SUPPORTING INFORMATION

Enantioselective Oxidative Multi-Functionalization of Terminal Alkynes with Nitrones and Alcohols for Expeditious Assembly of Chiral α-Alkoxy-β-amino-ketones

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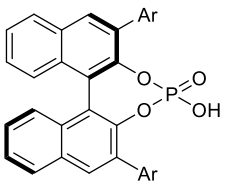
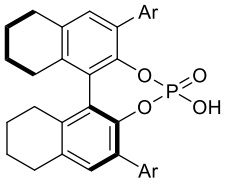
General Information

All reactions were performed in oven-dried glassware under atmosphere of argon. Solvents were dried and distilled followed the standard methods before using. Chiral phosphoric acids (CPAs), gold and other metal catalysts purchased from chemical vendors and used directly without any treatment. Analytical thin-layer chromatography was performed using glass plates pre-coated with 200-300 mesh silica gel impregnated with a fluorescent indicator (254 nm). Flash column chromatography was performed using silica gel (300-400 mesh). ^{1}H NMR and ^{13}C NMR spectra were recorded in $CDCl_3$ on 400/500 MHz spectrometer; chemical shifts are reported in ppm with the solvent signals as reference, and coupling constants (J) are given in Hertz. The peak information is described as: br = broad, s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet, comp = composite. Enantioselectivity was determined on HPLC using Chiralpak IB-3, ID-3, IF-3, IG-3, Y1 column. High-resolution mass spectra (HRMS) were recorded on a commercial apparatus (ESI Source) and (CI Source). Nitrones were prepared according to the known procedure and had physical and spectral properties identical to those earlier reported.[1]

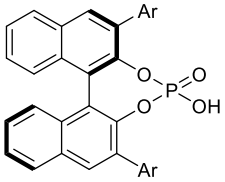
Condition Optimization



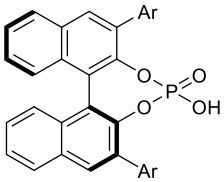
6a, Ar = ph
6b, Ar = *p*-$CF_3C_6H_4$
6c, Ar = 2,4,6-(*i*Pr)$_3C_6H_2$
6d, Ar = 3,5-$Cl_2C_6H_4$
6e, Ar = 3,5-$(CF_3)_2C_6H_4$
6f, Ar = 9-phenanthryl
6g, Ar = 9-anthracenyl



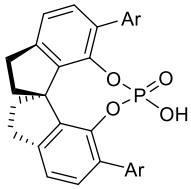
6h, Ar = 1-pyrenyl
6i, Ar = 9-phenanthryl
6j, Ar = 2,4,6-(*i*Pr)$_3C_6H_2$
6k, Ar = 3,5-$(CF_3)_2C_6H_4$



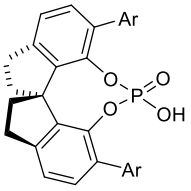
6l, Ar = *p*-NO_2
6m, Ar = biphenyl
6n, Ar = b-naphthyl
6o, Ar = $SiPh_3$



6p, Ar = 1-pyrenyl
6q, Ar = 4-(β-naphthyl)C_6H_4
6r, Ar = 2,4,6-$Me_3C_6H_2$
6s, Ar = 2,4,6-$Cy_3C_6H_2$



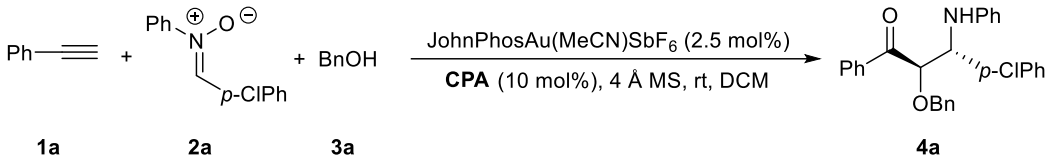
7a, Ar = 9-phenanthryl
7b, Ar = 9-anthracenyl
7c, Ar = 1-pyrenyl
7d, Ar = 3,5-$Ph_2C_6H_4$
7e, Ar = 2,4,6-$Me_3C_6H_2$



7f, Ar = 3,5-$(CF_3)_2C_6H_4$
7g, Ar = 2,4,6-(*i*Pr)$_3C_6H_2$

Scheme S1. Used Chiral Phosphoric Acids (CPA)

Table S1. Screening of Chiral Phosphoric Acids (CPA)[a]

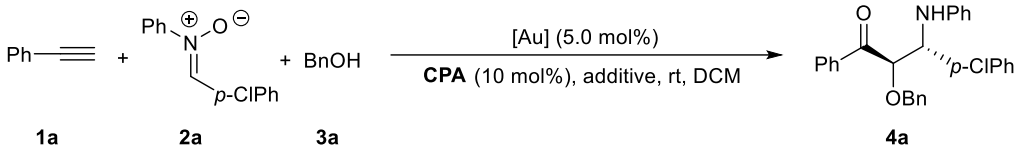


1a **2a** **3a** **4a**

entry	**CPA**	yield (%)[b]	*dr*[c]	*ee* (%)[c]
1	**6a**	26	60:40	10(0)
2	**6b**	29	57:43	22(3)
3	**6c**	20	50:50	3(0)
4	**6d**	31	62:38	33(17)
5	**6e**	50	76:24	50(35)
6	**6f**	33	69:31	59(53)
7	**6g**	43	76:24	64(10)
8	*ent*-**6f**	42	67:33	59(67)
9	*ent*-**6g**	40	83:17	74(3)
10	**6h**	39	72:28	47(36)
11	**6i**	41	66:34	59(43)
12	**6j**	33	48:52	52(18)
13	**6k**	51	77:23	51(42)
14	**6l**	31	65:35	36(22)
15	**6m**	41	60:40	35(55)
16	**6n**	39	61:39	30(40)
17	**6o**	19	51:49	0(0)
18	*ent*-**6o**	11	64:36	12(3)
19	**6p**	41	74:26	52(23)
20	**6q**	39	72:28	40(42)
21	**6r**	43	83:17	51(16)
22	**6s**	40	70:30	76(51)
23	**7a**	37	85:15	88(39)
24	*ent*-7**a**	38	78:22	78(24)
25	**7b**	33	75:25	75(61)
26	*ent*-7**b**	31	70:30	62(33)
27	**7c**	41	73:27	65(28)
28	**7d**	42	78:22	54(26)
29	**7e**	33	75:25	75(61)
30	**7f**	44	82:18	62(27)
31	**7g**	21	50:50	3(2)

[a]Unless otherwise noted, the reaction was carried out on a 0.2 mmol scale: **1a** (20.4 mg, 0.2 mmol), **2a** (60.0 mg, 0.26 mmol), and **3a** (216 mg, 2.0 mmol) in the presence of chiral phosphoric acid (CPA) (10 mol%), JohnphosAu(MeCN)SbF_6 (7.8 mg, 5.0 mol%), and 4 Å molecular sieves (100 mg) in DCM (4.0 mL) under argon atmosphere at room temperature, and the reaction was running for 6 hours under these conditions. [b]Isolated yields of **4a**. [c]The *dr* ratios and *ee* values were determined by chiral HPLC analysis.

Table S2. Screening of Gold Catalysts[a]

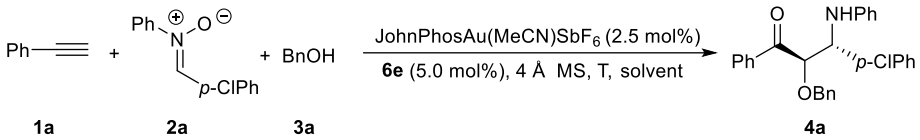


1a **2a** **3a** **4a**

entry	[Au]	**CAP**	addictive	yield (%)[b]	*dr*[c]	*ee* (%)[c]
1	JohnphosAu(MeCN)SbF_6	*ent*-**6g**	4 Å MS	40	83:17	74(3)
2	JohnphosAuNTf_2	*ent*-**6g**	4 Å MS	35	79:21	82(46)
3	BrettphosAuNTf_2	*ent*-**6g**	4 Å MS	50	80:20	71(17)
4	XPhosAuNTf_2	*ent*-**6g**	4 Å MS	26	83:17	75(13)
5	Me4*t*BuXPhosAuNTf_2	*ent*-**6g**	4 Å MS	50	87:13	80(38)
6	Me_3OMe*t*BuXPhosAuNTf_2	*ent*-**6g**	4 Å MS	52	88:12	82(51)
7	Me_3OMe*t*BuXPhosAuSbF_6	*ent*-**6g**	4 Å MS	54	87:13	79(31)
8	Me_3OMe*t*BuXPhosAuOTf	*ent*-**6g**	4 Å MS	50	87:13	78(7)
9	Me_3OMe*t*BuXPhosAuBArF	*ent*-**6g**	4 Å MS	52	80:20	73(6)
10	Me_3OMe*t*BuXPhosAuMe	*ent*-**6g**	4 Å MS	NR	-	-
11	Me_3OMe*t*BuXPhosAuNTf_2	*ent*-**6g**	3 Å MS	50	88:12	80(31)
12	Me_3OMe*t*BuXPhosAuNTf_2	*ent*-**6g**	5 Å MS	48	87:13	78(27)
13	Me_3OMe*t*BuXPhosAuNTf_2	**7a**	4 Å MS	44	89:11	90(24)
14[d]	Me_3OMe*t*BuXPhosAuNTf_2	**7a**	4 Å MS	49	90:10	90(33)

[a]Unless otherwise noted, the reaction was carried out on a 0.2 mmol scale: **1a** (20.4 mg, 0.2 mmol), **2a** (60.0 mg, 0.26 mmol), and **3a** (216 mg, 2.0 mmol) in the presence of chiral phosphoric acid (CPA) (10 mol%), gold catalyst (5.0 mol%), and molecular sieves (100 mg) in DCM (4.0 mL) under argon atmosphere at room temperature, and the reaction was running for 6 hours under these conditions. [b]Isolated yields of **4a**. [c]The *dr* ratios and *ee* values were determined by chiral HPLC analysis. [d]The gold catalyst was added to the reaction mixture in 0.5 h.

Table S3: Optimization of Other Reaction Parameters[a]

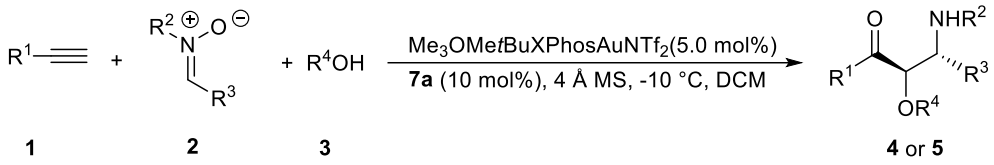


1a **2a** **3a** **4a**

entry	t (h)	solvent	T (°C)	yield (%)[b]	*dr*[c]	*ee* (%)[c]
1	4	DCM	rt	50	76:24	50(35)
2	4	DCE	rt	41	68:32	35(25)
3	4	$CHCl_3$	rt	33	57:43	35(21)
4[d]	4	$CHCl_3$	rt	26	63:37	20(33)
5	12	PhCl	rt	28	35:65	50(50)
6	12	PhMe	rt	21	40:60	51(65)
7	12	PhF	rt	37	31:69	52(49)
8	12	THF	rt	32	54:46	20(9)
9	8	DCM	0	40	75:25	51(41)

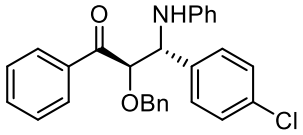
[a]Unless otherwise noted, the reaction was carried out on a 0.2 mmol scale: **1a** (20.4 mg, 0.2 mmol), **2a** (60.0 mg, 0.26 mmol), and **3a** (216 mg, 2.0 mmol) in the presence of chiral phosphoric acid **5e** (7.7 mg, 5.0 mol%), JohnphosAu(MeCN)SbF_6 (3.9 mg, 2.5 mol%), and 4 Å molecular sieves (100 mg) in indicated solvent (4.0 mL) under argon atmosphere at 0 °C or room temperature, and the reaction was running under these conditions for additional hours (as indicated). [b]Isolated yields of **4a**. [c]The *dr* ratios and *ee* values were determined by chiral HPLC analysis. [d]The reaction was conducted in the absence of molecular sieves.

General Procedure for the Asymmetric Three-component Reaction



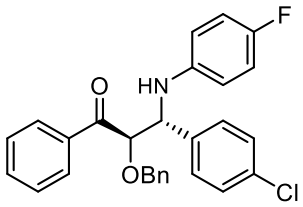
1 **2** **3** **4** or **5**

To a 10-mL oven-dried vial with a magnetic stirring bar, phenylacetylene **1** (0.6 mmol), nitrone **2** (0.2 mmol), alcohol **3** (6.0 mmol), chiral phosphoric acid **7a** (13.2 mg, 10 mol%), and 4Å MS (100 mg) in 2.0 mL DCM, a solution of $Me_3OMetBuXPhosAuNTf_2$ (9.8 mg, 5.0 mol%) in DCM (2.0 mL) was added *via* a syringe pump in 0.5 h under argon atmosphere at -10 ^oC. When the reaction was completed (monitored by TLC, about 12 h), the crude reaction mixture was quenched with saturated aqueous sodium bicarbonate (10 mL) and extracted with EtOAc (15 mL). The organic layer was washed with brine and dried over anhydrous Na_2SO_4. The solvent was evaporated in *vacuo* after filtration. The residue was purified by flash column chromatography on silica gel (Hexanes : EtOAc = 20:1 to 10:1) to give the pure products **4** or **5** in good to high yields.

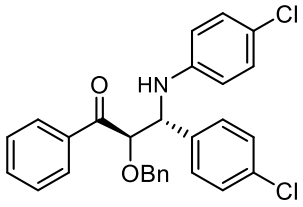


(2*R*,3*R*)-2-(Benzyloxy)-3-(4-chlorophenyl)-1-phenyl-3-(phenylamino)propan-1-one (4a) Yellow solid, 66.2 mg, 75% yield, 90:10 *dr*, 91%(44%) *ee*, $[\alpha]_D^{20}$ = 18.9^o (c = 0.45, MeOH), mp = 133 – 135 ^oC; ^1H NMR (500 MHz, $CDCl_3$) δ 7.78 (d, *J* = 7.9 Hz, 2H), 7.53 (t, *J* = 7.3 Hz, 1H), 7.37 (t, *J* = 7.5 Hz, 2H), 7.33 – 7.30 (comp, 3H), 7.22 – 7.14 (comp, 6H), 7.04 (t, *J* = 7.4 Hz, 2H), 6.63 (t, *J* = 7.2 Hz, 1H), 6.42 (d, *J* = 7.9 Hz, 2H), 4.90 (d, *J* = 5.3 Hz, 1H), 4.87 (s, 1H), 4.68 (d, *J* = 11.4 Hz, 2H), 4.33 (d, *J* = 11.8 Hz, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 199.0, 146.0, 137.2, 136.9, 135.9, 133.6, 133.5, 129.2, 129.1, 128.7, 128.6, 128.6, 128.5, 128.24, 128.18, 118.1, 113.9, 84.2, 72.7, 59.5; HRMS (TOF MS ESI$^+$) calculated for $C_{28}H_{25}NO_2Cl$ $[M + H]^+$: 442.1568, found 442.1573; HPLC conditions for determination of enantiomeric excess: Chiral

IB-3, λ = 254 nm, hexane : ethanol = 95:5, flow rate =1.0 mL/min, t_{major} = 8.9 min, t_{minor} = 10.6 min.

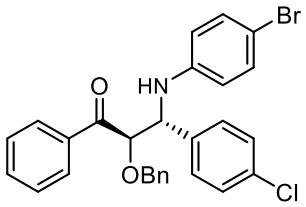


(2*R*,3*R*)-2-(Benzyloxy)-3-(4-chlorophenyl)-3-((4-fluorophenyl)amino)-1-phenylpropan-1-one (4b) White solid, 73.4 mg, 80% yield, 94:6 *dr*, 96%(3%) *ee*, $[\alpha]_D^{20}$ = 23.2° (c = 0.48, DCM), mp = 142 – 144 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.76 (d, *J* = 7.7 Hz, 2H), 7.53 (t, *J* = 7.3 Hz, 1H), 7.37 (t, *J* = 7.6 Hz, 2H), 7.34 – 7.27 (comp, 3H), 7.25 – 7.10 (comp, 6H), 6.74 (t, *J* = 8.5 Hz, 2H), 6.42 – 6.28 (m, 2H), 4.90 – 4.75 (m, 2H), 4.68 (d, *J* = 11.8 Hz, 1H), 4.58 (s, 1H), 4.33 (d, *J* = 11.8 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 199.0, 156.1 (d, *J* = 236.1 Hz), 142.3 (d, *J* = 3.2 Hz), 136.9, 136.8, 135.9, 133.6, 129.0, 128.7, 128.64, 128.62, 128.57, 128.55, 128.3, 128.2, 115.6 (d, *J* = 21.4 Hz), 114.9, 114.8, 89.0, 72.6, 60.2; ^{19}F NMR (376 MHz, $CDCl_3$) δ -127.0; HRMS (TOF MS ESI$^+$) calculated for $C_{28}H_{24}NO_2FCl$ $[M + H]^+$: 460.1474, found 460.1486; HPLC conditions for determination of enantiomeric excess: Chiral IF-3, λ = 254 nm, hexane : ethanol = 99:1, flow rate =1.0 mL/min, t_{major} = 19.3 min, t_{minor} = 18.5 min.

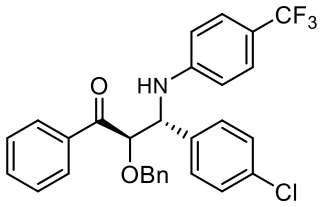


(2*R*,3*R*)-2-(Benzyloxy)-3-(4-chlorophenyl)-3-((4-chlorophenyl)amino)-1-phenylpropan-1-one (4c) White solid, 81.7 mg, 86% yield, 90:10 *dr*, 94%(18%) *ee*, $[\alpha]_D^{20}$ = 7.2° (c = 0.30, DCM), mp = 130 – 132 °C; ^{1}H NMR (500 MHz, $CDCl_3$) (δ, ppm) δ 7.75 (d, *J* = 7.6 Hz, 2H), 7.54 (t, *J* = 7.3 Hz, 1H), 7.37 (t, *J* = 7.6 Hz, 2H), 7.34 – 7.28 (comp, 3H), 7.20 (d, *J* = 3.5 Hz, 2H), 7.17 – 7.11 (comp, 4H), 6.98 (d, *J* = 8.6 Hz, 2H),

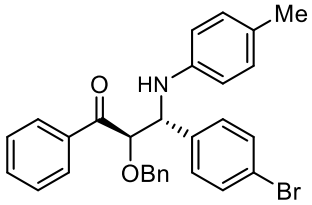
6.33 (d, *J* = 8.6 Hz, 2H), 4.90 (d, *J* = 5.2 Hz, 1H), 4.81 (s, 1H), 4.75 – 4.67 (m, 2H), 4.33 (d, *J* = 11.8 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) (δ, ppm) δ 198.9, 144.6, 136.73, 136.65, 135.9, 133.70, 133.68, 129.0, 128.68, 128.64, 128.61, 128.5, 128.3, 128.2, 122.8, 114.9, 83.8, 72.7, 59.6; HRMS (TOF MS ESI$^+$) calculated for $C_{28}H_{23}Cl_2NO_2Na$ [M + Na]$^+$: 498.0998, found 498.1000; HPLC conditions for determination of enantiomeric excess: Chiral IF-3, λ = 220 nm, hexane : ethanol = 97:3, flow rate =1.0 mL/min, t_{minor} = 11.9 min, t_{major} = 12.4 min.



(2*R*,3*R*)-2-(Benzyloxy)-3-((4-bromophenyl)amino)-3-(4-chlorophenyl)-1-phenylpropan-1-one (4d) White solid, 65.4 mg, 63% yield, 93:7 *dr*, 94%(11%) *ee*, $[\alpha]_D^{20}$ = 7.6^o (c = 0.40, DCM) , mp = 136 – 138 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.75 (d, *J* = 7.5 Hz, 2H), 7.54 (t, *J* = 7.4 Hz, 1H), 7.37 (t, *J* = 7.8 Hz, 2H), 7.34 – 7.28 (comp, 3H), 7.22 – 7.18 (m, 2H), 7.18 – 7.07 (comp, 6H), 6.29 (d, *J* = 8.8 Hz, 2H), 4.90 (d, *J* = 5.1 Hz, 1H), 4.80 (t, *J* = 5.3 Hz, 1H), 4.75 (d, *J* = 5.3 Hz, 1H), 4.69 (d, *J* = 11.8 Hz, 1H), 4.33 (d, *J* = 11.8 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 198.9, 145.0, 136.7, 136.6, 135.9, 133.7, 131.9, 129.0, 128.70, 128.65, 128.63, 128.5, 128.3, 128.2, 115.1, 109.8, 83.7, 72.6, 59.5; HRMS (TOF MS ESI$^+$) calculated for $C_{28}H_{24}NO_2ClBr$ [M + H]$^+$: 520.0673, found 520.0665; HPLC conditions for determination of enantiomeric excess: Chiral IB-3, λ = 260 nm, hexane : ethanol = 95:5, flow rate =1.0 mL/min, t_{major} = 10.4 min, t_{minor} = 9.8 min.

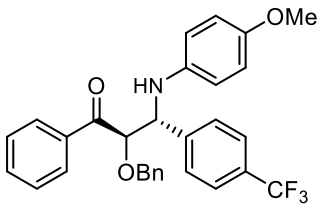


(2*R*,3*R*)-2-(Benzyloxy)-3-(4-chlorophenyl)-1-phenyl-3-((4-(trifluoromethyl)phenyl)amino)propan-1-one (4e) White solid, 87.5 mg, 86% yield, 94:6 *dr*, 95%(21%) *ee*, mp = 129 – 131 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.74 (d, *J* = 7.4 Hz, 2H), 7.54 (t, *J* = 7.4 Hz, 1H), 7.39 – 7.31 (comp, 5H), 7.28 – 7.24 (comp, 2H), 7.23 – 7.21 (comp, 2H), 7.19 – 7.10 (comp, 4H), 6.42 (d, *J* = 8.5 Hz, 2H), 5.10 (d, *J* = 6.5 Hz, 1H), 4.93 (d, *J* = 5.3 Hz, 1H), 4.91 – 4.85 (m, 1H), 4.70 (d, *J* = 11.8 Hz, 1H), 4.35 (d, *J* = 11.8 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 198.9, 148.6, 136.6, 136.3, 135.8, 133.9, 133.8, 128.9, 128.73, 128.69, 128.5, 128.4, 128.3, 126.5 (q, *J* = 3.4 Hz), 124.8 (q, *J* = 270.4 Hz), 119.6 (q, *J* = 32.6 Hz), 112.9, 83.3, 72.7, 59.1; ^{19}F NMR (376 MHz, $CDCl_3$) δ -61.2; HRMS (TOF MS ESI$^+$) calculated for $C_{29}H_{23}F_3ClNO_2Na$ $[M + Na]^+$: 532.1262, found 532.1270; HPLC conditions for determination of enantiomeric excess: Chiral IB-3, λ = 270 nm, hexane : ethanol = 97:3, flow rate =1.0 mL/min, t_{major} = 14.8 min, t_{minor} = 11.3 min.

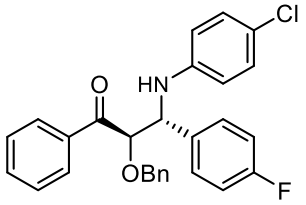


(2*R*,3*R*)-2-(Benzyloxy)-3-(4-bromophenyl)-1-phenyl-3-(p-tolylamino)propan-1-one (4f) White solid, 75.9 mg, 76% yield, 92:8 *dr*, 96%(26%) *ee*, $[\alpha]_D^{20}$ = 38.8° (c = 0.33, DCM), mp = 140 – 142 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.79 (d, *J* = 7.7 Hz, 2H), 7.53 (t, *J* = 7.3 Hz, 1H), 7.37 (t, *J* = 7.5 Hz, 2H), 7.35 – 7.27 (comp, 5H), 7.22 – 7.16 (comp, 2H), 7.10 (d, *J* = 7.9 Hz, 2H), 6.85 (d, *J* = 7.8 Hz, 2H), 6.35 (d, *J* = 7.8 Hz, 2H), 4.89 – 4.83 (m, 2H), 4.67 (d, *J* = 11.8 Hz, 1H), 4.54 (s, 1H), 4.32 (d, *J* = 11.8 Hz, 1H), 2.15 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 199.0, 143.7, 137.9, 136.9, 135.9, 133.5, 131.4, 129.7, 129.5, 128.7, 128.6, 128.19, 128.15, 127.4, 121.6, 114.1, 84.3,

72.7, 59.8, 20.4; HRMS (TOF MS ESI$^+$) calculated for $C_{29}H_{27}NO_2Br$ [M + H]$^+$: 522.1220, found 520.1222; HPLC conditions for determination of enantiomeric excess: Chiral IF-3, λ = 254 nm, hexane : ethanol = 98:2, flow rate =1.0 mL/min, t_{major} = 15.0 min, t_{minor} = 14.5 min.

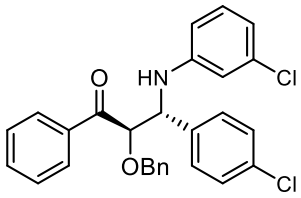


(2*R*,3*R*)-2-(Benzyloxy)-3-((4-methoxyphenyl)amino)-1-phenyl-3-(4-(trifluoromethyl)phenyl)propan-1-one (4g) White solid, 97.0 mg, 96% yield, 90:10 *dr*, 91%(16%) *ee*, mp = 136 – 138 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.77 (d, *J* = 7.6 Hz, 2H), 7.53 (t, *J* = 7.0 Hz, 1H), 7.44 (d, *J* = 7.8 Hz, 2H), 7.40 – 7.27 (comp, 7H), 7.17 (s, 2H), 6.64 (d, *J* = 8.4 Hz, 2H), 6.39 (d, *J* = 8.4 Hz, 2H), 4.91 – 4.87 (m, 2H), 4.69 (d, *J* = 11.8 Hz, 1H), 4.43 (s, 1H), 4.32 (d, *J* = 11.8 Hz, 1H), 3.66 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 198.9, 152.6, 143.1, 139.9, 136.8, 135.9, 133.6, 130.0 (q, *J* = 32.2 Hz), 128.7, 128.6, 128.5, 128.24, 128.17, 128.1, 125.3 (q, *J* = 3.5 Hz), 115.4, 114.8, 84.2, 72.7, 60.8, 55.6; ^{19}F NMR (471 MHz, $CDCl_3$) δ -62.5; HRMS (TOF MS ESI$^+$) calculated for $C_{30}H_{27}NO_3F_3$ [M + H]$^+$: 506.1938, found 506.1938; HPLC conditions for determination of enantiomeric excess: Chiral IB-3, λ = 254 nm, hexane : ethanol = 97:3, flow rate =1.0 mL/min, t_{major} = 13.2 min, t_{minor} = 15.7 min.

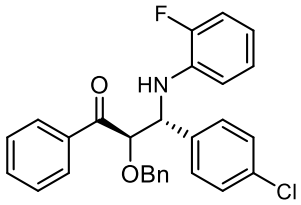


(2*R*,3*R*)-2-(Benzyloxy)-3-((4-chlorophenyl)amino)-3-(4-fluorophenyl)-1-phenylpropan-1-one (4h) White solid, 82.7 mg, 90% yield, 90:10 *dr*, 92%(12%) ee, $[\alpha]_D^{20}$ = 16.7° (c = 0.45, DCM), mp = 121 - 123 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.73 (d, *J* = 7.7 Hz, 2H), 7.52 (t, *J* = 7.3 Hz, 1H), 7.39 – 7.29 (comp, 5H), 7.22 – 7.14 (comp, 4H),

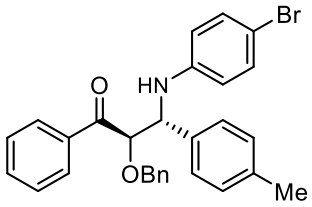
6.98 (d, *J* = 8.4 Hz, 2H), 6.87 (t, *J* = 8.3 Hz, 2H), 6.35 (d, *J* = 8.4 Hz, 2H), 4.91 (d, *J* = 4.4 Hz, 1H), 4.82 (s, 1H), 4.76 (s, 1H), 4.68 (d, *J* = 11.8 Hz, 1H), 4.33 (d, *J* = 11.8 Hz, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 199.1, 162.4 (*J* = 246.3 Hz), 144.7, 136.8, 136.0, 133.8 (d, *J* = 3.1 Hz), 133.6, 129.2 (d, *J* = 8.2 Hz), 129.0, 128.6, 128.5, 128.3, 128.2, 122.7, 115.4 (d, *J* = 21.5 Hz), 114.9, 83.8, 72.6, 59.5; ^{19}F NMR (471 MHz, $CDCl_3$) δ -114.3; HRMS (TOF MS ESI$^+$) calculated for $C_{28}H_{24}NO_2FCl$ $[M + H]^+$: 460.1474, found 460.1485; HPLC conditions for determination of enantiomeric excess: Chiral IB-3, λ = 254 nm, hexane : ethanol = 95:5, flow rate =1.0 mL/min, t_{major} = 9.1 min, t_{minor} = 8.8 min.



(2*R*,3*R*)-2-(Benzyloxy)-3-(4-chlorophenyl)-3-((3-chlorophenyl)amino)-1-phenylpropan-1-one (4i) White solid, 76.9 mg, 81% yield, 90:10 *dr*, 91%(11%) *ee*, $[\alpha]_D^{20}$ = 9.9^o (c = 0.30, DCM) , mp = 131 - 133 ^{o}C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.75 (d, *J* = 7.7 Hz, 2H), 7.54 (t, *J* = 7.4 Hz, 1H), 7.37 (t, *J* = 7.6 Hz, 2H), 7.34 – 7.28 (comp, 3H), 7.23 – 7.18 (m, 2H), 7.15 (q, *J* = 8.1 Hz, 4H), 6.93 (t, *J* = 7.9 Hz, 1H), 6.59 (d, *J* = 7.9 Hz, 1H), 6.39 (s, 1H), 6.29 (d, *J* = 8.2 Hz, 1H), 4.90 (s, 1H), 4.82 (s, 2H), 4.69 (d, *J* = 11.8 Hz, 1H), 4.33 (d, *J* = 11.8 Hz, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 198.8, 147.2, 136.7, 136.5, 135.9, 134.8, 133.8, 133.7, 130.1, 129.0, 128.71, 128.66, 128.6, 128.3, 128.2, 118.0, 113.6, 112.0, 83.6, 72.7, 59.3; HRMS (TOF MS ESI$^+$) calculated for $C_{28}H_{23}Cl_2NO_2Na$ $[M + Na]^+$: 498.0998, found 498.1016; HPLC conditions for determination of enantiomeric excess: Chiral ID-3, λ = 254 nm, hexane : ethanol = 98:2, flow rate =1.0 mL/min, t_{major} = 11.8 min, t_{minor} = 10.3 min.

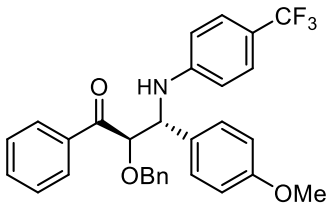


(2*R*,3*R*)-2-(Benzyloxy)-3-(4-chlorophenyl)-3-((2-fluorophenyl)amino)-1-phenylpropan-1-one (4j) Yellow oil, 55.1 mg, 60% yield, 80:20 *dr*, 90%(< 5%) *ee*; ^{1}H NMR (400 MHz, $CDCl_3$) δ major: 7.84 – 7.76 (comp, 2H), 7.56 (t, *J* = 7.5 Hz, 1H), 7.49 – 7.28 (comp, 5H), 7.25 – 7.03 (comp, 6H), 6.94 – 6.89 (m, 1H), 6.77 (t, *J* = 7.7 Hz, 1H), 6.59 – 6.53 (m, 1H), 6.34 (t, *J* = 7.7 Hz, 1H), 5.03 – 4.92 (m, 2H), 4.89 – 4.84 (comp, 1H), 4.70 (d, *J* = 11.9 Hz, 1H), 4.35 – 4.29 (m, 1H); minor: 7.91 – 7.89 (comp, 2H), 7.56 (t, *J* = 7.5 Hz, 1H), 7.49 – 7.28 (comp, 5H), 7.25 – 7.03 (comp, 6H), 6.94 – 6.89 (m, 1H), 6.70 (t, *J* = 7.7 Hz, 1H), 6.59 – 6.53 (m, 1H), 6.19 (t, *J* = 7.7 Hz, 1H), 5.15 – 5.12 (m, 1H), 4.89 – 4.84 (comp, 2H), 4.70 (d, *J* = 11.9 Hz, 1H), 4.35 – 4.29 (m, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ major: 198.8, 151.8 (d, *J* = 239.2 Hz), 138.0, 136.7 (d, *J* = 7.0 Hz), 135.9, 134.4 (d, *J* = 11.5 Hz), 133.6, 129.1, 128.8 (d, *J* = 1.2 Hz), 128.7, 128.63, 128.56, 128.5 (d, *J* = 4.4 Hz), 128.3, 128.2, 124.4 (d, *J* = 3.5 Hz), 117.6 (d, *J* = 7.2 Hz), 114.6 (d, *J* = 18.5 Hz), 113.5 (d, *J* = 2.9 Hz), 84.0, 72.7, 59.1; ^{19}F NMR (376 MHz, $CDCl_3$) δ minor: -135.1; major: -135.5; HRMS (TOF MS ESI^{+}) calculated for $C_{28}H_{23}FClNO_2Na$ $[M + Na]^{+}$: 482.1294, found 482.1299; HPLC conditions for determination of enantiomeric excess: Chiral IF-3, λ = 260 nm, hexane : ethanol = 97:3, flow rate =1.0 mL/min, t_{major} = 7.8 min, t_{minor} = 7.1 min.

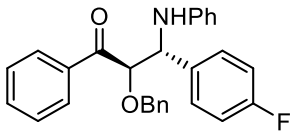


(2*R*,3*R*)-2-(Benzyloxy)-3-((4-bromophenyl)amino)-1-phenyl-3-(*p*-tolyl)propan-1-one (4k) White solid, 67.9 mg, 68% yield, 86:14 *dr*, 90%(20%) *ee*, mp = 138 – 140 ^{o}C; ^{1}H NMR (500 MHz, $CDCl_3$) δ major: 7.71 (d, *J* = 7.8 Hz, 2H), 7.51 – 7.43 (comp, 2H), 7.34 – 7.30 (comp, 4H), 7.20 (s, 2H), 7.17 – 7.02 (comp, 4H), 6.98 (d, *J* = 7.7 Hz,

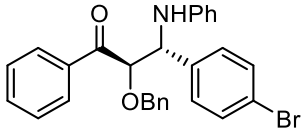
2H), 6.33 (d, *J* = 8.5 Hz, 2H), 4.92 (d, *J* = 4.7 Hz, 1H), 4.81 – 4.78 (comp, 2H), 4.66 (d, *J* = 11.9 Hz, 1H), 4.34 (d, *J* = 11.9 Hz, 1H), 2.24 (s, 3H); minor: 7.88 (d, *J* = 7.7 Hz, 2H), 7.59 – 7.55 (comp, 2H), 7.34 – 7.30 (comp, 4H), 7.20 (s, 2H), 7.17 – 7.02 (comp, 4H), 6.98 (d, *J* = 7.7 Hz, 2H), 6.27 (d, *J* = 8.5 Hz, 2H), 4.95 (d, *J* = 3.1 Hz, 1H), 4.81 – 4.78 (comp, 2H), 4.66 (d, *J* = 11.9 Hz, 1H), 4.30 (d, *J* = 11.9 Hz, 1H), 2.32 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ major: 199.4, 145.5, 137.6, 137.0, 136.1, 134.9, 133.4, 131.8 129.2, 128.6, 128.5, 128.15, 128.12, 127.5, 115.4, 115.2, 109.5, 84.0, 72.6, 59.8, 21.1; HRMS (TOF MS ESI$^+$) calculated for $C_{29}H_{26}BrNO_2Na$ [M + Na]$^+$: 522.1220, found 520.1227; HPLC conditions for determination of enantiomeric excess: Chiral IF-3, λ = 254 nm, hexane : ethanol = 97:3, flow rate =1.0 mL/min, t_{major} = 12.5 min, t_{minor} = 11.3 min.



(2*R*,3*R*)-2-(Benzyloxy)-3-(4-methoxyphenyl)-1-phenyl-3-((4-(trifluoromethyl)phenyl)amino)propan-1-one (4l) White solid, 84.9 mg, 84% yield, 89:11 *dr*, 92%(37%) *ee*, mp = 144 – 146 ºC; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.71 (d, *J* = 7.4 Hz, 2H), 7.50 (t, *J* = 7.4 Hz, 1H), 7.36 – 7.30 (comp, 4H), 7.26 (d, *J* = 7.0 Hz, 3H), 7.24 – 7.20 (comp, 2H), 7.12 (d, *J* = 8.6 Hz, 2H), 6.72 (d, *J* = 8.6 Hz, 2H), 6.46 (d, *J* = 8.5 Hz, 2H), 5.12 (d, *J* = 6.6 Hz, 1H), 4.93 (d, *J* = 5.2 Hz, 1H), 4.89 – 4.83 (m, 1H), 4.69 (d, *J* = 11.9 Hz, 1H), 4.36 (d, *J* = 11.9 Hz, 1H), 3.71 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 199.4, 159.3, 149.0, 136.9, 136.1, 133.5, 129.5, 128.7 (q, *J* = 270.4 Hz), 128.61, 128.58, 128.55, 128.3, 128.2, 126.4 (q, *J* = 3.6 Hz), 119.2 (q, *J* = 32.6 Hz), 114.0, 112.9, 83.5, 72.6, 59.0, 55.2; ^{19}F NMR (376 MHz, $CDCl_3$) δ -61.2; HRMS (TOF MS ESI$^+$) calculated for $C_{30}H_{26}F_3NO_3Na$ [M + Na]$^+$: 528.1757, found 528.1751; HPLC conditions for determination of enantiomeric excess: Chiral IB-3, λ = 254 nm, hexane : ethanol = 99:1, flow rate =1.0 mL/min, t_{major} = 21.9 min, t_{minor} = 19.3 min.

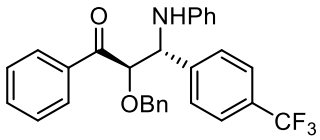


(2*R*,3*R*)-2-(Benzyloxy)-3-(4-fluorophenyl)-1-phenyl-3-(phenylamino)propan-1-one (4m) White solid, 61.2 mg, 72% yield, 90:10 *dr*, 90%(33%) *ee*, $[\alpha]_D^{20}$ = 12.5° (c = 0.47, MeOH), mp = 113 – 115 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ major: 7.88 – 7.75 (comp, 2H), 7.59 – 7.51 (m, 1H), 7.46 – 7.19 (comp, 9H), 7.04 (t, *J* = 7.2 Hz, 2H), 6.87 (t, *J* = 8.1 Hz, 2H), 6.65 – 6.58 (m, 1H), 6.44 (d, *J* = 7.8 Hz, 2H), 4.92 – 4.66 (comp, 4H), 4.35 – 4.28 (m, 1H); minor: 7.88 – 7.75 (comp, 2H), 7.59 – 7.51 (m, 1H), 7.46 – 7.19 (comp, 9H), 7.00 – 6.95 (comp, 4H), 6.65 – 6.58 (m, 1H), 6.38 (d, *J* = 7.8 Hz, 2H), 4.92 – 4.66 (comp, 4H), 4.35 – 4.28 (m, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ major: 199.2, 162.3 (d, *J* = 245.3 Hz), 146.1, 136.9, 136.0, 134.3 (d, *J* = 3.2 Hz), 133.5, 129.3 (d, *J* = 8.1 Hz), 129.1, 128.61, 128.59, 128.56, 128.20, 128.15, 118.0, 115.2 (d, *J* = 21.5 Hz), 113.86, 84.3, 72.6, 59.4; ^{19}F NMR (376 MHz, $CDCl_3$) δ major: -114.8; minor: -115.0; HRMS (TOF MS ESI$^+$) calculated for $C_{28}H_{25}FNO_2$ $[M + H]^+$: 426.1864, found 426.1863; HPLC conditions for determination of enantiomeric excess: Chiral IB-3, λ = 254 nm, hexane : ethanol = 97:3, flow rate =1.0 mL/min, t_{major} = 9.1 min, t_{minor} = 10.6 min.

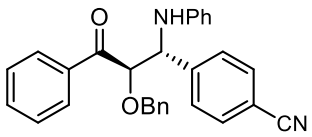


(2*R*,3*R*)-2-(Benzyloxy)-3-(4-bromophenyl)-1-phenyl-3-(phenylamino)propan-1-one (4n) White solid, 68.9 mg, 71% yield, 88:12 *dr*, 91%(26%) *ee*, $[\alpha]_D^{20}$ = 28.9° (c = 0.45, MeOH), mp = 125 – 127 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.79 (d, *J* = 7.7 Hz, 2H), 7.54 (t, *J* = 7.4 Hz, 1H), 7.38 (t, *J* = 7.7 Hz, 2H), 7.32 (t, *J* = 5.9 Hz, 5H), 7.22 – 7.17 (m, 2H), 7.10 (d, *J* = 8.3 Hz, 2H), 7.04 (t, *J* = 7.8 Hz, 2H), 6.64 (t, *J* = 7.3 Hz, 1H), 6.42 (d, *J* = 8.0 Hz, 2H), 4.90 (d, *J* = 5.4 Hz, 1H), 4.86 (s, 1H), 4.69 (d, *J* = 11.7 Hz, 2H), 4.33 (d, *J* = 11.7 Hz, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) (δ, ppm) δ 199.0, 146.0, 137.7, 136.8, 135.9, 133.6, 131.5, 129.4, 129.1, 128.7, 128.61, 128.57, 128.24,

128.18, 121.7, 118.1, 113.9, 84.1, 72.7, 59.5; HRMS (TOF MS ESI$^+$) calculated for $C_{28}H_{25}NO_2Br$ [M + H]$^+$: 486.1063, found 486.1066; HPLC conditions for determination of enantiomeric excess: Chiral IB-3, λ = 254 nm, hexane : ethanol = 97:3, flow rate =1.0 mL/min, t_{major} = 8.8 min, t_{minor} = 10.6 min.

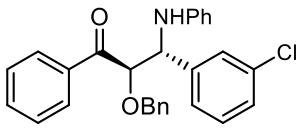


(2*R*,3*R*)-2-(Benzyloxy)-1-phenyl-3-(phenylamino)-3-(4-(trifluoromethyl)phenyl)propan-1-one (4o) White solid, 73.2 mg, 77% yield, 91:9 *dr*, 93%(10%) *ee*, $[\alpha]_D^{20}$ = 28.5^o (c = 0.47, DCM), mp = 126 – 128^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ major: 7.78 (d, *J* = 7.2 Hz, 2H), 7.53 (t, *J* = 7.4 Hz, 1H), 7.50 – 7.26 (comp, 9H), 7.23 – 7.15 (comp, 2H), 7.08 – 7.01 (comp, 2H), 6.64 (t, *J* = 7.3 Hz, 1H), 6.42 (d, *J* = 7.7 Hz, 2H), 4.95 – 4.91 (comp, 2H), 4.76 – 4.69 (comp, 2H), 4.33 (d, *J* = 11.9 Hz, 1H); minor: 7.89 (d, *J* = 7.2 Hz, 2H), 7.53 (t, *J* = 7.4 Hz, 1H), 7.50 – 7.26 (comp, 9H), 7.23 – 7.15 (comp, 2H), 6.96 – 6.92 (comp, 2H), 6.60 (t, *J* = 7.2 Hz, 1H), 6.37 (d, *J* = 7.7 Hz, 2H), 4.95 – 4.91 (comp, 2H), 4.76 – 4.69 (comp, 2H), 4.26 (d, *J* = 12.1 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ major: 198.8, 145.9, 142.9, 136.7, 135.8, 133.7, 129.2, 128.7, 128.63, 128.55, 128.3, 128.23 (q, *J* = 41.5 Hz), 128.20, 128.1, 128.0, 125.3 (q, *J* = 3.3 Hz), 118.3, 113.8, 84.1, 72.7, 59.7; ^{19}F NMR (376 MHz, $CDCl_3$) δ minor: -62.4; major: -62.5; HRMS (TOF MS ESI$^+$) calculated for $C_{29}H_{25}NO_2F_3$ [M + H]$^+$: 476.1832, found 476.1838; HPLC conditions for determination of enantiomeric excess: Chiral IB-3, λ = 254 nm, hexane : ethanol = 98:2, flow rate =1.0 mL/min, t_{major} = 9.1 min, t_{minor} = 11.1 min.



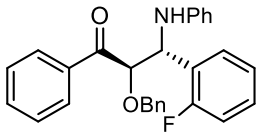
4-((1*R*,2*R*)-2-(Benzyloxy)-3-oxo-3-phenyl-1-(phenylamino)propyl)benzonitrile (4p) White solid, 48.4 mg, 56% yield, 93:7 *dr*, 95%(21%) *ee*, $[\alpha]_D^{20}$ = 2.3^o (c = 0.37,

MeOH), mp = 120 – 122 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.80 (d, *J* = 7.4 Hz, 2H), 7.56 (t, *J* = 7.4 Hz, 1H), 7.48 (d, *J* = 8.2 Hz, 2H), 7.39 (t, *J* = 7.8 Hz, 2H), 7.37 – 7.28 (comp, 5H), 7.23 – 7.16 (comp, 2H), 7.04 (t, *J* = 7.9 Hz, 2H), 6.66 (t, *J* = 7.3 Hz, 1H), 6.39 (d, *J* = 7.9 Hz, 2H), 4.93 (s, 2H), 4.70 (d, *J* = 11.7 Hz, 2H), 4.33 (d, *J* = 11.8 Hz, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 198.5, 145.6, 144.4, 136.5, 135.7, 133.9, 132.1, 129.2, 128.8, 128.7, 128.56, 128.55, 128.4, 128.3, 118.7, 118.4, 113.8, 111.6, 83.8, 72.7, 59.8; HRMS (TOF MS ESI$^+$) calculated for $C_{29}H_{25}N_2O_2$ $[M + H]^+$: 433.1911, found 433.1922; HPLC conditions for determination of enantiomeric excess: Chiral ID-3, λ = 240 nm, hexane : ethanol = 97:3, flow rate =1.0 mL/min, t_{major} = 32.9 min, t_{minor} = 26.4 min.

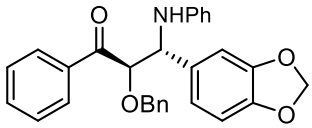


(2*R*,3*R*)-2-(Benzyloxy)-3-(3-chlorophenyl)-1-phenyl-3-(phenylamino)propan-1-one (4q) White solid, 70.6 mg, 80% yield, 84:16 *dr*, 87%(24%) *ee*, $[\alpha]_D^{20}$ = 23.3° (c = 0.37, DCM), mp = 130 – 132 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.80 (d, *J* = 7.4 Hz, 2H), 7.51 (t, *J* = 7.4 Hz, 1H), 7.47 – 7.43 (m, 1H), 7.35 (d, *J* = 7.6 Hz, 2H), 7.32 – 7.30 (comp, 2H), 7.25 – 7.22 (comp, 2H), 7.19 – 7.17 (comp, 2H), 7.13 – 7.10 (comp, 2H), 7.06 – 7.00 (comp, 2H), 6.66 – 6.57 (m, 1H), 6.43 (d, *J* = 7.9 Hz, 2H), 4.88 – 4.95 (comp, 2H), 4.76 – 4.64 (comp, 2H), 4.33 (d, *J* = 11.8 Hz, 1H); minor: 7.88 (d, *J* = 7.3 Hz, 2H), 7.51 (t, *J* = 7.4 Hz, 1H), 7.47 – 7.43 (m, 1H), 7.35 (d, *J* = 7.6 Hz, 2H), 7.32 – 7.30 (comp, 2H), 7.25 – 7.22 (comp, 2H), 7.19 – 7.17 (comp, 2H), 7.13 – 7.10 (comp, 2H), 7.06 – 7.00 (comp, 2H), 6.66 – 6.57 (m, 1H), 6.38 (d, *J* = 8.0 Hz, 2H), 4.95 – 4.92 (comp, 2H), 4.76 – 4.64 (comp, 2H), 4.28 (d, *J* = 11.9 Hz, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ major: 199.1, 146.1, 141.2, 136.9, 136.1, 134.4, 133.7, 129.7, 129.2, 128.74, 128.70, 128.67, 128.32, 128.25, 128.1, 128.0, 126.0, 118.2, 113.9, 84.1, 72.7, 59.8; HRMS (TOF MS ESI$^+$) calculated for $C_{28}H_{25}NO_2Cl$ $[M + H]^+$: 442.1568, found 442.1581; HPLC conditions for determination of enantiomeric excess: Chiral

Y1, λ = 254 nm, hexane : ethanol = 995:5, flow rate =1.0 mL/min, t_{major} = 31.1 min, t_{minor} = 45.6 min.

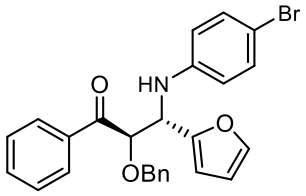


(2*R*,3*R*)-2-(Benzyloxy)-3-(2-fluorophenyl)-1-phenyl-3-(phenylamino)propan-1-one (4r) Yellow oil, 56.1 mg, 66% yield, >95:5 *dr*, 82% *ee*; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.82 (d, *J* = 8.0 Hz, 2H), 7.49 (t, *J* = 7.0 Hz, 1H), 7.36 – 7.27 (comp, 6H), 7.20 – 7.16 (comp, 2H), 7.15 – 7.10 (comp, 1H), 7.05 (t, *J* = 7.5 Hz, 2H), 6.98 – 6.90 (comp, 2H), 6.64 (t, *J* = 7.3 Hz, 1H), 6.48 (d, *J* = 8.3 Hz, 2H), 5.32 – 5.26 (m, 1H), 5.06 (d, *J* = 5.8 Hz, 1H), 4.76 – 4.67 (m, 2H), 4.40 (d, *J* = 12.0 Hz, 1H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 198.8, 160.9 (d, *J* = 244.9 Hz), 146.2, 137.0, 136.0, 133.5, 129.4 (d, *J* = 3.9 Hz), 129.3, 129.2, 129.1, 128.53, 128.51, 128.1, 128.0, 125.7 (d, *J* = 13.1 Hz), 124.3 (d, *J* = 3.1 Hz), 118.1, 115.1 (d, *J* = 22.0 Hz), 113.7, 82.3, 72.3, 53.7. ^{19}F NMR (376 MHz, $CDCl_3$) δ -118.6. HRMS (TOF MS ESI$^+$) calculated for $C_{28}H_{25}FNO_2$ $[M + H]^+$: 426.1864, found 426.1870; HPLC conditions for determination of enantiomeric excess: Chiral Y1, λ = 254 nm, hexane : ethanol = 97:3, flow rate =1.0 mL/min, t_{major} = 7.7 min, t_{minor} = 9.1 min.

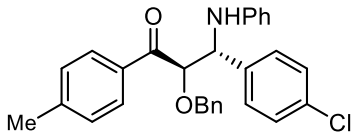


(2*R*,3*R*)-3-(Benzo[*d*][1,3]dioxol-5-yl)-2-(benzyloxy)-1-phenyl-3-(phenylamino)propan-1-one (4s) Yellow oil, 31.6 mg, 35% yield, 93:7 *dr*, 90%(31%) *ee*; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.77 (d, *J* = 7.3 Hz, 2H), 7.52 (d, *J* = 6.1 Hz, 1H), 7.40 – 7.25 (comp, 7H), 7.05 (t, *J* = 6.8 Hz, 2H), 6.75 (s, 1H), 6.66 – 6.57 (comp, 3H), 6.46 (d, *J* = 7.3 Hz, 2H), 5.85 (s, 2H), 4.92 (s, 1H), 4.82 (d, *J* = 2.0 Hz, 1H), 4.70 (d, *J* = 11.8 Hz, 2H), 4.35 (d, *J* = 11.7 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 199.2, 147.8, 147.1, 146.3, 137.1, 136.2, 133.4, 132.5, 129.9, 129.1, 128.56, 128.55, 128.54, 128.2, 121.1, 117.9, 113.9, 107.97, 107.95, 100.9, 84.2, 72.6, 59.7; HRMS (TOF MS ESI$^+$) calculated for

$C_{29}H_{26}NO_4$ $[M + H]^+$: 452.1856, found 452.1858; HPLC conditions for determination of enantiomeric excess: Chiral IF-3, λ = 254 nm, hexane : ethanol = 98:2, flow rate =1.0 mL/min, t_{major} = 26.4 min, t_{minor} = 23.2 min.

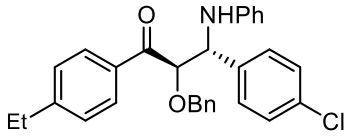


(2*R*,3*S*)-2-(Benzyloxy)-3-((4-bromophenyl)amino)-3-(furan-2-yl)-1-phenylpropan-1-one (4t) Yellow solid, 69.4 mg, 73% yield, 90:10 *dr*, 98% *ee*, $[\alpha]_D^{20}$ = 53.1° (c = 0.40, DCM), mp = 126 – 128 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.79 (d, *J* = 7.2 Hz, 2H), 7.54 (t, *J* = 7.4 Hz, 1H), 7.39 (t, *J* = 7.8 Hz, 2H), 7.32 – 7.29 (comp, 3H), 7.25 (d, *J* = 1.1 Hz, 1H), 7.20 (dd, *J* = 6.7, 2.9 Hz, 2H), 7.18 – 7.14 (comp, 2H), 6.44 – 6.39 (m, 2H), 6.19 (dd, *J* = 3.2, 1.8 Hz, 1H), 6.14 (d, *J* = 3.2 Hz, 1H), 5.01 (q, *J* = 5.6 Hz, 2H), 4.68 (d, *J* = 11.8 Hz, 1H), 4.53 (s, 1H), 4.38 (d, *J* = 11.8 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 199.1, 151.1, 145.2, 142.0, 136.8, 136.1, 133.4, 131.9, 128.60, 128.58, 128.55, 128.4, 128.2, 115.7, 110.5, 110.3, 108.7, 81.6, 72.7, 54.5; HRMS (TOF MS ESI$^+$) calculated for $C_{26}H_{22}BrNO_3Na$ $[M + Na]^+$: 498.0675, found 498.0667; HPLC conditions for determination of enantiomeric excess: Chiral ID-3, λ = 254 nm, hexane : ethanol = 96:4, flow rate =1.0 mL/min, t_{major} = 16.0 min, t_{minor} = 15.1 min.

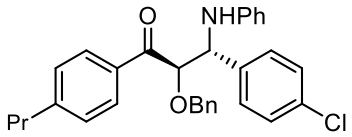


(2*R*,3*R*)-2-(Benzyloxy)-3-(4-chlorophenyl)-3-(phenylamino)-1-(*p*-tolyl)propan-1-one (5a) White solid, 65.5 mg, 72% yield, 89:11 *dr*, 91%(23%) *ee*, $[\alpha]_D^{20}$ = 44.9° (c = 0.37, DCM), mp = 110 – 112 °C; ^{1}H NMR (400 MHz, $CDCl_3$) (δ, ppm) δ 7.71 (d, *J* = 8.2 Hz, 2H), 7.32 – 7.29 (comp, 3H), 7.24 – 7.11 (comp, 8H), 7.04 (t, *J* = 7.9 Hz, 2H), 6.63 (t, *J* = 7.3 Hz, 1H), 6.42 (d, *J* = 8.0 Hz, 2H), 4.88 (d, *J* = 5.3 Hz, 2H), 4.68 (d, *J* = 11.8 Hz, 2H), 4.31 (d, *J* = 11.8 Hz, 1H), 2.39 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) (δ, ppm) δ 198.4, 146.0, 144.7, 137.3, 137.0, 133.44, 133.37, 129.4, 129.12, 129.07,

128.7, 128.6, 128.5, 128.2, 128.1, 118.0, 113.8, 84.1, 72.5, 59.5, 21.7; HRMS (TOF MS ESI$^+$) calculated for $C_{29}H_{27}NO_2Cl$ [M + H]$^+$: 456.1725, found 456.1733; HPLC conditions for determination of enantiomeric excess: Chiral IF-3, λ = 254 nm, hexane : ethanol = 99:1, flow rate =1.0 mL/min, t_{major} = 23.3 min, t_{minor} = 19.4 min.

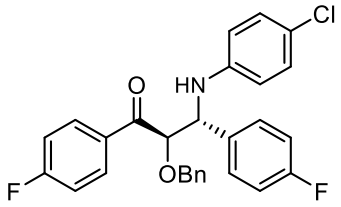


(2*R*,3*R*)-2-(Benzyloxy)-3-(4-chlorophenyl)-1-(4-ethylphenyl)-3-(phenylamino)propan-1-one (5b) White solid, 75.1 mg, 80% yield, 92:8 *dr*, 91%(40%) *ee*, $[\alpha]_D^{20}$ = 35.3^o (c = 0.45, DCM), mp = 109 – 111 ^{o}C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.73 (d, *J* = 7.9 Hz, 2H), 7.35 – 7.29 (comp, 3H), 7.19 (d, *J* = 7.6 Hz, 4H), 7.15 (s, 4H), 7.04 (t, *J* = 7.5 Hz, 2H), 6.63 (t, *J* = 7.3 Hz, 1H), 6.42 (d, *J* = 7.9 Hz, 2H), 4.88 (t, *J* = 8.9 Hz, 2H), 4.69 (d, *J* = 11.8 Hz, 2H), 4.32 (d, *J* = 11.9 Hz, 1H), 2.68 (q, *J* = 7.5 Hz, 2H), 1.25 (t, *J* = 7.6 Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 198.4, 150.8, 146.1, 137.3, 137.0, 133.6, 133.4, 129.11, 129.05, 128.8, 128.6, 128.5, 128.2, 128.1, 118.0, 113.8, 84.0, 72.5, 59.5, 29.0, 15.1; HRMS (TOF MS ESI$^+$) calculated for $C_{30}H_{29}NO_2Cl$ [M + H]$^+$: 470.1881, found 470.1885; HPLC conditions for determination of enantiomeric excess: Chiral IF-3, λ = 254 nm, hexane : ethanol = 99:1, flow rate =1.0 mL/min, t_{major} = 21.2 min, t_{minor} = 17.9 min.

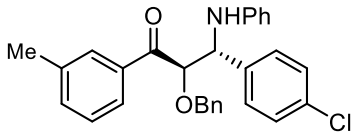


(2*R*,3*R*)-2-(Benzyloxy)-3-(4-chlorophenyl)-3-(phenylamino)-1-(4-propylphenyl)propan-1-one (5c) White solid, 67.8 mg, 70% yield, 87:13 *dr*, 90%(17%) *ee*, mp = 112 – 114 ^{o}C; ^{1}H NMR (500 MHz, $CDCl_3$) δ major: 7.71 (d, *J* = 7.7 Hz, 2H), 7.31 – 7.13 (comp, 11H), 7.03 (t, *J* = 7.5 Hz, 2H), 6.62 (t, *J* = 7.3 Hz, 1H), 6.42 (d, *J* = 7.9 Hz, 2H), 4.90 – 4.85 (comp, 2H), 4.73 – 4.67 (comp, 2H), 4.32 (d, *J* = 11.9 Hz, 1H), 2.61 (t, *J* = 7.6 Hz, 2H), 1.68 – 1.61 (m, 2H), 0.94 (t, *J* = 7.0 Hz, 3H); minor: 7.82 (d, *J* =

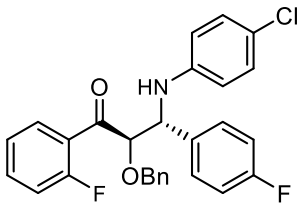
7.6 Hz, 2H), 7.31 – 7.13 (comp, 11H), 7.03 (t, *J* = 7.5 Hz, 2H), 6.58 (t, *J* = 7.3 Hz, 1H), 6.37 (d, *J* = 8.0 Hz, 2H), 4.90 – 4.85 (comp, 2H), 4.73 – 4.67 (comp, 2H), 4.26 (d, *J* = 11.9 Hz, 1H), 2.61 (t, *J* = 7.6 Hz, 2H), 1.68 – 1.61 (m, 2H), 0.88 (t, *J* = 6.5 Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ major: 198.4, 149.3, 146.1, 137.3, 137.0, 133.7, 133.4, 129.12, 129.06, 128.8, 128.7, 128.6, 128.5, 128.17, 128.16, 118.0, 113.8, 84.0, 72.5, 59.6, 38.1, 24.2, 13.8; HRMS (TOF MS ESI$^+$) calculated for $C_{31}H_{31}ClNO_2$ [M + H]$^+$: 484.2038, found 484.2040; HPLC conditions for determination of enantiomeric excess: Chiral IF-3, λ = 254 nm, hexane : ethanol = 99:1, flow rate =1.0 mL/min, t_{major} = 22.4 min, t_{minor} = 18.7 min.



(2*R*,3*R*)-2-(Benzyloxy)-3-((4-chlorophenyl)amino)-1,3-bis(4-fluorophenyl)propan-1-one (5d) White solid, 75.4 mg, 79% yield, 90:10 *dr*, 90%(6%) *ee*, $[\alpha]_D^{20}$ = 24.1° (c = 0.45, DCM), mp = 121 – 123 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.79 – 7.77 (comp, 2H), 7.31 (s, 3H), 7.22 – 7.14 (comp, 4H), 7.02 – 6.97 (comp, 4H), 6.89 (t, *J* = 8.1 Hz, 2H), 6.35 (d, *J* = 7.9 Hz, 2H), 4.83 – 4.77 (m, 2H), 4.70 (d, *J* = 5.5 Hz, 1H), 4.63 (d, *J* = 11.8 Hz, 1H), 4.33 (d, *J* = 11.8 Hz, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 197.9, 165.9 (d, *J* = 256.7 Hz), 162.4 (d, *J* = 246.8 Hz), 144.6, 136.6, 133.8 (d, *J* = 3.1 Hz), 132.2 (d, *J* = 2.9 Hz), 131.5 (d, *J* = 9.4 Hz), 129.2 (d, *J* = 8.5 Hz), 129.0, 128.7, 128.4, 128.2, 122.8, 115.7 (d, *J* = 21.8 Hz), 115.5 (d, *J* = 21.6 Hz), 114.9, 84.5, 72.8, 59.6; ^{19}F NMR (376 MHz, $CDCl_3$) δ -103.5, -114.1; HRMS (TOF MS ESI$^+$) calculated for $C_{28}H_{23}NO_2F_2Cl$ [M + H]$^+$: 478.1380, found 478.1391; HPLC conditions for determination of enantiomeric excess: Chiral IG-3, λ = 254 nm, hexane : ethanol = 96:4, flow rate =1.0 mL/min, t_{major} = 13.9 min, t_{minor} = 14.5 min.

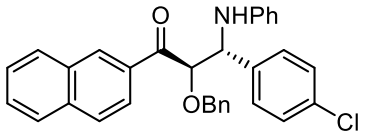


(2*R*,3*R*)-2-(Benzyloxy)-3-(4-chlorophenyl)-3-(phenylamino)-1-(*m*-tolyl)propan-1-one (5e) White solid, 67.4 mg, 74% yield, 95:5 *dr*, 91%(37%) *ee*, $[\alpha]_D^{20} = 25.3^o$ (c = 0.48, DCM), mp = 111 – 113 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.58 (d, *J* = 7.6 Hz, 1H), 7.48 (s, 1H), 7.38 – 7.29 (comp, 4H), 7.26 – 7.20 (comp, 3H), 7.16 (s, 4H), 7.05 (t, *J* = 7.6 Hz, 2H), 6.64 (t, *J* = 7.3 Hz, 1H), 6.43 (d, *J* = 8.1 Hz, 2H), 4.93 (d, *J* = 4.9 Hz, 1H), 4.87 (s, 1H), 4.70 – 4.67 (m, 2H), 4.33 (d, *J* = 11.8 Hz, 1H), 2.32 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 199.1, 146.1, 138.5, 137.2, 137.0, 136.0, 134.4, 133.5, 129.13, 129.11, 129.08, 128.6, 128.51, 128.47, 128.21, 128.16, 125.7, 118.1, 113.9, 83.9, 59.5, 21.3; HRMS (TOF MS ESI$^+$) calculated for $C_{29}H_{27}NO_2Cl$ $[M + H]^+$: 456.1725, found 456.1720; HPLC conditions for determination of enantiomeric excess: Chiral ID-3, λ = 254 nm, hexane : ethanol = 99:1, flow rate =1.0 mL/min, t_{major} = 15.2 min, t_{minor} = 13.1 min.

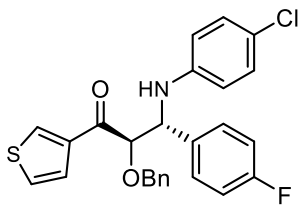


(2*R*,3*R*)-2-(Benzyloxy)-3-((4-chlorophenyl)amino)-1-(2-fluorophenyl)-3-(4-fluoro phenyl)propan-1-one (5f) White solid, 72.5 mg, 76% yield, >95:5 *dr*, 90% *ee*, mp = 116 – 118 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.48 (t, *J* = 7.2 Hz, 2H), 7.36 – 7.27 (comp, 5H), 7.16 – 7.10 (comp, 3H), 7.06 – 6.97 (comp, 3H), 6.83 (t, *J* = 8.5 Hz, 2H), 6.36 (d, *J* = 8.7 Hz, 2H), 5.14 (d, *J* = 4.7 Hz, 1H), 4.81 – 4.67 (m, 3H), 4.40 (d, *J* = 11.7 Hz, 1H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 197.3 (d, *J* = 4.3 Hz), 162.3 (d, *J* = 246.3 Hz), 160.8 (d, *J* = 253.2 Hz), 144.9, 137.1, 134.9 (d, *J* = 9.0 Hz), 133.3 (d, *J* = 3.0 Hz), 130.78, 129.3 (d, *J* = 8.2 Hz), 128.9, 128.6, 128.2, 127.6, 125.4 (d, *J* = 15.4 Hz), 124.8 (d, *J* = 3.1 Hz), 122.8, 116.5 (d, *J* = 23.5 Hz), 115.3, 115.1, 85.2, 72.9, 58.9. ^{19}F NMR (471 MHz, $CDCl_3$) δ -109.5, -114.4. HRMS (TOF MS ESI$^+$)

calculated for $C_{28}H_{23}NO_2F_2Cl$ $[M + H]^+$: 478.1380, found 478.1386; HPLC conditions for determination of enantiomeric excess: Chiral IF-3, λ = 254 nm, hexane : ethanol = 97:3, flow rate =1.0 mL/min, t_{major} = 9.1 min, t_{minor} = 8.6 min.

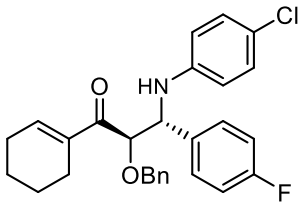


(2*R*,3*R*)-2-(Benzyloxy)-3-(4-chlorophenyl)-1-(naphthalen-2-yl)-3-(phenylamino)propan-1-one (5g) White solid, 77.6 mg, 79% yield, 82:18 *dr*, 90%(30%) *ee*, $[\alpha]_D^{20}$ = 19.8° (c = 0.47, DCM), mp = 148 – 150 °C; ^{1}H NMR (500 MHz, $CDCl_3$) (δ, ppm) δ 8.24 (s, 1H), 7.89 – 7.79 (comp, 4H), 7.60 (t, *J* = 6.9 Hz, 1H), 7.54 (t, *J* = 6.9 Hz, 1H), 7.32 (dd, *J* = 5.0, 1.8 Hz, 3H), 7.26 – 7.17 (comp, 4H), 7.16 – 7.12 (comp, 2H), 7.06 – 7.01 (comp, 2H), 6.63 (t, *J* = 7.3 Hz, 1H), 6.45 (d, *J* = 7.7 Hz, 2H), 5.05 (d, *J* = 5.2 Hz, 1H), 4.95 (t, *J* = 5.5 Hz, 1H), 4.73 (d, *J* = 11.9 Hz, 2H), 4.39 (d, *J* = 11.8 Hz, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) (δ, ppm) δ 198.8, 146.0, 137.2, 136.9, 135.7, 133.6, 133.2, 132.3, 130.6, 129.8, 129.2, 129.1, 128.9, 128.64, 128.60, 128.5, 128.3, 128.2, 127.8, 126.9, 124.0, 118.2, 113.9, 84.3, 72.7, 59.7; HRMS (TOF MS ESI$^+$) calculated for $C_{32}H_{26}ClNO_2Na$ $[M + Na]^+$: 514.1544, found 514.1548; HPLC conditions for determination of enantiomeric excess: Chiral IF-3, λ = 254 nm, hexane : ethanol = 97:3, flow rate =1.0 mL/min, t_{major} = 12.4 min, t_{minor} = 13.3 min.

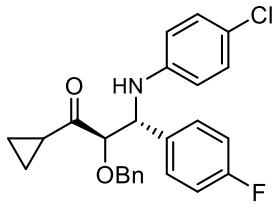


(2*R*,3*R*)-2-(Benzyloxy)-3-((4-chlorophenyl)amino)-3-(4-fluorophenyl)-1-(thiophen-3-yl)propan-1-one (5h) White solid, 84.6 mg, 91% yield, 88:12 *dr*, 90%(4%) *ee*, mp = 139 – 141 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.01 (s, 1H), 7.45 (d, *J* = 4.9 Hz, 1H), 7.32 (s, 3H), 7.24 - 7.18 (comp, 3H), 7.16 (s, 2H), 6.98 (d, *J* = 7.7 Hz, 2H), 6.90 (t, *J* = 8.1 Hz, 2H), 6.35 (d, *J* = 7.7 Hz, 2H), 4.75 (d, *J* = 4.9 Hz, 1H), 4.73 – 4.62 (m, 2H),

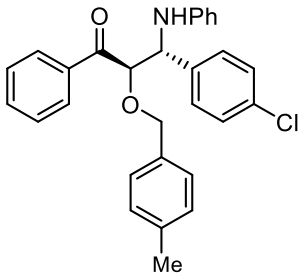
4.55 (d, *J* = 4.9 Hz, 1H), 4.32 (d, *J* = 11.8 Hz, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 194.0, 162.4 (d, *J* = 246.3 Hz), 144.6, 139.8, 136.6, 134.14 (d, *J* = 3.3 Hz), 134.12, 129.2 (d, *J* = 8.2 Hz), 129.0, 128.6, 128.3, 128.1, 127.4, 125.9, 122.7, 115.4 (d, *J* = 21.5 Hz), 114.9, 86.0, 72.9, 59.8; ^{19}F NMR (471 MHz, $CDCl_3$) δ -114.3; HRMS (TOF MS ESI$^+$) calculated for $C_{26}H_{21}NO_2SFClNa$ [M + Na]$^+$: 488.0858, found 488.0857; HPLC conditions for determination of enantiomeric excess: Chiral IB-3, λ = 254 nm, hexane : ethanol = 97:3, flow rate =1.0 mL/min, t_{major} = 14.5 min, t_{minor} = 13.8 min.



(2*R*,3*R*)-2-(Benzyloxy)-3-((4-chlorophenyl)amino)-1-(cyclohex-1-en-1-yl)-3-(4-fluorophenyl)propan-1-one (5i) Yellow oil, 50.0 mg, 54% yield, 93:7 *dr*, 92%(16%) *ee*; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.33 (d, *J* = 6.8 Hz, 3H), 7.25 (d, *J* = 8.7 Hz, 2H), 7.22 – 7.16 (comp, 2H), 6.99 (d, *J* = 7.5 Hz, 2H), 6.95 (t, *J* = 8.0 Hz, 2H), 6.52 (s, 1H), 6.36 (d, *J* = 7.5 Hz, 2H), 4.96 (bs, 1H), 4.75 (d, *J* = 4.1 Hz, 1H), 4.70 (d, *J* = 4.3 Hz, 1H), 4.63 (d, *J* = 11.9 Hz, 1H), 4.32 (d, *J* = 11.8 Hz, 1H), 2.21 (d, *J* = 16.8 Hz, 1H), 2.05 (d, *J* = 19.0 Hz, 1H), 1.98 – 1.88 (m, 2H), 1.55 – 1.43 (m, 4H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 199.0, 162.3 (d, *J* = 246.4 Hz), 145.2, 142.6, 139.5, 137.1, 134.5 (d, *J* = 3.0 Hz), 128.89, 128.87 (d, *J* = 8.0 Hz), 128.6, 128.2, 128.1, 122.3, 115.4 (d, *J* = 21.5 Hz), 114.7, 80.9, 72.0, 59.9, 26.2, 23.0, 21.7, 21.2; ^{19}F NMR (376 MHz, $CDCl_3$) δ -114.62; HRMS (TOF MS ESI$^+$) calculated for $C_{28}H_{28}NO_2FCl$ [M + H]$^+$: 464.1787, found 464.1801; HPLC conditions for determination of enantiomeric excess: Chiral IF-3, λ = 254 nm, hexane : ethanol = 97:3, flow rate =1.0 mL/min, t_{major} = 14.5 min, t_{minor} = 12.0 min.

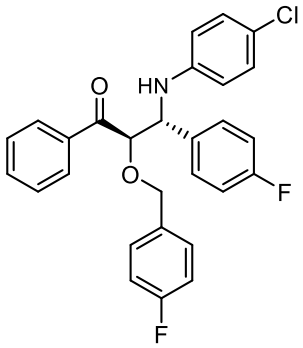


(2*R*,3*R*)-2-(Benzyloxy)-3-((4-chlorophenyl)amino)-1-cyclopropyl-3-(4-fluorophenyl)propan-1-one (5j) Yellow oil, 50.8 mg, 60% yield, 85:15 *dr*, 90%(14%) *ee*; ^{1}H NMR (400 MHz, $CDCl_3$) δ major: 7.41 – 7.27 (comp, 7H), 7.09 – 6.92 (comp, 4H), 6.43 – 6.34 (comp, 2H), 4.74 (d, *J* = 11.7 Hz, 1H), 4.70 – 4.52 (comp, 2H), 4.43 – 4.35 (m, 1H), 4.25 – 4.20 (m, 1H), 1.07 – 0.82 (comp, 4H), 0.671 – 0.65 (m, 1H); minor: 7.41 – 7.27 (comp, 7H), 7.16 – 7.11 (comp, 2H), 7.09 – 6.92 (comp, 2H), 6.43 – 6.34 (comp, 2H), 4.82 (s, 1H), 4.70 – 4.52 (comp, 2H), 4.43 – 4.35 (m, 1H), 4.15 – 4.14 (m, 1H), 1.16 – 1.09 (m, 2H), 1.07 – 0.82 (comp, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ major: 211.7, 162.4 (d, *J* = 246.3 Hz), 144.7, 136.8, 134.0 (d, *J* = 3.2 Hz), 129.6 (d, *J* = 8.1 Hz), 129.0, 128.7, 128.3, 128.0, 122.7, 115.3 (d, *J* = 21.5 Hz), 114.9, 87.2, 73.3, 58.7, 17.5, 12.52, 12.49; ^{19}F NMR (376 MHz, $CDCl_3$) δ major: -114.5; minor: -115.0; HRMS (TOF MS ESI$^+$) calculated for $C_{25}H_{24}NO_2FCl$ $[M + H]^+$: 424.1474, found 424.1480; HPLC conditions for determination of enantiomeric excess: Chiral IG-3, λ = 254 nm, hexane : ethanol : isopropanol = 98:1:1, flow rate =1.0 mL/min, t_{major} = 21.3 min, t_{minor} = 23.7 min.

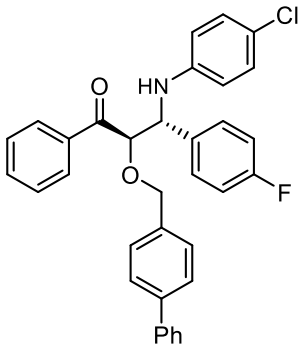


(2*R*,3*R*)-3-(4-Chlorophenyl)-2-((4-methylbenzyl)oxy)-1-phenyl-3-(phenylamino)propan-1-one (5k) White solid, 68.3 mg, 75% yield, 87:13 *dr*, 90%(15%) *ee*, $[\alpha]_D^{20}$ = 4.7^o (c = 0.40, DCM), mp = 120 – 122 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.77 (d, *J* = 7.2 Hz, 2H), 7.53 (t, *J* = 7.4 Hz, 1H), 7.36 (t, *J* = 7.8 Hz, 2H), 7.15 (s, 3H), 7.13 – 7.06 (comp, 7H), 6.63 (t, *J* = 7.3 Hz, 1H), 6.41 (d, *J* = 7.7 Hz, 2H), 4.90 – 4.83 (m,

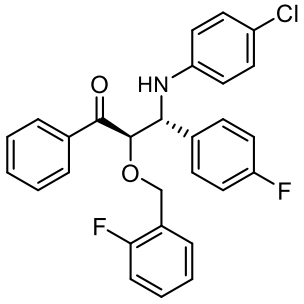
2H), 4.64 (d, *J* = 11.7 Hz, 2H), 4.28 (d, *J* = 11.7 Hz, 1H), 2.35 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 199.1, 146.0, 138.1, 137.2, 136.0, 133.8, 133.53, 133.46, 129.3, 129.12, 129.08, 128.62, 128.59, 128.5, 128.3, 118.0, 113.8, 84.0, 72.5, 59.4, 21.2; HRMS (TOF MS ESI$^+$) calculated for $C_{29}H_{27}NO_2Cl$ $[M + H]^+$: 456.1725, found 456.1737; HPLC conditions for determination of enantiomeric excess: Chiral IB-3, λ = 254 nm, hexane : ethanol = 95:5, flow rate =1.0 mL/min, t_{major} = 9.3 min, t_{minor} = 8.3 min.



(2*R*,3*R*)-3-((4-Chlorophenyl)amino)-2-((4-fluorobenzyl)oxy)-3-(4-fluorophenyl)-1-phenylpropan-1-one (5l) White solid, 79.2 mg, 83% yield, 93:7 *dr*, 90%(26%) *ee*, mp = 119 – 121 ^{o}C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.74 (d, *J* = 7.7 Hz, 2H), 7.53 (t, *J* = 7.3 Hz, 1H), 7.37 (t, *J* = 7.5 Hz, 2H), 7.16 (dd, *J* = 13.2, 7.5 Hz, 4H), 6.99 (comp, 4H), 6.88 (t, *J* = 8.3 Hz, 2H), 6.36 (d, *J* = 8.3 Hz, 2H), 4.83 (d, *J* = 4.8 Hz, 2H), 4.75 (s, 1H), 4.61 (d, *J* = 11.7 Hz, 1H), 4.32 (d, *J* = 11.7 Hz, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 199.02, 162.6 (d, *J* = 246.8 Hz), 162.4 (d, *J* = 246.6 Hz), 144.7, 135.9, 133.8 (d, *J* = 3.0 Hz), 133.7, 132.6 (d, *J* = 3.2 Hz), 130.0(d, *J* = 8.2 Hz), 129.2 (d, *J* = 8.1 Hz), 129.0, 128.7, 128.5, 122.8, 115.5 (d, *J* = 21.5 Hz), 115.4 (d, *J* = 21.2 Hz), 115.0, 83.8, 71.9, 59.6; ^{19}F NMR (471 MHz, $CDCl_3$) δ -113.6, -114.2; HRMS (TOF MS ESI$^+$) calculated for $C_{28}H_{23}NO_2F_2Cl$ $[M + H]^+$: 478.1380, found 478.1373; HPLC conditions for determination of enantiomeric excess: Chiral IB-3, λ = 254 nm, hexane : ethanol = 97:3, flow rate =1.0 mL/min, t_{major} = 12.1 min, t_{minor} = 11.4 min.

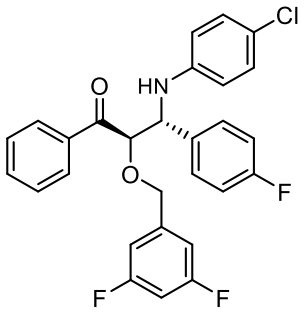


(2*R*,3*R*)-2-((1,1'-Biphenyl)-4-ylmethoxy)-3-((4-chlorophenyl)amino)-3-(4-fluorophenyl)-1-phenylpropan-1-one (5m) White solid, 45.0 mg, 42% yield, 96:4 *dr*, 97%(10%) *ee*, mp = 144 – 146 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.75 (d, *J* = 8.2 Hz, 2H), 7.61 – 7.51 (comp, 5H), 7.46 (t, *J* = 7.6 Hz, 2H), 7.37 (t, *J* = 7.4 Hz, 3H), 7.26 (s, 2H), 7.21 - 7.15 (comp, 2H), 6.98 (d, *J* = 8.0 Hz, 2H), 6.89 (t, *J* = 8.3 Hz, 2H), 6.36 (d, *J* = 8.1 Hz, 2H), 4.94 (d, *J* = 5.0 Hz, 1H), 4.85 (s, 1H), 4.78 (s, 1H), 4.72 (d, *J* = 11.9 Hz, 1H), 4.39 (d, *J* = 11.9 Hz, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 199.2, 162.4 (d, *J* = 246.6 Hz), 144.7, 140.9 (d, *J* = 8.9 Hz), 136.0, 135.7, 133.8 (d, *J* = 3.2 Hz), 133.6, 129.24, 129.18, 129.0, 128.9, 128.7, 128.6, 128.5, 127.5, 127.3, 127.1, 122.7, 115.4 (d, *J* = 21.5 Hz), 115.0, 83.8, 72.4, 59.6; ^{19}F NMR (471 MHz, $CDCl_3$) δ -114.3; HRMS (TOF MS ESI$^+$) calculated for $C_{34}H_{27}NO_2FClNa$ $[M + Na]^+$: 558.1607, found 558.1617; HPLC conditions for determination of enantiomeric excess: Chiral IF-3, λ = 254 nm, hexane : ethanol = 98:2, flow rate =1.0 mL/min, t_{major} = 21.6 min, t_{minor} = 18.5 min.



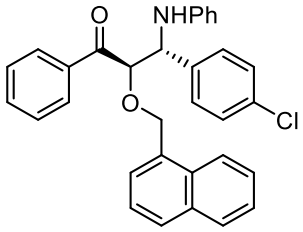
(2*R*,3*R*)-3-((4-Chlorophenyl)amino)-2-((2-fluorobenzyl)oxy)-3-(4-fluorophenyl)-1-phenylpropan-1-one (5n) White solid, 74.4 mg, 78% yield, 90:10 *dr*, 92%(15%) *ee*, mp = 120 - 122 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.73 (d, *J* = 7.4 Hz, 2H), 7.53 (t, *J*

= 7.4 Hz, 1H), 7.37 (t, *J* = 7.7 Hz, 2H), 7.34 – 7.28 (m, 1H), 7.26 – 7.21 (m, 1H), 7.20 – 7.09 (comp, 3H), 7.08 – 7.03 (m, 1H), 6.99 (d, *J* = 8.7 Hz, 2H), 6.85 (t, *J* = 8.6 Hz, 2H), 6.37 (d, *J* = 8.8 Hz, 2H), 4.99 (d, *J* = 4.5 Hz, 1H), 4.92 – 4.81 (comp, 2H), 4.70 (d, *J* = 11.9 Hz, 1H), 4.50 (d, *J* = 11.9 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 198.7, 162.4 (d, *J* = 246.4 Hz), 161.1 (d, *J* = 247.3 Hz), 144.7, 135.9, 133.6, 133.5 (d, *J* = 2.9 Hz), 130.8 (d, *J* = 4.0 Hz), 130.3 (d, *J* = 8.2 Hz), 129.2 (d, *J* = 8.2 Hz), 129.0, 128.7, 128.5, 124.3 (d, *J* = 2.5 Hz), 123.9 (d, *J* = 14.7 Hz), 122.6, 115.5 (d, *J* = 21.3 Hz), 115.3 (d, *J* = 21.6 Hz), 114.9, 84.2, 66.8 (d, *J* = 2.9 Hz), 59.3; ^{19}F NMR (376 MHz, $CDCl_3$) δ -114.4, -118.0; HRMS (TOF MS ESI$^+$) calculated for $C_{28}H_{22}NO_2F_2ClNa$ [M + Na]$^+$: 500.1199, found 500.1196; HPLC conditions for determination of enantiomeric excess: Chiral ID-3, λ = 254 nm, hexane : ethanol = 97:3, flow rate =1.0 mL/min, t_{major} = 11.7 min, t_{minor} = 9.7 min.

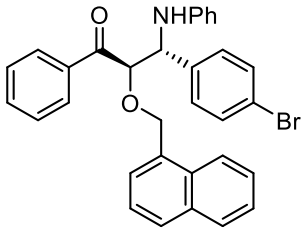


(2*R*,3*R*)-3-((4-Chlorophenyl)amino)-2-((3,5-difluorobenzyl)oxy)-3-(4-fluorophenyl)-1-phenylpropan-1-one (5o) Yellow oil, 54.5 mg, 55% yield, 94:6 *dr*, 93%(37%) *ee*; ^{1}H NMR (500 MHz, $CDCl_3$) δ major: 7.78 (d, *J* = 7.7 Hz, 2H), 7.62 – 7.53 (m, 1H), 7.41 – 7.32 (comp, 2H), 7.24 – 7.16 (comp, 2H), 7.05 – 6.99 (comp, 2H), 6.95 – 6.90 (comp, 2H), 6.74 – 6.68 (comp, 3H), 6.39 (d, *J* = 8.3 Hz, 2H), 4.93 – 4.81 (comp, 2H), 4.73 (s, 1H), 4.60 (d, *J* = 12.3 Hz, 1H), 4.31 (d, *J* = 12.3 Hz, 1H); minor: 7.88 (d, *J* = 7.7 Hz, 2H), 7.62 – 7.53 (m, 1H), 7.41 – 7.32 (comp, 4H), 7.05 – 6.99 (comp, 2H), 6.95 – 6.90 (comp, 2H), 6.50 (d, *J* = 6.3 Hz, 3H), 6.30 (d, *J* = 8.3 Hz, 2H), 4.93 – 4.81 (comp, 3H), 4.73 (s, 1H), 4.23 (d, *J* = 12.9 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ major: 198.6, 163.0 (d, *J* = 249.4 Hz), 162.5 (d, *J* = 247.0 Hz), 144.6, 140.8, 135.7, 133.7 (d, *J* = 2.9 Hz), 133.6, 129.2 (d, *J* = 8.2 Hz), 129.0, 128.8, 128.5, 123.0, 115.5

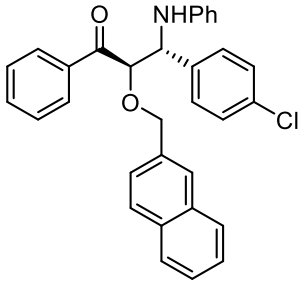
(d, *J* = 21.6 Hz), 115.1, 110.3 (d, *J* = 25.5 Hz), 103.4, 84.4, 71.3, 59.7; ^{19}F NMR (376 MHz, $CDCl_3$) δ major: -109.18, -113.9; minor: -109.24, -114.2; HRMS (TOF MS ESI$^+$) calculated for $C_{28}H_{22}NO_2F_3Cl$ $[M + H]^+$: 496.1286, found 496.1285; HPLC conditions for determination of enantiomeric excess: Chiral IF-3, λ = 254 nm, hexane : ethanol = 98:2, flow rate =1.0 mL/min, t_{major} = 15.2 min, t_{minor} = 13.7 min.



(2*R*,3*R*)-3-(4-Chlorophenyl)-2-(naphthalen-1-ylmethoxy)-1-phenyl-3-(phenylamino)propan-1-one (5p) White solid, 59.9 mg, 61% yield, 94:6 *dr*, 93%(18%) *ee*, $[\alpha]_D^{20}$ = 27.9^o (c = 0.43, DCM), mp = 144 – 146 ^{o}C; ^{1}H NMR (500 MHz, $CDCl_3$) (δ, ppm) δ 8.20 – 8.10 (m, 1H), 7.92 (d, *J* = 5.0 Hz, 1H), 7.87 (d, *J* = 8.1 Hz, 1H), 7.79 (d, *J* = 7.6 Hz, 2H), 7.64 – 7.51 (comp, 3H), 7.39 (t, *J* = 7.0 Hz, 3H), 7.27 (d, *J* = 6.6 Hz, 1H), 7.11 – 7.03 (comp, 4H), 6.94 (t, *J* = 7.4 Hz, 2H), 6.56 (t, *J* = 7.1 Hz, 1H), 6.12 (d, *J* = 7.8 Hz, 2H), 5.32 (d, *J* = 12.0 Hz, 1H), 4.96 (d, *J* = 4.5 Hz, 1H), 4.82 – 4.73 (m, 1H), 4.62 (d, *J* = 12.0 Hz, 1H), 4.45 (d, *J* = 6.9 Hz, 1H); δ ^{13}C NMR (125 MHz, $CDCl_3$) δ 198.7, 145.8, 136.8, 135.9, 134.0, 133.7, 133.5, 132.2, 131.9, 129.7, 129.05, 129.02, 128.9, 128.8, 128.6, 128.4, 128.0, 126.8, 126.2, 125.1, 124.2, 117.8, 113.5, 83.5, 71.1, 59.0; HRMS (TOF MS ESI$^+$) calculated for $C_{32}H_{27}NO_2Cl$ $[M + H]^+$: 492.1725, found 492.1724; HPLC conditions for determination of enantiomeric excess: Chiral IF-3, λ = 254 nm, hexane : ethanol = 95:5, flow rate =1.0 mL/min, t_{major} = 10.6 min, t_{minor} = 9.8 min.

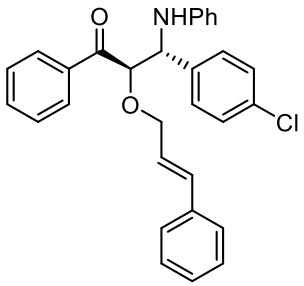


(2*R*,3*R*)-3-(4-Bromophenyl)-2-(naphthalen-1-ylmethoxy)-1-phenyl-3-(phenylamino)propan-1-one (5q) White solid, 67.4 mg, 63% yield, 86:14 *dr*, 90%(43%) *ee*, $[\alpha]_D^{20}$ = 24.0° (c = 0.30, DCM), mp = 149 – 151 °C; ^{1}H NMR (400 MHz, $CDCl_3$) (δ, ppm) δ 8.21 – 8.14 (m, 1H), 7.99 – 7.93 (comp, 1H), 7.90 (d, *J* = 8.2 Hz, 1H), 7.84 (d, *J* = 7.2 Hz, 2H), 7.64 – 7.56 (comp, 3H), 7.46 – 7.39 (comp, 3H), 7.33 – 7.27 (comp 3H), 7.05 – 6.95 (comp, 4H), 6.60 (t, *J* = 7.3 Hz, 1H), 6.17 (d, *J* = 7.7 Hz, 2H), 5.34 (d, *J* = 12.0 Hz, 1H), 4.99 (d, *J* = 5.0 Hz, 1H), 4.83 – 4.78 (m, 1H), 4.67 (d, *J* = 12.0 Hz, 1H), 4.48 (d, *J* = 7.4 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) (δ, ppm) δ 198.7, 145.7, 137.4, 135.9, 134.0, 133.7, 132.2, 131.9, 131.4, 129.7, 129.4, 129.0, 128.9, 128.8, 128.6, 128.0, 126.8, 126.2, 125.1, 124.2, 121.7, 117.9, 113.5, 83.4, 71.1, 59.1; HRMS (TOF MS ESI$^+$) calculated for $C_{32}H_{27}NO_2Br$ $[M + H]^+$: 536.1220, found 536.1229; HPLC conditions for determination of enantiomeric excess: Chiral IF-3, λ = 250 nm, hexane : ethanol = 95:5, flow rate =1.0 mL/min, t_{major} = 11.7 min, t_{minor} = 11.0 min.

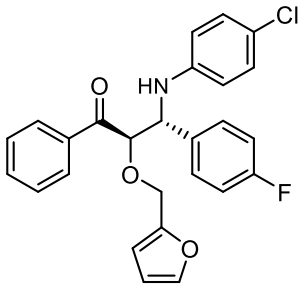


(2*R*,3*R*)-3-(4-Chlorophenyl)-2-(naphthalen-2-ylmethoxy)-1-phenyl-3-(phenylamino)propan-1-one (5r) White solid, 50.1 mg, 51% yield, 95:5 *dr*, 96%(7%) *ee*, $[\alpha]_D^{20}$ = 18.9° (c = 0.38, DCM), mp = 144 -146 °C; ^{1}H NMR (400 MHz, $CDCl_3$) (δ, ppm) δ 7.82 (m, 4H), 7.76 – 7.73 (comp, 1H), 7.57 (s, 1H), 7.56 – 7.47 (comp, 3H), 7.36 (t, *J* = 7.7 Hz, 2H), 7.30 (dd, *J* = 8.4, 1.3 Hz, 1H), 7.22 – 7.13 (comp, 4H), 7.02 (t, *J* = 7.9 Hz, 2H), 6.62 (t, *J* = 7.3 Hz, 1H), 6.41 (d, *J* = 7.9 Hz, 2H), 4.91 (dd, *J* = 11.9, 4.9 Hz,

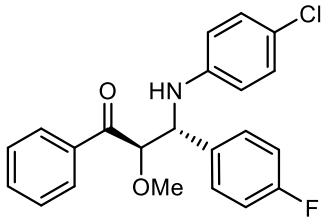
2H), 4.84 (d, *J* = 12.0 Hz, 1H), 4.68 (s, 1H), 4.48 (d, *J* = 12.0 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) (δ, ppm) δ 199.1, 146.0, 137.3, 135.9, 134.2, 133.6, 133.5, 133.16, 133.15, 129.13, 129.10, 128.7, 128.62, 128.55, 128.5, 128.0, 127.8, 127.3, 126.4, 126.3, 125.8, 118.1, 113.9, 84.1, 72.7, 59.5; HRMS (TOF MS ESI$^+$) calculated for $C_{32}H_{27}NO_2Cl$ [M + H]$^+$: 492.1725, found 492.1725; HPLC conditions for determination of enantiomeric excess: Chiral IF-3, λ = 254 nm, hexane : ethanol = 95:5, flow rate =1.0 mL/min, t_{major} = 11.7 min, t_{minor} = 11.0 min.



