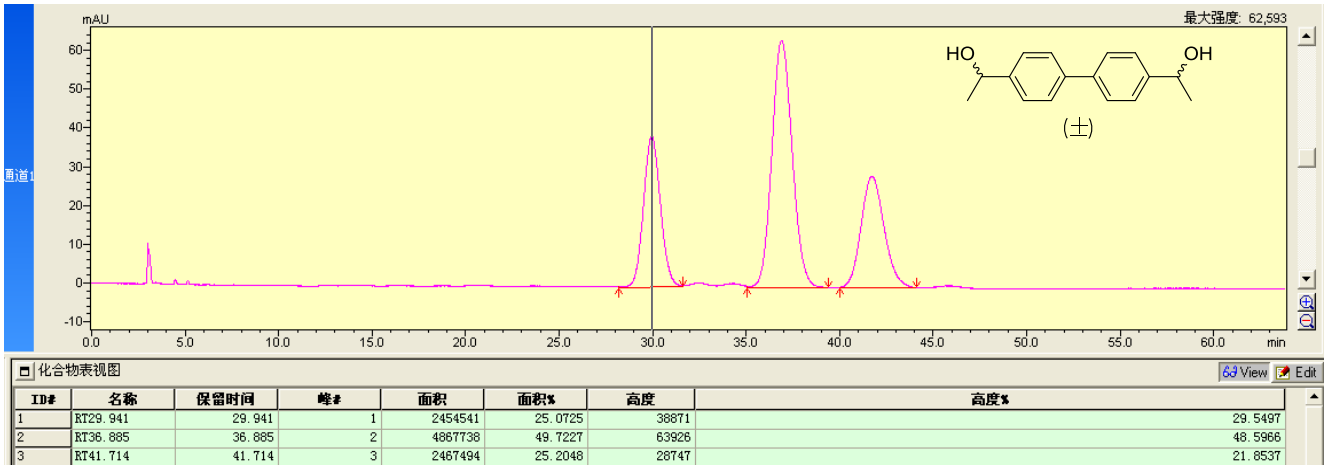
化合物表视图

ID#	名称	保留时间	峰#	面积	面积%	高度	高度%
1	RT19.225	19.225	1	38657841	90.4291	898010	92.3783
2	RT29.080	29.080	2	4091508	9.5709	74090	7.6217



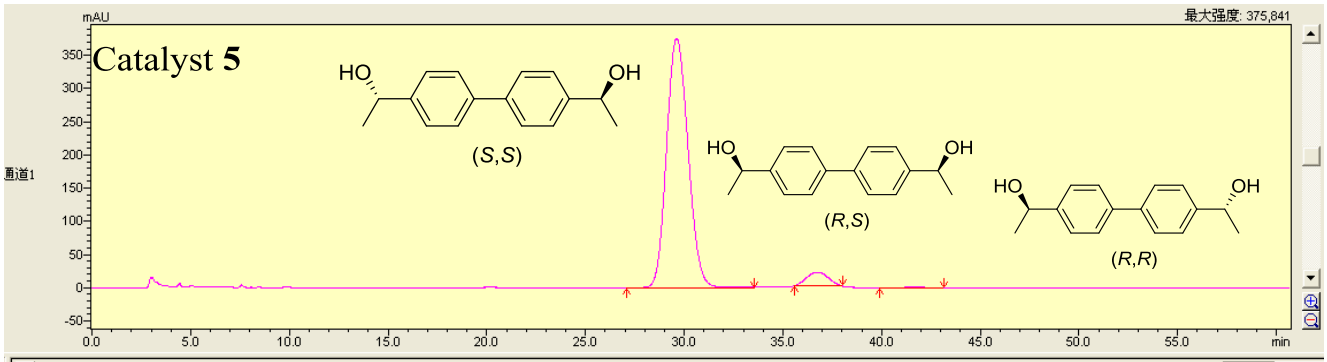
ID#	名称	保留时间	峰#	面积	面积%	高度	高度%
1	RT17.882	17.882	1	54328391	49.7262	1285639	50.7716

(*S*,*S*)−1,1'−([1,1'−biphenyl]−4,4'−diyl)diethanol (8t): (HPLC: Chiracel AD−H, detected at 254 nm, eluent: n−hexane/2−propanol = 92.5/7.5, flow rate = 1.0 mL/min, 25 ℃).



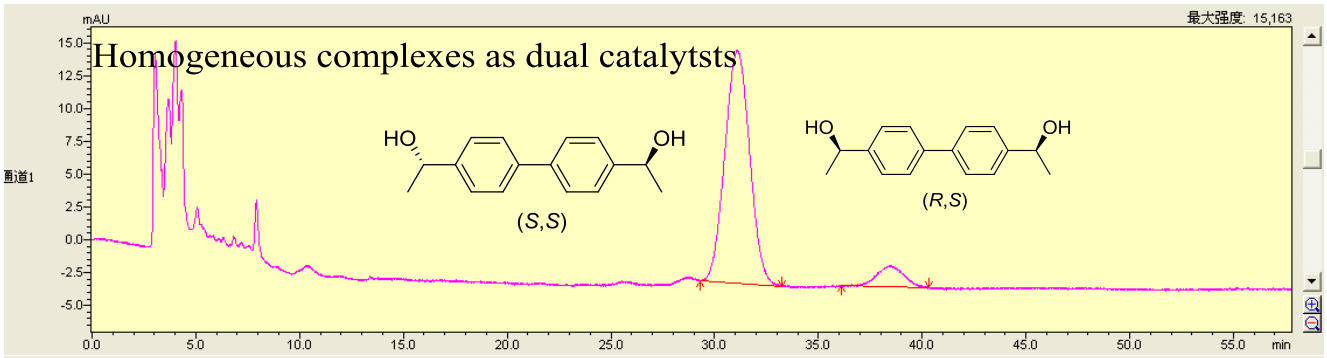
化合物表视图

ID#	名称	保留时间	峰#	面积	面积%	高度	高度%
1	RT29.941	29.941	1	2454541	25.0725	38871	29.5497
2	RT36.885	36.885	2	4867738	49.7227	63926	48.5966
3	RT41.714	41.714	3	2467494	25.2048	28747	21.8537



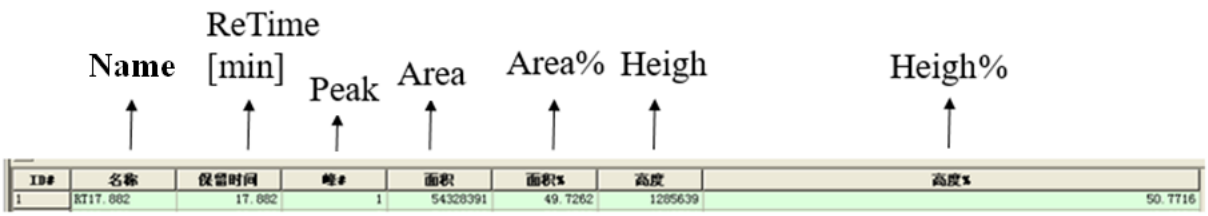
化合物表视图

ID#	名称	保留时间	峰#	面积	面积%	高度	高度%
1	RT29.615	29.615	1	28559029	94.5063	375885	94.5995
2	RT36.752	36.752	2	1587955	5.2548	20852	5.2481
3	RT41.658	41.658	3	72201	0.2389	606	0.1524



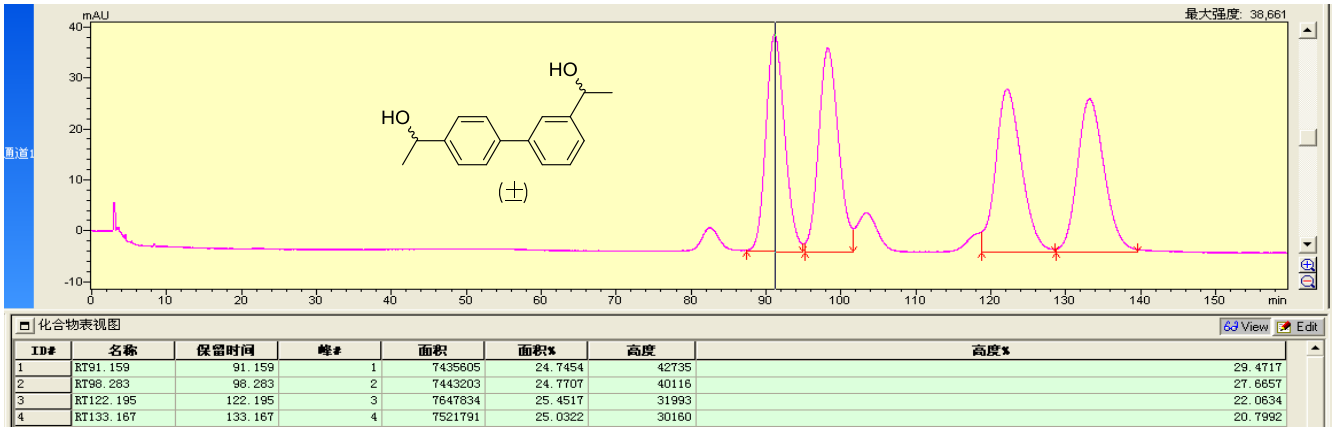
化合物表视图

ID#	名称	保留时间	峰#	面积	面积%	高度	高度%
1	RT31.096	31.096	1	1476876	91.1407	17725	91.5822
2	RT38.514	38.514	2	143559	8.8593	1629	8.4178



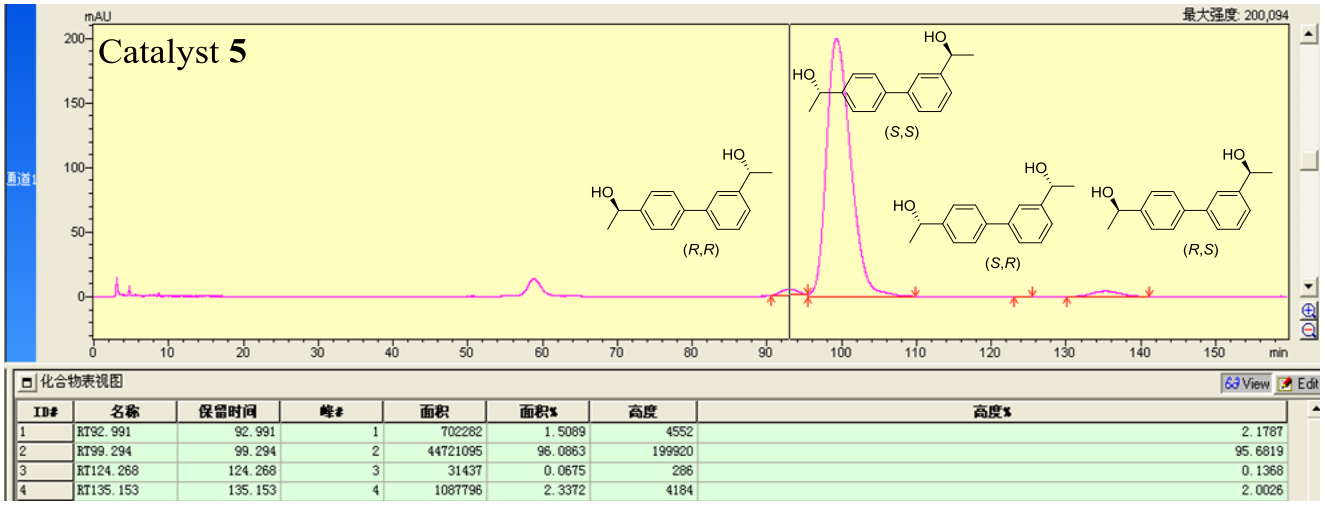
ID#	名称	保留时间	峰#	面积	面积%	高度	高度%
1	RT17.882	17.882	1	5432839	49.7262	1285639	50.7716

(*S*,*S*)−1,1'−([1,1'−biphenyl]−3,4'−diyl)diethanol (8u): (HPLC: Chiracel AD−H, detected at 254 nm, eluent: n−hexane/2−propanol = 96/4, flow rate = 1.0 mL/min, 25 ℃).



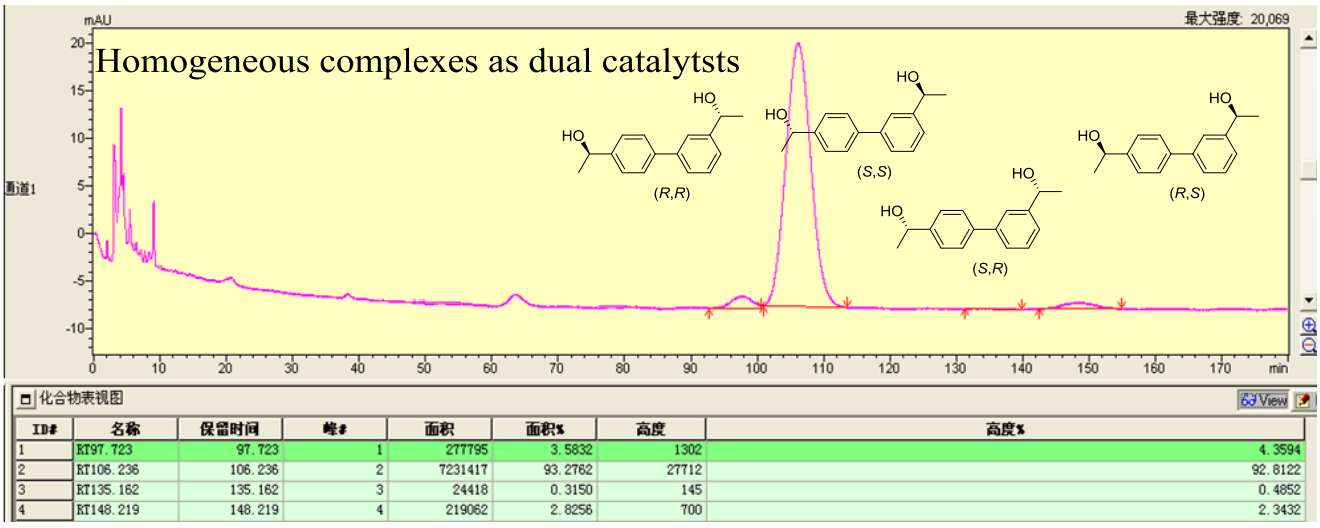
化合物表视图

ID#	名称	保留时间	峰#	面积	面积%	高度	高度%
1	RT91.159	91.159	1	7435605	24.7454	42735	29.4717
2	RT98.283	98.283	2	7443203	24.7707	40116	27.6657
3	RT122.195	122.195	3	7647834	25.4517	31993	22.0634
4	RT133.167	133.167	4	7521791	25.0322	30160	20.7992



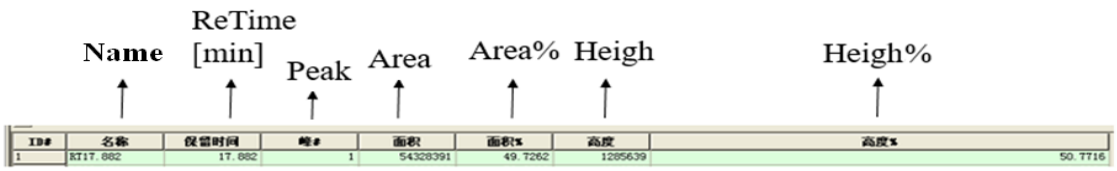
化合物表视图

ID#	名称	保留时间	峰#	面积	面积%	高度	高度%
1	RT92.991	92.991	1	702282	1.5089	4552	2.1787
2	RT99.294	99.294	2	44721095	96.0863	199920	95.6819
3	RT124.268	124.268	3	31437	0.0675	286	0.1368
4	RT135.153	135.153	4	1087796	2.3372	4184	2.0026



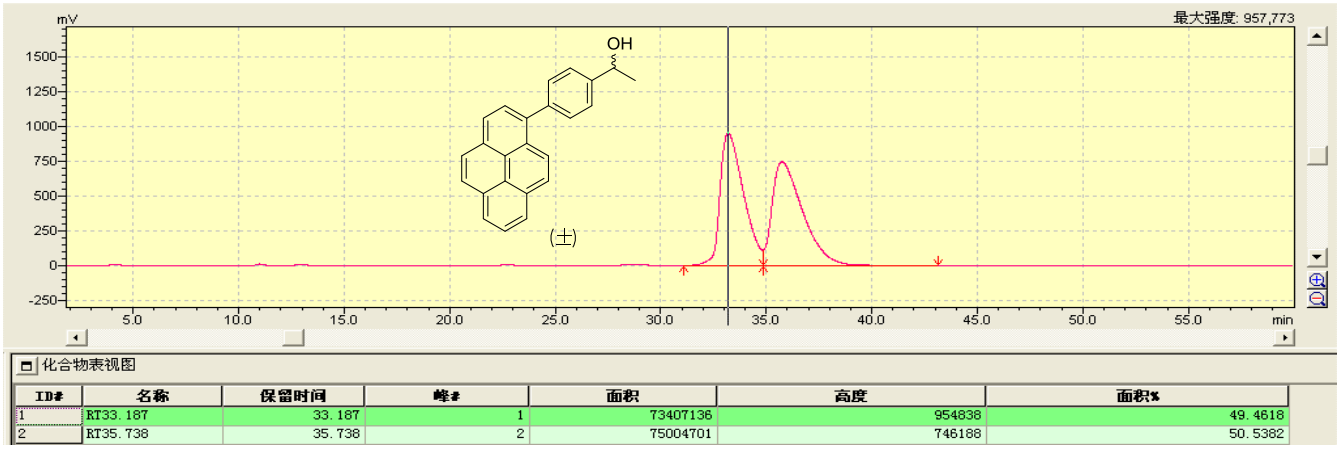
化合物表视图

ID#	名称	保留时间	峰#	面积	面积%	高度	高度%
1	RT97.723	97.723	1	277795	3.5832	1302	4.3594
2	RT106.236	106.236	2	7231417	93.2762	27712	92.8122
3	RT135.162	135.162	3	24418	0.3150	145	0.4852
4	RT148.219	148.219	4	219062	2.8256	700	2.3432



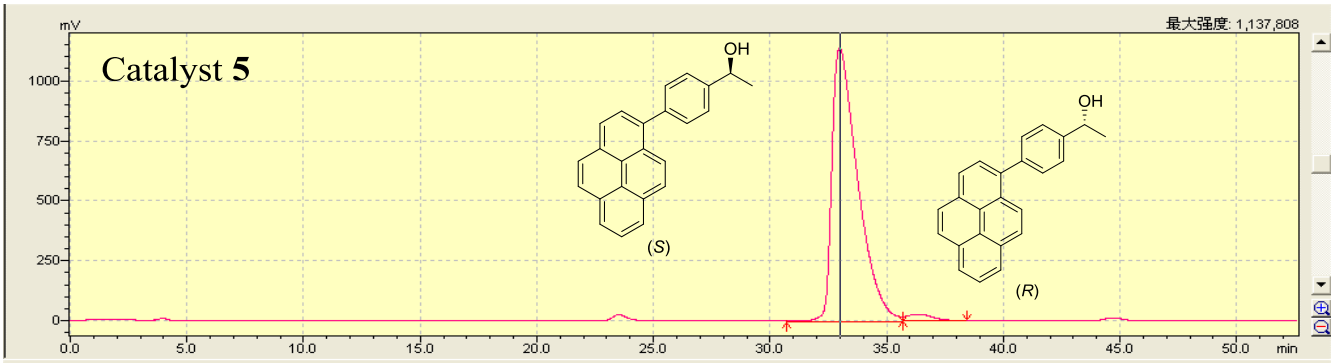
ID#	名称	保留时间	峰#	面积	面积%	高度	高度%
1	RT17.882	17.882	1	54328391	49.7262	1285639	50.7716

(*S*)−1−(4−(pyren−1−yl)phenyl)ethanol (8v): (HPLC: Chiracel OD−H, detected at 254 nm, eluent: n−hexane/2−propanol = 97/3, flow rate = 0.8 mL/min, 25 ℃).



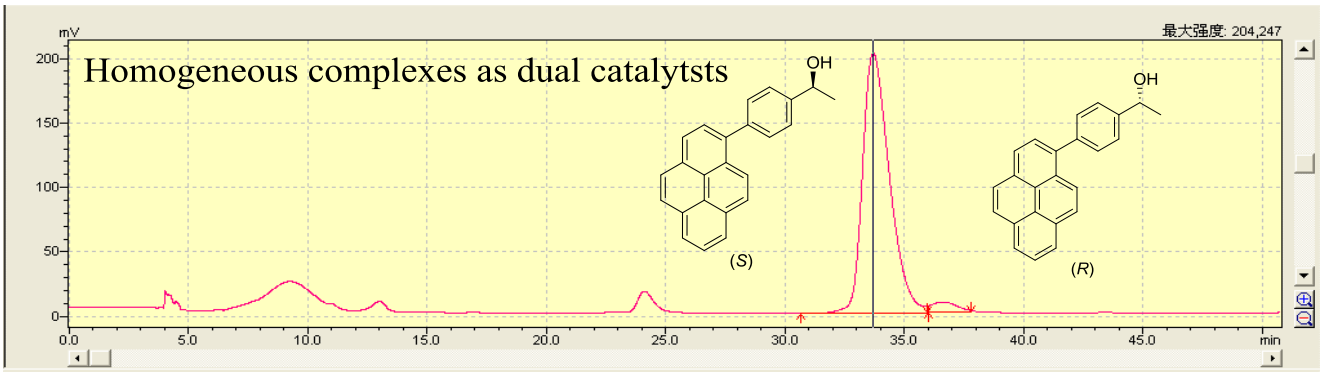
化合物表视图

ID#	名称	保留时间	峰#	面积	高度	面积%
1	RT33.187	33.187	1	73407136	954838	49.4618
2	RT35.738	35.738	2	75004701	746188	50.5382



化合物表视图

ID#	名称	保留时间	峰#	面积	高度	面积%
1	RT32.978	32.978	1	87776687	1139863	97.6482
2	RT36.340	36.340	2	2114036	26900	2.3518



化合物表视图

ID#	名称	保留时间	峰#	面积	高度	面积%
1	RT33.687	33.687	1	15910070	202084	96.4989
2	RT36.604	36.604	2	577236	7818	3.5011

ID#	名称	保留时间	峰#	面积	高度	面积%
1	RT27.188	27.188	1	6691012	167689	96.5063
2	RT31.439	31.439	2	242226	5230	3.4937

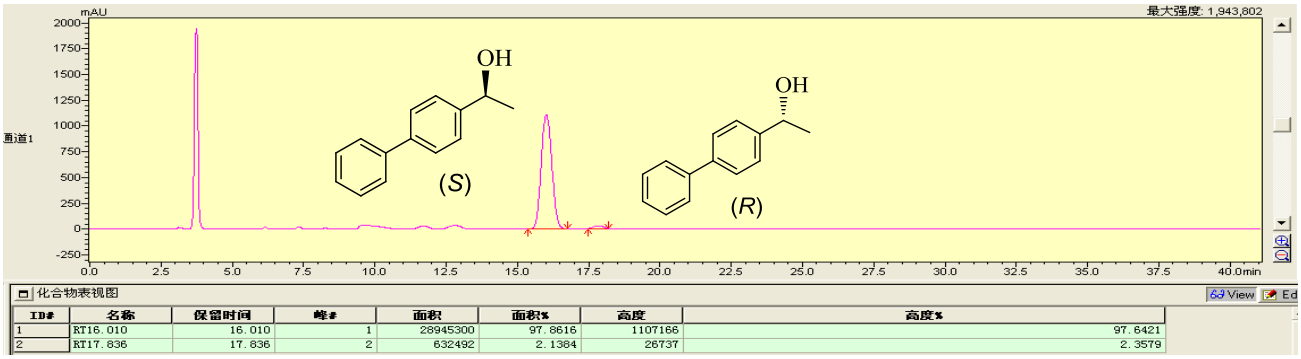
Table S2. Reusability of catalyst **5** in the Suzuki coupling–ATH of tandem reactions of 4−chloroacetophenone and phenylboronic acid.[a]

Entry	**1**	**2**	**3**	**4**	**5**	**6**	**7**	**8**
Yield [%]	97	96	94	95	93	92	87	82
ee [%]	96	96	96	96	94	95	95	95

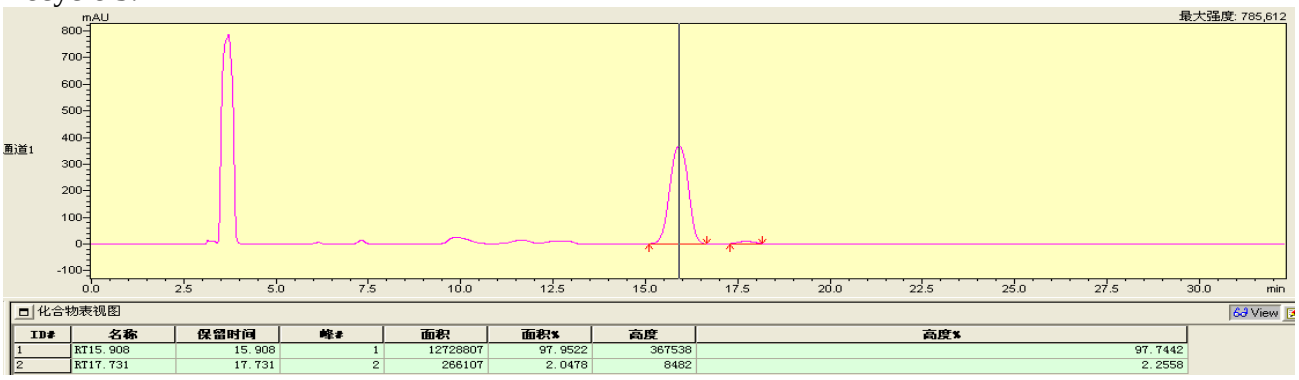
[a] Reaction conditions: catalyst **5** (133.5 mg, 20.0 μmol of Ru and 12.0 μmol of Pd, based on ICP analysis), Cs_2CO_3 (651.60 mg, 3.0 mmol), HCO_2Na (680.0 mg, 10.0 mmol), 4−chloroacetophenone (1.0 mmol) and phenylboronic acid (1.20 mmol), 20.0 mL of the mixed solvents (H_2O/^{i}PrOH v/v=1/3), reaction temperature (80 ℃), reaction time (0.5 h).

