Electronic Supplementary Material (ESI) for Green Chemistry.

Supporting Information

A chemo-enzymatic oxidation/Aldol sequential process directly converts arylbenzyl alcohols and cyclohexanol into chiral ß-hydroxy carbonyls

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CONTENTS

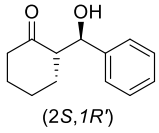
Experimental

1. General: All manipulations were carried out under an inert atmosphere using a nitrogen-filled glovebox or Schlenk techniques. Deuterated solvents were purchased commercially and were degassed and stored over activated 4 Å molecular sieves. All other reagents were obtained from commercial sources and used without further purification. The *Trametes versicolor* was obtained from Sigma−Aldrich Company Ltd and used as received. Enzymatic activity was 0.78 unit mg^{-1} protein (One unit is defined as the amount of enzyme that can reduce 1 μmol alcohol for a minute at pH 5.0 and 30 ℃).

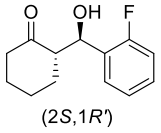
2. Characterization: The ^1H NMR spectra were performed on a Bruker Avance DPX-400 spectrometer in $CDCl_3$ solutions. Chemicals shifts are given in parts per million (δ units) downfield from tetramethylsilane using the residual solvent signal ($CHCl_3$, δ 7.26) as internal standard. ^1H NMR information is given in the following format: multiplicity (s, singlet; d, doublet; t, triplet; q, quartet; qui, quintet; sept, septet; m, multiplet), coupling constant(s) (J) in Hertz (Hz), the number of protons. The prefix app is occasionally applied when the true signal multiplicity was unresolved and br indicates the signal in question broadened. High-resolution mass spectrometry (HRMS) spectra were obtained on a micro TOF-QII Instrument.

3. Data of chiral products.

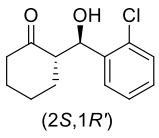
(*S,R*)-5a: (*S*)-2-((*R*)-hydroxy(phenyl)methyl)cyclohexan-1-one. (Laccase/**E** + catalyst **D**): 35% yield, 95% *ee*, 91/9 *dr*; (Laccase/**E** + catalyst **C**): 75% yield, 97% ee, 95/5 *dr*. ^1H NMR (400 MHz, Chloroform-*d*): δ 7.44 – 7.21 (m, 4H), 4.79 (d, J = 8.8 Hz, 1H), 2.70 – 2.28 (m, 2H), 2.09 (ddt, J = 12.5, 5.9, 3.1 Hz, 1H), 1.89 – 1.45 (m, 4H), 1.42 – 1.24 (m, 1H). HRMS (ESI): m/z $[M+H]^+$ calcd for $[C_{13}H_{16}NO_2]^+$ 205.1223; found: 205.1223. (HPLC: Chiracel OD-H, detected at 213 nm, eluent: n-hexane/2-propanol = 99/1, flow rate = 1.0 mL/min, 25 ℃).



(*S,R*)-5b: (*S*)-2-((*R*)-(2-fluorophenyl)(hydroxy)methyl)cyclohexan-1-one. (Laccase/**E** + catalyst **D**): 88% yield, 99% *ee*, 98/2 *dr*; (Laccase/**E** + catalyst **C**): 76% yield, 98% *ee*, 98/2 *dr*. ^1H NMR (400 MHz, Chloroform-*d*): δ 7.40 (td, J = 7.4, 1.9 Hz, 1H), 7.23 – 7.15 (m, 1H), 7.14 – 6.88 (m, 2H), 5.11 (d, J = 8.7 Hz, 1H), 2.69 – 2.55 (m, 1H), 2.48 – 2.21 (m, 2H), 2.02 (ddt, J = 12.2, 5.8, 2.9 Hz, 1H), 1.82 – 1.71 (m, 1H), 1.67 – 1.30 (m, 4H). HRMS (ESI): m/z $[M+H]^+$ calcd for $[C_{13}H_{15}FO_2]^+$ 223.1129; found: 223.1130. (HPLC: Chiracel AS-H, detected at 254 nm, eluent: n-hexane/2-propanol = 95/5, flow rate = 1.0 mL/min, 25 ℃).

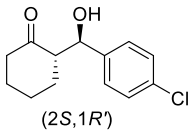


(*S,R*)-5c: (*S*)-2-((*R*)-(2-chlorophenyl)(hydroxy)methyl)cyclohexan-1-one. (Laccase/**E** + catalyst **D**): 68% yield, 96% *ee*, 98/2 *dr*; (Laccase/**E** + catalyst **C**): 76% yield, 93% *ee*, 90/10 *dr*. ^{1}H NMR (400 MHz, Chloroform-*d*): δ 7.55 – 7.08 (m, 4H), 5.67 – 5.23 (m, 1H), 2.79 – 2.55 (m, 1H), 2.45 – 2.22 (m, 2H), 2.07 – 1.97 (m, 1H), 1.82 – 1.41 (m, 5H)). HRMS (ESI): m/z $[M+H]^+$ calcd for $[C_{13}H_{16}ClO_2]^+$ 283.0328 ; found: 283.0834. (HPLC: Chiracel OD-H, detected at 220 nm, eluent: n-hexane/2-propanol = 99/1, flow rate = 1.0 mL/min, 25 ℃).



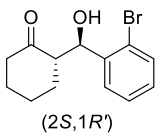
(2*S*,1*R*′)

(*S,R*)-5d: (*S*)-2-((*R*)-(4-chlorophenyl)(hydroxy)methyl)cyclohexan-1-one. (Laccase/**E** + catalyst **D**): 62% yield, 96% *ee*, 89/11 *dr*; (Laccase/**E** + catalyst **C**): 64% yield, 97% *ee*, 84/16 *dr*. ^{1}H NMR (400 MHz, Chloroform-*d*): δ 7.31 – 7.12 (m, 4H), 5.34 – 4.63 (m, 1H), 2.56 – 2.21 (m, 3H), 2.02 (ddt, J = 12.2, 5.8, 3.0 Hz, 1H), 1.82 – 1.39 (m, 4H), 1.22 (qd, J = 13.6, 12.9, 5.0 Hz, 1H). HRMS (ESI): m/z $[M+H]^+$ calcd for $[C_{13}H_{16}ClO_2]^+$ 283.0833; found: 283.0834. (HPLC: Chiracel AD-H, detected at 220 nm, eluent: n-hexane/2-propanol = 90/10, flow rate = 0.5 mL/min, 25 ℃).



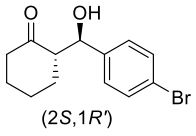
(2*S*,1*R*′)

(*S,R*)-5e: (*S*)-2-((*R*)-(2-bromophenyl)(hydroxy)methyl)cyclohexan-1-one. (Laccase/**E** + catalyst **D**): 80% yield, 94% *ee*, 93/7 *dr*; (Laccase/**E** + catalyst **C**): 84 %yield, 93% *ee*, 90/10 *dr*. ^{1}H NMR (400 MHz, Chloroform-*d*): δ 7.57 – 7.22 (m, 3H), 7.14 – 7.00 (m, 1H), 5.23 (d, J = 8.0 Hz, 1H), 2.83 – 2.43 (m, 1H), 2.43 – 2.18 (m, 2H), 2.10 – 1.93 (m, 1H), 1.83 – 1.34 (m, 5H). HRMS (ESI): m/z $[M+H]^+$ calcd for $[C_{13}H_{16}BrO_2]^+$283.0328; found: 283.0327. (HPLC: Chiracel OD-H, detected at 220 nm, eluent: n-hexane/2-propanol = 90/10, flow rate = 0.5 mL/min, 25 ℃).



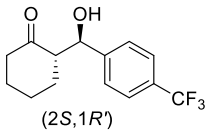
(2*S*,1*R*′)

(*S,R*)-5f: (*S*)-2-((*R*)-(4-bromophenyl)(hydroxy)methyl)cyclohexan-1-one. (Laccase/**E** + catalyst **D**): 71% yield, 95% *ee*, 88/12 *dr*; (Laccase/**E** + catalyst **C**): 78 %yield, 92% *ee*, 89/11 *dr*. ^{1}H NMR (400 MHz, Chloroform-*d*): δ 7.44 – 7.34 (m, 2H), 7.12 (dd, J = 8.6, 6.8 Hz, 2H), 5.32 – 4.61 (m, 1H), 2.55 – 2.21 (m, 3H), 2.02 (ddt, J = 12.2, 5.7, 2.9 Hz, 1H), 1.86 – 1.38 (m, 4H), 1.22 (qd, J = 13.6, 13.0, 5.0 Hz, 1H). HRMS (ESI): m/z $[M+H]^+$ calcd for $[C_{13}H_{16}BrO_2]^+$ 283.0328 ; found: 283.0319 (HPLC: Chiracel AD-H, detected at 220 nm, eluent: n-hexane/2-propanol = 90/10, flow rate = 1.0 mL/min, 25 ℃).



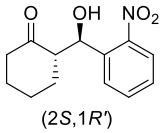
(2*S*,1*R*′)

(*S,R*)-5g: (*S*)-2-((*R*)-hydroxy(4-(trifluoromethyl)phenyl)methyl)cyclohexan-1-one. (Laccase/**E** + catalyst **D**): 29% yield, 98% *ee*, 91/9 *dr*; (Laccase/**E** + catalyst **C**): 75% yield, 98% *ee*, 91/9 *dr*. ^{1}H NMR (400 MHz, Chloroform-*d*): δ 7.59 – 7.15 (m, 4H), 5.42 – 4.70 (m, 1H), 2.57 – 2.21 (m, 3H), 2.03 (ddt, J = 12.2, 5.8, 3.0 Hz, 1H), 1.82 – 1.42 (m, 4H), 1.36 – 1.16 (m, 1H)). HRMS (ESI): m/z $[M+H]^+$ calcd for $[C_{14}H_{16}F_3O_2]^+$ 273.1097; found: 273.1098 (HPLC: Chiracel AD-H, detected at 220 nm, eluent: n-hexane/2-propanol = 90/10, flow rate = 0.5 mL/min, 25 ℃).

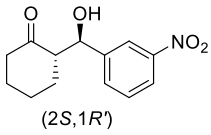


(2*S*,1*R*′)

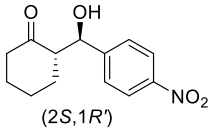
(*S*,*R*)-5h: (*S*)-2-((*R*)-hydroxy(2-nitrophenyl)methyl)cyclohexan-1-one. (Laccase/**E** + catalyst **D**): 90% yield, 99% *ee*, 98/2 *dr*; (Laccase/**E** + catalyst **C**): 85% yield, 99% *ee*, 98/2 *dr*. ^{1}H NMR (400 MHz, Chloroform-*d*): δ 7.95 – 7.30 (m, 4H), 5.37 (d, J = 7.0 Hz, 1H), 4.08 (d, J = 21.9 Hz, 1H), 2.86 – 2.60 (m, 1H), 2.44 – 2.22 (m, 2H), 2.02 (ddt, J = 12.6, 5.8, 3.0 Hz, 1H), 1.82 – 1.40 (m, 5H). HRMS (ESI): m/z $[M+H]^+$ calcd for $[C_{13}H_{15}NO_4]^+$ 250.1074; found: 250.1073. (HPLC: Chiracel AS-H, detected at 254 nm, eluent: n-hexane/2-propanol = 95/5, flow rate = 0.5 mL/min, 25 ℃).



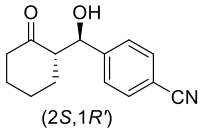
(*S*,*R*)-5i: (*S*)-2-((*R*)-hydroxy(3-nitrophenyl)methyl)cyclohexan-1-one. (Laccase/**E** + catalyst **D**): 87% yield, 98% *ee*, 89/11 *dr*; (Laccase/**E** + catalyst **C**): 80% yield, 99% *ee*, 95/5 *dr*. ^{1}H NMR (400 MHz, Chloroform-*d*): δ 8.19 – 8.01 (m, 2H), 7.59 (dq, J = 7.8, 1.9 Hz, 1H), 7.44 (td, J = 7.9, 3.6 Hz, 1H), 4.81 (dd, J = 8.5, 2.2 Hz, 1H), 4.23 – 3.83 (m, 1H), 2.63 – 2.24 (m, 3H), 2.11 – 1.94 (m, 1H), 1.86 – 1.14 (m, 5H). HRMS (ESI): m/z $[M+H]^+$ calcd for $[C_{13}H_{15}NO_4]^+$ 250.1074; found: 250.1073. (HPLC: Chiracel AD-H, detected at 254 nm, eluent: n-hexane/2-propanol = 95/5, flow rate = 0.8 mL/min, 25 ℃).



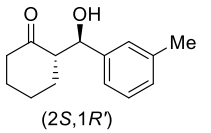
(*S*,*R*)-5j: (*S*)-2-((*R*)-hydroxy(4-nitrophenyl)methyl)cyclohexan-1-one. (Laccase/**E** + catalyst **D**): 91% yield, 99% *ee*, 93/7 *dr*; (Laccase/**E** + catalyst **C**): 82% yield, 99% *ee*, 92/8 *dr*. ^{1}H NMR (400 MHz, Chloroform-*d*): δ 7.31 – 7.12 (m, 4H), 5.34 – 4.63 (m, 1H), 2.56 – 2.21 (m, 3H), 2.02 (ddt, J = 12.2, 5.8, 3.0 Hz, 1H), 1.82 – 1.39 (m, 4H), 1.22 (qd, J = 13.5, 12.9, 5.0 Hz, 1H)). HRMS (ESI): m/z $[M+H]^+$ calcd for $[C_{13}H_{15}NO_4]^+$ 250.1074; found: 250.1073. (HPLC: Chiracel AD-H, detected at 254 nm, eluent: n-hexane/2-propanol = 90/10, flow rate = 1.0 mL/min, 25 ℃).



(*S*,*R*)-5k: 4-((*S*)-hydroxy((*R*)-2-oxocyclohexyl)methyl)benzonitrile. (Laccase/**E** + catalyst **D**): 91% yield, 87% *ee*, 82/18 *dr*; (Laccase/**E** + catalyst **C**): 89% yield, 96% *ee*, 90/10 *dr*. ^{1}H NMR (400 MHz, Chloroform-*d*): δ 7.61 – 7.30 (m, 4H), 5.39 – 4.71 (m, 1H), 3.55 (dd, J = 345.7, 3.2 Hz, 1H), 2.56 – 2.22 (m, 3H), 2.02 (ddt, J = 12.1, 5.9, 2.9 Hz, 1H), 1.81 – 1.40 (m, 4H), 1.33 – 1.15 (m, 1H). HRMS (ESI): m/z $[M+H]^+$ calcd for $[C_{14}H_{15}NO_2]^+$ 230.1176; found: 230.1175. (HPLC: Chiracel AD-H, detected at 220 nm, eluent: n-hexane/2-propanol = 90/10, flow rate = 0.5 mL/min, 25 ℃).

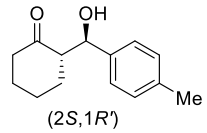


(*S*,*R*)-5l: (*S*)-2-((*R*)-hydroxy(m-tolyl)methyl)cyclohexan-1-one. (Laccase/**E** + catalyst **D**): 29% yield, 95% *ee*, 95/5 *dr*; (Laccase/**E** + catalyst **C**): 46% yield, 91% *ee*, 89/11 *dr*. ^{1}H NMR (400 MHz, Chloroform-*d*): δ 7.44 – 6.97 (m, 4H), 5.34 – 4.60 (m, 1H), 2.59 – 2.35 (m, 2H), 2.29 (d, J = 7.0 Hz, 3H), 2.01 (ddt, J = 12.3, 5.8, 3.0 Hz, 1H), 1.90 – 1.41 (m, 4H), 1.28 – 1.15 (m, 1H). HRMS (ESI): m/z $[M+H]^+$ calcd for $[C_{14}H_{18}O_2]^+$ 218.138; found:

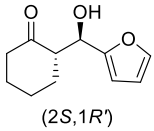


218.1378. (HPLC: Chiracel OD-H, detected at 254 nm, eluent: n-hexane/2-propanol = 97/3, flow rate = 0.5 mL/min, 25 ℃).

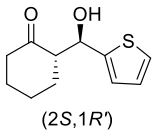
(*S,R*)-5m: (*S*)-2-((*R*)-hydroxy(p-tolyl)methyl)cyclohexan-1-one. (Laccase/**E** + catalyst **D**): 14% yield, 97% *ee*, 94/6 *dr*; (Laccase/**E** + catalyst **C**): 46% yield, 96% *ee*, 92/8 *dr*. ^{1}H NMR (400 MHz, Chloroform-*d*): δ 7.26 – 7.00 (m, 4H), 5.32 – 4.61 (m, 1H), 2.53 (dddd, J = 12.8, 8.8, 5.5, 1.2 Hz, 1H), 2.40 (dddd, J = 13.6, 4.6, 3.0, 1.7 Hz, 1H), 2.33 – 2.23 (m, 4H), 2.00 (ddq, J = 11.8, 5.7, 2.9 Hz, 1H), 1.75 – 1.40 (m, 4H), 1.27 – 1.14 (m, 1H). HRMS (ESI): m/z $[M+H]^+$ calcd for $[C_{14}H_{18}O_2]^+$ 218.138; found: 218.1376. (HPLC: Chiracel OD-H, detected at 254 nm, eluent: n-hexane/2-propanol = 97/3, flow rate = 0.5 mL/min, 25 ℃).



(*S,R*)-5n: (S)-2-((R)-furan-2-yl(hydroxy)methyl)cyclohexan-1-one. (Laccase/**E** + catalyst **D**): 64% yield, 87% *ee*, 94/6 *dr*; (Laccase/**E** + catalyst **C**): 77% yield, 90% *ee*, 80/20 *dr*. ^{1}H NMR (400 MHz, Chloroform-*d*): δ 7.47 (dd, J = 65.3, 1.7 Hz, 1H), 6.65 – 6.25 (m, 2H), 4.83 (d, J = 8.5 Hz, 1H), 2.92 (h, J = 6.9, 6.0 Hz, 1H), 2.55 – 2.32 (m, 2H), 2.17 – 1.52 (m, 5H), 1.41 – 1.23 (m, 1H). HRMS (ESI): m/z $[M+H]^+$ calcd for $[C_{11}H_{14}O_3]^+$ 211.0787; found: 211.0782. (HPLC: Chiracel AD-H, detected at 220 nm, eluent: n-hexane/2-propanol = 90/10, flow rate = 0.5 mL/min, 25 ℃).



(*S,R*)-5o: (*S*)-2-((*R*)-hydroxy(thiophen-2-yl)methyl)cyclohexan-1-one. (Laccase/**E** + catalyst **D**): 44% yield, 91% *ee*, 85/15 *dr*; (Laccase/**E** + catalyst **C**): 64 %yield, 68% *ee*, 72/28 *dr*. ^{1}H NMR (400 MHz, Chloroform-*d*): δ 7.34 – 6.83 (m, 3H), 5.53 – 4.96 (m, 1H), 2.66 – 2.54 (m, 1H), 2.46 – 2.23 (m, 2H), 1.80 – 1.47 (m, 4H), 1.33 – 1.14 (m, 1H). HRMS (ESI): m/z $[M+H]^+$ calcd for $[C_{11}H_{14}SO_2]^+$ 211.0787; found: 211.0782. (HPLC: Chiracel AD-H, detected at 254 nm, eluent: n-hexane/2-propanol = 90/10, flow rate = 1.0 mL/min, 25 ℃).



(*S,R*)-5p: (*S*)-2-((*R*)-hydroxy(naphthalen-1-yl)methyl)cyclohexan-1-one. (Laccase/**E** + catalyst **D**): 59% yield, 98% *ee*, 94/6 *dr*; (Laccase/**E** + catalyst **C**): 86% yield, 84% *ee*, 83/17 *dr*. ^{1}H NMR (400 MHz, Chloroform-*d*): δ 8.25 – 7.17 (m, 7H), 6.21 – 5.47 (m, 1H), 2.92 (dddd, J = 12.2, 8.7, 6.0, 1.2 Hz, 1H), 2.51 – 2.27 (m, 2H), 2.01 (dtd, J = 12.1, 6.0, 2.9 Hz, 1H), 1.70 – 1.16 (m, 6H). HRMS (ESI): m/z $[M+H]^+$ calcd for $[C_{17}H_{18}O_2]^+$255.138; found: 255.1372. (HPLC: Chiracel AD-H, detected at 254 nm, eluent: n-hexane/2-propanol = 95/5, flow rate = 1.0 mL/min, 25 ℃).

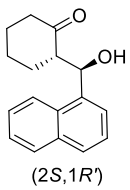
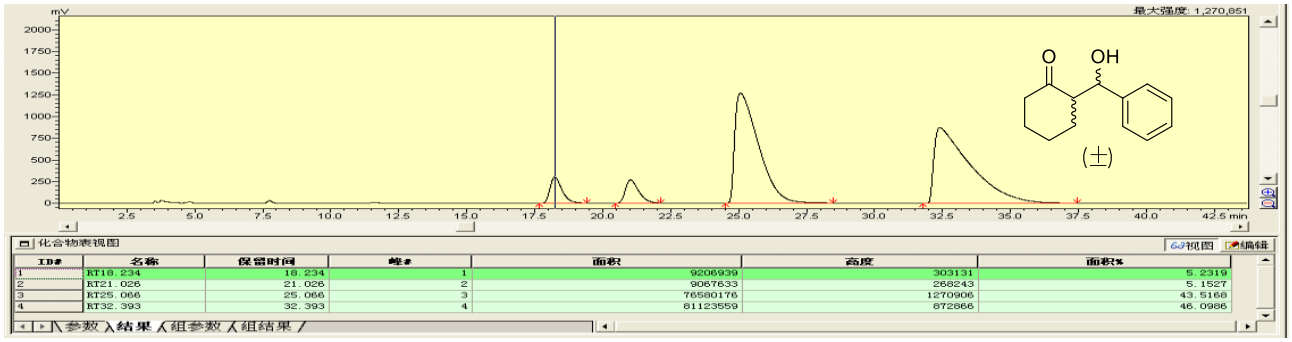
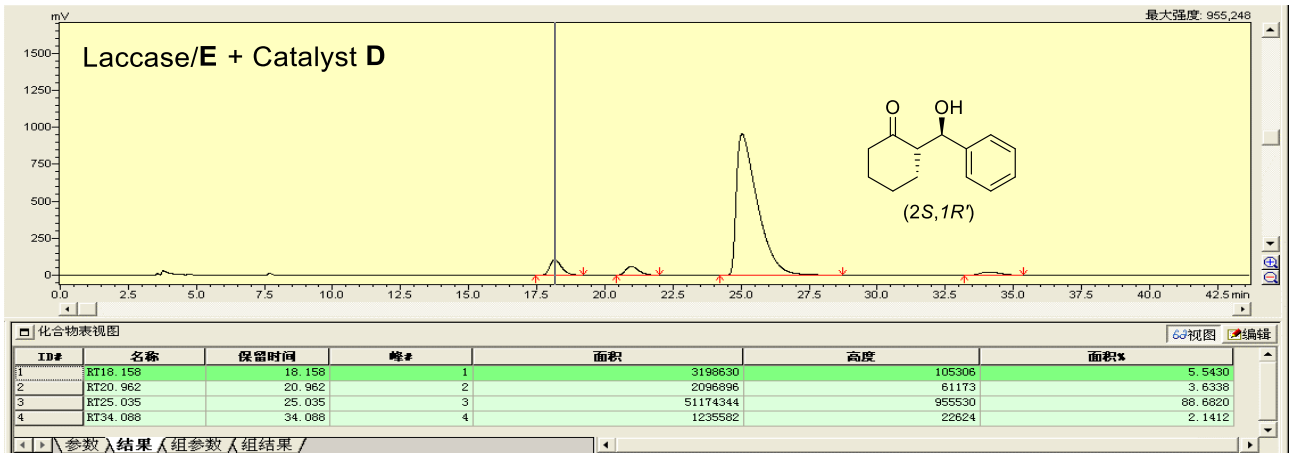
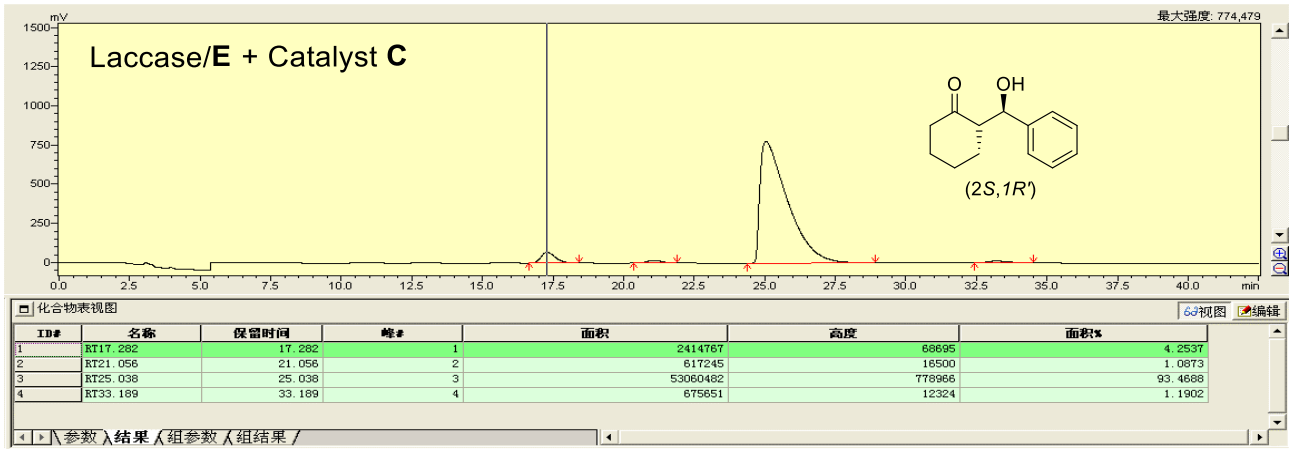


Figure S1. HPLC analyses for chiral products.

