Supporting Information

For

Asymmetric Ring-Opening of Oxabenzonorbornadiene with Amines Promoted by a Chiral Iridium-Monophosphine Catalyst

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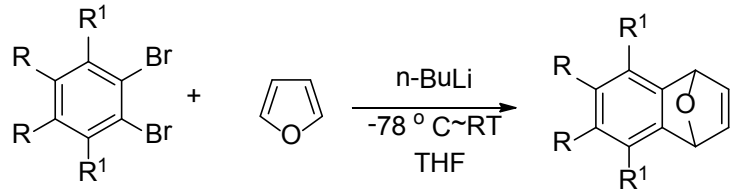
1. General Methods. All reactions were carried out under a nitrogen atomosphere unless otherwise specified. THF (<0.02% water content), Et_2O, dioxane, MTBE, DCM, DCE, Xylene and toluene were purchased from Sigma Aldrich and used directly without further purifications. Commercialized reagents were used without further purifications.

^1H, ^{31}P and ^{13}C NMR data were recorded on a Bruker-Topspin DRX400 or 500 NMR Spectrometer with $CDCl_3$ as the solvent. ^1H shifts were referenced to $CDCl_3$ at 7.27 ppm. ^{31}P shifts were referenced to 85% H_3PO_4 in D_2O at 0.0 ppm as external standard and obtained with ^1H decoupling. ^{13}C shifts were referenced to $CDCl_3$ at 77.23 ppm and obtained with ^1H decoupling. MS was measured on Agilent 1100 Series LC/MSD mass spectrometer. Chiral HPLC analyses wee performed on an Aglient 1200 system using a Chiralcel OD-H, Chiralpak AD-H column or Chiralcel Lu-Amy lose-2 column. Racemic compounds were prepared by reaction using $[IrCODCl]_2$ and NaI without using the ligand at 80 ^oC. The optical rotations were recorded on a Rudolph Research Automatic Polarimeter.

2. Synthesis of 1a~1e [1]



1a~1e

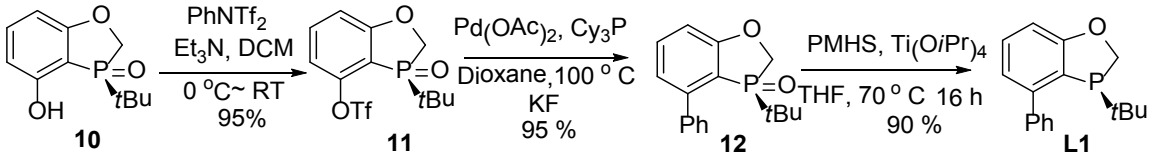
1a: R = OMe, R^1 = H; **1b**: R = H, R^1 = OMe;
1c: R = Br, R^1 = H; **1d**: R = F, R^1 = H;
1e: R = H, R^1 = H;

Under N_2 a stirred solution of substituted 1, 2-dibromobenzene (14.06 mmol) in anhydrous THF 25 mL Furan 30 mL was treated drop wise with 5.8 mL of BuLi (2.4 M in hexane) at -78°C. The solution was stirred at -78°C for 1.5 hr. 20 mL distillated water was added to reaction mixture and left to warm up to room temperature, diethyl ether was added to the reaction mixture, separated, extracted and dried over Na_2SO_4. The ether was then removed in *vacuo* and the resulting mixture was purified by flash chromatography (10%~50% ethyl acetate in hexanes) to give the product **1**. **1a:** White solid (2.5g, 87%). ^1H NMR (400MHz, $CDCl_3$) δ 6.97 (s, 2H), 6.90 (s, 2H), 5.60 (s, 2H), 3.77 (6H,

s); ^{13}C NMR (100MHz, $CDCl_3$) δ 146.0, 143.5, 141.9, 106.9, 82.7, 56.7, 56.6.; **1b**: White solid (1.8 g, 63%). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.01 (s, 2H), 6.94 (s, 2H), 5.65 (s, 2H), 3.82 (s, 6H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 145.8, 143.3, 141.7, 106.8, 82.6, 56.5.; **1c**: White solid (1.4 g, 43%). ^{1}H NMR (400MHz, $CDCl_3$): δ 7.45 (s, 2H), 6.97 (s, 2H), 5.64 (s, 2H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 150.1, 142.6, 125.3, 120.5, 81.6. **1d:** Yellow oil (2.5g, 87%).; ^{19}F NMR (376 MHz, $CDCl_3$) δ -142.39; ^{1}H NMR (400MHz, $CDCl_3$) δ 6.90-6.97 (m, 2H), 5.57 (s, 2H).; ^{13}C NMR (100MHz, $CDCl_3$) δ 148.5 (d, J= 15.0 Hz), 146.0 (d, J= 14.8 Hz), 145.3 (d, J= 4.7 Hz), 143.1, 110.7-110.9(m), 82.1 (d, J= 7.9 Hz).; **1e:** White solid (1.5g, 75%). ^{1}H NMR (400MHz, $CDCl_3$) δ 7.15-7.17 (m, 2H), 6.94 (s, 2H), 6.87-6.89 (m, 2H), 5.63 (s, 2H).; ^{13}C NMR (100MHz, $CDCl_3$) δ 149.0, 143.1, 125.1, 120.3, 82.4, 82.3.

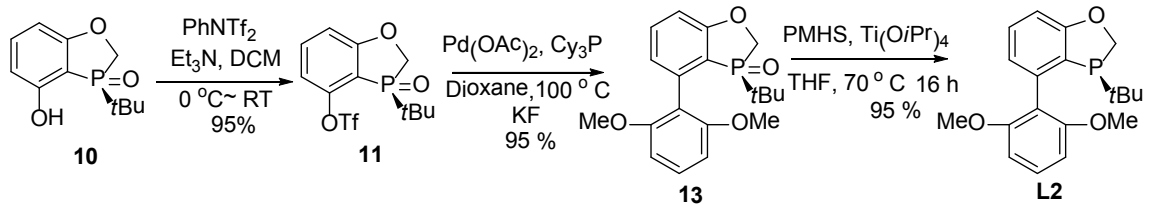
3. Synthetic procedures for ligand L1~L4 [2]

(1) Synthesis of ligand L1



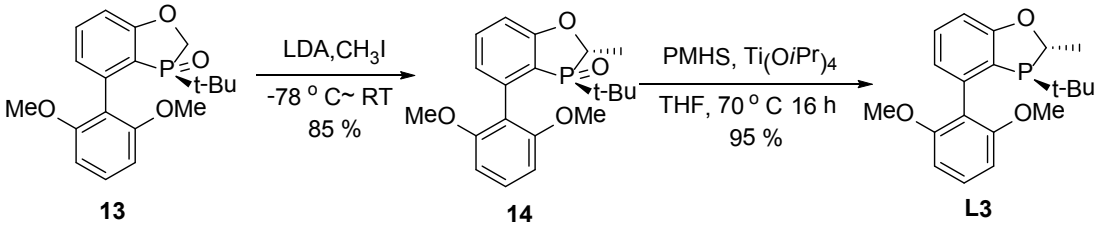
The ligand **L1** was synthesized from chiral **10** through a coupling reaction to obtain compound **12** followed by a stereospecific reduction of the **12** mediated by PMHS/Ti (O*i*-Pr)$_4$. The synthetic procedures were published in our previous paper [2]. ^{1}H NMR (400 MHz, CD_2Cl_2): δ 7.71 (m, 2H), 7.42 (m, 2H), 7.35 (m, 2H), 6.99 (m, 1H), 6.90 (dd, J = 8.1, 0.8 Hz, 1H), 4.87 (dd, J = 12.7, 1.9 Hz, 1H), 4.57 (dd, J = 25.9, 12.7 Hz, 1H), 0.64 (d, J = 12.1 Hz, 9H); ^{31}P NMR (162 MHz, CD_2Cl_2): δ -11.2; ^{13}C NMR (100 MHz, CD_2Cl_2): δ164.8, 146.5, 143.1, 131.9, 129.9, 129.8, 128.9, 127.9, 122.7 (d, J = 17.9 Hz), 122.3 (d, J = 3.1 Hz), 110.5, 70.5 (d, J = 26.9 Hz), 32.1 (d, J = 20.2 Hz), 27.0 (d, J = 13.8 Hz). ESI-MS: m/z 271 $[M+H]^+$.

(2) Synthesis of ligand L2



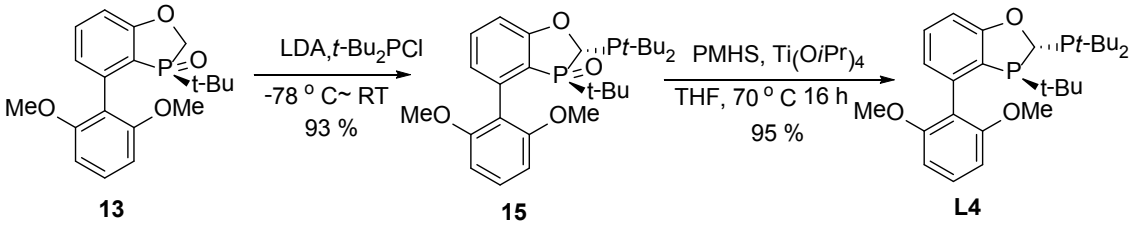
The ligand **L2** was synthesized out from chiral compound **10** by a coupling reaction to obtain compound **13** followed by a stereospecific reduction of **13** mediated by PMHS/Ti (O*i*-Pr)$_4$. The synthetic procedures were published in our previous paper [2]. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.29 (m, 2H), 6.87 (m, 2H), 6.65 (d, J = 8.2 Hz, 1H), 6.59 (d, J = 8.3 Hz, 1H), 4.81 (dd, J = 12.5, 1.8 Hz, 1H), 4.53 (dd, J = 25.2, 12.5 Hz, 1H), 3.77 (s, 3H), 3.71 (s, 3H), 0.73 (d, J = 12.1 Hz, 9H); ^{31}P NMR (162 MHz, $CDCl_3$): δ -7.9; ^{13}C NMR (100 MHz, $CDCl_3$): δ 163.4, 157.9. 157.1, 138.4 (d, J = 22.3 Hz), 130.5, 129.0, 125.0 (d, J = 16.4 Hz), 123.8 (d, J = 5.4 Hz), 119.6, 109.5, 104.5, 103.6, 70.4 (d, J = 33.8 Hz), 55.9, 55.4, 30.9 (d, J = 23.2 Hz), 26.6 (d, J = 18.1 Hz); ESI-MS: m/z 331 $[M+H]^+$.

(3) Synthesis of ligand L3



The ligand **L3** was synthesized from chiral compound **13** by a LDA-mediated homo-coupling reaction to obtain compound **14** followed by a stereospecific reduction of **14** mediated by PMHS/ Ti(O*i*-Pr)$_4$. The synthetic procedures were published in our previous paper [2]. ^{1}H NMR (400 MHz,CD_2Cl_2): δ 7.35-7.20 (m, 2H), 6.85-6.75 (m, 2H), 6.64 (d, J =8.4 Hz, 1H), 6.61 (d, J =8.4 Hz,1H), 4.97 (q, J =7.0 Hz, 1H), 3.73 (s, 3H), 3.71 (s, 3H), 1.40 (dd, J =16.4, 7.0 Hz, 3H), 0.71 (d, J=12.0 Hz, 9H); ^{31}P NMR (162 MHz, CD_2Cl_2): δ 9.9; ^{13}C NMR (100 MHz, CD_2Cl_2): δ 163.1, 158.2, 157.4, 139.5 (d, J=17.0 Hz), 130.7, 129.4, 125.78, 125.0 (d, J =6.0 Hz), 124.0, 120.0, 109.9, 104.6, 104.0, 79.2 (d, J=24.0 Hz), 56.0 (d, J =2.0 Hz), 31.1 (d, J =19.0 Hz), 25.6, 21.6 (d, J =29.0 Hz); HRMS calcd for $C_{20}H_{26}O_3P$ [M+H]+: 345.1614; found: 345.1605.

(4) Synthesis of ligand L4

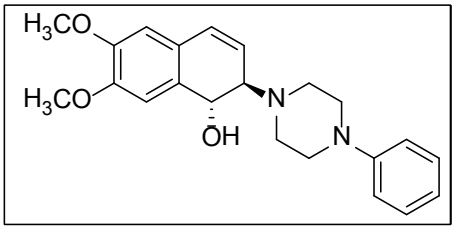


The ligand **L4** was synthesized from chiral compound **13** by a LDA-mediated homo-coupling reaction to obtain compound **15** followed by a stereospecific reduction of **15** mediated by PMHS/Ti(O*i*-Pr)$_4$. The synthetic procedures were published in our previous paper [2]. ^{1}H NMR (400 MHz, CD_2Cl_2) δ 7.42 (m, 1H), 7.25 (m, 1H), 6.90 (m, 1H), 6.81 (d, J = 8.0 Hz, 1H), 5.60 (dd, J = 5.4, 4.4 Hz, 1H), 1.37 (d, J = 11.0 Hz, 9H), 1.18 (d, J =11.1 Hz, 9H), 0.96 (d, J = 12.2 Hz, 9H); ^{31}P NMR (162 MHz, CD_2Cl_2): δ 52.0 (d, $^3J_{PP}$ = 146.1 Hz), 12.2 (d, $^3J_{PP}$ = 146.4 Hz); ^{13}C NMR (100 MHz, CD_2Cl_2) δ 164.7, 131.5,131.3, 121.1 (dd, J = 64.3, 6.4 Hz), 121.0 (d, J = 6.1 Hz), 111.3, 80.2 (dd, J = 45.3, 37.4 Hz), 34.6 (d, J = 24.4 Hz), 34.1 (dd, J = 22.4, 11.3 Hz), 32.0 (dd, J = 22.5, 7.6 Hz), 31.5(dd, J = 12.2, 3.6 Hz), 31.4 (d, J = 12.5 Hz), 26.3 (d, J = 14.7 Hz).

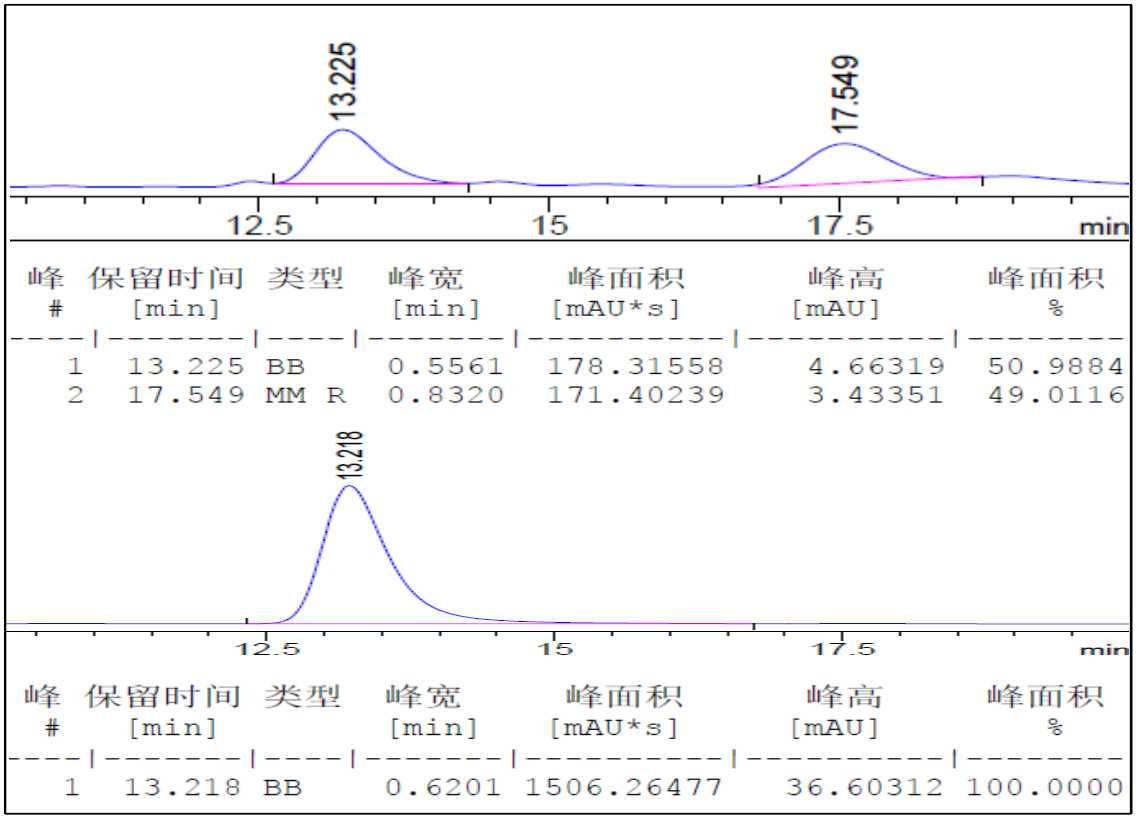
4. General procedure of asymmetric ring-opening of oxabenzonorbornadiene with amines

To a mixture of oxabenzonorbornadiene **1** (0.347 mmol, 1 equiv), amines **4** or **6** (1.041 mmol, 3 equiv), NaI (10.34 mg, 0.069 mmol, 0.2 equiv), ligand **L1** (4.5 mg, 0.0167 mmol, 4.8 mol %) and $[Ir(coe)_2Cl]_2$ (6.2 mg, 0.0069 mmol, 2.0 mol %) was added THF (2.0 mL). The mixture was stirred at reflux for 8~14 h and then the residue was directly subjected to silica gel column chromatography [ethyl acetate/hexanes (1:1~2:1 v/v) as the eluent] to afford the desired alcohol product **5** or **7**. The enantioselectivity was determined by chiral HPLC on a chiralcel OD-H, chiralcel AD-H, or Lux Amylose-2 column.

5. Analytical data of asymmetric addition products



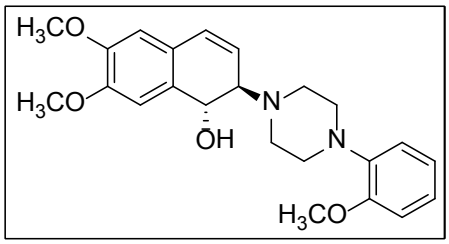
(1*R*, 2*R*)-6, 7-dimethoxy-2-(4-phenylpiperazin-1-yl)-1, 2-dihydronaphthalen-1-ol (3): White solid (91% yield); >99% *ee*; $[\alpha]_D^{27}$ = -225.27° (c = 0.62, $CHCl_3$); ^{1}H NMR (400MHz, $CDCl_3$) δ 7.17-7.21 (m, 2H), 7.06 (s, 1H), 6.77-6.86 (m, 3H), 6.56 (s, 1H), 6.39 (dd, *J* = 2.4 Hz, *J* = 9.9 Hz, 1H), 5.95 (dd, *J* = 2.6 Hz, *J* = 9.9 Hz, 1H), 4.78 (d, *J* = 11.8 Hz, 1H), 3.84 (s, 3H), 3.78 (s, 3H), 3.39 (td, *J* = 2.4 Hz, *J* = 11.2 Hz, 1H), 3.29 (br, 1H), 3.08-3.18 (m, 4H), 2.83-2.88 (m, 2H), 2.60-2.65 (m, 2H); ^{13}C NMR (100MHz, $CDCl_3$) δ 151.35, 148.71, 148.12, 129.92, 129.25, 129.05, 124.69, 122.52, 120.06, 116.35, 110.08, 108.77, 67.83, 67.72, 56.17, 56.14, 49.91, 49.11. ESI-MS: *m/z* 367 $[M+H]^+$. Chiral HPLC conditions: Chiralcel OD-H, 25 °C, flow rate: 1.0 mL/min, hexane/isopropanol: 75/25, 254 nm, 13.22 min (*major*), 17.55 min (*minor*).



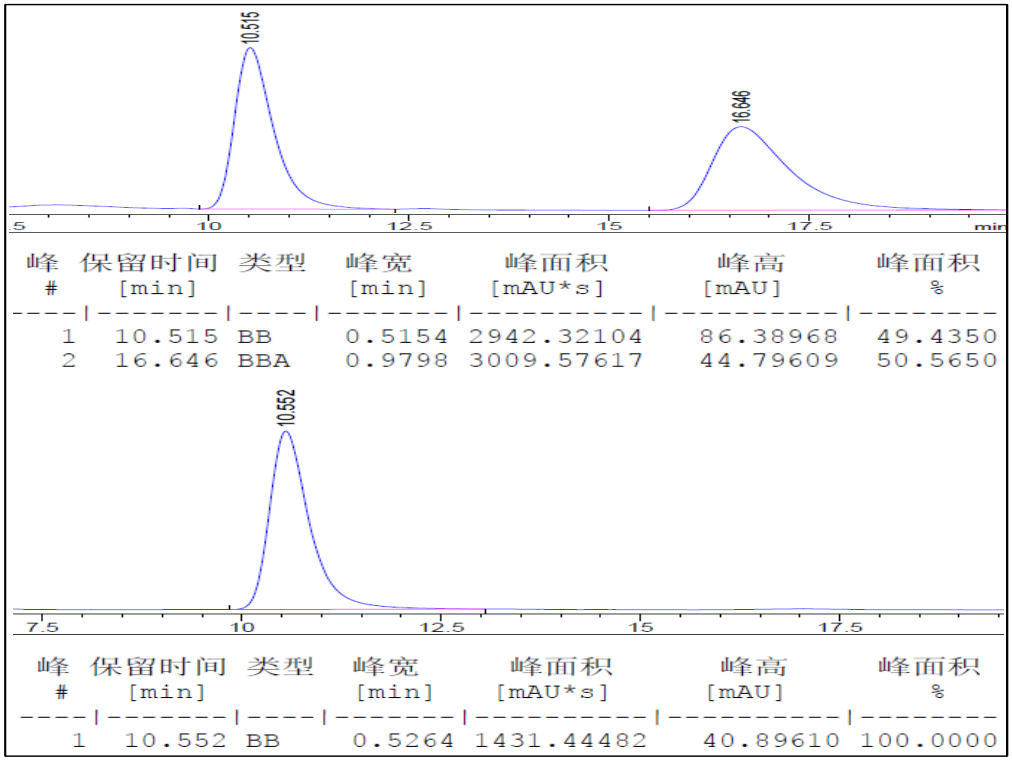
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	13.225	BB	0.5561	178.31558	4.66319	50.9884
2	17.549	MM R	0.8320	171.40239	3.43351	49.0116

峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	13.218	BB	0.6201	1506.26477	36.60312	100.0000

Table 2, Entry 1



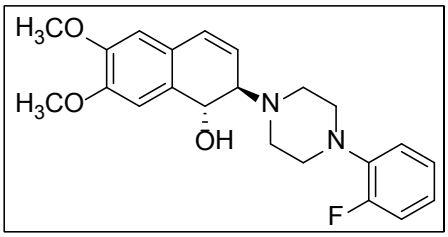
(1*R*, 2*R*)-6, 7-dimethoxy-2-(4-(2-methoxyphenyl-piperazin-1-yl)-1, 2-dihydronaphthalen-1-ol (5aa): White solid (93% yield); >99% *ee*; $[\alpha]_D^{27}$ = -199.43° (c = 0.82, $CHCl_3$); ^{1}H NMR (400MHz, $CDCl_3$) δ 7.06 (s, 1H), 6.91-6.94 (m, 1H), 6.84-6.87 (m, 2H), 6.78 (d, *J* = 7.8 Hz, 1H), 6.56 (s, 1H), 6.40 (dd, *J* = 2.4 Hz, *J* = 9.9 Hz, 1H), 6.00 (dd, *J* = 2.7 Hz, *J* = 9.8 Hz, 1H), 4.79 (d, *J* = 11.1 Hz, 1H), 3.84 (s, 3H), 3.79 (s, 3H), 3.78 (s, 3H), 3.43 (br, 1H), 3.39 (td, *J* = 2.4 Hz, *J* = 11.1 Hz, 1H), 3.02-3.06 (m, 4H), 2.88-2.92 (m, 2H), 2.66-2.70 (m, 2H); ^{13}C NMR (100MHz, $CDCl_3$) δ 152.18, 148.57, 148.00, 141.12, 129.90, 128.82, 124.63, 123.05, 122.77, 120.97, 118.21, 111.07, 109.99, 108.76, 67.58, 60.36, 56.03 (d, *J* = 1.5 Hz), 55.31, 51.15, 21.02, 14.19. ESI-MS: *m/z* 397 $[M+H]^+$. Chiral HPLC conditions: Chiralcel OD-H, 25 °C, flow rate: 1.0 mL/min, hexane/isopropanol: 75/25, 254 nm, 10.52 min (*major*), 16.65 min (*minor*).



峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	10.515	BB	0.5154	2942.32104	86.38968	49.4350
2	16.646	BBA	0.9798	3009.57617	44.79609	50.5650

峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	10.552	BB	0.5264	1431.44482	40.89610	100.0000

Table 2, Entry 2



(1*R*, 2*R*)- 2-(4-(2-fluorophenyl)piperazin-1-yl)-6, 7-dimethoxy-1, 2-dihydronaphthalen-1-ol (5ab): White solid (93% yield); >99% *ee*; $[\alpha]_D^{27}$ = -198.32° (c = 1.07, $CHCl_3$); ^{19}F NMR (376 MHz, $CDCl_3$) δ -119.78; ^{1}H NMR (400MHz, $CDCl_3$) δ 7.14 (s, 1H), 7.00-7.14 (m, 2H), 6.92-6.97 (m, 2H), 6.65 (s, 1H), 6.48 (dd, J = 2.5 Hz, J = 9.9 Hz, 1H), 6.06 (dd, J = 2.7 Hz, J = 9.9 Hz, 1H), 4.86 (d, J = 11.3 Hz, 1H), 3.93 (s, 3H), 3.87 (s, 3H), 3.47 (td, J = 2.5 Hz, J = 11.3 Hz, 1H), 3.28 (br, 1H), 3.09-3.17 (m, 4H), 2.94-2.98 (m, 2H), 2.72-2.76 (m, 2H); ^{13}C NMR (100MHz, $CDCl_3$) δ 156.83, 154.87, 148.47 (d, J = 72.5 Hz), 140.15 (d, J = 8.5 Hz), 129.98, 129.03, 124.75, 124.61 (d, J = 3.5 Hz), 122.76, 122.71, 119.11 (d, J = 2.9 Hz), 116.26 (d, J = 20.7 Hz), 110.16, 108.85, 67.84, 67.80, 56.19, 56.17, 51.23 (d, J = 3.2 Hz), 49.22. ESI-MS: *m/z* 385 $[M+H]^+$. Chiral HPLC conditions: Chiralcel OD-H, 25 °C, flow rate: 1.0 mL/min, hexane/isopropanol: 75/25, 254 nm, 10.19 min (*major*), 13.82 min (*minor*).

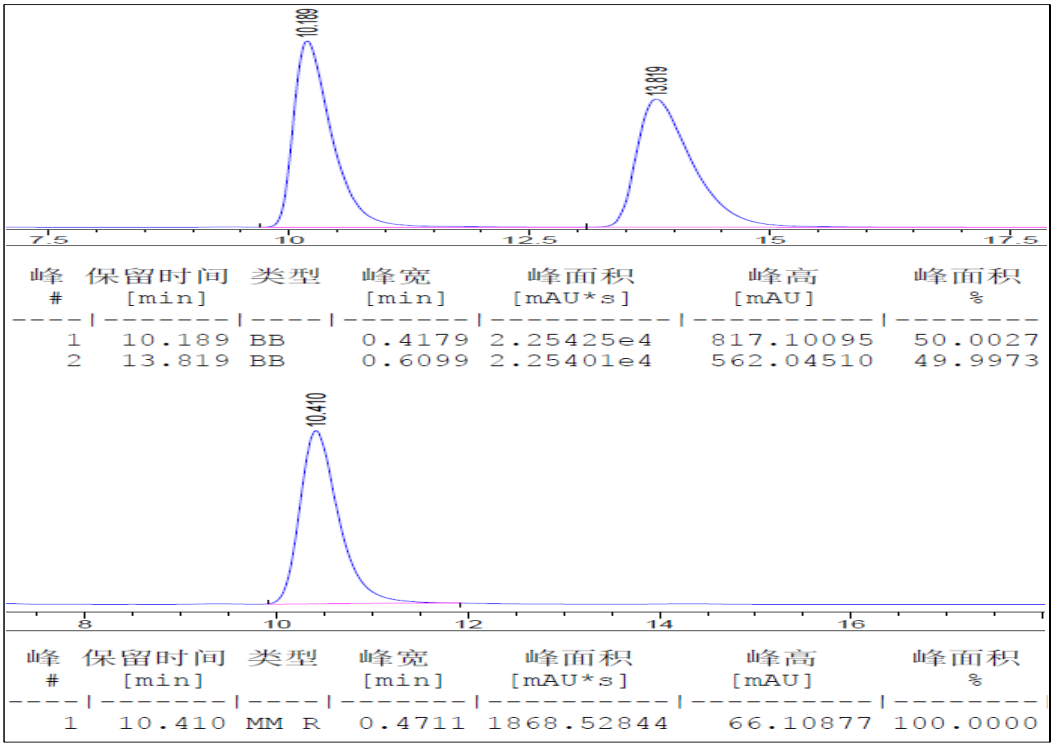
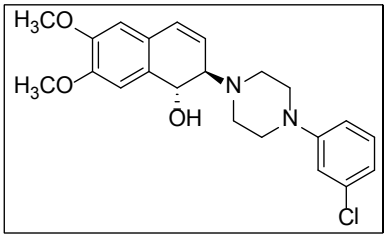


Table 2, Entry 3



(1*R*, 2*R*)-2-(4-(3-chlorophenyl)piperazin-1-yl)-6, 7-dimethoxy-1, 2-dihydronaphthalen-1-ol (5ac): White solid (95% yield); 95% *ee*; $[\alpha]_D^{27}$ = -177.95° (c = 1.20, $CHCl_3$); ^{1}H NMR (400MHz, $CDCl_3$) δ 7.14-7.27 (m, 2H), 6.88 (t, *J* = 2.1 Hz, 1H), 6.77-6.82 (m, 2H), 6.65 (s, 1H), 6.48 (dd, *J* = 2.5 Hz, *J* = 9.9 Hz, 1H), 6.00 (dd, *J* = 2.7 Hz, *J* = 9.8 Hz, 1H), 4.85 (d, *J* = 11.2 Hz, 1H), 3.93 (s, 3H), 3.87 (s, 3H), 3.47 (td, *J* = 2.6 Hz, *J* = 11.2 Hz, 1H), 3.16-3.25 (m, 4H), 3.04 (br, 1H), 2.89-2.93 (m, 2H), 2.67-2.71 (m, 2H); ^{13}C NMR (100MHz, $CDCl_3$) δ 152.26， 148.67， 148.08， 134.94， 130.05， 129.74， 129.02， 124.55， 122.19，119.46， 115.88， 114.02, 110.04， 108.75， 67.78， 67.62， 56.07， 56.04， 49.28， 48.83. ESI-MS: *m/z* 401 $[M+H]^+$. Chiral HPLC conditions: Chiralcel OD-H, 25 °C, flow rate: 1.0 mL/min, hexane/isopropanol: 75/25, 254 nm, 14.87 min (*major*), 19.19 min (*minor*).

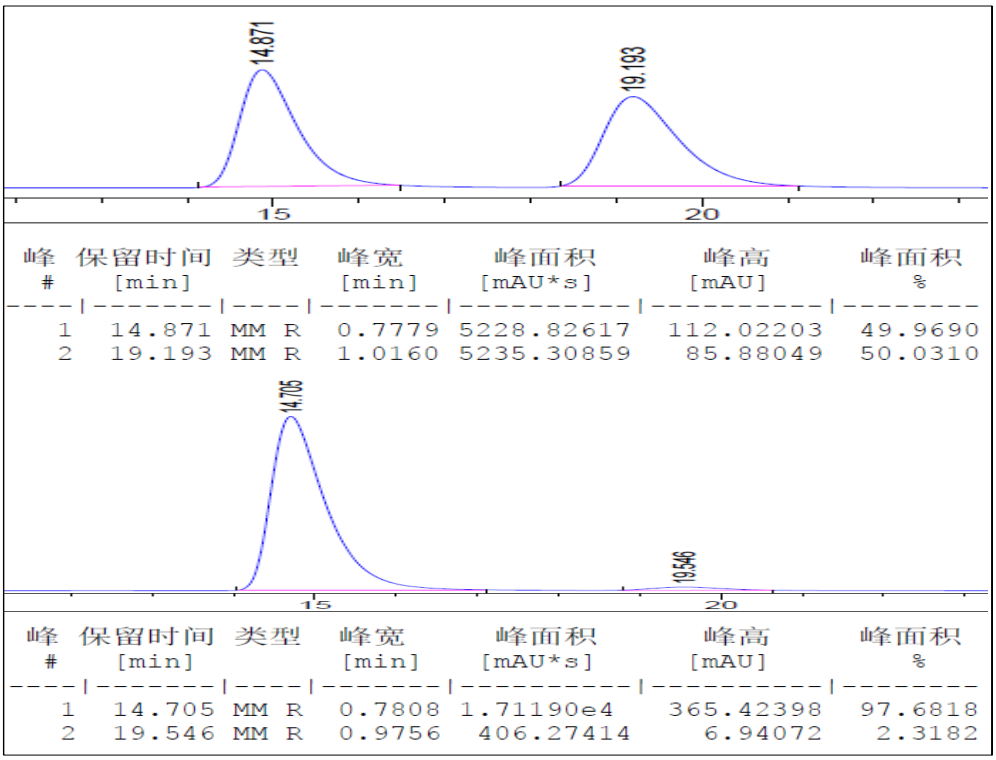
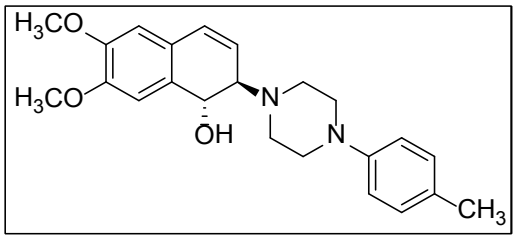


Table 2, Entry 4



(1*R*, 2*R*)-6, 7-dimethoxy-2-(4-*p*-tolylpiperazin-1-yl)-1, 2-dihydronaphthalen-1-ol (5ad): White solid (97% yield); >99% *ee*; $[\alpha]_D^{27}$ = -202.68° (c = 0.88, $CHCl_3$); ^{1}H NMR (400MHz, $CDCl_3$) δ 7.15 (s, 1H), 7.09 (d, J = 8.2 Hz, 1H), 6.86-6.88 (m, 2H), 6.66 (s, 1H), 6.49 (dd, J = 2.5 Hz, J = 9.9 Hz, 1H), 6.05 (dd, J = 2.6 Hz, J = 9.9 Hz, 1H), 4.87 (d, J = 11.4 Hz, 1H), 3.94 (s, 3H), 3.89 (s, 3H), 3.49 (td, J = 2.6 Hz, J = 11.4 Hz, 1H), 3.28 (br, 1H), 3.14-3.28 (m, 4H), 2.94-2.98 (m, 2H), 2.70-2.75 (m, 2H); ^{13}C NMR (100MHz, $CDCl_3$) δ 149.33, 148.80, 148.20, 130.03, 129.82，129.64, 129.06, 124.76, 122.64, 116.75, 110.18, 108.82, 67.90，67.83，56.24, 56.21，50.56, 49.22, 20.61. ESI-MS: *m/z* 381 $[M+H]^+$. Chiral HPLC conditions: Chiralcel OD-H, 25 °C, flow rate: 1.0 mL/min, hexane/isopropanol: 75/25, 254 nm, 9.95 min (*major*), 12.48 min (*minor*).

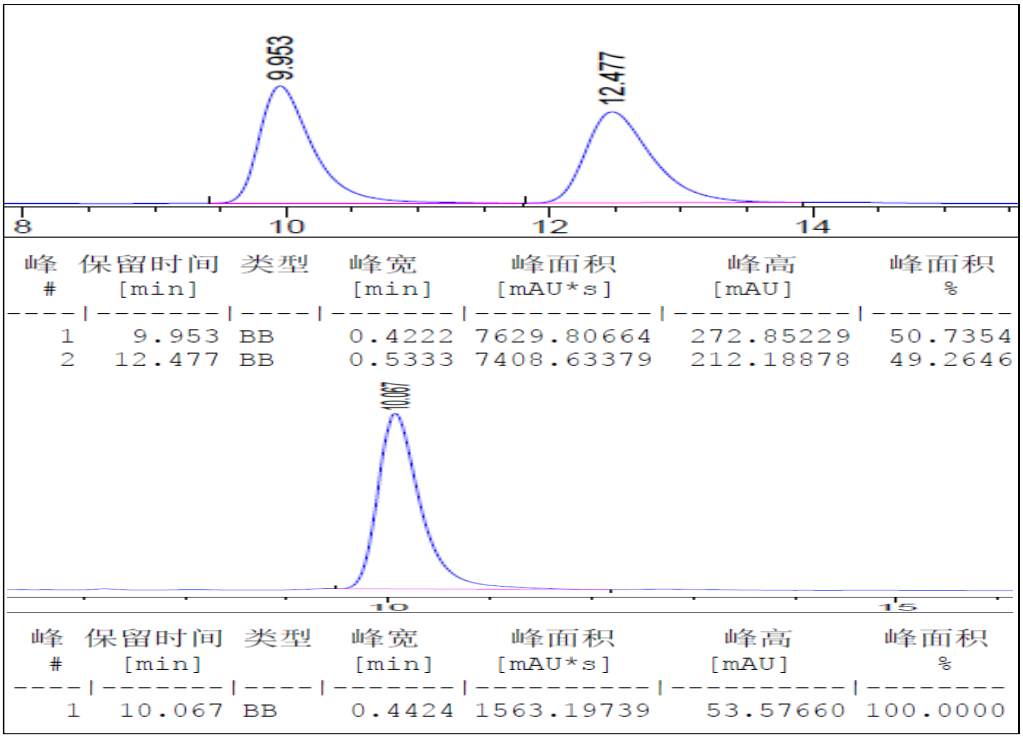
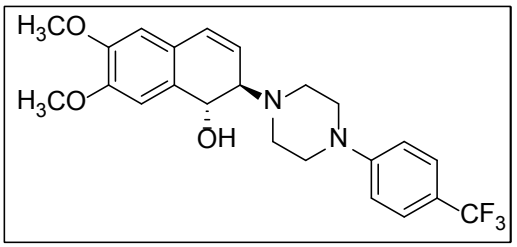


Table 2, Entry 5



(1*R*, 2*R*)-6, 7-dimethoxy-2-(4-(4-(trifluoromethyl)phenylpiperazin-1-yl)-1, 2-dihydronaphthalen-1-ol (5ae) White solid (81% yield); >99% *ee*; $[\alpha]_D^{27}$ = -198.38° (c = 1.23, $CHCl_3$); ^{19}F NMR (376 MHz, $CDCl_3$) δ -61.45; ^1H NMR (400MHz, $CDCl_3$) δ 7.40 (d, J = 8.6 Hz, 1H), 7.06 (s, 1H), 6.83 (d, J = 8.6 Hz, 1H), 6.57 (s, 1H), 6.41 (dd, J = 2.1 Hz, J = 9.9 Hz, 1H), 5.91 (dd, J = 2.6 Hz, J = 9.8 Hz, 1H), 4.78 (d, J = 11.0 Hz, 1H), 3.84 (s, 3H), 3.79 (s, 3H), 3.49 (td, J = 2.4 Hz, J = 11.2 Hz, 1H), 3.27 (br, 1H), 3.17-3.26 (m, 4H), 2.82-2.86 (m, 2H), 2.61-2.65 (m, 2H); ^{13}C NMR (100MHz, $CDCl_3$) δ 153.38, 148.86, 148.29, 129.29, 129.83, 129.26, 126.57, 126.54, 124.71, 122.21, 114.80, 110.21, 108.97, 67.98, 67.78, 56.22, 56.19, 48.91, 48.72. ESI-MS: *m/z* 435 $[M+H]^+$. Chiral HPLC conditions: Chiralcel OD-H, 25 °C, flow rate: 1.0 mL/min, hexane/isopropanol: 75/25, 230 nm, 11.64 min (*major*), 14.27 min (*minor*).