Figure S11. Reusability of catalyst **5** in the Suzuki coupling–ATH of tandem reactions of 4−chloroacetophenone and phenylboronic acid.

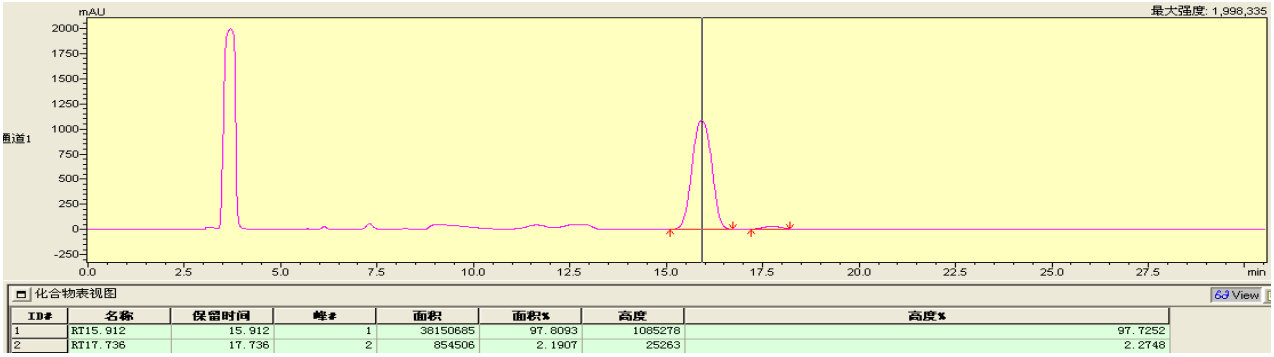
Recycling experiment part: Recycle 2.



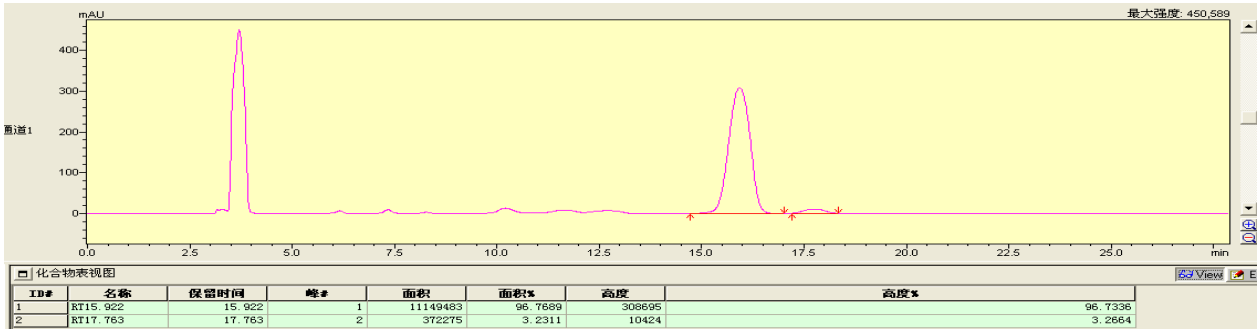
Recycle 3.



Recycle 4.



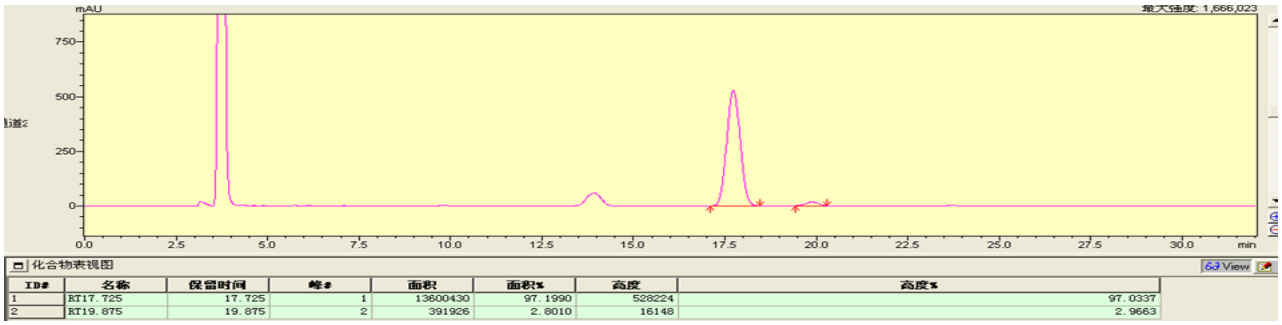
Recycle 5.



化合物表视图

ID#	名称	保留时间	峰#	面积	面积%	高度	高度%
1	RT15.922	15.922	1	11149483	96.7689	308695	96.7336
2	RT17.763	17.763	2	372275	3.2311	10424	3.2664

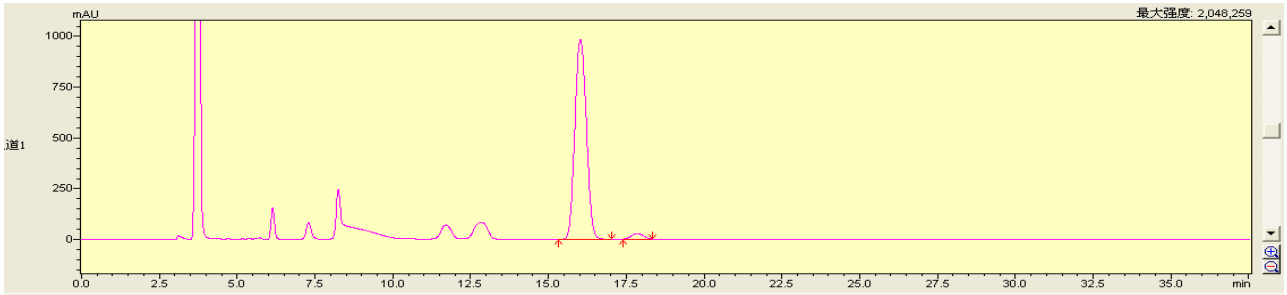
Recycle 6.



化合物表视图

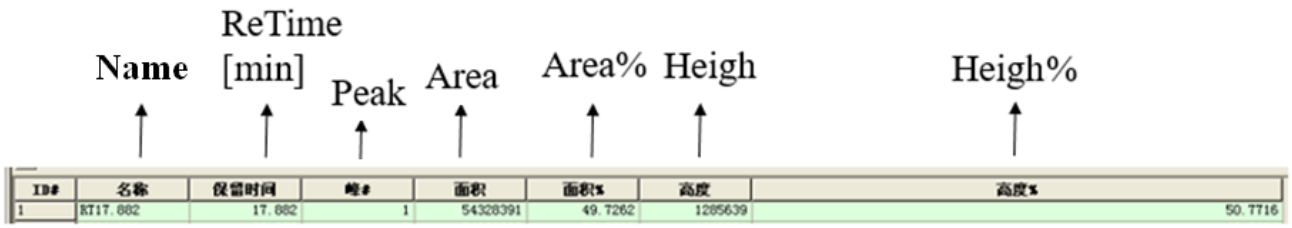
ID#	名称	保留时间	峰#	面积	面积%	高度	高度%
1	RT17.725	17.725	1	13600430	97.1990	528224	97.0337
2	RT19.875	19.875	2	391926	2.8010	16148	2.9663

Recycle 7.



化合物表视图

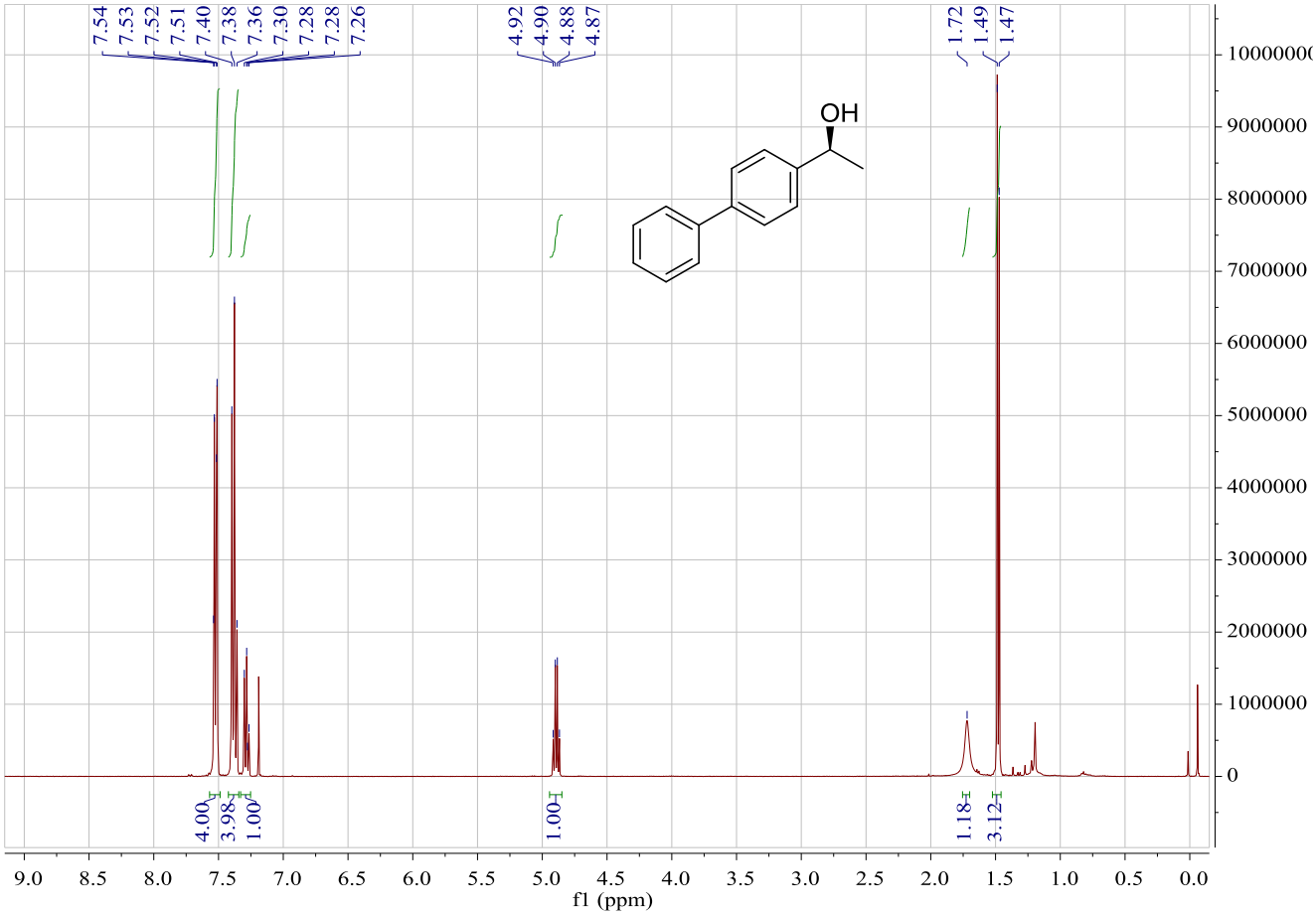
ID#	名称	保留时间	峰#	面积	面积%	高度	高度%
1	RT16.023	16.023	1	25207891	97.3253	983325	97.4105
2	RT17.844	17.844	2	692767	2.6747	26140	2.5895

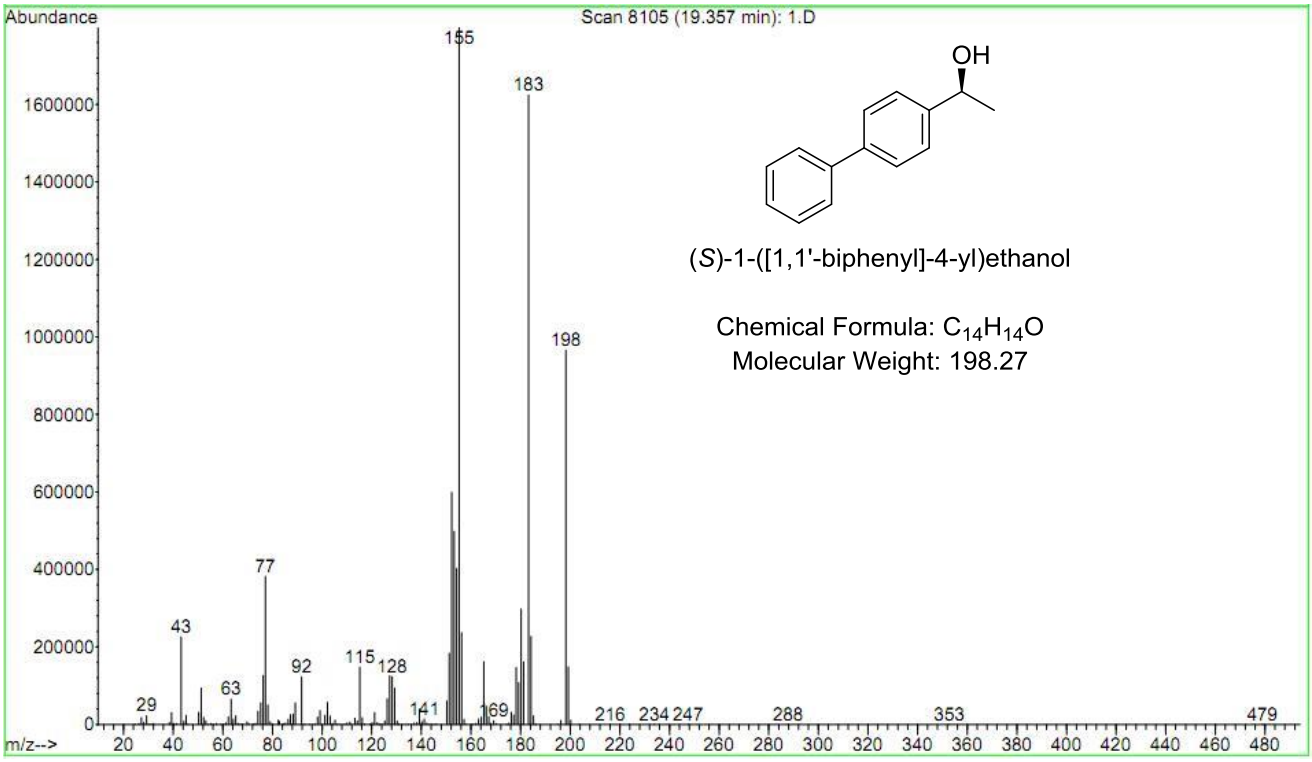


ID#	名称	保留时间	峰#	面积	面积%	高度	高度%
1	RT17.882	17.882	1	54328391	49.7262	1285639	50.7716

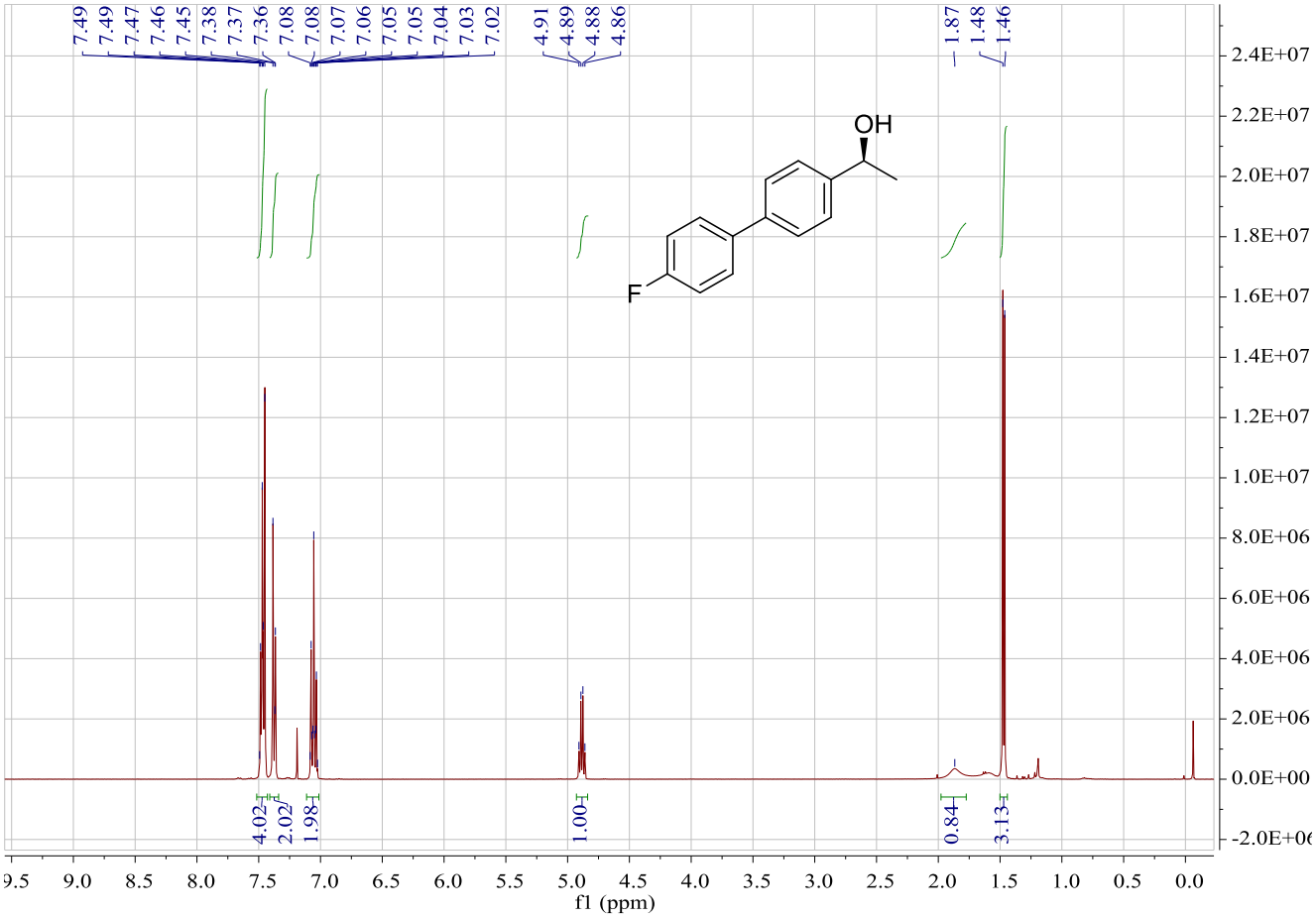
Figure S12. Characterization of chiral products **(**The ^{1}H NMR and GC−MS spectra of all chiral products).

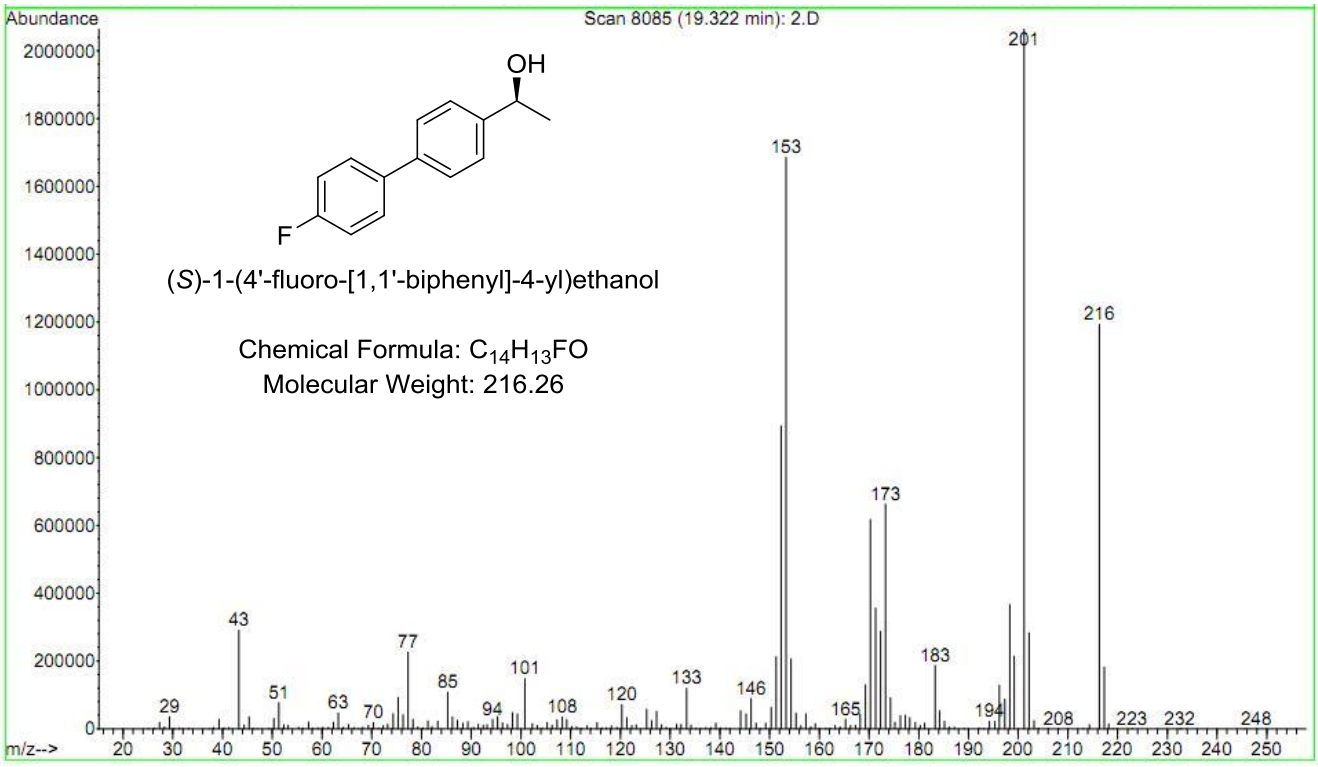
(*S*)−4−phenylacetophenol (8a).



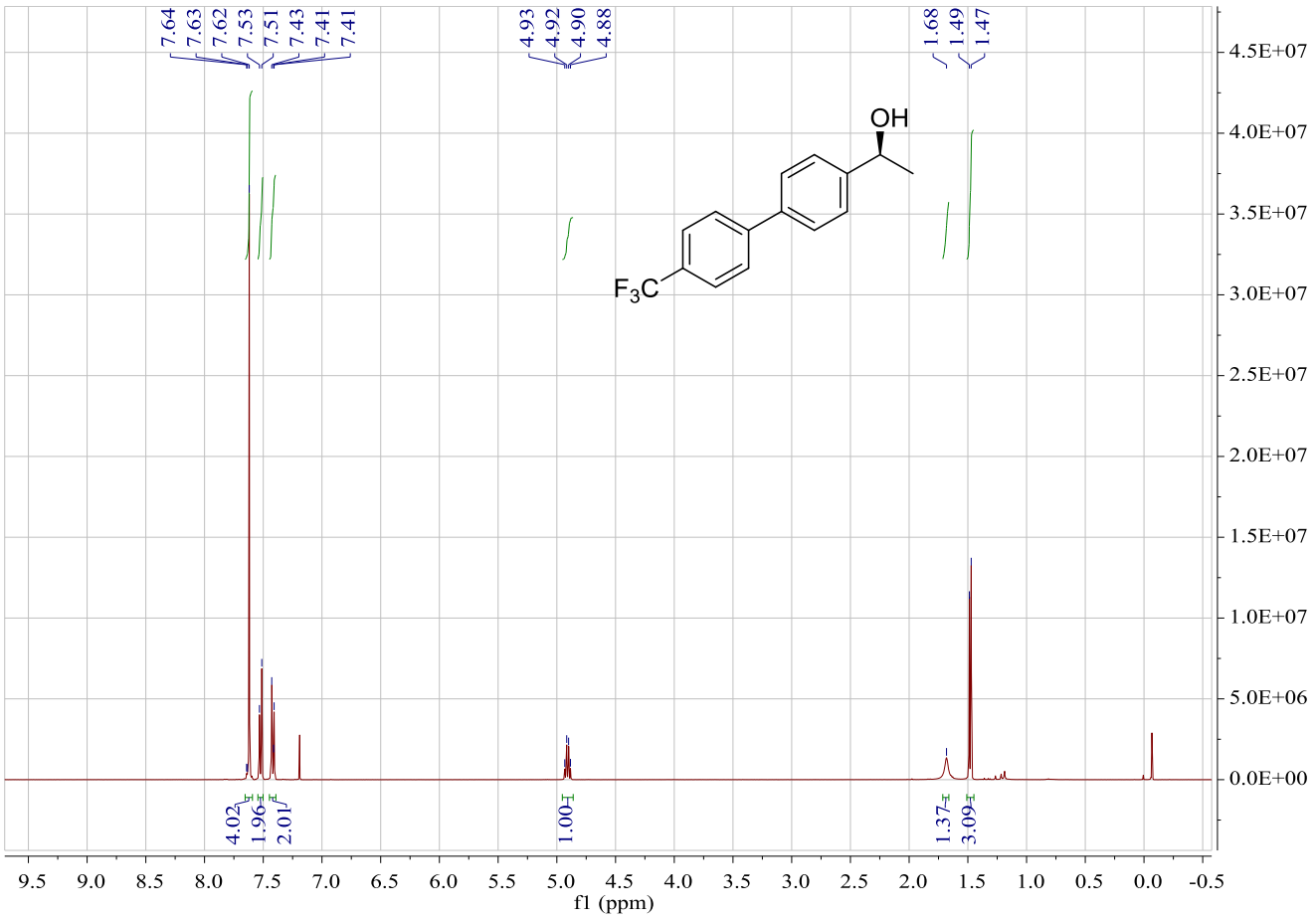


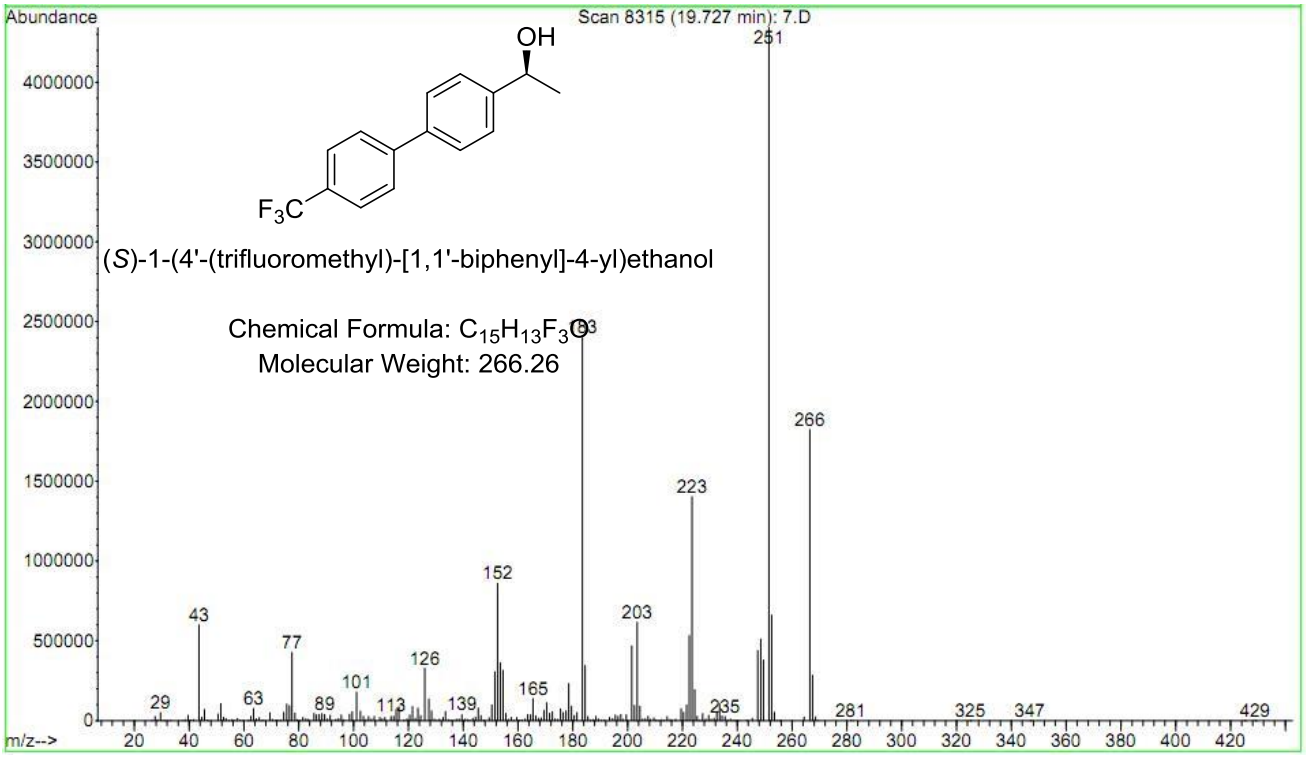
(*S*)−1−(4−(4−floro)phenyl)ethanol (8b).



