

Supporting Information

**Chiral Oxalamide Phosphine (COAP)-Pd-Catalyzed Enantioselective Cascade
Formal [4+1] Annulation for Enantioenriched 2,3-Disubstituted Indolines and
Further DFT Study on Regio- and Stereocontrol**

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1. General methods and materials

Unless otherwise stated, all reagents were purchased from commercial suppliers and used without further purification unless otherwise noted. Some commonly used solvents for asymmetric catalysis were dried with different drying agents through standard methods reported, including of methylene chloride (DCM), dichloroethane (DCE), tetrahydrofuran (THF), toluene, acetonitrile, trichloromethane, carbon tetrachloride, methyl tert-butyl ether (MTBE) as well as acetone. All other reaction media were used as obtained unless otherwise noted. Some reactions for the ligand synthesis were carried out in air and using undistilled solvents, without any precautions to exclude moisture unless otherwise noted. Flash Chromatography was performed with silica gel (300–400 mesh) from Yantai Chemical Industry Research Institute, P. R. China. Analytical thin-layer chromatography (TLC) was performed with 0.2 ± 0.03 mm coated commercial silica gel plates (GF-254, particle size 0.04–0.05 mm). The ^1H and ^{13}C NMR spectra were recorded in CDCl_3 on Varian Inova (400 MHz and 100 MHz, respectively) spectrometer. Chemical shifts (δ ppm) are relative to the resonance of the deuterated solvent as the internal standard (CDCl_3 , δ 7.26 ppm for proton NMR, δ 77.10 ppm for carbon NMR). The ^1H NMR data were reported as follows: chemical shift (δ , ppm), multiplicity (s = singlet, d = doublet, q = quartet, m = multiplet, td = triplet of doublets, dt = doublet of triplets, dd = doublet of doublets), coupling constants (J) and assignment. The data for ^{13}C NMR are reported in terms of chemical shift (δ , ppm). The IR spectra were recorded on a Varian 1000 FT-IR spectrometer. High-resolution mass spectra (HRMS) for all the compounds were determined on Micromass GCT-TOF mass spectrometer with ESI resource. High performance liquid chromatography (HPLC) was performed on an Agilent 1200 Series chromatographs using Chiralpak AD-H, AS-H column. The X-ray data were recorded on a Rigaku Mercury CCD/AFC diffractometer. Optical rotations were performed on Rudolph Aupol IV and reported as follows: $[\alpha]_{\text{D}}^{25}$ (c in g per 100 mL, solvent).

2. Preparation of L11–L13

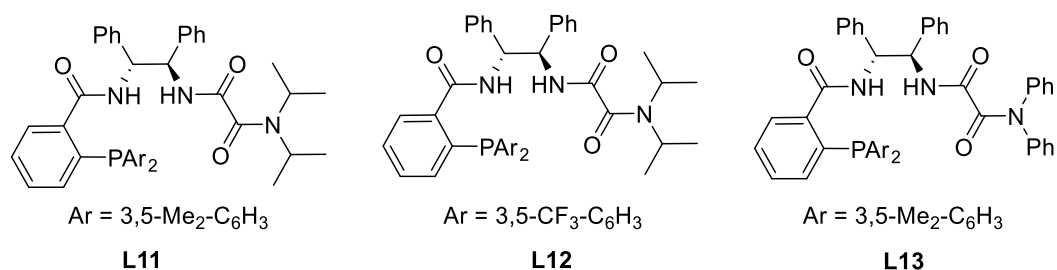


Figure S1. The structure of modified chiral oxalamide-phosphine (COAP) ligands **L11–L13**

2.1 Preparation of L11–L13

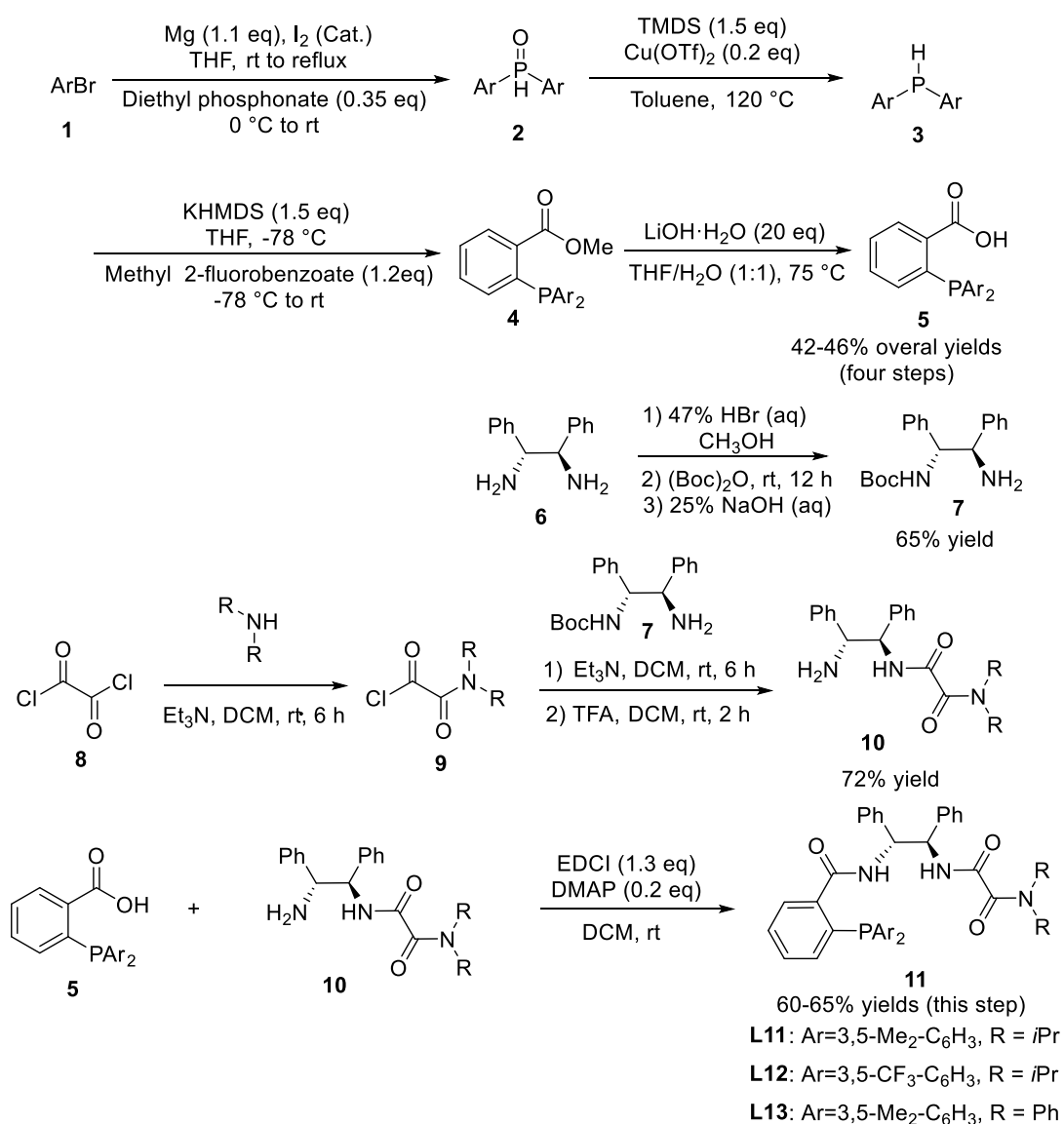


Figure S2. Synthetic scheme of the modified COAP

General procedures: The modified chiral oxalamide-phosphine (COAP) ligands **L11–L13** were synthesized according to literature methods with modification.¹⁻⁵

Diethylphosphonate (1.35 mL, 10.5 mmol) was added dropwise at 0 °C to a solution of arylmagnesium bromide in THF (40 mL) which was prepared intermediately from aryl bromides **1** (30.0 mmol) and magnesium (0.79 g, 33.0 mmol). The mixture was stirred for 2 hours at room temperature. Upon completion (monitored by TLC), the mixture was quenched by a saturated aq. NH₄Cl (30 mL), extracted with EtOAc (3×30 mL), and dried over Na₂SO₄. The organic phase was concentrated in vacuum and the residue was purified by column chromatography on silica gel using petroleum ether/ethyl acetate= 20/1 as eluent to give the diarylphosphine oxides **2**.

The corresponding diarylphosphine oxides **2** (2.56 g, 10.0 mmol) and Cu(OTf)₂ (0.72 g, 2.0 mmol, 0.2 equiv.) were added in a 50 mL Schlenk tube at room temperature. Then TMDS (2.65 mL, 15 mmol, 1.5 equiv.) and toluene (20 mL) were added under nitrogen protection. The reaction mixture was stirred for 12 h at 120 °C. After the reaction was completed, the solvent was removed under vacuum. The residue diarylphosphane **3** was used intermediately for the next step without any purification.

The corresponding diarylphosphanes **3** were placed in a Schlenk flask and dissolved in anhydrous THF (20 mL). The reaction mixture was cooled to –78 °C, KHMDS (1.0 M in THF, 15mL, 15 mmol, 1.5 equiv.) was added via syringe. The reaction mixture was then warmed to room temperature and stirred for 1 hour. The reaction mixture was cooled to –78 °C again and methyl-2-fluorobenzoate (1.5 mL, 12 mmol, 1.2 equiv.) was added dropwise. After the addition, the reaction mixture was warmed to room temperature and stirred overnight. The mixture was quenched with NH₄Cl aqueous (20mL) and was extracted with EtOAc (3×30mL). The combined organic layers were dried over Na₂SO₄, filtered and evaporated in vacuo. The crude was purified by flash chromatography on silica gel using petroleum ether/ethyl acetate = 20:1 as eluent to provide the products **4**.

The corresponding compounds **4** were charged into a round bottom flask equipped with reflux condenser and dissolved in THF (20 mL) at room temperature. Water (20 mL) was added into this solution followed by LiOH H₂O (7.80 g, 186 mmol, 20 equiv.). The reaction mixture was stirred at 75 °C for 36 h. Then the mixture was cooled to room temperature and extracted with EtOAc (3×30mL). The combined organic layers were dried over Na₂SO₄, filtered and evaporated in vacuo.

The crude was purified by flash chromatography on silica gel using petroleum ether/ethyl acetate = 5:1 as eluent to provide the corresponding products **5** (four steps, 42–46% yields).

To a solution of (*1R,2R*)-1,2-diphenylethane-1,2-diamine **6** (20 g, 94.0 mmol) in MeOH (250 mL) was added 47% HBr (aq., 11 mL, 94 mmol) at room temperature. Then both H₂O (30 mL) and Boc₂O (23 g, 104 mmol) were added. After stirring for 12 hours, H₂O (200 mL) was added to the mixture. The precipitated byproduct (diBoc compound) was filtered off, and the MeOH was removed under reduced pressure. The residue was basified with 25% aq. NaOH until pH values were over 14. The mixture was further cooled to 0 °C. After stirring for 1.0 hour, the precipitate was collected by filtration to afford wet crude product. The crude product was purified by column chromatography on silica gel (petroleum ether/EtOAc/CH₃OH 3:1:0.1 v/v) to give the corresponding product **7** (65% yield).

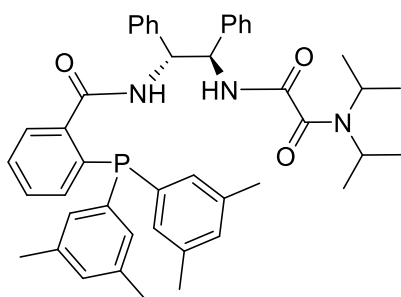
Amines of NHRR (10 mmol) in anhydrous CH₂Cl₂ (10 mL) were respectively added dropwise to a solution of oxalyl chloride **8** (1.29 mL, 15 mmol) in anhydrous CH₂Cl₂ (20 mL) at 0 °C. After stirring for 5 minutes, dry Et₃N (1.46 mL, 10.5 mmol) was added dropwise at 0 °C. Then, the mixture was further stirred for 6 hours at room temperature. The excess of oxalyl chloride and the solvent were removed under reduce pressure. The crude products **9** were dissolved in CH₂Cl₂ (15 mL) and cooled to 0 °C. And then a solution of the compound **7** (2.5 g, 8 mmol) in anhydrous CH₂Cl₂ (10 mL) was added dropwise at 0 °C, followed by the addition of Et₃N (1.15 mL, 8.4 mmol). Then the mixture was stirred for 12 hours at room temperature before being quenched by water (20 mL). The organic layer was separated and the aqueous layer was extracted with CH₂Cl₂ (10 mL×3). The combined organic phase was washed with brine (20 mL), and then dried over anhydrous Na₂SO₄. After removing the solvent under reduce pressure, the product was used for next step without further purification.

At room temperature, TFA (5.95 mL, 80 mmol) was added to a solution of the above product in anhydrous CH₂Cl₂ (100 mL). After stirring for 2 hours, the mixture was poured into saturated NaHCO₃ solution (50 mL). The organic layer was separated and the aqueous layer was extracted with CH₂Cl₂ (50 mL×3). The combined organic phase was washed with brine (50 mL), and then dried over anhydrous Na₂SO₄. The resulting residue was purified by column chromatography on silica gel to give the corresponding product **10** (two steps, 72% yield).

To an oven-dried flask was added **5** (1.81 g, 5.0 mmol), **10** (1.93 g, 6 mmol, 1.2 equiv.), DMAP (122.0 mg, 1 mmol, 0.2 equiv.) and EDCI (1.25 g, 6.5 mmol, 1.3 equiv.), followed by the addition of DCM (20 mL). The reaction mixture was stirred for 6 h at room temperature. After completion (monitored by TLC), the reaction mixture was directly subjected to by flash chromatography on silica gel using petroleum ether/ethyl acetate = 5:1 as eluent to provide the product **11** (60–65% yield).

***N*¹-((1*R*,2*R*)-2-(2-(bis(3,5-dimethylphenyl)phosphaneyl)benzamido)-1,2-diphenylethyl)-*N*²,*N*²-diisopropylloxalamide (L11)**

Following *General procedure A*, the product **L11** was obtained after column chromatography



(petroleum ether/EtOAc 5:1 v/v); white solid; mp 109 –

110 °C; 25.2% yield (2.7 g); $[\alpha]_D^{25} = -50.0$ (c 0.1, CHCl₃);

¹H NMR (400 MHz, CDCl₃) δ 8.09 (d, *J* = 8.0 Hz, 1H),

7.72 (ddd, *J* = 7.6, 3.8, 1.4 Hz, 1H), 7.36 (td, *J* = 7.4, 1.4

Hz, 1H), 7.32 – 7.28 (m, 1H), 7.17 – 7.07 (m, 8H), 6.99 –

6.92 (m, 3H), 6.89 (s, 1H), 6.87 – 6.80 (m, 2H), 6.80 – 6.68 (m, 4H), 5.41 (dd, *J* = 10.0, 8.0 Hz,

1H), 5.18 (dd, *J* = 10.0, 8.0 Hz, 1H), 4.46 (p, *J* = 6.6 Hz, 1H), 3.43 (p, *J* = 6.8 Hz, 1H), 2.20 (d, *J*

= 9.0 Hz, 12H), 1.40 (dd, *J* = 10.4, 6.8 Hz, 6H), 1.10 (d, *J* = 6.6 Hz, 3H), 1.02 (d, *J* = 6.6 Hz, 3H);

¹³C NMR (101 MHz, CDCl₃) δ 169.5, 163.8, 163.1, 141.0, 140.7, 138.4, 138.0, 137.9, 137.8,

137.7, 136.7, 136.6, 136.5, 136.4, 136.1, 134.4, 131.8, 131.6, 131.5, 131.3, 130.6, 130.6, 130.2,

128.7, 128.4, 128.4, 127.6, 127.6, 127.5, 127.5, 59.3, 58.6, 49.8, 46.3, 21.3, 20.8, 20.7, 20.2, 20.0;

³¹P NMR (162MHz, CDCl₃) δ -11.34; IR (KBr) ν_{\max} : 1671, 1639, 1497, 1245, 697 cm⁻¹; HRMS

(ESI): *m/z* = 712.3671 (calcd for C₄₅H₅₀N₃O₃P+H⁺ = 712.3663).

***N*¹-((1*R*,2*R*)-2-(2-(bis(3,5-bis(trifluoromethyl)phenyl)phosphaneyl)benzamido)-1,2-diphenylethyl)-*N*²,*N*²-diisopropylloxalamide (L12)**

Following *General procedure A*, the product **L12** was obtained after column chromatography

(petroleum ether/EtOAc 5:1 v/v); white solid; mp 122–123 °C; 29.9% yield (3.2 g); $[\alpha]_D^{25} = -34.0$

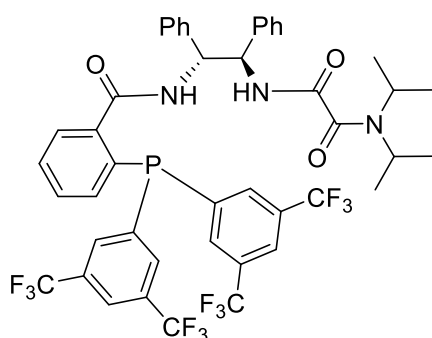
(c 0.1, CHCl₃); ¹H NMR (400 MHz, CDCl₃) δ 8.09 (s, 1H), 7.76 (d, *J* = 7.4 Hz, 2H), 7.67 (s, 2H),

7.50 (dd, *J* = 11.2, 6.2 Hz, 4H), 7.38 (d, *J* = 7.4 Hz, 1H), 7.33 (d, *J* = 7.4 Hz, 1H), 7.08 (d, *J* = 27.4

Hz, 10H), 6.74 (s, 1H), 5.49 (t, *J* = 8.6 Hz, 1H), 5.40 (d, *J* = 8.2 Hz, 1H), 4.07 – 3.91 (m, 1H),

3.37 – 3.22 (m, 1H), 1.19 (d, *J* = 6.4 Hz, 3H), 1.13 (d, *J* = 7.0 Hz, 3H), 0.97 (d, *J* = 6.8 Hz, 3H),

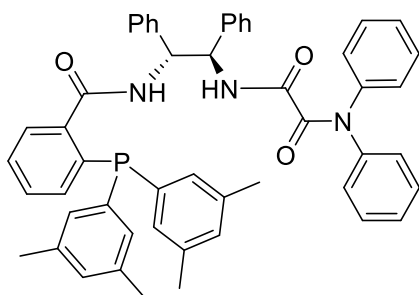
0.87 (d, $J = 6.6$ Hz, 3H); ^{13}C NMR (101 MHz, CDCl_3) δ 167.2, 164.3, 163.6, 141.5, 141.3, 141.1, 139.3, 139.1, 138.6, 137.2, 135.1, 134.9, 134.4, 133.6, 133.3, 133.1, 132.02, 131.95, 131.9, 131.8,



131.7, 131.62, 131.55, 131.51, 130.2, 128.7, 128.5, 128.1, 127.7, 127.4, 127.0, 124.44, 124.39, 122.9, 121.7, 121.7, 58.9, 58.4, 51.6, 50.3, 46.4, 33.05, 20.7, 20.5, 19.9, 19.8; ^{31}P NMR (162MHz, CDCl_3) δ -6.963; ^{19}F NMR (564 MHz, CDCl_3) δ -62.96; IR (KBr) ν_{max} : 1665, 1610, 1527, 1352, 1277, 1122, 896, 698, 681 cm^{-1} ;

HRMS (ESI): $m/z = 950.2350$ (calcd for $\text{C}_{45}\text{H}_{38}\text{F}_{12}\text{N}_3\text{O}_3\text{PNa}^+ = 950.2352$).

N^1 -((1*R*,2*R*)-2-(2-(bis(3,5-dimethylphenyl)phosphaneyl)benzamido)-1,2-diphenylethyl)- N^2,N^2 -diphenyloxalamidee (L13)



Following *General procedure A*, the product **L13** was obtained after column chromatography (petroleum ether/EtOAc 5:1 v/v); white solid; mp 123–124 °C; 23.5% yield (2.8 g); $[\alpha]_{\text{D}}^{25} = -27.8$ (c 0.2, CHCl_3); ^1H NMR (400 MHz, CDCl_3) δ 8.71 (d, $J = 7.8$ Hz, 1H), 7.75 (d, $J = 3.6$ Hz, 1H), 7.39 (q, $J = 6.8, 6.2$ Hz, 2H), 7.25 –

7.00 (m, 20H), 6.97 (s, 1H), 6.92 (d, $J = 8.0$ Hz, 1H), 6.83 (t, $J = 7.2$ Hz, 6H), 5.53 – 5.43 (m, 1H), 5.15 – 5.05 (m, 1H), 2.25 (s, 12H); ^{13}C NMR (101 MHz, CDCl_3) δ 170.2, 163.0, 161.6, 142.2, 141.3, 141.0, 138.5, 138.3, 138.2, 138.0, 137.9, 137.6, 136.7, 136.6, 136.2, 136.1, 135.9, 135.7, 134.5, 131.8, 131.6, 131.5, 131.3, 130.8, 130.4, 129.0, 128.9, 128.8, 128.7, 128.5, 128.2, 127.8, 60.3, 21.4; ^{31}P NMR (162MHz, CDCl_3) δ -11.87; IR (KBr) ν_{max} : 1656, 1491, 1028, 846, 753, 694 cm^{-1} ; HRMS (ESI): $m/z = 780.3355$ (calcd for $\text{C}_{51}\text{H}_{46}\text{N}_3\text{O}_3\text{P} + \text{H}^+ = 780.3350$).

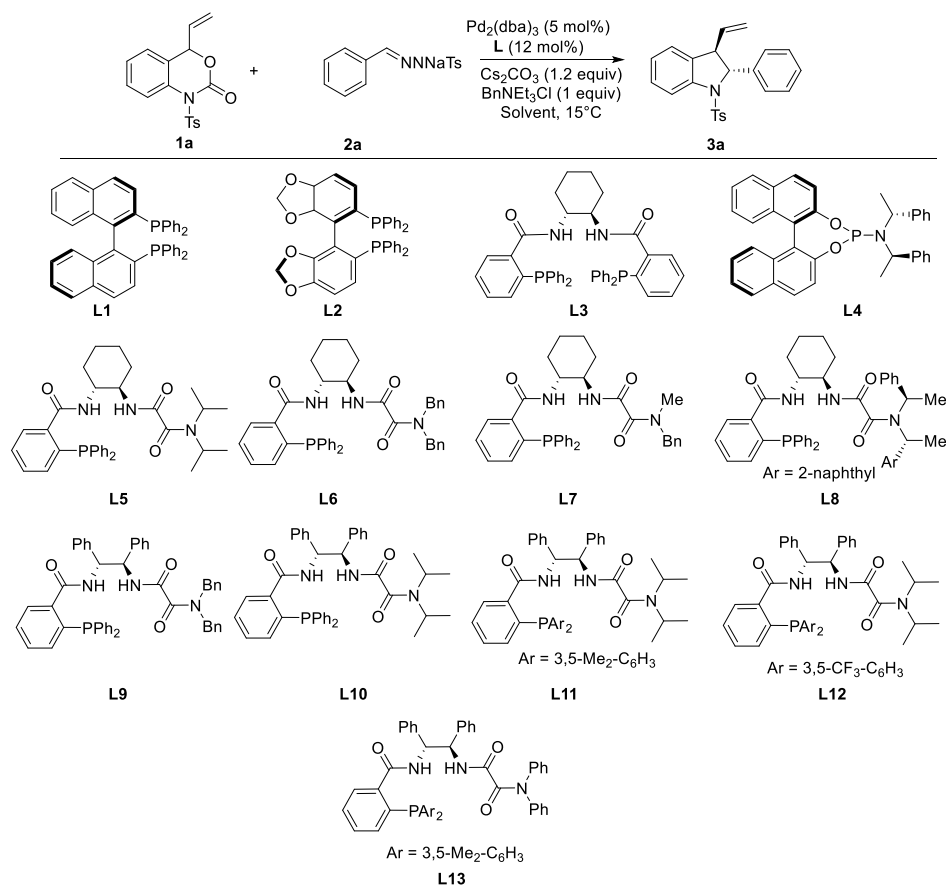
3. Preparation of vinyl benzoxazinaone and N-tosylhydrazone sodium

Vinyl benzoxazinaone was prepared according to the same procedure in the literature reported.^[6-8]

N-tosylhydrazone sodium was prepared according to the same procedure in the literature reported.^[9,10]

4. Optimization of reaction conditions

Table S1. Screening of ligands ^[a]



entry	Ligand	Solvent	Yield (%)	<i>dr</i>	<i>ee</i> (%)
1	L1	DCM	NR	--	--
2	L2	DCM	NR	--	--
3	L3	DCM	NR	--	--
4	L4	DCM	35	>20:1	0
5 ^b	L5	DCM	38	>20:1	57
6 ^b	L6	DCM	40	>20:1	36
7 ^b	L7	DCM	39	>20:1	55
8 ^b	L8	DCM	41	>20:1	38
9 ^b	L9	DCM	40	>20:1	36
10 ^b	L10	DCM	45	>20:1	87
11	L10	DCM	71	>20:1	76
12	L10	DCM/ <i>i</i> -PrOH ^c	71	>20:1	84
13	L11	DCM/ <i>i</i> -PrOH ^c	78	>20:1	91
14	L12	DCM/ <i>i</i> -PrOH ^c	56	>20:1	11

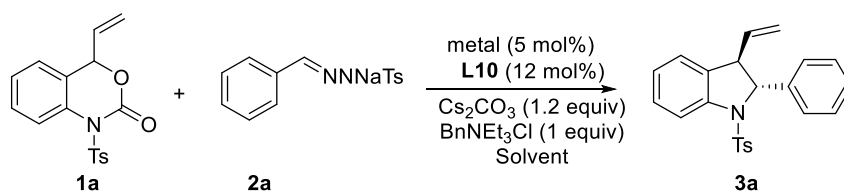
15 **L13** DCM/*i*-PrOH^c 65 >20:1 73

^a Reaction conditions: **1a** (0.1 mmol), **2a** (0.12 mmol), Pd₂(dba)₃ (5 mol%), ligand (12 mol%), Cs₂CO₃ (0.12 mmol), BnNEt₃Cl (0.1 mmol), 1 mL of dichloromethane/*i*-PrOH (10:1) at 15°C for 24 hours. Isolated yield. The *dr* values were determined by ¹H NMR. The *ee* values were determined by chiral HPLC.

^b at -10°C

^c a mixture of DCM and *i*-PrOH (10:1 v/v, 1 mL)

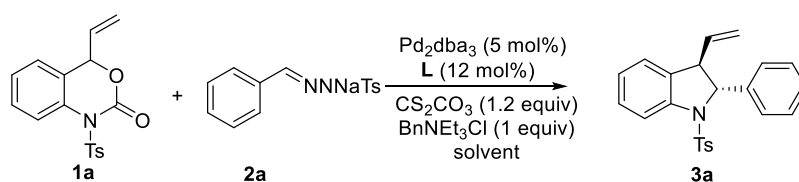
Table S2. Screening of the metal salt ^[a]



Entry	Metal	Solvent	Ligand	Temp. (°C)	Yield (%)	<i>dr</i>	<i>ee</i> (%)
1	Pd ₂ (dba) ₃	DCM	L10	15	71	>20:1	76
2	Pd ₂ (dba) ₃ ·CHCl ₃	DCM	L10	15	70	>20:1	76
3	Pd(dba) ₂	DCM	L10	-10	39	>20:1	76
4	Pd(PPh ₃) ₄	DCE	L10	-10	nr	>20:1	--
5	(PPh ₃) ₂ PdCl ₂	DCM	L10	-10	nr	>20:1	--
6	Pd(R-BINAP)Cl ₂	DCM	L10	-10	nr	>20:1	--
7	Pd(PhCN) ₂ Cl ₂	DCM	L10	-10	nr	>20:1	--
8	Pd[P(<i>t</i> Bu) ₃] ₂	DCM	L10	-10	nr	>20:1	--
9	NiCl ₂ (PPh ₃) ₂	DCE	L10	-10	nr	>20:1	--
10	RhCl(P(C ₆ H ₅) ₃) ₃	DCM	L10	-10	nr	>20:1	--

^a Reaction conditions: **1a** (0.1 mmol), **2a** (0.12 mmol), metal (5 mol%), ligand (12 mol%), Cs₂CO₃ (0.12 mmol), BnNEt₃Cl (0.1 mmol), 1 mL of solvent for 24 hours. Isolated yield. The *dr* values were determined by ¹H NMR. The *ee* values were determined by chiral HPLC.

Table S3. Screening of the solvents and reaction temperature ^[a]

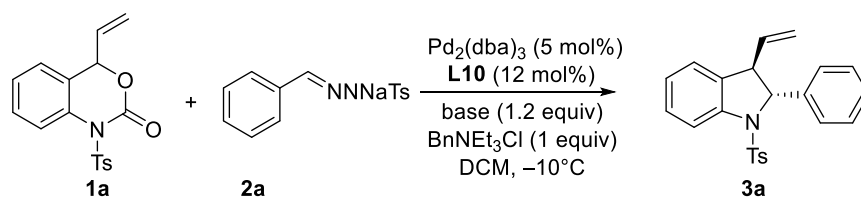


Entry	Solvent	Ligand	Temp. (°C)	Yield (%)	<i>dr</i>	<i>ee</i> (%)
1	DCE	L10	-10	45	> 20 : 1	73

2	CH ₃ CN	L10	-10	39	> 20 : 1	81
3	Toluene	L10	-10	33	> 20 : 1	49
4	CHCl ₃	L10	-10	Trace	--	--
5	CCl ₄	L10	-10	Trace	--	--
6	MTBE	L10	-10	Trace	--	--
7	Acetone	L10	-10	Trace	--	--
8	DCM	L10	-10	45	> 20 : 1	87
9	DCM	L10	15	71	> 20 : 1	76
10	DCM +Toluene	L10	15	65	> 20 : 1	77
11	DCM + DMSO	L10	15	70	> 20 : 1	72
12	DCM+CH ₃ OH	L10	15	72	> 20 : 1	80
13	DCM+ <i>i</i> -PrOH	L10	15	71	> 20 : 1	84
14	DCM	L10	25	78	> 20 : 1	74
15	DCM	L11	-10	45	> 20 : 1	86
16	Toluene	L11	25	68	> 20 : 1	44
17	MeCN	L11	25	69	> 20 : 1	64
18	DCE	L11	25	78	> 20 : 1	72
19	DCM/ <i>i</i> -PrOH	L11	15	78	> 20 : 1	91

^a Reaction conditions: **1a** (0.1 mmol), **2a** (0.12 mmol), metal (5 mol%), ligand (12 mol%), Cs₂CO₃ (0.12 mmol), BnNEt₃Cl (0.1 mmol), 1 mL of solvent for 24 hours. Isolated yield. The *dr* values were determined by ¹H NMR. The *ee* values were determined by chiral HPLC.

Table S4. Screening of the base ^[a]

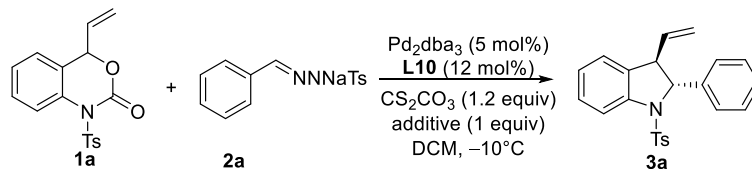


Entry	Base	Solvent	Temp. (°C)	Yield (%)	<i>dr</i>	<i>ee</i> (%)
1	CS ₂ CO ₃	DCM	-10	45	> 20 : 1	87
2	K ₂ CO ₃	DCM	-10	44	> 20 : 1	65
3	Li ₂ CO ₃	DCM	-10	40	> 20 : 1	74
4	Na ₂ CO ₃	DCM	-10	43	> 20 : 1	78
5	KHCO ₃	DCM	-10	41	> 20 : 1	70
6	Et ₃ N	DCM	-10	39	> 20 : 1	70
7	Quinoline	DCM	-10	38	> 20 : 1	71

^a Reaction conditions: **1a** (0.1 mmol), **2a** (0.12 mmol), metal (5 mol%), ligand (12 mol%), Cs₂CO₃

(0.12 mmol), BnNEt₃Cl (0.1 mmol), 1 mL of solvent for 24 hours. Isolated yield. The *dr* values were determined by ¹H NMR. The *ee* values were determined by chiral HPLC.

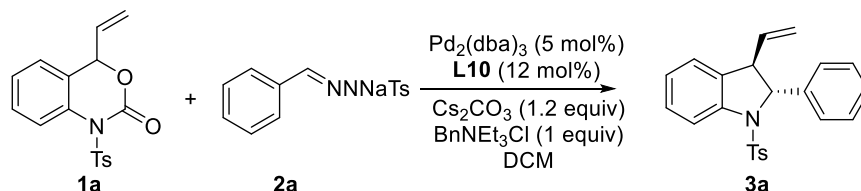
Table S5. Screening of the additives ^[a]



Entry	Additive	Yield (%)	<i>dr</i>	<i>ee</i> (%)
1	Benzyltriethylammonium chloride	45	>20 : 1	87
2	Tetrabutylammonium iodide	44	>20 : 1	69
3	Tetrabutylammonium chloride	40	>20 : 1	78
4	Tetrabutylammonium hydrogen sulfate	42	>20 : 1	71

^a Reaction conditions: **1a** (0.1 mmol), **2a** (0.12 mmol), Pd₂(dba)₃ (5 mol%), ligand (12 mol%), Cs₂CO₃ (0.12 mmol), BnNEt₃Cl (0.1 mmol), 1 mL of dichloromethane/*i*-PrOH (10:1) for 24 hours. Isolated yield. The *dr* values were determined by ¹H NMR. The *ee* values were determined by chiral HPLC.

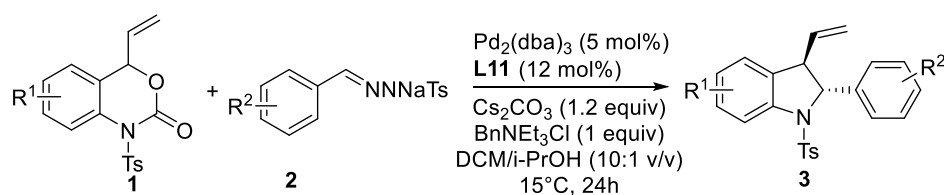
Table S6. Screening of the concentration ^[a]



entry	Solvent	Concentration(M)	Temp. (°C)	Yield (%)	<i>dr</i>	<i>ee</i> (%)
1	DCM	0.1	-10	45	>20 : 1	87
2	DCM	0.05	-10	45	>20 : 1	77
3	DCM	0.025	-10	45	>20 : 1	76

^a Reaction conditions: **1a** (0.1 mmol), **2a** (0.12 mmol), Pd₂(dba)₃ (5 mol%), ligand (12 mol%), Cs₂CO₃ (0.12 mmol), BnNEt₃Cl (0.1 mmol), 1 mL of solvent for 24 hours. Isolated yield. The *dr* values were determined by ¹H NMR. The *ee* values were determined by chiral HPLC.

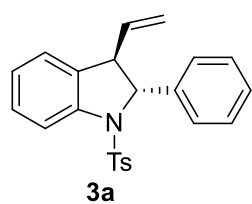
5. General procedure for the preparation of 3



To a flame dried schlenk tube, Pd₂(dba)₃ (4.6 mg, 0.005 mmol), (*R, R*)-**L11** (8.6 mg, 0.012 mmol) and dry DCM (1 mL) were added under nitrogen atmosphere. The mixture was stirred at 25 °C for 0.5 hour to produce a dark red solution and then *i*-PrOH (100 μL) was added. After that, vinyl benzoxazinone **1** (0.1 mmol), *N*-tosylhydrazone sodium salt **2** (0.12 mmol), Cs₂CO₃ (0.12 mmol, 39.10mg), BnNEt₃Cl (0.1 mmol, 22.50mg) were added. The mixture was stirred at 15 °C for 24 hours (monitored by TLC analysis) and then it was subjected to silica gel column to afford the desired products **3**.

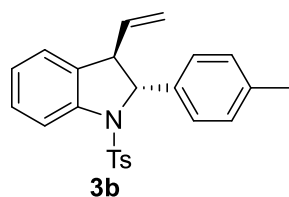
The racemic samples **3** were synthesized according to the literature method without any modification.¹¹ To a flame-dried schlenk tube, Pd₂(dba)₃ (4.6 mg, 0.005 mmol), dry THF (1 mL), vinyl benzoxazinone **1** (0.1 mmol), *N*-tosylhydrazone (0.12 mmol), and Cs₂CO₃ (0.12 mmol, 39.10mg) were added. The mixture was stirred at 60 °C for 4 hours (monitored by TLC analysis) and then it was subjected to silica gel column to afford the desired racemic products **3**.

(2*R,3R*)-2-phenyl-1-tosyl-3-vinylindoline (**3a**)



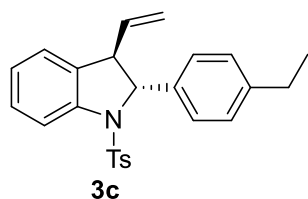
Following *General Procedure B*, the product **3a** was obtained after column chromatography (petroleum ether/EtOAc 50:1 v/v); light yellow oil; 78% yield (29.3 mg), >20:1 *dr*, 91% *ee* [Daicel Chiralpak AD-H, hexanes/*i*-propanol = 90/10, flow rate = 1.0 mL/min, λ = 254.4 nm, t (major) = 10.164, t (minor) = 18.572]; [α]_D²⁵ = -45.7 (c 0.10, CHCl₃); ¹H NMR (400 MHz, CDCl₃) δ 7.72 (d, *J* = 8.0 Hz, 1H), 7.53 – 7.49 (m, 2H), 7.25 – 7.17 (m, 6H), 7.11 (d, *J* = 8.0 Hz, 2H), 6.98 (td, *J* = 7.4, 1.0 Hz, 1H), 6.91 (d, *J* = 7.6 Hz, 1H), 5.17 – 5.07 (m, 1H), 4.84 (d, *J* = 3.6 Hz, 1H), 4.76 – 4.69 (m, 2H), 3.56 (dd, *J* = 8.2, 3.6 Hz, 1H), 2.29 (s, 3H); ¹³C NMR (101 MHz, CDCl₃) δ 143.0, 141.3, 140.8, 137.2, 133.7, 131.4, 128.5, 127.7, 127.6, 126.7, 126.4, 124.8, 124.7, 123.4, 115.0, 114.7, 70.1, 54.8, 20.5; IR (KBr) ν_{max}: 2963, 2923, 1475, 1499, 1367, 1168, 662 cm⁻¹; HRMS (ESI): *m/z* = 398.1161 (calcd for C₂₃H₂₁NO₂S+Na⁺ = 398.1185). The NMR data of **3a** was consistent with the data reported in the literature.^[11]

(2*R*,3*R*)-2-(*p*-tolyl)-1-tosyl-3-vinylindoline (**3b**)



Following *General Procedure B*, the product **3b** was obtained after column chromatography (petroleum ether/EtOAc 50:1 v/v); light yellow oil ; 71% yield (27.70 mg), >20:1 *dr*, 90% *ee* [Daicel Chiralpak AD-H, hexanes/*i*-propanol = 90/10, flow rate = 1.0 mL/min, $\lambda = 254.4$ nm, t (major) = 8.343, t (minor) = 17.096]; $[\alpha]_D^{25} = -51.02$ (c 0.10, CHCl₃); ¹H NMR (400 MHz, CDCl₃) δ 7.71 (d, $J = 8.2$ Hz, 1H), 7.51 (d, $J = 8.0$ Hz, 2H), 7.24 – 7.19 (m, 1H), 7.12 (dd, $J = 12.4, 8.0$ Hz, 4H), 7.04 (d, $J = 7.8$ Hz, 2H), 6.97 (d, $J = 7.4$ Hz, 1H), 6.91 (d, $J = 7.4$ Hz, 1H), 5.16 – 5.04 (m, 1H), 4.78 (d, $J = 3.8$ Hz, 1H), 4.75 – 4.67 (m, 2H), 3.54 (dd, $J = 8.2, 3.8$ Hz, 1H), 2.29 (s, 3H), 2.25 (s, 3H); ¹³C NMR (101 MHz, CDCl₃) δ 148.3, 143.9, 141.8, 139.6, 138.5, 134.9, 132.6, 129.4, 128.5, 127.4, 126.7, 125.8, 125.7, 124.4, 116.0, 115.5, 70.9, 55.6, 33.8, 24.0, 21.5; IR (KBr) ν_{\max} : 2961, 2922, 2851, 1718, 1361, 1259, 1070, 797 cm⁻¹; HRMS (ESI): $m/z = 390.1526$ (calcd for C₂₄H₂₃NO₂S+H⁺ = 390.1523).

(2*R*,3*R*)-2-(4-ethylphenyl)-1-tosyl-3-vinylindoline (**3c**)

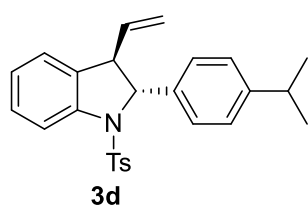


Following *General Procedure B*, the product **3c** was obtained after column chromatography (petroleum ether/EtOAc 50:1 v/v); light yellow oil ; 72% yield (27.70 mg), >20:1 *dr*, 93% *ee* [Daicel Chiralpak AD-H, hexanes/*i*-propanol = 90/10, flow rate = 1.0 mL/min, $\lambda = 254.4$ nm, t (major) = 9.302, t (minor) = 15.676]; $[\alpha]_D^{25} = -53.14$ (c 0.10, CHCl₃); ¹H NMR (400 MHz, CDCl₃) δ 7.79 (d, $J = 8.2$ Hz, 1H), 7.58 (d, $J = 8.0$ Hz, 2H), 7.32 – 7.27 (m, 1H), 7.23 (d, $J = 7.8$ Hz, 2H), 7.15 (dd, $J = 16.4, 8.0$ Hz, 4H), 7.05 (t, $J = 7.4$ Hz, 1H), 6.99 (d, $J = 7.4$ Hz, 1H), 5.19 (ddd, $J = 17.4, 9.6, 8.2$ Hz, 1H), 4.90 (d, $J = 3.6$ Hz, 1H), 4.79 (dd, $J = 13.4, 2.6$ Hz, 2H), 3.64 (dd, $J = 8.2, 3.6$ Hz, 1H), 2.62 (q, $J = 7.6$ Hz, 2H), 2.36 (s, 3H), 1.22 (t, $J = 7.6$ Hz, 3H); ¹³C NMR (101 MHz, CDCl₃) δ 143.9, 143.7, 141.8, 139.6, 138.4, 134.8, 132.5, 129.5, 128.6, 128.2, 127.4, 125.8, 125.7, 124.4, 116.0, 115.6, 71.4, 60.0, 28.5, 20.9, 15.5; IR (KBr) ν_{\max} : 2958, 2925, 2870, 1725, 1598, 1460, 1359, 1285, 1261, 1168, 773, 705 cm⁻¹; HRMS (ESI): $m/z = 404.1674$ (calcd for C₂₅H₂₅NO₂S+H⁺ = 404.1679).

(2*R*,3*R*)-2-(4-isopropylphenyl)-1-tosyl-3-vinylindoline (**3d**)

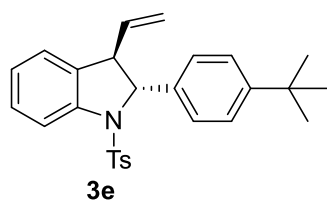
Following *General Procedure B*, the product **3d** was obtained after column chromatography

(petroleum ether/EtOAc 50:1 v/v); light yellow oil ; 74% yield (30.86 mg), >20:1 *dr*, 90% *ee*
 [Daicel Chiralpak AD-H, hexanes/*i*-propanol = 90/10, flow rate = 1.0 mL/min, λ = 254.4 nm, t



(major) = 7.454, t (minor) = 10.327]; $[\alpha]_D^{25}$ = -49.32 (c 0.10, CHCl₃); ¹H NMR (400 MHz, CDCl₃) δ 7.78 (d, *J* = 8.0 Hz, 1H), 7.56 (d, *J* = 8.2 Hz, 2H), 7.32 – 7.27 (m, 1H), 7.22 (d, *J* = 8.2 Hz, 2H), 7.15 (t, *J* = 7.8 Hz, 4H), 7.05 (t, *J* = 7.4 Hz, 1H), 6.99 (d, *J* = 7.2 Hz, 1H), 5.18 (ddd, *J* = 17.6, 9.6, 8.2 Hz, 1H), 4.91 (d, *J* = 3.4 Hz, 1H), 4.83 – 4.74 (m, 2H), 3.64 (dd, *J* = 8.2, 3.4 Hz, 1H), 2.87 (p, *J* = 6.8 Hz, 1H), 2.36 (s, 3H), 1.23 (d, *J* = 6.8 Hz, 6H); ¹³C NMR (101 MHz, CDCl₃) δ 148.1, 143.5, 141.8, 138.4, 134.8, 132.5, 129.4, 128.5, 127.4, 126.7, 125.8, 125.7, 124.4, 115.9, 115.5, 71.4, 56.5, 33.8, 23.99, 23.97, 21.5; IR (KBr) ν_{\max} : 2958, 2924, 2870, 1725, 1598, 1476, 1460, 1360, 1168, 749, 663 cm⁻¹; HRMS (ESI): *m/z* = 440.1648 (calcd for C₂₆H₂₇NO₂S+Na⁺ = 440.1655).

(2R,3R)-2-(4-(*tert*-butyl)phenyl)-1-tosyl-3-vinylindoline (3e)

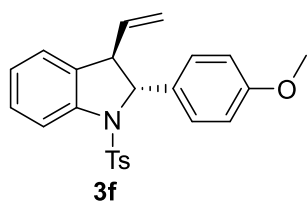


Following *General Procedure B*, the product **3e** was obtained after column chromatography (petroleum ether/EtOAc 50:1 v/v); light yellow oil ; 70% yield (30.17 mg), >20:1 *dr*, 89% *ee* [Daicel Chiralpak AD-H, hexanes/*i*-propanol = 90/10, flow rate = 1.0 mL/min, λ = 254.4 nm, t (major) = 7.479, t (minor) = 8.208]; $[\alpha]_D^{25}$ = -51.02 (c 0.10, CHCl₃); ¹H NMR (400 MHz, CDCl₃) δ 7.78 (d, *J* = 8.0 Hz, 1H), 7.56 (d, *J* = 8.2 Hz, 2H), 7.30 (d, *J* = 8.4 Hz, 3H), 7.23 (d, *J* = 8.4 Hz, 2H), 7.16 (d, *J* = 8.0 Hz, 2H), 7.05 (t, *J* = 6.8 Hz, 1H), 6.99 (d, *J* = 7.4 Hz, 1H), 5.19 (ddd, *J* = 17.6, 10.0, 8.2 Hz, 1H), 4.92 (d, *J* = 3.2 Hz, 1H), 4.84 – 4.74 (m, 2H), 3.65 (dd, *J* = 8.2, 3.2 Hz, 1H), 2.36 (s, 3H), 1.29 (s, 9H); ¹³C NMR (101 MHz, CDCl₃) δ 150.5, 143.9, 141.8, 139.2, 138.5, 135.0, 132.6, 129.4, 128.5, 127.4, 125.7, 125.6, 125.5, 124.4, 116.0, 115.4, 70.8, 55.6, 34.9, 31.4, 21.5; IR (KBr) ν_{\max} : 2961, 2923, 2852, 1359, 1259, 1091, 1017, 799, 663 cm⁻¹; HRMS (ESI): *m/z* = 454.1828 (calcd for C₂₇H₂₉NO₂S+Na⁺ = 454.1811).

(2R,3R)-2-(4-methoxyphenyl)-1-tosyl-3-vinylindoline (3f)

Following *General Procedure B*, the product **3f** was obtained after column chromatography (petroleum ether/EtOAc 40:1 v/v); light yellow oil; 78% yield (31.59 mg), >20:1 *dr*, 90% *ee* [Daicel Chiralpak AD-H, hexanes/*i*-propanol = 90/10, flow rate = 1.0 mL/min, λ = 254.4 nm, t

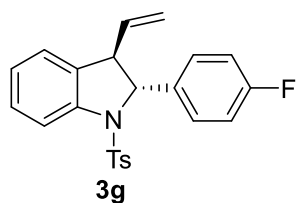
(major) = 13.375, t (minor) = 31.645]; $[\alpha]_D^{25} = -53.25$ (c 0.10, CHCl₃); ¹H NMR (400 MHz, CDCl₃) δ 7.80 (d, *J* = 8.0 Hz, 1H), 7.60 (d, *J* = 8.4 Hz, 2H), 7.34 – 7.25 (m, 3H), 7.20 (d, *J* = 8.0 Hz,



2H), 7.11 – 7.00 (m, 2H), 6.86 (d, *J* = 8.6 Hz, 2H), 5.26 – 5.16 (m, 1H), 4.88 (d, *J* = 3.6 Hz, 1H), 4.85 – 4.76 (m, 2H), 3.81 (s, 3H), 3.64 (dd, *J* = 8.2, 3.8 Hz, 1H), 2.39 (s, 3H); ¹³C NMR (101 MHz, CDCl₃) δ 143.9, 141.7, 138.3, 134.8, 134.5, 132.5, 132.0, 129.5, 128.6, 127.4,

127.2, 125.7, 124.4, 115.9, 115.7, 114.1, 70.8, 55.8, 55.3, 20.2; IR (KBr) ν_{\max} : 2958, 2922, 2851, 1724, 1355, 1260, 1168, 1074, 662 cm⁻¹; HRMS (ESI): *m/z* = 428.1296 (calcd for C₂₄H₂₃NO₃S+Na⁺ = 428.1291).

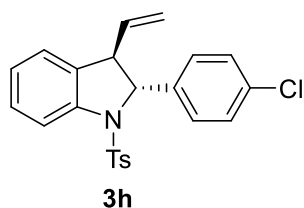
(2*R*,3*R*)-2-(4-fluorophenyl)-1-tosyl-3-vinylindoline (**3g**)



Following *General Procedure B*, the product **3g** was obtained after column chromatography (petroleum ether/EtOAc 50:1 v/v); light yellow oil ; 72% yield (28.30 mg), >20:1 *dr*, 91% *ee* [Daicel Chiralpak AD-H, hexanes/*i*-propanol = 90/10, flow rate = 1.0

mL/min, λ = 254.4 nm, t (major) = 8.446, t (minor) = 14.942]; $[\alpha]_D^{25} = -45.78$ (c 0.10, CHCl₃); ¹H NMR (400 MHz, CDCl₃) δ 7.73 (d, *J* = 8.2 Hz, 1H), 7.52 (d, *J* = 8.0 Hz, 2H), 7.25 – 7.19 (m, 3H), 7.13 (d, *J* = 8.0 Hz, 2H), 7.00 (t, *J* = 5.8 Hz, 1H), 6.96 – 6.90 (m, 3H), 5.11 (ddd, *J* = 16.6, 10.0, 8.2 Hz, 1H), 4.80 (d, *J* = 3.8 Hz, 1H), 4.78 – 4.70 (m, 2H), 3.52 (dd, *J* = 8.2, 3.8 Hz, 1H), 2.31 (s, 3H); ¹³C NMR (101 MHz, CDCl₃) δ 162.6 (d, *J*_{C-F} = 183.4 Hz), 144.2, 141.6, 138.0, 134.5, 132.2, 129.5, 129.0, 128.7, 128.4, 127.59 (d, *J*_{C-F} = 8.2 Hz), 127.4, 125.7, 124.6, 116.0 (d, *J*_{C-F} = 2.3 Hz), 115.6 (d, *J*_{C-F} = 8.2 Hz), 70.53, 55.9, 20.7.; ¹⁹F NMR (564 MHz, CDCl₃) δ -114.85; IR (KBr) ν_{\max} : 2921, 2851, 1354, 1260, 1164, 1089, 811, 662 cm⁻¹; HRMS (ESI): *m/z* = 416.1090 (calcd for C₂₃H₂₀FNO₂S+Na⁺ = 416.1091).

(2*R*,3*R*)-2-(4-chlorophenyl)-1-tosyl-3-vinylindoline (**3h**)



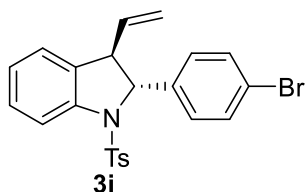
Following *General Procedure B*, the product **3h** was obtained after column chromatography (petroleum ether/EtOAc 50:1 v/v); light yellow oil ; 76% yield (31.08 mg), >20:1 *dr*, 91% *ee* [Daicel Chiralpak AD-H, hexanes/*i*-propanol = 90/10, flow rate = 1.0

mL/min, λ = 254.4 nm, t (major) = 8.471, t (minor) = 16.007]; $[\alpha]_D^{25} = -43.13$ (c 0.10, CHCl₃); ¹H

NMR (400 MHz, CDCl₃) δ 7.79 (d, *J* = 8.0 Hz, 1H), 7.58 (d, *J* = 8.2 Hz, 2H), 7.34 – 7.26 (m, 5H), 7.19 (d, *J* = 8.0 Hz, 2H), 7.09 – 7.04 (m, 1H), 6.98 (d, *J* = 7.4 Hz, 1H), 5.18 (ddd, *J* = 16.8, 10.0, 8.2 Hz, 1H), 4.86 – 4.76 (m, 3H), 3.57 (dd, *J* = 8.4, 3.8 Hz, 1H), 2.37 (s, 3H); ¹³C NMR (101 MHz, CDCl₃) δ 144.2, 141.6, 140.8, 137.9, 134.4, 133.5, 132.0, 129.6, 128.9, 128.7, 127.4, 127.3, 125.7, 124.6, 116.1, 116.0, 70.5, 55.8, 21.5; IR (KBr) ν_{\max} : 2956, 2920, 2851, 1725, 1358, 1168, 1090, 664 cm⁻¹; HRMS (ESI): *m/z* = 432.0792 (calcd for C₂₃H₂₀ClNO₂S+Na⁺ = 432.0796).

(2*R*,3*R*)-2-(4-bromophenyl)-1-tosyl-3-vinylindoline (3i)

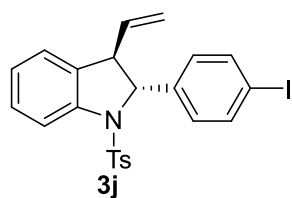
Following *General Procedure B*, the product **3i** was obtained after column chromatography (petroleum ether/EtOAc 50:1 v/v); light yellow oil ; 73% yield (33.07 mg), >20:1 *dr*, 91% *ee*



[Daicel Chiralpak AD-H, hexanes/*i*-propanol = 90/10, flow rate = 1.0 mL/min, λ = 254.4 nm, *t* (major) = 8.841, *t* (minor) = 16.814]; [α]_D²⁵ = -44.57 (c 0.10, CHCl₃); ¹H NMR (400 MHz, CDCl₃) δ 7.80 (d, *J* = 8.2 Hz, 1H), 7.58 (d, *J* = 8.2 Hz, 2H), 7.43

(d, *J* = 8.4 Hz, 2H), 7.34 – 7.28 (m, 1H), 7.20 (dd, *J* = 8.0, 5.0 Hz, 4H), 7.07 (t, *J* = 7.4 Hz, 1H), 6.98 (d, *J* = 7.4 Hz, 1H), 5.18 (ddd, *J* = 16.8, 10.0, 8.2 Hz, 1H), 4.86 – 4.76 (m, 3H), 3.57 (dd, *J* = 8.2, 3.8 Hz, 1H), 2.37 (s, 3H); ¹³C NMR (101 MHz, CDCl₃) δ 144.3, 142.1, 141.3, 137.9, 134.4, 132.0, 131.8, 130.0, 128.8, 127.7, 127.4, 125.7, 124.6, 121.6, 116.1, 116.0, 70.6, 55.7, 21.6; IR (KBr) ν_{\max} : 2956, 2922, 2854, 1724, 1598, 1357, 1168, 664 cm⁻¹; HRMS (ESI): *m/z* = 476.0298 (calcd for C₂₃H₂₀NO₂SBr+Na⁺ = 476.0291).

(2*R*,3*R*)-2-(4-iodophenyl)-1-tosyl-3-vinylindoline (3j)

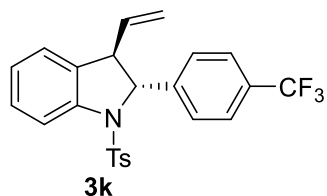


Following *General Procedure B*, the product **3j** was obtained after column chromatography (petroleum ether/EtOAc 50:1 v/v); light yellow oil ; 70% yield (35.07 mg), >20:1 *dr*, 90% *ee* [Daicel Chiralpak AD-H, hexanes/*i*-propanol = 90/10, flow rate = 1.0

mL/min, λ = 254.4 nm, *t* (major) = 10.362, *t* (minor) = 19.189]; [α]_D²⁵ = -45.15 (c 0.10, CHCl₃); ¹H NMR (400 MHz, CDCl₃) δ 7.79 (d, *J* = 8.0 Hz, 1H), 7.63 (d, *J* = 8.2 Hz, 2H), 7.57 (d, *J* = 8.2 Hz, 2H), 7.29 (d, *J* = 8.0 Hz, 1H), 7.19 (d, *J* = 8.0 Hz, 2H), 7.06 (t, *J* = 7.8 Hz, 3H), 6.98 (d, *J* = 7.4 Hz, 1H), 5.18 (ddd, *J* = 16.8, 10.0, 8.2 Hz, 1H), 4.88 – 4.75 (m, 3H), 3.57 (dd, *J* = 8.2, 3.8 Hz, 1H), 2.37 (s, 3H); ¹³C NMR (101 MHz, CDCl₃) δ 144.2, 142.0, 141.4, 137.9, 137.8, 134.4, 132.0,

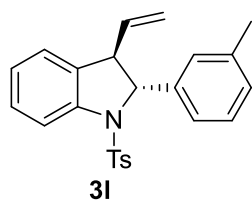
129.6, 128.8, 127.9, 127.4, 125.7, 124.6, 116.1, 90.2, 115.9, 70.7, 55.7, 21.6; IR (KBr) ν_{\max} : 2959, 2923, 2852, 1718, 1357, 1167, 812, 665 cm^{-1} ; HRMS (ESI): $m/z = 524.0159$ (calcd for $\text{C}_{23}\text{H}_{20}\text{NO}_2\text{S}+\text{Na}^+ = 524.0152$).

(2R,3R)-1-tosyl-2-(4-(trifluoromethyl)phenyl)-3-vinylindoline (3k)



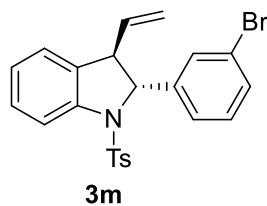
Following *General Procedure B*, the product **3k** was obtained after column chromatography (petroleum ether/EtOAc 50:1 v/v); light yellow oil ; 67% yield (29.68 mg), >20:1 *dr*, 82% *ee* [Daicel Chiralpak AD-H, hexanes/*i*-propanol = 90/10, flow rate = 1.0 mL/min, $\lambda = 254.4$ nm, t (major) = 7.803, t (minor) = 11.386]; $[\alpha]_{\text{D}}^{25} = -39.59$ (c 0.10, CHCl_3); ^1H NMR (400 MHz, CDCl_3) δ 7.82 (d, $J = 8.0$ Hz, 1H), 7.58 (dd, $J = 8.2, 6.2$ Hz, 4H), 7.45 (d, $J = 8.0$ Hz, 2H), 7.32 (t, $J = 7.6$ Hz, 1H), 7.20 (d, $J = 8.0$ Hz, 2H), 7.08 (t, $J = 7.4$ Hz, 1H), 6.99 (d, $J = 7.4$ Hz, 1H), 5.20 (ddd, $J = 16.8, 10.0, 8.2$ Hz, 1H), 4.92 (d, $J = 4.0$ Hz, 1H), 4.88 – 4.77 (m, 2H), 3.59 (dd, $J = 8.4, 3.8$ Hz, 1H), 2.37 (s, 3H); ^{13}C NMR (101 MHz, CDCl_3) δ 146.1, 144.3, 141.6, 137.8, 134.3, 131.8, 129.6, 128.8, 127.4, 126.2, 125.80, 125.77, 125.73, 125.72, 124.7, 116.3, 116.0, 70.6, 55.7, 21.5; IR (KBr) ν_{\max} : 2957, 2921, 2851, 1724, 1259, 1087, 662 cm^{-1} ; HRMS (ESI): $m/z = 466.1057$ (calcd for $\text{C}_{24}\text{H}_{20}\text{F}_3\text{NO}_2\text{S}+\text{Na}^+ = 466.1059$).

(2R,3R)-2-(*m*-tolyl)-1-tosyl-3-vinylindoline (3l)



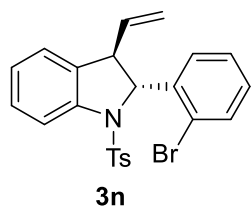
Following *General Procedure B*, the product **3l** was obtained after column chromatography (petroleum ether/EtOAc 50:1 v/v); light yellow oil ; 59% yield (22.95 mg), >20:1 *dr*, 91% *ee* [Daicel Chiralpak AD-H, hexanes/*i*-propanol = 90/10, flow rate = 1.0 mL/min, $\lambda = 254.4$ nm, t (major) = 10.912, t (minor) = 16.770]; $[\alpha]_{\text{D}}^{25} = -45.76$ (c 0.10, CHCl_3); ^1H NMR (400 MHz, CDCl_3) δ 7.80 (d, $J = 8.0$ Hz, 1H), 7.58 (d, $J = 8.2$ Hz, 2H), 7.32 – 7.28 (m, 1H), 7.22 – 7.15 (m, 3H), 7.11 – 7.03 (m, 4H), 6.98 (d, $J = 7.4$ Hz, 1H), 5.24 – 5.14 (m, 1H), 4.87 (d, $J = 3.6$ Hz, 1H), 4.83 – 4.76 (m, 2H), 3.62 (dd, $J = 8.2, 3.6$ Hz, 1H), 2.37 (s, 3H), 2.30 (s, 3H); ^{13}C NMR (101 MHz, CDCl_3) δ 144.0, 143.4, 142.2, 141.8, 138.4, 134.8, 132.5, 129.5, 128.60, 128.57, 128.5, 127.4, 126.4, 125.7, 124.4, 122.9, 116.0, 115.6, 70.7, 55.8, 21.53, 21.50; IR (KBr) ν_{\max} : 2920, 2851, 1597, 1356, 1167, 702, 664 cm^{-1} ; HRMS (ESI): $m/z = 412.1343$ (calcd for $\text{C}_{24}\text{H}_{23}\text{NO}_2\text{S}+\text{Na}^+ = 412.1342$).

(2*R*,3*R*)-2-(3-bromophenyl)-1-tosyl-3-vinylindoline (**3m**)



Following *General Procedure B*, the product **3m** was obtained after column chromatography (petroleum ether/EtOAc 50:1 v/v); light yellow oil ; 51% yield (23.10 mg), >20:1 *dr*, 88% *ee* [Daicel Chiralpak AD-H, hexanes/*i*-propanol = 90/10, flow rate = 1.0 mL/min, λ = 254.4 nm, t (major) = 11.875, t (minor) = 17.487]; $[\alpha]_D^{25} = -46.73$ (c 0.10, CHCl₃); ¹H NMR (400 MHz, CDCl₃) δ 7.81 (d, *J* = 8.2 Hz, 1H), 7.58 (d, *J* = 8.0 Hz, 2H), 7.44 – 7.36 (m, 2H), 7.30 (dd, *J* = 15.4, 7.7 Hz, 2H), 7.19 (d, *J* = 7.8 Hz, 3H), 7.07 (t, *J* = 7.4 Hz, 1H), 6.98 (d, *J* = 7.4 Hz, 1H), 5.17 (ddd, *J* = 16.6, 10.0, 8.2 Hz, 1H), 4.88 – 4.75 (m, 3H), 3.59 (dd, *J* = 8.2, 3.9 Hz, 1H), 2.37 (s, 3H); ¹³C NMR (101 MHz, CDCl₃) δ 144.5, 144.3, 141.6, 137.9, 134.3, 132.0, 130.8, 130.3, 129.6, 128.9, 128.8, 127.4, 125.7, 124.7, 124.6, 122.8, 116.2, 116.0, 70.5, 55.7, 21.6; IR (KBr) ν_{\max} : 2959, 2928, 2873, 1724, 1281, 1169, 1121, 1074, 745, 662 cm⁻¹; HRMS (ESI): *m/z* = 476.0287 (calcd for C₂₃H₂₀NO₂SBr+Na⁺ = 476.0291).

(2*R*,3*R*)-2-(2-bromophenyl)-1-tosyl-3-vinylindoline (**3n**)

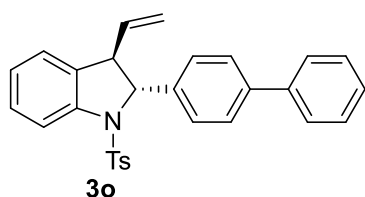


Following *General Procedure B*, the product **3n** was obtained after column chromatography (petroleum ether/EtOAc 50:1 v/v); light yellow oil ; 61% yield (27.63 mg), >20:1 *dr*, 75% *ee* [Daicel Chiralpak AD-H, hexanes/*i*-propanol = 90/10, flow rate = 1.0 mL/min, λ = 254.4 nm, t (major) = 8.505, t (minor) = 15.619]; $[\alpha]_D^{25} = -37.15$ (c 0.10, CHCl₃); ¹H NMR (400 MHz, CDCl₃) δ 7.88 (d, *J* = 8.0 Hz, 1H), 7.70 (d, *J* = 7.8 Hz, 2H), 7.59 (d, *J* = 7.8 Hz, 1H), 7.42 (d, *J* = 7.8 Hz, 1H), 7.35 (t, *J* = 7.6 Hz, 1H), 7.24 (d, *J* = 8.2 Hz, 3H), 7.14 (t, *J* = 7.6 Hz, 1H), 7.09 (t, *J* = 7.4 Hz, 1H), 6.98 (d, *J* = 7.4 Hz, 1H), 5.34 (d, *J* = 18.6 Hz, 2H), 4.67 (dd, *J* = 34.6, 13.4 Hz, 2H), 3.54 (d, *J* = 8.8 Hz, 1H), 2.40 (s, 3H); ¹³C NMR (101 MHz, CDCl₃) δ 144.2, 141.6, 140.8, 137.6, 134.4, 132.9, 131.8, 129.6, 129.0, 128.7, 128.4, 127.9, 127.8, 127.5, 126.2, 124.7, 116.0, 115.8, 70.3, 54.6, 21.6.; IR (KBr) ν_{\max} : 2959, 2929, 2873, 1723, 1475, 1460, 1361, 1278, 1169, 1120, 1073, 745, 662 cm⁻¹; 476.0289 (calcd for C₂₃H₂₀NO₂SBr+Na⁺ = 476.0291).