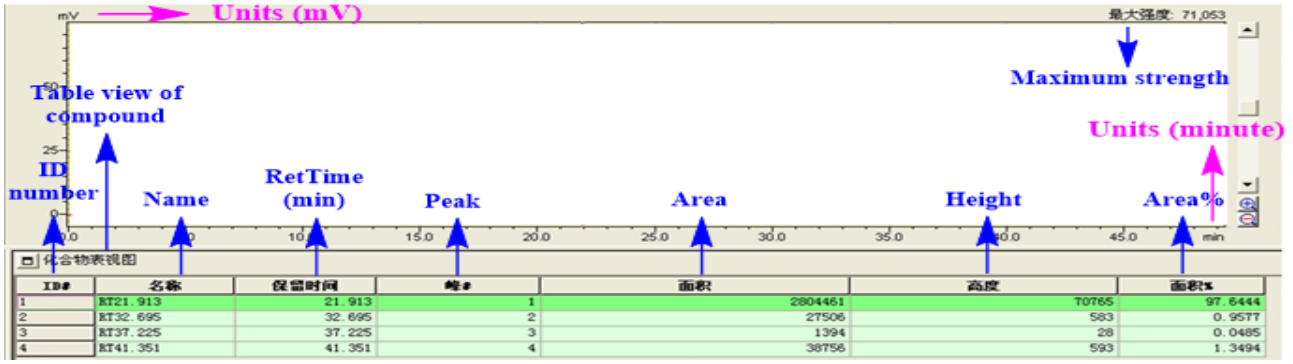
(*S,R*)-5a: (*S*)-2-((*R*)-hydroxy(phenyl)methyl)cyclohexan-1-one.



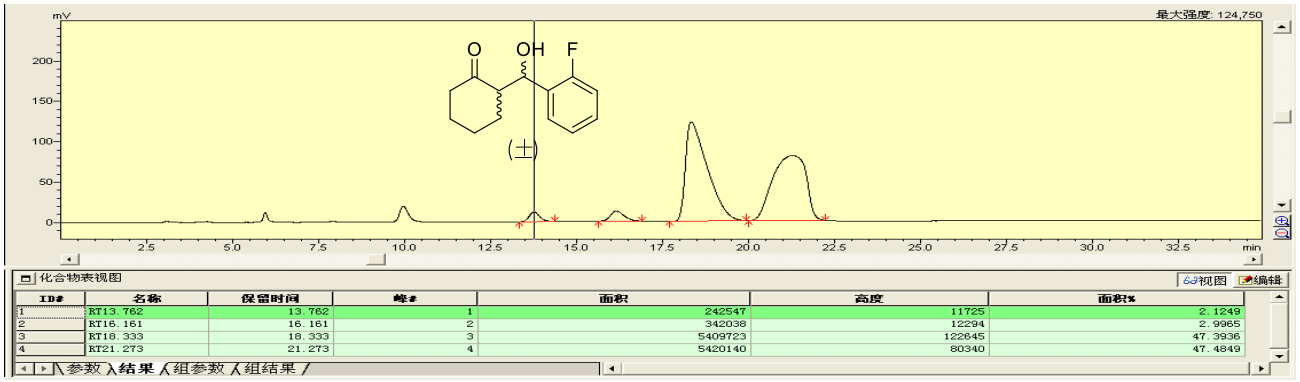


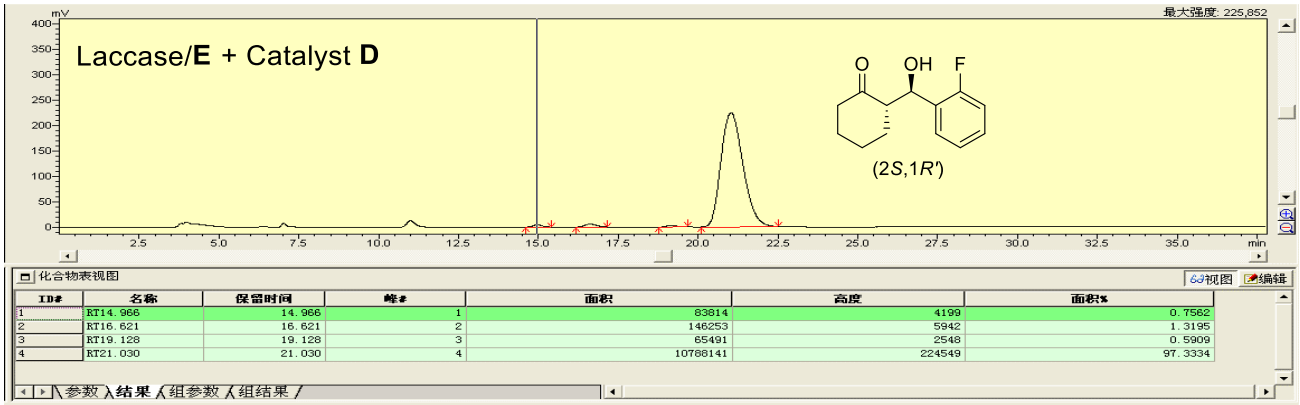


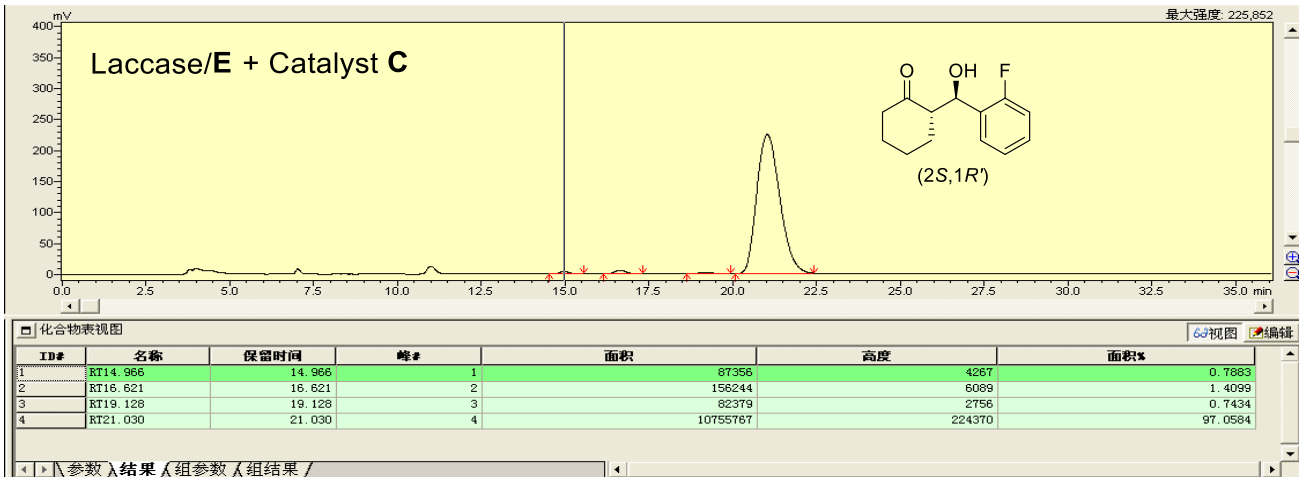
<u>Translation of all characters (Chinese) in the above two frameworks to English is as follows:</u>



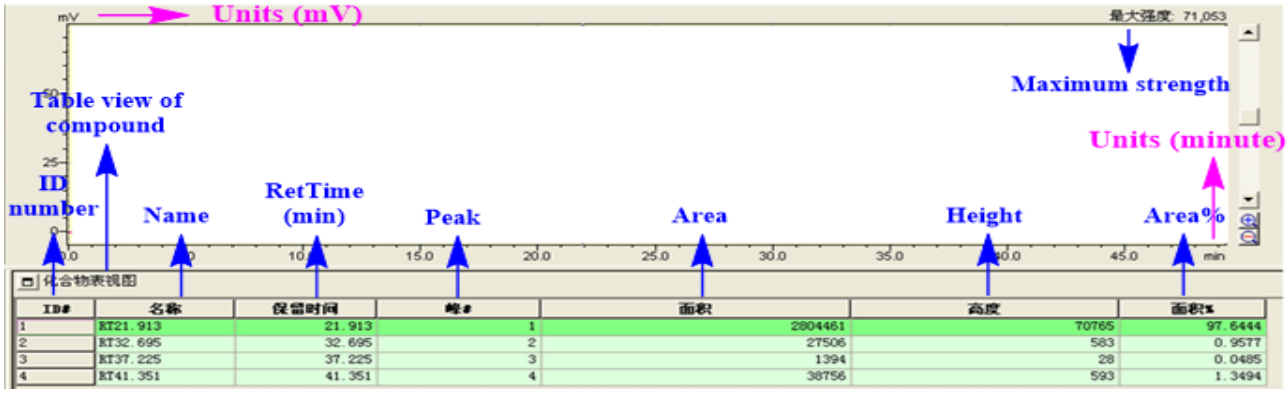
(*S*,*R*)-5b: (*S*)-2-((*R*)-(2-fluorophenyl)(hydroxy)methyl)cyclohexan-1-one.



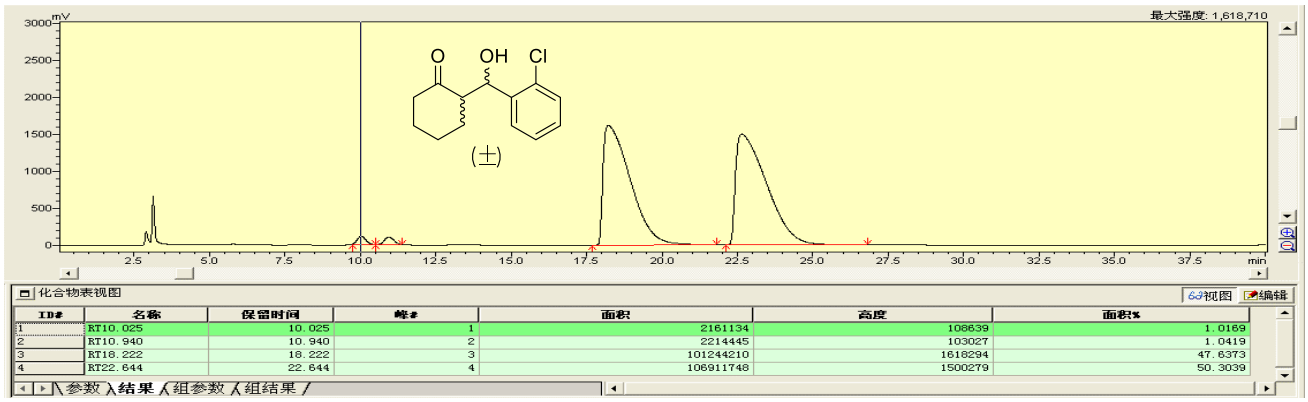


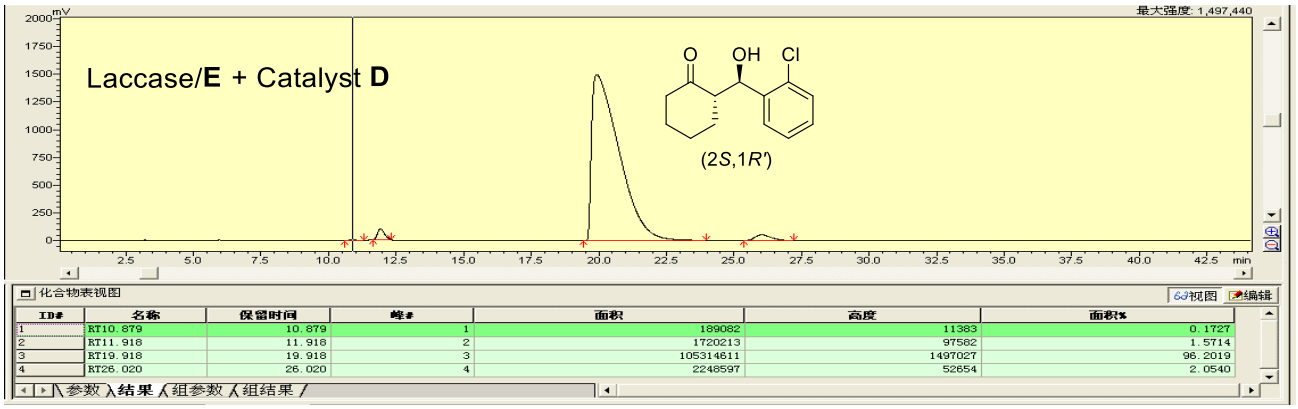


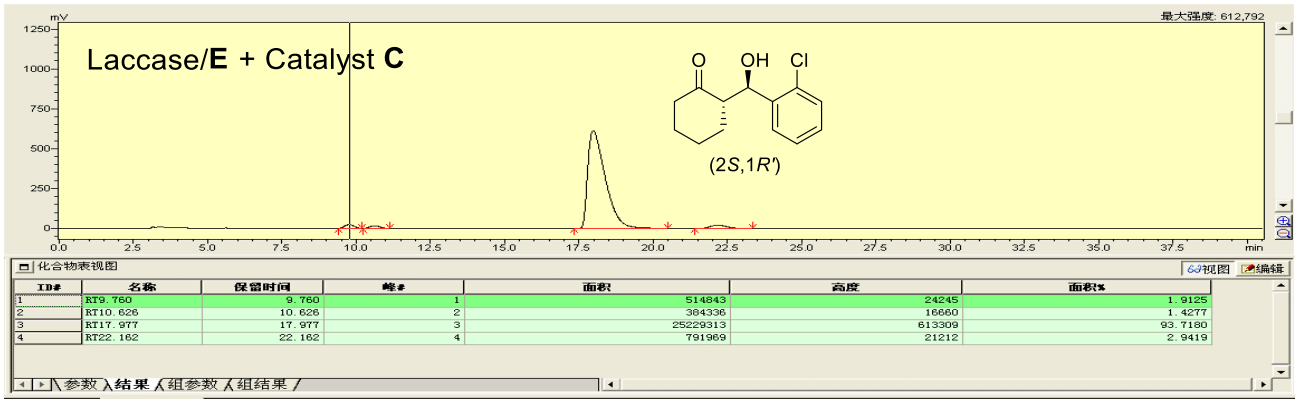
Translation of all characters (Chinese) in the above two frameworks to English is as follows:



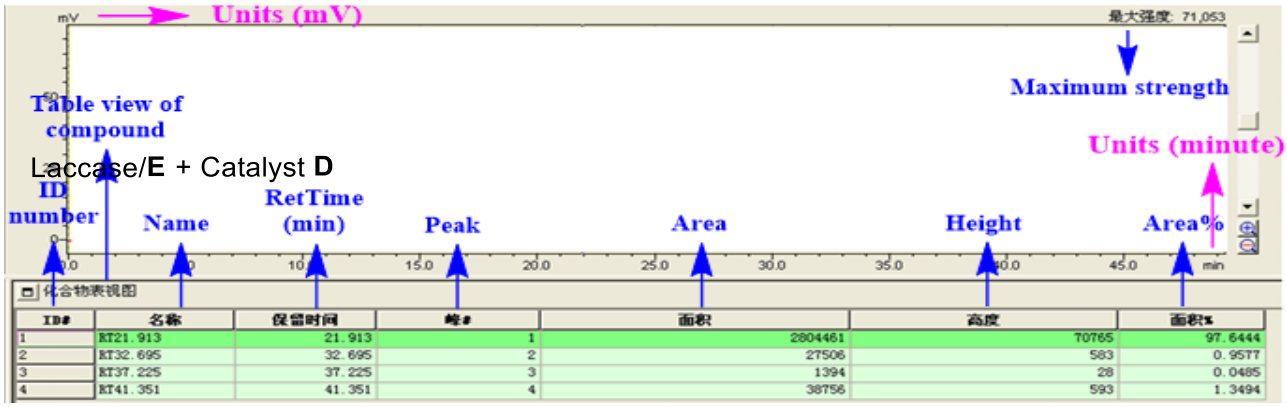
(*S*,*R*)-5c: (S)-2-((R)-(2-chlorophenyl)(hydroxy)methyl)cyclohexan-1-one (HPLC: Chiracel OD-H, detected at 220 nm, eluent: n-hexane/2-propanol = 99/1, flow rate = 1.0 mL/min, 25 ℃).



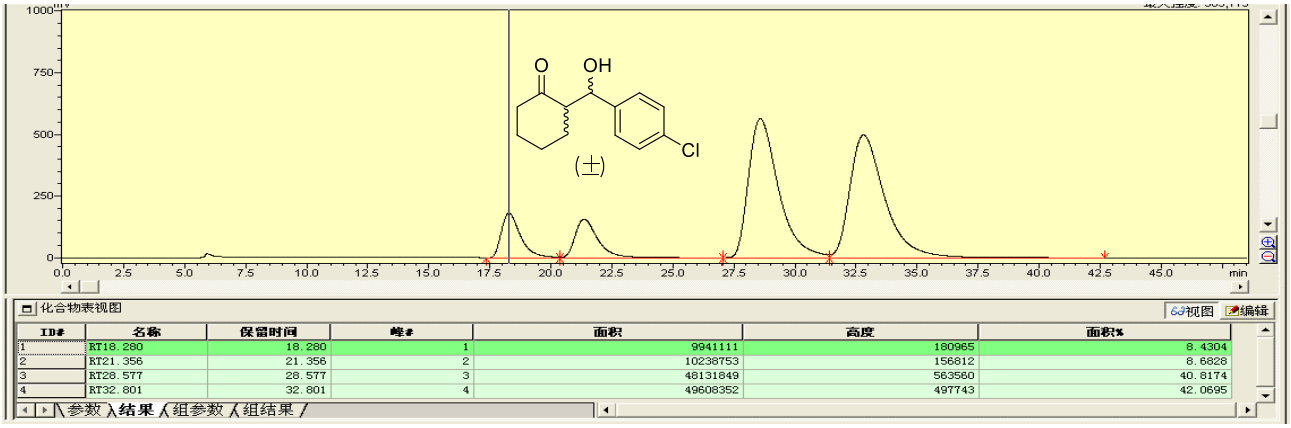




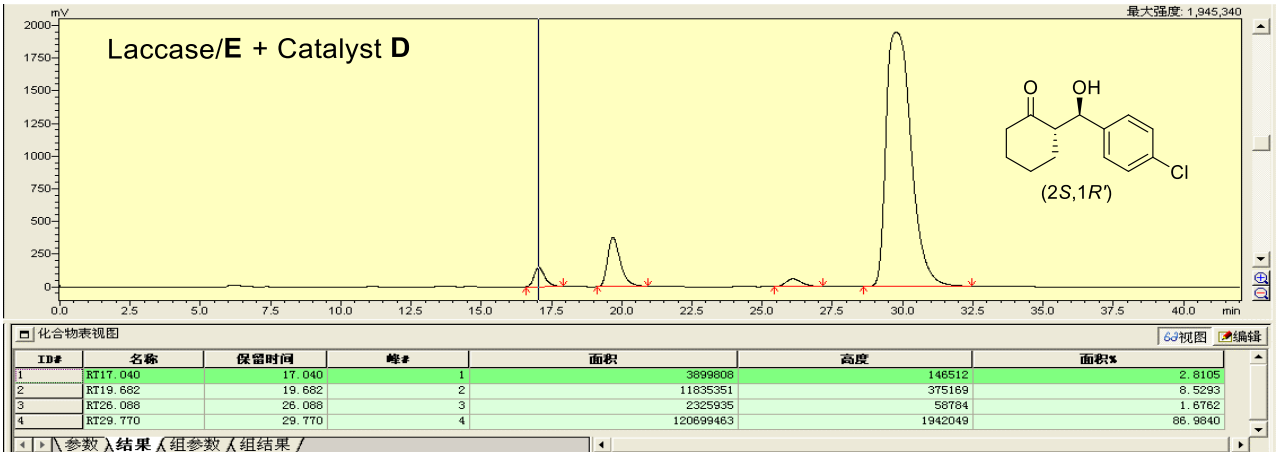
Translation of all characters (Chinese) in the above two frameworks to English is as follows:



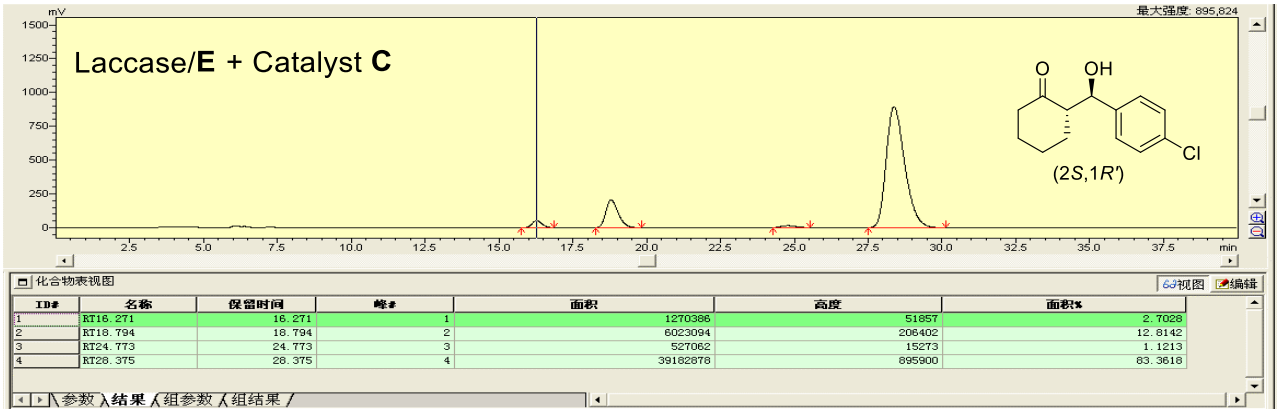
(*S,R*)-5d: (S)-2-((R)-(4-chlorophenyl)(hydroxy)methyl)cyclohexan-1-one.