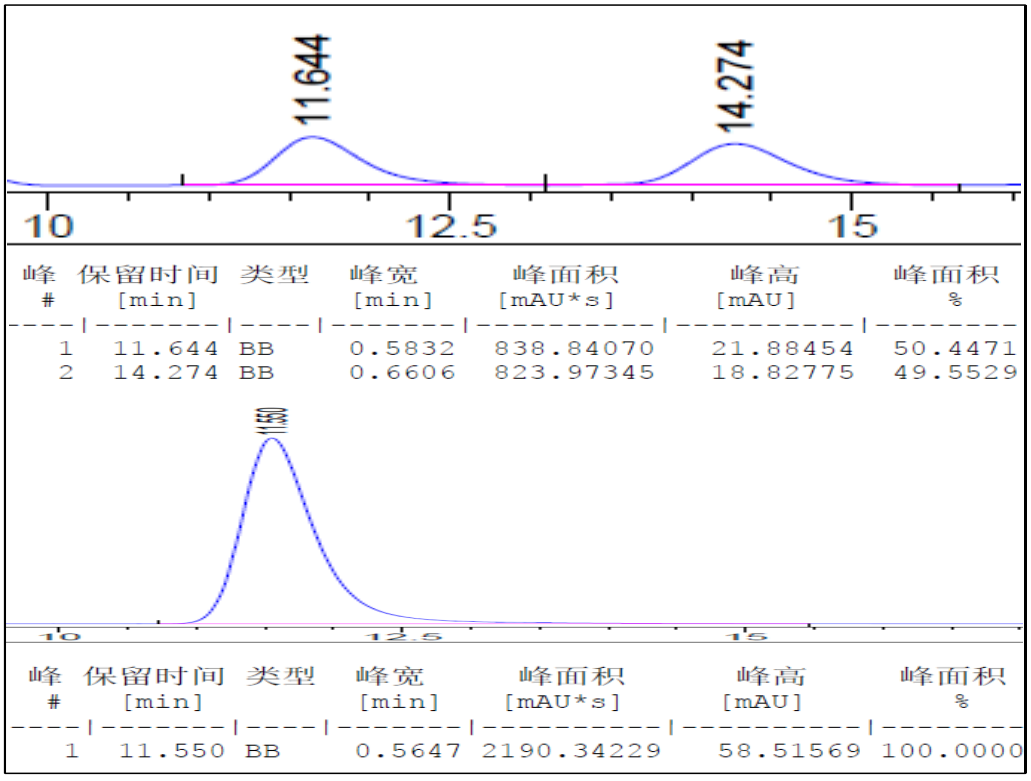
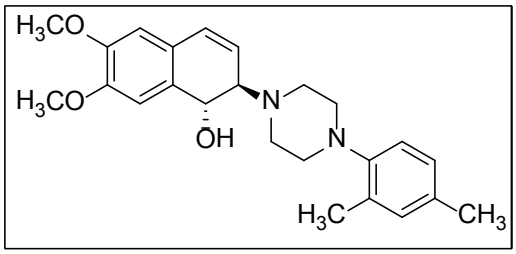
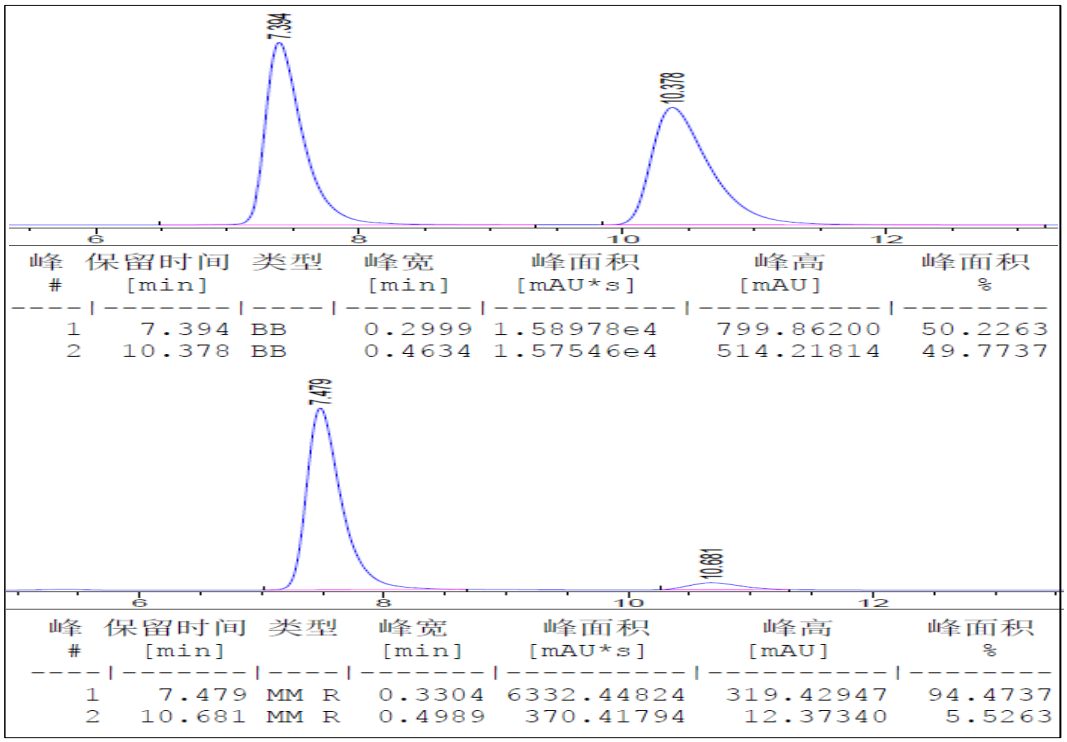


Table 2, Entry 6



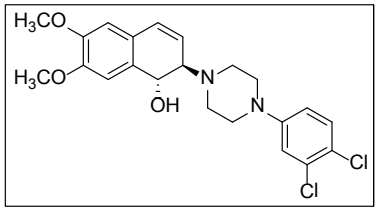
(1*R*, 2*R*)-2-(4-(2, 4-dimethylphenyl)piperazin-1-yl)- 6, 7-dimethoxy-1, 2-dihydronaphthalen-1-ol (5af): White solid (93% yield); 89% *ee*; $[\alpha]_D^{27}$ = -178.97° (c = 0.93, $CHCl_3$); ^1H NMR (400MHz, $CDCl_3$) δ 7.19 (s, 1H), 6.95-7.02 (m, 3H), 6.67 (s, 1H), 6.50 (dd, *J* = 2.5 Hz, *J* = 9.9 Hz, 1H), 6.12 (dd, *J* = 2.5 Hz, *J* = 9.9 Hz, 1H), 4.89 (d, *J* = 11.6 Hz, 1H), 3.96 (s, 3H), 3.89 (s, 3H), 3.49 (td, *J* = 2.5 Hz, *J* = 11.6 Hz, 1H), 3.34 (br, 1H), 2.92-2.99 (m, 6H), 2.70-2.74 (m, 2H), 2.31 (s, 3H), 2.30 (s, 3H)); ^{13}C NMR (100MHz, $CDCl_3$) δ 148.95, 148.61, 147.99, 132.63, 132.45, 131.83, 130.03, 128.76, 127.04, 124.64, 122.86, 118.93, 110.00, 108.62, 67.77, 56.08, 56.04, 52.47, 49.59, 20.71, 17.75. ESI-MS: *m/z* 395 $[M+H]^+$. Chiral HPLC conditions: Chiralcel OD-H, 25 °C, flow rate: 1.0 mL/min, hexane/isopropanol: 75/25, 254 nm, 7.39 min (*major*), 10.38 min (*minor*).



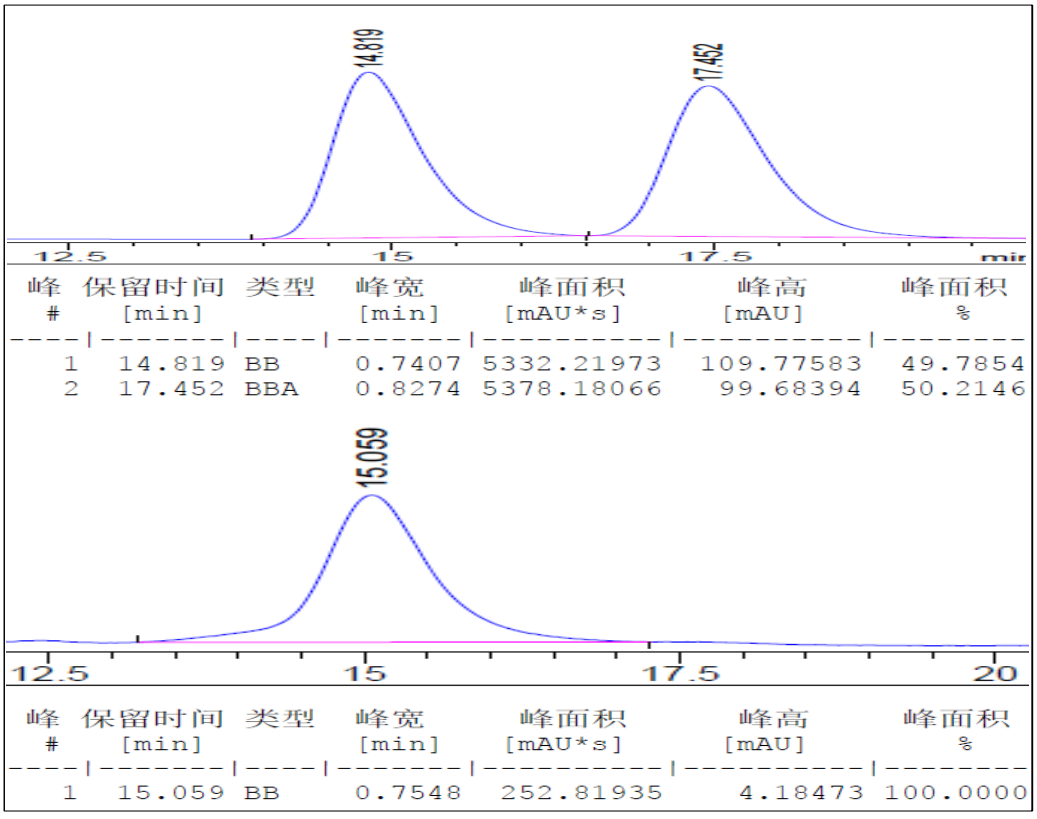
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	7.394	BB	0.2999	1.58978e4	799.86200	50.2263
2	10.378	BB	0.4634	1.57546e4	514.21814	49.7737

峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	7.479	MM R	0.3304	6332.44824	319.42947	94.4737
2	10.681	MM R	0.4989	370.41794	12.37340	5.5263

Table 2, Entry 7



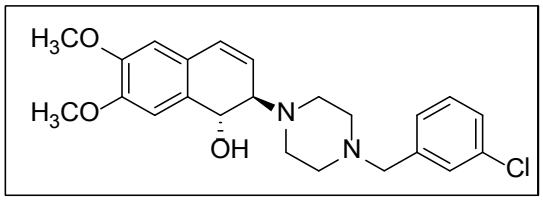
(1*R*, 2*R*)-2-(4-(3-3, 4-dichlorophenyl)piperazin-1-yl)-6,7-dimethoxy-1,2-dihydronaphthalen-1-ol (5ag): White solid (92% yield); >99% *ee*; $[\alpha]_D^{27}$ = -210.27° (c = 0.85, $CHCl_3$); ^{1}H NMR (400MHz, $CDCl_3$) δ 7.24 (d, J = 8.9 Hz, 1H), 7.12 (s, 1H), 6.93 (d, J = 2.8 Hz, 1H), 6.69-6.72 (m, 1H), 6.63 (s, 1H), 6.47 (dd, J = 2.4 Hz, J = 9.9 Hz, 1H), 5.97 (dd, J = 2.7 Hz, J = 9.9 Hz, 1H), 4.83 (d, J = 11.0 Hz, 1H), 3.84 (s, 3H), 3.91 (s, 3H), 3.85 (s, 3H), 3.46 (td, J = 2.5 Hz, J = 11.0 Hz, 1H), 3.12-3.20 (m, 4H), 3.08 (br, 1H), 2.86-2.90 (m, 2H), 2.65-2.69 (m, 2H); ^{13}C NMR (100MHz, $CDCl_3$) δ 150.58, 148.66, 148.10, 132.74, 130.43, 129.67, 129.08, 124.54, 122.22, 122.09, 117.28, 115.40, 110.04, 108.82, 67.79, 67.55, 56.06, 56.03, 49.21, 48.70. ESI-MS: *m/z* 435 $[M+H]^+$. Chiral HPLC conditions: Chiralcel OD-H, 25 °C, flow rate: 1.0 mL/min, hexane/isopropanol: 75/25, 254 nm, 14.82 min (*major*), 17.45 min (*minor*).



峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	14.819	BB	0.7407	5332.21973	109.77583	49.7854
2	17.452	BBA	0.8274	5378.18066	99.68394	50.2146

峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	15.059	BB	0.7548	252.81935	4.18473	100.0000

Table 2, Entry 8



1-(1*R*, 2*R*)-2-(4-(3-chlorobenzyl)piperazin-1-yl)-6,7-dimethoxy-1,2-dihydronaphthalen-1-ol (5ah): White solid (95% yield); >99% *ee*; $[\alpha]_D^{27}$ = -160.47° (c = 0.89, $CHCl_3$); ^{1}H NMR (400MHz, $CDCl_3$) δ 7.26 (s, 1H), 7.10-7.19 (m, 3H), 7.04 (s, 1H), 6.55 (s, 1H), 6.37 (dd, *J* = 2.5 Hz, *J* = 9.9 Hz, 1H), 5.940 (dd, *J* = 2.6 Hz, *J* = 9.9 Hz, 1H), 4.72 (d, *J* = 11.4 Hz, 1H), 3.84 (s, 3H), 3.78 (s, 3H), 3.40 (s, 2H), 3.32 (td, *J* = 2.5 Hz, *J* = 11.4 Hz, 1H), 3.17 (br, 1H), 2.71-2.75 (m,2H), 2.42-2.51 (m, 6H); ^{13}C NMR (100MHz, $CDCl_3$) δ 148.71， 148.12， 140.43， 134.32， 130.08， 129.62， 129.19， 128.88， 127.41， 127.34， 124.76， 122.91， 110.12， 108.77， 67.83， 67.65， 62.54， 56.19， 56.17， 53.68， 48.96. ESI-MS: *m/z* 415 $[M+H]^+$. Chiral HPLC conditions: Chiralcel OD-H, 25 °C, flow rate: 1.0 mL/min, hexane/isopropanol: 75/25, 254 nm, 7.16 min (*major*), 9.89 min (*minor*).

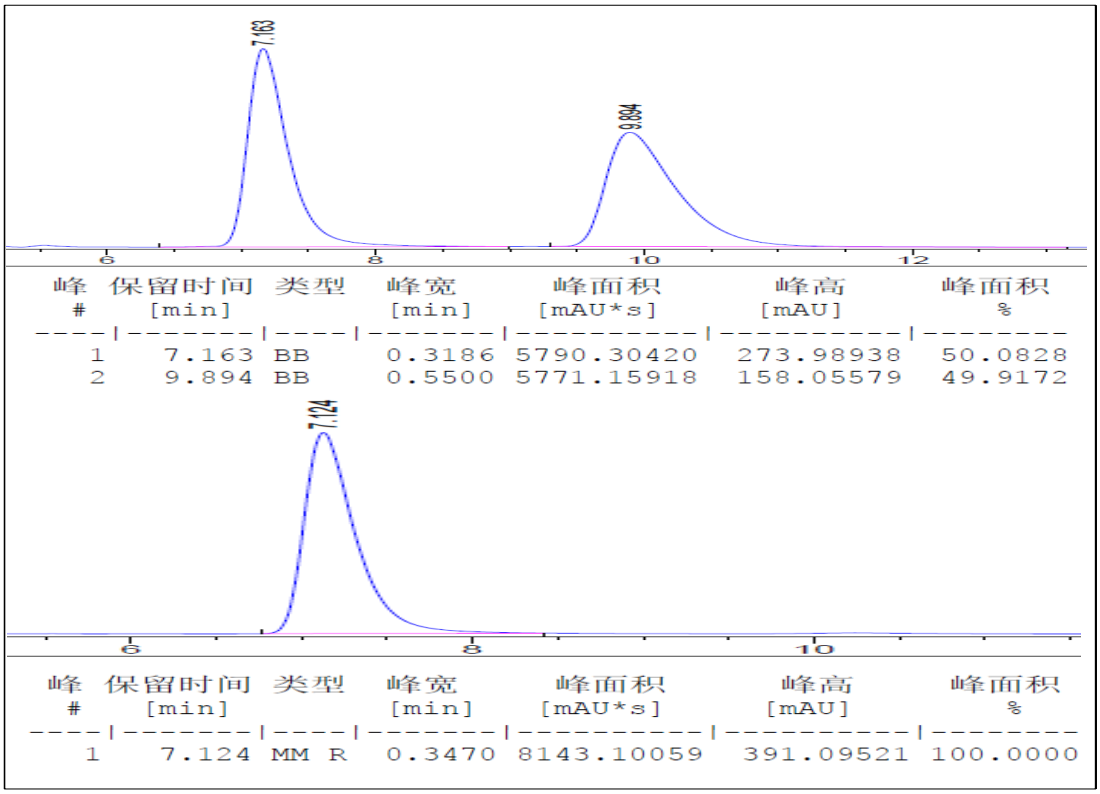
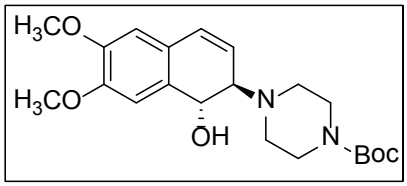
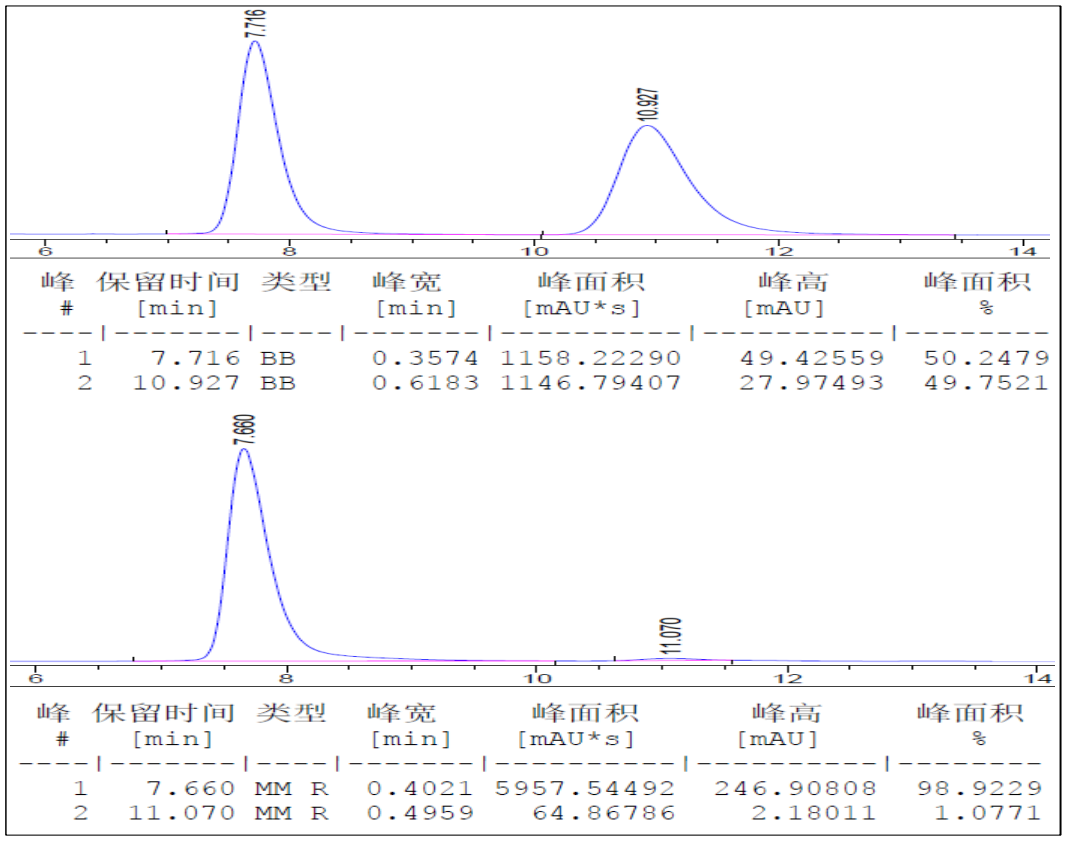


Table 2, Entry 9



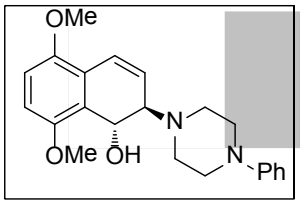
***tert*-butyl 4-((1*R*, 2*R*)-1-hydroxy-6, 7-dimethoxy-1, 2-dihydronaphthalen-2-yl)piperazine-1-carboxylate (5ai)**: White solid (93% yield); 98% *ee*; $[\alpha]_D^{27}$ = -172.45° (c = 1.19, $CHCl_3$); ^{1}H NMR (400MHz, $CDCl_3$) δ 7.04 (s, 1H), 6.56 (s, 1H), 6.39 (dd, *J* = 2.4 Hz, *J* = 9.9 Hz, 1H), 5.87 (dd, *J* = 2.7 Hz, *J* = 9.9 Hz, 1H), 4.74 (d, *J* = 11.1 Hz, 1H), 3.86 (s, 3H), 3.79 (s, 3H), 3.34-3.40 (m, 5H)，3.10 (br, 1H), 2.64-3.06 (m, 4H), 2.64-2.67 (m, 2H), 2.41-2.46 (m, 2H); ^{13}C NMR (100MHz, $CDCl_3$) δ 154.82， 148.81， 148.24， 129.87， 129.13， 124.69， 122.42， 110.17， 108.92， 79.90， 68.02， 67.95， 56.22， 56.19， 49.14， 28.58. ESI-MS: *m/z* 391 $[M+H]^+$. Chiral HPLC conditions: Chiralcel OD-H, 25 °C, flow rate: 1.0 mL/min, hexane/isopropanol: 75/25, 254 nm, 7.72 min (*major*), 10.93min (*minor*).



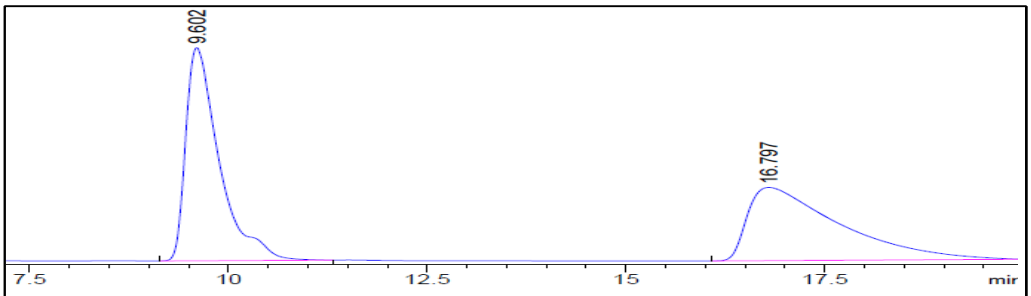
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	7.716	BB	0.3574	1158.22290	49.42559	50.2479
2	10.927	BB	0.6183	1146.79407	27.97493	49.7521

峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	7.660	MM R	0.4021	5957.54492	246.90808	98.9229
2	11.070	MM R	0.4959	64.86786	2.18011	1.0771

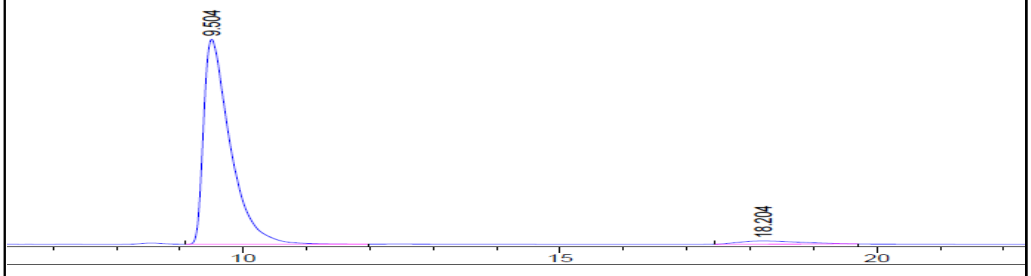
Table 2, Entry 10



(1*R*, 2*R*)-5, 8-Dimethoxy-2-(4-phenylpiperazin-1-yl)-1, 2-dihydronaphthalen-1-ol (5ba): White solid (93%). 93% *ee*; $[\alpha]_D^{27}$ = -202.55° (c = 0.38, $CHCl_3$); ^1H NMR (400 MHz, $CDCl_3$): δ 7.24-7.19 (m, 2H), 7.11 (d, *J* = 12 Hz, 1H), 6.86-6.74 (m, 5H), 5.99-5.95 (m, 1H), 5.28 (d, *J* = 12 Hz, 2H), 3.82 (s, 3H), 3.79 (s, 3H), 3.56 (d, *J* = 5.2 Hz, 1H), 3.09 (td, *J* = 4.8, 5.2 Hz, 4H), 2.84-2.78 (m, 2H), 2.56-2.50 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 151.4, 150.7, 149.7, 129.0, 124.9, 124.4, 122.7, 121.8, 119.6, 116.1, 111.1, 110.4, 63.7, 61.2, 56.1, 55.8, 49.6, 48.3. ESI-MS: *m/z* 367 $[M+H]^+$. Chiral HPLC conditions: Chiralcel OD-H, 25 °C, flow rate: 1.0 mL/min, hexane/isopropanol: 85/15, 254 nm, 9.60 min (*major*), 16.80 min (*minor*).

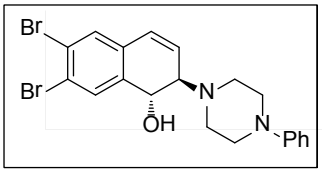


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	9.602	BB	0.4356	1.94741e4	665.09131	51.5111
2	16.797	BBA	1.1537	1.83316e4	228.55994	48.4889

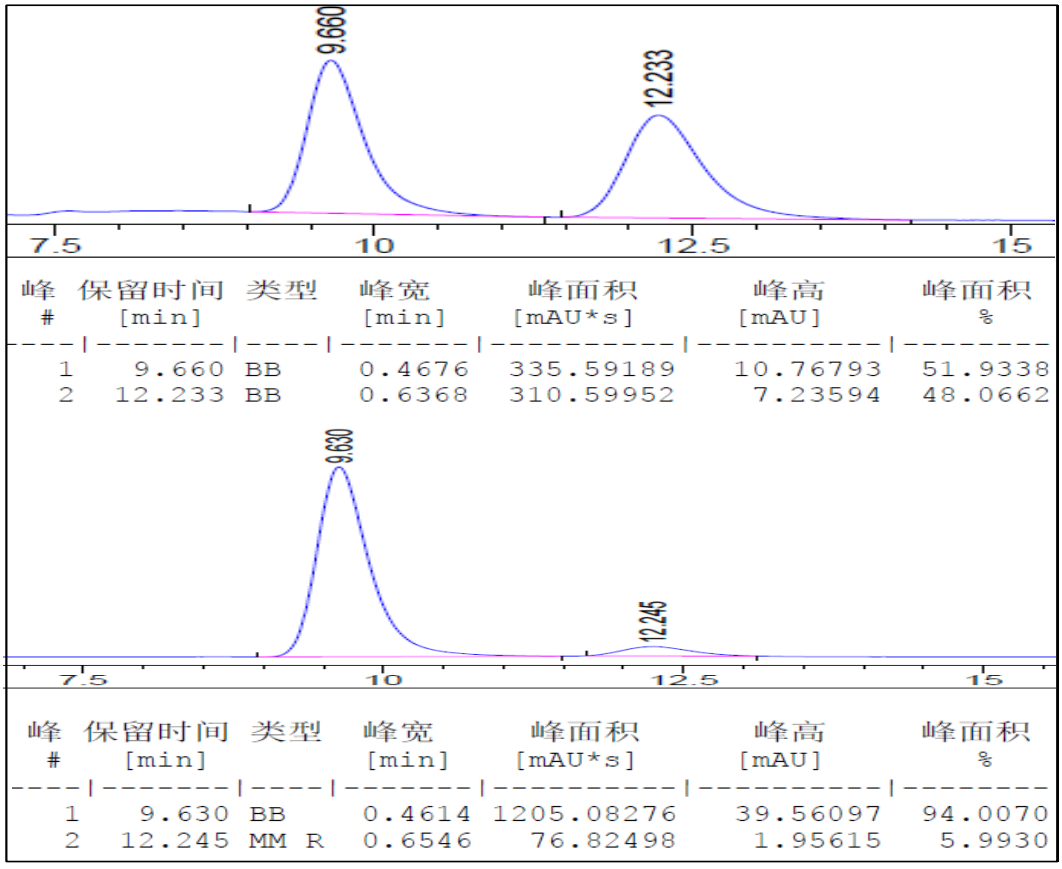


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	9.504	VB	0.4341	4.44619e4	1525.34045	96.4538
2	18.204	MM R	1.1353	1634.66174	23.99658	3.5462

Table 2, Entry 11



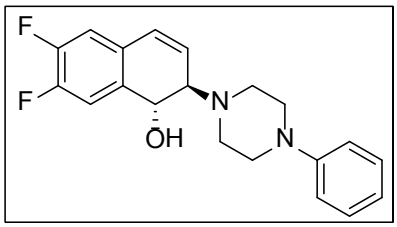
(1*R*, 2*R*)-6, 7-dibromo-2-(4-phenylpiperazin-1-yl)-1, 2-dihydronaphthalen-1-ol (5ca): White solid (95% yield); 88% *ee*; $[\alpha]_D^{27}$ = -172.55° (c = 0.26, $CHCl_3$); ^{1}H NMR (400MHz, $CDCl_3$) δ 7.41-7.44 (m, 1H), 7.26-7.31 (m, 2H), 6.96 (d, *J* = 8.0 Hz, 2H), 6.88-6.91 (m, 2H), 6.45 (dd, *J* = 9.9 Hz, *J* = 2.7 Hz, 1H), 6.19 (dd, *J* = 9.9 Hz, *J* = 1.8 Hz, 1H), 4.84 (d, *J* = 12.5 Hz, 1H), 3.49 (td, *J* = 2.5 Hz, *J* = 11.5 Hz, 1H), 3.41 (s, 1H), 3.21-3.30 (m, 4H), 2.99-3.03 (m, 2H), 2.70-2.74 (m, 2H); ^{13}C NMR (100MHz, $CDCl_3$) δ 150.1, 147.4, 128.1, 126.7, 124.3, 124.2, 119.1, 115.3, 114.0, 113.8, 113.4, 113.3, 66.3, 66.1, 48.8, 48.0. ESI-MS: *m/z* 463 $[M+H]^+$. Chiral HPLC conditions: Chiralcel OD-H, 25 °C, flow rate: 1.0 mL/min, hexane/isopropanol: 90/10, 254 nm, 9.66 min (*major*), 12.23 min (*minor*).



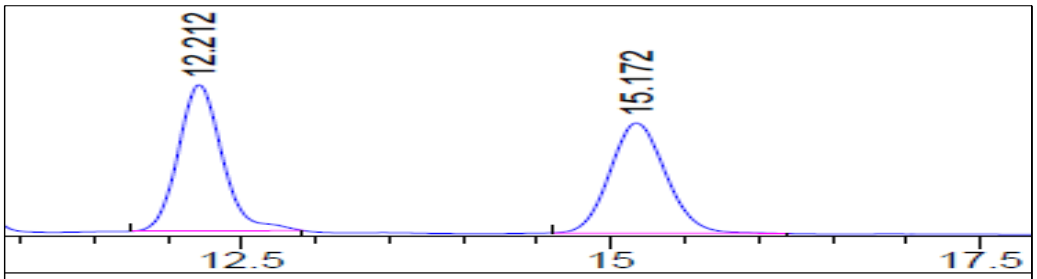
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	9.660	BB	0.4676	335.59189	10.76793	51.9338
2	12.233	BB	0.6368	310.59952	7.23594	48.0662

峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	9.630	BB	0.4614	1205.08276	39.56097	94.0070
2	12.245	MM R	0.6546	76.82498	1.95615	5.9930

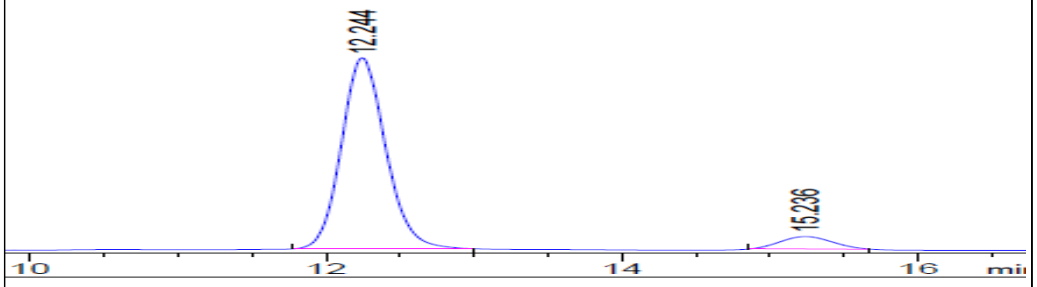
Table 2, Entry 12



(1*R*, 2*R*)-6, 7-difluoro-2-(4-phenylpiperazin-1-yl)-1, 2-dihydronaphthalen-1-ol (5da): White solid (97% yield); 86% *ee*; $[\alpha]_D^{27}$ = -72.55° (c = 0.28, $CHCl_3$); ^{19}F NMR (376 MHz, $CDCl_3$) δ -138.43, -140.87; ^{1}H NMR (400MHz, $CDCl_3$) δ 7.41-7.44 (m, 1H), 7.26-7.31 (m, 2H), 6.88-6.96 (m, 4H), 6.45 (dd, *J* = 2.7 Hz, *J* = 9.9 Hz, 1H), 6.19 (dd, *J* = 1.8 Hz, *J* = 9.9 Hz, 1H), 4.84 (d, *J* = 12.5 Hz, 1H), 3.48 (td, *J* = 2.5 Hz, *J* = 11.5 Hz, 1H), 3.41 (br, 1H), 3.21-3.30 (m, 4H), 2.99-3.03 (m, 2H), 2.70-2.74 (m, 2H); ^{13}C NMR (100MHz, $CDCl_3$) δ 151.39, 148.65, 129.39, 127.94, 125.53, 125.52, 120.32, 116.54, 115.22, 115.08, 114.67, 114.52, 67.57, 67.33, 50.05, 49.29. ESI-MS: *m/z* 343 $[M+H]^+$. Chiral HPLC conditions: Chiralcel OD-H, 25 °C, flow rate: 1.0 mL/min, hexane/isopropanol: 90/10, 254 nm, 12.21 min (*major*), 15.17 min (*minor*).

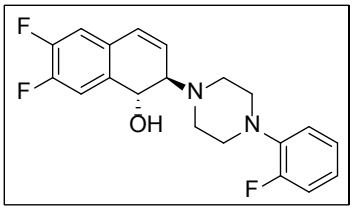


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	12.212	MM R	0.3444	397.65598	19.24551	50.9773
2	15.172	MM R	0.4386	382.40826	14.53155	49.0227



峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	12.244	MM R	0.3457	1932.72168	93.18774	93.0099
2	15.236	MM R	0.4002	145.25226	6.04981	6.9901

Table 2, Entry 13



(1*R*, 2*R*)-6, 7-difluoro-2-(4-(2-fluorophenyl)piperazin-1-yl)-1, 2-dihydronaphthalen-1-ol (5db): White solid (96% yield); 86% *ee*; $[\alpha]_D^{27}$ = -113.03° (c = 0.73, $CHCl_3$); ^{19}F NMR (376 MHz, $CDCl_3$) δ -122.91, -138.47, -140.86; ^1H NMR (400MHz, $CDCl_3$) δ 7.40-7.44 (m, 1H), 7.02-7.10 (m, 2H), 6.91-6.99 (m, 2H), 6.87-6.89 (m, 1H), 6.44 (dd, *J* = 2.7 Hz, *J* = 10.0 Hz, 1H), 6.22 (dd, *J* = 1.9 Hz, *J* = 10.0 Hz, 1H), 4.84 (d, *J* = 12.5 Hz, 1H), 3.48 (td, *J* = 2.5 Hz, *J* = 11.5 Hz, 1H), 3.43 (br, 1H), 3.12-3.21 (m, 4H), 3.00-3.04 (m, 2H), 2.72-2.76 (m, 2H); ^{13}C NMR (100MHz, $CDCl_3$) δ 156.92, 154.96, 150.73(dd, *J* = 13.0Hz, *J* = 23.4Hz), 148.76(dd, *J* = 13.0Hz, *J* = 21.0Hz), 140.11(d, *J* = 8.64Hz), 134.37 (dd, *J* = 3.7Hz, *J* = 5.7Hz), 128.69 (dd, *J* = 4.0Hz, *J* = 6.3Hz), 127.87, 125.73 (d, *J* = 2.5Hz), 124.71 (d, *J* = 3.6Hz), 122.93 (d, *J* = 7.9Hzz), 119.21 (d, *J* = 3.0Hz), 116.337 (d, *J* = 20.8Hz), 114.84 (dd, *J* = 18.60Hz, *J* = 70.1Hz), 67.56, 67.27, 51.26 (d, *J* = 3.2Hz), 49.32. ESI-MS: *m/z* 361 $[M+H]^+$. Chiral HPLC conditions: Chiralcel OD-H, 25 °C, flow rate: 1.0 mL/min, hexane/isopropanol: 90/10, 254 nm, 8.10 min (*major*), 9.77 min (*minor*).

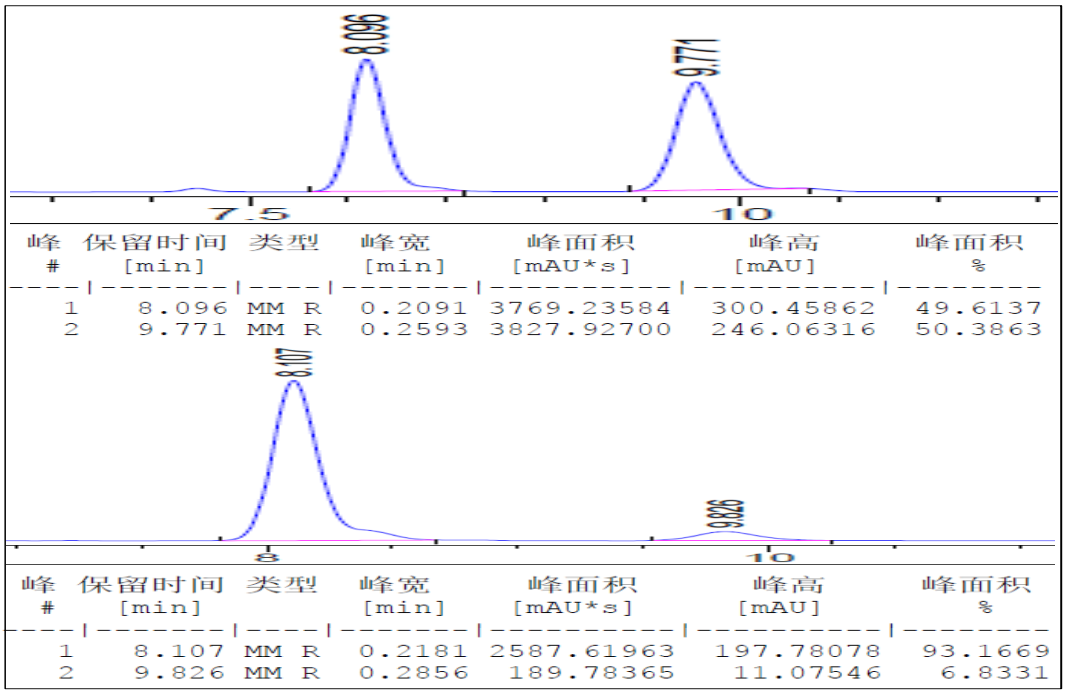
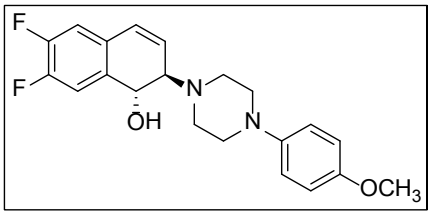
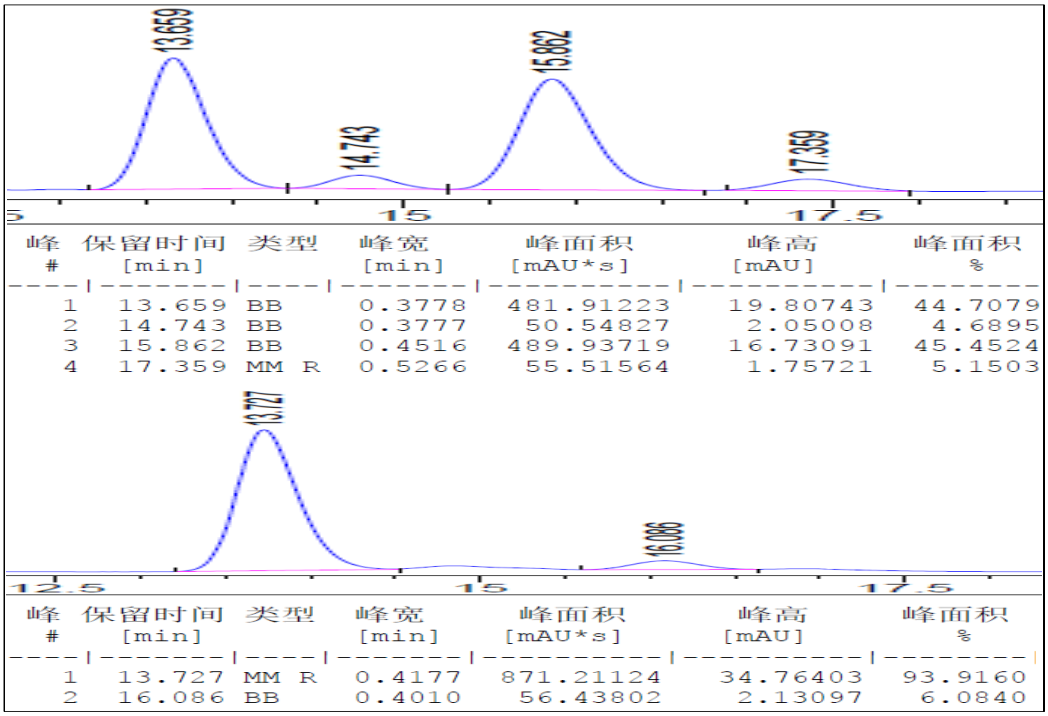


Table 2, Entry 14



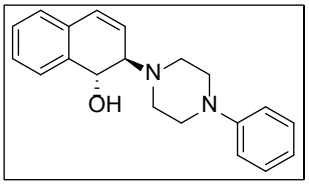
(1*R*, 2*R*)-6, 7-difluoro-2-(4-(4-methoxyphenyl)-piperazin-1-yl)-1, 2-dihydronaphthalen-1-ol (5dc): White solid (98% yield); 88% *ee*; $[\alpha]_D^{27}$ = -113.86° (c = 0.89, $CHCl_3$); ^{19}F NMR (376 MHz, $CDCl_3$) δ -138.47, -140.88; ^1H NMR (400MHz, $CDCl_3$) δ 7.31-7.35 (m, 1H), 6.76-6.85 (m, 5H), 6.35 (dd, *J* = 2.6 Hz, *J* = 10.0 Hz, 1H), 6.11 (dd, *J* = 1.7 Hz, *J* = 10.0 Hz, 1H), 4.74 (d, *J* = 12.5 Hz, 1H), 3.69 (s, 3H), 3.40 (td, *J* = 2.5 Hz, *J* = 11.5 Hz, 1H), 3.37 (br, 1H), 3.00-3.10 (m, 4H), 2.88-2.93 (m, 2H), 2.60-2.65 (m, 2H); ^{13}C NMR (100MHz, $CDCl_3$) δ 154.20, 150.93(dd, *J* = 13.0Hz, *J* = 19.2Hz), 148.47(dd, *J* = 12.7Hz, *J* = 16.6Hz), 145.67, 134.36 (dd, *J* = 3.7Hz, *J* = 5.4Hz), 128.66 (dd, *J* = 3.9Hz, *J* = 6.2Hz), 127.84, 125.64, 118.60, 115.09 (d, *J* = 18.1Hz), 114.63, 114.44, 67.42, 67.24, 55.72, 51.43, 49.28. ESI-MS: *m/z* 373 [M +H]$^+$. Chiral HPLC conditions: OD-H, 25 °C, flow rate: 1.0 mL/min, hexane/isopropanol: 90/10, 254 nm, 13.66 min (*major*), 15.86 min (*minor*).