(2*R*,3*R*)-2-([1,1'-biphenyl]-4-yl)-1-tosyl-3-vinylindoline (**3o**)

Following *General Procedure B*, the product **3o** was obtained after column chromatography (petroleum ether/EtOAc 50:1 v/v); light yellow oil ; 73% yield (32.92 mg), >20:1 *dr*, 90% *ee*

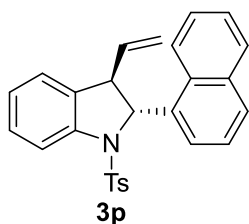
[Daicel Chiralpak AD-H, hexanes/*i*-propanol = 90/10, flow rate = 1.0 mL/min, λ = 254.4 nm, t (major) = 14.433, t (minor) = 26.772]; $[\alpha]_D^{25} = -48.09$ (c 0.10, CHCl₃) δ 7.83 (d, J = 8.0 Hz, 1H),



7.61 (d, J = 8.0 Hz, 2H), 7.58 – 7.51 (m, 4H), 7.41 (t, J = 8.4 Hz, 4H), 7.33 (q, J = 7.2 Hz, 2H), 7.19 (d, J = 8.0 Hz, 2H), 7.08 (t, J = 7.4 Hz, 1H), 7.02 (d, J = 7.4 Hz, 1H), 5.29 – 5.17 (m, 1H), 4.97 (d, J = 3.6 Hz, 1H), 4.89 – 4.78 (m, 2H), 3.69

(dd, J = 8.2, 3.6 Hz, 1H), 2.37 (s, 3H); ¹³C NMR (101 MHz, CDCl₃) δ 144.1, 141.8, 141.3, 140.8, 140.7, 138.3, 134.7, 132.4, 129.5, 128.8, 128.7, 127.5, 127.4, 127.3, 127.1, 126.3, 125.8, 124.5, 116.0, 115.8, 70.9, 56.3, 20.7; IR (KBr) ν_{\max} : 2961, 2921, 2851, 1457, 1360, 1261, 1091, 806 cm⁻¹; HRMS (ESI): m/z = 474.1489 (calcd for C₂₉H₂₅NO₂S+Na⁺ = 474.1499).

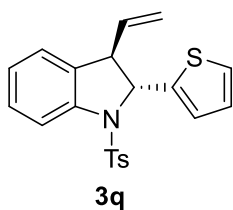
(2R,3R)-2-(naphthalen-1-yl)-1-tosyl-3-vinylindoline (3p)



Following *General Procedure B*, the product **3p** was obtained after column chromatography (petroleum ether/EtOAc 50:1 v/v); light yellow oil ; 65% yield (29.32 mg), >20:1 *dr*, 75% *ee* [Daicel Chiralpak AD-H, hexanes/*i*-propanol = 90/10, flow rate = 1.0 mL/min, λ = 254.4 nm, t

(major) = 27.343, t (minor) = 16.267]; $[\alpha]_D^{25} = 26.14$ (c 0.10, CHCl₃); ¹H NMR (400 MHz, CDCl₃) δ 7.93 (t, J = 8.8 Hz, 3H), 7.76 (d, J = 8.2 Hz, 1H), 7.65 (dd, J = 15.6, 7.4 Hz, 3H), 7.56 – 7.47 (m, 2H), 7.37 (dt, J = 19.8, 7.8 Hz, 2H), 7.24 (d, J = 7.6 Hz, 2H), 7.06 (t, J = 7.4 Hz, 1H), 6.92 (d, J = 7.4 Hz, 1H), 5.70 (s, 1H), 5.13 (dt, J = 18.2, 9.4 Hz, 1H), 4.96 – 4.77 (m, 2H), 3.61 (d, J = 9.0 Hz, 1H), 2.40 (s, 3H); ¹³C NMR (101 MHz, CDCl₃) δ 141.6, 138.5, 137.2, 135.0, 134.2, 132.8, 129.8, 129.6, 129.2, 128.7, 128.1, 127.4, 126.1, 126.0, 125.7, 125.6, 124.8, 123.4, 116.3, 116.0, 55.4, 29.7, 21.6; IR (KBr) ν_{\max} : 2960, 2920, 2851, 1463, 1261, 1170, 1093, 802 cm⁻¹; HRMS (ESI): m/z = 448.1349 (calcd for C₂₇H₂₃NO₂S+Na⁺ = 448.1342).

(2R,3R)-2-(thiophen-2-yl)-1-tosyl-3-vinylindoline (3q)



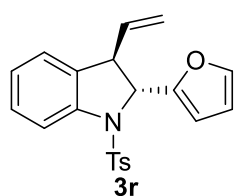
Following *General Procedure B*, the product **3q** was obtained after column chromatography (petroleum ether/EtOAc 50:1 v/v); light yellow oil ; 55% yield (20.98 mg), >20:1 *dr*, 76% *ee* [Daicel Chiralpak AD-H, hexanes/*i*-propanol = 90/10, flow rate = 1.0 mL/min, λ = 254.4 nm, t

(major) = 15.617, t (minor) = 33.683]; $[\alpha]_D^{25} = -60.04$ (c 0.10, CHCl₃); ¹H NMR (400 MHz,

CDCl₃) δ 7.65 (d, J = 8.2 Hz, 1H), 7.50 (d, J = 8.4 Hz, 2H), 7.25 – 7.19 (m, 1H), 7.13 – 7.07 (m, 3H), 7.02 – 6.94 (m, 3H), 6.85 (dd, J = 5.0, 3.4 Hz, 1H), 5.15 – 5.02 (m, 2H), 4.75 – 4.68 (m, 2H), 3.71 (dd, J = 8.0, 3.0 Hz, 1H), 2.29 (s, 3H). ¹³C NMR (101 MHz, CDCl₃) δ 144.4, 143.0, 139.9, 136.6, 133.8, 131.3, 128.5, 127.7, 126.4, 125.7, 124.7, 123.73, 123.68, 123.6, 115.4, 115.0, 66.2, 55.5, 20.5; IR (KBr) ν_{max} : 1723, 1461, 1358, 1288, 1013 cm⁻¹; HRMS (ESI): m/z = 404.0764 (calcd for C₂₁H₁₉NO₂S₂+Na⁺ = 404.0749).

(2*R*,3*R*)-2-(furan-2-yl)-1-tosyl-3-vinylindoline (**3r**)

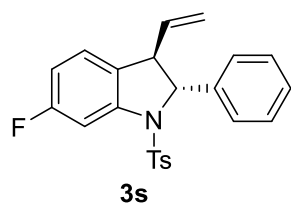
Following *General Procedure B*, the product **3r** was obtained after column chromatography (petroleum ether/EtOAc 50:1 v/v); light yellow oil; 54% yield (19.73 mg), >20:1 *dr*, 72% *ee*



[Daicel Chiralpak AD-H, hexanes/*i*-propanol = 90/10, flow rate = 1.0 mL/min, λ = 254.4 nm, t (major) = 10.949, t (minor) = 18.357]; $[\alpha]_{\text{D}}^{25}$ = -83.38 (c 0.10, CHCl₃); ¹H NMR (400 MHz, CDCl₃) δ 7.72 (d, J = 8.2 Hz, 1H), 7.59 (d, J = 8.4 Hz, 2H), 7.35 – 7.28 (m, 2H), 7.20 (d, J = 8.0 Hz,

2H), 7.07 (qd, J = 7.4, 1.4 Hz, 2H), 6.42 (d, J = 3.2 Hz, 1H), 6.34 (dd, J = 3.2, 1.8 Hz, 1H), 5.21 (ddd, J = 17.4, 9.8, 8.0 Hz, 1H), 5.03 (d, J = 3.4 Hz, 1H), 4.85 – 4.79 (m, 2H), 3.91 (dd, J = 8.0, 3.4 Hz, 1H), 2.38 (s, 3H). ¹³C NMR (101 MHz, CDCl₃) δ 153.2, 144.0, 142.4, 141.1, 137.6, 134.8, 132.4, 130.9, 129.5, 128.5, 127.4, 125.6, 124.4, 116.1, 111.9, 107.7, 65.0, 51.3, 21.1. IR (KBr) ν_{max} : 1723, 1460, 1358, 1288, 1188 cm⁻¹; HRMS (ESI): m/z = 388.0953 (calcd for C₂₁H₁₉NO₃S+Na⁺ = 388.0978).

(2*R*,3*R*)-6-fluoro-2-phenyl-1-tosyl-3-vinylindoline (**3s**)

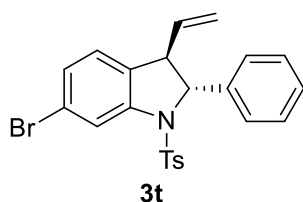


Following *General Procedure B*, the product **3s** was obtained after column chromatography (petroleum ether/EtOAc 50:1 v/v); light yellow oil ; 75% yield (29.48 mg), >20:1 *dr*, 90% *ee* [Daicel Chiralpak AD-H, hexanes/*i*-propanol = 90/10, flow rate = 1.0 mL/min,

λ = 254.4 nm, t (major) = 13.767, t (minor) = 22.474]; $[\alpha]_{\text{D}}^{25}$ = -45.36 (c 0.10, CHCl₃); ¹H NMR (400 MHz, CDCl₃) δ 7.62 (d, J = 8.2 Hz, 2H), 7.55 (dd, J = 9.8, 2.4 Hz, 1H), 7.32 (d, J = 5.0 Hz, 5H), 7.24 (d, J = 8.0 Hz, 2H), 6.94 (dd, J = 8.2, 5.6 Hz, 1H), 6.77 (td, J = 8.4, 2.4 Hz, 1H), 5.25 (ddd, J = 17.0, 10.0, 8.2 Hz, 1H), 4.95 (d, J = 3.8 Hz, 1H), 4.89 – 4.76 (m, 2H), 3.62 (dd, J = 8.2, 3.6 Hz, 1H), 2.41 (s, 3H); ¹³C NMR (101 MHz, CDCl₃) δ 162.2 (d, $J_{\text{C-F}}$ = 241.4 Hz), 143.3, 142.1

(d, $J_{C-F} = 13.4$ Hz), 140.86, 137.03, 133.54, 128.59, 127.73, 126.75 (d, $J_{C-F} = 15.4$ Hz), 126.36, 125.4 (d, $J_{C-F} = 9.8$ Hz), 124.78, 114.95, 110.1 (d, $J_{C-F} = 23.74$ Hz), 102.92, 102.64, 71.04, 54.07, 20.52.; ^{19}F NMR (376 MHz, CDCl_3) δ -112.60; IR (KBr) ν_{max} : 2959, 2921, 2851, 1729, 1350, 1092, 811, 662 cm^{-1} ; HRMS (ESI): $m/z = 416.1091$ (calcd for $\text{C}_{23}\text{H}_{20}\text{NO}_2\text{SF}+\text{Na}^+ = 416.1091$).

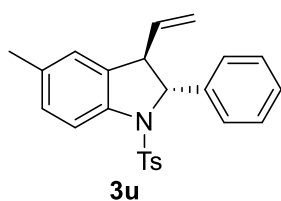
(2*R*,3*R*)-6-bromo-2-phenyl-1-tosyl-3-vinylindoline (3t)



Following *General Procedure B*, the product **3t** was obtained after column chromatography (petroleum ether/EtOAc 50:1 v/v); light yellow oil ; 73% yield (33.07 mg), >20:1 *dr*, 89% *ee* [Daicel Chiralpak AD-H, hexanes/*i*-propanol = 90/10, flow rate = 1.0

mL/min, $\lambda = 254.4$ nm, t (major) = 11.219, t (minor) = 20.702]; $[\alpha]_{\text{D}}^{25} = -44.27$ (c 0.10, CHCl_3); ^1H NMR (400 MHz, CDCl_3) δ 7.95 (d, $J = 1.8$ Hz, 1H), 7.59 (dd, $J = 8.4, 2.2$ Hz, 2H), 7.34 – 7.27 (m, 5H), 7.22 (d, $J = 8.2$ Hz, 2H), 7.18 (dd, $J = 8.0, 1.8$ Hz, 1H), 6.85 (d, $J = 8.0$ Hz, 1H), 5.26 – 5.15 (m, 1H), 4.91 (d, $J = 3.6$ Hz, 1H), 4.85 – 4.74 (m, 2H), 3.58 (dd, $J = 8.0, 3.6$ Hz, 1H), 2.39 (s, 3H); ^{13}C NMR (101 MHz, CDCl_3) δ 144.4, 143.1, 141.8, 137.7, 134.7, 131.4, 129.7, 128.8, 127.9, 127.42, 127.36, 126.9, 125.8, 122.2, 118.9, 116.2, 71.6, 55.3, 21.6; IR (KBr) ν_{max} : 2962, 2926, 2854, 1729, 1362, 1097, 1030, 811 cm^{-1} ; HRMS (ESI): $m/z = 476.0292$ (calcd for $\text{C}_{23}\text{H}_{20}\text{NO}_2\text{SBr}+\text{Na}^+ = 476.0291$).

(2*R*,3*R*)-5-methyl-2-phenyl-1-tosyl-3-vinylindoline (3u)

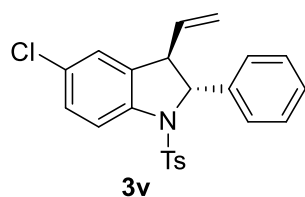


Following *General Procedure B*, the product **3u** was obtained after column chromatography (petroleum ether/EtOAc 50:1 v/v); light yellow oil ; 71% yield (27.62 mg), >20:1 *dr*, 90% *ee* [Daicel Chiralpak AD-H, hexanes/*i*-propanol = 90/10, flow rate = 1.0 mL/min, $\lambda = 254.4$

nm, t (major) = 13.135, t (minor) = 17.148]; $[\alpha]_{\text{D}}^{25} = -47.65$ (c 0.10, CHCl_3); ^1H NMR (400 MHz, CDCl_3) δ 7.68 (d, $J = 8.2$ Hz, 1H), 7.65 – 7.61 (m, 1H), 7.59 (d, $J = 7.8$ Hz, 2H), 7.31 (d, $J = 6.0$ Hz, 4H), 7.19 (d, $J = 8.0$ Hz, 2H), 7.08 (d, $J = 5.4$ Hz, 1H), 6.78 (s, 1H), 5.10 (dd, $J = 17.2, 8.6$ Hz, 1H), 4.87 (d, $J = 3.6$ Hz, 1H), 4.84 – 4.75 (m, 2H), 3.57 (dd, $J = 8.2, 3.6$ Hz, 1H), 2.37 (s, 3H), 2.28 (s, 3H); ^{13}C NMR (101 MHz, CDCl_3) δ 143.9, 143.0, 142.4, 134.3, 132.6, 129.5, 129.3, 129.0, 128.7, 128.4, 127.6, 127.5, 125.8, 125.4, 115.9, 115.5, 69.7, 53.0, 21.5, 21.0; IR (KBr) ν_{max} : 2963, 2924, 2872, 2852, 1476, 1460, 1168, 1091, 662 cm^{-1} ; HRMS (ESI): $m/z = 412.1340$ (calcd

for $C_{24}H_{23}NO_2S+Na^+ = 412.1342$).

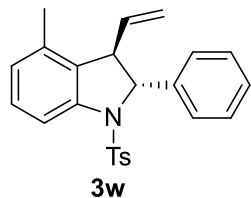
(2R,3R)-5-chloro-2-phenyl-1-tosyl-3-vinylindoline (3v)



Following *General Procedure B*, the product **3v** was obtained after column chromatography (petroleum ether/EtOAc 50:1 v/v); light yellow oil; 70% yield (28.63 mg), >20:1 *dr*, 92% *ee* [Daicel Chiralpak AD-H, hexanes/*i*-propanol = 90/10, flow rate = 1.0

mL/min, $\lambda = 254.4$ nm, t (major) = 10.283, t (minor) = 20.834]; $[\alpha]_D^{25} = -48.79$ (c 0.10, $CHCl_3$); 1H NMR (400 MHz, $CDCl_3$) δ 7.73 (dd, $J = 8.6, 2.0$ Hz, 1H), 7.58 (dd, $J = 8.2, 2.2$ Hz, 2H), 7.36 – 7.26 (m, 6H), 7.22 (dd, $J = 8.4, 2.1$ Hz, 2H), 6.96 (s, 1H), 5.21 – 5.09 (m, 1H), 4.92 – 4.87 (m, 1H), 4.87 – 4.76 (m, 2H), 3.60 (d, $J = 7.6$ Hz, 1H), 2.39 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 144.3, 141.8, 140.5, 137.5, 134.4, 129.7, 129.6, 128.8, 128.7, 127.9, 127.4, 125.9, 125.8, 117.0, 116.4, 71.5, 54.7, 21.6; IR (KBr) ν_{max} : 2958, 2921, 2851, 1724, 1597, 1475, 1460, 1357, 1167, 1004, 705 cm^{-1} ; HRMS (ESI): $m/z = 432.0792$ (calcd for $C_{23}H_{20}ClNO_2S+Na^+ = 432.0796$).

(2R,3R)-4-methyl-2-phenyl-1-tosyl-3-vinylindoline (3w)



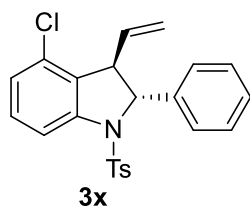
Following *General Procedure B*, the product **3w** was obtained after column chromatography (petroleum ether/EtOAc 50:1 v/v); light yellow oil ; 64% yield (25.29 mg), >20:1 *dr*, 70% *ee* [Daicel Chiralpak AD-H, hexanes/*i*-propanol = 90/10, flow rate = 1.0 mL/min, $\lambda = 254.4$ nm, t

(major) = 13.874, t (minor) = 16.110]; $[\alpha]_D^{25} = -40.08$ (c 0.10, $CHCl_3$); 1H NMR (400 MHz, $CDCl_3$) δ 7.66 (ddd, $J = 11.4, 7.4, 4.4$ Hz, 3H), 7.35 – 7.15 (m, 8H), 6.88 (dd, $J = 7.4, 4.4$ Hz, 1H), 5.09 (ddt, $J = 17.2, 8.4, 4.2$ Hz, 1H), 5.04 – 4.98 (m, 1H), 4.83 – 4.64 (m, 2H), 3.66 – 3.56 (m, 1H), 2.39 (s, 3H), 2.07 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 143.9, 142.4, 140.8, 137.2, 136.0, 135.3, 130.4, 129.5, 128.7, 127.7, 127.3, 126.1, 125.6, 115.2, 113.1, 69.1, 53.7, 21.5, 18.1; IR (KBr) ν_{max} : 2956, 2921, 2850, 1476, 1460, 1353, 1167, 1091, 758, 702, 664 cm^{-1} ; HRMS (ESI): $m/z = 412.1350$ (calcd for $C_{24}H_{23}NO_2S+Na^+ = 412.1342$).

(2R,3R)-4-chloro-2-phenyl-1-tosyl-3-vinylindoline (3x)

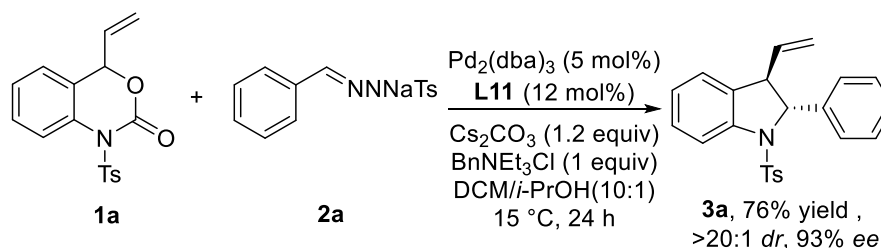
Following *General Procedure B*, the product **3x** was obtained after column chromatography (petroleum ether/EtOAc 50:1 v/v); light yellow oil ; 61% yield (24.95 mg), >20:1 *dr*, 60% *ee* [Daicel Chiralpak AD-H, hexanes/*i*-propanol = 90/10, flow rate = 1.0 mL/min, $\lambda = 254.4$ nm, t

(major) = 9.565, t (minor) = 12.434]; $[\alpha]_D^{25} = -38.65$ (c 0.10, CHCl_3); $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.73 (d, $J = 8.0$ Hz, 1H), 7.63 (d, $J = 8.0$ Hz, 2H), 7.47 – 7.41 (m, 1H), 7.35 – 7.29 (m, 5H), 7.23 (d, $J = 8.0$ Hz, 2H), 7.05 (d, $J = 8.0$ Hz, 1H), 5.15 (ddd, $J = 17.4, 10.0, 7.8$ Hz, 1H), 5.07 (d, $J = 2.2$ Hz, 1H), 4.87 – 4.74 (m, 2H), 3.79 – 3.73 (m, 1H), 2.40 (s, 3H); $^{13}\text{C NMR}$ (101 MHz, CDCl_3) δ 144.3, 143.4, 143.1, 141.6, 135.8, 135.1, 131.9, 130.1, 129.6, 128.8, 127.9, 127.3, 125.6, 125.0, 116.4, 114.2, 71.1, 54.4, 21.6; IR (KBr) ν_{max} : 2957, 2920, 2850, 1648, 1449, 1260, 1187, 1091, 803, 697, 662 cm^{-1} ; HRMS (ESI): $m/z = 432.0799$ (calcd for $\text{C}_{23}\text{H}_{20}\text{NO}_2\text{Scl} + \text{Na}^+ = 432.0796$).



6. Scale-up synthesis and further transformations

6.1 Gram scale synthesis of 3a



To a flame-dried schlenk tube, $\text{Pd}_2(\text{dba})_3$ (138 mg, 0.15 mmol, 5 mol%), (*R, R*)-**L11** (258 mg, 0.36 mmol) and dry DCM (30 mL) were added under nitrogen atmosphere. The mixture was stirred at 25 °C for 0.5 hour to produce a dark red solution and then *i*-PrOH (3 mL) was added. After that, vinyl benzoxazinone **1** (3.0 mmol, 0.99 g), *N*-tosylhydrazone sodium salt **2** (3.6 mmol, 1.07 g), Cs_2CO_3 (3.6 mmol, 1.17 g), BnNEt_3Cl (3 mmol, 675 mg) were added. The mixture was stirred at 15 °C for 24 hours (monitored by TLC analysis) and then it was subjected to silica gel column to afford the desired products **3a** in 76% yield with >20: *dr* and 93% *ee*.

6.2 Further transformation of the products

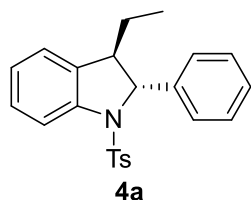
Hydrogenation reaction: To a flame dried schlenk tube, Pd/C (0.4 mmol, wt 10%) and **3a** (0.20 mmol) were added, then Methanol (2 mL) was added. The mixture was replaced with N_2 for three times, then inserted with a H_2 balloon. The reaction mixture was stirred at 30 °C under H_2 atmosphere for 24 hours. The reaction mixture was filtered and the filtrate was concentrated and purified by column chromatography on silica gel to afforded product **4a** in 71% yield with >20:1

dr and 93% *ee*.

Suzuki-coupling reaction: To a flame dried schlenk tube, **3i** (0.45 mmol), 4-Methoxyphenylboronic acid (0.9 mmol) and Na₂CO₃ (0.95 mmol) were added and then 2 mL of mixed solvents (toluene/EtOH/H₂O = 7:1.5:1.7, v/v/v) was added. The reaction mixture was stirred at 90 °C for 24 hours. The reaction mixture was allowed to cool to room temperature and 20 mL of water was added. The mixture was extracted with ethyl acetate. The organic phase was concentrated and purified by column chromatography on silica gel to afford product **4b** in 81% yield, with >20:1 *dr* and 90% *ee*.

Dihydroxylation reaction: To a three necked flask, **3i** (0.2 mmol) was added and then 3.5 mL acetone and 0.5 mL H₂O was added, then K₂OsO₄·2H₂O (0.02 mmol) was added, after that NMO (0.4 mmol) was added by portions. Stir at room temperature overnight. Add 5 mL of sat. NaHCO₃ solution and stir for half an hour. Concentrate to remove acetone, add ethyl acetate and allow to stand, collect organic phase and concentrate to obtained the **4c** in 85% yield with 5:1 *dr* and 90% *ee* for the major diastereomer.

(2*R*, 3*R*)-3-ethyl-2-phenyl-1-tosylindoline (**4a**)

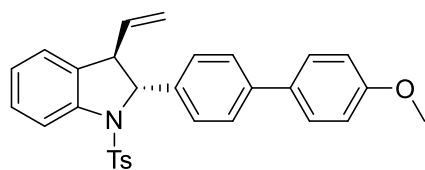


Following *General Procedure C*, the product **4a** was obtained after column chromatography (petroleum ether/EtOAc 50:1 v/v); light yellow oil; 71% yield (26.80 mg), >20:1 *dr*, 93% *ee* [Daicel Chiralpak AD-H, hexanes/*i*-propanol = 90/10, flow rate = 1.0 mL/min, λ = 254.4 nm, t (major) = 13.478, t (minor) = 25.975]; [α]_D²⁵ = -24.34 (c 0.10, CHCl₃); ¹H NMR (400 MHz, CDCl₃) δ 7.68 (d, *J* = 8.0 Hz, 1H), 7.52 (d, *J* = 8.2 Hz, 2H), 7.21 – 7.13 (m, 6H), 7.10 (d, *J* = 8.0 Hz, 2H), 6.96 (d, *J* = 3.4 Hz, 2H), 4.85 (d, *J* = 2.6 Hz, 1H), 2.84 (ddd, *J* = 8.4, 5.4, 2.6 Hz, 1H), 2.27 (s, 3H), 1.18 (s, 2H), 0.78 – 0.71 (m, 3H).; ¹³C NMR (101 MHz, CDCl₃) δ 143.9, 142.9, 141.5, 135.4, 134.7, 129.5, 128.7, 128.2, 127.5, 127.1, 126.2, 125.0, 124.1, 115.6, 69.9, 53.0, 29.5, 21.5, 11.2; IR (KBr) ν_{max} : 2963, 2927, 1724, 1460, 1165, 926, 812, 660, 574, 537 cm⁻¹; HRMS (ESI): *m/z* = 400.1311 (calcd for C₂₃H₂₃NO₂S+Na⁺ = 390.1342).

(2*R*, 3*R*)-2-(4'-methoxy-[1,1'-biphenyl]-4-yl)-1-tosyl-3-vinylindoline (**4b**)

Following *General Procedure D*, the product **4b** was obtained after column chromatography (petroleum ether/EtOAc 50:1 v/v); light yellow oil; 81% yield (39.01 mg), >20:1 *dr*, 90% *ee*

[Daicel Chiralpak AD-H, hexanes/*i*-propanol = 85/15, flow rate = 1.0 mL/min, λ = 254.4 nm, t (major) = 19.576, t (minor) = 30.161]; $[\alpha]_D^{25} = -26.67$ (c 0.10, CHCl₃); ¹H NMR (400 MHz, CDCl₃) δ 7.73 (d, J = 8.0 Hz, 1H), 7.52 (d, J = 7.8 Hz,

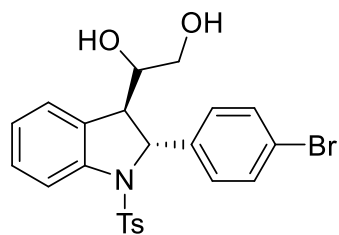


4b

2H), 7.40 (dd, J = 8.2, 4.0 Hz, 4H), 7.28 (d, J = 7.8 Hz, 2H), 7.23 (t, J = 7.6 Hz, 1H), 7.10 (d, J = 7.8 Hz, 2H), 6.99 (t, J = 7.4 Hz, 1H), 6.93 (d, J = 7.4 Hz, 1H), 6.88 (d,

J = 8.2 Hz, 2H), 5.13 (dt, J = 17.6, 8.8 Hz, 1H), 4.87 (d, J = 3.6 Hz, 1H), 4.79 – 4.68 (m, 2H), 3.76 (s, 3H), 3.63 – 3.55 (m, 1H), 2.28 (s, 3H); ¹³C NMR (101 MHz, CDCl₃) δ 159.2, 144.0, 141.8, 140.7, 139.9, 138.3, 134.8, 133.4, 132.5, 129.5, 128.6, 128.1, 127.4, 127.0, 126.3, 125.7, 124.5, 116.0, 115.8, 114.2, 71.0, 55.8, 55.4, 21.5.; IR (KBr) ν_{\max} : 2959, 2921, 2852, 1651, 1595, 1448, 1345, 1052, 696, 660, 575, 542 cm⁻¹; HRMS (ESI): m/z = 504.1615 (calcd for C₃₀H₂₇NO₃S+Na⁺ = 504.1604).

1-((2*R*,3*R*)-2-(4-bromophenyl)-1-tosylindolin-3-yl)ethane-1,2-diol (**4c**)



4c

Following *General Procedure E*, the product **4c** was obtained after column chromatography (petroleum ether/EtOAc 50:1 v/v); light yellow oil; 85% yield (41.51 mg), 5:1 *dr*, 90% *ee* [Daicel Chiralpak AS-H, hexanes/*i*-propanol = 82/18, flow rate = 1.0 mL/min, λ = 254.4 nm, t (major) = 30.969, t (minor) = 36.800];

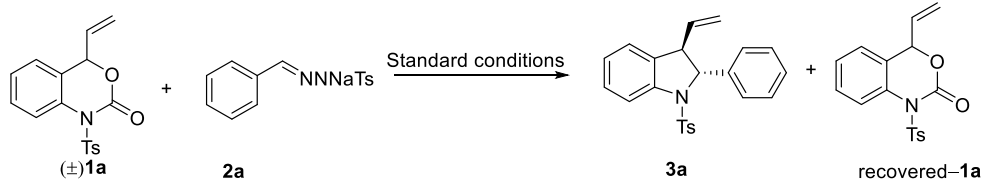
$[\alpha]_D^{25} = -15.67$ (c 0.10, CHCl₃); ¹H NMR (400 MHz, CDCl₃) δ 7.68 (d, J = 8.0 Hz, 1H), 7.59 (d, J = 8.0 Hz, 2H), 7.31 (d, J = 8.2 Hz, 2H), 7.24 (t, J = 7.2 Hz, 1H), 7.12 (t, J = 7.8 Hz, 4H), 6.99 (d, J = 10.6 Hz, 2H), 5.39 (s, 1H), 5.28 (d, J = 5.2 Hz, 1H), 3.51 – 3.46 (m, 1H), 3.02 (d, J = 7.6 Hz, 1H), 2.80 (d, J = 9.2 Hz, 1H), 2.30 (s, 3H); ¹³C NMR (101 MHz, CDCl₃) δ 143.2, 141.2, 140.6, 134.4, 130.7, 128.5, 128.1, 126.7, 126.2, 125.2, 123.2, 120.4, 114.6, 72.0, 65.3, 61.4, 53.0, 20.5.; IR (KBr) ν_{\max} : 2962, 2921, 2851, 1260, 1091, 1025, 799, 666, 569 cm⁻¹; HRMS (ESI): m/z = 510.0368 (calcd for C₂₃H₂₂BrNO₄S+Na⁺ = 510.0345).

7. DYKAT Studies

Five experiments were performed at the same time and respectively quenched at 3.0 hours, 6.0 hours, 9.0 hours, 12.0 hours and 24.0 hours. To five flame-dried schlenk tube, Pd₂(dba)₃ (4.6 mg,

0.005 mmol) and (*R,R*)-**L11** (8.6 mg, 0.012 mmol) were respectively added in dry DCM (1 mL) under nitrogen atmosphere. The mixture was stirred at 25 °C for 0.5 hours. Then *i*-PrOH (100 μL) was added into the resulted dark red solution. After that, vinyl benzoxazinone **1a** (0.1 mmol), *N*-tosylhydrazone sodium salt **2a** (0.12 mmol), Cs₂CO₃ (0.12 mmol, 39.10mg), BnNEt₃Cl (0.1 mmol, 22.50mg) were included. The mixture was stirred at 15 °C. The reasubstrate **1a** was recovered at different times and analyzed by HPLC (CHIRALPAK AD-H column, hexane/*i*-PrOH=85/15, 254nm, 1 mL/min). And the product **3a** was analyzed by HPLC (CHIRALPAK AD-H column, hexane/*i*-PrOH=90/10, 254nm, 1 mL/min) at different times.

Table S7. Test results of DYKAT studies



Time (h)	Recovered yield of 1a	ee of recovered 1a ^a (%)	Conv. of 1a %	<i>dr</i> of 3a (%)	<i>ee</i> of 3a ^b (%)
3	85	0	11	>20:1	91
6	74	0	22	>20:1	91
9	66	0	30	>20:1	91
12	43	0	55	>20:1	91
24	17	0	80	>20:1	91

^aDetermined by HPLC analysis CHIRALPAK AD-H column, hexane/*i*-PrOH=85/15, 254nm, 1 mL/min). ^bDetermined by HPLC analysis CHIRALPAK AD-H column, hexane/*i*-PrOH=90/10, 254nm, 1 mL/min).

8. The study of the non-linear effect

To a flame-dried schlenk tube, Pd₂dba₃ (4.6 mg, 0.005 mmol), (*R,R*)-**L10** (x mg) / *ent*-**L10** (y mg) and dry DCM (1 mL) were added under a nitrogen atmosphere. The mixture was stirred at 25 °C for 0.5 hour to produce a dark red solution and then *i*-PrOH (100 μL) was added. After that, vinyl benzoxazinone **1** (0.1 mmol), *N*-tosylhydrazone sodium salt **2** (0.12 mmol), Cs₂CO₃ (0.12 mmol, 39.10mg), BnNEt₃Cl (0.1 mmol, 22.50mg) were added. The mixture was stirred at 15 °C for 24 hours (monitored by TLC analysis) and then it was subjected to silica gel column to afford the desired products **3**.

Table S8. The study of the non-linear effect ^[a]

entry	x/y (mg)	ee (%) (L10 + ent-L10)	yield ^[b]	dr ^[c]	ee (%) ^[d] of 3a
1	2.35/1.60	20	68	>20:1	18
2	2.75/1.18	40	67	>20:1	37
3	3.14/0.79	60	69	>20:1	53
4	3.53/0.40	80	72	>20:1	68
5	3.93/0	100	71	>20:1	84

^[a]Reaction conditions: **1a** (0.05 mmol), **2a** (0.06 mmol), Pd₂(dba)₃ (5 mol%), ligand (12 mol%), Cs₂CO₃ (0.06 mmol), BnNEt₃Cl (0.05 mmol), 0.5 mL of dichloromethane/*i*-PrOH(10:1) at 15°C for 24 hours. ^[b] Isolated yield. ^[c] Determined by ¹H NMR analysis. ^[d] Determined by chiral HPLC.

9. The X-ray data of 3s

Table S9. Crystal data and structure refinement for **3s**.

Identification code	mo_b20220719bb_0m
Empirical formula	C ₂₃ H ₂₀ FNO ₂ S
Formula weight	393.46
Temperature	120(2) K
Wavelength	0.71073 Å
Crystal system, space group	Monoclinic, P 21
Unit cell dimensions	a = 11.2213(4) Å alpha = 90 deg. b = 10.9116(3) Å beta = 101.3400(10) deg. c = 16.2561(5) Å gamma = 90 deg.
Volume	1951.58(11) Å ³
Z, Calculated density	4, 1.339 Mg/m ³
Absorption coefficient	0.194 mm ⁻¹
F (000)	824
Crystal size	0.100 x 0.050 x 0.030 mm
Theta range for data collection	2.262 to 24.982 deg.
Limiting indices	-13<=h<=13, -12<=k<=12, -19<=l<=19

Reflections collected / unique	31994 / 6875 [R(int) = 0.0972]
Completeness to theta = 24.982	99.9 %
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	6875 / 1 / 507
Goodness-of-fit on F ²	1.039
Final R indices [I>2sigma(I)]	R1 = 0.0496, wR2 = 0.1160
R indices (all data)	R1 = 0.0611, wR2 = 0.1252
Absolute structure parameter	-0.06(8)
Extinction coefficient	n/a
Largest diff. peak and hole	0.233 and -0.431 e.A ⁻³

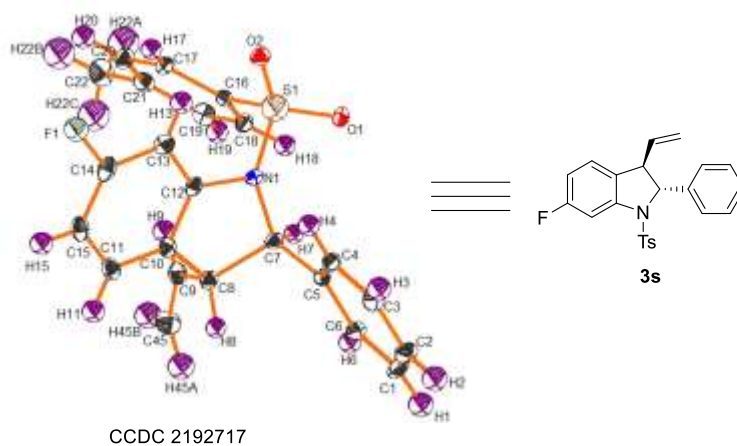


Figure S3. ORTEP drawing of **3s** (30% thermal ellipsoids)

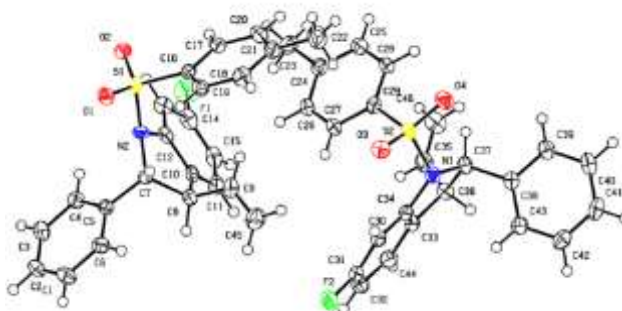
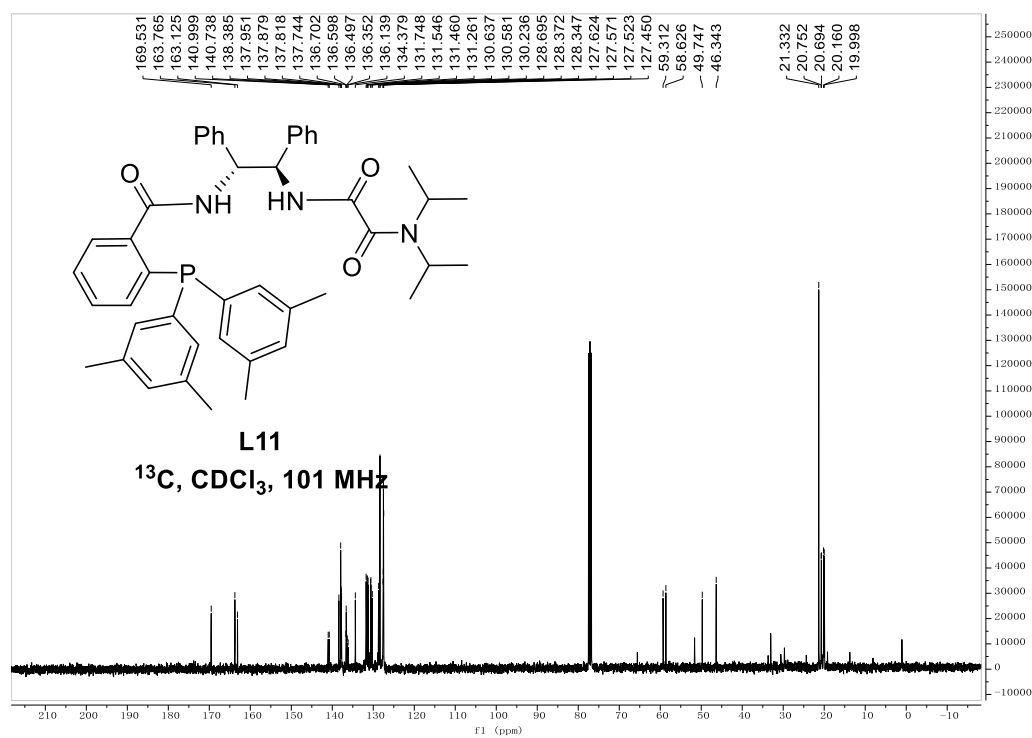
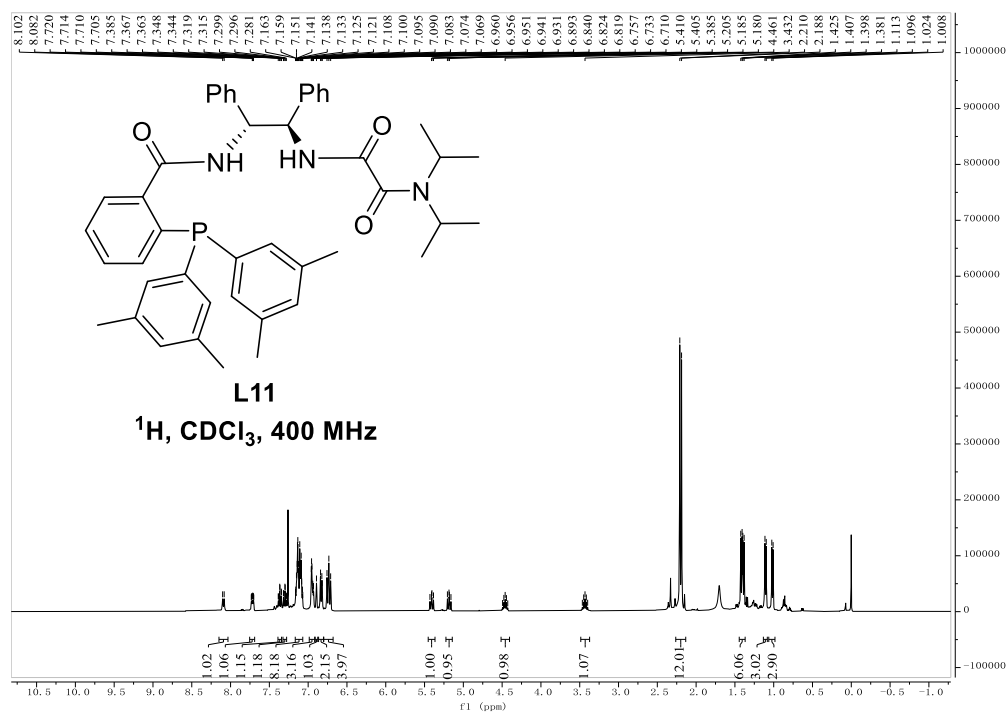


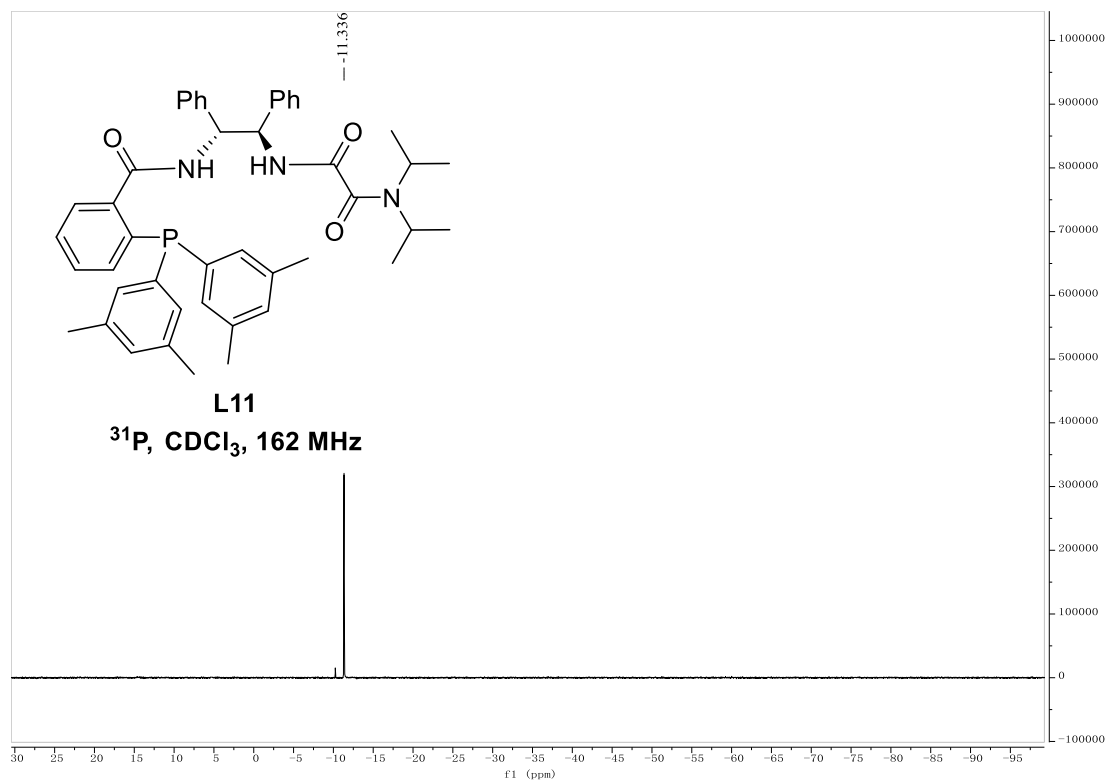
Figure S4. Packing of molecules in a unit cell of **3s**

The crystal was obtained through vapor diffusion with pentanes/CH₂Cl₂ at -20 °C. It should be noted that **3s** crystallizes in monoclinic space group P 1 21 1, which contains two molecules in the asymmetric unit. CCDC of **3s** is 2192717, which can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.

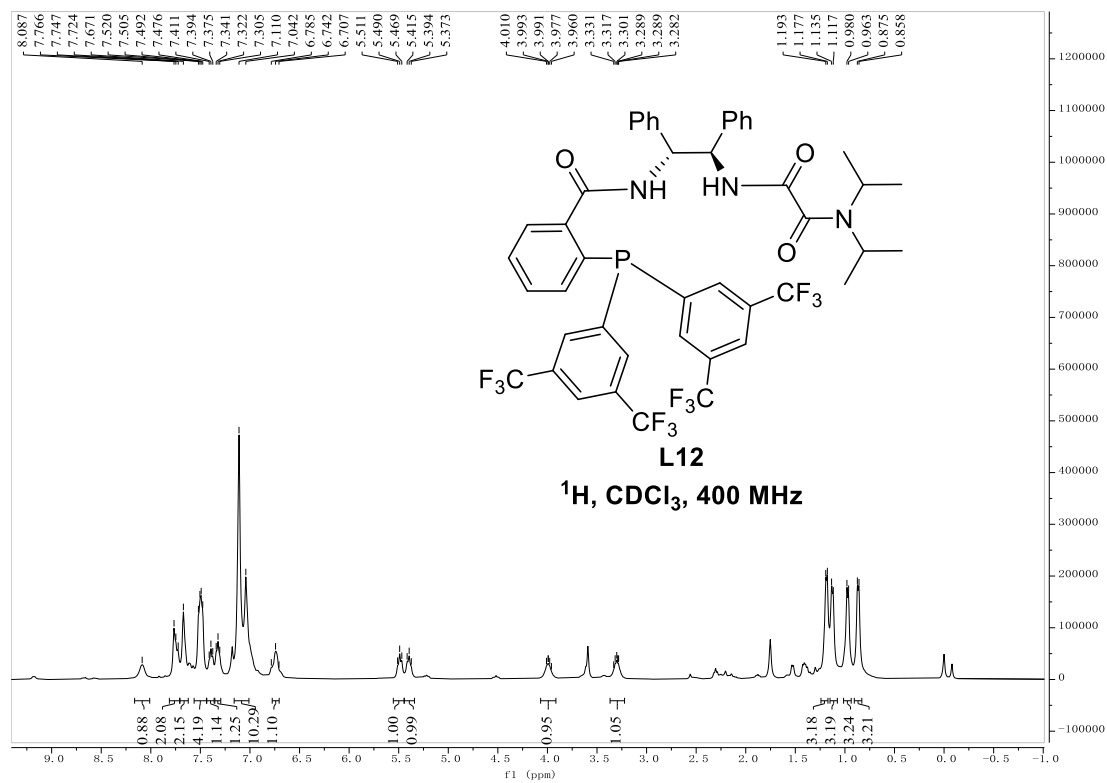
10. NMR spectra

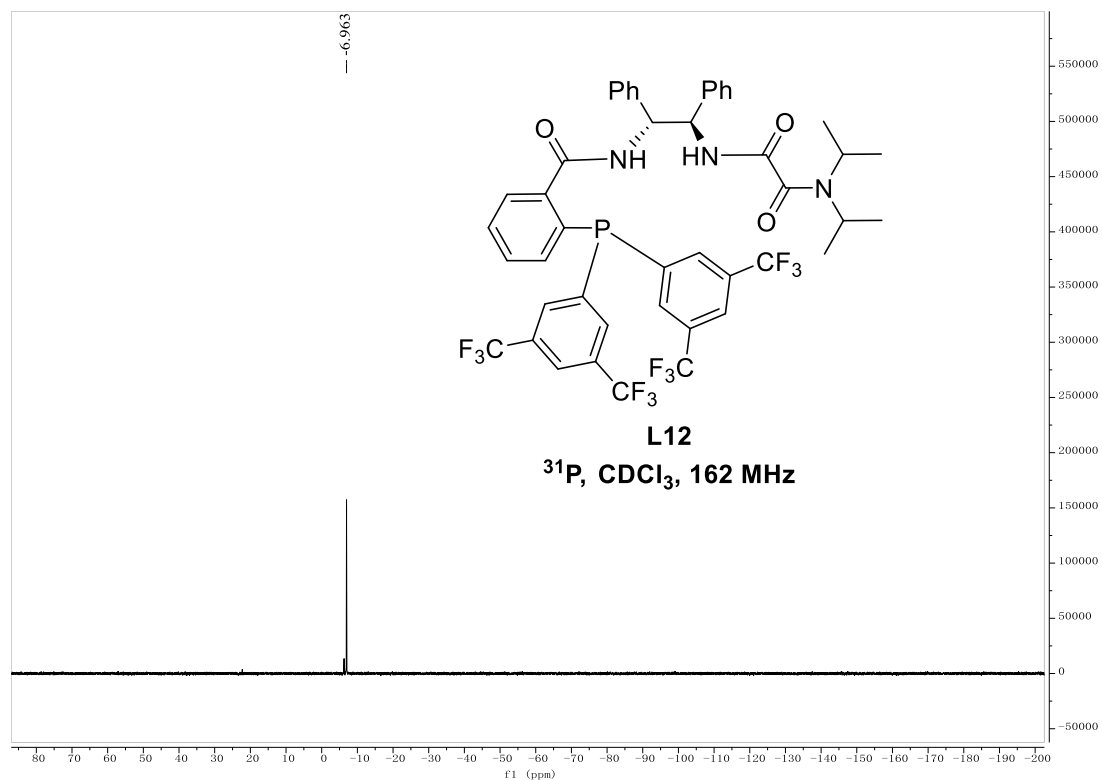
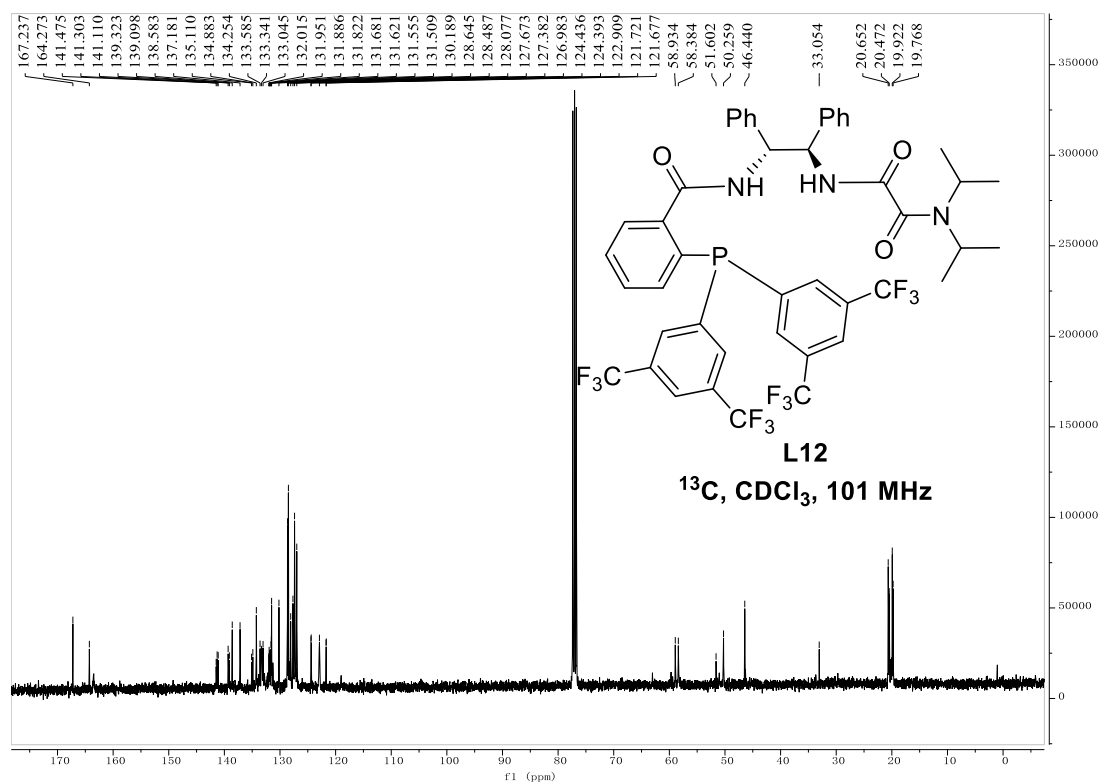
N^1 -(*(1R,2R)*-2-(2-(bis(3,5-dimethylphenyl)phosphaneyl)benzamido)-1,2-diphenylethyl)- N^2,N^2 -diisopropylamide (L11)

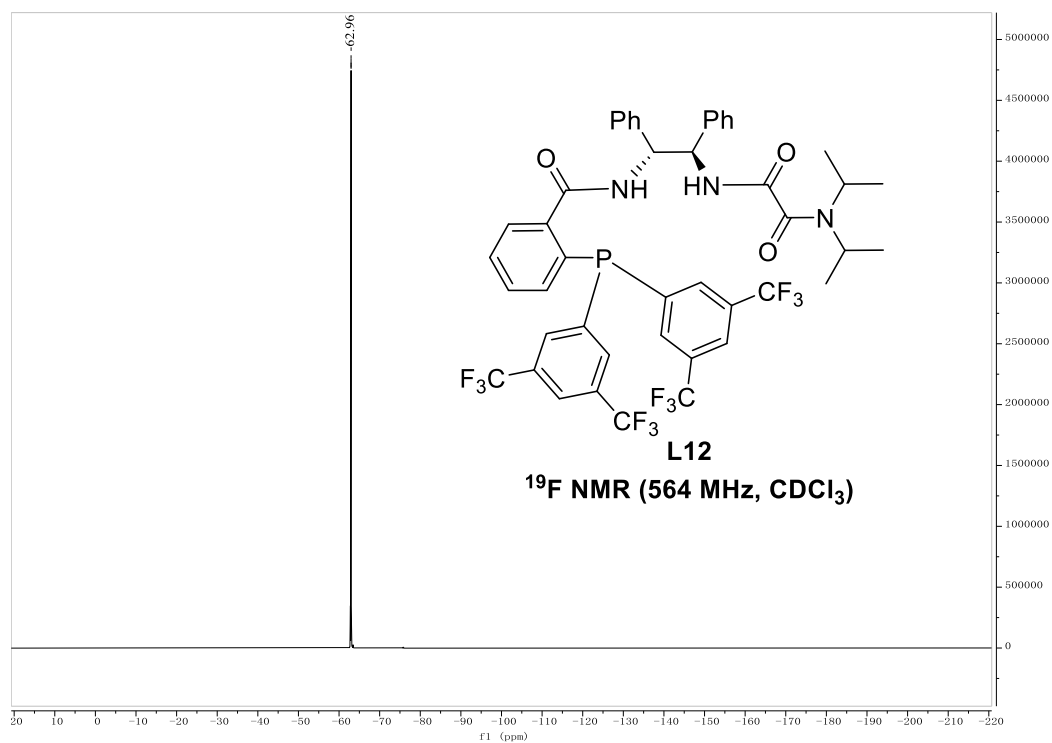




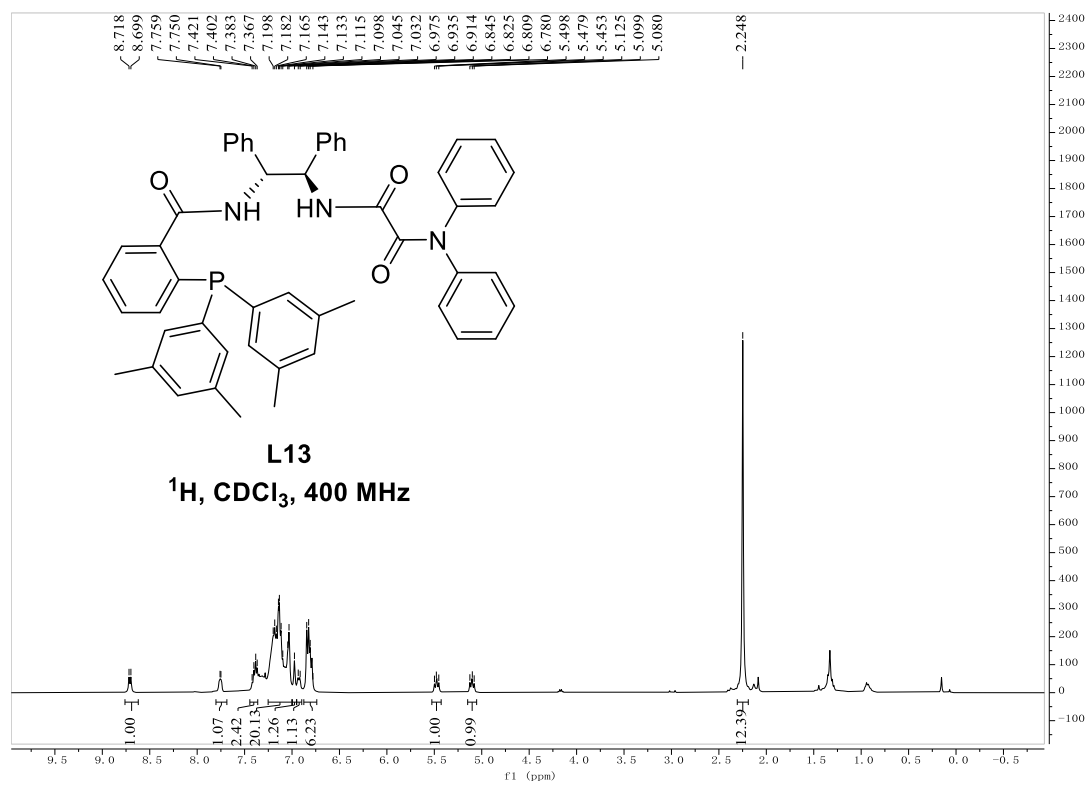
N^1 -((*1R,2R*)-2-(2-(bis(3,5-bis(trifluoromethyl)phenyl)phosphanyl)benzamido)-1,2-diphenylethyl)- N^2, N^2 -diisopropylamide (L12)

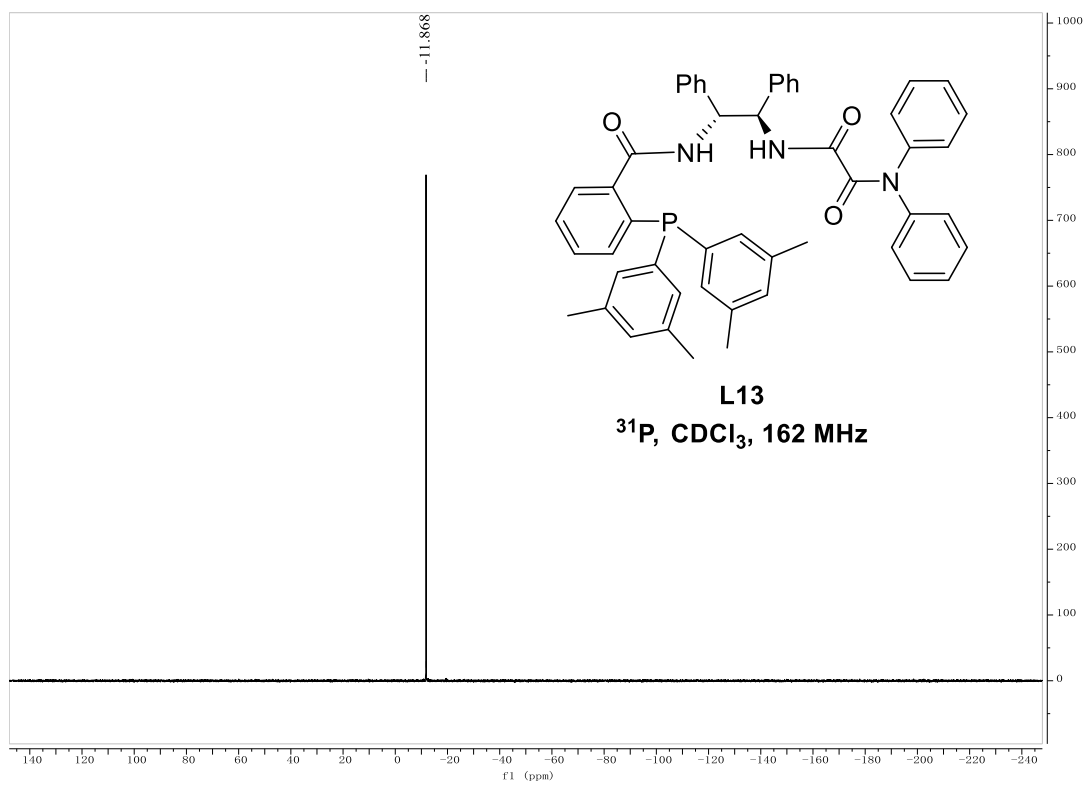
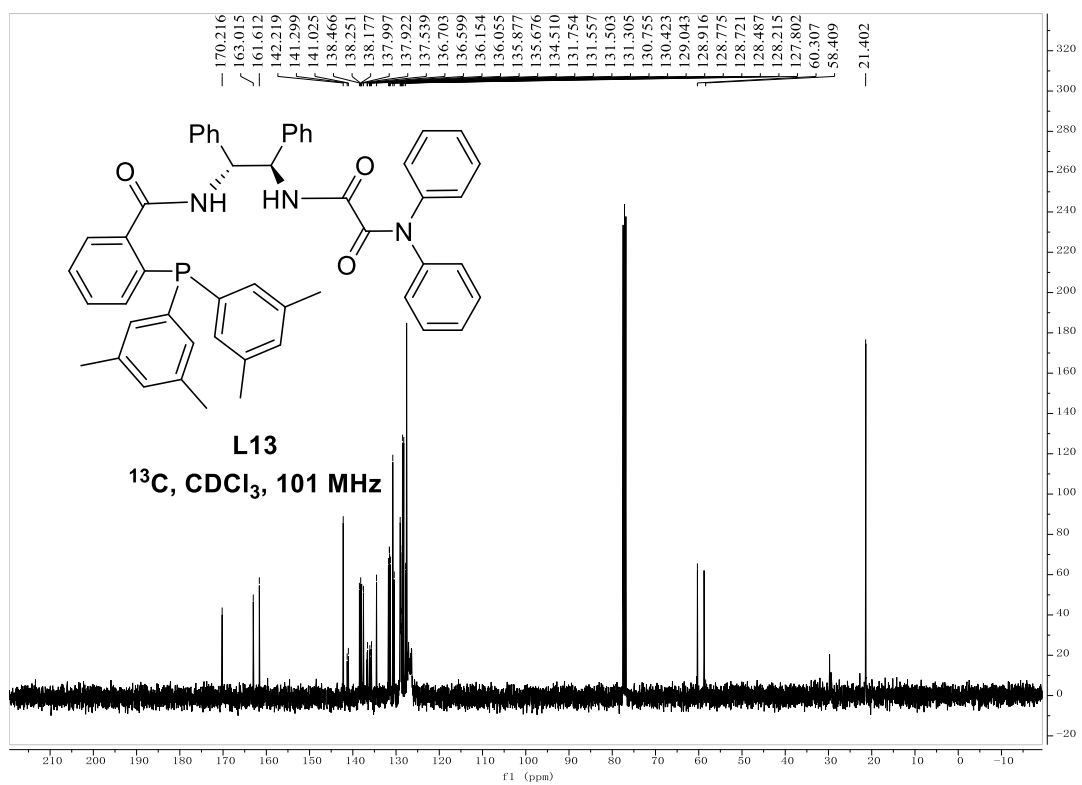




