

Asymmetric hydrolytic kinetic resolution with recyclable polymeric Co(III)-salen complexes: A practical strategy in the preparation of (S)-Metoprolol, (S)-Toliprolol and (S)-Alprenolol: computational rationale for enantioselectivity

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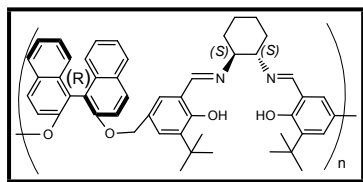
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Characterization data of ligands



1': Yield 96 %; yellow crystalline solid; Melting Point: 218 °C;

$[\alpha]_D^{27} = +158.34$ ($c = 0.125$, CHCl_3); ^1H NMR (200 MHz,

CDCl_3) δ in ppm: 1.22 (s, 18H), 1.56-1.69 (m, 3H), 1.80-1.90

(m, 5H), 4.70-4.92 (m, 6H), 6.23-6.51 (m, 2H), 6.61-6.95 (m, 3H), 7.21-7.26 (m, 3H), 7.30-

7.46 (m, 5H), 7.68-7.70 (m, 2H), 7.77-8.03 (m, 6H), 13.75 (bs, 2H); ^{13}C NMR (50 MHz,

CDCl_3) δ in ppm: 23.8, 24.3, 28.6, 34.0, 69.8, 72.00, 114.1, 115.9, 117.5, 122.8, 123.3, 125.0,

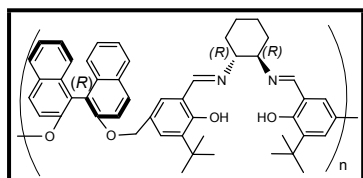
125.6, 126.1, 127.9, 128.7, 129.1, 133.5, 133.7, 153.5, 164.63; IR (KBr, $\nu \text{ cm}^{-1}$): 3432, 3056,

2931, 2860, 1722, 1626, 1591, 1442, 1358, 1264, 1156, 1086, 1013, 869, 745, 696; GPC:

Average molecular weight (M_n) 13658, polymer molecular weight distribution (PDI) 1.06,

Elemental analysis found: C 80.09, H 7.18, N 3.35; $\text{C}_{51}\text{H}_{56}\text{N}_2\text{O}_4$ calcd. C 80.49, H 7.42, N

3.68; UV-Vis.: (MeOH) λ_{max} 330 nm.



2': Yield 95 %; yellow crystalline solid; Melting Point: 215 °C;

$[\alpha]_D^{27} = +136.54$ ($c = 0.01$, CHCl_3); ^1H NMR (200 MHz, CDCl_3)

δ in ppm: 1.22 (s, 18H), 1.57-1.69 (m, 3H), 1.78-1.91 (m, 5H),

4.70-4.92 (m, 6H), 6.23-6.31 (m, 2H), 6.44-6.66 (m, 2H), 6.84-6.98 (m, 2H), 7.11-7.16 (m,

3H), 7.21-7.23 (m, 2H), 7.30-7.45 (m, 4H), 7.68-7.71 (m, 2H), 7.76-7.92 (m, 5H), 13.72 (bs,

2H); ^{13}C NMR (50 MHz, CDCl_3) δ in ppm: 23.8, 24.3, 28.6, 34.0, 35.97, 69.8, 72.0, 114.1,

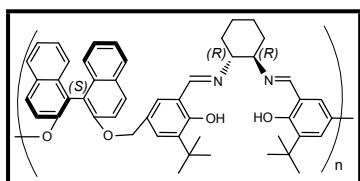
115.9, 117.5, 120.6, 122.8, 123.3, 125.0, 125.6, 125.8, 126.1, 127.3, 127.8, 127.9, 128.7,

128.9, 128.9, 133.5, 133.6, 153.6, 164.7; IR (KBr, $\nu \text{ cm}^{-1}$): 3430, 3055, 2931, 2860, 1811,

1736, 1627, 1592, 1443, 1324, 1265, 1155, 1082, 1013, 870, 744, 696, 580; GPC: Average

molecular weight (M_n) 13435, polymer molecular weight distribution (PDI) 1.09; Elemental

analysis found: C 80.23, H 7.32, N 3.48; C₅₁H₅₆N₂O₄calcd. C 80.49, H 7.42, N 3.68; UV-Vis.: (MeOH) λ_{max} 330 nm.

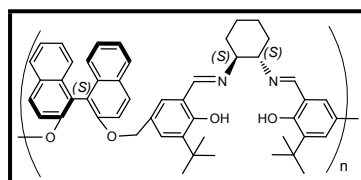


3': Yield 98 %; yellow crystalline solid; Melting Point: 220 °C;

$[\alpha]^{27}_{\text{D}} = -151.27$ (c=0.25, CHCl₃); ¹H NMR (200 MHz, CDCl₃)

δ in ppm: 1.22 (s, 18H), 1.61-1.65 (m, 3H), 1.76-1.88 (m, 5H),

4.71-4.91 (m, 6H), 6.24-6.51(m, 2H), 6.84-6.95 (m, 2H), 7.15-7.42 (m, 10H), 7.68-7.76 (m, 2H), 7.84-7.92 (m, 6H), 13.72 (bs, 2H); ¹³C NMR (50 MHz, CDCl₃) δ in ppm: 25.6, 26.1, 30.6, 33.3, 71.8, 73.9, 116.1, 117.9, 124.7, 125.2, 126.9, 127.6, 127.8, 129.2, 129.6, 130.5, 135.5, 138.31, 138.4, 138.5, 155.5, 166.5; IR (KBr, ν cm⁻¹): 3431, 3055, 2930, 2860, 1627, 1592, 1506, 1442, 1357, 1212, 1155, 1082, 1015, 869, 744, 580; GPC: Average molecular weight (M_n) 13999, polymer molecular weight distribution (PDI) 1.08; Elemental analysis found: C 80.04; H 7.16; N 3.45; C₅₁H₅₆N₂O₄calcd. C 80.49; H 7.42; N 3.68; UV-Vis.: (MeOH) λ_{max} 330 nm.



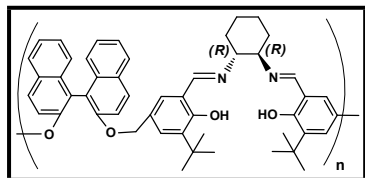
4':Yield 96 %; yellow crystalline solid; Melting Point: 210 °C;

$[\alpha]^{27}_{\text{D}} = +165.25$ (c= 0.25, CHCl₃); ¹H NMR (200 MHz,

CDCl₃) δ in ppm: 1.18(s, 18H), 1.60-1.65 (m, 3H), 1.78-1.92

(m, 5H), 4.43-4.92 (m, 6H), 5.90-5.94 (m, 2H), 6.61-6.83 (m, 3H), 6.89-7.04 (m, 3H), 7.08-7.19 (m, 6H), 7.46-7.49 (m, 2H), 7.64-7.68 (m, 2H), 7.72-7.85 (m, 4H), 13.91 (bs, 2H); ¹³C NMR (50 MHz, CDCl₃) δ in ppm: 24.2, 24.9, 29.2, 34.5, 70.4, 72.5, 114.7, 116.5, 118.0, 121.0, 123.3, 123.8, 125.5, 126.4, 127.8, 128.2, 129.1, 129.2, 129.4, 129.5, 129.6, 134.0, 134.2, 154.1, 165.1; IR (KBr, ν cm⁻¹): 3432, 3057, 2930, 2859, 1812, 1711, 1626, 1593, 1444, 1358, 1264, 1215, 1156, 1040, 869, 745, 696, 589; GPC: Average molecular weight (M_n) 13448, polymer molecular weight distribution (PDI) 1.07; Elemental analysis found: C

80.41, H 7.26, N 3.55; C₅₁H₅₆N₂O₄ calcd. C 80.49, H 7.42, N 3.68; UV-Vis.: (MeOH) $\lambda_{\max}$ 330 nm.



5': Yield 98 %; yellow crystalline solid; Melting Point: 225°C;

$[\alpha]_{\text{D}}^{27} = -142.91$ (c= 0.25, CHCl₃); ¹H NMR (200 MHz, CDCl₃)

δ in ppm: 1.18 (s, 18H), 1.62-1.68 (m, 3H), 1.78-1.83 (m, 5H),

4.41-4.72 (m, 6H), 5.90-5.96 (m, 2H), 6.61-6.84 (m, 3H), 7.00-7.06 (m, 3H), 7.10-7.19 (m,

5H), 7.46-7.49 (m, 2H), 7.64-7.70 (m, 2H), 7.76-7.94 (m, 6H), 13.91 (bs, 2H); ¹³C NMR (50

MHz, CDCl₃) δ in ppm: 25.6, 26.3, 30.0, 35.9, 71.8, 73.9, 116.1, 117.9, 124.7, 125.2,

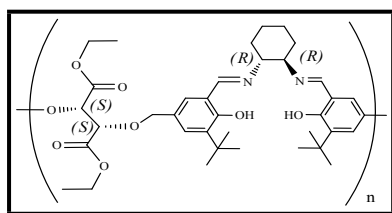
126.9, 127.6, 127.8, 129.2, 129.6, 129.9, 130.5, 135.5, 155.59, 165.5. IR (KBr, ν cm⁻¹): 3431,

3055, 2931, 2860, 1806, 1736, 1627, 1592, 1443, 1356, 1264, 1155, 1082, 1013, 869, 744,

580; GPC: Average molecular weight (M_n) 13208, polymer molecular weight distribution

(PDI) 1.04; Elemental analysis found: C 80.38, H 7.38, N 3.55; C₅₁H₅₆N₂O₄ calcd. C 80.49, H

7.42, N 3.68; UV-Vis: (MeOH) $\lambda_{\max}$ 330 nm.



6': Yield 95 %; yellow crystalline solid; Melting Point:

110°C; $[\alpha]_{\text{D}}^{27} = +187.09$ (c= 0.01, CHCl₃); ¹H NMR (200

MHz, CDCl₃) δ in ppm: 0.97 (t, $J=7$ Hz, 6H), 1.34 (s, 18H),

1.74-1.90 (m, 8H), 3.32-3.36 (m, 2H), 3.87-4.14 (m, 5H), 4.23-4.28 (m, 6H), 4.59-4.74 (m,

3H), 6.95 (s, 2H), 7.11 (s, 2H), 8.24 (s, 2H), 13.86 (bs, 2H); ¹³C NMR (50 MHz, CDCl₃) δ in

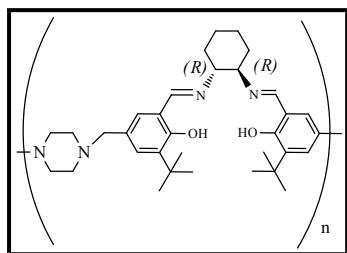
ppm: 13.9, 14.1, 24.2, 24.6, 29.3, 33.1, 33.6, 34.6, 54.6, 61.1, 72.3, 73.3, 76.4, 78.3, 118.1,

125.9, 130.1, 137.3, 160.4, 165.1, 169.2; IR (KBr, ν cm⁻¹): 3437, 2932, 2862, 1755, 1629,

1446, 1390, 1268, 1204, 1158, 1027, 863, 704, 554; GPC: Average molecular weight (M_n)

3466, polymer molecular weight distribution (PDI) 1.21; Elemental analysis found: C 68.76,

H 7.98, N 4.05; C₃₉H₅₆N₂O₈calcd. C 68.80, H 8.29, N 4.11; UV-Vis.: (MeOH) λ_{max} 260 nm and 330 nm.



7': Yield 96 %; yellow crystalline solid; Melting Point: 215 °C;

$[\alpha]_{\text{D}}^{27} = +93.35$ (c= 0.25, CHCl₃); ¹H NMR (200 MHz, CDCl₃) δ

in ppm: 1.29 (s, 18H), 1.47-1.66 (m, 3H), 1.7-1.81 (m, 5H),

2.07(s, 2H), 2.29 (m, 8H), 2.79 (bs, 1H), 3.25-3.35 (m, 6H), 6.86

(m, 2H), 7.00-7.17 (m, 2H), 8.17 (s, 2H), 13.69 (bs, 2H); ¹³C NMR (50 MHz, CDCl₃) δ in

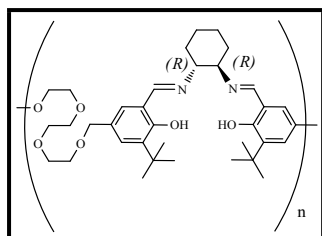
ppm: 24.3, 29.4, 30.9, 34.7, 52.8, 62.5, 72.3, 118.2, 126.6, 130.3, 136.7, 151.7, 159.3, 165.4;

IR (KBr, ν cm⁻¹): 3421, 2934, 2863, 2807, 1629, 1443, 1359, 1264, 1159, 1013, 878, 730,

621; GPC: Average molecular weight (M_n) 4529, polymer molecular weight distribution

(PDI) 1.42; Elemental analysis found: C 74.86, H 9.08, N 9.69; C₃₅H₅₂N₄O₂calcd. C 74.96, H

9.35, N 9.99; UV-Vis.: (MeOH) λ_{max} 262 nm and 330 nm.



