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1. General information

¹H and ¹³C NMR spectra were measured respectively at 400 and 100 MHz, respectively. The solvent used for NMR spectroscopy were CDCl₃ and acetone-*d*₆, using tetramethylsilane as the internal reference. HRMS (ESI) was determined by a HRMS/MS instrument. Enantiomeric excesses (*ee*) were determined by chiral high-performance liquid chromatography (chiral HPLC). The chiral columns used for the determination of enantiomeric ratios by chiral HPLC were Chiralpak columns. Optical rotation values were measured with instruments operating at $\lambda = 589$ nm, corresponding to the sodium D line at the temperatures indicated. The X-ray source used for the single crystal X-ray diffraction analysis of compounds **3ab** and **7ah** was GaK α ($\lambda = 1.34139$), and the thermal ellipsoid was drawn at the 30% probability level. Analytical grade solvents for the column chromatography were distilled before use. All starting materials commercially available were used directly. Substrates **1-2** and **6** were synthesized according to the literature methods.

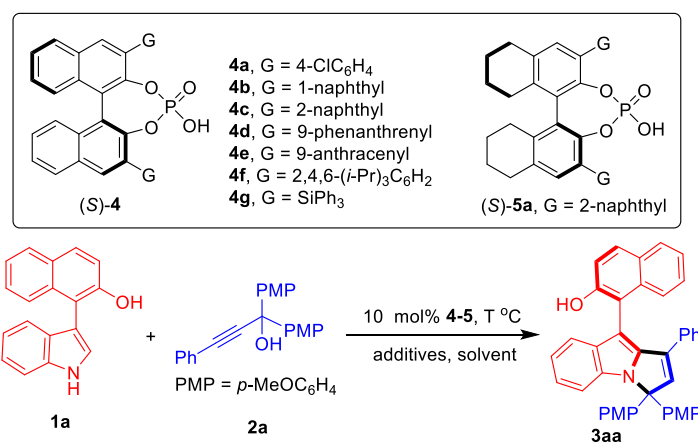
2. Evaluation of catalysts and optimization of reaction conditions

Condition optimization for the synthesis of axially chiral aryl-pyrroloindole **3aa**:

The reaction of 3-aryloindole **1a** with propargylic alcohol **2a** was utilized as a model reaction to test the feasibility of our design (**Table S1**). Gratifyingly, in the presence of CPA **4a**, asymmetric (2+3) cyclization between **1a** and **2a** successfully occurred in a regiospecific manner to generate axially chiral aryl-pyrroloindole **3aa** in a high yield of 95% with a moderate enantioselectivity of 60% *ee* (entry 1). This preliminary result demonstrated the feasibility of our strategy for designing and constructing this class of new axially chiral scaffolds. The screening of BINOL-derived CPAs **4a-4g** (entries 1-7) revealed that CPA **4c** bearing 2-naphthyl groups at the 3,3'-positions could give product **3aa** in better enantioselectivity than the others (entry 3 vs. entries 1-2 and 4-7). Then, changing the backbone of CPA **4c** from BINOL to H₈-BINOL, namely, using CPA **5a** as a catalyst, led to a further increase in the enantioselectivity to 70% *ee* (entry 8 vs. entry 3). Therefore, H₈-BINOL-derived CPA **5a** was chosen as the optimal catalyst for subsequent condition optimization. The evaluation of solvents (entries 8-13) demonstrated that DCM could facilitate (2+3) cyclization with a higher enantioselectivity than other solvents (entry 9 vs. entries 8 and 10-13). Thus, DCM was selected as the most suitable solvent for this reaction. Although

modulation of the reagent ratio did not improve the enantioselectivity (entries 14-16), the addition of additives such as molecular sieves (MS) and anhydrous sulfates contributed to improving the enantioselectivity (entries 17-21 vs. entry 9). Among these additives, 5 Å MS was the most efficient, enhancing the enantioselectivity from 75% ee to 86% ee (entry 19 vs. entry 9). In the presence of 5 Å MS as additives, lowering the catalyst loading of CPA **5a** from 10 mol% (entry 19) to 5 mol% (entry 22) led to an evident decrease in both the yield (from 81% to 68%) and the enantioselectivity (from 86% ee to 67% ee), which indicated that the catalyst loading of 10 mol% of CPA **5a** was necessary for controlling the reactivity and the enantioselectivity of the reaction. Next, adjusting the reaction concentration (entries 23-26) revealed that suitably diluting the reaction concentration could slightly increase the enantioselectivity (entry 25 vs. entry 19). In addition, either lowering or elevating the reaction temperature did not further improve the enantioselectivity (entries 27-28 vs. entry 25), which indicated that 20 °C was still the best reaction temperature. Therefore, the optimal reaction conditions were those described in entry 29, which could afford axially chiral aryl-pyrroloindole **3aa** in a high yield of 82% with a good enantioselectivity of 88% ee.

Table S1. Conditions optimization for the synthesis of axially chiral aryl-pyrroloindole **3aa**^a



entry	Cat.	solvent	T (°C)	1a:2a	additives	yield (%) ^b	ee (%) ^c
1	(S)- 4a	DCE (0.5 mL)	20	1:1.2	-	95	60
2	(S)- 4b	DCE (0.5 mL)	20	1:1.2	-	18	6
3	(S)- 4c	DCE (0.5 mL)	20	1:1.2	-	86	65
4	(S)- 4d	DCE (0.5 mL)	20	1:1.2	-	95	50
5	(S)- 4e	DCE (0.5 mL)	20	1:1.2	-	trace	-
6	(S)- 4f	DCE (0.5 mL)	20	1:1.2	-	75	60
7	(S)- 4g	DCE (0.5 mL)	20	1:1.2	-	10	<5
8	(S)- 5a	DCE (0.5 mL)	20	1:1.2	-	78	70

9	(<i>S</i>)- 5a	DCM (0.5 mL)	20	1:1.2	-	70	75
10	(<i>S</i>)- 5a	CHCl ₃ (0.5 mL)	20	1:1.2	-	65	66
11	(<i>S</i>)- 5a	CCl ₄ (0.5 mL)	20	1:1.2	-	66	36
12	(<i>S</i>)- 5a	toluene (0.5 mL)	20	1:1.2	-	55	66
13	(<i>S</i>)- 5a	CH ₃ CN (0.5 mL)	20	1:1.2	-	62	66
14	(<i>S</i>)- 5a	DCM (0.5 mL)	20	1:2	-	56	72
15	(<i>S</i>)- 5a	DCM (0.5 mL)	20	1.2:1	-	55	69
16	(<i>S</i>)- 5a	DCM (0.5 mL)	20	2:1	-	75	63
17	(<i>S</i>)- 5a	DCM (0.5 mL)	20	1:1.2	3 Å MS	90	83
18	(<i>S</i>)- 5a	DCM (0.5 mL)	20	1:1.2	4 Å MS	88	84
19	(<i>S</i>)- 5a	DCM (0.5 mL)	20	1:1.2	5 Å MS	81	86
20	(<i>S</i>)- 5a	DCM (0.5 mL)	20	1:1.2	Na ₂ SO ₄	89	73
21	(<i>S</i>)- 5a	DCM (0.5 mL)	20	1:1.2	MgSO ₄	80	77
22 ^d	(<i>S</i>)- 5a	DCM (0.5 mL)	20	1:1.2	5 Å MS	68	67
23	(<i>S</i>)- 5a	DCM (0.25mL)	20	1:1.2	5 Å MS	77	82
24	(<i>S</i>)- 5a	DCM (1.0 mL)	20	1:1.2	5 Å MS	79	86
25	(<i>S</i>)- 5a	DCM (1.5 mL)	20	1:1.2	5 Å MS	80	87
26	(<i>S</i>)- 5a	DCM (2.0 mL)	20	1:1.2	5 Å MS	83	86
27	(<i>S</i>)- 5a	DCM (1.5 mL)	0	1:1.2	5 Å MS	69	84
28	(<i>S</i>)- 5a	DCM (1.5 mL)	30	1:1.2	5 Å MS	79	86
29 ^e	(<i>S</i>)- 5a	DCM (3.0 mL)	20	1:1.2	5 Å MS	82	88

^aUnless indicated otherwise, the reaction was carried out in 0.05 mmol scale in a solvent with additives (50 mg) for 4 h. ^bIsolated yield. ^cThe enantiomeric excess (ee) was determined by HPLC. ^dCatalyzed by 5 mol% (*S*)-**5a**. ^eThe reaction was carried out in 0.1 mmol scale with 5 Å MS (100 mg) as additives. DCE = 1,2-dichloroethane, DCM = dichloromethane.

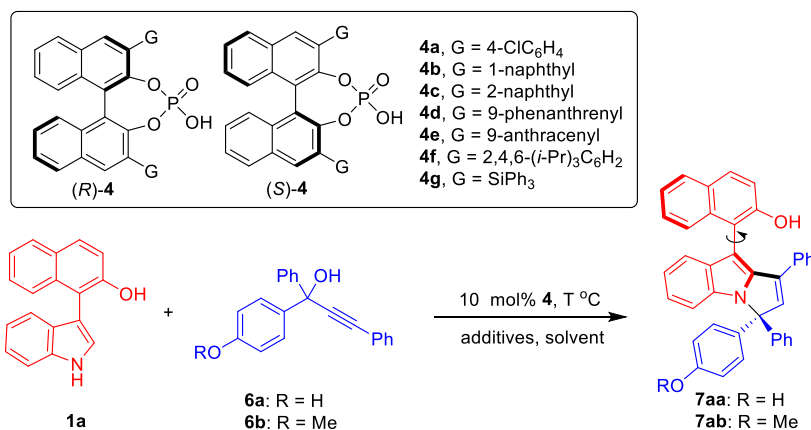
Condition optimization for the synthesis of aryl-pyrroloindoles **7** bearing both axial and central chirality:

After establishing the construction of axially chiral aryl-pyrroloindoles **3**, we aimed to construct aryl-pyrroloindole frameworks bearing both axial and central chirality, which is far more challenging due to the difficulty of simultaneous control of multiple chiral elements in one molecule. Initially, racemic propargylic alcohol **6a** bearing a *para*-hydroxyphenyl group was utilized as a substrate in the (2+3) cyclization with 3-aryloindole **1a** for condition optimization (Table S2, entries 1-11). As shown in entry 1, in the presence of CPA (*R*)-**4a**, the (2+3) cyclization of **6a** with **1a** rapidly occurred to afford aryl-pyrroloindole product **7aa** bearing both axial and central chirality in a high yield of 86% and a good diastereoselectivity of 87:13 dr, albeit with a low enantioselectivity of 26% ee. However, other CPAs **4b-4g** could not catalyze the reaction with a higher enantio-control than **4a** (entries 2-7 vs. entry 1). Therefore, solvents were evaluated in the

presence of (*R*)-**4a** (entries 8-11), indicating that using ethyl acetate as a solvent could enhance the enantioselectivity of product **7aa** to 68% ee with a prolonged reaction time (entry 8). To further improve the enantio-control of the reaction, racemic propargylic alcohol **6b** bearing a *para*-methoxyphenyl group was employed as a substrate for subsequent condition optimization (entries 12-39). The re-evaluation of solvents (entries 12-16) disclosed that using 1,2-dichloroethane or ethyl acetate as a solvent for the reaction could give product **7ab** in a much higher enantioselectivity than using other solvents (entries 12-13 vs. entries 14-16). In addition, slightly diluting the reaction concentration in the two solvents resulted in a further increased enantioselectivity (entries 17-18). Although ethyl acetate could deliver the reaction in a higher enantioselectivity than 1,2-dichloroethane, the reaction in ethyl acetate was very sluggish, and a reaction time of fifty hours was needed to complete the reaction (entry 17). Therefore, considering the high efficiency of the reaction in 1,2-dichloroethane with promising enantio-control (entry 18), the reaction concentration was further reduced in 1,2-dichloroethane (entries 19-22), and the enantioselectivity of product **7ab** could be enhanced to 85% ee (entry 21). Under this concentration, several chlorinated solvents were evaluated (entries 23-25), and dichloromethane was found to support the reaction to achieve a higher enantioselectivity of 88% ee (entry 23). Moreover, the conditions were further optimized by adding molecular sieves (MS) or anhydrous sulfates as additives to the reaction (entries 26-30). However, in this reaction for the synthesis of aryl-pyrroloindole **7ab** bearing both axial and central chirality, the addition of these additives could not improve the diastereoselectivity and the enantioselectivity (entries 26-30 vs. entry 23), which indicated that these additives were not necessary for this reaction. So, in the absence of additives, we further modulated the reagent ratio (entries 31-33) and changed the reaction temperature (entries 34-37). Nevertheless, the enantioselectivity of product **7ab** could not be enhanced under these conditions. Considering that the use of ethyl acetate as a solvent could improve the enantioselectivity with a long reaction time (entry 17), we tried using a mixed solvent of dichloromethane with ethyl acetate (4:1 v/v), and the enantioselectivity was indeed increased to 92% ee (entry 38). Therefore, the mixed solvent was selected as the most suitable medium for this reaction. In this mixed solvent, when the catalyst loading of CPA **4a** was lowered from 10 mol% (entry 38) to 5 mol% (entry 39), the yield of product **7ab** was greatly decreased from 94% to 32% albeit with a nearly retained stereoselectivity, which implied that 10 mol% catalyst loading of CPA

4a was a necessity to control the reactivity of the reaction. Finally, the optimal reaction conditions were set as illustrated in entry 40, which could afford product **7ab** in an excellent yield of 94% with high diastereo- and enantioselectivity (84:16 dr, 92% ee).

Table S2. Conditions optimization for the synthesis of aryl-pyrroloindoles **7** bearing both axial and central chirality^a



entry	Cat.	6	solvent	T (°C)	1a:6	additives	Time (h)	7	yield (%) ^b	dr ^c	ee (%) ^d
1	(<i>R</i>)- 4a	6a	DCM (0.5 mL)	20	1:1.2	-	1	7aa	86	87:13	26
2	(<i>S</i>)- 4b	6a	DCM (0.5 mL)	20	1:1.2	-	10	7aa	77	67:33	-17
3	(<i>S</i>)- 4c	6a	DCM (0.5 mL)	20	1:1.2	-	1	7aa	80	83:17	-16
4	(<i>S</i>)- 4d	6a	DCM (0.5 mL)	20	1:1.2	-	1	7aa	81	76:24	-19
5	(<i>R</i>)- 4e	6a	DCM (0.5 mL)	20	1:1.2	-	10	7aa	84	62:38	<5
6	(<i>S</i>)- 4f	6a	DCM (0.5 mL)	20	1:1.2	-	1	7aa	85	70:30	-12
7	(<i>R</i>)- 4g	6a	DCM (0.5 mL)	20	1:1.2	-	1	7aa	82	73:27	13
8	(<i>R</i>)- 4a	6a	DCE (0.5 mL)	20	1:1.2	-	1	7aa	98	87:13	27
9	(<i>R</i>)- 4a	6a	CHCl ₃ (0.5 mL)	20	1:1.2	-	1	7aa	74	89:11	20
10	(<i>R</i>)- 4a	6a	toluene (0.5 mL)	20	1:1.2	-	1	7aa	98	88:12	15
11	(<i>R</i>)- 4a	6a	EtOAc (0.5 mL)	20	1:1.2	-	12	7aa	80	79:21	68
12	(<i>R</i>)- 4a	6b	DCE (0.5 mL)	20	1:1.2	-	2	7ab	88	82:18	76
13	(<i>R</i>)- 4a	6b	EtOAc (0.5 mL)	20	1:1.2	-	24	7ab	80	80:20	80
14	(<i>R</i>)- 4a	6b	toluene (0.5 mL)	20	1:1.2	-	4	7ab	98	77:23	46
15	(<i>R</i>)- 4a	6b	acetone (0.5 mL)	20	1:1.2	-	50	7ab	95	78:22	74
16	(<i>R</i>)- 4a	6b	CH ₃ CN (0.5 mL)	20	1:1.2	-	10	7ab	89	75:25	65
17	(<i>R</i>)- 4a	6b	EtOAc (1.0 mL)	20	1:1.2	-	50	7ab	52	81:19	86
18	(<i>R</i>)- 4a	6b	DCE (1.0 mL)	20	1:1.2	-	4	7ab	98	83:17	80
19	(<i>R</i>)- 4a	6b	DCE (1.5 mL)	20	1:1.2	-	4	7ab	98	82:18	83
20	(<i>R</i>)- 4a	6b	DCE (2.0 mL)	20	1:1.2	-	4	7ab	98	81:19	85
21	(<i>R</i>)- 4a	6b	DCE (2.5 mL)	20	1:1.2	-	4	7ab	98	84:16	85
22	(<i>R</i>)- 4a	6b	DCE (3.0 mL)	20	1:1.2	-	4	7ab	98	83:17	85
23	(<i>R</i>)- 4a	6b	DCM (2.5 mL)	20	1:1.2	-	4	7ab	94	83:17	88
24	(<i>R</i>)- 4a	6b	CHCl ₃ (2.5 mL)	20	1:1.2	-	8	7ab	92	82:18	80

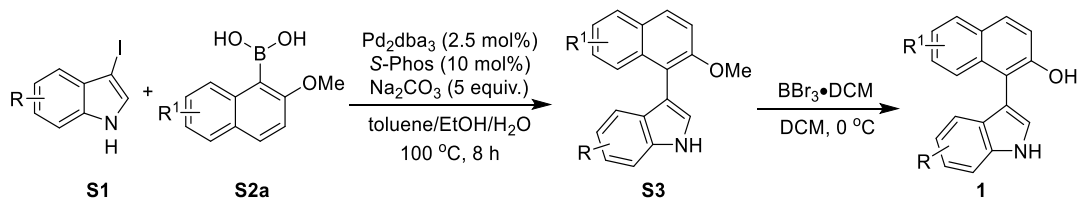
25	(<i>R</i>)- 4a	6b	CCl ₄ (2.5 mL)	20	1:1.2	-	4	7ab	95	84:16	46
26	(<i>R</i>)- 4a	6b	DCM (2.5 mL)	20	1:1.2	3 Å MS	10	7ab	64	81:19	86
27	(<i>R</i>)- 4a	6b	DCM (2.5 mL)	20	1:1.2	4 Å MS	10	7ab	77	80:20	84
28	(<i>R</i>)- 4a	6b	DCM (2.5 mL)	20	1:1.2	5 Å MS	4	7ab	91	81:19	88
29	(<i>R</i>)- 4a	6b	DCM (2.5 mL)	20	1:1.2	Na ₂ SO ₄	4	7ab	95	81:19	83
30	(<i>R</i>)- 4a	6b	DCM (2.5 mL)	20	1:1.2	MgSO ₄	4	7ab	95	78:22	83
31	(<i>R</i>)- 4a	6b	DCM (2.5 mL)	20	1:2	-	4	7ab	88	82:18	86
32	(<i>R</i>)- 4a	6b	DCM (2.5 mL)	20	1:2.1	-	4	7ab	94	82:18	87
33	(<i>R</i>)- 4a	6b	DCM (2.5 mL)	20	2:1	-	4	7ab	97	82:18	86
34	(<i>R</i>)- 4a	6b	DCM (2.5 mL)	-10	1:1.2	-	36	7ab	98	86:14	78
35	(<i>R</i>)- 4a	6b	DCM (2.5 mL)	10	1:1.2	-	24	7ab	97	84:16	84
36	(<i>R</i>)- 4a	6b	DCM (2.5 mL)	30	1:1.2	-	4	7ab	98	82:18	88
37	(<i>R</i>)- 4a	6b	DCM (2.5 mL)	50	1:1.2	-	2	7ab	98	80:20	88
38	(<i>R</i>)- 4a	6b	DCM:EtOAc (2.0 mL:0.5 mL)	20	1:1.2	-	10	7ab	94	83:17	92
39 ^e	(<i>R</i>)- 4a	6b	DCM:EtOAc (2.0 mL:0.5 mL)	20	1:1.2	-	20	7ab	32	81:19	91
40 ^f	(<i>R</i>)- 4a	6b	DCM:EtOAc (4 mL:1 mL)	20	1:1.2	-	10	7ab	94	84:16	92

^aUnless indicated otherwise, the reaction was carried out in 0.05 mmol scale in a solvent with additives (50 mg) for 1-50 h. ^bIsolated yield. ^cThe dr value was determined by HPLC and ¹H NMR. ^dThe enantiomeric excess (ee) referred to that of the major diastereomer and was determined by HPLC. ^eCatalyzed by 5 mol% (*R*)-**4a**. ^fThe reaction was carried out in 0.1 mmol scale under the catalysis of 15 mol% (*R*)-**4a**.

3. Synthetic procedures and characterization data of substrates 1, 2 and 6

General synthetic procedures for substrates 1:

3-Naphthylindoles **1** were synthesized according to the literature procedures.¹

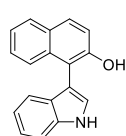


S1 to S3: Under argon atmosphere, to the mixture of **S1** (5.2 mmol), **S2a** (5.7 mmol), Pd_2dba_3 (2.5 mol%), *S*-Phos (CAS 657408-07-6, 10 mol%) and Na_2CO_3 (26 mmol) was added the mixed solvent of toluene (30 mL), ethanol (10 mL) and H_2O (10 mL). Then, the reaction mixture was stirred at $100\text{ }^\circ\text{C}$ for 8 h. After the completion of the reaction which was indicated by TLC, the reaction mixture was cooled to room temperature and quenched with water and extracted with ethyl acetate. The combined organic layer was washed with brine and dried over anhydrous Na_2SO_4 . Then, the organic layer was concentrated in vacuo to give a residue, which was purified by flash column chromatography (PE:EA = 20:1) to afford compounds **S3**.

S3 to substrates 1: Under argon atmosphere, to a stirring solution of BBr_3 (8 mL, 8 mmol, 1.0 M solution in DCM) in an ice bath was added dropwise the solution of **S3** (2 mmol) in DCM (10 mL) over a period of 30 min. Then, the reaction mixture was warmed to room temperature and stirred for 2 h. After the completion of the reaction which was indicated by TLC, water (50 mL) was added to the reaction mixture in an ice bath, and the aqueous layer was extracted three times with DCM. The combined organic layers were washed with brine, dried over anhydrous Na_2SO_4 , and concentrated in vacuo to give a residue, which was purified by flash column chromatography (PE:EA = 20:1) to afford substrates **1**.

Characterization data of substrates 1:

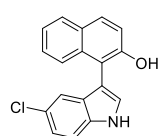
1-(1*H*-indol-3-yl)naphthalen-2-ol (**1a**)¹:



92% yield (0.48 g); white solid; m.p. $128\text{--}129\text{ }^\circ\text{C}$; $^1\text{H NMR}$ (400 MHz, CDCl_3): δ 8.53 (s, 1H), 7.91 – 7.80 (m, 2H), 7.61 – 7.50 (m, 2H), 7.43 – 7.37 (m, 1H), 7.36 – 7.28 (m, 5H), 7.16 – 7.11 (m, 1H), 5.56 (s, 1H).

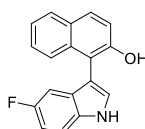
¹F. Jiang, K.-W. Chen, P. Wu, Y.-C. Zhang, Y. Jiao, F. Shi, *Angew. Chem. Int. Ed.* **2019**, 58, 15104.

1-(5-chloro-1H-indol-3-yl)naphthalen-2-ol (1b)¹:



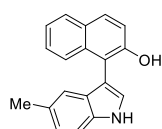
89% yield (0.52 g); white solid; m.p. 158.1-158.5 °C; ¹H NMR (400 MHz, CDCl₃) δ 8.55 (s, 1H), 7.91 – 7.78 (m, 2H), 7.52 – 7.36 (m, 3H), 7.35 – 7.28 (m, 3H), 7.25 – 7.18 (m, 2H), 5.35 (s, 1H).

1-(5-fluoro-1H-indol-3-yl)naphthalen-2-ol (1c)¹:



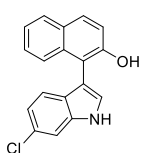
98% yield (0.54 g); white solid; m.p. 151-153 °C; ¹H NMR (400 MHz, CDCl₃) δ 8.55 (s, 1H), 7.90 – 7.80 (m, 2H), 7.54 – 7.41 (m, 3H), 7.39 – 7.28 (m, 3H), 7.10 – 7.02 (m, 1H), 6.93 (d, *J* = 9.2 Hz, 1H), 5.46 (s, 1H).

1-(5-methyl-1H-indol-3-yl)naphthalen-2-ol (1d)¹:



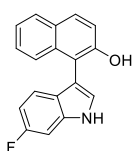
99% yield (0.54 g); white solid; m.p. 112-114 °C; ¹H NMR (400 MHz, CDCl₃) δ 8.45 (s, 1H), 7.89 – 7.82 (m, 2H), 7.61 – 7.55 (m, 1H), 7.43 (d, *J* = 8.4 Hz, 1H), 7.36 – 7.30 (m, 4H), 7.15 (d, *J* = 8.4 Hz, 1H), 7.09 (s, 1H), 5.57 (s, 1H), 2.37 (s, 3H).

1-(6-chloro-1H-indol-3-yl)naphthalen-2-ol (1e)¹:



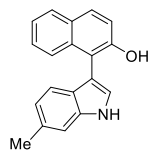
92% yield (0.54 g); white solid; m.p. 117-118 °C; ¹H NMR (400 MHz, CDCl₃) δ 8.52 (s, 1H), 7.92 – 7.79 (m, 2H), 7.57 – 7.45 (m, 2H), 7.40 – 7.28 (m, 4H), 7.19 (d, *J* = 8.8 Hz, 1H), 7.09 (d, *J* = 8.4 Hz, 1H), 5.46 (s, 1H).

1-(6-fluoro-1H-indol-3-yl)naphthalen-2-ol (1f)¹:



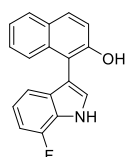
98% yield (0.54 g); white solid; m.p. 93-94 °C; ¹H NMR (400 MHz, CDCl₃) δ 8.52 (s, 1H), 7.92 – 7.78 (m, 2H), 7.55 – 7.49 (m, 1H), 7.42 – 7.28 (m, 4H), 7.24 – 7.13 (m, 2H), 6.94 – 6.82 (m, 1H), 5.51 (s, 1H).

1-(6-methyl-1H-indol-3-yl)naphthalen-2-ol (1g)¹:



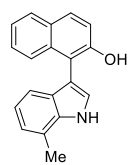
93% yield (0.51 g); white solid; m.p. 161-163 °C; ¹H NMR (400 MHz, CDCl₃) δ 8.41 (s, 1H), 7.84 (d, *J* = 8.8 Hz, 2H), 7.62 – 7.54 (m, 1H), 7.40 – 7.28 (m, 5H), 7.19 (d, *J* = 8.0 Hz, 1H), 6.97 (d, *J* = 8.4 Hz, 1H), 5.59 (s, 1H), 2.52 (s, 3H).

(5-fluoro-1H-indol-2-yl)diphenylmethanol (1h)¹:



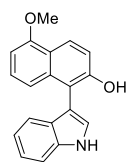
89% yield (0.49 g); white solid; m.p. 75-76 °C; ¹H NMR (400 MHz, CDCl₃) δ 8.73 (s, 1H), 7.89 – 7.81 (m, 2H), 7.56 – 7.49 (m, 1H), 7.45 – 7.40 (m, 1H), 7.37 – 7.29 (m, 3H), 7.09 – 6.99 (m, 3H), 5.46 (s, 1H).

1-(7-methyl-1H-indol-3-yl)naphthalen-2-ol (1i)¹:



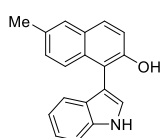
84% yield (0.46 g); brown solid; m.p. 105.2-105.8 °C; ¹H NMR (400 MHz, CDCl₃) δ 8.48 (s, 1H), 7.90 – 7.81 (m, 2H), 7.58 (d, *J* = 8.0 Hz, 1H), 7.40 (d, *J* = 2.0 Hz, 1H), 7.36 – 7.28 (m, 3H), 7.19 – 7.10 (m, 2H), 7.09 – 7.03 (m, 1H), 5.57 (s, 1H), 2.62 (s, 3H).

1-(1H-indol-3-yl)-5-methoxynaphthalen-2-ol (1j)¹:



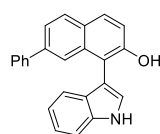
81% yield (0.47 g); yellow solid; m.p. 77-79 °C; ¹H NMR (400 MHz, CDCl₃) δ 8.54 (s, 1H), 8.30 (d, *J* = 8.8 Hz, 1H), 7.55 – 7.51 (m, 1H), 7.39 – 7.37 (m, 1H), 7.34 – 7.28 (m, 3H), 7.24 – 7.18 (m, 1H), 7.16 – 7.08 (m, 2H), 6.69 (d, *J* = 7.6 Hz, 1H), 5.54 (s, 1H), 4.02 (s, 3H).

1-(1H-indol-3-yl)-6-methylnaphthalen-2-ol (1k):



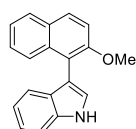
75% yield (0.41 g); white solid; m.p. 120-122 °C; ¹H NMR (400 MHz, CDCl₃) δ 8.54 (s, 1H), 7.76 (d, *J* = 8.8 Hz, 1H), 7.62 (s, 1H), 7.55 – 7.51 (m, 1H), 7.48 – 7.44 (m, 1H), 7.40 – 7.37 (m, 1H), 7.35 – 7.28 (m, 3H), 7.18 – 7.10 (m, 2H), 5.49 (s, 1H), 2.47 (s, 3H); ¹³C NMR (100 MHz, CDCl₃) δ 151.2, 136.6, 132.6, 132.5, 129.2, 128.8, 128.6, 127.5, 127.1, 125.1, 124.9, 123.1, 120.6, 120.3, 117.1, 112.9, 111.5, 108.6, 21.3; IR (KBr): 3329, 3041, 2915, 1600, 1474, 1378, 1232, 1146, 1100, 940, 672 cm⁻¹; ESI FTMS exact mass calcd for (C₁₉H₁₅NO-H)⁻ requires m/z 272.1081, found m/z 272.1084.

1-(1H-indol-3-yl)-7-phenylnaphthalen-2-ol (1l)¹:



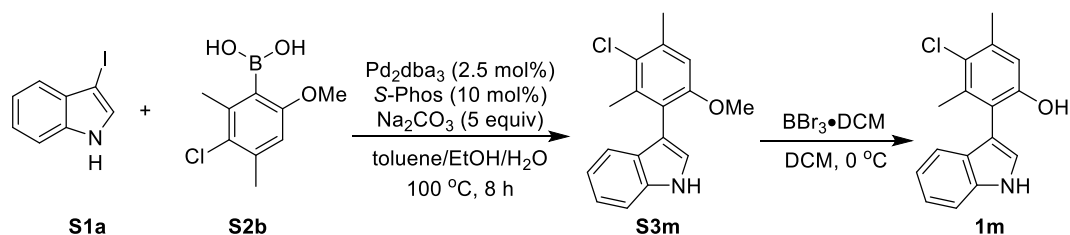
87% yield (0.58 g); yellow solid; m.p. 113-115 °C; ¹H NMR (400 MHz, CDCl₃) δ 8.54 (s, 1H), 7.98 – 7.84 (m, 2H), 7.80 (s, 1H), 7.60 (d, *J* = 8.4 Hz, 1H), 7.57 – 7.46 (m, 3H), 7.44 – 7.40 (m, 1H), 7.40 – 7.34 (m, 3H), 7.34 – 7.26 (m, 3H), 7.20 – 7.13 (m, 1H), 5.57 (s, 1H).

3-(2-methoxynaphthalen-1-yl)-1H-indole (1n)¹:



79% yield (0.43 g); white solid; m.p. 125-127 °C; ¹H NMR (400 MHz, CDCl₃) δ 8.36 (s, 1H), 7.91 (d, *J* = 8.8 Hz, 1H), 7.85 (d, *J* = 8.0 Hz, 1H), 7.74 (d, *J* = 8.4 Hz, 1H), 7.48 (d, *J* = 8.0 Hz, 1H), 7.42 (d, *J* = 9.2 Hz, 1H), 7.37 – 7.29 (m, 3H), 7.28 – 7.27 (m, 1H), 7.25 – 7.22 (m, 1H), 7.11 – 7.04 (m, 1H), 3.84 (s, 3H).

Synthetic procedure and characterization data of substrate **1m**:



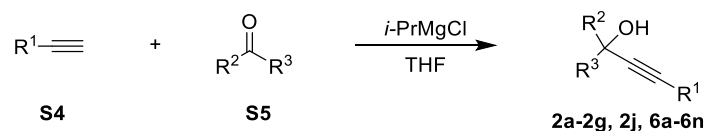
Following the literature method¹ and the general synthetic procedures for substrates **1**, a mixture of **S1a** (0.73 g, 3.0 mmol), **S2b** (0.71 g, 3.3 mmol), Pd₂dba₃ (69.0 mg, 2.5 mol%), S-Phos (123 mg, 10.0 mol%) and Na₂CO₃ (1.06 g, 10.0 mmol) in toluene/ethanol/H₂O (18/6/6 mL) was heated to reflux for 10 h, which afforded **S3m** (0.68 g, 79% yield). Then, the reaction of **S3m** (855 mg, 3 mmol) and BBr₃ (12 mL, 12 mmol, 1.0 M solution in DCM) in DCM (15 mL) at 0 °C for 2 h afforded substrate **1m** (0.80 g, 98% yield) as a white solid.

4-chloro-2-(1H-indol-3-yl)-3,5-dimethylphenol (1m**)**¹: m.p. 108-110 °C; ¹H NMR (400 MHz, CDCl₃) δ 8.46 (s, 1H), 7.49 (d, *J* = 8.4 Hz, 1H), 7.35 – 7.27 (m, 2H), 7.25 – 7.20 (m, 1H), 7.19 – 7.13 (m, 1H), 6.83 (s, 1H), 5.10 (s, 1H), 2.42 (s, 3H), 2.17 (s, 3H).

General synthetic procedures for substrates **2** and **6**:

Propargylic alcohols **2** and **6** were synthesized according to the literature procedures.^{2,3}

Synthetic Procedure A: (for the synthesis of substrates **2a-2g**, **2j**, **6a-6n**):



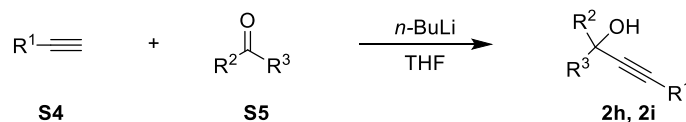
Under argon atmosphere, to an oven-dried flask charged with a solution of alkyne **S4** (12.5 mmol, 2.5 equiv) in dry THF (30 mL) was added *i*-PrMgCl (12.6 mmol, 6.3 mL, 2.0 M solution in THF) dropwise at 0 °C. After addition, the mixture was warmed to room temperature and stirred at the same temperature for 1 hour. Next, the reaction mixture was cooled to 0 °C, and a solution of ketone **S5** (5.0 mmol) in THF (5 mL) was added dropwise. The reaction mixture was then warmed to 60 °C and stirred for 6-12 h. After completion of the reaction which was indicated by TLC, the reaction mixture was cooled to 0 °C and slowly treated with saturated aqueous NH₄Cl solution (10

² D. Qian, L. Wu, Z. Lin, J. Sun, *Nat. Commun.* **2017**, *8*, 567.

³ W. Zhang, S. Wei, J. Qu, B. Wang, *Org. Biomol. Chem.* **2021**, *19*, 4992.

mL). The organic layer was separated and the aqueous layer was extracted with EtOAc for three times. The combined organic layers were dried over anhydrous Na₂SO₄, filtered, and concentrated to give a residue, which was purified through flash column chromatography on silica gel to afford pure substrates **2** or **6**.

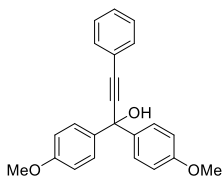
Synthetic Procedure B (for the synthesis of substrates **2h**, **2i**):



Under argon atmosphere, to an oven-dried flask charged with a solution of alkyne **S4** (7.5 mmol, 1.5 equiv.) in dry THF (10 mL) was added *n*-BuLi (7.7 mmol, 3.2 mL, 2.4 M in hexane) dropwise at -78 °C. The mixture was stirred at -78 °C for 1 h, then a solution of ketone **S5** (5.0 mmol, 1.0 equiv) in THF (5 mL) was added slowly via syringe. Then, the reaction mixture was gradually warmed up to room temperature and stirred for 3 h. After completion of the reaction which was indicated by TLC, the reaction mixture was cooled to 0 °C and the solution of saturated aqueous NH₄Cl (10 mL) was added to the mixture dropwise. The organic layer was separated and the aqueous layer was extracted with ethyl acetate for three times. The combined organic layers were washed with brine (50 mL), dried over anhydrous Na₂SO₄, filtered, and concentrated to give a residue, which was purified through flash column chromatography on silica gel to afford pure substrate **2h** or **2i**.

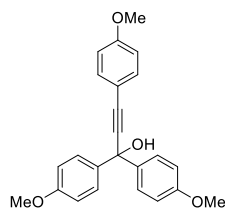
Characterization data of substrates 2 and 6:

1,1-bis(4-methoxyphenyl)-3-phenylprop-2-yn-1-ol (2a)²:

 92% yield (1.59 g); yellow solid; m.p. 77-78 °C; ¹H NMR (400 MHz, CDCl₃) δ 7.58 (d, *J* = 8.8 Hz, 4H), 7.53 – 7.48 (m, 2H), 7.36 – 7.29 (m, 3H), 6.88 (d, *J* = 8.8 Hz, 4H), 3.80 (s, 6H), 2.88 (s, 1H); ¹³C NMR (100 MHz, CDCl₃) δ 159.1, 137.6, 131.8, 128.6, 128.4, 127.5, 122.6, 113.6, 92.2, 86.9, 74.2, 55.3; IR (KBr): 3008, 2975, 2838, 1608, 1507, 1445, 1246, 899, 781, 695 cm⁻¹; ESI FTMS exact mass calcd for (C₂₃H₂₀O₃+Na)⁺ requires *m/z* 367.1305, found *m/z* 367.1307.

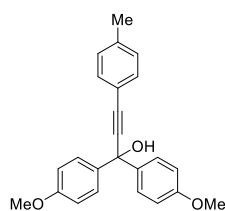
1,1,3-tris(4-methoxyphenyl)prop-2-yn-1-ol (2b)⁴:

⁴ C. D. Gabbutt, B. M. Heron, A. C. Instone, D. A. Thomas, S. M. Partington, M. B. Hursthouse, T. Gelbrich, *Eur. J. Org. Chem.* **2003**, 2003, 1220.



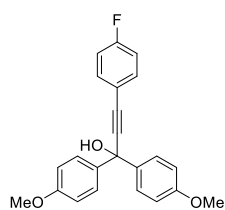
87% yield (1.62 g); yellow oil; ^1H NMR (400 MHz, CDCl_3) δ 7.57 (d, J = 8.8 Hz, 4H), 7.43 (d, J = 8.8 Hz, 2H), 6.93 – 6.79 (m, 6H), 3.81 (s, 3H), 3.80 (s, 6H), 2.85 (s, 1H); ^{13}C NMR (100 MHz, CDCl_3) δ 159.9, 159.1, 137.9, 133.3, 131.5, 131.1, 130.3, 127.5, 121.9, 114.7, 114.0, 113.8, 113.6, 113.5, 90.9, 86.9, 74.3, 55.4; IR (KBr): 3001, 2955, 2836, 1606, 1463, 1248, 1170, 1031, 831, 591 cm^{-1} ; ESI FTMS exact mass calcd for $(\text{C}_{24}\text{H}_{22}\text{O}_4+\text{Na})^+$ requires m/z 397.1410, found m/z 397.1411.

1,1-bis(4-methoxyphenyl)-3-(p-tolyl)prop-2-yn-1-ol (2c)⁵:



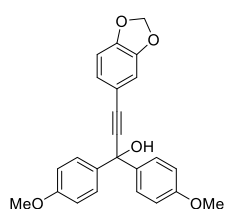
81% yield (1.45 g); yellow oil; ^1H NMR (400 MHz, CDCl_3) δ 7.58 (d, J = 8.8 Hz, 4H), 7.40 (d, J = 8.4 Hz, 2H), 7.14 (d, J = 8.0 Hz, 2H), 6.88 (d, J = 8.8 Hz, 4H), 3.80 (s, 6H), 2.87 (s, 1H), 2.36 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 159.1, 138.8, 137.8, 131.7, 129.2, 127.5, 119.6, 113.6, 91.5, 87.1, 74.3, 55.4, 21.6; IR (KBr): 3002, 2954, 2832, 1608, 1508, 1249, 1171, 1033, 819, 591 cm^{-1} ; ESI FTMS exact mass calcd for $(\text{C}_{24}\text{H}_{22}\text{O}_3+\text{Na})^+$ requires m/z 381.1461, found m/z 381.1478.

3-(4-fluorophenyl)-1,1-bis(4-methoxyphenyl)prop-2-yn-1-ol (2d):



83% yield (1.50 g); yellow oil; ^1H NMR (400 MHz, CDCl_3) δ 7.55 (d, J = 8.4 Hz, 4H), 7.51 – 7.43 (m, 2H), 7.06 – 6.98 (m, 2H), 6.87 (d, J = 8.8 Hz, 4H), 3.80 (s, 6H), 2.85 (s, 1H); ^{13}C NMR (100 MHz, CDCl_3) δ 162.8 (d, J = 248.5 Hz), 159.2, 137.5, 133.8 (d, J = 8.5 Hz), 127.5, 118.7, 115.7 (d, J = 21.9 Hz), 113.7, 91.9, 85.9, 74.3, 55.4; ^{19}F NMR (376 MHz, CDCl_3) δ -110.43; IR (KBr): 2836, 2360, 1601, 1507, 1249, 1172, 988, 832, 591 cm^{-1} ; ESI FTMS exact mass calcd for $(\text{C}_{23}\text{H}_{19}\text{FO}_3+\text{Na})^+$ requires m/z 385.1210, found m/z 385.1227.

3-(benzo[*d*][1,3]dioxol-5-yl)-1,1-bis(4-methoxyphenyl)prop-2-yn-1-ol (2e):

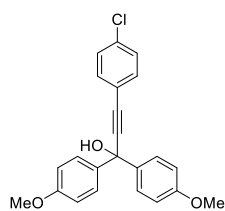


71% yield (1.38 g); yellow oil; ^1H NMR (400 MHz, CDCl_3) δ 7.55 (d, J = 8.8 Hz, 4H), 7.02 (d, J = 8.0 Hz, 1H), 6.86 (d, J = 8.4 Hz, 5H), 6.76 (d, J = 8.0 Hz, 1H), 5.96 (s, 2H), 3.79 (s, 6H), 2.94 (s, 1H); ^{13}C NMR (100 MHz, CDCl_3) δ 159.0, 148.1, 147.4, 137.7, 136.4, 129.1, 128.3, 127.8, 127.4, 126.5, 115.8, 113.9, 113.6, 111.7, 108.5, 101.4, 90.6, 86.7, 75.4, 74.2, 55.3; IR (KBr): 3002, 2956, 2836, 2360, 1507, 1249, 1172, 1036, 831, 591 cm^{-1} ; ESI FTMS exact mass calcd for

⁵ S. Aiken, B. Allsopp, K. Booth, C. D. Gabbutt, B. M. Heron, C. R. Rice, *Tetrahedron* **2014**, *70*, 9352.

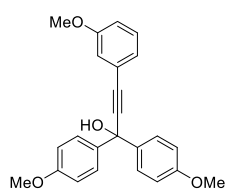
(C₂₄H₂₀O₅+Na)⁺ requires m/z 411.1203, found m/z 411.1225.

3-(4-chlorophenyl)-1,1-bis(4-methoxyphenyl)prop-2-yn-1-ol (2f):



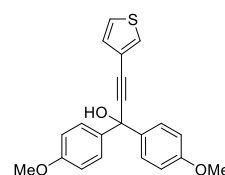
79% yield (1.49 g); yellow oil; ¹H NMR (400 MHz, CDCl₃) δ 7.54 (d, *J* = 8.4 Hz, 4H), 7.42 (d, *J* = 8.0 Hz, 2H), 7.30 (d, *J* = 8.0 Hz, 2H), 6.87 (d, *J* = 8.4 Hz, 4H), 3.80 (s, 6H), 2.86 (s, 1H); ¹³C NMR (100 MHz, CDCl₃) δ 159.2, 137.4, 134.7, 133.1, 128.8, 127.5, 121.1, 113.7, 93.2, 85.8, 74.3, 55.4; IR (KBr): 2980, 2931, 2837, 1606, 1508, 1331, 1248, 839, 751, 592 cm⁻¹; ESI FTMS exact mass calcd for (C₂₃H₁₉ClO₃+Na)⁺ requires m/z 401.0915, found m/z 401.0933.

3-(3-methoxyphenyl)-1,1-bis(4-methoxyphenyl)prop-2-yn-1-ol (2g):



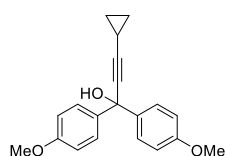
81% yield (1.51 g); yellow oil; ¹H NMR (400 MHz, CDCl₃) δ 7.57 (d, *J* = 8.8 Hz, 4H), 7.26 – 7.16 (m, 1H), 7.11 (d, *J* = 7.6 Hz, 1H), 7.02 (s, 1H), 6.95 – 6.82 (m, 5H), 3.80 (s, 9H), 3.01 (s, 1H); ¹³C NMR (100 MHz, CDCl₃) δ 159.3, 159.1, 137.6, 129.4, 127.4, 124.4, 123.6, 116.6, 115.2, 113.6, 92.0, 86.8, 74.2, 55.4, 55.3; IR (KBr): 3002, 2960, 2836, 2360, 1605, 1508, 1250, 1038, 831, 742 cm⁻¹; ESI FTMS exact mass calcd for (C₂₄H₂₂O₄+Na)⁺ requires m/z 397.1410, found m/z 397.1406.

1,1-bis(4-methoxyphenyl)-3-(thiophen-3-yl)prop-2-yn-1-ol (2h)⁶:



87% yield (1.53 g); yellow oil; ¹H NMR (400 MHz, CDCl₃) δ 7.53 (d, *J* = 8.4 Hz, 4H), 7.49 – 7.45 (m, 1H), 7.25 – 7.22 (m, 1H), 7.16 – 7.11 (m, 1H), 6.85 (d, *J* = 8.4 Hz, 4H), 3.77 (s, 6H), 2.94 (s, 1H); ¹³C NMR (100 MHz, CDCl₃) δ 159.1, 137.6, 123.0, 129.2, 127.5, 125.4, 121.6, 113.6, 91.7, 82.0, 74.3, 55.4; IR (KBr): 3104, 2953, 2834, 1607, 1507, 1247, 1080, 938, 824, 590 cm⁻¹; ESI FTMS exact mass calcd for (C₂₁H₁₈O₃S+H)⁺ requires m/z 351.1049, found m/z 351.1040.

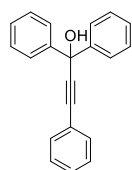
3-cyclopropyl-1,1-bis(4-methoxyphenyl)prop-2-yn-1-ol (2i):



80% yield (1.23 g); yellow oil; ¹H NMR (400 MHz, CDCl₃) δ 7.53 (d, *J* = 8.8 Hz, 4H), 6.89 (d, *J* = 8.8 Hz, 4H), 3.84 (s, 6H), 2.83 (s, 1H), 1.47 – 1.37 (m, 1H), 0.91 – 0.76 (m, 4H); ¹³C NMR (100 MHz, CDCl₃) δ 158.8, 138.0, 127.2, 113.3, 90.7, 78.4, 73.7, 55.2, 8.3, -0.4; IR (KBr): 3005, 2954, 2836, 2234, 1607, 1508, 1248, 1058, 939, 833, 635 cm⁻¹; ESI FTMS exact mass calcd for (C₂₀H₂₀O₃+H)⁺ requires m/z 309.1485, found m/z 309.1478.

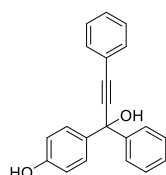
⁶ N. Cabrera-Lobera, N. Velasco, R. Sanz, M. A. Fernández-Rodríguez, *Tetrahedron* **2019**, *75*, 4071.

1,1,3-triphenylprop-2-yn-1-ol (2j)²:



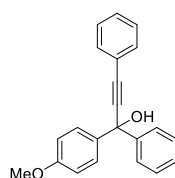
81% yield (1.15 g); white solid; m.p. 102–105 °C; ¹H NMR (400 MHz, CDCl₃) δ 7.70 (d, *J* = 7.6 Hz, 4H), 7.55 – 7.49 (m, 2H), 7.40 – 7.33 (m, 7H), 7.32 – 7.27 (m, 2H), 2.91 (s, 1H); ¹³C NMR (100 MHz, CDCl₃) δ 145.0, 131.8, 128.8, 128.4, 127.8, 126.1, 122.4, 91.7, 87.3, 74.9; IR (KBr): 3002, 2956, 2836, 2361, 1508, 1249, 1171, 1037, 832, 591 cm⁻¹.

4-(1-hydroxy-1,3-diphenylprop-2-yn-1-yl)phenol (6a)³:



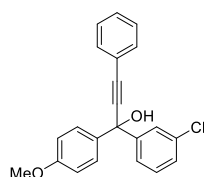
88% yield (1.32 g); yellow solid; m.p. 121–123 °C; ¹H NMR (400 MHz, CDCl₃) δ 7.66 (d, *J* = 8.0 Hz, 2H), 7.58 – 7.43 (m, 4H), 7.40 – 7.27 (m, 6H), 6.79 (d, *J* = 8.4 Hz, 2H), 5.00 (s, 1H), 2.87 (s, 1H).

1-(4-methoxyphenyl)-1,3-diphenylprop-2-yn-1-ol (6b)⁷:



90% yield (1.41 g); white solid; m.p. 102–103 °C; ¹H NMR (400 MHz, CDCl₃) δ 7.67 (d, *J* = 7.6 Hz, 2H), 7.58 (d, *J* = 8.8 Hz, 2H), 7.54 – 7.48 (m, 2H), 7.39 – 7.27 (m, 6H), 6.88 (d, *J* = 8.8 Hz, 2H), 3.80 (s, 3H), 2.84 (s, 1H); ¹³C NMR (100 MHz, CDCl₃) δ 159.2, 145.3, 137.4, 131.9, 128.7, 128.4, 127.8, 127.6, 126.1, 122.6, 113.7, 92.0, 87.1, 74.6, 55.4; IR (KBr): 3055, 2962, 2837, 2360, 1508, 1170, 1024, 829, 724, 525 cm⁻¹; ESI FTMS exact mass calcd for (C₂₂H₁₈O₂+Na)⁺ requires *m/z* 337.1199, found *m/z* 337.1198.

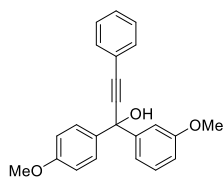
1-(3-chlorophenyl)-1-(4-methoxyphenyl)-3-phenylprop-2-yn-1-ol (6c):



87% yield (1.51 g); yellow solid; m.p. 88–90 °C; ¹H NMR (400 MHz, CDCl₃) δ 7.98 (d, *J* = 7.6 Hz, 1H), 7.57 – 7.47 (m, 4H), 7.40 – 7.27 (m, 6H), 6.88 (d, *J* = 8.4 Hz, 2H), 3.81 (s, 3H), 3.24 (s, 1H); ¹³C NMR (100 MHz, CDCl₃) δ 159.4, 147.4, 136.8, 134.3, 131.9, 129.6, 128.9, 128.5, 127.9, 127.5, 126.3, 124.4, 122.3, 113.8, 91.3, 87.6, 74.2, 55.4; IR (KBr): 3011, 2971, 2837, 2360, 1507, 1245, 1053, 789, 756, 525 cm⁻¹; ESI FTMS exact mass calcd for (C₂₂H₁₇ClO₂+Na)⁺ requires *m/z* 371.0809, found *m/z* 371.0818.

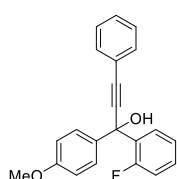
1-(3-methoxyphenyl)-1-(4-methoxyphenyl)-3-phenylprop-2-yn-1-ol (6d):

⁷ Y.-W. Dong, G.-W. Wang, L. Wang, *Tetrahedron* **2008**, *64*, 10148.



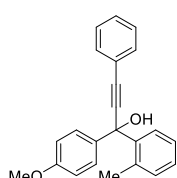
78% yield (1.34 g); yellow oil; ^1H NMR (400 MHz, CDCl_3) δ 7.60 (d, $J = 8.8$ Hz, 2H), 7.53 – 7.50 (m, 2H), 7.37 – 7.32 (m, 4H), 7.29 – 7.27 (m, 2H), 6.88 (d, $J = 8.8$ Hz, 2H), 6.85 – 6.81 (m, 1H), 3.81 (s, 3H), 3.80 (s, 3H), 2.94 (s, 1H); ^{13}C NMR (100 MHz, CDCl_3) δ 147.0, 137.3, 131.9, 129.4, 128.7, 128.4, 127.5, 122.6, 118.6, 113.7, 113.1, 112.0, 91.9, 87.1, 74.5, 56.1, 55.4; IR (KBr): 3448, 2360, 2342, 1607, 1508, 1275, 1036, 999, 751, 692 cm^{-1} ; ESI FTMS exact mass calcd for $(\text{C}_{23}\text{H}_{20}\text{O}_3+\text{Na})^+$ requires m/z 367.1305, found m/z 367.1324.

1-(2-fluorophenyl)-1-(4-methoxyphenyl)-3-phenylprop-2-yn-1-ol (6e):



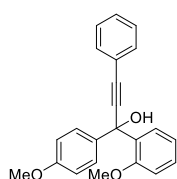
75% yield (1.25 g); yellow solid; ^1H NMR (400 MHz, CDCl_3) δ 7.82 – 7.71 (m, 1H), 7.59 (d, $J = 8.8$ Hz, 2H), 7.54 – 7.47 (m, 2H), 7.37 – 7.30 (m, 4H), 7.20 – 7.18 (m, 1H), 7.05 – 6.99 (m, 1H), 6.89 (d, $J = 8.8$ Hz, 2H), 3.81 (s, 3H), 3.10 (s, 1H); ^{13}C NMR (100 MHz, CDCl_3) δ 160.1 (d, $J = 244.3$ Hz), 159.4, 138.1, 136.0, 132.2 (d, $J = 10.0$ Hz), 131.9, 129.9 (d, $J = 8.4$ Hz), 128.9, 128.7, 128.4, 127.7, 127.4, 123.9 (d, $J = 3.3$ Hz), 122.5, 116.4 (d, $J = 21.6$ Hz), 113.7, 113.3, 90.3, 86.9, 72.2, 55.4; ^{19}F NMR (376 MHz, CDCl_3) δ -111.08; IR (KBr): 3007, 2936, 2837, 2360, 1609, 1508, 1026, 863, 760, 567 cm^{-1} ; ESI FTMS exact mass calcd for $(\text{C}_{22}\text{H}_{17}\text{FO}_2+\text{Na})^+$ requires m/z 355.1105, found m/z 355.1104.

1-(4-methoxyphenyl)-3-phenyl-1-(*o*-tolyl)prop-2-yn-1-ol (6f):



71% yield (1.16 g); yellow oil; ^1H NMR (400 MHz, CDCl_3) δ 7.98 (d, $J = 7.6$ Hz, 1H), 7.52 – 7.46 (m, 4H), 7.37 – 7.27 (m, 5H), 7.15 (d, $J = 7.2$ Hz, 1H), 6.86 (d, $J = 8.8$ Hz, 2H), 3.81 (s, 3H), 2.77 (s, 1H), 2.21 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 159.3, 141.8, 136.4, 132.1, 131.9, 131.7, 129.5, 128.6, 128.4, 128.0, 125.8, 125.6, 122.6, 113.9, 113.7, 91.1, 87.1, 74.0, 55.3, 21.1; IR (KBr): 3057, 2360, 2342, 1541, 1250, 1034, 788, 752, 691, 593 cm^{-1} ; ESI FTMS exact mass calcd for $(\text{C}_{23}\text{H}_{20}\text{O}_2+\text{Na})^+$ requires m/z 351.1356, found m/z 351.1381.

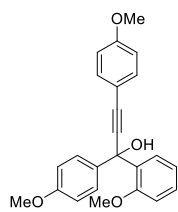
1-(2-methoxyphenyl)-1-(4-methoxyphenyl)-3-phenylprop-2-yn-1-ol (6g):



93% yield (1.60 g); yellow solid; m.p. 84-86 $^{\circ}\text{C}$; ^1H NMR (400 MHz, CDCl_3) δ 7.54 (d, $J = 8.8$ Hz, 2H), 7.51 – 7.45 (m, 2H), 7.39 (dd, $J = 8.0, 1.6$ Hz, 1H), 7.34 – 7.27 (m, 4H), 7.00 – 6.93 (m, 2H), 6.89 (d, $J = 8.8$ Hz, 2H), 4.98 (s, 1H), 3.83 (s, 3H), 3.82 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 159.1, 157.0, 136.7, 133.0, 131.8, 129.5, 128.5, 128.4, 128.3, 127.8, 123.1, 121.0, 113.4, 112.3, 91.5, 86.6, 74.6, 56.1,

55.4; IR (KBr): 3057, 2360, 2342, 1541, 1250, 1238, 1061, 807, 757, 525 cm^{-1} ; ESI FTMS exact mass calcd for $(\text{C}_{23}\text{H}_{20}\text{O}_3+\text{Na})^+$ requires m/z 367.1305, found m/z 367.1326.

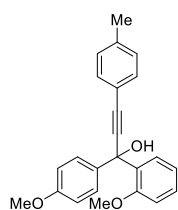
1-(2-methoxyphenyl)-1,3-bis(4-methoxyphenyl)prop-2-yn-1-ol (6h):



91% yield (1.70 g); white solid; ^1H NMR (400 MHz, CDCl_3) δ 7.52 (d, $J = 8.8$ Hz, 2H), 7.45 – 7.37 (m, 3H), 7.33 – 7.28 (m, 1H), 6.98 – 6.93 (m, 2H), 6.88 (d, $J = 8.8$ Hz, 2H), 6.82 (d, $J = 8.8$ Hz, 2H), 4.95 (s, 1H), 3.82 (s, 6H), 3.80 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 159.6, 158.9, 157.0, 136.9, 133.2, 133.1, 129.3,

128.5, 127.7, 120.9, 115.1, 113.8, 113.3, 112.3, 90.0, 86.5, 74.6, 56.0, 55.3; IR (KBr): 3006, 2979, 2838, 1599, 1461, 1238, 1061, 807, 757, 525 cm^{-1} ; ESI FTMS exact mass calcd for $(\text{C}_{24}\text{H}_{22}\text{O}_4+\text{Na})^+$ requires m/z 397.1410, found m/z 397.1410.

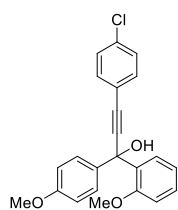
1-(2-methoxyphenyl)-1-(4-methoxyphenyl)-3-(p-tolyl)prop-2-yn-1-ol (6i):



84% yield (1.50 g); white solid; m.p. 97-99 $^{\circ}\text{C}$; ^1H NMR (400 MHz, CDCl_3) δ 7.52 (d, $J = 8.8$ Hz, 2H), 7.42 – 7.35 (m, 3H), 7.33 – 7.28 (m, 1H), 7.10 (d, $J = 8.0$ Hz, 2H), 6.98 – 6.93 (m, 2H), 6.88 (d, $J = 8.8$ Hz, 2H), 4.96 (s, 1H), 3.82 (s, 6H), 2.34 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 159.0, 157.0, 138.4, 136.7,

133.1, 131.7, 129.4, 129.0, 128.5, 127.7, 120.9, 119.9, 113.3, 112.3, 90.7, 86.7, 74.2, 56.0, 55.3, 21.5; IR (KBr): 3026, 2967, 2837, 2360, 1509, 1241, 1181, 1043, 778, 528 cm^{-1} ; ESI FTMS exact mass calcd for $(\text{C}_{24}\text{H}_{22}\text{O}_3+\text{Na})^+$ requires m/z 381.1461, found m/z 381.1478.

3-(4-chlorophenyl)-1-(2-methoxyphenyl)-1-(4-methoxyphenyl)prop-2-yn-1-ol (6j):

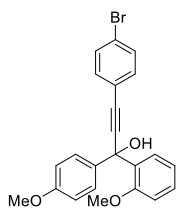


81% yield (1.53 g); yellow solid; ^1H NMR (400 MHz, CDCl_3) δ 7.50 (d, $J = 8.4$ Hz, 2H), 7.43 – 7.35 (m, 3H), 7.34 – 7.27 (m, 3H), 7.01 – 6.93 (m, 2H), 6.89 (d, $J = 8.8$ Hz, 2H), 4.97 (s, 1H), 3.82 (s, 6H); ^{13}C NMR (100 MHz, CDCl_3) δ 159.1,

156.9, 136.4, 134.4, 133.0, 132.7, 129.5, 128.6, 128.4, 127.7, 121.5, 121.0, 113.4, 112.2, 92.4, 85.4, 74.5, 56.0, 55.3; IR (KBr): 3003, 2963, 2837, 2360, 1608, 1487, 1181, 835, 777, 526 cm^{-1} ; ESI FTMS exact mass calcd for $(\text{C}_{23}\text{H}_{19}\text{ClO}_3+\text{Na})^+$ requires m/z 401.0915, found m/z 401.0928.

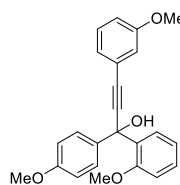
3-(4-bromophenyl)-1-(2-methoxyphenyl)-1-(4-methoxyphenyl)prop-2-yn-1-ol (6k):

75% yield (1.58 g); yellow solid; m.p. 127-129 $^{\circ}\text{C}$; ^1H NMR (400 MHz, CDCl_3) δ 7.55 (d, $J = 8.4$ Hz, 2H), 7.48 (d, $J = 8.4$ Hz, 2H), 7.43 – 7.34 (m, 4H), 7.05 – 6.98 (m, 2H), 6.94 (d, $J = 8.8$ Hz, 2H), 5.02 (s, 1H), 3.88 (s, 6H); ^{13}C NMR (100 MHz, CDCl_3) δ 159.1, 156.9, 136.3, 133.2, 132.7,



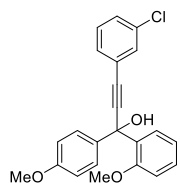
131.5, 129.5, 128.4, 127.7, 122.6, 121.9, 121.0, 113.4, 112.2, 92.6, 85.4, 74.5, 56.0, 55.3; IR (KBr): 3066, 2962, 2836, 2360, 1609, 1508, 1241, 1043, 785, 575 cm^{-1} ; ESI FTMS exact mass calcd for $(\text{C}_{23}\text{H}_{19}\text{BrO}_3+\text{Na})^+$ requires m/z 445.0410, found m/z 445.0430.

1-(2-methoxyphenyl)-3-(3-methoxyphenyl)-1-(4-methoxyphenyl)prop-2-yn-1-ol (6l):



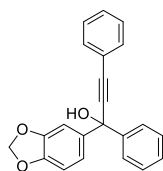
79% yield (1.48 g); yellow oil; ^1H NMR (400 MHz, CDCl_3) δ 7.52 (d, $J = 8.8$ Hz, 2H), 7.39 (d, $J = 8.0$ Hz, 1H), 7.35 – 7.29 (m, 1H), 7.23 – 7.17 (m, 1H), 7.08 (d, $J = 7.2$ Hz, 1H), 7.02 – 6.93 (m, 3H), 6.91 – 6.84 (m, 3H), 4.98 (s, 1H), 3.82 (s, 6H), 3.78 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 159.2, 159.0, 157.0, 136.6, 132.9, 129.4, 129.3, 128.4, 127.8, 124.3, 124.0, 121.0, 116.6, 115.0, 113.3, 112.3, 91.3, 86.4, 74.5, 56.0, 55.3; IR (KBr): 3002, 2957, 2835, 2360, 1608, 1275, 1026, 788, 692, 525 cm^{-1} ; ESI FTMS exact mass calcd for $(\text{C}_{24}\text{H}_{22}\text{O}_4+\text{Na})^+$ requires m/z 397.1410, found m/z 397.1412.

3-(3-chlorophenyl)-1-(2-methoxyphenyl)-1-(4-methoxyphenyl)prop-2-yn-1-ol (6m):



85% yield (1.61 g); yellow solid; m.p. 92-94 $^{\circ}\text{C}$; ^1H NMR (400 MHz, CDCl_3) δ 7.50 (d, $J = 8.8$ Hz, 2H), 7.45 (s, 1H), 7.39 – 7.27 (m, 4H), 7.25 – 7.19 (m, 1H), 6.99 – 6.93 (m, 2H), 6.89 (d, $J = 8.8$ Hz, 2H), 4.97 (s, 1H), 3.83 (s, 3H), 3.82 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 159.2, 157.0, 136.3, 134.1, 133.7, 132.7, 131.7, 130.0, 129.6, 129.5, 128.7, 128.4, 127.8, 124.7, 121.0, 114.0, 113.5, 112.3, 92.8, 85.1, 74.5, 56.1, 55.4; IR (KBr): 3065, 2997, 2837, 2360, 1606, 1507, 1248, 1078, 849, 689 cm^{-1} ; ESI FTMS exact mass calcd for $(\text{C}_{23}\text{H}_{19}\text{ClO}_3+\text{Na})^+$ requires m/z 401.0915, found m/z 401.0934.

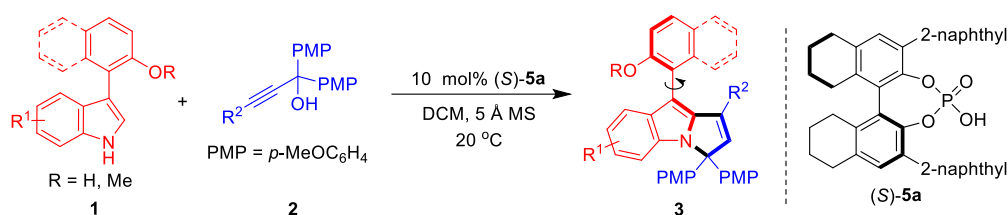
1-(benzo[d][1,3]dioxol-5-yl)-1,3-diphenylprop-2-yn-1-ol (6n):



85% yield (1.39 g); yellow oil; ^1H NMR (400 MHz, CDCl_3) δ 7.68 (d, $J = 7.6$ Hz, 2H), 7.53 – 7.50 (m, 2H), 7.42 – 7.27 (m, 7H), 7.21 (d, $J = 8.4$ Hz, 1H), 7.13 (s, 1H), 6.78 (d, $J = 8.0$ Hz, 1H), 5.94 (s, 2H); ^{13}C NMR (100 MHz, CDCl_3) δ 147.7, 147.2, 145.1, 139.3, 131.9, 128.8, 128.4, 127.8, 126.0, 122.4, 121.4, 120.0, 119.6, 108.6, 107.8, 107.2, 101.2, 101.1, 91.7, 87.2, 74.7; IR (KBr): 3053, 2880, 2777, 2360, 1500, 1484, 1242, 1054, 788, 585 cm^{-1} ; ESI FTMS exact mass calcd for $(\text{C}_{22}\text{H}_{16}\text{O}_3+\text{Na})^+$ requires m/z 351.0992, found m/z 351.0982.

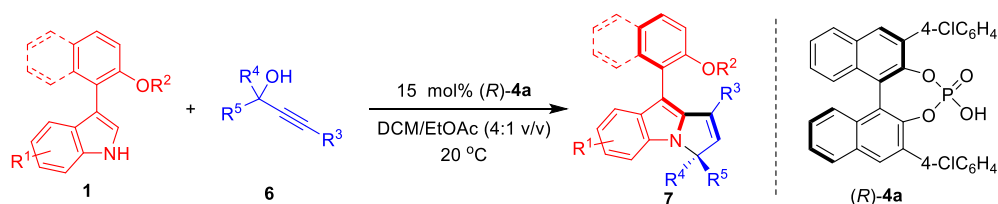
4. Synthetic procedures and characterization data of products 3 and 7

General synthetic procedures for products 3:



3-Arylindoles **1** (0.1 mmol), propargylic alcohols **2** (0.12 mmol), catalyst (S)-**5a** (6.0 mg, 0.01 mmol) and 5 Å MS (100 mg) were added to a reaction tube. Then, DCM (3 mL) was added to the reaction mixture, which was stirred at 20 °C for 4-10 h. After the completion of the reaction which was indicated by TLC, the reaction mixture was directly purified through preparative thin layer chromatography on silica gel to afford pure products **3**.

General synthetic procedures for products 7:

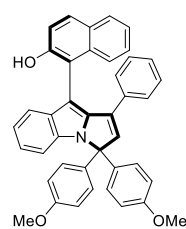


3-Arylindoles **1** (0.1 mmol), propargylic alcohols **6** (0.12 mmol), catalyst (R)-**4a** (8.5 mg, 0.015 mmol) were added to a reaction tube. Then, DCM:EA (4 mL:1 mL) were added to the reaction mixture, which was stirred at 20 °C for 10-90 h. After the completion of the reaction which was indicated by TLC, the reaction mixture was directly purified through preparative thin layer chromatography on silica gel to afford pure products **7**.

Synthetic procedures and characterization data of products 3 and 7:

(*R_a*)-1-(3,3-bis(4-methoxyphenyl)-1-phenyl-3*H*-pyrrolo[1,2-*a*]indol-9-yl)naphthalen-2-ol

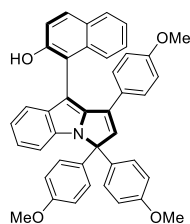
(**3aa**):



Following the general procedure, 3-naphthylindole **1a** (25.9 mg, 0.1 mmol), propargylic alcohol **2a** (41.3 mg, 0.12 mmol), catalyst (S)-**5a** (6.0 mg, 0.01 mmol) and 5 Å MS (100 mg) were added to a reaction tube. Then, DCM (3 mL) was added to the reaction mixture, which was stirred at 20 °C for 4 h. After the

completion of the reaction which was indicated by TLC, the reaction mixture was directly purified through preparative thin layer chromatography (PE:DCM = 1:2) on silica gel to afford pure compound **3aa** in 82% yield (48.0 mg) as a white solid. m.p. 133-135 °C; $[\alpha]_D^{20} = -43.3$ (c = 0.40, acetone); $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.80 – 7.73 (m, 2H), 7.48 (d, $J = 8.0$ Hz, 1H), 7.32 – 7.26 (m, 5H), 7.25 – 7.10 (m, 5H), 7.08 – 6.97 (m, 4H), 6.96 – 6.86 (m, 5H), 6.85 – 6.78 (m, 2H), 5.43 (s, 1H), 3.83 (s, 3H), 3.82 (s, 3H); $^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ 159.3, 152.1, 142.7, 141.1, 135.2, 134.8, 134.4, 133.0, 131.5, 129.6, 129.4, 129.0, 128.2, 127.9, 127.6, 127.3, 126.3, 125.2, 123.0, 122.8, 121.2, 120.1, 116.8, 114.2, 113.0, 111.1, 98.6, 75.5, 55.4; IR (KBr): 3499, 3053, 2924, 2284, 1606, 1508, 1251, 831, 780, 586 cm^{-1} ; ESI FTMS exact mass calcd for $(\text{C}_{41}\text{H}_{31}\text{NO}_3\text{-H})^-$ requires m/z 584.2231, found m/z 584.2238; The enantiomeric excess: 88%, determined by HPLC (Daicel Chiralpak IA, hexane/isopropanol = 70/30, flow rate 1.0 mL/min, T = 30 °C, 254 nm): $t_R = 5.273$ (minor), $t_R = 7.856$ (major).

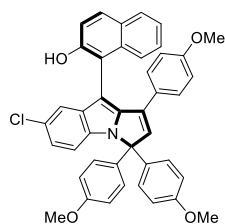
(*R_a*)-1-(1,3,3-tris(4-methoxyphenyl)-3H-pyrrolo[1,2-a]indol-9-yl)naphthalen-2-ol (3ab):



Following the general procedure, 3-naphthylindole **1a** (25.9 mg, 0.1 mmol), propargylic alcohol **2b** (44.9 mg, 0.12 mmol), catalyst (*S*)-**5a** (6.0 mg, 0.01 mmol) and 5 Å MS (100 mg) were added to a reaction tube. Then, DCM (3 mL) was added to the reaction mixture, which was stirred at 20 °C for 4 h. After the completion of the reaction which was indicated by TLC, the reaction mixture was directly purified through preparative thin layer chromatography (PE:DCM = 1:2) on silica gel to afford pure compound **3ab** in 78% yield (48.0 mg) as a white solid. m.p. 137-139 °C; $[\alpha]_D^{20} = -37.8$ (c = 0.75, acetone); $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.82 – 7.76 (m, 2H), 7.49 (d, $J = 8.0$ Hz, 1H), 7.33 – 7.27 (m, 5H), 7.25 – 7.20 (m, 2H), 7.18 – 7.10 (m, 3H), 7.06 – 6.98 (m, 3H), 6.96 – 6.88 (m, 4H), 6.81 (s, 1H), 6.35 (d, $J = 8.8$ Hz, 2H), 5.45 (s, 1H), 3.83 (s, 3H), 3.81 (s, 3H), 3.63 (s, 3H); $^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ 159.5, 159.2, 152.1, 143.1, 134.8, 134.6, 134.4, 133.0, 131.7, 129.6, 129.4, 129.0, 128.6, 127.9, 126.4, 125.3, 124.1, 123.1, 122.7, 121.1, 120.0, 116.9, 114.2, 113.1, 111.1, 98.5, 75.3, 55.4, 55.2; IR (KBr): 3426, 3053, 2833, 2050, 1507, 1462, 1336, 1250, 858, 584 cm^{-1} ; ESI FTMS exact mass calcd for $(\text{C}_{42}\text{H}_{33}\text{NO}_4\text{-H})^-$ requires m/z 614.2337, found m/z 614.2336; The enantiomeric excess: 93%, determined by HPLC (Daicel Chiralpak IA, hexane/isopropanol = 70/30, flow rate 1.0 mL/min, T = 30 °C, 254 nm): $t_R = 6.493$ (minor), $t_R = 10.606$ (major).

(*R_a*)-1-(7-chloro-1,3,3-tris(4-methoxyphenyl)-3*H*-pyrrolo[1,2-*a*]indol-9-yl)naphthalen-2-ol

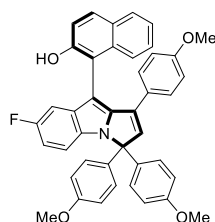
(3bb):



Following the general procedure, 3-naphthylindole **1b** (29.3 mg, 0.1 mmol), propargylic alcohol **2b** (44.9 mg, 0.12 mmol), catalyst (*S*)-**5a** (6.0 mg, 0.01 mmol) and 5 Å MS (100 mg) were added to a reaction tube. Then, DCM (3 mL) was added to the reaction mixture, which was stirred at 20 °C for 4 h. After the completion of the reaction which was indicated by TLC, the reaction mixture was directly purified through preparative thin layer chromatography (PE:DCM = 1:2) on silica gel to afford pure compound **3bb** in 84% yield (54.5 mg) as a white solid. m.p. 128-130 °C; $[\alpha]_D^{20} = -63.0$ (c = 1.04, acetone); $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.84 – 7.74 (m, 2H), 7.49 – 7.39 (m, 1H), 7.32 – 7.27 (m, 2H), 7.25 – 7.22 (m, 4H), 7.20 (s, 1H), 7.16 (d, $J = 8.8$ Hz, 1H), 7.06 (s, 2H), 7.00 (d, $J = 8.4$ Hz, 2H), 6.96 – 6.90 (m, 4H), 6.84 (s, 1H), 6.36 (d, $J = 8.4$ Hz, 2H), 5.35 (s, 1H), 3.83 (s, 3H), 3.82 (s, 3H), 3.63 (s, 3H); $^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ 159.5, 159.3, 152.1, 144.4, 140.3, 134.5, 134.2, 133.0, 131.2, 129.9, 129.2, 129.0, 128.7, 128.0, 126.6, 126.0, 124.9, 123.7, 123.2, 123.0, 120.3, 116.9, 114.2, 113.1, 112.3, 111.8, 98.1, 75.4, 55.4, 55.2; IR (KBr): 3745, 2930, 2833, 2359, 1507, 1251, 1058, 963, 830, 551 cm^{-1} ; ESI FTMS exact mass calcd for $(\text{C}_{42}\text{H}_{32}\text{ClNO}_4\text{-H})^-$ requires m/z 648.1947, found m/z 648.1943; The enantiomeric excess: 93%, determined by HPLC (Daicel Chiralpak IB, hexane/isopropanol = 70/30, flow rate 1.0 mL/min, T = 30 °C, 254 nm): $t_R = 6.980$ (major), $t_R = 8.477$ (minor).

(*R_a*)-1-(7-fluoro-1,3,3-tris(4-methoxyphenyl)-3*H*-pyrrolo[1,2-*a*]indol-9-yl)naphthalen-2-ol

(3cb):

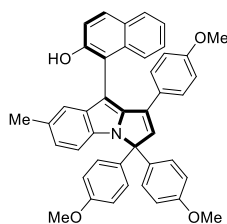


Following the general procedure, 3-naphthylindole **1c** (27.7 mg, 0.1 mmol), propargylic alcohol **2b** (44.9 mg, 0.12 mmol), catalyst (*S*)-**5a** (6.0 mg, 0.01 mmol) and 5 Å MS (100 mg) were added to a reaction tube. Then, DCM (3 mL) was added to the reaction mixture, which was stirred at 20 °C for 4 h. After the completion of the reaction which was indicated by TLC, the reaction mixture was directly purified through preparative thin layer chromatography (PE:DCM = 1:2) on silica gel to afford pure compound **3cb** in 82% yield (52.1 mg) as a white solid. m.p. 134-136 °C; $[\alpha]_D^{20} = -88.7$ (c = 0.67, acetone); $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.84 – 7.76 (m, 2H), 7.47 – 7.42 (m, 1H),

7.34 – 7.27 (m, 3H), 7.25 – 7.22 (m, 3H), 7.20 (s, 1H), 7.16 (d, $J = 9.2$ Hz, 1H), 7.06 (s, 2H), 7.00 (d, $J = 8.4$ Hz, 2H), 6.97 – 6.89 (m, 4H), 6.84 (s, 1H), 6.36 (d, $J = 8.4$ Hz, 2H), 5.35 (s, 1H), 3.83 (s, 3H), 3.82 (s, 3H), 3.63 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 159.5, 159.3, 158.1 (d, $J = 231.8$ Hz), 152.0, 144.6, 140.2, 134.6, 134.2, 131.4, 131.3, 129.8, 129.2, 129.0, 128.6, 128.0, 126.5, 126.0, 125.0, 123.8, 123.1, 123.0, 120.4, 116.9, 114.2, 113.1, 112.3, 111.5 (d, $J = 9.4$ Hz), 111.0 (d, $J = 26.1$ Hz), 106.1 (d, $J = 23.6$ Hz), 98.5 (d, $J = 4.6$ Hz), 75.4, 55.4, 55.2; ^{19}F NMR (376 MHz, CDCl_3) δ -123.60; IR (KBr): 3505, 2999, 2834, 1607, 1508, 1251, 1174, 1028, 830, 552 cm^{-1} ; ESI FTMS exact mass calcd for $(\text{C}_{42}\text{H}_{32}\text{FNO}_4+\text{Na})^+$ requires m/z 656.2208, found m/z 656.2187; The enantiomeric excess: 91%, determined by HPLC (Daicel Chiralpak IB, hexane/isopropanol = 70/30, flow rate 1.0 mL/min, $T = 30$ °C, 254 nm): $t_R = 6.070$ (major), $t_R = 7.746$ (minor).

(R_a)-1-(1,3,3-tris(4-methoxyphenyl)-7-methyl-3H-pyrrolo[1,2-*a*]indol-9-yl)naphthalen-2-ol

(3db):



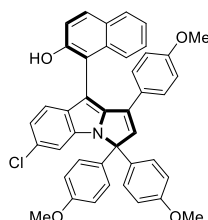
Following the general procedure, 3-naphthylindole **1d** (27.3 mg, 0.1 mmol), propargylic alcohol **2b** (44.9 mg, 0.12 mmol), catalyst (*S*)-**5a** (6.0 mg, 0.01 mmol) and 5 Å MS (100 mg) were added to a reaction tube. Then, DCM (3 mL) was added to the reaction mixture, which was stirred at 20 °C for 4 h.

After the completion of the reaction which was indicated by TLC, the reaction mixture was directly purified through preparative thin layer chromatography (PE:DCM = 1:2) on silica gel to afford pure compound **3db** in 71% yield (44.8 mg) as a white solid. m.p. 123-125 °C; $[\alpha]_D^{20} = -57.2$ ($c = 0.43$, acetone); ^1H NMR (400 MHz, CDCl_3) δ 7.82 – 7.75 (m, 2H), 7.49 (d, $J = 7.6$ Hz, 1H), 7.31 – 7.27 (m, 3H), 7.25 – 7.19 (m, 3H), 7.17 (d, $J = 8.8$ Hz, 1H), 7.07 – 7.02 (m, 2H), 7.00 – 6.92 (m, 4H), 6.92 – 6.86 (m, 3H), 6.79 (s, 1H), 6.33 (d, $J = 8.8$ Hz, 2H), 5.46 (s, 1H), 3.82 (s, 3H), 3.81 (s, 3H), 3.62 (s, 3H), 2.30 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 159.4, 159.2, 152.1, 143.2, 139.7, 134.7, 134.5, 133.3, 133.1, 129.5, 129.3, 129.0, 128.6, 127.9, 126.3, 125.3, 124.3, 123.1, 120.6, 116.8, 114.1, 113.3, 113.0, 110.7, 97.8, 75.2, 55.4, 55.2, 21.4; IR (KBr): 3854, 2930, 2833, 2362, 1508, 1251, 1175, 830, 779, 590 cm^{-1} ; ESI FTMS exact mass calcd for $(\text{C}_{43}\text{H}_{35}\text{NO}_4-\text{H})^-$ requires m/z 628.2493, found m/z 628.2496; The enantiomeric excess: 91%,

determined by HPLC (Daicel Chiralpak IB, hexane/isopropanol = 95/5, flow rate 1.0 mL/min, T = 30 °C, 254 nm): t_R = 20.693 (minor), t_R = 23.470 (major).

(*R_a*)-1-(6-chloro-1,3,3-tris(4-methoxyphenyl)-3*H*-pyrrolo[1,2-*a*]indol-9-yl)naphthalen-2-ol

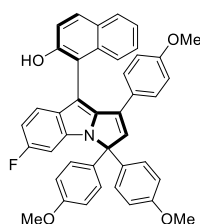
(3eb):



Following the general procedure, 3-naphthylindole **1e** (29.3 mg, 0.1 mmol), propargylic alcohol **2b** (44.9 mg, 0.12 mmol), catalyst (*S*)-**5a** (6.0 mg, 0.01 mmol) and 5 Å MS (100 mg) were added to a reaction tube. Then, DCM (3 mL) was added to the reaction mixture, which was stirred at 20 °C for 4 h. After the completion of the reaction which was indicated by TLC, the reaction mixture was directly purified through preparative thin layer chromatography (PE:DCM = 1:2) on silica gel to afford pure compound **3eb** in 92% yield (59.9 mg) as a white solid. m.p. 244-246 °C; $[\alpha]_D^{20}$ = -67.4 (c = 0.78, acetone); ¹H NMR (400 MHz, CDCl₃) δ 7.82 – 7.76 (m, 2H), 7.44 (d, *J* = 7.6 Hz, 1H), 7.31 – 7.27 (m, 3H), 7.25 – 7.21 (m, 3H), 7.17 – 7.11 (m, 3H), 7.01 – 6.90 (m, 7H), 6.81 (s, 1H), 6.36 (d, *J* = 8.8 Hz, 2H), 5.35 (s, 1H), 3.84 (s, 3H), 3.83 (s, 3H), 3.63 (s, 3H); ¹³C NMR (100 MHz, CDCl₃) δ 159.5, 159.3, 152.1, 143.7, 140.2, 134.9, 134.3, 134.2, 131.6, 131.1, 129.8, 129.2, 129.0, 128.7, 128.6, 128.0, 126.5, 125.0, 123.8, 123.2, 121.9, 120.7, 116.9, 114.3, 113.1, 112.4, 110.8, 98.7, 75.4, 55.4, 55.2; IR (KBr): 3503, 2999, 2884, 2360, 1508, 1202, 1031, 998, 829, 563 cm⁻¹; ESI FTMS exact mass calcd for (C₄₂H₃₂ClNO₄-H)⁻ requires m/z 648.1947, found m/z 648.1959; The enantiomeric excess: 98%, determined by HPLC (Daicel Chiralpak IB, hexane/isopropanol = 70/30, flow rate 1.0 mL/min, T = 30 °C, 254 nm): t_R = 6.163 (major), t_R = 8.373 (minor).

(*R_a*)-1-(6-fluoro-1,3,3-tris(4-methoxyphenyl)-3*H*-pyrrolo[1,2-*a*]indol-9-yl)naphthalen-2-ol

(3fb):

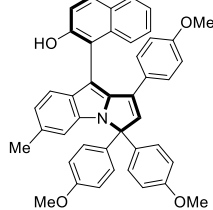


Following the general procedure, 3-naphthylindole **1f** (27.7 mg, 0.1 mmol), propargylic alcohol **2b** (44.9 mg, 0.12 mmol), catalyst (*S*)-**5a** (6.0 mg, 0.01 mmol) and 5 Å MS (100 mg) were added to a reaction tube. Then, DCM (3 mL) was added to the reaction mixture, which was stirred at 20 °C for 4 h. After the completion of the reaction which was indicated by TLC, the reaction mixture was

directly purified through preparative thin layer chromatography (PE:DCM = 1:2) on silica gel to afford pure compound **3fb** in 90% yield (56.9, mg) as a white solid. m.p. 115-117 °C; $[\alpha]_D^{20} = -41.9$ (c = 0.87, acetone); $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.82 – 7.76 (m, 2H), 7.47 (d, $J = 7.2$ Hz, 1H), 7.30 – 7.27 (m, 4H), 7.25 – 7.23 (m, 2H), 7.17 – 7.11 (m, 2H), 7.00 (d, $J = 8.8$ Hz, 2H), 6.97 – 6.89 (m, 4H), 6.84 (dd, $J = 9.6, 2.0$ Hz, 1H), 6.80 – 6.74 (m, 2H), 6.36 (d, $J = 8.4$ Hz, 2H), 5.40 (s, 1H), 3.84 (s, 3H), 3.83 (s, 3H), 3.63 (s, 3H); $^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ 160.2 (d, $J = 238.2$ Hz), 159.5, 159.3, 152.0, 143.5, 139.6, 134.7, 134.5, 134.2, 131.2, 129.7, 129.4, 129.2, 129.0, 128.6, 128.0, 126.4, 125.1, 123.9, 123.1, 121.8 (d, $J = 9.9$ Hz), 116.9, 114.2, 113.1, 112.6, 108.6 (d, $J = 24.6$ Hz), 108.4, 98.6, 97.6 (d, $J = 26.7$ Hz), 75.3, 55.4, 55.2; $^{19}\text{F NMR}$ (376 MHz, CDCl_3) δ -118.94; IR (KBr): 3508, 2995, 2834, 1607, 1508, 1252, 1032, 831, 775, 563 cm^{-1} ; ESI FTMS exact mass calcd for $(\text{C}_{42}\text{H}_{32}\text{FNO}_4\text{-H})^-$ requires m/z 632.2242, found m/z 632.2241; The enantiomeric excess: 97%, determined by HPLC (Daicel Chiralpak IB, hexane/isopropanol = 70/30, flow rate 1.0 mL/min, T = 30 °C, 254 nm): $t_R = 6.043$ (major), $t_R = 7.820$ (minor).

(R_a)-1-(1,3,3-tris(4-methoxyphenyl)-6-methyl-3H-pyrrolo[1,2-a]indol-9-yl)naphthalen-2-ol

(3gb):



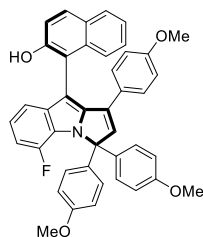
Following the general procedure, 3-naphthylindole **1g** (27.3 mg, 0.1 mmol), propargylic alcohol **2b** (44.9 mg, 0.12 mmol), catalyst (*S*)-**5a** (6.0 mg, 0.01 mmol) and 5 Å MS (100 mg) were added to a reaction tube. Then, DCM (3 mL) was added to the reaction mixture, which was stirred at 20 °C for 4 h.

After the completion of the reaction which was indicated by TLC, the reaction mixture was directly purified through preparative thin layer chromatography (PE:DCM = 1:2) on silica gel to afford pure compound **3gb** in 96% yield (60.6 mg) as a white solid. m.p. 263-265 °C; $[\alpha]_D^{20} = -22.1$ (c = 0.52, acetone); $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.78 (d, $J = 8.8$ Hz, 2H), 7.50 (d, $J = 8.0$ Hz, 1H), 7.32 – 7.27 (m, 4H), 7.25 – 7.19 (m, 2H), 7.18 – 7.11 (m, 2H), 6.99 (d, $J = 8.8$ Hz, 2H), 6.96 – 6.89 (m, 5H), 6.86 (d, $J = 8.0$ Hz, 1H), 6.76 (s, 1H), 6.35 (d, $J = 8.4$ Hz, 2H), 5.46 (s, 1H), 3.83 (s, 3H), 3.82 (s, 3H), 3.63 (s, 3H), 2.37 (s, 3H); $^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ 159.4, 159.2, 152.0, 142.4, 139.5, 135.2, 134.5, 134.3, 132.6, 131.6, 130.8, 129.3, 128.9, 128.5, 127.8, 126.2, 125.3, 124.1, 123.0, 121.7, 120.7, 116.8, 114.1, 113.2, 113.0, 111.0, 98.2, 75.1, 55.3, 55.2, 22.0; IR (KBr): 3398, 2952, 2361, 1608, 1509, 1251, 1032, 832, 780, 583 cm^{-1} ; ESI

FTMS exact mass calcd for (C₄₃H₃₅NO₄-H)⁻ requires m/z 628.2493, found m/z 628.2493; The enantiomeric excess: 95%, determined by HPLC (Daicel Chiralpak IB, hexane/isopropanol = 70/30, flow rate 1.0 mL/min, T = 30 °C, 254 nm): t_R = 5.717 (major), t_R = 6.840 (minor).

(R_a)-1-(5-fluoro-1,3,3-tris(4-methoxyphenyl)-3H-pyrrolo[1,2-a]indol-9-yl)naphthalen-2-ol

(3hb):



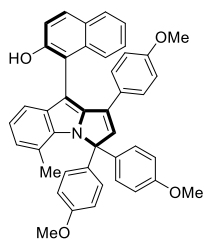
Following the general procedure, 3-naphthylindole **1h** (27.7 mg, 0.1 mmol), propargylic alcohol **2b** (44.9 mg, 0.12 mmol), catalyst (*S*)-**5a** (6.0 mg, 0.01 mmol) and 5 Å MS (100 mg) were added to a reaction tube. Then, DCM (3 mL) was added to the reaction mixture, which was stirred at 20 °C for 4 h.

After the completion of the reaction which was indicated by TLC, the reaction mixture was directly purified through preparative thin layer chromatography (PE:DCM = 1:2) on silica gel to afford pure compound **3hb** in 79% yield (49.9 mg) as a white solid. m.p. 120-122 °C; [α]_D²⁰ = -56.6 (c = 1.02, acetone); ¹H NMR (400 MHz, CDCl₃) δ 7.82 – 7.77 (m, 2H), 7.49 – 7.44 (m, 1H), 7.35 – 7.30 (m, 4H), 7.29 – 7.27 (m, 1H), 7.24 (s, 1H), 7.16 (d, *J* = 8.8 Hz, 1H), 7.02 – 6.98 (m, 2H), 6.98 – 6.96 (m, 1H), 6.95 – 6.88 (m, 5H), 6.87 – 6.81 (m, 1H), 6.79 (s, 1H), 6.35 (d, *J* = 8.4 Hz, 2H), 5.38 (s, 1H), 3.84 (s, 3H), 3.82 (s, 3H), 3.63 (s, 3H); ¹³C NMR (100 MHz, CDCl₃) δ 159.5, 159.2, 150.2 (d, *J* = 245.5 Hz), 144.6, 141.0, 136.9, 134.3, 133.2, 131.5 (d, *J* = 5.9 Hz), 129.8, 129.3 (d, *J* = 2.0 Hz), 129.0, 128.6, 128.0, 126.5, 125.1, 123.7, 123.4, 123.2, 120.4 (d, *J* = 5.7 Hz), 116.9, 116.8, 114.1, 113.8, 113.0, 112.6, 108.7 (d, *J* = 18.1 Hz), 99.1, 76.3, 55.4, 55.2; ¹⁹F NMR (376 MHz, CDCl₃) δ -126.71; IR (KBr): 3673, 2929, 2358, 1607, 1508, 1251, 1031, 832, 774, 553 cm⁻¹; ESI FTMS exact mass calcd for (C₄₂H₃₂FNO₄-H)⁻ requires m/z 632.2242, found m/z 632.2239; The enantiomeric excess: 98%, determined by HPLC (Daicel Chiralpak IB, hexane/isopropanol = 70/30, flow rate 1.0 mL/min, T = 30 °C, 254 nm): t_R = 5.790 (major), t_R = 7.357 (minor).

(R_a)-1-(1,3,3-tris(4-methoxyphenyl)-5-methyl-3H-pyrrolo[1,2-a]indol-9-yl)naphthalen-2-ol

(3ib):

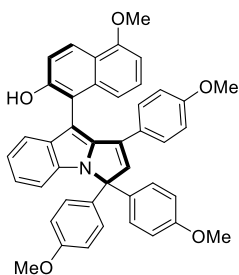
Following the general procedure, 3-naphthylindole **1i** (27.3 mg, 0.1 mmol), propargylic alcohol **2b** (44.9 mg, 0.12 mmol), catalyst (*S*)-**5a** (6.0 mg, 0.01 mmol) and 5 Å MS (100 mg) were added to a



reaction tube. Then, DCM (3 mL) was added to the reaction mixture, which was stirred at 20 °C for 4 h. After the completion of the reaction which was indicated by TLC, the reaction mixture was directly purified through preparative thin layer chromatography (PE:DCM = 1:2) on silica gel to afford pure compound **3ib** in 95% yield (59.9 mg) as a white solid. m.p. 134-136 °C; $[\alpha]_D^{20} = -24.1$ (c = 0.69, acetone); $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.78 (d, $J = 8.8$ Hz, 2H), 7.53 – 7.48 (m, 1H), 7.37 – 7.27 (m, 5H), 7.25 – 7.21 (m, 1H), 7.17 – 7.10 (m, 2H), 7.00 – 6.88 (m, 8H), 6.71 (s, 1H), 6.30 (d, $J = 8.8$ Hz, 2H), 5.44 (s, 1H), 3.84 (s, 3H), 3.83 (s, 3H), 3.61 (s, 3H), 1.96 (s, 3H); $^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ 159.2, 159.1, 152.0, 144.5, 141.8, 135.4, 134.4, 133.8, 131.6, 131.4, 129.5, 129.3, 129.0, 128.6, 127.9, 126.3, 125.6, 125.3, 124.0, 123.0, 121.6, 120.4, 118.7, 116.8, 113.9, 113.2, 112.8, 98.6, 76.2, 55.4, 55.2, 21.1; IR (KBr): 2930, 2835, 2361, 1607, 1509, 1254, 1031, 831, 780, 591 cm^{-1} ; ESI FTMS exact mass calcd for $(\text{C}_{43}\text{H}_{35}\text{NO}_4\text{-H})^-$ requires m/z 628.2493, found m/z 628.2498; The enantiomeric excess: 96%, determined by HPLC (Daicel Chiralpak IB, hexane/isopropanol = 70/30, flow rate 1.0 mL/min, T = 30 °C, 254 nm): $t_R = 5.750$ (major), $t_R = 6.577$ (minor).

(*R_a*)-5-methoxy-1-(1,3,3-tris(4-methoxyphenyl)-3H-pyrrolo[1,2-a]indol-9-yl)naphthalen-2-ol

(3jb):

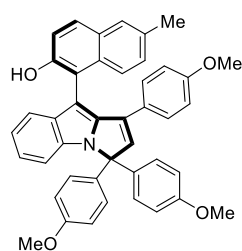


Following the general procedure, 3-naphthylindole **1j** (28.9 mg, 0.1 mmol), propargylic alcohol **2b** (44.9 mg, 0.12 mmol), catalyst (*S*)-**5a** (6.0 mg, 0.01 mmol) and 5 Å MS (100 mg) were added to a reaction tube. Then, DCM (3 mL) was added to the reaction mixture, which was stirred at 20 °C for 4 h. After the completion of the reaction which was indicated by TLC, the reaction mixture was directly purified through preparative thin layer chromatography (PE:DCM = 1:2) on silica gel to afford pure compound **3jb** in 79% yield (51.2 mg) as a white solid. m.p. 99-101 °C; $[\alpha]_D^{20} = -53.3$ (c = 0.34, acetone); $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 8.24 (d, $J = 8.8$ Hz, 1H), 7.32 – 7.27 (m, 3H), 7.25 – 7.20 (m, 2H), 7.19 – 7.06 (m, 5H), 7.05 – 6.99 (m, 3H), 6.98 – 6.84 (m, 4H), 6.81 (s, 1H), 6.64 (d, $J = 7.6$ Hz, 1H), 6.38 (d, $J = 8.4$ Hz, 2H), 5.43 (s, 1H), 4.01 (s, 3H), 3.82 (s, 3H), 3.81 (s, 3H), 3.64 (s, 3H); $^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ 159.5, 159.2, 155.6, 152.6, 143.0, 139.8, 135.7, 134.7, 134.6, 133.1, 131.6, 129.3, 128.6, 126.5, 124.1, 123.6,

122.6, 121.1, 120.8, 119.9, 118.0, 115.8, 114.1, 113.1, 113.0, 111.0, 101.6, 98.8, 75.2, 55.5, 55.4, 55.2; IR (KBr): 2955, 2835, 2364, 1654, 1560, 1248, 1032, 831, 799, 586 cm^{-1} ; ESI FTMS exact mass calcd for $(\text{C}_{43}\text{H}_{35}\text{NO}_5+\text{Na})^+$ requires m/z 668.2407, found m/z 668.2394; The enantiomeric excess: 92%, determined by HPLC (Daicel Chiralpak IB, hexane/isopropanol = 85/15, flow rate 1.0 mL/min, T = 30 °C, 254 nm): t_R = 8.700 (major), t_R = 10.070 (minor).

(*R_a*)-6-methyl-1-(1,3,3-tris(4-methoxyphenyl)-3*H*-pyrrolo[1,2-*a*]indol-9-yl)naphthalen-2-ol

(3kb):

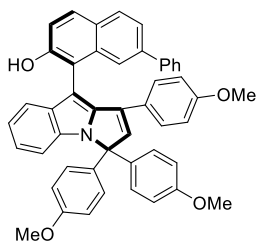


Following the general procedure, 3-naphthylindole **1k** (27.3 mg, 0.1 mmol), propargylic alcohol **2b** (44.9 mg, 0.12 mmol), catalyst (*S*)-**5a** (6.0 mg, 0.01 mmol) and 5 Å MS (100 mg) were added to a reaction tube. Then, DCM (3 mL) was added to the reaction mixture, which was stirred at 20 °C for 4 h. After the completion of the reaction which was indicated by TLC, the reaction mixture was directly purified through preparative thin layer chromatography (PE:DCM = 1:2) on silica gel to afford pure compound **3kb** in 80% yield (50.6 mg) as a white solid. m.p. 84-86 °C; $[\alpha]_D^{20} = -46.5$ (c = 0.88, acetone); ^1H NMR (400 MHz, CDCl_3) δ 7.71 (d, $J = 8.8$ Hz, 1H), 7.57 (s, 1H), 7.42 (d, $J = 8.8$ Hz, 1H), 7.32 – 7.27 (m, 4H), 7.25 – 7.22 (m, 1H), 7.19 – 7.15 (m, 1H), 7.14 – 7.07 (m, 3H), 7.06 – 7.00 (m, 3H), 6.97 – 6.89 (m, 4H), 6.83 (s, 1H), 6.39 (d, $J = 8.8$ Hz, 2H), 5.38 (s, 1H), 3.83 (s, 3H), 3.82 (s, 3H), 3.64 (s, 3H), 2.46 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 159.5, 159.2, 151.4, 142.9, 139.8, 134.8, 134.6, 133.2, 132.5, 132.3, 131.7, 131.6, 129.3, 129.2, 128.9, 128.6, 127.0, 125.2, 124.1, 122.6, 121.2, 119.9, 116.8, 114.1, 113.1, 113.0, 111.0, 98.7, 75.2, 55.4, 55.2, 21.4; IR (KBr): 2954, 2931, 2363, 1654, 1508, 1252, 1200, 831, 780, 587 cm^{-1} ; ESI FTMS exact mass calcd for $(\text{C}_{43}\text{H}_{35}\text{NO}_4+\text{Na})^+$ requires m/z 652.2458, found m/z 652.2430; The enantiomeric excess: 90%, determined by HPLC (Daicel Chiralpak IB, hexane/isopropanol = 70/30, flow rate 1.0 mL/min, T = 30 °C, 254 nm): t_R = 5.780 (major), t_R = 7.217 (minor).

(*R_a*)-7-phenyl-1-(1,3,3-tris(4-methoxyphenyl)-3*H*-pyrrolo[1,2-*a*]indol-9-yl)naphthalen-2-ol

(3lb):

Following the general procedure, 3-naphthylindole **1l** (33.5 mg, 0.1 mmol), propargylic alcohol **2b**

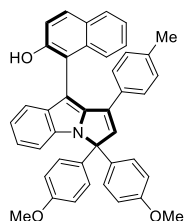


(44.9 mg, 0.12 mmol), catalyst (*S*)-**5a** (6.0 mg, 0.01 mmol) and 5 Å MS (100 mg) were added to a reaction tube. Then, DCM (3 mL) was added to the reaction mixture, which was stirred at 20 °C for 12 h. After the completion of the reaction which was indicated by TLC, the reaction mixture was directly purified through preparative thin layer

chromatography (PE:DCM = 1:2) on silica gel to afford pure compound **3b** in 60% yield (41.5 mg) as a white solid. m.p. 136-138 °C; $[\alpha]_D^{20} = -61.2$ ($c = 0.19$, acetone); $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.80 (d, $J = 9.2$ Hz, 1H), 7.76 (d, $J = 8.4$ Hz, 1H), 7.62 (s, 1H), 7.46 – 7.40 (m, 3H), 7.39 – 7.32 (m, 5H), 7.31 – 7.27 (m, 2H), 7.22 (d, $J = 8.6$ Hz, 2H), 7.18 – 7.10 (m, 2H), 7.09 – 7.04 (m, 1H), 6.99 (d, $J = 8.8$ Hz, 2H), 6.94 (d, $J = 8.8$ Hz, 2H), 6.89 – 6.81 (m, 3H), 6.30 (d, $J = 8.4$ Hz, 2H), 5.64 (s, 1H), 3.83 (s, 3H), 3.80 (s, 3H), 3.59 (s, 3H); $^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ 159.3, 159.2, 159.1, 152.2, 143.8, 141.6, 140.0, 138.5, 134.8, 134.6, 132.6, 132.0, 131.1, 129.4, 129.2, 128.6, 128.4, 128.2, 128.1, 127.3, 127.0, 124.2, 123.4, 122.7, 122.5, 120.7, 120.1, 116.9, 114.2, 114.1, 113.5, 113.0, 111.1, 98.3, 75.5, 55.4, 55.3, 55.2; IR (KBr): 2954, 2931, 2835, 2364, 1654, 1508, 1252, 1200, 818, 746, 587 cm^{-1} ; ESI FTMS exact mass calcd for $(\text{C}_{48}\text{H}_{37}\text{NO}_4 + \text{H})^+$ requires m/z 692.2795, found m/z 692.2779; The enantiomeric excess: 86%, determined by HPLC (Daicel Chiralpak IA, hexane/isopropanol = 70/30, flow rate 1.0 mL/min, $T = 30$ °C, 254 nm): $t_R = 6.126$ (minor), $t_R = 14.026$ (major).

(*R_a*)-1-(3,3-bis(4-methoxyphenyl)-1-(*p*-tolyl)-3*H*-pyrrolo[1,2-*a*]indol-9-yl)naphthalen-2-ol

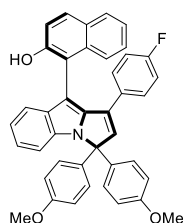
(3ac):



Following the general procedure, 3-naphthylindole **1a** (25.9 mg, 0.1 mmol), propargylic alcohol **2c** (43.0 mg, 0.12 mmol), catalyst (*S*)-**5a** (6.0 mg, 0.01 mmol) and 5 Å MS (100 mg) were added to a reaction tube. Then, DCM (3 mL) was added to the reaction mixture, which was stirred at 20 °C for 4 h. After the completion of the reaction which was indicated by TLC, the reaction mixture was directly purified through preparative thin layer chromatography (PE:DCM = 1:2) on silica gel to afford pure compound **3ac** in 89% yield (53.5 mg) as a white solid. m.p. 130-132 °C; $[\alpha]_D^{20} = -47.7$ ($c = 0.43$, acetone); $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.87 – 7.79 (m, 2H), 7.54 (d, $J = 8.4$ Hz, 1H), 7.36 – 7.31 (m, 4H), 7.31 – 7.24 (m, 3H), 7.23 – 7.14 (m, 3H), 7.10 – 7.05 (m, 1H), 7.04 – 6.92 (m, 6H), 6.91

(s, 1H), 6.68 (d, $J = 8.0$ Hz, 2H), 5.49 (s, 1H), 3.88 (s, 3H), 3.87 (s, 3H), 2.18 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 159.2, 152.1, 143.0, 140.7, 138.0, 137.9, 135.0, 134.8, 134.4, 133.0, 131.6, 129.5, 129.3, 129.0, 128.6, 128.3, 127.9, 127.2, 126.3, 125.2, 123.0, 122.7, 121.1, 121.0, 120.0, 116.8, 114.1, 113.1, 111.0, 98.5, 75.3, 55.4, 55.3, 21.2; IR (KBr): 3501, 3049, 2950, 2835, 1607, 1463, 1251, 1031, 778, 556 cm^{-1} ; ESI FTMS exact mass calcd for $(\text{C}_{42}\text{H}_{33}\text{NO}_3\text{-H})^-$ requires m/z 598.2387, found m/z 598.2380; The enantiomeric excess: 91%, determined by HPLC (Daicel Chiralpak IA, hexane/isopropanol = 95/5, flow rate 1.0 mL/min, $T = 30$ °C, 254 nm): $t_R = 8.943$ (major), $t_R = 10.406$ (minor).

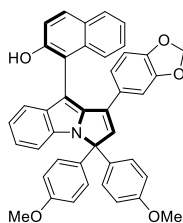
(*R_a*)-1-(1-(4-fluorophenyl)-3,3-bis(4-methoxyphenyl)-3*H*-pyrrolo[1,2-*a*]indol-9-yl)naphthalen-2-ol (3ad):



Following the general procedure, 3-naphthylindole **1a** (25.9 mg, 0.1 mmol), propargylic alcohol **2d** (43.4 mg, 0.12 mmol), catalyst (*S*)-**5a** (6.0 mg, 0.01 mmol) and 5 Å MS (100 mg) were added to a reaction tube. Then, DCM (3 mL) was added to the reaction mixture, which was stirred at 20 °C for 4 h. After the completion of the reaction which was indicated by TLC, the reaction mixture was directly purified through preparative thin layer chromatography (PE:DCM = 1:2) on silica gel to afford pure compound **3ad** in 81% yield (48.9 mg) as a white solid. m.p. 241-243 °C; $[\alpha]_D^{20} = -43.7$ ($c = 0.88$, acetone); ^1H NMR (400 MHz, CDCl_3) δ 7.83 – 7.76 (m, 2H), 7.48 (d, $J = 8.0$ Hz, 1H), 7.31 – 7.27 (m, 5H), 7.25 – 7.20 (m, 2H), 7.20 – 7.12 (m, 3H), 7.08 – 7.01 (m, 3H), 6.97 – 6.89 (m, 4H), 6.86 (s, 1H), 6.56 – 6.48 (m, 2H), 5.44 (s, 1H), 3.83 (s, 3H), 3.82 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 162.4 (d, $J = 247.4$ Hz), 159.3, 152.0, 142.6, 140.9, 134.8, 134.2 (d, $J = 23.7$ Hz), 132.8, 131.3, 129.7, 129.3, 129.0 (d, $J = 7.7$ Hz), 128.9, 127.9, 127.6, 126.4, 125.0, 123.1, 122.8, 121.1, 120.1, 116.8, 114.5 (d, $J = 21.3$ Hz), 114.3, 114.1, 112.7, 111.1, 98.5, 75.4, 55.3; ^{19}F NMR (376 MHz, CDCl_3) δ -113.27; IR (KBr): 3421, 2931, 2834, 1733, 1508, 1251, 1058, 831, 669, 563 cm^{-1} ; ESI FTMS exact mass calcd for $(\text{C}_{41}\text{H}_{30}\text{FNO}_3\text{-H})^-$ requires m/z 602.2137, found m/z 602.2140; The enantiomeric excess: 88%, determined by HPLC (Daicel Chiralpak IA, hexane/isopropanol = 70/30, flow rate 1.0 mL/min, $T = 30$ °C, 254 nm): $t_R = 5.393$ (minor), $t_R = 7.150$ (major).

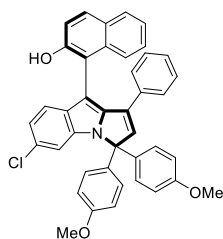
(*R_a*)-1-(1-(benzo[*d*][1,3]dioxol-5-yl)-3,3-bis(4-methoxyphenyl)-3*H*-pyrrolo[1,2-*a*]indol-9-yl)

naphthalen-2-ol (**3ae**):



Following the general procedure, 3-naphthylindole **1a** (25.9 mg, 0.1 mmol), propargylic alcohol **2e** (46.6 mg, 0.12 mmol), catalyst (*S*)-**5a** (6.0 mg, 0.01 mmol) and 5 Å MS (100 mg) were added to a reaction tube. Then, DCM (3 mL) was added to the reaction mixture, which was stirred at 20 °C for 10 h. After the completion of the reaction which was indicated by TLC, the reaction mixture was directly purified through preparative thin layer chromatography (PE:DCM = 1:2) on silica gel to afford pure compound **3ae** in 91% yield (57.2 mg) as a white solid. m.p. 142-144 °C; $[\alpha]_D^{20} = -56.8$ ($c = 1.01$, acetone); $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.81 – 7.75 (m, 2H), 7.45 (d, $J = 8.0$ Hz, 1H), 7.30 – 7.27 (m, 2H), 7.25 – 7.17 (m, 6H), 7.16 – 7.10 (m, 2H), 7.04 – 7.00 (m, 1H), 6.94 – 6.88 (m, 4H), 6.79 (s, 1H), 6.56 (s, 1H), 6.52 (d, $J = 8.4$ Hz, 1H), 6.20 (d, $J = 8.0$ Hz, 1H), 5.75 (d, $J = 7.2$ Hz, 2H), 5.44 (s, 1H), 3.82 (s, 3H), 3.81 (s, 3H); $^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ 159.2, 152.0, 147.4, 147.0, 142.8, 140.2, 134.7, 134.4, 132.9, 131.4, 129.6, 129.5, 129.3, 129.0, 127.9, 126.3, 125.4, 125.2, 123.0, 122.7, 121.4, 121.0, 120.0, 116.8, 114.1, 113.7, 113.0, 111.0, 107.8, 107.4, 100.9, 98.5, 75.2, 55.3; IR (KBr): 3498, 3054, 2897, 2834, 1607, 1508, 1251, 1074, 831, 587 cm^{-1} ; ESI FTMS exact mass calcd for $(\text{C}_{42}\text{H}_{31}\text{NO}_5\text{-H})^-$ requires m/z 628.2129, found m/z 628.2148; The enantiomeric excess: 90%, determined by HPLC (Daicel Chiralpak IB, hexane/isopropanol = 95/5, flow rate 0.5 mL/min, $T = 30$ °C, 254 nm): $t_R = 30.980$ (major), $t_R = 35.487$ (minor).

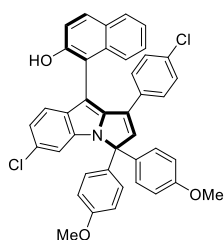
(*R_a*)-1-(6-chloro-3,3-bis(4-methoxyphenyl)-1-phenyl-3*H*-pyrrolo[1,2-*a*]indol-9-yl)naphthalen-2-ol (**3ea**):



Following the general procedure, 3-naphthylindole **1e** (29.3 mg, 0.1 mmol), propargylic alcohol **2a** (41.3 mg, 0.12 mmol), catalyst (*S*)-**5a** (6.0 mg, 0.01 mmol) and 5 Å MS (100 mg) were added to a reaction tube. Then, DCM (3 mL) was added to the reaction mixture, which was stirred at 20 °C for 4 h. After the completion of the reaction which was indicated by TLC, the reaction mixture was directly purified through preparative thin layer chromatography (PE:DCM = 1:2) on silica gel to afford pure compound **3ea** in 97% yield (59.8 mg) as a white solid. m.p. 127-129 °C; $[\alpha]_D^{20} = -69.7$ ($c = 1.28$, acetone); $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.81 –

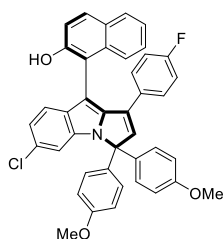
7.74 (m, 2H), 7.42 (d, $J = 7.2$ Hz, 1H), 7.30 – 7.27 (m, 2H), 7.25 – 7.20 (m, 4H), 7.16 – 7.10 (m, 3H), 7.04 (d, $J = 7.6$ Hz, 2H), 7.01 – 6.91 (m, 6H), 6.87 (s, 1H), 6.85 – 6.79 (m, 2H), 5.33 (s, 1H), 3.84 (s, 3H), 3.83 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 159.4, 159.3, 152.0, 143.7, 140.2, 134.9, 134.3, 134.2, 131.6, 131.1, 129.8, 129.2, 129.0, 128.7, 128.6, 128.0, 126.5, 125.0, 123.8, 123.2, 121.9, 120.7, 116.9, 114.3, 113.1, 112.4, 110.8, 98.8, 75.6, 55.4; IR (KBr): 2930, 2835, 2360, 1607, 1509, 1279, 1030, 831, 751, 591 cm^{-1} ; ESI FTMS exact mass calcd for $(\text{C}_{41}\text{H}_{30}\text{ClNO}_3\text{-H})^-$ requires m/z 618.1841, found m/z 618.1842; The enantiomeric excess: 94%, determined by HPLC (Daicel Chiralpak IB, hexane/isopropanol = 70/30, flow rate 1.0 mL/min, $T = 30$ °C, 254 nm): $t_{\text{R}} = 5.103$ (major), $t_{\text{R}} = 5.920$ (minor).

(*R_a*)-1-(6-chloro-1-(4-chlorophenyl)-3,3-bis(4-methoxyphenyl)-3H-pyrrolo[1,2-*a*]indol-9-yl)naphthalen-2-ol (3ef):



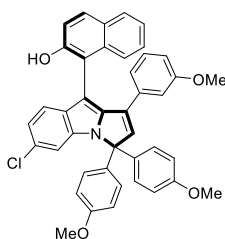
Following the general procedure, 3-naphthylindole **1e** (29.3 mg, 0.1 mmol), propargylic alcohol **2f** (45.4 mg, 0.12 mmol), catalyst (*S*)-**5a** (6.0 mg, 0.01 mmol) and 5 Å MS (100 mg) were added to a reaction tube. Then, DCM (3 mL) was added to the reaction mixture, which was stirred at 20 °C for 4 h. After the completion of the reaction which was indicated by TLC, the reaction mixture was directly purified through preparative thin layer chromatography (PE:DCM = 1:2) on silica gel to afford pure compound **3ef** in 88% yield (57.8 mg) as a white solid. m.p. 150-152 °C; $[\alpha]_{\text{D}}^{20} = -73.9$ ($c = 1.59$, acetone); ^1H NMR (400 MHz, CDCl_3) δ 7.86 – 7.74 (m, 2H), 7.40 (d, $J = 8.0$ Hz, 1H), 7.31 – 7.27 (m, 1H), 7.25 – 7.20 (m, 5H), 7.17 – 7.10 (m, 3H), 7.02 – 6.91 (m, 7H), 6.87 (s, 1H), 6.79 (d, $J = 8.4$ Hz, 2H), 5.30 (s, 1H), 3.84 (s, 3H), 3.83 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 159.5, 159.4, 152.0, 143.0, 141.7, 135.0, 134.2, 134.1, 133.8, 131.5, 130.7, 130.0, 129.8, 129.2, 129.1, 129.0, 128.9, 128.5, 128.1, 127.8, 126.6, 124.8, 123.3, 121.9, 120.9, 116.9, 114.4, 112.0, 110.8, 98.9, 75.6, 55.4; IR (KBr): 2953, 2929, 2360, 1607, 1507, 1252, 1032, 830, 707, 590 cm^{-1} ; ESI FTMS exact mass calcd for $(\text{C}_{41}\text{H}_{29}\text{Cl}_2\text{NO}_3\text{-H})^-$ requires m/z 652.1451, found m/z 652.1430; The enantiomeric excess: 96%, determined by HPLC (Daicel Chiralpak IB, hexane/isopropanol = 70/30, flow rate 1.0 mL/min, $T = 30$ °C, 254 nm): $t_{\text{R}} = 5.176$ (major), $t_{\text{R}} = 5.910$ (minor).

(*R_a*)-1-(6-chloro-1-(4-fluorophenyl)-3,3-bis(4-methoxyphenyl)-3*H*-pyrrolo[1,2-*a*]indol-9-yl)naphthalen-2-ol (3ed):



Following the general procedure, 3-naphthylindole **1e** (29.3 mg, 0.1 mmol), propargylic alcohol **2d** (43.4 mg, 0.12 mmol), catalyst (*S*)-**5a** (6.0 mg, 0.01 mmol) and 5 Å MS (100 mg) were added to a reaction tube. Then, DCM (3 mL) was added to the reaction mixture, which was stirred at 20 °C for 4 h. After the completion of the reaction which was indicated by TLC, the reaction mixture was directly purified through preparative thin layer chromatography (PE:DCM = 1:2) on silica gel to afford pure compound **3ed** in 95% yield (60.5 mg) as a white solid. m.p. 263-265 °C; $[\alpha]_D^{20} = -42.6$ ($c = 1.28$, acetone); $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.84 – 7.72 (m, 2H), 7.40 (d, $J = 8.0$ Hz, 1H), 7.30 – 7.27 (m, 1H), 7.25 – 7.20 (m, 5H), 7.18 – 7.09 (m, 3H), 7.06 – 6.89 (m, 7H), 6.83 (s, 1H), 6.56 – 6.43 (m, 2H), 5.31 (s, 1H), 3.84 (s, 3H), 3.83 (s, 3H); $^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ 162.5 (d, $J = 246.5$ Hz), 159.5, 159.4 (d, $J = 5.1$ Hz), 152.0, 143.3, 141.3, 135.0, 134.2, 133.8, 131.5, 130.8 (d, $J = 2.5$ Hz), 130.0, 129.2, 129.1, 129.0, 128.9, 128.8, 128.1, 127.4, 127.3, 126.6, 124.8, 123.2, 121.9, 120.9, 116.8, 114.6 (d, $J = 21.5$ Hz), 114.4, 112.1, 110.8, 98.8, 75.6, 55.4; $^{19}\text{F NMR}$ (376 MHz, CDCl_3) δ -113.03; IR (KBr): 2999, 2930, 2834, 2360, 1607, 1509, 1252, 1032, 834, 749 cm^{-1} ; ESI FTMS exact mass calcd for $(\text{C}_{41}\text{H}_{29}\text{ClFNO}_3\text{-H})^-$ requires m/z 636.1747, found m/z 636.1758; The enantiomeric excess: 95%, determined by HPLC (Daicel Chiralpak IB, hexane/isopropanol = 95/5, flow rate 1.0 mL/min, $T = 30$ °C, 254 nm): $t_R = 10.730$ (major), $t_R = 11.973$ (minor).

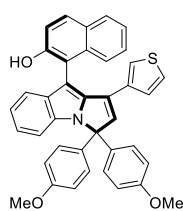
(*R_a*)-1-(6-chloro-1-(3-methoxyphenyl)-3,3-bis(4-methoxyphenyl)-3*H*-pyrrolo[1,2-*a*]indol-9-yl)naphthalen-2-ol (3eg):



Following the general procedure, 3-naphthylindole **1e** (29.3 mg, 0.1 mmol), propargylic alcohol **2g** (44.9 mg, 0.12 mmol), catalyst (*S*)-**5a** (6.0 mg, 0.01 mmol) and 5 Å MS (100 mg) were added to a reaction tube. Then, DCM (3 mL) was added to the reaction mixture, which was stirred at 20 °C for 4 h. After the completion of the reaction which was indicated by TLC, the reaction mixture was directly purified through preparative thin layer chromatography (PE:DCM = 1:2) on silica gel to afford pure compound **3eg** in 95% yield (61.8

mg) as a white solid. m.p. 143-145 °C; $[\alpha]_D^{20} = -126.1$ (c = 1.31, acetone); $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.77 (d, $J = 9.2$ Hz, 2H), 7.50 – 7.44 (m, 1H), 7.30 – 7.27 (m, 2H), 7.25 – 7.23 (m, 4H), 7.15 – 7.08 (m, 3H), 7.00 – 6.91 (m, 5H), 6.90 – 6.85 (m, 2H), 6.84 – 6.78 (m, 1H), 6.59 (dd, $J = 8.0, 2.0$ Hz, 1H), 6.49 (s, 1H), 5.34 (s, 1H), 3.84 (s, 3H), 3.83 (s, 3H), 2.98 (s, 3H); $^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ 159.4, 159.3, 158.9, 152.0, 143.2, 141.9, 135.0, 134.8, 134.1, 132.7, 131.6, 130.9, 130.8, 129.8, 129.2, 129.1, 128.9, 128.8, 128.0, 126.6, 124.9, 123.2, 122.0, 120.7, 119.6, 117.0, 115.8, 114.4, 114.3, 112.3, 111.3, 110.8, 98.7, 75.5, 55.4, 54.5; IR (KBr): 3475, 3046, 2834, 1606, 1507, 1258, 1040, 831, 705, 531 cm^{-1} ; ESI FTMS exact mass calcd for $(\text{C}_{42}\text{H}_{32}\text{ClNO}_4\text{-H})^-$ requires m/z 648.1947, found m/z 648.1925; The enantiomeric excess: 97%, determined by HPLC (Daicel Chiralpak IB, hexane/isopropanol = 70/30, flow rate 1.0 mL/min, T = 30 °C, 254 nm): $t_R = 5.713$ (major), $t_R = 7.000$ (minor).

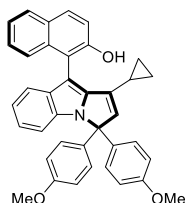
(*R_a*)-1-(3,3-bis(4-methoxyphenyl)-1-(thiophen-3-yl)-3H-pyrrolo[1,2-*a*]indol-9-yl)naphthalen-2-ol (3ah):



Following the general procedure, 3-naphthylindole **1a** (25.9 mg, 0.1 mmol), propargylic alcohol **2h** (42.0 mg, 0.12 mmol), catalyst (*S*)-**5a** (6.0 mg, 0.01 mmol) and 5 Å MS (100 mg) were added to a reaction tube. Then, DCM (3 mL) was added to the reaction mixture, which was stirred at 20 °C for 4 h. After the completion of the reaction which was indicated by TLC, the reaction mixture was directly purified through preparative thin layer chromatography (PE:DCM = 1:2) on silica gel to afford pure compound **3ah** in 82% yield (48.4 mg) as a white solid. m.p. 66-68 °C; $[\alpha]_D^{20} = -81.4$ (c = 0.81, acetone); $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.87 (d, $J = 8.8$ Hz, 1H), 7.82 (d, $J = 7.6$ Hz, 1H), 7.48 (d, $J = 8.0$ Hz, 1H), 7.33 – 7.27 (m, 5H), 7.25 – 7.21 (m, 3H), 7.17 – 7.10 (m, 2H), 7.05 – 6.99 (m, 1H), 6.97 – 6.87 (m, 7H), 6.65 – 6.59 (m, 1H), 5.49 (s, 1H), 3.82 (s, 3H), 3.81 (s, 3H); $^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ 159.3, 159.2, 152.3, 142.7, 140.4, 134.6, 134.5, 133.0, 132.0, 131.4, 131.3, 129.9, 129.5, 129.4, 129.3, 129.0, 128.0, 126.7, 126.51, 125.3, 124.9, 123.7, 123.2, 122.8, 121.1, 120.0, 117.0, 114.1, 113.0, 111.0, 98.4, 75.1, 55.4; IR (KBr): 3501, 3054, 2928, 2834, 2359, 1704, 1508, 1251, 1031, 787, 585 cm^{-1} ; ESI FTMS exact mass calcd for $(\text{C}_{39}\text{H}_{29}\text{NO}_3\text{S+H})^+$ requires m/z 592.1941, found m/z 592.1928; The enantiomeric excess: 90%, determined by HPLC (Daicel Chiralpak OD-H, hexane/isopropanol = 70/30, flow rate 1.0 mL/min, T = 30 °C, 254 nm): $t_R =$

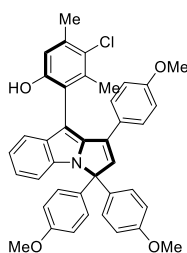
5.883 (major), $t_R = 11.323$ (minor).

(*S_a*)-1-(1-cyclopropyl-3,3-bis(4-methoxyphenyl)-3*H*-pyrrolo[1,2-*a*]indol-9-yl)naphthalen-2-ol (3ai):



3-Naphthylindole **1a** (25.9 mg, 0.1 mmol), propargylic alcohol **2i** (29.4 mg, 0.12 mmol), catalyst (*R*)-**4e** (14.0 mg, 0.02 mmol) were added to a reaction tube. Then, toluene (1 mL) was added to the reaction mixture, which was stirred at 20 °C for 24 h. After the completion of the reaction which was indicated by TLC, the reaction mixture was directly purified through preparative thin layer chromatography (PE:DCM = 1:1) on silica gel to afford pure compound **3ai** in 53% yield (29.0 mg) as a white solid. m.p. 71-73 °C; $[\alpha]_D^{20} = -46.0$ ($c = 0.35$, acetone); $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.90 – 7.79 (m, 2H), 7.60 – 7.53 (m, 1H), 7.38 – 7.29 (m, 3H), 7.24 (s, 1H), 7.22 – 7.14 (m, 4H), 7.14 – 7.06 (m, 2H), 7.05 – 6.98 (m, 1H), 6.95 – 6.83 (m, 4H), 6.23 (s, 1H), 5.60 (s, 1H), 3.82 (s, 3H), 3.80 (s, 3H), 1.19 – 1.11 (m, 1H), 0.57 – 0.37 (m, 3H), 0.33 – 0.25 (m, 1H); $^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ 159.2, 159.1, 152.3, 145.6, 137.2, 136.3, 134.8, 134.6, 132.8, 131.9, 131.8, 129.5, 129.2, 129.1, 129.0, 128.0, 126.3, 125.5, 123.1, 122.3, 120.7, 119.8, 116.9, 114.0, 112.6, 111.0, 97.2, 75.3, 55.4, 7.9, 7.6, 7.4; IR (KBr): 3048, 2961, 2834, 2359, 2341, 1597, 1508, 830, 745, 585 cm^{-1} ; ESI FTMS exact mass calcd for $(\text{C}_{38}\text{H}_{31}\text{NO}_3+\text{H})^+$ requires m/z 550.2377, found m/z 550.2353; The enantiomeric excess: 82%, determined by HPLC (Daicel Chiralpak AD-H, hexane/isopropanol = 90/10, flow rate 1.0 mL/min, $T = 30$ °C, 254 nm): $t_R = 6.760$ (minor), $t_R = 8.260$ (major).

(*R_a*)-4-chloro-3,5-dimethyl-2-(1,3,3-tris(4-methoxyphenyl)-3*H*-pyrrolo[1,2-*a*]indol-9-yl)phenol (3mb):

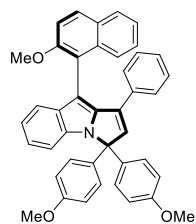


Following the general procedure, 3-phenylindole **1m** (27.1 mg, 0.1 mmol), propargylic alcohol **2b** (44.9 mg, 0.12 mmol), catalyst (*S*)-**5a** (6.0 mg, 0.01 mmol) and 5 Å MS (100 mg) were added to a reaction tube. Then, DCM (3 mL) was added to the reaction mixture, which was stirred at 20 °C for 4 h. After the completion of the reaction which was indicated by TLC, the reaction mixture was directly purified through preparative thin layer chromatography (PE:DCM = 1:2) on

silica gel to afford pure compound **3mb** in 63% yield (39.5 mg) as a white solid. m.p. 117-119 °C; $[\alpha]_D^{20} = -52.4$ ($c = 0.89$, acetone); $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.34 – 7.30 (m, 1H), 7.29 – 7.27 (m, 1H), 7.25 – 7.24 (m, 1H), 7.18 – 7.13 (m, 3H), 7.12 – 7.04 (m, 4H), 6.92 – 6.84 (m, 4H), 6.82 – 6.76 (m, 2H), 6.60 (d, $J = 8.8$ Hz, 2H), 5.13 (s, 1H), 3.80 (s, 3H), 3.79 (s, 3H), 3.75 (s, 3H), 2.40 (s, 3H), 1.90 (s, 3H); $^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ 159.8, 159.2, 152.3, 142.8, 140.0, 137.2, 136.7, 134.4, 132.0, 131.6, 131.3, 129.3, 129.2, 128.7, 126.2, 124.1, 122.7, 120.5, 120.1, 119.1, 114.3, 114.1, 113.3, 111.1, 99.6, 75.3, 55.4, 55.3, 21.1, 18.7; IR (KBr): 3504, 2998, 1608, 1606, 1508, 1251, 1175, 829, 744, 506 cm^{-1} ; ESI FTMS exact mass calcd for $(\text{C}_{40}\text{H}_{34}\text{ClNO}_4\text{-H})^-$ requires m/z 626.2103, found m/z 626.2092; The enantiomeric excess: 87%, determined by HPLC (Daicel Chiralpak IB, hexane/isopropanol = 85/15, flow rate 1.0 mL/min, $T = 30$ °C, 254 nm): $t_R = 6.777$ (major), $t_R = 7.730$ (minor).

(*R_a*)-9-(2-methoxynaphthalen-1-yl)-3,3-bis(4-methoxyphenyl)-1-phenyl-3H-pyrrolo[1,2-*a*]

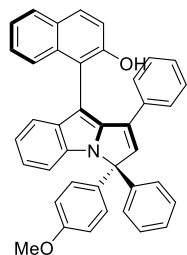
indole (3na):



Following the general procedure, 3-naphthylindole **1n** (27.3 mg, 0.1 mmol), propargylic alcohol **2a** (41.3 mg, 0.12 mmol), catalyst (*S*)-**5a** (6.0 mg, 0.01 mmol) and 5 Å MS (100 mg) were added to a reaction tube. Then, DCM (3 mL) was added to the reaction mixture, which was stirred at 20 °C for 4 h. After the completion of the reaction which was indicated by TLC, the reaction mixture was directly purified through preparative thin layer chromatography (PE:DCM = 1:2) on silica gel to afford pure compound **3na** in 88% yield (52.5 mg) as a white solid. m.p. 71-73 °C; $[\alpha]_D^{20} = -4.7$ ($c = 1.12$ acetone); $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.90 – 7.81 (m, 3H), 7.41 (d, $J = 8.8$ Hz, 2H), 7.39 – 7.33 (m, 2H), 7.29 – 7.27 (m, 1H), 7.25 – 7.20 (m, 2H), 7.14 – 7.09 (m, 3H), 7.08 – 6.98 (m, 4H), 6.96 (d, $J = 9.2$ Hz, 2H), 6.92 – 6.84 (m, 5H), 3.84 (s, 3H), 3.81 (s, 3H), 3.30 (s, 3H); $^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ 159.1, 155.2, 142.5, 136.1, 134.5, 134.1, 133.7, 132.9, 132.5, 131.7, 129.4, 129.0, 128.9, 127.9, 127.7, 127.4, 127.3, 126.4, 126.1, 123.3, 121.6, 121.5, 119.3, 117.4, 114.0, 113.9, 113.1, 110.8, 101.8, 75.0, 55.6, 55.4, 55.3; IR (KBr): 3565, 3049, 2930, 2359, 1733, 1558, 1252, 907, 761, 586 cm^{-1} ; ESI FTMS exact mass calcd for $(\text{C}_{42}\text{H}_{33}\text{NO}_3+\text{Na})^+$ requires m/z 622.2353, found m/z 622.2329; The enantiomeric excess: 20%, determined by HPLC (Daicel Chiralpak IA, hexane/isopropanol = 85/15, flow rate 1.0 mL/min, $T = 30$ °C, 254 nm): $t_R = 5.063$ (minor), $t_R =$

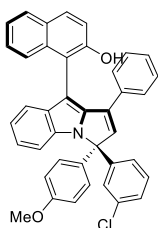
5.923 (major).

(*S,S*)-1-(3-(4-methoxyphenyl)-1,3-diphenyl-3*H*-pyrrolo[1,2-*a*]indol-9-yl)naphthalen-2-ol (7ab):



Following the general procedure, 3-naphthylindole **1a** (25.9 mg, 0.1 mmol), propargylic alcohol **6b** (37.7 mg, 0.12 mmol), catalyst (*R*)-**4a** (8.5 mg, 0.015 mmol) were added to a reaction tube. Then, DCM:EA (4 mL:1 mL) were added to the reaction mixture, which was stirred at 20 °C for 10 h. After the completion of the reaction which was indicated by TLC, the reaction mixture was directly purified through preparative thin layer chromatography (toluene) on silica gel to afford pure compound **7ab** in 96% yield (53.3 mg) as a white solid. 84:16 dr; m.p. 138-140 °C; $[\alpha]_D^{20} = +23.1$ (c = 0.46, acetone); $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.82 – 7.74 (m, 2H), 7.50 (d, $J = 8.0$ Hz, 1H), 7.45 – 7.39 (m, 2H), 7.36 (m, 3H), 7.33 – 7.27 (m, 3H), 7.25 – 7.18 (m, 2H), 7.17 – 7.09 (m, 3H), 7.09 – 6.97 (m, 4H), 6.94 – 6.88 (m, 3H), 6.86 – 6.79 (m, 2H), 5.43 (s, 1H), 3.81 (s, 3H); $^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ 159.5, 152.1, 142.9, 141.0, 139.6, 135.6, 134.9, 134.5, 133.1, 131.6, 131.4, 129.7, 129.5, 129.0, 128.8, 128.3, 128.2, 128.0, 127.9, 127.8, 127.7, 127.6, 127.4, 127.3, 126.4, 125.3, 123.1, 122.9, 121.3, 120.2, 116.8, 114.3, 114.2, 113.0, 111.2, 98.8, 76.0, 55.5; IR (KBr): 3505, 3055, 2927, 1654, 1509, 1251, 1031, 833, 745, 592 cm^{-1} ; ESI FTMS exact mass calcd for $(\text{C}_{40}\text{H}_{29}\text{NO}_2\text{-H})^-$ requires m/z 554.2125, found m/z 554.2134; The enantiomeric excess: 92%, determined by HPLC (Daicel Chiralpak IA, hexane/isopropanol = 70/30, flow rate 1.0 mL/min, T = 30 °C, 254 nm): $t_R = 4.607$ (major), $t_R = 6.407$ (minor).

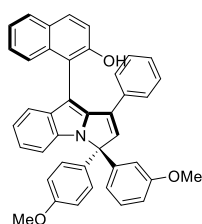
(*S,R*)-1-(3-(3-chlorophenyl)-3-(4-methoxyphenyl)-1-phenyl-3*H*-pyrrolo[1,2-*a*]indol-9-yl)naphthalen-2-ol (7ac):



Following the general procedure, 3-naphthylindole **1a** (25.9 mg, 0.1 mmol), propargylic alcohol **6c** (41.8 mg, 0.12 mmol), catalyst (*R*)-**4a** (8.5 mg, 0.015 mmol) were added to a reaction tube. Then, DCM:EA (4 mL:1 mL) were added to the reaction mixture, which was stirred at 20 °C for 48 h. After the completion of the reaction which was indicated by TLC, the reaction mixture was directly purified through preparative thin layer chromatography (toluene) on silica gel to afford pure

compound **7ac** in 56% yield (33.0 mg) as a white solid. 91:9 dr; m.p. 141-143 °C; $[\alpha]_D^{20} = +10.6$ (c = 0.60, acetone); $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.82 – 7.72 (m, 2H), 7.53 – 7.47 (m, 1H), 7.39 (s, 1H), 7.35 (d, $J = 5.2$ Hz, 2H), 7.32 – 7.27 (m, 4H), 7.25 – 7.20 (m, 2H), 7.18 – 7.11 (m, 3H), 7.10 – 6.98 (m, 4H), 6.93 (d, $J = 8.8$ Hz, 2H), 6.89 – 6.79 (m, 3H), 5.38 (s, 1H), 3.82 (s, 3H); $^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ 159.6, 152.1, 142.7, 141.9, 140.2, 136.0, 134.9, 134.8, 134.4, 133.1, 131.3, 130.6, 130.2, 129.7, 129.4, 129.0, 128.4, 128.3, 128.0, 127.7, 127.3, 126.5, 126.2, 125.2, 123.1, 121.4, 120.3, 116.9, 114.4, 112.8, 111.0, 99.3, 75.5, 55.5; IR (KBr): 3506, 3056, 2930, 1594, 1510, 1253, 1029, 833, 745, 694 cm^{-1} ; ESI FTMS exact mass calcd for $(\text{C}_{40}\text{H}_{28}\text{ClNO}_2\text{-H})^-$ requires m/z 588.1736, found m/z 588.1747; The enantiomeric excess: 95%, determined by HPLC (Daicel Chiralpak AD-H, hexane/isopropanol = 70/30, flow rate 1.0 mL/min, T = 30 °C, 254 nm): $t_R = 4.266$ (major), $t_R = 6.990$ (minor).

(*S_w*,*R*)-1-(3-(3-methoxyphenyl)-3-(4-methoxyphenyl)-1-phenyl-3*H*-pyrrolo[1,2-*a*]indol-9-yl)naphthalen-2-ol (7ad**):**

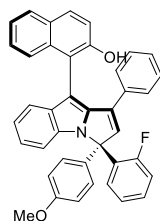


Following the general procedure, 3-naphthylindole **1a** (25.9 mg, 0.1 mmol), propargylic alcohol **6d** (41.3 mg, 0.12 mmol), catalyst (*R*)-**4a** (8.5 mg, 0.015 mmol) were added to a reaction tube. Then, DCM:EA (4 mL:1 mL) were added to the reaction mixture, which was stirred at 20 °C for 10 h. After the completion of the reaction which was indicated by TLC, the reaction mixture was directly purified through preparative thin layer chromatography (toluene) on silica gel to afford pure compound **7ad** in 91% yield (53.2 mg) as a white solid. 88:12 dr; m.p. 148-150 °C; $[\alpha]_D^{20} = +11.8$ (c = 0.94, acetone); $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.81 – 7.74 (m, 2H), 7.50 (d, $J = 8.0$ Hz, 1H), 7.37 – 7.27 (m, 4H), 7.25 – 7.18 (m, 3H), 7.16 – 7.11 (m, 2H), 7.10 – 7.06 (m, 2H), 7.05 – 6.98 (m, 2H), 6.97 – 6.88 (m, 6H), 6.86 – 6.80 (m, 2H), 5.44 (s, 1H), 3.82 (s, 3H), 3.76 (s, 3H); $^{13}\text{C NMR}$ (100 MHz,) δ 159.9, 159.4, 152.0, 142.9, 141.2, 140.8, 135.5, 134.9, 134.4, 133.0, 131.5, 131.2, 129.9, 129.6, 129.5, 129.0, 128.2, 127.9, 127.6, 127.3, 126.3, 125.2, 123.0, 122.8, 121.1, 120.5, 120.1, 116.8, 114.3, 114.2, 112.9, 111.2, 98.8, 75.8, 55.4, 55.3; IR (KBr): 3054, 2931, 2834, 1598, 1510, 1253, 1032, 830, 760, 697 cm^{-1} ; ESI FTMS exact mass calcd for $(\text{C}_{41}\text{H}_{31}\text{NO}_3\text{-H})^-$ requires m/z 584.2231, found m/z 584.2230; The enantiomeric excess: 91%, determined by HPLC (Daicel Chiralpak IA, hexane/isopropanol = 85/15, flow rate 1.0 mL/min, T = 30 °C, 254 nm): $t_R = 6.253$ (major), $t_R =$

11.493 (minor).

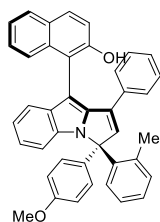
(*S_w*,*R*)-1-(3-(2-fluorophenyl)-3-(4-methoxyphenyl)-1-phenyl-3*H*-pyrrolo[1,2-*a*]indol-9-yl)

naphthalen-2-ol (7ae):



Following the general procedure, 3-naphthylindole **1a** (25.9 mg, 0.1 mmol), propargylic alcohol **6e** (39.9 mg, 0.12 mmol), catalyst (*R*)-**4a** (8.5 mg, 0.015 mmol) were added to a reaction tube. Then, DCM:EA (4 mL:1 mL) were added to the reaction mixture, which was stirred at 20 °C for 36 h. After the completion of the reaction which was indicated by TLC, the reaction mixture was directly purified through preparative thin layer chromatography (toluene) on silica gel to afford pure compound **7ae** in 74% yield (42.6 mg) as a white solid. 86:14 dr; m.p. 233-235 °C; $[\alpha]_D^{20} = +20.8$ ($c = 0.36$, acetone); ¹H NMR (400 MHz, CDCl₃) δ 7.83 (d, $J = 8.4$ Hz, 2H), 7.58 (d, $J = 7.6$ Hz, 1H), 7.51 – 7.46 (m, 1H), 7.34 (s, 1H), 7.31 – 7.22 (m, 7H), 7.21 – 7.04 (m, 8H), 6.96 – 6.85 (m, 4H), 5.41 (s, 1H), 3.84 (s, 3H); ¹³C NMR (100 MHz, CDCl₃) δ 160.8 (d, $J = 246.6$ Hz), 159.5, 152.0, 142.6, 138.4, 138.4, 136.5, 135.1, 134.4, 133.1, 131.3, 130.6, 130.0 (d, $J = 8.1$ Hz), 129.6, 129.0, 128.6 (d, $J = 3.3$ Hz), 128.3, 128.2, 127.9, 127.6, 127.3, 126.4, 126.2, 125.1, 125.0 (d, $J = 3.3$ Hz), 123.1, 123.0, 121.2, 120.2, 116.8, 116.4 (d, $J = 21.8$ Hz), 114.2, 112.8, 110.9, 99.1, 73.8, 55.3; ¹⁹F NMR (376 MHz, CDCl₃) δ -107.64; IR (KBr): 3498, 3056, 2929, 1620, 1462, 1270, 1029, 858, 762, 598 cm⁻¹; ESI FTMS exact mass calcd for (C₄₀H₂₈FN₂O₂-H)⁻ requires m/z 572.2031, found m/z 572.2054; The enantiomeric excess: 94%, determined by HPLC (Daicel Chiralpak AD-H, hexane/isopropanol = 98/2, flow rate 1.0 mL/min, T = 30 °C, 254 nm): $t_R = 16.420$ (major), $t_R = 20.623$ (minor).

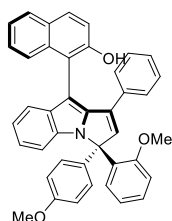
(*S_w*,*R*)-1-(3-(4-methoxyphenyl)-1-phenyl-3-(*o*-tolyl)-3*H*-pyrrolo[1,2-*a*]indol-9-yl)naphthalen-2-ol (7af):



Following the general procedure, 3-naphthylindole **1a** (25.9 mg, 0.1 mmol), propargylic alcohol **6f** (39.4 mg, 0.12 mmol), catalyst (*R*)-**4a** (8.5 mg, 0.015 mmol) were added to a reaction tube. Then, DCM:EA (4 mL:1 mL) were added to the reaction mixture, which was stirred at 20 °C for 86 h. After the completion of the reaction which was indicated by TLC, the reaction mixture was directly purified through preparative thin layer chromatography (toluene) on silica gel to afford pure compound **7af** in 68%

yield (38.7 mg) as a white solid. >95:5 dr; m.p. 175-177 °C; $[\alpha]_{\text{D}}^{20} = +11.3$ (c = 0.65, acetone); ^1H NMR (400 MHz, CDCl_3) δ 7.82 (d, $J = 8.8$ Hz, 2H), 7.58 (d, $J = 8.0$ Hz, 1H), 7.42 – 7.34 (m, 3H), 7.34 – 7.32 (m, 2H), 7.31 – 7.25 (m, 3H), 7.23 – 7.19 (m, 2H), 7.19 – 7.15 (m, 3H), 7.15 – 7.13 (m, 1H), 7.13 – 7.04 (m, 3H), 6.95 – 6.85 (m, 4H), 5.43 (s, 1H), 3.84 (s, 3H), 2.23 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 159.4, 152.0, 142.3, 137.7, 137.1, 136.8, 135.2, 134.4, 133.1, 132.6, 131.7, 131.6, 129.6, 129.0, 128.6, 128.3, 128.1, 127.9, 127.8, 127.6, 127.3, 126.8, 126.4, 126.0, 125.2, 123.1, 122.8, 121.2, 120.1, 116.8, 114.4, 113.8, 112.9, 111.4, 98.8, 76.7, 55.4, 21.9; IR (KBr): 3055, 1597, 1443, 1252, 1200, 1031, 915, 835, 743 cm^{-1} ; ESI FTMS exact mass calcd for $(\text{C}_{41}\text{H}_{31}\text{NO}_2\text{-H})^-$ requires m/z 568.2282, found m/z 568.2293; The enantiomeric excess: 93%, determined by HPLC (Daicel Chiralpak AD-H, hexane/isopropanol = 98/2, flow rate 1.0 mL/min, T = 30 °C, 254 nm): $t_{\text{R}} = 11.650$ (major), $t_{\text{R}} = 15.353$ (minor).

(*S_w*,*R*)-1-(3-(2-methoxyphenyl)-3-(4-methoxyphenyl)-1-phenyl-3*H*-pyrrolo[1,2-*a*]indol-9-yl)naphthalen-2-ol (7ag):

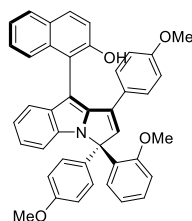


Following the general procedure, 3-naphthylindole **1a** (25.9 mg, 0.1 mmol), propargylic alcohol **6g** (41.3 mg, 0.12 mmol), catalyst (*R*)-**4a** (8.5 mg, 0.015 mmol) were added to a reaction tube. Then, DCM:EA (4 mL:1 mL) were added to the reaction mixture, which was stirred at 20 °C for 36 h. After the completion of the reaction which was indicated by TLC, the reaction mixture was directly purified through preparative thin layer chromatography (toluene) on silica gel to afford pure compound **7ag** in 74% yield (43.3 mg) as a white solid. 94:6 dr; m.p. 144-146 °C; $[\alpha]_{\text{D}}^{20} = -72.7$ (c = 0.39, acetone); ^1H NMR (400 MHz, CDCl_3) δ 7.80 – 7.75 (m, 2H), 7.56 (d, $J = 7.6$ Hz, 1H), 7.45 – 7.39 (m, 1H), 7.33 (s, 1H), 7.29 – 7.27 (m, 1H), 7.25 – 7.22 (m, 2H), 7.20 – 7.14 (m, 3H), 7.12 – 7.07 (m, 5H), 7.05 – 7.04 (m, 1H), 7.03 – 6.98 (m, 3H), 6.85 – 6.79 (m, 4H), 5.38 (s, 1H), 3.78 (s, 3H), 3.72 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 159.0, 157.8, 152.1, 142.9, 139.5, 136.0, 135.3, 134.5, 133.2, 131.9, 131.8, 129.5, 129.0, 128.2, 128.1, 128.0, 127.9, 127.6, 127.3, 126.8, 126.4, 125.3, 123.1, 122.6, 121.4, 121.0, 120.0, 116.8, 113.8, 113.1, 111.8, 111.3, 98.3, 75.2, 55.5, 55.3; IR (KBr): 3054, 2962, 2834, 1596, 1558, 1256, 1025, 909, 810, 696 cm^{-1} ; ESI FTMS exact mass calcd for $(\text{C}_{41}\text{H}_{31}\text{NO}_3\text{-H})^-$ requires m/z 584.2231, found m/z 584.2278; The enantiomeric excess: 93%, determined by HPLC (Daicel Chiralpak AD-H, hexane/isopropanol = 95/5, flow rate 0.5

mL/min, T = 30 °C, 254 nm): t_R = 11.796 (major), t_R = 13.530 (minor).