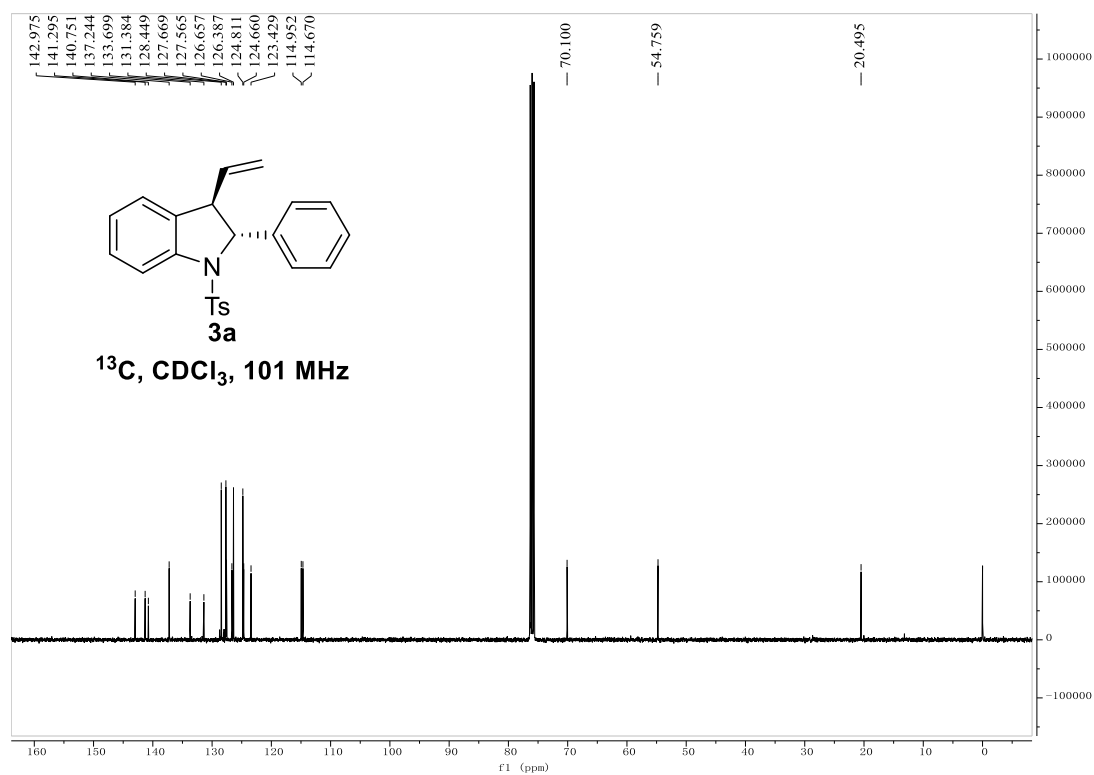
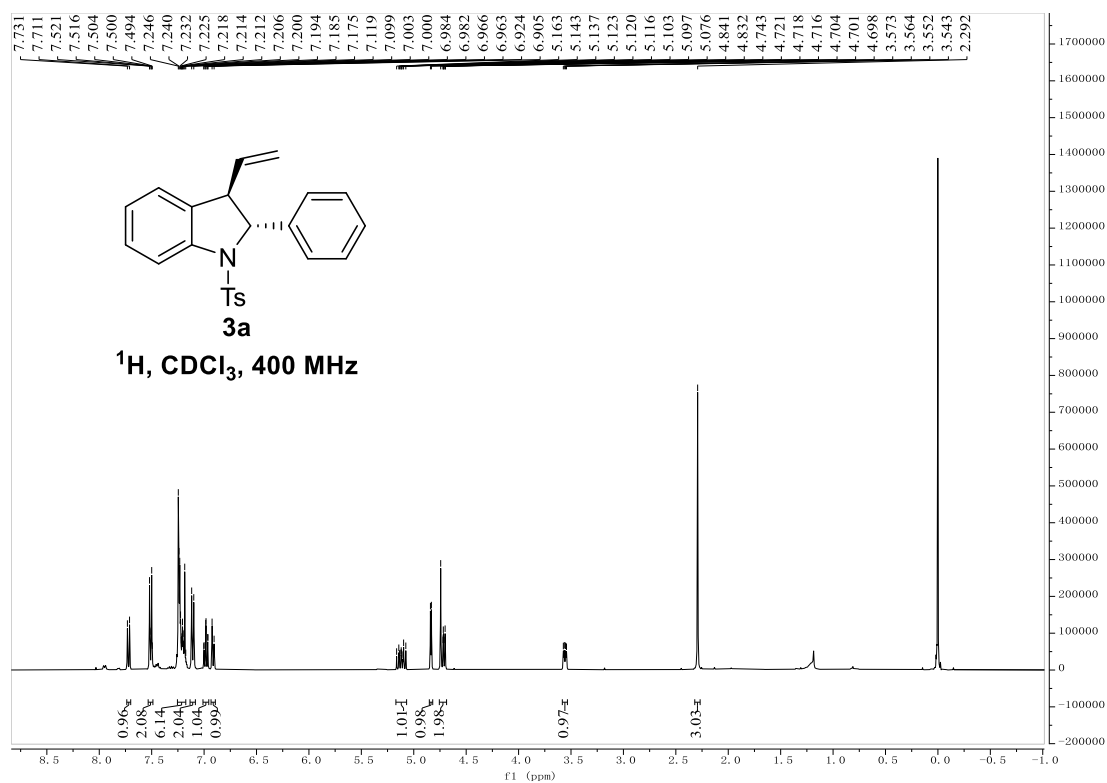


***N*¹-((1*R*,2*R*)-2-(2-(bis(3,5-dimethylphenyl)phosphaneyl)benzamido)-1,2-diphenylethyl)-*N*²,*N*²-diphenyloxalamidee (L13)**

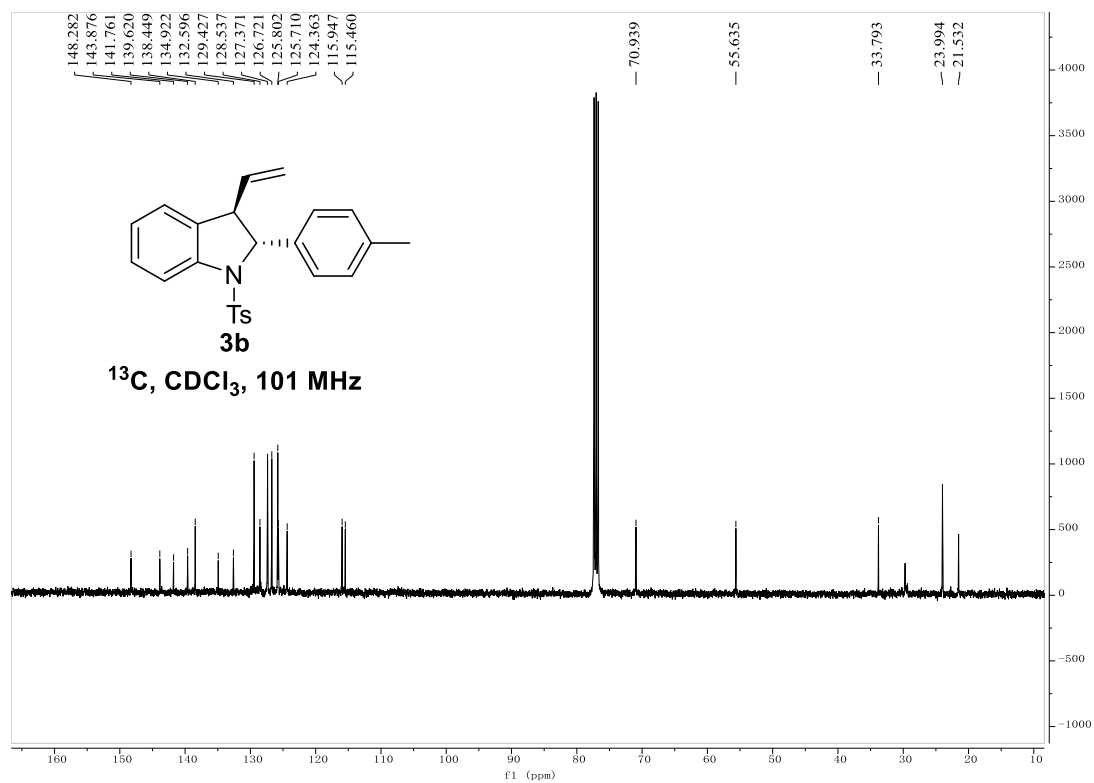
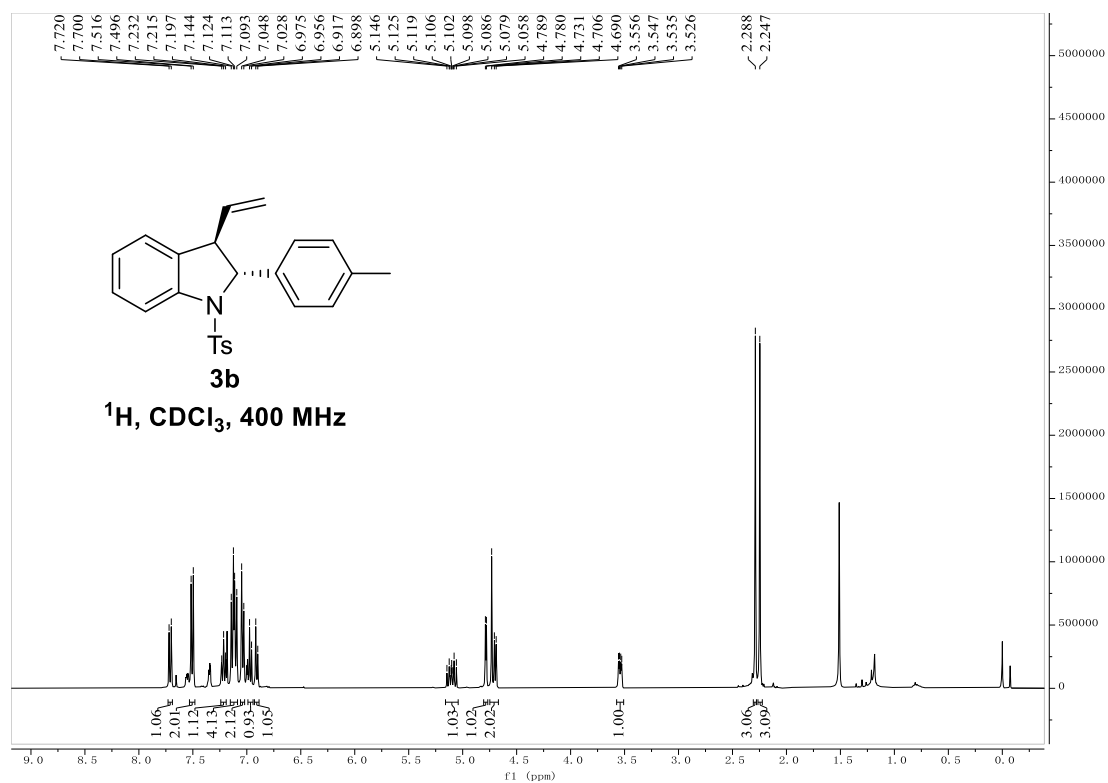




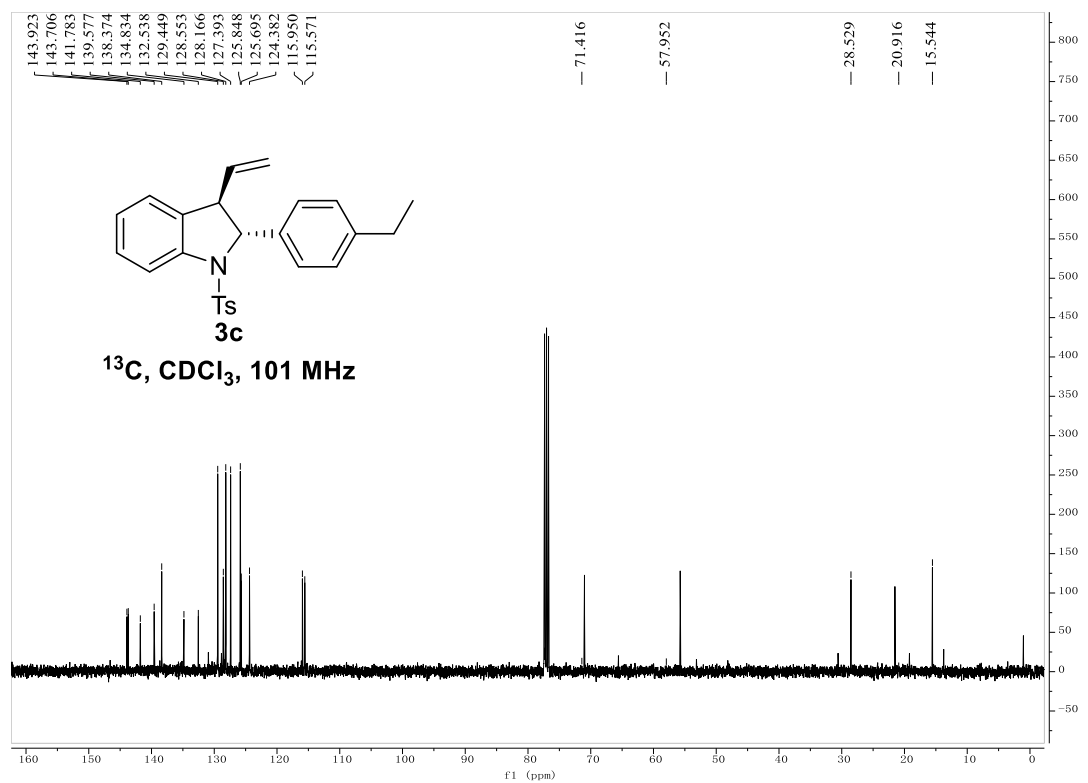
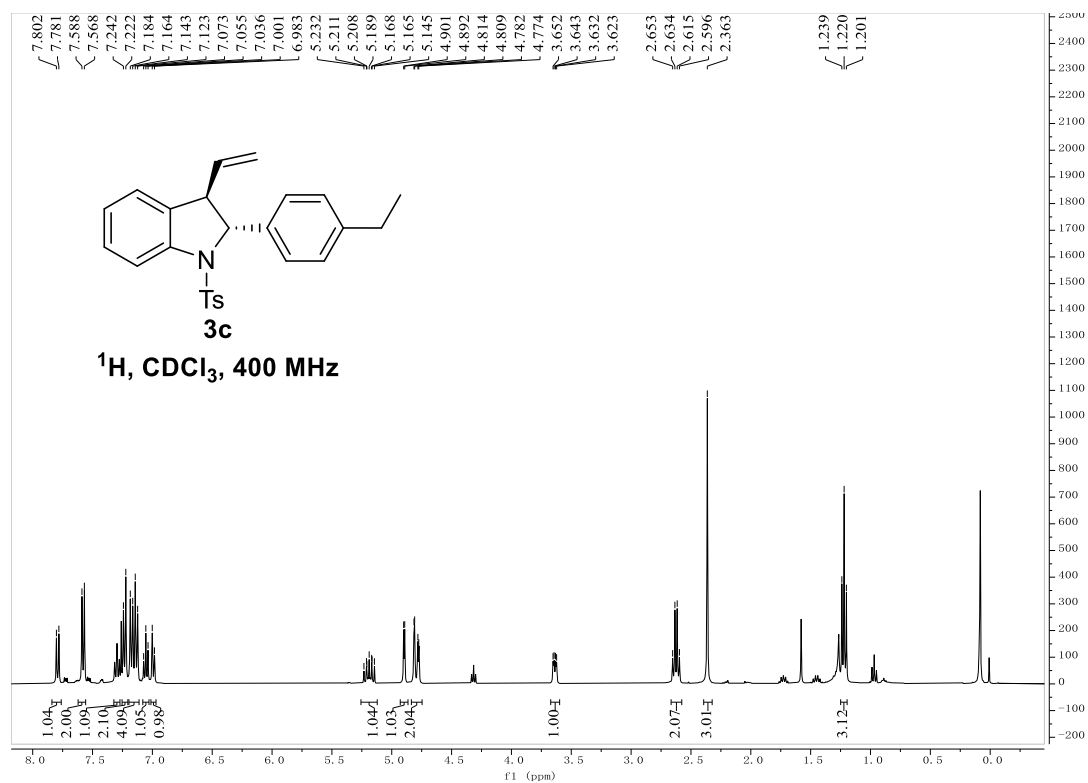
(2*R*,3*R*)-2-phenyl-1-tosyl-3-vinylindoline (3a)



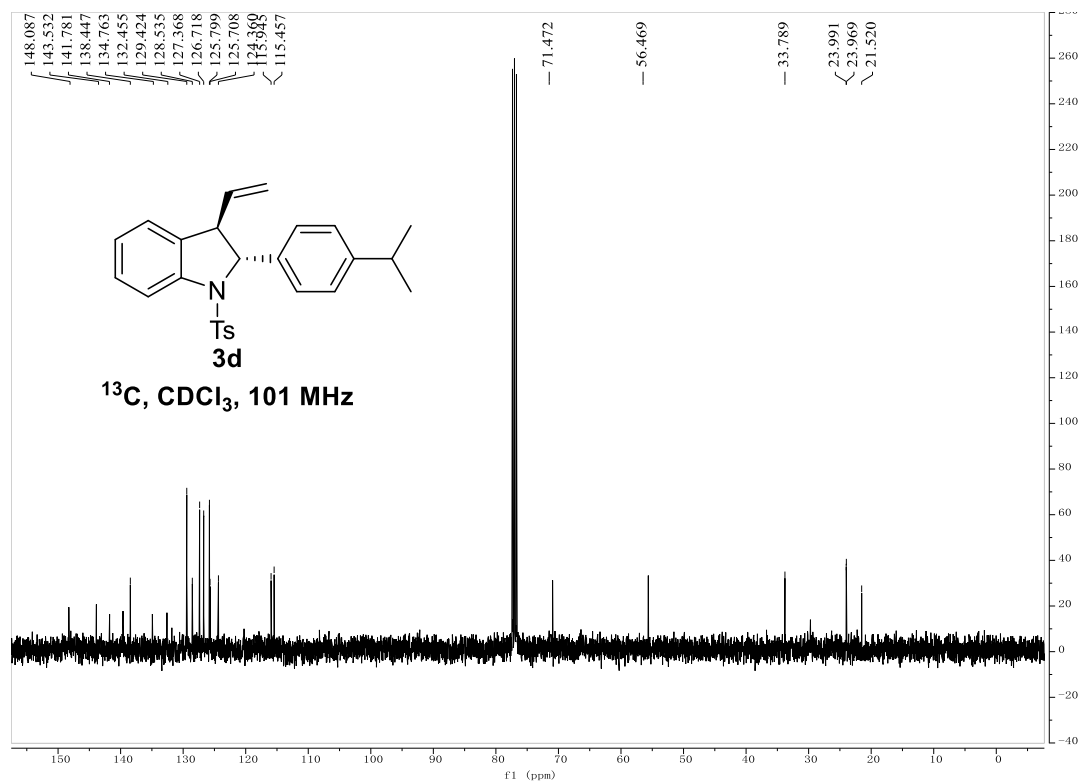
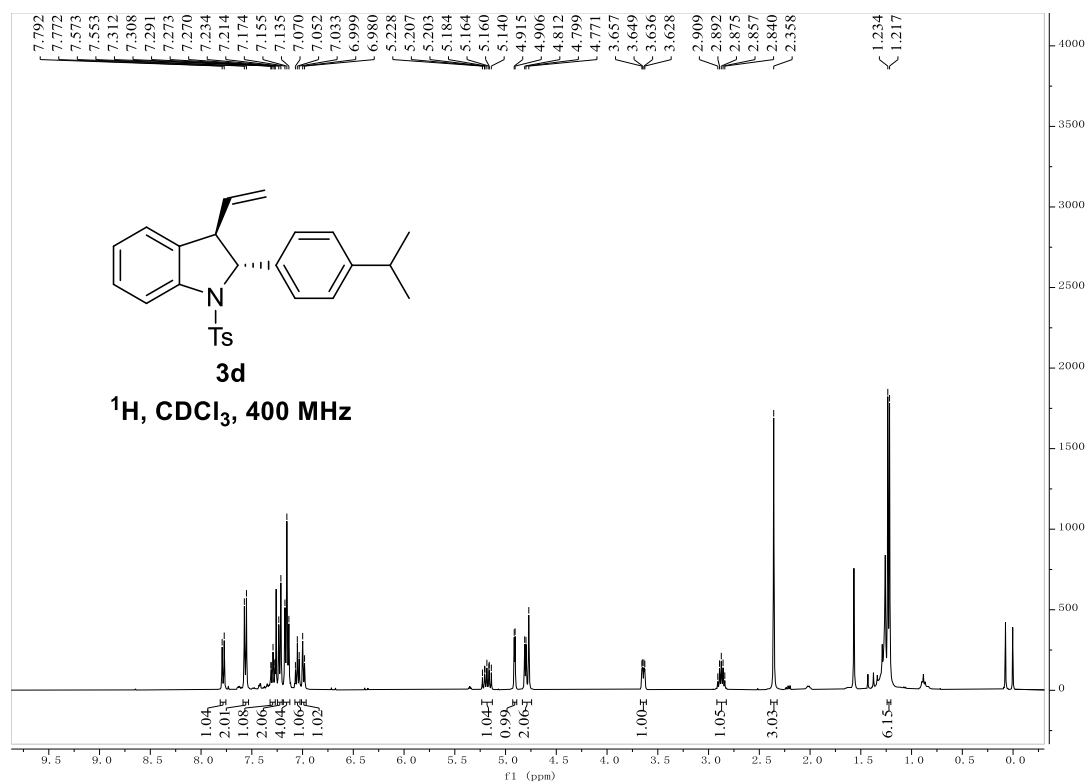
(2*R*,3*R*)-2-(*p*-tolyl)-1-tosyl-3-vinylindoline (3b**)**



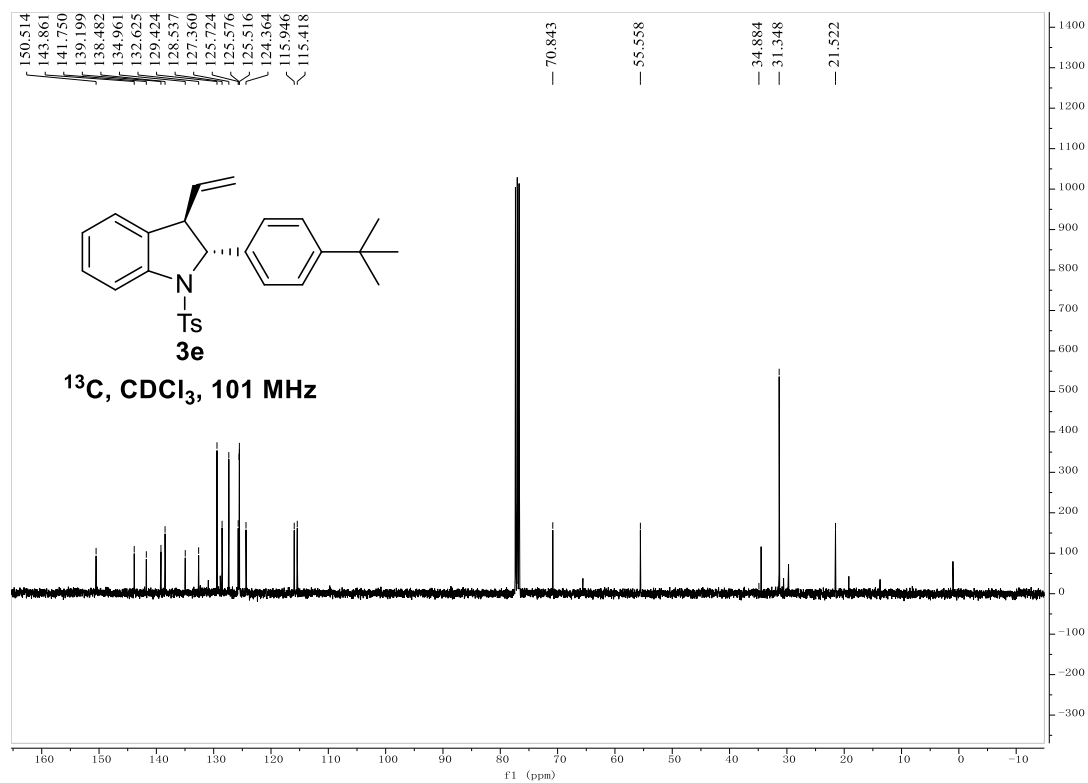
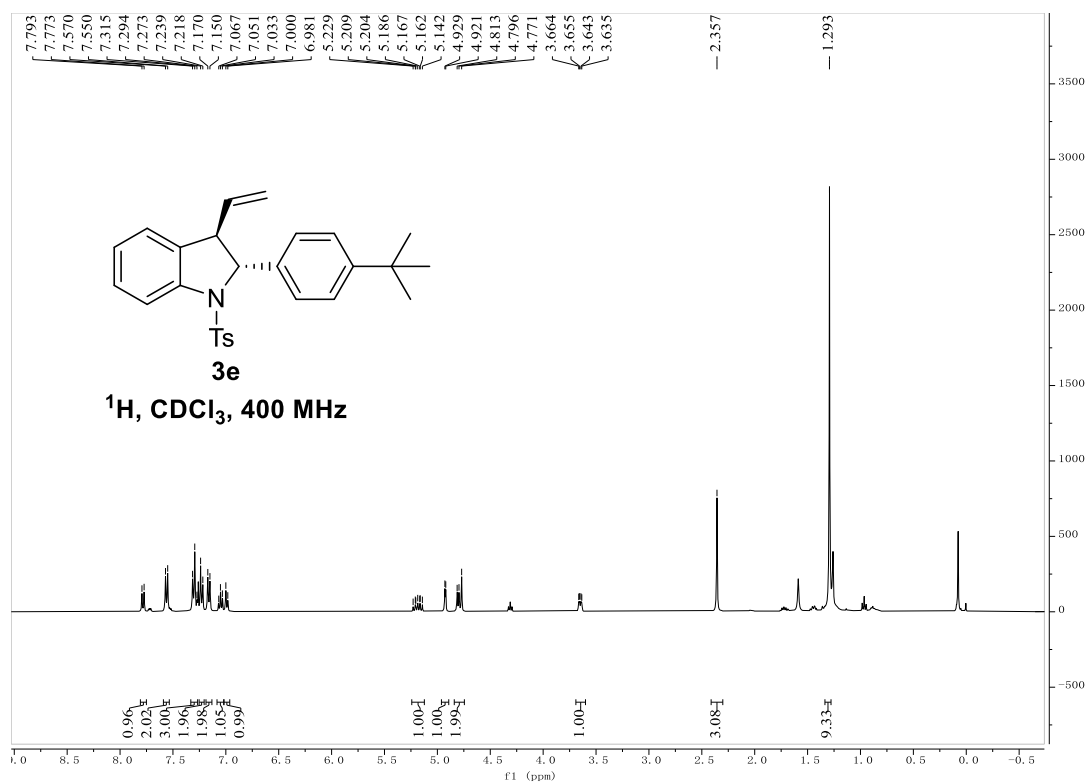
(2*R*,3*R*)-2-(4-ethylphenyl)-1-tosyl-3-vinylindoline (3c)



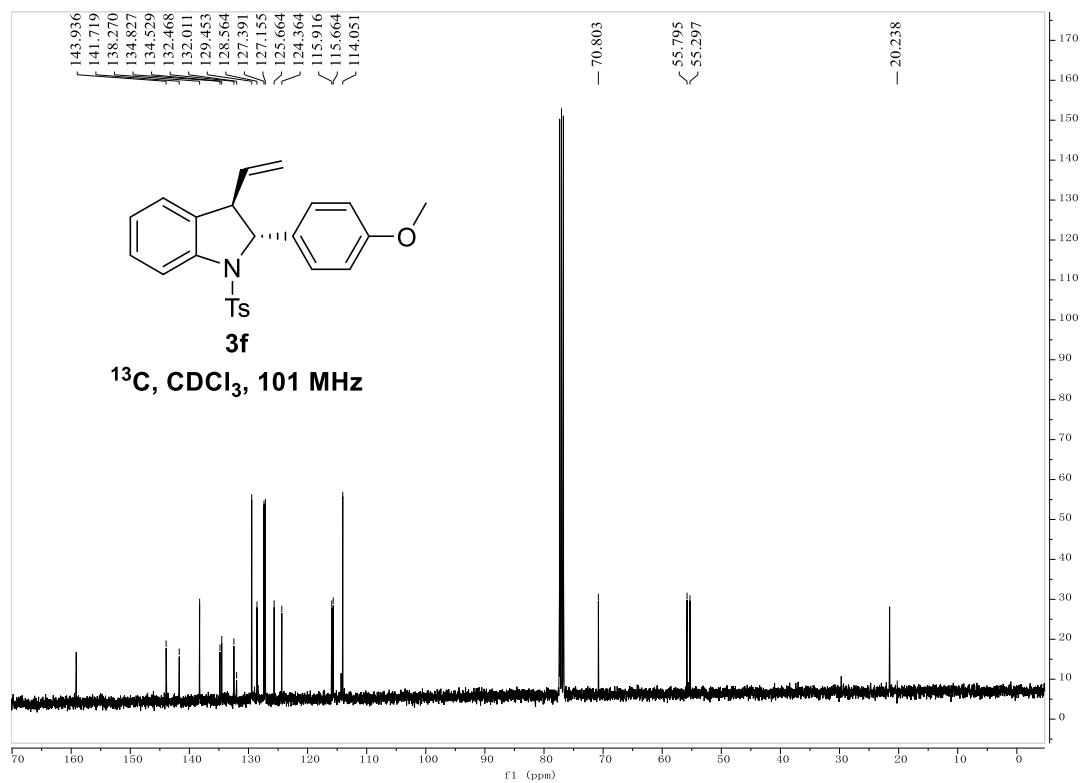
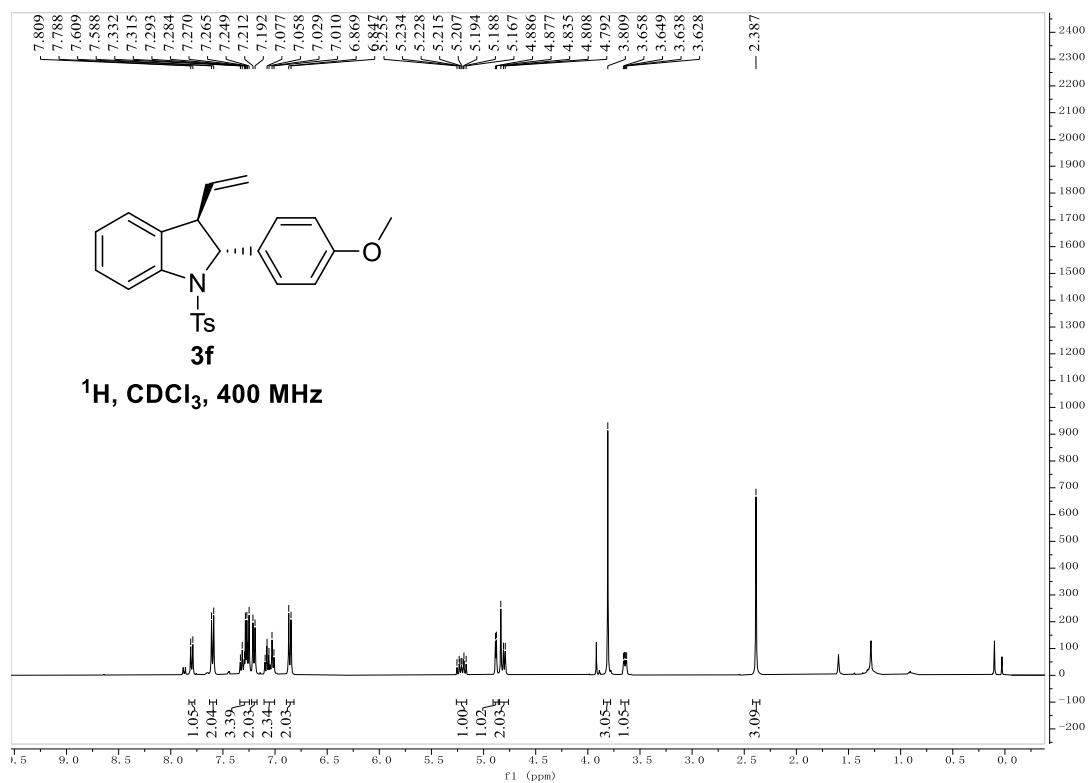
(2*R*,3*R*)-2-(4-isopropylphenyl)-1-tosyl-3-vinylindoline (3d)



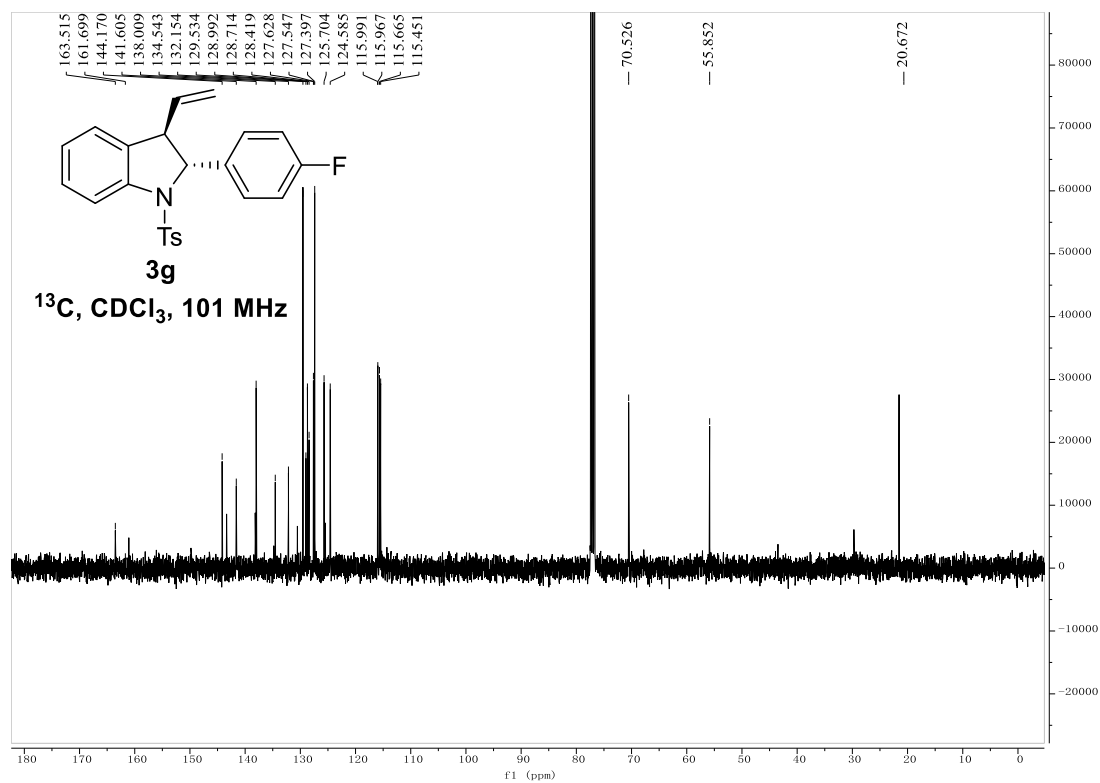
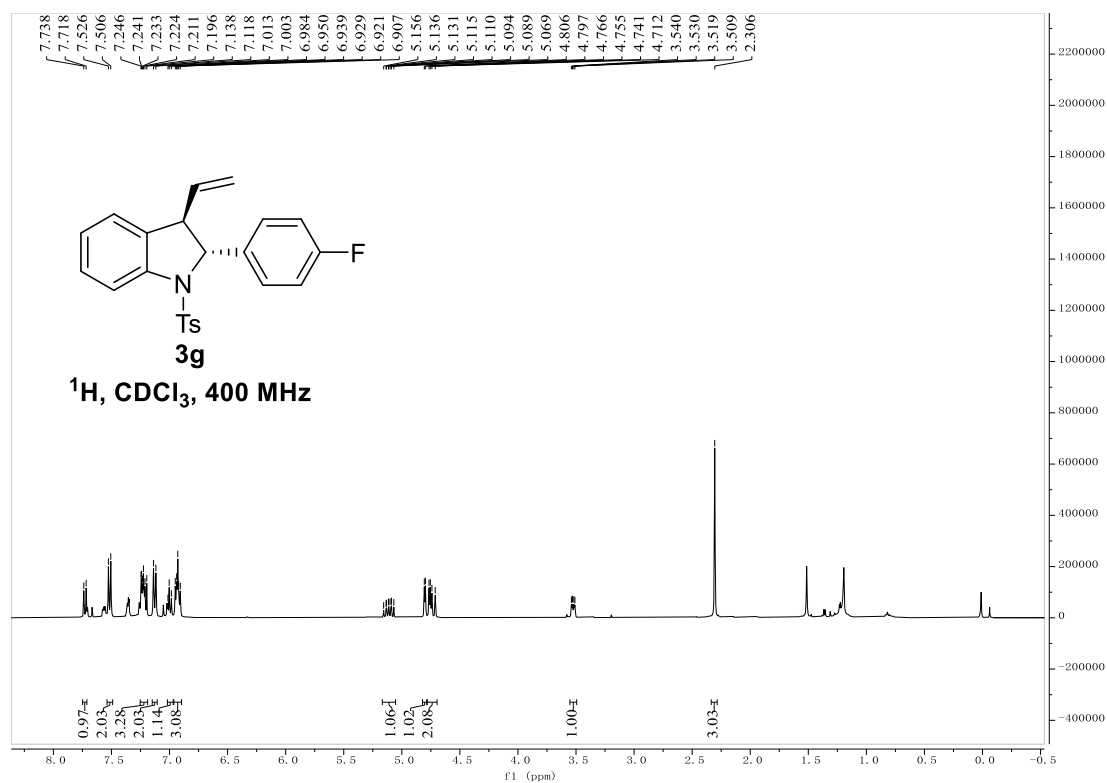
(2*R*,3*R*)-2-(4-(*tert*-butyl)phenyl)-1-tosyl-3-vinylindoline (3e)

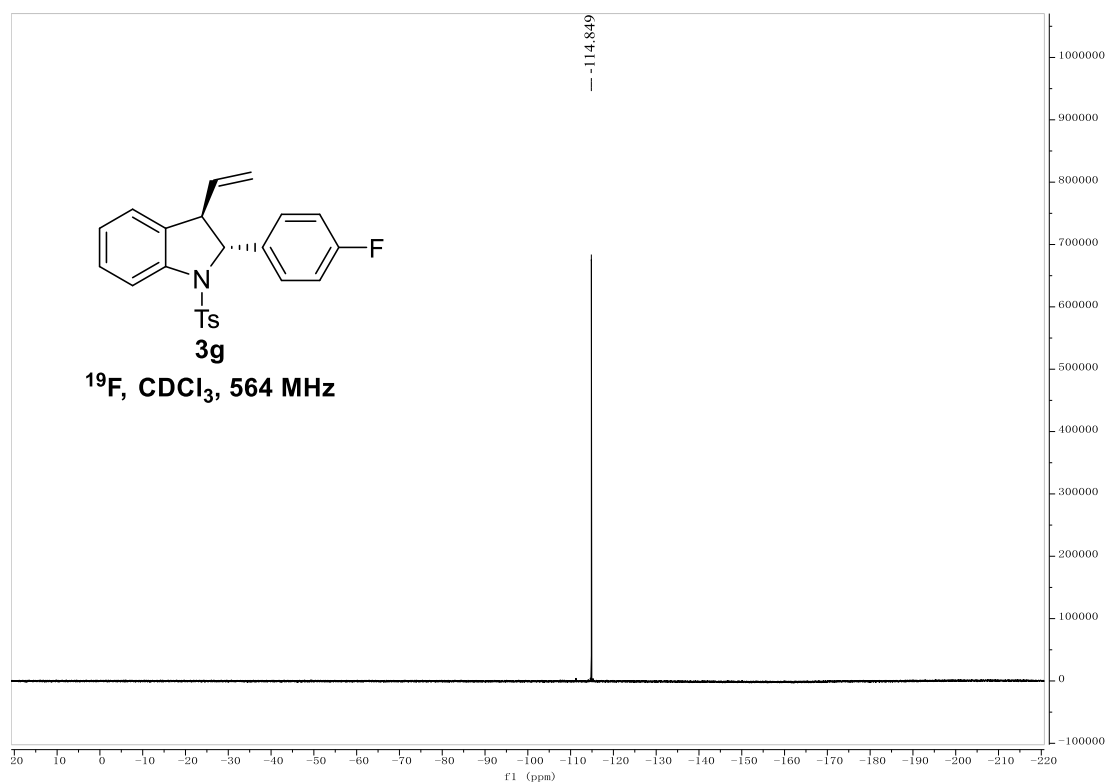


(2*R*,3*R*)-2-(4-methoxyphenyl)-1-tosyl-3-vinylindoline (3f)

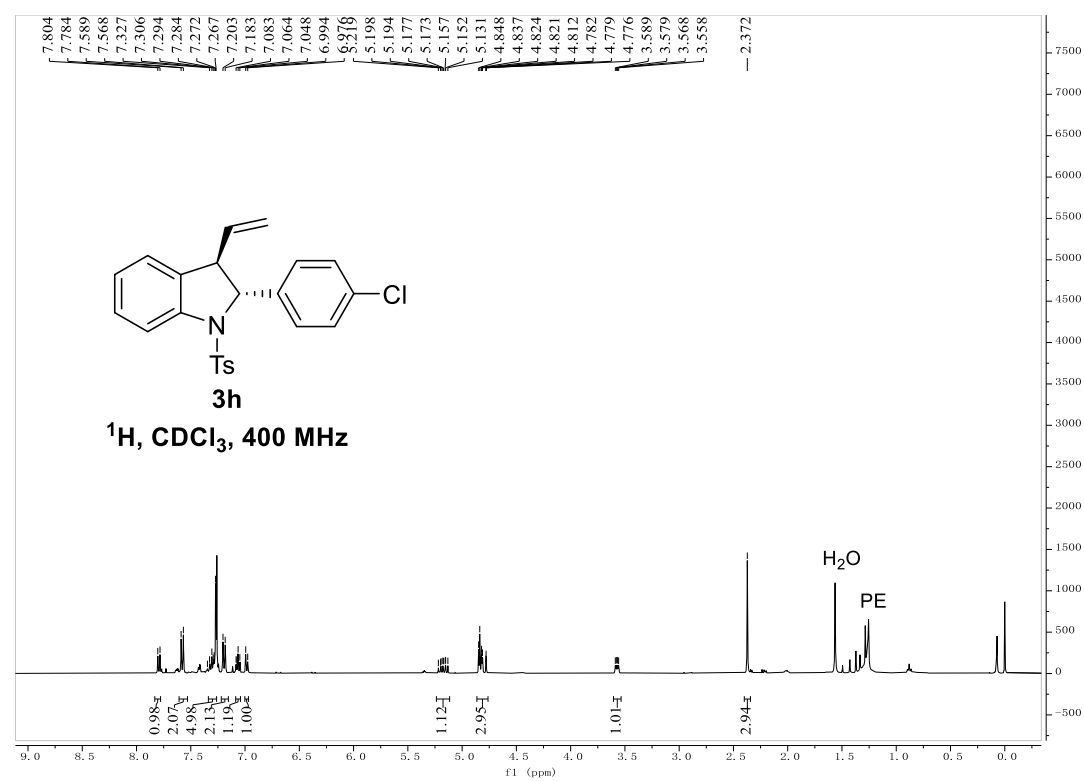


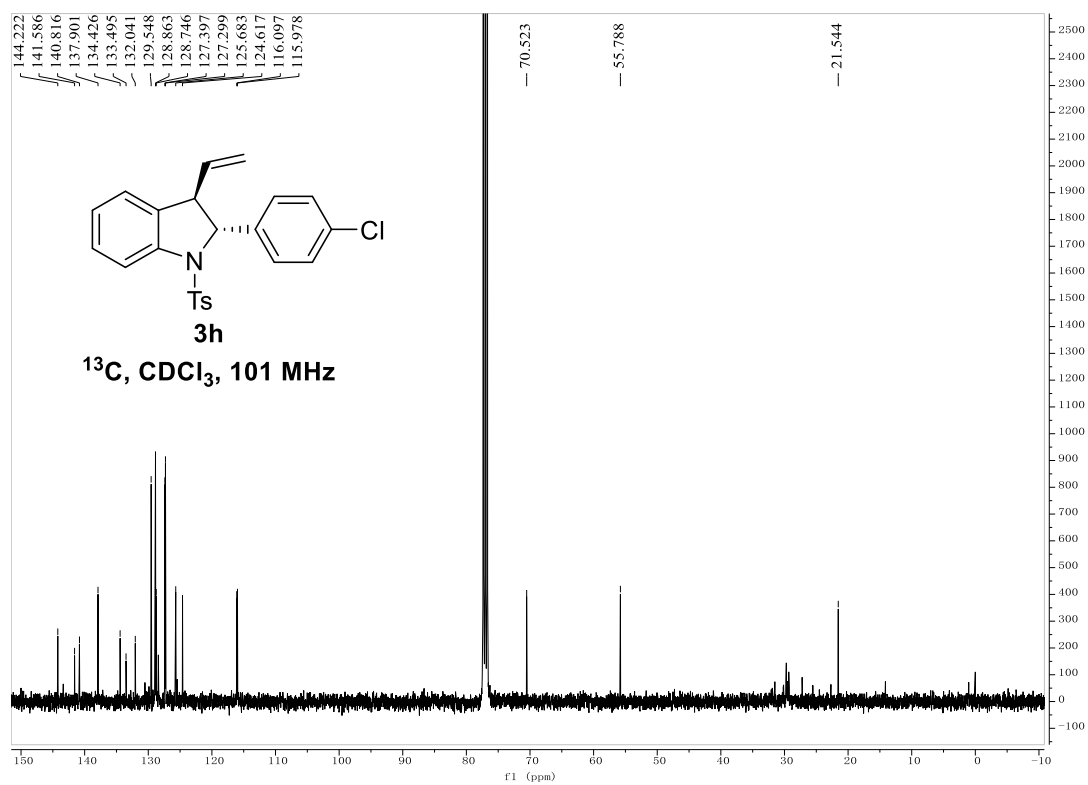
(2*R*,3*R*)-2-(4-fluorophenyl)-1-tosyl-3-vinylindoline (3g)



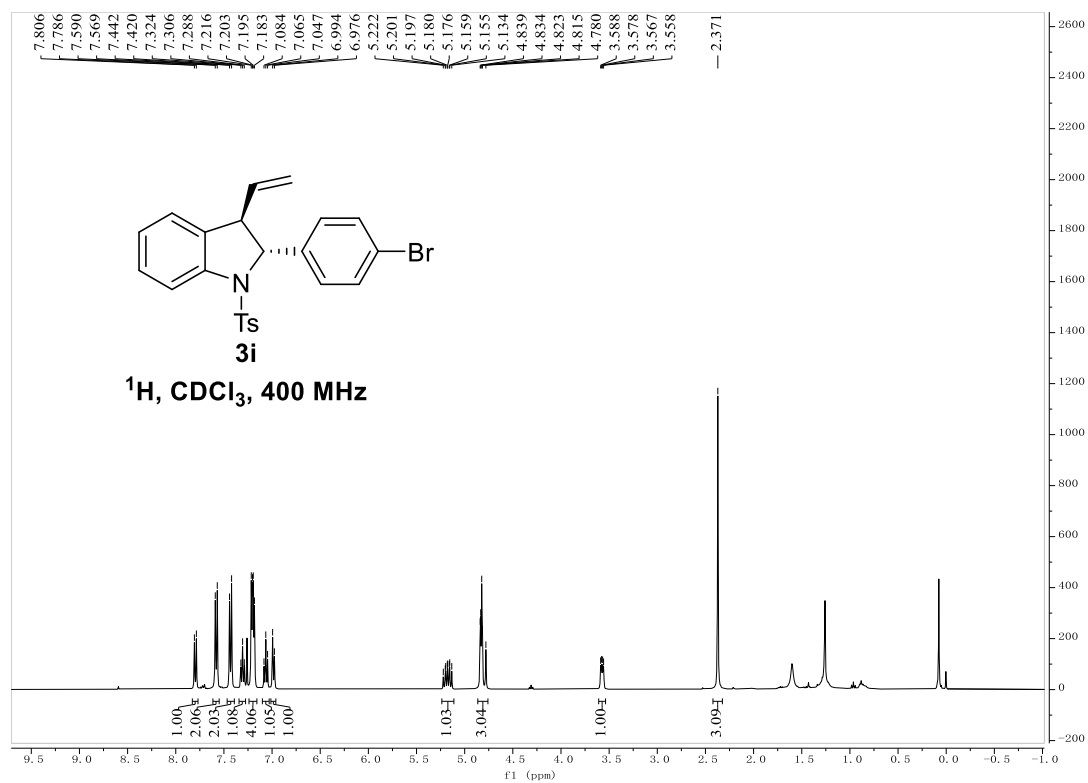


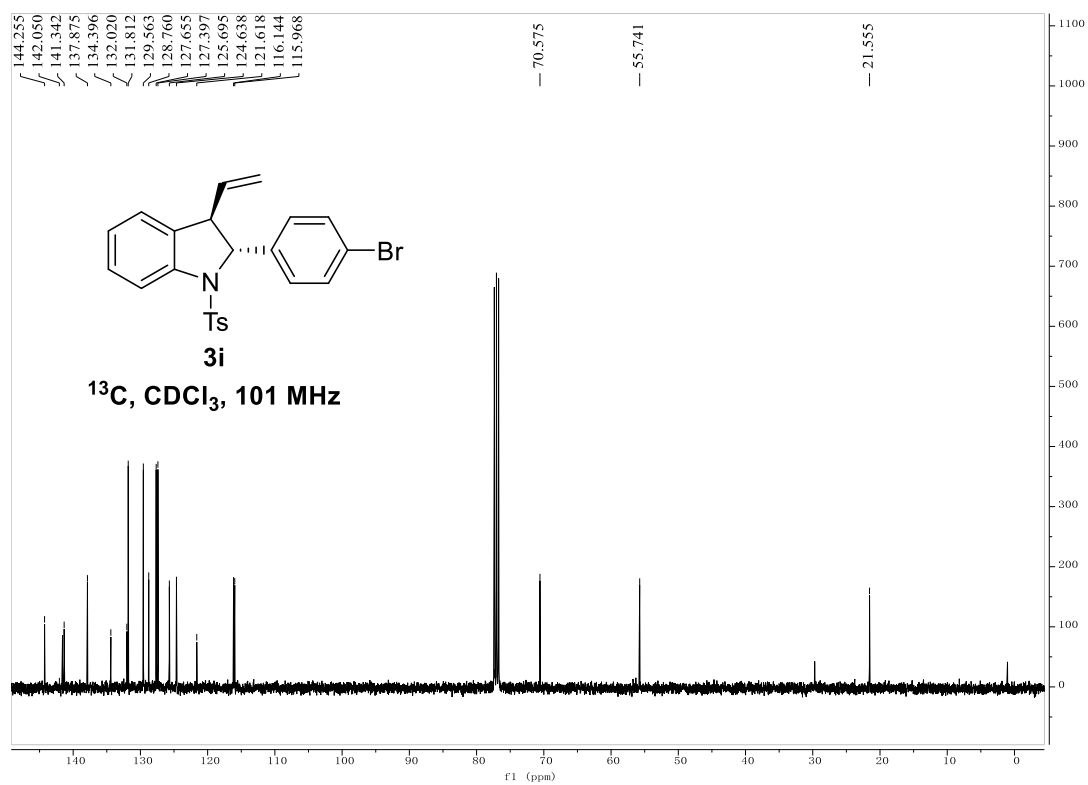
(2R,3R)-2-(4-chlorophenyl)-1-tosyl-3-vinylindoline (3h)



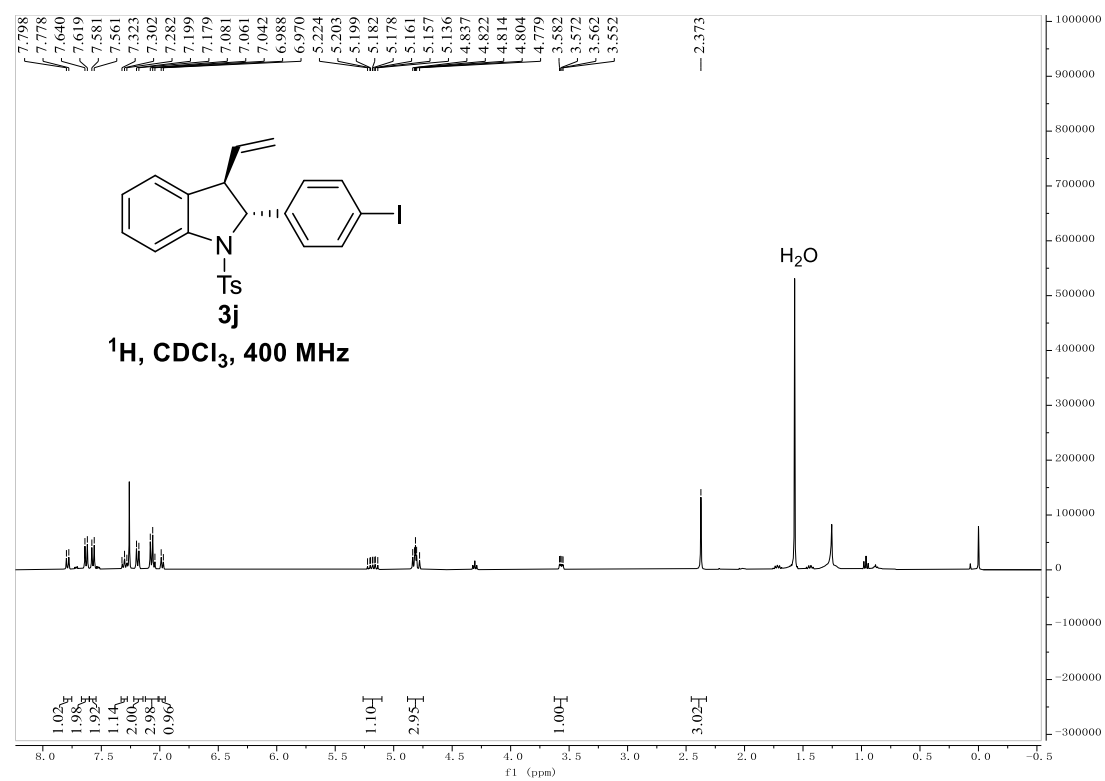


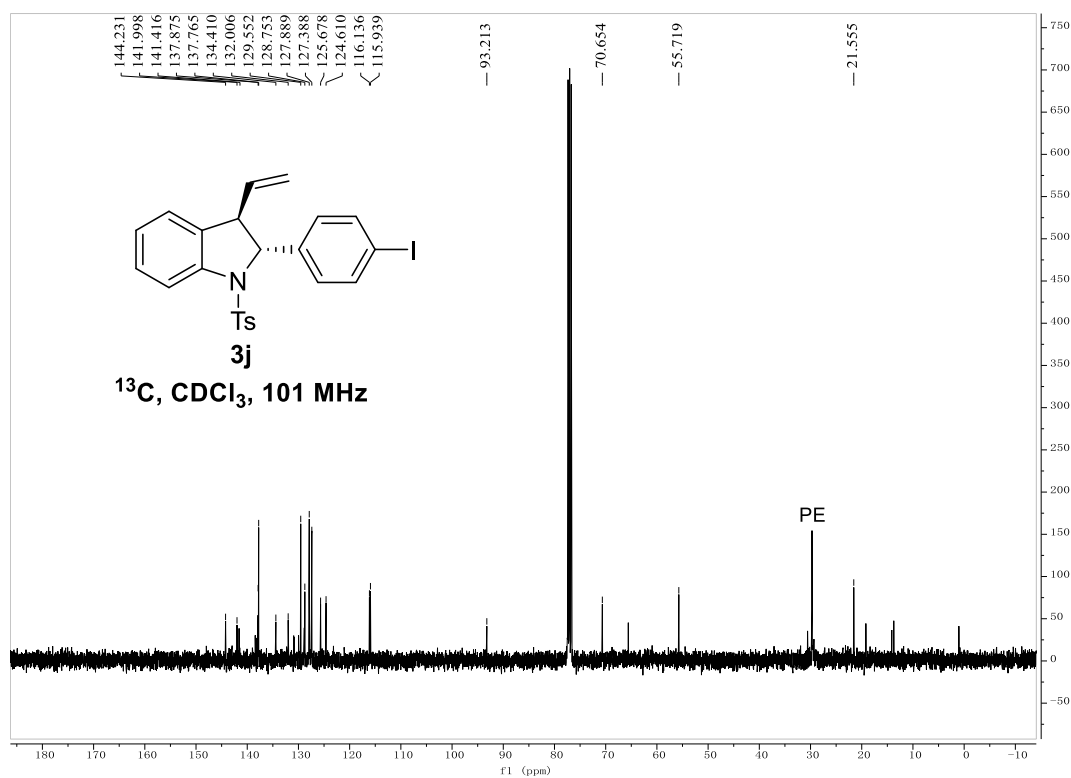
(2*R*,3*R*)-2-(4-bromophenyl)-1-tosyl-3-vinylindoline (3i)



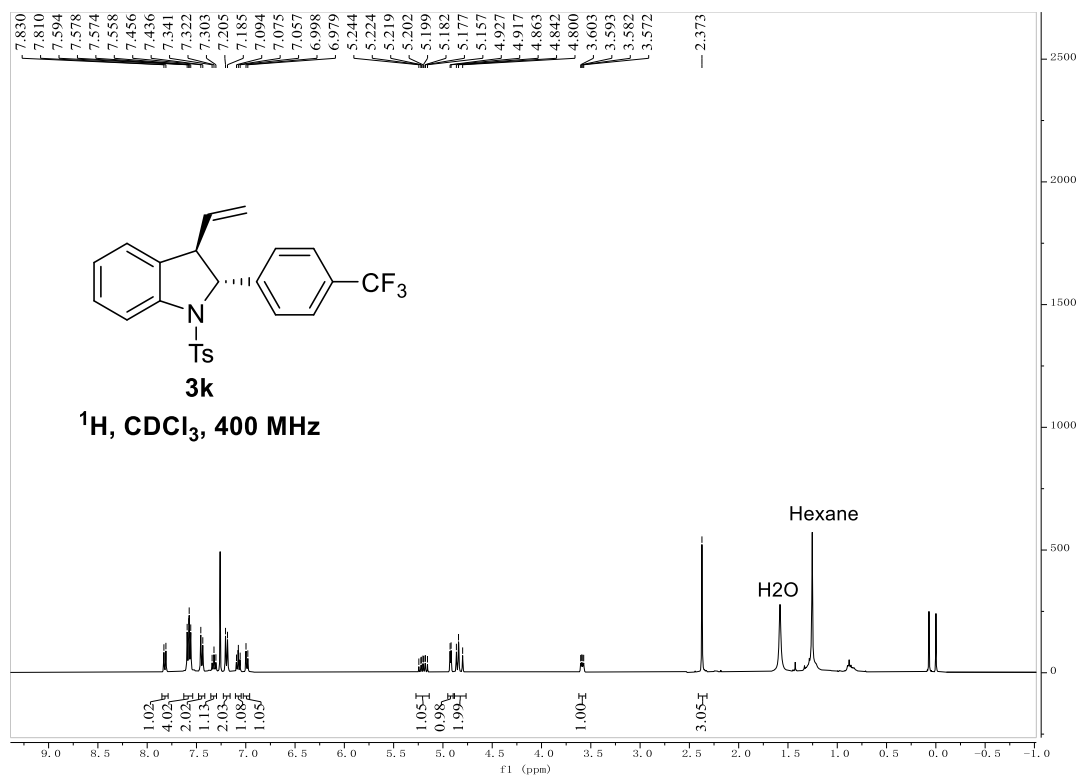


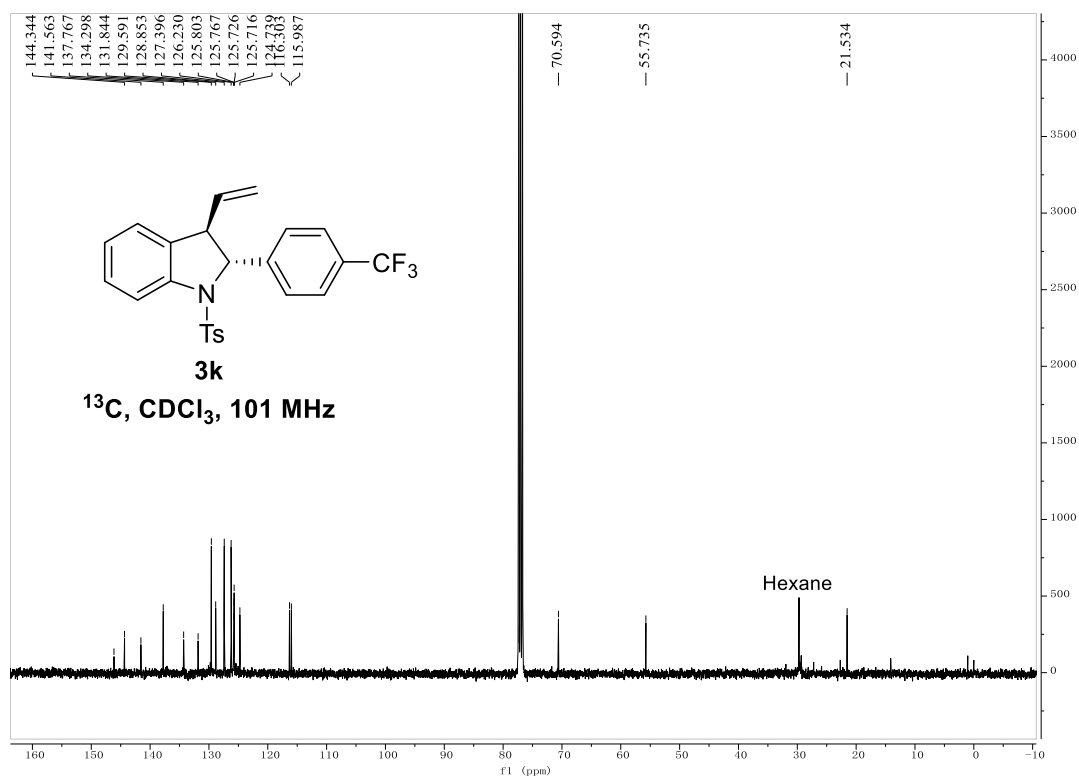
(2*R*,3*R*)-2-(4-iodophenyl)-1-tosyl-3-vinylindoline (3j)



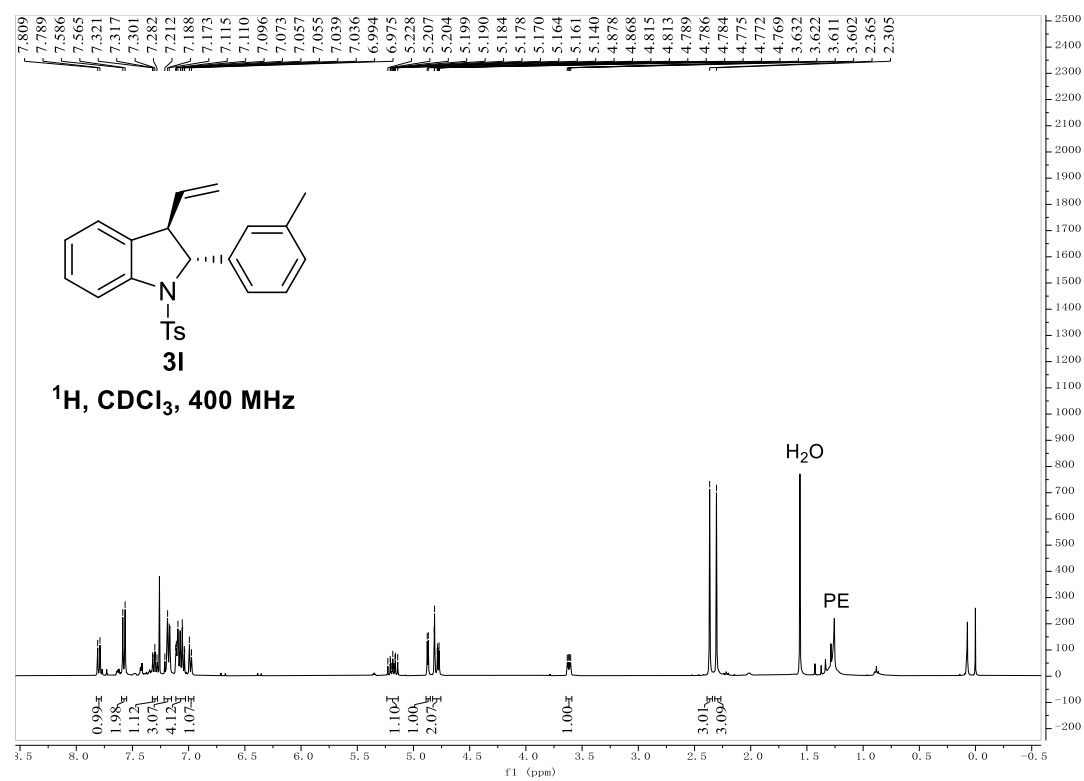


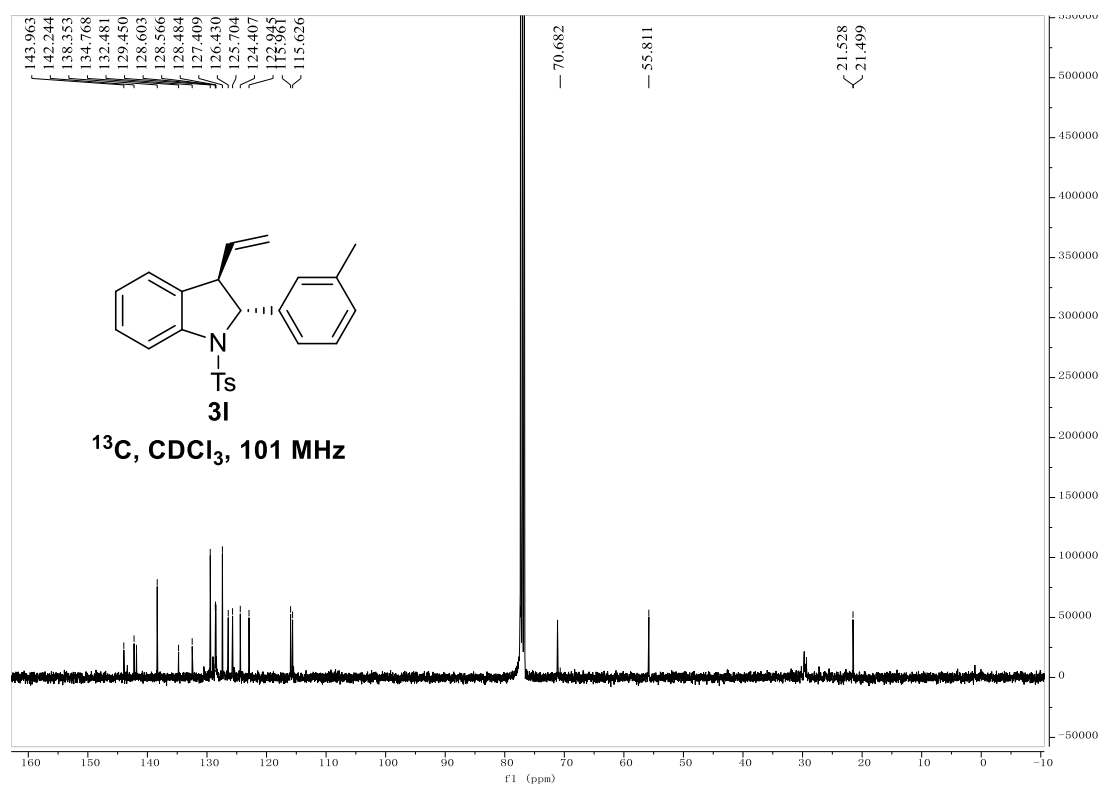
(2*R*,3*R*)-1-tosyl-2-(4-(trifluoromethyl)phenyl)-3-vinylindoline (3k)