ID#	名称	保留时间	峰#	面积	高度	面积%
1	RT18.280	18.280	1	9941111	180965	8.4304
2	RT21.356	21.356	2	10238753	156812	8.6828
3	RT28.577	28.577	3	48131849	563560	40.8174
4	RT32.801	32.801	4	49608352	497743	42.0695

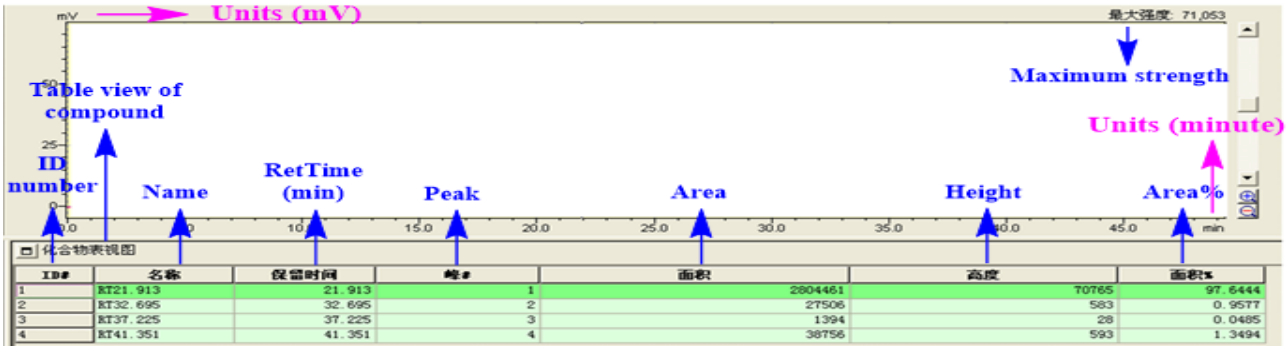


ID#	名称	保留时间	峰#	面积	高度	面积%
1	RT17.040	17.040	1	3899808	146512	2.8105
2	RT19.682	19.682	2	11835351	375169	8.5293
3	RT26.088	26.088	3	2325935	58784	1.6762
4	RT29.770	29.770	4	120699463	1942049	86.9840



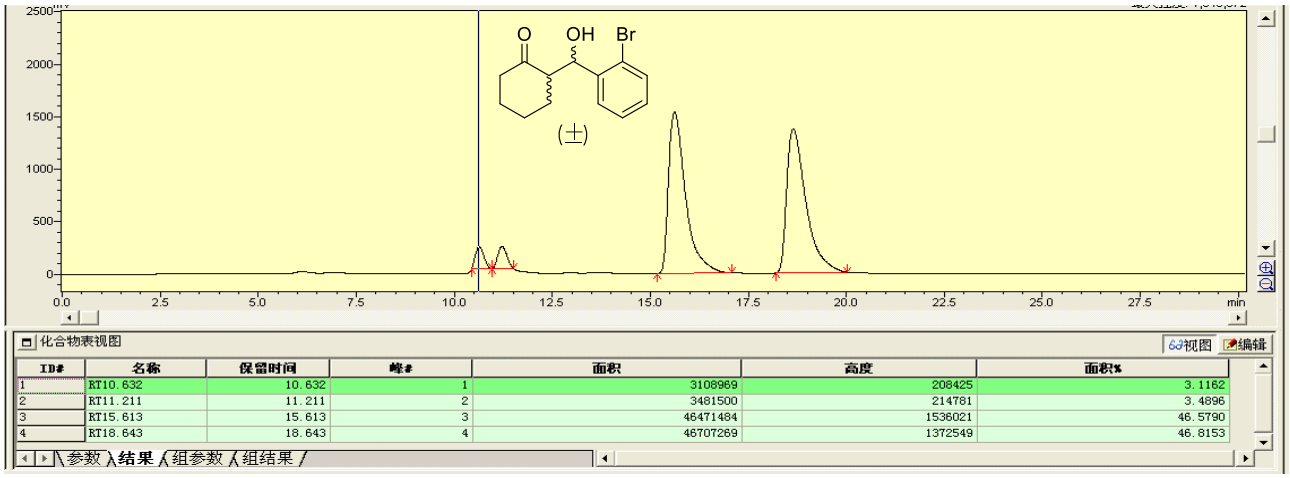
ID#	名称	保留时间	峰#	面积	高度	面积%
1	RT16.271	16.271	1	1270386	51857	2.7028
2	RT18.794	18.794	2	6023094	206402	12.8142
3	RT24.773	24.773	3	527062	15273	1.1213
4	RT28.375	28.375	4	39182878	895900	83.3618

Translation of all characters (Chinese) in the above two frameworks to English is as follows:



ID#	名称	保留时间	峰#	面积	高度	面积%
1	RT21.913	21.913	1	2804461	70765	97.6444
2	RT32.695	32.695	2	27506	583	0.9577
3	RT37.225	37.225	3	1394	28	0.0485
4	RT41.351	41.351	4	38756	593	1.3494

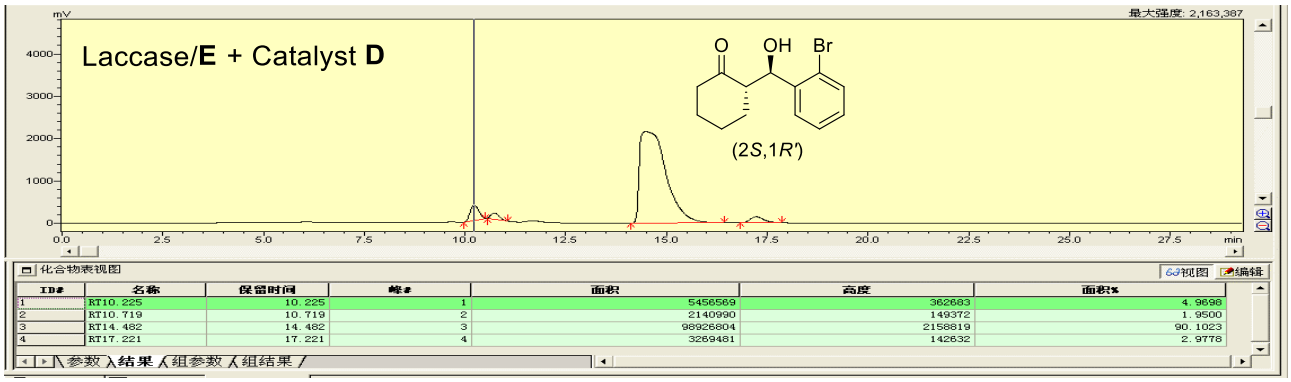
(*S,R*)-5e: (S)-2-((R)-(2-bromophenyl)(hydroxy)methyl)cyclohexan-1-one.



化合物表视图

ID#	名称	保留时间	峰#	面积	高度	面积%
1	RT10.632	10.632	1	3108969	208425	3.1162
2	RT11.211	11.211	2	3481500	214781	3.4896
3	RT15.613	15.613	3	46471484	1536021	46.5790
4	RT18.643	18.643	4	46707269	1372549	46.8153

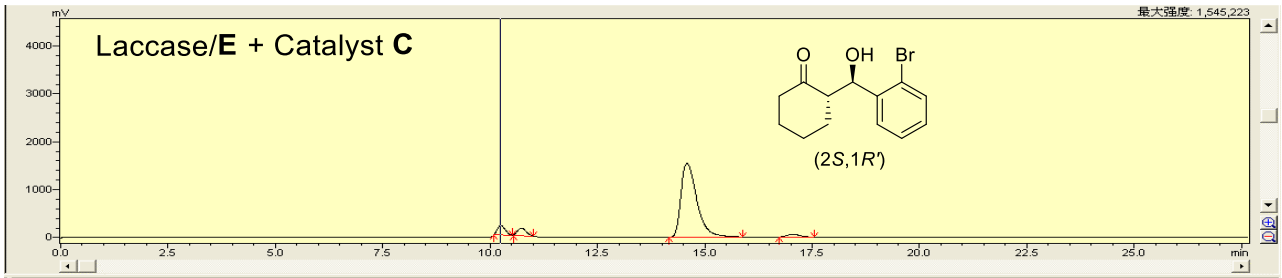
参数 结果 组参数 组结果



化合物表视图

ID#	名称	保留时间	峰#	面积	高度	面积%
1	RT10.225	10.225	1	5456569	362683	4.9698
2	RT10.719	10.719	2	2140990	149372	1.9500
3	RT14.482	14.482	3	98926804	2158819	90.1023
4	RT17.221	17.221	4	3269481	142632	2.9778

参数 结果 组参数 组结果

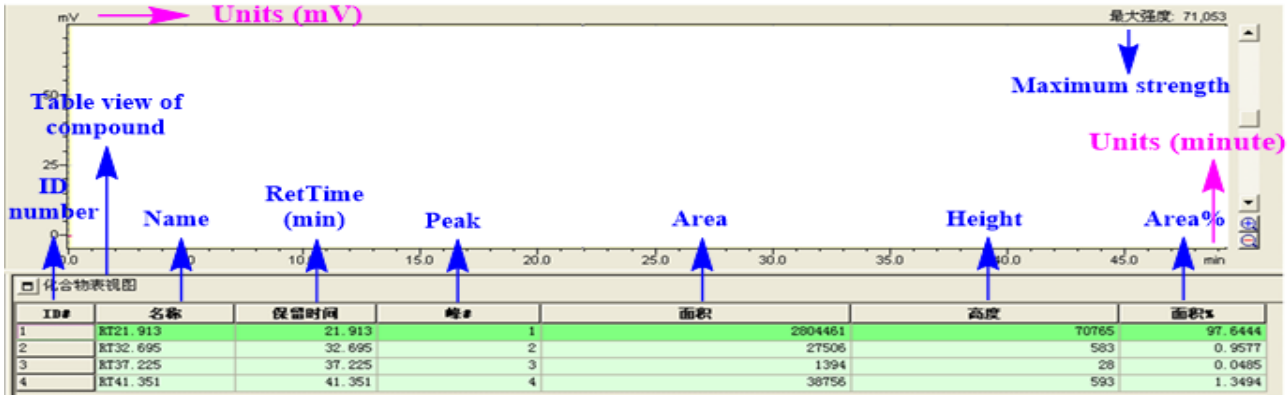


化合物表视图

ID#	名称	保留时间	峰#	面积	高度	面积%
1	RT10.244	10.244	1	2484882	197450	5.4127
2	RT10.723	10.723	2	2060631	150370	4.4885
3	RT14.582	14.582	3	40007556	1540846	87.1460
4	RT17.044	17.044	4	1355570	58748	2.9528

参数 结果 组参数 组结果

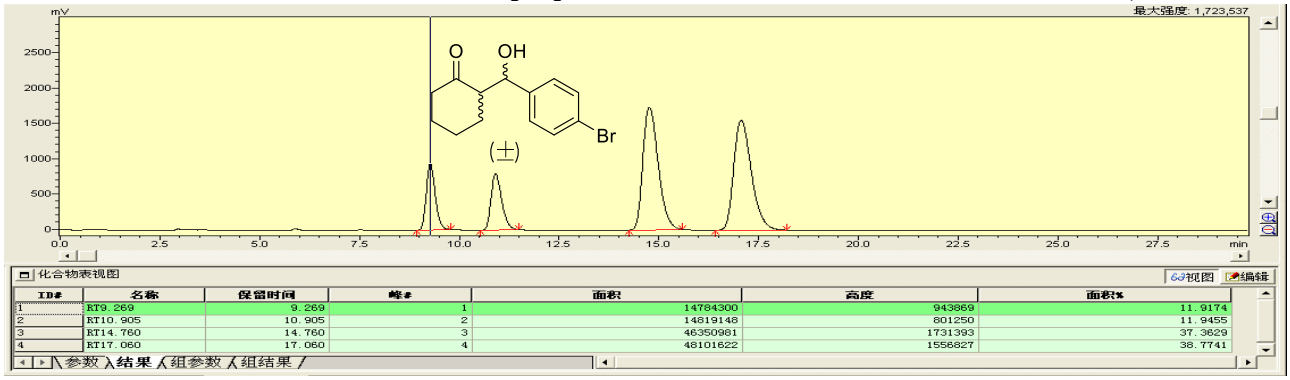
<u>Translation of all characters (Chinese) in the above two frameworks to English is as follows:</u>



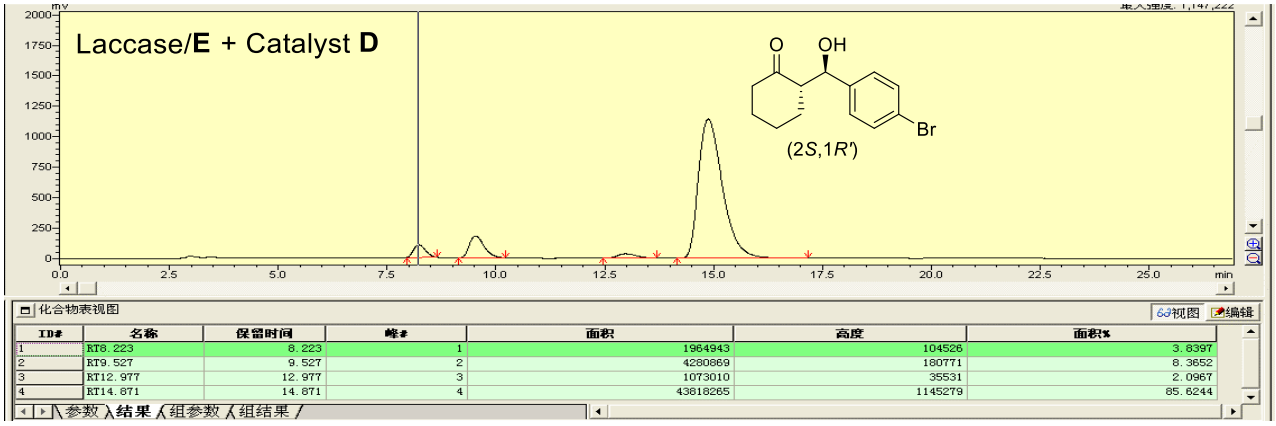
化合物表视图

ID#	名称	保留时间	峰#	面积	高度	面积%
1	RT21.913	21.913	1	2804461	70765	97.6444
2	RT32.695	32.695	2	27506	583	0.9577
3	RT37.225	37.225	3	1394	28	0.0485
4	RT41.351	41.351	4	38756	593	1.3494

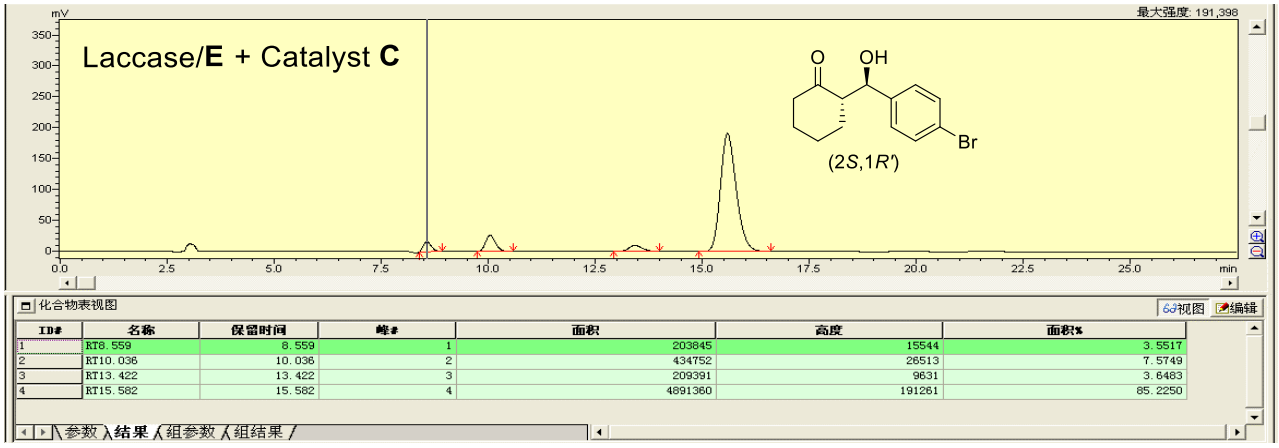
(*S*,*R*)-5f: (S)-2-((R)-(4-bromophenyl)(hydroxy)methyl)cyclohexan-1-one (HPLC: Chiracel AD-H, detected at 220 nm, eluent: n-hexane/2-propanol = 90/10, flow rate = 1.0 mL/min, 25 ℃).



ID#	名称	保留时间	峰#	面积	高度	面积%
1	RT9.269	9.269	1	14784300	943869	11.9174
2	RT10.905	10.905	2	14819148	801250	11.9455
3	RT14.760	14.760	3	46350981	1731393	37.3629
4	RT17.060	17.060	4	48101622	1556827	38.7741

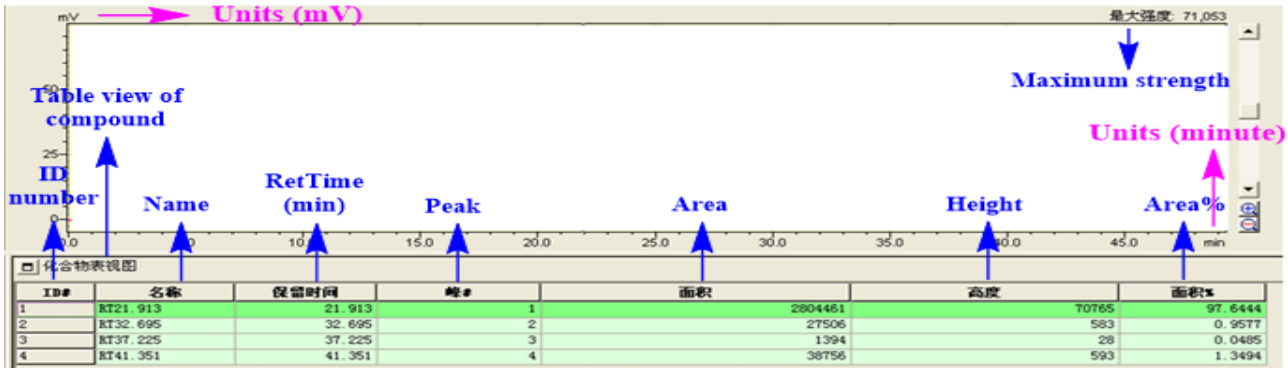


ID#	名称	保留时间	峰#	面积	高度	面积%
1	RT8.223	8.223	1	1964943	104526	3.8397
2	RT9.527	9.527	2	4280869	180771	8.3652
3	RT12.977	12.977	3	1073010	35531	2.0967
4	RT14.871	14.871	4	43818265	1145279	85.6244



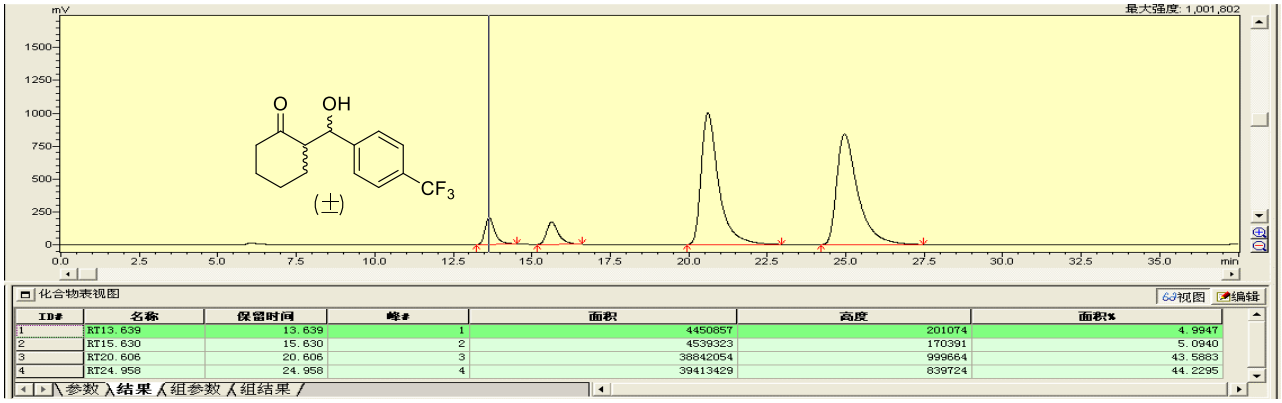
ID#	名称	保留时间	峰#	面积	高度	面积%
1	RT8.559	8.559	1	203845	15544	3.5517
2	RT10.036	10.036	2	434752	26513	7.5749
3	RT13.422	13.422	3	209391	9631	3.6483
4	RT15.582	15.582	4	4891360	191261	85.2250

Translation of all characters (Chinese) in the above two frameworks to English is as follows:



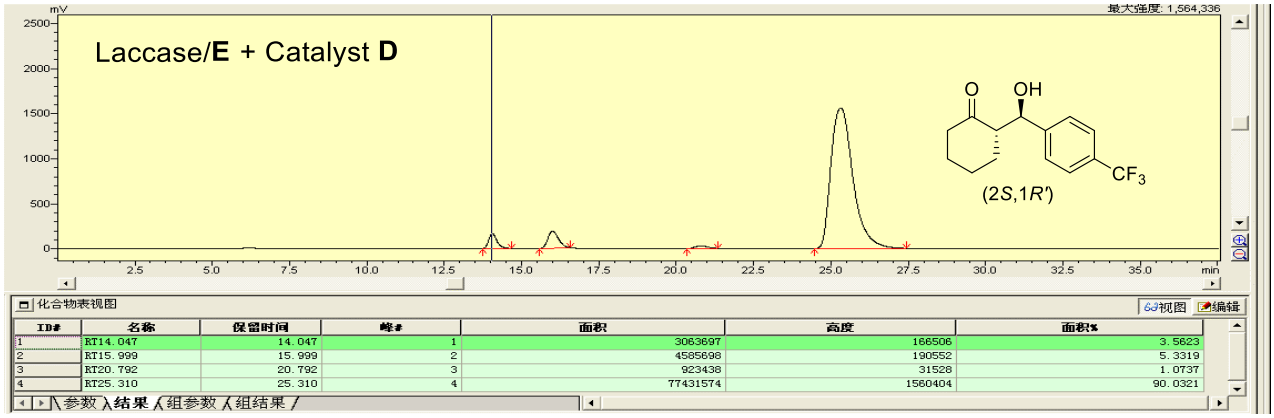
ID#	名称	保留时间	峰#	面积	高度	面积%
1	RT21.913	21.913	1	2804461	70765	97.6444
2	RT32.695	32.695	2	27506	583	0.9577
3	RT37.225	37.225	3	1394	28	0.0485
4	RT41.351	41.351	4	38756	593	1.3494

(*S*,*R*)-5g: (S)-2-((R)-hydroxy(4-(trifluoromethyl)phenyl)methyl)cyclohexan-1-one.