(*S_w*,*R*)-1-(3-(2-methoxyphenyl)-1,3-bis(4-methoxyphenyl)-3*H*-pyrrolo[1,2-*a*]indol-9-yl)

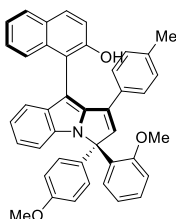
naphthalen-2-ol (7ah):



Following the general procedure, 3-naphthylindole **1a** (25.9 mg, 0.1 mmol), propargylic alcohol **6h** (44.9 mg, 0.12 mmol), catalyst (*R*)-**4a** (8.5 mg, 0.015 mmol) were added to a reaction tube. Then, DCM:EA (4 mL:1 mL) were added to the reaction mixture, which was stirred at 20 °C for 48 h. After the completion of the reaction which was indicated by TLC, the reaction mixture was directly purified through preparative thin layer chromatography (toluene) on silica gel to afford pure compound **7ah** in 98% yield (60.4 mg) as a white solid. 95:5 dr; m.p. 133-135 °C; $[\alpha]_D^{20}$ = -145.1 (c = 0.37, acetone); ¹H NMR (400 MHz, CDCl₃) δ 7.82 – 7.76 (m, 2H), 7.56 (d, *J* = 7.6 Hz, 1H), 7.44 – 7.39 (m, 1H), 7.32 – 7.27 (m, 2H), 7.25 – 7.21 (m, 2H), 7.20 – 7.16 (m, 2H), 7.15 – 7.08 (m, 4H), 7.06 – 6.98 (m, 5H), 6.81 (d, *J* = 8.4 Hz, 2H), 6.36 (d, *J* = 8.8 Hz, 2H), 5.39 (s, 1H), 3.77 (s, 3H), 3.72 (s, 3H), 3.63 (s, 3H); ¹³C NMR (100 MHz, CDCl₃) δ 159.4, 158.9, 157.7, 152.1, 143.1, 138.1, 135.4, 135.2, 134.4, 133.2, 132.0, 129.5, 129.4, 128.9, 128.6, 128.1, 128.0, 127.9, 126.9, 126.3, 125.4, 124.4, 123.1, 122.5, 121.3, 121.0, 119.9, 116.8, 113.8, 113.2, 113.0, 111.7, 111.2, 98.2, 75.0, 55.5, 55.2; IR (KBr): 3054, 2962, 2834, 1596, 1558, 1256, 1024, 908, 746, 696 cm⁻¹; ESI FTMS exact mass calcd for (C₄₂H₃₃NO₄-H)⁻ requires m/z 614.2337, found m/z 614.2338; The enantiomeric excess: 94%, determined by HPLC (Daicel Chiralpak OD-H, hexane/isopropanol = 95/5, flow rate 0.5 mL/min, T = 30 °C, 254 nm): t_R = 18.767 (minor), t_R = 20.930 (major).

(*S_w*,*R*)-1-(3-(2-methoxyphenyl)-3-(4-methoxyphenyl)-1-(*p*-tolyl)-3*H*-pyrrolo[1,2-*a*]indol-9-yl)

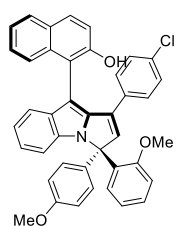
naphthalen-2-ol (7ai):



Following the general procedure, 3-naphthylindole **1a** (25.9 mg, 0.1 mmol), propargylic alcohol **6i** (43.0 mg, 0.12 mmol), catalyst (*R*)-**4a** (8.5 mg, 0.015 mmol) were added to a reaction tube. Then, DCM:EA (4 mL:1 mL) were added to the reaction mixture, which was stirred at 20 °C for 50 h. After the completion of the reaction which was indicated by TLC, the reaction mixture was directly purified through preparative thin layer chromatography (toluene) on silica gel to afford pure compound **7ai**

in 86% yield (51.6 mg) as a white solid. >95:5 dr; m.p. 139-141 °C; $[\alpha]_{\text{D}}^{20} = -133.1$ ($c = 0.78$, acetone); ^1H NMR (400 MHz, CDCl_3) δ 7.87 – 7.73 (m, 2H), 7.56 (d, $J = 8.0$ Hz, 1H), 7.47 – 7.38 (m, 1H), 7.33 – 7.27 (m, 2H), 7.25 – 7.21 (m, 2H), 7.21 – 7.07 (m, 6H), 7.06 – 6.94 (m, 5H), 6.82 (d, $J = 8.4$ Hz, 2H), 6.64 (d, $J = 8.0$ Hz, 2H), 5.39 (s, 1H), 3.77 (s, 3H), 3.72 (s, 3H), 2.14 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 159.0, 157.8, 152.1, 143.0, 138.9, 137.7, 135.9, 135.2, 134.5, 133.2, 131.9, 129.4, 129.0, 128.9, 128.3, 128.2, 128.1, 127.9, 127.2, 126.9, 126.3, 125.4, 123.0, 122.5, 121.3, 121.0, 119.9, 116.8, 113.8, 113.2, 111.7, 111.2, 98.2, 75.0, 55.5, 55.2, 21.2; IR (KBr): 3502, 2929, 2834, 1597, 1488, 1338, 1250, 1028, 830, 746 cm^{-1} ; ESI FTMS exact mass calcd for $(\text{C}_{42}\text{H}_{33}\text{NO}_3\text{-H})^-$ requires m/z 598.2387, found m/z 598.2386; The enantiomeric excess: 92%, determined by HPLC (Daicel Chiralpak AD-H, hexane/isopropanol = 98/2, flow rate 1.0 mL/min, $T = 30$ °C, 254 nm): $t_{\text{R}} = 11.926$ (major), $t_{\text{R}} = 17.390$ (minor).

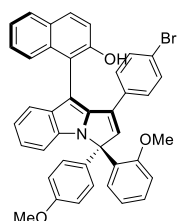
(*S_w*,*R*)-1-(1-(4-chlorophenyl)-3-(2-methoxyphenyl)-3-(4-methoxyphenyl)-3*H*-pyrrolo[1,2-*a*]indol-9-yl)naphthalen-2-ol (7aj):



Following the general procedure, 3-naphthylindole **1a** (25.9 mg, 0.1 mmol), propargylic alcohol **6j** (45.4 mg, 0.12 mmol), catalyst (*R*)-**4a** (8.5 mg, 0.015 mmol) were added to a reaction tube. Then, DCM:EA (4 mL:1 mL) were added to the reaction mixture, which was stirred at 20 °C for 50 h. After the completion of the reaction which was indicated by TLC, the reaction mixture was directly purified through preparative thin layer chromatography (toluene) on silica gel to afford pure compound **7aj** in 95% yield (58.8 mg) as a white solid. 92:8 dr; m.p. 132-134 °C; $[\alpha]_{\text{D}}^{20} = -135.9$ ($c = 1.48$, acetone); ^1H NMR (400 MHz, CDCl_3) δ 7.81 (d, $J = 8.4$ Hz, 2H), 7.53 (d, $J = 8.0$ Hz, 1H), 7.45 – 7.40 (m, 1H), 7.33 (s, 1H), 7.31 – 7.27 (m, 2H), 7.25 – 7.23 (m, 1H), 7.20 – 7.17 (m, 1H), 7.16 – 7.12 (m, 3H), 7.12 – 7.08 (m, 2H), 7.07 – 6.97 (m, 5H), 6.85 – 6.77 (m, 4H), 5.37 (s, 1H), 3.78 (s, 3H), 3.73 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 159.0, 157.7, 152.0, 142.4, 139.7, 135.3, 134.9, 134.4, 133.8, 133.0, 131.5, 130.4, 129.7, 129.6, 129.0, 128.6, 128.2, 128.0, 127.9, 127.7, 126.5, 126.4, 125.1, 123.2, 122.7, 121.4, 121.0, 120.1, 116.8, 113.8, 112.8, 111.8, 111.3, 98.4, 75.2, 55.5, 55.3; IR (KBr): 3054, 2930, 2834, 1596, 1488, 1248, 1025, 831, 744, 510 cm^{-1} ; ESI FTMS exact mass calcd for $(\text{C}_{41}\text{H}_{30}\text{ClNO}_3\text{-H})^-$ requires m/z 618.1841, found m/z 618.1844; The enantiomeric excess: 94%, determined by HPLC (Daicel Chiralpak AD-H, hexane/isopropanol = 98/2, flow rate 1.0

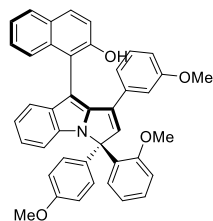
mL/min, T = 30 °C, 254 nm): t_R = 13.850 (major), t_R = 17.826 (minor).

(*S_w*,*R*)-1-(1-(4-bromophenyl)-3-(2-methoxyphenyl)-3-(4-methoxyphenyl)-3*H*-pyrrolo[1,2-*a*]indol-9-yl)naphthalen-2-ol (7ak):



Following the general procedure, 3-naphthylindole **1a** (25.9 mg, 0.1 mmol), propargylic alcohol **6k** (50.6 mg, 0.12 mmol), catalyst (*R*)-**4a** (8.5 mg, 0.015 mmol) were added to a reaction tube. Then, DCM:EA (4 mL:1 mL) were added to the reaction mixture, which was stirred at 20 °C for 50 h. After the completion of the reaction which was indicated by TLC, the reaction mixture was directly purified through preparative thin layer chromatography (toluene) on silica gel to afford pure compound **7ak** in 94% yield (62.2 mg) as a white solid. 92:8 dr; m.p. 135-137 °C; $[\alpha]_D^{20}$ = -114.8 (c = 0.80, acetone); ¹H NMR (400 MHz, CDCl₃) δ 7.81 (d, *J* = 8.4 Hz, 2H), 7.52 (d, *J* = 8.4 Hz, 1H), 7.45 – 7.40 (m, 1H), 7.33 (s, 1H), 7.31 – 7.27 (m, 1H), 7.25 – 7.21 (m, 2H), 7.19 – 7.12 (m, 4H), 7.11 – 7.07 (m, 2H), 7.06 – 7.00 (m, 3H), 6.94 (s, 4H), 6.81 (d, *J* = 8.8 Hz, 2H), 5.35 (s, 1H), 3.77 (s, 3H), 3.72 (s, 3H); ¹³C NMR (100 MHz, CDCl₃) δ 159.0, 157.7, 152.0, 142.3, 139.8, 135.3, 134.9, 134.4, 133.0, 131.5, 130.8, 130.6, 129.7, 129.6, 129.0, 128.9, 128.2, 128.0, 127.9, 126.5, 126.4, 125.1, 123.2, 122.8, 122.1, 121.4, 121.0, 120.1, 116.8, 113.8, 112.8, 111.8, 111.3, 100.0, 98.4, 75.2, 55.5, 55.3; IR (KBr): 3052, 2930, 2834, 1597, 1509, 1249, 1027, 918, 783, 510 cm⁻¹; ESI FTMS exact mass calcd for (C₄₁H₃₀BrNO₃-H)⁻ requires m/z 662.1336, found m/z 662.1339; The enantiomeric excess: 91%, determined by HPLC (Daicel Chiralpak AD-H, hexane/isopropanol = 98/2, flow rate 1.0 mL/min, T = 30 °C, 254 nm): t_R = 15.216 (major), t_R = 19.813 (minor).

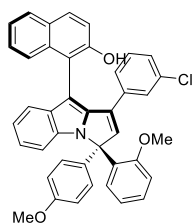
(*S_w*,*R*)-1-(3-(2-methoxyphenyl)-1-(3-methoxyphenyl)-3-(4-methoxyphenyl)-3*H*-pyrrolo[1,2-*a*]indol-9-yl)naphthalen-2-ol (7al):



Following the general procedure, 3-naphthylindole **1a** (25.9 mg, 0.1 mmol), propargylic alcohol **6l** (44.9 mg, 0.12 mmol), catalyst (*R*)-**4a** (8.5 mg, 0.015 mmol) were added to a reaction tube. Then, DCM:EA (4 mL:1 mL) were added to the reaction mixture, which was stirred at 20 °C for 90 h. After the completion of the reaction which was indicated by TLC, the reaction mixture was directly purified through preparative thin layer chromatography (toluene) on silica gel to afford pure compound **7al**

in 76% yield (46.6 mg) as a white solid. 94:6 dr; m.p. 143-145 °C; $[\alpha]_D^{20} = -94.8$ (c = 0.46, acetone); $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.83 – 7.77 (m, 2H), 7.53 – 7.48 (m, 1H), 7.45 – 7.39 (m, 1H), 7.34 – 7.27 (m, 4H), 7.18 – 7.15 (m, 1H), 7.14 – 7.09 (m, 4H), 7.06 – 7.01 (m, 4H), 7.00 – 6.95 (m, 2H), 6.81 (d, $J = 8.4$ Hz, 2H), 6.35 (d, $J = 8.4$ Hz, 2H), 5.27 (s, 1H), 3.78 (s, 3H), 3.72 (s, 3H), 3.63 (s, 3H); $^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ 159.5, 159.1, 157.7, 152.2, 144.5, 138.6, 135.4, 134.4, 134.3, 133.6, 131.7, 129.8, 129.7, 129.1, 128.6, 128.1, 127.9, 126.6, 126.0, 125.1, 124.1, 123.3, 123.0, 121.4, 120.3, 116.9, 113.9, 113.1, 112.5, 112.1, 111.8, 98.0, 75.3, 55.5, 55.3, 55.2; IR (KBr): 3054, 2961, 2834, 1606, 1508, 1252, 1030, 934, 861, 585 cm^{-1} ; ESI FTMS exact mass calcd for $(\text{C}_{42}\text{H}_{33}\text{NO}_4\text{-H})^-$ requires m/z 614.2337, found m/z 614.2341; The enantiomeric excess: 95%, determined by HPLC (Daicel Chiralpak IB, hexane/isopropanol = 95/5, flow rate 1.0 mL/min, T = 30 °C, 254 nm): $t_R = 7.456$ (minor), $t_R = 9.203$ (major).

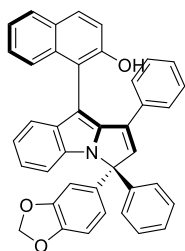
(*S_w*,*R*)-(1-(3-chlorophenyl)-3-(2-methoxyphenyl)-3-(4-methoxyphenyl)-3*H*-pyrrolo[1,2-*a*]indol-9-yl)naphthalen-2-ol (7am):



Following the general procedure, 3-naphthylindole **1a** (25.9 mg, 0.1 mmol), propargylic alcohol **6m** (45.4 mg, 0.12 mmol), catalyst (*R*)-**4a** (8.5 mg, 0.015 mmol) were added to a reaction tube. Then, DCM:EA (4 mL:1 mL) were added to the reaction mixture, which was stirred at 20 °C for 48 h. After the completion of the reaction which was indicated by TLC, the reaction mixture was directly purified through preparative thin layer chromatography (toluene) on silica gel to afford pure compound **7am** in 79% yield (48.9 mg) as a white solid. 95:5 dr; m.p. 122-124 °C; $[\alpha]_D^{20} = -147.0$ (c = 0.54, acetone); $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.80 (d, $J = 8.8$ Hz, 2H), 7.53 (d, $J = 8.0$ Hz, 1H), 7.46 – 7.40 (m, 1H), 7.35 (s, 1H), 7.31 – 7.27 (m, 2H), 7.25 – 7.21 (m, 1H), 7.18 – 7.12 (m, 4H), 7.10 – 7.08 (m, 3H), 7.06 – 7.01 (m, 3H), 6.99 – 6.92 (m, 2H), 6.82 (d, $J = 8.4$ Hz, 2H), 6.77 – 6.71 (m, 1H), 5.35 (s, 1H), 3.78 (s, 3H), 3.73 (s, 3H); $^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ 159.1, 157.7, 152.0, 142.3, 140.2, 135.3, 134.8, 134.4, 133.6, 133.5, 133.0, 131.5, 129.9, 129.6, 129.1, 128.7, 128.3, 128.0, 127.9, 127.5, 126.5, 126.4, 125.4, 125.1, 123.1, 122.8, 121.4, 121.0, 120.1, 116.8, 113.9, 112.7, 111.8, 111.3, 100.0, 98.5, 75.2, 55.5, 55.3; IR (KBr): 3056, 2929, 2834, 1596, 1488, 1429, 1338, 1108, 1026, 745 cm^{-1} ; ESI FTMS exact mass calcd for $(\text{C}_{41}\text{H}_{30}\text{ClNO}_3\text{-H})^-$ requires m/z 618.1841, found m/z 618.1840; The enantiomeric excess: 92%, determined by HPLC (Daicel

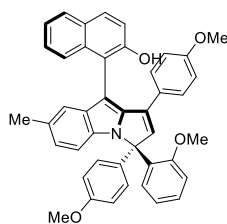
Chiralpak IB, hexane/isopropanol = 95/5, flow rate 1.0 mL/min, T = 30 °C, 254 nm): t_R = 6.840 (minor), t_R = 7.790 (major).

(*S,S*)-1-(3-(benzo[*d*][1,3]dioxol-5-yl)-1,3-diphenyl-3*H*-pyrrolo[1,2-*a*]indol-9-yl)naphthalen-2-ol (7an):



Following the general procedure, 3-naphthylindole **1a** (25.9 mg, 0.1 mmol), propargylic alcohol **6n** (39.4 mg, 0.12 mmol), catalyst (*R*)-**4a** (8.5 mg, 0.015 mmol) were added to a reaction tube. Then, DCM:EA (4 mL:1 mL) were added to the reaction mixture, which was stirred at 20 °C for 60 h. After the completion of the reaction which was indicated by TLC, the reaction mixture was directly purified through preparative thin layer chromatography (toluene) on silica gel to afford pure compound **7an** in 77% yield (43.7 mg) as a white solid. 91:9 dr; m.p. 153-155 °C; $[\alpha]_D^{20}$ = -46.1 (c = 0.46, acetone); $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.81 – 7.72 (m, 2H), 7.51 – 7.40 (m, 3H), 7.39 – 7.33 (m, 3H), 7.30 – 7.27 (m, 1H), 7.25 – 7.17 (m, 3H), 7.17 – 7.10 (m, 2H), 7.09 – 6.95 (m, 4H), 6.92 – 6.70 (m, 6H), 5.98 (d, J = 8.0 Hz, 2H), 5.41 (s, 1H); $^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ 152.1, 148.2, 147.6, 142.7, 140.8, 139.2, 135.7, 134.9, 134.4, 133.3, 133.0, 131.4, 129.7, 129.0, 128.9, 128.3, 128.1, 127.9, 127.6, 127.3, 126.4, 125.2, 123.1, 122.9, 121.9, 121.2, 120.2, 116.9, 112.9, 111.2, 108.8, 108.4, 101.5, 99.0, 76.1; IR (KBr): 3055, 2893, 1596, 1502, 1485, 1233, 1197, 1036, 758, 557 cm^{-1} ; ESI FTMS exact mass calcd for $(\text{C}_{40}\text{H}_{27}\text{NO}_3\text{-H})^-$ requires m/z 568.1918, found m/z 568.1906; The enantiomeric excess: 94%, determined by HPLC (Daicel Chiralpak IA, hexane/isopropanol = 95/5, flow rate 1.0 mL/min, T = 30 °C, 254 nm): t_R = 10.780 (major), t_R = 16.910 (minor).

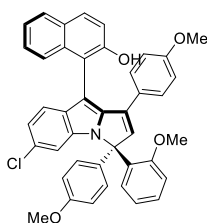
(*S,R*)-1-(3-(2-methoxyphenyl)-1,3-bis(4-methoxyphenyl)-7-methyl-3*H*-pyrrolo[1,2-*a*]indol-9-yl)naphthalen-2-ol (7dh):



Following the general procedure, 3-naphthylindole **1d** (27.3 mg, 0.1 mmol), propargylic alcohol **6h** (44.9 mg, 0.12 mmol), catalyst (*R*)-**4a** (8.5 mg, 0.015 mmol) were added to a reaction tube. Then, DCM:EA (4 mL:1 mL) were added to the reaction mixture, which was stirred at 20 °C for 18 h. After the completion of the reaction which was indicated by TLC, the reaction mixture was

directly purified through preparative thin layer chromatography (toluene) on silica gel to afford pure compound **7dh** in 91% yield (57.4 mg) as a white solid. 95:5 dr; m.p. 143-145 °C; $[\alpha]_D^{20} = -107.0$ (c = 0.80, acetone); $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.82 – 7.74 (m, 2H), 7.54 (d, $J = 8.0$ Hz, 1H), 7.46 – 7.39 (m, 1H), 7.31 – 7.27 (m, 2H), 7.25 – 7.20 (m, 2H), 7.13 – 7.05 (m, 4H), 7.04 – 7.01 (m, 2H), 6.99 – 6.87 (m, 4H), 6.82 (d, $J = 8.8$ Hz, 2H), 6.32 (d, $J = 8.8$ Hz, 2H), 5.43 (s, 1H), 3.86 (s, 3H), 3.80 (s, 3H), 3.62 (s, 3H), 1.91 (s, 3H); $^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ 159.2, 159.1, 157.5, 152.0, 144.6, 139.6, 135.7, 134.5, 134.0, 132.8, 131.3, 129.6, 129.4, 129.0, 128.7, 128.5, 127.9, 127.4, 126.3, 125.6, 125.4, 124.4, 123.0, 121.7, 121.5, 120.3, 118.6, 116.8, 113.4, 112.8, 111.5, 98.2, 55.3, 55.2, 21.2; IR (KBr): 2999, 2930, 2834, 1610, 1508, 1249, 1074, 919, 832, 564 cm^{-1} ; ESI FTMS exact mass calcd for $(\text{C}_{43}\text{H}_{35}\text{NO}_4\text{-H})^-$ requires m/z 628.2493, found m/z 628.2467; The enantiomeric excess: 92%, determined by HPLC (Daicel Chiralpak IB, hexane/isopropanol = 99/1, flow rate 1.0 mL/min, T = 30 °C, 254 nm): $t_R = 23.450$ (major), $t_R = 30.760$ (minor).

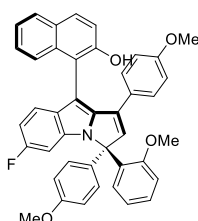
(*S_w*,*R*)-1-(6-chloro-3-(2-methoxyphenyl))-1,3-bis(4-methoxyphenyl)-3*H*-pyrrolo[1,2-*a*]indol-9-yl)naphthalen-2-ol (7eh**):**



Following the general procedure, 3-naphthylindole **1e** (29.3 mg, 0.1 mmol), propargylic alcohol **6h** (44.9 mg, 0.12 mmol), catalyst (*R*)-**4a** (8.5 mg, 0.015 mmol) were added to a reaction tube. Then, DCM:EA (4 mL:1 mL) were added to the reaction mixture, which was stirred at 20 °C for 90 h. After the completion of the reaction which was indicated by TLC, the reaction mixture was directly purified through preparative thin layer chromatography (toluene) on silica gel to afford pure compound **7eh** in 77% yield (50.2mg) as a white solid. 95:5 dr; m.p. 135-137 °C; $[\alpha]_D^{20} = -104.8$ (c = 0.78, acetone); $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.84 – 7.73 (m, 2H), 7.53 – 7.47 (m, 1H), 7.46 – 7.38 (m, 1H), 7.33 – 7.27 (m, 2H), 7.25 (s, 1H), 7.17 – 7.10 (m, 5H), 7.08 – 7.04 (m, 3H), 7.03 – 7.00 (m, 1H), 6.99 – 6.96 (m, 2H), 6.84 (d, $J = 8.8$ Hz, 2H), 6.36 (d, $J = 8.8$ Hz, 2H), 5.30 (s, 1H), 3.80 (s, 3H), 3.72 (s, 3H), 3.63 (s, 3H); $^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ 159.5, 159.1, 157.7, 152.1, 143.8, 138.4, 135.4, 135.2, 134.3, 131.8, 131.5, 129.7, 129.6, 129.0, 128.6, 128.5, 128.0, 127.9, 127.8, 126.5, 125.1, 124.1, 123.2, 121.6, 121.5, 120.6, 116.9, 113.9, 113.0, 112.6, 111.9, 110.9, 98.40, 75.2, 55.5, 55.3, 55.2; IR (KBr): 2999, 2931, 2834, 1609, 1508, 1249, 1028, 833, 784, 595 cm^{-1} ; ESI FTMS exact mass calcd for $(\text{C}_{42}\text{H}_{32}\text{ClNO}_4\text{-H})^-$ requires m/z 648.1947, found m/z 648.1928;

The enantiomeric excess: 96%, determined by HPLC (Daicel Chiralpak IB, hexane/isopropanol = 95/5, flow rate 1.0 mL/min, T = 30 °C, 254 nm): t_R = 9.227 (minor), t_R = 11.893 (major).

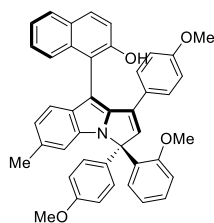
(*S_w*,*R*)-1-(6-fluoro-3-(2-methoxyphenyl)-1,3-bis(4-methoxyphenyl)-3*H*-pyrrolo[1,2-*a*]indol-9-yl)naphthalen-2-ol (7fh):



Following the general procedure, 3-naphthylindole **1f** (27.7 mg, 0.1 mmol), propargylic alcohol **6h** (44.9 mg, 0.12 mmol), catalyst (*R*)-**4a** (8.5 mg, 0.015 mmol) were added to a reaction tube. Then, DCM:EA (4 mL:1 mL) were added to the reaction mixture, which was stirred at 20 °C for 42 h. After the completion of the reaction which was indicated by TLC, the reaction mixture was directly purified through preparative thin layer chromatography (toluene) on silica gel to afford pure compound **7fh** in 73% yield (46.1 mg) as a white solid. >95:5 dr; m.p. 126-127 °C; $[\alpha]_D^{20}$ = -101.6 (c = 1.11, acetone); ¹H NMR (400 MHz, CDCl₃) δ 7.84 – 7.75 (m, 2H), 7.57 – 7.51 (m, 1H), 7.46 – 7.39 (m, 1H), 7.32 – 7.27 (m, 2H), 7.23 (s, 1H), 7.17 – 7.08 (m, 5H), 7.07 – 6.99 (m, 4H), 6.83 (d, *J* = 8.8 Hz, 2H), 6.79 – 6.73 (m, 2H), 6.36 (d, *J* = 8.4 Hz, 2H), 5.34 (s, 1H), 3.79 (s, 3H), 3.72 (s, 3H), 3.63 (s, 3H); ¹³C NMR (100 MHz, CDCl₃) δ 160.1 (d, *J* = 237.5 Hz), 159.4, 159.1, 157.6, 152.1, 143.5 (d, *J* = 3.5 Hz), 137.8, 135.3, 135.1 (d, *J* = 12.7 Hz), 134.3, 131.6, 129.6, 129.5, 129.0, 128.6, 128.0, 127.9, 127.8, 126.6, 126.4, 125.2, 124.2, 123.1, 121.6 (d, *J* = 10.1 Hz), 121.4, 116.9, 113.9, 113.0, 112.8, 111.9, 108.4 (d, *J* = 24.5 Hz), 98.3, 97.9, 97.6, 75.1, 55.5, 55.3, 55.2; ¹⁹F NMR (376 MHz, CDCl₃) δ -119.19; IR (KBr): 3392, 2931, 2834, 1621, 1508, 1436, 1248, 1029, 828, 785, 751 cm⁻¹; ESI FTMS exact mass calcd for (C₄₂H₃₂FNO₄-H)⁻ requires *m/z* 632.2242, found *m/z* 632.2240; The enantiomeric excess: 95%, determined by HPLC (Daicel Chiralpak IB, hexane/isopropanol = 95/5, flow rate 1.0 mL/min, T = 30 °C, 254 nm): t_R = 8.506 (minor), t_R = 10.453 (major).

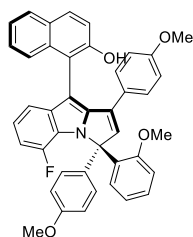
(*S_w*,*R*)-1-(3-(2-methoxyphenyl)-1,3-bis(4-methoxyphenyl)-6-methyl-3*H*-pyrrolo[1,2-*a*]indol-9-yl)naphthalen-2-ol (7gh):

Following the general procedure, 3-naphthylindole **1g** (27.3 mg, 0.1 mmol), propargylic alcohol **6h** (44.9 mg, 0.12 mmol), catalyst (*R*)-**4a** (8.5 mg, 0.015 mmol) were added to a reaction tube. Then, DCM:EA (4 mL:1 mL) were added to the reaction mixture, which was stirred at 20 °C for



18 h. After the completion of the reaction which was indicated by TLC, the reaction mixture was directly purified through preparative thin layer chromatography (toluene) on silica gel to afford pure compound **7gh** in 95% yield (59.8 mg) as a white solid. >95:5 dr; m.p. 140-142 °C; $[\alpha]_D^{20} = -146.3$ (c = 0.76, acetone); $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.83 – 7.75 (m, 2H), 7.58 (d, $J = 8.0$ Hz, 1H), 7.44 – 7.38 (m, 1H), 7.30 – 7.27 (m, 1H), 7.25 – 7.17 (m, 3H), 7.17 – 7.10 (m, 3H), 7.06 – 6.99 (m, 5H), 6.98 – 6.84 (m, 2H), 6.83 – 6.76 (m, 2H), 6.35 (d, $J = 8.4$ Hz, 2H), 5.41 (s, 1H), 3.77 (s, 3H), 3.72 (s, 3H), 3.63 (s, 3H), 2.29 (s, 3H); $^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ 159.3, 158.9, 157.7, 152.1, 143.2, 137.9, 137.7, 135.7, 135.6, 134.5, 133.6, 133.5, 132.1, 129.4, 129.3, 129.0, 128.6, 128.2, 128.1, 128.0, 127.9, 127.0, 126.3, 125.4, 124.5, 124.1, 123.0, 121.6, 121.3, 120.5, 116.8, 113.7, 113.4, 113.0, 111.7, 111.3, 110.9, 97.6, 74.9, 55.5, 55.2, 21.4; IR (KBr): 2999, 2930, 2833, 2359, 1609, 1248, 1075, 1058, 807, 568 cm^{-1} ; ESI FTMS exact mass calcd for $(\text{C}_{43}\text{H}_{35}\text{NO}_4\text{-H})^-$ requires m/z 628.2493, found m/z 628.2511; The enantiomeric excess: 97%, determined by HPLC (Daicel Chiralpak IB, hexane/isopropanol = 95/5, flow rate 0.5 mL/min, T = 30 °C, 254 nm): $t_R = 14.940$ (minor), $t_R = 16.680$ (major).

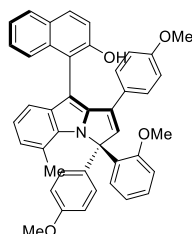
(*S_a*,*R*)-1-(5-fluoro-3-(2-methoxyphenyl)-1,3-bis(4-methoxyphenyl)-3*H*-pyrrolo[1,2-*a*]indol-9-yl)naphthalen-2-ol (7hh):



Following the general procedure, 3-naphthylindole **1h** (27.7 mg, 0.1 mmol), propargylic alcohol **6h** (44.9 mg, 0.12 mmol), catalyst (*R*)-**4a** (8.5 mg, 0.015 mmol) were added to a reaction tube. Then, DCM:EA (4 mL:1 mL) were added to the reaction mixture, which was stirred at 20 °C for 90 h. After the completion of the reaction which was indicated by TLC, the reaction mixture was directly purified through preparative thin layer chromatography (toluene) on silica gel to afford pure compound **7hh** in 82% yield (52.0 mg) as a white solid. 94:6 dr; m.p. 137-139 °C; $[\alpha]_D^{20} = -48.4$ (c = 0.76, acetone); $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.85 – 7.74 (m, 2H), 7.54 – 7.49 (m, 1H), 7.45 – 7.39 (m, 1H), 7.33 – 7.27 (m, 3H), 7.25 – 7.22 (m, 1H), 7.15 – 7.02 (m, 5H), 7.01 – 6.93 (m, 3H), 6.92 – 6.86 (m, 1H), 6.84 – 6.72 (m, 3H), 6.34 (d, $J = 8.8$ Hz, 2H), 5.32 (s, 1H), 3.78 (s, 3H), 3.74 (s, 3H), 3.63 (s, 3H); $^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ 159.3, 158.9, 157.5, 152.1, 147.6 (d, $J = 249.4$ Hz), 144.6, 139.1, 137.1, 134.2 (d, $J = 17.3$ Hz), 131.5, 129.7, 129.4, 129.0,

128.6, 128.0, 126.8, 126.4, 125.2, 124.1, 123.1, 121.2, 120.3 (d, $J = 5.9$ Hz), 116.7 (d, $J = 19.8$ Hz), 113.2, 113.0, 112.7, 111.5, 108.6 (d, $J = 18.1$ Hz), 98.7, 76.1, 55.4, 55.2; ^{19}F NMR (376 MHz, CDCl_3) δ -126.41; IR (KBr): 3384, 2930, 2834, 1597, 1489, 1248, 1176, 1027, 831, 591 cm^{-1} ; ESI FTMS exact mass calcd for $(\text{C}_{42}\text{H}_{32}\text{FNO}_4\text{-H})^-$ requires m/z 632.2242, found m/z 632.2245; The enantiomeric excess: 98%, determined by HPLC (Daicel Chiralpak IB, hexane/isopropanol = 95/5, flow rate 1.0 mL/min, $T = 30$ °C, 254 nm): $t_{\text{R}} = 8.346$ (minor), $t_{\text{R}} = 9.820$ (major).

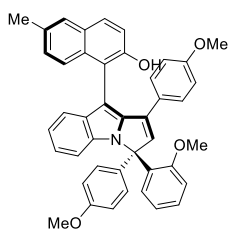
(*S_wR*)-1-(3-(2-methoxyphenyl)-1,3-bis(4-methoxyphenyl)-5-methyl-3*H*-pyrrolo[1,2-*a*]indol-9-yl)naphthalen-2-ol (7ih):



Following the general procedure, 3-naphthylindole **1i** (27.3 mg, 0.1 mmol), propargylic alcohol **6h** (44.9 mg, 0.12 mmol), catalyst (*R*)-**4a** (8.5 mg, 0.015 mmol) were added to a reaction tube. Then, DCM:EA (4 mL:1 mL) were added to the reaction mixture, which was stirred at 20 °C for 18 h. After the completion of the reaction which was indicated by TLC, the reaction mixture

was directly purified through preparative thin layer chromatography (toluene) on silica gel to afford pure compound **7ih** in 93% yield (58.8 mg) as a white solid. >95:5 dr; m.p. 144-146 °C; $[\alpha]_{\text{D}}^{20} = -30.6$ ($c = 0.71$, acetone); ^1H NMR (400 MHz, CDCl_3) δ 7.80 – 7.73 (m, 2H), 7.51 (d, $J = 8.0$ Hz, 1H), 7.44 – 7.39 (m, 1H), 7.29 – 7.27 (m, 1H), 7.25 – 7.18 (m, 3H), 7.12 – 7.05 (m, 3H), 7.05 – 6.99 (m, 3H), 6.97 – 6.92 (m, 1H), 6.91 – 6.86 (m, 3H), 6.80 (d, $J = 8.4$ Hz, 2H), 6.30 (d, $J = 8.8$ Hz, 2H), 5.40 (s, 1H), 3.85 (s, 3H), 3.79 (s, 3H), 3.61 (s, 3H), 1.89 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 159.1, 157.5, 152.0, 144.6, 139.6, 135.7, 134.4, 134.0, 132.8, 131.2, 129.5, 129.4, 129.0, 128.6, 128.5, 127.9, 127.4, 126.3, 125.5, 125.4, 124.4, 123.0, 121.7, 121.4, 120.2, 118.6, 116.8, 113.3, 112.8, 111.4, 98.2, 76.7, 55.3, 55.2, 21.2; IR (KBr): 2930, 2833, 1597, 1508, 1488, 1249, 1028, 831, 780, 521 cm^{-1} ; ESI FTMS exact mass calcd for $(\text{C}_{43}\text{H}_{35}\text{NO}_4\text{-H})^-$ requires m/z 628.2493, found m/z 628.2500; The enantiomeric excess: 99%, determined by HPLC (Daicel Chiralpak IB, hexane/isopropanol = 95/5, flow rate 1.0 mL/min, $T = 30$ °C, 254 nm): $t_{\text{R}} = 8.113$ (minor), $t_{\text{R}} = 10.343$ (major).

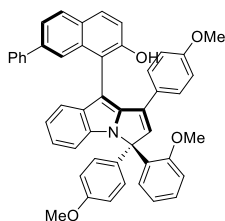
(*S_wR*)-1-(3-(2-methoxyphenyl)-1,3-bis(4-methoxyphenyl)-3*H*-pyrrolo[1,2-*a*]indol-9-yl)-6-methylnaphthalen-2-ol (7kh):



Following the general procedure, 3-naphthylindole **1k** (27.3 mg, 0.1 mmol), propargylic alcohol **6h** (44.9 mg, 0.12 mmol), catalyst (*R*)-**4a** (8.5 mg, 0.015 mmol) were added to a reaction tube. Then, DCM:EA (4 mL:1 mL) were added to the reaction mixture, which was stirred at 20 °C for 36 h.

After the completion of the reaction which was indicated by TLC, the reaction mixture was directly purified through preparative thin layer chromatography (toluene) on silica gel to afford pure compound **7kh** in 96% yield (60.4 mg) as a white solid. 91:9 dr; m.p. 142-145 °C; $[\alpha]_D^{20} = -143.7$ ($c = 0.57$, acetone); $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.74 (d, $J = 9.2$ Hz, 1H), 7.62 (s, 1H), 7.51 (d, $J = 8.4$ Hz, 1H), 7.49 – 7.44 (m, 1H), 7.31 – 7.29 (m, 1H), 7.28 – 7.22 (m, 2H), 7.21 – 7.17 (m, 2H), 7.16 – 7.06 (m, 8H), 7.05 – 7.03 (m, 1H), 6.85 (d, $J = 8.8$ Hz, 2H), 6.43 (d, $J = 8.8$ Hz, 2H), 5.34 (s, 1H), 3.82 (s, 3H), 3.77 (s, 3H), 3.70 (s, 3H), 2.51 (s, 3H); $^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ 159.4, 158.9, 157.7, 151.4, 142.9, 138.0, 135.4, 135.2, 133.3, 132.5, 132.3, 132.0, 129.4, 129.2, 128.7, 128.6, 128.5, 128.1, 128.0, 127.0, 126.9, 125.3, 124.4, 122.4, 121.3, 121.0, 119.8, 116.8, 113.7, 113.0, 111.7, 111.2, 98.4, 75.0, 55.4, 55.2, 55.1, 21.4; IR (KBr): 3651, 2954, 2835, 2363, 1654, 1508, 1474, 1335, 1200, 1077, 830, 587 cm^{-1} ; ESI FTMS exact mass calcd for $(\text{C}_{43}\text{H}_{35}\text{NO}_4 + \text{H})^+$ requires m/z 630.2639, found m/z 630.2624; The enantiomeric excess: 92%, determined by HPLC (Daicel Chiralpak AD-H, hexane/isopropanol = 85/15, flow rate 1.0 mL/min, $T = 30$ °C, 254 nm): $t_R = 4.353$ (major), $t_R = 5.197$ (minor).

(*S,R*)-1-(3-(2-methoxyphenyl))-1,3-bis(4-methoxyphenyl)-3H-pyrrolo[1,2-a]indol-9-yl)-7-phenylnaphthalen-2-ol (7lh**):**

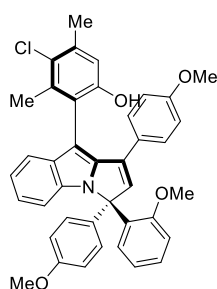


Following the general procedure, 3-naphthylindole **1l** (33.5 mg, 0.1 mmol), propargylic alcohol **6h** (44.9 mg, 0.12 mmol), catalyst (*R*)-**4a** (8.5 mg, 0.015 mmol) were added to a reaction tube. Then, DCM:EA (4 mL:1 mL) were added to the reaction mixture, which was stirred at 20 °C for 72 h.

After the completion of the reaction which was indicated by TLC, the reaction mixture was directly purified through preparative thin layer chromatography (toluene) on silica gel to afford pure compound **7lh** in 69% yield (47.5 mg) as a white solid. 90:10 dr; m.p. 189-191 °C; $[\alpha]_D^{20} = -62.6$ ($c = 0.84$, acetone); $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.83 – 7.77 (m, 2H), 7.71 (s, 1H), 7.50 (d, $J = 8.4$ Hz, 1H), 7.43 – 7.37 (m, 3H), 7.32 (d, $J = 7.6$ Hz, 1H), 7.29 – 7.27 (m, 1H), 7.24 (s, 3H),

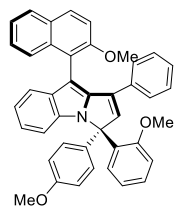
7.22 – 7.15 (m, 3H), 7.13 – 7.07 (m, 2H), 7.06 – 6.94 (m, 6H), 6.82 (d, $J = 8.8$ Hz, 2H), 6.33 (d, $J = 8.4$ Hz, 2H), 5.50 (s, 1H), 3.78 (s, 3H), 3.69 (s, 3H), 3.62 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 159.3, 158.9, 157.6, 152.4, 143.4, 141.4, 138.6, 138.3, 135.4, 135.2, 134.8, 132.9, 131.9, 129.3, 129.1, 128.6, 128.5, 128.3, 128.2, 128.1, 127.8, 127.2, 127.1, 126.9, 124.5, 123.3, 122.6, 121.5, 120.8, 120.0, 116.9, 113.7, 113.6, 113.0, 111.8, 111.2, 98.0, 75.1, 55.4, 55.3, 55.2; IR (KBr): 3502, 3053, 2931, 1608, 1508, 1454, 1337, 1252, 1033, 831, 746 cm^{-1} ; ESI FTMS exact mass calcd for $(\text{C}_{48}\text{H}_{37}\text{NO}_4+\text{Na})^+$ requires m/z 714.2615, found m/z 714.2594; The enantiomeric excess: 79%, determined by HPLC (Daicel Chiralpak IC, hexane/isopropanol = 95/5, flow rate 1.0 mL/min, $T = 30$ °C, 254 nm): $t_R = 6.493$ (minor), $t_R = 7.163$ (major).

(*S_a*,*R*)-4-chloro-2-(3-(2-methoxyphenyl)-1,3-bis(4-methoxyphenyl)-5-methyl-3*H*-pyrrolo[1,2-*a*]indol-9-yl)-3,5-dimethylphenol (7mh):



Following the general procedure, 3-phenylindole **1m** (27.1 mg, 0.1 mmol), propargylic alcohol **6h** (44.9 mg, 0.12 mmol), catalyst (*R*)-**4a** (8.5 mg, 0.015 mmol) were added to a reaction tube. Then, DCM:EA (4 mL:1 mL) were added to the reaction mixture, which was stirred at 20 °C for 90 h. After the completion of the reaction which was indicated by TLC, the reaction mixture was directly purified through preparative thin layer chromatography (toluene) on silica gel to afford pure compound **7mh** in 90% yield (56.4 mg) as a white solid. 92:8 dr; m.p. 132-134 °C; $[\alpha]_D^{20} = -166.9$ ($c = 0.79$, acetone); ^1H NMR (400 MHz, CDCl_3) δ 7.42 – 7.36 (m, 1H), 7.33 – 7.29 (m, 1H), 7.23 (s, 1H), 7.15 – 7.09 (m, 4H), 7.08 – 7.01 (m, 4H), 7.00 – 6.93 (m, 2H), 6.78 (d, $J = 8.4$ Hz, 2H), 6.72 (s, 1H), 6.60 (d, $J = 8.4$ Hz, 2H), 5.06 (s, 1H), 3.76 (s, 3H), 3.75 (s, 3H), 3.70 (s, 3H), 2.40 (s, 3H), 1.99 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 159.7, 159.0, 157.8, 152.4, 142.7, 138.4, 137.1, 136.6, 135.3, 134.9, 132.2, 131.8, 129.4, 128.8, 128.0, 126.9, 126.2, 124.6, 122.6, 121.3, 120.4, 120.0, 119.3, 114.3, 113.8, 113.3, 111.8, 111.3, 99.4, 75.0, 55.5, 55.4, 55.3, 21.1, 18.8; IR (KBr): 3502, 2930, 2833, 1597, 1508, 1249, 1028, 831, 780, 559 cm^{-1} ; ESI FTMS exact mass calcd for $(\text{C}_{40}\text{H}_{34}\text{ClNO}_4-\text{H})^-$ requires m/z 626.2103, found m/z 626.2103; The enantiomeric excess: 92%, determined by HPLC (Daicel Chiralpak IB, hexane/isopropanol = 98/2, flow rate 1.0 mL/min, $T = 30$ °C, 254 nm): $t_R = 9.603$ (minor), $t_R = 10.673$ (major).

(*S_aR*)-9-(2-methoxynaphthalen-1-yl)-3-(2-methoxyphenyl)-3-(4-methoxyphenyl)-1-phenyl-3*H*-pyrrolo[1,2-*a*]indole (7ng):



Following the general procedure, 3-naphthylindole **1n** (27.3 mg, 0.1 mmol), propargylic alcohol **6g** (41.3 mg, 0.12 mmol), catalyst (*R*)-**4a** (8.5 mg, 0.015 mmol) were added to a reaction tube. Then, DCM:EA (4 mL:1 mL) were added to the reaction mixture, which was stirred at 20 °C for 10 h. After the completion of the reaction which was indicated by TLC, the reaction mixture was directly purified through preparative thin layer chromatography (PE:DCM = 1:2) on silica gel to afford pure compound **7ng** in 86% yield (51.7 mg) with 63:37 dr.

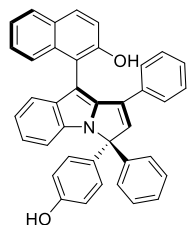
Major diastereomer of **7ng**: white solid; m.p. 138-140 °C; $[\alpha]_D^{20} = +22.2$ (c = 0.61, acetone); $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.99 – 7.92 (m, 1H), 7.90 – 7.84 (m, 1H), 7.81 (d, $J = 8.8$ Hz, 1H), 7.43 – 7.35 (m, 4H), 7.33 (s, 1H), 7.19 (d, $J = 8.0$ Hz, 1H), 7.16 – 7.09 (m, 4H), 7.08 – 7.02 (m, 3H), 7.01 – 6.93 (m, 4H), 6.92 – 6.86 (m, 2H), 6.79 (d, $J = 8.8$ Hz, 2H), 3.78 (s, 3H), 3.76 (s, 3H), 3.26 (s, 3H); $^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ 158.7, 157.6, 155.2, 142.9, 138.2, 137.0, 135.1, 134.0, 133.8, 133.3, 132.4, 129.3, 129.0, 128.8, 128.5, 128.2, 127.9, 127.6, 127.4, 127.2, 127.0, 126.4, 126.1, 123.3, 121.5, 121.4, 121.2, 119.3, 117.5, 113.6, 113.0, 111.4, 111.0, 101.6, 74.9, 55.7, 55.4, 55.2; IR (KBr): 3448, 3054, 2931, 2360, 1508, 1251, 1109, 806, 761, 697 cm^{-1} ; ESI FTMS exact mass calcd for $(\text{C}_{42}\text{H}_{33}\text{NO}_3+\text{Na})^+$ requires m/z 622.2353, found m/z 622.2351; The enantiomeric excess: 11%, determined by HPLC (Daicel Chiralpak IB, hexane/isopropanol = 95/5, flow rate 0.5 mL/min, T = 30 °C, 254 nm): $t_R = 12.573$ (major), $t_R = 13.483$ (minor).

Minor diastereomer of **7ng**: white solid; m.p. 138-140 °C; $[\alpha]_D^{20} = -84.7$ (c = 0.22, acetone); $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.84 – 7.76 (m, 2H), 7.68 (d, $J = 8.0$ Hz, 1H), 7.42 – 7.37 (m, 1H), 7.31 – 7.27 (m, 2H), 7.22 – 7.14 (m, 5H), 7.13 – 7.06 (m, 3H), 7.05 – 6.92 (m, 6H), 6.87 – 6.76 (m, 4H), 3.77 (s, 3H), 3.71 (s, 3H), 3.36 (s, 3H); $^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ 158.7, 157.8, 155.3, 142.1, 138.4, 136.8, 134.6, 134.3, 133.6, 133.3, 132.5, 129.1, 129.0, 128.8, 128.7, 128.1, 127.7, 127.4, 127.3, 127.2, 126.3, 125.9, 123.2, 121.4, 121.3, 121.2, 119.1, 117.6, 113.6, 113.4, 111.6, 110.8, 101.6, 74.6, 55.9, 55.5, 55.2; IR (KBr): 3049, 2930, 2833, 1508, 1268, 1108, 1020, 805, 758, 536 cm^{-1} ; ESI FTMS exact mass calcd for $(\text{C}_{42}\text{H}_{33}\text{NO}_3+\text{Na})^+$ requires m/z 622.2353, found m/z 622.2360; The enantiomeric excess: 22%, determined by HPLC (Daicel Chiralpak IC, hexane/isopropanol = 98/2, flow rate 0.5 mL/min, T = 30 °C, 254 nm): $t_R = 11.890$ (minor), $t_R =$

13.317 (major).

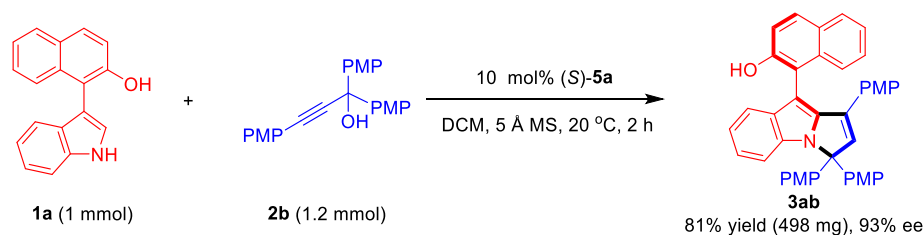
(*S,S*)-1-(3-(4-hydroxyphenyl)-1,3-diphenyl-3*H*-pyrrolo[1,2-*a*]indol-9-yl)naphthalen-2-ol

(7aa):

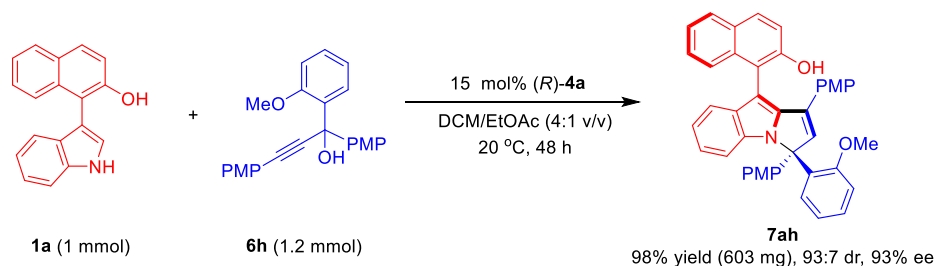


Following the general procedure, 3-naphthylindoles **1a** (25.9 mg, 0.1 mmol), alcohol **6a** (36.0 mg, 0.12 mmol), catalyst (*R*)-**4a** (8.5 mg, 0.015 mmol) were added to a reaction tube. Then, DCM:EA (4 mL:1 mL) were added to the reaction mixture, which was stirred at 20 °C for 60 h. After the completion of the reaction which was indicated by TLC, the reaction mixture was directly purified through preparative thin layer chromatography (PE:DCM = 1:2) on silica gel to afford pure compound **7aa** in 65% yield (35.0 mg) as a white solid. 81:19 dr; m.p. 133-135 °C; $[\alpha]_D^{20} = +21.5$ (c = 0.69, acetone); $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.84 – 7.71 (m, 2H), 7.49 (d, $J = 7.6$ Hz, 1H), 7.45 – 7.31 (m, 5H), 7.30 – 7.27 (m, 1H), 7.25 – 7.18 (m, 4H), 7.18 – 7.09 (m, 3H), 7.08 – 6.96 (m, 4H), 6.89 (s, 1H), 6.86 – 6.75 (m, 4H), 5.44 (s, 1H), 4.97 (s, 1H); $^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ 155.4, 152.0, 142.8, 140.9, 139.4, 135.5, 134.8, 134.4, 133.0, 131.5, 131.4, 129.7, 129.6, 128.9, 128.8, 128.2, 128.0, 127.9, 127.8, 127.6, 127.3, 126.3, 125.2, 123.0, 122.8, 121.1, 120.1, 116.8, 115.6, 112.9, 111.0, 98.7, 75.8; IR (KBr): 3502, 3055, 2931, 2359, 1596, 1487, 1052, 917, 781, 593 cm^{-1} ; ESI FTMS exact mass calcd for $(\text{C}_{39}\text{H}_{27}\text{NO}_2\text{-H})^-$ requires m/z 540.1969, found m/z 540.1954; The enantiomeric excess: 68%, determined by HPLC (Daicel Chiralpak AD-H, hexane/isopropanol = 85/15, flow rate 1.0 mL/min, T = 30 °C, 254 nm): $t_R = 6.077$ (major), $t_R = 21.103$ (minor).

5. Procedure for one-mmol-scale reaction



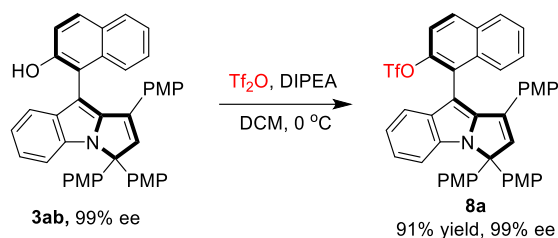
3-Naphthylindole **1a** (259.1mg, 1.0 mmol), propargylic alcohol **2b** (450.1mg, 1.2 mmol), catalyst *(S)*-**5a** (60.8 mg, 0.10 mmol) and 5 Å MS (1.0 g) were added to a reaction bottle. Then, DCM (30 mL) was added to the reaction mixture, which was stirred at 20 °C for 2 h. After the completion of the reaction which was indicated by TLC, the reaction mixture was concentrated in vacuo to give a residue, which was purified by flash column chromatography (PE:DCM = 2:1) to afford compound **3ab** (498 mg, 81% yield, 93% ee).



3-Naphthylindole **1a** (259.1mg, 1.0 mmol), propargylic alcohol **6h** (450.1mg, 1.2 mmol), catalyst *(R)*-**4a** (85.2 mg, 0.15 mmol) were added to a reaction bottle. Then, DCM:EA (40 mL:10 mL) were added to the reaction mixture, which was stirred at 20 °C for 48 h. After the completion of the reaction which was indicated by TLC, the reaction mixture was concentrated in vacuo to give a residue, which was purified by flash column chromatography (PE:DCM = 2:1) to afford compound **7ah** (603 mg, 98% yield, 93:7 dr, 93% ee).

6. Synthetic procedures and characterization data of compounds 8-10, 13, 16

Synthetic procedure and characterization data of compound 8a:

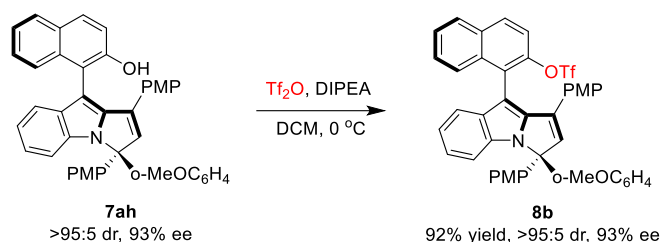


Under argon atmosphere at 0 °C, to the solution of **3ab** (309 mg, 0.5 mmol) in dichloromethane (15 mL) was added *i*-Pr₂NEt (DIPEA, 0.26 mL, 1.5 mmol). Then, Tf₂O (0.17 mL, 1.0 mmol) was added dropwise to the reaction mixture, which was further stirred at 0 °C for 10 min. After the completion of the reaction which was indicated by TLC, the reaction mixture was diluted by dichloromethane and quenched by hydrochloric acid (1 M). The resultant mixture was extracted by dichloromethane, and the organic layer was washed successively by saturated NaHCO₃ aqueous solution and saturated NaCl aqueous solution. Subsequently, the resultant organic layer was dried by anhydrous Na₂SO₄ and concentrated in vacuo to give a residue, which was purified by flash column chromatography (PE:DCM = 2:1) to afford pure product **8a**.

(*R_a*)-1-(1,3,3-tris(4-methoxyphenyl)-3*H*-pyrrolo[1,2-*a*]indol-9-yl)naphthalen-2-yl

trifluoromethanesulfonate (8a): 91% yield (340.4 mg); white solid; m.p. 76-78 °C; [α]_D²⁰ = +27.5 (c = 0.28, acetone); ¹H NMR (400 MHz, CDCl₃) δ 7.97 – 7.90 (m, 2H), 7.88 (d, *J* = 9.2 Hz, 1H), 7.56 – 7.51 (m, 1H), 7.44 – 7.39 (m, 1H), 7.36 (d, *J* = 8.4 Hz, 2H), 7.25 – 7.19 (m, 3H), 7.13 – 7.06 (m, 2H), 7.04 – 6.99 (m, 1H), 6.97 – 6.91 (m, 4H), 6.87 (d, *J* = 8.4 Hz, 2H), 6.79 (s, 1H), 6.37 (d, *J* = 8.4 Hz, 2H), 3.82 (s, 3H), 3.80 (s, 3H), 3.66 (s, 3H); ¹³C NMR (100 MHz, CDCl₃) δ 159.3, 159.2, 159.1, 145.9, 143.0, 140.6, 134.7, 134.2, 133.9, 133.1, 132.5, 131.5, 131.4, 129.6, 129.4, 128.6, 128.0, 127.7, 127.2, 126.8, 125.9, 124.9, 122.1, 121.1, 119.7, 119.3, 114.0, 113.9, 113.0, 110.8, 98.5, 75.3, 55.4, 55.3, 55.2; IR (KBr): 3546, 3054, 2930, 2340, 1569, 1509, 1028, 888, 691, 557 cm⁻¹; ESI FTMS exact mass calcd for (C₄₃H₃₂F₃NO₆S+Na)⁺ requires m/z 770.1795, found m/z 770.1797; The enantiomeric excess: 99%, determined by HPLC (Daicel Chiralpak AD-H, hexane/isopropanol = 95/5, flow rate 1.0 mL/min, T = 30 °C, 254 nm): t_R = 5.193 (minor), t_R = 7.066 (major).

Synthetic procedure and characterization data of compound **8b**:

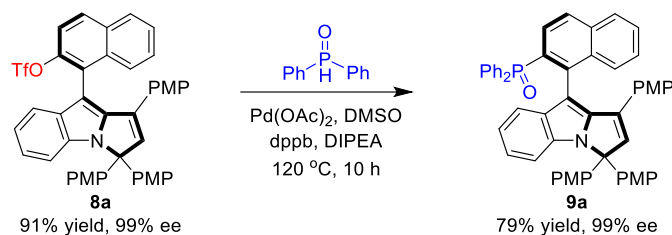


Under argon atmosphere at 0 °C, to the solution of **7ah** (309 mg, 0.5 mmol) in dichloromethane (15 mL) was added *i*-Pr₂NEt (DIPEA, 0.26 mL, 1.5 mmol). Then, Tf₂O (0.17 mL, 1.0 mmol) was added dropwise to the reaction mixture, which was further stirred at 0 °C for 10 min. After the completion of the reaction which was indicated by TLC, the reaction mixture was diluted by dichloromethane and quenched by hydrochloric acid (1 M). The resultant mixture was extracted by dichloromethane, and the organic layer was washed successively by saturated NaHCO₃ aqueous solution and saturated NaCl aqueous solution. Subsequently, the resultant organic layer was dried by anhydrous Na₂SO₄ and concentrated in vacuo to give a residue, which was purified by flash column chromatography (PE:DCM = 2:1) to afford pure product **8b**.

(S_o,R)-1-(3-(2-methoxyphenyl)-1,3-bis(4-methoxyphenyl)-3H-pyrrolo[1,2-a]indol-9-yl)

naphthalen-2-yl trifluoromethanesulfonate (8b): 92% yield (344.5 mg); > 95:5 dr; white solid; m.p. 106-108 °C; [α]_D²⁰ = -179.9 (c = 0.74, acetone); ¹H NMR (400 MHz, CDCl₃) δ 8.00 (d, *J* = 8.4 Hz, 1H), 7.93 (d, *J* = 8.0 Hz, 1H), 7.87 (d, *J* = 9.2 Hz, 1H), 7.58 – 7.53 (m, 1H), 7.47 – 7.38 (m, 2H), 7.27 (s, 1H), 7.25 – 7.21 (m, 2H), 7.20 – 7.15 (m, 3H), 7.08 – 6.98 (m, 5H), 6.95 (d, *J* = 8.4 Hz, 2H), 6.79 (d, *J* = 8.4 Hz, 2H), 6.39 (d, *J* = 8.4 Hz, 2H), 3.77 (s, 3H), 3.75 (s, 3H), 3.67 (s, 3H); ¹³C NMR (100 MHz, CDCl₃) δ 159.2, 158.9, 157.7, 146.1, 143.2, 138.9, 135.6, 134.7, 133.9, 133.4, 132.5, 131.5, 129.4, 129.3, 128.6, 128.5, 128.1, 128.0, 127.8, 127.2, 127.0, 126.8, 125.8, 125.3, 122.0, 121.3, 120.9, 119.7, 119.2, 113.4, 113.0, 111.6, 111.1, 98.3, 75.3, 55.4, 55.2; IR (KBr): 3048, 2836, 2048, 1609, 1509, 1251, 1032, 831, 638 cm⁻¹; ESI FTMS exact mass calcd for (C₄₃H₃₂F₃NO₆S+Na)⁺ requires *m/z* 770.1795, found *m/z* 770.1776; The enantiomeric excess: 93%, determined by HPLC (Daicel Chiralpak OD-H, hexane/isopropanol = 99/1, flow rate 0.2 mL/min, T = 30 °C, 254 nm): *t_R* = 49.843 (major), *t_R* = 53.133 (minor).

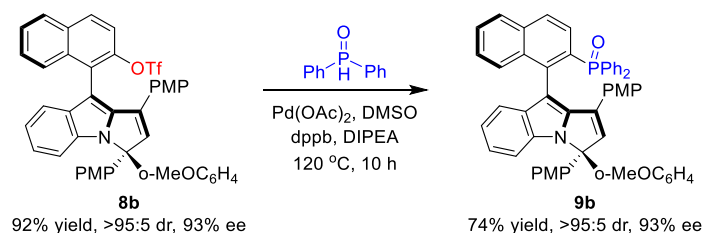
Synthetic procedure and characterization data of compound **9a**:



Under argon atmosphere, DMSO (1 mL, pre-deoxygenized by ultrasonic) was added to the mixture of **8a** (71.7 mg, 0.1 mmol), $\text{Ph}_2\text{P}(\text{O})\text{H}$ (80.8 mg, 0.4 mmol), $\text{Pd}(\text{OAc})_2$ (6.7 mg, 0.03 mmol) and dppb (12.8 mg, 0.03 mmol). Then, *i*-Pr₂NEt (DIPEA, 84 μL , 0.5 mmol) was added to the reaction mixture, which was stirred at 120 °C for 10 h. After the completion of the reaction which was indicated by TLC, the reaction mixture was diluted with dichloromethane and quenched with hydrochloric acid (1 M). The resultant mixture was extracted with dichloromethane, and the organic layer was washed successively with saturated NaHCO_3 aqueous solution and brine. Subsequently, the resultant organic layer was dried with anhydrous Na_2SO_4 and concentrated in vacuo to give a residue, which was purified by flash column chromatography (PE:EA = 4:1) to afford pure product **9a**.

(*R_a*)-diphenyl(1-(1,3,3-tris(4-methoxyphenyl)-3*H*-pyrrolo[1,2-*a*]indol-9-yl)naphthalen-2-yl)phosphine oxide (9a**):** 79% yield (63.5 mg); white solid; m.p. 96-98 °C; $[\alpha]_{\text{D}}^{20} = +38.5$ (c = 0.20, acetone); ¹H NMR (400 MHz, CDCl_3) δ 7.91 (d, *J* = 8.4 Hz, 1H), 7.84 (d, *J* = 8.8 Hz, 1H), 7.74 (dd, *J* = 8.4, 2.0 Hz, 1H), 7.61 – 7.55 (m, 1H), 7.53 (d, *J* = 8.8 Hz, 2H), 7.42 – 7.33 (m, 3H), 7.31 – 7.27 (m, 4H), 7.21 (s, 1H), 7.16 (d, *J* = 7.2 Hz, 1H), 7.13 – 7.02 (m, 3H), 7.01 – 6.94 (m, 5H), 6.87 (d, *J* = 8.8 Hz, 2H), 6.82 – 6.71 (m, 4H), 6.48 – 6.42 (m, 1H), 6.37 (d, *J* = 8.4 Hz, 2H), 6.31 (d, *J* = 8.0 Hz, 1H), 3.79 (s, 3H), 3.74 (s, 3H), 3.69 (s, 3H); ¹³C NMR (100 MHz, CDCl_3) δ 158.7, 158.6, 157.8, 145.4, 140.6, 137.2, 137.1, 134.8, 134.6, 134.5, 133.6, 133.4, 133.2, 132.8, 132.6, 132.2, 132.0, 131.9, 131.6, 131.5, 131.0, 130.5, 129.3, 129.2, 129.0, 128.9, 128.2, 128.1, 127.8, 127.7, 127.6, 127.4, 127.3, 127.0, 126.9, 126.7, 126.6, 121.1, 120.6, 120.2, 118.7, 113.2, 112.6, 111.4, 110.1, 102.2, 74.8, 55.4, 55.3, 55.2; ³¹P NMR (162 MHz, CDCl_3) δ 27.2; IR (KBr): 3050, 2833, 2359, 1606, 1508, 1200, 1027, 830, 720 cm^{-1} ; ESI FTMS exact mass calcd for $(\text{C}_{54}\text{H}_{42}\text{NO}_4\text{P}+\text{H})^+$ requires *m/z* 800.2924, found *m/z* 800.2925; The enantiomeric excess: 99%, determined by HPLC (Daicel Chiralpak IC, hexane/isopropanol = 85/15, flow rate 1.0 mL/min, T = 30 °C, 254 nm): *t_R* = 17.820 (minor), *t_R* = 21.170 (major).

Synthetic procedure and characterization data of compound **9b**:

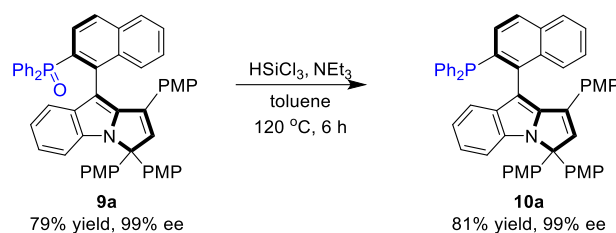


Under argon atmosphere, DMSO (1 mL, pre-deoxygenized by ultrasonic) was added to the mixture of **8b** (71.7 mg, 0.1 mmol), Ph₂P(O)H (80.8 mg, 0.4 mmol), Pd(OAc)₂ (6.7 mg, 0.03 mmol) and dppb (12.8 mg, 0.03 mmol). Then, *i*-Pr₂NEt (DIPEA, 84 uL, 0.5 mmol) was added to the reaction mixture, which was stirred at 120 °C for 10 h. After the completion of the reaction which was indicated by TLC, the reaction mixture was diluted with dichloromethane and quenched with hydrochloric acid (1 M). The resultant mixture was extracted with dichloromethane, and the organic layer was washed successively with saturated NaHCO₃ aqueous solution and brine. Subsequently, the resultant organic layer was dried with anhydrous Na₂SO₄ and concentrated in vacuo to give a residue, which was purified by flash column chromatography (PE:EA = 4:1) to afford pure product **9b**.

(*S_w*,*R*)-(1-(3-(2-methoxyphenyl)-1,3-bis(4-methoxyphenyl)-3*H*-pyrrolo[1,2-*a*]indol-9-yl)

naphthalen-2-yl)diphenylphosphine oxide (9b**):** 74% yield (59.1 mg); > 95:5 dr; white solid; m.p. 119-121 °C; [α]_D²⁰ = -79.1 (c = 0.33, acetone); ¹H NMR (400 MHz, CDCl₃) δ 7.92 (d, *J* = 8.0 Hz, 1H), 7.82 (d, *J* = 8.4 Hz, 1H), 7.76 (dd, *J* = 8.8, 2.4 Hz, 1H), 7.62 – 7.55 (m, 3H), 7.43 – 7.36 (m, 2H), 7.35 – 7.27 (m, 4H), 7.25 – 7.22 (m, 2H), 7.15 – 7.07 (m, 3H), 7.00 – 6.88 (m, 7H), 6.87 – 6.83 (m, 1H), 6.82 – 6.75 (m, 3H), 6.73 (s, 1H), 6.56 – 6.50 (m, 1H), 6.48 – 6.43 (m, 1H), 6.36 (d, *J* = 8.8 Hz, 2H), 3.83 (s, 3H), 3.80 (s, 3H), 3.68 (s, 3H); ¹³C NMR (100 MHz, CDCl₃) δ 159.1, 158.8, 158.7, 145.3, 140.3, 140.2, 139.0, 136.1, 134.7, 134.6, 134.5, 133.4, 133.1, 133.0, 132.9, 132.8, 132.1, 131.9, 131.8, 131.4, 131.3, 131.1, 130.4, 129.2, 129.1, 128.9, 128.8, 128.2, 128.1, 127.9, 127.8, 127.7, 127.5, 127.3, 127.0, 126.8, 126.7, 126.5, 120.9, 120.6, 118.7, 113.9, 113.6, 112.6, 109.9, 102.6, 74.9, 55.4, 55.3; ³¹P NMR (162 MHz, CDCl₃) δ 26.9; IR (KBr): 3049, 2833, 2358, 1607, 1508, 1248, 1025, 744, 542 cm⁻¹; ESI FTMS exact mass calcd for (C₅₄H₄₂NO₄P+Na)⁺ requires m/z 822.2744, found m/z 822.2719; The enantiomeric excess: 93%, determined by HPLC (Daicel Chiralpak IC, hexane/isopropanol = 90/10, flow rate 0.5 mL/min, T = 30 °C, 254 nm): t_R = 32.990 (major), t_R = 37.297 (minor).

Synthetic procedure and characterization data of compound **10a**:

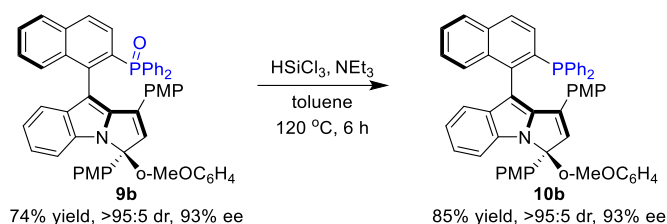


Under argon atmosphere, to the solution of compound **9a** (79.9 mg, 0.1 mmol) in anhydrous toluene (1 mL) was successively added NEt_3 (0.36 mL, 2.5 mmol) and HSiCl_3 (0.1 mL, 1 mmol). Then, the reaction mixture was heated to 120 °C and refluxed for 6 h. After the completion of the reaction which was indicated by TLC, the reaction mixture was quenched with saturated NaHCO_3 aqueous solution. The resultant mixture was filtered and the solid powder was washed with ethyl acetate. Subsequently, the filtrate was extracted with ethyl acetate, and the organic layer was dried over anhydrous Na_2SO_4 and concentrated in vacuo to give a residue, which was further purified by flash column chromatography (PE:EA = 10:1) to afford pure product **10a**.

(*R_a*)-9-(2-(diphenylphosphanyl)naphthalen-1-yl)-1,3,3-tris(4-methoxyphenyl)-3*H*-pyrrolo

[1,2-*a*]indole (10a**):** 81% yield (63.4 mg); white solid; m.p. 74-76 °C; $[\alpha]_{\text{D}}^{20} = -95.3$ (c = 0.51, acetone); $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.94 – 7.87 (m, 2H), 7.73 (d, $J = 8.4$ Hz, 1H), 7.55 – 7.50 (m, 1H), 7.43 – 7.36 (m, 3H), 7.31 – 7.27 (m, 1H), 7.25 – 7.19 (m, 3H), 7.17 – 7.11 (m, 2H), 7.05 – 6.94 (m, 6H), 6.93 – 6.81 (m, 6H), 6.77 (d, $J = 8.8$ Hz, 2H), 6.65 – 6.55 (m, 4H), 6.37 (d, $J = 8.4$ Hz, 2H), 3.78 (s, 3H), 3.76 (s, 3H), 3.70 (s, 3H); $^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ 159.2, 158.7, 157.6, 142.2, 138.7, 137.2, 136.2, 134.5, 134.3, 134.1, 133.9, 133.5, 132.9, 132.8, 132.3, 129.4, 129.1, 128.9, 128.4, 128.1, 128.0, 127.8, 127.5, 127.4, 127.2, 126.4, 126.3, 125.8, 121.3, 120.6, 119.0, 113.2, 113.0, 111.4, 110.5, 74.7, 55.4, 55.3, 55.2; $^{31}\text{P NMR}$ (162 MHz, CDCl_3) δ -12.6; IR (KBr): 3048, 2928, 2833, 2363, 1608, 1510, 1250, 1025, 695, 548 cm^{-1} ; ESI FTMS exact mass calcd for $(\text{C}_{54}\text{H}_{42}\text{NO}_3\text{P}+\text{H})^+$ requires m/z 784.2975, found m/z 784.2965; The enantiomeric excess: 99%, determined by HPLC (Daicel Chiralpak IA, hexane/isopropanol = 95/5, flow rate 1.0 mL/min, T = 30 °C, 254 nm): $t_{\text{R}} = 6.343$ (minor), $t_{\text{R}} = 13.553$ (major).

Synthetic procedure and characterization data of compound 10b:

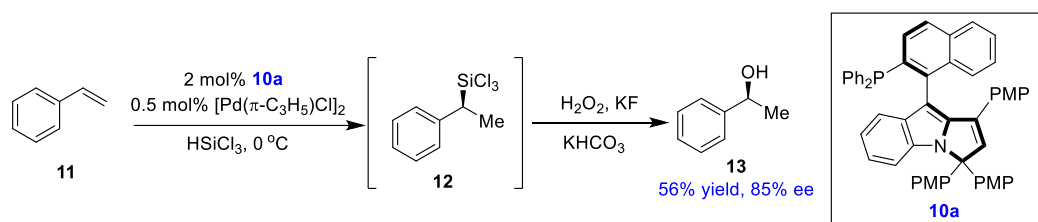


Under argon atmosphere, to the solution of compound **9b** (79.9 mg, 0.1 mmol) in anhydrous toluene (1 mL) was successively added NEt₃ (0.36 mL, 2.5 mmol) and HSiCl₃ (0.1 mL, 1 mmol). Then, the reaction mixture was heated to 120 °C and refluxed for 6 h. After the completion of the reaction which was indicated by TLC, the reaction mixture was quenched with saturated NaHCO₃ aqueous solution. The resultant mixture was filtered and the solid powder was washed with ethyl acetate. Subsequently, the filtrate was extracted with ethyl acetate, and the organic layer was dried over anhydrous Na₂SO₄ and concentrated in vacuo to give a residue, which was further purified by flash column chromatography (PE:EA = 10:1) to afford pure product **10b**.

(*S_wR*)-9-(2-(diphenylphosphanyl)naphthalen-1-yl)-3-(2-methoxyphenyl)-1,3-bis

(4-methoxyphenyl)-3*H*-pyrrolo[1,2-*a*]indole (**10b**): 85% yield (66.6 mg); > 95:5 dr; white solid; m.p. 119.0-121.0 °C; [α]_D²⁰ = -18.2 (c = 0.29, acetone); ¹H NMR (400 MHz, CDCl₃) δ 7.90 (d, *J* = 8.0 Hz, 2H), 7.75 (d, *J* = 8.4 Hz, 1H), 7.56 – 7.50 (m, 1H), 7.47 – 7.37 (m, 3H), 7.31 (d, *J* = 8.4 Hz, 2H), 7.22 – 7.17 (m, 1H), 7.16 – 7.09 (m, 2H), 7.08 – 6.82 (m, 14H), 6.79 (s, 1H), 6.74 – 6.64 (m, 2H), 6.63 – 6.52 (m, 2H), 6.38 (d, *J* = 8.4 Hz, 2H), 3.83 (s, 3H), 3.81 (s, 3H), 3.70 (s, 3H); ¹³C NMR (100 MHz, CDCl₃) δ 159.3, 159.0, 142.1, 139.4, 139.1, 139.0, 138.8, 138.6, 138.5, 137.5, 137.3, 135.3, 134.1, 134.0, 133.9, 133.8, 133.7, 133.5, 133.1, 132.9, 132.7, 131.5, 129.8, 129.5, 129.4, 129.1, 128.1, 128.0, 127.9, 127.8, 127.6, 127.4, 126.5, 126.4, 125.4, 121.5, 120.9, 119.0, 114.0, 113.7, 113.0, 110.3, 105.7, 105.6, 74.7, 55.3; ³¹P NMR (162 MHz, CDCl₃) δ -12.2; IR (KBr): 3051, 2833, 2360, 1606, 1509, 1246, 1070, 747, 532 cm⁻¹; ESI FTMS exact mass calcd for (C₅₄H₄₂NO₃P+Na)⁺ requires m/z 806.2795, found m/z 806.2754; The enantiomeric excess: 93%, determined by HPLC (Daicel Chiralpak AD-H, hexane/isopropanol = 90/10, flow rate 1.0 mL/min, T = 30 °C, 254 nm): t_R = 3.526 (major), t_R = 4.860 (minor).

Synthetic procedure and characterization data of compound **13**:



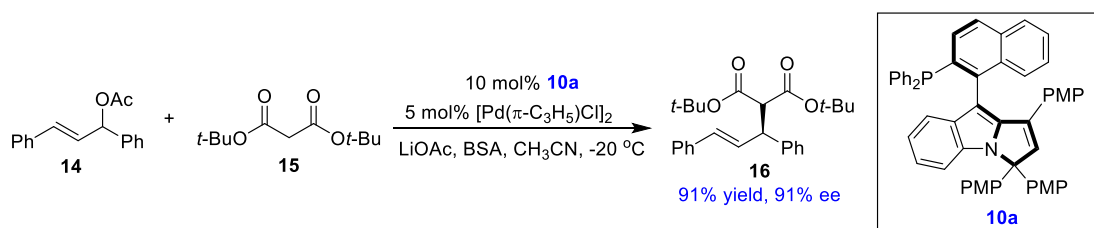
Under argon atmosphere, to the mixture of chiral phosphine ligand **10a** (15.7 mg, 0.02 mmol) and $[\text{Pd}(\pi\text{-C}_3\text{H}_5)\text{Cl}]_2$ (1.8 mg, 0.005 mmol) was added styrene **11** (103.2 mg, 1.0 mmol), and the reaction mixture was stirred at room temperature for 1 h. Then, trichlorosilane (0.20 mL, 2.0 mmol) was added to the reaction mixture, which was stirred at $0\text{ }^\circ\text{C}$ for 48 h. Then, the reaction mixture was subjected to distillation under reduced pressure to afford intermediate product **12** as colorless oil, which was directly subjected to the subsequent reaction. Namely, to the mixture of intermediate product **12**, KF (6.0 mmol), KHCO_3 (9.0 mmol) in THF (5 mL)/MeOH (5 mL) was added hydrogen peroxide (30 wt.%, 12.0 mmol) at room temperature. Then, the reaction mixture was stirred at room temperature for 16 h. After the completion of the reaction which was indicated by TLC, saturated $\text{Na}_2\text{S}_2\text{O}_3$ aqueous solution was added to the reaction mixture, which was extracted with ethyl acetate. The organic layer was washed with water and brine, dried over Na_2SO_4 and concentrated in vacuo to give a residue, which was further purified by preparative thin layer chromatography (PE:EA = 5:1) to afford pure product **13**.

(S)-1-phenylethanol (**13**)⁸:

56% yield (68.3 mg); colorless oil; $[\alpha]_{\text{D}}^{20} = -36.2$ ($c = 0.78$, CHCl_3); ^1H NMR (400 MHz, CDCl_3) δ 7.42 – 7.33 (m, 4H), 7.32 – 7.27 (m, 1H), 4.92 – 4.83 (m, 1H), 2.14 (s, 1H), 1.49 (d, $J = 6.4$ Hz, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 145.9, 128.5, 127.5, 125.5, 70.4, 25.2; IR (KBr): 3366, 3063, 2973, 1452, 1204, 1099, 1029, 761, 700, 541 cm^{-1} ; The enantiomeric excess: 85%, determined by HPLC (Daicel Chiralpak AD-H, hexane/isopropanol = 95/5, flow rate 0.6 mL/min, $T = 30\text{ }^\circ\text{C}$, 254 nm): $t_{\text{R}} = 14.787$ (minor), $t_{\text{R}} = 17.227$ (major).

⁸ P. Du, Y.-L. Liu, X.-B. Lu, *Tetrahedron Lett.* **2020**, *61*, 152386.

Synthetic procedure and characterization data of compound **16**:



Under argon atmosphere, to the mixture of chiral phosphine ligand **10a** (0.01 mmol, 7.8 mg), $[\text{Pd}(\pi\text{-C}_3\text{H}_5)\text{Cl}]_2$ (0.005 mmol, 1.8 mg) and LiOAc (0.02 mmol, 1.3 mg) in acetonitrile (1.5 mL) were added *N,O*-bis(trimethylsilyl)acetamide (BSA, 0.3 mmol, 61.0 mg) and allylic ester **14** (0.1 mmol, 25.2 mg), which was stirred at room temperature for 30 min. Then, malonate **15** (0.3 mmol, 64.8 mg) was added and the reaction mixture was stirred at $-20\text{ }^\circ\text{C}$ for 24 h. After the completion of the reaction which was indicated by TLC, the reaction mixture was quenched with water, diluted and extracted with ethyl acetate. The organic layer was washed with brine, dried over Na_2SO_4 , and concentrated in vacuo to give a residue, which was further purified by column chromatography to afford product **16**.

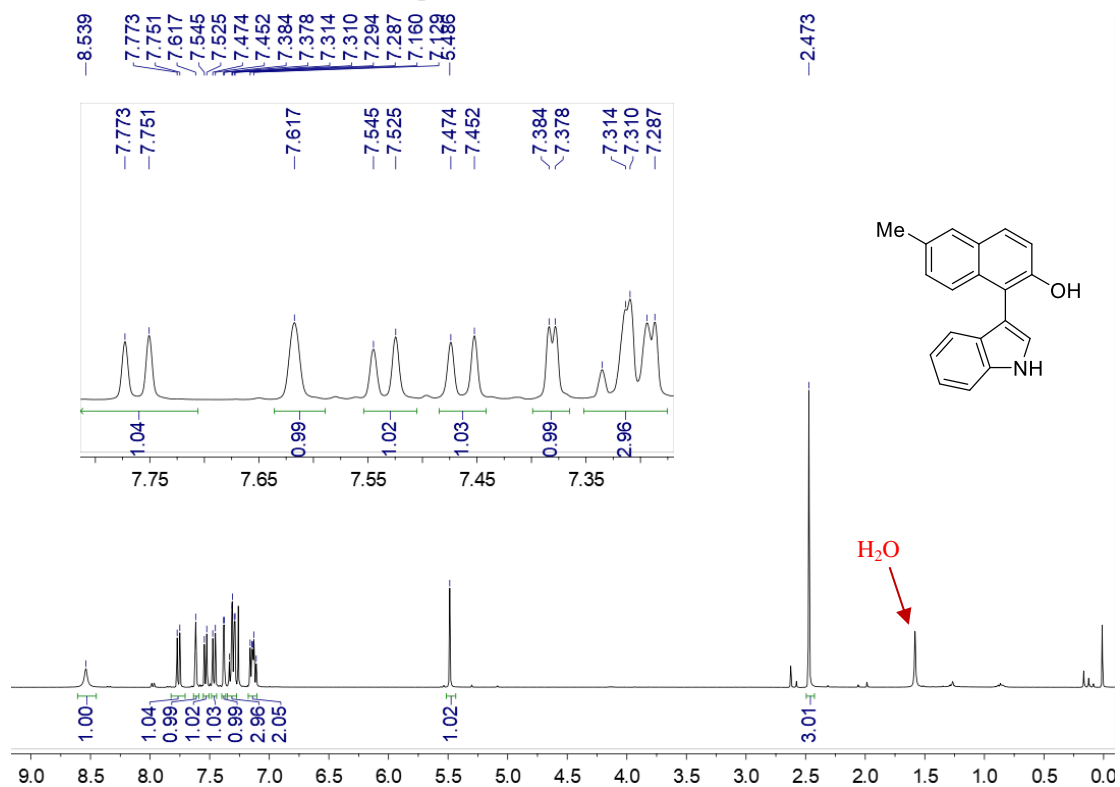
(*S*)-di-*tert*-butyl -2-(1,3-diphenylallyl)malonate (**16**)⁹:

91% yield (37.1 mg); colorless oil; $[\alpha]_{\text{D}}^{20} = -14.8$ ($c = 0.24$, CHCl_3); ^1H NMR (400 MHz, CDCl_3) δ 7.34 – 7.27 (m, 7H), 7.25 – 7.15 (m, 3H), 6.49 – 6.41 (m, 1H), 6.37 – 6.29 (m, 1H), 4.19 – 4.12 (m, 1H), 3.74 (d, $J = 10.8$ Hz, 1H), 1.42 (s, 9H), 1.22 (s, 9H); ^{13}C NMR (100 MHz, CDCl_3) δ 167.3, 166.8, 140.8, 137.1, 131.3, 130.2, 128.5, 128.2, 127.4, 126.9, 126.3, 81.8, 81.6, 59.4, 49.1, 28.0, 27.6; IR (KBr): 3061, 2979, 2360, 1730, 1478, 1369, 1246, 1141, 745, 698. 531 cm^{-1} ; ESI FTMS exact mass calcd for $(\text{C}_{26}\text{H}_{32}\text{O}_4 + \text{Na})^+$ requires m/z 431.2193, found m/z 431.2182; The enantiomeric excess: 91%, determined by HPLC (Daicel Chiralpak IA, hexane/isopropanol = 90/10, flow rate 1.0 mL/min, $T = 30\text{ }^\circ\text{C}$, 254 nm): $t_{\text{R}} = 5.667$ (minor), $t_{\text{R}} = 7.163$ (major).

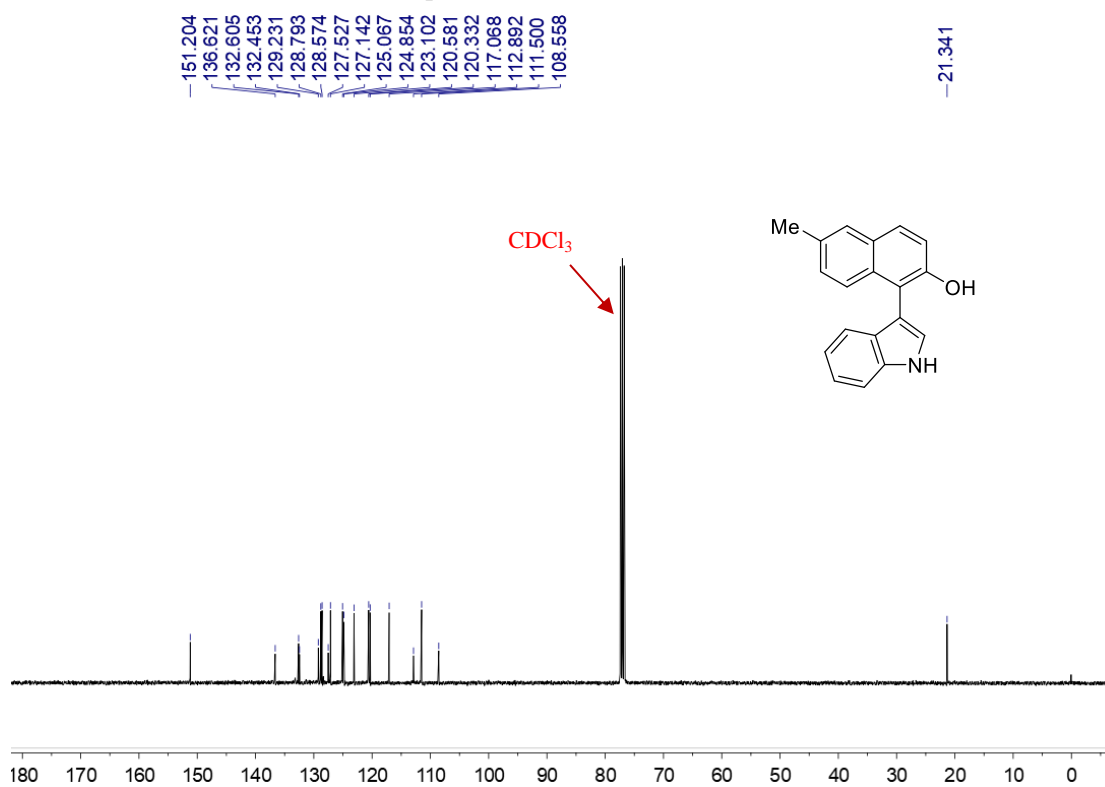
⁹ Y. Tanaka, T. Mino, K. Akita, M. Sakamoto, T. Fujita, *J. Org. Chem.* **2004**, *69*, 6679.

7. NMR spectra of substrates **1k**, **2** and **6** as new compounds

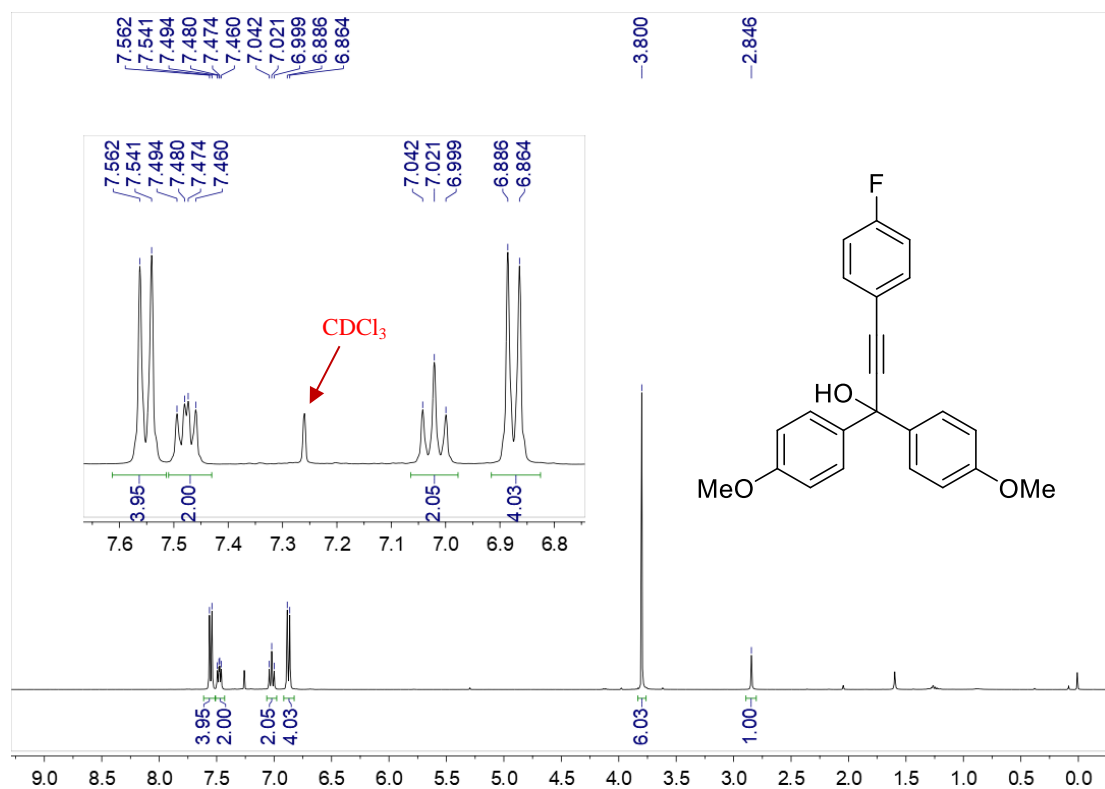
^1H NMR (400 MHz, CDCl_3) of compound **1k**:



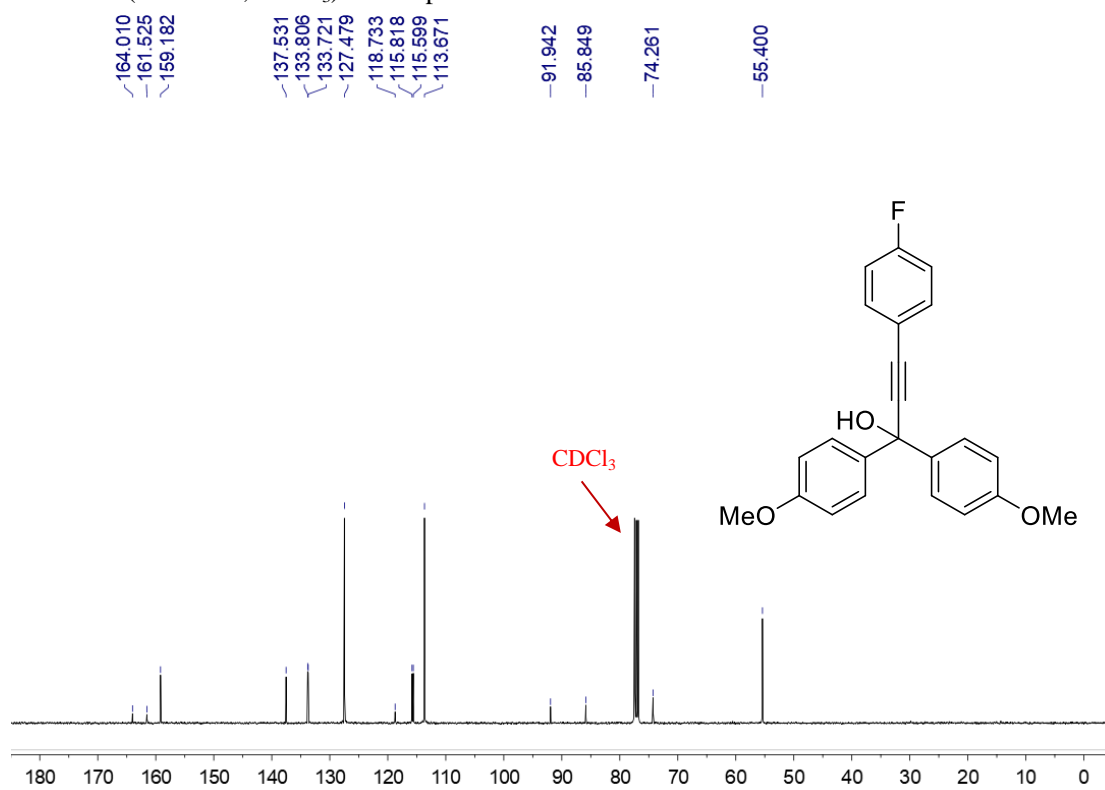
^{13}C NMR (100 MHz, CDCl_3) of compound **1k**:



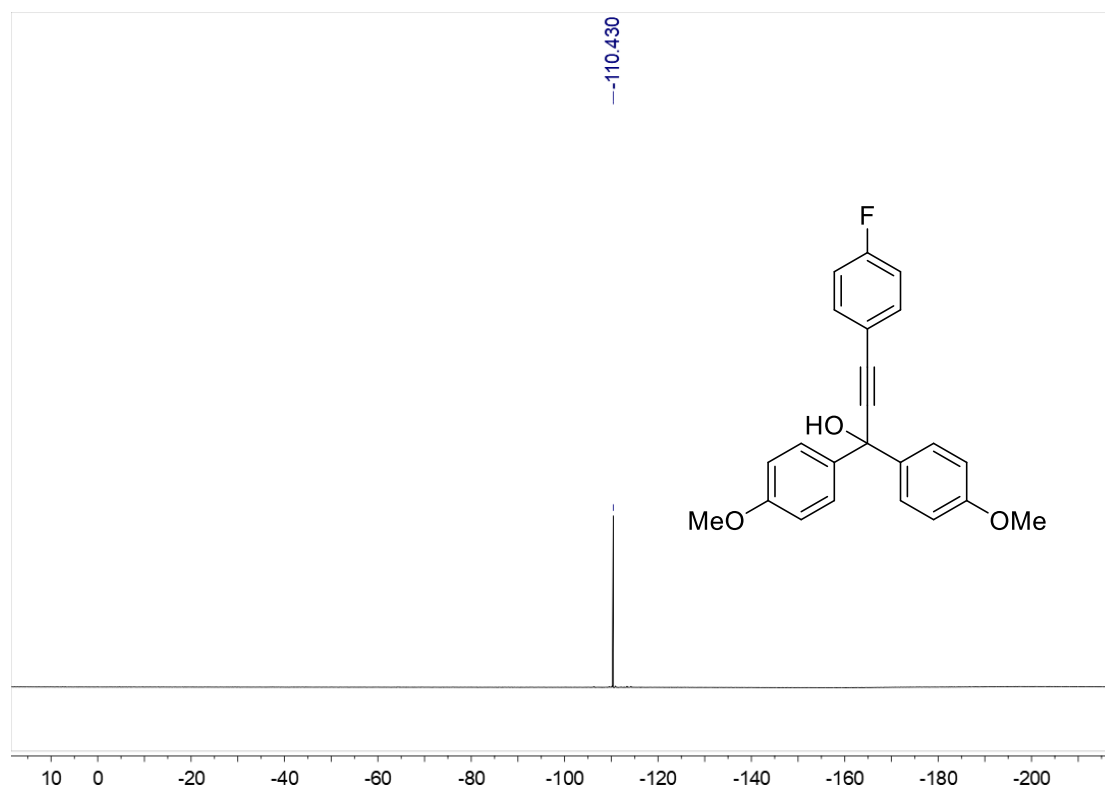
^1H NMR (400 MHz, CDCl_3) of compound **2d**:



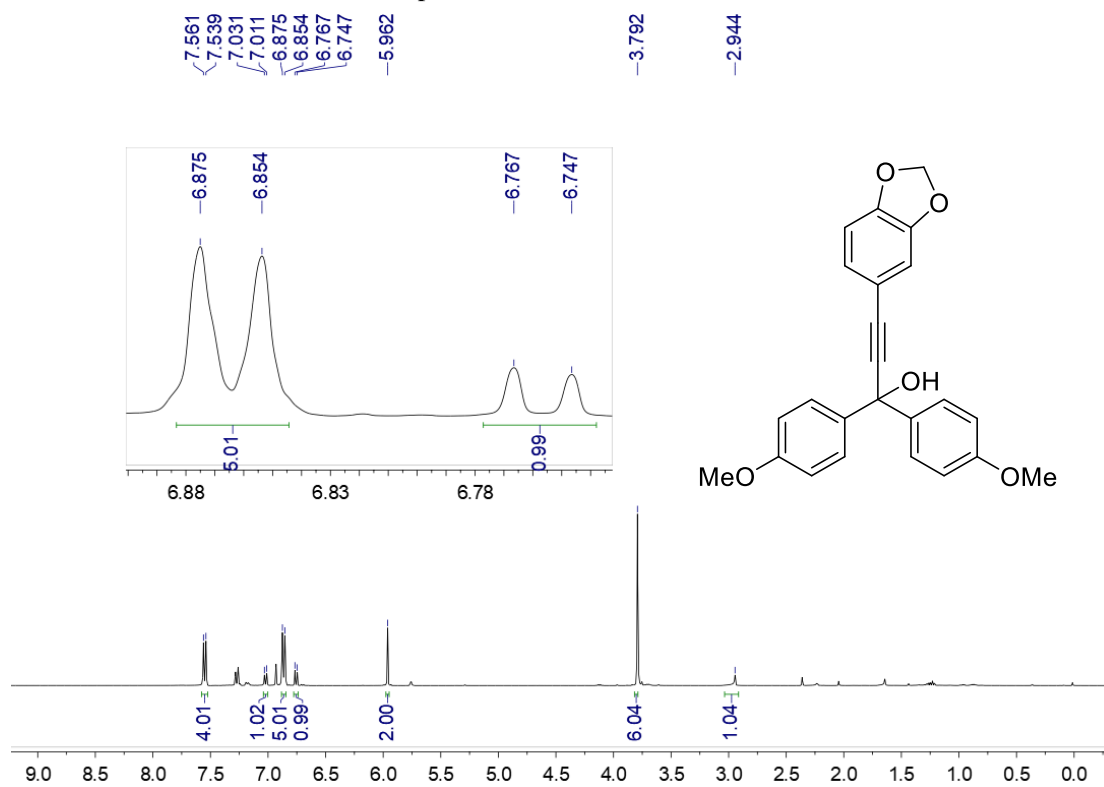
^{13}C NMR (100 MHz, CDCl_3) of compound **2d**:



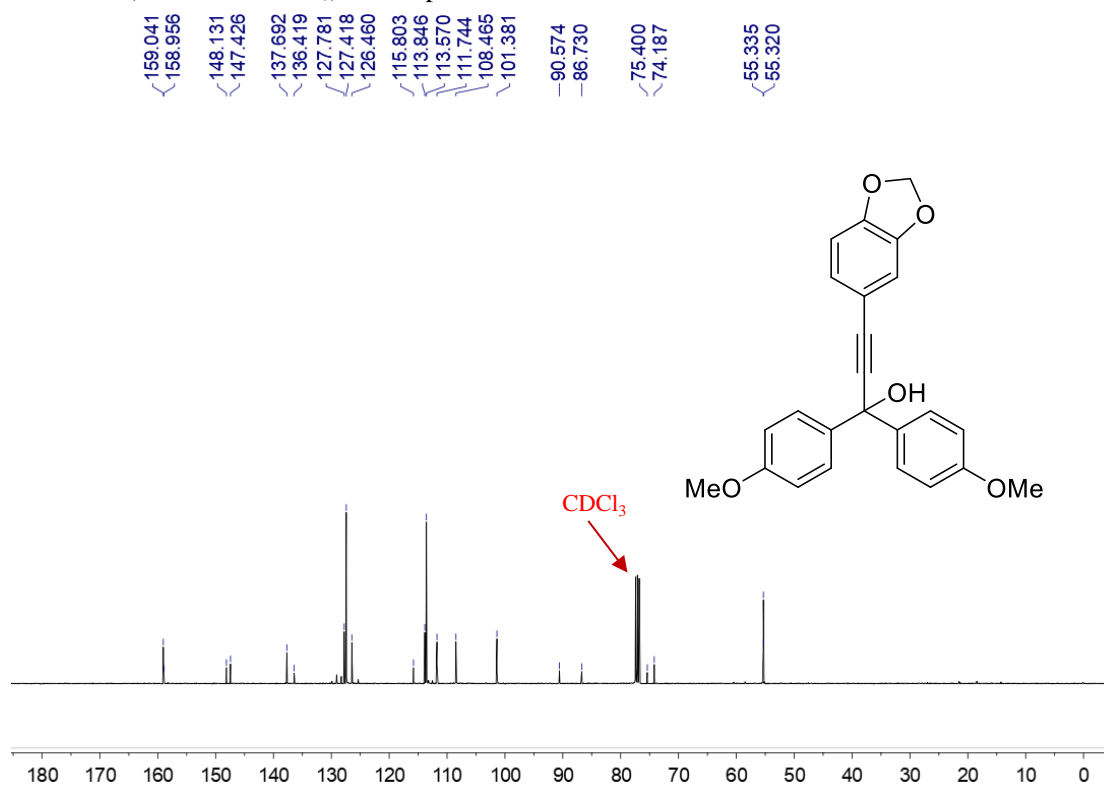
^{19}F NMR (376 MHz, CDCl_3) of compound **2d**:



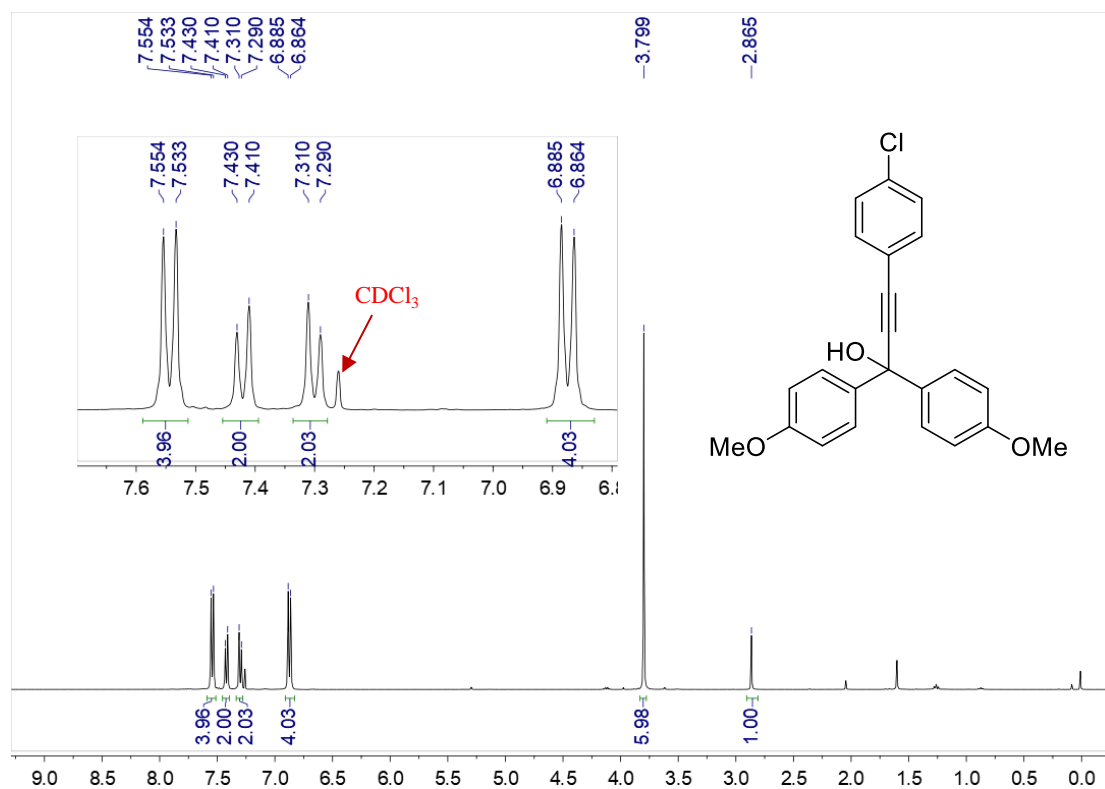
^1H NMR (400 MHz, CDCl_3) of compound **2e**:



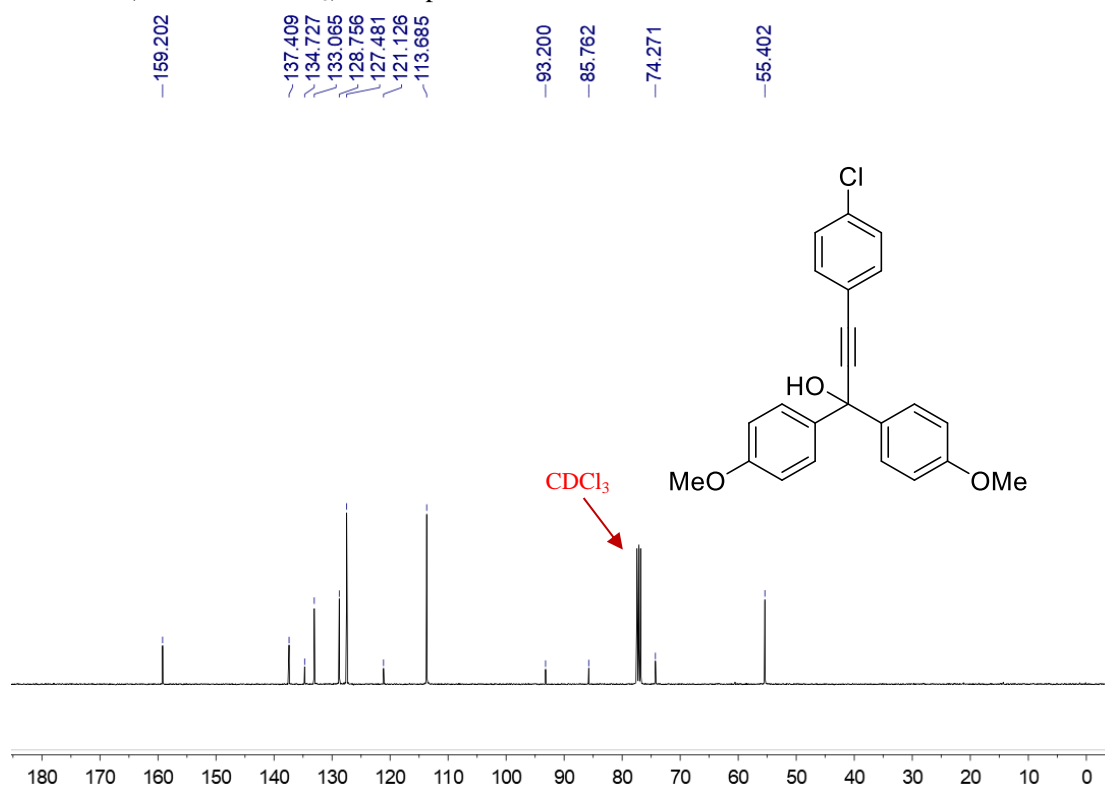
^{13}C NMR (100 MHz, CDCl_3) of compound **2e**:



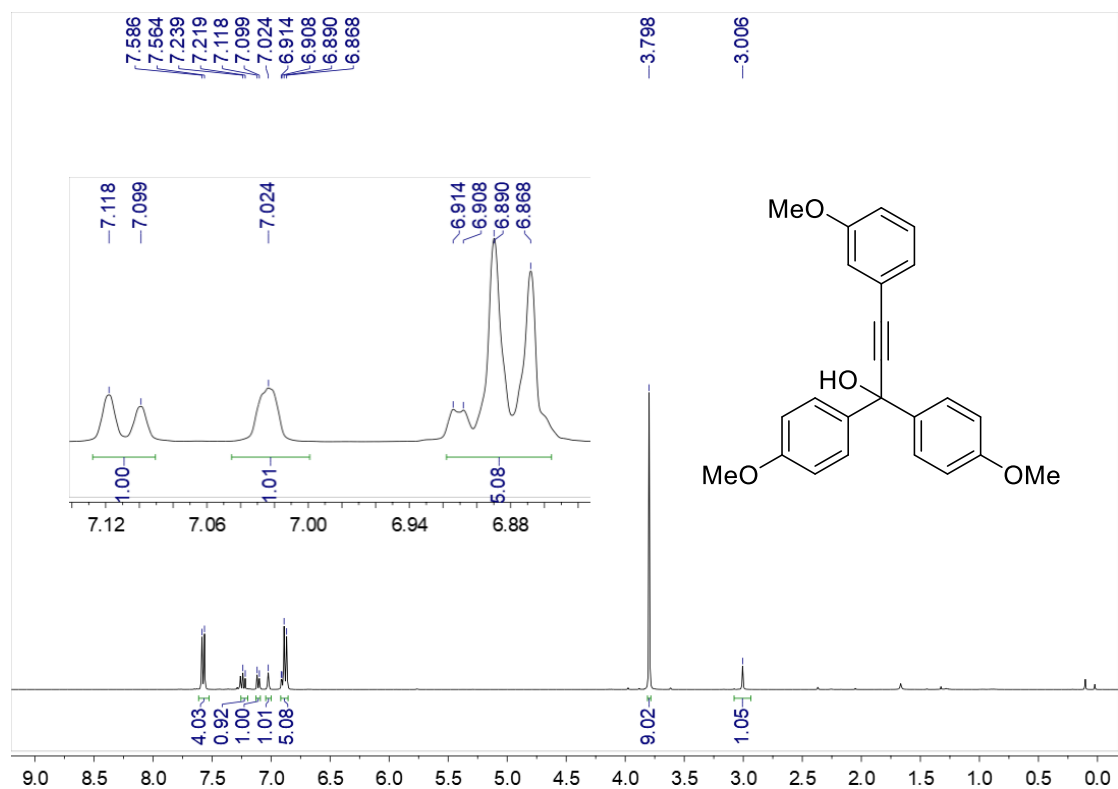
^1H NMR (400 MHz, CDCl_3) of compound **2f**:



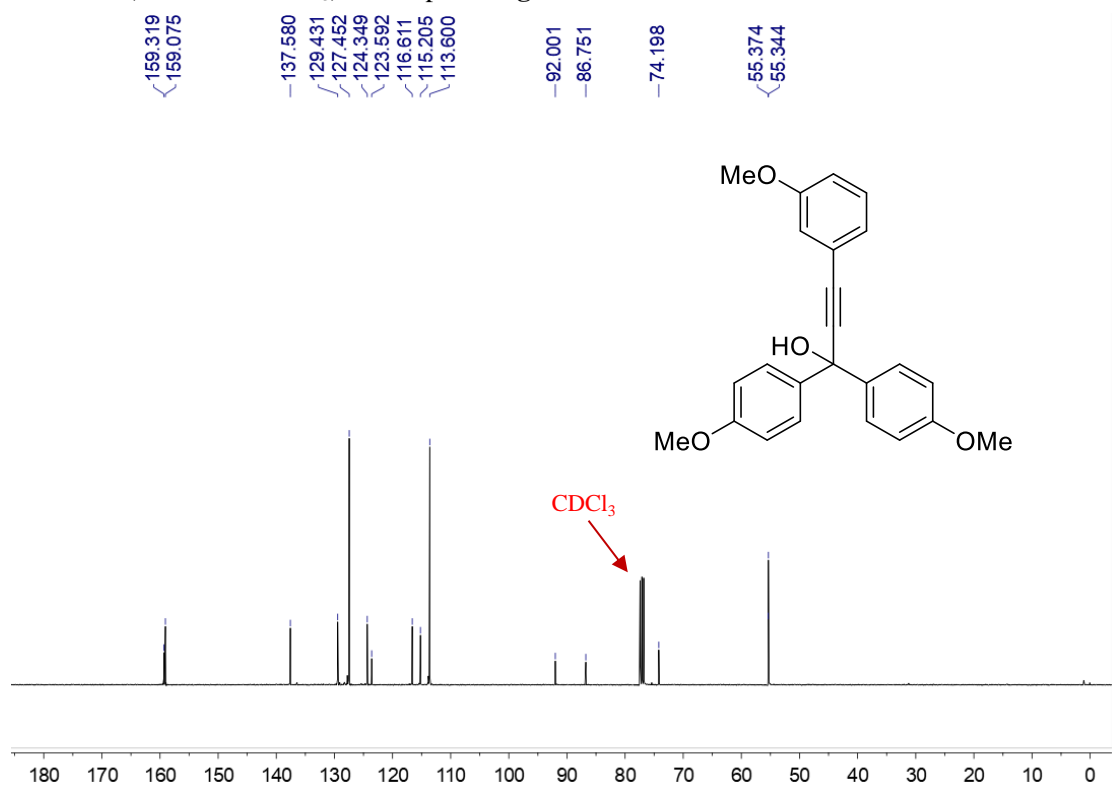
^{13}C NMR (100 MHz, CDCl_3) of compound **2f**:



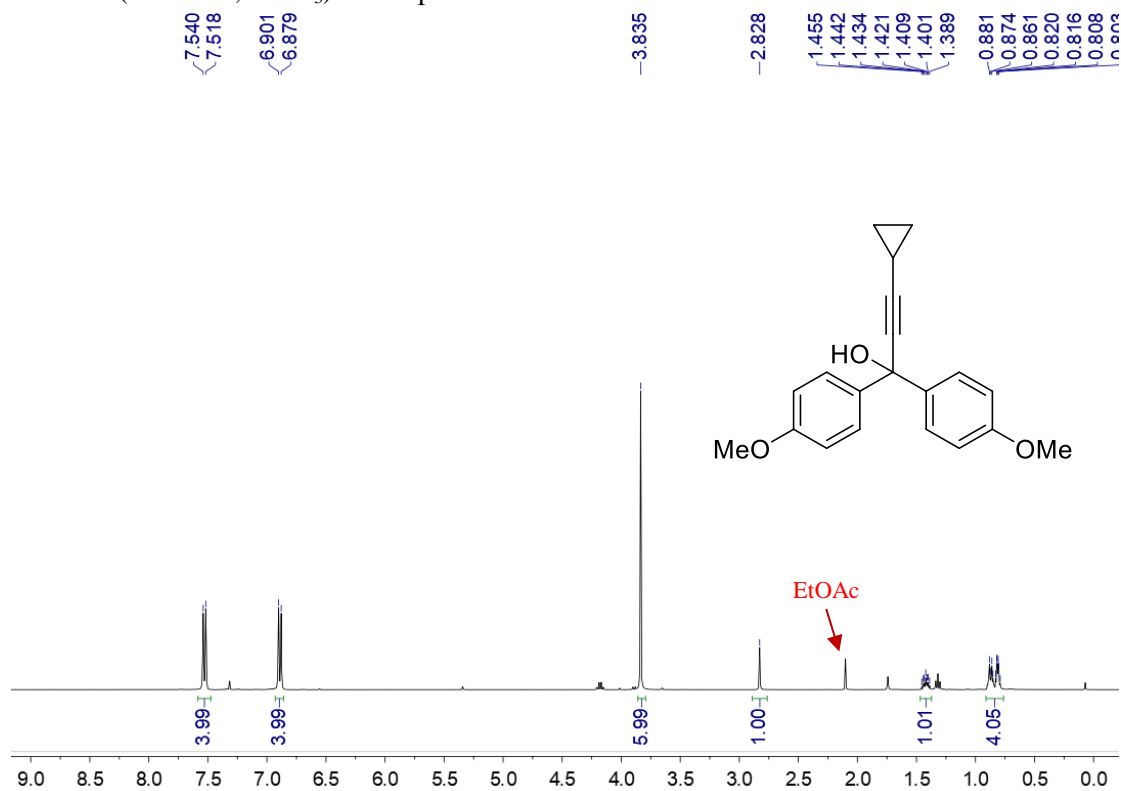
^1H NMR (400 MHz, CDCl_3) of compound **2g**:



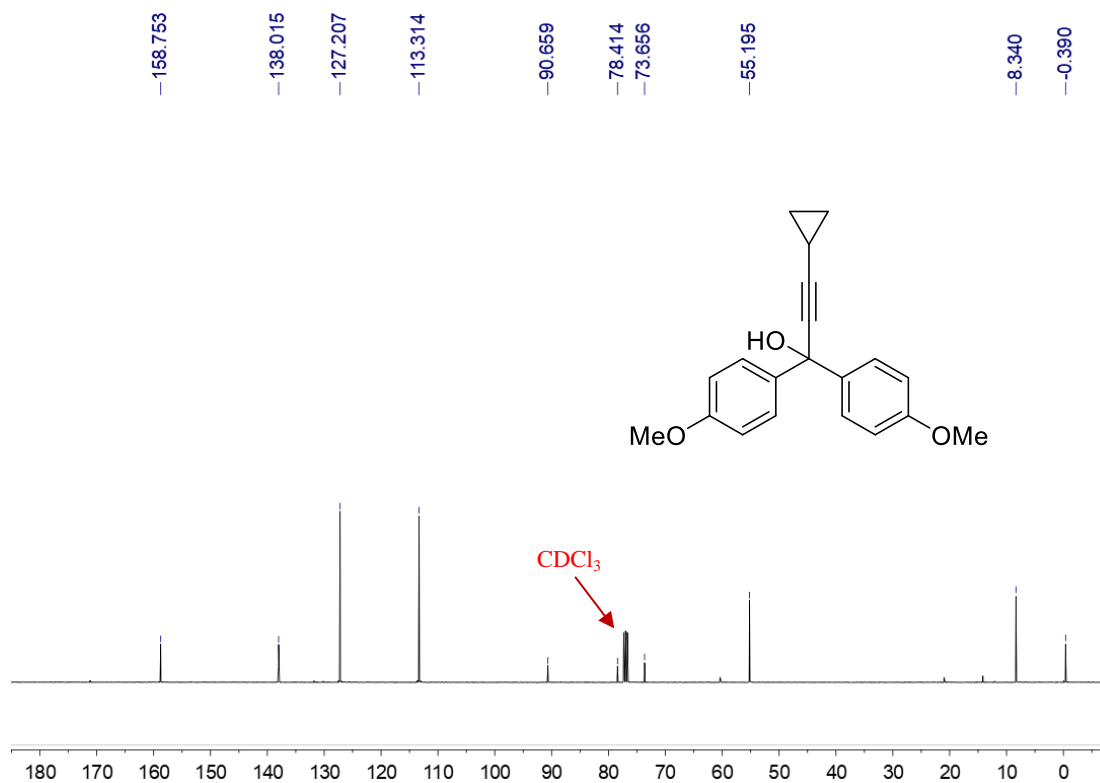
^{13}C NMR (100 MHz, CDCl_3) of compound **2g**:



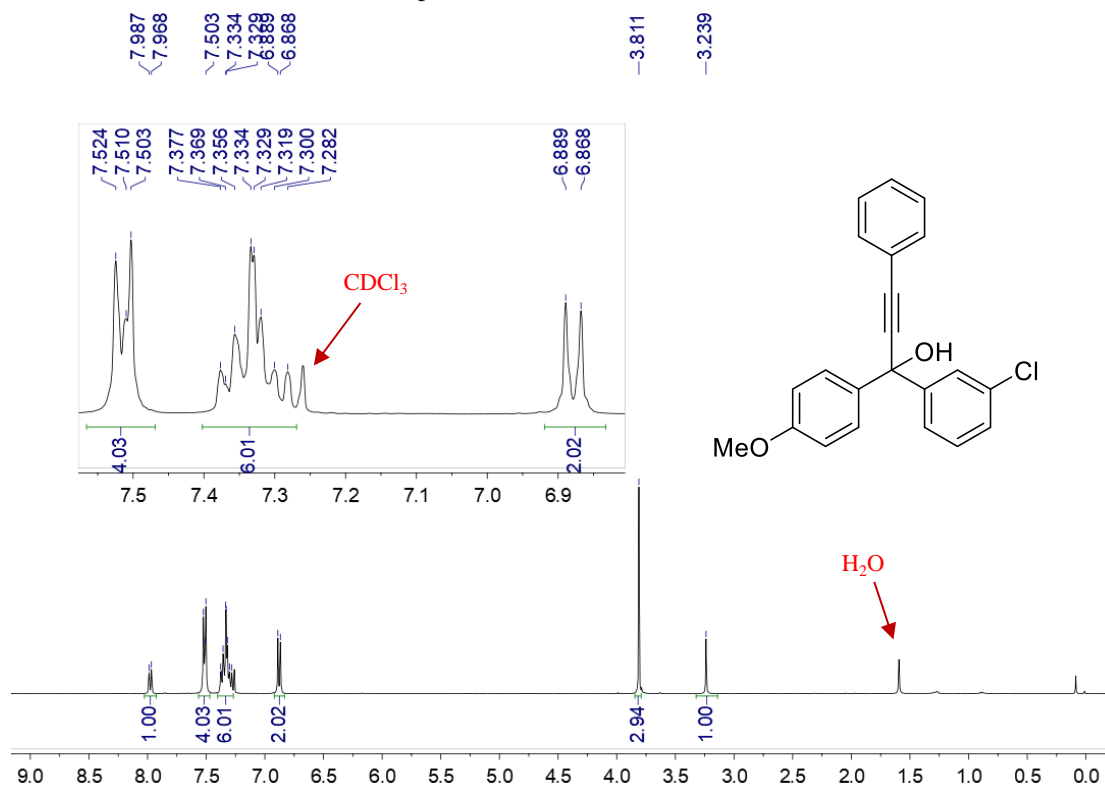
^1H NMR (400 MHz, CDCl_3) of compound **2i**:



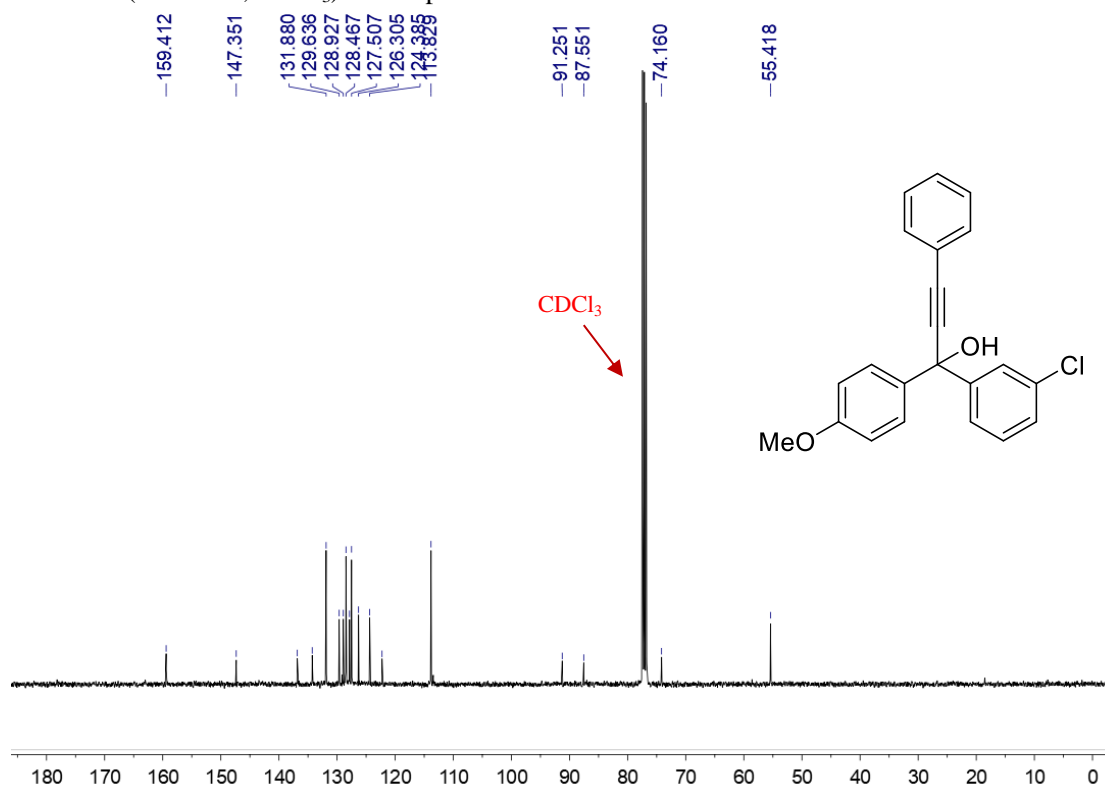
^{13}C NMR (100 MHz, CDCl_3) of compound **2i**:



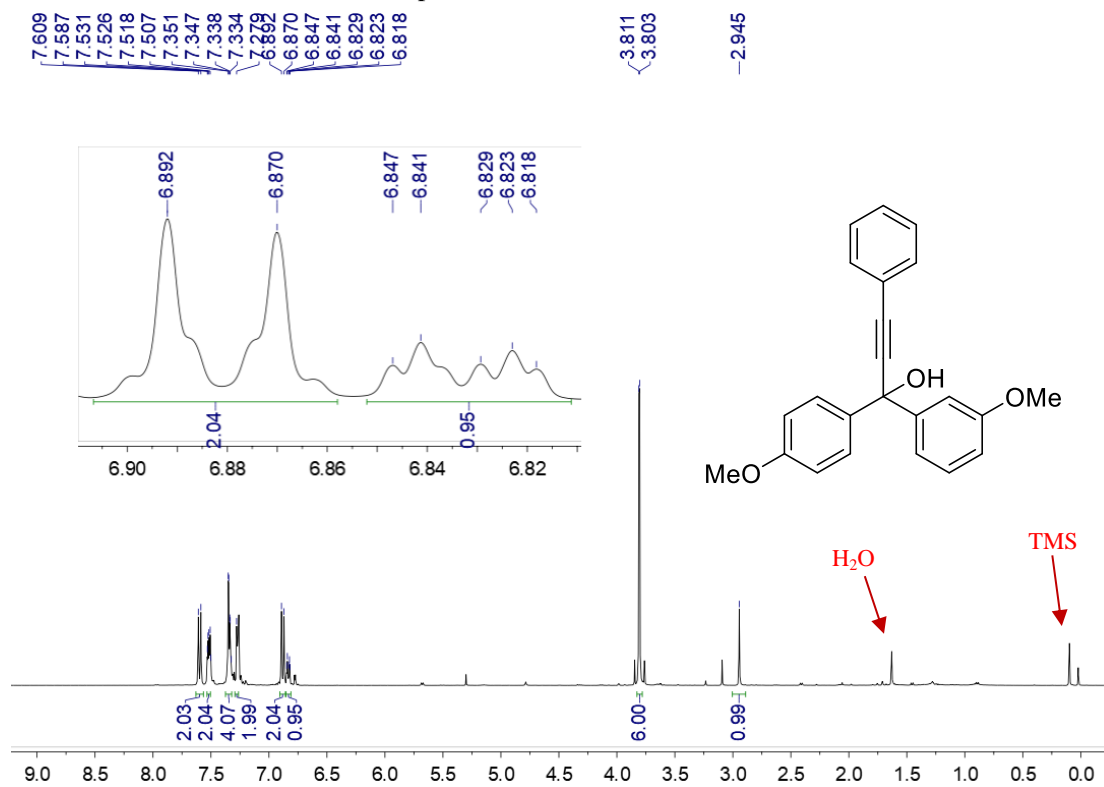
^1H NMR (400 MHz, CDCl_3) of compound **6c**:



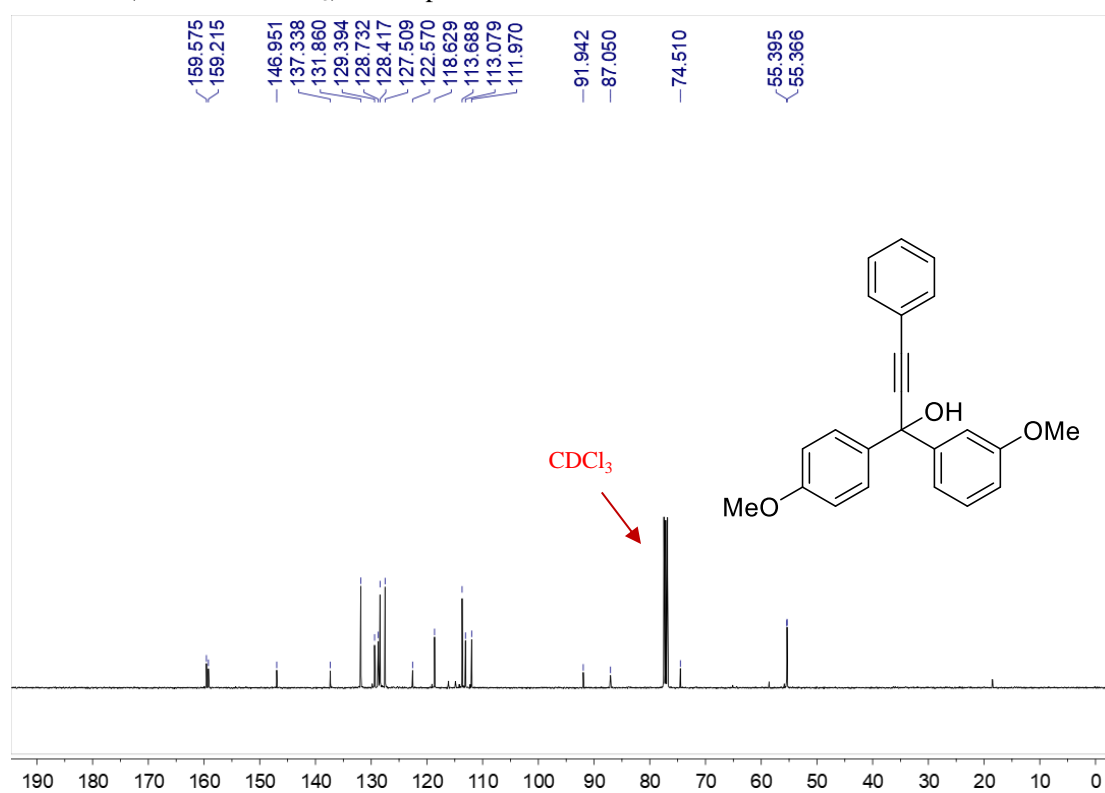
^{13}C NMR (100 MHz, CDCl_3) of compound **6c**:



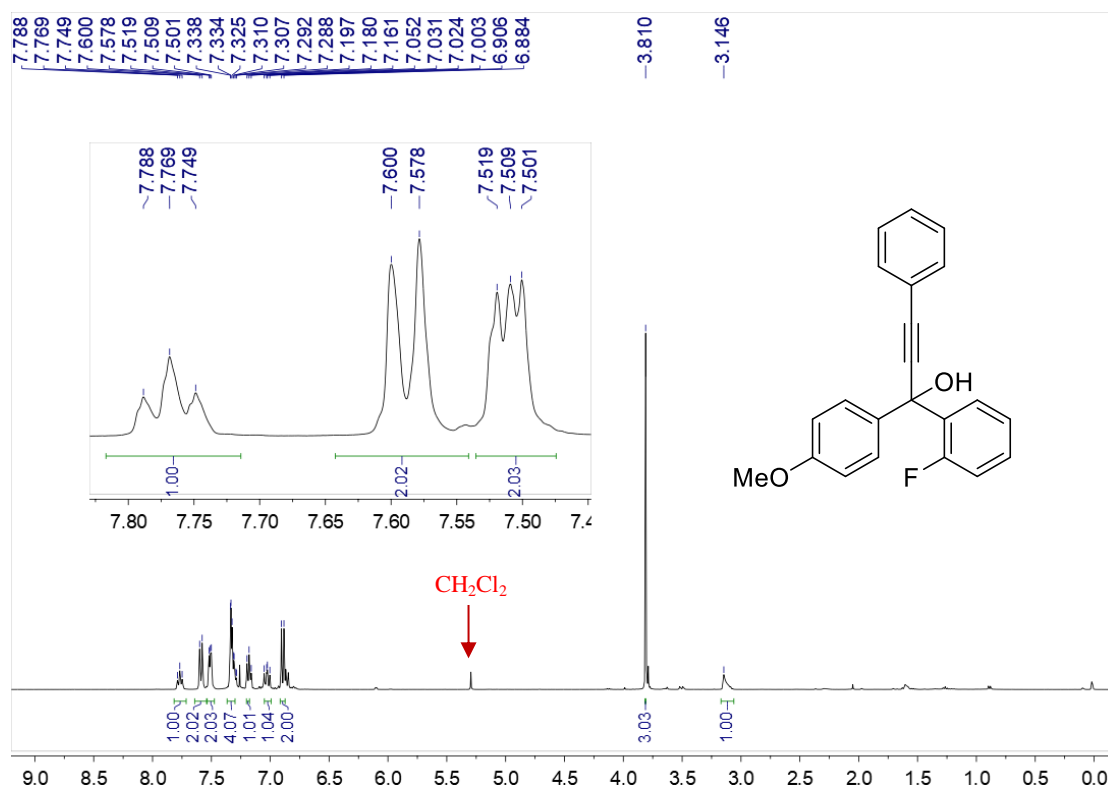
^1H NMR (400 MHz, CDCl_3) of compound **6d**:



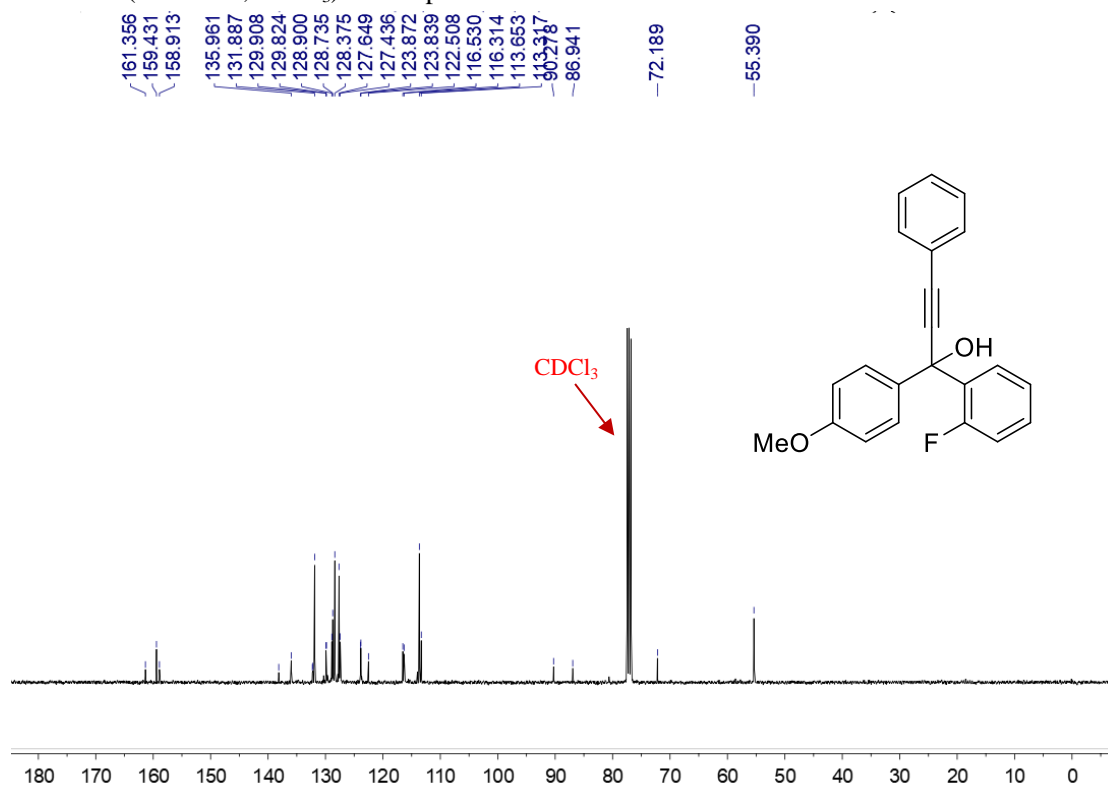
^{13}C NMR (100 MHz, CDCl_3) of compound **6d**:



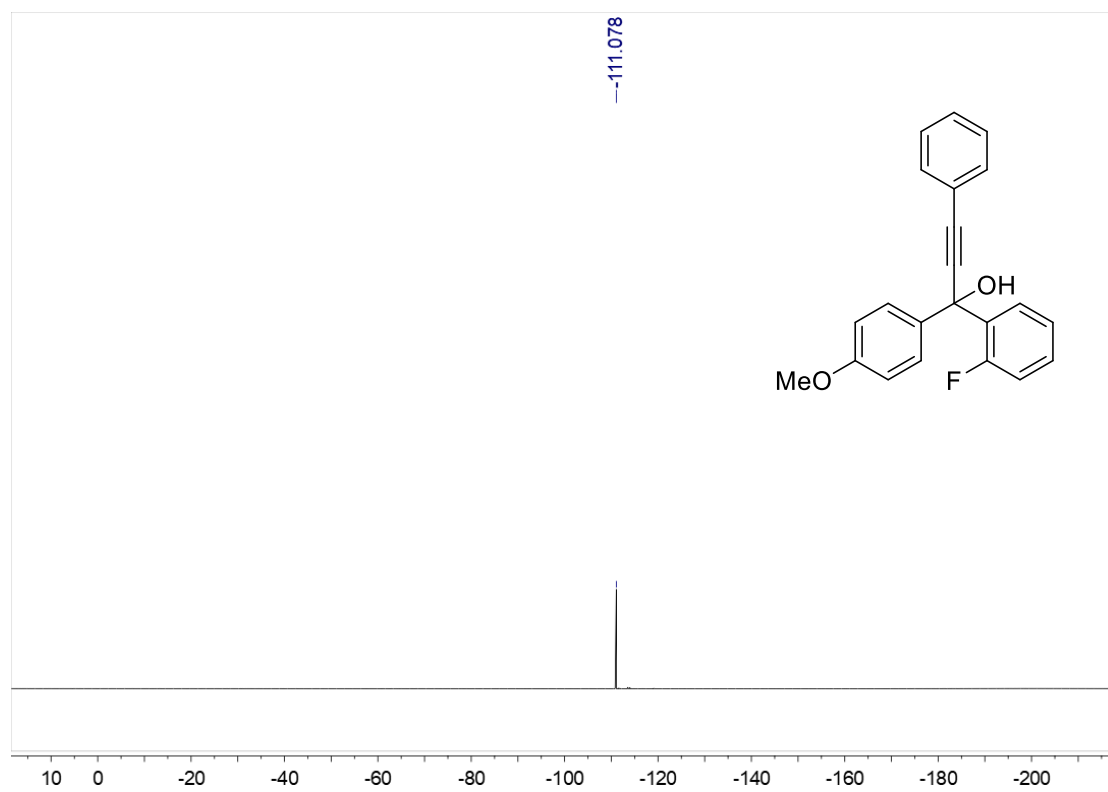
¹H NMR (400 MHz, CDCl₃) of compound **6e**:



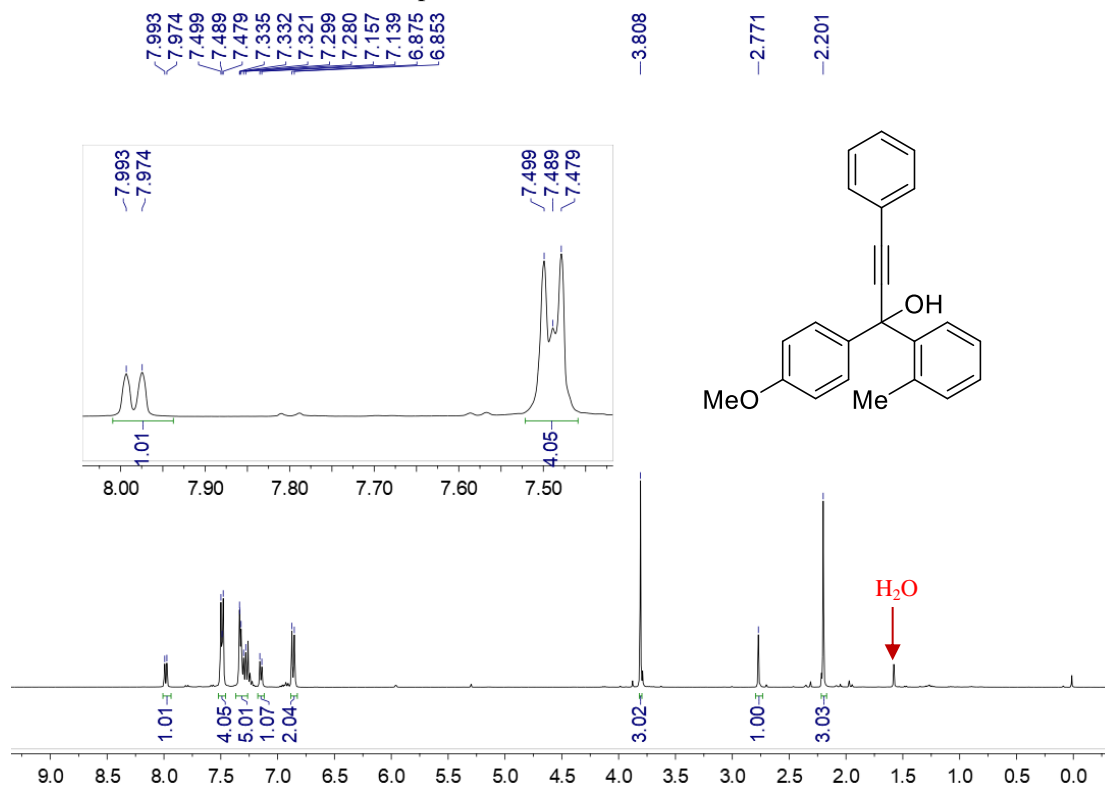
¹³C NMR (100 MHz, CDCl₃) of compound **6e**:



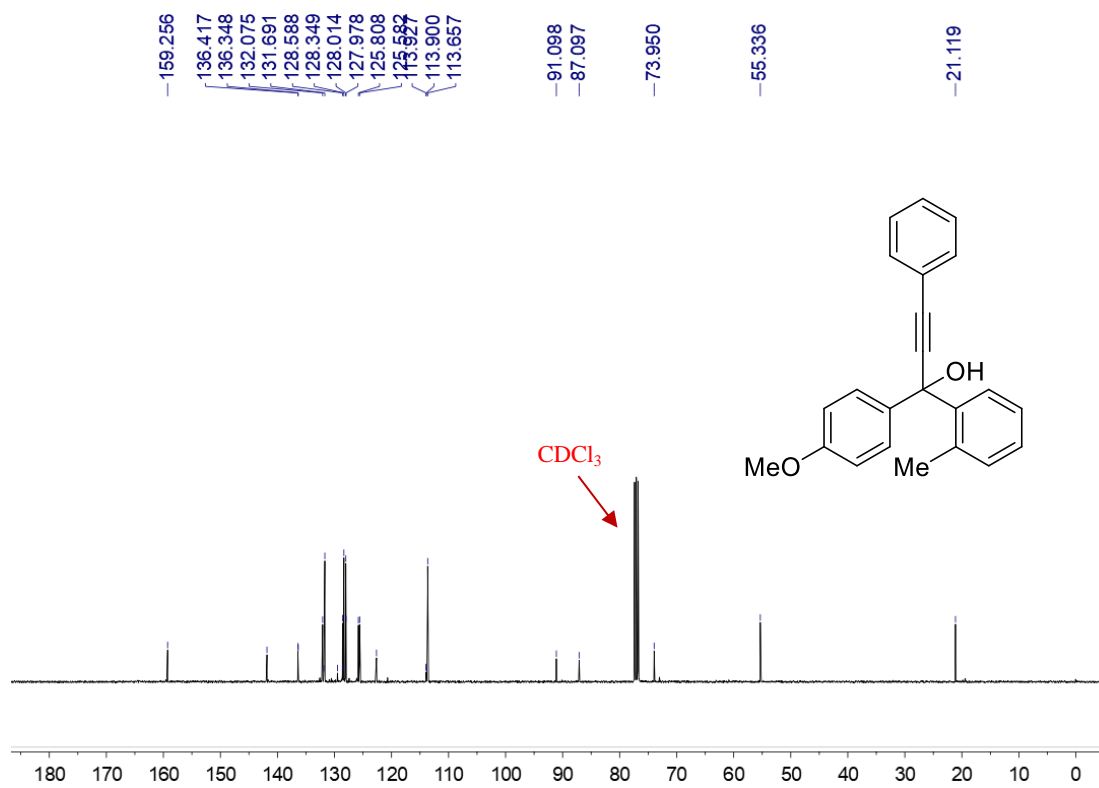
^{19}F NMR (376 MHz, CDCl_3) of compound **6e**:



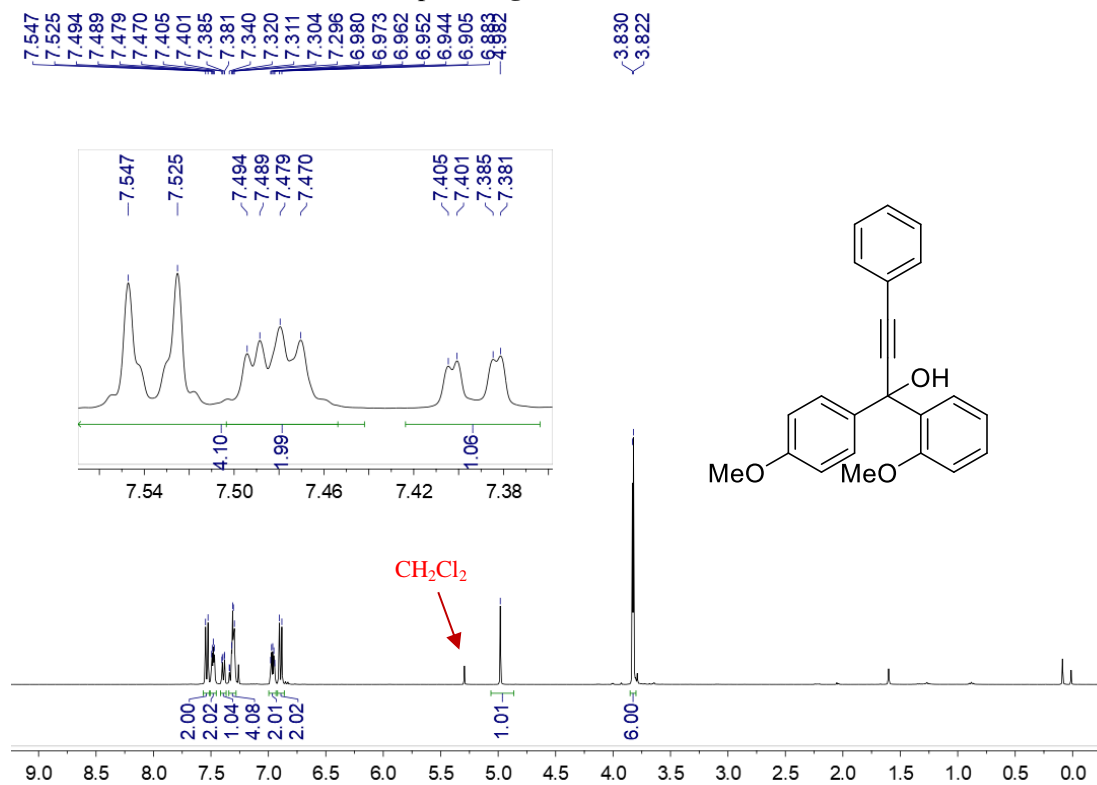
^1H NMR (400 MHz, CDCl_3) of compound **6f**:



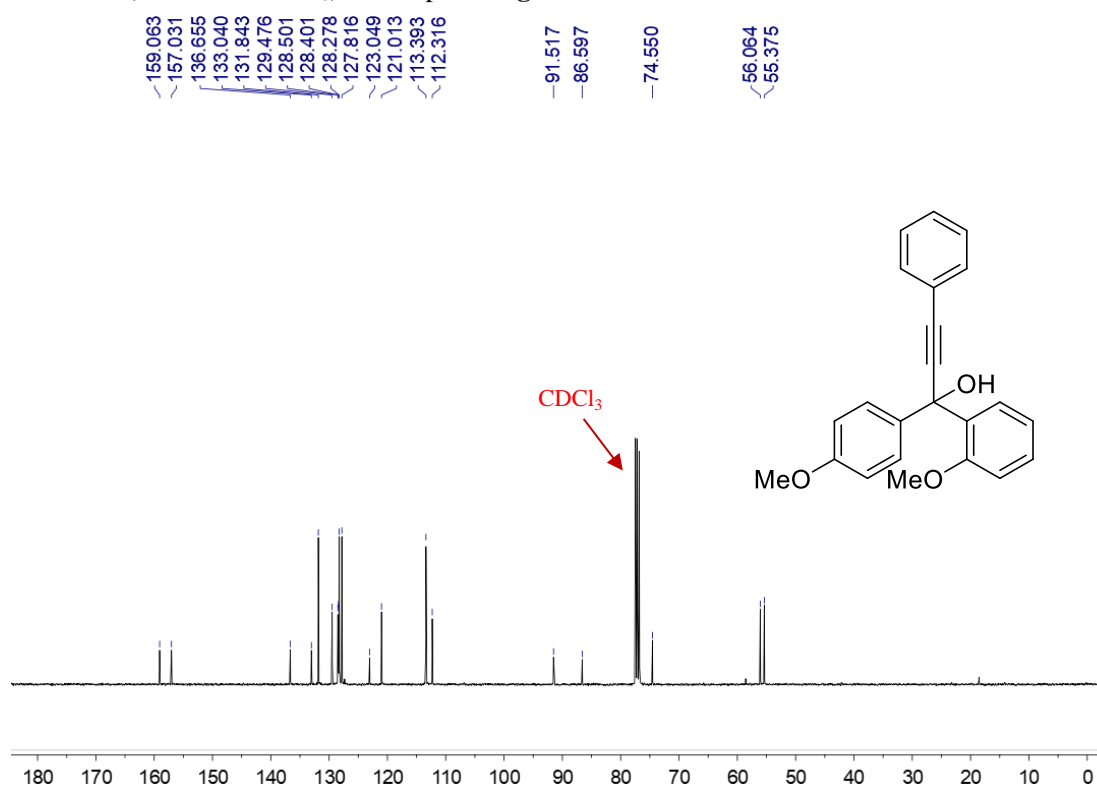
^{13}C NMR (100 MHz, CDCl_3) of compound **6f**:



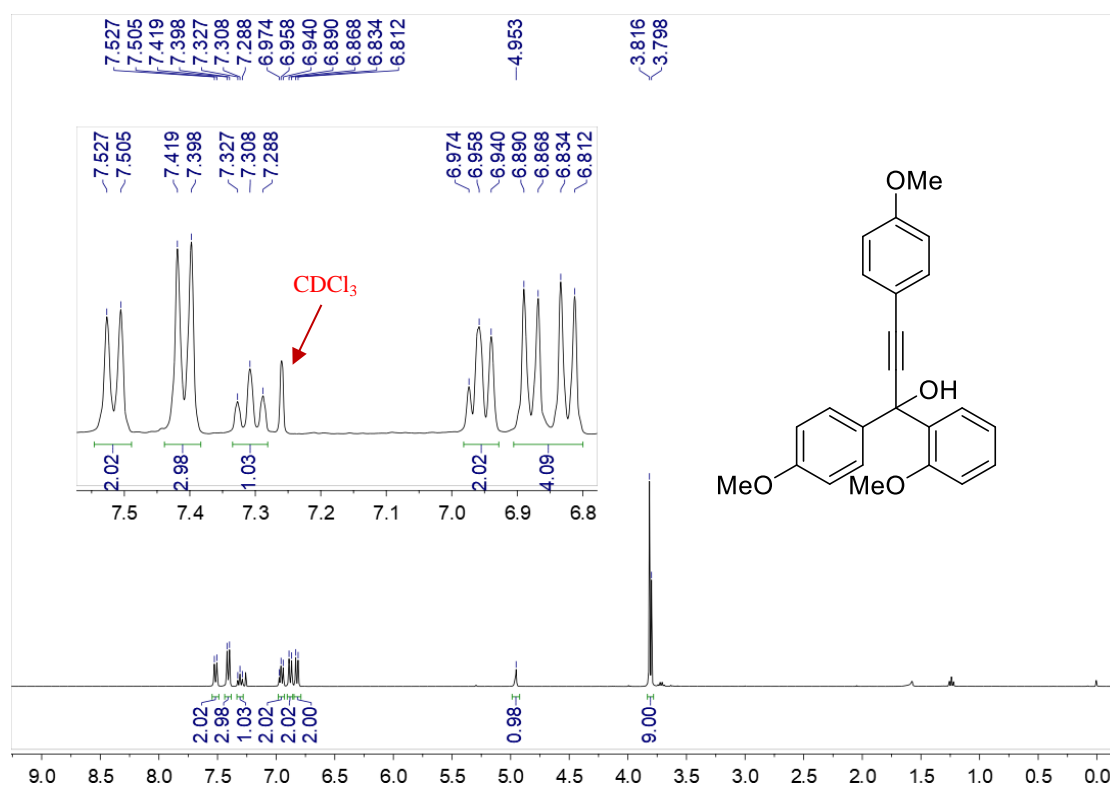
^1H NMR (400 MHz, CDCl_3) of compound **6g**:



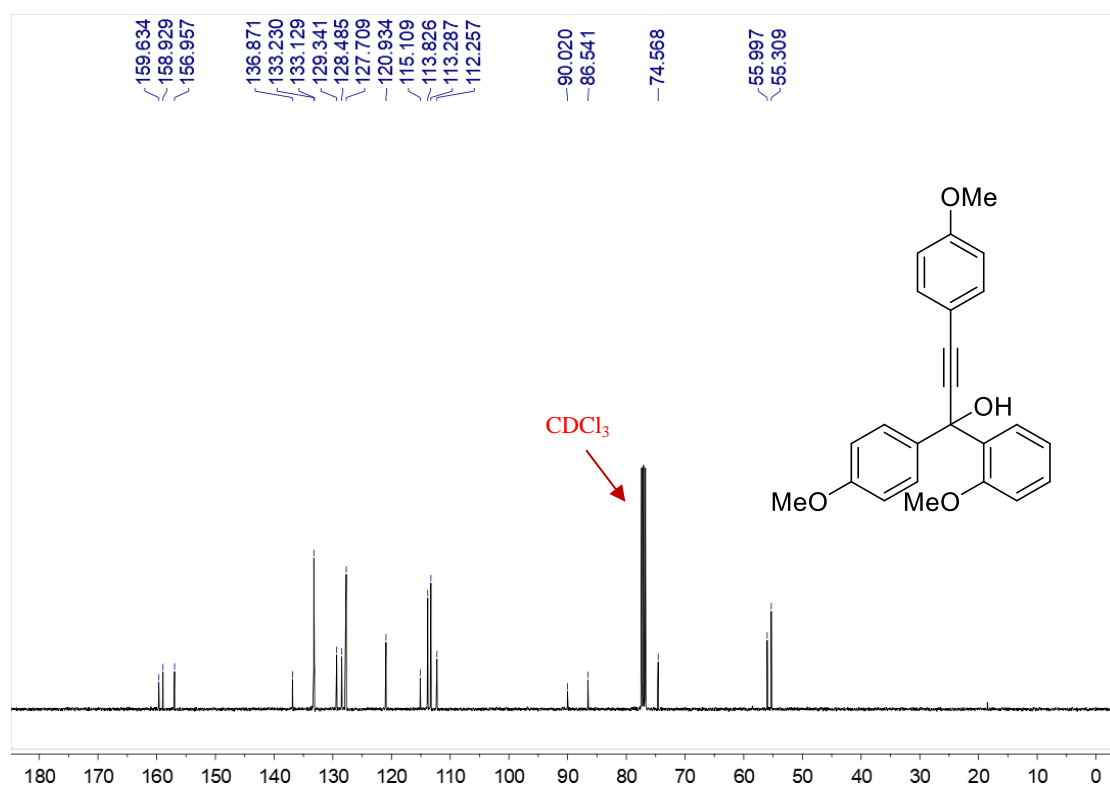
^{13}C NMR (100 MHz, CDCl_3) of compound **6g**:



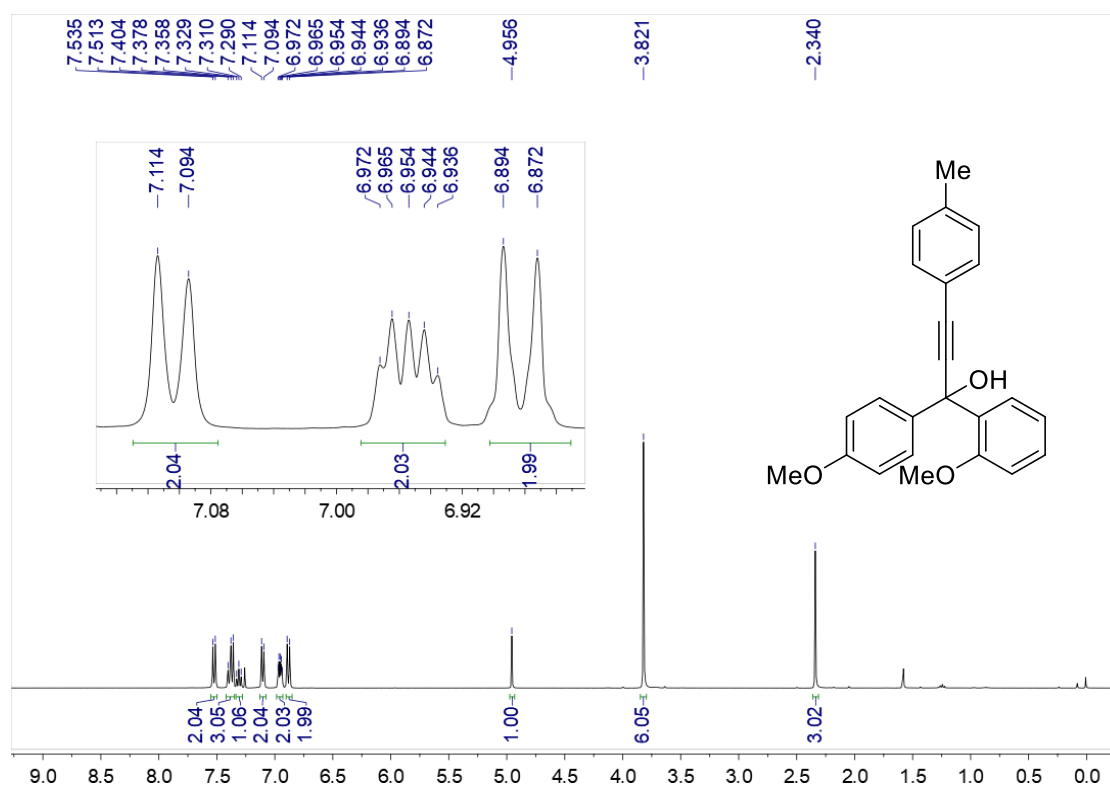
^1H NMR (400 MHz, CDCl_3) of compound **6h**:



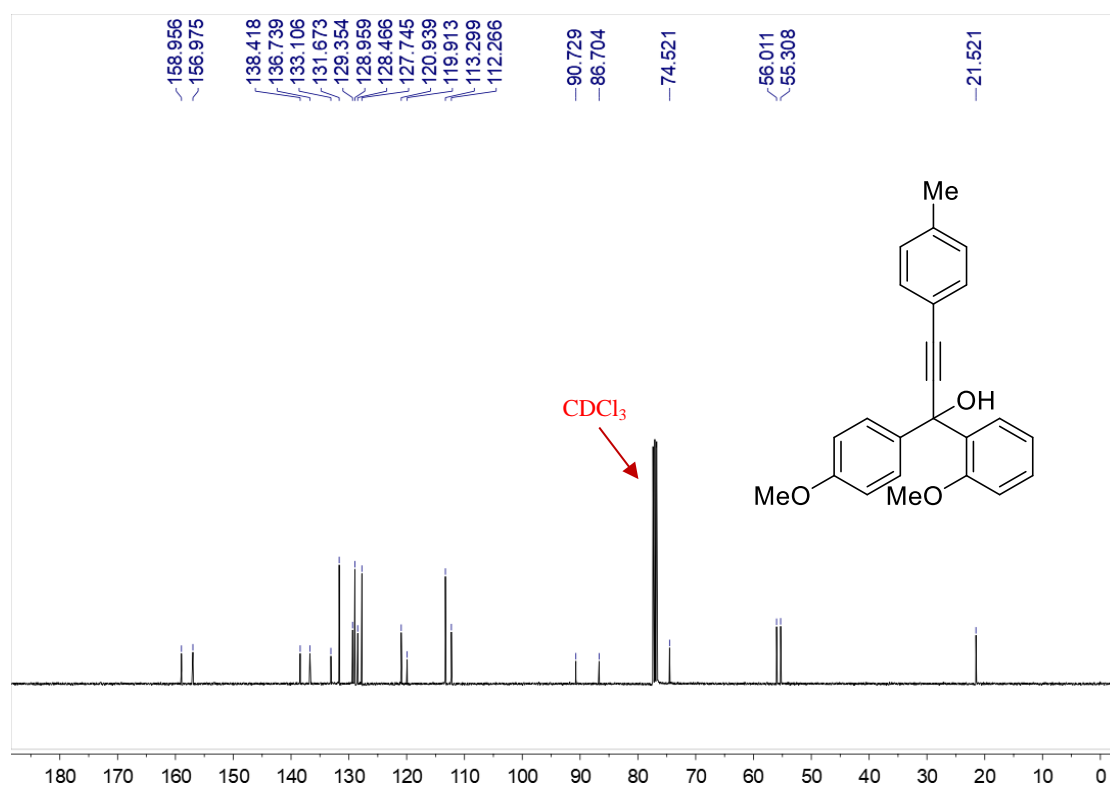
^{13}C NMR (100 MHz, CDCl_3) of compound **6h**:



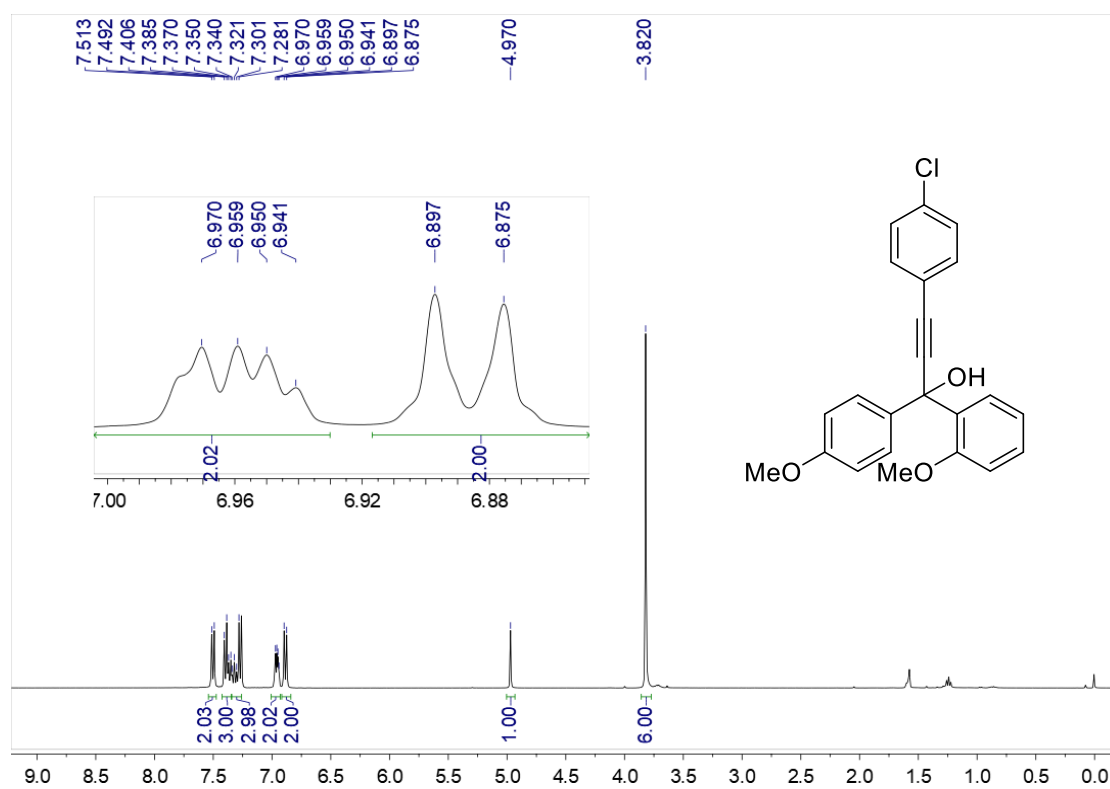
¹H NMR (400 MHz, CDCl₃) of compound **6i**:



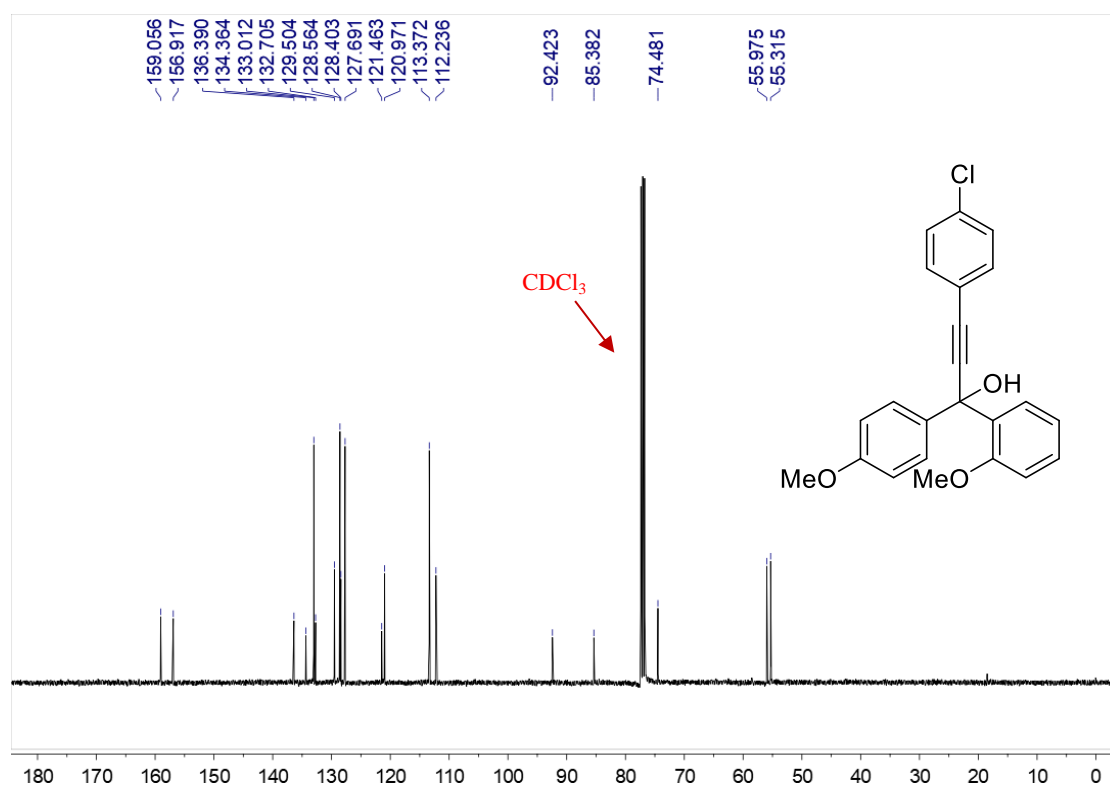
¹³C NMR (100 MHz, CDCl₃) of compound **6i**:



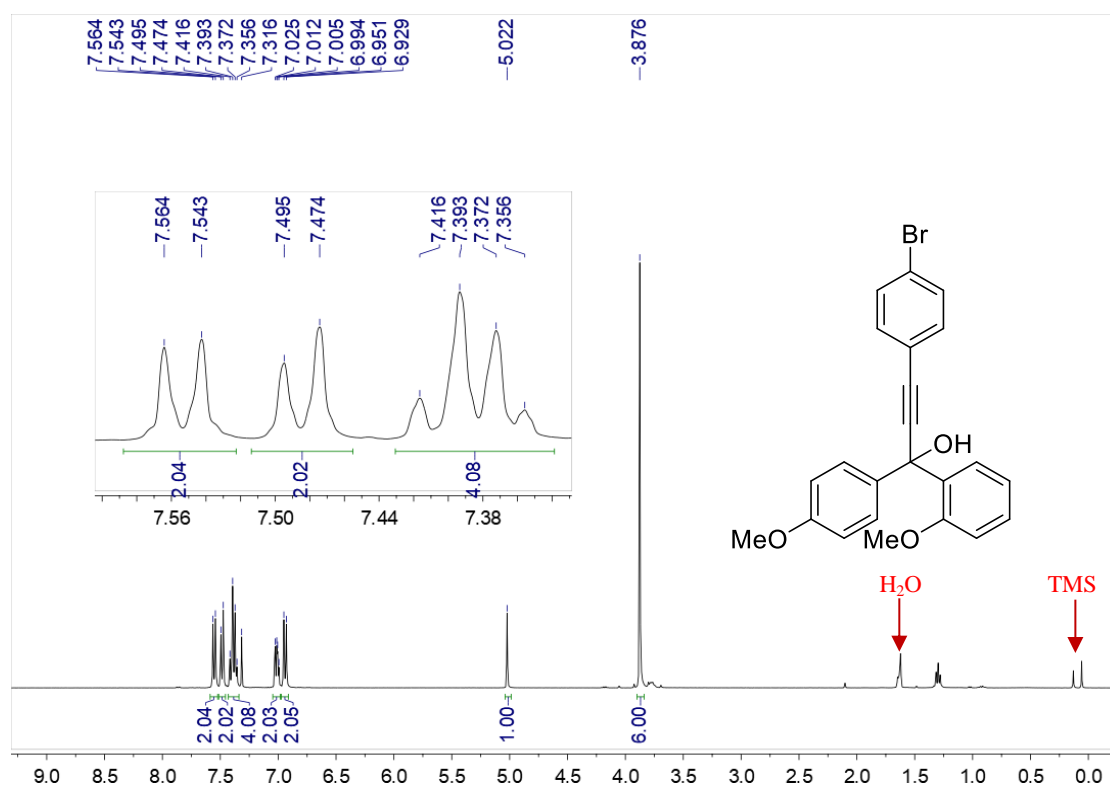
^1H NMR (400 MHz, CDCl_3) of compound **6j**:



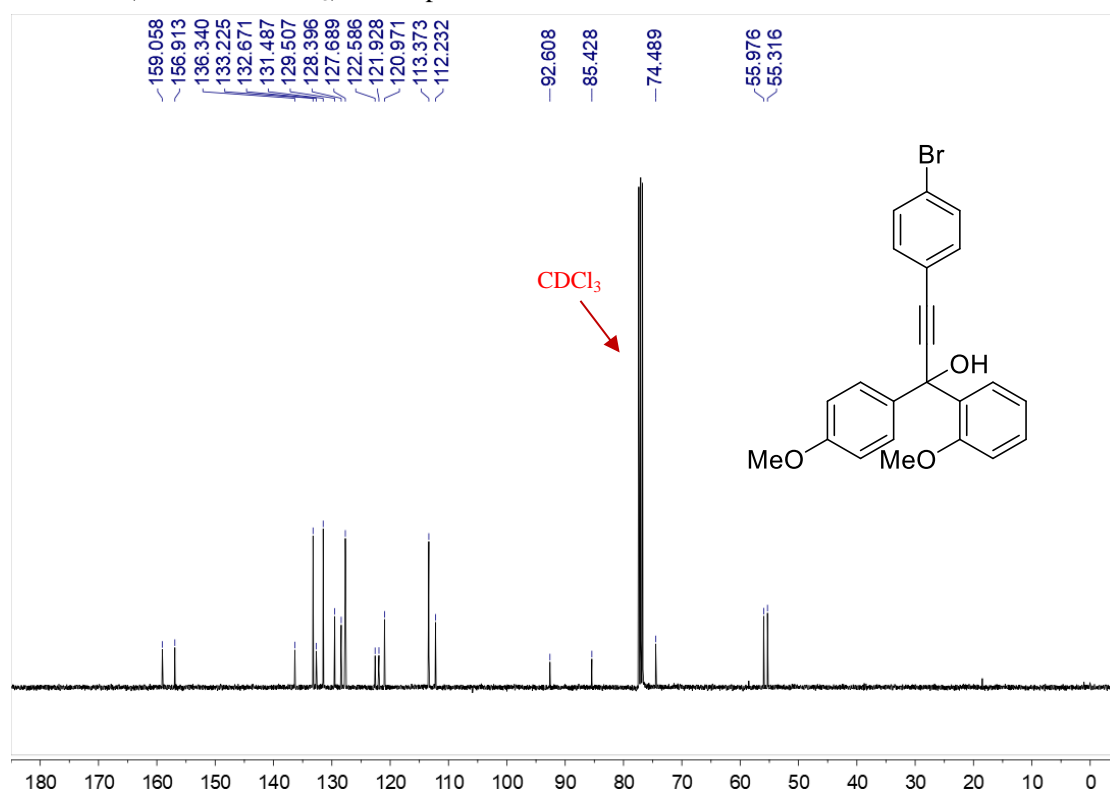
^{13}C NMR (100 MHz, CDCl_3) of compound **6j**:



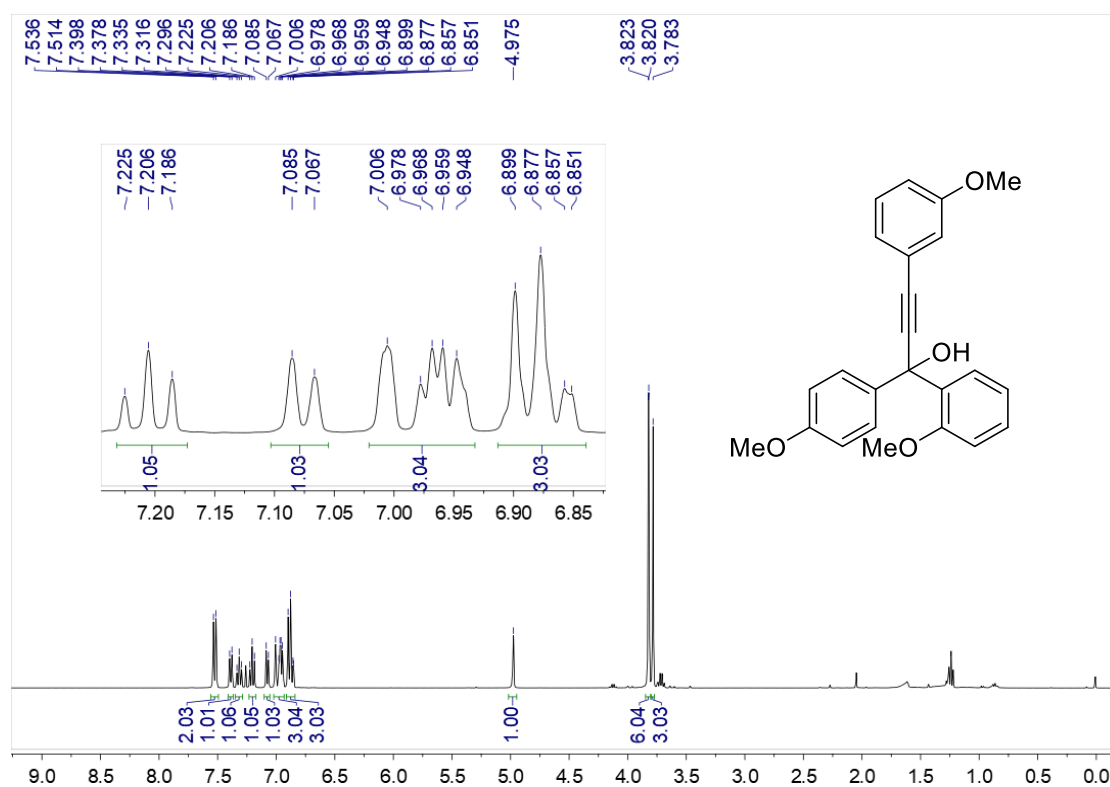
^1H NMR (400 MHz, CDCl_3) of compound **6k**:



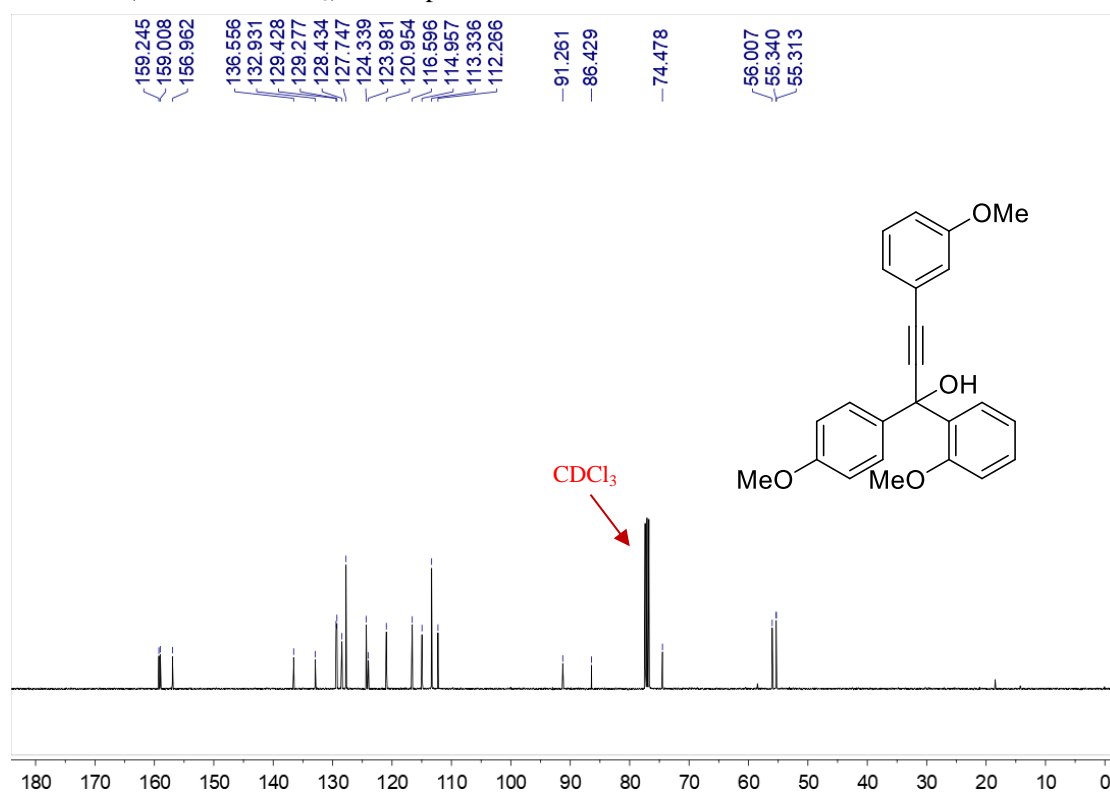
^{13}C NMR (100 MHz, CDCl_3) of compound **6k**:



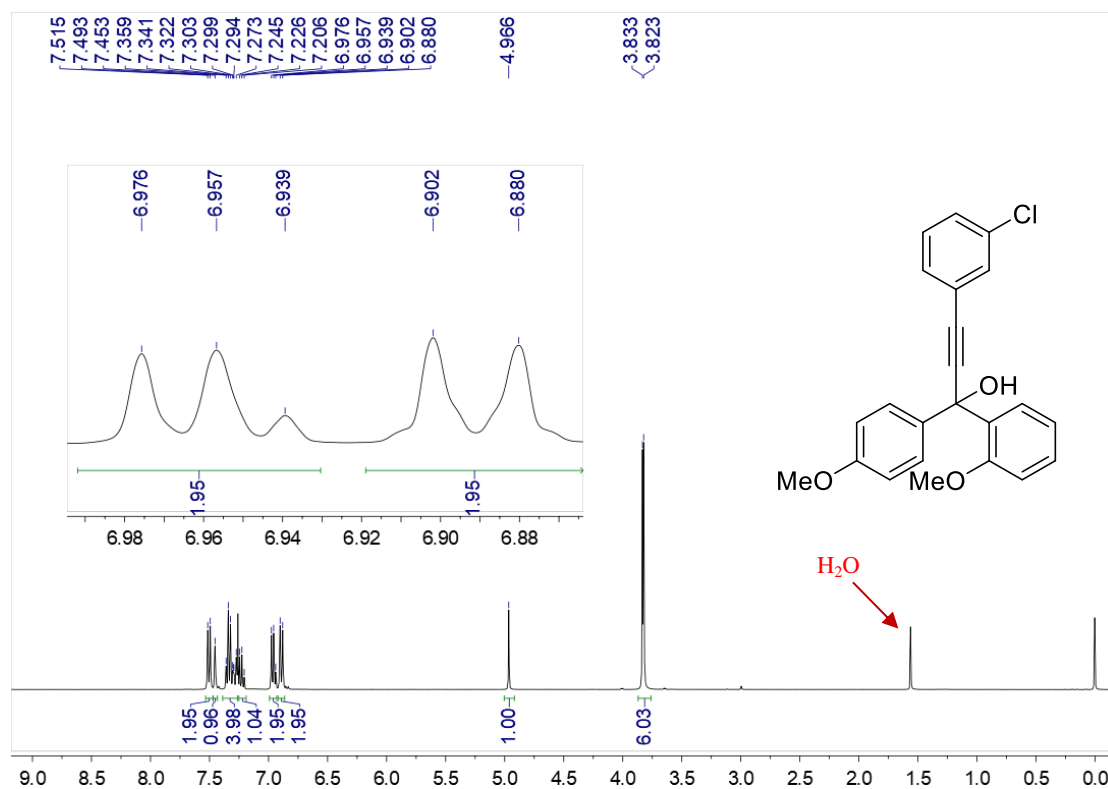
¹H NMR (400 MHz, CDCl₃) of compound **6l**:



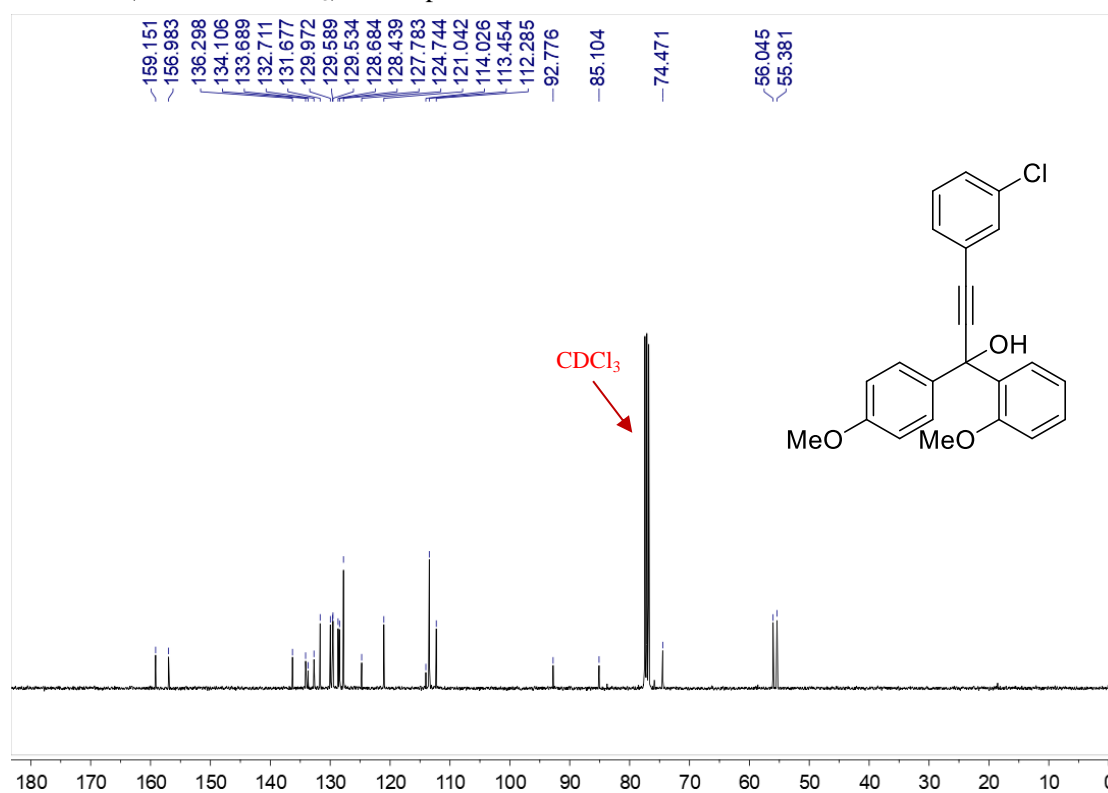
¹³C NMR (100 MHz, CDCl₃) of compound **6l**:



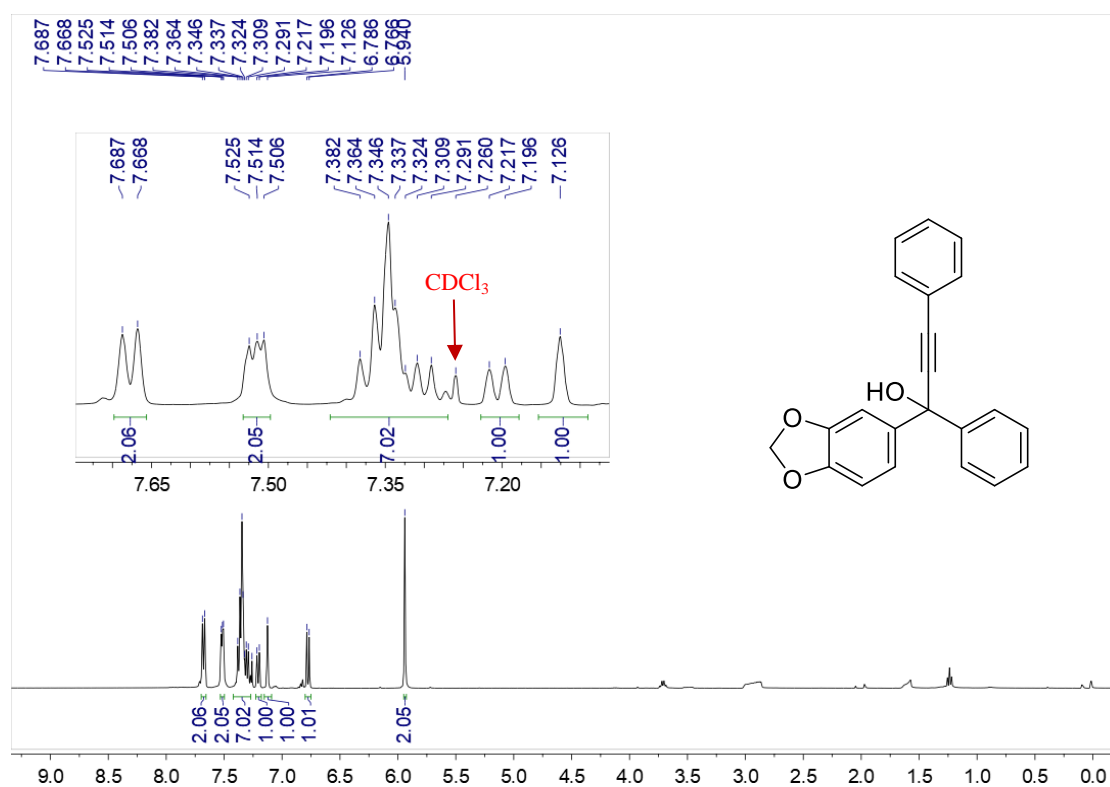
^1H NMR (400 MHz, CDCl_3) of compound **6m**:



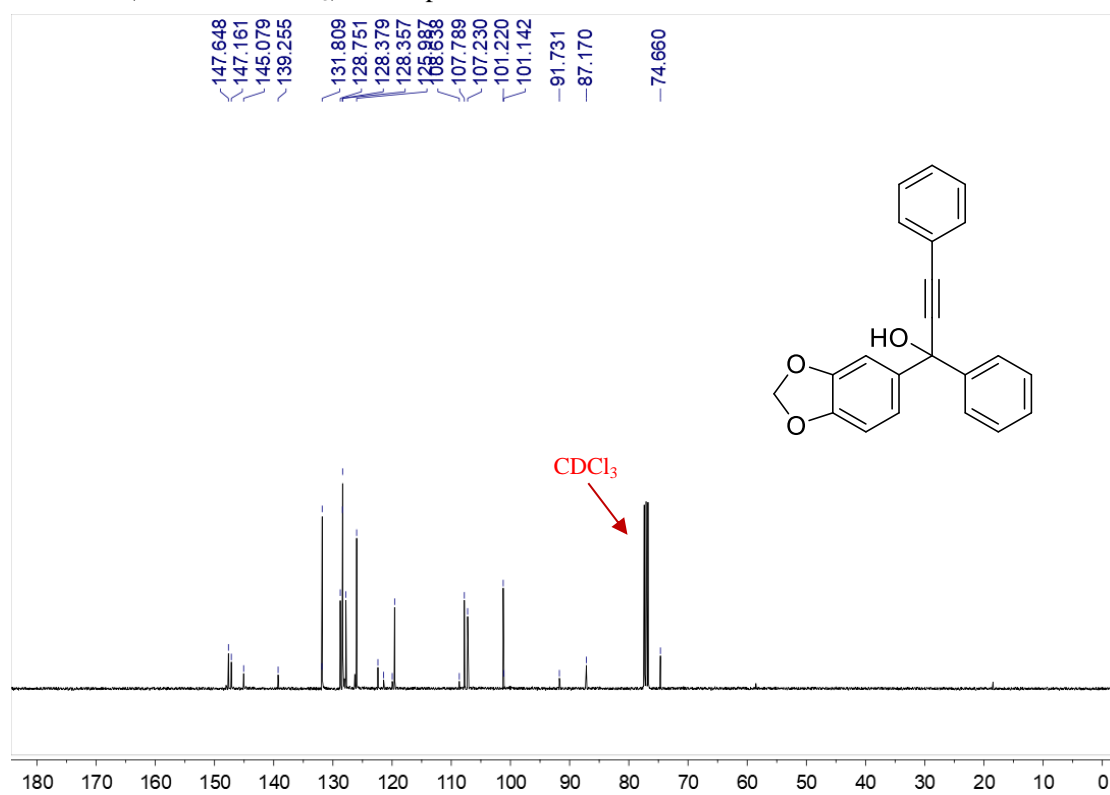
^{13}C NMR (100 MHz, CDCl_3) of compound **6m**:



^1H NMR (400 MHz, CDCl_3) of compound **6n**:

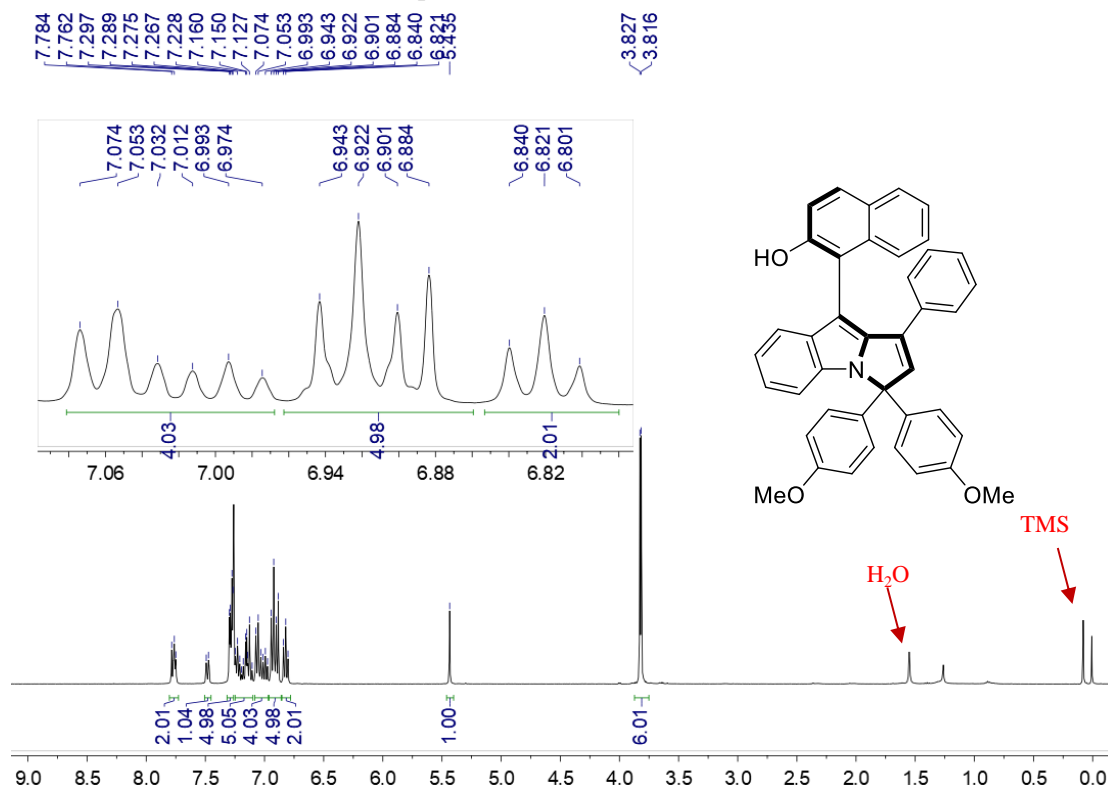


^{13}C NMR (100 MHz, CDCl_3) of compound **6n**:

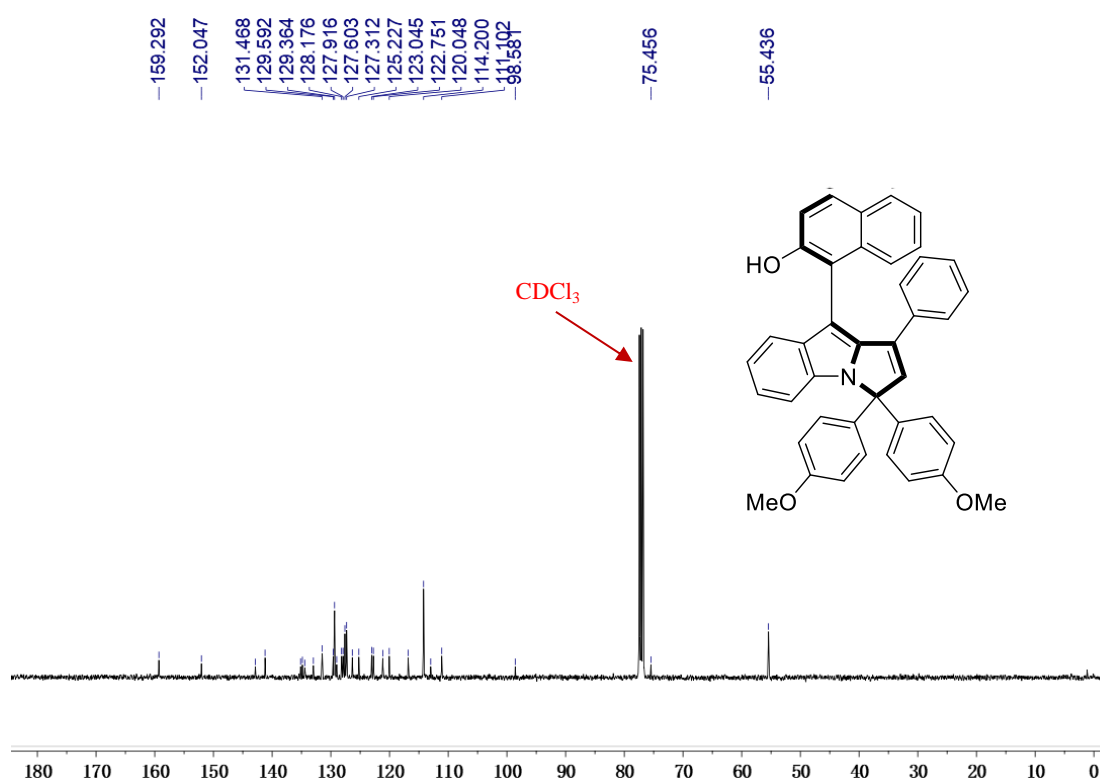


8. NMR spectra of all products 3, 7-10, 13, 16

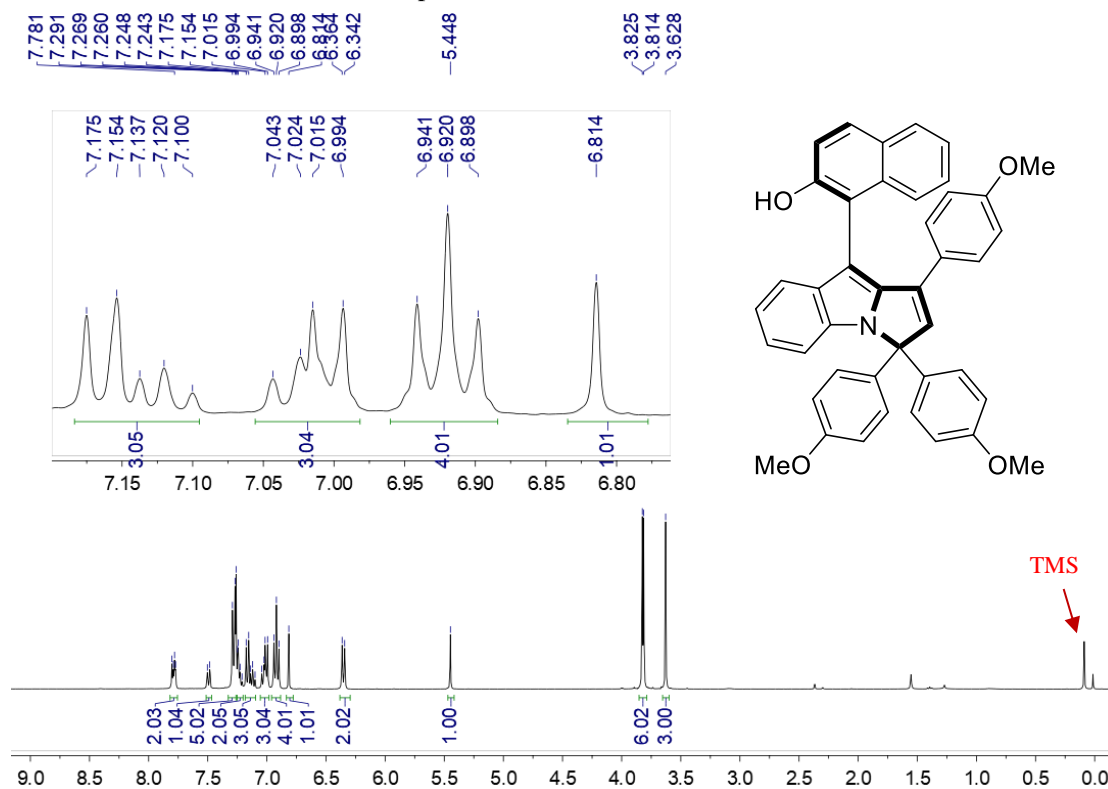
^1H NMR (400 MHz, CDCl_3) of compound **3aa**:



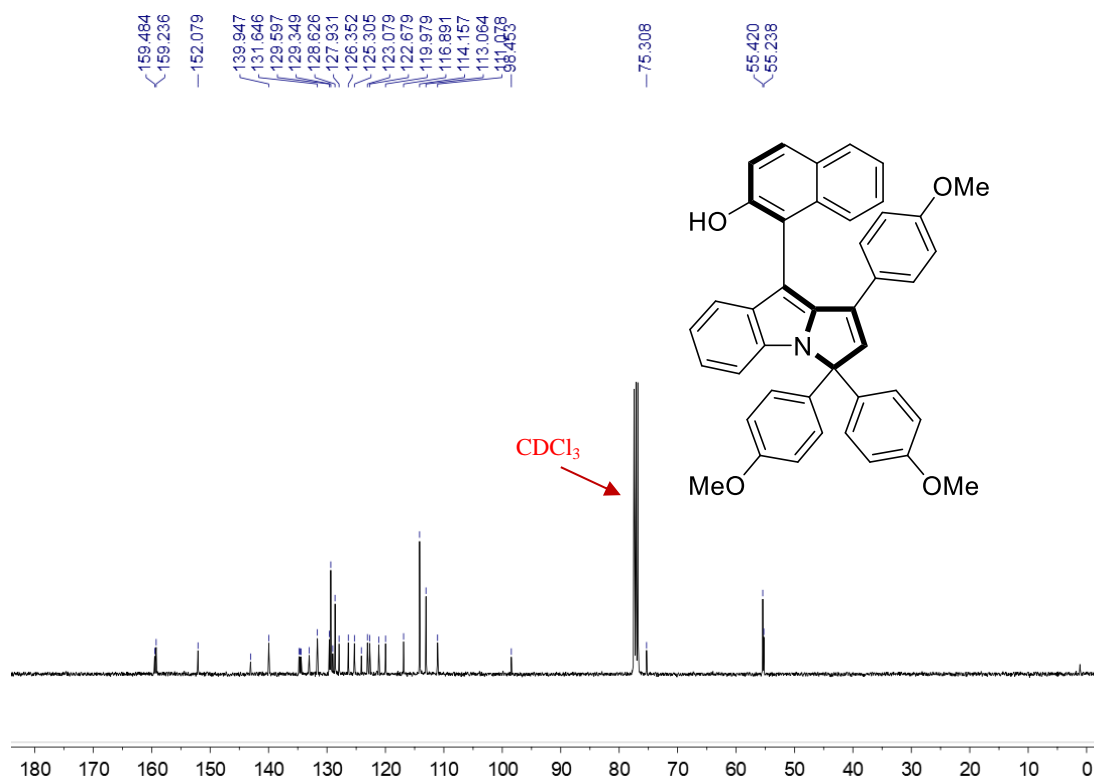
^{13}C NMR (100 MHz, CDCl_3) of compound **3aa**:



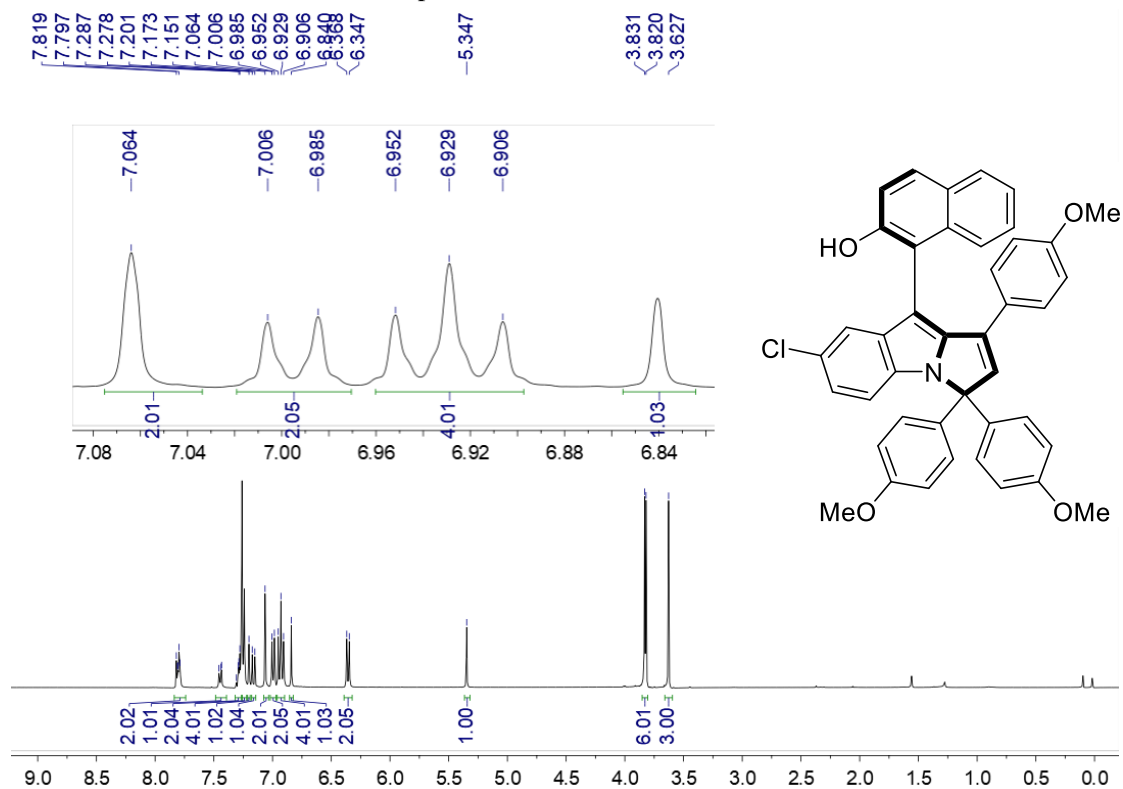
^1H NMR (400 MHz, CDCl_3) of compound **3ab**:



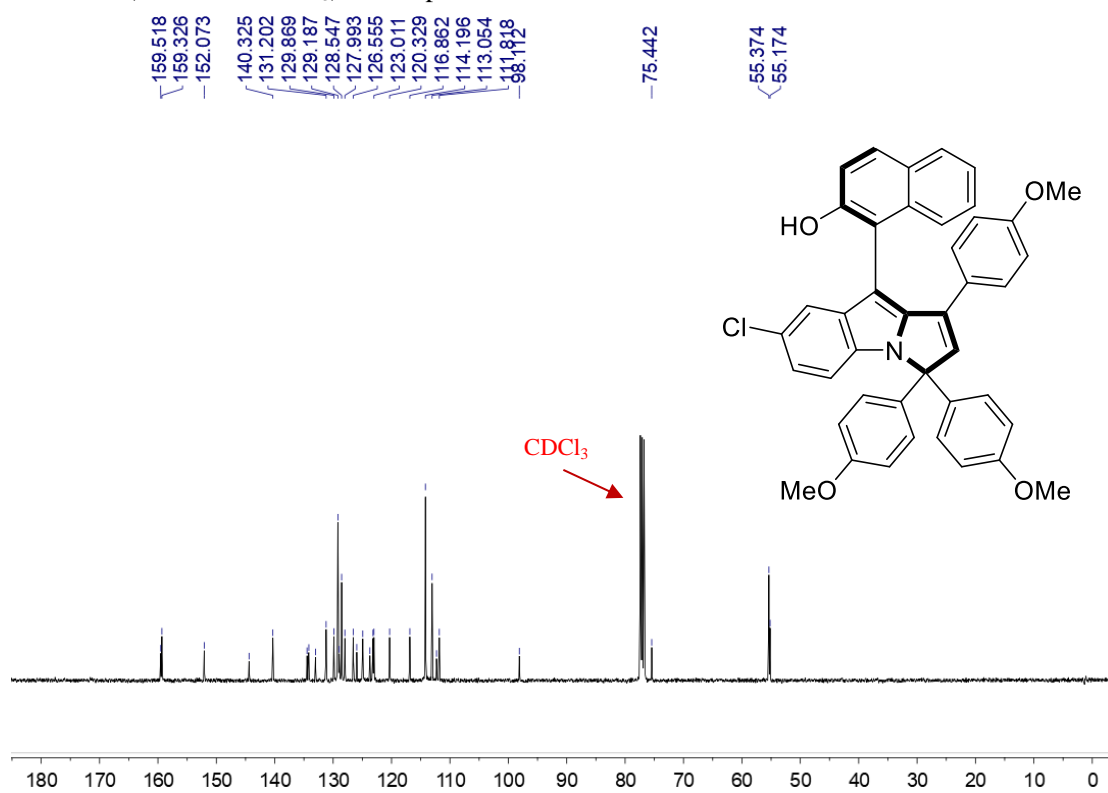
^{13}C NMR (100 MHz, CDCl_3) of compound **3ab**:



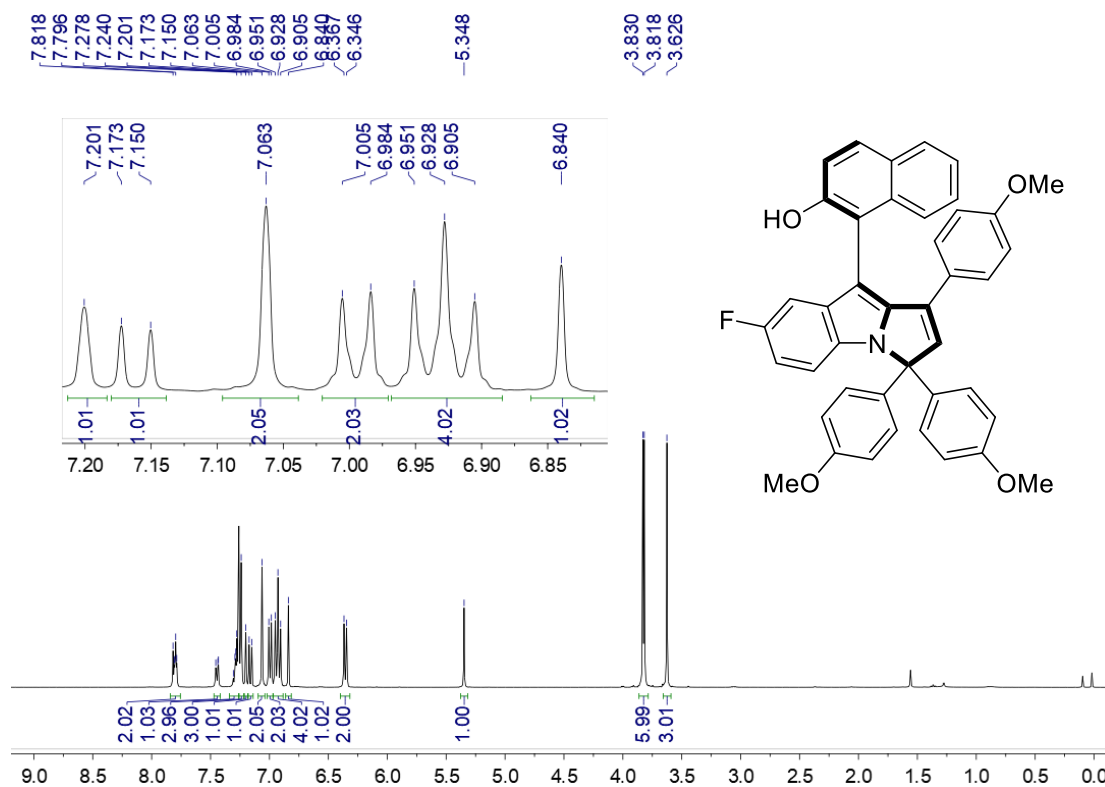
^1H NMR (400 MHz, CDCl_3) of compound **3bb**:



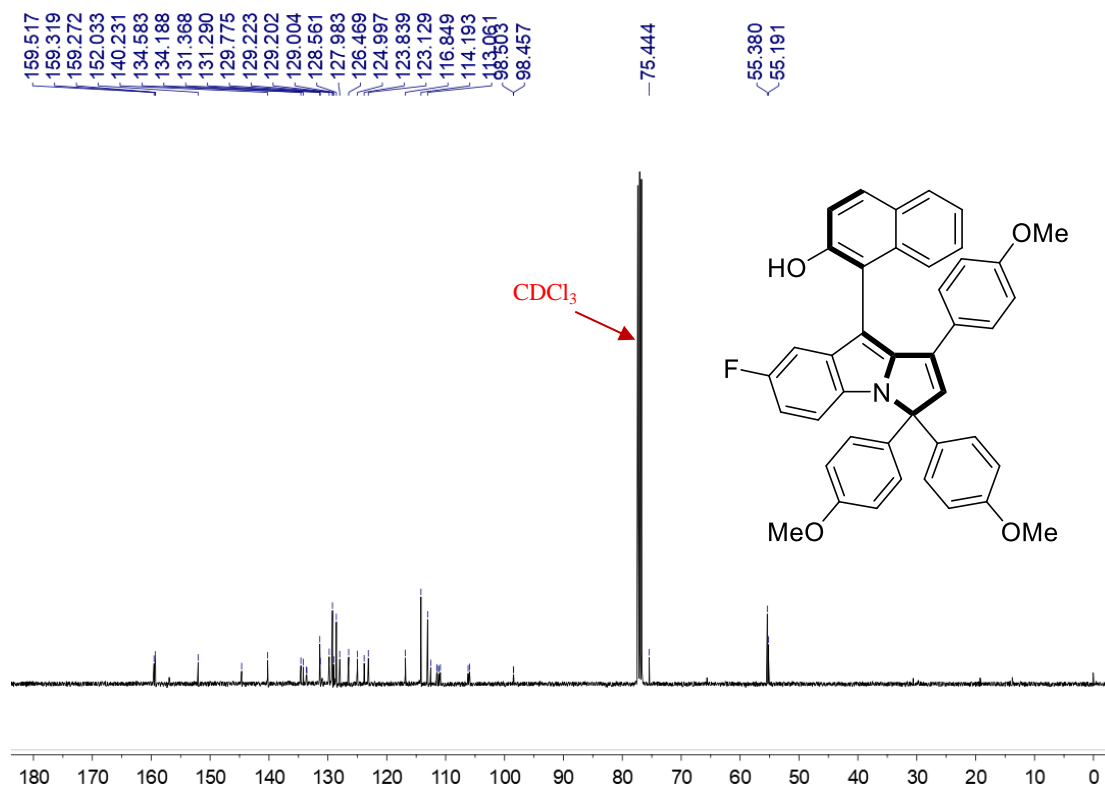
^{13}C NMR (100 MHz, CDCl_3) of compound **3bb**:



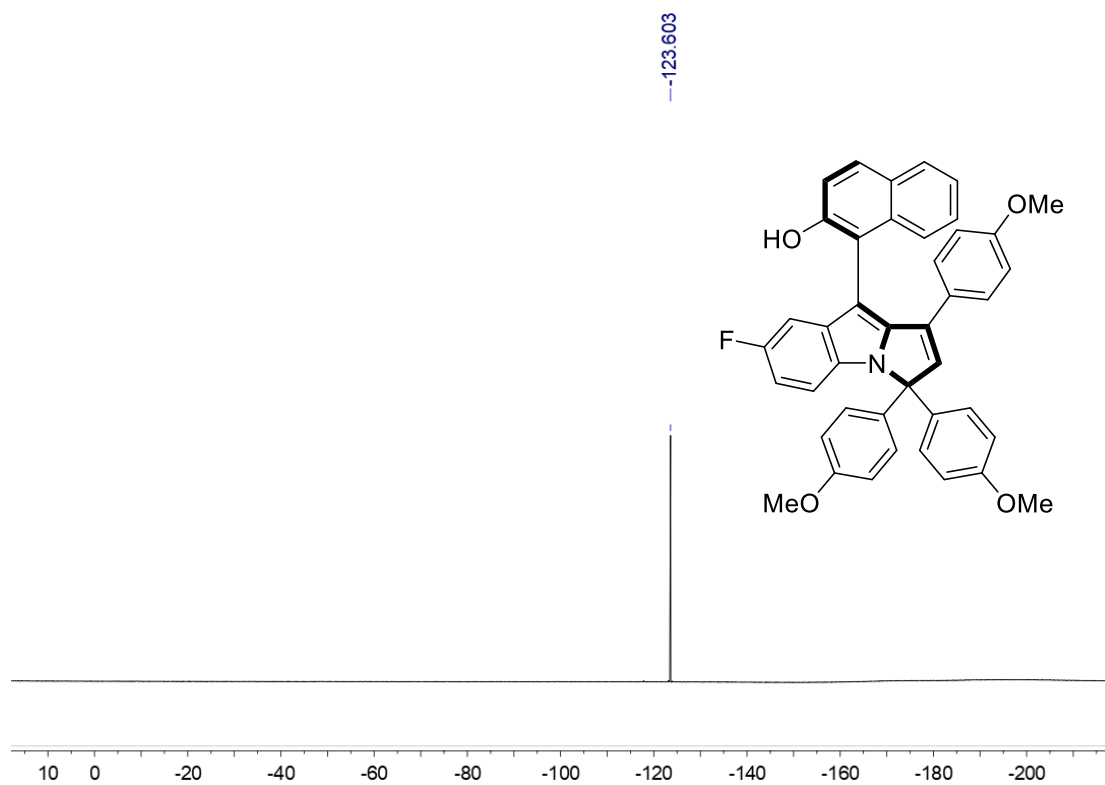
^1H NMR (400 MHz, CDCl_3) of compound **3cb**:



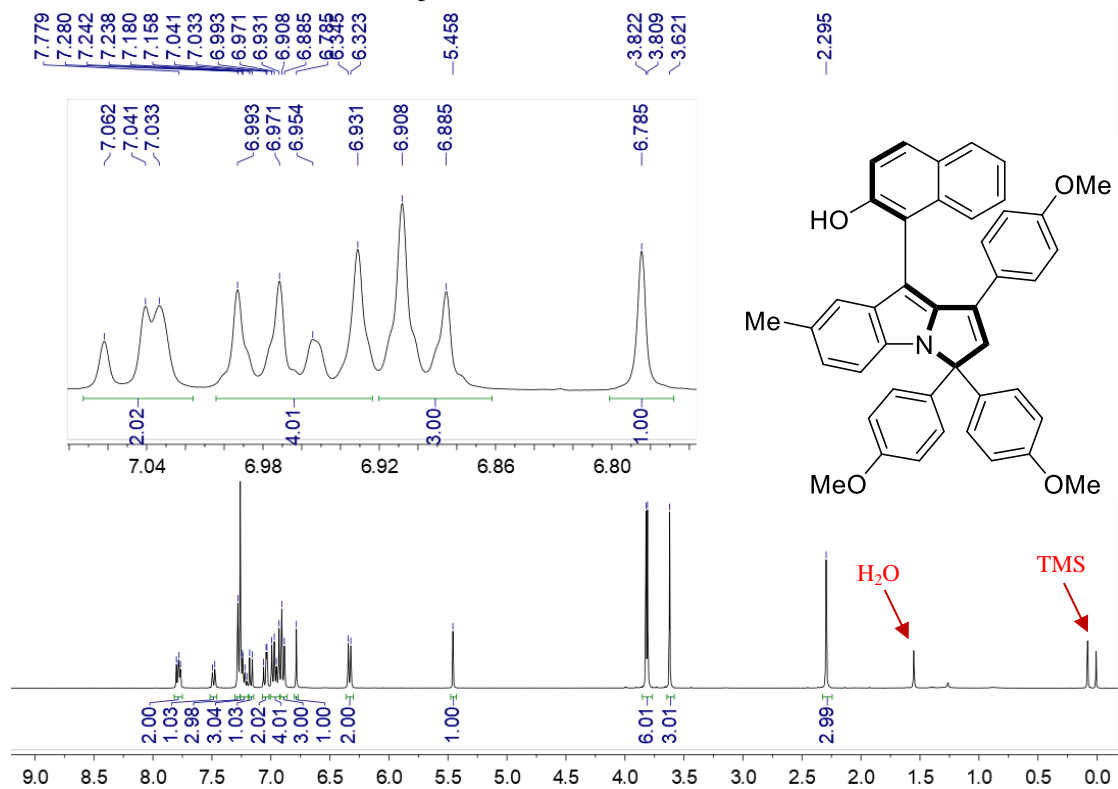
^{13}C NMR (100 MHz, CDCl_3) of compound **3cb**:



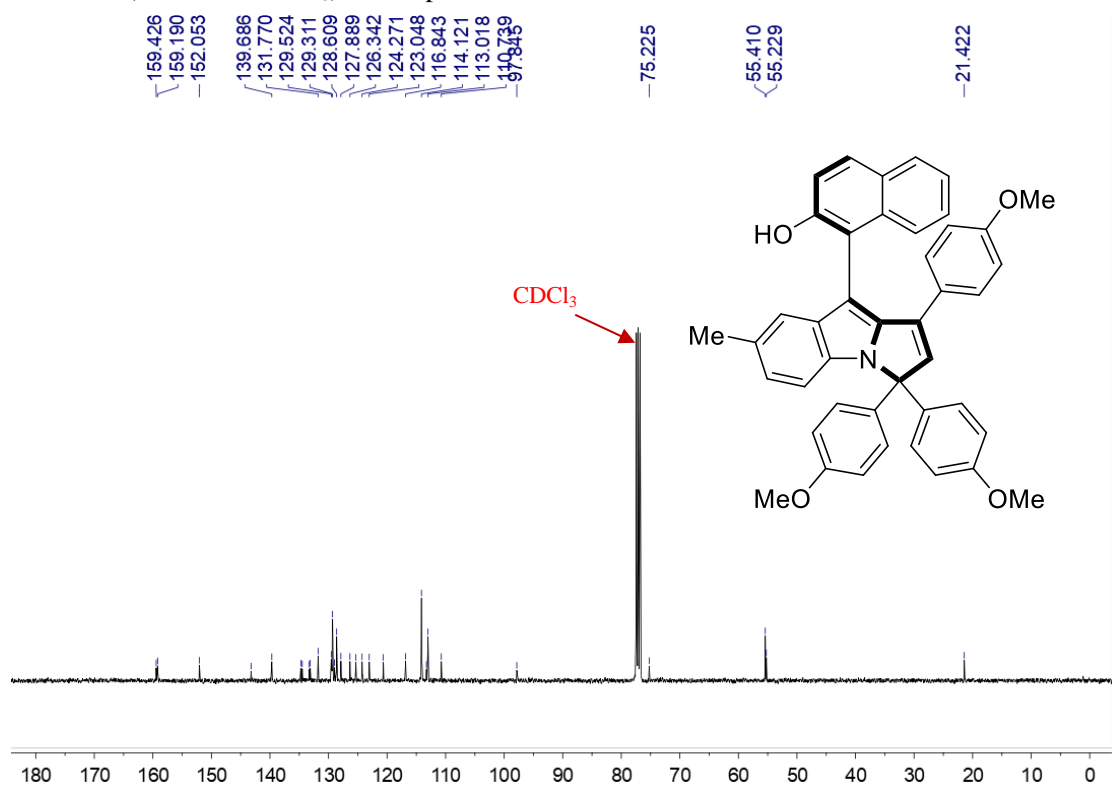
^{19}F NMR (376 MHz, CDCl_3) of compound **3cb**:



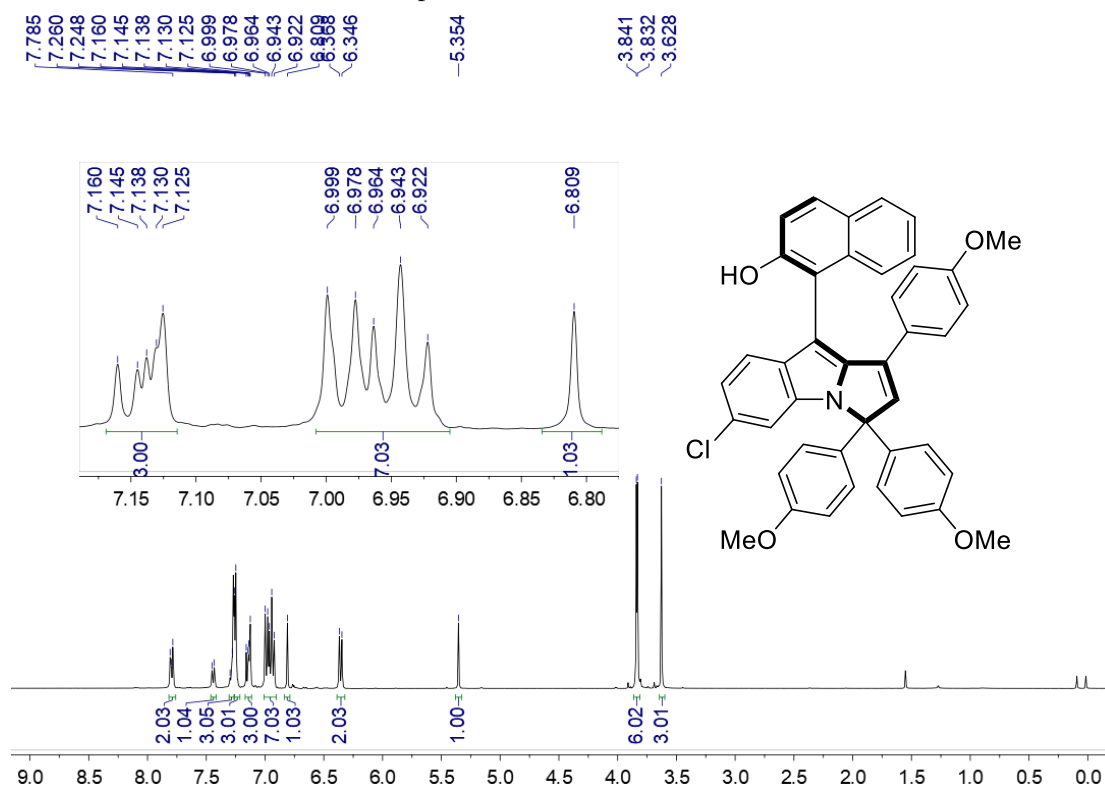
^1H NMR (400 MHz, CDCl_3) of compound **3db**:



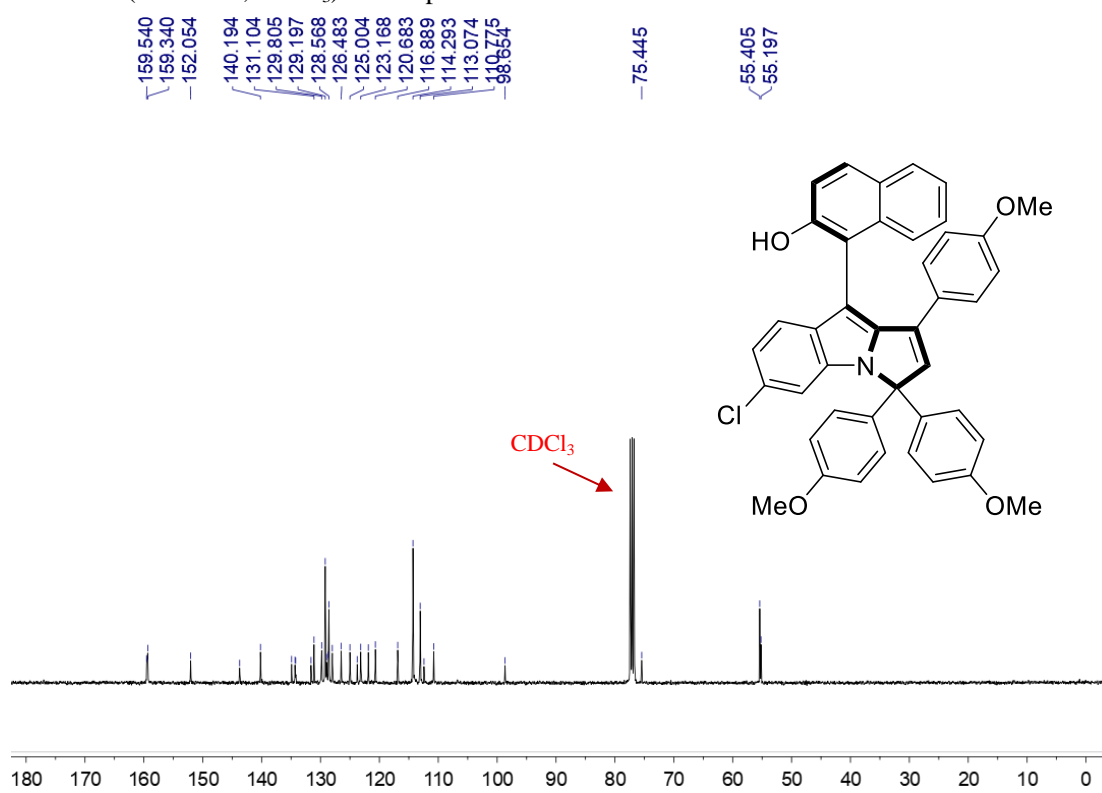
^{13}C NMR (100 MHz, CDCl_3) of compound **3db**:



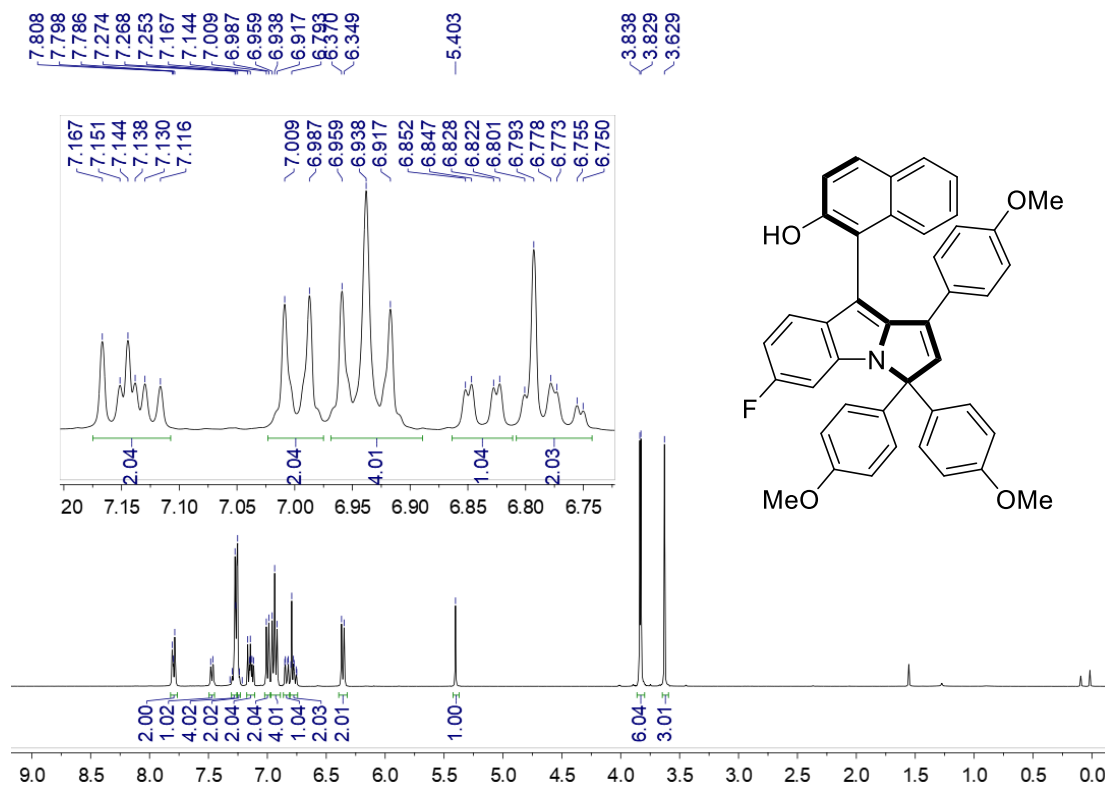
¹H NMR (400 MHz, CDCl₃) of compound **3eb**:



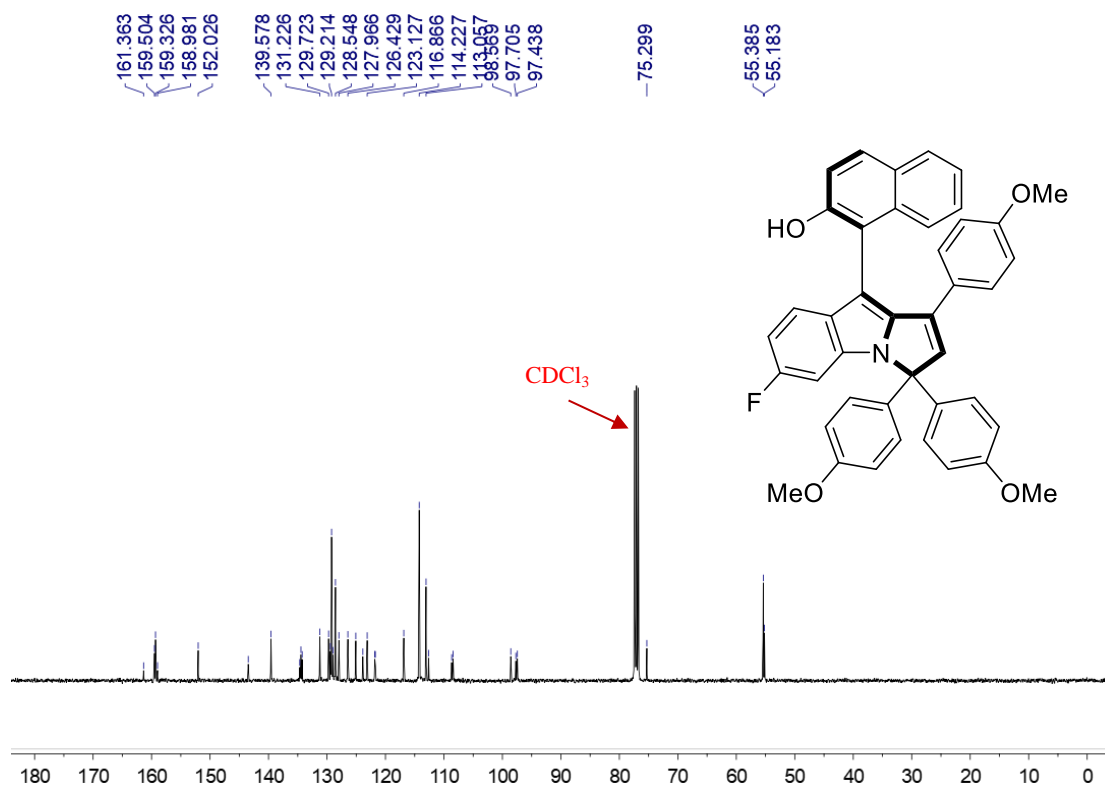
¹³C NMR (100 MHz, CDCl₃) of compound **3eb**:



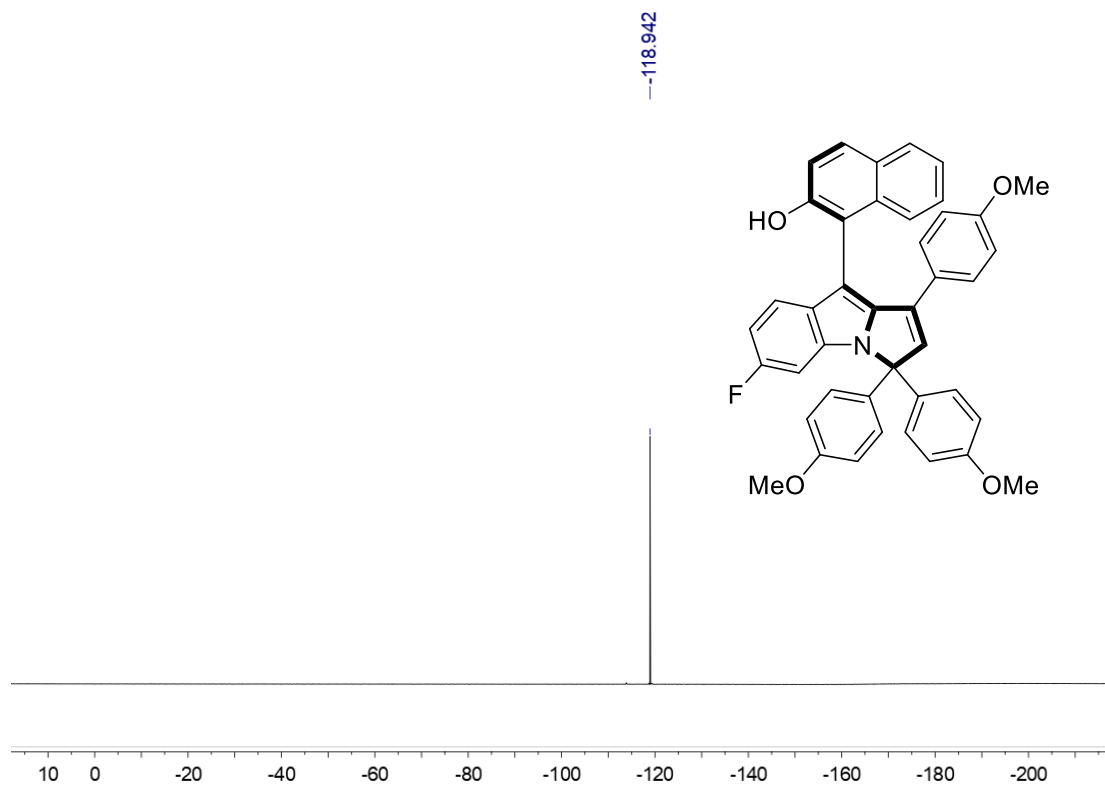
^1H NMR (400 MHz, CDCl_3) of compound **3fb**:



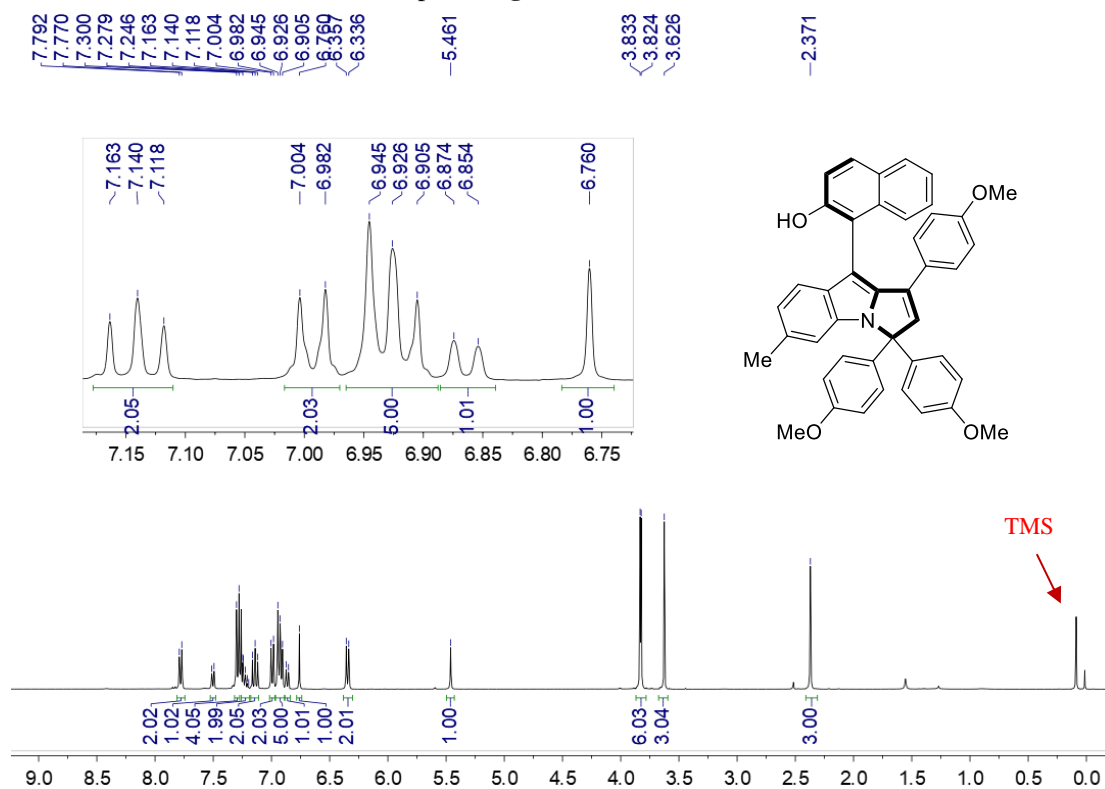
^{13}C NMR (100 MHz, CDCl_3) of compound **3fb**:



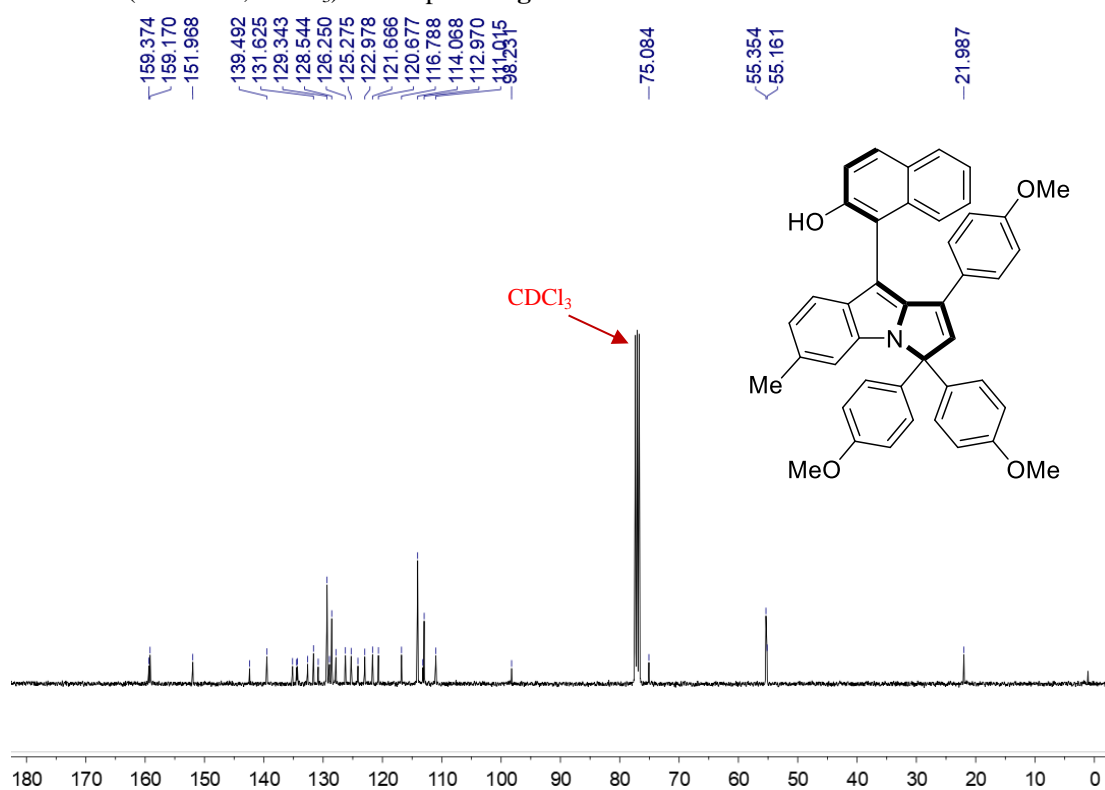
^{19}F NMR (376 MHz, CDCl_3) of compound **3fb**:



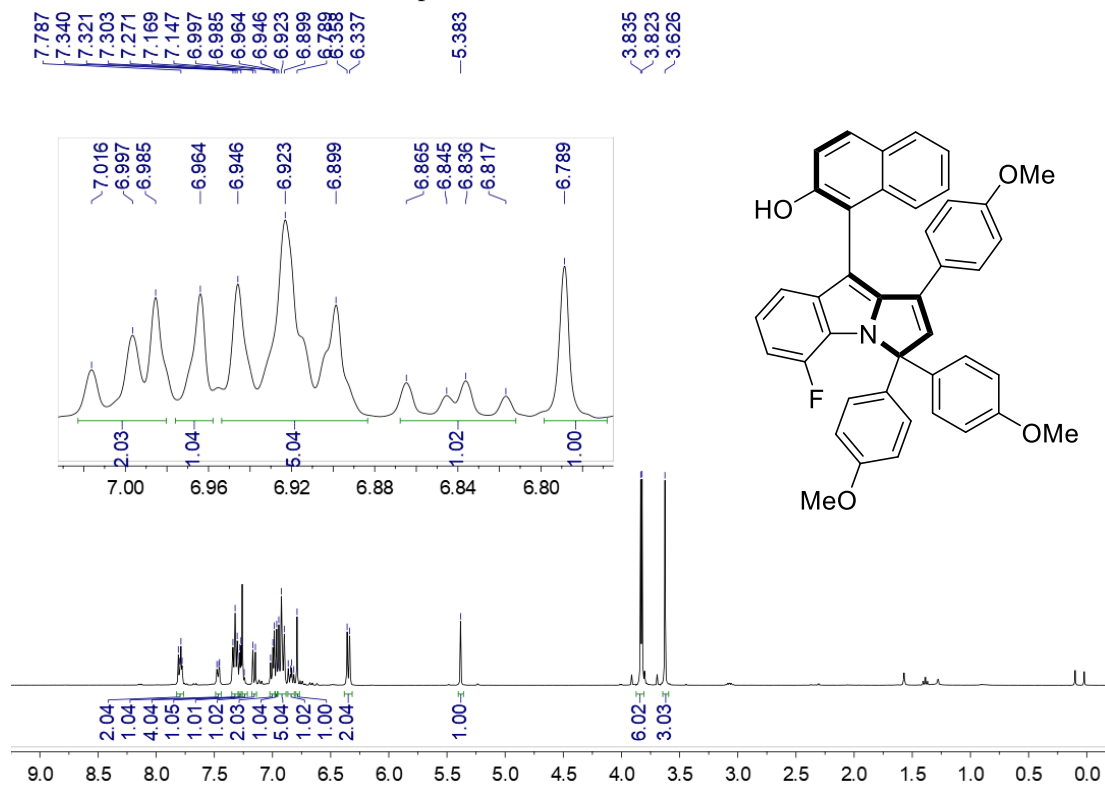
^1H NMR (400 MHz, CDCl_3) of compound **3gb**:



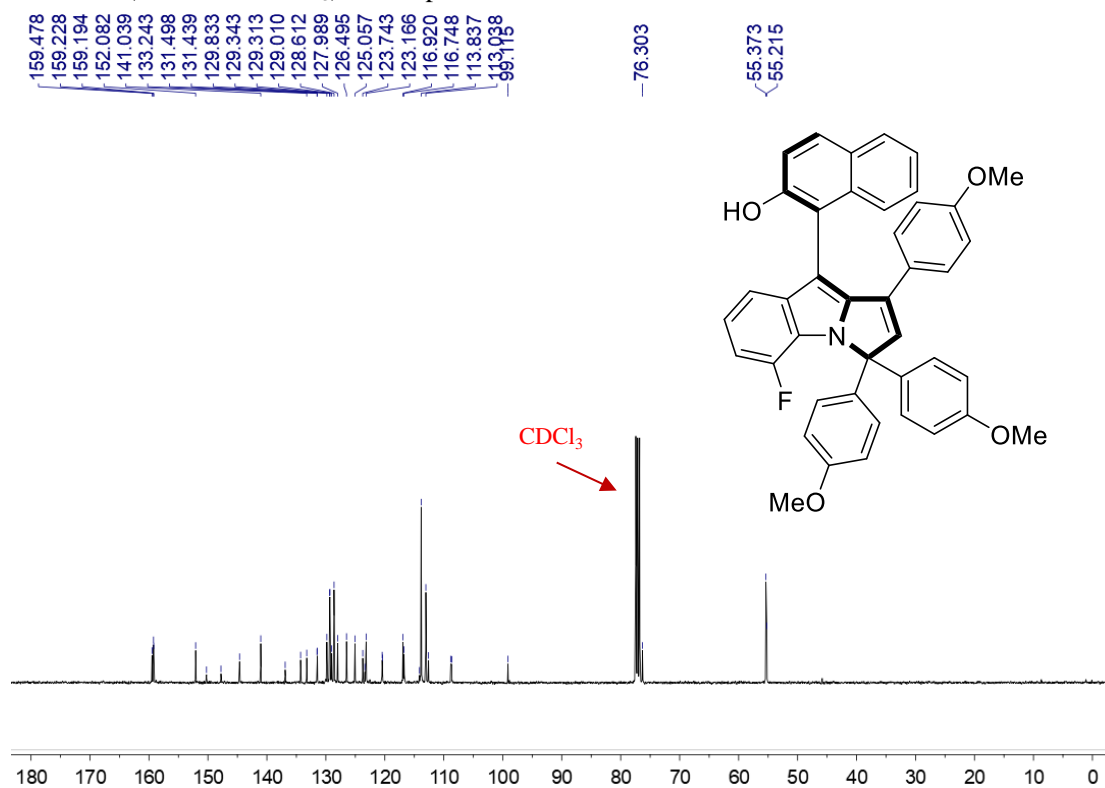
^{13}C NMR (100 MHz, CDCl_3) of compound **3gb**:



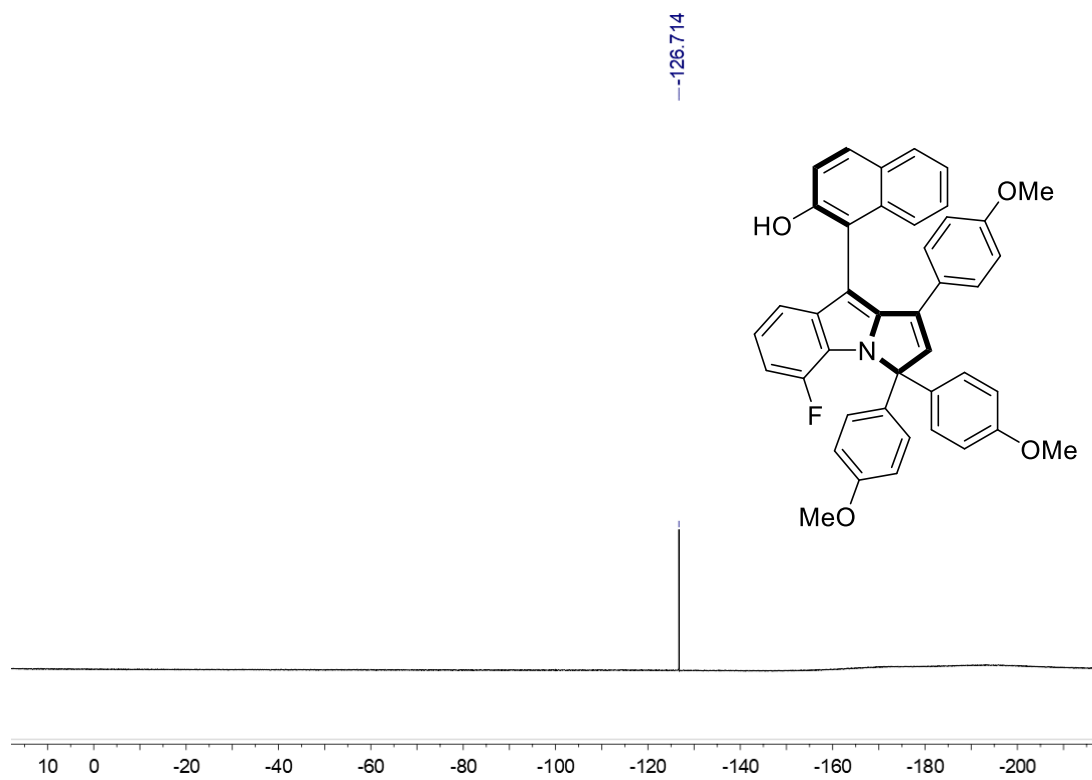
^1H NMR (400 MHz, CDCl_3) of compound **3hb**:



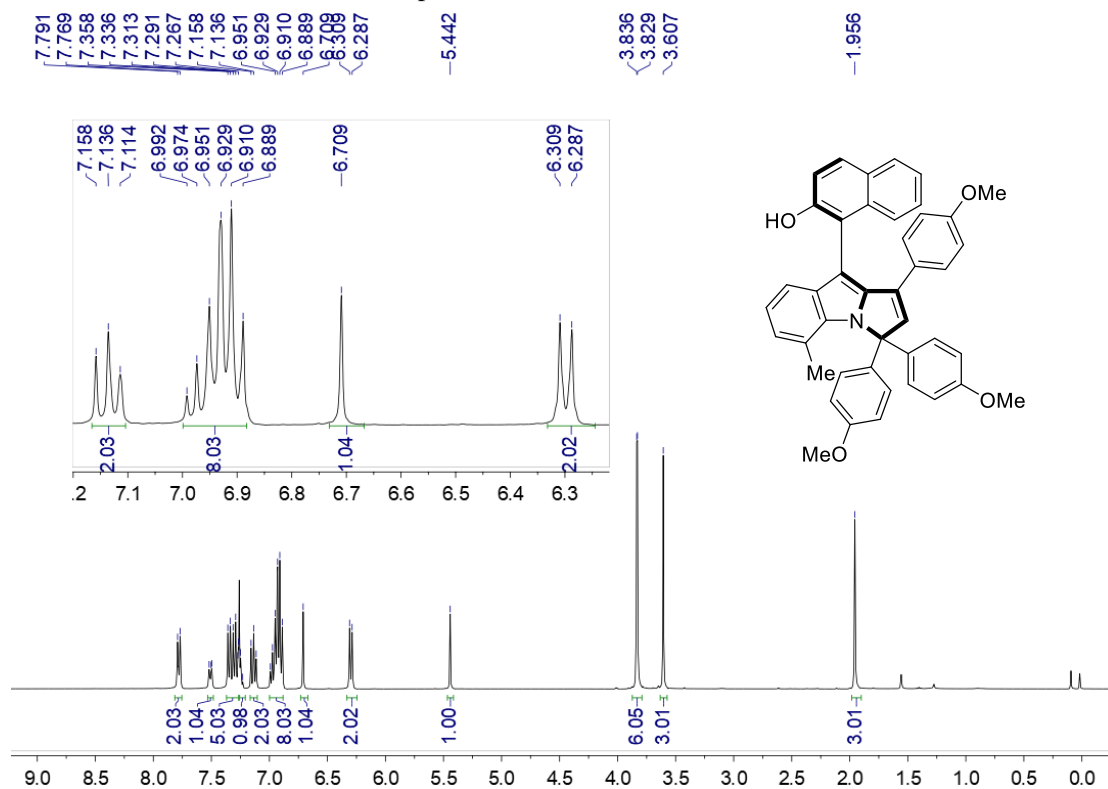
^{13}C NMR (100 MHz, CDCl_3) of compound **3hb**:



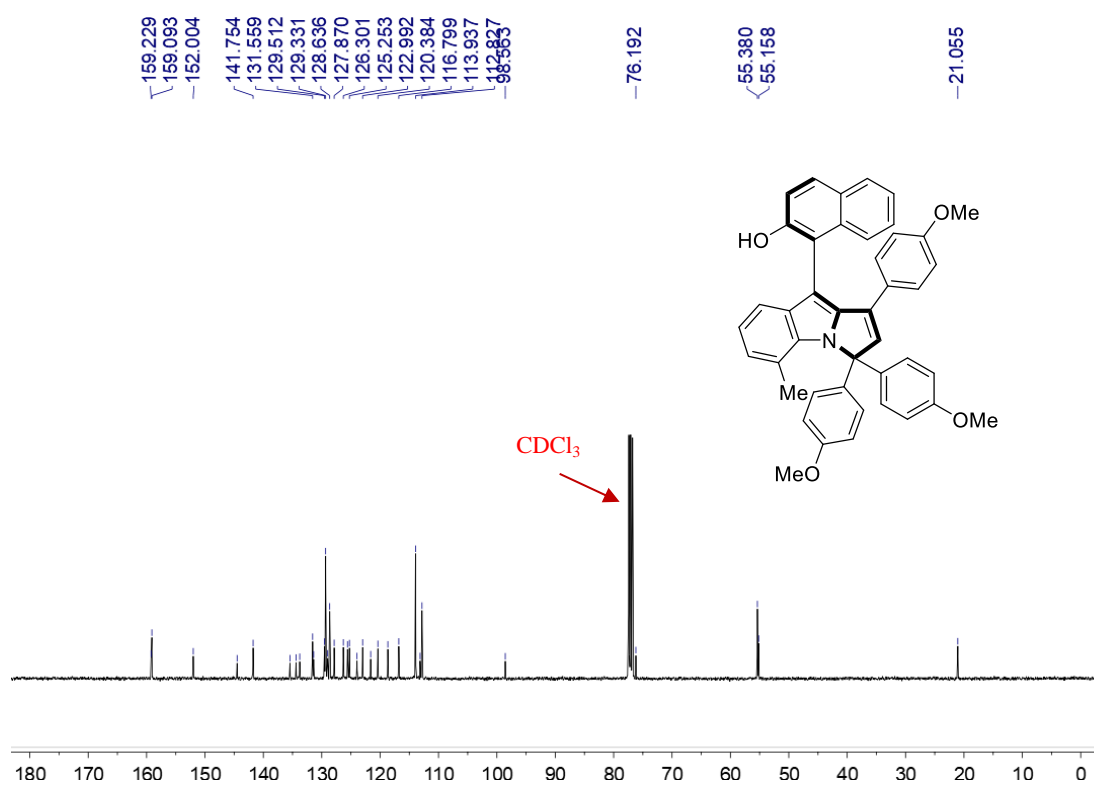
^{19}F NMR (376 MHz, CDCl_3) of compound **3hb**:



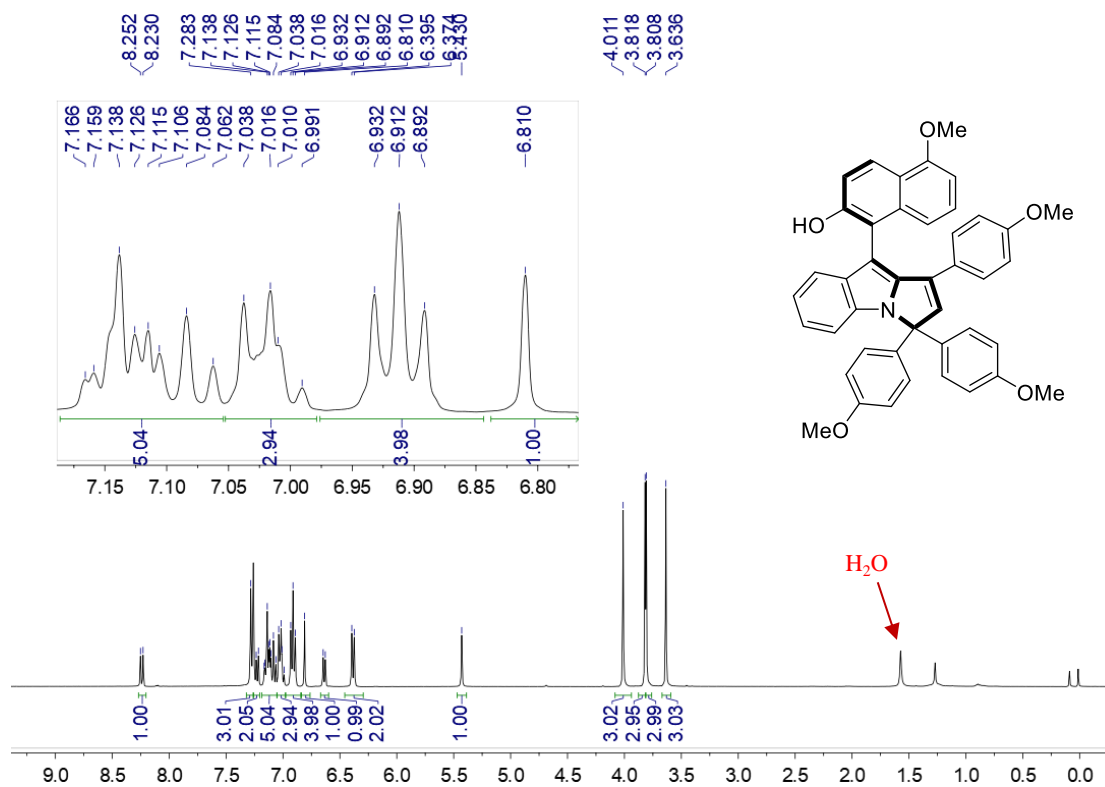
^1H NMR (400 MHz, CDCl_3) of compound **3ib**:



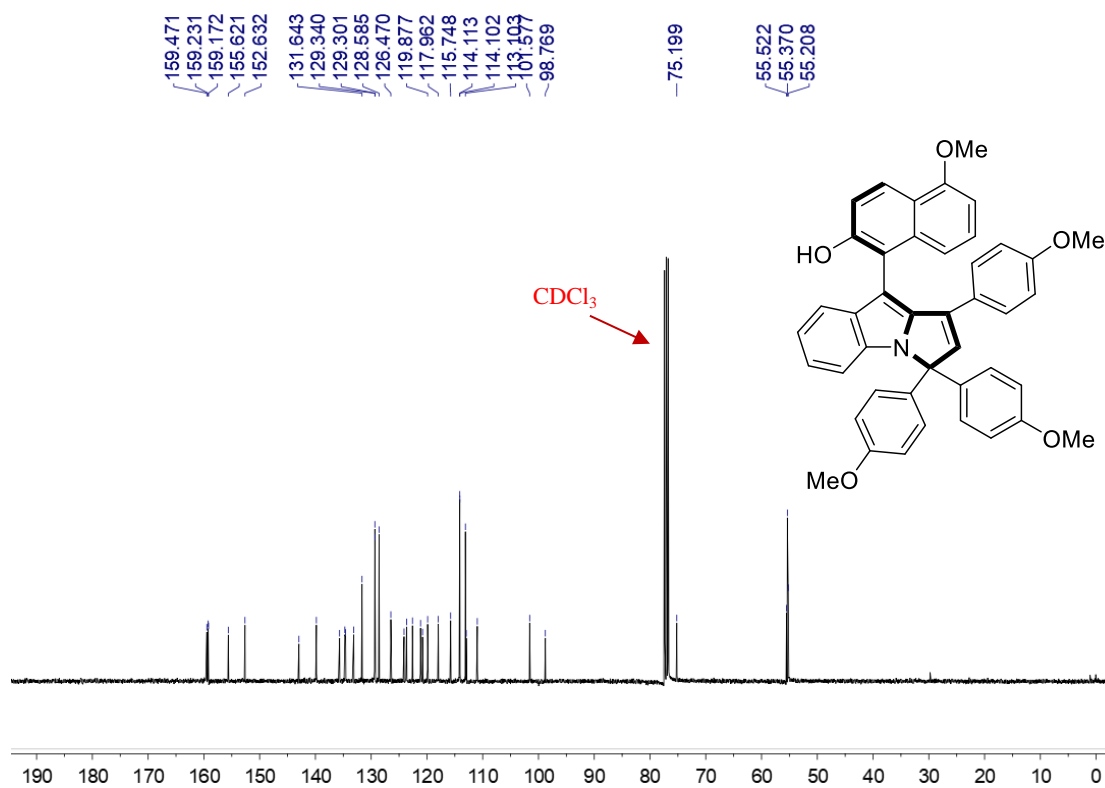
^{13}C NMR (100 MHz, CDCl_3) of compound **3ib**:



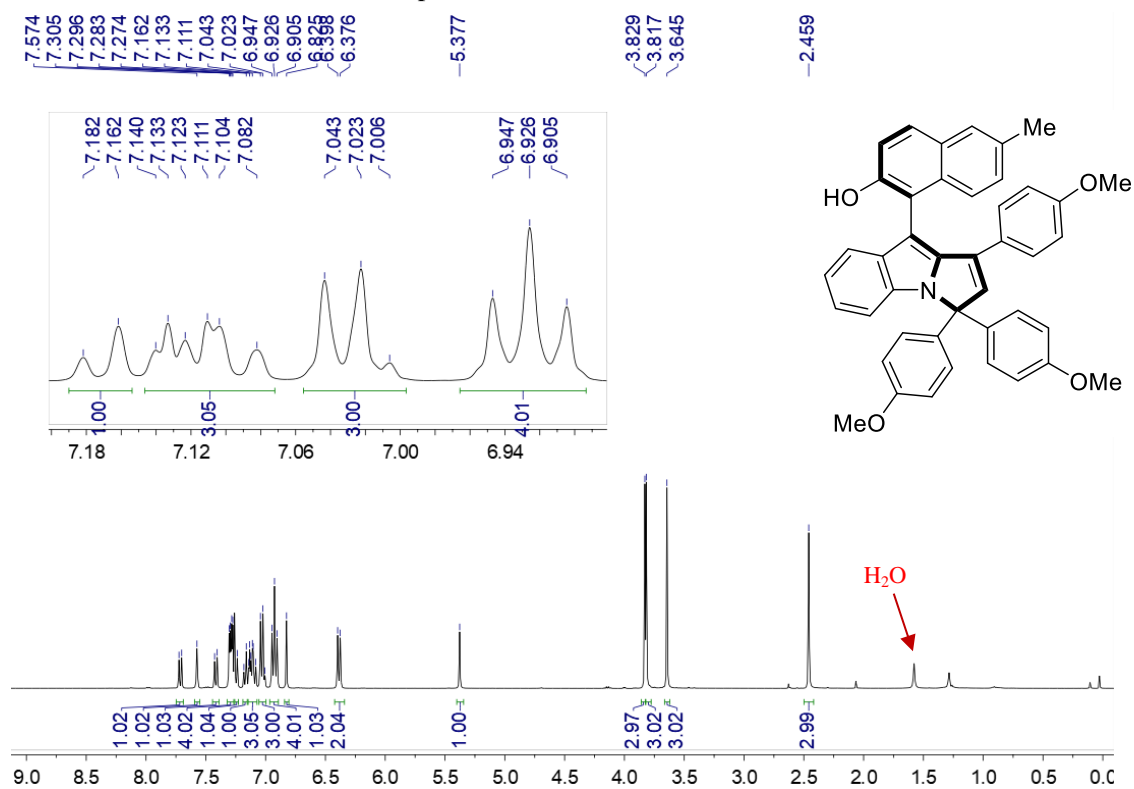
^1H NMR (400 MHz, CDCl_3) of compound **3jb**:



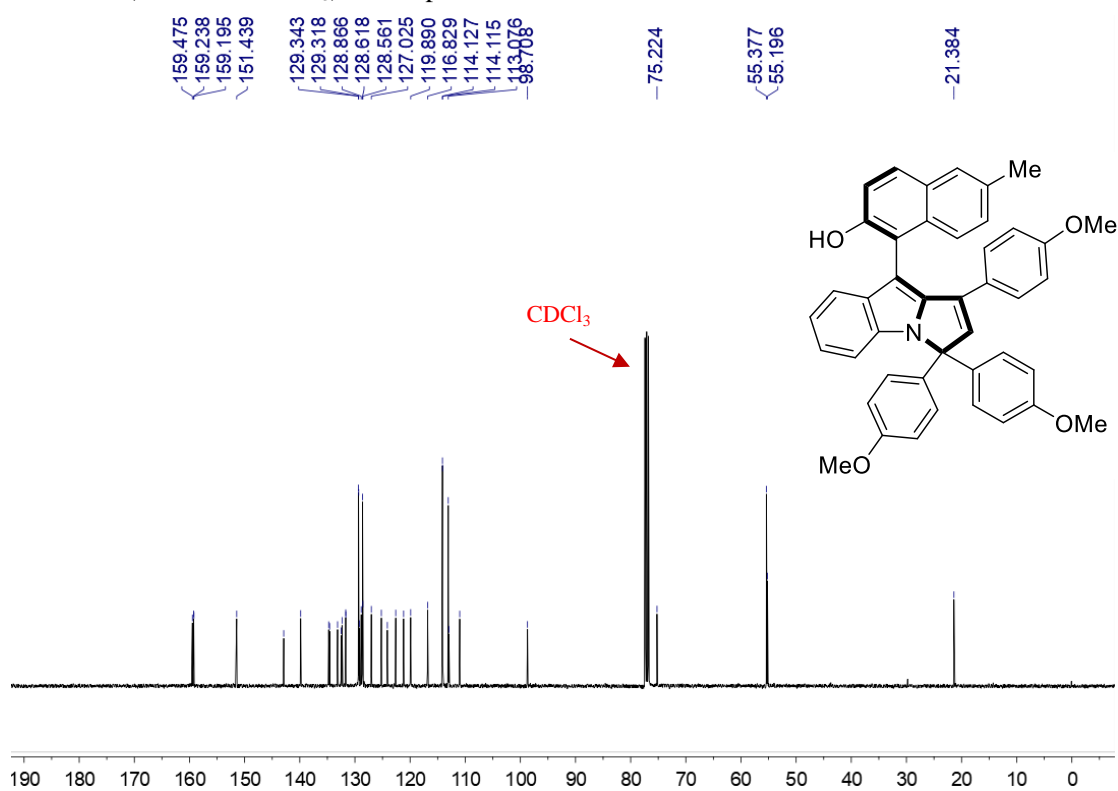
^{13}C NMR (100 MHz, CDCl_3) of compound **3jb**:



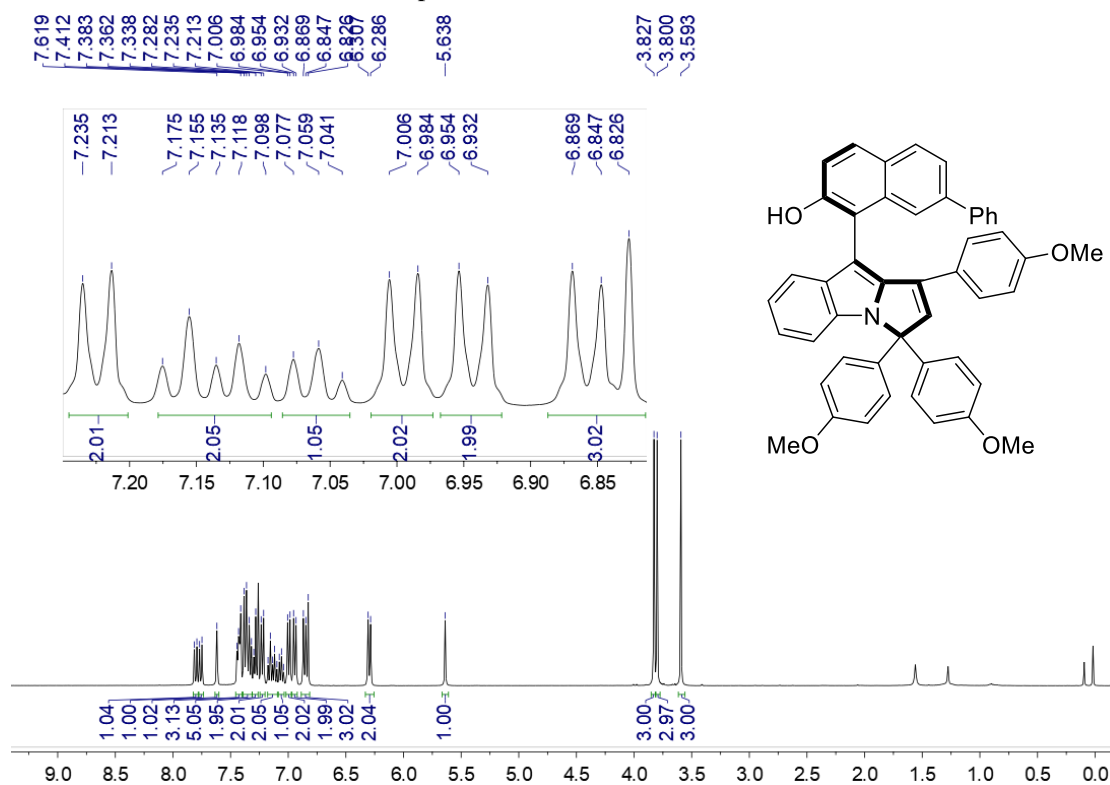
^1H NMR (400 MHz, CDCl_3) of compound **3kb**:



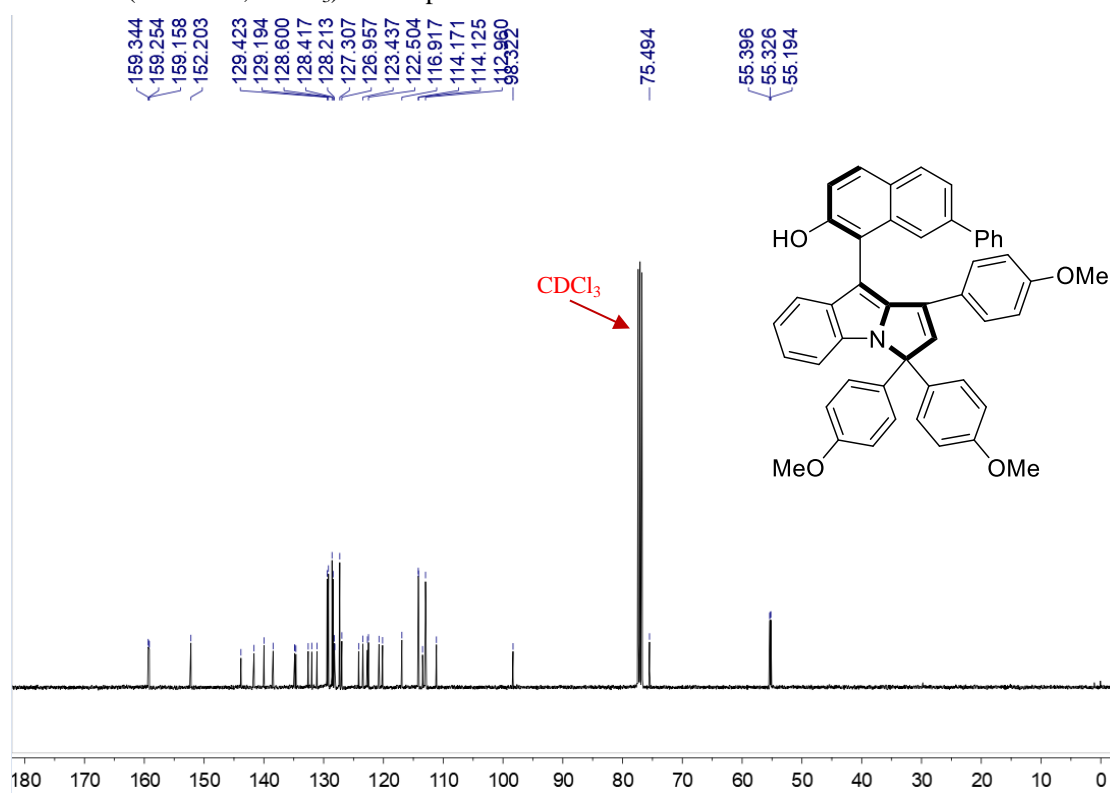
^{13}C NMR (100 MHz, CDCl_3) of compound **3kb**:



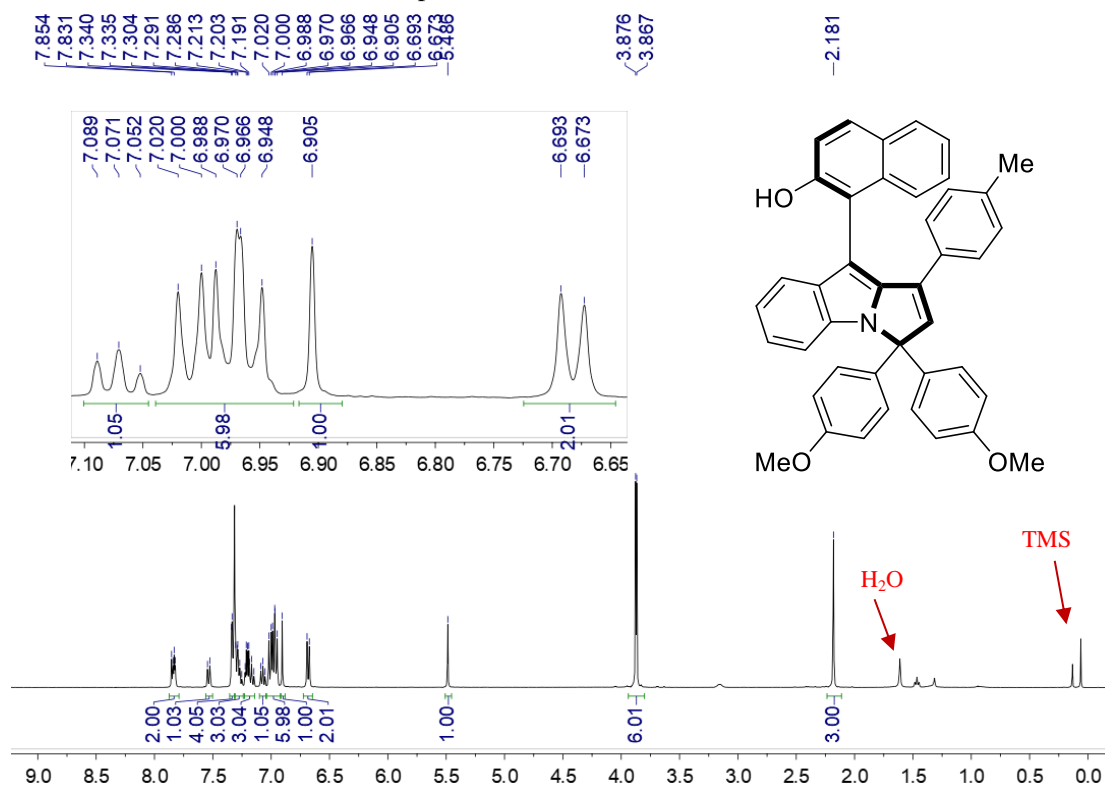
^1H NMR (400 MHz, CDCl_3) of compound **31b**:



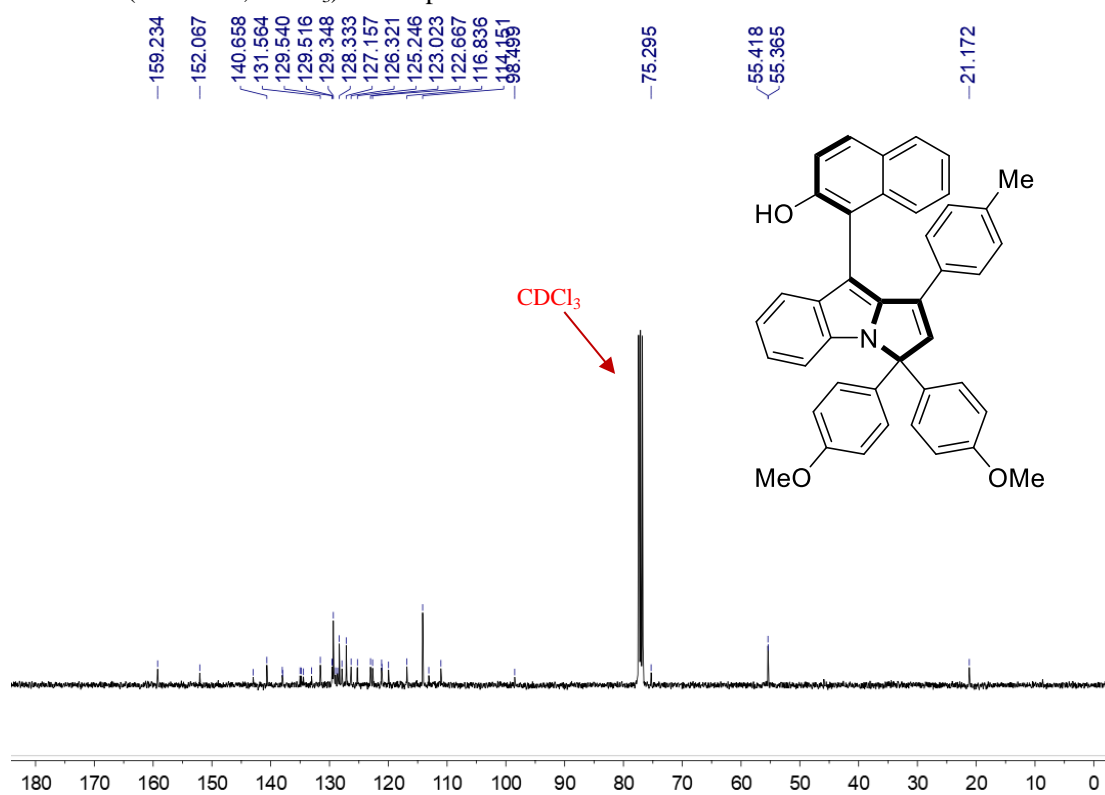
^{13}C NMR (100 MHz, CDCl_3) of compound **31b**:



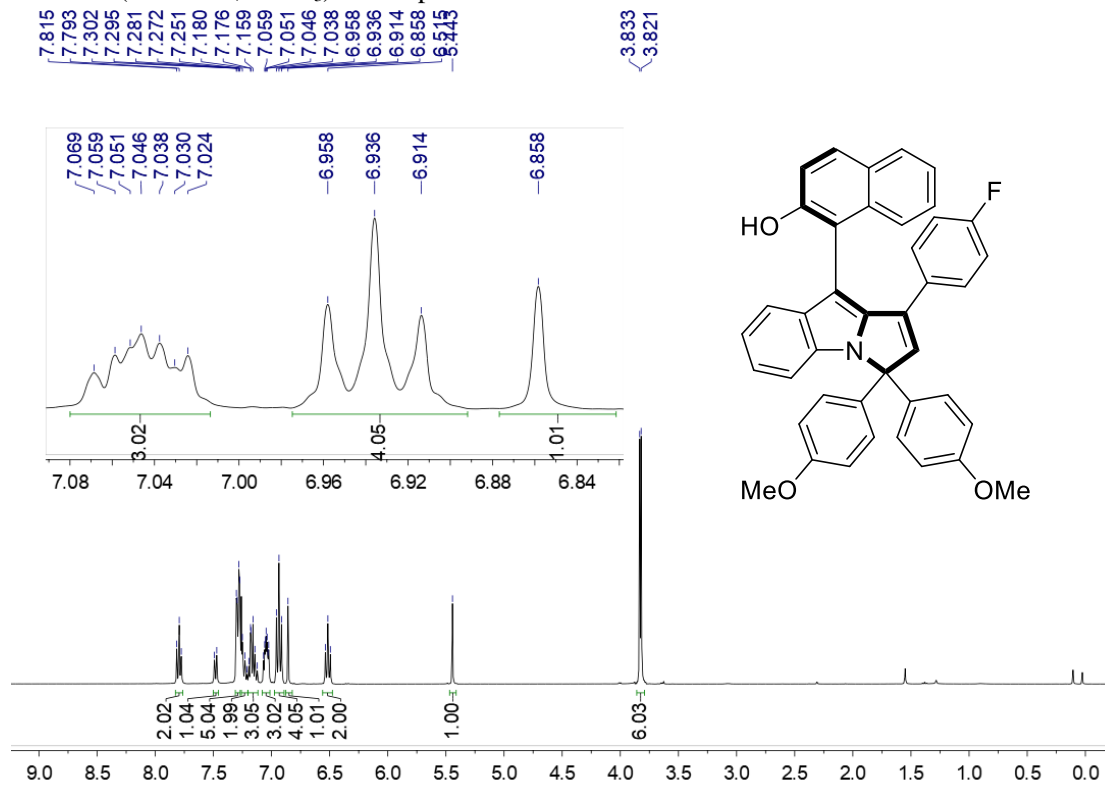
^1H NMR (400 MHz, CDCl_3) of compound **3ac**:



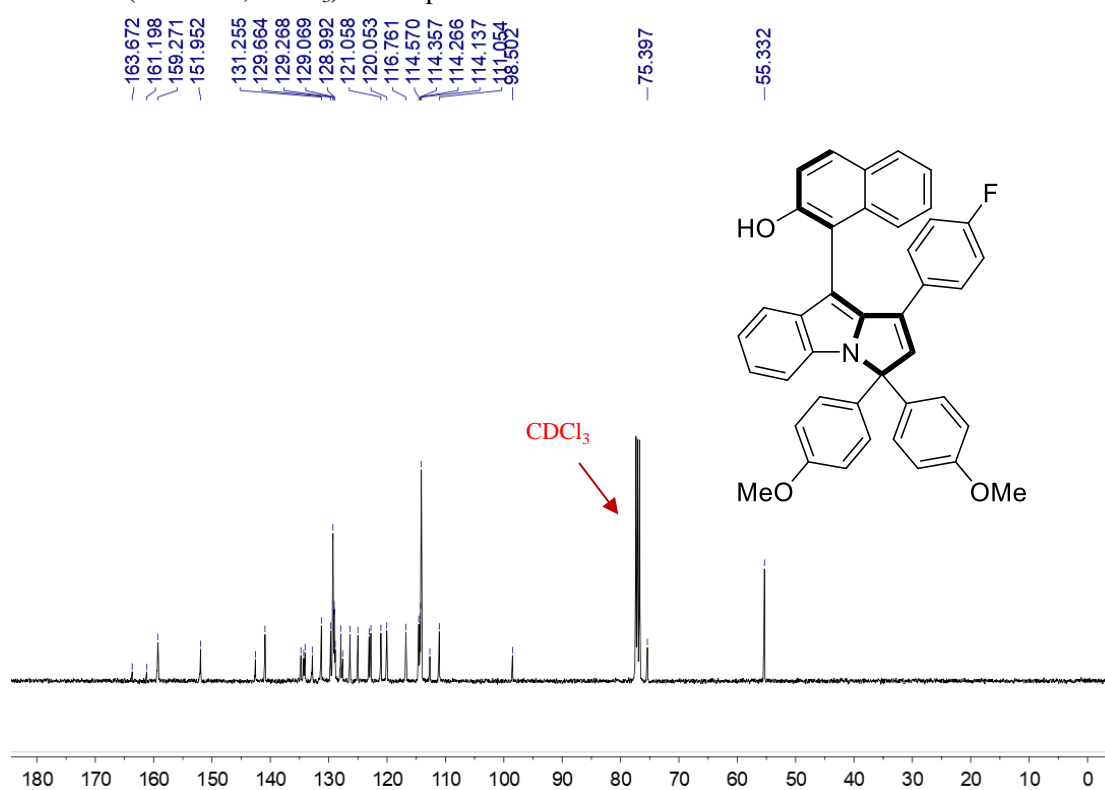
^{13}C NMR (100 MHz, CDCl_3) of compound **3ac**:



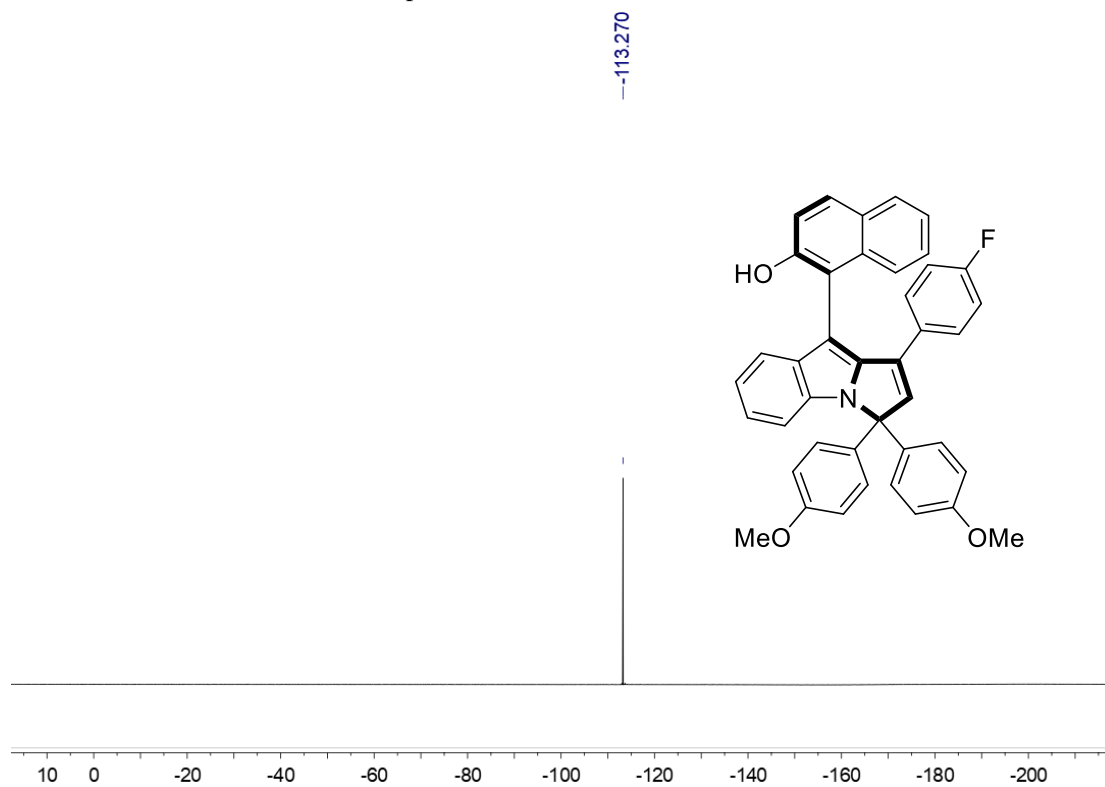
^1H NMR (400 MHz, CDCl_3) of compound **3ad**:



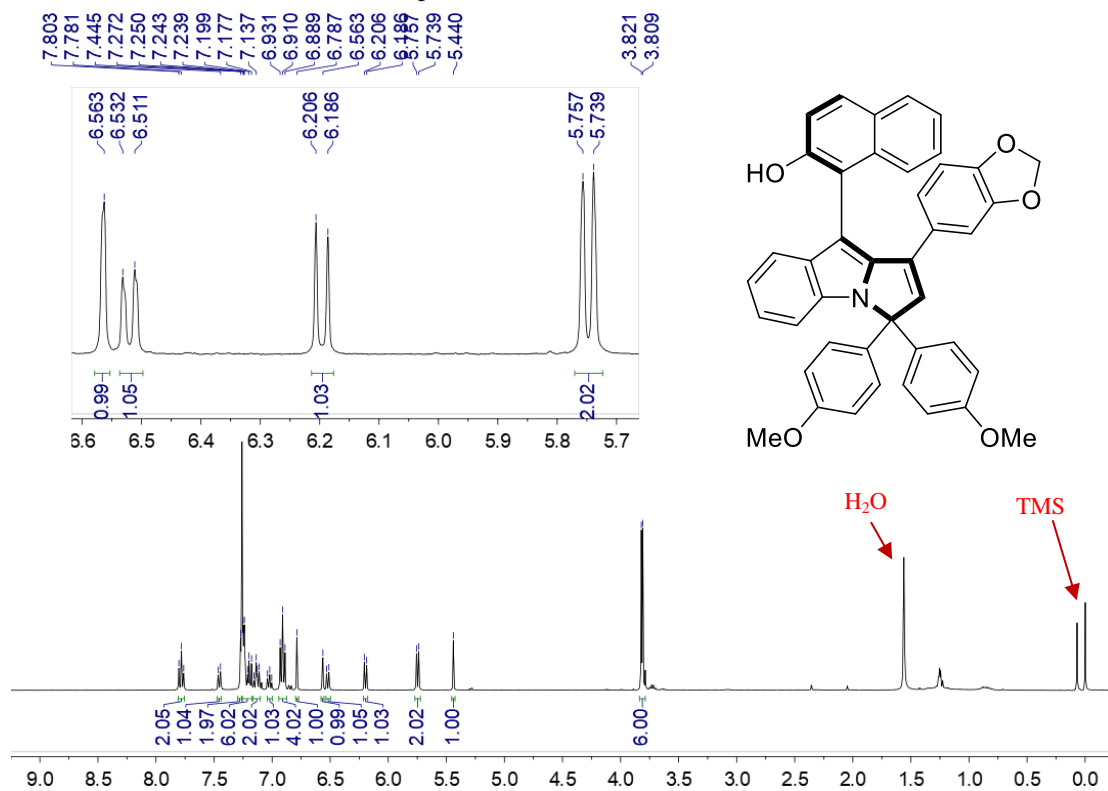
^{13}C NMR (100 MHz, CDCl_3) of compound **3ad**:



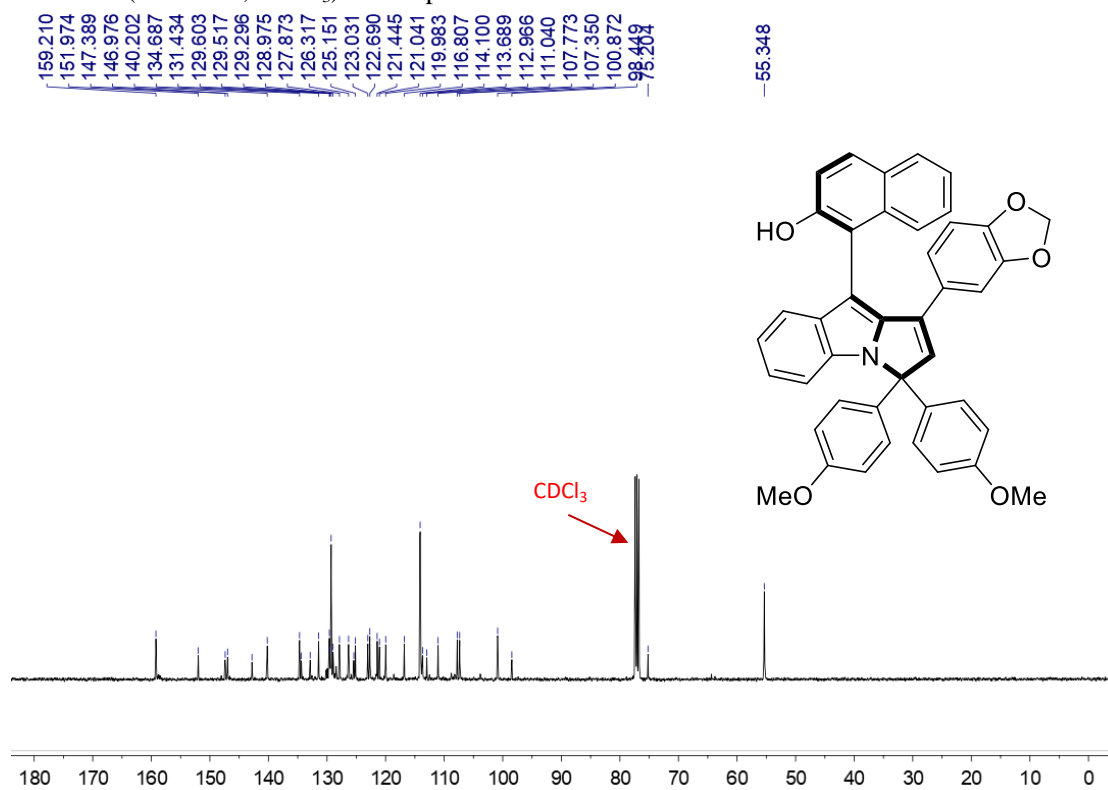
^{19}F NMR (376 MHz, CDCl_3) of compound **3ad**:



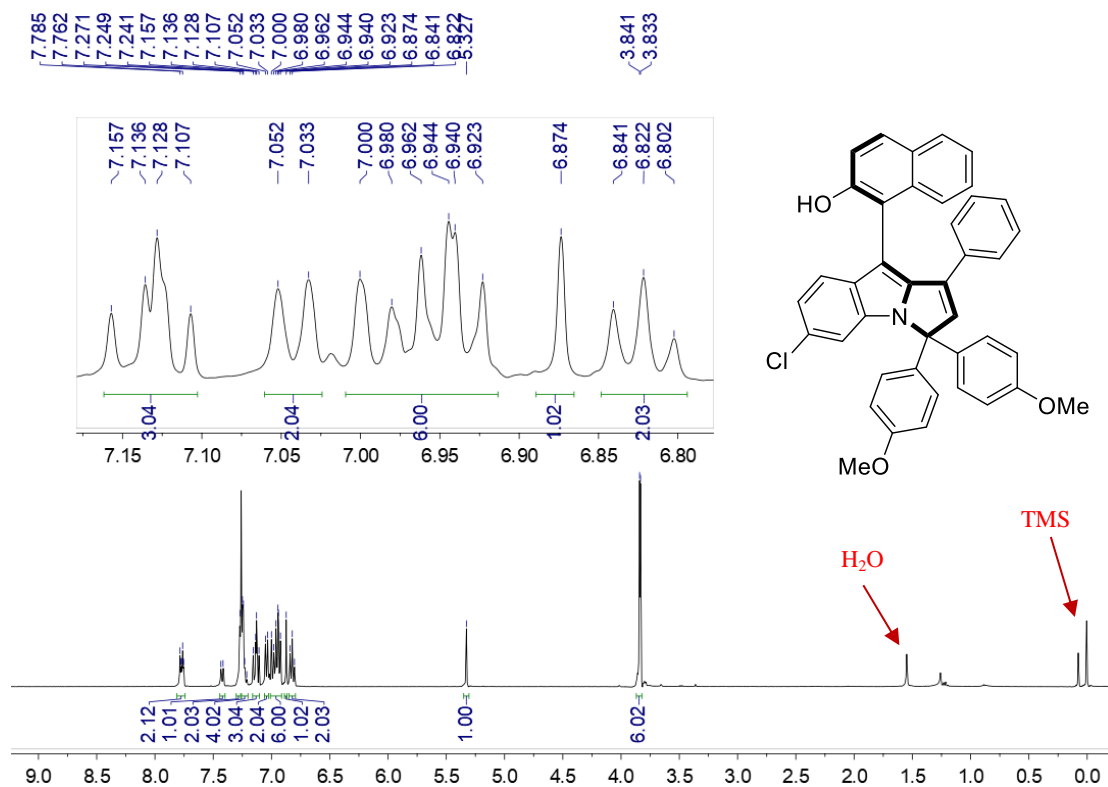
^1H NMR (400 MHz, CDCl_3) of compound **3ae**:



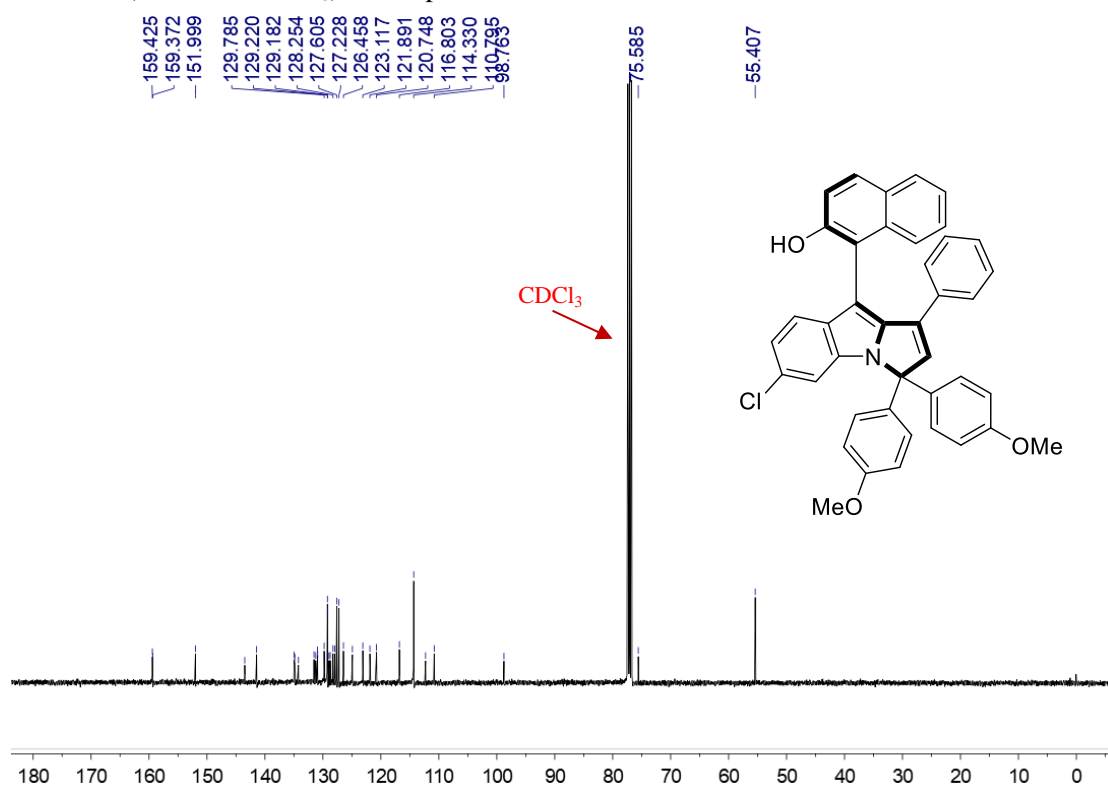
^{13}C NMR (100 MHz, CDCl_3) of compound **3ae**:



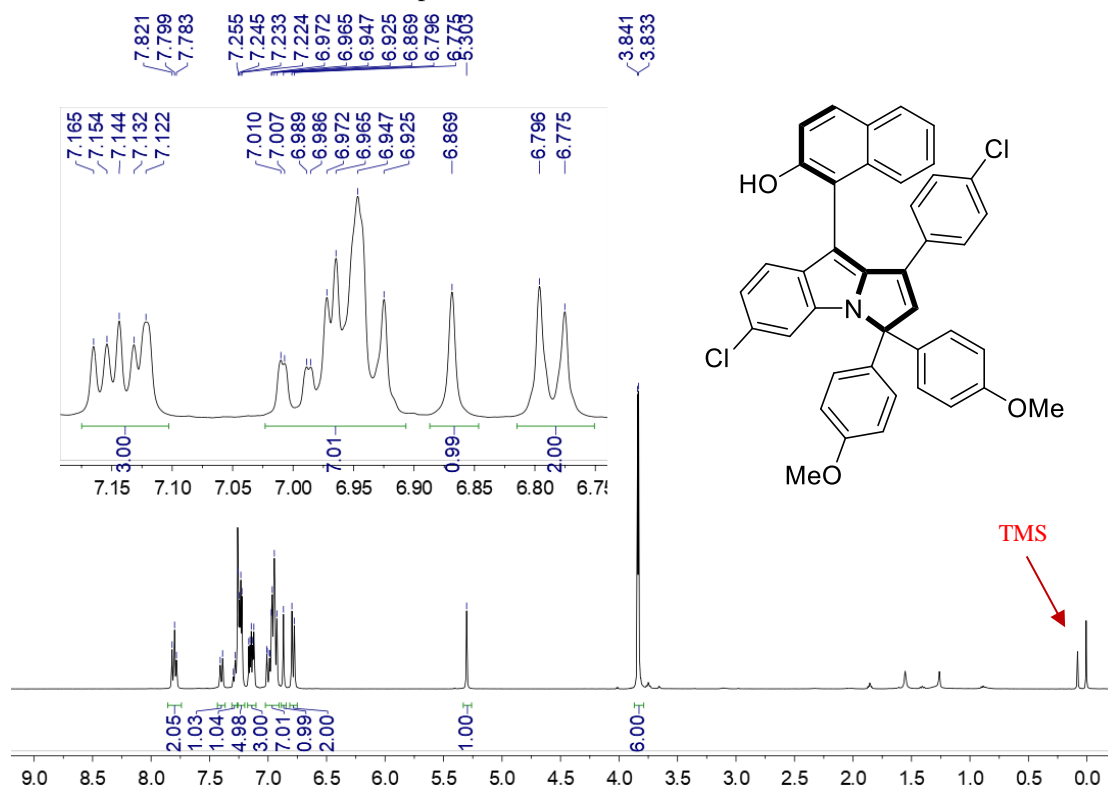
^1H NMR (400 MHz, CDCl_3) of compound **3ea**:



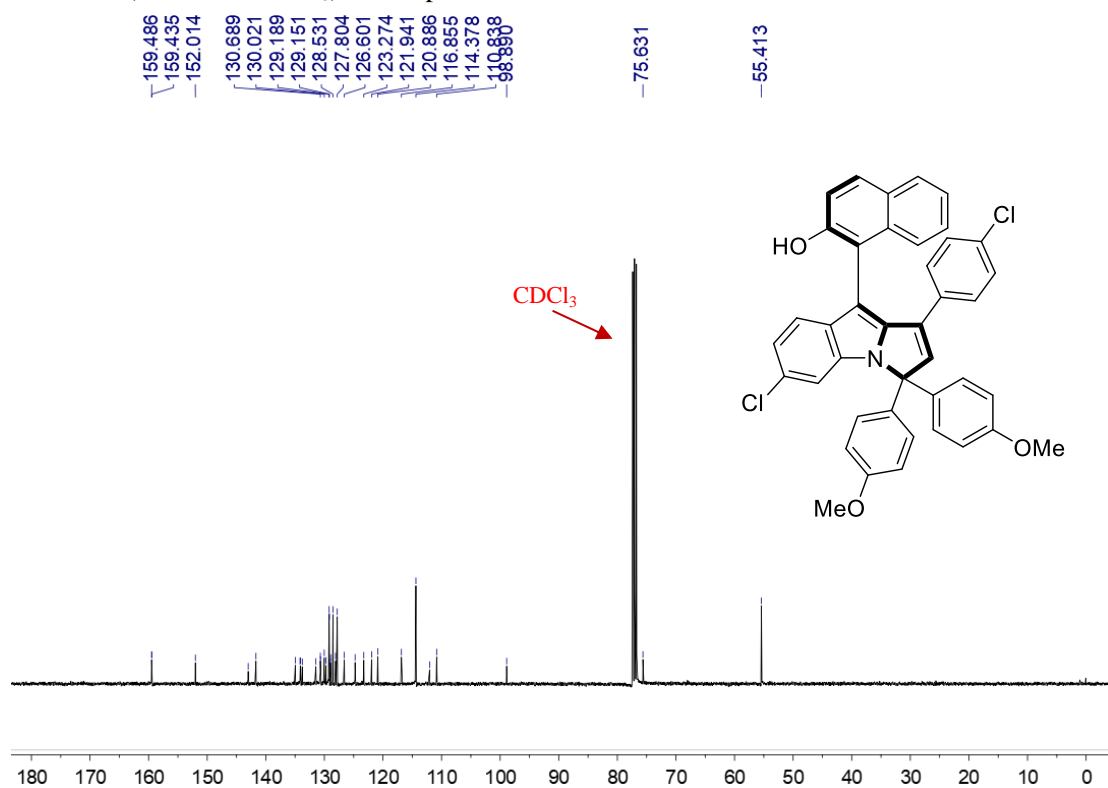
^{13}C NMR (100 MHz, CDCl_3) of compound **3ea**:



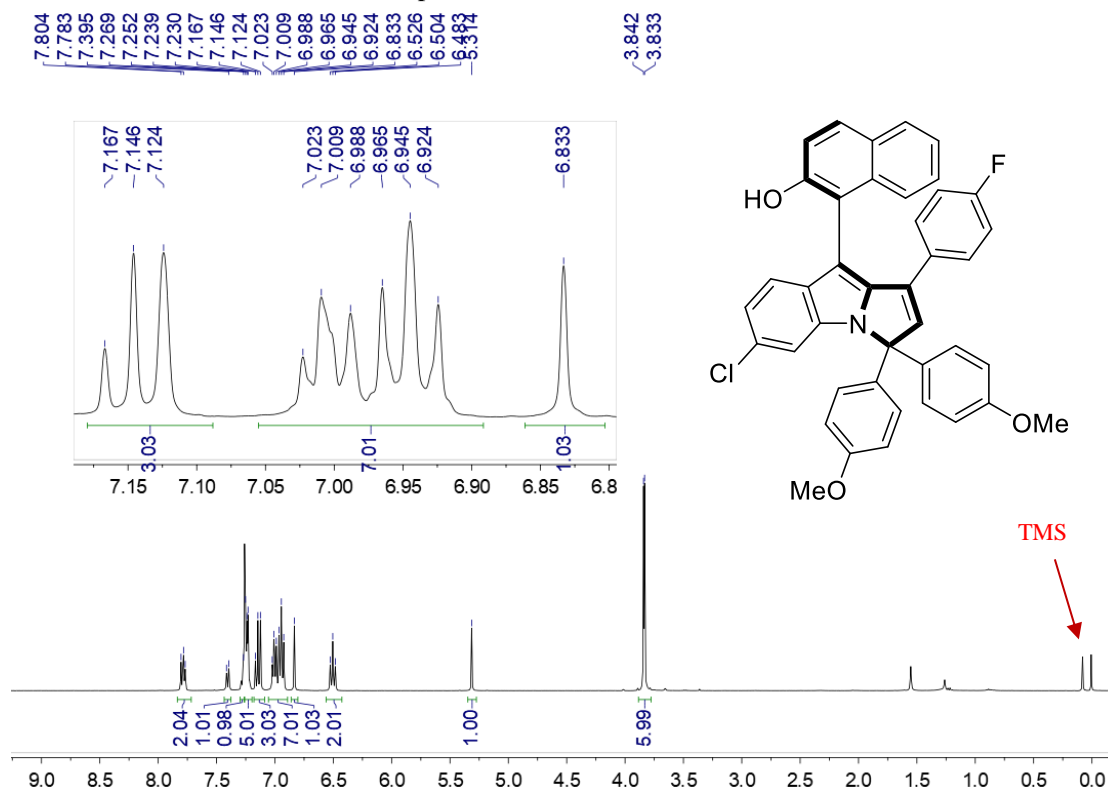
^1H NMR (400 MHz, CDCl_3) of compound **3ef**:



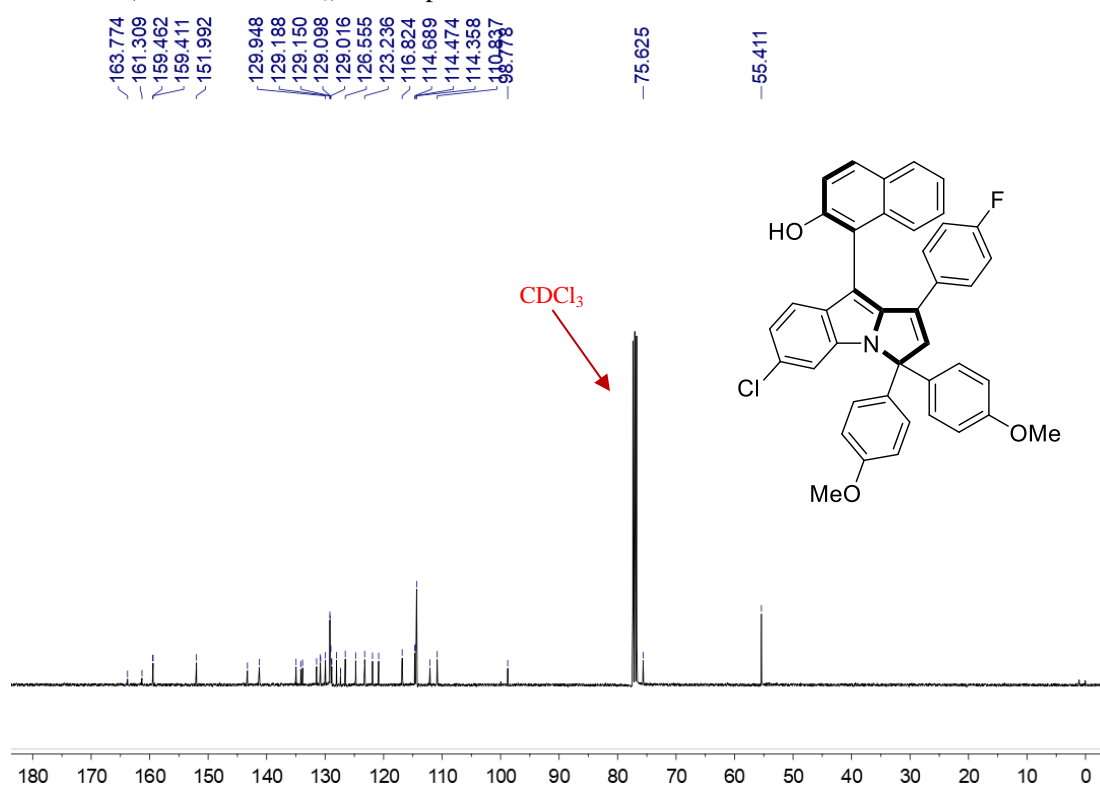
^{13}C NMR (100 MHz, CDCl_3) of compound **3ef**:



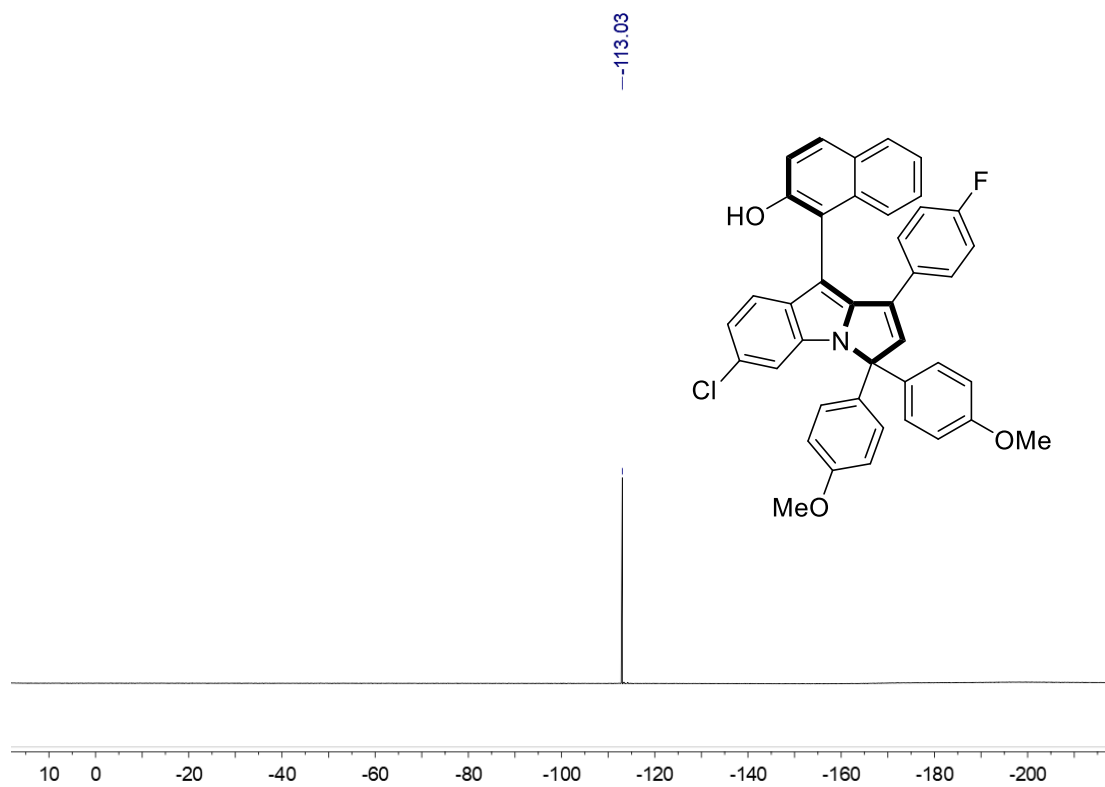
^1H NMR (400 MHz, CDCl_3) of compound **3ed**:



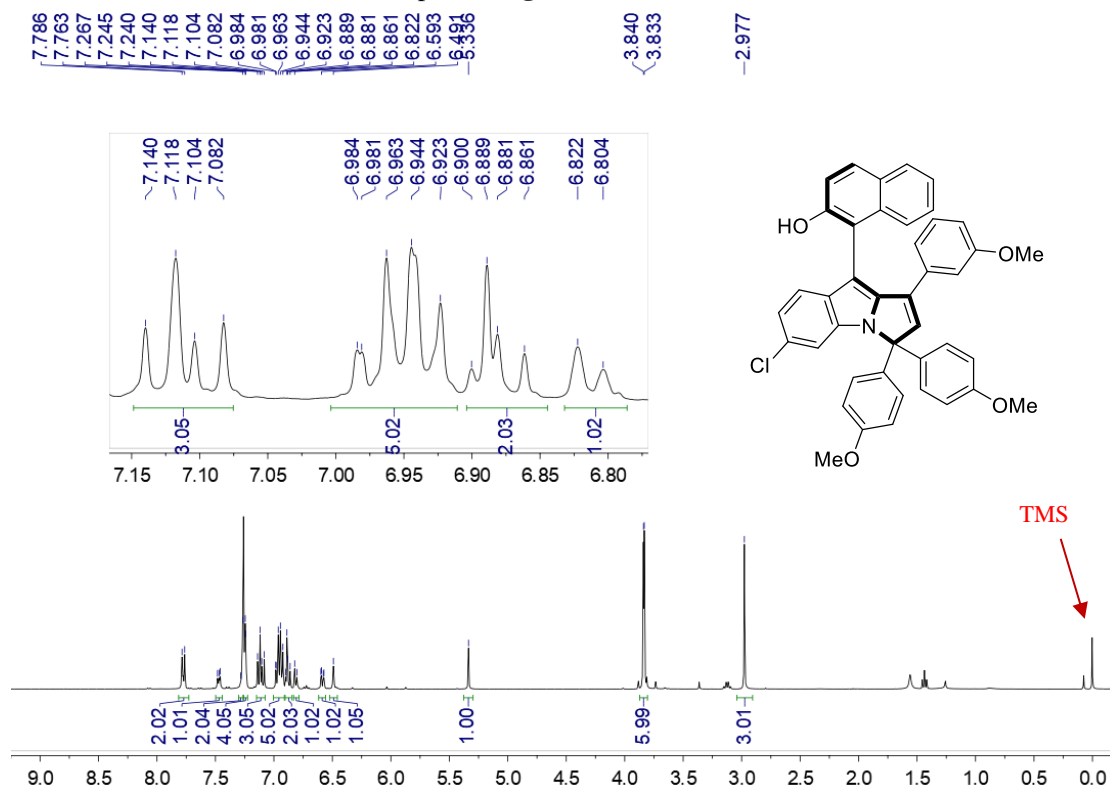
^{13}C NMR (100 MHz, CDCl_3) of compound **3ed**:



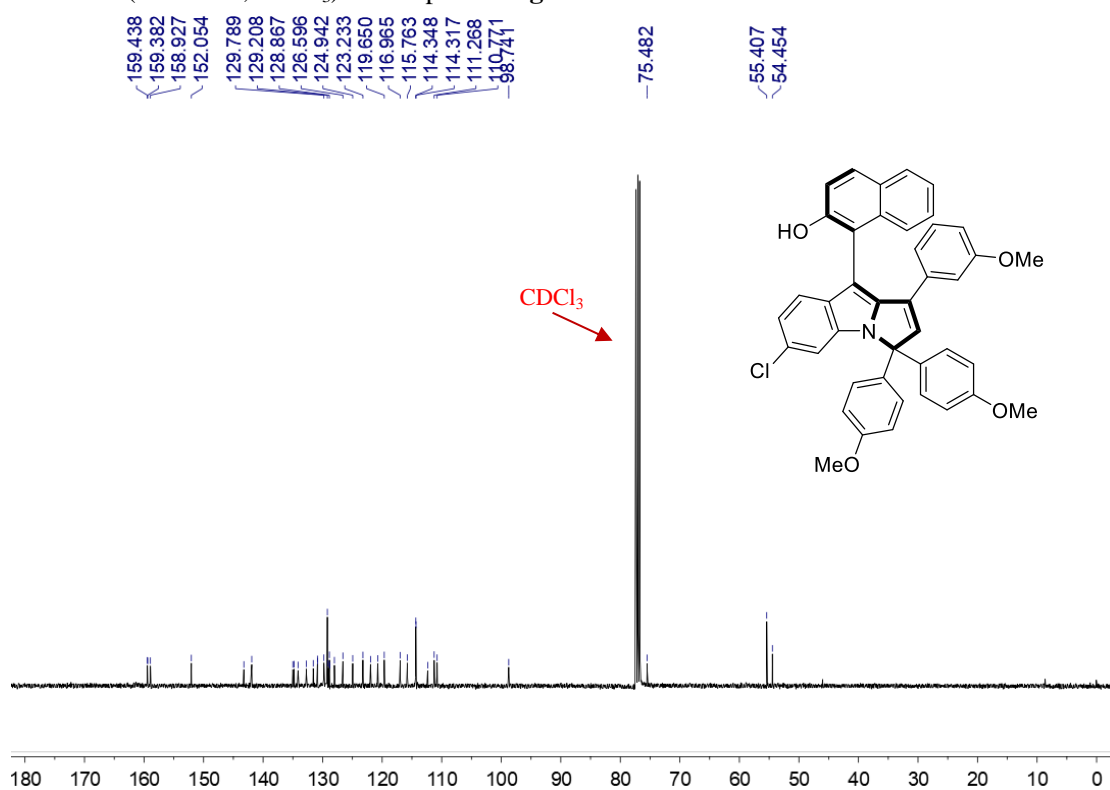
^{19}F NMR (376 MHz, CDCl_3) of compound **3ed**:



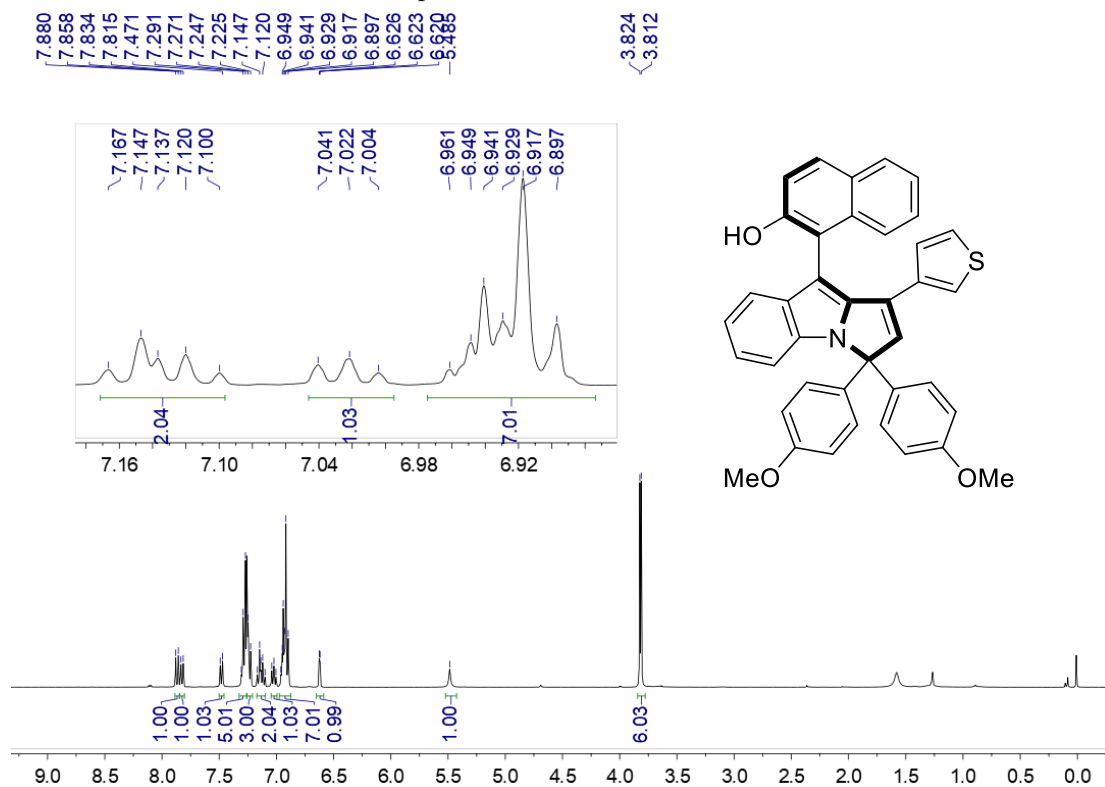
^1H NMR (400 MHz, CDCl_3) of compound **3eg**:



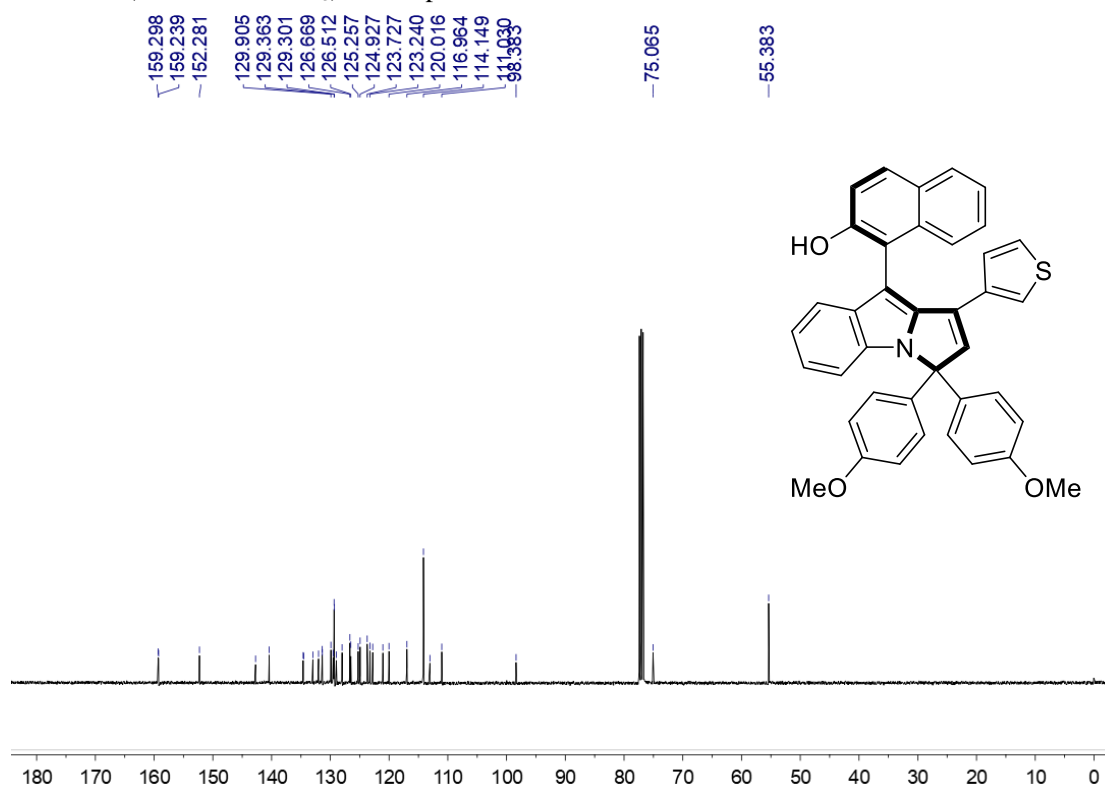
^{13}C NMR (100 MHz, CDCl_3) of compound **3eg**:



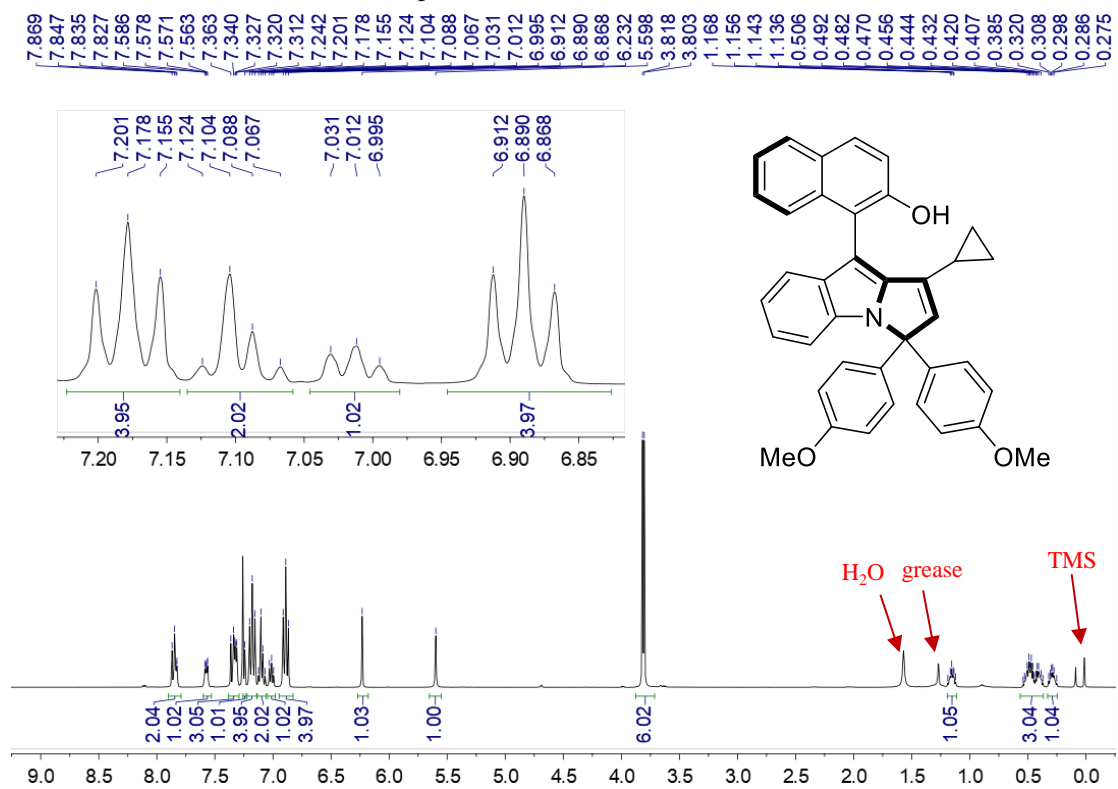
¹H NMR (400 MHz, CDCl₃) of compound **3ah**:



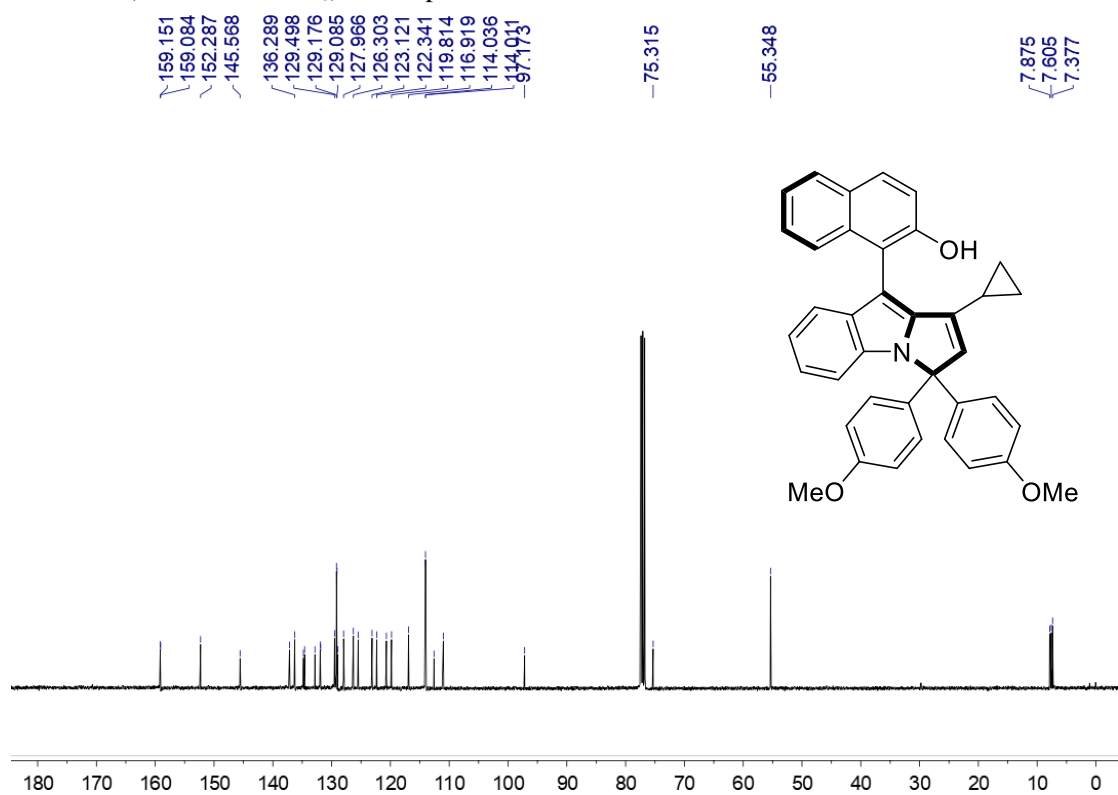
¹³C NMR (100 MHz, CDCl₃) of compound **3ah**:



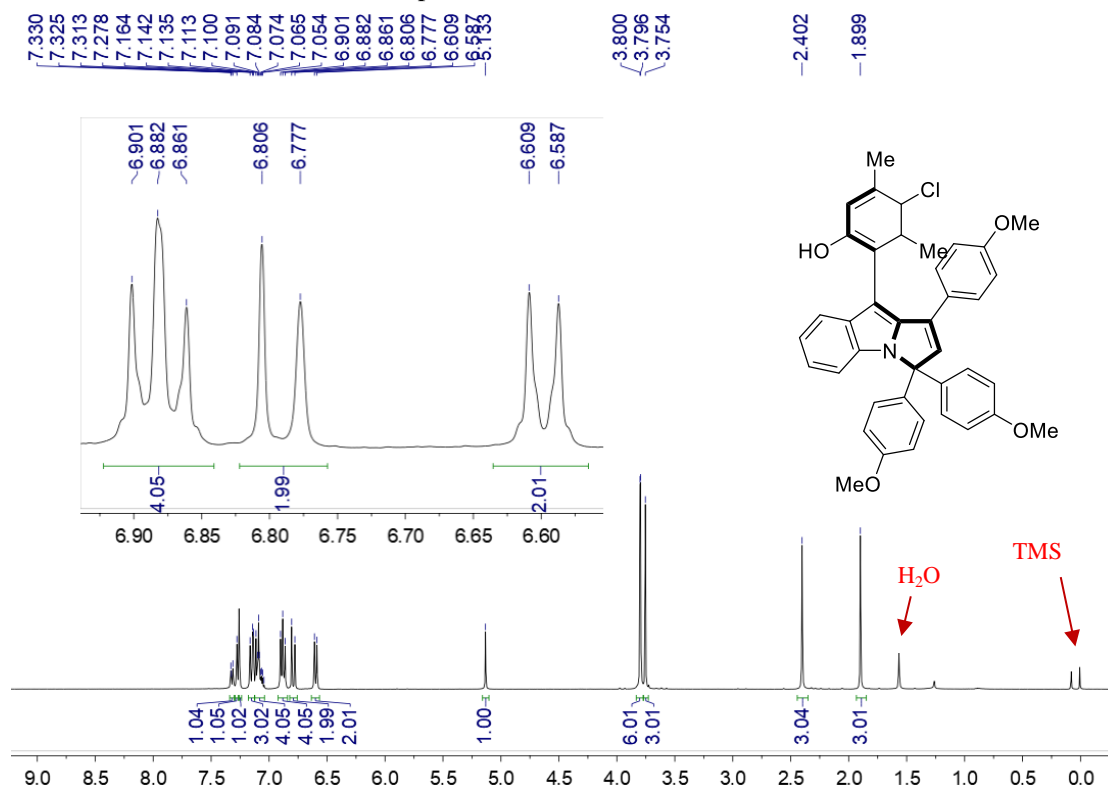
¹H NMR (400 MHz, CDCl₃) of compound **3ai**:



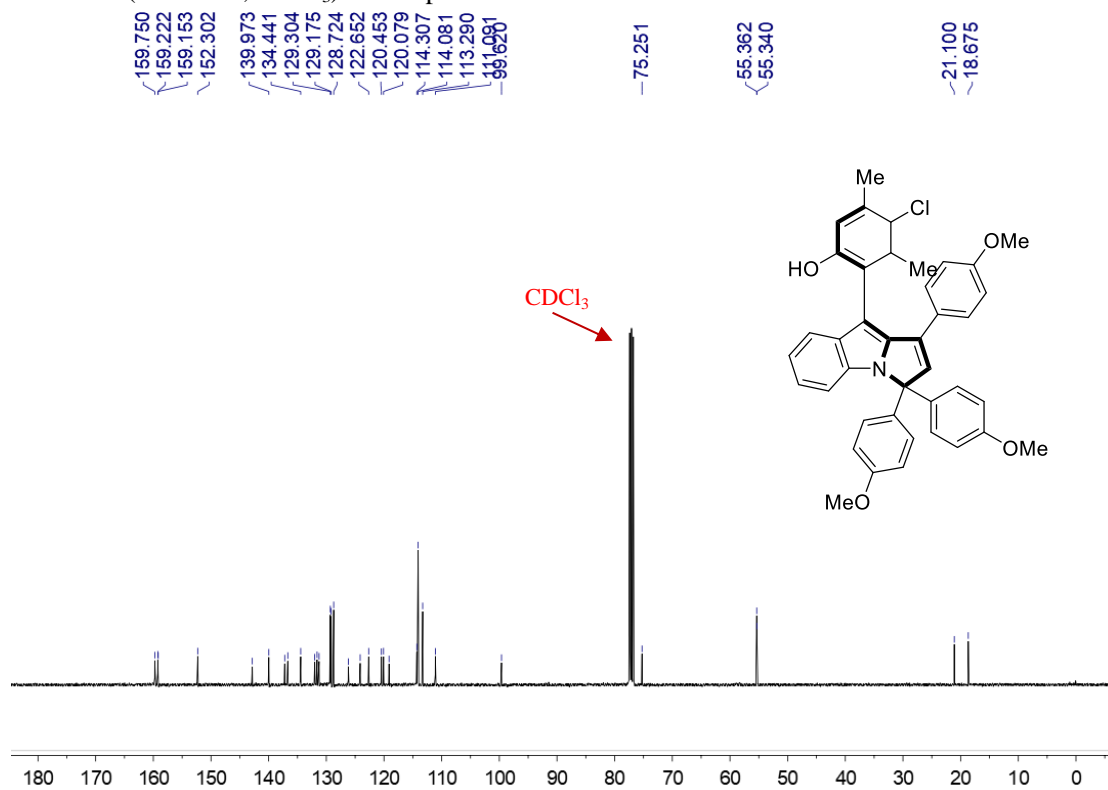
¹³C NMR (100 MHz, CDCl₃) of compound **3ai**:



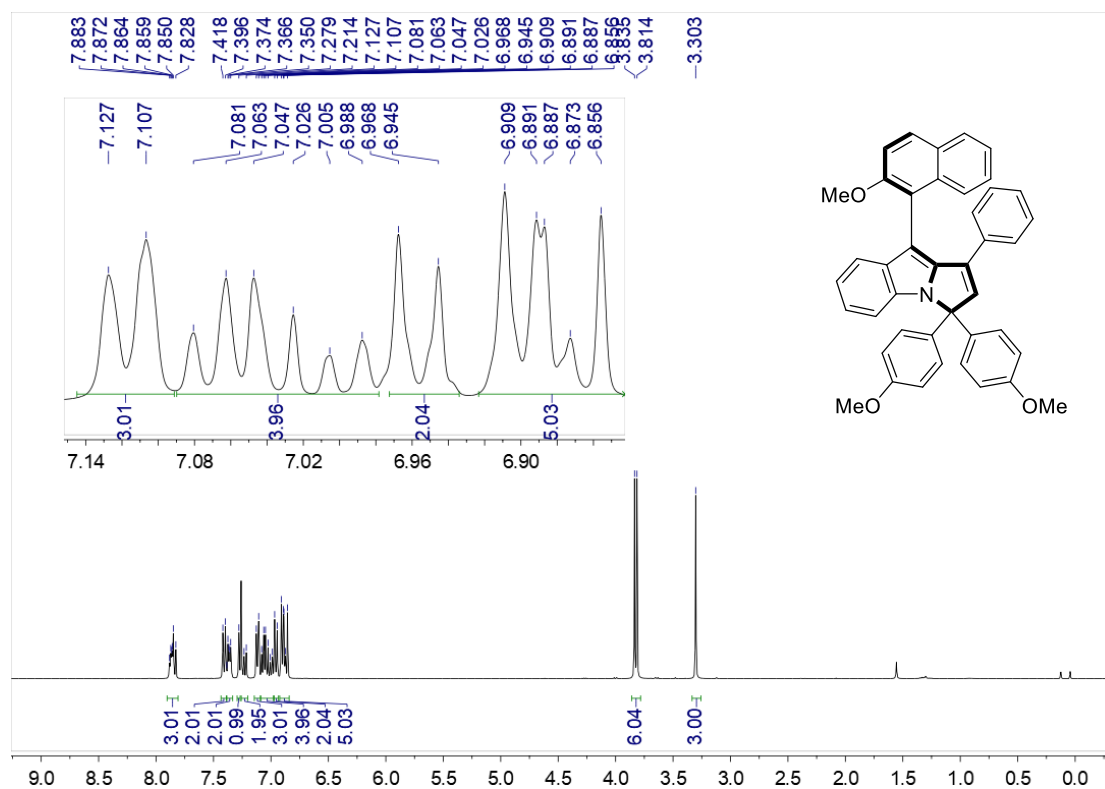
^1H NMR (400 MHz, CDCl_3) of compound **3mb**:



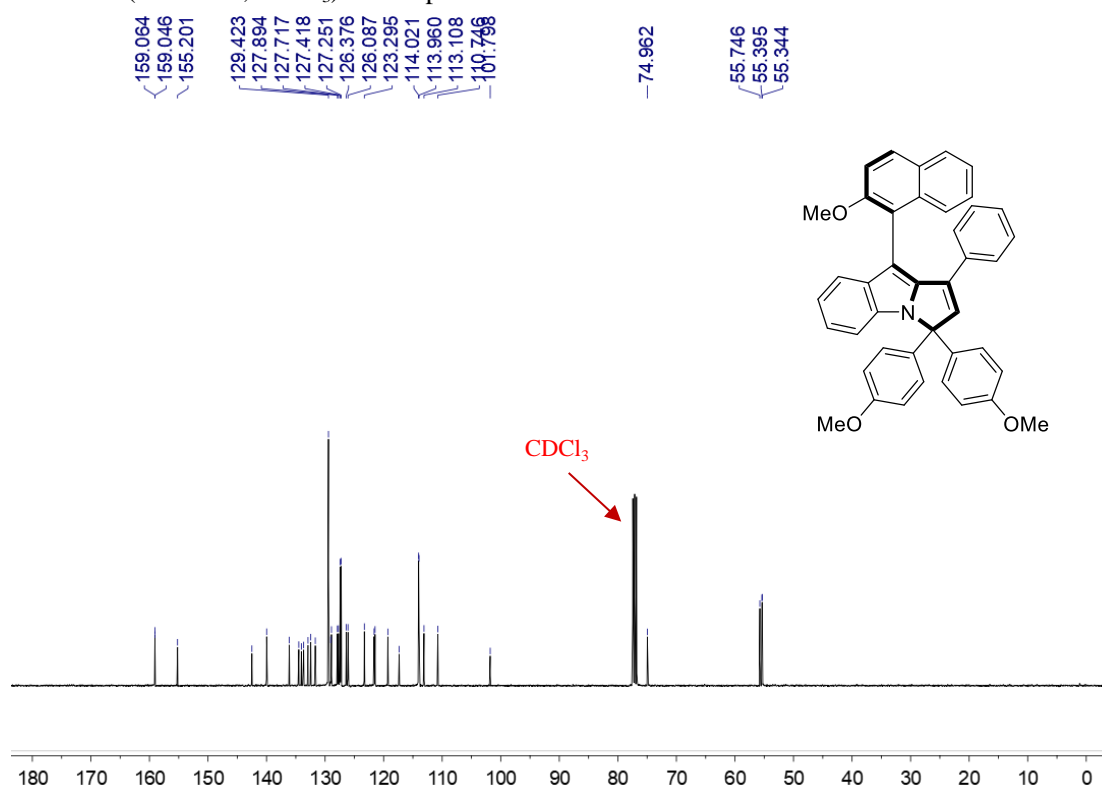
^{13}C NMR (100 MHz, CDCl_3) of compound **3mb**:



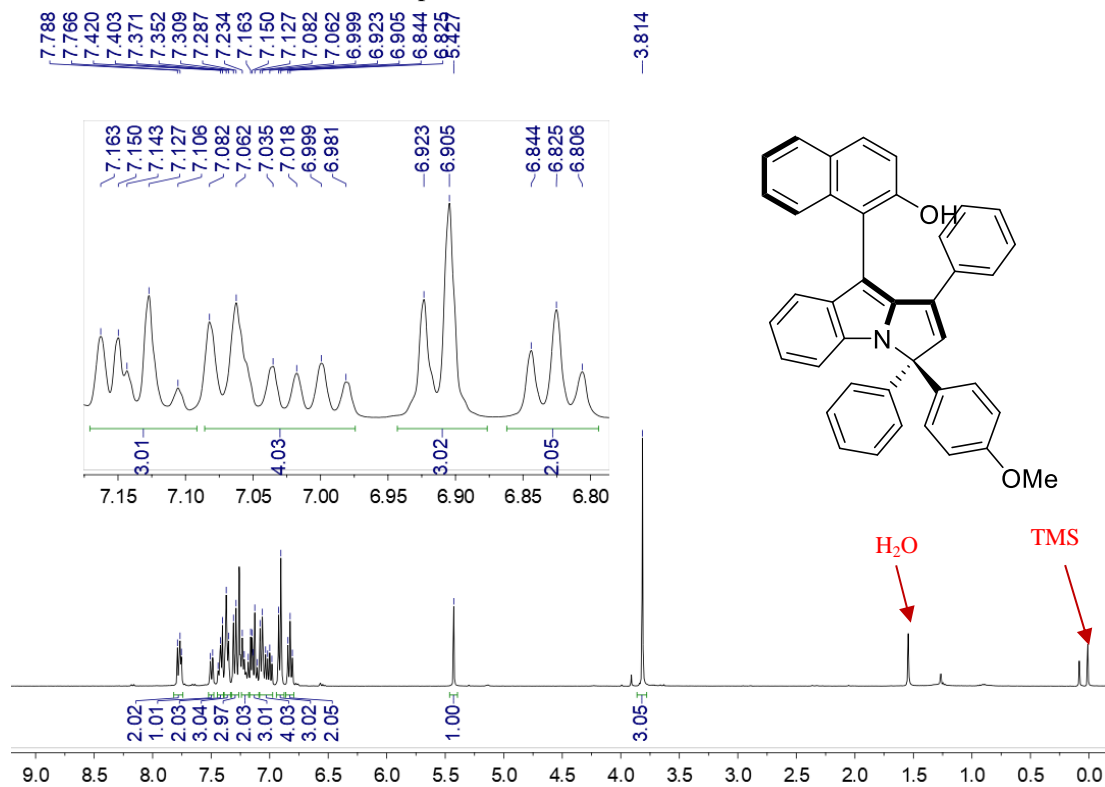
^1H NMR (400 MHz, CDCl_3) of compound **3na**:



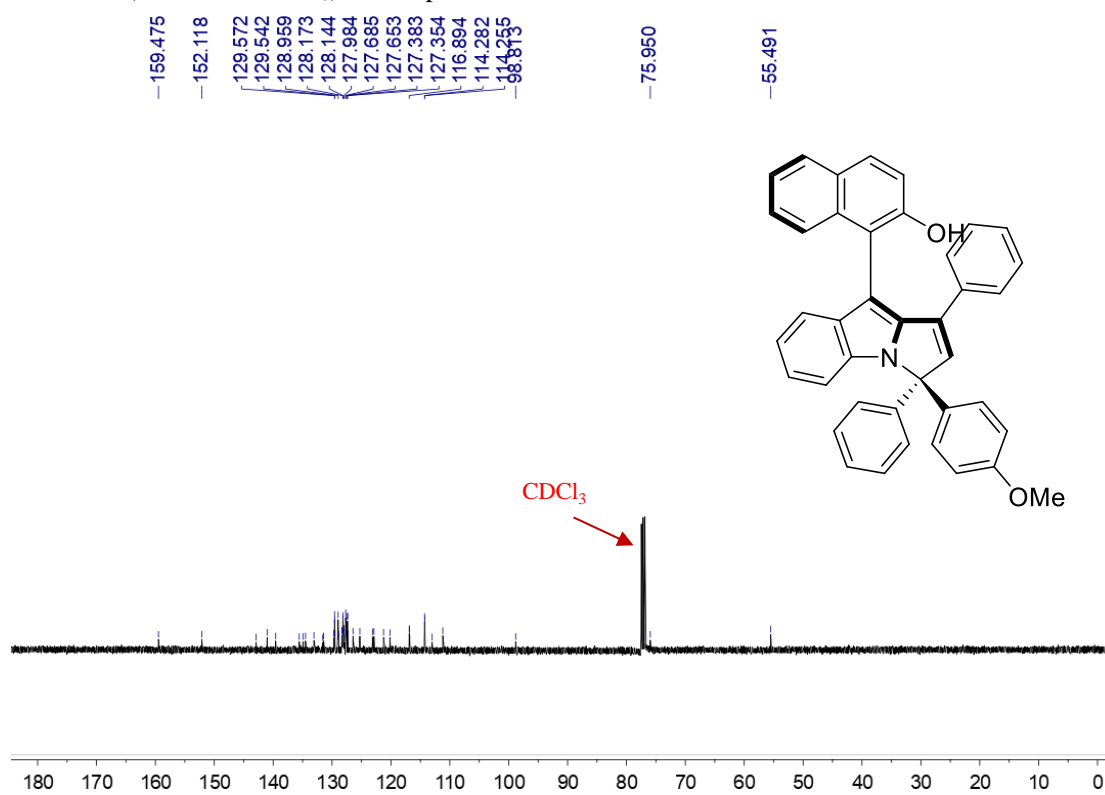
^{13}C NMR (100 MHz, CDCl_3) of compound **3na**:



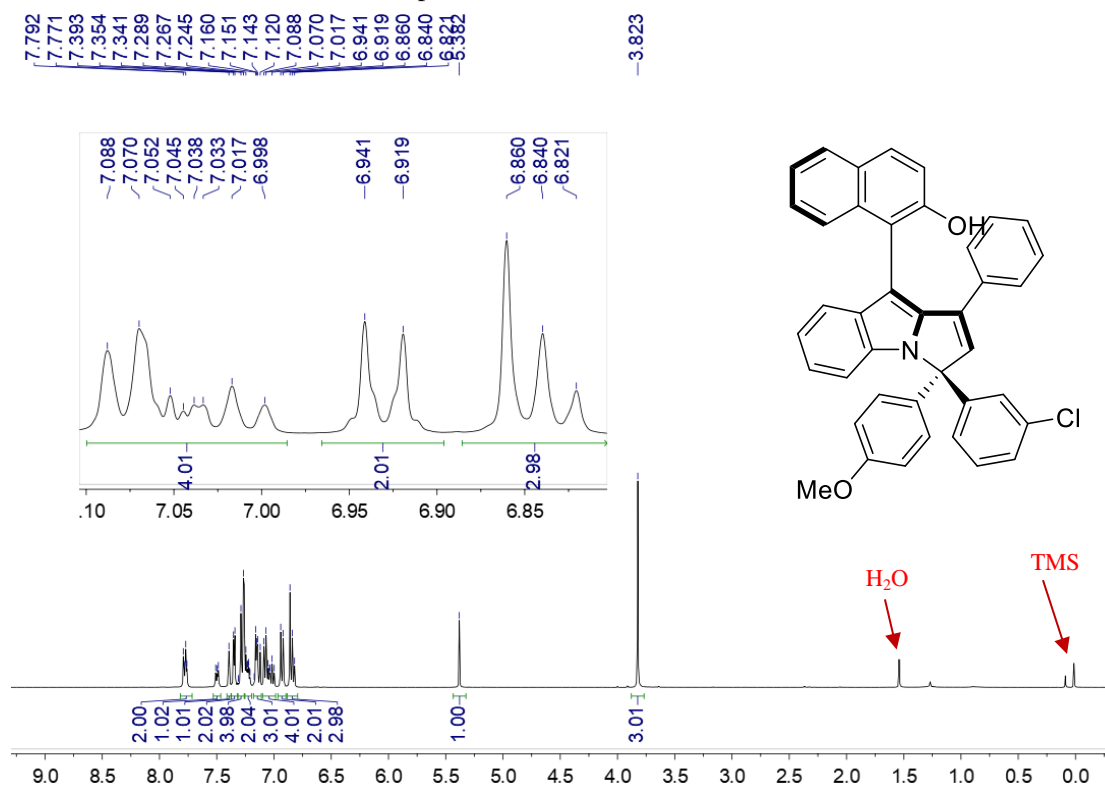
^1H NMR (400 MHz, CDCl_3) of compound **7ab**:



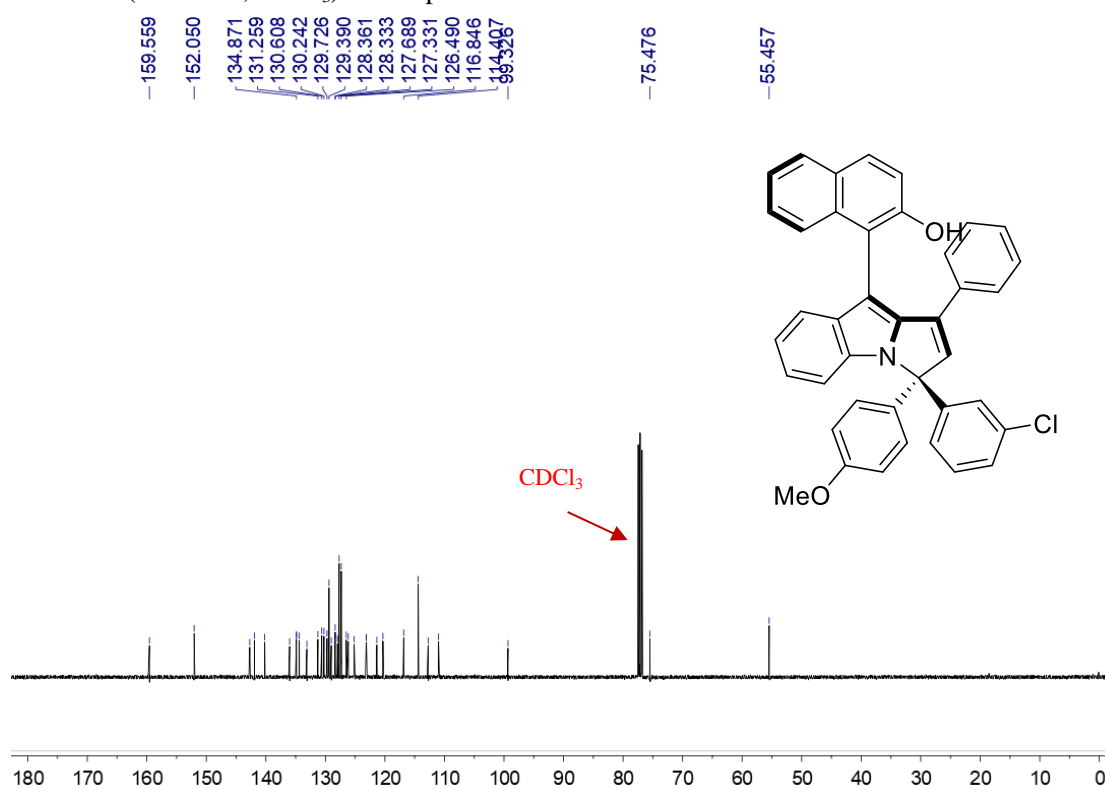
^{13}C NMR (100 MHz, CDCl_3) of compound **7ab**:



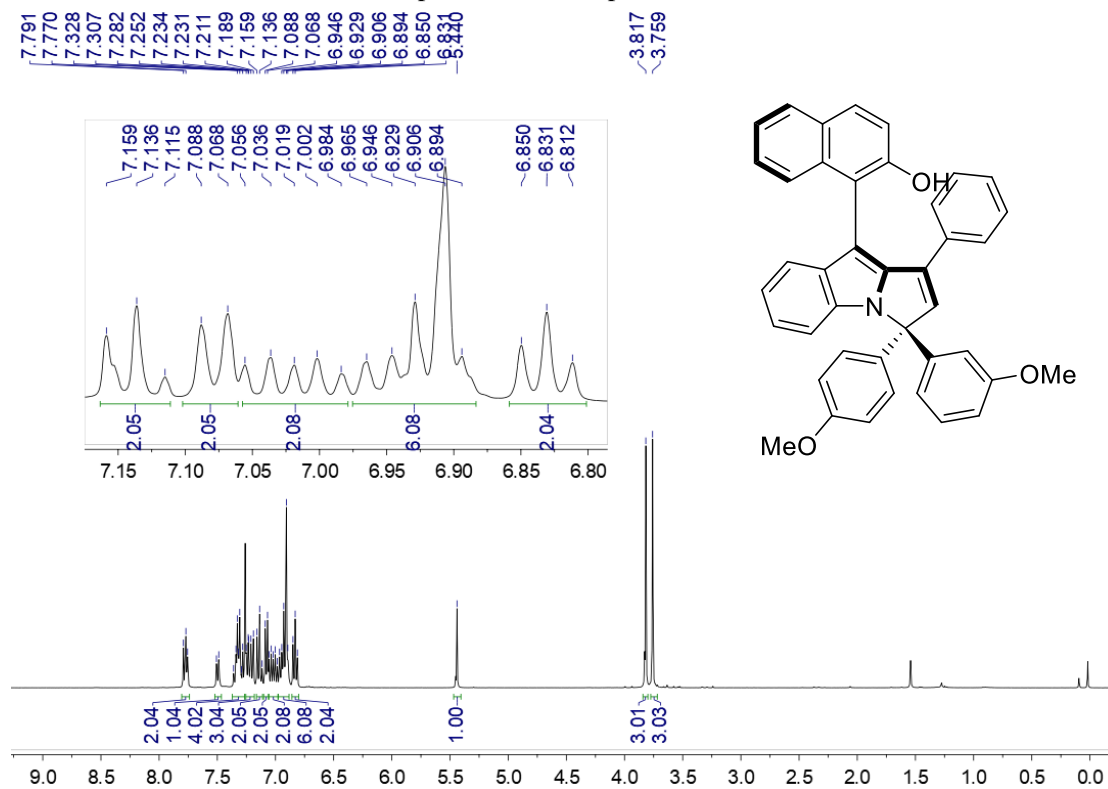
^1H NMR (400 MHz, CDCl_3) of compound **7ac**:



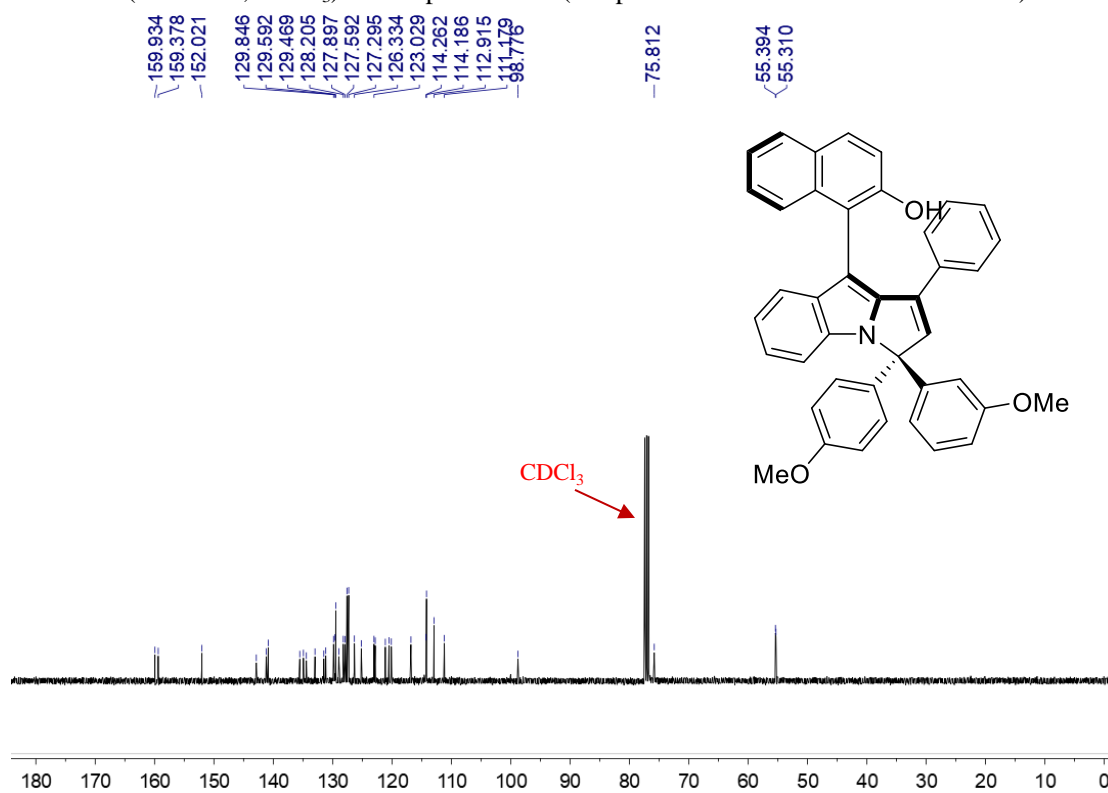
^{13}C NMR (100 MHz, CDCl_3) of compound **7ac**:



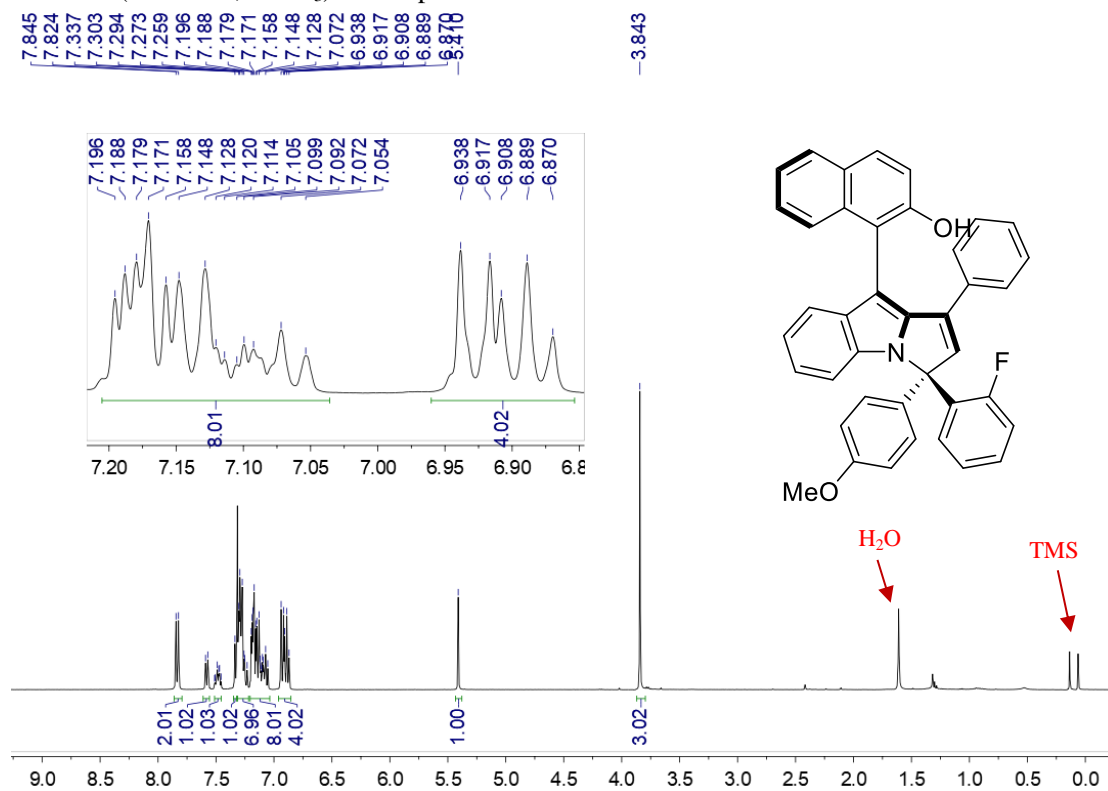
^1H NMR (400 MHz, CDCl_3) of compound **7ad**: (inseparable diastereomers with 88:12 dr)



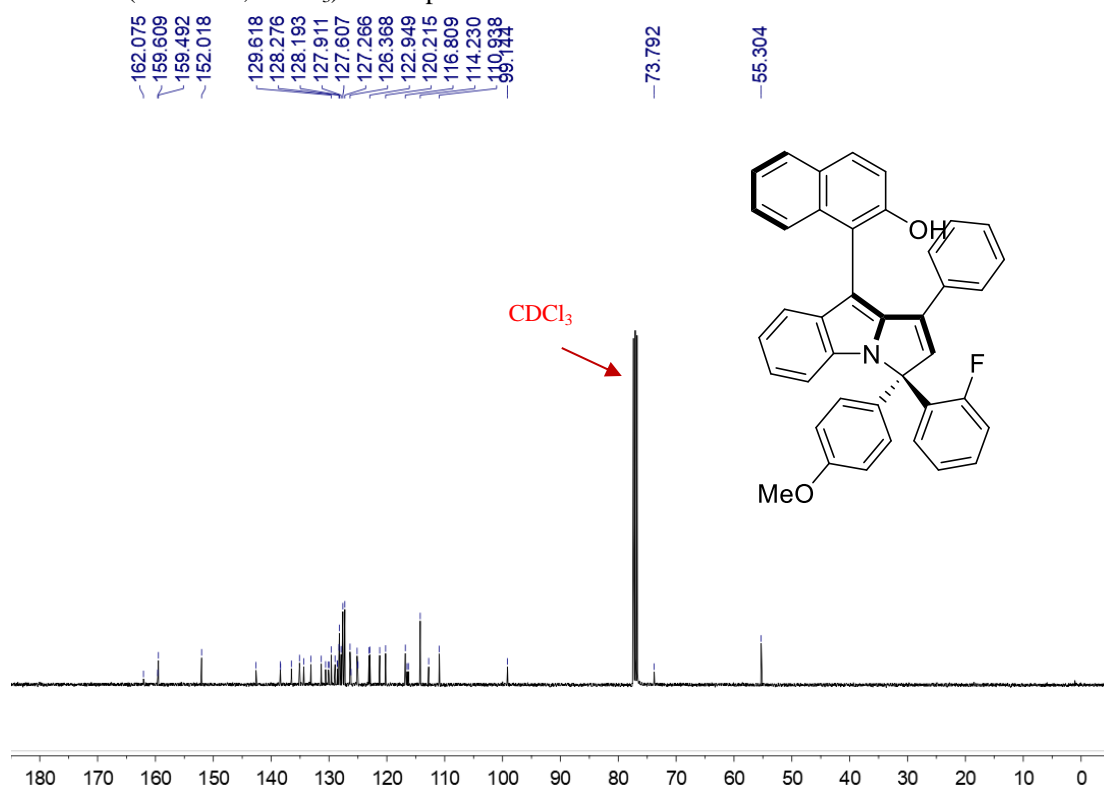
^{13}C NMR (100 MHz, CDCl_3) of compound **7ad**: (inseparable diastereomers with 88:12 dr)



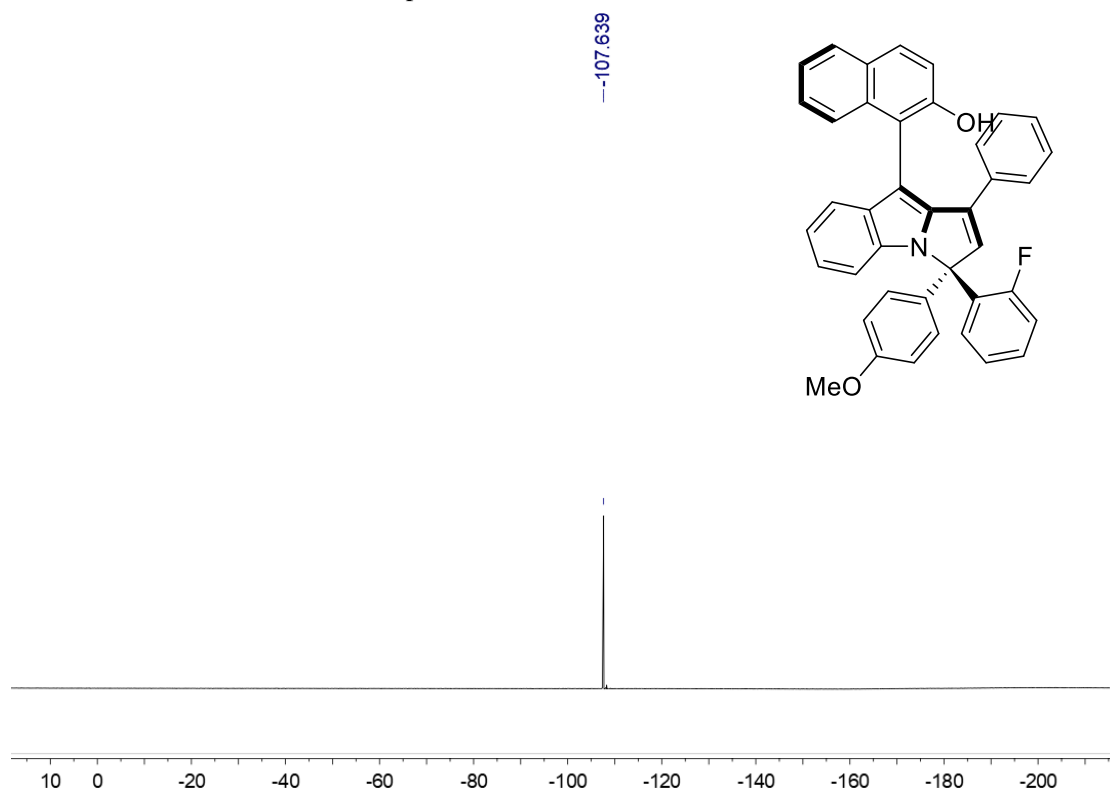
^1H NMR (400 MHz, CDCl_3) of compound **7ae**:



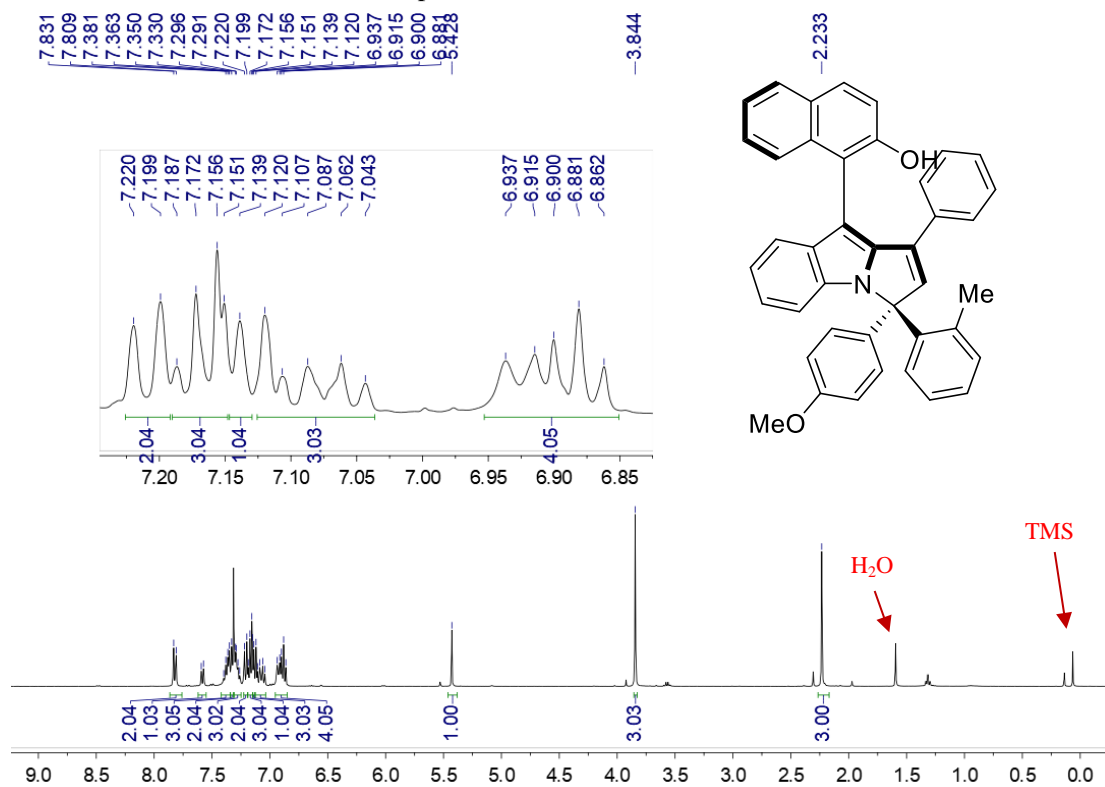
^{13}C NMR (100 MHz, CDCl_3) of compound **7ae**:



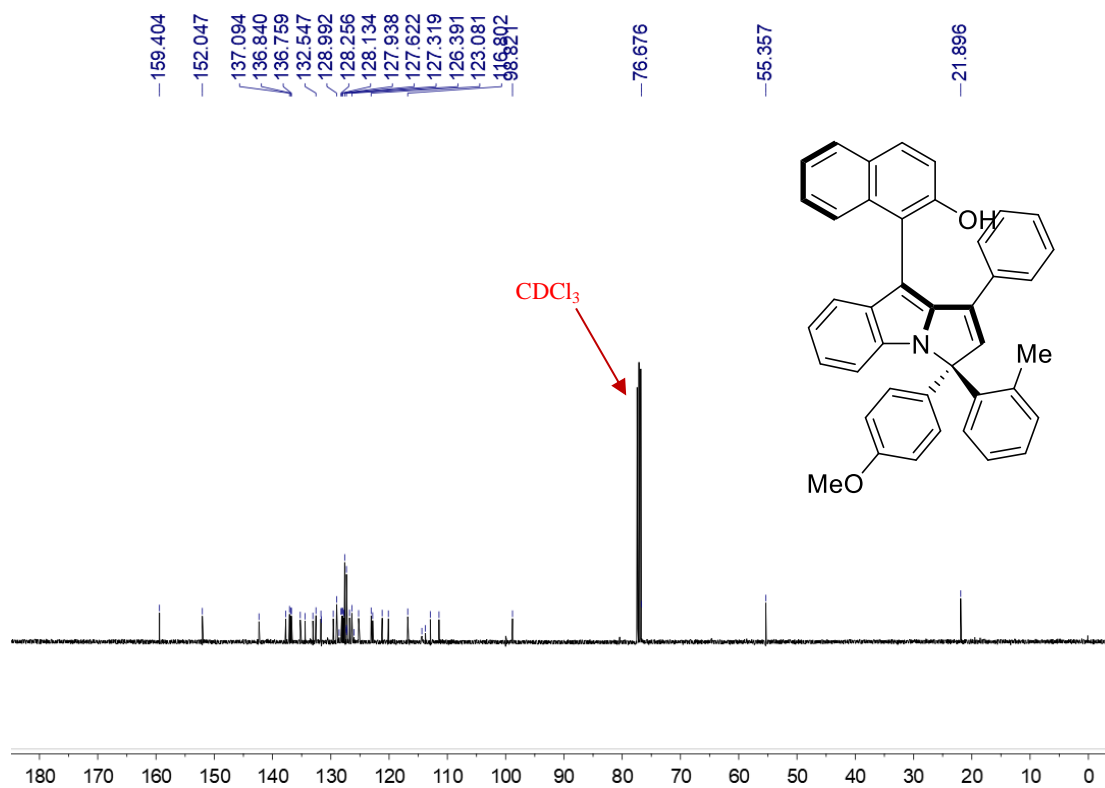
^{19}F NMR (376 MHz, CDCl_3) of compound **7ae**:



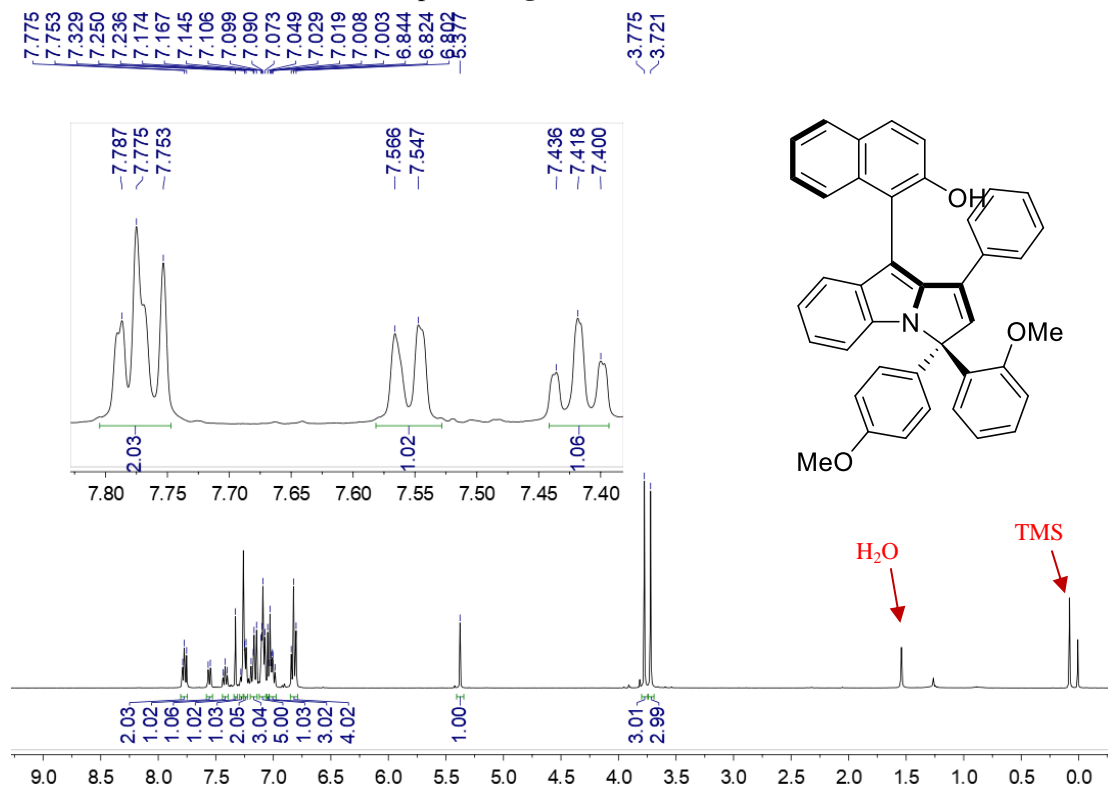
^1H NMR (400 MHz, CDCl_3) of compound **7af**:



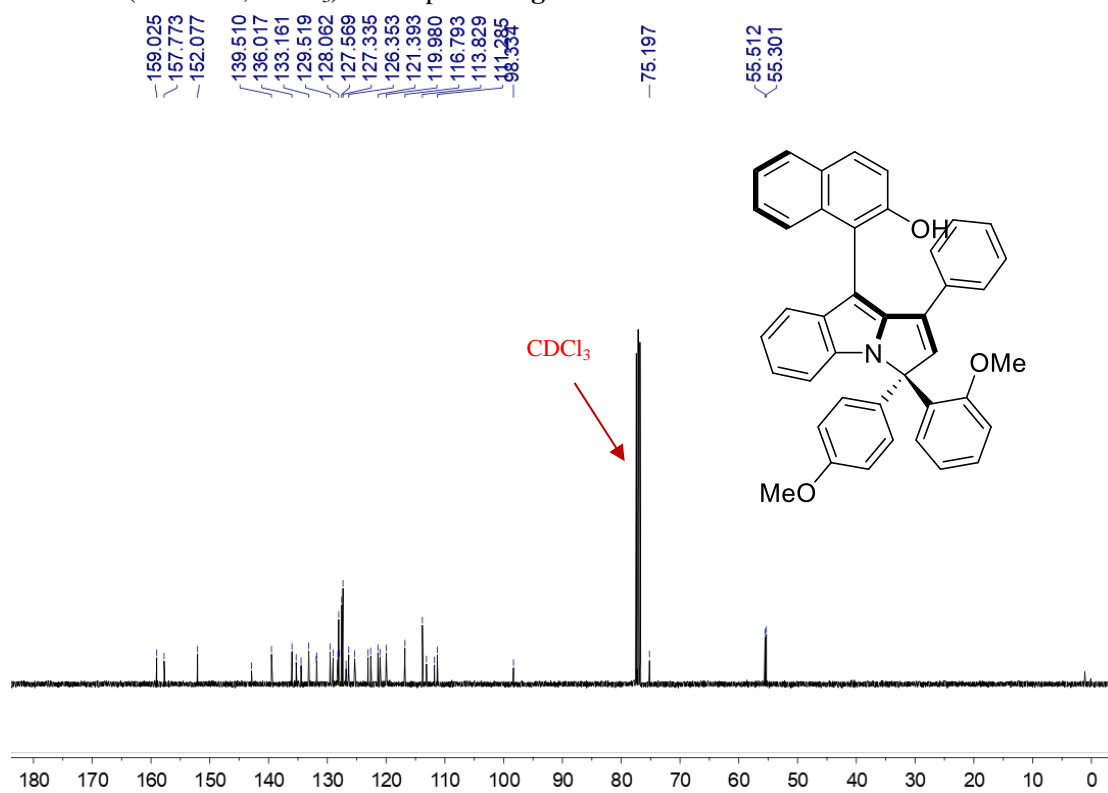
^{13}C NMR (100 MHz, CDCl_3) of compound **7af**:



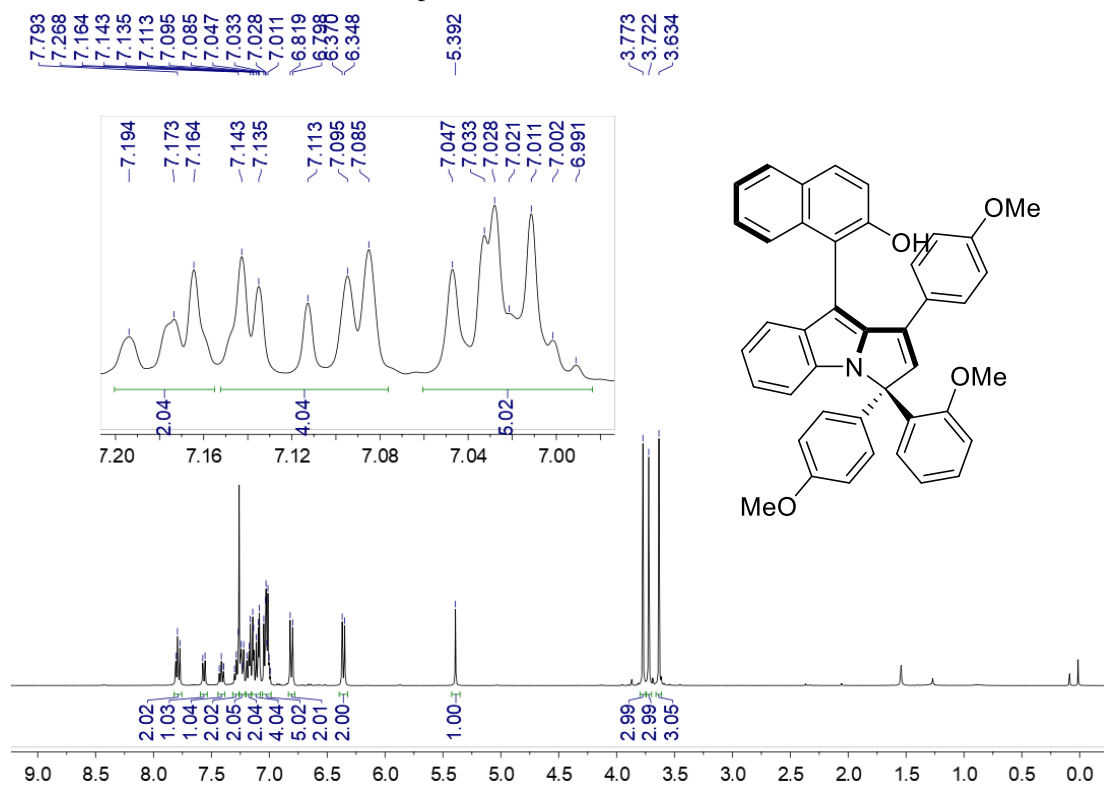
^1H NMR (400 MHz, CDCl_3) of compound **7ag**:



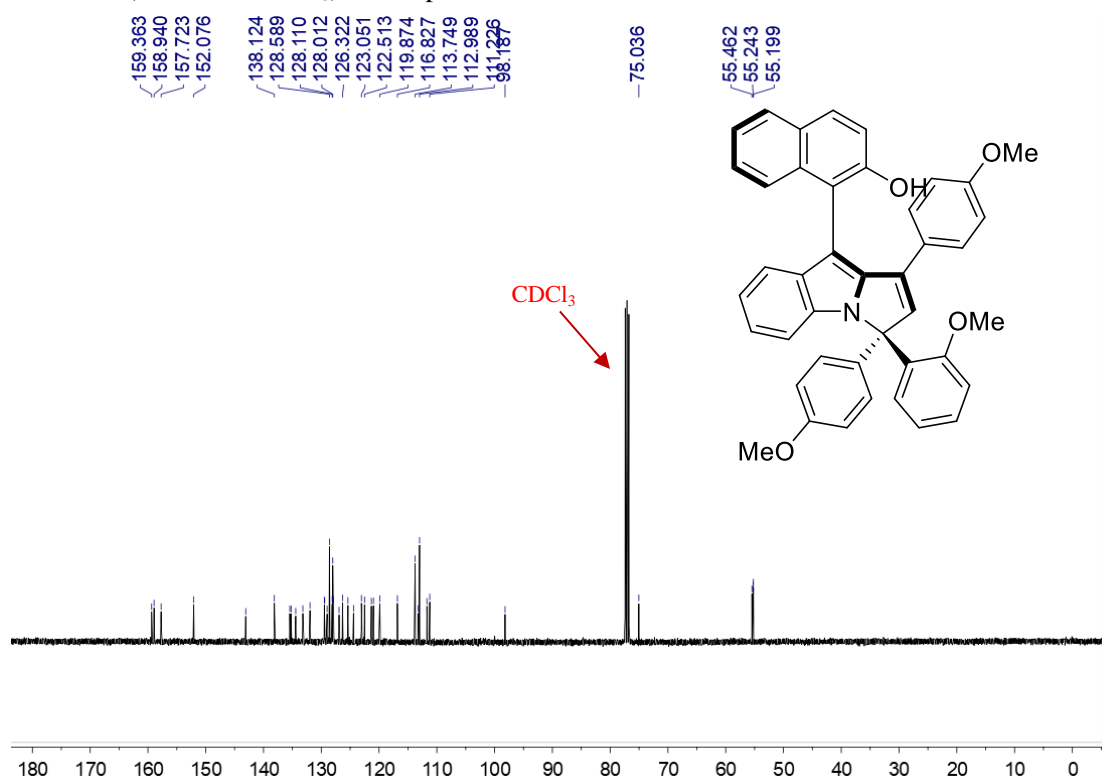
^{13}C NMR (100 MHz, CDCl_3) of compound **7ag**:



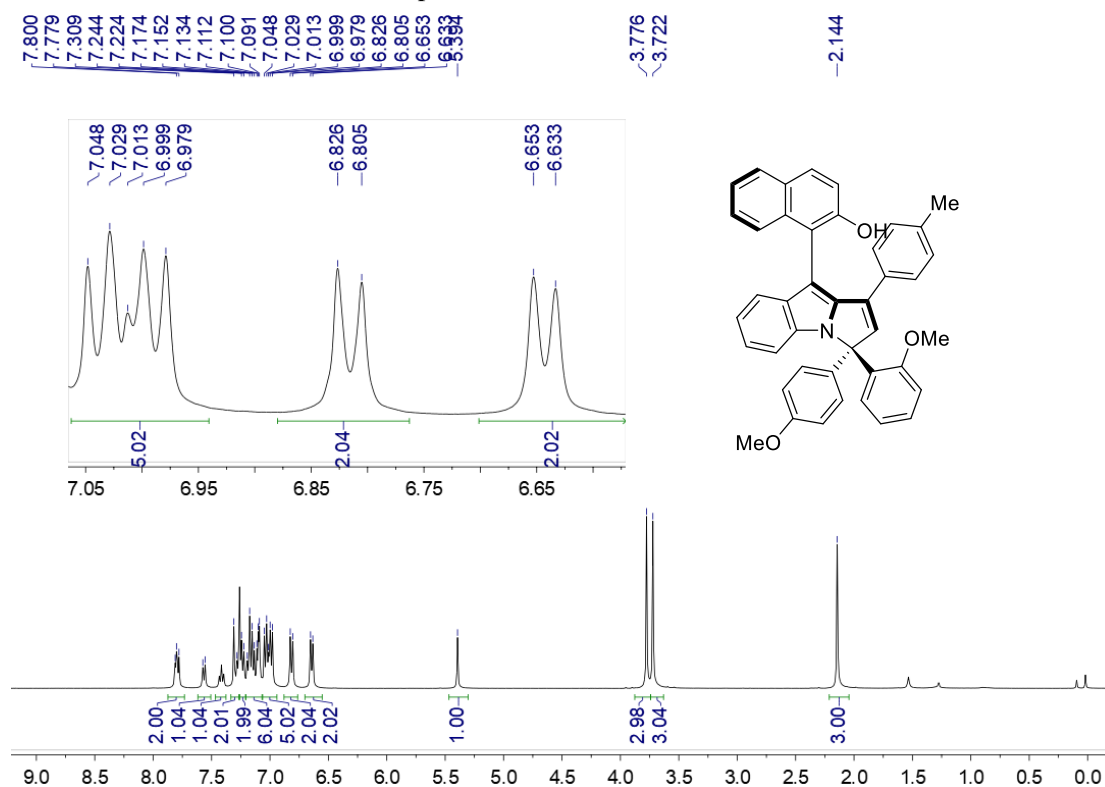
^1H NMR (400 MHz, CDCl_3) of compound **7ah**:



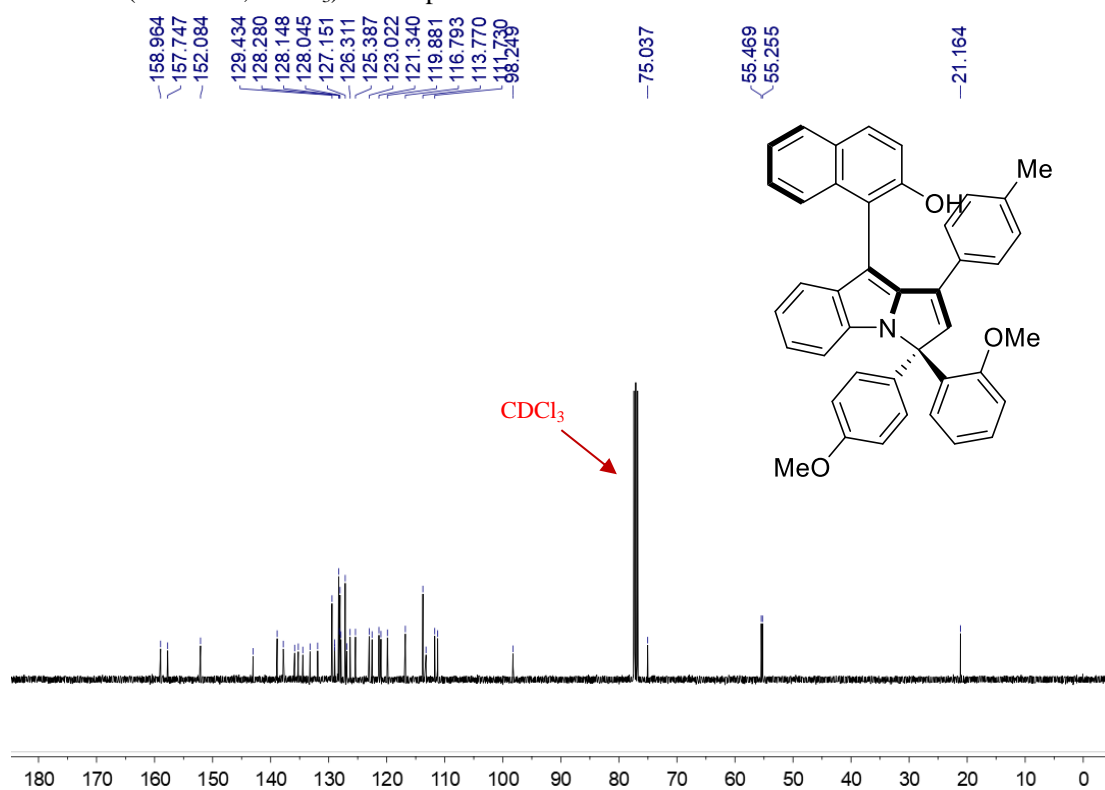
^{13}C NMR (100 MHz, CDCl_3) of compound **7ah**:



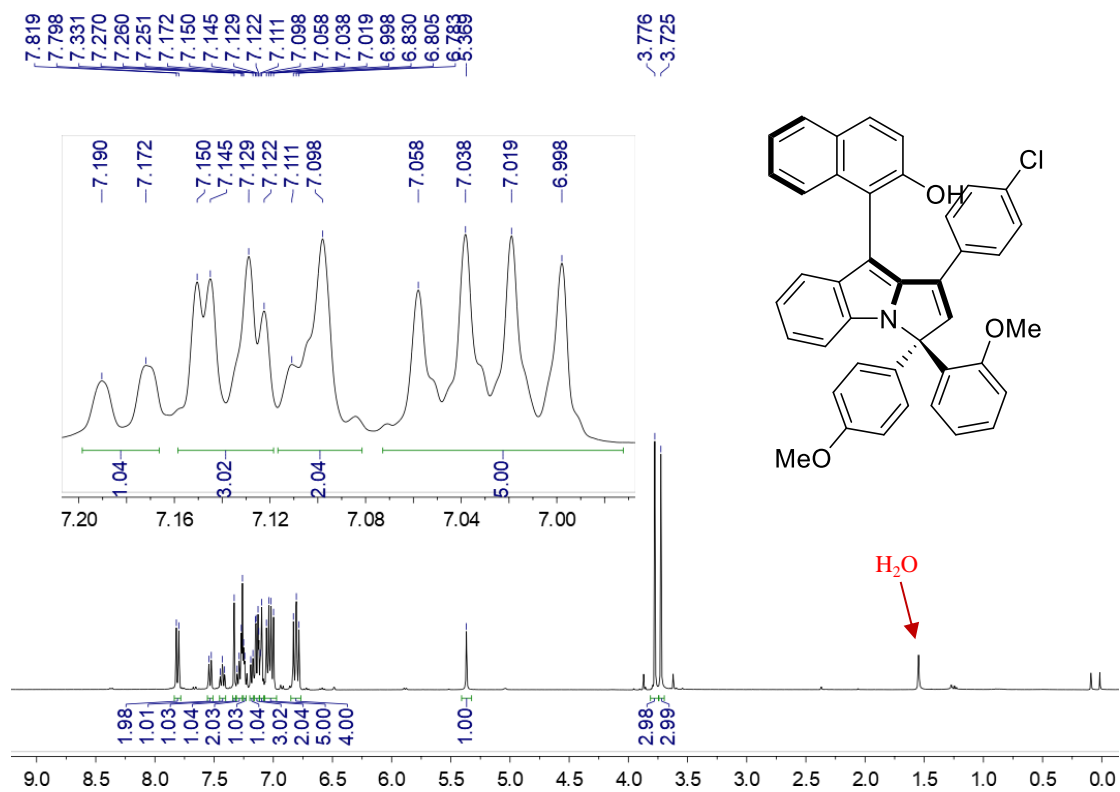
^1H NMR (400 MHz, CDCl_3) of compound **7ai**:



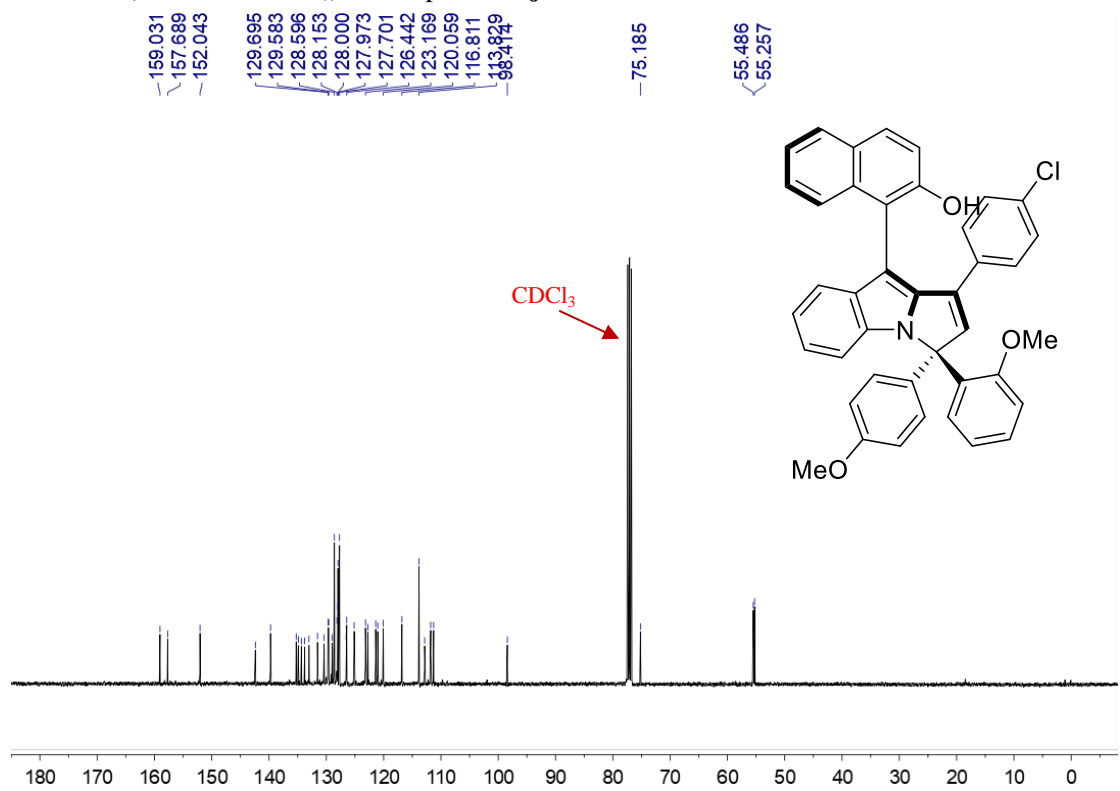
^{13}C NMR (100 MHz, CDCl_3) of compound **7ai**:



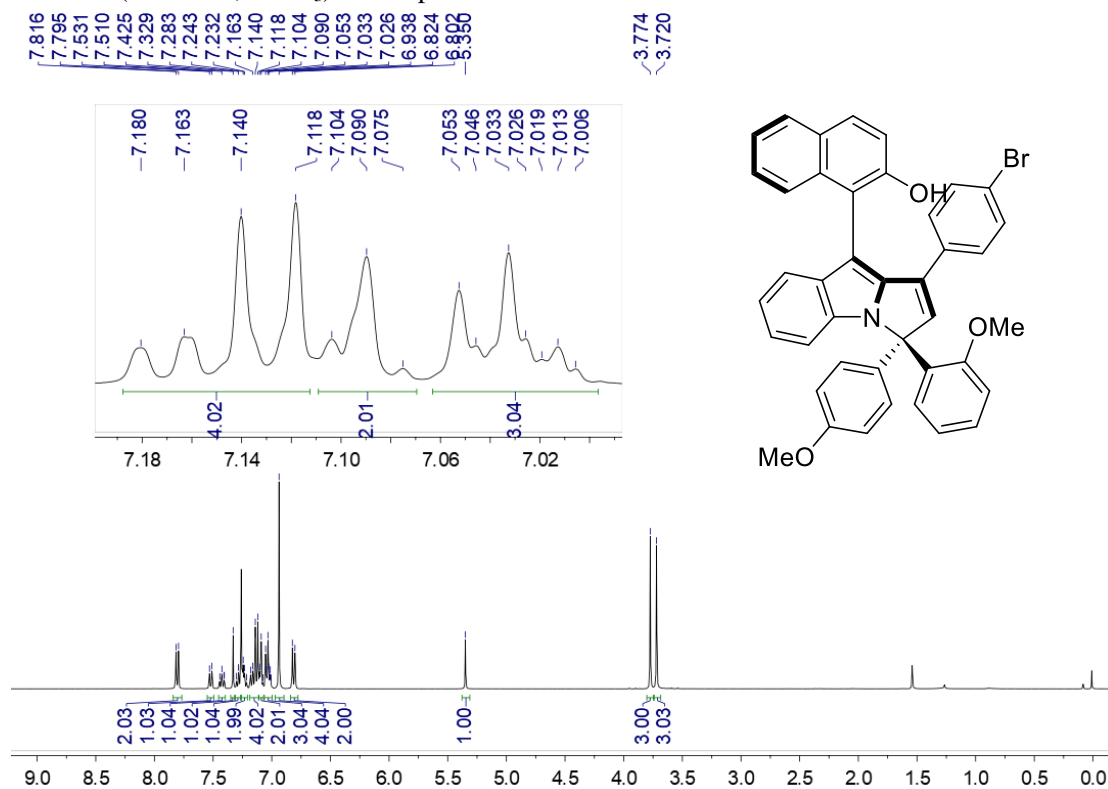
¹H NMR (400 MHz, CDCl₃) of compound **7aj**:



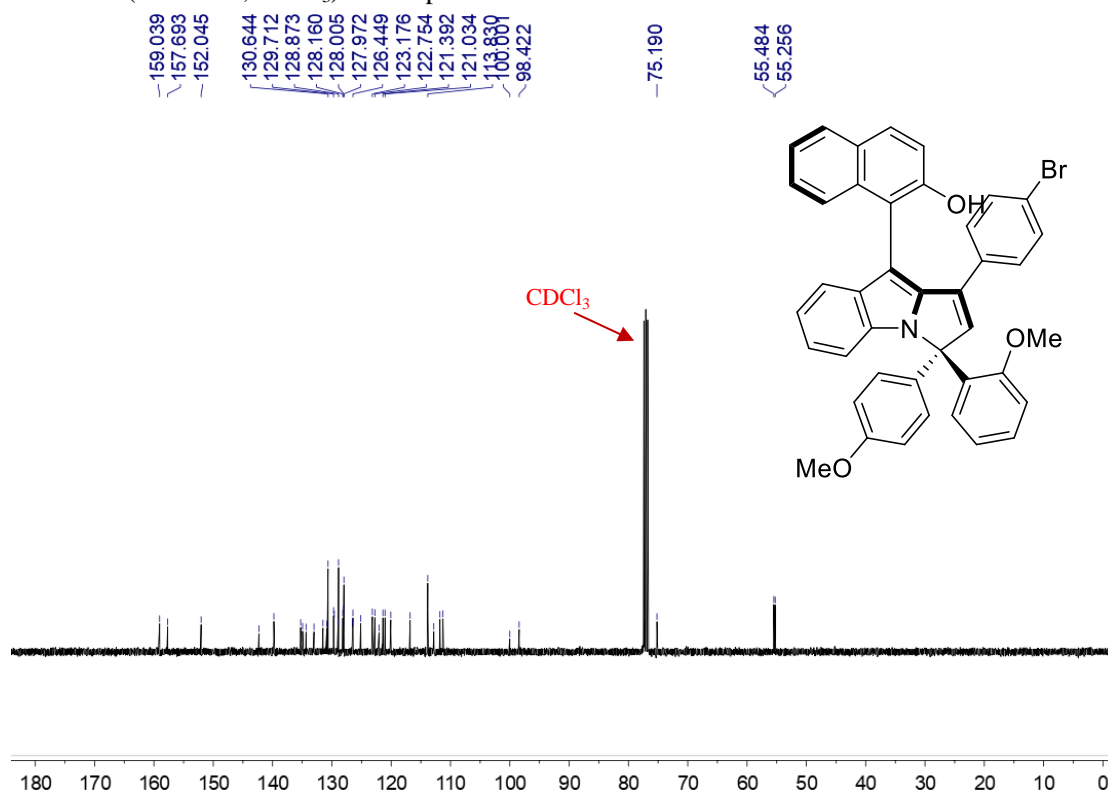
¹³C NMR (100 MHz, CDCl₃) of compound **7aj**:



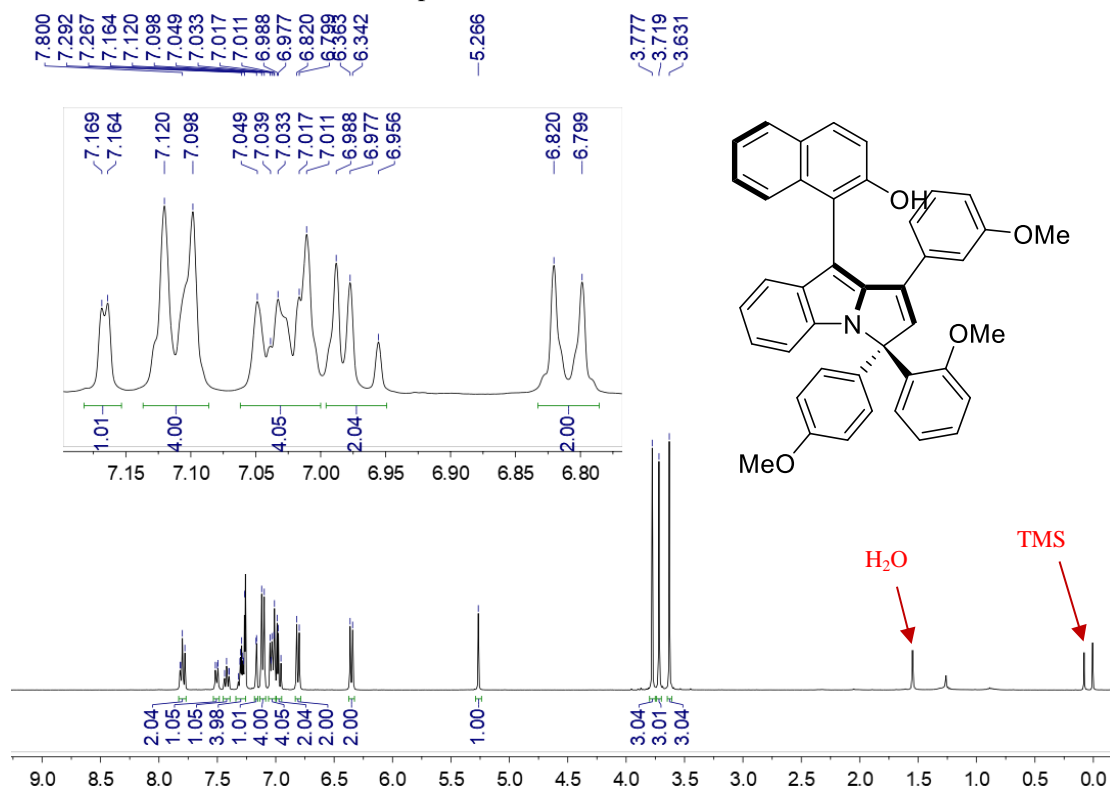
^1H NMR (400 MHz, CDCl_3) of compound **7ak**:



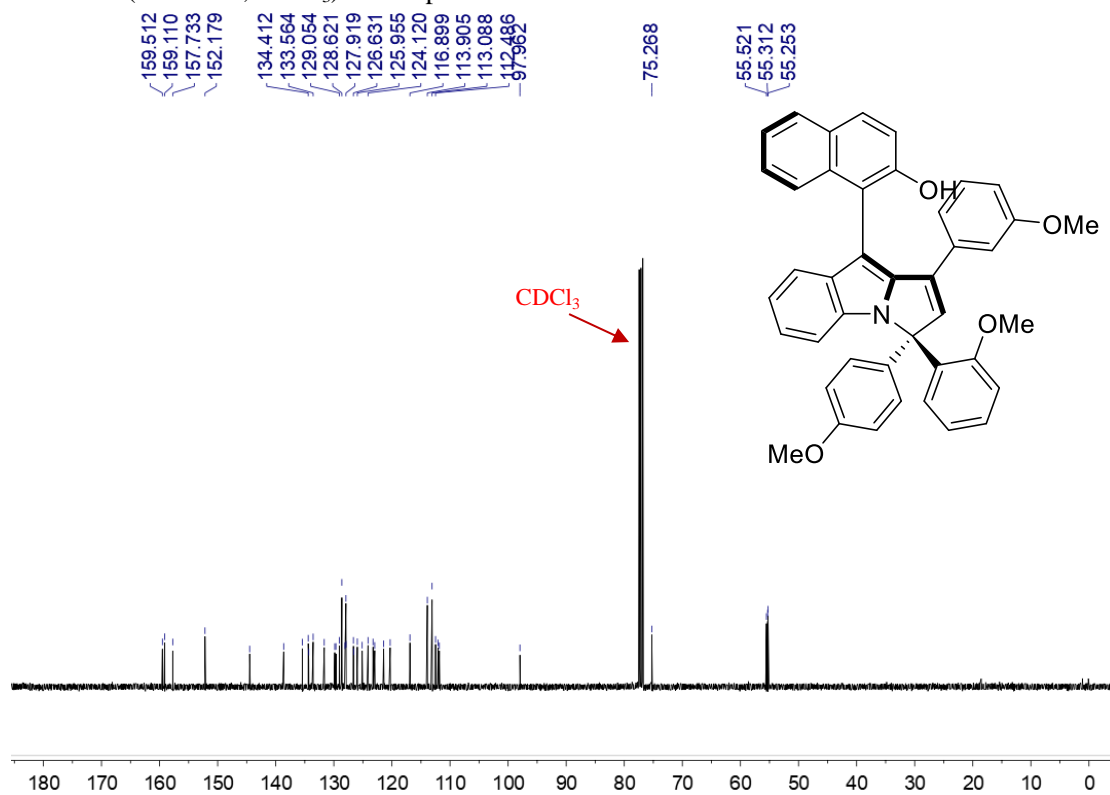
^{13}C NMR (100 MHz, CDCl_3) of compound **7ak**:



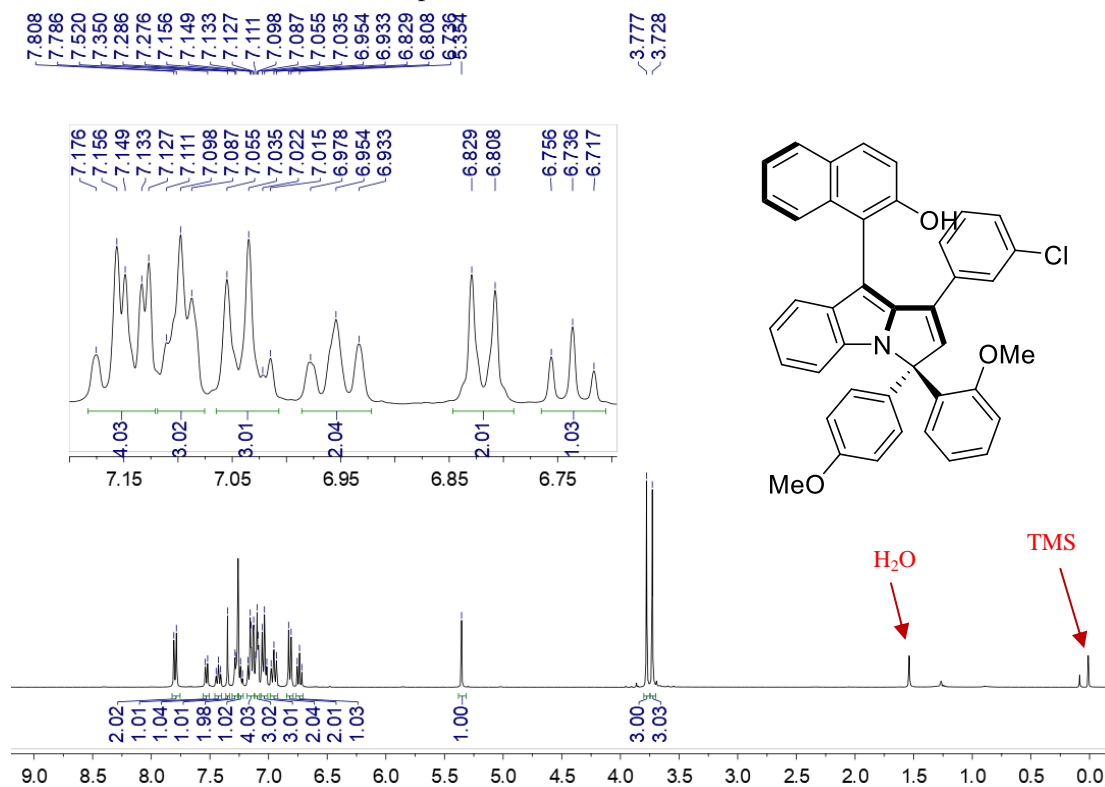
^1H NMR (400 MHz, CDCl_3) of compound **7al**:



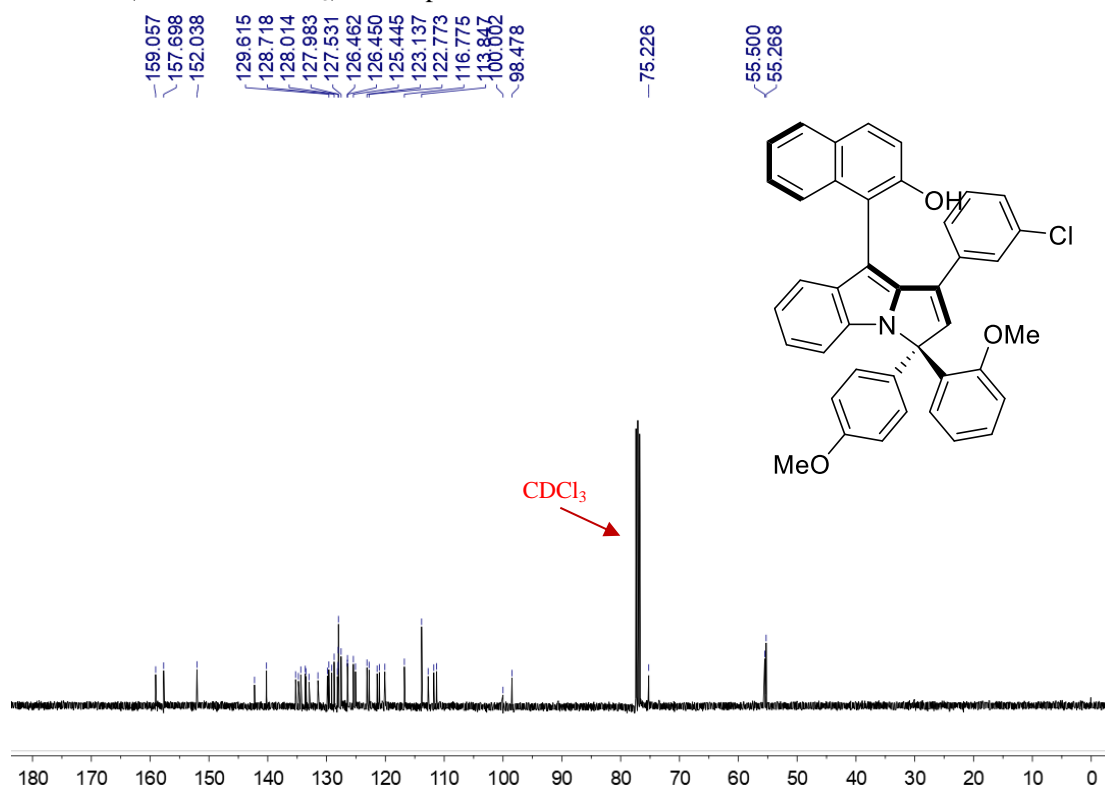
^{13}C NMR (100 MHz, CDCl_3) of compound **7al**:



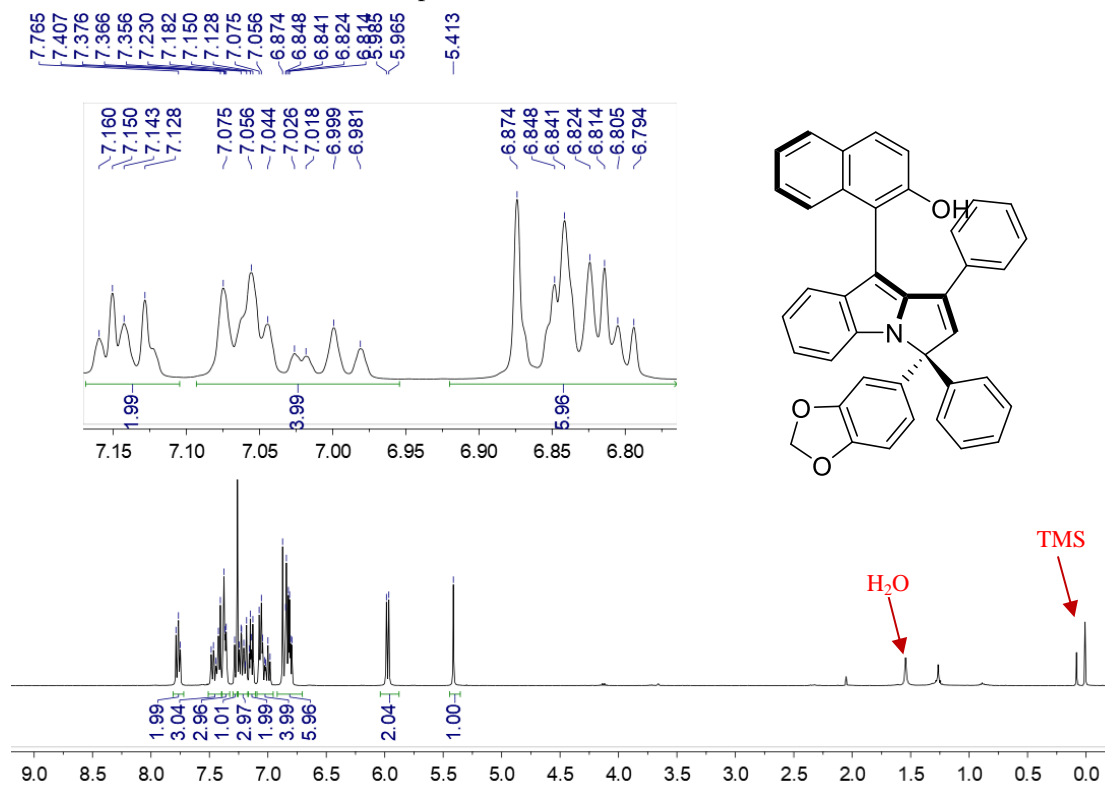
^1H NMR (400 MHz, CDCl_3) of compound **7am**:



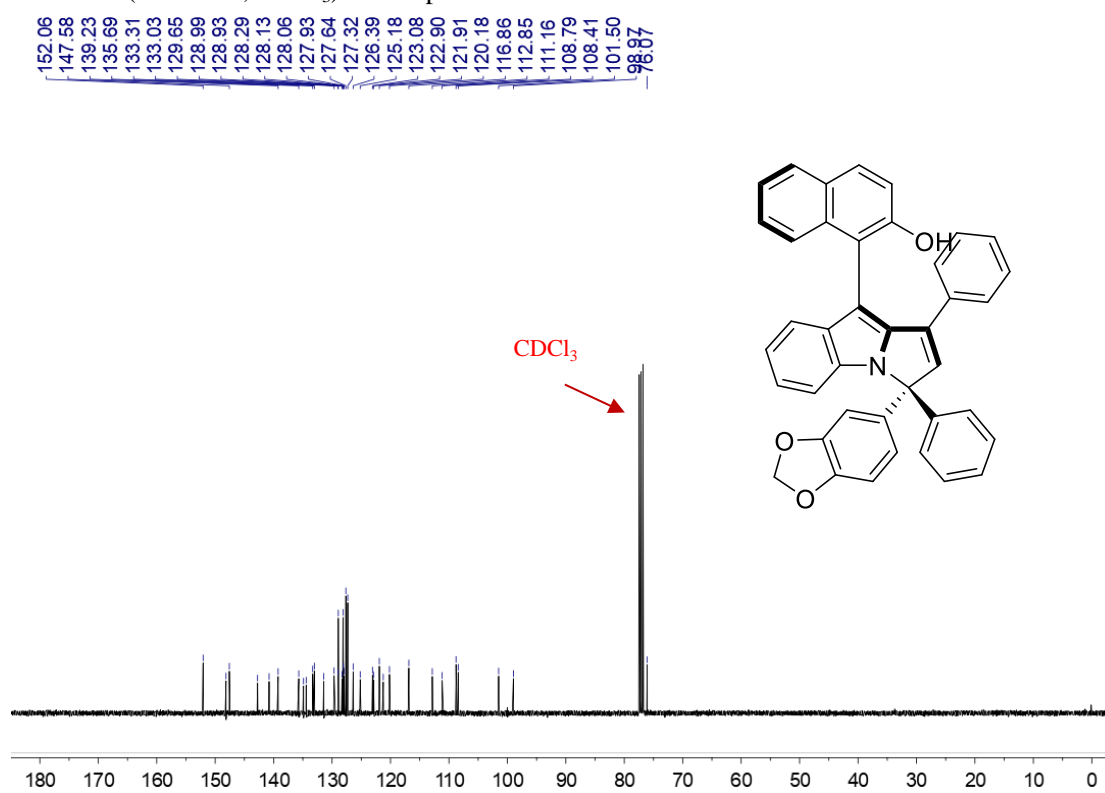
^{13}C NMR (100 MHz, CDCl_3) of compound **7am**:



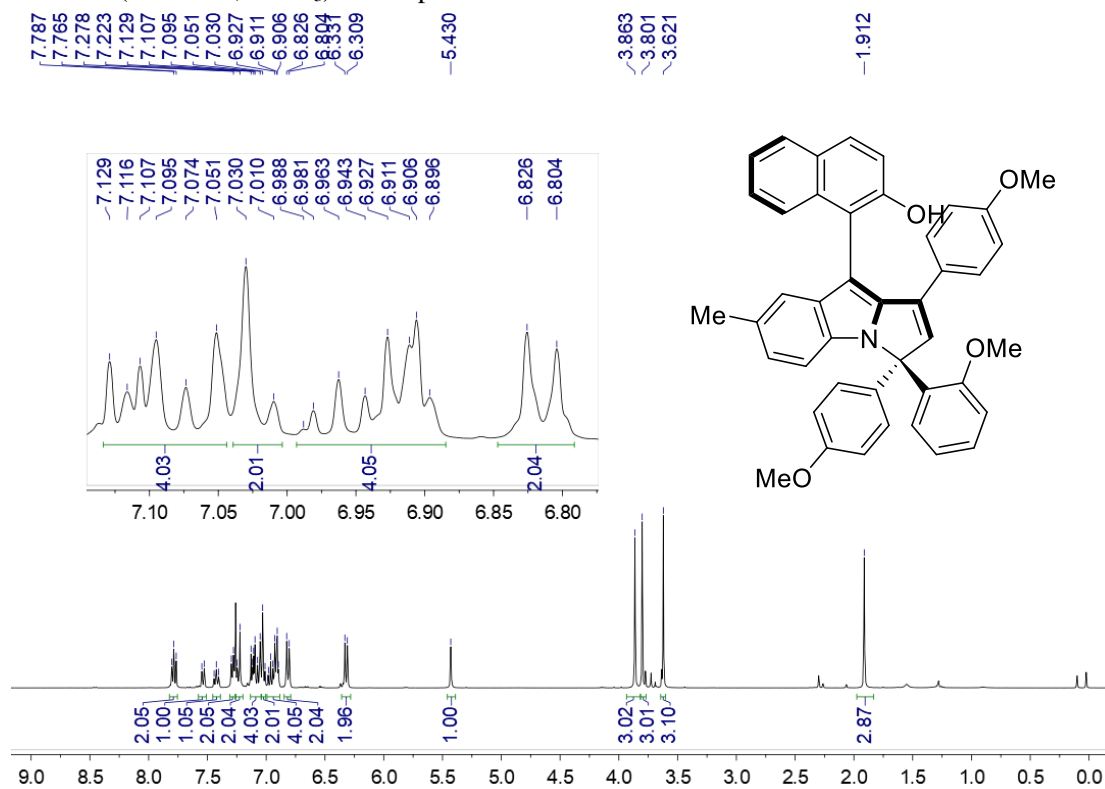
^1H NMR (400 MHz, CDCl_3) of compound **7an**:



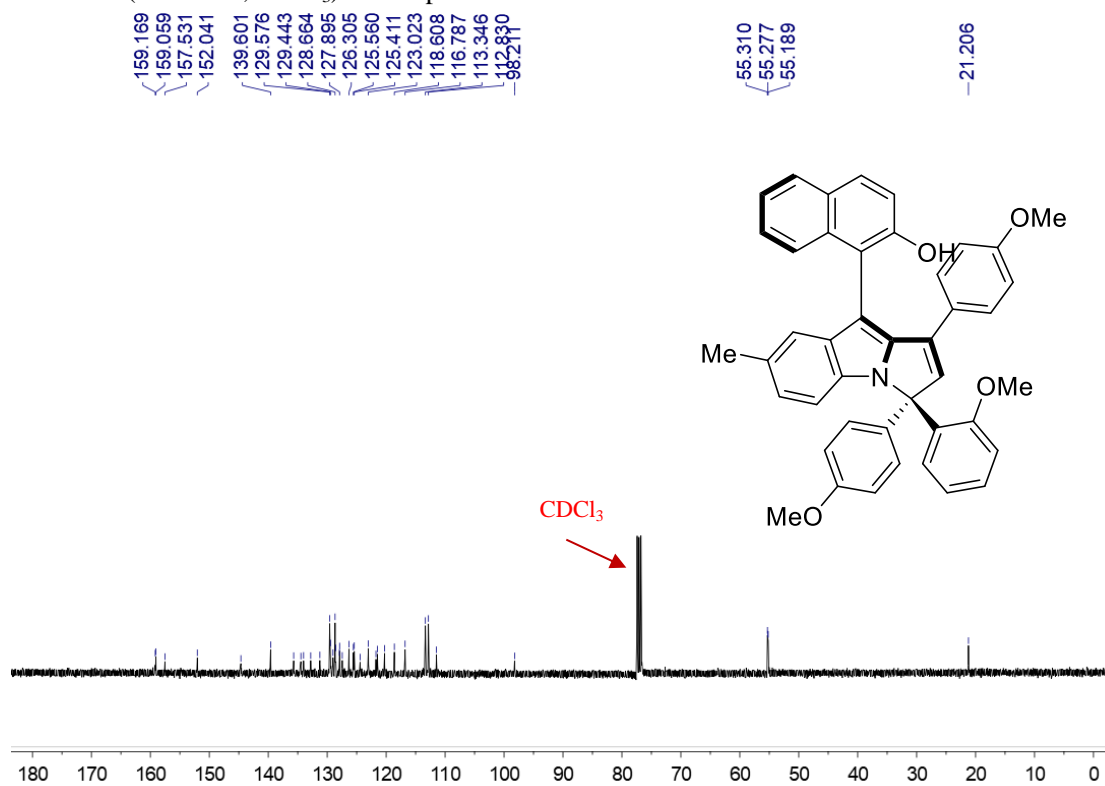
^{13}C NMR (100 MHz, CDCl_3) of compound **7an**:



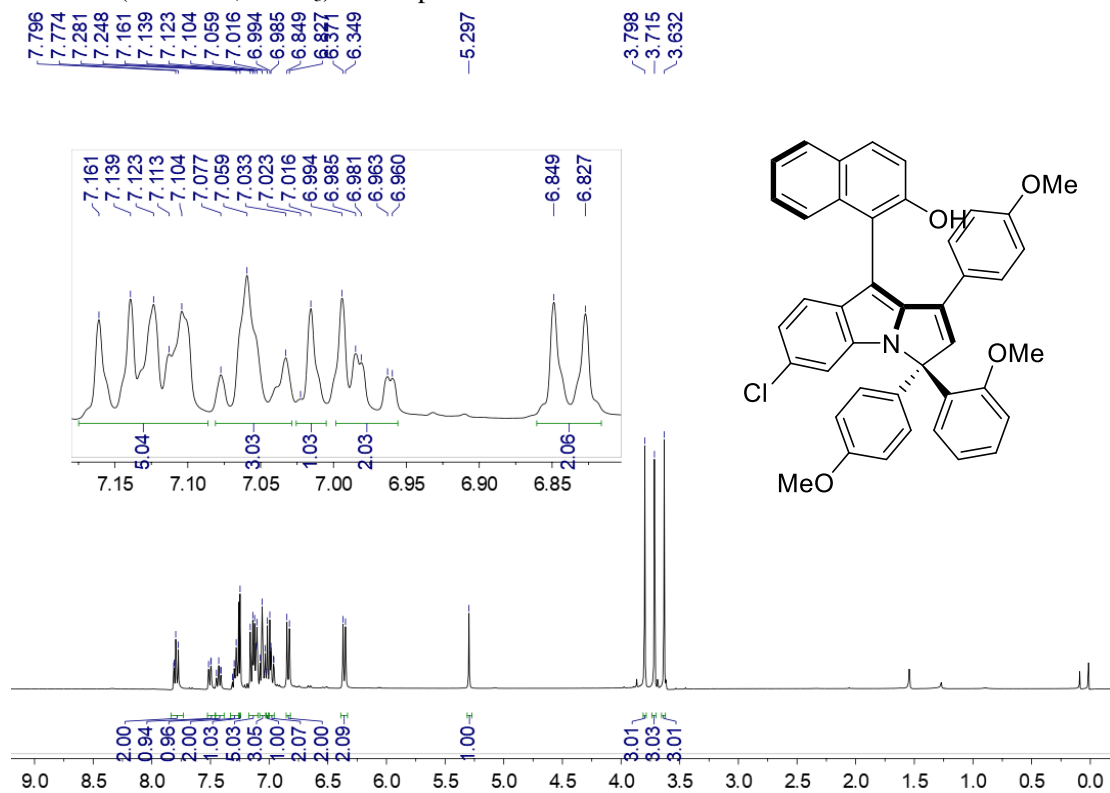
¹H NMR (400 MHz, CDCl₃) of compound **7dh**:



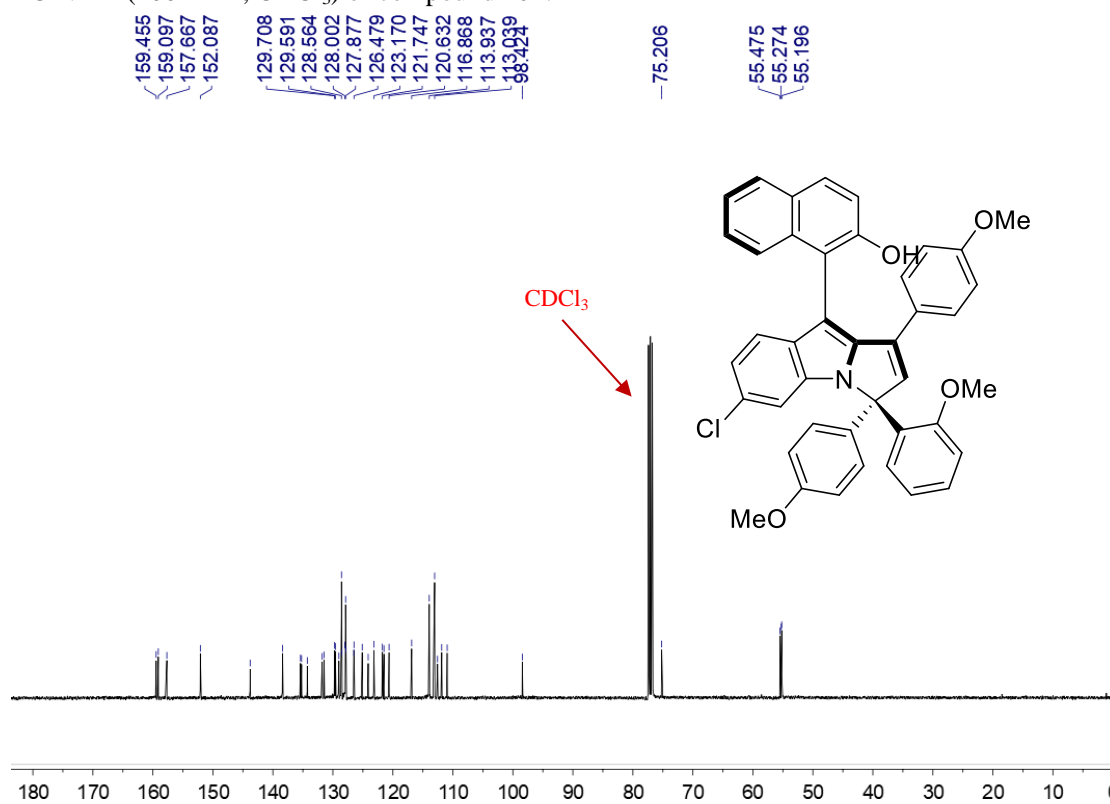
¹³C NMR (100 MHz, CDCl₃) of compound **7dh**:



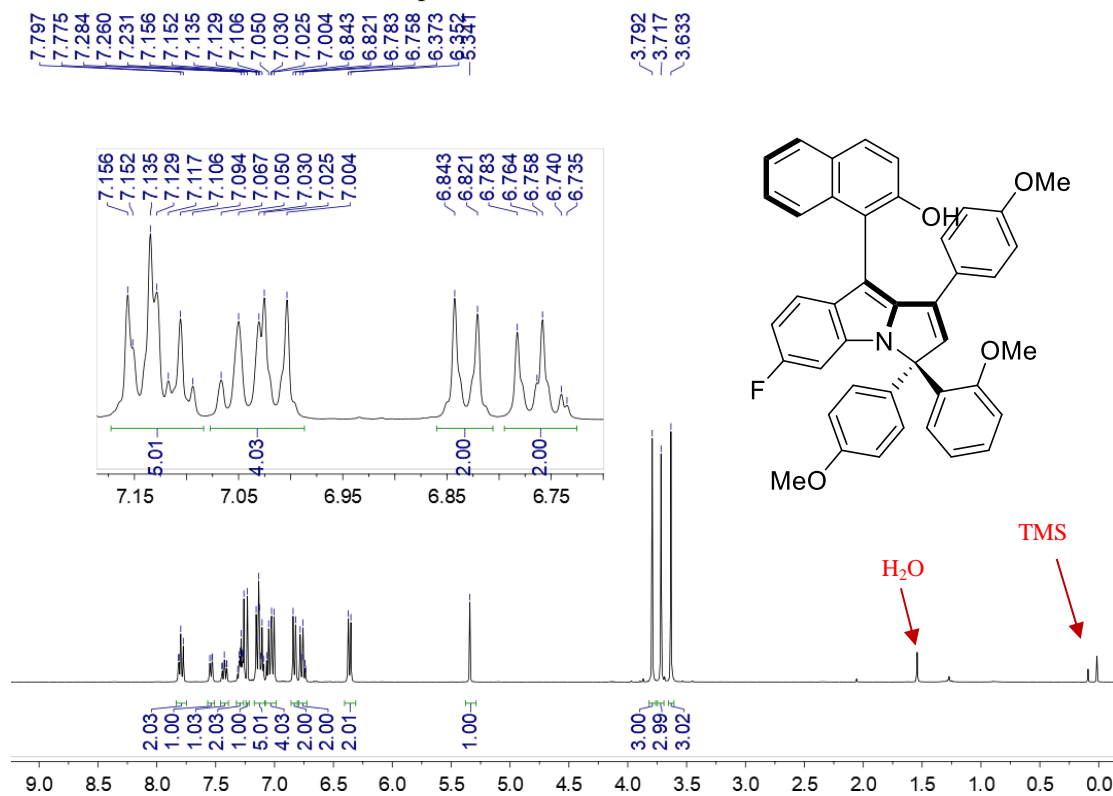
^1H NMR (400 MHz, CDCl_3) of compound **7eh**:



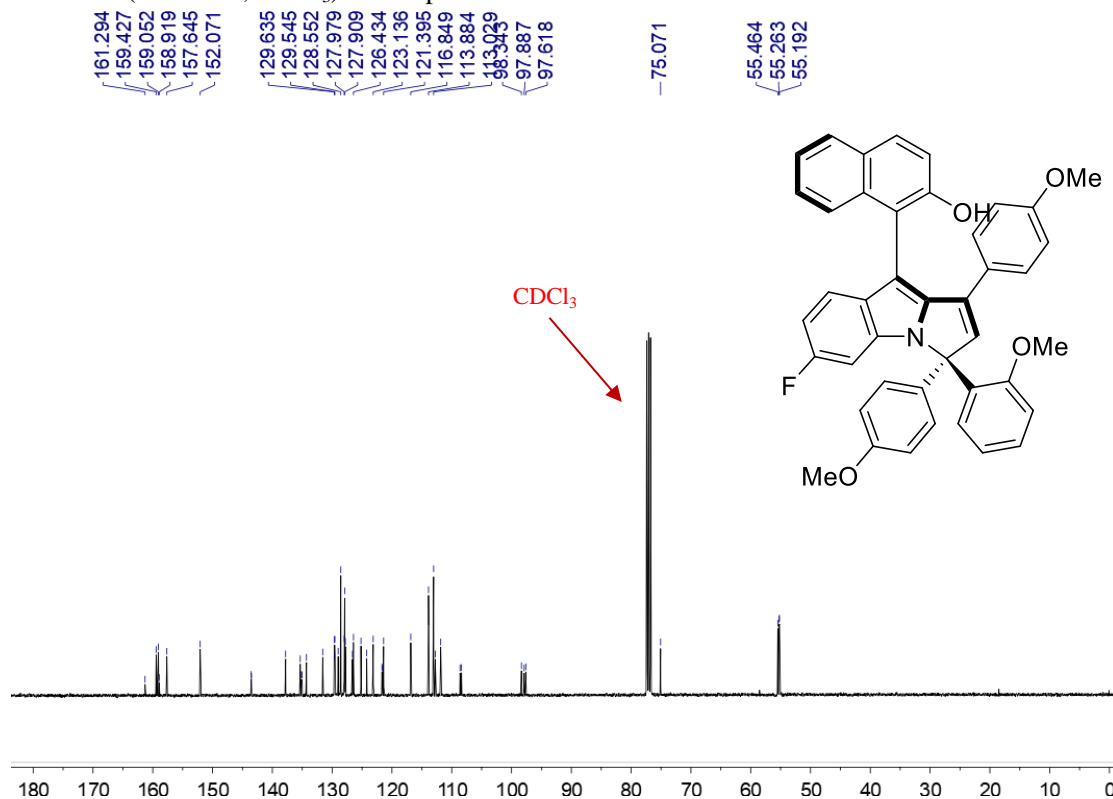
^{13}C NMR (100 MHz, CDCl_3) of compound **7eh**:



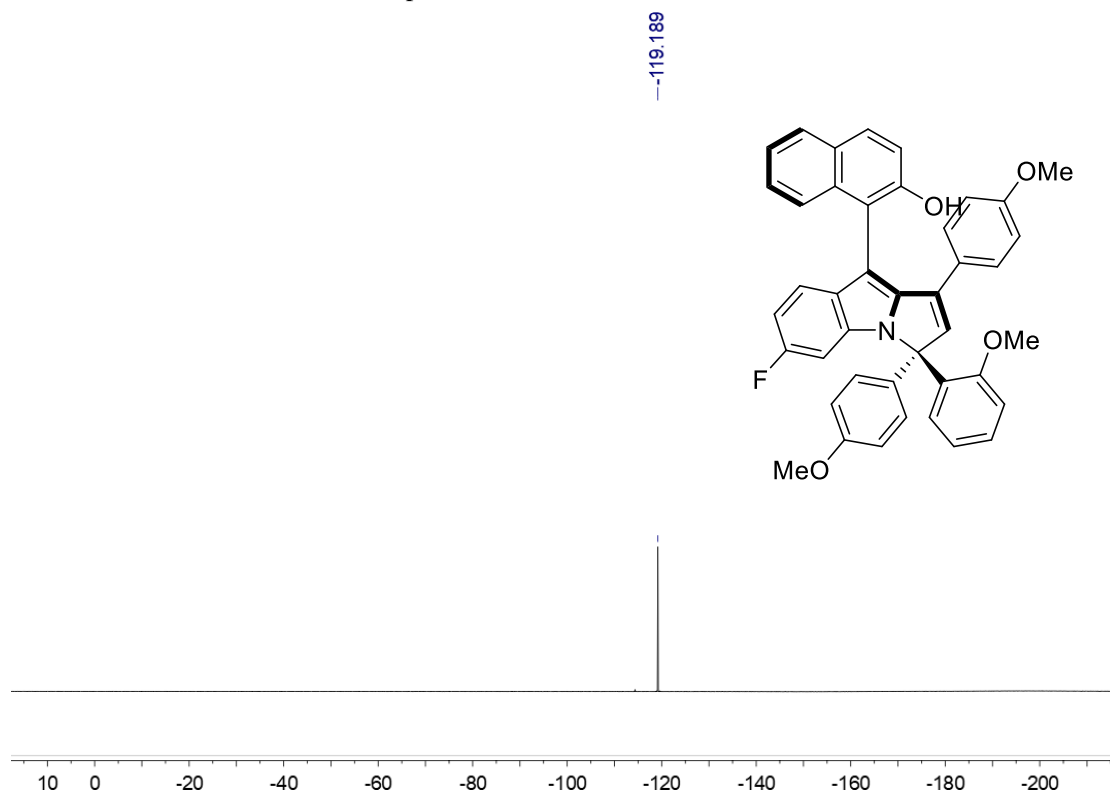
^1H NMR (400 MHz, CDCl_3) of compound **7fh**:



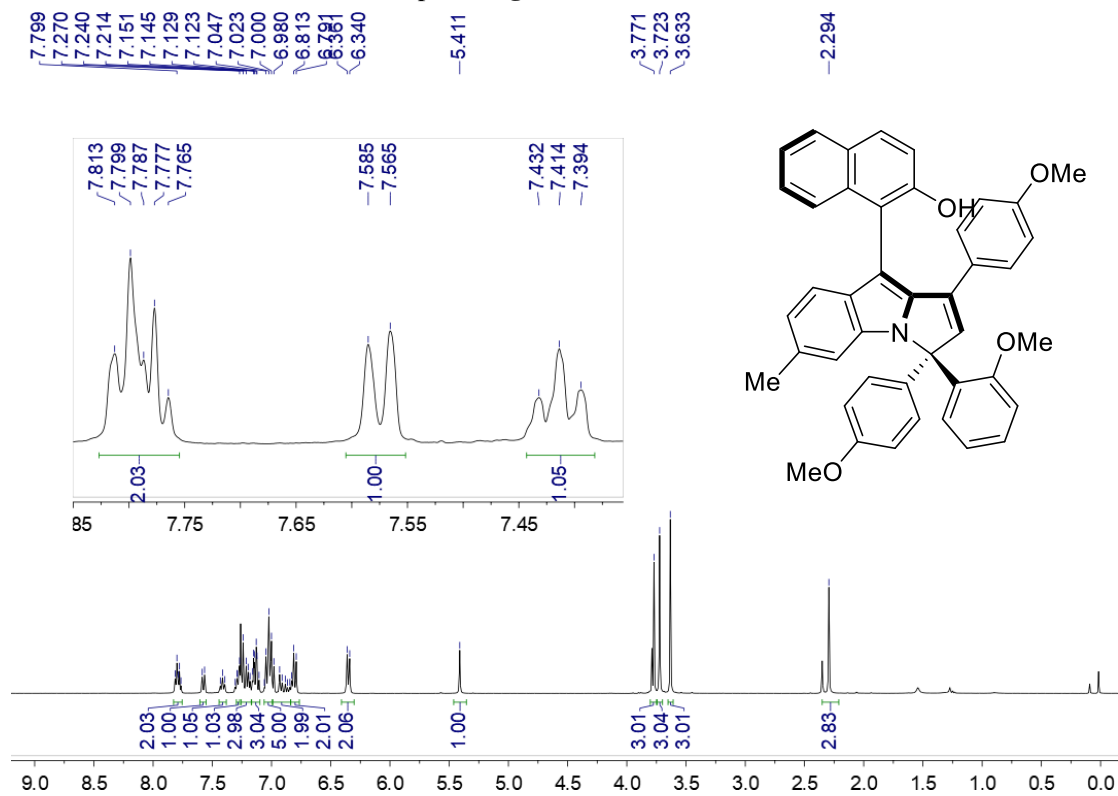
^{13}C NMR (100 MHz, CDCl_3) of compound **7fh**:



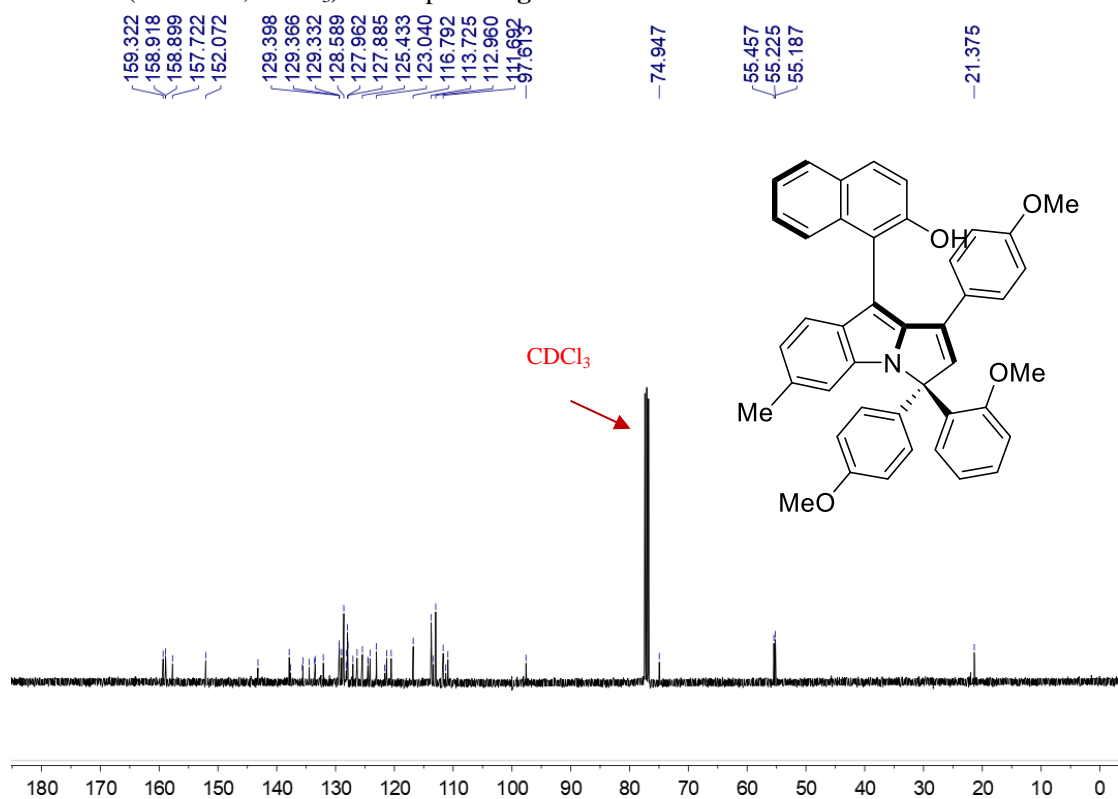
^{19}F NMR (376 MHz, CDCl_3) of compound **7fh**:



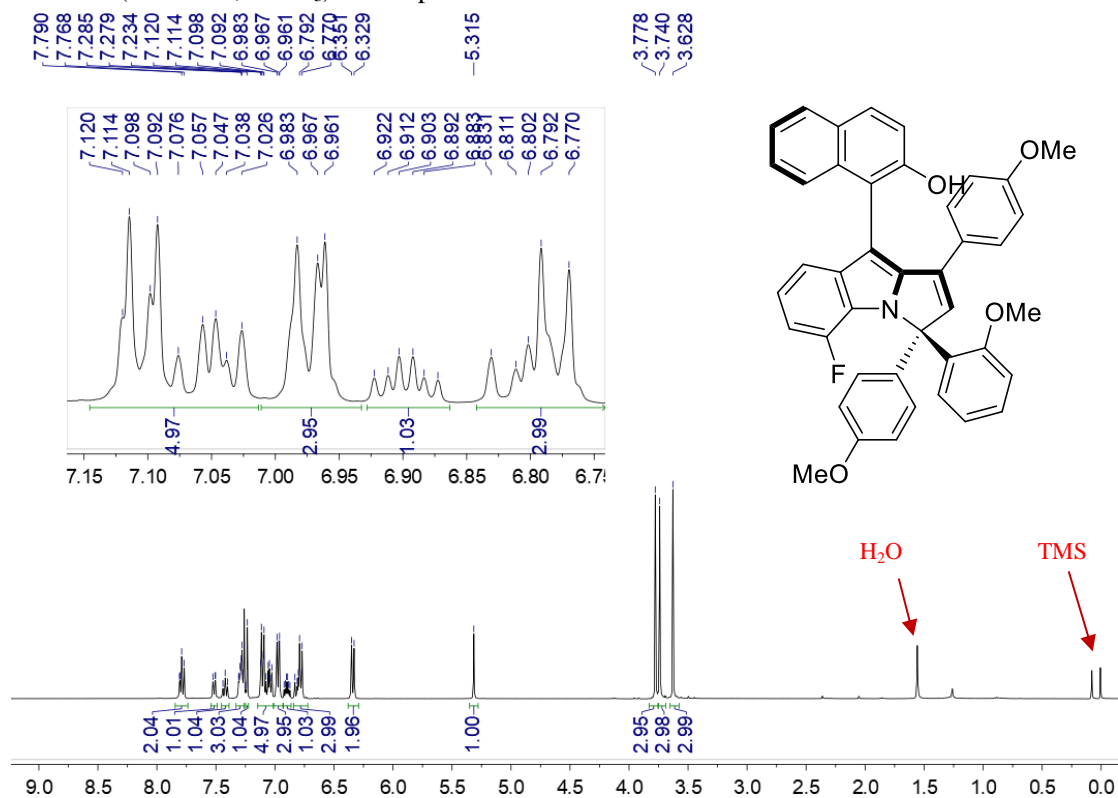
^1H NMR (400 MHz, CDCl_3) of compound **7gh**:



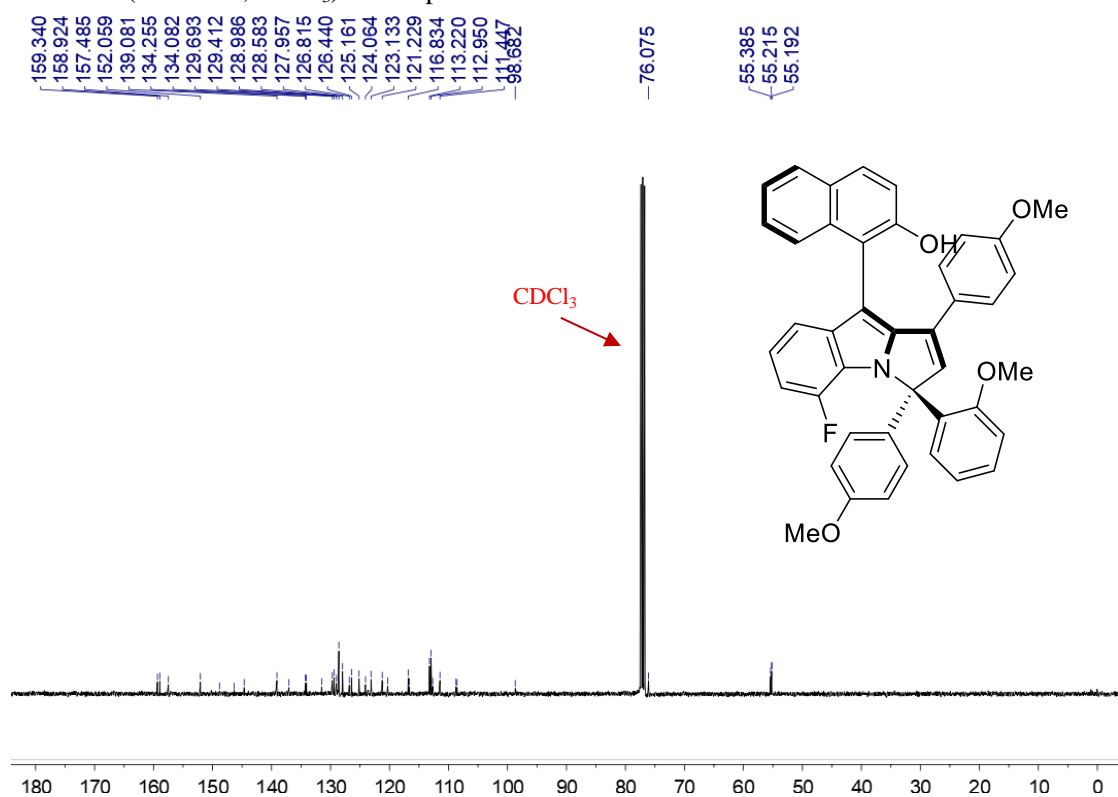
^{13}C NMR (100 MHz, CDCl_3) of compound **7gh**:



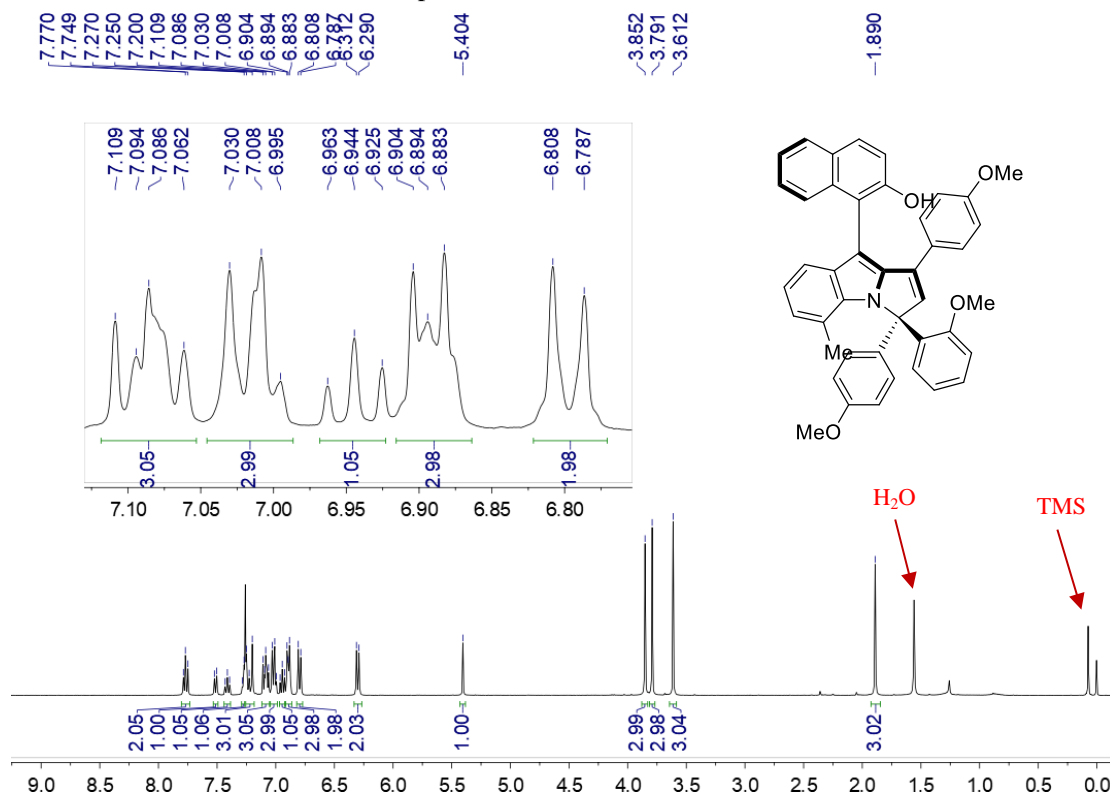
^1H NMR (400 MHz, CDCl_3) of compound **7hh**:



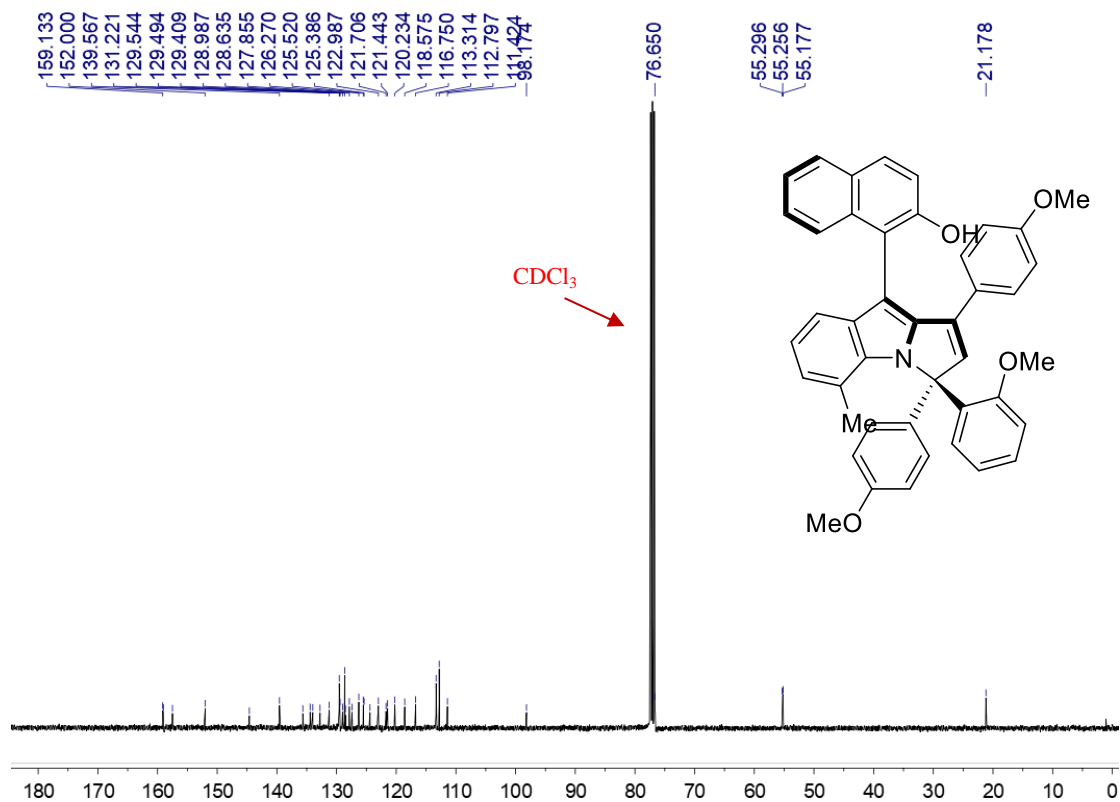
^{13}C NMR (100 MHz, CDCl_3) of compound **7hh**:



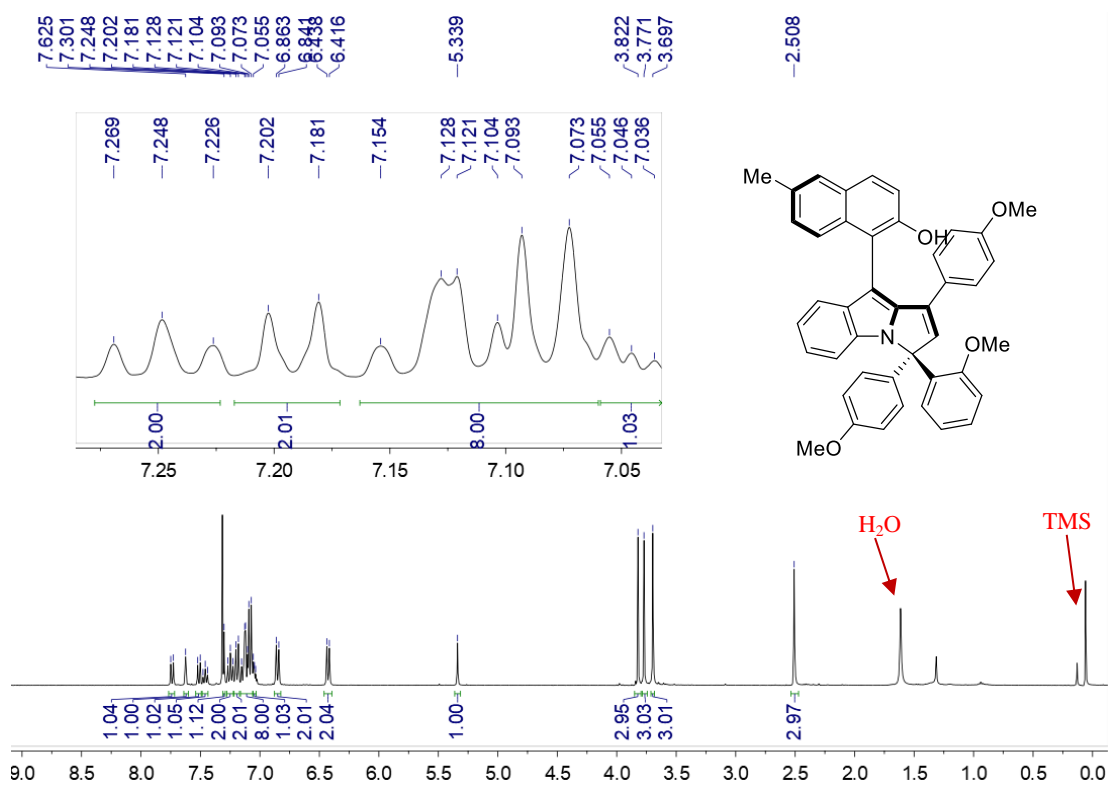
^1H NMR (400 MHz, CDCl_3) of compound **7ih**:



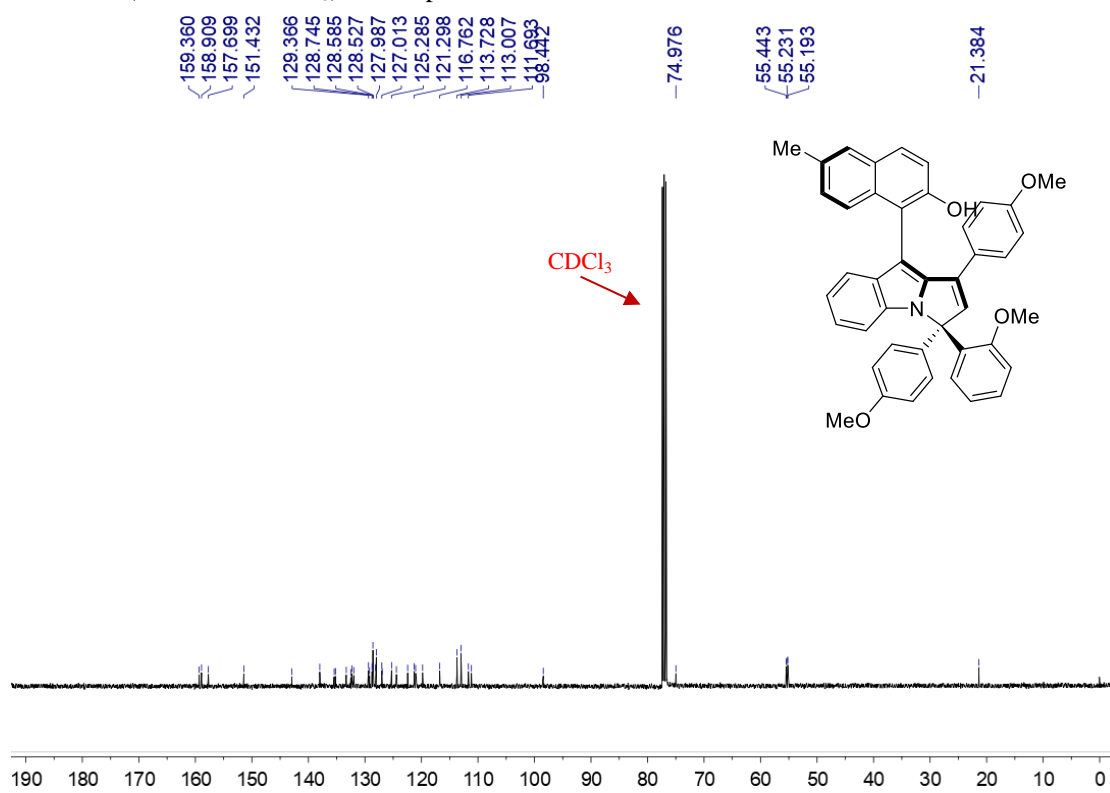
^{13}C NMR (100 MHz, CDCl_3) of compound **7ih**:



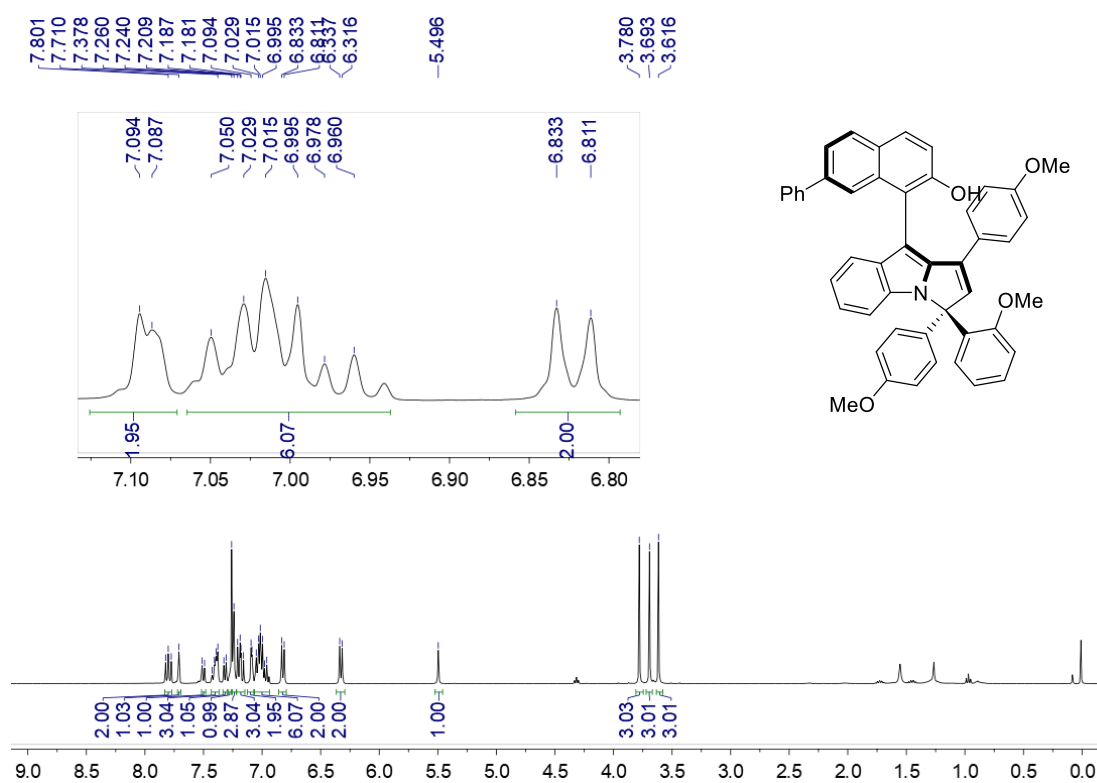
^1H NMR (400 MHz, CDCl_3) of compound **7kh**:



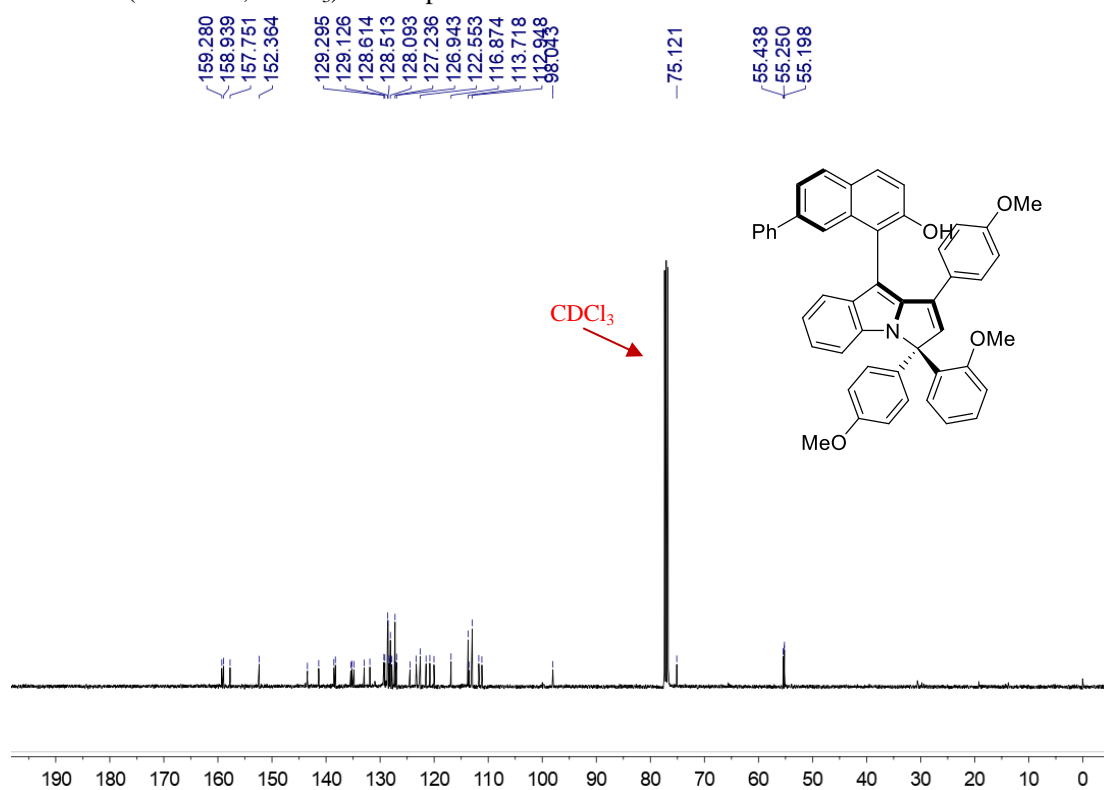
^{13}C NMR (100 MHz, CDCl_3) of compound **7kh**:



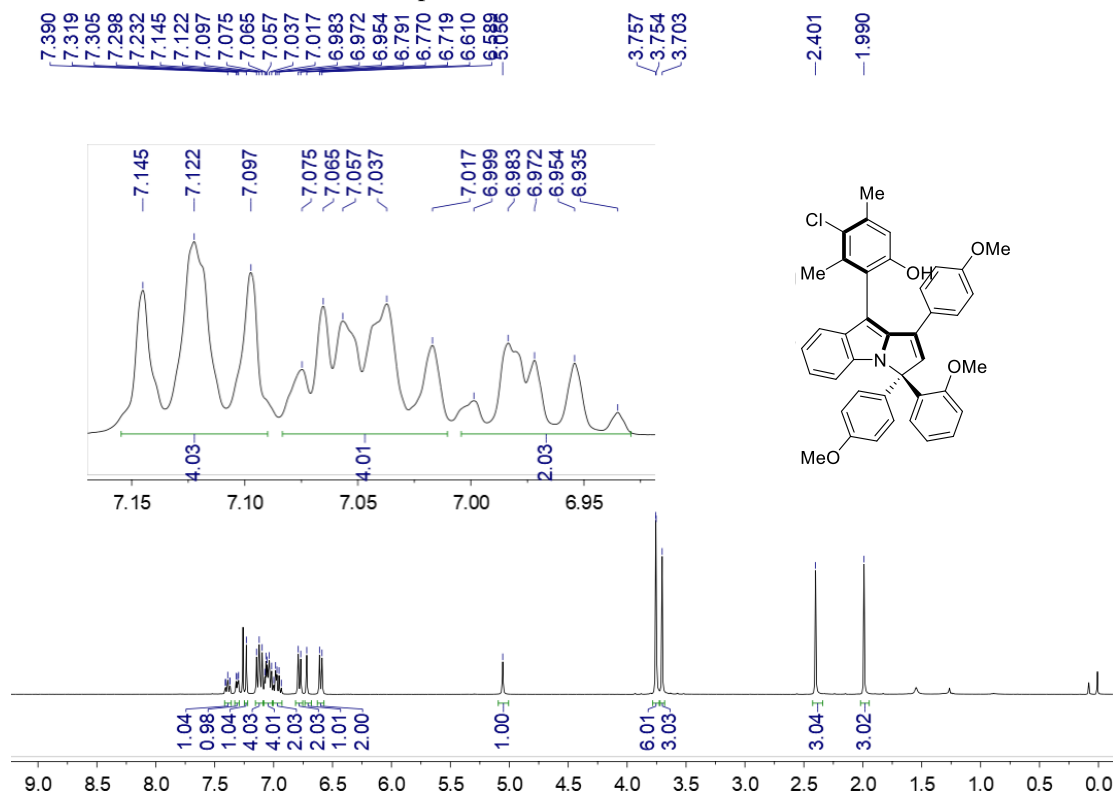
^1H NMR (400 MHz, CDCl_3) of compound **7lh**:



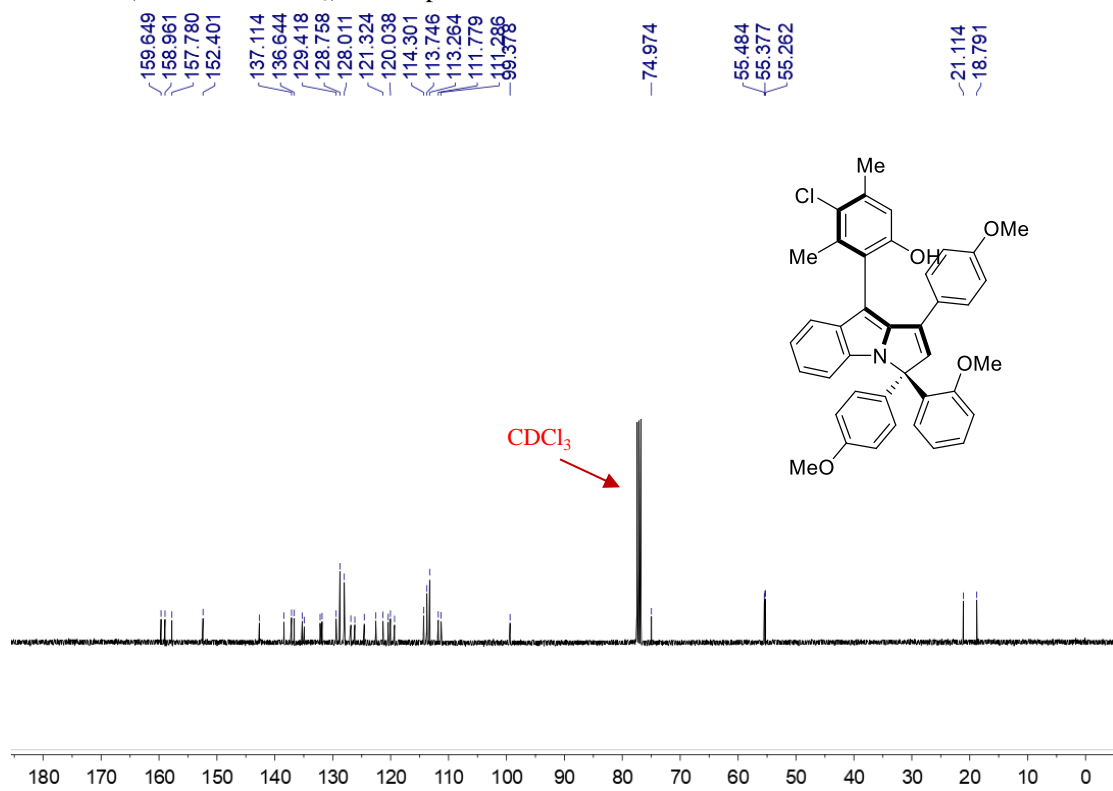
^{13}C NMR (100 MHz, CDCl_3) of compound **7lh**:



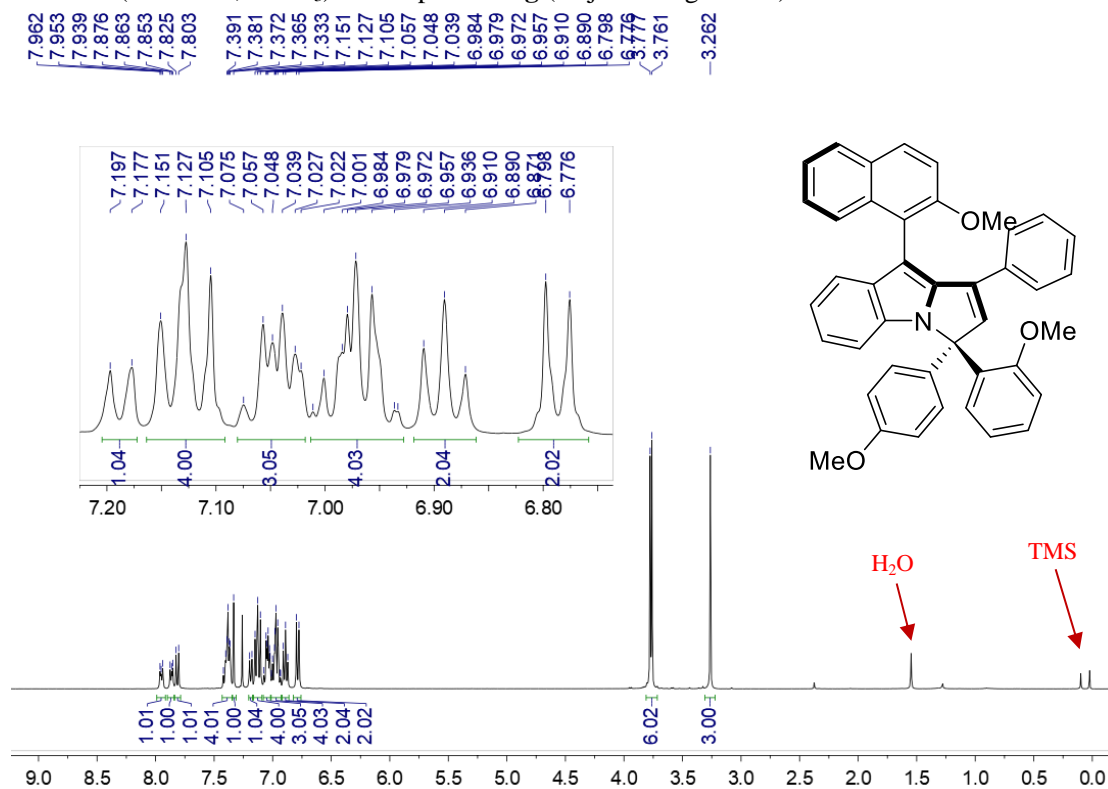
¹H NMR (400 MHz, CDCl₃) of compound **7mh**:



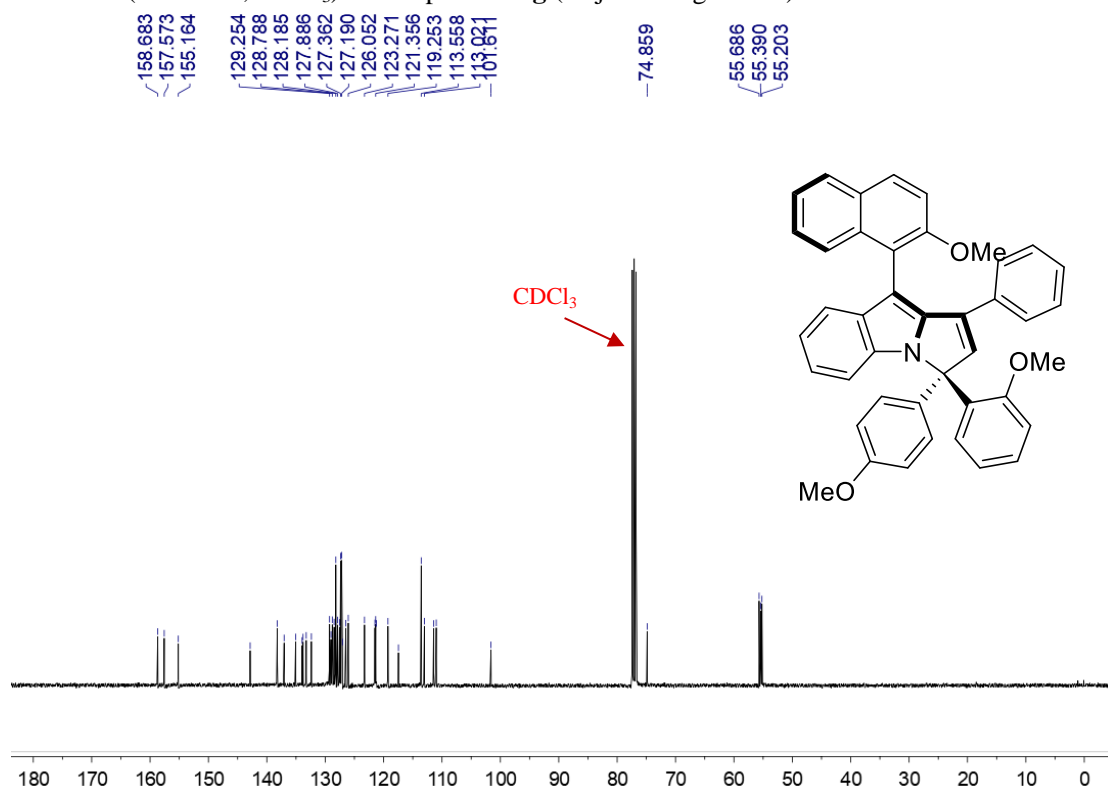
¹³C NMR (100 MHz, CDCl₃) of compound **7mh**:



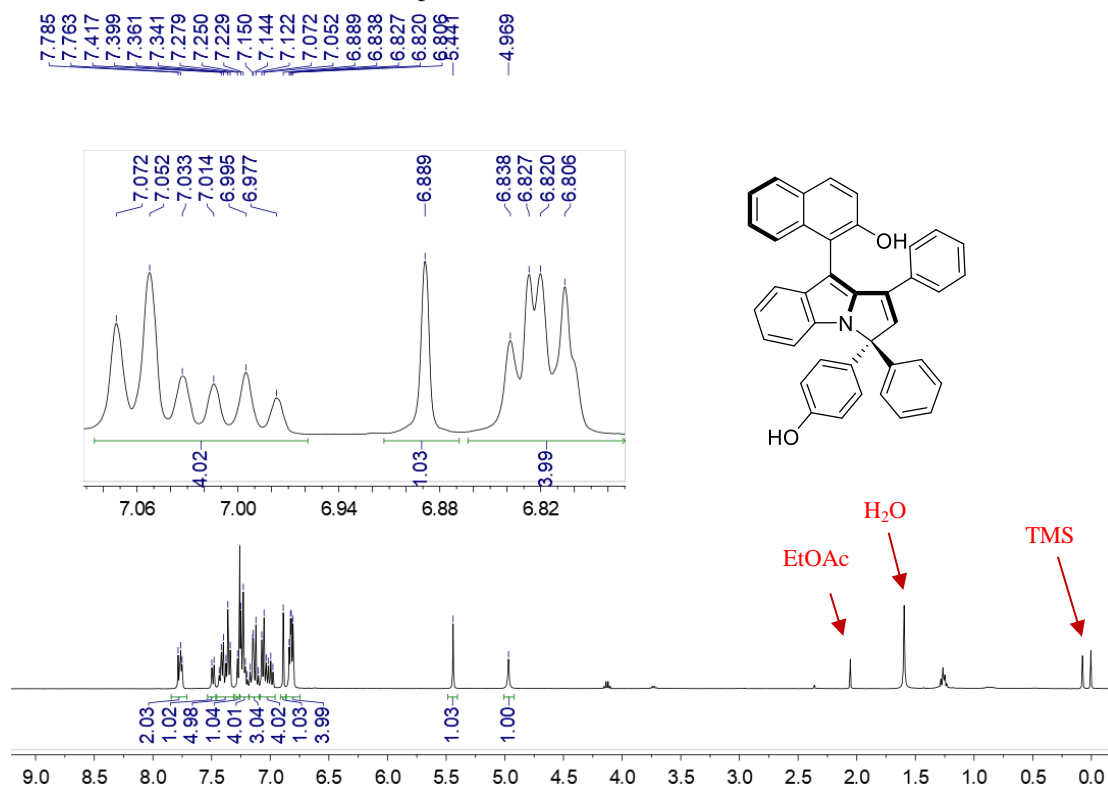
^1H NMR (400 MHz, CDCl_3) of compound **7ng** (major configuration):



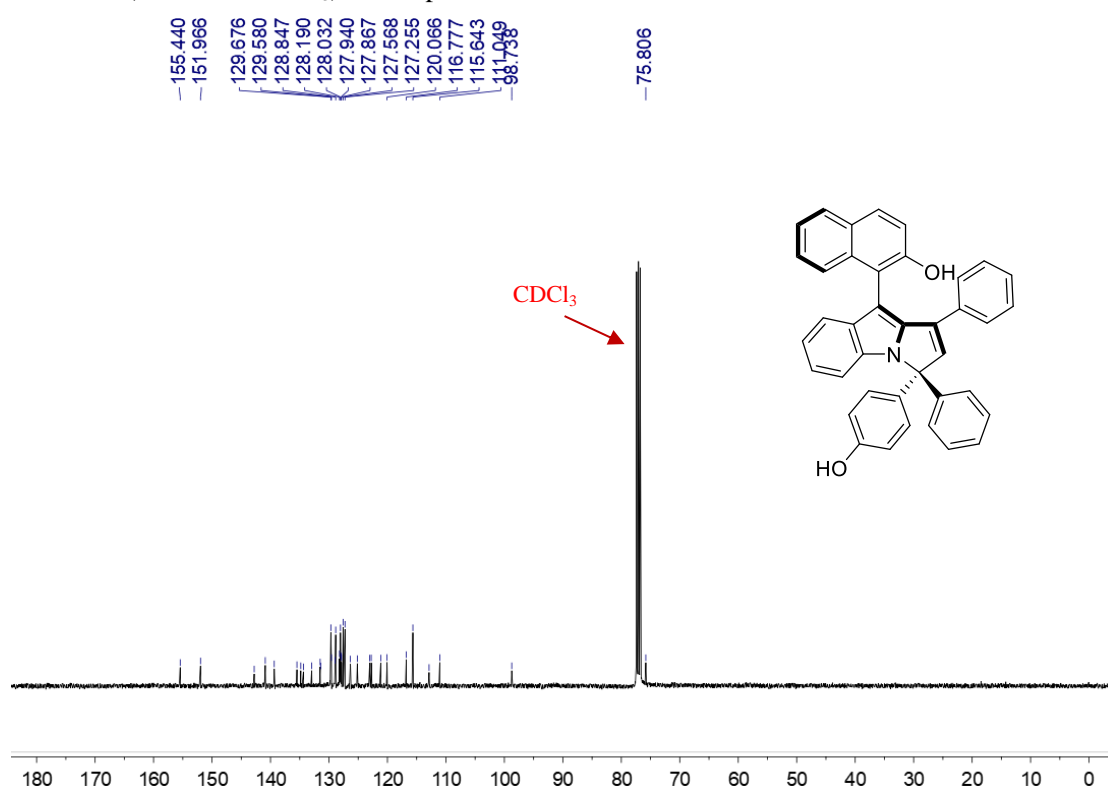
^{13}C NMR (100 MHz, CDCl_3) of compound **7ng** (major configuration):



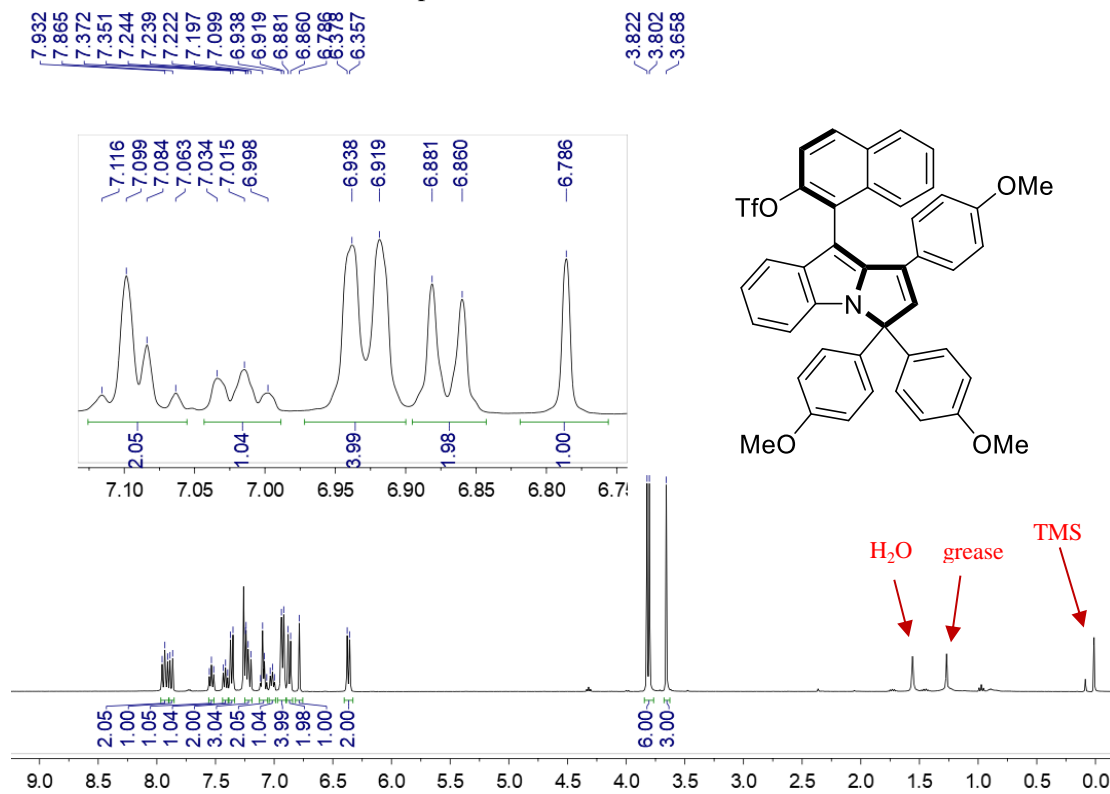
^1H NMR (400 MHz, CDCl_3) of compound **7aa**:



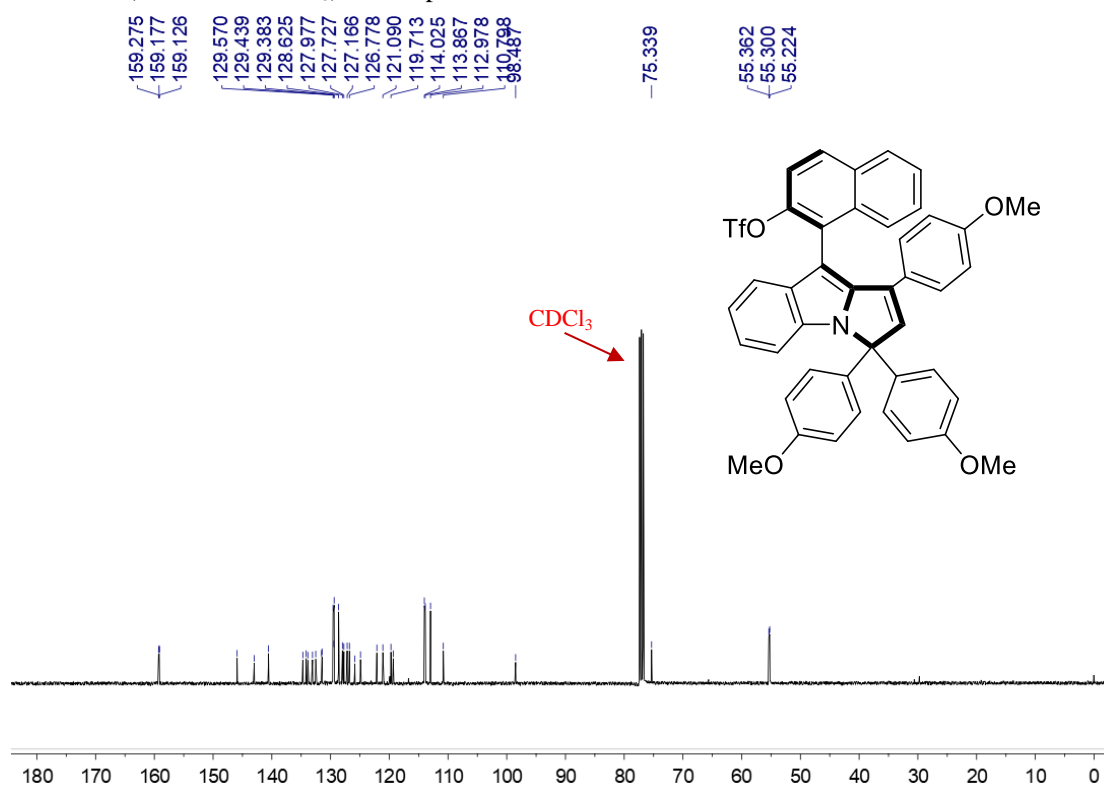
^{13}C NMR (100 MHz, CDCl_3) of compound **7aa**:



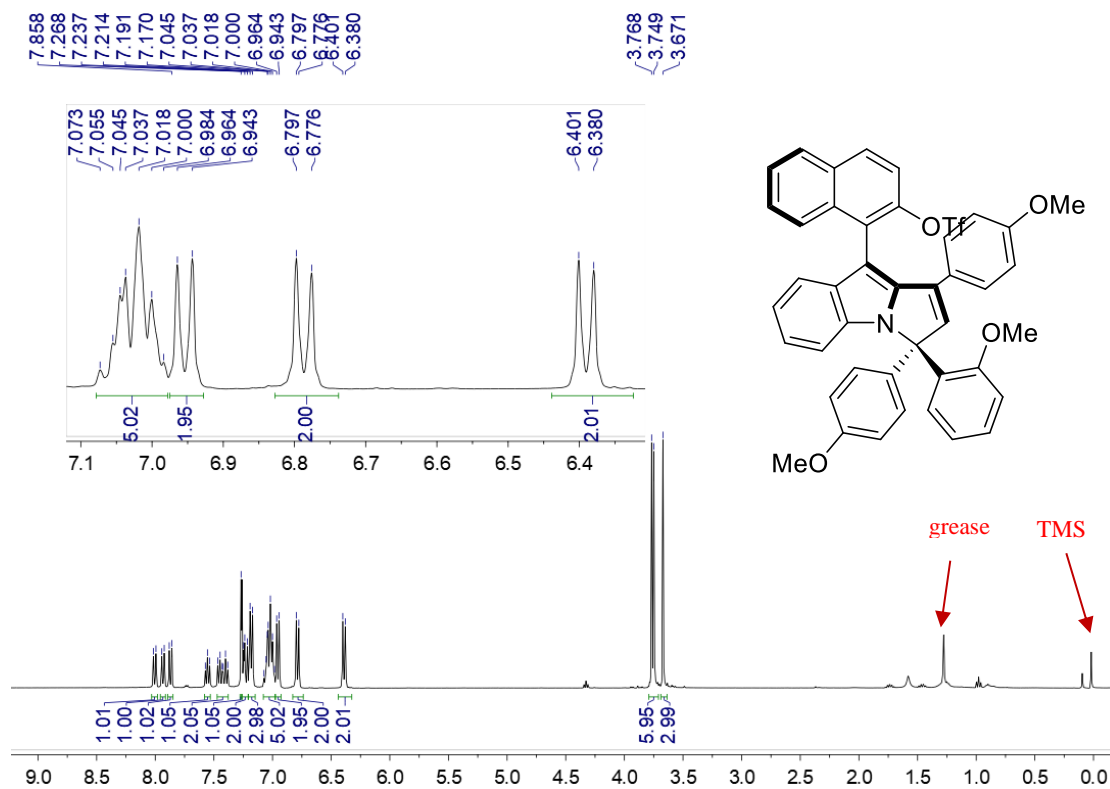
^1H NMR (400 MHz, CDCl_3) of compound **8a**:



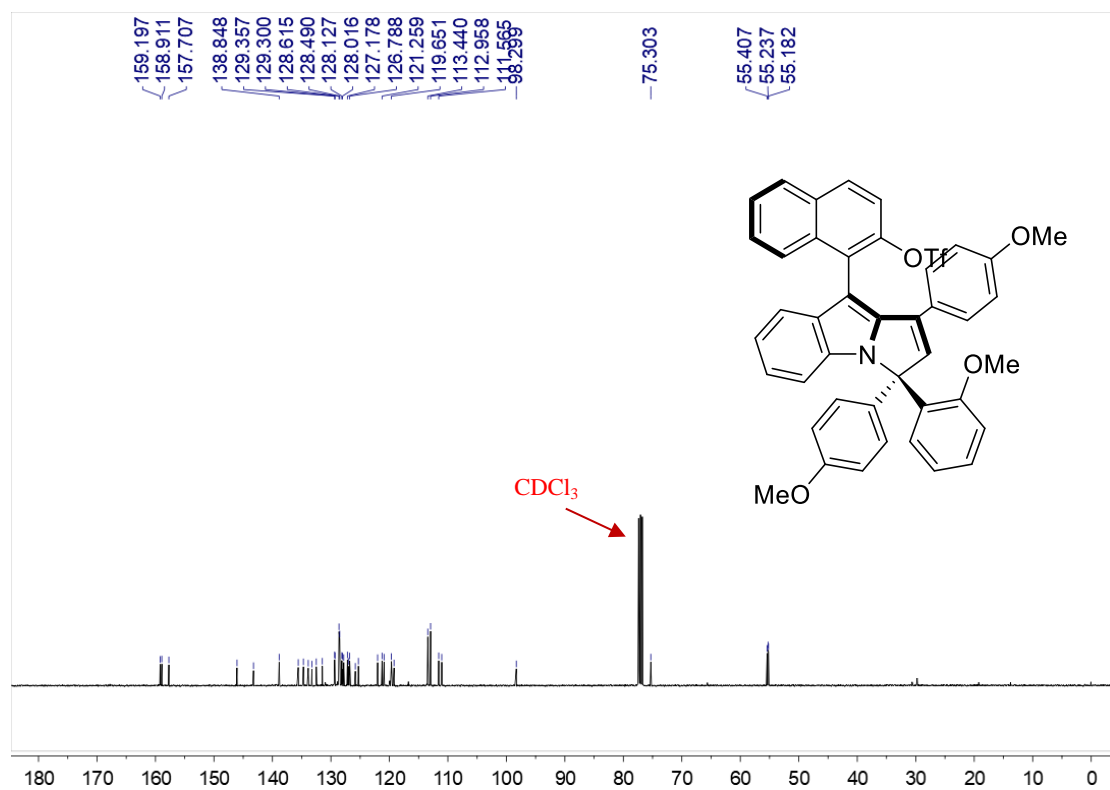
^{13}C NMR (100 MHz, CDCl_3) of compound **8a**:



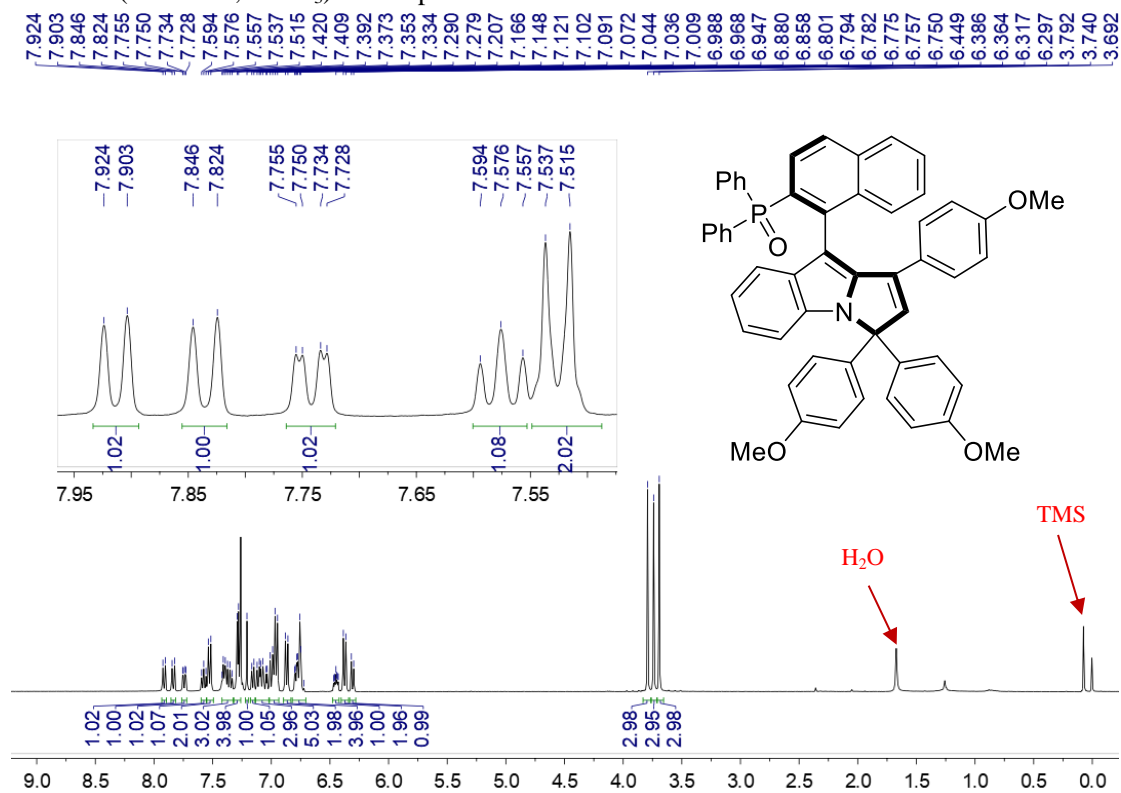
^1H NMR (400 MHz, CDCl_3) of compound **8b**:



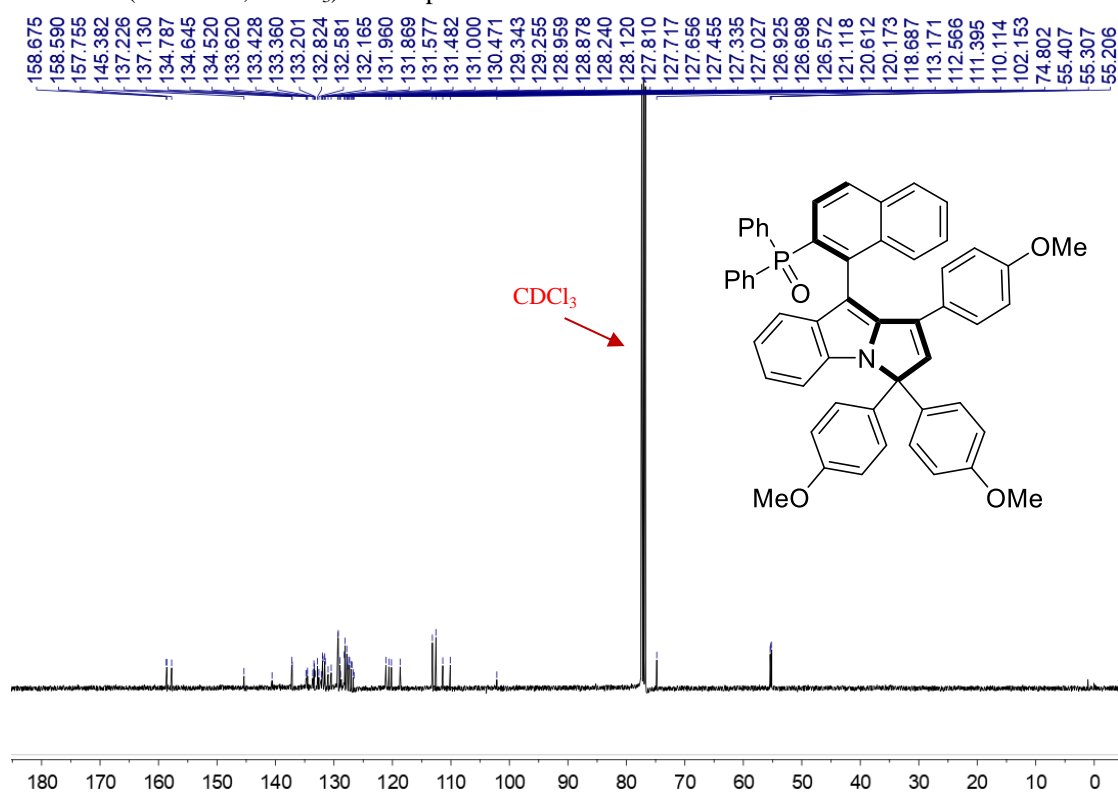
^{13}C NMR (100 MHz, CDCl_3) of compound **8b**:



¹H NMR (400 MHz, CDCl₃) of compound **9a**:

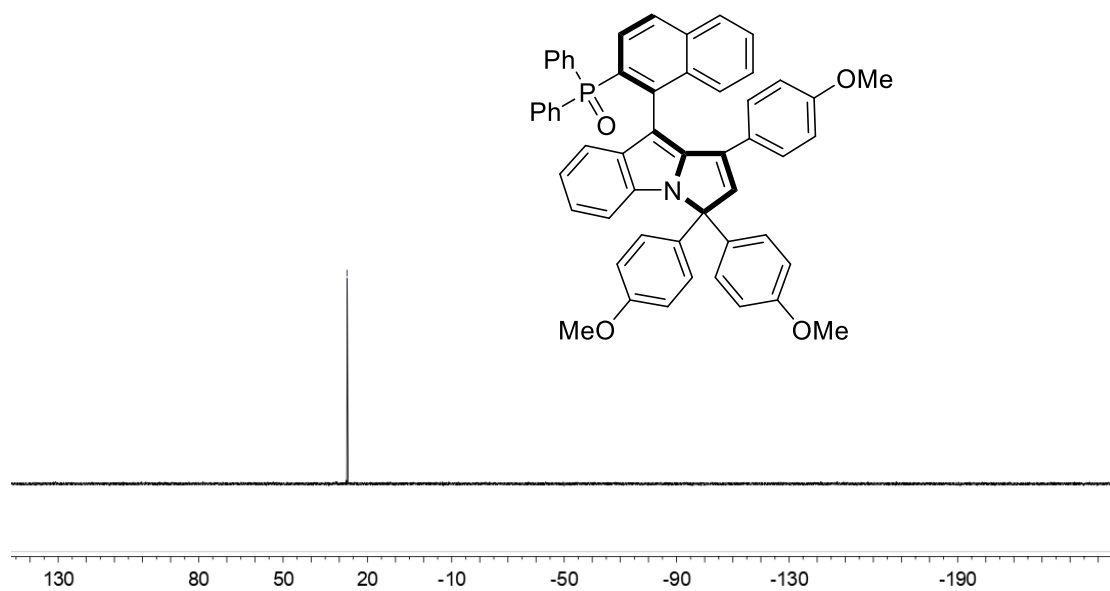


¹³C NMR (100 MHz, CDCl₃) of compound **9a**:

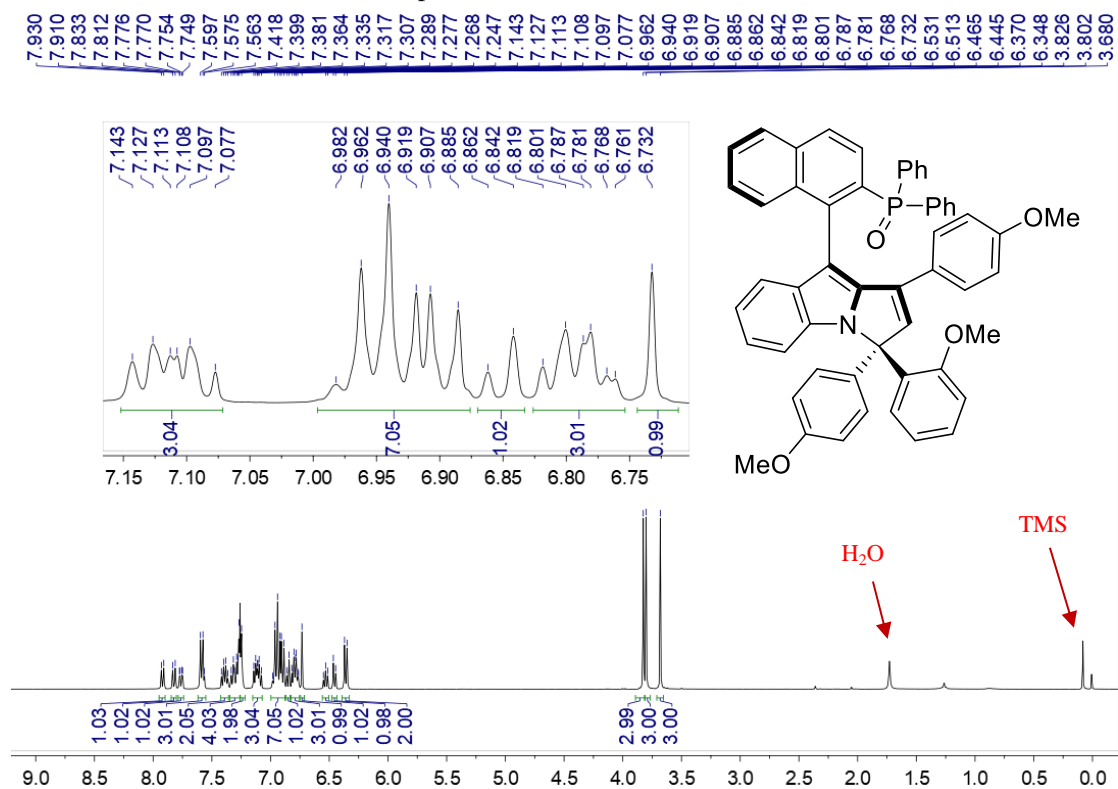


^{31}P NMR (162 MHz, CDCl_3) of compound **9a**:

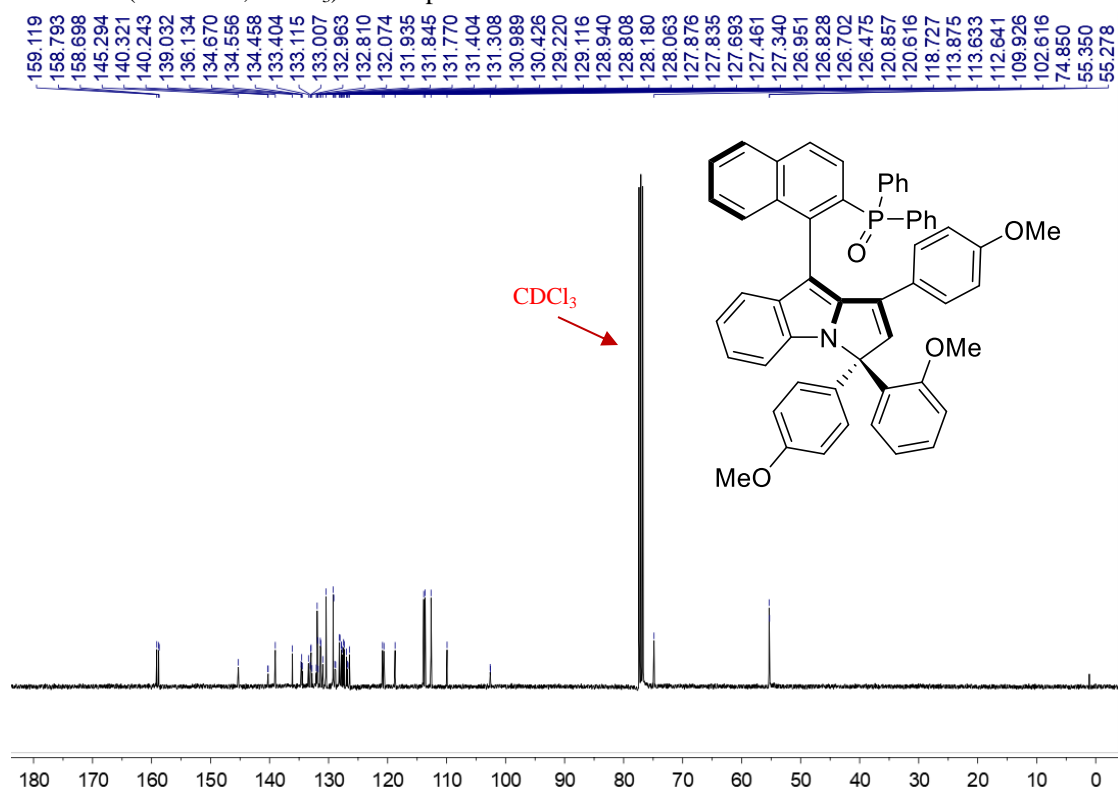
-27.197



¹H NMR (400 MHz, CDCl₃) of compound **9b**:

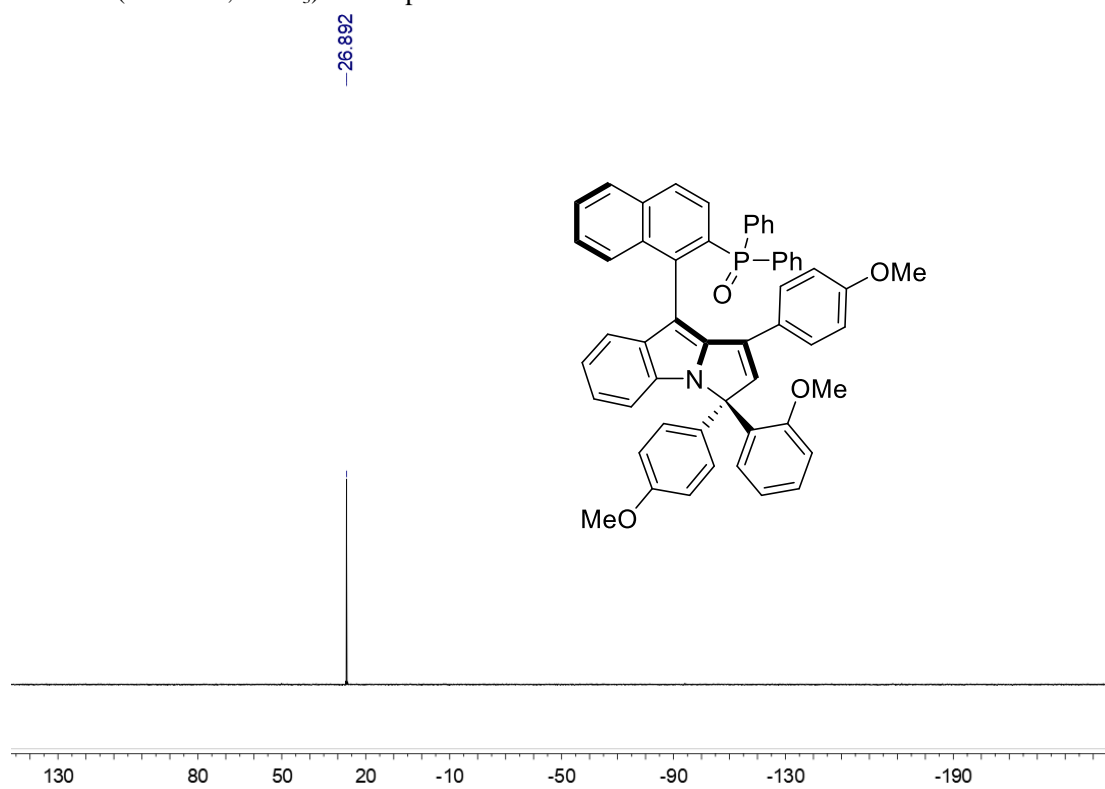


¹³C NMR (100 MHz, CDCl₃) of compound **9b**:



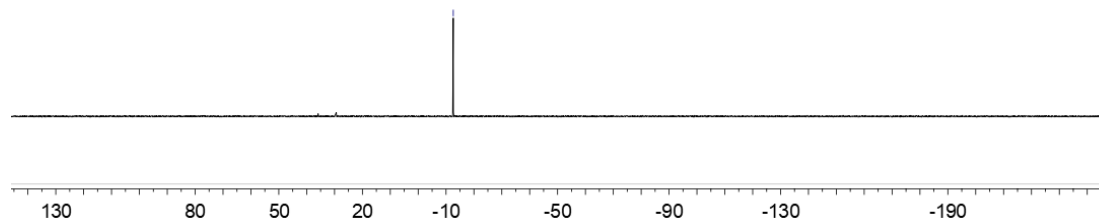
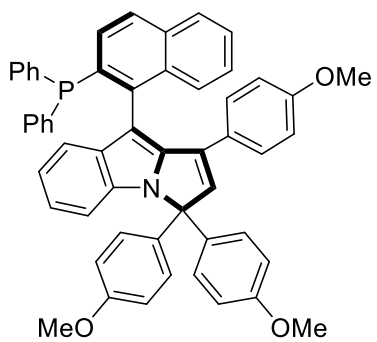
³¹P NMR (162 MHz, CDCl₃) of compound **9b**:

-26.892

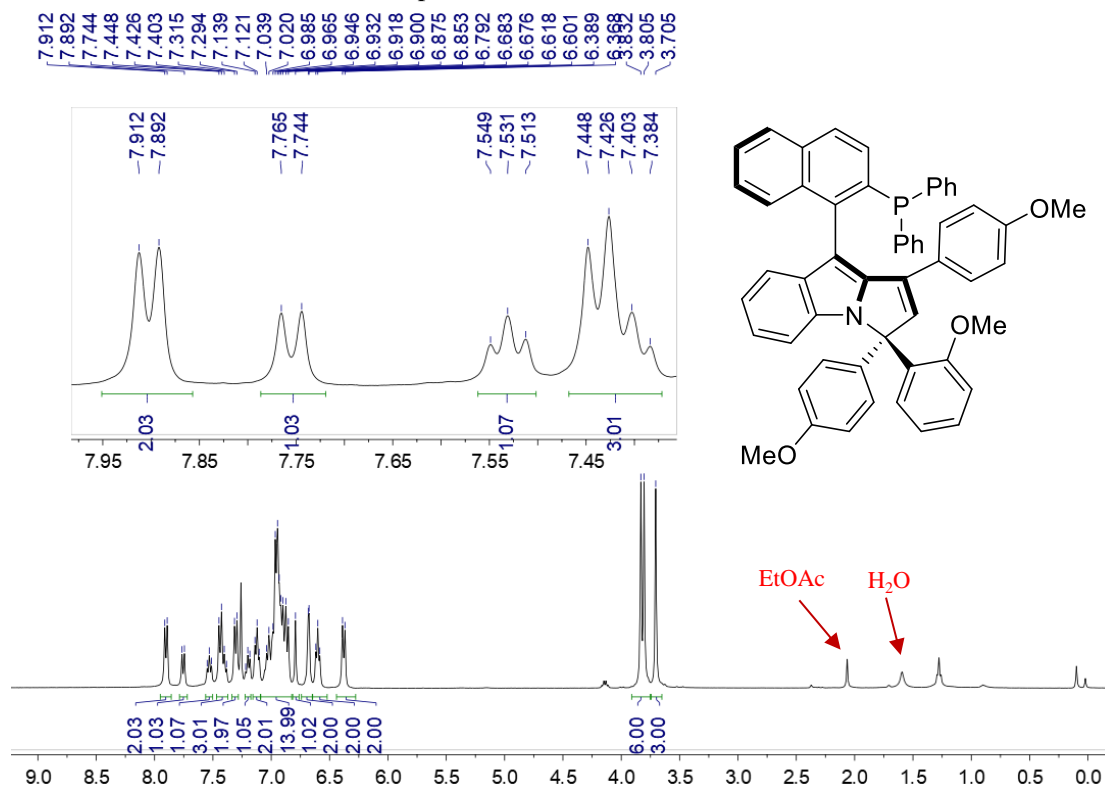


^{31}P NMR (162 MHz, CDCl_3) of compound **10a**:

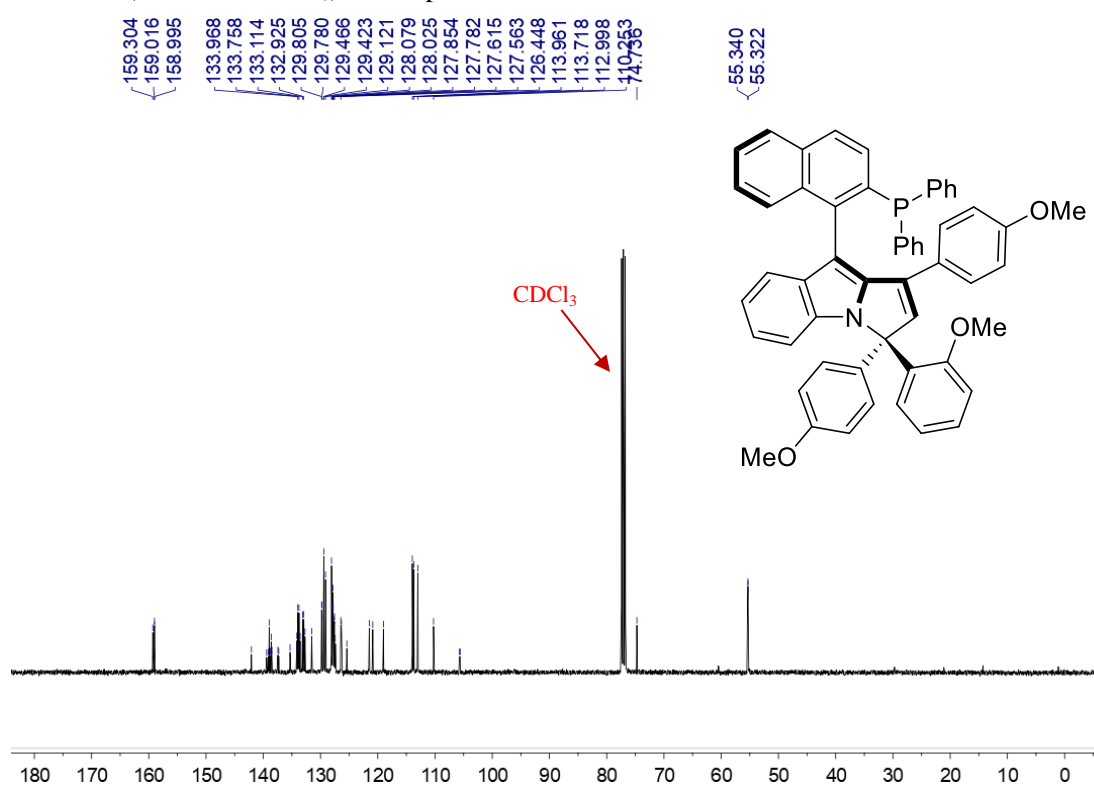
---12.590



^1H NMR (400 MHz, CDCl_3) of compound **10b**:

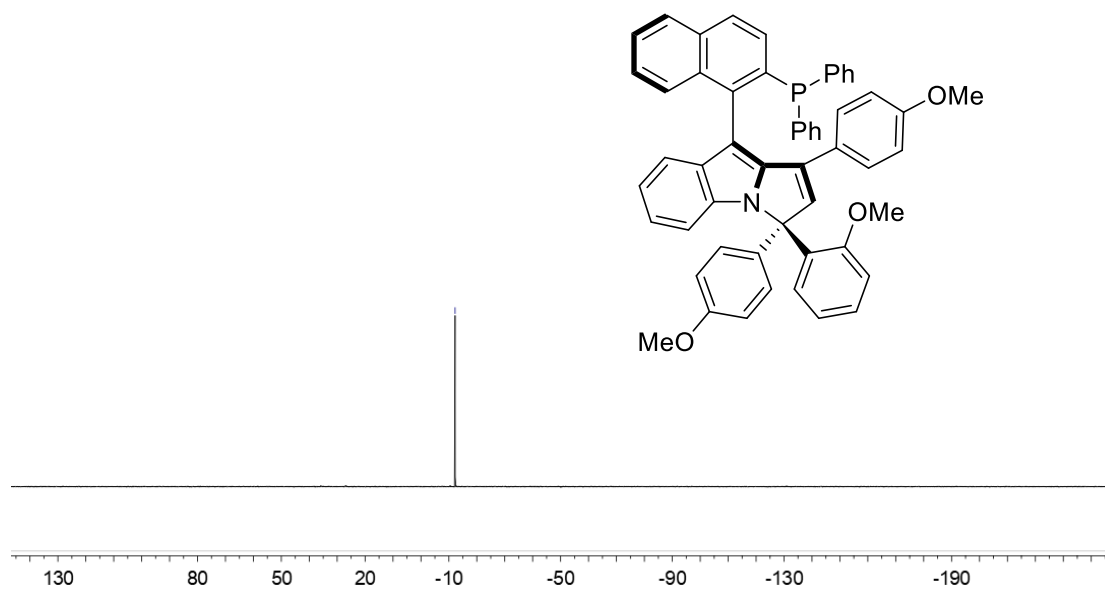


^{13}C NMR (100 MHz, CDCl_3) of compound **10b**:

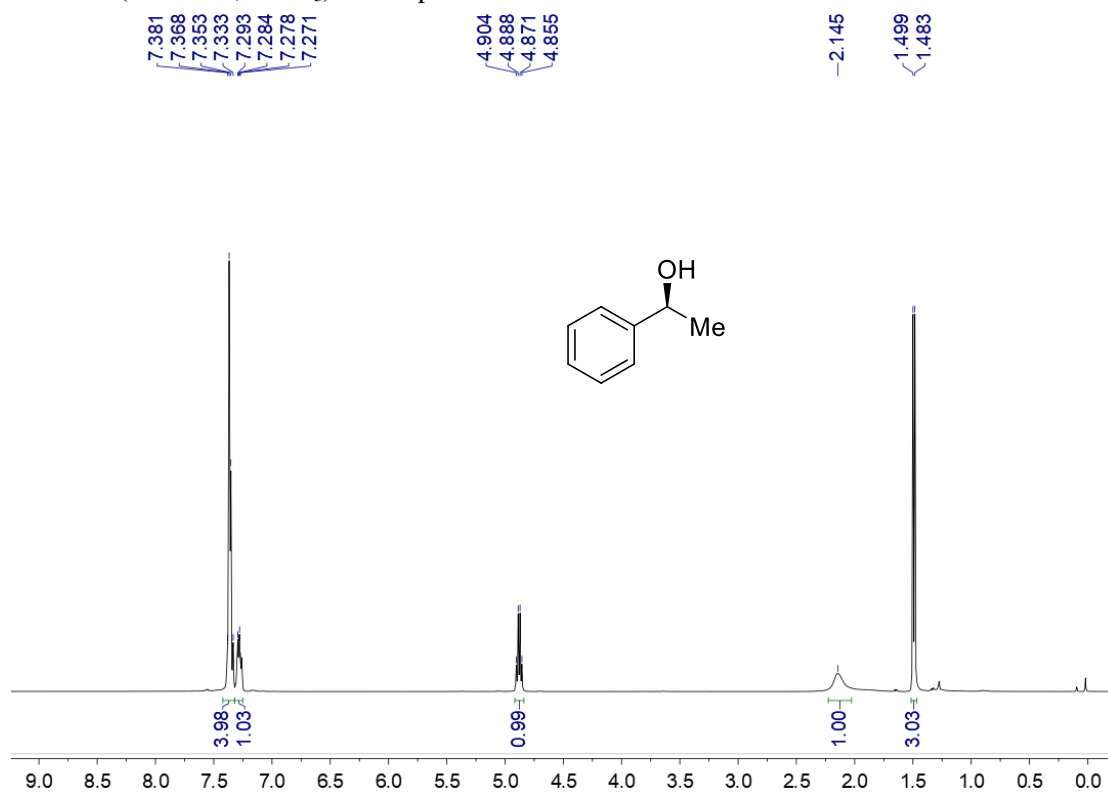


³¹P NMR (162 MHz, CDCl₃) of compound **10b**:

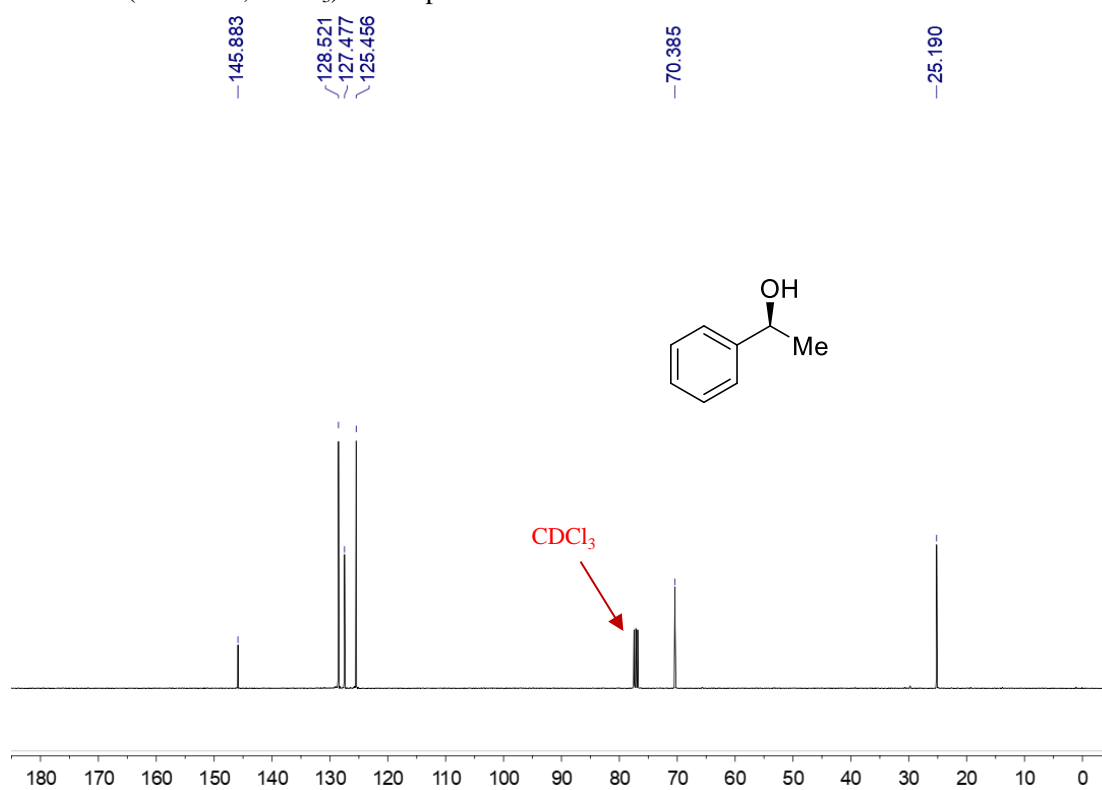
---12.223



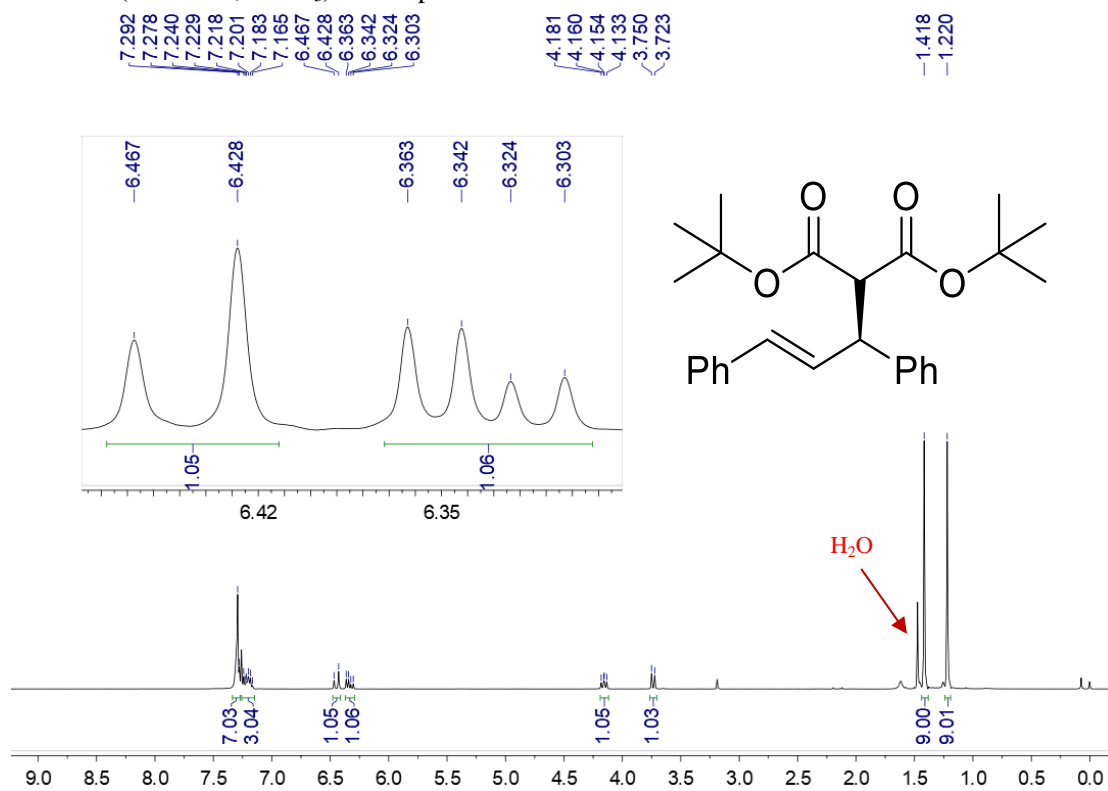
^1H NMR (400 MHz, CDCl_3) of compound **13**:



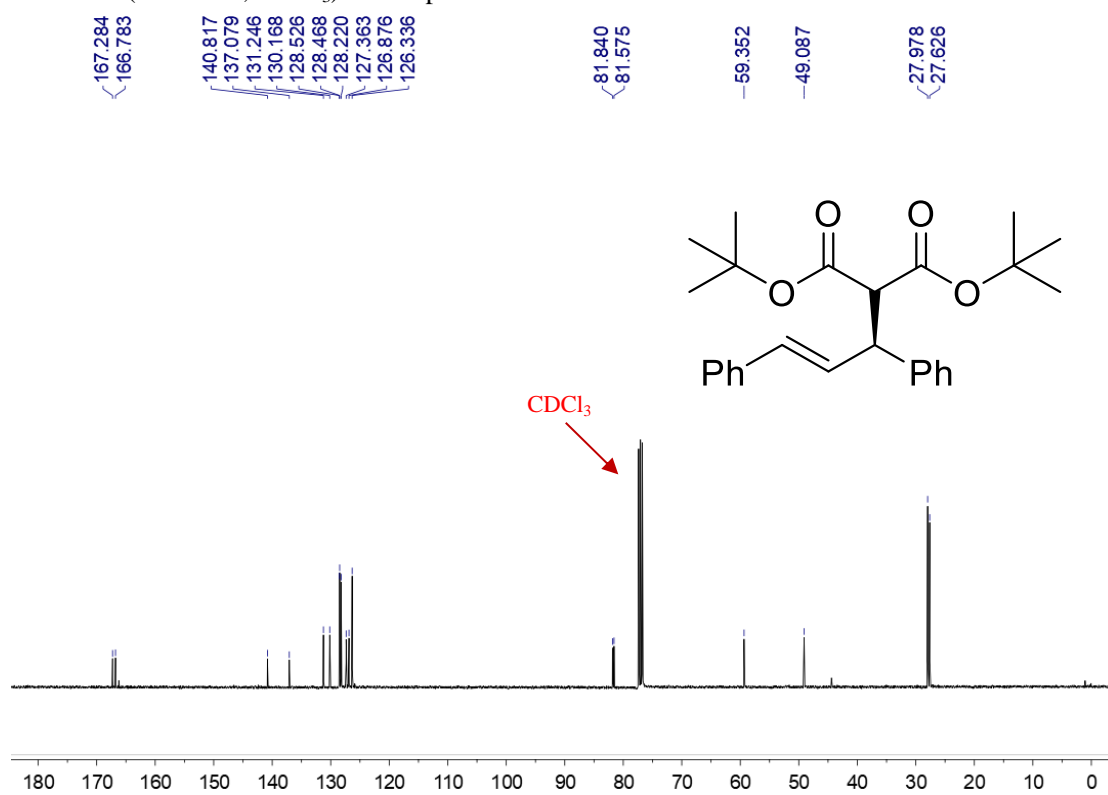
^{13}C NMR (100 MHz, CDCl_3) of compound **13**:



^1H NMR (400 MHz, CDCl_3) of compound **16**:



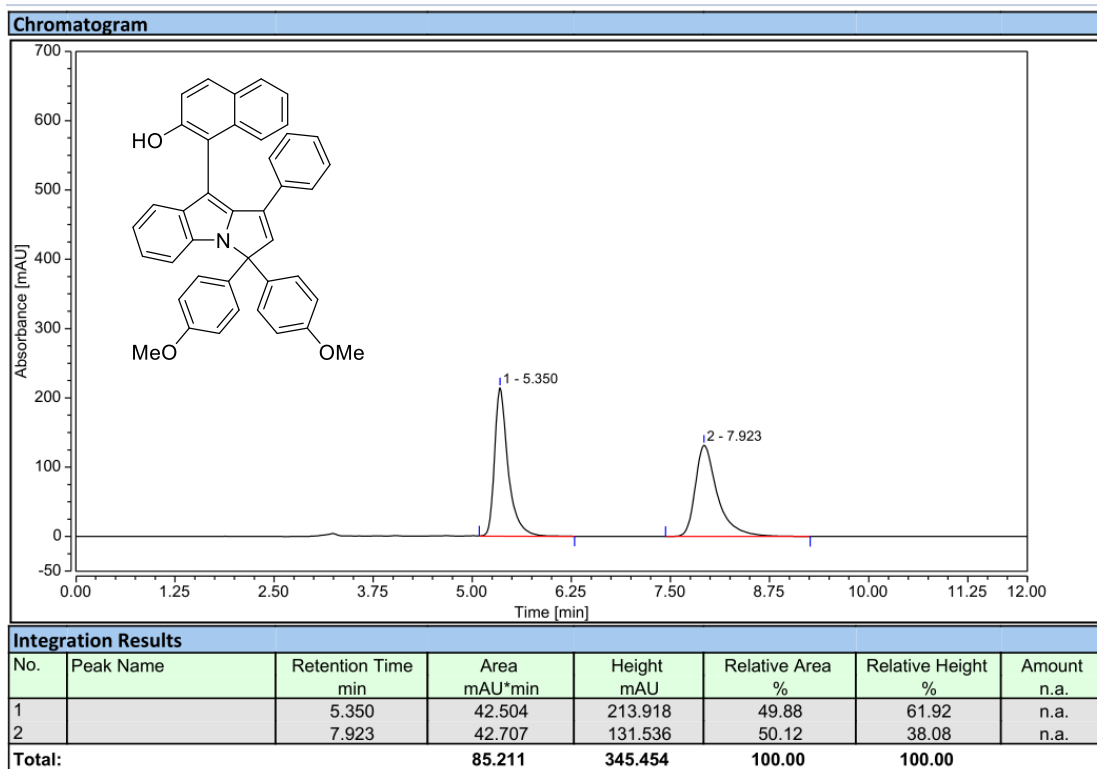
^{13}C NMR (100 MHz, CDCl_3) of compound **16**:



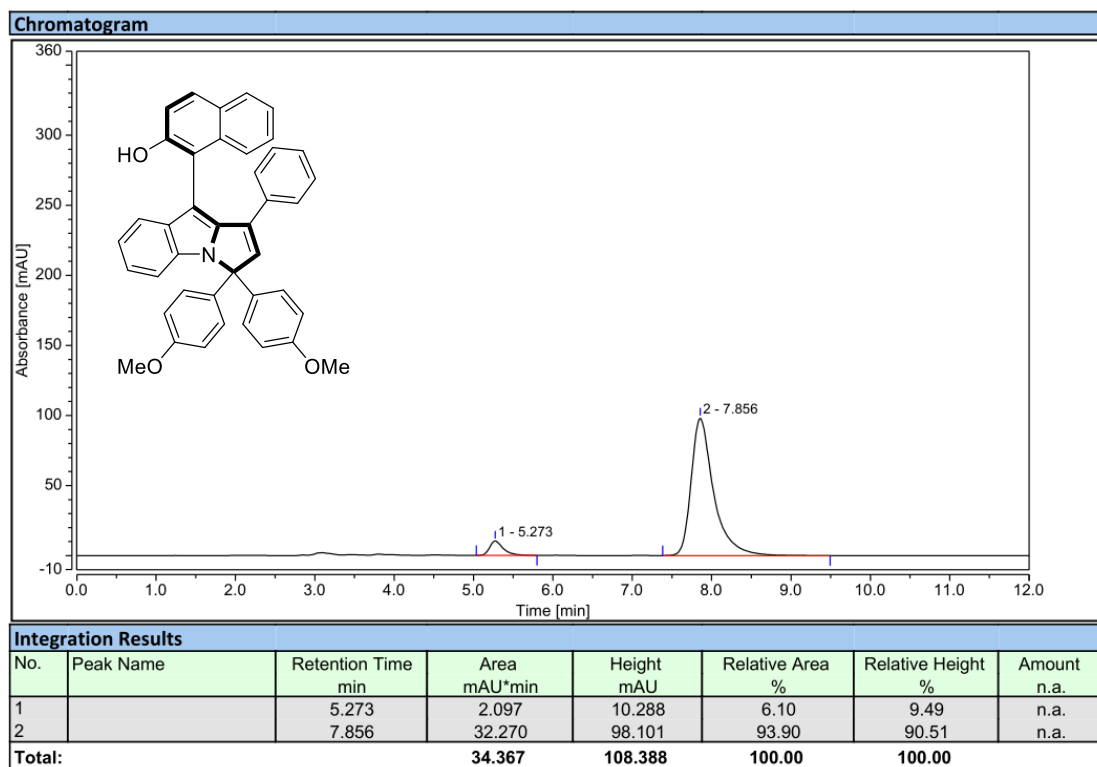
9. HPLC traces of all products 3, 7-10, 13, 16

3aa

Racemic:

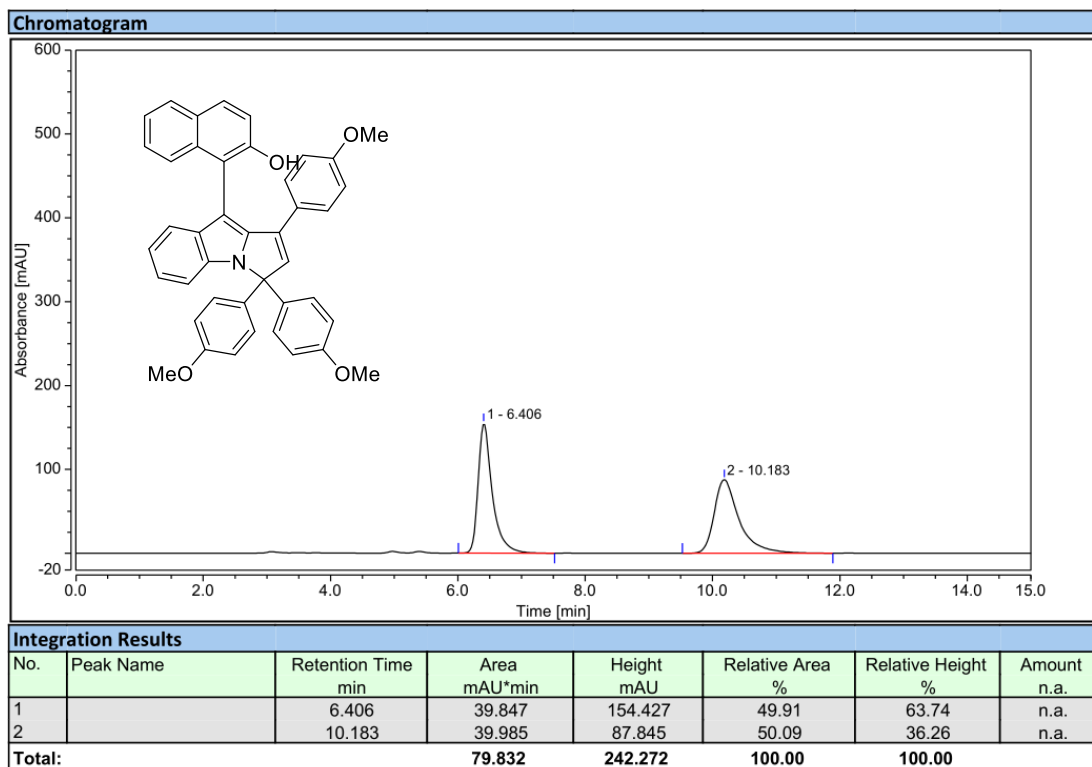


Enantioselective:

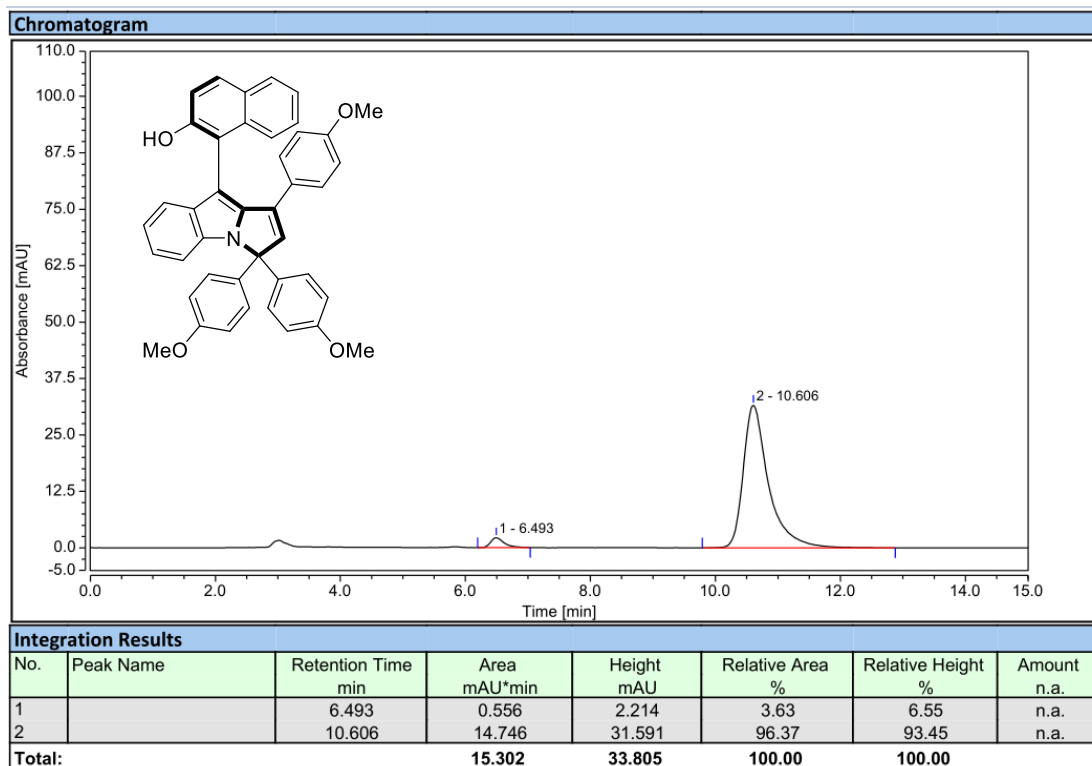


3ab

Racemic:

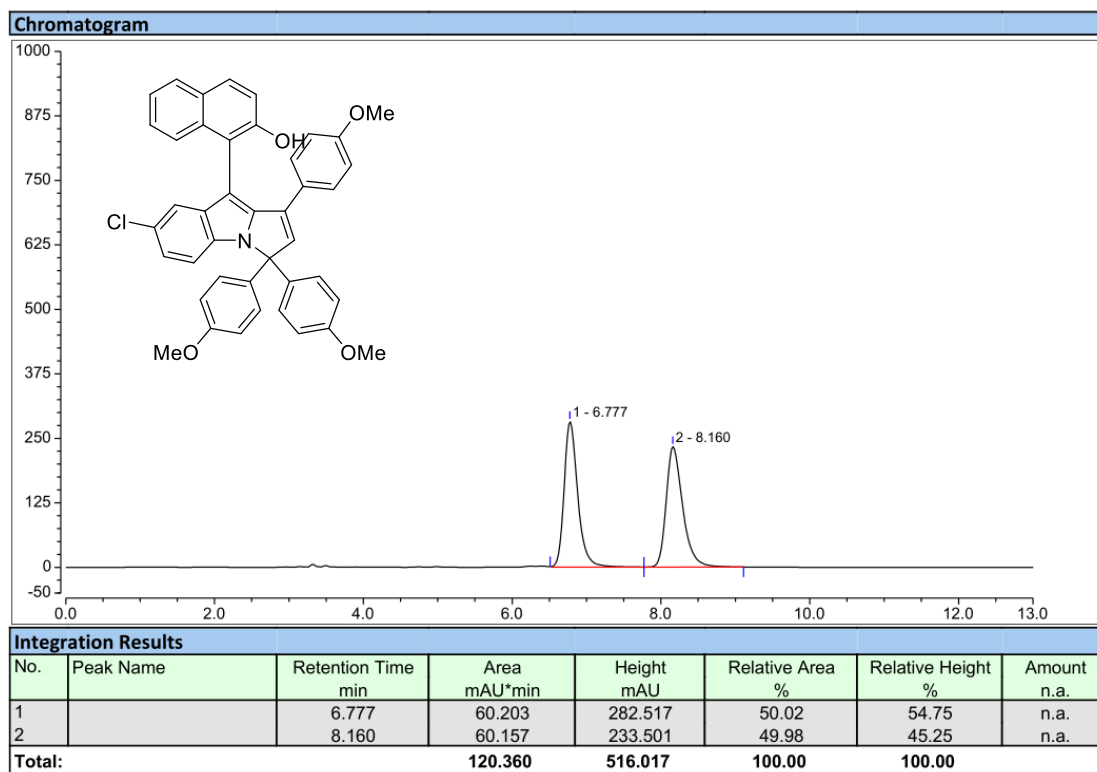


Enantioselective:

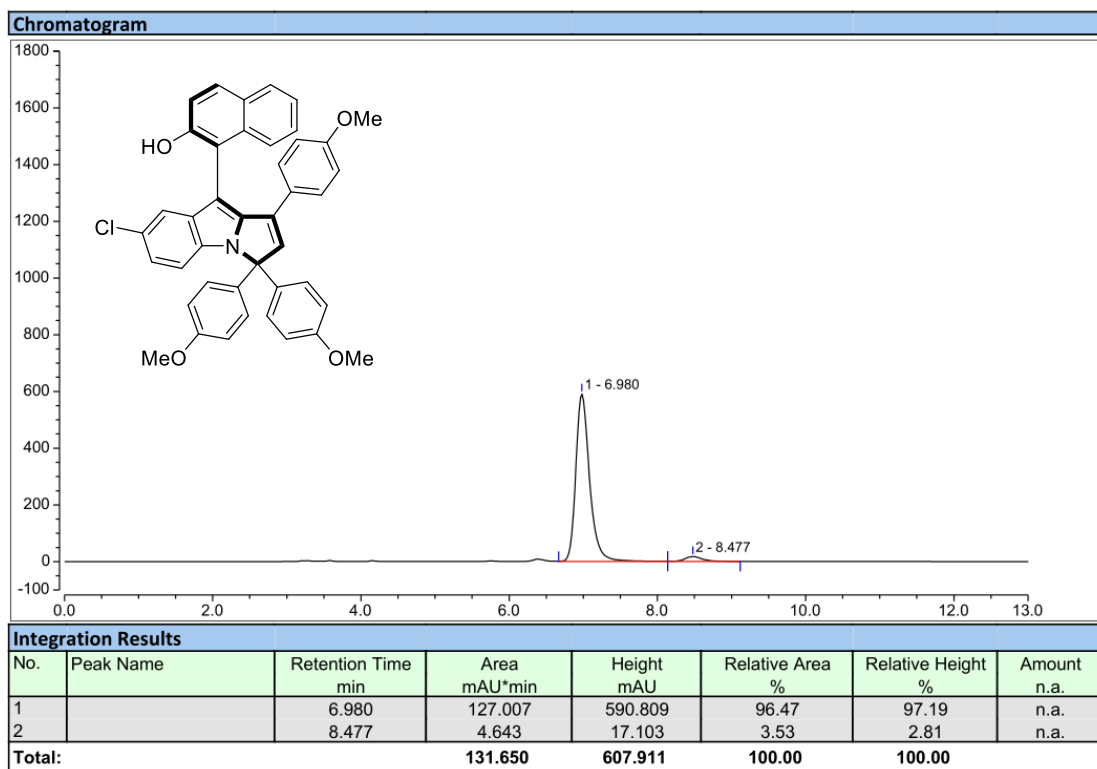


3bb

Racemic:

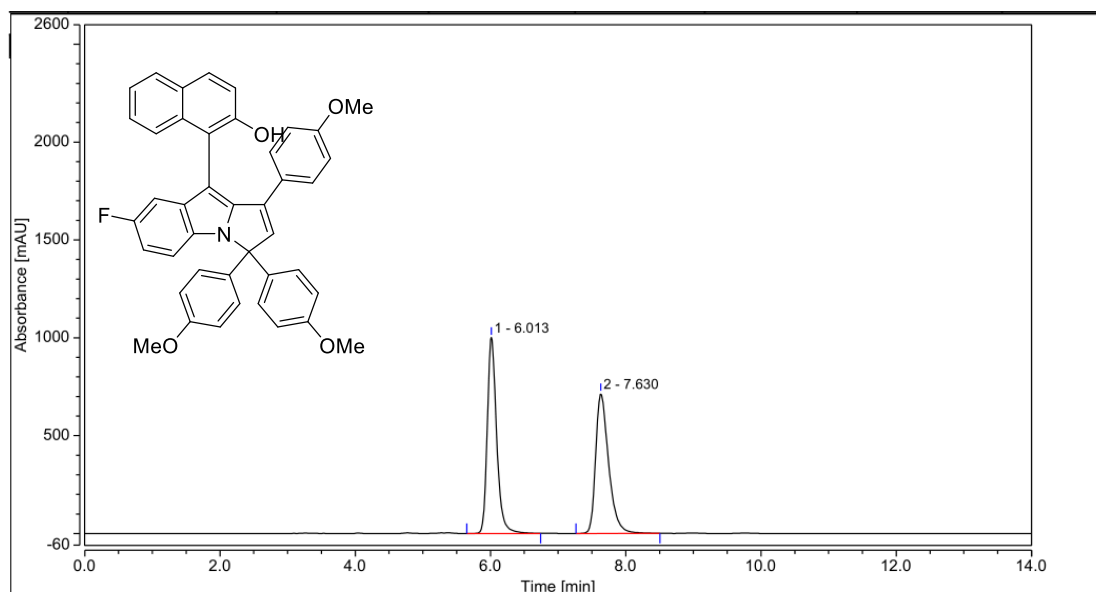


Enantioselective:



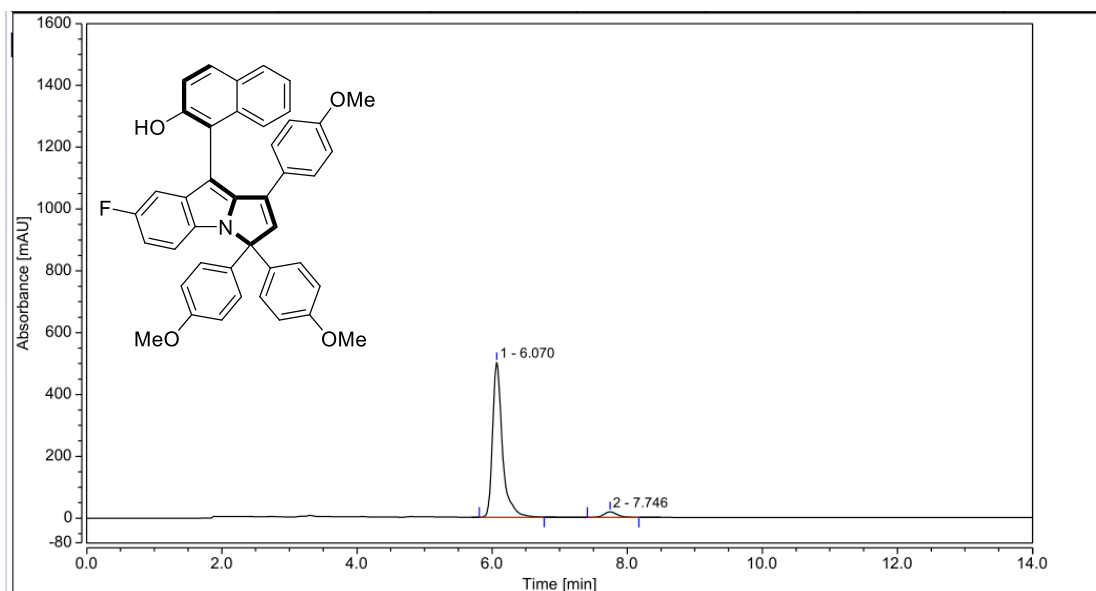
3cb

Racemic:



Integration Results							
No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount
1		6.013	160.716	1002.044	50.33	58.35	n.a.
2		7.630	158.621	715.273	49.67	41.65	n.a.
Total:			319.337	1717.317	100.00	100.00	

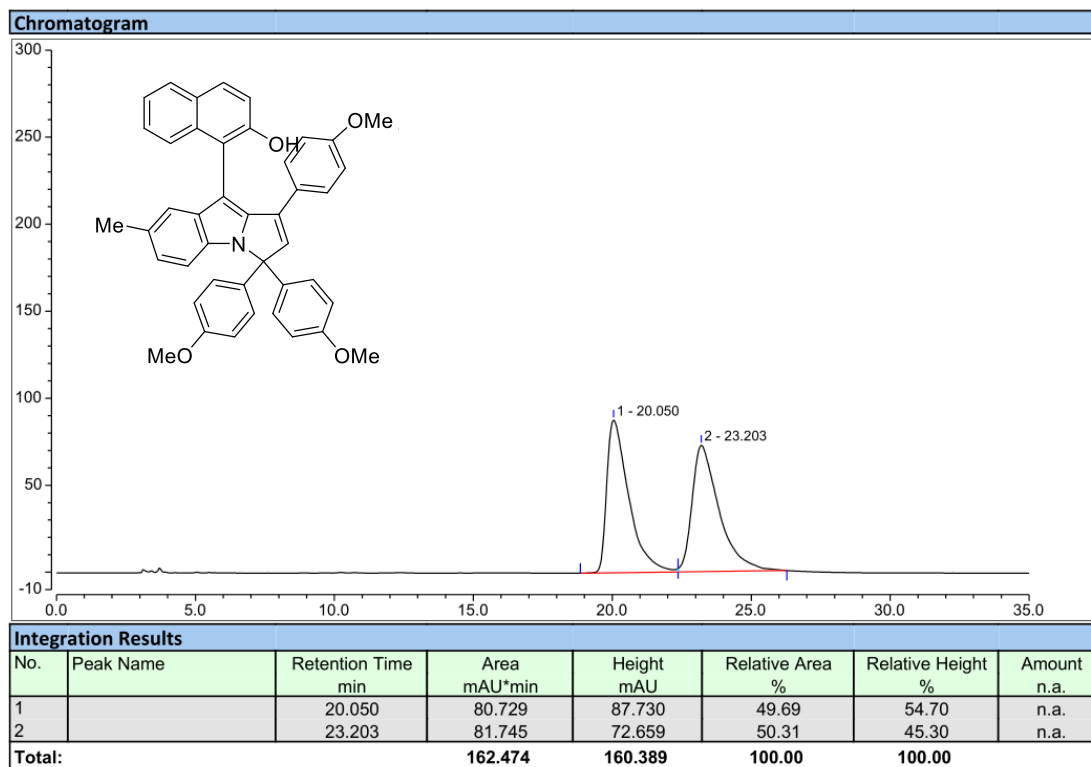
Enantioselective:



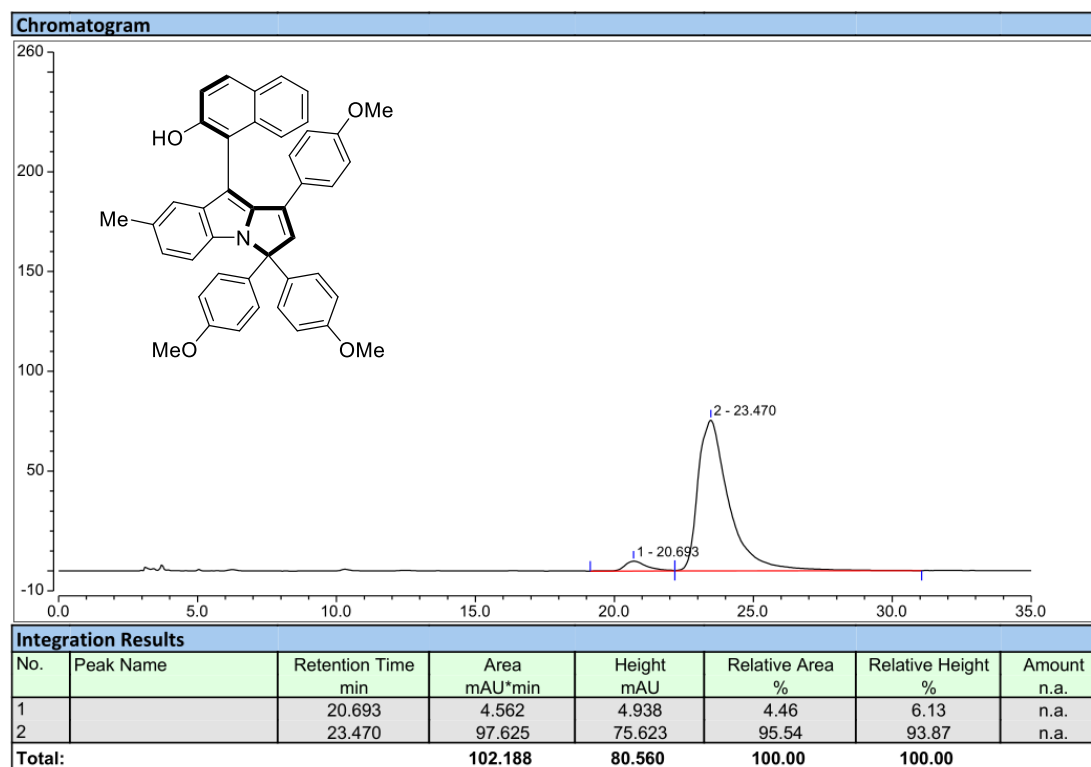
Integration Results							
No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount
1		6.070	84.972	500.787	95.41	96.57	n.a.
2		7.746	4.089	17.768	4.59	3.43	n.a.
Total:			89.061	518.555	100.00	100.00	

3db

Racemic:

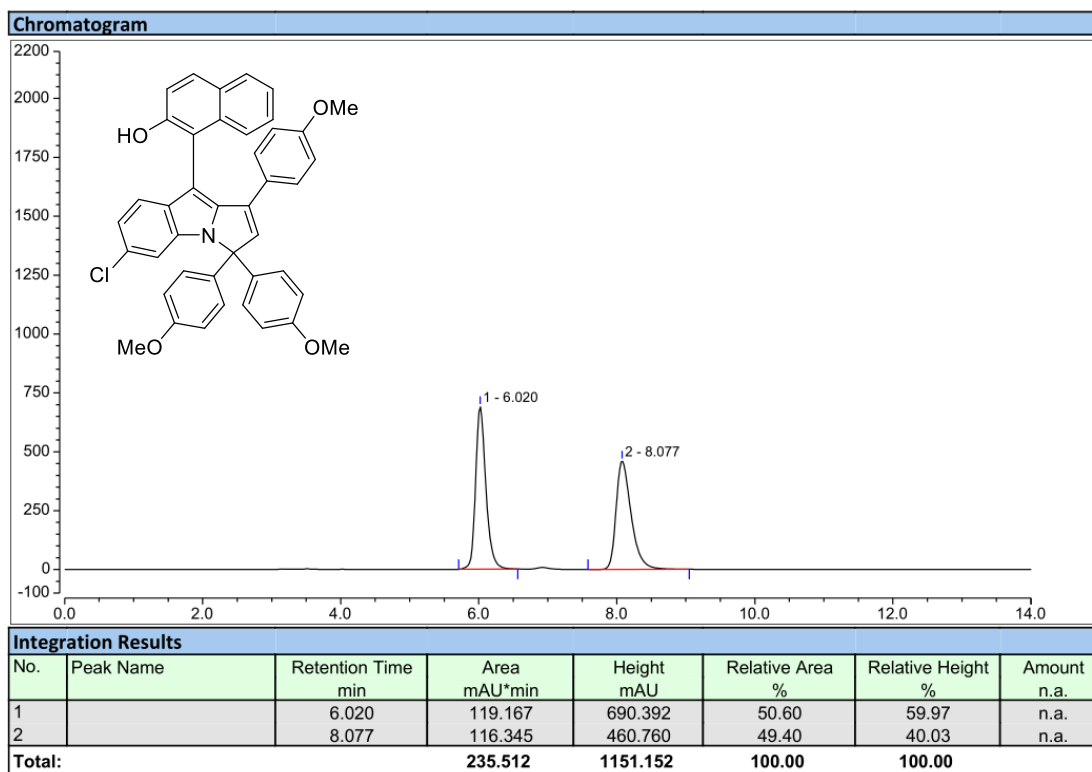


Enantioselective:

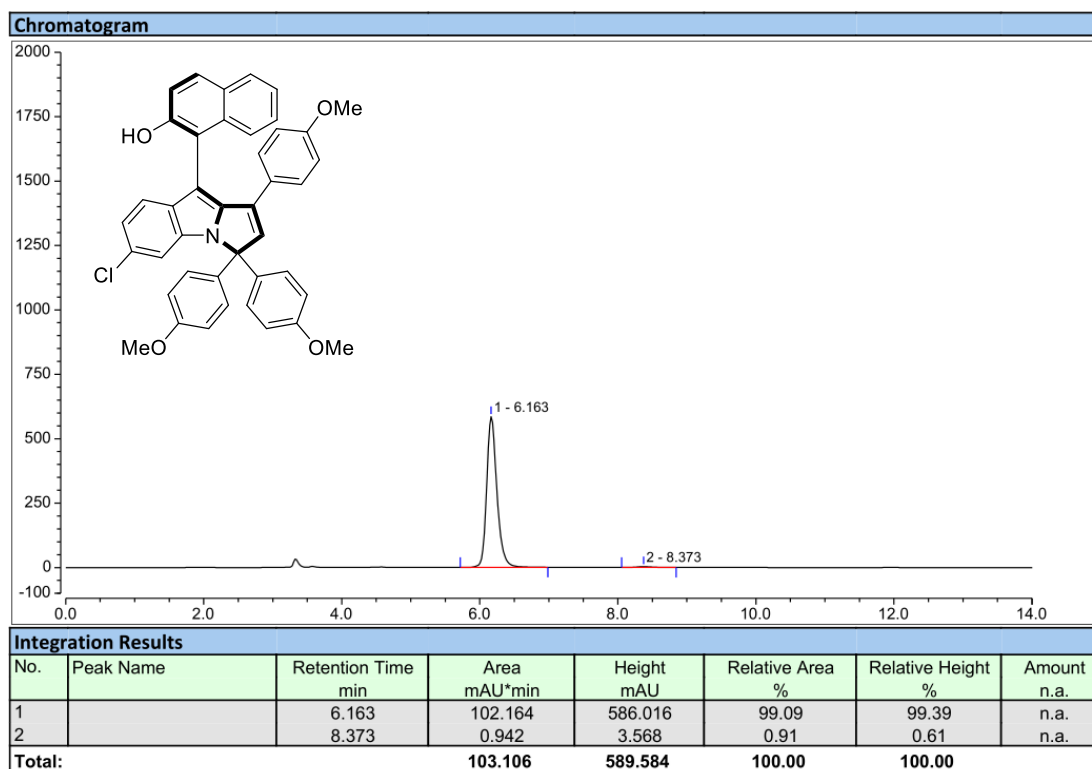


3eb

Racemic:

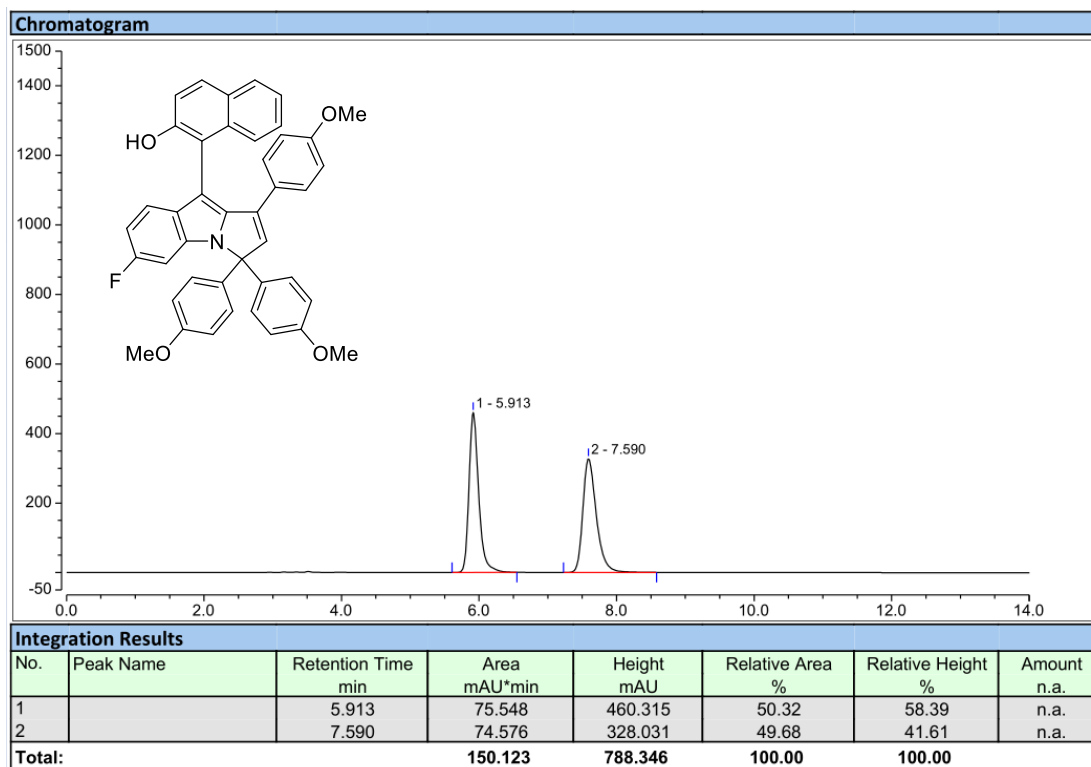


Enantioselective:

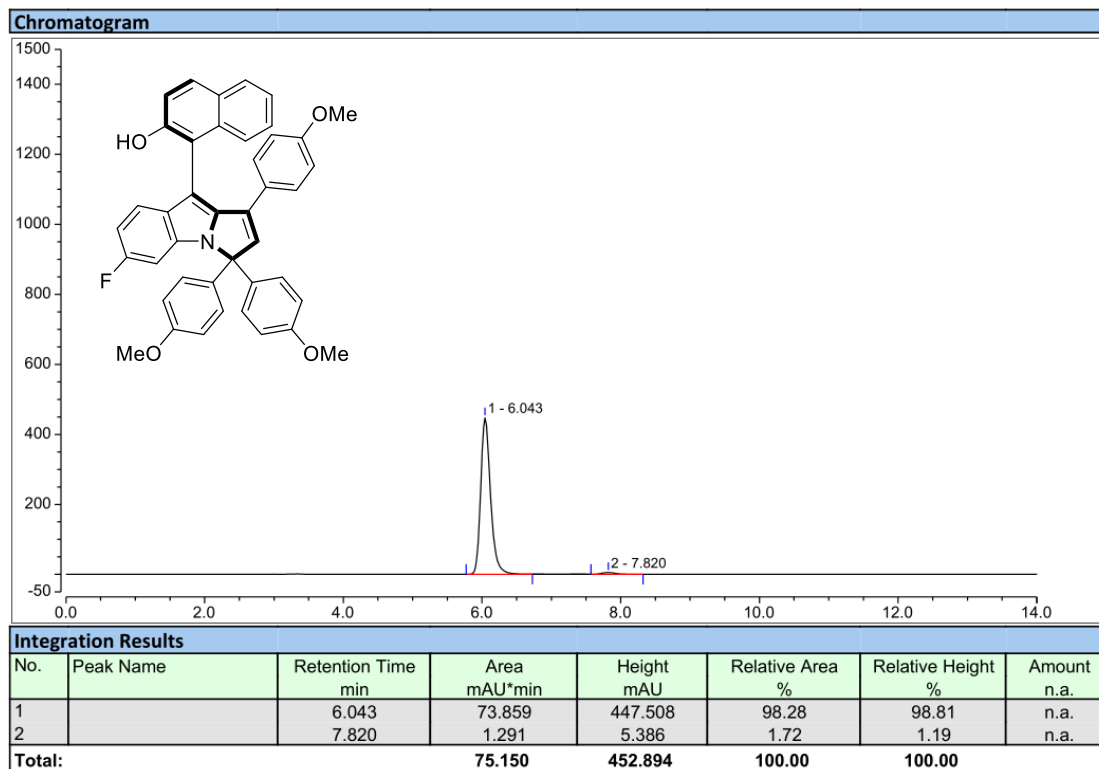


3fb

Racemic:

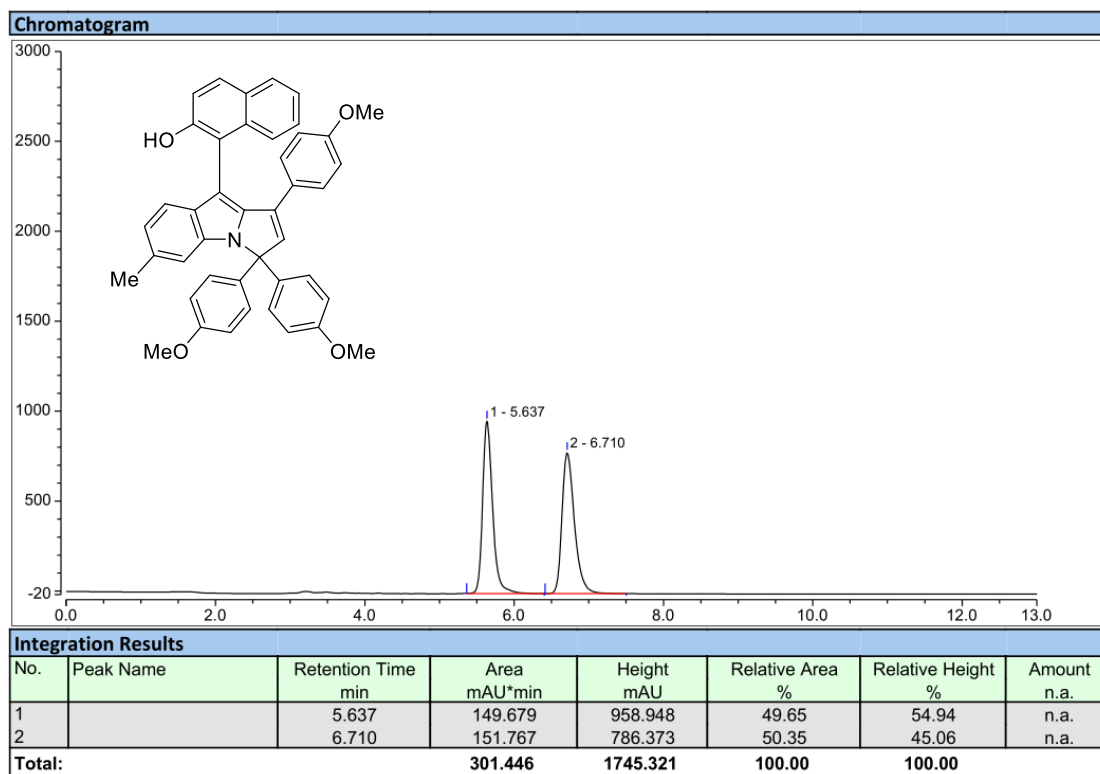


Enantioselective:

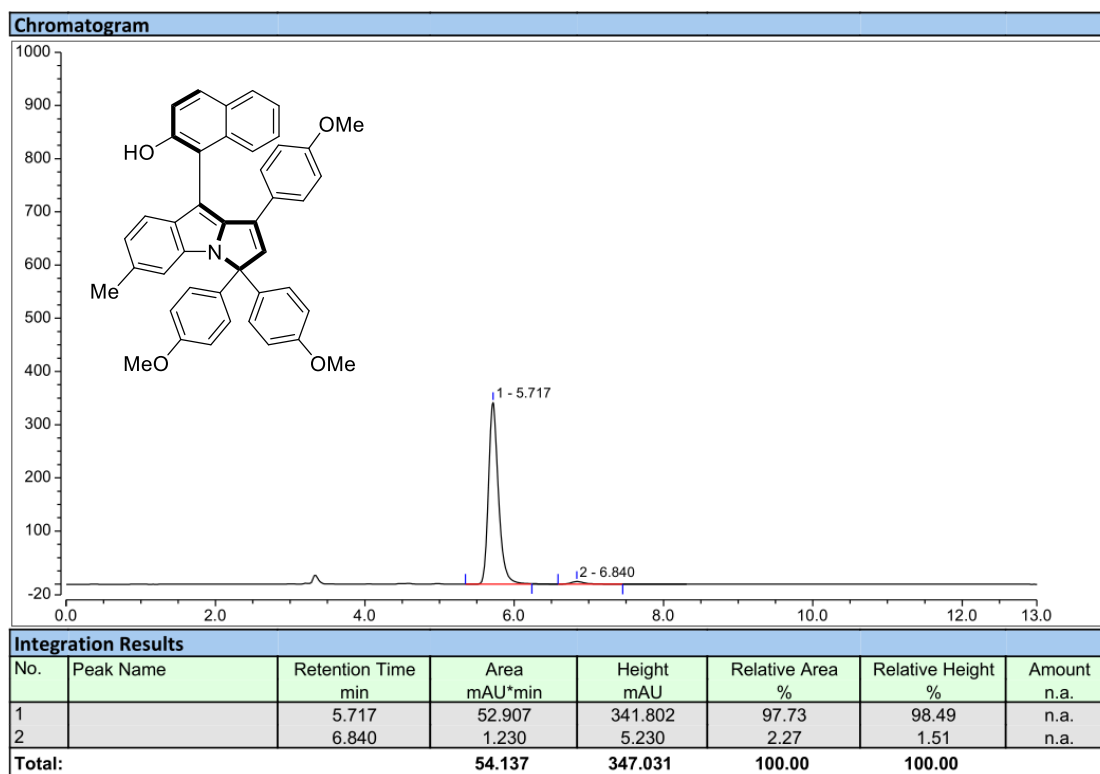


3gb

Racemic:

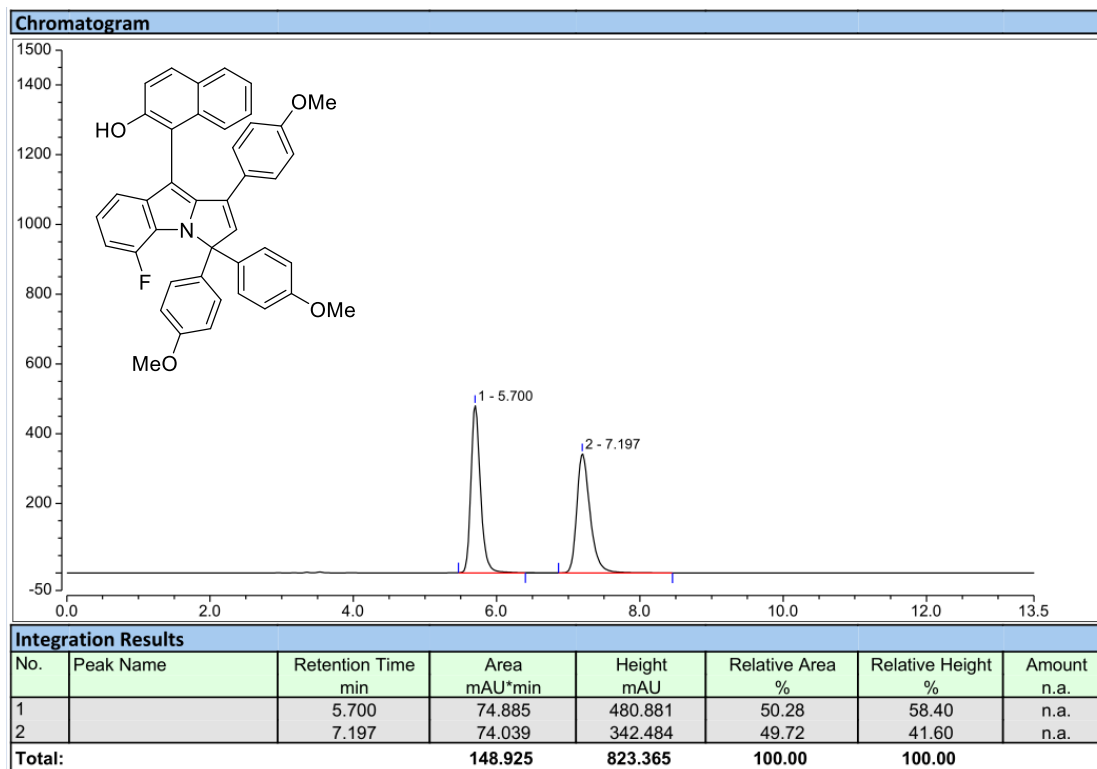


Enantioselective:

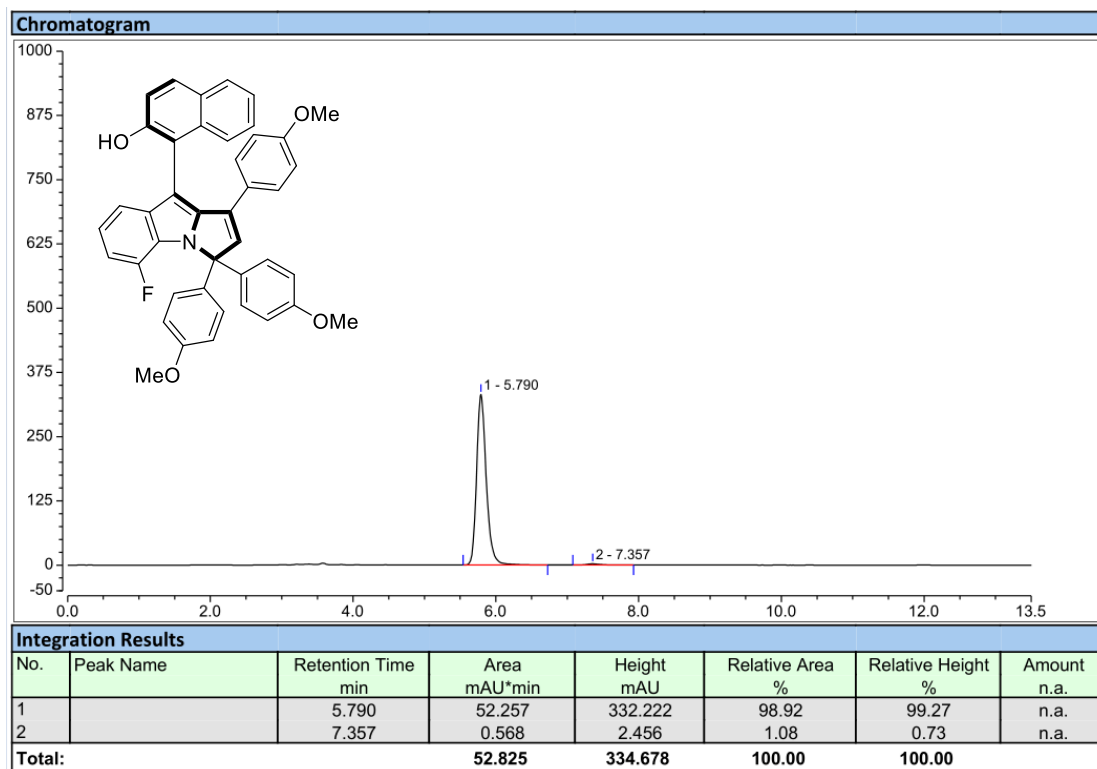


3hb

Racemic:

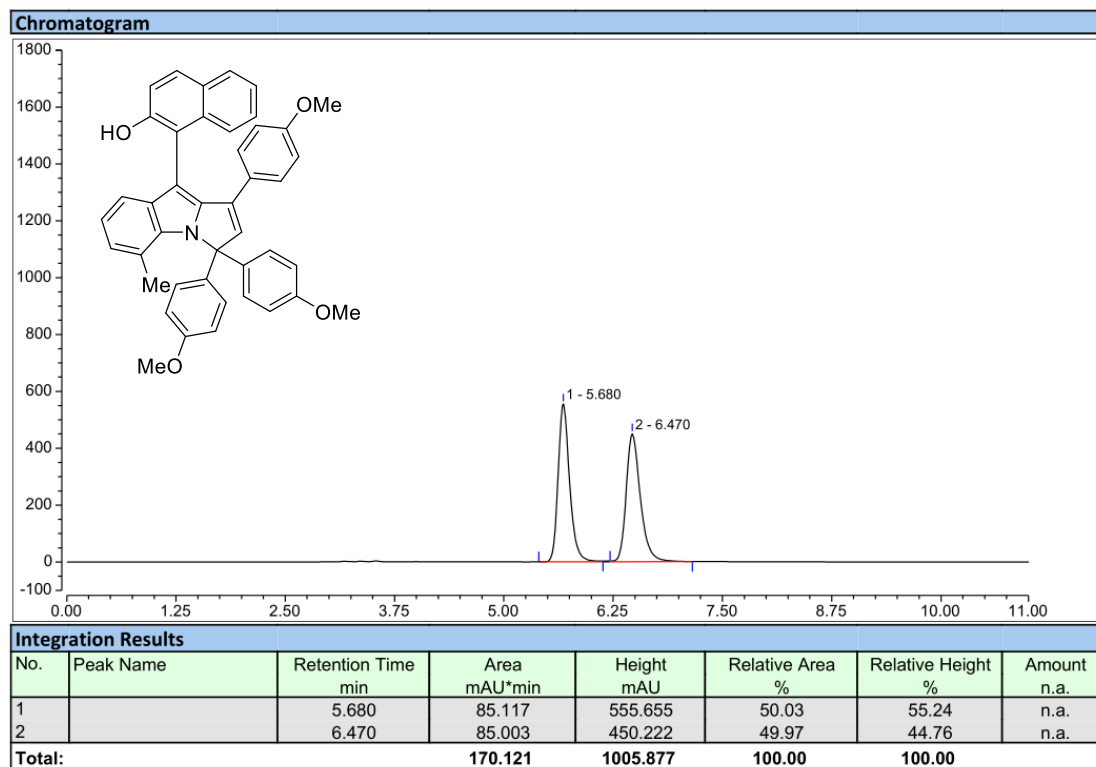


Enantioselective:

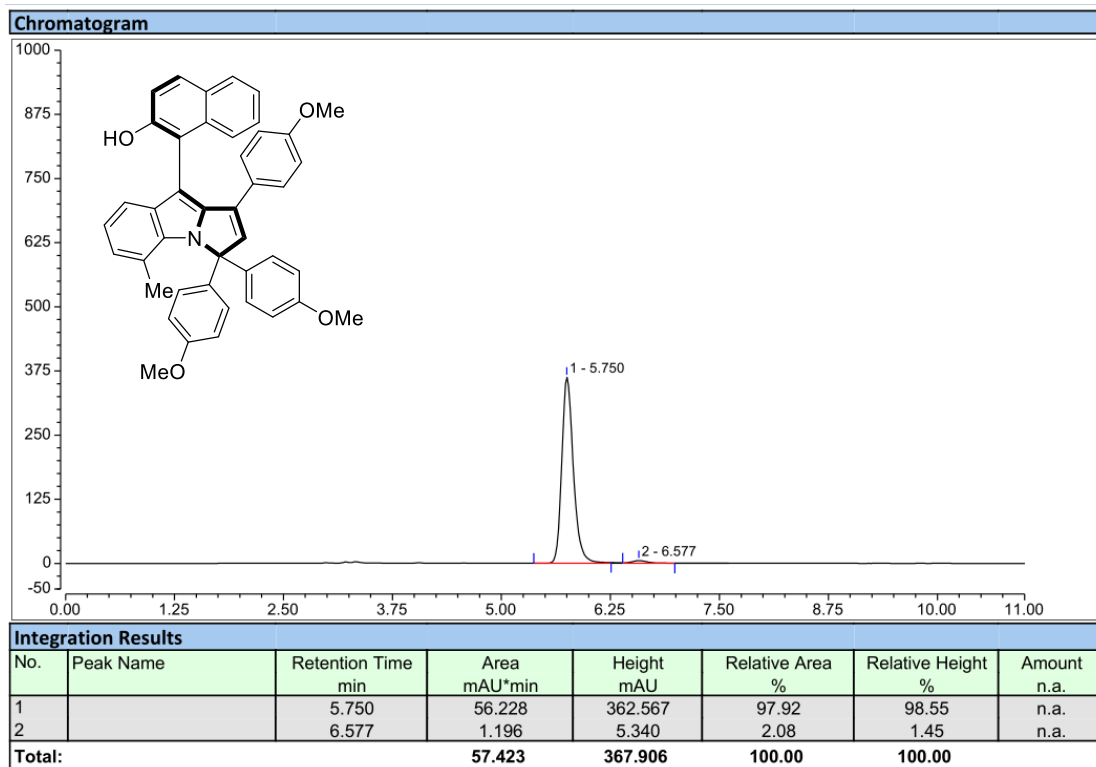


3ib

Racemic:

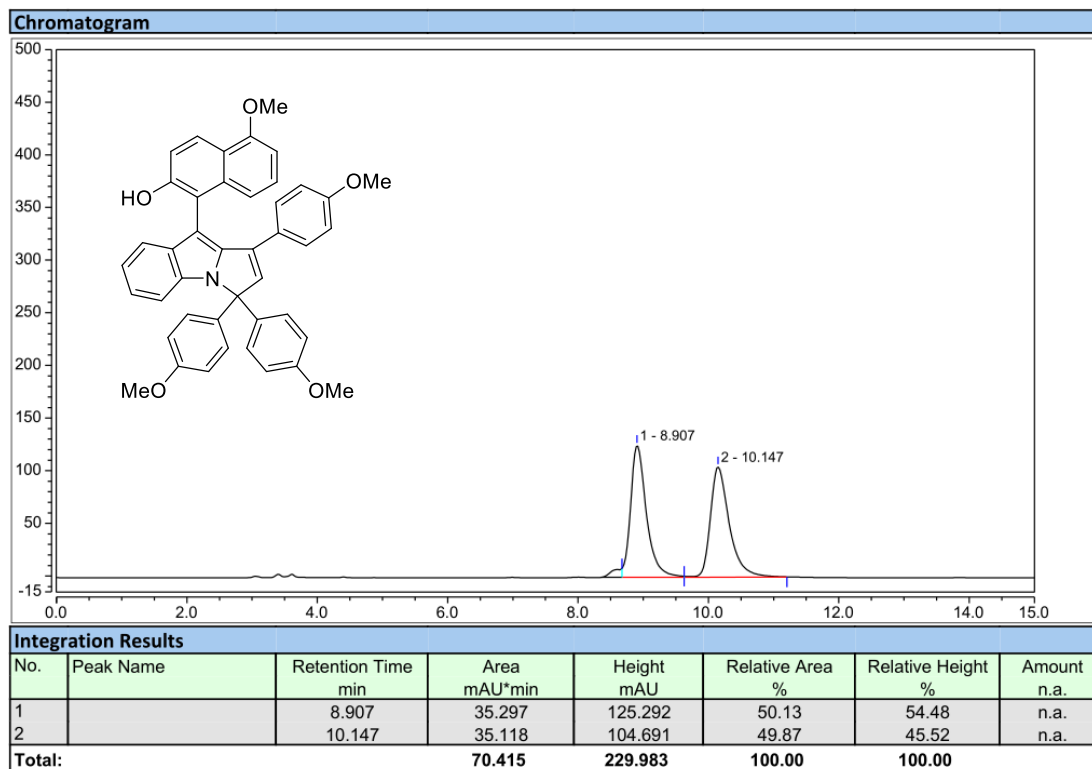


Enantioselective:

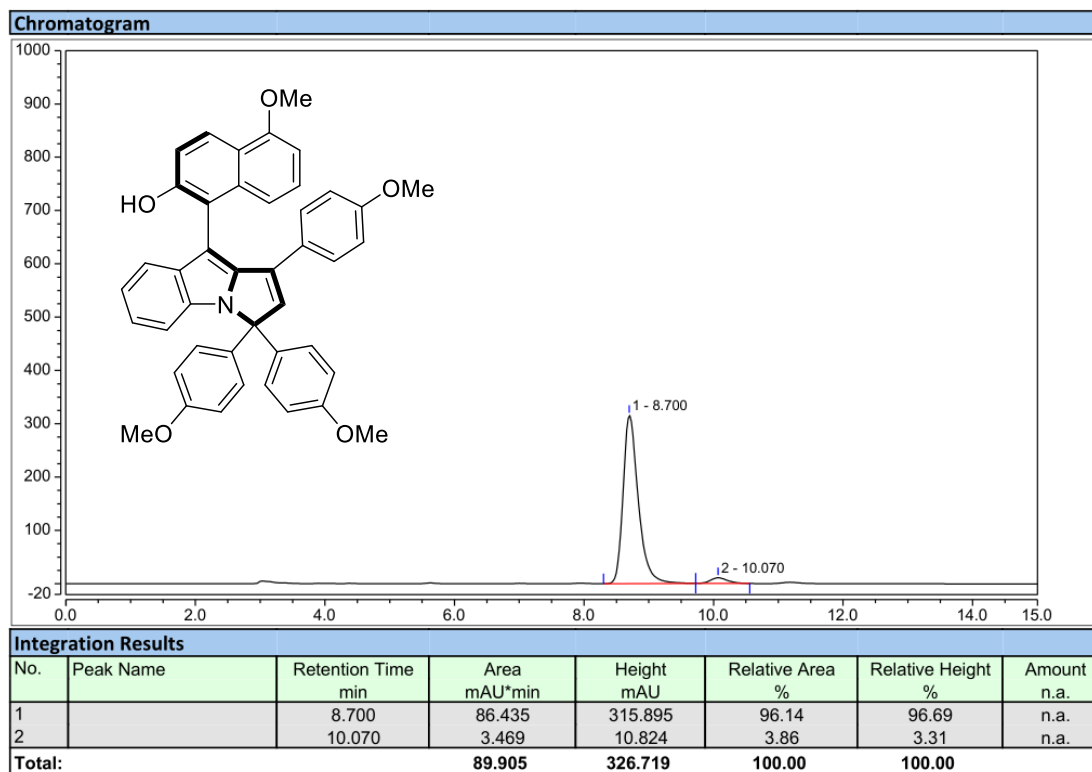


3jb

Racemic:

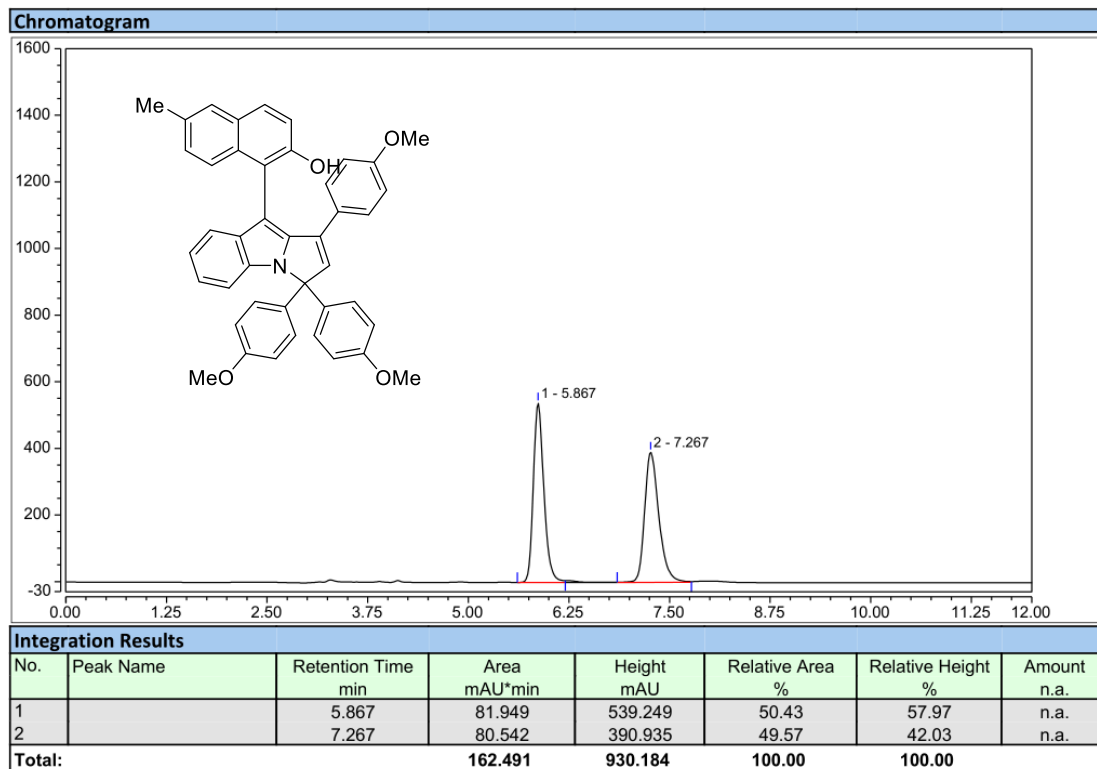


Enantioselective:

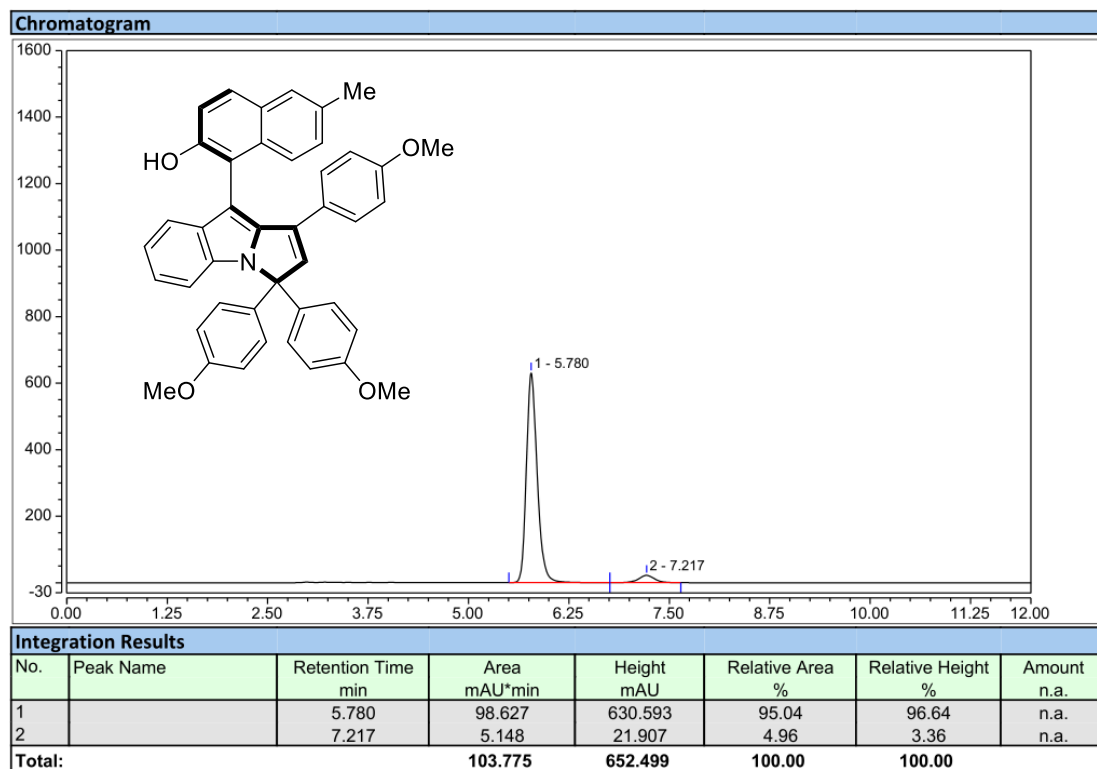


3kb

Racemic:

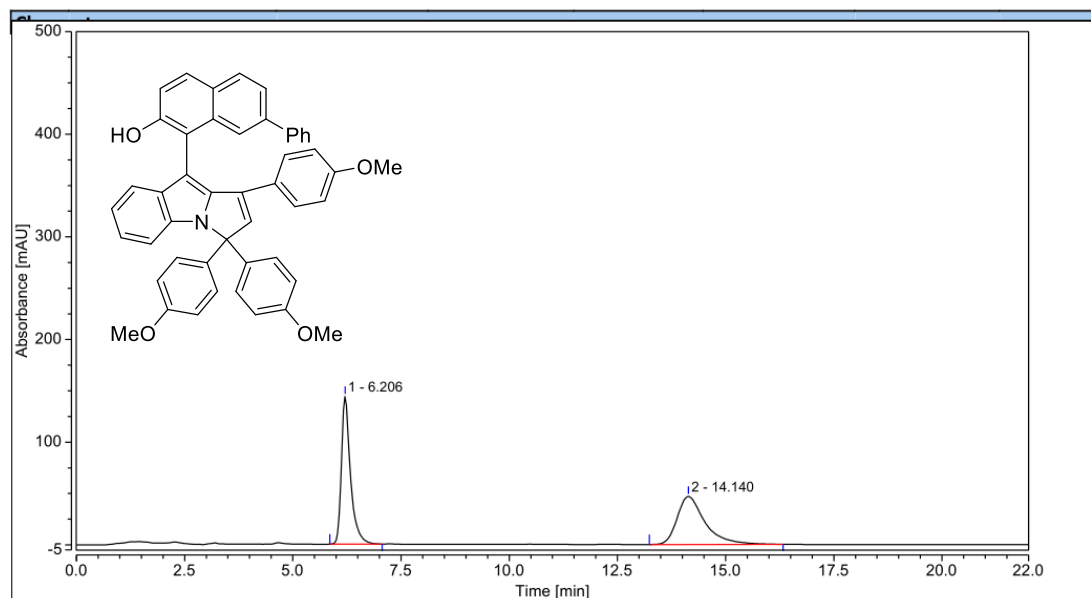


Enantioselective:



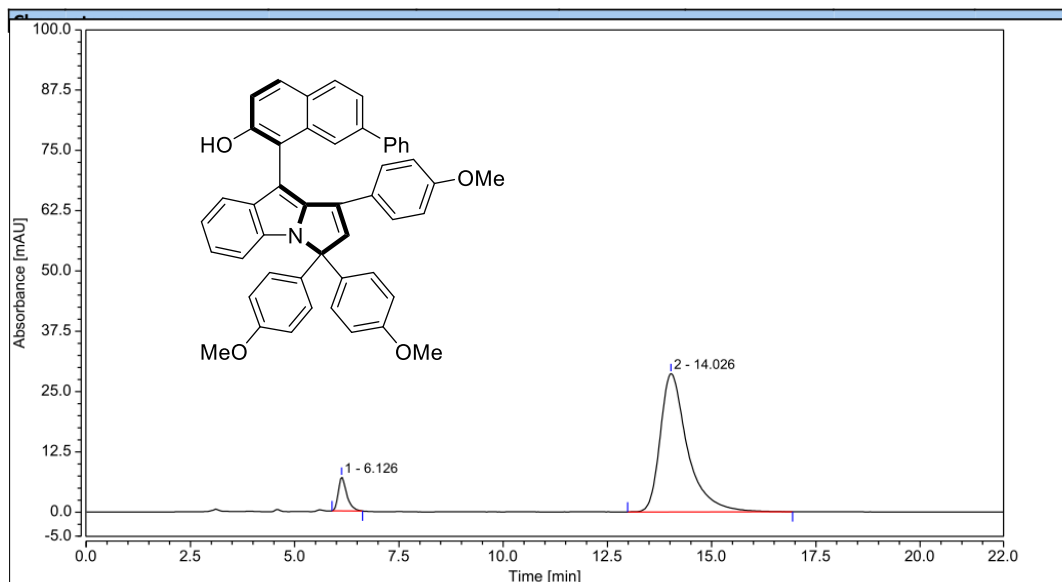
31b

Racemic:



Integration Results							
No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		6.206	35.239	143.904	50.27	75.48	n.a.
2		14.140	34.860	46.738	49.73	24.52	n.a.
Total:			70.099	190.642	100.00	100.00	

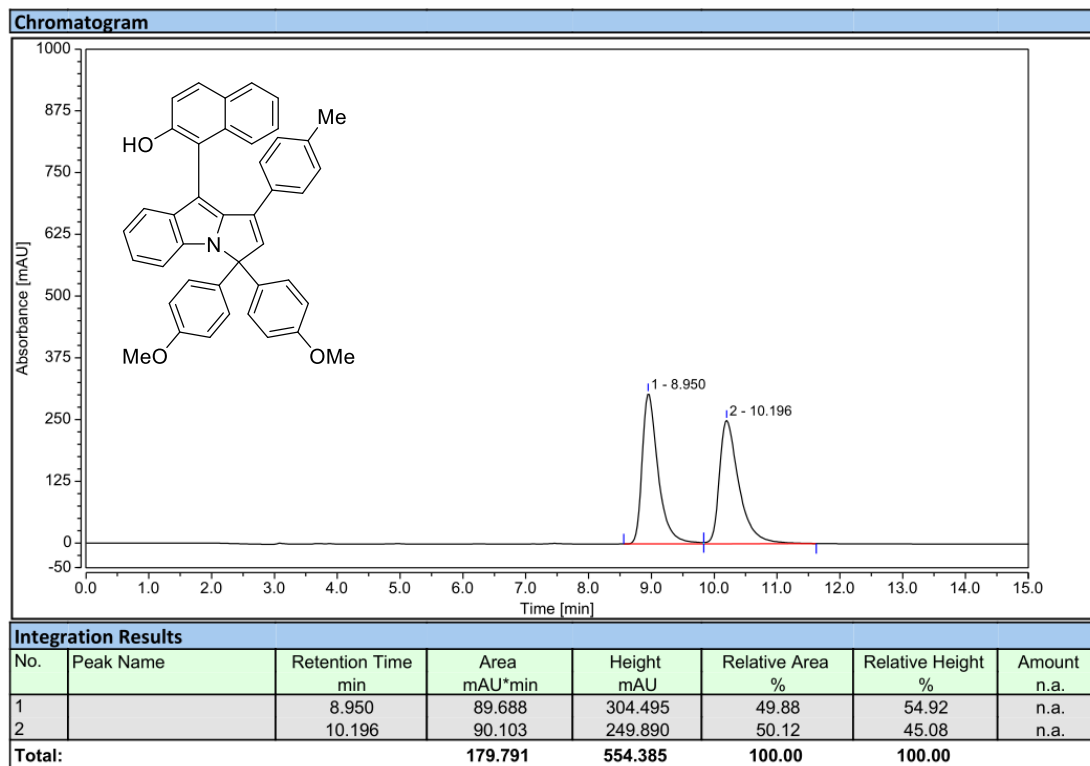
Enantioselective:



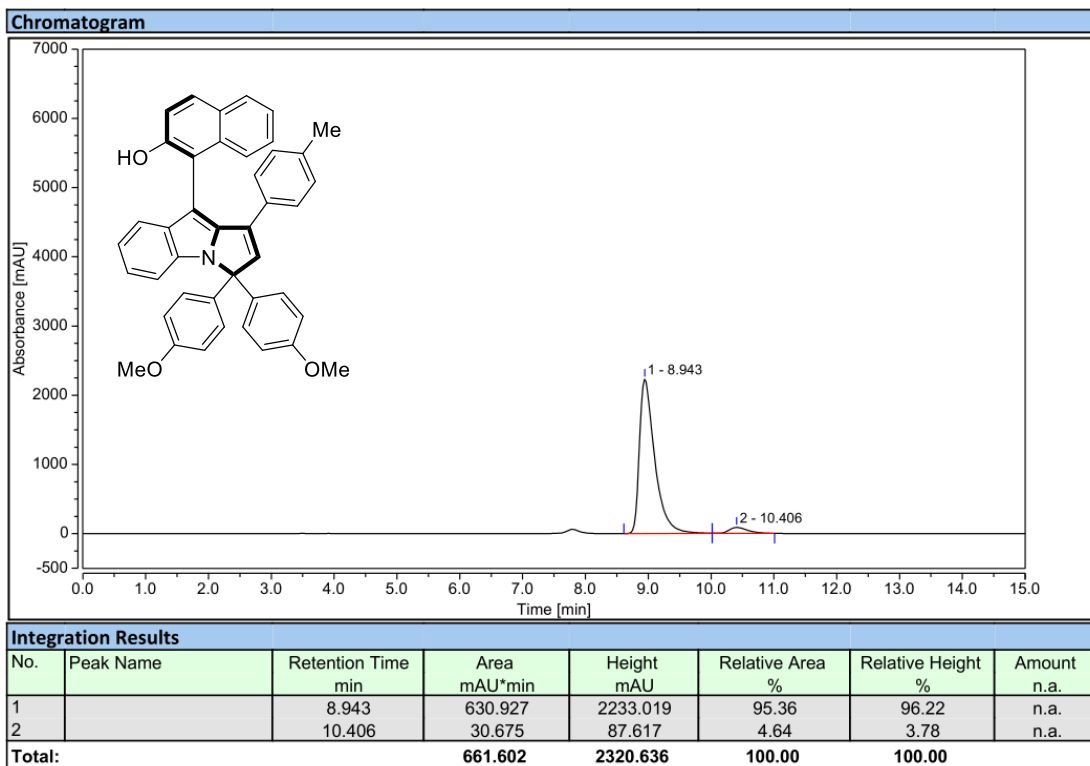
Integration Results							
No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		6.126	1.661	6.981	7.09	19.58	n.a.
2		14.026	21.769	28.674	92.91	80.42	n.a.
Total:			23.430	35.655	100.00	100.00	

3ac

Racemic:

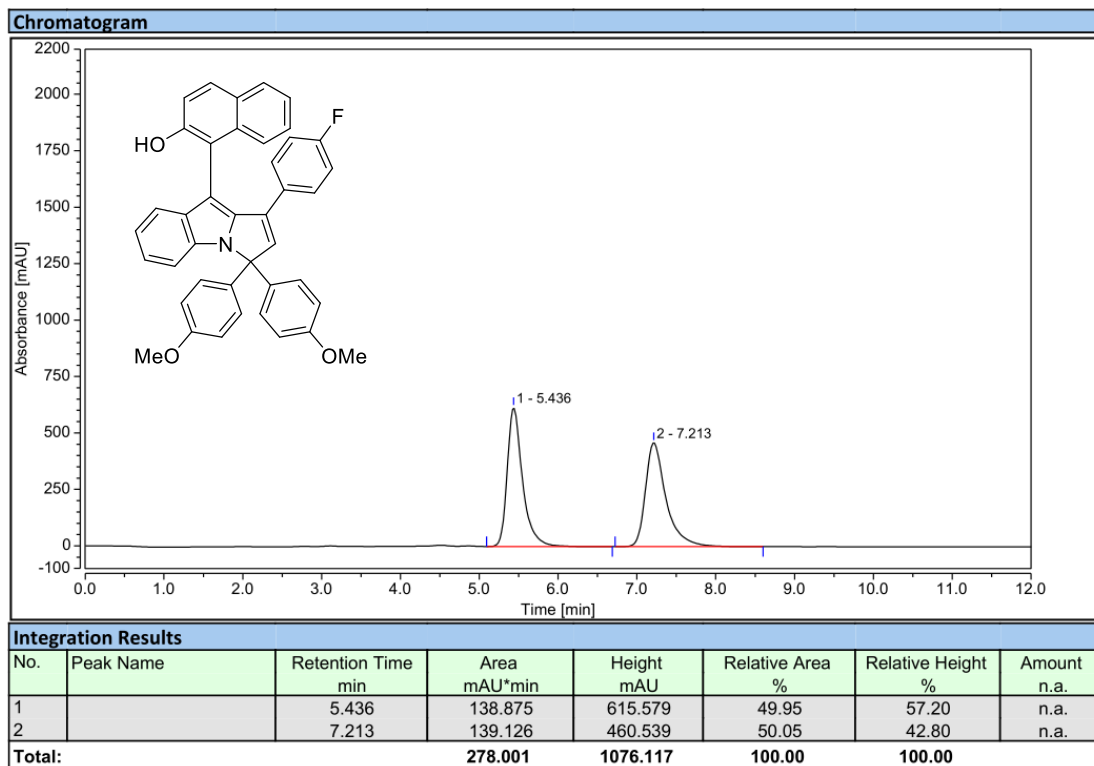


Enantioselective:

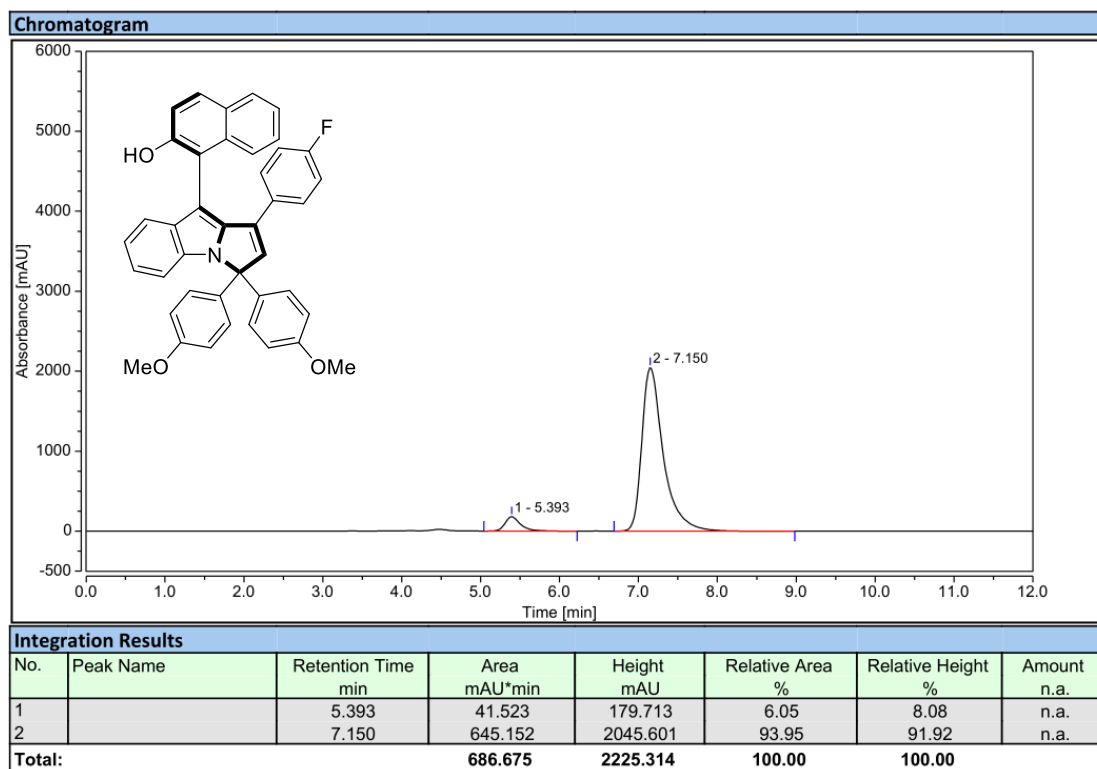


3ad

Racemic:

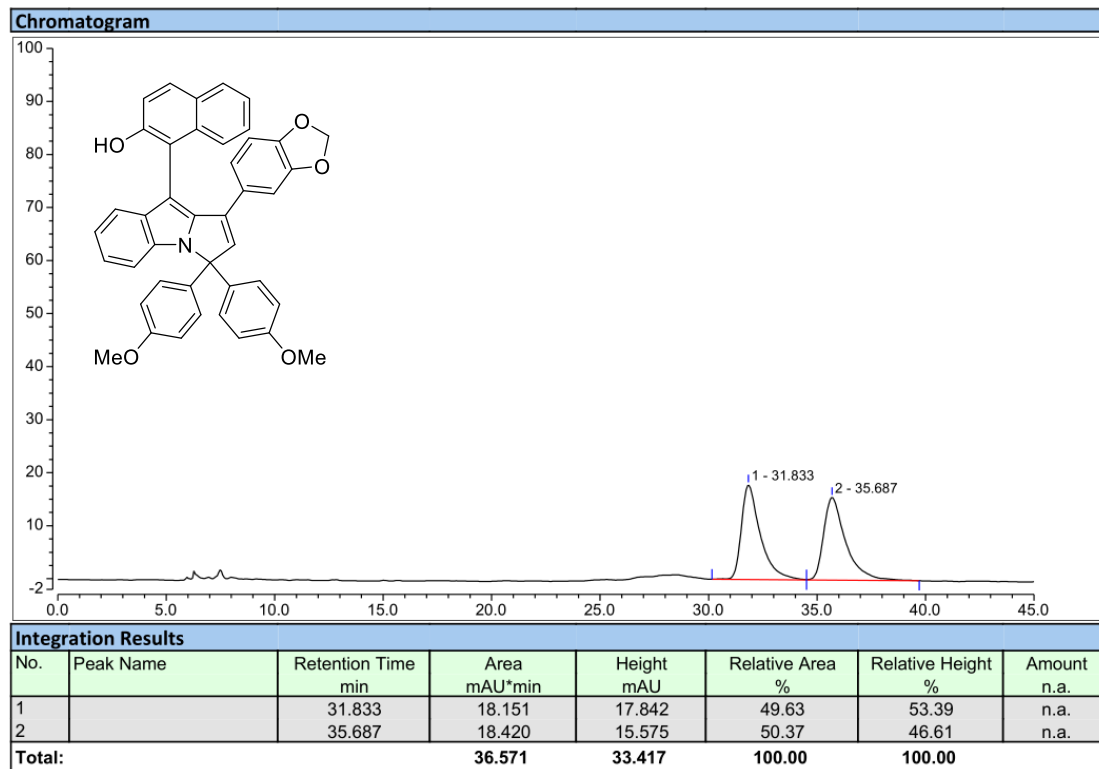


Enantioselective:

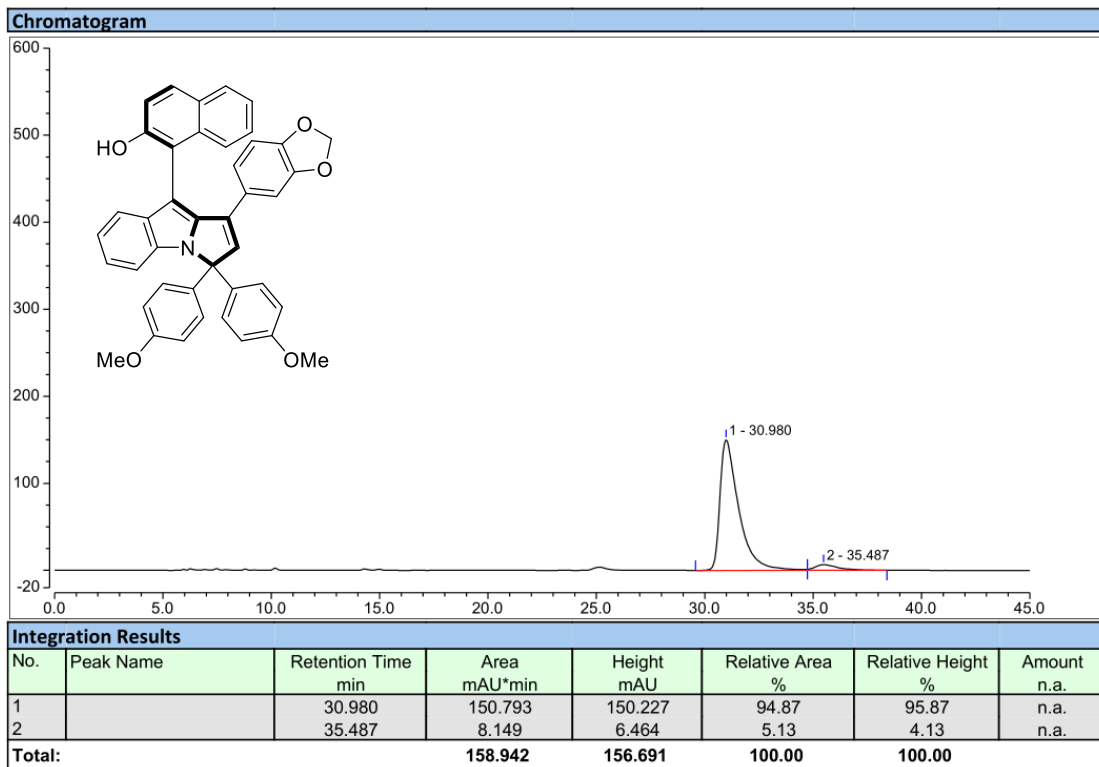


3ae

Racemic:

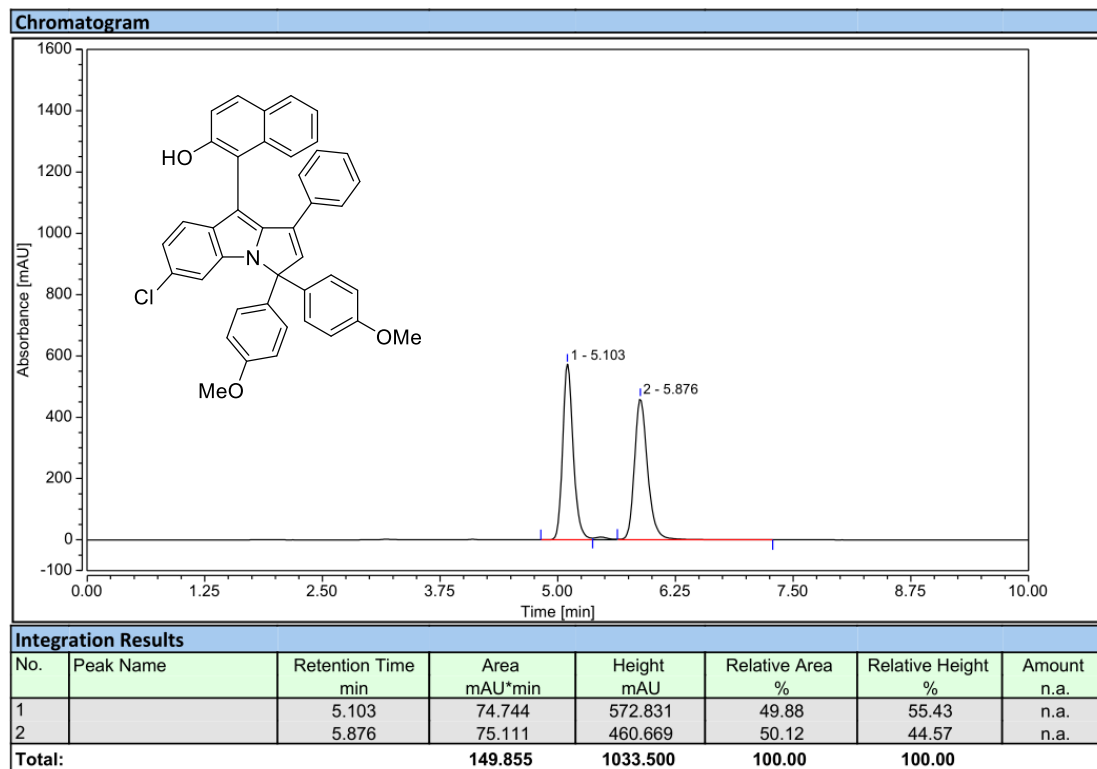


Enantioselective:

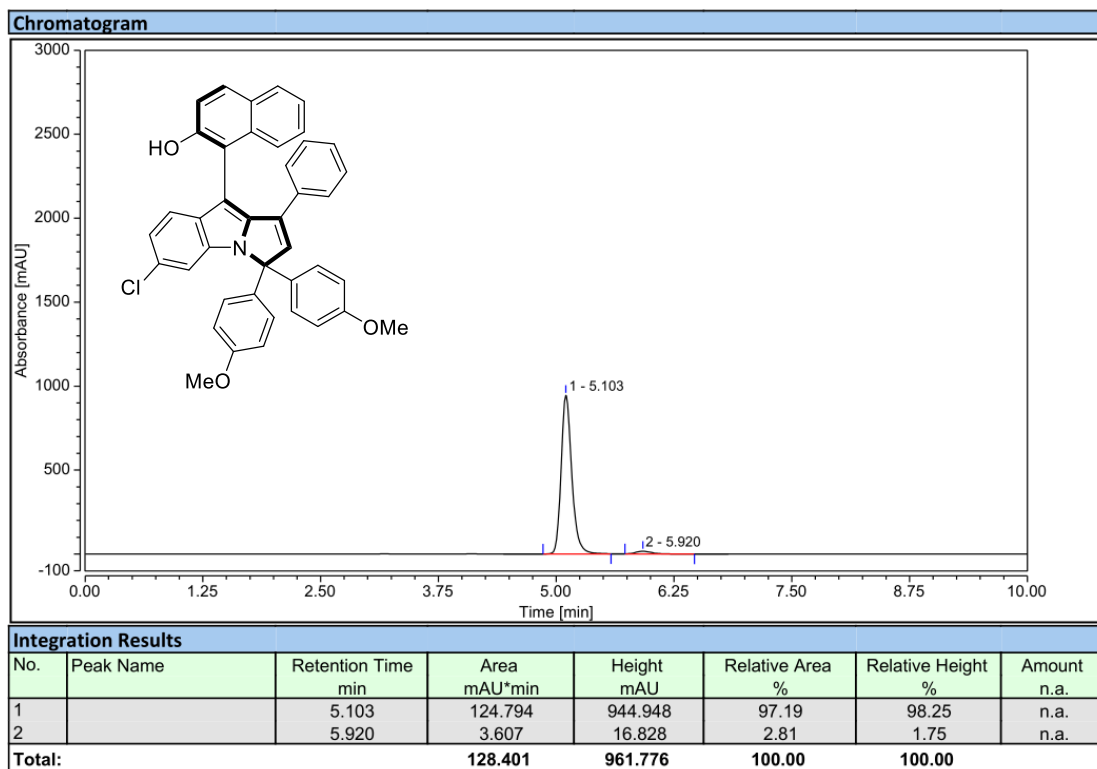


3ea

Racemic:

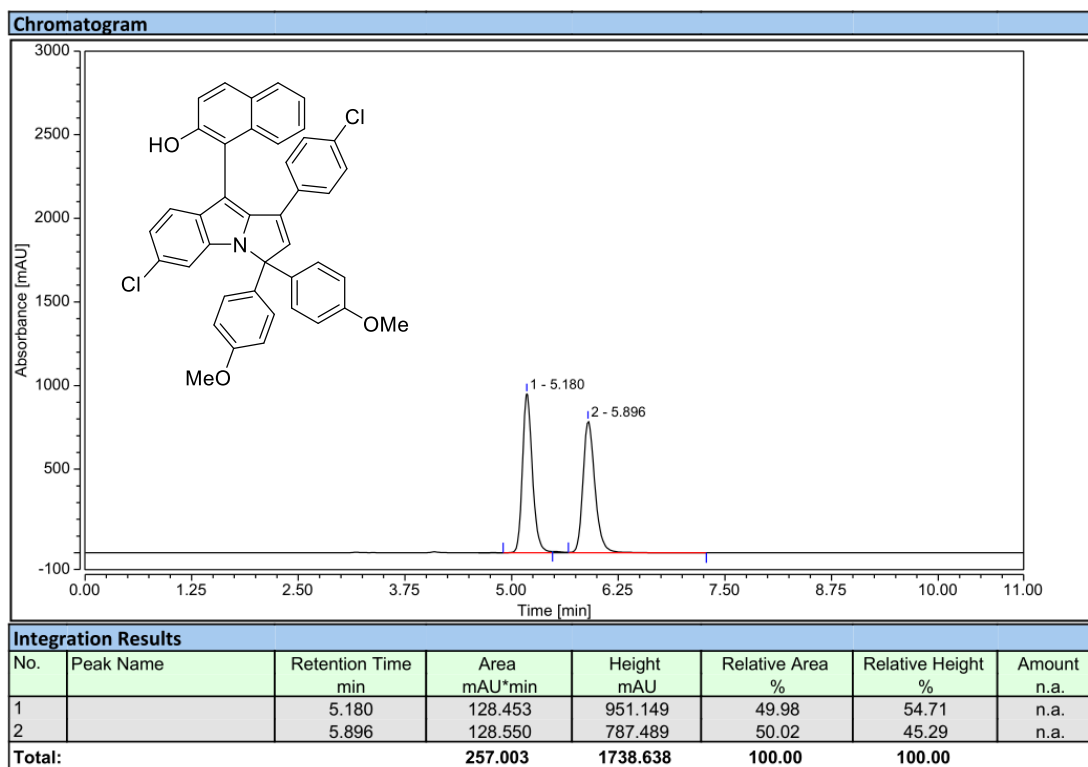


Enantioselective:

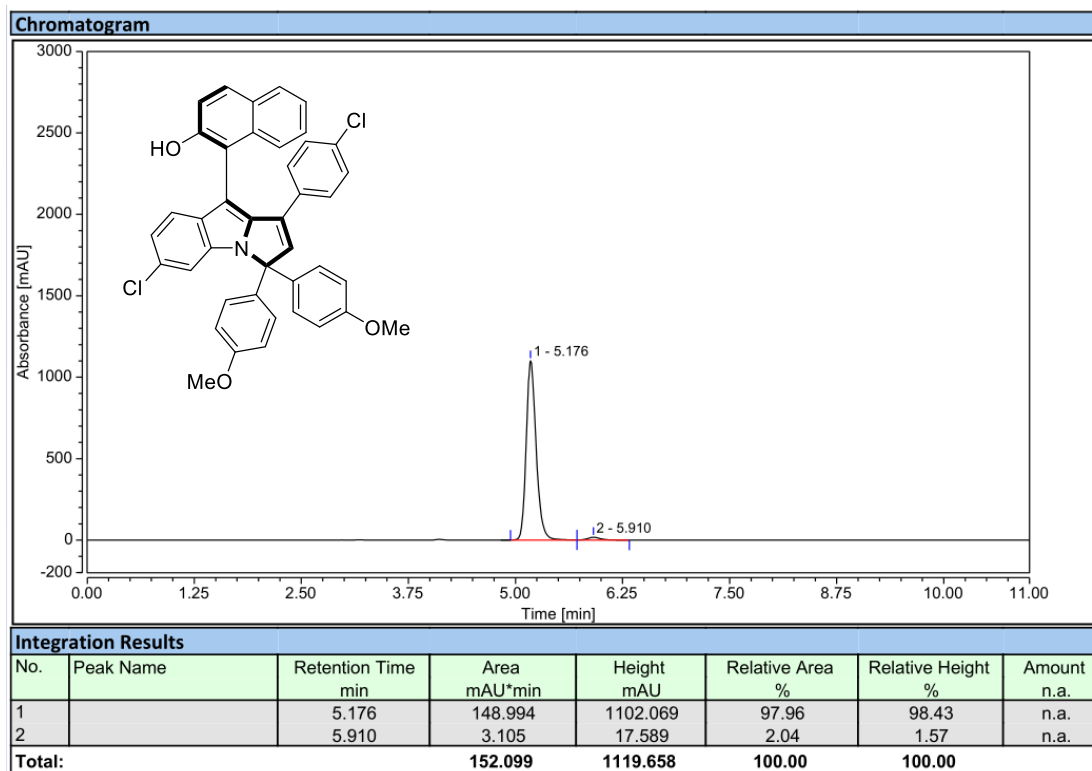


3ef

Racemic:

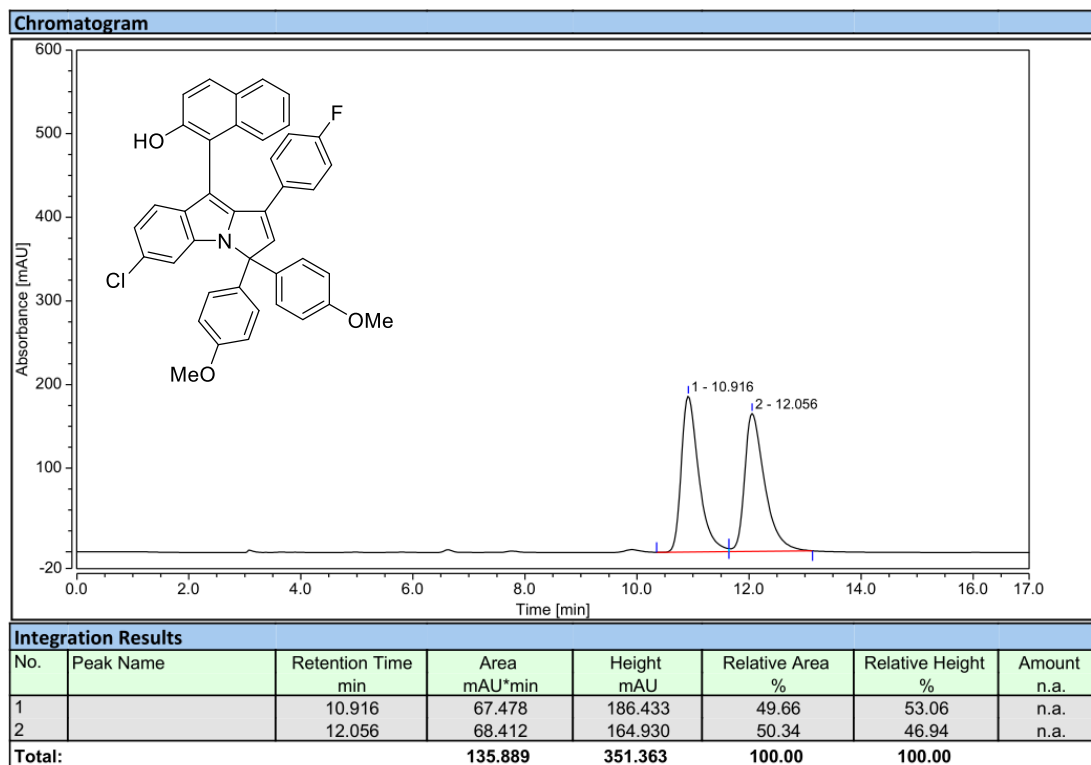


Enantioselective:

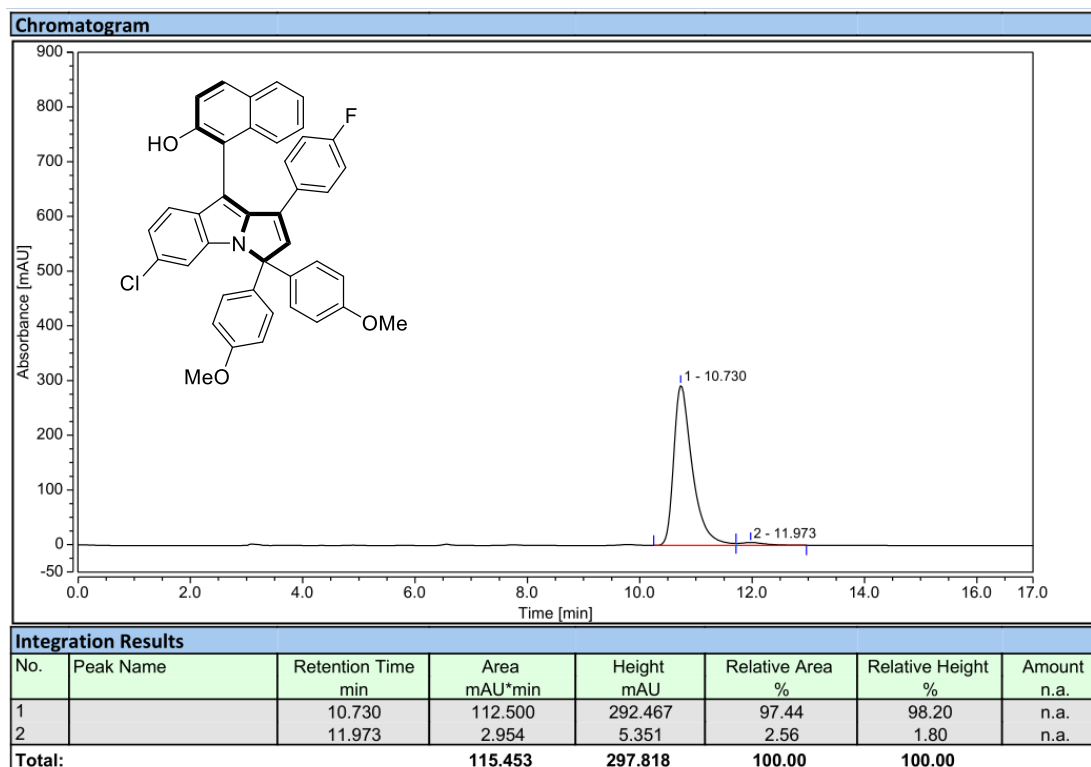


3ed

Racemic:

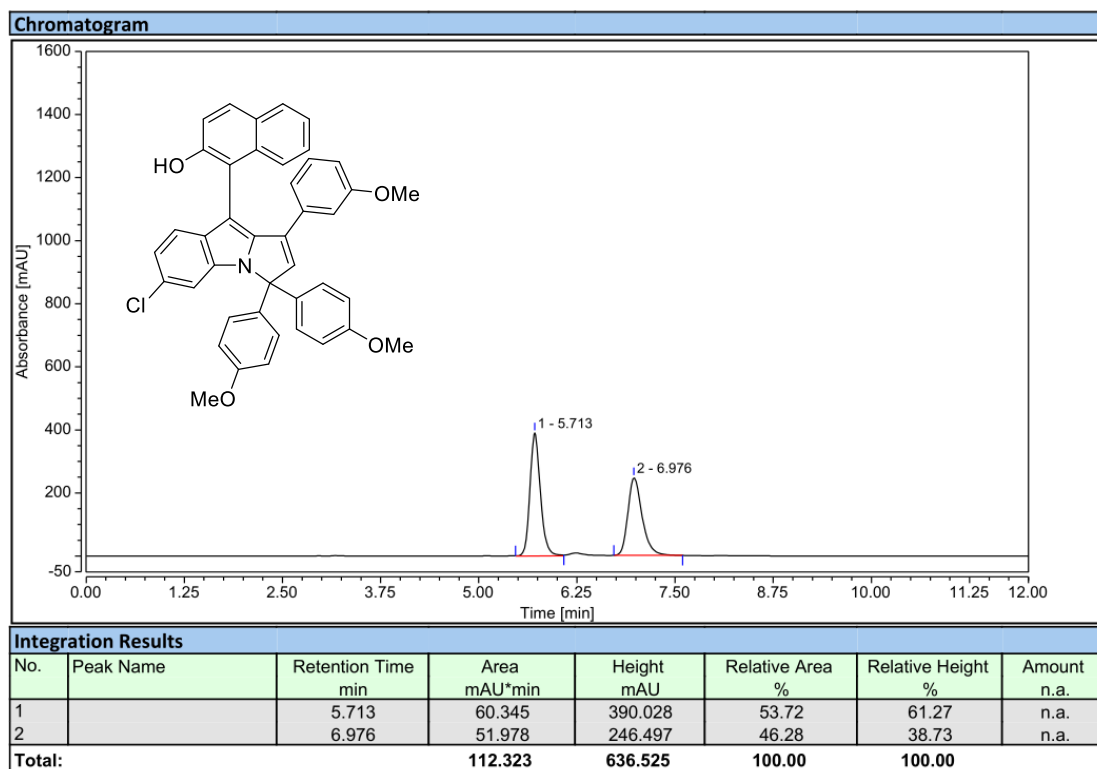


Enantioselective:

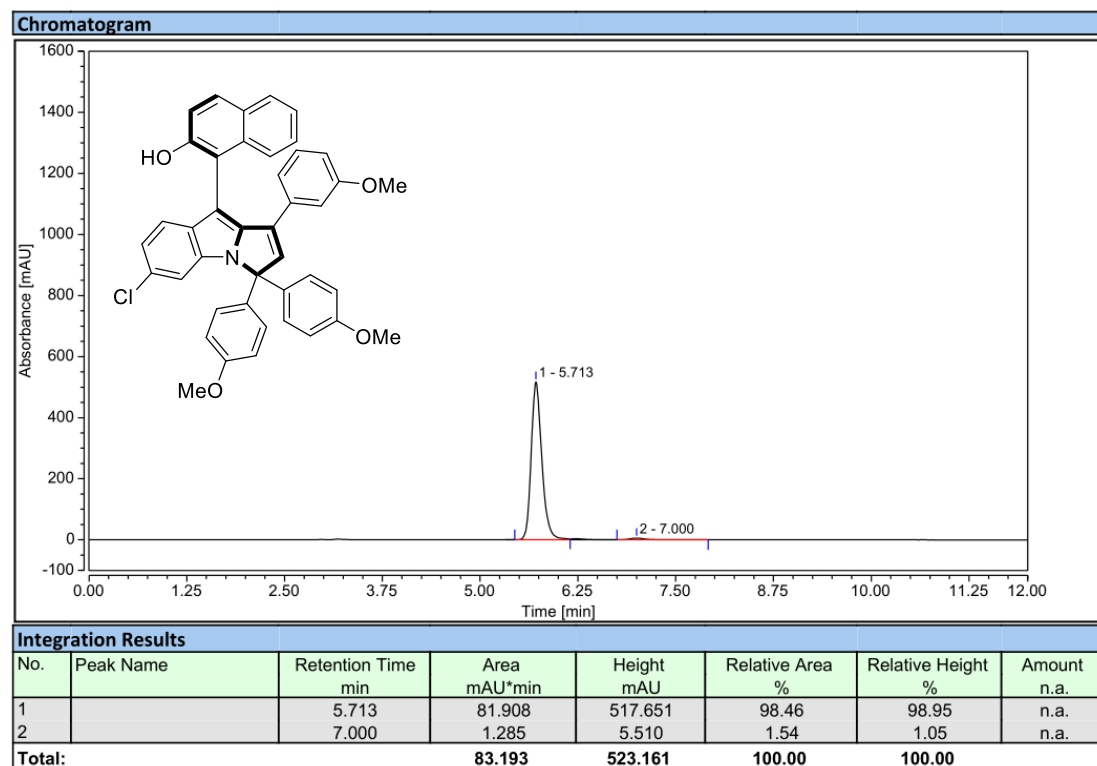


3eg

Racemic:

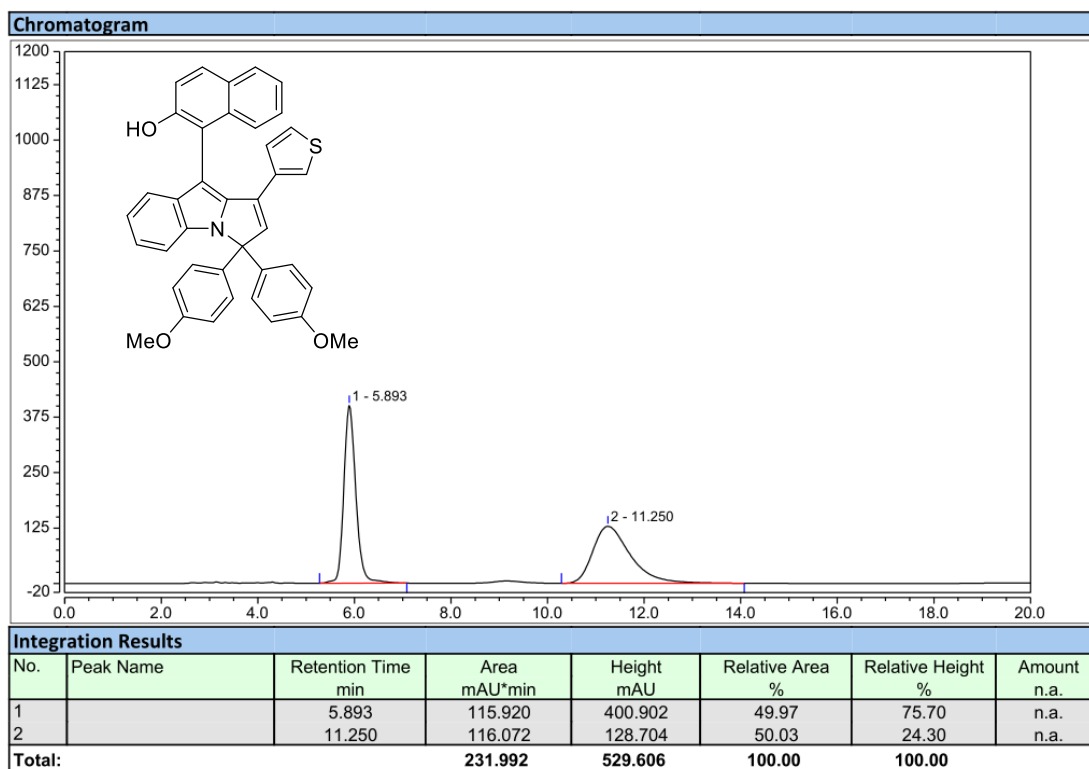


Enantioselective:

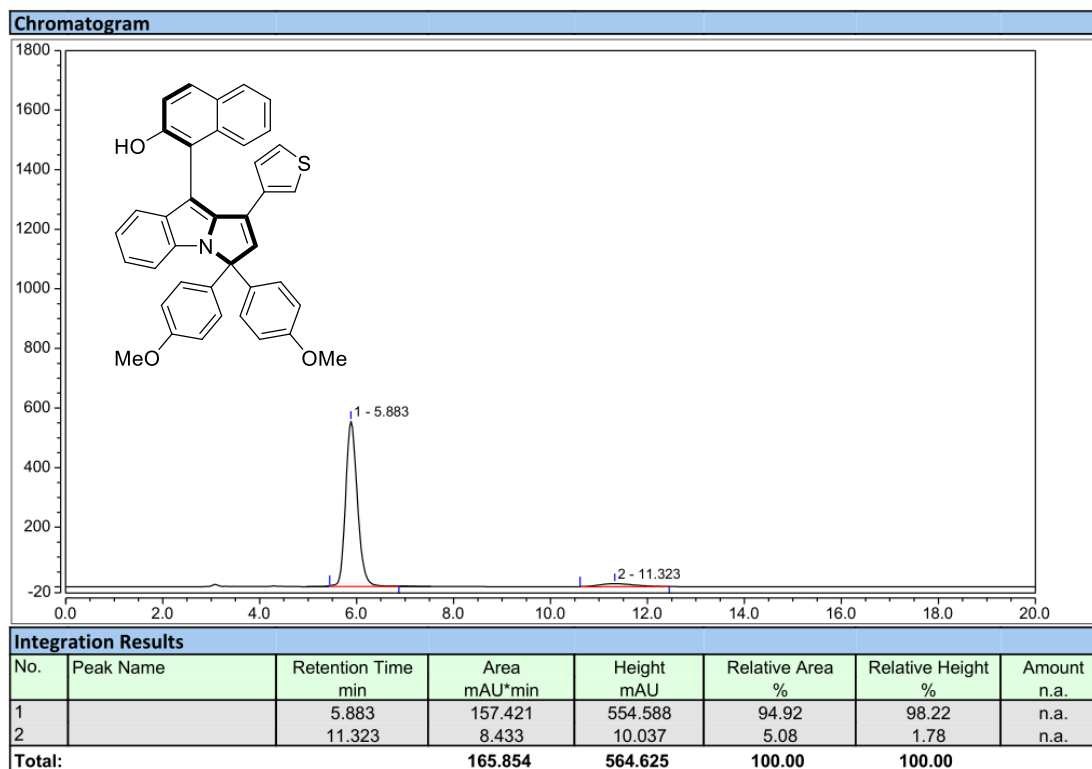


3ah

Racemic:

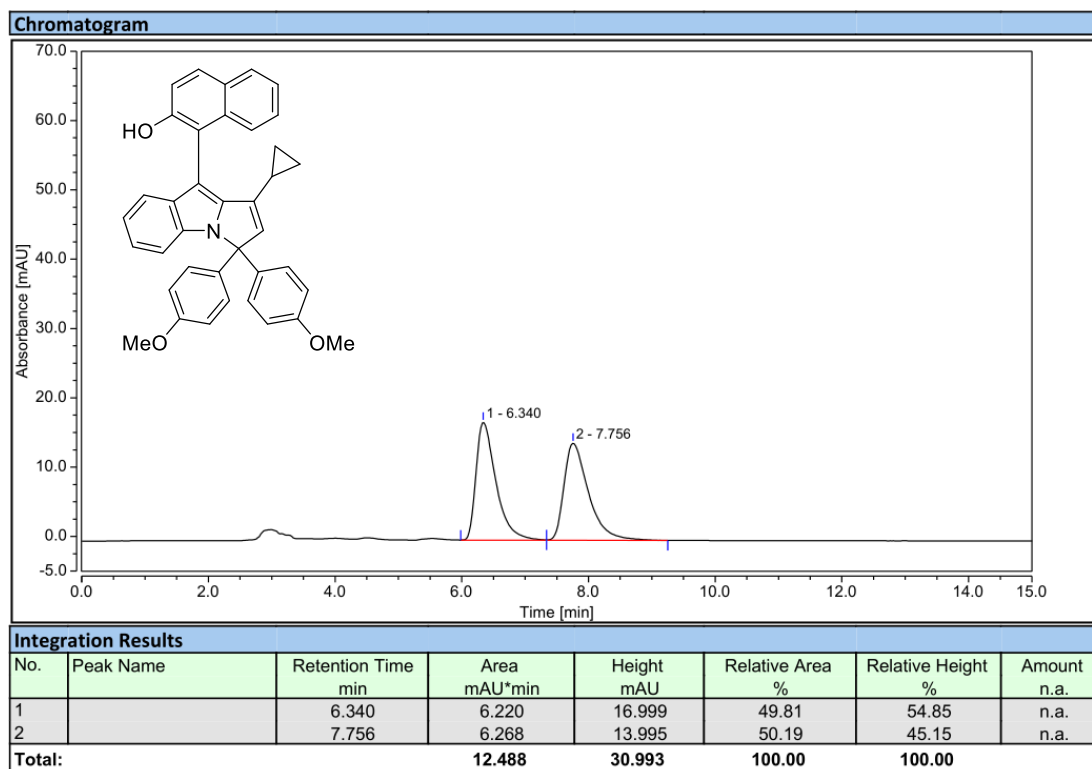


Enantioselective:

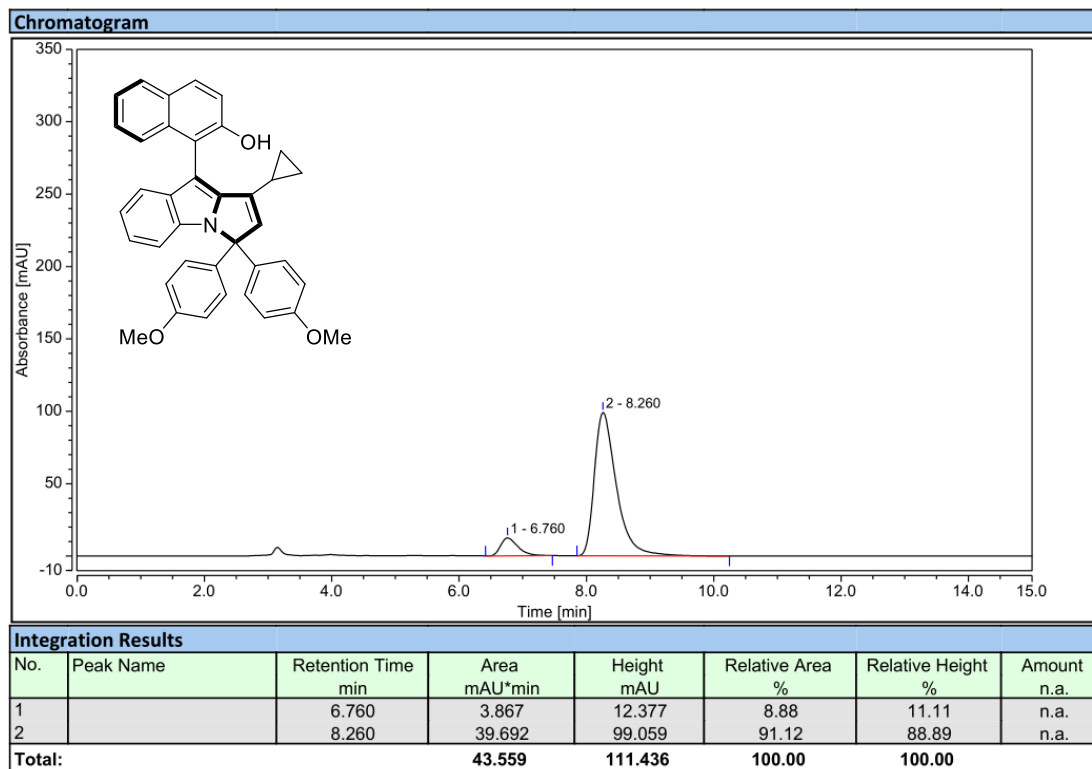


3ai

Racemic:

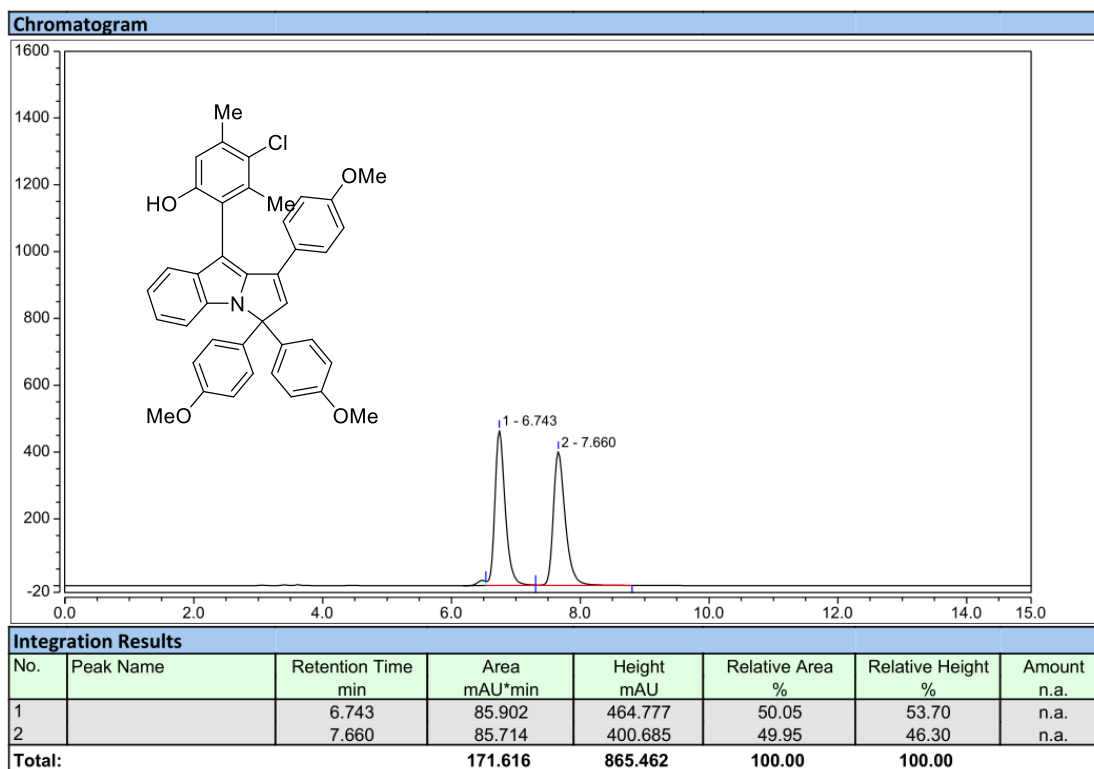


Enantioselective:

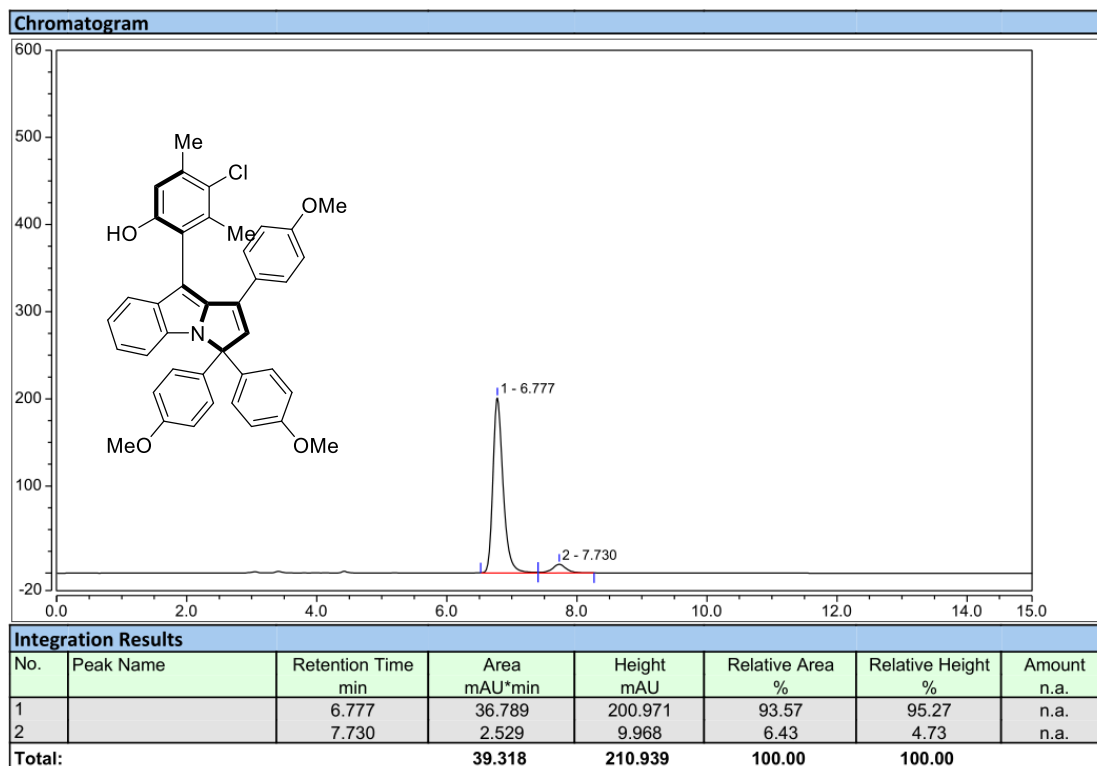


3mb

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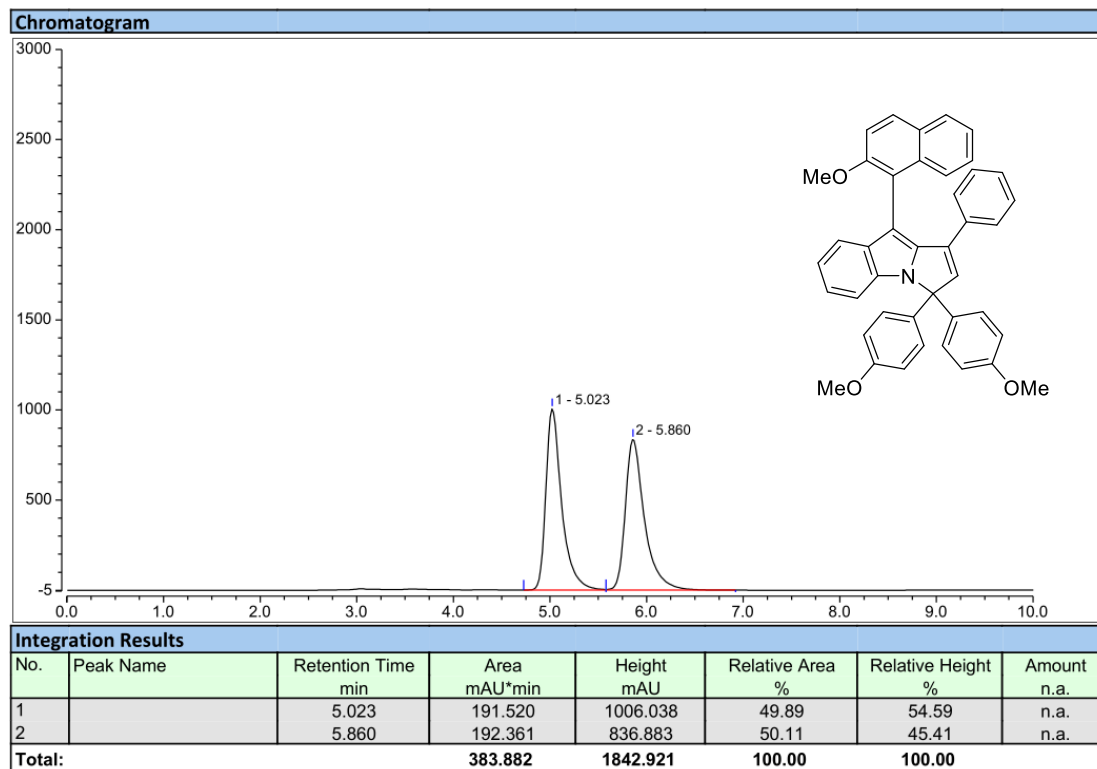


Enantioselective:

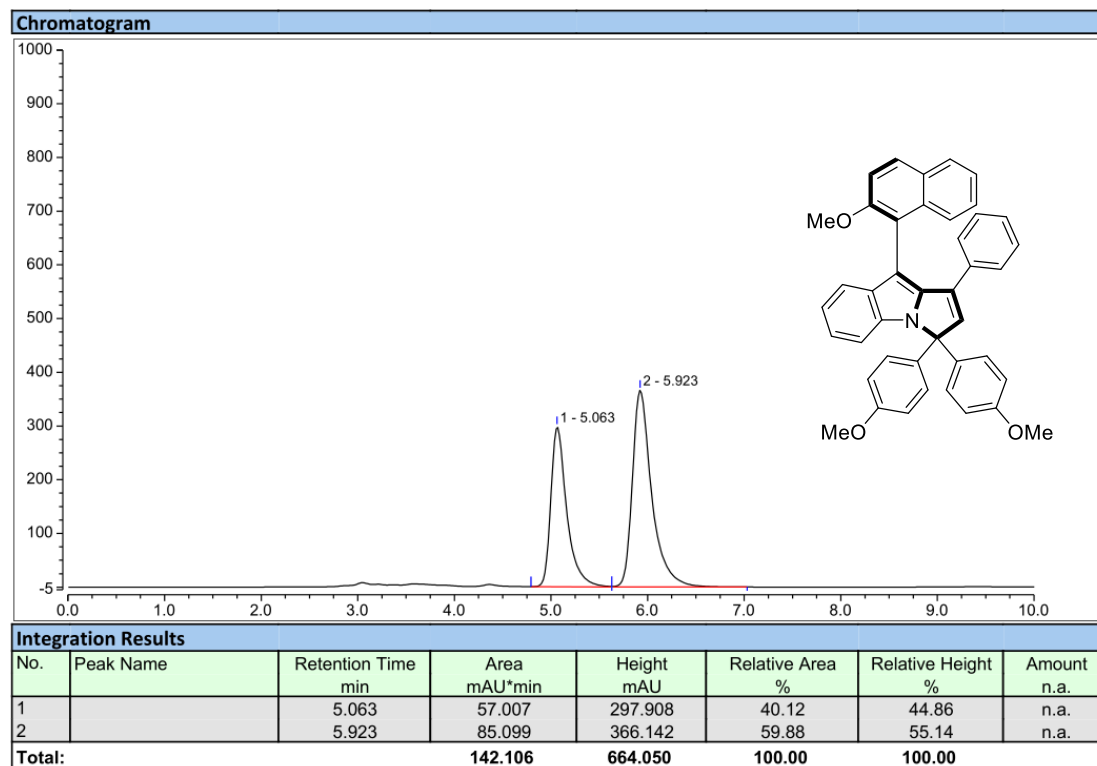


3na

Racemic:

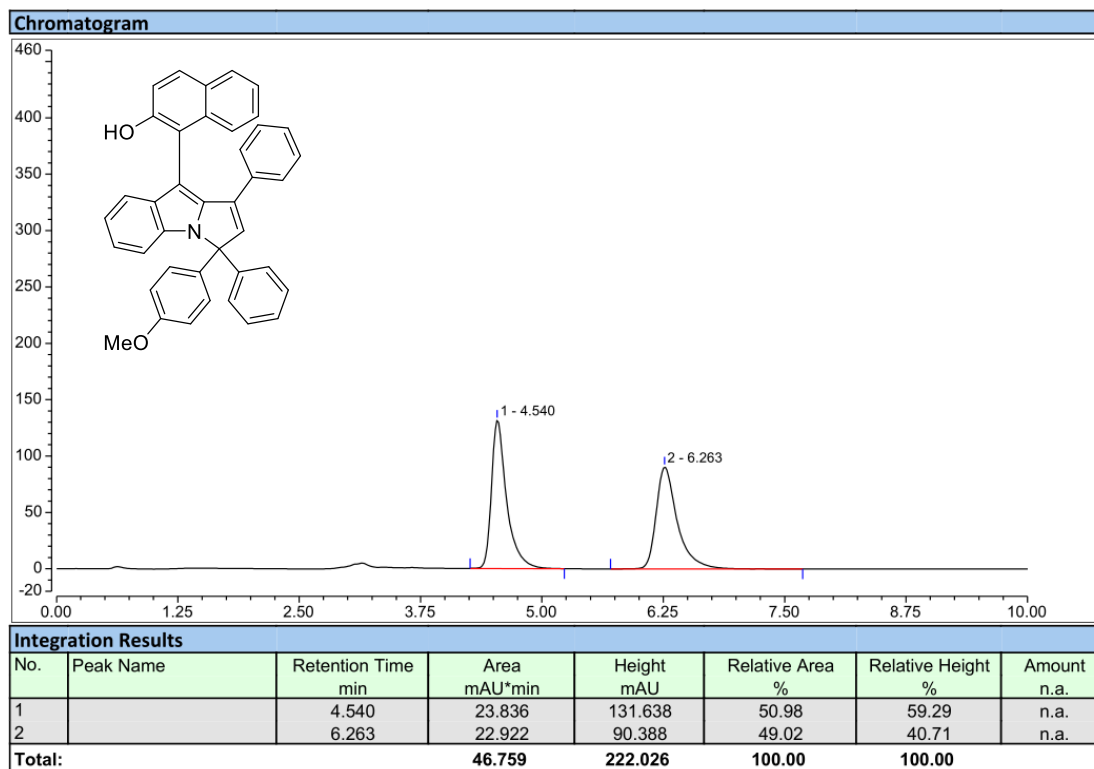


Enantioselective:

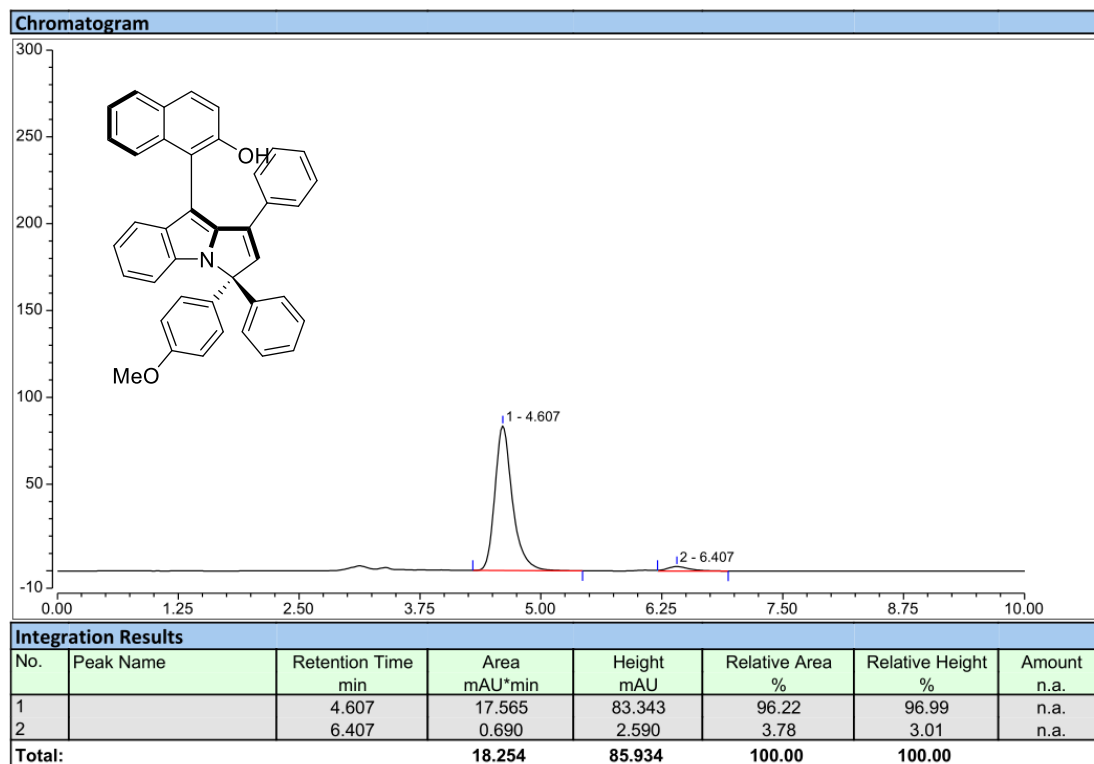


7ab

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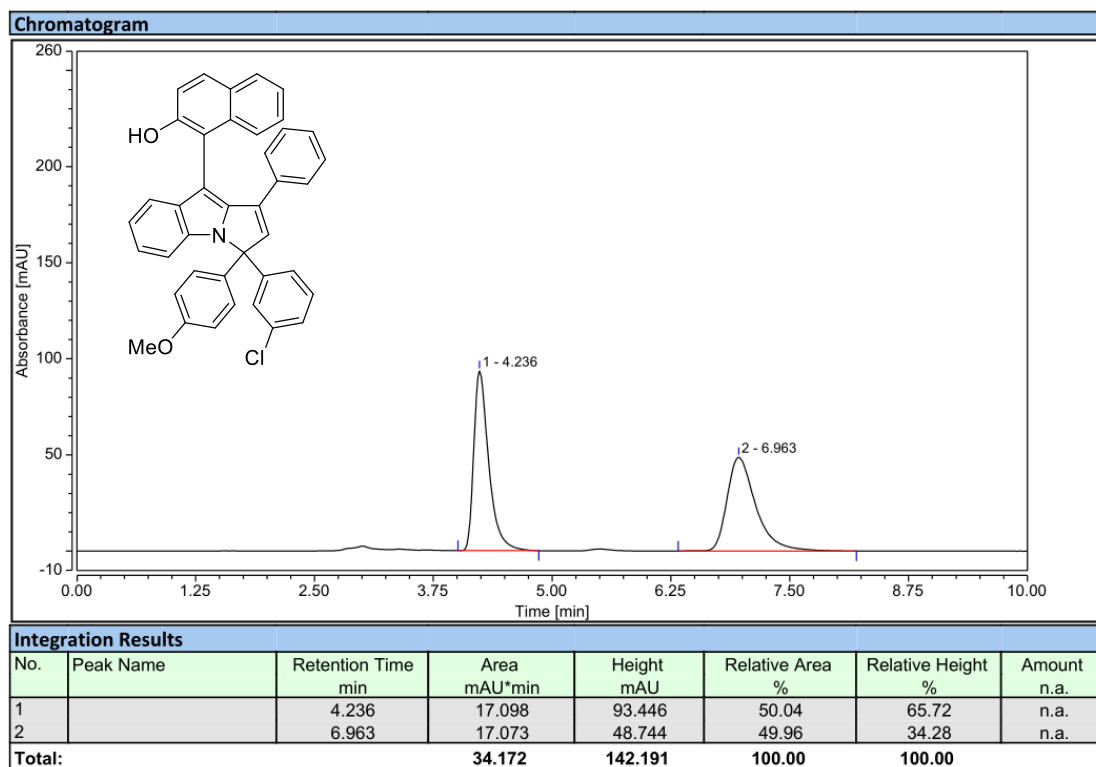


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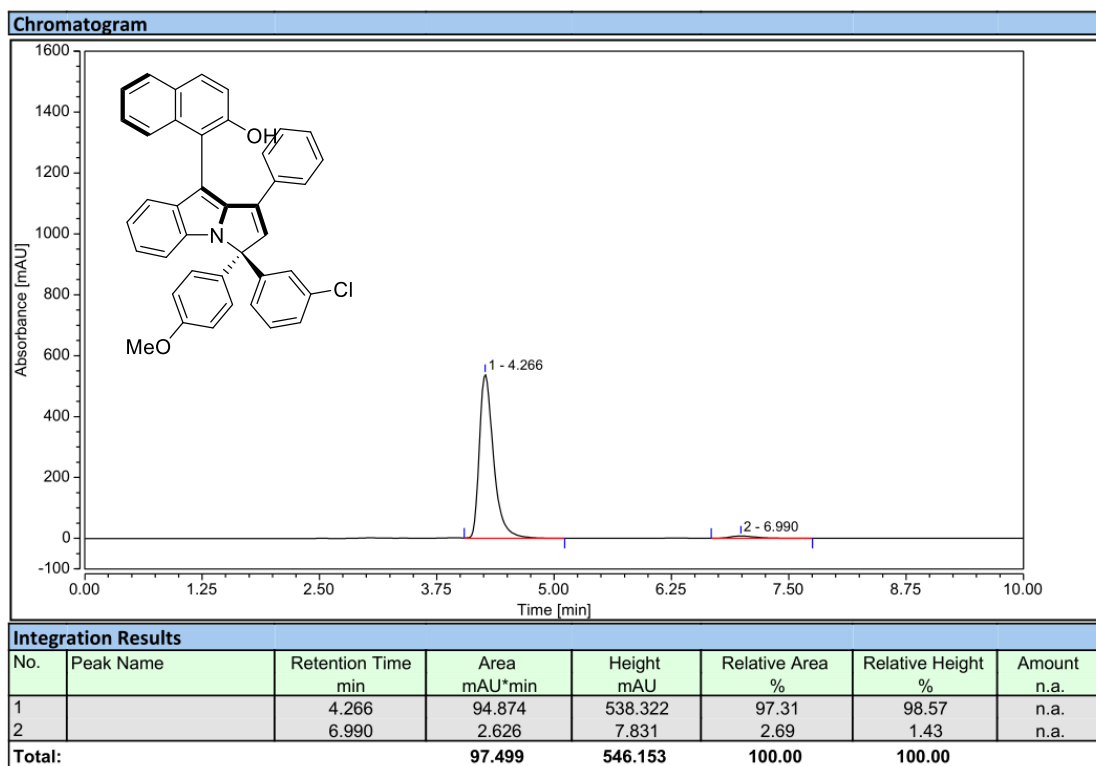


7ac

Racemic:

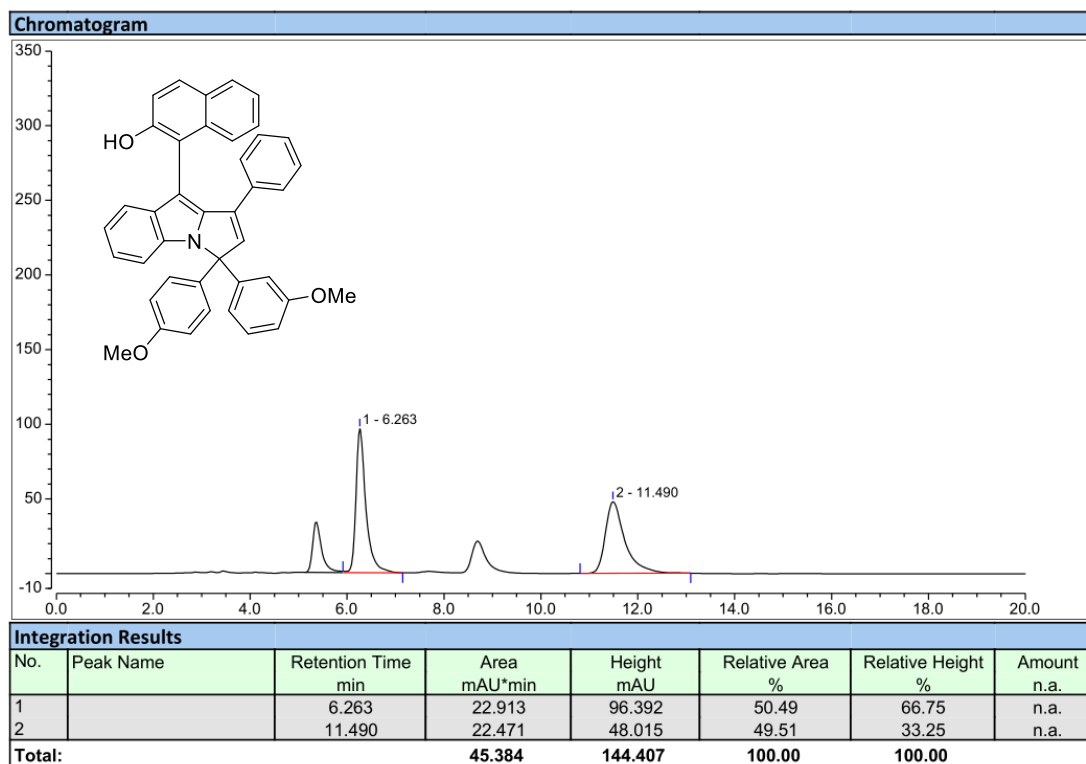


Enantioselective:

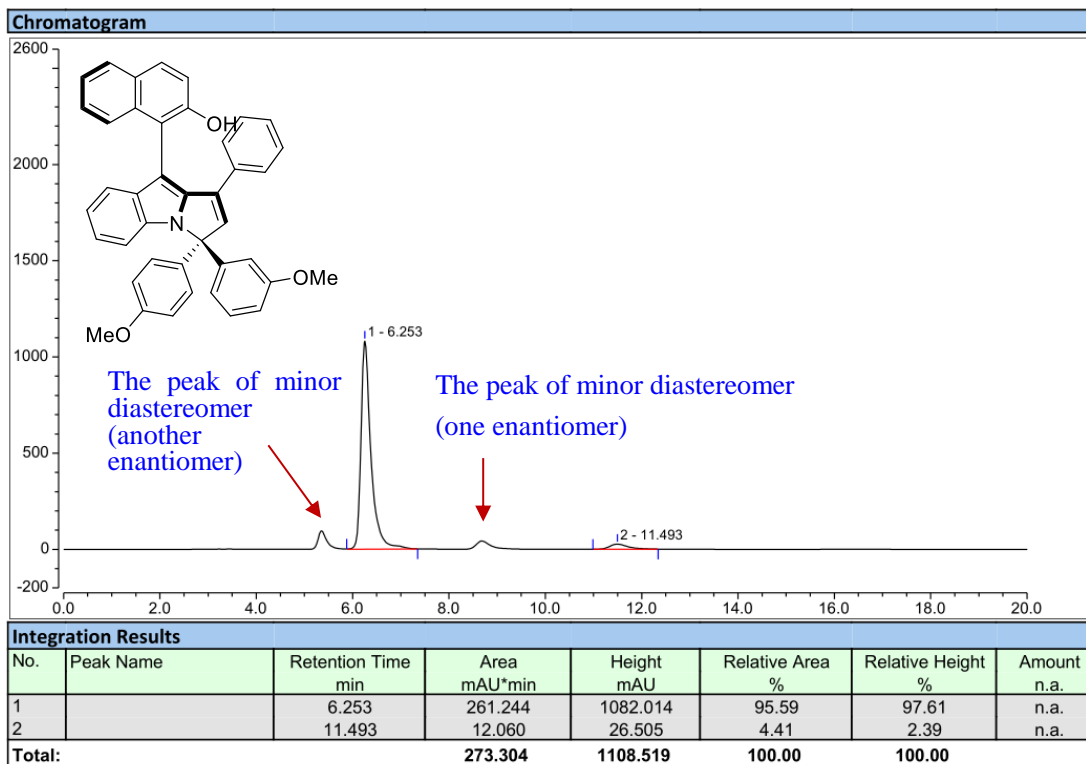


7ad (inseparable diastereomers with 88:12 dr)

Racemic:

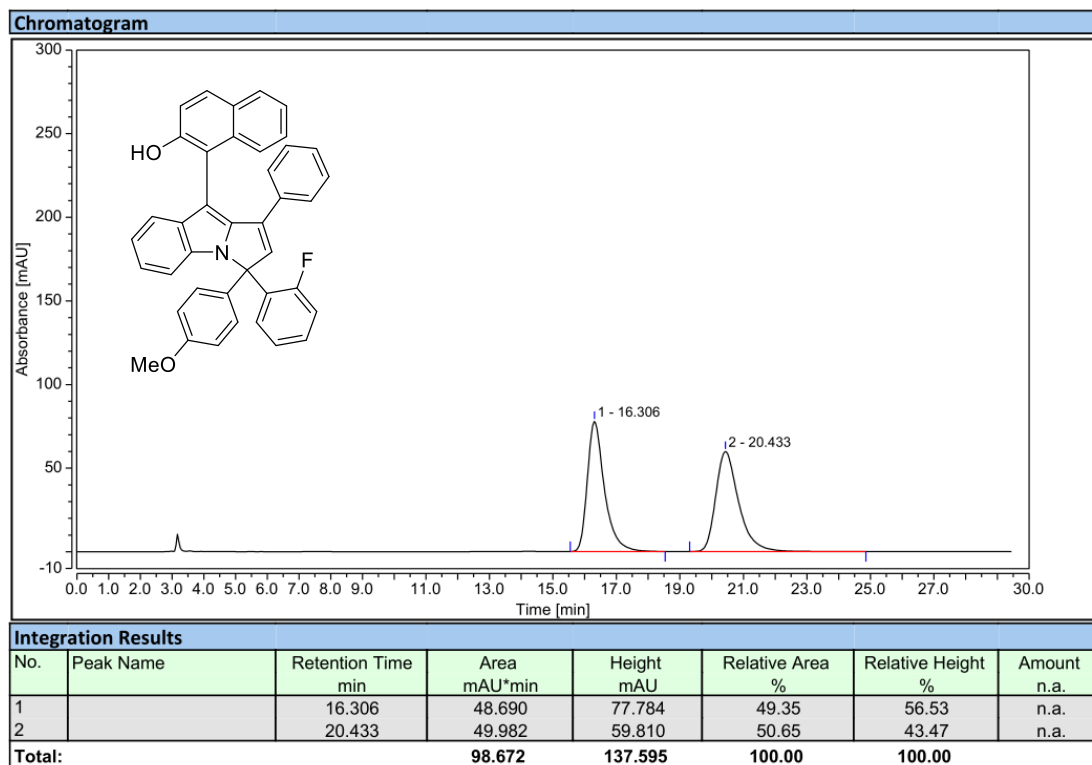


Enantioselective: (inseparable diastereomers with 88:12 dr)

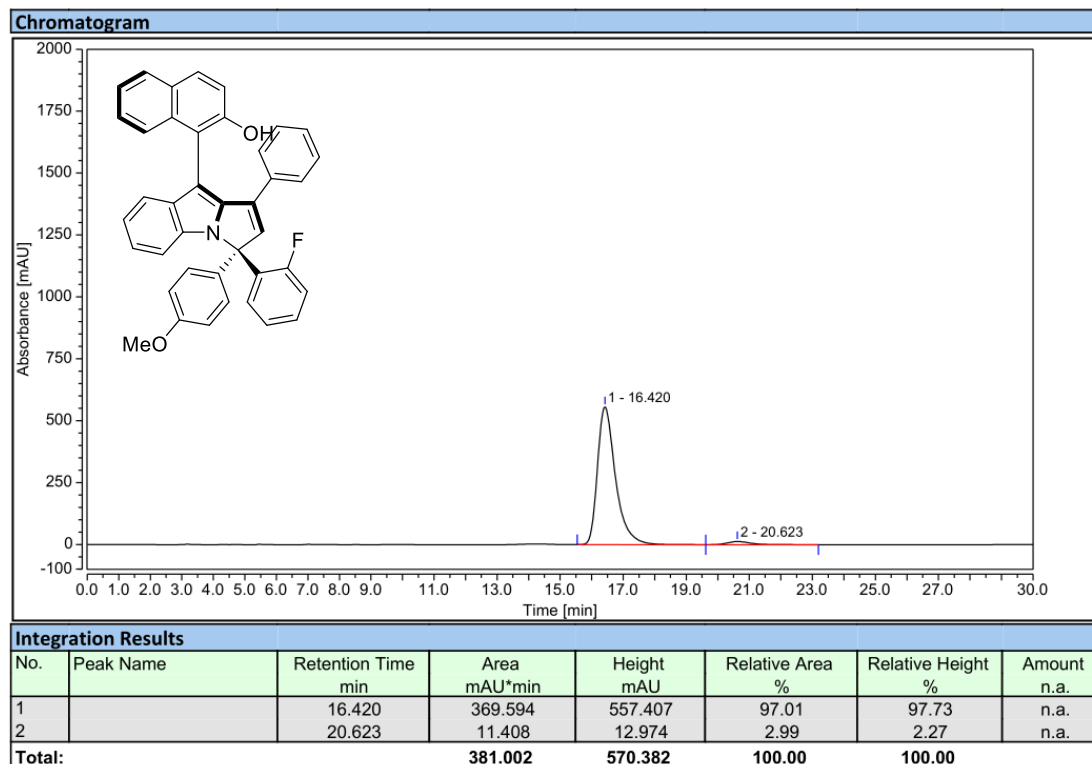


7ae

Racemic:

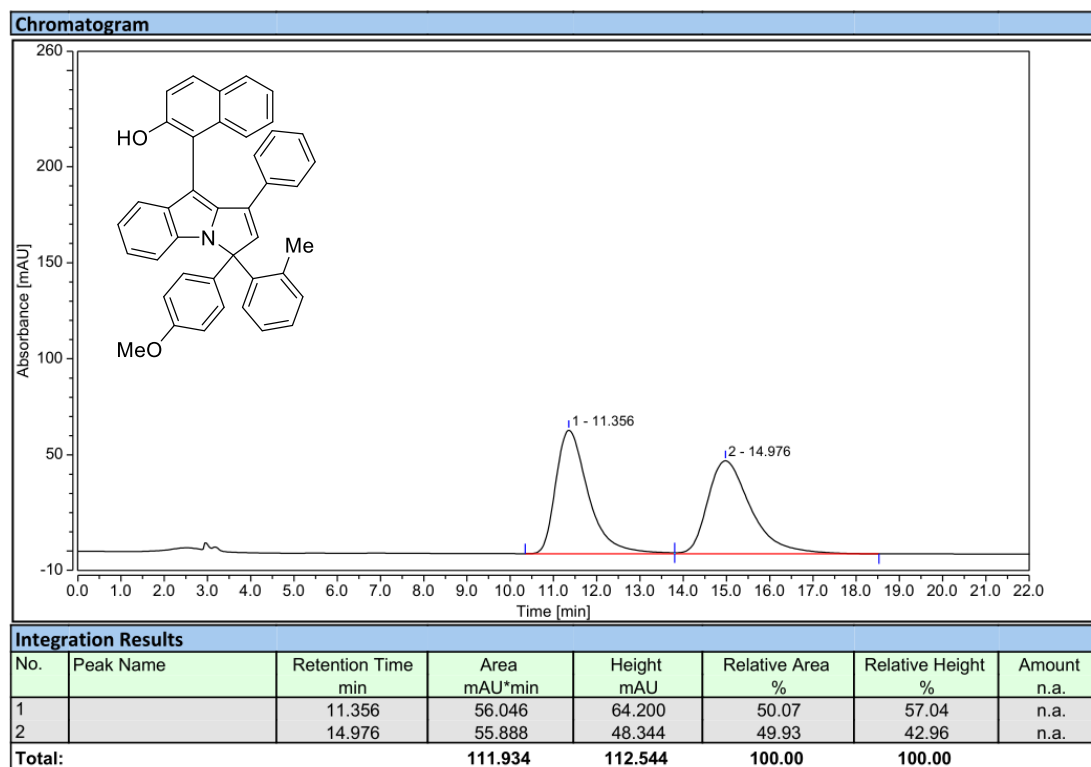


Enantioselective:

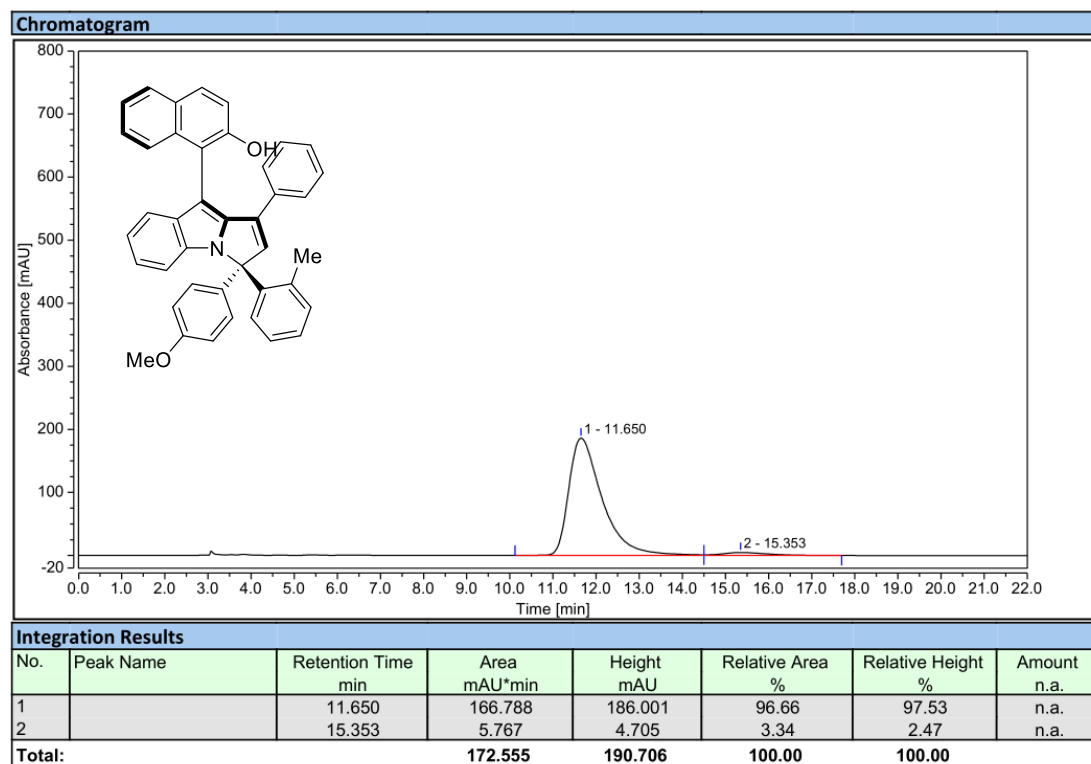


7af

Racemic:

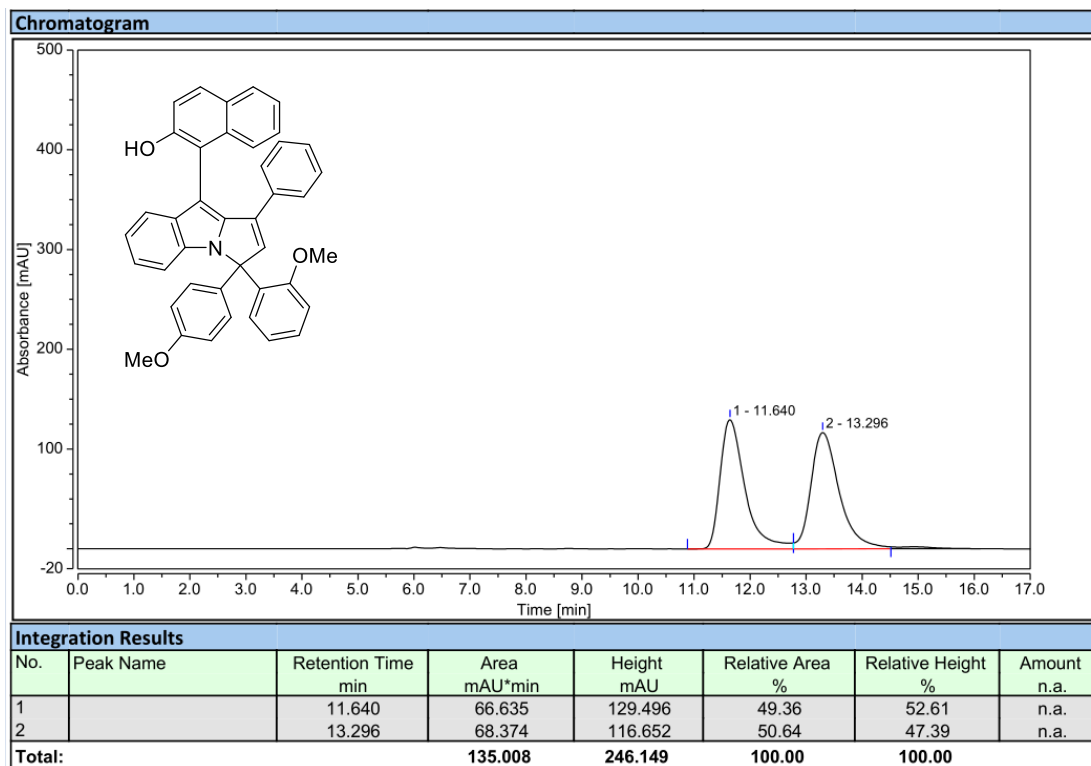


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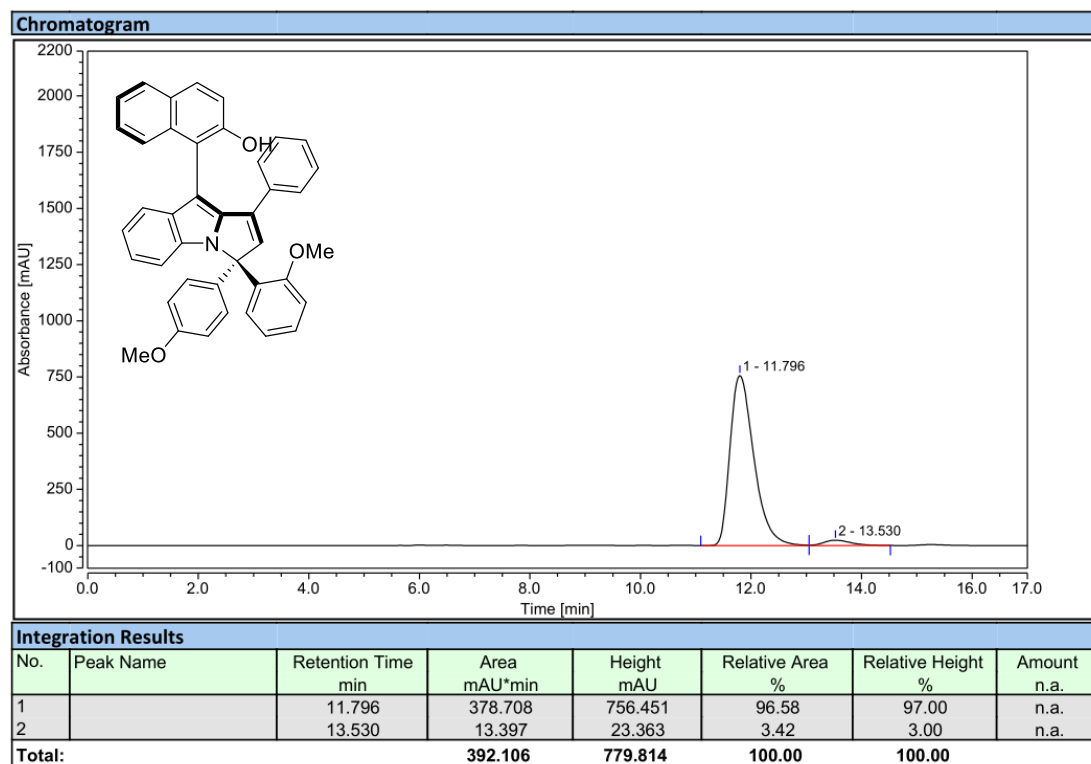


7ag

Racemic:

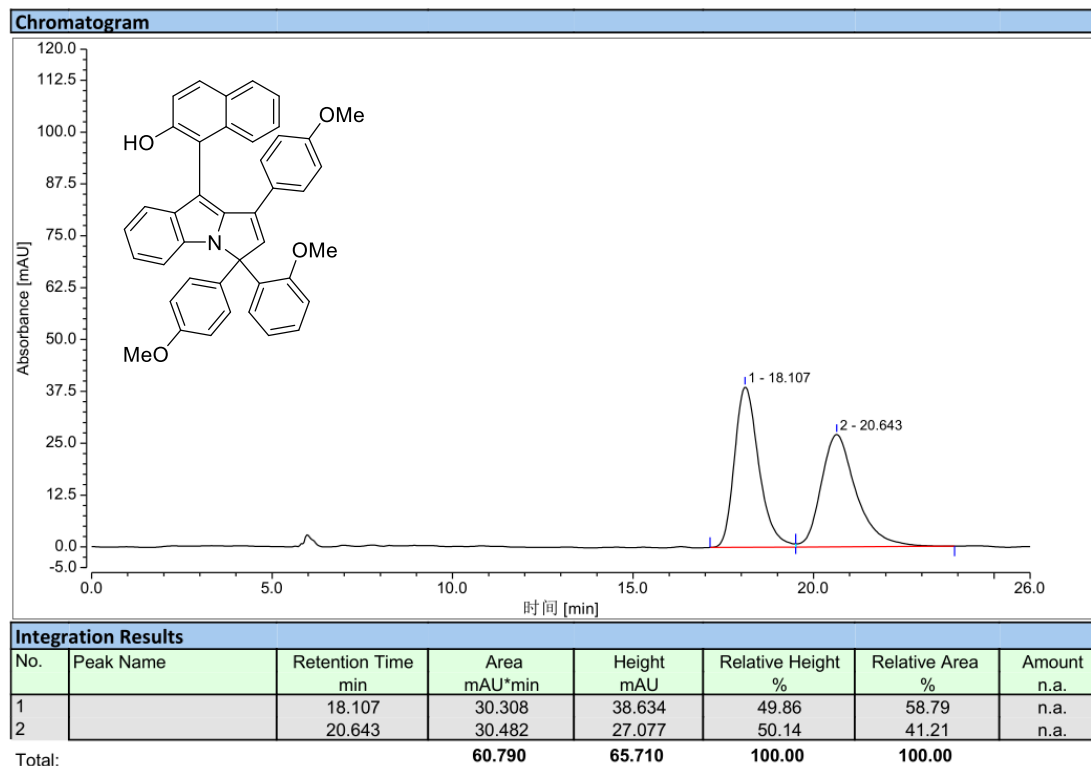


Enantioselective:

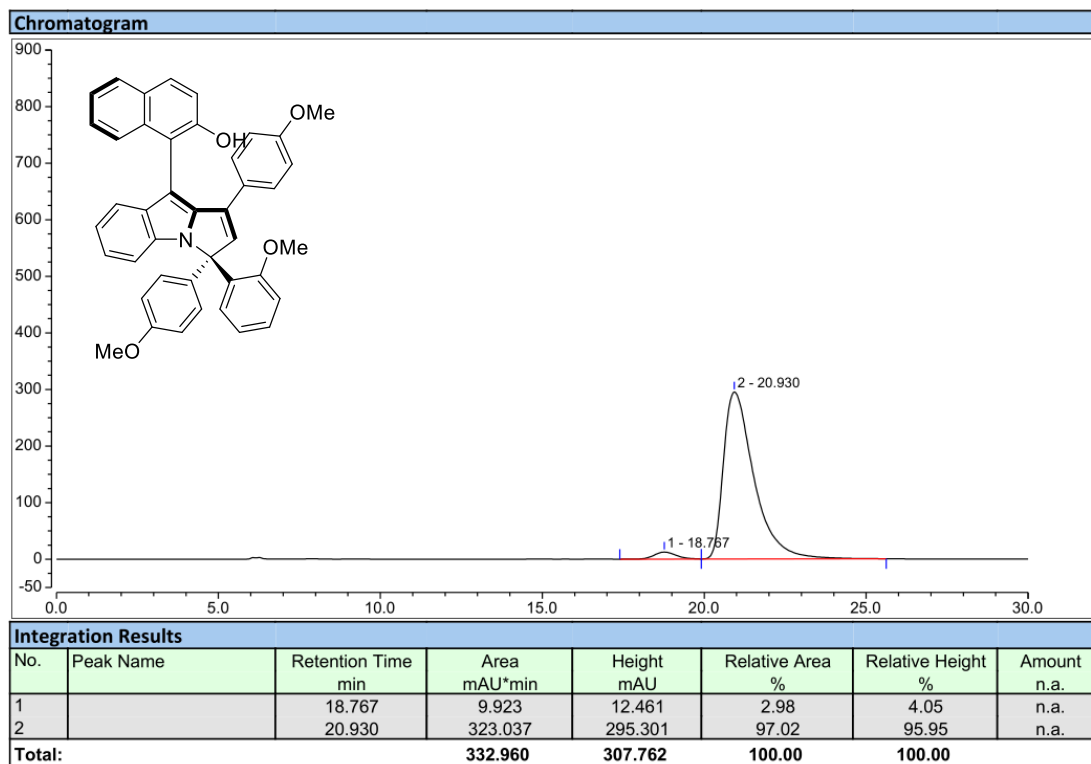


7ah

Racemic:

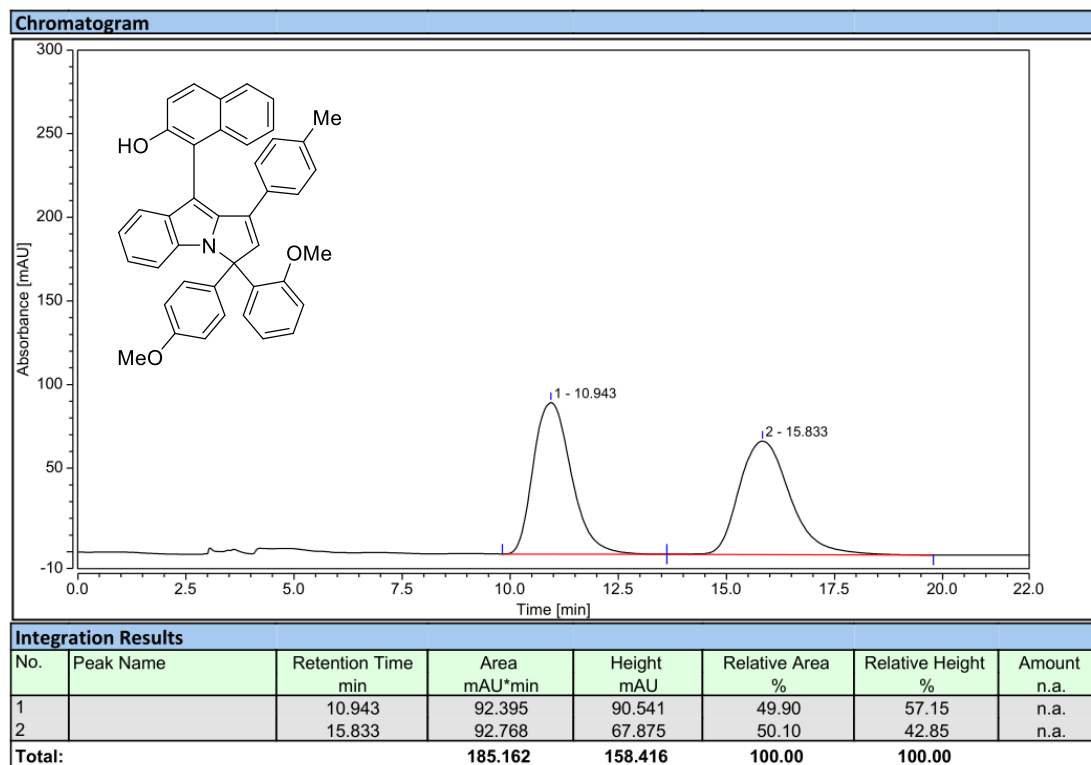


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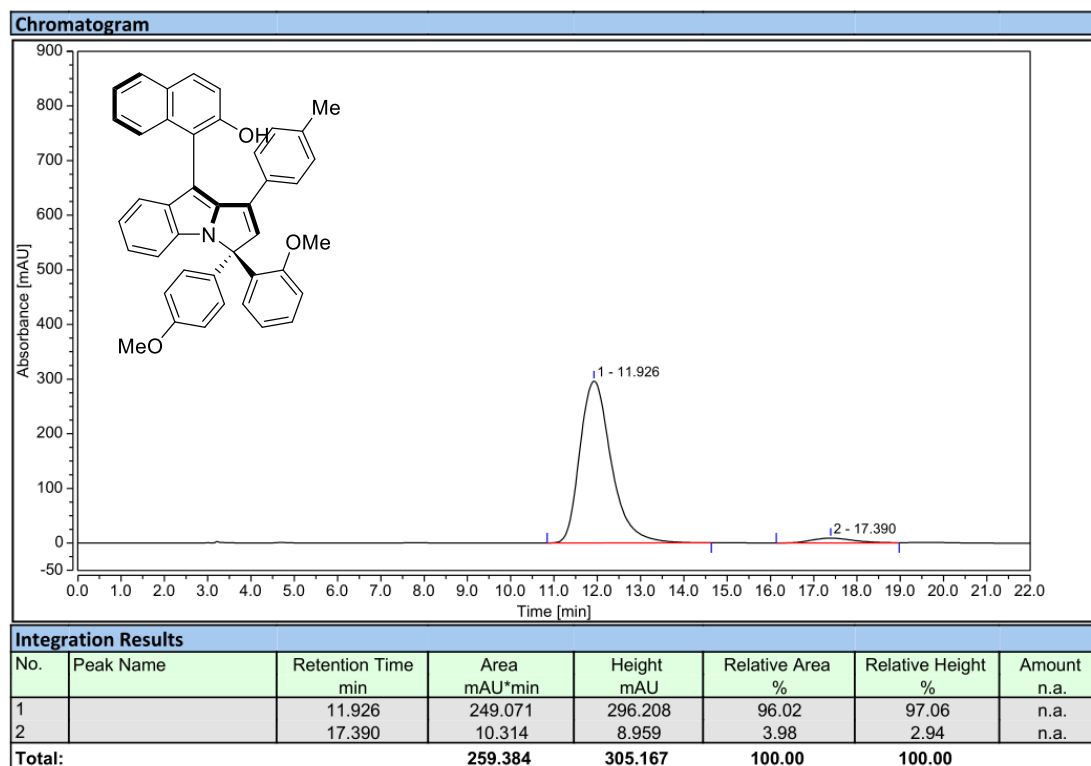


7ai

Racemic:

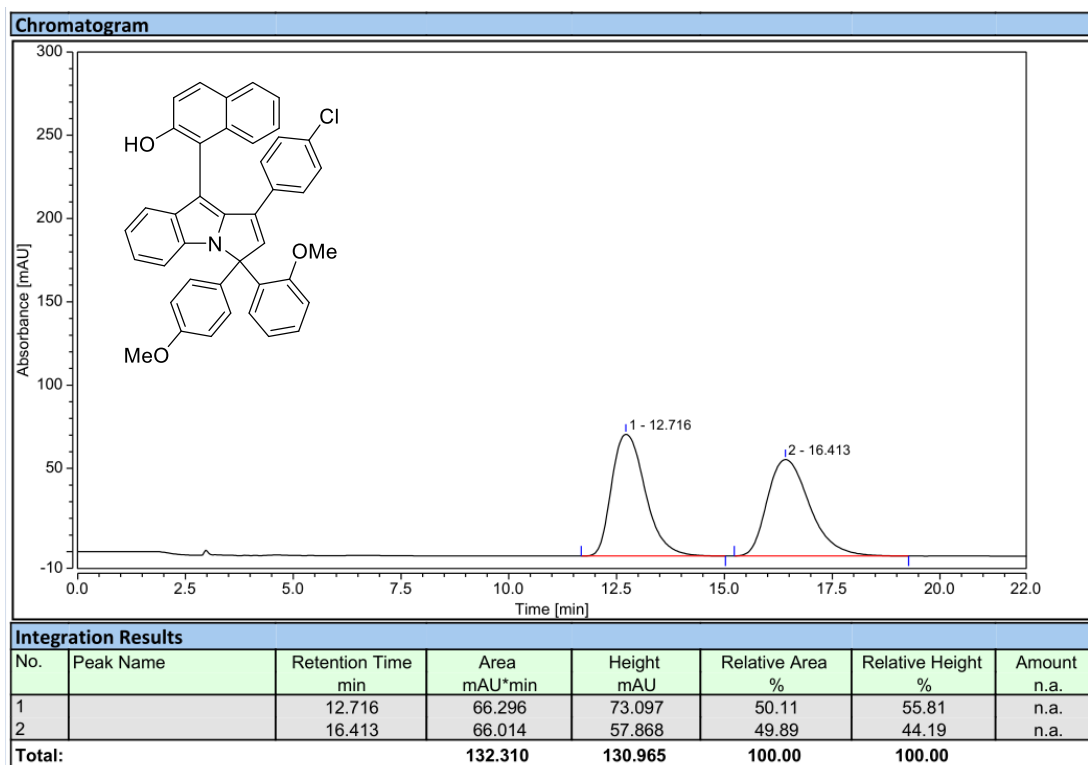


Enantioselective:

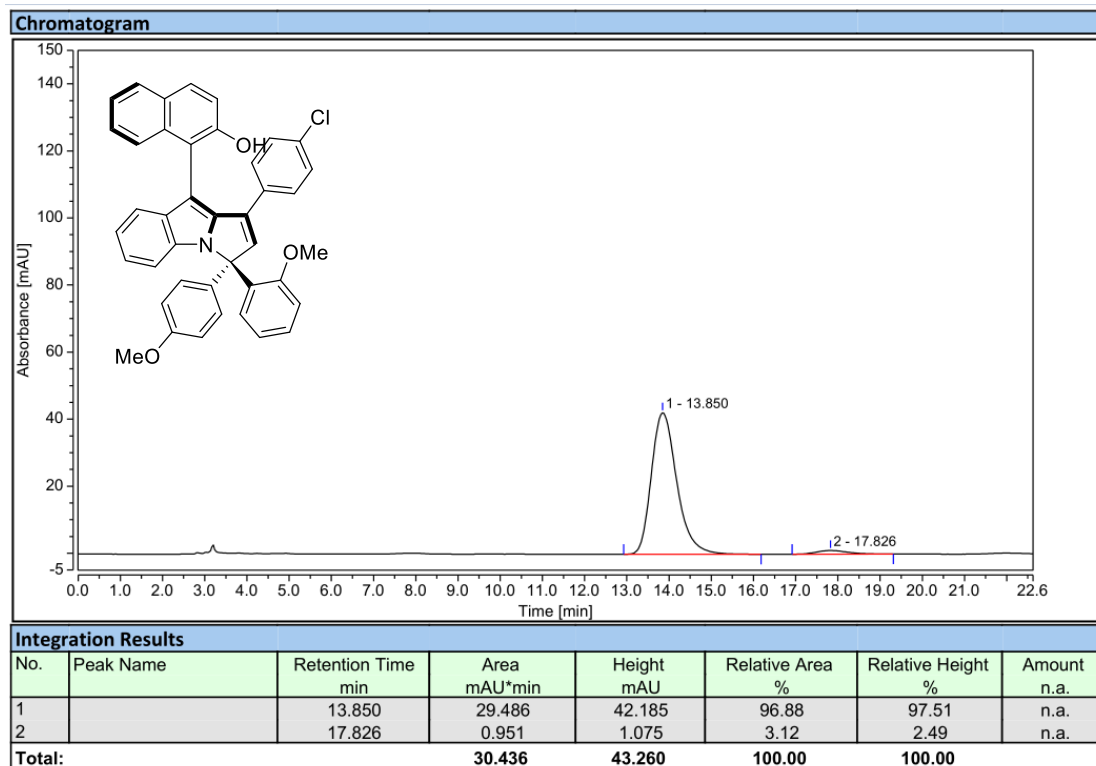


7aj

Racemic:

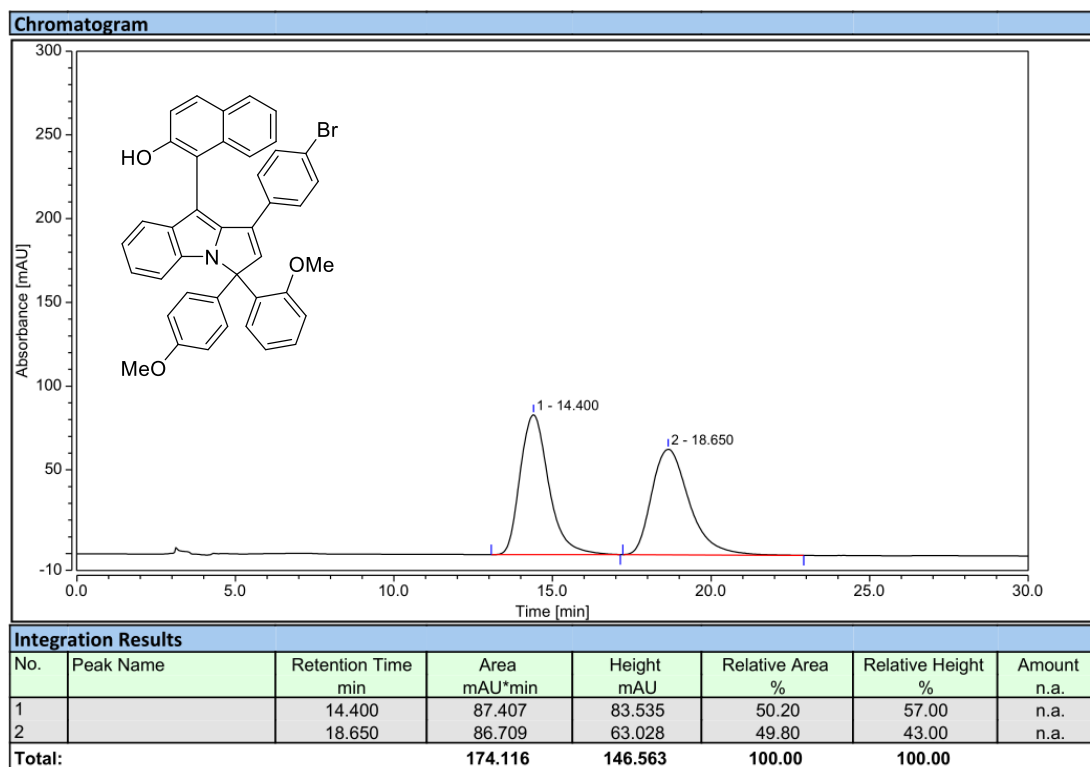


Enantioselective:

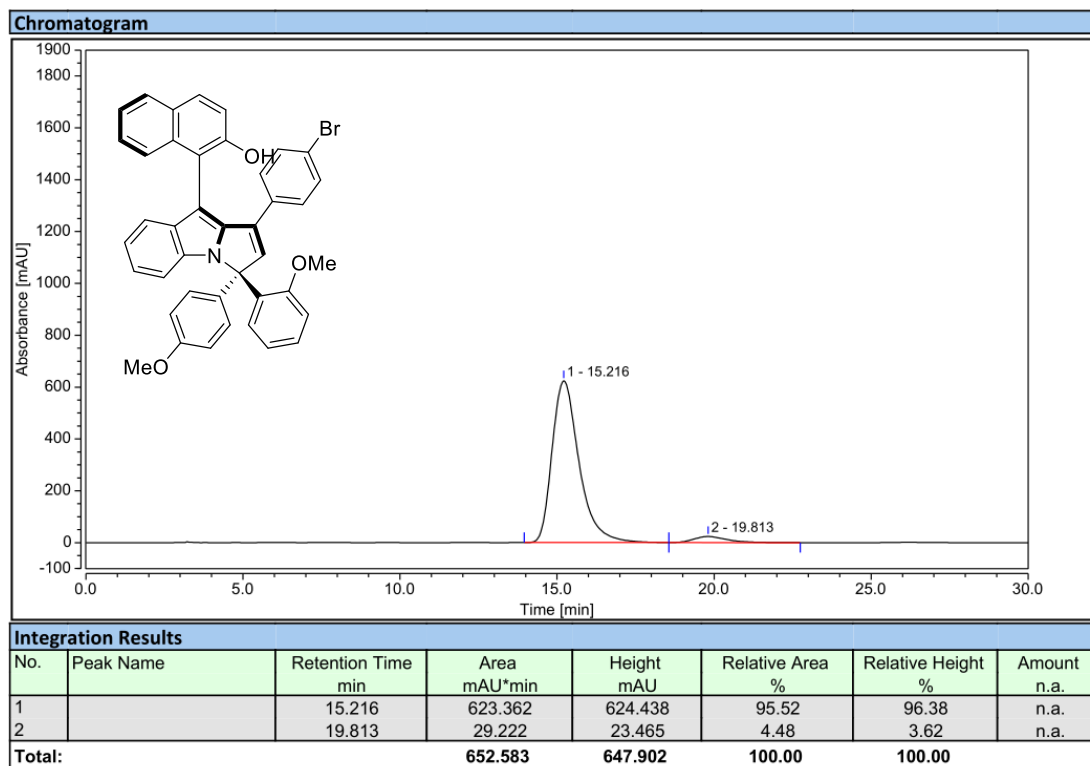


7ak

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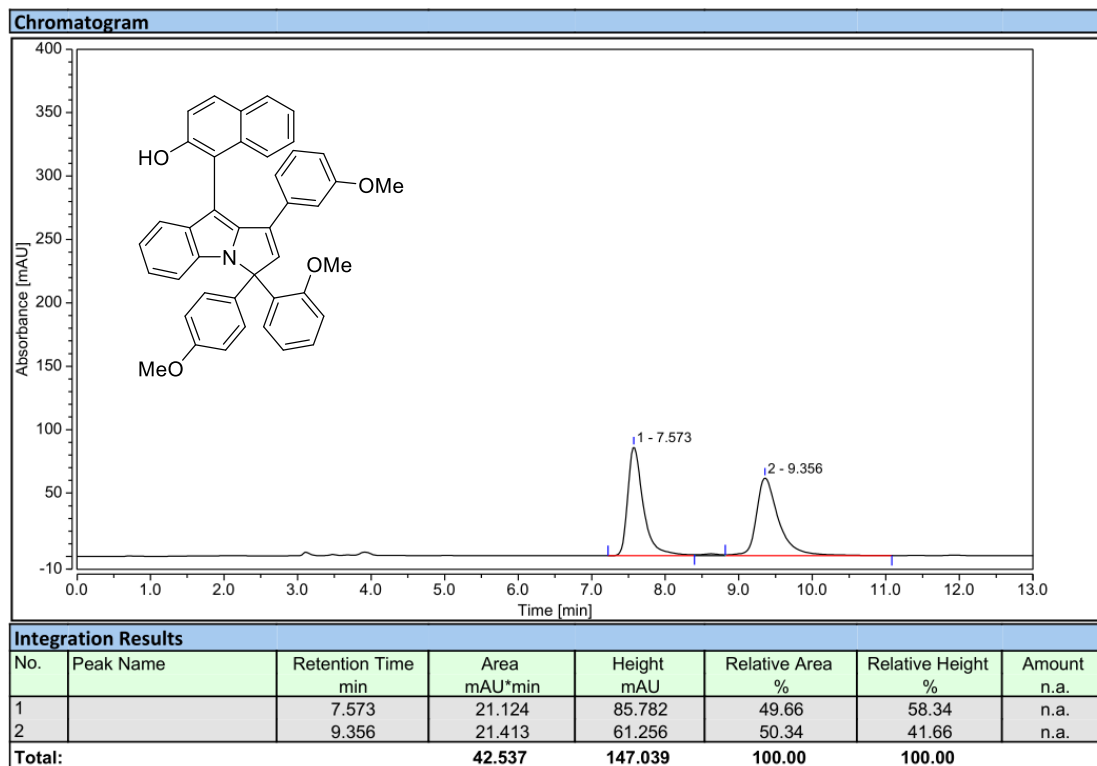


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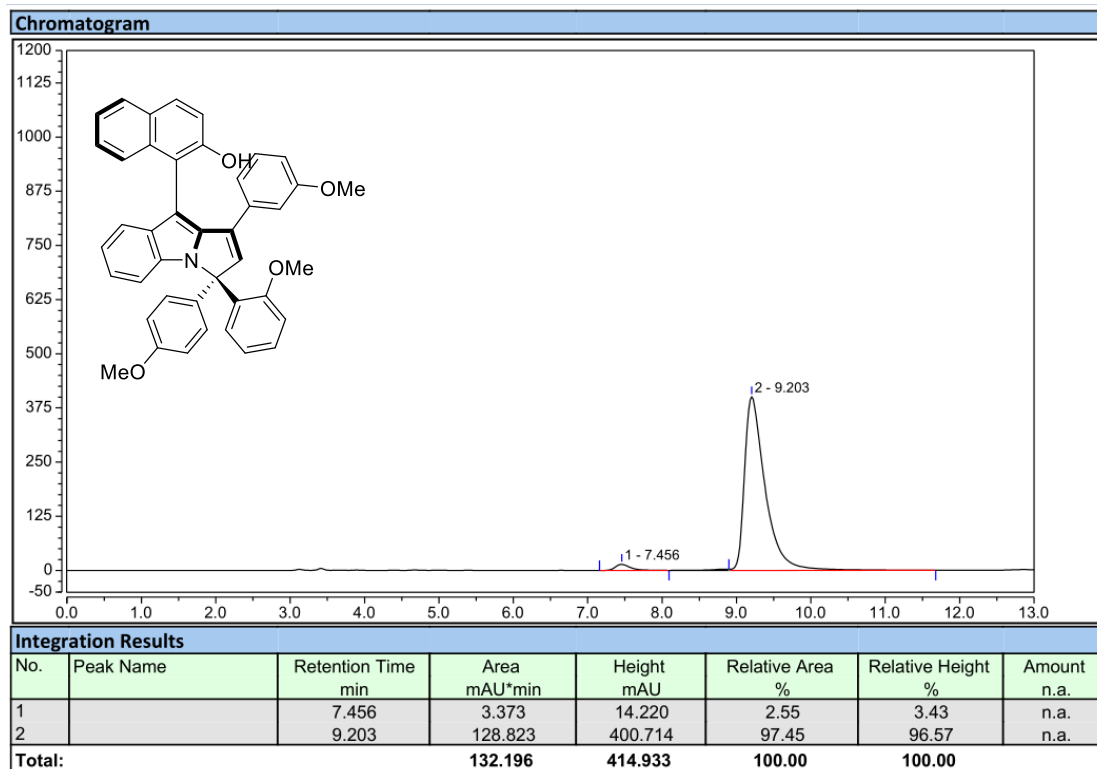


7al

Racemic:

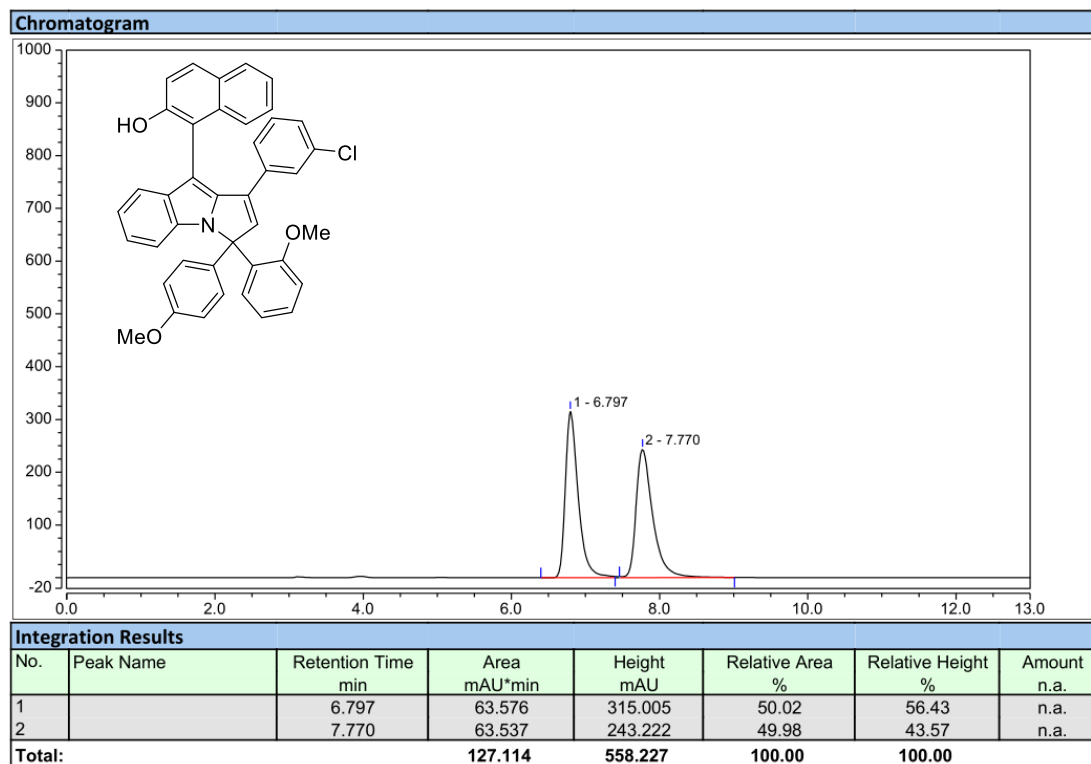


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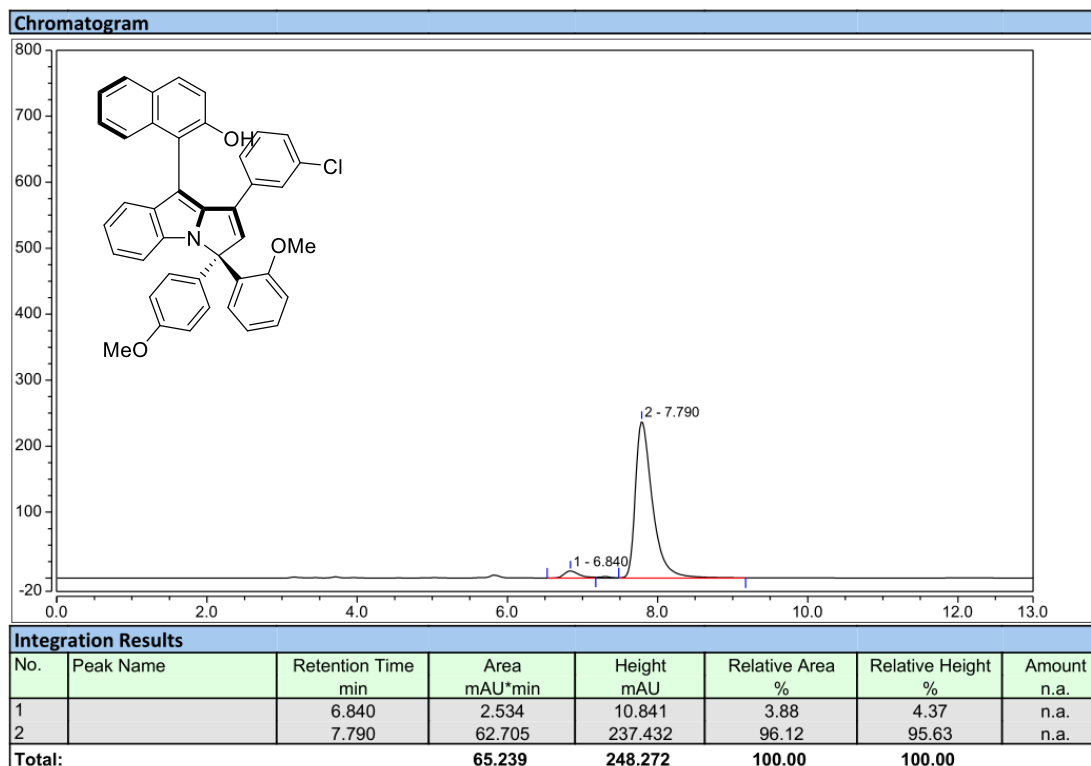


7am

Racemic:

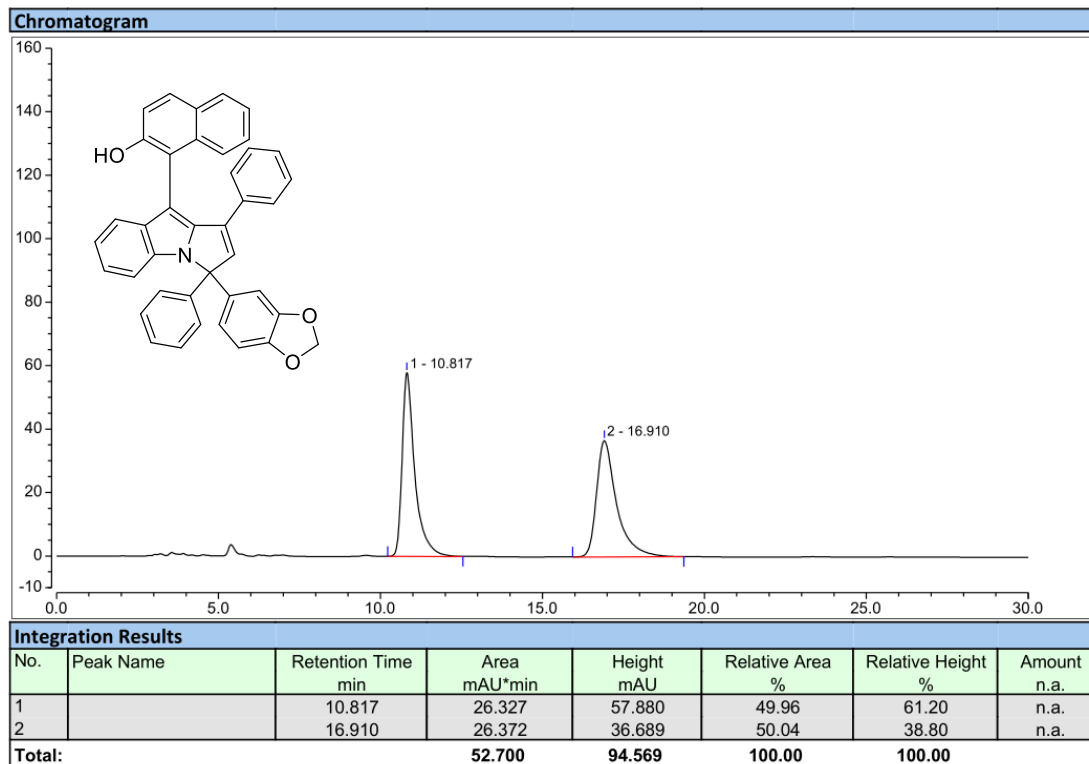


Enantioselective:

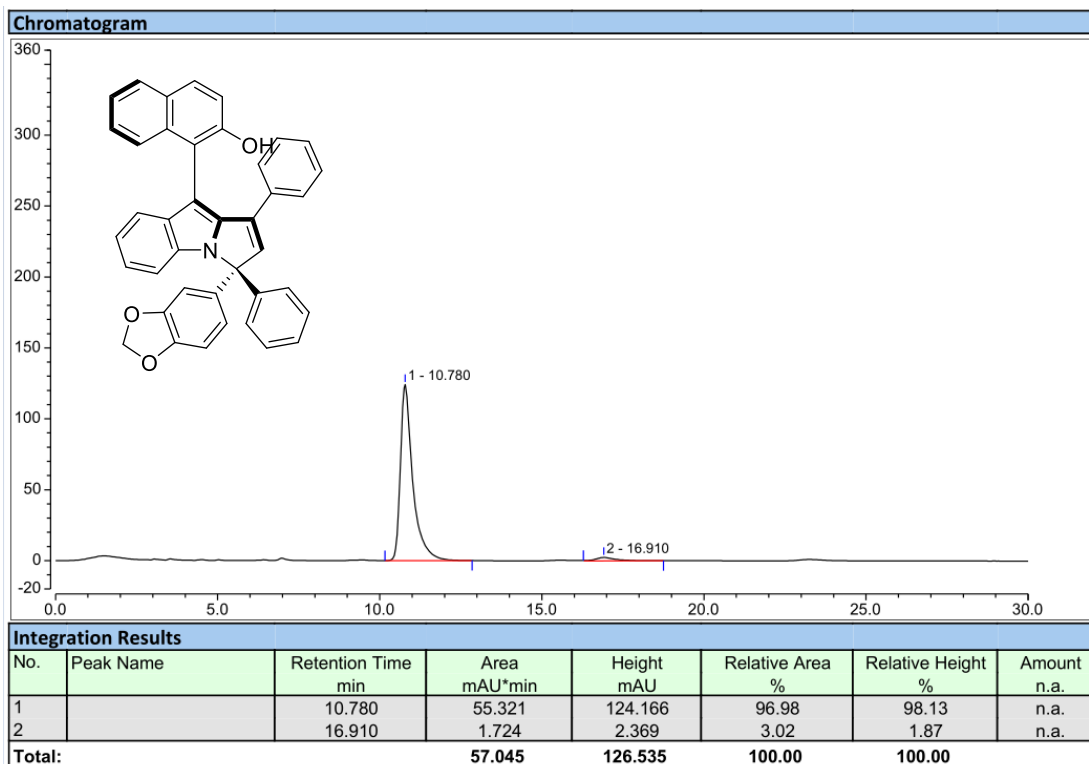


7an

Racemic:

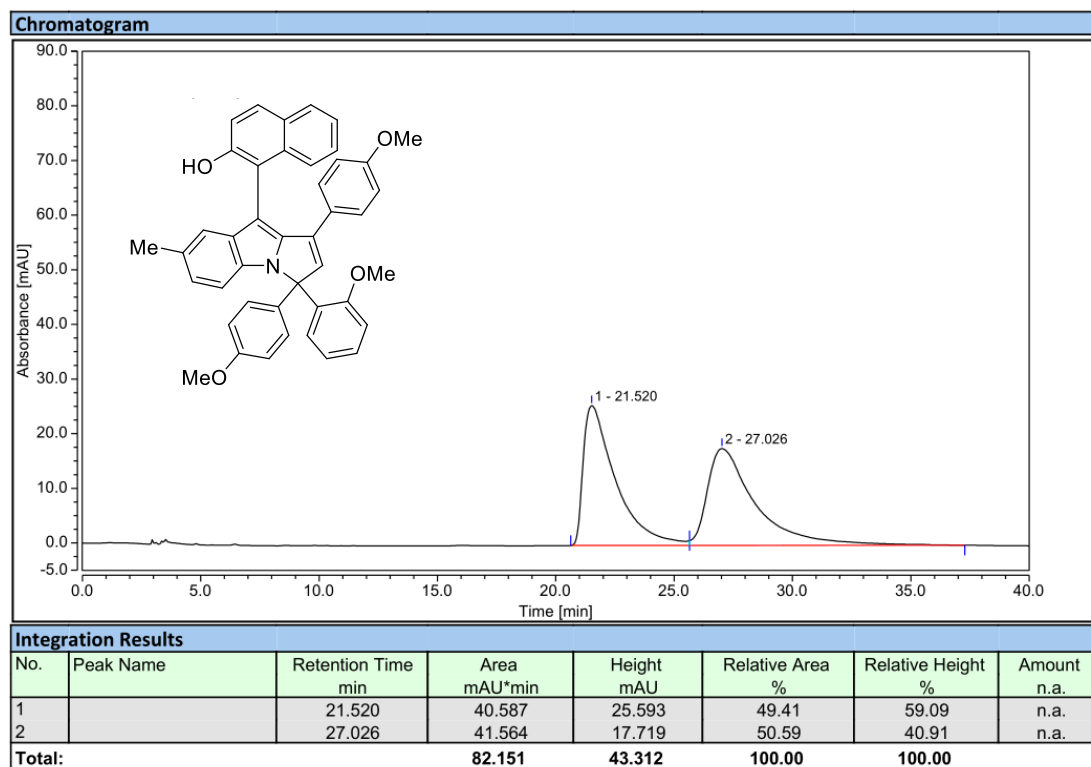


Enantioselective:

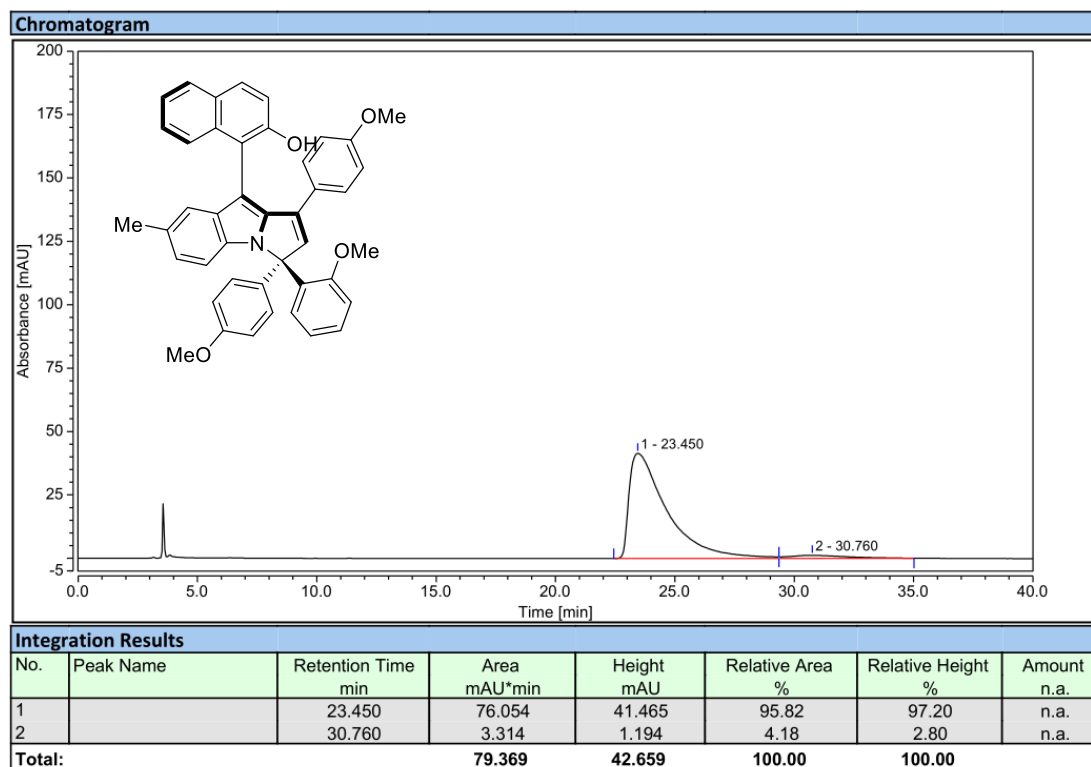


7dh

Racemic:

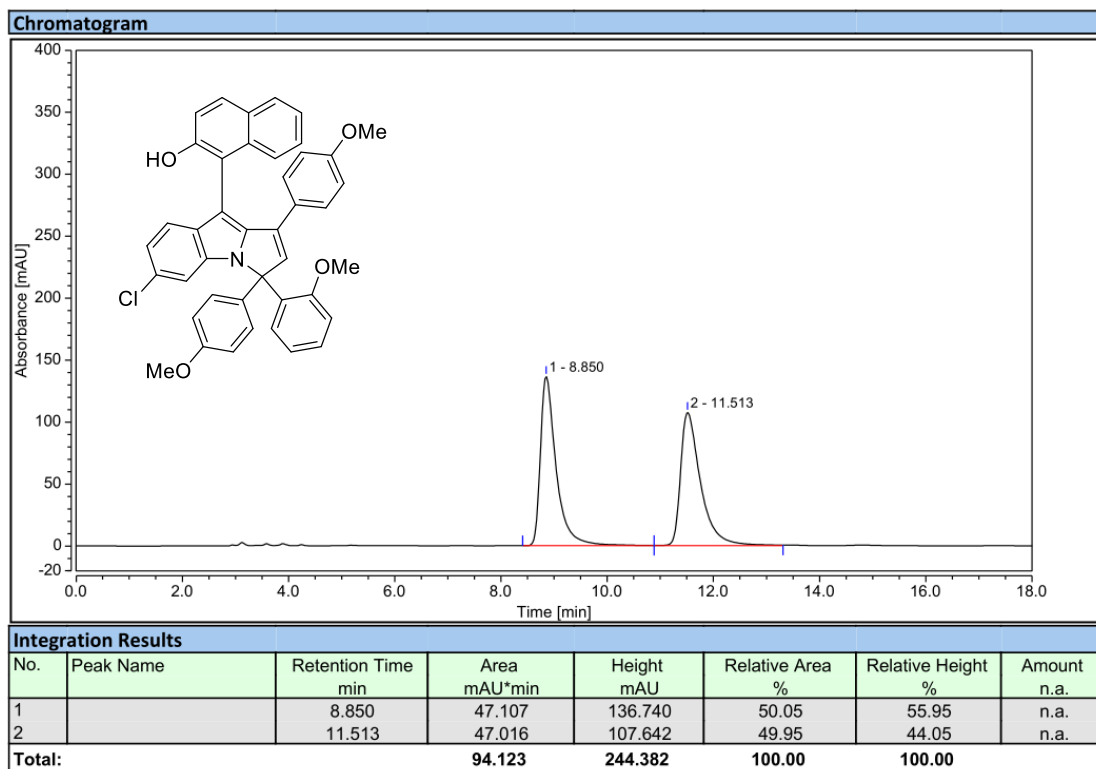


Enantioselective:

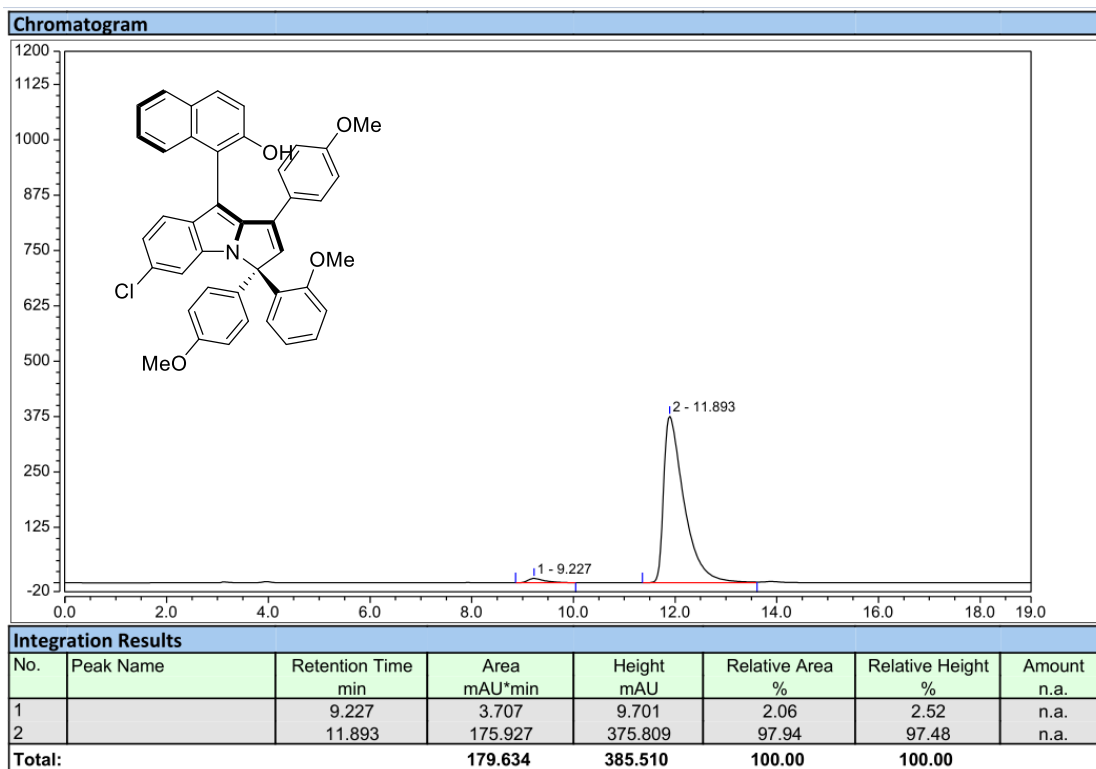


7eh

Racemic:

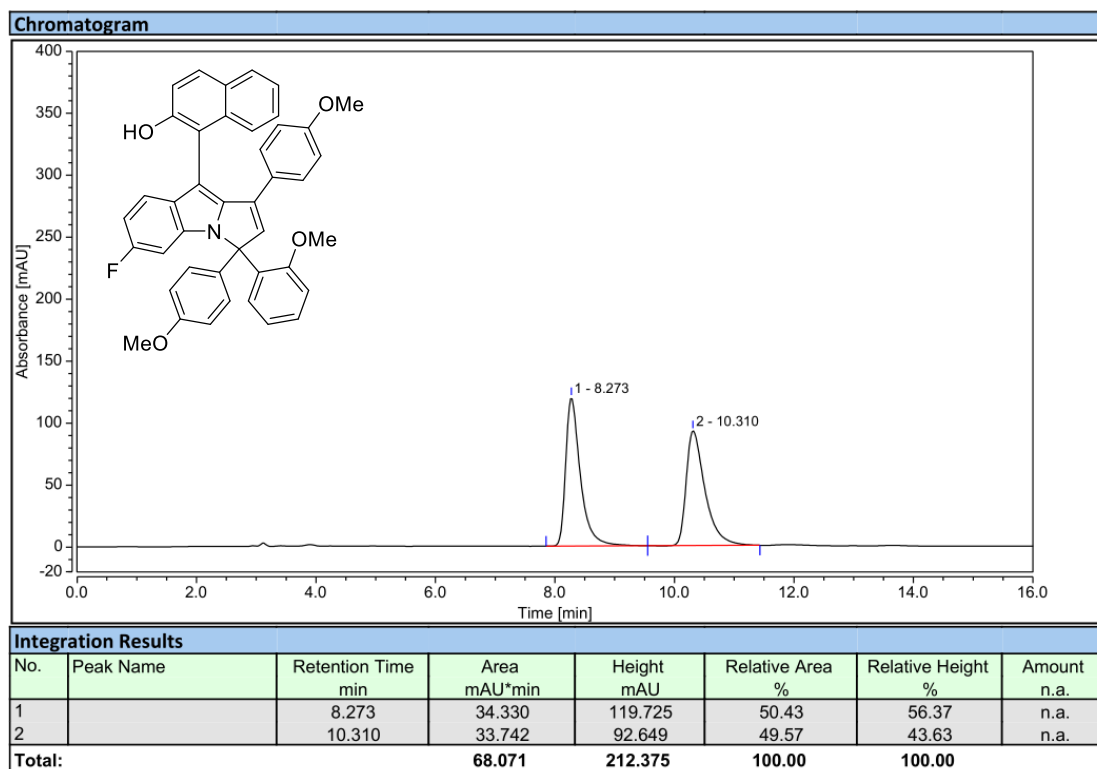


Enantioselective:

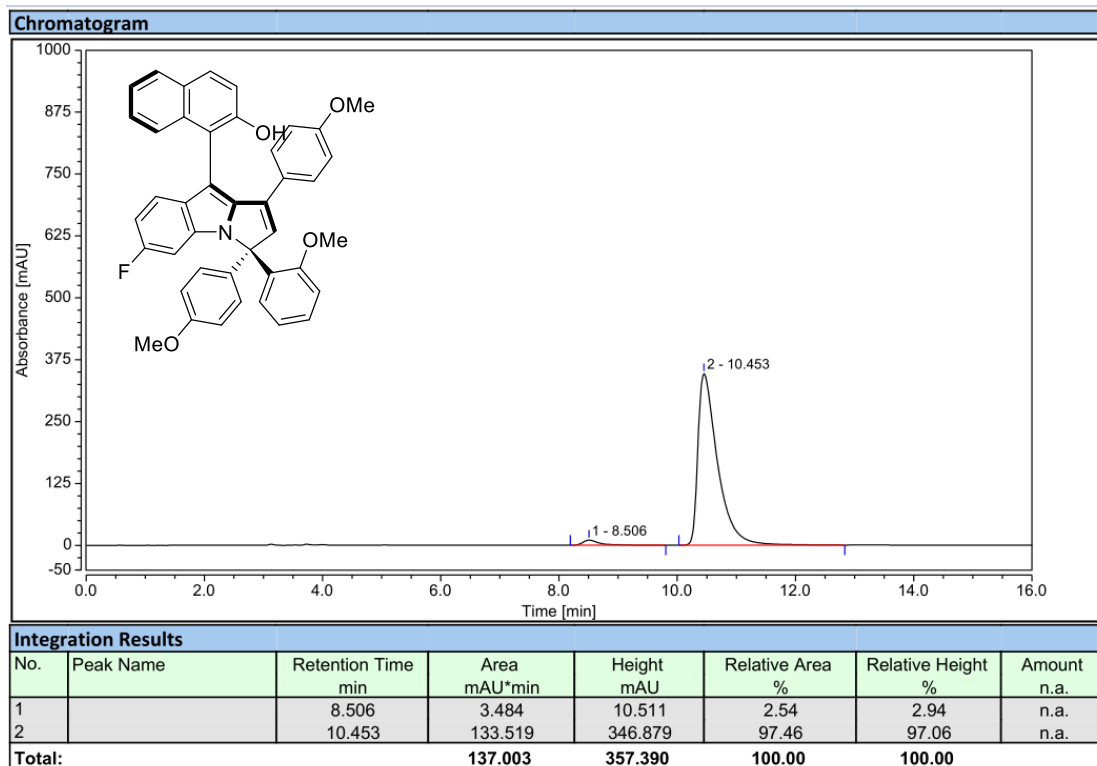


7fh

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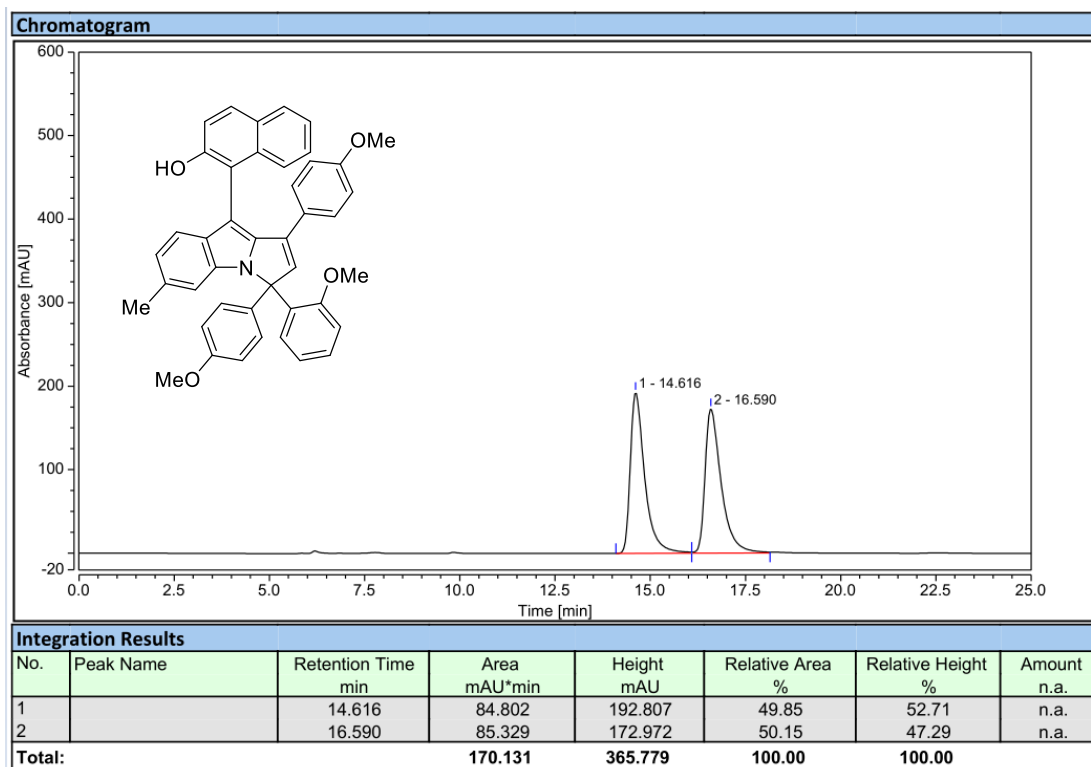


Enantioselective:

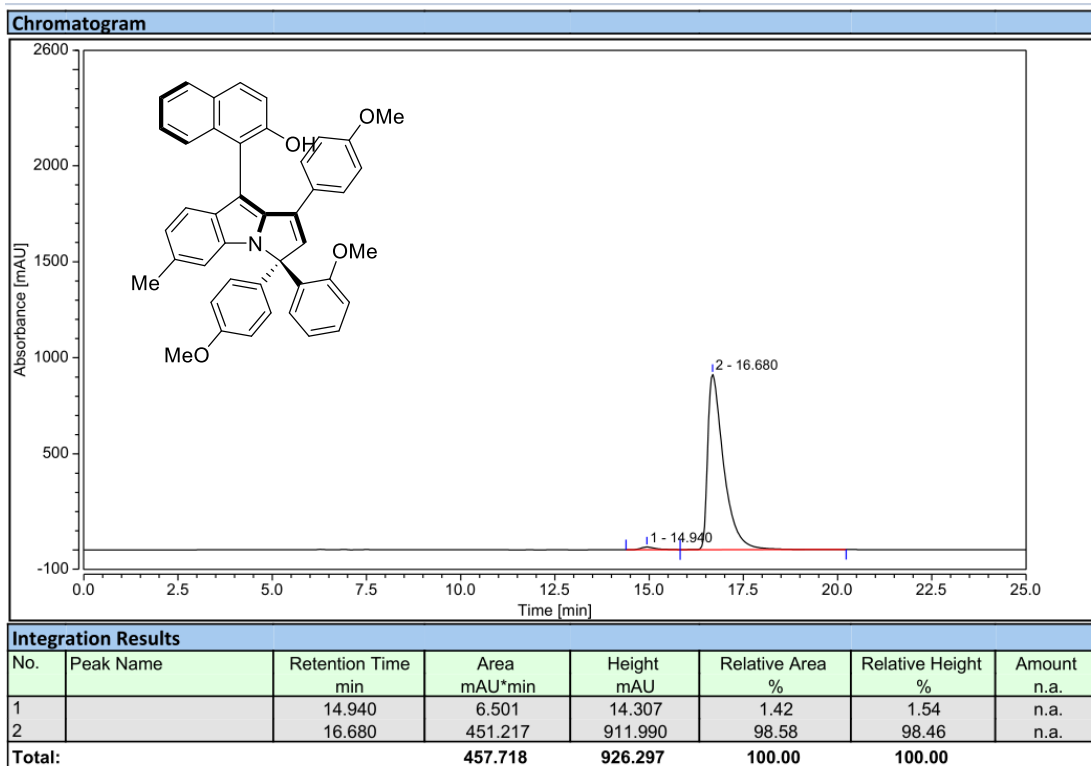


7gh

Racemic:

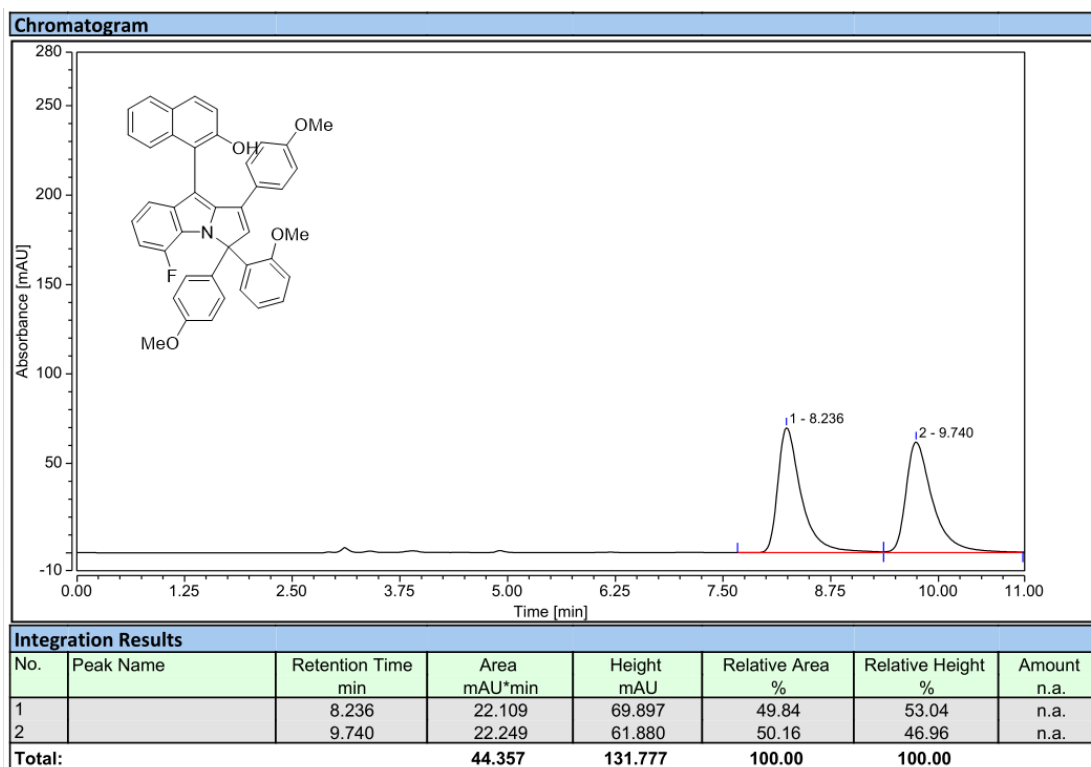


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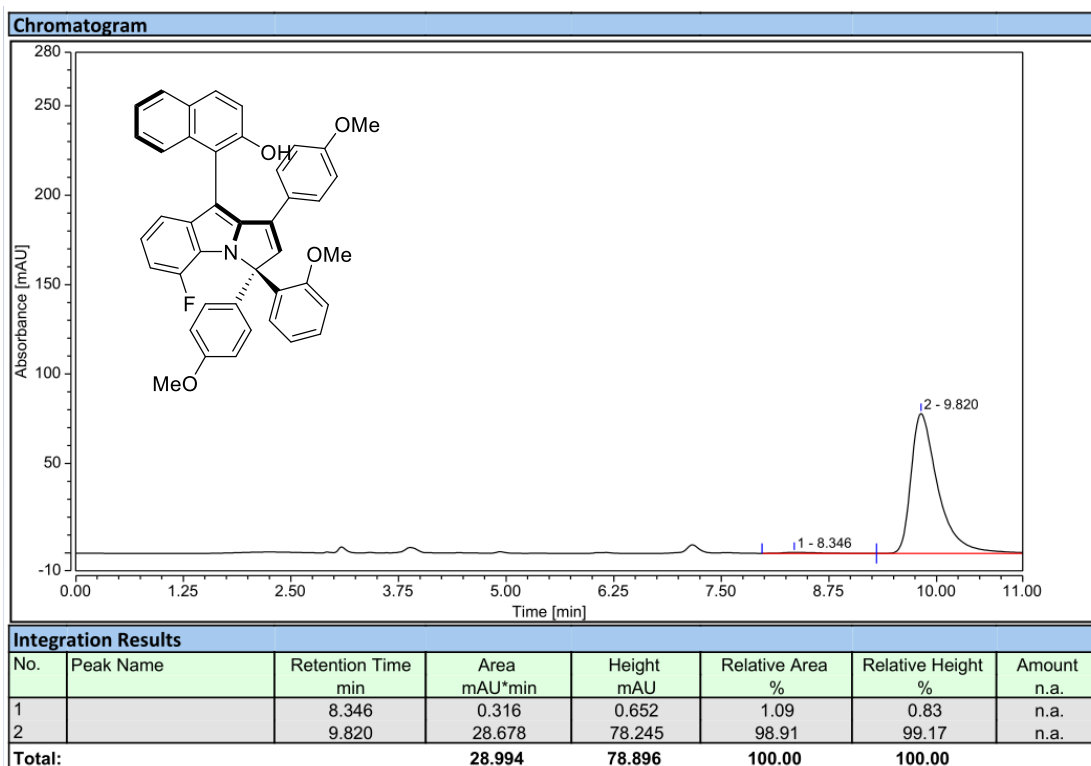


7hh

Racemic:

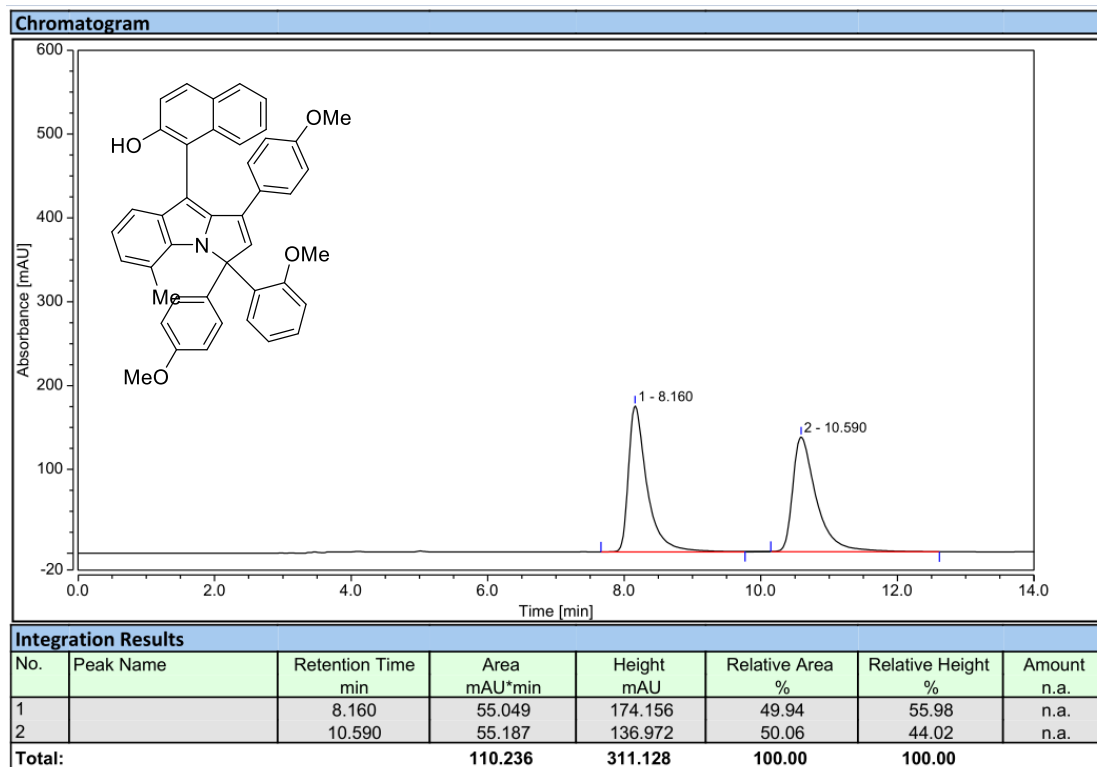


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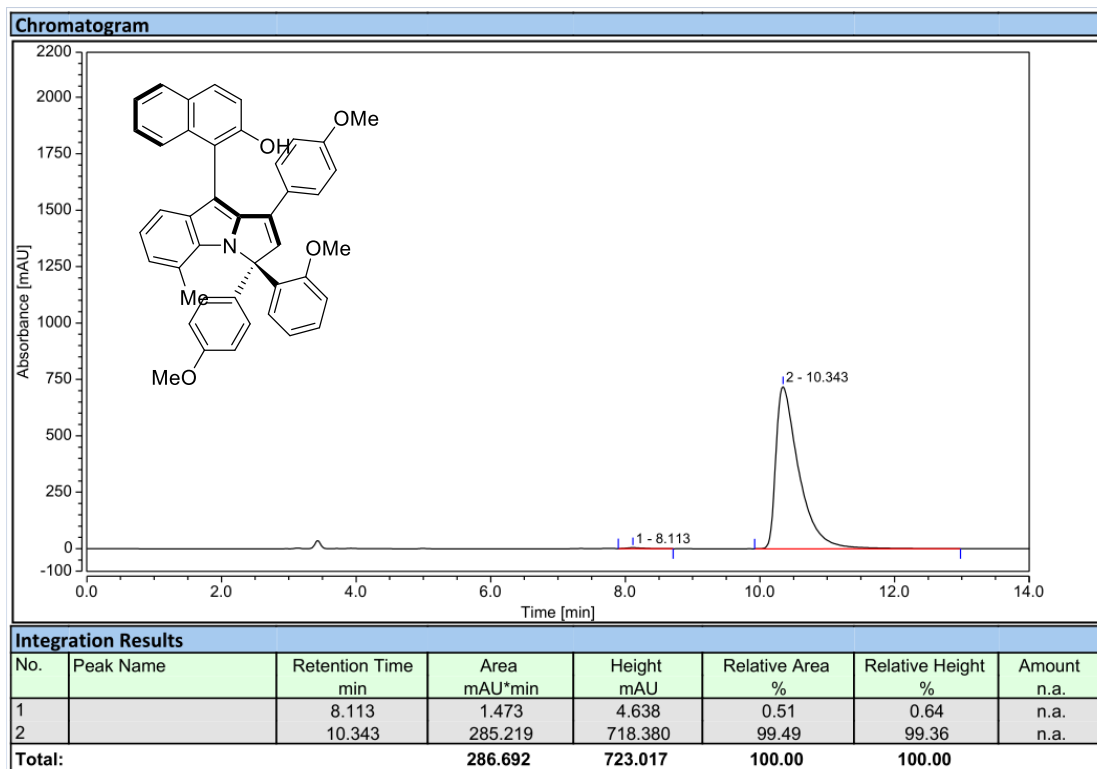


7ih

Racemic:

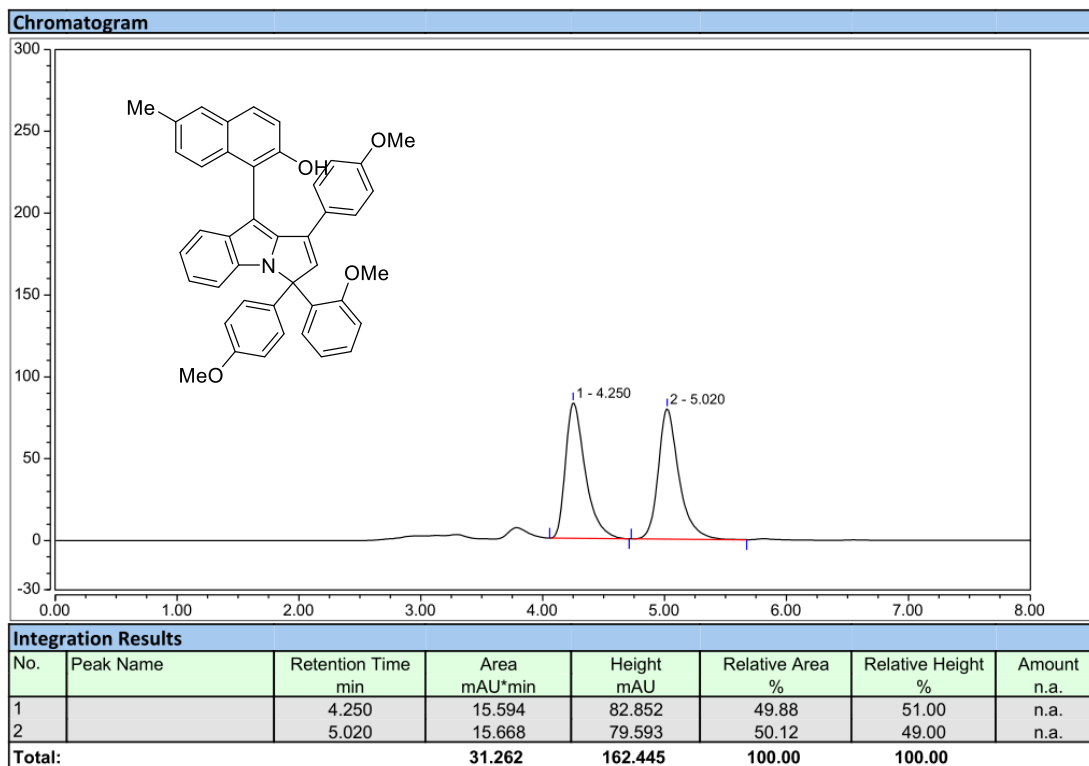


Enantioselective:

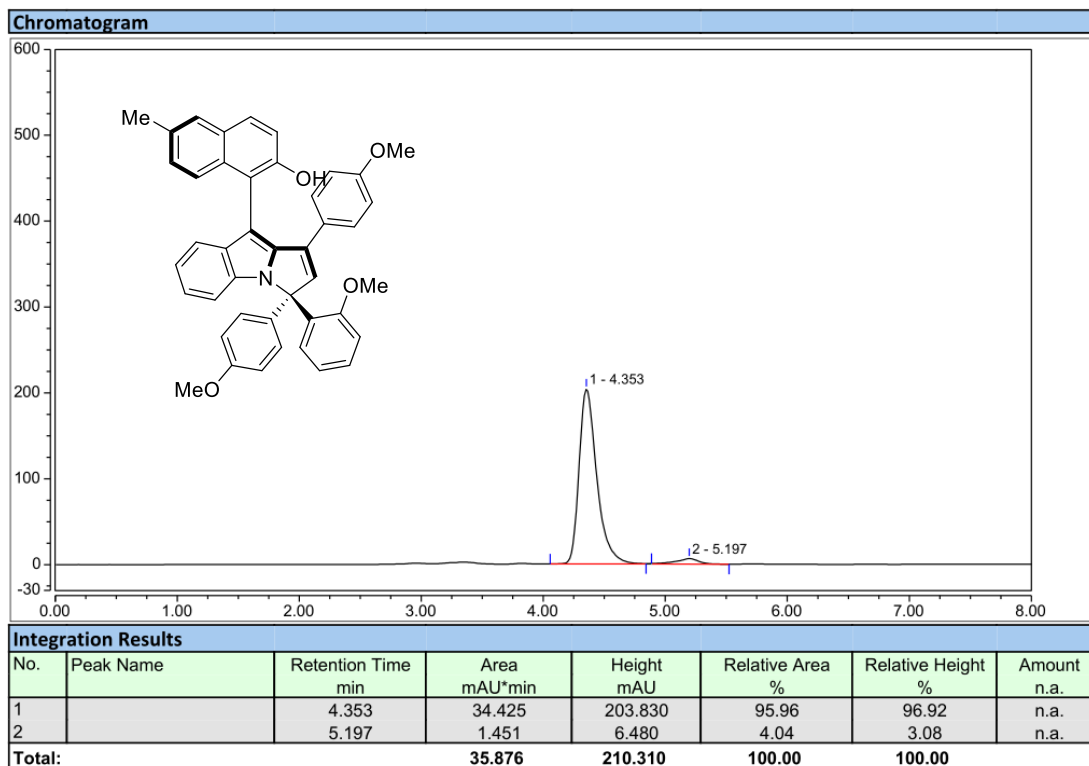


7kh

Racemic:

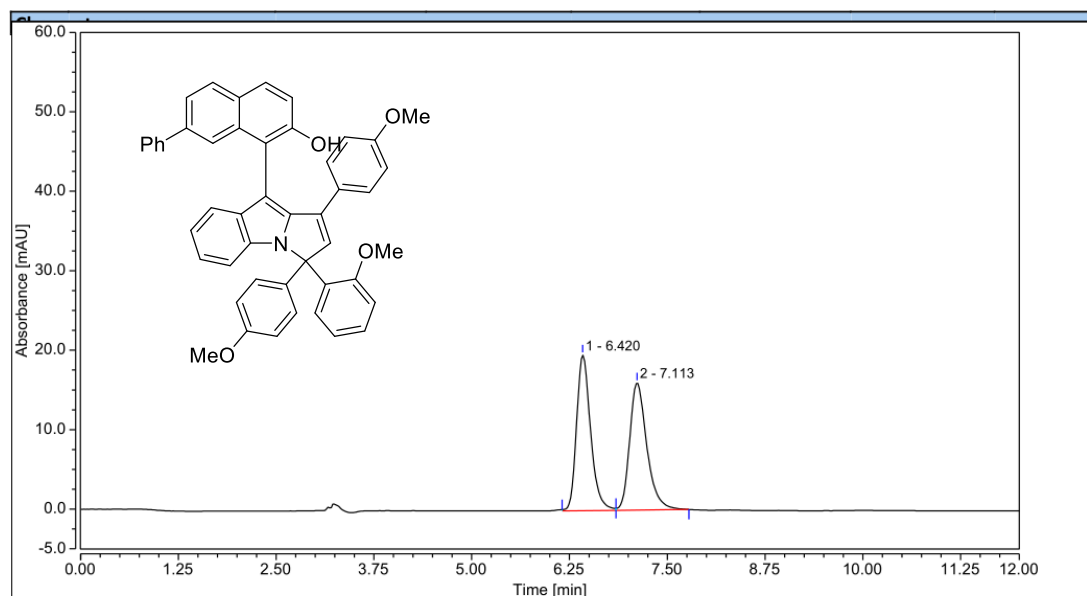


Enantioselective:



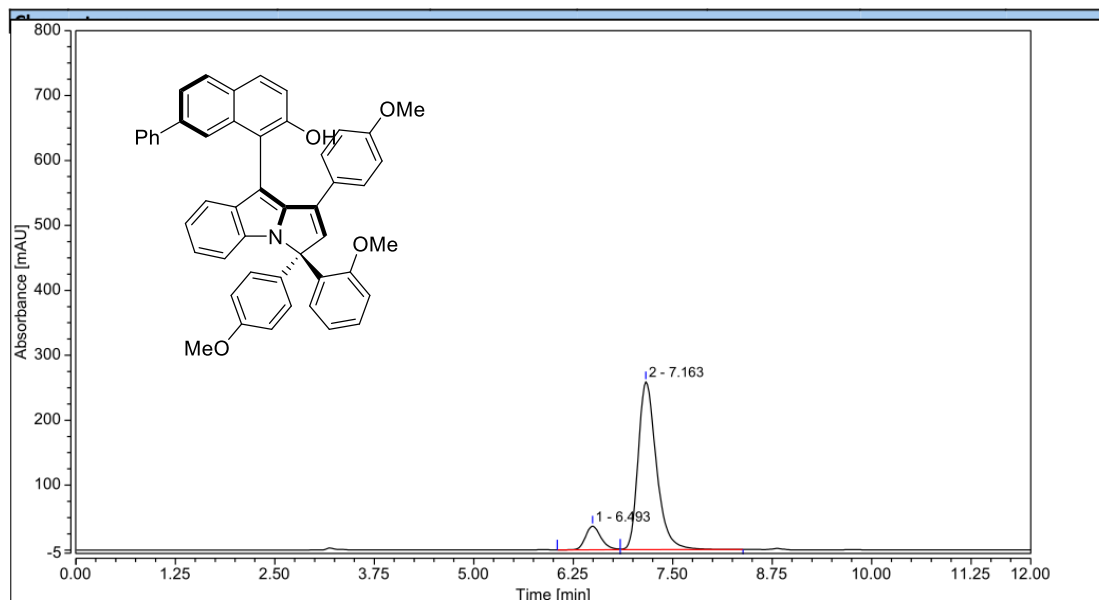
7lh

Racemic:



Integration Results							
No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount
1		6.420	4.081	19.581	49.99	55.00	n.a.
2		7.113	4.083	16.020	50.01	45.00	n.a.
Total:			8.164	35.601	100.00	100.00	

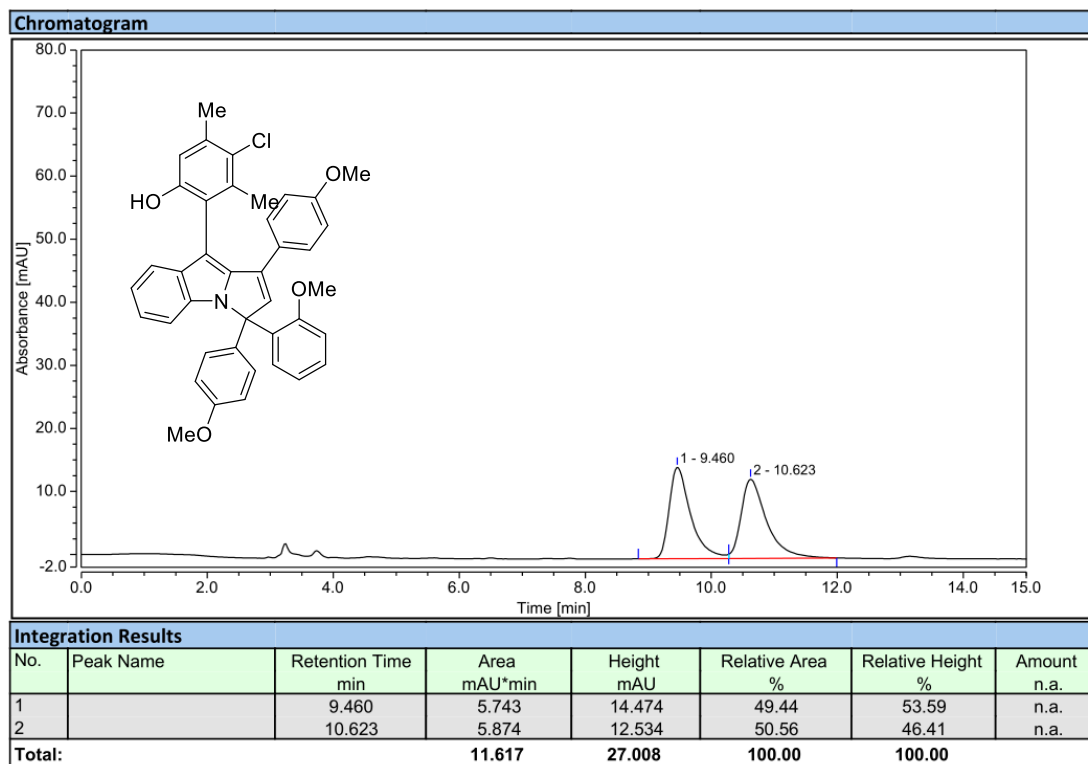
Enantioselective:



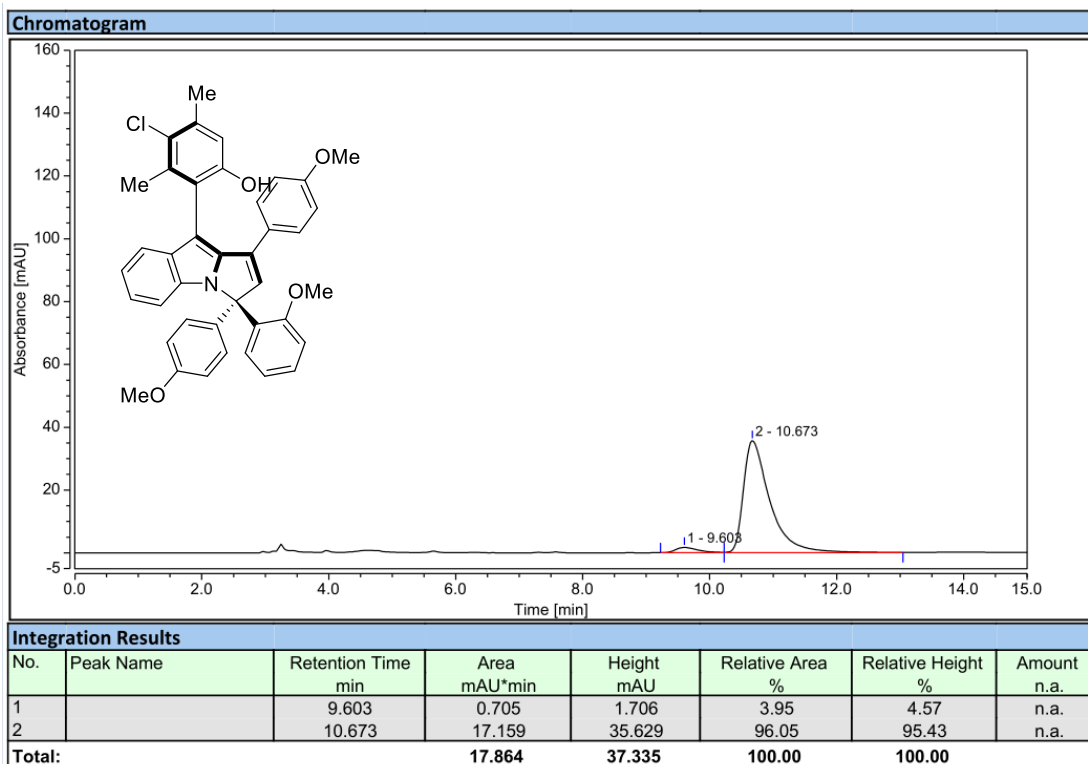
Integration Results							
No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount
1		6.493	8.205	36.457	10.64	12.36	n.a.
2		7.163	68.928	258.566	89.36	87.64	n.a.
Total:			77.133	295.023	100.00	100.00	

7mh

Racemic:

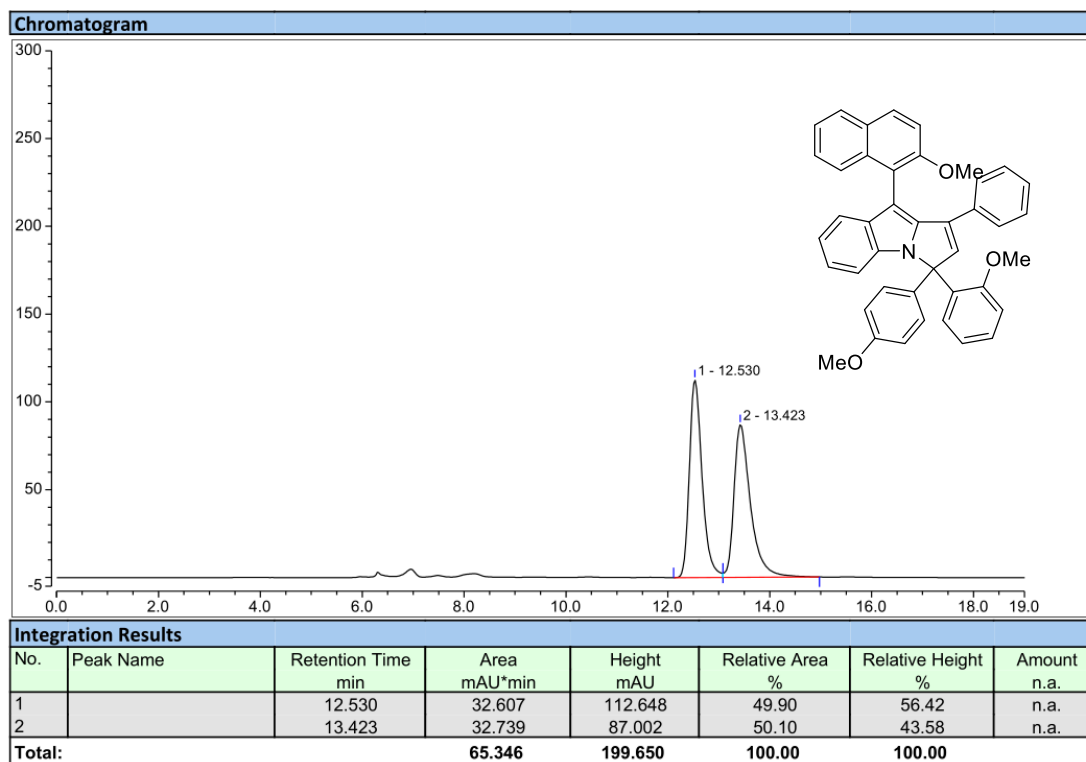


Enantioselective:

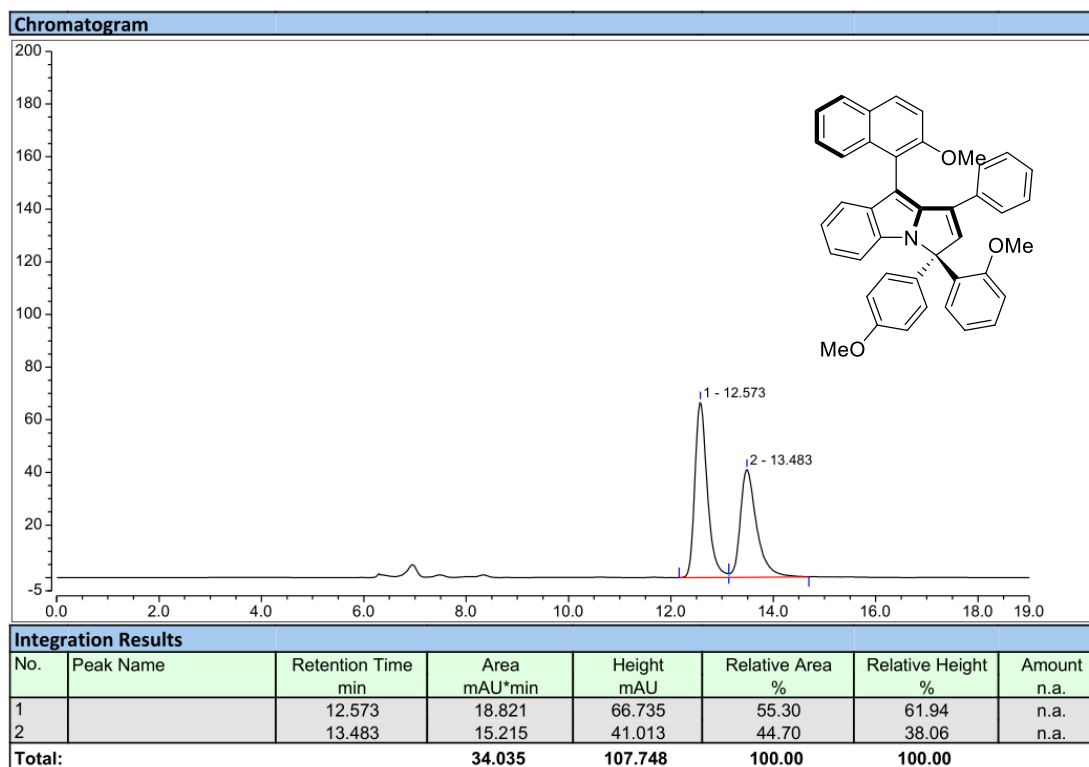


7ng (major configuration)

Racemic:

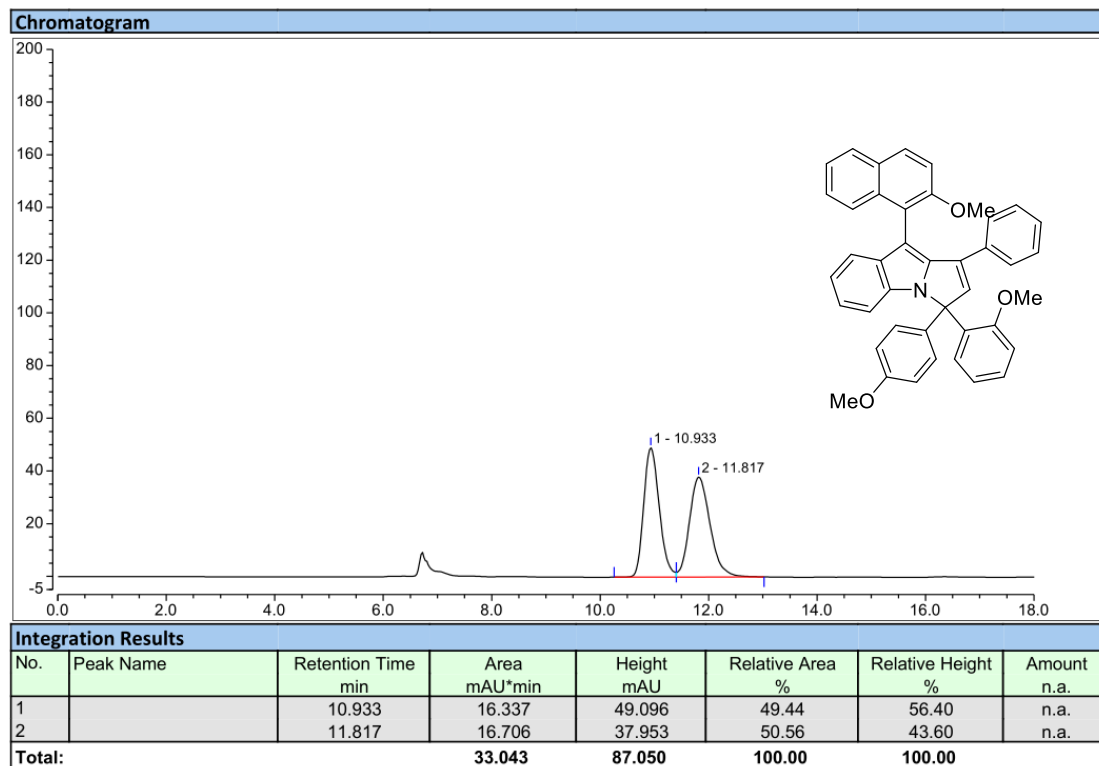


Enantioselective:

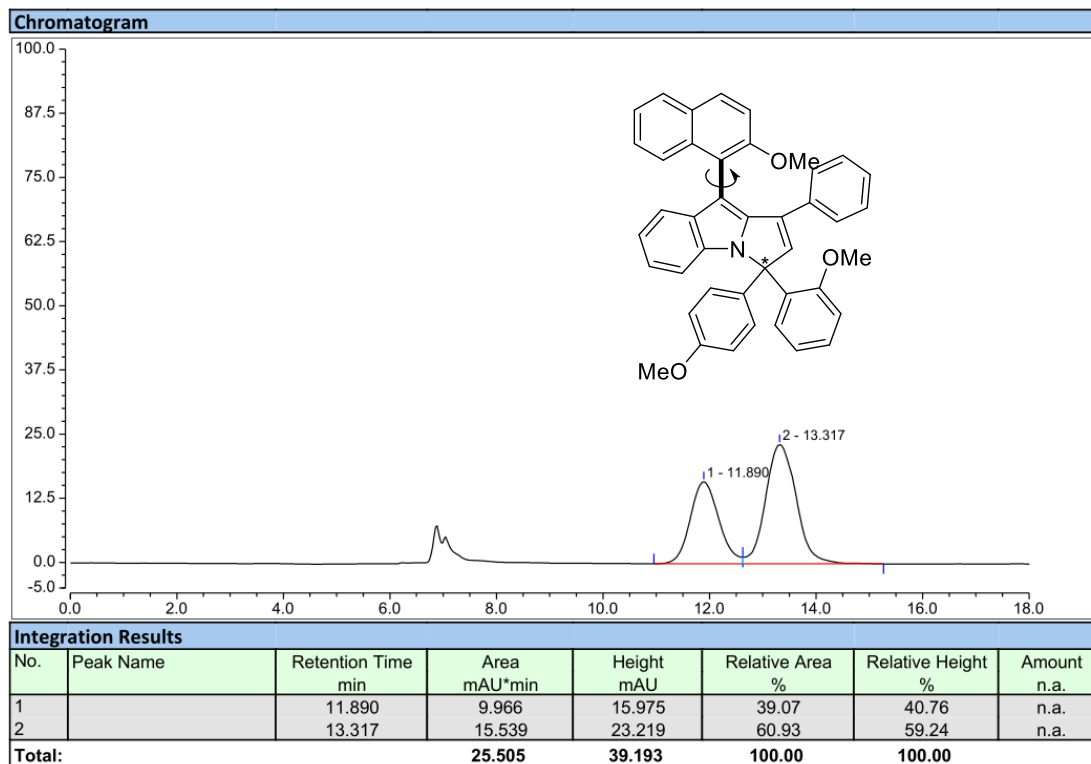


7ng (minor configuration)

Racemic:

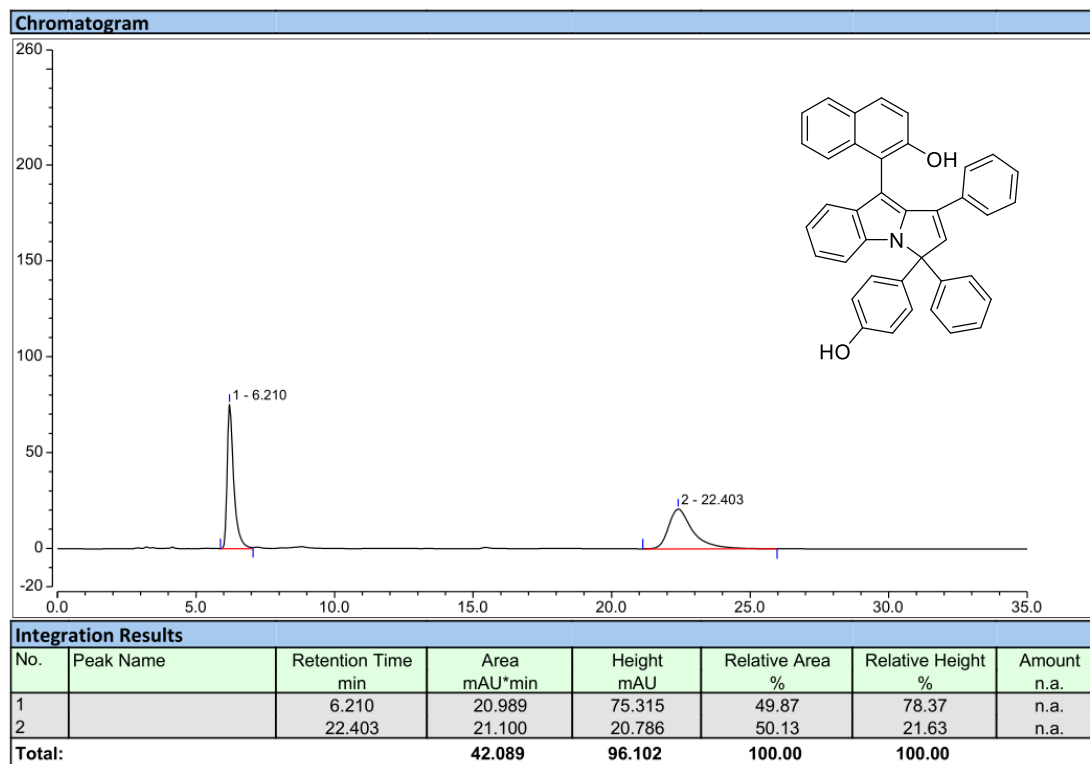


Enantioselective:

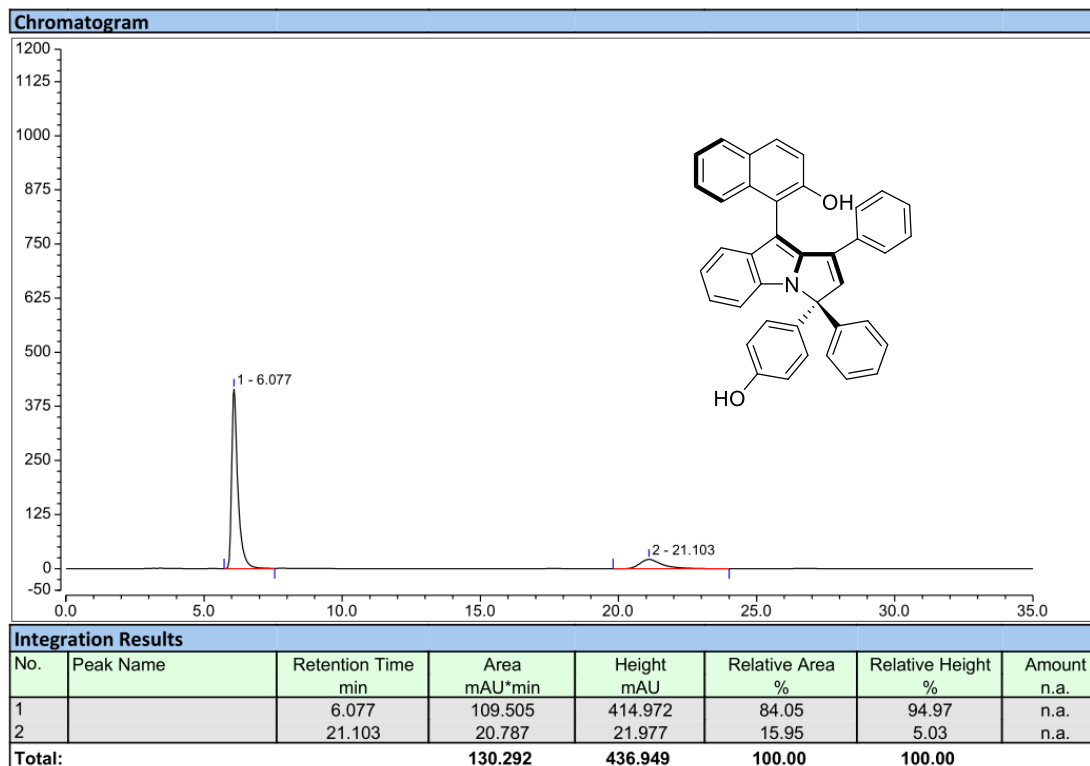


7aa

Racemic:

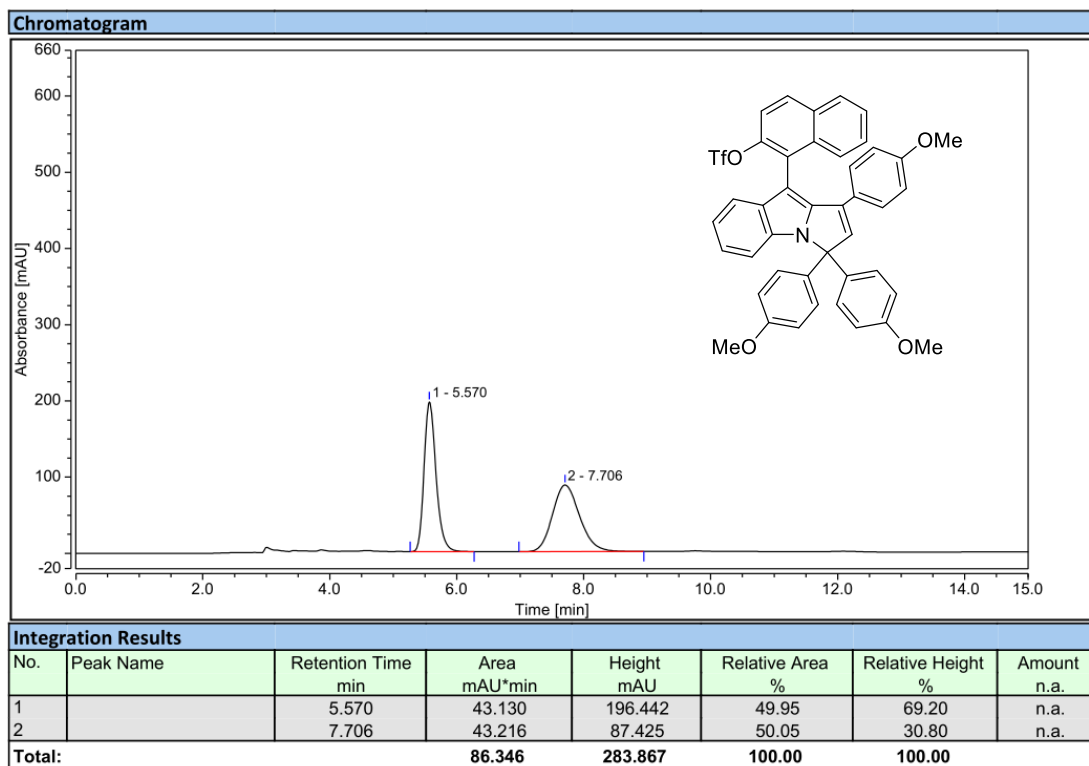


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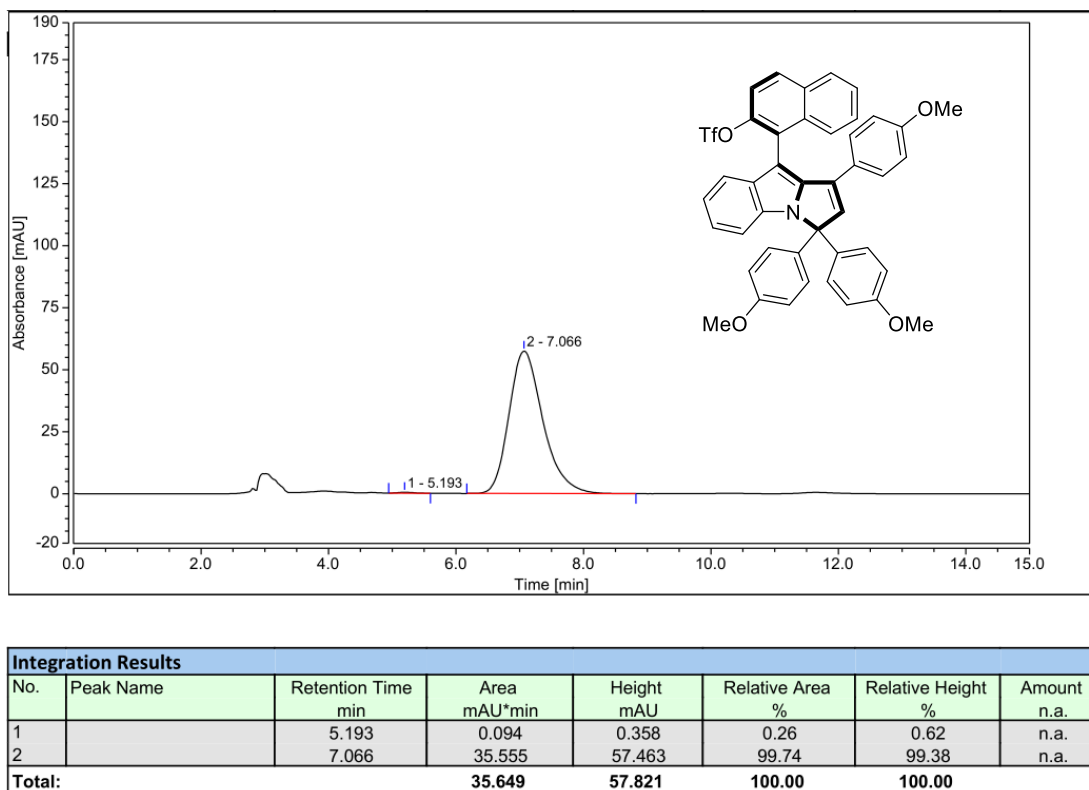


8a

Racemic:

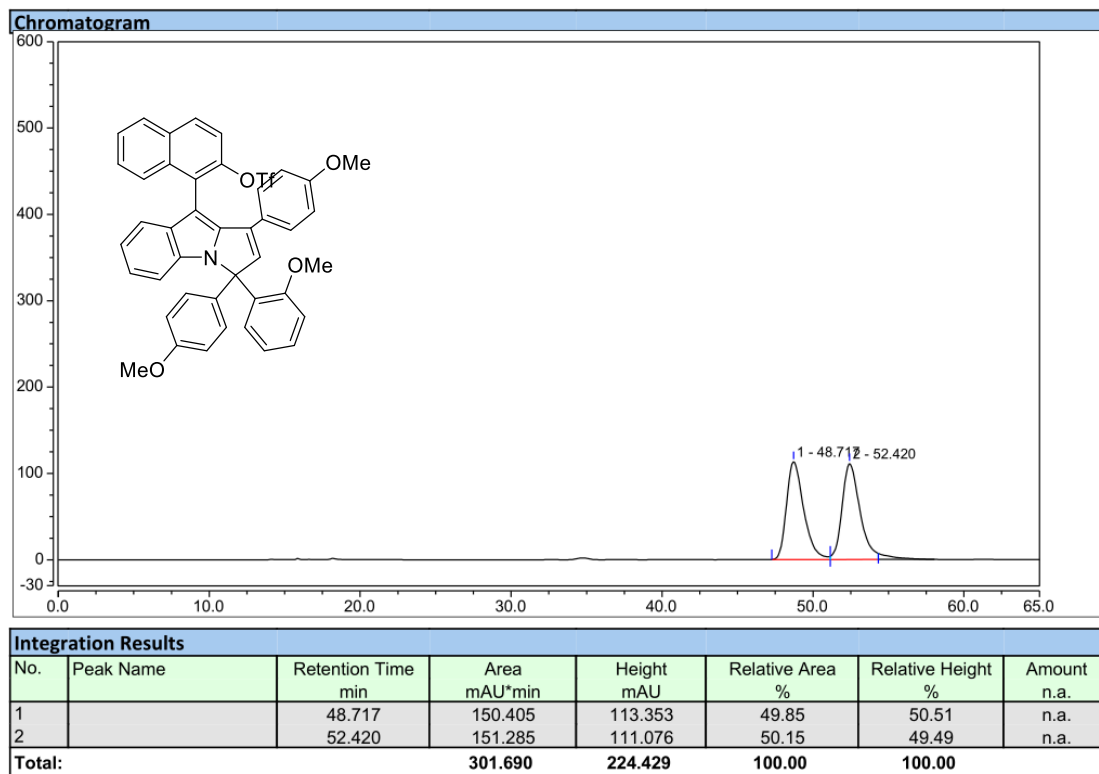


Enantioselective:

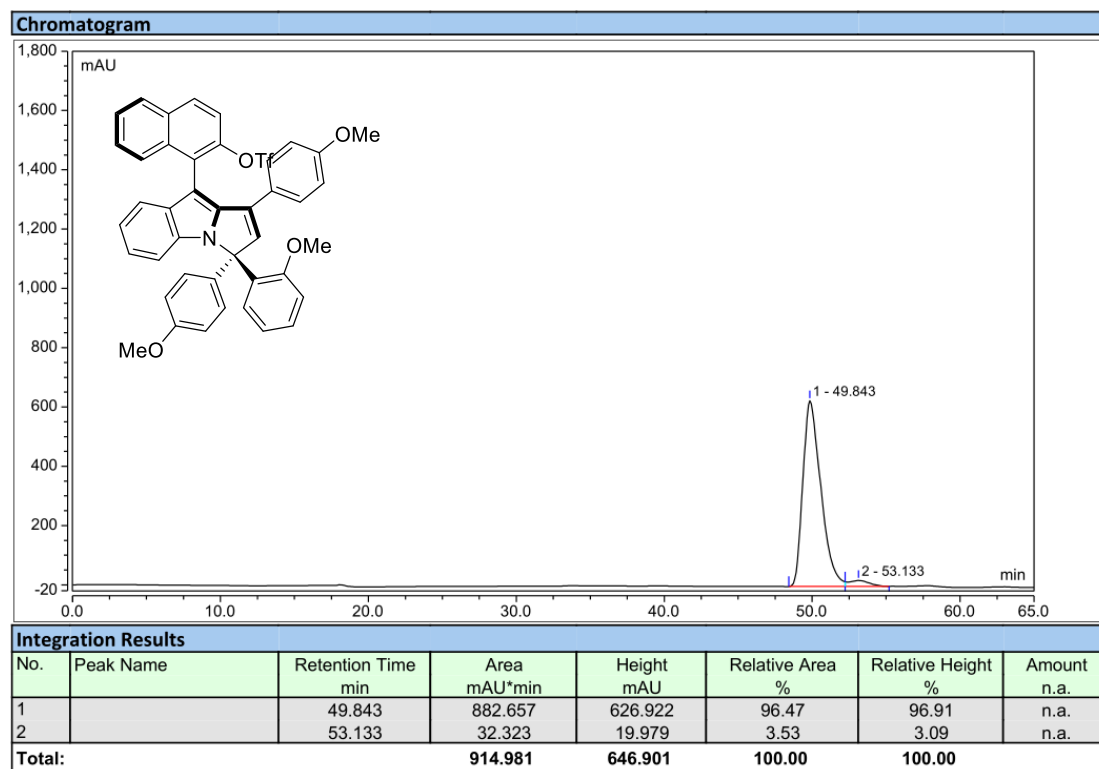


8b

Racemic:

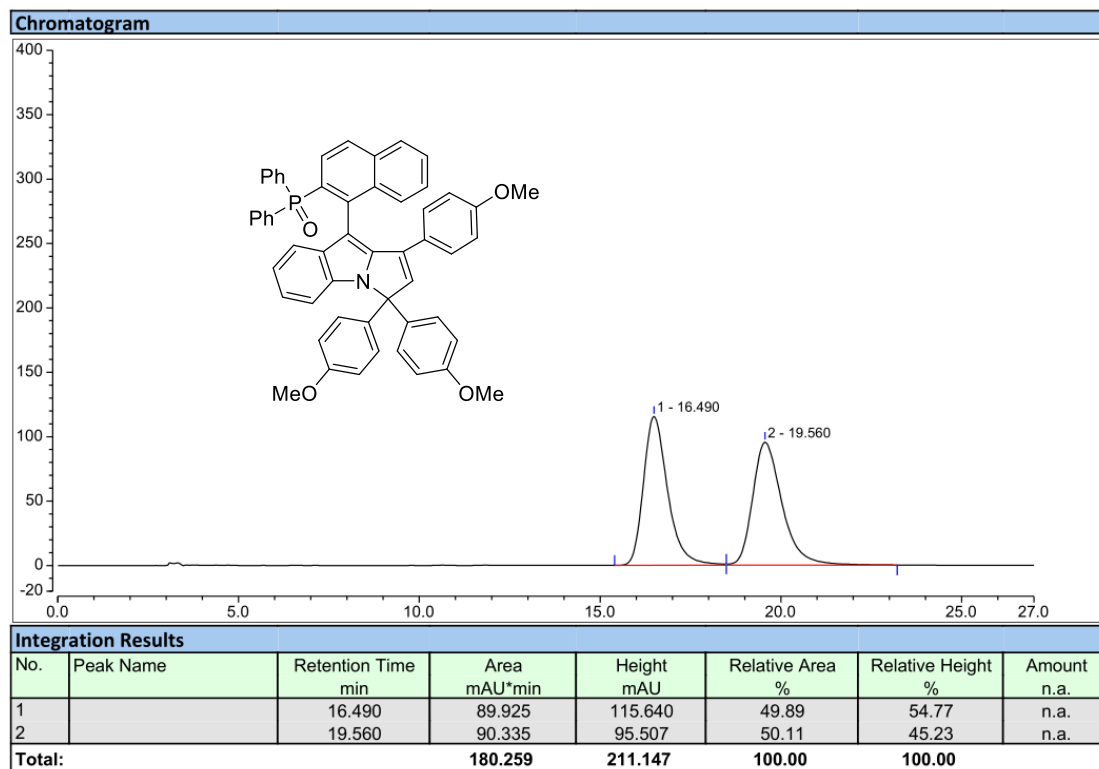


Enantioselective:

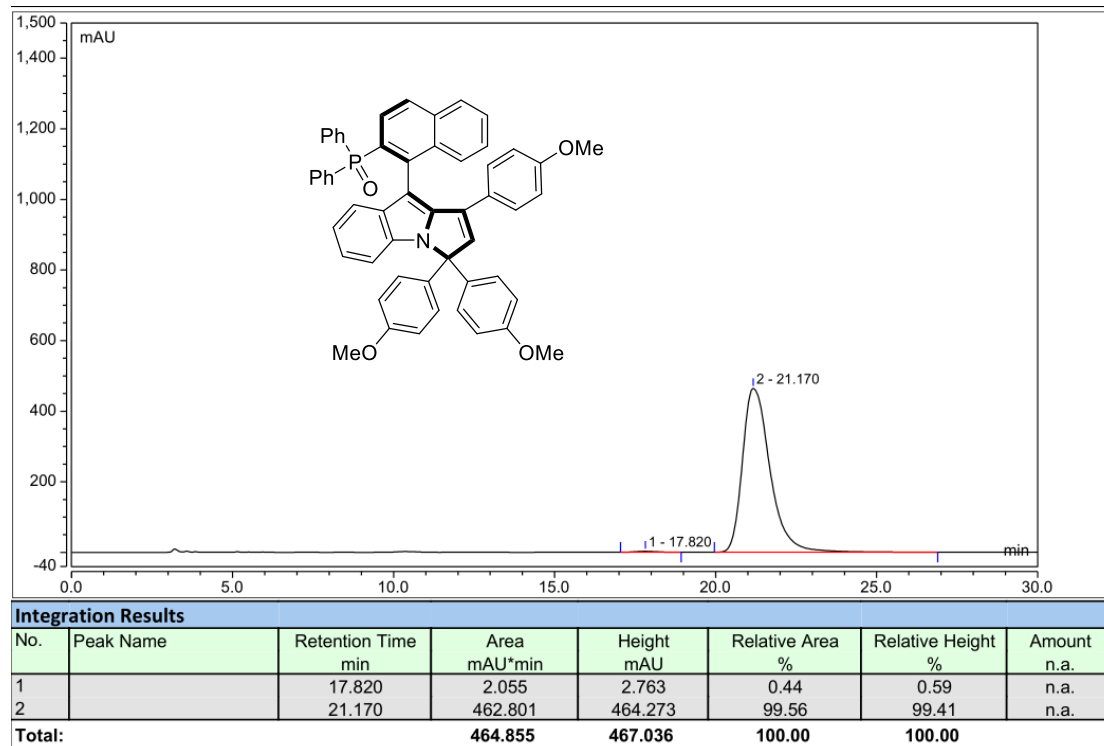


9a

Racemic:

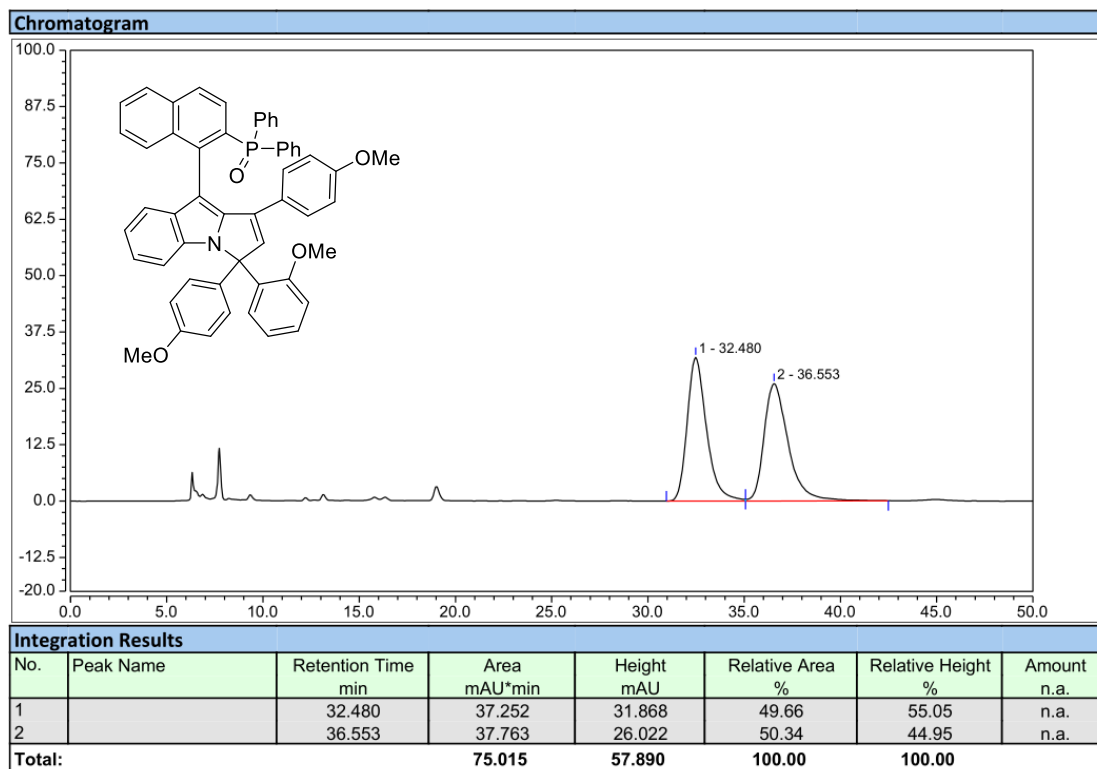


Enantioselective:

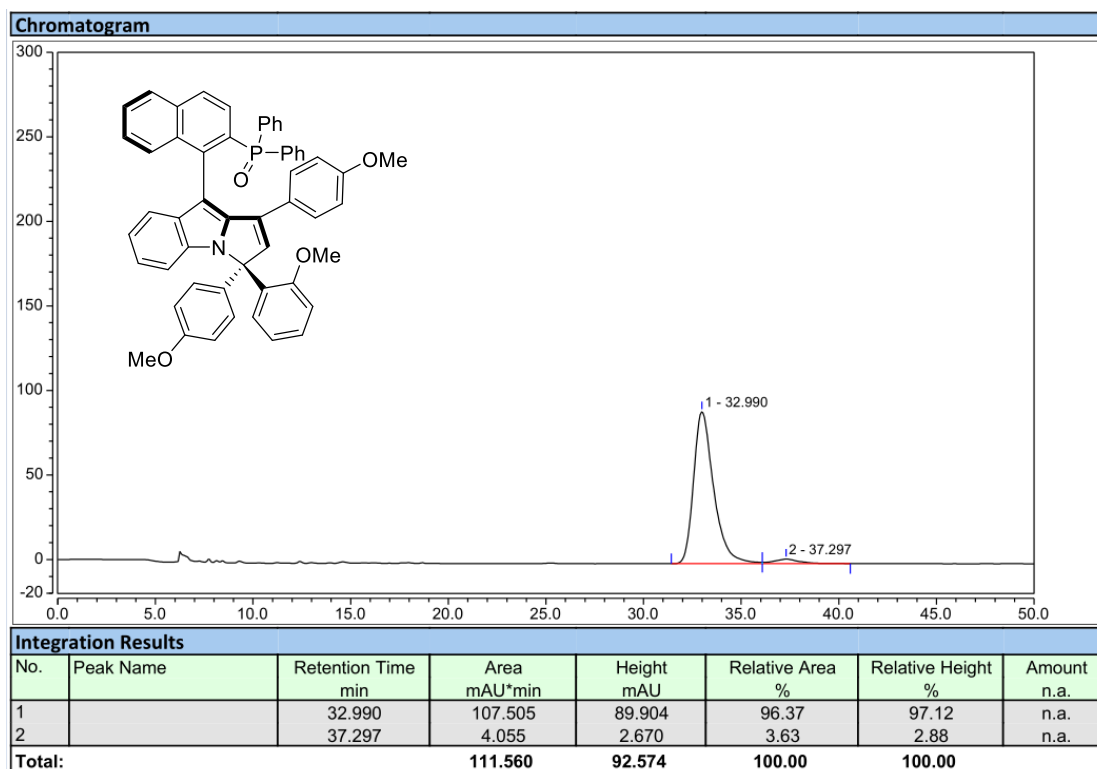


9b

Racemic:

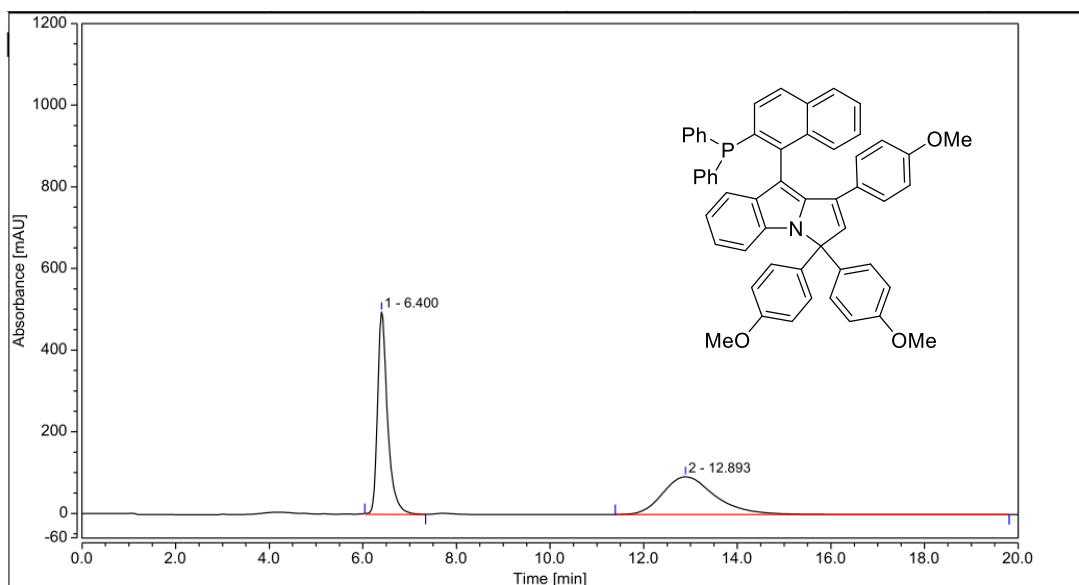


Enantioselective:



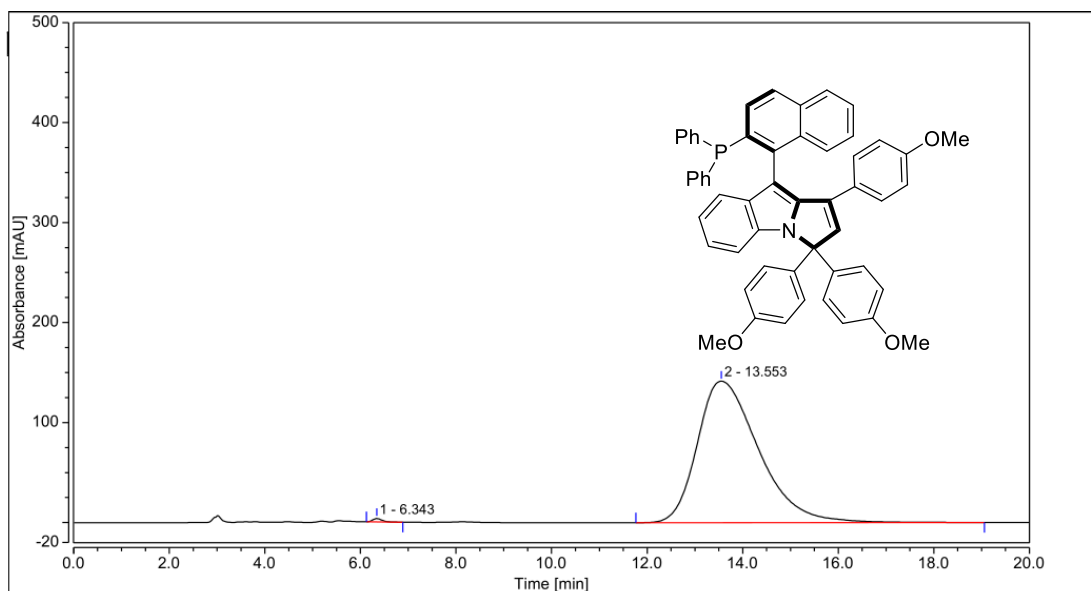
10a

Racemic:



Integration Results							
No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount
1		6.400	123.650	495.505	50.68	84.28	n.a.
2		12.893	120.328	92.413	49.32	15.72	n.a.
Total:			243.978	587.918	100.00	100.00	

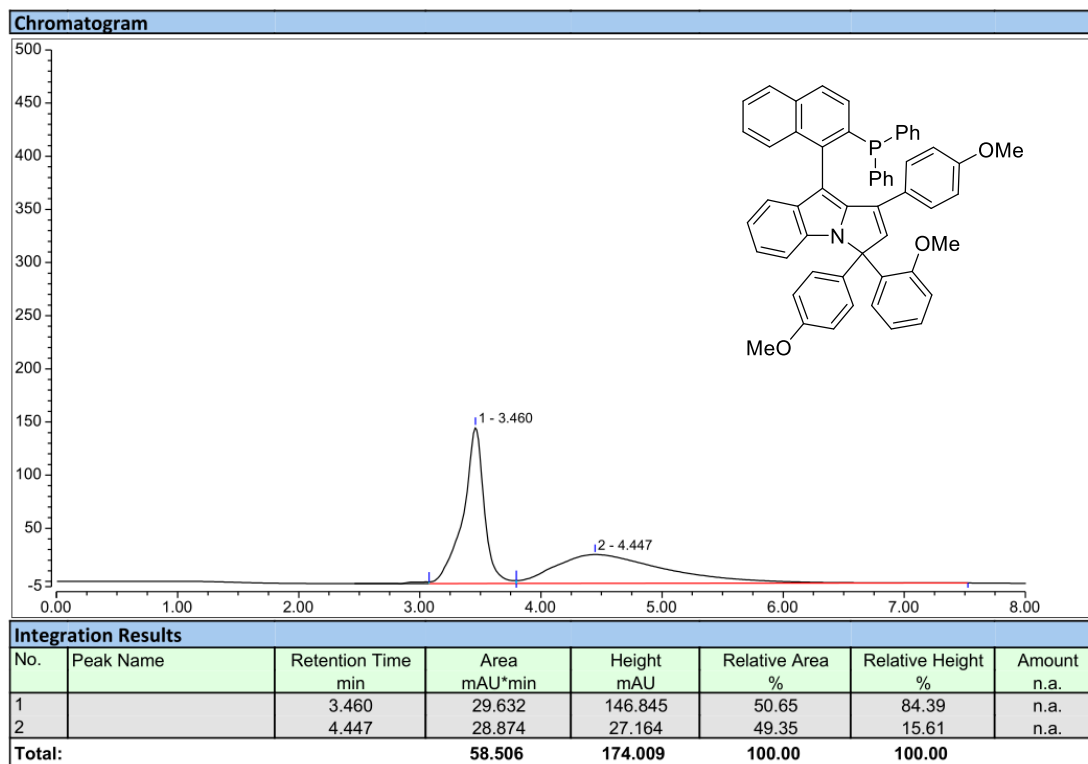
Enantioselective:



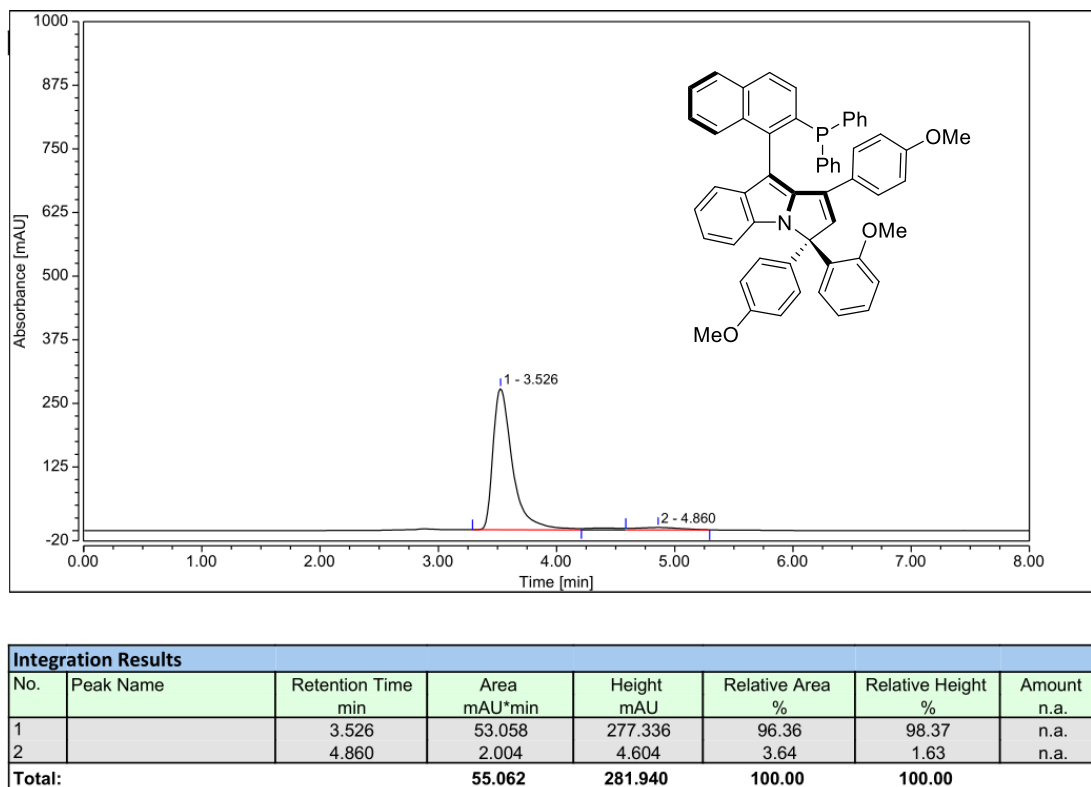
Integration Results							
No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount
1		6.343	0.768	3.413	0.36	2.36	n.a.
2		13.553	210.463	141.467	99.64	97.64	n.a.
Total:			211.231	144.880	100.00	100.00	

10b

Racemic:

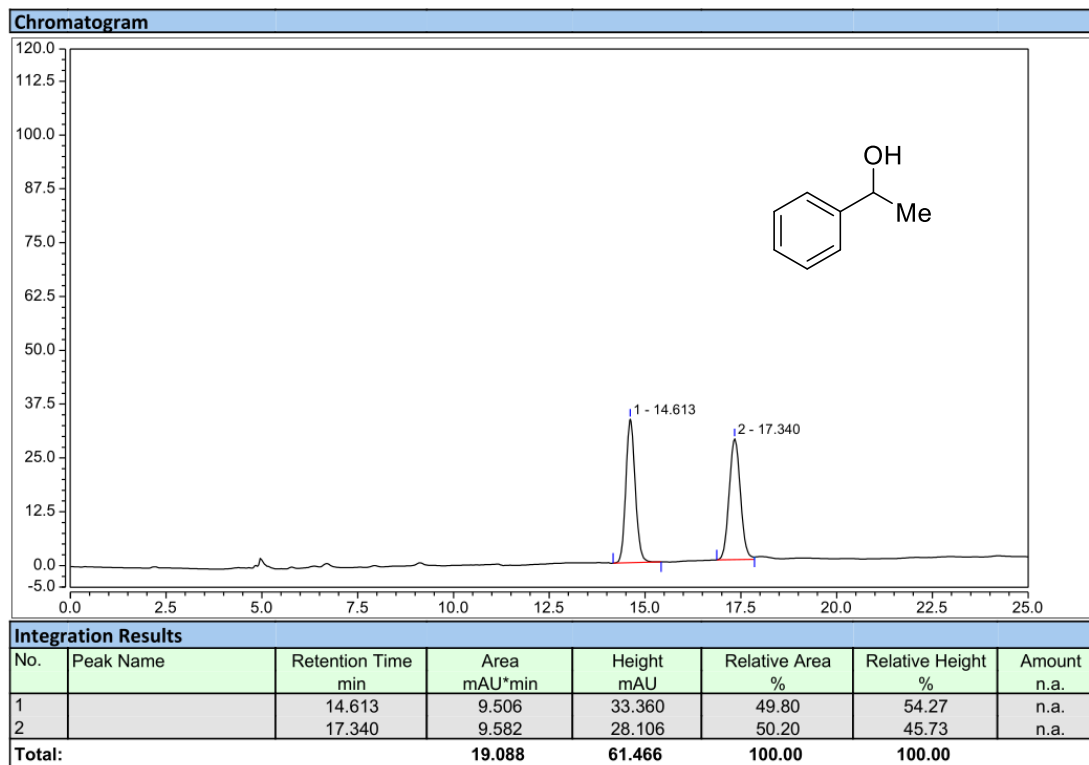


Enantioselective:

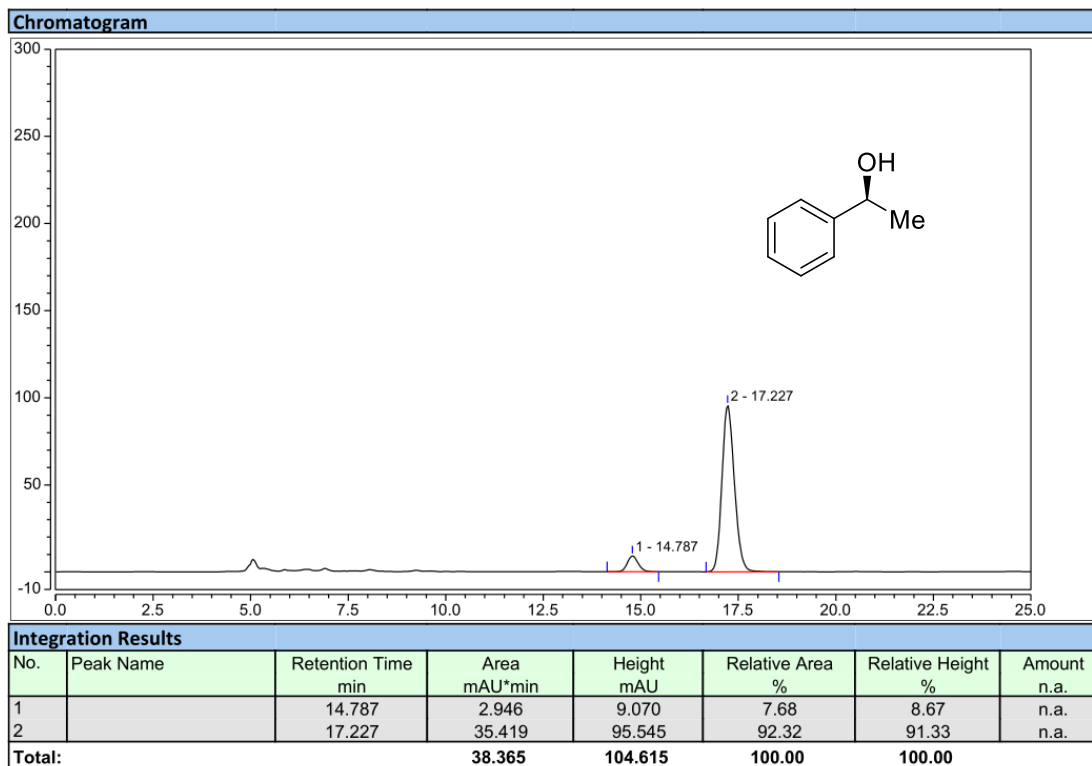


13

Racemic:

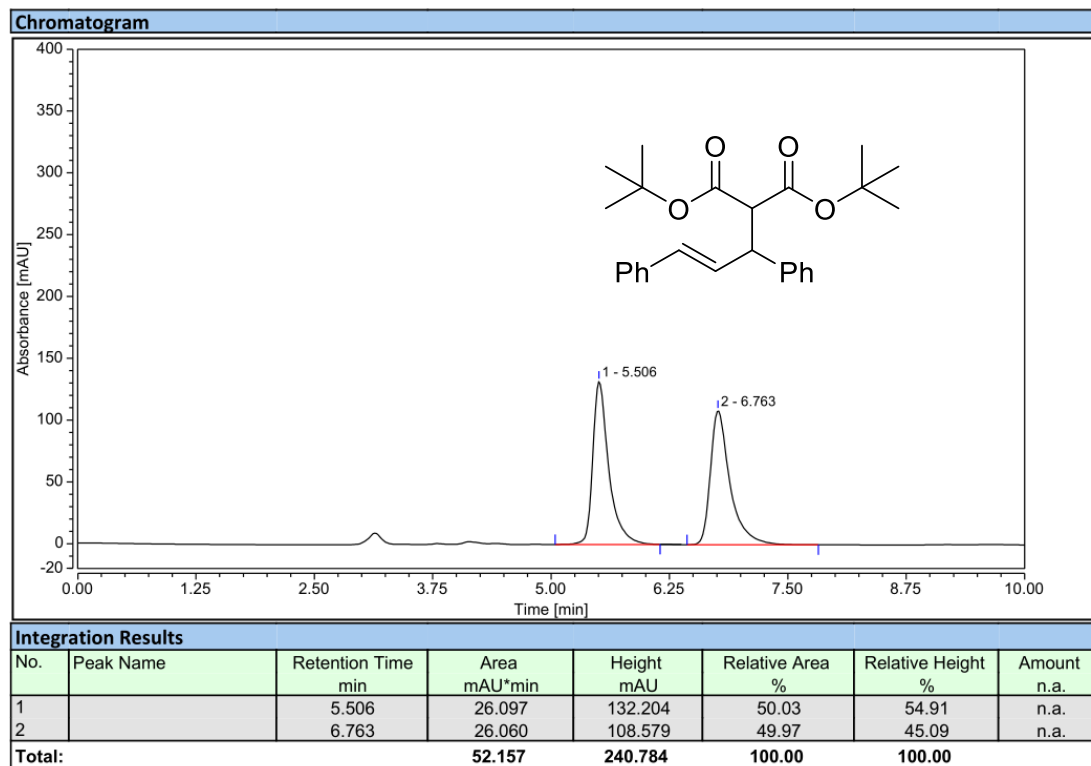


Enantioselective:

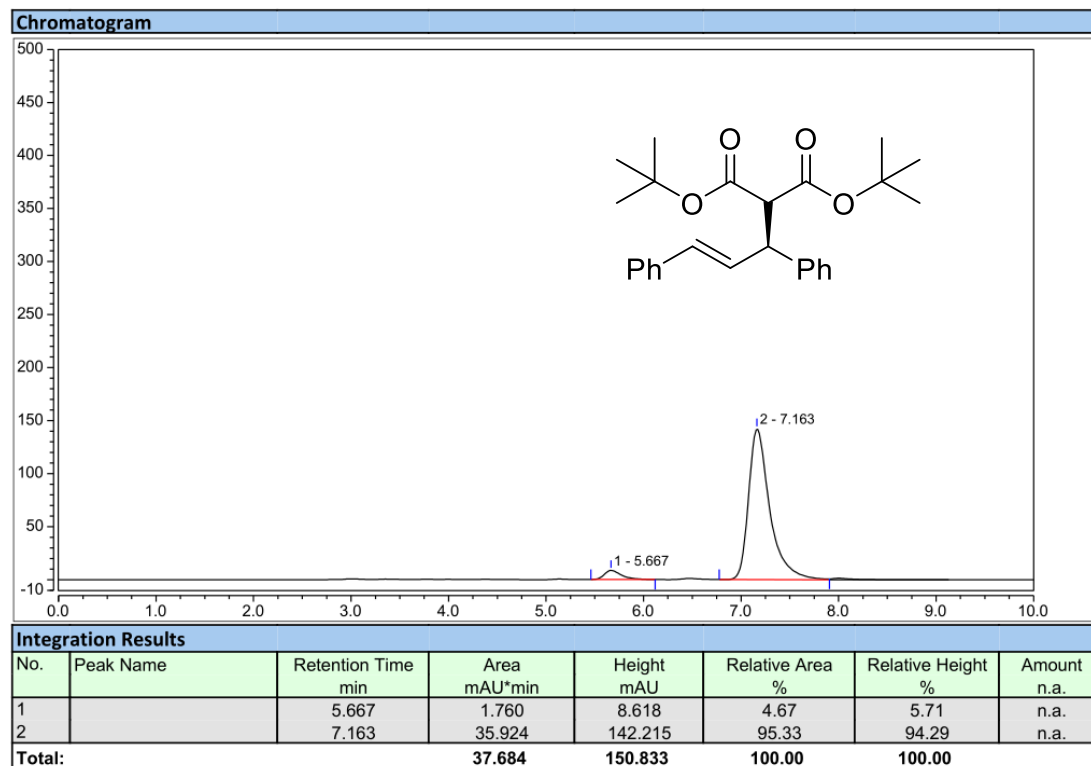


16

Racemic:

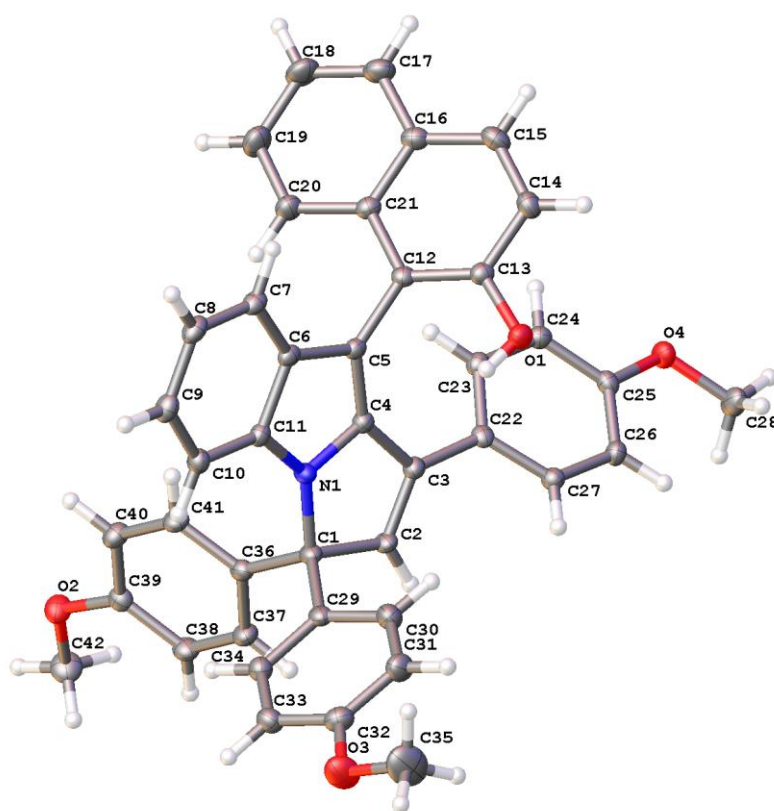
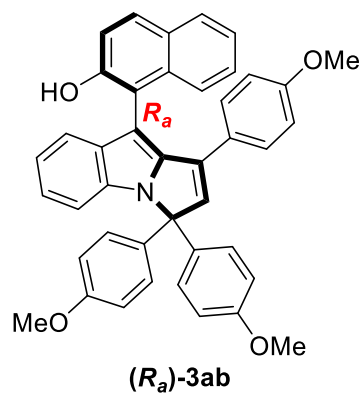


Enantioselective:



10. X-ray single-crystal data for products 3ab and 7ah

Compound 3ab:



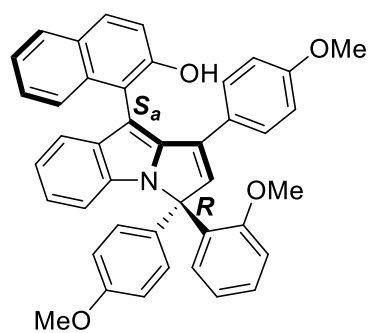
The single-crystal of **3ab** was grown from the mixed solution of dichloromethane and petrol ether (V/V = 1:2).

The X-ray source used for the single crystal X-ray diffraction analysis was GaK α ($\lambda = 1.34139$), and the thermal ellipsoid was drawn at the 30% probability level.

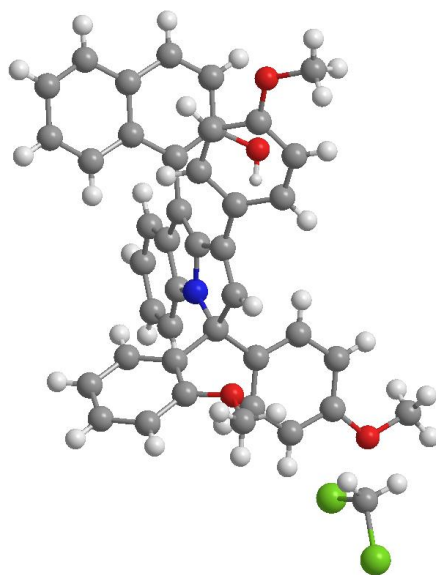
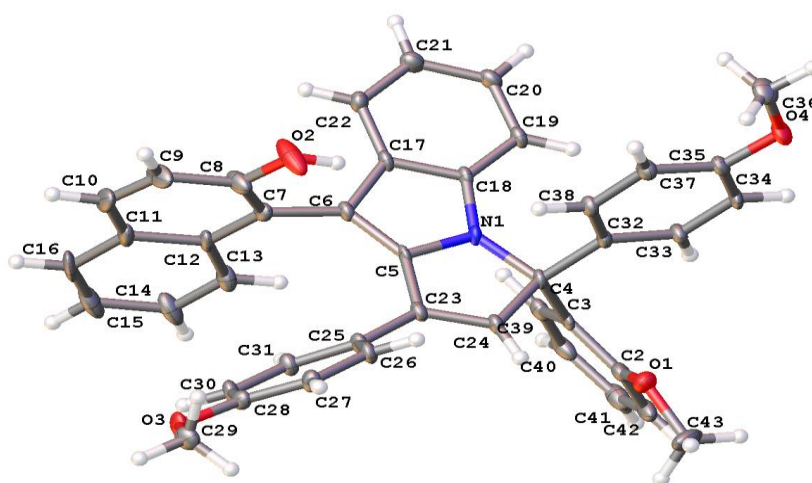
Identification code	201201sf_0m
Empirical formula	C ₄₂ H ₃₃ N O ₄
Formula weight	615.69
Temperature	181.01 K

Wavelength	1.34139 Å	
Crystal system	Orthorhombic	
Space group	P2 ₁ 2 ₁ 2 ₁	
Unit cell dimensions	a = 12.5522(3) Å	= 90°.
	b = 14.1223(4) Å	= 90°.
	c = 18.6257(5) Å	= 90°.
Volume	3301.70(15) Å ³	
Z	4	
Density (calculated)	1.239 Mg/m ³	
Absorption coefficient	0.404 mm ⁻¹	
F(000)	1296	
Crystal size	0.09 x 0.08 x 0.06 mm ³	
Theta range for data collection	3.417 to 54.962 °	
Index ranges	-15<=h<=15, -17<=k<=16, -22<=l<=20	
Reflections collected	36416	
Independent reflections	6264 [R(int) = 0.0473]	
Completeness to theta = 53.594 °	99.8 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7508 and 0.6698	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	6264 / 0 / 428	
Goodness-of-fit on F ²	1.066	
Final R indices [I>2sigma(I)]	R1 = 0.0356, wR2 = 0.0779	
R indices (all data)	R1 = 0.0441, wR2 = 0.0831	
Absolute structure parameter	0.09(10)	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.133 and -0.172 e.Å ⁻³	

Compound 7ah:



(S_a,R)-7ah



(with CH₂Cl₂)

The single-crystal of **7ah** was grown from the mixed solution of dichloromethane and petrol ether (V/V = 1:2).

The X-ray source used for the single crystal X-ray diffraction analysis was GaK α ($\lambda = 1.34139$), and the thermal ellipsoid was drawn at the 30% probability level.

Identification code	210317sf_0m
Empirical formula	C43 H35 Cl2 N O4
Formula weight	700.62
Temperature	173.0 K
Wavelength	1.34139 Å
Crystal system	Monoclinic
Space group	P 1 21 1
Unit cell dimensions	a = 10.5890(4) Å = 90°. b = 11.6002(5) Å = 100.037(2)°. c = 14.4543(6) Å = 90°.
Volume	1748.31(12) Å ³
Z	2
Density (calculated)	1.331 Mg/m ³
Absorption coefficient	1.323 mm ⁻¹
F(000)	732
Crystal size	0.07 x 0.05 x 0.05 mm ³
Theta range for data collection	3.688 to 54.967 °
Index ranges	-12<=h<=12, -14<=k<=13, -17<=l<=17
Reflections collected	26306
Independent reflections	6603 [R(int) = 0.1098]
Completeness to theta = 53.594 °	99.8 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.7508 and 0.3587
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	6603 / 1 / 455
Goodness-of-fit on F ²	1.015
Final R indices [I>2sigma(I)]	R1 = 0.0602, wR2 = 0.1475
R indices (all data)	R1 = 0.0675, wR2 = 0.1564
Absolute structure parameter	0.034(14)
Extinction coefficient	n/a
Largest diff. peak and hole	0.415 and -0.517 e.Å ⁻³

11. Theoretical calculations on the rotational barrier and reaction pathway

Computational Methods: The DFT calculations were performed by using the Gaussian 16 package.¹⁰ The geometry optimizations of minima and transition states were carried out at the B3LYP-D3¹¹ with a Becke–Johnson (BJ)¹² damping function and the 6-31G(d,p)¹³ (6-31G* for rotational barriers) basis set. The vibrational frequencies were computed at the same level to check whether each optimized structure is an energy minimum (zero imaginary frequency) or a transition state (one imaginary frequency) and to evaluate its zero-point vibration energy (ZPE) and thermal corrections at 298 K in kcal·mol⁻¹. The single-point energies and solvent effects were computed with the dispersion-corrected density functional method B3LYP-D3 with a Becke–Johnson (BJ) damping function and the 6-311+G (d,p) basis set using the SMD solvation model.¹⁴ DFT-optimized structures are illustrated using CYLView.¹⁵

Theoretical calculations on the rotational barriers of **3ab**, **7ad** and **10a**:

As shown in **Fig. S1**, there are two transition states account for the interconversion of the two enantiomers of compounds **3ab**, **7ad** and **10a** according to the rotation direction of the chiral axis. In this study, both **TS-cis** and **TS-trans** of these compounds have been considered. The rotational barriers of compounds **3ab**, **7ad** and **10a** were calculated to be 35.15, 32.93 and 37.70 kcal·mol⁻¹. The calculated electronic energies, enthalpies and free energies are listed in **Table S3**. The calculated structures of **3ab**, **10a** and **7ad** are shown in **Fig. S2**.

¹⁰ In Gaussian 16, rev. C.01.

¹¹ a) S. Grimme, J. Antony, S. Ehrlich, H. Krieg, *J. Chem. Phys.* **2010**, *132*, 154104; b) C. Lee, W. Yang, R. G. Parr, *Phys. Rev. B*, **1988**, *37*, 785.

¹² a) T. Korona, M. Przybytek, B. Jeziorski, *Mol. Phys.* **2006**, *104*, 2303; b) S. Grimme, S. Ehrlich, L. Goerigk, *J. Comput. Chem.* **2011**, *32*, 1456.

¹³ a) A. V. Marenich, C. J. Cramer, D. G. Truhlar, *Theory Comput.* **2009**, *5*, 2447; b) A. V. Marenich, C. J. Cramer, D. G. Truhlar, *J. Phys. Chem. B*, **2009**, *113*, 6378.

¹⁴ a) H. Puthoff, *Phys. Rev. A*, **1989**, *40*, 4857; b) A. V. Marenich, C. J. Cramer, D. G. Truhlar, *J. Phys. Chem. B*, **2009**, *113*, 4538.

¹⁵ C. Y. Legault, CYLView, 1.0b, Universit e de Sherbrook, **2009**; www.cylview.org.

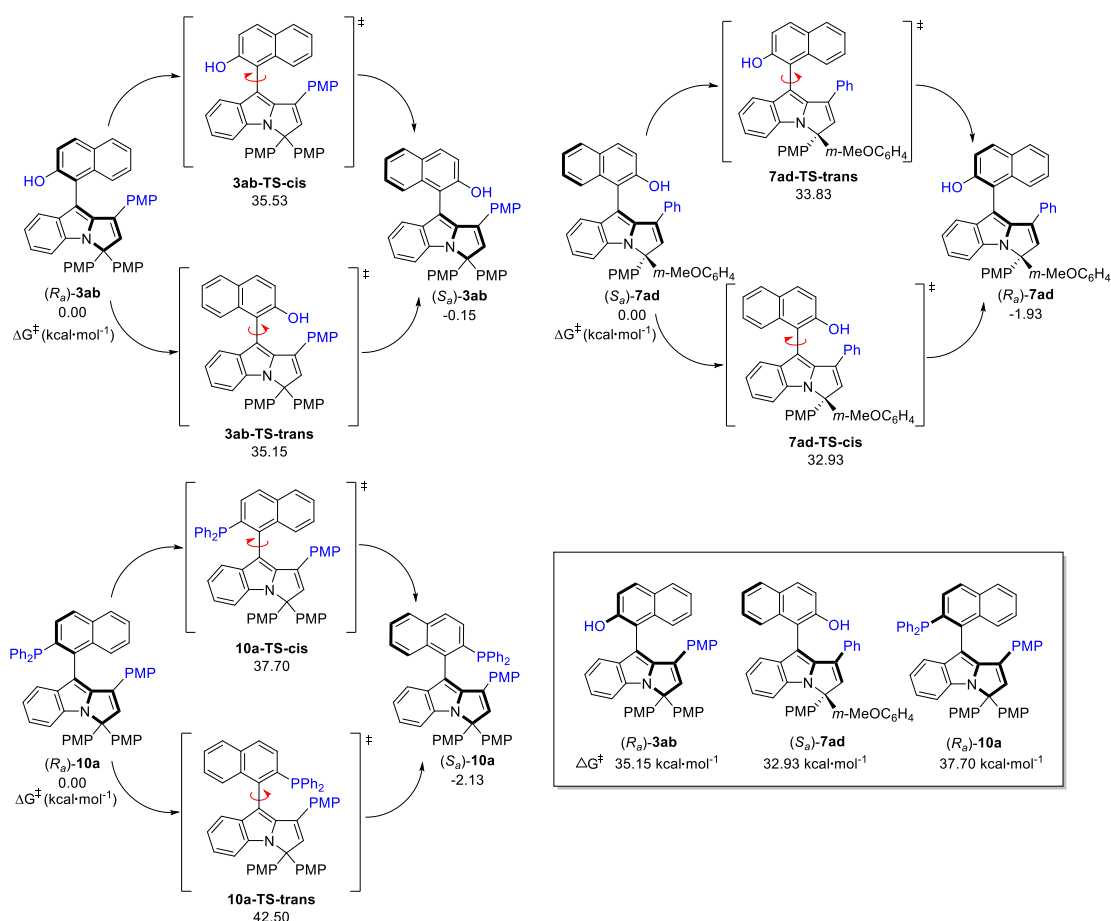


Fig. S1 Calculated rotational barriers of **3ab**, **7ad** and **10a**

Table S3. Electronic energies, enthalpies and free energies (in hartrees) computed at the level of B3LYP-D3(BJ)-SMD (**10a**: *o*-xylene, **3ab** and **7ad**: 2-propanol) /6-311+G(d,p)//B3LYP-D3(BJ)/6-31G(d)

Structure	ZPE	$\Delta H_{0 \rightarrow T}$	$\Delta G_{0 \rightarrow T}$	E	H	G	Imaginary Frequency
(R_a)-3ab	0.644707	0.684496	0.570186	-1976.722091	-1976.037595	-1976.151905	
3ab-TS-cis	0.644611	0.683176	0.57408	-1976.669361	-1975.986185	-1976.095281	-26.20i
3ab-TS-trans	0.64407	0.682875	0.572341	-1976.668235	-1975.98536	-1976.095894	-31.33i
(S_a)-3ab	0.644457	0.684264	0.570326	-1976.722466	-1976.038202	-1976.15214	
(R_a)-10a	0.814588	0.864717	0.728188	-2705.735016	-2704.870299	-2705.006828	
10a-TS-cis	0.813311	0.862563	0.727493	-2705.674244	-2704.811681	-2704.946751	-12.86i
10a-TS-trans	0.813466	0.862581	0.728757	-2705.667863	-2704.805282	-2704.939106	-13.50i
(S_a)-10a	0.814316	0.864562	0.726595	-2705.736821	-2704.872259	-2705.010226	
(S_a)-7ad	0.611353	0.648716	0.540778	-1862.15352	-1861.504804	-1861.612742	
7ad-TS-trans	0.610918	0.647217	0.54308	-1862.101907	-1861.45469	-1861.558827	-27.23i
7ad-TS-cis	0.611093	0.64734	0.542521	-1862.10278	-1861.45544	-1861.560259	-34.37i
(R_a)-7ad	0.611846	0.649068	0.540667	-1862.15649	-1861.507422	-1861.615823	

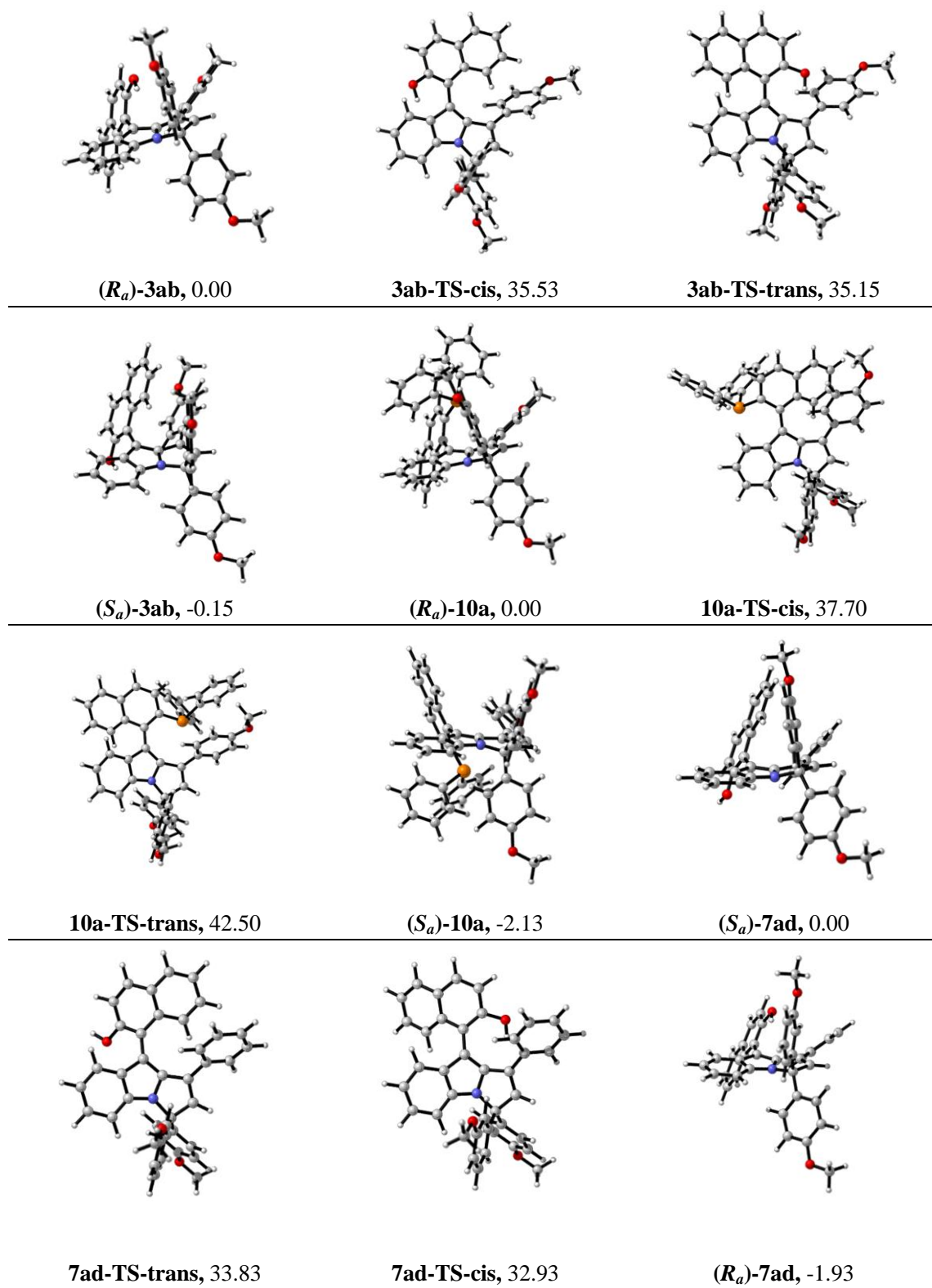


Fig. S2. The calculated structures of **3ab**, **10a** and **7ad**. The relative free energies (G_g , 298.15 K) are in kcal/mol.

Theoretical calculations on the reaction pathway:

To provide an in-depth understanding of the CPA-catalyzed asymmetric (2+3) cyclization for the construction of axially chiral aryl-pyrroloindole scaffolds, we performed theoretical calculations of the possible reaction pathway and activation mode for the synthesis of product (*R_a*)-**3ab**. The optimal reaction pathway is illustrated **Fig. S3**, thus providing an in-depth understanding of the reaction mechanism and the process of dynamic kinetic resolution for the construction of axially chiral aryl-pyrroloindole scaffolds. The calculated electronic energies, enthalpies and free energies are listed in **Table S4**. The calculated structures of substrates, intermediates and transition states are shown in **Fig. S4**.

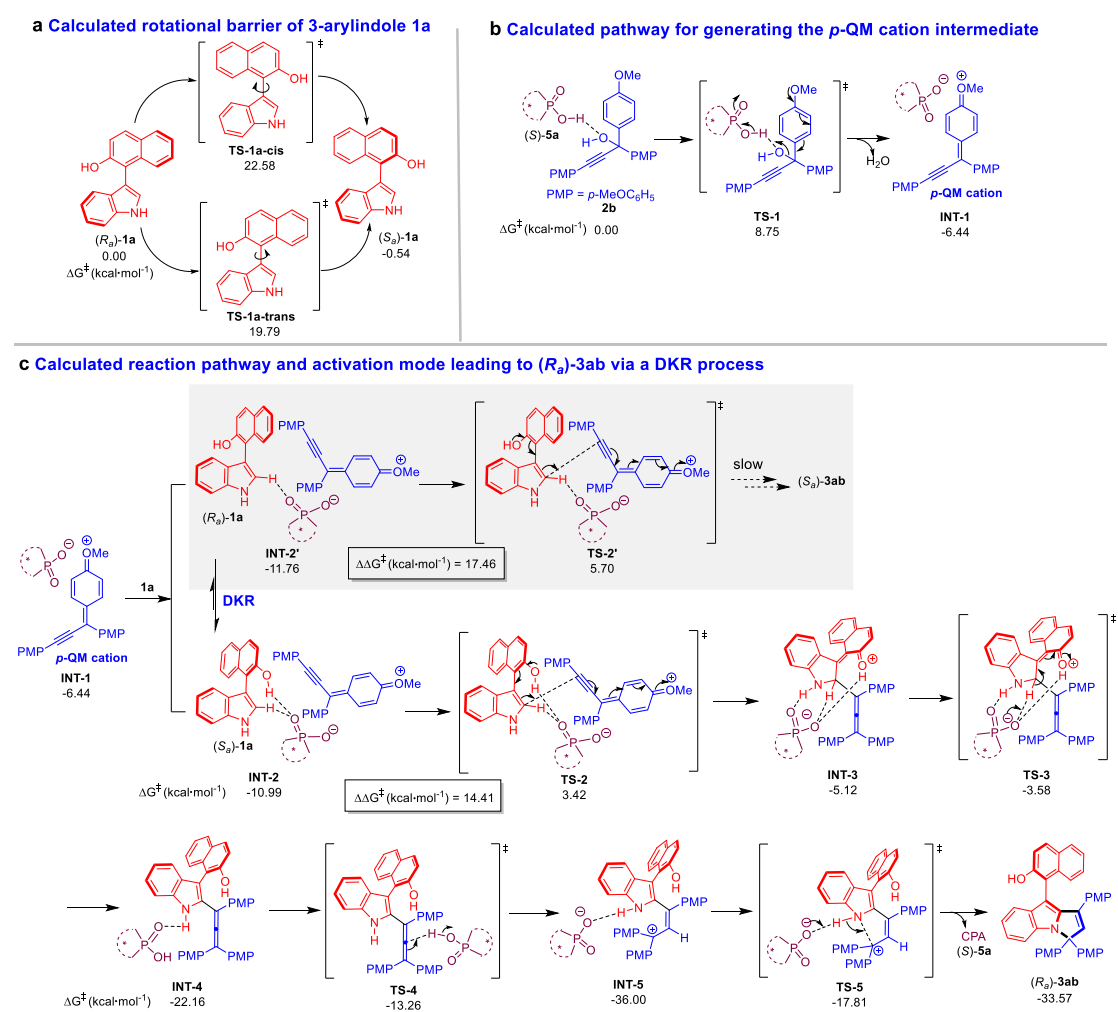
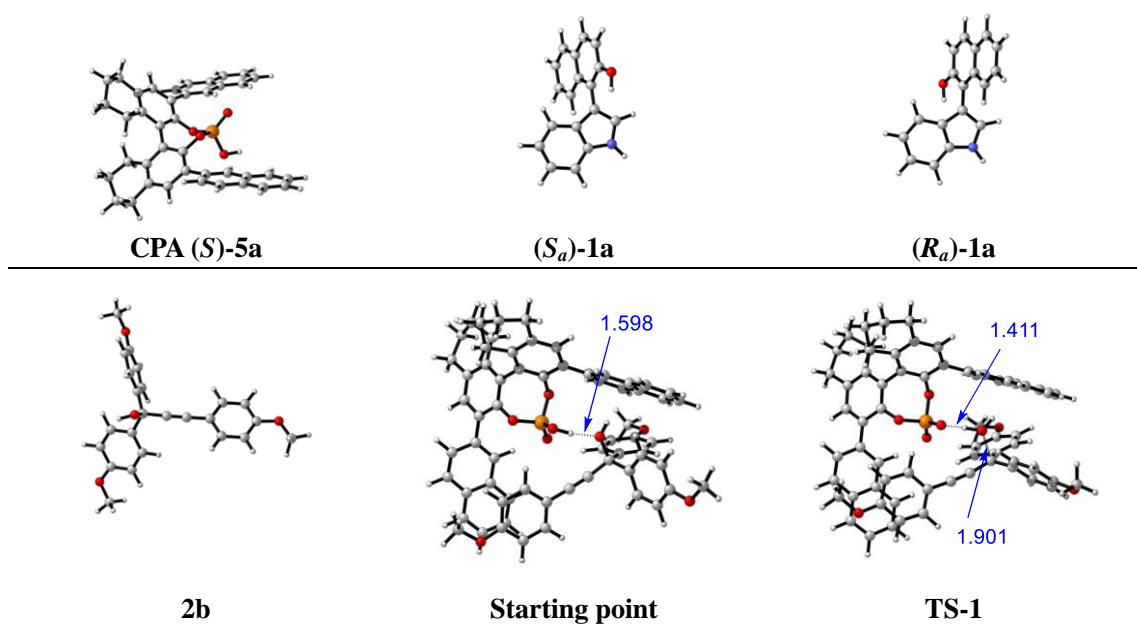
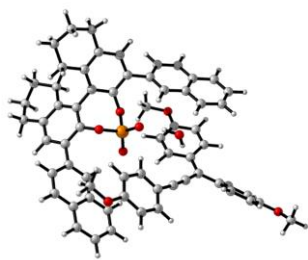


Table S4. Electronic energies, enthalpies and free energies (in hartrees) computed at the level of B3LYP-D3(BJ)-SMD(dichloro-methane)/6-311+G(d,p)//B3LYP-D3(BJ)/6-31G(d,p)

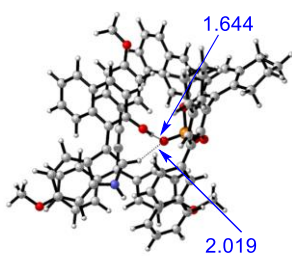
Structure	ZPE	$\Delta H_{0 \rightarrow T}$	$\Delta G_{0 \rightarrow T}$	E	H	G	Imaginary Frequency
CPA (S)-5a	0.633111	0.669494	0.56528	-2187.274838	-2186.605344	-2186.709558	
(S _a)-1a	0.262697	0.278286	0.220851	-824.059974	-823.781688	-823.839123	
(R _a)-1a	0.262646	0.278256	0.220801	-824.05906	-823.780804	-823.838259	
2b	0.402914	0.430004	0.34263	-1229.0641	-1228.634096	-1228.72147	
H ₂ O	0.021364	0.025143	0.003707	-76.467093	-76.44195	-76.463386	
Start point	1.039352	1.102227	0.940509	-3416.38247	-3415.280243	-3415.441961	
TS-1	1.036156	1.099073	0.935652	-3416.363673	-3415.2646	-3415.428021	-244.01i
INT-1	1.038023	1.10237	0.937362	-3416.389579	-3415.287209	-3415.452217	
INT-2	1.277368	1.354393	1.164286	-4163.999503	-4162.64511	-4162.835217	
TS-2	1.276099	1.352533	1.161515	-4163.973756	-4162.621223	-4162.812241	-404.69i
INT-3	1.277209	1.353474	1.164101	-4163.989957	-4162.636483	-4162.825856	
TS-3	1.274454	1.350104	1.163361	-4163.986757	-4162.636653	-4162.823396	-259.06i
INT-4	1.278018	1.354928	1.163119	-4164.016133	-4162.661205	-4162.853014	
TS-4	1.272856	1.349214	1.159432	-4163.998257	-4162.649043	-4162.838825	-1219.76i
INT-5	1.279977	1.35613	1.166716	-4164.041785	-4162.685655	-4162.875069	
TS-5	1.27693	1.352173	1.166029	-4164.012104	-4162.659931	-4162.846075	-268.47i
(R _a)-3ab	0.643468	0.683356	0.568323	-1976.729963	-1976.046607	-1976.16164	
INT-2'	1.277668	1.355212	1.162248	-4163.998686	-4162.643474	-4162.836438	
TS-2'	1.276493	1.353356	1.162089	-4163.970702	-4162.617346	-4162.808613	-398.75i
TS-1a-trans	0.262433	0.277229	0.222653	-824.029368	-823.752139	-823.806715	-54.46i
TS-1a-cis	0.262418	0.277329	0.222229	-824.024506	-823.747177	-823.802277	-99.31i

Fig. S4. Quantum chemistry method-optimized structures (distances are shown in angstroms).

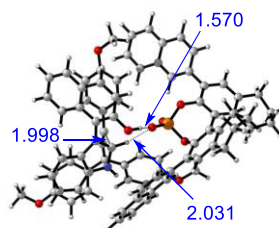




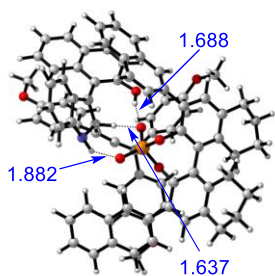
INT-1



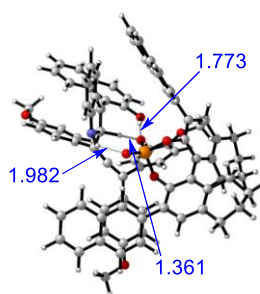
INT-2



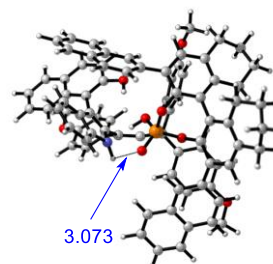
TS-2



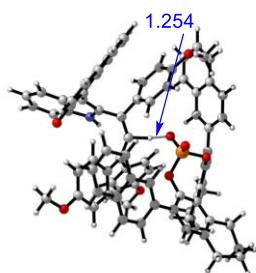
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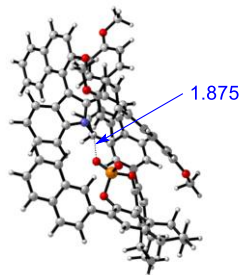
TS-3



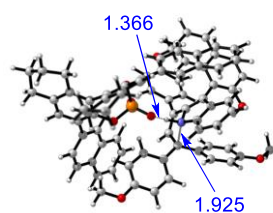
INT-4



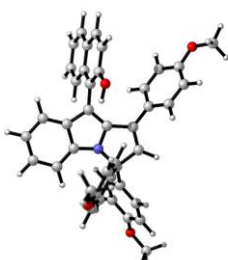
TS-4



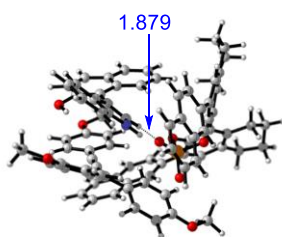
INT-5



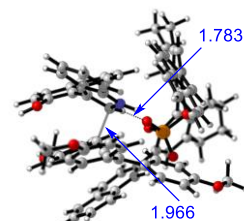
TS-5



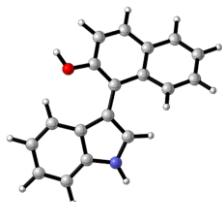
(*R_a*)-3ab



INT-2'



TS-2'



TS-1a-trans



TS-1a-cis

Cartesian coordinates of DFT-computed structures in calculation of rotational barriers:

(R_a)-3ab

E(RB3LYP) = -1976.722091 Hartree

Sum of electronic and thermal Free Energies = -1976.151905 Hartree

O	2.25775300	2.43119000	0.16166600
H	1.34270700	2.16583100	-0.04787600
O	-5.21003300	-4.84366800	0.29180100
O	-4.70355300	4.81516800	0.49135800
O	5.15320000	-0.74877000	4.09852500
N	-1.00179800	-0.10684600	-0.67887500
C	-1.93636600	-0.17844100	0.46225400
C	-0.93165400	-0.35085100	1.60057100
H	-1.26410800	-0.55428800	2.61032800
C	0.35180900	-0.28617000	1.17346600
C	0.32083600	-0.05250300	-0.26996400
C	1.13689600	0.30261900	-1.33215200
C	0.24474000	0.47507100	-2.46279300
C	0.46161500	0.81861000	-3.80516000
H	1.47129900	0.99353000	-4.16459400
C	-0.63315900	0.92909400	-4.65425600
H	-0.47921100	1.19599400	-5.69586000
C	-1.94304400	0.69987600	-4.18818800
H	-2.77778800	0.79585100	-4.87653700
C	-2.19187500	0.34959100	-2.86467500
H	-3.19888100	0.17144700	-2.50614600
C	-1.09118000	0.24002800	-2.01139600
C	2.59400900	0.53561900	-1.28749800
C	3.08073400	1.58568100	-0.51750700
C	4.46993600	1.82468000	-0.39197400
H	4.79386000	2.65314100	0.22916700
C	5.36581300	1.01499600	-1.04138400
H	6.43351000	1.19359900	-0.94271300
C	4.92568200	-0.06739200	-1.84917000
C	5.83856200	-0.91904900	-2.52112600
H	6.90305400	-0.72006000	-2.42094500
C	5.39405300	-1.97817400	-3.28031200
H	6.10380100	-2.62390400	-3.78937300
C	4.00668200	-2.22849100	-3.39189000
H	3.65848200	-3.06945100	-3.98541300
C	3.09270500	-1.41858000	-2.75404400
H	2.02996700	-1.61637800	-2.84245900
C	3.51898300	-0.31051700	-1.97328200

C	1.58233300	-0.40775500	1.96520200
C	2.71070400	-1.06615900	1.44272800
H	2.66546600	-1.50471500	0.45276300
C	3.88088100	-1.16550900	2.17653500
H	4.75514200	-1.66428100	1.77221200
C	3.95584900	-0.60902100	3.46151900
C	2.83972200	0.03962500	4.00304300
H	2.87518900	0.48391000	4.99051500
C	1.66951700	0.13569500	3.25070200
H	0.81607000	0.66755800	3.66196200
C	5.28388200	-0.19692000	5.39749800
H	5.13238300	0.89057700	5.38964100
H	6.30383200	-0.41764800	5.71664300
H	4.57591900	-0.65304200	6.10216400
C	-2.70518900	1.14807700	0.55093200
C	-2.06373500	2.28968300	1.03679100
H	-1.05353800	2.20915800	1.42668800
C	-2.69048600	3.53534200	1.03599100
H	-2.15923000	4.39675700	1.42276600
C	-3.99362000	3.65257600	0.53821600
C	-4.64821800	2.51551700	0.04796900
H	-5.65738900	2.62295300	-0.33620000
C	-4.00824400	1.28299100	0.05411000
H	-4.53103900	0.41287700	-0.32781000
C	-4.07202000	5.99775000	0.95413200
H	-3.16816200	6.22393200	0.37370100
H	-3.80768000	5.92343700	2.01728400
H	-4.79976000	6.79931200	0.81803000
C	-2.84061100	-1.40681000	0.39720300
C	-3.80871800	-1.60507500	1.38510400
H	-3.94428800	-0.85650100	2.16086900
C	-4.62160700	-2.73812800	1.39184400
H	-5.36263600	-2.85491800	2.17360900
C	-4.46920600	-3.70254400	0.38815000
C	-3.49966800	-3.51548400	-0.60443500
H	-3.39350000	-4.27194100	-1.37514000
C	-2.69392700	-2.38338800	-0.59452700
H	-1.94505200	-2.25578100	-1.36755400
C	-6.19977500	-5.07788700	1.27931400
H	-5.75866800	-5.15211400	2.28206500
H	-6.66515300	-6.02970600	1.01820600
H	-6.96282000	-4.28822400	1.28006600

3ab-TS-cis

E(RB3LYP) = -1976.669361 Hartree

Sum of electronic and thermal Free Energies = -1976.095281 Hartree

O	-1.62638300	-4.33371100	-1.27285600
H	-0.77252800	-3.92845900	-1.04730400
O	4.89270300	4.09701100	-2.65933400
O	4.61578100	-3.24528500	3.77508600
O	-4.65216300	4.66694300	0.88290900
N	0.96000500	-0.48506800	-0.50272500
C	1.81336100	0.35755400	0.35022600
C	0.73151000	1.19874300	0.99895600
H	0.97872200	2.10918600	1.52863900
C	-0.51421900	0.83388100	0.61363700
C	-0.40705500	-0.39093300	-0.22033000
C	-1.08225600	-1.43855000	-0.88525300
C	-0.05313900	-2.00302800	-1.78332100
C	-0.10829200	-2.81751800	-2.93516300
H	-1.05626200	-3.18469000	-3.30623200
C	1.06431200	-3.13834500	-3.60716100
H	1.01280100	-3.76729000	-4.49092300
C	2.31168300	-2.65004000	-3.17589500
H	3.21337100	-2.92588100	-3.71485200
C	2.39904100	-1.77917400	-2.09847000
H	3.34324000	-1.34099200	-1.80102100
C	1.20960300	-1.44206000	-1.44313200
C	-2.43125100	-2.05110900	-0.81297700
C	-2.61011600	-3.39224800	-1.20521900
C	-3.88339000	-3.90357500	-1.56832000
H	-3.91162400	-4.90981900	-1.97377900
C	-5.01360300	-3.15082600	-1.41628100
H	-5.98211800	-3.52463400	-1.73703700
C	-4.93414900	-1.91767300	-0.71725200
C	-6.10341300	-1.24057600	-0.29252700
H	-7.06575000	-1.61229300	-0.63671600
C	-6.03536000	-0.18162100	0.58752400
H	-6.94099700	0.31711900	0.92084200
C	-4.78197200	0.19706200	1.10629800
H	-4.71216800	0.96344000	1.87183200
C	-3.62856000	-0.41025700	0.65316900
H	-2.69037300	-0.16525200	1.11716000
C	-3.64517900	-1.42176800	-0.32908900
C	-1.64755300	1.77396200	0.74790800

C	-2.36950300	2.16164500	-0.39503700
H	-2.15444100	1.68209400	-1.34476000
C	-3.35365500	3.13144600	-0.31970400
H	-3.91704200	3.43152500	-1.19686300
C	-3.65608300	3.73562200	0.90996300
C	-2.94807400	3.36236000	2.05669900
H	-3.16262800	3.81226200	3.01868500
C	-1.94737800	2.39090100	1.96293000
H	-1.40412700	2.09791000	2.85701600
C	-5.01149000	5.28915700	2.10440000
H	-5.36286000	4.55484700	2.84144700
H	-5.82350700	5.97721600	1.86381200
H	-4.17189300	5.85319600	2.53204000
C	2.59064900	-0.54398600	1.31691300
C	1.96701100	-1.02627200	2.46831000
H	0.96043200	-0.69512500	2.70379400
C	2.60307900	-1.93013300	3.31965700
H	2.08579800	-2.28006000	4.20505900
C	3.89710600	-2.36910100	3.01767500
C	4.53478400	-1.89294400	1.86456300
H	5.53783400	-2.24334400	1.64422300
C	3.88596900	-0.99540200	1.02775700
H	4.39953200	-0.63248800	0.14427100
C	4.00146300	-3.77692600	4.93755600
H	3.08945500	-4.33559100	4.69020400
H	3.75493100	-2.98736200	5.65959100
H	4.73290800	-4.45522700	5.37970100
C	2.69213100	1.31047300	-0.46235500
C	3.72276100	2.01765600	0.16142300
H	3.94689400	1.82867900	1.20684200
C	4.48392400	2.95874900	-0.53260400
H	5.27925500	3.48238400	-0.01587400
C	4.21073500	3.20827800	-1.88234900
C	3.17009400	2.51495500	-2.51401300
H	2.96736300	2.72276500	-3.55947000
C	2.41794300	1.58555400	-1.80859500
H	1.61013800	1.06495200	-2.30939400
C	5.95230500	4.82519600	-2.06146800
H	5.59479900	5.44719900	-1.23030500
H	6.35515700	5.46744400	-2.84620900
H	6.74350100	4.15732900	-1.69608500

3ab-TS-trans

E(RB3LYP) = -1976.668235 Hartree

Sum of electronic and thermal Free Energies = -1976.095894 Hartree

O	-3.23295000	1.05915900	1.24107000
H	-2.30920600	0.89568400	1.48281500
O	4.88217800	0.75448700	-4.58654100
O	4.58496400	-1.16689800	4.96186800
O	-3.67434300	5.85601300	-0.52477000
N	0.69303900	-0.59276400	-0.07613100
C	1.80915000	0.31735800	0.20002300
C	1.02036000	1.59208500	0.42831600
H	1.50674700	2.55544400	0.49845700
C	-0.31872200	1.40072000	0.35133000
C	-0.57324900	-0.04466400	0.13442800
C	-1.54844700	-1.03736700	-0.13499400
C	-0.78708100	-2.10178200	-0.81531800
C	-1.14186000	-3.18694500	-1.64188900
H	-2.17956500	-3.40032800	-1.85659700
C	-0.15070300	-3.98010800	-2.20472300
H	-0.43780400	-4.81049400	-2.84323400
C	1.21364100	-3.72275000	-1.97410300
H	1.96703100	-4.36808500	-2.41654500
C	1.60894100	-2.62319000	-1.22567700
H	2.65370400	-2.36969100	-1.09304500
C	0.60033400	-1.80886900	-0.69801000
C	-2.98728600	-1.12087300	0.18179400
C	-3.75520400	-0.04812800	0.65341000
C	-5.16693900	-0.02583900	0.54775900
H	-5.66705300	0.90188800	0.80659100
C	-5.85129500	-1.13525600	0.13446600
H	-6.93062700	-1.11394100	0.01229900
C	-5.15588700	-2.36604200	0.00037200
C	-5.86775000	-3.58577300	-0.12324400
H	-6.94563600	-3.53879900	-0.25910000
C	-5.22885800	-4.79924000	-0.00631600
H	-5.78779400	-5.72770300	-0.07952800
C	-3.84803400	-4.81911600	0.27960300
H	-3.34695600	-5.76436600	0.46927500
C	-3.12397200	-3.64638700	0.34134300
H	-2.07408700	-3.69268300	0.59389600
C	-3.72611000	-2.37879400	0.12222500
C	-1.24124200	2.54681500	0.20196100

C	-2.12332600	2.60421200	-0.89261800
H	-2.18974400	1.75438200	-1.56541800
C	-2.91328000	3.71843800	-1.10898200
H	-3.59669300	3.77071600	-1.95014200
C	-2.84895900	4.81097900	-0.22904200
C	-1.97772600	4.77049800	0.86248300
H	-1.91436000	5.59724500	1.55971500
C	-1.18071500	3.64079700	1.06523000
H	-0.51160900	3.60733100	1.92054800
C	-3.65938100	6.97759900	0.34151500
H	-3.95550200	6.70141500	1.36210900
H	-4.38471500	7.68293600	-0.06739800
H	-2.66878800	7.45069700	0.37074600
C	2.56373500	-0.08674400	1.46973500
C	3.46870800	0.80845300	2.04654500
H	3.64499300	1.77220100	1.57702000
C	4.16890200	0.49107300	3.21019100
H	4.86228900	1.21211500	3.62632600
C	3.95990700	-0.75024100	3.82336400
C	3.05297800	-1.65330800	3.25634900
H	2.90069900	-2.61058900	3.74408700
C	2.36465100	-1.32275600	2.09498500
H	1.66560400	-2.03520100	1.67283600
C	5.50444900	-0.28040500	5.57667600
H	5.01781700	0.65411600	5.88569100
H	6.34432300	-0.04451400	4.90971100
H	5.87951800	-0.80136300	6.45905200
C	2.70613600	0.44746200	-1.03819500
C	4.05717000	0.11079300	-1.04011300
H	4.52937100	-0.23530700	-0.12777600
C	4.82571100	0.19890600	-2.20573000
H	5.87339500	-0.07479600	-2.16956300
C	4.23291400	0.63081500	-3.39450300
C	2.87070100	0.96988600	-3.40436000
H	2.42439200	1.29756300	-4.33749800
C	2.12429200	0.87759400	-2.24199300
H	1.06892700	1.13149900	-2.26221700
C	6.25556800	0.40538200	-4.63259100
H	6.85396400	1.03727800	-3.96307200
H	6.57258100	0.56921100	-5.66374300
H	6.41139300	-0.64833800	-4.36659900

(S₀)-3ab

E(RB3LYP) = -1976.722466 Hartree

Sum of electronic and thermal Free Energies = -1976.15214 Hartree

O	-2.21091600	-2.13410900	3.24650300
H	-1.27847300	-1.87555400	3.12934100
O	6.05938000	-4.09919700	-0.58149700
O	3.67794300	5.25684200	-1.07500900
O	-5.63165600	-1.72366700	-2.52746900
N	1.15654700	-0.18995800	0.75319100
C	1.94560800	-0.15229300	-0.49647500
C	0.86319700	-0.57505700	-1.49569600
H	1.10202800	-0.74499600	-2.53766400
C	-0.34091400	-0.74307500	-0.90435100
C	-0.18243100	-0.42906600	0.51037800
C	-0.93693500	-0.17466500	1.64017400
C	0.01762400	0.24271400	2.65083800
C	-0.11407200	0.62025100	3.99655700
H	-1.09297000	0.62059200	4.46791000
C	1.02222500	0.99867700	4.70204400
H	0.93232700	1.29579900	5.74292300
C	2.29153700	1.00696300	4.09064700
H	3.15912500	1.31169900	4.66864800
C	2.45933300	0.63243000	2.76060000
H	3.43524700	0.64052900	2.28889000
C	1.31897200	0.25124500	2.05065800
C	-2.40783800	-0.26968500	1.73689400
C	-2.97180600	-1.27830600	2.50648300
C	-4.36855600	-1.50587600	2.51733500
H	-4.75305100	-2.31864200	3.12483800
C	-5.19304700	-0.72916100	1.74307100
H	-6.26339400	-0.91773200	1.72793300
C	-4.67467600	0.32924800	0.95126200
C	-5.51493600	1.13399900	0.14074900
H	-6.58153100	0.92230100	0.13060700
C	-4.99744800	2.16198400	-0.61489200
H	-5.65149500	2.77548900	-1.22846600
C	-3.60948300	2.43068600	-0.57534900
H	-3.20523500	3.25389600	-1.15856000
C	-2.76605100	1.65916400	0.19184100
H	-1.70246800	1.87114400	0.21885800
C	-3.26460400	0.57865100	0.96706500
C	-1.65078100	-1.09912600	-1.47007000

C	-2.45348000	-2.06025100	-0.83016000
H	-2.05094400	-2.61831900	0.00876300
C	-3.76302800	-2.27055600	-1.22568300
H	-4.39896800	-2.98308400	-0.71222800
C	-4.31170900	-1.50471100	-2.26423900
C	-3.51337800	-0.57987900	-2.94413800
H	-3.91675500	0.01965300	-3.75084300
C	-2.19175500	-0.38675200	-2.54166200
H	-1.59103000	0.37488200	-3.03034800
C	-6.27967700	-0.83233300	-3.41980100
H	-6.17888100	0.20633800	-3.07981500
H	-7.33290200	-1.11874000	-3.41863400
H	-5.88427300	-0.92038800	-4.44054500
C	2.42700800	1.28744500	-0.72730200
C	1.51119400	2.26557700	-1.12179800
H	0.48458600	1.98092100	-1.33056000
C	1.88279500	3.60302600	-1.25079900
H	1.14321600	4.33176400	-1.56050900
C	3.20255400	3.98290300	-0.97826700
C	4.12919400	3.01267800	-0.57731800
H	5.14719900	3.32350100	-0.36615400
C	3.74179100	1.68449000	-0.45238200
H	4.47361800	0.94681600	-0.14166600
C	2.77017000	6.27696200	-1.45736600
H	1.94232400	6.36740700	-0.74209000
H	2.36119300	6.09668200	-2.46030800
H	3.34595500	7.20383100	-1.46343800
C	3.07076600	-1.18373300	-0.50489200
C	3.91387300	-1.27522500	-1.61550400
H	3.79227900	-0.57768000	-2.43958000
C	4.92452200	-2.23326500	-1.68638700
H	5.55902300	-2.27187800	-2.56364000
C	5.10383500	-3.12701200	-0.62336500
C	4.26345300	-3.04546800	0.49331600
H	4.41537200	-3.74463800	1.30910400
C	3.25782600	-2.08778100	0.54677900
H	2.61268300	-2.04068500	1.41631000
C	6.92785700	-4.22543200	-1.69493300
H	6.37342700	-4.45786100	-2.61370400
H	7.59954700	-5.05240900	-1.45914900
H	7.51699800	-3.31218600	-1.85195400

(R_a)-10a

E(RB3LYP) = -2705.735016 Hartree

Sum of electronic and thermal Free Energies = -2705.006828 Hartree

O	7.41204100	-3.43394400	-0.48939600
O	3.27769700	5.27552900	-1.51630600
O	-4.07113900	-3.90958700	-3.12785200
N	1.86798700	-0.39908700	0.58482700
C	2.63054700	-0.33045300	-0.67529600
C	1.63859000	-1.02457500	-1.60471700
H	1.90696200	-1.26614400	-2.62471800
C	0.47631300	-1.33817500	-0.98508900
C	0.57258600	-0.86330500	0.39656700
C	-0.19275000	-0.58268600	1.51438600
C	0.69560300	0.09691500	2.43863400
C	0.52060400	0.61663600	3.73027200
H	-0.42854300	0.49510400	4.24437400
C	1.57817600	1.28624800	4.33469300
H	1.45216100	1.69676900	5.33261200
C	2.81432900	1.44052700	3.67644800
H	3.61879100	1.97728300	4.17086800
C	3.02796400	0.91540300	2.40562900
H	3.97629100	1.03419900	1.89407600
C	1.96429600	0.24099000	1.80183900
C	-1.63326500	-0.82657300	1.74278200
C	-2.60785600	-0.15756400	0.99962200
C	-3.98201500	-0.40111400	1.26770500
H	-4.73493700	0.11694200	0.68622800
C	-4.37383300	-1.27681200	2.24945300
H	-5.43047100	-1.44458100	2.44359200
C	-3.41593500	-1.97624300	3.02379900
C	-3.79719500	-2.89970600	4.03170300
H	-4.85680400	-3.05720400	4.21729700
C	-2.84963800	-3.58602900	4.75513400
H	-3.15314200	-4.29139600	5.52360600
C	-1.47446200	-3.37860000	4.49431800
H	-0.73032300	-3.93051100	5.06153500
C	-1.07274900	-2.48541500	3.52699000
H	-0.01825600	-2.33142700	3.33055000
C	-2.02557600	-1.74954900	2.76896500
C	-0.68932300	-2.01351100	-1.56727700
C	-1.53139900	-2.82025700	-0.78095800
H	-1.30894500	-2.96243800	0.26993300