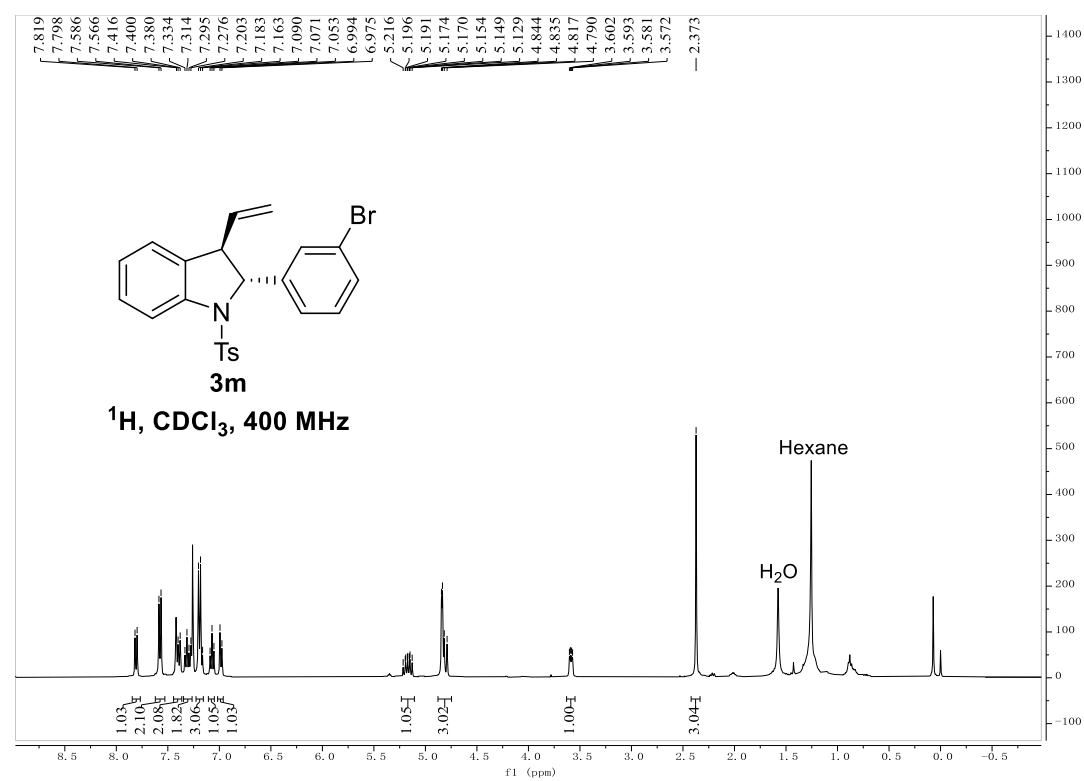


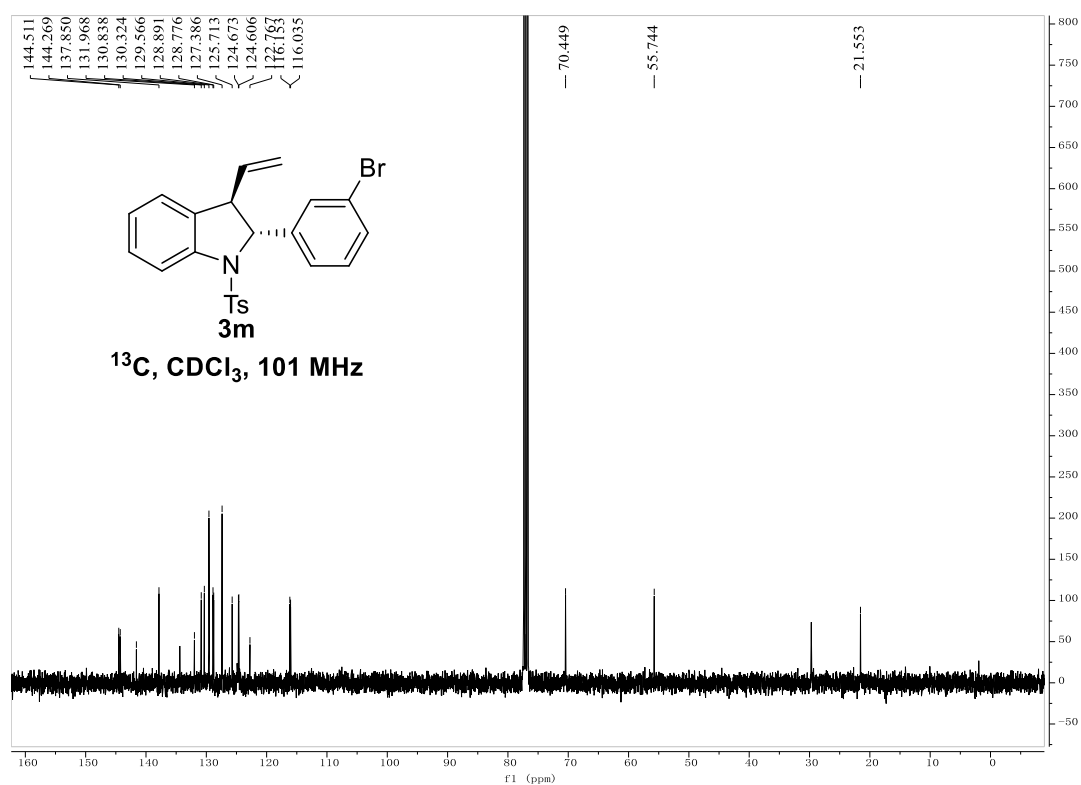
(2*R*,3*R*)-2-(*m*-tolyl)-1-tosyl-3-vinylindoline (3l)



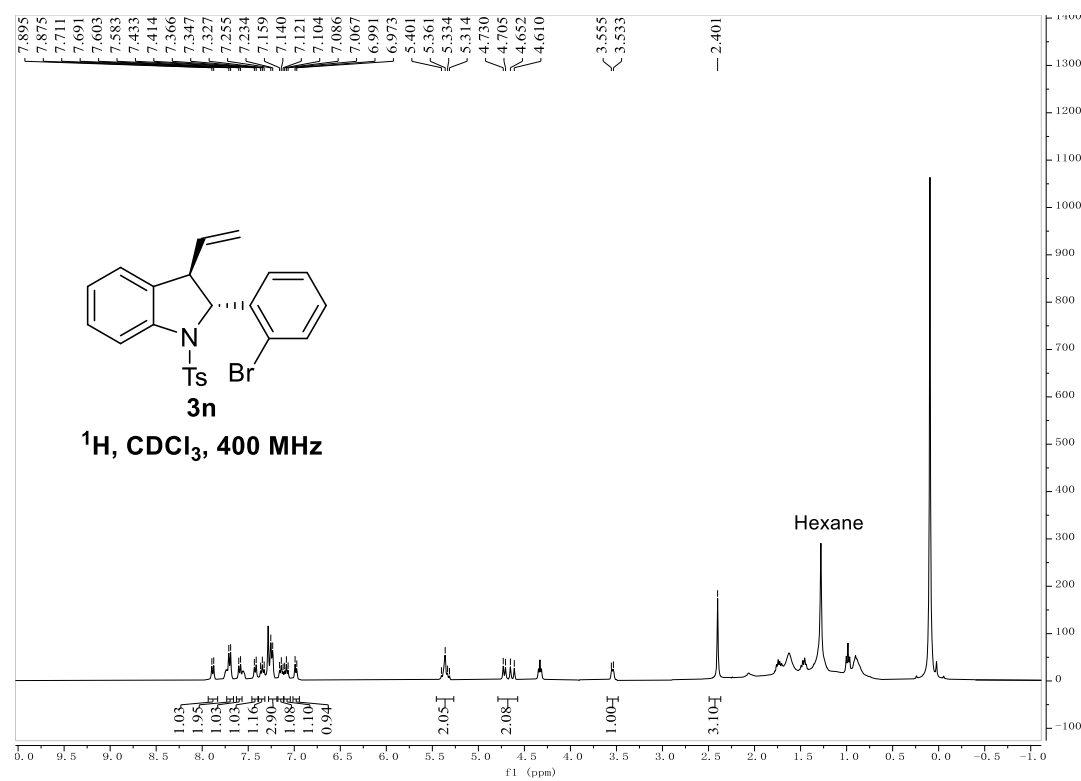


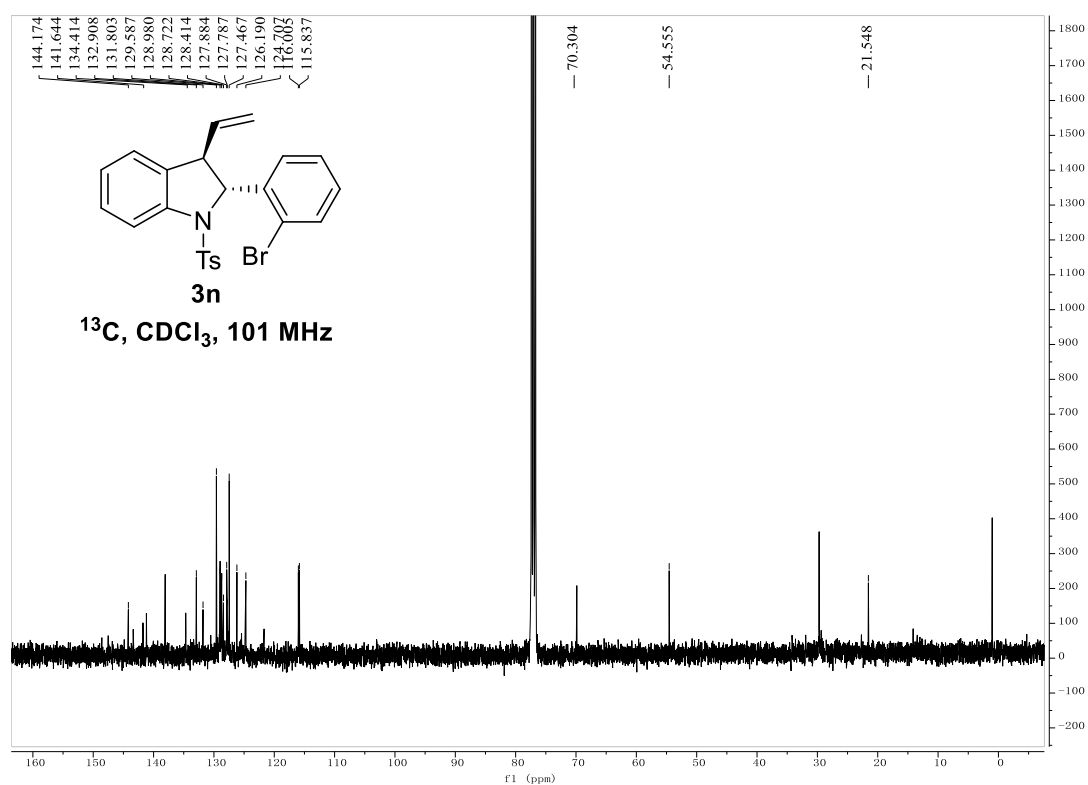
(2*R*,3*R*)-2-(3-bromophenyl)-1-tosyl-3-vinylindoline (3m)



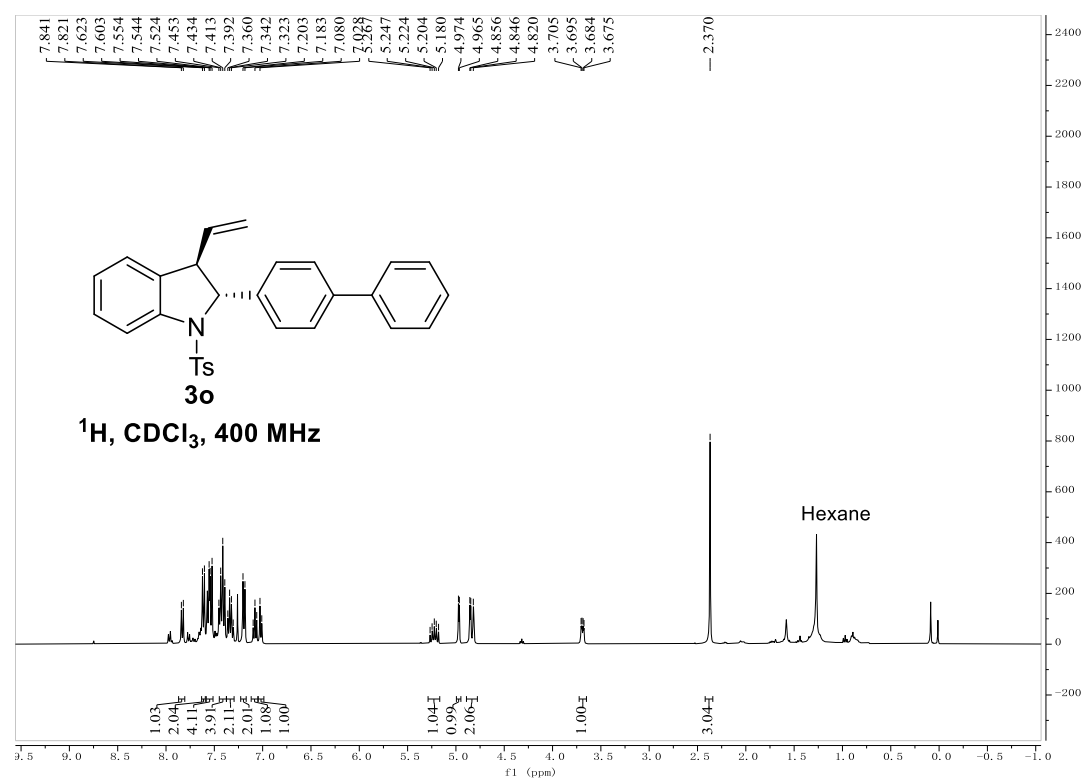


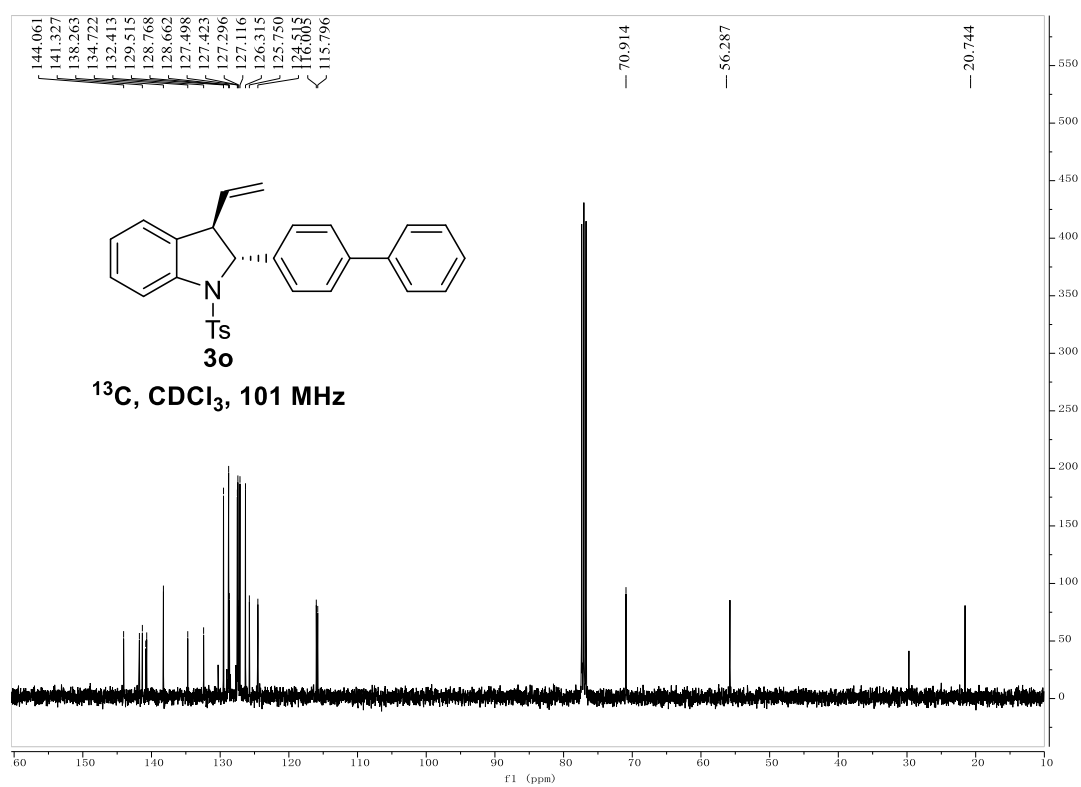
(2*R*,3*R*)-2-(2-bromophenyl)-1-tosyl-3-vinylindoline (3n**)**



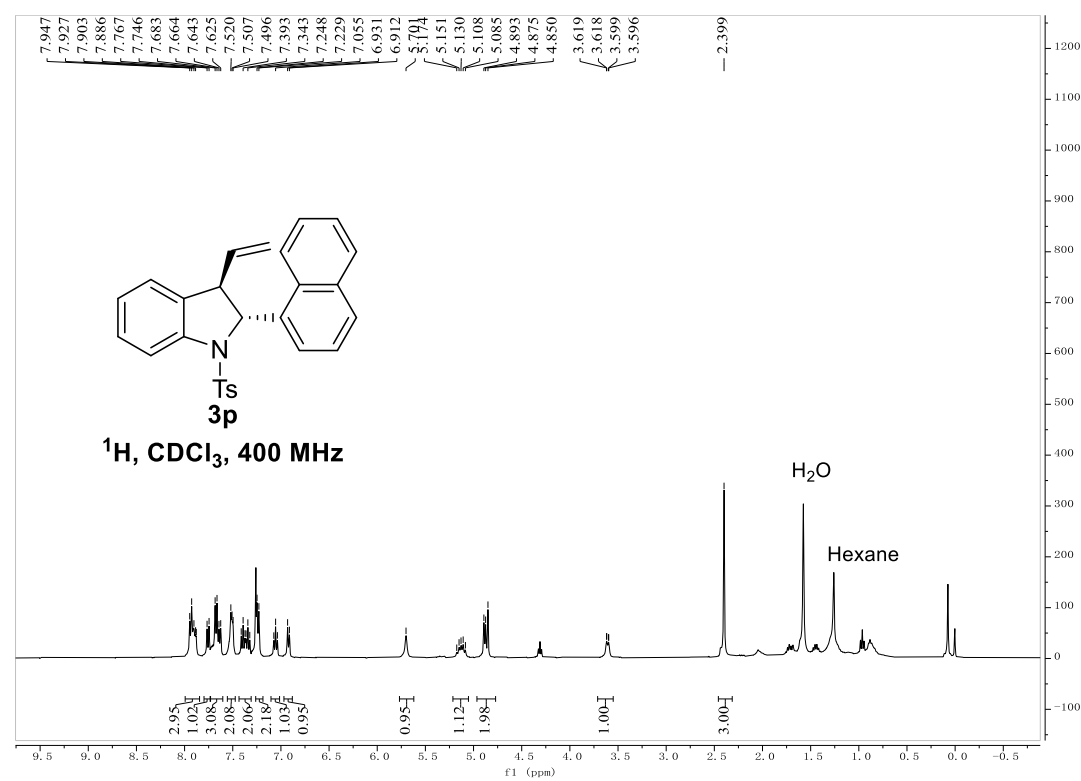


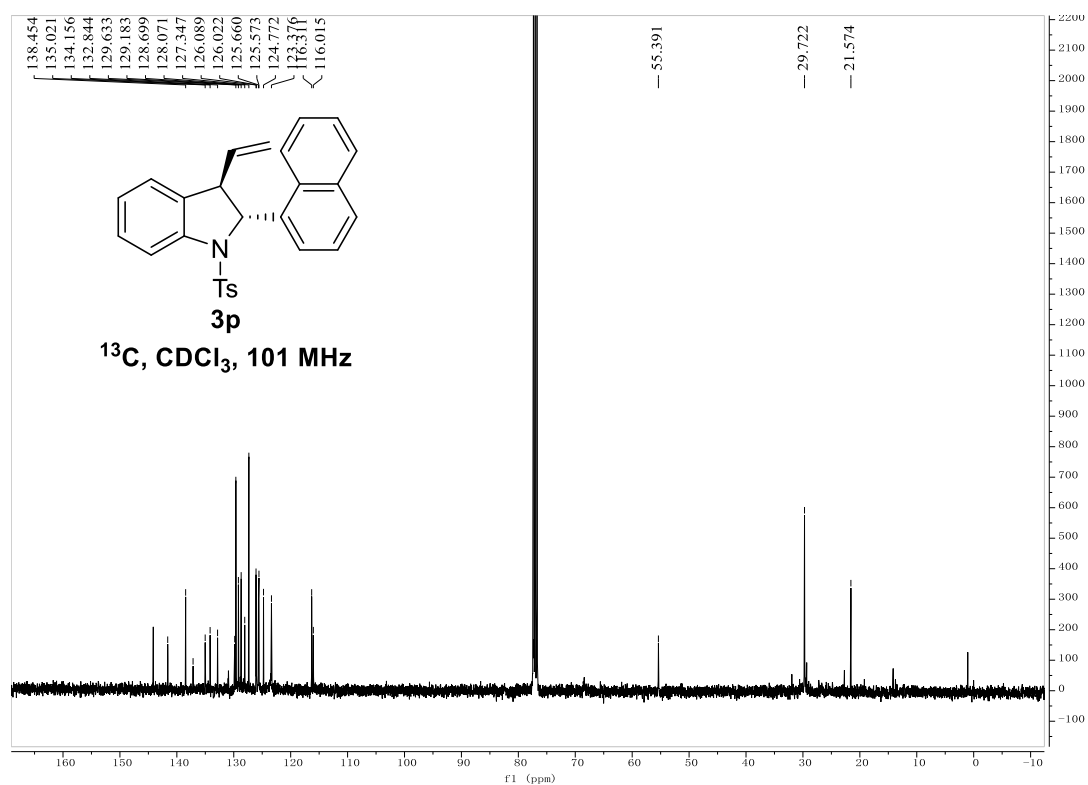
(2*R*,3*R*)-2-([1,1'-biphenyl]-4-yl)-1-tosyl-3-vinylindoline (3o)



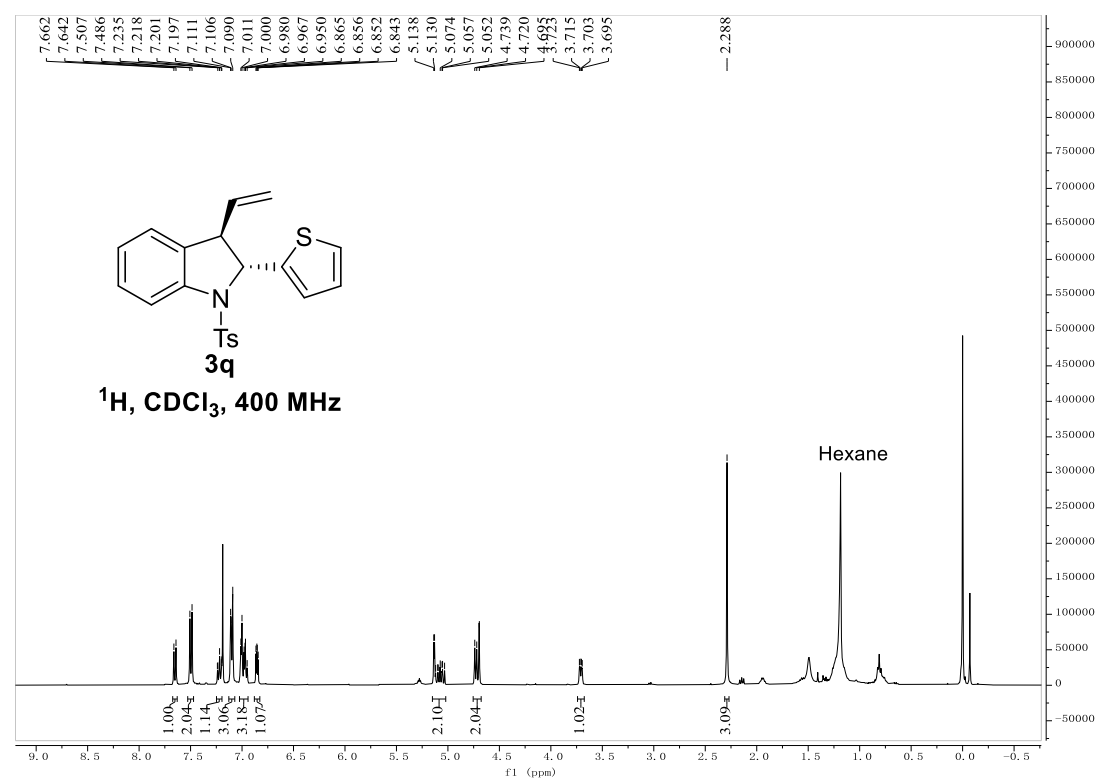


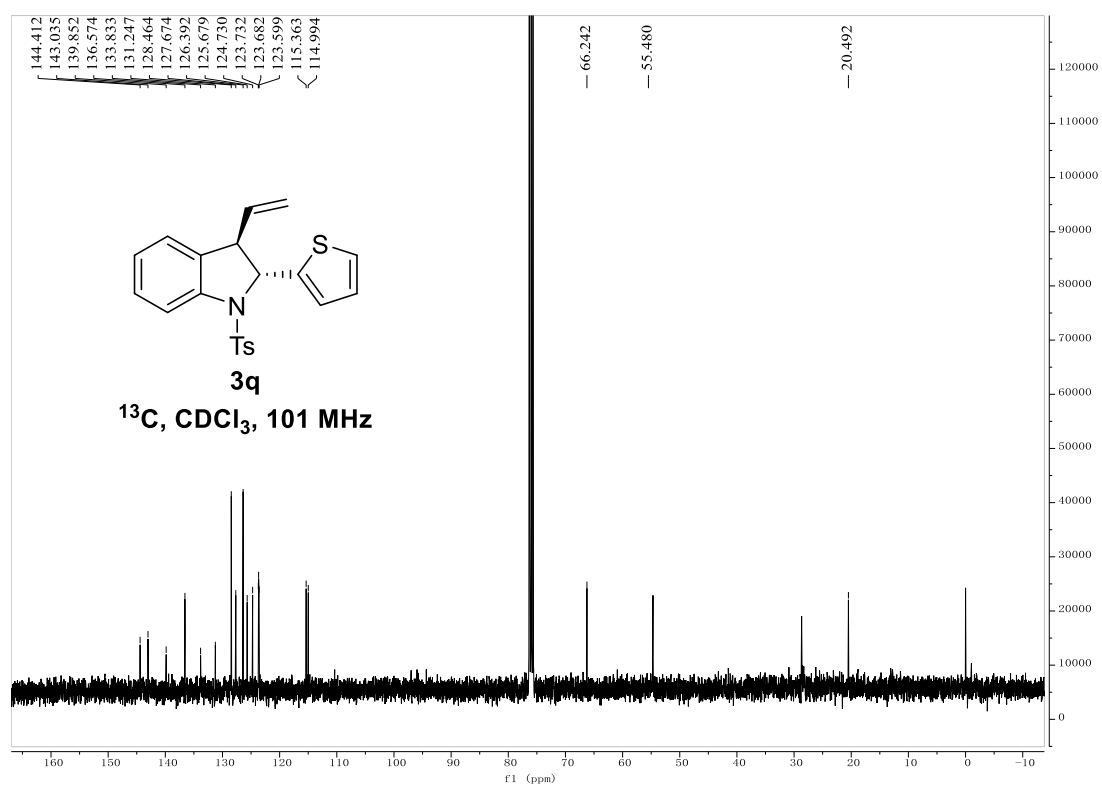
(2R,3R)-2-(naphthalen-1-yl)-1-tosyl-3-vinylindoline (3p)



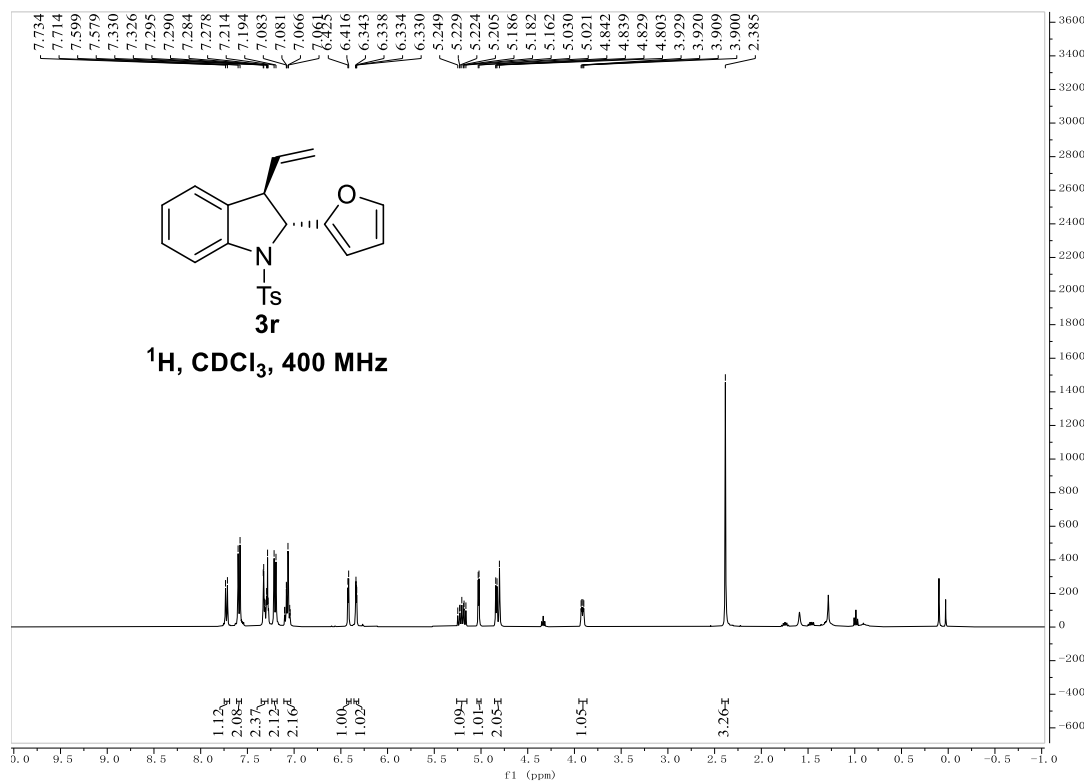


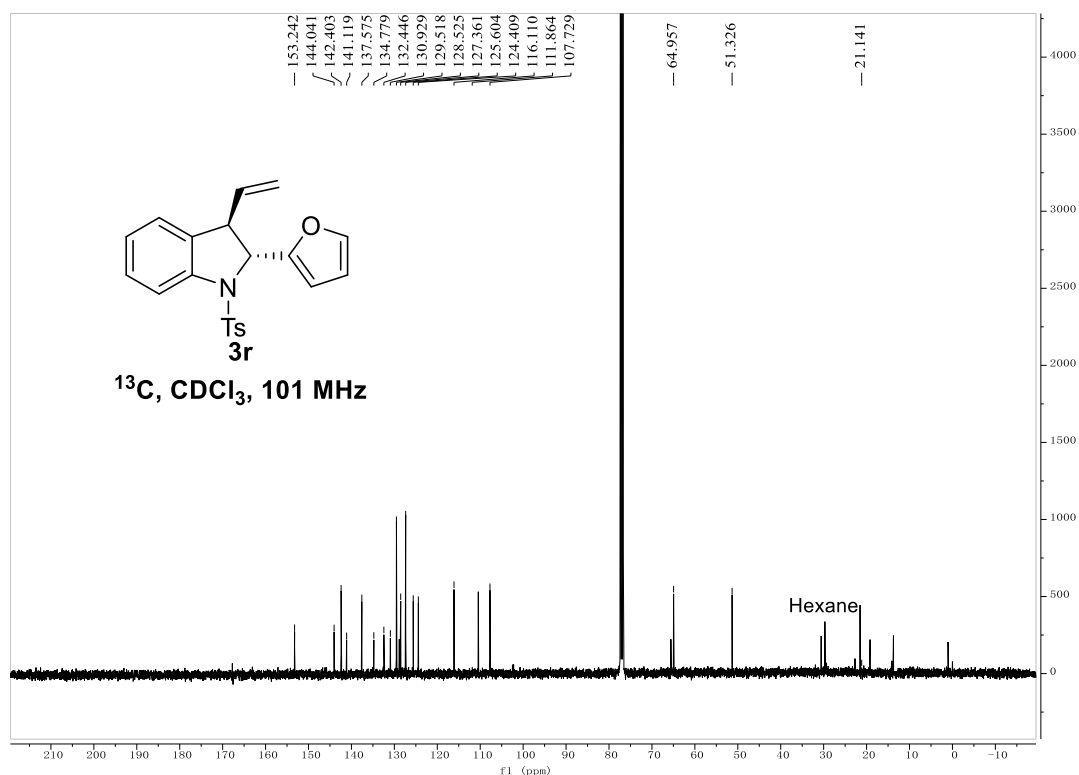
(2*R*,3*R*)-2-(thiophen-2-yl)-1-tosyl-3-vinylindoline (3q)



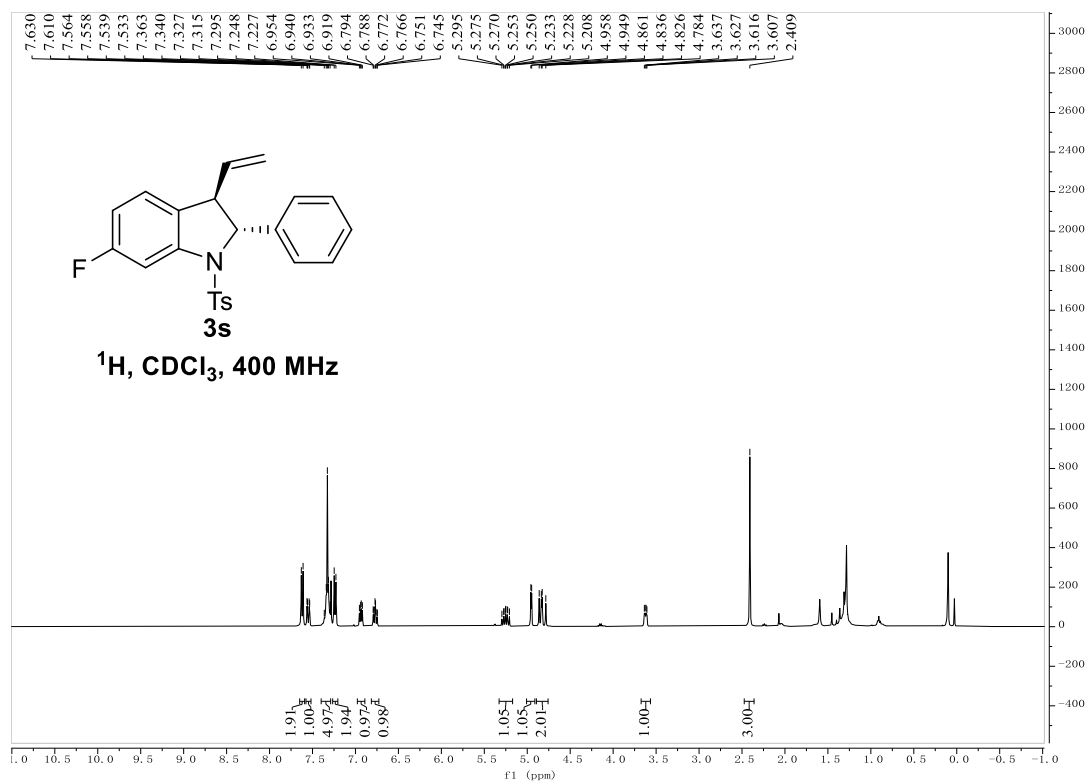


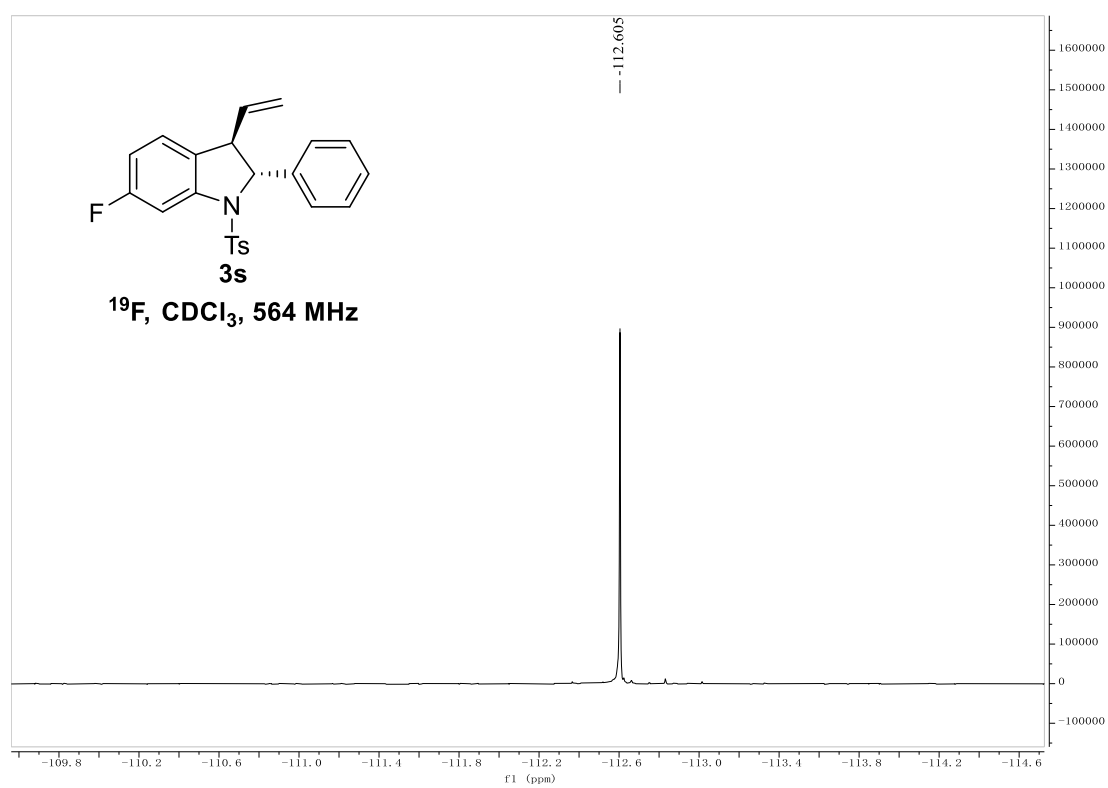
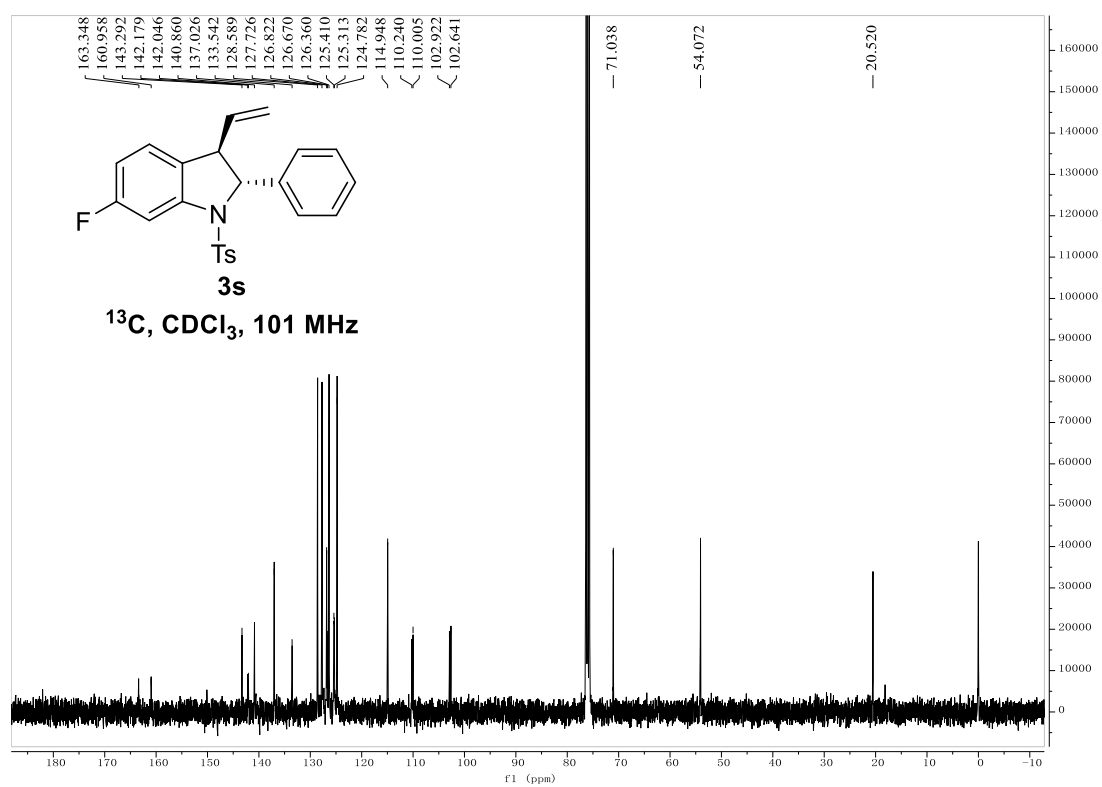
(2*R*,3*R*)-2-(furan-2-yl)-1-tosyl-3-vinylindoline (3r)



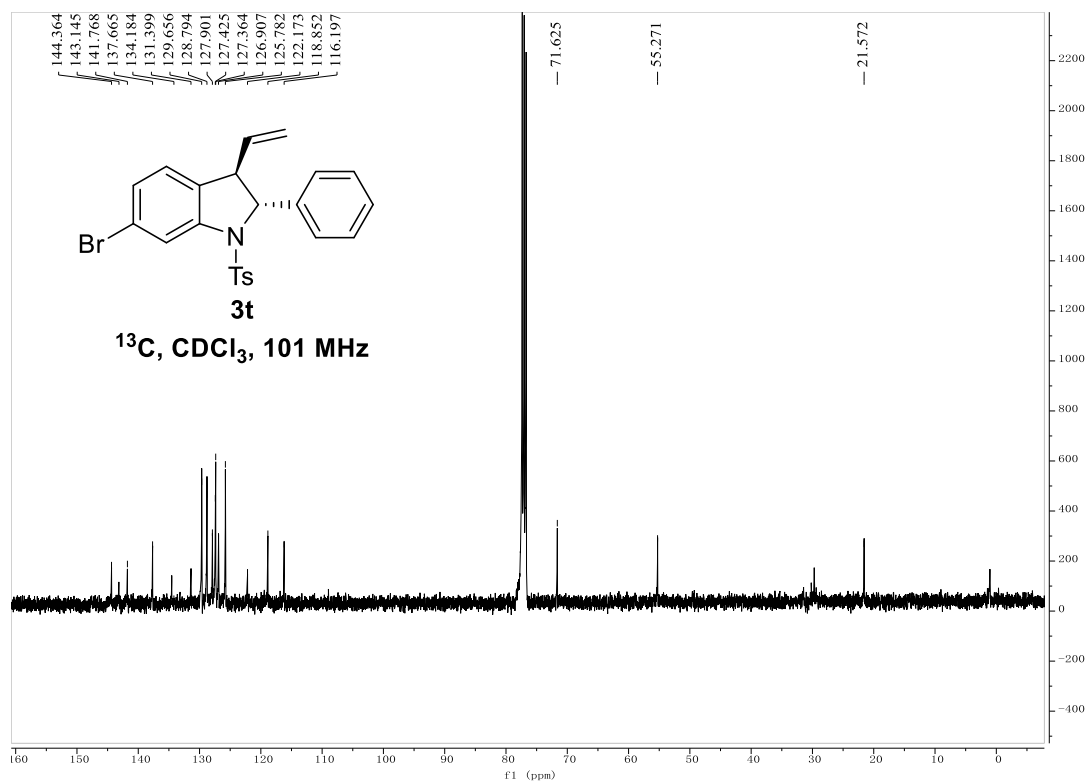
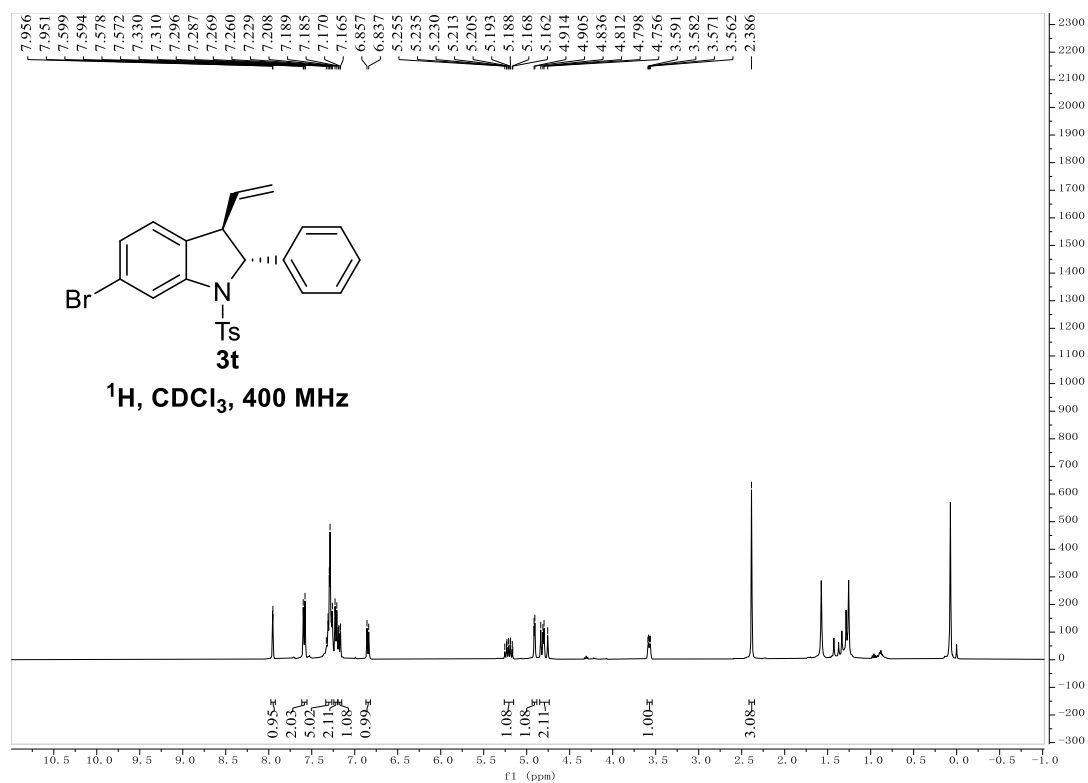


(2*R*,3*R*)-6-fluoro-2-phenyl-1-tosyl-3-vinylindoline (3s)

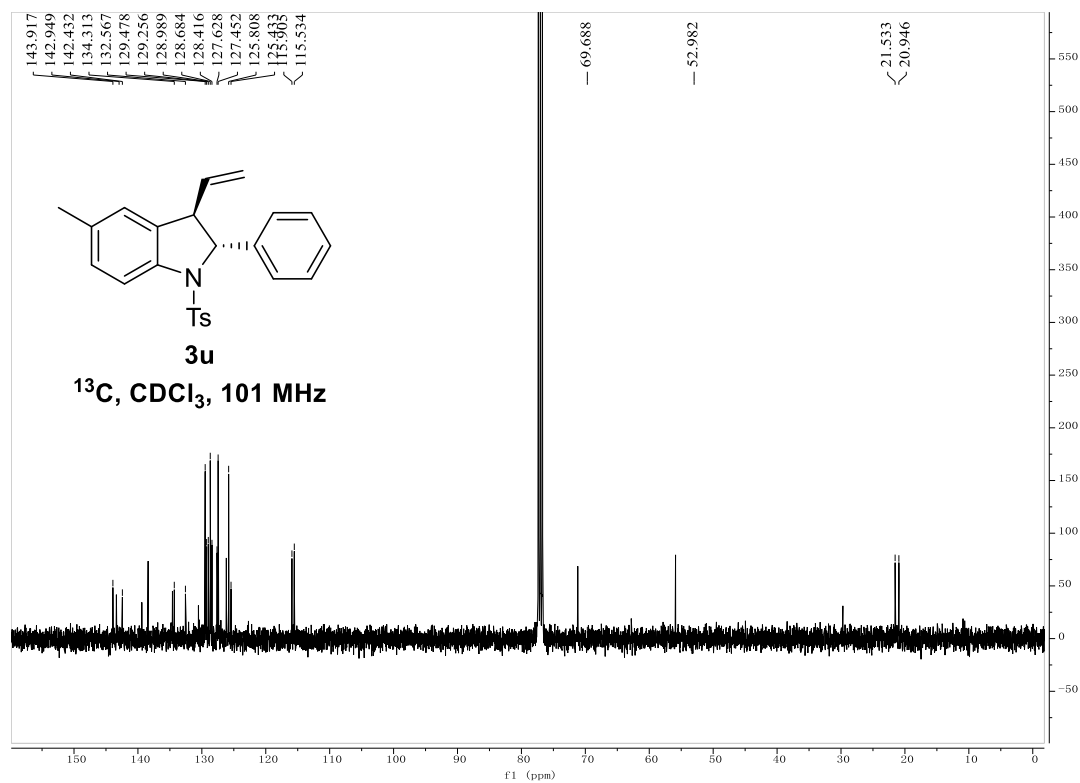
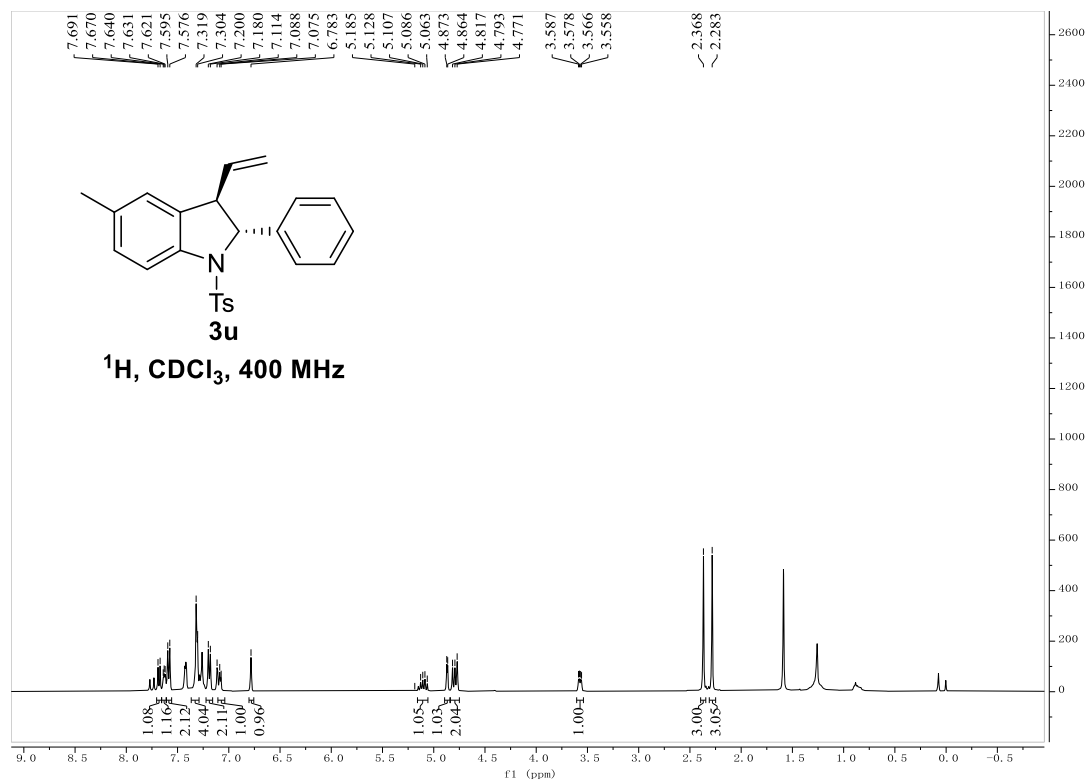




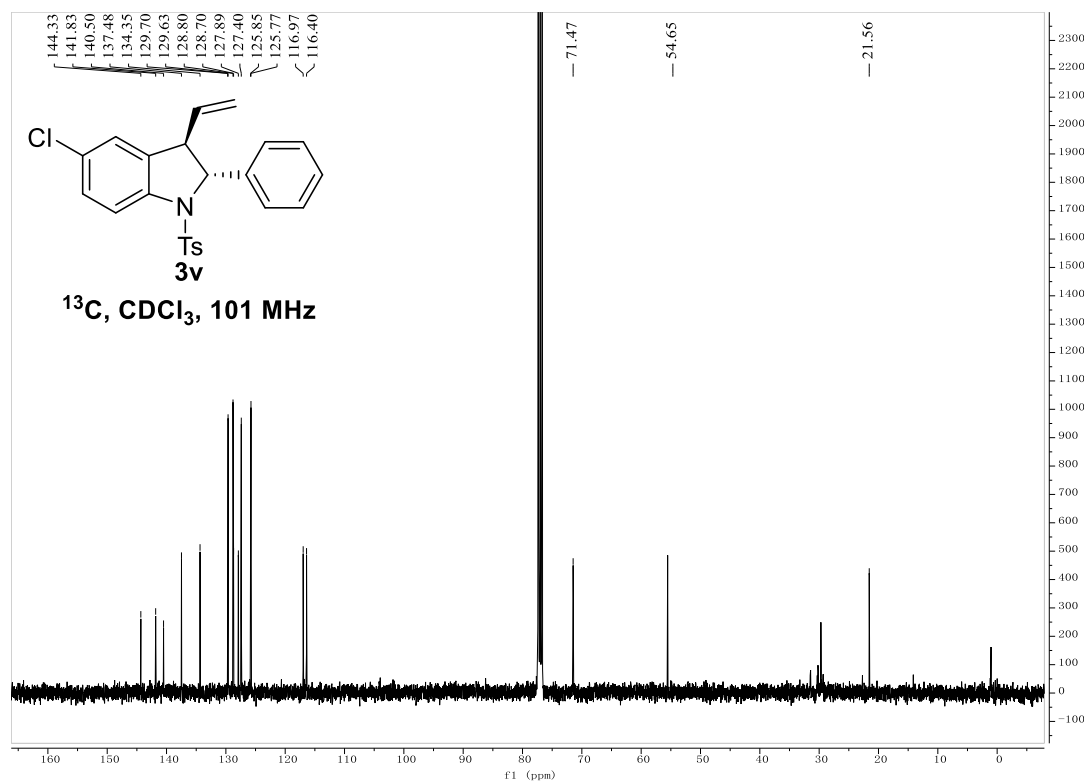
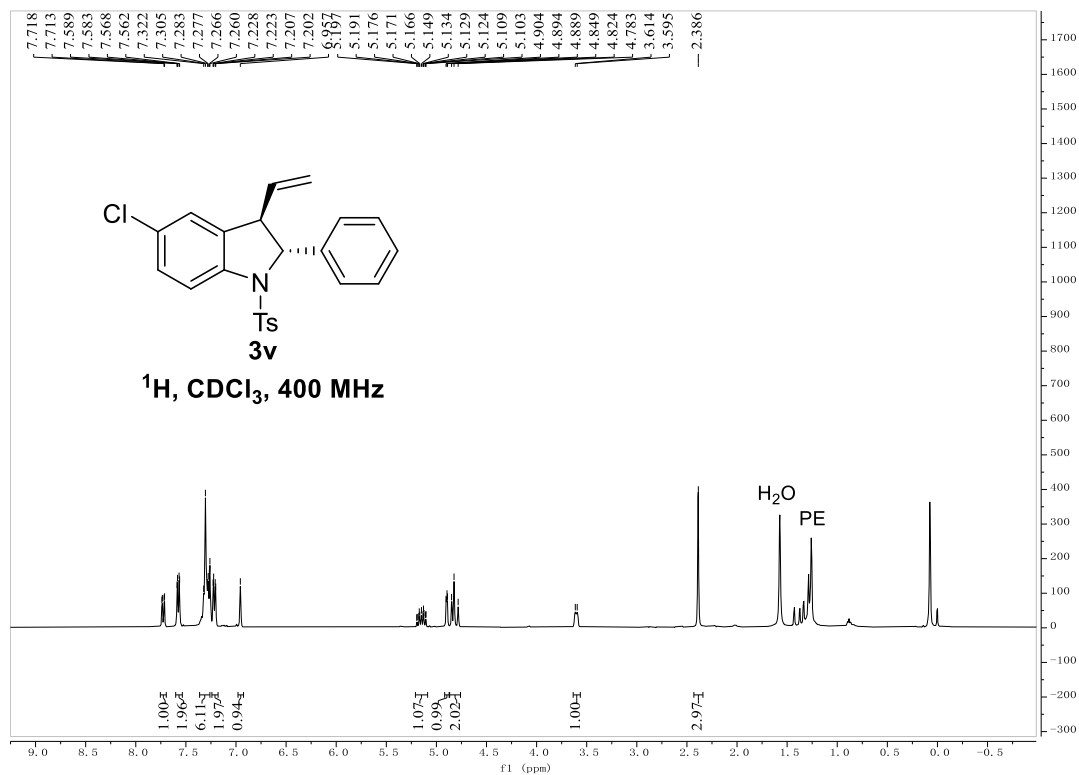
(2*R*,3*R*)-6-bromo-2-phenyl-1-tosyl-3-vinylindoline (3t)



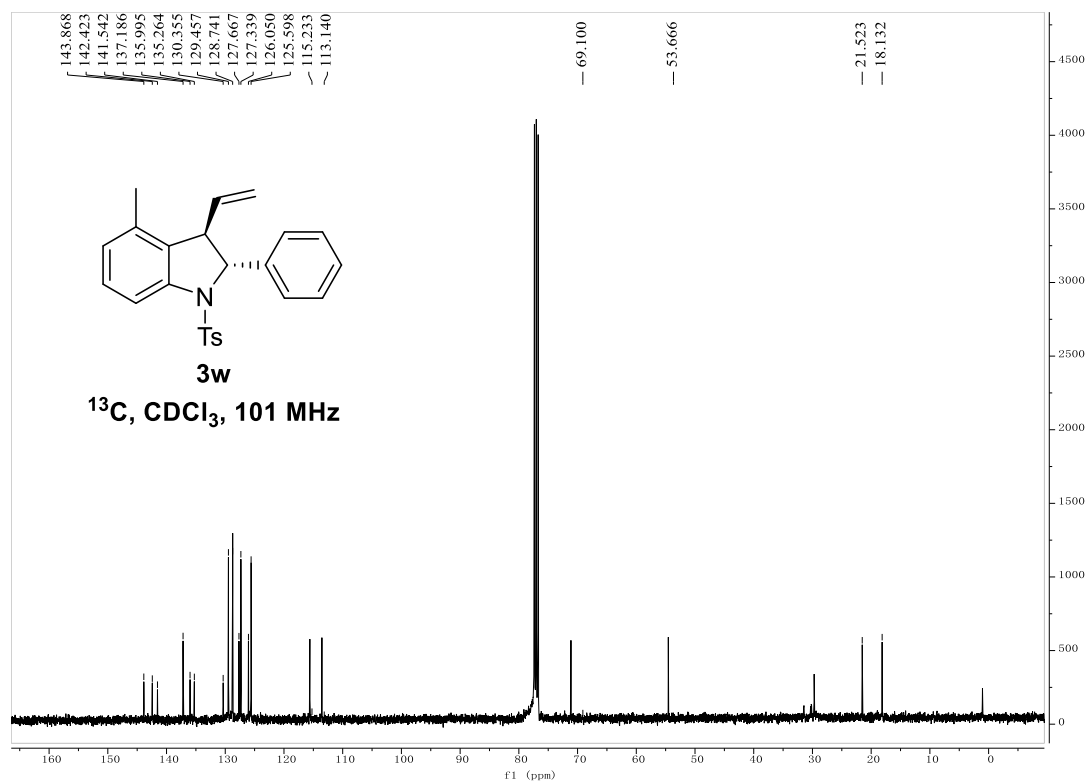
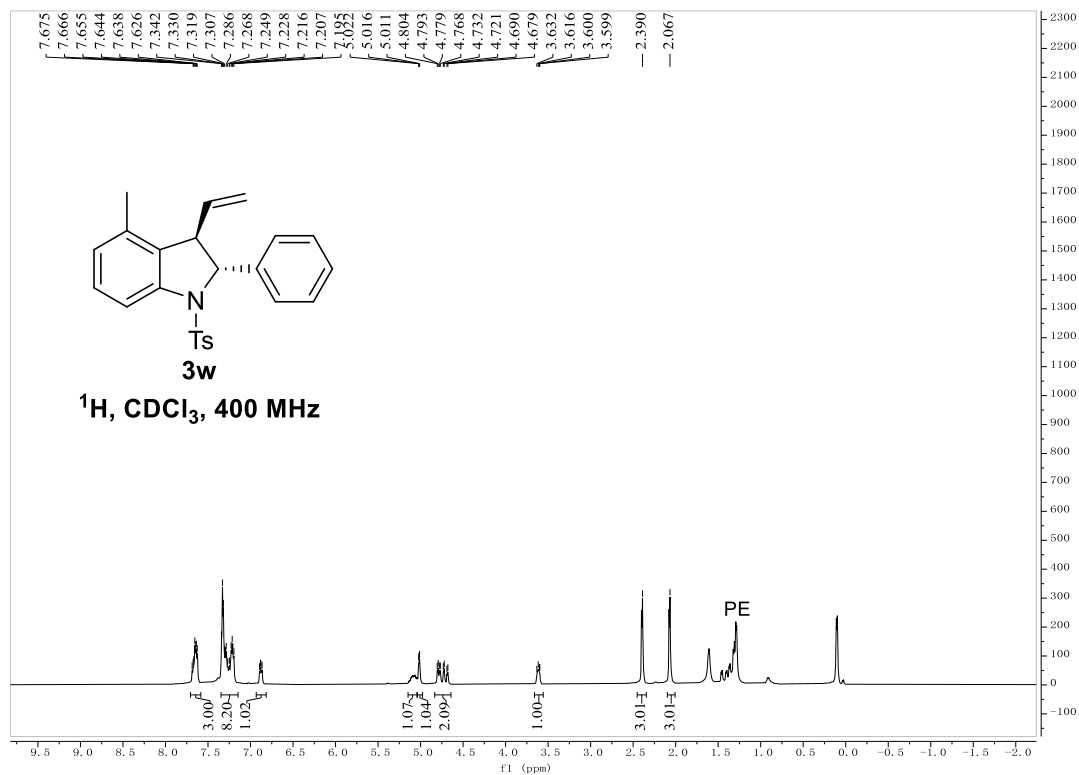
(2*R*,3*R*)-5-methyl-2-phenyl-1-tosyl-3-vinylindoline (3u)



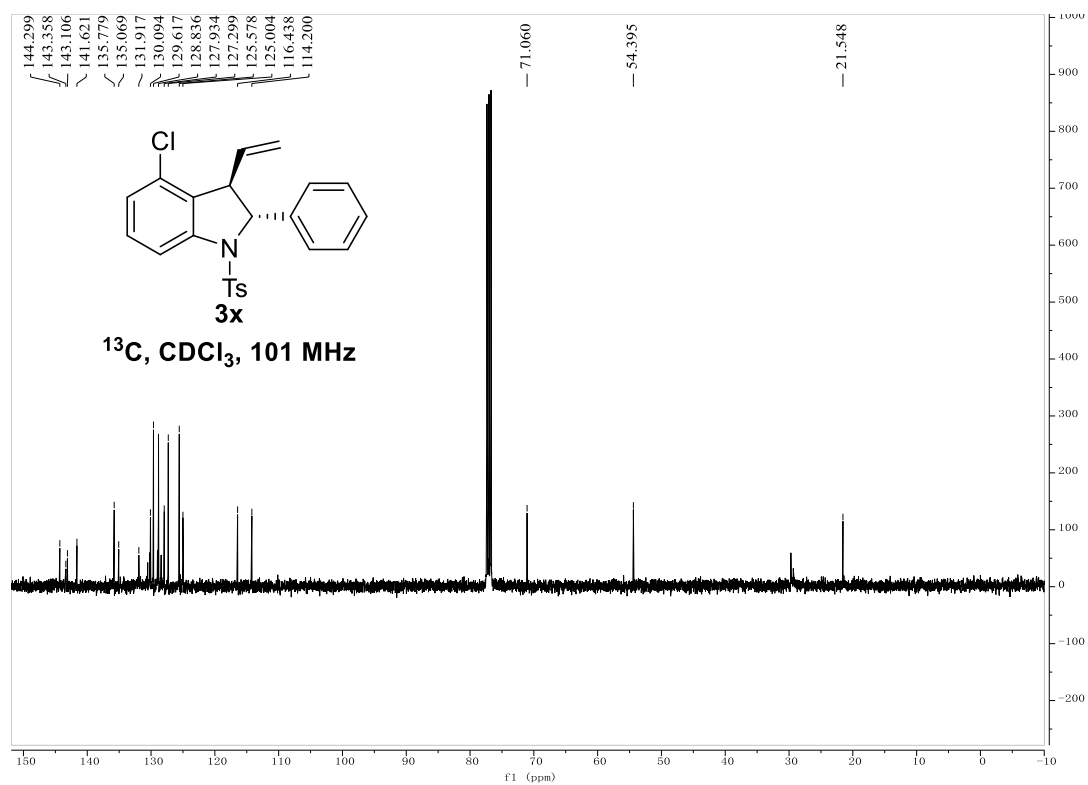
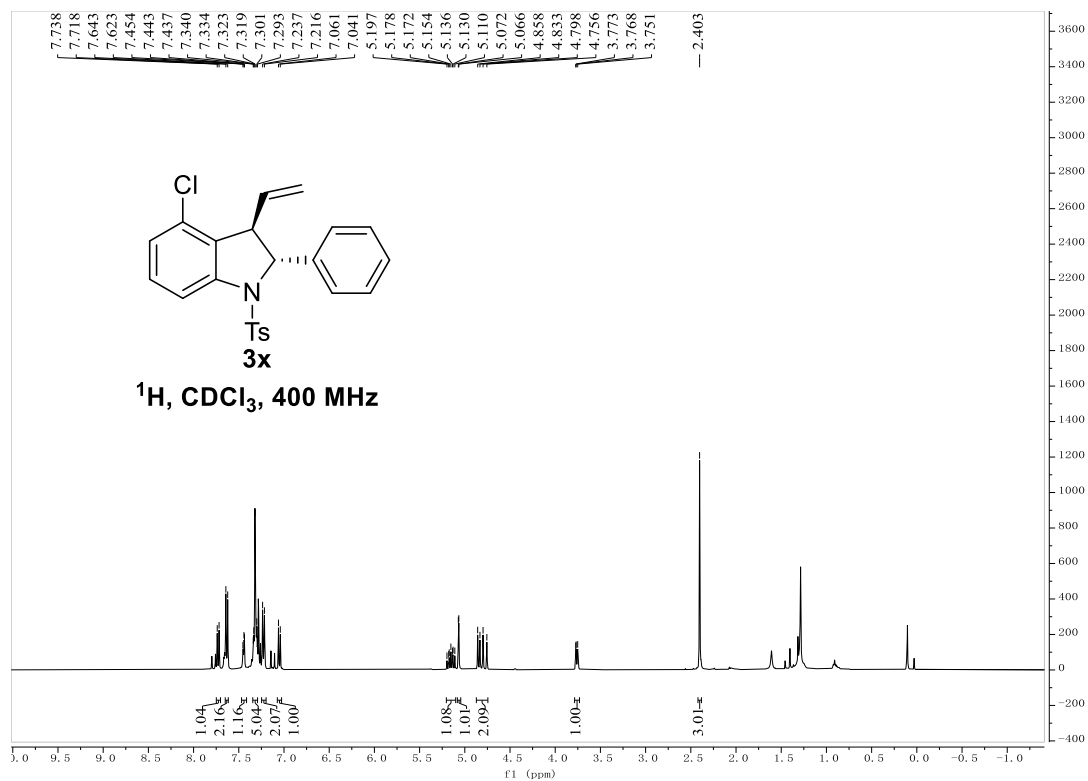
(2*R*,3*R*)-5-chloro-2-phenyl-1-tosyl-3-vinylindoline (3v)