8':Yield 96 %; yellow crystalline solid; Melting Point: 100 °C;

$[\alpha]_{\text{D}}^{27} = -160.01$ (c= 0.25, CHCl₃); ¹H NMR (200 MHz,

CDCl₃) δ in ppm: 1.38 (s, 18H), 1.69-1.75 (m, 3H), 1.85-2.06 (m,

5H), 3.30-3.32 (m, 3H), 3.56-3.63 (m, 14H), 4.38 (m, 5H), 6.98 (m, 2H), 7.20 (m, 2H), 8.26

(s, 2H), 13.55 (bs, 2H); ¹³C NMR (50 MHz, CDCl₃) δ in ppm: 23.7, 28.8, 32.5, 34.2, 68.5,

70.0, 71.8, 72.6, 117.6, 126.5, 129.0, 136.6, 159.4, 164.8; IR (KBr, ν cm⁻¹): 3432, 2927,

2862, 1629, 1444, 1385, 1358, 1265, 1098, 1026, 870, 706, 517; GPC: Average molecular

weight (M_n) 4543, polymer molecular weight distribution (PDI) 1.66, Elemental analysis

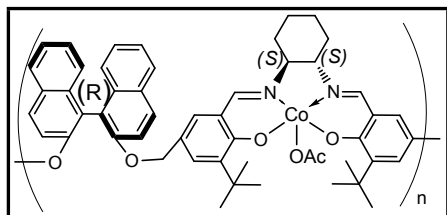
found: C 70.98, H 9.08, N 4.20; C₃₇H₅₆N₂O₆ calcd. C 71.12, H 9.03, N 4.48; UV-Vis.:

(MeOH) λ_{max} 260, 330 nm.

Table 3: GPC analysis data of polymeric ligands 1'-8'

Ligands	Average Molecular Weight (M_n)	No of monomeric units	PDI
1'	13568	18	1.06
2'	13435	18	1.09
3'	13999	18	1.08
4'	13448	18	1.07
5'	13208	17	1.04
6'	3466	5	1.21
7'	4529	8	1.42
8'	4543	7	1.66

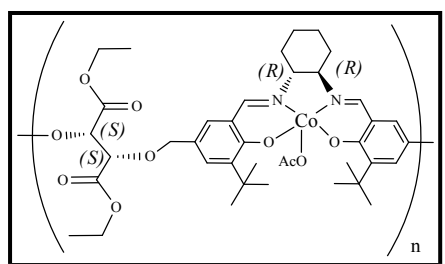
Characterization data of Co(III) salen complexes



1: Yield 99 %; dark brown solid; Melting Point: >200 °C; $[\alpha]_D^{27} = 921.54$ ($c = 0.025$, CHCl_3); IR (KBr, $\nu \text{ cm}^{-1}$): 3428, 3054, 2935, 2845, 1696, 1592, 1382, 1262, 1240,

1162, 1016, 870, 721, 567; Elemental analysis found: C 72.82, H 6.45, N 3.17;

$\text{C}_{53}\text{H}_{57}\text{CoN}_2\text{O}_6$ calcd. C 72.59, H 6.55, N 3.19; UV-Vis.: (MeOH) λ_{max} 330, 400 nm.

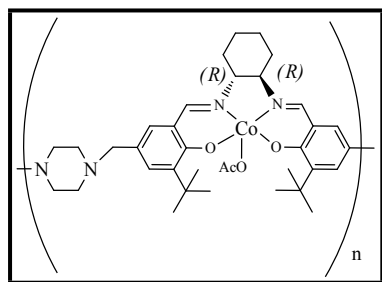


6: Yield 97 %; dark brown solid; Melting Point: 135 °C;

$[\alpha]_D^{27} = -724.72$ ($c = 0.025$, CHCl_3); IR (KBr, $\nu \text{ cm}^{-1}$): 3426, 3115, 2929, 2852, 1946, 1749, 1642, 1528, 1342, 1258, 1157, 1098, 870, 794, 562; Elemental analysis

found: C 61.42, H 7.44, N 3.60; $\text{C}_{41}\text{H}_{57}\text{CoN}_2\text{O}_{10}$ calcd. C 61.80, H 7.21, N 3.52; UV-Vis.:

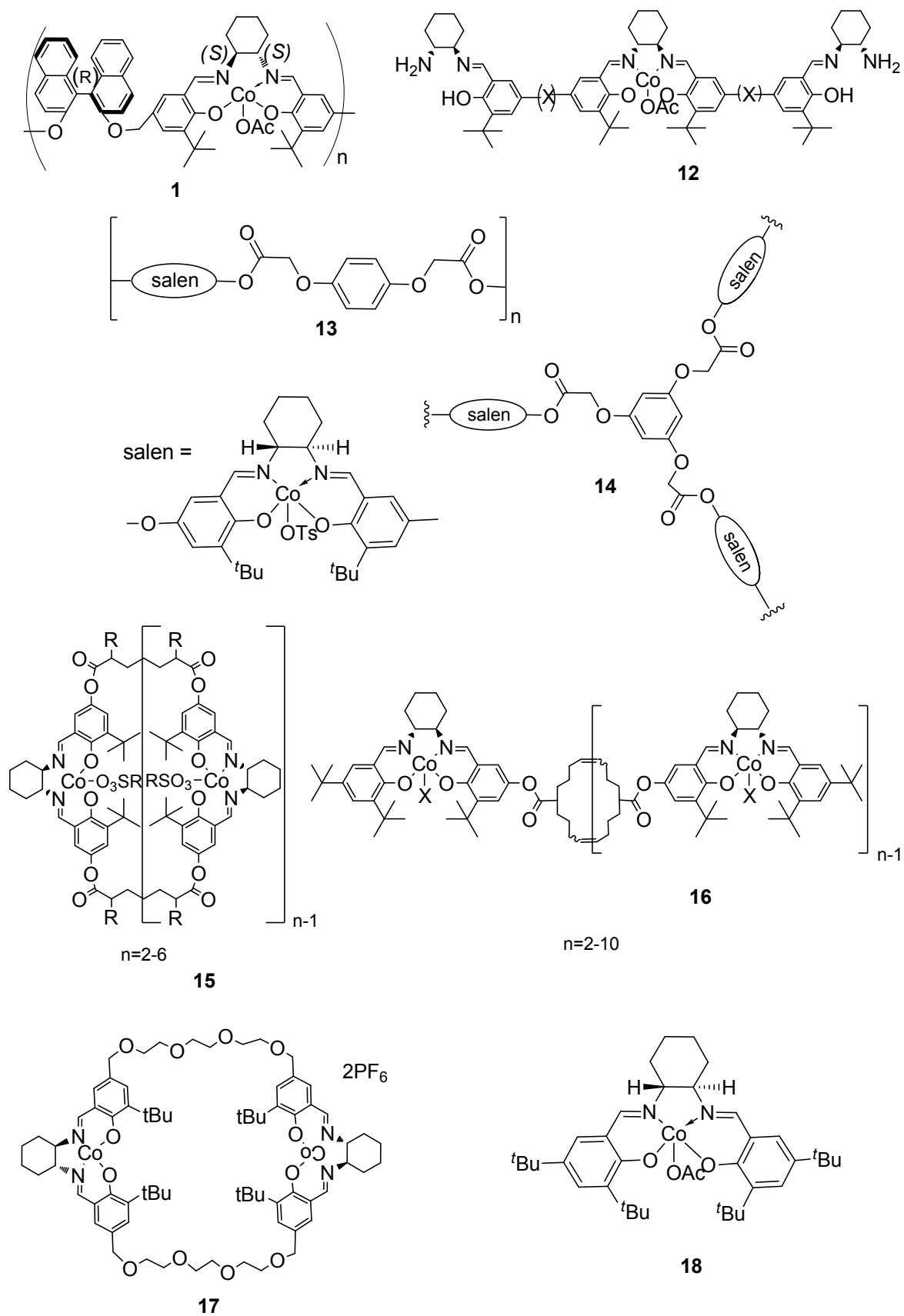
(MeOH) λ_{max} 400 nm.



7: Yield 98 %; dark brown solid; Melting Point: 220 °C; $[\alpha]_D^{27} = -245.75$ ($c = 0.025$, CHCl_3); IR (KBr, $\nu \text{ cm}^{-1}$): 3434, 2928, 2862, 1634, 1540, 1434, 1340, 1262, 1172, 1092, 872, 794, 513; Elemental analysis Found: C 65.35, H 7.80, N 8.12;

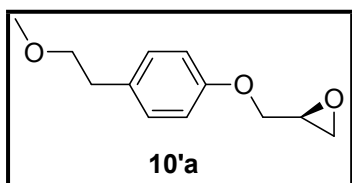
$\text{C}_{37}\text{H}_{53}\text{CoN}_4\text{O}_4$ calcd. C 65.66, H 7.89, N 8.28; UV-Vis.: (MeOH) λ_{max} 262, 400 nm.

Table 4: Comparison of catalytic activity of complex 1 with some of the literature reported catalysts.

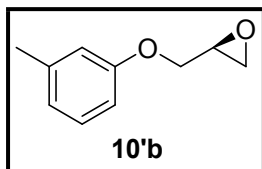


Catalyst	Substrate	Solvent	Catalyst loading (mol %)	Time (h)	Water equivalent	Ee of unreacted epoxide (%)	Ee of diol (%)
1	Epichlorohydrin	-	0.005	5	0.5	99	96
1	Styrene Oxide	-	0.05	12	0.5	99	94
1	1,2-epoxyhexane	-	0.05	6	0.5	99	96
12	Epichlorohydrin	THF	0.5	12	0.55	97	94
13	Epichlorohydrin	-	0.02	14	0.6	98	97
14	Epichlorohydrin	-	0.02	11	0.6	99	86
13	Styrene Oxide	-	0.16	14	0.6	98	89
14	Styrene Oxide	-	0.16	21	0.6	95	92
15	Styrene Oxide	-	0.04	24	0.6	99	-
16	Epichlorohydrin	-	0.01	2	0.6	99	-
16	Styrene oxide	-	0.1	3.5	0.6	99	-
17	Epichlorohydrin	-	0.008	3	0.5	99	96
17	Styrene oxide	-	0.075	16	0.5	99	92
18	Epichlorohydrin	-	0.5	16	0.55	99	-
18	Styrene Oxide	-	0.8	48	0.55	99	-
18	1,2-epoxyhexane	-	0.15	3	0.6	99	-

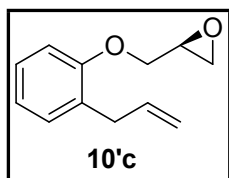
NMR Spectral data of 10'a-c:



^1H NMR (200 MHz, CDCl_3) δ in ppm: 2.72-2.91 (m, 4H), 3.34 (s, 4H), 3.52 (t, J = 7.2 Hz, 2H), 3.89 (dd, J = 5.6, 5.4 Hz, 1H), 4.15 (dd, J = 3.0, 8.0 Hz, 1H), 6.83 (d, J = 8.4 Hz, 2H), 7.11 (d, J = 8.4 Hz, 2H); ^{13}C NMR (50 MHz, CDCl_3) δ in ppm: 35.3, 44.7, 50.2, 58.6, 68.8, 73.8, 114.6, 129.8, 131.7, 157.0.

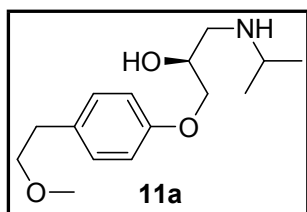


^1H NMR (200 MHz, CDCl_3) δ in ppm: 2.32 (s, 3H), 2.72-2.76 (m, 1H), 2.87 (t, J = 4.4 Hz), 3.34 (m, 1H), 3.89 (dd, J = 5.6, 5.4 Hz, 1H), 4.15 (dd, J = 3.2, 8.0 Hz, 1H), 6.7-6.8 (m, 3H), 7.12 (dd, J = 7.8, 8.2 Hz, 1H); ^{13}C NMR (50 MHz, CDCl_3) δ in ppm: 21.5, 44.5, 50.2, 68.6, 111.5, 115.5, 122.1, 129.2, 139.6, 158.5.