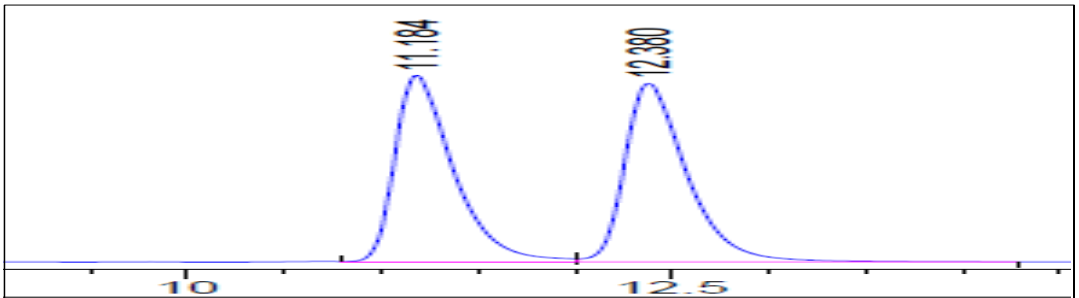
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	13.659	BB	0.3778	481.91223	19.80743	44.7079
2	14.743	BB	0.3777	50.54827	2.05008	4.6895
3	15.862	BB	0.4516	489.93719	16.73091	45.4524
4	17.359	MM R	0.5266	55.51564	1.75721	5.1503

峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	13.727	MM R	0.4177	871.21124	34.76403	93.9160
2	16.086	BB	0.4010	56.43802	2.13097	6.0840

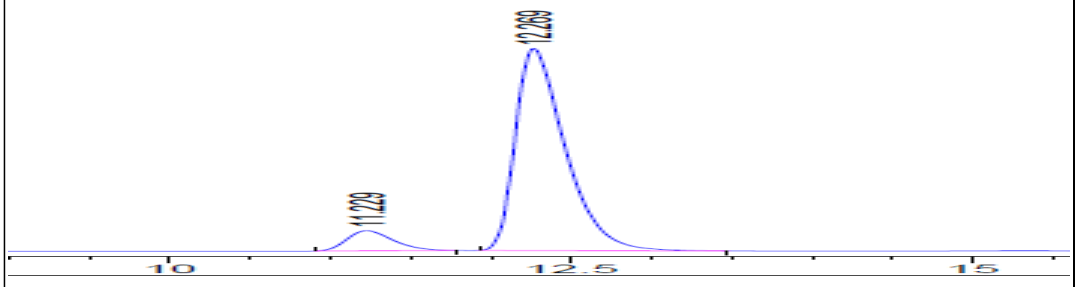
Table 2, Entry 15



(1*R*, 2*R*)-2-(4-phenylpiperazin-1-yl)-1, 2-dihydronaphthalen-1-ol (5ea): White solid (93% yield); 83% *ee*; $[\alpha]_D^{27}$ = -158.92° (c = 0.53, $CHCl_3$); ^1H NMR (400MHz, $CDCl_3$) δ 7.50 (d, J = 7.1 Hz, 1H), 7.14-7.21 (m, 4H), 6.99-7.01 (m, 1H), 6.77-6.86 (m, 3H), 6.47 (dd, J = 2.5 Hz, J = 9.9 Hz, 1H), 6.04 (dd, J = 2.5 Hz, J = 9.9 Hz, 1H), 4.84 (d, J = 11.6 Hz, 1H), 3.45 (td, J = 2.5 Hz, J = 11.5 Hz, 1H), 3.28 (br, 1H), 3.08-3.19 (m, 4H), 2.85-3.08 (m, 2H), 2.60-2.65 (m, 2H); ^{13}C NMR (100MHz, $CDCl_3$) δ 151.42, 137.17, 131.91, 129.60, 129.32, 128.09, 127.65, 126.40, 124.97, 124.58, 120.13, 116.43, 67.91, 67.62 (d, J = 2.9 Hz), 49.98, 49.13; ESI-MS: *m/z* 307 $[M+H]^+$. Chiral HPLC conditions: Chiralcel OD-H, 25 °C, flow rate: 1.0 mL/min, hexane/isopropanol: 90/10, 254 nm, 11.18 min (*minor*), 12.38 min (*major*).

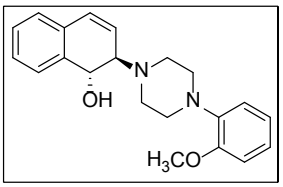


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	11.184	VV	0.3154	5341.83252	253.98758	49.7077
2	12.380	VB	0.3375	5404.65918	242.98349	50.2923



峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	11.229	MM R	0.3324	801.20343	40.17772	8.4802
2	12.269	MM R	0.3598	8646.75000	400.54092	91.5198

Table 2, Entry 16



(1*R*, 2*R*)-2-(4-(2-methoxyphenylpiperazin-1-yl)-1, 2-dihydro-naphthalen-1-ol (5eb): White solid (95% yield); 85% *ee*; $[\alpha]_D^{27}$ = -131.84° (c = 0.57, $CHCl_3$); ^1H NMR (400MHz, $CDCl_3$) δ 7.50 (d, J = 7.1 Hz, 1H), 7.12-7.20 (m, 2H), 6.98-7.00 (m, 1H), 6.90-6.94 (m, 1H), 6.81-6.87 (m, 2H), 6.76-6.78 (m, 1H), 6.46 (dd, J = 2.5 Hz, J = 9.9 Hz, 1H), 6.09 (dd, J = 2.5 Hz, J = 9.9 Hz, 1H), 4.84 (d, J = 11.5 Hz, 1H), 3.77 (s, 3H), 3.70 (s, 1H), 3.42 (td, J = 2.5 Hz, J = 11.5 Hz, 1H), 2.89-3.03 (m, 6H), 2.64-2.69 (m, 2H); ^{13}C NMR (100MHz, $CDCl_3$) δ 152.31, 141.23, 137.21, 131.92, 129.44, 127.95, 127.55, 126.31, 124.94, 124.91, 123.21, 121.11, 118.37, 112.21, 67.75, 67.55 (d, J = 2.9 Hz), 55.44 (d, J = 5.8 Hz), 51.27, 49.22; ESI-MS: *m/z* 337 $[M+H]^+$. Chiral HPLC conditions: Chiralcel OD-H, 25 °C, flow rate: 1.0 mL/min, hexane/isopropanol: 90/10, 254 nm, 10.14 min (*major*), 10.94 min (*minor*).

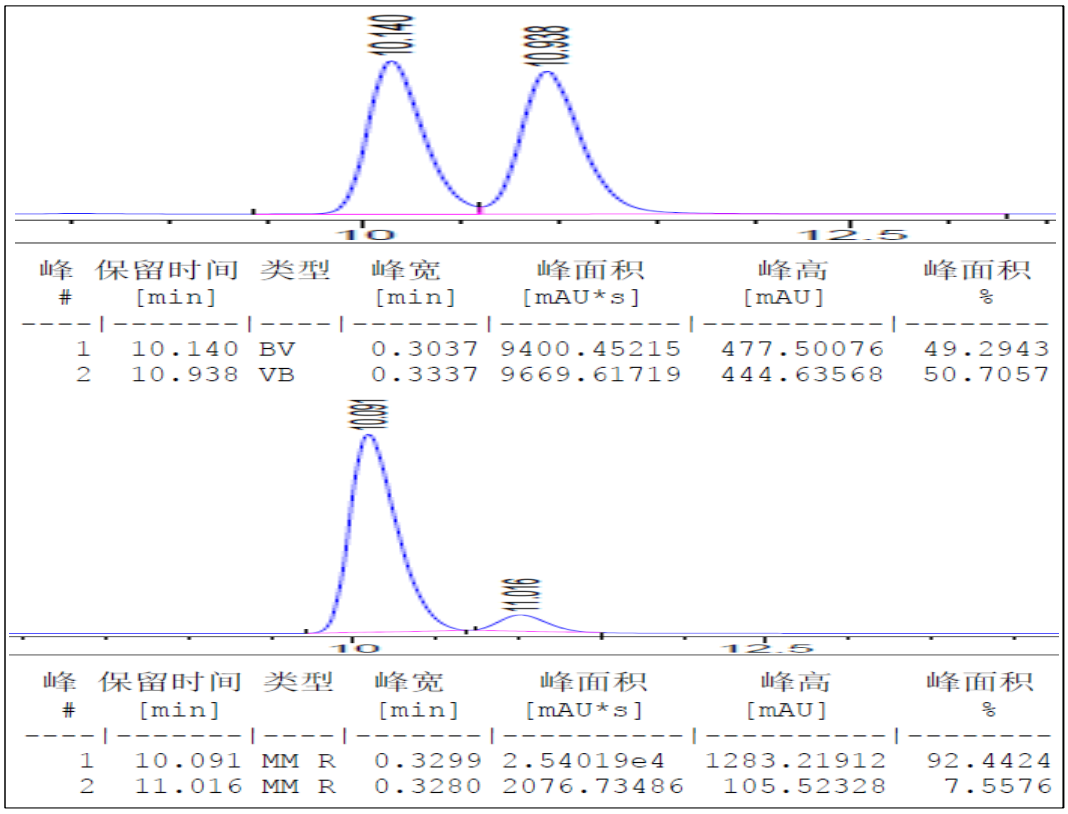
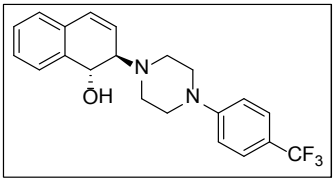
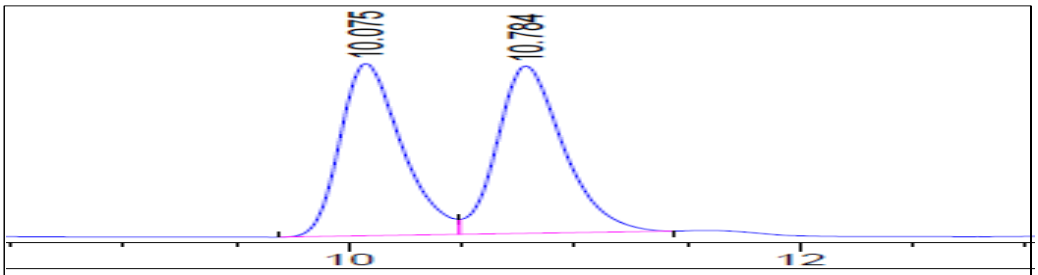


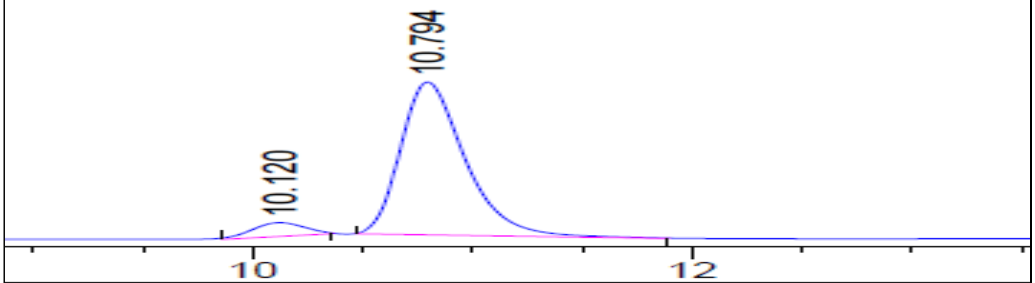
Table 2, Entry 17



(1*R*, 2*R*)-2-(4-(4-(trifluoromethyl)phenylpiperazin-1-yl)-1, 2-dihydronaphthalen-1-ol (5ec): White solid (87% yield); 86% *ee*; $[\alpha]_D^{27}$ = -161.89° (c = 0.45, $CHCl_3$); ^{19}F NMR (376 MHz, $CDCl_3$) δ -58.33; ^{1}H NMR (500MHz, $CDCl_3$) δ 7.59-7.61 (m, 1H), 7.50-7.51 (m, 2H), 7.27-7.31(m, 2H), 7.11-7.12 (m, 1H), 6.94-6.96 (m, 2H), 6.59(dd, *J* = 2.4 Hz, *J* = 9.9 Hz, 1H), 6.11 (dd, *J* = 2.5 Hz, *J* = 9.9 Hz, 1H), 4.96 (d, *J* = 11.3 Hz, 1H), 3.57 (td, *J* = 2.4 Hz, *J* = 11.2 Hz, 1H), 3.33-3.37 (m, 4H), 3.27(br, 1H), 2.97-3.01 (2H, m), 2.73-2.77 (2H, m); ^{13}C NMR (125 MHz, $CDCl_3$) δ 153.41, 137.01, 131.85, 129.95, 128.27, 127.84, 126.65 (td, *J* = 3.7 Hz), 126.55, 125.98, 125.15, 124.06, 114.96, 67.99, 67.78, 48.97, 48.80; ESI-MS: *m/z* 375 $[M+H]^+$. Chiral HPLC conditions: Chiralcel Lu-Amy lose-2, 25 °C, flow rate: 1.0 mL/min, hexane/isopropanol: 90/10, 254 nm, 10.08 min (*minor*), 10.78 min (*major*).

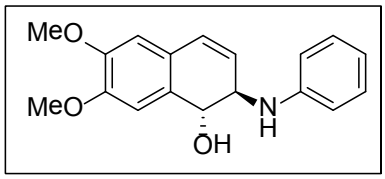


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	10.075	BV	0.2896	2076.13306	109.28251	48.9538
2	10.784	VB	0.3099	2164.87354	106.15694	51.0462

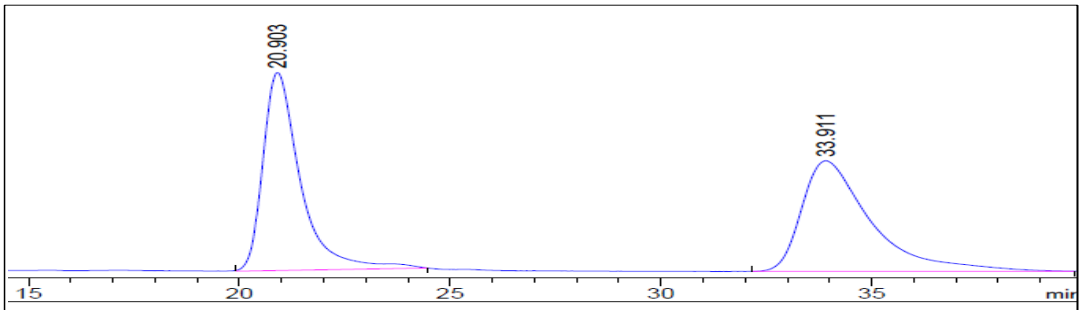


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	10.120	MM R	0.2764	105.17548	6.34239	6.8253
2	10.794	MM R	0.3414	1435.79480	70.10091	93.1747

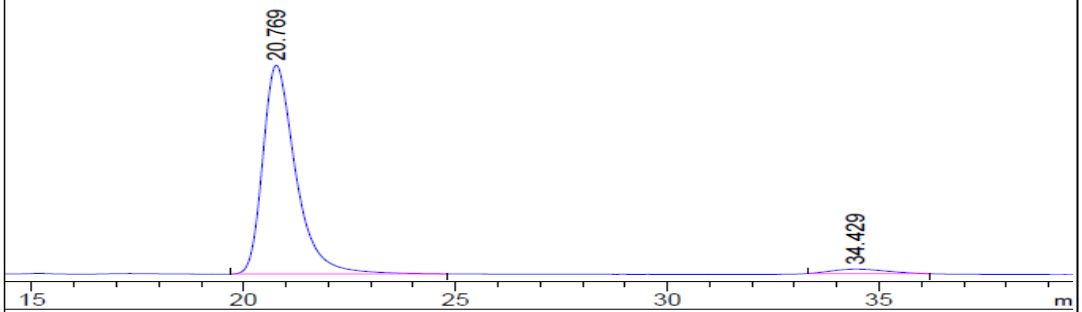
Table 3, Entry 1



(1*R*, 2*R*)-6, 7-dimethoxy-2-(phenylamino)-1, 2-dihydronaphthalen-1-ol (7aa): White solid (81% yield); 93% *ee*; $[\alpha]_D^{27}$ = -152.93° (c = 0.68, CH_2Cl_2); ^{1}H NMR (500MHz, $CDCl_3$) δ 7.18-7.26 (m, 2H), 7.03 (s, 1H), 6.69-6.78 (m, 4H), 6.48 (dd, *J* = 3.0 Hz, *J* = 9.5 Hz, 1H), 5.93 (dd, *J* = 3.4 Hz, *J* = 9.5 Hz, 1H), 4.78 (d, *J* = 7.2 Hz, 1H), 4.30 (td, *J* = 2.7 Hz, *J* = 9.8 Hz, 1H), 3.90 (s, 3H), 3.89 (s, 3H), 2.60 (br, 3H); ^{13}C NMR (125MHz, $CDCl_3$) δ 148.96, 146.80, 129.67, 128.42, 128.40, 125.90, 124.89, 118.59, 114.25, 111.00, 110.46, 110.19, 71.54, 56.27, 56.26, 55.78. ESI-MS: *m/z* 298 $[M+H]^+$. Chiral HPLC conditions: Chiralcel OD-H, 25 °C, flow rate: 1.0 mL/min, hexane/isopropanol: 90/10, 254 nm, 20.90min (*major*), 33.91 min (*minor*).

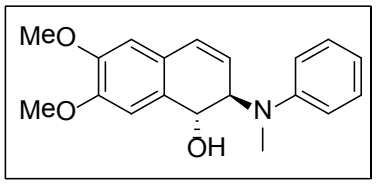


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	20.903	MM R	1.0316	1223.28296	19.76399	49.2943
2	33.911	BB	1.5054	1258.31055	11.04288	50.7057

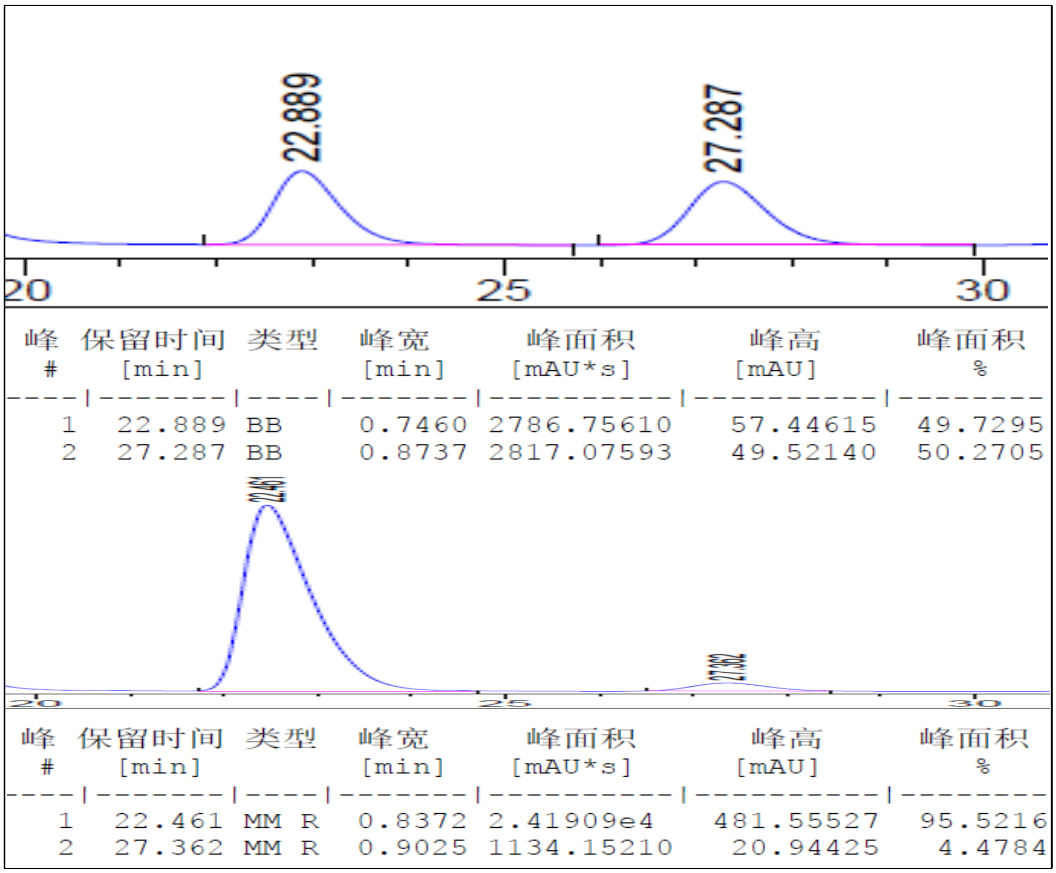


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	20.769	BB	0.8028	1453.90662	26.80604	96.5499
2	34.429	MM R	1.5076	51.95430	5.74356e-1	3.4501

Table 3, Entry 2



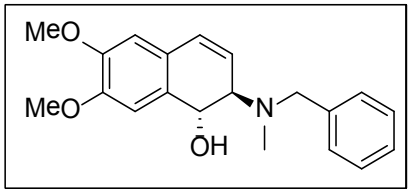
(1*R*, 2*R*)-6, 7-dimethoxy-2-(methyl(phenyl)amino)-1, 2-dihydronaphthalen-1-ol (7ab): Colorless liquid (55% yield); 93% *ee*; $[\alpha]_D^{27}$ = -146.04° (c = 0.72, CH_2Cl_2); ^{1}H NMR (500MHz, $CDCl_3$) δ 7.24-7.27 (m, 2H), 7.11 (s, 1H), 6.95-6.97 (s, 1H), 6.52 (dd, *J* = 2.5 Hz, *J* = 9.8 Hz, 1H), 5.83 (dd, *J* = 3.2 Hz, *J* = 9.7 Hz, 1H), 5.02 (d, *J* = 9.3 Hz, 1H), 4.71 (td, *J* = 2.8 Hz, *J* = 9.3 Hz, 1H), 3.89 (s, 3H), 3.88 (s, 3H), 2.81 (s, 3H), 2.65 (br, 1H); ^{13}C NMR (125MHz, $CDCl_3$) δ 150.16, 148.67, 148.37, 129.36, 129.26, 129.24, 125.66, 124.93, 117.90, 114.48, 110.17, 109.62, 70.06, 63.33, 56.04, 56.01, 33.34. ESI-MS: *m/z* 312 $[M+H]^+$. Chiral HPLC conditions: Chiralcel OD-H, 25 °C, flow rate: 1.0 mL/min, hexane/isopropanol: 90/10, 254 nm, 22.89 min (*major*), 27.29 min (*minor*).



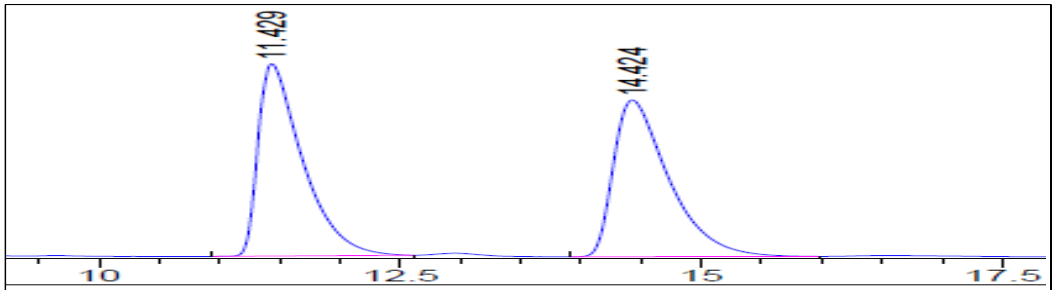
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	22.889	BB	0.7460	2786.75610	57.44615	49.7295
2	27.287	BB	0.8737	2817.07593	49.52140	50.2705

峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	22.461	MM R	0.8372	2.41909e4	481.55527	95.5216
2	27.362	MM R	0.9025	1134.15210	20.94425	4.4784

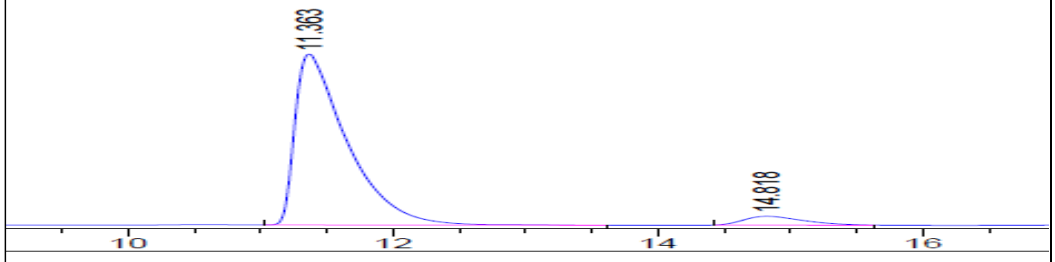
Table 3, Entry 4



(1*R*, 2*R*)-2-(benzyl(methyl)amino)-6, 7-dimethoxy-1, 2-dihydronaphthalen-1-ol (7ac): Colorless liquid (95% yield); 89% *ee*; $[\alpha]_D^{27}$ = -172.39° (c = 0.62, CH_2Cl_2); ^{1}H NMR (500MHz, $CDCl_3$) δ 7.24-7.32 (m, 5H), 7.14 (s, 1H), 6.63 (s, 1H), 6.47 (dd, *J* = 2.6 Hz, *J* = 9.9 Hz, 1H), 6.04 (dd, *J* = 2.4 Hz, *J* = 9.9 Hz, 1H), 4.88 (d, *J* = 12.0 Hz, 1H), 3.92 (s, 3H), 3.86 (s, 3H), 3.83 (s, 1H), 3.56-3.60 (m, 2H), 3.35 (br, 1H), 2.33 (s, 3H); ^{13}C NMR (125MHz, $CDCl_3$) δ 148.72, 148.04, 139.09, 130.14, 129.19, 129.02, 128.60, 127.39, 124.80, 123.14, 110.13, 108.59, 68.87, 66.70, 58.93, 56.20, 56.18, 38.12. ESI-MS: *m/z* 326 $[M+H]^+$. Chiral HPLC conditions: Chiralcel OD-H, 25 °C, flow rate: 1.0 mL/min, hexane/isopropanol: 85/15, 254 nm, 11.43 min (*major*), 14.42 min (*minor*).

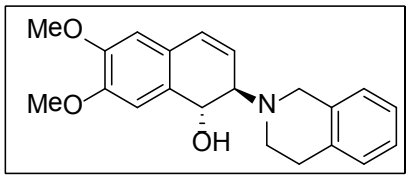


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	11.429	BB	0.3820	3123.69312	121.46868	49.6938
2	14.424	BB	0.4807	3162.18433	98.97977	50.3062

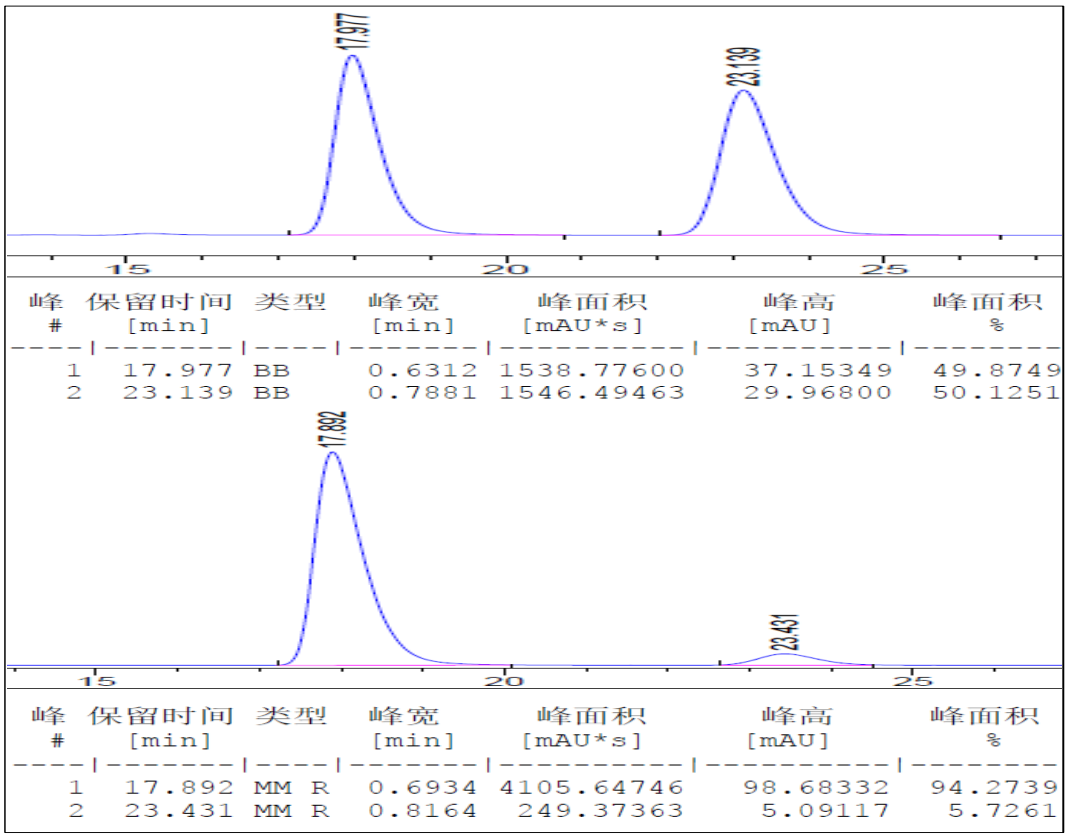


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	11.363	BB	0.3984	7280.04883	266.75061	94.4102
2	14.818	MM R	0.5200	431.03433	13.81604	5.5898

Table 3, Entry 5



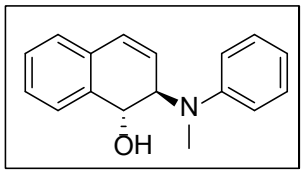
(1*R*, 2*R*)-2-(3,4-dihydroisoquinolin-2(1H)-yl)-6, 7-dimethoxy-1, 2-dihydronaphthalen-1-ol (7ad): Colorless liquid (93% yield); 89% *ee*; $[\alpha]_D^{27}$ = -163.7° (c = 0.83, CH_2Cl_2); ^{1}H NMR (500MHz, $CDCl_3$) δ 7.05-7.09 (m, 4H), 6.94-6.96 (m, 1H), 6.58 (s, 1H), 6.41 (dd, *J* = 2.5 Hz, *J* = 9.9 Hz, 1H), 5.96 (dd, *J* = 2.5 Hz, *J* = 9.9 Hz, 1H), 4.87 (d, *J* = 11.9 Hz, 1H), 3.91 (d, *J* = 14.9 Hz, 1H), 3.85 (s, 3H), 3.80 (s, 3H), 3.71 (d, *J* = 14.9 Hz, 1H), 3.53 (td, *J* = 2.5 Hz, *J* = 11.9 Hz, 1H), 3.32 (br, 1H), 3.03-3.05 (m, 1H), 2.83-2.87 (m, 2H), 2.70-2.74 (m, 1H); ^{13}C NMR (125MHz, $CDCl_3$) δ 148.80, 148.12, 134.98, 134.61, 130.12, 129.33, 128.98, 126.84, 126.40, 125.89, 124.77, 122.68, 110.16, 108.72, 68.29, 68.08, 56.23, 56.21, 52.18, 47.22, 30.12. ESI-MS: *m/z* 338 $[M+H]^+$. Chiral HPLC conditions: Chiralcel OD-H, 25 °C, flow rate: 1.0 mL/min, hexane/isopropanol: 85/15, 254 nm, 17.98 min (*major*), 23.14 min (*minor*).



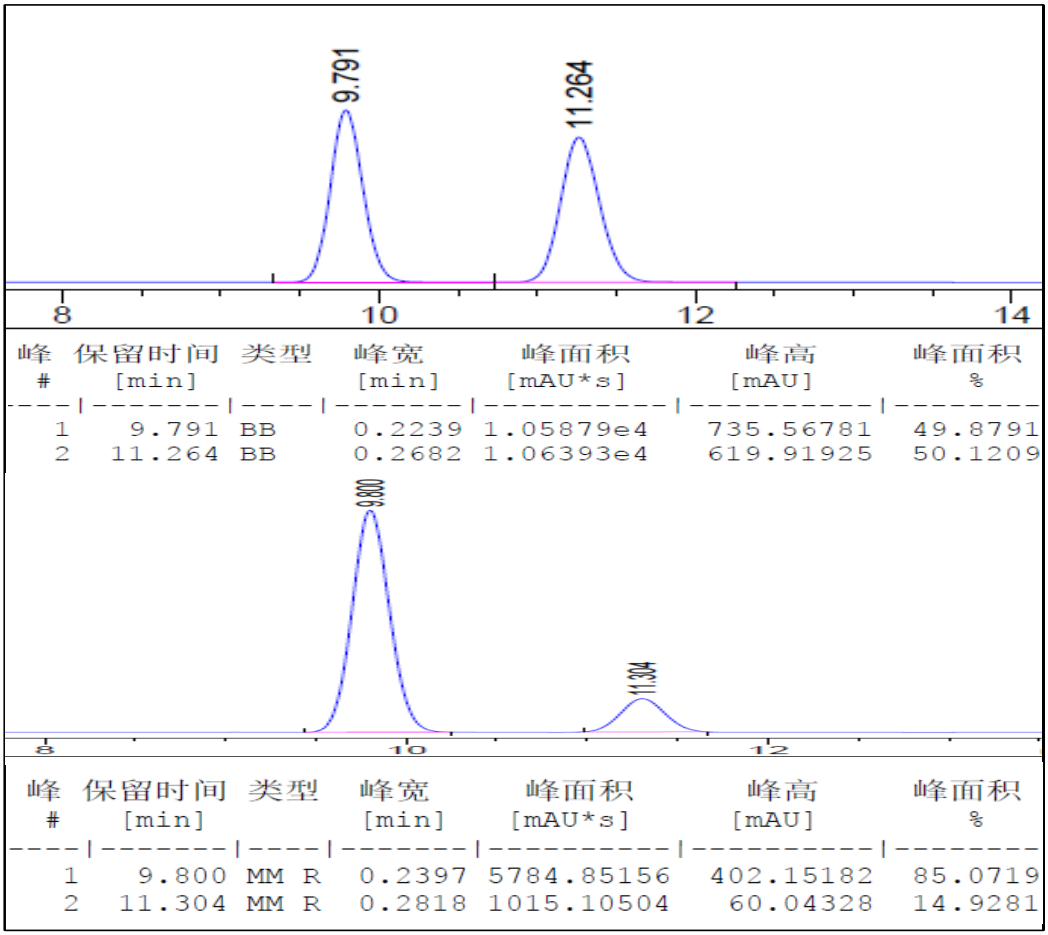
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	17.977	BB	0.6312	1538.77600	37.15349	49.8749
2	23.139	BB	0.7881	1546.49463	29.96800	50.1251

峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	17.892	MM R	0.6934	4105.64746	98.68332	94.2739
2	23.431	MM R	0.8164	249.37363	5.09117	5.7261

Table 3, Entry 7



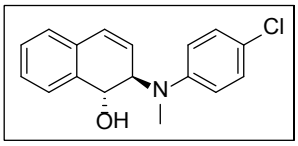
(1*R*, 2*R*)-2-[methyl(phenyl)amino]-1,2-dihydronaphthalen-1-ol (7ca): Colorless liquid (95% yield); 70% *ee*; $[\alpha]_D^{27}$ = -112.93° (c = 0.72, CH_2Cl_2); ^{1}H NMR (500MHz, $CDCl_3$) δ 7.52-7.54 (m, 1H), 7.22-7.27 (m, 4H), 7.09-7.11 (m, 1H), 6.94-6.95 (m, 1H), 6.77-6.80 (m, 1H), 6.57 (dd, *J* = 2.5 Hz, *J* = 9.8 Hz, 1H), 5.91 (dd, *J* = 3.0 Hz, *J* = 9.8 Hz, 1H), 5.08 (d, *J* = 9.8 Hz, 1H), 4.72 (td, *J* = 2.7 Hz, *J* = 9.8 Hz, 1H), 2.83 (s, 3H), 2.38 (s, 1H); ^{13}C NMR (125MHz, $CDCl_3$) δ 150.44, 136.72, 132.16, 129.86, 129.46, 128.29, 128.13, 127.95, 126.65, 125.80, 118.29, 114.85, 70.27, 63.70, 33.56. ESI-MS: *m/z* 252 $[M+H]^+$. Chiral HPLC conditions: Chiralcel AD-H, 25 °C, flow rate: 1.0 mL/min, hexane/isopropanol: 90/10, 254 nm, 9.79 min (*major*), 11.26 min (*minor*).



峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	9.791	BB	0.2239	1.05879e4	735.56781	49.8791
2	11.264	BB	0.2682	1.06393e4	619.91925	50.1209

峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	9.800	MM R	0.2397	5784.85156	402.15182	85.0719
2	11.304	MM R	0.2818	1015.10504	60.04328	14.9281

Table 3, Entry 8



(1*R*, 2*R*)-2-((4-chlorophenyl)(methyl)amino)-1,2-dihydro-naphthalen-1-ol (7cb): White solid (91% yield); 77% *ee*; $[\alpha]_D^{27}$ = -112.04° (c = 0.82, CH_2Cl_2); ^{1}H NMR (500MHz, $CDCl_3$) δ 7.53-7.54 (m, 1H), 7.29-7.31 (m, 2H), 7.20-7.22 (m, 2H), 7.14-7.16 (m, 1H), 6.86-6.88 (m, 2H), 6.63 (dd, *J* = 2.5 Hz, *J* = 9.8 Hz, 1H), 5.91 (dd, *J* = 3.1 Hz, *J* = 9.8 Hz, 1H), 5.08 (d, *J* = 9.5 Hz, 1H), 4.68 (td, *J* = 2.8 Hz, *J* = 9.5 Hz, 1H), 2.82 (s, 3H), 2.38 (s, 1H); ^{13}C NMR (125MHz, $CDCl_3$) δ 148.82, 136.37, 131.91, 129.93, 129.04, 128.24, 128.12, 127.32, 126.61, 125.73, 122.81, 115.67, 70.12, 63.57, 33.53. ESI-MS: *m/z* 286 $[M+H]^+$. Chiral HPLC conditions: Chiralcel AD-H, 25 °C, flow rate: 1.0 mL/min, hexane/isopropanol: 90/10, 254 nm, 11.08 min (*major*), 13.04 min (*minor*).