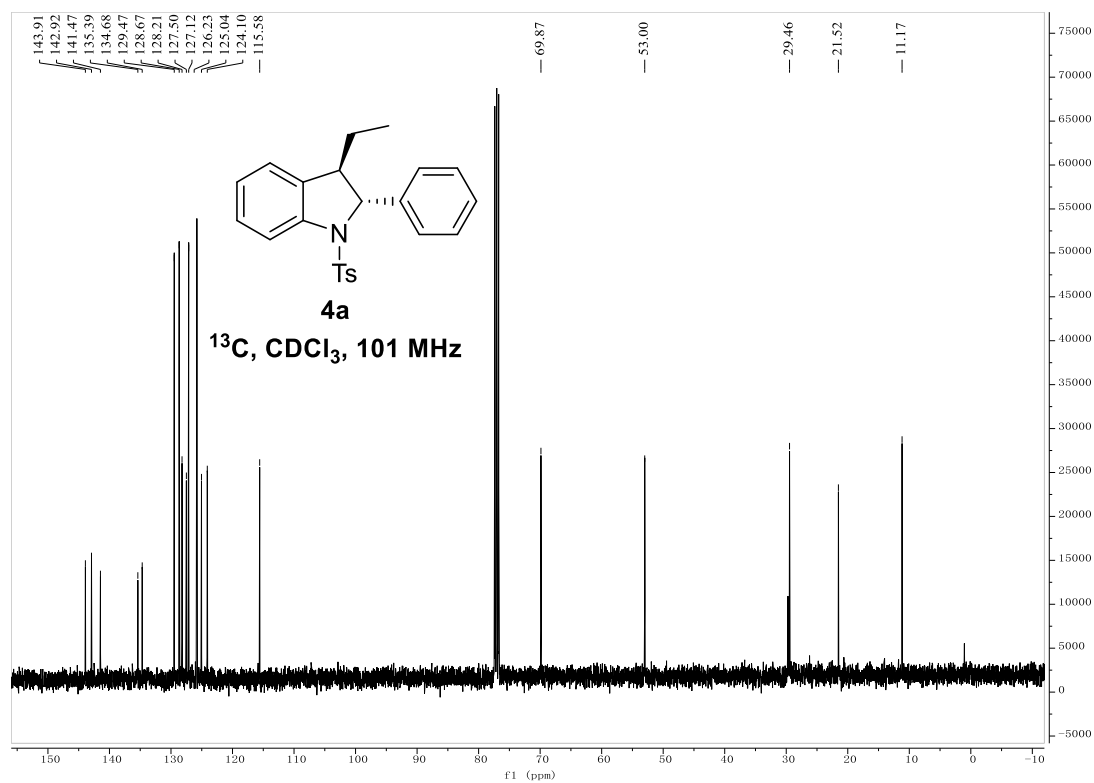
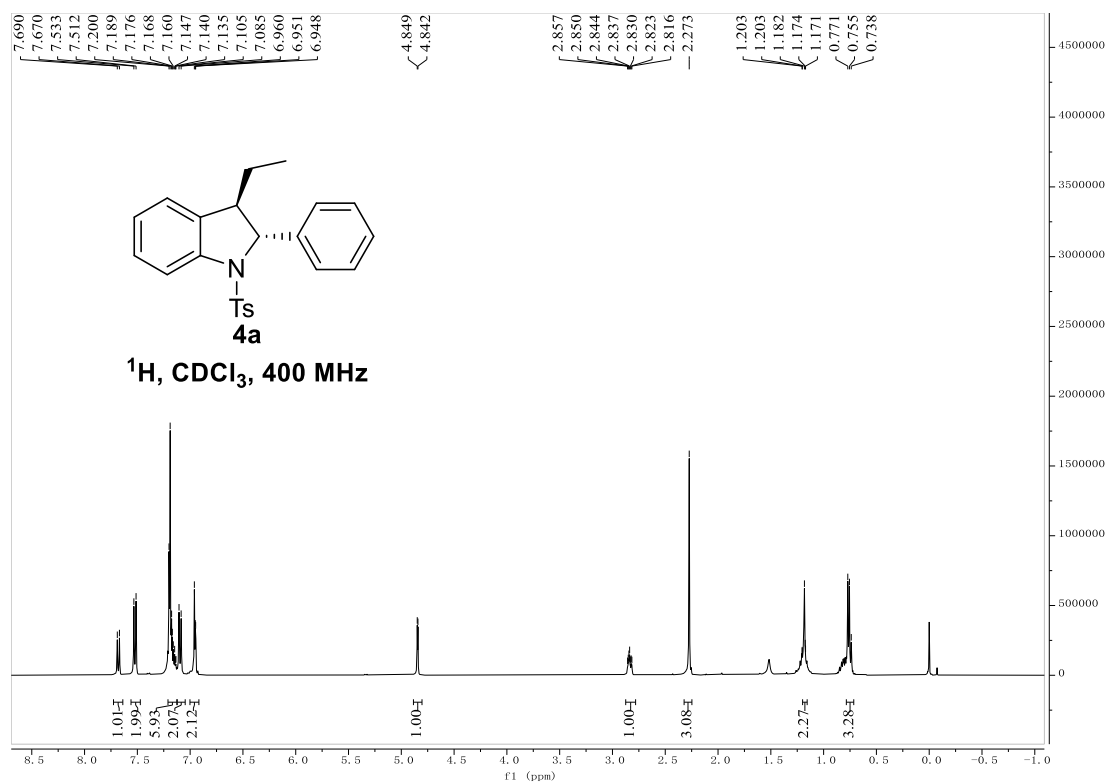
(2*R*,3*R*)-4-methyl-2-phenyl-1-tosyl-3-vinylindoline (3w)



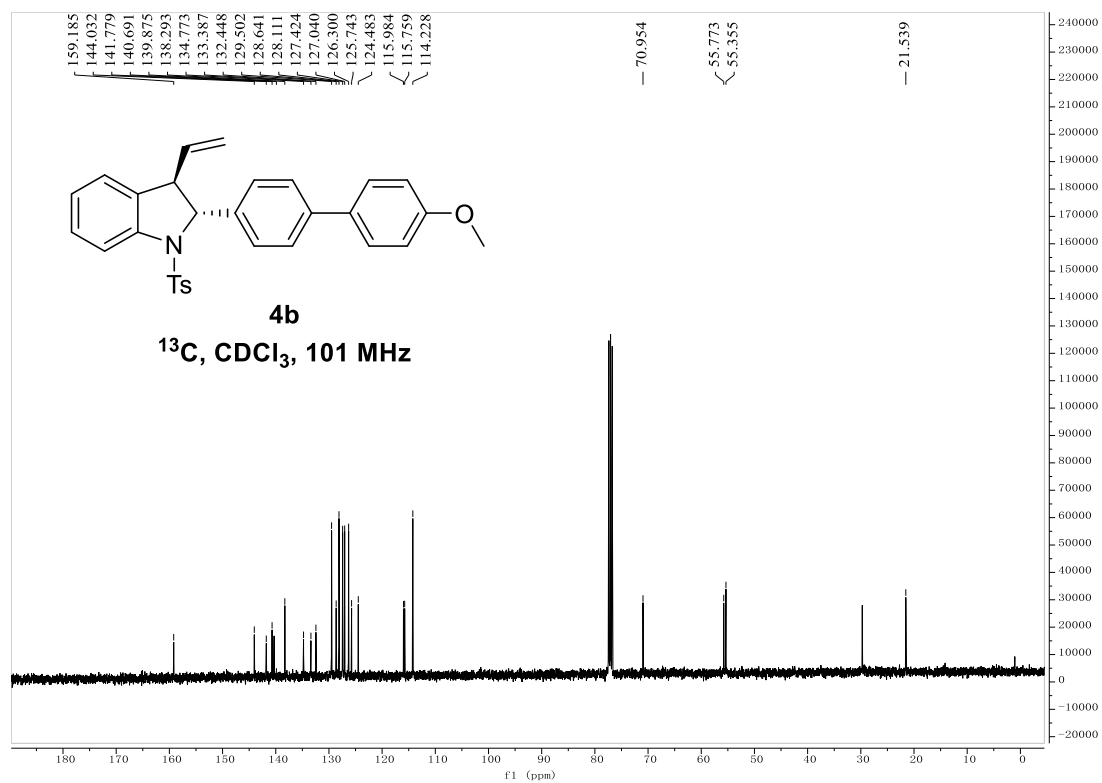
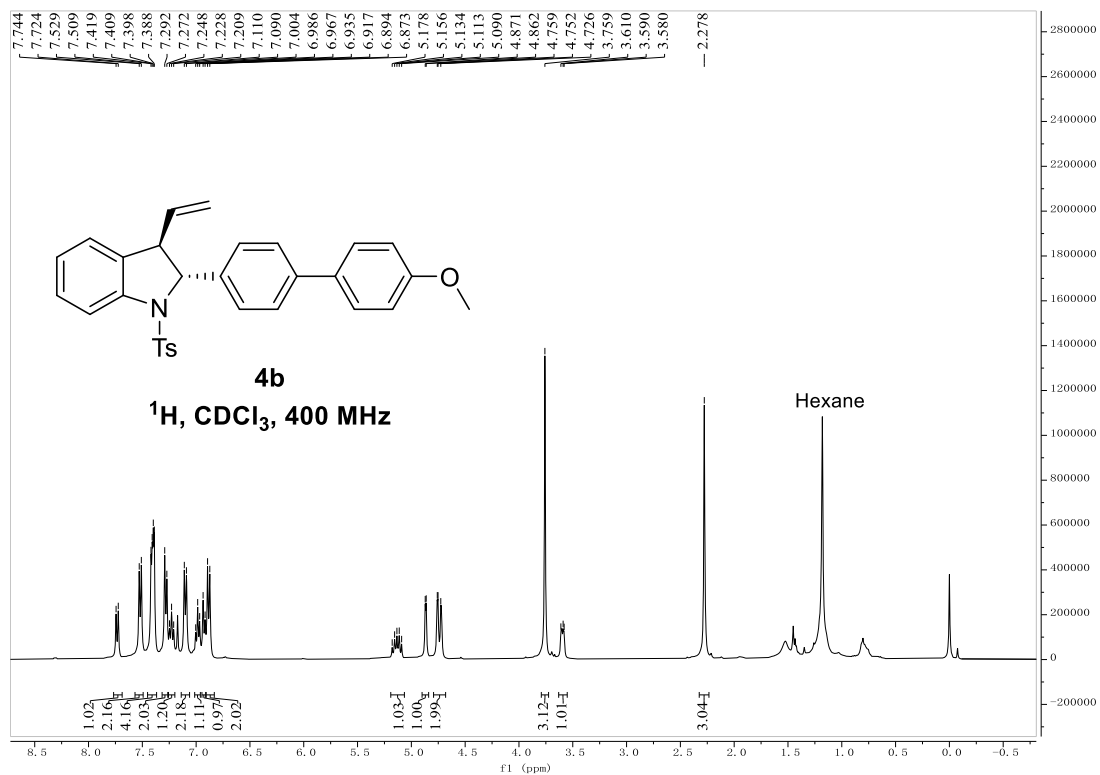
(2*R*,3*R*)-4-chloro-2-phenyl-1-tosyl-3-vinylindoline (3x)



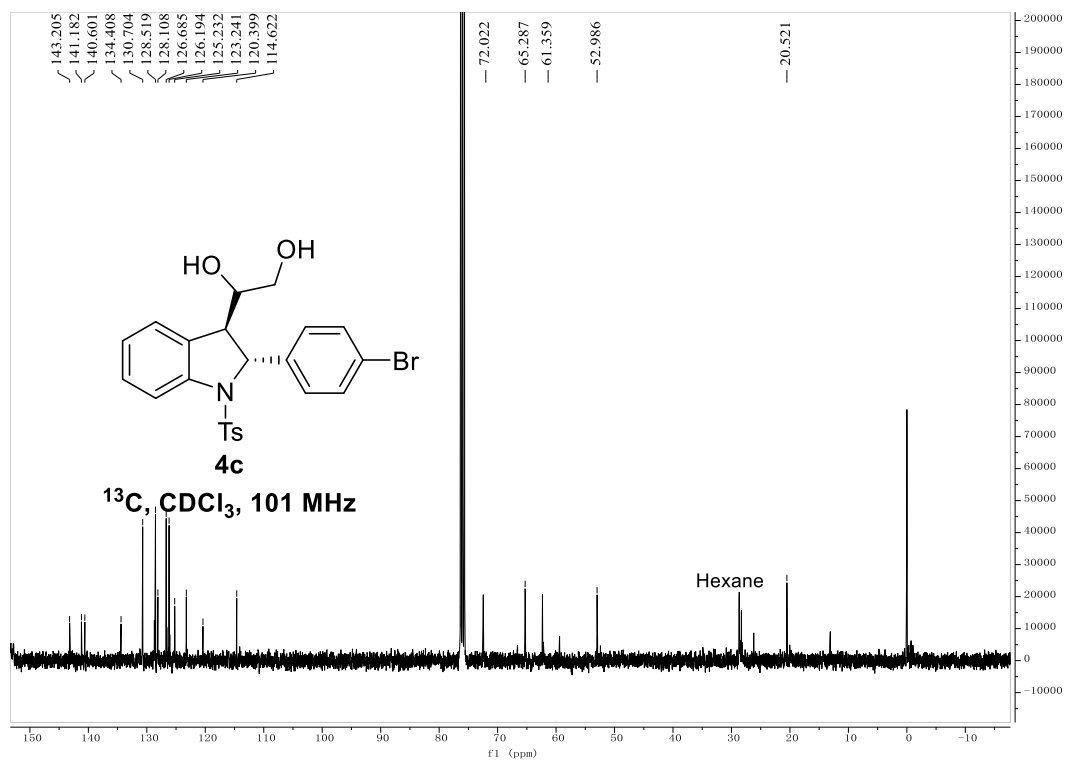
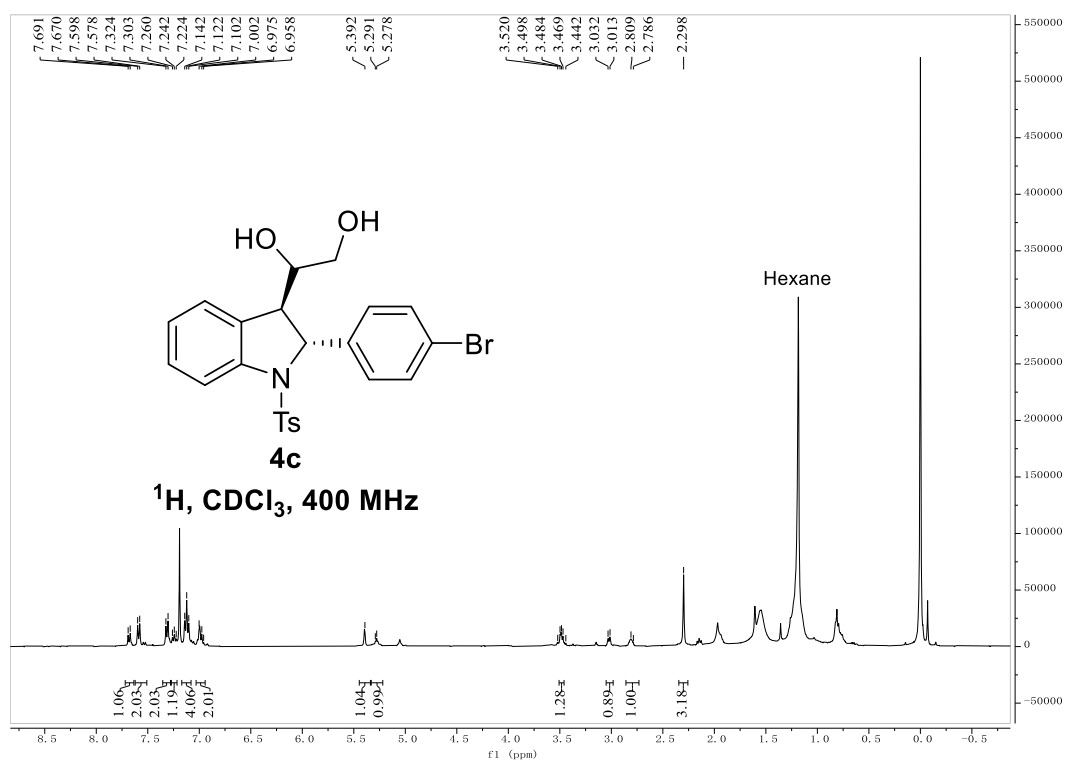
(2*R*,3*R*)-3-ethyl-2-phenyl-1-tosylindoline (4a)



(2*R*,3*R*)-2-(4'-methoxy-[1,1'-biphenyl]-4-yl)-1-tosyl-3-vinylindoline (4b)

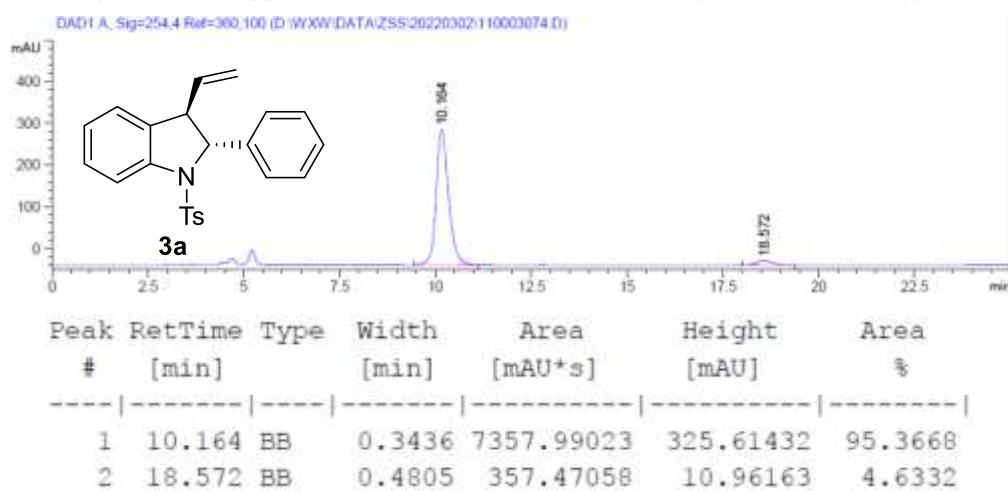
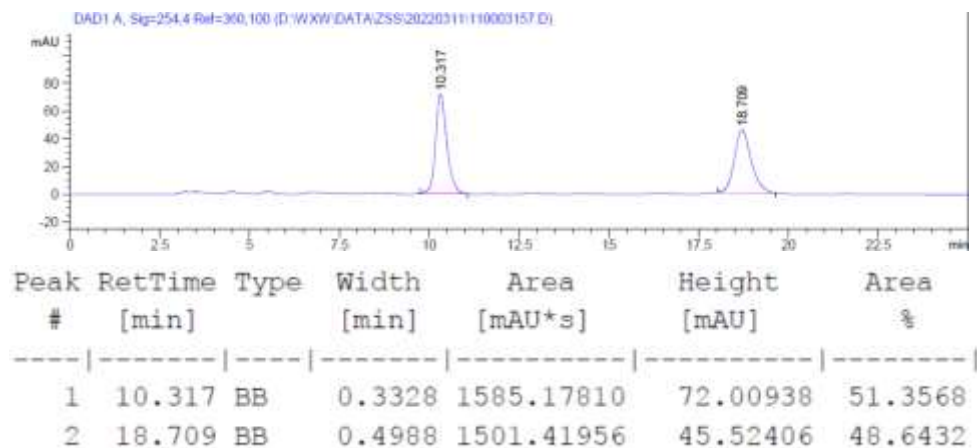


1-((2*R*,3*R*)-2-(4-bromophenyl)-1-tosylindolin-3-yl)ethane-1,2-diol (4c**)**

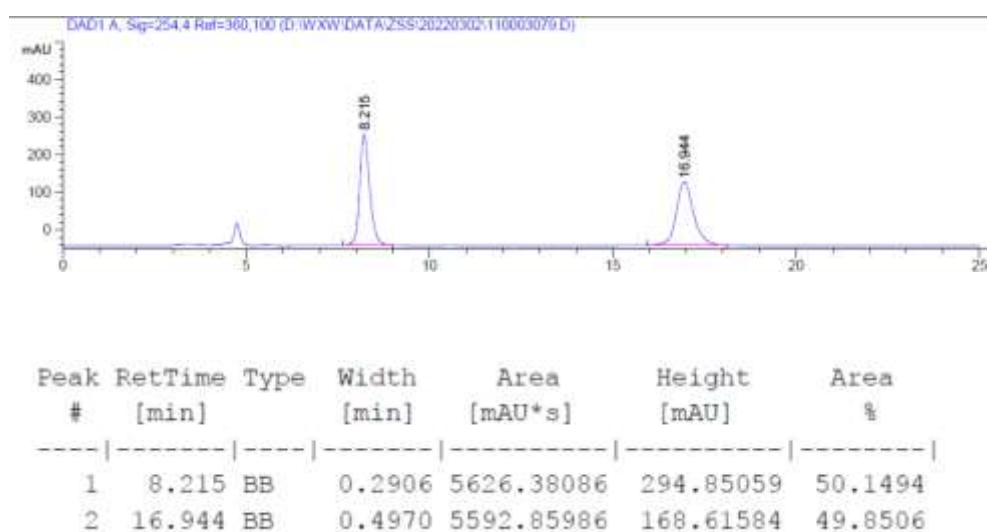


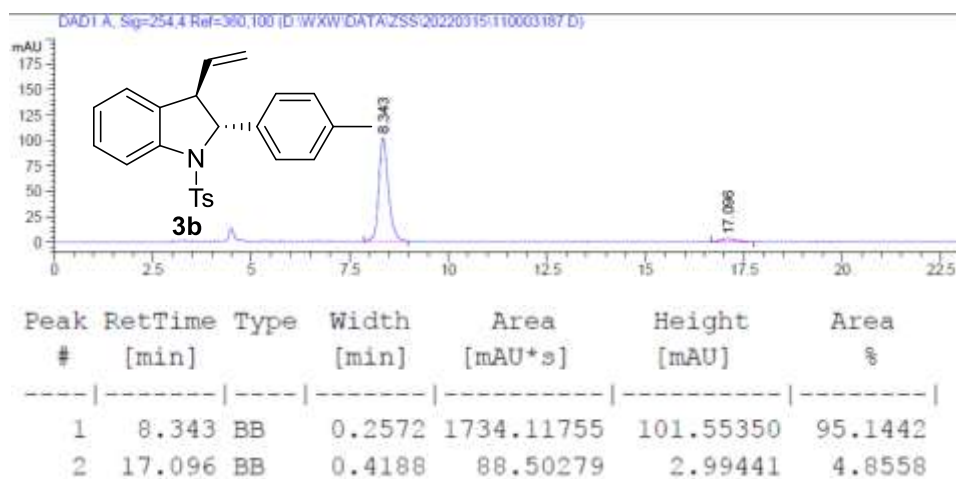
11. HPLC analysis

(2*R*,3*R*)-2-phenyl-1-tosyl-3-vinylindoline (3a)

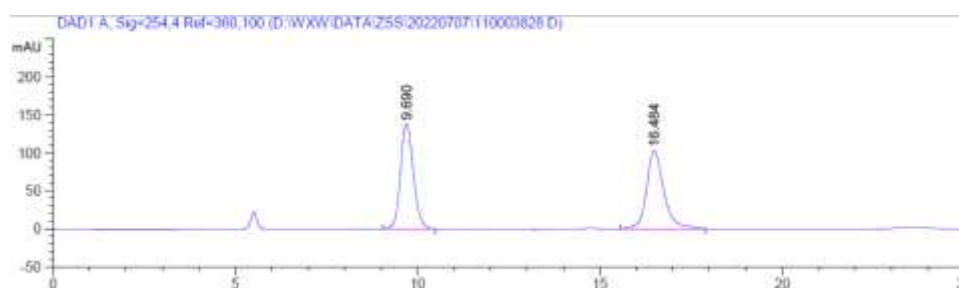


(2*R*,3*R*)-2-(*p*-tolyl)-1-tosyl-3-vinylindoline (3b)

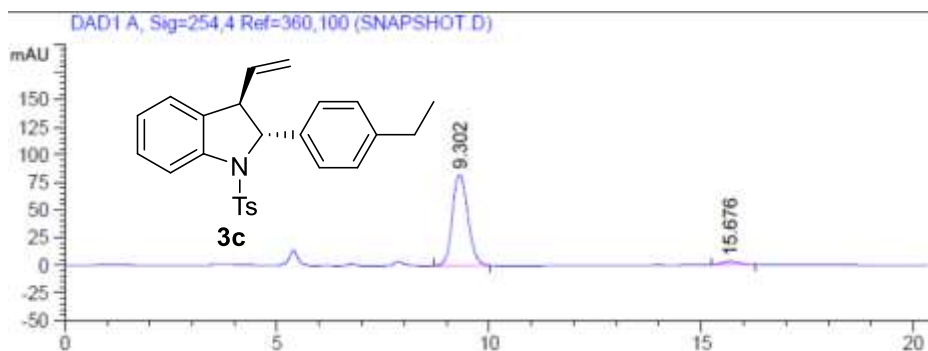




(2*R*,3*R*)-2-(4-ethylphenyl)-1-tosyl-3-vinylindoline (3c)

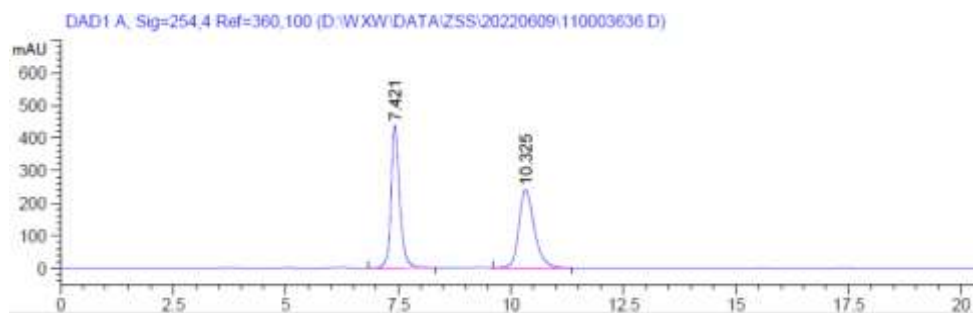


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	9.690	BB	0.3838	3429.79614	139.03056	49.9244
2	16.484	BB	0.4911	3440.19043	103.69138	50.0756

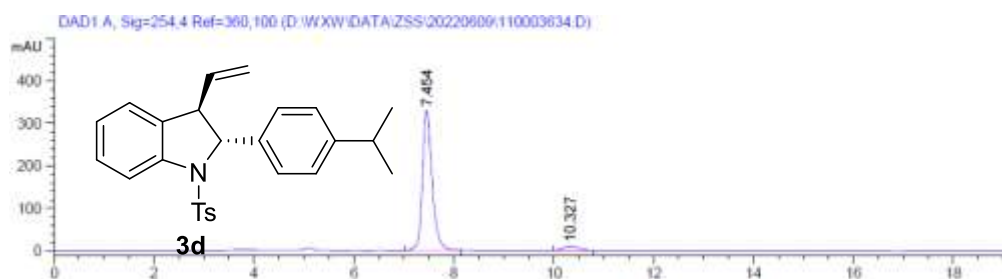


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	9.302	BB	0.4011	2101.55420	82.51653	96.4430
2	15.676	BB	0.3939	77.50844	2.82654	3.5570

(2*R*,3*R*)-2-(4-isopropylphenyl)-1-tosyl-3-vinylindoline (3d)

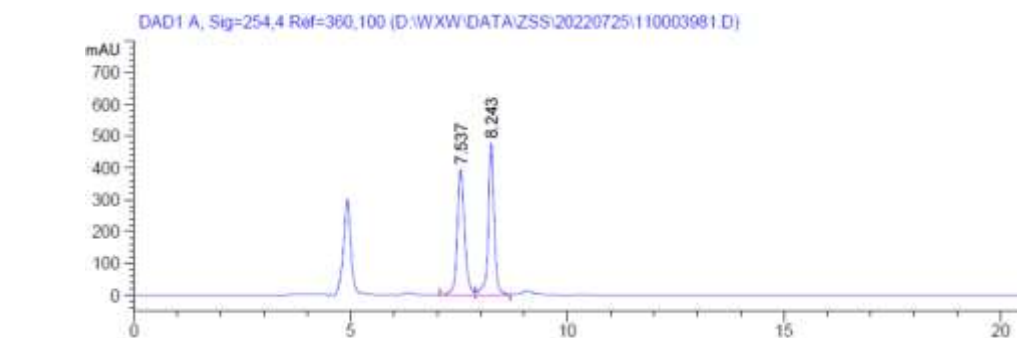


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	7.421	BB	0.2002	5852.98730	437.08771	50.2761
2	10.325	VB	0.3679	5788.70703	239.55563	49.7239



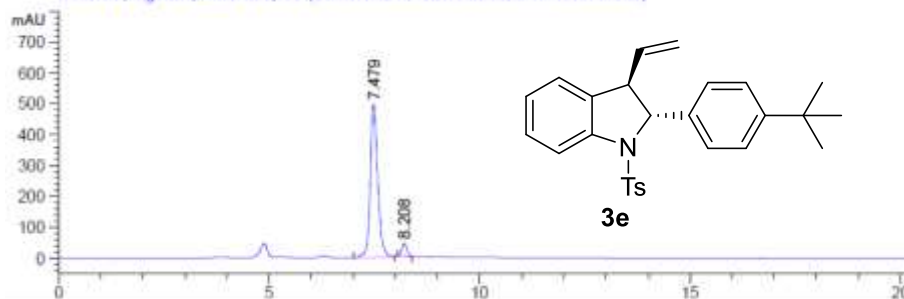
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	7.454	BB	0.2035	4460.32031	330.32062	95.0328
2	10.327	MM R	0.3667	233.13147	10.59655	4.9672

(2*R*,3*R*)-2-(4-(*tert*-butyl)phenyl)-1-tosyl-3-vinylindoline (3e)



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	7.537	VV	0.1776	4662.08984	395.25165	50.2194
2	8.243	VV	0.1451	4621.36133	476.49939	49.7806

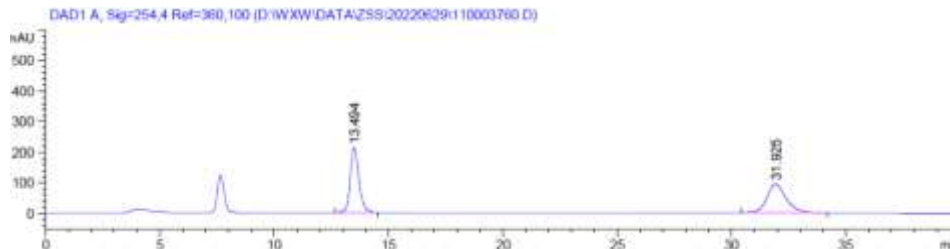
DAD1 A, Sig=254,4 Ref=360,100 (D:\WXW\DATA\ZSS\20220725\110003979.D)



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	7.479	BB	0.1858	6114.15479	495.87891	94.5317
2	8.208	MM R	0.1433	353.68399	41.12835	5.4683

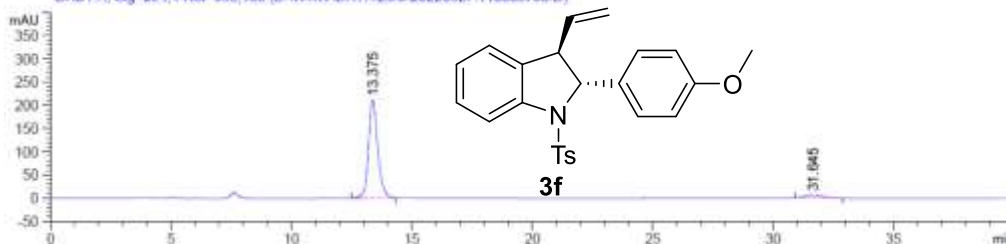
(2R,3R)-2-(4-methoxyphenyl)-1-tosyl-3-vinylindoline (3f)

DAD1 A, Sig=254,4 Ref=360,100 (D:\WXW\DATA\ZSS\20220629\110003760.D)



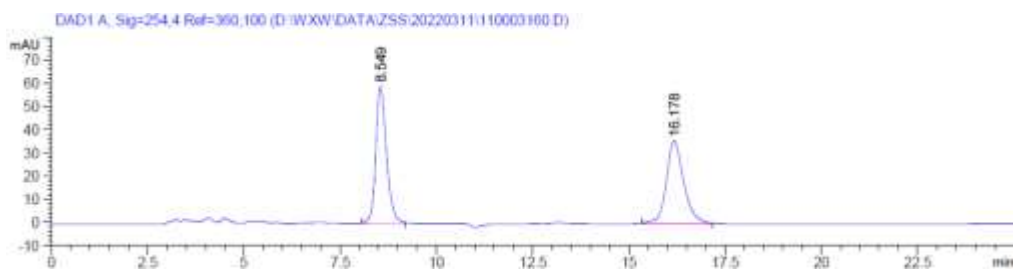
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	13.494	BB	0.4046	5713.43066	213.24898	50.7554
2	31.925	MM R	0.9775	5543.36084	94.52052	49.2446

DAD1 A, Sig=254,4 Ref=360,100 (D:\WXW\DATA\ZSS\20220627\110003750.D)

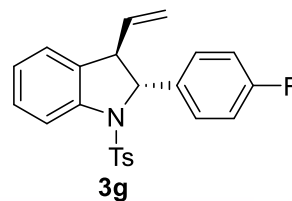
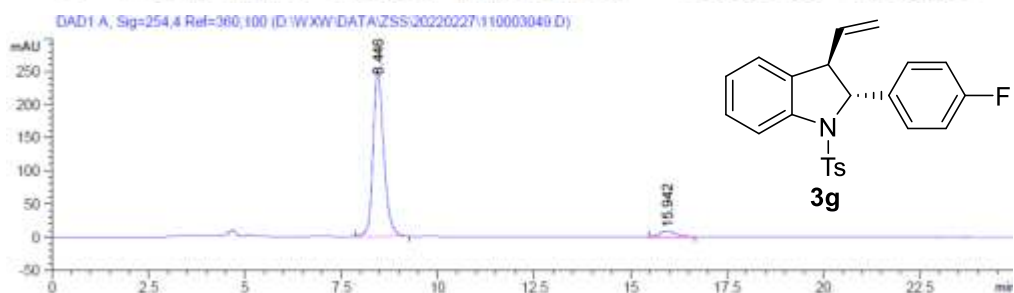


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	13.375	MM R	0.4434	5635.15820	211.83868	94.2314
2	31.645	BB	0.6595	344.97128	6.64739	5.7686

(2R,3R)-2-(4-fluorophenyl)-1-tosyl-3-vinylindoline (3g)

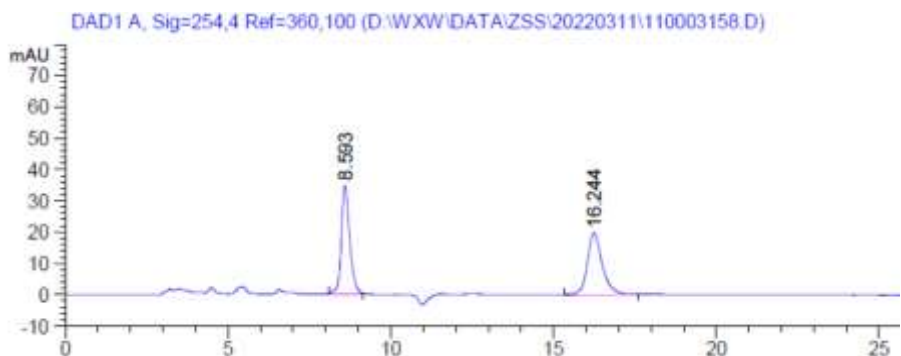


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	8.549	BB	0.2927	1139.11401	59.13330	50.4415
2	16.178	MM R	0.5231	1119.17529	35.66105	49.5585

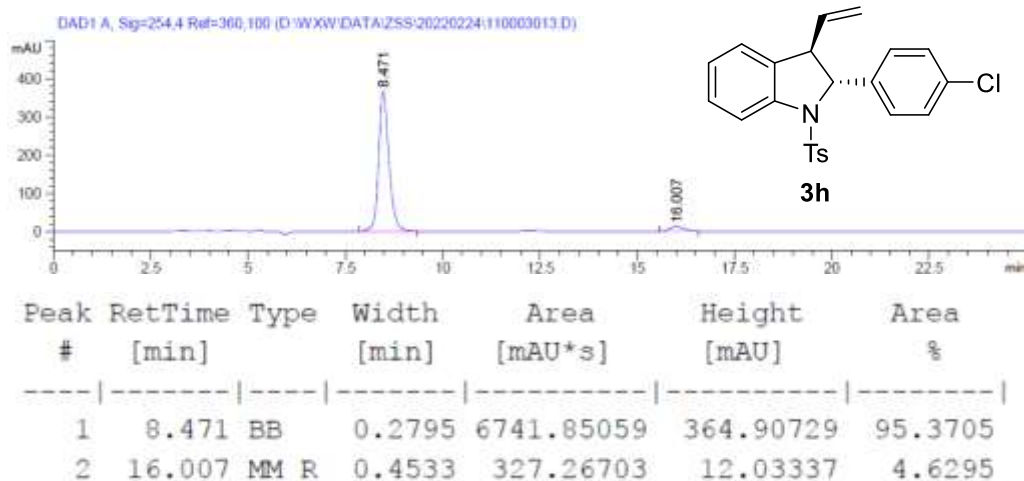


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	8.446	BB	0.2966	4852.62744	249.85382	95.3624
2	15.942	BB	0.4272	235.98837	8.31376	4.6376

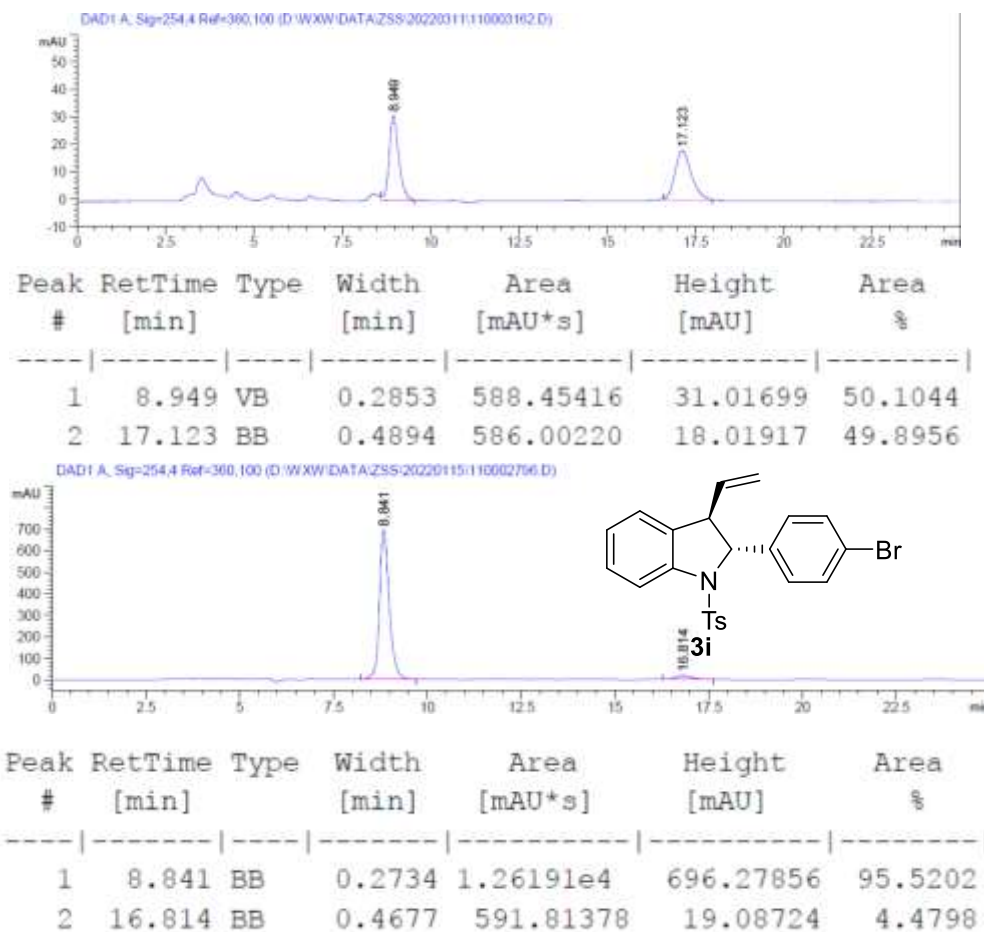
(2R,3R)-2-(4-chlorophenyl)-1-tosyl-3-vinylindoline (3h)



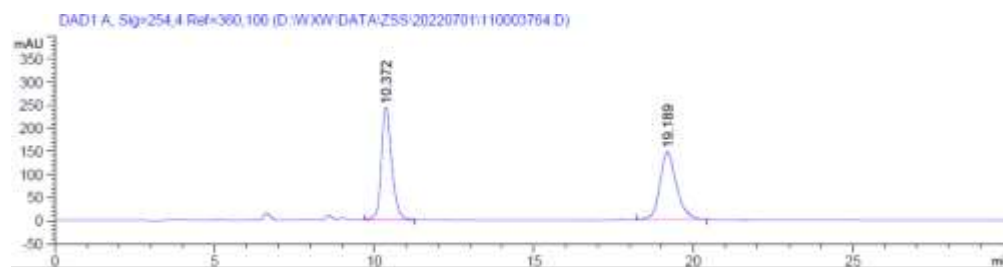
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	8.593	BB	0.2741	630.80493	34.70299	49.2547
2	16.244	MM R	0.5477	649.89423	19.77561	50.7453



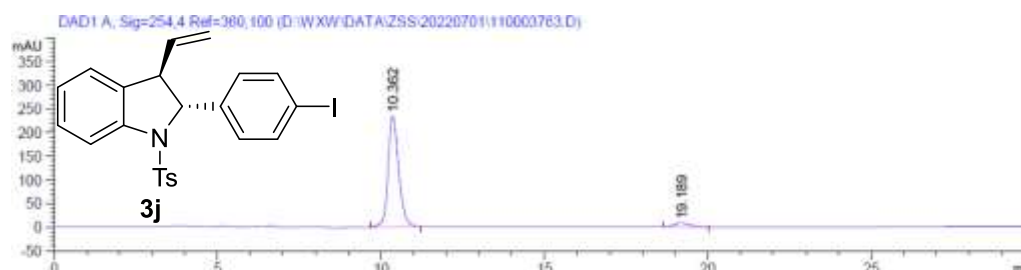
(2R,3R)-2-(4-bromophenyl)-1-tosyl-3-vinylindoline (3i)



(2R,3R)-2-(4-iodophenyl)-1-tosyl-3-vinylindoline (3j)

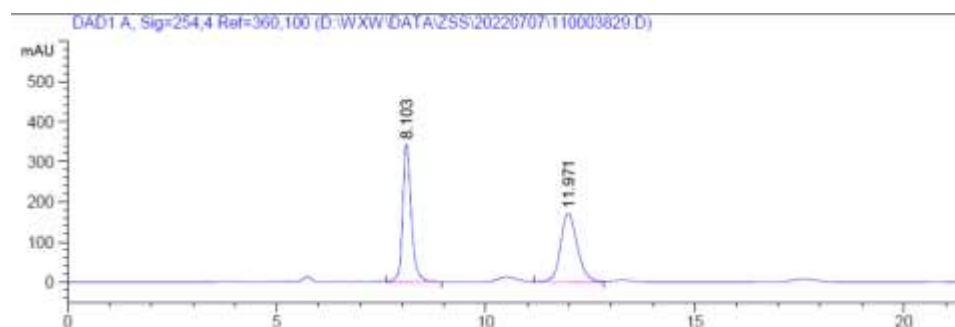


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	10.372	BB	0.3443	5455.82227	242.68387	50.7596
2	19.189	BB	0.5458	5292.52783	146.38052	49.2404

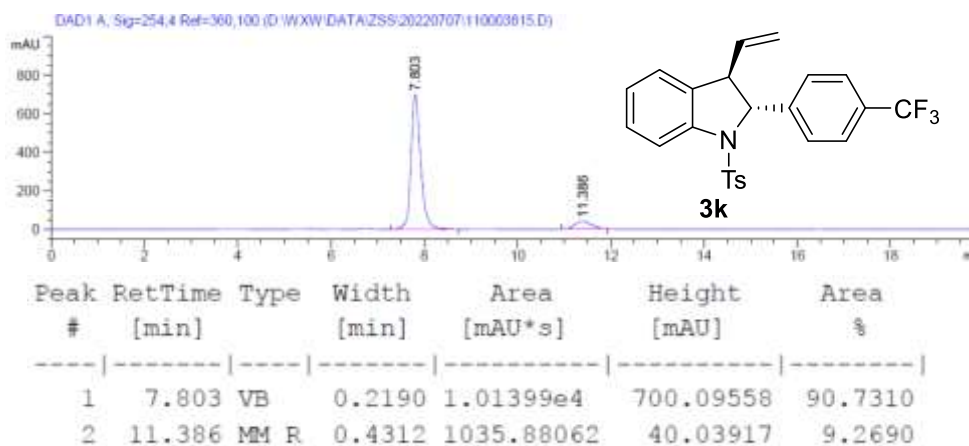


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	10.362	BB	0.3436	5280.59961	233.70644	94.9877
2	19.189	BB	0.4992	278.64383	8.14332	5.0123

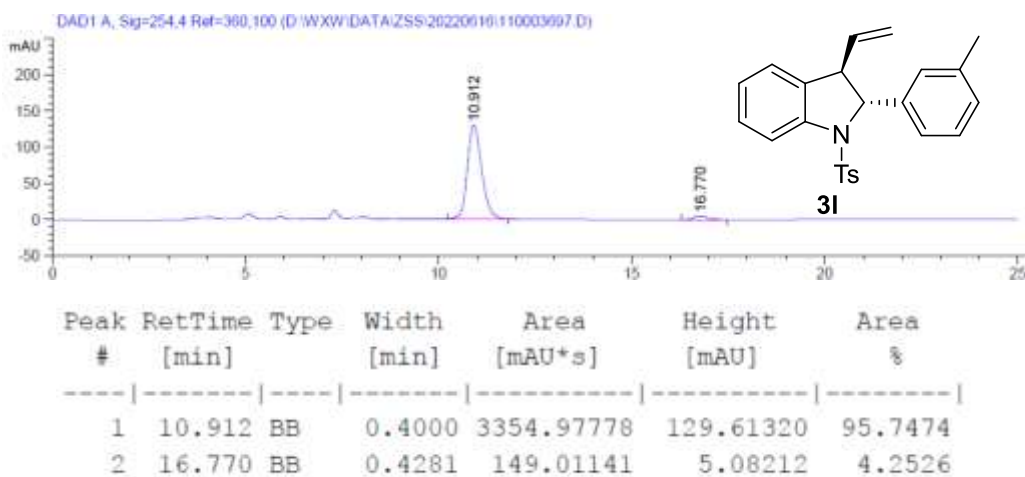
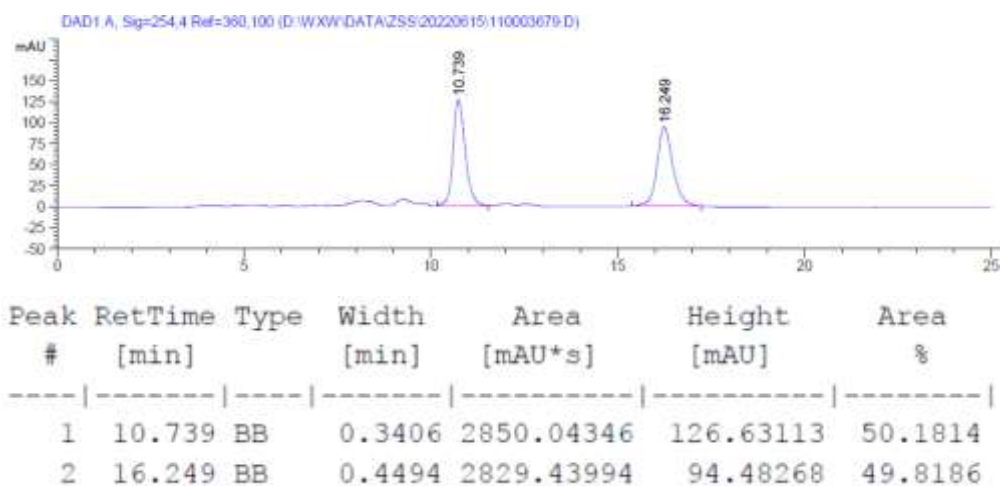
(2R,3R)-1-tosyl-2-(4-(trifluoromethyl)phenyl)-3-vinylindoline (3k)



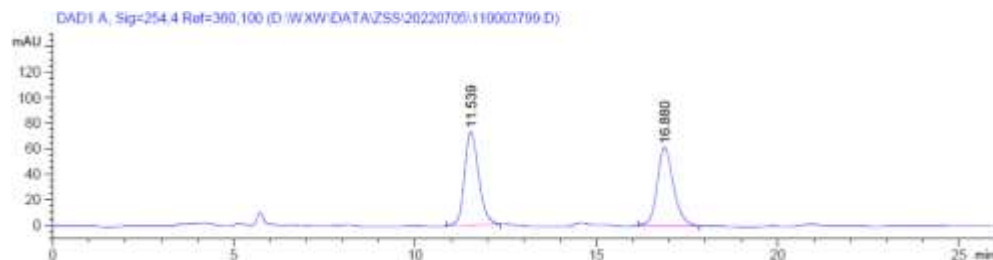
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	8.103	VB	0.2133	4945.30225	344.84058	50.6083
2	11.971	VB	0.4310	4826.41748	172.17607	49.3917



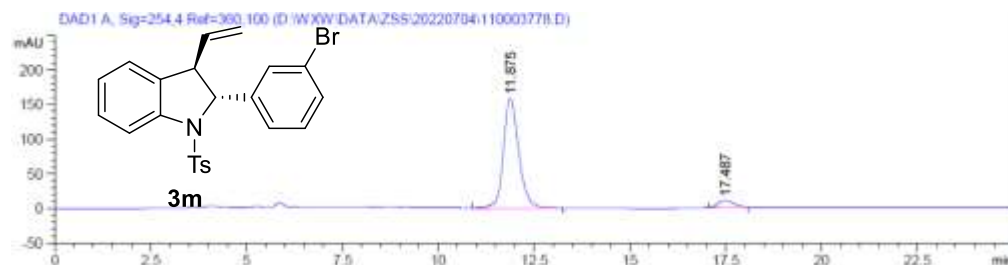
(2*R*,3*R*)-2-(*m*-tolyl)-1-tosyl-3-vinylindoline (3l)



(2*R*,3*R*)-2-(3-bromophenyl)-1-tosyl-3-vinylindoline (3m)

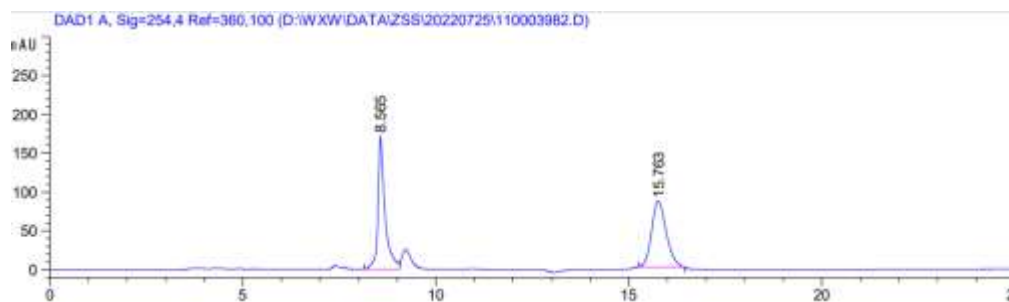


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	11.539	BB	0.4159	1986.04688	73.33987	50.5219
2	16.880	BB	0.4718	1945.01367	61.70187	49.4781

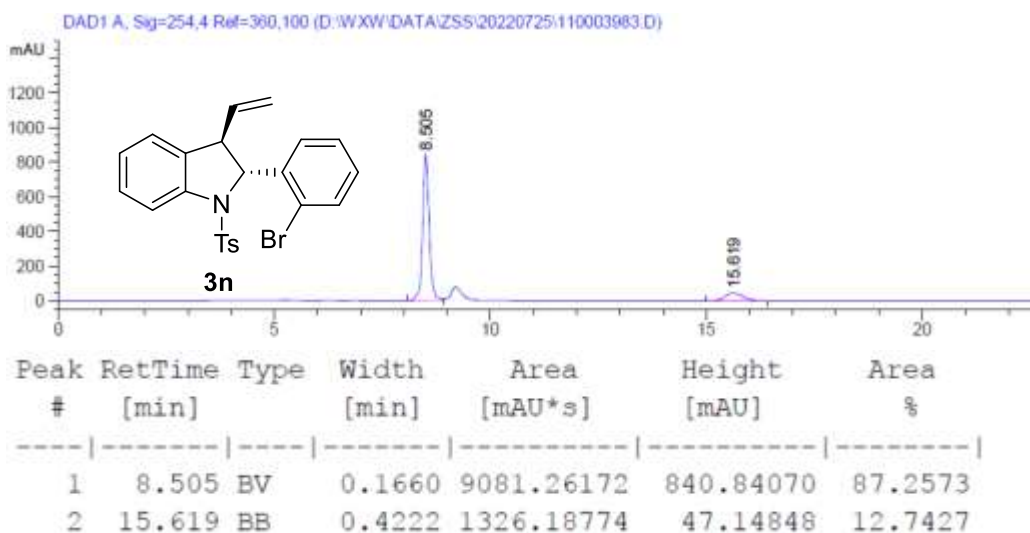


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	11.875	MM R	0.4656	4438.21094	158.86264	93.8518
2	17.487	MM R	0.4752	290.74591	10.19701	6.1482

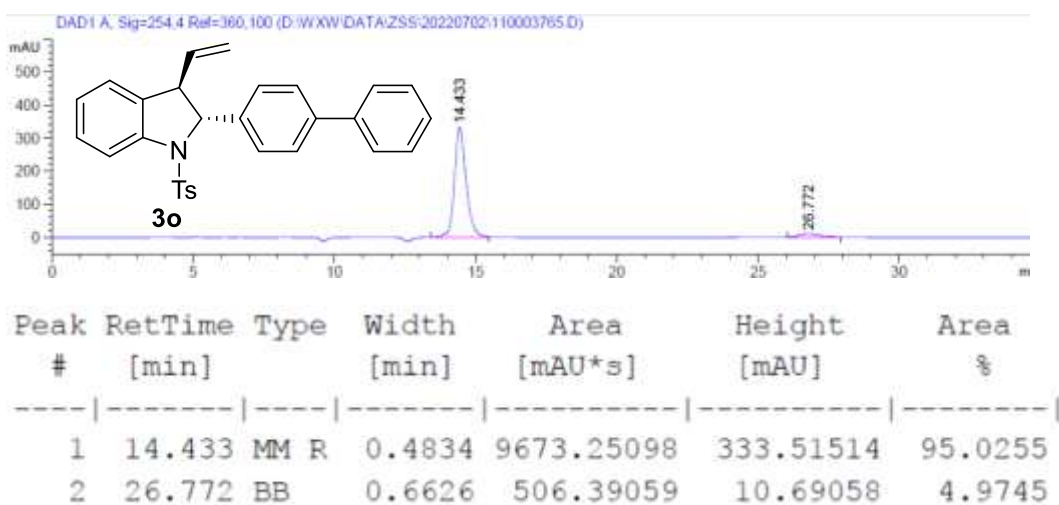
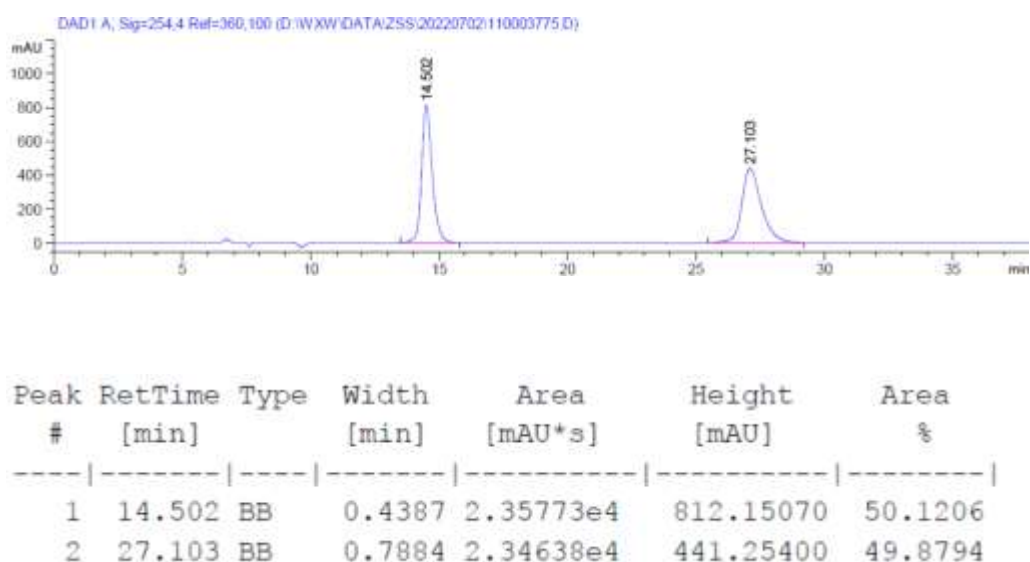
(2*R*,3*R*)-2-(2-bromophenyl)-1-tosyl-3-vinylindoline (3n)



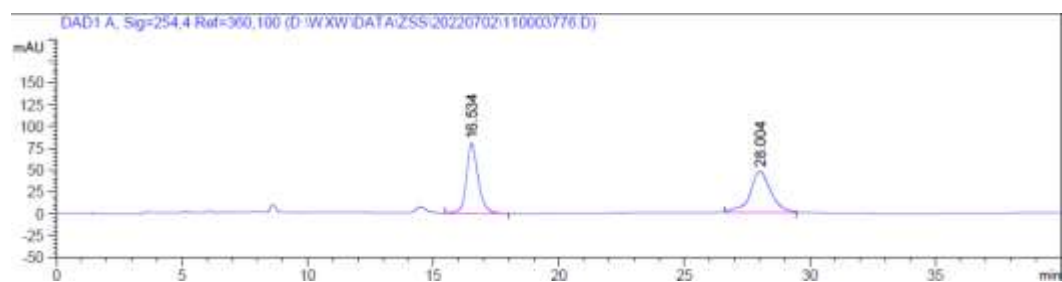
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	8.565	MF R	0.2118	2167.82471	170.61145	49.1029
2	15.763	MM R	0.4399	2247.03467	85.13592	50.8971



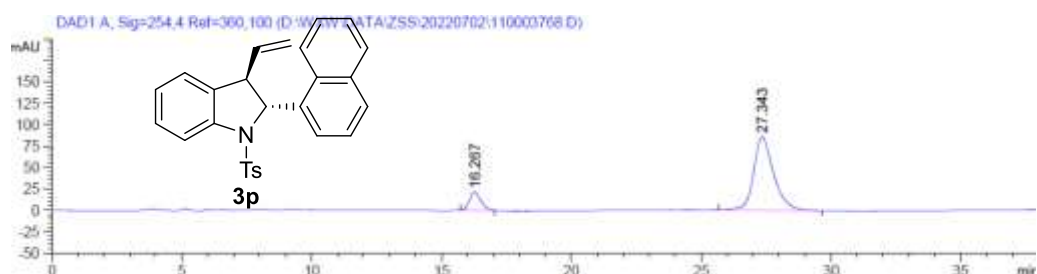
(2*R*,3*R*)-2-([1,1'-biphenyl]-4-yl)-1-tosyl-3-vinylindoline (3o)



(2*R*,3*R*)-2-(naphthalen-1-yl)-1-tosyl-3-vinylindoline (3p)

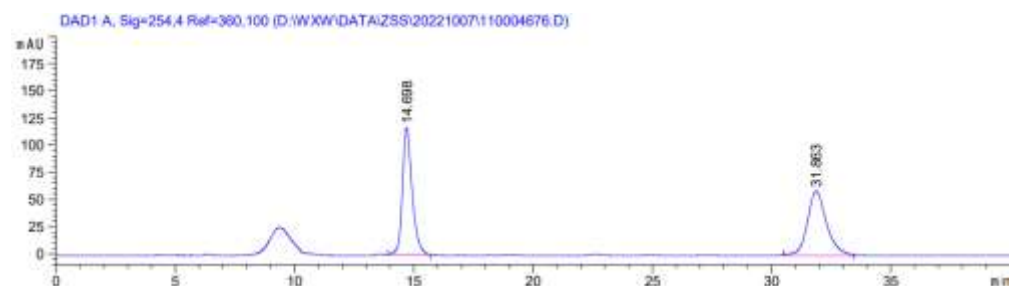


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	16.534	MM R	0.5360	2580.15234	80.22732	49.3679
2	28.004	BB	0.8166	2646.22485	47.02003	50.6321

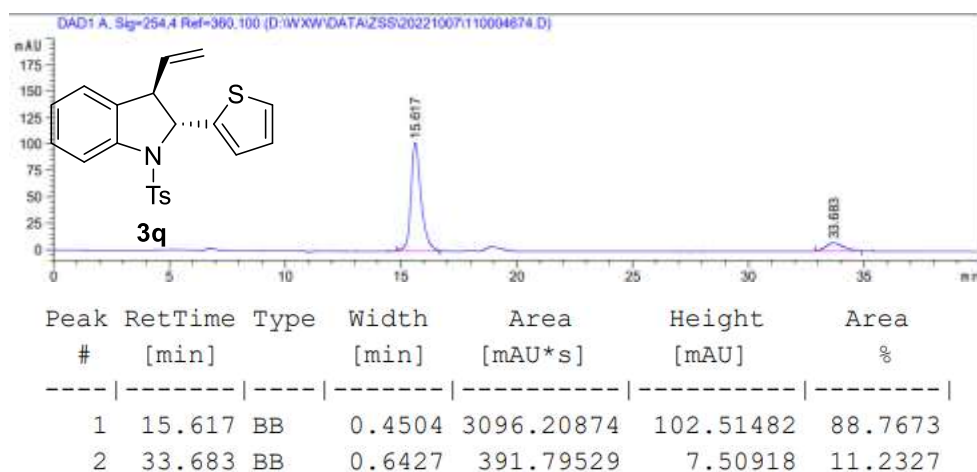


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	16.267	BB	0.4525	643.44244	21.41450	12.2268
2	27.343	MM R	0.9007	4619.13330	85.47237	87.7732

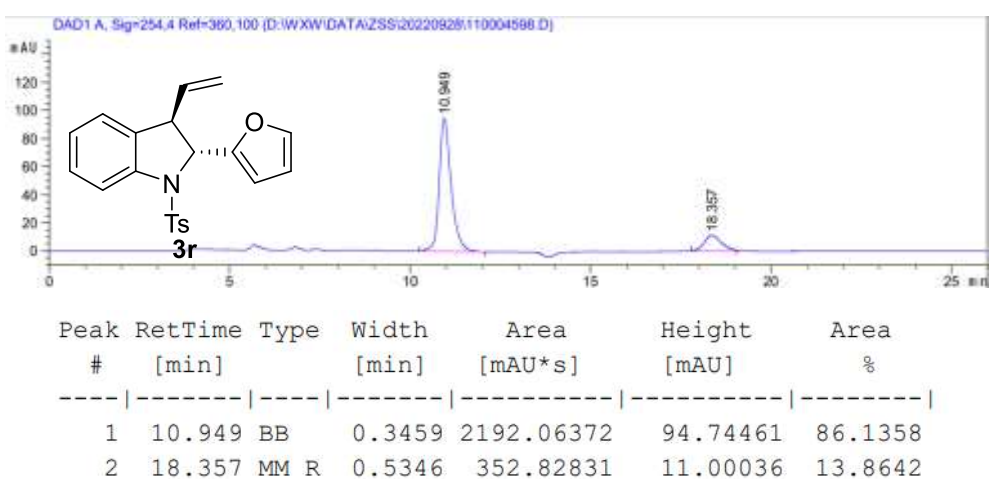
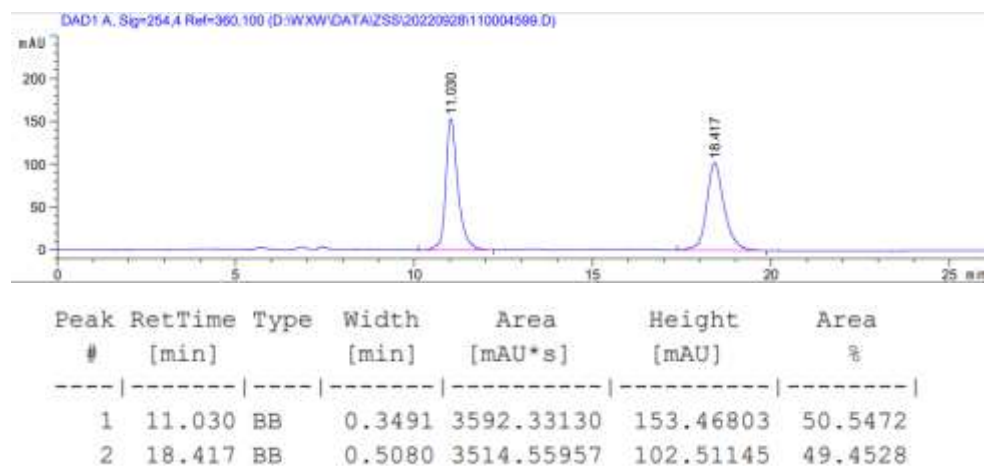
(2*R*,3*R*)-2-(thiophen-2-yl)-1-tosyl-3-vinylindoline (3q)