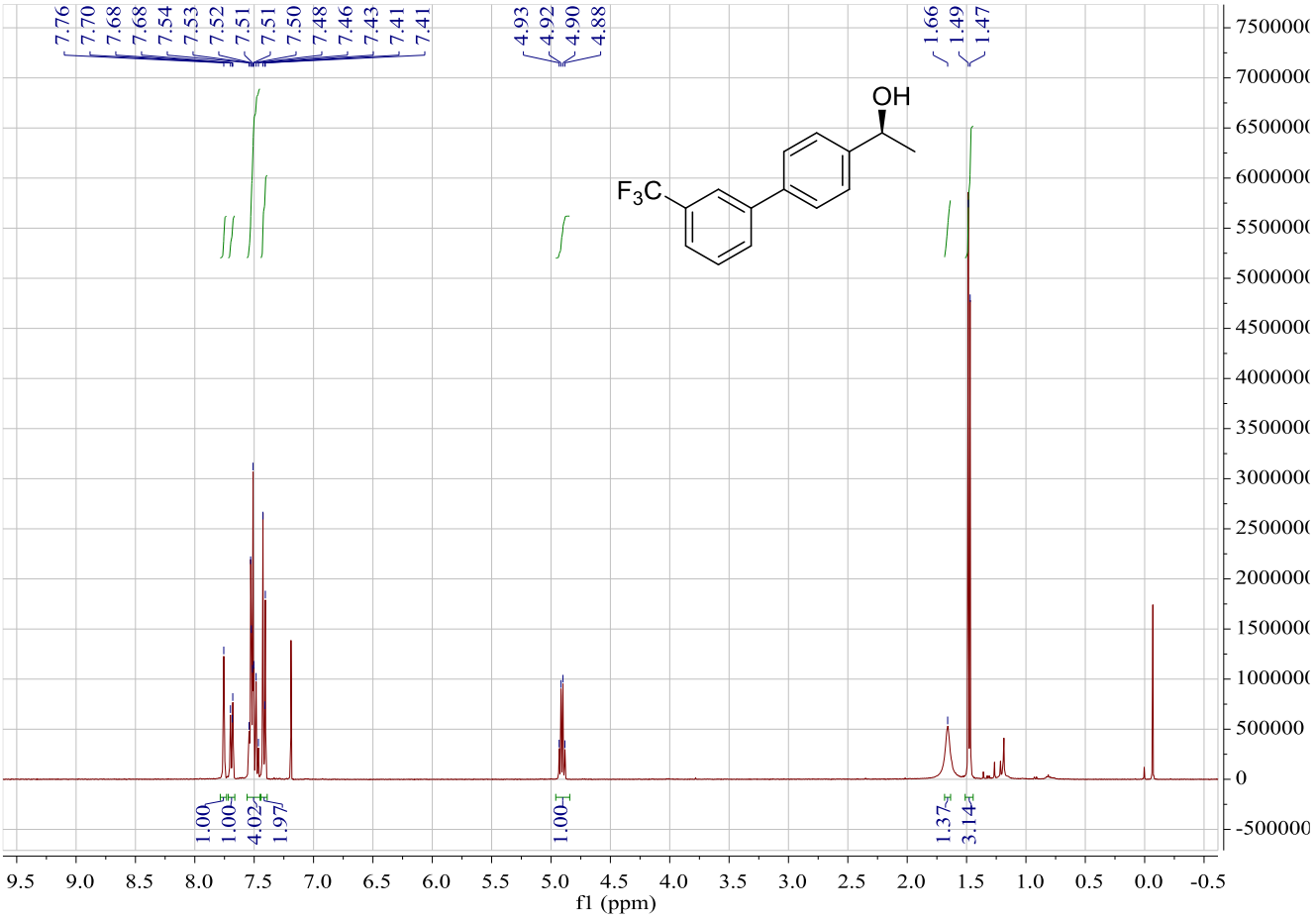


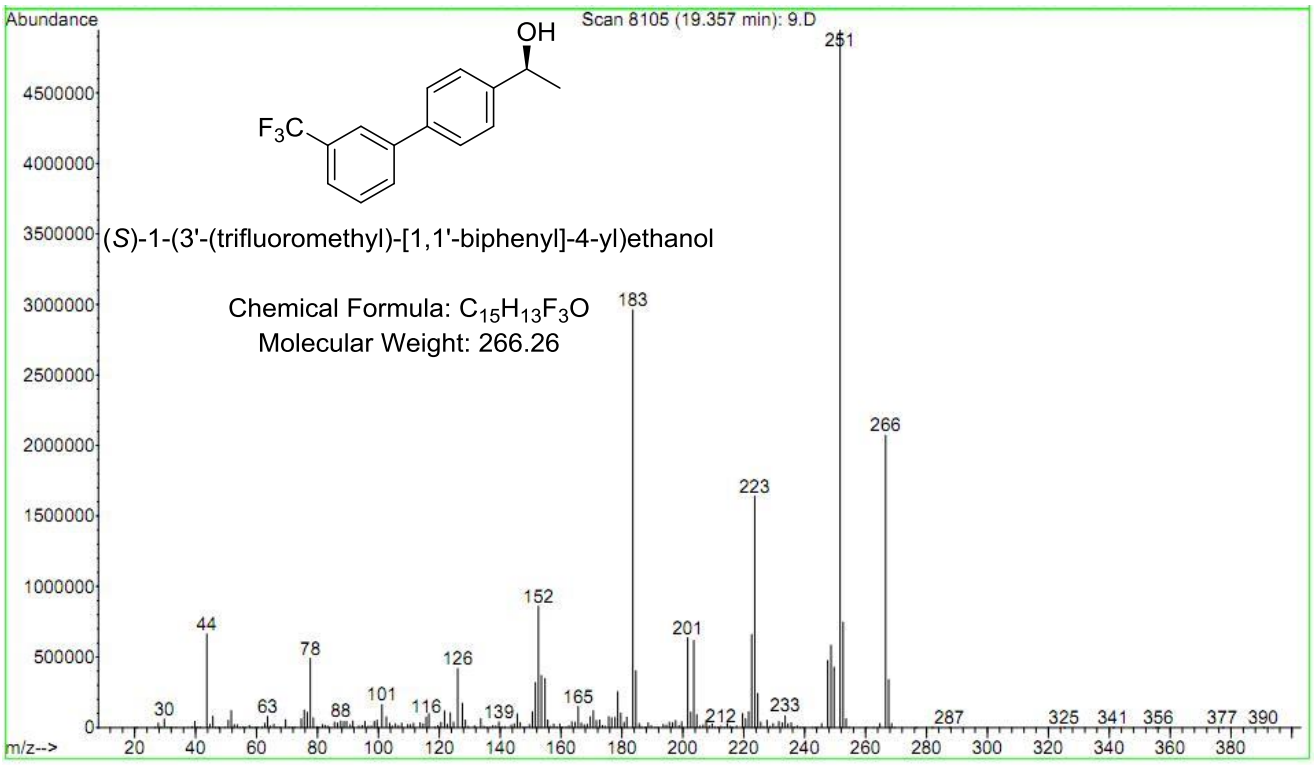
(*S*)−1−(4−(4−trifluoromethyl)phenyl)ethanol (8c).



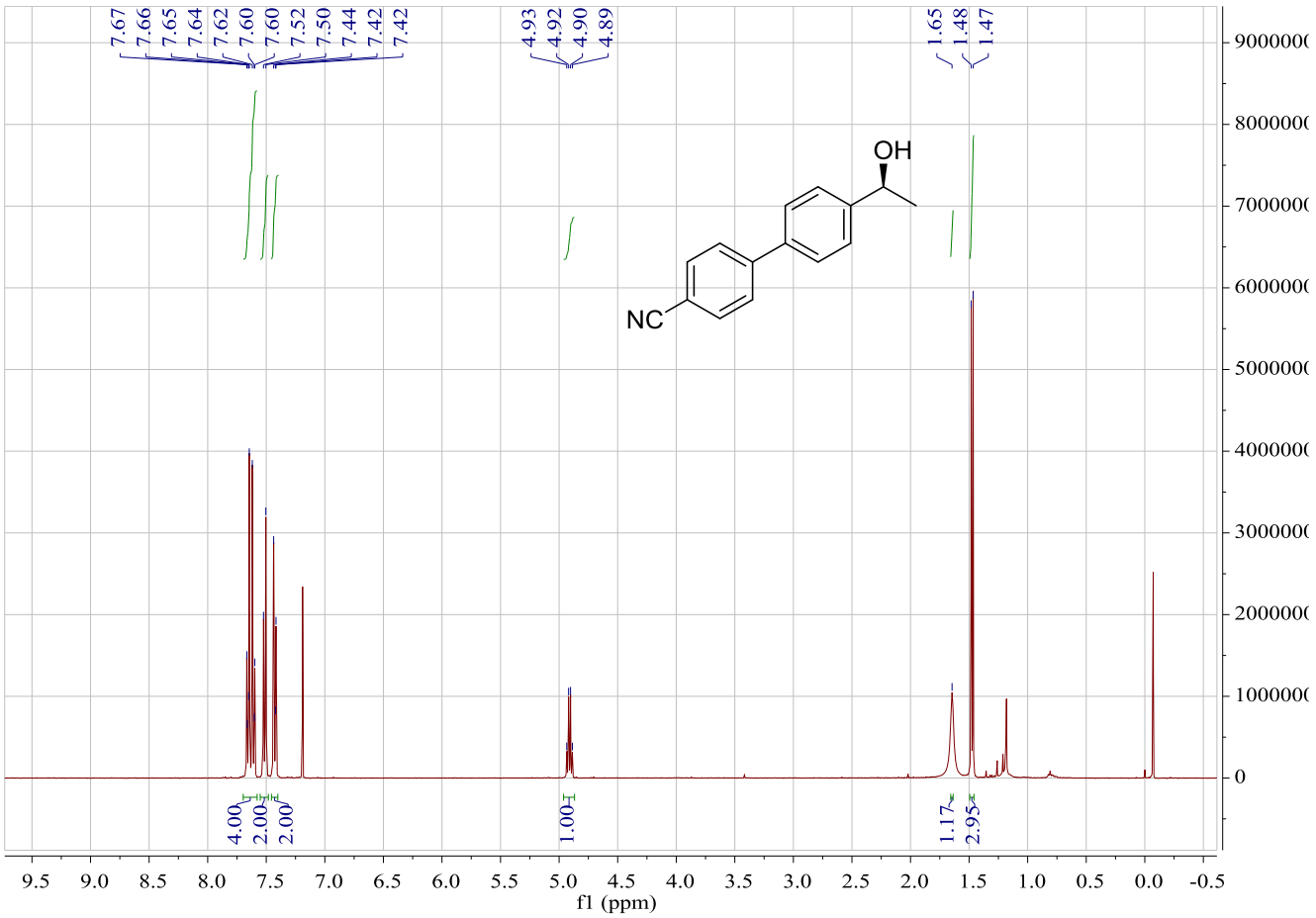


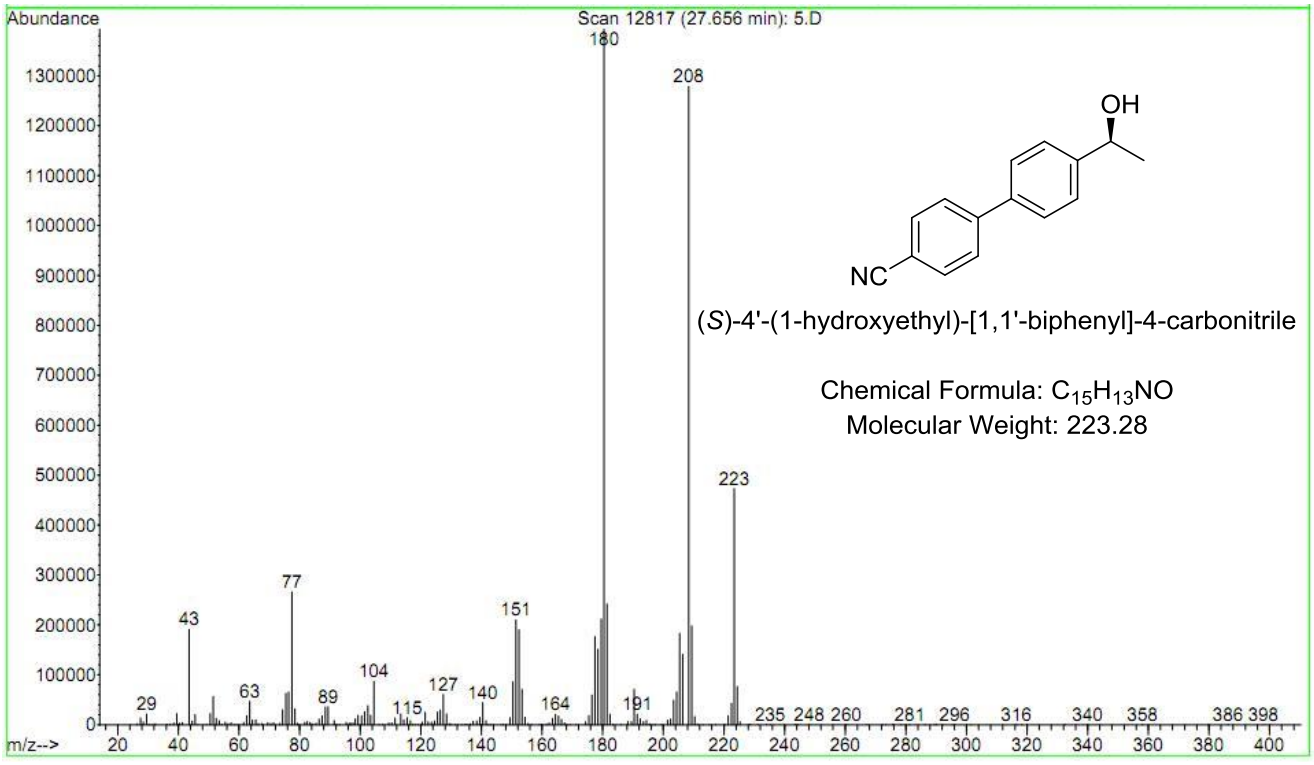
(*S*)−1−(4−(3−trifluouomethyl)phenyl)ethanol (8d).



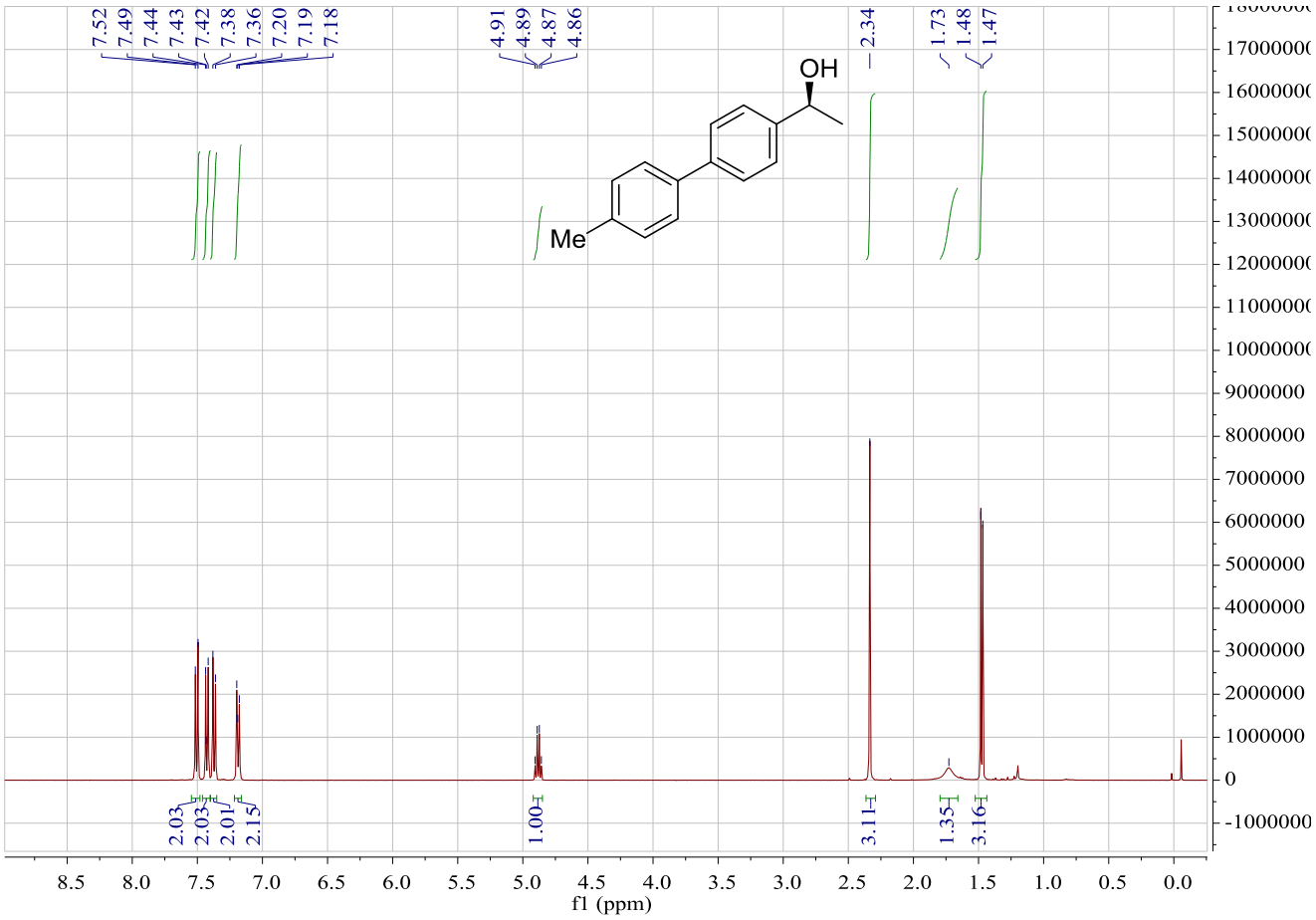


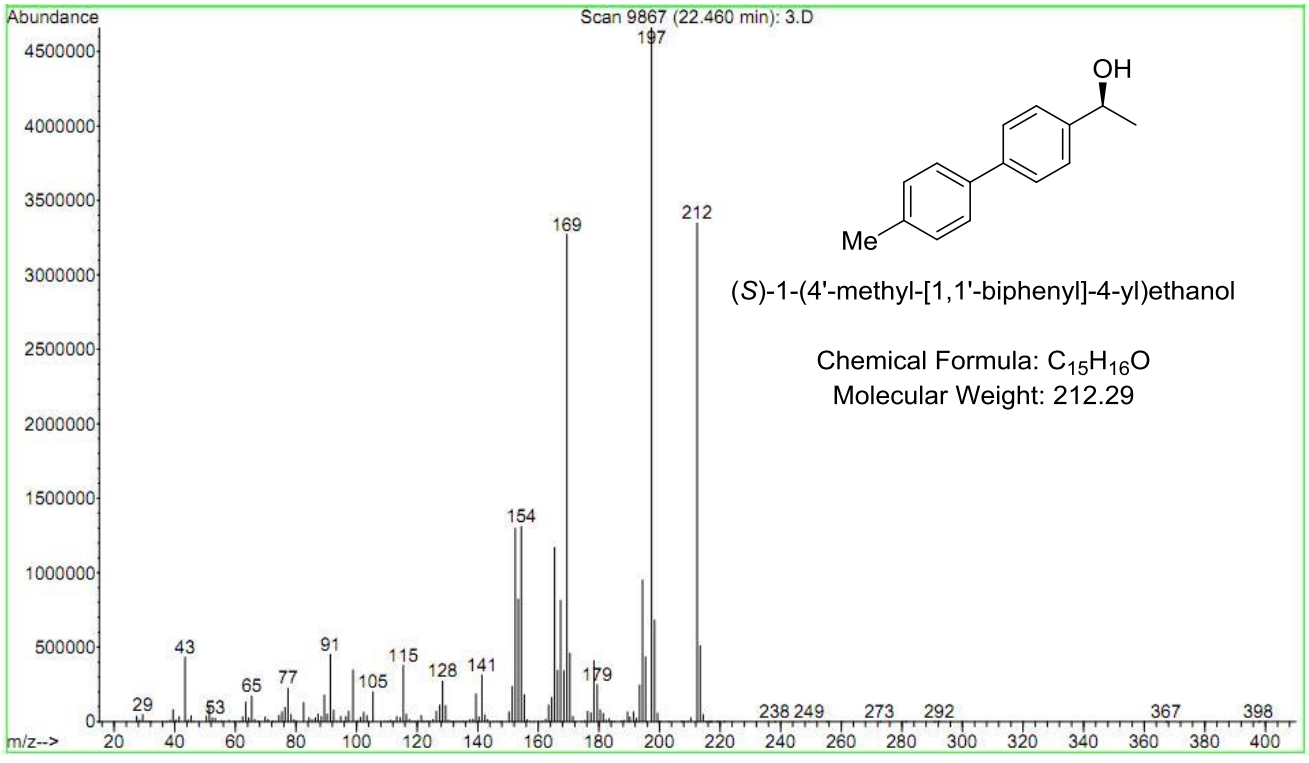
(*S*)−1−(4−(4−cyano)phenyl)ethanol (8e).