(2*R*,3*R*)-3-(4-Chlorophenyl)-2-(cinnamyloxy)-1-phenyl-3-(phenylamino)propan-1-one (5s) Yellow oil, 42.0 mg, 45% yield, 96:4 *dr*, 94%(15%) *ee*, ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.81 (d, *J* = 7.7 Hz, 2H), 7.52 (t, *J* = 7.2 Hz, 1H), 7.36 (t, *J* = 7.5 Hz, 2H), 7.30 – 7.15 (comp, 9H), 7.05 (t, *J* = 7.7 Hz, 2H), 6.65 (t, *J* = 7.3 Hz, 1H), 6.50 – 6.43 (comp, 3H), 6.13 – 6.06 (m, 1H), 4.97 – 4.90 (comp, 2H), 4.78 (s, 1H), 4.29 – 4.25 (m, 1H), 4.07 – 4.02 (m, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 199.2, 146.1, 137.3, 136.2, 136.0, 133.9, 133.6, 129.2, 129.1, 128.7, 128.63, 128.62, 128.58, 128.1, 126.6, 124.7, 118.2, 114.0, 84.1, 71.5, 59.5; HRMS (TOF MS ESI$^+$) calculated for $C_{30}H_{27}NO_2Cl$ [M + H]$^+$: 468.1725, found 468.1725; HPLC conditions for determination of enantiomeric excess: Chiral IB-3, λ = 254 nm, hexane : ethanol = 99:1, flow rate =1.0 mL/min, t_{major} = 20.2 min, t_{minor} = 22.9 min.

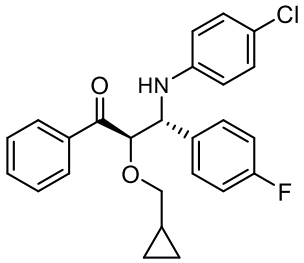


(2*R*,3*R*)-3-((4-Chlorophenyl)amino)-3-(4-fluorophenyl)-2-(furan-2-ylmethoxy)-1-phenylpropan-1-one (5t) Yellow oil, 60.2 mg, 67% yield, 88:12 *dr*, 90%(9%) *ee*; ^{1}H NMR (400 MHz, $CDCl_3$) δ major: 7.68 (d, *J* = 7.5 Hz, 2H), 7.57 – 7.50 (m, 1H), 7.46 – 7.32 (comp, 3H), 7.13 – 7.10 (comp, 2H), 7.01 – 6.91 (comp, 2H), 6.84 (t, *J* = 8.6 Hz, 2H), 6.44 – 6.28 (comp, 3H), 6.26 (d, *J* = 3.0 Hz, 1H), 5.01 (d, *J* = 4.3 Hz, 1H), 4.91 – 4.72 (comp, 2H), 4.67 (d, *J* = 13.3 Hz, 1H), 4.39 – 4.33 (m, 1H); minor: 7.85 (d, *J* = 7.5 Hz, 2H), 7.57 – 7.50 (m, 1H), 7.46 – 7.32 (comp, 3H), 7.13 – 7.10 (comp, 2H), 7.01 – 6.91 (comp, 4H), 6.44 – 6.28 (comp, 3H), 6.13 (d, *J* = 3.1 Hz, 1H), 4.91 – 4.72 (comp, 3H), 4.59 (d, *J* = 13.2 Hz, 1H), 4.39 – 4.33 (m, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ major: 198.6, 162.4 (d, *J* = 246.5 Hz), 150.5, 144.9, 143.5, 136.1, 133.6, 133.5 (d, *J* = 3.2 Hz), 129.3 (d, *J* = 8.1 Hz), 129.1, 128.7, 128.6, 122.7, 115.4 (d, *J* = 21.6 Hz), 115.0, 111.0, 110.7, 82.9, 64.2, 59.3; ^{19}F NMR (376 MHz, $CDCl_3$) δ major: -114.4; minor: -114.7; HRMS (TOF MS ESI$^+$) calculated for $C_{26}H_{22}NO_3FCl$ $[M + H]^+$: 450.1267, found 450.1276; HPLC conditions for determination of enantiomeric excess: Chiral IF-3, λ = 254 nm, hexane : ethanol = 98:2, flow rate =1.0 mL/min, t_{major} = 16.2 min, t_{minor} = 14.3 min.

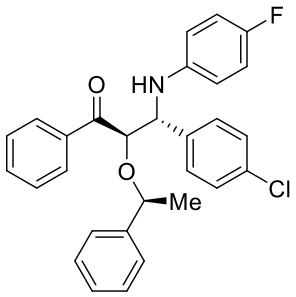


(2*R*,3*R*)-3-((4-chlorophenyl)amino)-3-(4-fluorophenyl)-2-methoxy-1-phenylpropan-1-one (5u) Yellow oil, 45.2 mg, 59% yield, >95:5 *dr*, 92% *ee*; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.75 (d, *J* = 7.9 Hz, 2H), 7.53 (t, *J* = 7.4 Hz, 1H), 7.37 (t, *J* = 7.6 Hz, 2H), 7.19 – 7.11 (comp, 2H), 7.00 (d, *J* = 8.4 Hz, 2H), 6.86 (t, *J* = 8.4 Hz, 2H), 6.42 (d, *J* =

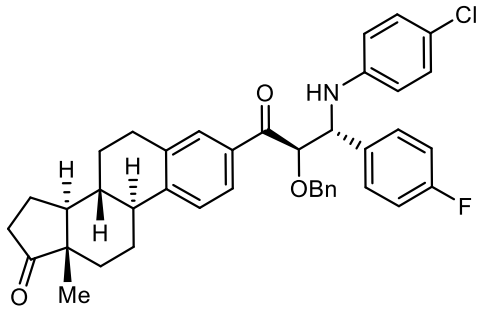
8.4 Hz, 2H), 4.85 – 4.81 (comp 3H), 3.39 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 198.9, 162.5(d, *J* = 246.4Hz), 144.9, 136.1, 133.8, 133.6 (d, *J* = 3.1 Hz), 129.3 (d, *J* = 8.2 Hz), 129.1, 128.8, 128.5, 122.8, 115.5 (d, *J* = 21.5 Hz), 115.1, 86.5, 59.4, 58.8; ^{19}F NMR (376 MHz, $CDCl_3$) δ -114.3; HRMS (TOF MS ESI$^+$) calculated for $C_{22}H_{19}NO_2FCl$ [M + H]$^+$: 384.1161, found 384.1159; HPLC conditions for determination of enantiomeric excess: Chiral Y1, λ = 254 nm, hexane : ethanol = 98:2, flow rate =1.0 mL/min, t_{major} = 12.6 min, t_{minor} = 13.6 min.



(2*R*,3*R*)-3-((4-Chlorophenyl)amino)-2-(cyclopropylmethoxy)-3-(4-fluorophenyl)-1-phenylpropan-1-one (5v) Yellow oil, 60.9 mg, 72% yield, 89:11 *dr*, 90%(3%) *ee*; ^{1}H NMR (400 MHz, $CDCl_3$) δ major: 7.78 (d, *J* = 7.3 Hz, 2H), 7.58 – 7.45 (comp, 1H), 7.35 (t, *J* = 7.8 Hz, 2H), 7.25 – 7.20 (comp, 2H), 7.01 – 6.94 (comp, 2H), 6.88 (t, *J* = 8.6 Hz, 2H), 6.42 (d, *J* = 8.8 Hz, 2H), 4.88 – 4.83 (comp, 3H), 3.38 – 3.32 (m, 1H), 3.28 – 3.23 (m, 1H), 1.01 – 0.93 (m, 1H), 0.52 – 0.42 (comp, 2H), 0.11 – 0.07 (comp, 2H); minor: 7.93 (d, *J* = 7.8 Hz, 2H), 7.58 – 7.45 (comp, 5H), 7.01 – 6.94 (comp, 4H), 6.35 (d, *J* = 8.8 Hz, 2H), 4.77 – 4.75 (comp, 3H), 3.44 (d, *J* = 7.0 Hz, 1H), 3.20 – 3.17 (m, 1H), 1.01 – 0.93 (m, 1H), 0.52 – 0.42 (comp, 2H), 0.11 – 0.07 (comp, 2H); ^{13}C NMR (125 MHz, $CDCl_3$) δ major: 199.6, 162.3 (d, *J* = 246.2 Hz), 144.8, 135.9, 134.0 (d, *J* = 3.0 Hz), 133.5, 129.2 (d, *J* = 8.1 Hz), 129.0, 128.6, 128.5, 122.6, 115.3 (d, *J* = 21.5 Hz), 115.0, 84.9, 75.6, 59.5, 10.5, 3.3, 3.0; ^{19}F NMR (376 MHz, $CDCl_3$) δ major: -114.49; minor: -114.54; HRMS (TOF MS ESI$^+$) calculated for $C_{25}H_{23}NO_2FClNa$ [M + Na]$^+$: 446.1294, found 446.1293; HPLC conditions for determination of enantiomeric excess: Chiral IG-3, λ = 254 nm, hexane : ethanol = 97:3, flow rate =1.0 mL/min, t_{major} = 16.1 min, t_{minor} = 17.6 min.

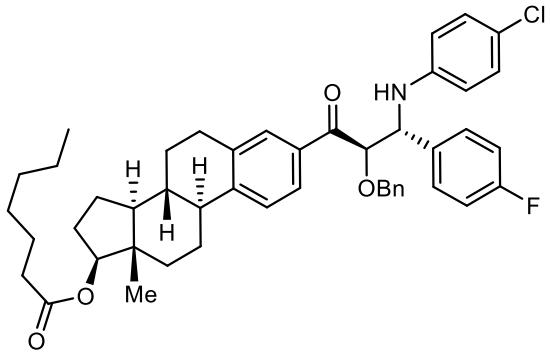


(2*R*,3*R*)-3-(4-Chlorophenyl)-3-((4-fluorophenyl)amino)-1-phenyl-2-((*S*)-1-phenylethoxy)propan-1-one (5w) White solid, 79.5 mg, 84% yield, 88:12 *dr*, mp = 133 –135 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.54 (dd, *J* = 8.3, 1.2 Hz, 2H), 7.44 (t, *J* = 7.4 Hz, 1H), 7.29 – 7.23 (m, 4H), 7.23 – 7.18 (comp, 5H), 7.16 – 7.11 (comp, 2H), 6.80 – 6.72 (m, 2H), 6.44 – 6.30 (m, 2H), 4.77 (s, 1H), 4.68 (d, *J* = 6.5 Hz, 1H), 4.57 (s, 1H), 4.31 (q, *J* = 6.4 Hz, 1H), 1.38 (d, *J* = 6.4 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 199.2, 156.0 (d, *J* = 236.0 Hz), 142.5 (d, *J* = 2.0 Hz), 141.9, 137.7, 135.9, 133.5, 133.0, 128.9, 128.64, 128.61, 128.5, 128.3, 128.1, 126.7, 115.6 (d, *J* = 22.4 Hz), 114.6 (d, *J* = 7.4 Hz), 82.4, 79.1, 60.2, 22.7; ^{19}F NMR (376 MHz, $CDCl_3$) δ -127.2; HRMS (TOF MS ESI^{+}) calculated for $C_{29}H_{26}NO_2FCl$ $[M + H]^{+}$: 474.1631, found 474.1623.



(8*R*,9*S*,13*S*,14*S*)-3-((2*R*,3*R*)-2-(Benzyloxy)-3-((4-chlorophenyl)amino)-3-(4-fluorophenyl)propanoyl)-13-methyl-6,7,8,9,11,12,13,14,15,16-decahydro-17*H*-cyclopenta[*a*]phenanthren-17-one (5x) White solid, 110.5 mg, 87% yield, 84:16 *dr*; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.59 (d, *J* = 8.0 Hz, 1H), 7.42 (s, 1H), 7.35 (d, *J* = 4.7 Hz, 3H), 7.30 (s, 1H), 7.25 – 7.18 (comp, 4H), 7.00 (d, *J* = 8.5 Hz, 2H), 6.90 (t, *J* = 8.4 Hz, 2H), 6.38 (d, *J* = 8.5 Hz, 2H), 4.90 (d, *J* = 4.6 Hz, 1H), 4.88 – 4.75 (m, 2H), 4.71 (d, *J* = 11.8 Hz, 1H), 4.35 (d, *J* = 11.8 Hz, 1H), 2.89 – 2.82 (m, 2H), 2.57 – 2.52 (m, 1H), 2.44 (d, *J* = 12.7 Hz, 1H), 2.33 (t, *J* = 8.3 Hz, 1H), 2.20 – 2.16 (m, 1H), 2.11 – 2.00

(m, 3H), 1.69 – 1.59 (m, 3H), 1.58 – 1.51 (m, 3H), 0.95 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 220.4, 198.7, 162.3 (d, *J* = 246.3 Hz), 146.3, 144.8, 137.0 (d, *J* = 8.1 Hz), 133.9 (d, *J* = 2.8 Hz), 133.6, 129.3, 129.2, 129.1, 128.9, 128.6, 128.2, 128.1, 125.9, 125.6, 122.6, 122.2, 115.3 (d, *J* = 21.5 Hz), 114.9, 83.7, 72.4, 59.6, 50.5, 47.9, 44.7, 37.7, 35.8, 31.5, 29.2, 26.2, 25.5, 21.6, 13.8; ^{19}F NMR (376 MHz, $CDCl_3$) δ -114.6; HRMS (TOF MS ESI$^+$) calculated for $C_{40}H_{39}NO_3FClNa$ [M + Na]$^+$: 658.2495, found 658.2489.

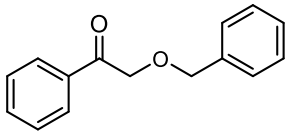


(8*R*,9*S*,13*S*,14*S*,17*S*)-3-((2*R*,3*R*)-2-(benzyloxy)-3-((4-chlorophenyl)amino)-3-(4-fluorophenyl)propanoyl)-13-methyl-7,8,9,11,12,13,14,15,16,17-decahydro-6*H*-cyclopenta[*a*]phenanthren-17-yl heptanoate (5y) Yellow oil, 122.9 mg, 82% yield, 78:22 *dr*; ^{1}H NMR (500 MHz, $CDCl_3$) δ major: 7.59 – 7.54 (m, 1H), 7.38 – 7.30 (comp, 4H), 7.26 – 7.13 (comp, 5H), 6.98 (t, *J* = 8.9 Hz, 2H), 6.93 – 6.86 (comp, 2H), 6.35 (d, *J* = 8.5 Hz, 2H), 4.92 – 4.88 (m, 1H), 4.85 – 4.76 (comp, 2H), 4.74 – 4.65 (comp, 2H), 4.31 (d, *J* = 11.8 Hz, 1H), 2.79 (d, *J* = 6.7 Hz, 2H), 2.31 (t, *J* = 7.4 Hz, 5H), 1.90 (d, *J* = 11.9 Hz, 2H), 1.76 – 1.73 (comp, 2H), 1.64 – 1.35 (comp, 14H), 0.89 (t, *J* = 6.4 Hz, 3H), 0.84 (s, 3H); minor: 7.64 (d, *J* = 7.2 Hz, 1H), 7.38 – 7.30 (comp, 4H), 7.26 – 7.13 (comp, 5H), 6.98 (t, *J* = 8.9 Hz, 2H), 6.93 – 6.86 (comp, 2H), 6.29 (d, *J* = 8.7 Hz, 2H), 4.92 – 4.88 (m, 1H), 4.85 – 4.76 (comp, 2H), 4.74 – 4.65 (comp, 2H), 4.26 (d, *J* = 11.9 Hz, 1H), 2.88 (d, *J* = 4.5 Hz, 2H), 2.31 (t, *J* = 7.4 Hz, 5H), 1.90 (d, *J* = 11.9 Hz, 2H), 1.76 – 1.73 (comp, 2H), 1.64 – 1.35 (comp, 14H), 0.89 (t, *J* = 6.4 Hz, 3H), 0.84 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ major: 198.7, 174.0, 145.8 (d, *J* = 257.1 Hz), 137.2, 137.0, 133.9 (d, *J* = 2.8 Hz), 133.4, 129.23, 129.17, 128.9, 128.8, 128.6, 128.4, 128.2, 128.1, 125.8, 125.7, 122.5, 115.3 (d, *J* = 21.4 Hz), 114.9, 83.6, 82.3, 72.4, 59.6,

50.0, 44.6, 42.9, 37.9, 36.9, 34.6, 31.5, 29.3, 28.9, 27.6, 26.9, 25.8, 25.1, 23.3, 22.5, 14.1, 12.1; ^{19}F NMR (471 MHz, $CDCl_3$) δ major: -114.5; minor: -114.8; HRMS (TOF MS ESI$^+$) calculated for $C_{47}H_{53}NO_4FClNa$ [M + Na]$^+$: 772.3552, found 772.3539.

Control Experiments

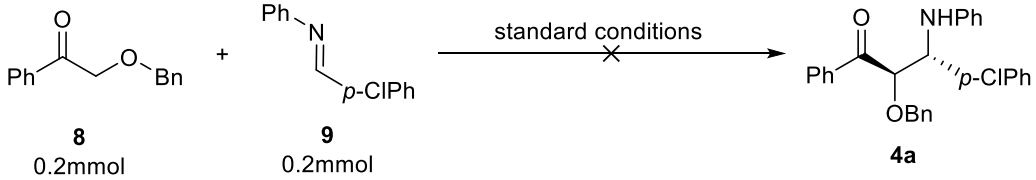
Compound **8** was prepared according to the reported synthetic method using 2-diazo-1-phenylethan-1-one.[2]



2-(Benzyloxy)-1-phenylethan-1-one (8)

White solid; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.92 (d, *J* = 7.5 Hz, 2H), 7.57 (t, *J* = 7.4 Hz, 1H), 7.45 (t, *J* = 7.7 Hz, 2H), 7.39 – 7.34 (comp, 5H), 4.76 (s, 2H), 4.70 (s, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 196.3, 137.3, 134.9, 133.6, 128.7, 128.6, 128.1, 128.0, 127.9, 73.4, 72.6.

Control experimental with 8



To a 10-mL oven-dried vial with a magnetic stirring bar, **8** (45.2 mg, 0.2 mmol), imine **9** (43.0 mg, 0.2 mmol), chiral phosphoric acid **7a** (13.2 mg, 10 mol%), 4Å MS (100.0 mg) in 2.0 mL DCM, a solution of $Me_3OMe^tBuXPhosAuNTf_2$ (9.8 mg, 1.0 μmol, 5.0 mol %) in DCM (2.0 mL) was added via a syringe pump in 0.5 h under argon atmosphere at -10 ^{o}C. After addition, the reaction mixture was stirred under these conditions until consumption of the material. The reaction was monitored by proton NMR (see Figure S1).

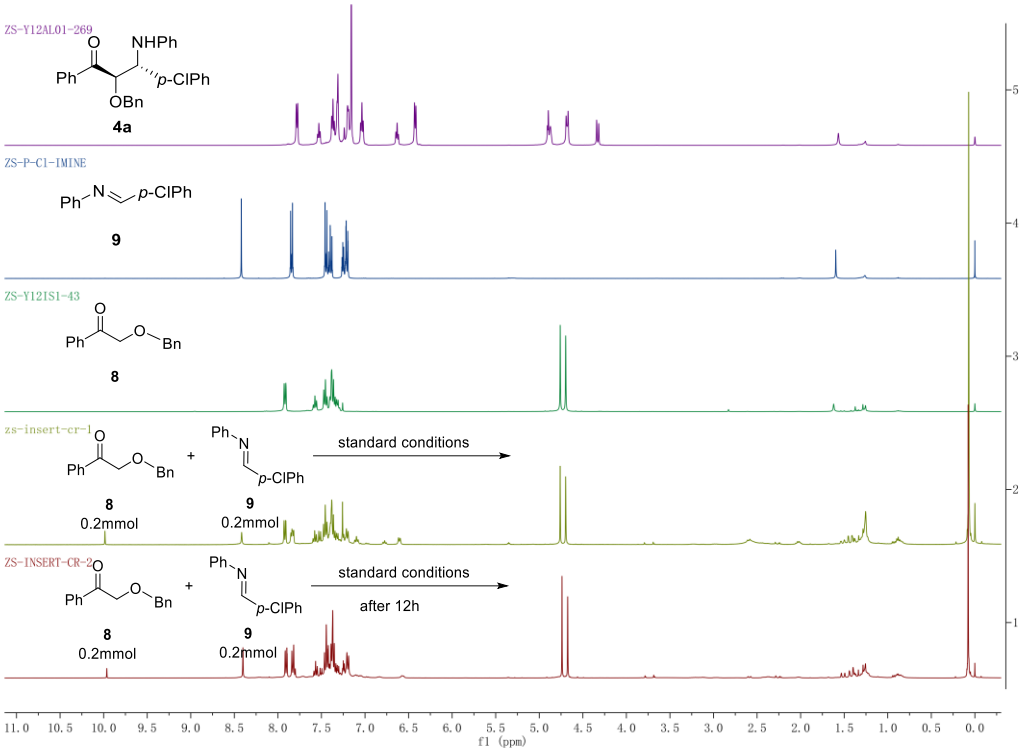
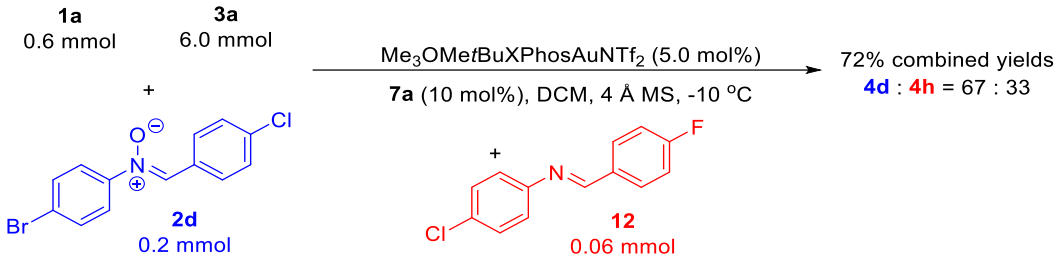


Figure S1. Control experimental of **8** with imine **9**.

Crossover experiments



To a 10-mL oven-dried vial with a magnetic stirring bar, phenylacetylene **1a** (61.2 mg, 0.6 mmol) , nitrone **2d** (62.2 mg, 0.2 mmol), imine **12** (14.0 mg, 0.06 mmol), Benzyl alcohol **3a** (648.6 mg, 6.0 mmol), chiral phosphoric acid **7a** (13.2 mg, 10.0 mol %), 4 Å MS (100.0 mg) in 2.0 mL DCM, a solution of $Me_3OMe^tBuXPhosAuNTf_2$ (9.8 mg, 1.0 μmol, 5.0 mol%) in DCM (2.0 mL) was added via a syringe pump in 0.5 h under argon atmosphere at -10 °C. After addition, the reaction mixture was stirred under these conditions until consumption of the material. When the reaction was completed (monitored by TLC), the crude reaction mixture was subjected to proton NMR analysis (Figure S2, the first spectrum), and the reaction mixture was purified by

column chromatography on silica gel without any additional treatment (Hexanes : EtOAc = 20:1 to 10:1) to give 74.5 mg of products **4d** and **4h** in 72% combined yields with **4d** : **4h** = 67 : 33 (see Figure 2 for detail).

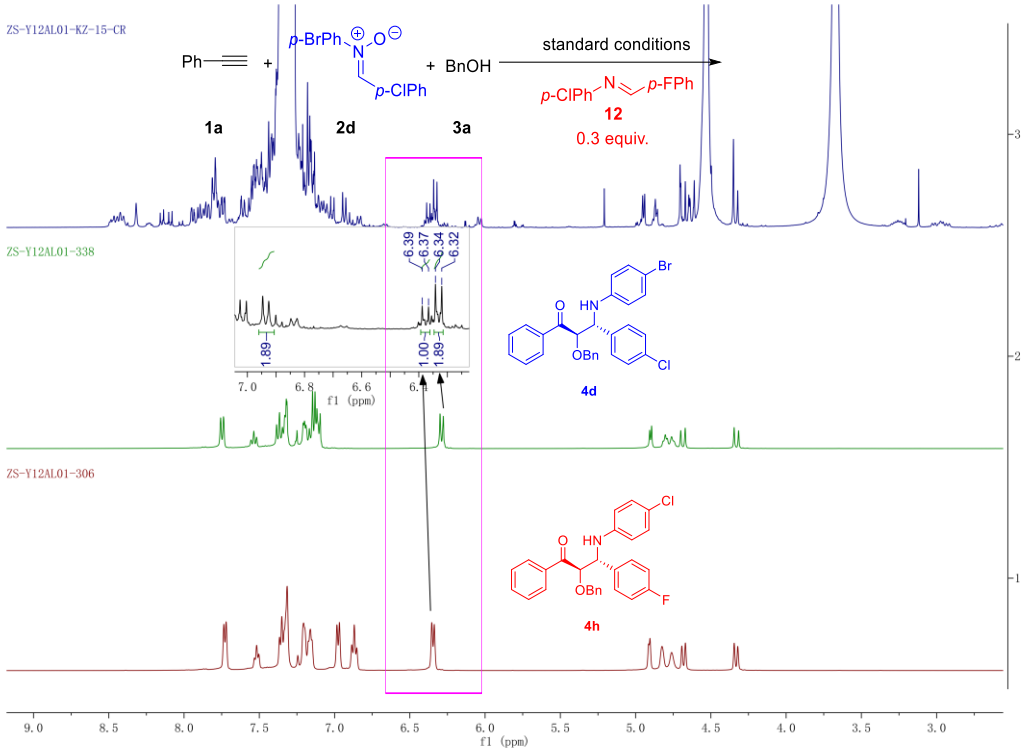
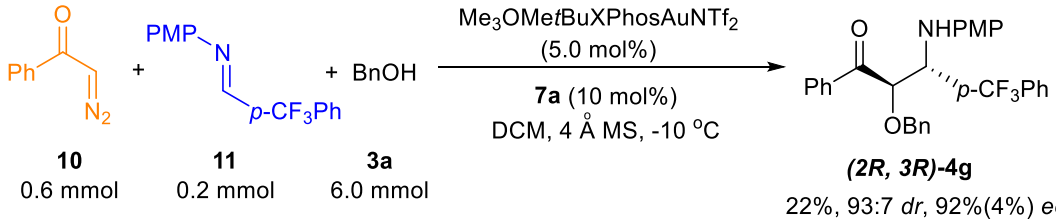


Figure S2. NMR analysis of products in crossover experiment.

Control experimental with diazo compound 10



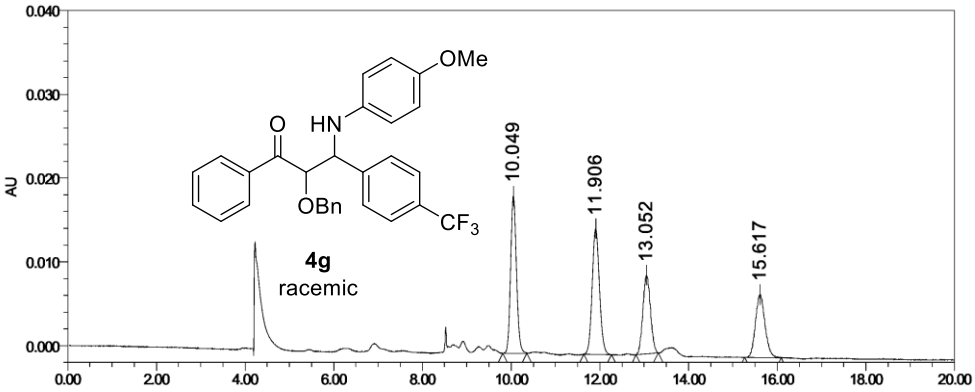
10 0.6 mmol | **11** 0.2 mmol | **3a** 6.0 mmol

***(2R, 3R)*-4g**

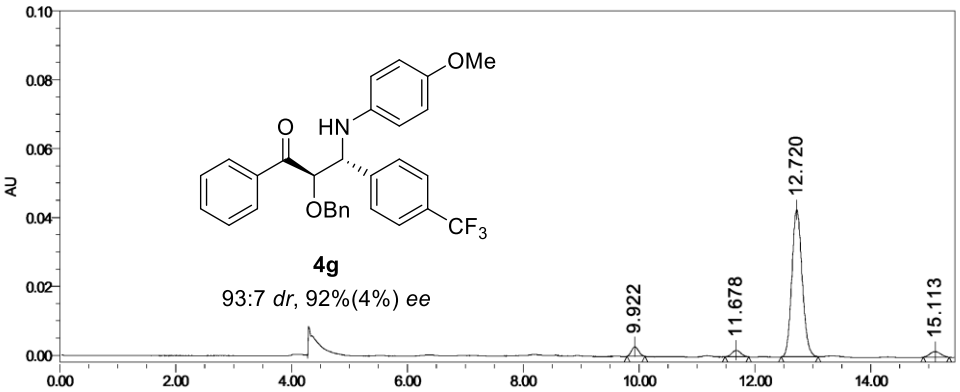
22%, 93:7 *dr*, 92%(4%) *ee*

To a 10-mL oven-dried vial with a magnetic stirring bar, diazo compound **10** (87.6 mg, 0.6 mmol), imine **11** (56.0 mg, 0.2 mmol), benzyl alcohol **3a** (648.6 mg, 6.0 mmol), chiral phosphoric acid **7a** (13.2 mg, 10 mol%), and 4Å MS (100 mg) in 2.0 mL DCM, a solution of $Me_3OMetBuXPhosAuNTf_2$ (9.8 mg, 5.0 mol%) in DCM (2.0 mL) was added *via* a syringe pump in 0.5 h under argon atmosphere at -10 °C. After addition, the reaction mixture was stirred under these conditions until consumption of the

material(monitored by TLC), the reaction mixture was purified by column chromatography on silica gel without any additional treatment (Hexanes : EtOAc = 20:1 to 10:1) to give 21.6 mg of products **4g** in 22% yields with 93:7 *dr*, 92%(4%) *ee*.The chiral HPLC analysis (conditions: Chiral IB-3, λ = 254 nm, hexane : enathol = 97:3, flow rate = 1.0 mL/min, t_{major} = 12.7 min; t_{minor} = 15.1 min.

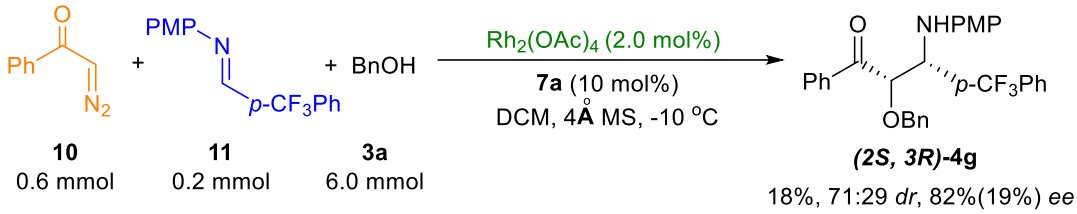


Entry	RT min	Height mV	Area mV.sec	% Area %
1	10.049	18783	170283	30.16
2	11.906	15007	169750	30.07
3	13.052	9410	112360	19.90
4	15.617	7525	112215	19.87



Entry	RT min	Height mV	Area mV.sec	% Area %
1	9.922	2702	22619	3.84
2	11.678	1898	20708	3.51
3	12.72	42744	524540	88.96
4	15.113	1650	21800	3.70

Control experimental with diazo compound 10 in the presence of $Rh_2(OAc)_4$

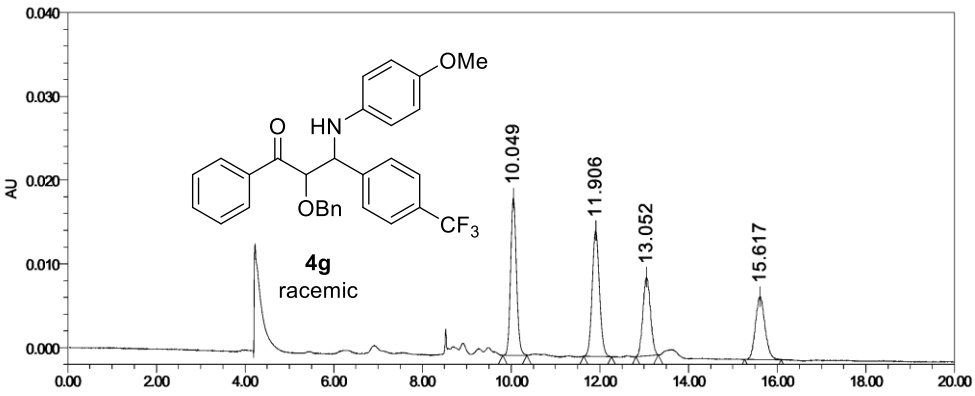


10 0.6 mmol | **11** 0.2 mmol | **3a** 6.0 mmol

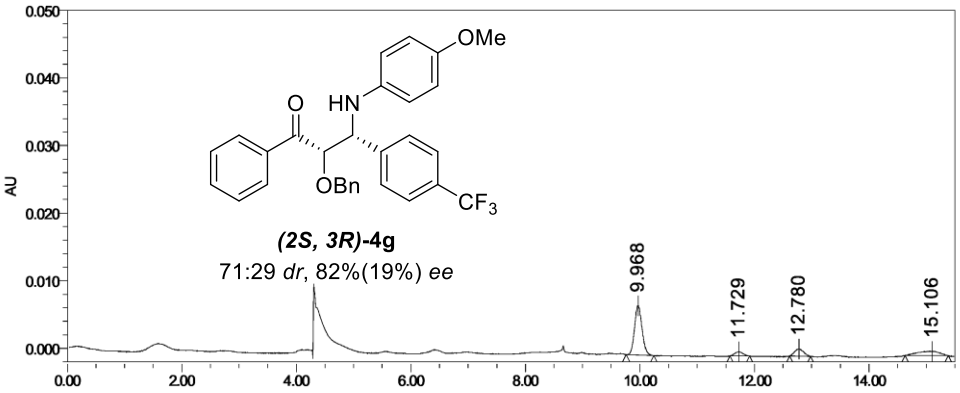
***(2S, 3R)*-4g**

18%, 71:29 *dr*, 82%(19%) *ee*

To a 10-mL oven-dried vial with a magnetic stirring bar, diazo compound **10** (87.6 mg, 0.6 mmol), imine **9** (56.0 mg, 0.2 mmol), benzyl alcohol **3a** (648.6 mg, 6.0 mmol), chiral phosphoric acid **7a** (13.2 mg, 10 mol%), and 4Å MS (100 mg) in 2.0 mL DCM, a solution of $Rh_2(OAc)_4$ (4.4 mg, 1.0 μmol, 5.0 mol%) in DCM (2.0 mL) was added *via* a syringe pump in 0.5 h under argon atmosphere at -10 °C. After addition, the reaction mixture was stirred under these conditions until consumption of the material (monitored by TLC), the reaction mixture was purified by column chromatography on silica gel without any additional treatment (Hexanes : EtOAc = 20:1 to 10:1) to give 21.6 mg of products **4q** in 18% yields with 71:29 *dr*, 82%(19%) *ee*. The chiral HPLC analysis (conditions: Chiral IB-3, λ = 254 nm, hexane : enathol = 97:3, flow rate = 1.0 mL/min, t_{major} = 10.0 min; t_{minor} = 11.7 min.

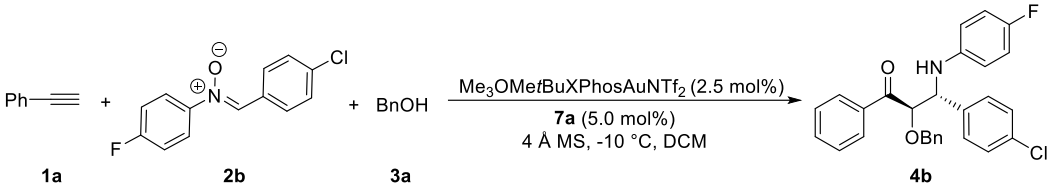


Entry	RT min	Height mV	Area mV.sec	% Area %
1	10.049	18783	170283	30.16
2	11.906	15007	169750	30.07
3	13.052	9410	112360	19.90
4	15.617	7525	112215	19.87



Entry	RT min	Height mV	Area mV.sec	% Area %
1	9.968	7315	66782	65.85
2	11.729	648	6458	6.37
3	12.780	1044	11477	11.32
4	15.106	632	16692	16.46

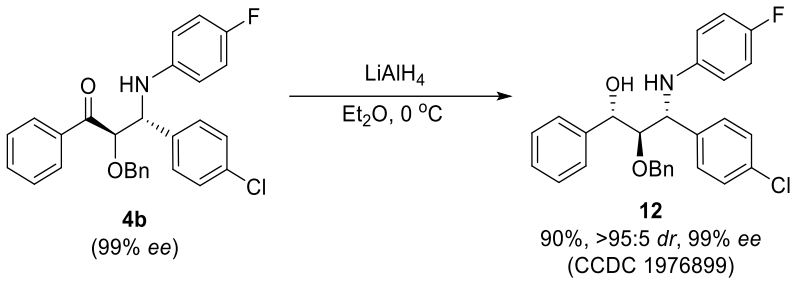
Procedure of the Scale Up



To a 100-mL oven-dried vial with a magnetic stirring bar, phenylacetylene **1a** (918 mg, 9.0 mmol), nitrone **2b** (747 mg, 3.0 mmol) and benzyl alcohol **3a** (9.73 g, 90.0 mmol), chiral phosphoric acid **7a** (99.9 mg, 0.15 mmol, 5.0 mol%), 4Å MS (1.5 g) in 30 mL DCM, a solution of $Me_3OMe^tBuXPhosAuNTf_2$ (75.0 mg, 0.075 mmol, 2.5 mol%) in DCM (30 mL) was added *via* a syringe pump in 0.5 hour under argon atmosphere at -10 ^oC. After addition, the reaction mixture was stirred under these conditions until consumption of the material (monitored by TLC, about 24 h), the crude reaction mixture was quenched with saturated aqueous sodium bicarbonate (20 mL) and extracted with EtOAc (30 mL). The organic phase was washed with brine and dried over anhydrous Na_2SO_4. The solvent was evaporated in *vacuo* after filtration. The residue was purified by flash column chromatography on silica gel

(Hexanes : EtOAc = 20:1 to 10:1) to give the 1.06 g pure products **4b** in 76% yields with 94:6 *dr* and 95%(12%) *ee*. Recrystallization in DCM and hexane gives the pure product **4b** in 63% yield with > 99% *ee*.

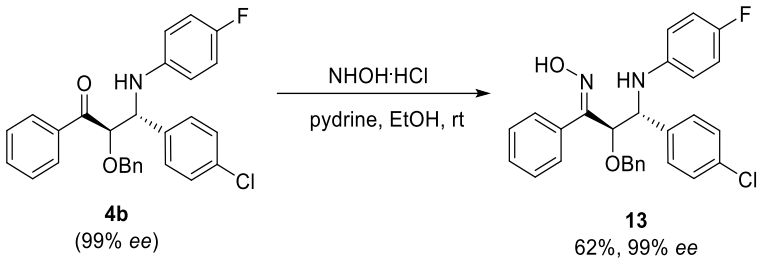
Derivatizations



4b
(99% *ee*)

12
90%, >95:5 *dr*, 99% *ee*
(CCDC 1976899)

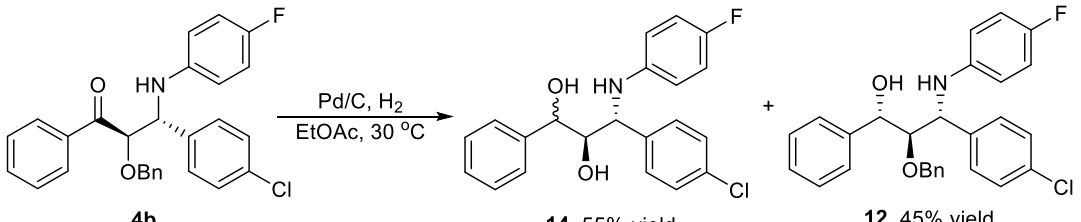
***Synthesis of 12*:** To a 10-mL oven-dried round-bottom flask with a magnetic stirring bar, a solution of **4b** (46.0 mg, 0.1 mmol) in Et_2O (2.0 mL), was added $LiAlH_4$ (3.8 mg, 0.1 mmol, 1.0 equiv) under stirring at 0 °C, and the reaction mixture was stirred at room temperature for 1 h. When the reaction was completed (monitored by TLC), the solvent was evaporated under vacuum after filtering through a pad of Celite. The residue was purified by column chromatography on silica gel (Hexanes : EtOAc = 5:1) to give 41.9 mg of pure product **12** as white solid in 90% yield with 99% *ee*, mp = 135 – 137 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.41 – 7.24 (comp, 12H), 7.05 – 6.96 (m, 2H), 6.73 (t, *J* = 8.7 Hz, 2H), 6.29 – 6.20 (m, 2H), 4.68 (d, *J* = 4.5 Hz, 1H), 4.43 (d, *J* = 8.0 Hz, 1H), 4.19 (s, 1H), 3.89 – 3.80 (m, 2H), 3.68 (d, *J* = 11.3 Hz, 1H), 2.42 (s, 1H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 156.0 (d, *J* = 235.6 Hz), 142.6 (d, *J* = 1.8 Hz), 141.7, 138.2, 137.6, 133.1, 129.8, 128.61, 128.56, 128.44, 128.41, 128.38, 128.2, 127.3, 115.6 (d, *J* = 22.3 Hz), 114.8 (d, *J* = 7.4 Hz), 85.3, 74.9, 74.5, 59.1; ^{19}F NMR (376 MHz, $CDCl_3$) δ -127.4; HRMS (TOF MS ESI+) calculated for $C_{28}H_{26}NO_2FCl$ $[M + H]^+$: 462.1631, found 462.1635; HPLC conditions for determination of enantiomeric excess: Chiral IF-3, λ = 254 nm, hexane : ethanol = 97:3, flow rate =1.0 mL/min, t_{major} = 18.7 min, t_{minor} = 14.6 min.



4b
(99% *ee*)

13
62%, 99% *ee*

Synthesis of 13: To a 10-mL oven-dried round-bottom flask with a magnetic stirring bar, a solution of **4b** (46.0 mg, 0.1 mmol) in EtOH (2.0 mL), was added NHOH·HCl (10.4 mg, 0.3 mmol, 3.0 equiv), and pydrine (12.0 mg, 0.3 mmol, 3.0 equiv.) under tirring at room temperature, and the reaction mixture was stirring for 12 h. When the reaction was completed (monitored by TLC), the solvent was evaporated under vacuum after filtering through a pad of Celite. The residue was purified by column chromatography on silica gel (Hexanes : EtOAc = 5:1) to give 29.4 mg of pure product **13** as white solid in 62% yield with 99% *ee*, $[\alpha]_D^{20} = 15.9^o$ (c = 0.44, DCM), mp = 150 – 152 ^{o}C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.14 (s, 1H), 7.39 – 7.32 (comp, 5H), 7.26 – 7.22 (comp, 3H), 7.20 (d, *J* = 8.4 Hz, 2H), 7.16 (d, *J* = 7.8 Hz, 2H), 6.96 (d, *J* = 6.3 Hz, 2H), 6.70 (t, *J* = 8.0 Hz, 2H), 6.26 – 6.21 (m, 2H), 4.70 (d, *J* = 11.9 Hz, 1H), 4.34 (d, *J* = 12.0 Hz, 1H), 4.17 (s, 2H), 4.09 (s, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 157.1, 156.0 (d, *J* = 235.7 Hz), 149.5, 142.1 (d, *J* = 1.8 Hz), 138.6, 136.8, 133.2, 130.2, 129.3, 129.2, 128.4, 128.33, 128.27, 128.0, 127.8, 115.6 (d, *J* = 22.4 Hz), 114.5 (d, *J* = 7.4 Hz), 83.3, 71.3, 58.8; ^{19}F NMR (376 MHz, $CDCl_3$) δ -127.2; HRMS (TOF MS ESI+) calculated for $C_{28}H_{25}N_2O_2FCl$ $[M + H]^+$: 475.1583, found 475.1583; HPLC conditions for determination of enantiomeric excess: Chiral IF-3, λ = 254 nm, hexane : ethanol = 97:3, flow rate =1.0 mL/min, t_{major} = 16.8 min, t_{minor} = 35.1 min.



4b
(99% *ee* after recrystallization)

14, 55% yield
84:16 *dr*, 99%(99%) *ee*

12, 45% yield
86:14 *dr,* 99%(99%) *ee*

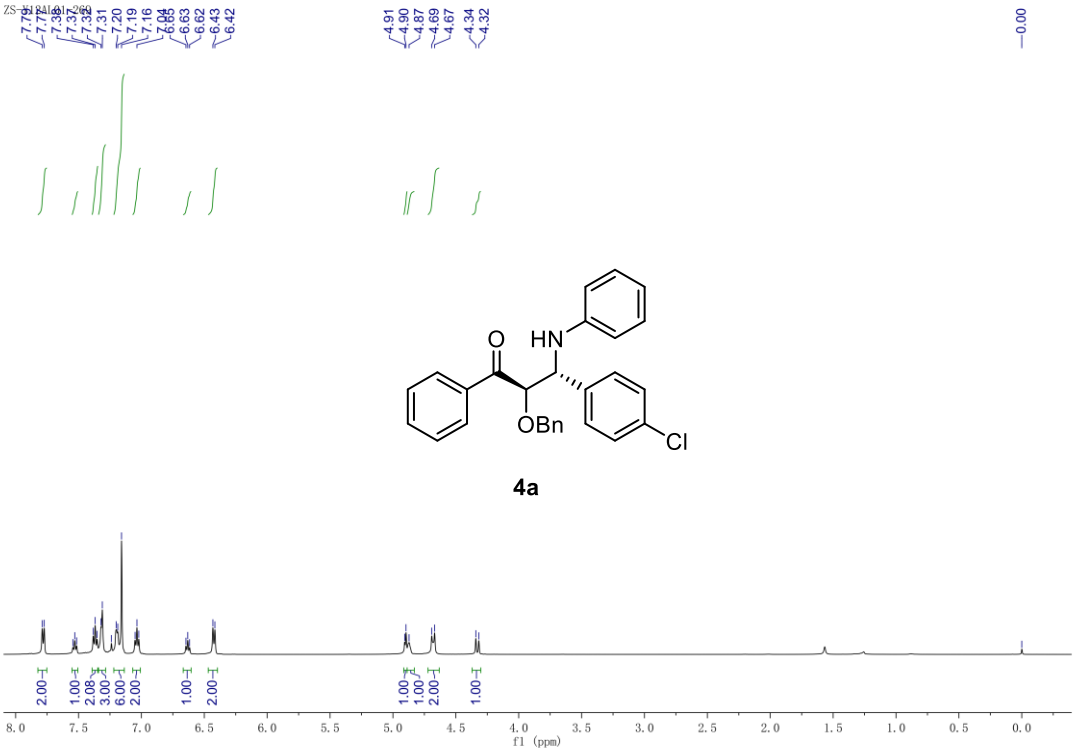
Synthesis of 14: To a 10 mL hydrogenation reactor containing a magnetic stirring bar,

4b (23.0 mg, 0.05 mmol) in 3.0 mL of ethyl acetate, was added wet 10% Pd/C (9.2 mg, 40 %). The heterogeneous mixture was charged with a hydrogen balloon (with a long needle inserted into the reaction mixture and bubbling hydrogen slowly). The reaction mixture stirred overnight at room temperature under these conditions. After completion of the reaction, the mixture was filtered through a pad of Celite to remove Pd/C and the residue was purified by flash chromatography after evaporation of the solvent in *vacuo* (Petroleum ether : EtOAc = 4:1) to give 10.3 mg **14** as yellow oil (55% yield, 84:16 *dr*, 99% *ee*),[3] contaminated with **12** in 45% yield with 86:14 *dr* and 99% *ee*.

The major diastereomer of **14**: ^{1}H NMR (400 MHz, $CDCl_3$) δ major: 7.42 – 7.26 (comp, 10H), 6.77 (t, *J* = 8.6 Hz, 2H), 6.42 – 6.39 (comp, 2H), 4.47 (d, *J* = 4.6 Hz, 1H), 4.39 (d, *J* = 4.3 Hz, 1H), 4.13 (t, *J* = 4.5 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 156.2 (d, *J* = 236.7 Hz), 142.8 (d, *J* = 1.4 Hz), 140.8, 137.8, 133.7, 129.4, 129.0, 128.9, 128.6, 126.9, 115.8 (d, *J* = 22.4 Hz), 114.9 (d, *J* = 7.3 Hz), 77.1, 73.9, 60.4; ^{19}F NMR (376 MHz, $CDCl_3$) δ-127.1; HPLC conditions for determination of enantiomeric excess: Chiral IG-3, λ = 230 nm, hexane : ethanol = 90:10, flow rate =1.0 mL/min, t_{major} = 29.5 min.

The minor diastereomer of **14**: ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.44 – 7.24 (comp, 10H), 6.79 (t, *J* = 8.7 Hz, 2H), 6.50 – 6.40 (comp, 2H), 4.76 (d, *J* = 4.3 Hz, 1H), 4.29 (d, *J* = 8.1 Hz, 1H), 4.09 (dd, *J* = 7.5, 3.9 Hz, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 156.2 (d, *J* = 235.6 Hz), 142.8 (d, *J* = 1.0 Hz), 140.8, 137.4, 133.5, 129.9, 129.0, 128.9, 128.7, 127.4, 115.8 (d, *J* = 22.4 Hz), 115.0 (d, *J* = 7.4 Hz), 76.9, 75.3, 59.0; ^{19}F NMR (376 MHz, $CDCl_3$) δ-127.3; HPLC conditions for determination of enantiomeric excess: Chiral IC, λ = 240 nm, hexane : ethanol = 97:3, flow rate =1.0 mL/min, t_{major} = 13.8 min.

HRMS (TOF MS ESI$^+$) calculated for $C_{21}H_{19}NO_2FCl$ $[M + H]^+$: 372.1161, found 372.1160.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HN
OBn
Cl
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1.00
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3.00
6.00
2.00
1.00
2.00
1.00
1.00
2.00
1.00
f1 (ppm)

4a


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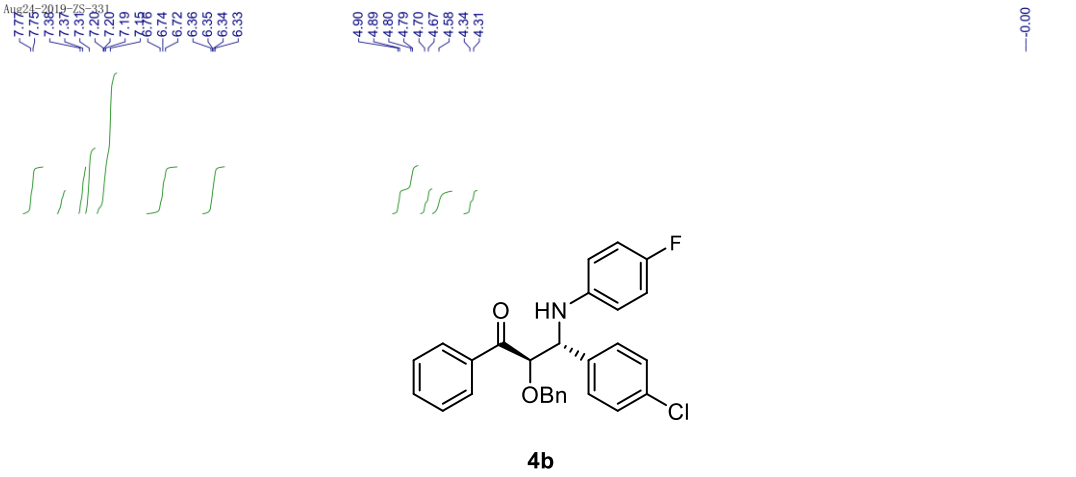
Cl
f1 (ppm)

4a


Aug24-2019-ZS-331
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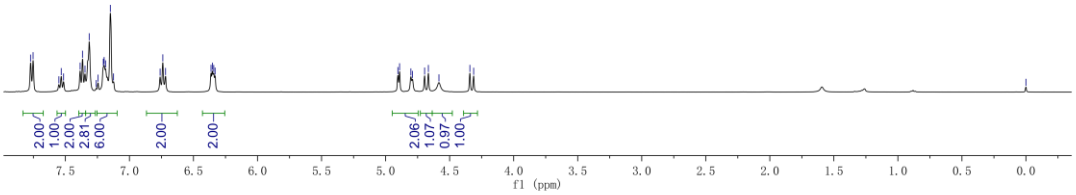
Cl

4b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1.5
1.0
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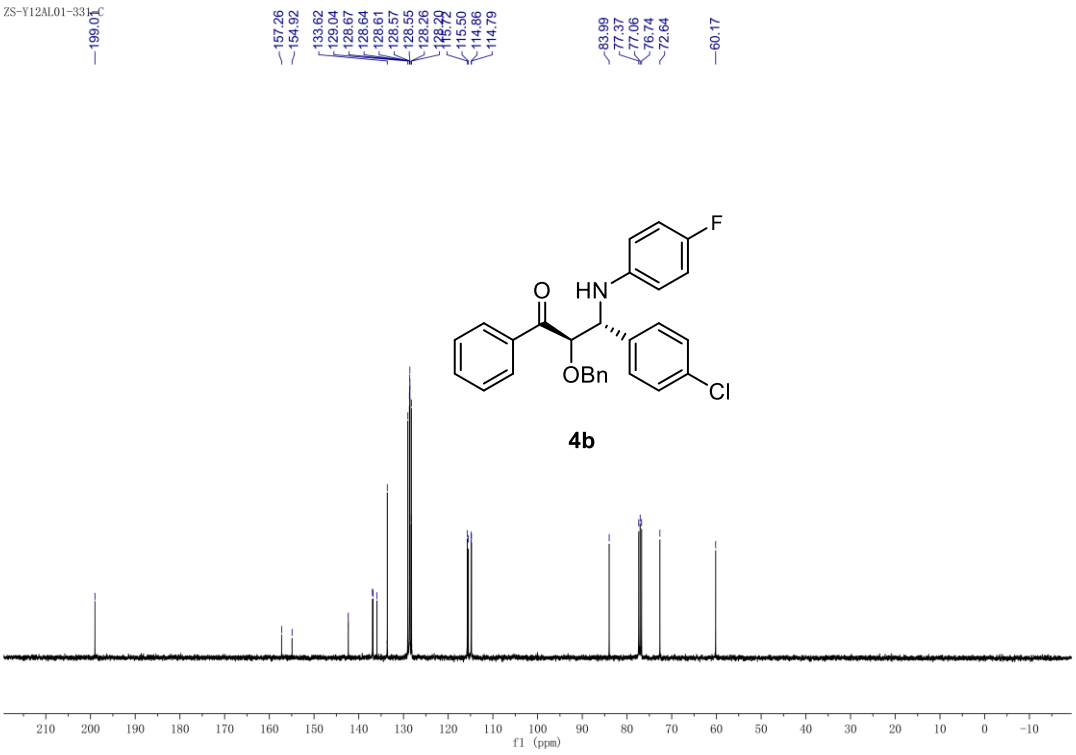
f1 (ppm)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77.06
76.74
72.64
60.17
F
O
HN
OBn
Cl
210
200
190
180
170
160
150
140
130
120
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100
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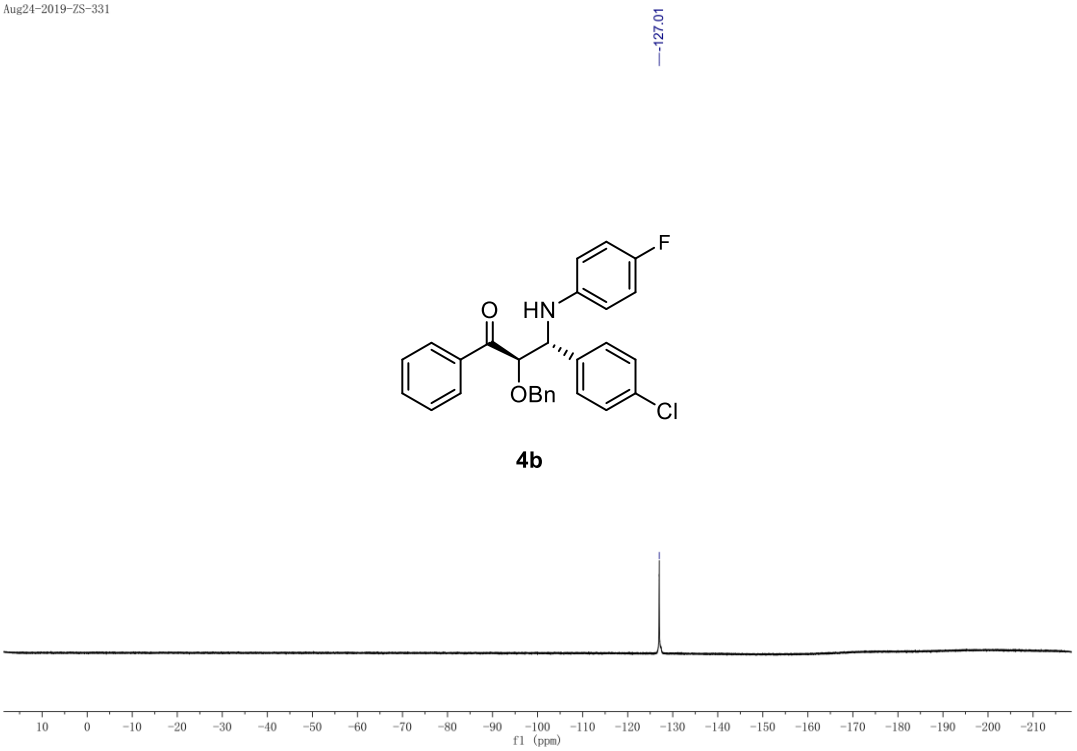
60
50
40
30
20
10
0
-10
f1 (ppm)

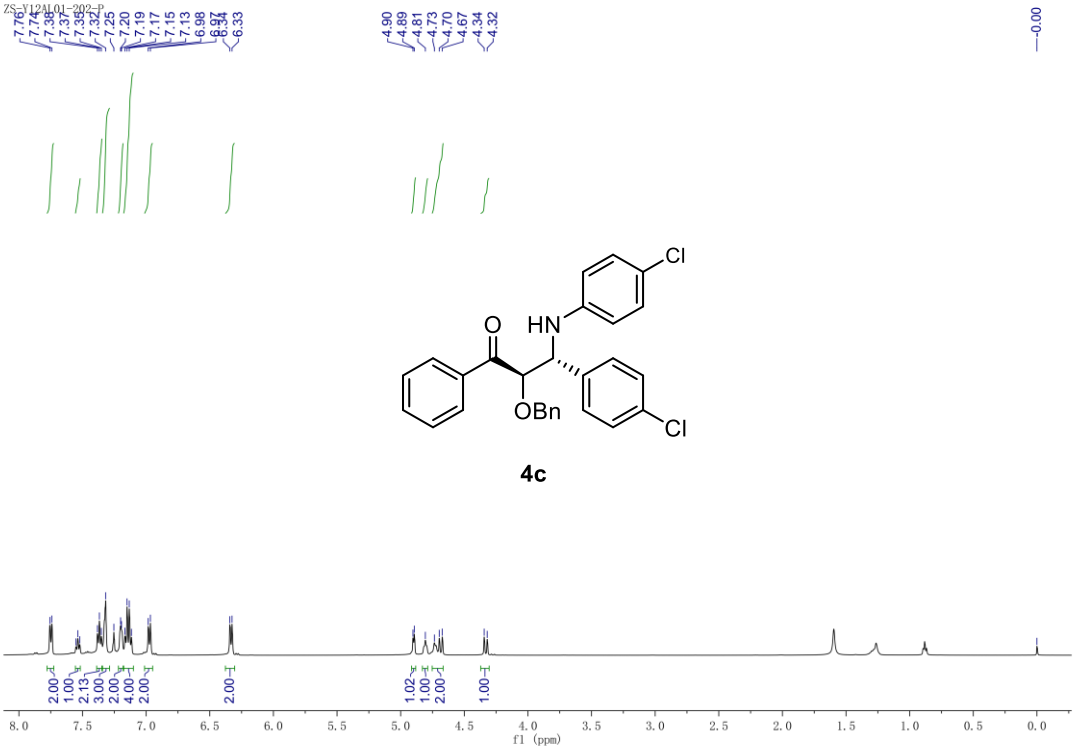
4b

Aug24-2019-ZS-331

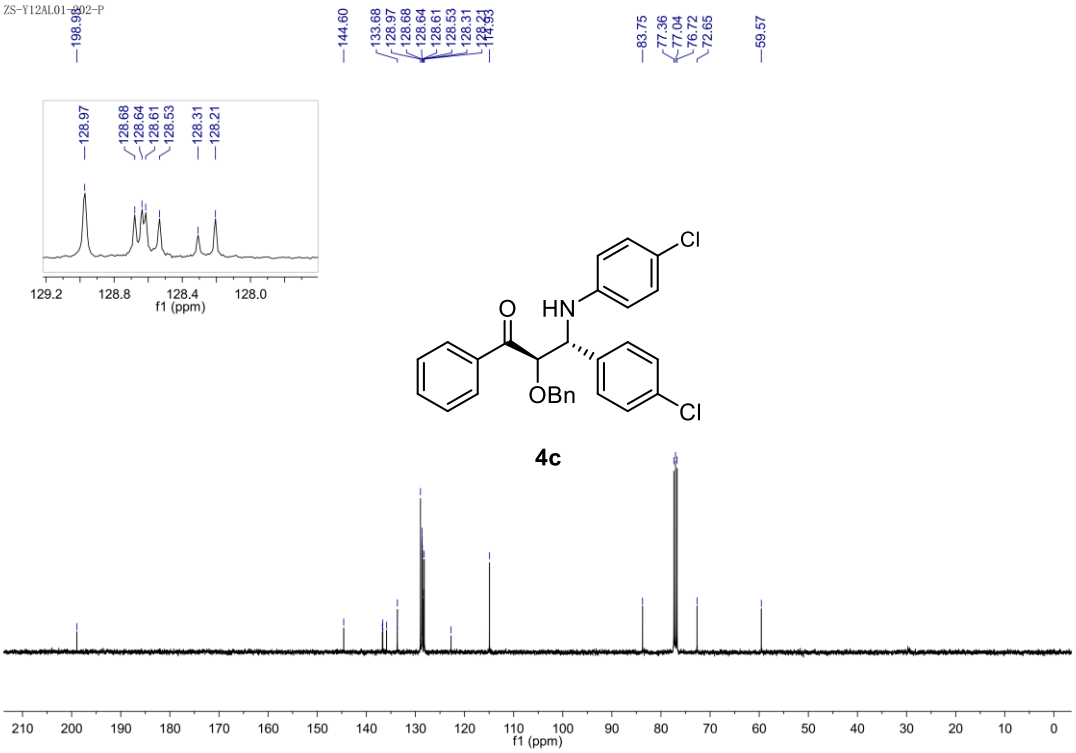


4b

ZS-Y12AL01-202-P



4c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72.65
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128.0
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HN
OBn
Cl
4c
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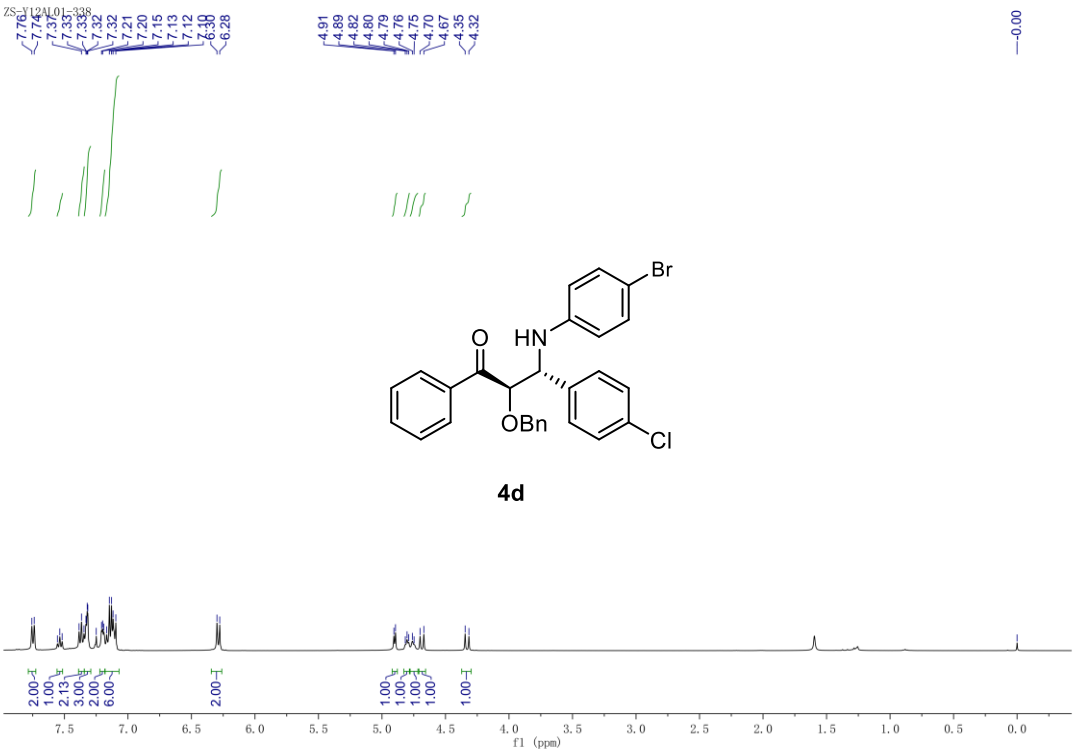
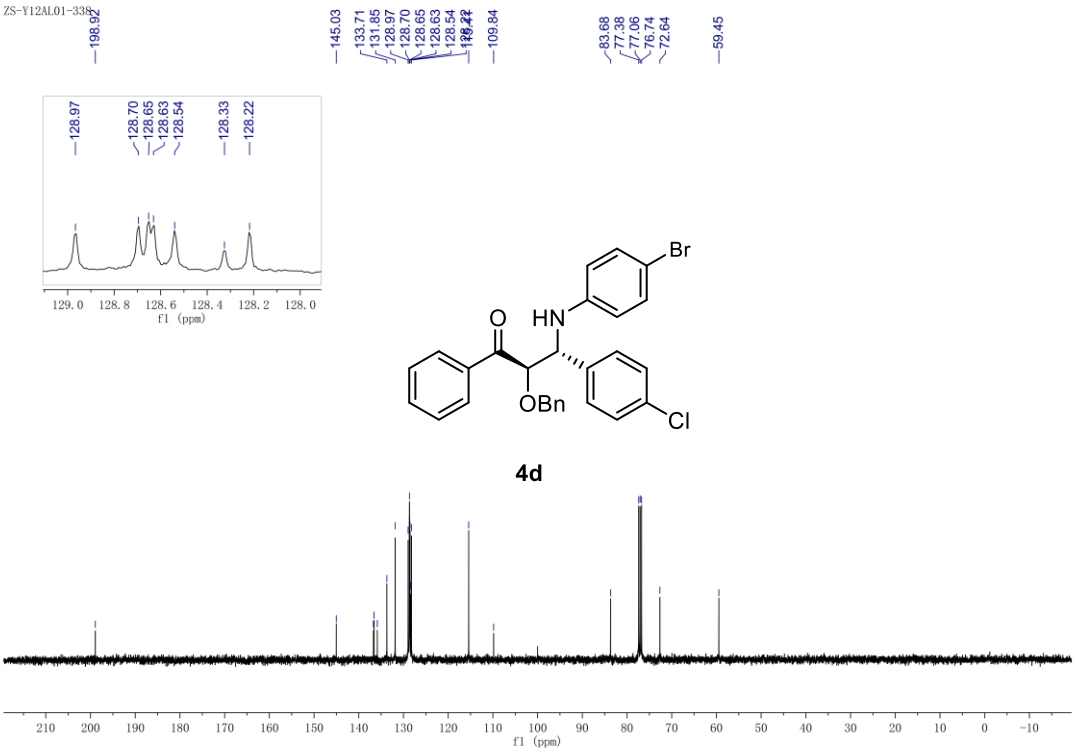
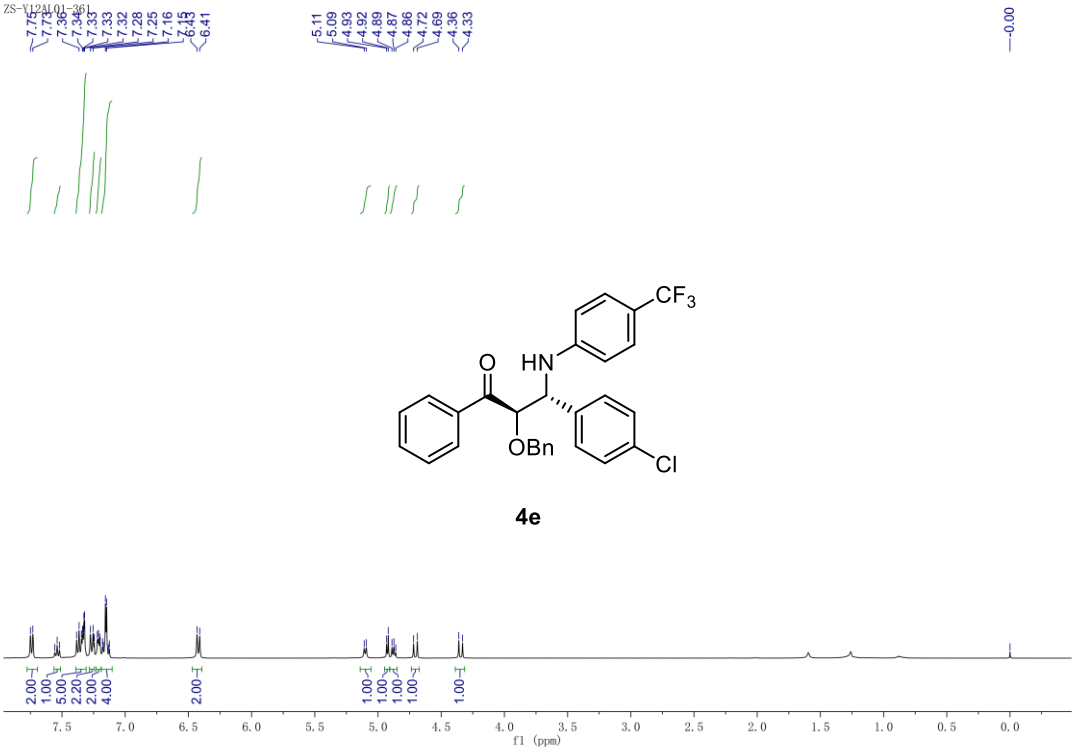
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


ZS-Y12AL01-338
7.76
7.74
7.37
7.33
7.32
7.21
7.20
7.15
7.13
7.12
6.30
6.28
4.91
4.89
4.82
4.80
4.79
4.76
4.75
4.70
4.67
4.35
4.32
0.00
Br
O
HN
OBn
Cl
4d
2.00
1.00
2.13
3.00
2.00
6.00
2.00
1.00
1.00
1.00
1.00
1.00
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

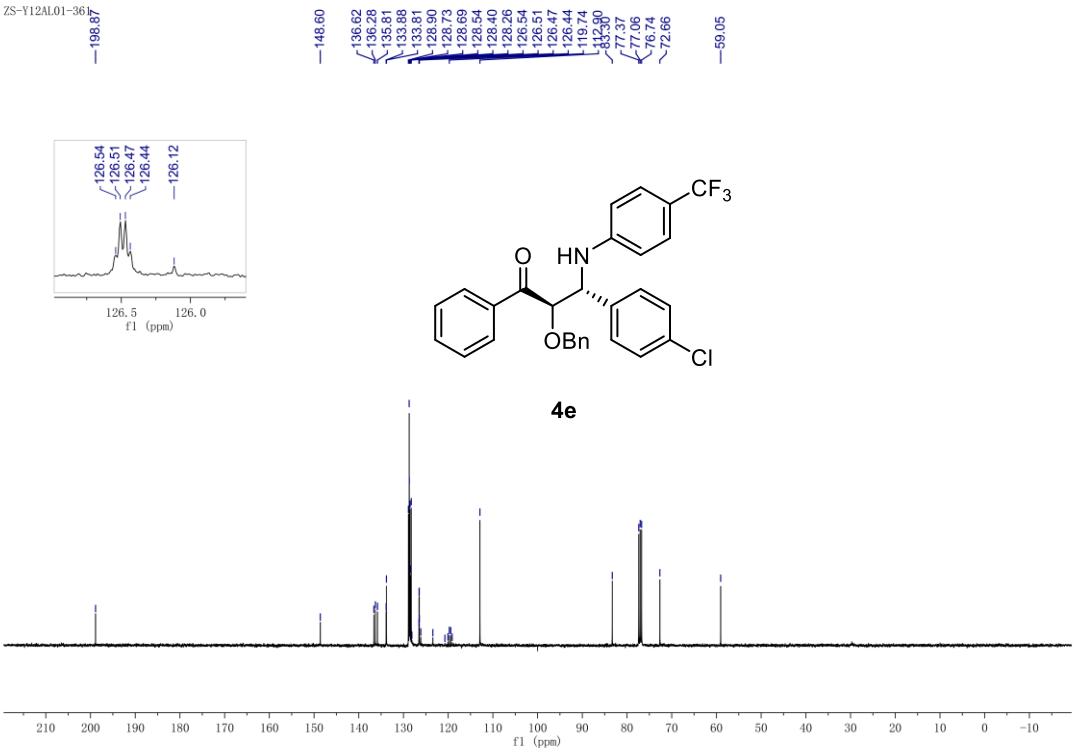

ZS-Y12AL01-338
198.92
145.03
133.71
131.85
128.97
128.70
128.65
128.63
128.54
128.33
128.22
109.84
83.68
77.38
77.06
76.74
72.64
59.45
f1 (ppm)
Br
HN
O
OBn
Cl

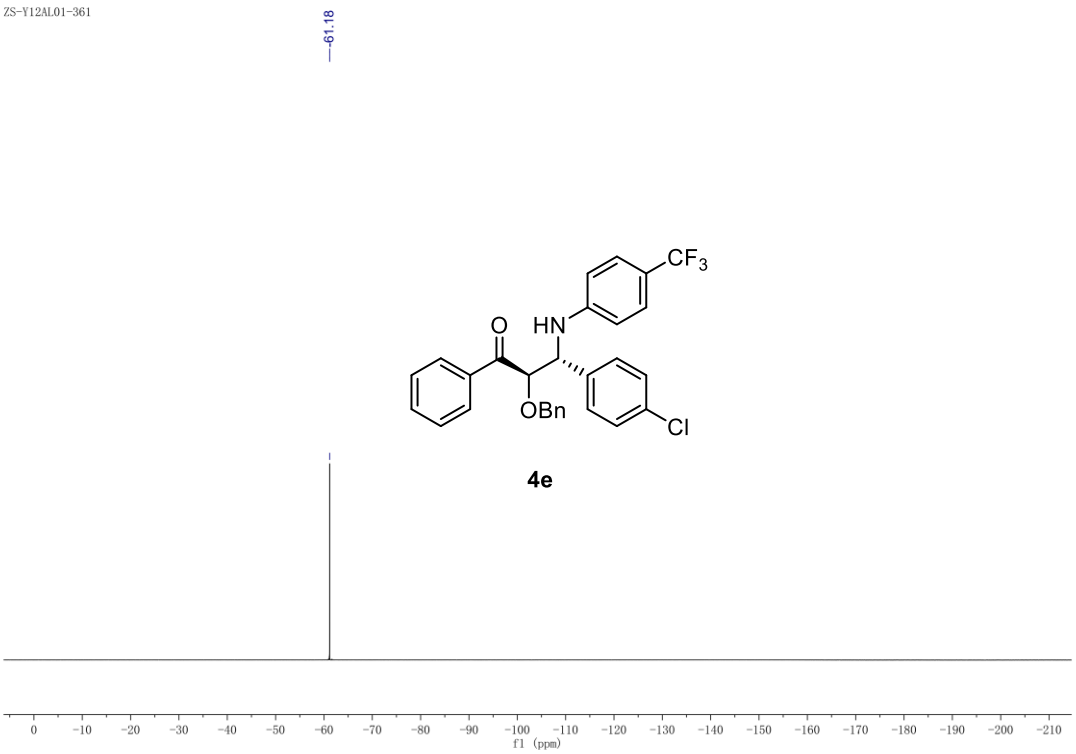
4d

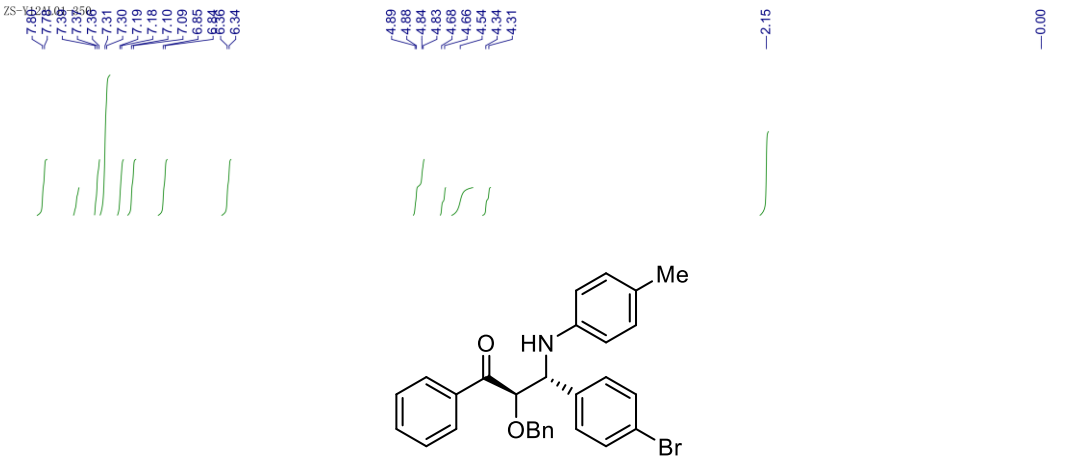
f1 (ppm)


ZS-Y12AL01-361
7.75
7.73
7.36
7.34
7.33
7.32
7.28
7.25
7.16
6.43
6.41
5.11
5.09
4.93
4.92
4.89
4.87
4.86
4.72
4.69
4.36
4.33
0.00
CF3
HN
O
OBn
Cl
2.00
1.00
5.00
2.20
2.00
4.00
2.00
1.00
1.00
1.00
1.00
f1 (ppm)

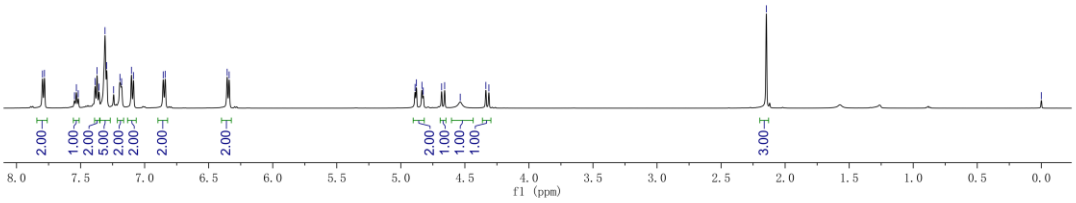
4e

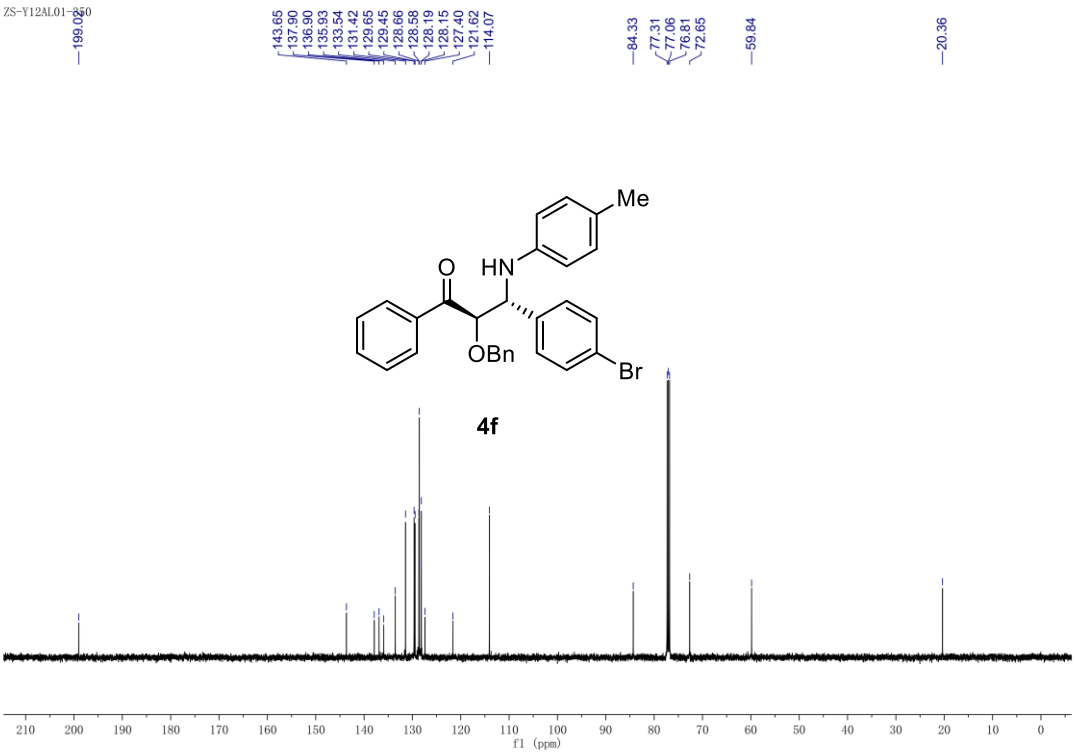

ZS-Y12AL01-361
198.87
148.60
136.62
136.28
135.81
133.88
133.81
128.90
128.73
128.69
128.54
128.40
128.26
126.54
126.51
126.47
126.44
119.74
112.90
83.30
77.37
77.06
76.74
72.66
59.05
126.54
126.51
126.47
126.44
126.12
126.5
126.0
f1 (ppm)
CF3
HN
O
OBn
Cl
4e
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


ZS-Y12AL01-361
61.18
CF3
HN
O
OBn
Cl
4e
0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)

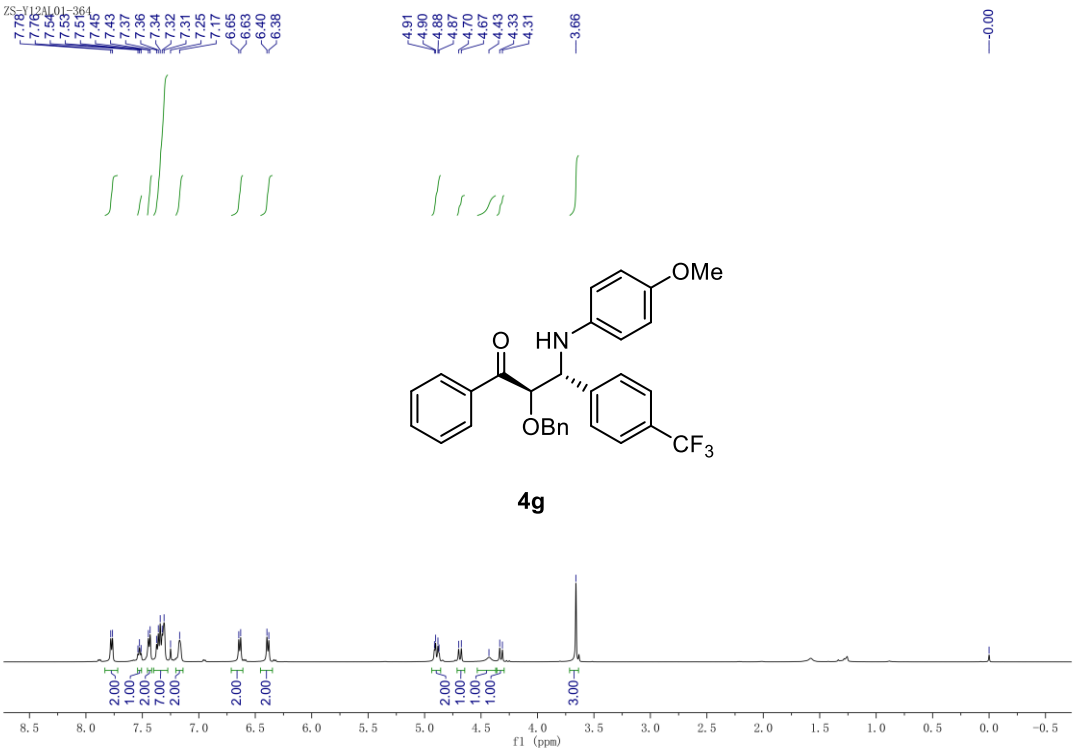


4f

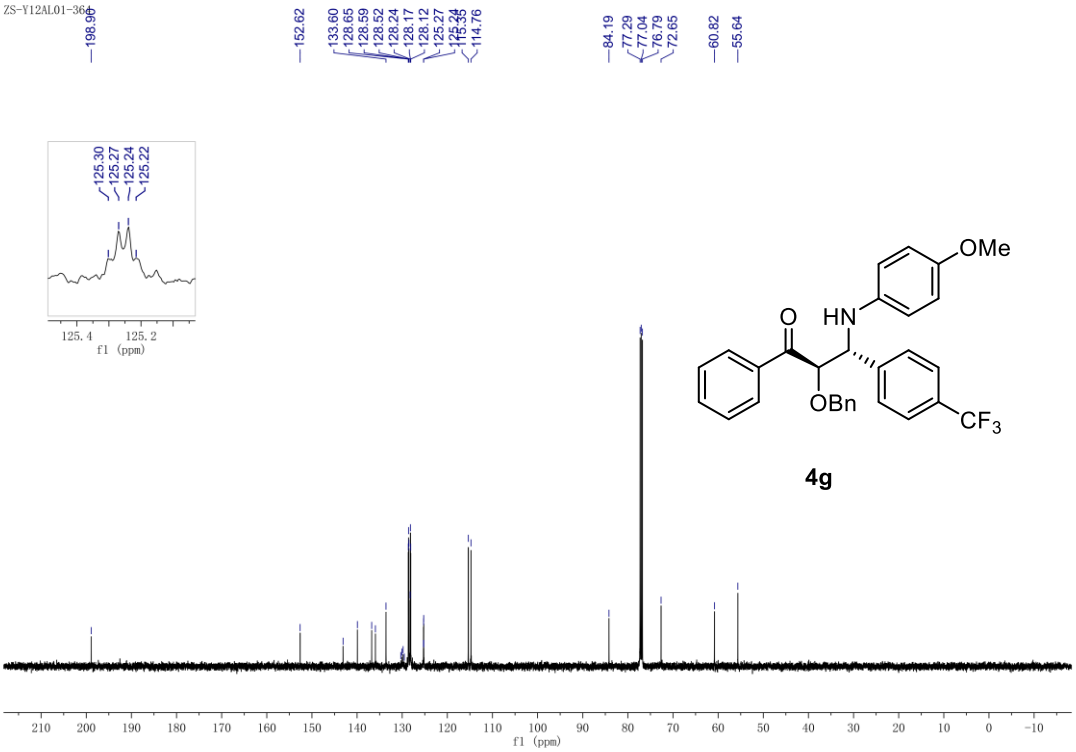




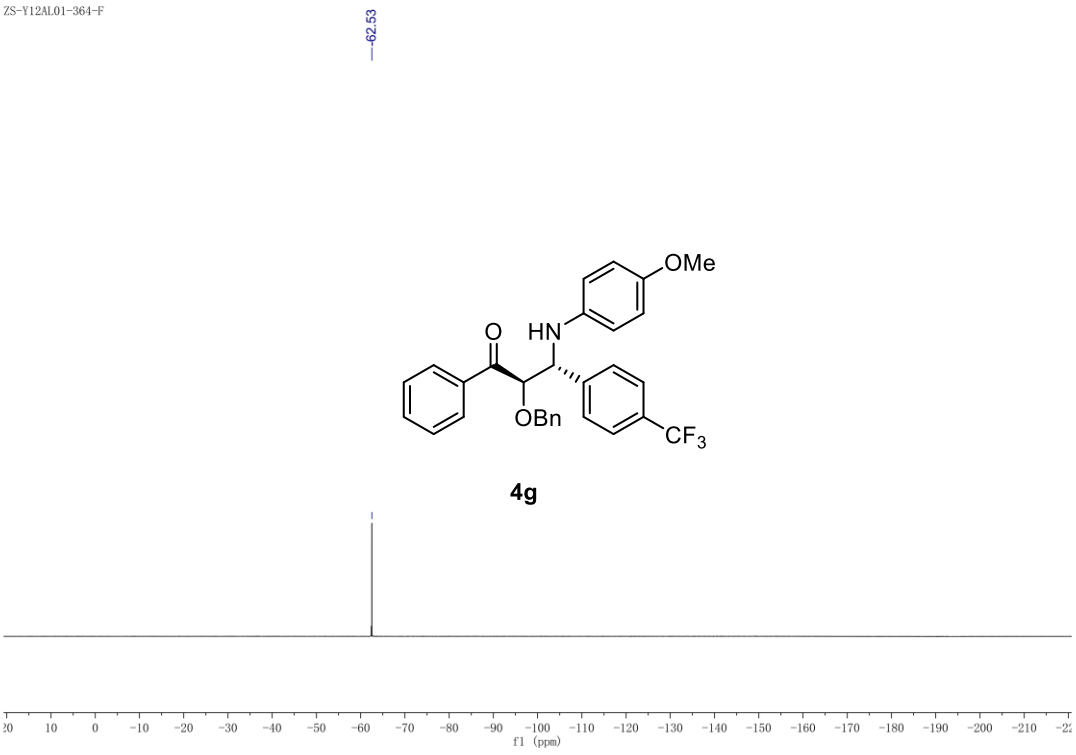
4f


ZS-Y12AL01-364
7.78
7.76
7.54
7.53
7.51
7.45
7.43
7.37
7.36
7.34
7.32
7.31
7.25
7.17
6.65
6.63
6.40
6.38
4.91
4.90
4.88
4.87
4.70
4.67
4.43
4.33
4.31
3.66
0.00
OMe
HN
O
OBn
CF3
2.00
1.00
2.00
7.00
2.00
2.00
2.00
2.00
1.00
1.00
1.00
3.00
f1 (ppm)

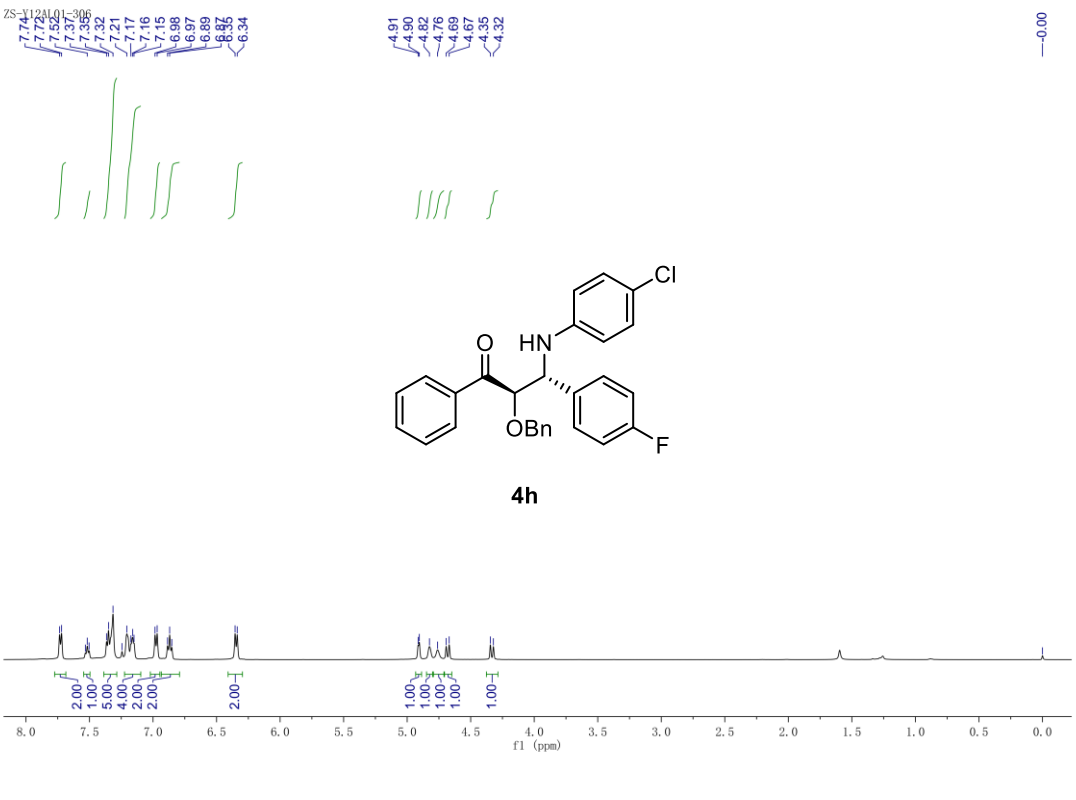
4g


ZS-Y12AL01-364
198.96
152.62
133.60
128.65
128.59
128.52
128.24
128.17
128.12
125.27
125.24
125.22
114.76
84.19
77.29
77.04
76.79
72.65
60.82
55.64
125.30
125.27
125.24
125.22
125.4
125.2
f1 (ppm)
OMe
HN
O
OBn
CF3
f1 (ppm)