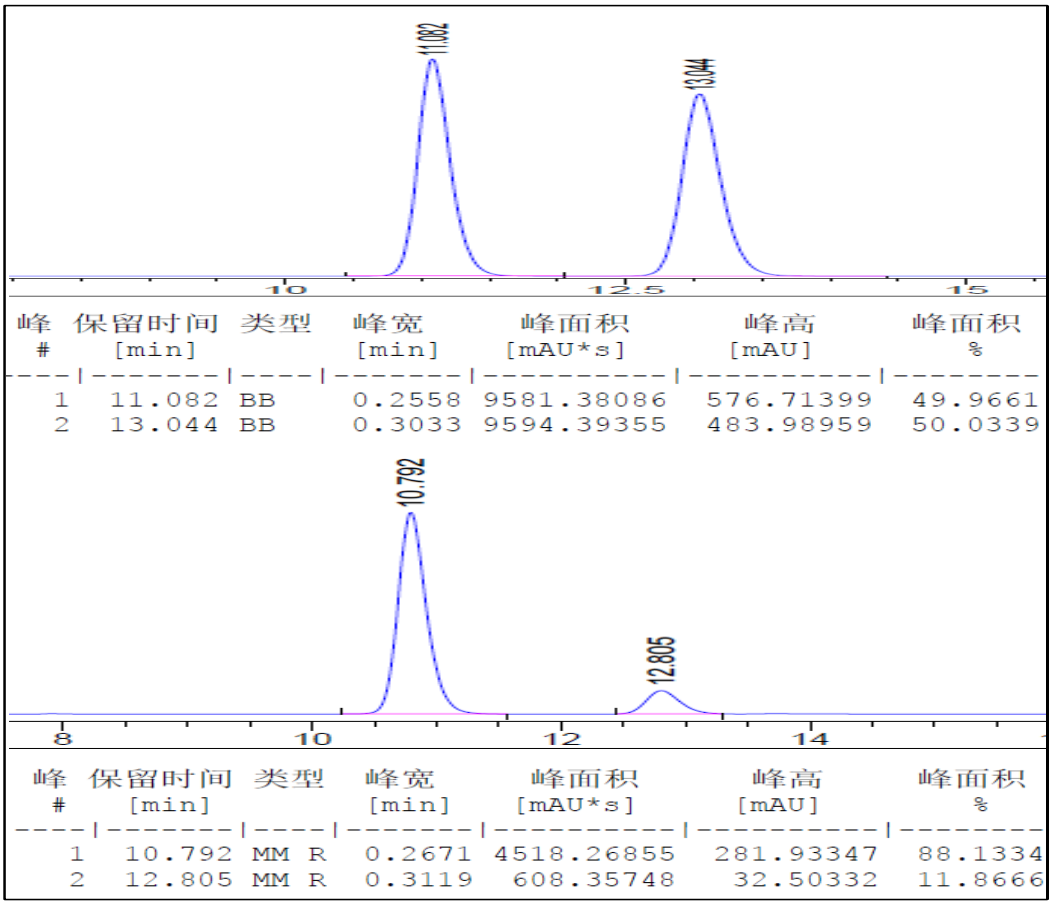
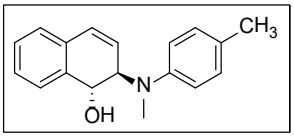
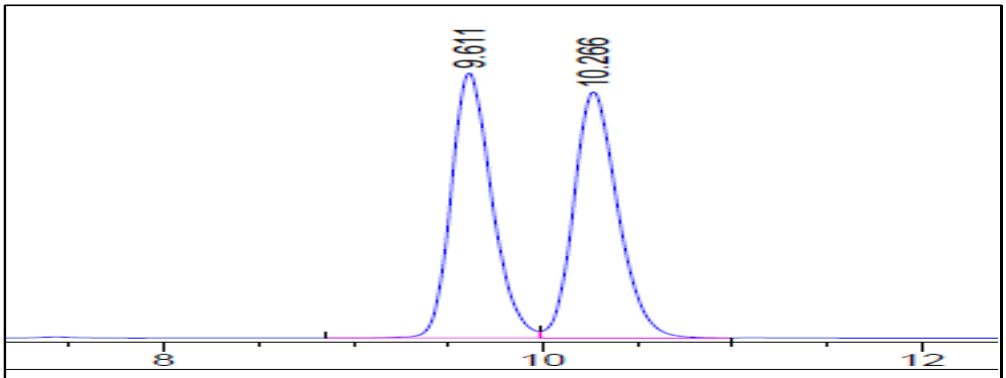


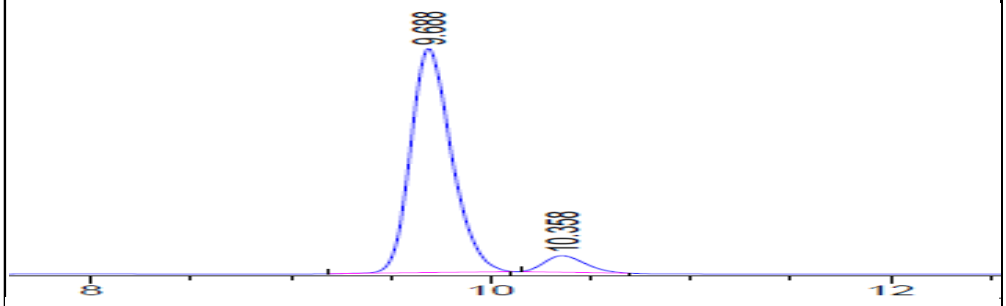
Table 3, Entry 9



(1*R*, 2*R*)-2-(methyl(p-tolyl)amino)-1,2-dihydronaphthalen-1-ol (7cc): Colorless liquid (95% yield); 87% *ee*; $[\alpha]_D^{27}$ = -132.39° (c = 0.62, CH_2Cl_2); ^{1}H NMR (500MHz, $CDCl_3$) δ 7.58-7.60 (m, 1H), 7.27-7.31 (m, 2H), 7.10-7.15 (m, 3H), 6.91-6.93 (m, 2H), 6.60 (dd, *J* = 2.5 Hz, *J* = 9.8 Hz, 1H), 5.96 (dd, *J* = 2.9 Hz, *J* = 9.8 Hz, 1H), 5.13 (d, *J* = 10.1 Hz, 1H), 4.69 (td, *J* = 2.7 Hz, *J* = 10.1 Hz, 1H), 2.85 (s, 3H), 2.51 (s, 1H), 2.31 (s, 3H); ^{13}C NMR (125MHz, $CDCl_3$) δ 148.41, 136.83, 132.19, 129.96, 129.77, 128.22, 128.02, 127.92, 126.59, 125.64, 115.50, 70.11, 64.36, 33.71, 20.47. ESI-MS: *m/z* 266 $[M+H]^+$. Chiral HPLC conditions: Chiralcel AD-H, 25 °C, flow rate: 1.0 mL/min, hexane/isopropanol: 90/10, 254 nm, 9.61 min (*major*), 10.27 min (*minor*).

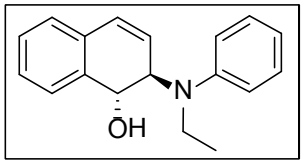


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	9.611	BV	0.2301	1.02606e4	687.48340	49.9288
2	10.266	VB	0.2481	1.02899e4	638.33307	50.0712

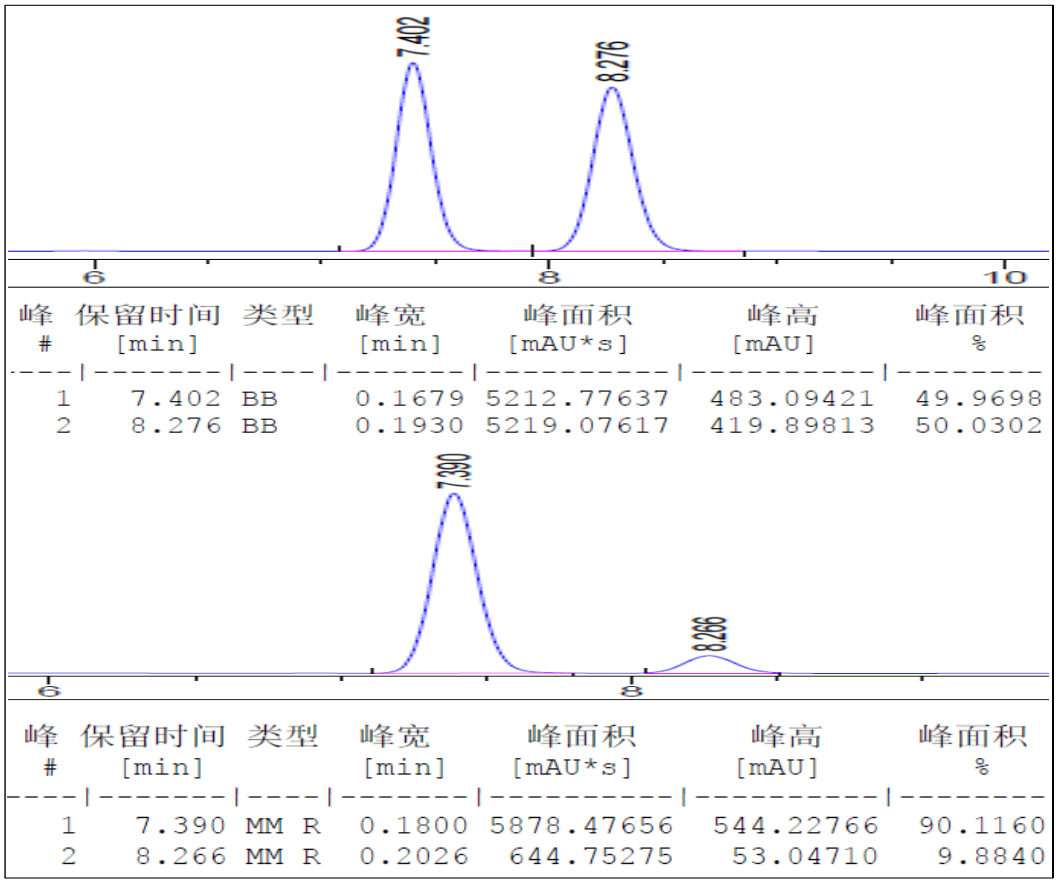


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	9.688	MM R	0.2374	1.68046e4	1180.01733	93.2048
2	10.358	MM R	0.2346	1225.15625	87.04253	6.7952

Table 3, Entry 10

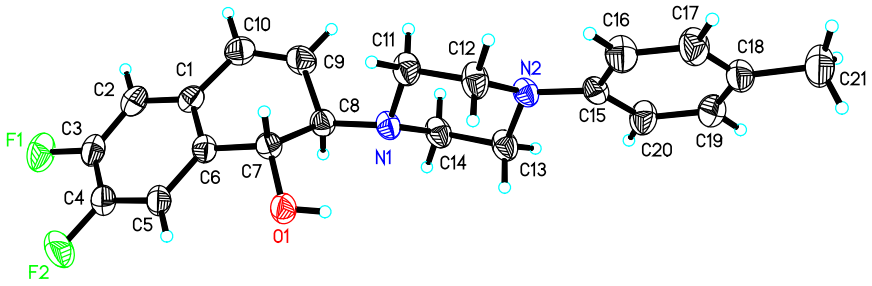


(1*R*, 2*R*)-2-(ethyl(phenyl)amino)-1, 2-dihydronaphthalen-1-ol (7cd): Colorless liquid (91% yield); 80% *ee*; $[\alpha]_D^{27}$ = -160.7° (c = 0.85, CH_2Cl_2); ^{1}H NMR (500MHz, $CDCl_3$) δ 7.56-7.58 (m, 1H), 7.28-7.33 (m, 4H), 7.16-7.18 (m, 1H), 6.99-7.00 (m, 2H), 6.81-6.84 (m, 1H), 6.64 (dd, *J* = 2.4 Hz, *J* = 9.8 Hz, 1H), 6.00 (dd, *J* = 3.2 Hz, *J* = 9.8 Hz, 1H), 5.15 (d, *J* = 9.8 Hz, 1H), 4.71 (td, *J* = 2.8 Hz, *J* = 9.2 Hz, 1H), 3.39 (q, *J* = 7.0 Hz, 2H), 2.47 (s, 1H), 5.15 (t, *J* = 7.08 Hz, 3H); ^{13}C NMR (125MHz, $CDCl_3$) δ 148.40, 136.57, 132.16, 129.61, 129.48, 128.81, 128.24, 128.21, 126.71, 126.19, 117.80, 114.95, 70.47, 63.39, 41.72, 14.67. ESI-MS: *m/z* 266 $[M+H]^+$. Chiral HPLC conditions: Chiralcel OD-H, 25 °C, flow rate: 1.0 mL/min, hexane/isopropanol: 90/10, 254 nm, 7.40 min (*major*), 8.28 min (*minor*).



峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	7.402	BB	0.1679	5212.77637	483.09421	49.9698
2	8.276	BB	0.1930	5219.07617	419.89813	50.0302

峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	7.390	MM R	0.1800	5878.47656	544.22766	90.1160
2	8.266	MM R	0.2026	644.75275	53.04710	9.8840



Scheme 4 The X-ray structure of the chiral **5ae** (the absolute configuration of the chiral center in **5ae** is *R,R*)

Table 4 *Crystal data*

$C_{23}H_{25}F_3N_2O_3$	$F(000) = 456$
$M_r = 434.45$	?
Triclinic, $P\bar{1}$	$D_x = 1.360$ Mg m^{-3}
Hall symbol: ?	Melting point: ? K
$a = 9.2387$ (9) Å	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
$b = 11.4941$ (11) Å	Cell parameters from 1996 reflections
$c = 11.8575$ (11) Å	$\theta = 5.1$–$47.6°$
$\alpha = 64.434$ (2)°	$\mu = 0.11$ mm^{-1}
$\beta = 69.340$ (2)°	$T = 293$ K
$\gamma = 84.039$ (2)°	Prismatic, colorless
$V = 1061.07$ (18) Å^3	0.25 × 0.18 × 0.12 mm
$Z = 2$	

Table 5 *Data collection*

CCD area detector diffractometer	5183 independent reflections
Radiation source: fine-focus sealed tube	4224 reflections with $I > 2\sigma(I)$
Graphite monochromator	$R_{int} = 0.024$
Detector resolution: ? pixels mm^{-1}	$\theta_{max} = 26.0°$, $\theta_{min} = 2.0°$
phi and ω scans	$h = 8$-11
Absorption correction: empirical (using intensity measurements) sadabs	$k = 13$-14

T_{min} = 0.137, T_{max} = 1.000	l = 13-14
6491 measured reflections	

Table 6 *Refinement*

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.047	H-atom parameters constrained
$wR(F^2)$ = 0.132	$w = 1/[\sigma^2(F_o^2) + (0.0729P)^2 + 0.0966P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.02	$(\Delta/\sigma)_{max}$ = 0.001
5183 reflections	$\Delta\rho_{max}$ = 0.17 e Å^{-3}
619 parameters	$\Delta\rho_{min}$ = −0.20 e Å^{-3}

Table 7 Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	y	z	U_{iso}*/U_{eq}	Occ. (<1)
N1	0.4371 (3)	0.1827 (2)	0.3605 (3)	0.0486 (6)	
N2	0.4202 (4)	0.3525 (3)	0.4844 (3)	0.0509 (7)	
N1'	0.8962 (3)	0.9144 (3)	0.6387 (3)	0.0552 (7)	
N2'	0.9490 (4)	0.7734 (3)	0.4795 (3)	0.0569 (7)	
O1	0.3350 (3)	0.1553 (3)	0.1754 (3)	0.0705 (7)	
H1	0.3040	0.2041	0.2118	0.106*	
O2	0.4461 (3)	−0.1474 (3)	−0.0488 (3)	0.0680 (7)	
O3	0.6647 (4)	−0.2896 (2)	0.0182 (3)	0.0706 (8)	
O1'	1.0414 (3)	0.9807 (2)	0.7772 (3)	0.0628 (7)	
H1'	1.0579	0.9217	0.7537	0.094*	
O2'	0.9293 (4)	1.2851 (3)	0.9994 (3)	0.0758 (8)	
O3'	0.7059 (4)	1.4208 (3)	0.9390 (3)	0.0728 (8)	
F1	0.1741 (14)	0.6984 (12)	0.8046 (12)	0.108 (5)	0.50
F2	0.4104 (17)	0.7078 (15)	0.769 (2)	0.122 (5)	0.50
F3	0.313 (2)	0.8305 (7)	0.6304 (8)	0.102 (3)	0.50

F4	1.067 (2)	0.3198 (10)	0.2958 (13)	0.127 (7)	0.50
F5	1.2455 (10)	0.4447 (15)	0.1500 (17)	0.109 (2)	0.50
F6	1.032 (3)	0.4712 (19)	0.128 (2)	0.154 (7)	0.50
F1'	0.183 (2)	0.760 (2)	0.724 (3)	0.177 (8)	0.50
F2'	0.305 (3)	0.6596 (11)	0.8338 (11)	0.138 (5)	0.50
F3'	0.417 (2)	0.8071 (18)	0.6529 (18)	0.160 (6)	0.50
F4'	1.154 (4)	0.347 (2)	0.267 (3)	0.183 (10)	0.50
F5'	1.160 (3)	0.4986 (15)	0.0883 (11)	0.177 (7)	0.50
F6'	0.9556 (11)	0.3946 (14)	0.2250 (16)	0.116 (3)	0.50
C1	0.5238 (4)	0.0010 (3)	0.1455 (3)	0.0459 (7)	
C2	0.4581 (4)	−0.0197 (3)	0.0672 (3)	0.0508 (8)	
H2	0.3817	0.0330	0.0410	0.061*	
C3	0.5054 (4)	−0.1188 (3)	0.0272 (3)	0.0500 (8)	
C4	0.6231 (4)	−0.1945 (3)	0.0634 (3)	0.0515 (8)	
C5	0.6897 (4)	−0.1731 (3)	0.1405 (3)	0.0537 (8)	
H5	0.7686	−0.2240	0.1640	0.064*	
C6	0.6399 (4)	−0.0763 (3)	0.1836 (3)	0.0464 (8)	
C7	0.7034 (4)	−0.0555 (3)	0.2715 (4)	0.0564 (9)	
H7	0.7951	−0.0923	0.2815	0.068*	
C8	0.6321 (5)	0.0144 (4)	0.3361 (4)	0.0578 (9)	
H8	0.6748	0.0270	0.3905	0.069*	
C9	0.4826 (4)	0.0743 (3)	0.3233 (3)	0.0474 (7)	
H9	0.4006	0.0058	0.3833	0.057*	
C10	0.4816 (4)	0.1132 (3)	0.1846 (3)	0.0485 (7)	
H10	0.5592	0.1847	0.1222	0.058*	
C11	0.5618 (5)	0.2803 (3)	0.3096 (3)	0.0599 (9)	
H11A	0.6092	0.3101	0.2139	0.072*	
H11B	0.6407	0.2421	0.3491	0.072*	
C12	0.5004 (5)	0.3938 (3)	0.3415 (3)	0.0624 (10)	
H12A	0.5858	0.4549	0.3110	0.075*	
H12B	0.4294	0.4373	0.2944	0.075*	
C13	0.3015 (4)	0.2517 (3)	0.5380 (4)	0.0534 (8)	

H13A	0.2190	0.2863	0.5021	0.064*
H13B	0.2578	0.2210	0.6340	0.064*
C14	0.3676 (4)	0.1402 (3)	0.5035 (3)	0.0508 (7)
H14A	0.4453	0.1021	0.5445	0.061*
H14B	0.2857	0.0745	0.5390	0.061*
C15	0.3890 (4)	0.4456 (3)	0.5352 (4)	0.0499 (8)
C16	0.4742 (6)	0.5608 (4)	0.4734 (4)	0.0853 (15)
H16	0.5504	0.5824	0.3903	0.102*
C17	0.4491 (6)	0.6457 (4)	0.5324 (5)	0.0859 (15)
H17	0.5098	0.7225	0.4882	0.103*
C18	0.3394 (5)	0.6199 (3)	0.6515 (4)	0.0558 (9)
C19	0.2493 (7)	0.5092 (4)	0.7122 (5)	0.102 (2)
H19	0.1713	0.4899	0.7941	0.122*
C20	0.2725 (7)	0.4244 (5)	0.6531 (5)	0.104 (2)
H20	0.2066	0.3507	0.6951	0.124*
C21	0.3116 (5)	0.7110 (4)	0.7136 (4)	0.0624 (10)
C22	0.3339 (6)	−0.0669 (5)	−0.0945 (5)	0.0807 (13)
H22A	0.2404	−0.0789	−0.0205	0.121*
H22B	0.3128	−0.0887	−0.1569	0.121*
H22C	0.3723	0.0216	−0.1373	0.121*
C23	0.8029 (6)	−0.3507 (4)	0.0294 (5)	0.0781 (12)
H23A	0.8862	−0.2865	−0.0102	0.117*
H23B	0.8267	−0.4061	−0.0157	0.117*
H23C	0.7898	−0.4011	0.1217	0.117*
C1'	0.8772 (4)	1.1564 (3)	0.7795 (3)	0.0469 (7)
C2'	0.9367 (4)	1.1730 (3)	0.8643 (3)	0.0518 (8)
H2'	1.0170	1.1235	0.8866	0.062*
C3'	0.8780 (4)	1.2623 (3)	0.9163 (3)	0.0561 (9)
C4'	0.7564 (5)	1.3357 (3)	0.8830 (3)	0.0569 (9)
C5'	0.6959 (5)	1.3176 (3)	0.8014 (3)	0.0566 (9)
H5'	0.6139	1.3655	0.7808	0.068*

C6'	0.7559 (4)	1.2276 (3)	0.7485 (3)	0.0525 (8)
C7'	0.6909 (5)	1.2035 (4)	0.6639 (4)	0.0628 (10)
H7'	0.6241	1.2616	0.6276	0.075*
C8'	0.7248 (5)	1.1015 (4)	0.6380 (4)	0.0659 (10)
H8'	0.6862	1.0909	0.5802	0.079*
C9'	0.8251 (4)	1.0022 (3)	0.7008 (3)	0.0553 (8)
H9'	0.7588	0.9481	0.7918	0.066*
C10'	0.9479 (4)	1.0693 (3)	0.7124 (3)	0.0509 (8)
H10'	1.0152	1.1236	0.6219	0.061*
C11'	0.7824 (5)	0.8175 (4)	0.6675 (4)	0.0687 (10)
H11C	0.7086	0.8590	0.6229	0.082*
H11D	0.7259	0.7771	0.7625	0.082*
C12'	0.8585 (6)	0.7164 (4)	0.6225 (4)	0.0748 (12)
H12C	0.9263	0.6705	0.6721	0.090*
H12D	0.7800	0.6546	0.6408	0.090*
C13'	1.0573 (4)	0.8779 (4)	0.4435 (4)	0.0581 (9)
H13C	1.1040	0.9210	0.3474	0.070*
H13D	1.1394	0.8422	0.4796	0.070*
C14'	0.9771 (4)	0.9745 (3)	0.4957 (4)	0.0584 (8)
H14C	1.0531	1.0395	0.4748	0.070*
H14D	0.9034	1.0174	0.4514	0.070*
C15'	0.9898 (4)	0.6922 (3)	0.4151 (3)	0.0546 (8)
C16'	0.9016 (7)	0.5819 (5)	0.4610 (5)	0.1042 (19)
H16'	0.8167	0.5591	0.5393	0.125*
C17'	0.9343 (7)	0.5034 (5)	0.3954 (6)	0.1057 (19)
H17'	0.8700	0.4303	0.4293	0.127*
C18'	1.0582 (5)	0.5306 (4)	0.2827 (4)	0.0628 (10)
C19'	1.1498 (7)	0.6376 (5)	0.2372 (5)	0.0910 (15)
H19'	1.2361	0.6578	0.1603	0.109*
C20'	1.1189 (6)	0.7170 (4)	0.3013 (4)	0.0840 (13)
H20'	1.1855	0.7886	0.2679	0.101*

C21'	1.0915 (7)	0.4434 (5)	0.2144 (5)	0.0828 (14)
C22'	1.0432 (7)	1.2053 (5)	1.0455 (5)	0.0869 (14)
H22D	1.0035	1.1169	1.0934	0.130*
H22E	1.0685	1.2315	1.1033	0.130*
H22F	1.1346	1.2136	0.9709	0.130*
C23'	0.5668 (6)	1.4808 (4)	0.9263 (5)	0.0837 (13)
H23D	0.5824	1.5342	0.8340	0.126*
H23E	0.5381	1.5331	0.9749	0.126*
H23F	0.4857	1.4158	0.9613	0.126*

Table 8 Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0512 (15)	0.0523 (14)	0.0510 (14)	−0.0001 (12)	−0.0175 (13)	−0.0289 (12)
N2	0.0544 (16)	0.0486 (14)	0.0535 (14)	−0.0037 (13)	−0.0123 (13)	−0.0283 (12)
N1'	0.0536 (17)	0.0655 (17)	0.0564 (16)	−0.0012 (14)	−0.0169 (13)	−0.0352 (14)
N2'	0.0566 (18)	0.0653 (17)	0.0543 (16)	−0.0096 (15)	−0.0105 (14)	−0.0340 (14)
O1	0.0752 (17)	0.0875 (18)	0.0912 (18)	0.0410 (15)	−0.0540 (16)	−0.0632 (16)
O2	0.0795 (19)	0.0814 (17)	0.0784 (17)	0.0205 (15)	−0.0427 (15)	−0.0561 (15)
O3	0.0839 (19)	0.0694 (15)	0.0802 (16)	0.0258 (15)	−0.0341 (15)	−0.0510 (14)
O1'	0.0645 (16)	0.0716 (16)	0.0831 (17)	0.0245 (14)	−0.0413 (15)	−0.0520 (15)
O2'	0.091 (2)	0.0841 (18)	0.0865 (18)	0.0192 (17)	−0.0454 (17)	−0.0580 (16)
O3'	0.086 (2)	0.0619 (15)	0.0810 (18)	0.0191 (15)	−0.0257 (16)	−0.0457 (14)
F1	0.098 (8)	0.109 (7)	0.106 (6)	−0.033 (7)	0.024 (7)	−0.075 (5)
F2	0.119 (7)	0.131 (10)	0.232 (15)	0.067 (6)	−0.128 (9)	−0.140 (11)
F3	0.184 (10)	0.044 (3)	0.081 (4)	0.029 (5)	−0.054 (6)	−0.028 (3)
F4	0.190 (15)	0.062 (5)	0.112 (7)	−0.008 (8)	−0.011 (10)	−0.050 (4)
F5	0.104 (5)	0.134 (7)	0.122 (7)	0.035 (5)	−0.027 (5)	−0.100 (6)
F6	0.230 (15)	0.193 (15)	0.196 (13)	0.162 (13)	−0.184 (13)	−0.165 (12)
F1'	0.166 (15)	0.233 (18)	0.32 (2)	0.141 (14)	−0.170 (16)	−0.245 (18)
F2'	0.269 (16)	0.090 (6)	0.098 (6)	0.065 (9)	−0.098 (9)	−0.063 (5)
F3'	0.169 (11)	0.135 (9)	0.172 (12)	−0.085 (9)	0.034 (8)	−0.115 (9)
F4'	0.29 (2)	0.176 (17)	0.25 (3)	0.187 (17)	−0.22 (2)	−0.176 (18)
F5'	0.265 (18)	0.166 (11)	0.090 (6)	−0.028 (14)	0.011 (10)	−0.094 (7)
F6'	0.123 (6)	0.128 (8)	0.160 (8)	0.019 (6)	−0.059 (7)	−0.110 (6)

C1	0.0517 (18)	0.0467 (16)	0.0406 (15)	0.0043 (15)	−0.0157 (14)	−0.0200 (13)
C2	0.0532 (19)	0.0586 (19)	0.0489 (16)	0.0096 (16)	−0.0209 (15)	−0.0288 (15)
C3	0.053 (2)	0.0547 (18)	0.0497 (17)	0.0036 (16)	−0.0191 (16)	−0.0276 (16)
C4	0.059 (2)	0.0484 (17)	0.0491 (17)	0.0056 (16)	−0.0134 (16)	−0.0271 (15)
C5	0.0520 (19)	0.0545 (18)	0.0534 (18)	0.0118 (16)	−0.0188 (16)	−0.0232 (16)
C6	0.0462 (18)	0.0505 (18)	0.0420 (16)	0.0036 (15)	−0.0134 (14)	−0.0207 (14)
C7	0.0520 (19)	0.064 (2)	0.067 (2)	0.0163 (17)	−0.0319 (18)	−0.0332 (18)
C8	0.064 (2)	0.066 (2)	0.064 (2)	0.0103 (18)	−0.0379 (19)	−0.0339 (18)
C9	0.0520 (18)	0.0483 (16)	0.0500 (16)	0.0042 (14)	−0.0203 (14)	−0.0262 (14)
C10	0.0543 (19)	0.0487 (17)	0.0527 (17)	0.0072 (15)	−0.0240 (15)	−0.0269 (14)
C11	0.064 (2)	0.064 (2)	0.0520 (18)	−0.0057 (17)	−0.0090 (17)	−0.0314 (16)
C12	0.075 (3)	0.0571 (19)	0.0501 (18)	−0.0165 (18)	−0.0105 (18)	−0.0223 (16)
C13	0.0528 (19)	0.0519 (17)	0.0578 (18)	−0.0062 (15)	−0.0086 (15)	−0.0314 (15)
C14	0.0496 (18)	0.0543 (17)	0.0517 (17)	−0.0048 (15)	−0.0126 (15)	−0.0274 (15)
C15	0.0541 (19)	0.0447 (16)	0.0556 (17)	0.0014 (15)	−0.0206 (16)	−0.0238 (15)
C16	0.097 (3)	0.064 (2)	0.075 (3)	−0.028 (2)	0.017 (2)	−0.042 (2)
C17	0.101 (3)	0.063 (2)	0.081 (3)	−0.032 (2)	0.008 (3)	−0.041 (2)
C18	0.061 (2)	0.0478 (19)	0.069 (2)	0.0087 (17)	−0.0294 (19)	−0.0288 (17)
C19	0.129 (5)	0.077 (3)	0.081 (3)	−0.032 (3)	0.024 (3)	−0.056 (3)
C20	0.120 (4)	0.076 (3)	0.085 (3)	−0.050 (3)	0.034 (3)	−0.051 (2)
C21	0.072 (3)	0.051 (2)	0.076 (2)	0.015 (2)	−0.035 (2)	−0.0325 (19)
C22	0.091 (3)	0.100 (3)	0.094 (3)	0.031 (3)	−0.058 (3)	−0.064 (3)
C23	0.082 (3)	0.075 (3)	0.088 (3)	0.030 (2)	−0.028 (2)	−0.051 (2)
C1'	0.0393 (16)	0.0524 (18)	0.0510 (17)	−0.0005 (14)	−0.0133 (14)	−0.0246 (14)
C2'	0.0487 (18)	0.0578 (19)	0.0580 (18)	0.0047 (16)	−0.0211 (16)	−0.0307 (16)
C3'	0.061 (2)	0.060 (2)	0.0526 (18)	0.0007 (18)	−0.0171 (17)	−0.0298 (17)
C4'	0.065 (2)	0.0493 (19)	0.0532 (18)	0.0051 (17)	−0.0156 (17)	−0.0229 (16)
C5'	0.055 (2)	0.0502 (18)	0.0571 (19)	0.0085 (17)	−0.0168 (17)	−0.0192 (16)
C6'	0.052 (2)	0.0539 (19)	0.0498 (18)	0.0027 (16)	−0.0149 (16)	−0.0218 (15)
C7'	0.054 (2)	0.077 (3)	0.068 (2)	0.016 (2)	−0.0304 (18)	−0.035 (2)
C8'	0.054 (2)	0.095 (3)	0.075 (2)	0.015 (2)	−0.0318 (19)	−0.054 (2)
C9'	0.0490 (18)	0.069 (2)	0.0544 (18)	−0.0028 (16)	−0.0167 (15)	−0.0318 (16)
C10'	0.0445 (17)	0.0631 (19)	0.0581 (19)	0.0042 (15)	−0.0202 (15)	−0.0355 (16)
C11'	0.068 (2)	0.083 (2)	0.0572 (19)	−0.019 (2)	−0.0069 (18)	−0.0379 (19)
C12'	0.093 (3)	0.071 (2)	0.058 (2)	−0.015 (2)	−0.007 (2)	−0.0363 (19)

C13'	0.0511 (19)	0.068 (2)	0.062 (2)	−0.0035 (17)	−0.0155 (17)	−0.0346 (17)
C14'	0.059 (2)	0.0585 (19)	0.067 (2)	−0.0020 (16)	−0.0224 (18)	−0.0329 (17)
C15'	0.054 (2)	0.059 (2)	0.0543 (18)	0.0029 (17)	−0.0153 (16)	−0.0300 (17)
C16'	0.105 (4)	0.104 (3)	0.090 (3)	−0.047 (3)	0.026 (3)	−0.064 (3)
C17'	0.111 (4)	0.092 (3)	0.107 (4)	−0.036 (3)	0.010 (3)	−0.065 (3)
C18'	0.071 (3)	0.060 (2)	0.066 (2)	0.013 (2)	−0.023 (2)	−0.0368 (19)
C19'	0.091 (3)	0.090 (3)	0.077 (3)	−0.009 (3)	0.009 (2)	−0.049 (3)
C20'	0.085 (3)	0.071 (3)	0.083 (3)	−0.020 (2)	0.007 (2)	−0.044 (2)
C21'	0.098 (4)	0.087 (3)	0.090 (3)	0.030 (3)	−0.039 (3)	−0.061 (3)
C22'	0.102 (4)	0.105 (3)	0.100 (3)	0.023 (3)	−0.061 (3)	−0.068 (3)
C23'	0.089 (3)	0.067 (2)	0.092 (3)	0.022 (2)	−0.016 (3)	−0.048 (2)

Table 9 Geometric parameters (Å,°)

N1—C14	1.451 (4)	C14—H14B	0.9700
N1—C11	1.465 (4)	C15—C20	1.368 (6)
N1—C9	1.469 (4)	C15—C16	1.372 (5)
N2—C15	1.401 (4)	C16—C17	1.386 (6)
N2—C13	1.444 (4)	C16—H16	0.9300
N2—C12	1.462 (4)	C17—C18	1.342 (6)
N1'—C14'	1.453 (5)	C17—H17	0.9300
N1'—C11'	1.458 (5)	C18—C19	1.355 (6)
N1'—C9'	1.468 (4)	C18—C21	1.477 (5)
N2'—C15'	1.392 (5)	C19—C20	1.388 (7)
N2'—C13'	1.460 (4)	C19—H19	0.9300
N2'—C12'	1.468 (5)	C20—H20	0.9300
O1—C10	1.415 (4)	C22—H22A	0.9600
O1—H1	0.8200	C22—H22B	0.9600
O2—C3	1.366 (4)	C22—H22C	0.9600
O2—C22	1.410 (5)	C23—H23A	0.9600
O3—C4	1.379 (4)	C23—H23B	0.9600
O3—C23	1.413 (5)	C23—H23C	0.9600
O1'—C10'	1.408 (4)	C1'—C6'	1.379 (5)
O1'—H1'	0.8200	C1'—C2'	1.388 (5)
O2'—C3'	1.357 (4)	C1'—C10'	1.499 (5)
O2'—C22'	1.421 (6)	C2'—C3'	1.387 (5)

O3'—C4'	1.365 (5)	C2'—H2'	0.9300
O3'—C23'	1.419 (6)	C3'—C4'	1.400 (5)
F1—C21	1.317 (9)	C4'—C5'	1.368 (5)
F2—C21	1.288 (8)	C5'—C6'	1.403 (5)
F3—C21	1.298 (7)	C5'—H5'	0.9300
F4—C21'	1.316 (11)	C6'—C7'	1.463 (5)
F5—C21'	1.355 (10)	C7'—C8'	1.317 (6)
F6—C21'	1.240 (9)	C7'—H7'	0.9300
F1'—C21	1.245 (11)	C8'—C9'	1.499 (5)
F2'—C21	1.266 (9)	C8'—H8'	0.9300
F3'—C21	1.314 (8)	C9'—C10'	1.512 (4)
F4'—C21'	1.216 (12)	C9'—H9'	0.9800
F5'—C21'	1.279 (11)	C10'—H10'	0.9800
F6'—C21'	1.371 (10)	C11'—C12'	1.493 (6)
C1—C2	1.381 (5)	C11'—H11C	0.9700
C1—C6	1.393 (5)	C11'—H11D	0.9700
C1—C10	1.521 (4)	C12'—H12C	0.9700
C2—C3	1.388 (5)	C12'—H12D	0.9700
C2—H2	0.9300	C13'—C14'	1.505 (5)
C3—C4	1.391 (5)	C13'—H13C	0.9700
C4—C5	1.377 (5)	C13'—H13D	0.9700
C5—C6	1.389 (5)	C14'—H14C	0.9700
C5—H5	0.9300	C14'—H14D	0.9700
C6—C7	1.471 (5)	C15'—C16'	1.368 (6)
C7—C8	1.316 (5)	C15'—C20'	1.389 (6)
C7—H7	0.9300	C16'—C17'	1.375 (7)
C8—C9	1.505 (5)	C16'—H16'	0.9300
C8—H8	0.9300	C17'—C18'	1.352 (7)
C9—C10	1.511 (4)	C17'—H17'	0.9300
C9—H9	0.9800	C18'—C19'	1.357 (6)
C10—H10	0.9800	C18'—C21'	1.488 (6)
C11—C12	1.512 (5)	C19'—C20'	1.371 (7)
C11—H11A	0.9700	C19'—H19'	0.9300
C11—H11B	0.9700	C20'—H20'	0.9300
C12—H12A	0.9700	C22'—H22D	0.9600

C12—H12B	0.9700	C22'—H22E	0.9600
C13—C14	1.516 (5)	C22'—H22F	0.9600
C13—H13A	0.9700	C23'—H23D	0.9600
C13—H13B	0.9700	C23'—H23E	0.9600
C14—H14A	0.9700	C23'—H23F	0.9600
C14—N1—C11	108.4 (3)	O2—C22—H22C	109.5
C14—N1—C9	112.5 (2)	H22A—C22—H22C	109.5
C11—N1—C9	114.9 (3)	H22B—C22—H22C	109.5
C15—N2—C13	117.5 (3)	O3—C23—H23A	109.5
C15—N2—C12	118.8 (3)	O3—C23—H23B	109.5
C13—N2—C12	111.8 (3)	H23A—C23—H23B	109.5
C14'—N1'—C11'	108.2 (3)	O3—C23—H23C	109.5
C14'—N1'—C9'	116.2 (3)	H23A—C23—H23C	109.5
C11'—N1'—C9'	111.2 (3)	H23B—C23—H23C	109.5
C15'—N2'—C13'	120.1 (3)	C6'—C1'—C2'	119.8 (3)
C15'—N2'—C12'	118.0 (3)	C6'—C1'—C10'	118.2 (3)
C13'—N2'—C12'	111.8 (3)	C2'—C1'—C10'	121.9 (3)
C10—O1—H1	109.5	C3'—C2'—C1'	120.9 (3)
C3—O2—C22	117.4 (3)	C3'—C2'—H2'	119.5
C4—O3—C23	117.2 (3)	C1'—C2'—H2'	119.5
C10'—O1'—H1'	109.5	O2'—C3'—C2'	124.9 (3)
C3'—O2'—C22'	118.1 (3)	O2'—C3'—C4'	116.0 (3)
C4'—O3'—C23'	116.6 (4)	C2'—C3'—C4'	119.2 (3)
C2—C1—C6	120.2 (3)	O3'—C4'—C5'	125.1 (4)
C2—C1—C10	121.8 (3)	O3'—C4'—C3'	115.1 (3)
C6—C1—C10	117.8 (3)	C5'—C4'—C3'	119.9 (3)
C1—C2—C3	120.4 (3)	C4'—C5'—C6'	120.9 (4)
C1—C2—H2	119.8	C4'—C5'—H5'	119.6
C3—C2—H2	119.8	C6'—C5'—H5'	119.6
O2—C3—C2	124.6 (3)	C1'—C6'—C5'	119.4 (3)
O2—C3—C4	116.1 (3)	C1'—C6'—C7'	118.5 (3)
C2—C3—C4	119.4 (3)	C5'—C6'—C7'	122.1 (3)
C5—C4—O3	124.0 (3)	C8'—C7'—C6'	121.5 (4)
C5—C4—C3	120.3 (3)	C8'—C7'—H7'	119.3
O3—C4—C3	115.7 (3)	C6'—C7'—H7'	119.3

C4—C5—C6	120.5 (3)	C7'—C8'—C9'	120.6 (3)
C4—C5—H5	119.7	C7'—C8'—H8'	119.7
C6—C5—H5	119.7	C9'—C8'—H8'	119.7
C5—C6—C1	119.2 (3)	N1'—C9'—C8'	117.3 (3)
C5—C6—C7	121.7 (3)	N1'—C9'—C10'	110.3 (3)
C1—C6—C7	119.0 (3)	C8'—C9'—C10'	109.0 (3)
C8—C7—C6	120.9 (3)	N1'—C9'—H9'	106.6
C8—C7—H7	119.5	C8'—C9'—H9'	106.6
C6—C7—H7	119.5	C10'—C9'—H9'	106.6
C7—C8—C9	121.0 (3)	O1'—C10'—C1'	111.3 (3)
C7—C8—H8	119.5	O1'—C10'—C9'	111.9 (3)
C9—C8—H8	119.5	C1'—C10'—C9'	111.1 (3)
N1—C9—C8	117.5 (3)	O1'—C10'—H10'	107.4
N1—C9—C10	109.5 (2)	C1'—C10'—H10'	107.4
C8—C9—C10	110.3 (3)	C9'—C10'—H10'	107.4
N1—C9—H9	106.3	N1'—C11'—C12'	111.1 (3)
C8—C9—H9	106.3	N1'—C11'—H11C	109.4
C10—C9—H9	106.3	C12'—C11'—H11C	109.4
O1—C10—C9	111.0 (3)	N1'—C11'—H11D	109.4
O1—C10—C1	109.8 (3)	C12'—C11'—H11D	109.4
C9—C10—C1	110.4 (2)	H11C—C11'—H11D	108.0
O1—C10—H10	108.5	N2'—C12'—C11'	111.4 (3)
C9—C10—H10	108.5	N2'—C12'—H12C	109.3
C1—C10—H10	108.5	C11'—C12'—H12C	109.3
N1—C11—C12	110.9 (3)	N2'—C12'—H12D	109.3
N1—C11—H11A	109.5	C11'—C12'—H12D	109.3
C12—C11—H11A	109.5	H12C—C12'—H12D	108.0
N1—C11—H11B	109.5	N2'—C13'—C14'	111.2 (3)
C12—C11—H11B	109.5	N2'—C13'—H13C	109.4
H11A—C11—H11B	108.1	C14'—C13'—H13C	109.4
N2—C12—C11	111.4 (3)	N2'—C13'—H13D	109.4
N2—C12—H12A	109.3	C14'—C13'—H13D	109.4
C11—C12—H12A	109.3	H13C—C13'—H13D	108.0
N2—C12—H12B	109.3	N1'—C14'—C13'	112.2 (3)
C11—C12—H12B	109.3	N1'—C14'—H14C	109.2