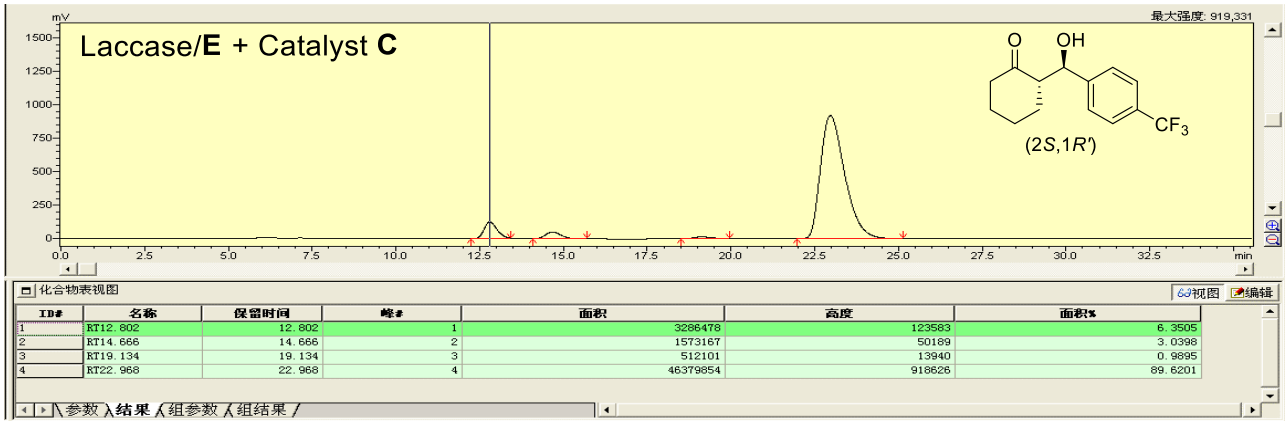
化合物表视图

ID#	名称	保留时间	峰#	面积	高度	面积%
1	RT13.639	13.639	1	4450857	201074	4.9947
2	RT15.630	15.630	2	4539323	170391	5.0940
3	RT20.606	20.606	3	38842054	999664	43.5883
4	RT24.958	24.958	4	39413429	839724	44.2295



化合物表视图

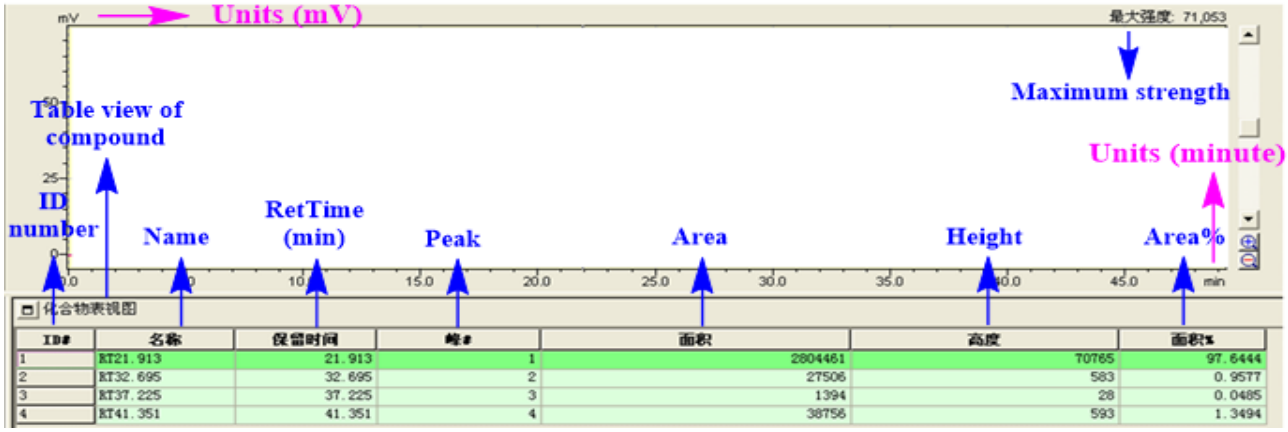
ID#	名称	保留时间	峰#	面积	高度	面积%
1	RT14.047	14.047	1	3083697	166506	3.5823
2	RT15.999	15.999	2	4585698	190552	5.3319
3	RT20.792	20.792	3	923438	31528	1.0737
4	RT25.310	25.310	4	77431574	1560404	90.0321



化合物表视图

ID#	名称	保留时间	峰#	面积	高度	面积%
1	RT12.802	12.802	1	3286478	123583	6.3505
2	RT14.666	14.666	2	1573167	50189	3.0398
3	RT19.134	19.134	3	512101	13940	0.9895
4	RT22.968	22.968	4	46379854	918626	89.6201

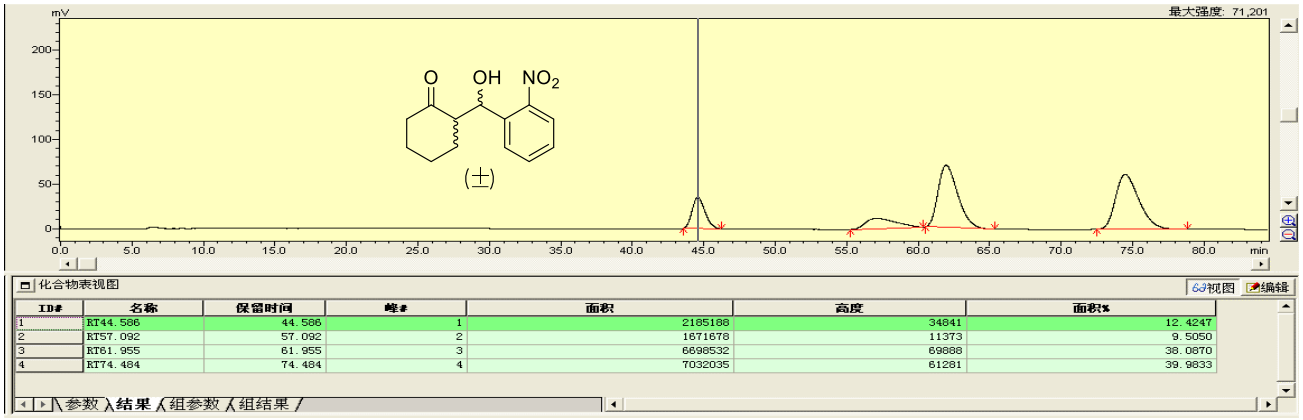
<u>Translation of all characters (Chinese) in the above two frameworks to English is as follows:</u>

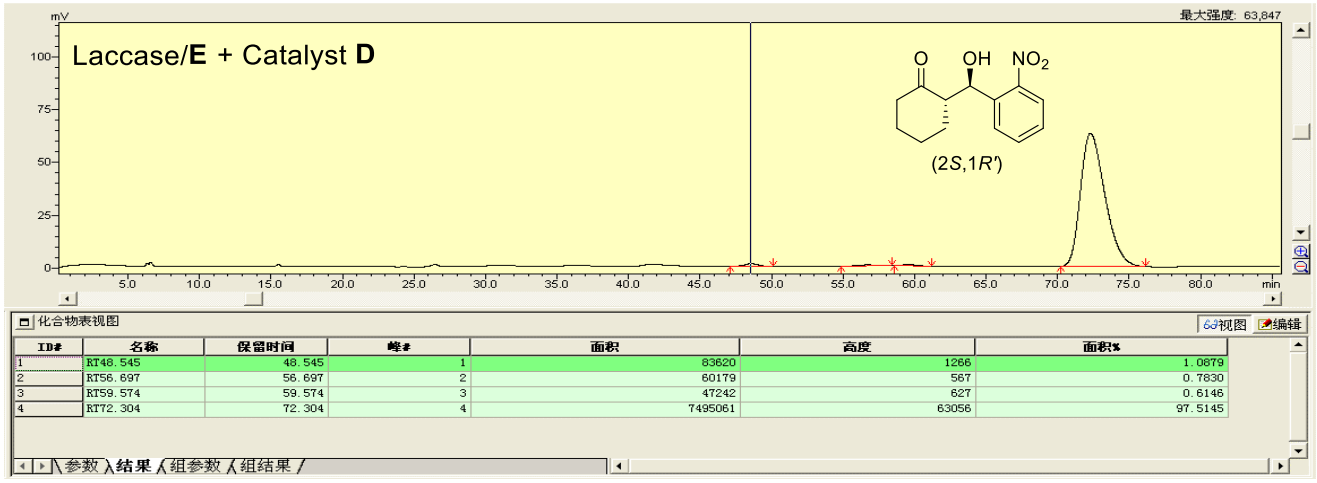


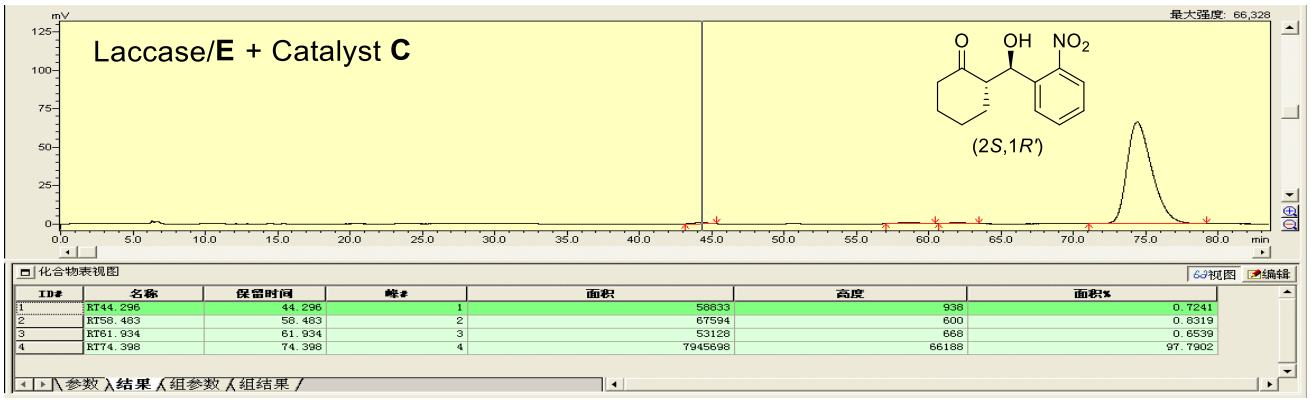
化合物表视图

ID#	名称	保留时间	峰#	面积	高度	面积%
1	RT21.913	21.913	1	2804461	70765	97.6444
2	RT32.695	32.695	2	27506	583	0.9577
3	RT37.225	37.225	3	1394	28	0.0485
4	RT41.351	41.351	4	38756	593	1.3494

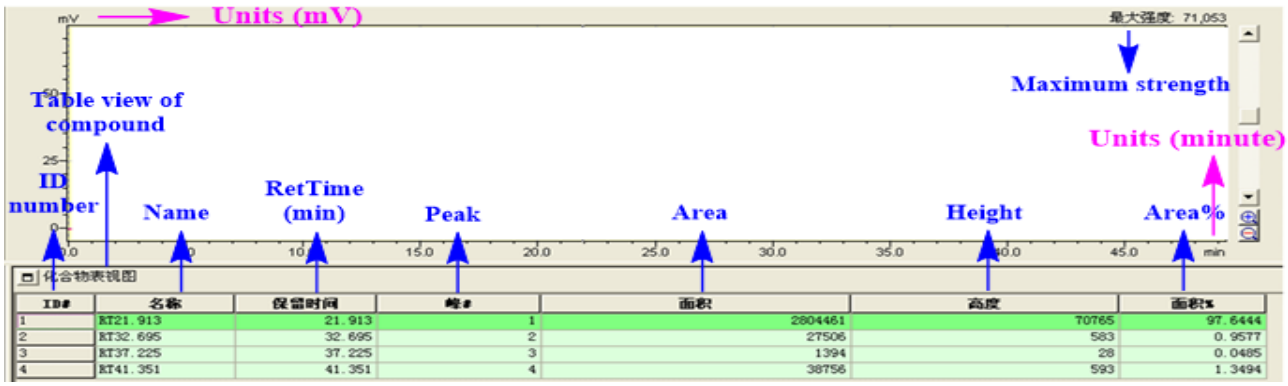
(*S,R*)-5h:(S)-2-((R)-hydroxy(2-nitrophenyl)methyl)cyclohexan-1-one.



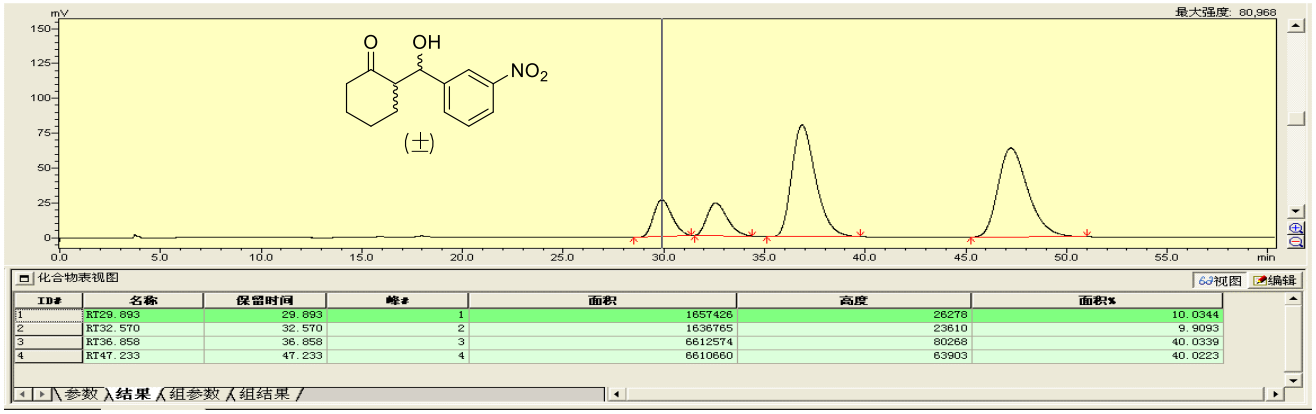


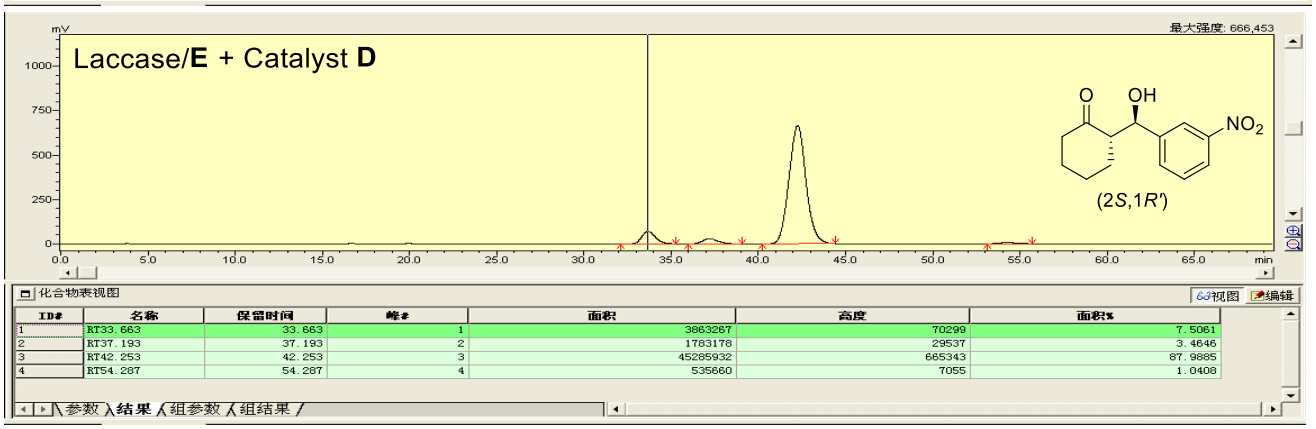


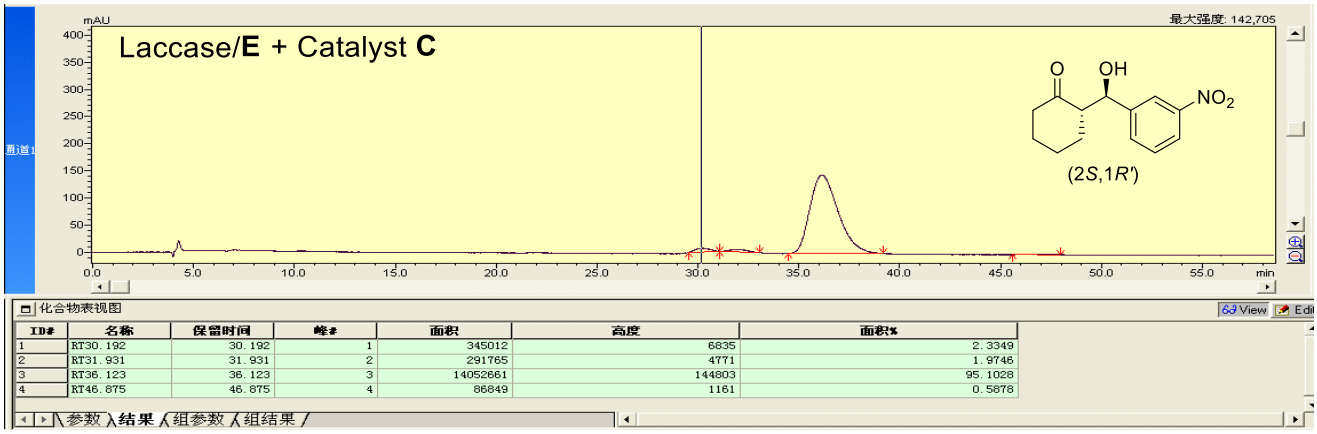
<u>Translation of all characters (Chinese) in the above two frameworks to English is as follows:</u>



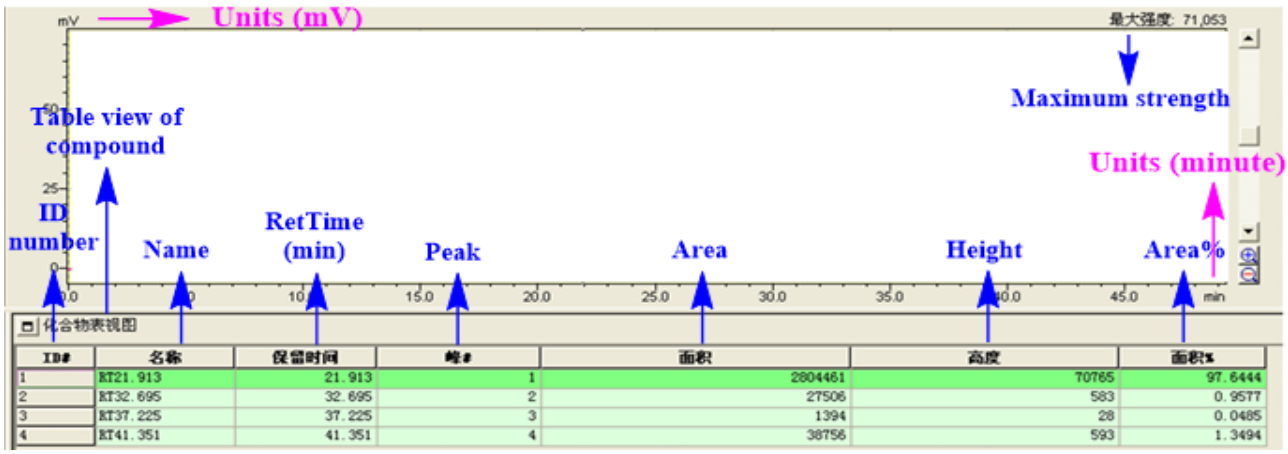
(*S,R*)-5i: (S)-2-((R)-hydroxy(3-nitrophenyl)methyl)cyclohexan-1-one.



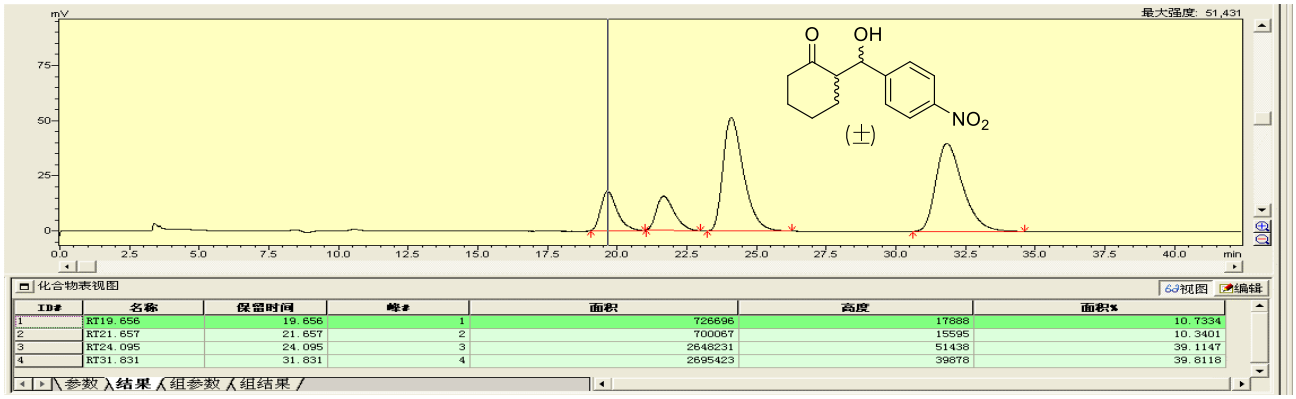


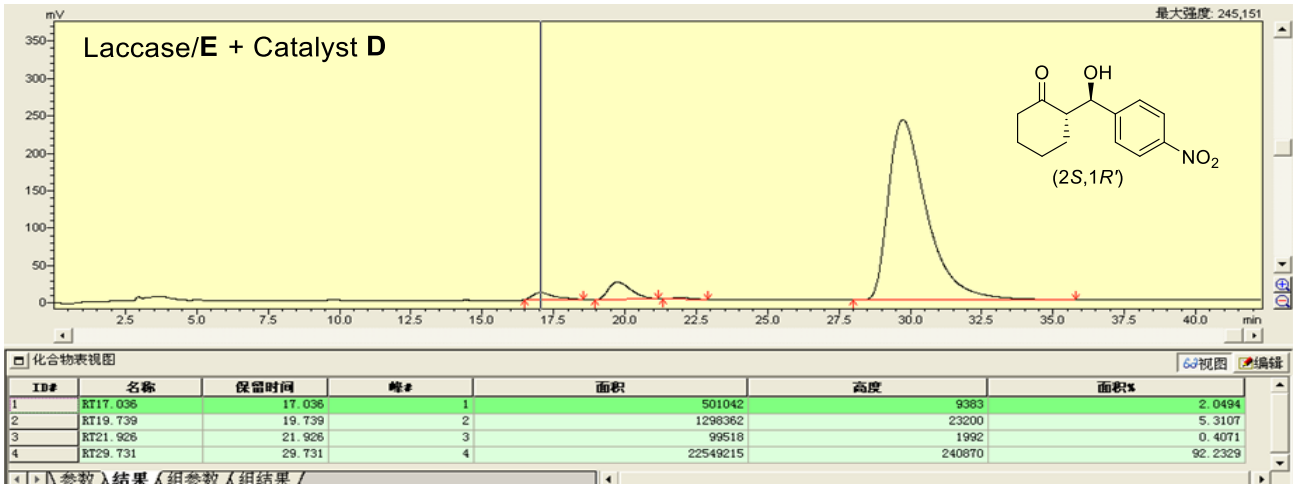


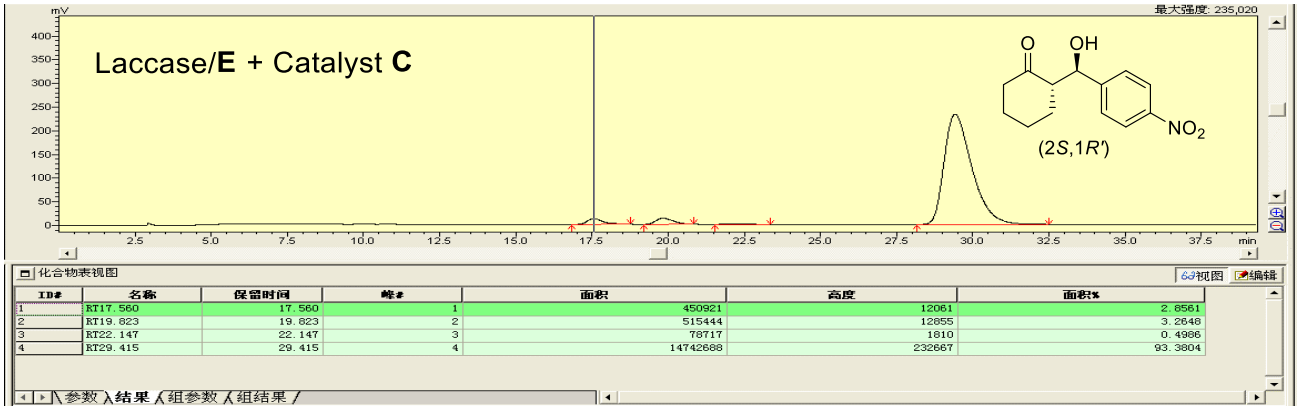
Translation of all characters (Chinese) in the above two frameworks to English is as follows:



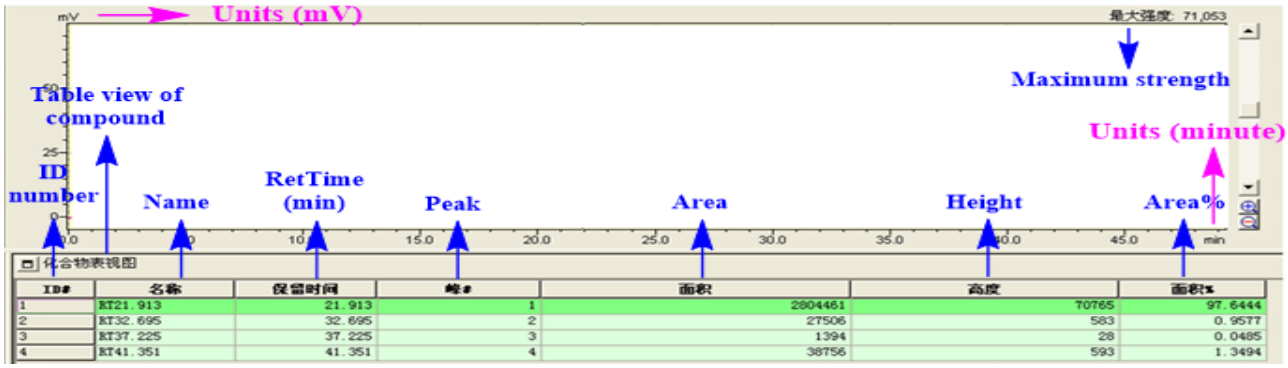
(*S,R*)-5j: (S)-2-((R)-hydroxy(4-nitrophenyl)methyl)cyclohexan-1-one.