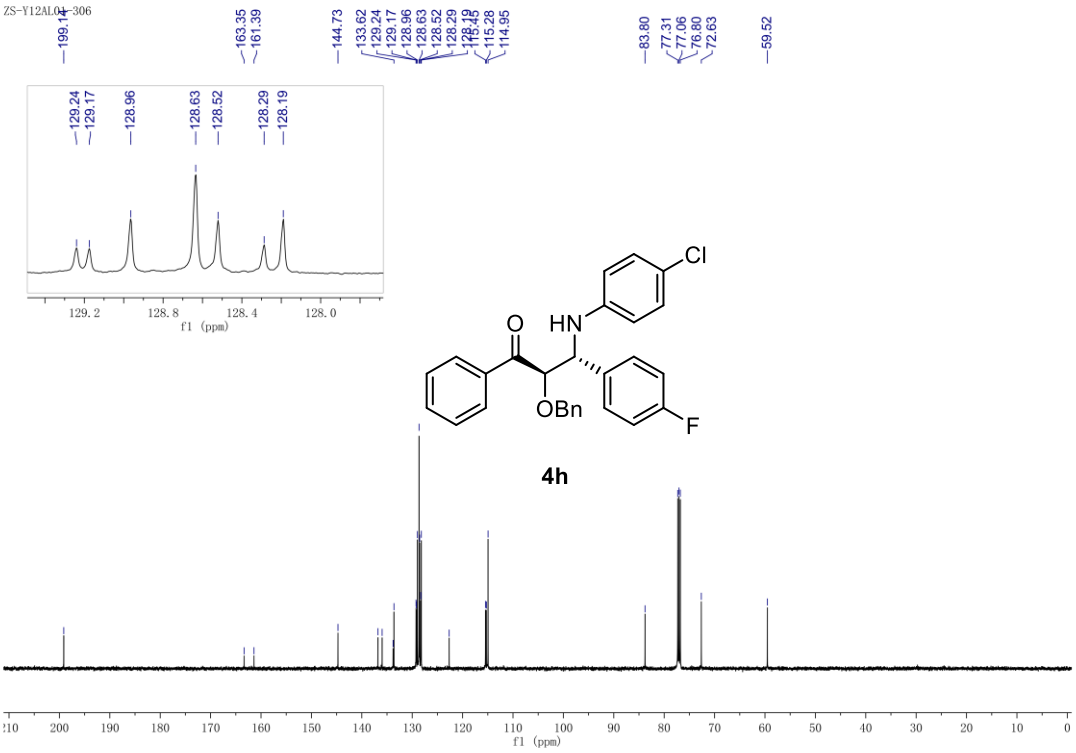
4g

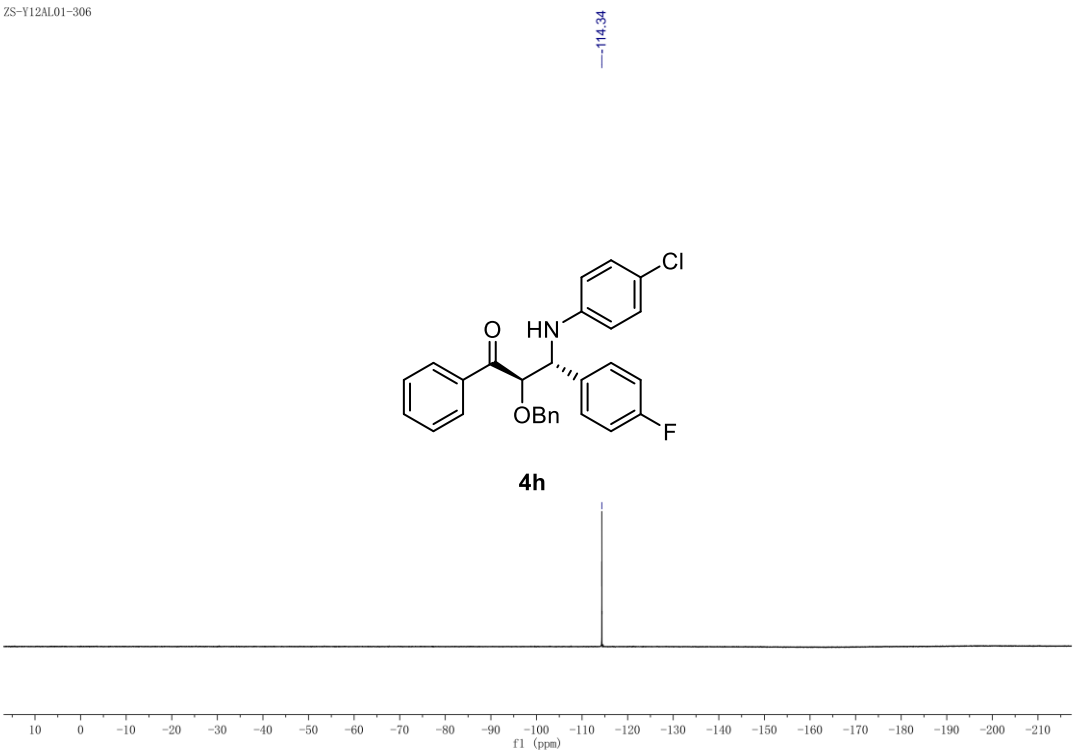

ZS-Y12AL01-364-F
-62.53
OMe
HN
O
OBn
CF3
f1 (ppm)

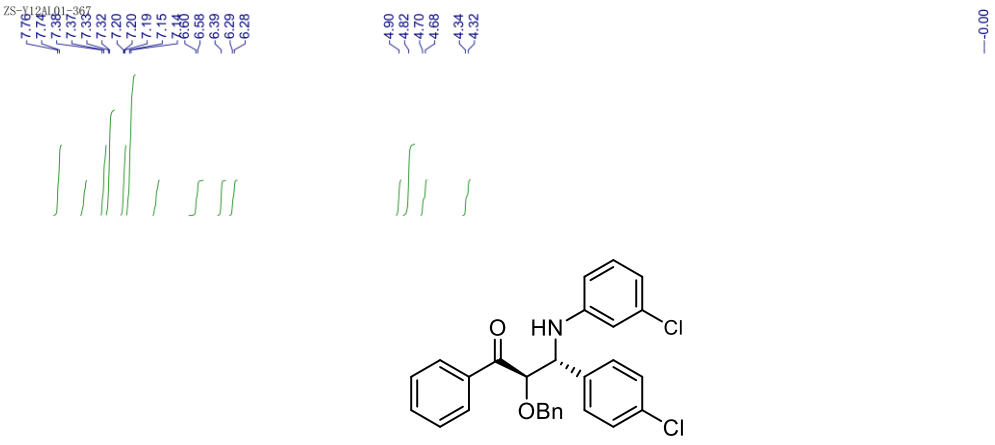
4g


ZS-Y12AL01-306
7.74
7.72
7.58
7.57
7.34
7.32
7.21
7.17
7.16
7.15
6.98
6.97
6.89
6.87
6.35
6.34
4.91
4.90
4.82
4.76
4.69
4.67
4.35
4.32
-0.00
Cl
HN
O
OBn
F
2.00
1.00
5.00
4.00
2.00
2.00
2.00
1.00
1.00
1.00
1.00
1.00
f1 (ppm)

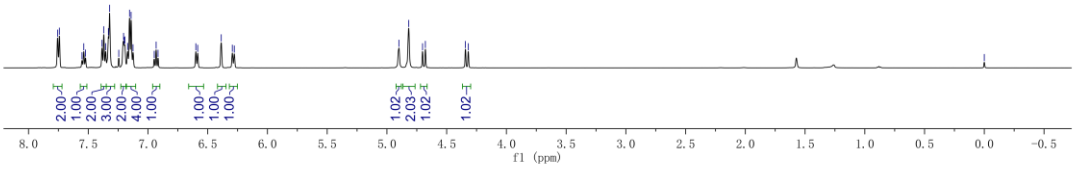
4h

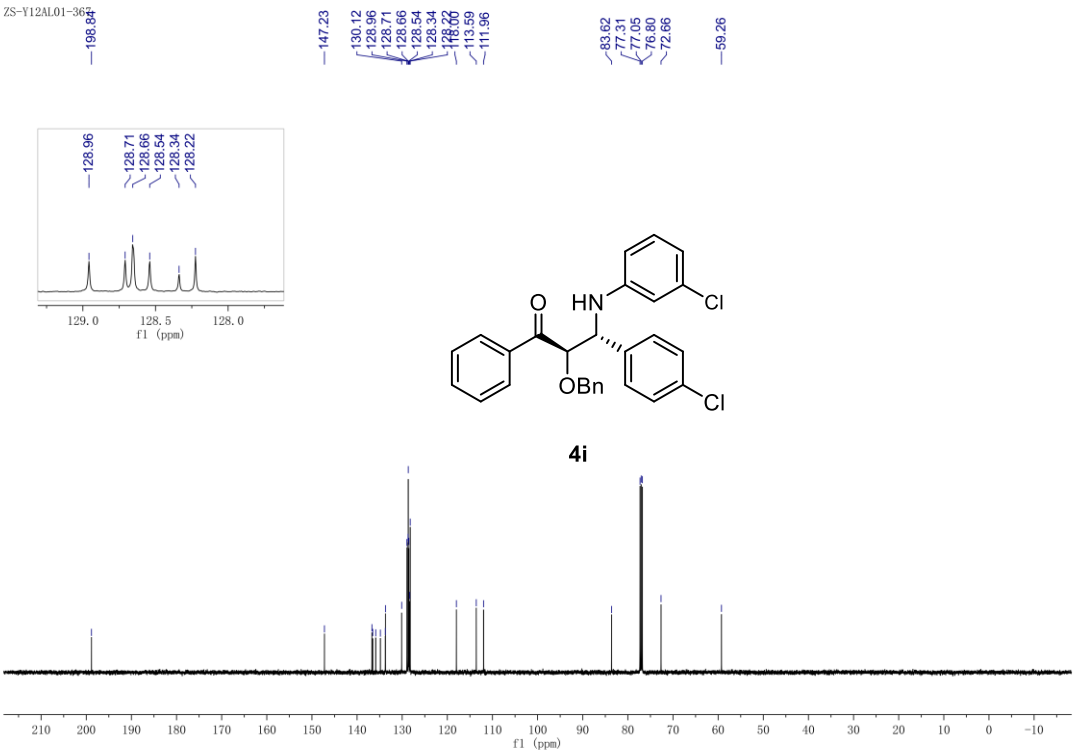

ZS-Y12AL01-306
199.14
163.35
161.39
144.73
133.62
129.24
129.17
128.96
128.63
128.52
128.29
128.19
115.45
115.28
114.95
83.80
77.31
77.06
76.80
72.63
59.52
129.24
129.17
128.96
128.63
128.52
128.29
128.19
129.2
128.8
128.4
128.0
f1 (ppm)
Cl
HN
O
OBn
F
4h
f1 (ppm)


ZS-Y12AL01-306
114.34
Cl
HN
O
OBn
F
4h
f1 (ppm)

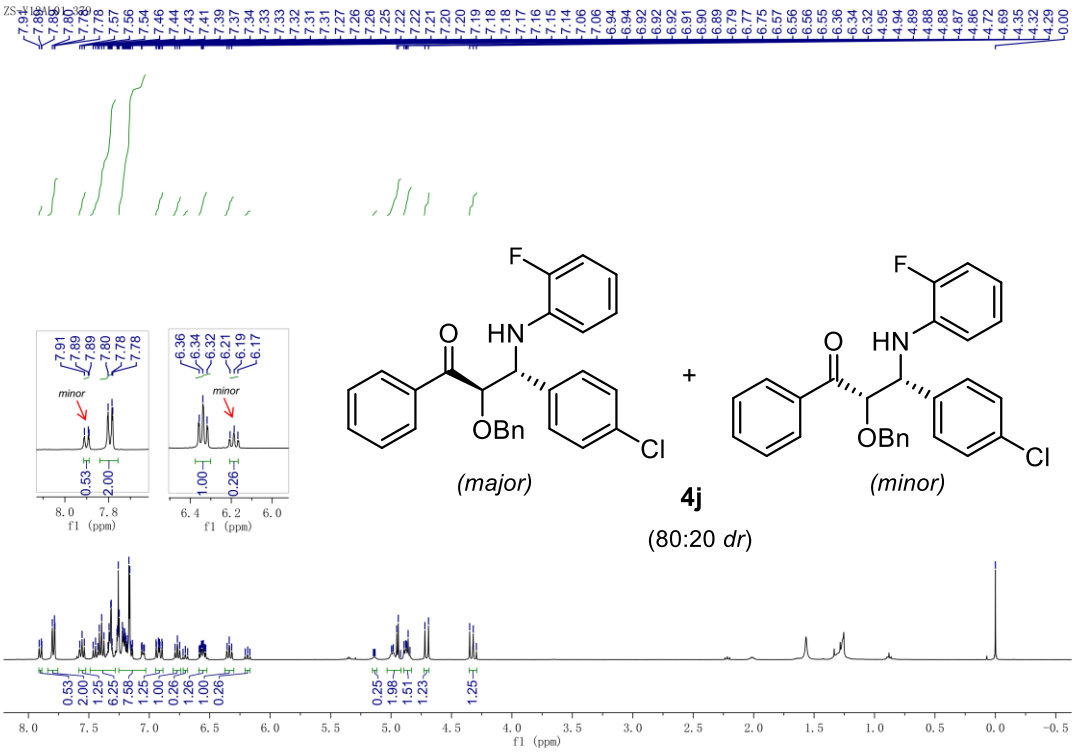

ZS-Y12AL01-367
7.76
7.74
7.38
7.37
7.33
7.32
7.20
7.20
7.19
7.15
7.14
7.00
6.58
6.39
6.29
6.28
4.90
4.82
4.70
4.68
4.34
4.32
0.00
O
HN
Cl
OBn
Cl

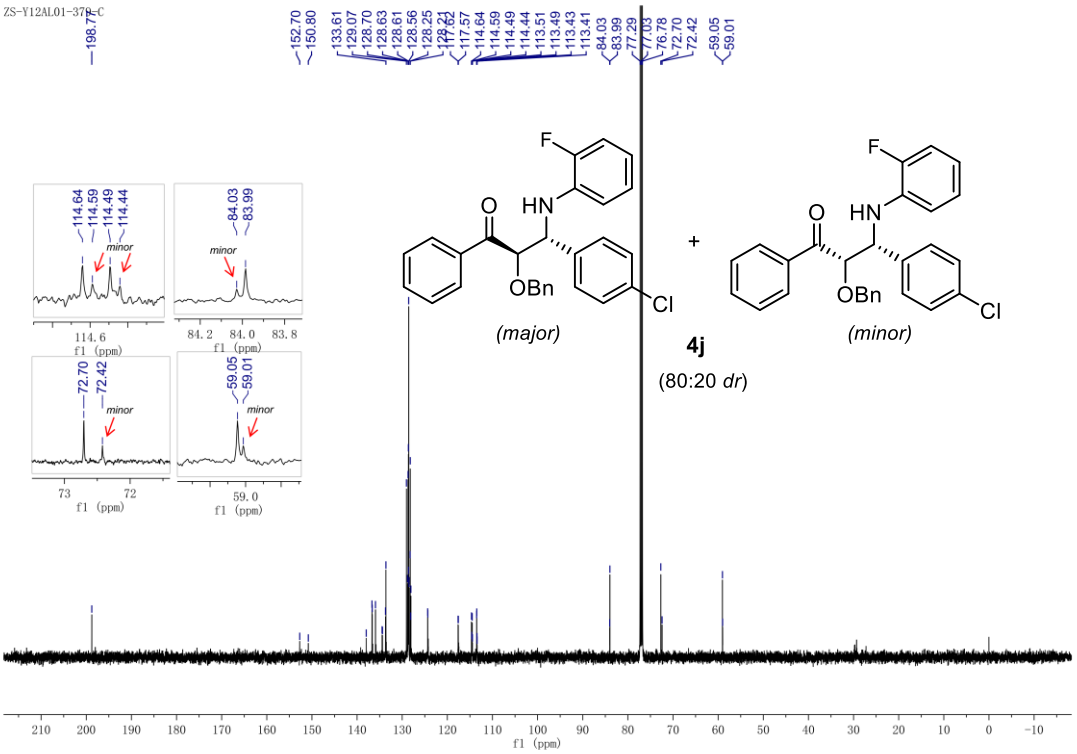
4i

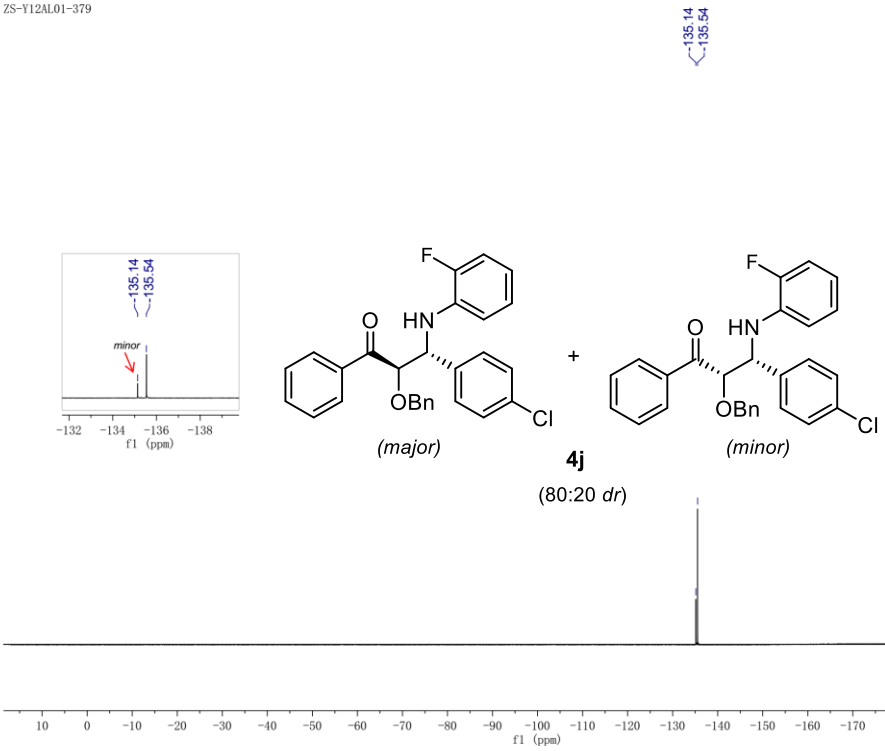

2.00
1.00
2.00
3.00
2.00
4.00
1.00
1.00
1.00
1.00
1.02
2.03
1.02
1.02
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

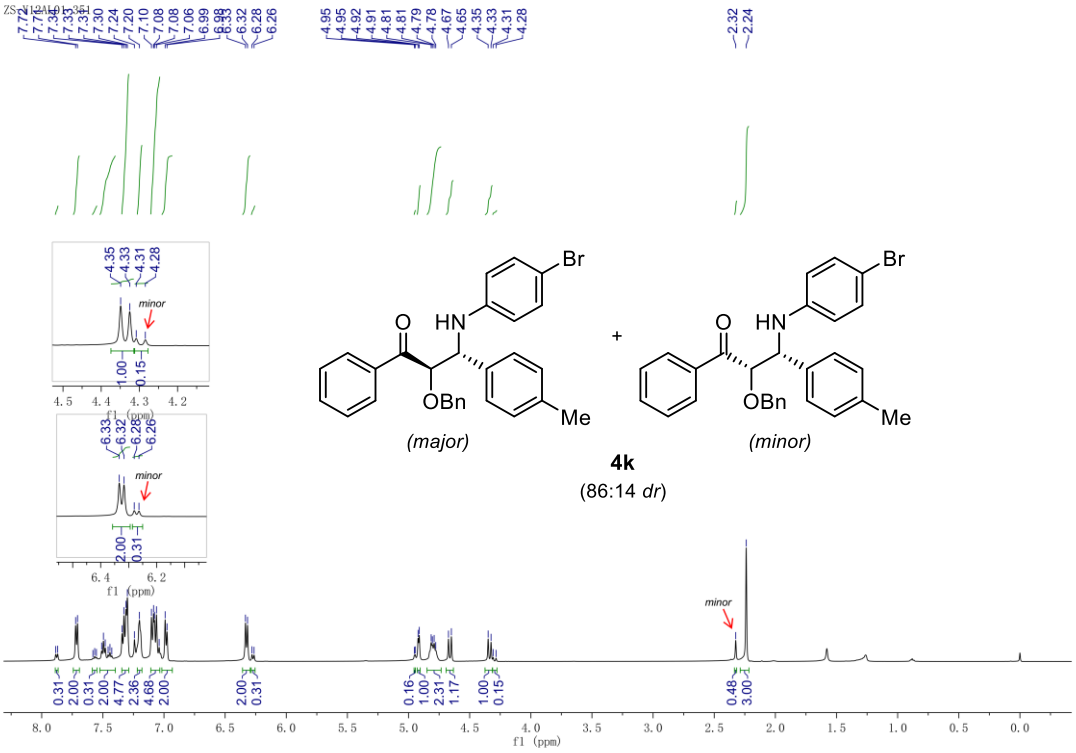

ZS-Y12AL01-367
198.84
147.23
130.12
128.96
128.71
128.66
128.54
128.34
128.22
113.59
111.96
83.62
77.31
77.05
76.80
72.66
59.26
128.96
128.71
128.66
128.54
128.34
128.22
129.0
128.5
128.0
f1 (ppm)
O
HN
Cl
OBn
Cl
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

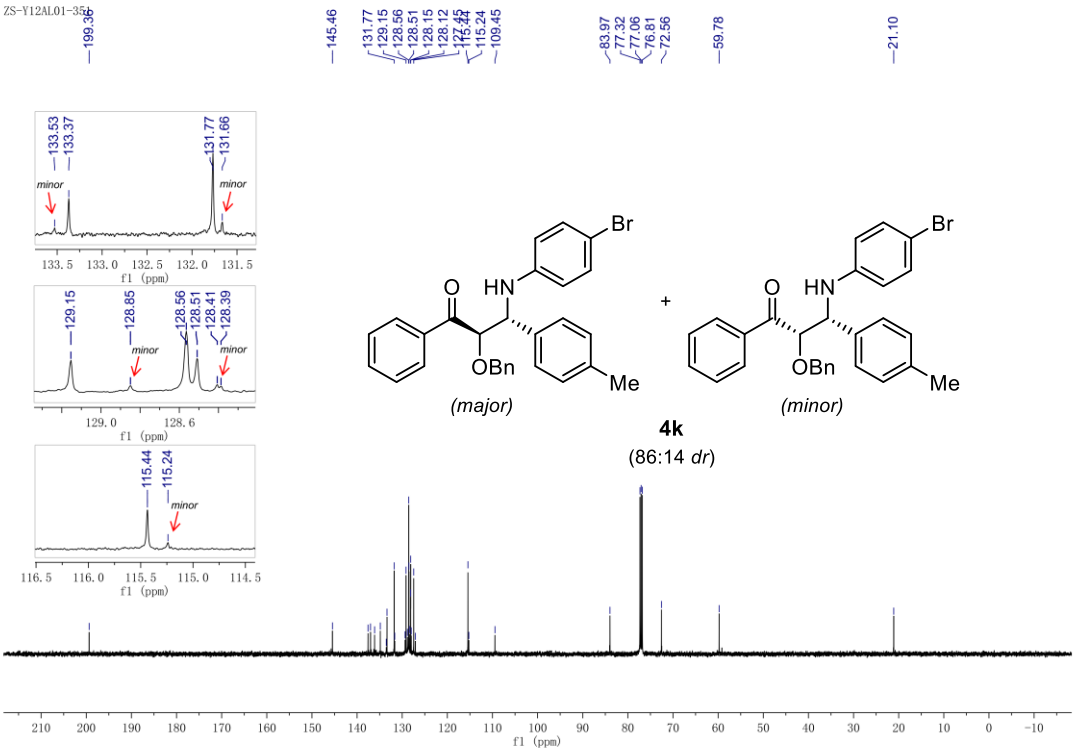
4i

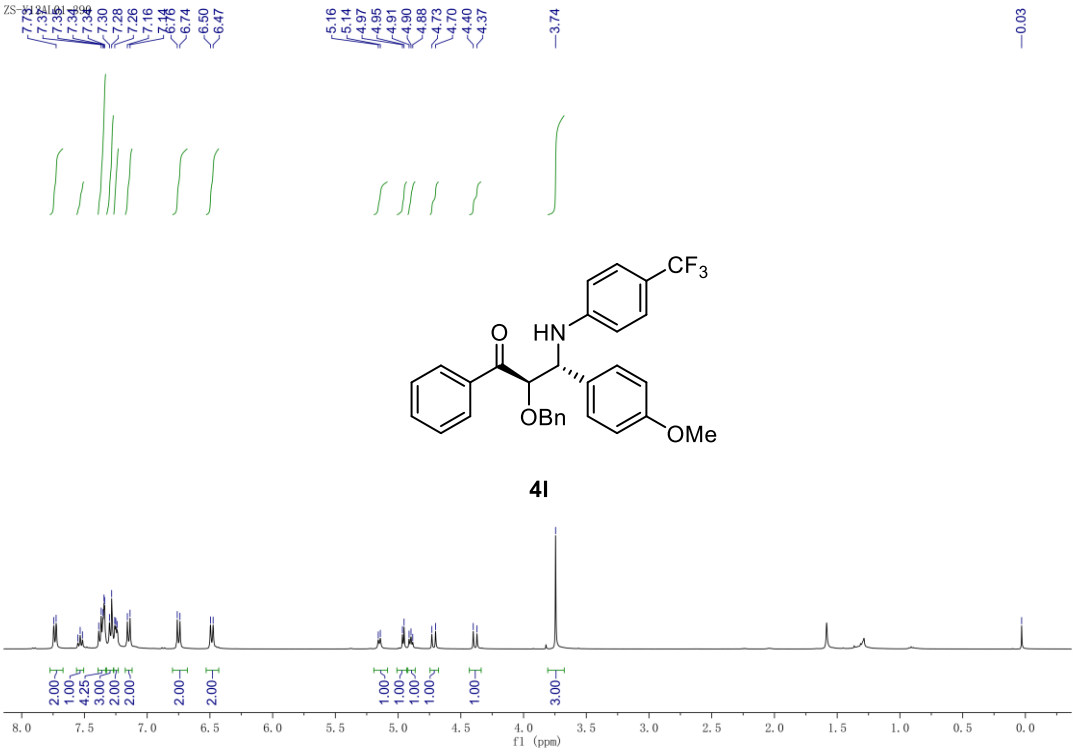

F
HN
O
OBn
Cl
(major)
+
(minor)
4j
(80:20 dr)
minor
f1 (ppm)

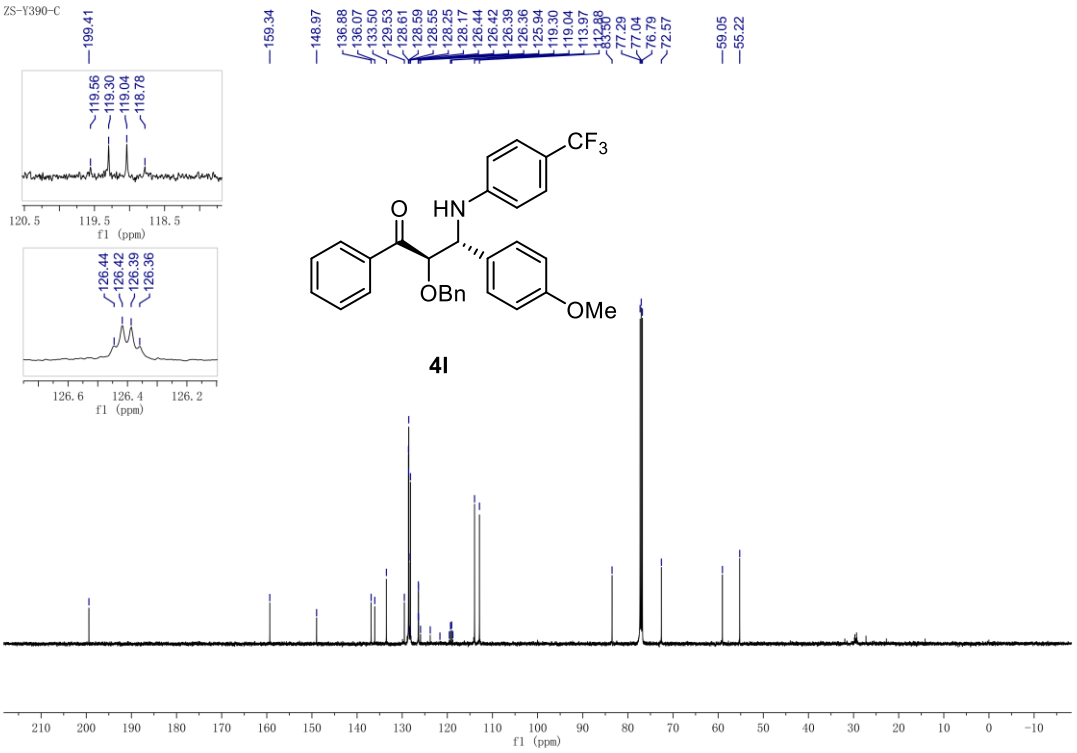

F
HN
O
OBn
Cl
(major)
+
(minor)
4j
(80:20 dr)
minor
f1 (ppm)

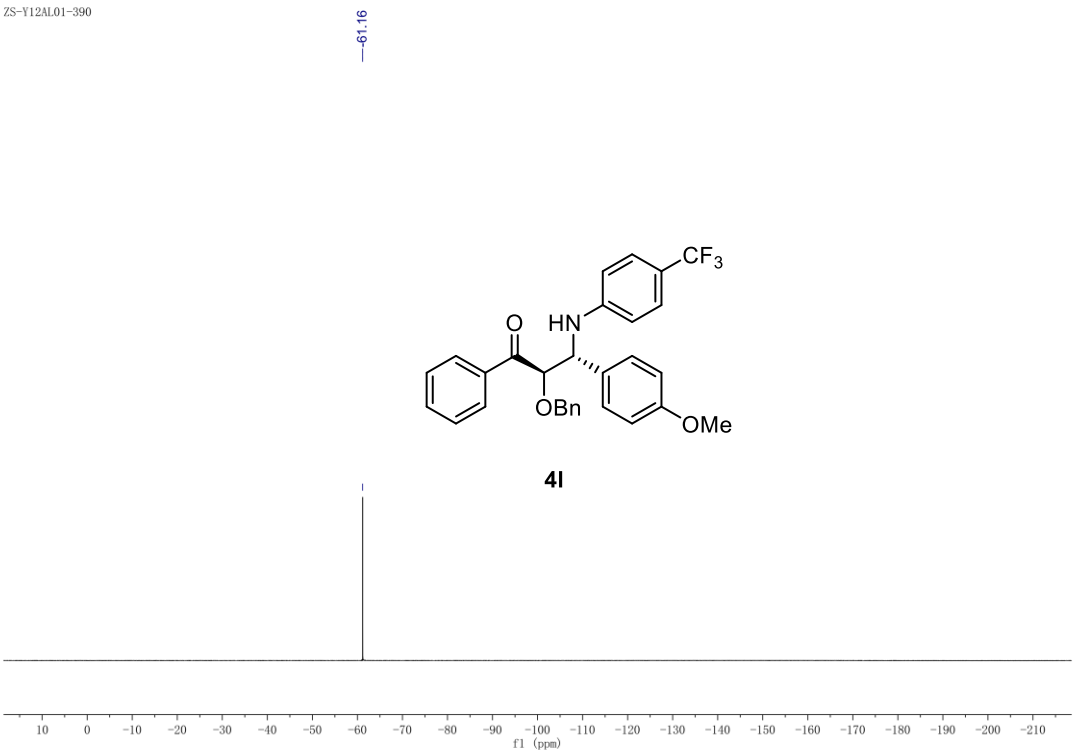

ZS-Y12AL01-379
135.14
135.54
minor
F
HN
O
OBn
Cl
(major)
+
(minor)
4j
(80:20 dr)

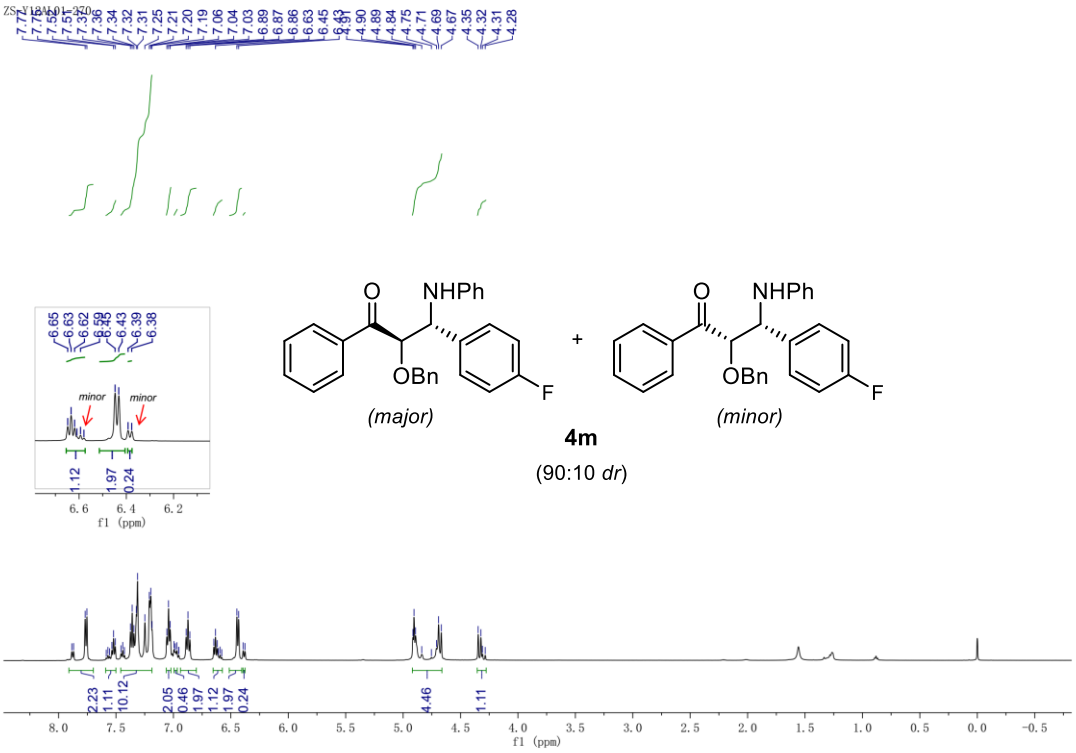

7.72
7.76
7.34
7.33
7.31
7.30
7.24
7.20
7.10
7.08
7.08
7.06
6.99
6.32
6.28
6.26
4.95
4.92
4.91
4.81
4.79
4.78
4.67
4.65
4.35
4.33
4.31
4.28
2.32
2.24
minor
Br
Me
(major)
+
(minor)
4k
(86:14 dr)

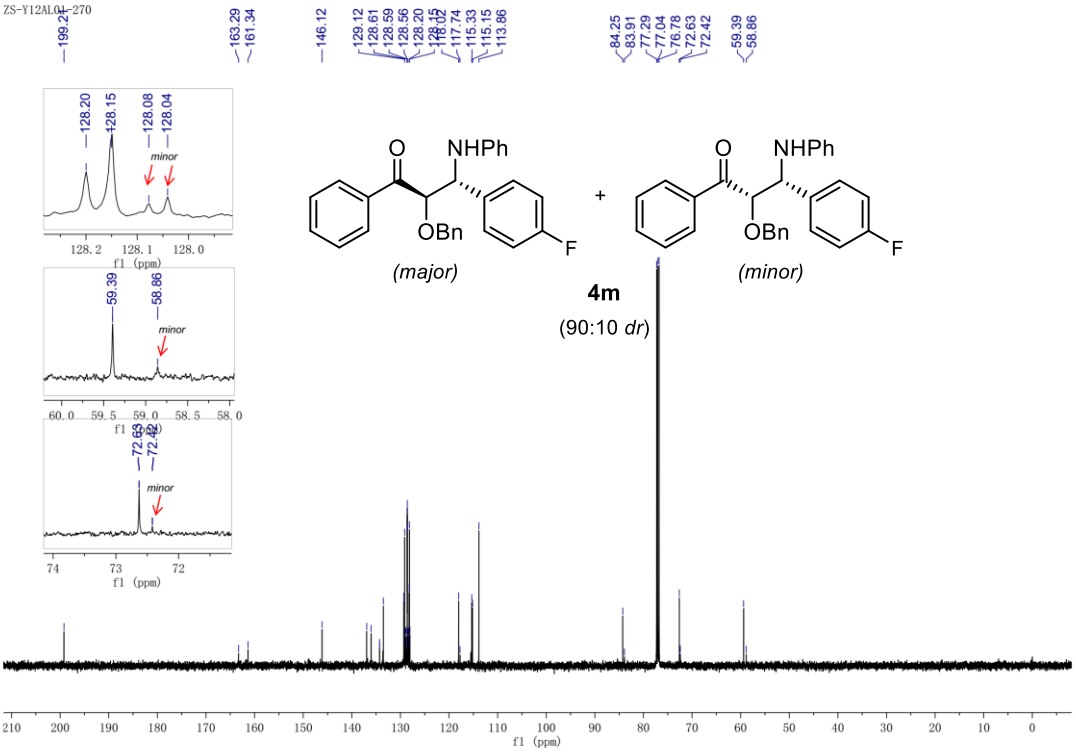

ZS-Y12AL01-3
199.36
145.46
131.77
129.15
128.56
128.51
128.15
128.12
115.44
115.24
109.45
83.97
77.32
77.06
76.81
72.56
59.78
21.10
133.53
133.37
131.77
131.66
minor
minor
129.15
128.85
128.56
128.51
128.41
128.39
minor
minor
115.44
115.24
minor
f1 (ppm)
Br
O
HN
OBn
Me
(major)
+
(minor)
4k
(86:14 dr)

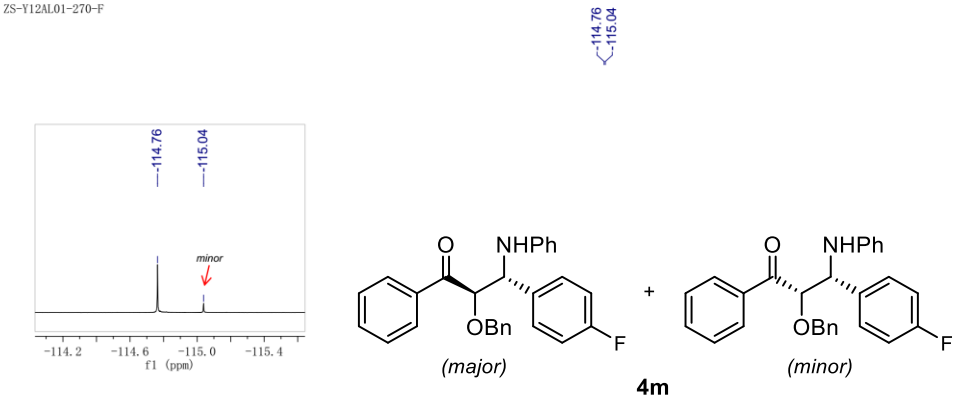

7.72
7.32
7.34
7.30
7.28
7.26
7.16
7.14
6.76
6.74
6.50
6.47
5.16
5.14
4.97
4.95
4.91
4.90
4.88
4.73
4.70
4.40
4.37
3.74
0.03
CF3
O
HN
OBn
OMe
4l
2.00
1.00
4.25
3.00
2.00
2.00
2.00
2.00
1.00
1.00
1.00
1.00
1.00
3.00
f1 (ppm)


ZS-Y390-C
199.41
159.34
148.97
136.88
136.07
133.50
129.53
128.61
128.59
128.55
128.25
128.17
126.44
126.42
126.39
126.36
125.94
119.30
119.04
113.97
112.88
83.50
77.29
77.04
76.79
72.57
59.05
55.22
119.56
119.30
119.04
118.78
126.44
126.42
126.39
126.36
CF3
O
HN
OBn
OMe
4l
f1 (ppm)


ZS-Y12AL01-390
61.16
CF3
O
HN
OBn
OMe
4l
f1 (ppm)

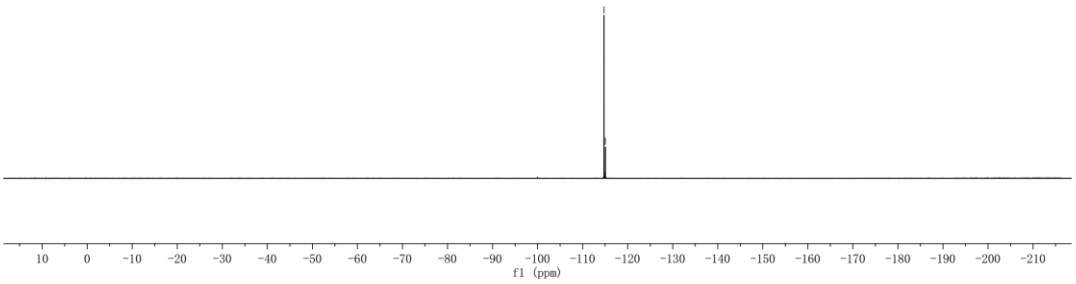

ZS-Y12AL01-270
7.72 7.70 7.55 7.53 7.36 7.34 7.32 7.31 7.25 7.21 7.20 7.19 7.06 7.04 7.03 6.89 6.87 6.86 6.63 6.45 6.43 4.91 4.90 4.89 4.84 4.75 4.71 4.69 4.67 4.35 4.32 4.31 4.28
6.65 6.63 6.62 6.59 6.55 6.43 6.39 6.38
minor
minor
1.12 1.97 0.24
6.6 6.4 6.2
f1 (ppm)
O NHPh
OBn
F
(major)
+
O NHPh
OBn
F
(minor)
4m
(90:10 dr)
2.23 1.11 10.12 2.05 0.46 1.97 1.12 1.97 0.24 4.46 1.11
8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

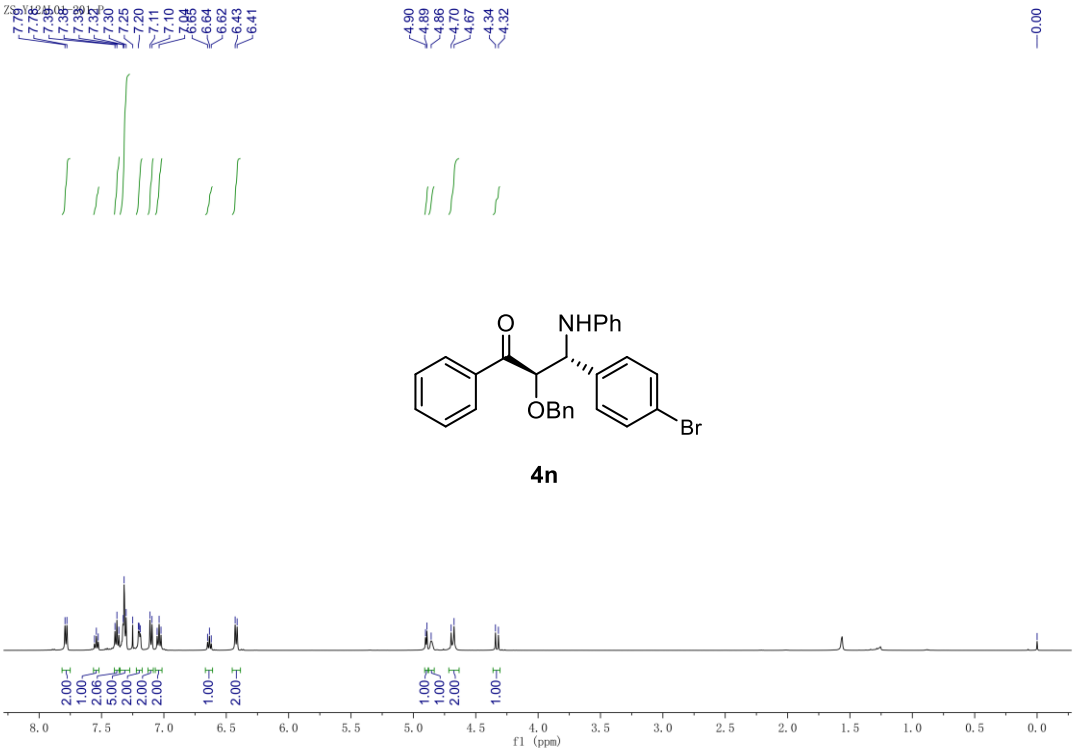

ZS-Y12AL01-270
199.25
163.29 161.34 146.12 129.12 128.61 128.59 128.56 128.20 128.15 128.12 117.74 115.33 115.15 113.86
84.25 83.91 77.29 77.04 76.78 72.63 72.42 59.39 58.86
128.20 128.15 128.08 128.04
minor
128.2 128.1 128.0
f1 (ppm)
59.39 58.86
minor
60.0 59.5 59.0 58.5 58.0
f1 (ppm)
72.63 72.42
minor
74 73 72
f1 (ppm)
O NHPh
OBn
F
(major)
+
O NHPh
OBn
F
(minor)
4m
(90:10 dr)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


ZS-Y12AL01-270-F
-114.76
-115.04
minor
-114.2
-114.6
-115.0
-115.4
f1 (ppm)
O
NHPh
OBn
F
+
(major)
(minor)

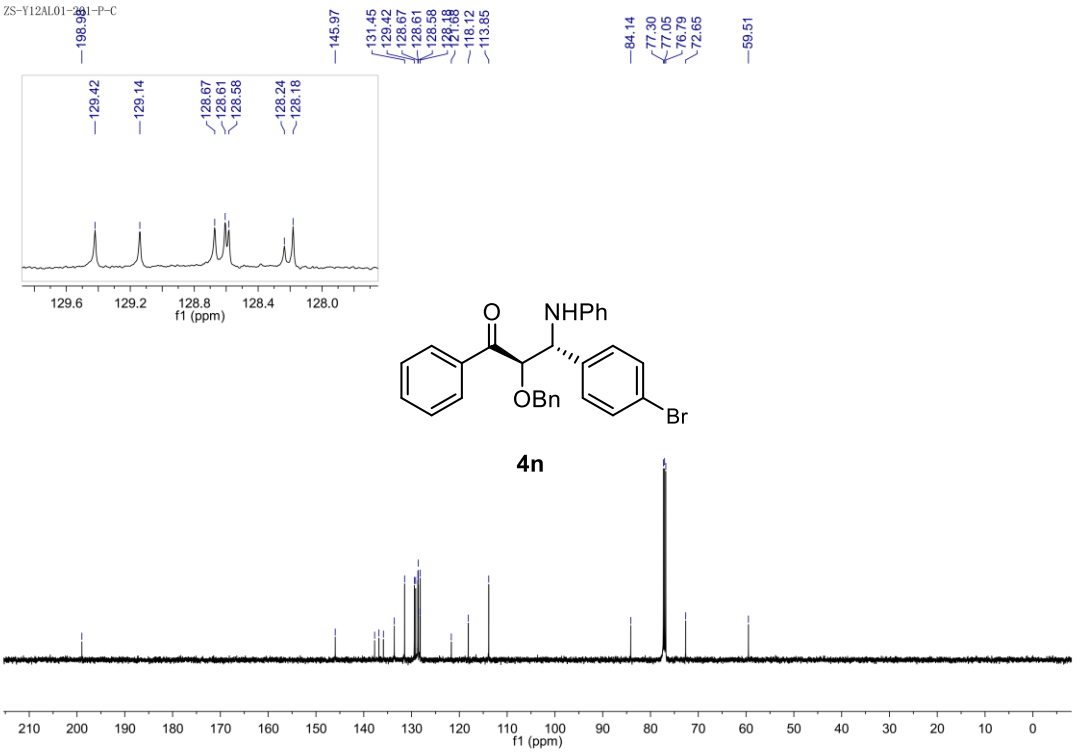
4m

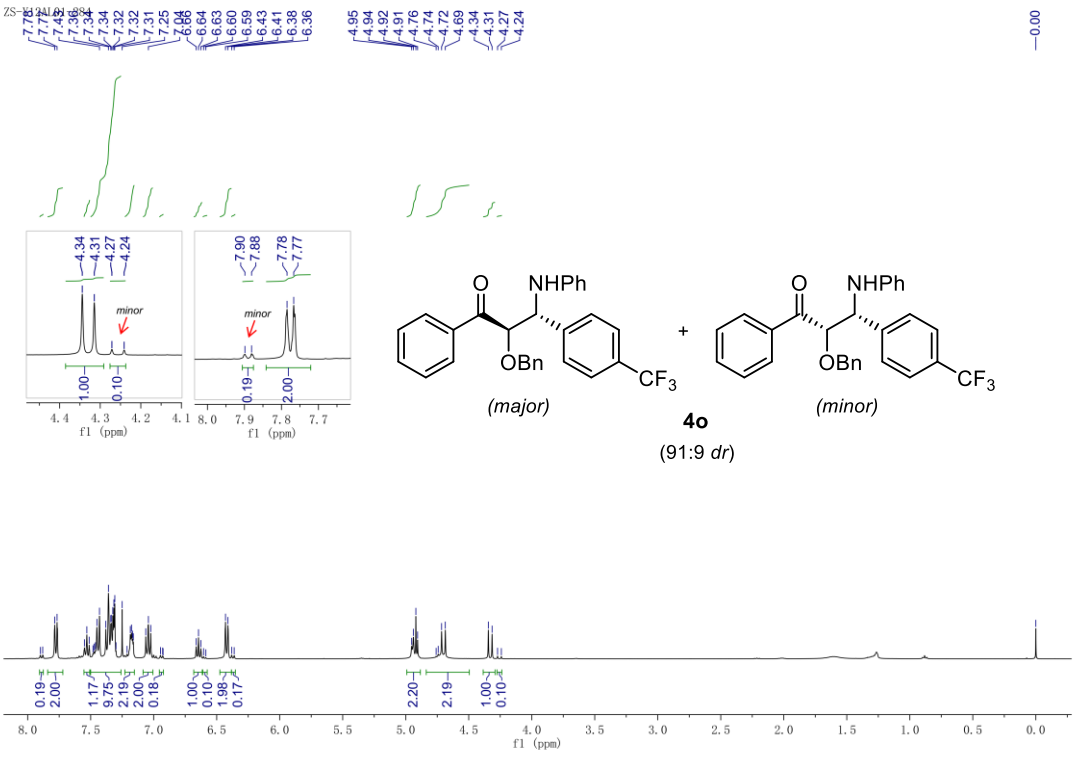
(90:10 *dr*)

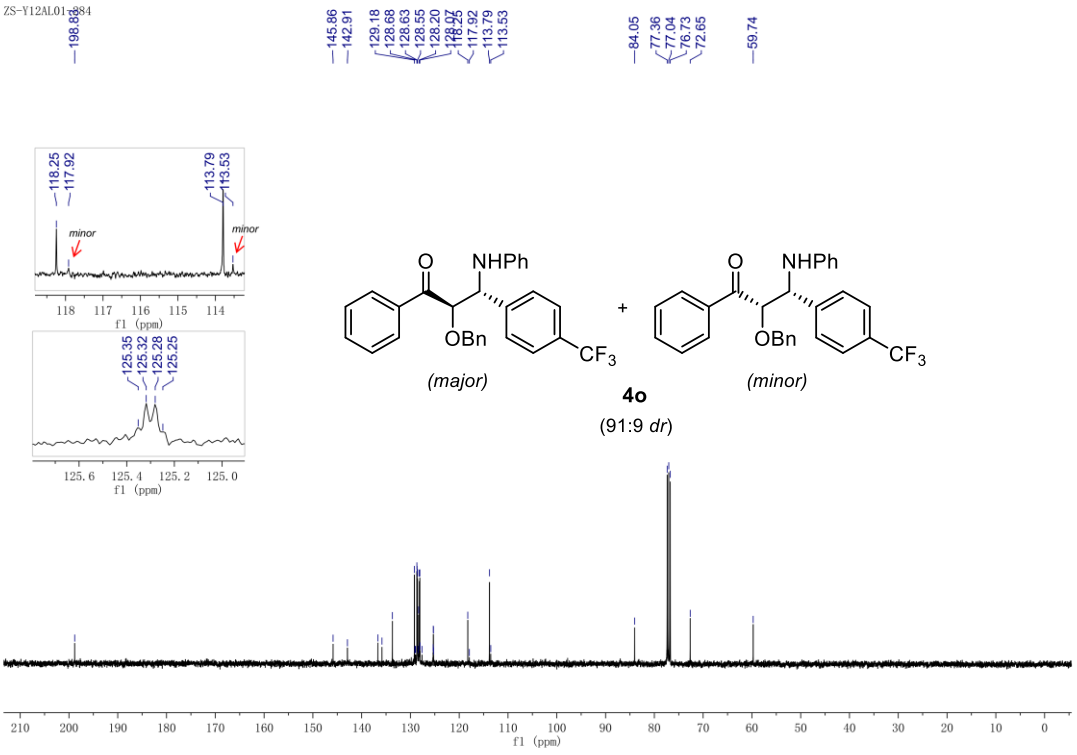

10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
f1 (ppm)

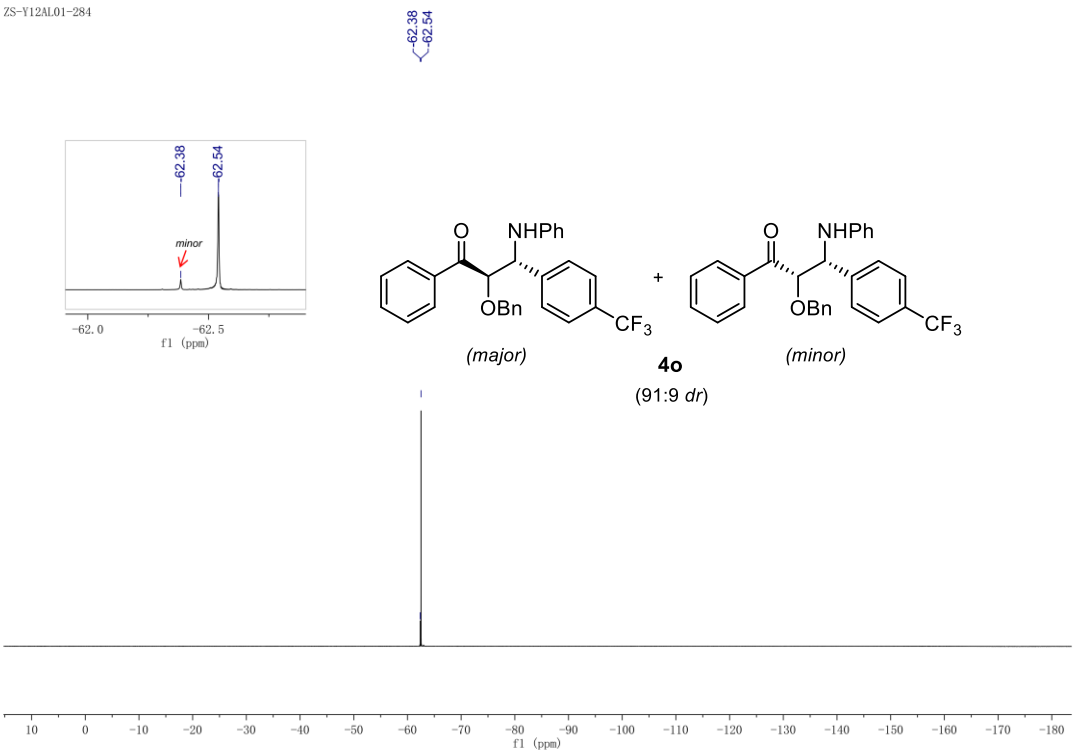

7.79
7.78
7.39
7.38
7.38
7.37
7.36
7.30
7.25
7.20
7.11
7.10
6.64
6.62
6.43
6.41
4.90
4.89
4.86
4.70
4.67
4.34
4.32
0.00
O
NHPh
OBn
Br
2.00
1.00
2.06
5.00
2.00
2.00
2.00
1.00
2.00
1.00
1.00
2.00
1.00
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

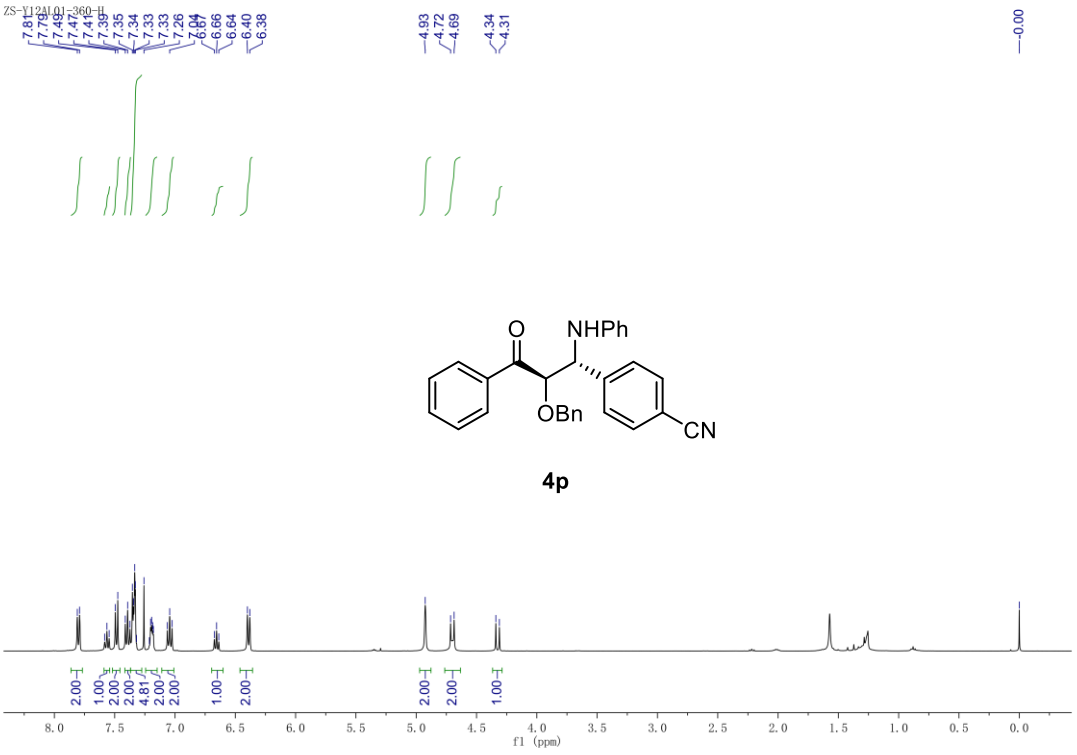
4n

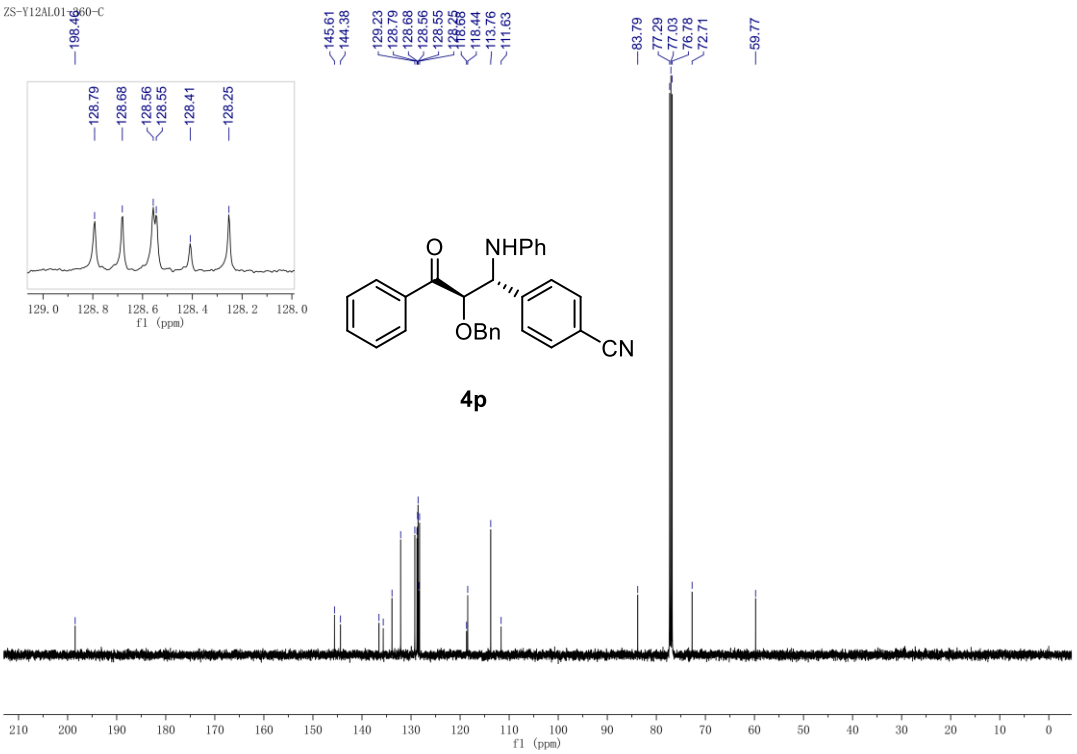

ZS-Y12AL01-201-P-C
198.98
145.97
131.45
129.42
128.67
128.61
128.58
84.14
77.30
77.05
76.79
72.65
59.51
129.42
129.14
128.67
128.61
128.58
128.24
128.18
129.6
129.2
128.8
128.4
128.0
f1 (ppm)
O
NHPh
OBn
Br
4n
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

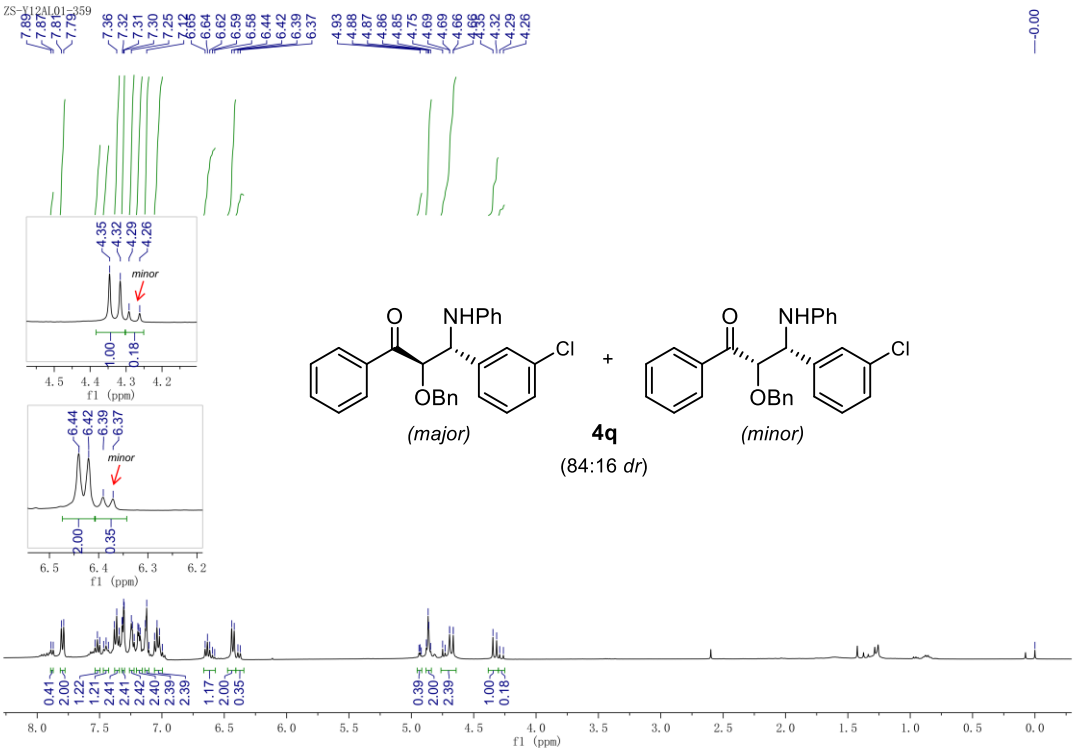

7.78
7.77
7.43
7.36
7.34
7.34
7.32
7.32
7.31
7.25
7.04
6.66
6.64
6.63
6.60
6.59
6.43
6.41
6.38
6.36
4.95
4.94
4.92
4.91
4.76
4.74
4.72
4.69
4.34
4.31
4.27
4.24
0.00
4.34
4.31
4.27
4.24
minor
1.00
0.10
7.90
7.88
7.78
7.77
minor
0.19
2.00
4.4
4.3
4.2
4.1
8.0
7.9
7.8
7.7
f1 (ppm)
O
NHPh
OBn
CF3
(major)
+
O
NHPh
OBn
CF3
(minor)
4o
(91:9 dr)
0.19
2.00
1.17
9.75
2.19
2.00
0.18
1.00
0.10
1.98
0.17
2.20
2.19
1.00
0.10
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

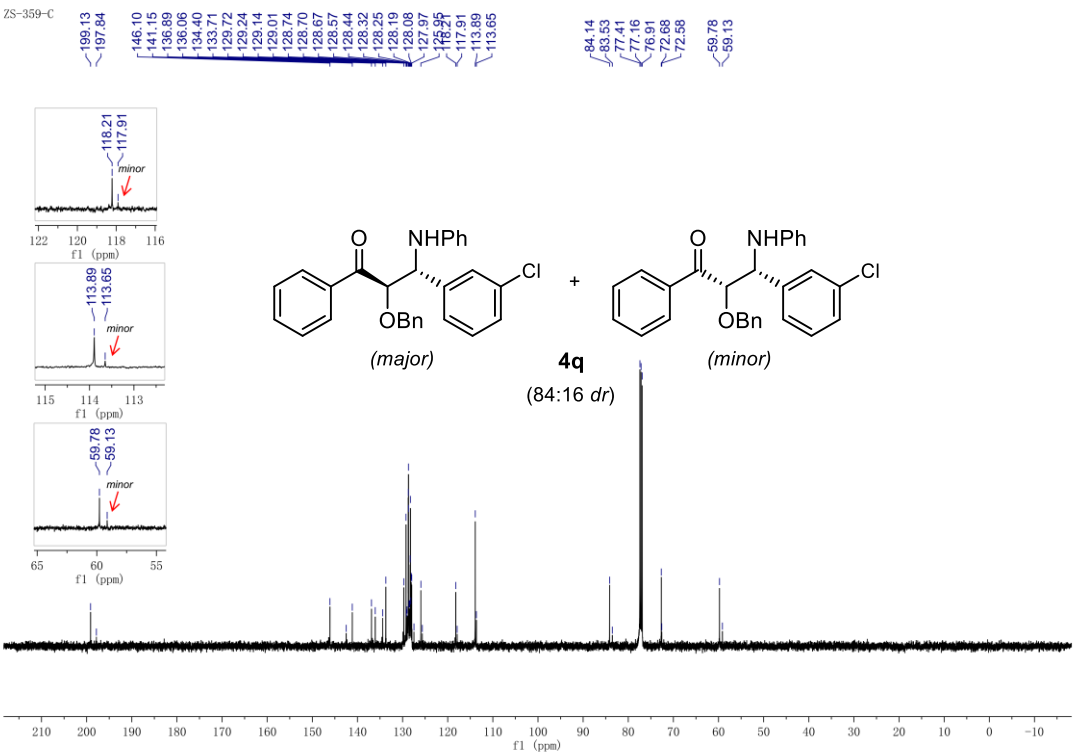

ZS-Y12AL01-284
198.83
145.86
142.91
129.18
128.68
128.63
128.55
128.20
117.92
113.79
113.53
84.05
77.36
77.04
76.73
72.65
59.74
118.25
117.92
113.79
113.53
minor
minor
125.35
125.32
125.28
125.25
O
NHPh
OBn
CF3
(major)
+
O
NHPh
OBn
CF3
(minor)
4o
(91:9 dr)
f1 (ppm)

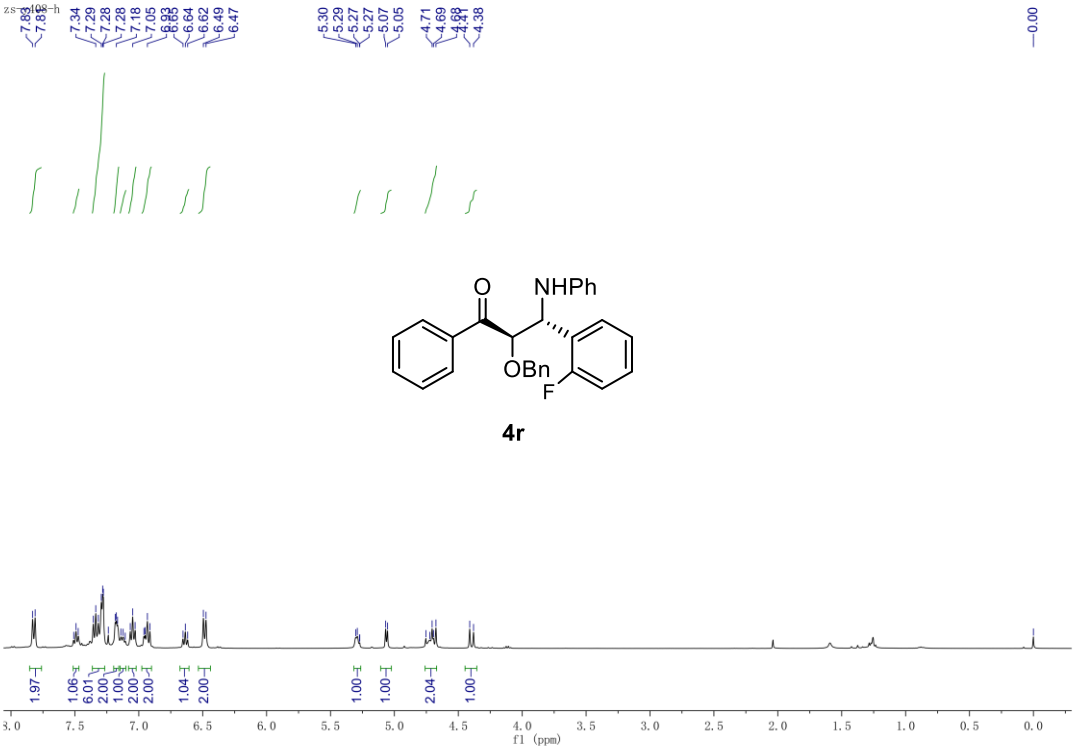

ZS-Y12AL01-284
62.38
62.54
minor
O
NHPh
OBn
CF3
(major)
+
O
NHPh
OBn
CF3
(minor)
4o
(91:9 dr)
f1 (ppm)

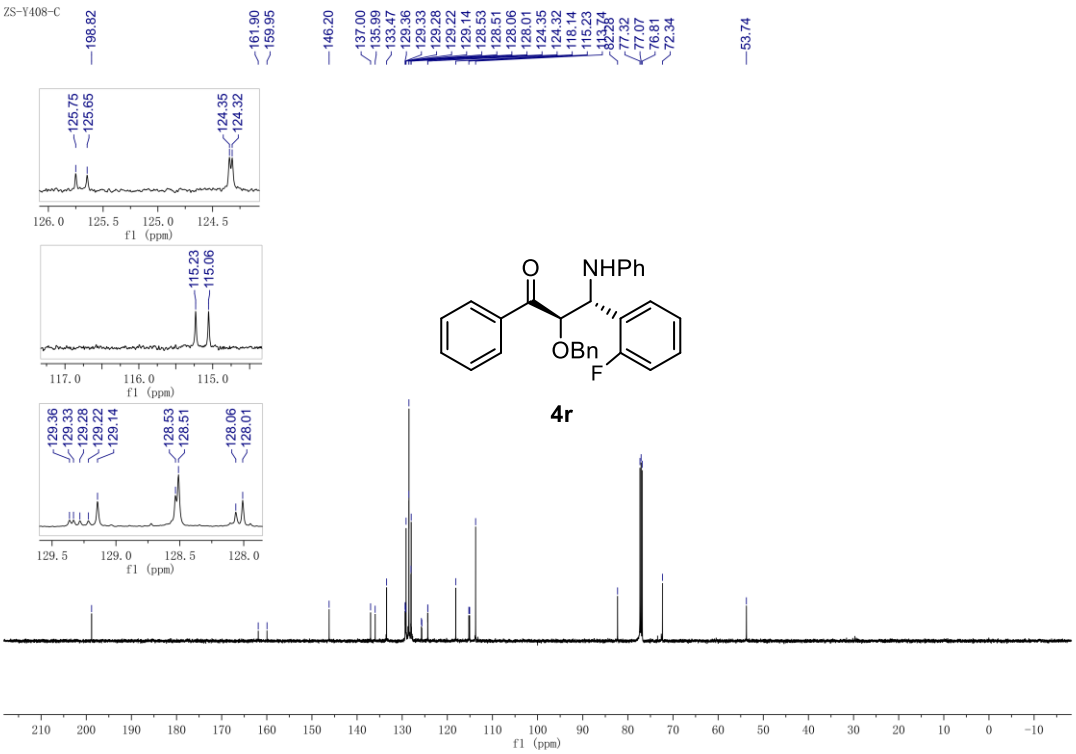

ZS-Y12AL01-360-H
7.81
7.79
7.49
7.47
7.41
7.39
7.35
7.34
7.33
7.26
6.67
6.66
6.64
6.40
6.38
4.93
4.72
4.69
4.34
4.31
0.00
O
NHPh
OBn
CN
4p
2.00
1.00
2.00
2.00
4.81
2.00
2.00
1.00
2.00
2.00
2.00
1.00
f1 (ppm)


ZS-Y12AL01-360-C
198.46
145.61
144.38
129.23
128.79
128.68
128.56
128.55
128.41
128.25
118.44
113.76
111.63
83.79
77.29
77.03
76.78
72.71
59.77
128.79
128.68
128.56
128.55
128.41
128.25
129.0
128.8
128.6
128.4
128.2
128.0
f1 (ppm)
O
NHPh
OBn
CN
4p
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

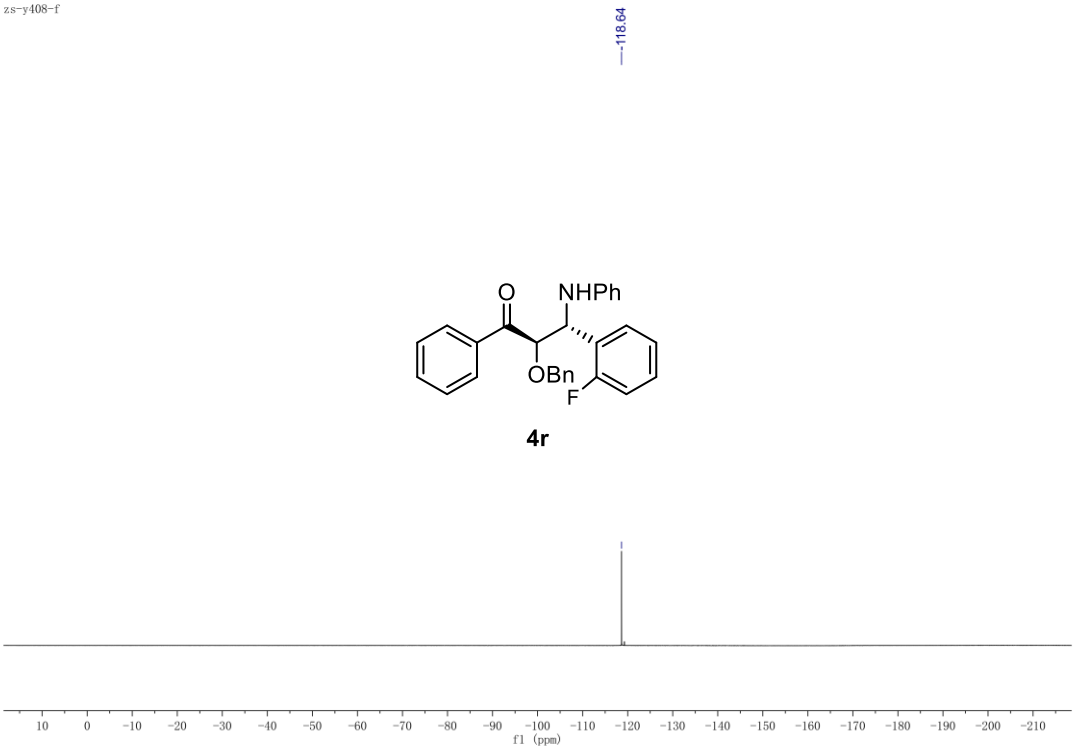

ZS-X12AL01-359
4.35
4.32
4.29
4.26
minor
1.00
0.18
6.44
6.42
6.39
6.37
minor
2.00
0.35
f1 (ppm)
O
NHPh
Cl
OBn
(major)
4q
(minor)
(84:16 dr)


ZS-359-C
199.13
197.84
146.10
141.15
136.89
136.06
134.40
133.71
129.72
129.24
129.14
129.01
128.74
128.70
128.67
128.57
128.44
128.32
128.25
128.19
128.08
127.97
118.21
117.91
113.89
113.65
84.14
83.53
77.41
77.16
76.91
72.68
72.58
59.78
59.13
minor
f1 (ppm)
O
NHPh
Cl
OBn
(major)
4q
(minor)
(84:16 dr)

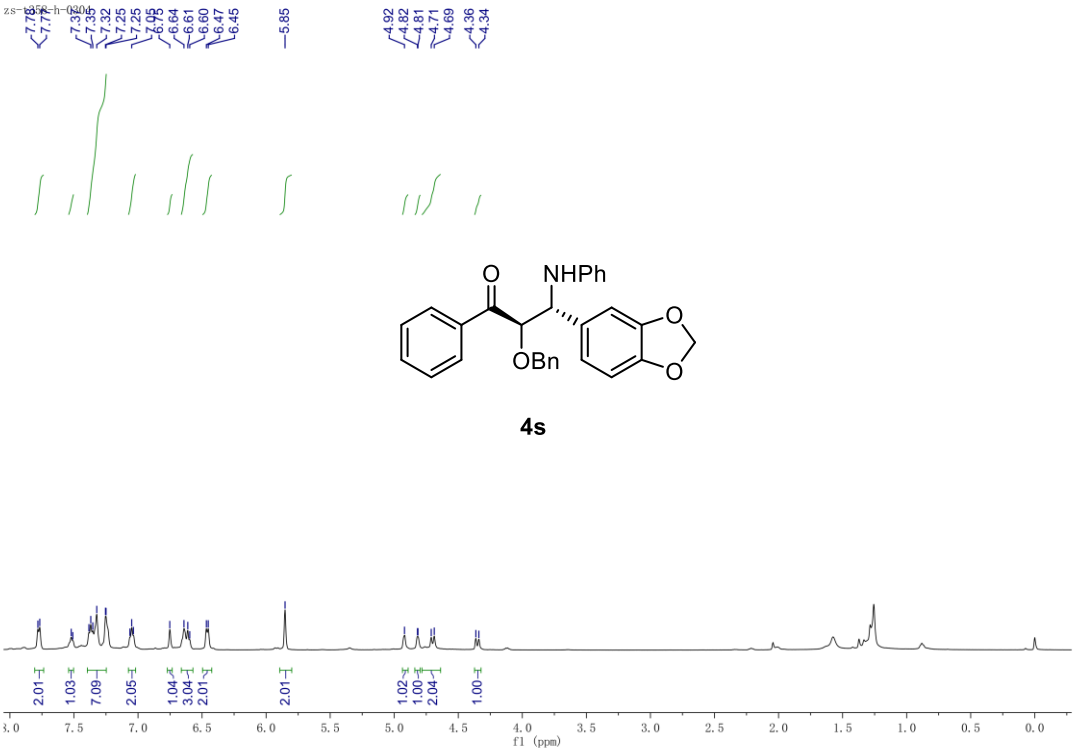

zs-y408-h
7.85
7.83
7.34
7.29
7.28
7.28
7.18
7.05
6.65
6.64
6.62
6.49
6.47
5.30
5.29
5.27
5.27
5.07
5.05
4.71
4.69
4.68
4.41
4.38
0.00
O
NHPh
OBn
F
4r
1.97
1.06
6.01
2.00
1.00
2.00
2.00
1.04
2.00
1.00
1.00
2.04
1.00
f1 (ppm)


ZS-Y408-C
198.82
161.90
159.95
146.20
137.00
135.99
133.47
129.36
129.33
129.28
129.22
129.14
128.53
128.51
128.06
128.01
124.35
124.32
118.14
115.23
115.06
77.32
77.07
76.81
72.34
53.74
125.75
125.65
O
NHPh
OBn
F
4r
f1 (ppm)

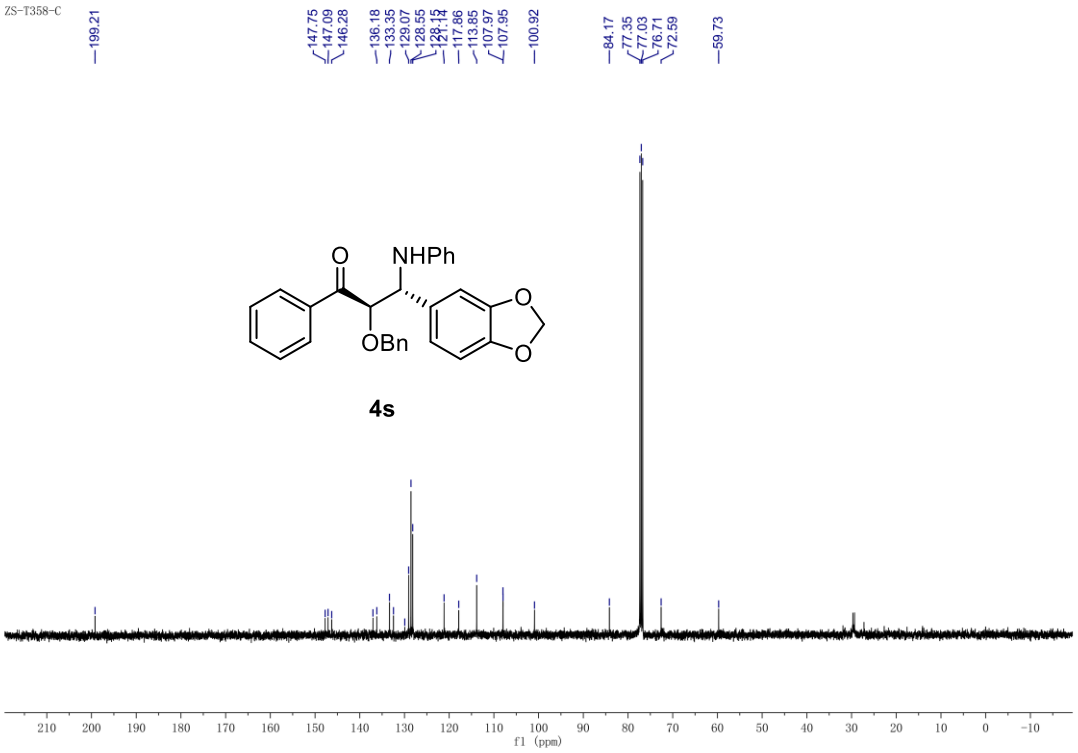
zs-y408-f

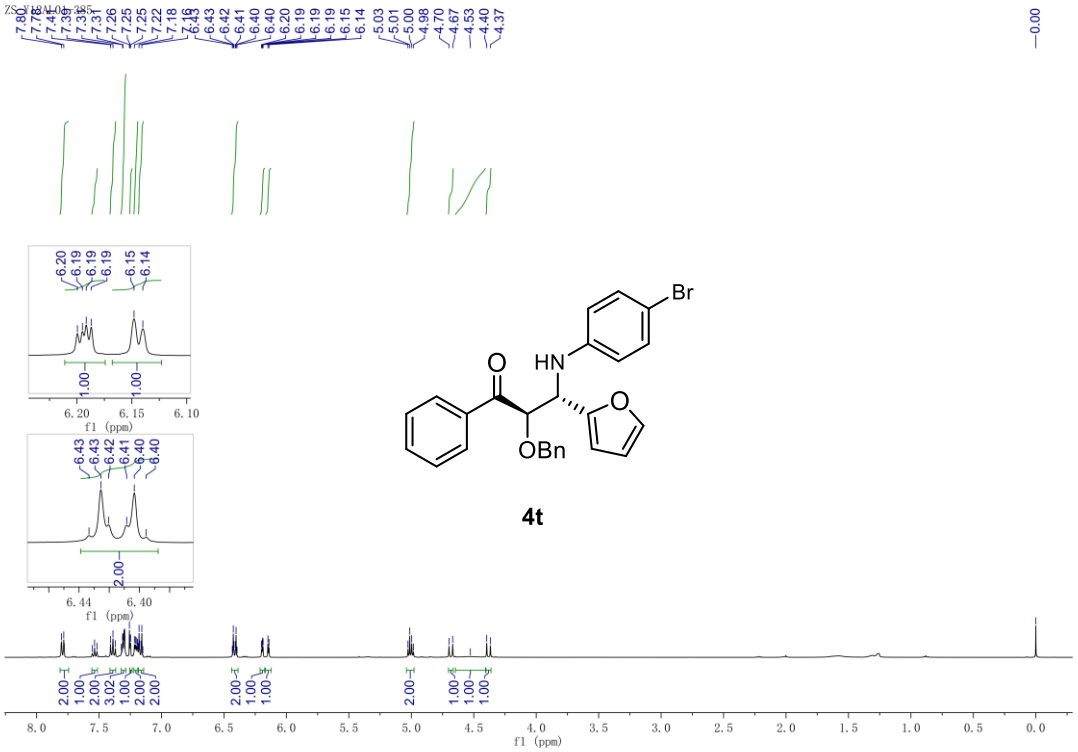


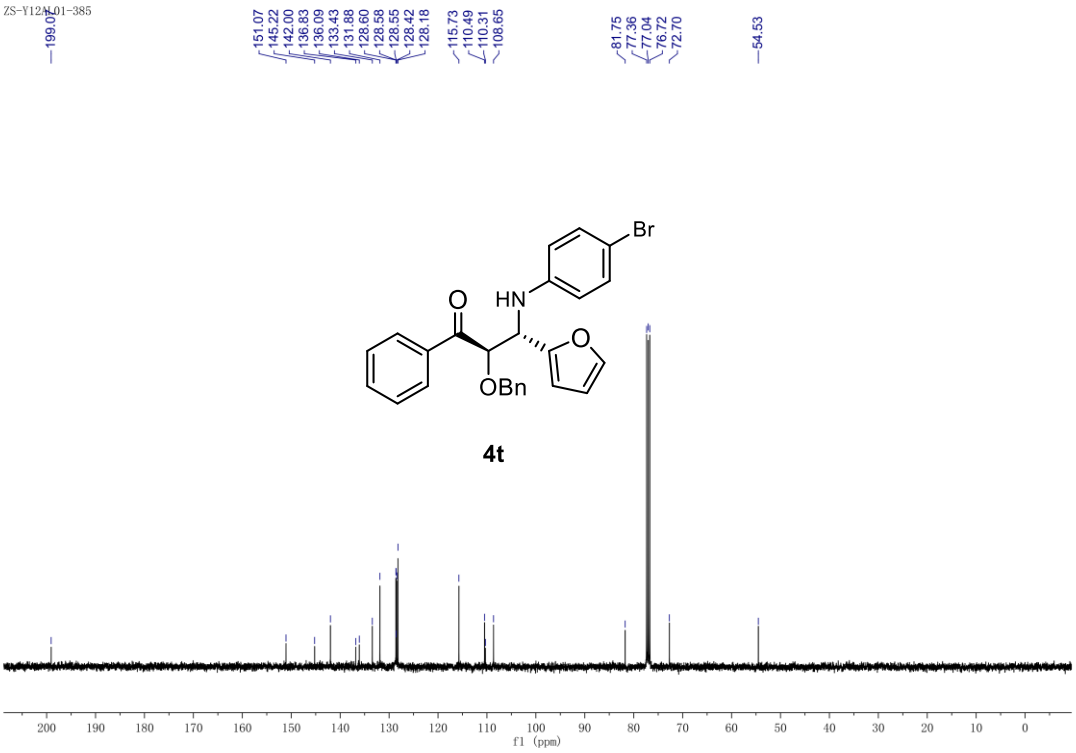
4r

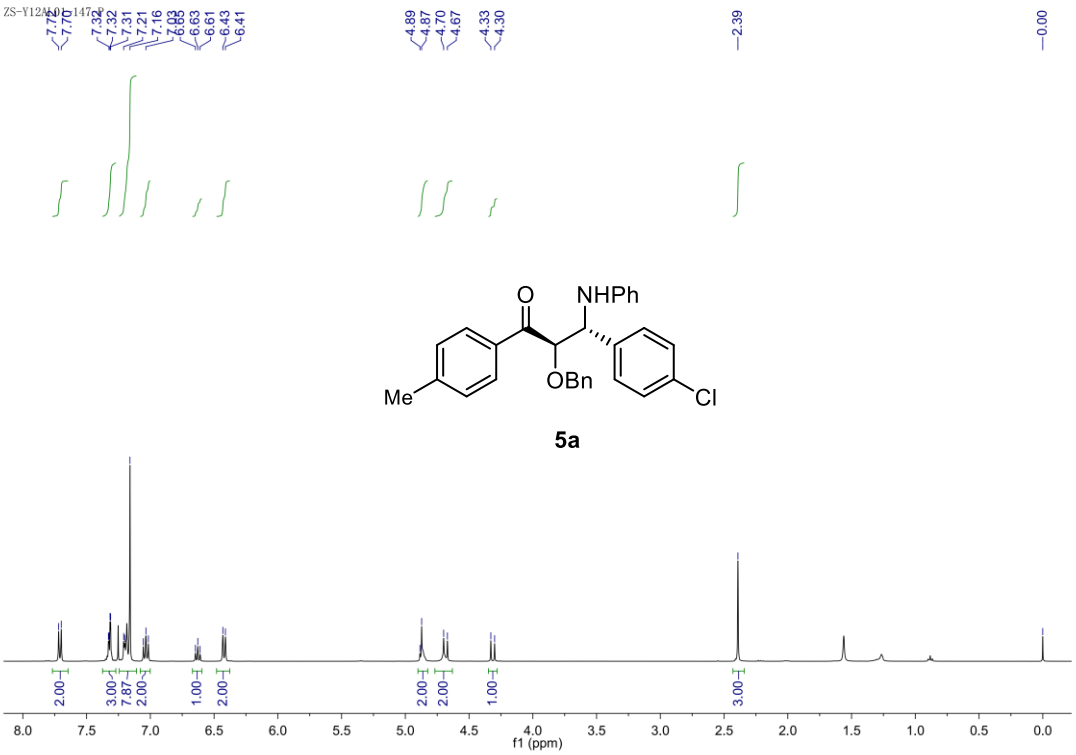


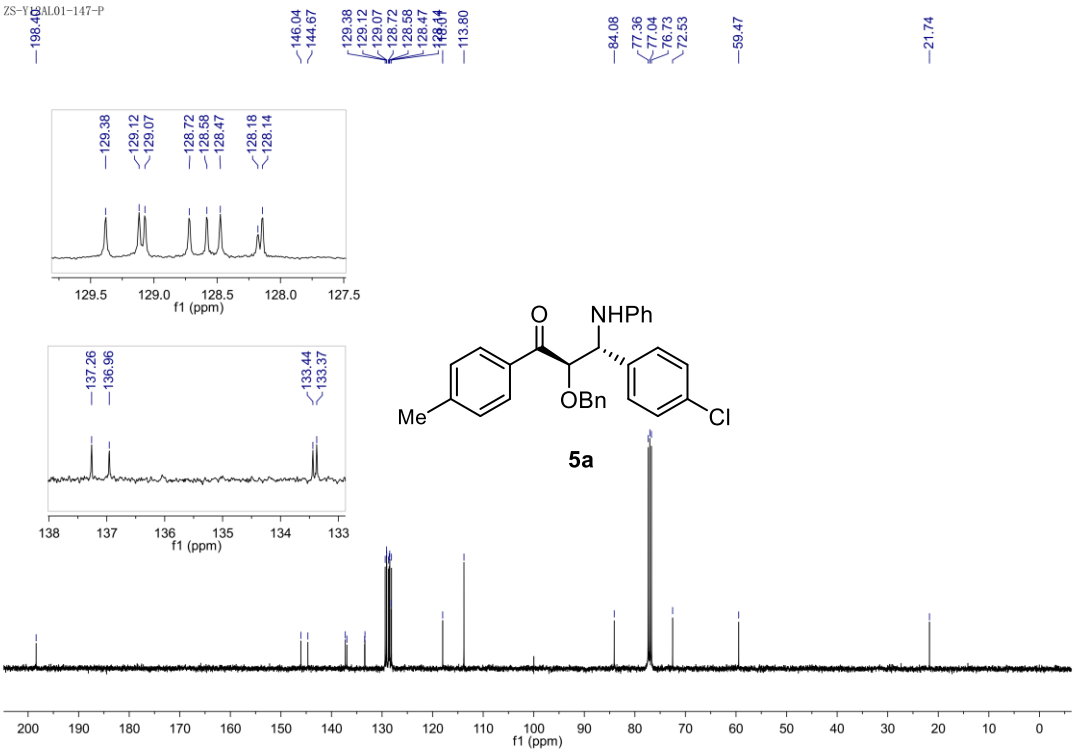
4s


ZS-T358-C
199.21
147.75
147.09
146.28
136.18
133.35
129.07
128.55
128.13
127.15
117.86
113.85
107.97
107.95
100.92
84.17
77.35
77.03
76.71
72.59
59.73
O
NHPh
OBn
O
O
4s
f1 (ppm)

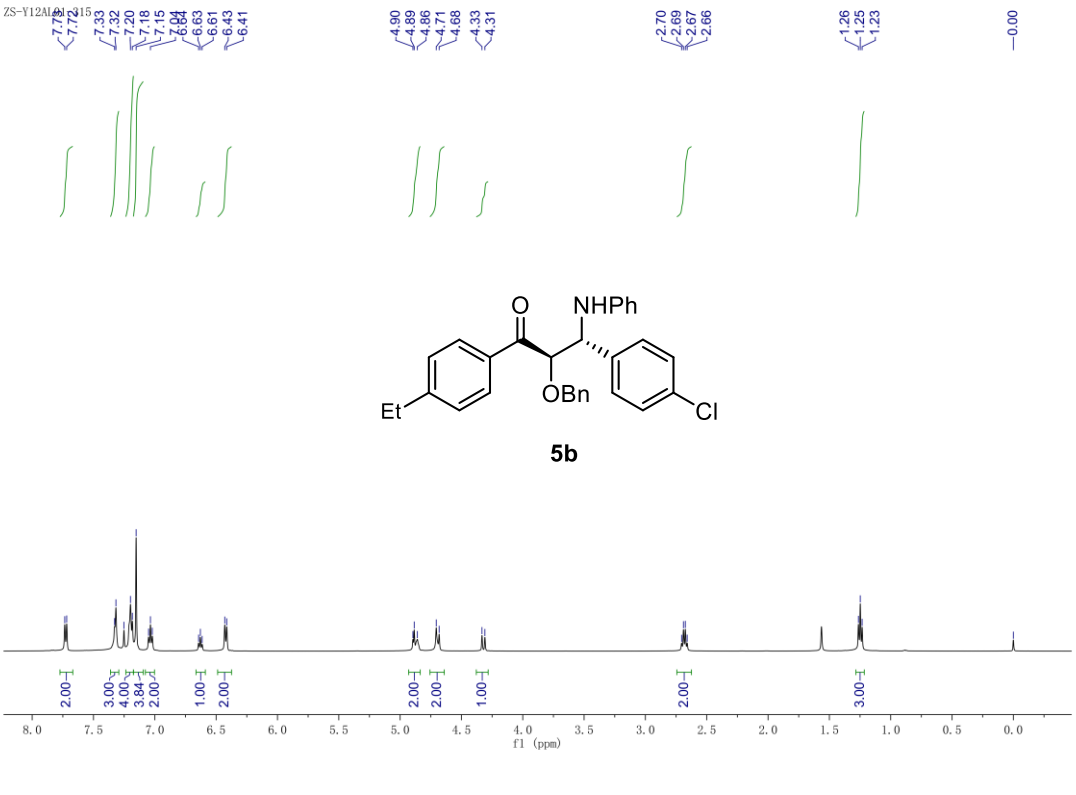

7.80
7.78
7.44
7.36
7.33
7.31
7.26
7.25
7.25
7.22
7.18
6.43
6.42
6.41
6.40
6.40
6.20
6.19
6.19
6.19
6.15
6.14
5.03
5.01
5.00
4.98
4.70
4.67
4.53
4.40
4.37
0.00
6.20
6.19
6.19
6.19
6.15
6.14
1.00
1.00
f1 (ppm)
6.43
6.43
6.42
6.42
6.41
6.40
6.40
6.40
2.00
f1 (ppm)
Br
HN
O
O
OBn
4t
2.00
1.00
2.00
3.02
1.00
2.00
2.00
2.00
1.00
1.00
2.00
1.00
1.00
1.00
f1 (ppm)