H12A—C12—H12B	108.0	C13'—C14'—H14C	109.2
N2—C13—C14	110.7 (3)	N1'—C14'—H14D	109.2
N2—C13—H13A	109.5	C13'—C14'—H14D	109.2
C14—C13—H13A	109.5	H14C—C14'—H14D	107.9
N2—C13—H13B	109.5	C16'—C15'—C20'	115.8 (4)
C14—C13—H13B	109.5	C16'—C15'—N2'	121.0 (3)
H13A—C13—H13B	108.1	C20'—C15'—N2'	123.2 (3)
N1—C14—C13	111.3 (3)	C15'—C16'—C17'	122.3 (4)
N1—C14—H14A	109.4	C15'—C16'—H16'	118.9
C13—C14—H14A	109.4	C17'—C16'—H16'	118.9
N1—C14—H14B	109.4	C18'—C17'—C16'	121.3 (4)
C13—C14—H14B	109.4	C18'—C17'—H17'	119.4
H14A—C14—H14B	108.0	C16'—C17'—H17'	119.4
C20—C15—C16	115.9 (4)	C17'—C18'—C19'	117.5 (4)
C20—C15—N2	121.1 (3)	C17'—C18'—C21'	120.1 (4)
C16—C15—N2	122.9 (3)	C19'—C18'—C21'	122.4 (4)
C15—C16—C17	121.4 (4)	C18'—C19'—C20'	122.0 (4)
C15—C16—H16	119.3	C18'—C19'—H19'	119.0
C17—C16—H16	119.3	C20'—C19'—H19'	119.0
C18—C17—C16	121.7 (4)	C19'—C20'—C15'	121.1 (4)
C18—C17—H17	119.2	C19'—C20'—H20'	119.5
C16—C17—H17	119.2	C15'—C20'—H20'	119.5
C17—C18—C19	118.1 (4)	F4'—C21'—F6	130.3 (9)
C17—C18—C21	121.7 (3)	F4'—C21'—F5'	111.9 (12)
C19—C18—C21	120.2 (4)	F6—C21'—F5'	53.4 (9)
C18—C19—C20	120.5 (4)	F4'—C21'—F4	36.0 (13)
C18—C19—H19	119.7	F6—C21'—F4	111.2 (12)
C20—C19—H19	119.7	F5'—C21'—F4	129.9 (9)
C15—C20—C19	122.2 (4)	F4'—C21'—F5	65.1 (12)
C15—C20—H20	118.9	F6—C21'—F5	104.8 (10)
C19—C20—H20	118.9	F5'—C21'—F5	54.5 (11)
F1'—C21—F2'	100.7 (11)	F4—C21'—F5	98.7 (8)
F1'—C21—F2	130.2 (7)	F4'—C21'—F6'	102.8 (13)
F2'—C21—F2	47.6 (7)	F6—C21'—F6'	51.0 (9)
F1'—C21—F3	63.9 (10)	F5'—C21'—F6'	102.2 (11)

F2'—C21—F3	132.2 (6)	F4—C21'—F6'	68.9 (8)
F2—C21—F3	106.1 (8)	F5—C21'—F6'	138.4 (6)
F1'—C21—F3'	106.7 (10)	F4'—C21'—C18'	113.5 (8)
F2'—C21—F3'	105.3 (9)	F6—C21'—C18'	115.2 (6)
F2—C21—F3'	62.0 (8)	F5'—C21'—C18'	115.0 (7)
F3—C21—F3'	48.0 (8)	F4—C21'—C18'	114.1 (7)
F1'—C21—F1	40.4 (10)	F5—C21'—C18'	111.2 (5)
F2'—C21—F1	63.1 (9)	F6'—C21'—C18'	110.1 (6)
F2—C21—F1	105.8 (9)	O2'—C22'—H22D	109.5
F3—C21—F1	100.6 (7)	O2'—C22'—H22E	109.5
F3'—C21—F1	128.7 (7)	H22D—C22'—H22E	109.5
F1'—C21—C18	114.4 (6)	O2'—C22'—H22F	109.5
F2'—C21—C18	114.2 (5)	H22D—C22'—H22F	109.5
F2—C21—C18	114.0 (5)	H22E—C22'—H22F	109.5
F3—C21—C18	113.2 (5)	O3'—C23'—H23D	109.5
F3'—C21—C18	114.2 (5)	O3'—C23'—H23E	109.5
F1—C21—C18	115.8 (5)	H23D—C23'—H23E	109.5
O2—C22—H22A	109.5	O3'—C23'—H23F	109.5
O2—C22—H22B	109.5	H23D—C23'—H23F	109.5
H22A—C22—H22B	109.5	H23E—C23'—H23F	109.5
C6—C1—C2—C3	0.9 (5)	C6'—C1'—C2'—C3'	−1.4 (5)
C10—C1—C2—C3	176.4 (3)	C10'—C1'—C2'—C3'	174.4 (3)
C22—O2—C3—C2	2.9 (5)	C22'—O2'—C3'—C2'	−5.1 (6)
C22—O2—C3—C4	−175.9 (4)	C22'—O2'—C3'—C4'	174.6 (4)
C1—C2—C3—O2	179.2 (3)	C1'—C2'—C3'—O2'	−179.9 (3)
C1—C2—C3—C4	−2.0 (5)	C1'—C2'—C3'—C4'	0.5 (5)
C23—O3—C4—C5	−13.0 (5)	C23'—O3'—C4'—C5'	9.4 (5)
C23—O3—C4—C3	167.5 (3)	C23'—O3'—C4'—C3'	−169.7 (3)
O2—C3—C4—C5	−179.7 (3)	O2'—C3'—C4'—O3'	0.1 (5)
C2—C3—C4—C5	1.4 (5)	C2'—C3'—C4'—O3'	179.8 (3)
O2—C3—C4—O3	−0.3 (4)	O2'—C3'—C4'—C5'	−179.0 (3)
C2—C3—C4—O3	−179.1 (3)	C2'—C3'—C4'—C5'	0.8 (5)
O3—C4—C5—C6	−179.2 (3)	O3'—C4'—C5'—C6'	180.0 (3)
C3—C4—C5—C6	0.3 (5)	C3'—C4'—C5'—C6'	−1.1 (5)
C4—C5—C6—C1	−1.3 (5)	C2'—C1'—C6'—C5'	1.1 (5)

C4—C5—C6—C7	176.9 (3)	C10'—C1'—C6'—C5'	−174.8 (3)
C2—C1—C6—C5	0.7 (5)	C2'—C1'—C6'—C7'	−177.2 (3)
C10—C1—C6—C5	−174.9 (3)	C10'—C1'—C6'—C7'	6.9 (5)
C2—C1—C6—C7	−177.5 (3)	C4'—C5'—C6'—C1'	0.2 (5)
C10—C1—C6—C7	6.8 (4)	C4'—C5'—C6'—C7'	178.3 (3)
C5—C6—C7—C8	−164.0 (3)	C1'—C6'—C7'—C8'	12.8 (6)
C1—C6—C7—C8	14.2 (5)	C5'—C6'—C7'—C8'	−165.4 (4)
C6—C7—C8—C9	0.6 (5)	C6'—C7'—C8'—C9'	3.4 (6)
C14—N1—C9—C8	−79.6 (4)	C14'—N1'—C9'—C8'	49.8 (4)
C11—N1—C9—C8	45.0 (4)	C11'—N1'—C9'—C8'	−74.5 (4)
C14—N1—C9—C10	153.6 (3)	C14'—N1'—C9'—C10'	−75.6 (3)
C11—N1—C9—C10	−81.9 (3)	C11'—N1'—C9'—C10'	160.0 (3)
C7—C8—C9—N1	−160.4 (3)	C7'—C8'—C9'—N1'	−161.9 (4)
C7—C8—C9—C10	−33.9 (4)	C7'—C8'—C9'—C10'	−35.8 (5)
N1—C9—C10—O1	−56.3 (3)	C6'—C1'—C10'—O1'	−165.2 (3)
C8—C9—C10—O1	172.9 (3)	C2'—C1'—C10'—O1'	18.9 (4)
N1—C9—C10—C1	−178.3 (3)	C6'—C1'—C10'—C9'	−39.8 (4)
C8—C9—C10—C1	50.9 (4)	C2'—C1'—C10'—C9'	144.4 (3)
C2—C1—C10—O1	22.3 (4)	N1'—C9'—C10'—O1'	−53.1 (3)
C6—C1—C10—O1	−162.2 (3)	C8'—C9'—C10'—O1'	176.9 (3)
C2—C1—C10—C9	145.0 (3)	N1'—C9'—C10'—C1'	−178.2 (3)
C6—C1—C10—C9	−39.4 (4)	C8'—C9'—C10'—C1'	51.8 (4)
C14—N1—C11—C12	−58.9 (4)	C14'—N1'—C11'—C12'	60.0 (4)
C9—N1—C11—C12	174.4 (3)	C9'—N1'—C11'—C12'	−171.3 (3)
C15—N2—C12—C11	164.8 (3)	C15'—N2'—C12'—C11'	−162.1 (3)
C13—N2—C12—C11	−53.3 (4)	C13'—N2'—C12'—C11'	52.5 (5)
N1—C11—C12—N2	56.0 (4)	N1'—C11'—C12'—N2'	−57.6 (5)
C15—N2—C13—C14	−163.9 (3)	C15'—N2'—C13'—C14'	164.4 (3)
C12—N2—C13—C14	53.6 (4)	C12'—N2'—C13'—C14'	−51.0 (4)
C11—N1—C14—C13	59.9 (3)	C11'—N1'—C14'—C13'	−59.1 (4)
C9—N1—C14—C13	−172.0 (3)	C9'—N1'—C14'—C13'	175.1 (3)
N2—C13—C14—N1	−58.0 (4)	N2'—C13'—C14'—N1'	55.4 (4)
C13—N2—C15—C20	17.3 (6)	C13'—N2'—C15'—C16'	169.4 (4)
C12—N2—C15—C20	157.1 (5)	C12'—N2'—C15'—C16'	26.9 (6)
C13—N2—C15—C16	−164.6 (4)	C13'—N2'—C15'—C20'	−11.3 (6)

C12—N2—C15—C16	−24.8 (5)	C12'—N2'—C15'—C20'	−153.8 (4)
C20—C15—C16—C17	4.1 (8)	C20'—C15'—C16'—C17'	−2.9 (9)
N2—C15—C16—C17	−174.1 (4)	N2'—C15'—C16'—C17'	176.4 (5)
C15—C16—C17—C18	−0.8 (9)	C15'—C16'—C17'—C18'	1.3 (10)
C16—C17—C18—C19	−1.9 (8)	C16'—C17'—C18'—C19'	0.5 (9)
C16—C17—C18—C21	−179.4 (5)	C16'—C17'—C18'—C21'	179.5 (6)
C17—C18—C19—C20	1.1 (9)	C17'—C18'—C19'—C20'	−0.6 (8)
C21—C18—C19—C20	178.6 (5)	C21'—C18'—C19'—C20'	−179.5 (5)
C16—C15—C20—C19	−4.9 (9)	C18'—C19'—C20'—C15'	−1.2 (9)
N2—C15—C20—C19	173.3 (5)	C16'—C15'—C20'—C19'	2.8 (8)
C18—C19—C20—C15	2.4 (10)	N2'—C15'—C20'—C19'	−176.5 (4)
C17—C18—C21—F1'	113.6 (18)	C17'—C18'—C21'—F4'	−79 (2)
C19—C18—C21—F1'	−63.8 (18)	C19'—C18'—C21'—F4'	100 (2)
C17—C18—C21—F2'	−131.0 (14)	C17'—C18'—C21'—F6	91.1 (17)
C19—C18—C21—F2'	51.5 (15)	C19'—C18'—C21'—F6	−90.0 (17)
C17—C18—C21—F2	−78.5 (12)	C17'—C18'—C21'—F5'	150.6 (18)
C19—C18—C21—F2	104.1 (12)	C19'—C18'—C21'—F5'	−30.5 (19)
C17—C18—C21—F3	42.9 (11)	C17'—C18'—C21'—F4	−39.3 (11)
C19—C18—C21—F3	−134.5 (11)	C19'—C18'—C21'—F4	139.6 (10)
C17—C18—C21—F3'	−9.8 (16)	C17'—C18'—C21'—F5	−149.9 (10)
C19—C18—C21—F3'	172.8 (15)	C19'—C18'—C21'—F5	29.0 (11)
C17—C18—C21—F1	158.4 (10)	C17'—C18'—C21'—F6'	35.8 (10)
C19—C18—C21—F1	−19.0 (11)	C19'—C18'—C21'—F6'	−145.3 (9)

Table 10 Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1′—H1′···N1′	0.82	2.38	2.815 (4)	114
O1—H1···N1	0.82	2.40	2.816 (4)	112

6. References:

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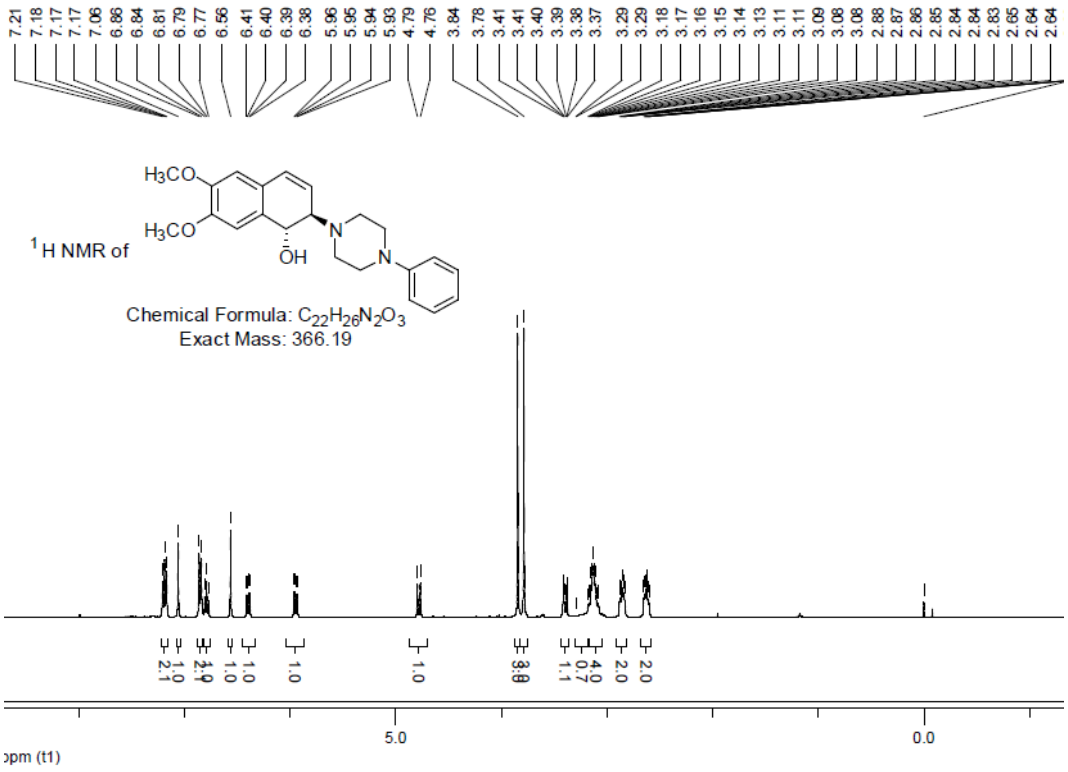
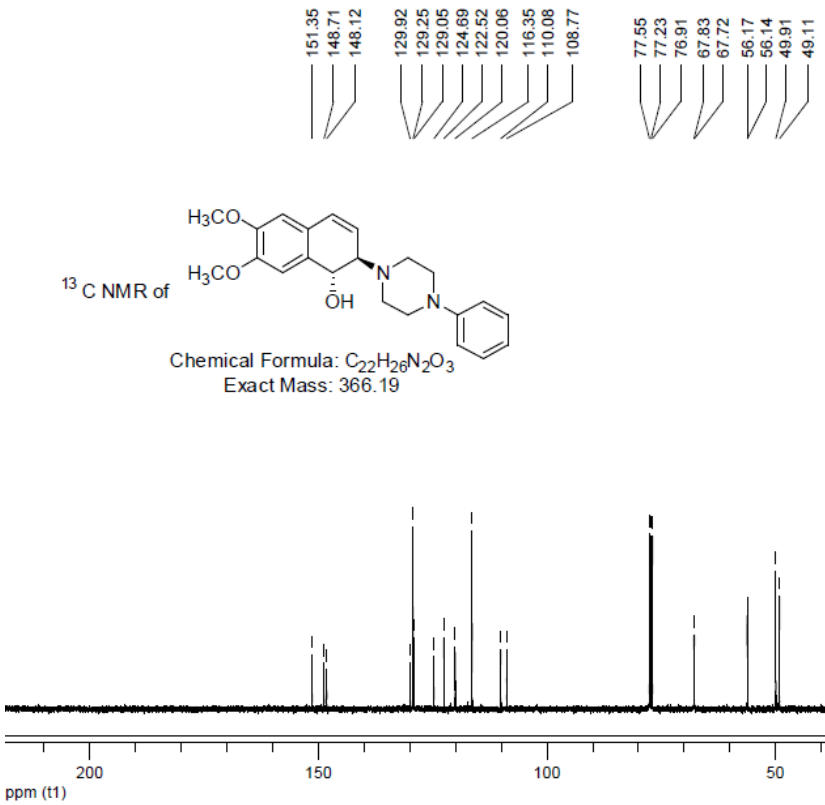
7. NMR spectra

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77.23
76.91
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67.72
56.17
56.14
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49.11
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H3CO
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Exact Mass: 366.19
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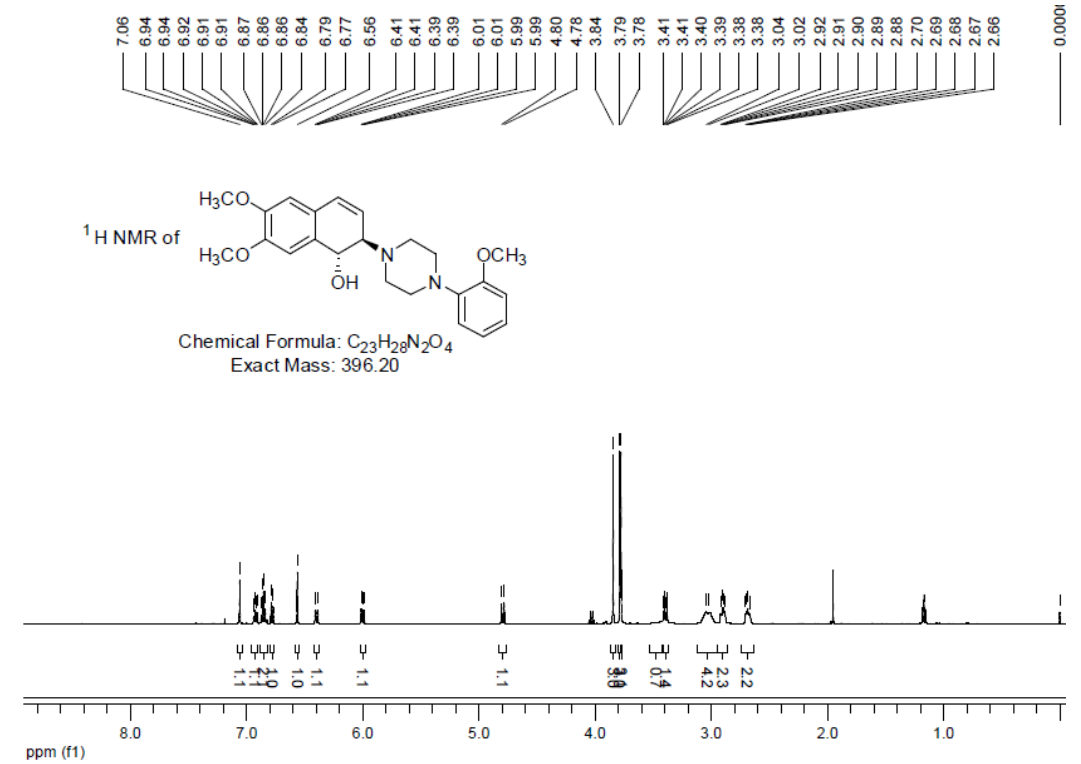
ppm (t1)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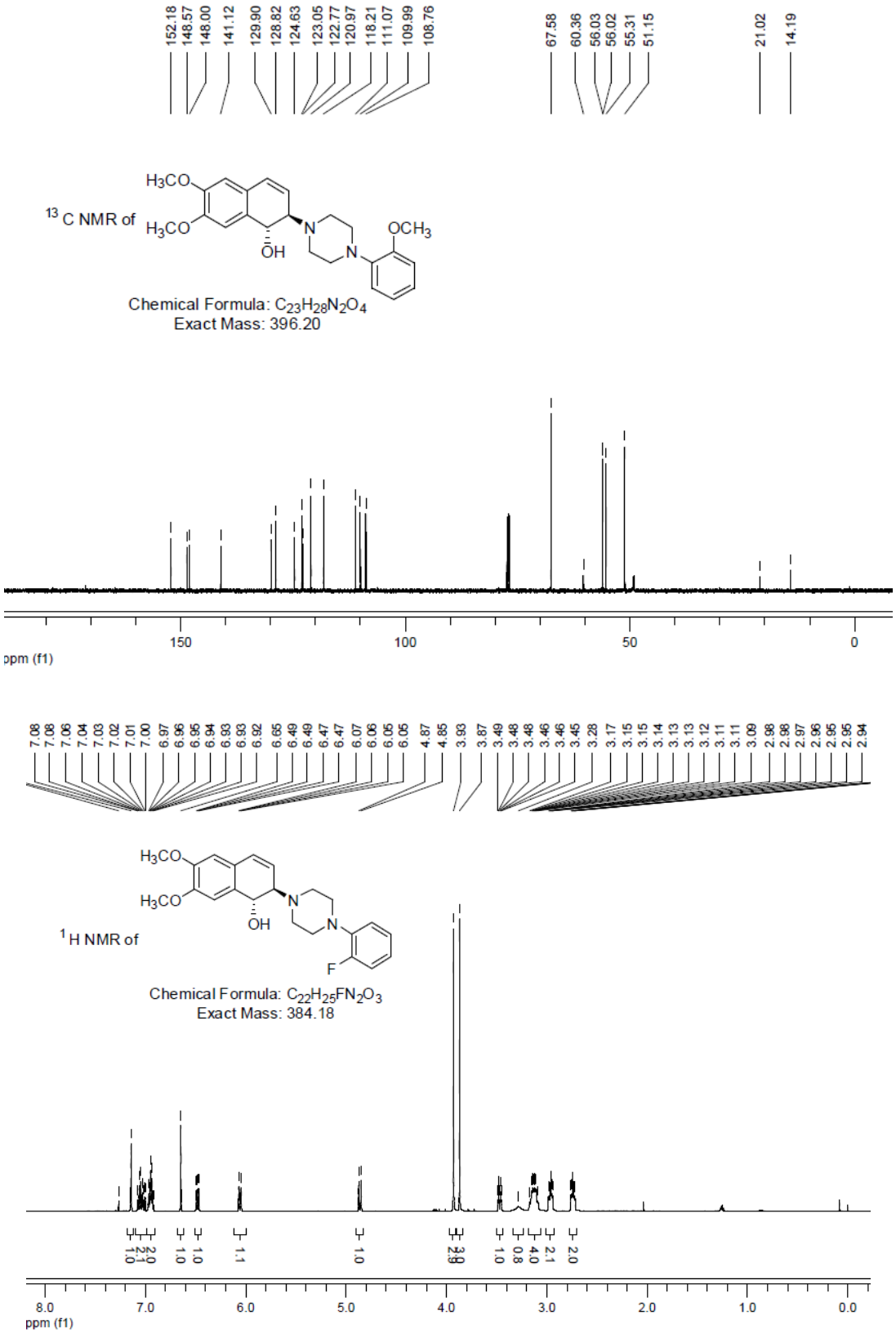
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OH
N
N
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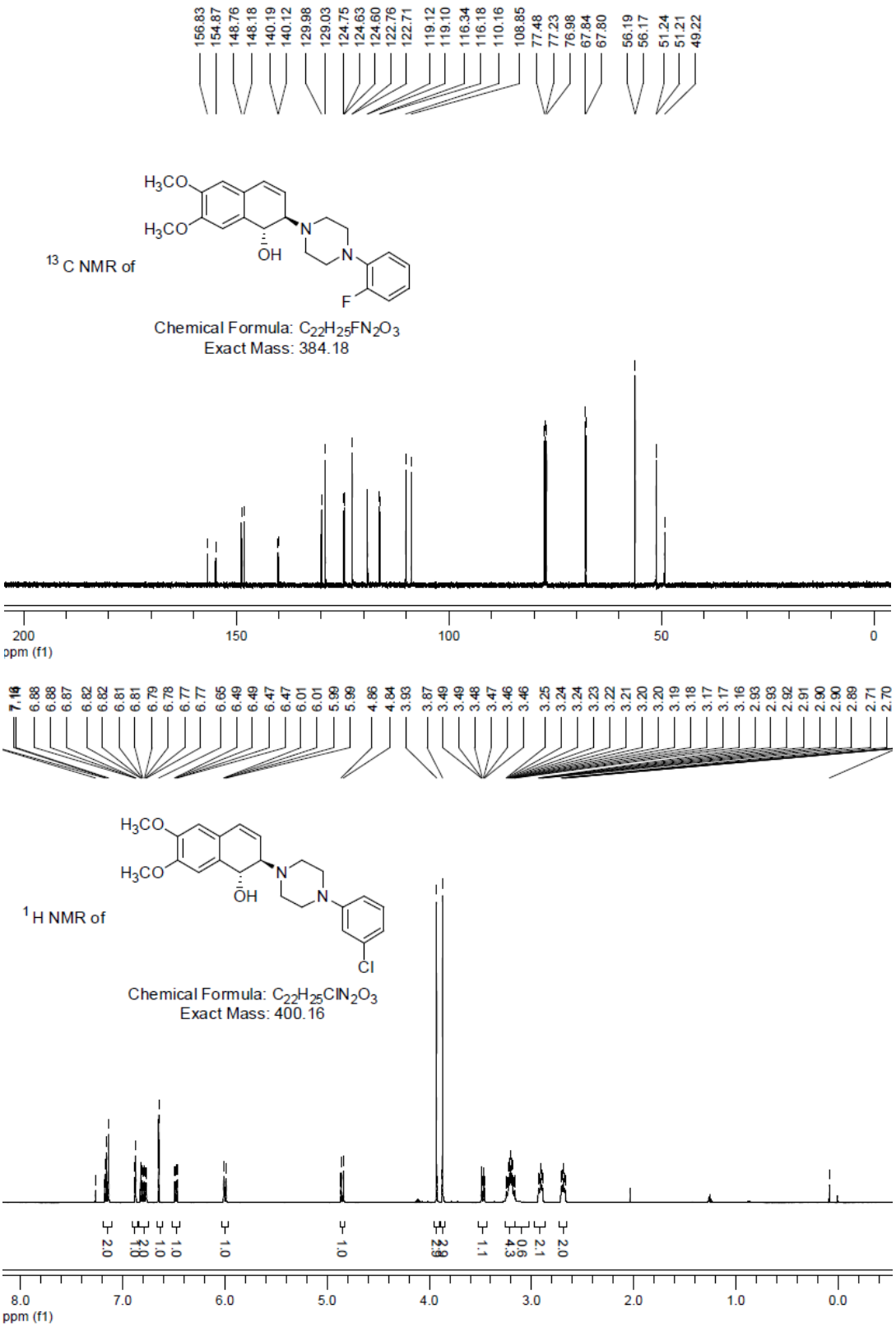
ppm (f1)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H3CO
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F
13 C NMR of
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ppm (f1)
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6.88
6.88
6.87
6.82
6.82
6.81
6.81
6.79
6.78
6.77
6.77
6.65
6.49
6.49
6.47
6.47
6.01
6.01
5.99
5.99
4.86
4.84
3.93
3.87
3.49
3.49
3.48
3.47
3.46
3.46
3.25
3.24
3.24
3.23
3.22
3.21
3.20
3.20
3.19
3.18
3.17
3.16
2.93
2.93
2.92
2.91
2.90
2.90
2.89
2.71
2.70
H3CO
H3CO
OH
N
N
Cl
1 H NMR of
Chemical Formula: C22H25ClN2O3
Exact Mass: 400.16
2.0
1.8
2.0
1.0
1.0
1.0
1.0
2.9
2.9
1.1
0.9
1.3
1.1
2.0
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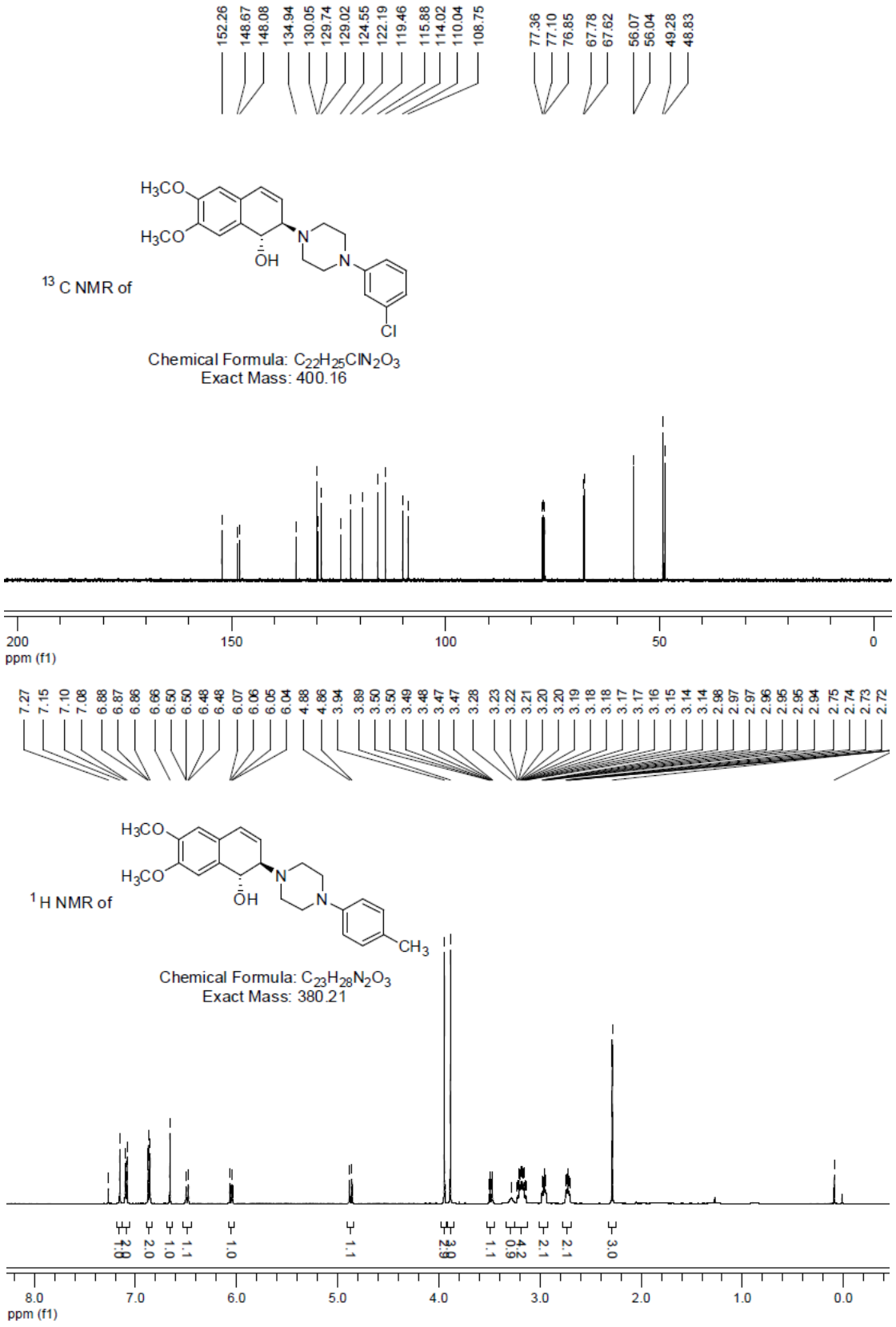
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm (f1)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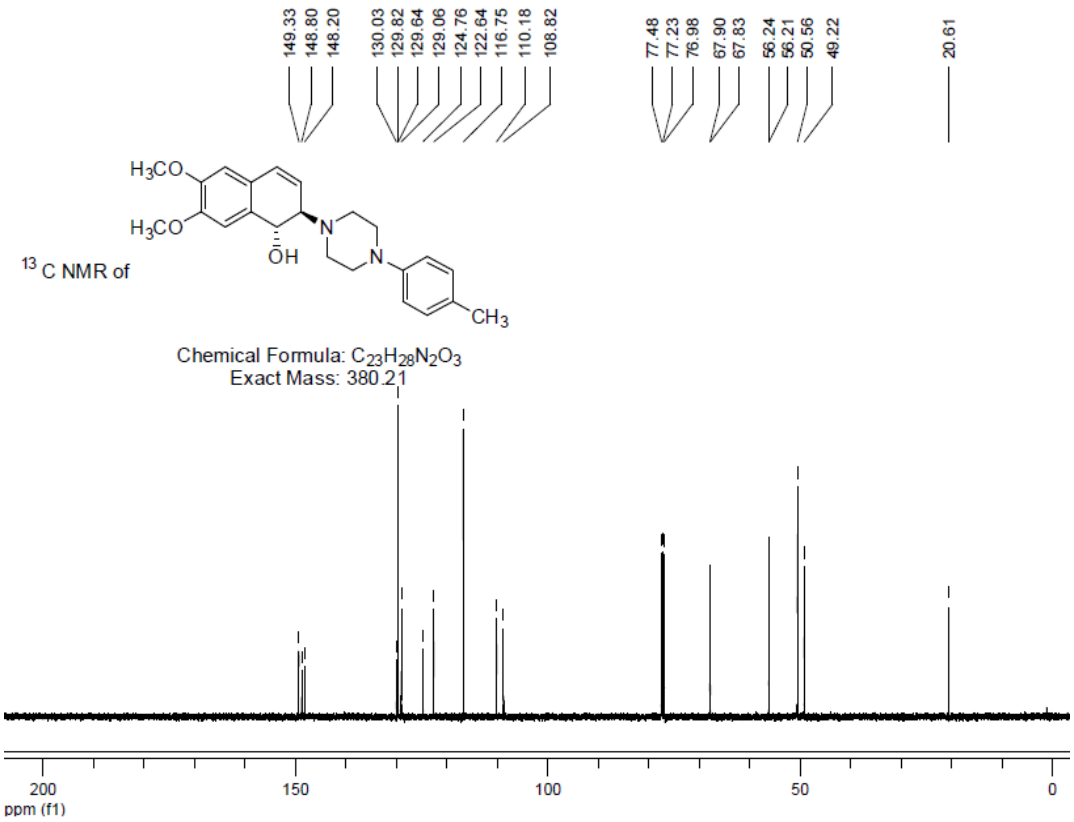
148.67
148.08
134.94
130.05
129.74
129.02
124.55
122.19
119.46
115.88
114.02
110.04
108.75
77.36
77.10
76.85
67.78
67.62
56.07
56.04
49.28
48.83
H3CO
H3CO
OH
N
N
Cl
13 C NMR of
Chemical Formula: C22H25ClN2O3
Exact Mass: 400.16
200
150
100
50
0
ppm (f1)
7.27
7.15
7.10
7.06
6.88
6.87
6.86
6.66
6.50
6.50
6.48
6.48
6.07
6.06
6.05
6.04
4.88
4.86
3.94
3.89
3.50
3.50
3.49
3.48
3.47
3.47
3.28
3.23
3.22
3.21
3.20
3.20
3.19
3.18
3.18
3.17
3.17
3.16
3.15
3.14
3.14
2.98
2.97
2.97
2.96
2.95
2.95
2.94
2.75
2.74
2.73
2.72
H3CO
H3CO
OH
N
N
CH3
1H NMR of
Chemical Formula: C23H28N2O3
Exact Mass: 380.21
2.8
2.0
1.0
1.1
1.0
1.1
3.9
1.1
0.6
1.2
2.1
3.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm (f1)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148.80
148.20
130.03
129.82
129.64
129.06
124.76
122.64
116.75
110.18
108.82
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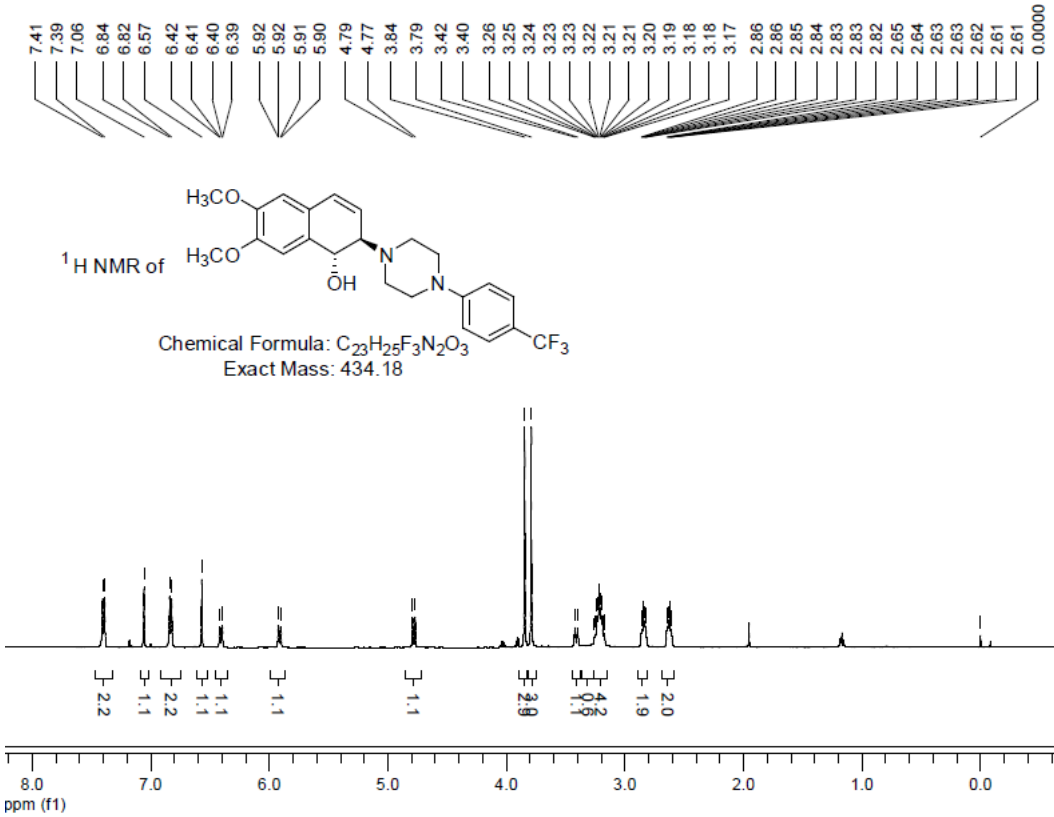
77.23
76.98
67.90
67.83
56.24
56.21
50.56
49.22
20.61
H3CO
H3CO
OH
N
N
CH3
13 C NMR of
Chemical Formula: C23H28N2O3
Exact Mass: 380.21
200
150
100
50
0
ppm (f1)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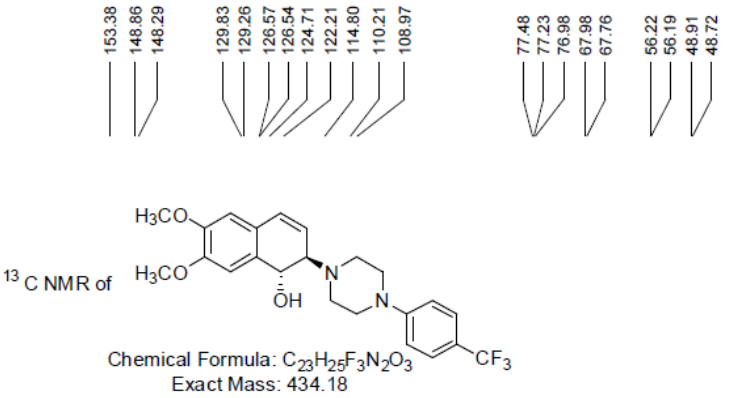
7.39
7.06
6.84
6.82
6.57
6.42
6.41
6.40
6.39
5.92
5.92
5.91
5.90
4.79
4.77
3.84
3.79
3.42
3.40
3.26
3.25
3.24
3.23
3.23
3.22
3.21
3.21
3.20
3.19
3.18
3.18
3.17
2.86
2.86
2.85
2.84
2.83
2.83
2.82
2.65
2.64
2.63
2.63
2.62
2.61
2.61
0.0000
H3CO
H3CO
OH
N
N
CF3
1H NMR of
Chemical Formula: C23H25F3N2O3
Exact Mass: 434.18
2.2
1.1
2.2
1.1
1.1
1.1
1.1
2.9
1.7
4.2
1.9
2.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm (f1)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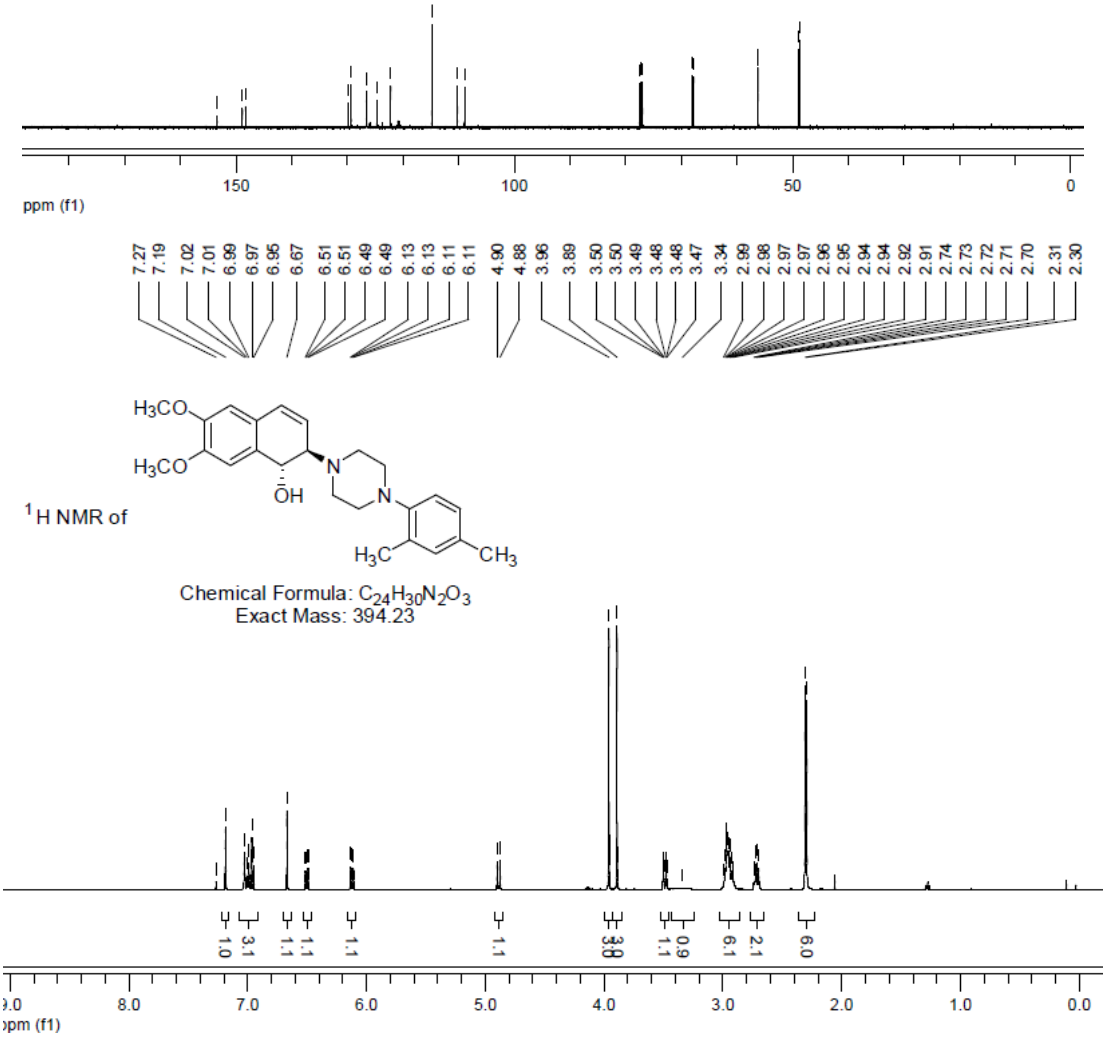
129.26
126.57
126.54
124.71
122.21
114.80
110.21
108.97
77.48
77.23
76.98
67.98
67.76
56.22
56.19
48.91
48.72
^{13}C NMR of
H_3CO
H_3CO
OH
N
N
CF_3
Chemical Formula: $C_{23}H_{25}F_3N_2O_3$
Exact Mass: 434.18