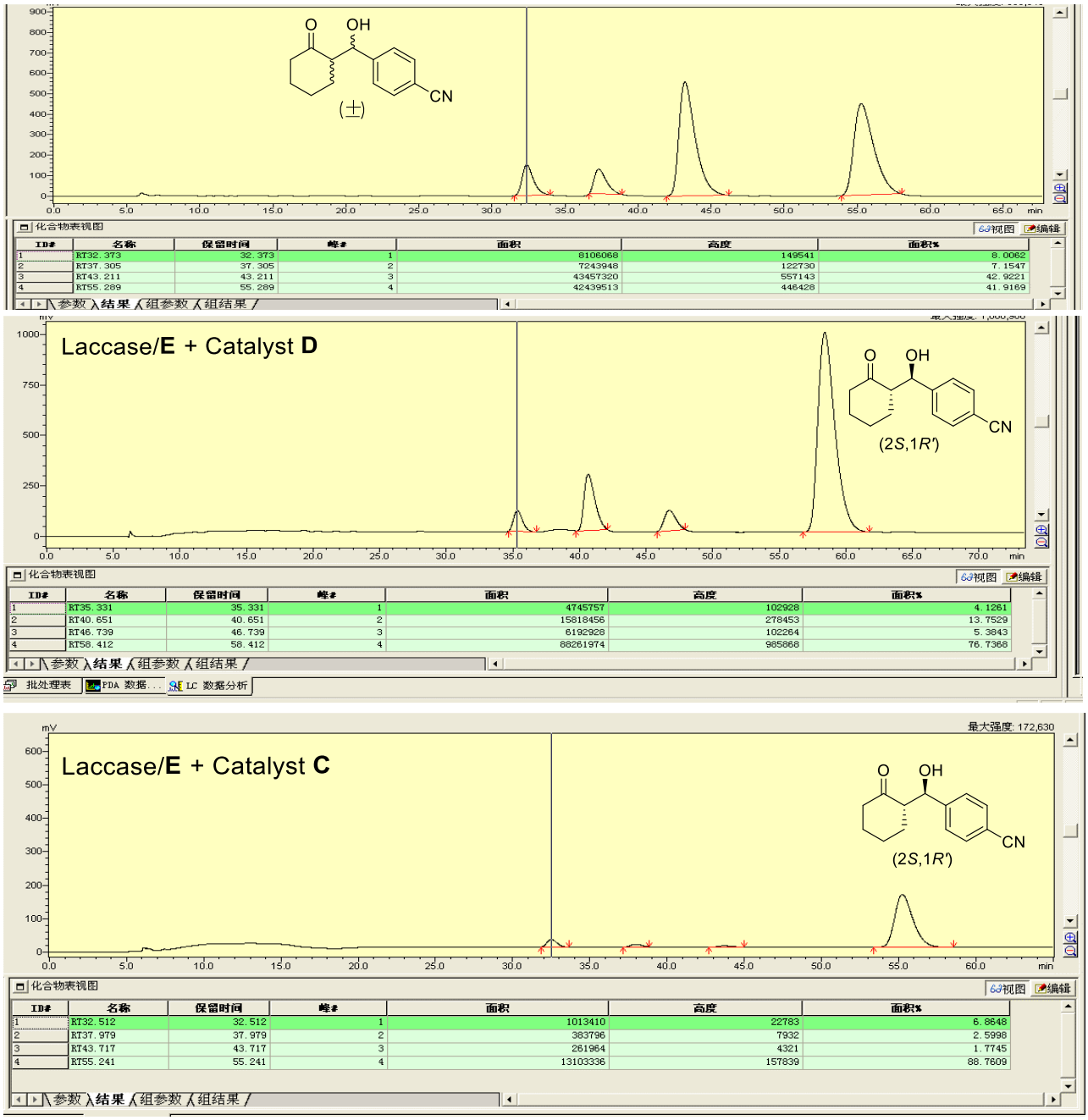




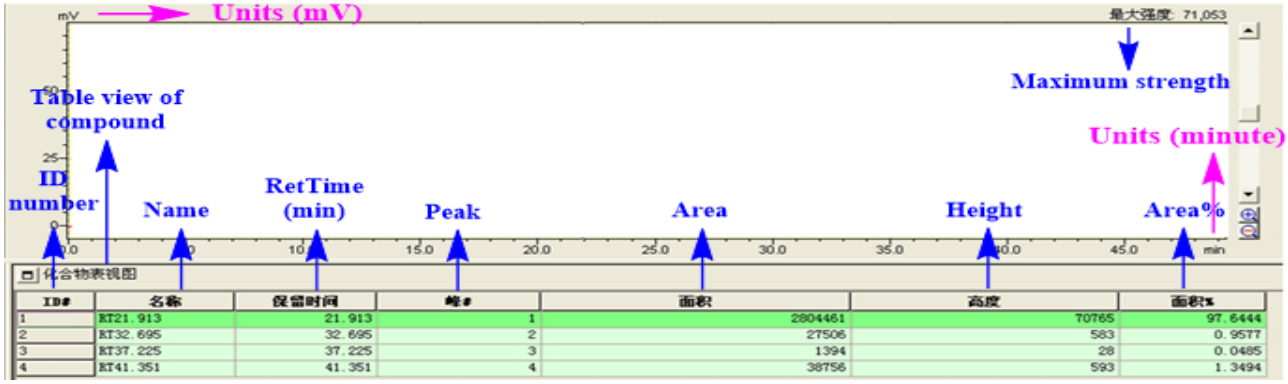
Translation of all characters (Chinese) in the above two frameworks to English is as follows:



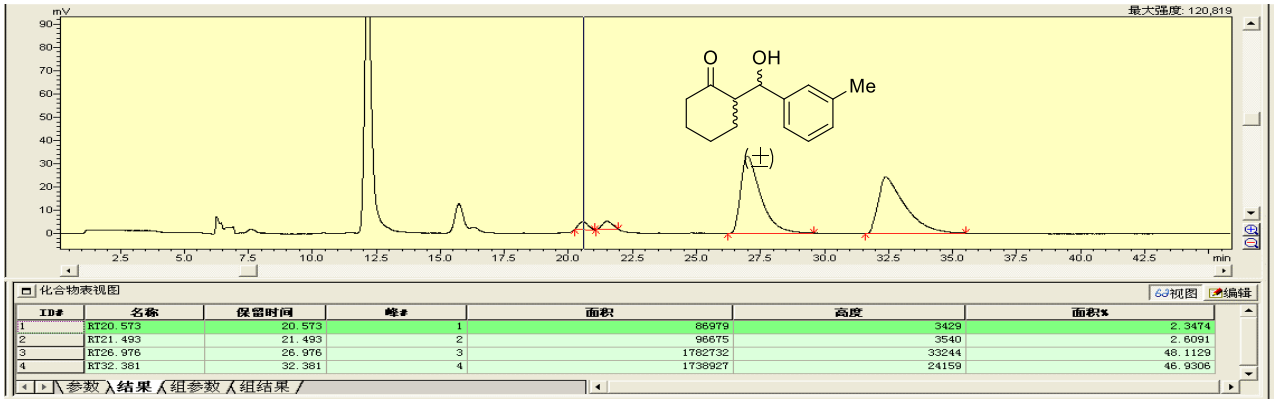
(*S,R*)-5k: 4-((S)-hydroxy((R)-2-oxocyclohexyl)methyl)benzonitrile.



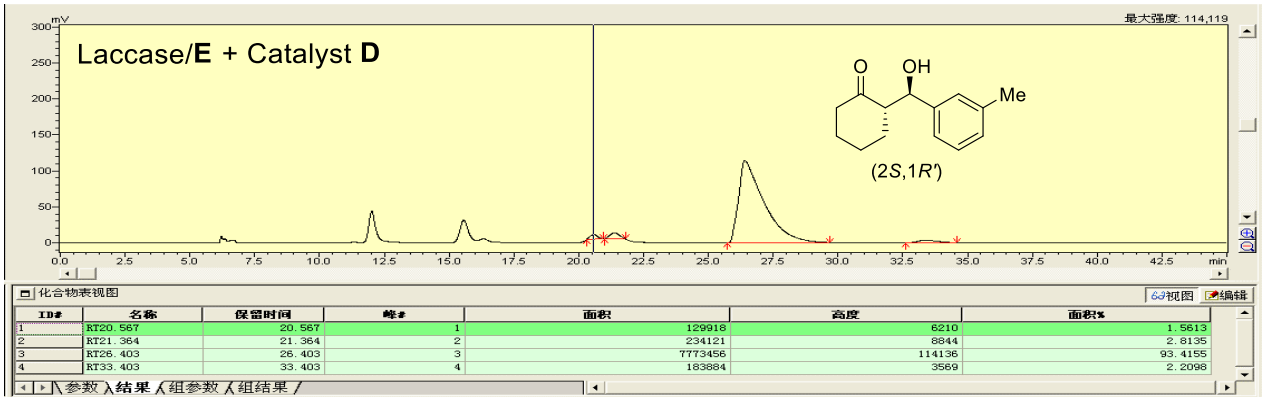
Translation of all characters (Chinese) in the above two frameworks to English is as follows:



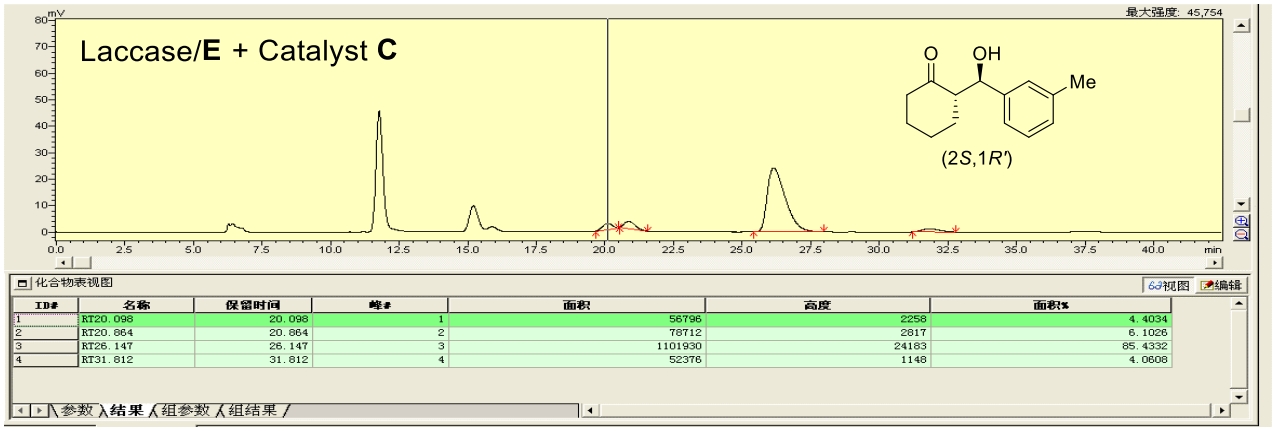
(*S*,*R*)-5l: (S)-2-((R)-hydroxy(m-tolyl)methyl)cyclohexan-1-one.



ID#	名称	保留时间	峰#	面积	高度	面积%
1	RT20.573	20.573	1	86979	3429	2.3474
2	RT21.493	21.493	2	96675	3540	2.6091
3	RT26.976	26.976	3	1782732	33244	48.1129
4	RT32.381	32.381	4	1738927	24159	46.9306

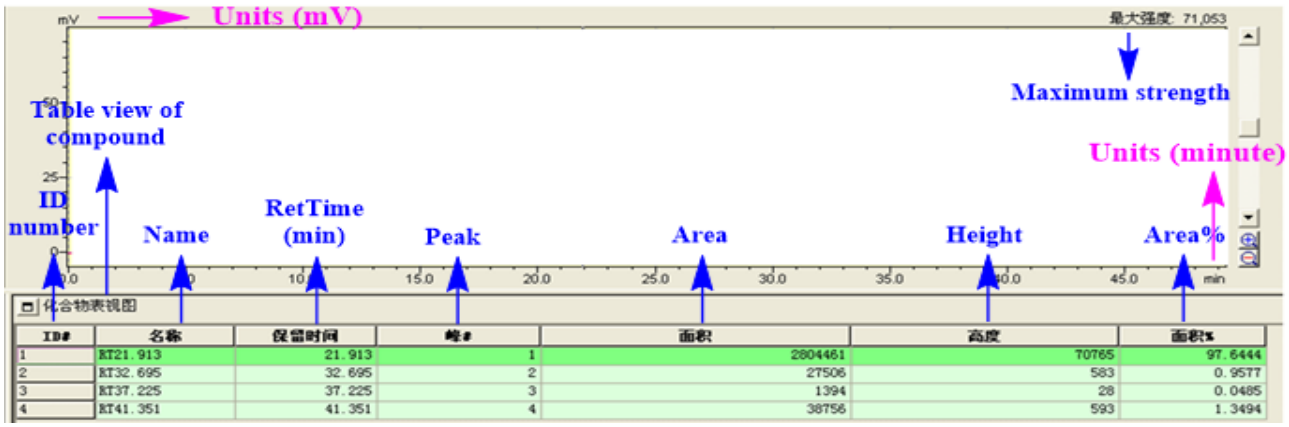


ID#	名称	保留时间	峰#	面积	高度	面积%
1	RT20.567	20.567	1	129918	6210	1.5613
2	RT21.364	21.364	2	234121	8844	2.8135
3	RT26.403	26.403	3	7773456	114136	93.4155
4	RT33.403	33.403	4	183884	3569	2.2098



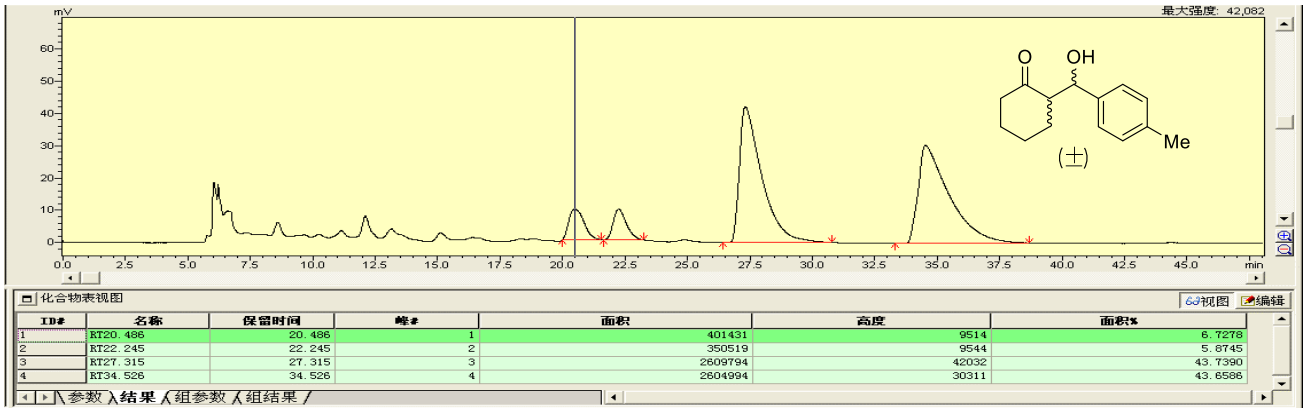
ID#	名称	保留时间	峰#	面积	高度	面积%
1	RT20.098	20.098	1	56796	2258	4.4034
2	RT20.864	20.864	2	78712	2617	6.1026
3	RT26.147	26.147	3	1101930	24183	85.4332
4	RT31.812	31.812	4	52376	1148	4.0608

<u>Translation of all characters (Chinese) in the above two frameworks to English is as follows:</u>

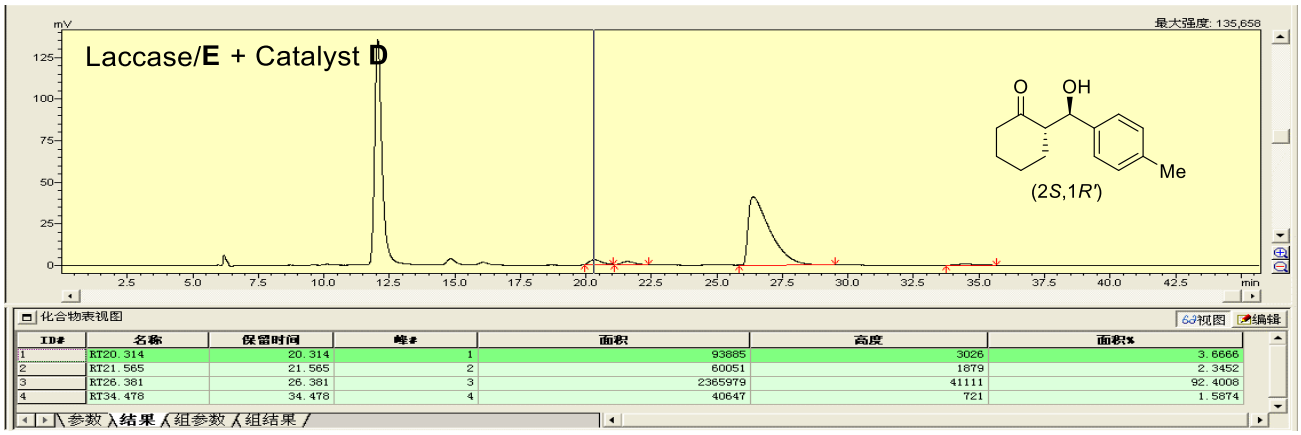


ID#	名称	保留时间	峰#	面积	高度	面积%
1	RT21.913	21.913	1	2804461	70765	97.6444
2	RT32.695	32.695	2	27506	583	0.9577
3	RT37.225	37.225	3	1394	28	0.0485
4	RT41.351	41.351	4	38756	593	1.3494

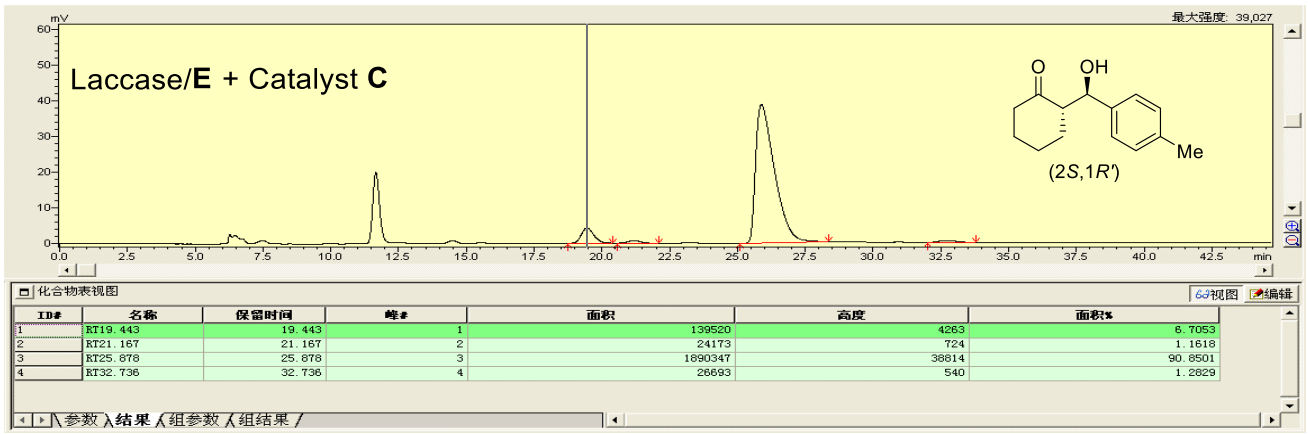
(*S*,*R*)-5m: (*S*)-2-((*R*)-hydroxy(p-tolyl)methyl)cyclohexan-1-one (HPLC: Chiracel OD-H, detected at 254 nm, eluent: n-hexane/2-propanol = 97/3, flow rate = 0.5 mL/min, 25 ℃).



ID#	名称	保留时间	峰#	面积	高度	面积%
1	RT20.486	20.486	1	401431	9514	6.7278
2	RT22.245	22.245	2	350519	9544	5.8745
3	RT27.315	27.315	3	2609794	42032	43.7390
4	RT34.526	34.526	4	2604994	30311	43.6586

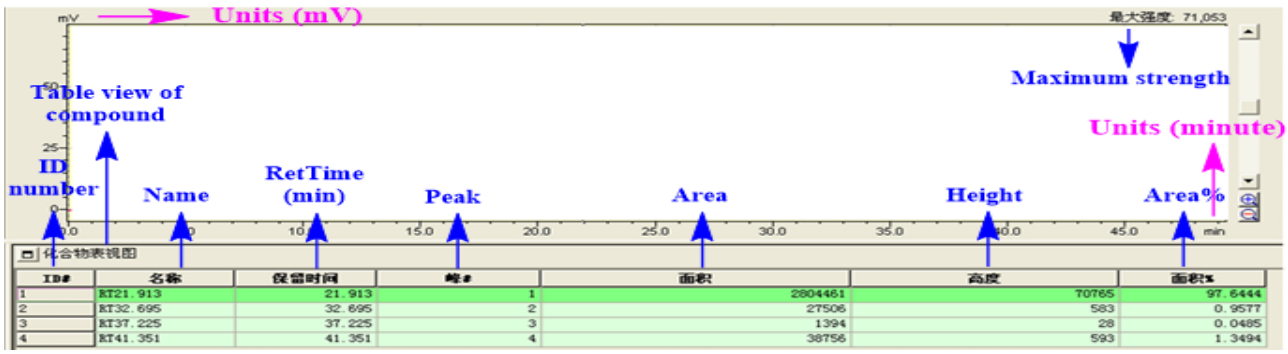


ID#	名称	保留时间	峰#	面积	高度	面积%
1	RT20.314	20.314	1	93885	3026	3.6666
2	RT21.565	21.565	2	60051	1879	2.3452
3	RT26.381	26.381	3	2365979	41111	92.4008
4	RT34.478	34.478	4	40647	721	1.5874



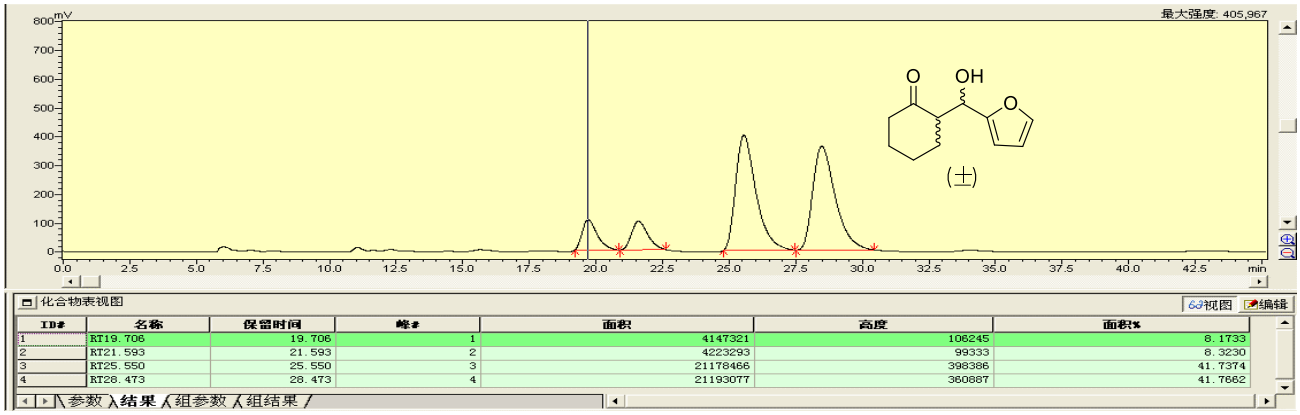
ID#	名称	保留时间	峰#	面积	高度	面积%
1	RT19.443	19.443	1	139520	4263	6.7053
2	RT21.167	21.167	2	24173	724	1.1618
3	RT25.878	25.878	3	1890347	38814	90.8501
4	RT32.736	32.736	4	26693	540	1.2829

<u>Translation of all characters (Chinese) in the above two frameworks to English is as follows:</u>



ID#	名称	保留时间	峰#	面积	高度	面积%
1	RT21.913	21.913	1	2804461	70765	97.6444
2	RT32.695	32.695	2	27506	583	0.9577
3	RT37.225	37.225	3	1394	28	0.0485
4	RT41.351	41.351	4	38756	593	1.3494

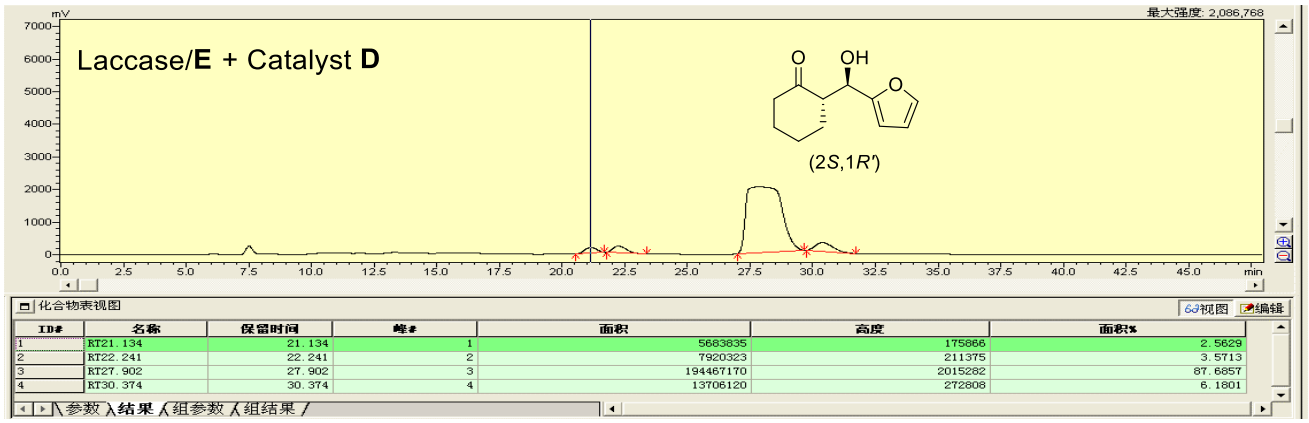
(*S*,*R*)-5n: (S)-2-((R)-furan-2-yl(hydroxy)methyl)cyclohexan-1-one.