ZS-Y12A-01-385
199.07
151.07
145.22
142.00
136.83
136.09
133.43
131.88
128.60
128.58
128.55
128.42
128.18
115.73
110.49
110.31
108.65
81.75
77.36
77.04
76.72
72.70
54.53
Br
HN
O
O
OBn
4t
f1 (ppm)

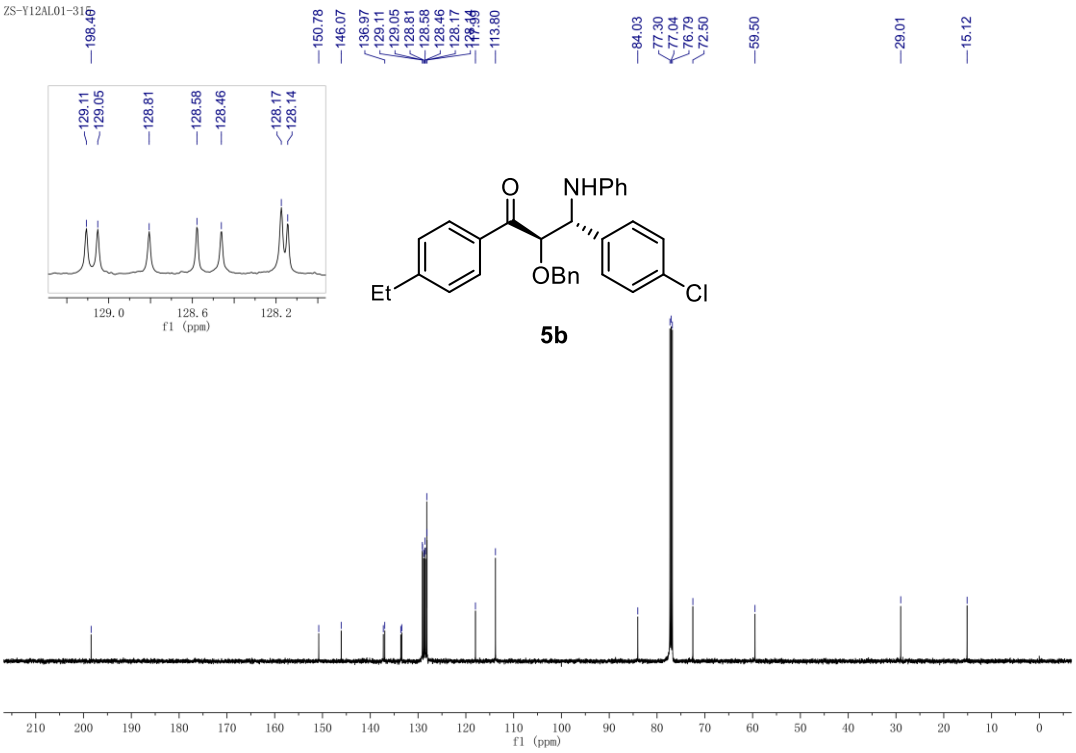

ZS-Y12A-01-147-P
7.77
7.77
7.32
7.32
7.31
7.21
7.16
6.63
6.61
6.43
6.41
4.89
4.87
4.70
4.67
4.33
4.30
2.39
0.00
O
NHPh
OBn
Me
Cl
5a
2.00
3.00
7.87
2.00
1.00
2.00
2.00
2.00
1.00
3.00
f1 (ppm)

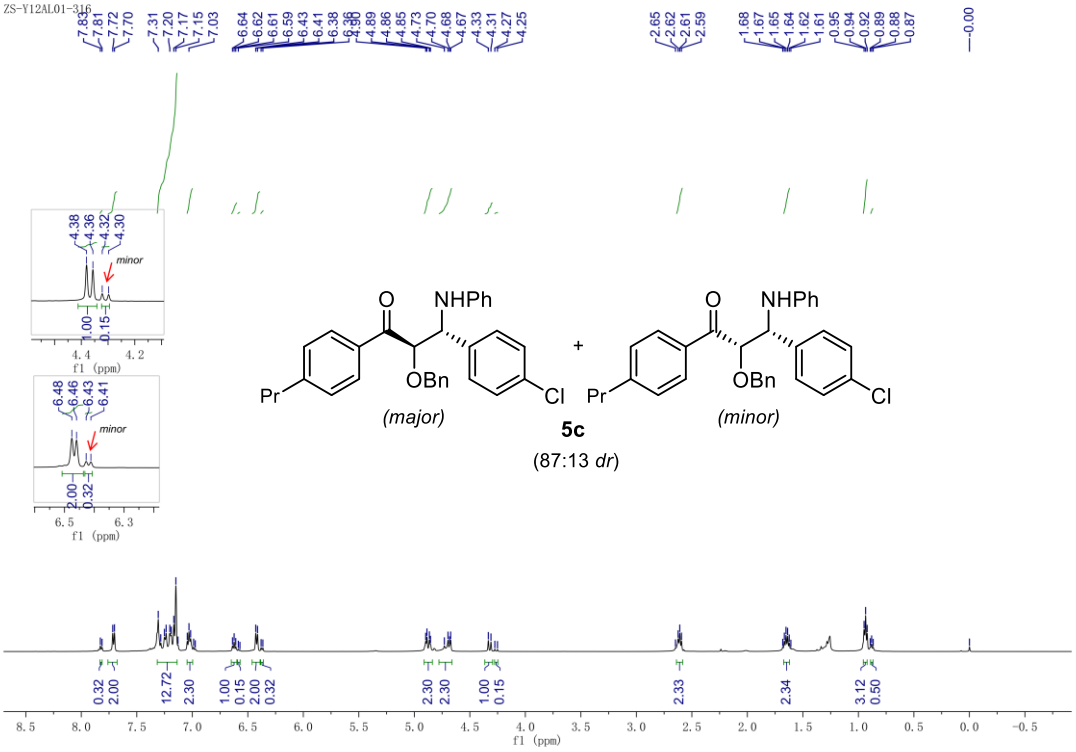

198.40
146.04
144.67
129.38
129.12
129.07
128.72
128.58
128.47
128.18
128.14
113.80
84.08
77.36
77.04
76.73
72.53
59.47
21.74
f1 (ppm)
O
NHPh
OBn
Me
Cl

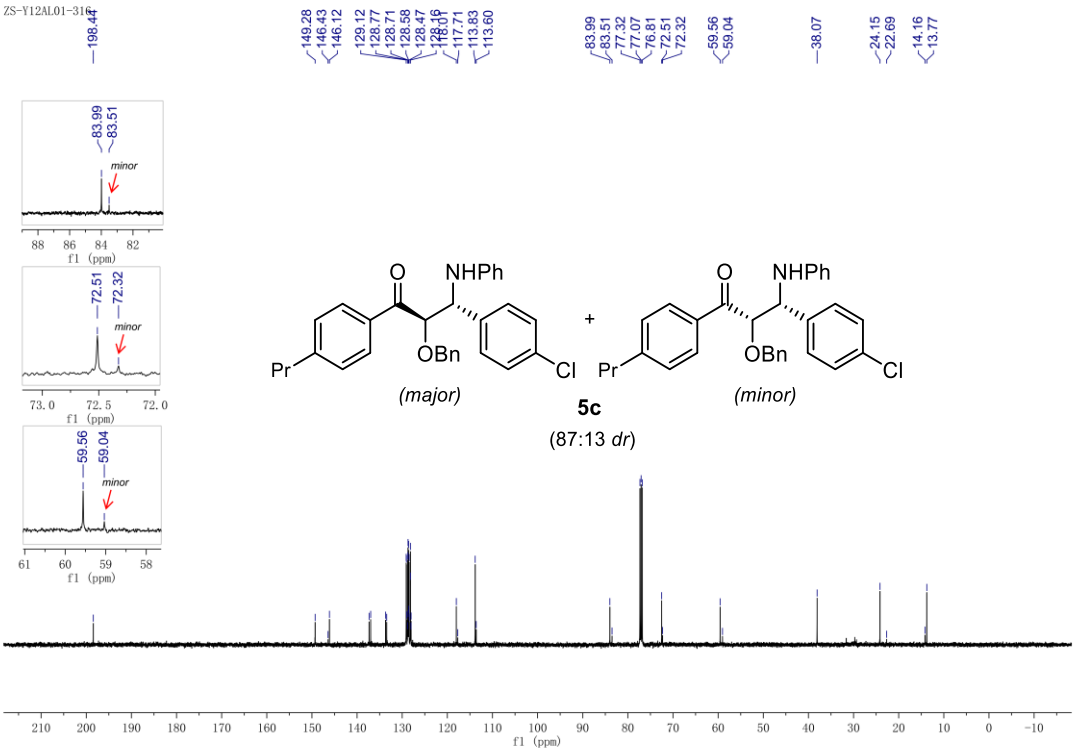
5a


7.73
7.72
7.33
7.32
7.20
7.18
7.15
7.04
6.64
6.63
6.61
6.43
6.41
4.90
4.89
4.86
4.71
4.68
4.33
4.31
2.70
2.69
2.67
2.66
1.26
1.25
1.23
0.00
2.00
3.00
4.00
3.84
2.00
1.00
2.00
2.00
2.00
1.00
2.00
3.00
f1 (ppm)
O
NHPh
OBn
Et
Cl

5b

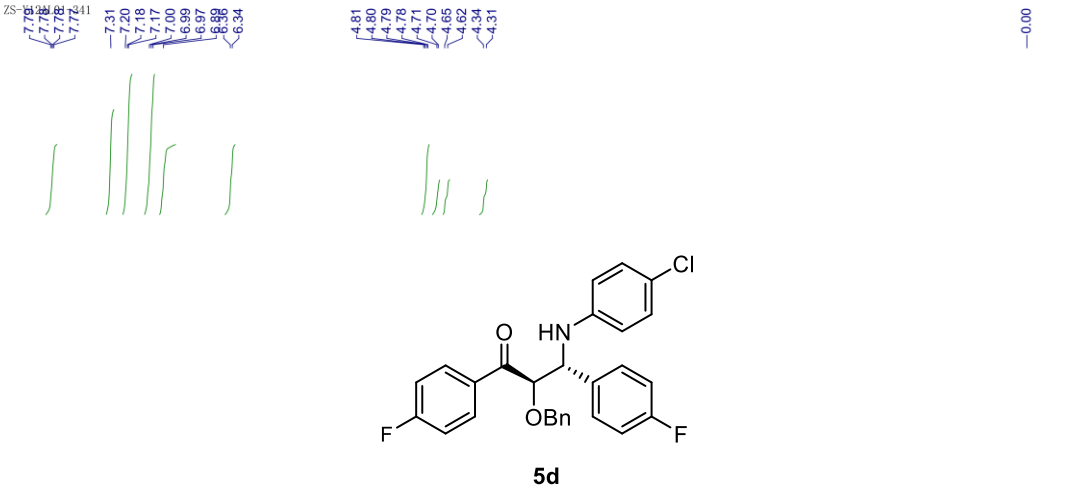

ZS-Y12AL01-316
198.46
150.78
146.07
136.97
129.11
129.05
128.81
128.58
128.46
128.17
128.14
113.80
84.03
77.30
77.04
76.79
72.50
59.50
29.01
15.12
129.11
129.05
128.81
128.58
128.46
128.17
128.14
129.0
128.6
128.2
f1 (ppm)
O
NHPh
OBn
Et
Cl
5b
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


ZS-Y12AL01-316
7.83
7.81
7.72
7.70
7.31
7.20
7.17
7.15
7.03
6.64
6.62
6.61
6.59
6.43
6.41
6.38
4.89
4.86
4.85
4.73
4.70
4.68
4.67
4.33
4.31
4.27
4.25
2.65
2.62
2.61
2.59
1.68
1.67
1.65
1.64
1.62
1.61
0.95
0.94
0.92
0.89
0.88
0.87
0.00
4.38
4.36
4.32
4.30
minor
1.00
0.15
4.4
4.2
f1 (ppm)
6.48
6.46
6.43
6.41
minor
2.00
0.32
6.5
6.3
f1 (ppm)
O
NHPh
OBn
Pr
Cl
(major)
+
(minor)
5c
(87:13 dr)
0.32
2.00
12.72
2.30
1.00
0.15
2.00
0.32
2.30
2.30
1.00
0.15
2.33
2.34
3.12
0.50
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)


ZS-Y12AL01-316
198.44
149.28
146.43
146.12
129.12
128.77
128.71
128.58
128.47
128.16
128.01
117.71
113.83
113.60
83.99
83.51
77.32
77.07
76.81
72.51
72.32
59.56
59.04
38.07
24.15
22.69
14.16
13.77
minor
f1 (ppm)
O
NHPh
OBn
Pr
Cl
(major)
+
(minor)

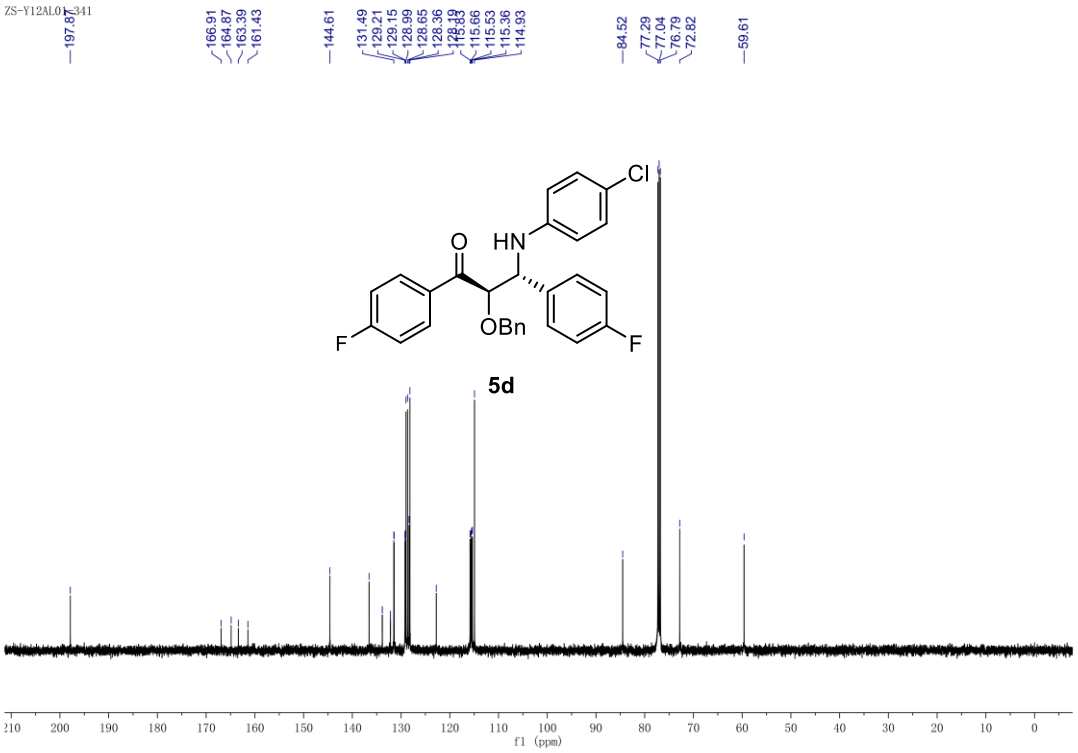
5c

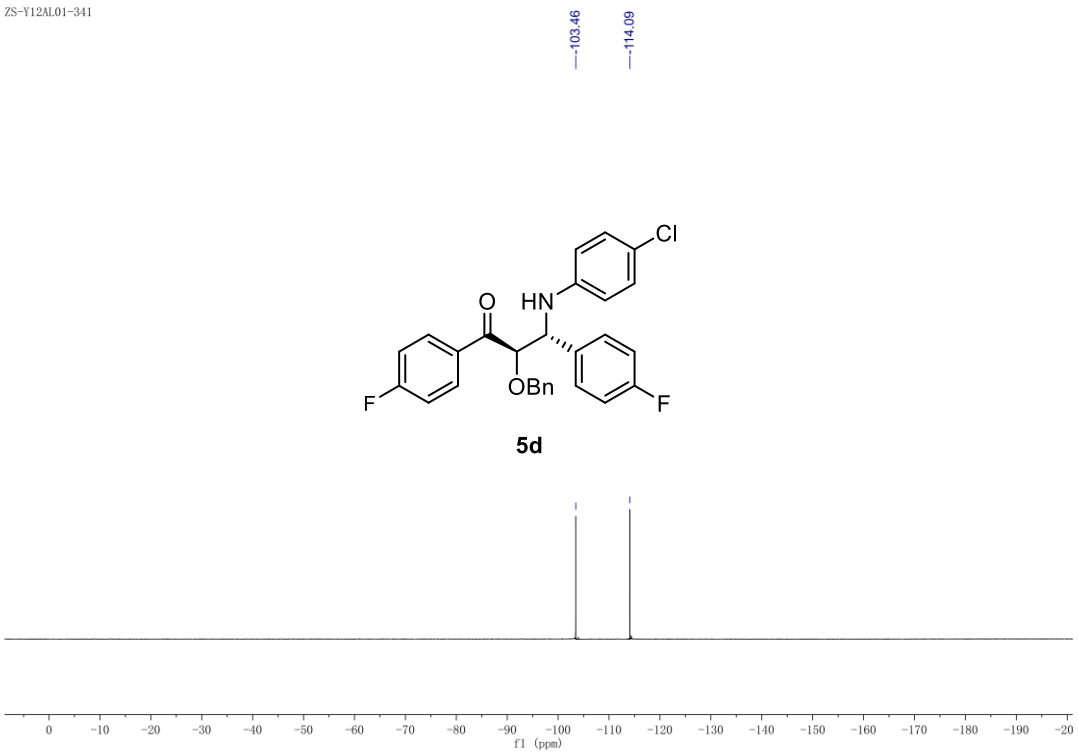
(87:13 *dr*)

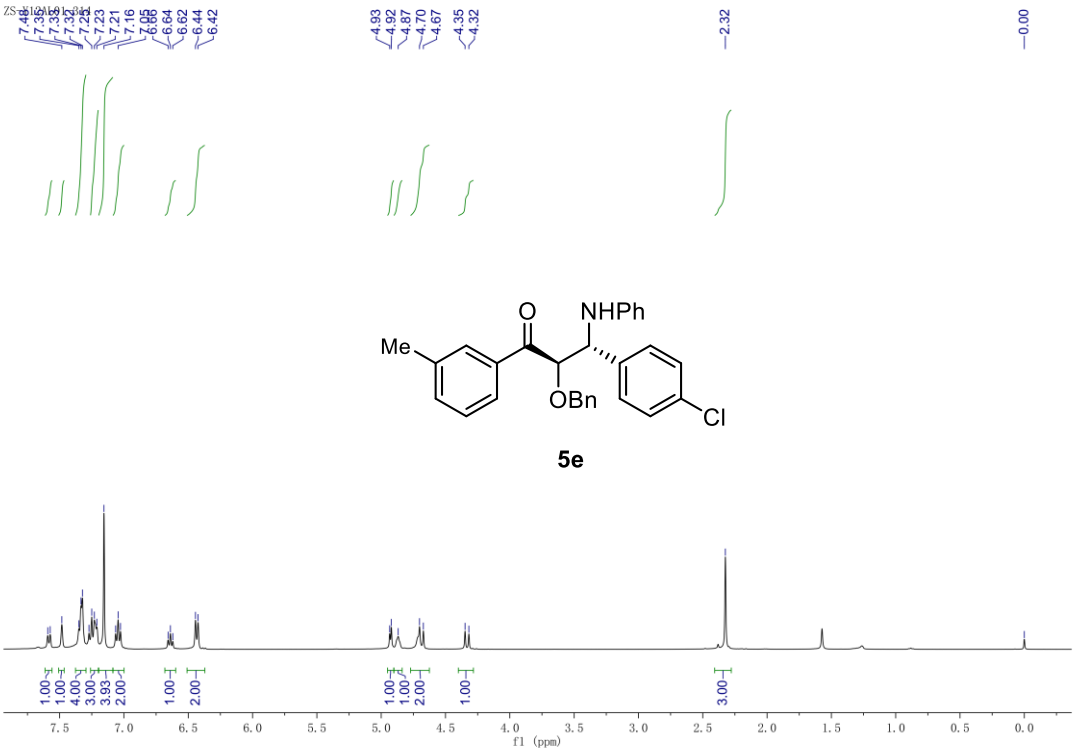

7.31
7.20
7.18
7.17
7.00
6.99
6.97
6.34
4.81
4.80
4.79
4.78
4.71
4.70
4.65
4.62
4.34
4.31
0.00
2.00
3.00
4.00
4.00
2.00
2.00
2.00
1.00
1.00
f1 (ppm)

Cl
O
HN
OBn
F
F

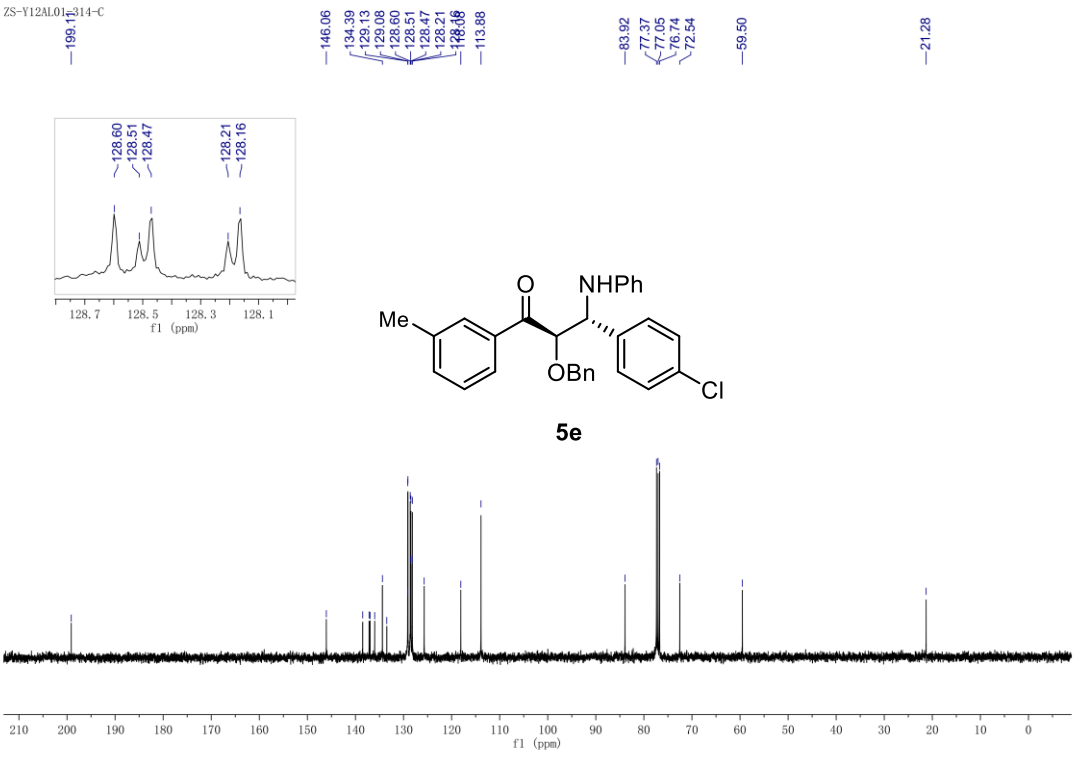
5d


ZS-Y12AL01-341
197.87
166.91
164.87
163.39
161.43
144.61
131.49
129.21
129.15
128.99
128.65
128.36
115.66
115.53
115.36
114.93
84.52
77.29
77.04
76.79
72.82
59.61
Cl
O
HN
OBn
F
F
5d
f1 (ppm)

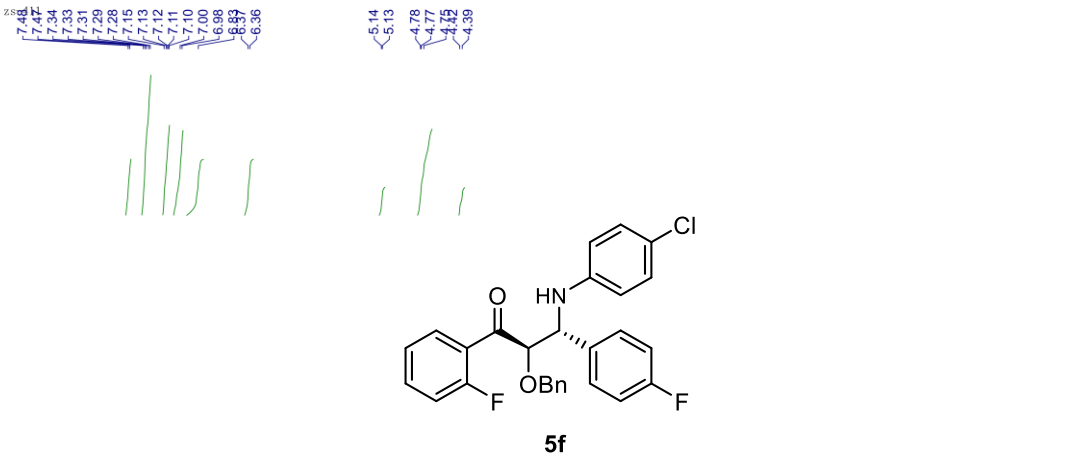

ZS-Y12AL01-341
103.46
114.09
Cl
O
HN
OBn
F
F
5d
f1 (ppm)

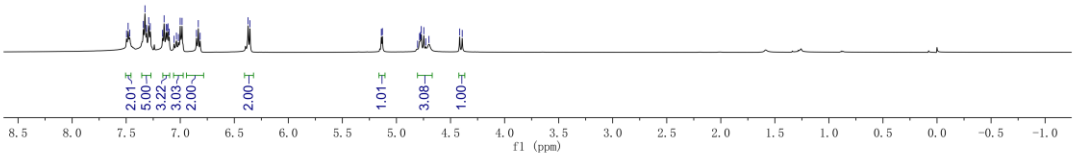

7.46
7.36
7.33
7.32
7.29
7.23
7.21
7.16
7.05
6.66
6.64
6.62
6.44
6.42
4.93
4.92
4.87
4.70
4.67
4.35
4.32
2.32
0.00
O
NHPh
Me
OBn
Cl
1.00
1.00
4.00
3.00
3.93
2.00
1.00
2.00
1.00
1.00
2.00
1.00
3.00
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

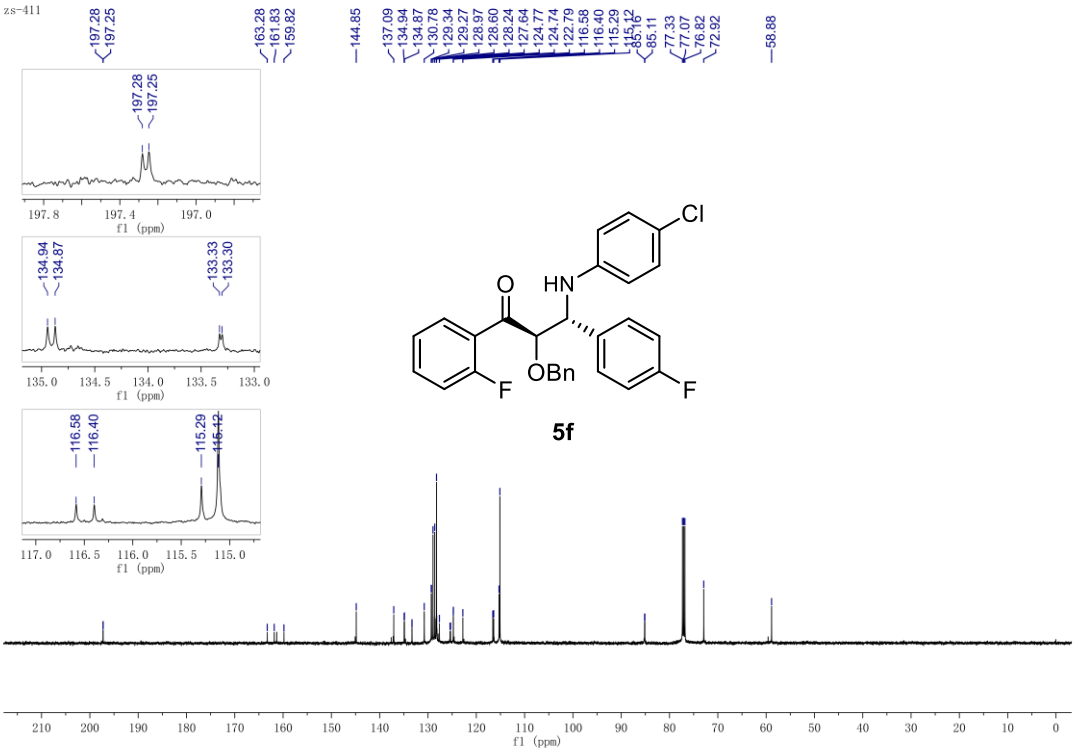
5e


ZS-Y12AL01-314-C
199.11
146.06
134.39
129.13
129.08
128.60
128.51
128.47
128.21
128.16
113.88
83.92
77.37
77.05
76.74
72.54
59.50
21.28
128.60
128.51
128.47
128.21
128.16
128.7
128.5
128.3
128.1
f1 (ppm)
O
NHPh
Me
OBn
Cl
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

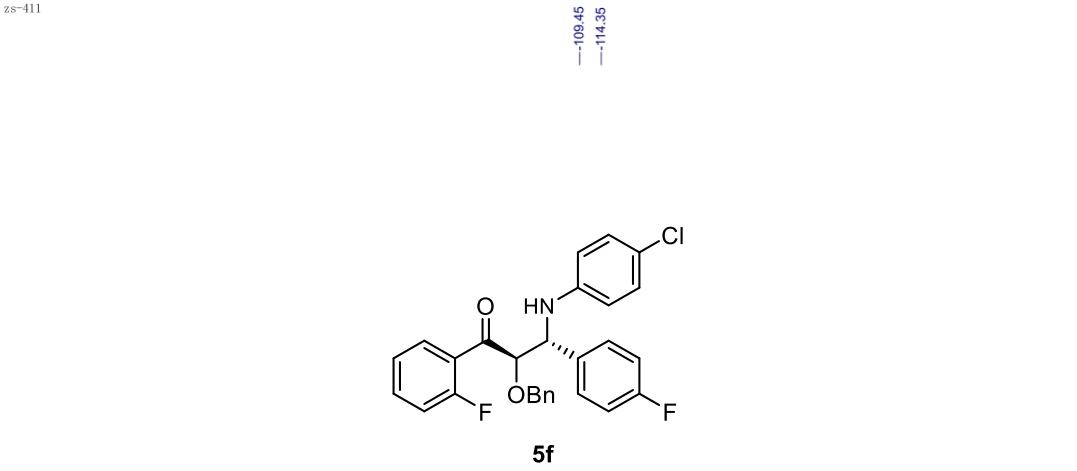
5e


Cl
HN
O
OBn
F
F
5f



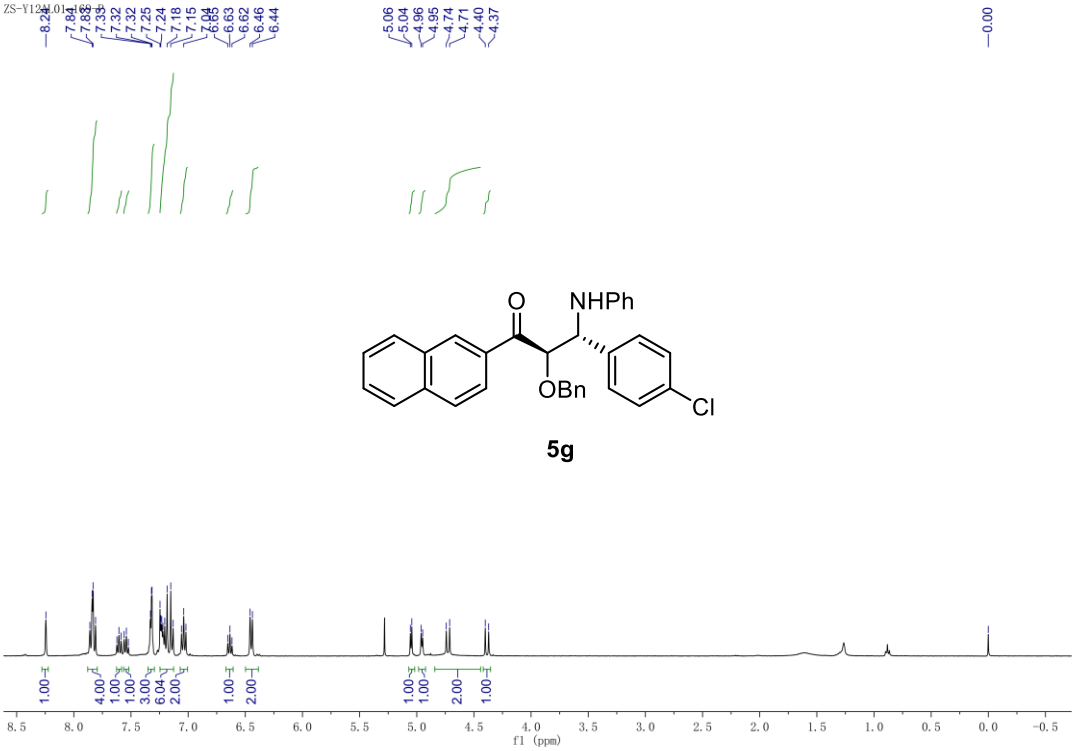

Cl
HN
O
OBn
F
F
5f

zs-411

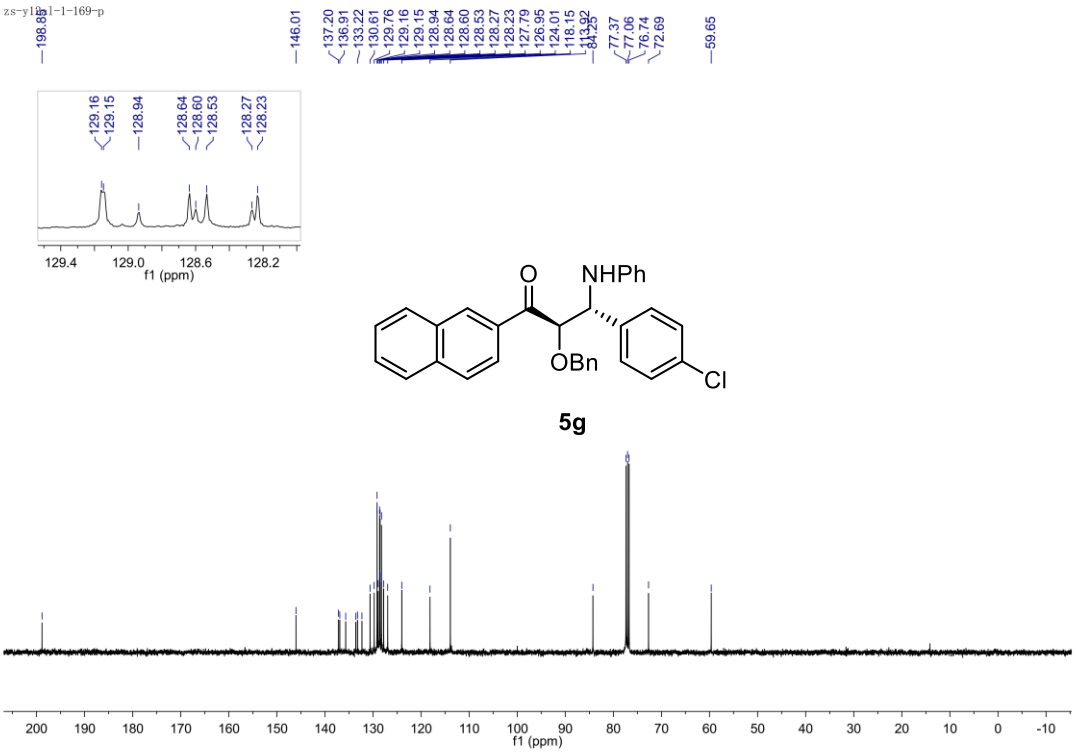


5f

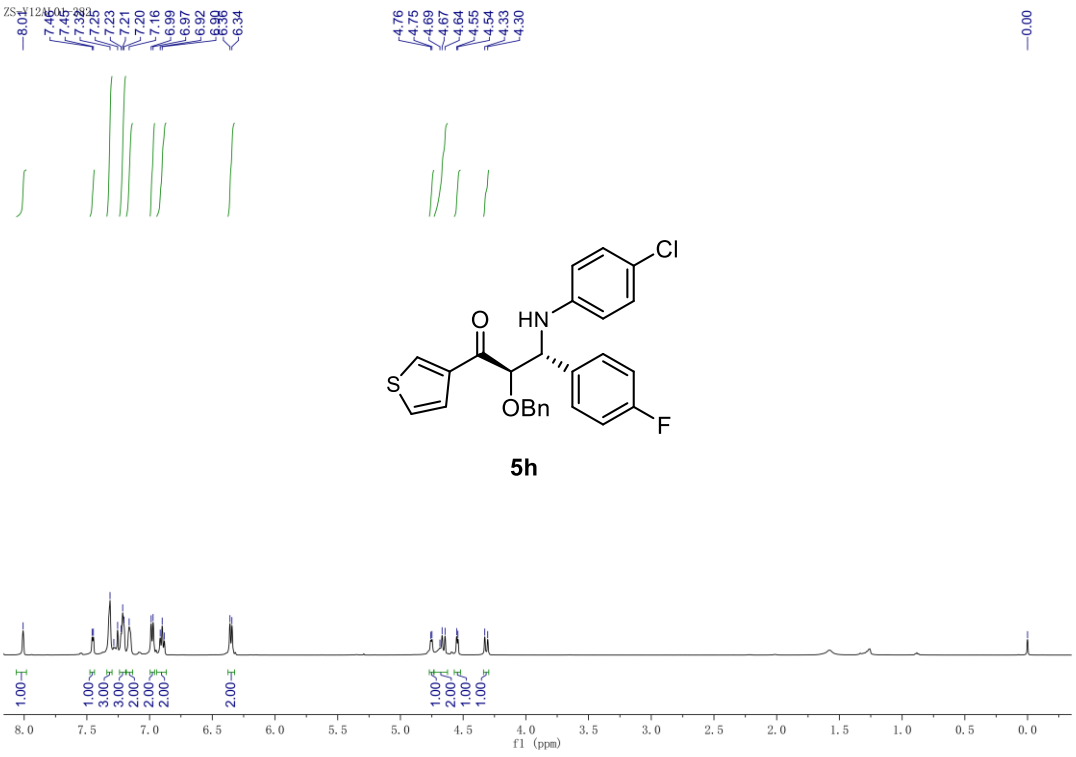
ZS-Y12M01-100-D



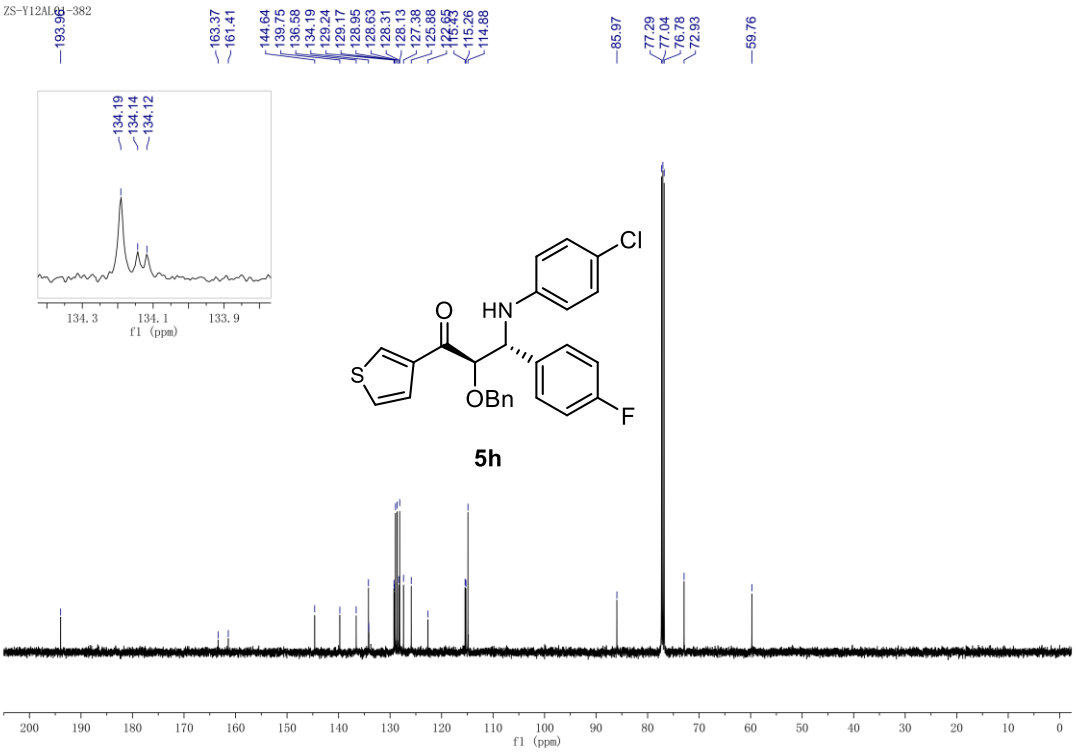
5g

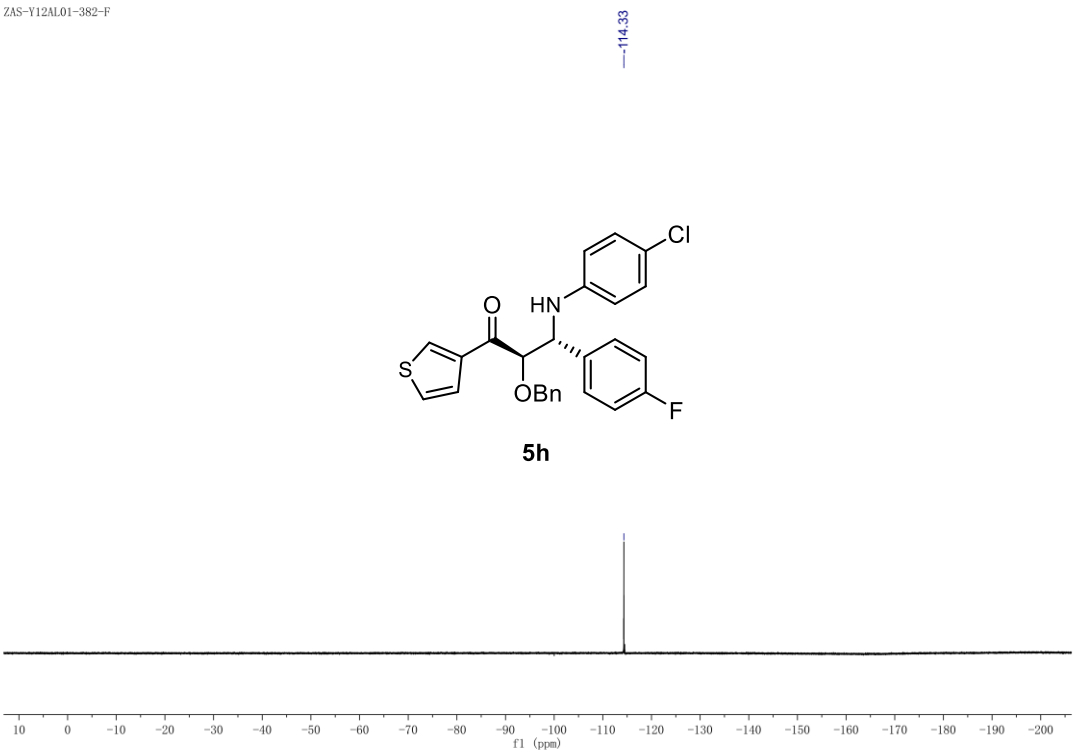

zs-y1
198.88
146.01
137.20
136.91
133.22
130.61
129.76
129.16
129.15
128.94
128.64
128.60
128.53
128.27
128.23
127.79
126.95
124.01
118.15
113.92
84.25
77.37
77.06
76.74
72.69
59.65
129.4
129.0
128.6
128.2
f1 (ppm)
O
NHPh
OBn
Cl
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

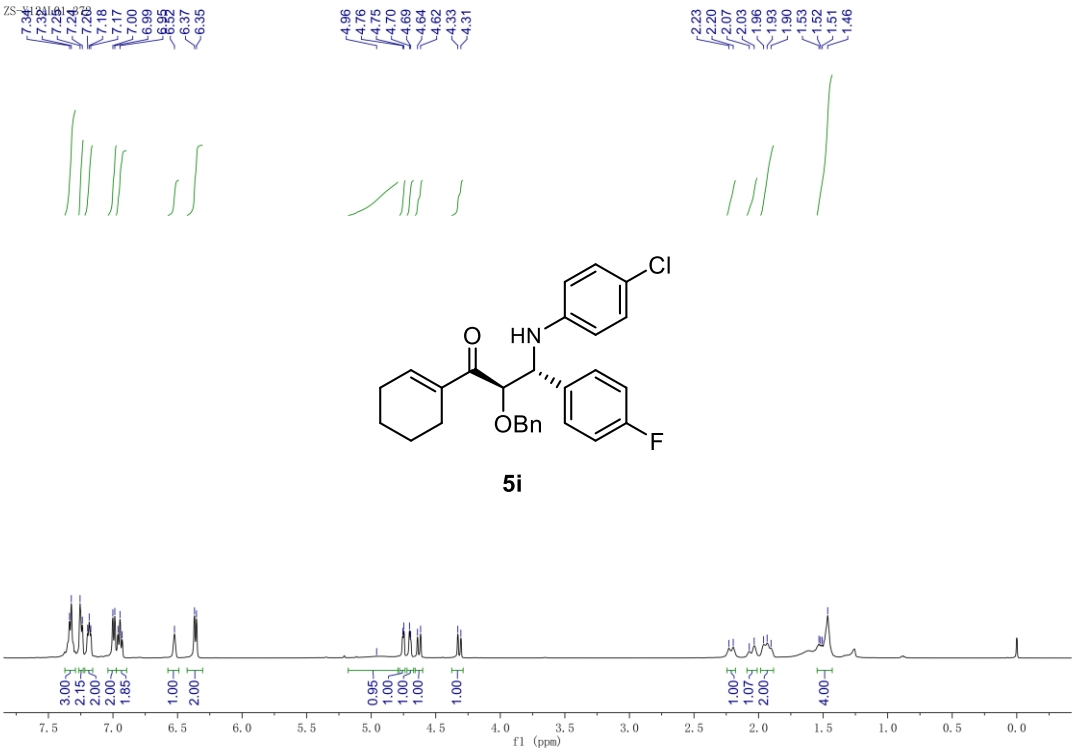
5g

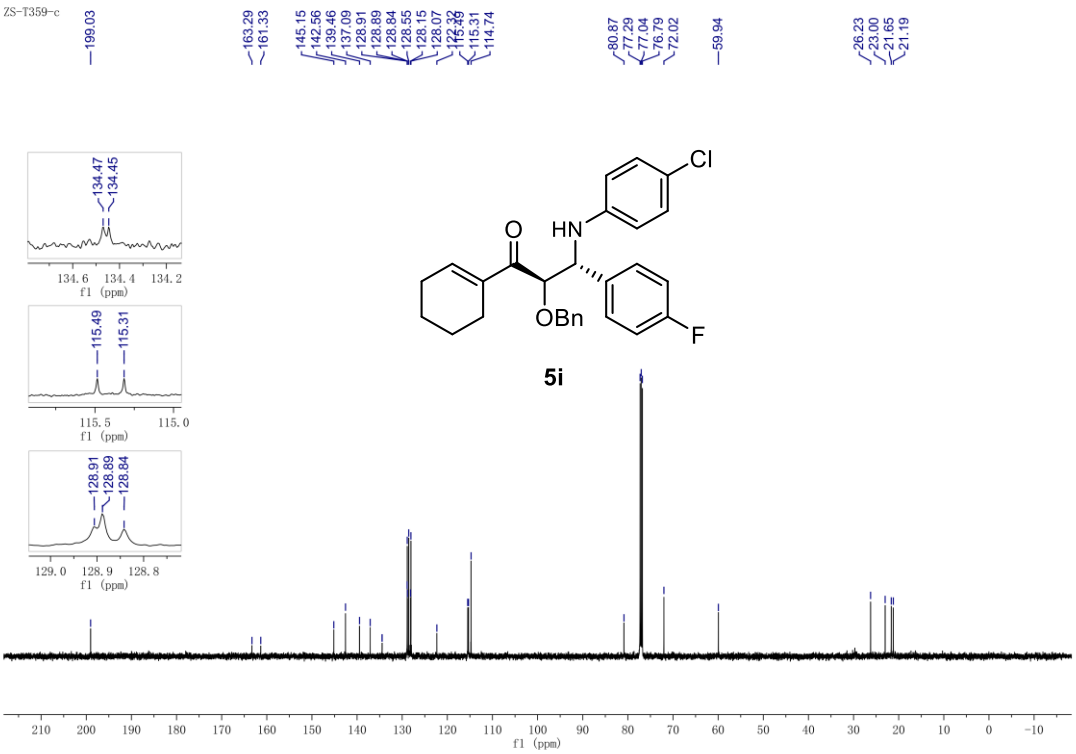

8.01
7.46
7.45
7.38
7.25
7.23
7.21
7.20
7.16
6.99
6.97
6.92
6.90
6.36
6.34
4.76
4.75
4.69
4.67
4.64
4.55
4.54
4.33
4.30
0.00
Cl
O
HN
S
OBn
F
1.00
3.00
2.00
2.00
2.00
1.00
2.00
1.00
1.00
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

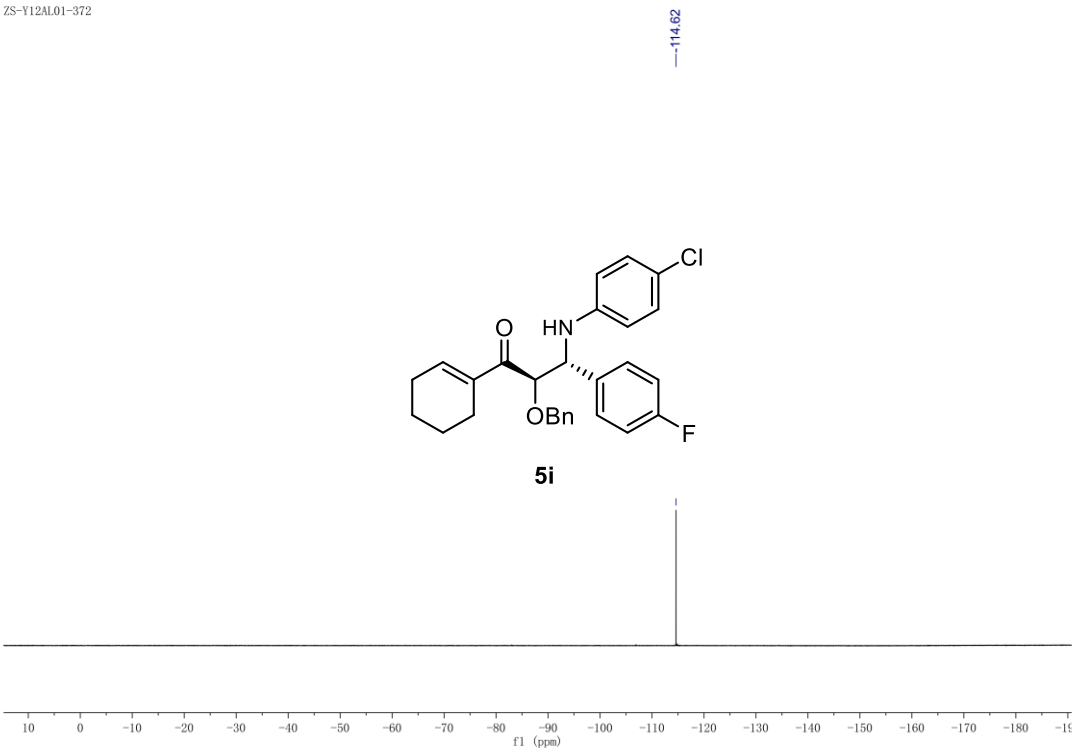
5h


ZS-Y12AL01-382
193.96
163.37
161.41
144.64
139.75
136.58
134.19
129.24
129.17
128.95
128.63
128.31
128.13
127.38
125.88
115.26
114.88
85.97
77.29
77.04
76.78
72.93
59.76
134.19
134.14
134.12
134.3
134.1
133.9
f1 (ppm)
Cl
HN
O
S
OBn
F
5h
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

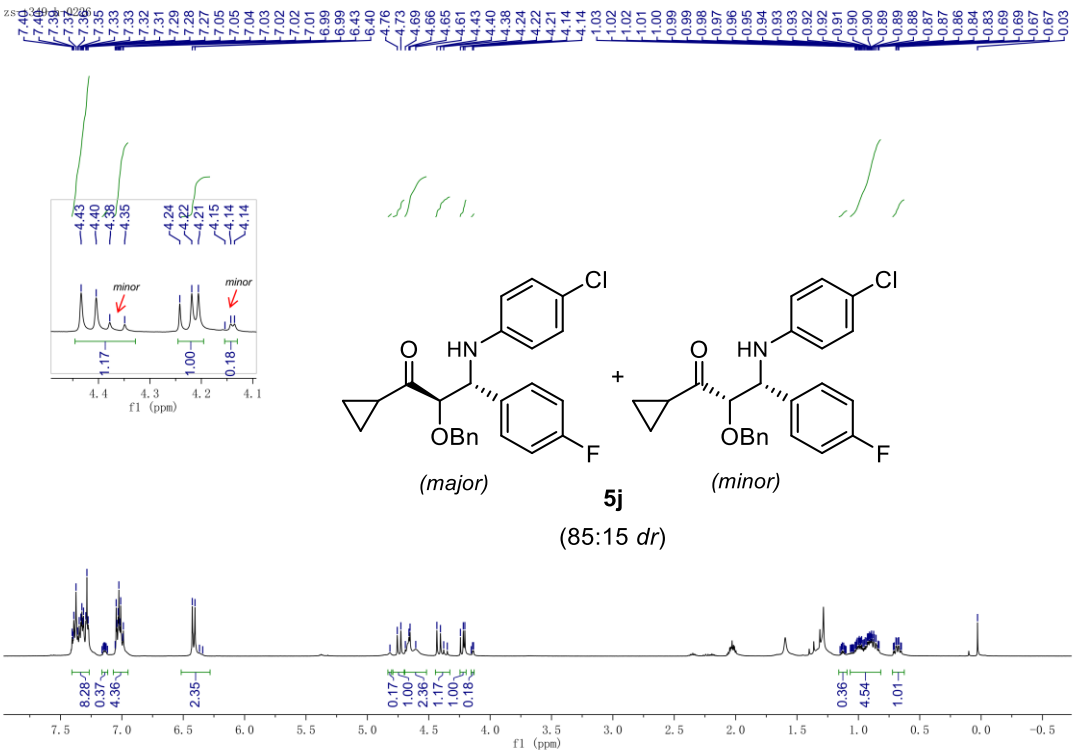

ZAS-Y12AL01-382-F
114.33
Cl
HN
O
S
OBn
F
5h
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
f1 (ppm)


7.34
7.32
7.26
7.24
7.20
7.18
7.17
7.00
6.99
6.95
6.52
6.37
6.35
4.96
4.76
4.75
4.70
4.69
4.64
4.62
4.33
4.31
2.23
2.20
2.07
2.03
1.96
1.93
1.90
1.53
1.52
1.51
1.46
Cl
HN
O
OBn
F
5i
3.00
2.15
2.00
2.00
1.85
1.00
2.00
0.95
1.00
1.00
1.00
1.00
1.00
1.07
2.00
4.00
f1 (ppm)


ZS-T359-c
199.03
163.29
161.33
145.15
142.56
139.46
137.09
128.91
128.89
128.84
128.55
128.15
128.07
115.49
115.31
114.74
80.87
77.29
77.04
76.79
72.02
59.94
26.23
23.00
21.65
21.19
134.47
134.45
115.49
115.31
128.91
128.89
128.84
Cl
HN
O
OBn
F
5i
f1 (ppm)

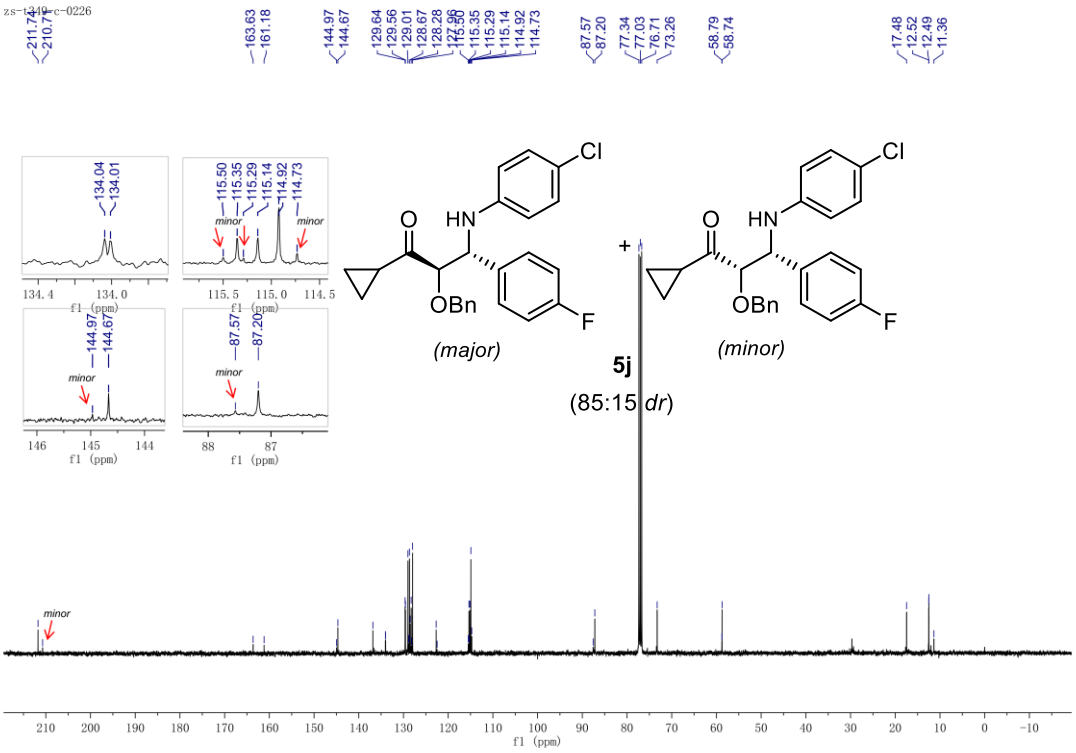


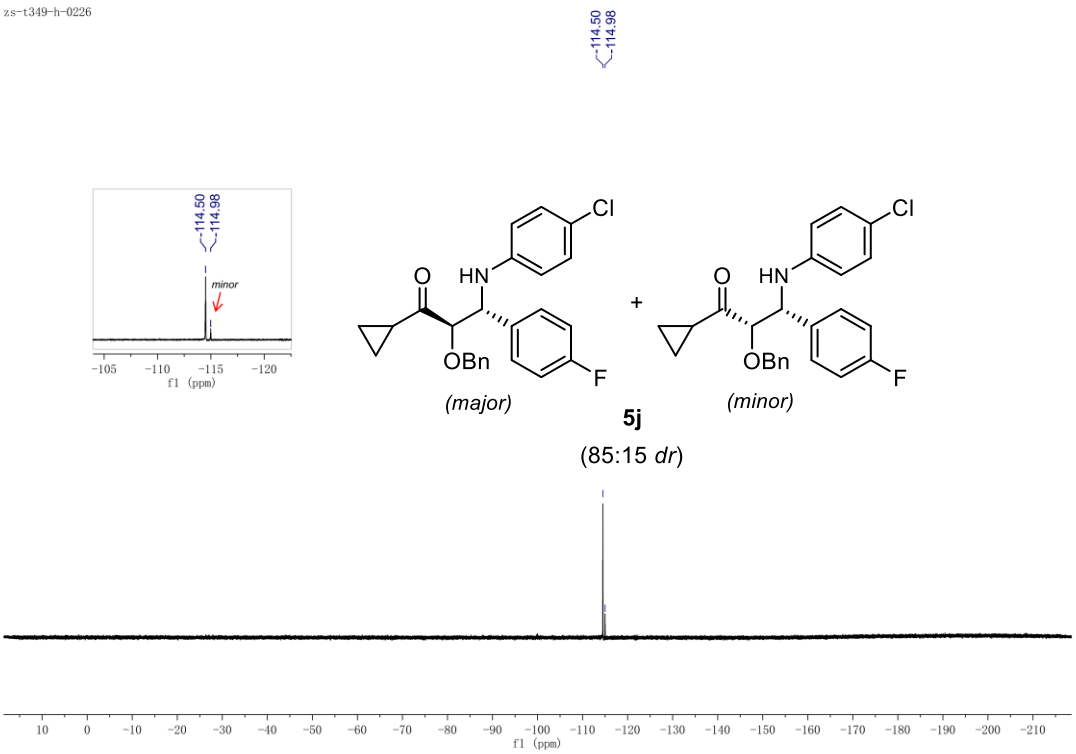
5i

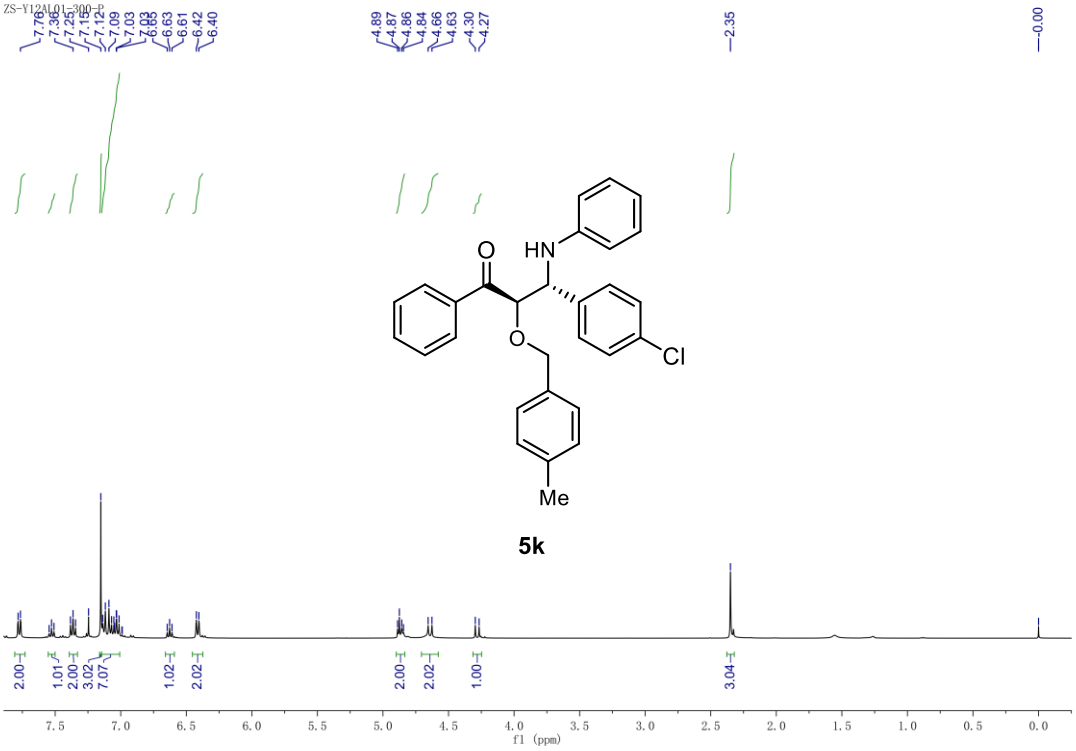


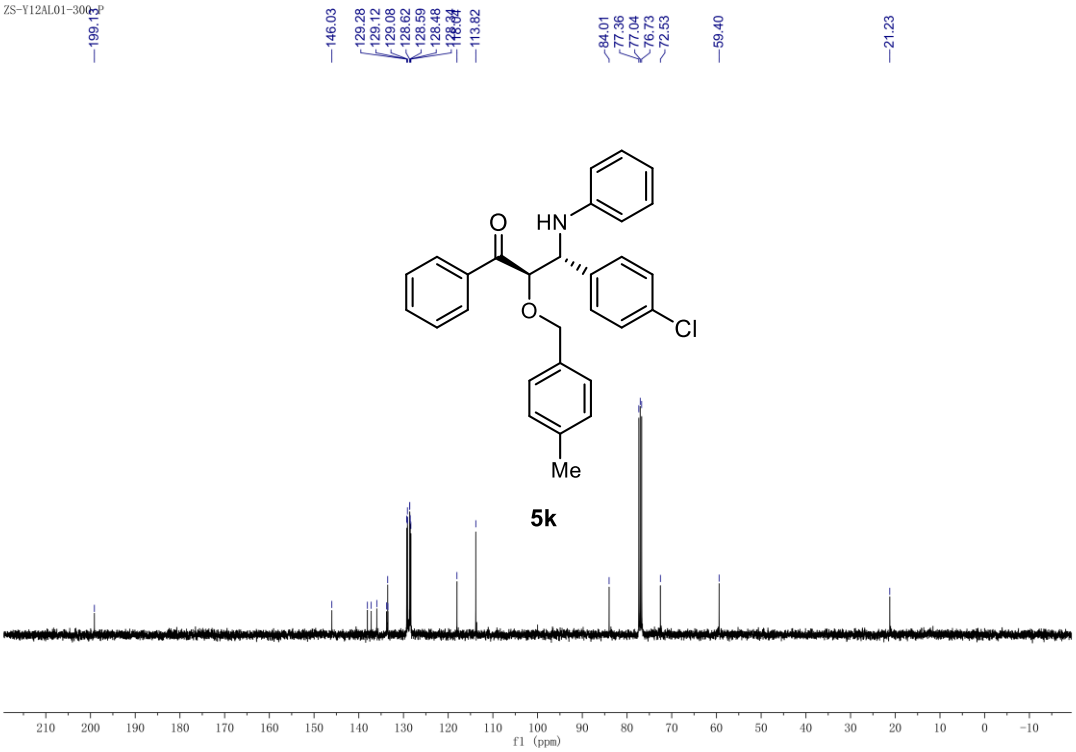
(major) **5j** *(minor)*

(85:15 *dr*)

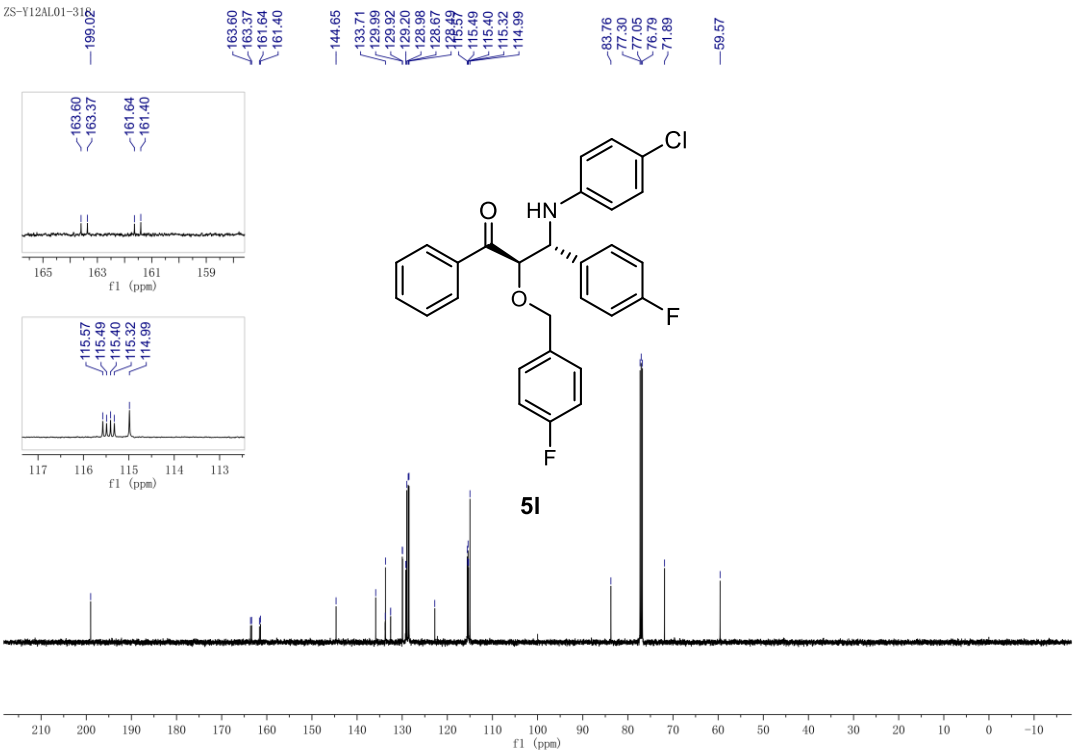

zs-t349-c-0226
211.74
210.71
163.63
161.18
144.97
144.67
129.64
129.56
129.01
128.67
128.28
127.96
115.50
115.35
115.29
115.14
114.92
114.73
87.57
87.20
77.34
77.03
76.71
73.26
58.79
58.74
17.48
12.52
12.49
11.36
134.04
134.01
minor
144.97
144.67
87.57
87.20
f1 (ppm)
Cl
O
HN
OBn
F
(major)
+
(minor)
5j
(85:15 dr)


zs-t349-h-0226
114.50
114.98
minor
f1 (ppm)
Cl
O
HN
OBn
F
(major)
+
(minor)
5j
(85:15 dr)

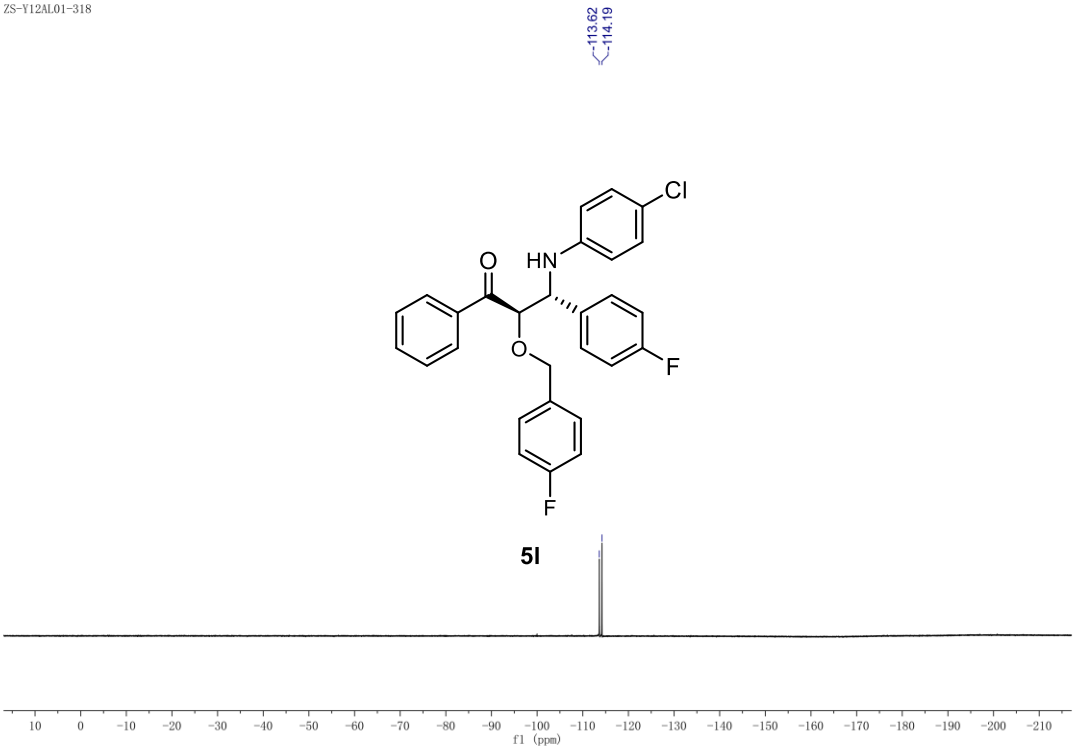

ZS-Y12AL01-300-P
7.76
7.36
7.25
7.15
7.12
7.09
7.03
6.63
6.61
6.42
6.40
4.89
4.87
4.86
4.84
4.66
4.63
4.30
4.27
2.35
0.00
O
HN
Cl
O
Me
5k
2.00
1.01
2.00
3.02
7.07
1.02
2.02
2.00
2.02
1.00
3.04
f1 (ppm)


ZS-Y12AL01-300-P
199.17
146.03
129.28
129.12
129.08
128.62
128.59
128.48
113.82
84.01
77.36
77.04
76.73
72.53
59.40
21.23
O
HN
Cl
O
Me
5k
f1 (ppm)

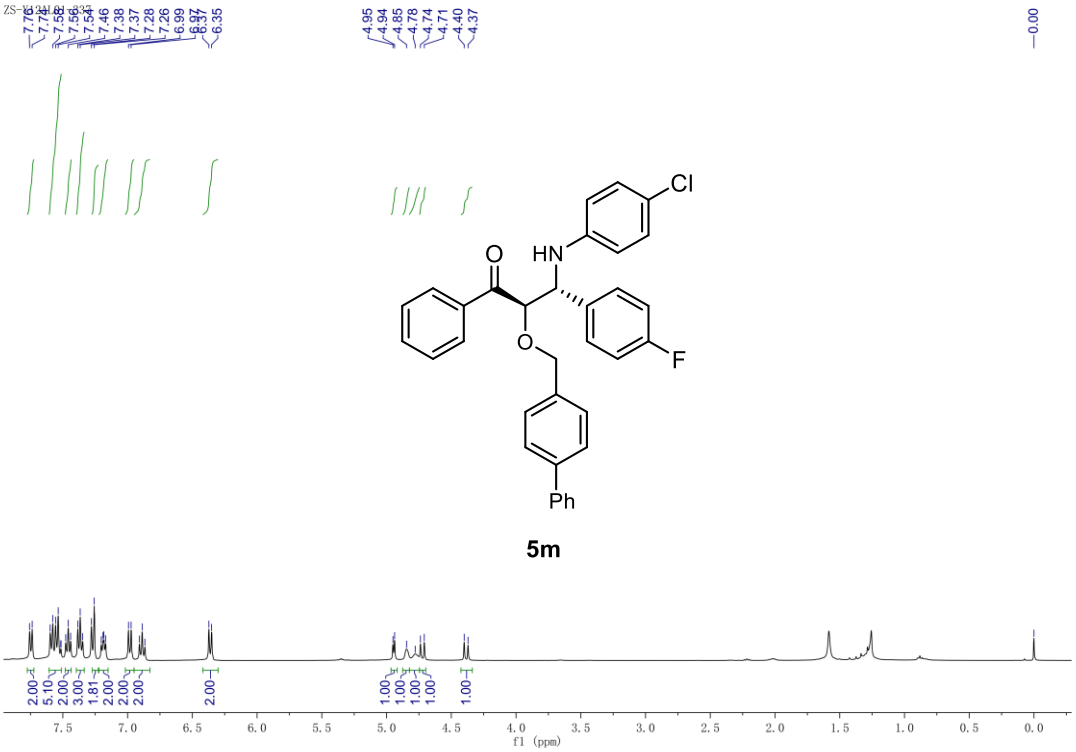

ZS-Y12AL01-318
7.74
7.73
7.38
7.37
7.18
7.16
7.15
7.14
7.01
6.99
6.98
6.36
4.83
4.82
4.75
4.62
4.60
4.33
4.30
0.00
Cl
HN
O
O
F
F
5l
2.00
1.00
2.00
4.00
3.86
2.00
2.00
2.00
0.95
1.00
1.00
f1 (ppm)


ZS-Y12AL01-318
199.02
163.60
163.37
161.64
161.40
144.65
133.71
129.99
129.92
129.20
128.98
128.67
115.49
115.40
115.32
114.99
83.76
77.30
77.05
76.79
71.89
59.57
115.57
f1 (ppm)
Cl
HN
O
O
F
F
5l
f1 (ppm)

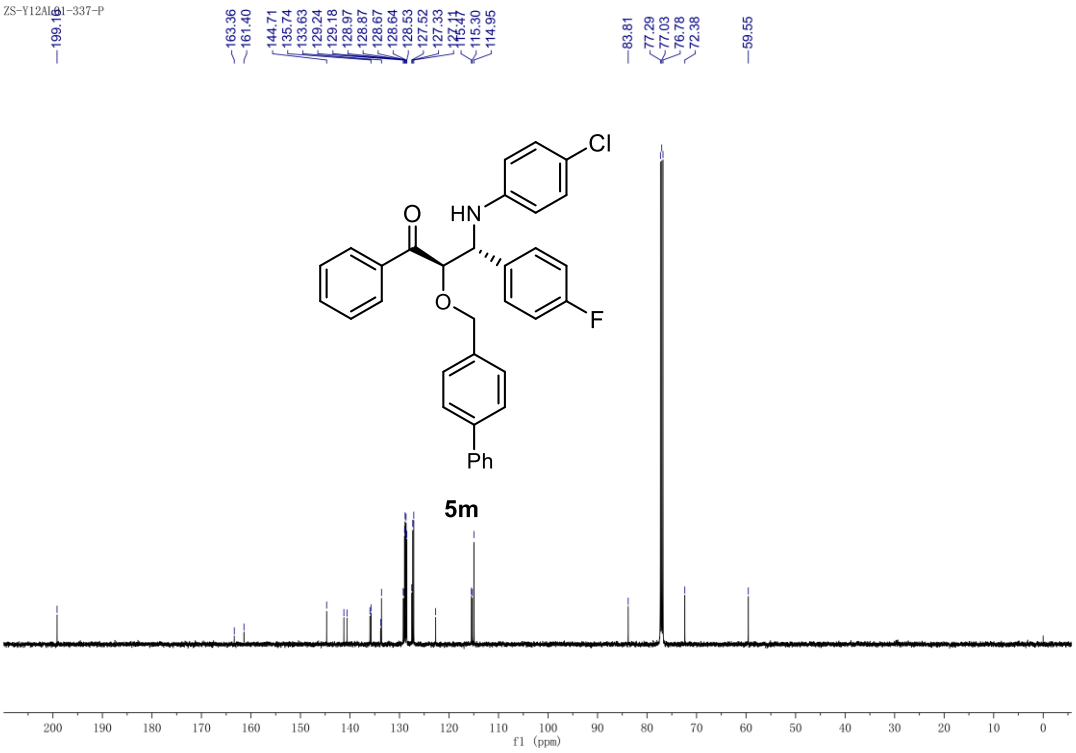
ZS-Y12AL01-318

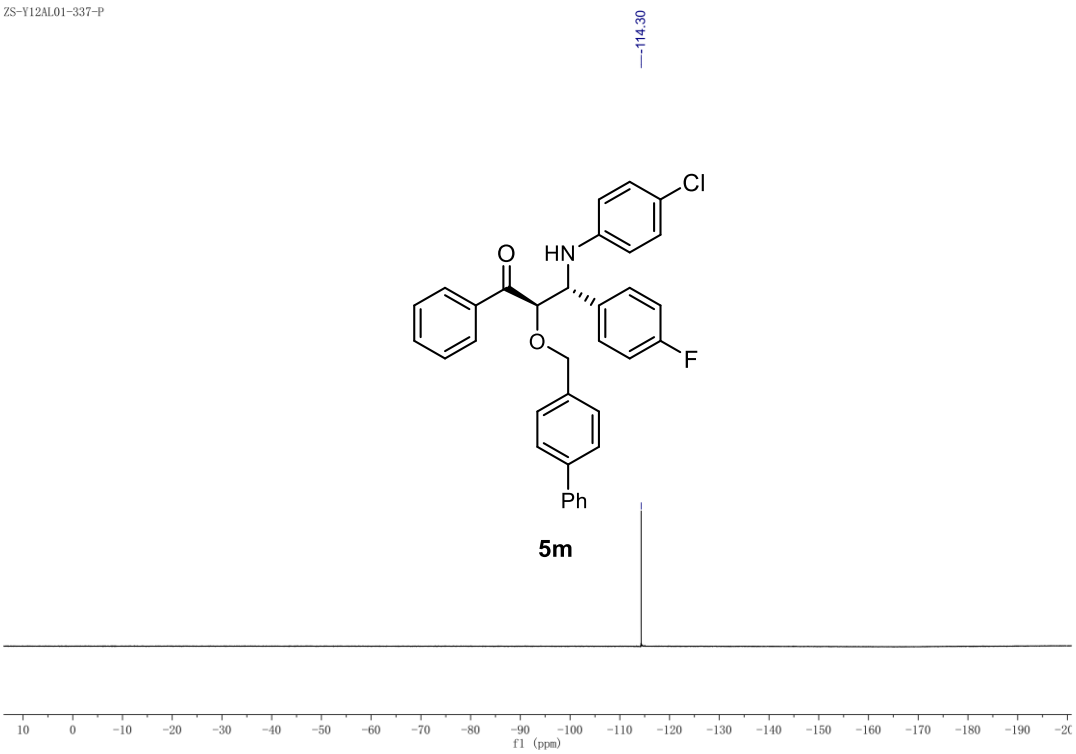


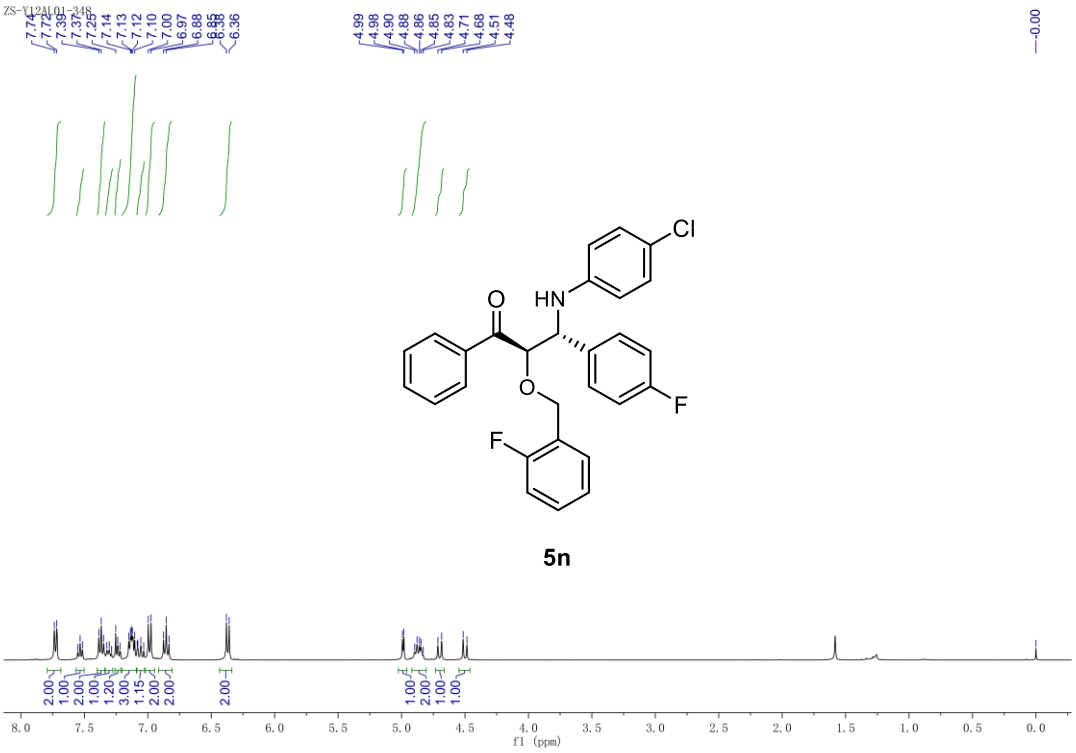
5l



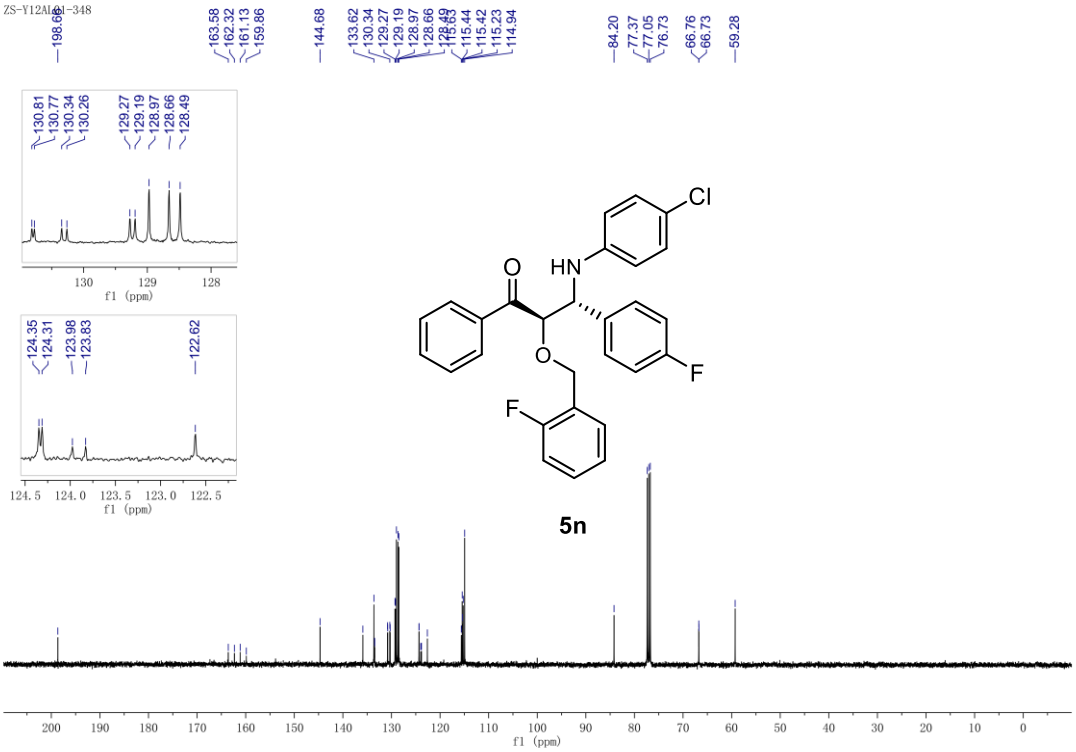
5m


ZS-Y12AL01-337-P
199.16
163.36
161.40
144.71
135.74
133.63
129.24
129.18
128.97
128.87
128.67
128.64
128.53
127.52
127.33
115.41
115.30
114.95
83.81
77.29
77.03
76.78
72.38
59.55
Cl
HN
O
O
F
Ph
5m
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


ZS-Y12AL01-337-P
-114.30
Cl
HN
O
O
F
Ph
5m
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -20
f1 (ppm)

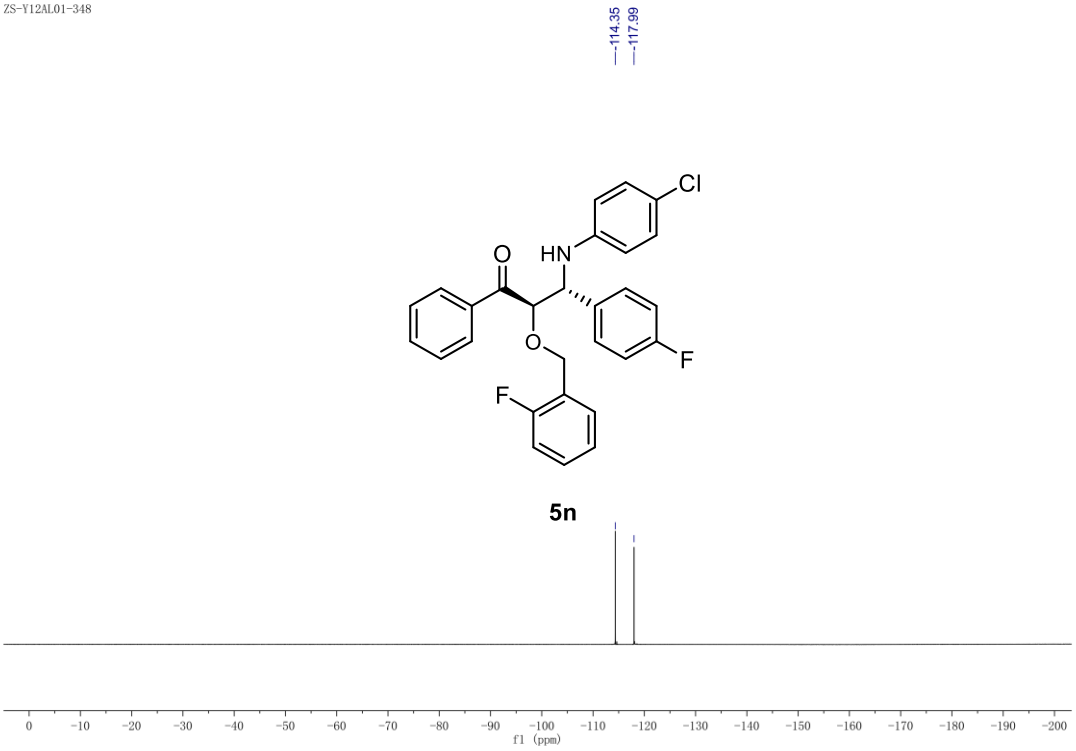

ZS-Y12AL01-348
7.74
7.72
7.39
7.37
7.25
7.14
7.13
7.12
7.10
7.00
6.97
6.88
6.36
4.99
4.98
4.90
4.88
4.86
4.85
4.83
4.71
4.68
4.51
4.48
0.00
Cl
HN
O
O
F
F
2.00
1.00
2.00
1.00
1.20
3.00
1.15
2.00
2.00
2.00
1.00
2.00
1.00
1.00
f1 (ppm)

5n

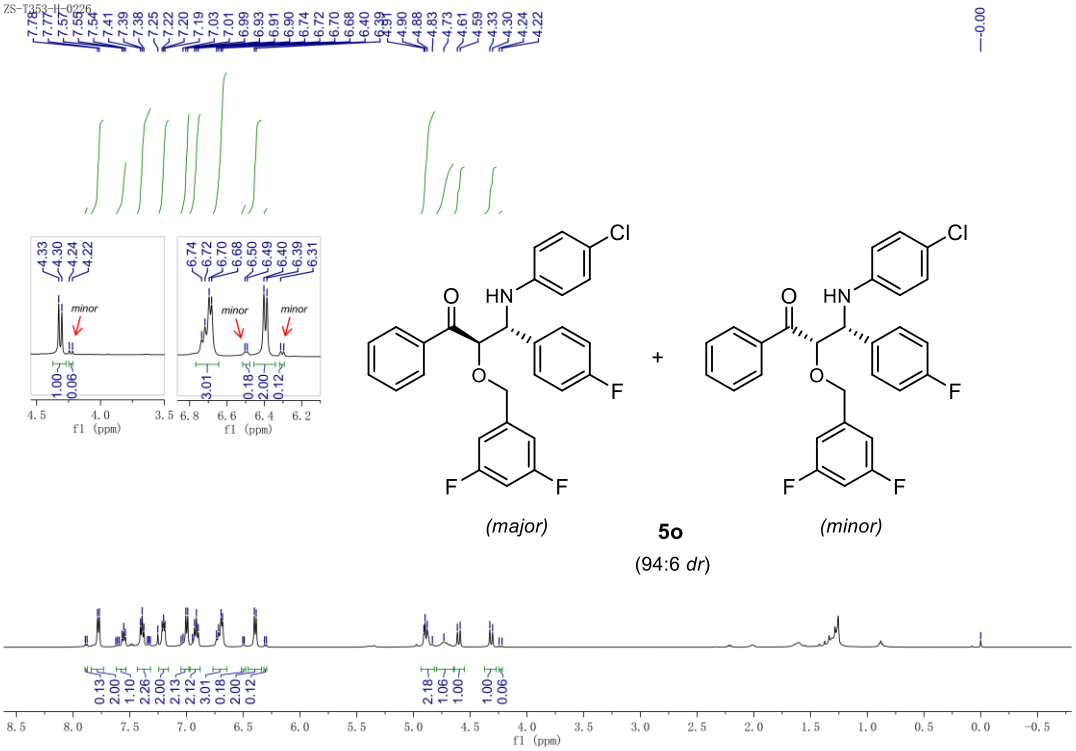

ZS-Y12AL01-348
198.68
163.58
162.32
161.13
159.86
144.68
133.62
130.34
129.27
129.19
128.97
128.66
128.49
115.44
115.42
115.23
114.94
84.20
77.37
77.05
76.73
66.76
66.73
59.28
130.81
130.77
130.34
130.26
129.27
129.19
128.97
128.66
128.49
124.35
124.31
123.98
123.83
122.62
Cl
HN
O
O
F
F
f1 (ppm)