150
100
50
0
ppm (f1)
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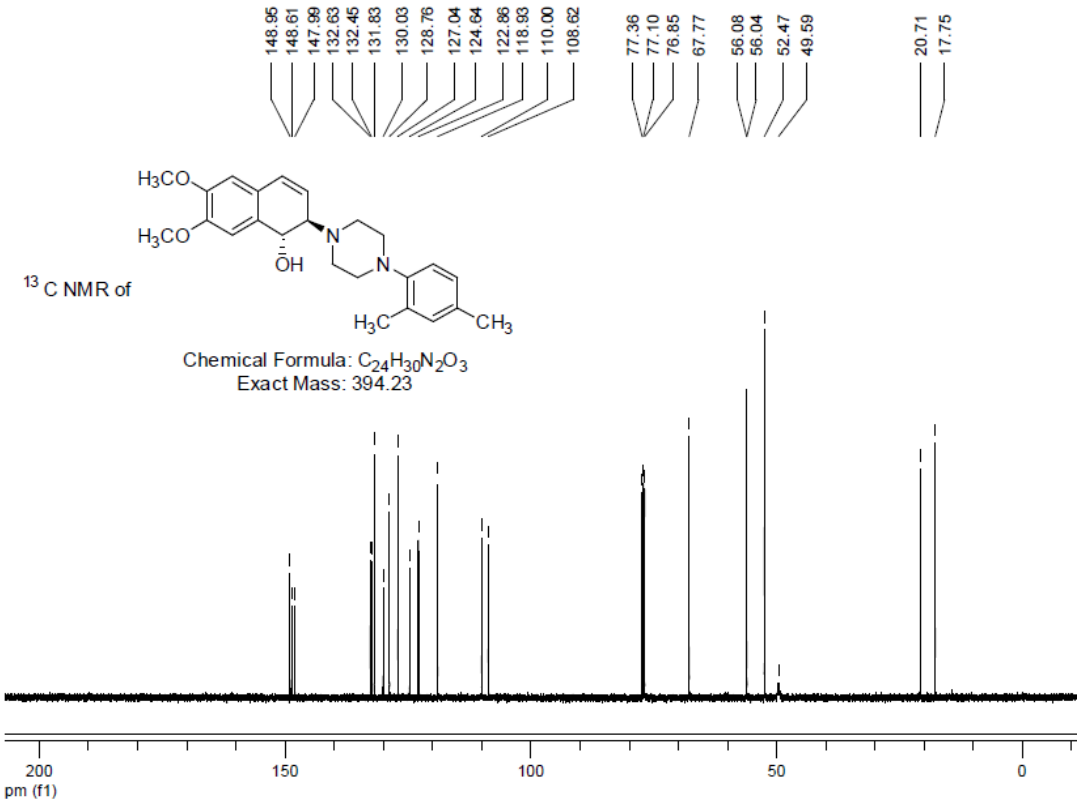
7.19
7.02
7.01
6.99
6.97
6.95
6.67
6.51
6.51
6.49
6.49
6.13
6.13
6.11
6.11
4.90
4.88
3.96
3.89
3.50
3.50
3.49
3.48
3.48
3.47
3.34
2.99
2.98
2.97
2.97
2.96
2.95
2.94
2.94
2.92
2.91
2.74
2.73
2.72
2.71
2.70
2.31
2.30
^{1}H NMR of
H_3CO
H_3CO
OH
N
N
H_3C
CH_3
Chemical Formula: $C_{24}H_{30}N_2O_3$
Exact Mass: 394.23
1.0
3.1
1.1
1.1
1.1
1.1
3.8
1.1
0.9
6.1
2.1
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm (f1)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148.61
147.99
132.63
132.45
131.83
130.03
128.76
127.04
124.64
122.86
118.93
110.00
108.62
77.36
77.10
76.85
67.77
56.08
56.04
52.47
49.59
20.71
17.75
H3CO
H3CO
OH
N
N
H3C
CH3
13 C NMR of
Chemical Formula: C24H30N2O3
Exact Mass: 394.23
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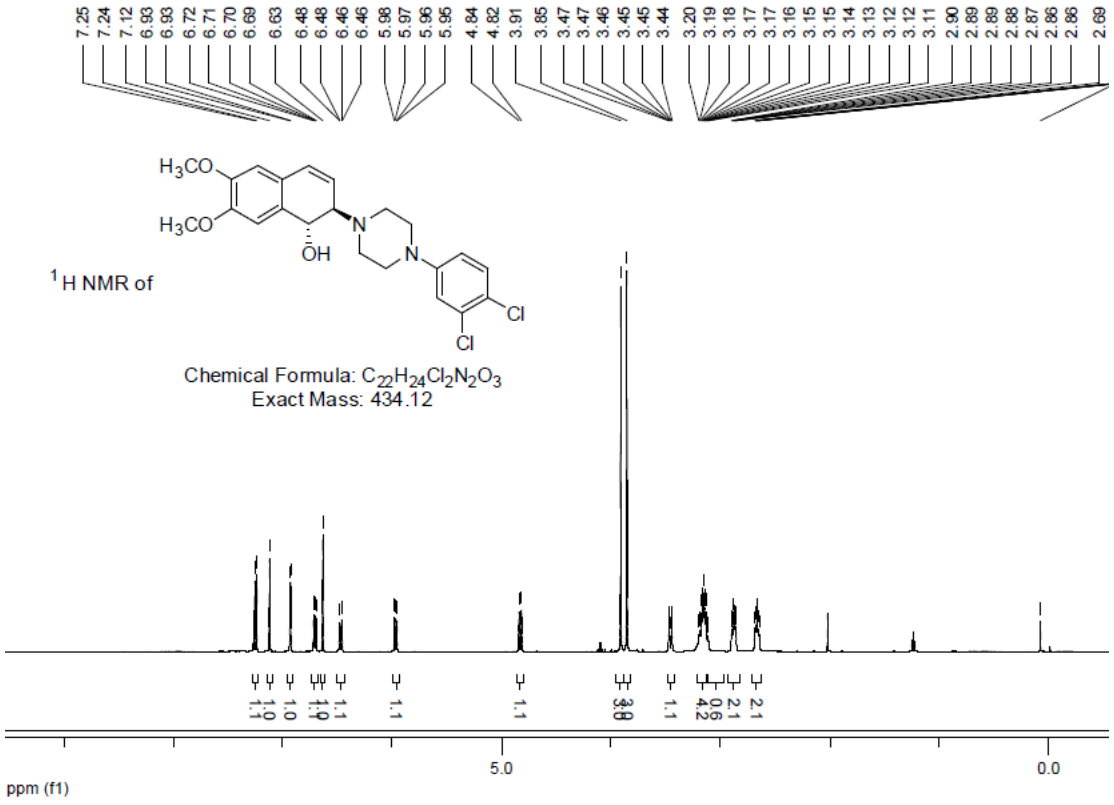
150
100
50
0
pm (f1)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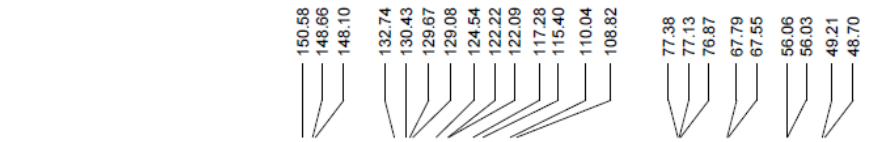
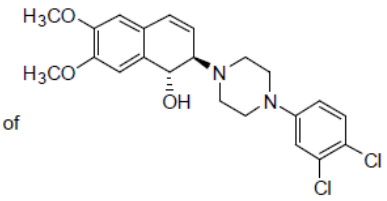
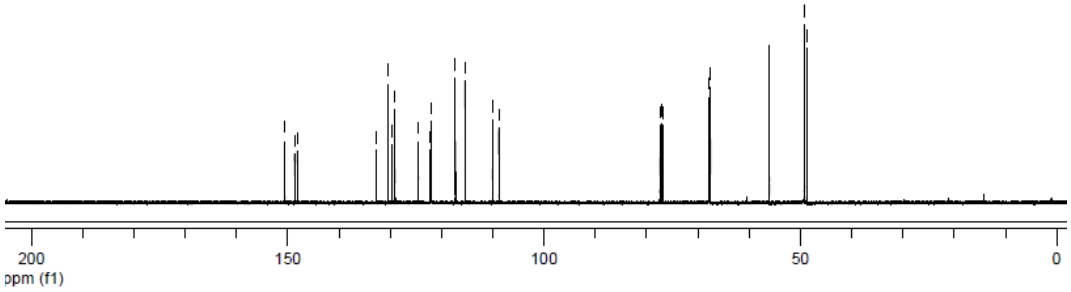
7.24
7.12
6.93
6.93
6.72
6.71
6.70
6.69
6.63
6.48
6.48
6.46
6.46
5.98
5.97
5.96
5.95
4.84
4.82
3.91
3.85
3.47
3.47
3.46
3.45
3.45
3.44
3.20
3.19
3.18
3.17
3.17
3.16
3.15
3.15
3.14
3.13
3.12
3.12
3.11
2.90
2.89
2.89
2.88
2.87
2.86
2.86
2.69
H3CO
H3CO
OH
N
N
Cl
Cl
1 H NMR of
Chemical Formula: C22H24Cl2N2O3
Exact Mass: 434.12
1.10
1.10
1.01
1.19
1.19
1.11
1.11
1.11
3.00
1.11
4.29
2.11
2.11
5.0
0.0
ppm (f1)

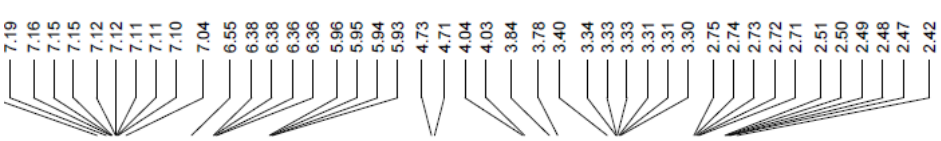


^{13}C NMR of

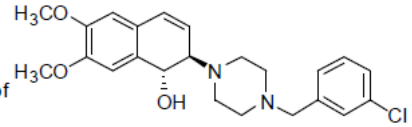


Chemical Formula: $C_{22}H_{24}Cl_2N_2O_3$
Exact Mass: 434.12

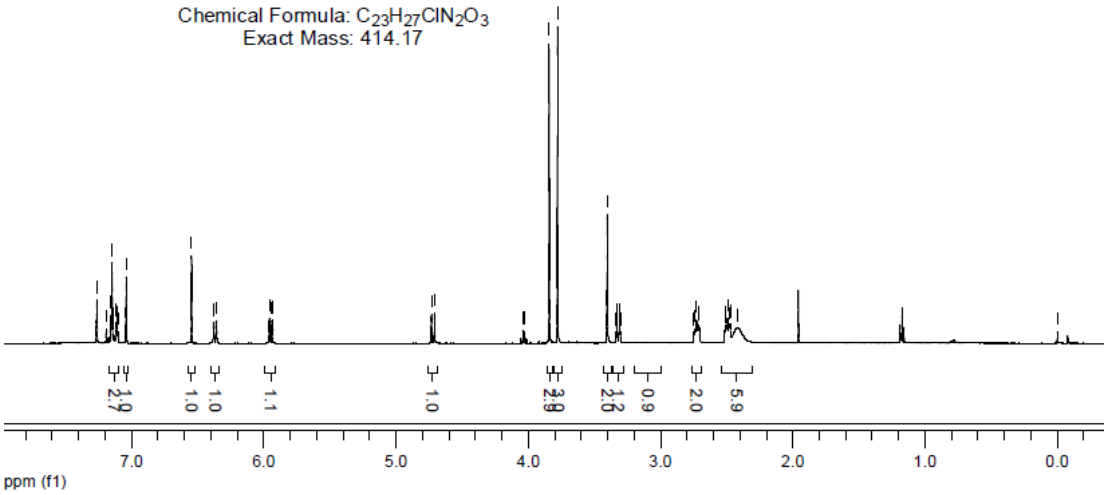


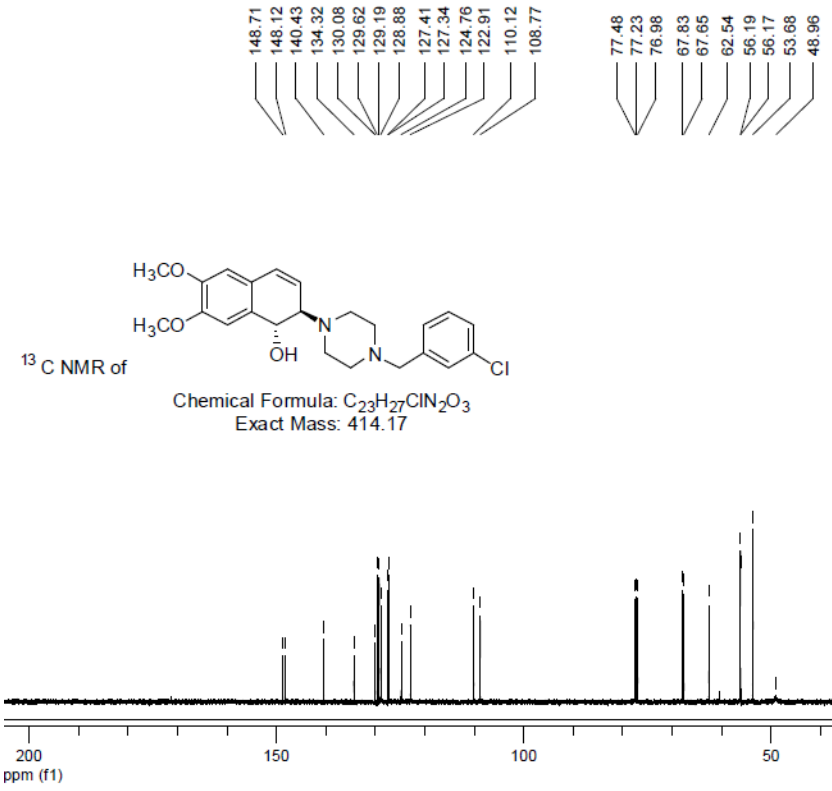


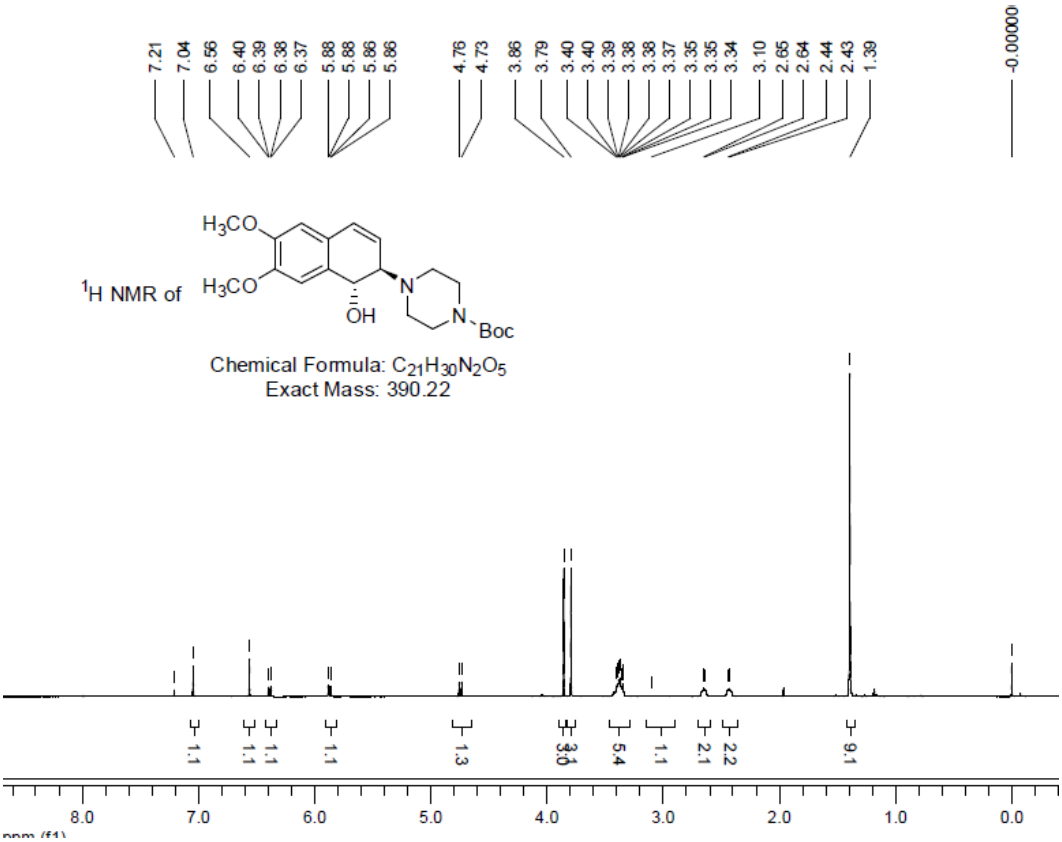
^{1}H NMR of

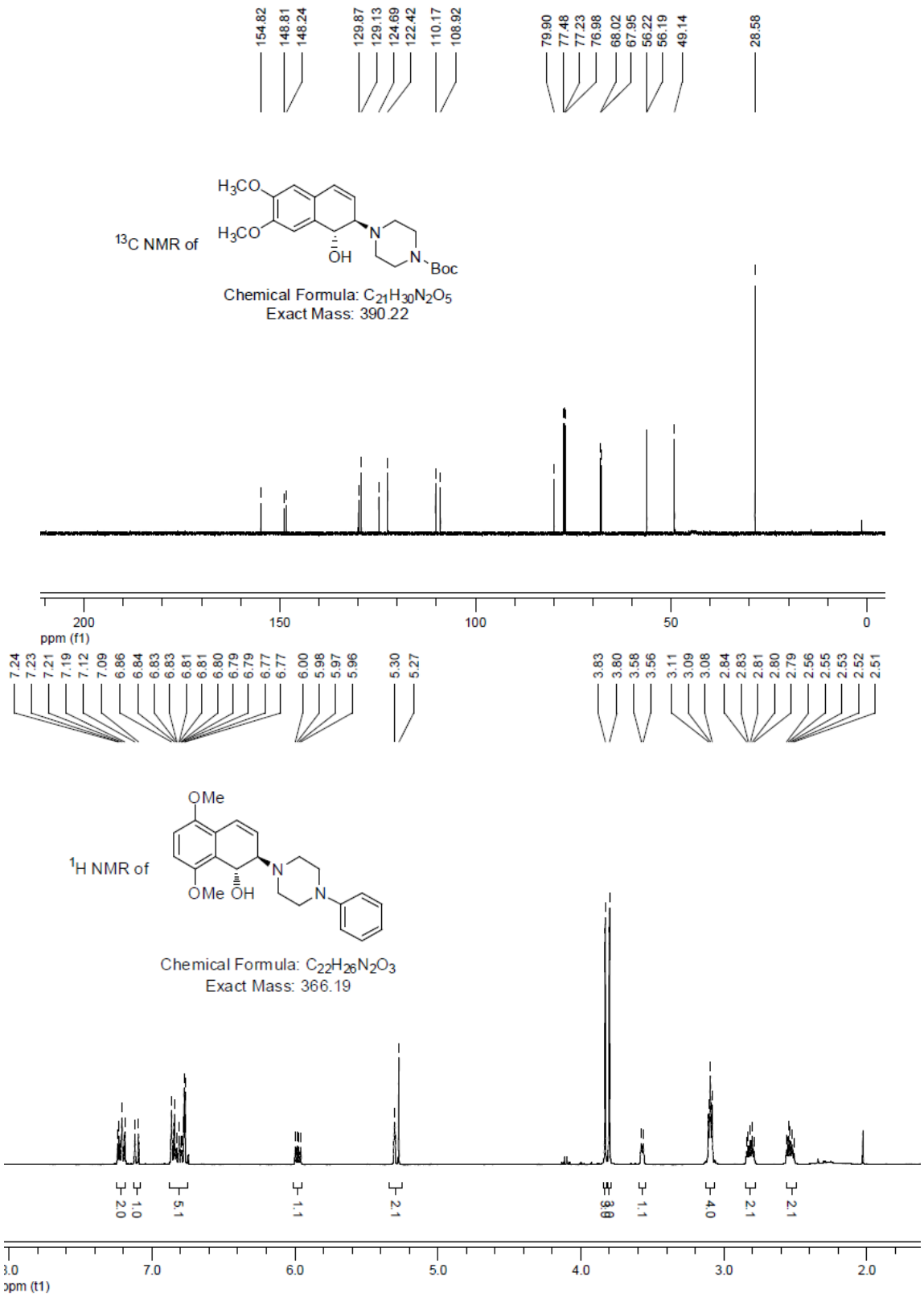


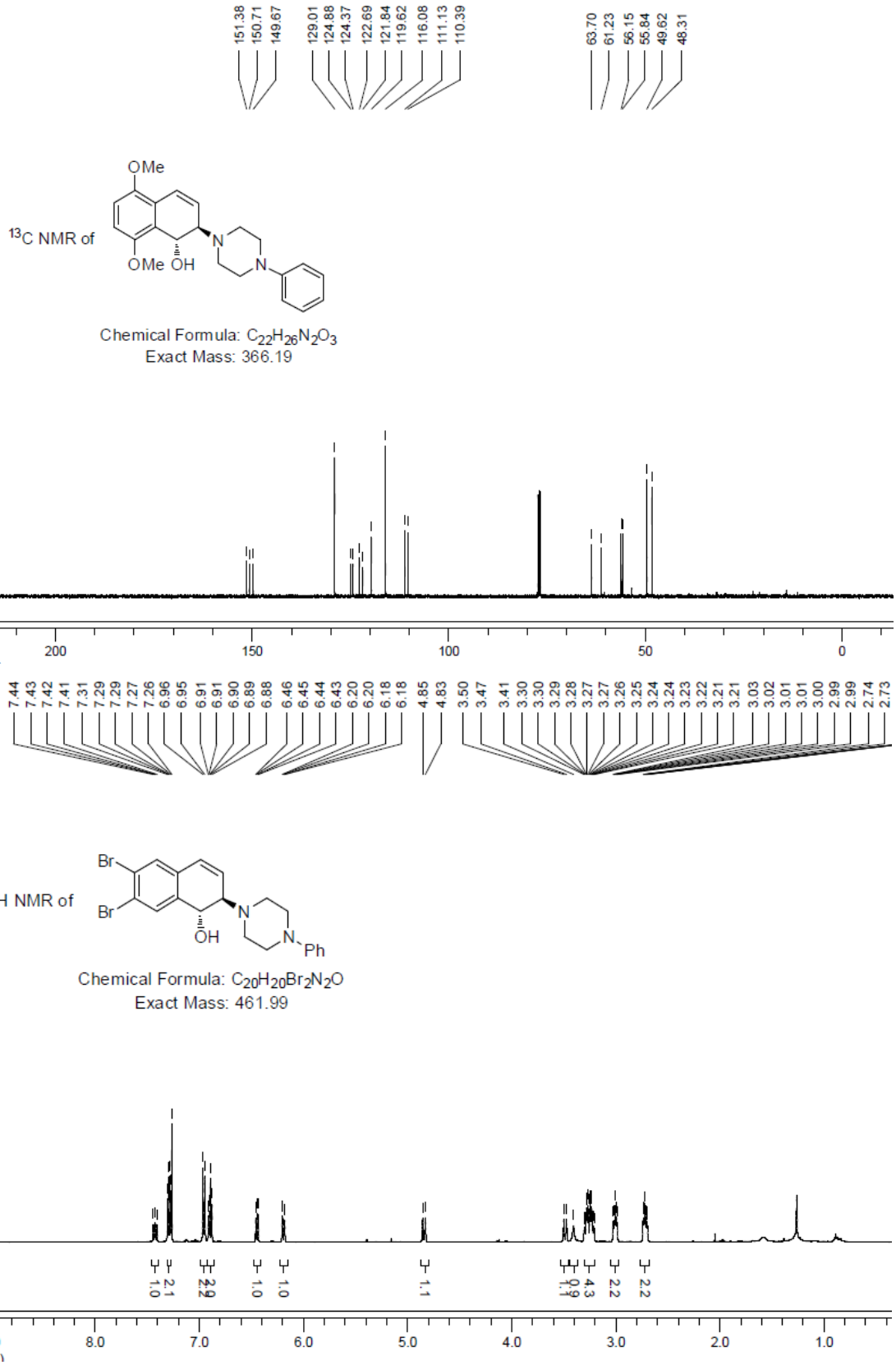
Chemical Formula: $C_{23}H_{27}ClN_2O_3$
Exact Mass: 414.17

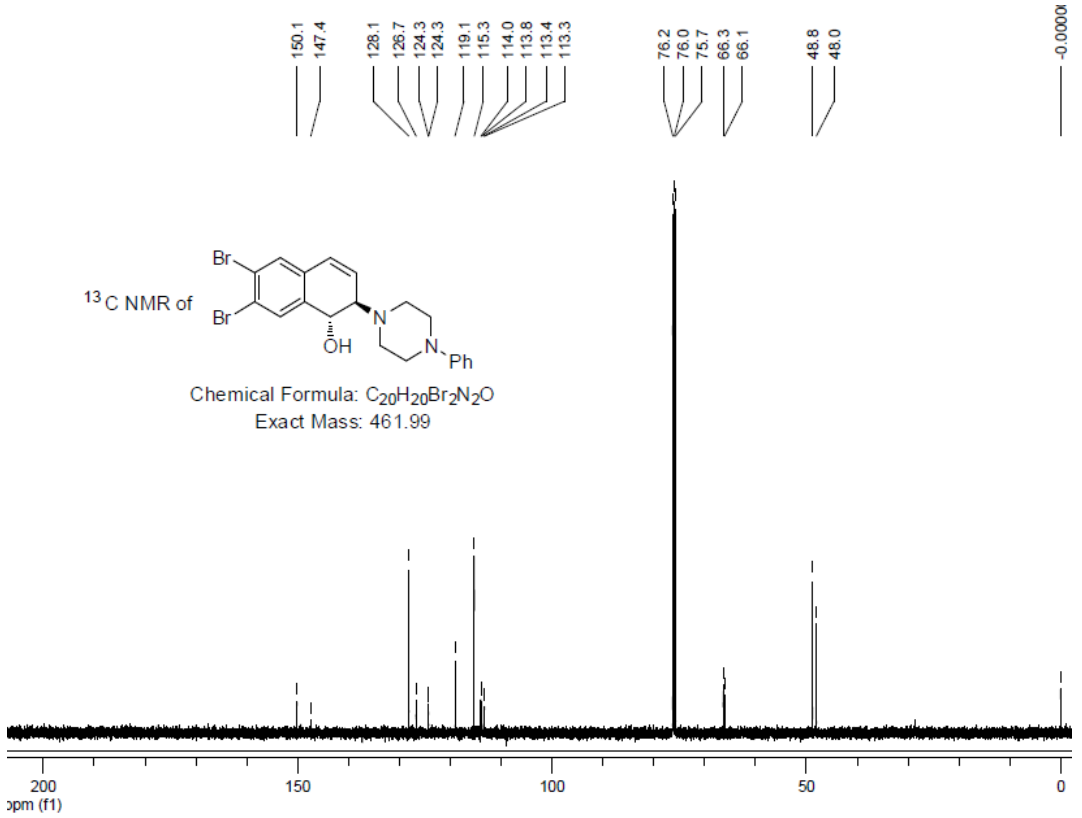



148.71
148.12
140.43
134.32
130.08
129.62
129.19
128.88
127.41
127.34
124.76
122.91
110.12
108.77
77.48
77.23
76.98
67.83
67.65
62.54
56.19
56.17
53.68
48.96
H3CO
H3CO
OH
N
N
Cl
13 C NMR of
Chemical Formula: C23H27ClN2O3
Exact Mass: 414.17
200
150
100
50
0
ppm (f1)


7.21
7.04
6.56
6.40
6.39
6.38
6.37
5.88
5.88
5.86
5.86
4.76
4.73
3.86
3.79
3.40
3.40
3.39
3.38
3.38
3.37
3.35
3.35
3.34
3.10
2.65
2.64
2.44
2.43
1.39
-0.00000
H3CO
H3CO
OH
N
N
Boc
1H NMR of
Chemical Formula: C21H30N2O5
Exact Mass: 390.22
1.1
1.1
1.1
1.1
1.3
3.0
5.4
1.1
2.1
2.2
9.1
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0

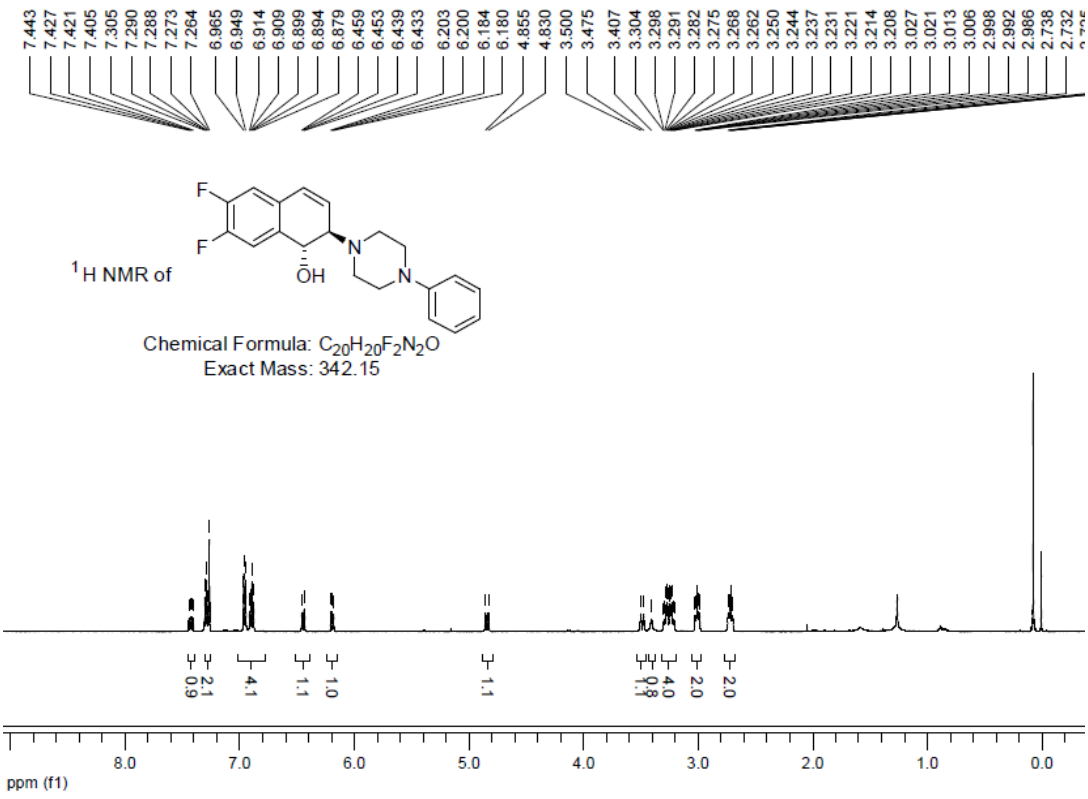

154.82
148.81
148.24
129.87
129.13
124.69
122.42
110.17
108.92
79.90
77.48
77.23
76.98
68.02
67.95
56.22
56.19
49.14
28.58
^{13}C NMR of
H_3CO
H_3CO
OH
N
N
Boc
Chemical Formula: $C_{21}H_{30}N_2O_5$
Exact Mass: 390.22
200
150
100
50
0
ppm (f1)
7.24
7.23
7.21
7.19
7.12
7.09
6.86
6.84
6.83
6.83
6.81
6.81
6.80
6.79
6.79
6.77
6.77
6.00
5.98
5.97
5.96
5.30
5.27
3.83
3.80
3.58
3.56
3.11
3.09
3.08
2.84
2.83
2.81
2.80
2.79
2.56
2.55
2.53
2.52
2.51
^{1}H NMR of
OMe
OMe
OH
N
N
Chemical Formula: $C_{22}H_{26}N_2O_3$
Exact Mass: 366.19
2.0
1.0
5.1
1.1
2.1
3.0
1.1
4.0
2.1
2.1
7.0
6.0
5.0
4.0
3.0
2.0
ppm (t1)


151.38
150.71
149.67
129.01
124.88
124.37
122.69
121.84
119.62
116.08
111.13
110.39
63.70
61.23
56.15
55.84
49.62
48.31
^{13}C NMR of
OMe
OMe OH
N
N
Chemical Formula: $C_{22}H_{26}N_2O_3$
Exact Mass: 366.19
200
150
100
50
0
7.44
7.43
7.42
7.41
7.31
7.29
7.29
7.27
7.26
6.96
6.95
6.91
6.91
6.90
6.89
6.88
6.46
6.45
6.44
6.43
6.20
6.20
6.18
6.18
4.85
4.83
3.50
3.47
3.41
3.30
3.30
3.29
3.28
3.27
3.27
3.26
3.25
3.24
3.24
3.23
3.22
3.21
3.21
3.03
3.02
3.01
3.01
3.00
2.99
2.99
2.74
2.73
^{1}H NMR of
Br
Br
OH
N
N
Ph
Chemical Formula: $C_{20}H_{20}Br_2N_2O$
Exact Mass: 461.99
1.0
2.1
2.2
2.9
1.0
1.0
1.1
1.1
0.9
4.3
2.2
2.2
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
ppm (t1)