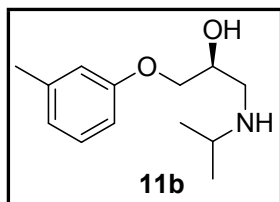
^1H NMR (200 MHz, CDCl_3) δ in ppm: 2.74 (dd, J = 2.6, 2.0 Hz, 1H), 2.86 (t, J = 4.4 Hz, 1H), 3.32-3.37 (m, 1H), 3.39 (d, J = 6.4 Hz, 2H), 3.92 (dd, J = 5.4, 5.8 Hz, 1H), 4.18 (dd, J = 3.0, 8.0 Hz, 1H), 5.01-5.10 (m, 2H), 5.89-6.09 (m, 1H), 6.80-6.94 (m, 2H), 7.13-7.20 (m, 2H); ^{13}C NMR (50 MHz, CDCl_3) δ in ppm: 34.4, 44.6, 50.3, 68.8, 111.6, 115.5, 121.2, 127.3, 129.1, 130.0, 136.9, 156.2.

NMR Spectral data of 11a-c:



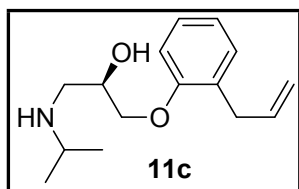
^1H NMR (500 MHz, CDCl_3) δ in ppm: 1.07 (dd, J = 2.0, 4.0 Hz, 6H), 2.65-2.69 (m, 1H), 2.79-2.85 (m, 4H), 3.33 (s, 3H), 3.53 (t, J = 7.0 Hz, 2H), 3.87-3.94 (m, 2H), 4.04-4.07 (m, 1H), 6.82 (d, J = 8.5

Hz, 2H), 7.09 (d, J = 8.5 Hz, 2H); ^{13}C NMR (125MHz, CDCl_3) δ in ppm: 22.8, 22.9, 35.3, 48.9, 49.7, 58.6, 68.4, 70.9, 73.8, 114.5, 129.8, 131.2, 157.2.



^1H NMR (500 MHz, CDCl_3) δ in ppm: 1.08 (d, J = 5.0 Hz, 6H), 2.32 (s, 3H), 2.69-2.73 (m, 1H), 2.81-2.88 (m, 2H), 3.95-4.01 (m, 3H), 6.71-6.78 (m, 3H), 7.14 (t, J = 7.0 Hz, 1H); ^{13}C NMR (125MHz,

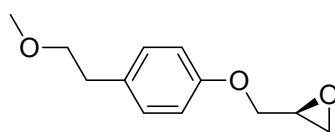
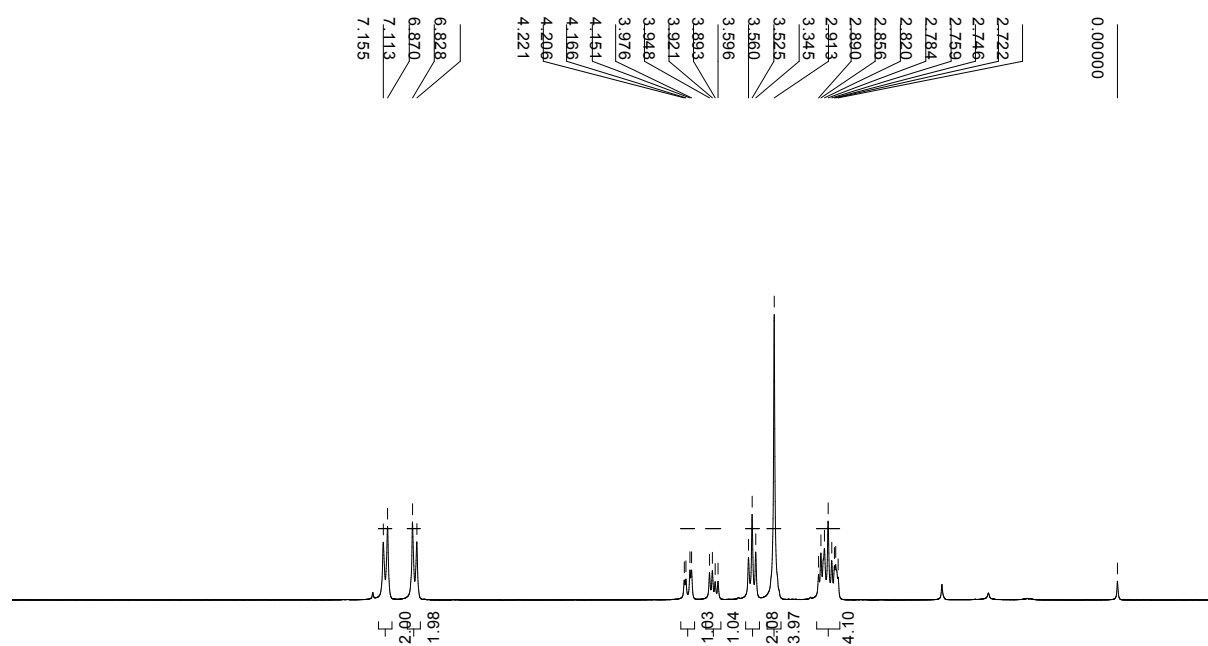
CDCl_3) δ in ppm: 21.5, 23.0, 23.1, 48.9, 49.4, 68.5, 70.4, 111.4, 115.4, 121.8, 129.2, 139.5, 158.7.



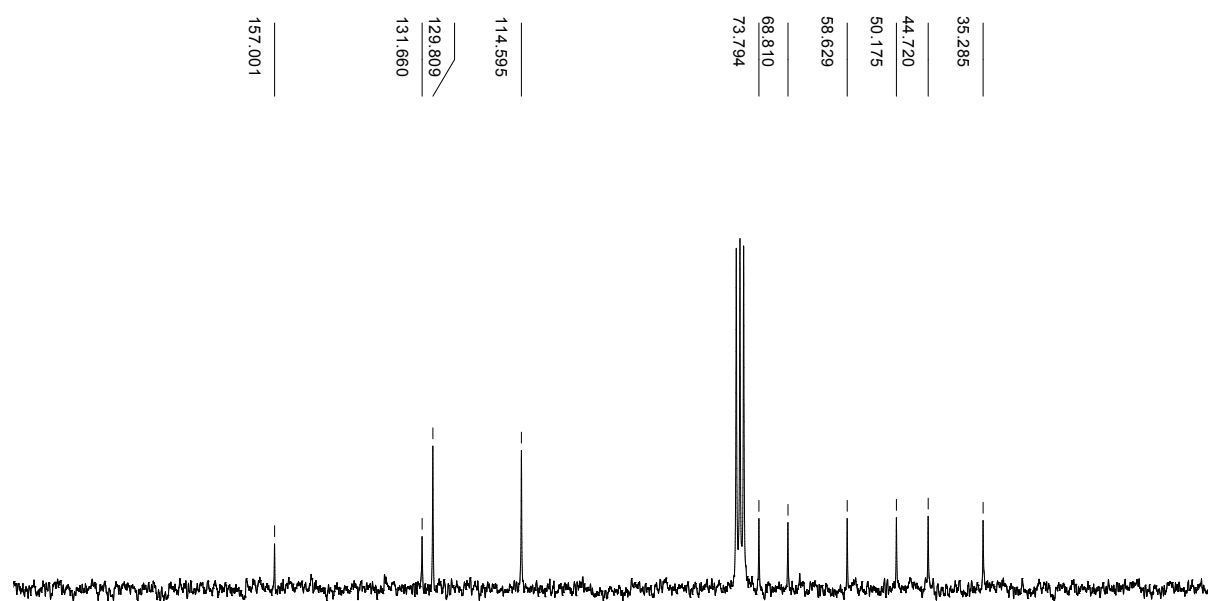
^1H NMR (500 MHz, CDCl_3) δ in ppm: 1.08 (d, J = 6.0 Hz, 6H), 2.73-2.77 (m, 1H), 2.79-2.84 (m, 1H), 2.86 (dd, J = 4.0, 8.0 Hz, 1H), 3.38 (dd, J = 1.0, 5.5 Hz, 1H), 3.95-4.00 (m, 2H), 4.02-4.06 (m, 1H),

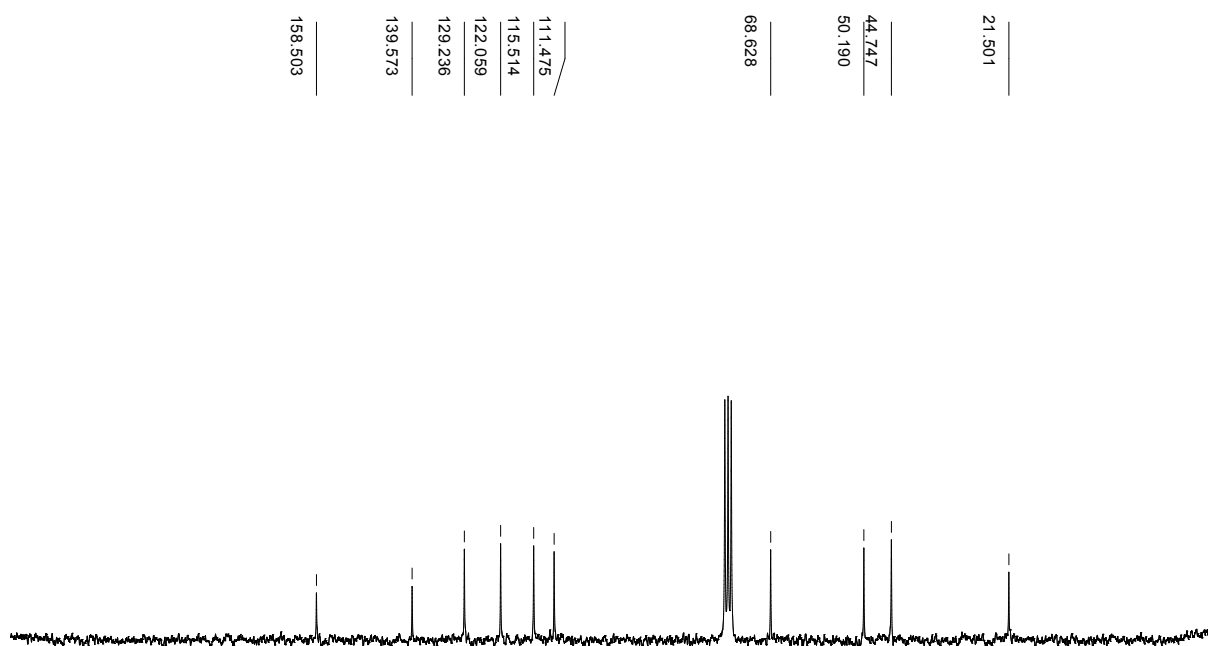
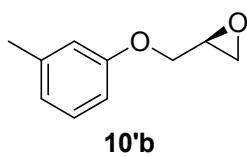
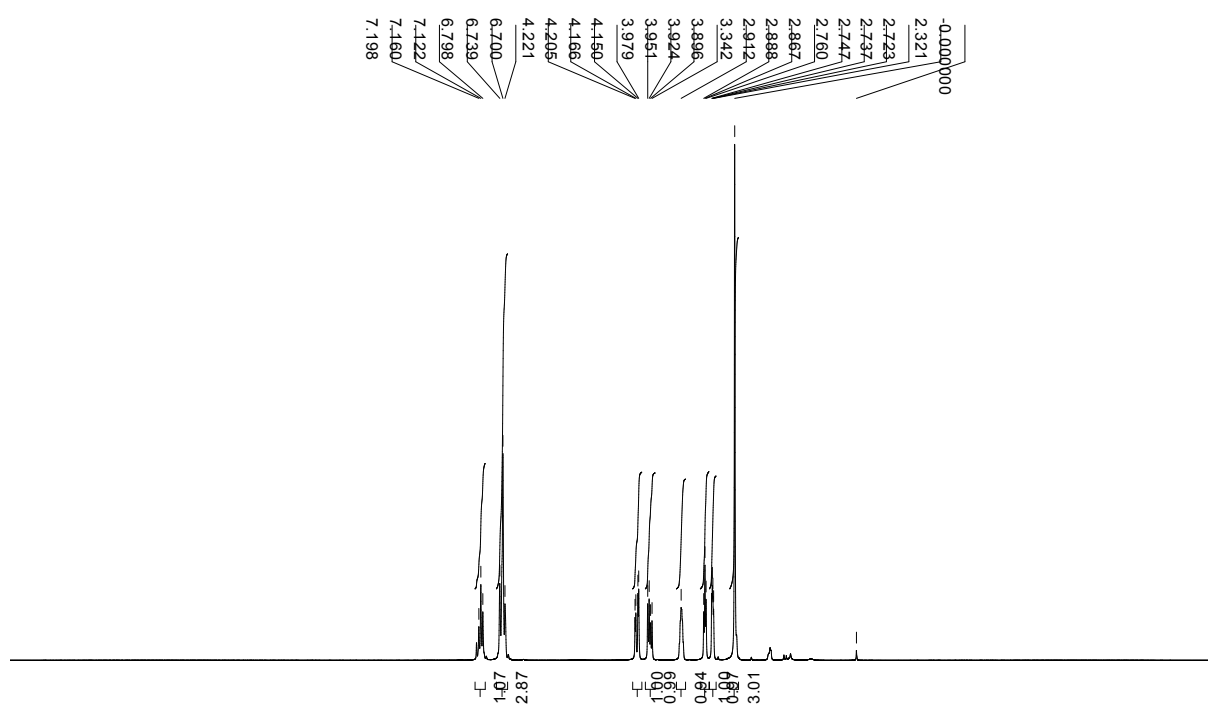
5.01-5.03 (m, 1H), 5.04 (t, J = 1.5 Hz, 1H), 5.94-6.02 (m, 1H), 6.83 (d, J = 8.0 Hz, 1H), 6.89 (dt, J = 7.5, 1.0 Hz, 1H), 7.13 (dd, J = 1.5, 5.5 Hz, 1H), 7.16 (dt, J = 8.0, 1.5 Hz, 1H); ^{13}C NMR (125MHz, CDCl_3) δ in ppm: 23.0, 23.1, 34.7, 48.9, 49.5, 68.7, 70.6, 111.3, 115.3, 120.9, 127.5, 128.5, 130.0, 137.2, 156.4.