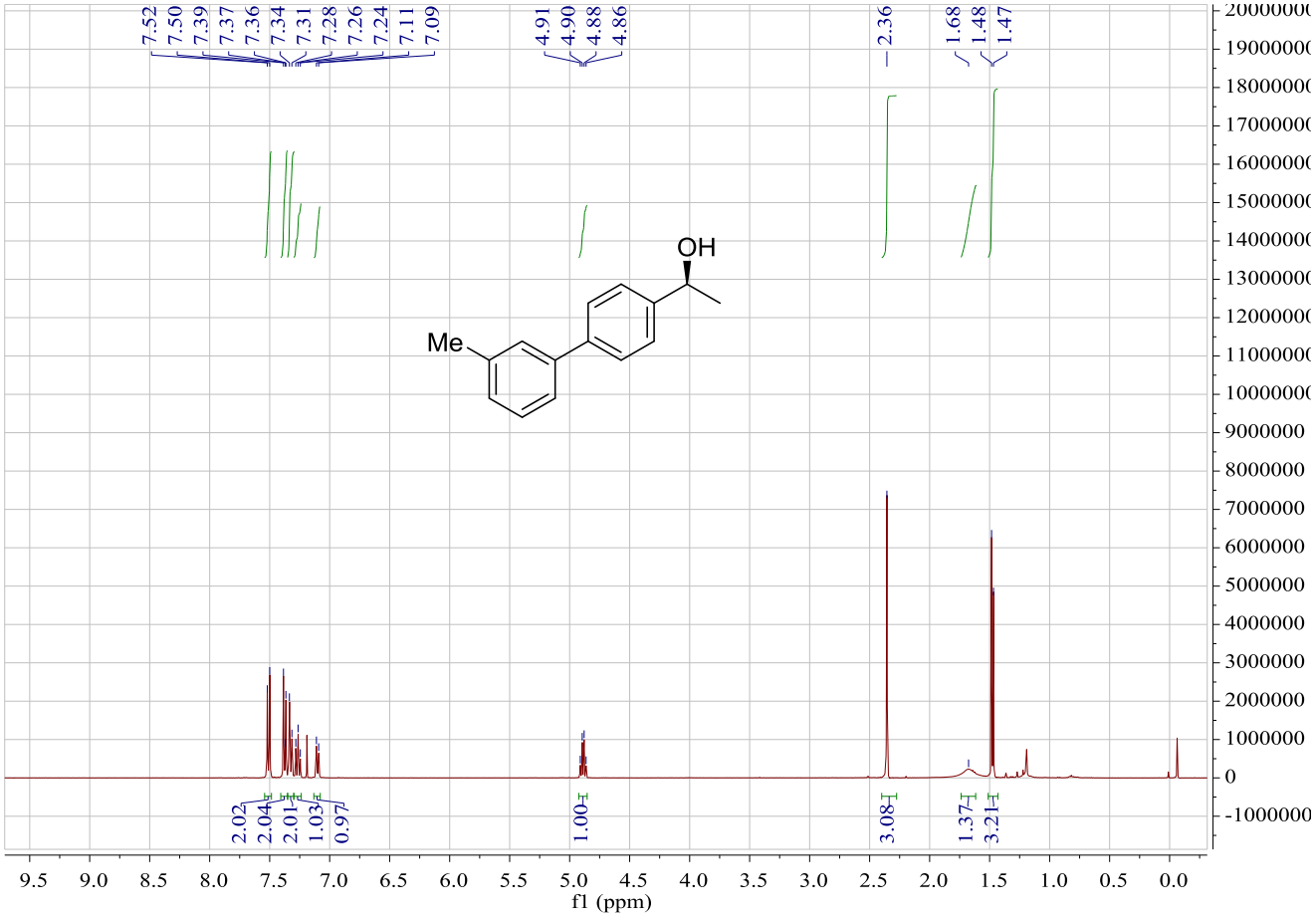


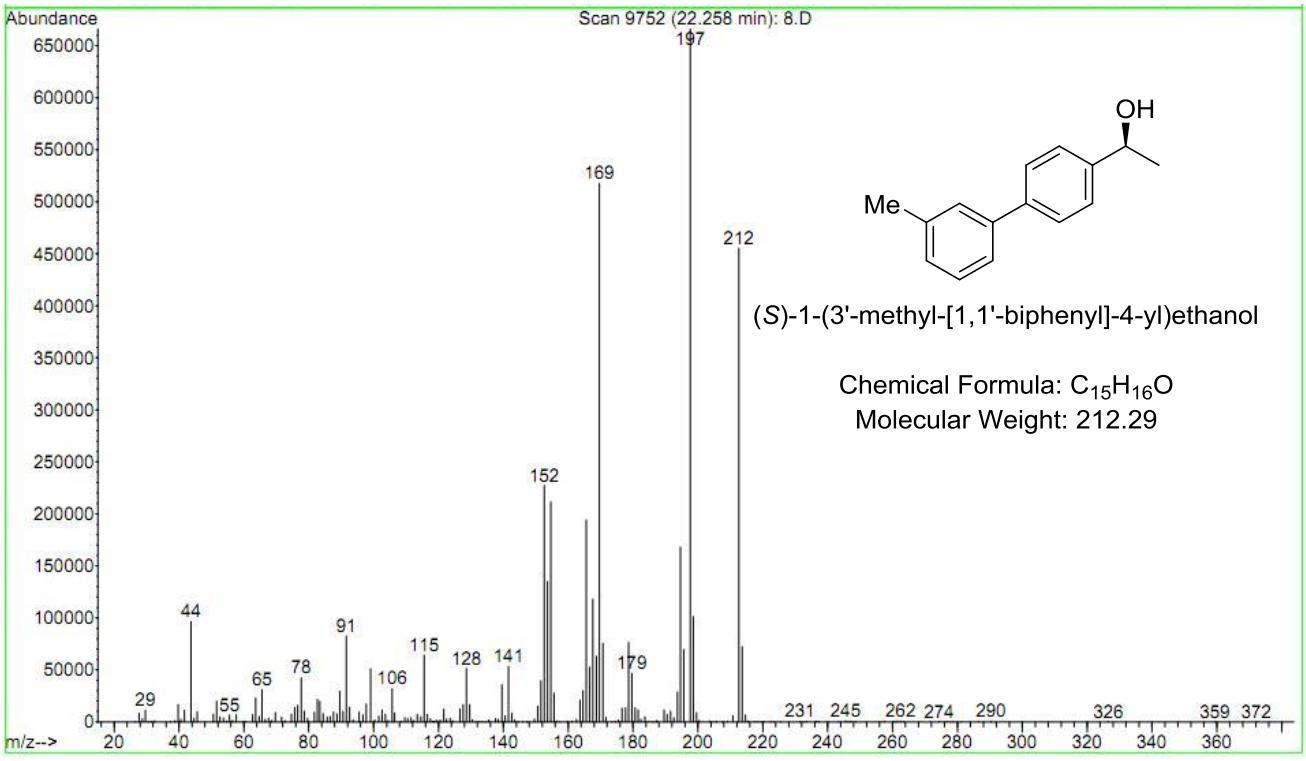
(*S*)−1−(4−(4−methyl)phenyl)ethanol (8f).



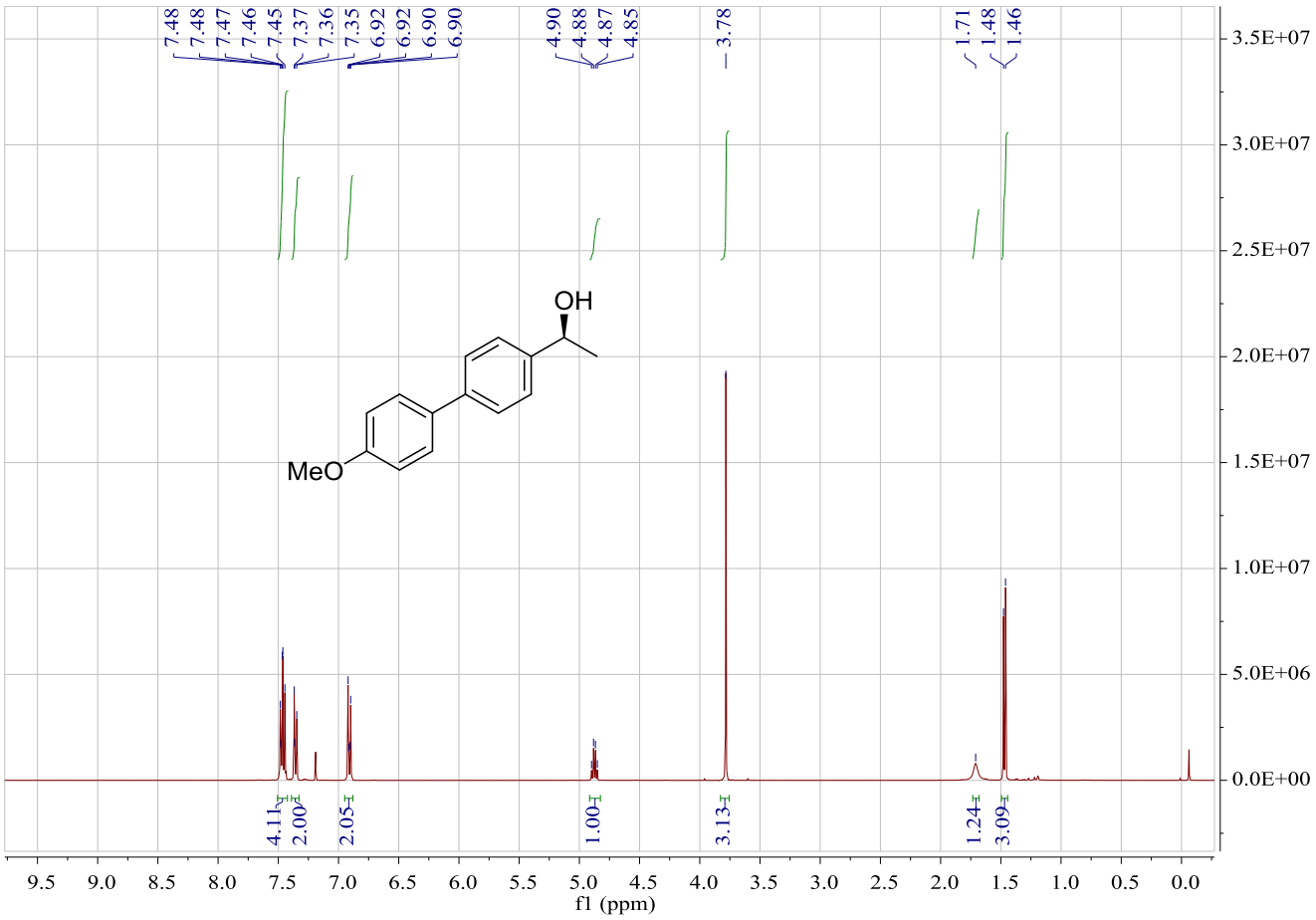


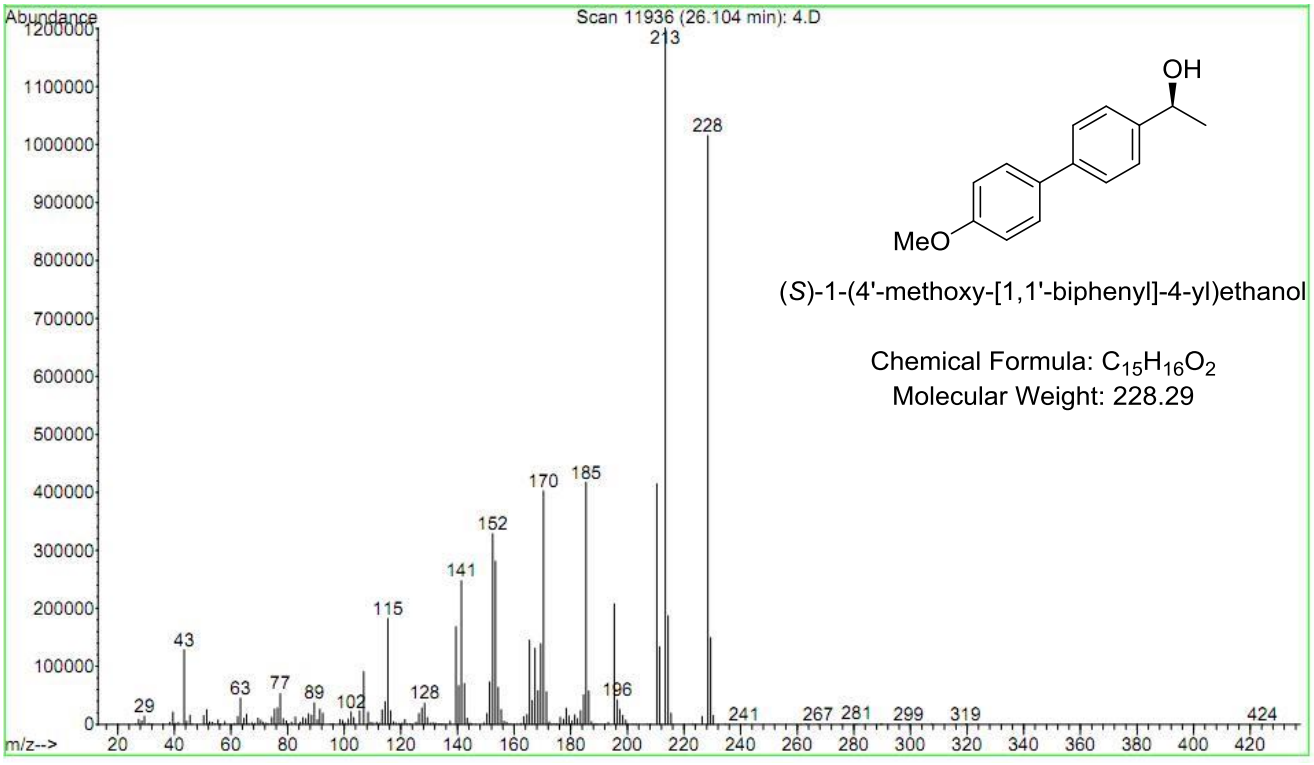
(*S*)−1−(4−(3−methyl)phenyl)ethanol (8g).



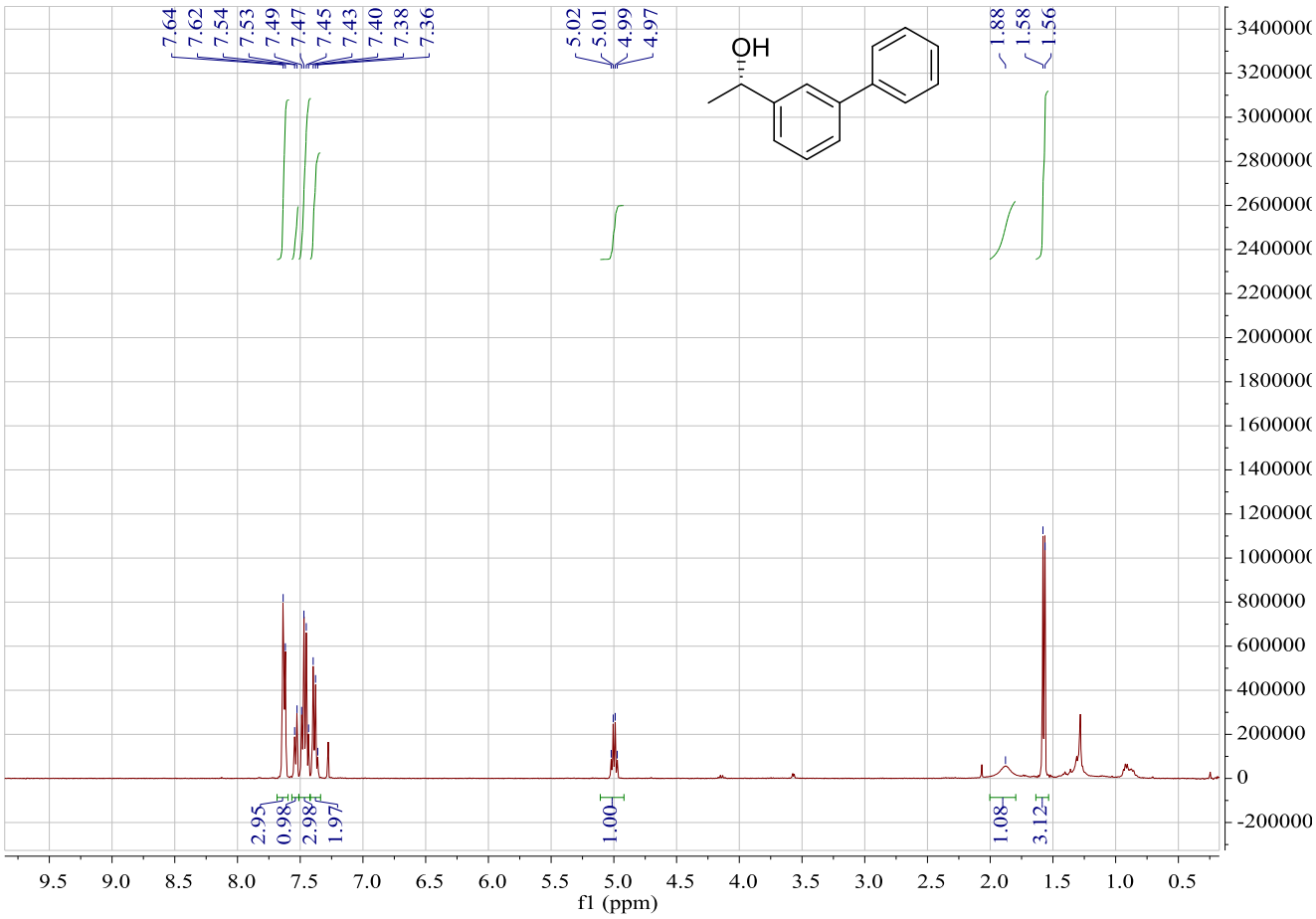


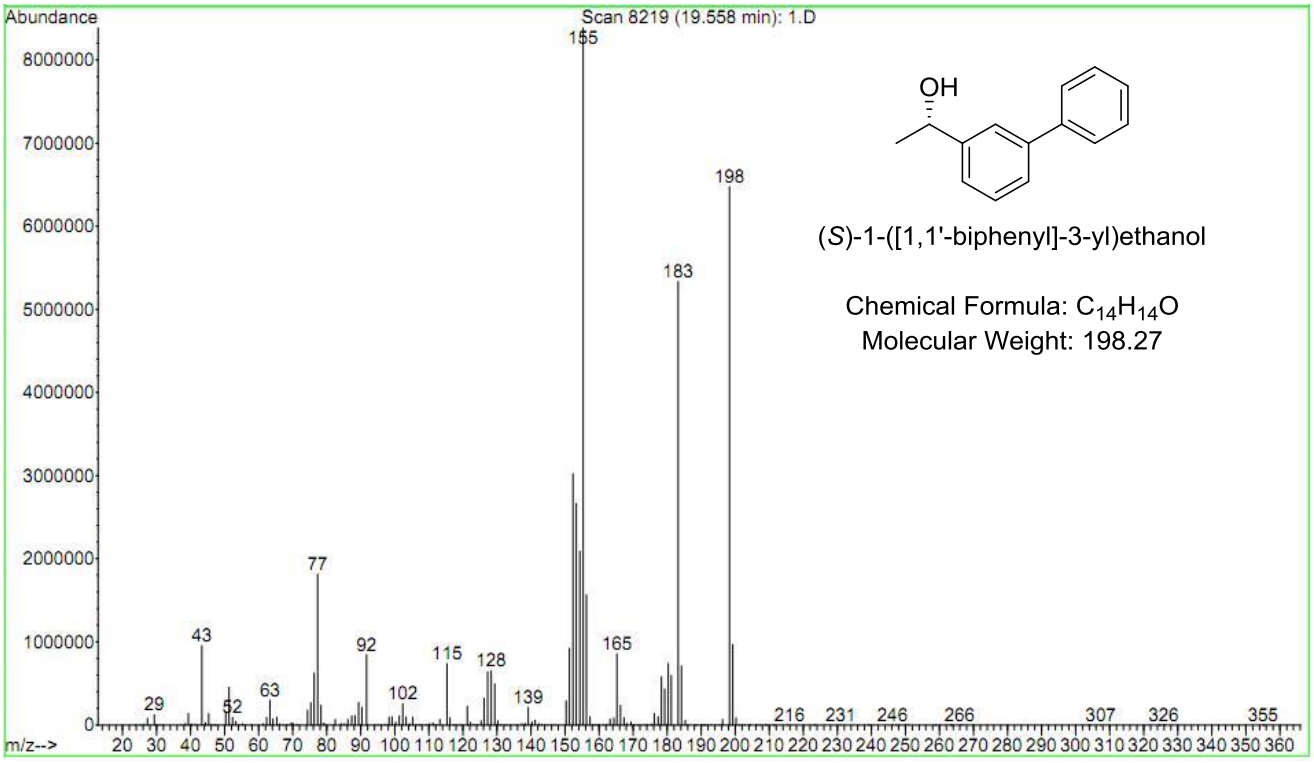
(*S*)−1−(4−(4−methoxy)phenyl)ethanol (8h).



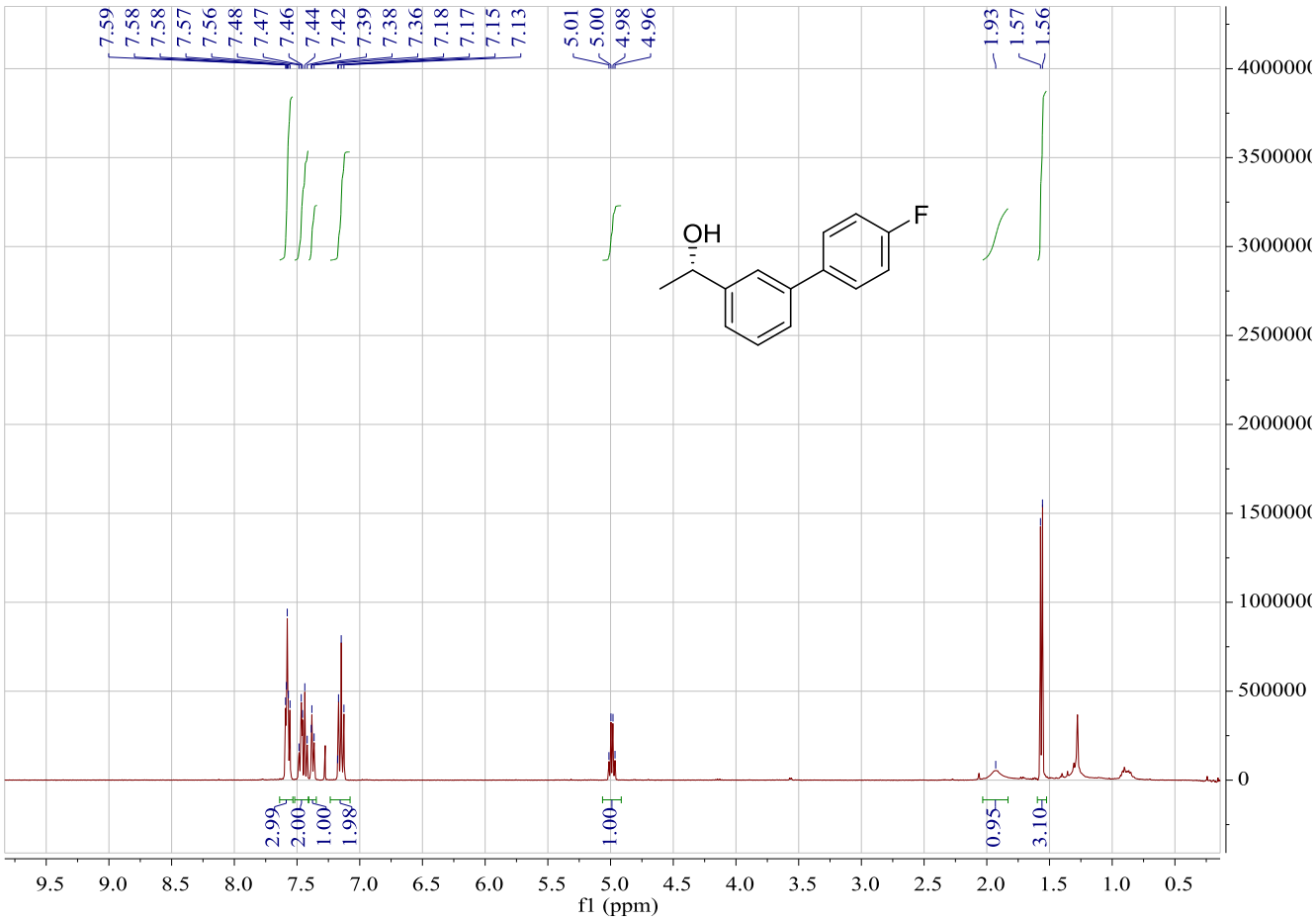


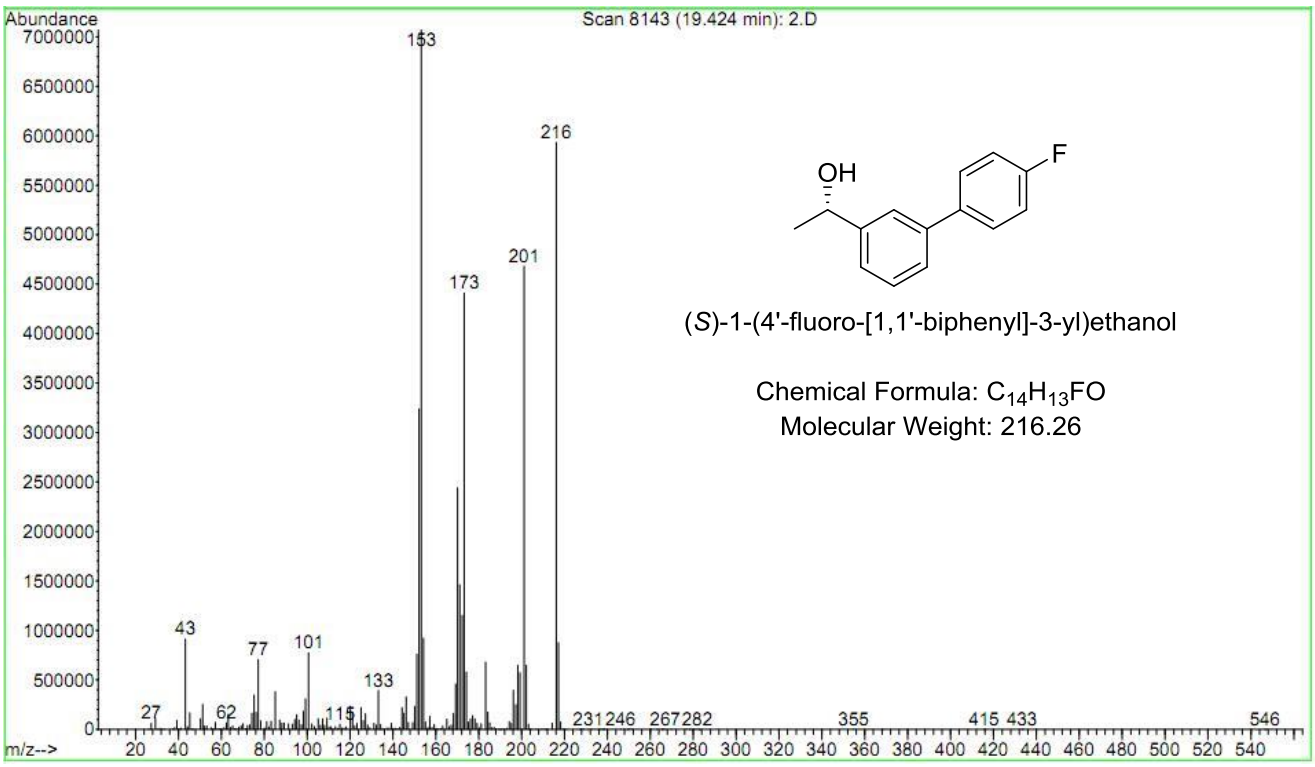
(*S*)−3−phenylacetophenol (8i).