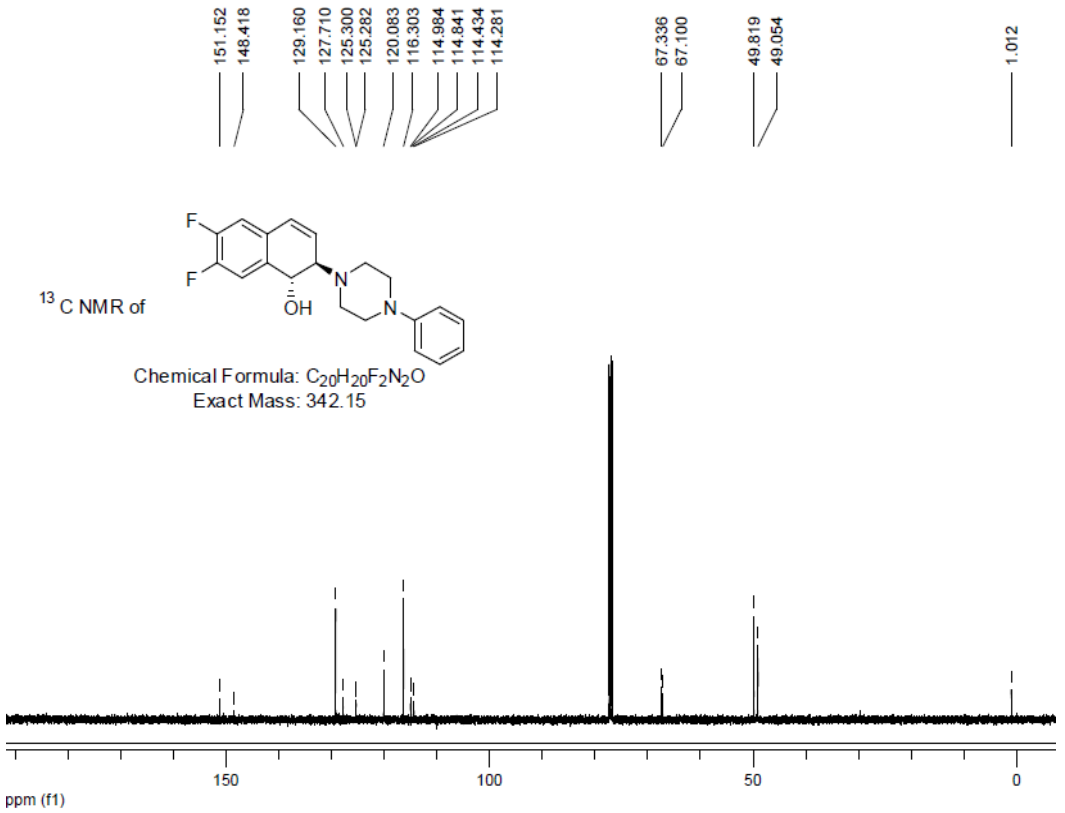
^{13}C NMR of

Chemical Formula: $C_{20}H_{20}Br_2N_2O$
Exact Mass: 461.99



^{1}H NMR of

Chemical Formula: $C_{20}H_{20}F_2N_2O$
Exact Mass: 342.15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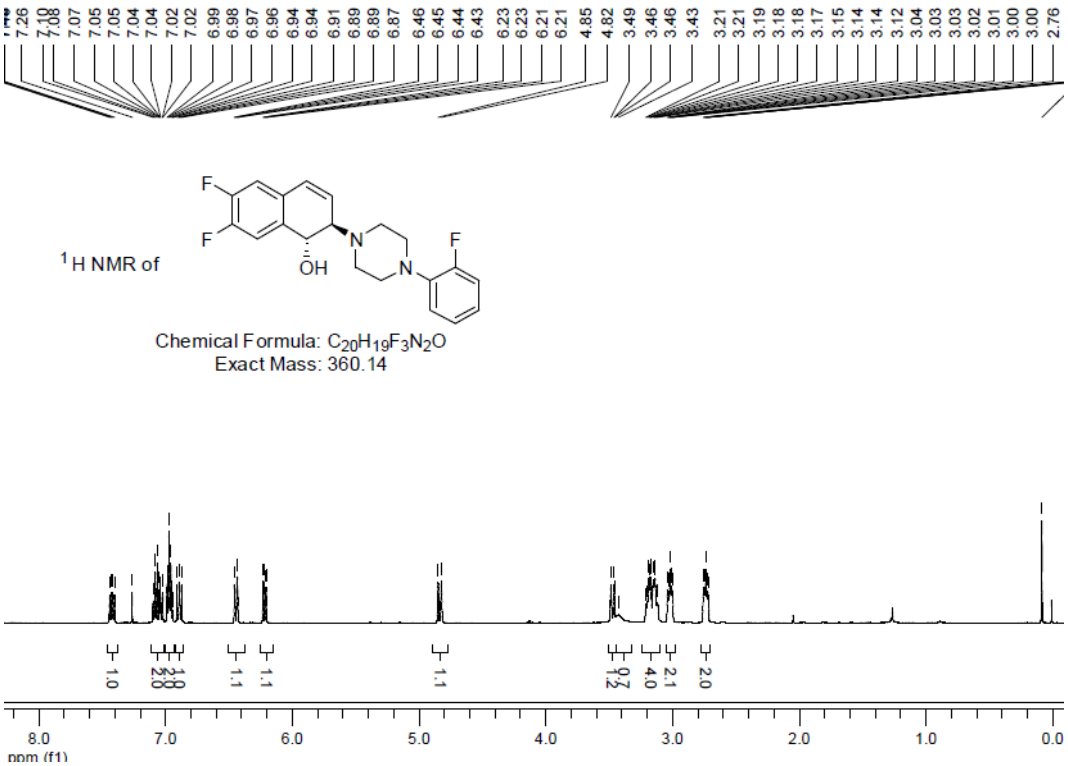
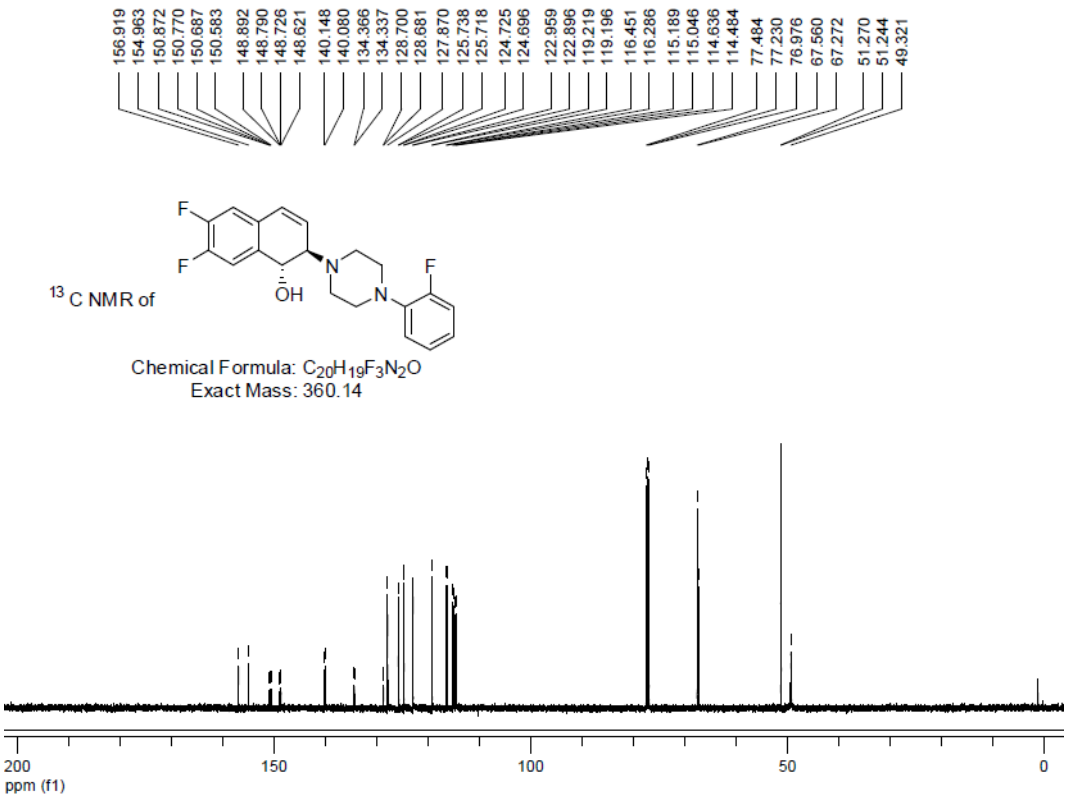
148.418
129.160
127.710
125.300
125.282
120.083
116.303
114.984
114.841
114.434
114.281
67.336
67.100
49.819
49.054
1.012
F
F
OH
N
N
13 C NMR of
Chemical Formula: C20H20F2N2O
Exact Mass: 342.15
150
100
50
0
ppm (f1)