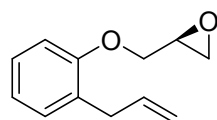
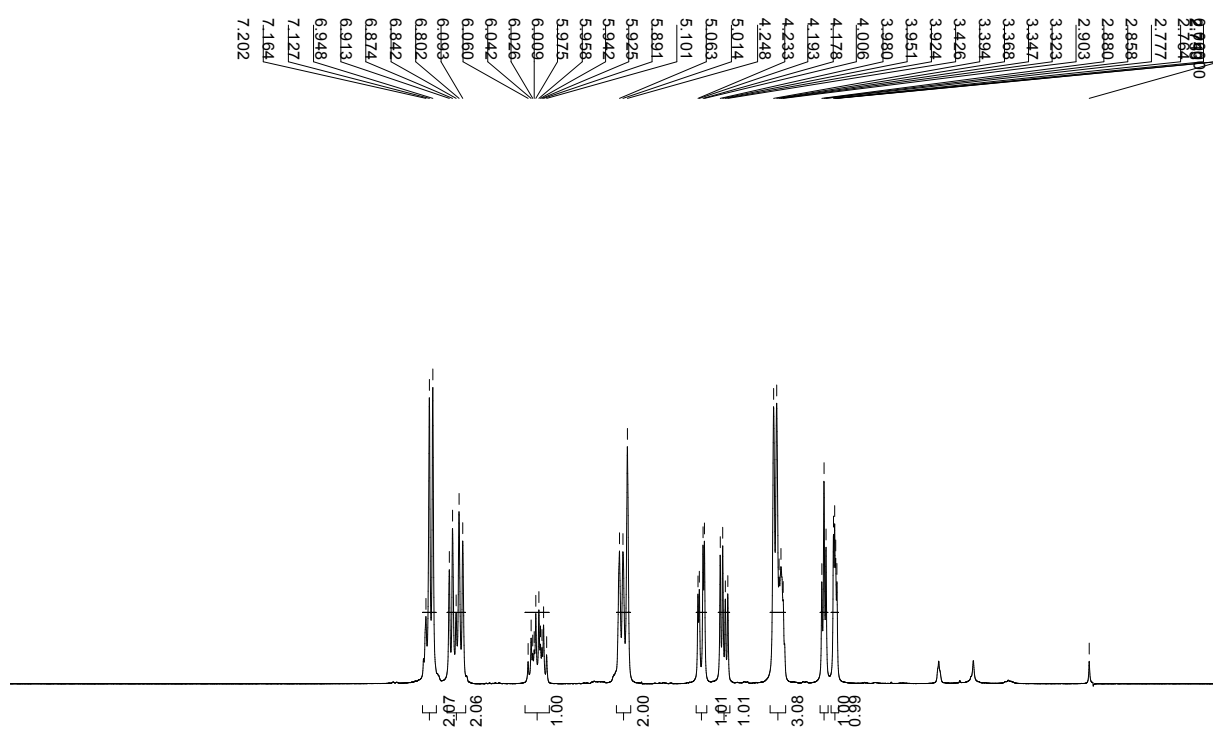
NMR spectra of β -blockers and their intermediate epoxides



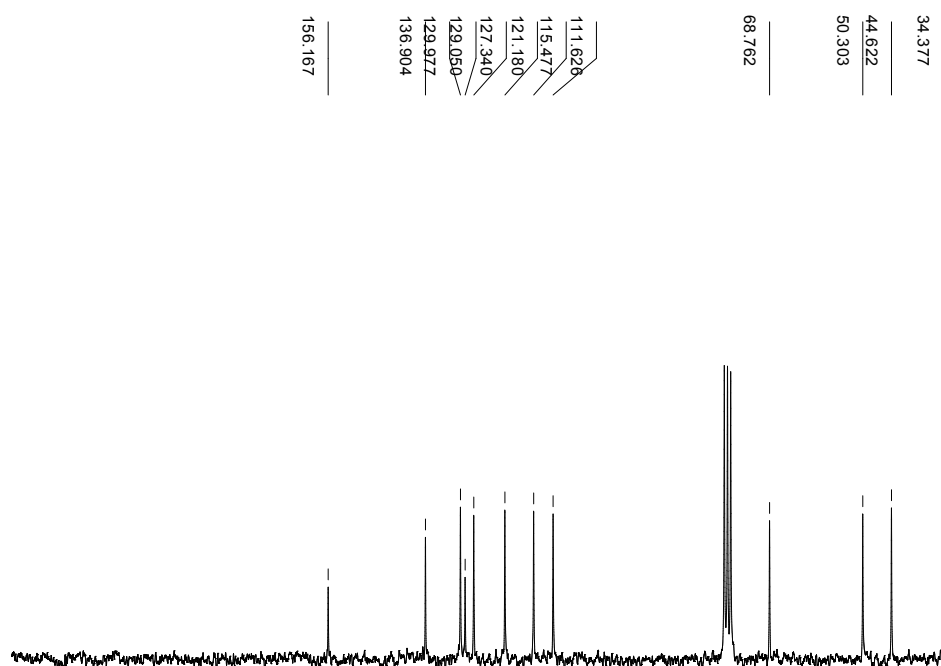
10'a

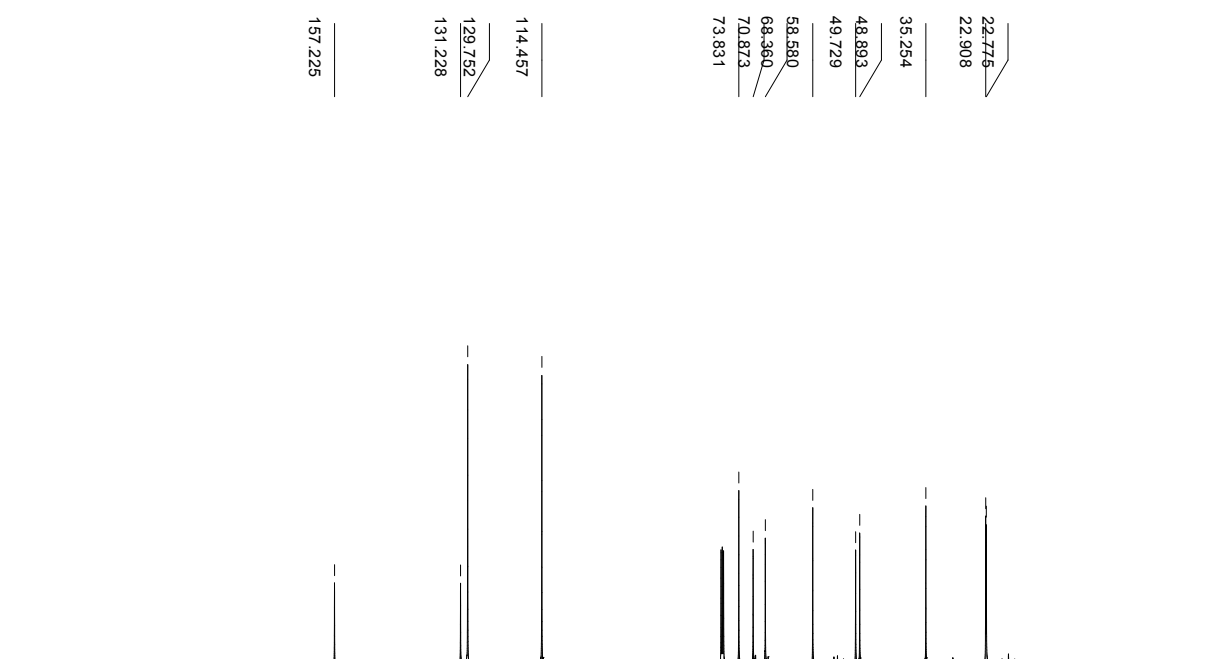
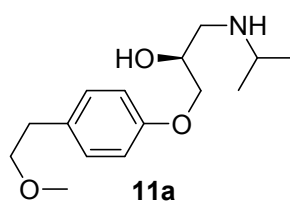
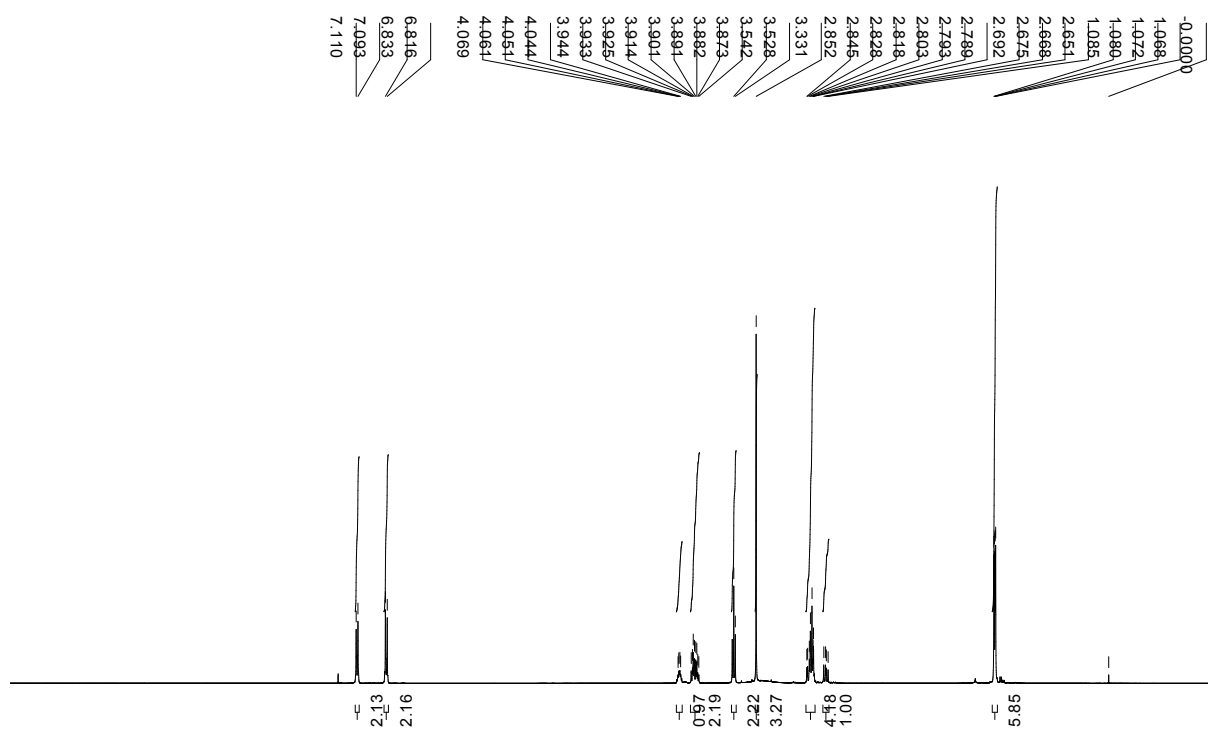