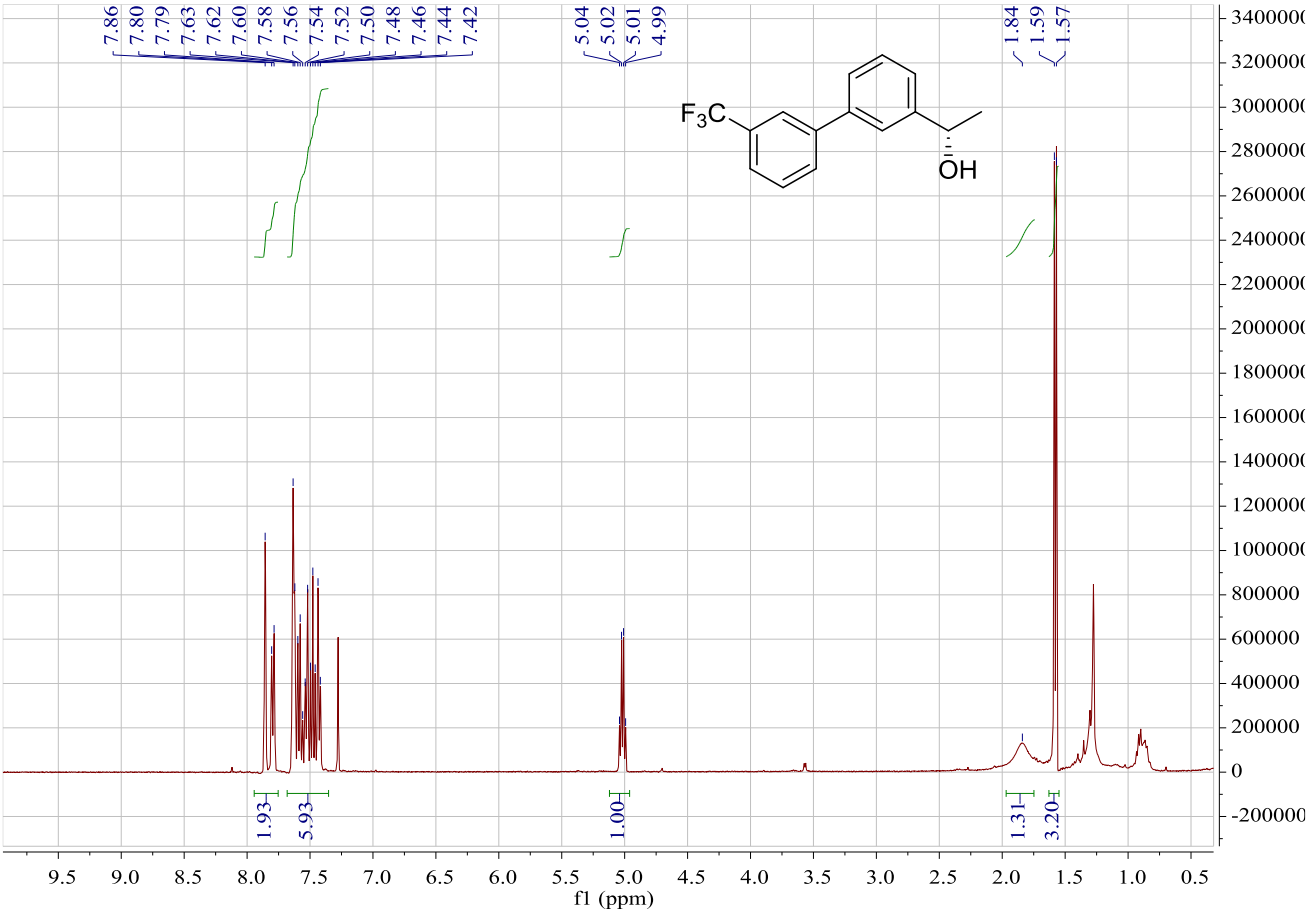


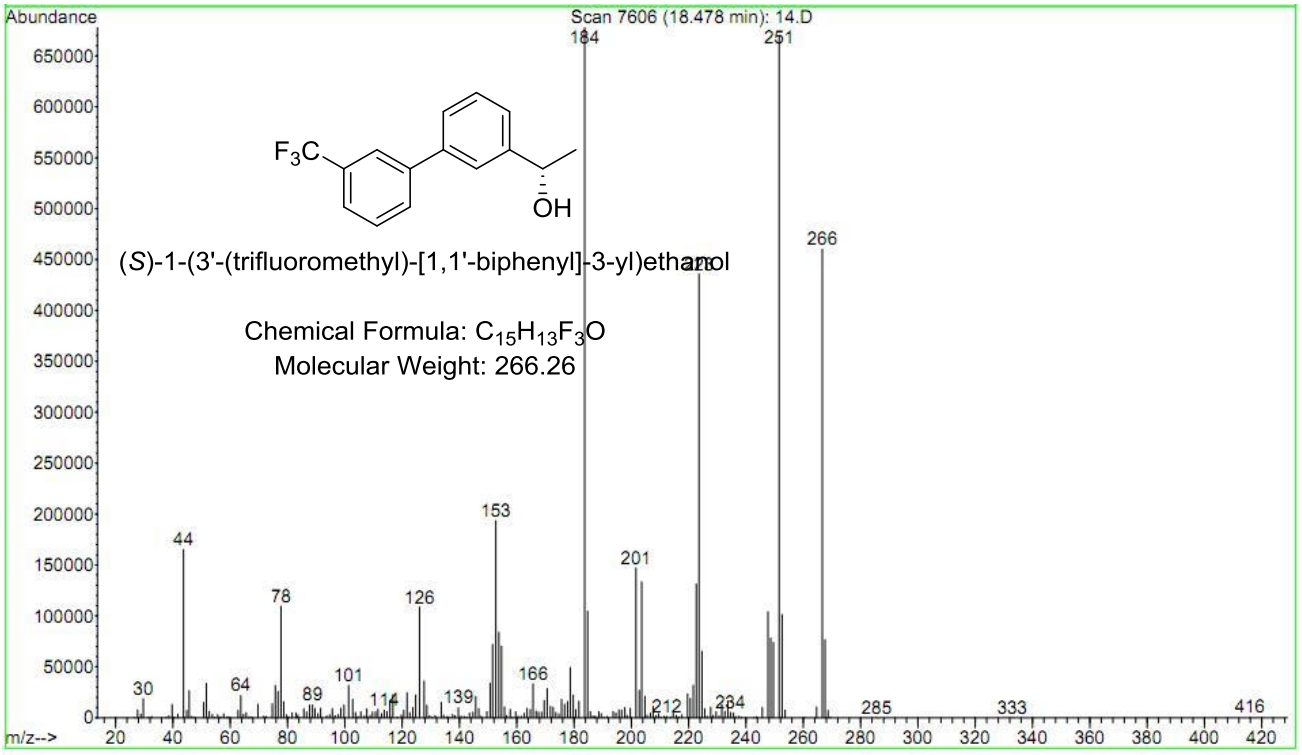
(*S*)−1−(3−(4−fluoro)phenyl)ethanol (8j).



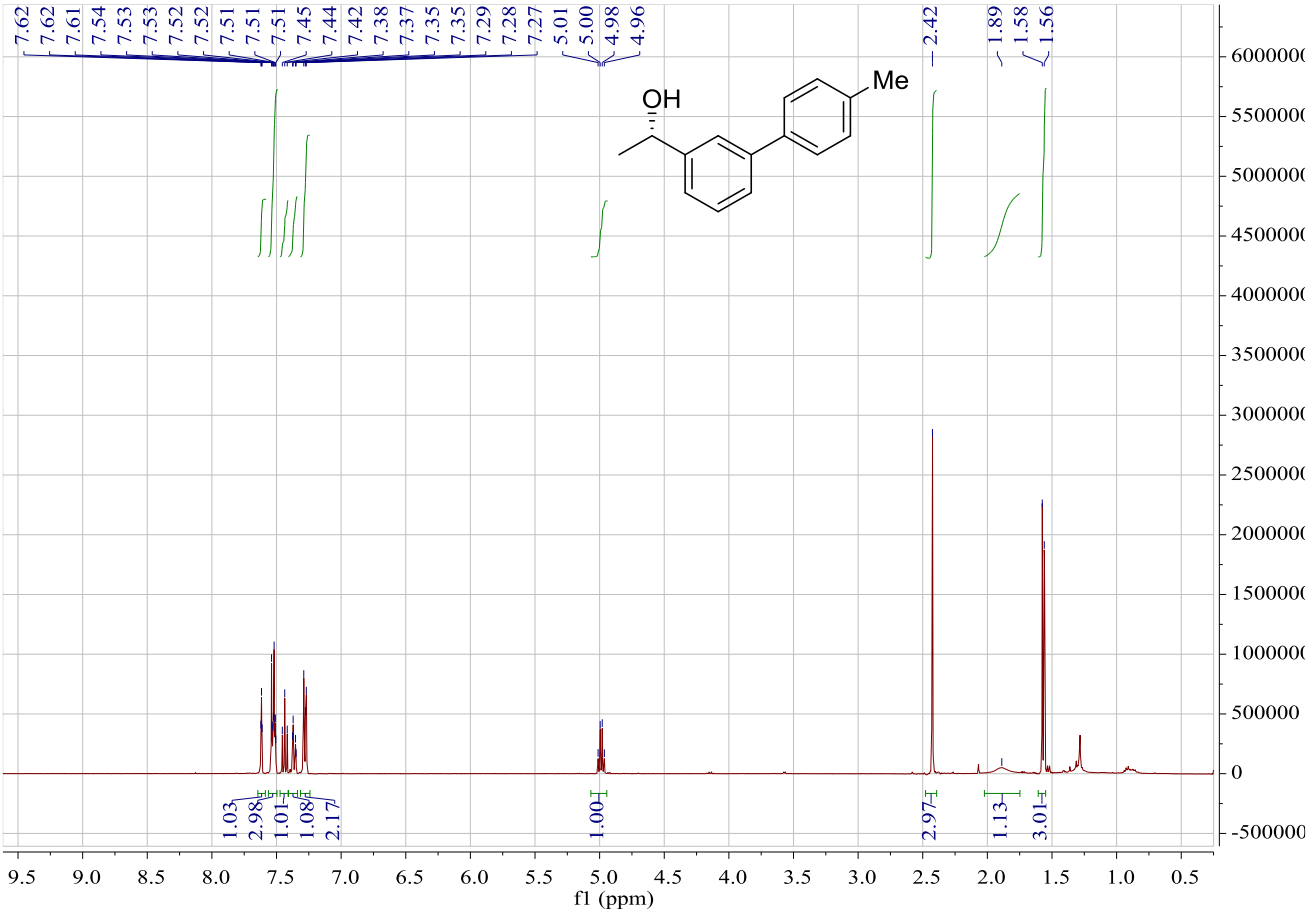


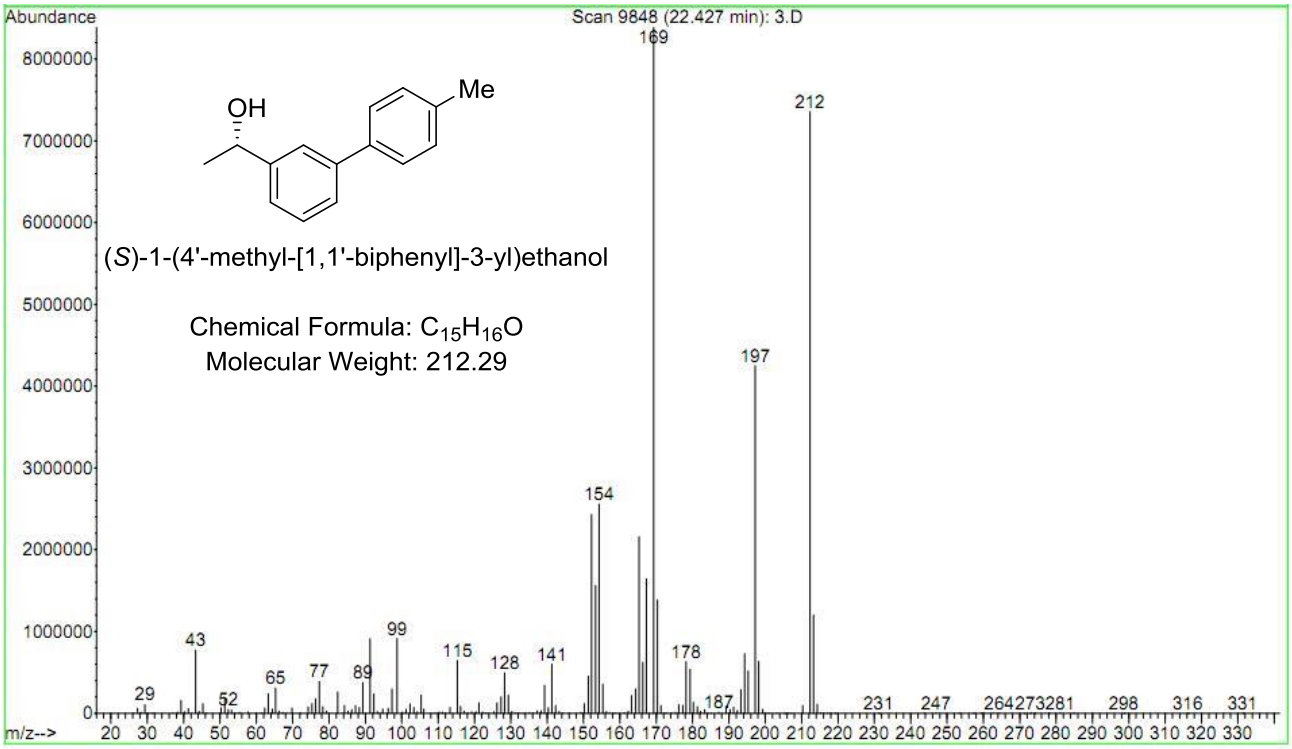
(*S*)−1−(3−(3−trifluouomethyl)phenyl)ethanol (8k).



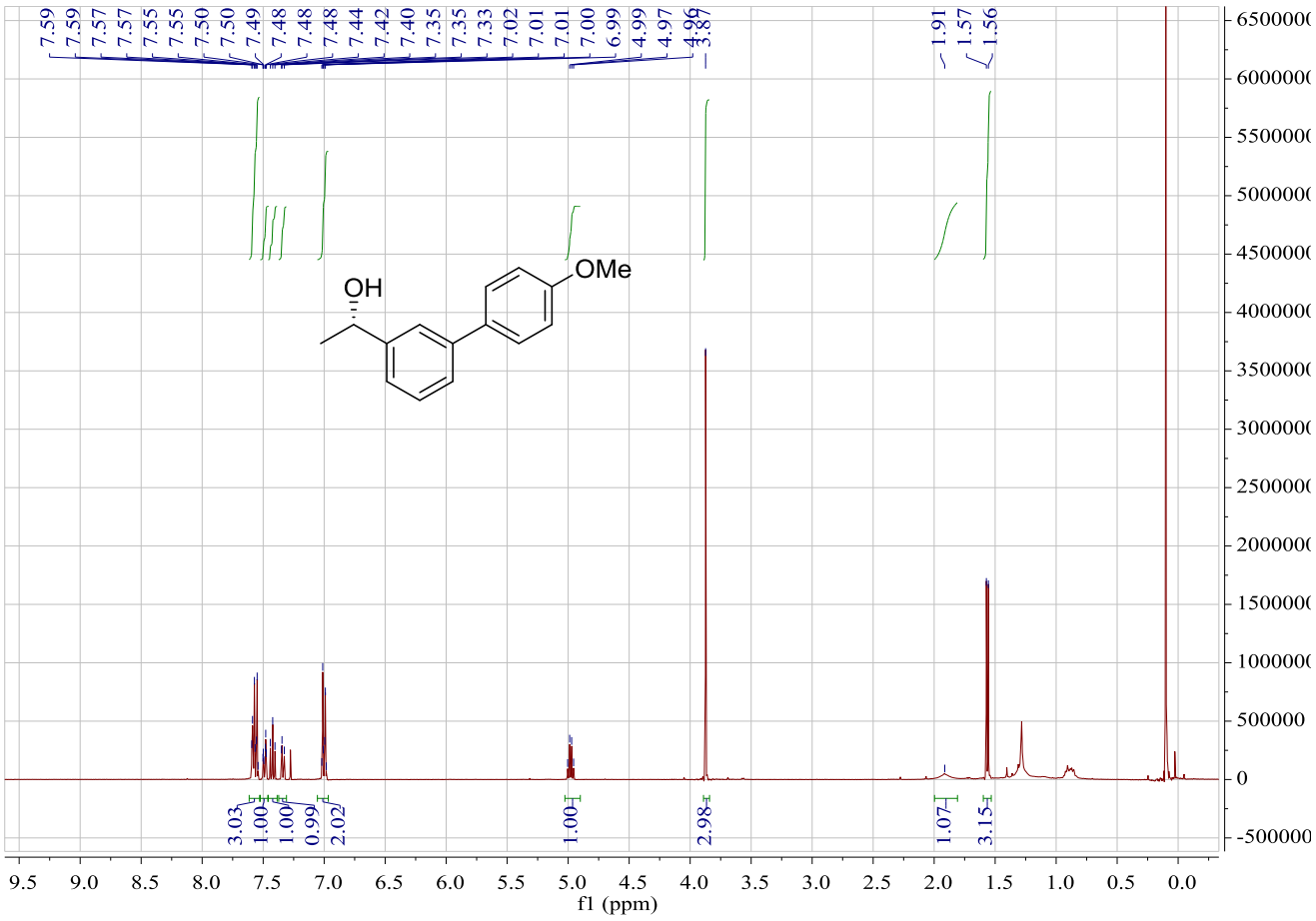


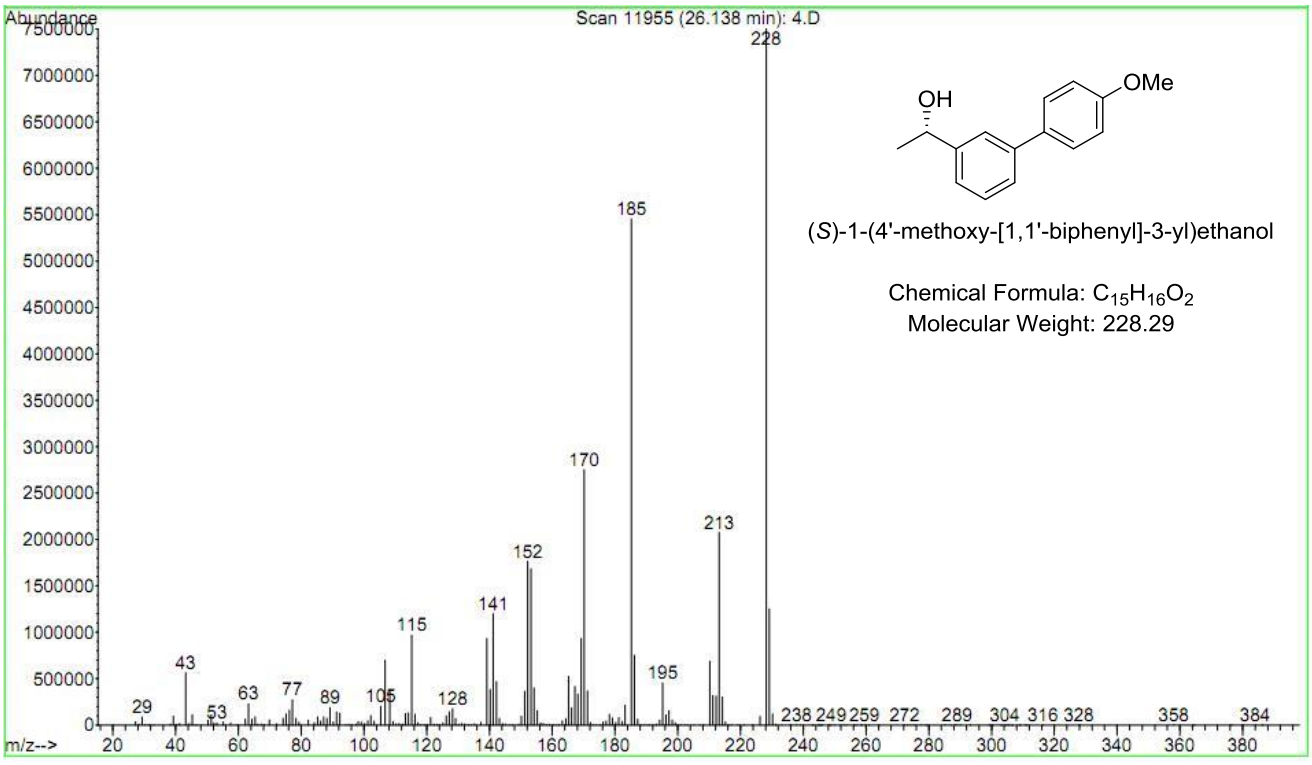
(*S*)−1−(3−(4−methyl)phenyl)ethanol (8l).



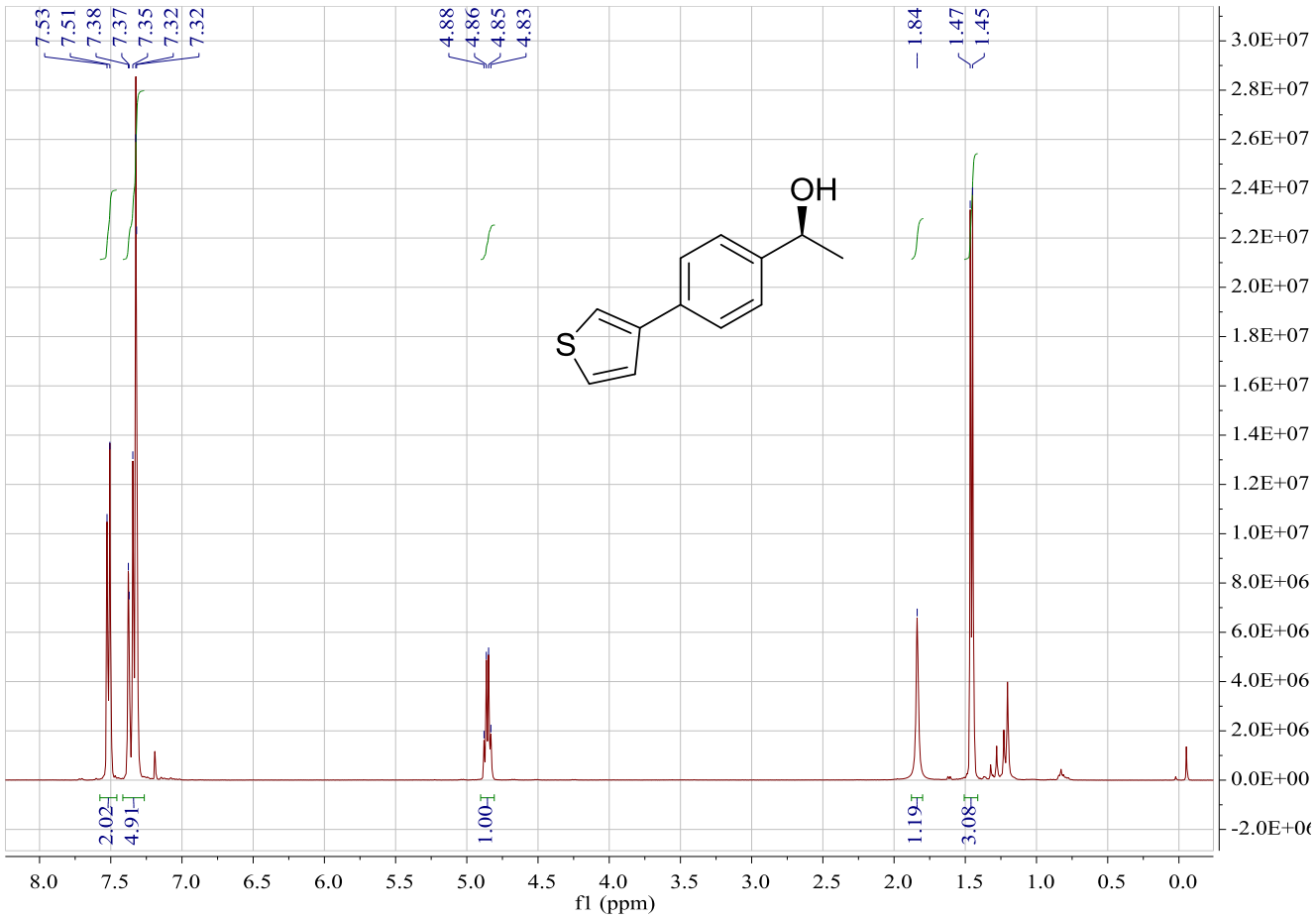


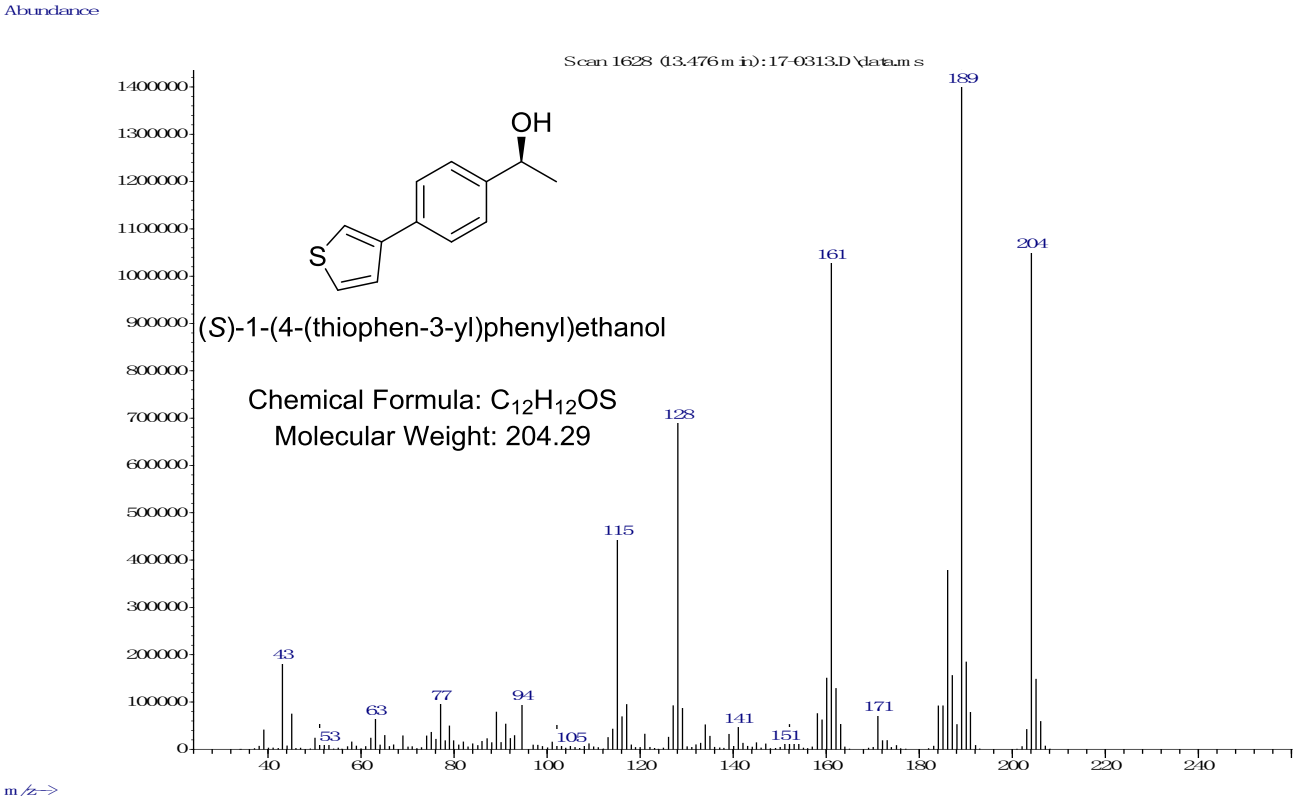
(*S*)−1−(3−(4−methoxy)phenyl)ethanol (8m).