7.26
7.10
7.08
7.07
7.05
7.05
7.04
7.04
7.02
7.02
6.99
6.98
6.97
6.96
6.94
6.94
6.91
6.89
6.89
6.87
6.46
6.45
6.44
6.43
6.23
6.23
6.21
6.21
4.85
4.82
3.49
3.46
3.46
3.43
3.21
3.21
3.19
3.18
3.18
3.17
3.15
3.14
3.14
3.12
3.04
3.03
3.03
3.02
3.01
3.00
3.00
2.76
F
F
OH
N
N
F
1H NMR of
Chemical Formula: C20H19F3N2O
Exact Mass: 360.14
1.0
2.8
1.1
1.1
1.1
0.7
2.1
4.0
2.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm (f1)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150.872
150.770
150.687
150.583
148.892
148.790
148.726
148.621
140.148
140.080
134.366
134.337
128.700
128.681
127.870
125.738
125.718
124.725
124.696
122.959
122.896
119.219
119.196
116.451
116.286
115.189
115.046
114.636
114.484
77.484
77.230
76.976
67.560
67.272
51.270
51.244
49.321
F
F
OH
N
N
F
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Chemical Formula: C20H19F3N2O
Exact Mass: 360.14
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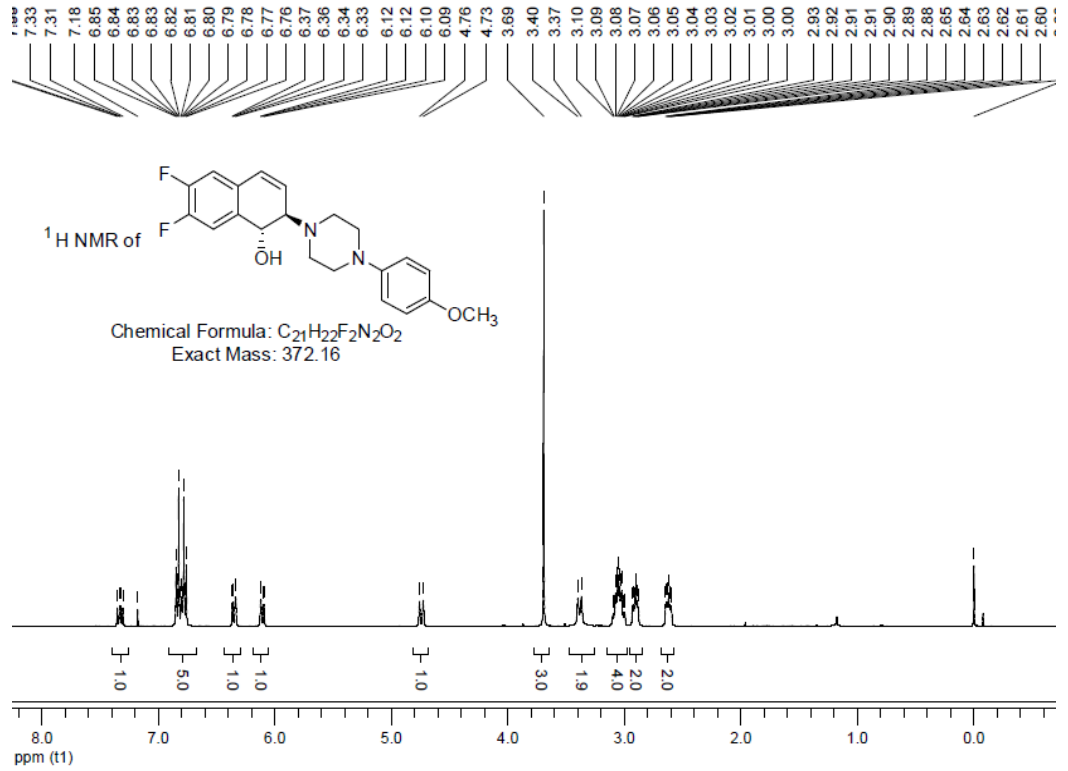
150
100
50
0
ppm (f1)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7.18
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6.84
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6.82
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6.80
6.79
6.78
6.77
6.76
6.37
6.36
6.34
6.33
6.12
6.12
6.10
6.09
4.76
4.73
3.69
3.40
3.37
3.10
3.09
3.08
3.07
3.06
3.05
3.04
3.03
3.02
3.01
3.00
3.00
2.93
2.92
2.91
2.91
2.90
2.89
2.88
2.65
2.64
2.63
2.62
2.61
2.60
F
F
OH
N
N
OCH3
1 H NMR of
Chemical Formula: C21H22F2N2O2
Exact Mass: 372.16
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5.0
1.0
1.0
1.0
3.0
1.9
4.0
2.0
2.0
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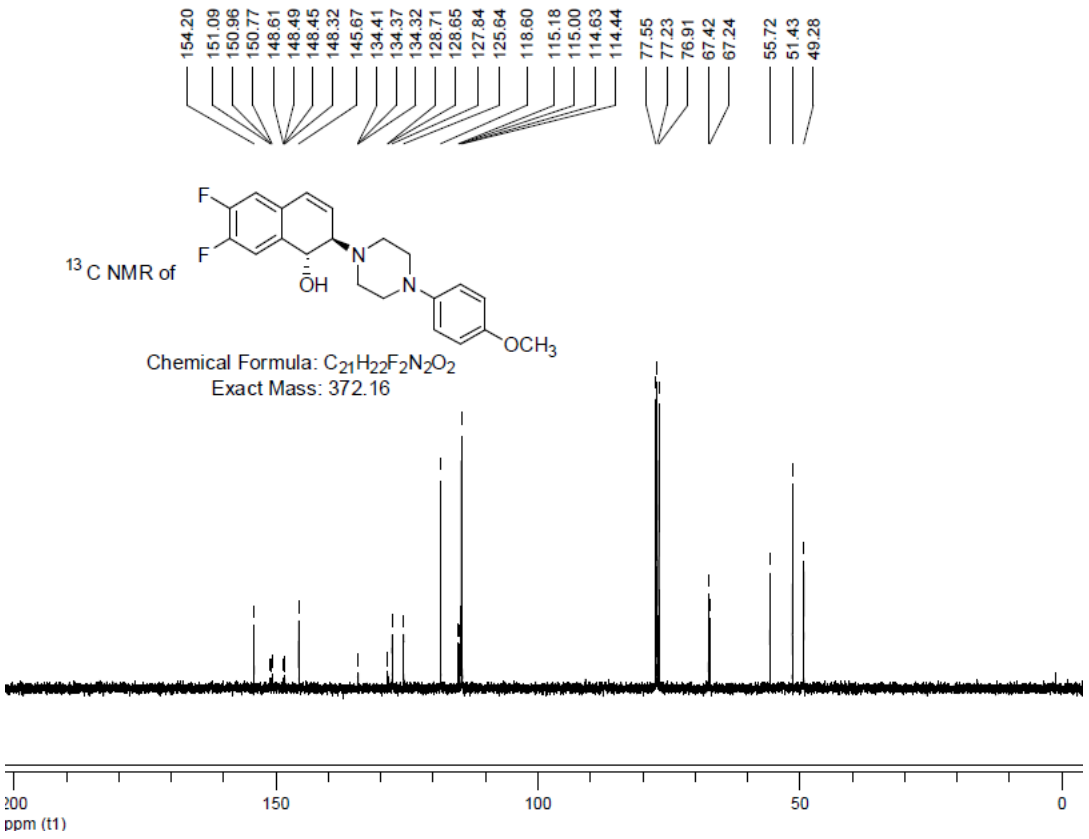
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm (t1)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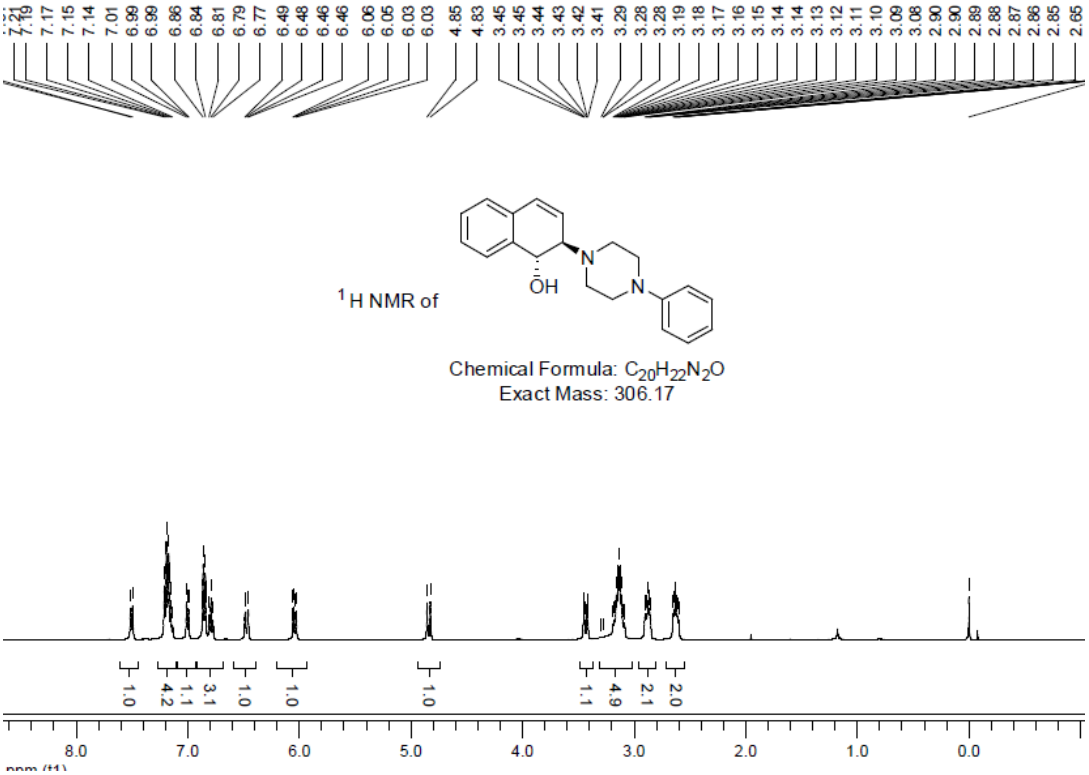
151.09
150.96
150.77
148.61
148.49
148.45
148.32
145.67
134.41
134.37
134.32
128.71
128.65
127.84
125.64
118.60
115.18
115.00
114.63
114.44
77.55
77.23
76.91
67.42
67.24
55.72
51.43
49.28
13 C NMR of
F
F
OH
N
N
OCH3
Chemical Formula: C21H22F2N2O2
Exact Mass: 372.16
200
150
100
50
0
ppm (t1)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7.15
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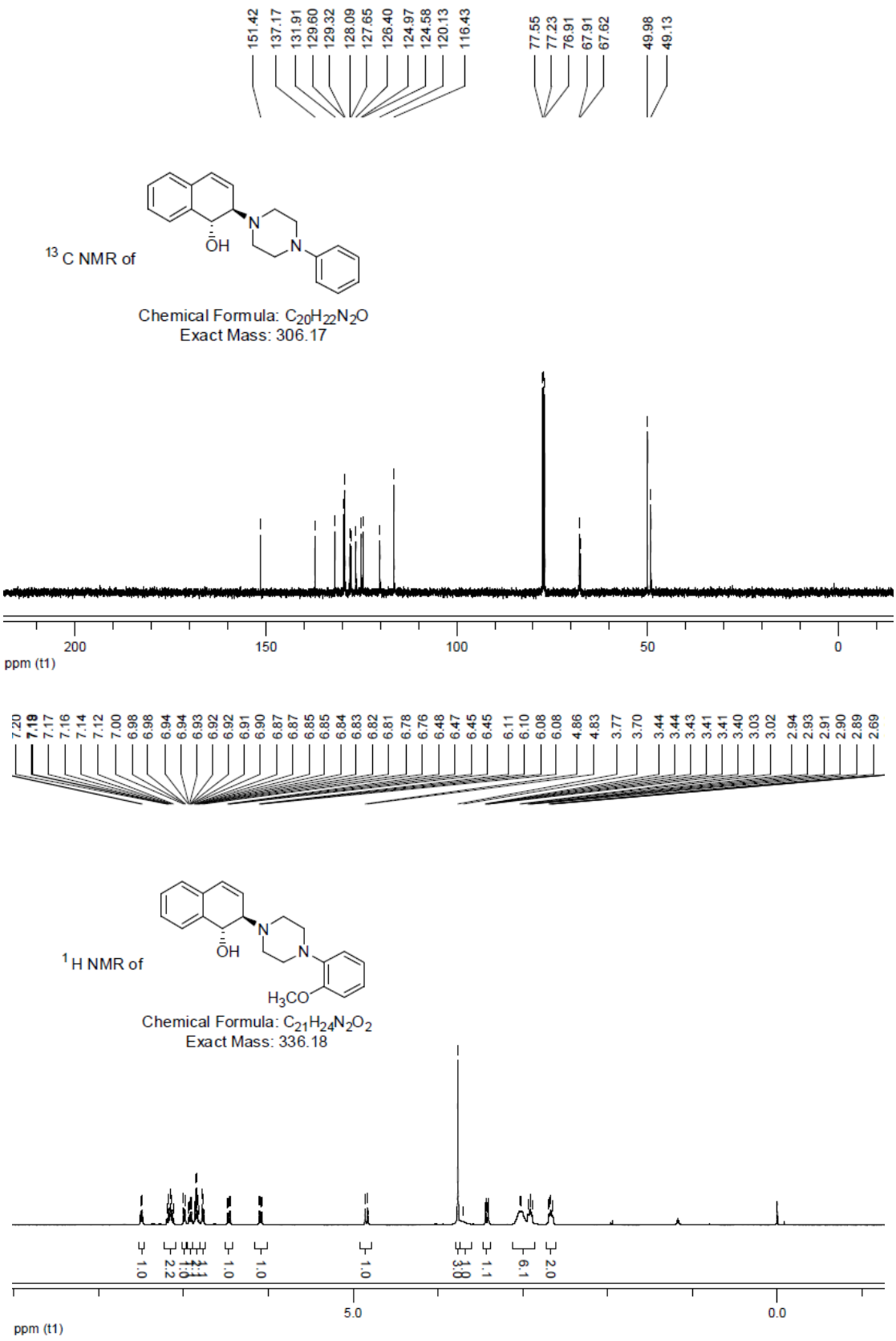
6.99
6.86
6.84
6.81
6.79
6.77
6.49
6.48
6.46
6.46
6.06
6.05
6.03
6.03
4.85
4.83
3.45
3.45
3.44
3.43
3.42
3.41
3.29
3.28
3.28
3.19
3.18
3.17
3.16
3.15
3.14
3.14
3.13
3.12
3.11
3.10
3.09
3.08
2.90
2.90
2.89
2.88
2.87
2.86
2.85
2.65
1 H NMR of
OH
N
N
Chemical Formula: C20H22N2O
Exact Mass: 306.17
1.0
4.2
1.1
3.1
1.0
1.0
1.0
1.1
4.9
2.1
2.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0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137.17
131.91
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129.32
128.09
127.65
126.40
124.97
124.58
120.13
116.43
77.55
77.23
76.91
67.91
67.62
49.98
49.13
OH
N
N
13 C NMR of
Chemical Formula: C20H22N2O
Exact Mass: 306.17
200
150
100
50
0
ppm (t1)
7.20
7.19
7.17
7.16
7.14
7.12
7.00
6.98
6.98
6.94
6.94
6.93
6.92
6.92
6.91
6.90
6.87
6.87
6.85
6.85
6.84
6.83
6.82
6.81
6.78
6.76
6.48
6.47
6.45
6.45
6.11
6.10
6.08
6.08
4.86
4.83
3.77
3.70
3.44
3.44
3.43
3.41
3.41
3.40
3.03
3.02
2.94
2.93
2.91
2.90
2.89
2.69
OH
N
N
H3CO
1 H NMR of
Chemical Formula: C21H24N2O2
Exact Mass: 336.18
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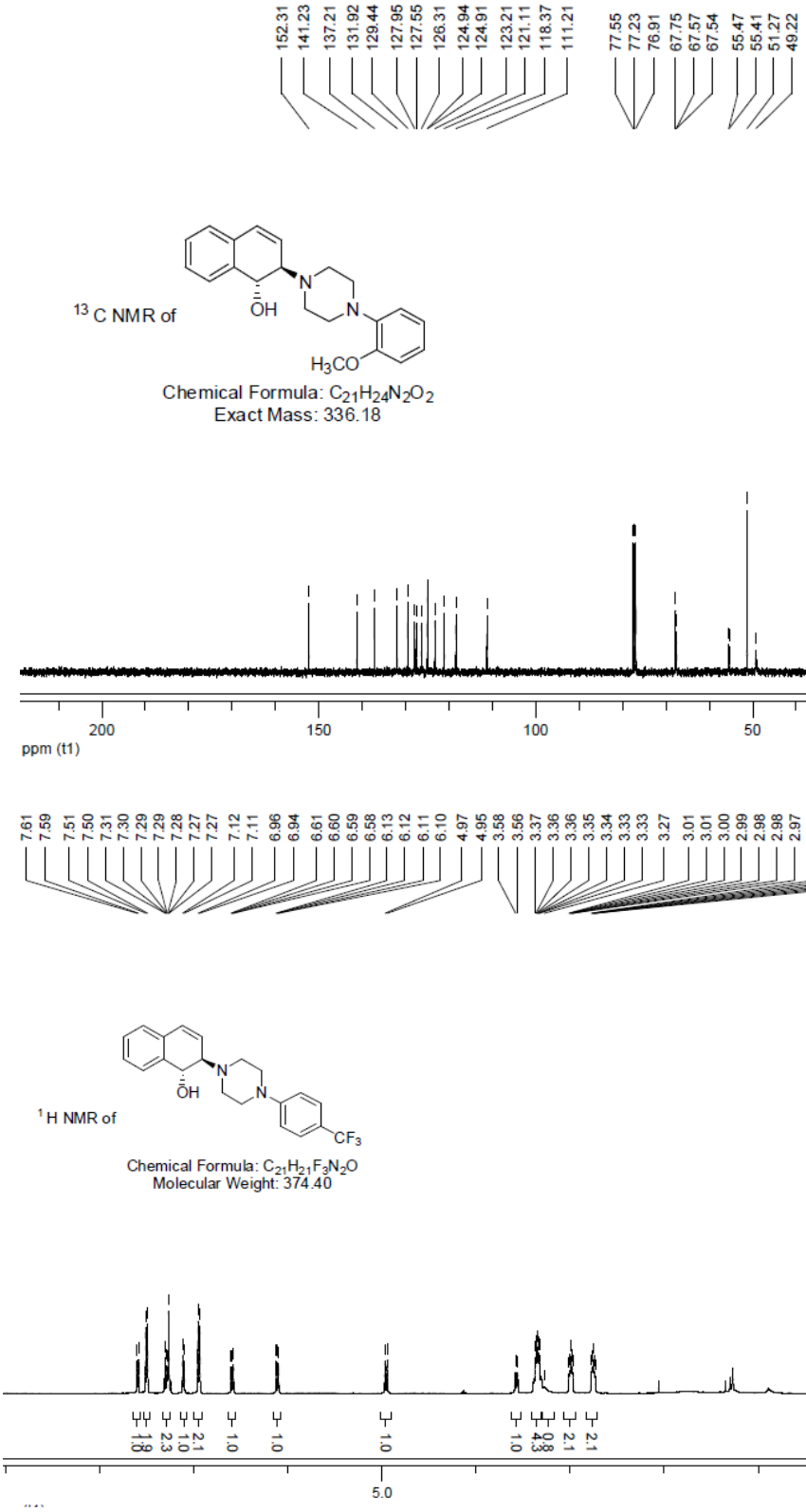
2.2
1.0
1.0
1.0
3.8
1.1
9.1
2.0
5.0
0.0
ppm (t1)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141.23
137.21
131.92
129.44
127.95
127.55
126.31
124.94
124.91
123.21
121.11
118.37
111.21
77.55
77.23
76.91
67.75
67.57
67.54
55.47
55.41
51.27
49.22
13 C NMR of
OH
N
N
H3CO
Chemical Formula: C21H24N2O2
Exact Mass: 336.18
200
150
100
50
0
ppm (t1)
7.61
7.59
7.51
7.50
7.31
7.30
7.29
7.29
7.28
7.27
7.27
7.12
7.11
6.96
6.94
6.61
6.60
6.59
6.58
6.13
6.12
6.11
6.10
4.97
4.95
3.58
3.56
3.37
3.36
3.36
3.35
3.34
3.33
3.33
3.27
3.01
3.01
3.00
2.99
2.98
2.98
2.97
2.77
2.77
2.76
2.75
2.75
2.74
2.73
1500
1000
500
0
1 H NMR of
OH
N
N
CF3
Chemical Formula: C21H21F3N2O
Molecular Weight: 374.40
11.8
2.3
10.0
2.1
1.0
1.0
1.0
1.0
0.8
0.3
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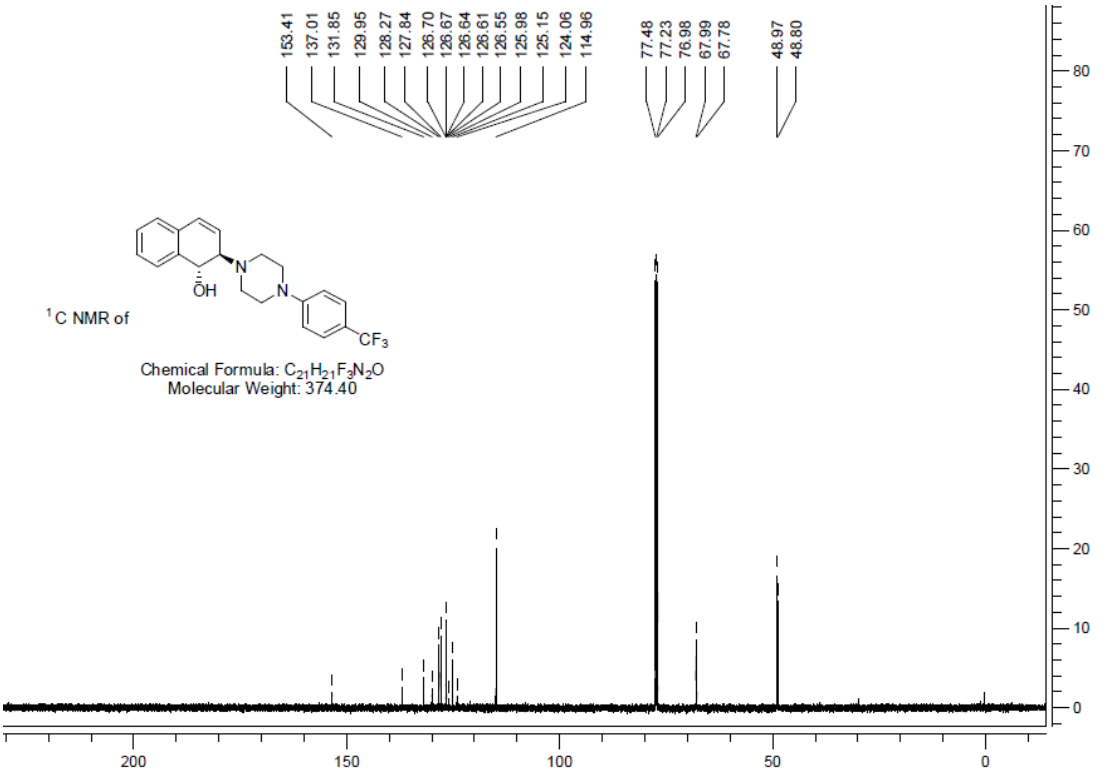
2.1
5.0
0.0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137.01
131.85
129.95
128.27
127.84
126.70
126.67
126.64
126.61
126.55
125.98
125.15
124.06
114.96
77.48
77.23
76.98
67.99
67.78
48.97
48.80
OH
N
N
CF3
1C NMR of
Chemical Formula: C21H21F3N2O
Molecular Weight: 374.40
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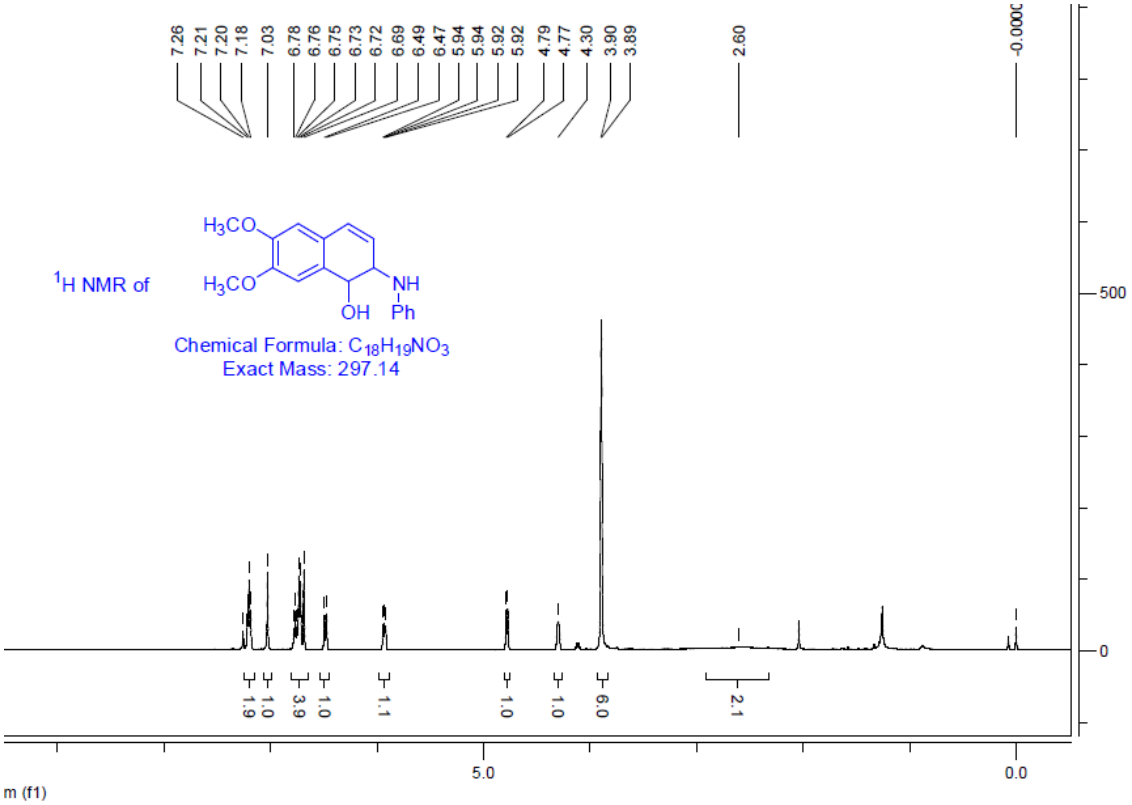
150
100
50
0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7.21
7.20
7.18
7.03
6.78
6.76
6.75
6.73
6.72
6.69
6.49
6.47
5.94
5.94
5.92
5.92
4.79
4.77
4.30
3.90
3.89
2.60
-0.000
H3CO
H3CO
OH
NH
Ph
1H NMR of
Chemical Formula: C18H19NO3
Exact Mass: 297.14
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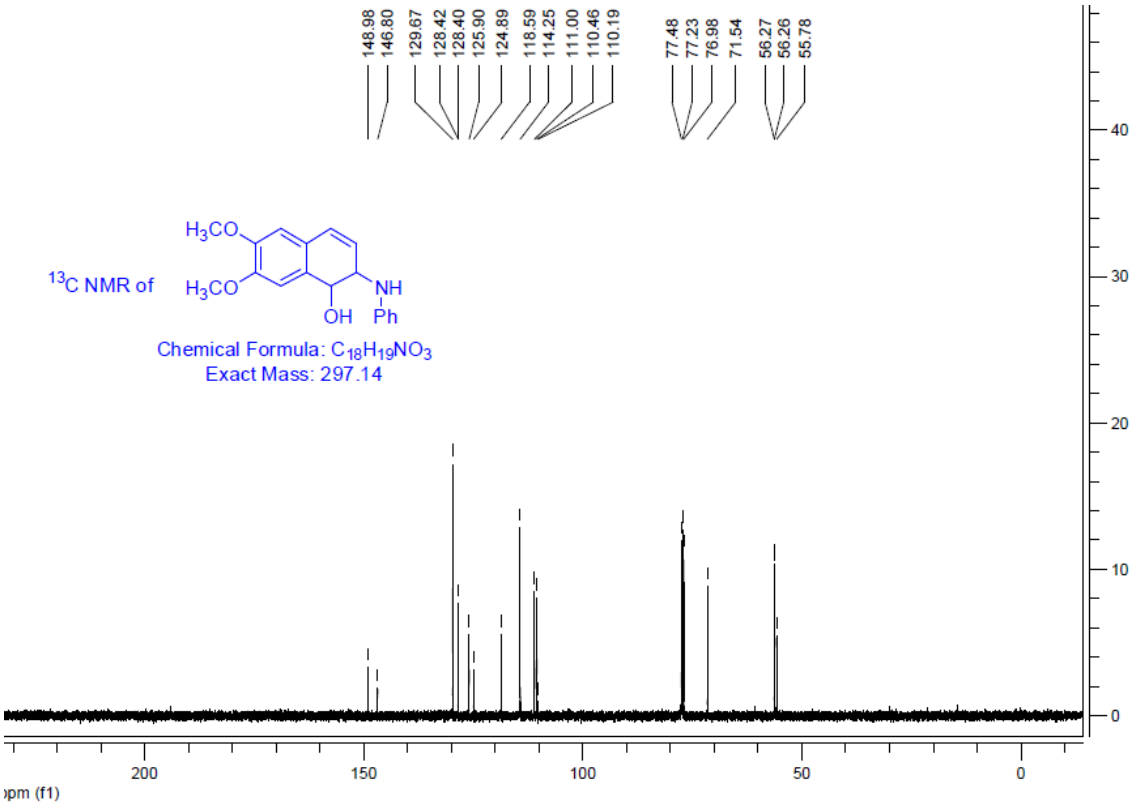
1.0
3.9
1.0
1.1
1.0
1.0
6.0
2.1
5.0
0.0
m (f1)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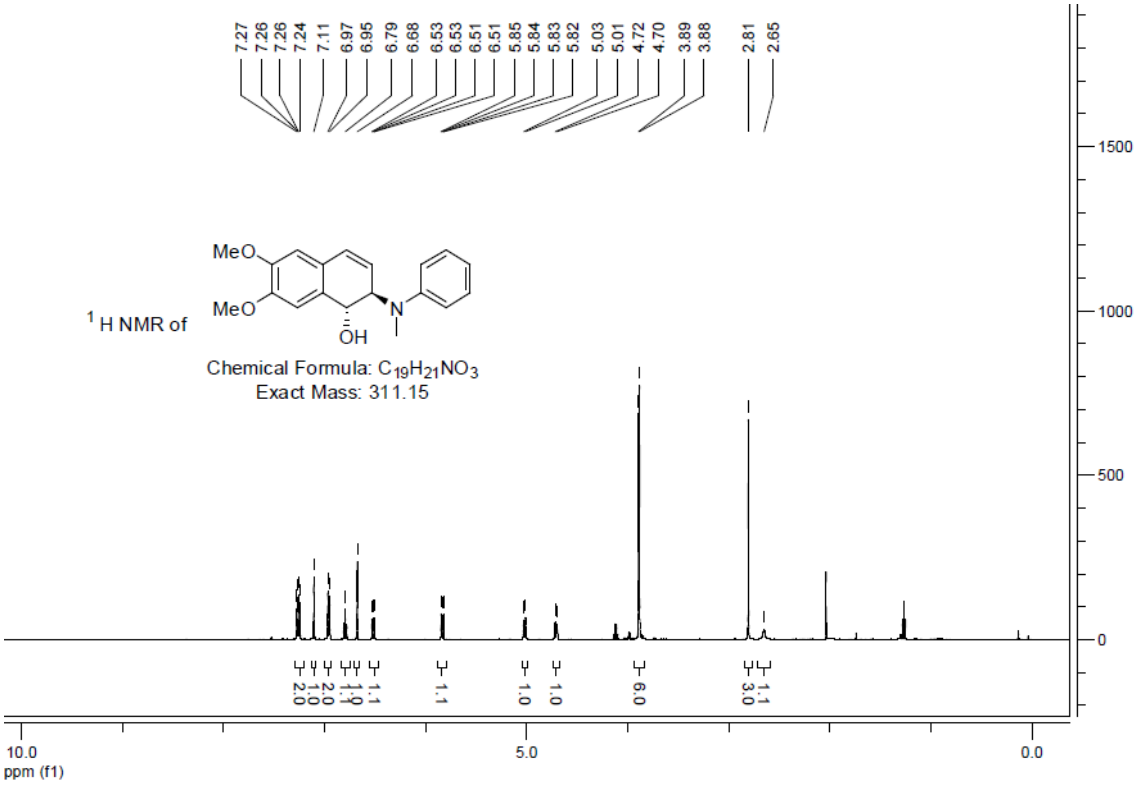
146.80
129.67
128.42
128.40
125.90
124.89
118.59
114.25
111.00
110.46
110.19
77.48
77.23
76.98
71.54
56.27
56.26
55.78
^{13}C NMR of
H_3CO
H_3CO
NH
Ph
OH
Chemical Formula: $C_{18}H_{19}NO_3$
Exact Mass: 297.14
40
30
20
10
0
200
150
100
50
0
ppm (f1)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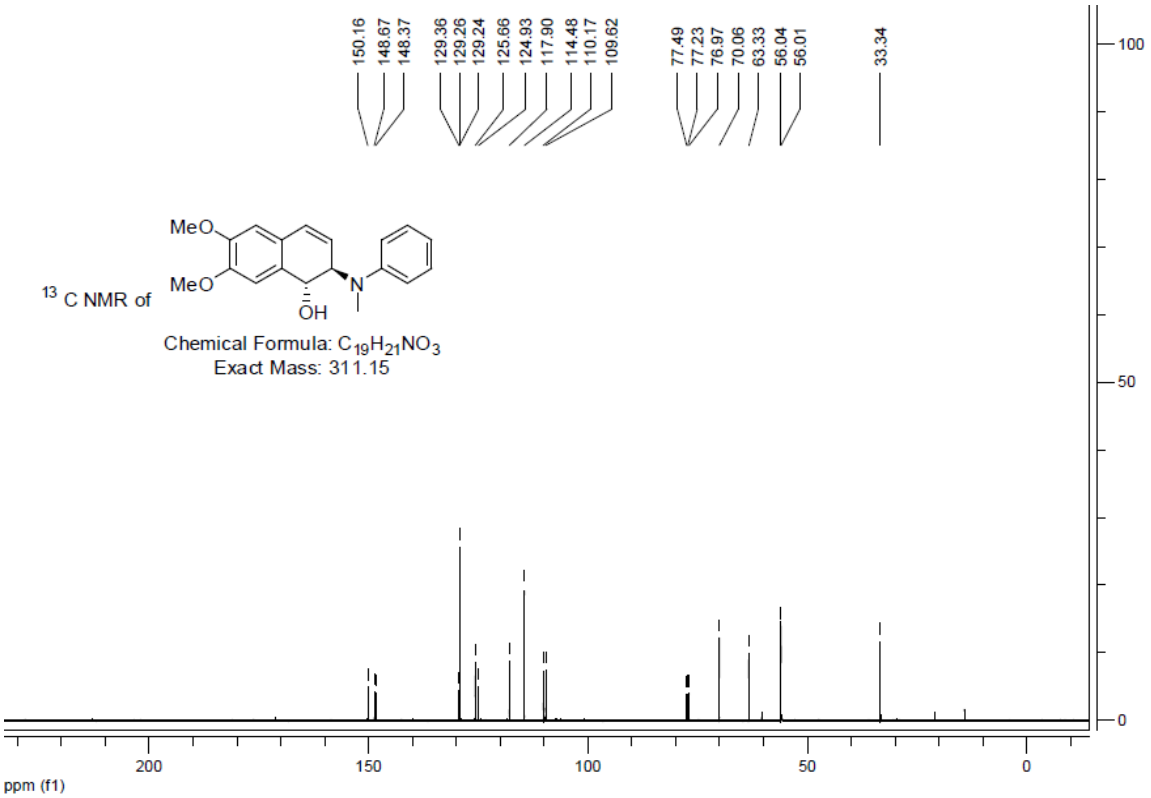
7.26
7.26
7.24
7.11
6.97
6.95
6.79
6.68
6.53
6.53
6.51
6.51
5.85
5.84
5.83
5.82
5.03
5.01
4.72
4.70
3.89
3.88
2.81
2.65
^{1}H NMR of
MeO
MeO
N
OH
Chemical Formula: $C_{19}H_{21}NO_3$
Exact Mass: 311.15
1500
1000
500
0
2.0
1.0
1.0
1.1
1.1
1.1
1.1
1.0
1.0
6.0
3.0
1.1
10.0
5.0
0.0
ppm (f1)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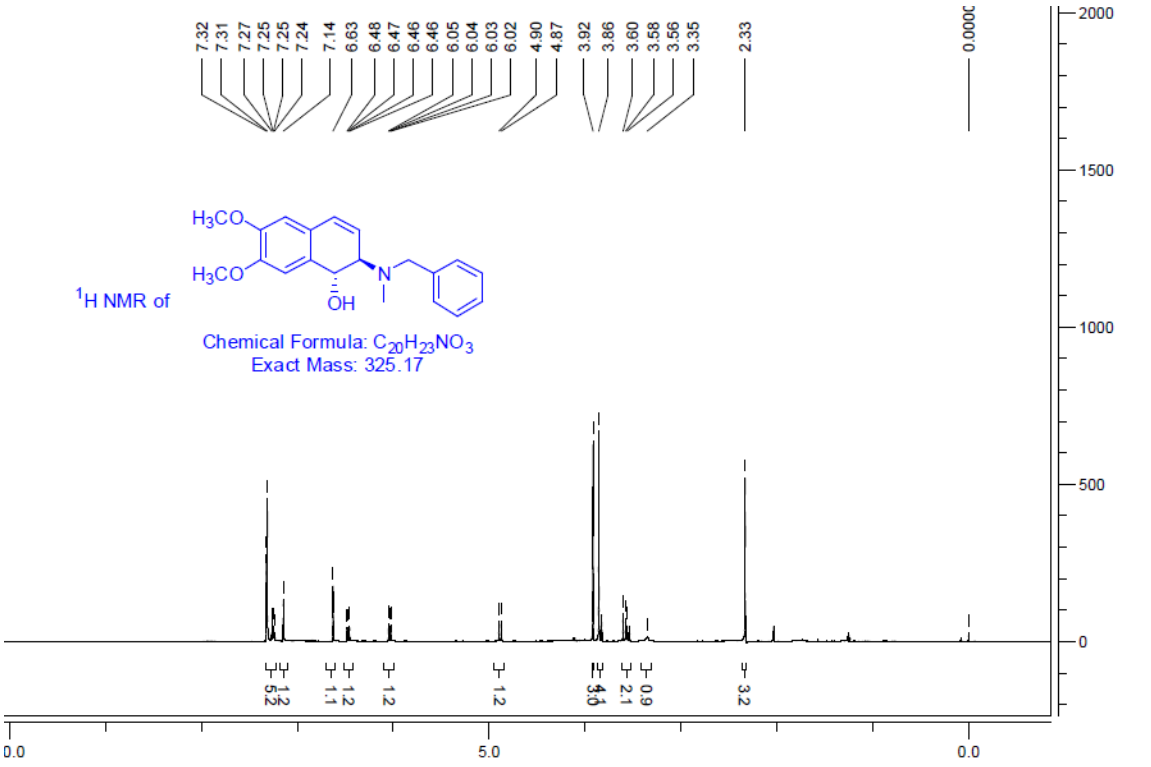
148.67
148.37
129.36
129.26
129.24
125.66
124.93
117.90
114.48
110.17
109.62
77.49
77.23
76.97
70.06
63.33
56.04
56.01
33.34
MeO
MeO
N
OH
13 C NMR of
Chemical Formula: C19H21NO3
Exact Mass: 311.15
100
50
0
200
150
100
50
0
ppm (f1)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7.31
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7.24
7.14
6.63
6.48
6.47
6.46
6.46
6.05
6.04
6.03
6.02
4.90
4.87
3.92
3.86
3.60
3.58
3.56
3.35
2.33
0.0000
H3CO
H3CO
N
OH
1H NMR of
Chemical Formula: C20H23NO3
Exact Mass: 325.17
2000
1500
1000
500
0
5.2
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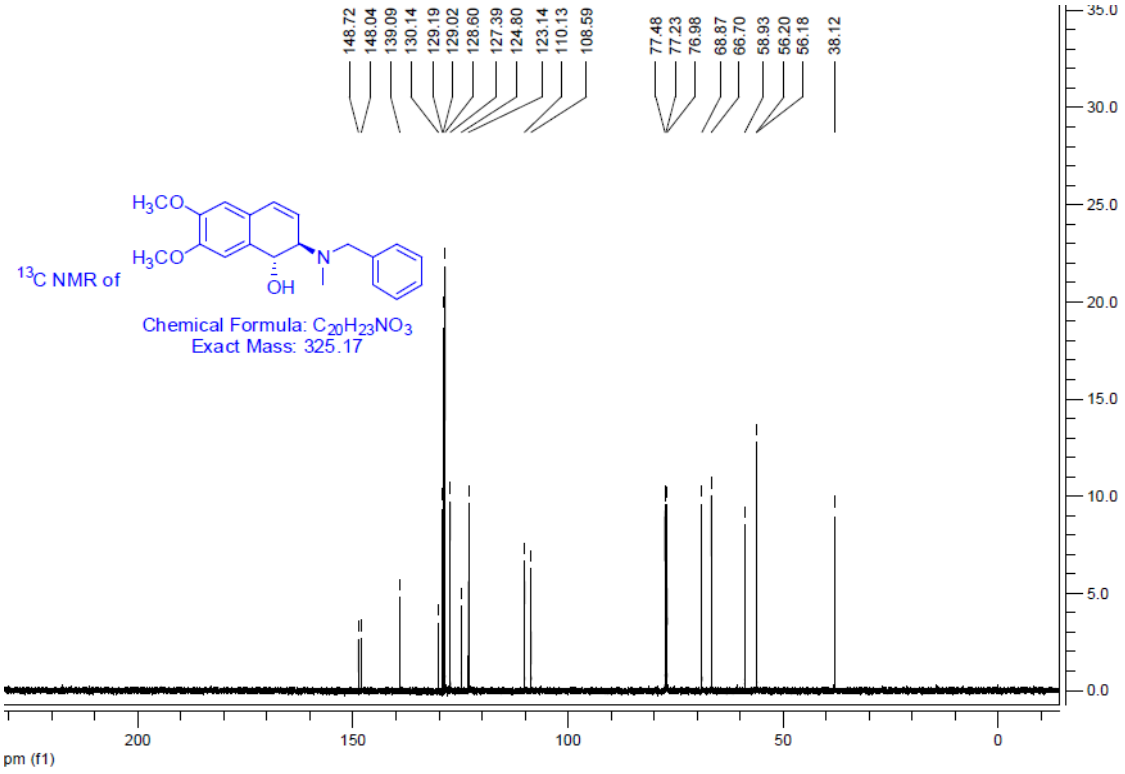
1.1
1.2
1.2
1.2
3.0
2.1
0.9
3.2
0.0
5.0
0.0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139.09
130.14
129.19
129.02
128.60
127.39
124.80
123.14
110.13
108.59
77.48
77.23
76.98
68.87
66.70
58.93
56.20
56.18
38.12
H3CO
H3CO
N
OH
13C NMR of
Chemical Formula: C20H23NO3
Exact Mass: 325.17
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25.0
20.0
15.0
10.0
5.0
0.0
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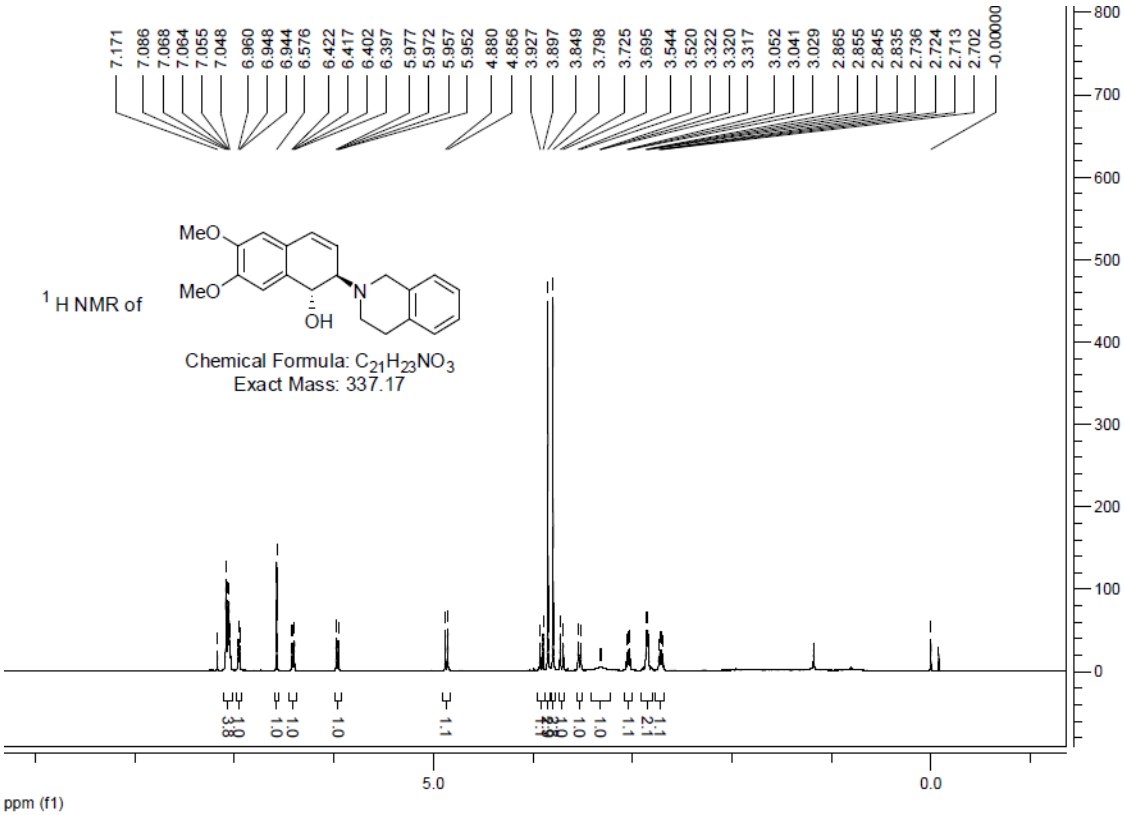
150
100
50
0
pm (f1)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7.068
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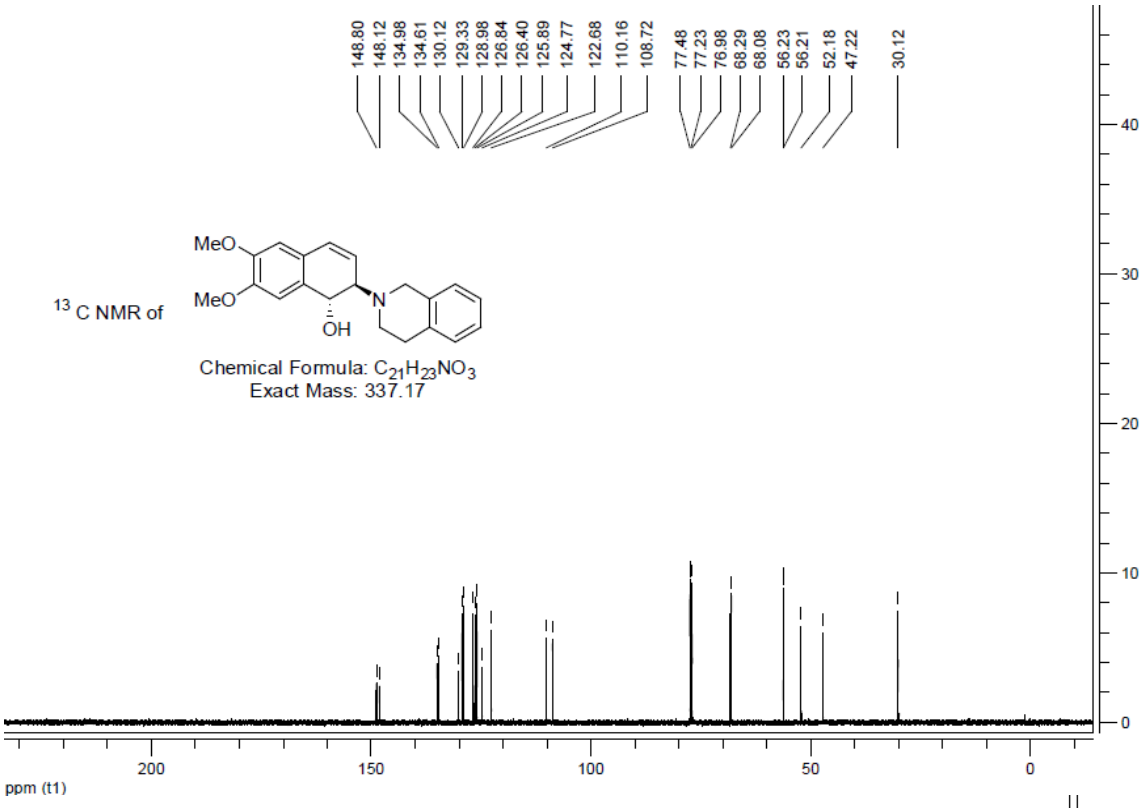
7.055
7.048
6.960
6.948
6.944
6.576
6.422
6.417
6.402
6.397
5.977
5.972
5.957
5.952
4.880
4.856
3.927
3.897
3.849
3.798
3.725
3.695
3.544
3.520
3.322
3.320
3.317
3.052
3.041
3.029
2.865
2.855
2.845
2.835
2.736
2.724
2.713
2.702
-0.00000
MeO
MeO
N
OH
1H NMR of
Chemical Formula: C21H23NO3
Exact Mass: 337.17
800
700
600
500
400
300
200
100
0
5.0
0.0
ppm (f1)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134.61
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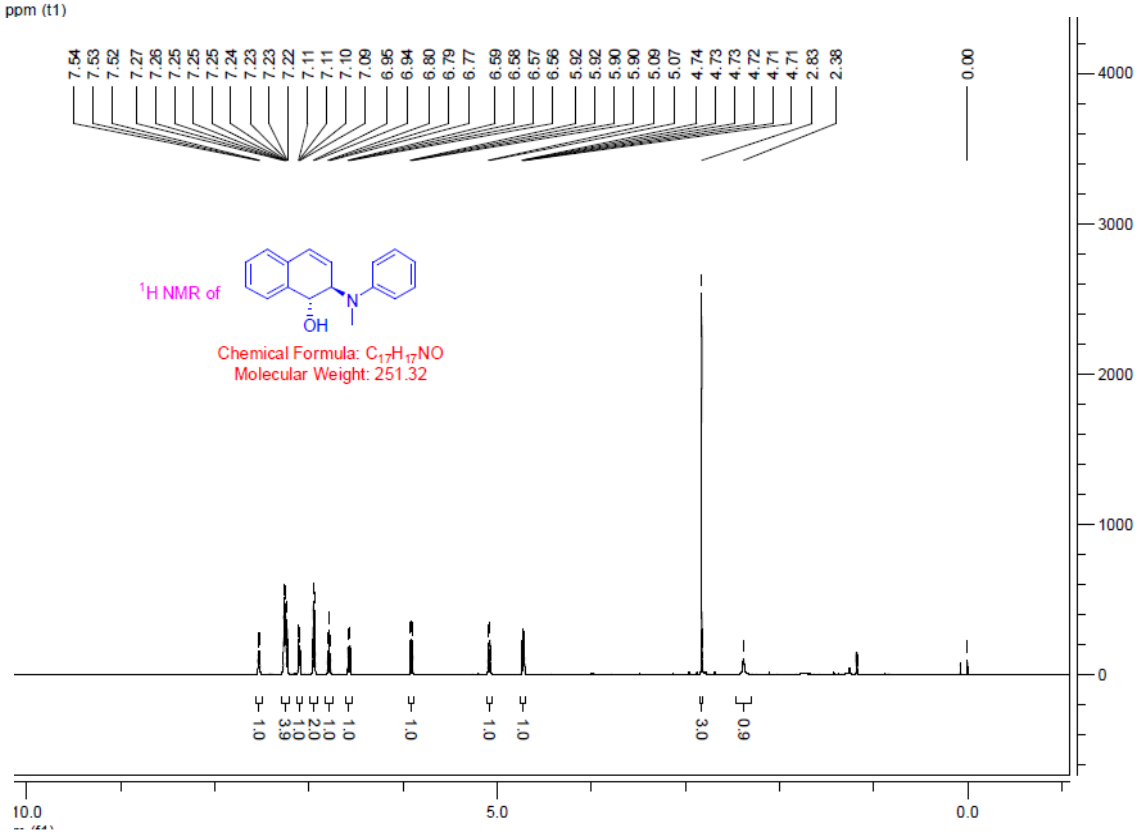
129.33
128.98
126.84
126.40
125.89
124.77
122.68
110.16
108.72
77.48
77.23
76.98
68.29
68.08
56.23
56.21
52.18
47.22
30.12
MeO
MeO
N
OH
13 C NMR of
Chemical Formula: C21H23NO3
Exact Mass: 337.17
40
30
20
10
0
200
150
100
50
0
ppm (t1)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7.26
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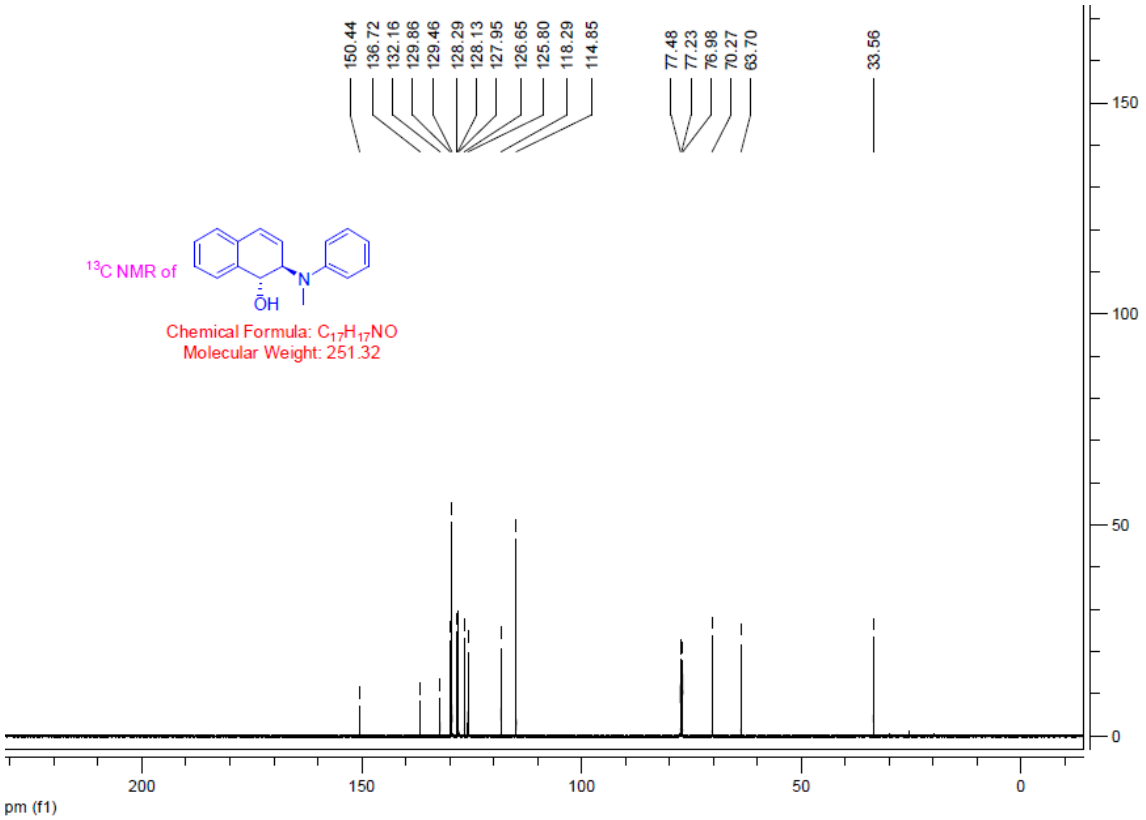
7.25
7.25
7.24
7.23
7.23
7.22
7.11
7.11
7.10
7.09
6.95
6.94
6.80
6.79
6.77
6.59
6.58
6.57
6.56
5.92
5.92
5.90
5.90
5.09
5.07
4.74
4.73
4.73
4.72
4.71
4.71
2.83
2.38
0.00
1H NMR of
N
OH
Chemical Formula: C17H17NO
Molecular Weight: 251.32
4000
3000
2000
1000
0
1.0
3.9
1.0
2.0
1.0
1.0
1.0
1.0
1.0
3.0
0.9
10.0
5.0
0.0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132.16
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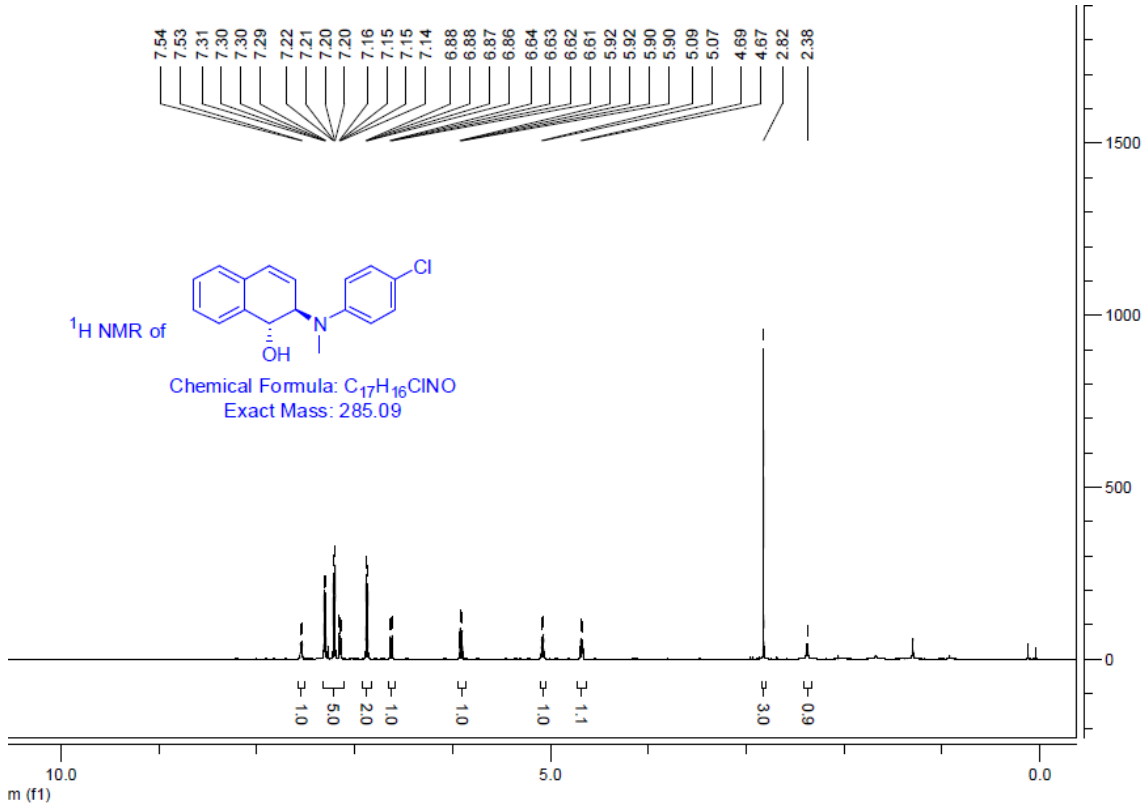
129.46
128.29
128.13
127.95
126.65
125.80
118.29
114.85
77.48
77.23
76.98
70.27
63.70
33.56
13C NMR of
OH
N
Chemical Formula: C17H17NO
Molecular Weight: 251.32
150
100
50
0
200
150
100
50
0
pm (f1)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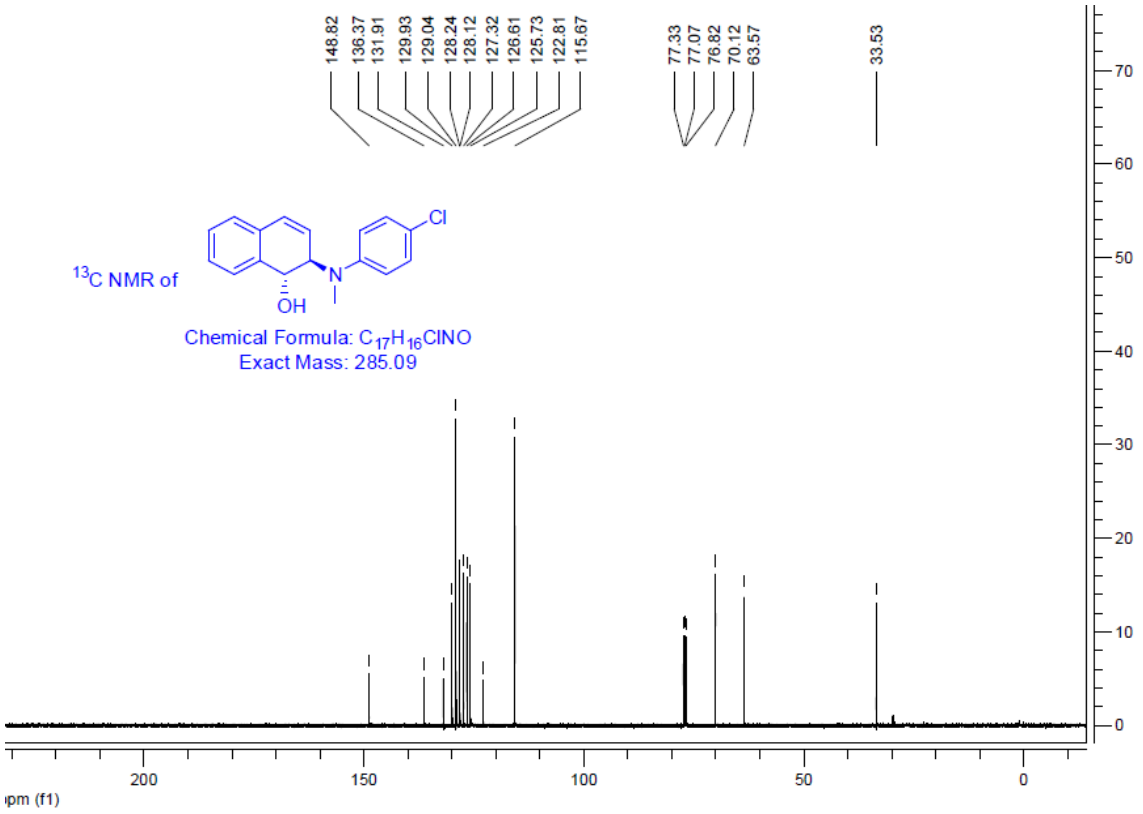
7.53
7.31
7.30
7.30
7.29
7.22
7.21
7.20
7.20
7.16
7.15
7.15
7.14
6.88
6.88
6.87
6.86
6.64
6.63
6.62
6.61
5.92
5.92
5.90
5.90
5.09
5.07
4.69
4.67
2.82
2.38
1H NMR of
Cl
OH
N
Chemical Formula: C17H16ClNO
Exact Mass: 285.09
1.0
5.0
2.0
1.0
1.0
1.0
1.1
3.0
0.9
1500
1000
500
0
10.0
5.0
0.0
m (f1)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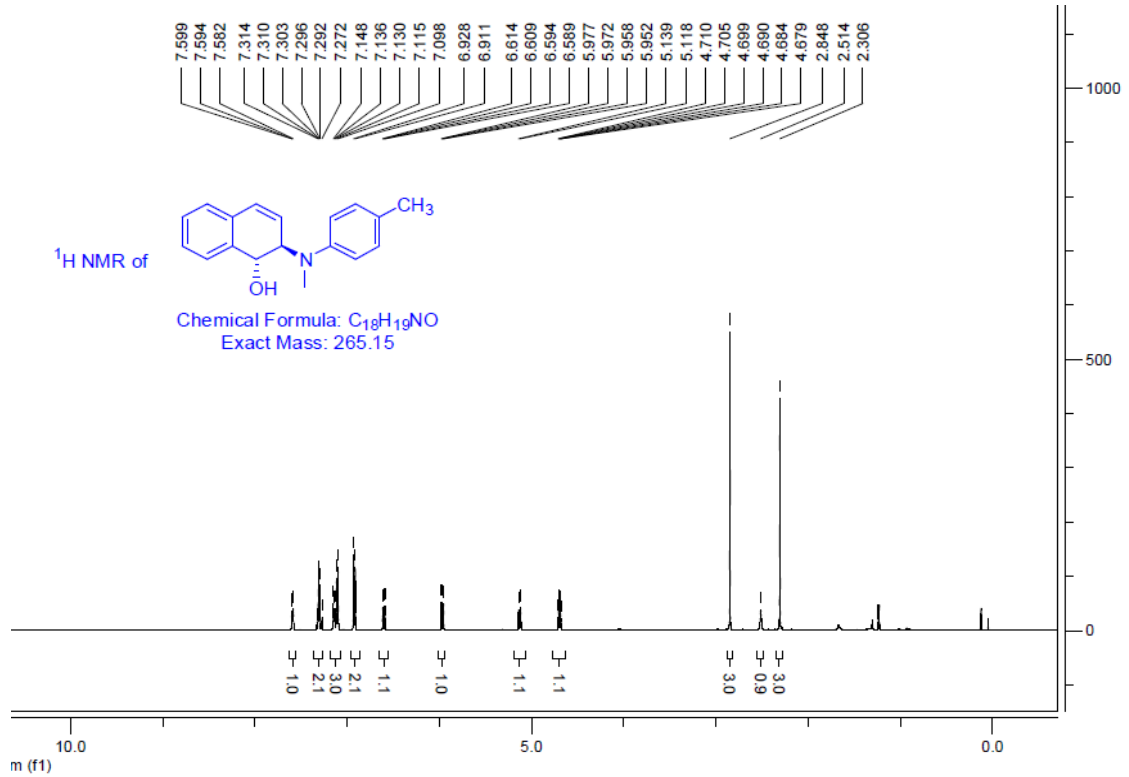
129.93
129.04
128.24
128.12
127.32
126.61
125.73
122.81
115.67
77.33
77.07
76.82
70.12
63.57
33.53
Cl
N
OH
13C NMR of
Chemical Formula: C17H16ClNO
Exact Mass: 285.09
200
150
100
50
0
ppm (f1)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7.303
7.296
7.292
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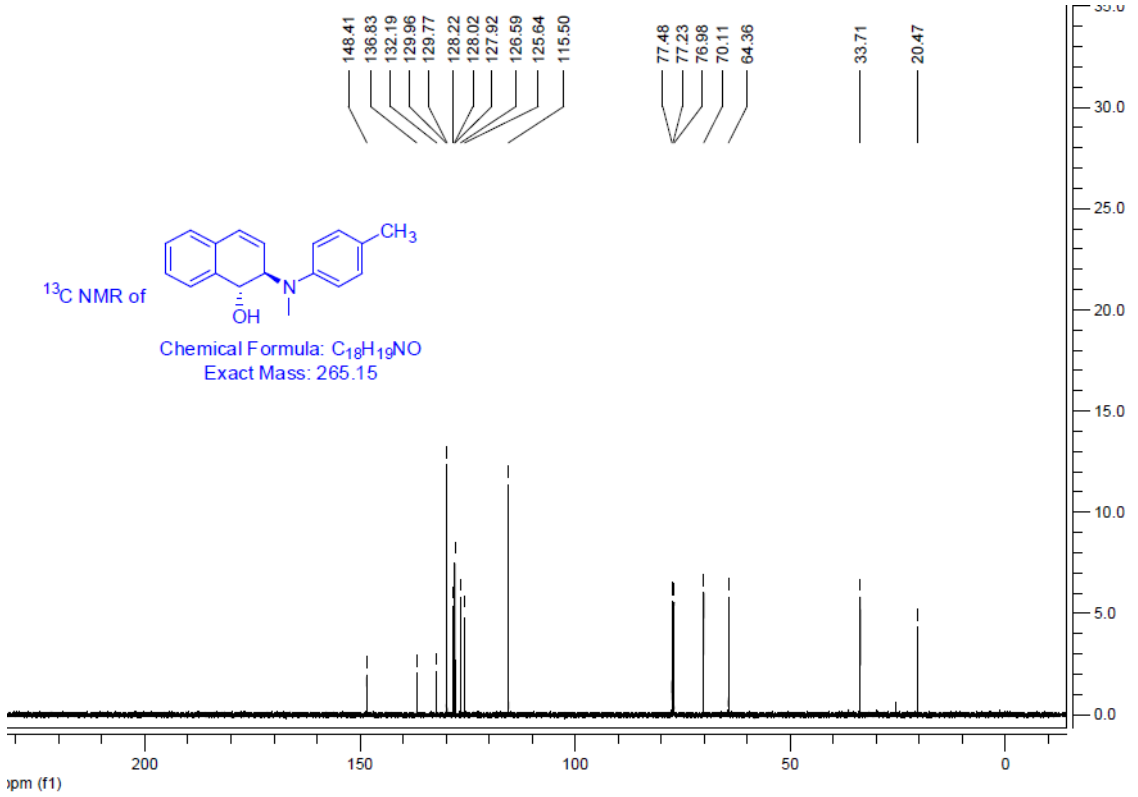
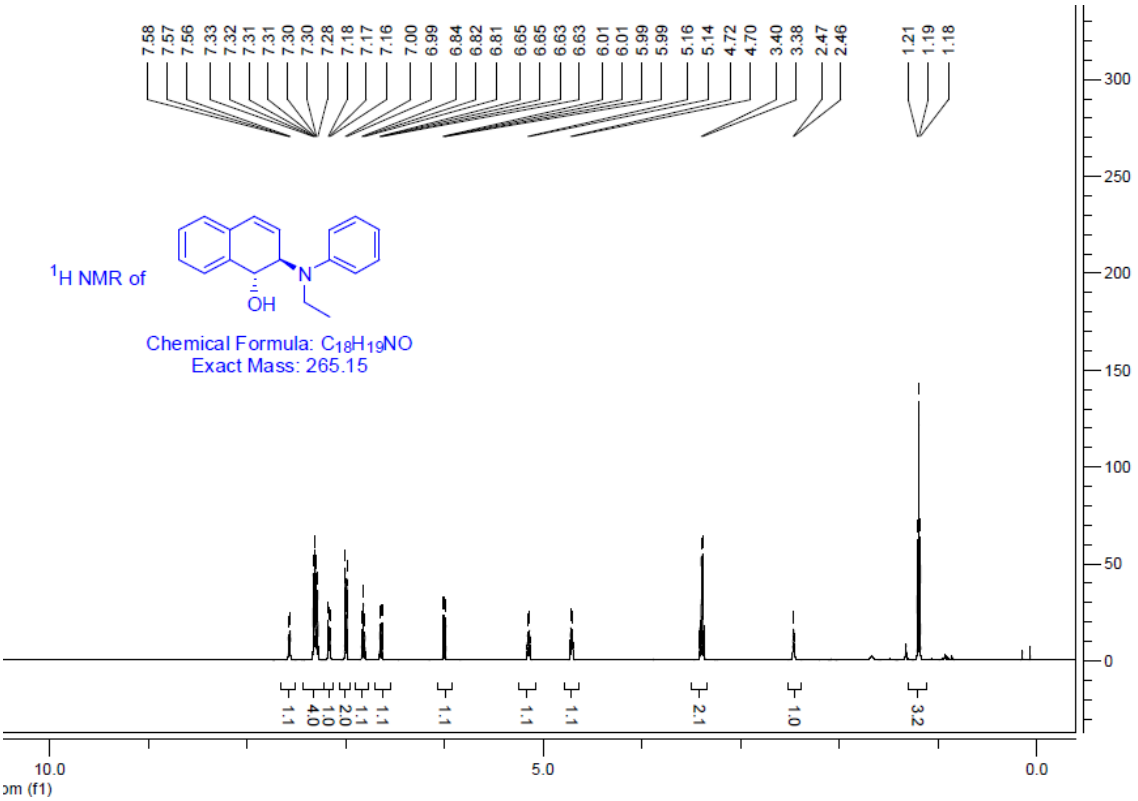
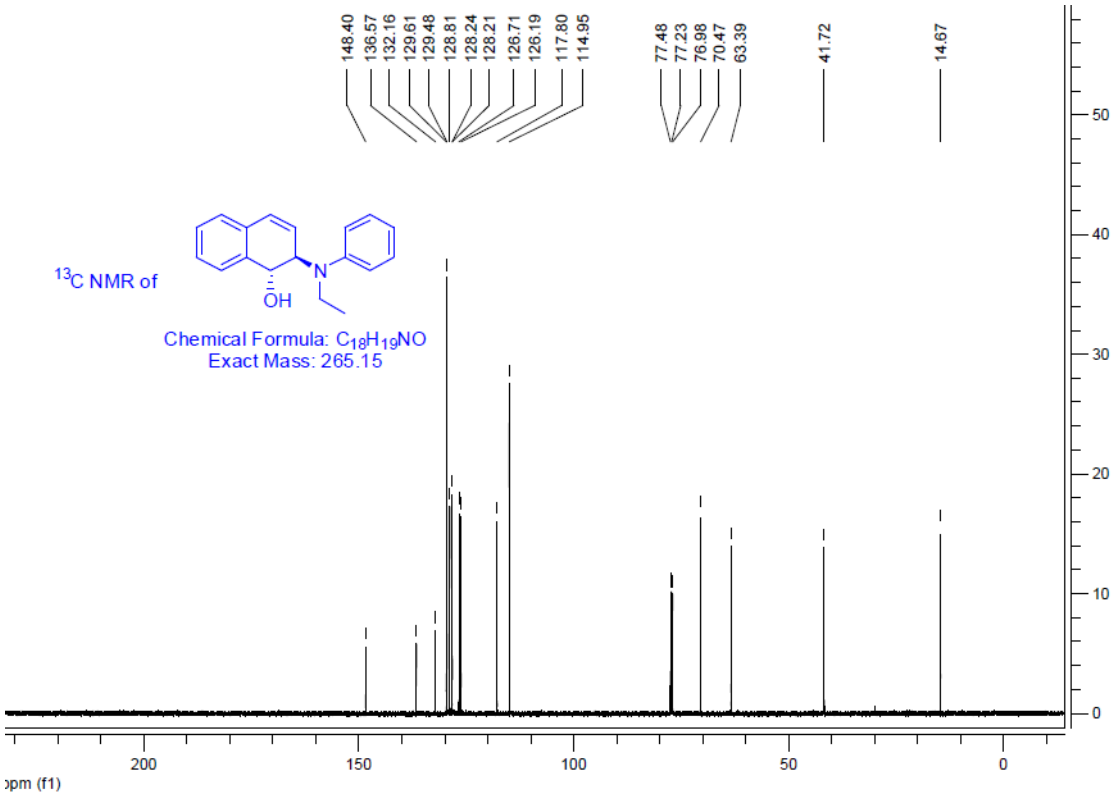
7.148
7.136
7.130
7.115
7.098
6.928
6.911
6.614
6.609
6.594
6.589
5.977
5.972
5.958
5.952
5.139
5.118
4.710
4.705
4.699
4.690
4.684
4.679
2.848
2.514
2.306
CH3
N
OH
1H NMR of
Chemical Formula: C18H19NO
Exact Mass: 265.15
1.0
2.1
3.0
2.1
1.1
1.0
1.1
1.1
3.0
0.9
3.0
10.0
5.0
0.0
m (f1)


148.41
136.83
132.19
129.96
129.77
128.22
128.02
127.92
126.59
125.64
115.50
77.48
77.23
76.98
70.11
64.36
33.71
20.47
CH3
N
OH
13C NMR of
Chemical Formula: C18H19NO
Exact Mass: 265.15
200
150
100
50
0
ppm (f1)


7.58
7.57
7.56
7.33
7.32
7.31
7.31
7.30
7.30
7.28
7.18
7.17
7.16
7.00
6.99
6.84
6.82
6.81
6.65
6.65
6.63
6.63
6.01
6.01
5.99
5.99
5.16
5.14
4.72
4.70
3.40
3.38
2.47
2.46
1.21
1.19
1.18
N
OH
1H NMR of
Chemical Formula: C18H19NO
Exact Mass: 265.15
1.1
4.0
1.0
2.0
1.1
1.1
1.1
1.1
2.1
1.0
3.2
10.0
5.0
0.0
pm (f1)


148.40
136.57
132.16
129.61
129.48
128.81
128.24
128.21
126.71
126.19
117.80
114.95
77.48
77.23
76.98
70.47
63.39
41.72
14.67
^{13}C NMR of
N
OH
Chemical Formula: $C_{18}H_{19}NO$
Exact Mass: 265.15
50
40
30
20
10
0
200
150
100
50
0
ppm (f1)