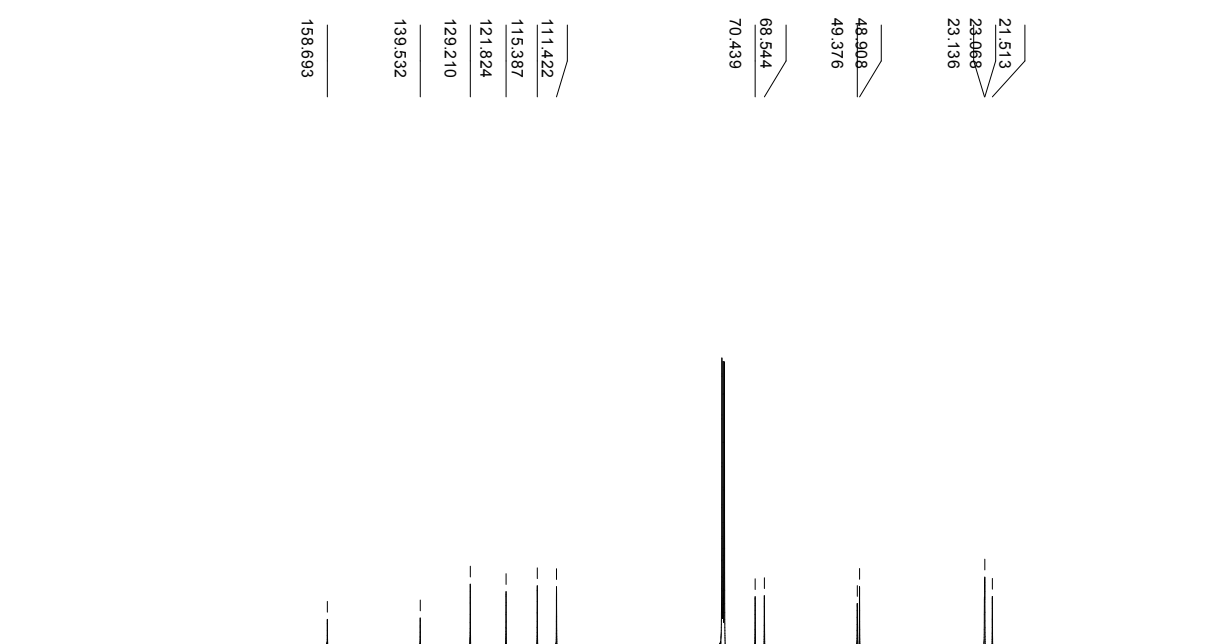
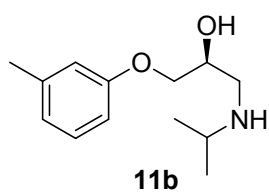
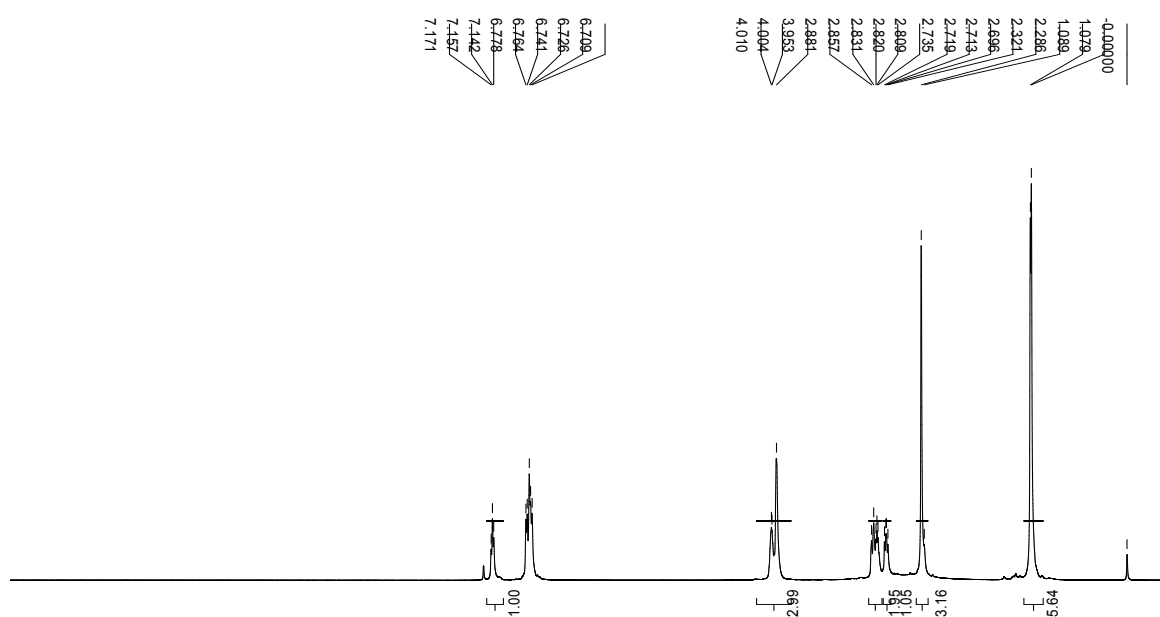


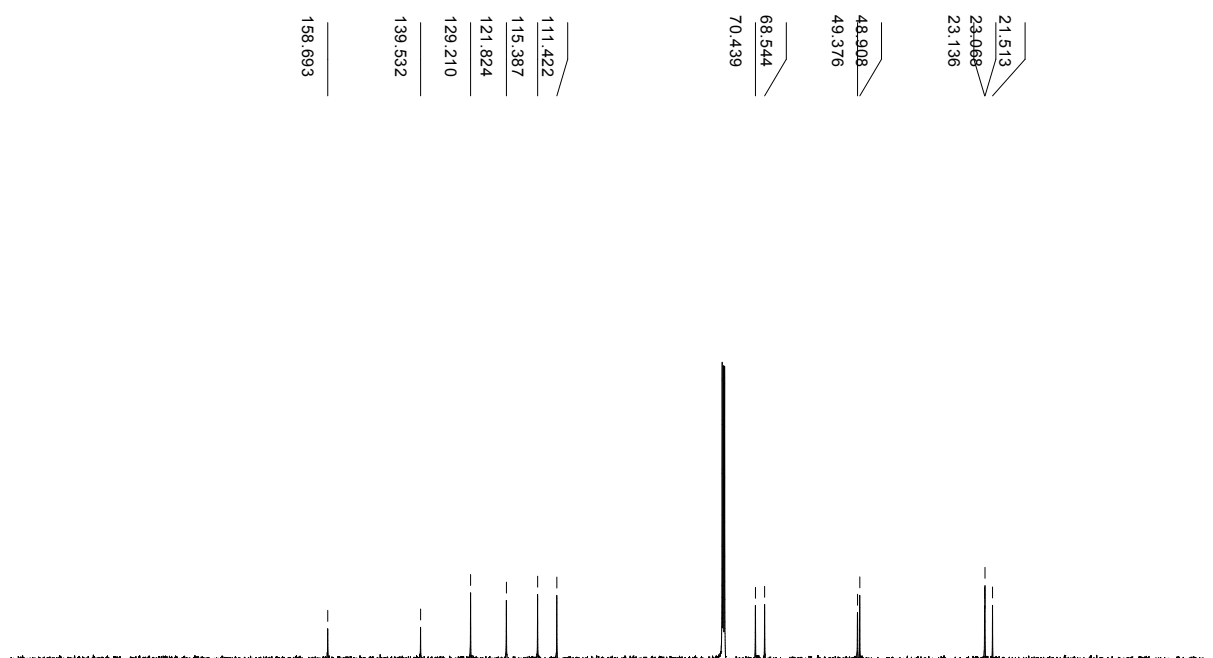


10°C









Transition State - 1 (TS-1)

ONIOM(B3LYP/6-31G*:STO3G) level of theory:

Charge: 0

Spin Multiplicity: 1

Imaginary frequency: -454.51 cm⁻¹

Electronic Energy (au): -5555.03346581

Gibbs Free Energy at 298.150 K (au): -5553.058248

Electronic Energy (au): -8072.39994429 at M06-L/6-31+G**//ONIOM (B3LYP/6-31G*:STO3G)

Co	3.01190600	2.96437100	0.15346500	O	4.55203800	3.24222500	-0.90090400
N	3.61384300	4.07585300	1.58709600	O	1.34147200	2.76088300	1.19876800
N	3.72172800	1.52392900	1.16899300	C	0.31991100	1.21215500	0.98316300
C	4.05624200	0.37288100	0.70358200	C	0.07014000	2.60891900	0.59448800
H	4.53694700	-0.34043400	1.37403500	H	0.22781400	0.95281900	2.02682400
C	3.35983100	5.33484300	1.69468800	H	0.97549500	0.63184300	0.35571800
H	3.72605500	5.85027600	2.58462400	H	0.08339100	2.79085400	-0.48323100
C	3.85973800	-0.09223600	-0.66195000	C	3.86361900	1.90327200	2.58532400
C	3.01559600	0.65159200	-1.58758200	C	4.41725400	3.33786700	2.58366700
C	4.48325400	-1.29743500	-1.04623700	H	2.84091700	1.93439200	2.98435400
C	2.85827900	0.09590800	-2.92410500	H	5.43457700	3.29029000	2.18051700
H	5.11950500	-1.82337700	-0.31496800	C	4.43367600	3.91940400	4.03177700
C	3.52910400	-1.08081300	-3.26457000	H	4.86773200	4.93284800	4.03119600
H	3.43854000	-1.47686800	-4.28300900	H	3.40103700	3.98914400	4.41574500
C	2.65401600	6.18251500	0.76161500	C	4.73505900	0.96865800	3.47701300
C	2.16389500	5.67276800	-0.50712100	C	1.86411200	8.43677800	0.25517900
C	2.48626800	7.54642600	1.11483000	C	4.34319000	-1.80019800	-2.34100700
C	1.56922700	6.64384800	-1.42431600	C	-6.60221400	0.39424900	-0.41037800
H	2.86571900	7.88421100	2.08928800	C	2.85052700	-2.34135900	4.36680200
C	1.42734700	7.96982300	-1.01911000	H	4.30582100	-0.04739800	3.49483800
H	0.97493900	8.69675600	-1.70320500	H	5.75374500	0.91094200	3.05694000
O	2.39349700	1.73637500	-1.24956500	C	5.29196300	3.00256500	4.95812500
O	2.23387200	4.42777500	-0.84662900	C	4.78632100	1.52919700	4.93223600

H	5.45088800	0.89608800	5.54479500	C	-1.78468700	-3.13840000	-2.83259500
H	3.77652400	1.47922300	5.37564100	H	-2.79586200	-3.55523900	-2.97575100
H	5.26011800	3.39120200	5.99059000	H	-1.73970100	-2.15662000	-3.33453900
H	6.34247400	3.03405100	4.62097200	C	0.71847100	-3.58931800	-3.20293600
N	0.01224100	-2.22574800	0.39986600	C	-0.72965200	-4.10210700	-3.45744200
N	-2.39176700	-2.06635400	-0.56355600	H	-0.91196600	-4.18626300	-4.54229300
C	-3.48919300	-1.59082300	-1.04222700	H	-0.85089400	-5.10794900	-3.01894600
H	-3.75101300	-1.83342900	-2.07256300	H	1.44667600	-4.31469500	-3.60368300
C	1.10983400	-2.38093900	1.06190500	H	0.87156400	-2.63510400	-3.73579900
H	1.99561500	-2.70070000	0.51327100	H	-1.95978400	0.63443100	0.90487000
C	-4.46722500	-0.79257500	-0.32803100	Co	-1.63901600	-1.59656500	1.12366000
C	-4.38753200	-0.62880100	1.10617600	O	-2.19564500	-3.42329500	1.91892800
C	-5.56534600	-0.28079200	-1.05376700	H	-3.09290700	-3.09573200	2.13899500
C	-5.49058000	0.01976800	1.77637400	H	-1.71471200	-3.37166600	2.76645200
H	-5.59425300	-0.42818800	-2.14267100	H	1.72974600	9.48922800	0.52960300
C	-6.54937800	0.51781600	1.01008600	H	3.82288800	-2.62398400	4.78713100
H	-7.38290700	1.02663200	1.50872300	C	-1.05495500	3.35073200	1.30558900
C	1.31426400	-2.16818400	2.47949100	H	-2.01267400	2.96581500	0.91767400
C	0.28351300	-1.60073000	3.32372000	H	-1.01724400	3.09818500	2.37497200
C	2.57662200	-2.52142000	3.01833300	C	-1.01384800	4.87275400	1.13168100
C	0.58931600	-1.40503800	4.72691000	H	-0.04712700	5.24840800	1.48502000
H	3.33536900	-2.94558900	2.34583700	H	-1.06330600	5.11862800	0.06134900
C	1.84760800	-1.78037300	5.20654600	C	-2.14854000	5.59118600	1.87323700
H	2.08378100	-1.64062900	6.26779800	H	-3.11788800	5.20133100	1.52820100
O	-3.36771900	-1.07023300	1.81057500	H	-2.08954400	5.35154700	2.94499000
O	-0.90096600	-1.26657500	2.87554100	C	-2.11442600	7.11186700	1.68736100
O	-1.25811500	0.10695100	0.48664600	H	-2.92220400	7.60304600	2.24264600
C	-1.49282000	-2.96239200	-1.31303700	H	-1.16248800	7.53023100	2.03612500
C	-0.07250100	-2.42474700	-1.06375700	H	-2.22224700	7.38273000	0.62987700
H	-1.56771500	-3.94410700	-0.82427100	C	5.03827300	-3.11436500	-2.76844200
H	0.00659100	-1.43117200	-1.52515700	H	5.18140300	-3.14064500	-3.87068700
C	1.00051500	-3.37177500	-1.68409500	H	4.41959600	-3.99831500	-2.49484000
H	2.00377000	-2.92672500	-1.57203400	C	10.59172600	-6.60230800	-1.53800000
H	0.98314900	-4.33924200	-1.15284900	C	9.95333200	-5.37166400	-1.55415000