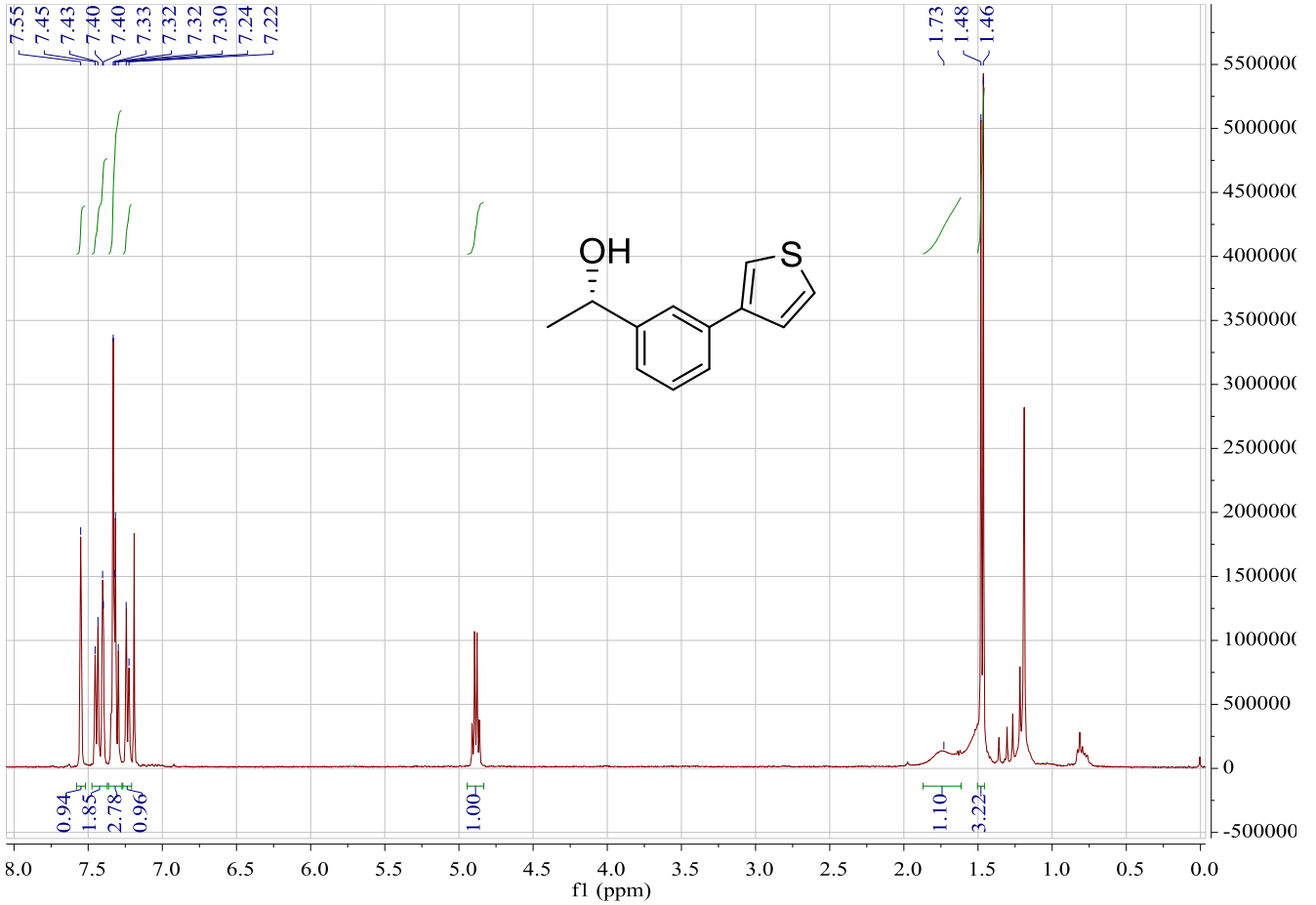


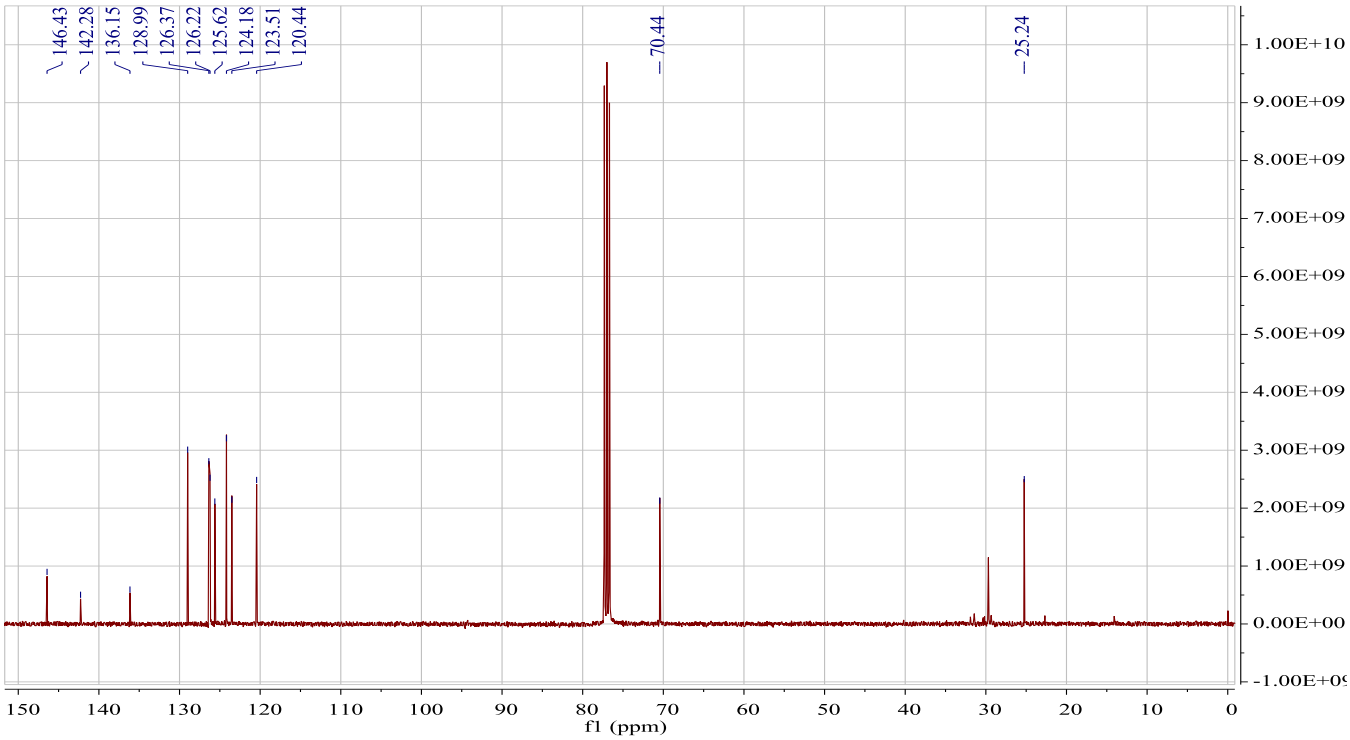
(*S*)−1−(4−(thiophen−3−yl)phenyl)ethanol (8n).

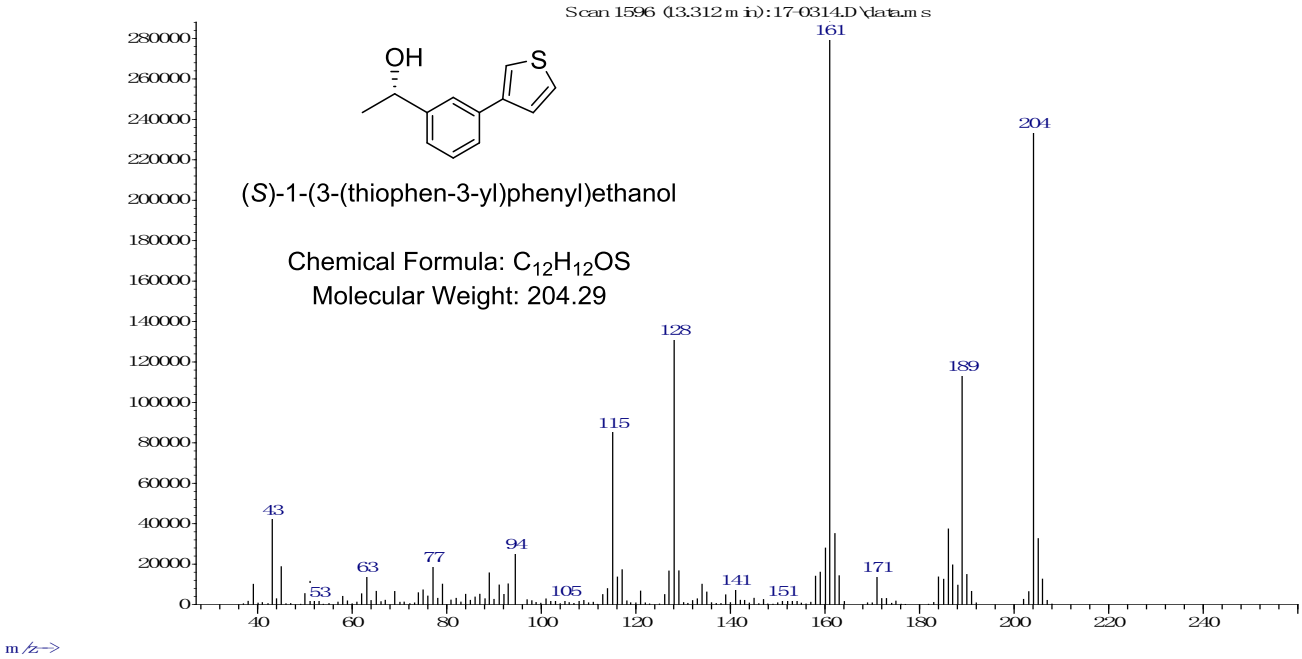




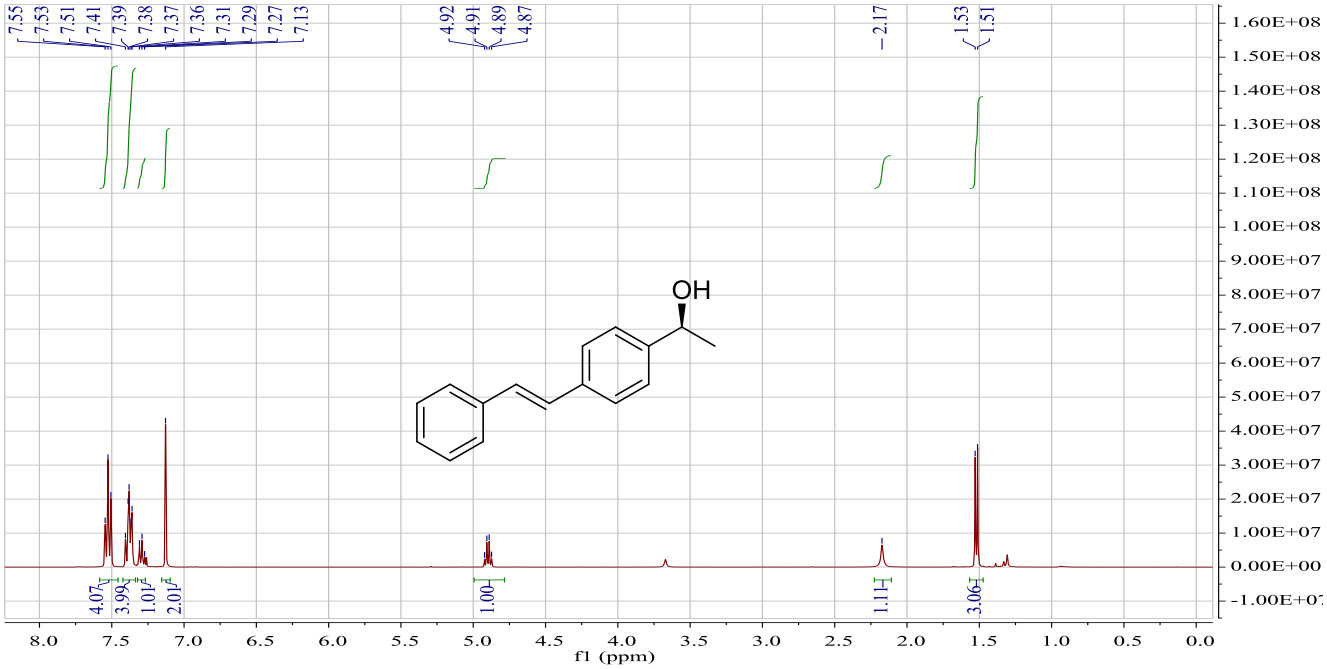
(*S*)−1−(3−(thiophen−3−yl)phenyl)ethanol (8o).

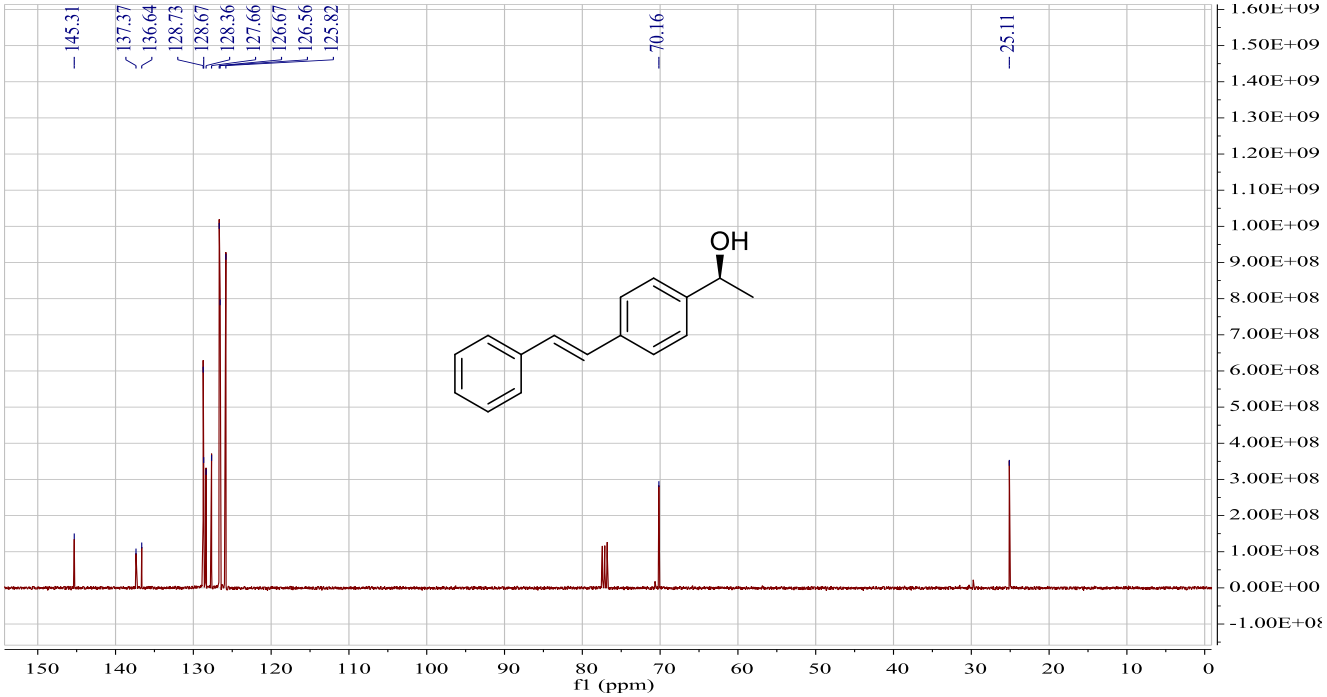


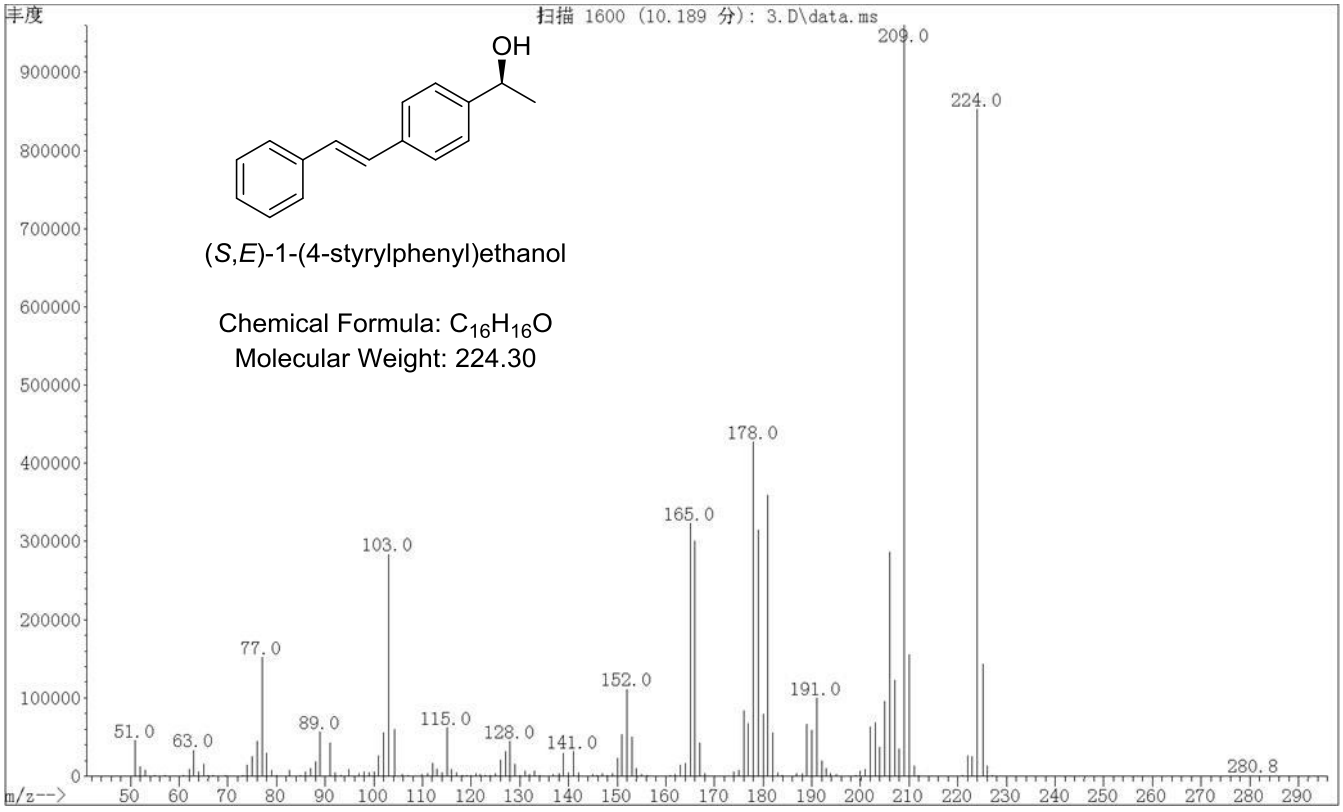



Abundance
Scan 1596 (13.312 min): 17-0314.D\data.ms
OH
S
(S)-1-(3-(thiophen-3-yl)phenyl)ethanol
Chemical Formula: C12H12OS
Molecular Weight: 204.29
161
204
128
189
115
43
94
77
63
171
141
151
105
53
m/z-->

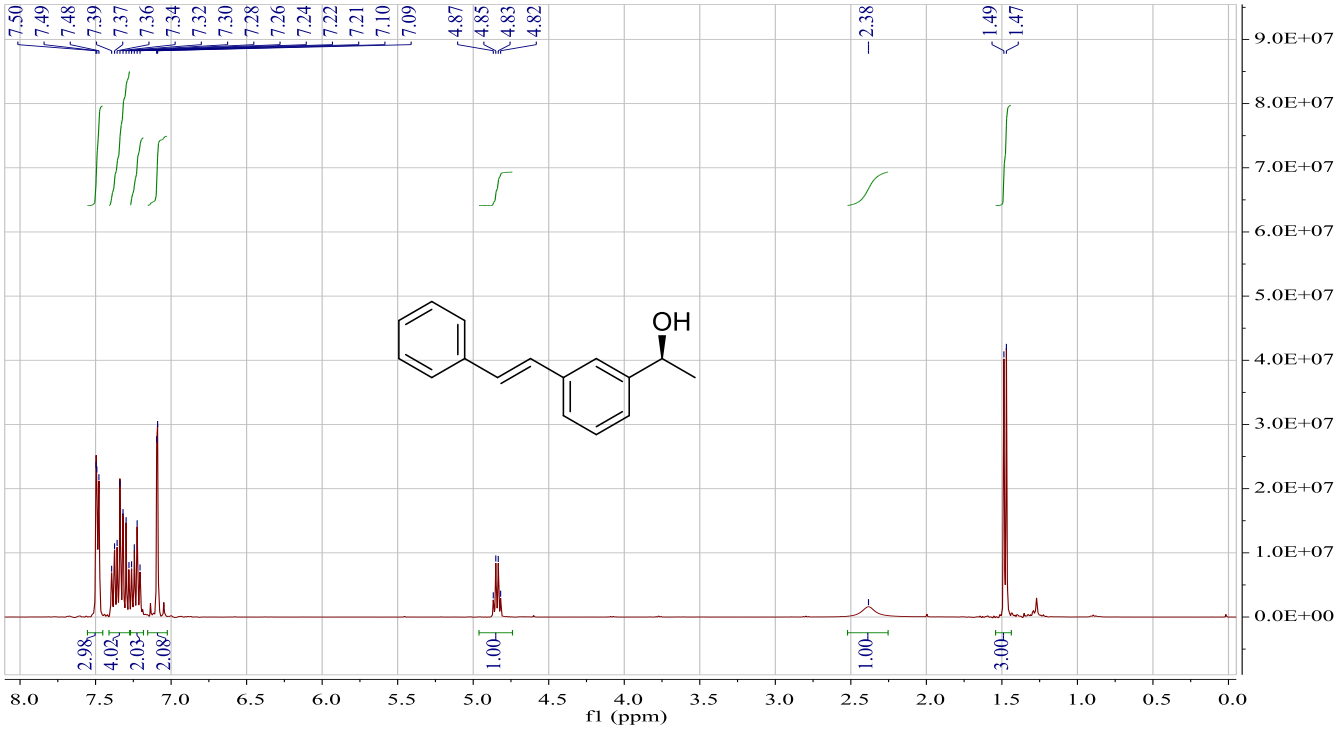
(*S*,*E*)−1−(4−styrylphenyl)ethanol (8p).