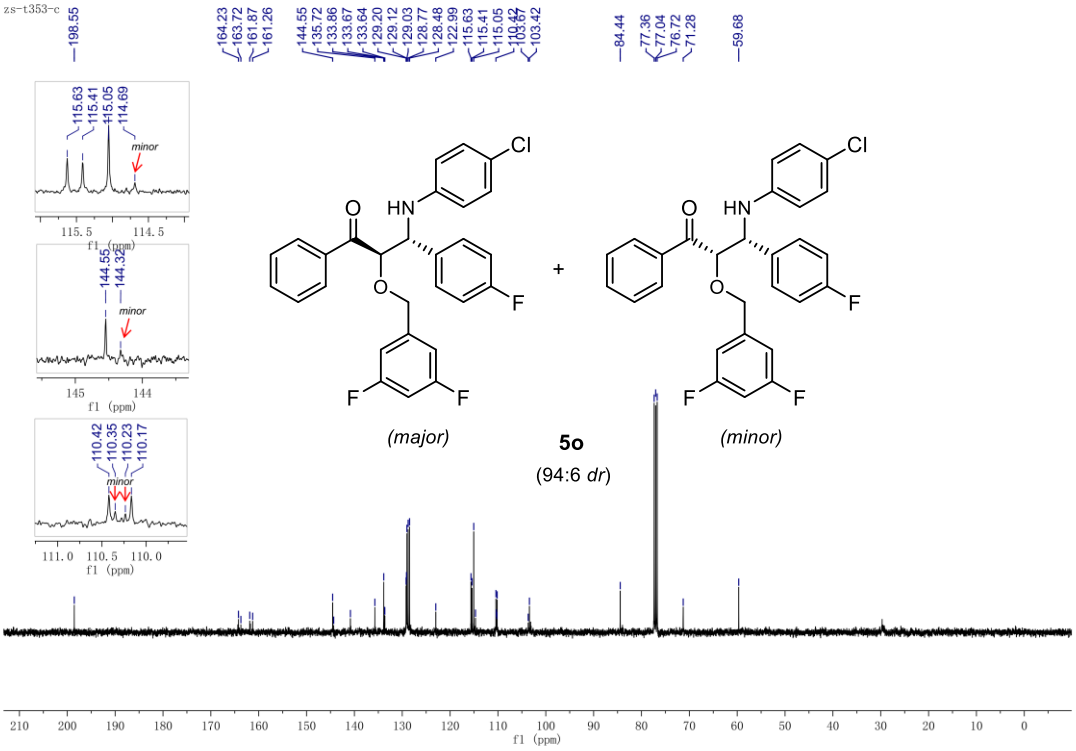
5n

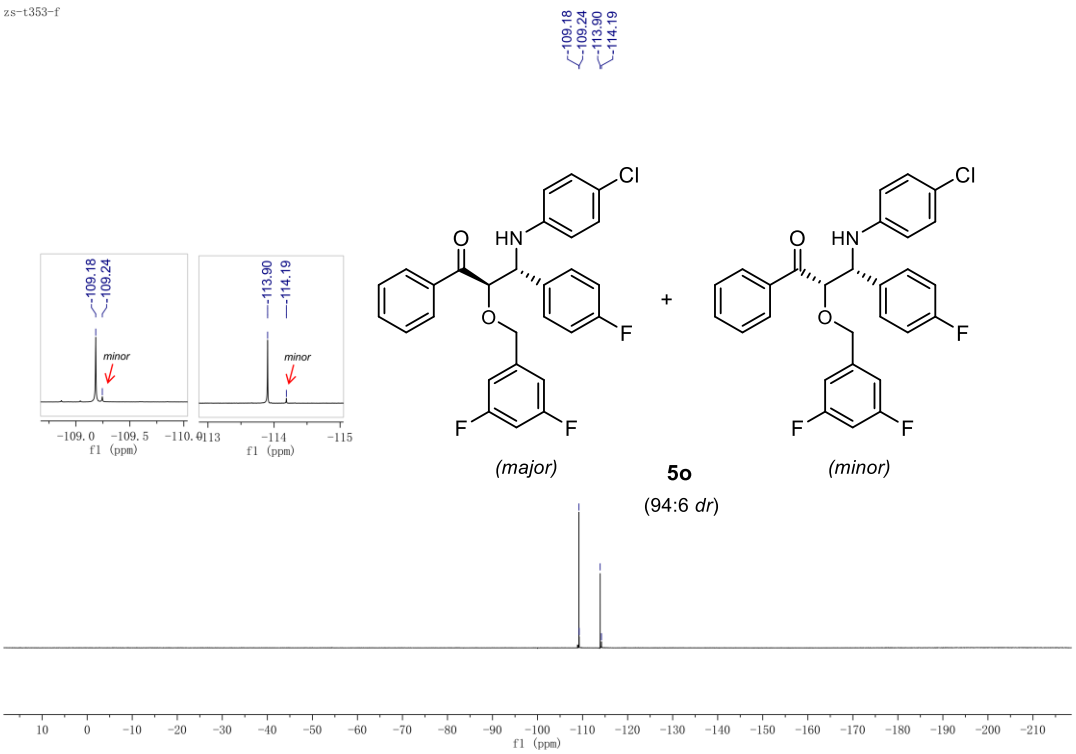
ZS-Y12AL01-348

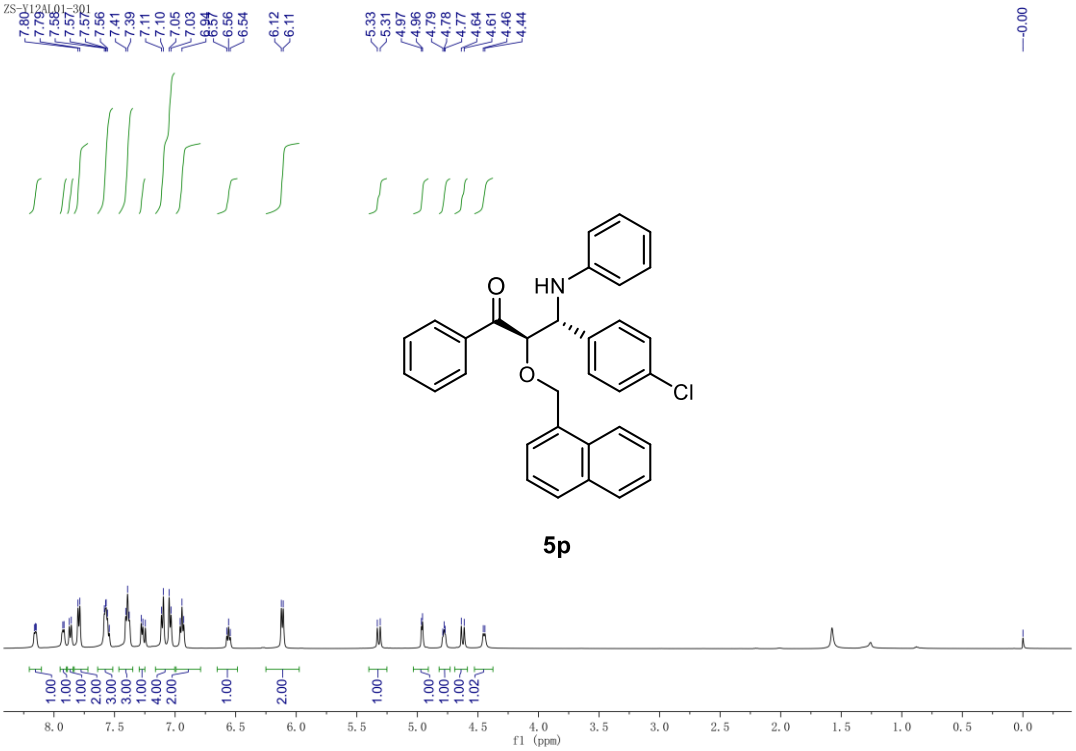


ZS-T353-H-0226

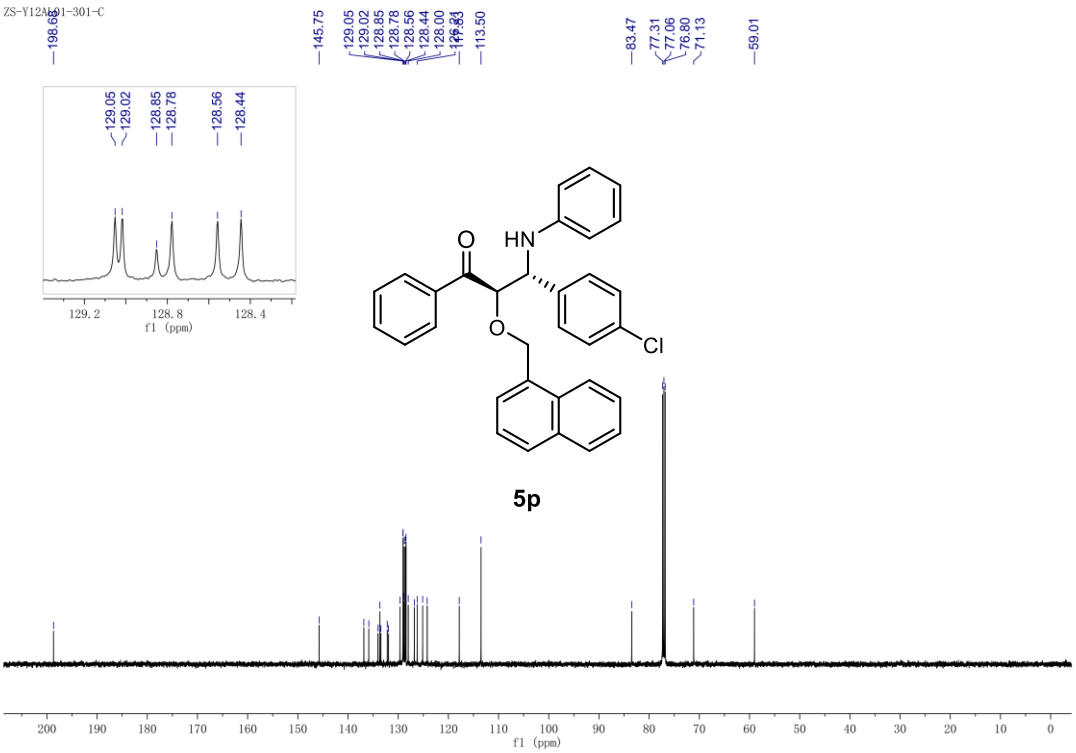



zs-t353-c
198.55
164.23
163.72
161.87
161.26
144.55
135.72
133.86
133.67
133.64
129.20
129.12
129.03
128.77
128.48
122.99
115.63
115.41
115.05
110.42
103.67
103.42
84.44
77.36
77.04
76.72
71.28
59.68
115.63
115.41
115.05
114.69
minor
144.55
144.32
minor
110.42
110.35
110.23
110.17
minor
Cl
HN
O
O
F
F
F
+
(major)
5o
(94:6 dr)
(minor)
f1 (ppm)

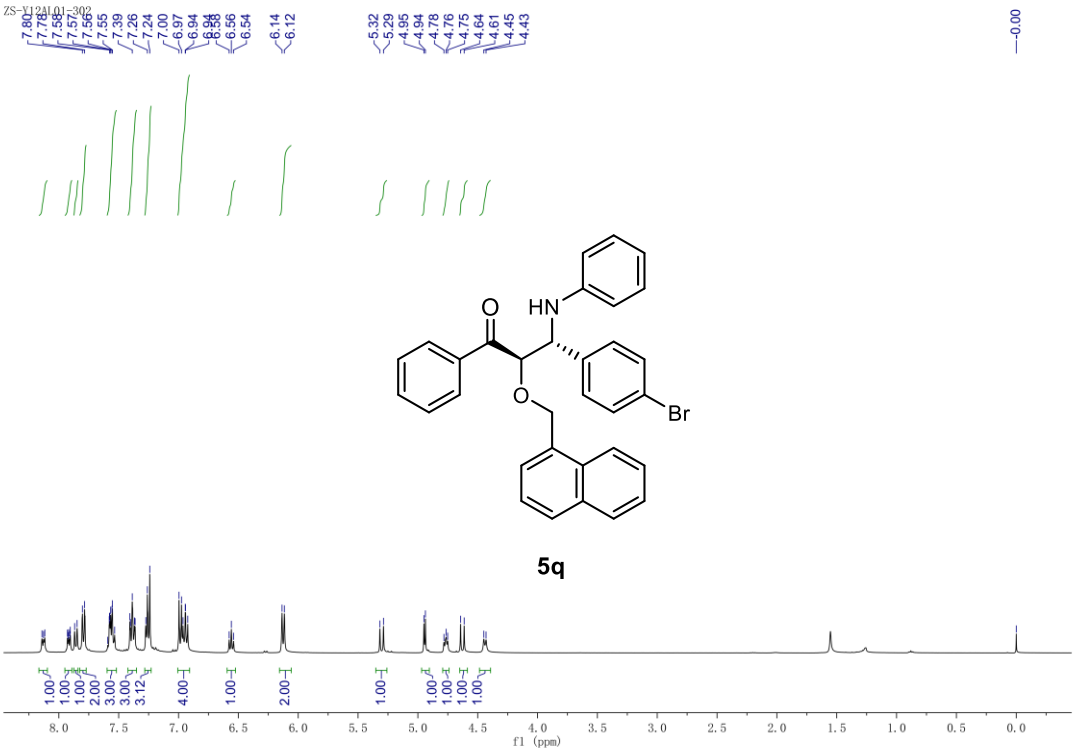

zs-t353-f
109.18
109.24
113.90
114.19
minor
minor
Cl
HN
O
O
F
F
F
+
(major)
5o
(94:6 dr)
(minor)
f1 (ppm)

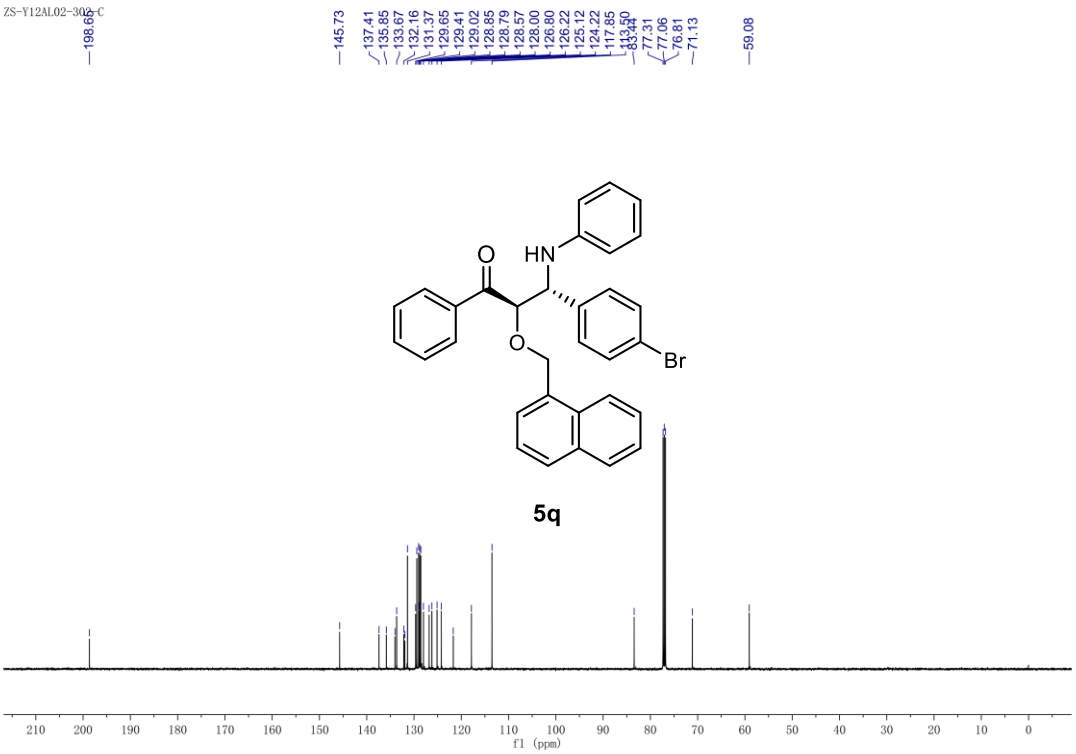

ZS-Y12A101-301
7.80
7.78
7.58
7.57
7.57
7.56
7.41
7.39
7.11
7.10
7.05
7.03
6.57
6.56
6.54
6.12
6.11
5.33
5.31
4.97
4.96
4.79
4.78
4.77
4.64
4.61
4.46
4.44
0.00
O
HN
O
Cl
1.00
1.00
1.00
2.00
3.00
3.00
1.00
4.00
2.00
1.00
2.00
1.00
1.00
1.00
1.00
1.02
f1 (ppm)

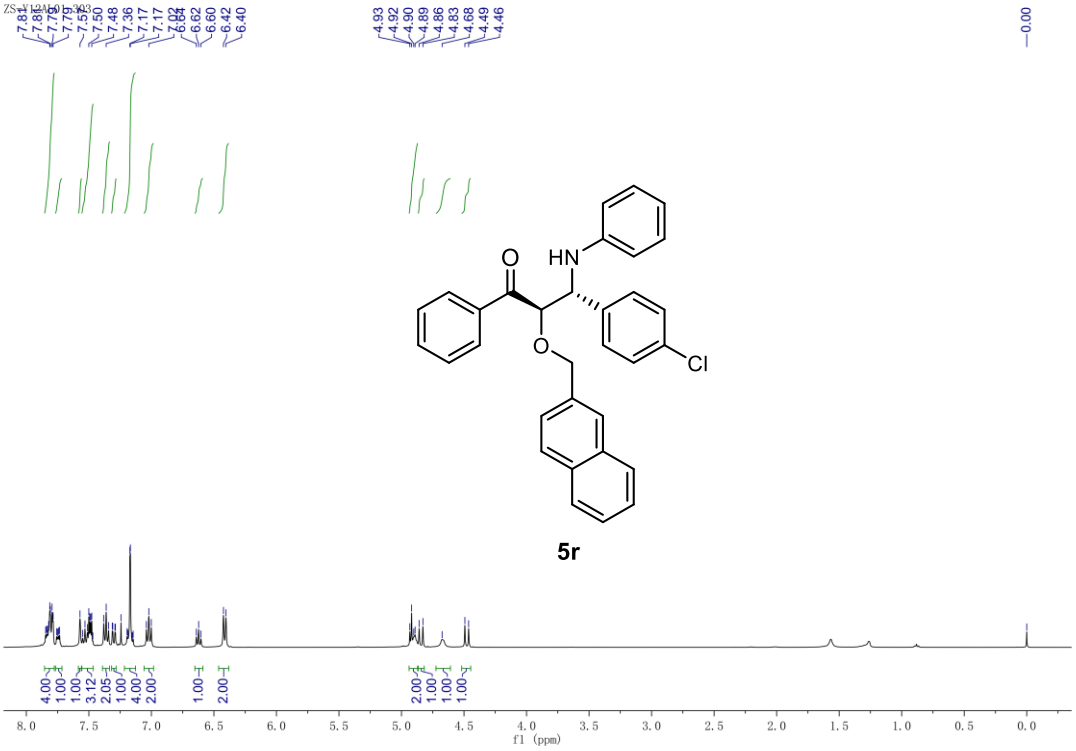
5p

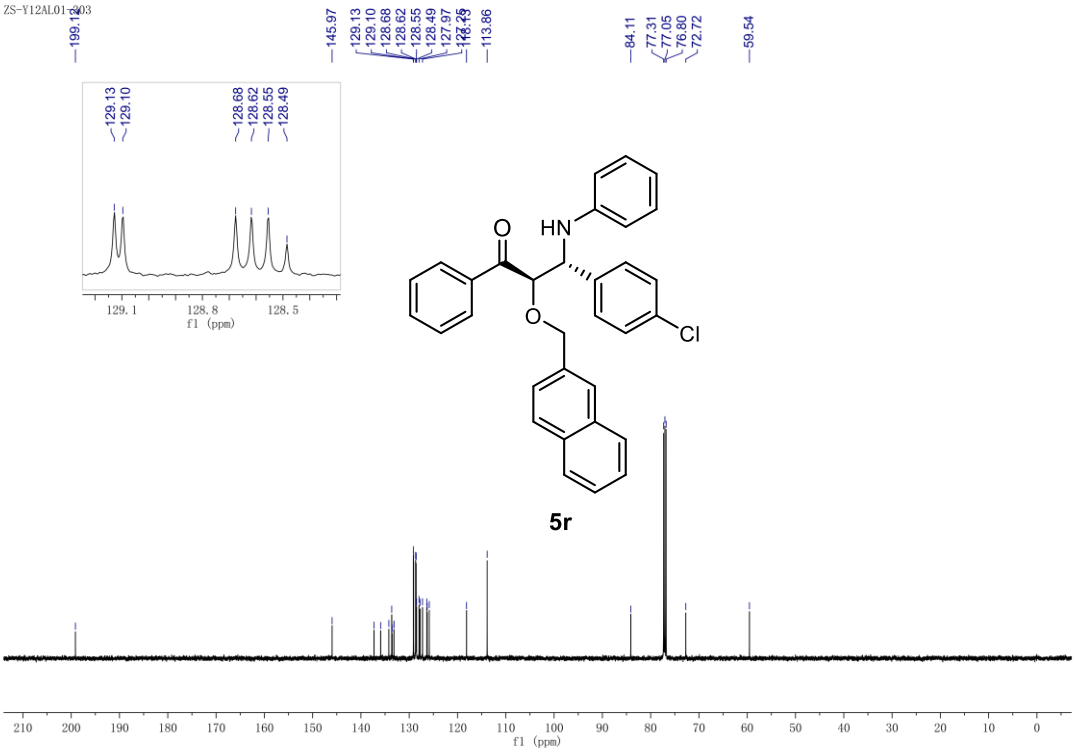

ZS-Y12A101-301-C
198.66
145.75
129.05
129.02
128.85
128.78
128.56
128.44
128.00
113.50
83.47
77.31
77.06
76.80
71.13
59.01
129.2
128.8
128.4
f1 (ppm)
O
HN
O
Cl
f1 (ppm)

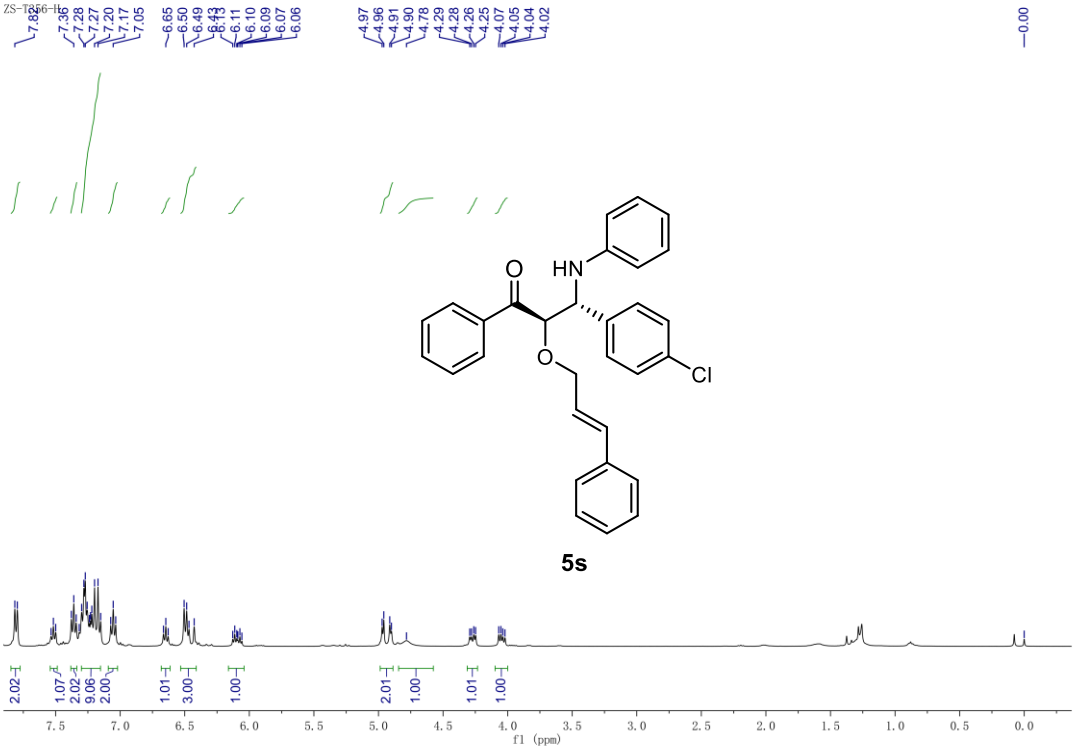
5p

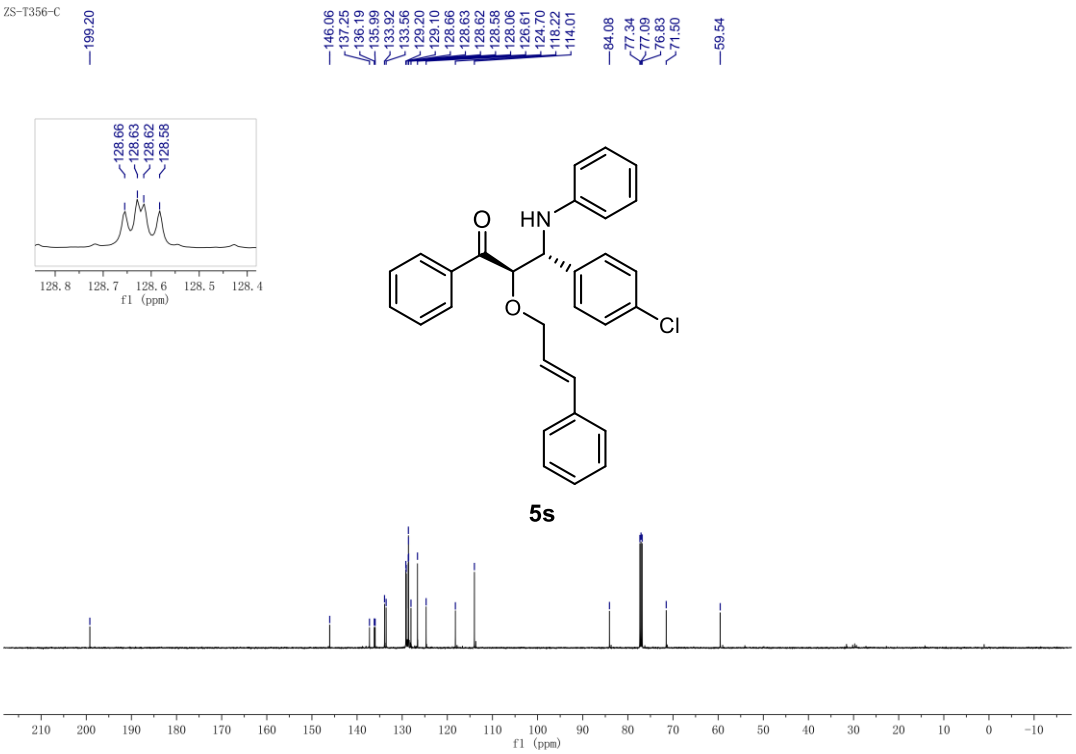

ZS-Y12AL01-302
7.80
7.78
7.58
7.57
7.56
7.55
7.39
7.26
7.24
7.00
6.97
6.94
6.58
6.56
6.54
6.14
6.12
5.32
5.29
4.95
4.94
4.78
4.76
4.75
4.64
4.61
4.45
4.43
0.00
O
HN
O
Br
5q
1.00
1.00
1.00
2.00
3.00
3.00
3.12
4.00
1.00
2.00
1.00
1.00
1.00
1.00
1.00
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

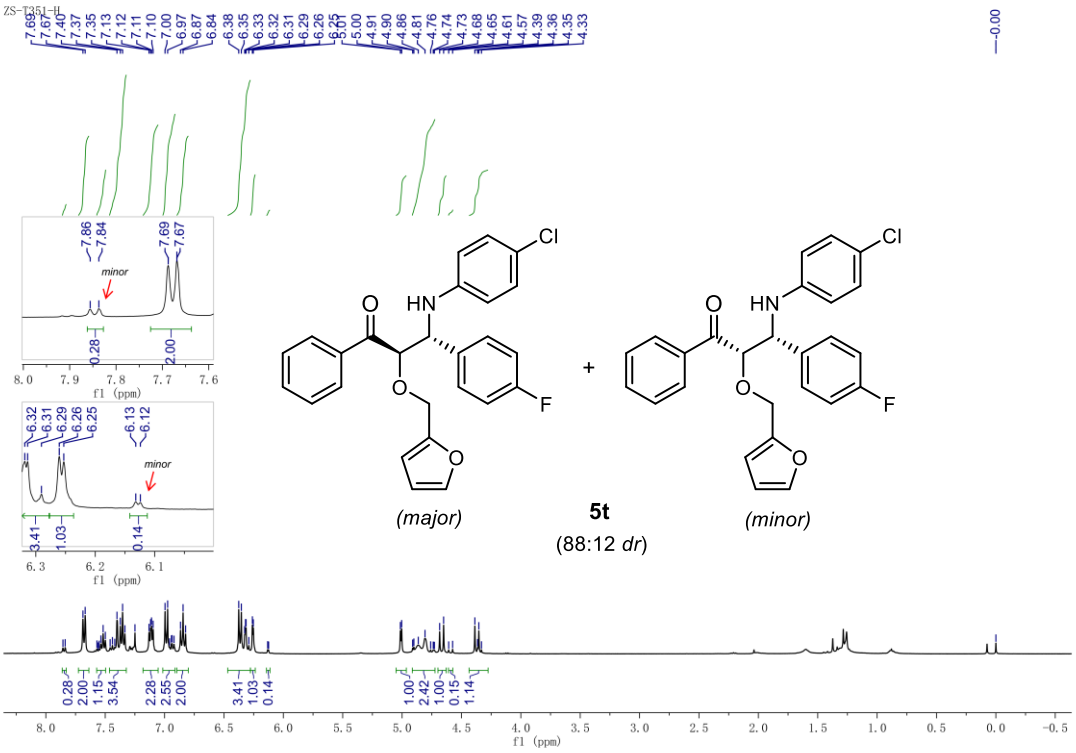

ZS-Y12AL02-302-C
198.65
145.73
137.41
135.85
133.67
132.16
131.37
129.65
129.41
129.02
128.85
128.79
128.57
128.00
126.80
126.22
125.12
124.22
117.85
113.50
83.44
77.31
77.06
76.81
71.13
59.08
O
HN
O
Br
5q
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

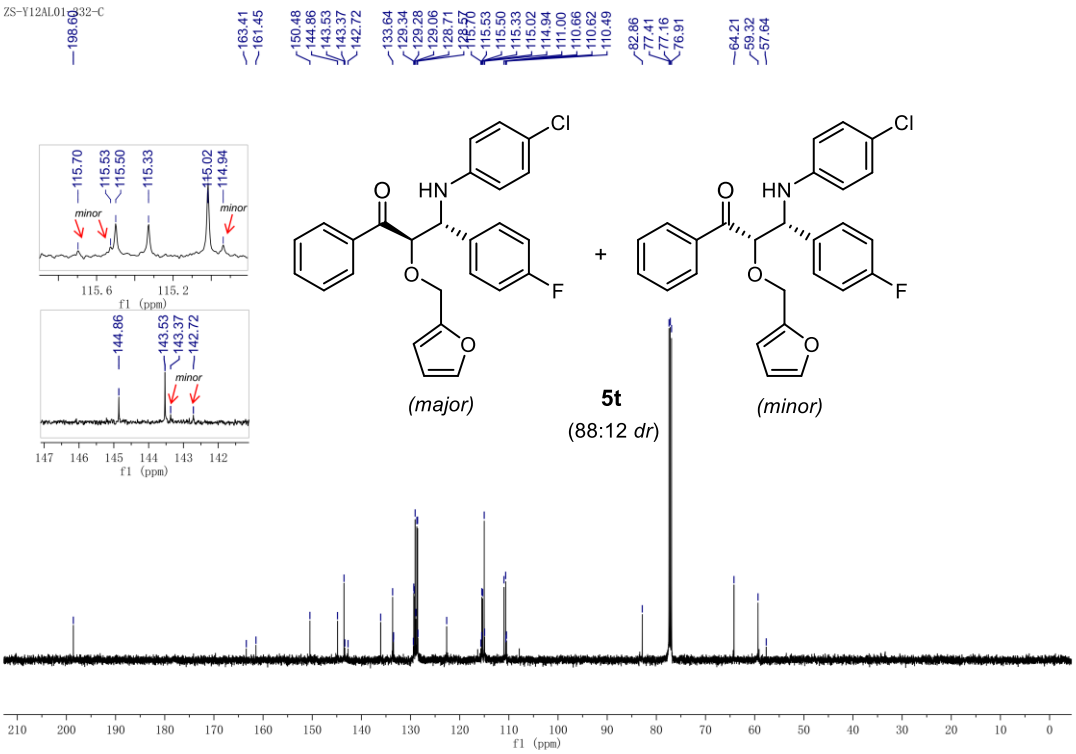

ZS-Y12AL01-303
7.84
7.83
7.78
7.77
7.76
7.51
7.50
7.48
7.36
7.17
7.17
7.02
6.84
6.62
6.60
6.42
6.40
4.93
4.92
4.90
4.89
4.86
4.83
4.68
4.49
4.46
0.00
O
HN
O
Cl
5r
4.00
1.00
1.00
3.12
2.05
1.00
4.00
2.00
1.00
2.00
2.00
1.00
1.00
1.00
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

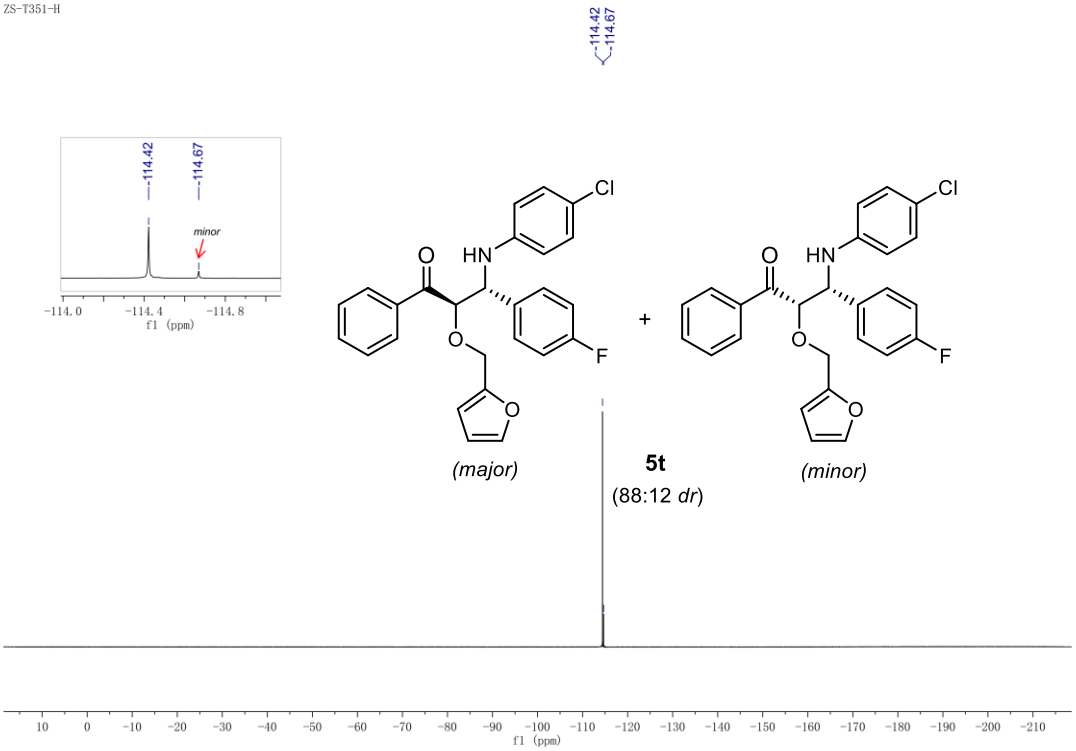

ZS-Y12AL01-303
199.12
145.97
129.13
129.10
128.68
128.62
128.55
128.49
127.97
113.86
84.11
77.31
77.05
76.80
72.72
59.54
129.13
129.10
128.68
128.62
128.55
128.49
129.1
128.8
128.5
f1 (ppm)
O
HN
O
Cl
5r
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

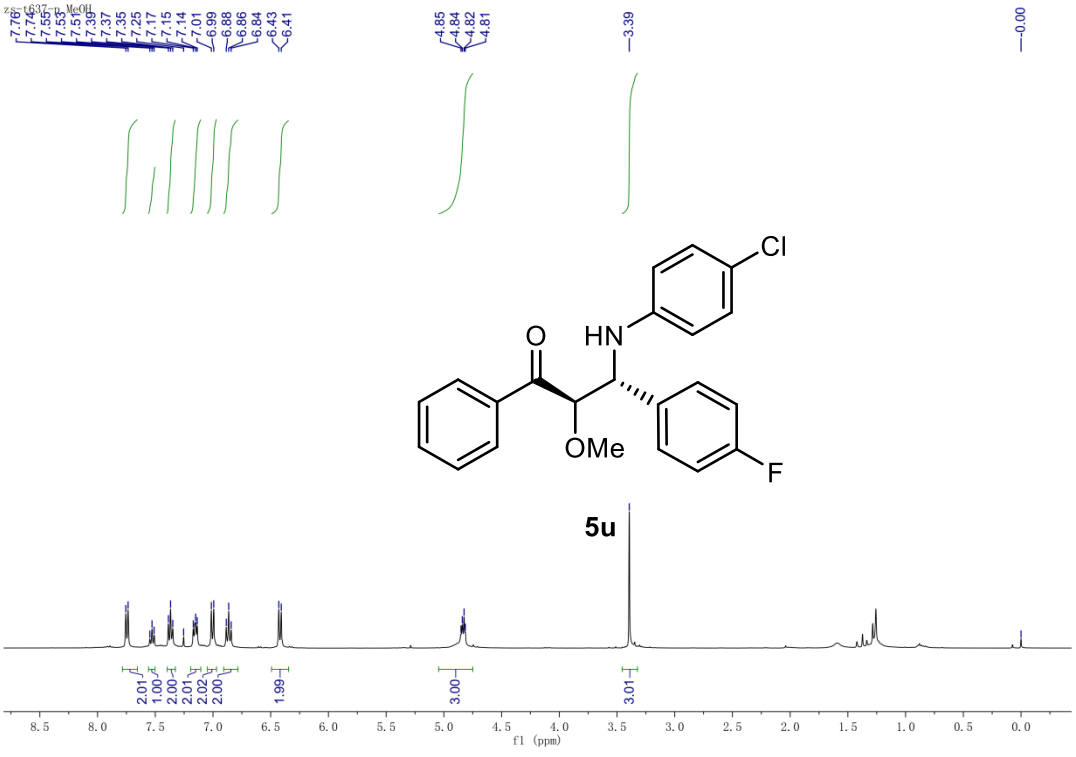

ZS-T356-H
7.82
7.36
7.28
7.27
7.20
7.17
7.05
6.65
6.50
6.49
6.43
6.11
6.10
6.09
6.07
6.06
4.97
4.96
4.91
4.90
4.78
4.29
4.28
4.26
4.25
4.07
4.05
4.04
4.02
0.00
O
HN
O
Cl
5s
2.02
1.07
2.02
9.06
2.00
1.01
3.00
1.00
2.01
1.00
1.01
1.00
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

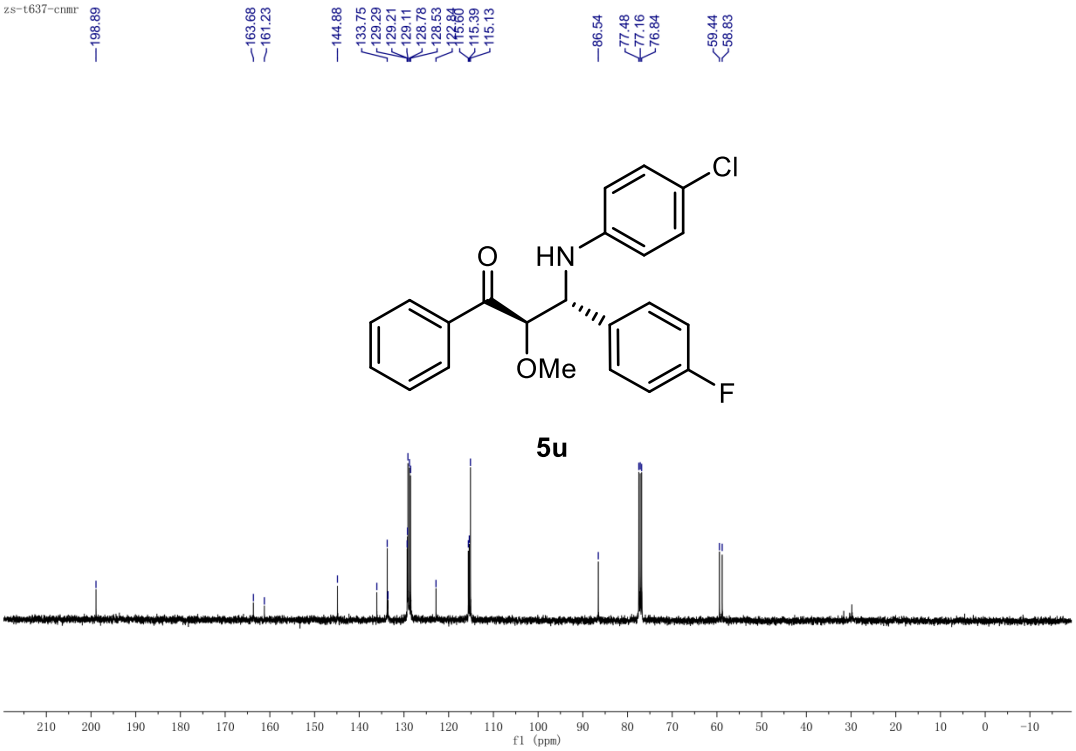

ZS-T356-C
199.20
146.06
137.25
136.19
135.99
133.92
133.56
129.20
129.10
128.66
128.63
128.62
128.58
128.06
126.61
124.70
118.22
114.01
84.08
77.34
77.09
76.83
71.50
59.54
128.66
128.63
128.62
128.58
128.8
128.7
128.6
128.5
128.4
f1 (ppm)
O
HN
O
Cl
5s
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−10
f1 (ppm)

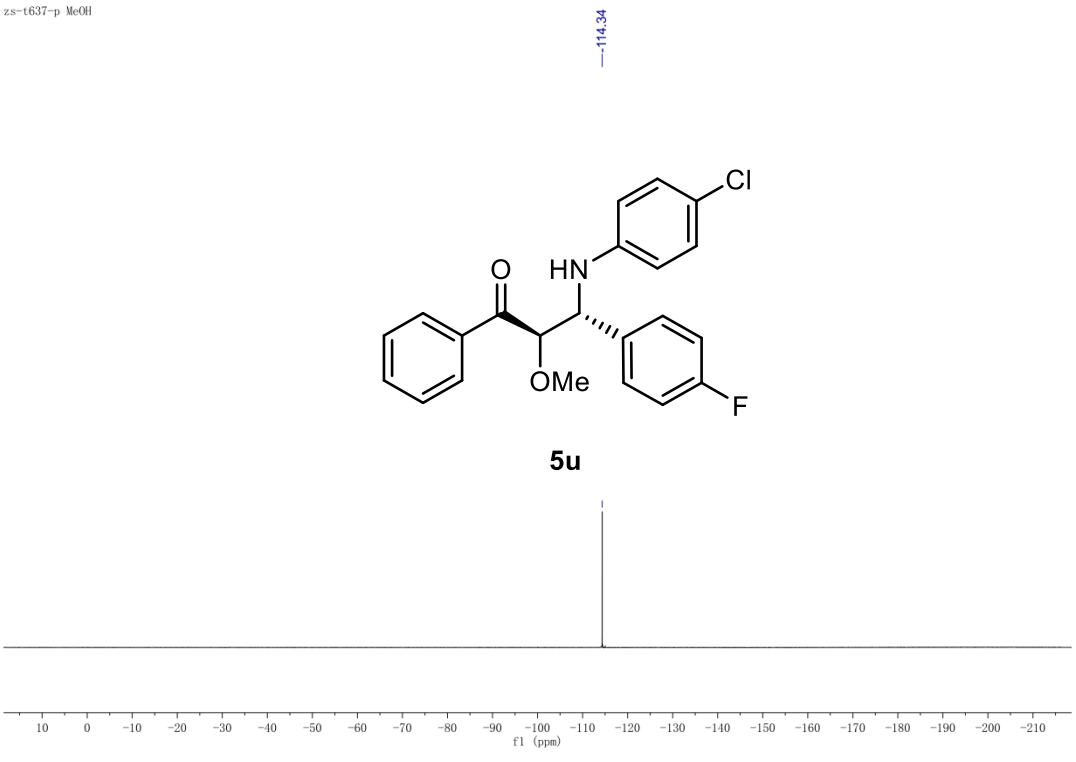

ZS-T351-H1
minor
minor
Cl
HN
O
O
F
O
(major)
+
Cl
HN
O
O
F
O
(minor)
5t
(88:12 dr)
f1 (ppm)

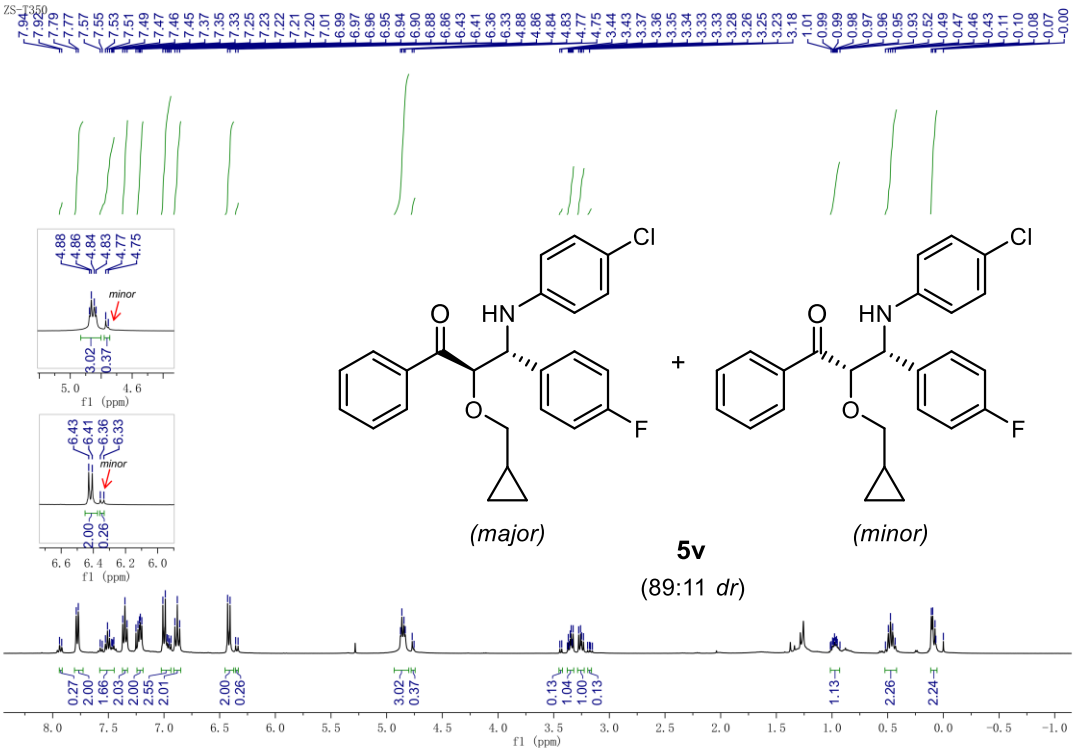

ZS-Y12AL01-332-C
minor
minor
minor
Cl
HN
O
O
F
O
(major)
+
Cl
HN
O
O
F
O
(minor)
5t
(88:12 dr)
f1 (ppm)

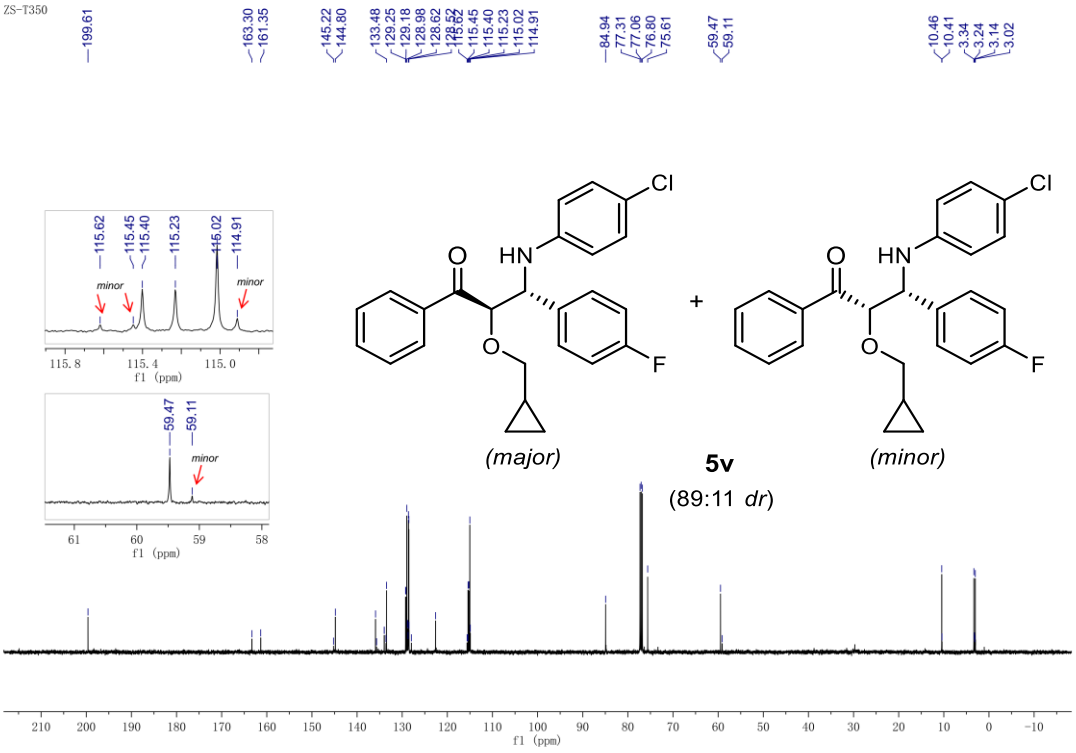

ZS-T351-H
-114.42
-114.67
minor
-114.0
-114.4
-114.8
f1 (ppm)
Cl
HN
O
O
F
O
(major)
+
(minor)
5t
(88:12 dr)
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
f1 (ppm)

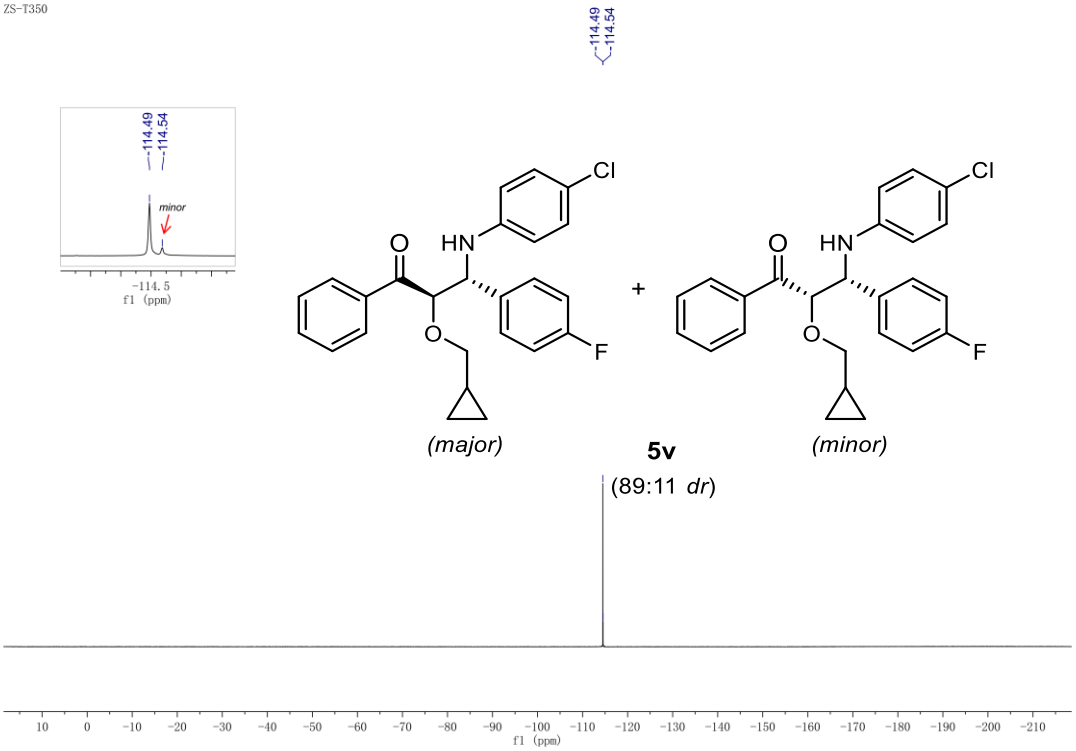

7.76
7.74
7.55
7.53
7.51
7.39
7.37
7.35
7.25
7.17
7.15
7.14
7.01
6.99
6.88
6.86
6.84
6.43
6.41
4.85
4.84
4.82
4.81
3.39
0.00
Cl
HN
O
OMe
F
5u
2.01
1.00
2.00
2.01
2.02
2.00
1.99
3.00
3.01
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

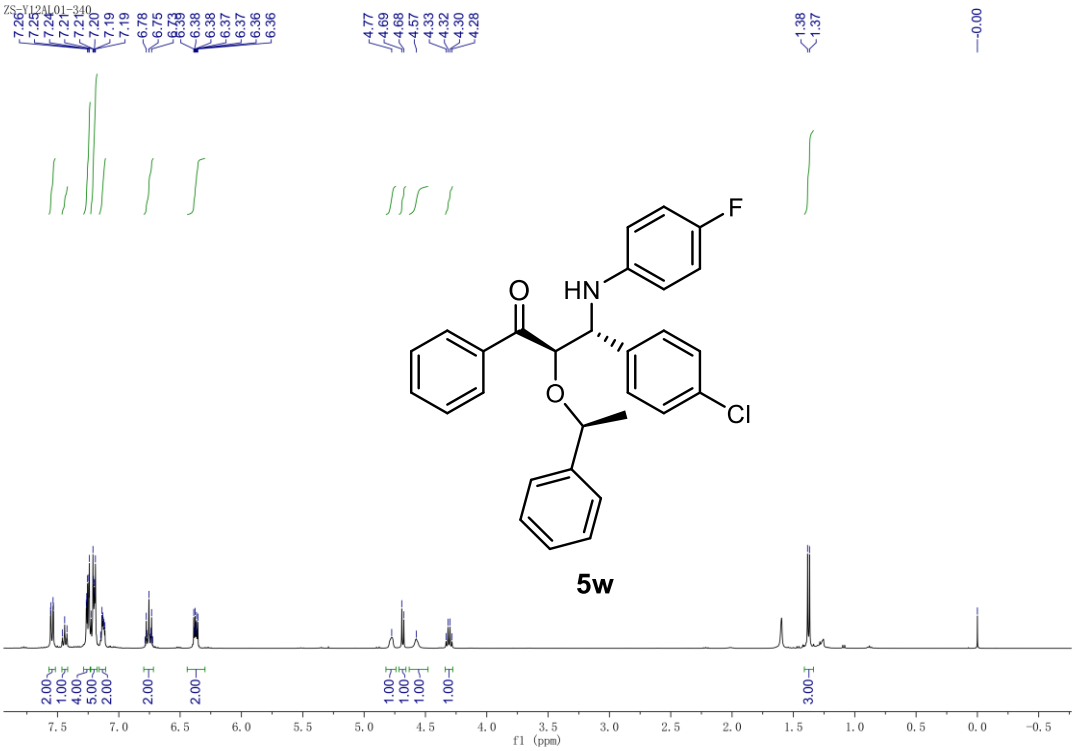

zs-t637-cnmr
198.89
163.68
161.23
144.88
133.75
129.29
129.21
129.11
128.78
128.53
115.39
115.13
86.54
77.48
77.16
76.84
59.44
58.83
Cl
HN
O
OMe
F
5u
f1 (ppm)

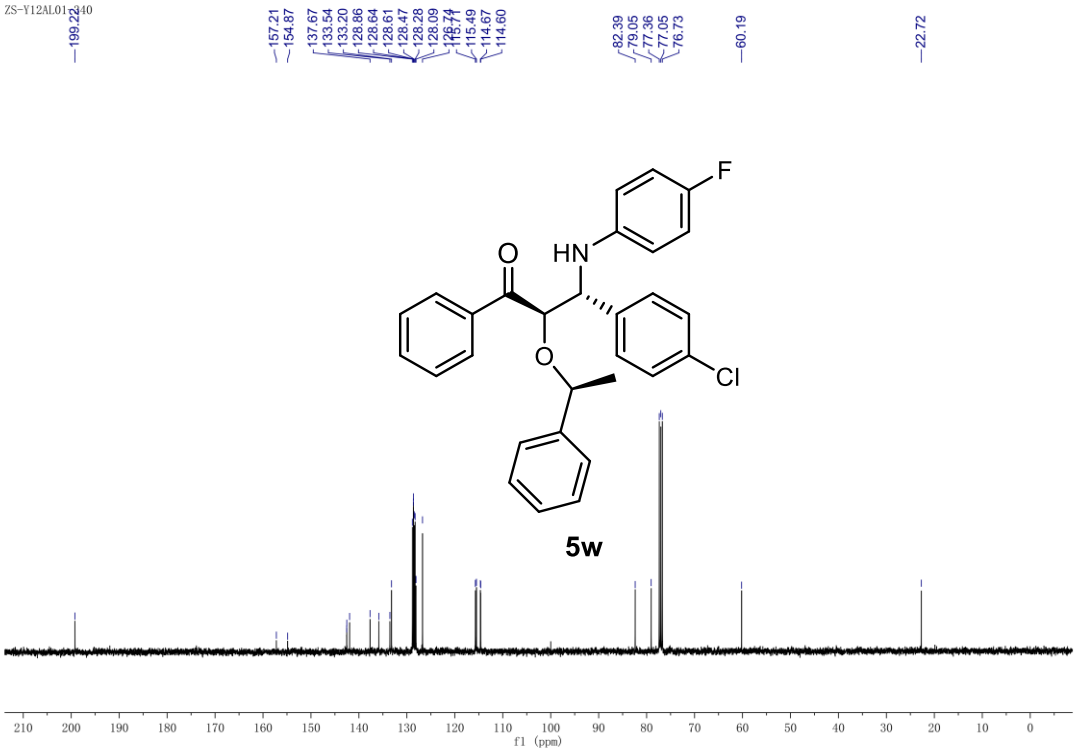

zs-t637-p MeOH
114.34
Cl
HN
O
OMe
F
5u
f1 (ppm)

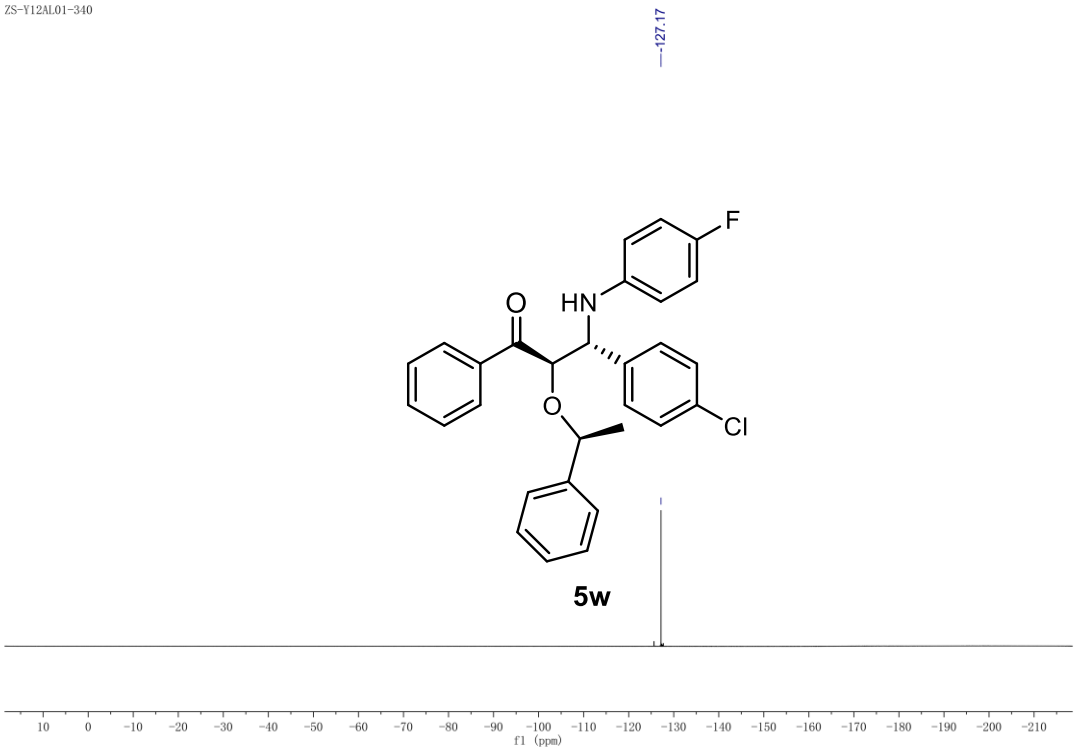

ZS-T350
minor
f1 (ppm)
Cl
O
HN
O
F
+
(major)
5v
(minor)
(89:11 dr)

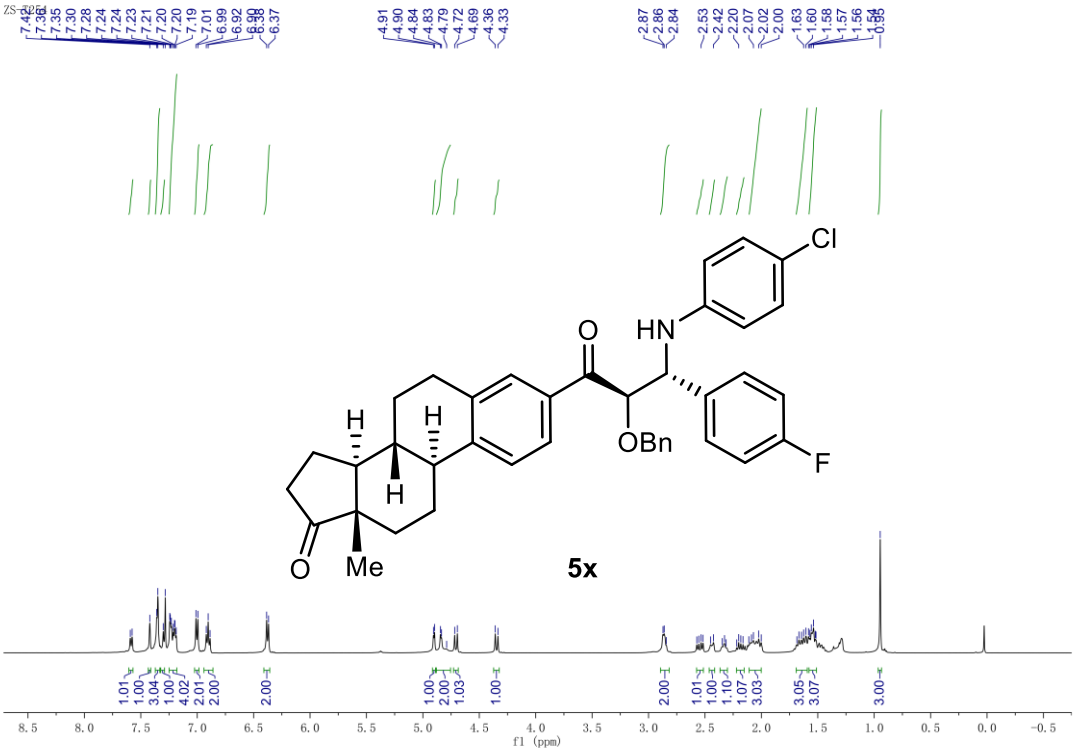

ZS-T350
minor
f1 (ppm)
Cl
O
HN
O
F
+
(major)
5v
(minor)
(89:11 dr)

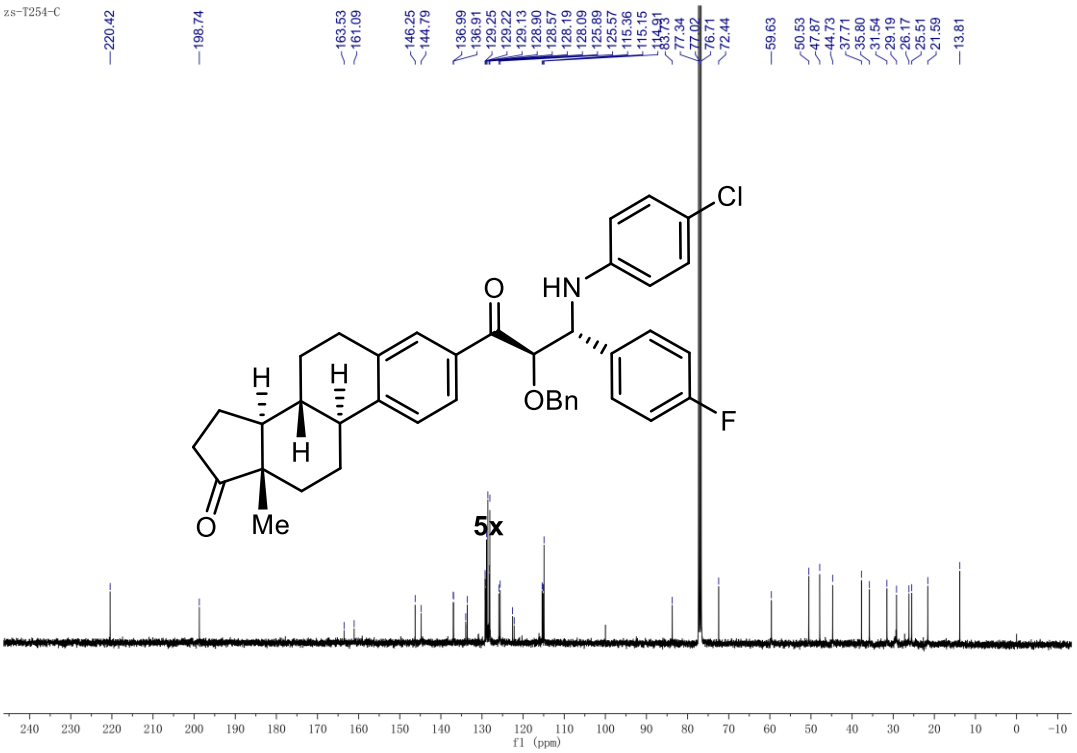

ZS-T350
-114.49
-114.54
minor
-114.5
f1 (ppm)
Cl
HN
O
O
F
(major)
+
(minor)
5v
(89:11 dr)
f1 (ppm)

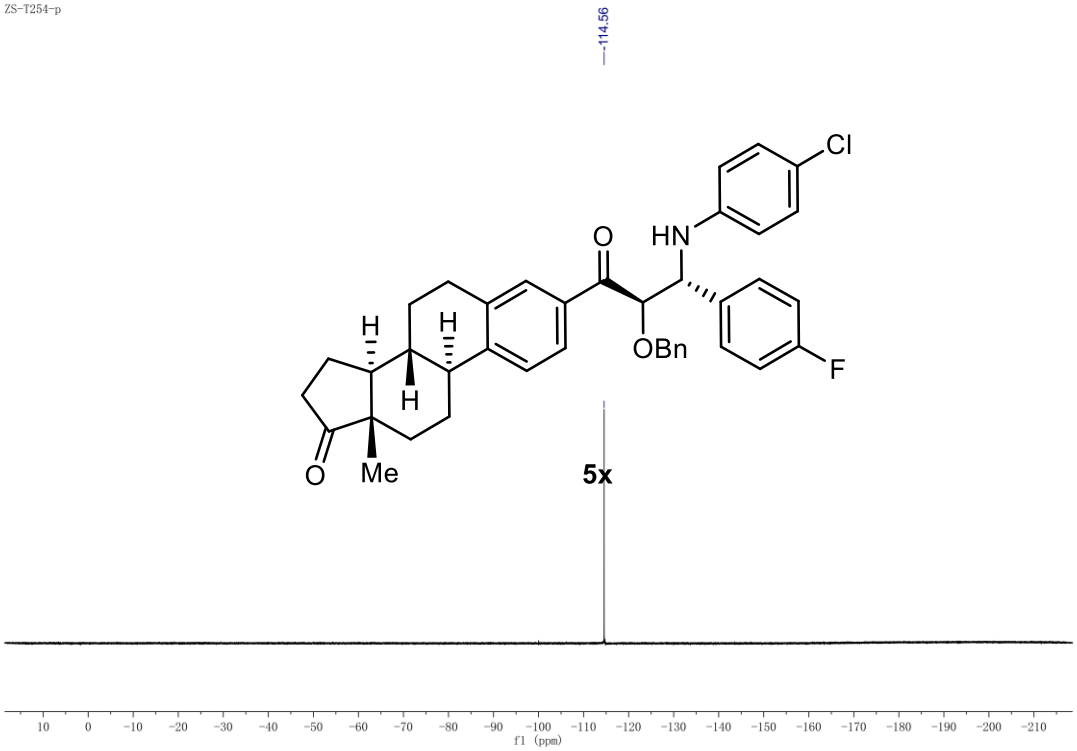

ZS-Y12AL01-340
7.26
7.25
7.24
7.21
7.21
7.20
7.19
7.19
6.78
6.75
6.38
6.38
6.37
6.37
6.36
6.36
4.77
4.69
4.68
4.57
4.33
4.32
4.30
4.28
1.38
1.37
0.00
F
HN
O
O
Cl
5w
2.00
1.00
4.00
5.00
2.00
2.00
2.00
1.00
1.00
1.00
3.00
f1 (ppm)

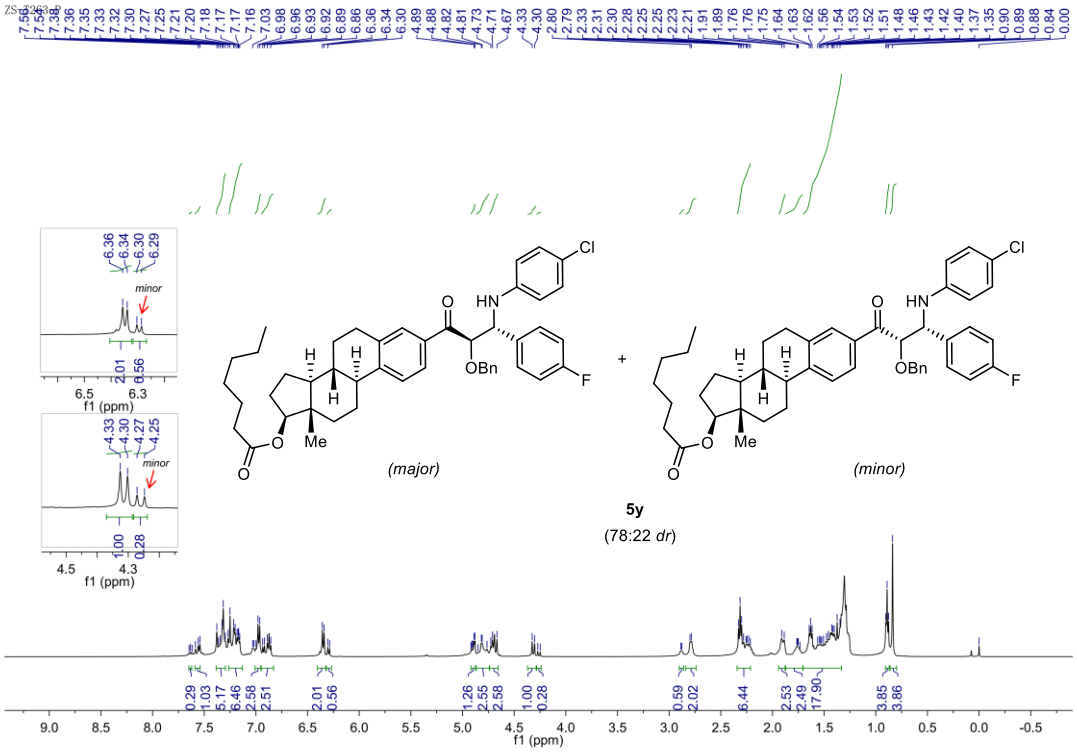

ZS-Y12AL01-340
199.22
157.21
154.87
137.67
133.54
133.20
128.86
128.64
128.61
128.47
128.28
128.09
115.49
114.67
114.60
82.39
79.05
77.36
77.05
76.73
60.19
22.72
F
HN
O
O
Cl
5w
f1 (ppm)

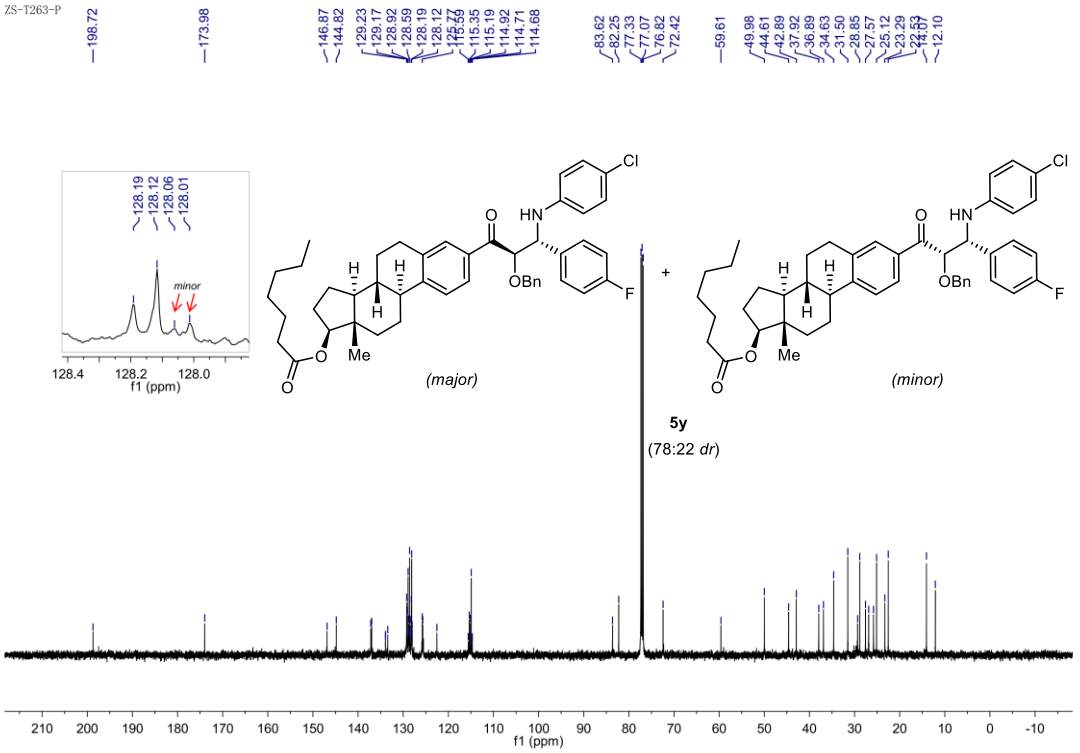

ZS-Y12AL01-340
127.17
F
HN
O
O
Cl
5w
f1 (ppm)

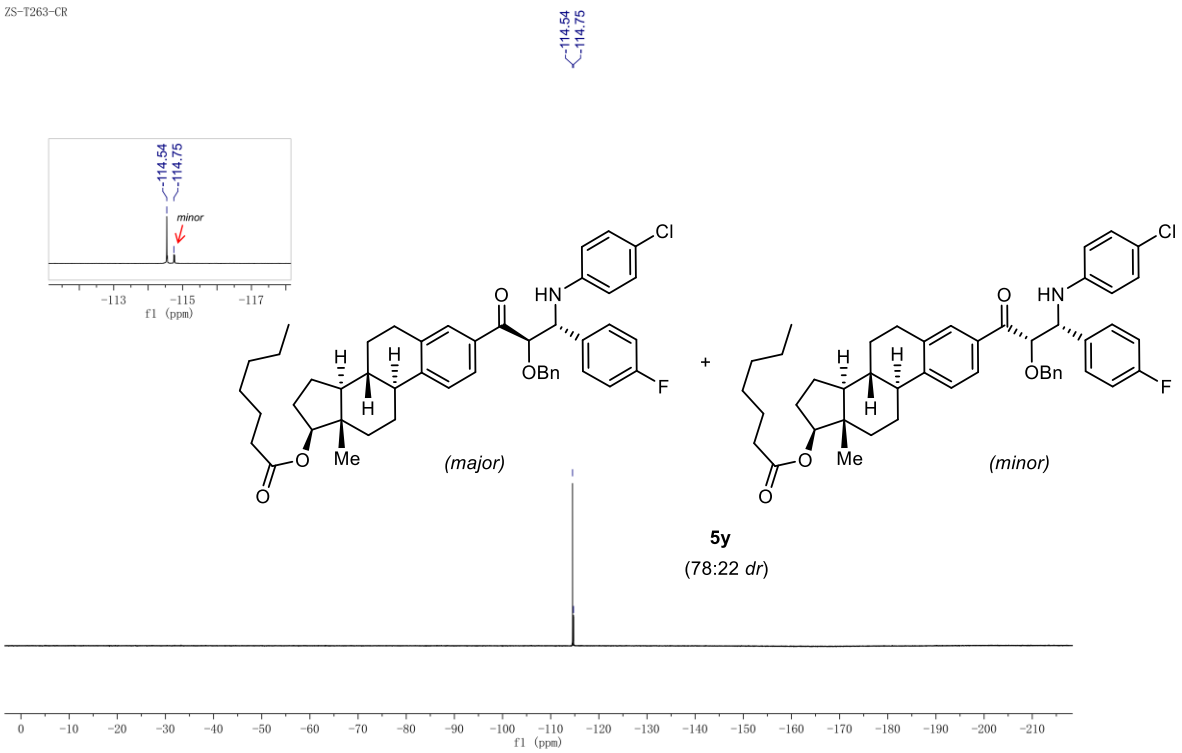

Cl
HN
O
OBn
F
H
H
H
O
Me
5x

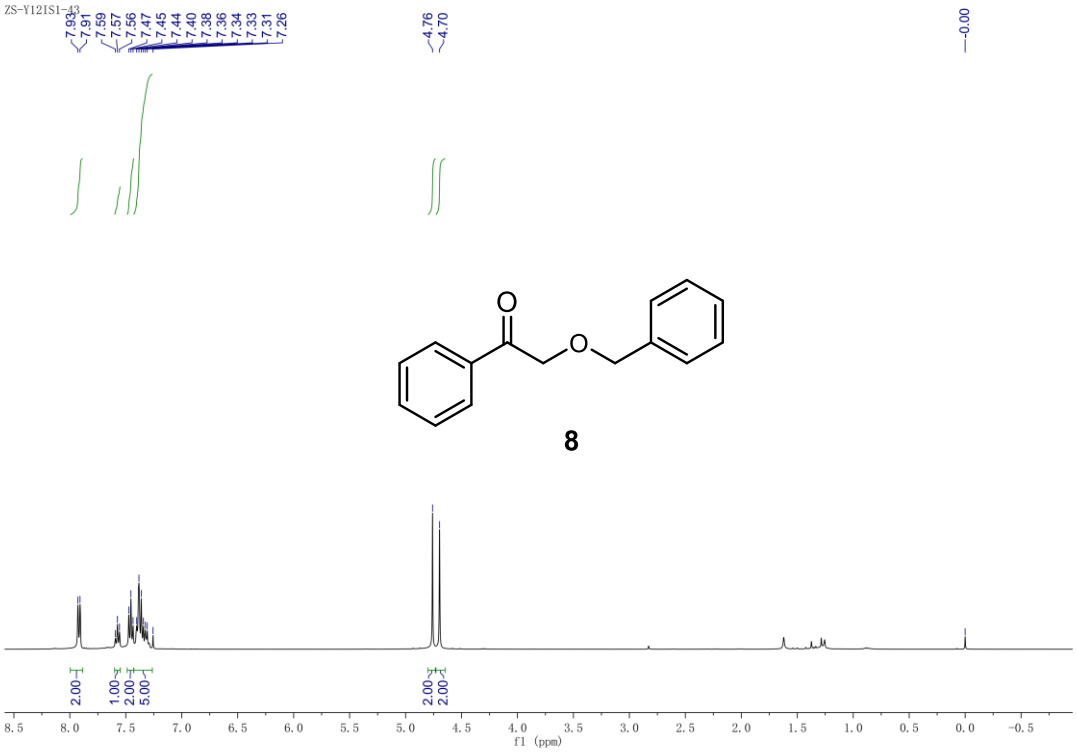

zs-T254-C
Cl
HN
O
OBn
F
H
H
H
O
Me
5x


ZS-T254-p
-114.56
Cl
HN
O
H
H
OBn
F
H
O
Me
5x
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)


ZS-T263-p
6.36
6.34
6.30
6.29
minor
2.01
0.56
6.5
6.3
f1 (ppm)
4.33
4.30
4.27
4.25
minor
1.00
0.28
4.5
4.3
f1 (ppm)
Cl
HN
O
OBn
F
H
H
H
O
Me
O
(major)
+
(minor)
5y
(78:22 dr)
0.29 1.03 5.17 6.46 2.58 2.51 2.01 0.56 1.26 2.55 2.58 1.00 0.28 0.59 2.02 6.44 2.53 2.49 17.90 3.85 3.86
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


ZS-T263-P
198.72
173.98
146.87
144.82
129.23
129.17
128.92
128.59
128.19
128.12
125.77
125.58
115.35
115.19
114.92
114.71
114.68
83.62
82.25
77.33
77.07
76.82
72.42
59.61
49.98
44.61
42.89
37.92
36.89
34.63
31.50
28.85
27.57
25.12
23.29
14.07
12.10
128.19
128.12
128.06
128.01
minor
128.4
128.2
128.0
f1 (ppm)
Cl
HN
O
OBn
F
H
Me
(major)
(minor)
5y
(78:22 dr)
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


ZS-T263-CR
114.54
114.75
minor
-113
-115
-117
f1 (ppm)
Cl
HN
O
OBn
F
H
Me
(major)
(minor)
5y
(78:22 dr)
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
f1 (ppm)


ZS-Y12IS1-43
7.93
7.91
7.59
7.57
7.56
7.47
7.45
7.44
7.40
7.38
7.36
7.34
7.33
7.31
7.26
4.76
4.70
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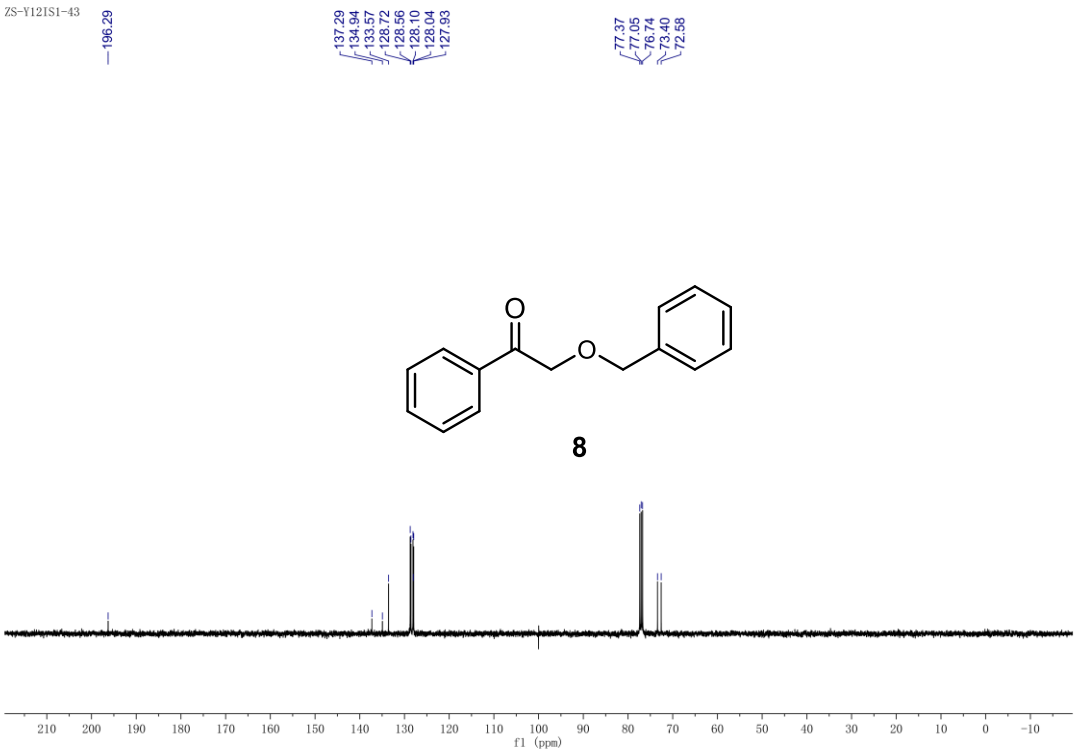
O
O
8
2.00
1.00
2.00
5.00
2.00
2.00
f1 (ppm)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196.29
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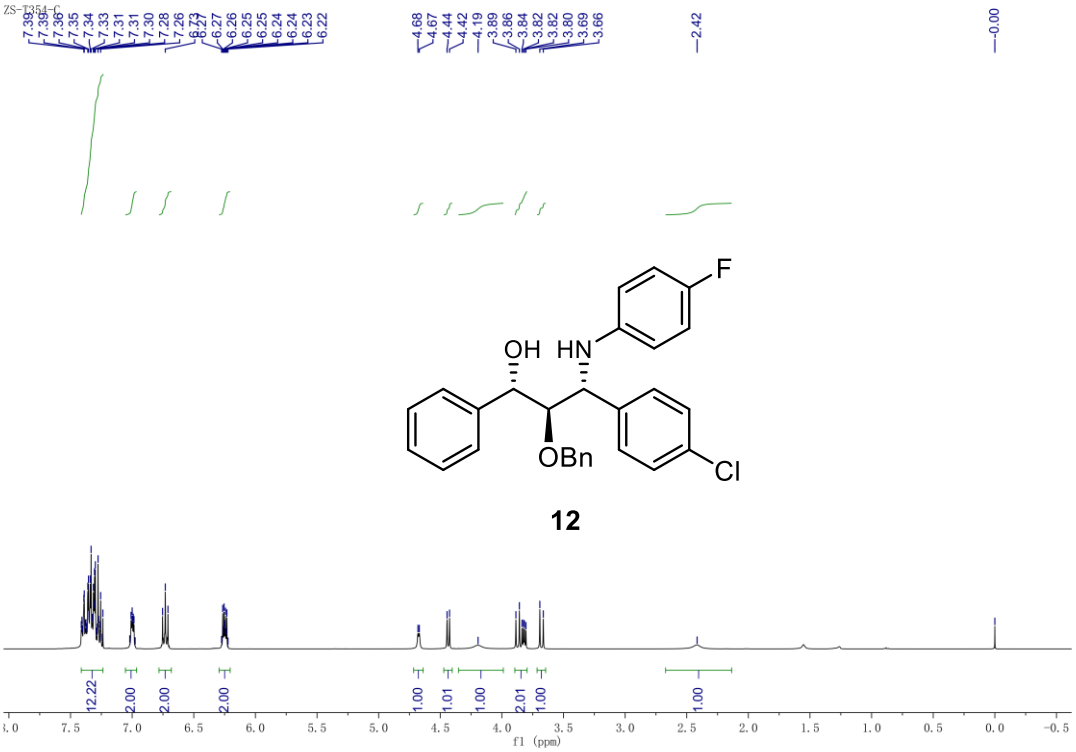
127.93
77.37
77.05
76.74
73.40
72.58
O
O
8
f1 (ppm)


ZS-T354-C
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7.38
7.36
7.35
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7.33
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7.30
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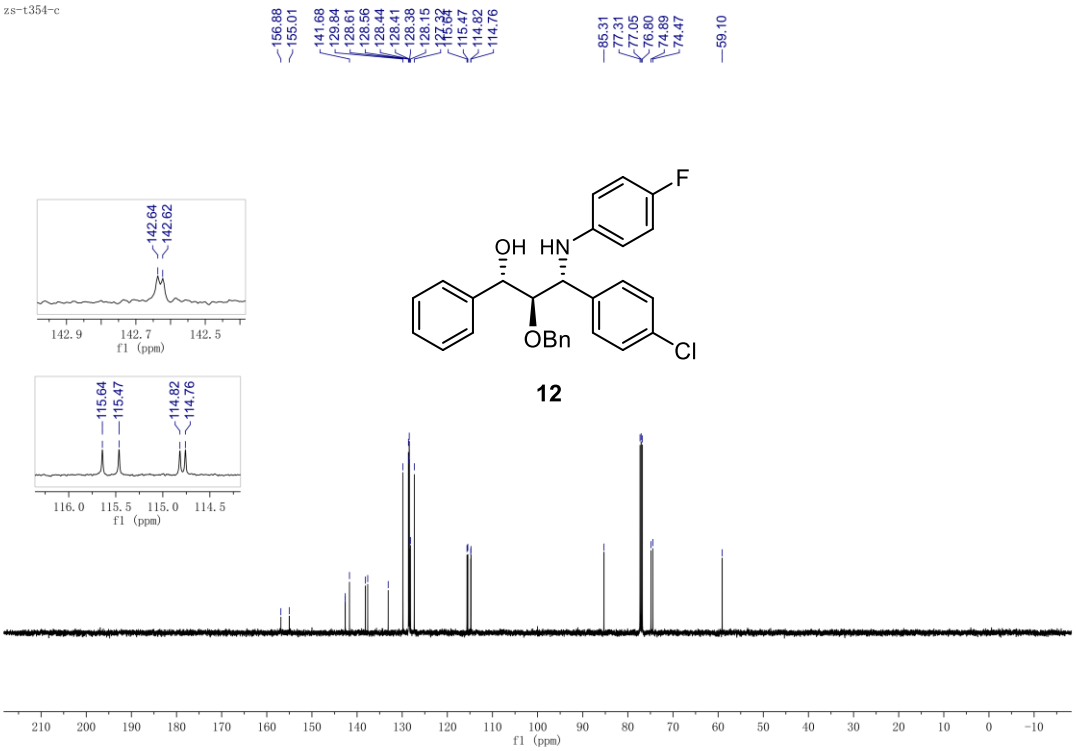
7.26
6.27
6.26
6.25
6.25
6.24
6.24
6.23
6.22
4.68
4.67
4.44
4.42
4.19
3.89
3.86
3.84
3.82
3.82
3.80
3.69
3.66
2.42
0.00
F
OH HN
OBn
Cl
12
12.22
2.00
2.00
2.00
1.00
1.01
1.00
2.01
1.00
1.00
f1 (ppm)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128.61
128.56
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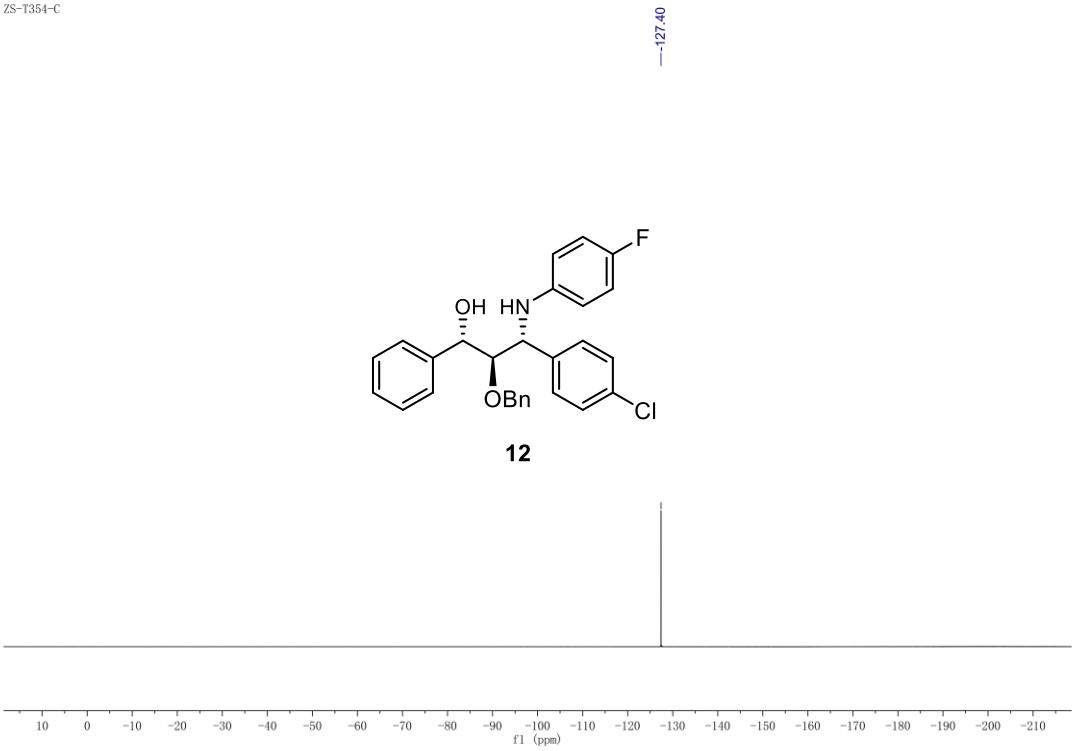
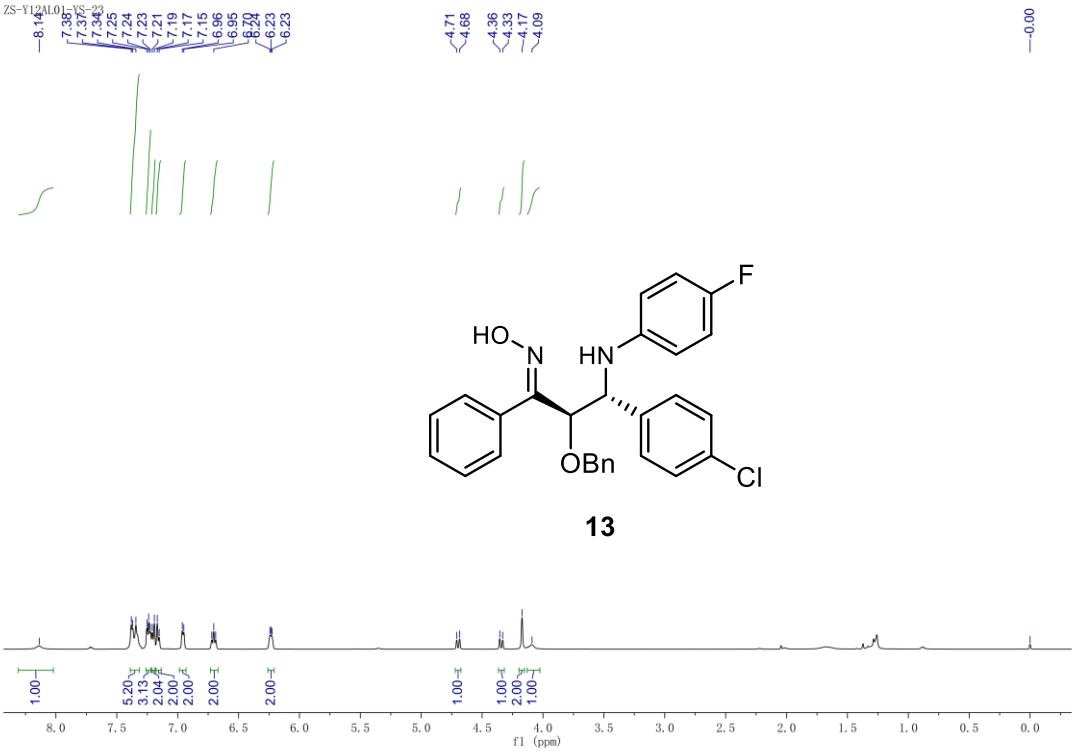
128.41
128.38
128.15
115.47
114.82
114.76
85.31
77.31
77.05
76.80
74.89
74.47
59.10
142.64
142.62
142.9
142.7
142.5
f1 (ppm)
115.64
115.47
114.82
114.76
116.0
115.5
115.0
114.5
f1 (ppm)
F
OH HN
OBn
Cl
12
f1 (ppm)