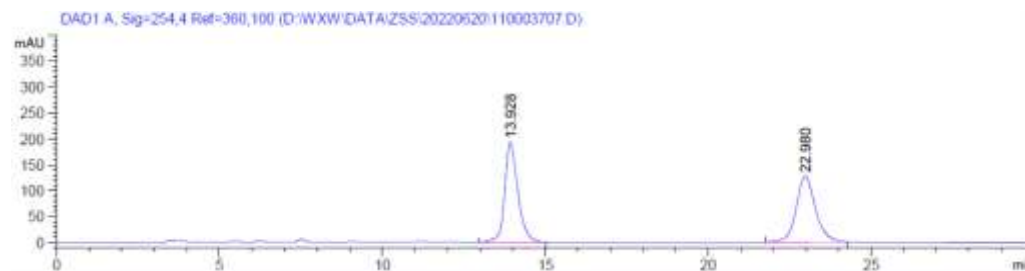
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	14.698	BB	0.4230	3318.68188	116.98586	49.6141
2	31.863	MM R	0.9454	3370.31421	59.41882	50.3859



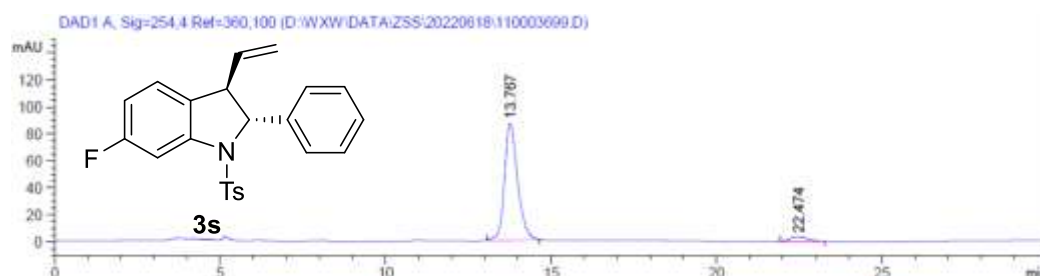
(2R,3R)-2-(furan-2-yl)-1-tosyl-3-vinylindoline (3r)



(2*R*,3*R*)-6-fluoro-2-phenyl-1-tosyl-3-vinylindoline (3s)

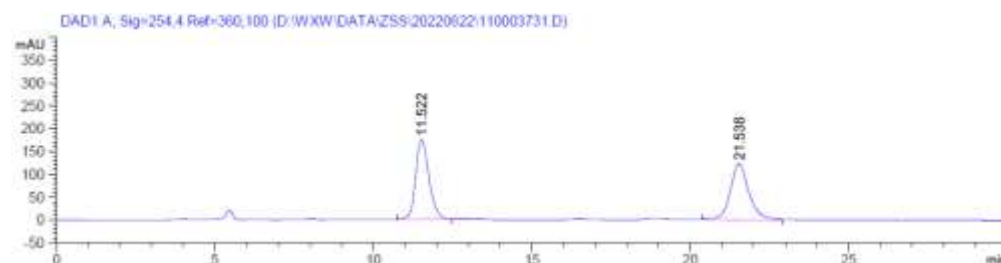


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	13.928	BB	0.4255	5491.58105	193.26498	50.8560
2	22.980	BB	0.6274	5306.70703	127.53449	49.1440

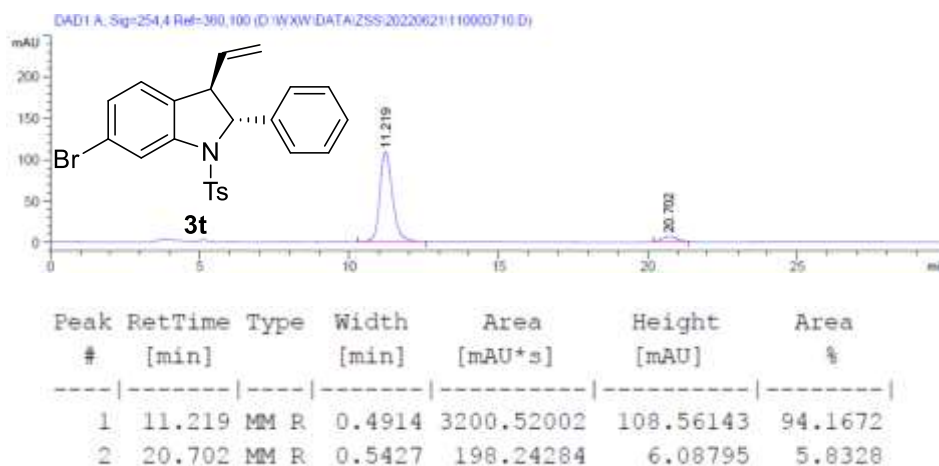


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	13.767	BB	0.4244	2413.32227	86.80238	95.0439
2	22.474	BB	0.4418	125.84332	3.43154	4.9561

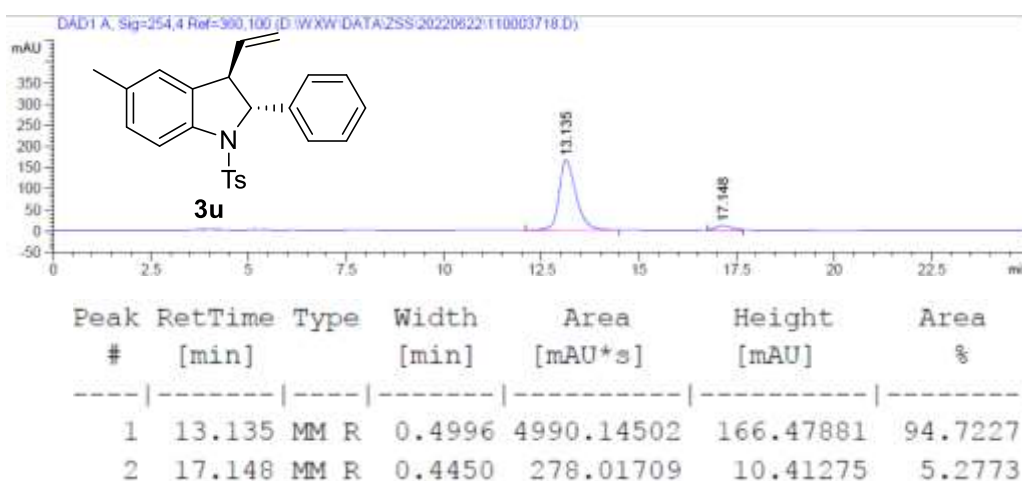
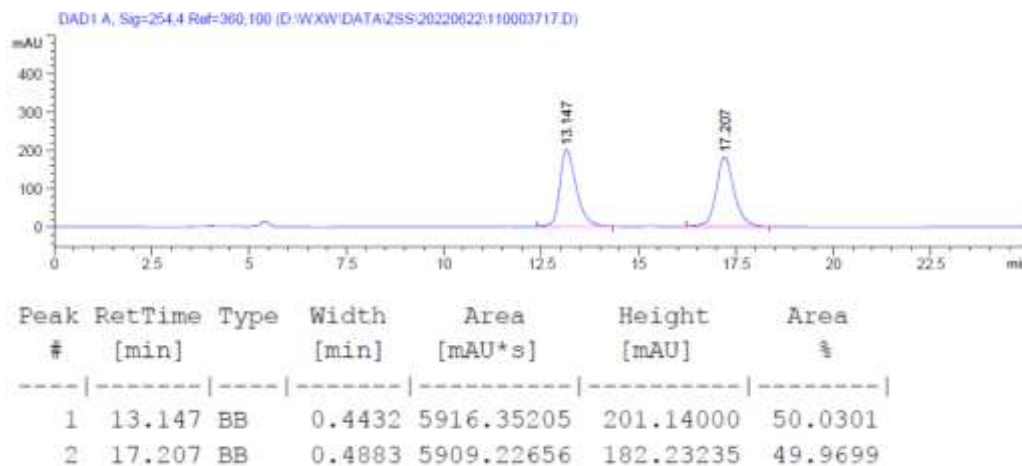
(2*R*,3*R*)-6-bromo-2-phenyl-1-tosyl-3-vinylindoline (3t)



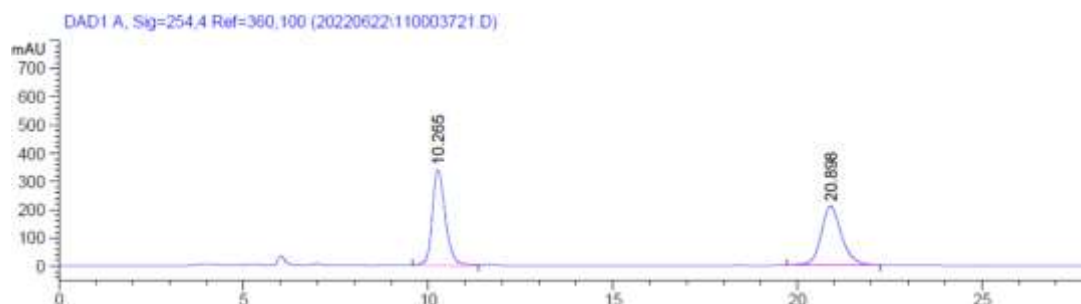
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	11.522	BB	0.4523	5112.61475	174.25105	50.2499
2	21.538	MM R	0.6897	5061.75830	122.31786	49.7501



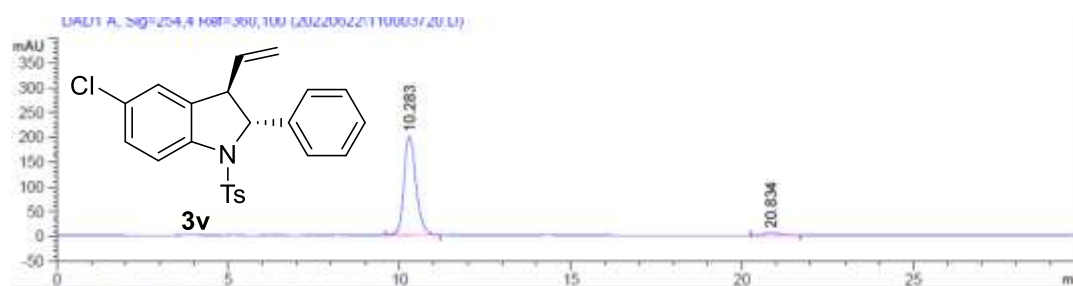
(2R,3R)-5-methyl-2-phenyl-1-tosyl-3-vinylindoline (3u)



(2R,3R)-5-chloro-2-phenyl-1-tosyl-3-vinylindoline (3v)

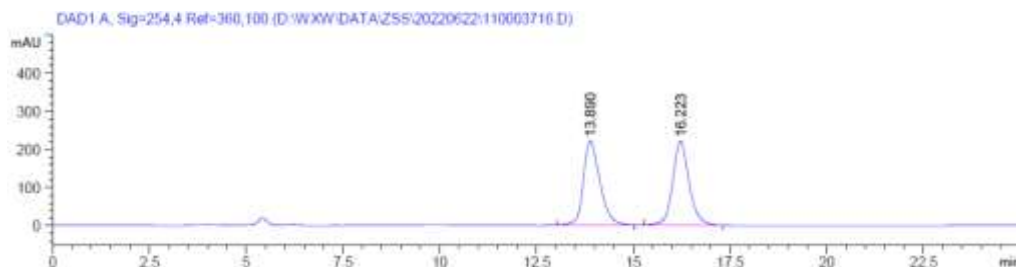


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	10.265	BB	0.3777	8356.94238	338.87027	50.6096
2	20.898	BB	0.5861	8155.62891	210.44855	49.3904

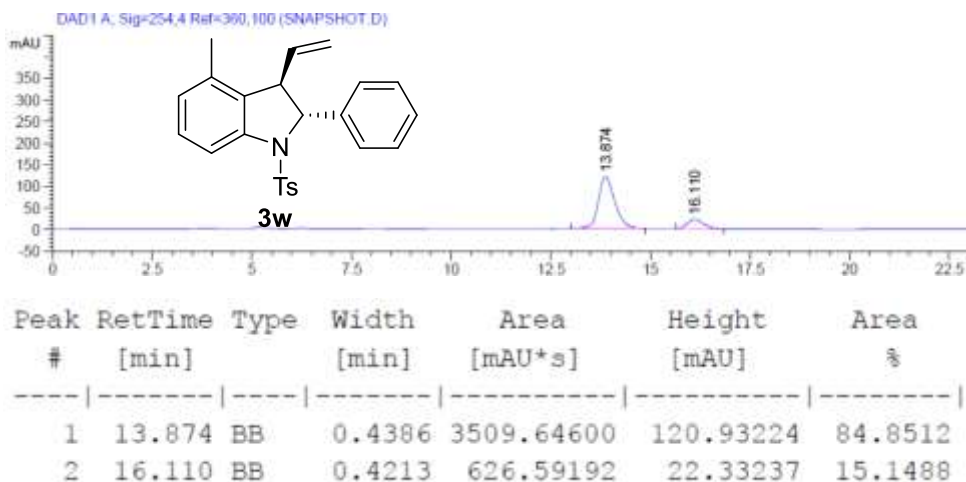


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	10.283	BB	0.3780	4902.43555	199.99683	95.7233
2	20.834	BB	0.5161	219.03055	6.11145	4.2767

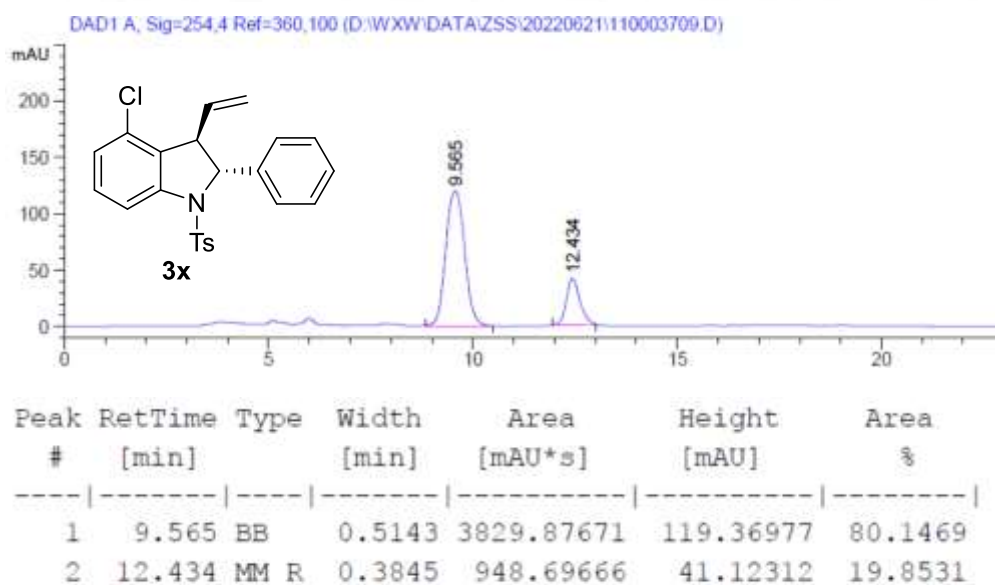
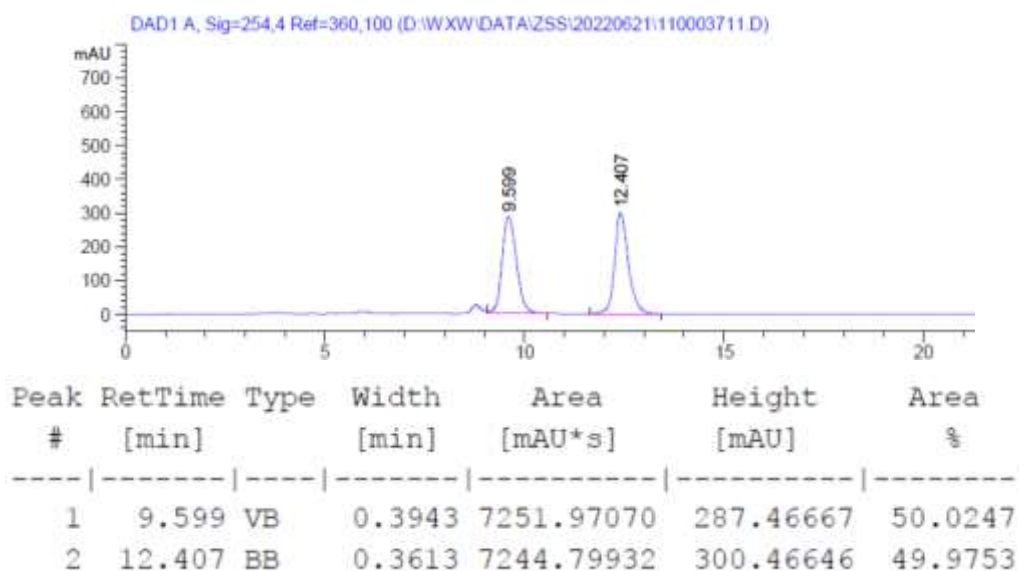
(2R,3R)-4-methyl-2-phenyl-1-tosyl-3-vinylindoline (3w)



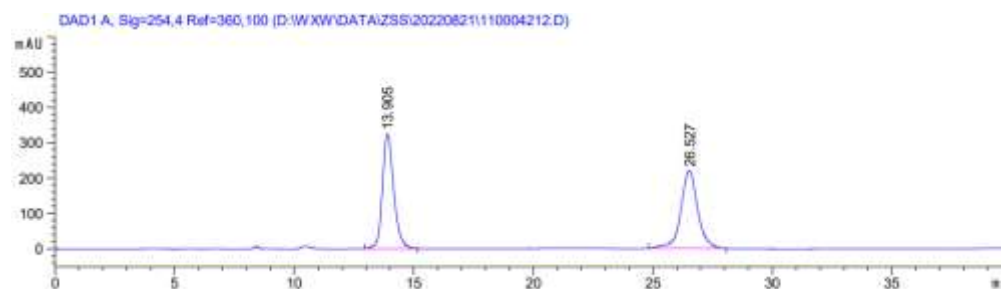
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	13.890	BB	0.4528	6572.88330	221.11736	50.2050
2	16.223	BB	0.4454	6519.20850	220.17848	49.7950



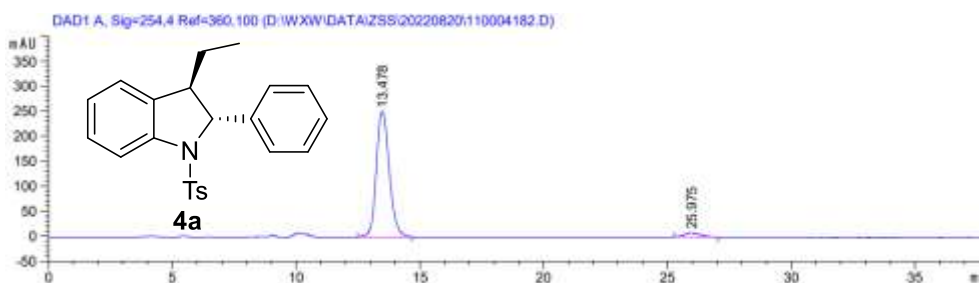
(2R,3R)-4-chloro-2-phenyl-1-tosyl-3-vinylindoline (3x)



(2R,3R)-3-ethyl-2-phenyl-1-tosylindoline (4a)

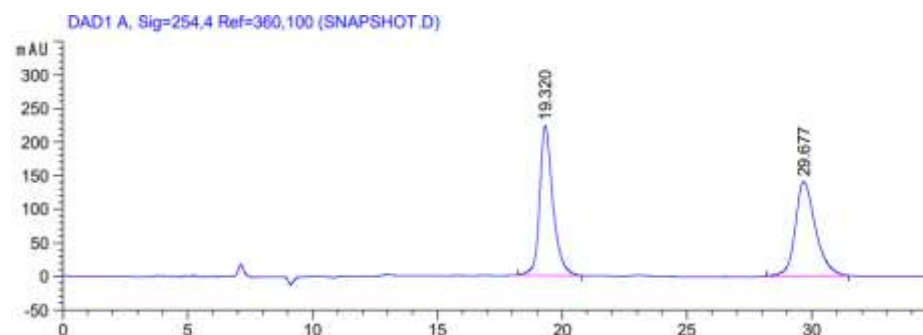


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	13.905	BB	0.4985	1.06665e4	325.34390	49.6478
2	26.527	BB	0.7300	1.08178e4	220.65262	50.3522

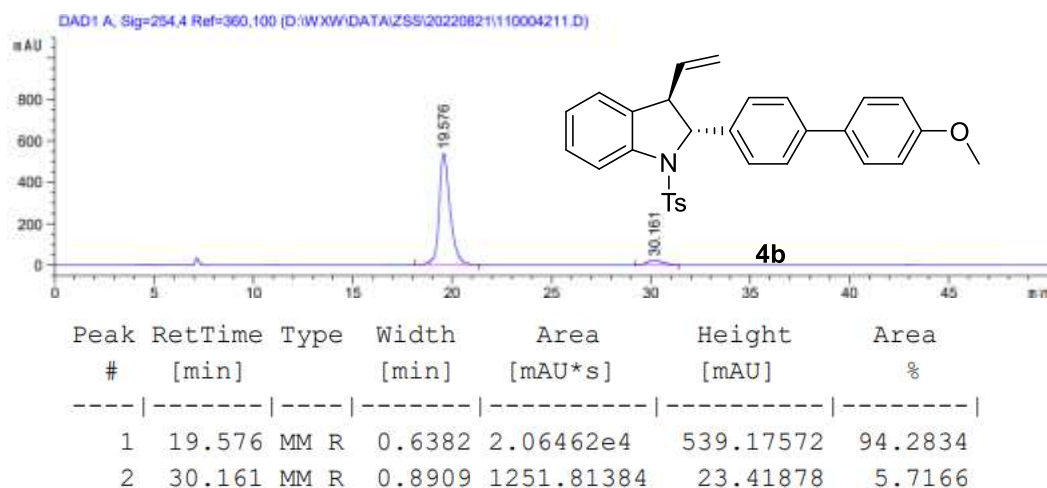


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	13.478	BB	0.5663	9148.49121	251.53532	96.2031
2	25.975	BB	0.5912	361.06888	8.24104	3.7969

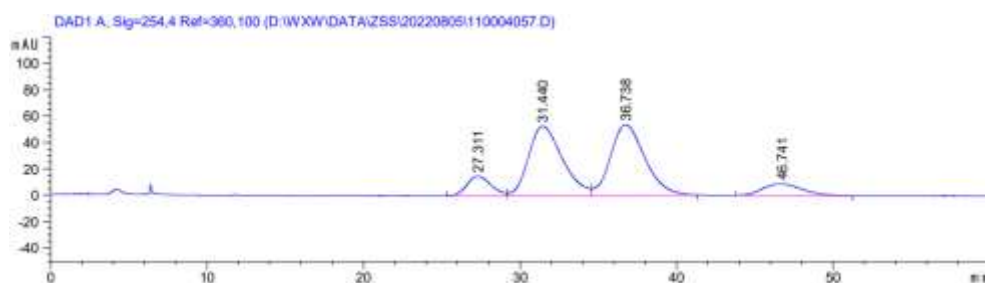
(2R,3R)-2-(4'-methoxy-[1,1'-biphenyl]-4-yl)-1-tosyl-3-vinylindoline (4b)



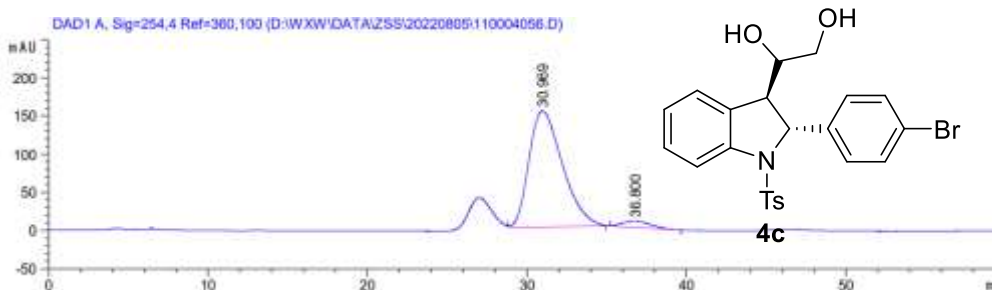
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	19.320	BB	0.5470	8203.08008	223.08563	50.6355
2	29.677	BB	0.8509	7997.17139	140.75565	49.3645



1-((2R,3R)-2-(4-bromophenyl)-1-tosylindolin-3-yl)ethane-1,2-diol (4c)



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	27.311	BV	1.3733	1593.60742	14.93011	8.2503
2	31.440	VV	2.0058	7937.14111	52.79854	41.0914
3	36.738	VB	2.0759	8196.69434	53.60564	42.4352
4	46.741	BB	2.0907	1588.36292	8.93189	8.2231



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	30.969	MM R	2.4381	2.21437e4	151.37483	95.5183
2	36.800	MM R	2.0613	1038.97473	8.40071	4.4817

12. Computational details

All density functional theory (DFT) calculations were performed using Gaussian 16.¹² Transition-state and intermediate geometries were calculated with the B3LYP density functional^{13,14}, and the SDD basis set with effective core potential was used for Pd and the 6-31G(d) basis set was used for other atoms. The D3 version of Grimme's dispersion with Becke-Johnson damping was added.^{15,16} The `integral=(finegrid,acc2e=10)` keyword and options were added in the optimizations of geometries. Normal mode frequency analysis was used to confirm that the transition-state structures are saddle points (with a single imaginary frequency) and the intermediate structures are minima (without imaginary frequency) on the potential energy surfaces. All saddle points were analyzed with the intrinsic reaction coordinate calculations to verify that they connect the expected minima. Single-point energies were calculated at the MN15/SDD,6-311++G(d,p), SMD(dichloromethane) level of theory. The refined energies were corrected to Gibbs free energies at 298.15 K and 1 atm, using the gas-phase B3LYP-D3(BJ)/SDD,6-31G(d,p) harmonic frequencies. Free energies obtained from the level of MN15/SDD,6-311++G(d,p), SMD(dichloromethane) // B3LYP-D3(BJ)/SDD,6-31G(d) calculations were discussed.

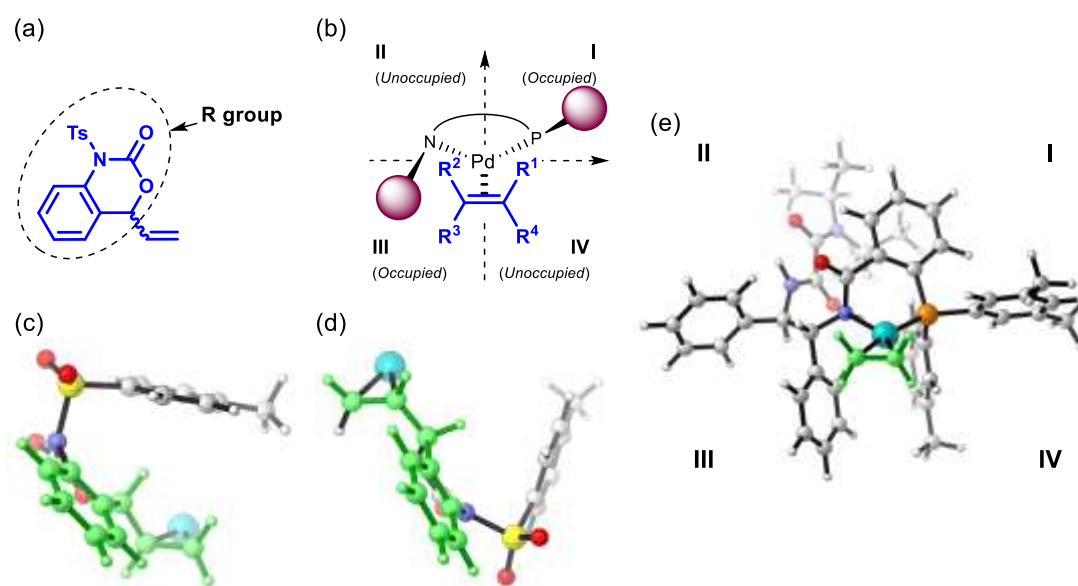


Figure S5. (a) Structural formula of racemic vinyl benzoxazinone (*R*)/(*S*)-**1a**. (b) Quadrant diagram of alkylene-coordinated Pd complex. (c) 3D representation of (*R*)-**1a** coordinating to a Pd

atom. (d) 3D representation of (*S*)-**1a** coordinating to a Pd atom. (e) 3D representation of an ethylene coordinating to the **L11**-coordinated Pd catalyst.

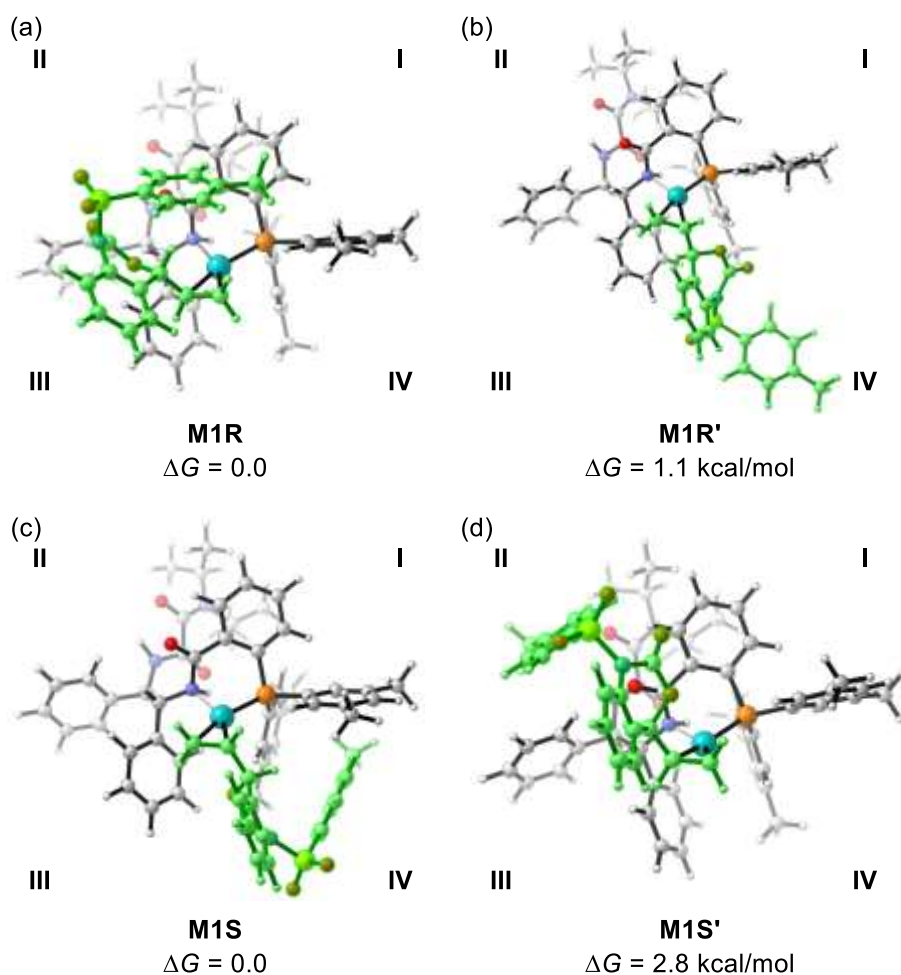


Figure S6. DFT-calculated geometries and relative free energies for the intermediate of R group of (*R*)-**1a** located in quadrant II (**M1R**), IV (**M1R'**) and (*S*)-**1a** located in quadrant IV (**M1S**), II (**M1S'**).

Table S10. DFT-calculated thermal corrections to Gibbs free energies at the level of B3LYP-D3(BJ)/SDD,6-31G(d) (G_{corr}), and single-point energies at the level of MN15/SDD,6-311++G(d,p), SMD(dichloromethane) (E_{sol}). All energies are given in hartree.

Species	G_{corr}	E_{sol}	$G_{\text{corr}} + E_{\text{sol}}$
(<i>R</i>)- 1a	0.240308	-1409.6440866	-1409.4037786
CO ₂	-0.009125	-188.4518434	-188.4609684

N₂	-0.012851	-109.4276648	-109.4405158
(2R,3R)-3a	0.331049	-1491.2960088	-1490.9649598
M1R	1.036819	-4011.5452773	-4010.5084583
M1R'	1.035401	-4011.5420284	-4010.5066274
TS1R	1.038718	-4011.5163742	-4010.4776562
M2R	1.041523	-4011.5474052	-4010.5058822
TS2R	1.037973	-4011.5368027	-4010.4988297
M3R	1.026061	-3823.0878320	-3822.0617710
M1S	1.042361	-4011.5471041	-4010.5047431
M1S'	1.040354	-4011.5406933	-4010.5003393
TS1S	1.037593	-4011.5101543	-4010.4725613
M2S	1.041697	-4011.5308611	-4010.4891641
TS2S	1.039530	-4011.5180625	-4010.4785325
M3S	1.029603	-3823.0837778	-3822.0541748
TS3S	1.027589	-3823.0488874	-3822.0212984
M4S	1.028020	-3823.0800823	-3822.0520623
M5	1.029493	-3823.1083111	-3822.0788181
M6	1.125632	-4093.1272420	-4092.0016100
M6_{dia}	1.124199	-4093.1220337	-4091.9978347
TS4	1.125709	-4093.1168410	-4091.9911320
TS4_{dia}	1.126224	-4093.1118677	-4091.9856437
M7	1.129126	-4093.1816482	-4092.0525222
M7_{dia}	1.134194	-4093.1892371	-4092.0550431
TS5	1.128413	-4093.1441840	-4092.0157710
M8	1.129734	-4093.1913442	-4092.0616102

Table S11. DFT-calculated imaginary frequencies of the transition states.

Species	Imaginary frequencies/cm⁻¹	Species	Imaginary frequencies/cm⁻¹
TS1R	187.55i	TS2R	204.08i
TS1S	114.64i	TS2S	252.79i
TS3S	155.78i	TS4	136.08i
TS4_{dia}	123.63i	TS5	214.95i

Cartesian coordinates of the transition-state and intermediate structures

(R)-1a

C	-2.48032100	-1.95236000	-0.35832600
C	-1.89571200	-0.72319700	-0.04849900
C	-2.60453600	0.46875300	-0.23967000
C	-3.89063900	0.43334900	-0.77124400
C	-4.46877500	-0.78774600	-1.11903300
C	-3.76238200	-1.97152000	-0.90744700
H	-1.94559200	-2.87629600	-0.18705000
H	-4.42978600	1.36411200	-0.91633900
H	-5.46819600	-0.81439500	-1.54207900
H	-4.21292000	-2.92680900	-1.15905300
C	-1.88569200	1.72624400	0.17850500
H	-1.11888200	1.98820200	-0.56392200
O	-1.19040800	1.46301200	1.43730600
C	-0.33926800	0.41576800	1.47950700
O	0.56977200	0.37012600	2.27191800
N	-0.59707000	-0.58764900	0.52941600
S	0.68257500	-1.75207900	0.21849200
C	2.06851900	-0.69019400	-0.11709700
C	3.01601400	-0.44913300	0.87615300
C	2.18823400	-0.14291700	-1.39533200
C	4.10388000	0.36385900	0.57327900
H	2.88413500	-0.87853600	1.86090900
C	3.28041200	0.67258800	-1.67328300
H	1.44515600	-0.36486200	-2.15339500
C	4.25253500	0.93560900	-0.69763700
H	4.84725200	0.56462200	1.33978200
H	3.38541900	1.10666300	-2.66386200
O	0.27833100	-2.39167200	-1.03263900
O	0.92588000	-2.53756000	1.42109200
C	5.45052000	1.79358500	-1.01747300
H	6.29859200	1.17429400	-1.33732300
H	5.23483000	2.49697500	-1.82758300
H	5.77655900	2.36565600	-0.14309400
C	-2.77679100	2.90103400	0.43429400
H	-3.46124000	2.79004100	1.27290000
C	-2.77311800	4.00250000	-0.31269000
H	-2.09103700	4.12168900	-1.15146400
H	-3.45187900	4.82688300	-0.11568400

CO₂

C	0.00000000	0.00000000	0.00000000
O	0.00000000	0.00000000	1.16913100

O 0.00000000 0.00000000 -1.16913100

N₂

N 0.00000000 0.00000000 0.55275000

N 0.00000000 0.00000000 -0.55275000

(2*R*,3*R*)-**3a**

C 1.72003600 1.68618500 -0.94937200

C 0.42093200 1.36262000 -0.56946400

C -0.44805000 2.33120300 -0.05390200

C -0.02034500 3.64094200 0.11495500

C 1.29389000 3.97237700 -0.23453300

C 2.15027500 3.00415900 -0.76438400

H 2.37819600 0.94154200 -1.38034200

H -0.70141900 4.39110300 0.50679400

H 1.64499400 4.99253400 -0.10853500

H 3.16156300 3.27691500 -1.05192600

C -1.80507100 1.71186800 0.21209000

H -1.86335700 1.42161300 1.26684200

N -0.23021300 0.08144200 -0.71010700

S 0.21181600 -1.07793800 0.52018800

C 1.98460800 -1.10652500 0.34332000

C 2.54273100 -1.79729000 -0.73211200

C 2.77884800 -0.42991200 1.26515500

C 3.92499700 -1.78733000 -0.89104800

H 1.89915200 -2.32546600 -1.42702900

C 4.16082900 -0.43752000 1.09448100

H 2.31131600 0.09939200 2.08743100

C 4.75267300 -1.10928800 0.01686800

H 4.37193400 -2.31652700 -1.72856000

H 4.79021600 0.09239100 1.80437600

O -0.10348200 -0.55014200 1.85955700

O -0.31141900 -2.37368400 0.08826600

C 6.25140300 -1.13131300 -0.14885700

H 6.71905300 -0.26051100 0.32076800

H 6.53719300 -1.14655200 -1.20560800

H 6.68192100 -2.02672000 0.31789800

C -2.97123500 2.58588600 -0.13510400

H -3.00427500 2.94160400 -1.16586700

C -3.93020400 2.93971400 0.71958200

H -3.92402800 2.59958900 1.75264600

H -4.75889800 3.57446700 0.41934700

C -4.08878500 -1.99536600 1.04116500

C -3.17896400 -0.95646900 0.85326000

C	-2.68537400	-0.67090400	-0.42349300
C	-3.12636500	-1.43960000	-1.50604100
C	-4.03222700	-2.48049100	-1.32107900
C	-4.51707600	-2.76082000	-0.04295500
H	-4.45956300	-2.20896400	2.03959300
H	-2.83459900	-0.38941600	1.70977200
H	-2.74481000	-1.22204900	-2.50050300
H	-4.36063800	-3.07037800	-2.17220500
H	-5.22564000	-3.57074800	0.10659600
C	-1.71141800	0.44890100	-0.68958700
H	-1.87330400	0.78755100	-1.71999800

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C	0.80257800	3.04885300	-1.35947700
C	-0.03141500	1.72136500	-1.37102200
H	1.61809600	2.92874400	-2.07661100
N	1.44383900	3.29364400	-0.07730400
N	0.61114300	0.67172200	-0.56767800
H	1.56083000	0.45442500	-0.86015300
C	1.38056100	-0.12211700	1.64688700
C	1.89700600	-1.39813500	1.30872900
C	2.70482700	-2.05745300	2.24764500
C	2.99994400	-1.48539800	3.48453600
C	2.48817200	-0.22935200	3.80999500
C	1.68585000	0.44408900	2.89351800
P	1.38756700	-2.25270000	-0.25336200
H	3.08642600	-3.04542700	2.01587400
H	3.62200500	-2.02541900	4.19286600
H	2.70299700	0.22159800	4.77336200
H	1.27294500	1.41919500	3.12616200
Pd	-0.64007200	-1.41799800	-0.94972100
C	2.71489000	-1.82170700	-1.44497700
C	3.79193200	-0.98635900	-1.14099900
C	4.69718100	-0.59488100	-2.14106300
C	4.51321000	-1.08134100	-3.43607400
C	3.44924900	-1.93656300	-3.76286200
C	2.54656700	-2.28513000	-2.76061800
H	3.92580400	-0.61818100	-0.12899100
H	5.20971000	-0.78186400	-4.21655700
H	1.68469200	-2.90207400	-3.00180300
C	1.68830300	-4.02650300	0.08372800
C	0.58031600	-4.80842200	0.41783400
C	0.72620300	-6.16935500	0.71720600
C	2.00288300	-6.73136100	0.64750500

C	3.12832300	-5.97529200	0.28575700
C	2.95821900	-4.61801900	0.00663000
H	-0.40296200	-4.34643700	0.42929000
H	2.12743400	-7.79006600	0.86733600
H	3.81555800	-4.01646800	-0.28345600
C	2.66782700	2.81658400	0.20005100
O	3.32505500	2.13720200	-0.60047500
H	0.96518300	3.77906500	0.67440900
H	-0.99743200	1.89250500	-0.90200700
C	0.43627100	0.70684700	0.81318200
O	-0.42634000	1.39310600	1.34637900
C	-0.22932600	1.26592500	-2.79815700
C	-1.45986600	1.46853900	-3.42919900
C	0.82047200	0.67960700	-3.51665100
C	-1.64918900	1.06558900	-4.75124800
H	-2.27034900	1.92405100	-2.87083000
C	0.62906600	0.26801700	-4.83460500
H	1.79233400	0.53401300	-3.05374000
C	-0.60779100	0.45693100	-5.45479100
H	-2.61123500	1.22545900	-5.23029200
H	1.44886900	-0.19493300	-5.37532900
H	-0.75646700	0.13967300	-6.48336800
C	-0.07209400	4.21451400	-1.76200000
C	0.22509600	4.96171600	-2.90449000
C	-1.20593900	4.53401000	-1.00456200
C	-0.59788600	6.02123400	-3.28810500
H	1.09859700	4.70648500	-3.49889400
C	-2.02736900	5.59343100	-1.38767900
H	-1.47810500	3.94101800	-0.13699800
C	-1.72498600	6.33985800	-2.52863900
H	-0.36054800	6.59401600	-4.18036400
H	-2.90995600	5.82072600	-0.79730000
H	-2.36883000	7.16194800	-2.82902800
C	3.10103300	3.25795700	1.63170000
O	2.25147300	3.87378000	2.28813200
N	4.35268600	3.01837700	2.08906200
C	5.35070300	2.15572600	1.41287500
C	4.77474800	3.67282500	3.35688800
H	5.83038400	3.41132400	3.45979600
C	4.03921500	3.11207000	4.57852200
C	3.28715600	-2.46577000	-5.16731500
H	3.62852400	-1.73788300	-5.91139900
H	3.87493700	-3.38110000	-5.31537300
H	2.24132400	-2.70854700	-5.38065700

C	5.81999500	0.35965500	-1.82217400
H	6.56486200	0.38445800	-2.62355900
H	5.42410200	1.37122100	-1.68308400
H	6.32955800	0.07790000	-0.89320900
C	4.48770700	-6.62552000	0.18949600
H	4.74117000	-7.16057200	1.11237800
H	4.51983700	-7.35790600	-0.62677000
H	5.27087100	-5.88453500	0.00231600
C	-0.47383500	-6.99546600	1.11282800
H	-0.25423700	-8.06690900	1.07532800
H	-0.79561900	-6.75871700	2.13535500
H	-1.32603500	-6.79927000	0.45239200
H	4.82781200	1.70227200	0.57922100
H	4.17055200	2.02807900	4.64136000
H	4.44854500	3.56018100	5.49098300
H	2.97326700	3.33809400	4.52383300
C	4.69747600	5.20129600	3.26598600
H	3.66349200	5.53915800	3.18778800
H	5.14418100	5.64105400	4.16464900
H	5.25436100	5.56301600	2.39505200
C	5.83194600	1.02689100	2.33130200
H	4.98489000	0.44284000	2.70160400
H	6.48541000	0.35767000	1.76035300
H	6.40750500	1.38994800	3.18994500
C	6.50105800	2.99181600	0.84405600
H	6.11608200	3.73334400	0.13696300
H	7.05943400	3.51739400	1.62717200
H	7.20554800	2.34402300	0.31132300
C	-7.19382800	0.25578300	-0.15478700
C	-5.80115300	0.26060300	-0.07719900
C	-5.03522400	-0.66801000	-0.78950300
C	-5.67114800	-1.61796400	-1.58393600
C	-7.06597200	-1.64674100	-1.65057400
C	-7.82178700	-0.71494300	-0.93584000
H	-7.76404500	0.99056100	0.39890700
H	-5.07150500	-2.33405300	-2.13608900
H	-7.56192500	-2.39201300	-2.26565000
H	-8.90598100	-0.73321300	-0.99421900
C	-3.54286700	-0.54847000	-0.60080500
H	-3.28270500	-0.89333700	0.40401700
O	-3.21821300	0.88691800	-0.65092000
C	-3.84270800	1.70828300	0.21583100
O	-3.37121500	2.77295100	0.52739800
N	-5.10459600	1.24485300	0.69654800

S	-5.28098600	1.16396800	2.44350500
C	-4.13883500	-0.15413300	2.80131700
C	-2.78228100	0.15105100	2.93321300
C	-4.59401600	-1.47383000	2.76336300
C	-1.87134800	-0.89582800	3.03270600
H	-2.43945000	1.17837200	2.91670800
C	-3.66146400	-2.50490600	2.86230100
H	-5.65225500	-1.67821300	2.64758100
C	-2.29209500	-2.23209600	2.99562300
H	-0.81561900	-0.66882500	3.12114400
H	-4.00159400	-3.53681500	2.83186700
O	-6.64457000	0.69165600	2.66795100
O	-4.79062100	2.41274800	3.00266500
C	-1.28228900	-3.34429000	3.11957800
H	-1.05231800	-3.54686500	4.17396800
H	-1.65292500	-4.27531200	2.67938000
H	-0.34318400	-3.08117800	2.62455800
C	-2.67953200	-1.25607900	-1.59803000
H	-2.73099700	-0.87036500	-2.61475700
C	-2.32189100	-2.60625800	-1.38373200
H	-2.65706000	-3.12119800	-0.48296800
H	-2.12234600	-3.25849000	-2.23174800

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C	-3.08170500	2.84352800	0.48673900
C	-1.95945600	2.24468400	-0.43651000
H	-2.78144400	2.67384400	1.52353300
N	-4.35451700	2.16369100	0.31976000
N	-2.12013100	0.80283900	-0.62063400
H	-2.11002100	0.26759500	0.24392300
C	-3.35799500	-1.12882400	-1.50394700
C	-2.48076100	-2.17556600	-1.11856700
C	-2.97627600	-3.48780100	-1.12336500
C	-4.28640400	-3.77250500	-1.50486500
C	-5.13694700	-2.73870400	-1.89710900
C	-4.67197500	-1.42722300	-1.89178100
P	-0.67715000	-1.87879600	-0.77174300
H	-2.31452600	-4.30263800	-0.85096500
H	-4.63590100	-4.80127100	-1.50523000
H	-6.15383300	-2.95120700	-2.21162500
H	-5.31416500	-0.60567600	-2.18866300
Pd	-0.13535900	0.10074500	-1.83909700
C	-0.59252000	-1.81881200	1.05941300
C	-1.72594800	-1.78842100	1.87610400

C	-1.60221700	-1.59969700	3.26311500
C	-0.32529500	-1.46478700	3.80534900
C	0.83134100	-1.51265500	3.00988600
C	0.68516200	-1.67699900	1.63244800
H	-2.71434900	-1.90340800	1.44321300
H	-0.21972800	-1.31853600	4.87866000
H	1.56891700	-1.69187600	1.00147900
C	0.11532800	-3.47580900	-1.18392100
C	0.62563400	-3.61995600	-2.47727300
C	1.24262300	-4.81164600	-2.87439800
C	1.34590500	-5.85015500	-1.94407200
C	0.85918600	-5.72408000	-0.63622600
C	0.23860600	-4.52787600	-0.26696300
H	0.54786600	-2.78496300	-3.17032100
H	1.82654600	-6.78039900	-2.24144000
H	-0.14300800	-4.40918100	0.74304800
C	-4.66549100	1.06124900	1.02353800
O	-3.90820400	0.56563500	1.86598800
H	-5.01711000	2.43072200	-0.40064400
H	-2.07310000	2.67097200	-1.43225300
C	-3.01339000	0.33566400	-1.58130700
O	-3.51577900	1.07456500	-2.42143400
C	-0.58548400	2.58314000	0.10630700
C	0.07038000	3.73470700	-0.34216400
C	0.05062600	1.76525100	1.05025100
C	1.35265100	4.04507300	0.11417900
H	-0.42126600	4.37919300	-1.06561400
C	1.33746600	2.06734300	1.49876400
H	-0.43549100	0.87337700	1.42942500
C	1.99568500	3.20629000	1.02761600
H	1.85464300	4.93504500	-0.25486000
H	1.83546500	1.40674400	2.20014700
H	3.00248300	3.43249700	1.36449100
C	-3.22228400	4.32392700	0.21540300
C	-2.85376000	5.26563800	1.17830700
C	-3.68396300	4.76420200	-1.03272700
C	-2.94905000	6.63096200	0.90436500
H	-2.48190000	4.92729200	2.14144900
C	-3.78715700	6.12742000	-1.30443200
H	-3.94926800	4.03714100	-1.79753800
C	-3.41846700	7.06435300	-0.33591700
H	-2.65568200	7.35422200	1.65988100
H	-4.14888500	6.45796100	-2.27387100
H	-3.49343800	8.12675500	-0.54964400

C	-6.08398700	0.55584200	0.61400000
O	-6.63034500	1.17550700	-0.30855900
N	-6.68064700	-0.46626900	1.26950600
C	-6.02208200	-1.32393200	2.28409200
C	-8.10468200	-0.76576400	0.95795400
H	-8.37256200	-1.56491200	1.65267000
C	-8.29265300	-1.30970300	-0.46191900
C	2.19784300	-1.39946300	3.64080500
H	2.20332000	-0.65222900	4.44221300
H	2.49702100	-2.35699700	4.08856200
H	2.95617100	-1.12098800	2.90787300
C	-2.82774500	-1.52833900	4.13970700
H	-2.56238000	-1.58251400	5.20019700
H	-3.36918400	-0.59300000	3.96422300
H	-3.51940700	-2.35101200	3.92203500
C	1.02532800	-6.84702900	0.35945700
H	0.90894300	-7.82667300	-0.11703700
H	2.02316900	-6.82340200	0.81658100
H	0.29330300	-6.77227200	1.16996600
C	1.81337700	-4.95063300	-4.26524500
H	2.01739700	-5.99743100	-4.51201700
H	1.12779300	-4.54975400	-5.02004800
H	2.75694800	-4.39759500	-4.35853800
H	-4.99109900	-0.99411300	2.32233300
H	-7.65947300	-2.18633600	-0.62250200
H	-9.33739500	-1.60887100	-0.60383700
H	-8.03979300	-0.55044700	-1.20329700
C	-9.02010800	0.42488600	1.26538700
H	-8.82692600	1.25478100	0.58446900
H	-10.06597500	0.11672800	1.15629500
H	-8.87099900	0.76962000	2.29412700
C	-6.02578700	-2.79634100	1.85882400
H	-5.55890000	-2.91688400	0.87753400
H	-5.44922100	-3.37980700	2.58530000
H	-7.03308500	-3.22619500	1.82018100
C	-6.63273200	-1.10298600	3.67137100
H	-6.56142000	-0.04816200	3.95513400
H	-7.68563300	-1.40357700	3.71811600
H	-6.08573000	-1.69392200	4.41372100
C	6.31391000	1.88886900	-1.60556500
C	5.05108300	1.37849300	-1.31124800
C	4.02293800	1.40524600	-2.25865500
C	4.25490800	1.96868100	-3.50972600
C	5.50739300	2.50944100	-3.80764100

C	6.52848500	2.46821200	-2.85696200
H	7.11417500	1.84104400	-0.87836500
H	3.44838900	1.99406200	-4.23505600
H	5.68654500	2.95788900	-4.78015800
H	7.50625000	2.87947800	-3.08968100
C	2.71877100	0.81826600	-1.78608500
H	2.30253900	1.46995600	-1.01130500
O	3.04109500	-0.45634800	-1.11679200
C	3.89630400	-0.41433000	-0.09513600
O	3.96346900	-1.30725700	0.72325600
N	4.72953100	0.73107600	-0.07400200
S	5.31953800	1.32777000	1.44035400
C	6.83912300	0.43948700	1.71241300
C	8.03645900	1.15303800	1.70029800
C	6.80671000	-0.93611000	1.95802800
C	9.22873400	0.46754400	1.92982800
H	8.02568900	2.22218800	1.52063400
C	8.00928000	-1.59741100	2.17982300
H	5.86112200	-1.46537500	1.94660300
C	9.23427300	-0.91103500	2.17137400
H	10.16787400	1.01382000	1.92328600
H	7.99945200	-2.66861500	2.36341900
O	4.33874400	0.94728800	2.45020500
O	5.64097700	2.73242100	1.19756000
C	10.52326900	-1.64985900	2.43054200
H	10.57600700	-1.99292200	3.47134200
H	10.60603700	-2.53792400	1.79372800
H	11.39411200	-1.01481600	2.24370400
C	0.74700500	1.57753500	-3.11722000
H	0.81531600	2.53316100	-2.60265800
C	1.67256900	0.55147500	-2.82750000
H	1.94151700	-0.18671300	-3.58188800
H	0.24696100	1.60007400	-4.08317500

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C	0.76249900	-3.19947300	1.12835200
C	-0.04576700	-1.85322900	1.19700300
H	1.43820300	-3.22746000	1.98597200
N	1.61895900	-3.29160000	-0.04535200
N	0.60364000	-0.75480500	0.45906800
H	1.50942200	-0.50399600	0.85041600
C	1.55461200	0.14556000	-1.63721000
C	1.95304900	1.42708900	-1.18936900
C	2.84162500	2.17175200	-1.97999300

C	3.31822900	1.67670000	-3.19266900
C	2.90926200	0.41883200	-3.63739500
C	2.03900100	-0.34005300	-2.85997100
P	1.19431000	2.20192200	0.30249000
H	3.13507500	3.16448700	-1.65564500
H	3.99668300	2.27751600	-3.79146700
H	3.26235500	0.02933300	-4.58651800
H	1.71872800	-1.32462700	-3.18147200
Pd	-0.76465900	1.20695400	0.84386300
C	2.38273900	1.89458800	1.65852200
C	3.53333100	1.11521700	1.50485800
C	4.31951300	0.78245800	2.61764900
C	3.94430100	1.27079100	3.87211300
C	2.80295100	2.06438800	4.04850000
C	2.02082200	2.35820500	2.93202600
H	3.81495600	0.74584200	0.52408000
H	4.55053600	1.01795000	4.73925900
H	1.10451800	2.93070500	3.05305700
C	1.28666200	3.99337600	-0.02734400
C	0.21377700	4.57287100	-0.71314200
C	0.22227000	5.93354400	-1.03586600
C	1.31801700	6.70500200	-0.63465600
C	2.39591900	6.15275800	0.07015400
C	2.37205900	4.78640100	0.36637300
H	-0.63352500	3.95470800	-0.99321500
H	1.33010400	7.76781600	-0.86895500
H	3.19758400	4.33888200	0.91243300
C	2.84040500	-2.74011400	-0.07698800
O	3.31730100	-2.09739600	0.87101200
H	1.29830700	-3.74000600	-0.89739000
H	-1.01475700	-1.98140100	0.72350700
C	0.58436600	-0.77571000	-0.94051300
O	-0.15796500	-1.50120300	-1.57989700
C	-0.23894600	-1.42467700	2.63684800
C	-1.52413000	-1.35593600	3.18478500
C	0.86596700	-1.08119800	3.42865200
C	-1.70211800	-0.93901400	4.50522700
H	-2.37463400	-1.60503700	2.56068500
C	0.68534800	-0.66089100	4.74518900
H	1.87104100	-1.13897400	3.01786100
C	-0.60020700	-0.58699800	5.28700500
H	-2.70462700	-0.89224400	4.92234900
H	1.55040900	-0.39677700	5.34590000
H	-0.74062000	-0.26697600	6.31616300

C	-0.18817900	-4.37457000	1.18667400
C	-0.04909200	-5.34547100	2.18210300
C	-1.22418500	-4.48700700	0.24962700
C	-0.93430500	-6.42240100	2.24507200
H	0.75002900	-5.25293300	2.91357800
C	-2.10760700	-5.56372400	0.31473600
H	-1.37846900	-3.72496100	-0.50942500
C	-1.96465600	-6.53330600	1.30964000
H	-0.82154000	-7.16999000	3.02552400
H	-2.91611400	-5.62589900	-0.40740900
H	-2.65841300	-7.36804900	1.36176200
C	3.52844800	-3.04654600	-1.44423200
O	2.84406100	-3.66861100	-2.26642000
N	4.81464100	-2.69269000	-1.67729300
C	5.62010900	-1.80654200	-0.80508000
C	5.48095100	-3.22433000	-2.89716400
H	6.51381400	-2.87885900	-2.81475900
C	4.90281100	-2.63866500	-4.18952000
C	2.39448500	2.55864000	5.41460200
H	2.33245200	3.65300900	5.44162000
H	1.40627600	2.16896900	5.68621900
H	3.10585900	2.24308100	6.18391300
C	5.52228500	-0.11353700	2.46336200
H	6.13686800	-0.11821000	3.36876900
H	5.20191200	-1.14031600	2.25673400
H	6.15378900	0.20685500	1.62663300
C	3.54844400	7.02192500	0.51285600
H	3.90750300	7.65662200	-0.30522800
H	3.24904400	7.68849700	1.33150300
H	4.38900100	6.41824300	0.86843600
C	-0.91749000	6.54290300	-1.81592400
H	-1.86054700	6.02545500	-1.61089300
H	-1.04990600	7.60223700	-1.57394900
H	-0.73584700	6.47454600	-2.89669900
H	4.94690000	-1.47669700	-0.02282800
H	4.95128300	-1.54630400	-4.17176000
H	5.48828200	-2.99343100	-5.04529100
H	3.86470700	-2.94675900	-4.32234400
C	5.51708700	-4.75687300	-2.90422700
H	4.51472000	-5.17315400	-3.01248500
H	6.13333600	-5.10193600	-3.74184800
H	5.95837200	-5.13541400	-1.97616900
C	6.10125200	-0.56458500	-1.56423900
H	5.25519900	-0.02805500	-2.00327900

H	6.60846200	0.10981100	-0.86505600
H	6.81331300	-0.80211900	-2.36225600
C	6.76303800	-2.57848300	-0.13824200
H	6.36512400	-3.41733500	0.44126500
H	7.48300000	-2.97049400	-0.86541400
H	7.30842600	-1.91865300	0.54490100
C	-7.02004300	-0.97622000	0.41054800
C	-5.70290500	-0.56580400	0.21687700
C	-5.08143000	0.29640100	1.14120700
C	-5.78216400	0.69713200	2.28378900
C	-7.09850700	0.28151400	2.48109300
C	-7.71971500	-0.53798200	1.53571900
H	-7.47953100	-1.63908300	-0.31343200
H	-5.30563500	1.36826400	2.99148700
H	-7.64250500	0.60681600	3.36287900
H	-8.74872500	-0.85305700	1.68181500
C	-3.75974800	0.82183400	0.78882000
H	-3.65577400	1.09194500	-0.25847700
O	-2.99742300	-1.01506100	0.42300300
C	-3.57060700	-1.58533500	-0.57766100
O	-3.12360200	-2.45931200	-1.30494900
N	-4.92422700	-1.07963600	-0.85172500
S	-5.29979400	-0.67585600	-2.47774900
C	-3.91197700	0.37710400	-2.89741400
C	-2.68928800	-0.19384400	-3.26089400
C	-4.05816400	1.76043700	-2.77922700
C	-1.60424900	0.64347400	-3.50040000
H	-2.58490200	-1.26909700	-3.31845300
C	-2.95901500	2.58115000	-3.03530600
H	-5.02140300	2.17630700	-2.50386500
C	-1.72039000	2.03669800	-3.40210300
H	-0.64837300	0.20200100	-3.76181200
H	-3.07052300	3.66079100	-2.96758700
O	-6.50438000	0.15515500	-2.39443300
O	-5.26547700	-1.86542100	-3.31804300
C	-0.53635200	2.91634300	-3.71826700
H	-0.21445800	2.77682700	-4.75749800
H	-0.77232800	3.97561000	-3.58051600
H	0.32135700	2.67520700	-3.08256600
C	-2.90767600	1.52167200	1.66949800
H	-2.95843100	1.30655600	2.73318000
C	-2.14850700	2.65256800	1.21402300
H	-2.42610700	3.10336600	0.25983700
H	-1.82340200	3.38008500	1.95718600

M2R

C	0.82892600	-2.98381900	0.89433200
C	-0.30158500	-1.92801300	0.73740700
H	1.46198300	-2.65798700	1.72512000
N	1.71944100	-3.03116300	-0.26229200
N	0.27461000	-0.63002200	0.29189700
H	1.11342000	-0.41243500	0.83196600
C	1.51933100	0.62156000	-1.45763700
C	1.75225400	1.82168400	-0.74906300
C	2.72219200	2.71623000	-1.22477200
C	3.44883100	2.43991600	-2.38082700
C	3.20232800	1.26316900	-3.08861900
C	2.24697100	0.36252900	-2.62670400
P	0.76102300	2.31016000	0.72007900
H	2.89038500	3.64863300	-0.69601800
H	4.19137100	3.14924600	-2.73412100
H	3.74747900	1.04835400	-4.00155400
H	2.04596600	-0.56195200	-3.15636200
Pd	-1.15638200	1.11366800	0.78773500
C	1.77054500	1.85916300	2.16956700
C	2.96570600	1.15063100	2.04258800
C	3.62300800	0.65695000	3.18136300
C	3.07101100	0.91666000	4.43565700
C	1.87919700	1.64508100	4.58868300
C	1.22861500	2.10013900	3.44450800
H	3.37710300	0.93710700	1.06315800
H	3.57038200	0.53231900	5.32254100
H	0.27930800	2.62109000	3.53758300
C	0.71359700	4.12688200	0.66273100
C	-0.20849700	4.72059400	-0.20479100
C	-0.25966300	6.11279900	-0.34192700
C	0.61737100	6.88844800	0.42269900
C	1.53813100	6.31542100	1.31073400
C	1.58252600	4.92280000	1.42060300
H	-0.88111100	4.09124400	-0.78031600
H	0.58125700	7.97175200	0.32801000
H	2.29320700	4.45658500	2.09618400
C	2.85473300	-2.31989100	-0.31760900
O	3.18840100	-1.49801000	0.55076900
H	1.46449600	-3.55421800	-1.09454800
H	-1.02205400	-2.23623500	-0.02346300
C	0.52959300	-0.45669300	-1.09477300
O	0.00405200	-1.14345500	-1.94215200

C	-1.00115600	-1.74172500	2.06607400
C	-2.27808100	-2.27682700	2.25810700
C	-0.36378500	-1.07295700	3.12356400
C	-2.90984900	-2.13805900	3.49563500
H	-2.76675400	-2.77636700	1.42733100
C	-1.00667300	-0.91818600	4.35038600
H	0.63723500	-0.66891300	3.00079200
C	-2.28352700	-1.45422200	4.53865500
H	-3.90161900	-2.55504200	3.63395500
H	-0.50560400	-0.39168800	5.15778700
H	-2.78293800	-1.34710000	5.49810900
C	0.29175700	-4.36716000	1.19956600
C	0.81744100	-5.07930400	2.28260100
C	-0.70044700	-4.95152300	0.40187700
C	0.36210600	-6.36465500	2.57347900
H	1.58449900	-4.62147300	2.90297700
C	-1.15215700	-6.23887100	0.69633000
H	-1.16646500	-4.39677900	-0.40973400
C	-0.62408100	-6.94832600	1.77619000
H	0.77387600	-6.90674700	3.42042000
H	-1.93038300	-6.67994500	0.08026200
H	-0.98402300	-7.94872500	2.00106200
C	3.63428700	-2.62634400	-1.62342900
O	2.97234500	-3.11384100	-2.54631900
N	4.95806200	-2.35359100	-1.71612700
C	5.78548200	-1.80911300	-0.61380300
C	5.64288600	-2.61998300	-3.01044400
H	6.67101500	-2.28790900	-2.85066200
C	5.07597800	-1.77750400	-4.15753400
C	1.31449600	1.91386900	5.96227600
H	1.85349400	2.73019100	6.46001600
H	0.25878400	2.19749100	5.90946100
H	1.39845100	1.03168800	6.60639000
C	4.87193500	-0.17341400	3.02791300
H	5.36279600	-0.34404500	3.99074100
H	4.62028500	-1.14253900	2.58411600
H	5.59019200	0.30999800	2.35579400
C	2.45122200	7.18726800	2.13837100
H	2.90236500	7.98075300	1.53235400
H	1.89971900	7.67529000	2.95191900
H	3.25868600	6.60298000	2.58995000
C	-1.23603500	6.74880100	-1.30112400
H	-2.25916700	6.40284200	-1.11421800
H	-1.22765900	7.83934900	-1.21657900

H	-0.99222000	6.49005300	-2.33863300
H	5.14992900	-1.80448600	0.26429200
H	5.12191400	-0.71397400	-3.90579700
H	5.67664600	-1.94150800	-5.05905700
H	4.04200300	-2.05054600	-4.37219500
C	5.68352900	-4.11705100	-3.33861300
H	4.67970200	-4.49884200	-3.53034100
H	6.29847600	-4.27978900	-4.23075100
H	6.12478100	-4.68324000	-2.51195200
C	6.17451400	-0.35540600	-0.90143700
H	5.27667400	0.25310200	-1.04611600
H	6.74116000	0.05502400	-0.05787000
H	6.80086300	-0.26673100	-1.79672600
C	6.99389700	-2.70261000	-0.31074000
H	6.67671300	-3.73272500	-0.12002200
H	7.73342100	-2.71349100	-1.11801300
H	7.49683800	-2.32902100	0.58783800
C	-5.55634400	-2.50226500	-0.30229200
C	-4.72097200	-1.38713500	-0.40173700
C	-4.61114200	-0.49762500	0.69021500
C	-5.37145500	-0.74592100	1.84936000
C	-6.20313300	-1.85293500	1.93544600
C	-6.28860500	-2.74057400	0.85597700
H	-5.60661100	-3.18254400	-1.14461000
H	-5.31890700	-0.04741200	2.67832200
H	-6.79135000	-2.02239900	2.83274400
H	-6.93710900	-3.60987100	0.91503400
C	-3.77775900	0.68370900	0.57876100
H	-3.60335000	1.05049300	-0.42549600
O	-2.69363900	-3.02859700	-0.92168900
C	-2.93794300	-2.31745400	-1.92318600
O	-2.52793400	-2.32335000	-3.07823700
N	-3.93168700	-1.21214700	-1.57593100
S	-4.51869000	-0.13848700	-2.75300500
C	-3.12841300	0.96952000	-3.04021900
C	-1.95086300	0.51852600	-3.63662400
C	-3.28292500	2.31158400	-2.68131900
C	-0.91172500	1.42615500	-3.83780800
H	-1.85250500	-0.52928700	-3.89394900
C	-2.23639600	3.20456000	-2.90650800
H	-4.22229200	2.64119300	-2.25101000
C	-1.03019000	2.77396600	-3.47968800
H	0.01232800	1.07538700	-4.28704600
H	-2.37002900	4.25519100	-2.65923400