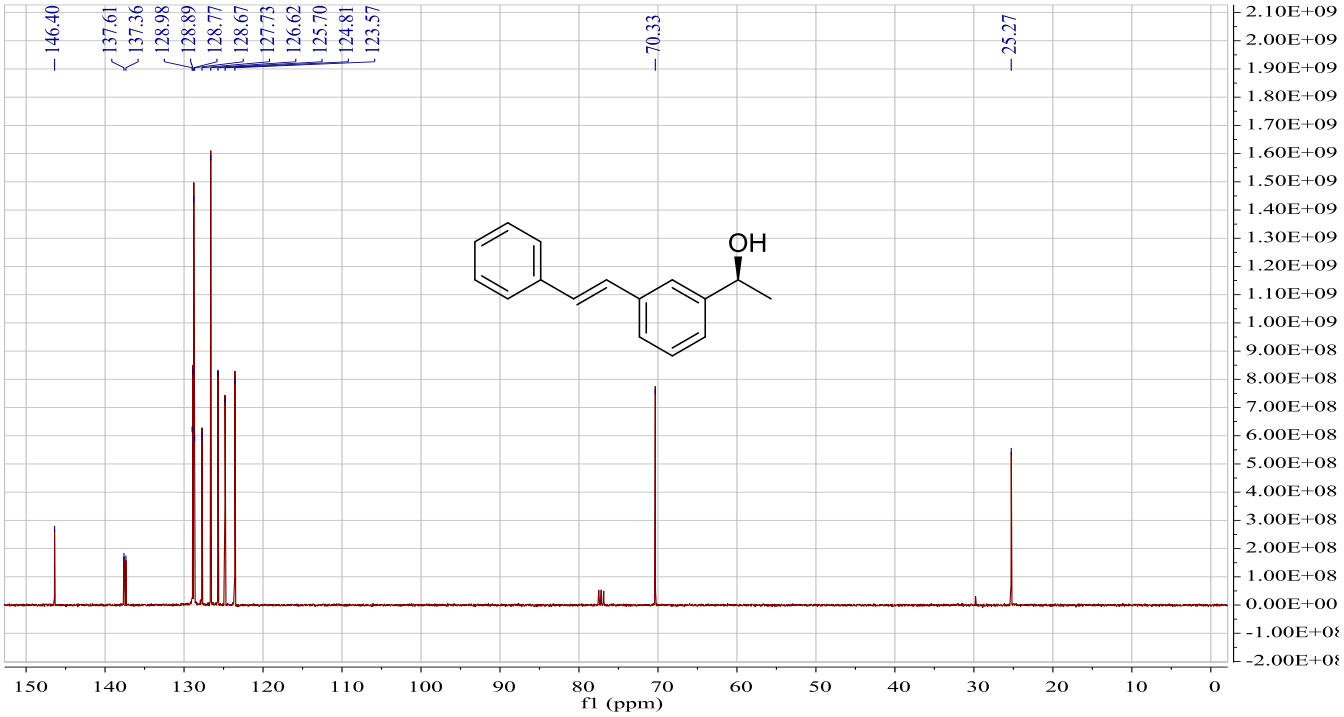


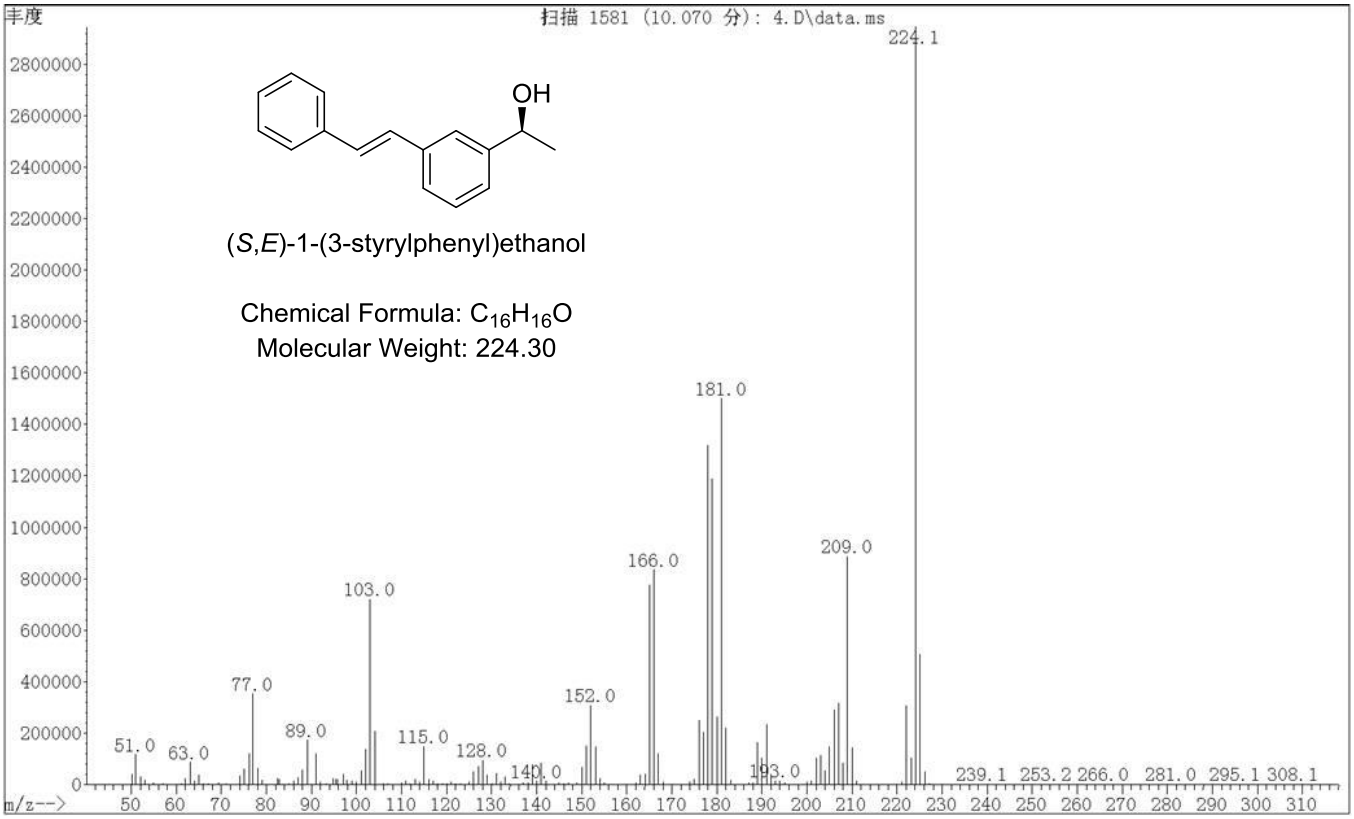



丰度
扫描 1600 (10.189 分): 3.D\data.ms
OH
(S,E)-1-(4-styrylphenyl)ethanol
Chemical Formula: C16H16O
Molecular Weight: 224.30
209.0
224.0
178.0
165.0
103.0
77.0
152.0
191.0
51.0
63.0
89.0
115.0
128.0
141.0
280.8
m/z-->

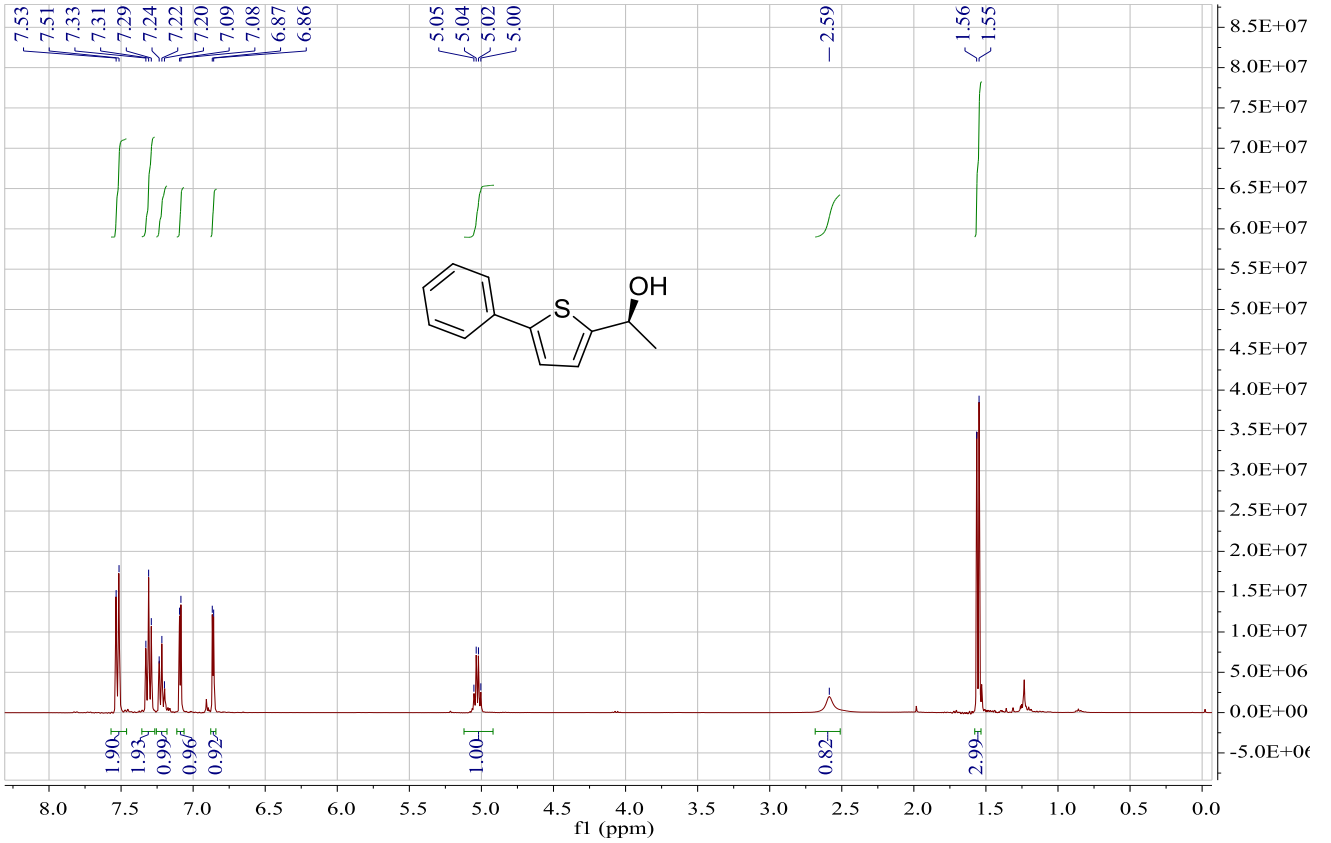
(*S*,*E*)−1−(3−styrylphenyl)ethanol (8q).

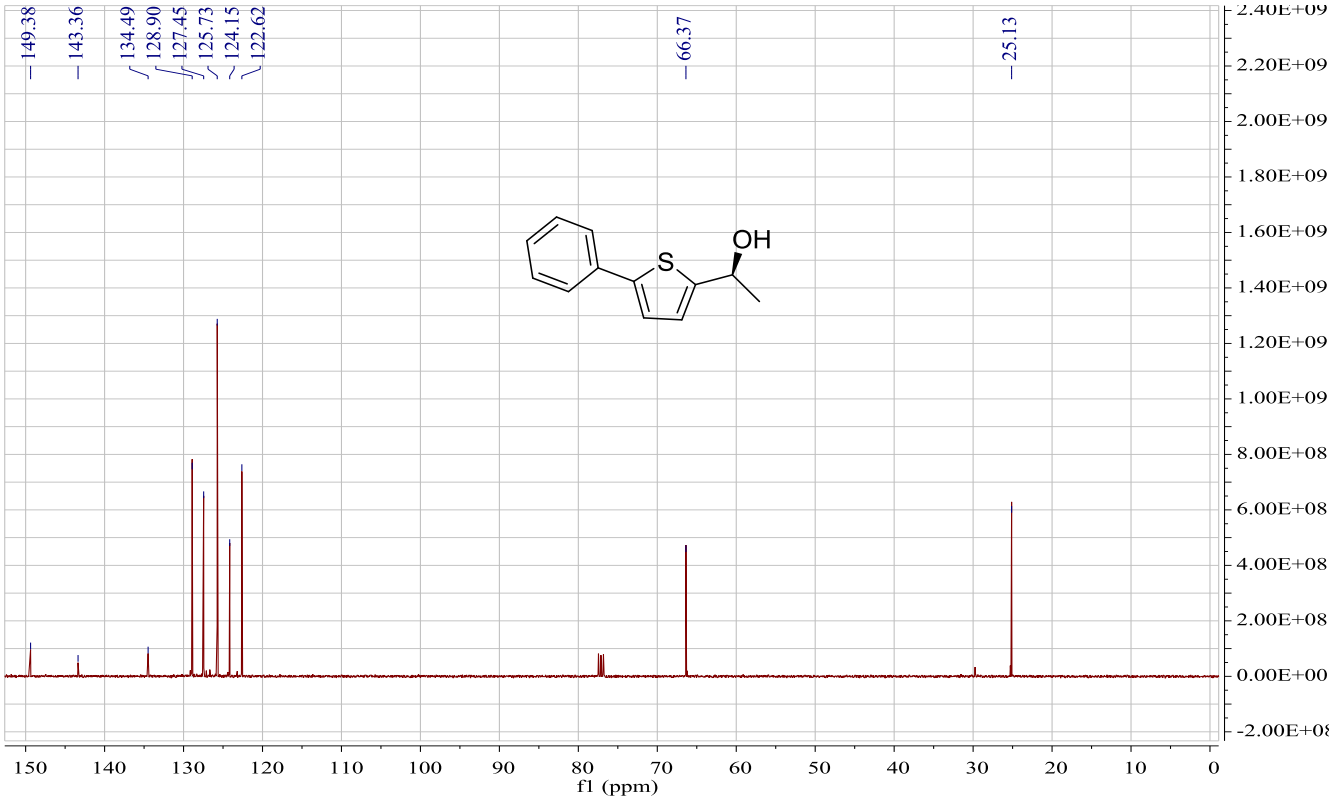


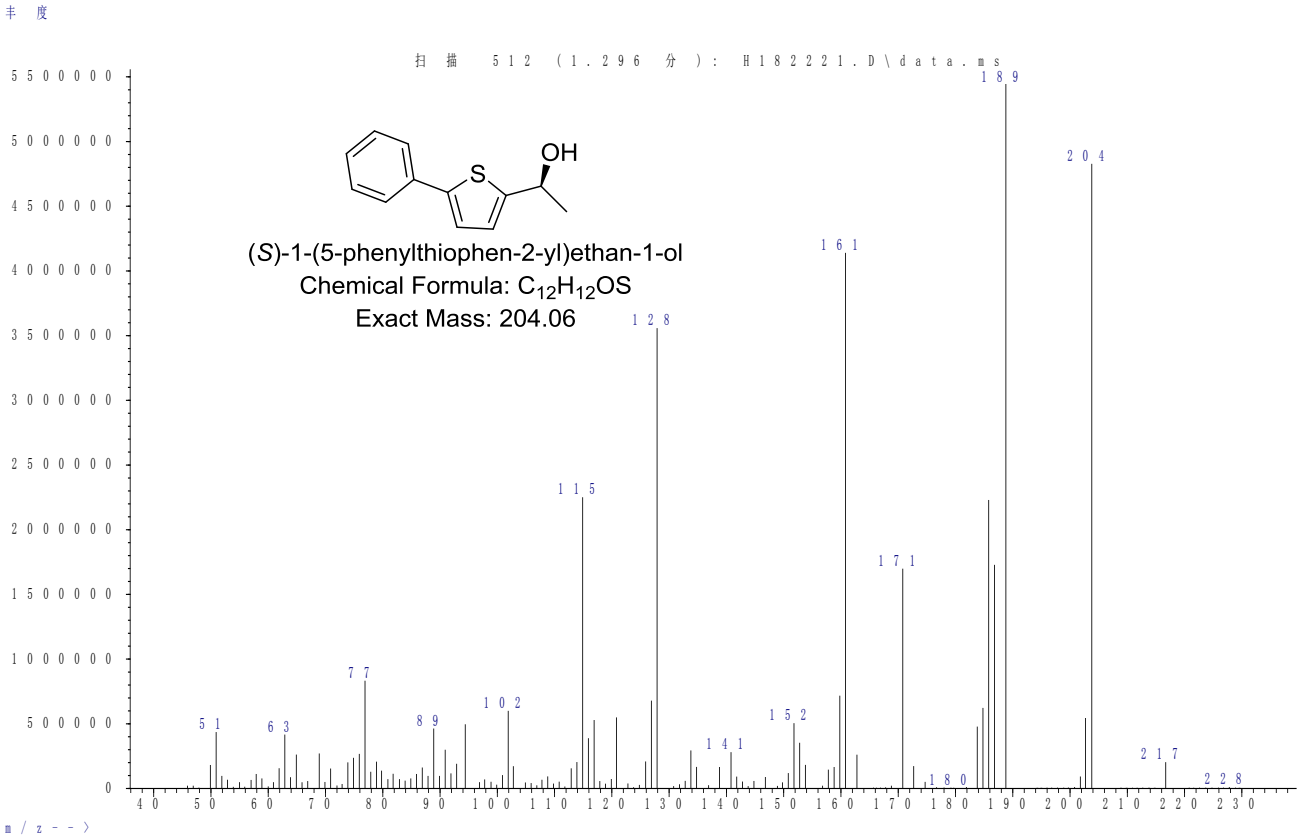



丰度
扫描 1581 (10.070 分): 4.D\data.ms
OH
(S,E)-1-(3-styrylphenyl)ethanol
Chemical Formula: C16H16O
Molecular Weight: 224.30
224.1
181.0
209.0
166.0
103.0
77.0
152.0
89.0
115.0
128.0
51.0
63.0
141.0
193.0
239.1
253.2
266.0
281.0
295.1
308.1
m/z-->

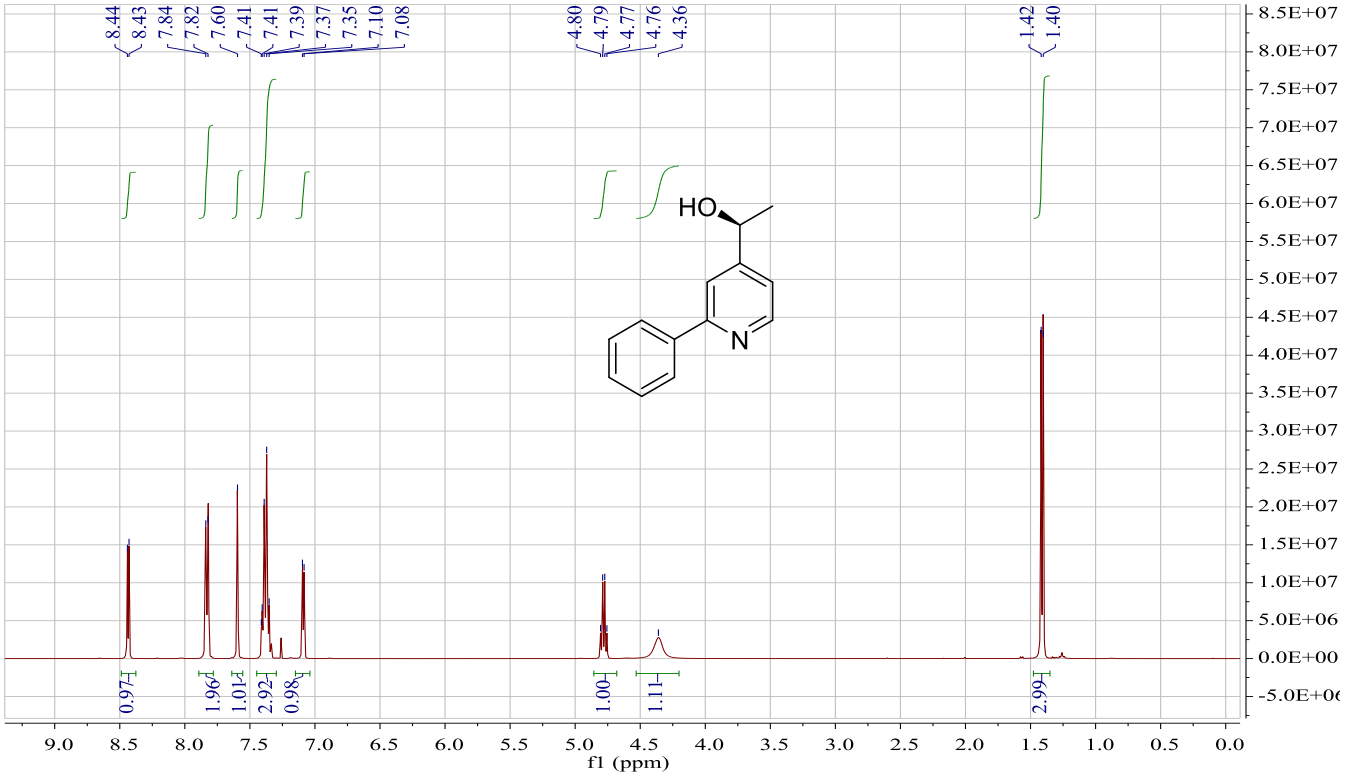
(*S*)−1−(5−phenylthiophen−2−yl)ethanol (8r).

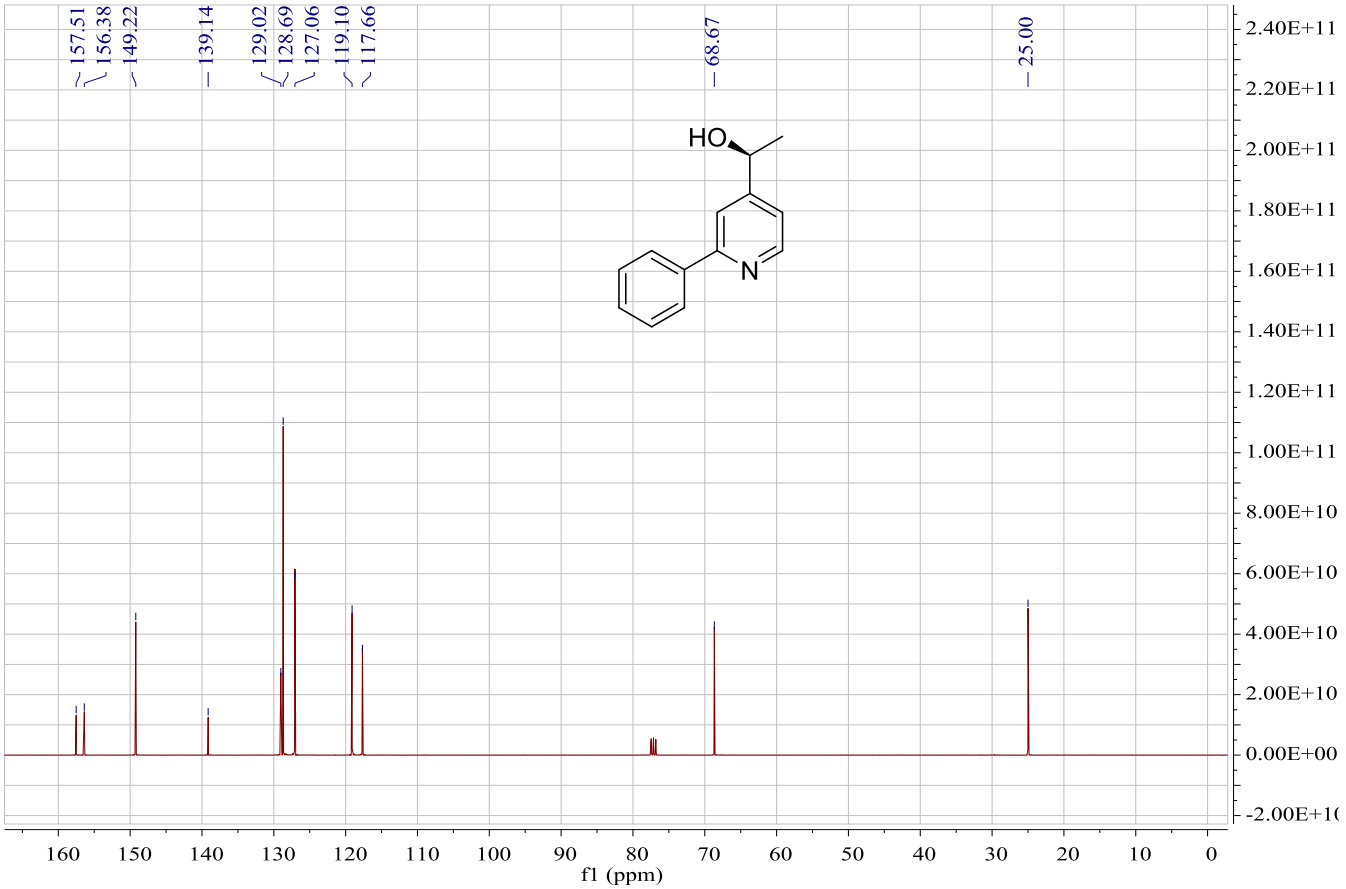


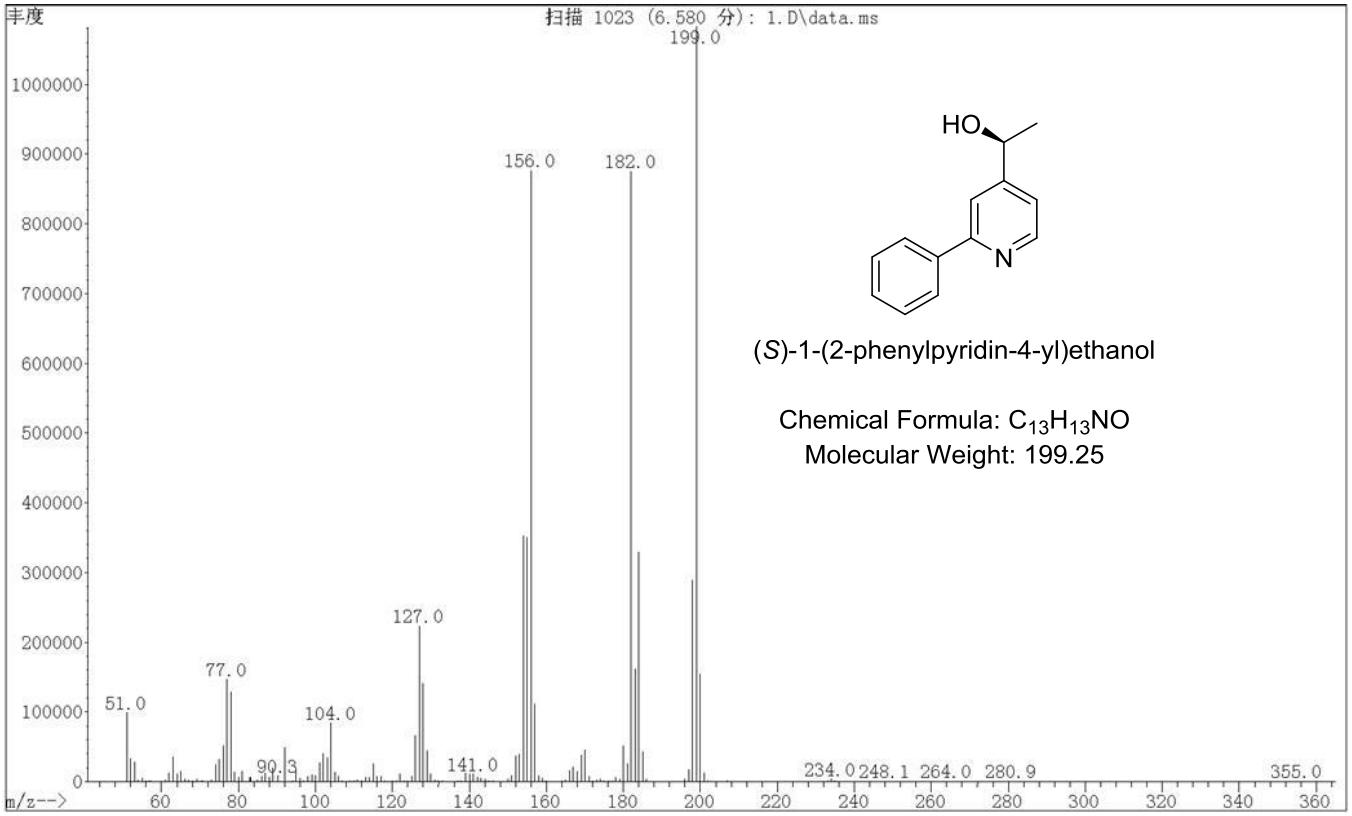



丰 度
扫 描 512 (1.296 分): H182221.D\data.ms
OH
S
(S)-1-(5-phenylthiophen-2-yl)ethan-1-ol
Chemical Formula: C12H12OS
Exact Mass: 204.06
m/z-->
189
204
161
128
115
171
77
102
89
152
51
63
141
180
217
228

(*S*)−1−(2−phenylpyridin−4−yl)ethanol (8s).