化合物表视图

ID#	名称	保留时间	峰#	面积	高度	面积%
1	RT19.706	19.706	1	4147321	106245	8.1733
2	RT21.593	21.593	2	4223293	99333	8.3230
3	RT25.550	25.550	3	21178466	398386	41.7374
4	RT28.473	28.473	4	21193077	360887	41.7662

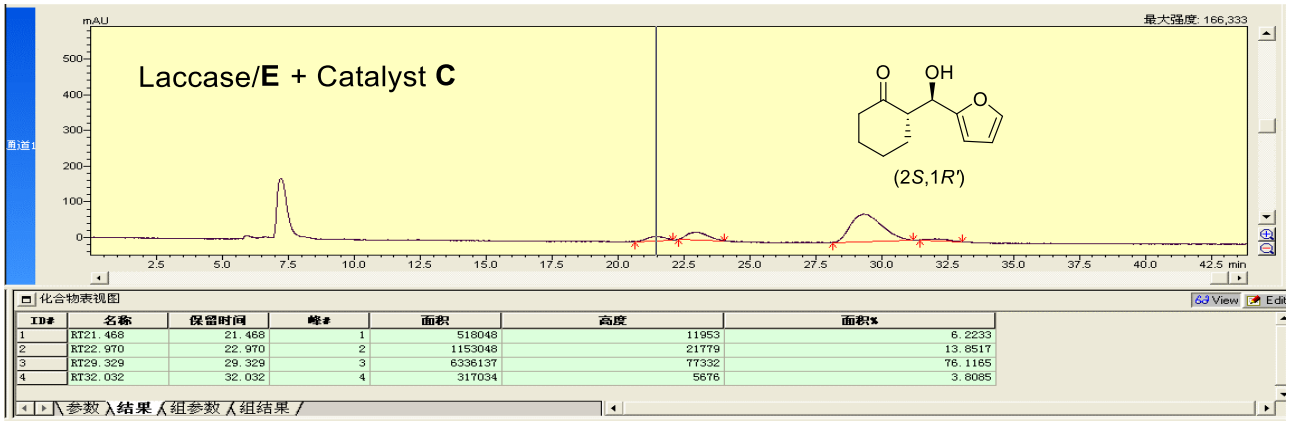
参数 结果 组参数 组结果



化合物表视图

ID#	名称	保留时间	峰#	面积	高度	面积%
1	RT21.134	21.134	1	5683835	175866	2.5629
2	RT22.241	22.241	2	7920323	211375	3.5713
3	RT27.902	27.902	3	194467170	2015282	87.6857
4	RT30.374	30.374	4	13706120	272808	6.1801

参数 结果 组参数 组结果

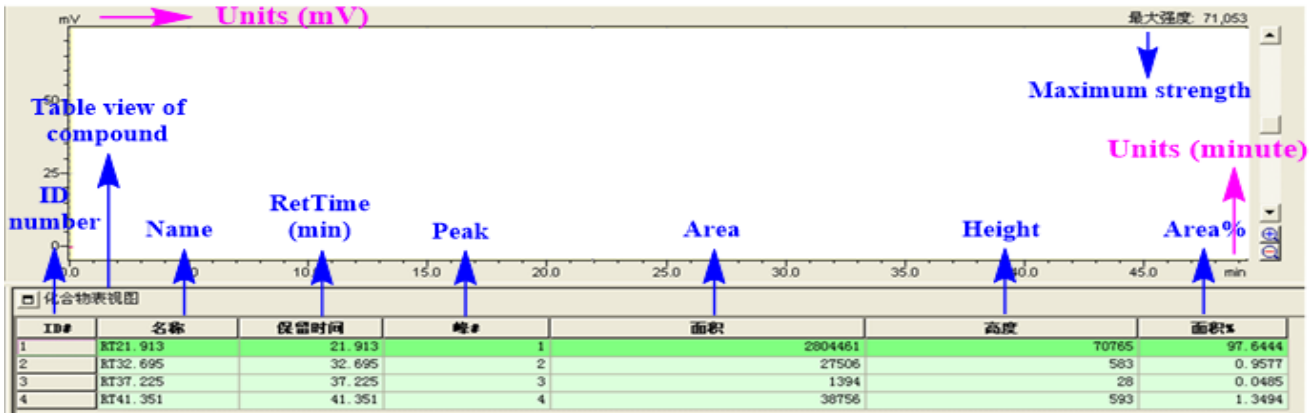


化合物表视图

ID#	名称	保留时间	峰#	面积	高度	面积%
1	RT21.468	21.468	1	518048	11953	6.2233
2	RT22.970	22.970	2	1153048	21779	13.8517
3	RT29.329	29.329	3	6336137	77332	76.1165
4	RT32.032	32.032	4	317034	5676	3.8085

参数 结果 组参数 组结果

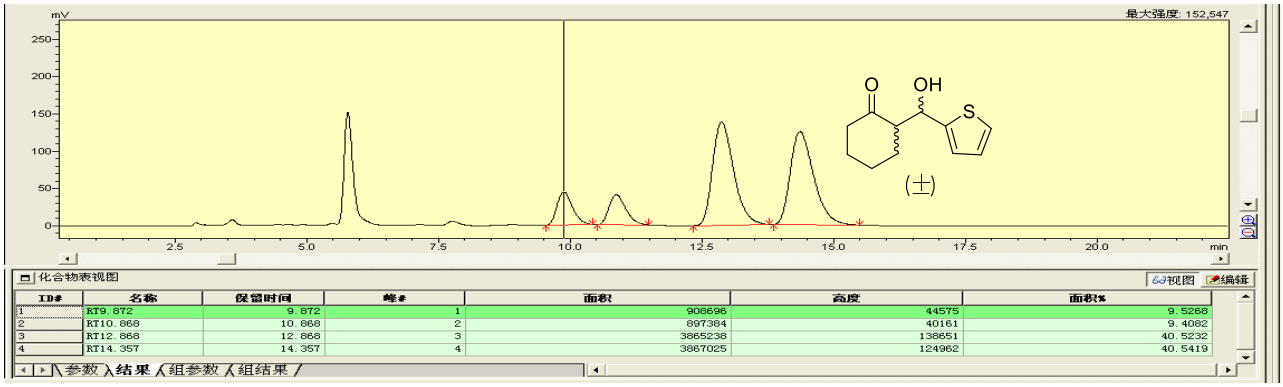
<u>Translation of all characters (Chinese) in the above two frameworks to English is as follows:</u>

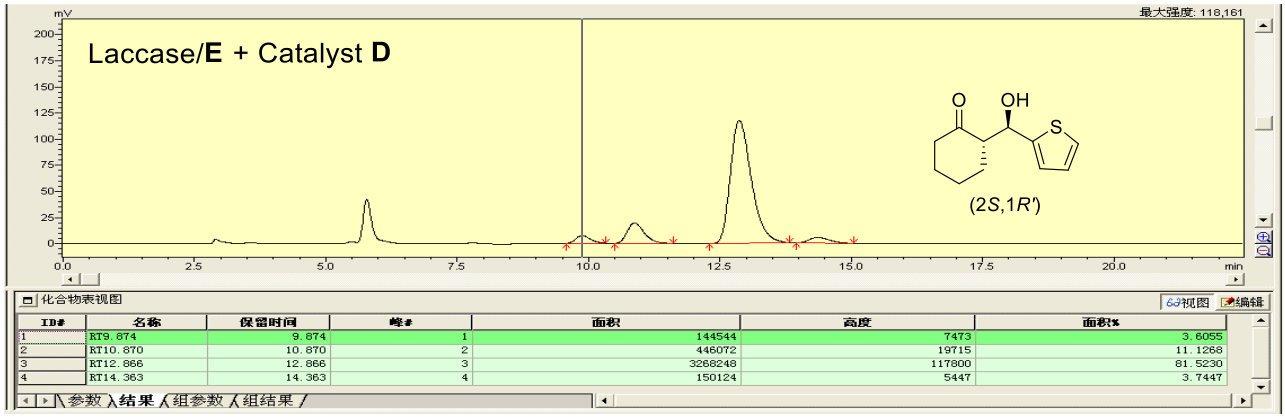


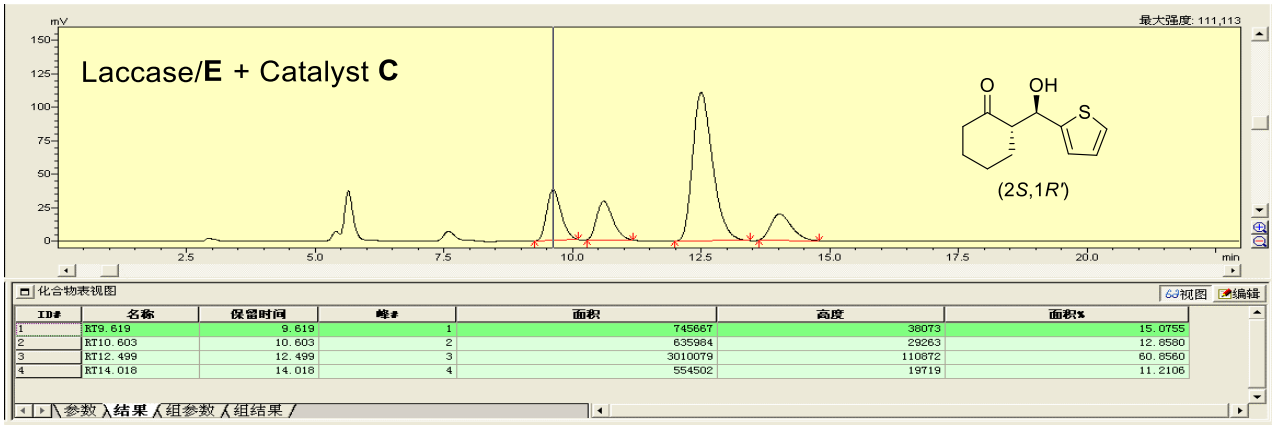
化合物表视图

ID#	名称	保留时间	峰#	面积	高度	面积%
1	RT21.913	21.913	1	2804461	70765	97.6444
2	RT32.695	32.695	2	27506	583	0.9577
3	RT37.225	37.225	3	1394	28	0.0485
4	RT41.351	41.351	4	38756	593	1.3494

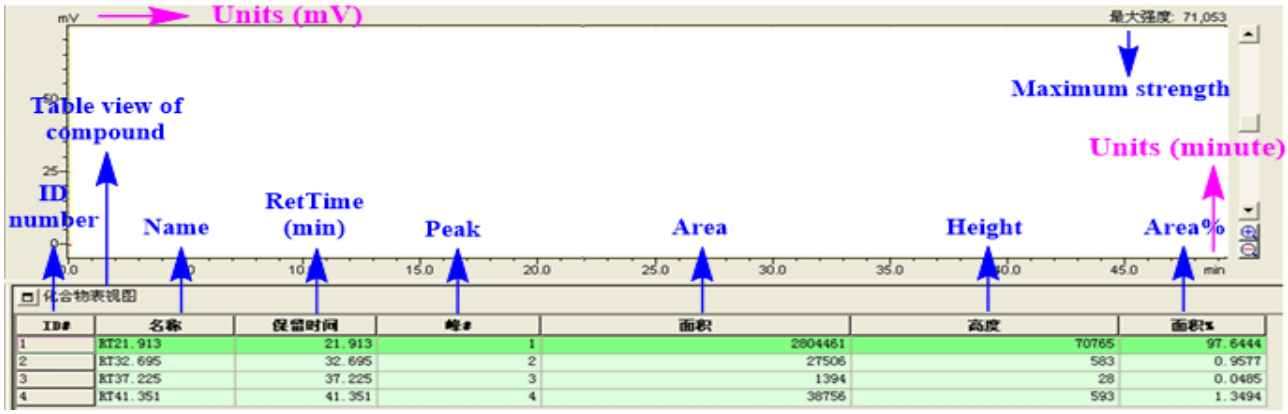
(*S*,*R*)-5o: (S)-2-((R)-hydroxy(thiophen-2-yl)methyl)cyclohexan-1-one.



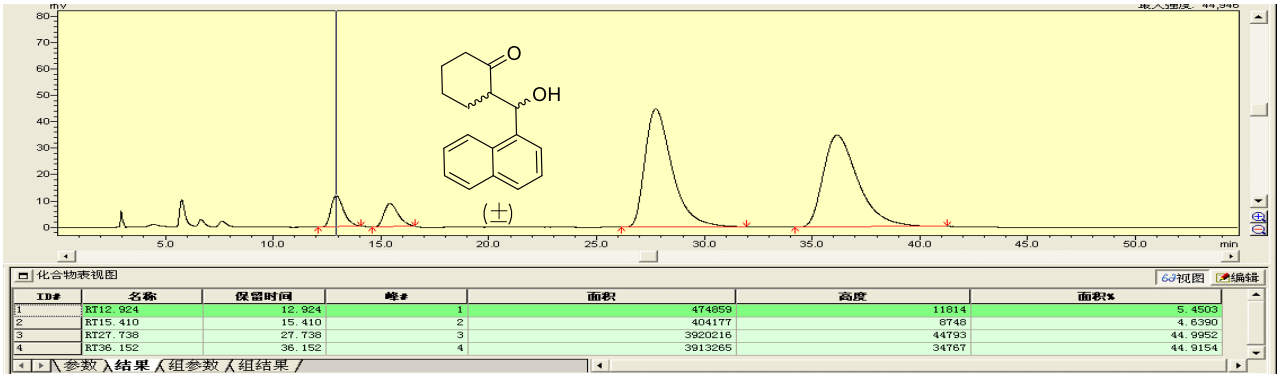




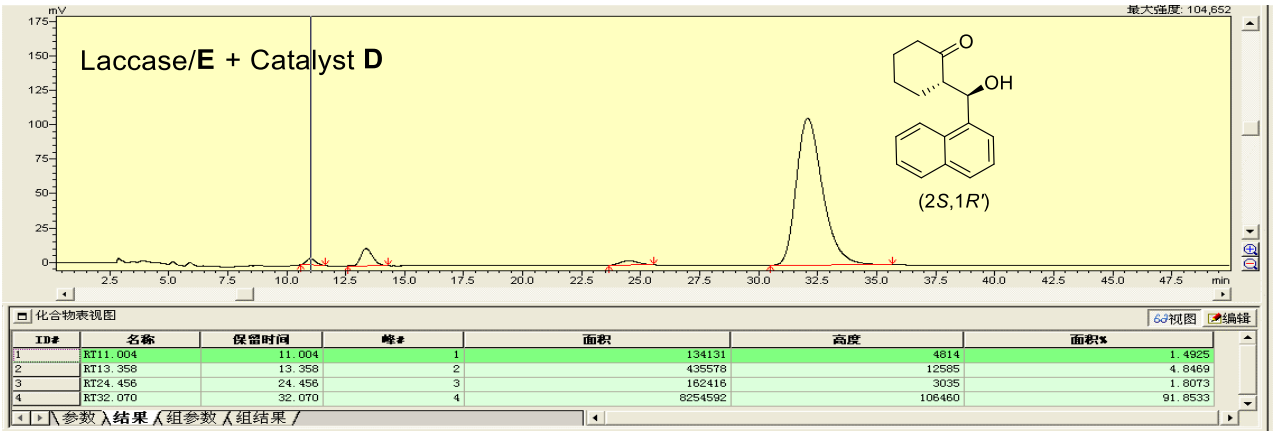
<u>Translation of all characters (Chinese) in the above two frameworks to English is as follows:</u>



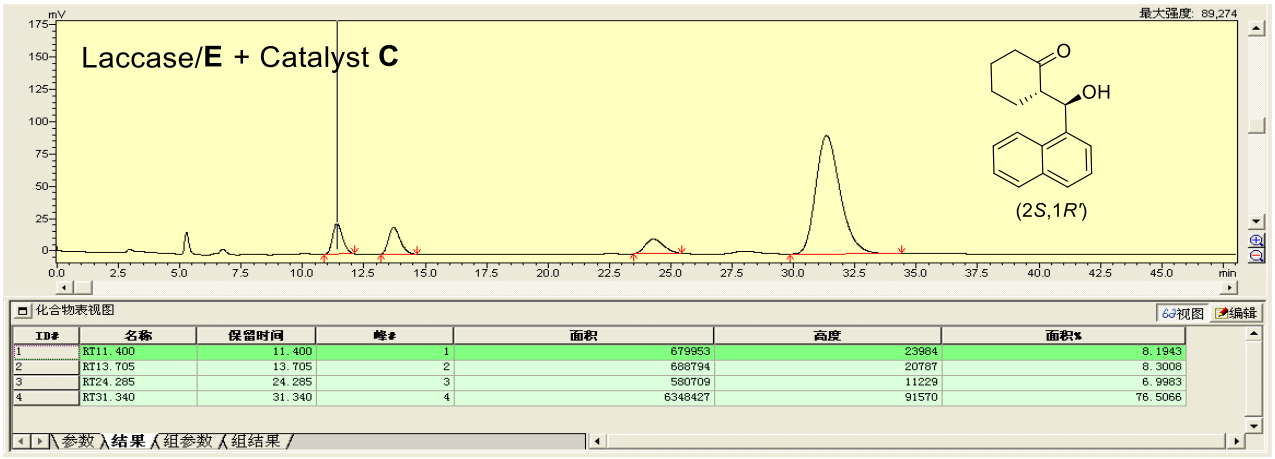
(*S*,*R*)-5p: (S)-2-((R)-hydroxy(naphthalen-1-yl)methyl)cyclohexan-1-one.



ID#	名称	保留时间	峰#	面积	高度	面积%
1	RT12.924	12.924	1	474859	11814	5.4503
2	RT15.410	15.410	2	404177	8748	4.6390
3	RT27.738	27.738	3	3920216	44793	44.9952
4	RT36.152	36.152	4	3913265	34767	44.9154

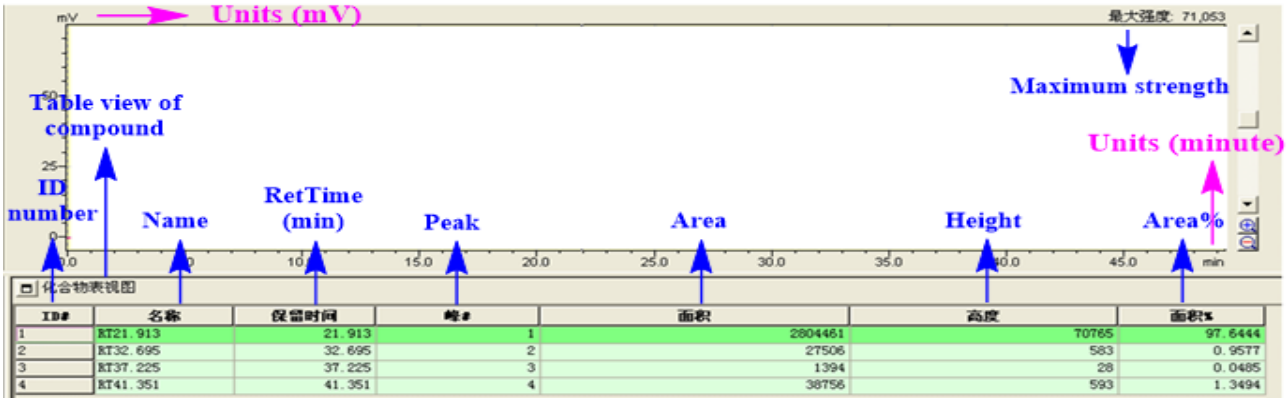


ID#	名称	保留时间	峰#	面积	高度	面积%
1	RT11.004	11.004	1	134131	4814	1.4925
2	RT13.358	13.358	2	435578	12585	4.8469
3	RT24.456	24.456	3	162416	3035	1.8073
4	RT32.070	32.070	4	8254592	106460	91.8533



ID#	名称	保留时间	峰#	面积	高度	面积%
1	RT11.400	11.400	1	679953	23984	8.1943
2	RT13.705	13.705	2	688794	20787	8.3008
3	RT24.285	24.285	3	580709	11229	6.9983
4	RT31.340	31.340	4	6348427	91570	76.5066

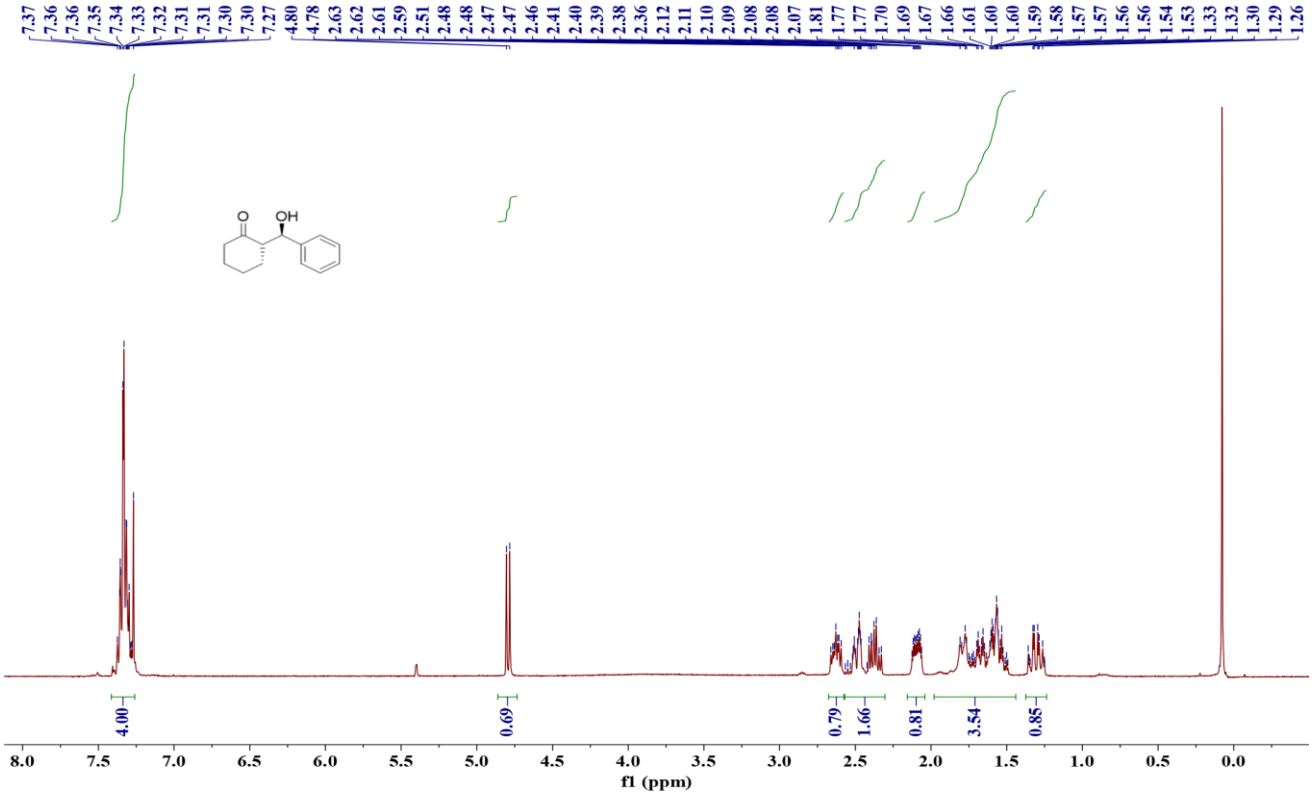
<u>Translation of all characters (Chinese) in the above two frameworks to English is as follows:</u>