O	-5.54366000	0.66500500	-2.06242500
O	-4.85639900	-0.81166300	-4.00400100
C	0.10360800	3.74197500	-3.71548200
H	0.92382200	3.26514600	-4.25933300
H	-0.22895500	4.61160700	-4.29556500
H	0.51377600	4.11779500	-2.77047300
C	-3.30559300	1.45847500	1.62169000
H	-3.43352200	1.12315400	2.64839500
C	-2.47506000	2.60266000	1.34737700
H	-2.67772000	3.17247800	0.44097900
H	-2.14919400	3.21589000	2.18477000

TS2R

C	-0.37674900	3.10014200	0.86603300
C	0.61564700	1.90444300	0.72758900
H	-1.04196800	2.86084500	1.70040700
N	-1.25161900	3.24380600	-0.29089000
N	-0.12211100	0.68917700	0.29625600
H	-0.99177000	0.59446400	0.82261000
C	-1.48763100	-0.39311000	-1.48073100
C	-1.89717800	-1.55616900	-0.78788000
C	-2.94409900	-2.32515100	-1.31641300
C	-3.57721200	-1.96221600	-2.50351300
C	-3.16535100	-0.81831300	-3.18706800
C	-2.13013100	-0.04139400	-2.67533700
P	-1.04516800	-2.15817300	0.72836800
H	-3.24915400	-3.23162200	-0.80435800
H	-4.37954200	-2.57935400	-2.89702700
H	-3.63944200	-0.53620000	-4.12110200
H	-1.79336700	0.85125500	-3.19032100
Pd	1.03258000	-1.26333800	0.84802800
C	-2.03840700	-1.52561600	2.12414100
C	-3.17411700	-0.73752000	1.94193200
C	-3.82292400	-0.16073700	3.04604000
C	-3.32741600	-0.42088300	4.32317500
C	-2.19545700	-1.22687100	4.53274200
C	-1.54968800	-1.76289300	3.42175800
H	-3.54301600	-0.53023400	0.94439700
H	-3.82336500	0.02427300	5.18328500
H	-0.64433500	-2.34946600	3.55553000
C	-1.29673700	-3.96138600	0.73370600
C	-0.41391200	-4.74829700	-0.01219400
C	-0.57632300	-6.13805800	-0.07087300
C	-1.62819000	-6.71605200	0.64589300

C	-2.51806600	-5.94853300	1.41002600
C	-2.34497200	-4.56255300	1.44447300
H	0.39536000	-4.27437800	-0.55923400
H	-1.75761900	-7.79592100	0.61299200
H	-3.02524100	-3.94967600	2.02785100
C	-2.46439900	2.66993300	-0.34173400
O	-2.89582900	1.91595200	0.54324700
H	-0.94270600	3.72271300	-1.13122800
H	1.36047200	2.10885800	-0.04154300
C	-0.36846600	0.53732800	-1.09162600
O	0.26791000	1.14157200	-1.92914300
C	1.28212000	1.67275500	2.06424000
C	2.57133600	2.15806800	2.29346300
C	0.58484600	1.04723500	3.10938100
C	3.15403400	2.02135600	3.55470600
H	3.11597400	2.63149000	1.48300200
C	1.17825900	0.88893100	4.36025600
H	-0.42604800	0.68246600	2.95907100
C	2.46611900	1.38170900	4.58620200
H	4.15618300	2.40155700	3.71917500
H	0.62942700	0.39452100	5.15694300
H	2.92783800	1.27319500	5.56392600
C	0.34049500	4.39901700	1.16362500
C	0.06049600	5.08792300	2.34719700
C	1.28721300	4.91683000	0.27167500
C	0.71626500	6.28295200	2.64217300
H	-0.66760200	4.68044300	3.04409500
C	1.94056400	6.11311200	0.56728000
H	1.55515700	4.37329700	-0.62919700
C	1.65711900	6.79912000	1.74976600
H	0.49447300	6.80749100	3.56738400
H	2.68102000	6.50060200	-0.12626300
H	2.17181900	7.72826300	1.97823000
C	-3.18750700	3.04853000	-1.66417100
O	-2.46261600	3.49020200	-2.56370900
N	-4.52641800	2.89786900	-1.79444500
C	-5.42829300	2.37986200	-0.73881000
C	-5.15647300	3.29658000	-3.08347000
H	-6.21858500	3.08201400	-2.94685800
C	-4.67319600	2.44189700	-4.25943700
C	-1.68770600	-1.48806200	5.92985900
H	-2.36159800	-2.15790000	6.47869300
H	-0.69779100	-1.95423400	5.91213600
H	-1.61581600	-0.55932200	6.50733000

C	-4.99778000	0.75980100	2.83391600
H	-5.54592700	0.93542000	3.76450000
H	-4.64836500	1.72444100	2.44896900
H	-5.69632600	0.35107300	2.09512300
C	-3.62757400	-6.61046700	2.19091500
H	-4.15844700	-7.35028600	1.58143000
H	-3.23223200	-7.13797200	3.06820200
H	-4.35693300	-5.87655300	2.54689600
C	0.36070300	-6.98022900	-0.90164800
H	1.40766700	-6.73267700	-0.69407600
H	0.21911900	-8.04733100	-0.70677900
H	0.19516700	-6.80997300	-1.97251700
H	-4.80248600	2.20686600	0.12881500
H	-4.83919400	1.38072300	-4.05200600
H	-5.24049000	2.70716400	-5.15844800
H	-3.61261700	2.60635900	-4.45434200
C	-5.01990300	4.80089200	-3.34470200
H	-3.97695200	5.07281000	-3.51214400
H	-5.60143300	5.07189500	-4.23285800
H	-5.40389500	5.37680400	-2.49629700
C	-6.02450400	1.02886500	-1.14888100
H	-5.22846600	0.30900000	-1.36163100
H	-6.64106200	0.63355300	-0.33370000
H	-6.66275500	1.10924300	-2.03612600
C	-6.49686300	3.40860400	-0.35199900
H	-6.03379400	4.35736300	-0.06227900
H	-7.21113400	3.60691100	-1.15832500
H	-7.06623000	3.03149200	0.50462300
C	5.59725400	1.89937900	-0.39885800
C	4.72688200	0.79908200	-0.48280700
C	4.54634800	-0.00075600	0.68240300
C	5.27954400	0.29145100	1.84986900
C	6.15216800	1.36600400	1.89857000
C	6.29549700	2.18311000	0.76829200
H	5.71663400	2.51862600	-1.27974500
H	5.16613200	-0.34781300	2.72003700
H	6.72229000	1.56846300	2.80066000
H	6.97546300	3.03043600	0.79398700
C	3.64351900	-1.12511700	0.62977800
H	3.42211000	-1.50835100	-0.35782200
O	2.97553700	2.86398800	-1.36862000
C	3.03130400	2.14081500	-2.33374100
O	2.75350900	1.95211600	-3.47650500
N	4.00030400	0.58320100	-1.66174700

S	4.46777800	-0.64320600	-2.65297900
C	2.96920500	-1.62688900	-2.86874400
C	1.82973100	-1.07153100	-3.45207000
C	2.98984500	-2.97175500	-2.49446000
C	0.70560500	-1.87325000	-3.64085600
H	1.82873000	-0.02996900	-3.74843200
C	1.85704900	-3.76133700	-2.69772400
H	3.89925300	-3.38521700	-2.07131300
C	0.69614900	-3.22449700	-3.27207900
H	-0.18020000	-1.44373300	-4.09879300
H	1.88932000	-4.81734600	-2.43821900
O	5.42000300	-1.52281900	-1.93949500
O	4.82557100	-0.14449700	-3.98471500
C	-0.52643500	-4.07997600	-3.50170700
H	-0.26327900	-5.03371600	-3.97465100
H	-1.03774100	-4.31298900	-2.55970900
H	-1.24924400	-3.57015100	-4.14550900
C	3.10841100	-1.82825600	1.69959900
H	3.27731000	-1.48915500	2.71912300
C	2.16957400	-2.88841100	1.44917000
H	2.30776600	-3.48738800	0.54949500
H	1.77629100	-3.44717000	2.29623900

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C	-2.18303800	-2.11675100	1.12118300
C	-1.74352300	-0.59733300	1.07016100
H	-1.96013200	-2.48129300	2.12740300
N	-1.44578100	-2.97557400	0.20657800
N	-0.40211800	-0.39010900	0.50437600
H	0.31910400	-0.85886700	1.05162000
C	1.16209900	-0.78106500	-1.37916800
C	2.30110900	-0.10324300	-0.88730600
C	3.54489000	-0.35030800	-1.48853300
C	3.66677000	-1.23433500	-2.55872000
C	2.53605700	-1.88551400	-3.05242500
C	1.29678100	-1.66059900	-2.46274600
P	2.19773100	1.20984700	0.40315800
H	4.42135800	0.18066000	-1.13238700
H	4.63960300	-1.40128100	-3.01204000
H	2.61551000	-2.56143700	-3.89735600
H	0.40716300	-2.16006800	-2.82640400
Pd	0.06303200	1.90816800	0.76460200
C	2.74482100	0.42723400	1.95962900
C	2.90372000	-0.95404000	2.08995900

C	3.07390000	-1.53283500	3.35874100
C	3.11200500	-0.69777200	4.47580400
C	2.97709300	0.69539300	4.36769100
C	2.77786300	1.24428500	3.10325500
H	2.86240800	-1.59256500	1.21365400
H	3.23500900	-1.14108400	5.46152700
H	2.61162100	2.31352100	3.00166100
C	3.49964200	2.37750400	-0.10431600
C	3.19969500	3.20871100	-1.19004100
C	4.15989900	4.08876900	-1.69883800
C	5.41263600	4.13739100	-1.07674100
C	5.72702700	3.33160100	0.02504600
C	4.75950200	2.44001100	0.50111700
H	2.21543300	3.15315200	-1.64898000
H	6.16497700	4.82396100	-1.45921000
H	4.98896900	1.79205100	1.34209700
C	-0.20414400	-3.41172200	0.45619000
O	0.44680800	-3.06835000	1.45617700
H	-1.85121800	-3.25624600	-0.68082000
H	-2.41915600	-0.06481000	0.40207100
C	-0.24731900	-0.63975800	-0.87554100
O	-1.19948400	-0.78077300	-1.61573900
C	-1.83574500	-0.01271000	2.46333000
C	-3.08233100	0.42139000	2.92419100
C	-0.72908100	0.05955400	3.32321000
C	-3.21725700	0.94913900	4.20862500
H	-3.94405800	0.36484500	2.26999600
C	-0.86298100	0.59797400	4.60286700
H	0.24621900	-0.29883300	3.01515100
C	-2.10710300	1.04969000	5.04832000
H	-4.19100500	1.29790800	4.53915600
H	0.00942300	0.65755400	5.24714700
H	-2.21137800	1.46959500	6.04511100
C	-3.66769300	-2.20553000	0.84131900
C	-4.55284400	-2.66603200	1.81935500
C	-4.16588500	-1.76547900	-0.39316100
C	-5.92618200	-2.68807000	1.56891100
H	-4.16795200	-2.99454900	2.78154100
C	-5.53626100	-1.79366800	-0.64276500
H	-3.50393100	-1.36693100	-1.15656300
C	-6.41907600	-2.25345000	0.33697500
H	-6.60885100	-3.04128800	2.33694000
H	-5.89615400	-1.43404500	-1.60136700
H	-7.48863700	-2.26580800	0.14543400

C	0.25372700	-4.37382400	-0.68706100
O	-0.53607500	-4.50012000	-1.63153700
N	1.42237700	-5.05257100	-0.61329800
C	2.46661200	-4.83275000	0.41330500
C	1.69516100	-6.09651400	-1.63869300
H	2.64633300	-6.53649100	-1.33120400
C	1.89499800	-5.50994000	-3.03990700
C	3.03407100	1.57339300	5.59401200
H	4.07132800	1.81192900	5.86271200
H	2.50998000	2.52014600	5.42954400
H	2.58101100	1.07869800	6.45978800
C	3.16747600	-3.03005800	3.50786000
H	3.42247100	-3.31402100	4.53319000
H	2.21085200	-3.49476400	3.24648900
H	3.92954400	-3.44931300	2.84095800
C	7.07576100	3.43491700	0.69537700
H	7.86988100	3.63584600	-0.03142300
H	7.08980200	4.25317400	1.42706900
H	7.32731900	2.51361500	1.23040400
C	3.84368300	4.94954900	-2.89808000
H	2.91327900	5.50998700	-2.75072300
H	4.64343200	5.66876900	-3.09817100
H	3.71087900	4.33592500	-3.79775400
H	2.10397000	-4.01728000	1.02775500
H	2.68506900	-4.75381000	-3.03001700
H	2.19252100	-6.30735100	-3.73020200
H	0.97297500	-5.05502900	-3.40437200
C	0.64752300	-7.21500900	-1.60431400
H	-0.32897400	-6.84843200	-1.92338000
H	0.95601400	-8.02346600	-2.27637300
H	0.55766800	-7.62628500	-0.59333600
C	3.78780300	-4.38943600	-0.22604000
H	3.64089500	-3.49355500	-0.83633200
H	4.51037000	-4.15145900	0.56271300
H	4.23614200	-5.16652600	-0.85501500
C	2.62330100	-6.06135800	1.31523400
H	1.66625000	-6.31404000	1.78244800
H	2.98362600	-6.94007300	0.76875500
H	3.34580300	-5.84829700	2.11021400
C	-5.34803000	1.77177200	-0.45008600
C	-3.97157000	2.14581700	-0.45853700
C	-3.46778900	2.85462300	0.69805900
C	-4.30361900	3.08236200	1.81515800
C	-5.62315700	2.68097700	1.80217900

C	-6.13277800	2.02349100	0.65563800
H	-5.75568400	1.25233500	-1.30911200
H	-3.89748300	3.60878600	2.67451100
H	-6.27127000	2.87894300	2.65040300
H	-7.17172400	1.70284100	0.64712600
C	-2.12740300	3.32512800	0.60434000
H	-1.78088100	3.46734000	-0.41812200
N	-3.04971700	1.84853700	-1.39531700
S	-3.43730600	1.42622100	-2.91926100
C	-1.76331600	1.46519800	-3.57888200
C	-1.27115000	0.38568200	-4.30056600
C	-0.95662500	2.57923300	-3.33481300
C	0.05271800	0.40471000	-4.74734600
H	-1.91022800	-0.47448900	-4.46284900
C	0.36196600	2.58263500	-3.77666800
H	-1.35866100	3.42162200	-2.78398600
C	0.89479400	1.48592100	-4.47219400
H	0.44436900	-0.44866600	-5.29526400
H	0.98958800	3.45058100	-3.58570700
O	-4.22651200	2.47169500	-3.60462400
O	-3.93449300	0.03430600	-3.05005000
C	2.34608200	1.48175600	-4.88678000
H	2.60696000	0.56228000	-5.41948100
H	2.57967800	2.32901700	-5.54414300
H	3.00369200	1.55534600	-4.01138200
C	-1.21033000	3.59489200	1.62587700
H	-1.48412000	3.40781700	2.66220100
C	0.14484300	3.92871500	1.29543400
H	0.34450900	4.47444800	0.37320700
H	0.83591000	4.15886100	2.10389400

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C	-3.38933700	2.57442600	0.57006800
C	-2.14331500	2.54648300	-0.37420400
H	-3.06431700	2.22285300	1.55349800
N	-4.43268700	1.65803200	0.13492700
N	-1.82875700	1.15916200	-0.75358500
H	-1.87908200	0.51434200	0.03393100
C	-2.59031400	-0.82011800	-2.06154000
C	-1.63521400	-1.80113700	-1.69486900
C	-1.91439700	-3.14119300	-2.00325000
C	-3.10022300	-3.51795300	-2.63241700
C	-4.04120400	-2.54840000	-2.97462800
C	-3.78013500	-1.21145700	-2.69323700

P	-0.00881200	-1.30901900	-0.95239900
H	-1.17889800	-3.90289000	-1.77456600
H	-3.27991000	-4.56496600	-2.86051900
H	-4.96474600	-2.82510900	-3.47245600
H	-4.49215500	-0.44046500	-2.96279200
Pd	0.45559000	0.87812000	-1.51268500
C	-0.27238900	-1.54641400	0.85467600
C	-1.22135800	-2.41975500	1.39947800
C	-1.36291100	-2.54040200	2.78684200
C	-0.55386600	-1.75625700	3.61500500
C	0.38787900	-0.85893900	3.09817200
C	0.53238500	-0.77628600	1.70916300
H	-1.86617700	-2.99882200	0.74476100
H	-0.66893200	-1.83695000	4.69448300
H	1.26149100	-0.09138800	1.28488800
C	1.12603100	-2.69088300	-1.38310000
C	2.12960300	-2.41298500	-2.31369700
C	3.06345400	-3.39117500	-2.68485400
C	2.95831200	-4.66093200	-2.11224300
C	1.96091800	-4.96837700	-1.17327000
C	1.06103600	-3.96736700	-0.80380100
H	2.18259300	-1.41472300	-2.74091600
H	3.67758400	-5.42890800	-2.39025700
H	0.31699600	-4.17667500	-0.04132600
C	-4.47993800	0.37161100	0.52687000
O	-3.61260000	-0.15555700	1.23326300
H	-5.16427300	1.94547900	-0.50667200
H	-2.40070700	3.04578000	-1.30728900
C	-2.46117300	0.67437800	-1.90608100
O	-2.94081400	1.42743600	-2.74380600
C	-0.98040500	3.25666100	0.27428100
C	-0.67127200	4.56484800	-0.10679800
C	-0.21869900	2.63620500	1.27071000
C	0.40132000	5.23651200	0.48013800
H	-1.26893600	5.05176800	-0.87234500
C	0.86301400	3.29888500	1.84880100
H	-0.44675900	1.62084600	1.57891900
C	1.17630600	4.59975800	1.45117200
H	0.63765500	6.25058000	0.16990300
H	1.48281700	2.78843100	2.57638600
H	2.02557200	5.11210900	1.89429600
C	-3.92516000	3.98442800	0.67535900
C	-3.78716600	4.70917900	1.86090900
C	-4.51884600	4.59706000	-0.43576500

C	-4.24184700	6.02576000	1.94183000
H	-3.30908300	4.24313000	2.71790400
C	-4.98130300	5.90975700	-0.35428400
H	-4.60683800	4.05252600	-1.37362600
C	-4.84299700	6.62751700	0.83578600
H	-4.12501200	6.58054700	2.86833800
H	-5.44231900	6.37379700	-1.22143700
H	-5.19804700	7.65216800	0.89815500
C	-5.76047100	-0.30033700	-0.05782000
O	-6.37117700	0.36071900	-0.90963700
N	-6.18549200	-1.50604400	0.38066800
C	-5.45335200	-2.37496700	1.33414700
C	-7.49188000	-2.01458400	-0.12065900
H	-7.63562900	-2.96101700	0.40457600
C	-7.46474600	-2.32791800	-1.61990500
C	1.18799300	0.03579100	4.01205000
H	0.59315500	0.91232600	4.30273800
H	1.46786200	-0.48283100	4.93584600
H	2.09255700	0.39956900	3.52186600
C	-2.39092900	-3.46975900	3.38377700
H	-2.06569200	-3.85419600	4.35621700
H	-3.34370500	-2.94901400	3.54040300
H	-2.58667000	-4.32481100	2.72886400
C	1.88825200	-6.34631900	-0.56020300
H	1.71525800	-7.11362800	-1.32455900
H	2.82412500	-6.60687500	-0.05069800
H	1.07762800	-6.41347000	0.17159500
C	4.14733200	-3.06813500	-3.68496400
H	4.92171700	-3.84099900	-3.70076100
H	3.73687600	-2.98603300	-4.69929700
H	4.62786900	-2.11041000	-3.45396000
H	-4.53228600	-1.85113100	1.56984600
H	-6.66258600	-3.03489100	-1.84938100
H	-8.41761300	-2.78276400	-1.91360300
H	-7.31394400	-1.41928300	-2.20428100
C	-8.65359500	-1.09667600	0.27681500
H	-8.59084300	-0.13851900	-0.24037200
H	-9.60262000	-1.57719500	0.01400900
H	-8.64964900	-0.91618800	1.35696600
C	-5.07843600	-3.70735500	0.67571700
H	-4.47440200	-3.53392800	-0.21930700
H	-4.49126200	-4.30712200	1.37818100
H	-5.95572300	-4.29971000	0.39301800
C	-6.24635800	-2.55324400	2.63403600

H	-6.45825600	-1.58123200	3.09096200
H	-7.19679100	-3.07602900	2.48056900
H	-5.65912800	-3.14438000	3.34484600
C	7.03608300	2.23587300	-0.89175200
C	5.74542400	1.74564300	-0.69748200
C	4.79233000	1.79098700	-1.72131100
C	5.13505600	2.33862300	-2.95413700
C	6.43252000	2.80739800	-3.17095300
C	7.37628600	2.74870200	-2.14428300
H	7.76023300	2.21271700	-0.08746400
H	4.38729800	2.39750800	-3.73791100
H	6.70236500	3.22584800	-4.13588900
H	8.38291400	3.12139200	-2.30813900
C	3.44864100	1.20890600	-1.35790500
H	3.55926200	0.12137100	-1.24121300
O	3.09257600	1.72061600	-0.03163000
C	3.95649200	1.48178100	0.96478500
O	3.60786500	1.45176000	2.12600900
N	5.28048100	1.24923600	0.55725900
S	6.28290900	0.25749300	1.59498100
C	5.15337300	-1.07437300	1.91727600
C	4.60009100	-1.21812600	3.18591500
C	4.80006000	-1.91903500	0.86284300
C	3.66705200	-2.23092100	3.39437500
H	4.88162900	-0.53178400	3.97524200
C	3.85563000	-2.91298400	1.08759900
H	5.25640900	-1.79772400	-0.11408600
C	3.26676100	-3.07503900	2.35197100
H	3.22057800	-2.35015200	4.37708700
H	3.56692800	-3.56425200	0.27172000
O	7.35145800	-0.20513000	0.71089300
O	6.58657400	0.97081900	2.82931200
C	2.19450600	-4.10937900	2.57325200
H	2.38695100	-5.01634400	1.99256500
H	1.22009200	-3.71579700	2.26296200
H	2.11723200	-4.38357300	3.62986700
C	2.31151800	1.48907200	-2.30136900
H	2.45711200	1.00989300	-3.26993500
C	1.48820000	2.62916500	-2.21722400
H	1.60966100	3.33755500	-1.40328900
H	1.00143500	3.01012700	-3.11225000

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C	-0.26079500	-2.49625500	2.13048500
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C	-0.04634300	-0.93121500	2.17147000
H	0.60337200	-2.95825400	2.60969000
N	-0.28993300	-3.03439200	0.78186700
N	0.56198000	-0.41030000	0.94906600
H	1.53429400	-0.67799100	0.82197600
C	0.54504900	-0.14025800	-1.48902100
C	1.74312400	0.60808000	-1.62804100
C	2.32805800	0.68630400	-2.89969700
C	1.74500200	0.07296400	-4.00915100
C	0.55181600	-0.63356800	-3.86677600
C	-0.03585700	-0.74211900	-2.61062700
P	2.39753900	1.67451600	-0.25374400
H	3.23417100	1.26755500	-3.03027200
H	2.21532200	0.16605100	-4.98410300
H	0.07259700	-1.08597000	-4.72880600
H	-0.96379000	-1.28110100	-2.47323700
Pd	0.53970000	2.04181500	1.06516100
C	3.70918700	0.67258100	0.54722700
C	4.08469000	-0.60924900	0.13231700
C	5.01354400	-1.35462600	0.87394100
C	5.57945700	-0.77634700	2.01333100
C	5.23006600	0.51108100	2.44158600
C	4.27704100	1.21724700	1.70833500
H	3.65183700	-1.03413200	-0.76869600
H	6.30557100	-1.34650700	2.58906900
H	3.95076700	2.19701100	2.04916300
C	3.32180600	2.97262300	-1.15193100
C	2.59340200	4.08913600	-1.57354900
C	3.21245800	5.11324300	-2.29996900
C	4.57893500	5.00258200	-2.57402900
C	5.33470000	3.90238000	-2.14616300
C	4.69076100	2.88430200	-1.43803100
H	1.53502200	4.15319900	-1.33050500
H	5.07163500	5.79665300	-3.13182500
H	5.25623700	2.01777500	-1.10716200
C	0.84402700	-3.35326100	0.13277200
O	1.96747300	-3.23279700	0.63694100
H	-1.15489800	-3.10030100	0.25776200
H	-1.02367900	-0.45748000	2.23394700
C	-0.21018900	-0.34829500	-0.20879700
O	-1.42764300	-0.51695000	-0.17547000
C	0.78583400	-0.53677400	3.36946200
C	0.25997300	0.31688200	4.34293300
C	2.09594600	-1.01194100	3.50942500

C	1.03071700	0.69779700	5.44163600
H	-0.75659200	0.68423200	4.23556200
C	2.86601900	-0.63250900	4.60734400
H	2.51873300	-1.67320700	2.75726400
C	2.33680900	0.22329400	5.57551800
H	0.61066300	1.36134800	6.19216800
H	3.88120200	-1.00482500	4.70124700
H	2.93744500	0.51466100	6.43283400
C	-1.51506900	-2.85321700	2.89436600
C	-1.43953200	-3.62854100	4.05392600
C	-2.76079000	-2.36977900	2.47002900
C	-2.59155000	-3.92416300	4.78464700
H	-0.47300100	-3.99540900	4.38906400
C	-3.91067900	-2.66521000	3.20114500
H	-2.82549300	-1.75924300	1.57332500
C	-3.82977800	-3.44229600	4.35933800
H	-2.51995600	-4.52648800	5.68579200
H	-4.86916900	-2.27760500	2.87022000
H	-4.72710100	-3.66573100	4.92937900
C	0.51757900	-3.92225200	-1.28156600
O	-0.68544000	-4.06027900	-1.54735600
N	1.50103100	-4.29732200	-2.12707000
C	2.94061800	-3.99261000	-1.94201300
C	1.13147700	-5.07061900	-3.34466600
H	2.08958900	-5.33367700	-3.79779800
C	0.35694800	-4.23321700	-4.36668500
C	5.83826000	1.11585000	3.68312800
H	6.51757400	0.41496600	4.17865700
H	6.40683200	2.02333800	3.44665600
H	5.05784100	1.39737900	4.39950100
C	5.37246800	-2.76058600	0.46427600
H	6.25021800	-3.12361900	1.00795900
H	4.53741600	-3.43993000	0.66701000
H	5.59152300	-2.81942900	-0.60804800
C	6.81583200	3.83006500	-2.43106400
H	7.04682800	4.18393100	-3.44197900
H	7.38458500	4.45575200	-1.73088800
H	7.19031800	2.80603800	-2.33438300
C	2.41317000	6.30509100	-2.76887200
H	3.04680600	7.03625600	-3.28027800
H	1.62097600	6.00110600	-3.46364900
H	1.92541700	6.81049700	-1.92684900
H	2.99740500	-3.36271000	-1.06234400
H	0.91397100	-3.32967200	-4.62680200

H	0.20642100	-4.82049600	-5.27955100
H	-0.61771800	-3.94238300	-3.97259300
C	0.42550700	-6.38466900	-2.99210900
H	-0.55923900	-6.19990500	-2.56129900
H	0.30362100	-6.98511100	-3.90028600
H	1.02078900	-6.96218900	-2.27700300
C	3.50050600	-3.19600400	-3.12553000
H	2.92520500	-2.27992700	-3.28419900
H	4.53619400	-2.91389900	-2.90548000
H	3.51062900	-3.76741600	-4.05994400
C	3.73136000	-5.27113700	-1.65020900
H	3.34574700	-5.75391700	-0.74699000
H	3.68130500	-5.98844000	-2.47718700
H	4.78605300	-5.02882900	-1.48616700
C	-5.75385100	3.81490200	-0.27123900
C	-4.58634600	3.05476700	-0.17217400
C	-3.70086300	3.24775400	0.89767200
C	-3.99945000	4.18616900	1.88125800
C	-5.18740300	4.91593000	1.81577900
C	-6.05526200	4.72795800	0.74018500
H	-6.41901200	3.69042500	-1.11358800
H	-3.29506200	4.34723500	2.69067200
H	-5.42369000	5.63988700	2.58996500
H	-6.97013600	5.30892400	0.66984000
C	-2.43971300	2.42341800	0.84142200
H	-2.67791000	1.36845900	1.03223500
O	-1.96698700	2.47983200	-0.54492800
C	-2.79543100	1.97846400	-1.47985300
O	-2.38723900	1.47568000	-2.49925300
N	-4.16672100	2.11750500	-1.16947100
S	-5.30261500	1.10958300	-2.04542800
C	-4.80259200	-0.53094900	-1.57227800
C	-3.82969000	-1.21751700	-2.29627200
C	-5.45181400	-1.11622300	-0.48167700
C	-3.48949200	-2.51040700	-1.90062000
H	-3.34338400	-0.73386800	-3.13385000
C	-5.10722200	-2.41158900	-0.11551500
H	-6.22291800	-0.56644100	0.04554800
C	-4.11735300	-3.12466900	-0.80891200
H	-2.71334700	-3.04996100	-2.43235400
H	-5.61435300	-2.88429100	0.72042600
O	-6.59464900	1.37971200	-1.41468300
O	-5.11190000	1.30807800	-3.47493000
C	-3.76195200	-4.53020500	-0.39130900

H	-4.47805600	-5.25159600	-0.80665900
H	-3.79101800	-4.63188700	0.69897000
H	-2.76465300	-4.80493500	-0.74199900
C	-1.31232100	2.85433000	1.74471200
H	-1.48411400	2.61195500	2.79288200
C	-0.42456200	3.89740900	1.41169700
H	-0.53701000	4.43368900	0.47290100
H	0.09480000	4.43925000	2.19924200

TS1S

C	-3.21355200	2.57282100	0.71101600
C	-1.86782800	2.35220400	-0.06401500
H	-3.05001600	2.25336700	1.74265800
N	-4.30433100	1.75483200	0.20778100
N	-1.72608800	0.96142500	-0.52156400
H	-1.77178100	0.29093900	0.24392200
C	-2.56113600	-0.93133400	-1.86588800
C	-1.62948600	-1.92772500	-1.47216600
C	-1.95028300	-3.26751400	-1.73054700
C	-3.13888800	-3.62721700	-2.36550800
C	-4.04021700	-2.64087200	-2.76216900
C	-3.75033500	-1.30372400	-2.50770800
P	0.04009000	-1.49680800	-0.77067900
H	-1.24499600	-4.04302500	-1.45607000
H	-3.35038600	-4.67531100	-2.55778200
H	-4.96062000	-2.90659100	-3.27165000
H	-4.44008000	-0.51976000	-2.79846800
Pd	0.40457900	0.69321700	-1.49580900
C	-0.15519300	-1.72007000	1.03494500
C	-1.37979100	-2.04386800	1.62792900
C	-1.50159800	-2.08951500	3.02450400
C	-0.37001300	-1.83408800	3.80032400
C	0.87341700	-1.52449000	3.22875800
C	0.96783400	-1.45324100	1.83686900
H	-2.25045000	-2.24150300	1.01201300
H	-0.45589600	-1.86637800	4.88470900
H	1.90940400	-1.15672700	1.38752900
C	1.10752000	-2.90002800	-1.26645200
C	1.95165000	-2.71960400	-2.36601200
C	2.77266800	-3.75890600	-2.82012700
C	2.71146900	-4.99050600	-2.15908200
C	1.88000900	-5.19589900	-1.04939800
C	1.09529500	-4.13135100	-0.59704400
H	1.97099600	-1.75255800	-2.86307900

H	3.33839900	-5.80897100	-2.50727300
H	0.46590400	-4.26024100	0.27942100
C	-4.52376100	0.50853100	0.66078500
O	-3.79921300	-0.03808200	1.50161600
H	-4.91501300	2.06910400	-0.53887900
H	-1.88261200	2.95562400	-0.97036500
C	-2.41222800	0.55642800	-1.67628700
O	-2.89773900	1.36305500	-2.45858600
C	-0.69143800	2.73849600	0.80249100
C	0.03340500	3.89962500	0.52568200
C	-0.31023000	1.93322200	1.88405400
C	1.14808900	4.23575000	1.29461800
H	-0.27496600	4.53584700	-0.29983000
C	0.80753400	2.26325400	2.64486600
H	-0.86212200	1.02695300	2.12101900
C	1.54137100	3.41271800	2.34900500
H	1.71615500	5.13124200	1.05857500
H	1.12697600	1.60508700	3.44464300
H	2.43008300	3.64892900	2.92606000
C	-3.57266900	4.04053300	0.66983000
C	-3.47244000	4.82933600	1.81758800
C	-3.96089900	4.63326300	-0.53916000
C	-3.76646500	6.19264200	1.76479300
H	-3.15282100	4.37504100	2.75119600
C	-4.26384100	5.99286000	-0.59078200
H	-4.01113400	4.03120500	-1.44425600
C	-4.16717300	6.77566600	0.56221000
H	-3.68210000	6.79755000	2.66301500
H	-4.56837200	6.44226800	-1.53163000
H	-4.39848000	7.83619300	0.52107200
C	-5.78981900	-0.08747100	-0.03045400
O	-6.27499700	0.59635800	-0.94237500
N	-6.33440000	-1.25289300	0.38634700
C	-5.73206600	-2.15951500	1.39340000
C	-7.64248700	-1.66612700	-0.19164200
H	-7.89971300	-2.58159600	0.34534000
C	-7.54089400	-2.02039100	-1.67858500
C	2.08192300	-1.26769000	4.09353700
H	1.78827800	-0.91082300	5.08697200
H	2.66049700	-2.18989400	4.23380700
H	2.74125000	-0.53575100	3.62166100
C	-2.83491700	-2.37476000	3.66953000
H	-2.72281400	-2.60539600	4.73359100
H	-3.49636500	-1.50687300	3.57303600

H	-3.33751900	-3.22312500	3.19037400
C	1.81408800	-6.54596800	-0.37712800
H	1.13215800	-7.21854500	-0.91357100
H	2.79527100	-7.03188500	-0.35448600
H	1.45221500	-6.46144400	0.65193800
C	3.73027600	-3.53901100	-3.96579200
H	4.69167100	-3.15204000	-3.60329000
H	3.93533400	-4.47089100	-4.50218300
H	3.33504600	-2.81181900	-4.68264700
H	-4.78010200	-1.71459800	1.65652600
H	-6.79257700	-2.80214700	-1.83657500
H	-8.50807000	-2.39570500	-2.03160200
H	-7.26812200	-1.14325000	-2.26718500
C	-8.74663200	-0.64424700	0.10325900
H	-8.56776100	0.29134800	-0.42804200
H	-9.71247600	-1.05130700	-0.21604800
H	-8.80174200	-0.43606200	1.17698200
C	-5.45169700	-3.54288700	0.79637400
H	-4.80833800	-3.45889800	-0.08392100
H	-4.93546900	-4.15881200	1.54104800
H	-6.36597200	-4.07451400	0.51016400
C	-6.58583300	-2.22137800	2.66403300
H	-6.72523400	-1.21834000	3.07971200
H	-7.57318900	-2.66203100	2.48630600
H	-6.07978800	-2.83531200	3.41663700
C	5.77719900	3.53117000	-0.43627100
C	4.87565700	2.49467500	-0.69630600
C	3.91400400	2.63329100	-1.72814300
C	3.84272400	3.84464700	-2.44159400
C	4.74466700	4.86814800	-2.18194700
C	5.71938000	4.70036900	-1.19073400
H	6.49541400	3.42770000	0.36899200
H	3.10734300	3.94473500	-3.23191600
H	4.70094600	5.78928700	-2.75485200
H	6.42733000	5.49851100	-0.98670100
C	3.12217700	1.47989000	-2.09163200
H	3.63378200	0.52470400	-2.00562200
O	2.50472100	1.26386600	0.06427000
C	3.49518500	1.06659000	0.81174000
O	3.57706100	0.68435700	1.97542900
N	4.79726500	1.33479700	0.09729000
S	6.24360100	0.65631100	0.72268900
C	5.64065500	-0.97607700	1.10444500
C	5.69088900	-1.42628600	2.41842400

C	5.06369700	-1.74368800	0.09268200
C	5.12113100	-2.65902000	2.72646800
H	6.12671500	-0.79361500	3.18234100
C	4.47592500	-2.96028100	0.42154500
H	5.04982900	-1.37965400	-0.92909000
C	4.47870500	-3.42371400	1.74579300
H	5.14263100	-3.01557000	3.75278800
H	3.99785800	-3.55028400	-0.35208600
O	7.14983100	0.59838700	-0.43089500
O	6.69888800	1.30678100	1.95528300
C	3.75532700	-4.69516500	2.10981900
H	2.67301900	-4.51558000	2.15159400
H	4.06966800	-5.07079700	3.08855600
H	3.92504100	-5.48240300	1.36852400
C	1.91874000	1.49960600	-2.84147900
H	1.81252700	0.73509800	-3.61351100
C	0.87651100	2.44107600	-2.63395900
H	1.05402300	3.28425900	-1.97377200
H	0.10434100	2.57424400	-3.38867100

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C	-3.48287600	2.06414400	0.88843300
C	-2.03631900	2.23451900	0.30317200
H	-3.37993400	1.66075300	1.89759900
N	-4.30572500	1.11135200	0.16254300
N	-1.53351600	0.97937900	-0.29667500
H	-1.50750300	0.21073700	0.37437700
C	-2.00696700	-0.82274300	-1.94976300
C	-0.95343000	-1.71845400	-1.64274000
C	-1.04826500	-3.03385500	-2.11571700
C	-2.13773700	-3.45885600	-2.87800300
C	-3.16232300	-2.56696700	-3.18593000
C	-3.09389900	-1.25690800	-2.71986700
P	0.59181000	-1.15154400	-0.77532700
H	-0.24352800	-3.73035700	-1.91372700
H	-2.17207100	-4.48254500	-3.23993600
H	-4.00612400	-2.88074100	-3.79100600
H	-3.88280100	-0.54777300	-2.94042800
Pd	0.60720400	1.17538400	-1.21724200
C	0.25773800	-1.49121400	0.99326800
C	-0.87274200	-2.18888200	1.43610500
C	-1.11122500	-2.35032300	2.80789000
C	-0.19699700	-1.80632300	3.71382300
C	0.94622400	-1.11341300	3.29396100

C	1.16468600	-0.96201300	1.92326300
H	-1.58047400	-2.59407800	0.72026900
H	-0.38575300	-1.91419600	4.78037600
H	2.03305900	-0.40591300	1.59731800
C	1.82268900	-2.41505200	-1.24690500
C	2.74958800	-2.11906800	-2.24525200
C	3.72697900	-3.05021800	-2.62452500
C	3.72862800	-4.29666600	-1.99613500
C	2.80465900	-4.62303800	-0.99053600
C	1.86258600	-3.66697500	-0.61136300
H	2.76010900	-1.13572800	-2.69395600
H	4.48624800	-5.02675300	-2.27315600
H	1.16850500	-3.88498100	0.19509600
C	-4.35243500	-0.18970800	0.49962600
O	-3.63770800	-0.68121800	1.38013600
H	-4.91800400	1.39684000	-0.59402200
H	-2.08237900	2.94475900	-0.51823300
C	-2.08003700	0.62464900	-1.55115400
O	-2.63066900	1.45392600	-2.26457200
C	-1.10998400	2.74713400	1.37420600
C	-0.57287200	4.03037900	1.27359200
C	-0.79997100	1.95403100	2.48487400
C	0.28256300	4.51516000	2.26101300
H	-0.81810500	4.64612800	0.41211200
C	0.06001600	2.43581700	3.46707100
H	-1.21186100	0.95198400	2.57963400
C	0.60502000	3.71539800	3.35558400
H	0.70819800	5.50993900	2.16645200
H	0.31323300	1.80853900	4.31472000
H	1.28782600	4.08200600	4.11624700
C	-4.14950800	3.42059400	0.93623900
C	-4.36848800	4.06344400	2.15616500
C	-4.51037700	4.06477100	-0.25469800
C	-4.95248700	5.33062300	2.19038400
H	-4.06915500	3.57422600	3.07872400
C	-5.10166300	5.32654300	-0.22083100
H	-4.31376100	3.58202300	-1.20984700
C	-5.32406600	5.96212400	1.00307300
H	-5.11537600	5.82350100	3.14450900
H	-5.38208400	5.81624100	-1.14896800
H	-5.77987800	6.94772100	1.02969100
C	-5.42987300	-0.91865500	-0.36352300
O	-5.98924900	-0.22493000	-1.22447600
N	-5.75914700	-2.20893100	-0.12948200

C	-5.02641000	-3.11664200	0.78575500
C	-6.95409600	-2.76798600	-0.81908700
H	-7.06255400	-3.77210300	-0.40371100
C	-6.74487200	-2.91490000	-2.32950200
C	1.91575200	-0.52410500	4.28719200
H	1.40160700	-0.21709500	5.20517500
H	2.67885600	-1.25871900	4.56792100
H	2.43261600	0.33494600	3.85081000
C	-2.35427500	-3.05118300	3.29554600
H	-2.23851400	-3.39942400	4.32682100
H	-3.21149100	-2.37010300	3.25774100
H	-2.59614300	-3.91813800	2.67022300
C	2.85329000	-5.97455500	-0.31902500
H	2.61600200	-6.77932500	-1.02586800
H	3.85258700	-6.18321700	0.08124400
H	2.13920600	-6.03378700	0.50815300
C	4.78654300	-2.66019000	-3.62229000
H	5.41900600	-1.87583100	-3.19091700
H	5.41820100	-3.51195500	-3.89201700
H	4.34270000	-2.25947000	-4.54119700
H	-4.16197700	-2.55735200	1.12314500
H	-5.86292700	-3.52737400	-2.53710100
H	-7.61656300	-3.40852900	-2.77365600
H	-6.61760000	-1.93771500	-2.79771500
C	-8.23077200	-1.99535900	-0.46760600
H	-8.20545300	-0.98521000	-0.87815000
H	-9.09813300	-2.52133200	-0.88155900
H	-8.35588100	-1.93261800	0.61856100
C	-4.51965200	-4.36216000	0.05039400
H	-3.90167400	-4.07944300	-0.80635400
H	-3.90303900	-4.95461000	0.73551100
H	-5.32962000	-5.01046400	-0.30172900
C	-5.87309000	-3.45419600	2.01654600
H	-6.15593900	-2.53815900	2.54470400
H	-6.78690000	-4.00058800	1.75699800
H	-5.29563700	-4.08085800	2.70413200
C	4.87448100	3.45220500	-0.97992000
C	3.95197700	2.43131400	-1.25045000
C	3.12233300	2.52881200	-2.37993800
C	3.27196000	3.64196400	-3.22734000
C	4.21671800	4.63154000	-2.97501800
C	5.01885600	4.53770500	-1.83926700
H	5.47933100	3.37567000	-0.08613800
H	2.63430500	3.71767000	-4.10233700

H	4.31517000	5.47217600	-3.65589300
H	5.74842500	5.30978400	-1.61291900
C	2.07771400	1.53755300	-2.76001700
H	2.44278800	0.61108800	-3.19049500
O	1.84541100	2.20275500	0.53386700
C	2.94979600	1.71817800	0.88326600
O	3.40614800	1.48199900	2.00421300
N	3.80748600	1.35321500	-0.30120200
S	5.27687300	0.47111500	-0.09825300
C	4.96160100	-0.75814900	1.16063100
C	5.33327700	-0.48597500	2.47914600
C	4.49168600	-2.01198000	0.78959800
C	5.18933700	-1.48157600	3.43641700
H	5.71328600	0.49330300	2.73455600
C	4.33492800	-2.99365100	1.76832200
H	4.27188800	-2.21882400	-0.24601000
C	4.66900300	-2.74181600	3.10151400
H	5.47203200	-1.27643800	4.46577400
H	3.95423200	-3.96970000	1.48576600
O	5.46025400	-0.22173500	-1.38654000
O	6.37194900	1.31371000	0.40747700
C	4.44672300	-3.78953100	4.16334400
H	3.46323700	-3.66096700	4.63582900
H	5.19948600	-3.72551100	4.95604100
H	4.47611100	-4.79994800	3.74267100
C	0.78549500	1.99927300	-3.17836600
H	0.18624500	1.44409800	-3.89473000
C	0.21492200	3.01345800	-2.38535100
H	0.83823800	3.73701400	-1.87173000
H	-0.83555600	3.25495500	-2.51317300

TS2S

C	-3.55724600	2.07334300	0.86269600
C	-2.09556000	2.19518300	0.29282100
H	-3.47287300	1.72101400	1.89250900
N	-4.38166800	1.09475600	0.17575100
N	-1.61848700	0.93388700	-0.31002500
H	-1.57683900	0.17259800	0.36795200
C	-2.08340800	-0.89253900	-1.91968600
C	-1.01306700	-1.76221500	-1.59129500
C	-1.09395000	-3.09334500	-2.02253200
C	-2.18028400	-3.55660100	-2.76595000
C	-3.21765600	-2.68844000	-3.09966700
C	-3.16688900	-1.36482500	-2.67288700

P	0.55065200	-1.16014500	-0.77438000
H	-0.27856100	-3.77209800	-1.80323600
H	-2.20260100	-4.59197000	-3.09393200
H	-4.05836300	-3.03253800	-3.69248200
H	-3.96776100	-0.67407400	-2.90853200
Pd	0.49239500	1.17057300	-1.25707200
C	0.28504800	-1.49273400	1.00783200
C	-0.88047100	-2.08340700	1.50869000
C	-1.06772100	-2.22124700	2.89238700
C	-0.06861500	-1.75568200	3.74972300
C	1.11434900	-1.17416600	3.27186800
C	1.28228600	-1.05215000	1.89181000
H	-1.65237000	-2.43069500	0.83017500
H	-0.21356100	-1.84477100	4.82456400
H	2.19330300	-0.61072400	1.50778400
C	1.78332000	-2.40426000	-1.27854800
C	2.62226900	-2.11804400	-2.35490400
C	3.59409700	-3.03833400	-2.77387500
C	3.68101600	-4.25760900	-2.09950700
C	2.84716300	-4.57203700	-1.01471600
C	1.90341400	-3.63115100	-0.60425200
H	2.55585000	-1.15673000	-2.84938000
H	4.43729700	-4.97637700	-2.40785400
H	1.27181000	-3.83908300	0.25440800
C	-4.40923900	-0.19476300	0.55408600
O	-3.68202000	-0.64441400	1.44732500
H	-4.99673800	1.34989900	-0.58941400
H	-2.10417900	2.91921400	-0.51834400
C	-2.18448900	0.55891700	-1.54898000
O	-2.76373400	1.36968900	-2.26033800
C	-1.16064300	2.65235500	1.38472000
C	-0.60421900	3.93142500	1.34094600
C	-0.86074200	1.80647100	2.46021500
C	0.25899300	4.35921900	2.34917000
H	-0.84181300	4.58960100	0.50934300
C	0.00821800	2.23065900	3.46174100
H	-1.29334100	0.81035100	2.51654800
C	0.57135600	3.50692000	3.40755400
H	0.69742000	5.35155600	2.29922500
H	0.25111900	1.55967900	4.27911000
H	1.25844000	3.83102000	4.18349300
C	-4.20608600	3.43852100	0.83170800
C	-4.44512400	4.13943600	2.01525100
C	-4.53238800	4.02969200	-0.39662800

C	-5.01511700	5.41307100	1.97715600
H	-4.17567100	3.68937800	2.96656900
C	-5.11010900	5.29756300	-0.43437900
H	-4.31919800	3.49935000	-1.32250400
C	-5.35244000	5.99193600	0.75344800
H	-5.19487000	5.95138900	2.90325700
H	-5.36467800	5.74625900	-1.39025300
H	-5.79780100	6.98218000	0.72368000
C	-5.47869300	-0.96866500	-0.27788100
O	-6.05623000	-0.31068800	-1.15450200
N	-5.78151300	-2.25698900	-0.00163000
C	-5.02101100	-3.12429000	0.93024600
C	-6.97239300	-2.85915500	-0.66160500
H	-7.05732900	-3.85169400	-0.21421100
C	-6.77591600	-3.04841300	-2.16900400
C	2.17769600	-0.68680800	4.22312800
H	1.74390800	-0.41310100	5.19127300
H	2.92450500	-1.46791500	4.40249500
H	2.70683800	0.17571100	3.81040000
C	-2.33379700	-2.83015300	3.44098700
H	-2.22118700	-3.09956900	4.49571200
H	-3.16670100	-2.12532000	3.35011600
H	-2.61058100	-3.73586600	2.88877200
C	3.00203200	-5.88695900	-0.28928400
H	3.99010100	-5.96244500	0.18137800
H	2.24799200	-6.00006800	0.49594900
H	2.90649600	-6.73669600	-0.97566700
C	4.56181300	-2.66879100	-3.86662400
H	5.25307600	-1.90892600	-3.48535800
H	5.13879300	-3.53553100	-4.20334900
H	4.04327700	-2.24362300	-4.73378100
H	-4.16368400	-2.53992200	1.24149300
H	-5.88379900	-3.64875700	-2.36800000
H	-7.64193900	-3.57332200	-2.58758200
H	-6.67429500	-2.08392600	-2.66882100
C	-8.25938500	-2.09930700	-0.32033000
H	-8.25616500	-1.10157900	-0.76097000
H	-9.12088100	-2.65261400	-0.71009200
H	-8.37553500	-2.00657300	0.76467700
C	-4.49842900	-4.38032100	0.22469300
H	-3.89835500	-4.11038000	-0.64868600
H	-3.85981500	-4.93888200	0.91809200
H	-5.29933400	-5.05535600	-0.09665800
C	-5.84586400	-3.44140400	2.18098700

H	-6.14359900	-2.51567300	2.68337000
H	-6.74956700	-4.01672000	1.95002500
H	-5.24609200	-4.03237400	2.88103200
C	4.91809300	3.50839300	-0.78612900
C	4.01389700	2.49503000	-1.15920700
C	3.04415900	2.77938000	-2.14548300
C	3.00516000	4.06326200	-2.72796600
C	3.90862900	5.04877900	-2.35555200
C	4.86850000	4.76423000	-1.37845700
H	5.64927600	3.28726000	-0.02063600
H	2.28186500	4.26536100	-3.51096300
H	3.87548900	6.02490100	-2.83085200
H	5.57753800	5.52864900	-1.07187400
C	2.14493200	1.72901300	-2.65174600
H	2.63651900	0.81338800	-2.96345900
O	1.85714500	2.07946800	0.68239300
C	2.91908800	1.73251500	1.13169800
O	3.59643400	1.58428600	2.10655200
N	3.93573600	1.25415500	-0.47781900
S	5.35874600	0.38815000	-0.46429000
C	5.16161500	-0.74644000	0.90663000
C	5.71003900	-0.41906900	2.14653300
C	4.55416100	-1.98011900	0.69836000
C	5.62300600	-1.33592700	3.18939600
H	6.19310300	0.54037300	2.27982100
C	4.45749900	-2.88163500	1.75689800
H	4.18144100	-2.22942300	-0.28269300
C	4.99226800	-2.57605600	3.01352300
H	6.04409300	-1.08435100	4.15960400
H	3.96640800	-3.83759500	1.59978700
O	5.39915800	-0.42833100	-1.69918000
O	6.55957900	1.19503300	-0.15988900
C	4.91690700	-3.57343200	4.14414700
H	4.94552800	-3.07700600	5.11981100
H	5.76125600	-4.27465600	4.11067700
H	3.99813800	-4.16765200	4.09074700
C	0.85216100	2.03703500	-3.17702700
H	0.39800100	1.41758900	-3.94614600
C	0.07124500	2.96171600	-2.45211200
H	0.53753300	3.75303400	-1.87610300
H	-0.97819300	3.07984800	-2.70418300

M3S

C	-3.86199400	1.87418100	0.45337700
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C	-2.49790800	2.14566700	-0.29747800
H	-3.62469500	1.80300000	1.51745900
N	-4.49129900	0.61141100	0.10255800
N	-1.84862200	0.89717800	-0.72823600
H	-1.65798100	0.27581100	0.05812300
C	-2.17478200	-1.23981600	-1.93961800
C	-0.96471900	-1.89468200	-1.59617700
C	-0.89041300	-3.28177700	-1.78682600
C	-1.96722400	-4.00744500	-2.29678000
C	-3.14864400	-3.35285900	-2.64034300
C	-3.24654800	-1.97661500	-2.46173900
P	0.55415300	-0.94261700	-1.12606600
H	0.03748500	-3.79748400	-1.57168100
H	-1.87147100	-5.08005600	-2.43963500
H	-3.98657500	-3.90430400	-3.05282600
H	-4.15755200	-1.44839200	-2.71541200
Pd	0.20484200	1.27093700	-1.75436900
C	0.61563500	-0.91986100	0.70270700
C	-0.25264400	-1.63450800	1.53274000
C	-0.18563900	-1.47493000	2.92386100
C	0.77946200	-0.61142300	3.45499600
C	1.66646400	0.10609100	2.64125800
C	1.56382100	-0.04807800	1.25765400
H	-0.99656400	-2.29610000	1.10040100
H	0.83524300	-0.48469400	4.53439400
H	2.22446900	0.51623200	0.60622600
C	1.95594700	-2.00225500	-1.59626800
C	2.74677600	-1.60594300	-2.67694300
C	3.88339300	-2.33935100	-3.03821100
C	4.19595700	-3.48093400	-2.29402800
C	3.42143300	-3.89824600	-1.20355800
C	2.29492200	-3.14792600	-0.86050600
H	2.49242600	-0.70001700	-3.21876700
H	5.09075700	-4.04349900	-2.54976400
H	1.70684000	-3.42652500	0.01029500
C	-4.16346500	-0.53555700	0.72520300
O	-3.22412500	-0.61155000	1.52680700
H	-5.26707900	0.56171500	-0.54937000
H	-2.70671000	2.69314300	-1.21376100
C	-2.44637700	0.23195100	-1.82233700
O	-3.17942200	0.82095200	-2.60348400
C	-1.61526000	2.96941000	0.60817800
C	-1.54745500	4.35418100	0.42779500
C	-0.95141200	2.38715500	1.69626300

C	-0.81457700	5.14920100	1.31056300
H	-2.08090700	4.80973000	-0.40198600
C	-0.21630000	3.18043000	2.57469400
H	-1.01255900	1.31790400	1.87375800
C	-0.14717600	4.56187800	2.38585300
H	-0.76899400	6.22374000	1.15855100
H	0.29970700	2.71531900	3.40781000
H	0.42423100	5.17664200	3.07488300
C	-4.80892500	3.02610400	0.20964400
C	-5.16386200	3.88611300	1.25101300
C	-5.31289100	3.25734300	-1.07802200
C	-6.02092000	4.96238300	1.01529200
H	-4.76275800	3.71503300	2.24616100
C	-6.17623100	4.32670800	-1.31084500
H	-5.01383100	2.60661500	-1.89692800
C	-6.53169400	5.18150600	-0.26437100
H	-6.28948900	5.62712300	1.83126500
H	-6.56577200	4.49690300	-2.31034500
H	-7.20059700	6.01741200	-0.44779100
C	-5.13483400	-1.67421600	0.28466700
O	-5.96110600	-1.36446600	-0.58496400
N	-5.09596300	-2.89339300	0.86596300
C	-4.05455500	-3.34897800	1.81871700
C	-6.17890800	-3.86385400	0.54263600
H	-5.96883000	-4.72680100	1.17808000
C	-6.12501300	-4.34315600	-0.91098700
C	2.69778200	1.03900100	3.22022500
H	2.61111200	1.10261000	4.31002100
H	3.70883900	0.69955500	2.97748300
H	2.59204000	2.04433000	2.80031700
C	-1.16672000	-2.18448500	3.82294800
H	-0.83855900	-2.16857000	4.86687500
H	-2.14942200	-1.70195500	3.76684600
H	-1.29865300	-3.23105100	3.52515800
C	3.84873300	-5.07511400	-0.36192900
H	4.58206800	-4.75670400	0.39016300
H	3.00051000	-5.51824000	0.17059800
H	4.31849100	-5.85554300	-0.96941100
C	4.78500000	-1.86032900	-4.14374500
H	5.54308900	-1.19840300	-3.70996900
H	5.29740300	-2.69432000	-4.63445100
H	4.22698900	-1.30187400	-4.90276000
H	-3.34711500	-2.53184800	1.89632400
H	-5.14891600	-4.78218200	-1.13534800

H	-6.89101400	-5.11040800	-1.06998300
H	-6.30795400	-3.51552800	-1.59770000
C	-7.55928700	-3.33255300	0.94522800
H	-7.84929500	-2.48146900	0.32770300
H	-8.30368400	-4.12662800	0.82063000
H	-7.56178200	-3.02426800	1.99603900
C	-3.30311200	-4.56932800	1.27508000
H	-2.86497800	-4.34808800	0.29770100
H	-2.49141900	-4.82874700	1.96377700
H	-3.94276100	-5.45318600	1.17661400
C	-4.64790100	-3.58576300	3.21125700
H	-5.13033500	-2.67517200	3.58048000
H	-5.38567800	-4.39561200	3.22066300
H	-3.85030800	-3.85709100	3.91053500
C	4.85939900	2.79209100	0.77416700
C	4.24871900	2.18256300	-0.37359200
C	3.01006000	2.79445500	-0.86190800
C	2.43921000	3.87631700	-0.13374600
C	3.03878700	4.39555300	0.98670100
C	4.26867000	3.84716000	1.42479400
H	5.81531700	2.41899500	1.11153200
H	1.51852700	4.32197300	-0.48185300
H	2.58657400	5.22728000	1.51561600
H	4.76215800	4.27097100	2.29657300
C	2.49053500	2.30715600	-2.08934800
H	3.14833200	1.57927100	-2.55745000
N	4.69856700	1.09811500	-1.02832500
S	6.09496500	0.34214000	-0.60923700
C	5.65774500	-0.52291300	0.90469000
C	6.33986800	-0.28954200	2.09484800
C	4.59667000	-1.42669600	0.85769400
C	5.93471200	-0.95807300	3.25387400
H	7.17102300	0.40728900	2.10406900
C	4.20175800	-2.08344200	2.01573100
H	4.08085200	-1.58930500	-0.07691500
C	4.85712000	-1.85105600	3.23491800
H	6.45638900	-0.77205600	4.18952500
H	3.35463200	-2.76373100	1.98178800
O	6.32465700	-0.68876000	-1.63381500
O	7.21133200	1.24993200	-0.27144500
C	4.37655000	-2.53094400	4.49299100
H	4.97592600	-2.24076500	5.36136800
H	4.42299900	-3.62322100	4.40182600
H	3.33076000	-2.26960600	4.69937400

C	1.37326400	2.68872700	-2.89895300
H	1.42292300	2.33883500	-3.92908200
C	0.17440000	3.31038900	-2.49062700
H	0.10107300	3.92613200	-1.60436700
H	-0.58126600	3.50333800	-3.24845300

TS3S

C	-4.01335800	2.06334000	0.86140400
C	-2.54325300	2.27930400	0.31361900
H	-3.92487500	1.76316900	1.90745100
N	-4.72642500	0.98678600	0.19778500
N	-2.02578300	1.10195800	-0.38680900
H	-1.86507000	0.30169700	0.21997700
C	-2.37517600	-0.61087500	-2.13653700
C	-1.20808800	-1.40080500	-1.98136800
C	-1.18842800	-2.68049200	-2.55363200
C	-2.28622700	-3.17892600	-3.25494300
C	-3.43038200	-2.39578900	-3.40378600
C	-3.46866500	-1.11890800	-2.85025500
P	0.30494300	-0.66267800	-1.22944400
H	-0.28932300	-3.28067900	-2.47838200
H	-2.23910200	-4.17159000	-3.69401000
H	-4.28540600	-2.76815800	-3.95804800
H	-4.34743800	-0.49466800	-2.96066300
Pd	0.28579600	1.65159600	-1.23168400
C	0.22579600	-1.11927500	0.55151100
C	-0.75622500	-1.93405900	1.12270200
C	-0.78184200	-2.14967200	2.50931600
C	0.20852800	-1.55878100	3.30073900
C	1.21038500	-0.74810800	2.74986400
C	1.19563600	-0.52673000	1.37370100
H	-1.51199700	-2.39660300	0.49447300
H	0.19525100	-1.72668800	4.37594200
H	1.95187100	0.11648400	0.93437900
C	1.74191300	-1.64683000	-1.79499900
C	2.71632400	-0.96949500	-2.53807400
C	3.93416100	-1.57991100	-2.86041700
C	4.13714500	-2.90376700	-2.45475900
C	3.17328100	-3.61296900	-1.72651400
C	1.97969600	-2.96746700	-1.38923900
H	2.52902400	0.05803400	-2.83488100
H	5.08884100	-3.38126800	-2.67607400
H	1.24918300	-3.48542500	-0.77287100
C	-4.59083600	-0.29593000	0.57483300

O	-3.80928400	-0.66136000	1.46180000
H	-5.39527500	1.16720400	-0.54318600
H	-2.56704600	3.07462300	-0.42861900
C	-2.56006500	0.79869500	-1.63684800
O	-3.18827400	1.62544000	-2.28895800
C	-1.63159900	2.66805800	1.45309900
C	-1.08777000	3.95322000	1.51287700
C	-1.35540300	1.75806600	2.48192800
C	-0.26298700	4.32462200	2.57556800
H	-1.30821600	4.66053900	0.71868700
C	-0.53233800	2.12831200	3.54330200
H	-1.78648700	0.76070000	2.45845200
C	0.01900500	3.41074500	3.59229800
H	0.15587400	5.32639800	2.60970600
H	-0.32433000	1.41177300	4.33163500
H	0.65868000	3.69822800	4.42208300
C	-4.79127500	3.35527300	0.76487500
C	-5.20029300	4.02542000	1.91995500
C	-5.08643500	3.90434900	-0.49126900
C	-5.90363100	5.22777600	1.82737700
H	-4.96298300	3.60587200	2.89396900
C	-5.79772100	5.09956600	-0.58282900
H	-4.74192100	3.39935300	-1.39086700
C	-6.20748800	5.76416500	0.57589100
H	-6.21484700	5.74221400	2.73213000
H	-6.02588400	5.51635000	-1.55969400
H	-6.75731700	6.69818500	0.50239700
C	-5.57899800	-1.19084300	-0.23649600
O	-6.31254200	-0.59624900	-1.03802300
N	-5.66007900	-2.52139500	-0.00973200
C	-4.69166400	-3.30194300	0.79645900
C	-6.80014400	-3.27003600	-0.60539700
H	-6.70452400	-4.27928900	-0.19901100
C	-6.70283400	-3.37618400	-2.13036500
C	2.26493900	-0.09604400	3.60730000
H	3.25611400	-0.19760800	3.15623500
H	2.06026600	0.97592100	3.71634100
H	2.29873000	-0.53829400	4.60792700
C	-1.87961000	-2.97277800	3.13471700
H	-1.63852600	-3.24434600	4.16726500
H	-2.81887000	-2.40859800	3.13910300
H	-2.05533100	-3.89803000	2.57368700
C	3.46256900	-5.00827100	-1.23027800
H	4.07511200	-4.96951500	-0.32020700

H	2.54081100	-5.54681900	-0.98668600
H	4.01520300	-5.59298000	-1.97302000
C	5.02739600	-0.81356000	-3.56045300
H	4.68176200	0.17881300	-3.86643000
H	5.88054700	-0.68928800	-2.88382900
H	5.38071500	-1.34314600	-4.45299500
H	-3.90213900	-2.60854000	1.06121900
H	-5.75359000	-3.83218100	-2.42437100
H	-7.51726600	-4.00604600	-2.50582400
H	-6.77949500	-2.39017800	-2.59112600
C	-8.15102300	-2.72144200	-0.13194000
H	-8.32965500	-1.72059800	-0.52697600
H	-8.95242500	-3.38392100	-0.47719400
H	-8.18757400	-2.68138500	0.96189800
C	-4.06437900	-4.43521100	-0.02347600
H	-3.59968000	-4.04448500	-0.93315500
H	-3.28608000	-4.91938900	0.57693300
H	-4.78685900	-5.20888400	-0.30459300
C	-5.33640500	-3.79122000	2.09686300
H	-5.68841400	-2.93882300	2.68608300
H	-6.18456000	-4.46052800	1.91315500
H	-4.60309400	-4.34197400	2.69482300
C	6.90706200	2.55869800	-0.69667100
C	5.59194200	1.95792500	-0.58783500
C	4.45127000	2.73865400	-1.14764500
C	4.70532900	4.04016700	-1.72853300
C	5.96141200	4.54583000	-1.79398500
C	7.06589300	3.78223600	-1.27105200
H	7.75505100	2.02409100	-0.28932100
H	3.85193800	4.59598700	-2.10312700
H	6.14914700	5.52179600	-2.23034200
H	8.06450300	4.20776700	-1.33173000
C	3.20760500	2.17924900	-1.14768700
H	3.14431200	1.19704700	-0.69203400
N	5.30959500	0.78840500	-0.06218400
S	6.48908800	-0.28256300	0.42879200
C	5.49044200	-1.33702900	1.46767700
C	5.91548500	-1.61026300	2.76503800
C	4.33447300	-1.92230900	0.94767700
C	5.15961700	-2.47864300	3.55521200
H	6.81536200	-1.13773100	3.14236200
C	3.59666000	-2.78585500	1.74753000
H	4.01076800	-1.68539100	-0.05601600
C	3.99337500	-3.07413200	3.06223000

H	5.47695600	-2.68740700	4.57356500
H	2.68040700	-3.21661100	1.35653200
O	6.91818500	-1.05616300	-0.75254400
O	7.52876600	0.32405900	1.28188400
C	3.15244100	-3.98635600	3.91914100
H	2.10886500	-3.65020500	3.92962400
H	3.51484000	-4.01602500	4.95121700
H	3.15800200	-5.01322400	3.53237800
C	1.98920300	2.73290800	-1.78960500
H	2.04812200	2.75182500	-2.88201400
C	1.08891700	3.64523600	-1.18373600
H	1.23404500	3.95985800	-0.15337600
H	0.52305600	4.32876300	-1.81369100