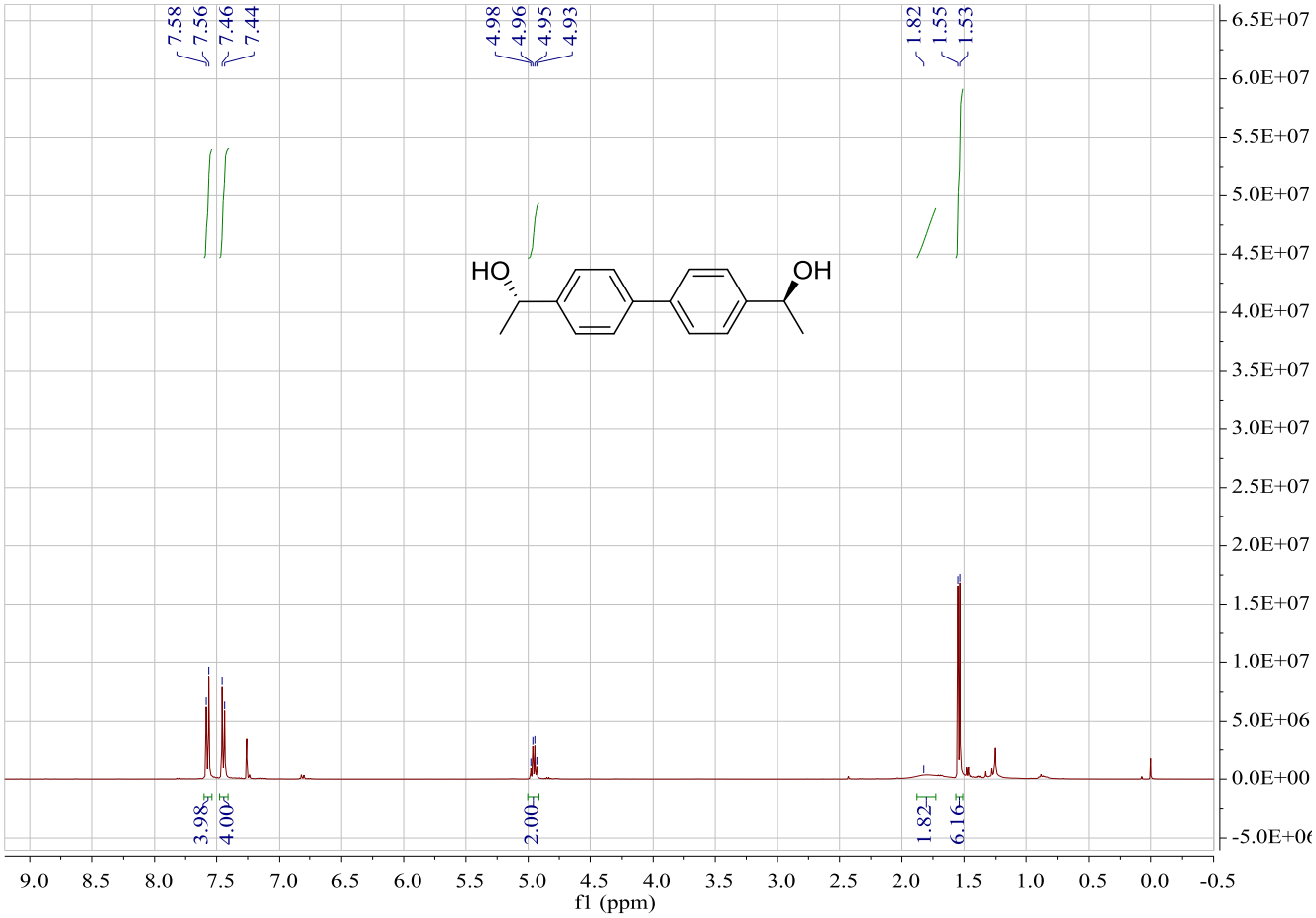




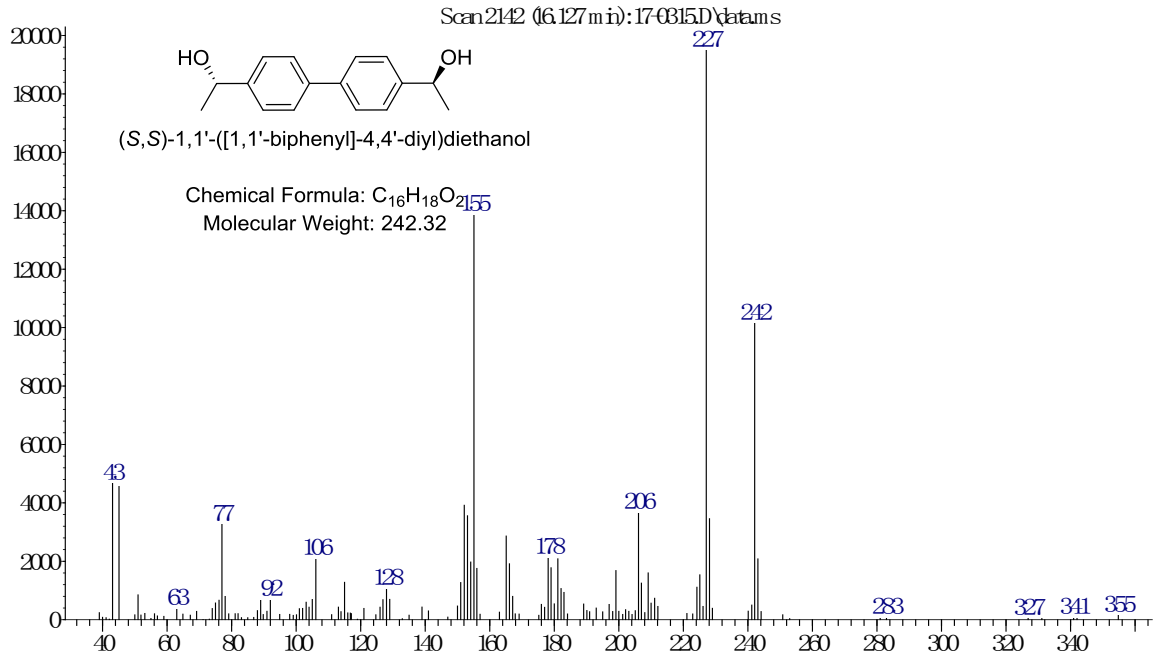
(*S*)-1-(2-phenylpyridin-4-yl)ethanol

Chemical Formula: $C_{13}H_{13}NO$
Molecular Weight: 199.25

(*S*,*S*)−1,1'−([1,1'−biphenyl]−4,4'−diyl)diethanol (8t).

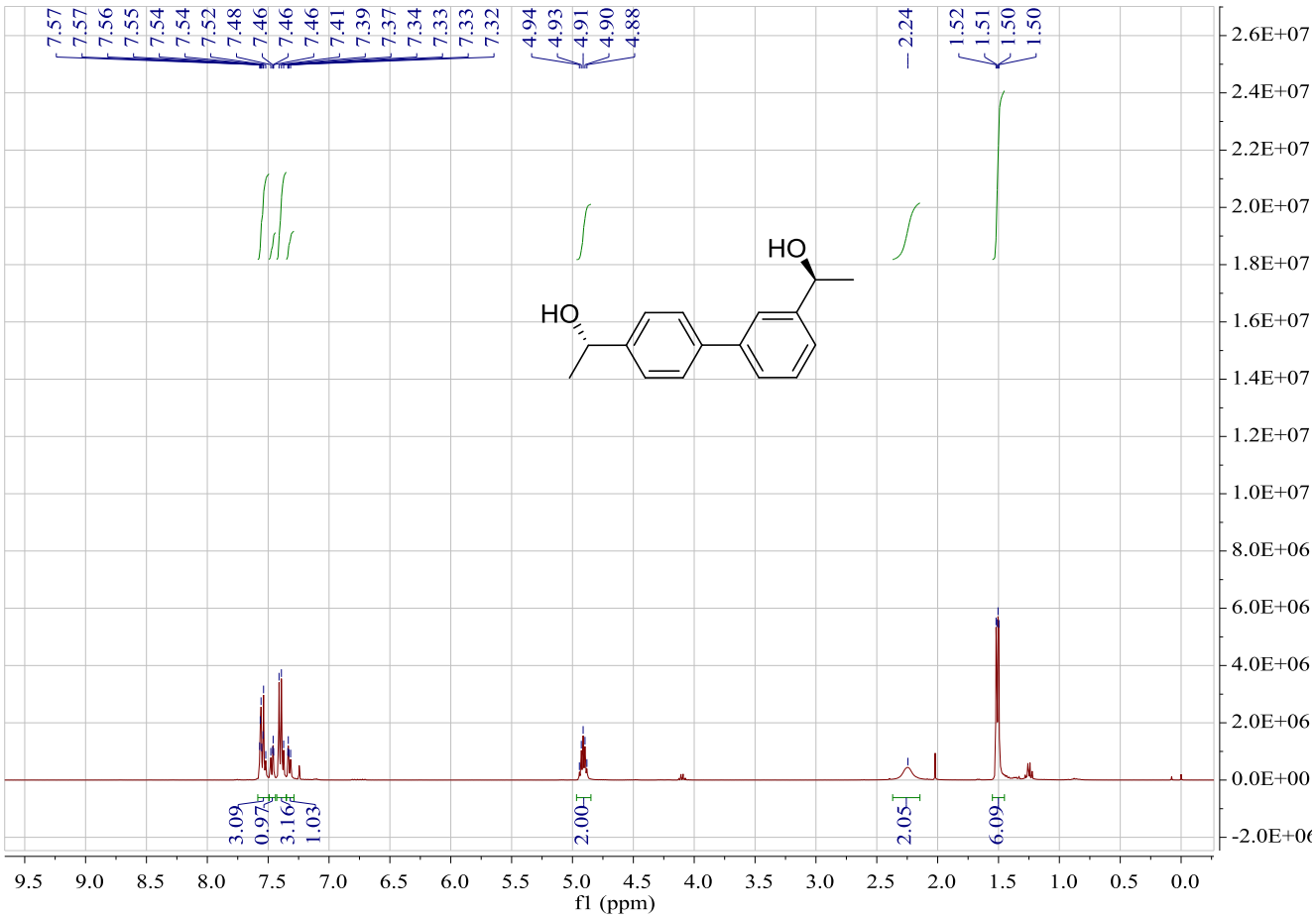


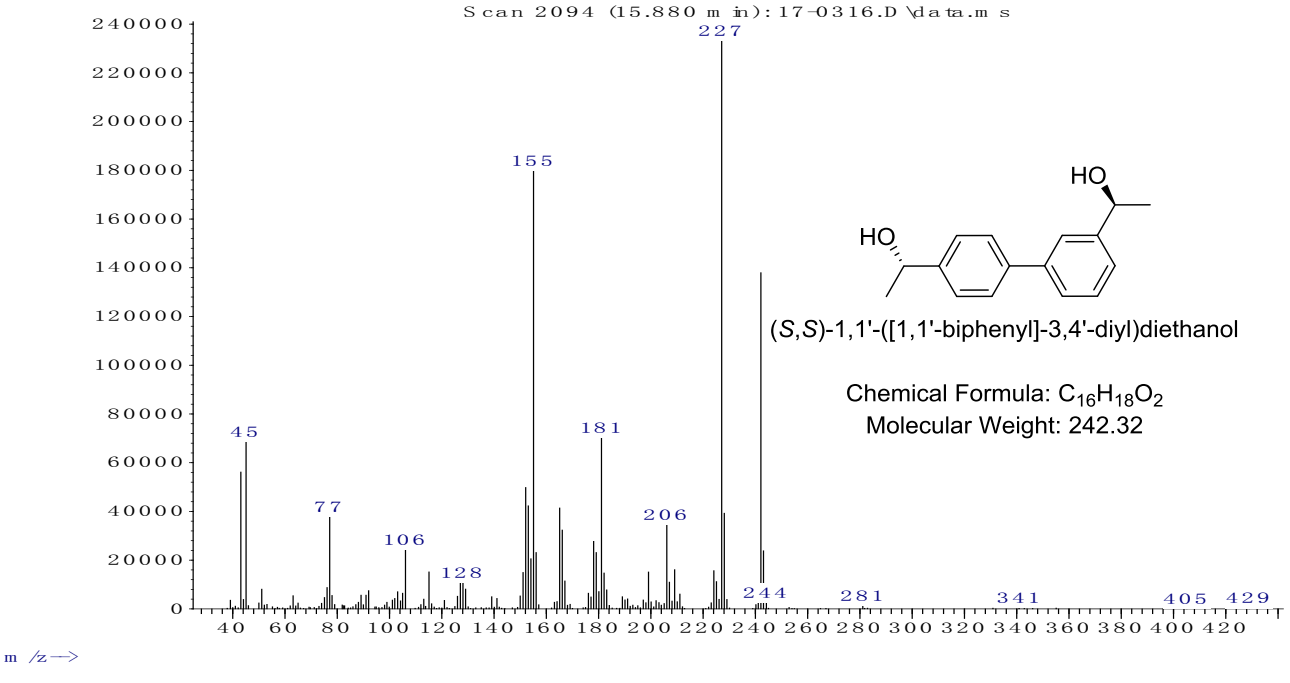
Abundance



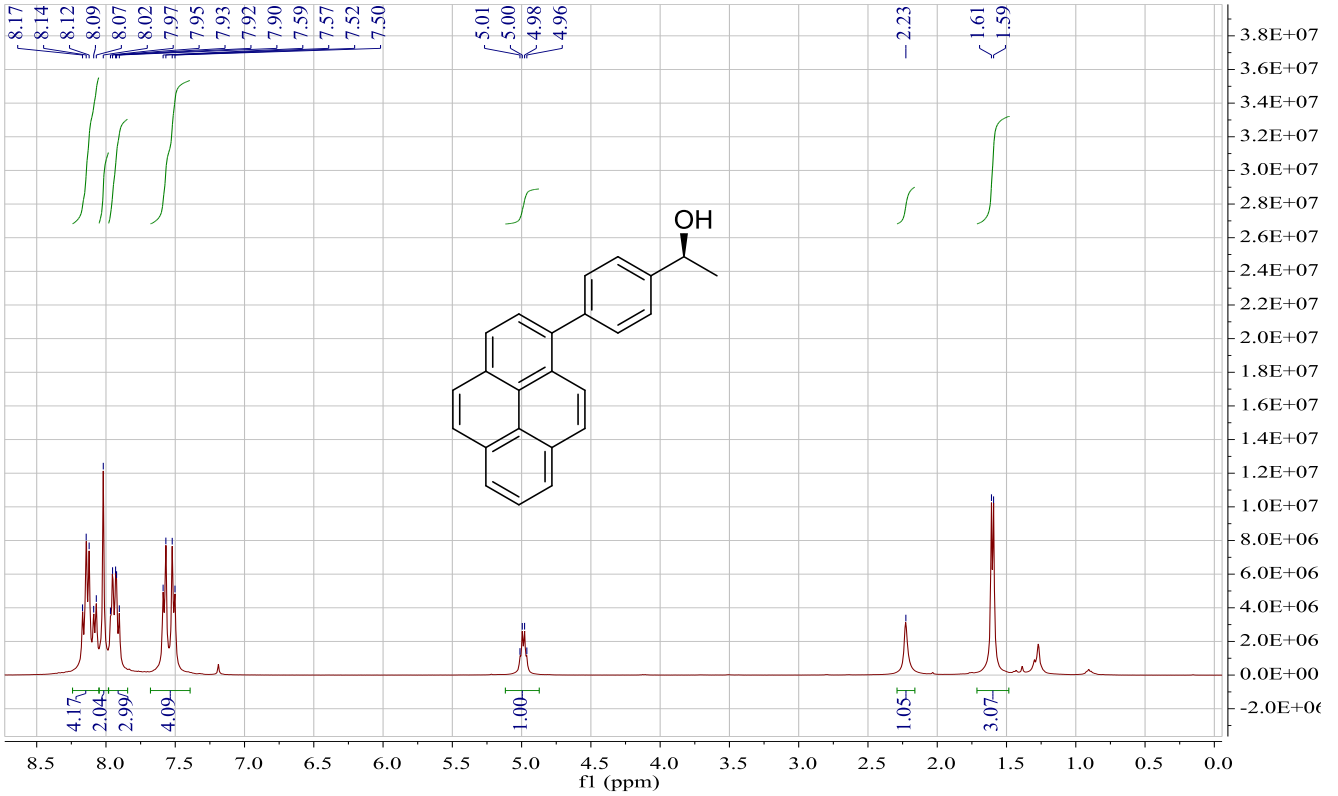
m/z→

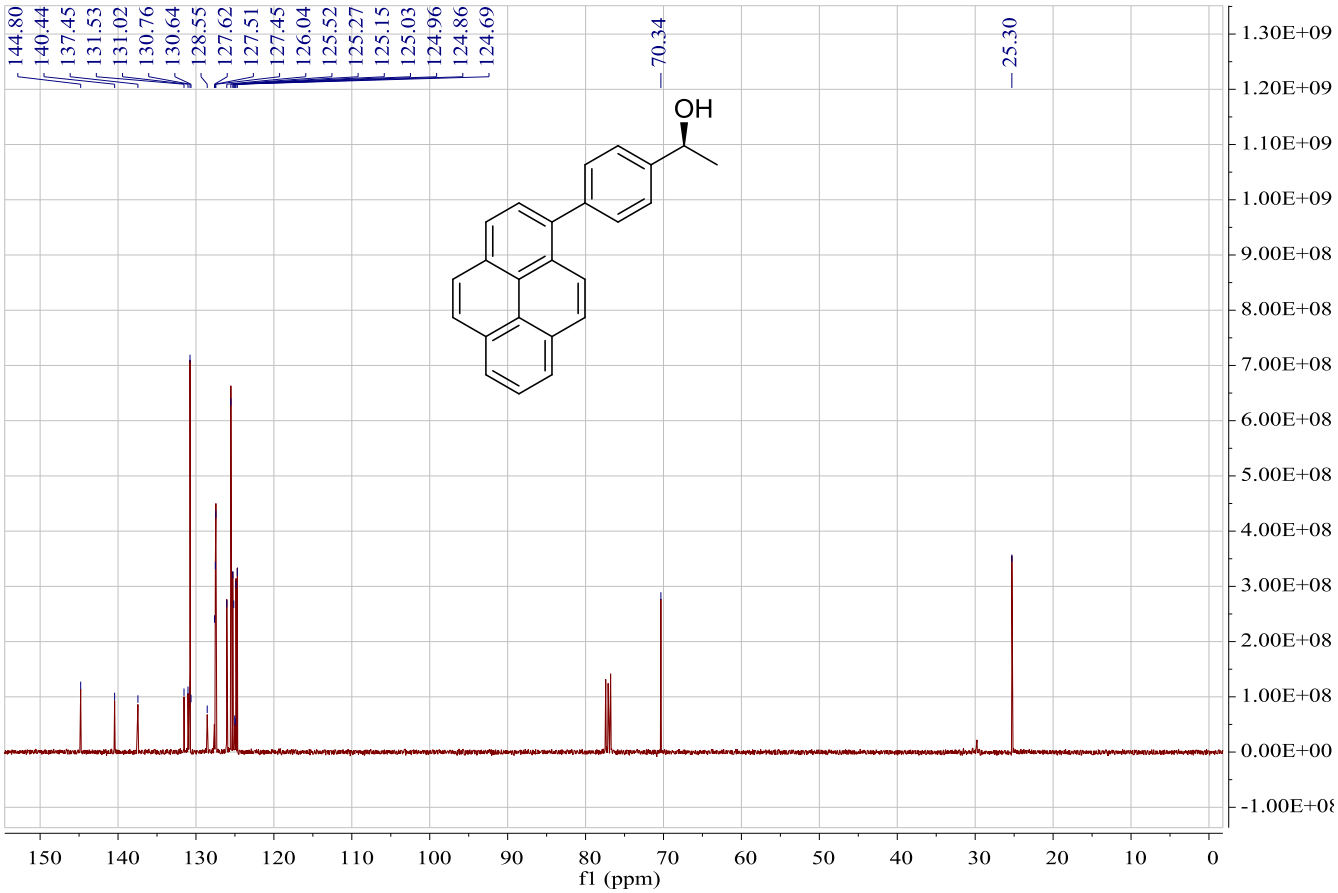
(*S*,*S*)−1,1'−([1,1'−biphenyl]−3,4'−diyl)diethanol (8u).



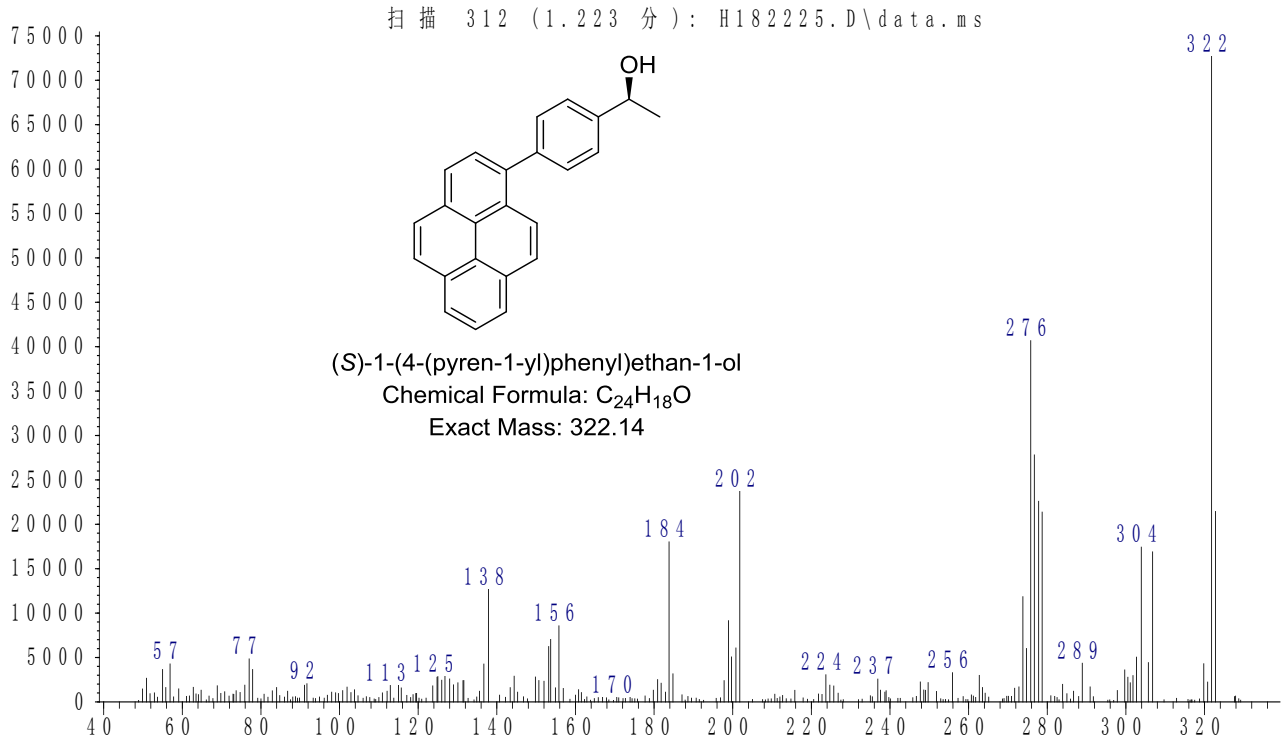


(*S*)−1−(4−(pyren−1−yl)phenyl)ethanol (8v).





丰 度


扫 描 312 (1.223 分): H182225.D\data.ms
OH
(S)-1-(4-(pyren-1-yl)phenyl)ethan-1-ol
Chemical Formula: C24H18O
Exact Mass: 322.14
75000
70000
65000
60000
55000
50000
45000
40000
35000
30000
25000
20000
15000
10000
5000
0
40 60 80 100 120 140 160 180 200 220 240 260 280 300 320
322
276
202
184
304
138
156
57
77
92
113
125
170
224
237
256
289
m/z-->
S64