ZS-T354-C

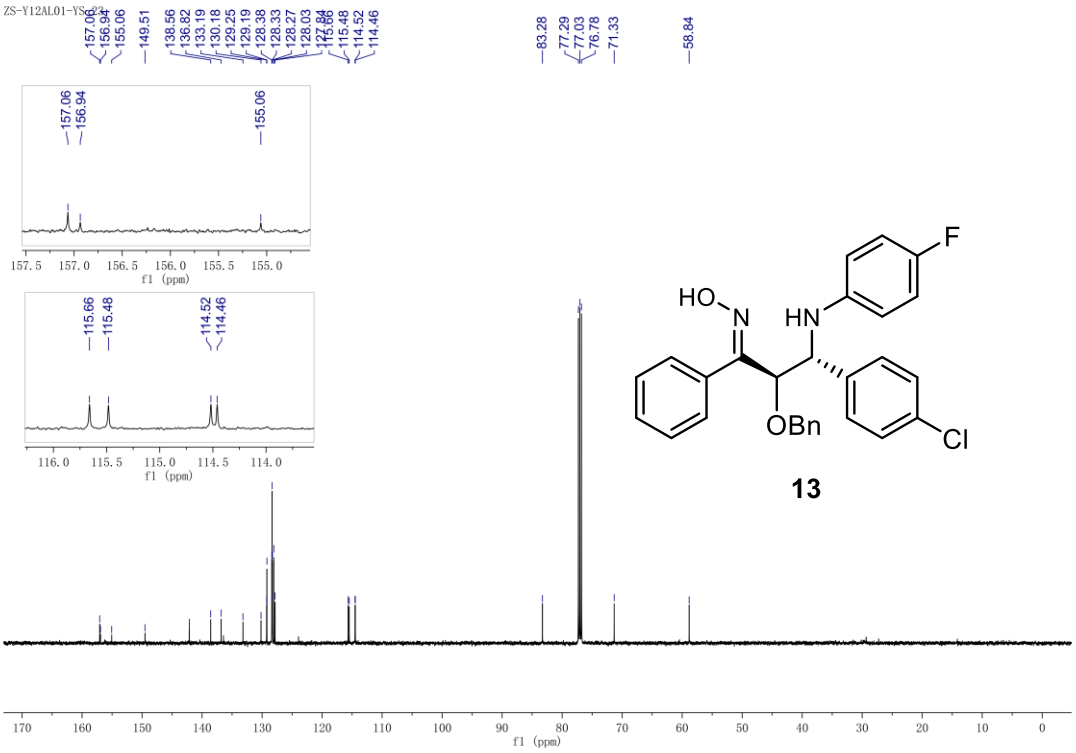


12

ZS-Y12AL01-YS-23



13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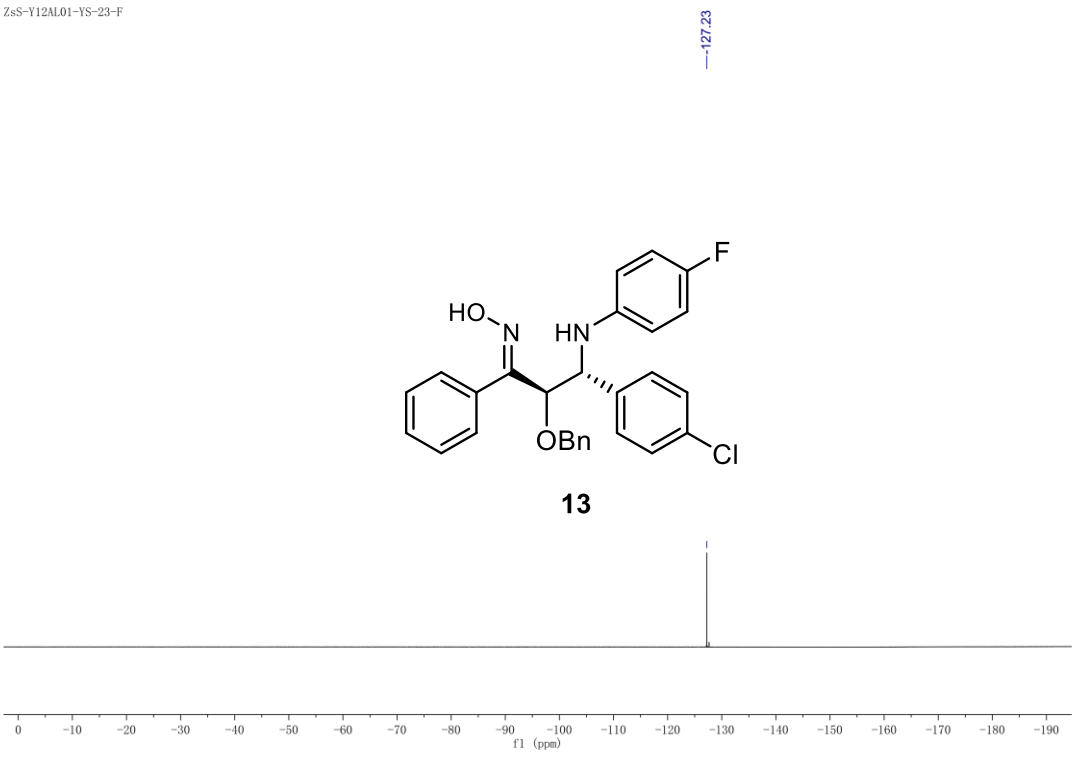
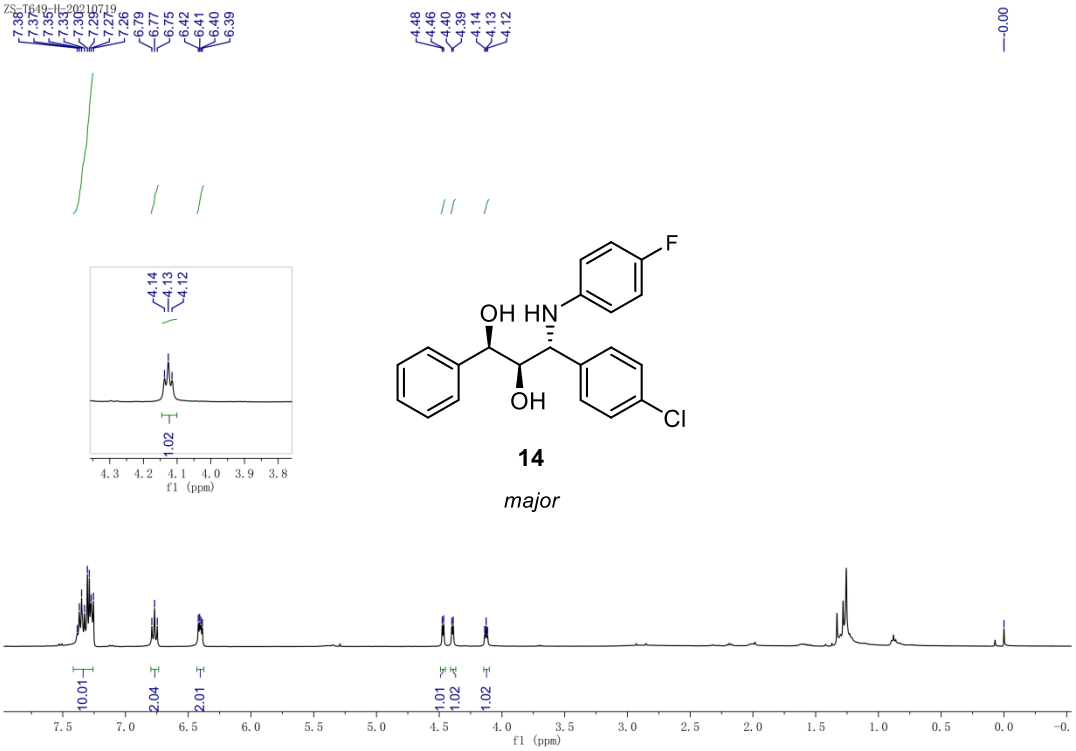
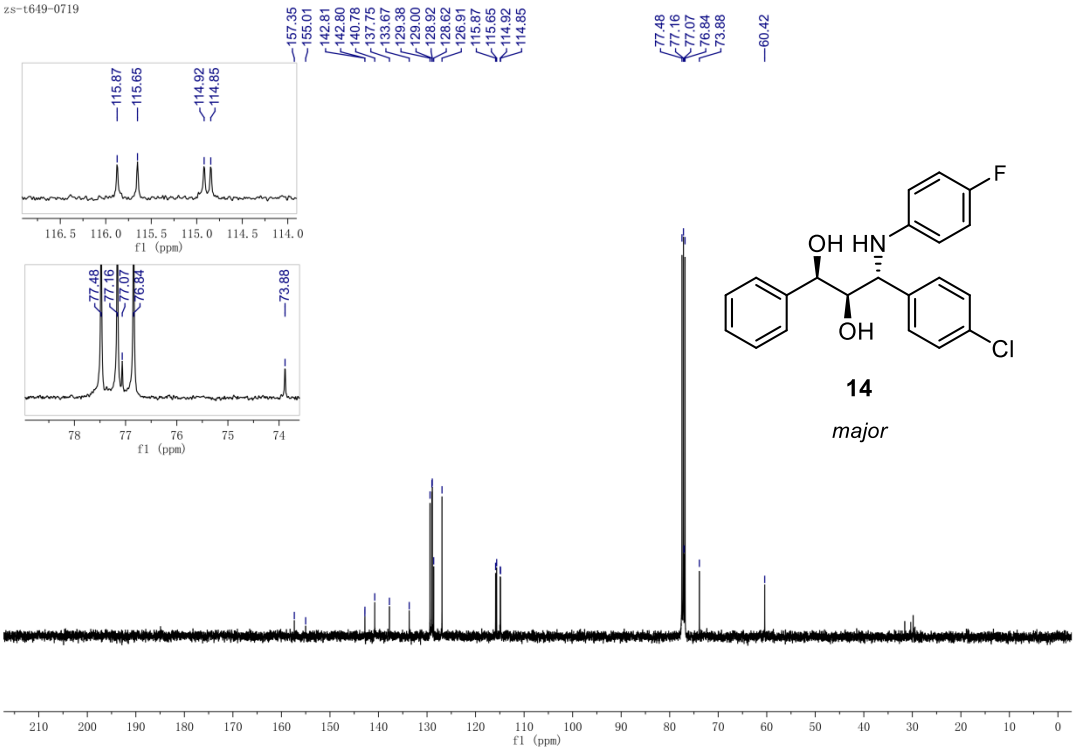
130.18
129.25
129.19
128.38
128.33
128.27
128.03
115.66
115.48
114.52
114.46
83.28
77.29
77.03
76.78
71.33
58.84
f1 (ppm)
HO
N
HN
F
OBn
Cl

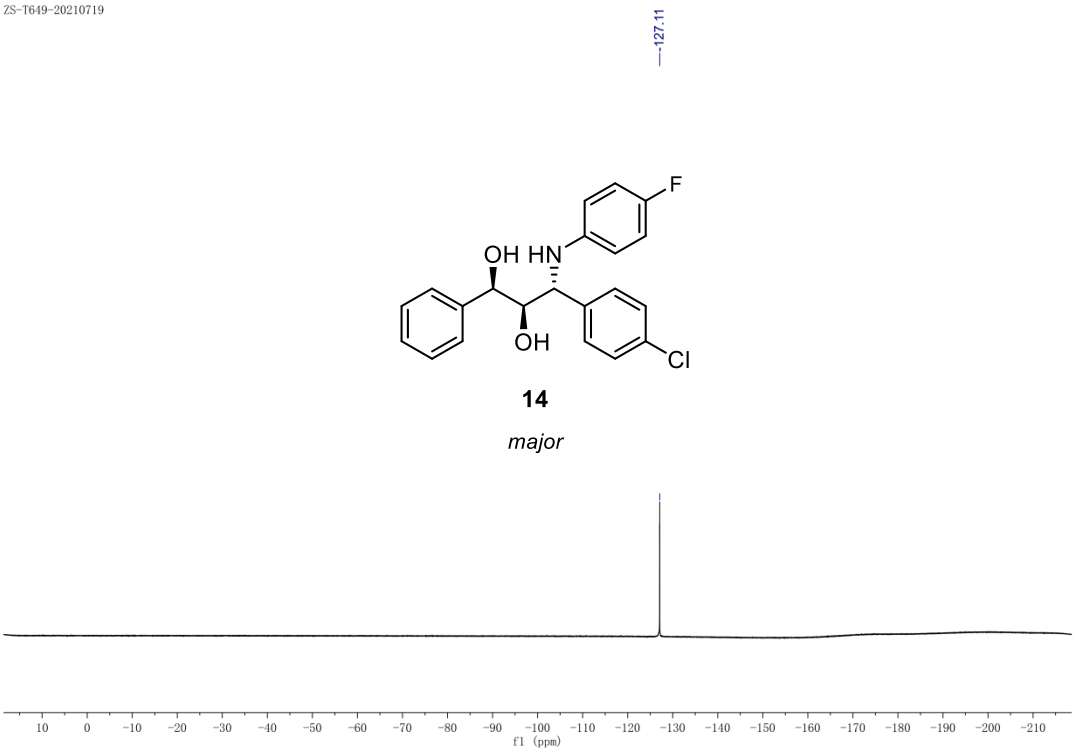
13


ZsS-Y12AL01-YS-23-F
127.23
f1 (ppm)
HO
N
HN
F
OBn
Cl

13


OH HN
OH
F
Cl
14
major


OH HN
OH
F
Cl
14
major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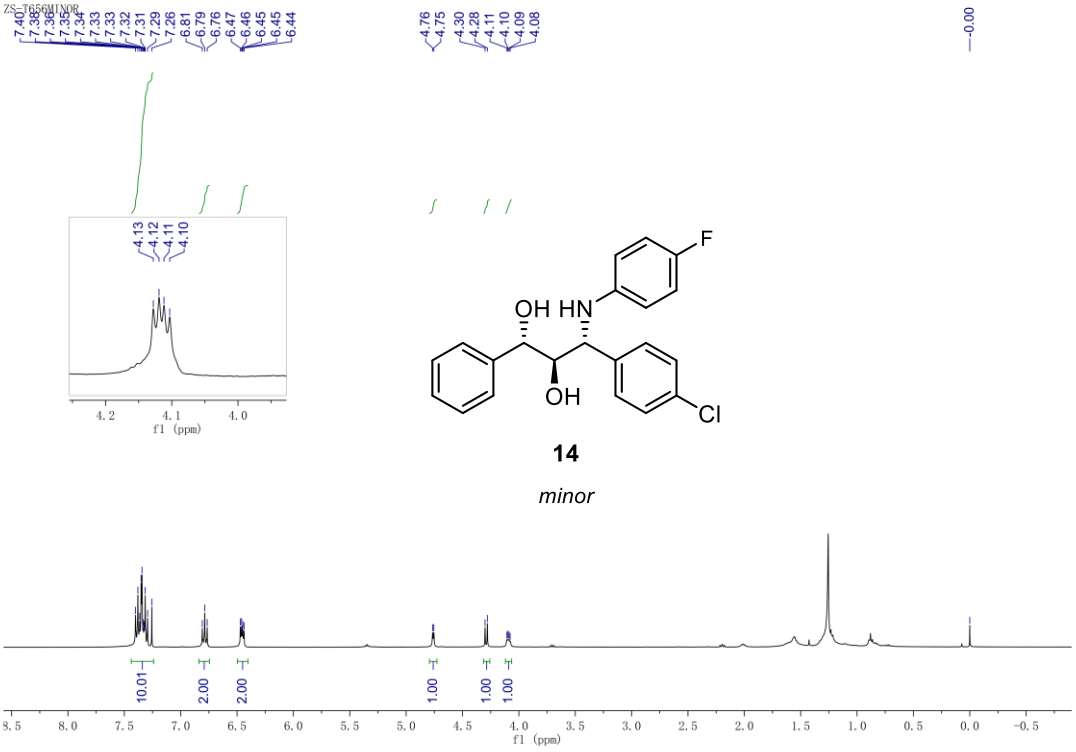
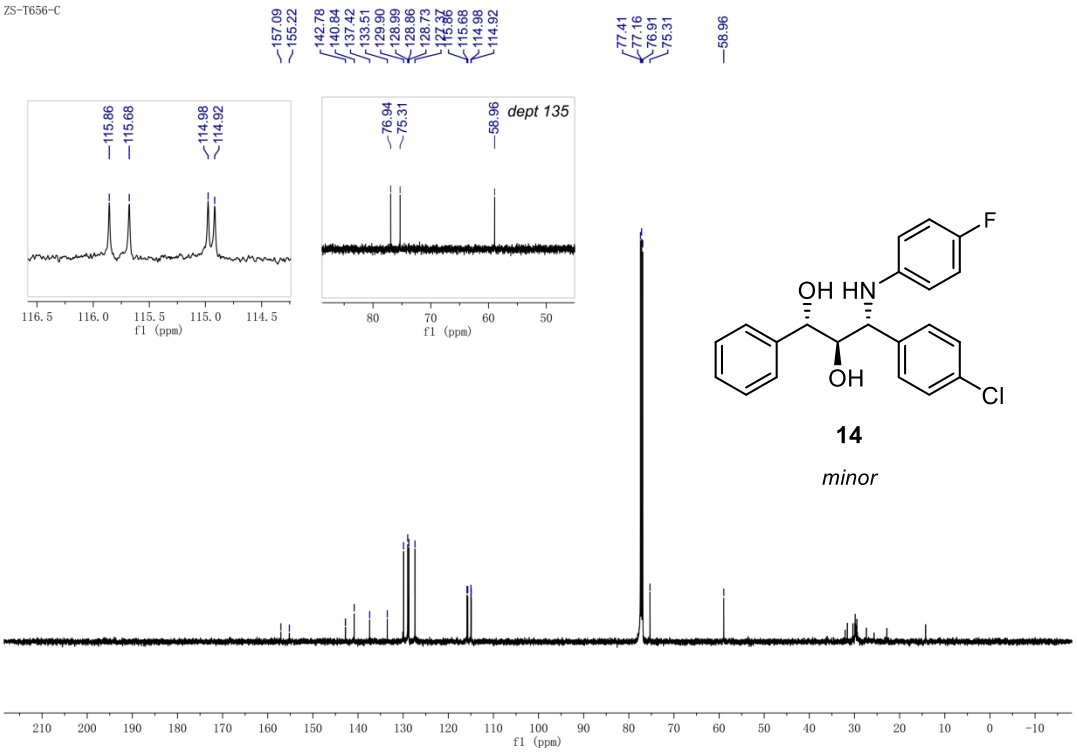
-127.11
F
OH HN
OH
Cl
14
major
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)


ZS-T656HTNOR
7.40 7.38 7.36 7.35 7.34 7.33 7.32 7.31 7.29 7.26 6.81 6.79 6.76 6.47 6.46 6.45 6.45 6.44
4.76 4.75 4.30 4.28 4.11 4.10 4.09 4.08
-0.00
4.13 4.12 4.11 4.10
4.2 4.1 4.0
f1 (ppm)
F
OH HN
OH
Cl
14
minor
10.01 2.00 2.00 1.00 1.00 1.00
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


ZS-T656-C
157.09
155.22
142.78
140.84
137.42
133.51
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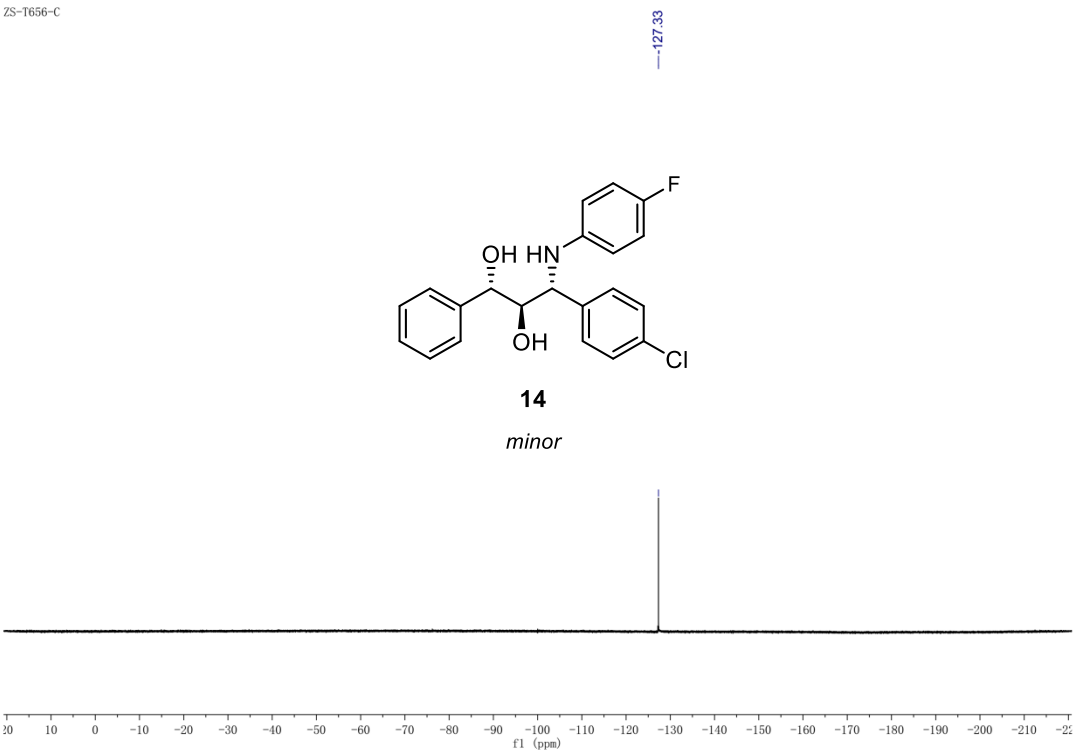
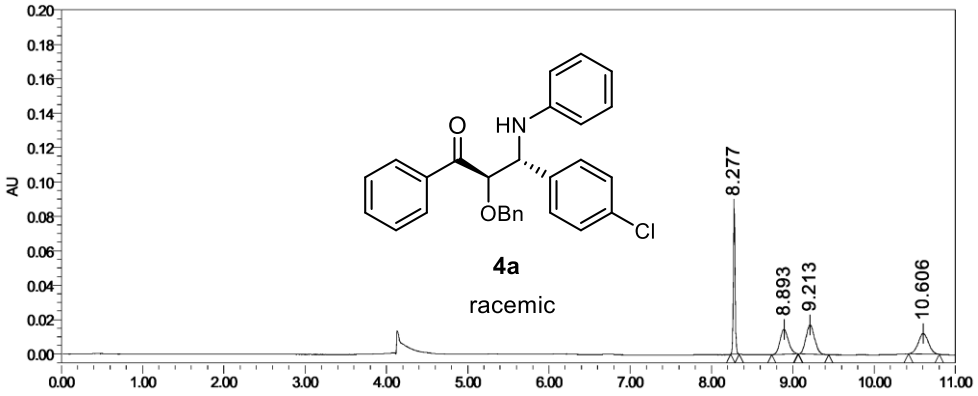
128.99
128.86
128.73
127.37
115.86
115.68
114.98
114.92
77.41
77.16
76.91
75.31
58.96
dept 135
F
OH HN
OH
Cl
14
minor
f1 (ppm)

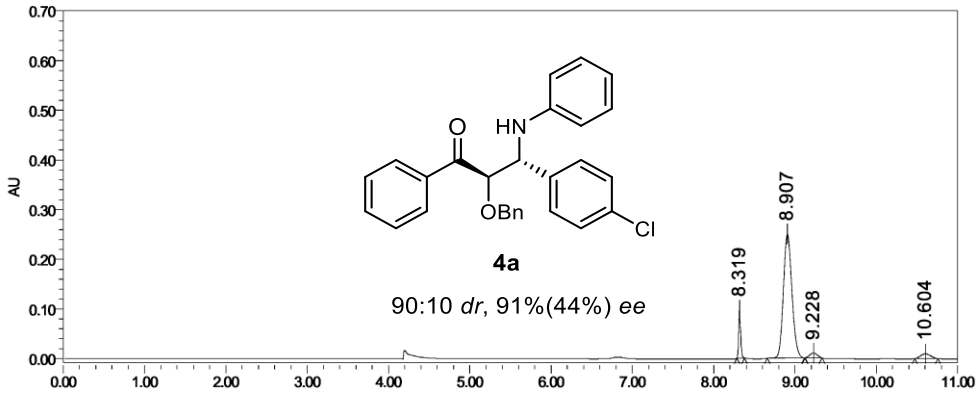

ZS-T656-C
-127.33
F
OH HN
OH
Cl
14
minor
f1 (ppm)

Condition：Chrial IB-3, λ = 254 nm, hexane/ethanol = 95:5

flow rate = 1.0 mL/min



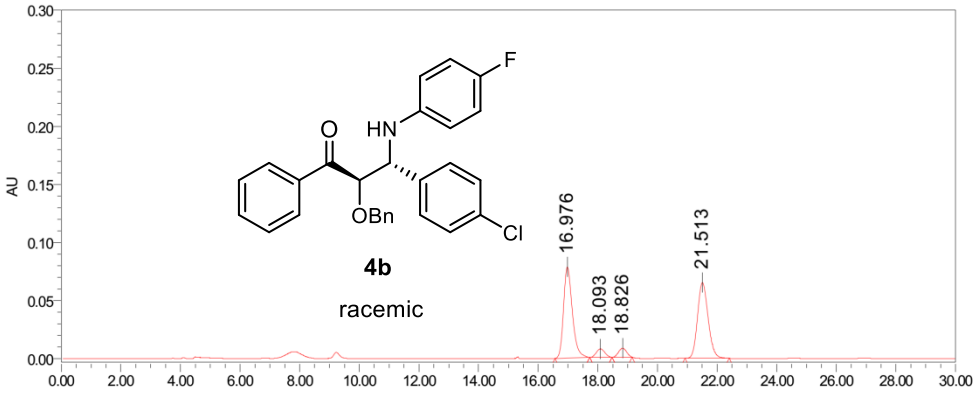
Entry	RT min	Height mV	Area mV.sec	% Area %
1	8.277	84956	133283	28.59
2	8.893	14513	103713	22.25
3	9.213	16988	124964	26.81
4	10.606	11873	104150	22.34



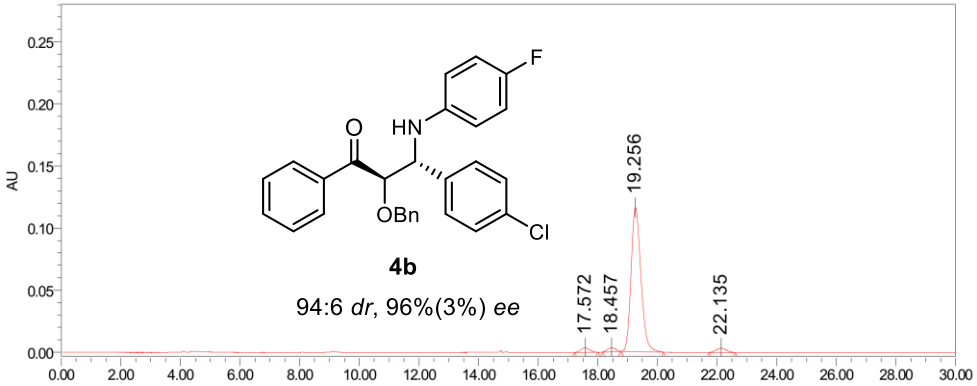
Entry	RT min	Height mV	Area mV.sec	% Area %
1	8.319	96982	158989	7.47
2	8.907	249675	1826673	85.81
3	9.228	9587	60997	2.87
4	10.604	9735	82087	3.86

Condition：Chrial IF-3, λ = 254 nm, hexane/ethanol = 99:1

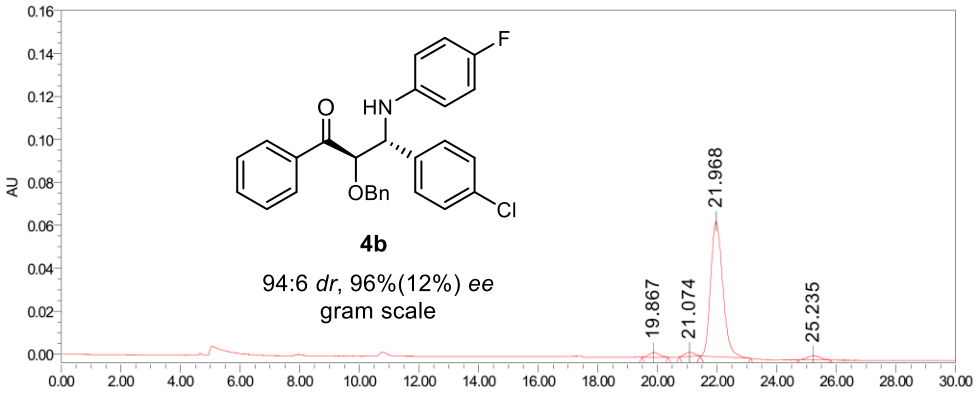
flow rate = 1.0 mL/min



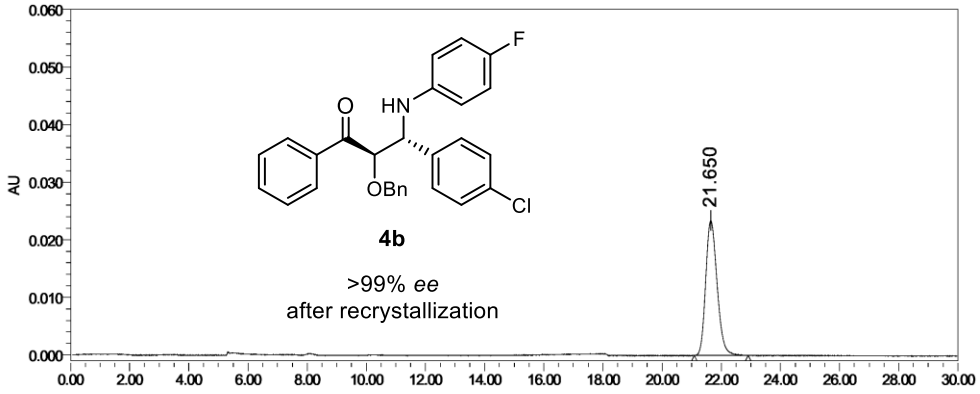
Entry	RT min	Height mV	Area mV.sec	% Area %
1	16.976	78243	1606349	45.94
2	18.093	7217	142489	4.07
3	18.826	7708	142503	4.08
4	21.513	65112	1605627	45.91



Entry	RT min	Height mV	Area mV.sec	% Area %
1	17.572	3712	77226	2.68
2	18.457	3243	61019	2.12
3	19.256	116121	2659701	92.30
4	22.135	3480	83531	2.90



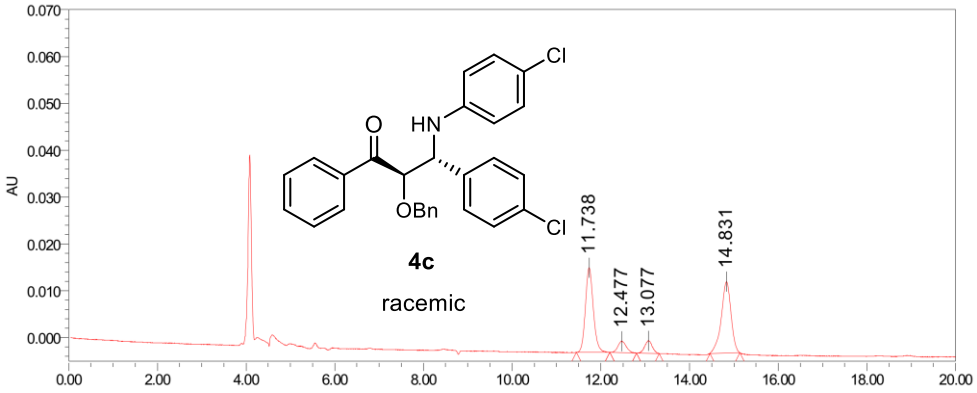
Entry	RT min	Height mV	Area mV.sec	% Area %
1	19.867	2124	50363	2.64
2	21.074	1912	42092	2.21
3	21.968	63021	1757268	92.23
4	25.235	1849	55504	2.91



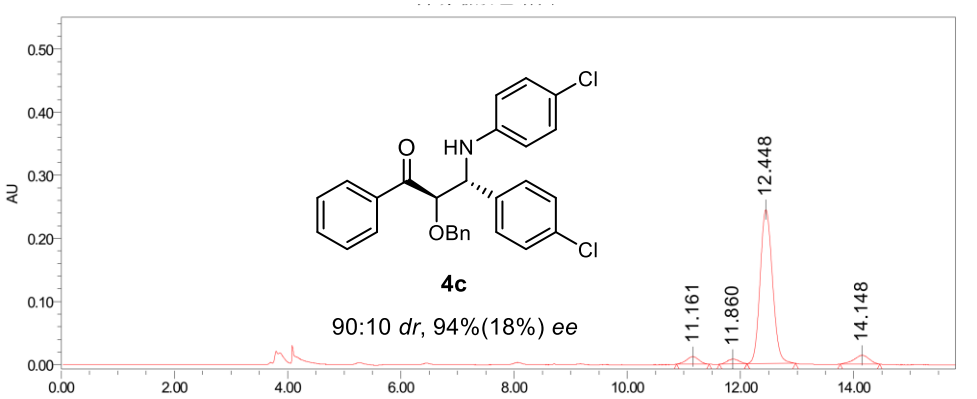
Entry	RT min	Height mV	Area mV.sec	% Area %
1	21.650	23449	624324	>99.9

Condition：Chrial IF-3, λ = 220 nm, hexane/ethanol = 97:3

flow rate = 1.0 mL/min



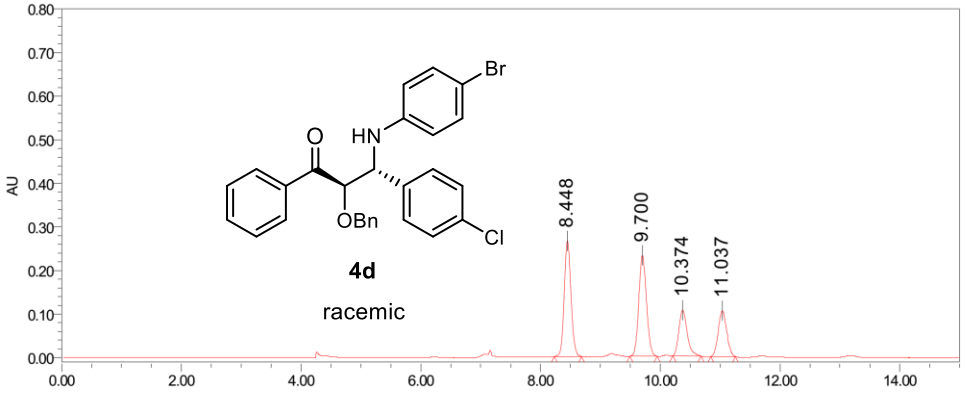
Entry	RT min	Height mV	Area mV.sec	% Area %
1	11.738	18060	221898	42.96
2	12.477	2434	31444	6.09
3	13.077	2690	31337	6.07
4	14.831	15259	231841	44.98



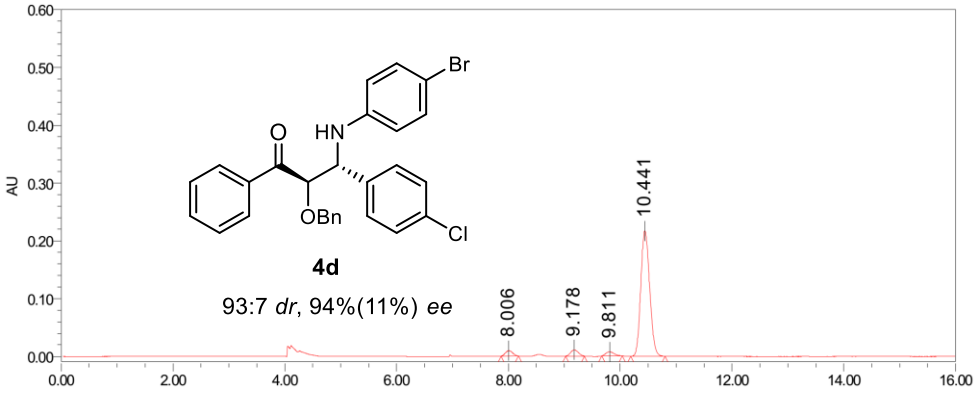
Entry	RT min	Height mV	Area mV.sec	% Area %
1	11.161	11817	180121	4.25
2	11.860	7531	108177	2.55
3	12.448	243713	3692271	87.11
4	14.148	13786	258222	6.09

Condition：Chrial IB-3, λ = 260 nm, hexane/ethanol = 95:5

flow rate = 1.0 mL/min



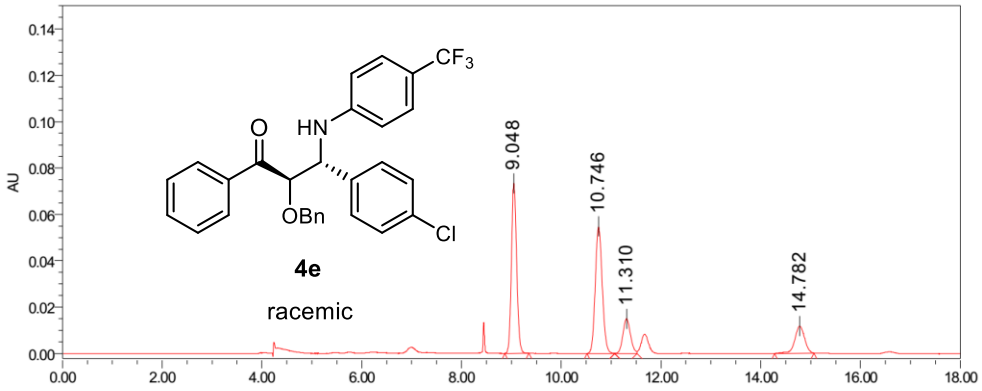
Entry	RT min	Height mV	Area mV.sec	% Area %
1	8.448	265014	2081843	33.55
2	9.700	231773	2081095	33.54
3	10.374	104998	1020552	16.45
4	11.037	104803	1021154	16.46



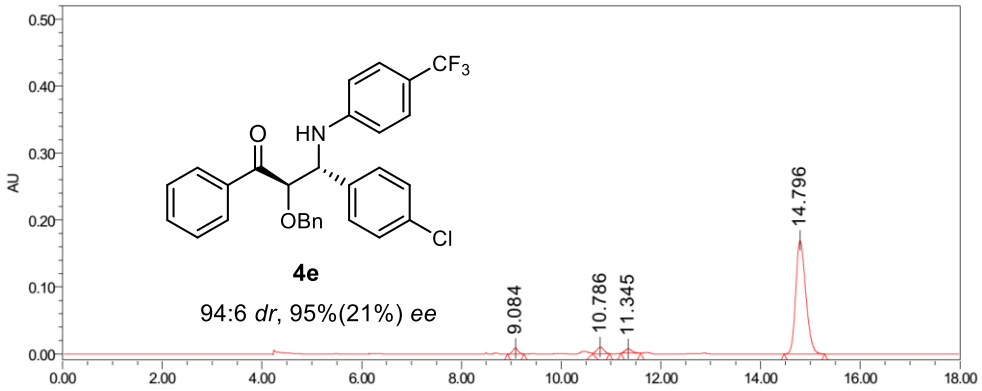
Entry	RT min	Height mV	Area mV.sec	% Area %
1	8.006	9311	82090	3.09
2	9.178	10588	102607	3.87
3	9.811	7103	74763	2.82
4	10.441	217040	2393844	90.22

Condition：Chrial IB-3, λ = 270 nm, hexane/ethanol = 97:3

flow rate = 1.0 mL/min



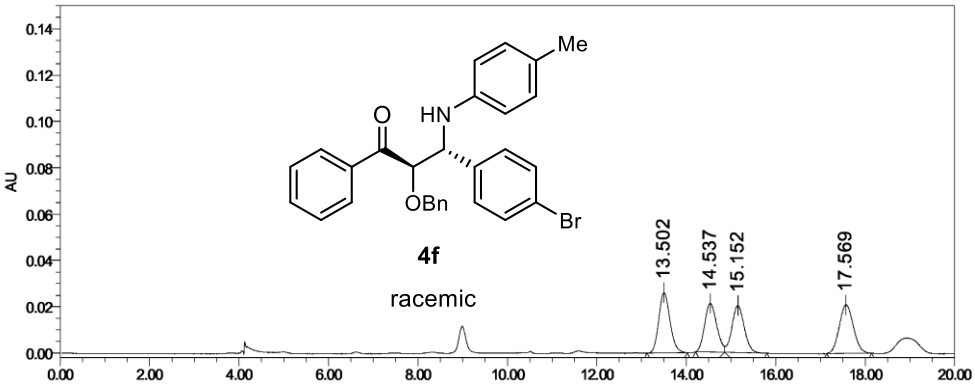
Entry	RT min	Height mV	Area mV.sec	% Area %
1	9.048	73413	533839	38.56
2	10.746	54804	534827	38.63
3	11.31	14971	158018	11.41
4	14.782	11641	157904	11.40



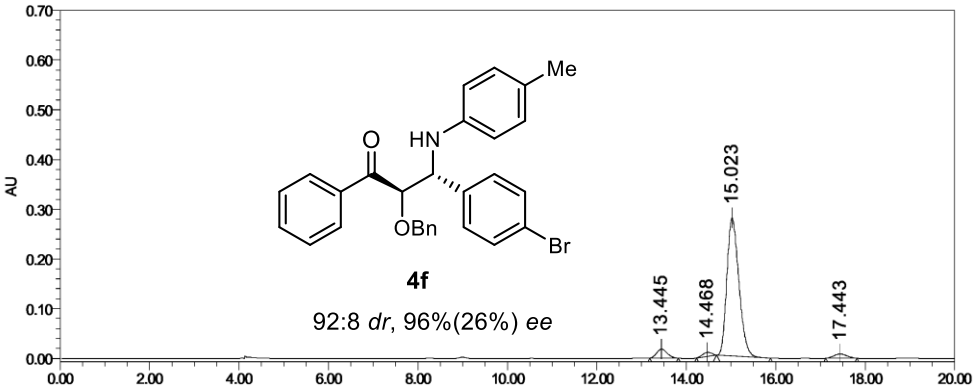
Entry	RT min	Height mV	Area mV.sec	% Area %
1	9.084	8498	62327	2.41
2	10.786	9964	96457	3.74
3	11.345	6377	65459	2.54
4	14.796	169151	2357518	91.31

Condition：Chrial IF-3, λ = 254 nm, hexane/ethanol = 98:2

flow rate = 1.0 mL/min



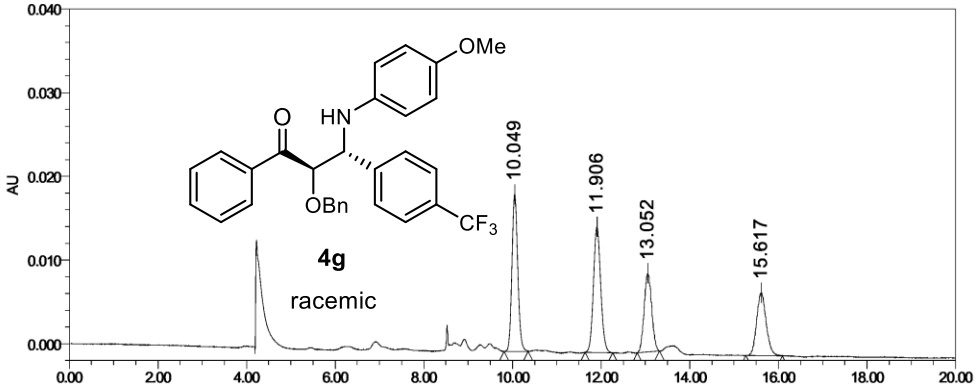
Entry	RT min	Height mV	Area mV.sec	% Area %
1	13.502	26083	456580	26.84
2	14.537	21039	395844	23.27
3	15.152	20337	390969	22.99
4	17.569	20940	457502	26.90



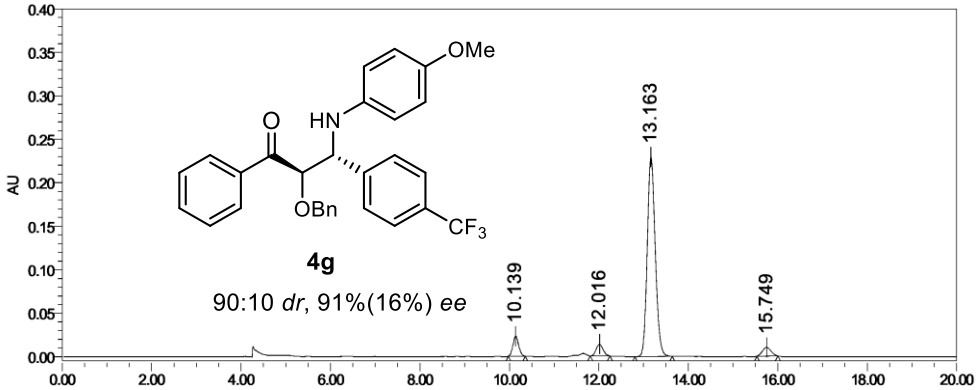
Entry	RT min	Height mV	Area mV.sec	% Area %
1	13.445	17867	293089	5.09
2	14.468	8023	115002	2.00
3	15.023	277846	5182175	89.97
4	17.443	8547	169871	2.95

Condition：Chrial IB-3, λ = 254 nm, hexane/ethanol = 97:3

flow rate = 1.0 mL/min



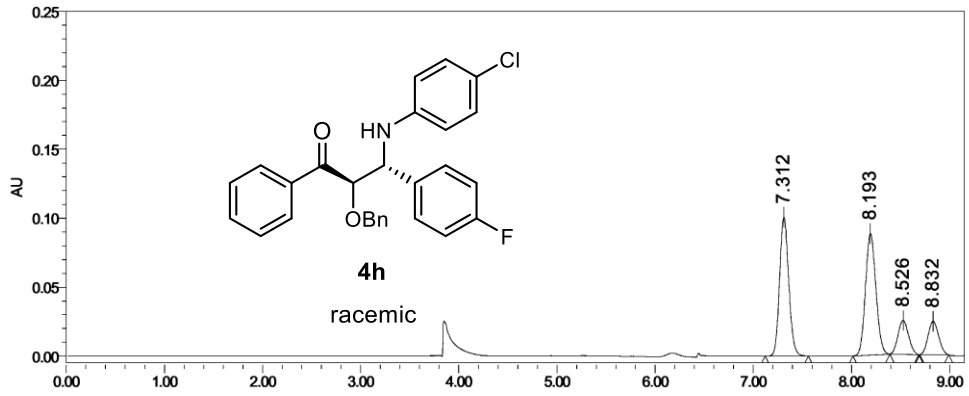
Entry	RT min	Height mV	Area mV.sec	% Area %
1	10.049	18783	170283	30.16
2	11.906	15007	169750	30.07
3	13.052	9410	112360	19.90
4	15.617	7525	112215	19.87



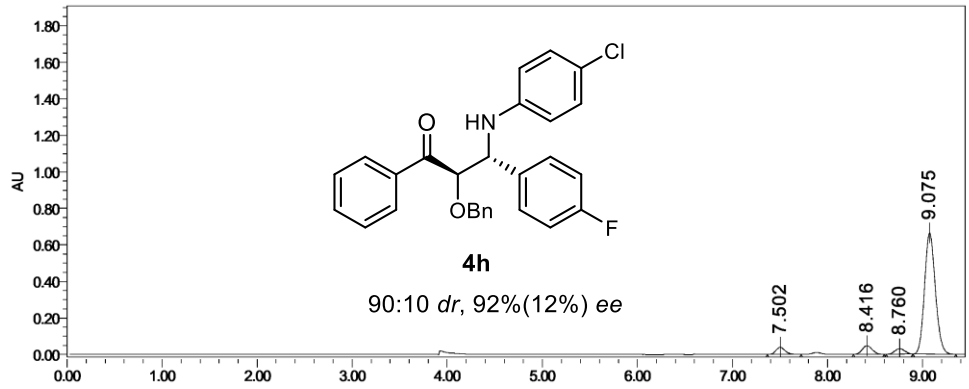
Entry	RT min	Height mV	Area mV.sec	% Area %
1	10.139	22887	203662	6.11
2	12.016	13473	145227	4.35
3	13.163	229635	2852491	85.53
4	15.749	9858	133855	4.01

Condition：Chrial IB-3, λ = 254 nm, hexane/ethanol = 95:5

flow rate = 1.0 mL/min



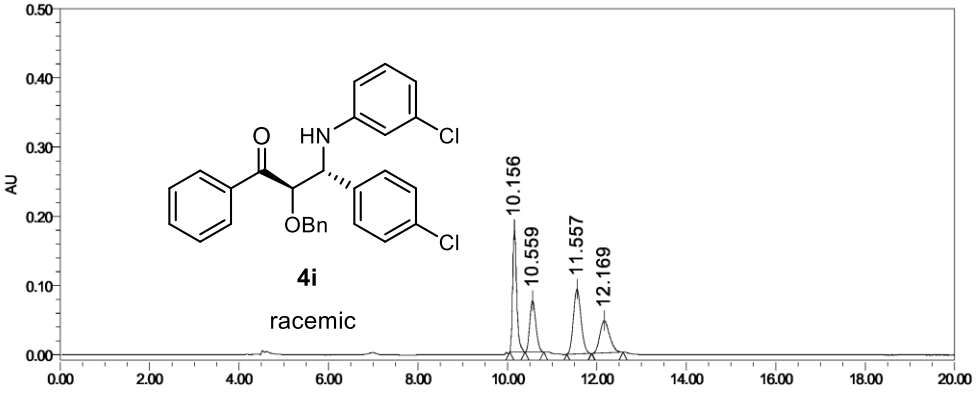
Entry	RT min	Height mV	Area mV.sec	% Area %
1	7.312	100587	651267	39.06
2	8.193	88189	651503	39.08
3	8.526	24525	182191	10.93
4	8.832	24221	182342	10.94



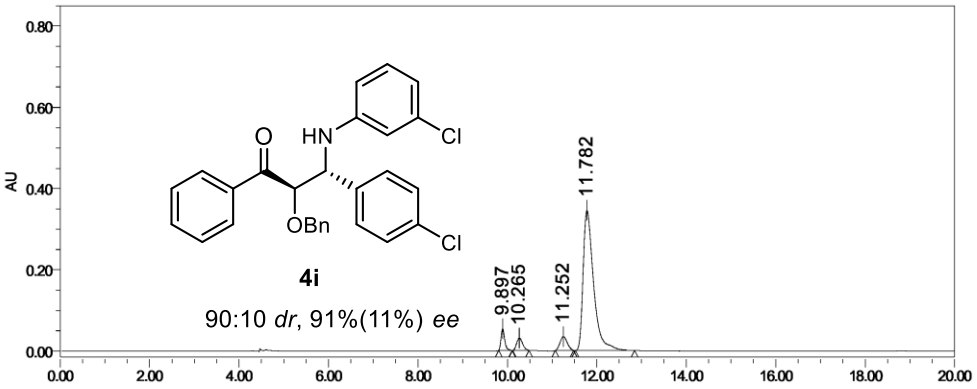
Entry	RT min	Height mV	Area mV.sec	% Area %
1	7.502	39727	268508	4.39
2	8.416	47296	345087	5.64
3	8.76	29574	215418	3.52
4	9.075	662767	5288067	86.45

Condition：Chrial ID-3, λ = 254 nm, hexane/ethanol = 98:2

flow rate = 1.0 mL/min



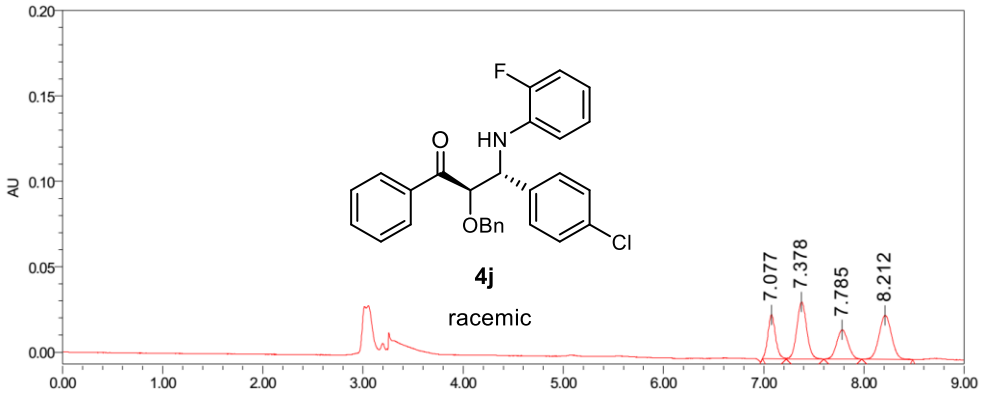
Entry	RT min	Height mV	Area mV.sec	% Area %
1	10.156	176607	1110540	30.56
2	10.559	74451	707054	19.46
3	11.557	93608	1114630	30.68
4	12.169	46415	701159	19.30



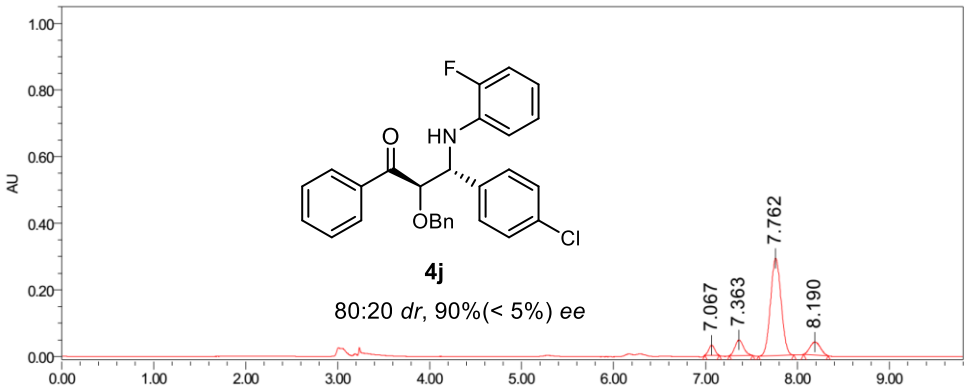
Entry	RT min	Height mV	Area mV.sec	% Area %
1	9.897	53517	302998	4.61
2	10.265	30248	279383	4.25
3	11.252	33853	377044	5.74
4	11.782	345139	5609154	85.39

Condition：Chrial IF-3, λ = 220 nm, hexane/ethanol = 97:3

flow rate = 1.0 mL/min



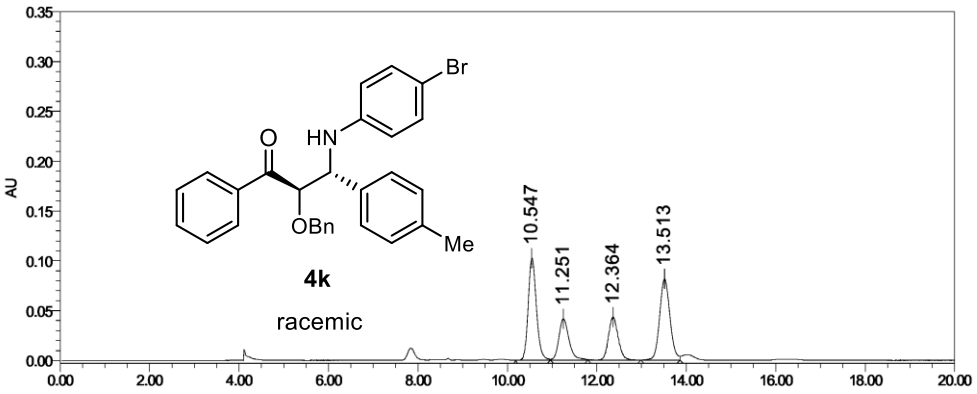
Entry	RT min	Height mV	Area mV.sec	% Area %
1	7.077	25728	134934	18.61
2	7.378	33312	228615	31.53
3	7.785	17137	136931	18.89
4	8.212	25683	224566	30.97



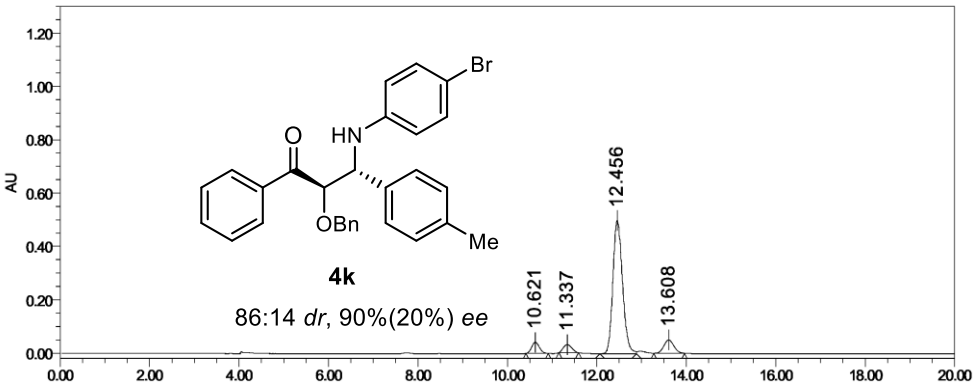
Entry	RT min	Height mV	Area mV.sec	% Area %
1	7.067	30558	139587	4.54
2	7.363	46731	302100	9.83
3	7.762	292063	2324321	75.66
4	8.190	39258	306140	9.97

Condition：Chrial IF-3, λ = 254 nm, hexane/ethanol = 97:3

flow rate = 1.0 mL/min



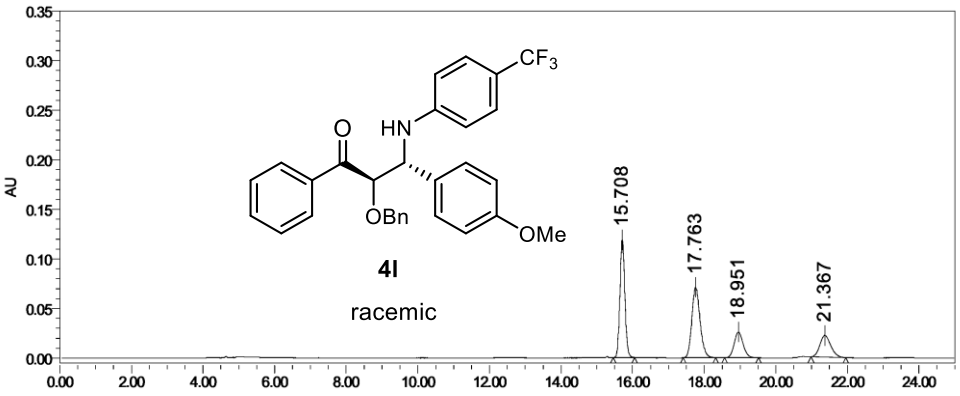
Entry	RT min	Height mV	Area mV.sec	% Area %
1	10.547	102469	1301965	33.21
2	11.251	41473	657304	16.77
3	12.364	43136	649888	16.58
4	13.513	81400	1311246	33.45



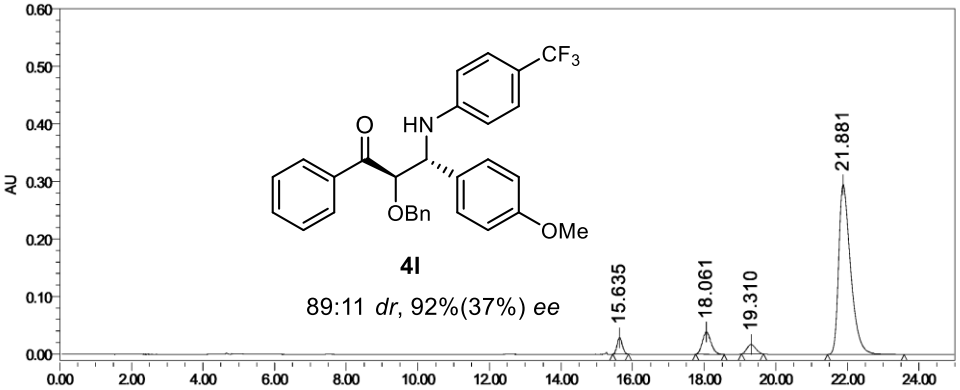
Entry	RT min	Height mV	Area mV.sec	% Area %
1	10.621	42065	507151	5.60
2	11.337	30107	400597	4.42
3	12.456	499064	7378670	81.46
4	13.608	49591	771259	8.51

Condition：Chrial IB-3, λ = 254 nm, hexane/ethanol = 99:1

flow rate = 1.0 mL/min



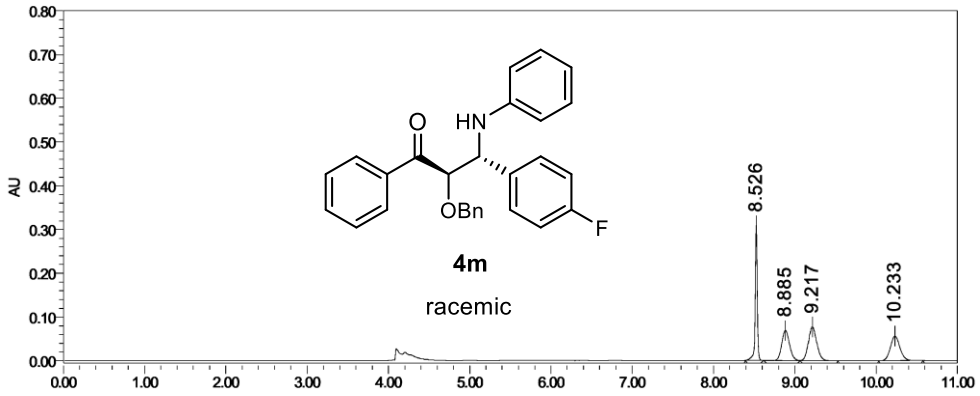
Entry	RT min	Height mV	Area mV.sec	% Area %
1	15.708	118791	1131646	35.55
2	17.763	70916	1127958	35.43
3	18.951	26156	457981	14.39
4	21.367	21875	465922	14.64



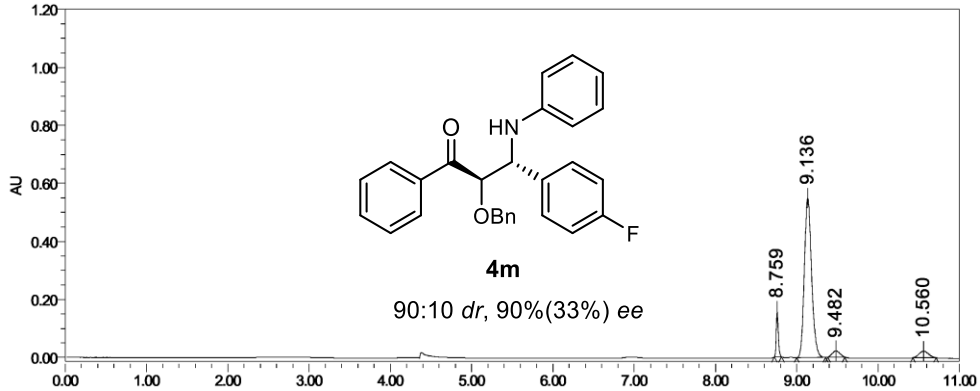
Entry	RT min	Height mV	Area mV.sec	% Area %
1	15.635	28585	291109	3.61
2	18.061	38567	640337	7.94
3	19.310	16390	279045	3.46
4	21.881	295063	6850690	84.98

Condition：Chrial IB-3, λ = 254 nm, hexane/ethanol = 97:3

flow rate = 1.0 mL/min



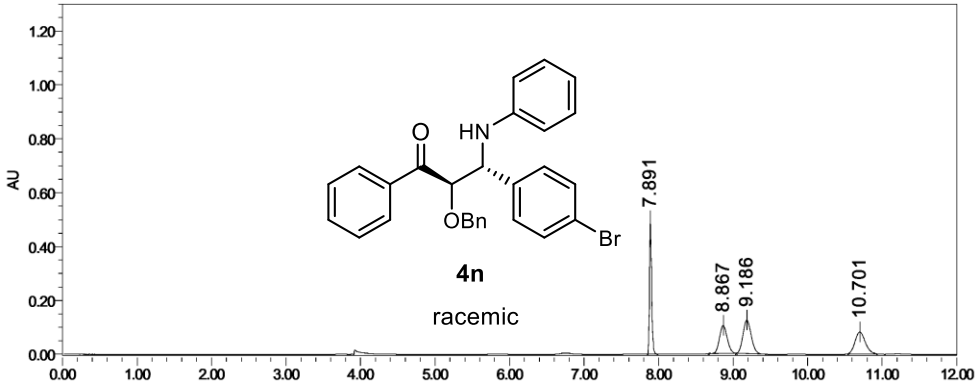
Entry	RT min	Height mV	Area mV.sec	% Area %
1	8.526	312219	553046	27.35
2	8.885	68755	460755	22.78
3	9.217	76982	548552	27.12
4	10.233	56089	459997	22.75



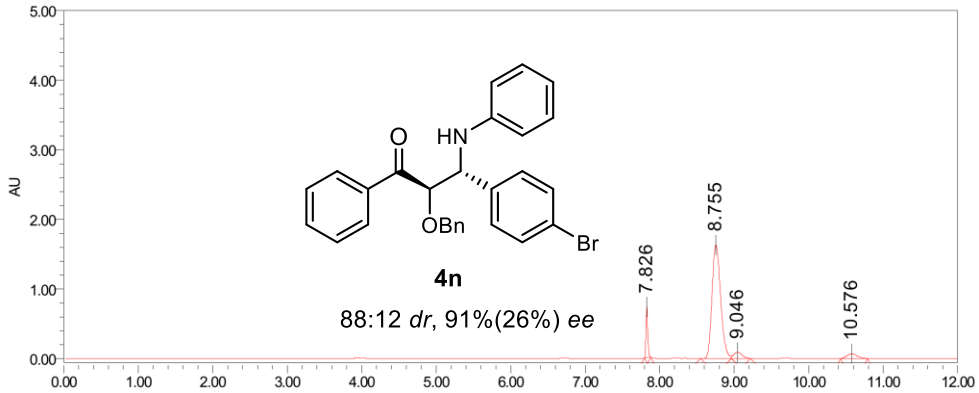
Entry	RT min	Height mV	Area mV.sec	% Area %
1	8.759	159030	278818	6.94
2	9.136	551014	3413702	84.98
3	9.482	21288	138927	3.46
4	10.560	22501	185709	4.62

Condition：Chrial IB-3, λ = 254 nm, hexane/ethanol = 97:3

flow rate = 1.0 mL/min



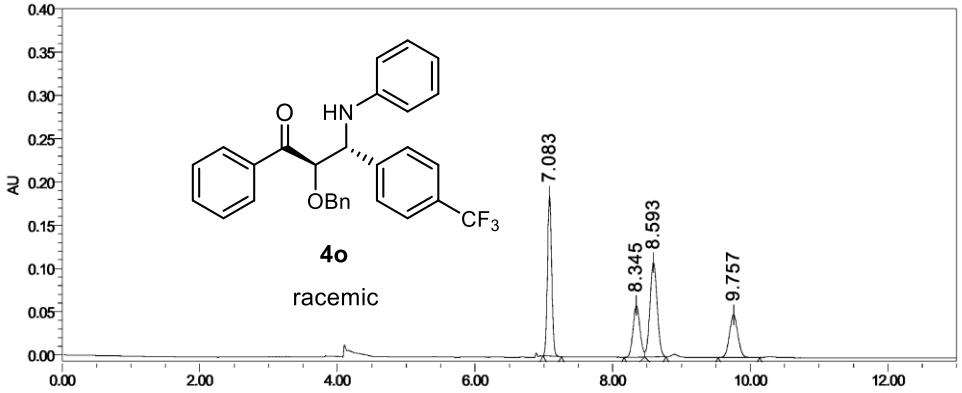
Entry	RT min	Height mV	Area mV.sec	% Area %
1	7.891	494367	1001021	28.78
2	8.867	103229	743659	21.38
3	9.186	124458	963936	27.72
4	10.701	81288	768969	22.11



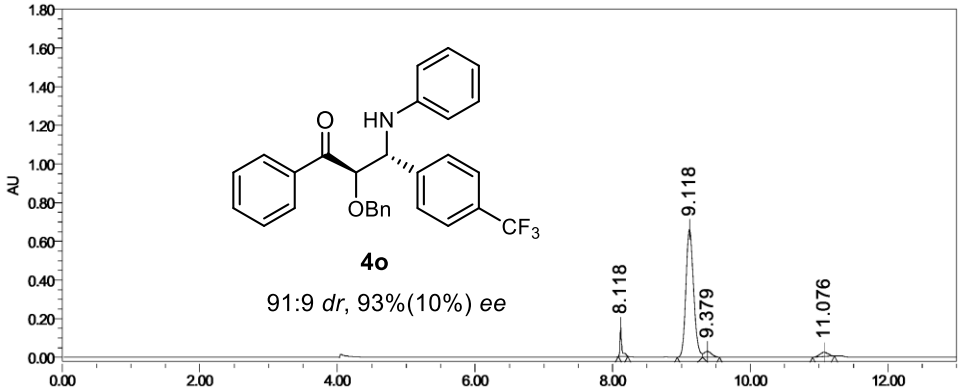
Entry	RT min	Height mV	Area mV.sec	% Area %
1	7.826	728246	1192234	7.67
2	8.755	1631199	13016271	83.73
3	9.051	89270	701904	4.51
4	10.576	66538	635685	4.09

Condition：Chrial IB-3, λ = 254 nm, hexane/ethanol = 98:2

flow rate = 1.0 mL/min



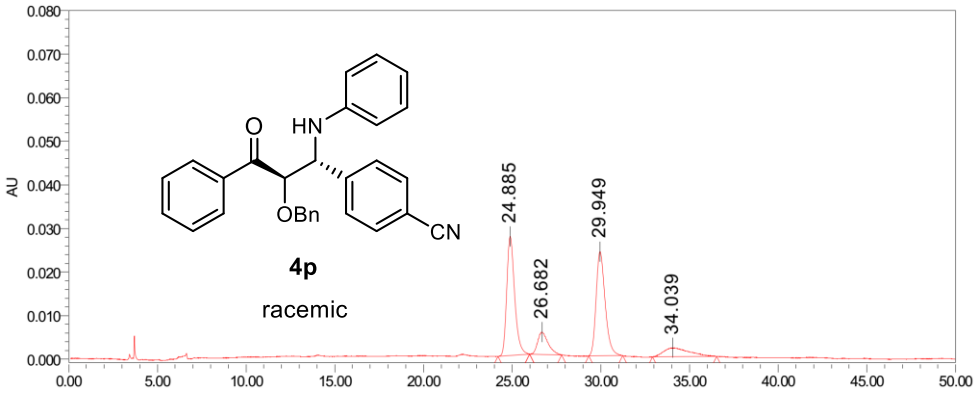
Entry	RT min	Height mV	Area mV.sec	% Area %
1	7.083	185221	790831	32.66
2	8.345	59600	414817	17.13
3	8.593	108966	795201	32.84
4	9.757	49570	420615	17.37



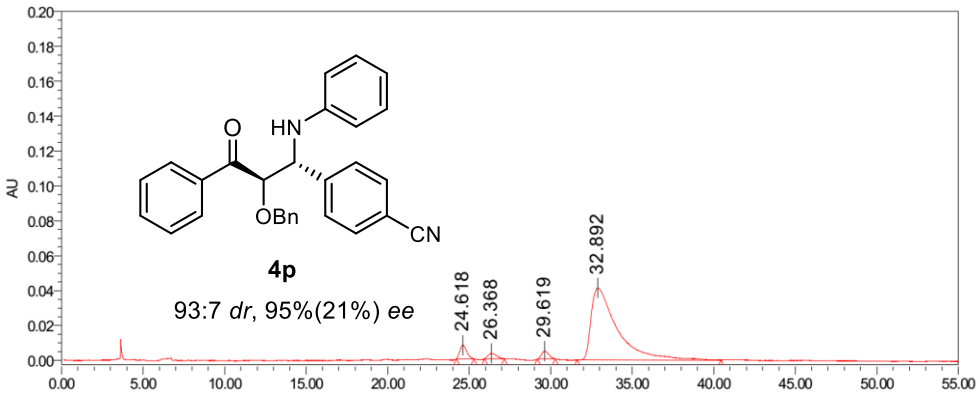
Entry	RT min	Height mV	Area mV.sec	% Area %
1	8.118	150948	283809	4.86
2	9.118	661007	5132698	87.98
3	9.379	29494	231737	3.97
4	11.076	21791	185708	3.18

Condition：Chrial ID-3, λ = 240 nm, hexane/ethanol = 97:3

flow rate = 1.0 mL/min



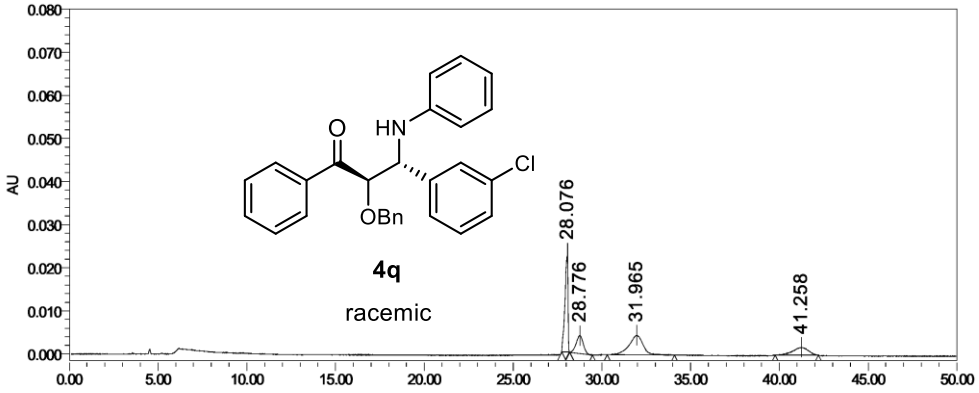
Entry	RT min	Height mV	Area mV.sec	% Area %
1	24.885	27309	840811	40.09
2	26.682	5080	208804	9.96
3	29.949	23880	841464	40.12
4	34.039	2046	206082	9.83



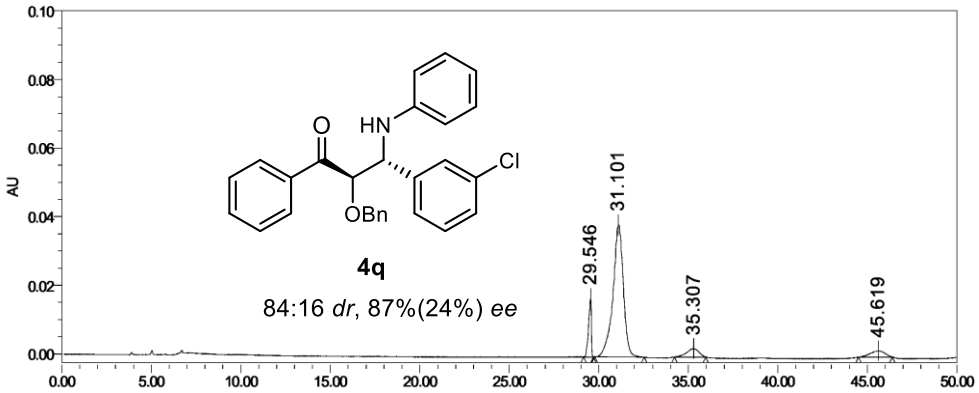
Entry	RT min	Height mV	Area mV.sec	% Area %
1	24.618	7884	229013	4.50
2	26.368	3026	109754	2.15
3	29.619	4490	142052	2.79
4	32.892	41348	4613428	90.56

Condition：Chrial Y1, λ = 254 nm, hexane/ethanol = 995:5

flow rate = 1.0 mL/min



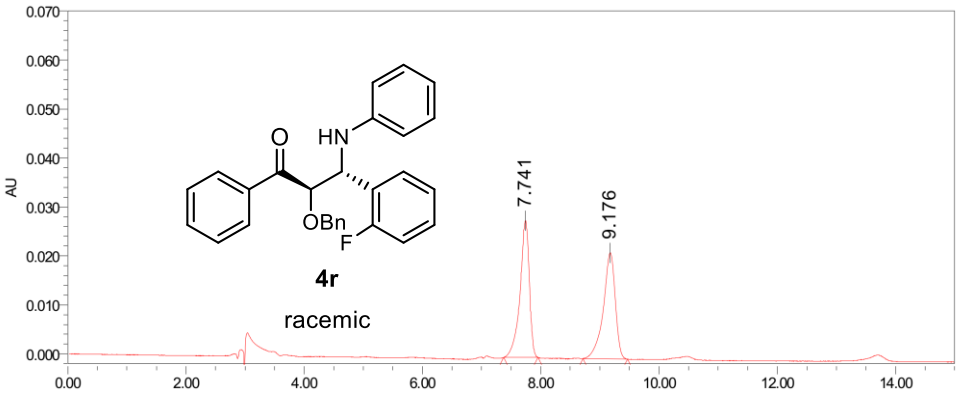
Entry	RT min	Height mV	Area mV.sec	% Area %
1	28.076	22922	265884	35.83
2	28.776	4170	114371	15.41
3	31.965	4528	247970	33.42
4	41.258	1824	113786	15.33



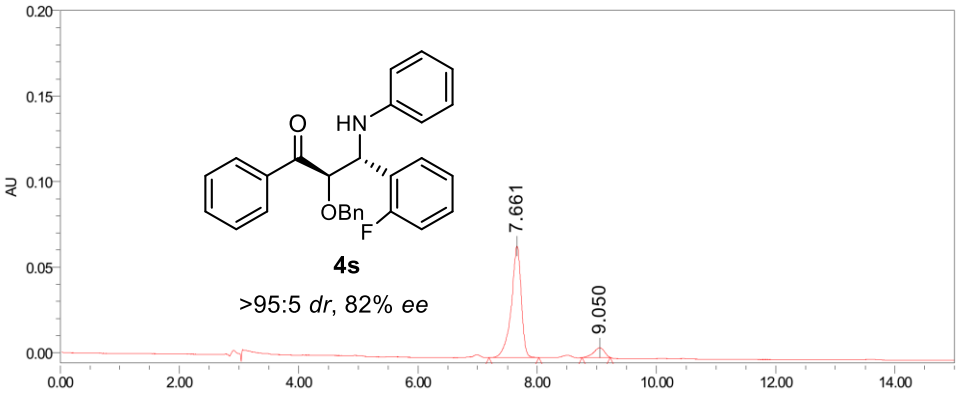
Entry	RT min	Height mV	Area mV.sec	% Area %
1	29.546	17086	188181	9.65
2	31.101	38594	1541608	79.06
3	35.307	2468	115273	5.91
4	45.619	1829	104918	5.38

Condition：Chrial Y1, λ = 254 nm, hexane/ethanol = 97:3

flow rate = 1.0 mL/min



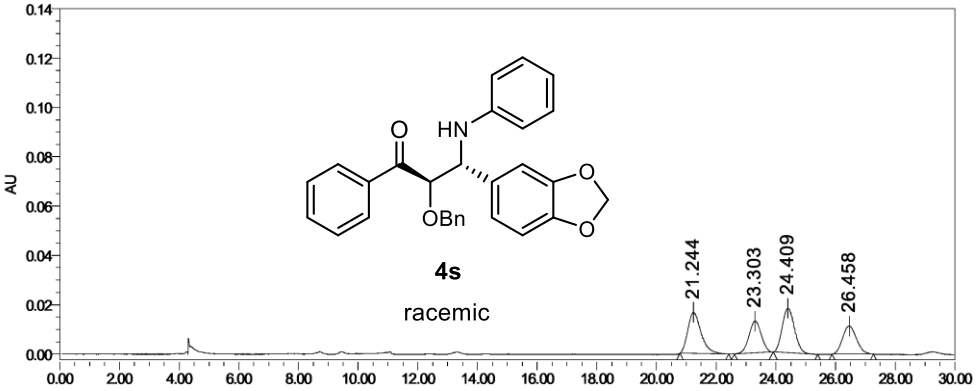
Entry	RT min	Height mV	Area mV.sec	% Area %
1	7.741	27922	305210	50.19
2	9.176	21685	302912	49.81



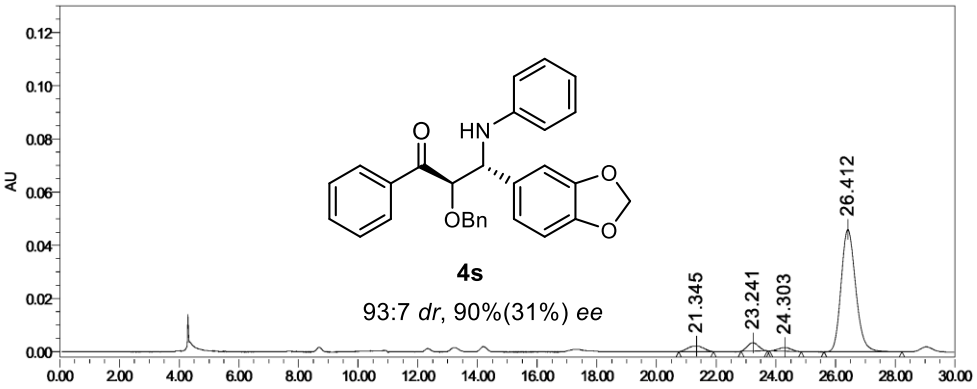
Entry	RT min	Height mV	Area mV.sec	% Area %
1	7.661	65131	750499	91.33
2	9.050	5698	71290	8.67

Condition：Chrial IF-3, λ = 254 nm, hexane/ethanol = 98:2

flow rate = 1.0 mL/min



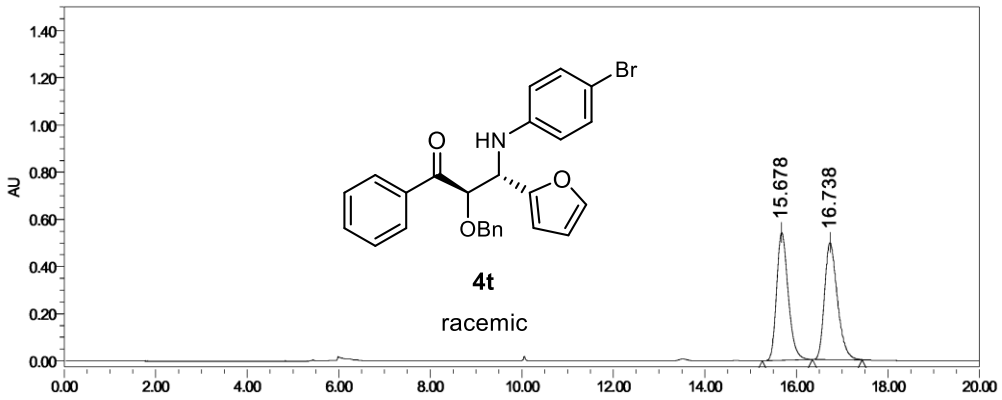
Entry	RT min	Height mV	Area mV.sec	% Area %
1	21.244	16628	513969	29.10
2	23.303	12871	368603	20.87
3	24.409	18046	512331	29.01
4	26.458	11419	371387	21.03



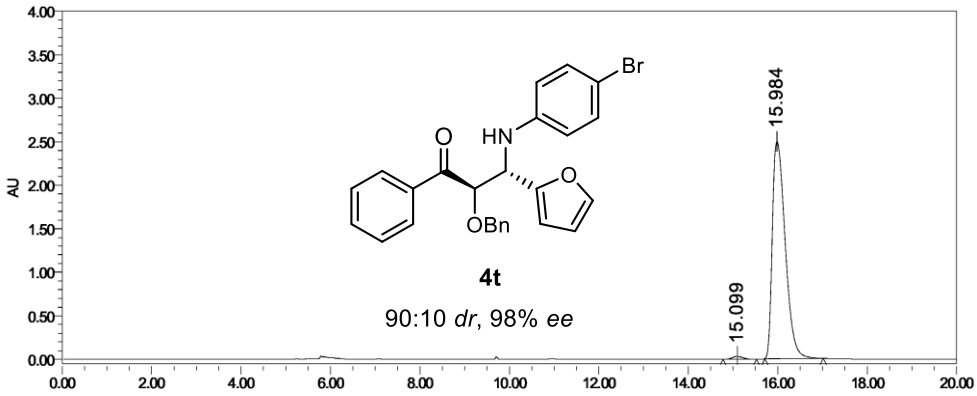
Entry	RT min	Height mV	Area mV.sec	% Area %
1	21.345	2081	77388	4.37
2	23.241	3083	79806	4.51
3	24.303	1410	40697	2.30
4	26.412	45992	1571760	88.82

Condition：Chrial ID-3, λ = 254 nm, hexane/ethanol = 96:4

flow rate = 1.0 mL/min



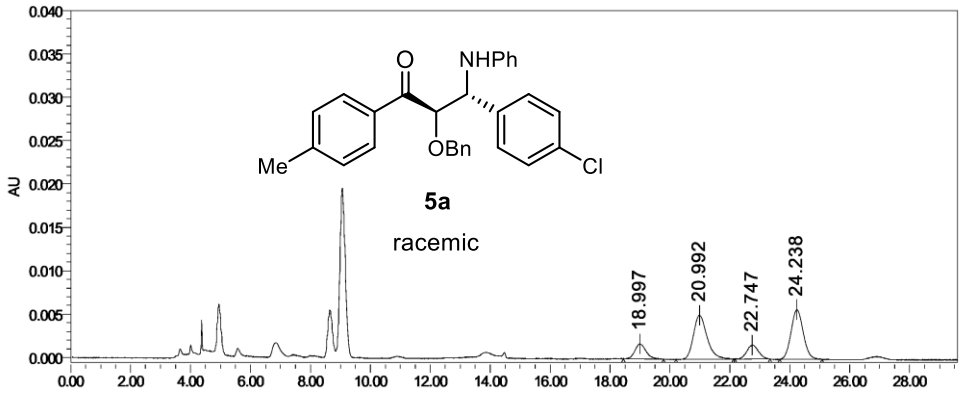
Entry	RT min	Height mV	Area mV.sec	% Area %
1	15.678	542171	9632691	49.93
2	16.738	495828	9659664	50.07



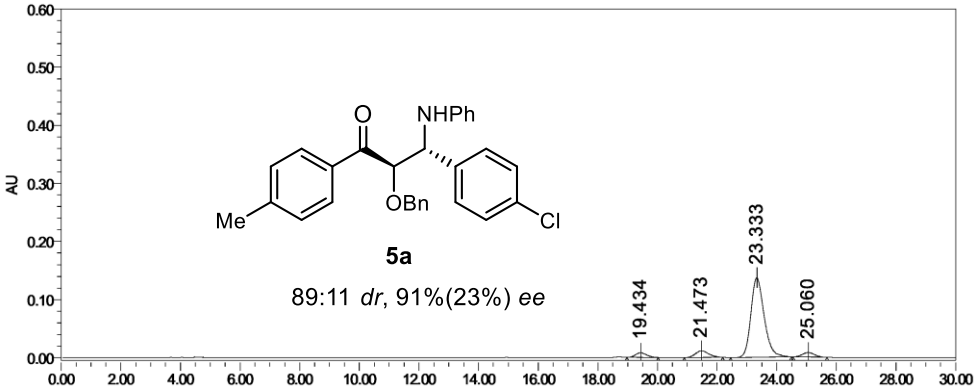
Entry	RT min	Height mV	Area mV.sec	% Area %
1	15.099	32803	539051	1.07
2	15.984	2497375	49982496	98.93

Condition：Chrial IF-3, λ = 254 nm, hexane/ethanol = 99:1

flow rate = 1.0 mL/min



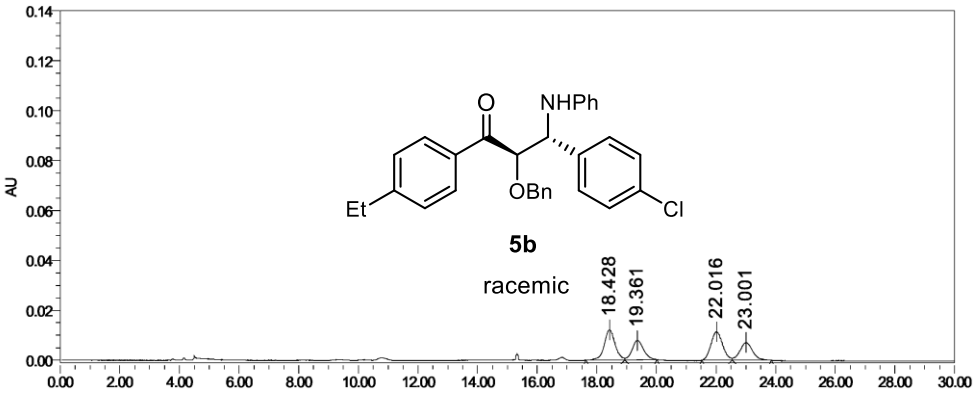
Entry	RT min	Height mV	Area mV.sec	% Area %
1	18.997	1736	43843	10.78
2	20.992	5086	159109	39.13
3	22.747	1608	43488	10.69
4	24.238	5716	160193	39.39



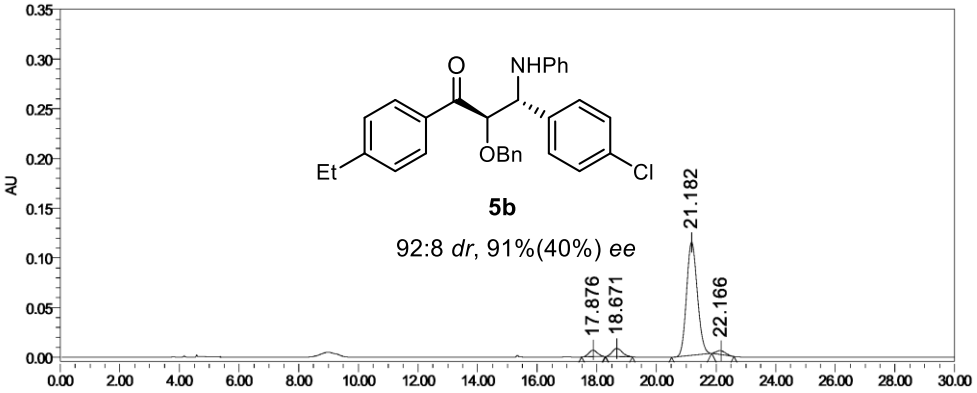
Entry	RT min	Height mV	Area mV.sec	% Area %
1	19.434	7912	200159	4.00
2	21.473	11466	355179	7.09
3	23.333	136739	4229451	84.47
4	25.060	7804	221969	4.43

Condition：Chrial IF-3, λ = 254 nm, hexane/ethanol = 99:1

flow rate = 1.0 mL/min



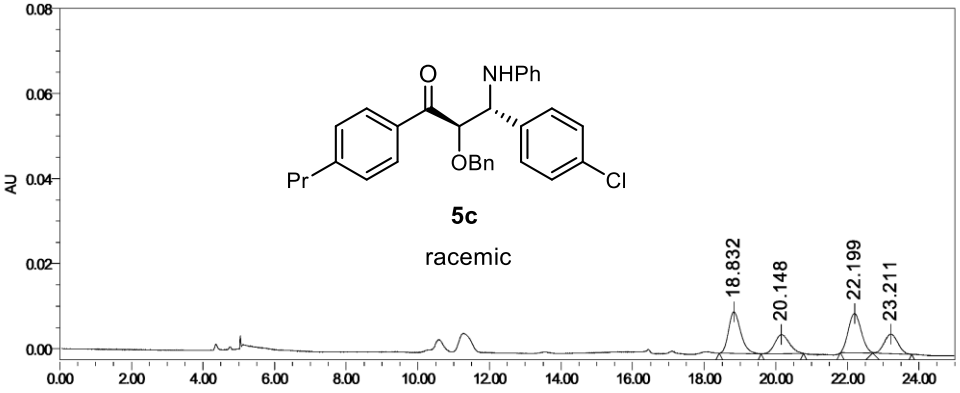
Entry	RT min	Height mV	Area mV.sec	% Area %
1	18.428	12139	305904	29.71
2	19.361	7758	207981	20.20
3	22.016	11391	306541	29.77
4	23.001	7071	209242	20.32



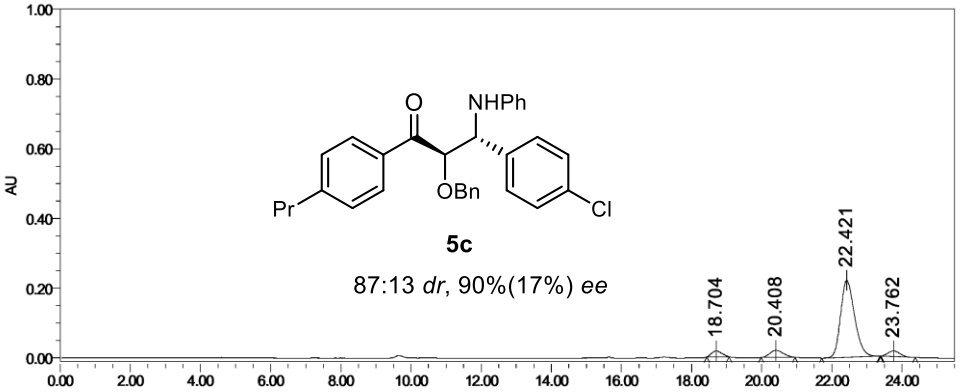
Entry	RT min	Height mV	Area mV.sec	% Area %
1	17.876	6576	132858	4.08
2	18.671	8222	187521	5.75
3	21.182	113760	2858993	87.73
4	22.166	3809	79401	2.44