C	9.14982200	-4.93490000	-0.43772300	C	-12.01443400	-1.40511900	0.94412300
C	9.01595200	-5.82427500	0.69724500	C	-11.24074500	-2.37088100	0.20238100
C	9.69604900	-7.09241600	0.67921800	C	-10.94294600	-3.63959000	0.83300300
C	10.46676900	-7.47384700	-0.40853900	C	-11.42919000	-3.89254700	2.16332300
H	11.19942600	-6.91762500	-2.39693700	C	-12.17259400	-2.94041300	2.84477100
H	10.04874500	-4.70621700	-2.42176400	H	-13.05416000	-0.93609800	2.77544000
C	8.47045400	-3.65699900	-0.42877900	H	-12.24011500	-0.44084100	0.47064100
C	8.19621000	-5.41921600	1.81238400	C	-10.75733400	-2.10774800	-1.13580100
H	9.58970500	-7.75598700	1.54833700	C	-10.16504400	-4.61582600	0.10963400
H	10.98133900	-8.44365600	-0.41284900	H	-11.19869600	-4.85994600	2.63029400
C	7.54293100	-4.20217200	1.81214400	H	-12.53962100	-3.14323700	3.85942000
C	7.67921700	-3.30913100	0.68691400	C	-9.70275700	-4.35720400	-1.16554600
H	8.09891800	-6.09973200	2.66935300	C	-9.99745700	-3.09304900	-1.79835800
H	6.92028600	-3.88498900	2.65870700	H	-9.94531500	-5.57742700	0.59351600
C	12.04357600	-1.25145500	-1.39104500	H	-9.11231400	-5.09524300	-1.72397300
C	10.92271700	-2.00949400	-1.09096100	C	-14.54719200	-1.28361300	-3.19761000
C	9.72299600	-1.90893200	-1.88764700	C	-13.34872600	-1.53875000	-2.55049600
C	9.71697000	-0.98453800	-3.00069200	C	-12.29660200	-0.55006600	-2.51912600
C	10.90020200	-0.21401700	-3.28300200	C	-12.52552900	0.71354300	-3.18590000
C	12.03687100	-0.34445300	-2.50060200	C	-13.78358100	0.94337900	-3.84856900
H	12.94837700	-1.34046600	-0.77452200	C	-14.77082900	-0.02907800	-3.85474800
H	10.92904800	-2.70156600	-0.23903700	H	-15.33793400	-2.04610200	-3.21127400
C	8.53597100	-2.68335900	-1.59590600	H	-13.17809900	-2.49939300	-2.04719300
C	8.51796800	-0.85111800	-3.78586600	C	-11.03565100	-0.79249100	-1.85268400
H	10.88118900	0.48379200	-4.13137700	C	-11.48295200	1.70415000	-3.16651500
H	12.93489000	0.24746700	-2.72131300	H	-13.94389700	1.90767100	-4.35007000
C	7.38139900	-1.58873400	-3.50476800	H	-15.72764100	0.15294500	-4.36176300
C	7.38209700	-2.52510800	-2.40470600	C	-10.27592800	1.47314500	-2.52929800
H	8.51265200	-0.13755800	-4.62164900	C	-10.03854900	0.21470300	-1.85982300
H	6.47827000	-1.45306000	-4.10904300	H	-11.65773700	2.66384200	-3.67281600
O	6.98742600	-2.08313700	0.77129000	H	-9.50435800	2.24996600	-2.53214300
O	6.30729100	-3.37773500	-2.04664000	O	-9.49448400	-2.91310900	-3.10108200
H	7.31954300	-1.59044300	-0.06750000	O	-8.84804100	-0.13724500	-1.17396400
C	-12.46574800	-1.68303600	2.22548900	H	-9.83646300	-1.97076800	-3.33254700

C	-7.80971600	0.93419200	-1.19369800	C	-0.48345400	-0.76281400	5.66984100
H	-8.20248600	1.85847500	-0.71590700	C	-0.00824000	-0.68295900	7.16049700
H	-7.51855800	1.17120600	-2.24040100	H	0.21061900	-1.68279800	7.56424200
C	5.81541000	3.03238100	-0.65398500	H	0.88927600	-0.05504300	7.26120700
O	6.32897500	2.63797600	0.39427100	H	-0.80790300	-0.23475500	7.76953400
C	1.18153100	6.19606600	-2.87279300	C	-1.80149200	-1.61488500	5.62076400
C	0.46311100	7.32442600	-3.68967000	H	-2.16309700	-1.65086700	4.58323000
H	1.11724100	8.19728400	-3.83176100	H	-1.61438000	-2.63841600	5.98055900
H	0.19521700	6.93498800	-4.68387500	H	-2.57624600	-1.15734900	6.25361600
H	-0.46055700	7.65240300	-3.18946600	C	-0.78306800	0.69470600	5.16685800
C	0.23180500	4.94954900	-2.81409300	H	-1.12408600	0.66074200	4.12232200
H	0.72673000	4.17441500	-2.21069800	H	-1.56739900	1.15949600	5.78298500
H	-0.72883000	5.21846500	-2.34886000	H	0.12398700	1.31500900	5.22726700
H	0.03725700	4.56581300	-3.82664200	C	1.99242300	0.87171500	-3.97066300
C	2.50921400	5.81257500	-3.62194700	C	2.67081100	2.26213900	-4.23229800
H	3.16604500	6.69186700	-3.70467400	H	2.05786300	2.86588400	-4.91813000
H	3.03937400	5.02712600	-3.06391500	H	2.77984100	2.79895100	-3.27902900
H	2.28807800	5.44363200	-4.63499700	H	3.66708200	2.12412500	-4.67856200
C	-5.47796800	0.15514500	3.33619600	C	1.85782000	0.11930800	-5.33845700
C	-6.76409500	0.85464700	3.89251900	H	1.21635900	0.70733200	-6.01264900
H	-6.85808200	1.88105000	3.50793800	H	2.83650100	-0.00593000	-5.82490200
H	-7.67140400	0.29084000	3.62894300	H	1.39913300	-0.87291000	-5.20955200
H	-6.69898600	0.90635700	4.98991000	C	0.55529100	1.10123400	-3.38211700
C	-5.38549300	-1.27910100	3.97054500	H	0.03120100	0.14232300	-3.24815300
H	-6.26504800	-1.88115300	3.69565900	H	0.66282500	1.59744800	-2.40591200
H	-4.47777300	-1.77939900	3.60403000	H	-0.04129100	1.73573200	-4.05440300
H	-5.33523300	-1.20908300	5.06753700	C	6.67764100	3.34802500	-1.87709500
C	-4.22581900	0.99826600	3.76498700	H	7.72675700	3.13971100	-1.65594200
H	-3.31463600	0.50955800	3.39196100	H	6.34845300	2.74914000	-2.73268400
H	-4.28574000	2.01560400	3.34968600	H	6.55842800	4.40142400	-2.15316200
H	-4.17110400	1.06980400	4.86143600				

Transition State - 2 (TS-2)

ONIOM(B3LYP/6-31G*:STO3G) level of theory:

Charge: 0

Spin Multiplicity: 1

Imaginary frequency: -468.57 cm⁻¹

Electronic Energy (au): -5555.02979529

Gibbs Free Energy at 298.150 K (au): -5553.053132

Electronic Energy (au): -8072.38746294 at M06-L/6-31+G**//ONIOM (B3LYP/6-31G*:STO3G)

Co	-2.64188900	2.64749400	2.20868600	O	-2.38290300	4.02952100	0.87174900
N	-2.79206500	1.30713900	3.55833000	O	-3.38235800	1.51505400	0.81055500
N	-1.87753700	3.73086800	3.57058400	O	-4.40473400	3.28322600	2.41708000
C	-1.81080200	5.01695000	3.53633800	O	-0.83553200	1.88217900	1.90383000
H	-1.44535700	5.53649700	4.42295000	C	0.16455000	2.51761900	1.13445000
C	-3.10348600	0.07454500	3.34182200	H	-0.17926800	3.45722200	0.69421100
H	-3.07908100	-0.61252900	4.18920700	C	-1.41673200	2.91771600	4.70762500
C	-2.16014000	5.87012900	2.42059100	C	-2.47857000	1.82311800	4.90732500
C	-2.41133400	5.30812400	1.10641100	H	-0.48803900	2.43401900	4.37652400
C	-2.15976500	7.27065100	2.62753100	H	-3.38923400	2.32438800	5.25354700
C	-2.65216300	6.24374600	0.01873000	C	-1.99962800	0.78057600	5.96491100
C	-2.40976900	8.14646300	1.58026200	H	-2.77978400	0.01947400	6.13132300
H	-1.95761500	7.65220000	3.63803100	H	-1.09260600	0.26788000	5.59998000
C	-2.65322000	7.61509400	0.28265400	C	-1.14934900	3.67296800	6.04489000
H	-2.85195200	8.32015900	-0.53265700	H	-0.37112400	4.44088400	5.90027800
C	-3.53859400	-0.52440900	2.09636200	H	-2.07717100	4.17509600	6.36843900
C	-3.72822900	0.27766900	0.89805500	C	-1.70244200	1.50231500	7.31668500
C	-3.87108100	-1.90027000	2.10904500	C	-0.67732400	2.66151100	7.13499300
C	-4.35996500	-0.37953000	-0.24646600	H	-0.54124700	3.19205600	8.09297200
C	-4.39766100	-2.52974600	0.98570800	H	0.30223000	2.24396600	6.84330300
H	-3.71168500	-2.46862100	3.03672200	H	-1.31442700	0.77063800	8.04615900
C	-4.64879000	-1.73885600	-0.18001900	H	-3.93770200	7.48716600	-2.26381900
H	-5.12545500	-2.23678100	-1.03266100	H	-2.17407900	7.42302700	-2.55368700