M4S

C	-4.09920200	1.81420400	0.64427300
C	-2.60894800	2.20453900	0.27374600
H	-4.08907800	1.51056400	1.69343100
N	-4.61384600	0.67218600	-0.09263800
N	-1.87955100	1.09412700	-0.35753900
H	-1.77067600	0.29092800	0.25979800
C	-1.98993200	-0.64636100	-2.12274300
C	-0.82422400	-1.39847800	-1.83180600
C	-0.71901400	-2.69020700	-2.36694600
C	-1.72813600	-3.23239200	-3.16328400
C	-2.86682700	-2.48211200	-3.45143700
C	-2.99081700	-1.19598600	-2.93470500
P	0.61640300	-0.61791900	-0.97825600
H	0.18131100	-3.26641800	-2.18917800
H	-1.61203800	-4.23335300	-3.56922800
H	-3.65067400	-2.88706400	-4.08226000
H	-3.86935200	-0.59917700	-3.14678100
Pd	0.37327600	1.70590400	-0.95192300
C	0.40520800	-0.96743900	0.81211400
C	-0.56606900	-1.81658900	1.34859000
C	-0.69264000	-1.95662300	2.73946700
C	0.17821000	-1.24119800	3.56834200
C	1.16294600	-0.38784200	3.05102800
C	1.26341300	-0.25792100	1.66631700
H	-1.23329100	-2.36464100	0.69014000
H	0.08342600	-1.34597300	4.64750500
H	2.02853300	0.38885000	1.24501800
C	2.06159800	-1.64178100	-1.40667800
C	3.04310300	-1.10172600	-2.24374100

C	4.20815900	-1.82610400	-2.52909100
C	4.35811200	-3.09530500	-1.95985300
C	3.39292900	-3.65387700	-1.11335900
C	2.24008700	-2.91419800	-0.84247000
H	2.91890600	-0.09914700	-2.64200500
H	5.27118700	-3.65258300	-2.15726900
H	1.49621300	-3.31266900	-0.15755500
C	-4.38568600	-0.58703700	0.32249600
O	-3.62159100	-0.85012500	1.25906200
H	-5.26925700	0.78108300	-0.85918900
H	-2.63624400	2.99494400	-0.47309900
C	-2.27430200	0.75632800	-1.66424200
O	-2.86500800	1.55603900	-2.37825300
C	-1.92348900	2.69893500	1.52359600
C	-1.75968000	4.07150500	1.72940200
C	-1.53793700	1.80527600	2.53083300
C	-1.18971800	4.54895700	2.91031900
H	-2.07899300	4.76740900	0.95875100
C	-0.97286600	2.28172100	3.71200800
H	-1.69046700	0.73764000	2.40664200
C	-0.79107600	3.65326300	3.90370500
H	-1.06106700	5.61784700	3.05404800
H	-0.68084700	1.57626200	4.48304900
H	-0.34945900	4.02171600	4.82517900
C	-4.99984900	3.01397500	0.46533300
C	-5.58893200	3.62886300	1.57238000
C	-5.22747600	3.53612600	-0.81597800
C	-6.40523600	4.74896900	1.40586400
H	-5.40318500	3.23177400	2.56661300
C	-6.05106100	4.64839000	-0.98215900
H	-4.74363400	3.07743400	-1.67524800
C	-6.64124300	5.25731400	0.12829200
H	-6.85693200	5.22143300	2.27340700
H	-6.22616400	5.04452400	-1.97829300
H	-7.27863600	6.12710100	-0.00249900
C	-5.23365400	-1.58919800	-0.51940100
O	-5.94504300	-1.08369300	-1.39862100
N	-5.22535400	-2.91241500	-0.24405500
C	-4.28440000	-3.57918600	0.68843100
C	-6.23304600	-3.77975900	-0.91466000
H	-6.08280200	-4.76500000	-0.46812000
C	-5.98496600	-3.91527000	-2.41986400
C	2.07202200	0.41040100	3.94920200
H	3.06723100	0.50987300	3.51004200

H	1.67114900	1.42120900	4.09684200
H	2.17835700	-0.05687600	4.93311000
C	-1.77280800	-2.83252300	3.32294100
H	-1.61134300	-3.01025200	4.39064300
H	-2.75325900	-2.35958300	3.19784200
H	-1.81267700	-3.80618700	2.82049900
C	3.63349400	-4.98411400	-0.44309000
H	4.26770300	-4.85500800	0.44345900
H	2.69547100	-5.44417600	-0.11498100
H	4.14413300	-5.68542600	-1.11135100
C	5.30896800	-1.23715300	-3.36985700
H	4.96794600	-0.35621900	-3.91952300
H	6.13334900	-0.92748500	-2.71861400
H	5.69602200	-1.97050900	-4.08669600
H	-3.60175000	-2.80649500	1.02104100
H	-4.97525400	-4.28892900	-2.61170400
H	-6.70124300	-4.62743300	-2.84476000
H	-6.10730900	-2.95282000	-2.91882900
C	-7.66610300	-3.34800300	-0.58342000
H	-7.89688800	-2.37836800	-1.02640200
H	-8.36866300	-4.09050000	-0.97750800
H	-7.80813300	-3.28442900	0.50058100
C	-3.46032500	-4.65525400	-0.02698800
H	-2.93157700	-4.22854800	-0.88411000
H	-2.71579400	-5.05709300	0.66942800
H	-4.06776500	-5.49715400	-0.37678000
C	-5.02108000	-4.10974700	1.92215000
H	-5.53593500	-3.29214300	2.43643800
H	-5.75887700	-4.87885100	1.66808300
H	-4.30459100	-4.55564500	2.61966000
C	6.22552000	1.84342800	-2.14716500
C	5.01336300	1.80633200	-1.36669400
C	3.85112000	2.47042100	-1.95168800
C	3.89520500	2.87005600	-3.32340300
C	5.04295100	2.77936900	-4.06443500
C	6.22623400	2.29795100	-3.43907000
H	7.13692800	1.45056700	-1.71798200
H	3.00396200	3.29382300	-3.77456500
H	5.06435300	3.10727300	-5.09886100
H	7.15500600	2.27691000	-4.00389500
C	2.75865100	2.79308200	-1.12307500
H	2.90426200	2.61438800	-0.06009200
N	4.85826200	1.21633100	-0.17506600
S	6.15646500	0.47919800	0.53774100

C	5.32869200	-0.51532700	1.77271700
C	5.73009600	-0.43608400	3.10263100
C	4.37993300	-1.45157100	1.36364000
C	5.15429500	-1.30075400	4.03716700
H	6.47859400	0.29486800	3.38832100
C	3.80914800	-2.29757400	2.30560400
H	4.08753900	-1.49615000	0.32476100
C	4.18363700	-2.23348100	3.65646800
H	5.45491700	-1.23887700	5.08011600
H	3.04369600	-3.00284600	1.99340600
O	6.81642700	-0.48178700	-0.37775500
O	7.01839400	1.44364600	1.24861300
C	3.51758300	-3.13316100	4.66749100
H	2.43363400	-2.96201200	4.68199800
H	3.90295800	-2.95905200	5.67685800
H	3.67256200	-4.19201700	4.42632200
C	1.56746100	3.46217100	-1.52578100
H	1.43338700	3.70485800	-2.57622900
C	0.54312100	3.82030900	-0.63073300
H	0.73517800	3.87988500	0.43886100
H	-0.28333000	4.42644100	-0.99147200

M5

C	-2.95422800	2.71816000	0.25995500
C	-1.42118500	2.29632600	0.37593100
H	-3.36550700	2.70706600	1.27182100
N	-3.73058200	1.75251700	-0.49694700
N	-1.19704800	0.92361400	-0.04326300
H	-1.54530400	0.18894800	0.55718100
C	-1.19897300	-0.75691100	-1.84830300
C	-0.51166800	-1.87053500	-1.32434800
C	-0.71698700	-3.12669000	-1.91971300
C	-1.55931800	-3.28717300	-3.01540900
C	-2.22920600	-2.18071600	-3.53734700
C	-2.04559000	-0.93317100	-2.95456300
P	0.65780300	-1.79775000	0.10214800
H	-0.18986100	-3.99101800	-1.53342200
H	-1.68868000	-4.27128900	-3.45692700
H	-2.88894400	-2.28625600	-4.39267300
H	-2.55347100	-0.06195100	-3.35020500
Pd	1.77123300	0.12641000	0.76781700
C	-0.36884300	-2.60116300	1.40393800
C	-0.58155900	-3.98692600	1.44341800
C	-1.45431600	-4.54848000	2.37610100

C	-2.13872100	-3.69568200	3.25608100
C	-1.94900900	-2.31290400	3.23754800
C	-1.03255500	-1.78082600	2.31806900
H	-0.05287700	-4.63610600	0.75270500
H	-2.83312500	-4.12506200	3.97557400
H	-0.82368000	-0.71643100	2.32616000
C	1.95563600	-3.03715800	-0.26213700
C	2.41179200	-3.27246800	-1.56139700
C	3.54856000	-4.06197600	-1.78491700
C	4.21020400	-4.61660800	-0.68770700
C	3.76864300	-4.39880200	0.62582500
C	2.64281700	-3.59988700	0.82616200
H	1.92573700	-2.79063800	-2.40066500
H	5.09610400	-5.22620700	-0.85448200
H	2.29864100	-3.40845700	1.83897500
C	-4.08590300	0.57440100	0.03991200
O	-3.81720000	0.24732200	1.20456500
H	-4.01822700	1.92668100	-1.45328500
H	-0.85360400	2.89894800	-0.32944100
C	-1.12638100	0.67515700	-1.38665300
O	-1.10148600	1.57823000	-2.21967100
C	-0.93900500	2.59645200	1.77502900
C	-0.10385500	3.69449300	1.99545700
C	-1.39442100	1.85580700	2.87515200
C	0.29400700	4.03386100	3.29049500
H	0.24376700	4.28098200	1.15231600
C	-0.98304500	2.18208000	4.16670600
H	-2.10522900	1.05234700	2.71526000
C	-0.13488600	3.27385000	4.37894100
H	0.95214800	4.88455200	3.43880700
H	-1.34139500	1.59889700	5.01086700
H	0.17924900	3.53336600	5.38608700
C	-3.08989600	4.10640800	-0.31973000
C	-3.66982200	5.12933600	0.43536500
C	-2.61305500	4.38768300	-1.60838500
C	-3.78047800	6.41917700	-0.08660900
H	-4.03192800	4.91447800	1.43755300
C	-2.73242600	5.67443400	-2.13136800
H	-2.13103400	3.60000300	-2.18148900
C	-3.31504200	6.69286000	-1.37301700
H	-4.23021600	7.20716300	0.51107200
H	-2.36118700	5.88346800	-3.13074800
H	-3.40117300	7.69593500	-1.78157100
C	-4.90100700	-0.27141700	-0.97274800

O	-5.28597600	0.31440900	-1.99266100
N	-5.21442800	-1.55436800	-0.67721700
C	-4.54306400	-2.36368100	0.37217100
C	-6.27182600	-2.22163700	-1.48095100
H	-6.43773100	-3.17682700	-0.97764700
C	-5.82249700	-2.51680500	-2.91616500
C	-2.72314100	-1.40091300	4.15590300
H	-3.42197900	-0.78640200	3.57663000
H	-3.29809300	-1.96992400	4.89275000
H	-2.05556500	-0.72069200	4.69685400
C	-1.69319600	-6.03866400	2.41609100
H	-1.66182800	-6.42160900	3.44225400
H	-2.68019800	-6.29053600	2.00688100
H	-0.94433500	-6.57820200	1.82847700
C	4.48894100	-5.02907900	1.79365600
H	4.22835800	-6.09063700	1.89544100
H	5.57606200	-4.97445900	1.66862700
H	4.22997400	-4.53505200	2.73557900
C	4.06759700	-4.24497700	-3.18971900
H	4.85701600	-5.00174000	-3.23169300
H	3.26744000	-4.54487800	-3.87547600
H	4.48057600	-3.30299700	-3.57177600
H	-3.68483100	-1.78825400	0.70216700
H	-4.89897300	-3.10151500	-2.92104400
H	-6.59891900	-3.09184200	-3.43384900
H	-5.64979100	-1.58643300	-3.45960300
C	-7.59625200	-1.45169500	-1.42340800
H	-7.51568300	-0.48974500	-1.93182600
H	-8.38029100	-2.04136300	-1.91134600
H	-7.89438600	-1.27825400	-0.38384600
C	-4.01177600	-3.68622300	-0.18968300
H	-3.36591100	-3.51070800	-1.05255500
H	-3.41151600	-4.17108800	0.58452700
H	-4.80846900	-4.37976900	-0.47983700
C	-5.45998800	-2.56210300	1.58055500
H	-5.74419200	-1.59152400	1.99547600
H	-6.36923300	-3.11506100	1.31583800
H	-4.93295600	-3.13015900	2.35468100
C	1.83648300	3.91619200	-1.16929000
C	2.15985200	2.76237400	-0.44282600
C	2.83269700	2.88369400	0.79406100
C	3.18818500	4.14361800	1.27559100
C	2.86838400	5.29109600	0.54531900
C	2.19250200	5.17126200	-0.67281100

H	1.30568600	3.80499900	-2.10688900
H	3.70403200	4.22503000	2.22897900
H	3.13479700	6.27147800	0.92972500
H	1.92958800	6.06219500	-1.23641800
C	3.12275200	1.60499300	1.51468800
H	4.07756300	1.12376800	1.29042900
N	1.78649500	1.45745800	-0.88455100
S	2.55003900	0.90395300	-2.23266600
C	4.23731400	0.64842300	-1.65968600
C	5.09454300	1.74647400	-1.57540400
C	4.61077900	-0.58473400	-1.12408200
C	6.32646000	1.60292000	-0.93701000
H	4.79130400	2.69809800	-1.99721600
C	5.84757800	-0.71568800	-0.49778200
H	3.93532500	-1.42653300	-1.18946700
C	6.72119400	0.37586900	-0.38657100
H	6.99206200	2.45953000	-0.86298300
H	6.13408200	-1.68095200	-0.08665000
O	1.98108600	-0.42211600	-2.53686700
O	2.60998600	1.92843500	-3.28668100
C	8.06814700	0.22330300	0.27693400
H	8.40198500	1.16420100	0.72665600
H	8.83405400	-0.08050100	-0.44908700
H	8.04326400	-0.54023500	1.06166500
C	2.35464000	1.11047100	2.59454300
H	1.55386500	1.71886900	3.00344400
C	2.35897200	-0.29335700	2.82807200
H	3.27379600	-0.86777500	2.68979400
H	1.64375800	-0.71133500	3.53051600

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C	-2.98102700	-0.12177700	2.47728100
C	-1.56911900	0.32707100	1.91847700
H	-2.81832100	-0.94015900	3.18094600
N	-3.83446600	-0.65379500	1.43537900
N	-1.18980000	-0.38735600	0.71671300
H	-0.78855100	-1.30869800	0.82338900
C	-1.23083800	-0.79837000	-1.68250600
C	0.05496500	-1.35306900	-1.87590400
C	0.29965800	-2.07438700	-3.05492100
C	-0.67885100	-2.21931500	-4.03495900
C	-1.93485200	-1.64173400	-3.85367600
C	-2.20567700	-0.94882500	-2.67837200
P	1.47404500	-1.08675000	-0.72596400

H	1.28073100	-2.50214900	-3.22350100
H	-0.45281200	-2.77318900	-4.94154500
H	-2.69933500	-1.73311700	-4.61917400
H	-3.17776700	-0.50119200	-2.50249200
Pd	1.86992500	1.04895500	0.31144900
C	1.33767100	-2.47622200	0.47724600
C	0.30036800	-3.41650000	0.44726100
C	0.21611200	-4.42242400	1.42285500
C	1.21198900	-4.49569400	2.40103700
C	2.27475900	-3.58645400	2.43632500
C	2.30884900	-2.57201700	1.48116200
H	-0.45145200	-3.37246200	-0.33509700
H	1.15850000	-5.28067000	3.15206800
H	3.11998800	-1.85532700	1.51034400
C	2.96637700	-1.51531400	-1.71244900
C	3.30608600	-0.66201500	-2.77671400
C	4.48590000	-0.85830800	-3.49580100
C	5.34321300	-1.90099300	-3.11673700
C	5.03362800	-2.75074100	-2.05377300
C	3.82723400	-2.56042400	-1.36692900
H	2.64120600	0.15627800	-3.03635100
H	6.27709500	-2.04550000	-3.65727900
H	3.57879400	-3.22957400	-0.55116100
C	-3.72104600	-1.92143000	1.00660700
O	-3.01646200	-2.77574400	1.55955700
H	-4.37251700	-0.03632900	0.83703400
H	-1.64098500	1.37451400	1.62907000
C	-1.68612500	-0.00528100	-0.49222400
O	-2.51432200	0.89792400	-0.61554400
C	-0.52472000	0.17206500	2.99883800
C	0.04308800	1.30236800	3.59294200
C	-0.15092100	-1.10036000	3.44949600
C	0.98324500	1.16370900	4.61537800
H	-0.24769400	2.28957100	3.24997100
C	0.79200300	-1.23834500	4.46691700
H	-0.60489100	-1.98727400	3.01453100
C	1.36574100	-0.10655400	5.05140600
H	1.40947500	2.05012700	5.07689400
H	1.06558100	-2.23101200	4.81048400
H	2.09108200	-0.21382000	5.85374100
C	-3.62878400	1.04815500	3.18030800
C	-3.80044700	1.04215100	4.56621100
C	-4.01148500	2.17887800	2.44587500
C	-4.35569900	2.14665700	5.21473400

H	-3.49142300	0.17150800	5.13856900
C	-4.57375600	3.27774500	3.09195600
H	-3.84261700	2.20366700	1.37250700
C	-4.74729900	3.26479600	4.47793600
H	-4.48193300	2.13234000	6.29374000
H	-4.86757400	4.14931600	2.51408700
H	-5.18034900	4.12481700	4.98109700
C	-4.63500000	-2.13492200	-0.24176600
O	-5.36515300	-1.18652600	-0.55374900
N	-4.64356500	-3.31660900	-0.90539300
C	-3.66424900	-4.40746500	-0.69705900
C	-5.70752300	-3.54729100	-1.91805900
H	-5.56504400	-4.58369900	-2.23233300
C	-5.54170700	-2.66185200	-3.15788600
C	3.35413000	-3.66664800	3.48806200
H	3.23685200	-4.55365600	4.11786100
H	4.35014500	-3.70388100	3.03107100
H	3.32950600	-2.78449300	4.13967000
C	-0.93624500	-5.39386300	1.42711400
H	-0.74865800	-6.23154100	2.10597000
H	-1.85379300	-4.88798600	1.74493600
H	-1.11405700	-5.80284300	0.42634300
C	5.99603900	-3.82426100	-1.60736900
H	6.68716100	-4.10510800	-2.40865300
H	6.59820800	-3.47299700	-0.75856300
H	5.46803100	-4.72642700	-1.27967800
C	4.82700700	0.04542100	-4.65632700
H	5.89701000	0.28231900	-4.68027900
H	4.58050100	-0.43171000	-5.61384200
H	4.26605600	0.98303200	-4.60228000
H	-2.91794700	-4.00491600	-0.02294100
H	-4.54460100	-2.78721200	-3.58860100
H	-6.28151700	-2.94694100	-3.91469300
H	-5.68651600	-1.61144400	-2.90119100
C	-7.10950300	-3.45296200	-1.30516700
H	-7.33327900	-2.43247200	-0.99162700
H	-7.85287600	-3.76386900	-2.04781300
H	-7.19457600	-4.11560900	-0.43731700
C	-2.95539000	-4.78941600	-2.00185800
H	-2.48507800	-3.91477100	-2.45882200
H	-2.17076600	-5.52160200	-1.78010500
H	-3.62654400	-5.24682700	-2.73690400
C	-4.32248200	-5.60229500	-0.00109300
H	-4.72273200	-5.29420300	0.96949100

H	-5.13848100	-6.02649200	-0.59708000
H	-3.58635200	-6.39573300	0.16634900
C	-1.36080600	3.70430400	0.15558700
C	-0.06443400	3.18790900	0.15287000
C	0.88070400	3.62408200	1.10288300
C	0.49802300	4.57250400	2.05566100
C	-0.80605700	5.08245700	2.06882400
C	-1.72868000	4.65166000	1.11802300
H	-2.08067900	3.32712600	-0.55898500
H	1.22541600	4.91860100	2.78469300
H	-1.09534000	5.80938500	2.82291500
H	-2.74493400	5.03494300	1.13074000
C	2.26210500	3.03525900	1.02399100
H	2.79894500	3.41621100	0.14870100
N	0.33942200	2.11919500	-0.71848200
S	0.78310700	2.56426800	-2.24042000
C	-0.65136200	3.39682300	-2.91060500
C	-1.74944600	2.63684100	-3.31518100
C	-0.68639200	4.78798800	-2.94375400
C	-2.89714400	3.28883100	-3.75208200
H	-1.70074200	1.55687600	-3.27307800
C	-1.84496200	5.42619600	-3.38537000
H	0.18184200	5.35065800	-2.62034100
C	-2.96445000	4.69026500	-3.79083400
H	-3.76039400	2.70340000	-4.05946200
H	-1.88246800	6.51235700	-3.40846600
O	1.89582900	3.54091600	-2.26721800
O	0.96307500	1.31331900	-3.01228700
C	-4.21454200	5.38174600	-4.27729100
H	-5.11399100	4.92987100	-3.84382600
H	-4.30946100	5.30683000	-5.36850400
H	-4.20975900	6.44522700	-4.01879200
C	3.07503200	3.13787700	2.25396500
H	2.56571400	2.86792200	3.17892400
C	4.36523100	3.50017800	2.31326500
H	4.91654000	3.78280900	1.41909400
H	4.91198600	3.51126400	3.25224100
C	6.40202200	0.16394100	-0.61019900
C	5.11297700	0.50655000	-0.22749600
C	4.65347200	0.21886600	1.07864600
C	5.53600800	-0.40692400	1.99100300
C	6.81517100	-0.77577800	1.59579100
C	7.24688500	-0.48806000	0.29466400
H	6.74427700	0.38293800	-1.61555900

H	4.43412800	0.99543800	-0.91642600
H	5.18792900	-0.61414300	2.99952500
H	7.48268700	-1.27265600	2.29344400
H	8.25053400	-0.76919800	-0.01253900
C	3.29133000	0.47964600	1.44638500
H	3.08504800	0.34754700	2.51509100

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C	-2.48995900	0.55757600	2.72875300
C	-1.15336200	0.81714500	1.91161800
H	-2.25376000	-0.13377000	3.53941300
N	-3.50722700	-0.09937100	1.93613800
N	-0.97569900	-0.11611200	0.81897200
H	-0.56813400	-1.01806300	1.02262000
C	-1.50262700	-0.96702100	-1.41190200
C	-0.30549000	-1.63175400	-1.75856500
C	-0.33299900	-2.54196400	-2.82760100
C	-1.49969800	-2.78440500	-3.54711800
C	-2.67552700	-2.11517300	-3.20996900
C	-2.67135100	-1.22070600	-2.14525600
P	1.32869700	-1.30843900	-0.96561000
H	0.57904800	-3.04783700	-3.11949300
H	-1.48298400	-3.48667400	-4.37550000
H	-3.58754800	-2.28367700	-3.77409000
H	-3.56901300	-0.68197100	-1.86341900
Pd	2.14199900	0.92230200	-0.54508100
C	1.32968900	-2.39028700	0.52443000
C	0.26232000	-3.22165700	0.88499300
C	0.32575900	-3.99819000	2.05432200
C	1.48065800	-3.93941600	2.83834600
C	2.57061500	-3.13324700	2.48714500
C	2.47501500	-2.36213800	1.33084300
H	-0.62135900	-3.27795200	0.25620300
H	1.53581900	-4.54398000	3.74117500
H	3.30878500	-1.73751200	1.04588100
C	2.54390200	-2.13232300	-2.06609300
C	3.01246000	-1.40273400	-3.17016400
C	3.97620500	-1.94864800	-4.02046000
C	4.47325200	-3.22961300	-3.74075700
C	4.02042300	-3.97288700	-2.64774400
C	3.04291100	-3.41345500	-1.81367800
H	2.59458700	-0.42169400	-3.37568800
H	5.23067700	-3.65886300	-4.39444900
H	2.67772800	-3.98282300	-0.96486200

C	-3.53191600	-1.43255200	1.77706000
O	-2.79798300	-2.21447900	2.39391400
H	-4.10746500	0.43001800	1.31364400
H	-1.22856100	1.80105400	1.45232800
C	-1.67562400	0.06443000	-0.33524400
O	-2.47973700	0.98588600	-0.48445100
C	0.00376300	0.79924100	2.88171100
C	0.62010600	1.99941000	3.24983700
C	0.38826500	-0.39161800	3.51327800
C	1.58768400	2.01484200	4.25685600
H	0.33153700	2.92123600	2.75579600
C	1.35924800	-0.37695600	4.51337900
H	-0.09502100	-1.32883600	3.24928300
C	1.94827700	0.82949900	4.90066600
H	2.04828000	2.95593300	4.54432100
H	1.63790400	-1.30586600	5.00236600
H	2.67797600	0.84579500	5.70597900
C	-2.98601600	1.86816700	3.29324300
C	-2.94489000	2.11260600	4.66764500
C	-3.44082600	2.87418900	2.43022000
C	-3.36130400	3.34256300	5.17997900
H	-2.57842700	1.33837700	5.33646300
C	-3.86528100	4.09856200	2.94225400
H	-3.43696900	2.70143900	1.35739500
C	-3.82640500	4.33627700	4.31815500
H	-3.32277300	3.52276300	6.25070300
H	-4.21832800	4.87160400	2.26560500
H	-4.15251100	5.29348100	4.71535900
C	-4.64652700	-1.82009500	0.75526300
O	-5.38495500	-0.90338300	0.37508000
N	-4.80943200	-3.10686900	0.36205300
C	-3.83333400	-4.19178700	0.61202700
C	-6.04726600	-3.46626800	-0.37875800
H	-5.99514300	-4.55195100	-0.48736200
C	-6.09072300	-2.86231400	-1.78658100
C	3.80533200	-3.06283900	3.35093100
H	3.94529900	-3.98322500	3.92706000
H	4.70369300	-2.88885000	2.75013000
H	3.73321700	-2.22970300	4.06067500
C	-0.83216900	-4.87300800	2.46156600
H	-0.54918900	-5.55425000	3.27003300
H	-1.67105400	-4.25805100	2.80200100
H	-1.18610600	-5.47816100	1.61938700
C	4.58631100	-5.34109000	-2.34928700

H	4.95219400	-5.82989000	-3.25808800
H	5.42992400	-5.27742400	-1.64930200
H	3.83423000	-5.99220100	-1.89104400
C	4.46128000	-1.17674200	-5.22399200
H	5.55647900	-1.15770900	-5.27281200
H	4.10408600	-1.63413800	-6.15533500
H	4.09985700	-0.14481700	-5.20138100
H	-2.96650900	-3.70978200	1.04796600
H	-5.19689300	-3.13964400	-2.35164700
H	-6.96768800	-3.24331000	-2.32238400
H	-6.15349800	-1.77434600	-1.73543100
C	-7.30827400	-3.15638900	0.43614400
H	-7.43727600	-2.08092100	0.56534600
H	-8.18564400	-3.55521000	-0.08527700
H	-7.25362700	-3.62684400	1.42365900
C	-3.38496000	-4.86339400	-0.69127500
H	-2.98574100	-4.12514000	-1.39163600
H	-2.59076500	-5.58372100	-0.46471900
H	-4.19020500	-5.41494800	-1.18855600
C	-4.37870700	-5.18658900	1.64051700
H	-4.58783800	-4.67110000	2.58250300
H	-5.29869500	-5.67149800	1.29451200
H	-3.64199800	-5.97324200	1.83441900
C	-1.06781700	3.69038200	-0.45515500
C	0.19019200	3.09701500	-0.58259500
C	1.30443300	3.62840800	0.09085600
C	1.12715000	4.74503600	0.91521300
C	-0.13578700	5.32876300	1.06406100
C	-1.22763800	4.80608600	0.37271000
H	-1.91334100	3.24423700	-0.96093900
H	1.98524400	5.16741000	1.43012800
H	-0.26120000	6.18863300	1.71658700
H	-2.21146900	5.25131000	0.48901600
C	2.65053700	2.99202900	-0.14519900
H	3.03622200	3.26763600	-1.13177100
N	0.39812000	1.87959500	-1.30914900
S	0.57966400	2.05001400	-2.94525000
C	-0.97281400	2.73299200	-3.51179100
C	-2.07675100	1.89349000	-3.65299700
C	-1.07967800	4.10528600	-3.72760400
C	-3.30437600	2.44321400	-4.00637100
H	-1.96808800	0.83097200	-3.48336500
C	-2.31718500	4.64053600	-4.08076900
H	-0.20402100	4.73325000	-3.61114000

C	-3.44509000	3.82218700	-4.22094800
H	-4.17114100	1.79469400	-4.10849000
H	-2.41032400	5.71125500	-4.24429600
O	1.62729200	3.02821400	-3.31300700
O	0.69718000	0.68044400	-3.49703300
C	-4.77945400	4.40374200	-4.61930400
H	-5.60376100	3.90456100	-4.09827900
H	-4.95693500	4.28464100	-5.69644200
H	-4.83240800	5.47390000	-4.39507100
C	3.62888200	3.25554500	0.92507800
H	3.26914600	3.09853100	1.94248800
C	4.88933500	3.67680900	0.75457900
H	5.29799100	3.86005300	-0.23722000
H	5.55468800	3.83871000	1.59821300
C	5.05001500	0.40838100	3.37436600
C	4.23367800	0.50396100	2.25770000
C	4.75762400	0.25938900	0.96540600
C	6.12724600	-0.07631400	0.83913400
C	6.94484900	-0.15917300	1.95899500
C	6.40360800	0.08180800	3.22676400
H	4.63657200	0.59217900	4.35943400
H	3.18267400	0.74799000	2.35399800
H	6.53048200	-0.26619600	-0.15184600
H	7.99546500	-0.41215200	1.85357800
H	7.04015800	0.01376000	4.10479300
C	3.92491600	0.33373700	-0.19277600
H	4.44698700	0.01551300	-1.10590300

TS4

C	-3.08229400	0.10794800	2.40999600
C	-1.62388600	0.38486200	1.85449500
H	-3.01329600	-0.69114900	3.15105400
N	-3.97408300	-0.36964400	1.37336400
N	-1.34079600	-0.34560100	0.63791500
H	-1.06197000	-1.31361300	0.71928100
C	-1.41545800	-0.69179500	-1.76436200
C	-0.21123600	-1.40769800	-1.95191800
C	-0.04742000	-2.13993300	-3.13816900
C	-1.02885600	-2.14737500	-4.12666000
C	-2.20048200	-1.41263100	-3.94842400
C	-2.39050700	-0.69952300	-2.76914300
P	1.23447800	-1.32011500	-0.80832000
H	0.87526600	-2.68383600	-3.30494500
H	-0.86841100	-2.71516600	-5.03854200

H	-2.96191100	-1.39473000	-4.72208900
H	-3.29797000	-0.13131400	-2.59717400
Pd	1.73177300	0.62007700	0.22129400
C	1.03390500	-2.72305200	0.35307400
C	-0.08861100	-3.55394600	0.36113600
C	-0.22033500	-4.56515700	1.32941300
C	0.81257800	-4.74914100	2.24964500
C	1.96083200	-3.94275300	2.24419400
C	2.04522500	-2.91855200	1.30611400
H	-0.86945000	-3.42077700	-0.38188000
H	0.72317100	-5.54059100	2.99097200
H	2.90888200	-2.26474700	1.30865600
C	2.67807900	-1.74684000	-1.85045000
C	3.03404100	-0.82035900	-2.84432800
C	4.19977900	-0.99887800	-3.59043600
C	5.01394200	-2.10671400	-3.31417700
C	4.67961500	-3.03578800	-2.32663200
C	3.49234000	-2.85458700	-1.60502700
H	2.40131000	0.04475000	-3.02526200
H	5.93633000	-2.24050900	-3.87674200
H	3.22550200	-3.57354100	-0.83835100
C	-3.94224300	-1.64083900	0.94076600
O	-3.27867200	-2.53407900	1.48280700
H	-4.50004300	0.27699500	0.79527700
H	-1.57240000	1.43640700	1.57813400
C	-1.76612900	0.13145100	-0.56188600
O	-2.44787800	1.15393700	-0.66647800
C	-0.59253400	0.10080200	2.92001900
C	0.06411800	1.16473200	3.54363900
C	-0.30384300	-1.21150500	3.31524300
C	1.02315200	0.92397300	4.52811600
H	-0.17033800	2.18083200	3.25075700
C	0.65382200	-1.45177700	4.29933200
H	-0.82956200	-2.04695700	2.86034900
C	1.32577400	-0.38630000	4.90442000
H	1.53050800	1.76251400	4.99730300
H	0.86710900	-2.47343600	4.59665500
H	2.07015300	-0.57709200	5.67302600
C	-3.61051800	1.37275300	3.04621700
C	-3.79639200	1.45742900	4.42725600
C	-3.86089900	2.49901100	2.24863800
C	-4.23595000	2.64809100	5.00980100
H	-3.59002300	0.58997800	5.04855900
C	-4.30962800	3.68359800	2.82890100

H	-3.67777900	2.44716400	1.17814800
C	-4.49715300	3.76180200	4.21141300
H	-4.37458700	2.70344000	6.08589300
H	-4.50606000	4.54917000	2.20213000
H	-4.84125000	4.68785300	4.66341000
C	-4.88123600	-1.79318600	-0.29828800
O	-5.54314800	-0.79375400	-0.60548700
N	-4.98050400	-2.97102300	-0.95919900
C	-4.08330100	-4.13182800	-0.75725700
C	-6.05472000	-3.11888800	-1.97717300
H	-5.98531200	-4.16111000	-2.29679100
C	-5.82155900	-2.24141200	-3.21183700
C	3.06644100	-4.15087000	3.25029700
H	3.98424000	-3.64506700	2.93501900
H	2.78923000	-3.74655100	4.23239300
H	3.28830800	-5.21489900	3.38776800
C	-1.46031200	-5.42129900	1.37853000
H	-1.33988900	-6.25578700	2.07611600
H	-2.32180900	-4.82530400	1.69752200
H	-1.69447800	-5.83746400	0.39211000
C	5.60478200	-4.17871800	-1.98806700
H	6.25222000	-3.90878100	-1.14297600
H	5.04692300	-5.07558600	-1.69768400
H	6.25272700	-4.43710800	-2.83194800
C	4.56566300	-0.00727700	-4.66848000
H	4.12488200	0.97293200	-4.46333100
H	5.65168700	0.10957600	-4.75385800
H	4.19461400	-0.33581000	-5.64817100
H	-3.32408300	-3.79641400	-0.06075000
H	-4.83232700	-2.43132400	-3.63689300
H	-6.57443600	-2.47370200	-3.97376500
H	-5.89674700	-1.18438300	-2.95264500
C	-7.44799300	-2.92795100	-1.36709300
H	-7.59823400	-1.89612200	-1.04684800
H	-8.20970000	-3.17879700	-2.11381200
H	-7.58343400	-3.58903200	-0.50449000
C	-3.38057400	-4.53384800	-2.05929600
H	-2.83786600	-3.68632300	-2.48604100
H	-2.65825800	-5.32952300	-1.84492600
H	-4.07216100	-4.91820000	-2.81688900
C	-4.83614100	-5.29259400	-0.10031400
H	-5.24040900	-4.97776300	0.86657000
H	-5.66305300	-5.65393900	-0.72238500
H	-4.15681400	-6.13452800	0.06876200

C	-0.65049700	3.81405500	0.66632300
C	0.52063700	3.08838700	0.42328400
C	1.61758000	3.19070700	1.33089300
C	1.48749600	4.07043700	2.41618400
C	0.31698000	4.79851400	2.64097300
C	-0.76072900	4.66217000	1.76910900
H	-1.48168400	3.66991600	-0.01261900
H	2.32208200	4.19758500	3.09594400
H	0.25237600	5.46204900	3.49876500
H	-1.68887700	5.19590100	1.94981800
C	2.90822500	2.41129600	1.13502800
H	3.32596800	2.57531200	0.13858800
N	0.52614100	2.13586700	-0.64428800
S	1.02291000	2.61100100	-2.12351200
C	-0.16647600	3.85703200	-2.61525500
C	-1.51595600	3.50525700	-2.70882600
C	0.25916200	5.15598300	-2.87342800
C	-2.43998200	4.47948400	-3.07146500
H	-1.83658800	2.50133400	-2.45321100
C	-0.68280700	6.11967800	-3.23703000
H	1.31243500	5.39653000	-2.78262900
C	-2.03987900	5.79745500	-3.34453300
H	-3.49344300	4.21694400	-3.13543700
H	-0.35766400	7.13801900	-3.43555400
O	2.35560600	3.26325300	-2.12824300
O	0.84429400	1.44546700	-3.01855200
C	-3.05386700	6.83546200	-3.75939500
H	-2.66918500	7.85036600	-3.61712600
H	-3.98231100	6.73910800	-3.18549300
H	-3.31748900	6.72866800	-4.81997200
C	3.93625500	2.63185200	2.17999900
H	3.63231400	2.44971300	3.21038800
C	5.19047000	3.02410200	1.93248100
H	5.53596700	3.21623800	0.91996400
H	5.91229600	3.15497400	2.73344800
C	6.27598500	-0.58957500	-0.36217100
C	5.02823700	-0.04679700	-0.07947500
C	4.46939100	-0.16690500	1.20905100
C	5.21201900	-0.83120900	2.20707800
C	6.45246900	-1.39236400	1.91711600
C	6.98678700	-1.27212200	0.63046400
H	6.68598900	-0.49850200	-1.36263100
H	4.45957000	0.45735200	-0.85285100
H	4.79197600	-0.91385500	3.20625500

H	7.00797500	-1.91384500	2.69166100
H	7.95786600	-1.70369700	0.40368000
C	3.12008700	0.28707500	1.49384500
H	2.81640100	0.17512900	2.53797500

TS4_{dia}

C	-2.70198900	0.76554700	2.47052100
C	-1.23109800	0.79226500	1.84403400
H	-2.64785600	0.19078300	3.39729000
N	-3.66184500	0.08663000	1.62817900
N	-1.05703300	-0.15192000	0.76237300
H	-0.76599700	-1.09440500	0.98413100
C	-1.51490600	-0.93671100	-1.50365800
C	-0.38228700	-1.73865000	-1.76491600
C	-0.45889200	-2.68298700	-2.80149900
C	-1.60501100	-2.81522400	-3.58194000
C	-2.70728600	-1.99751100	-3.33955900
C	-2.66061000	-1.07603900	-2.29858100
P	1.25761400	-1.52322500	-0.94131500
H	0.40167200	-3.30252400	-3.02240400
H	-1.62644600	-3.54684100	-4.38441100
H	-3.59808100	-2.07553400	-3.95456200
H	-3.51213400	-0.44311100	-2.07539000
Pd	2.12405500	0.53252700	-0.60401200
C	1.19468300	-2.55753600	0.56725600
C	0.10248400	-3.37046400	0.88982200
C	0.08523000	-4.09019800	2.09505700
C	1.19110000	-4.00005800	2.94396600
C	2.30197500	-3.20316500	2.63492000
C	2.28586200	-2.47833200	1.44422300
H	-0.73939500	-3.44536300	0.20737600
H	1.18516300	-4.56084000	3.87650900
H	3.11988500	-1.83358700	1.19726300
C	2.41703000	-2.36503400	-2.07688000
C	2.74122000	-1.68317500	-3.26285800
C	3.65807800	-2.23113200	-4.15822100
C	4.25282500	-3.46409500	-3.84253700
C	3.94341300	-4.15482700	-2.67028000
C	3.00839500	-3.59361200	-1.78590700
H	2.26153000	-0.73189300	-3.48345800
H	4.97739400	-3.89294800	-4.53238700
H	2.75375900	-4.11854600	-0.86988100
C	-3.71053300	-1.25168200	1.53474600
O	-3.03676900	-2.01736100	2.23568500

H	-4.22003400	0.59763700	0.95387300
H	-1.08654900	1.77527700	1.40213000
C	-1.63256800	0.11500200	-0.44113200
O	-2.29536100	1.13363000	-0.64213200
C	-0.24319200	0.59734700	2.96599400
C	0.41057300	1.71145700	3.50214700
C	-0.07928100	-0.65459000	3.57317600
C	1.19713700	1.58154000	4.64839600
H	0.29002300	2.68014800	3.02876900
C	0.72159500	-0.78634400	4.70565100
H	-0.61059900	-1.51881000	3.18642200
C	1.34761900	0.33423600	5.25698200
H	1.69009500	2.45661000	5.06288800
H	0.83781000	-1.76224100	5.16787100
H	1.94715900	0.23405300	6.15805700
C	-3.12560300	2.18562800	2.76723000
C	-3.14515200	2.65620500	4.08240600
C	-3.41902000	3.06958400	1.71837400
C	-3.45973500	3.98959100	4.35310100
H	-2.90436400	1.97760000	4.89637500
C	-3.74335600	4.39748500	1.98987100
H	-3.35623300	2.71875900	0.69261500
C	-3.76254100	4.86244400	3.30781200
H	-3.46924000	4.34378400	5.38016100
H	-3.97046900	5.07240300	1.16911400
H	-4.01004700	5.89938100	3.51743300
C	-4.76757300	-1.66332500	0.46230300
O	-5.45366200	-0.74819700	-0.01094200
N	-4.94408200	-2.96370600	0.12808400
C	-4.00614100	-4.05520100	0.47797300
C	-6.14630600	-3.33279500	-0.66498400
H	-6.11605800	-4.42364600	-0.71357400
C	-6.09635800	-2.80572600	-2.10286500
C	3.46162300	-3.07996200	3.59025600
H	4.38594600	-2.81819400	3.06724300
H	3.27150600	-2.28107800	4.31708500
H	3.62372800	-4.00923700	4.14679500
C	-1.11595600	-4.91710800	2.47778800
H	-0.89384100	-5.57372700	3.32463500
H	-1.95137700	-4.26602200	2.75762400
H	-1.45080400	-5.54302700	1.64317900
C	4.60251300	-5.47290700	-2.34068300
H	5.29001700	-5.37149900	-1.49133600
H	3.86096100	-6.23180000	-2.06456700

H	5.17734100	-5.85507200	-3.18982400
C	4.00079900	-1.51582700	-5.44272900
H	5.08601500	-1.43292300	-5.57506300
H	3.60938600	-2.05715600	-6.31345100
H	3.57592800	-0.50820800	-5.45700500
H	-3.16112300	-3.57286900	0.95565600
H	-5.18454400	-3.14021600	-2.60428400
H	-6.95677900	-3.18932200	-2.66315500
H	-6.12610700	-1.71519000	-2.11378600
C	-7.44139000	-2.95076900	0.06078300
H	-7.54812500	-1.86722500	0.12903300
H	-8.29921000	-3.35398000	-0.48883500
H	-7.45348500	-3.37121200	1.07194700
C	-3.48821200	-4.77442300	-0.77290200
H	-3.02413400	-4.06653400	-1.46482500
H	-2.73008700	-5.50733400	-0.47439800
H	-4.27298400	-5.31953600	-1.30840400
C	-4.63570000	-5.00740900	1.49889100
H	-4.89205500	-4.45992000	2.41073300
H	-5.54207500	-5.48677600	1.11159300
H	-3.92874400	-5.80111200	1.76112500
C	-0.19001400	3.75179500	0.14901500
C	0.87429900	2.98737400	-0.33283100
C	2.18896500	3.18664900	0.18975700
C	2.35399100	4.11548900	1.22447500
C	1.27448100	4.85774900	1.71621100
C	0.00387400	4.68690200	1.17032800
H	-1.17526600	3.56471700	-0.26021500
H	3.34223100	4.28844000	1.63608500
H	1.43609100	5.57176000	2.51917100
H	-0.84437500	5.24641800	1.55365800
C	3.36310500	2.46672300	-0.43968400
H	3.28640500	2.50224800	-1.52950200
N	0.61967700	1.89986800	-1.22372200
S	0.66067500	2.17400500	-2.83899800
C	-0.78631400	3.17883100	-3.14829800
C	-2.02922100	2.56496200	-3.30098100
C	-0.66864500	4.56783500	-3.12154600
C	-3.16442600	3.35961300	-3.42523300
H	-2.09740600	1.48543100	-3.30992400
C	-1.81690100	5.34892300	-3.24203300
H	0.31032100	5.01877000	-3.00558800
C	-3.07821700	4.75899400	-3.39235500
H	-4.13716000	2.88701500	-3.53814500

H	-1.73257700	6.43258600	-3.21629900
O	1.83078900	2.98387100	-3.25674200
O	0.46252100	0.86256100	-3.49125200
C	-4.31725600	5.60765500	-3.54288800
H	-4.58331400	5.73582200	-4.60056500
H	-4.17211600	6.60678700	-3.11934000
H	-5.17887700	5.14803400	-3.04636700
C	4.71505500	2.90350500	-0.01769600
H	4.91619600	2.93885700	1.05079700
C	5.68931300	3.22937200	-0.87490300
H	5.53153100	3.20398000	-1.95060600
H	6.67055400	3.53730000	-0.52530100
C	4.43319000	0.39791200	3.72349900
C	3.82192700	0.53760900	2.48249800
C	4.54700700	0.27995000	1.30011800
C	5.89037000	-0.13896600	1.41043300
C	6.48732800	-0.31049000	2.65573900
C	5.76074200	-0.03227300	3.81620900
H	3.86658500	0.61306600	4.62120100
H	2.78535000	0.84942500	2.41144400
H	6.45741800	-0.32398400	0.50232400
H	7.51976500	-0.64174800	2.72257800
H	6.22658800	-0.14938800	4.79075000
C	3.95285600	0.43197100	-0.01608200
H	4.68323500	0.30584400	-0.82096800

M7

C	-3.20898100	0.60699000	1.76235800
C	-1.64812900	0.51637100	1.46071100
H	-3.37932500	0.15435500	2.74090500
N	-3.99227100	-0.16109600	0.81554300
N	-1.32343600	-0.53167000	0.50654200
H	-1.00316300	-1.42034000	0.86860300
C	-1.12738700	-1.51202900	-1.70894800
C	0.10813000	-2.19214000	-1.62182300
C	0.34604300	-3.25274400	-2.51199000
C	-0.59061500	-3.60956100	-3.47915800
C	-1.78681200	-2.89882000	-3.58841800
C	-2.05227500	-1.85978200	-2.70234900
P	1.48153900	-1.65291900	-0.49384700
H	1.28746700	-3.78716300	-2.46343400
H	-0.37644200	-4.43124500	-4.15636200
H	-2.50954800	-3.15301500	-4.35729800
H	-2.97929800	-1.29959000	-2.75788700

Pd	1.36543700	0.64370800	-0.38265400
C	1.23007900	-2.65658200	1.01406600
C	0.13090800	-3.51057500	1.17101800
C	-0.08772500	-4.17465000	2.38587200
C	0.83730700	-4.00167700	3.41831400
C	1.95057800	-3.16431500	3.28018800
C	2.12696900	-2.48431400	2.07489400
H	-0.56111300	-3.66501300	0.34764100
H	0.68022200	-4.52161100	4.36093900
H	2.97213700	-1.81839700	1.95443900
C	2.95162300	-2.31630400	-1.34605900
C	3.24795900	-1.75447300	-2.59931400
C	4.35197900	-2.19075200	-3.32706600
C	5.17496600	-3.17884200	-2.76582500
C	4.91741900	-3.72541700	-1.50873900
C	3.78102400	-3.29677900	-0.80741100
H	2.61435200	-0.96684700	-3.00147000
H	6.04976400	-3.51517600	-3.31924000
H	3.55673600	-3.72844000	0.16300600
C	-4.04346000	-1.50296400	0.86979300
O	-3.58820700	-2.17524600	1.80313900
H	-4.36378300	0.26741600	-0.02459600
H	-1.34861800	1.45369500	0.99145500
C	-1.54894400	-0.37687400	-0.82172000
O	-2.10591000	0.61896700	-1.29066900
C	-0.86316900	0.31723800	2.73755700
C	0.01705700	1.30892400	3.17525500
C	-1.01926300	-0.84873100	3.49906400
C	0.75264800	1.13474900	4.34798100
H	0.12535000	2.21706200	2.60016800
C	-0.28486500	-1.02162400	4.67147300
H	-1.72720300	-1.60780700	3.17843400
C	0.60469800	-0.03236500	5.09899600
H	1.43051700	1.92026300	4.66975300
H	-0.41073100	-1.92987500	5.25317500
H	1.16635400	-0.16548900	6.02008500
C	-3.62721300	2.05973900	1.79160900
C	-3.96269700	2.67041300	3.00243000
C	-3.60538500	2.82936400	0.61941900
C	-4.27933400	4.02970200	3.04681400
H	-3.96667500	2.08112400	3.91568900
C	-3.93107300	4.18367200	0.66202000
H	-3.28890700	2.37541300	-0.31480100
C	-4.26764100	4.78840800	1.87582200

H	-4.53382300	4.49337500	3.99576600
H	-3.89138500	4.76927200	-0.25137700
H	-4.51377100	5.84622300	1.90860900
C	-4.79387200	-2.06415600	-0.37302500
O	-5.36805600	-1.23672500	-1.09184300
N	-4.84363100	-3.40047300	-0.59363400
C	-3.96386000	-4.39343500	0.06866100
C	-5.83043800	-3.91691100	-1.57865800
H	-5.76789300	-5.00346600	-1.48422600
C	-5.47131000	-3.55198900	-3.02309800
C	2.91123800	-2.94547700	4.42130600
H	3.94491600	-2.87530600	4.06558600
H	2.67679600	-2.00624700	4.93751800
H	2.85595200	-3.75459000	5.15635300
C	-1.31927700	-5.02331100	2.57999500
H	-1.24884300	-5.62773900	3.48942100
H	-2.21121800	-4.39057400	2.66128400
H	-1.47575100	-5.70131300	1.73359000
C	5.85693500	-4.72549700	-0.88301900
H	6.47714000	-4.23800200	-0.11925900
H	5.31219400	-5.53756000	-0.38860600
H	6.52905100	-5.16705400	-1.62537000
C	4.69256200	-1.57084200	-4.65963100
H	3.84560000	-1.01177900	-5.06789000
H	5.53125000	-0.86908700	-4.55973100
H	4.99076300	-2.32933400	-5.39217400
H	-3.23199000	-3.81670400	0.62362300
H	-4.46408600	-3.89840300	-3.26935900
H	-6.17681800	-4.03292200	-3.71017800
H	-5.51998700	-2.47160500	-3.16750700
C	-7.26323900	-3.51656000	-1.20842900
H	-7.40726900	-2.43913900	-1.30119900
H	-7.96637700	-4.02321400	-1.87874700
H	-7.49266500	-3.81654700	-0.18048100
C	-3.20290800	-5.24442800	-0.95520100
H	-2.63239900	-4.61215800	-1.64034100
H	-2.49892900	-5.89359000	-0.42289700
H	-3.85819400	-5.89382200	-1.54513200
C	-4.75349100	-5.23347400	1.07533500
H	-5.18363300	-4.58314500	1.84196700
H	-5.56191800	-5.79535100	0.59333800
H	-4.09336300	-5.95655200	1.56598700
C	-0.29828500	4.21238000	0.87587000
C	0.83464200	3.46536200	0.52986000

C	1.98041700	3.48402300	1.35026800
C	1.94939500	4.26069300	2.51313100
C	0.81377500	4.99526600	2.86518500
C	-0.31335900	4.97278800	2.04350300
H	-1.17229600	4.15739200	0.23987100
H	2.82865000	4.30668300	3.14709500
H	0.81456500	5.58143500	3.77995800
H	-1.21056500	5.52200300	2.31367700
C	3.19040100	2.66817500	0.92649400
H	3.47161000	2.99547500	-0.07962200
N	0.78591800	2.57935600	-0.56938700
S	1.08935700	3.12705400	-2.09145300
C	-0.37248500	4.08504000	-2.46849300
C	-1.58359800	3.41442700	-2.65985000
C	-0.31063200	5.47563100	-2.45159200
C	-2.74281500	4.16210500	-2.83805700
H	-1.61715900	2.33163400	-2.63550100
C	-1.48515800	6.20826900	-2.62954000
H	0.64359500	5.96462800	-2.29101600
C	-2.71378500	5.56652500	-2.82258400
H	-3.69045500	3.64844800	-2.98276800
H	-1.44640800	7.29444700	-2.61106200
O	2.24597800	4.04140600	-2.16694200
O	1.08627200	1.91266200	-2.93921200
C	-3.98229300	6.35870600	-3.02617100
H	-3.85660400	7.40178800	-2.71972400
H	-4.81548100	5.93356700	-2.45454300
H	-4.28348500	6.35763500	-4.08175800
C	4.37277700	2.89321600	1.84107600
H	4.27235100	2.50609600	2.85619600
C	5.50427000	3.49358000	1.47623600
H	5.64117800	3.87972600	0.46897800
H	6.33303600	3.62009300	2.16766500
C	5.88811200	-0.06723700	-1.20777100
C	4.70241600	0.56135700	-0.84278500
C	4.17089100	0.39686800	0.44641800
C	4.87666500	-0.40269900	1.35787600
C	6.06130600	-1.04178900	0.99111200
C	6.56947900	-0.87945200	-0.29725700
H	6.27690800	0.06411000	-2.21334300
H	4.16276100	1.17179500	-1.56157200
H	4.51229700	-0.48876300	2.37843900
H	6.59179100	-1.65424800	1.71574300
H	7.48864400	-1.37799800	-0.59138400

C	2.94135700	1.12702900	0.87180600
H	2.58257300	0.77547100	1.84588300

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C	-2.87749300	0.61538400	1.87111200
C	-1.39096700	0.74777800	1.34577700
H	-2.84235800	0.04831200	2.80310500
N	-3.74983300	-0.13314700	0.98759800
N	-1.00849900	-0.26037600	0.35171500
H	-0.83775900	-1.18236400	0.74345600
C	-1.24727400	-1.43071200	-1.78840700
C	-0.06280800	-2.20627800	-1.71885100
C	0.07938100	-3.28759700	-2.60084500
C	-0.90036900	-3.58620900	-3.54646300
C	-2.04827700	-2.79859100	-3.63012800
C	-2.21963300	-1.73527800	-2.74886700
P	1.37958200	-1.76942500	-0.64262900
H	0.98480800	-3.88365000	-2.56570800
H	-0.75759300	-4.42383300	-4.22299200
H	-2.80633100	-3.00908100	-4.37787800
H	-3.10751600	-1.11441400	-2.78534100
Pd	1.25416500	0.49460800	-0.40808200
C	1.17042300	-2.78059400	0.86564700
C	0.03074100	-3.56523200	1.08417300
C	-0.14794400	-4.23358300	2.30311600
C	0.84997400	-4.12504200	3.27559100
C	2.00214300	-3.35517600	3.07540500
C	2.14514100	-2.66748800	1.86837300
H	-0.72585000	-3.65598600	0.31094900
H	0.72428000	-4.65138700	4.21941400
H	3.01308400	-2.03824800	1.71301900
C	2.81829700	-2.44518600	-1.53093500
C	3.18800500	-1.79104300	-2.71887600
C	4.35070600	-2.15283300	-3.39634000
C	5.14441200	-3.18042100	-2.85950100
C	4.79211900	-3.84868800	-1.68641800
C	3.61184500	-3.47445900	-1.02680600
H	2.56822400	-0.98365500	-3.10226300
H	6.06330000	-3.45951800	-3.37142500
H	3.33384600	-3.97438500	-0.10456100
C	-3.72882900	-1.47402500	0.94008100
O	-3.03222300	-2.17169200	1.69068000
H	-4.28380600	0.32893400	0.25948600
H	-1.27766300	1.70329100	0.83676000

C	-1.58263600	-0.25472300	-0.91584200
O	-2.32440600	0.64159000	-1.29009300
C	-0.45374700	0.69034400	2.53377700
C	0.18644200	1.84974900	2.97614300
C	-0.27808000	-0.50198500	3.24961500
C	1.01137400	1.82168400	4.10127300
H	0.04902700	2.77613300	2.43504100
C	0.54333400	-0.53042100	4.37491400
H	-0.80007000	-1.40531000	2.94599900
C	1.19278000	0.62976900	4.80363000
H	1.51051800	2.73315600	4.41770500
H	0.66755500	-1.46120400	4.91897800
H	1.82777300	0.60472600	5.68528800
C	-3.41493100	2.00418700	2.13703600
C	-3.76996400	2.39244500	3.43051600
C	-3.49873800	2.93581000	1.09217700
C	-4.20690300	3.69455900	3.68256100
H	-3.69331500	1.67595100	4.24417500
C	-3.93427100	4.23532400	1.34337300
H	-3.20298000	2.65052400	0.08692900
C	-4.28868600	4.61772500	2.63975200
H	-4.47634800	3.98711600	4.69356100
H	-3.97679200	4.94757000	0.52589000
H	-4.62098200	5.63329000	2.83654400
C	-4.70514300	-1.97519800	-0.17182100
O	-5.33201500	-1.09662300	-0.77696900
N	-4.86980900	-3.29657600	-0.41832500
C	-4.03132500	-4.37582900	0.15322200
C	-5.96191500	-3.70869000	-1.34117000
H	-5.94452400	-4.80049300	-1.31366800
C	-5.70012100	-3.28113400	-2.78928200
C	3.04997700	-3.23246700	4.15298600
H	4.05158800	-3.43032700	3.75780500
H	3.06709600	-2.21391300	4.55676600
H	2.85840900	-3.92675500	4.97718400
C	-1.39909300	-5.03241500	2.56787600
H	-1.29163600	-5.65519600	3.46127000
H	-2.25346600	-4.36297200	2.71521900
H	-1.63823800	-5.68986200	1.72446700
C	5.66860300	-4.93256000	-1.10678900
H	6.10035400	-4.61594900	-0.14886300
H	5.09775200	-5.84862400	-0.91486400
H	6.49428900	-5.18245400	-1.77961800
C	4.76602200	-1.43985800	-4.65986400

H	5.72805000	-0.93066500	-4.52572000
H	4.88376300	-2.14209300	-5.49386500
H	4.02740500	-0.68763200	-4.95103500
H	-3.25658900	-3.87431100	0.72107300
H	-4.73002900	-3.65305600	-3.13030400
H	-6.47622000	-3.69927200	-3.44036700
H	-5.71352300	-2.19399400	-2.87951400
C	-7.33836900	-3.26747400	-0.83114700
H	-7.43779500	-2.18168200	-0.85956900
H	-8.11803900	-3.70865400	-1.46207000
H	-7.49576400	-3.61025700	0.19701300
C	-3.34824800	-5.19758700	-0.94596800
H	-2.76244100	-4.55178800	-1.60522200
H	-2.66822600	-5.92088000	-0.48236500
H	-4.05757700	-5.76456100	-1.55873900
C	-4.83813000	-5.23834200	1.12835300
H	-5.24912700	-4.61785600	1.93070600
H	-5.66552800	-5.76078100	0.63491600
H	-4.19017500	-5.99710800	1.57950200
C	0.81170600	4.41885800	0.89750600
C	1.48511300	3.45666100	0.13554100
C	2.89296300	3.36314100	0.19668600
C	3.57839800	4.21003500	1.07139000
C	2.90032200	5.14644900	1.85656500
C	1.51438700	5.26312400	1.75845400
H	-0.26979600	4.47812200	0.81768900
H	4.66064000	4.15618200	1.12584900
H	3.45906300	5.79257400	2.52818400
H	0.97922300	5.99917900	2.35247100
C	3.59120000	2.40633200	-0.75722000
H	3.23219900	2.66789300	-1.75506100
N	0.74055400	2.51703800	-0.63135400
S	0.45483300	2.91384400	-2.21859000
C	-0.96014300	4.01526000	-2.16710200
C	-2.24256900	3.50702500	-2.36840100
C	-0.75821600	5.37233800	-1.90839300
C	-3.33330300	4.37179800	-2.29232200
H	-2.37289400	2.45098900	-2.56661900
C	-1.86119700	6.21932400	-1.82356100
H	0.24879800	5.75281700	-1.78248000
C	-3.16252500	5.73515000	-2.01495900
H	-4.33568700	3.97979100	-2.44805700
H	-1.70914400	7.27538900	-1.61421300
O	1.55318600	3.71343900	-2.80172000

O	0.03549100	1.67502500	-2.90034800
C	-4.35042700	6.66510700	-1.95813700
H	-4.59170900	7.05904400	-2.95421700
H	-4.15637600	7.52388000	-1.30695300
H	-5.24400600	6.15076400	-1.58822800
C	5.09440400	2.55709700	-0.76668100
H	5.61867700	2.31814800	0.15742900
C	5.79298700	2.91299500	-1.84516700
H	5.30062400	3.15285100	-2.78530200
H	6.87733200	2.98830000	-1.82505800
C	4.29686900	0.09062500	3.01168700
C	3.62210600	0.64755400	1.92845200
C	3.93447100	0.26414200	0.61152600
C	4.93520300	-0.70390800	0.42029800
C	5.60871400	-1.26513600	1.50630300
C	5.29709600	-0.86530600	2.80715100
H	4.03156500	0.39914000	4.01832000
H	2.83603000	1.37308900	2.09866800
H	5.19204100	-1.00627700	-0.58977200
H	6.38228200	-2.00909300	1.33297800
H	5.82372700	-1.29614600	3.65415500
C	3.26858300	0.89454800	-0.57085500
H	3.59092400	0.38880300	-1.48272700

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C	-2.76683900	2.19408800	1.44997900
C	-1.47969300	1.27327700	1.26664100
H	-3.15884200	2.01459600	2.45251400
N	-3.82308000	1.82354100	0.52810100
N	-1.74655200	0.13229900	0.40763500
H	-1.84439800	-0.77638800	0.84042300
C	-1.90661900	-1.01567700	-1.72561900
C	-1.07953700	-2.14385400	-1.54175100
C	-1.29752500	-3.26684200	-2.35423400
C	-2.29069100	-3.26601500	-3.33284700
C	-3.07980900	-2.13143900	-3.52873300
C	-2.88637200	-1.01045100	-2.72484500
P	0.36885300	-2.08771700	-0.38332300
H	-0.66443000	-4.13937900	-2.23611900
H	-2.43504800	-4.14631700	-3.95289600
H	-3.83827100	-2.11723200	-4.30543000
H	-3.48824000	-0.11728900	-2.85645200
Pd	1.46419300	-0.14992400	-0.28396700
C	-0.32316500	-2.77509100	1.17511900

C	-1.65887900	-3.16883100	1.31417200
C	-2.15961000	-3.58053700	2.55850900
C	-1.28388100	-3.64491200	3.64292200
C	0.06252600	-3.27326900	3.52734500
C	0.52117500	-2.81484500	2.29361300
H	-2.32210800	-3.15106500	0.45306900
H	-1.66150400	-3.96889400	4.61039200
H	1.54491800	-2.46263800	2.20159400
C	1.44038200	-3.41866600	-1.04551300
C	2.32483000	-3.04848500	-2.06536600
C	3.18248800	-3.99047900	-2.64242700
C	3.15181000	-5.30283000	-2.16072600
C	2.28770400	-5.69382500	-1.12820200
C	1.42882900	-4.73784600	-0.57604700
H	2.37470200	-2.00684000	-2.37745000
H	3.83046000	-6.03882700	-2.58814500
H	0.75124700	-5.02039200	0.22486900
C	-4.54830200	0.70507100	0.71140800
O	-4.55208600	0.04287600	1.75439300
H	-3.87481100	2.24366300	-0.39289500
H	-0.71934700	1.86650100	0.75715800
C	-1.75743000	0.25297900	-0.94060600
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C	-0.93496800	0.80432700	2.59855300
C	0.36283700	1.15320500	2.98301800
C	-1.71940300	0.02441100	3.45811200
C	0.87276200	0.73525400	4.21255600
H	0.96732100	1.76257600	2.32653300
C	-1.20534900	-0.39821200	4.68381400
H	-2.73318100	-0.23801900	3.16747000
C	0.08876200	-0.04068900	5.06747200
H	1.87606700	1.03554000	4.50305500
H	-1.82018700	-1.00544400	5.34181800
H	0.48065900	-0.36181700	6.02873500
C	-2.40906200	3.65700700	1.30193000
C	-2.54399500	4.53019200	2.38386000
C	-1.92105600	4.14977200	0.08210200
C	-2.21159200	5.88036700	2.25253200
H	-2.91128000	4.15105800	3.33393500
C	-1.59215400	5.49772200	-0.05028300
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C	-1.74014500	6.36842200	1.03311200
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H	-1.19956000	5.86174500	-0.99492800

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C	-7.16294100	-0.90336100	-1.63707700
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C	-6.65337600	-0.91748100	-3.08247000
C	0.99489300	-3.35539300	4.70977500
H	1.73506100	-2.54995500	4.68114900
H	0.44809600	-3.27840600	5.65481200
H	1.53903300	-4.30896300	4.71925000
C	-3.62488600	-3.89939800	2.72385300
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H	3.27801500	-7.54606400	-0.59810100
H	1.82505600	-7.19792400	0.35712500
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H	3.60792400	-3.36913000	-4.66841500
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C	-8.25474400	0.14848200	-1.40970800
H	-7.88214900	1.15265400	-1.61764800
H	-9.10085700	-0.05601100	-2.07511400
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C	-5.44313400	-3.19049100	-0.73041000
H	-4.64453900	-2.96245200	-1.44091500
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C	4.44013500	1.42170200	1.53667700
H	5.25150400	1.76563300	0.88749100
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C	0.87644600	2.58084800	-2.82010400
C	2.48283700	4.40266700	-2.71229600
C	-0.09592600	3.47119700	-3.25926700
H	0.62526800	1.54165500	-2.64159600
C	1.49645100	5.28135900	-3.16255800
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C	6.23352700	-2.75820100	-0.94416900
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M8

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O	4.85225900	1.62635500	-2.53972000
O	4.24004400	-0.81071100	-2.09380700
C	-1.35103100	1.26390400	-5.15944100

H	-1.74785700	0.34408000	-5.60131800
H	-1.35054800	2.04766400	-5.92343800
H	-2.03253000	1.56562800	-4.35462000
C	5.29268100	2.93891100	1.86475400
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C	4.16409000	1.08928300	0.55481100
H	3.50758800	1.04910800	1.43145000

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