Condition：Chrial IF-3, λ = 254 nm, hexane/ethanol = 99:1

flow rate = 1.0 mL/min



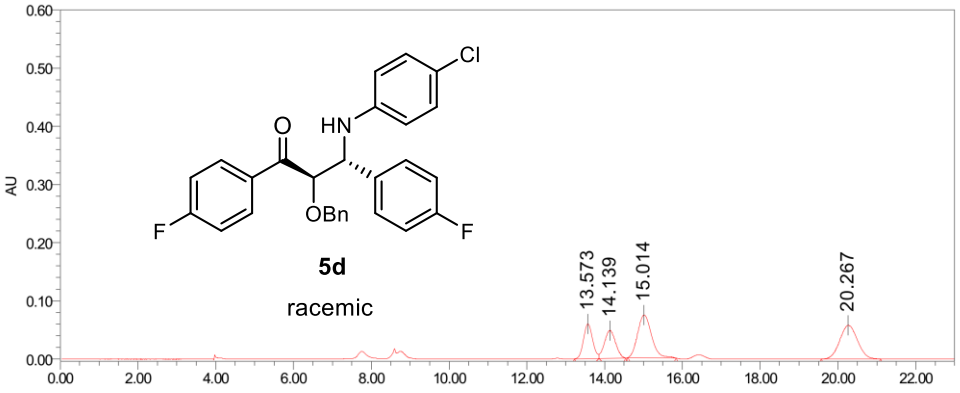
Entry	RT min	Height mV	Area mV.sec	% Area %
1	18.832	9782	229192	32.41
2	20.148	4497	125670	17.77
3	22.199	9282	231682	32.76
4	23.211	4623	120706	17.07



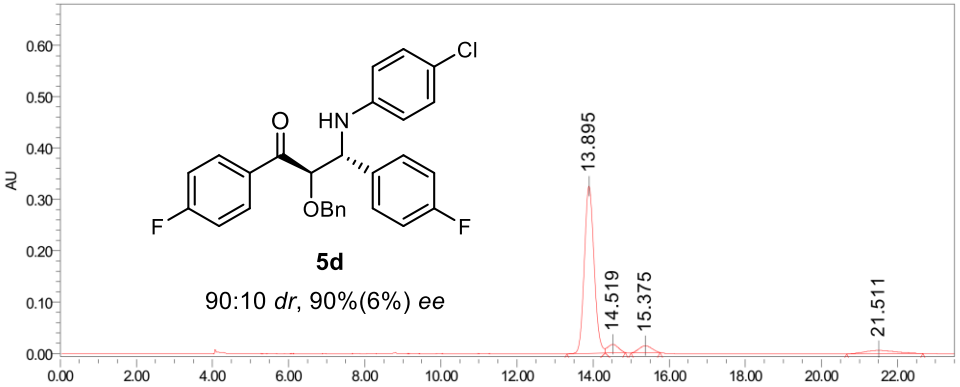
Entry	RT min	Height mV	Area mV.sec	% Area %
1	18.704	16599	334242	4.56
2	20.408	20205	542548	7.40
3	22.421	220387	6070458	82.76
4	23.762	16027	388110	5.29

Condition：Chrial IG-3, λ = 254 nm, hexane/ethanol = 96:4

flow rate = 1.0 mL/min



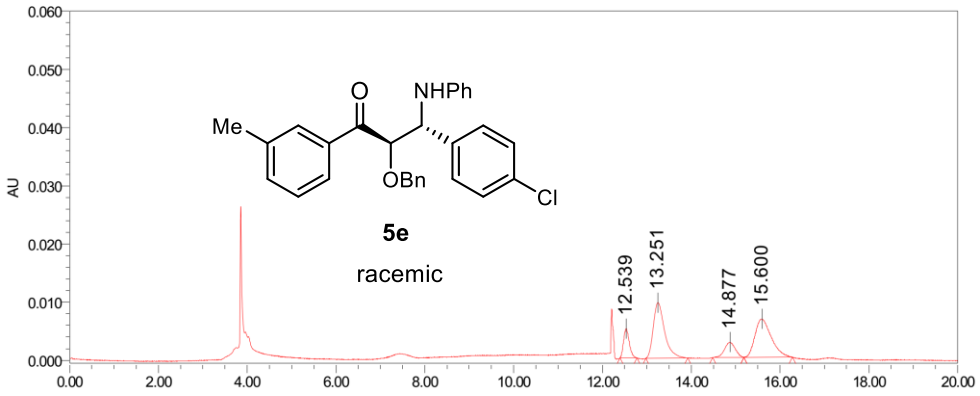
Entry	RT min	Height mV	Area mV.sec	% Area %
1	13.573	59576	963962	17.41
2	14.139	47518	932968	16.85
3	15.014	73352	1819433	32.86
4	20.267	57927	1820335	32.88



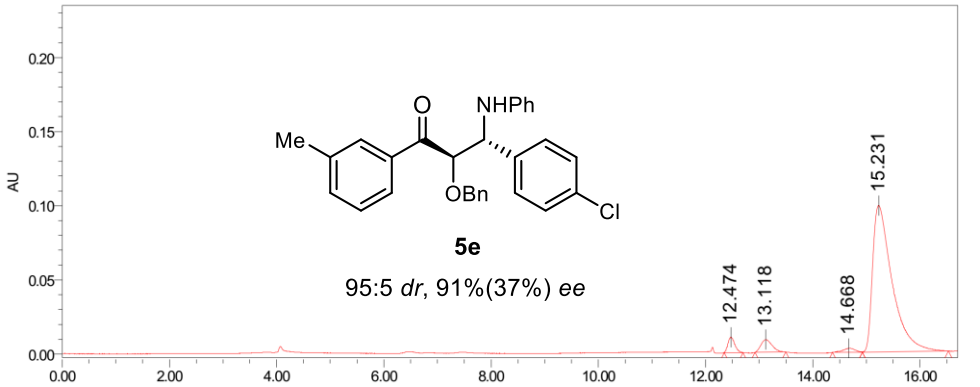
Entry	RT min	Height mV	Area mV.sec	% Area %
1	13.895	325493	5791032	85.34
2	14.519	16206	315403	4.65
3	15.375	13580	318830	4.70
4	21.511	6260	360300	5.31

Condition：Chrial ID-3, λ = 254 nm, hexane/ethanol = 99:1

flow rate = 1.0 mL/min



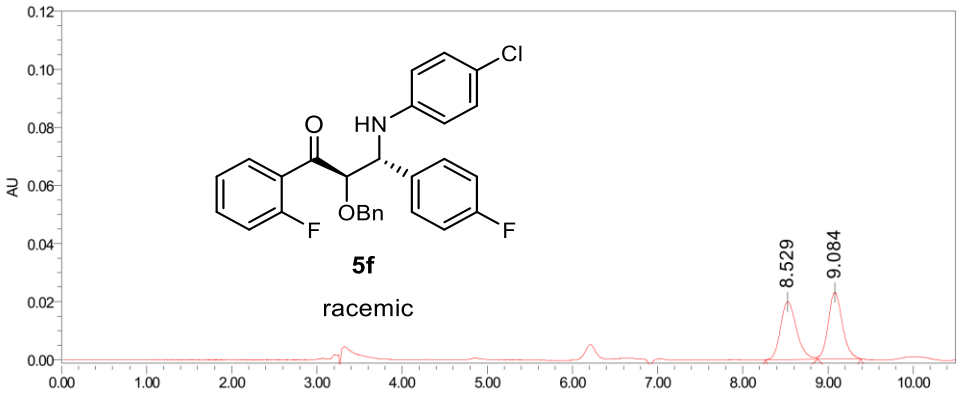
Entry	RT min	Height mV	Area mV.sec	% Area %
1	12.539	5006	44501	10.52
2	13.251	9537	167224	39.52
3	14.877	2630	44290	10.47
4	15.600	6598	167158	39.50



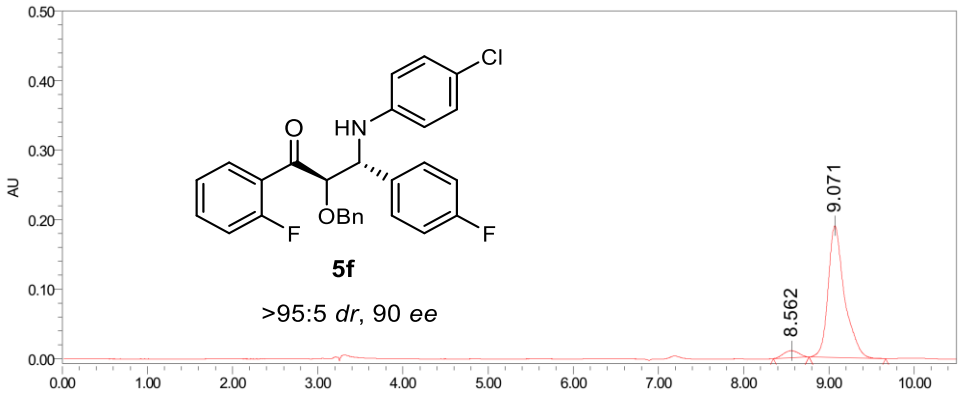
Entry	RT min	Height mV	Area mV.sec	% Area %
1	12.474	10442	90201	3.30
2	13.118	8441	122126	4.46
3	14.668	2639	41034	1.50
4	15.231	98713	2482669	90.74

Condition：Chrial IF-3, λ = 254 nm, hexane/ethanol = 97:3

flow rate = 1.0 mL/min



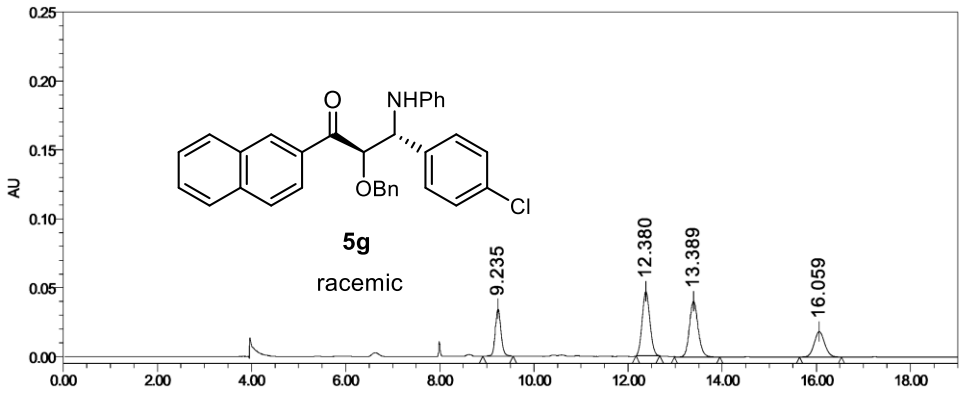
Entry	RT min	Height mV	Area mV.sec	% Area %
1	8.529	19913	260300	49.78
2	9.084	22916	262578	50.22



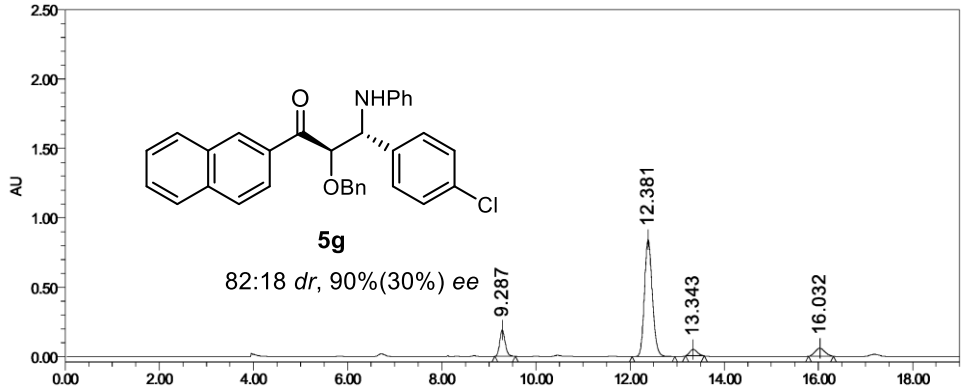
Entry	RT min	Height mV	Area mV.sec	% Area %
1	8.562	9991	125418	4.76
2	9.071	189174	2511677	95.24

Condition：Chrial IF-3, λ = 254 nm, hexane/ethanol = 97:3

flow rate = 1.0 mL/min



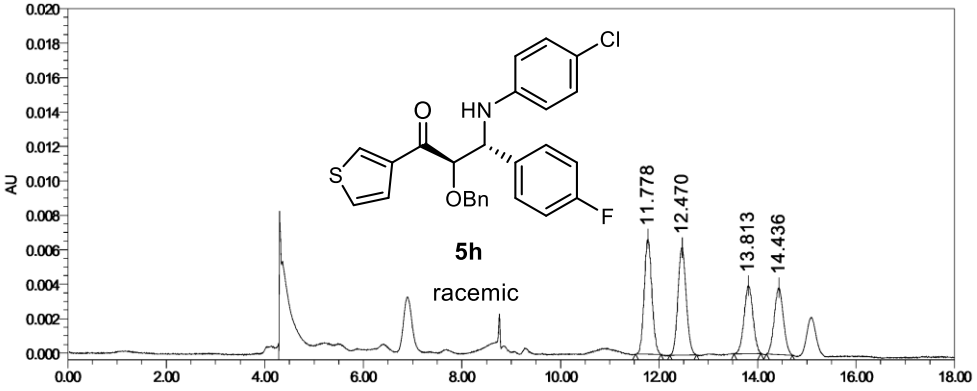
Entry	RT min	Height mV	Area mV.sec	% Area %
1	9.235	34290	285172	17.63
2	12.38	46741	532290	32.92
3	13.389	40321	514945	31.84
4	16.059	18414	284742	17.61



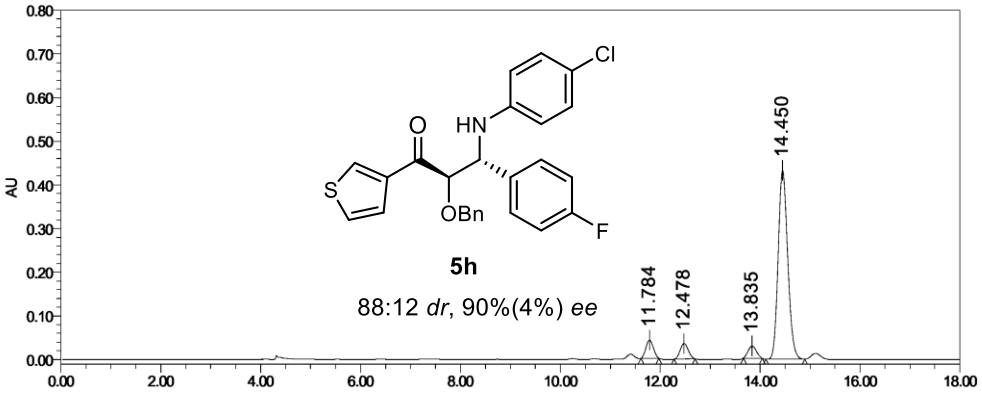
Entry	RT min	Height mV	Area mV.sec	% Area %
1	9.287	188734	1526895	12.06
2	12.381	842877	9797550	77.37
3	13.343	45336	513104	4.05
4	16.032	57356	825649	6.52

Condition：Chrial IB-3, λ = 254 nm, hexane/ethanol = 97:3

flow rate = 1.0 mL/min



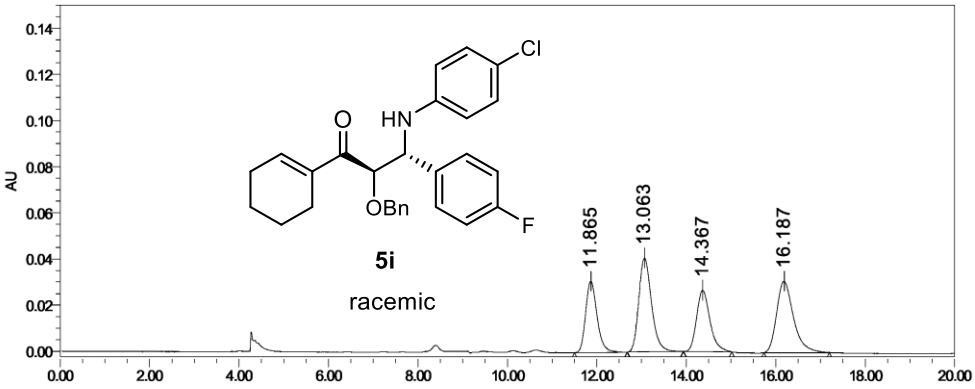
Entry	RT min	Height mV	Area mV.sec	% Area %
1	11.778	6687	72392	29.62
2	12.470	6235	72406	29.63
3	13.813	3956	49815	20.38
4	14.436	3871	49790	20.37



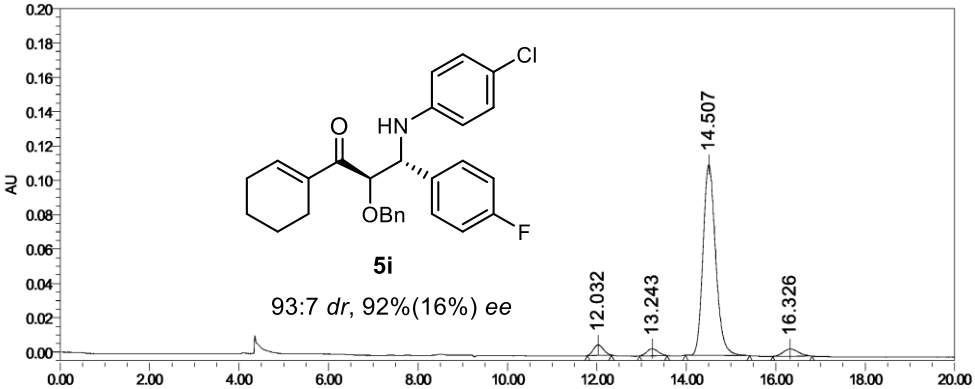
Entry	RT min	Height mV	Area mV.sec	% Area %
1	11.784	41467	427374	6.20
2	12.478	35207	398865	5.79
3	13.835	27702	318879	4.63
4	14.450	432710	5748305	83.39

Condition：Chrial IF-3, λ = 254 nm, hexane/ethanol = 97:3

flow rate = 1.0 mL/min



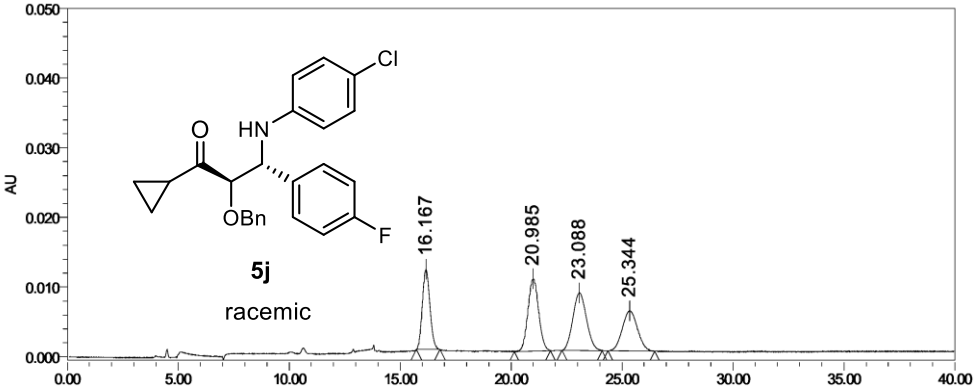
Entry	RT min	Height mV	Area mV.sec	% Area %
1	11.865	30919	546854	20.11
2	13.063	40618	807745	29.70
3	14.367	26603	554640	20.39
4	16.187	30910	810363	29.80



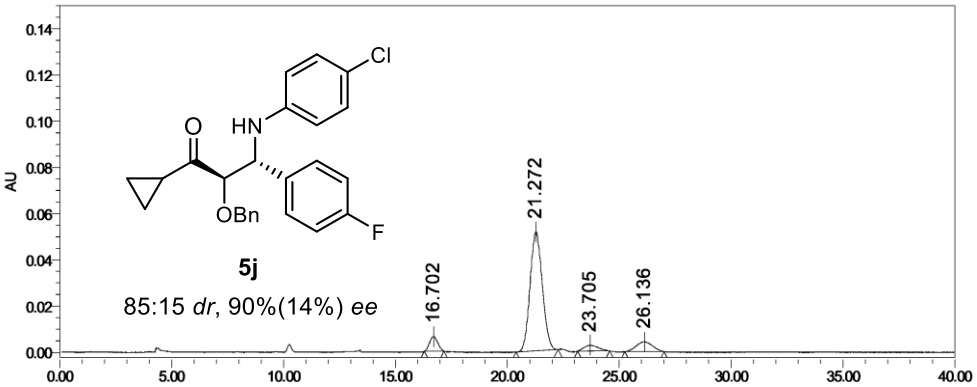
Entry	RT min	Height mV	Area mV.sec	% Area %
1	12.032	6035	92817	3.81
2	13.243	4041	69930	2.87
3	14.507	111140	2176486	89.31
4	16.326	4183	97757	4.01

Condition：Chrial IG-3, λ = 254 nm, hexane/ethanol/2-propanol = 98:1:1

flow rate = 1.0 mL/min



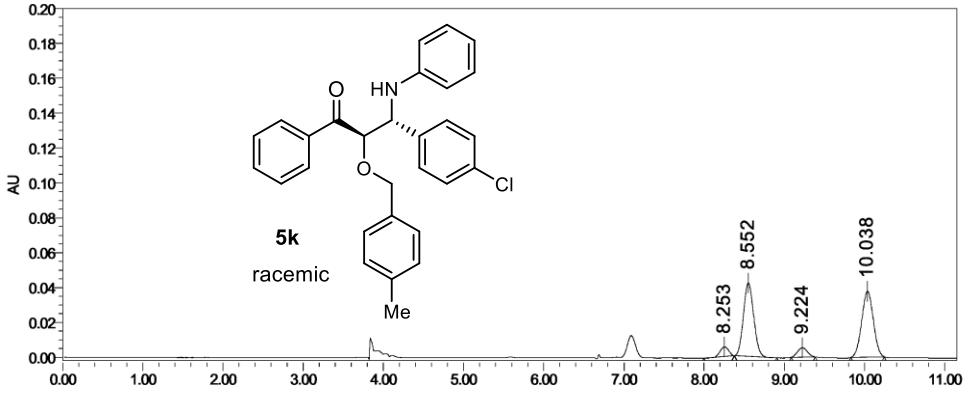
Entry	RT min	Height mV	Area mV.sec	% Area %
1	16.167	11551	275820	22.05
2	20.985	10346	350087	27.99
3	23.088	8277	350388	28.01
4	25.344	5784	274588	21.95



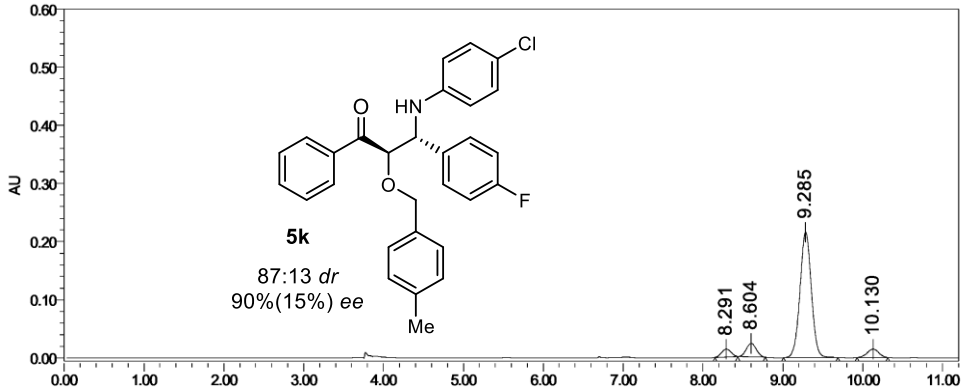
Entry	RT min	Height mV	Area mV.sec	% Area %
1	16.702	6362	161815	6.66
2	21.272	51510	1943866	80.05
3	23.705	2450	108581	4.47
4	26.136	4223	214201	8.82

Condition：Chrial IB-3, λ = 254 nm, hexane/ethanol = 95:5

flow rate = 1.0 mL/min



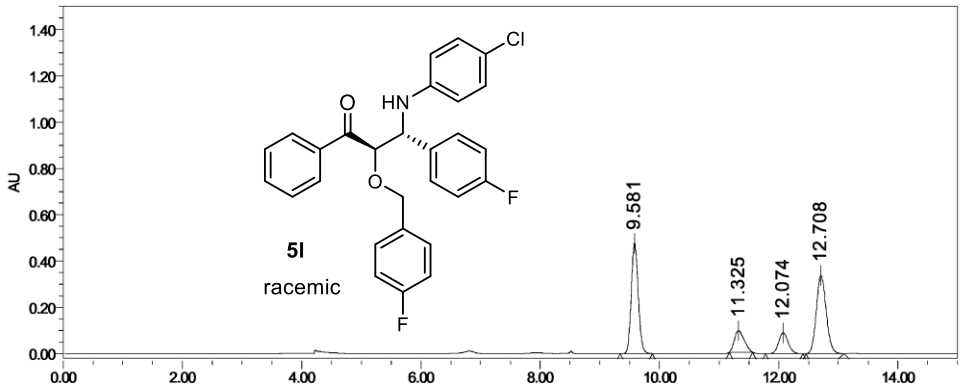
Entry	RT min	Height mV	Area mV.sec	% Area %
1	8.253	5473	41269	4.92
2	8.552	42226	374724	44.67
3	9.224	5357	45263	5.40
4	10.038	37741	377600	45.01



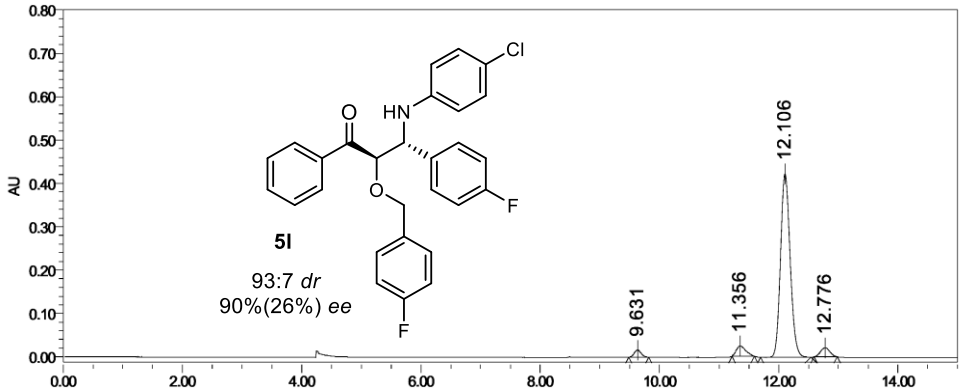
Entry	RT min	Height mV	Area mV.sec	% Area %
1	8.291	13360	110217	4.25
2	8.604	23090	200090	7.72
3	9.285	216098	2134553	82.37
4	10.130	14462	146501	5.65

Condition：Chrial IB-3, λ = 254 nm, hexane/ethanol = 97:3

flow rate = 1.0 mL/min



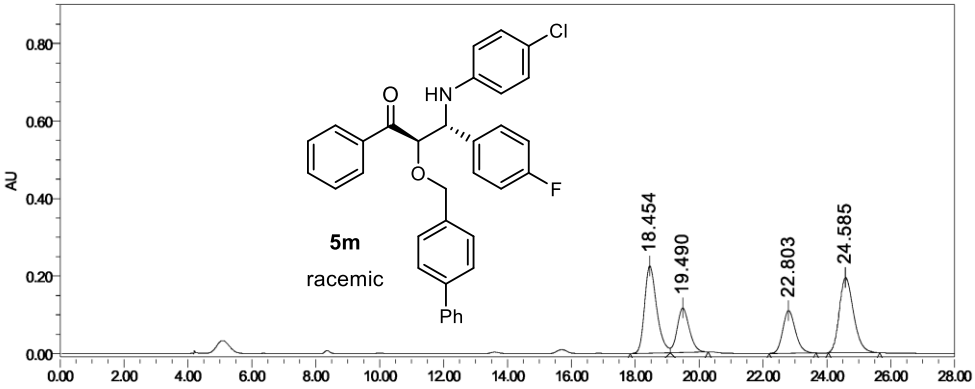
Entry	RT min	Height mV	Area mV.sec	% Area %
1	9.581	477851	3875240	39.52
2	11.325	93533	1058691	10.80
3	12.074	89778	998667	10.18
4	12.708	338095	3872708	39.50



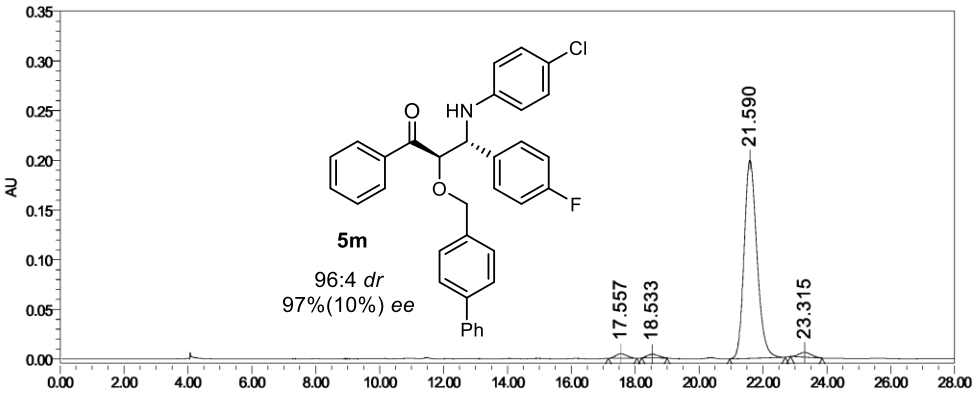
Entry	RT min	Height mV	Area mV.sec	% Area %
1	9.631	16556	131840	2.45
2	11.356	23653	259052	4.81
3	12.106	423470	4767393	88.58
4	12.776	20856	223843	4.16

Condition：Chrial IF-3, λ = 254 nm, hexane/ethanol = 98:2

flow rate = 1.0 mL/min



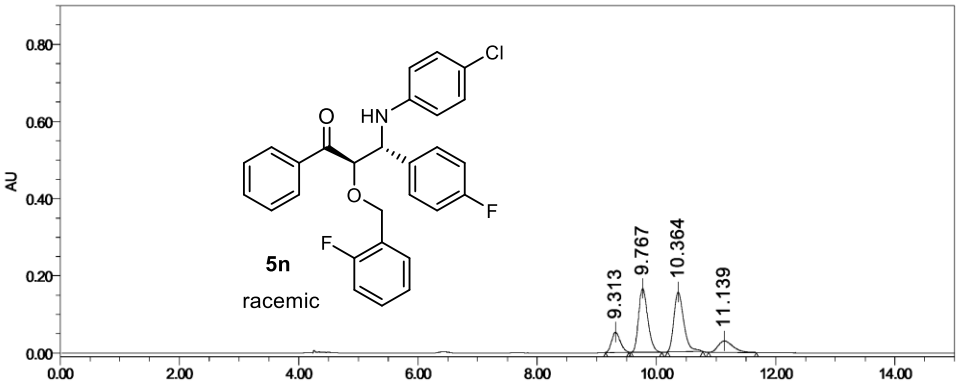
Entry	RT min	Height mV	Area mV.sec	% Area %
1	18.454	224675	5949964	33.10
2	19.49	114232	3027305	16.84
3	22.803	110103	3039566	16.91
4	24.585	193678	5960346	33.16



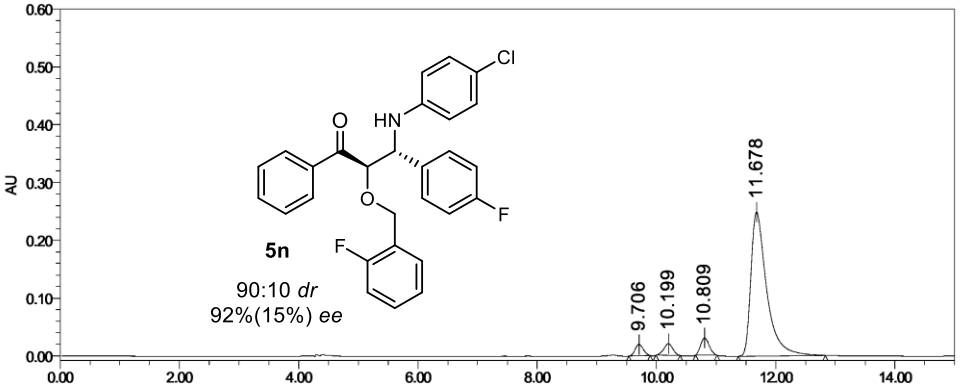
Entry	RT min	Height mV	Area mV.sec	% Area %
1	17.557	4508	107328	1.83
2	18.533	3580	88331	1.50
3	21.590	199396	5546963	94.44
4	23.315	4783	130779	2.23

Condition：Chrial ID-3, λ = 254 nm, hexane/ethanol = 97:3

flow rate = 1.0 mL/min



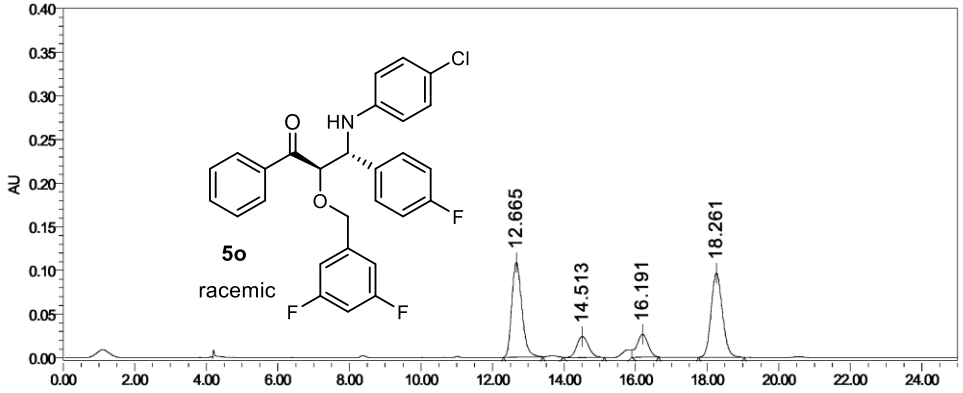
Entry	RT min	Height mV	Area mV.sec	% Area %
1	9.313	52192	516553	11.33
2	9.767	165251	1765485	38.71
3	10.364	154194	1761470	38.63
4	11.139	29581	516912	11.33



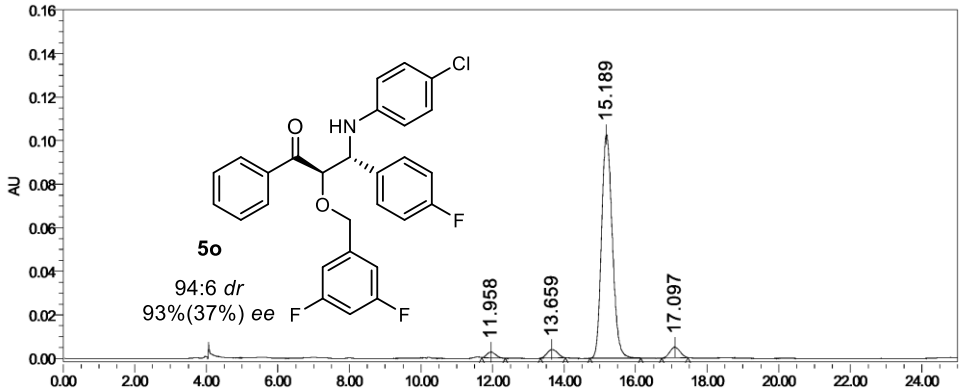
Entry	RT min	Height mV	Area mV.sec	% Area %
1	9.706	19878	188242	3.56
2	10.199	20322	216496	4.10
3	10.809	29323	292344	5.54
4	11.678	248965	4584526	86.80

Condition：Chrial IF-3, λ = 254 nm, hexane/ethanol = 98:2

flow rate = 1.0 mL/min



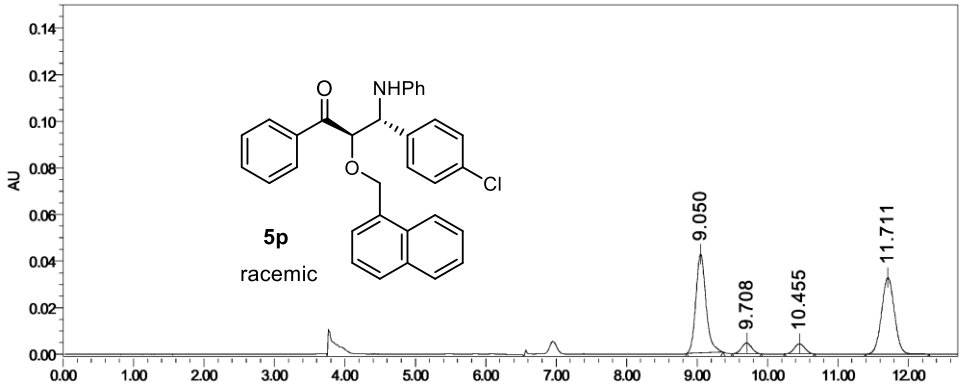
Entry	RT min	Height mV	Area mV.sec	% Area %
1	12.665	108674	2101178	39.51
2	14.513	24057	548557	10.32
3	16.191	26115	566036	10.64
4	18.261	96518	2101737	39.52



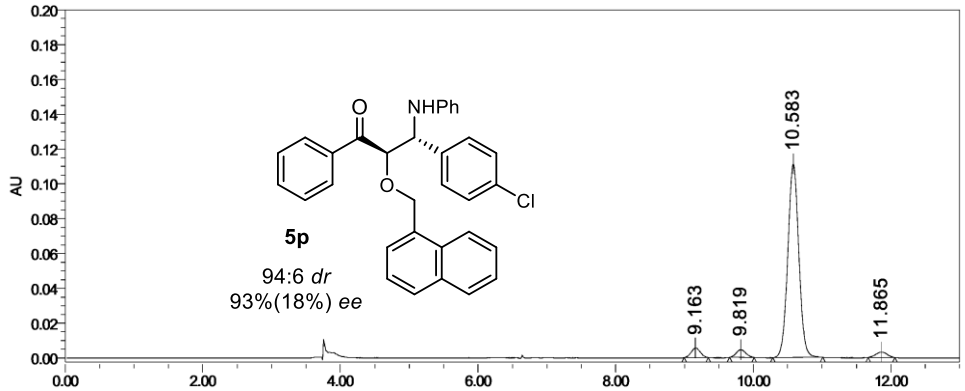
Entry	RT min	Height mV	Area mV.sec	% Area %
1	11.958	2640	44696	1.90
2	13.659	3841	77711	3.30
3	15.189	102726	2138156	90.66
4	17.097	4899	97847	4.15

Condition：Chrial IF-3, λ = 254 nm, hexane/ethanol = 95:5

flow rate = 1.0 mL/min



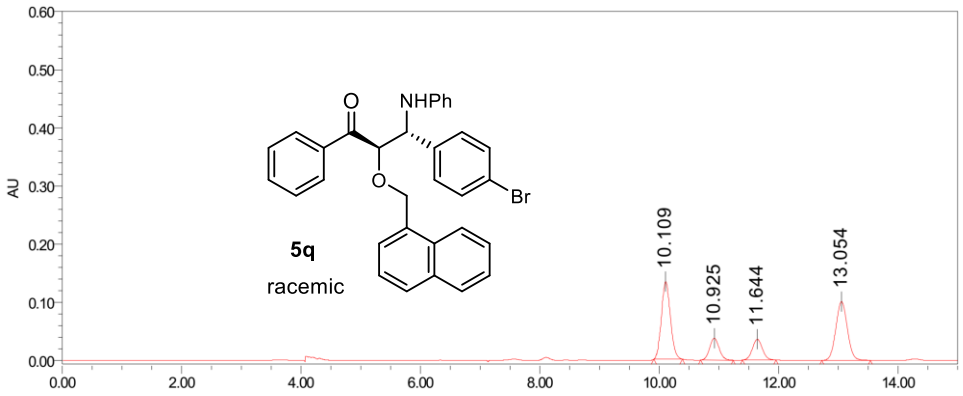
Entry	RT min	Height mV	Area mV.sec	% Area %
1	9.05	42317	421857	45.26
2	9.708	4583	45811	4.91
3	10.455	4373	46190	4.96
4	11.711	32848	418300	44.87



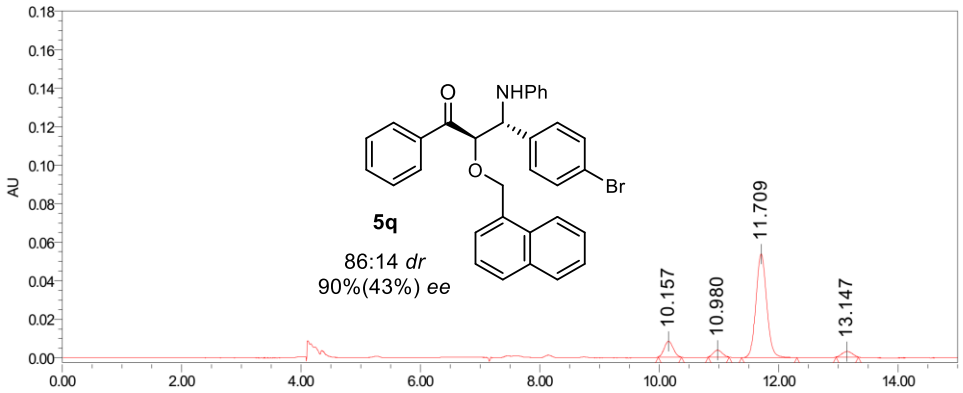
Entry	RT min	Height mV	Area mV.sec	% Area %
1	9.163	5460	50174	3.67
2	9.819	4408	42505	3.11
3	10.583	111279	1238605	90.69
4	11.865	3098	34456	2.52

Condition：Chrial IF-3, λ = 250 nm, hexane/ethanol = 95:5

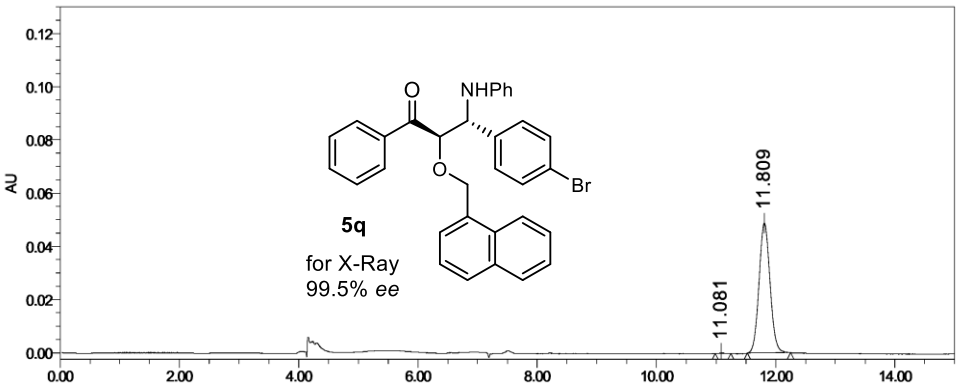
flow rate = 1.0 mL/min



Entry	RT min	Height mV	Area mV.sec	% Area %
1	10.109	133225	1383186	38.76
2	10.925	37805	418107	11.72
3	11.644	35692	417372	11.69
4	13.054	100992	1350270	37.87



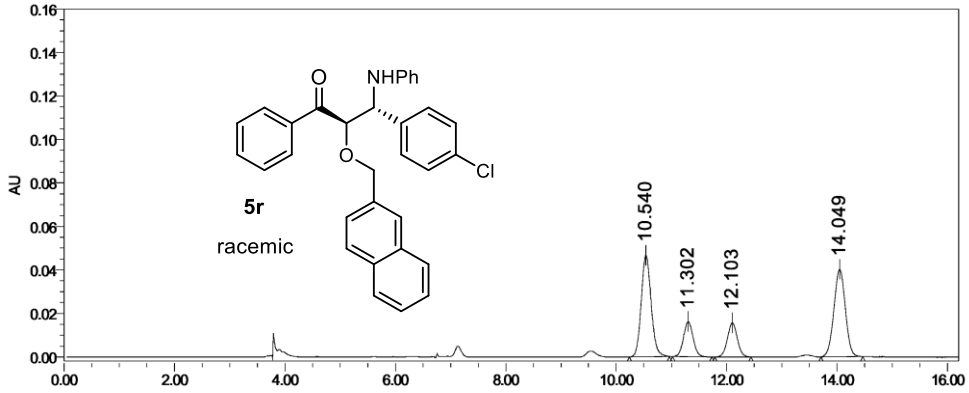
Entry	RT min	Height mV	Area mV.sec	% Area %
1	10.157	8194	84518	10.18
2	10.98	3613	37501	4.52
3	11.709	53868	674532	81.24
4	13.147	2853	33714	4.06



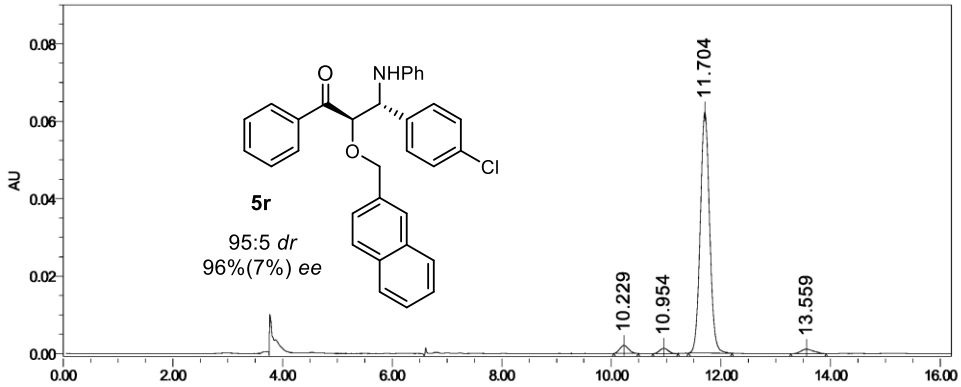
Entry	RT min	Height mV	Area mV.sec	% Area %
1	11.081	170	1382	0.22
2	11.809	48815	626341	99.78

Condition：Chrial IF-3, λ = 254 nm, hexane/ethanol = 95:5

flow rate = 1.0 mL/min



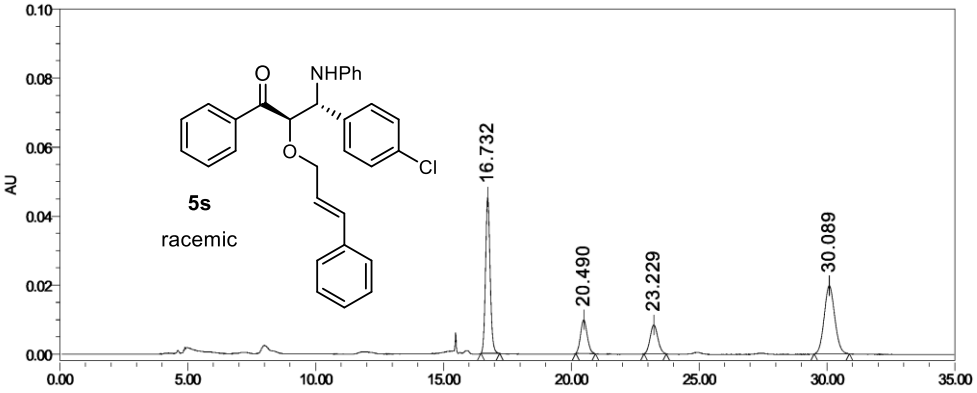
Entry	RT min	Height mV	Area mV.sec	% Area %
1	10.549	45313	566368	38.22
2	11.302	9717	174938	11.80
3	12.103	8354	173288	11.69
4	14.049	19732	567453	38.29



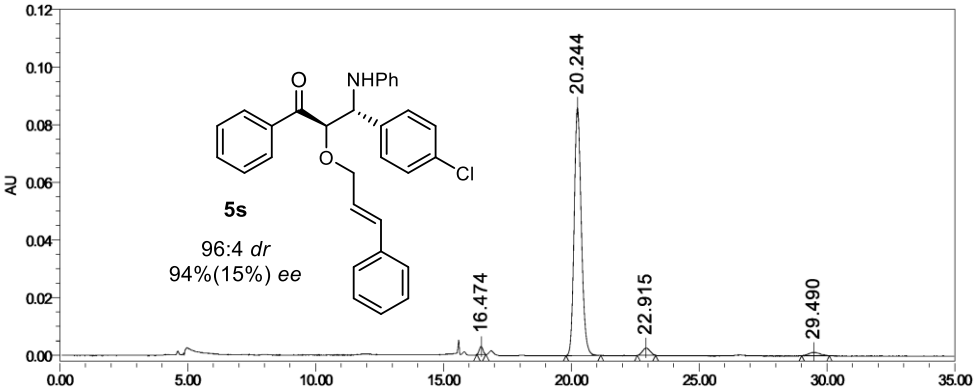
Entry	RT min	Height mV	Area mV.sec	% Area %
1	10.229	2085	23177	2.92
2	10.954	1366	14570	1.83
3	11.704	62237	737190	92.72
4	13.559	1205	20102	2.53

Condition：Chrial IB-3, λ = 254 nm, hexane/ethanol = 99:1

flow rate = 1.0 mL/min



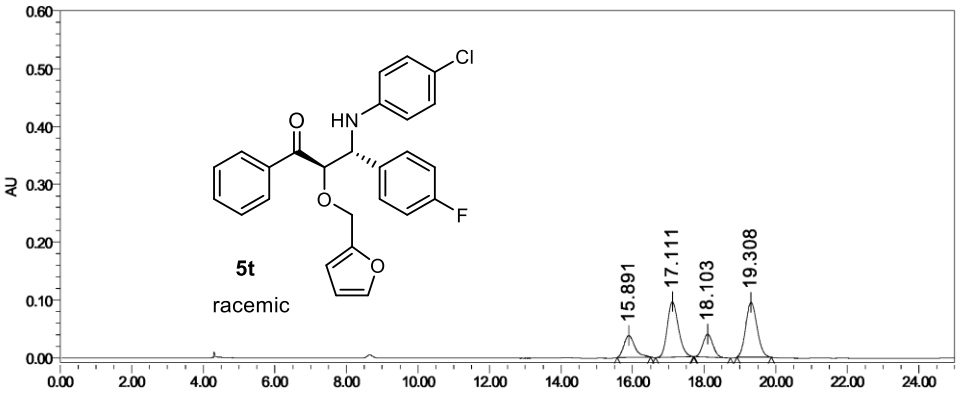
Entry	RT min	Height mV	Area mV.sec	% Area %
1	16.732	45313	566368	38.22
2	20.49	9717	174938	11.80
3	23.229	8354	173288	11.69
4	30.089	19732	567453	38.29



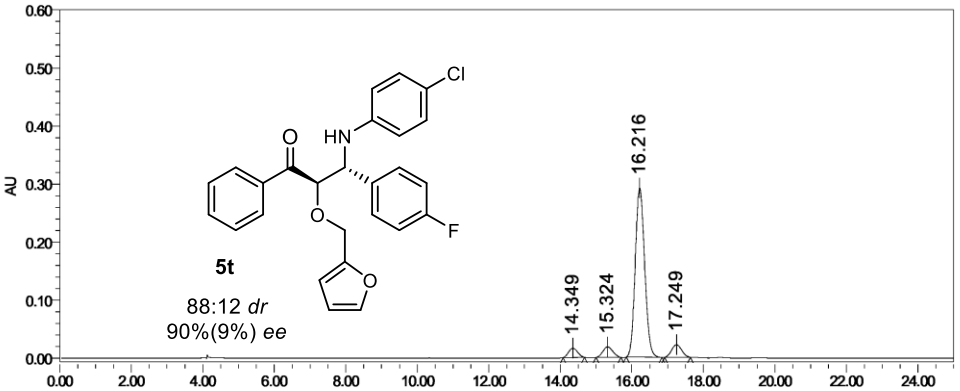
Entry	RT min	Height mV	Area mV.sec	% Area %
1	16.474	2748	27510	1.53
2	20.244	86142	1682889	93.49
3	22.915	2526	52283	2.90
4	29.490	1179	37324	2.07

Condition：Chrial IF-3, λ = 254 nm, hexane/ethanol = 98:2

flow rate = 1.0 mL/min



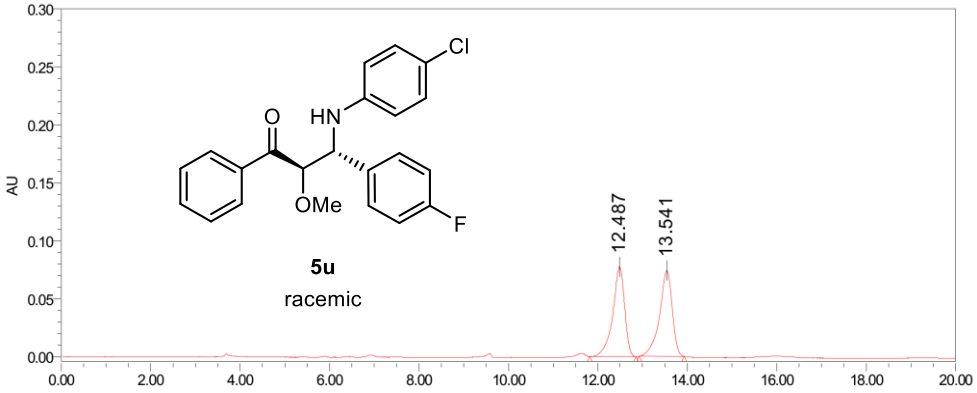
Entry	RT min	Height mV	Area mV.sec	% Area %
1	15.891	37429	782068	13.72
2	17.111	95750	2072847	36.36
3	18.103	39584	765408	13.43
4	19.308	94648	2080325	36.49



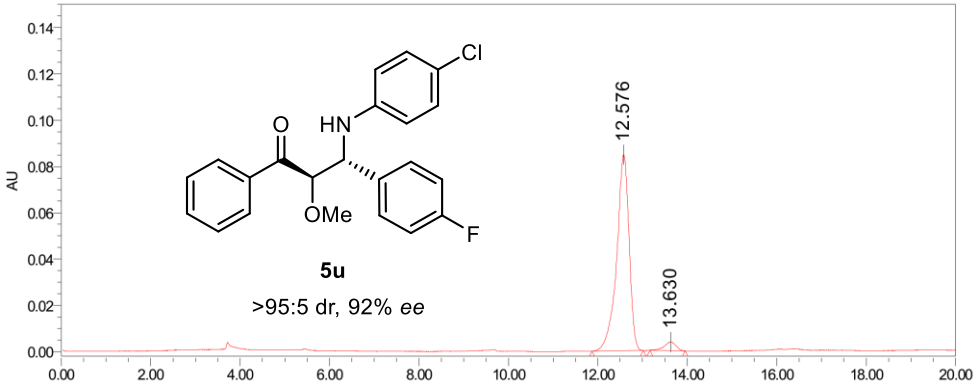
Entry	RT min	Height mV	Area mV.sec	% Area %
1	14.349	15753	275639	4.33
2	15.324	18000	347231	5.46
3	16.216	291220	5321140	83.63
4	17.249	21458	418694	6.58

Condition：Chrial Y1, λ = 254 nm, hexane/ethanol = 98:2

flow rate = 1.0 mL/min



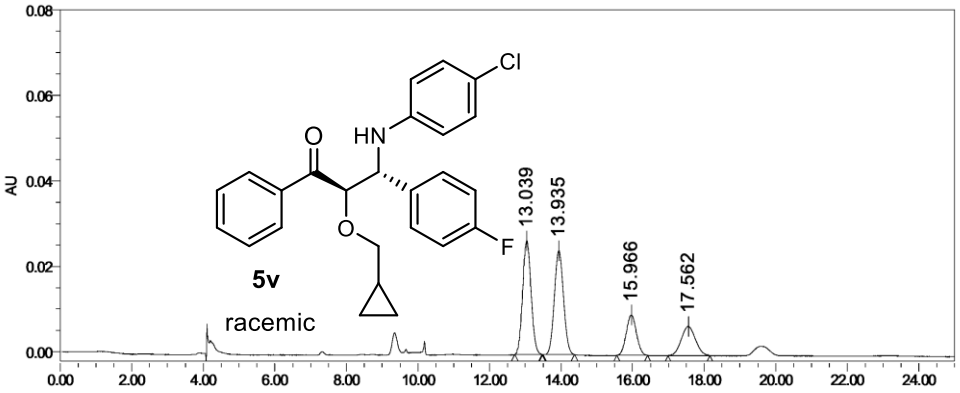
Entry	RT min	Height mV	Area mV.sec	% Area %
1	12.487	77585	1412678	49.03
2	13.541	73953	1466479	50.97



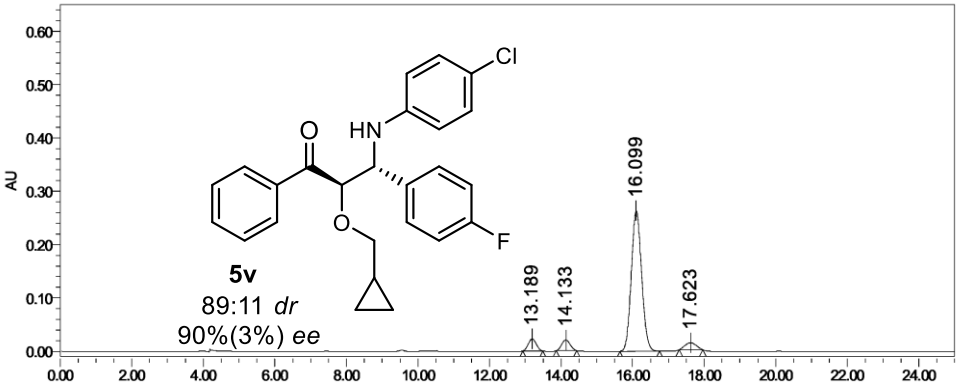
Entry	RT min	Height mV	Area mV.sec	% Area %
1	12.576	84679	1614481	95.98
2	13.630	3710	67588	4.02

Condition：Chrial IG-3, λ = 254 nm, hexane/ethanol = 97:3

flow rate = 1.0 mL/min



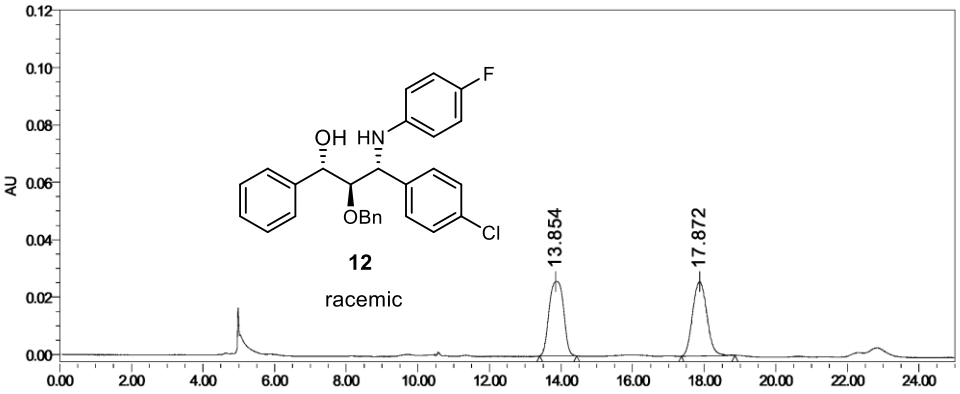
Entry	RT min	Height mV	Area mV.sec	% Area %
1	13.039	26590	433782	34.96
2	13.935	24300	433394	34.93
3	15.966	9410	186378	15.02
4	17.562	6803	187348	15.10



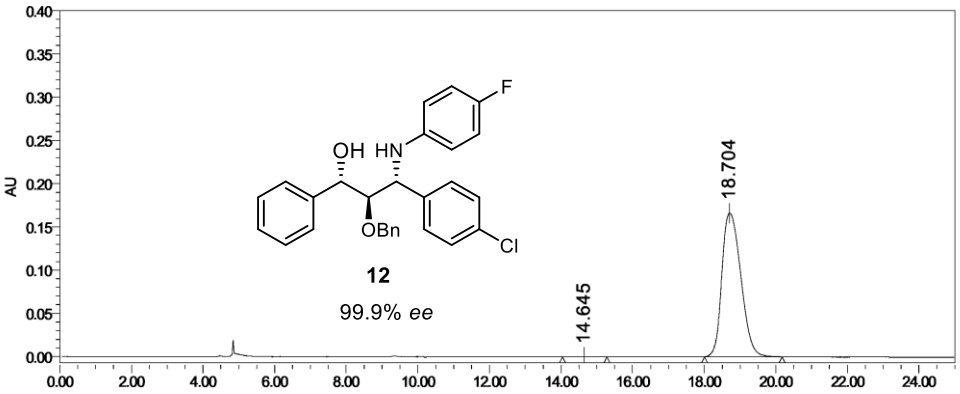
Entry	RT min	Height mV	Area mV.sec	% Area %
1	13.189	22644	350505	5.60
2	14.133	20131	332820	5.32
3	16.099	263514	5291145	84.52
4	17.623	13000	286021	4.57

Condition：Chrial IF-3, λ = 254 nm, hexane/ethanol = 97:3

flow rate = 1.0 mL/min



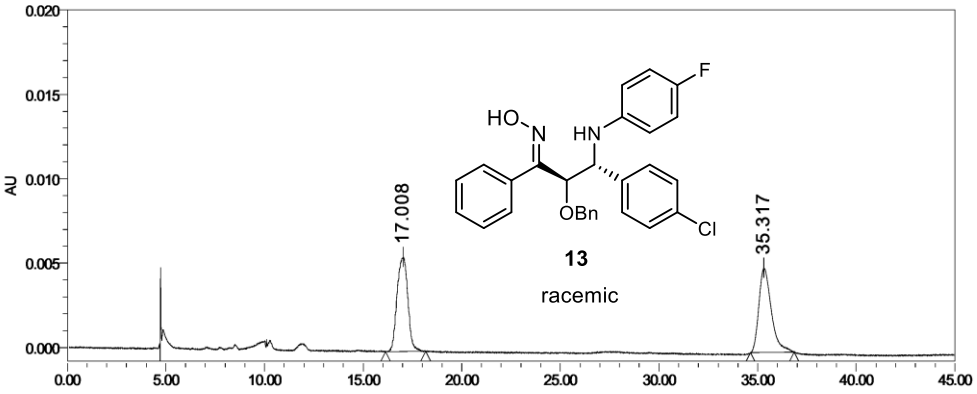
Entry	RT min	Height mV	Area mV.sec	% Area %
1	13.854	25904	725719	50.63
2	17.872	25890	707773	49.37



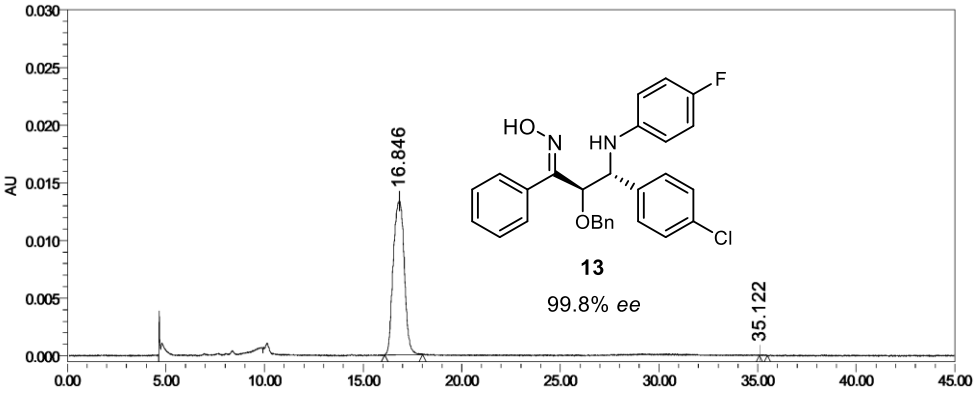
Entry	RT min	Height mV	Area mV.sec	% Area %
1	14.645	103	3081	0.05
2	18.704	166100	6127448	99.95

Condition：Chrial IF-3, λ = 254 nm, hexane/ethanol = 97:3

flow rate = 1.0 mL/min



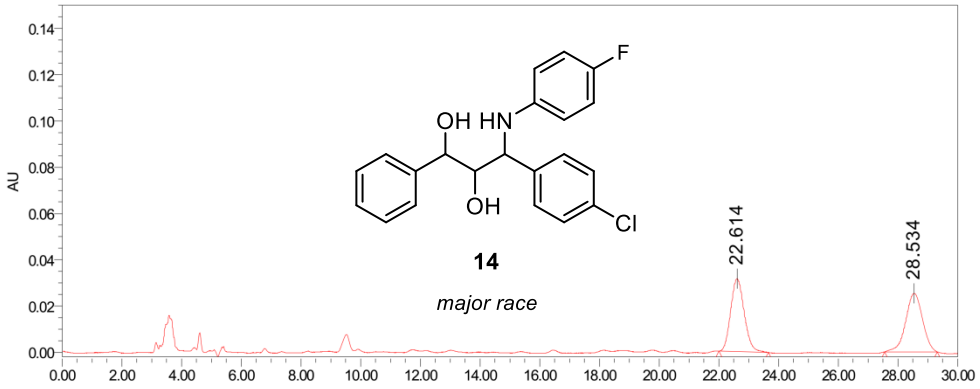
Entry	RT min	Height mV	Area mV.sec	% Area %
1	17.008	5577	212993	49.28
2	35.317	5017	219258	50.72



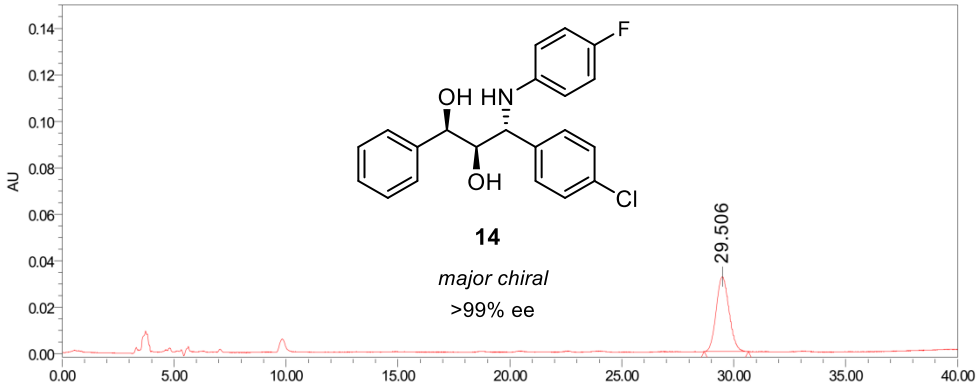
Entry	RT min	Height mV	Area mV.sec	% Area %
1	16.846	13293	521788	99.94
2	35.122	40	320	0.06

Condition: Chrial IG-3, λ = 230 nm, hexane/ethanol = 90:10

flow rate = 1.0 mL/min



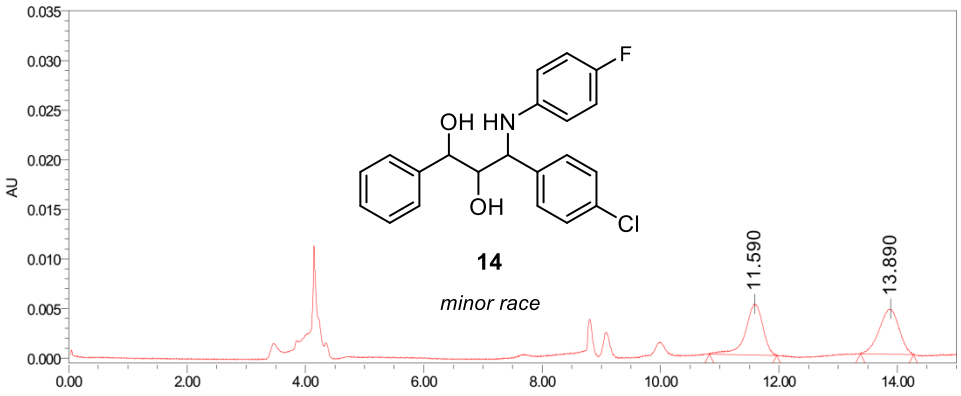
Entry	RT min	Height mV	Area mV.sec	% Area %
1	22.614	31559	988106	50.08
2	28.534	25325	984867	49.92



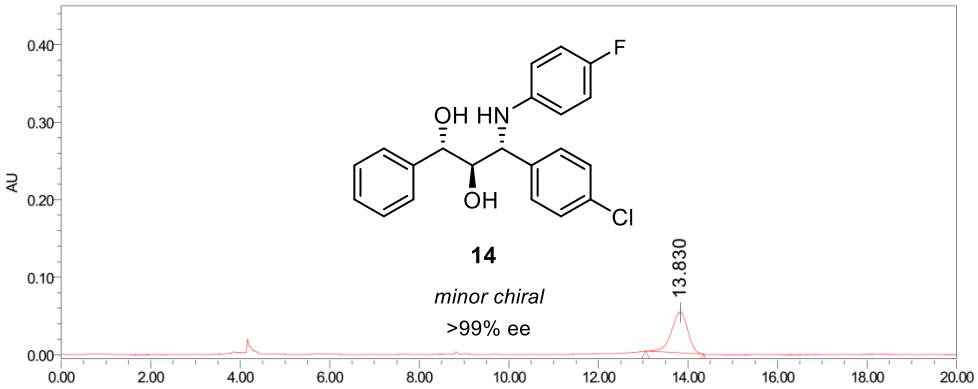
Entry	RT min	Height mV	Area mV.sec	% Area %
1	29.506	32172	1276895	100.00

Condition: Chrial IC, λ = 240 nm, hexane/ethanol = 97:3

flow rate = 1.0 mL/min

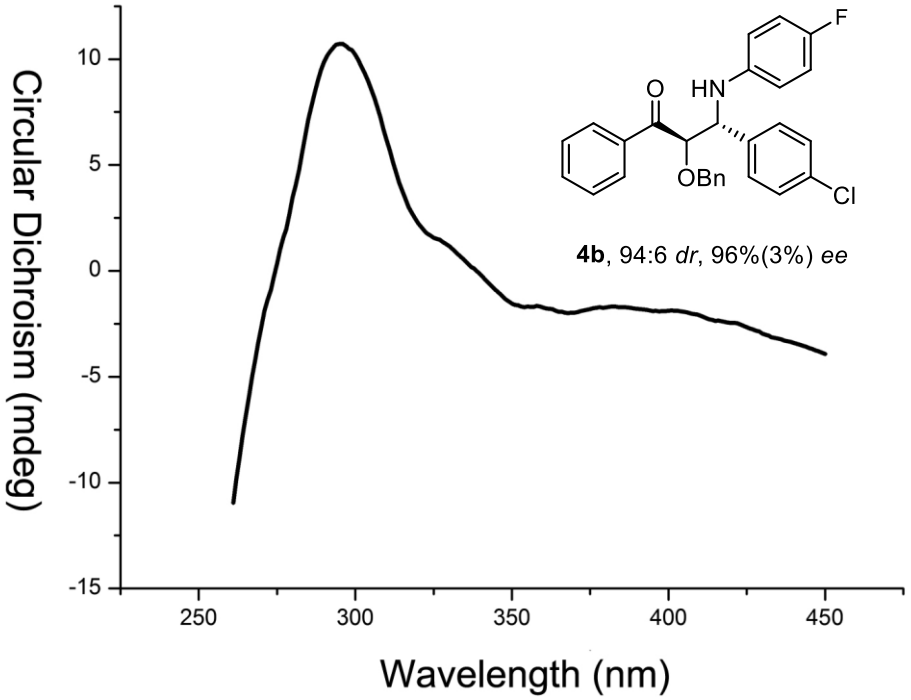


Entry	RT min	Height mV	Area mV.sec	% Area %
1	11.590	5132	105181	49.74
2	13.890	4571	106286	50.26

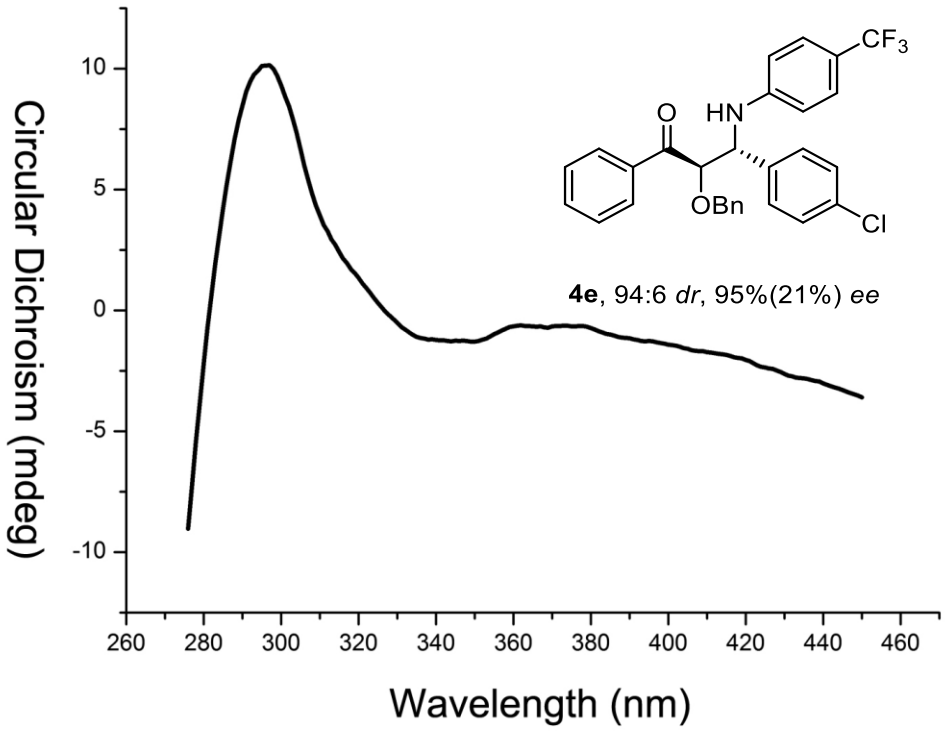


Entry	RT min	Height mV	Area mV.sec	% Area %
1	13.830	52600	1343022	100.00

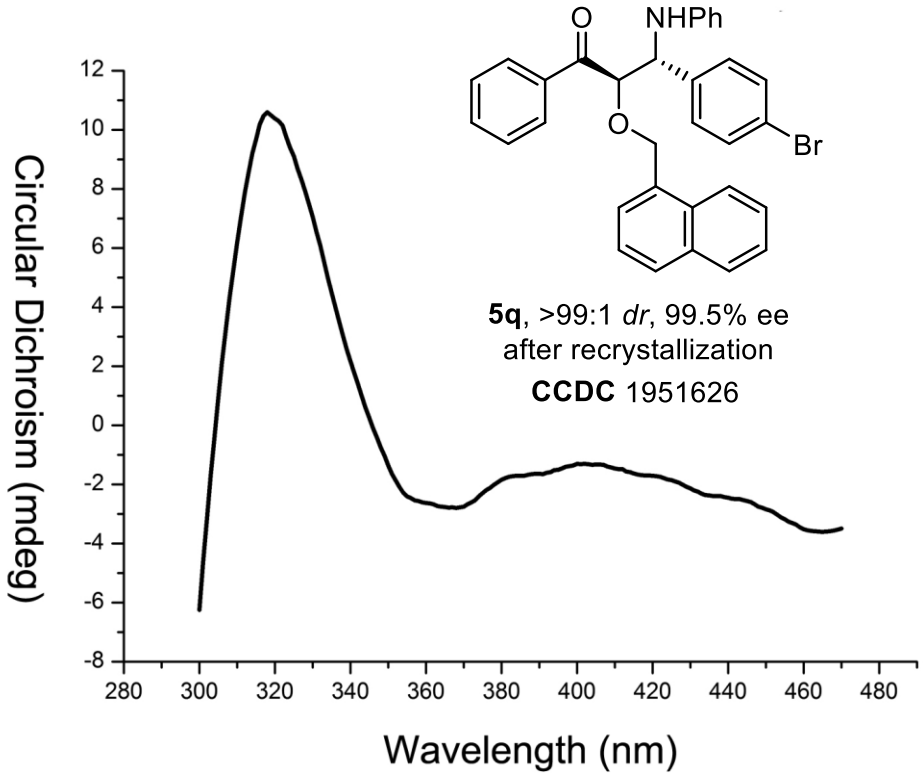
Circular Dichroism Spectra for Products 4b, 4e, and 5q.



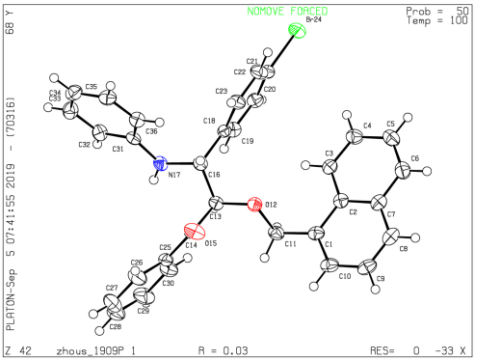
4b, 94:6 *dr*, 96%(3%) *ee*

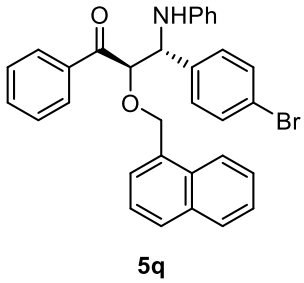


4e, 94:6 *dr*, 95%(21%) *ee*


O
NHPh
O
Br
5q, >99:1 *dr*, 99.5% ee
after recrystallization
CCDC 1951626
Circular Dichroism (mdeg)
12
10
8
6
4
2
0
-2
-4
-6
-8
280
300
320
340
360
380
400
420
440
460
480
Wavelength (nm)

Crystallographic Data for 5q.





5q

CCDC 1951626

Bond precision: C-C = 0.0052 A Wavelength=1.54184

Cell: a=5.3961(1) b=10.3004(1) c=12.1257(1)
alpha=106.609(1) beta=92.180(1) gamma=98.022(1)
Temperature: 100 K

	Calculated	Reported
Volume	637.371(15)	637.370(15)
Space group	P 1	P 1
Hall group	P 1	P 1
Moiety formula	C32 H26 Br N O2	C32 H26 Br N O2
Sum formula	C32 H26 Br N O2	C32 H26 Br N O2
Mr	536.44	536.45
Dx,g cm-3	1.398	1.398
Z	1	1
Mu (mm-1)	2.428	2.428
F000	276.0	276.0
F000'	276.00	
h,k,lmax	6,13,15	6,12,15
Nref	5368[2684]	4978
Tmin,Tmax	0.747,0.784	0.814,1.000
Tmin'	0.483	

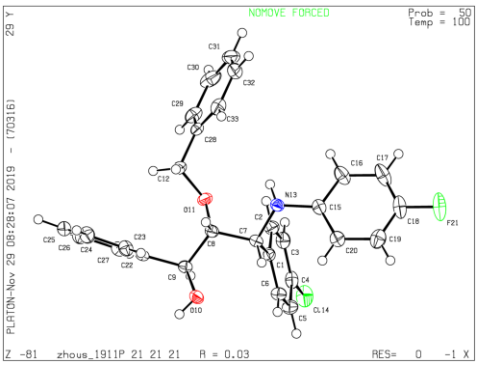
Correction method= # Reported T Limits: Tmin=0.814 Tmax=1.000
AbsCorr = MULTI-SCAN

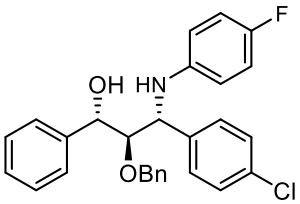
Data completeness= 1.85/0.93 Theta(max)= 76.856

R(reflections)= 0.0263(4909) wR2(reflections)= 0.0639(4978)

S = 1.083 Npar= 326

Crystallographic Data for 12.





12

CCDC 1976899

Bond precision: C-C = 0.0029 A Wavelength=1.54184

Cell: a=9.6668(1) b=14.4575(1) c=16.9589(1)
alpha=90 beta=90 gamma=90
Temperature: 100 K

	Calculated	Reported
Volume	2370.14(3)	2370.14(3)
Space group	P 21 21 21	P 21 21 21
Hall group	P 2ac 2ab	P 2ac 2ab
Moiety formula	C28 H25 Cl F N O2	C28 H25 Cl F N O2
Sum formula	C28 H25 Cl F N O2	C28 H25 Cl F N O2
Mr	461.94	461.94
Dx,g cm-3	1.295	1.295
Z	4	4
Mu (mm-1)	1.697	1.697
F000	968.0	968.0
F000'	972.18	
h,k,lmax	12,18,21	12,18,21
Nref	5017[2841]	4921
Tmin,Tmax	0.844,0.844	0.832,1.000
Tmin'	0.844	

Correction method= # Reported T Limits: Tmin=0.832 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 1.73/0.98 Theta(max)= 77.038

R(reflections)= 0.0272(4781) wR2(reflections)= 0.0708(4921)

S = 1.047 Npar= 300

General Procedure for the *in vitro* Anti-tumor Activity Study

Cell viability was measured by CCK-8 assay

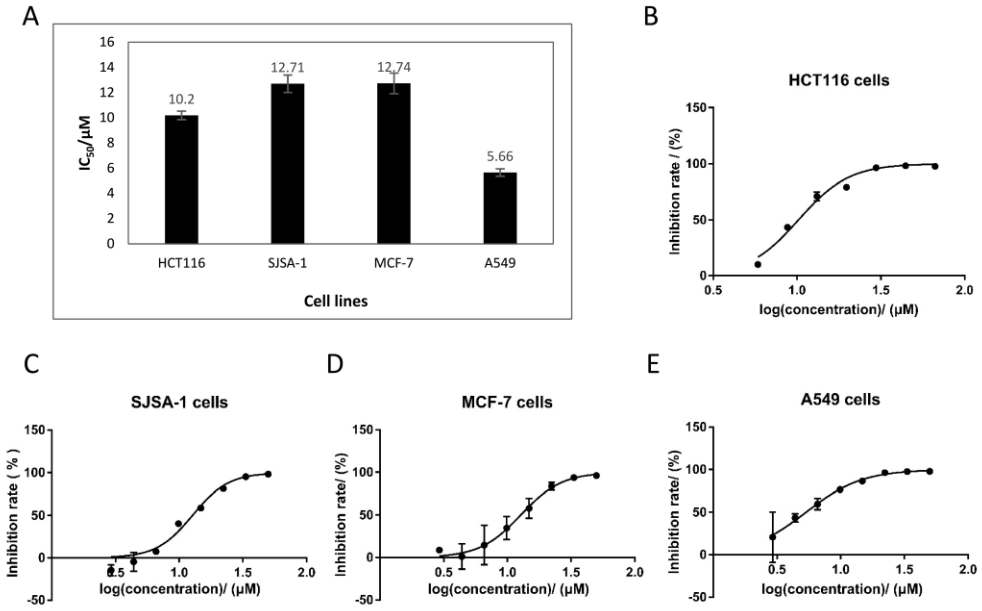
Human cancer cell lines HCT116, A549, and SJSA-1 were obtained from Cell Cook. Cells were cultured in RPMI1640 medium containing 10% fetal bovine serum and 1% penicillin/streptomycin (Gibco) in a humidified incubator containing 5% CO_2 at 37 °C. Human cancer cell lines MCF-7 was obtained from Procell and cells were cultured in MEM medium containing 10% fetal bovine serum, 1% penicillin/streptomycin (Gibco) and 0.01 mg/mL insulin (Procell) in a humidified incubator containing 5% CO_2 at 37 °C. For cell viability, cells were seeded in 96-well plates at 5000 cells per well. After 24 hours, serially diluted compounds were added and cells were cultured for another 48 hours. Cell viability was measured using a Cell Counting Kit-8 (CCK-8) assay according to the manufacturer's instructions (Yeasen Biotechnology, China).

These representative products **4a**, **4b**, **4c**, **4e**, **4h**, **4j**, **4l**, **4m**, **4p**, **5a**, **5f**, **5g**, **5k**, **5n**, and **5q** on cell viability was evaluated *via* CCK8 assay in HCT116 (colon cancer), MCF-7 (breast cancer), A549 (lung adenocarcinoma) and SJSA-1 (osteosarcoma cancer) human cancer cell lines, and the *in vitro* anti-tumor activity results have been listed in Table S4.

According these results, compound **4e** exhibits significant and broad anticancer potency than other tested compounds with more than 90% inhibitory rate towards four kind of cancer cells (HCT116 cells, IC_{50}=10.29 μM; MCF-7 cells, IC_{50}=12.74 μM; A549 cells, IC_{50}=5.66 μM; SJSA-1 cells, IC_{50}=12.71 μM, see Table S5 for detail).

Table S4. Anti-tumor Activity Study of Compounds **4a**, **4b**, **4c**, **4e**, **4h**, **4j**, **4l**, **4m**, **4p**, **5a**, **5f**, **5g**, **5k**, **5n**, and **5q (**Inhibitory rate at 20 μM**)**

Compound	HCT116	MCF-7	A549	SJSA-1
4a	36.43±0.98	55.40±6.15	7.69±5.68	＜30
4b	54.29±0.04	71.17±4.83	32.14±3.60	＜30
4c	49.78±1.96	35.46±8.80	62.24±6.74	＜30
4e	94.98±0.65	92.56±0.56	97.24±0.77	93.95±0.15
4h	47.14±6.53	42.82±0.47	45.13±9.63	＜30
4j	28.90±8.39	43.49±2.84	41.87±5.73	＜30
4l	43.97±1.05	41.82±7.61	41.72±22.86	＜30
4m	37.58±4.57	58.93±0.22	55.36±11.20	＜30
4p	26.64±4.37	57.04±6.87	＜30	＜30
5a	＜30	17.10±2.69	63.95±13.61	＜30
5f	41.06±14.83	28.52±1.70	70.40±7.41	＜30
5g	＜30	26.25±12.31	33.28±4.49	42.88±11.41
5k	31.81±16.55	68.11±1.68	39.47±0.74	31.39±9.32
5n	29.01±7.15	48.43±14.48	32.37±6.61	＜30
5q	＜30	53.50±4.70	＜30	48.60±5.34



Scheme S2. Anti-tumor Activity Study of Compound **4e** on the inhibition of HCT116, SJSA-1, MCF-7 and A549 cells (vehicle-treated cells set at 5000).

Computational Studies

Using Gaussian 09 program[4], all of the structures were optimized by the density functional theory (DFT)[5, 6] with the M06-2X functional[7] with basis sets I (BSI, lanl2dz[8-10] for metal atom and 6-31G (d, p)[11, 12] for nonmetal atoms) in the gas phase. Frequency analysis calculations based on optimized structures were performed to characterize the structures to be minima (no imaginary frequency) or transition states (one imaginary frequency). IRC calculations were taken to confirm the connection between two correct minima for a transition state. The multilayered quantum mechanical and molecular mechanical (QM/MM) method,[13-15] specifically, the two-layer ONIOM method,[16, 17] was employed in phosphoric acid and Au complex. The two-layer structures are shown in Figure S1, in which the QM parts were highlighted. The QM part and MM parts were treated with the M06-2X functional and the universal force field,[18] respectively. Based on M06-2X/BSI optimized geometries, the energy results were further refined by calculating the single-point energy at the M06-2X/BSII level of theory (BSII designates SDD[19, 20] for metal atom and 6-311++G (d, p)[21, 22] for nonmetal atoms). The bulky solvation effect of dichloromethane (ε = 8.93) were simulated by the PCM[23-25] continuum solvent model at the M06-2X/BSII level of theory. The 3D optimized structures were displayed by CYLview visualization program.[26]

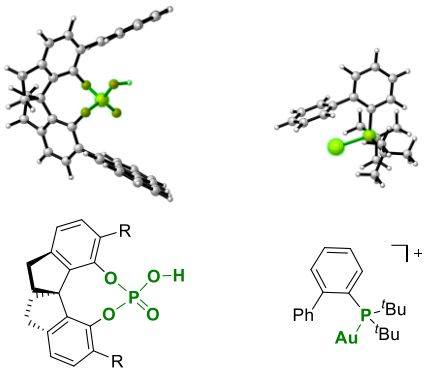


Figure S3. ONIOM model for the phosphoric acid **7a** (Ar = 9-phenanthryl) and Au complex. QM for the highlighted part, MM for the rest part.

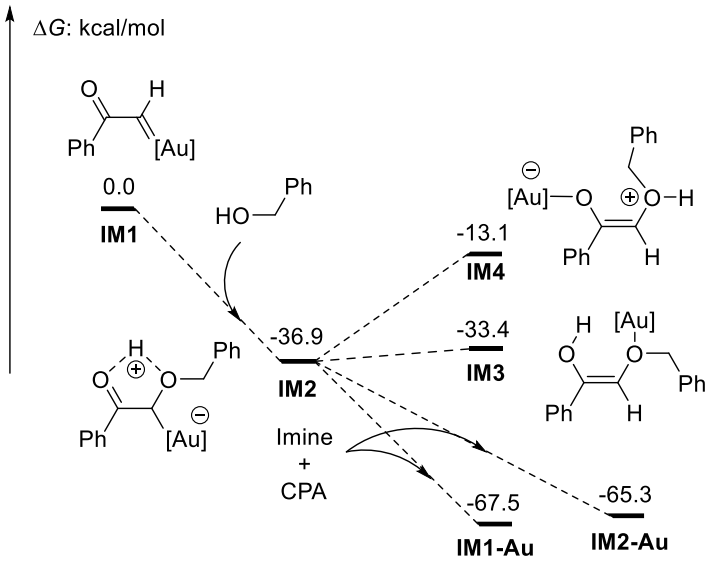


Figure S4. Free energy profiles for the [Au] assists the formation of enol.

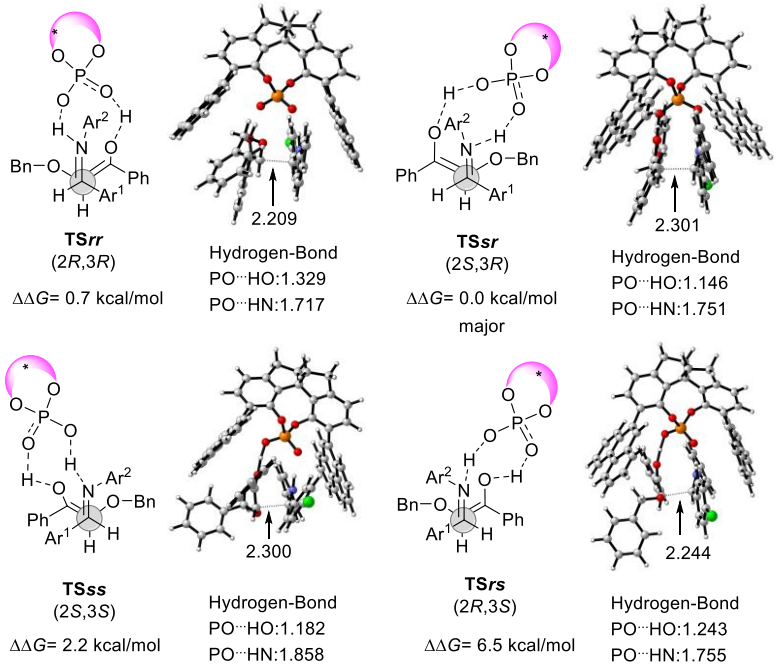


Figure S5. Transition states for the stereoselectivity of the Mannich-type addition with enol species. Bond lengths are in Å.