C	-4.77913200	0.48055400	-1.48526600	H	4.21934000	4.34681500	-5.24416000
C	-5.87497900	1.50324700	-1.00940700	H	3.44030100	2.81955000	-4.73524400
C	-3.53879100	1.27490200	-2.02383400	H	2.80754900	6.27838200	-6.05453200
C	-5.37235000	-0.38136700	-2.65277700	H	2.10588700	5.25629300	-7.33402300
H	-6.77050600	0.96807800	-0.65910100	H	1.03750900	6.15268900	-6.21201000
H	-5.48168200	2.11687100	-0.18488400	C	-4.75991300	-4.02849500	0.97679900
H	-6.16543400	2.16530300	-1.83912800	H	-2.64553700	1.90950200	7.72037100
H	-2.76734400	0.58458700	-2.39515800	C	-0.10170800	1.34802500	0.27792400
H	-3.83604400	1.94264300	-2.84564200	H	0.26738700	0.38774700	0.60308800
H	-3.12823900	1.86952900	-1.19454600	H	-0.98751400	1.37758400	-0.34038600
H	-5.64829500	0.28593700	-3.48344300	N	0.11536300	-0.27752800	-3.12678100
H	-4.62742300	-1.09965400	-3.02838900	N	2.03673500	-1.15247700	-1.62629600
H	-6.27371300	-0.93926600	-2.33958400	C	2.95410300	-1.33948700	-0.73575800
C	6.02659300	2.57007900	-1.96774400	H	2.92059700	-2.26005600	-0.15212000
C	6.21428500	2.03641600	-3.43327100	C	-0.61439800	0.14185200	-4.10533100
C	4.88696800	3.64878200	-1.93809900	H	-1.54110100	-0.39144200	-4.31918900
C	7.36488200	3.25114500	-1.52165300	C	4.07597700	-0.47265100	-0.44883600
H	7.02556900	1.29341800	-3.47257300	C	4.40171200	0.64171600	-1.31609300
H	5.27998000	1.56619900	-3.77110500	C	4.92014100	-0.82117500	0.62972500
H	6.46192600	2.86492100	-4.11372300	C	5.61769800	1.37548000	-1.04216800
H	4.77140600	4.05581300	-0.92227300	C	6.08084700	-0.09806500	0.90045900
H	5.12634200	4.47627600	-2.62243400	H	4.65225400	-1.68770600	1.25075200
H	3.93924300	3.18737300	-2.24927200	C	6.40965900	0.99612000	0.04530900
H	7.59313500	4.07911700	-2.20983100	H	7.32991100	1.55170000	0.26111600
H	7.28231500	3.66500100	-0.50569200	C	-0.35289200	1.27459200	-4.96738900
H	8.20482000	2.54105000	-1.55010800	C	0.74072700	2.18891300	-4.70850500
C	2.01203600	4.38582400	-5.29553900	C	-1.25937400	1.51376100	-6.03079600
C	1.87698300	4.94980800	-3.83622500	C	0.85944600	3.35845600	-5.55459900
C	3.39167100	3.65234600	-5.45093700	C	-1.11735500	2.62445800	-6.84950400
C	1.98076900	5.59254500	-6.29392100	H	-2.08274000	0.80360300	-6.18982000
H	0.92637300	5.49208000	-3.72139300	C	-0.05799500	3.53995600	-6.59405500
H	1.90233900	4.11740200	-3.11881600	H	0.03122700	4.41838800	-7.24363500
H	2.70523000	5.63955800	-3.61501600	O	3.66496000	0.96670600	-2.34850100
H	3.50925500	3.26244400	-6.47379500	O	1.61865400	1.99659600	-3.75585300

O	1.19895800	1.38351900	-1.20004100	C	1.50953400	2.69197200	1.83248000
C	1.02585300	-2.17229300	-1.97065400	C	2.03347300	1.46049900	2.58012800
C	-0.27504100	-1.40032800	-2.25151900	H	2.24143400	3.01700400	1.07972900
H	1.35661400	-2.62251600	-2.91766200	C	3.26461200	1.76528200	3.44349500
H	-0.62435700	-0.95885300	-1.30929600	H	1.23164500	1.05862900	3.21255300
C	-1.38237600	-2.35540000	-2.79392500	H	2.29239800	0.67318100	1.85893700
H	-2.32207300	-1.79719000	-2.93960900	H	4.07608300	2.13859400	2.80229400
H	-1.06846000	-2.76922500	-3.76792100	C	12.38012400	-1.35949300	-1.30756100
C	0.79357600	-3.31004500	-0.93029500	C	11.57220100	-1.86245600	-0.29904100
H	1.72624700	-3.87801700	-0.77628600	C	10.55044100	-2.84068500	-0.58291400
H	0.49332100	-2.86940800	0.03594500	C	10.38637600	-3.28178700	-1.95203900
C	-1.63288000	-3.50980900	-1.77543200	C	11.24416000	-2.73836100	-2.97141000
C	-0.31824600	-4.27660400	-1.44436700	C	12.21785900	-1.80109900	-2.66000800
H	-0.51524100	-5.04269700	-0.67530100	H	13.15344300	-0.61543000	-1.07316300
H	0.04435300	-4.79691300	-2.34800700	H	11.69784600	-1.52282800	0.73719500
H	-2.37477000	-4.20819600	-2.19848800	C	9.69342400	-3.38250600	0.44944900
H	-2.06348500	-3.08647400	-0.85115400	C	9.36529400	-4.25423000	-2.25708800
H	1.08594200	2.26659300	-1.59280000	H	11.11149500	-3.08277600	-4.00621600
Co	1.83141400	0.42945400	-2.66639700	H	12.86779400	-1.39268500	-3.44496000
O	2.74898200	-0.47488200	-4.28837600	C	8.54738600	-4.76423300	-1.26832200
H	3.61719700	-0.11670600	-3.99845300	C	8.70753900	-4.32712200	0.09858900
H	2.48483400	0.08603600	-5.03970500	H	9.24854500	-4.58632700	-3.29784500
C	-2.95519800	5.68977700	-1.41234200	H	7.76972900	-5.50632400	-1.49123800
C	-1.79658000	4.72625800	-1.85022100	C	12.72633500	-5.04107200	3.15966900
C	-4.30494600	4.89000200	-1.35315500	C	11.76626200	-4.51561700	2.30977000
C	-3.09236000	6.82014200	-2.48864500	C	10.82823000	-3.52043500	2.77373900
H	-0.84876800	5.27854200	-1.93962600	C	10.91443500	-3.08995200	4.15251100
H	-1.69427600	3.94891800	-1.07870100	C	11.92533100	-3.65816400	5.00681300
H	-2.02703900	4.25967900	-2.81969700	C	12.81022400	-4.60918900	4.52426000
H	-5.13370100	5.55978900	-1.07839000	H	13.43312900	-5.79674900	2.79056100
H	-4.52804700	4.43801200	-2.33146700	H	11.70272700	-4.84662100	1.26495400
H	-4.22809100	4.09389000	-0.59870900	C	9.81489000	-2.95835800	1.90765300
H	-3.27306600	6.36181600	-3.47311600	C	9.98130900	-2.10436600	4.62844900
C	7.02491200	-0.50333700	2.04358100	H	11.97971800	-3.32116700	6.05109700

H	13.57852100	-5.03808800	5.18110400	C	-12.04554200	-2.82953300	2.47977400
C	9.01082300	-1.56640600	3.80082800	H	-13.06926400	-3.30162400	0.60052200
C	8.91744300	-1.98915400	2.42202600	H	-10.98320800	-3.94272100	-0.60796000
H	10.04793400	-1.77741300	5.67560700	C	-8.43153200	-3.92807100	0.41229100
H	8.31763600	-0.81610000	4.19486000	C	-8.32849300	-3.06508500	3.13113800
O	7.83793600	-4.90185100	1.04528100	H	-10.77587400	-2.43573800	4.18677900
O	7.97183700	-1.51033200	1.48014400	H	-12.97358200	-2.55032800	2.99584800
H	8.14864700	-4.45426700	1.91799000	C	-7.15883400	-3.41602200	2.48092800
H	6.45121800	-0.94619300	2.88703900	C	-7.19784200	-3.86188500	1.10606400
H	7.58292900	0.38187600	2.41933700	H	-8.29131200	-2.72409400	4.17521300
C	-9.38939100	-8.03850000	-0.89420600	H	-6.20134500	-3.34627100	3.00664800
C	-9.08749800	-6.74839300	-0.48551800	O	-7.79688500	-2.08273300	-1.72358300
C	-8.75535000	-5.72326000	-1.44486100	O	-6.08329100	-4.30535000	0.35229100
C	-8.74127100	-6.07678200	-2.84875100	H	-7.86815800	-2.07517800	-0.69810800
C	-9.06097500	-7.42564300	-3.23481300	H	-4.69225300	-4.45872200	1.99897200
C	-9.37789900	-8.38412000	-2.28392200	H	-4.06687900	-4.60201300	0.32283300
H	-9.64036500	-8.80672000	-0.15032800	H	-1.81486300	2.80916800	-7.67500800
H	-9.09611700	-6.48373300	0.57986200	H	-2.42001600	9.23059300	1.74059400
C	-8.43664600	-4.36983800	-1.04556800	H	1.39554800	3.52611000	2.53922900
C	-8.40604400	-5.06639400	-3.82217400	H	3.02663800	2.58234500	4.13958200
H	-9.04879700	-7.68171900	-4.30313300	C	3.75703500	0.55047900	4.23684600
H	-9.62070800	-9.41049800	-2.58879500	H	4.03557700	-0.27161400	3.56532000
C	-8.09901400	-3.77647300	-3.43528900	H	4.63423500	0.79607800	4.84680600
C	-8.11151700	-3.42126700	-2.03635100	H	2.97748200	0.17462600	4.91110500
H	-8.39968200	-5.34117000	-4.88587500	C	-5.02802400	3.78448800	3.44775100
H	-7.84542300	-3.00079800	-4.16960200	O	-4.63023600	3.86479100	4.61114800
C	-12.09872400	-3.25839400	1.11327300	C	-6.40590000	4.31745300	3.05444300
C	-10.94152500	-3.61510200	0.43900000	H	-6.96511900	3.55679700	2.50046100
C	-9.65585400	-3.56693000	1.09390800	H	-6.95793200	4.61576100	3.94843900
C	-9.60629200	-3.13029500	2.47206400	H	-6.28588500	5.18168600	2.39142400
C	-10.82859700	-2.76652400	3.14043200				

R-BINOL with (S,S)-Co(III) salen complex

B3LYP/ 6-31G* level of theory:

Charge: 0

Spin Multiplicity: 1

Electronic Energy (au): -2681.36454876

Co	2.93023000	0.60860500	-0.43442700	C	3.09910300	4.84291600	-0.34639600
O	4.58134300	-0.25121100	-0.17880100	C	1.87924500	5.78130500	-0.31597700
N	3.67873500	2.34238100	-0.19885300	C	0.81929100	5.38216100	-1.35185500
C	5.97873100	1.65532000	0.21988200	C	0.38363300	3.91440900	-1.19275300
C	7.26903600	2.16792400	0.49669600	H	3.79032900	5.12987900	0.45357500
C	8.32654900	1.31428900	0.69494800	H	2.17180700	3.29282200	0.82007100
C	8.09999600	-0.07648700	0.64086100	H	2.09841400	3.11911400	-2.21774700
C	6.86053600	-0.64816300	0.38393500	H	1.43478100	5.75500000	0.68858200
C	5.74940600	0.24162600	0.13628800	H	2.20511600	6.81415500	-0.48668100
H	7.40384100	3.24600500	0.55342100	H	-0.05727200	6.03523800	-1.26890100
H	8.94865700	-0.72629400	0.82094900	H	1.22430000	5.52975000	-2.36333400
C	4.92317400	2.59998700	0.06137500	H	-0.14291800	3.77648400	-0.23837800
N	1.38475600	1.54967700	-1.06676300	H	-0.32237400	3.65770300	-1.99073600
O	2.26572600	-1.02912600	-1.12213900	H	3.63686400	4.95127400	-1.29957400
C	1.01612200	-1.37761700	-1.24203100	H	9.32146300	1.69435000	0.90554600
C	0.65577000	-2.76964800	-1.40034200	C	2.42546100	0.86744700	2.35084000
C	-0.69318400	-3.08108400	-1.50613600	O	3.06901400	1.89546600	2.51615800
C	-1.73345500	-2.12506800	-1.50754600	C	1.77581600	0.12321900	3.51859700
C	-1.39172600	-0.79456100	-1.41271200	H	2.31046300	-0.81726200	3.69078100
C	-0.04133000	-0.40643500	-1.27045800	H	1.82960800	0.74186400	4.41649300
H	-0.98001500	-4.12421600	-1.59741100	H	0.73556300	-0.12662700	3.29046800
H	-2.15980200	-0.02649400	-1.43752800	C	-9.13144400	-0.93201800	-0.80229000
C	0.23060200	0.99714300	-1.27185500	C	-7.84645700	-0.80239100	-0.32184300
H	-0.62114400	1.64141200	-1.49472000	C	-7.01218500	0.27162600	-0.73879400
H	5.21030000	3.64419200	0.18662300	C	-7.54450000	1.21622000	-1.67857600
C	1.61272900	2.99842200	-1.23574700	C	-8.87306000	1.05333400	-2.15238400
C	2.64214000	3.39055400	-0.16694200	C	-9.65523400	0.00331400	-1.72621800