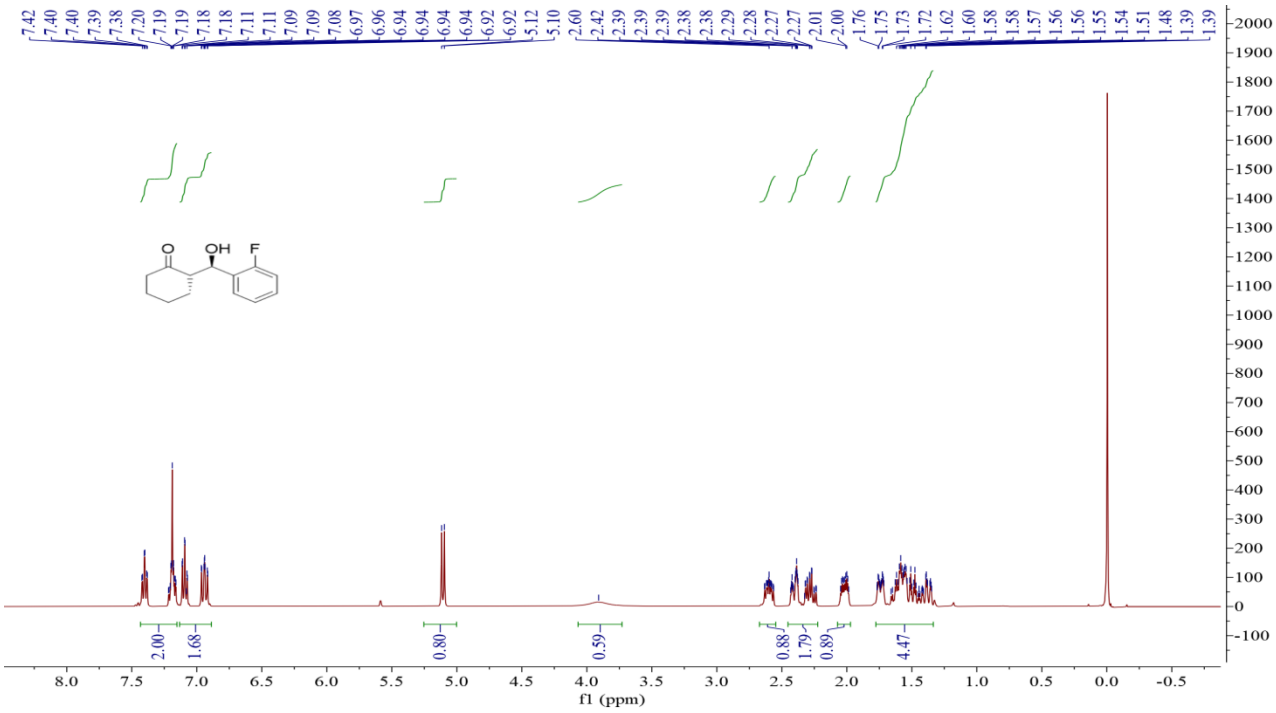
ID#	名称	保留时间	峰#	面积	高度	面积%
1	RT21.913	21.913	1	2804461	70765	97.6444
2	RT32.695	32.695	2	27506	583	0.9577
3	RT37.225	37.225	3	1394	28	0.0485
4	RT41.351	41.351	4	38756	593	1.3494

Figure S2. Characterization of chiral products (The ^{1}H NMR of all chiral products).

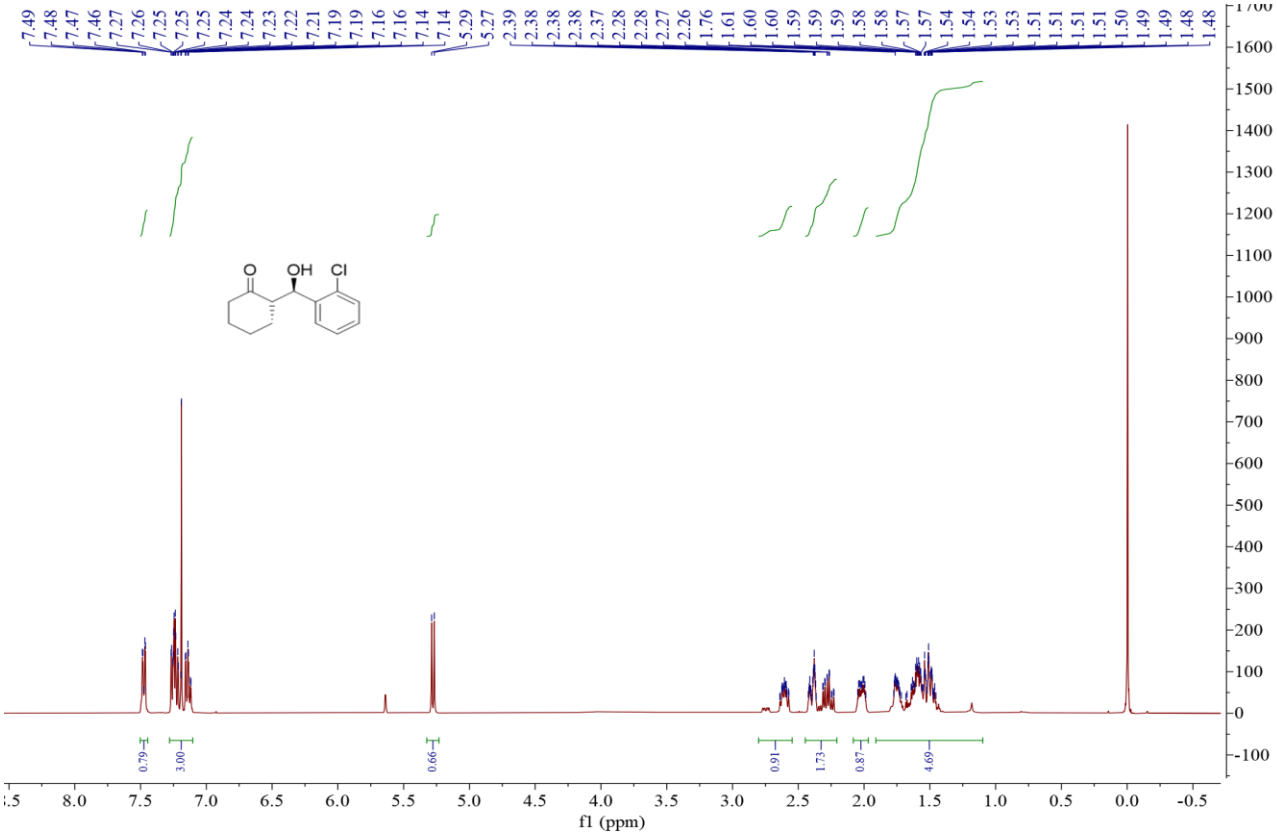
(*S,R*)-5a: (*S*)-2-((*R*)-hydroxy(phenyl)methyl)cyclohexan-1-one.



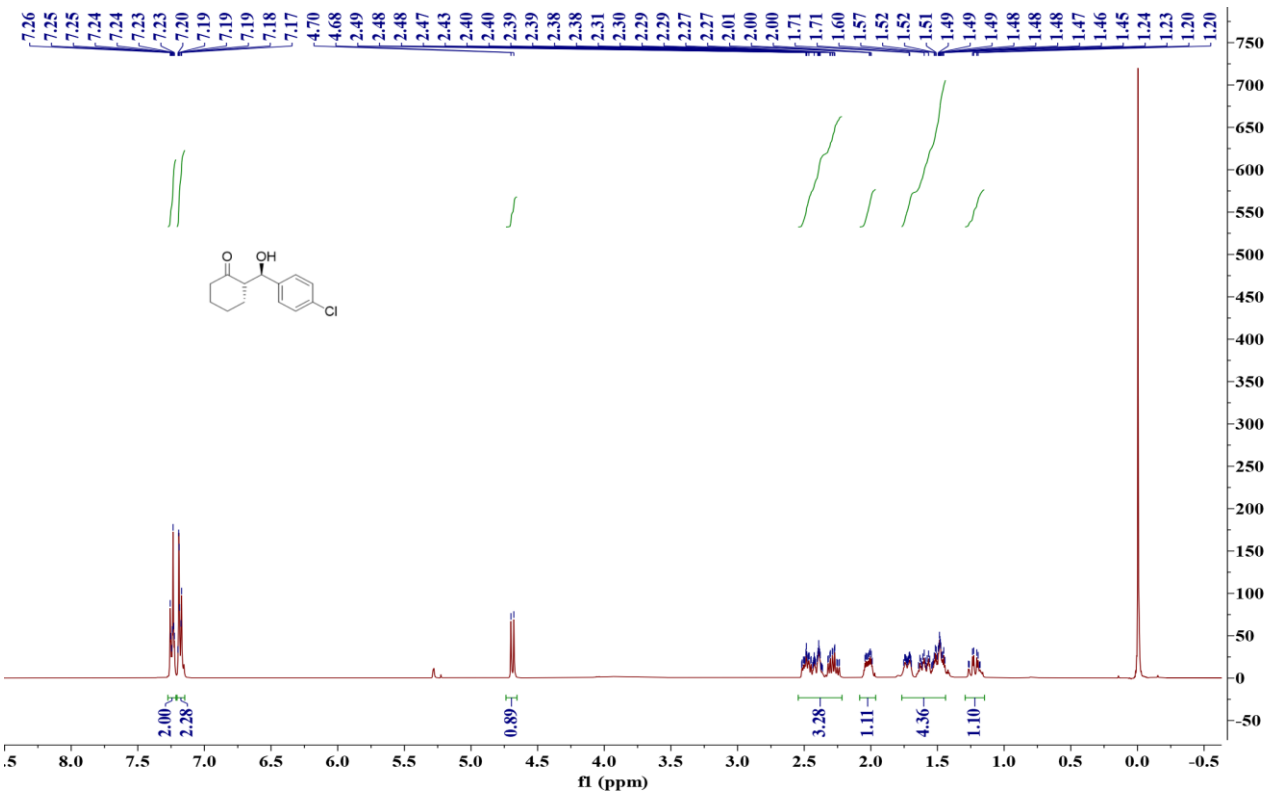
(*S,R*)-5b: (*S*)-2-((*R*)-(2-fluorophenyl)(hydroxy)methyl)cyclohexan-1-one.



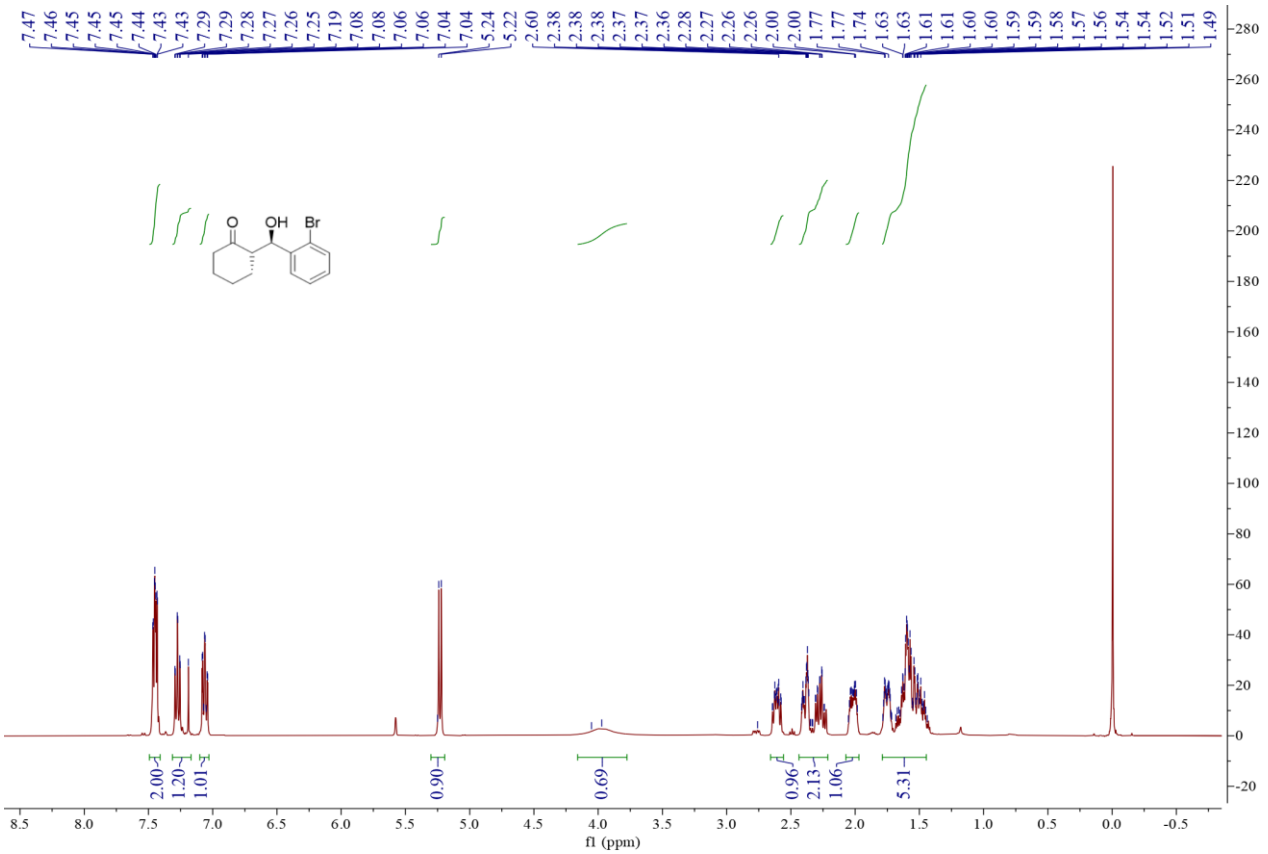
(*S,R*)-5c: (*S*)-2-((*R*)-(2-chlorophenyl)(hydroxy)methyl)cyclohexan-1-one.



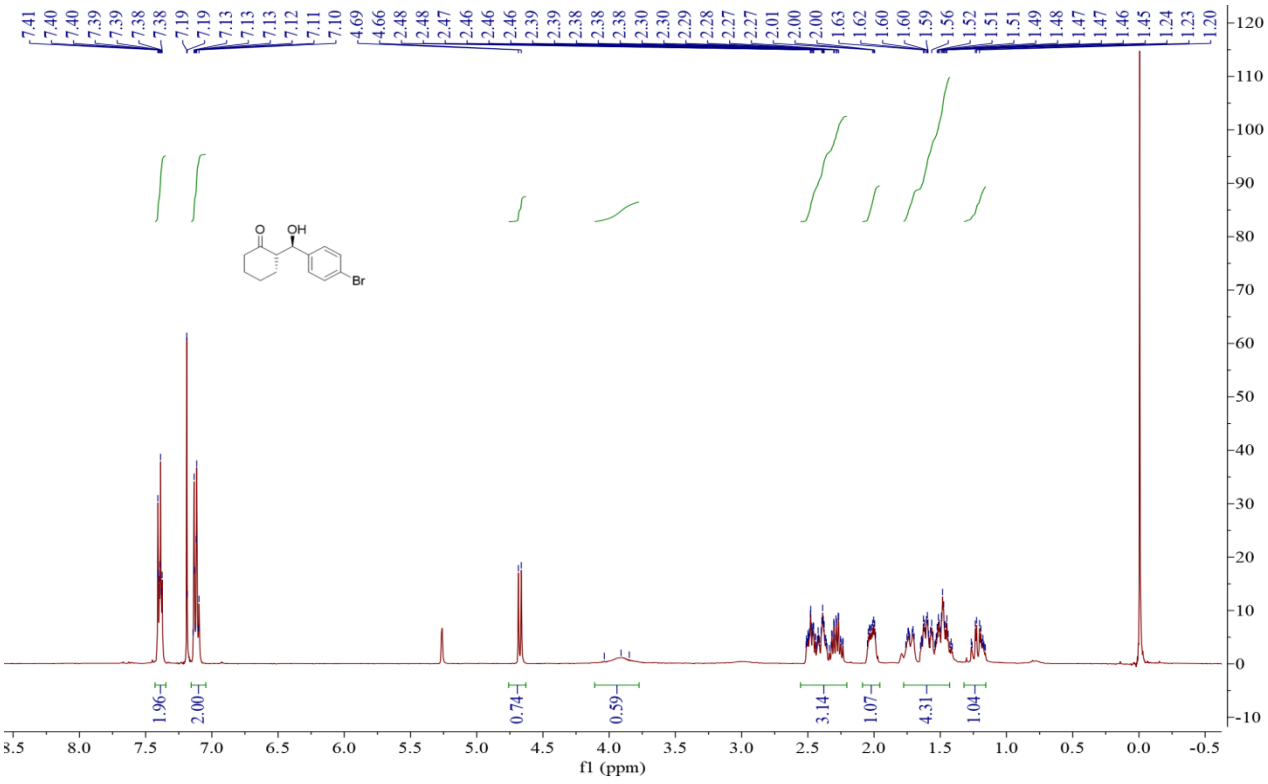
(*S,R*)-5d: (*S*)-2-((*R*)-(4-chlorophenyl)(hydroxy)methyl)cyclohexan-1-one.



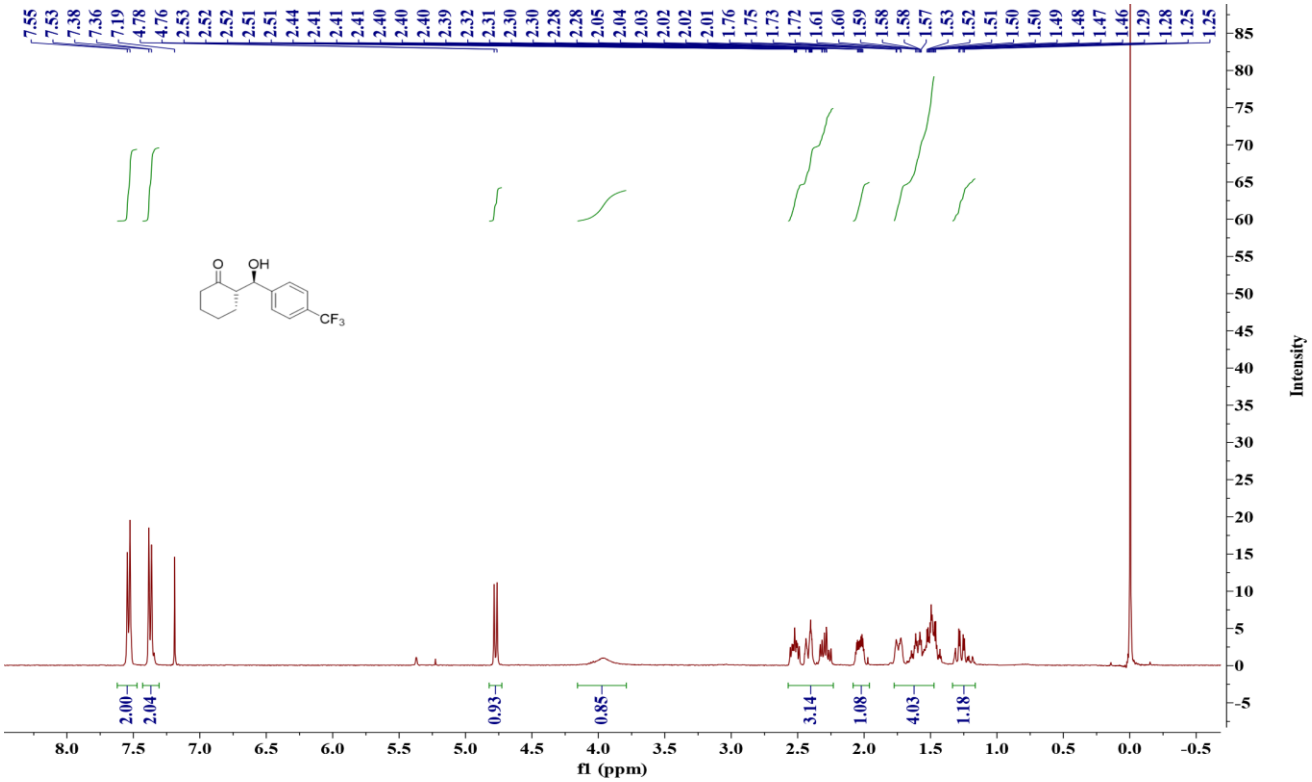
(*S,R*)-5e: (*S*)-2-((*R*)-(2-bromophenyl)(hydroxy)methyl)cyclohexan-1-one.



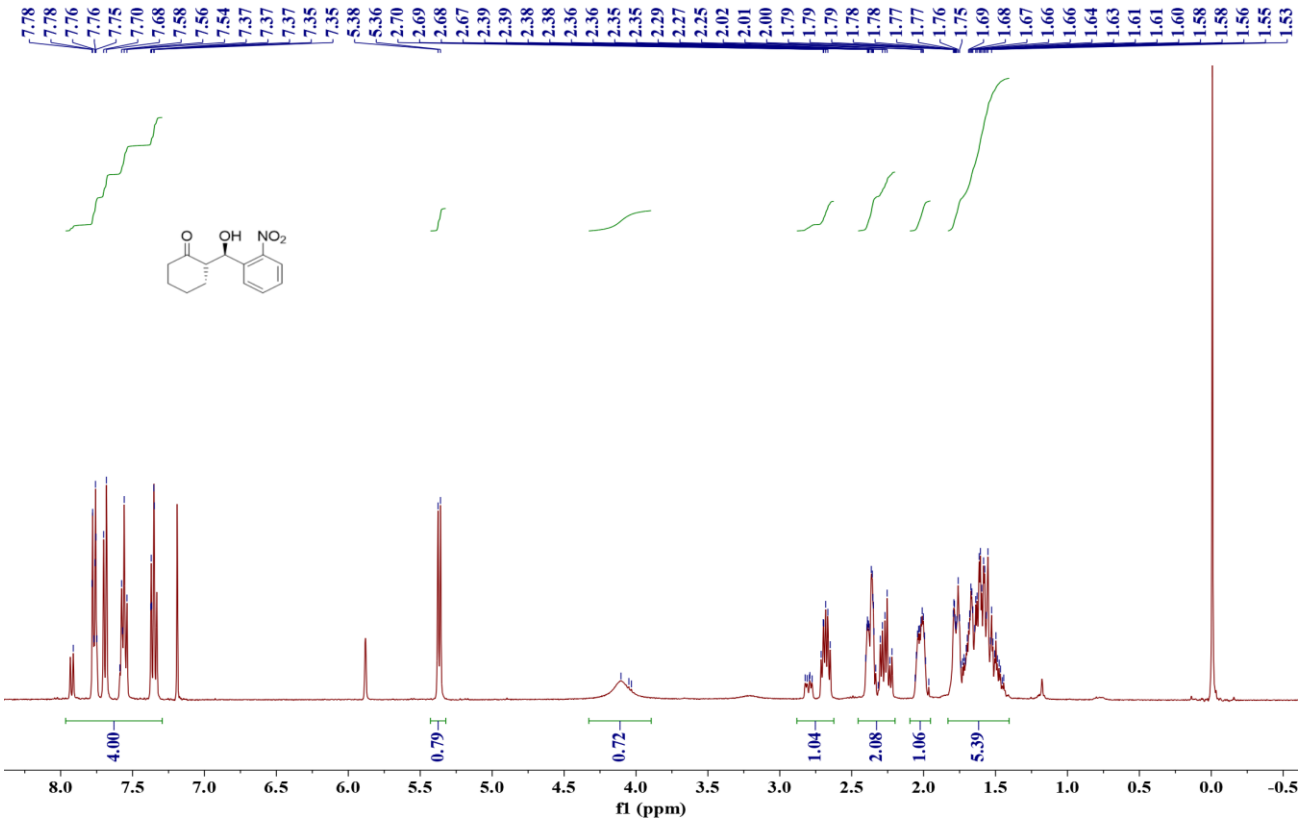
(*S,R*)-5f: (*S*)-2-((*R*)-(4-bromophenyl)(hydroxy)methyl)cyclohexan-1-one.