Cartesian Coordinates of Computed Structures

CPA		C	0.432782 4.561487 -1.205057
0 1		C	-0.012705 3.683801 -0.008239
C	-0.815802 4.733253 -2.086163	C	-1.172015 2.927037 -0.586605

C	-1.676118 3.594755 -1.679727	H	0.783045 -1.706049 1.014903
C	-2.851038 3.181040 -2.305655	C	-3.625843 0.045272 -0.317527
C	-3.505547 2.039680 -1.826973	C	-4.037158 -0.009612 0.957048
C	-2.942597 1.278622 -0.780224	C	-3.886239 -1.104002 -1.239301
C	-1.737550 1.711366 -0.172005	C	-4.784969 -1.165510 1.482202
C	1.136140 2.919278 0.586117	H	-3.847078 0.829590 1.618155
C	1.635050 3.592873 1.679108	C	-4.620783 -2.230766 -0.779819
C	0.785767 4.745151 2.066978	C	-3.376469 -1.102475 -2.554410
C	-0.454300 4.583748 1.174367	C	-5.200384 -1.160532 2.822532
C	2.809190 3.186774 2.310698	C	-5.097218 -2.258161 0.641910
C	3.472225 2.048958 1.837609	C	-4.855699 -3.299740 -1.674336
C	2.920562 1.283518 0.788489	H	-2.772678 -0.285340 -2.923212
C	1.715422 1.707206 0.173124	C	-3.619461 -2.170667 -3.414637
O	1.080106 0.903218 -0.737804	C	-5.926376 -2.232465 3.338798
P	-0.032742 -0.081114 -0.086393	H	-4.964459 -0.323795 3.468863
O	0.618685 -0.771715 1.198530	C	-5.837381 -3.333432 1.185536
O	-1.057852 0.897036 0.694459	C	-4.362474 -3.261887 -2.978365
O	-0.561151 -1.004031 -1.092363	H	-5.409755 -4.178658 -1.389676
H	4.399187 1.744143 2.307622	H	-3.224837 -2.154246 -4.422476
H	3.206630 3.744448 3.148903	C	-6.245024 -3.314912 2.521863
H	-3.252123 3.731727 -3.146746	H	-6.244972 -2.222782 4.373207
H	-4.430699 1.725510 -2.294425	H	-6.114473 -4.196238 0.602899
H	-0.552659 4.668955 -3.163954	H	-4.548087 -4.089959 -3.650543
H	-1.330926 5.693188 -1.867416	H	-6.811068 -4.144854 2.925239
H	1.213252 4.028695 -1.794400	C	3.620362 0.058047 0.325660
H	0.847175 5.545567 -0.893419	C	4.016369 0.001474 -0.953872
H	1.315944 5.696363 1.846189	C	3.909776 -1.083316 1.250233
H	0.510650 4.692859 3.142433	C	4.763988 -1.151170 -1.485770
H	-1.249892 4.072457 1.762672	H	3.808625 0.835026 -1.616751
H	-0.848571 5.571241 0.847741	C	4.646800 -2.205943 0.783843

C	3.425241 -1.079767 2.575207	C	-2.208420 2.328312 -0.033649
C	5.153505 -1.151128 -2.833878	H	-3.170737 1.845454 -0.033179
C	5.097393 -2.237838 -0.646145	C	1.510804 1.566744 0.005085
C	4.908735 -3.267418 1.679974	C	2.156227 1.258672 -1.202187
H	2.819952 -0.267788 2.951939	H	1.693477 1.506640 -2.149468
C	3.693851 -2.140906 3.436335	C	3.402768 0.624901 -1.187598
C	5.874299 -2.222322 -3.358709	H	3.896299 0.381496 -2.119523
H	4.900040 -0.319419 -3.480057	C	4.012903 0.307232 0.029951
C	5.831825 -3.312604 -1.198615	H	4.977495 -0.183483 0.039655
C	4.438981 -3.227282 2.992440	C	3.380286 0.628244 1.235043
H	5.466633 -4.142245 1.390482	H	3.856689 0.388187 2.176706
H	3.317283 -2.122721 4.451031	C	2.134366 1.262999 1.224742
C	6.213552 -3.299106 -2.542646	H	1.657371 1.517832 2.162738
H	6.172076 -2.216808 -4.399315	C	-1.830297 -0.805862 1.649738
H	6.123030 -4.171808 -0.617621	C	-0.816548 -0.422214 2.743997
H	4.644628 -4.049838 3.665550	H	-1.175911 -0.740220 3.746795
H	6.774967 -4.128853 -2.952879	H	-0.662760 0.677948 2.768666
		H	0.166187 -0.907165 2.558110
JohnPhosAu		C	-3.174011 -0.128241 1.979310
1 1		H	-3.598509 -0.553274 2.914531
Au	0.996613 -1.170332 -0.051099	H	-3.921522 -0.275326 1.180389
P	-1.113078 -0.254927 0.018199	H	-3.041218 0.959241 2.151726
C	-1.020354 1.576505 -0.003164	C	-1.999044 -2.334887 1.668528
C	0.217964 2.266392 -0.009316	H	-2.254957 -2.688032 2.691026
C	0.236258 3.670067 -0.036817	H	-1.057717 -2.837011 1.357575
H	1.178509 4.205171 -0.040929	H	-2.819278 -2.659218 1.000724
C	-0.954848 4.393788 -0.061332	C	-1.964102 -0.860946 -1.531655
H	-0.931255 5.475666 -0.082656	C	-3.499615 -0.864370 -1.434437
C	-2.175344 3.723360 -0.060546	H	-3.942463 -1.184784 -2.402362
H	-3.100039 4.285585 -0.081272	H	-3.897586 0.142794 -1.214498

H	-3.857183	-1.579405 -0.670464
C	-1.477187	-2.290365 -1.835347
H	-1.915771	-2.660692 -2.787378
H	-1.770272	-2.997777 -1.036021
H	-0.371123	-2.316413 -1.935796
C	-1.542703	0.042707 -2.706990
H	-1.940859	-0.347473 -3.668774
H	-0.435245	0.092369 -2.785938
H	-1.932546	1.073827 -2.576675

$PhCH_2OH$

0 1

C	2.295968	0.329868 -0.014910
C	1.351160	1.350112 0.015777
C	-0.010009	1.051006 0.036471
C	-0.433854	-0.275350 0.023916
C	0.517096	-1.297073 -0.010659
C	1.874664	-0.998620 -0.028042
H	3.355290	0.565417 -0.031120
H	1.673149	2.386925 0.023399
H	-0.753098	1.839718 0.058050
H	0.190095	-2.334644 -0.026187
H	2.604223	-1.801994 -0.056453
C	-1.901291	-0.627189 0.066505
H	-2.121066	-1.113093 1.030276
H	-2.113883	-1.365163 -0.722402
O	-2.674413	0.540004 -0.100939
H	-3.601814	0.306279 -0.002406

Enol

0 1

C	0.544402	-0.371205 -0.490402
C	1.478103	0.373118 0.117456
O	1.130632	1.488162 0.814665
C	2.928442	0.119423 0.056096
C	3.436295	-1.153837 -0.226434
C	3.819710	1.170220 0.292250
C	4.807200	-1.362990 -0.302548
H	2.754700	-1.987643 -0.363720
C	5.192362	0.955108 0.222758
H	3.423675	2.151805 0.527049
C	5.690968	-0.308408 -0.080093
H	5.188464	-2.355484 -0.520872
H	5.875131	1.778913 0.405263
H	6.761971	-0.475135 -0.132917
H	0.758362	-1.237128 -1.108207
O	-0.767527	0.038579 -0.396383
C	-1.663056	-0.998046 -0.023492
H	-1.389998	-1.395900 0.963575
H	-1.574791	-1.823260 -0.747658
C	-3.070499	-0.462629 -0.009563
C	-3.455855	0.548428 -0.890171
C	-4.011080	-1.000802 0.868311
C	-4.767530	1.013427 -0.889592
H	-2.718262	0.971866 -1.563842
C	-5.325055	-0.542158 0.862422
H	-3.711744	-1.779977 1.564994
C	-5.705773	0.467948 -0.016451
H	-5.058605	1.804654 -1.573343
H	-6.048085	-0.966010 1.551968

H -6.727995 0.832239 -0.017730

H 0.170523 1.581549 0.725889

Imine

0 1

C -0.505914 0.571610 -0.000015

N -1.338856 -0.394448 -0.000003

C -2.736132 -0.167161 0.000000

C -3.530514 -1.319411 0.000005

C -3.362364 1.088499 -0.000002

C -4.918698 -1.229068 0.000009

H -3.031157 -2.283549 0.000007

C -4.749486 1.174325 0.000001

H -2.779212 2.003460 -0.000005

H -5.518069 -2.134069 0.000013

H -5.223096 2.151417 0.000000

H -0.800597 1.627175 -0.000018

C 0.946173 0.332910 -0.000009

C 1.813500 1.429006 0.000001

C 1.476957 -0.963285 -0.000014

C 3.192415 1.246354 0.000006

H 1.406665 2.436584 0.000004

C 2.849630 -1.161938 -0.000008

H 0.800135 -1.811220 -0.000022

C 3.691494 -0.050590 0.000001

H 3.867836 2.094486 0.000014

H 3.267405 -2.162666 -0.000012

C -5.534022 0.020034 0.000006

H -6.616607 0.097685 0.000009

Cl 5.423556 -0.299169 0.000008

IM1

1 1

C -2.200333 0.078558 -1.473277

C -3.401760 -0.372717 -0.857009

O -3.058933 -1.272798 -1.675051

C -4.464125 -0.234052 0.064880

C -4.530802 0.937304 0.840312

C -5.422422 -1.258845 0.189995

C -5.563157 1.081241 1.750633

H -3.778690 1.708760 0.715113

C -6.449419 -1.099552 1.102951

H -5.343966 -2.149597 -0.425920

C -6.514181 0.064609 1.877215

H -5.635309 1.974564 2.359888

H -7.201250 -1.871386 1.219701

H -7.322190 0.180734 2.592599

Au -0.319504 -0.197417 -0.656669

P 1.805743 -0.859137 0.192711

C 1.436955 -1.868961 1.726669

C 2.616670 -1.782820 -1.215965

C 1.261618 -0.903685 2.916014

H 2.219967 -0.404086 3.168934

H 0.508647 -0.121198 2.678739

H 0.919183 -1.449301 3.821994

C 2.517235 -2.904491 2.085639

H 2.241363 -3.430772 3.025181

H 2.612301 -3.683086 1.306971

H 3.498848 -2.430799 2.263070

C 0.096933 -2.599404 1.513523

H	-0.714406 -1.875658 1.283819	C	-1.093132 3.026638 0.333720
H	0.159019 -3.326071 0.680642	H	0.251674 2.435990 1.902480
H	-0.195457 -3.160792 2.427382	C	-1.262548 3.206652 -1.042245
C	2.597969 -0.841001 -2.435158	H	-0.348928 3.047164 -2.986164
H	1.556858 -0.544406 -2.688271	H	-1.897980 3.269553 1.014682
H	3.180994 0.081921 -2.227589	H	-2.204201 3.575856 -1.427293
H	3.044135 -1.334709 -3.325802	H	-2.376176 0.699057 -2.351471
C	1.793078 -3.033405 -1.571827		
H	2.152490 -3.482055 -2.523319	**IM2**	
H	1.884001 -3.814168 -0.793966	1 1	
H	0.720120 -2.773231 -1.699577	C	2.070699 0.894775 -0.717913
C	4.080147 -2.181544 -0.943666	C	2.235038 2.141760 -0.057383
H	4.190148 -2.767477 -0.015658	O	2.978539 2.154731 1.014973
H	4.466791 -2.807746 -1.776719	C	1.640258 3.414047 -0.455525
H	4.735038 -1.288375 -0.888057	C	0.724504 3.487491 -1.516536
C	2.900732 0.536584 0.658047	C	2.007215 4.577135 0.233451
C	4.165739 0.281793 1.218466	C	0.185478 4.709840 -1.880207
C	2.493033 1.883002 0.493662	H	0.421663 2.589086 -2.046191
C	5.011516 1.328037 1.589691	C	1.460362 5.799717 -0.135761
H	4.514527 -0.723832 1.372159	H	2.717041 4.514260 1.050312
C	3.353727 2.925841 0.873238	C	0.550987 5.866759 -1.187543
C	4.607294 2.648740 1.415423	H	-0.524788 4.766712 -2.697430
H	5.983178 1.112757 2.015393	H	1.743157 6.699236 0.399175
H	3.049150 3.958659 0.751211	H	0.120952 6.821734 -1.470904
H	5.263813 3.459120 1.705075	H	2.075385 0.933214 -1.809797
C	1.174724 2.251252 -0.044582	O	2.881652 -0.087878 -0.139193
C	1.002342 2.435083 -1.424656	C	3.585546 -0.921109 -1.075841
C	0.122164 2.550300 0.833235	H	4.314740 -0.310845 -1.623762
C	-0.217205 2.905886 -1.921329	H	2.858705 -1.327664 -1.791601
H	1.815687 2.233736 -2.110239	C	4.248094 -2.019044 -0.301062

C	3.548824 -3.193189 -0.019628	C	-0.246665 -3.138699 -1.739055
C	5.540183 -1.851831 0.196845	H	0.316025 -4.088758 -1.610876
C	4.132704 -4.191630 0.751666	H	-0.796330 -3.219264 -2.695331
H	2.546352 -3.327631 -0.417107	H	0.490468 -2.310772 -1.812324
C	6.127559 -2.849466 0.969070	C	-2.285227 -4.006828 -0.541485
H	6.091030 -0.941961 -0.027666	H	-2.986143 -3.913109 -1.388874
C	5.423421 -4.018341 1.247198	H	-1.813141 -5.010734 -0.610951
H	3.587351 -5.105515 0.961781	H	-2.859279 -3.990348 0.407316
H	7.134762 -2.718080 1.349665	C	-3.141217 -1.003000 0.723136
H	5.883410 -4.798137 1.844972	C	-4.333614 -1.747667 0.658814
Au	0.023423 0.194397 -0.368618	C	-2.962963 -0.107025 1.804508
P	-1.891379 -1.172241 -0.607713	C	-5.315397 -1.621653 1.642349
C	-2.661577 -0.643609 -2.230885	H	-4.518637 -2.434860 -0.147410
C	-1.203413 -2.910055 -0.555635	C	-3.961409 0.011819 2.785900
C	-3.563320 0.578088 -1.964218	C	-5.129552 -0.743331 2.705623
H	-4.438081 0.299184 -1.340359	H	-6.224289 -2.205889 1.577315
H	-2.996299 1.376579 -1.437913	H	-3.833282 0.695336 3.617044
H	-3.951703 0.999839 -2.916628	H	-5.892553 -0.644687 3.466923
C	-3.497862 -1.735528 -2.921166	C	-1.768489 0.737225 1.952236
H	-3.949682 -1.334931 -3.854498	C	-0.645657 0.250500 2.638010
H	-2.876016 -2.599517 -3.218469	C	-1.822245 2.088103 1.577031
H	-4.332702 -2.078360 -2.284917	C	0.407098 1.112663 2.957630
C	-1.537333 -0.197659 -3.185494	H	-0.603914 -0.782672 2.958382
H	-0.925096 0.605173 -2.724122	C	-0.771013 2.948274 1.904174
H	-0.866825 -1.038219 -3.446809	H	-2.693127 2.480360 1.066243
H	-1.960453 0.198711 -4.134015	C	0.334582 2.464442 2.608983
C	-0.384694 -3.027019 0.744351	H	1.268362 0.738663 3.495748
H	0.423886 -2.264354 0.771251	H	-0.820493 3.993185 1.626323
H	-1.034968 -2.875399 1.632419	H	1.140050 3.135664 2.876599
H	0.083964 -4.031540 0.830298	H	3.373845 1.261976 1.112626

IM3

1 1

C	-4.231180 0.926132 -0.519680	H	-1.638843 -2.675595 -3.213631
C	-3.069976 1.020772 0.141911	H	-0.757188 -4.415119 -1.680448
O	-2.332403 -0.028795 0.722297	Au	-0.175866 0.223880 0.153542
C	-2.380336 2.310050 0.354844	P	1.886918 0.295426 -0.824804
C	-2.311322 3.278901 -0.653523	C	1.614386 -0.487196 -2.502145
C	-1.739074 2.549936 1.580641	C	2.425349 2.083313 -0.829500
C	-1.634913 4.473603 -0.429527	C	1.640684 -2.018629 -2.330533
H	-2.775042 3.087119 -1.616397	H	2.659989 -2.372562 -2.070067
C	-1.049167 3.740828 1.792210	H	0.945561 -2.332664 -1.522786
H	-1.827343 1.818817 2.378438	H	1.336932 -2.530037 -3.269651
C	-0.996165 4.704118 0.787881	C	2.650981 -0.088050 -3.566765
H	-1.590731 5.220299 -1.215365	H	2.448089 -0.630376 -4.515681
H	-0.569745 3.920500 2.748728	H	2.596918 0.990673 -3.803339
H	-0.464842 5.634928 0.954406	H	3.678762 -0.351662 -3.261534
H	-4.653789 1.857914 -0.879425	C	0.211739 -0.090258 -3.003151
O	-5.019061 -0.118981 -0.857586	H	-0.564831 -0.355415 -2.256025
C	-4.927114 -1.348691 -0.157917	H	0.142001 0.996534 -3.200236
H	-5.859421 -1.869810 -0.390110	H	-0.031393 -0.616134 -3.951827
H	-4.907305 -1.164405 0.925143	C	2.332940 2.587551 0.621578
C	-3.742886 -2.190347 -0.588368	H	1.310417 2.433389 1.024132
C	-3.239778 -3.170947 0.273559	H	3.049160 2.041374 1.271424
C	-3.151301 -2.005972 -1.842812	H	2.573443 3.671067 0.684292
C	-2.165468 -3.968191 -0.117677	C	1.465776 2.921572 -1.690683
H	-3.696883 -3.316669 1.249578	H	1.636621 4.008113 -1.529882
C	-2.079546 -2.806350 -2.230489	H	1.616319 2.727740 -2.769476
H	-3.546744 -1.245990 -2.509763	H	0.411923 2.695727 -1.427465
C	-1.585717 -3.786858 -1.370528	C	3.873937 2.286128 -1.313554
H	-1.787933 -4.731629 0.554091	H	4.043670 1.859718 -2.316929
		H	4.109384 3.370997 -1.370002
		H	4.599200 1.836170 -0.605407

C	3.120965 -0.689171 0.106545	C	-1.580740 2.315584 2.189746
C	4.412935 -0.864303 -0.421151	C	-2.611767 3.922594 0.156163
C	2.800006 -1.320207 1.334817	H	-3.546436 2.116523 -0.580462
C	5.359493 -1.648081 0.240077	C	-1.286894 3.673968 2.161853
H	4.703814 -0.397712 -1.345769	H	-1.194998 1.678905 2.981917
C	3.761454 -2.110294 1.985980	C	-1.803778 4.477761 1.144965
C	5.033279 -2.273806 1.440047	H	-3.002420 4.547867 -0.639691
H	6.348644 -1.771849 -0.181721	H	-0.660727 4.108473 2.934077
H	3.525409 -2.596030 2.925403	H	-1.572769 5.537557 1.123564
H	5.768154 -2.882544 1.950789	H	-4.909584 0.573979 1.231668
C	1.491486 -1.166090 1.990372	O	-4.303153 -1.462611 1.400216
C	1.257438 -0.074077 2.839949	C	-3.814999 -2.424189 0.331667
C	0.523189 -2.175276 1.875446	H	-4.478055 -3.282148 0.457075
C	0.056250 0.019834 3.547779	H	-2.805408 -2.645087 0.664298
H	2.012369 0.689312 2.972993	C	-3.857622 -1.810895 -1.023138
C	-0.672225 -2.083031 2.595378	C	-2.661701 -1.575862 -1.701645
H	0.702086 -3.037230 1.244282	C	-5.076503 -1.488837 -1.626072
C	-0.908654 -0.983503 3.425159	C	-2.685515 -1.034625 -2.983748
H	-0.121704 0.864701 4.200373	H	-1.718188 -1.837134 -1.228421
H	-1.411511 -2.868021 2.520257	C	-5.097441 -0.919340 -2.892577
H	-1.836258 -0.912590 3.978076	H	-6.012676 -1.689832 -1.109451
H	-2.660744 -0.907245 0.448058	C	-3.900054 -0.696319 -3.572963
		H	-1.759118 -0.883604 -3.526960
IM4		H	-6.043450 -0.666982 -3.359025
1 1		H	-3.918255 -0.269985 -4.570451
C	-4.030637 -0.042781 1.309144	H	-5.205768 -1.642136 1.700239
C	-2.730437 0.308109 1.289449	Au	0.065252 -0.011988 0.483345
O	-1.768256 -0.572816 1.365330	P	1.956282 0.660620 -0.609803
C	-2.414311 1.761702 1.210113	C	1.452905 0.781548 -2.408989
C	-2.922417 2.564451 0.188441	C	2.484902 2.262895 0.196106

C	1.414792 -0.645730 -2.989633	C	5.436951 -2.416987 -0.303856
H	2.430195 -1.094293 -3.009739	H	6.522743 -1.049258 -1.552898
H	0.754198 -1.299239 -2.379294	H	4.130542 -3.588201 0.921847
H	1.028923 -0.640311 -4.032122	H	6.248814 -3.130405 -0.245265
C	2.390519 1.644188 -3.271833	C	1.935556 -2.099833 0.999065
H	2.028431 1.661637 -4.322690	C	1.727182 -1.656308 2.313920
H	2.412038 2.693906 -2.927345	C	1.024856 -2.992688 0.414529
H	3.416940 1.238458 -3.297508	C	0.610209 -2.094468 3.032213
C	0.026100 1.361638 -2.490240	H	2.437828 -0.991057 2.787258
H	-0.666128 0.807032 -1.822546	C	-0.084587 -3.436539 1.139160
H	-0.000574 2.430242 -2.207243	H	1.186962 -3.359787 -0.591564
H	-0.367296 1.294110 -3.527623	C	-0.291006 -2.990017 2.448008
C	2.499128 2.014665 1.715937	H	0.450052 -1.750198 4.045642
H	1.495464 1.696785 2.072529	H	-0.779589 -4.133105 0.688732
H	3.229692 1.218873 1.975246	H	-1.151870 -3.333353 3.006903
H	2.786811 2.936342 2.266933		
C	1.461614 3.372046 -0.097477	**IM1-Au**	
H	1.620057 4.245275 0.571910	1 1	
H	1.553338 3.743703 -1.135779	C	-0.112958 -1.120701 -0.328843
H	0.431147 2.996666 0.062610	C	1.152452 -0.992826 0.136182
C	3.888879 2.732575 -0.228790	O	1.967059 -0.040740 -0.280370
H	3.982311 2.817307 -1.326371	C	-0.100050 0.443368 2.894365
H	4.104942 3.734008 0.202604	N	-1.198204 -0.185806 2.639224
H	4.672337 2.045021 0.150743	C	-1.684639 -1.314838 3.355150
C	3.323467 -0.554757 -0.455805	C	-3.065543 -1.511480 3.387211
C	4.543843 -0.325953 -1.118483	C	-0.802454 -2.206311 3.963318
C	3.175496 -1.751760 0.288903	C	-3.567661 -2.598110 4.092048
C	5.590127 -1.245978 -1.039895	H	-3.720980 -0.818892 2.869292
H	4.707674 0.566828 -1.694433	C	-1.323241 -3.290183 4.659203
C	4.236212 -2.670228 0.355675	H	0.271718 -2.084124 3.858101

H	-4.639032 -2.759726 4.132196	H	0.279113 -1.049297 -2.961232
H	-0.645583 -3.997896 5.124609	H	1.010027 0.410492 -2.252558
H	0.448675 0.133804 3.782770	C	-0.782227 0.762172 -3.433592
C	0.462334 1.490164 2.073004	C	-1.598810 1.784252 -2.942224
C	-0.061148 1.826728 0.814260	C	-0.752752 0.516312 -4.805522
C	1.628814 2.119612 2.533175	C	-2.382300 2.536454 -3.810478
C	0.601316 2.738405 0.011885	H	-1.653861 1.969609 -1.871701
H	-0.967787 1.360221 0.445885	C	-1.516901 1.285679 -5.677830
C	2.276070 3.059894 1.750011	H	-0.132766 -0.288101 -5.192609
H	2.025469 1.871798 3.514514	C	-2.337163 2.294268 -5.180829
C	1.766263 3.340872 0.481601	H	-3.041084 3.301403 -3.416027
H	0.226976 2.985484 -0.975962	H	-1.485372 1.084340 -6.743425
H	3.158150 3.575635 2.110488	H	-2.948284 2.883168 -5.856524
C	1.587299 -1.914075 1.225490	Au	4.038225 0.114795 -0.133030
C	2.419611 -1.427491 2.241659	P	6.279887 0.601657 0.064451
C	1.199515 -3.257656 1.269445	C	7.368431 -0.597119 -0.808196
C	2.872353 -2.260551 3.261840	C	6.844715 -1.703979 -1.521980
H	2.689215 -0.376801 2.229265	C	7.717319 -2.624076 -2.128230
C	1.647131 -4.091920 2.289142	H	7.324203 -3.473309 -2.674841
H	0.589651 -3.654198 0.465814	C	9.097197 -2.460082 -2.039060
C	2.489424 -3.600404 3.285277	H	9.760184 -3.173206 -2.511735
H	3.524289 -1.865521 4.035249	C	9.621576 -1.378005 -1.340546
H	1.359614 -5.137575 2.293975	H	10.694097 -1.249308 -1.270836
H	2.851993 -4.259424 4.067177	C	8.768062 -0.459803 -0.728289
H	-0.817213 -1.845891 0.062848	H	9.220698 0.362232 -0.204543
C	-2.701461 -3.479546 4.736563	C	5.403922 -1.959249 -1.656916
H	-3.100608 -4.330421 5.278117	C	4.814801 -3.003875 -0.928948
Cl	2.595399 4.468763 -0.538412	H	5.388711 -3.547898 -0.188622
O	-0.668311 -0.280194 -1.290045	C	3.494730 -3.378140 -1.185952
C	0.065110 -0.073654 -2.512885	H	3.051099 -4.200541 -0.641051

C	2.752962 -2.701935 -2.157019	H	5.617253 -1.469778 1.987796
H	1.729558 -2.986618 -2.344156	H	7.399988 -1.585662 1.759571
C	3.332453 -1.657322 -2.882107	C	-5.603438 1.858545 0.061471
H	2.760943 -1.144108 -3.644242	C	-6.876160 1.285448 0.233072
C	4.659680 -1.292890 -2.641959	C	-7.655434 1.621899 1.317768
H	5.114841 -0.517981 -3.243756	C	-7.274340 2.625653 2.204341
C	6.528634 2.298212 -0.693529	C	-6.052238 3.274348 2.004442
C	5.758807 2.307200 -2.026988	C	-5.191697 2.879365 0.957734
H	5.830261 3.299962 -2.522244	C	-8.877065 0.788478 1.417622
H	6.177721 1.549709 -2.722424	C	-8.651585 -0.293918 0.352569
H	4.683095 2.079054 -1.863318	C	-7.588424 0.277583 -0.622015
C	8.000804 2.640548 -0.989776	C	-6.791336 -0.820913 -1.261955
H	8.081532 3.677767 -1.381657	C	-7.331671 -1.139525 -2.487214
H	8.627328 2.585458 -0.080917	C	-8.375377 -0.171936 -2.908511
H	8.418441 1.972094 -1.770391	C	-8.281499 0.932211 -1.842129
C	5.933077 3.387836 0.209500	C	-6.896001 -2.250924 -3.206012
H	5.858148 4.355239 -0.332933	C	-5.857977 -3.029752 -2.681627
H	4.916454 3.097960 0.538389	C	-5.210590 -2.649234 -1.486518
H	6.572921 3.567891 1.095140	C	-5.668970 -1.512490 -0.773344
C	6.636464 0.472617 1.901273	O	-4.940753 -1.004760 0.222773
C	7.998122 1.051004 2.324491	P	-3.889510 0.124694 -0.261865
H	8.094452 1.017670 3.431523	O	-3.160018 -0.392871 -1.525237
H	8.840602 0.458788 1.923952	O	-4.757265 1.353771 -0.835516
H	8.100907 2.109445 2.025261	O	-3.019884 0.483609 0.890948
C	5.523565 1.188968 2.695146	H	-5.758363 4.063204 2.686052
H	5.529438 0.874420 3.761294	H	-7.908922 2.896083 3.038473
H	5.654215 2.286959 2.694214	H	-7.351231 -2.508997 -4.153449
H	4.526626 0.957630 2.274948	H	-5.525664 -3.903428 -3.228761
C	6.593724 -1.022672 2.275459	H	-8.157460 0.233389 -3.920033
H	6.732397 -1.163955 3.369316	H	-9.373118 -0.660638 -2.891141

H	-7.647731 1.757626 -2.238732	C	-1.557210 -3.239714 -3.864065
H	-9.283648 1.350142 -1.600829	H	-3.420217 -2.317843 -3.441562
H	-9.772941 1.401841 1.181221	C	-0.670835 -4.731860 -2.185746
H	-8.969800 0.336810 2.428850	C	-1.934309 -5.169428 -0.011843
H	-8.255357 -1.205619 0.855007	C	-3.211049 -5.450469 2.053820
H	-9.604324 -0.567683 -0.152046	C	-0.561802 -4.103977 -3.426460
C	-3.873075 3.545150 0.818163	H	-1.454147 -2.733905 -4.815484
C	-2.913075 3.631773 1.956994	H	0.150260 -5.363059 -1.890230
C	-3.579318 4.195495 -0.377109	C	-0.969478 -6.064501 0.507306
C	-3.090128 2.828524 3.102203	H	-4.081995 -5.233188 2.659982
C	-1.786262 4.493541 1.875656	C	-2.238557 -6.314438 2.551522
C	-2.393584 5.058023 -0.499392	H	0.311718 -4.273136 -4.043128
H	-4.275392 4.132399 -1.205945	C	-1.123007 -6.623450 1.778403
C	-2.207615 2.913668 4.175504	H	-0.087566 -6.346474 -0.042944
H	-3.901245 2.116057 3.167699	H	-2.353591 -6.750147 3.535581
C	-0.910756 4.566233 2.984077	H	-0.371742 -7.300150 2.164979
C	-1.528810 5.251009 0.603911	C	-1.059724 6.572336 -1.846418
C	-2.154192 5.721014 -1.712473	H	-0.879032 7.078544 -2.785861
C	-1.128605 3.788439 4.121379	C	-0.205562 6.781595 -0.767083
H	-2.355301 2.290485 5.048070	H	0.640654 7.448439 -0.872212
H	-0.036917 5.195561 2.989597	H	0.260454 6.337920 1.245796
C	-0.434928 6.134032 0.449007	H	-0.440550 3.846055 4.955010
H	-2.820902 5.586802 -2.554963	H	-1.829128 0.118702 1.851908
C	-4.049745 -3.432680 -0.996542	H	-2.135926 -0.370965 -1.466980
C	-2.836221 -3.669147 -1.834226		
C	-4.121648 -3.985154 0.279332	**IM2-Au**	
C	-2.681811 -3.016712 -3.075563	1 1	
C	-1.803746 -4.526981 -1.364553	C	1.649017 -2.436005 0.579841
C	-3.064941 -4.873069 0.784160	C	0.404253 -1.957846 0.734061
H	-4.997571 -3.804258 0.892691	O	-0.051092 -1.084274 -0.187665

H	-2.384743 0.523277 1.433491	H	1.173798 -2.619326 3.265099
H	-1.026989 -0.998543 -0.234273	C	-2.100952 -3.176766 3.975453
C	-0.223601 2.035670 1.559195	H	-3.732803 -2.850514 2.597617
N	-0.959826 1.069450 1.971282	H	-0.279251 -3.375424 5.107474
C	-0.745984 0.628199 3.308905	H	-2.737490 -3.484624 4.798528
C	-1.849260 0.267442 4.084048	H	2.096209 -3.185068 1.216392
C	0.541748 0.547141 3.851841	C	-5.634084 1.325619 0.034634
C	-1.666146 -0.093587 5.414232	C	-6.793922 0.576031 0.297057
H	-2.842247 0.289759 3.648499	C	-7.582724 0.857856 1.388469
C	0.715622 0.172412 5.178231	C	-7.361567 1.990062 2.167997
H	1.403362 0.743051 3.220349	C	-6.297417 2.837011 1.839122
H	-2.529665 -0.353145 6.017736	C	-5.405941 2.501613 0.795290
H	1.716669 0.109884 5.592906	C	-8.660561 -0.145543 1.575676
H	0.456976 2.517275 2.270043	C	-8.330212 -1.215073 0.521169
C	-0.190296 2.591327 0.207570	C	-7.428226 -0.507682 -0.519499
C	-0.872769 2.013330 -0.866345	C	-6.541477 -1.468748 -1.250312
C	0.586509 3.735319 -0.012792	C	-7.091006 -1.785098 -2.472990
C	-0.775439 2.557835 -2.137619	C	-8.283571 -0.963360 -2.787424
H	-1.470200 1.123218 -0.725214	C	-8.294149 0.082739 -1.664082
C	0.702675 4.283785 -1.282670	C	-6.543520 -2.777374 -3.281245
H	1.092804 4.212326 0.821966	C	-5.394545 -3.443079 -2.845368
C	0.026317 3.679753 -2.338939	C	-4.763842 -3.072584 -1.638409
H	-1.313810 2.111236 -2.967013	C	-5.329118 -2.045593 -0.836556
H	1.298919 5.171471 -1.459631	O	-4.683098 -1.561515 0.226088
C	-0.449965 -2.380602 1.863842	P	-3.754047 -0.281829 -0.118237
C	-1.831857 -2.437687 1.703880	O	-2.612530 -0.592089 -1.017688
C	0.103958 -2.713314 3.106032	O	-4.690222 0.856951 -0.785987
C	-2.659421 -2.821958 2.753425	O	-3.355919 0.198205 1.314379
H	-2.264172 -2.233562 0.733489	H	-6.149734 3.741569 2.416160
C	-0.717262 -3.123533 4.147223	H	-8.014429 2.224962 2.998718

H	-7.001823 -3.035095 -4.227361	H	-0.941974 7.137317 0.268787
H	-4.978695 -4.232240 -3.459932	H	-2.291644 6.931342 -3.762533
H	-8.181876 -0.478100 -3.782068	H	-0.892312 7.967214 -2.008072
H	-9.197073 -1.595114 -2.753641	C	-3.534001 -3.786499 -1.228862
H	-7.828919 1.018509 -2.049487	C	-2.316639 -3.815629 -2.092244
H	-9.332898 0.322440 -1.346546	C	-3.581129 -4.575529 -0.081146
H	-9.649402 0.319830 1.374802	C	-2.238128 -3.028410 -3.258808
H	-8.632130 -0.573703 2.600695	C	-1.231312 -4.664461 -1.754352
H	-7.765604 -2.039278 1.013250	C	-2.403831 -5.343456 0.358315
H	-9.253861 -1.645065 0.074867	H	-4.483637 -4.594861 0.519504
C	-4.266469 3.404231 0.491167	C	-1.159843 -3.158392 -4.132353
C	-3.335221 3.895168 1.549786	H	-3.013188 -2.316359 -3.507555
C	-4.140300 3.890204 -0.808451	C	-0.182089 -4.827639 -2.685269
C	-3.314714 3.288689 2.822033	C	-1.231900 -5.365596 -0.431187
C	-2.421440 4.945852 1.263692	C	-2.432276 -5.995068 1.600220
C	-3.199935 4.975040 -1.126237	C	-0.152325 -4.079826 -3.863401
H	-4.812819 3.535097 -1.581265	H	-1.116173 -2.557289 -5.031387
C	-2.434490 3.727439 3.807872	H	0.626042 -5.522648 -2.518071
H	-3.961558 2.455463 3.056405	C	-0.079675 -5.993367 0.091689
C	-1.530247 5.362700 2.279522	H	-3.328760 -5.981226 2.208064
C	-2.388011 5.539363 -0.115438	C	-1.291968 -6.633289 2.085922
C	-3.155679 5.477391 -2.435348	H	0.670202 -4.197045 -4.557228
C	-1.545670 4.760938 3.537436	C	-0.115877 -6.622814 1.338284
H	-2.428613 3.250288 4.779443	H	0.864140 -5.981640 -0.431171
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C	-1.565534 6.638828 -0.454506	H	0.774813 -7.097680 1.729215
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C	-1.533215 7.130450 -1.761663	O	2.435111 -2.000736 -0.492859

C	1.983609 -2.377840 -1.832075	H	5.169396 -3.979034 -2.093644
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H	0.907754 -2.511404 -1.755224	H	4.074783 -4.945665 -0.092945
C	2.309578 -1.284302 -2.800985	C	4.945303 -3.521482 1.267720
C	3.519438 -1.277205 -3.502411	H	4.478728 -3.953952 2.143291
C	1.383670 -0.254977 -3.008993	C	5.785245 -2.412402 1.400380
C	3.803965 -0.251835 -4.402597	H	5.988495 -2.016746 2.386611
H	4.224527 -2.093433 -3.374734	C	4.830071 1.919843 1.944050
C	1.663700 0.758336 -3.919647	C	4.672578 0.746343 2.928848
H	0.446098 -0.266645 -2.459444	H	4.297188 1.100755 3.913551
C	2.872967 0.762000 -4.614235	H	5.649242 0.245811 3.097712
H	4.737617 -0.259770 -4.955172	H	3.954533 -0.005911 2.535290
H	0.938920 1.546104 -4.095888	C	5.833896 2.921672 2.545425
H	3.082504 1.551844 -5.328261	H	5.409956 3.385497 3.462329
Au	3.917421 -0.469371 -0.179198	H	6.078110 3.738066 1.843310
P	5.388282 1.198935 0.313114	H	6.772851 2.413826 2.846821
C	7.103049 0.577849 0.510440	C	3.457332 2.592094 1.786018
C	7.416393 -0.802977 0.430739	H	3.020936 2.836340 2.778746
C	8.752998 -1.222903 0.537065	H	2.753250 1.915430 1.256361
H	9.002093 -2.275954 0.478531	H	3.536994 3.545181 1.230603
C	9.775876 -0.296712 0.728519	C	5.317950 2.350585 -1.161391
H	10.801777 -0.631413 0.812248	C	5.798907 3.784741 -0.877354
C	9.475602 1.058717 0.820600	H	5.740226 4.393777 -1.805492
H	10.269357 1.777942 0.976541	H	6.851698 3.811608 -0.547638
C	8.153711 1.491935 0.712384	H	5.160185 4.289210 -0.129410
H	7.965391 2.546809 0.797972	C	3.864465 2.409799 -1.662952
C	6.395325 -1.850261 0.268556	H	3.796103 2.963286 -2.624549
C	6.167642 -2.417691 -0.994400	H	3.208067 2.925034 -0.940032
H	6.656772 -2.013555 -1.872281	H	3.466454 1.388468 -1.819797
C	5.333770 -3.533435 -1.121462	C	6.183056 1.746311 -2.284585

H	6.073215 2.325836 -3.226856	O	-1.240504 -1.358019 0.691119
H	5.884072 0.695077 -2.486645	C	-2.569562 -0.929112 0.414786
H	7.257814 1.756189 -2.006929	H	-2.600525 0.102243 0.773790
		H	-2.721770 -0.941907 -0.668764
TS*rr*		C	-3.586953 -1.792705 1.111079
0 1		C	-4.391237 -2.678915 0.395621
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C	-0.619234 -2.646784 -1.171219	C	-5.316630 -3.483795 1.056381
H	0.864999 -0.634190 1.664561	H	-4.298363 -2.728600 -0.686660
C	2.649271 -3.638606 -0.423667	C	-4.607535 -2.553167 3.165365
C	2.008591 -2.481674 0.034051	H	-3.043005 -1.075790 3.062646
C	2.211091 -1.277320 -0.643861	C	-5.428255 -3.417914 2.442109
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C	3.610450 -2.399670 -2.232425	H	-4.681814 -2.505422 4.247601
H	2.492218 -4.583479 0.089163	H	-6.152129 -4.040273 2.958815
H	1.744477 -0.368929 -0.288870	C	-1.575544 -1.875051 5.455492
H	3.108583 -0.303722 -2.333488	H	-2.187107 -1.924083 6.350240
C	1.059924 -2.604465 1.150658	C	-1.252815 3.464423 -0.904146
H	0.947151 -3.613095 1.535878	C	-0.406997 4.524187 -1.269663
N	0.828067 -1.617716 2.011507	C	-0.503071 5.104546 -2.513906
C	0.010679 -1.751697 3.155825	C	-1.530162 4.769748 -3.392237
C	-0.436640 -2.985717 3.632475	C	-2.471625 3.814700 -2.994981
C	-0.354299 -0.574853 3.822477	C	-2.338527 3.142840 -1.759583
C	-1.228385 -3.038124 4.777111	C	0.557715 6.113964 -2.748576
H	-0.182144 -3.912918 3.131570	C	1.466109 5.960796 -1.519129
C	-1.133219 -0.644600 4.968800	C	0.604838 5.253722 -0.440899
H	-0.039177 0.377702 3.409748	C	1.448255 4.467139 0.512014
H	-1.575264 -4.001826 5.135715	C	1.712730 5.214997 1.636060
H	-1.405408 0.273180 5.480155	C	0.906684 6.459691 1.683797
H	-1.337241 -3.455267 0.705020	C	-0.052247 6.302257 0.492209

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C	3.011996 2.774930 1.262049	C	-5.796190 1.707214 1.410866
C	2.006670 3.190361 0.348826	C	-4.397203 -1.151136 -3.930108
O	1.509693 2.351111 -0.561245	H	-2.632361 -0.637532 -5.038984
P	0.143516 1.589798 -0.038594	H	-6.043677 -1.503174 -2.653784
O	0.400150 0.979048 1.303247	C	-6.715576 -0.330774 -0.264593
O	-1.000203 2.741062 0.186691	H	-5.452253 2.494344 2.070796
O	-0.255445 0.715534 -1.207087	C	-6.867247 0.908707 1.807862
H	-3.299925 3.587828 -3.654983	H	-4.653205 -1.979101 -4.578743
H	-1.617188 5.260298 -4.353118	C	-7.327770 -0.104705 0.970489
H	2.889433 5.422437 3.431154	H	-7.108936 -1.134428 -0.864578
H	4.117426 3.306496 3.052839	H	-7.343271 1.077980 2.765024
H	0.345780 6.534084 2.640222	H	-8.160259 -0.722753 1.281424
H	1.567364 7.342984 1.549572	C	3.772397 1.518643 1.056092
H	-1.026927 5.916945 0.868780	C	3.794460 0.430323 2.083097
H	-0.237188 7.276928 -0.010787	C	4.526970 1.416473 -0.046511
H	0.109867 7.130163 -2.788249	C	3.010260 0.524884 3.251020
H	1.113861 5.896325 -3.685701	C	4.596195 -0.725130 1.876708
H	2.331746 5.317166 -1.796400	C	5.401649 0.254553 -0.283542
H	1.862205 6.944635 -1.183806	H	4.525426 2.221874 -0.773615
C	-3.369102 2.150433 -1.364560	C	3.026118 -0.489942 4.205142
C	-3.735148 1.007390 -2.256255	H	2.364713 1.372827 3.428756
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C	-4.866440 0.202340 -1.953100	C	6.189126 0.216222 -1.444107
C	-5.168965 1.488457 0.175290	C	3.798081 -1.627314 4.000384
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C	-3.260578 -0.393968 -4.191853	H	5.149935 -2.655323 2.745939
H	-2.021167 1.222200 -3.581402	C	6.268611 -1.922291 0.352086

H	6.162695 1.033528 -2.154425	C	0.340215 5.307545 -1.621856
C	7.009762 -0.880159 -1.702034	C	0.089845 4.276816 -0.688024
H	3.793249 -2.420576 4.736885	C	4.122898 5.577214 -1.200889
C	7.044356 -1.948870 -0.809357	C	4.796096 4.591963 -0.230655
H	6.337656 -2.776901 1.004105	C	3.678470 4.125407 0.734729
H	7.611546 -0.906388 -2.601221	C	3.958933 2.769890 1.311114
H	7.675314 -2.803345 -1.017748	C	4.505837 2.891752 2.568837
O	-0.394489 -1.591976 -1.877389	C	4.493845 4.292033 3.055825
H	-0.379688 -0.588934 -1.427293	C	3.653767 5.024316 1.998719
C	-0.389039 -3.936640 -1.854058	C	4.983070 1.783656 3.264591
C	0.454947 -3.954802 -2.970024	C	4.877567 0.520090 2.674648
C	-0.963034 -5.130384 -1.401648	C	4.238249 0.361577 1.426597
C	0.743944 -5.154749 -3.607310	C	3.736940 1.502773 0.746122
H	0.889738 -3.019451 -3.307687	O	2.951214 1.376423 -0.323047
C	-0.674979 -6.328446 -2.045343	P	1.372305 1.269623 0.079525
H	-1.659734 -5.120336 -0.569228	O	1.095590 0.169516 1.046306
C	0.182829 -6.343352 -3.143698	O	1.000855 2.669336 0.832298
H	1.408569 -5.162640 -4.465218	O	0.672226 1.194304 -1.282191
H	-1.128159 -7.250634 -1.696536	H	-0.474171 5.743894 -2.187000
H	0.405659 -7.280764 -3.643480	H	1.840272 6.508489 -2.610058
C	3.468698 -3.600023 -1.543113	H	5.433450 1.897038 4.242289
H	3.964590 -4.494274 -1.902103	H	5.272379 -0.341220 3.199613
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		H	5.531002 4.689509 3.087825

TS*rs*

0 1

C	1.169832 3.744355 0.063677	H	2.610863 5.117047 2.378529
C	2.444805 4.311385 -0.096932	H	4.043558 6.049383 1.812817
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C	1.645521 5.754616 -1.858219	H	4.490868 5.428361 -2.238794
		H	5.179283 3.723863 -0.813580
		H	5.656116 5.062858 0.294540

C	-1.303225	3.794654	-0.482788	C	1.978705	-2.895642	3.323271
C	-2.167480	3.368124	-1.628845	H	2.582167	-0.869250	3.106028
C	-1.806207	3.812170	0.760831	C	2.789476	-4.458502	1.671139
C	-1.620920	3.189571	-2.916305	C	4.319500	-3.686142	-0.215482
C	-3.545512	3.093261	-1.416739	C	5.622926	-2.775278	-2.069401
C	-3.217024	3.486182	1.033820	C	2.029358	-4.185884	2.808097
H	-1.182237	4.131940	1.588616	H	1.380652	-2.688261	4.201323
C	-2.423030	2.794158	-3.984276	H	2.771140	-5.471051	1.302906
H	-0.564953	3.323561	-3.103190	C	4.520150	-4.978509	-0.751152
C	-4.336754	2.692290	-2.517044	H	6.064342	-1.932348	-2.586916
C	-4.099239	3.183432	-0.026942	C	5.788341	-4.056089	-2.594102
C	-3.684287	3.518630	2.356422	H	1.469458	-4.978849	3.287095
C	-3.776973	2.551006	-3.786067	C	5.244526	-5.155095	-1.932612
H	-1.987968	2.658994	-4.966196	H	4.131347	-5.864696	-0.276991
H	-5.385752	2.468540	-2.421303	H	6.346633	-4.197968	-3.510358
C	-5.460395	2.949042	0.276430	H	5.383117	-6.149414	-2.337296
H	-3.010085	3.747726	3.172792	C	-2.707475	-1.730968	-0.535718
C	-5.025581	3.262559	2.635916	C	-1.879584	-0.925623	-1.327661
H	-4.394566	2.235735	-4.617305	O	-1.439459	0.168661	-0.828133
C	-5.912259	2.985447	1.597764	H	0.585474	-1.394005	0.432620
H	-6.191398	2.729489	-0.483820	H	-0.434852	0.644588	-1.150379
H	-5.380086	3.288047	3.658239	C	-0.952842	-2.765931	0.404309
H	-6.954890	2.794371	1.817173	N	0.238556	-2.283527	0.026406
C	4.146359	-0.995675	0.835738	C	0.945946	-2.812902	-1.081461
C	3.450461	-2.114355	1.544680	C	1.631559	-1.950882	-1.938797
C	4.782950	-1.226001	-0.320855	C	0.959145	-4.189936	-1.316558
C	2.676457	-1.865521	2.696905	C	2.281022	-2.469416	-3.052184
C	3.519022	-3.434677	1.025759	H	1.608890	-0.879207	-1.765371
C	4.898579	-2.583559	-0.883182	C	1.604836	-4.694903	-2.439147
H	5.290262	-0.410253	-0.825164	H	0.491815	-4.866985	-0.608334

H	2.796185 -1.791295 -3.724708	C	-5.885538 -2.326324 0.582278
H	1.612926 -5.765956 -2.613780	C	-6.482599 -0.670886 -1.060653
H	-1.236597 -3.694413 -0.082664	C	-7.025146 -3.055884 0.261299
C	-1.443238 -2.586733 1.775402	H	-5.191826 -2.677738 1.342445
C	-2.355607 -3.521473 2.272395	C	-7.628659 -1.396343 -1.378125
C	-1.051582 -1.507655 2.574683	H	-6.263253 0.254862 -1.585290
C	-2.855039 -3.410869 3.562026	C	-7.901068 -2.590645 -0.718309
H	-2.679310 -4.346286 1.642065	H	-7.234407 -3.988303 0.776619
C	-1.549038 -1.387829 3.865199	H	-8.303086 -1.032739 -2.146949
H	-0.364051 -0.756104 2.196441	H	-8.790602 -3.159971 -0.968242
C	-2.441832 -2.339262 4.347856	C	2.261939 -3.837442 -3.315805
H	-3.552895 -4.138814 3.959441	H	2.769342 -4.233033 -4.189256
H	-1.250857 -0.557448 4.494590	Cl	-3.060093 -2.188574 5.970246
C	-1.444644 -1.350797 -2.682548		
C	-0.878547 -0.398487 -3.534280	**TS*sr***	
C	-1.586654 -2.669151 -3.133766	0 1	
C	-0.472893 -0.750997 -4.816094	C	-0.732852 -2.836277 -1.196824
H	-0.731351 0.613044 -3.180815	C	-1.913973 -2.259893 -0.727001
C	-1.163145 -3.024012 -4.406613	O	-1.980117 -1.018973 -0.440798
H	-1.992060 -3.432248 -2.476633	H	0.028490 -0.983366 1.545384
C	-0.612419 -2.063333 -5.254565	H	-1.100184 -0.188753 -0.841483
H	-0.038177 0.000423 -5.466950	C	-0.081772 -2.981726 1.005699
H	-1.253405 -4.053819 -4.736107	N	-0.438388 -1.893364 1.694035
H	-0.285079 -2.343916 -6.250612	C	-1.580947 -1.830562 2.529834
O	-3.268058 -1.165715 0.587170	C	-2.225963 -0.601495 2.710958
H	-3.276063 -2.539574 -0.992972	C	-2.053039 -2.966827 3.190158
C	-4.381206 -0.331708 0.304074	C	-3.365164 -0.536595 3.502076
H	-4.557386 0.227643 1.228265	H	-1.838651 0.279145 2.213542
H	-4.121778 0.379695 -0.487921	C	-3.208029 -2.891240 3.961511
C	-5.608987 -1.125818 -0.075698	H	-1.525910 -3.911359 3.108864

H	-3.863888 0.418278 3.629946	C	2.134792 -0.333649 -2.738663
H	-3.577324 -3.785124 4.453556	C	3.327136 -2.226057 -3.642204
H	-0.666910 -3.872946 1.212684	C	3.245367 0.471773 -2.985642
C	1.295939 -3.207890 0.560005	H	1.248526 0.081269 -2.271564
C	1.733787 -4.531754 0.416898	C	4.430307 -1.417852 -3.896157
C	2.140016 -2.159971 0.179439	H	3.375196 -3.289941 -3.864647
C	2.989346 -4.816047 -0.098440	C	4.393184 -0.064756 -3.563345
H	1.078097 -5.347563 0.709299	H	3.207266 1.521243 -2.710536
C	3.379532 -2.439143 -0.384380	H	5.325174 -1.849014 -4.333382
H	1.810194 -1.127517 0.260554	H	5.257966 0.563861 -3.749837
C	3.796221 -3.758036 -0.512327	C	1.679607 3.206887 0.636563
H	3.337886 -5.837501 -0.197820	C	1.053588 4.454532 0.797338
H	3.994317 -1.642566 -0.785619	C	1.224283 5.185648 1.951082
C	-3.071810 -3.133809 -0.394228	C	2.119714 4.784328 2.939167
C	-3.991277 -2.722770 0.575171	C	2.851006 3.607794 2.747822
C	-3.291305 -4.339994 -1.071230	C	2.635156 2.805781 1.606911
C	-5.079857 -3.524300 0.894907	C	0.362308 6.391474 1.987498
H	-3.835705 -1.774696 1.077404	C	-0.544490 6.213727 0.760288
C	-4.386960 -5.136089 -0.756443	C	0.179322 5.199603 -0.163523
H	-2.627688 -4.641405 -1.875146	C	-0.792086 4.415392 -0.989693
C	-5.279934 -4.733880 0.233793	C	-0.919974 4.983960 -2.235446
H	-5.771755 -3.199276 1.665357	C	0.086640 6.047938 -2.472737
H	-4.551296 -6.063714 -1.294907	C	1.003724 5.945269 -1.242834
H	-6.135030 -5.355297 0.479843	C	-1.919503 4.579237 -3.116529
O	0.197809 -2.007446 -1.746780	C	-2.793307 3.559676 -2.722297
H	-0.675045 -3.888939 -1.457074	C	-2.614804 2.894570 -1.488374
C	1.036103 -2.613920 -2.716891	C	-1.564492 3.301408 -0.624149
H	0.438051 -2.854094 -3.608898	O	-1.239112 2.579284 0.449112
H	1.443567 -3.555937 -2.317901	P	-0.040526 1.505513 0.163692
C	2.178491 -1.690204 -3.057792	O	-0.402862 0.687784 -1.084587

O	1.262929 2.365057 -0.311438	H	6.264643 1.450773 -1.492585
O	0.205581 0.754551 1.423169	C	7.318013 -0.317251 -0.900392
H	3.580486 3.313435 3.492630	H	3.227161 -2.607639 4.763709
H	2.262448 5.380912 3.830958	C	7.412832 -1.351944 0.027877
H	-2.034235 5.059231 -4.079840	H	6.623078 -2.256396 1.773353
H	-3.599224 3.273308 -3.386840	H	8.031004 -0.250950 -1.711945
H	0.653302 5.857627 -3.409525	H	8.201066 -2.087908 -0.065487
H	-0.414032 7.039047 -2.514657	C	-3.561762 1.816443 -1.102294
H	1.900300 5.344507 -1.517789	C	-3.854658 0.664973 -2.012523
H	1.349470 6.948519 -0.909554	C	-4.218574 1.932371 0.061364
H	0.987373 7.305276 1.892834	C	-3.032262 0.404147 -3.128433
H	-0.236535 6.424393 2.923121	C	-4.911038 -0.233440 -1.703576
H	-1.518241 5.792450 1.099124	C	-5.303972 1.008253 0.433979
H	-0.747033 7.187937 0.263234	H	-4.005907 2.769529 0.717696
C	3.476994 1.603010 1.416422	C	-3.266047 -0.700777 -3.943706
C	3.457966 0.469910 2.390943	H	-2.181723 1.030746 -3.358065
C	4.354053 1.605369 0.403559	C	-5.127157 -1.346486 -2.546951
C	2.468335 0.399659 3.391980	C	-5.701930 -0.019430 -0.449520
C	4.407804 -0.579258 2.276531	C	-5.973831 1.192754 1.652619
C	5.382603 0.558795 0.270557	C	-4.313138 -1.569742 -3.657004
H	4.367354 2.437886 -0.292309	H	-2.622114 -0.892478 -4.792336
C	2.391074 -0.702066 4.240871	H	-5.893909 -2.077508 -2.349371
H	1.732977 1.183578 3.509569	C	-6.812986 -0.817974 -0.095931
C	4.301706 -1.690655 3.142240	H	-5.669956 1.977954 2.334140
C	5.453920 -0.496949 1.207407	C	-7.044487 0.370419 1.999040
C	6.313889 0.641082 -0.774887	H	-4.482367 -2.434623 -4.285532
C	3.300285 -1.746705 4.111657	C	-7.469381 -0.625215 1.122099
H	1.614894 -0.751235 4.993717	H	-7.189458 -1.596762 -0.738850
H	4.964653 -2.537610 3.073376	H	-7.555123 0.515023 2.942287
C	6.495536 -1.443005 1.077775	H	-8.310816 -1.252506 1.386960

C	-3.877542 -1.680884 4.113017	H	4.924196 4.318476 2.759747
H	-4.777319 -1.624029 4.716400	H	5.387158 1.914577 2.388539
Cl	5.343740 -4.098027 -1.233366	H	2.803914 6.153729 2.121558
		H	4.101167 6.531753 0.892863
TS*ss*		H	1.142663 5.964243 0.509443
0 1		H	2.219541 6.997167 -0.499647
C	0.014251 3.633783 -1.085201	H	2.173577 6.661303 -3.324747
C	1.081859 4.395870 -1.589215	H	2.679850 5.153017 -4.221315
C	1.033665 4.917963 -2.861707	H	3.873361 4.318975 -2.417746
C	-0.117469 4.826282 -3.640903	H	3.953920 6.032325 -1.870915
C	-1.240638 4.181091 -3.112026	C	-2.412990 2.947524 -1.292134
C	-1.185953 3.572641 -1.840095	C	-3.076426 1.789187 -1.966459
C	2.310637 5.560797 -3.255707	C	-2.979499 3.514427 -0.217927
C	3.260473 5.194660 -2.104702	C	-2.451383 1.127486 -3.042678
C	2.353053 4.805898 -0.908667	C	-4.328340 1.314959 -1.492047
C	3.023200 3.817438 -0.005500	C	-4.300632 3.086972 0.276075
C	3.601743 4.463326 1.062017	H	-2.495878 4.360414 0.259345
C	3.219820 5.895693 1.123861	C	-3.033480 0.002116 -3.621989
C	2.146102 6.021784 0.029843	H	-1.499205 1.461935 -3.430208
C	4.448837 3.792734 1.941735	C	-4.889583 0.162643 -2.085757
C	4.695664 2.430532 1.733737	C	-4.994908 2.033257 -0.359629
C	4.035556 1.730100 0.700094	C	-4.878025 3.760625 1.362952
C	3.145761 2.427744 -0.156544	C	-4.245197 -0.481813 -3.140747
O	2.341478 1.771306 -0.991767	H	-2.537434 -0.502051 -4.441132
P	0.888613 1.441052 -0.326595	H	-5.814637 -0.269298 -1.740518
O	0.999609 0.683970 0.954483	C	-6.292004 1.708628 0.098183
O	0.180341 2.877612 0.000898	H	-4.346600 4.564775 1.857098
O	0.129488 0.761502 -1.466253	C	-6.148397 3.407621 1.815518
H	-2.152168 4.144841 -3.695953	H	-4.689980 -1.361329 -3.586721
H	-0.150995 5.264192 -4.630109	C	-6.856303 2.389763 1.179621

H	-6.888958 0.939069 -0.363284	C	-0.601624 -2.157110 2.750885
H	-6.589020 3.930741 2.654297	C	-0.103478 -0.954308 3.260619
H	-7.847222 2.125863 1.526109	C	-0.696850 -0.356231 4.365492
C	4.336575 0.291627 0.491652	C	-1.808554 -0.951548 4.945678
C	4.157408 -0.716350 1.581948	H	-2.095772 -3.692976 2.992938
C	4.865733 -0.078728 -0.683249	H	0.715829 -0.444063 2.771824
C	3.494807 -0.372370 2.777200	H	-0.316767 0.582452 4.751875
C	4.613542 -2.049188 1.399270	C	-0.023300 -2.799868 1.561691
C	5.367435 -1.445609 -0.910632	H	-0.049243 -3.883205 1.501687
H	5.000554 0.659079 -1.467234	N	0.907860 -2.201572 0.831155
C	3.290346 -1.320263 3.777493	C	1.651461 -2.858286 -0.185716
H	3.104865 0.623206 2.936876	C	2.106153 -4.164798 -0.004432
C	4.376793 -2.995927 2.421175	C	1.929831 -2.172628 -1.367717
C	5.289738 -2.415518 0.113706	C	2.786673 -4.804308 -1.032371
C	5.962189 -1.761906 -2.141418	H	1.934183 -4.676039 0.937166
C	3.724139 -2.628610 3.597362	C	2.625652 -2.819615 -2.383690
H	2.773255 -1.043256 4.687256	H	1.564857 -1.160861 -1.508224
H	4.667413 -4.029194 2.326640	H	3.135387 -5.821731 -0.889315
C	5.855544 -3.689243 -0.121185	H	2.834738 -2.284586 -3.304046
H	6.020057 -1.022438 -2.930765	H	-2.503861 -3.634794 0.726735
C	6.493536 -3.031754 -2.360877	O	-0.986469 -4.058657 -0.625787
H	3.545515 -3.365949 4.369451	C	-1.050947 -3.969778 -2.048020
C	6.446791 -3.990086 -1.350680	H	-0.293951 -4.681489 -2.395774
H	5.856399 -4.465516 0.626201	H	-0.758450 -2.969598 -2.379902
H	6.950690 -3.270418 -3.312386	C	-2.418712 -4.335619 -2.574939
H	6.869235 -4.972076 -1.520585	C	-2.872210 -3.813927 -3.786010
C	-1.751716 -3.176003 0.091440	C	-3.236209 -5.220380 -1.869328
C	-1.792678 -1.808474 -0.148706	C	-4.118717 -4.176388 -4.289581
H	0.942290 -1.168884 0.827317	H	-2.247342 -3.113942 -4.334518
C	-1.700232 -2.757784 3.378646	C	-4.487335 -5.573589 -2.363782

H	-2.878785 -5.628051 -0.928301	C	-0.212392 -0.426209 2.145324
C	-4.931665 -5.053654 -3.577514	N	-1.517516 -0.618160 2.411505
H	-4.461432 -3.761451 -5.232278	C	-2.040266 -1.785442 2.996151
H	-5.116012 -6.258623 -1.803157	C	-3.414583 -1.819718 3.263753
H	-5.907584 -5.329019 -3.964315	C	-1.232938 -2.873984 3.342701
C	3.042965 -4.138267 -2.229675	C	-3.959190 -2.914763 3.918159
H	3.580874 -4.638860 -3.027610	H	-4.033183 -0.980644 2.962102
O	-0.902079 -1.286053 -0.915834	C	-1.794853 -3.958524 4.009664
H	-0.521759 -0.169642 -1.142436	H	-0.173071 -2.891590 3.109325
C	-2.739829 -1.017792 0.674894	H	-5.023045 -2.931438 4.129343
C	-2.301160 0.149098 1.306690	H	-1.160826 -4.794786 4.286021
C	-4.024235 -1.506808 0.944426	H	0.460448 -1.009899 2.770179
C	-3.111685 0.774232 2.247879	C	0.275881 0.919571 1.805463
H	-1.297941 0.521521 1.123797	C	-0.458475 1.796268 1.000656
C	-4.840036 -0.863118 1.867098	C	1.534275 1.312091 2.274111
H	-4.380981 -2.384283 0.412688	C	0.080407 3.018279 0.629118
C	-4.375498 0.266292 2.538192	H	-1.442325 1.519567 0.636258
H	-2.748555 1.658324 2.762883	C	2.054931 2.559832 1.953805
H	-5.837576 -1.242650 2.063814	H	2.095289 0.649733 2.928849
H	-5.001965 0.758546 3.275308	C	1.328146 3.393717 1.110773
C	-2.315726 -2.157069 4.464293	H	-0.446937 3.662320 -0.061898
H	-3.185075 -2.604748 4.931447	H	2.999933 2.896238 2.362288
Cl	-2.602904 -0.167777 6.280582	C	2.041131 -2.565306 1.282681
		C	3.069140 -2.286705 2.189059
TS*rr*-Au		C	1.544063 -3.870656 1.193020
1 1		C	3.595142 -3.294758 2.989554
C	0.068869 -1.420062 0.346132	H	3.435236 -1.270029 2.289660
C	1.470600 -1.482505 0.440842	C	2.072831 -4.879401 1.989898
O	2.186732 -0.552882 -0.055741	H	0.766385 -4.095202 0.472799
H	-2.214623 0.025670 2.026686	C	3.098730 -4.592654 2.888547

H	4.384472 -3.067545 3.698272	C	9.859422 -0.517043 -1.650749
H	1.691173 -5.890762 1.901587	H	10.894893 -0.202045 -1.666510
H	3.511616 -5.380119 3.509929	C	8.907415 0.250684 -0.979321
H	-0.512523 -2.299953 0.615759	H	9.245139 1.148374 -0.494691
C	-3.151692 -3.980591 4.313002	C	5.793368 -1.827769 -1.639502
H	-3.582047 -4.829761 4.831986	C	5.442707 -2.936878 -0.855252
Cl	1.989887 4.935605 0.653756	H	6.151114 -3.356004 -0.151073
O	-0.563841 -0.571155 -0.540416	C	4.189358 -3.533786 -1.006466
C	-0.025018 -0.370591 -1.880201	H	3.930185 -4.400210 -0.412853
H	-0.773903 -0.774258 -2.563598	C	3.274439 -3.018352 -1.928307
H	0.900426 -0.933400 -1.983063	H	2.301254 -3.476254 -2.033604
C	0.170418 1.092262 -2.165740	C	3.616005 -1.910822 -2.709426
C	1.431790 1.683438 -2.088260	H	2.911045 -1.519679 -3.431433
C	-0.929687 1.876295 -2.524312	C	4.877413 -1.323193 -2.575713
C	1.592763 3.041431 -2.346497	H	5.149869 -0.499302 -3.221231
H	2.281780 1.064986 -1.818611	C	6.208638 2.548094 -0.851068
C	-0.769537 3.233448 -2.788712	C	5.539336 2.309707 -2.216711
H	-1.912847 1.420529 -2.607379	H	5.376035 3.269132 -2.754079
C	0.490559 3.820717 -2.692917	H	6.176756 1.664058 -2.857635
H	2.574639 3.498593 -2.273761	H	4.556311 1.811471 -2.089338
H	-1.627588 3.826993 -3.083692	C	7.565660 3.234402 -1.102920
H	0.615093 4.880288 -2.891963	H	7.407490 4.259738 -1.502075
Au	4.234600 -0.014978 -0.014358	H	8.166263 3.329162 -0.182714
P	6.345260 0.882907 -0.008280	H	8.157224 2.686031 -1.864134
C	7.553563 -0.133300 -0.945774	C	5.301868 3.480199 -0.032210
C	7.176291 -1.326908 -1.611874	H	5.042152 4.390566 -0.614871
C	8.148225 -2.092517 -2.278480	H	4.356631 2.962774 0.233036
H	7.869473 -3.007148 -2.788595	H	5.807250 3.822260 0.891155
C	9.481006 -1.688507 -2.298332	C	6.854600 0.914020 1.795072
H	10.220833 -2.284469 -2.816985	C	7.978763 1.911783 2.124153

H	8.240823 1.844762 3.202424	P	-4.171694 0.132135 -0.230190
H	8.903043 1.696988 1.561118	O	-3.076645 -0.252234 -1.295765
H	7.658771 2.955321 1.943475	O	-4.962597 1.296617 -1.014546
C	5.625495 1.266359 2.654045	O	-3.642841 0.510399 1.095996
H	5.848910 1.138798 3.735494	H	-6.579053 3.998415 2.269955
H	5.318166 2.317901 2.507569	H	-8.643548 2.640707 2.424974
H	4.766285 0.614566 2.403192	H	-6.947102 -2.476574 -4.796050
C	7.313168 -0.504658 2.186549	H	-5.163594 -3.820028 -3.732124
H	7.527875 -0.566917 3.275453	H	-7.989131 0.184691 -4.526548
H	6.525071 -1.251443 1.945543	H	-9.212249 -0.871027 -3.675135
H	8.241029 -0.785834 1.645802	H	-7.810719 1.652748 -2.738541
H	-2.202350 -0.446071 -0.864693	H	-9.445921 1.050391 -2.283053
C	-5.964397 1.795905 -0.289043	H	-10.179873 0.992171 0.401680
C	-7.201813 1.133101 -0.252851	H	-9.408378 -0.015530 1.715182
C	-8.112437 1.397416 0.744651	H	-8.401921 -1.464610 0.204859
C	-7.907852 2.427031 1.660386	H	-9.706158 -0.939333 -0.921502
C	-6.733502 3.182813 1.574120	C	-4.492257 3.657158 0.583168
C	-5.741758 2.860934 0.622840	C	-3.607106 3.803207 1.775425
C	-9.259644 0.457212 0.720482	C	-4.193134 4.354425 -0.583995
C	-8.835727 -0.586660 -0.325533	C	-3.788119 2.979550 2.905318
C	-7.746333 0.098247 -1.189409	C	-2.533394 4.734202 1.754748
C	-6.800084 -0.898606 -1.793595	C	-3.091409 5.328104 -0.624430
C	-7.186687 -1.189039 -3.083095	H	-4.830430 4.240070 -1.453883
C	-8.268235 -0.295484 -3.563990	C	-2.929807 3.069388 3.997908
C	-8.387670 0.747173 -2.442602	H	-4.578071 2.242118 2.941905
C	-6.608340 -2.235991 -3.796573	C	-1.679065 4.805826 2.879664
C	-5.594144 -2.985672 -3.192068	C	-2.297026 5.560760 0.522429
C	-5.112247 -2.640847 -1.910832	C	-2.860140 6.048573 -1.805753
C	-5.704254 -1.560239 -1.208879	C	-1.879745 3.980075 3.985351
O	-5.171678 -1.124863 -0.066221	H	-3.074083 2.422608 4.853759

H	-0.830482 5.468179 2.918105	H	-0.656619 6.793335 1.285286
C	-1.284669 6.545378 0.445939	H	-1.208572 4.039272 4.832598
H	-3.468161 5.873476 -2.685018		
C	-4.009511 -3.432182 -1.310653	**TS*rs*-Au**	
C	-2.704410 -3.634761 -2.007553	1 1	
C	-4.251195 -4.083868 -0.104367	C	0.156444 -1.094684 0.215838
C	-2.406898 -2.927698 -3.190516	C	1.552583 -1.229283 0.428316
C	-1.739666 -4.530662 -1.469612	O	2.314561 -0.221754 0.276723
C	-3.280108 -5.036798 0.452832	H	-1.550119 0.798195 1.683113
H	-5.202840 -3.946016 0.397072	C	-0.152428 -0.614035 2.150862
C	-1.204294 -3.133434 -3.861617	N	-0.622315 0.661409 2.092731
H	-3.092521 -2.198384 -3.598189	C	0.265983 1.750245 1.983564
C	-0.517270 -4.701496 -2.160413	C	-0.013991 2.762691 1.068755
C	-2.046584 -5.270570 -0.198191	C	1.401799 1.842257 2.793042
C	-3.613898 -5.745273 1.616116	C	0.856986 3.837787 0.926528
C	-0.262798 -4.015797 -3.347585	H	-0.921405 2.678599 0.478835
H	-0.992700 -2.588118 -4.772371	C	2.264128 2.922189 2.650519
H	0.259536 -5.358342 -1.806989	H	1.589921 1.092244 3.555326
C	-1.160522 -6.215796 0.370359	H	0.639207 4.613609 0.199581
H	-4.564879 -5.579080 2.107635	H	3.131814 2.999318 3.298562
C	-2.723760 -6.669606 2.158720	H	0.858534 -0.656744 2.546455
H	0.675221 -4.162961 -3.867384	C	-1.007504 -1.698095 2.705359
C	-1.497279 -6.898247 1.541334	C	-2.405584 -1.653018 2.655015
H	-0.206075 -6.451355 -0.069412	C	-0.382865 -2.753809 3.379976
H	-2.983552 -7.205400 3.062507	C	-3.161273 -2.618676 3.306268
H	-0.806069 -7.614542 1.966659	H	-2.915216 -0.848712 2.135327
C	-1.840041 6.995752 -1.865069	C	-1.132490 -3.726892 4.029053
H	-1.661209 7.542512 -2.781827	H	0.701796 -2.801135 3.434587
C	-1.057740 7.246363 -0.740681	C	-2.519665 -3.636757 4.007690
H	-0.272255 7.989777 -0.786661	H	-4.244169 -2.574965 3.286387

H	-0.649080 -4.531309 4.571398	H	-2.966766 2.445653 -5.186327
C	2.060721 -2.463395 1.072246	Au	4.374770 0.151770 0.092952
C	3.056947 -2.332825 2.049141	P	6.484479 1.018510 0.024020
C	1.537206 -3.726534 0.786518	C	7.581843 0.183217 -1.185744
C	3.525521 -3.449304 2.729145	C	7.121591 -0.872321 -2.011308
H	3.420016 -1.342083 2.307294	C	8.007429 -1.499671 -2.903307
C	2.016776 -4.845589 1.460074	H	7.663846 -2.308281 -3.537777
H	0.781613 -3.835188 0.018238	C	9.337280 -1.093101 -2.987279
C	3.005983 -4.708808 2.430854	H	10.011251 -1.582128 -3.678722
H	4.283615 -3.338677 3.497130	C	9.797504 -0.056816 -2.180769
H	1.624201 -5.828478 1.227335	H	10.830426 0.260150 -2.246237
H	3.371499 -5.584361 2.957005	C	8.930067 0.573563 -1.287841
H	-0.446570 -1.997665 0.174221	H	9.325906 1.371995 -0.686545
C	2.002192 3.921564 1.712956	C	5.736101 -1.363676 -1.982631
H	2.670055 4.770616 1.616017	C	5.426436 -2.527438 -1.263675
Cl	-3.462848 -4.800980 4.886519	H	6.175110 -3.002692 -0.641661
O	-0.373103 -0.067862 -0.538611	C	4.159970 -3.105403 -1.379257
C	0.477923 0.676064 -1.461203	H	3.931561 -4.013714 -0.837944
H	1.204039 -0.013747 -1.893389	C	3.194467 -2.519941 -2.203536
H	1.005070 1.452555 -0.904348	H	2.213137 -2.966521 -2.287338
C	-0.405033 1.239308 -2.535933	C	3.497789 -1.359415 -2.920533
C	-0.619007 0.501667 -3.700416	H	2.756409 -0.917819 -3.573635
C	-1.089514 2.444677 -2.359585	C	4.767462 -0.784096 -2.816183
C	-1.534847 0.930571 -4.655255	H	5.005969 0.088942 -3.409683
H	-0.053342 -0.412608 -3.853032	C	6.259868 2.792350 -0.521683
C	-2.009980 2.874377 -3.309092	C	5.437737 2.760629 -1.824084
H	-0.899164 3.050964 -1.480502	H	5.239437 3.789999 -2.194137
C	-2.242773 2.111554 -4.450610	H	5.985727 2.211917 -2.619543
H	-1.697517 0.344837 -5.553870	H	4.460012 2.256659 -1.661615
H	-2.547563 3.803719 -3.160504	C	7.584543 3.524976 -0.808593

H	7.388978 4.596398 -1.030662	C	-6.617494 -0.639680 -1.762385
H	8.277400 3.487309 0.049561	C	-7.062717 -0.899010 -3.039032
H	8.090704 3.101554 -1.700044	C	-8.164405 0.007383 -3.447055
C	5.451626 3.570197 0.529539	C	-8.234517 1.017527 -2.291049
H	5.129491 4.556256 0.130066	C	-6.515241 -1.925877 -3.803655
H	4.542661 3.000182 0.812651	C	-5.473427 -2.687014 -3.263648
H	6.051787 3.770631 1.436899	C	-4.928889 -2.367108 -2.000656
C	7.172669 0.770201 1.747804	C	-5.486767 -1.301771 -1.248075
C	8.297300 1.748438 2.130730	O	-4.861093 -0.844733 -0.160269
H	9.162772 1.670523 1.450084	P	-3.888397 0.420123 -0.445897
H	7.936731 2.793037 2.159688	O	-3.013147 0.047004 -1.699081
H	8.671956 1.515133 3.150991	O	-4.805020 1.600258 -1.044557
C	6.022668 0.917312 2.763108	O	-3.137074 0.761470 0.778644
H	6.374377 0.688521 3.792531	H	-6.217660 3.992214 2.567749
H	5.615478 1.946059 2.773379	H	-8.271217 2.623730 2.726173
H	5.195206 0.219156 2.523878	H	-6.899767 -2.144148 -4.791595
C	7.709603 -0.671035 1.850383	H	-5.069976 -3.509742 -3.841134
H	8.025439 -0.903498 2.890548	H	-7.926978 0.515517 -4.406405
H	6.926760 -1.403148 1.554376	H	-9.112532 -0.565569 -3.533851
H	8.591854 -0.814930 1.192247	H	-7.665010 1.929610 -2.581068
H	-2.070531 -0.038681 -1.448099	H	-9.283970 1.318305 -2.077945
C	-5.743300 1.999275 -0.185755	H	-9.908345 1.115939 0.668111
C	-6.970889 1.320368 -0.125732	H	-9.072237 0.033197 1.878417
C	-7.828100 1.508527 0.934806	H	-8.146144 -1.318085 0.238605
C	-7.576986 2.469928 1.910093	H	-9.496774 -0.724056 -0.793218
C	-6.407642 3.231489 1.820475	C	-4.217158 3.784412 0.761610
C	-5.467107 2.987078 0.796114	C	-3.328237 3.902239 1.953352
C	-8.972814 0.566760 0.908572	C	-3.939085 4.534674 -0.377544
C	-8.598791 -0.408433 -0.217680	C	-3.449411 2.994611 3.025148
C	-7.546035 0.326673 -1.087896	C	-2.313051 4.895360 1.989594

C	-2.869798 5.545314 -0.375513	C	-0.210457 -3.846419 -3.744695
H	-4.579141 4.444325 -1.248104	H	-0.973868 -2.365769 -5.095219
C	-2.611064 3.084774 4.133115	H	0.352779 -5.241590 -2.266176
H	-4.177476 2.194916 3.002207	C	-1.000407 -6.147735 -0.067452
C	-1.484961 4.973094 3.133767	H	-4.196613 -5.331388 1.962630
C	-2.100401 5.774038 0.789753	C	-2.426447 -6.529766 1.847395
C	-2.658114 6.316799 -1.527959	H	0.691298 -4.012007 -4.320365
C	-1.638180 4.076211 4.191001	C	-1.280493 -6.831617 1.117561
H	-2.711400 2.377669 4.946415	H	-0.112429 -6.443777 -0.600230
H	-0.688568 5.692957 3.221516	H	-2.644773 -7.069238 2.759832
C	-1.140109 6.811990 0.763891	H	-0.609494 -7.606505 1.465515
H	-3.250275 6.149091 -2.419312		
C	-1.689414 7.318145 -1.537304	**TS*sr*-Au**	
H	-0.984010 4.138452 5.051180	1 1	
C	-0.937034 7.568743 -0.392508	C	0.129612 -0.089588 1.103373
H	-0.533975 7.058454 1.619662	C	1.474711 -0.453151 1.312981
H	-1.530143 7.909210 -2.429921	O	2.323544 -0.330527 0.364572
H	-0.192952 8.354945 -0.399367	H	-1.802815 -1.385718 -0.905150
C	-3.801551 -3.172958 -1.469047	H	-2.056652 0.936573 0.292925
C	-2.551948 -3.409087 -2.251853	C	-0.268011 -1.982947 0.322880
C	-3.979494 -3.823248 -0.250685	N	-0.832891 -1.685345 -0.869423
C	-2.294426 -2.677558 -3.429127	C	-0.080688 -1.427021 -2.043406
C	-1.597357 -4.361292 -1.800441	C	-0.623122 -0.581889 -3.012039
C	-3.017905 -4.830930 0.219721	C	1.157120 -2.037772 -2.264442
H	-4.888268 -3.657125 0.317278	C	0.094081 -0.310949 -4.172573
C	-1.146892 -2.917452 -4.180209	H	-1.611962 -0.160655 -2.862455
H	-2.974307 -1.912095 -3.776194	C	1.854827 -1.769896 -3.435648
C	-0.422019 -4.554679 -2.562873	H	1.569122 -2.745099 -1.552843
C	-1.858014 -5.124190 -0.533334	H	-0.335282 0.356412 -4.912119
C	-3.298058 -5.541248 1.395582	H	2.799195 -2.274631 -3.614464

H	0.745841 -2.355345 0.217105	C	-8.684835 1.060827 0.095509
C	-1.020076 -2.645887 1.411947	C	-7.524024 0.267308 0.746206
C	-2.354455 -2.347322 1.700009	C	-6.520022 1.168845 1.407913
C	-0.357212 -3.601680 2.188933	C	-6.765306 1.234240 2.761777
C	-3.018138 -2.992279 2.732892	C	-7.804620 0.270094 3.195905
H	-2.892662 -1.606954 1.127326	C	-8.050079 -0.574984 1.937477
C	-1.009145 -4.251035 3.230011	C	-6.085555 2.131984 3.582181
H	0.678172 -3.850725 1.977095	C	-5.120707 2.969722 3.013463
C	-2.339207 -3.940995 3.494138	C	-4.794633 2.861797 1.645225
H	-4.056434 -2.763563 2.944735	C	-5.476486 1.919964 0.834112
H	-0.495933 -4.997171 3.825632	O	-5.042278 1.656611 -0.399775
C	1.822686 -1.211333 2.536151	P	-4.033302 0.403262 -0.487128
C	2.818539 -2.193231 2.447177	O	-2.914873 0.582164 0.621105
C	1.157046 -1.018028 3.751666	O	-4.783971 -0.876251 0.165910
C	3.142684 -2.970577 3.551931	O	-3.527166 0.207333 -1.855050
H	3.309612 -2.369950 1.494433	H	-6.690373 -3.100431 -3.315341
C	1.482844 -1.797359 4.856166	H	-8.755733 -1.746349 -3.097913
H	0.403316 -0.244070 3.846175	H	-6.308616 2.191195 4.639718
C	2.472575 -2.772895 4.758563	H	-4.612646 3.691354 3.641469
H	3.908264 -3.735018 3.471341	H	-7.436765 -0.361077 4.033426
H	0.968203 -1.638094 5.797339	H	-8.724816 0.816391 3.495174
H	2.725038 -3.376573 5.623890	H	-7.462561 -1.517203 2.025821
H	-0.569505 -0.133836 1.932074	H	-9.123620 -0.848409 1.837591
C	-5.840632 -1.260440 -0.548595	H	-10.094503 -0.406985 -0.735803
C	-7.070022 -0.608156 -0.381203	H	-9.440466 0.790911 -1.949414
C	-8.067547 -0.737518 -1.319088	H	-8.297705 2.012191 -0.334821
C	-7.952004 -1.632450 -2.382003	H	-9.496282 1.311602 0.813671
C	-6.778096 -2.386736 -2.505343	C	-4.454476 -2.967635 -1.781613
C	-5.703255 -2.188107 -1.612486	C	-3.609951 -2.868644 -3.008458
C	-9.204679 0.178083 -1.052888	C	-4.098329 -3.856811 -0.771628

C	-3.947882 -1.973975 -4.044335	C	-1.985974 5.874280 0.171233
C	-2.443076 -3.671275 -3.134384	C	-3.722986 6.597930 -1.389253
C	-2.874845 -4.666836 -0.867093	C	0.240445 3.949206 2.617831
H	-4.724994 -3.944659 0.109154	H	-0.278151 2.199782 3.746476
C	-3.183350 -1.907921 -5.206635	H	0.537895 5.631981 1.378613
H	-4.798732 -1.312709 -3.961071	C	-1.209319 6.984660 -0.233719
C	-1.701449 -3.603789 -4.336078	H	-4.700423 6.468299 -1.837811
C	-2.031216 -4.560058 -1.996303	C	-2.928038 7.668701 -1.793423
C	-2.535688 -5.519476 0.193818	H	1.247664 3.994620 3.008784
C	-2.073007 -2.730783 -5.358054	C	-1.678277 7.865870 -1.211081
H	-3.455702 -1.218037 -5.994884	H	-0.240715 7.195289 0.188384
H	-0.832383 -4.215987 -4.511497	H	-3.286033 8.353150 -2.551543
C	-0.810524 -5.273825 -1.988493	H	-1.068240 8.705651 -1.518164
H	-3.186776 -5.613112 1.054310	C	1.338382 -0.894800 -4.389323
C	-1.339821 -6.233823 0.168251	H	1.889278 -0.690455 -5.300655
H	-1.487199 -2.682692 -6.267027	Cl	-3.167637 -4.750761 4.783488
C	-0.473483 -6.100436 -0.913926	O	-0.289345 0.787731 0.134590
H	-0.093031 -5.196707 -2.788718	C	0.671850 1.597426 -0.572787
H	-1.075110 -6.875830 0.998425	H	1.375551 2.020560 0.149800
H	0.465129 -6.639514 -0.921007	H	1.225440 0.951994 -1.262341
C	-3.767968 3.763357 1.070376	C	-0.020237 2.692219 -1.332701
C	-2.383787 3.846036 1.620630	C	0.681559 3.869292 -1.595289
C	-4.152051 4.624701 0.045987	C	-1.290075 2.520520 -1.877321
C	-1.920096 2.884084 2.541094	C	0.130752 4.846568 -2.417548
C	-1.504941 4.873153 1.181669	H	1.666101 4.020025 -1.158607
C	-3.265478 5.706585 -0.407221	C	-1.853046 3.507234 -2.681439
H	-5.155183 4.559143 -0.360637	H	-1.838497 1.603289 -1.709846
C	-0.620499 2.942074 3.037613	C	-1.137947 4.666768 -2.964919
H	-2.553178 2.072189 2.871509	H	0.684835 5.757252 -2.619772
C	-0.186828 4.898719 1.691110	H	-2.847315 3.356367 -3.089556

H	-1.569955 5.433799 -3.598763	H	7.459897 1.151622 -4.309221
Au	4.384610 -0.224962 0.020742	H	8.218637 -0.173623 -3.387181
P	6.478746 -0.255294 -0.875584	H	8.262940 1.514084 -2.760611
C	7.702613 0.705905 0.093870	C	5.355300 -0.289567 -3.438660
C	7.337116 1.417264 1.263336	H	5.088824 0.265268 -4.364306
C	8.316268 2.109207 1.995279	H	4.415652 -0.513519 -2.891366
H	8.045820 2.654857 2.891634	H	5.826717 -1.238551 -3.755910
C	9.646509 2.106527 1.580178	C	6.974990 -2.060544 -0.869005
H	10.393451 2.643812 2.150192	C	8.025352 -2.433249 -1.929825
C	10.013508 1.411100 0.431670	H	8.300662 -3.505775 -1.831802
H	11.046911 1.407973 0.109641	H	8.956822 -1.852620 -1.809092
C	9.052355 0.715392 -0.302895	H	7.632647 -2.302020 -2.955032
H	9.377457 0.188338 -1.182389	C	5.713257 -2.916054 -1.097049
C	5.955732 1.465367 1.765528	H	5.955922 -3.999162 -1.035682
C	5.575367 0.647363 2.839694	H	5.268768 -2.730246 -2.093441
H	6.266306 -0.081946 3.244582	H	4.943530 -2.696595 -0.328169
C	4.309727 0.789755 3.413857	C	7.531834 -2.406680 0.526283
H	4.022290 0.164457 4.249022	H	7.726359 -3.497520 0.615920
C	3.416419 1.741284 2.913514	H	6.808823 -2.117654 1.320102
H	2.435360 1.843350 3.357269	H	8.490093 -1.879250 0.715052
C	3.788936 2.554843 1.839552		
H	3.101457 3.297114 1.456383	**TS*ss*-Au**	
C	5.059818 2.426236 1.272931	1 1	
H	5.353379 3.090409 0.470891	C	0.179892 0.974433 1.219042
C	6.300309 0.543056 -2.556284	C	1.540040 0.741181 1.407208
C	5.648007 1.920778 -2.334794	O	2.260628 0.311982 0.435405
H	5.479459 2.440845 -3.302798	H	-2.339431 -1.139092 1.323815
H	6.301243 2.567054 -1.710653	H	-2.250898 0.948344 -0.241207
H	4.666290 1.815220 -1.823475	C	-0.377253 -1.115721 1.826461
C	7.640654 0.760407 -3.284610	N	-1.682698 -0.983399 2.081374

C	-2.227442 -0.302482 3.191557	H	3.531152 1.115554 6.378236
C	-3.618036 -0.179270 3.264591	H	-0.416569 1.381968 2.028536
C	-1.418068 0.261182 4.180463	C	-5.480148 -2.116225 -0.137593
C	-4.190063 0.512910 4.322648	C	-6.811876 -1.722106 -0.329601
H	-4.234243 -0.620302 2.488254	C	-7.642371 -2.434069 -1.160906
C	-2.008132 0.951939 5.234742	C	-7.252276 -3.662909 -1.690914
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H	-5.269345 0.606473 4.376322	C	-5.065115 -3.375010 -0.636632
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H	0.267157 -1.139606 2.701071	C	-8.739239 -0.391751 -0.659798
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C	-0.037186 -2.322373 -1.724479	C	-8.197398 0.183057 2.584226
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H	1.872510 -2.522246 1.643112	C	-5.947459 3.106495 1.653595
C	1.195744 -2.966309 -1.641342	C	-5.420355 2.604716 0.444751
H	-0.573988 -2.274511 -2.665516	C	-5.865905 1.349723 -0.046330
H	2.811985 -3.613391 -0.379571	O	-5.301574 0.799629 -1.121935
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C	1.679740 1.887433 3.638779	O	-4.586357 -1.250745 0.337534
C	3.527999 0.003112 4.536603	O	-3.539823 -0.807310 -2.021989
H	3.309944 -0.903492 2.598318	H	-5.685922 -5.130289 -1.756379
C	2.198163 1.978615 4.925592	H	-7.929661 -4.237677 -2.309114
H	0.991007 2.642580 3.276011	H	-7.222144 2.719722 3.350706
C	3.123058 1.038197 5.376164	H	-5.628143 4.069920 2.031882
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C	3.689603 3.270581 -0.528325		

Reference

(1) (a) Wang, X.; Xu, X.; Zavalij, P. Y.; Doyle, M. P. Asymmeric Formal [3 + 3]-Cycloaddition Reactions of Nitrones with Electrophilic Vinylcarbene Intermediates. *J. Am. Chem. Soc.* **2011**, *133*, 16402-16405. (b) Sahani, R. L.; Patil, M. D.; Wagh, S. B.; Liu, R.-S. Catalytic Transformations of Alkynes into Either α-Alkoxy or α-Aryl Enolates: Mannich Reactions by Cooperative Catalysis and Evidence for Nucleophile-directed Chemoselectivity. *Angew. Chem. Int. Ed.* **2018**, *57*, 14878-14882.

(2) Tudjarian, A.; Minehan. T. [3,3]-Sigmatropic Rearrangement/5-*exo*-dig Cyclization Reactions of Benzyl Alkynyl Ethers: Synthesis of Substituted 2-Indanones and Indenes. *J. Org. Chem.* **2011**, *76*, 3576-3581.

(3) Luoab, L.; Yamamoto, H. Synthesis of Virtually Enantiopure Aminodiols with Three Adjacent Stereogenic Centers by Epoxidation and Ring-Opening. *Org. Biomol. Chem.* **2015**, *13*, 10466-10470.

(4) Gaussian 09, Revision D.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2013.

(5) Hohenberg, P.; Kohn, W. Inhomogeneous Electron Gas. *Phys. Rev.* **1964**, *136*, B864-B871.

(6) Kohn, W.; Sham, L. J. Self-Consistent Equations Including Exchange and Correlation Effects. *Phys. Rev.* **1965**, *140*, A1133-A1138.

(7) Zhao, Y.; Truhlar, D. G. The M06 Suite of Density Functionals for Main Group

Thermochemistry, Thermochemical Kinetics, Noncovalent Interactions, Excited States, and Transition Elements: Two New Functionals and Systematic Testing of Four M06-class Functionals and 12 Other Functionals. *Theor. Chem. Acc.* **2007**, *120*, 215-241.

(8) Hay, P. J.; Wadt, W. R. Ab initio Effective Core Potentials for Molecular Calculations. Potentials for the Transition Metal Atoms Sc to Hg. *J. Chem. Phys.* **1985**, *82*, 270-283.

(9) Hay, P. J.; Wadt, W. R. Ab initio Effective Core Potentials for Molecular Calculations. Potentials for K to Au Including the Outermost Core Orbitals. *J. Chem. Phys.* **1985**, *82*, 299-310.

(10) Wadt, W. R.; Hay, P. J. Ab initio Effective Core Potentials for Molecular Calculations. Potentials for Main Group Elements Na to Bi. *J. Chem. Phys.* **1985**, *82*, 284-298.

(11) Petersson, G. A.; Bennett, A.; Tensfeldt, T. G.; Al-Laham, M. A.; Shirley, W. A.; Mantzaris, J. A Complete Basis set Model Chemistry. I. The Total Energies of Closed-shell Atoms and Hydrides of the First-row Elements. *J. Chem. Phys.* **1988**, *89*, 2193-2218.

(12) Petersson, G. A.; Al-Laham, M. A. A Complete Basis set Model Chemistry. II. Open-shell Systems and the Total Energies of the First-row Atoms. *J. Chem. Phys.* **1991**, *94*, 6081-6090.

(13) Dapprich, S.; Komáromi, I.; Byun, K. S.; Morokuma, K.; Frisch, M. J. A New ONIOM Implementation in Gaussian98. Part I. The Calculation of Energies, Gradients, Vibrational Frequencies and Electric Field Derivatives. *J. Mol. Struc. Theochem* **1999**, *461-462*.

(14) Senn, H. M.; Thiel, W. QM/MM Methods for Biomolecular Systems. *Angew. Chem. Int. Ed.* **2009**, *48*, 1198-229.

(15) Menikarachchi, L. C.; Gascon, J. A. QM/MM Approaches in Medicinal Chemistry Research. *Curr. Top. Med. Chem.* **2010**, *10*, 46-54.

(16) Vreven, T.; Byun, K. S.; Komaromi, I.; Dapprich, S.; Montgomery, J. A.; Morokuma, K.; Frisch, M. J. Combining Quantum Mechanics Methods with Molecular Mechanics Methods in ONIOM. *J. Chem. Theory. Comput.* **2006**, *2*, 815-26.

(17) Chung, L. W.; Sameera, W. M.; Ramozzi, R.; Page, A. J.; Hatanaka, M.; Petrova, G. P.; Harris, T. V.; Li, X.; Ke, Z.; Liu, F.; Li, H. B.; Ding, L.; Morokuma, K. The ONIOM Method and Its Applications. *Chem. Rev.* **2015**, *115*, 5678-796.

(18) Rappe, A. K.; Casewit, C. J.; Colwell, K. S.; Goddard, W. A.; Skiff, W. M. UFF, a Full Periodic Table Force Field for Molecular Mechanics and Molecular Dynamics Simulations. *J. Am. Chem. Soc.* **1992**, *114*, 10024-10035.

(19) Andrae, D.; Huermann, U.; Dolg, M.; Stoll, H.; Preu, H. Energy-Adjustedab initio Pseudopotentials for the Second and Third Row Transition Elements. *Theoretica. Chimica. Acta.* **1990**, *77*, 123-141.

(20) Schwerdtfeger, P.; Dolg, M.; Schwarz, W. H. E.; Bowmaker, G. A.; Boyd, P. D. W. Relativistic Effects in Gold Chemistry. I. Diatomic Gold Compounds. *J. Chem. Phys.* **1989**, *91*, 1762-1774.

(21) Krishnan, R.; Binkley, J. S.; Seeger, R.; Pople, J. A. Self-consistent Molecular Orbital Methods. XX. A Basis Set for Correlated Wave Functions. *J. Chem. Phys.* **1980**, *72*, 650-654.

(22) McLean, A. D.; Chandler, G. S. Contracted Gaussian Basis Sets for Molecular Calculations. I. Second Row Atoms, Z=11–18. *J. Chem. Phys.* **1980**, *72*, 5639-5648.

(23) Tomasi, J.; Mennucci, B.; Cammi, R. Quantum Mechanical Continuum Solvation Models. *Chem. Rev.* **2005**, *105*, 2999-3093.

(24) Miertuš, S.; Scrocco, E.; Tomasi, J. Electrostatic Interaction of a Solute with a Continuum. A Direct Utilizaion of AB initio Molecular Potentials for the Prevision of Solvent Effects. *Chem. Phys.* **1981**, *55*, 117-129.

(25) Cossi, M.; Barone, V.; Cammi, R.; Tomasi, J. Ab initio Study of Solvated Molecules: A New Implementation of the Polarizable Continuum Model. *Chem. Phys. Lett.* **1996**, *255*, 327-335.

(26) Legault, C. Y. CYLview, 1.0b; Université de Sherbrooke 2009, http://www.cylview.org.