H	-9.74956200	-1.76169600	-0.46907900	H	-3.45708900	-2.57227800	-2.73877300
H	-7.45443100	-1.52633800	0.38537500	H	-3.32811300	-3.57737200	-1.29681500
C	-5.67337600	0.43180800	-0.25819800	O	2.18305900	0.24283900	1.21844600
C	-6.72265400	2.29119400	-2.11292600	C	1.73358200	-3.86865700	-1.43860800
H	-9.26260600	1.77803900	-2.86407300	C	6.66729300	-2.17603200	0.38909300
H	-10.67033200	-0.11061800	-2.09655300	C	2.51485100	-3.87695700	-0.10399200
C	-5.43917700	2.43338900	-1.64881800	H	2.98034300	-2.91052600	0.08592100
C	-4.91720000	1.49936600	-0.72117600	H	1.84482900	-4.11158500	0.73246100
H	-7.12735300	3.00709200	-2.82439200	H	3.29881200	-4.64399900	-0.13212700
H	-4.80244800	3.25118100	-1.97177400	C	2.69550800	-3.61093700	-2.62509200
C	-6.28966400	0.74914100	4.03423300	H	2.15267300	-3.65366800	-3.57766800
C	-6.09606500	0.64371500	2.67465900	H	3.17572800	-2.63495800	-2.54309600
C	-5.28065700	-0.38832000	2.12869200	H	3.47667600	-4.38072800	-2.64863400
C	-4.66340900	-1.31156300	3.03686900	C	1.13117400	-5.27489500	-1.63442600
C	-4.88392400	-1.17343900	4.43360600	H	0.46408900	-5.56004700	-0.81195500
C	-5.68065800	-0.16606200	4.92713400	H	0.57613500	-5.36243200	-2.57623800
H	-6.91785600	1.54418100	4.42726600	H	1.94338100	-6.00977700	-1.66349300
H	-6.56883600	1.34992800	2.00029600	C	5.66321300	-2.55411500	1.50626200
C	-5.05822200	-0.52249600	0.71874700	H	4.70865500	-2.04215600	1.37587200
C	-3.83749400	-2.33519100	2.50845200	H	5.48003000	-3.63575200	1.49980400
H	-4.40756700	-1.88225900	5.10713700	H	6.06876800	-2.28689100	2.48991100
H	-5.84373200	-0.06912400	5.99684600	C	6.15489700	-2.65695700	-0.98973300
C	-3.62526000	-2.46111500	1.15611900	H	6.01734300	-3.74549500	-0.97923100
C	-4.24704900	-1.55930900	0.25246100	H	5.20406500	-2.19007500	-1.24542300
H	-3.35686800	-3.02867100	3.19437000	H	6.88411400	-2.41904500	-1.77447000
H	-2.97198700	-3.24203900	0.78719600	C	7.98197000	-2.92949700	0.67833800
O	-3.62559100	1.71168700	-0.31434500	H	8.74681000	-2.73607800	-0.08334500
O	-4.11620200	-1.65190100	-1.10401200	H	8.39935000	-2.67496700	1.65967000
H	-3.41381100	1.03012500	0.34994500	H	7.78305800	-4.00710200	0.67693800
C	-3.17405100	-2.55948300	-1.68042300				

S-BINOL with (S,S)-Co(III) salen complex

B3LYP/ 6-31G* level of theory:

Charge: 0

Spin Multiplicity: 1

Electronic Energy (au): -2681.36299284

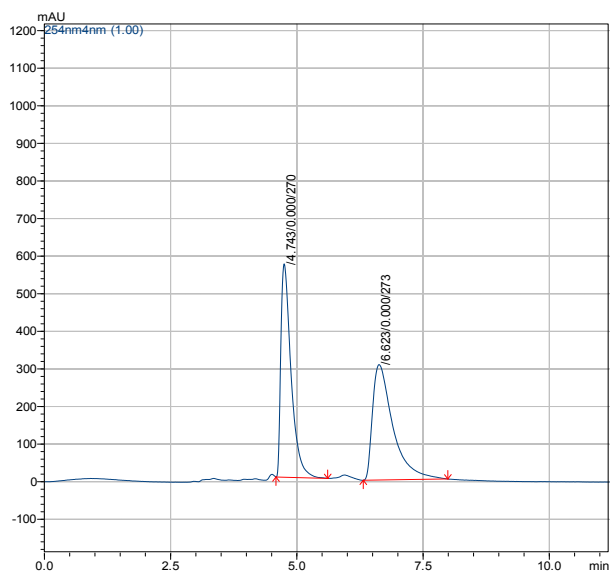
				C	-5.86769400	-5.09927400	-0.58133800
Co	-3.48789100	-0.38499800	-0.46041700	C	-4.86570900	-5.34386300	-1.71748100
O	-4.23728800	1.28520000	-0.04489700	C	-3.60108800	-4.48011100	-1.56279300
N	-5.12541900	-1.30946400	-0.16766300	H	-6.89953400	-3.48342500	0.41452900
C	-6.46723600	0.60770200	0.51314600	H	-4.46943700	-3.07048600	0.65381000
C	-7.76921400	0.97159100	0.93400400	H	-4.50657600	-2.70528400	-2.36820100
C	-8.05676500	2.27797000	1.24460800	H	-5.43397400	-5.44493400	0.36727900
C	-7.03131600	3.24219500	1.15739500	H	-6.77594500	-5.69128100	-0.74423800
C	-5.73131300	2.95518400	0.76134300	H	-4.58422700	-6.40280700	-1.75444800
C	-5.42744500	1.58995300	0.39897300	H	-5.34280200	-5.11413700	-2.68100700
H	-8.53128300	0.19888500	1.00948900	H	-3.04273000	-4.78627500	-0.66693300
H	-7.28374200	4.26138200	1.42627200	H	-2.94512700	-4.64053900	-2.42649700
C	-6.23654000	-0.76993500	0.22977400	H	-6.79055200	-3.27779600	-1.33867900
N	-2.89870500	-2.02715100	-1.25079900	H	-9.05121800	2.57143700	1.56644700
O	-2.00411600	0.53860200	-1.19997800	C	10.03669600	-0.19846900	-1.59767600
C	-0.81575600	0.05697000	-1.41900600	C	9.46313200	1.04437500	-1.74916000
C	0.31029900	0.94727000	-1.61618800	C	8.16347600	1.31775400	-1.24776000
C	1.55864100	0.37860100	-1.81324800	C	7.43862100	0.28174000	-0.56934800
C	1.79812400	-1.01707900	-1.87075800	C	8.05971900	-0.99089200	-0.43288400
C	0.72137800	-1.86387000	-1.74844100	C	9.32266300	-1.22357800	-0.93313900
C	-0.58103600	-1.35650700	-1.52879300	H	8.10683200	3.37808900	-1.91603300
H	2.42035400	1.02733500	-1.92257500	H	11.03218400	-0.39496300	-1.98637000
H	0.85592900	-2.94275200	-1.82232200	H	9.99974600	1.84082700	-2.26031200
C	-1.66190700	-2.28873800	-1.53955500	C	7.55592200	2.59347900	-1.40278700
H	-1.41015300	-3.30190700	-1.85809000	C	6.12810800	0.55401000	-0.06111700
H	-7.09593900	-1.42479800	0.37503500	H	7.52094700	-1.78522400	0.07383400
C	-3.98962600	-3.00174900	-1.44101500	H	9.77538000	-2.20499400	-0.81667500
C	-4.96520800	-2.77200700	-0.27841800	C	5.58203900	1.81617400	-0.25064200
C	-6.23708800	-3.61084400	-0.44856400	C	6.29631200	2.84105300	-0.91974600

H	5.81936700	3.80942000	-1.03379500	H	-2.27925800	-1.57094000	4.22279000
C	4.34349400	-1.19975200	-0.02003800	O	-4.09559900	-1.67248400	2.44094800
C	5.32685500	-0.48188400	0.66451400	C	0.12346400	2.47586100	-1.60752200
C	5.54792800	-0.75024000	2.05486500	C	1.43973900	3.22727100	-1.89464900
C	4.76507200	-1.75104500	2.72058000	H	2.21256400	3.03150400	-1.14356200
C	3.77919200	-2.44668100	1.97747400	H	1.84803800	2.97733400	-2.88156900
C	3.56404000	-2.18291000	0.64528600	H	1.23940400	4.30476900	-1.88727400
H	7.12286400	0.71314300	2.32773400	C	-0.88734900	2.88302300	-2.70867500
C	6.52557600	-0.04884700	2.81693200	H	-1.85801600	2.40784400	-2.56078700
C	4.98766500	-2.01242500	4.09945400	H	-1.02912900	3.97070700	-2.69911800
H	3.17657700	-3.19946700	2.48033200	H	-0.50931700	2.60362800	-3.70017800
H	2.78720600	-2.71554600	0.11215300	C	-0.38375900	2.92664100	-0.21779800
C	5.94303200	-1.31781700	4.80487900	H	-1.31749500	2.42933200	0.04349000
C	6.71595000	-0.32643400	4.15226400	H	0.36139500	2.70101800	0.55492300
H	4.38397000	-2.77415100	4.58784500	H	-0.55251400	4.01068200	-0.21427300
H	6.10579400	-1.52459100	5.85898700	C	-4.64414300	4.04562900	0.73468400
H	7.46788600	0.22238900	4.71310600	C	-3.52272200	3.66623100	1.73347900
O	4.33396700	2.15000800	0.19256400	H	-3.91628000	3.63890500	2.75717000
O	4.20830400	-0.90744800	-1.34716600	H	-3.09424000	2.68999100	1.50198800
H	3.94749300	1.36707600	0.62436700	H	-2.71989600	4.41288200	1.70104800
C	3.19247900	-1.53615800	-2.13773300	C	-4.07140500	4.19906000	-0.69486400
H	3.50480800	-1.30315000	-3.16116100	H	-3.30141100	4.98054700	-0.70680100
H	3.23270100	-2.62754700	-2.02320000	H	-3.62589300	3.26922600	-1.04791100
O	-2.55128500	-0.64426400	1.11451000	H	-4.86179100	4.49698000	-1.39539400
C	-3.00806600	-1.14622000	2.24107800	C	-5.19125200	5.42391800	1.15967800
C	-1.96998300	-0.98818700	3.35293300	H	-5.97812200	5.78375000	0.48593400
H	-0.98118400	-1.30741800	3.01128600	H	-5.58772500	5.41645800	2.18184500
H	-1.89599300	0.06903000	3.62998400	H	-4.37585000	6.15533200	1.13113500

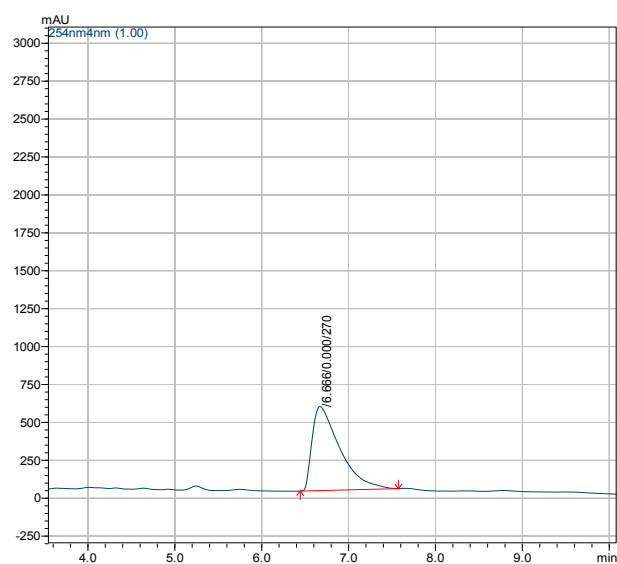
HPLC Chromatogram of (*S*)-Metoprolol and (*S*)-Toliprolol

(a) (*S*)-Metoprolol

Racemic

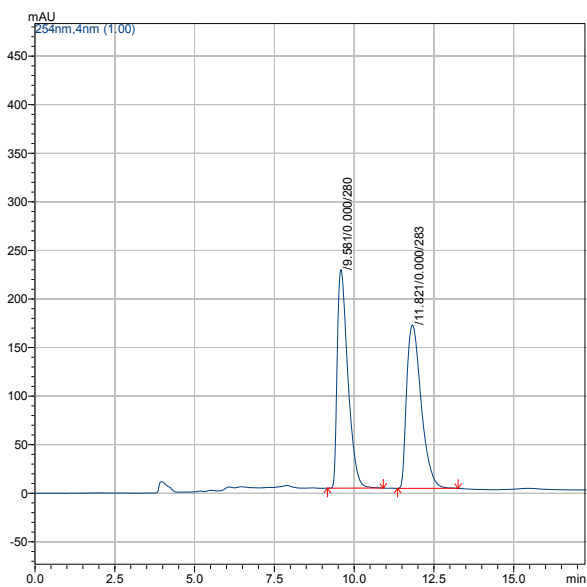


Chiral



(b) (*S*)-Toliprolol

Racemic



Chiral