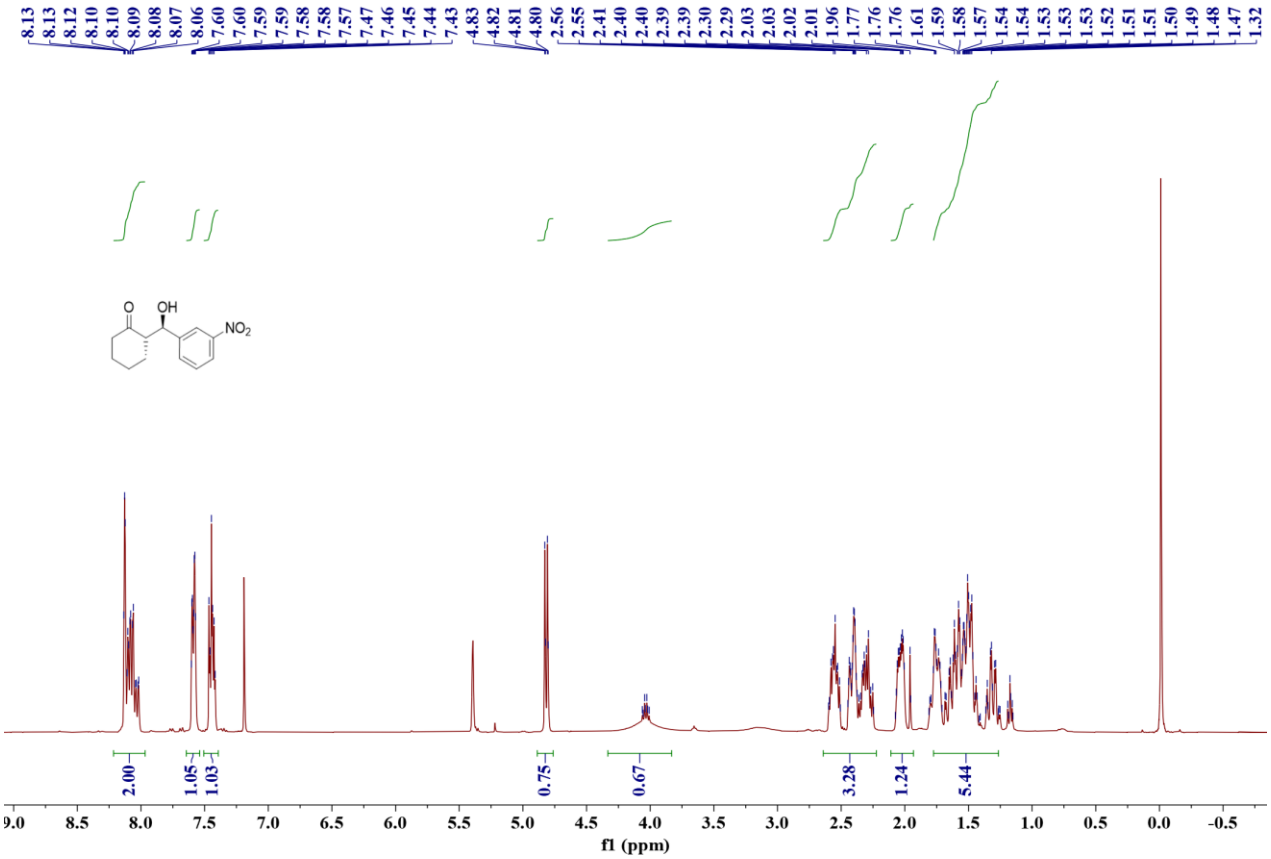
(*S,R*)-5g: (S)-2-((R)-hydroxy(4-(trifluoromethyl)phenyl)methyl)cyclohexan-1-one.



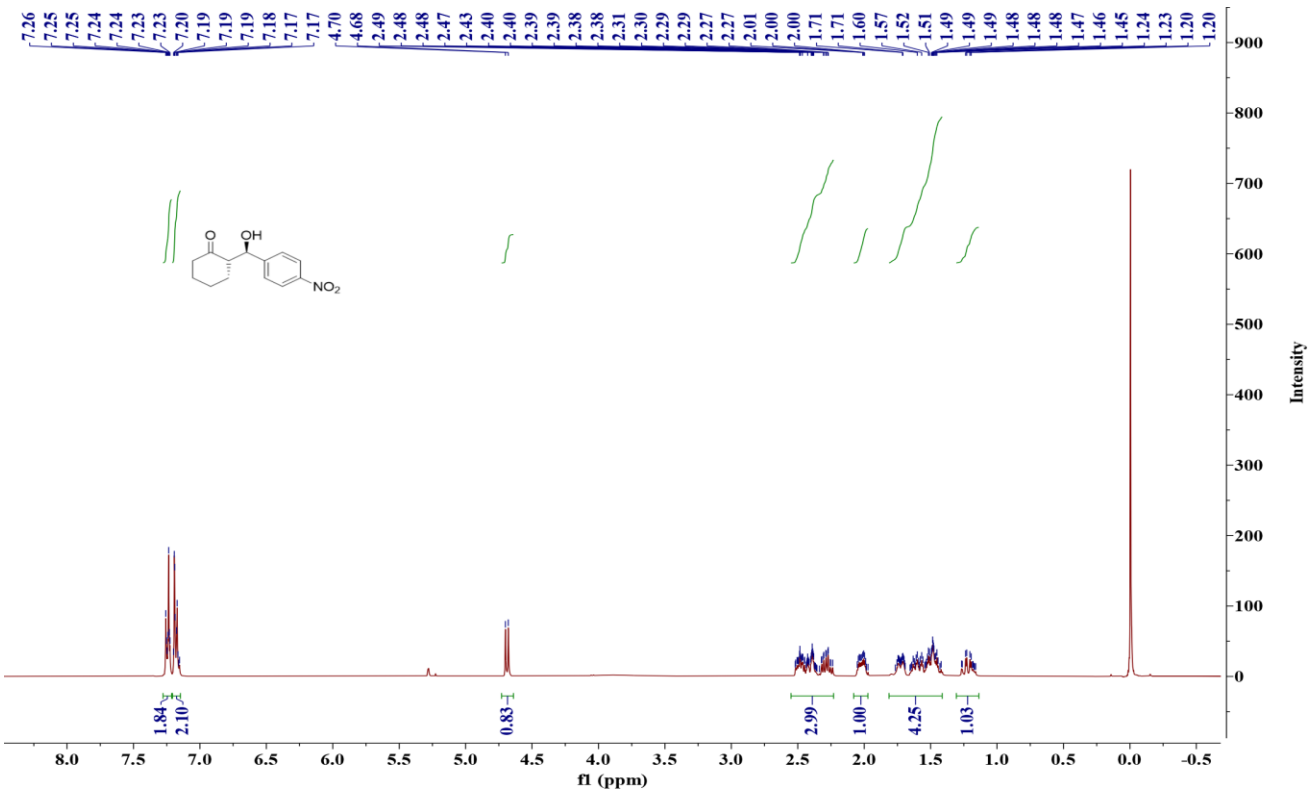
(*S,R*)-5h: (*S*)-2-((*R*)-hydroxy(2-nitrophenyl)methyl)cyclohexan-1-one.



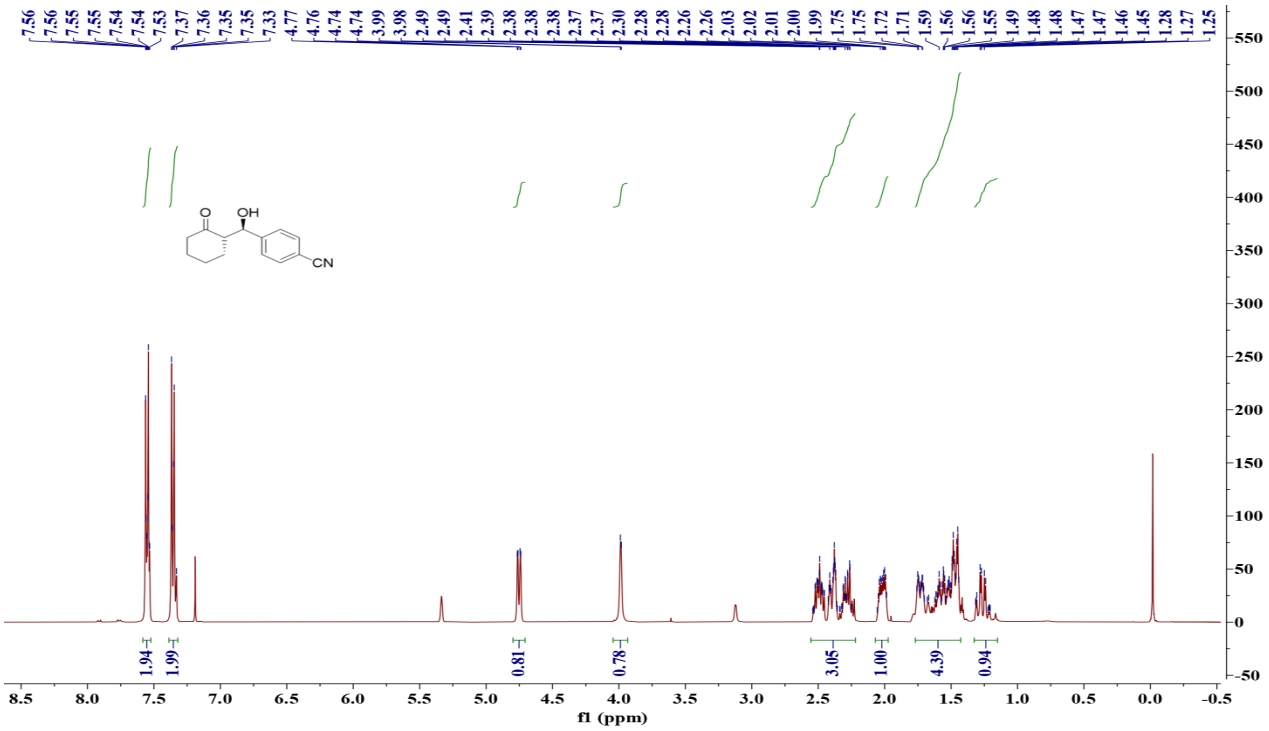
(*S,R*)-5i: (*S*)-2-((*R*)-hydroxy(3-nitrophenyl)methyl)cyclohexan-1-one.



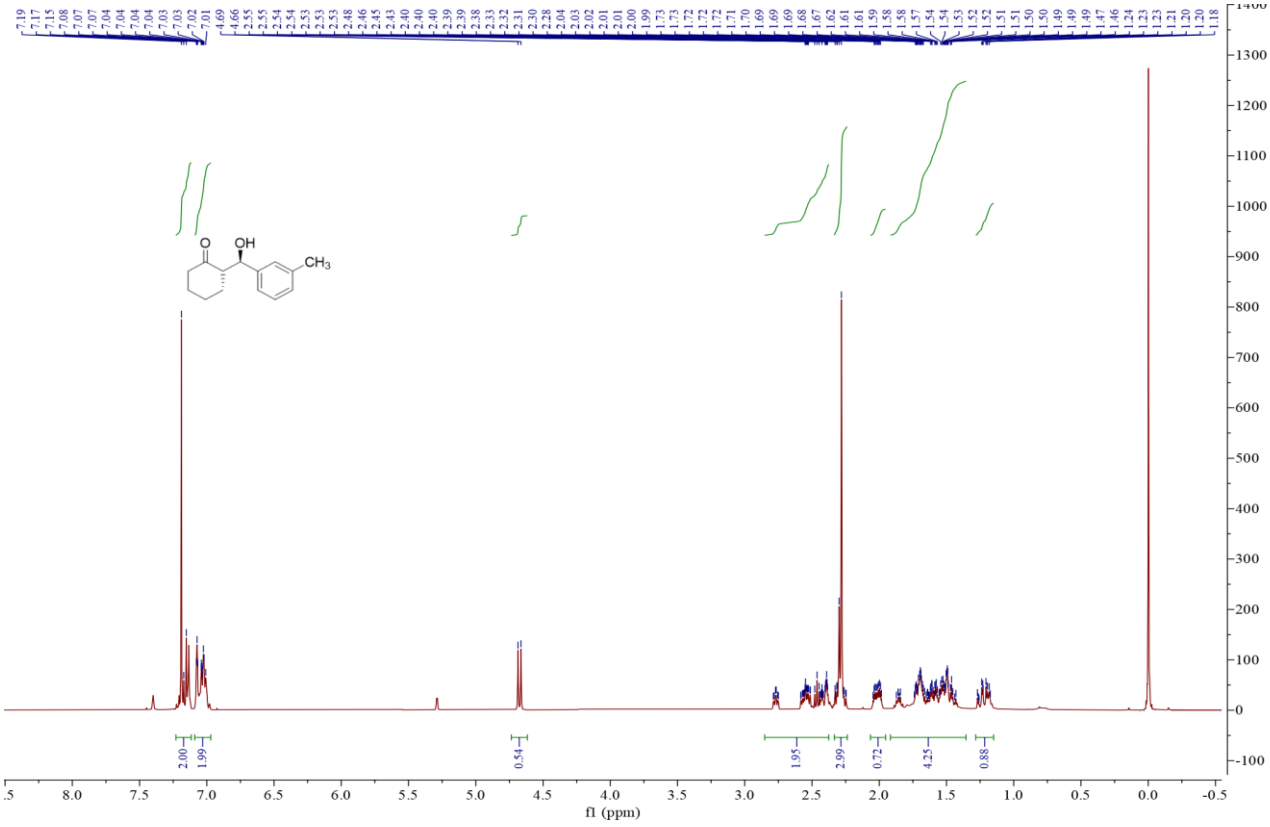
(*S,R*)-5j: (S)-2-((R)-hydroxy(4-nitrophenyl)methyl)cyclohexan-1-one.



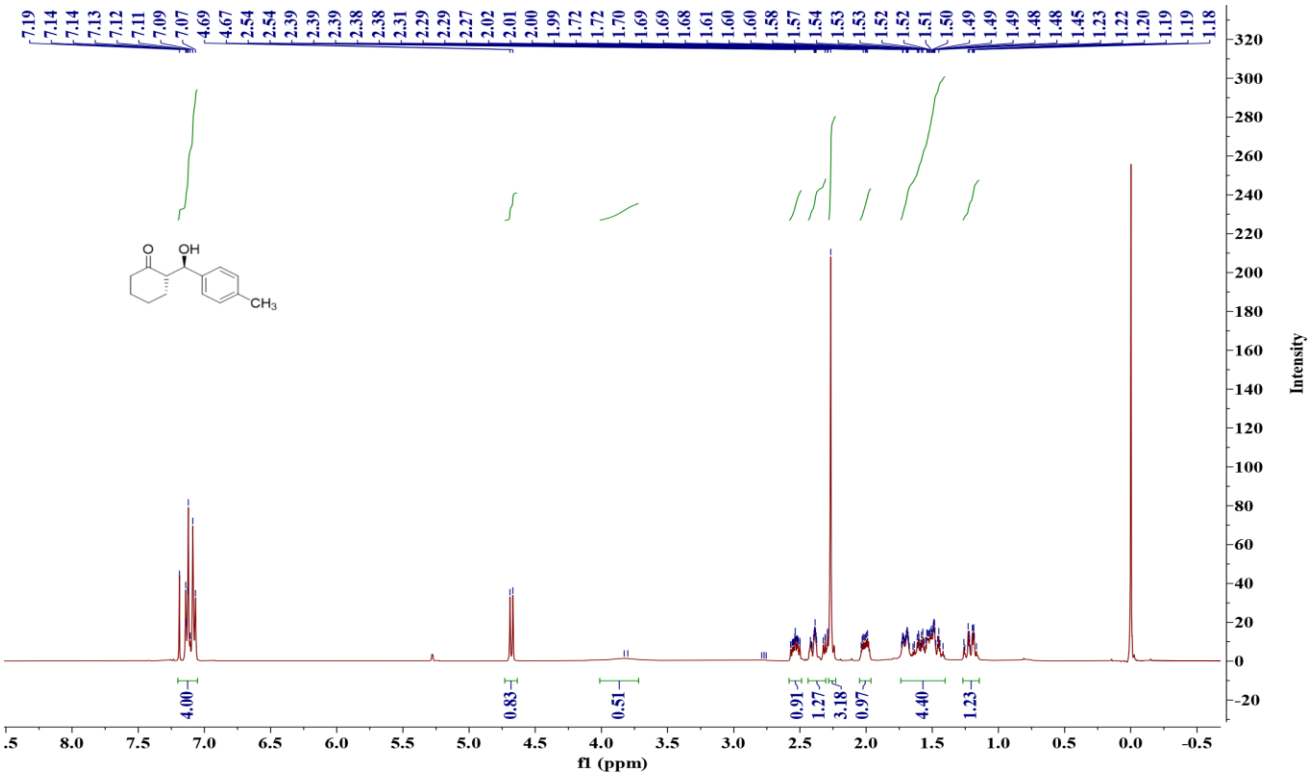
(*S,R*)-5k: 4-((S)-hydroxy((R)-2-oxocyclohexyl)methyl)benzonitrile.



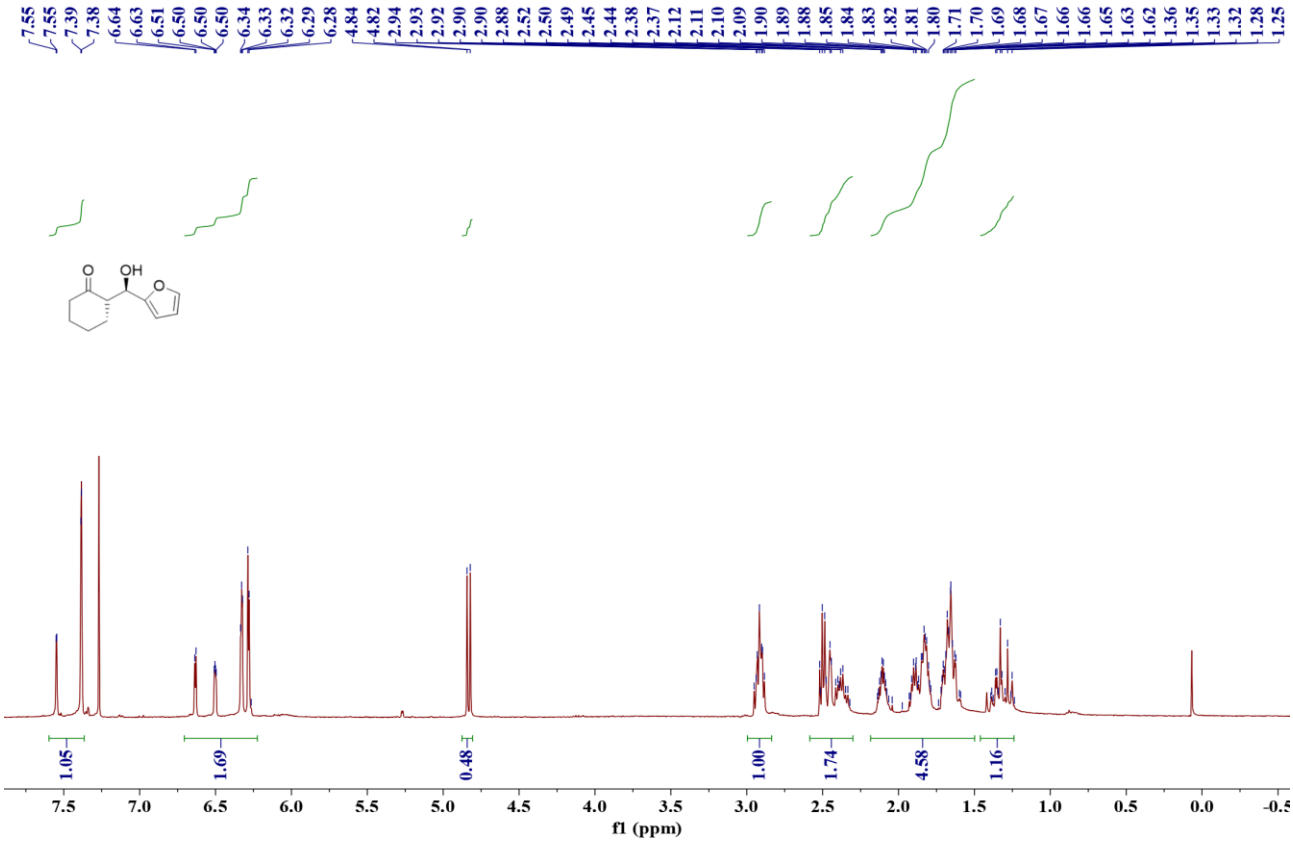
(*S,R*)-5l: (S)-2-((R)-hydroxy(m-tolyl)methyl)cyclohexan-1-one.



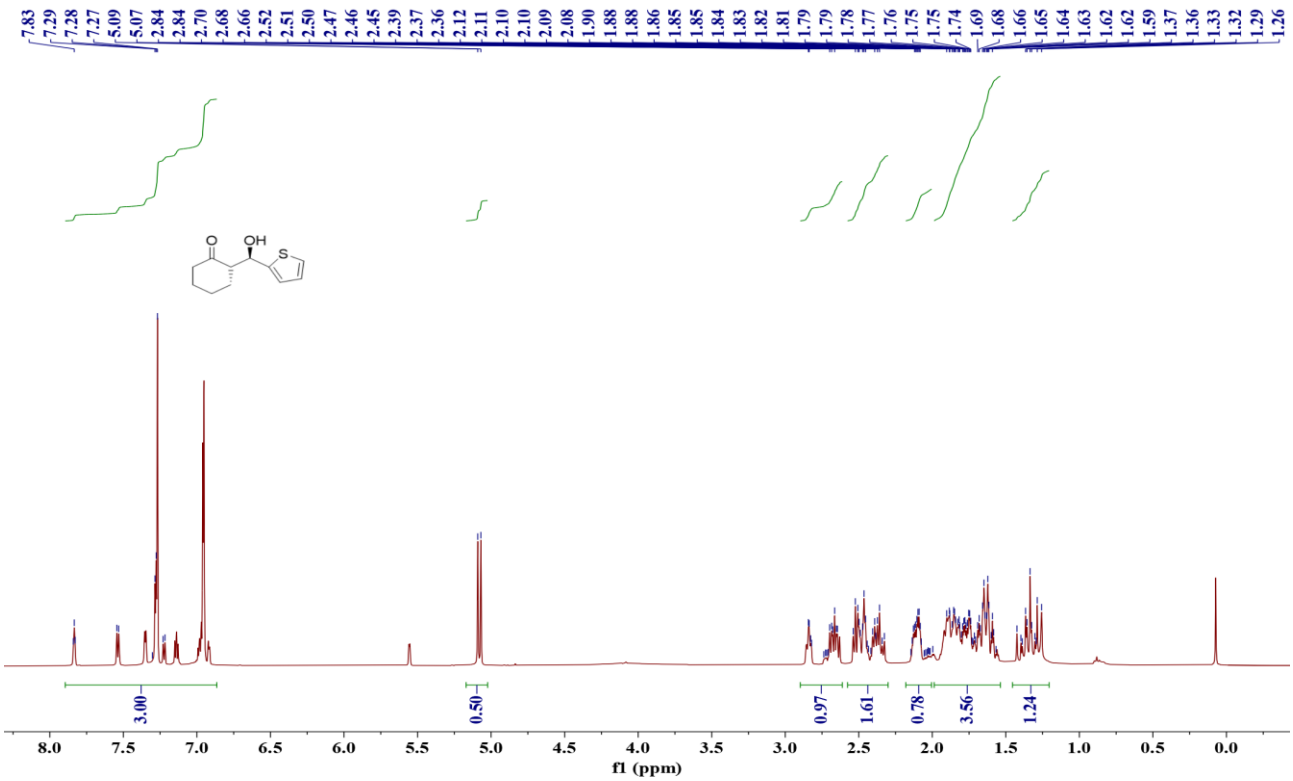
(*S,R*)-5m: (*S*)-2-((*R*)-hydroxy(p-tolyl)methyl)cyclohexan-1-one.



(*S,R*)-5n: (S)-2-((R)-furan-2-yl(hydroxy)methyl)cyclohexan-1-one.



(*S,R*)-5o: (S)-2-((R)-hydroxy(thiophen-2-yl)methyl)cyclohexan-1-one.



(*S,R*)-5p: (*S*)-2-((*R*)-hydroxy(naphthalen-1-yl)methyl)cyclohexan-1-one.