C	-2.64591300	-3.43778100	-1.32705800
H	-3.30415800	-4.04675000	-0.71663100
C	-2.94596200	-3.27743100	-2.68671100
C	-2.10759100	-2.49563300	-3.49196300
H	-2.32008400	-2.34841900	-4.54418800
C	-0.99887000	-1.86858300	-2.92457600
H	-0.38157100	-1.22449000	-3.54347900
C	-4.44883800	-3.72343500	-4.48068700
H	-4.63227200	-2.66353600	-4.70399300
H	-5.37361700	-4.28685100	-4.61491900
H	-3.68614600	-4.10763600	-5.17075000
C	2.83346900	1.15406400	-1.02069000
C	1.70092500	1.95164000	-1.21233900
H	0.71363000	1.50006100	-1.20001100
C	1.80572300	3.32803800	-1.38628200
H	0.90193400	3.91171200	-1.49828900
C	3.06774700	3.93435300	-1.37403400
C	4.20960800	3.14578000	-1.19833700
H	5.18077100	3.63006700	-1.18699500
C	4.08887800	1.77167500	-1.01593200
H	4.98374800	1.18085000	-0.85589900
C	2.13483900	6.11254300	-1.58833000
H	1.49867200	5.99784500	-0.70148800
H	1.53696100	5.90301700	-2.48559400
H	2.51393500	7.13483200	-1.63903000
C	3.92256200	-1.14057600	-0.62028100
C	4.71323500	-1.25790300	-1.76675500
H	4.42023500	-0.74006400	-2.67604300
C	5.88627500	-2.01210000	-1.77072500
H	6.47349700	-2.07631100	-2.67896500
C	6.28512900	-2.67268400	-0.60248300
C	5.49839800	-2.56685000	0.55032400
H	5.82023900	-3.08567800	1.44741600
C	4.33098600	-1.81267700	0.53718800
H	3.73117600	-1.74447200	1.43714200
C	8.23835900	-3.56842800	-1.63304000
H	7.70156500	-4.04400800	-2.46457700
H	9.07065200	-4.20538400	-1.32907400
H	8.62708600	-2.59684400	-1.96586900
P	-2.08821900	0.95178100	-0.39631000
C	-1.75023400	2.56502500	0.42809000
C	-1.62089800	3.70422500	-0.38568700
C	-1.48151500	2.68684200	1.79545900
C	-1.24479400	4.93013800	0.15908300

H	-1.82665400	3.63087400	-1.45108700
C	-1.07175700	3.90660200	2.33538100
H	-1.58293500	1.82427200	2.44155500
C	-0.95547600	5.03327600	1.52251400
H	-1.17190700	5.80508900	-0.48217200
H	-0.84311100	3.96972500	3.39543700
H	-0.64437600	5.98453400	1.94514200
C	-3.70890100	1.26703700	-1.22012400
C	-4.57713100	2.32010200	-0.89846000
C	-4.08639500	0.36056900	-2.22303500
C	-5.79311100	2.46416100	-1.56730900
H	-4.30039900	3.02607600	-0.12216900
C	-5.30831300	0.49692200	-2.88015300
H	-3.42042400	-0.45611900	-2.48325700
C	-6.16371200	1.55167700	-2.55706300
H	-6.45613400	3.28577900	-1.30922300
H	-5.58995000	-0.21797400	-3.64932600
H	-7.11297300	1.66369200	-3.07384200

10a-TS-cis

E(RB3LYP) = -2705.674244 Hartree

Sum of electronic and thermal Free Energies = -2704.946751 Hartree

O	-5.22515200	-1.41085600	5.33986900
O	-6.15946700	-2.31230600	-4.23135300
O	-0.00201700	6.79399000	-1.52737600
N	-1.76394100	-0.69891300	0.02197600
C	-3.15129200	-0.23918500	0.15434900
C	-2.91904100	1.25328000	0.02239100
H	-3.74498400	1.94768600	-0.04966500
C	-1.60929500	1.57085200	-0.11546300
C	-0.82722700	0.31650300	-0.03823200
C	0.46129000	-0.25048700	-0.21266200
C	0.18435900	-1.66021200	-0.55873200
C	0.89639000	-2.69820600	-1.18705100
H	1.90358500	-2.55369000	-1.54151900
C	0.28476200	-3.92363400	-1.42731000
H	0.85535800	-4.70661500	-1.91791700
C	-1.05003800	-4.16143000	-1.06188700
H	-1.49810700	-5.13364000	-1.24505300
C	-1.81982900	-3.14068700	-0.51952100

H	-2.87257300	-3.27461600	-0.30208300
C	-1.19970900	-1.90413000	-0.32501500
C	1.74676900	0.43188300	-0.08443200
C	3.00965100	-0.13209400	-0.41553500
C	4.06040900	0.73542500	-0.82030900
H	4.97750500	0.28487100	-1.18572800
C	3.96362600	2.10227000	-0.72842400
H	4.76004000	2.74939700	-1.08626000
C	2.89769300	2.64992500	0.02896900
C	2.92483000	3.99239200	0.48311000
H	3.72603400	4.63902600	0.13311500
C	2.00391700	4.44976200	1.39798800
H	2.04699600	5.47454800	1.75554600
C	1.03509600	3.56340700	1.91258500
H	0.35279500	3.89760700	2.68807500
C	0.93689700	2.27789800	1.42624300
H	0.18993300	1.60828200	1.83455600
C	1.81825300	1.79352200	0.42703900
C	-1.15629600	2.91998400	-0.49038600
C	-1.77185400	4.05758700	0.05631400
H	-2.53921800	3.93368200	0.81495000
C	-1.37911500	5.33321200	-0.31712200
H	-1.83300000	6.21569100	0.12187100
C	-0.35086400	5.50344300	-1.25408400
C	0.24932200	4.38117900	-1.83373700
H	1.04395200	4.48362400	-2.56220200
C	-0.15877400	3.10589600	-1.45133000
H	0.31962500	2.24027600	-1.89630600
C	1.10248000	7.00849300	-2.39027600
H	2.01190400	6.53414400	-1.99919400
H	1.24458400	8.08967800	-2.43363700
H	0.90534200	6.62846900	-3.40146100
C	-3.99725500	-0.76979400	-1.01127300
C	-3.60160500	-0.46285600	-2.31575300
H	-2.72896600	0.16375000	-2.47347900
C	-4.29168600	-0.95467400	-3.42103100
H	-3.95068600	-0.69889000	-4.41699400
C	-5.41022800	-1.77538600	-3.22715300
C	-5.81596700	-2.08988300	-1.92499400
H	-6.68061400	-2.73187500	-1.79174800
C	-5.11456000	-1.59270200	-0.83247500
H	-5.43743600	-1.85721000	0.16785600
C	-5.77054900	-2.04096200	-5.56808600
H	-4.75877700	-2.41289800	-5.77540500

H	-5.81137200	-0.96627800	-5.78887000
H	-6.48664500	-2.56729600	-6.20119800
C	-3.71924700	-0.56777400	1.53728800
C	-4.92482700	0.01061400	1.94365000
H	-5.46378300	0.66537200	1.26449300
C	-5.46822200	-0.24344900	3.20270800
H	-6.40603600	0.22259000	3.48043700
C	-4.79138000	-1.09231100	4.08702000
C	-3.58097100	-1.67390600	3.69159600
H	-3.06782400	-2.32869400	4.38821400
C	-3.05332000	-1.41252200	2.43287400
H	-2.11399600	-1.87115000	2.14674600
C	-6.44557200	-0.84315400	5.78492400
H	-6.39367100	0.25328000	5.81186500
H	-6.60166000	-1.22228900	6.79611500
H	-7.28719100	-1.14768500	5.14875700
P	3.47762000	-1.82072900	0.17442100
C	4.42229500	-1.41921000	1.71428300
C	4.72175900	-0.13209700	2.18120400
C	4.77943200	-2.52102300	2.51159800
C	5.38616300	0.04310800	3.39595900
H	4.43720200	0.73706300	1.60237500
C	5.46357200	-2.34581000	3.71338200
H	4.50985500	-3.52392000	2.18832600
C	5.76910500	-1.05917600	4.16024200
H	5.60641700	1.04909300	3.74351000
H	5.74148400	-3.21194400	4.30803500
H	6.28970600	-0.91725300	5.10335700
C	4.81344900	-2.26126700	-1.02686900
C	4.54106700	-2.16220400	-2.40270600
C	6.04386400	-2.80435800	-0.63107600
C	5.46663900	-2.59598200	-3.34976600
H	3.60883600	-1.71335700	-2.73516100
C	6.97025600	-3.23745900	-1.58031400
H	6.28754600	-2.87763200	0.42366900
C	6.68638900	-3.13910100	-2.94254200
H	5.23636300	-2.50282200	-4.40786300
H	7.92167700	-3.64699300	-1.25086000
H	7.41007600	-3.47571800	-3.67955400

10a-TS-trans

E(RB3LYP) = -2705.667863 Hartree

Sum of electronic and thermal Free Energies = -2704.939106 Hartree

O	-4.56371900	-3.15747100	4.64941000
O	-6.79833900	3.40140400	-2.10219800
O	3.10452700	5.41405200	0.81611800
N	-1.96492200	-0.32701700	-0.46026200
C	-2.74981500	0.38032400	0.55466300
C	-1.65851000	1.27549800	1.10758700
H	-1.88830400	2.10609600	1.76113100
C	-0.45163700	1.03961000	0.54134700
C	-0.59112200	-0.11224900	-0.38331700
C	0.04440000	-0.96795400	-1.31614000
C	-1.06403100	-1.46297400	-2.15749000
C	-1.13288100	-2.07851200	-3.42270600
H	-0.23126500	-2.30941100	-3.97466800
C	-2.37154000	-2.38095800	-3.97319600
H	-2.41485600	-2.85103500	-4.95145000
C	-3.56853700	-2.08891400	-3.29219000
H	-4.52214800	-2.35178900	-3.74080400
C	-3.54619400	-1.43031000	-2.07030800
H	-4.45808200	-1.14502700	-1.55988500
C	-2.29242900	-1.09482900	-1.54720400
C	1.42199200	-1.46405500	-1.51037300
C	2.63214300	-0.86047600	-1.10387700
C	3.84376400	-1.19641200	-1.76935300
H	4.74183800	-0.65222500	-1.49777300
C	3.90971800	-2.17843500	-2.72492500
H	4.83042800	-2.37715600	-3.26713600
C	2.80616500	-3.05511500	-2.86812900
C	2.92734900	-4.27843600	-3.57888800
H	3.84345900	-4.46265300	-4.13450100
C	1.94510900	-5.23834800	-3.50709000
H	2.06017800	-6.18263100	-4.03188500
C	0.81239200	-5.01334400	-2.69387000
H	0.07487100	-5.79959000	-2.56179500
C	0.63698300	-3.80350600	-2.05960900
H	-0.23171700	-3.65513900	-1.43262800
C	1.58706400	-2.75193600	-2.18006900
C	0.59375100	2.08258700	0.60123700
C	0.97013300	2.66301400	1.82304000
H	0.61365600	2.22163300	2.74916000
C	1.81557400	3.75998400	1.86126900
H	2.13047200	4.19691900	2.80332500
C	2.28592300	4.33208800	0.67021400
C	1.90385300	3.77870300	-0.55397700

H	2.26058000	4.19424800	-1.48827100
C	1.06943600	2.65909900	-0.58006600
H	0.78363500	2.22678500	-1.53510300
C	3.60416000	6.02677200	-0.35975600
H	4.21404700	5.32747400	-0.94326700
H	4.22673200	6.85784400	-0.02321600
H	2.79053100	6.41457200	-0.98779900
C	-3.84995800	1.21356100	-0.11568100
C	-3.47489200	2.19416000	-1.03787600
H	-2.42032600	2.36645400	-1.23133800
C	-4.42331300	2.94897000	-1.72419400
H	-4.09356700	3.69838300	-2.43364600
C	-5.78591600	2.72473200	-1.48938100
C	-6.17385400	1.74424200	-0.56867800
H	-7.23330300	1.57901800	-0.40191000
C	-5.21463000	0.99908000	0.10767900
H	-5.53422000	0.23817200	0.81051900
C	-6.45281500	4.39021800	-3.05847200
H	-5.89042200	3.95923200	-3.89695000
H	-5.86247300	5.19823400	-2.60679300
H	-7.39732300	4.79470100	-3.42587400
C	-3.26058800	-0.57339300	1.63794700
C	-3.83085800	-0.04517200	2.79958400
H	-3.93637100	1.03098300	2.90549800
C	-4.28328300	-0.86819600	3.83020900
H	-4.71964600	-0.41989200	4.71469200
C	-4.15984900	-2.25749500	3.70732800
C	-3.58666300	-2.79711600	2.55005200
H	-3.49606400	-3.87546900	2.47049500
C	-3.14274200	-1.96351500	1.53036600
H	-2.69965100	-2.40209300	0.64417500
C	-5.13551500	-2.65538100	5.84528300
H	-4.42952700	-2.01639800	6.39202700
H	-5.37672400	-3.52926900	6.45261900
H	-6.05382000	-2.08713200	5.64591400
P	2.69725800	-0.02347300	0.52662400
C	4.08974900	1.17681200	0.35125100
C	4.78494400	1.59788200	1.49565200
C	4.38270100	1.80190500	-0.86937200
C	5.74458300	2.60484000	1.42087900
H	4.57703900	1.13024500	2.45323100
C	5.35486500	2.79922200	-0.94826400
H	3.84556300	1.50913200	-1.76512200
C	6.03658200	3.20964600	0.19707600

H	6.26810000	2.91617700	2.32072200
H	5.57774100	3.25552600	-1.90979700
H	6.78996000	3.99024100	0.13774000
C	3.47331800	-1.33158200	1.59251100
C	4.22904000	-2.42796600	1.15572900
C	3.22971600	-1.19332700	2.96925700
C	4.74523500	-3.34361100	2.07254000
H	4.40914700	-2.57556000	0.09743700
C	3.76169500	-2.09791600	3.88840600
H	2.60814900	-0.37226400	3.31899500
C	4.52211500	-3.17803500	3.44057400
H	5.32606500	-4.19011100	1.71546400
H	3.56793000	-1.96792500	4.94985100
H	4.92825000	-3.89284200	4.15107000

(S_a)-10a

E(RB3LYP) = -2705.736821 Hartree

Sum of electronic and thermal Free Energies = -2705.010226 Hartree

O	-3.42141300	5.63731400	-0.73251400
O	-7.32051900	-3.24891400	-0.84607900
O	4.32094200	-1.45094300	-4.44239900
N	-1.78848200	-0.46027800	0.33338700
C	-2.62045100	-0.01403500	-0.79429800
C	-1.64583800	-0.27509800	-1.94217100
H	-1.93319000	-0.08681900	-2.96865600
C	-0.43838100	-0.70580600	-1.50825300
C	-0.50443800	-0.81021800	-0.05078300
C	0.26391700	-1.07931200	1.06803800
C	-0.61875100	-0.89735200	2.20183700
C	-0.43198000	-1.01522100	3.58722700
H	0.53192300	-1.32263400	3.98158100
C	-1.49420500	-0.73107200	4.43610100
H	-1.36001900	-0.81607300	5.51075900
C	-2.74567500	-0.33034000	3.92714600
H	-3.55638500	-0.11218500	4.61641500
C	-2.96688400	-0.20710400	2.55919400
H	-3.92995900	0.09895800	2.16797000
C	-1.89909500	-0.49707300	1.70581300
C	1.70459700	-1.40494600	1.12230200
C	2.65699800	-0.46223500	0.73270900

C	4.03519700	-0.80149700	0.77419600
H	4.77046000	-0.06611400	0.46968600
C	4.45166600	-2.03957000	1.19982800
H	5.51192800	-2.27963400	1.23274600
C	3.51555800	-3.01986600	1.61228400
C	3.92079400	-4.30794500	2.04968600
H	4.98368600	-4.53534600	2.07991400
C	2.99208200	-5.25118000	2.42421400
H	3.31426900	-6.23373600	2.75754000
C	1.61149800	-4.94426000	2.37085600
H	0.88218800	-5.69594800	2.65948300
C	1.18627900	-3.70265000	1.95581000
H	0.12824200	-3.47108700	1.91610100
C	2.12015900	-2.69930900	1.57484500
C	0.76531800	-0.97201600	-2.30604200
C	1.10318800	-0.15040800	-3.39520900
H	0.45394700	0.68090500	-3.65256900
C	2.27976200	-0.34812900	-4.10210400
H	2.55678200	0.29805800	-4.92884100
C	3.16388900	-1.37063300	-3.72436200
C	2.82990700	-2.21590100	-2.66127100
H	3.48892400	-3.01710600	-2.35081600
C	1.63621000	-2.01439600	-1.97083800
H	1.39070400	-2.67419700	-1.14712900
C	5.29301500	-2.39361900	-4.01925000
H	5.59639900	-2.21339500	-2.97977800
H	6.15115600	-2.25679300	-4.67936200
H	4.92427700	-3.42351800	-4.11269700
C	-3.89409600	-0.86015300	-0.87061200
C	-3.83351300	-2.15470200	-1.38855700
H	-2.89233000	-2.52342400	-1.78509300
C	-4.95142600	-2.98876800	-1.40200900
H	-4.86477000	-3.98632400	-1.81595000
C	-6.16499500	-2.52515800	-0.88126400
C	-6.23791900	-1.23041100	-0.35187100
H	-7.18520500	-0.88680600	0.05082100
C	-5.11519100	-0.41297500	-0.34868700
H	-5.19101400	0.58983700	0.05775300
C	-7.29122800	-4.56984200	-1.36026200
H	-6.58228400	-5.20089700	-0.80844700
H	-7.02790200	-4.58122100	-2.42616800
H	-8.30090100	-4.96381300	-1.23321600
C	-2.88182400	1.49552100	-0.74447100
C	-3.72517100	2.08186700	-1.69229200

H	-4.23989000	1.45338700	-2.41345500
C	-3.93542200	3.46045400	-1.72827400
H	-4.59978600	3.87691300	-2.47602500
C	-3.28731400	4.28037300	-0.79697800
C	-2.43374500	3.70357300	0.15037600
H	-1.93672800	4.34775700	0.86721100
C	-2.22874100	2.33005700	0.17092300
H	-1.55231400	1.91390800	0.90666500
C	-4.26557800	6.26511200	-1.68192100
H	-3.91356300	6.09596800	-2.70824200
H	-4.22780500	7.33263500	-1.45847700
H	-5.30204200	5.91253100	-1.59581900
P	2.07248400	1.17619400	0.08668100
C	3.67868000	1.99098900	-0.31182600
C	4.38757600	2.82030600	0.56746100
C	4.20179400	1.75512100	-1.59371000
C	5.59542200	3.39819900	0.17384300
H	3.99385400	3.01115500	1.56090500
C	5.41657000	2.31947000	-1.97977700
H	3.65322700	1.12259800	-2.28639400
C	6.11501800	3.14620100	-1.09713900
H	6.13472000	4.04211000	0.86376000
H	5.81170500	2.12104800	-2.97260200
H	7.05714200	3.59539800	-1.39957000
C	1.56885000	2.04365200	1.63376100
C	1.77808300	1.54758400	2.92602300
C	0.88546200	3.26071400	1.48088100
C	1.30242800	2.24236200	4.03853100
H	2.30077500	0.60693600	3.06096200
C	0.42920700	3.96603300	2.59307400
H	0.69893600	3.64730900	0.48219100
C	0.62920000	3.45284700	3.87646200
H	1.45544200	1.83308700	5.03328900
H	-0.09071000	4.91101600	2.45890100
H	0.25737600	3.99152300	4.74352400

(S₀)-7ad

E(RB3LYP) = -1862.15352 Hartree

Sum of electronic and thermal Free Energies = -1861.612742 Hartree

O	-2.52524000	-2.96191500	2.46104900
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H	-3.09749600	-3.68574300	2.75811100
O	6.89166000	-2.45878500	-0.59641100
N	0.96676900	-0.38593500	0.72638100
C	1.79088600	0.07235600	-0.41450900
C	0.93021100	-0.42715800	-1.57452200
H	1.28918300	-0.39285800	-2.59518400
C	-0.26905500	-0.88846000	-1.15197300
C	-0.29777500	-0.77571200	0.30128400
C	-1.18812800	-0.76770200	1.35265600
C	-0.42297700	-0.35020400	2.50751000
C	-0.75520700	-0.16009300	3.85556000
H	-1.76279300	-0.37264700	4.20038900
C	0.22092100	0.30492900	4.72931900
H	-0.02493400	0.45983200	5.77619100
C	1.52831800	0.57748900	4.28174200
H	2.26896800	0.94148200	4.98822400
C	1.89385800	0.38720100	2.95184400
H	2.90062200	0.59354400	2.60728000
C	0.91184900	-0.07489800	2.07366900
C	-2.64504800	-0.95500100	1.22542000
C	-3.28136200	-2.06885200	1.74810200
C	-4.65419000	-2.31221000	1.50212000
H	-5.11865800	-3.20674000	1.91390400
C	-5.38352000	-1.44653500	0.72276200
H	-6.43049600	-1.65142900	0.51473900
C	-4.79058600	-0.27726800	0.18486400
C	-5.52115100	0.63241300	-0.62392300
H	-6.56333400	0.41065700	-0.84171600
C	-4.92923800	1.76992300	-1.12249900
H	-5.49891200	2.45567700	-1.74338300
C	-3.57822700	2.05479600	-0.81037600
H	-3.10884900	2.96401100	-1.17598500
C	-2.84349000	1.18793000	-0.03539900
H	-1.81728100	1.42422600	0.21482300
C	-3.41199000	-0.01390800	0.46674500
C	-1.40291500	-1.37718500	-1.95027200
C	-2.16633000	-2.46573700	-1.50233600
H	-1.88154700	-2.97075700	-0.58579100
C	-3.28517700	-2.88311900	-2.21711900
H	-3.87592900	-3.71754400	-1.85068400
C	-3.65464400	-2.22287400	-3.39061300
C	-2.89374400	-1.14695200	-3.84997100
H	-3.18197900	-0.62303900	-4.75696800
C	-1.77582700	-0.72547600	-3.13322600

H	-1.20564000	0.13733300	-3.46510100
C	1.82929700	1.61441400	-0.36617700
C	0.70574600	2.33086100	-0.77476600
H	-0.14533800	1.82934900	-1.21801500
C	0.63768200	3.71662500	-0.60577000
C	1.71605300	4.40654700	-0.04164900
C	2.84531300	3.68485400	0.35129200
H	3.68437800	4.21610900	0.79203300
C	2.91108600	2.30238500	0.19785400
H	3.79461200	1.76059300	0.51467700
C	3.16862500	-0.57475800	-0.44635900
C	4.08990900	-0.19742900	-1.42632600
H	3.83358000	0.59184500	-2.12779300
C	5.34453100	-0.80006600	-1.51669100
H	6.03379600	-0.47935200	-2.28856500
C	5.69345500	-1.80553900	-0.60702100
C	4.77627600	-2.19324900	0.37725900
H	5.06268600	-2.97377000	1.07458200
C	3.52819000	-1.58681600	0.45099400
H	2.82376600	-1.89796000	1.21388600
C	7.84987500	-2.10272800	-1.57805900
H	7.47540400	-2.28873000	-2.59344100
H	8.71941300	-2.73544200	-1.39245500
H	8.14302900	-1.04796800	-1.49154300
H	-4.53587400	-2.54092300	-3.94072900
H	1.68807000	5.48086500	0.09564000
O	-0.52577900	4.29987900	-1.02587300
C	-0.67923600	5.69415600	-0.81965900
H	-1.67445300	5.94489700	-1.19016500
H	-0.61156600	5.95163700	0.24529700
H	0.07144800	6.26927200	-1.37773000

7ad-TS-trans

E(RB3LYP) = -1862.101907 Hartree

Sum of electronic and thermal Free Energies = -1861.558827 Hartree

O	-2.34000100	-2.77299800	2.70612100
H	-2.78560000	-3.27282700	3.40717600
O	4.93933800	-4.39121100	-1.72565100
N	0.71445500	-0.17632600	0.57556400
C	1.78634800	0.16499900	-0.35786700

C	0.94031300	0.56695400	-1.54876800
H	1.37044300	1.05692700	-2.41172500
C	-0.38436100	0.41048300	-1.32181100
C	-0.56931500	-0.19557200	0.01992900
C	-1.47589800	-0.64417000	1.00866000
C	-0.68986700	-0.61119200	2.25336900
C	-1.03262000	-0.63338900	3.61753700
H	-2.06851200	-0.70998800	3.92255300
C	-0.03937200	-0.51238700	4.57978500
H	-0.31345400	-0.51849800	5.63117100
C	1.31499900	-0.37282400	4.21997900
H	2.07306200	-0.29531000	4.99420200
C	1.68879700	-0.28913000	2.88612500
H	2.71800600	-0.12227100	2.59192500
C	0.67023400	-0.37109300	1.92981000
C	-2.86830300	-1.14887100	1.01781500
C	-3.27408100	-2.03550600	2.03248500
C	-4.63903100	-2.21308000	2.37061500
H	-4.88077600	-2.81289800	3.24698300
C	-5.63426700	-1.64297200	1.62237400
H	-6.67738900	-1.74431100	1.90829000
C	-5.29636000	-1.01348600	0.39927300
C	-6.29688400	-0.64140400	-0.53375100
H	-7.33835600	-0.73406700	-0.23465900
C	-5.96708200	-0.23582700	-1.80801800
H	-6.74374800	0.02656600	-2.52076900
C	-4.61271300	-0.23602600	-2.19997000
H	-4.33700900	-0.00942900	-3.22481800
C	-3.62447700	-0.53411200	-1.28608400
H	-2.60562200	-0.61031200	-1.61927700
C	-3.91090800	-0.85276400	0.05805200
C	-1.34907600	1.12577600	-2.19077300
C	-1.37457400	0.91728900	-3.57412300
H	-0.75606900	0.13457400	-4.00387800
C	-2.19651800	1.69686700	-4.39017300
H	-2.21350300	1.51995400	-5.46212800
C	-2.99073000	2.69922600	-3.83288200
C	-2.96301800	2.91645600	-2.45301300
H	-3.58089400	3.69267200	-2.01092900
C	-2.15185300	2.13470900	-1.63734200
H	-2.14077000	2.28793800	-0.56249100
C	2.58516000	1.36838500	0.17392900
C	1.89977200	2.56460800	0.37737200
H	0.84547900	2.64951300	0.13723000

C	2.55212800	3.68044500	0.91018100
C	3.91023000	3.60257000	1.24300200
C	4.58839600	2.40062100	1.03852600
H	5.64031300	2.33503400	1.30258400
C	3.94170900	1.28611600	0.50836500
H	4.48432400	0.35978900	0.36500100
C	2.64952900	-1.05090600	-0.70533600
C	3.58927000	-0.95277400	-1.73529500
H	3.72292100	-0.00683700	-2.25293100
C	4.37829600	-2.03998100	-2.10918700
H	5.09694400	-1.92356500	-2.91153000
C	4.22482900	-3.26308700	-1.44520400
C	3.28212200	-3.37404800	-0.41652100
H	3.17294900	-4.32924600	0.08656900
C	2.50391200	-2.28086700	-0.05407100
H	1.77735500	-2.38850000	0.74259800
C	5.89508100	-4.32849400	-2.77020900
H	5.42578400	-4.08082300	-3.73156000
H	6.33944500	-5.32332700	-2.83084300
H	6.68109700	-3.59244500	-2.55450400
H	-3.62951800	3.30591200	-4.46837900
H	4.43616400	4.45423400	1.65747800
O	1.78043200	4.79467400	1.06559600
C	2.38571700	5.94905300	1.62208300
H	1.60173300	6.70677700	1.66638800
H	2.76334300	5.75685100	2.63496700
H	3.20933700	6.31490800	0.99463400

7ad-TS-cis

E(RB3LYP) = -1862.10278 Hartree

Sum of electronic and thermal Free Energies = -1861.560259 Hartree

O	-2.74119500	0.48728100	-2.50591400
H	-1.86903300	0.08049500	-2.39341000
O	4.77418900	-4.41648700	-2.09278900
N	0.57143300	-0.27474000	0.36616200
C	1.88084100	0.10928600	-0.16631500
C	1.42132700	0.96247500	-1.33154300
H	2.11302400	1.57158200	-1.89720500
C	0.07265600	1.00230100	-1.44975900
C	-0.51609300	0.11458500	-0.41827500

C	-1.70727800	-0.34024800	0.20011300
C	-1.27027000	-0.74813300	1.54822100
C	-1.93571100	-0.96575900	2.77146900
H	-3.01111100	-0.87872900	2.83703900
C	-1.20415100	-1.27546700	3.91036100
H	-1.72898900	-1.43688800	4.84747200
C	0.19956000	-1.37260800	3.87660100
H	0.74478200	-1.62967600	4.78018800
C	0.89945500	-1.09646000	2.71076700
H	1.98232900	-1.10029600	2.68131300
C	0.15187000	-0.74716300	1.58066500
C	-3.09195600	-0.46466100	-0.29395500
C	-3.55440500	0.10351500	-1.48749800
C	-4.92923100	0.33481800	-1.73195200
H	-5.18499500	0.90428600	-2.61969400
C	-5.87828900	-0.14861400	-0.87386200
H	-6.93315000	0.05732400	-1.03267200
C	-5.48810600	-1.04627300	0.15487300
C	-6.46025400	-1.79699400	0.86297900
H	-7.50922600	-1.56253300	0.69813700
C	-6.09647800	-2.83899700	1.68519000
H	-6.85101600	-3.42225500	2.20508000
C	-4.73274600	-3.18319400	1.78939800
H	-4.43659300	-4.05993200	2.35872800
C	-3.76519800	-2.42854800	1.15893900
H	-2.73165800	-2.73640300	1.23170300
C	-4.09157100	-1.28299200	0.38529700
C	-0.57071900	2.05053700	-2.27594800
C	-0.19572700	2.24108600	-3.60994700
H	0.50111300	1.54636400	-4.07064200
C	-0.72397500	3.30203300	-4.34650900
H	-0.43290000	3.43419200	-5.38485100
C	-1.62505400	4.18491400	-3.75381500
C	-1.99843200	4.00257600	-2.41892100
H	-2.69963900	4.68780300	-1.95099200
C	-1.47801100	2.94319300	-1.68509300
H	-1.77664300	2.78896800	-0.65247100
C	2.63910200	0.96238800	0.86628500
C	2.03944600	2.14407100	1.29732100
H	1.08522700	2.46362800	0.89275400
C	2.64652600	2.93701500	2.27583500
C	3.87249900	2.54630200	2.82906400
C	4.46541500	1.36163200	2.39191700
H	5.41313900	1.05328000	2.82461400

C	3.86303300	0.56743200	1.41820200
H	4.33405100	-0.35407000	1.09927200
C	2.66758700	-1.10507100	-0.66633300
C	3.82216200	-0.90963400	-1.42916900
H	4.16681400	0.10001000	-1.63463200
C	4.55977600	-1.98443900	-1.92444400
H	5.45009400	-1.79233900	-2.51116700
C	4.13534400	-3.29230100	-1.65950300
C	2.97787100	-3.49935600	-0.89989400
H	2.66100800	-4.51860800	-0.70462000
C	2.25444100	-2.41757100	-0.41206300
H	1.35935500	-2.59859200	0.17139800
C	5.94469500	-4.25486300	-2.87628700
H	5.73445800	-3.71086900	-3.80652700
H	6.28658100	-5.26287500	-3.11637400
H	6.73133400	-3.72689900	-2.32115800
H	-2.03800100	5.00982900	-4.32744200
H	4.36049700	3.14499800	3.58865100
O	1.96701700	4.06742500	2.62141500
C	2.52182300	4.89516000	3.62971000
H	1.82063600	5.72119700	3.75839700
H	2.62685000	4.35565900	4.58016300
H	3.50090500	5.29294800	3.33139800

(R_a)-7ad

E(RB3LYP) = -1862.15649 Hartree

Sum of electronic and thermal Free Energies = -1861.615823 Hartree

O	2.59853600	2.34226600	0.15990500
H	1.70468100	2.08703300	-0.13496700
O	-5.36506800	-4.37220900	0.84187000
N	-0.73748700	-0.16996300	-0.56945400
C	-1.86737600	0.10136000	0.33673800
C	-1.10683500	0.25392900	1.65277000
H	-1.63349700	0.37081000	2.59098400
C	0.23310100	0.15452000	1.48948700
C	0.48916800	-0.04943900	0.06435400
C	1.51290000	-0.07006000	-0.86931100
C	0.85861200	-0.21103500	-2.15623100
C	1.34622900	-0.30082900	-3.46822200
H	2.41643200	-0.28510200	-3.65125600

C	0.43840600	-0.41017500	-4.51475000
H	0.80247400	-0.47884800	-5.53579600
C	-0.95011900	-0.43381000	-4.27536600
H	-1.63389500	-0.51800900	-5.11516300
C	-1.46644800	-0.35398900	-2.98583500
H	-2.53391200	-0.37044000	-2.80058800
C	-0.55288000	-0.24323000	-1.93474300
C	2.95757200	0.08606700	-0.60931300
C	3.42198100	1.28835000	-0.08849100
C	4.79031600	1.47611500	0.22208800
H	5.09545300	2.43288300	0.63256800
C	5.68767700	0.46234400	0.00681500
H	6.73837800	0.60360800	0.24720900
C	5.27089300	-0.78578300	-0.52861300
C	6.18401700	-1.84786100	-0.74801900
H	7.23325300	-1.68629400	-0.51180600
C	5.75776500	-3.05976000	-1.24336400
H	6.46730600	-3.86593700	-1.40609400
C	4.38812000	-3.25562600	-1.53556000
H	4.05236300	-4.21538200	-1.91879200
C	3.47514700	-2.24300400	-1.33754400
H	2.42612900	-2.39999300	-1.56374000
C	3.88508800	-0.97684700	-0.83935200
C	1.27811800	0.23523300	2.52112300
C	2.41081900	-0.59011900	2.45203500
H	2.50740100	-1.30050700	1.63927200
C	3.40747300	-0.50112100	3.42014100
H	4.28278600	-1.13965200	3.34623700
C	3.28461800	0.40714900	4.47279600
C	2.15624800	1.22545000	4.55495700
H	2.05818500	1.93949900	5.36781200
C	1.16130600	1.14241300	3.58394300
H	0.29862200	1.80126000	3.62736400
C	-2.54657600	1.40757800	-0.11044700
C	-1.91625800	2.62077200	0.15709300
H	-1.00249500	2.65851000	0.74015500
C	-2.44762300	3.82361000	-0.32155500
C	-3.62661900	3.81525700	-1.07598000
C	-4.25174400	2.59565200	-1.34020900
H	-5.16507200	2.58586600	-1.92854100
C	-3.72567400	1.39691400	-0.86639900
H	-4.22727100	0.46006700	-1.07840500
C	-2.82590500	-1.08230600	0.44434900
C	-3.96632300	-0.97705400	1.24477000

H	-4.18780700	-0.03661200	1.74187200
C	-4.84282500	-2.04917100	1.40851500
H	-5.71838300	-1.92850200	2.03507600
C	-4.57821800	-3.26151600	0.75962800
C	-3.43535000	-3.37896400	-0.04051300
H	-3.24422200	-4.32519300	-0.53602900
C	-2.56943000	-2.30274900	-0.19072200
H	-1.68722800	-2.41139900	-0.81072500
C	-6.53255500	-4.30202600	1.64313800
H	-6.28855500	-4.09414400	2.69326600
H	-7.00615500	-5.28230500	1.56957600
H	-7.22711300	-3.53450700	1.27673200
H	4.06652700	0.48096200	5.22342200
H	-4.05678000	4.73441100	-1.45498800
O	-1.74547500	4.94568200	0.00592000
C	-2.23012300	6.19372100	-0.46107000
H	-1.52603900	6.94337400	-0.09672800
H	-2.26256400	6.22792100	-1.55788300
H	-3.23068100	6.41069400	-0.06421000

Cartesian coordinates of DFT-computed structures in calculation of reaction pathway:

CPA (S)-5a

C	-0.68148300	1.66870300	-0.31856600
C	-1.54565300	0.59949200	-0.06720400
C	-2.90277000	0.62488100	-0.42076500
C	-3.33546300	1.74412300	-1.13694300
H	-4.37923200	1.78961800	-1.43441400
C	0.68427400	1.68755900	0.28796300
C	1.58328100	0.65693600	0.00904600
C	2.92701900	0.68861900	0.40523900
C	3.32165100	1.79726300	1.15814200
H	4.35608900	1.85184500	1.48539500
O	-1.04608700	-0.51558900	0.62124800
O	1.11491400	-0.42765100	-0.74903000
P	0.08349300	-1.45785200	-0.04899800
O	0.60613700	-2.45418400	0.90592600
O	-0.56571100	-2.08503600	-1.38505400
C	-2.47276000	2.76616300	-1.53982400
C	-3.03372700	3.90488400	-2.37284400
C	-1.12789500	2.73285100	-1.13914400
C	-1.96149200	4.69798600	-3.12190600
H	-3.57772000	4.58772700	-1.70415900
H	-3.78004000	3.51020400	-3.07100100
C	-0.14344500	3.76541600	-1.66307700
C	-0.81253700	5.04253600	-2.17370900
H	-2.40089100	5.60267000	-3.55520500
H	-1.57323600	4.09981900	-3.95639100
H	0.61011200	4.00424700	-0.91235700
H	0.41051800	3.29637900	-2.48924700
H	-0.06816000	5.67297900	-2.67135000
H	-1.20265100	5.62085800	-1.32493500
C	1.09037900	2.73853300	1.14550900
C	0.07424800	3.72970700	1.68873800
C	2.42975000	2.79337900	1.56411200
C	0.70477300	5.01030200	2.23836700
H	-0.47331700	3.22437100	2.49760800
H	-0.67979000	3.96959900	0.93872200
C	2.95258100	3.92531100	2.43051300
C	1.85367200	4.67187900	3.18869900
H	-0.06058300	5.60815800	2.74442100
H	1.08726800	5.62003000	1.40829600
H	3.70280400	3.53313800	3.12575500
H	3.48420200	4.63832900	1.78368300

H	2.26578900	5.57660700	3.64796600
H	1.47359000	4.04377200	4.00473000
C	-3.88357200	-0.41385800	-0.01716400
C	-3.67243400	-1.76479700	-0.21183600
C	-5.11002400	0.00881200	0.57303800
C	-4.64021900	-2.72714000	0.16806500
H	-2.76258100	-2.10427500	-0.68821300
C	-6.06827700	-0.89979700	0.95002300
H	-5.26984600	1.06892900	0.74198200
C	-5.86710000	-2.29172800	0.76240900
C	-4.43071800	-4.11814300	-0.02751900
H	-6.99382700	-0.56064500	1.40699600
C	-6.83113500	-3.26141800	1.14121500
C	-5.38422100	-5.03486800	0.34932200
H	-3.49793700	-4.44645600	-0.47785500
C	-6.59675000	-4.60233100	0.93992100
H	-7.75971000	-2.92544100	1.59451400
H	-5.21032200	-6.09560900	0.19717700
H	-7.34137200	-5.33558800	1.23393700
C	3.91790600	-0.35147800	0.03383800
C	3.68810100	-1.69679400	0.24799100
C	5.16074400	0.05612200	-0.53012300
C	4.65778400	-2.66991100	-0.09817100
H	2.76373100	-2.03107500	0.70400500
C	6.12037700	-0.86578600	-0.87172800
H	5.33389800	1.11322800	-0.70672900
C	5.90135500	-2.25359600	-0.67098700
C	4.42516700	-4.05554500	0.11153200
H	7.06031800	-0.54082700	-1.30950400
C	6.86274400	-3.23881100	-1.01560900
C	5.37735500	-4.98656100	-0.23319800
H	3.47738800	-4.35999400	0.54641600
C	6.60760800	-4.57427100	-0.80215500
H	7.80551900	-2.91987100	-1.45191700
H	5.18998000	-6.04359200	-0.07053100
H	7.35082400	-5.31932600	-1.06957200
H	-0.50180100	-3.05010700	-1.34523500

(S_a)-1a

O	0.45218800	3.13506300	-0.57386400
H	-0.46162400	2.90070000	-0.33918500
N	-2.74732600	1.17652800	1.41669000
C	-1.40744700	1.51434000	1.39852100
C	-0.74556700	0.76108300	0.44980400

C	-1.74630500	-0.08985500	-0.15845400
C	-1.70206200	-1.05471300	-1.17714800
H	-0.76178800	-1.28287900	-1.66772800
C	-2.87478700	-1.70744400	-1.53006800
H	-2.85701600	-2.45780000	-2.31406600
C	-4.09511700	-1.41285600	-0.88731700
H	-4.99491400	-1.94150400	-1.18594300
C	-4.16997400	-0.45946000	0.12050000
H	-5.11065500	-0.23217800	0.61282900
C	-2.98556100	0.19393600	0.47477600
C	0.68901300	0.83127900	0.10401100
C	1.21045800	2.01649600	-0.40343000
C	2.56949300	2.11940400	-0.78751100
H	2.91896700	3.06746500	-1.18125600
C	3.39988200	1.03547600	-0.66858600
H	4.44153400	1.11109400	-0.96759300
C	2.92329700	-0.20049300	-0.15706500
C	3.77315500	-1.32780300	-0.02441500
H	4.81045900	-1.23312400	-0.33456100
C	3.30199100	-2.51517400	0.48704300
H	3.96207200	-3.37155700	0.58306700
C	1.95228300	-2.61486900	0.89583000
H	1.58442600	-3.54895500	1.30995300
C	1.10014700	-1.53936700	0.77927000
H	0.06930600	-1.62542500	1.10155700
C	1.55052500	-0.30372900	0.24057400
H	-3.43797900	1.57662500	2.02966200
H	-1.00954600	2.24382800	2.08933200

(R_n)-1a

O	-0.40990700	2.51619000	-0.91544400
H	-1.17211200	1.92386500	-1.00826500
N	-2.27089500	-1.67955800	-1.36205800
C	-0.94394200	-1.31006900	-1.45658000
C	-0.67108600	-0.29815000	-0.56239000
C	-1.91743600	-0.02352100	0.12575900
C	-2.28629300	0.87453200	1.14296500
H	-1.55052400	1.55018100	1.56670200
C	-3.60032300	0.87544700	1.59002900
H	-3.89931700	1.56371500	2.37411600
C	-4.55715100	-0.00586700	1.04620900
H	-5.57665900	0.02019200	1.41768000
C	-4.22075700	-0.90945000	0.04550500
H	-4.95739600	-1.59113200	-0.36878200

C	-2.89766200	-0.90702100	-0.40472600
C	0.61611400	0.39654600	-0.36430800
C	0.67387400	1.77405400	-0.55265400
C	1.88398000	2.49144500	-0.39491500
H	1.86682600	3.56271400	-0.56268800
C	3.03585300	1.83014100	-0.05756200
H	3.96725700	2.37796500	0.05397900
C	3.03792400	0.42653100	0.15460900
C	4.22192700	-0.26692500	0.51267100
H	5.14366300	0.30066300	0.60967200
C	4.21000900	-1.62400100	0.73853800
H	5.12292800	-2.14306900	1.01322100
C	2.99685300	-2.34025600	0.62357000
H	2.98295500	-3.40788200	0.82238200
C	1.83098700	-1.69762000	0.27098100
H	0.90390400	-2.25428300	0.20178500
C	1.81054200	-0.30061800	0.01133400
H	-2.71354500	-2.39544000	-1.91403500
H	-0.28294300	-1.79130000	-2.16201600

2b

C	1.03827000	0.05385400	1.09121600
C	1.70500400	1.30658600	0.50774300
C	0.98368000	2.47224100	0.25574500
C	3.09534600	1.32712200	0.31440000
C	1.61619400	3.63672400	-0.18251600
H	-0.09160500	2.46789600	0.39695900
C	3.74032800	2.47823900	-0.11406600
H	3.67293900	0.42429000	0.48599500
C	3.00281100	3.64311500	-0.36755100
H	1.02300500	4.52183500	-0.37571200
H	4.81319600	2.49923500	-0.27147900
C	1.64828700	-1.23016000	0.50522500
C	1.74609200	-1.39546500	-0.88434200
C	2.07591600	-2.26122300	1.33351600
C	2.27121900	-2.55785200	-1.42545700
H	1.40972100	-0.60019500	-1.54217900
C	2.61105100	-3.43987800	0.80303700
H	1.98135400	-2.14211100	2.40630200
C	2.71094500	-3.59001000	-0.58194800
H	2.35536200	-2.69464200	-2.49814600
H	2.93690000	-4.22354000	1.47569400
C	-0.40561800	0.02645400	0.82208200
C	-1.58695700	-0.02771100	0.55886000

C	-2.97536900	-0.10451100	0.24681300
C	-3.88944800	0.81355700	0.78569600
C	-3.46478000	-1.10871800	-0.61415900
C	-5.24783300	0.74211700	0.48482500
H	-3.52682900	1.58937400	1.45156400
C	-4.81286600	-1.18507400	-0.92032400
H	-2.76900300	-1.82586300	-1.03608900
C	-5.71522200	-0.26075200	-0.37276500
H	-5.92602200	1.46532900	0.91995400
H	-5.19819200	-1.95373100	-1.58120900
O	1.18475400	0.08157100	2.52671500
H	2.06904700	0.43534900	2.69727500
O	3.21709100	-4.69197500	-1.21043300
O	3.72362800	4.71978900	-0.79308300
O	-7.01894200	-0.42234900	-0.73501600
C	3.66745800	-5.76464200	-0.40103600
H	4.02796200	-6.53159600	-1.08767600
H	4.48782500	-5.45592300	0.25959100
H	2.85532700	-6.17877500	0.21006300
C	3.02187000	5.92113900	-1.06856800
H	3.77372900	6.64304200	-1.38932400
H	2.28599100	5.78404900	-1.87093700
H	2.51025500	6.30360700	-0.17634600
C	-7.97445500	0.48101200	-0.20256800
H	-8.93819900	0.17601400	-0.61157400
H	-8.01262100	0.42825100	0.89271200
H	-7.76392200	1.51480900	-0.50405300

H₂O

O	0.00000000	0.00000000	0.11920900
H	0.00000000	0.75932100	-0.47683700
H	0.00000000	-0.75932100	-0.47683700

Start point

C	3.23580900	0.96064800	0.12237000
C	3.43629300	0.73156200	1.62468200
C	2.33056500	0.78400100	2.47855200
C	4.67406400	0.33425400	2.14608600
C	2.44510000	0.43343300	3.82258500
H	1.36101800	1.08046100	2.09262700
C	4.80171100	-0.00964700	3.48629600
H	5.54132800	0.28594500	1.49911500
C	3.68590500	0.03175500	4.33333300
H	1.56571300	0.47914300	4.45254400

H	5.75763100	-0.31009600	3.90206900
C	4.56022000	1.15492500	-0.61390600
C	5.23885700	2.37756400	-0.51856500
C	5.14933400	0.11321200	-1.32172500
C	6.48014100	2.54746900	-1.11180700
H	4.78371200	3.19922300	0.02547900
C	6.40020200	0.26936700	-1.92507300
H	4.63358700	-0.83302200	-1.40977100
C	7.07153100	1.48941800	-1.81880400
H	7.01373900	3.48935700	-1.04615700
H	6.82865700	-0.56524800	-2.46547000
C	2.31787100	2.06632500	-0.17199200
C	1.49589700	2.87411000	-0.54523300
C	0.49746400	3.77294000	-1.01986900
C	-0.70299300	3.26938000	-1.54667900
C	0.69313000	5.16802600	-1.00359400
C	-1.68136800	4.12348200	-2.04473000
H	-0.86497300	2.19924200	-1.57231400
C	-0.27821300	6.02206300	-1.49815300
H	1.61650500	5.57007000	-0.60025800
C	-1.47278400	5.50635500	-2.02235800
H	-2.60355600	3.70176500	-2.42239800
H	-0.14104100	7.09769600	-1.48857200
O	2.56892700	-0.23493800	-0.41137300
H	2.68061000	-0.94777200	0.23981200
O	8.29627700	1.75208400	-2.36401300
O	3.90920100	-0.33066700	5.62858800
O	-2.36297700	6.42821300	-2.48285700
C	8.92650600	0.71519700	-3.09552700
H	9.87619400	1.12345300	-3.44353100
H	9.11942800	-0.16401000	-2.46697000
H	8.32543400	0.40781700	-3.96084200
C	2.80718800	-0.30661300	6.52279800
H	3.19607400	-0.63033400	7.48885200
H	2.38842200	0.70255900	6.61990800
H	2.01325000	-0.99283100	6.20252300
C	-3.57001300	5.95077300	-3.05806200
H	-4.13350700	6.83760400	-3.35119500
H	-3.37338500	5.33641200	-3.94586800
H	-4.15437400	5.36891600	-2.33792900
H	1.03980100	-0.11657900	-0.82644900
C	-3.57103400	-2.01756500	0.08890200
C	-3.45668300	-0.62297300	0.02665800
C	-4.47169800	0.23655700	0.47230200

C	-5.61243700	-0.36844700	1.00659200
H	-6.41410600	0.27341600	1.36102800
C	-2.51041700	-2.88159100	-0.51446400
C	-1.19046200	-2.74708100	-0.07655500
C	-0.14397200	-3.56022700	-0.53405300
C	-0.49138700	-4.54658400	-1.46268000
H	0.27885900	-5.23058500	-1.80675600
O	-2.30869600	-0.07404000	-0.55310800
O	-0.90680800	-1.71458200	0.81842700
P	-0.88242300	-0.19438700	0.21701300
O	0.05711400	-0.18652700	-1.04454300
O	-0.62581100	0.75498900	1.32167200
C	-5.72829200	-1.74982200	1.17550100
C	-6.99190400	-2.30170600	1.81105600
C	-4.68888700	-2.58888300	0.74165300
C	-6.82108500	-3.70777800	2.38866700
H	-7.78143400	-2.32715200	1.04577800
H	-7.34400900	-1.60796800	2.58237800
C	-4.71542400	-4.07269400	1.07173600
C	-6.11706100	-4.60621500	1.37165500
H	-7.79718100	-4.11794400	2.66888300
H	-6.21860200	-3.66118200	3.30521700
H	-4.24614000	-4.66087100	0.28276800
H	-4.08051300	-4.22087400	1.95768200
H	-6.04751200	-5.63560400	1.73925100
H	-6.70676200	-4.63885500	0.44512200
C	-2.79979900	-3.81194000	-1.53899300
C	-4.15443100	-3.80983300	-2.22680600
C	-1.77978400	-4.66977800	-1.98623800
C	-4.46380700	-5.10929300	-2.97238500
H	-4.14918400	-2.97808000	-2.94645000
H	-4.95295300	-3.57423700	-1.52292500
C	-2.04481500	-5.75901800	-3.01044900
C	-3.28722600	-5.50316900	-3.86589100
H	-5.37868200	-4.98527900	-3.56143200
H	-4.65834600	-5.91374100	-2.24974800
H	-1.16013200	-5.88556800	-3.64420600
H	-2.17225800	-6.71219000	-2.47697700
H	-3.52235600	-6.39394500	-4.45810500
H	-3.08658700	-4.69065600	-4.57630800
C	-4.38468000	1.71713000	0.41072200
C	-3.29588700	2.39968500	0.91781400
C	-5.47859700	2.46069800	-0.11771200
C	-3.24731500	3.81404100	0.91494200

H	-2.45606700	1.86224400	1.34014200
C	-5.46296100	3.83553600	-0.12398000
H	-6.32828900	1.92396600	-0.52880200
C	-4.35239900	4.55563200	0.39130100
C	-2.11507400	4.51306400	1.40950700
H	-6.30532700	4.39010500	-0.52965300
C	-4.28723900	5.97345100	0.39154800
C	-2.07804300	5.88691700	1.38441500
H	-1.27123500	3.93614600	1.77434500
C	-3.17475700	6.62361400	0.87382400
H	-5.12706300	6.53781600	-0.00521900
H	-1.19952700	6.41349100	1.74248000
H	-3.12933900	7.70800800	0.85437900
C	1.26777600	-3.37043000	-0.12213500
C	2.28396600	-3.55974600	-1.04449000
C	1.62421600	-2.99462300	1.20832700
C	3.64981500	-3.40643400	-0.70127800
H	2.03651900	-3.79989000	-2.07357300
C	2.94086000	-2.82062400	1.56931000
H	0.84269900	-2.82717300	1.93715600
C	3.99312300	-3.02589500	0.63500100
C	4.69159500	-3.58862600	-1.65056000
H	3.19091300	-2.50671900	2.57800700
C	5.35838100	-2.83728500	0.97066600
C	6.00763900	-3.40471000	-1.29285700
H	4.42901300	-3.87362500	-2.66535900
C	6.34402700	-3.02234300	0.02863400
H	5.60601700	-2.53250100	1.98202900
H	6.79510200	-3.54807800	-2.02644900
H	7.38521000	-2.86875800	0.29357100

TS-1

C	3.52371600	1.05882700	0.26156400
C	3.37589300	0.44338900	1.59224100
C	2.20012800	0.65766200	2.32528900
C	4.31708900	-0.48619300	2.08549300
C	1.94265900	-0.03515900	3.49868700
H	1.43949100	1.32640300	1.94777300
C	4.08992500	-1.14785600	3.27621100
H	5.20762000	-0.71891500	1.51473800
C	2.88848300	-0.94826700	3.97856100
H	0.98278300	0.10946300	3.97372900
H	4.80041200	-1.86979900	3.66071400
C	4.88861800	1.20776700	-0.33632200

C	5.99003500	1.53311200	0.47277200
C	5.07283700	1.13587400	-1.72118100
C	7.23941800	1.75535800	-0.08661900
H	5.86088000	1.63160000	1.54409900
C	6.32543100	1.33896300	-2.29136900
H	4.22457300	0.89126000	-2.34780800
C	7.41938500	1.65045700	-1.47232200
H	8.09287400	2.01404900	0.52997700
H	6.43772400	1.25613900	-3.36490900
C	2.60398400	2.07635900	-0.11240100
C	1.75090500	2.83423000	-0.53221700
C	0.68362100	3.63731000	-1.00795300
C	-0.54819700	3.02425500	-1.29978000
C	0.82343800	5.02694800	-1.20107000
C	-1.61479100	3.77454700	-1.77771600
H	-0.65712800	1.95691000	-1.15473000
C	-0.24489700	5.77736400	-1.65577900
H	1.77075700	5.50553500	-0.97668900
C	-1.47020900	5.15650000	-1.95109300
H	-2.55691600	3.27873600	-1.97050400
H	-0.16408900	6.84943600	-1.79500900
O	2.78405300	-0.29909300	-0.84401200
H	3.11380500	-1.14829600	-0.50259600
O	8.68280700	1.87008800	-1.92376000
O	2.72390100	-1.71101100	5.08688000
O	-2.45083900	5.98080500	-2.39991400
C	8.91605500	1.79518000	-3.32302800
H	9.97639200	2.00697500	-3.46217100
H	8.69111200	0.79561300	-3.71482600
H	8.32239800	2.53779200	-3.86966200
C	1.48040700	-1.61715700	5.77818300
H	1.54162600	-2.33233200	6.59853000
H	1.32464900	-0.61026800	6.18153600
H	0.64213100	-1.87603200	5.12216800
C	-3.68089800	5.39247100	-2.80579500
H	-4.31174200	6.21925300	-3.13447200
H	-3.52972900	4.69612700	-3.63999700
H	-4.16547800	4.86659600	-1.97808500
H	1.75350800	-0.26523100	-0.61393300
C	-3.61184000	-1.75361500	-0.02554600
C	-3.33236300	-0.39110400	0.15534200
C	-4.29650600	0.49973000	0.66077600
C	-5.52630900	-0.04884400	1.03677300
H	-6.28415400	0.61597100	1.44253300

C	-2.60502400	-2.60582400	-0.72734900
C	-1.31501900	-2.69622400	-0.19686800
C	-0.31109300	-3.47098000	-0.79399500
C	-0.65096600	-4.16594300	-1.95653500
H	0.10049300	-4.79687800	-2.42382500
O	-2.09297200	0.08005200	-0.23892600
O	-1.01427800	-1.93485800	0.91960300
P	-0.73769000	-0.32006800	0.64257300
O	0.36652900	-0.15888300	-0.37912400
O	-0.71236400	0.35242400	1.97295800
C	-5.79626800	-1.41779700	0.97862500
C	-7.14774500	-1.91708000	1.45757100
C	-4.82671300	-2.28910600	0.45650600
C	-7.16250500	-3.41113000	1.78713000
H	-7.89192200	-1.72222900	0.67114700
H	-7.46733300	-1.32881700	2.32509500
C	-5.03382300	-3.79373000	0.51310500
C	-6.50105900	-4.20137300	0.65719500
H	-8.19146100	-3.74785800	1.95442600
H	-6.61175500	-3.58981800	2.71997400
H	-4.58416100	-4.28448500	-0.35150300
H	-4.47280000	-4.16966100	1.38138700
H	-6.56847800	-5.27928400	0.84078100
H	-7.03429400	-4.00576800	-0.28350800
C	-2.89575200	-3.25340500	-1.94969400
C	-4.20293700	-2.97691600	-2.67321000
C	-1.91204800	-4.06052400	-2.54835400
C	-4.54913100	-4.02102100	-3.73646200
H	-4.10434000	-1.99329400	-3.15545400
H	-5.02672600	-2.86637700	-1.96754300
C	-2.18705900	-4.84566900	-3.81829200
C	-3.34530000	-4.28038100	-4.64291000
H	-5.41230900	-3.68079200	-4.31884600
H	-4.84537700	-4.96042000	-3.24960400
H	-1.27315300	-4.89577000	-4.42096300
H	-2.42402500	-5.88408700	-3.54358900
H	-3.60213700	-4.97283700	-5.45199000
H	-3.03879400	-3.33695800	-5.11354300
C	-4.07586000	1.96399200	0.75864200
C	-2.91425500	2.50428100	1.27864600
C	-5.10325900	2.84831300	0.31674800
C	-2.71637800	3.90525600	1.33467300
H	-2.12987400	1.85596700	1.65192000
C	-4.94849900	4.21295400	0.38621400

H	-6.01527300	2.42753000	-0.09566000
C	-3.74540900	4.78644000	0.87702200
C	-1.49433500	4.45716000	1.80209000
H	-5.74423200	4.87215100	0.04804000
C	-3.51387000	6.18576100	0.89937500
C	-1.29570700	5.81770000	1.80314700
H	-0.71517400	3.77638800	2.13104400
C	-2.31472700	6.69009000	1.34823400
H	-4.29393800	6.85267400	0.54202400
H	-0.35067500	6.22979500	2.14335000
H	-2.14252200	7.76215400	1.34862200
C	1.06569700	-3.51433300	-0.25246700
C	2.15100600	-3.37775500	-1.09819000
C	1.30270100	-3.70166500	1.14069100
C	3.48442100	-3.41963800	-0.61116200
H	1.98627500	-3.18461800	-2.15379000
C	2.57970800	-3.78360700	1.63685000
H	0.45246500	-3.77554900	1.80713000
C	3.70775800	-3.65236300	0.78412100
C	4.60549300	-3.18651300	-1.45565600
H	2.74328000	-3.92543800	2.70103500
C	5.04137100	-3.70635900	1.26418700
C	5.88499800	-3.20661500	-0.95012200
H	4.43008900	-2.98195400	-2.50798800
C	6.10668300	-3.48457700	0.42101200
H	5.20626900	-3.91240400	2.31751400
H	6.73075200	-3.01411700	-1.60262600
H	7.12159700	-3.51658300	0.80496200

INT-1

C	-4.53287300	-0.00015200	-0.58605100
C	-3.68738900	-1.03585400	-1.10422800
C	-2.32763000	-0.74825900	-1.39610300
C	-4.13924300	-2.37447100	-1.29695500
C	-1.47771100	-1.70894200	-1.89139100
H	-1.92245600	0.24611900	-1.25588600
C	-3.29292800	-3.34290800	-1.77942100
H	-5.14105400	-2.65130300	-0.99461700
C	-1.94907400	-3.02229300	-2.07940100
H	-0.45565600	-1.42410400	-2.09433000
H	-3.60837400	-4.37463300	-1.86614100
C	-5.99131500	-0.05435800	-0.63473700
C	-6.67945200	-0.69692500	-1.68913700
C	-6.75334400	0.58074200	0.36373200

C	-8.06004700	-0.71978400	-1.72538600
H	-6.11597400	-1.14109200	-2.50079500
C	-8.14007500	0.54991000	0.34666000
H	-6.23773300	1.08056800	1.17661400
C	-8.80450500	-0.10600000	-0.70251500
H	-8.59569400	-1.19234800	-2.54079700
H	-8.69339900	1.02791500	1.14464100
C	-3.93940000	1.10885800	-0.00045300
C	-3.34341200	2.05260200	0.51694300
C	-2.54558900	3.04458300	1.09059800
C	-1.19075900	2.73890300	1.36771100
C	-3.03895900	4.34021600	1.39251400
C	-0.34899900	3.69090700	1.90791600
H	-0.81577500	1.74177900	1.17481800
C	-2.19830200	5.28980100	1.92582900
H	-4.07678800	4.57817800	1.18565900
C	-0.84380000	4.97664300	2.18171100
H	0.68599200	3.42977600	2.08324400
H	-2.54142200	6.29303600	2.14960300
O	-2.25404000	-0.19686400	2.60158500
H	-2.74508300	-0.06363200	1.78186200
O	-10.14757800	-0.19252100	-0.82309800
O	-1.19113800	-4.02674400	-2.52582400
O	-0.10861900	5.97723600	2.69489000
C	-10.96178700	0.42565700	0.16898300
H	-11.99169000	0.23352100	-0.13037100
H	-10.78203300	-0.00940500	1.15867200
H	-10.78829500	1.50704900	0.20828700
C	0.19962100	-3.76875800	-2.78058000
H	0.63757200	-4.74170900	-2.99639800
H	0.30976900	-3.10570200	-3.64474800
H	0.67842000	-3.32530600	-1.90679700
C	1.26830100	5.72809100	2.99144400
H	1.65609500	6.66804400	3.38328600
H	1.36683500	4.94431600	3.75002700
H	1.82003900	5.44808400	2.09042500
H	-1.33037400	-0.20692400	2.27817000
C	4.16979500	-0.27377600	-0.43875500
C	3.40420900	0.89388300	-0.32026800
C	3.77955800	2.09210700	-0.95089100
C	4.93587600	2.06819800	-1.73173700
H	5.24483300	2.98603400	-2.22559100
C	3.82129300	-1.47228700	0.38447300
C	2.54163800	-2.03543800	0.28573500

C	2.21694500	-3.25023000	0.91064800
C	3.21395700	-3.86432700	1.67001800
H	2.98266000	-4.80811400	2.15704900
O	2.28714400	0.87046600	0.48968000
O	1.59934800	-1.40523300	-0.50613600
P	0.93047300	0.04071500	0.00096800
O	0.13856600	-0.14816200	1.26342100
O	0.32219200	0.64268500	-1.22838100
C	5.66068900	0.89626600	-1.96447000
C	6.87507900	0.96126400	-2.87430200
C	5.26406900	-0.29588000	-1.33720400
C	7.29122900	-0.39923400	-3.43621100
H	7.71748800	1.37849400	-2.30280500
H	6.68432600	1.67077400	-3.68739900
C	5.93677800	-1.60952300	-1.70357100
C	7.32888000	-1.43524600	-2.31238100
H	8.26454000	-0.31801300	-3.93257900
H	6.56945200	-0.72218700	-4.19802600
H	5.97876000	-2.28286300	-0.84731000
H	5.28923600	-2.11420600	-2.43600900
H	7.69399900	-2.40051600	-2.68021200
H	8.03306400	-1.10421900	-1.53654400
C	4.76573700	-2.05411200	1.26445700
C	6.04823000	-1.31701900	1.61698800
C	4.46230000	-3.27536300	1.88748700
C	7.13307000	-2.22084900	2.20498800
H	5.78646500	-0.54711400	2.35759400
H	6.43563500	-0.76792100	0.75877500
C	5.46190000	-3.99568100	2.77529800
C	6.55667500	-3.08225400	3.32898600
H	7.96580400	-1.60830000	2.56780000
H	7.53821100	-2.87274200	1.41840500
H	4.92954400	-4.49602400	3.59192100
H	5.93503200	-4.79734000	2.18881000
H	7.33830600	-3.68231300	3.80785000
H	6.13611100	-2.42789300	4.10380100
C	3.00291100	3.35124000	-0.81706900
C	1.66108800	3.40552100	-1.14327500
C	3.65978800	4.54309400	-0.39908900
C	0.93576800	4.61859600	-1.06022000
H	1.14507000	2.50728200	-1.46661400
C	2.97812800	5.73489200	-0.30415500
H	4.71377800	4.49592500	-0.14166200
C	1.59611300	5.81078200	-0.62412800

C	-0.44508200	4.67636700	-1.38940900
H	3.49178600	6.63589100	0.02188700
C	0.84524200	7.01092900	-0.51591000
C	-1.14334800	5.85529700	-1.27978000
H	-0.93577400	3.76142800	-1.70671800
C	-0.49296000	7.03344900	-0.83549300
H	1.34571700	7.91327900	-0.17442500
H	-2.20129300	5.88623500	-1.52099000
H	-1.05746800	7.95667700	-0.74538300
C	0.88482300	-3.90096800	0.78961700
C	-0.27245200	-3.27468400	1.21192800
C	0.80573100	-5.23064500	0.28519400
C	-1.52407500	-3.94222200	1.17185800
H	-0.22651200	-2.26132300	1.59279700
C	-0.39899100	-5.88736200	0.19666600
H	1.71830000	-5.71585200	-0.04871900
C	-1.59679900	-5.27030600	0.64215200
C	-2.70605100	-3.32920800	1.66958800
H	-0.44641500	-6.89508000	-0.20756100
C	-2.85553200	-5.92549400	0.59990600
C	-3.90716400	-4.00129300	1.62894500
H	-2.63433700	-2.33133400	2.09639300
C	-3.98633200	-5.30597600	1.08374400
H	-2.90751600	-6.93165700	0.19186200
H	-4.80406400	-3.52917700	2.02005900
H	-4.94201000	-5.82198600	1.05726400

INT-2

O	-0.07483000	-0.68476300	-2.21082200
H	-0.11371700	-0.90127500	-1.23975700
O	8.51037500	0.97186800	-0.49826300
O	1.79085100	-4.01605900	5.03775700
O	-2.41083400	5.08174000	-0.80219300
N	3.74298700	-1.51514400	-0.75254100
C	3.55504000	0.38780900	2.04998700
C	2.58925300	1.33760800	1.73703800
C	1.70216900	2.11364700	1.40085300
C	2.54353600	-0.83815700	-0.77550000
C	2.61755700	0.22862200	-1.64833200
C	3.95317300	0.18335500	-2.22102700
C	4.64286500	0.94436000	-3.17966000
H	4.16075800	1.79223300	-3.65254900
C	5.94677500	0.59610300	-3.51718600
H	6.47653200	1.17620200	-4.26765300

C	6.58322900	-0.51660300	-2.93041600
H	7.59814900	-0.77053500	-3.22007800
C	5.92260100	-1.29974200	-1.99063700
H	6.40278100	-2.16234900	-1.53919400
C	4.62047800	-0.93672100	-1.64177400
C	1.51963800	1.13198600	-2.04267400
C	0.25838900	0.62064400	-2.37334300
C	-0.72829800	1.44916000	-2.96381700
H	-1.66969400	0.97607300	-3.22306700
C	-0.50295400	2.78351500	-3.18029300
H	-1.27113300	3.41193700	-3.62217300
C	0.71943000	3.37391300	-2.77419500
C	0.95033800	4.76606600	-2.91680200
H	0.17475200	5.36936000	-3.38234600
C	2.11620900	5.34705700	-2.47360200
H	2.27733200	6.41503400	-2.58643900
C	3.09923800	4.54338100	-1.85272900
H	4.01145800	5.00129300	-1.47924900
C	2.91109400	3.18529300	-1.71548900
H	3.66750600	2.58023800	-1.23440600
C	1.73224500	2.54532900	-2.18576900
C	0.65638800	2.92673200	0.94782800
C	0.81676800	4.31535700	0.77277600
H	1.75026100	4.78665700	1.05578100
C	-0.20798000	5.07467400	0.23574000
H	-0.07353100	6.14050000	0.11509100
C	-1.38673100	4.44088900	-0.19276500
C	-1.55075400	3.05691000	-0.02971100
H	-2.46183900	2.58776300	-0.37395900
C	-0.55649200	2.30892800	0.55760100
H	-0.66209300	1.23910800	0.65106800
C	-2.31344700	6.48870100	-0.98062800
H	-2.24195400	7.00026100	-0.01511800
H	-3.23293600	6.78949200	-1.48337800
H	-1.45221000	6.75005500	-1.60654400
C	3.12513200	-0.75675100	2.82556100
C	1.75660000	-1.11626400	2.80554600
H	1.06551400	-0.57796800	2.17154900
C	1.27271100	-2.19370800	3.51990800
H	0.21307900	-2.40687700	3.44116800
C	2.15744200	-2.94656200	4.30522000
C	3.51948500	-2.58658100	4.38095000
H	4.16814700	-3.15137400	5.04089700
C	3.99259300	-1.51120100	3.65980500

H	5.02249000	-1.20438600	3.79119600
C	0.39505300	-4.32146600	5.12444600
H	-0.02132900	-4.56010200	4.14209400
H	-0.16166100	-3.48208200	5.55215800
H	0.32462800	-5.18994300	5.77840100
C	4.89199600	0.57979400	1.52538300
C	5.22032400	1.79964300	0.89174400
H	4.49975800	2.60813800	0.91679800
C	6.41342800	1.97770400	0.21729500
H	6.60836500	2.91690200	-0.28274900
C	7.34151000	0.92399300	0.16447600
C	7.05389300	-0.28930100	0.81566300
H	7.76935300	-1.09833300	0.72939500
C	5.84704700	-0.46649000	1.45531700
H	5.60319300	-1.44630900	1.84001300
C	8.73926000	2.06619500	-1.38704000
H	7.93284000	2.13039000	-2.12439100
H	9.68288100	1.84761700	-1.88606600
H	8.82912700	3.01095600	-0.83948000
C	-3.72030500	-2.11547800	-1.19496300
C	-2.55294200	-2.77757300	-0.79654200
C	-1.68667100	-3.40353100	-1.70849100
C	-2.09389100	-3.40719100	-3.04602700
H	-1.47209400	-3.91208000	-3.77924000
C	-4.53308700	-1.38989700	-0.16907800
C	-3.91401400	-0.39058000	0.59242200
C	-4.64303800	0.48858400	1.40817400
C	-6.01991700	0.28476000	1.49375900
H	-6.60575900	0.95514200	2.11729900
O	-2.22833200	-2.73785900	0.54923000
O	-2.54848200	-0.21491900	0.48027100
P	-1.51561700	-1.35694600	1.11674600
O	-1.55845600	-1.43875800	2.60720300
O	-0.21912100	-1.07079400	0.39192400
C	-3.23373000	-2.73793300	-3.49081000
C	-3.56420400	-2.76880700	-4.97177600
C	-4.03496300	-2.03865900	-2.57053300
C	-4.39861500	-1.57051000	-5.42622300
H	-4.12323000	-3.69057400	-5.19116100
H	-2.63565500	-2.83282900	-5.54931800
C	-5.12355900	-1.09914800	-3.06406100
C	-5.59410300	-1.39029700	-4.49049100
H	-4.72671700	-1.71151900	-6.46198000
H	-3.78138900	-0.66244100	-5.40588100

H	-5.97516100	-1.08552500	-2.38355200
H	-4.70988600	-0.08039600	-3.02399800
H	-6.24464300	-0.57861100	-4.83446200
H	-6.20007500	-2.30689100	-4.49871000
C	-5.91045100	-1.64168200	0.02640300
C	-6.54865400	-2.88336300	-0.57264100
C	-6.65612900	-0.78494200	0.85340800
C	-8.07395000	-2.80499500	-0.65359200
H	-6.26892100	-3.73517700	0.06441900
H	-6.12112900	-3.10587100	-1.55162300
C	-8.15258200	-0.96195100	1.04404200
C	-8.65210700	-2.36486700	0.69223200
H	-8.47914400	-3.77706300	-0.95520800
H	-8.36780900	-2.08389000	-1.42894900
H	-8.42160400	-0.70688100	2.07531600
H	-8.67458600	-0.23168800	0.40805700
H	-9.74743000	-2.37853100	0.67510000
H	-8.33565800	-3.07518000	1.46734200
C	-0.33658100	-3.88383100	-1.32624100
C	-0.04750600	-4.44335600	-0.09328200
C	0.73793600	-3.67709800	-2.24250400
C	1.28346100	-4.74287300	0.28791600
H	-0.83980200	-4.60784800	0.62535300
C	2.03019700	-4.00623400	-1.92101200
H	0.53360400	-3.17785700	-3.18086300
C	2.35002500	-4.52555400	-0.64098200
C	1.60176000	-5.20870300	1.59103600
H	2.83362500	-3.80540200	-2.62364000
C	3.68588100	-4.77432300	-0.22468500
C	2.90622600	-5.41159800	1.97923800
H	0.78765000	-5.38589800	2.28687000
C	3.96123100	-5.19095500	1.06086400
H	4.49029000	-4.63012000	-0.94292400
H	3.12684000	-5.73240000	2.99210900
H	4.98775600	-5.36574700	1.36942800
C	-3.97131000	1.63322400	2.07701300
C	-4.38206900	2.92422500	1.80482500
C	-2.86345800	1.42630400	2.94766200
C	-3.69464300	4.04754000	2.33265000
H	-5.21536100	3.09226200	1.12795100
C	-2.18424300	2.49589000	3.47677500
H	-2.54311400	0.41319400	3.16443200
C	-2.55862700	3.83114300	3.17567500
C	-4.06774900	5.37939000	2.01590200

H	-1.32723100	2.32632000	4.12296400
C	-1.83795400	4.95287200	3.65880300
C	-3.35033300	6.44881700	2.50388300
H	-4.92762300	5.53982700	1.37157200
C	-2.22070000	6.23360300	3.33046600
H	-0.96983900	4.78095700	4.28918400
H	-3.65187000	7.46342800	2.25955600
H	-1.65908200	7.08405400	3.70532700
H	1.72022800	-1.16531900	-0.16094200
H	3.88677400	-2.38104100	-0.25487500

TS-2

O	-0.26976500	0.30068800	3.15762300
H	0.37274600	0.16173400	2.40116600
O	-9.06304500	-2.01153100	-1.98945300
O	0.41849700	-4.16306900	-4.42926200
O	-0.71533500	6.19930800	0.04548200
N	-2.95356100	-1.41349100	0.81363300
C	-3.53394100	-0.85042400	-2.12337300
C	-3.13269200	0.21867400	-1.41617100
C	-2.54446300	0.93806000	-0.54093300
C	-2.16127000	-0.28394600	0.99245700
C	-2.78894000	0.50883300	2.02437200
C	-4.05436700	-0.08596700	2.28234400
C	-5.11360800	0.23358100	3.16089000
H	-5.04805400	1.11200200	3.79235800
C	-6.22451600	-0.58587900	3.18868700
H	-7.05133600	-0.35567300	3.85214500
C	-6.30363900	-1.72620400	2.35209900
H	-7.20122000	-2.33656200	2.37809900
C	-5.26930600	-2.09133900	1.50609600
H	-5.33555100	-2.96510000	0.87377800
C	-4.12895500	-1.27740800	1.49270600
C	-2.15660200	1.67076000	2.62529400
C	-0.83996300	1.52421400	3.09142000
C	-0.13127000	2.64442300	3.58879100
H	0.88129100	2.48355100	3.94210700
C	-0.71757000	3.88332500	3.61813000
H	-0.16583100	4.74186300	3.99167100
C	-2.05560000	4.07642800	3.18117800
C	-2.65365300	5.36083500	3.20485700
H	-2.06668000	6.19771800	3.57244800
C	-3.94268300	5.55043900	2.76285200
H	-4.39069200	6.53866800	2.78442900

C	-4.67477400	4.45265100	2.26244900
H	-5.68341600	4.60388600	1.88976100
C	-4.11483900	3.19500300	2.21400700
H	-4.67681900	2.37929800	1.77942800
C	-2.80023500	2.95672000	2.69143100
C	-2.03829700	2.28291700	-0.40220300
C	-2.86833600	3.38677900	-0.68169200
H	-3.89115100	3.21342400	-0.99840600
C	-2.39255200	4.67845800	-0.54460100
H	-3.02150200	5.53676000	-0.75107600
C	-1.08238300	4.90074200	-0.09046500
C	-0.24706000	3.81295800	0.18709000
H	0.77501800	3.95586900	0.50902000
C	-0.72378100	2.51983800	0.02626700
H	-0.07428400	1.68431100	0.24456200
C	0.60554400	6.46694100	0.50525800
H	0.76577700	6.04721200	1.50594400
H	0.69070900	7.55313700	0.54798300
H	1.35610400	6.07267500	-0.18570100
C	-2.51124300	-1.71658100	-2.73512500
C	-1.14950500	-1.48351900	-2.46267500
H	-0.83800000	-0.65526500	-1.84037700
C	-0.14490600	-2.26498200	-3.00924700
H	0.87641900	-2.00762100	-2.76184600
C	-0.48356400	-3.32479200	-3.86132100
C	-1.83424400	-3.56003200	-4.17446300
H	-2.07468400	-4.36454200	-4.86088800
C	-2.82788200	-2.76321300	-3.62840300
H	-3.85833900	-2.94163600	-3.91078300
C	1.79634000	-3.94639200	-4.13282900
H	1.99060300	-4.02239400	-3.05686600
H	2.12969300	-2.96379000	-4.48418100
H	2.34063000	-4.72958800	-4.66062300
C	-4.98238700	-1.14633100	-2.19050000
C	-5.91586900	-0.11228300	-2.32767400
H	-5.55624500	0.89967000	-2.48325300
C	-7.28644700	-0.35485200	-2.27418800
H	-7.97677700	0.47033600	-2.39519800
C	-7.75047600	-1.65946500	-2.06705600
C	-6.82876600	-2.70595500	-1.91949200
H	-7.20663300	-3.70747400	-1.74444400
C	-5.46802200	-2.45207000	-1.98370700
H	-4.76750200	-3.26398900	-1.82615100
C	-10.03716900	-0.98705400	-2.12141100

H	-9.93400800	-0.22995400	-1.33420100
H	-11.00557600	-1.47856700	-2.02479000
H	-9.97544600	-0.49720600	-3.10098700
C	4.46684800	-1.66172200	0.96072300
C	3.15008400	-2.11921000	0.84480900
C	2.51460800	-2.85823300	1.85398500
C	3.28817900	-3.17143100	2.97661900
H	2.84613200	-3.77928500	3.76085700
C	5.03349200	-0.82277900	-0.13934000
C	4.38105400	0.37335600	-0.47555400
C	4.94082500	1.29446300	-1.37651500
C	6.15625800	0.93921000	-1.96863400
H	6.60679200	1.63208500	-2.67435300
O	2.44338200	-1.74395900	-0.28725600
O	3.18051200	0.66659600	0.14766600
P	1.82586100	-0.20384200	-0.25277800
O	1.33096700	0.09297500	-1.62831500
O	0.91620300	-0.05420000	0.94424100
C	4.59586800	-2.71307200	3.14480600
C	5.34527700	-3.10000100	4.40674500
C	5.18706300	-1.91509400	2.14943300
C	6.48283200	-2.13767900	4.75352100
H	5.76555600	-4.10736800	4.27041100
H	4.63876900	-3.17881500	5.24049200
C	6.51696200	-1.22752000	2.40967600
C	7.34429100	-1.88694300	3.51516400
H	7.08215800	-2.54551100	5.57483500
H	6.06660900	-1.18369400	5.10298600
H	7.10448600	-1.14631100	1.49478400
H	6.29348200	-0.19017100	2.69913000
H	8.20474300	-1.25366500	3.75739300
H	7.74652800	-2.84370800	3.15456100
C	6.20475000	-1.19634200	-0.83413300
C	6.77421900	-2.59691700	-0.67874700
C	6.77599900	-0.29251300	-1.74476300
C	8.22807400	-2.71708700	-1.13925200
H	6.15265500	-3.27379300	-1.28349900
H	6.66652400	-2.95141900	0.34759200
C	8.07054700	-0.60266900	-2.47498800
C	8.39738600	-2.09667800	-2.52671700
H	8.52946000	-3.77029800	-1.14092200
H	8.88584600	-2.19959400	-0.42729200
H	8.02906600	-0.18270700	-3.48622600
H	8.89332700	-0.07967400	-1.96544700

H	9.41531900	-2.24485200	-2.90346500
H	7.72011300	-2.59962400	-3.22964100
C	1.08670200	-3.24979600	1.79659100
C	0.46768400	-3.66480500	0.63043700
C	0.31723100	-3.21736100	2.99738100
C	-0.88215300	-4.09611800	0.62414200
H	1.01581800	-3.66511900	-0.30303400
C	-0.98662700	-3.64371100	3.02644300
H	0.77170500	-2.81786400	3.89694600
C	-1.62128900	-4.12036800	1.85119000
C	-1.53002800	-4.51050200	-0.57121600
H	-1.55444900	-3.60462300	3.95153400
C	-2.95882100	-4.59164600	1.84121300
C	-2.83442800	-4.95289000	-0.55108800
H	-0.98090400	-4.47219200	-1.50434600
C	-3.55228500	-5.00695000	0.66906700
H	-3.51408100	-4.60542400	2.77449400
H	-3.30739600	-5.27180100	-1.47478100
H	-4.57452100	-5.37368600	0.67605500
C	4.32404800	2.61006500	-1.68484600
C	2.99484500	2.73899800	-2.04455600
C	5.14142500	3.77663500	-1.64382700
C	2.44430500	4.00458500	-2.36884300
H	2.35573400	1.86430500	-2.10369800
C	4.63294700	5.01613600	-1.94982900
H	6.18055600	3.67572000	-1.34544600
C	3.27215500	5.17200500	-2.32192700
C	1.07994500	4.14426900	-2.74151800
H	5.26978600	5.89588300	-1.90598200
C	2.70330500	6.43185200	-2.64707800
C	0.55740900	5.37919900	-3.04921800
H	0.45703300	3.25584000	-2.75693600
C	1.37659100	6.53375300	-3.00252400
H	3.33453400	7.31603600	-2.61026300
H	-0.49117700	5.47388300	-3.31202000
H	0.95076200	7.50302800	-3.24400600
H	-1.08815700	-0.36565300	0.84325900
H	-2.73846100	-2.15535500	0.16347300

INT-3

O	-1.88428400	-1.60015500	1.00185300
H	-1.26456600	-1.28711300	0.30323400
O	4.30331300	5.11541900	2.56996200
O	-0.55352600	-3.44345200	4.69819500

O	-7.26847300	3.74774900	1.00307400
N	-1.67424200	1.49126400	-2.21706500
C	0.00967600	1.48512400	1.96688600
C	-1.02671700	1.70137800	1.18237300
C	-2.03101800	1.75415900	0.33764200
C	-1.96534700	0.88235700	-0.91850600
C	-3.16430000	0.03787000	-1.14104500
C	-3.44254500	0.05919900	-2.51700200
C	-4.37245000	-0.65751900	-3.31750600
H	-5.10888500	-1.29313200	-2.84450800
C	-4.28718300	-0.54371900	-4.68226400
H	-4.97757700	-1.08787700	-5.31772600
C	-3.28192500	0.26689400	-5.28896700
H	-3.23845900	0.31574300	-6.37286000
C	-2.36432500	0.97972200	-4.54984200
H	-1.59349700	1.58146100	-5.01712700
C	-2.45774400	0.89743900	-3.14362700
C	-3.87533300	-0.61416500	-0.06322700
C	-3.18293300	-1.31789400	0.94559100
C	-3.89883000	-1.89153900	2.03614900
H	-3.30663500	-2.41514500	2.77732000
C	-5.25386800	-1.78896600	2.12584300
H	-5.78181300	-2.24018400	2.96142500
C	-6.00336500	-1.07479600	1.15020000
C	-7.40114200	-0.90937200	1.29510300
H	-7.89231300	-1.39351100	2.13486100
C	-8.12189200	-0.13845100	0.40905900
H	-9.19344700	-0.01429900	0.52880400
C	-7.44432700	0.50899200	-0.64234900
H	-7.99061000	1.16070900	-1.31664700
C	-6.08426600	0.35124700	-0.81184200
H	-5.59372700	0.90695200	-1.59662700
C	-5.31657900	-0.46820500	0.05339300
C	-3.33895400	2.40716500	0.60635900
C	-3.97770300	3.15556500	-0.39525300
H	-3.45274100	3.35835900	-1.32372200
C	-5.27463600	3.61728400	-0.22100200
H	-5.78241200	4.18250400	-0.99517100
C	-5.97325300	3.32072200	0.95733200
C	-5.33744000	2.60812900	1.97873900
H	-5.85859500	2.35936200	2.89427000
C	-4.02987700	2.16069400	1.79456800
H	-3.55723900	1.55354700	2.55939900
C	-8.05710400	3.33308100	2.10758200

H	-8.09533200	2.23923400	2.17771500
H	-9.05967000	3.72222000	1.92487600
H	-7.67955700	3.74470500	3.05223300
C	-0.03127100	0.21809000	2.76695000
C	0.82298700	-0.84564200	2.45875100
H	1.55013800	-0.73557900	1.66582200
C	0.69473800	-2.07927400	3.09470700
H	1.34735400	-2.88844100	2.79391700
C	-0.30726500	-2.26151600	4.05265700
C	-1.14535700	-1.19404300	4.39674600
H	-1.90386300	-1.35099400	5.15636300
C	-1.00611500	0.03004200	3.75508800
H	-1.66611200	0.85279000	4.01189200
C	0.23994800	-4.55955400	4.33664000
H	1.30059400	-4.39361300	4.56379600
H	0.14215300	-4.79502600	3.26881100
H	-0.12710000	-5.39964900	4.92799800
C	1.14434200	2.43111600	2.07157300
C	0.95045600	3.78878400	1.78948900
H	-0.02640600	4.12594800	1.45838400
C	1.97430600	4.71851900	1.93920800
H	1.78535900	5.75704300	1.70110000
C	3.23383500	4.29087000	2.37065200
C	3.45073200	2.93329200	2.63669600
H	4.43700200	2.62076800	2.96162900
C	2.41675100	2.02047400	2.50189400
H	2.59625500	0.97892100	2.73508000
C	4.07502200	6.51401800	2.50938800
H	3.75476000	6.83036500	1.51182500
H	5.02866500	6.98617200	2.75073900
H	3.31887600	6.82583800	3.24144400
H	-0.66922800	1.57900600	-2.42986600
H	-1.09449300	0.19469100	-0.75951400
C	4.35202700	-1.24067000	-0.77620300
C	3.81018800	0.05386200	-0.76017900
C	4.58836700	1.19038100	-1.05328600
C	5.91817700	0.94710200	-1.42161600
H	6.54031700	1.79473000	-1.69094700
C	3.49486500	-2.39197600	-0.36103600
C	2.31397700	-2.63123600	-1.06851400
C	1.43247300	-3.67258500	-0.74552200
C	1.82535000	-4.51930900	0.29533200
H	1.18587000	-5.36115600	0.54645700
O	2.47603400	0.19194000	-0.39832800

O	1.95723900	-1.69725500	-2.04080700
P	1.26342000	-0.35332900	-1.38877800
O	0.16927700	-0.79522100	-0.43959400
O	0.95032900	0.62102300	-2.48400400
C	6.46618500	-0.33034000	-1.53183800
C	7.91141300	-0.46869200	-1.97507800
C	5.67593500	-1.44732400	-1.22027500
C	8.24717400	-1.85656500	-2.52397300
H	8.56324600	-0.26314200	-1.11317600
H	8.14042400	0.30526900	-2.71613500
C	6.19417500	-2.85316000	-1.47410000
C	7.71885100	-2.93178600	-1.57374100
H	9.32920400	-1.95229300	-2.66527900
H	7.78266300	-1.98777000	-3.51011000
H	5.82799500	-3.54930200	-0.71785100
H	5.75500200	-3.20030300	-2.42093200
H	8.01467500	-3.93194100	-1.90848200
H	8.16210200	-2.78539500	-0.57910500
C	3.80516400	-3.19705700	0.75577100
C	4.93062600	-2.80092400	1.69662800
C	2.97842400	-4.29617600	1.05269800
C	5.39462500	-3.93493900	2.61250700
H	4.55646300	-1.97167600	2.31508500
H	5.77547000	-2.38726800	1.14407600
C	3.31622100	-5.25636100	2.17892800
C	4.19422800	-4.62566200	3.26123300
H	6.07654300	-3.53855600	3.37224200
H	5.96252400	-4.67250800	2.02924600
H	2.39164000	-5.65513500	2.61039000
H	3.84655600	-6.12207800	1.75622000
H	4.51776900	-5.39063500	3.97536100
H	3.61421300	-3.88335300	3.82632700
C	4.10092400	2.59228300	-1.00229900
C	2.81224800	2.95384500	-1.35023700
C	5.01393900	3.62587300	-0.63429500
C	2.39704200	4.30675100	-1.34160000
H	2.10000300	2.20712500	-1.66771200
C	4.65308600	4.94942800	-0.66536700
H	6.01059600	3.35686700	-0.30221700
C	3.33545900	5.33550100	-1.01947400
C	1.05382600	4.66823300	-1.62816100
H	5.36894900	5.71537300	-0.38126600
C	2.90261000	6.68696100	-1.02618700
C	0.65496400	5.98453800	-1.59624800

H	0.34017800	3.87949800	-1.84743300
C	1.59095700	7.00605400	-1.29949200
H	3.62478200	7.46932400	-0.80641100
H	-0.37861800	6.24670800	-1.80119800
H	1.26972800	8.04335700	-1.29227200
C	0.09611400	-3.79201900	-1.37277800
C	-1.00508800	-4.05153700	-0.57774600
C	-0.10189600	-3.57950400	-2.76802000
C	-2.31652400	-4.09086400	-1.11189300
H	-0.88199400	-4.14766300	0.49561700
C	-1.36066800	-3.61534200	-3.31530800
H	0.75587700	-3.36955700	-3.39420900
C	-2.50471500	-3.86616500	-2.51221100
C	-3.45628500	-4.30205700	-0.29211300
H	-1.49687400	-3.44234800	-4.37927100
C	-3.82152900	-3.88736900	-3.03851400
C	-4.72372600	-4.28990200	-0.82674900
H	-3.30950100	-4.45056900	0.77282100
C	-4.90797900	-4.09013800	-2.21604100
H	-3.95837200	-3.72552300	-4.10383700
H	-5.58686000	-4.42777000	-0.18349800
H	-5.91198000	-4.09575800	-2.63033600

TS-3

O	-1.95525600	-1.45269200	1.19544200
H	-1.35721800	-1.18785400	0.47103200
O	4.81482600	4.93077500	2.29523300
O	-0.99853900	-2.90089100	4.95248100
O	-6.95971300	4.29939000	1.04709200
N	-1.59880900	1.50412100	-2.24133600
C	0.19942600	1.69457000	1.88159500
C	-0.82785000	1.93277100	1.09236400
C	-1.86780100	1.98397100	0.29080700
C	-3.07164400	0.18133700	-1.04254500
C	-3.28164100	-0.02877600	-2.41995800
C	-4.16008500	-0.87790900	-3.13398800
H	-4.88762700	-1.47647800	-2.60076400
C	-4.03647800	-0.93888100	-4.50181900
H	-4.68690100	-1.59213300	-5.07262500
C	-3.03841200	-0.18732400	-5.18318100
H	-2.95942500	-0.28339700	-6.26187500
C	-2.16372300	0.64833100	-4.51912000
H	-1.39165900	1.20246400	-5.04029500
C	-2.31191000	0.75547700	-3.12288900

C	-3.84487000	-0.34944500	0.08358600
C	-3.24026500	-1.06955300	1.11863400
C	-4.01114100	-1.52718800	2.22386800
H	-3.48136100	-2.07606200	2.99424200
C	-5.34994000	-1.27211700	2.30133300
H	-5.92551400	-1.62542500	3.15237000
C	-6.01222700	-0.52878100	1.28763500
C	-7.38961900	-0.21617800	1.39277000
H	-7.93896100	-0.59225700	2.25184000
C	-8.01854000	0.55313500	0.43922600
H	-9.07385200	0.79039800	0.52986800
C	-7.27357700	1.04219900	-0.65415300
H	-7.75417400	1.67547400	-1.39305800
C	-5.93465900	0.74534200	-0.78658100
H	-5.38349400	1.16521300	-1.61583600
C	-5.25712400	-0.05922900	0.16683700
C	-3.12906600	2.72163900	0.57822300
C	-3.75896900	3.46629700	-0.43163100
H	-3.25926200	3.59606900	-1.38697900
C	-5.02005800	4.00826000	-0.23448600
H	-5.52241700	4.57087900	-1.01394300
C	-5.69461500	3.79334600	0.97538100
C	-5.06771600	3.08008200	2.00143800
H	-5.57306100	2.89164400	2.93992200
C	-3.79292300	2.55374900	1.79477600
H	-3.33231900	1.94584700	2.56576100
C	-7.73763300	3.96152600	2.18472900
H	-7.83683000	2.87408300	2.28705700
H	-8.72110700	4.40365900	2.01928800
H	-7.30928600	4.37575500	3.10642200
C	0.02717900	0.50720400	2.78145200
C	0.73610200	-0.67763800	2.56072500
H	1.47377900	-0.72096100	1.76903500
C	0.44621500	-1.83221000	3.28822500
H	0.98034000	-2.74288500	3.05428800
C	-0.57568800	-1.80981600	4.24195600
C	-1.25804300	-0.61704100	4.50642800
H	-2.03357800	-0.61720900	5.26478400
C	-0.95611100	0.52583000	3.77971700
H	-1.49750500	1.44697800	3.96972300
C	-0.42051600	-4.15344600	4.63154100
H	0.65045800	-4.17877100	4.86771600
H	-0.55484200	-4.39629700	3.56964000
H	-0.93874000	-4.89425600	5.24219400

C	1.42152500	2.52593500	1.91880600
C	1.40268100	3.83369400	1.41826400
H	0.49626400	4.21067000	0.95507000
C	2.50984300	4.66901500	1.51937400
H	2.45457300	5.67254000	1.11812800
C	3.67991700	4.19189000	2.12018800
C	3.72649000	2.87627700	2.59618200
H	4.64497600	2.52306400	3.05206600
C	2.60773300	2.06158300	2.50932800
H	2.64840800	1.05744600	2.91339200
C	4.73017300	6.32841400	2.06537100
H	4.52252300	6.55686700	1.01560500
H	5.70368100	6.73855500	2.33889700
H	3.95297700	6.78720400	2.68990000
H	-0.60878700	1.66706900	-2.44719800
C	4.11777000	-1.58912500	-0.56862800
C	3.75236400	-0.23988900	-0.67453700
C	4.68277000	0.76125600	-1.00936800
C	5.98406400	0.32147500	-1.28614800
H	6.72176000	1.05966600	-1.58419400
C	3.09944000	-2.59002900	-0.13114000
C	1.93842500	-2.73855900	-0.89278600
C	0.93975100	-3.67041200	-0.58477900
C	1.17246500	-4.48850000	0.52394900
H	0.43502000	-5.24813000	0.76801500
O	2.42753400	0.09305300	-0.39578800
O	1.73269700	-1.82980300	-1.93623200
P	1.21643300	-0.36469200	-1.41491300
O	0.02056800	-0.60599400	-0.48148000
O	1.03539700	0.56671000	-2.56766900
C	6.36420500	-1.02002600	-1.27407400
C	7.79509900	-1.37717900	-1.63301600
C	5.42120400	-1.99900800	-0.92617300
C	7.96148800	-2.83028500	-2.08074200
H	8.43076000	-1.20391000	-0.75229700
H	8.15811800	-0.69054200	-2.40575200
C	5.75809100	-3.47518400	-1.05599900
C	7.26120600	-3.76002700	-1.08937800
H	9.02525700	-3.07642900	-2.16753000
H	7.51949200	-2.96465700	-3.07677800
H	5.28333200	-4.05849900	-0.26576000
H	5.30350300	-3.83456800	-1.99077400
H	7.42938800	-4.81062500	-1.34950400
H	7.68818600	-3.60859200	-0.08847700

C	3.25709400	-3.36195400	1.04062700
C	4.37200800	-3.04680300	2.02278200
C	2.29813500	-4.34598500	1.34053600
C	4.68115300	-4.19482000	2.98462200
H	4.05025100	-2.17025000	2.60445100
H	5.27485700	-2.72859500	1.50000700
C	2.47502700	-5.28573900	2.52006300
C	3.39066300	-4.72556700	3.61041000
H	5.37742300	-3.85113500	3.75674900
H	5.18312600	-5.00760200	2.44226700
H	1.49416700	-5.54696300	2.93090100
H	2.90415600	-6.22844500	2.15076700
H	3.60243500	-5.50010700	4.35533200
H	2.88699300	-3.90387000	4.13670300
C	4.38604900	2.21319600	-1.10039800
C	3.19166700	2.70743400	-1.59041300
C	5.40476600	3.14476500	-0.73789600
C	2.97289500	4.09885700	-1.73216700
H	2.40642100	2.03729800	-1.90861700
C	5.23853700	4.49524900	-0.91269800
H	6.32443900	2.77613700	-0.29712800
C	4.02001100	5.01846500	-1.41523900
C	1.72256400	4.60844300	-2.17142500
H	6.03157500	5.18179300	-0.63099800
C	3.78519700	6.40900200	-1.57325000
C	1.51323300	5.96342300	-2.28692100
H	0.92818800	3.90344200	-2.39902100
C	2.55772800	6.87361500	-1.99092400
H	4.59120900	7.10461400	-1.35341600
H	0.54815100	6.34130100	-2.61044800
H	2.38699400	7.94047500	-2.09919700
C	-0.32542400	-3.76146000	-1.35042100
C	-1.53269500	-3.82378100	-0.67957000
C	-0.32523900	-3.79756200	-2.77395700
C	-2.76301700	-3.93064500	-1.37553600
H	-1.55222300	-3.73695600	0.40063100
C	-1.49863100	-3.93887000	-3.47334300
H	0.61830300	-3.71980100	-3.30098800
C	-2.74718800	-4.02707100	-2.80315600
C	-4.01333900	-3.94180700	-0.70068600
H	-1.48425800	-3.98426300	-4.55870400
C	-3.97503400	-4.19601100	-3.49335800
C	-5.19009300	-4.08178300	-1.40102400
H	-4.02609000	-3.83119200	0.37901800

C	-5.16996800	-4.22872700	-2.81017300
H	-3.95494600	-4.28986300	-4.57558500
H	-6.13852600	-4.08224900	-0.87298800
H	-6.10354700	-4.35597000	-3.34997800
C	-1.93013100	1.05664900	-0.90634100
H	-1.01138000	0.24956700	-0.71836900

INT-4

O	-2.66843000	-1.33763800	0.99946300
H	-2.10438400	-1.00534500	0.28439300
O	4.39424900	4.91897000	2.36715200
O	-1.21788000	-2.98183500	4.86146100
O	-7.51790600	3.71130600	1.75315100
N	-1.47766600	1.31322800	-1.96976700
C	-0.15271300	1.62864600	1.74579500
C	-1.22202600	1.90860000	1.02741500
C	-2.34129900	1.95878900	0.33203700
C	-3.36857400	0.26308000	-1.27759500
C	-3.06086200	-0.18551000	-2.62061100
C	-3.65929500	-1.11137900	-3.48284200
H	-4.53402100	-1.66628800	-3.16602000
C	-3.09094400	-1.31106400	-4.73487400
H	-3.54155900	-2.02722400	-5.41431300
C	-1.92767000	-0.62489100	-5.12818600
H	-1.49834600	-0.81870100	-6.10601200
C	-1.30297800	0.28884300	-4.28190800
H	-0.37796900	0.78352000	-4.55289900
C	-1.89612000	0.50253900	-3.04084500
C	-4.38088200	-0.25032500	-0.33052700
C	-3.96120700	-0.98155600	0.77443000
C	-4.88023900	-1.40766500	1.76444600
H	-4.49102200	-1.96697500	2.60855300
C	-6.20780200	-1.08529900	1.65605300
H	-6.91009200	-1.39674200	2.42449000
C	-6.68915600	-0.33114200	0.55366600
C	-8.04976200	0.05297900	0.44691600
H	-8.74069100	-0.26338900	1.22441500
C	-8.49055300	0.81145500	-0.61380900
H	-9.53284200	1.10703800	-0.68050600
C	-7.58121700	1.20295400	-1.62303300
H	-7.93296300	1.79899600	-2.45970900
C	-6.25391100	0.84609600	-1.54834200
H	-5.55682200	1.16039200	-2.31674900
C	-5.76444400	0.07778800	-0.45984600

C	-3.62902500	2.54138700	0.80966000
C	-4.39968400	3.34028800	-0.04844600
H	-4.00068500	3.61868500	-1.01916100
C	-5.67845100	3.74066200	0.30437200
H	-6.29012600	4.33542300	-0.36444200
C	-6.23044800	3.32364000	1.52220500
C	-5.46561300	2.54899800	2.40085200
H	-5.87552500	2.20303300	3.34115400
C	-4.17340300	2.17012400	2.04020900
H	-3.60850800	1.51340600	2.69072400
C	-8.19013600	3.12868300	2.85682300
H	-8.19117300	2.03416700	2.78530600
H	-9.21616600	3.49675100	2.81448400
H	-7.74166700	3.42851800	3.81273200
C	-0.30449200	0.40700000	2.60689000
C	0.37750000	-0.78447600	2.34753000
H	1.09432800	-0.82879800	1.53735900
C	0.11308100	-1.93701900	3.09184100
H	0.64180900	-2.84624900	2.84556400
C	-0.85141200	-1.90522900	4.10389500
C	-1.51321000	-0.70722600	4.39754200
H	-2.24178200	-0.69692600	5.20094800
C	-1.23581200	0.43054800	3.65621400
H	-1.74826200	1.35983400	3.88063400
C	-0.59345700	-4.22259400	4.58805600
H	0.48526000	-4.18118500	4.78242400
H	-0.75611800	-4.53726200	3.54891600
H	-1.05175700	-4.94928600	5.26023200
C	1.07006700	2.45775300	1.79638100
C	1.08940200	3.73939400	1.22954400
H	0.21713200	4.09049300	0.68610400
C	2.18179400	4.58611300	1.37941100
H	2.15681500	5.57235400	0.93415400
C	3.29832100	4.14885600	2.10300500
C	3.32274600	2.84753000	2.61701800
H	4.20460300	2.52083800	3.15720300
C	2.21791300	2.02018500	2.47621800
H	2.23218900	1.03078800	2.91768400
C	4.26791200	6.32097900	2.18215600
H	4.13757600	6.58457900	1.12850400
H	5.19712500	6.75870200	2.55059000
H	3.42261300	6.72015500	2.75674900
H	-0.91684600	2.14486100	-2.10195400
C	4.40786400	-1.43133500	-0.36659200

C	4.02846500	-0.09941300	-0.56951400
C	4.95930300	0.91741000	-0.83857500
C	6.29434100	0.51092000	-0.95230700
H	7.04046000	1.26416500	-1.18587200
C	3.37711000	-2.42898200	0.04684500
C	2.26195100	-2.63812300	-0.76755100
C	1.25428700	-3.55909200	-0.46436000
C	1.44260200	-4.32496800	0.68934700
H	0.70154300	-5.08202400	0.92893700
O	2.66553900	0.20650600	-0.45751500
O	2.11539500	-1.82150900	-1.89987200
P	1.64060100	-0.29780000	-1.62086400
O	0.29077900	-0.40661800	-0.79742000
O	1.58274700	0.52110100	-2.85135500
C	6.70198300	-0.82011700	-0.85549400
C	8.17196100	-1.14768800	-1.04428200
C	5.75211500	-1.81431100	-0.57343400
C	8.42519300	-2.61255400	-1.40502500
H	8.70294000	-0.91605800	-0.10945900
H	8.59704100	-0.48323400	-1.80448700
C	6.13920100	-3.28332600	-0.60788900
C	7.64281700	-3.52263200	-0.45767100
H	9.49802500	-2.82837300	-1.36291600
H	8.10069100	-2.80114500	-2.43661900
H	5.58889900	-3.85229900	0.14272400
H	5.80731500	-3.68678900	-1.57570200
H	7.86741200	-4.57696800	-0.65078300
H	7.94840700	-3.31721100	0.57750700
C	3.47306500	-3.13299900	1.26830500
C	4.49945100	-2.72398600	2.31177200
C	2.52019200	-4.12589700	1.55612900
C	4.74099800	-3.78047300	3.39159900
H	4.11679100	-1.80835800	2.78635100
H	5.44181800	-2.43344700	1.84591000
C	2.64536600	-5.00018900	2.78943200
C	3.41294900	-4.32101600	3.92450100
H	5.34016600	-3.34710400	4.19918300
H	5.32597300	-4.61077500	2.97317200
H	1.64981400	-5.31322900	3.11919200
H	3.17206200	-5.92424300	2.51062600
H	3.57680400	-5.02826400	4.74453300
H	2.81932000	-3.48980300	4.32767400
C	4.62329000	2.35370900	-0.99695600
C	3.50525900	2.78656200	-1.68408900

C	5.52137800	3.33013600	-0.47494400
C	3.23507600	4.16452600	-1.85550300
H	2.82512600	2.07813500	-2.13489400
C	5.30669400	4.67229100	-0.66456300
H	6.37889300	3.00242700	0.10270700
C	4.15636200	5.13503000	-1.35321100
C	2.05761900	4.60792500	-2.51370100
H	6.00432300	5.39755500	-0.25664200
C	3.86819100	6.51275700	-1.53689600
C	1.79236500	5.95036400	-2.65523800
H	1.37347400	3.85786200	-2.90160100
C	2.70871600	6.91278600	-2.16332300
H	4.57895400	7.25017900	-1.17270600
H	0.88476700	6.27962800	-3.15184100
H	2.49606900	7.96981900	-2.29109800
C	0.02733800	-3.71327700	-1.28034300
C	-1.20960700	-3.70599000	-0.66249300
C	0.10039400	-3.91041100	-2.68789300
C	-2.40134800	-3.93210300	-1.39726600
H	-1.28364400	-3.49754000	0.40024100
C	-1.03574200	-4.15140800	-3.42021100
H	1.06884000	-3.88151700	-3.17389400
C	-2.31251900	-4.19276400	-2.80123700
C	-3.68073500	-3.91676300	-0.78076700
H	-0.96934000	-4.31566500	-4.49181300
C	-3.50074100	-4.47263900	-3.52340900
C	-4.81754000	-4.16853400	-1.51352400
H	-3.74510300	-3.69637600	0.27856300
C	-4.72590100	-4.46342500	-2.89593000
H	-3.42665000	-4.68521800	-4.58623100
H	-5.78944300	-4.14013700	-1.03096500
H	-5.62893900	-4.67298000	-3.46130700
C	-2.43642600	1.22061000	-0.94339600
H	-0.36588000	0.22811100	-1.18959700

TS-4

O	5.31319900	-2.54851300	0.77828500
H	5.00025200	-2.17530700	1.61791100
O	-3.62330000	0.20578300	5.24526100
O	1.90039300	-6.33367700	0.68049400
O	2.27013200	5.04885800	-2.89257200
N	2.93205500	0.36762700	3.03171700
C	0.37024100	-1.00318100	1.45297600
C	0.95953300	0.07848600	0.80722400

C	2.14038200	0.71746400	0.71452700
C	4.55976300	0.09733100	1.48602700
C	5.09578500	-0.19543300	2.79804200
C	6.36092200	-0.61066600	3.25138000
H	7.16960400	-0.75937100	2.54270800
C	6.54930200	-0.81559700	4.61136700
H	7.52093200	-1.13275200	4.97653700
C	5.50069100	-0.61267000	5.53230400
H	5.68188600	-0.77877400	6.58952800
C	4.23902200	-0.20529800	5.11412700
H	3.43215000	-0.05056600	5.82386600
C	4.04817400	-0.00929200	3.74391200
C	5.24353800	-0.19431800	0.20314200
C	5.55137000	-1.51913300	-0.09184200
C	6.11040900	-1.89347900	-1.33603000
H	6.31280600	-2.94480600	-1.50886600
C	6.36246700	-0.94045600	-2.28938400
H	6.77265000	-1.22707900	-3.25373100
C	6.11397500	0.43235200	-2.03039400
C	6.39154600	1.43409700	-2.99566400
H	6.77661000	1.12731100	-3.96450800
C	6.18285700	2.76382700	-2.71315800
H	6.39135600	3.52282200	-3.46073700
C	5.71052400	3.14471800	-1.43635100
H	5.55837100	4.19461700	-1.20973000
C	5.42832700	2.19522000	-0.48199900
H	5.06853400	2.49145400	0.49428100
C	5.58523100	0.81330900	-0.75467500
C	2.30228700	1.81461000	-0.27209600
C	2.11304100	1.58631200	-1.63379700
H	1.93204700	0.57759000	-1.98561300
C	2.10829600	2.63669300	-2.54678900
H	1.93408800	2.42150000	-3.59246700
C	2.28198200	3.94531700	-2.08768600
C	2.47391200	4.19123400	-0.72089600
H	2.57240500	5.21598600	-0.38549100
C	2.48757800	3.13286200	0.17170600
H	2.61099300	3.32914100	1.23302100
C	1.91766800	4.86186100	-4.25359600
H	2.65375700	4.24288300	-4.78184000
H	1.90053500	5.85697900	-4.70088800
H	0.92776600	4.39911700	-4.34930400
C	0.74905800	-2.37024200	1.15062900
C	2.07606700	-2.67020500	0.78578900

H	2.78407400	-1.86615800	0.64519400
C	2.50766100	-3.97731600	0.64304200
H	3.54388600	-4.15669600	0.39584200
C	1.58657000	-5.02439000	0.79302600
C	0.23425700	-4.74281600	1.05916300
H	-0.46717600	-5.56695400	1.09980100
C	-0.17567500	-3.43879400	1.23892900
H	-1.22156500	-3.22313700	1.41909200
C	3.27343200	-6.68334000	0.51449400
H	3.87645400	-6.31386700	1.35132400
H	3.66777500	-6.28648300	-0.42493000
H	3.30068900	-7.77290800	0.49575400
C	-0.71579300	-0.73221100	2.40367700
C	-0.91896200	-1.58846000	3.50293700
H	-0.29412200	-2.46592400	3.61714400
C	-1.87397500	-1.31236500	4.47594900
H	-1.98662200	-1.98543800	5.31625900
C	-2.66104900	-0.15971800	4.35934800
C	-2.47332700	0.70668900	3.27038800
H	-3.10598200	1.58039300	3.18120700
C	-1.51325400	0.43438100	2.31544400
H	-1.40557300	1.10223400	1.47041700
C	-3.90508100	-0.66318300	6.33531300
H	-4.21925400	-1.65313700	5.98452200
H	-4.72241200	-0.19657700	6.88481300
H	-3.03631800	-0.77046500	6.99536000
H	2.02552100	0.59061600	3.41173200
C	3.22324900	0.43726000	1.67769800
H	0.05487100	0.71374400	0.08827400
C	-4.31552900	-0.79490700	-1.16974000
C	-3.05673000	-1.38642200	-1.35976300
C	-2.90974100	-2.64748200	-1.96743000
C	-4.08133500	-3.25014800	-2.43988700
H	-4.00097800	-4.21049700	-2.94072800
C	-4.40890500	0.46862000	-0.37561400
C	-3.67218700	1.58079800	-0.79233800
C	-3.63910800	2.78407600	-0.07370200
C	-4.48031200	2.86707300	1.04036300
H	-4.52278100	3.80501400	1.58756900
O	-1.94126000	-0.70311200	-0.89363400
O	-2.87852900	1.43821700	-1.92551300
P	-1.44680300	0.67383200	-1.69527200
O	-0.72135500	1.44382400	-0.57270700
O	-0.79014600	0.40461800	-2.99585100

C	-5.33545500	-2.64191000	-2.36771000
C	-6.53221000	-3.36500700	-2.95969000
C	-5.46193300	-1.39313000	-1.73838000
C	-7.71232000	-2.43881400	-3.26049400
H	-6.86248000	-4.13693600	-2.24888400
H	-6.22247200	-3.90127200	-3.86359000
C	-6.78222300	-0.64194900	-1.77419200
C	-7.98781400	-1.54064900	-2.05405400
H	-8.59596900	-3.03079400	-3.52250600
H	-7.47744700	-1.81129800	-4.13007100
H	-6.93578600	-0.07476100	-0.85518400
H	-6.70731000	0.11402100	-2.56955000
H	-8.87719800	-0.92300300	-2.21920700
H	-8.19463500	-2.16699700	-1.17515000
C	-5.15941800	0.55046700	0.81820400
C	-5.76712200	-0.69178700	1.44381000
C	-5.23903200	1.78301500	1.49091600
C	-6.94206900	-0.38396000	2.37298500
H	-4.97100900	-1.18004400	2.02646500
H	-6.05660300	-1.41599500	0.68207500
C	-6.14736500	1.97915400	2.69296100
C	-6.54032200	0.67802900	3.39736200
H	-7.26887800	-1.30259700	2.87304600
H	-7.79533300	-0.02438600	1.78152900
H	-5.67280800	2.66649700	3.40293700
H	-7.05947400	2.48775400	2.34822000
H	-7.35614100	0.87246500	4.10274200
H	-5.68993000	0.31175900	3.98290100
C	-1.61164600	-3.35536000	-2.09945800
C	-0.43163400	-2.69664400	-2.39582100
C	-1.57450200	-4.77292100	-1.94313600
C	0.79278600	-3.39503300	-2.51668400
H	-0.42717700	-1.63131000	-2.57974000
C	-0.40646700	-5.48073500	-2.09212300
H	-2.48820800	-5.29702300	-1.68133900
C	0.81414100	-4.81770700	-2.38093200
C	2.00911400	-2.70652900	-2.77048600
H	-0.39883900	-6.55956500	-1.96282100
C	2.04901000	-5.50011200	-2.52285600
C	3.19575200	-3.39234900	-2.88555700
H	1.97937200	-1.62607300	-2.87444800
C	3.21317300	-4.80383300	-2.76677200
H	2.06020900	-6.58285100	-2.43196900
H	4.11951000	-2.85271400	-3.06175400

H	4.15271400	-5.33837900	-2.87799700
C	-2.68007800	3.86586300	-0.39969300
C	-1.95034400	4.45105200	0.61863300
C	-2.44501100	4.28664600	-1.73982300
C	-0.98047800	5.45053300	0.36263200
H	-2.08926700	4.11306800	1.64167900
C	-1.51249000	5.25465400	-2.01915800
H	-3.00606400	3.82432200	-2.54198100
C	-0.75538300	5.86843200	-0.98716400
C	-0.21677600	6.04662800	1.40063100
H	-1.34477600	5.56857000	-3.04581600
C	0.20828000	6.87587700	-1.24346300
C	0.71145400	7.02333600	1.12068600
H	-0.38284000	5.71988400	2.42376200
C	0.92272100	7.44589100	-0.21441100
H	0.38548300	7.17917800	-2.27015600
H	1.28618900	7.47477800	1.92390300
H	1.65956300	8.21502700	-0.42463400

INT-5

O	5.47227000	1.25847400	2.01354300
H	4.54521600	1.44964100	1.79310200
O	-4.00600400	-2.76929200	3.12634000
O	2.48404200	4.63143100	3.38057100
O	8.04898700	-3.82321100	0.84677100
N	1.86168500	0.67220600	-0.51982200
C	1.08511200	-0.68329800	2.09505700
C	2.09767100	-1.45908500	1.50044100
C	3.18563700	-0.99670700	0.73029300
C	4.10310700	1.07624900	-0.52538500
C	3.44000800	2.14007400	-1.19684300
C	3.89915000	3.32233300	-1.82066400
H	4.95796700	3.55880400	-1.82621800
C	2.96958700	4.14791700	-2.41840300
H	3.29377600	5.06332500	-2.90333400
C	1.58484000	3.82326300	-2.41839500
H	0.88529400	4.50472900	-2.88966800
C	1.09988000	2.67534400	-1.81916300
H	0.05060900	2.40696600	-1.81674400
C	2.04251200	1.84234700	-1.19344700
C	5.57158100	0.96832500	-0.37663800
C	6.17374800	1.03721800	0.87142000
C	7.56867000	0.85575100	1.02962000
H	7.97753100	0.90700500	2.03265600

C	8.35977900	0.61882000	-0.06311000
H	9.42901600	0.47069800	0.05752800
C	7.80333500	0.55949500	-1.36829200
C	8.60667000	0.28922300	-2.50506300
H	9.67589300	0.15689700	-2.36283700
C	8.04998500	0.18357900	-3.75928700
H	8.67465300	-0.02858000	-4.62109500
C	6.65563200	0.34848500	-3.92097300
H	6.21468800	0.25995600	-4.90921200
C	5.84882600	0.62296500	-2.83836900
H	4.78208600	0.75039500	-2.97782200
C	6.39310100	0.74491700	-1.53061400
C	4.41689200	-1.78406600	0.74334400
C	4.83058400	-2.40533700	1.93379200
H	4.21789300	-2.30319300	2.82331700
C	6.03288600	-3.09835500	2.01450300
H	6.33197500	-3.53953400	2.95647300
C	6.85164700	-3.18968800	0.87910800
C	6.44276200	-2.59817800	-0.32773100
H	7.08703600	-2.67976000	-1.19524900
C	5.24893300	-1.90980800	-0.38698200
H	4.93692400	-1.46784100	-1.31966100
C	8.52038200	-4.43750400	2.03908300
H	8.64993600	-3.70277200	2.84258900
H	9.48705200	-4.87435000	1.78844300
H	7.84058600	-5.22825700	2.37788100
C	1.40826100	0.70771800	2.46789000
C	2.63120300	0.96216200	3.11020100
H	3.28751200	0.13586400	3.35847000
C	3.01762900	2.25431100	3.45722100
H	3.96141500	2.40505100	3.96446100
C	2.18215900	3.33338000	3.13333300
C	0.94583200	3.09034500	2.51593300
H	0.31002400	3.93581100	2.27582000
C	0.55575500	1.80011600	2.20012500
H	-0.39618400	1.63194200	1.70057700
C	3.76876300	4.92958100	3.91193300
H	4.56589300	4.54850900	3.26251100
H	3.89370100	4.51269000	4.91868400
H	3.82673800	6.01687900	3.96267700
C	-0.18273600	-1.27857400	2.44284400
C	-0.55502900	-2.54249200	1.92301900
H	0.10898000	-3.07218400	1.25160400
C	-1.79092400	-3.09658900	2.18155000

H	-2.04767200	-4.04251900	1.72789200
C	-2.73394600	-2.36730300	2.92467100
C	-2.37490900	-1.13660200	3.49920100
H	-3.11430300	-0.59809100	4.07970700
C	-1.12505500	-0.60880300	3.26642800
H	-0.86704000	0.34770800	3.70035100
C	-4.47616200	-3.91827300	2.41828000
H	-4.34918700	-3.79155200	1.33901300
H	-5.53641100	-3.99542000	2.65681500
H	-3.96009400	-4.82558500	2.75211900
H	0.93516700	0.22765100	-0.48780500
C	3.08812800	0.17840400	-0.08896500
H	2.06747300	-2.53220400	1.65239300
C	-5.21269300	-0.10262100	-0.17795200
C	-4.50897700	1.04540000	-0.56847300
C	-4.96539900	2.33514100	-0.25263600
C	-6.12421800	2.42781100	0.51961400
H	-6.49439700	3.41693500	0.77660200
C	-4.82057900	-1.42628300	-0.74767200
C	-3.49887200	-1.87831700	-0.62546100
C	-3.09570800	-3.12276700	-1.14672000
C	-4.07280500	-3.92385800	-1.73853200
H	-3.77766100	-4.89005500	-2.13986100
O	-3.31466400	0.88551200	-1.25898100
O	-2.59150400	-1.14757000	0.09564000
P	-2.06384100	0.38288700	-0.28179600
O	-0.82385500	0.28831400	-1.13496700
O	-2.06638000	1.15212700	1.00209700
C	-6.76108100	1.30505100	1.05693400
C	-7.95568200	1.50771500	1.97164100
C	-6.29303400	0.02459900	0.72641200
C	-8.22801000	0.31008600	2.88394000
H	-8.84741800	1.69008500	1.35350100
H	-7.81032400	2.41728700	2.56493000
C	-6.84487300	-1.20270800	1.43395400
C	-8.22061700	-0.98130300	2.06462000
H	-9.18388000	0.44264900	3.40269100
H	-7.44950700	0.24936200	3.65575700
H	-6.86796100	-2.06435000	0.76448200
H	-6.12488400	-1.46292400	2.22310000
H	-8.48356200	-1.84253100	2.68933900
H	-8.98462300	-0.91606600	1.27749700
C	-5.75690400	-2.20821300	-1.47018600
C	-7.10815700	-1.63132500	-1.86478400

C	-5.38749600	-3.48775000	-1.91934800
C	-8.14353100	-2.69055600	-2.24591900
H	-6.93605900	-0.97327600	-2.72935500
H	-7.50371700	-0.97957200	-1.08696200
C	-6.37045000	-4.41399200	-2.61376200
C	-7.55179700	-3.67968000	-3.24930100
H	-9.03426800	-2.20178300	-2.65540600
H	-8.46578400	-3.23397700	-1.34662000
H	-5.83985100	-5.01259000	-3.36269500
H	-6.75895400	-5.13140800	-1.87526600
H	-8.30473600	-4.40041800	-3.58667300
H	-7.21161700	-3.13123400	-4.13731200
C	-4.27668600	3.57251600	-0.70330000
C	-2.94647900	3.81276100	-0.41612000
C	-5.01895000	4.56252600	-1.40710700
C	-2.31445700	5.01365000	-0.82103300
H	-2.38513500	3.08276700	0.15588500
C	-4.43186700	5.73809700	-1.81195700
H	-6.06273900	4.36786300	-1.63508100
C	-3.06484500	6.00110500	-1.53628700
C	-0.94668800	5.26675900	-0.53232200
H	-5.00991100	6.48087300	-2.35546400
C	-2.41634200	7.19809600	-1.93794200
C	-0.34557400	6.43696200	-0.93571700
H	-0.37678800	4.50685000	-0.00697500
C	-1.08819500	7.41271200	-1.64540800
H	-2.98800700	7.94452800	-2.48334900
H	0.70379400	6.61034300	-0.71711800
H	-0.60398900	8.33289100	-1.95893200
C	-1.67787700	-3.55193300	-1.15736600
C	-0.70656600	-2.71265000	-1.66740400
C	-1.29893300	-4.84722700	-0.70845500
C	0.64322300	-3.12197300	-1.76345500
H	-0.96368400	-1.71746100	-2.00681100
C	0.01380800	-5.26017000	-0.75248800
H	-2.06437300	-5.51073700	-0.31500900
C	1.02334500	-4.41880900	-1.29138100
C	1.62354900	-2.28777900	-2.36598200
H	0.28991700	-6.24890300	-0.39564000
C	2.37971500	-4.82163600	-1.41686600
C	2.91692300	-2.72744400	-2.51395800
H	1.31979400	-1.30648000	-2.71672000
C	3.30225600	-4.00072700	-2.02335200
H	2.67256000	-5.80041800	-1.04622200

H	3.65015300	-2.09766700	-3.00830500
H	4.33395800	-4.32186500	-2.12249800

TS-5

O	6.03964300	-0.46985100	-1.12012100
H	5.21916300	-0.24278100	-1.58364600
O	-3.26393600	3.48836500	-4.28607700
O	6.52034500	1.18686000	-4.45009400
O	3.44853900	2.11662100	5.97777900
N	1.45920600	0.20301600	-1.25175300
C	1.58956700	2.04318700	-1.80238300
C	1.70670800	2.51069500	-0.38202200
C	2.18080600	1.61608600	0.51104800
C	3.33014600	-0.64331900	-0.18708700
C	3.08212400	-1.41305600	-1.40922200
C	3.74071600	-2.48846800	-2.01125900
H	4.62012400	-2.92593200	-1.55550500
C	3.20797300	-3.00832900	-3.18902300
H	3.70192600	-3.84794400	-3.66564300
C	2.02024000	-2.50599100	-3.74537400
H	1.61624000	-2.96156100	-4.64359300
C	1.34731400	-1.43857900	-3.15252300
H	0.41636600	-1.04843700	-3.54834300
C	1.92750900	-0.87841100	-2.02149000
C	4.48490900	-0.83385800	0.70968100
C	5.77306900	-0.75111800	0.18905000
C	6.91178800	-0.93865600	1.00847100
H	7.88962700	-0.86209400	0.54560300
C	6.76322700	-1.18756400	2.34788500
H	7.63788800	-1.31786700	2.97890200
C	5.47519000	-1.26708900	2.93778300
C	5.31087100	-1.48599700	4.33016200
H	6.20013800	-1.60798900	4.94320400
C	4.05732200	-1.53946200	4.89440800
H	3.94077400	-1.69488000	5.96224300
C	2.91500400	-1.39439300	4.07423000
H	1.92509600	-1.43170100	4.51713800
C	3.04116700	-1.19352500	2.71870300
H	2.15502000	-1.08562900	2.10786500
C	4.31913500	-1.10399100	2.10850000
C	2.52074400	1.87313900	1.92940800
C	3.85297200	2.03461400	2.31204900
H	4.63412200	2.03159000	1.55850100
C	4.20688000	2.13460400	3.65626700

H	5.25164300	2.22267700	3.92416500
C	3.20924600	2.07978200	4.63492100
C	1.86552700	1.96588600	4.25539700
H	1.10973800	1.92580100	5.03228600
C	1.52241400	1.84917500	2.91550800
H	0.49435600	1.67100400	2.61882200
C	4.79995400	2.05995000	6.40533000
H	5.30062900	1.16461600	6.01718300
H	4.77028700	2.01879100	7.49501500
H	5.36192800	2.95078400	6.09607700
C	2.87471900	1.96536500	-2.55971900
C	4.07094000	2.41660600	-1.98634800
H	4.04220300	2.93255300	-1.03490000
C	5.30478100	2.20245200	-2.59548500
H	6.20367300	2.55147300	-2.10517700
C	5.36925700	1.50212200	-3.80640100
C	4.18094800	1.06671600	-4.41214000
H	4.24412000	0.51678300	-5.34408400
C	2.96162900	1.29355900	-3.79729100
H	2.06930600	0.89372900	-4.25724300
C	7.74565400	1.38702800	-3.74992100
H	7.73206700	0.86421000	-2.78728900
H	7.94660600	2.45325500	-3.58978900
H	8.52434900	0.96910200	-4.38822900
C	0.33909500	2.43285500	-2.48141600
C	-0.83729500	2.49676700	-1.71448000
H	-0.79571100	2.26484500	-0.65815400
C	-2.05710200	2.84550700	-2.27101400
H	-2.93347400	2.85149400	-1.63999000
C	-2.12297200	3.16090400	-3.63402200
C	-0.95024100	3.16141700	-4.40790200
H	-1.01719500	3.45247100	-5.45027100
C	0.25951000	2.80176100	-3.84020200
H	1.15333200	2.84461100	-4.44827000
C	-4.48228300	3.45305300	-3.54578200
H	-4.66381100	2.45525500	-3.13001300
H	-5.26926200	3.70337400	-4.25771000
H	-4.47385300	4.18010000	-2.72796000
H	0.35810100	0.01933700	-1.00515700
C	2.35166600	0.31774500	-0.12998600
H	1.42372900	3.52706100	-0.13385200
C	-4.24595500	-2.03603700	0.13846800
C	-2.90999100	-2.34258000	0.41709600
C	-2.27057100	-3.49159800	-0.07545900

C	-3.05273900	-4.34023100	-0.86531100
H	-2.61407500	-5.26687000	-1.22371900
C	-4.85361400	-0.81988600	0.76157800
C	-4.25826900	0.43207500	0.55273600
C	-4.84535900	1.62064100	1.01875200
C	-6.04935700	1.51048100	1.71454300
H	-6.52318100	2.41914800	2.07719600
O	-2.18968200	-1.42989200	1.17584300
O	-3.09666700	0.50818700	-0.19482800
P	-1.66216400	-0.08680600	0.38413200
O	-1.01190200	0.80472800	1.38839300
O	-0.90943400	-0.47278800	-0.87921500
C	-4.36523500	-4.03548800	-1.23267800
C	-5.11816500	-5.01389500	-2.11716600
C	-4.96731800	-2.85780900	-0.75689000
C	-6.29776900	-4.38134700	-2.85784100
H	-5.49521000	-5.83389800	-1.48838600
H	-4.42165100	-5.47549100	-2.82606200
C	-6.31901400	-2.41705900	-1.29350400
C	-7.14490100	-3.56126700	-1.88433700
H	-6.89662800	-5.16004300	-3.34264800
H	-5.92493800	-3.72243500	-3.65315500
H	-6.89182700	-1.88693300	-0.53201400
H	-6.12789800	-1.67213200	-2.08023300
H	-8.03280400	-3.15627000	-2.38198600
H	-7.50357300	-4.21356700	-1.07618900
C	-6.00756400	-0.90631600	1.57593000
C	-6.51127300	-2.25860800	2.05480200
C	-6.62277700	0.27441100	2.02549700
C	-7.96233800	-2.23476900	2.53784800
H	-5.86398400	-2.56940200	2.88806000
H	-6.37679800	-3.02295000	1.28903000
C	-7.91047200	0.25175200	2.83011800
C	-8.17337800	-1.08587800	3.52454700
H	-8.21375600	-3.19718500	2.99656600
H	-8.63641100	-2.10592000	1.67968900
H	-7.89838800	1.06863400	3.56026900
H	-8.74921300	0.46687100	2.15147900
H	-9.18807700	-1.10029600	3.93708600
H	-7.48272500	-1.20679900	4.36927600
C	-0.84205600	-3.79146900	0.18749000
C	-0.07499200	-4.43931000	-0.76650600
C	-0.23030900	-3.45942600	1.43324600
C	1.28066900	-4.78135400	-0.53301300

H	-0.50662600	-4.68573800	-1.73161300
C	1.09086000	-3.74214200	1.67241800
H	-0.82236000	-2.97372500	2.19655300
C	1.89248700	-4.39463700	0.70094200
C	2.05214300	-5.50980300	-1.47599600
H	1.54038000	-3.47968300	2.62365900
C	3.26034500	-4.69756800	0.92142100
C	3.36594600	-5.82809300	-1.21759100
H	1.58447700	-5.81241200	-2.40877400
C	3.98192700	-5.40330000	-0.01576500
H	3.72424400	-4.36804000	1.84665500
H	3.94150800	-6.39380300	-1.94445500
H	5.02577300	-5.64055800	0.16673500
C	-4.21818700	2.94475800	0.77915000
C	-2.91486600	3.19048200	1.16833200
C	-4.95093400	3.98135000	0.13667900
C	-2.28110100	4.42304200	0.88359600
H	-2.33977400	2.41714700	1.66300200
C	-4.36348100	5.19511200	-0.14373300
H	-5.98029700	3.79260800	-0.15407900
C	-3.00832000	5.44617600	0.19734500
C	-0.92384900	4.65548400	1.23704900
H	-4.93057600	5.97485500	-0.64574000
C	-2.34534100	6.65973300	-0.12395000
C	-0.30956600	5.84155400	0.90791400
H	-0.38349000	3.87498300	1.76391700
C	-1.02626000	6.85143900	0.21762200
H	-2.89660000	7.43460100	-0.65003400
H	0.72754300	6.01146600	1.18236700
H	-0.52882300	7.78211900	-0.03793900

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O	2.27823900	2.39301000	-0.47047700
H	1.36382600	2.09078900	-0.60267300
O	-5.15874900	-4.63620900	1.52471800
O	-4.74877200	4.75443000	-0.75778800
O	5.15200300	0.36989300	4.15690600
N	-0.99906900	-0.26337100	-0.62601900
C	-1.93389400	-0.04929400	0.49629300
C	-0.92903200	0.08307900	1.63988300
H	-1.26018000	0.14628200	2.66764900
C	0.35421700	0.04100900	1.20941600
C	0.32356800	-0.10563700	-0.24564500
C	1.13898200	-0.03990700	-1.36459000

C	0.24568500	-0.16605000	-2.50034000
C	0.46157300	-0.18273200	-3.88591800
H	1.47071500	-0.10856300	-4.27822900
C	-0.63382100	-0.29658800	-4.73328000
H	-0.48136800	-0.30946100	-5.80797700
C	-1.94306300	-0.39670600	-4.22270900
H	-2.77759200	-0.48277500	-4.91159200
C	-2.19125800	-0.39078500	-2.85388700
H	-3.19720000	-0.46939100	-2.46061900
C	-1.08988100	-0.27472600	-2.00249000
C	2.59736400	0.18784400	-1.38548800
C	3.09328200	1.39741600	-0.91269800
C	4.48437300	1.65119600	-0.85786700
H	4.81553500	2.60852000	-0.47118700
C	5.37259300	0.69629000	-1.28026200
H	6.44104800	0.88721000	-1.23416800
C	4.92268900	-0.55406300	-1.78201000
C	5.82769900	-1.55529100	-2.21608500
H	6.89302000	-1.34414900	-2.17411200
C	5.37395100	-2.77048100	-2.67664900
H	6.07729100	-3.52920900	-3.00531900
C	3.98505300	-3.03229200	-2.71541200
H	3.62995900	-3.99470400	-3.07172900
C	3.07857500	-2.08057700	-2.30358800
H	2.01490800	-2.28716600	-2.33445000
C	3.51427500	-0.81190500	-1.83490600
C	1.58448200	0.13314100	2.00557400
C	2.71583300	-0.63362600	1.67170700
H	2.67378900	-1.31155700	0.82810200
C	3.88509500	-0.53500600	2.40673100
H	4.76155600	-1.11738200	2.14620700
C	3.95557700	0.33511900	3.50383900
C	2.83706200	1.09854300	3.85757600
H	2.87040700	1.78413900	4.69485300
C	1.66792100	0.99195800	3.10574600
H	0.81279900	1.60948000	3.36344500
C	5.27728400	1.24222000	5.26761000
H	5.12082900	2.28901100	4.97812200
H	6.29662400	1.11878700	5.63498100
H	4.57085100	0.98309200	6.06643500
C	-2.71619500	1.24731200	0.24358200
C	-2.09153600	2.48182500	0.43120200
H	-1.08530900	2.51266900	0.83650300
C	-2.73072500	3.67899200	0.11142200

H	-2.21357400	4.61644100	0.27294400
C	-4.02843800	3.65002700	-0.41213500
C	-4.66643600	2.41838000	-0.60515300
H	-5.67162100	2.41357800	-1.01223300
C	-4.01459200	1.23571800	-0.28225800
H	-4.52353100	0.29088700	-0.43522800
C	-4.13370300	6.02349800	-0.60271100
H	-3.22516700	6.10822200	-1.21184600
H	-3.88144000	6.22448300	0.44610200
H	-4.86549700	6.75672500	-0.94316200
C	-2.82671000	-1.26258600	0.74689700
C	-3.79898700	-1.20939300	1.74878300
H	-3.94650200	-0.28724500	2.30280700
C	-4.60077700	-2.31095000	2.04444900
H	-5.34607000	-2.23131000	2.82582700
C	-4.43068100	-3.50012500	1.32524000
C	-3.45697600	-3.56531500	0.32163000
H	-3.33900500	-4.49370200	-0.22627900
C	-2.66353400	-2.45993900	0.04121200
H	-1.91136700	-2.52603300	-0.73547700
C	-6.15378700	-4.61836300	2.53486800
H	-5.72144100	-4.42330400	3.52443900
H	-6.60690700	-5.61022400	2.52966000
H	-6.92629900	-3.86688900	2.32798000

INT-2'

O	-3.37636200	3.32798500	2.37641000
H	-3.77625400	2.54453200	1.96756200
O	-9.43302300	-0.43336700	-0.09327800
O	-1.22913900	-3.32840300	-5.12805800
O	1.32600300	5.56866800	0.83123400
N	-3.17541000	-1.09699000	0.91744900
C	-4.09616700	0.12098200	-1.75754100
C	-3.37313600	1.19842100	-1.28387000
C	-2.58540100	2.06084400	-0.89478200
C	-2.10162700	-0.29092100	1.18381700
C	-2.44084000	0.63998200	2.15271600
C	-3.82237000	0.34971700	2.52264300
C	-4.72703100	0.87433100	3.46337300
H	-4.43636200	1.69981100	4.10333400
C	-6.00127300	0.32240600	3.55885400
H	-6.70399000	0.72834500	4.28015200
C	-6.39014900	-0.76143900	2.75090500

H	-7.38965900	-1.17425900	2.84902100
C	-5.50779600	-1.32281500	1.83262700
H	-5.79384800	-2.16599500	1.21627200
C	-4.23955600	-0.75498100	1.72571800
C	-1.58456300	1.71820400	2.66489300
C	-2.11230200	3.00516600	2.78310700
C	-1.35121300	4.08195800	3.28874600
H	-1.82744700	5.05341500	3.35705000
C	-0.03847600	3.89503200	3.63171000
H	0.55470500	4.72844100	3.99694500
C	0.57961100	2.62716100	3.47646800
C	1.95691900	2.44720200	3.76403100
H	2.51978300	3.29753400	4.14149200
C	2.56975800	1.23054000	3.56740000
H	3.62905400	1.10714600	3.77210000
C	1.80811000	0.13434700	3.11002500
H	2.28274700	-0.82585400	2.96063500
C	0.46114500	0.27020900	2.85532200
H	-0.09650400	-0.59324900	2.52240600
C	-0.19695200	1.51977200	2.99800300
C	-1.59839100	2.96764200	-0.50344600
C	-1.88455700	4.32762000	-0.22346500
H	-2.89967900	4.69288500	-0.32433800
C	-0.87503300	5.17223400	0.17386300
H	-1.06134600	6.21831700	0.38680800
C	0.43283700	4.67527000	0.36932900
C	0.72644000	3.32862500	0.10813100
H	1.71749900	2.91979400	0.24953500
C	-0.27316700	2.49210800	-0.34762000
H	-0.04798100	1.44586500	-0.52818500
C	2.64437300	5.10482000	1.13983400
H	2.60828700	4.30297500	1.88285400
H	3.16795700	5.96883500	1.54965000
H	3.15709300	4.75339400	0.24111700
C	-3.37570200	-0.83743200	-2.57847000
C	-1.96948000	-0.92892300	-2.46912600
H	-1.43358700	-0.37919200	-1.70657400
C	-1.22601900	-1.74626600	-3.29530500
H	-0.14858000	-1.74843100	-3.17467600
C	-1.87504700	-2.50382500	-4.28082000
C	-3.27430600	-2.42211700	-4.42649500
H	-3.74915900	-2.98700600	-5.22099900
C	-4.00959500	-1.60475500	-3.59076800
H	-5.07446400	-1.50287300	-3.75997100

C	0.20085300	-3.39139600	-5.03217000
H	0.51193600	-3.79885700	-4.06482800
H	0.65310100	-2.40337900	-5.15474100
H	0.51775200	-4.05661200	-5.83453000
C	-5.50779800	0.00554500	-1.42239200
C	-6.20514000	1.11971500	-0.91550700
H	-5.69347900	2.07445800	-0.85998500
C	-7.51590400	1.02346600	-0.47935800
H	-8.01266600	1.90155300	-0.08810900
C	-8.17203000	-0.21706100	-0.52940300
C	-7.49640500	-1.34196300	-1.02985900
H	-8.01079500	-2.29638700	-1.02590000
C	-6.18641700	-1.23517000	-1.45524800
H	-5.65366400	-2.13038400	-1.74970900
C	-10.12341100	0.64137700	0.53792900
H	-9.57327900	1.00077700	1.41476500
H	-11.08488100	0.23449500	0.85006400
H	-10.28854600	1.47269200	-0.15698600
C	4.03412300	-1.96627300	0.75570600
C	2.77828400	-2.51558900	0.46278200
C	2.01948600	-3.20826700	1.42458700
C	2.62948000	-3.41687000	2.66740000
H	2.09825200	-3.99127900	3.42042800
C	4.73367400	-1.14916700	-0.28394500
C	4.07197300	-0.03242400	-0.81447300
C	4.73642000	0.91176100	-1.61761900
C	6.07300500	0.65424700	-1.92706900
H	6.60872300	1.36790300	-2.54802900
O	2.28159200	-2.32829500	-0.80698000
O	2.74333300	0.16062500	-0.49369500
P	1.61886000	-0.84976900	-1.20346300
O	1.65756300	-0.78677800	-2.69919900
O	0.35591400	-0.61115800	-0.43055500
C	3.86819500	-2.86917800	3.00472000
C	4.41054700	-3.09350600	4.40381300
C	4.55959300	-2.08624400	2.06260000
C	5.33068300	-1.96324700	4.86747000
H	4.97404700	-4.03797500	4.42430200
H	3.57529900	-3.22286200	5.10064800
C	5.76075500	-1.25690500	2.48776100
C	6.39851500	-1.70678300	3.80400200
H	5.78717200	-2.21869000	5.82996300
H	4.74107200	-1.04989600	5.02336800
H	6.51431200	-1.21886100	1.70113500

H	5.40806700	-0.22011600	2.59202700
H	7.11521700	-0.94936400	4.13987600
H	6.96959800	-2.63087900	3.64010500
C	6.04891500	-1.43982600	-0.71172800
C	6.67930600	-2.78290600	-0.38294500
C	6.72345500	-0.51772300	-1.52885800
C	8.20123800	-2.79670800	-0.53462700
H	6.24638500	-3.52348600	-1.07120900
H	6.38926500	-3.11662200	0.61497700
C	8.16114900	-0.73940700	-1.96471500
C	8.60340400	-2.20176900	-1.88514800
H	8.57377100	-3.82165400	-0.43057100
H	8.66023200	-2.20869000	0.27241500
H	8.29853400	-0.35197700	-2.98052100
H	8.81952800	-0.13687100	-1.32136200
H	9.68519400	-2.27499100	-2.04212500
H	8.12404700	-2.77746700	-2.68776300
C	0.59906400	-3.58114500	1.21511800
C	0.07912100	-3.96556800	-0.00916200
C	-0.29608500	-3.47928200	2.32330300
C	-1.30473000	-4.21917600	-0.18019900
H	0.72939600	-4.03723800	-0.87073200
C	-1.63512500	-3.74970000	2.19755900
H	0.08868800	-3.13480700	3.27660700
C	-2.18537600	-4.12040100	0.94401400
C	-1.85900600	-4.52843900	-1.45185100
H	-2.29868200	-3.63760100	3.05012900
C	-3.57799700	-4.32532300	0.75294800
C	-3.21438700	-4.70064400	-1.61368700
H	-1.19335000	-4.60156400	-2.30565400
C	-4.08464100	-4.59667000	-0.49995200
H	-4.23888500	-4.23966700	1.61098900
H	-3.62073800	-4.90823600	-2.59777000
H	-5.15233300	-4.74445700	-0.63526300
C	4.07146000	2.16727500	-2.04619600
C	2.81029200	2.17104500	-2.61439000
C	4.72603800	3.41247000	-1.82390800
C	2.13289900	3.38317200	-2.88792900
H	2.31418900	1.23250300	-2.83722000
C	4.10300800	4.60580800	-2.10980200
H	5.72252000	3.40956800	-1.39215500
C	2.77440100	4.63113500	-2.61045100
C	0.79521700	3.38678100	-3.36693000
H	4.61008600	5.54840700	-1.91964400

C	2.04736800	5.83488700	-2.80260700
C	0.11246900	4.56881400	-3.53063300
H	0.31628800	2.43208700	-3.56342400
C	0.74388700	5.80443200	-3.24307800
H	2.53190000	6.78152900	-2.57872700
H	-0.91857500	4.55992500	-3.87038700
H	0.19162900	6.73070800	-3.36966300
H	-1.17263500	-0.42305000	0.64588000
H	-3.14122000	-1.90575900	0.31581300

TS-2'

O	3.35140900	3.26503100	-2.88532400
H	3.52242100	4.21561100	-2.88429400
O	9.51275200	-0.39788800	0.29789100
O	1.41527000	-3.63465600	5.19695400
O	-0.63217700	5.97256900	-0.37198000
N	2.93092800	-1.04698300	-1.03093400
C	4.03749600	-0.10613200	1.65851300
C	3.29165200	0.79923700	1.00112000
C	2.41416900	1.31364000	0.23238800
C	1.98592900	-0.03274300	-1.13452600
C	2.33020600	0.74202300	-2.30407900
C	3.60947500	0.28511600	-2.73046800
C	4.48684100	0.67246300	-3.76634700
H	4.23022800	1.50497300	-4.40883100
C	5.67618200	-0.01160500	-3.92278400
H	6.36720600	0.27665400	-4.70797600
C	6.01860300	-1.08218300	-3.06032200
H	6.97356600	-1.58147300	-3.19326300
C	5.17282700	-1.50896800	-2.05039800
H	5.44260600	-2.31779400	-1.38503700
C	3.95605400	-0.82964300	-1.90025900
C	1.48718600	1.79421400	-2.84677700
C	2.01948400	3.06158200	-3.09538300
C	1.19944500	4.14303800	-3.48291300
H	1.65026200	5.11965700	-3.63806500
C	-0.15463800	3.97244800	-3.60974800
H	-0.78382300	4.81579100	-3.87913500
C	-0.75890900	2.71229300	-3.38058700
C	-2.16386600	2.55133800	-3.47614500
H	-2.76650200	3.41467200	-3.74571200
C	-2.75032400	1.33279000	-3.22527200
H	-3.82780800	1.21751400	-3.27876600
C	-1.94064000	0.22136200	-2.91292700

H	-2.39729600	-0.74149600	-2.73234100
C	-0.57029700	0.34455400	-2.83509600
H	0.01551200	-0.53561500	-2.61156700
C	0.06476200	1.59813000	-3.01762600
C	1.60369200	2.50486100	0.12732300
C	2.20651500	3.77721000	0.08561600
H	3.28712300	3.85133600	0.14639800
C	1.43049900	4.91609600	-0.04176400
H	1.87480400	5.90529300	-0.06986300
C	0.03537500	4.80642500	-0.16943900
C	-0.57484100	3.54987000	-0.10198600
H	-1.64873700	3.43583200	-0.15919300
C	0.20605000	2.41247100	0.05153700
H	-0.26965100	1.44010200	0.10165300
C	-2.02405700	5.89121100	-0.65998500
H	-2.20541100	5.27859900	-1.55167700
H	-2.34989800	6.91532000	-0.84708800
H	-2.58536200	5.47423300	0.18044500
C	3.36129200	-1.05670800	2.55646400
C	1.95930900	-1.18988600	2.51131400
H	1.37139000	-0.63699900	1.78895200
C	1.27581500	-2.02766100	3.37698400
H	0.19469400	-2.04749900	3.30519100
C	1.99210400	-2.77933100	4.31697400
C	3.39079200	-2.66164100	4.38764700
H	3.92373300	-3.23061500	5.14180500
C	4.06055200	-1.80557100	3.52878300
H	5.13338100	-1.69231500	3.62963100
C	-0.00822400	-3.73847300	5.17484600
H	-0.36529500	-4.12750200	4.21448600
H	-0.48336200	-2.76921400	5.35716100
H	-0.26684700	-4.43603100	5.97159400
C	5.49308400	-0.14992900	1.40601800
C	6.21082200	1.02197400	1.13681600
H	5.70201600	1.97704100	1.21771700
C	7.55324100	0.98741600	0.76997000
H	8.07482200	1.91618900	0.57656800
C	8.20833500	-0.24509800	0.65662300
C	7.50449300	-1.42898200	0.91847100
H	8.02447600	-2.37485700	0.81207300
C	6.16981300	-1.38002000	1.28774100
H	5.62646800	-2.30458900	1.44644400
C	10.26515200	0.77046600	0.00779500
H	9.83530200	1.32629900	-0.83470200

H	11.26476900	0.42624200	-0.25884700
H	10.33078400	1.43362300	0.87919700
C	-4.19623000	-1.84323500	-0.69752500
C	-2.96072100	-2.47389600	-0.49157100
C	-2.28572600	-3.16127000	-1.51833300
C	-2.97173300	-3.29435800	-2.73176800
H	-2.50921600	-3.86130100	-3.53437200
C	-4.77169100	-1.00272800	0.39886300
C	-3.99868000	0.05325700	0.90665300
C	-4.54223100	1.02293000	1.76874500
C	-5.87351900	0.85438700	2.15425400
H	-6.31656800	1.58910300	2.82182500
O	-2.39087700	-2.35645400	0.75439900
O	-2.68186100	0.15903000	0.50891800
P	-1.58675700	-0.94369300	1.12833500
O	-1.51469700	-0.90362200	2.62066900
O	-0.37433200	-0.78652800	0.26002100
C	-4.20081500	-2.67979600	-2.97843700
C	-4.83226000	-2.83758700	-4.34929900
C	-4.80088600	-1.89753100	-1.97421400
C	-5.74146700	-1.66532300	-4.72138200
H	-5.42612000	-3.76327100	-4.36626400
H	-4.04441100	-2.96963000	-5.09904500
C	-5.99137400	-1.01024500	-2.30332000
C	-6.72888400	-1.40540500	-3.58416600
H	-6.26689500	-1.87766100	-5.65889100
H	-5.13329100	-0.76629500	-4.89018000
H	-6.69149300	-0.96181900	-1.46981900
H	-5.60914500	0.01587800	-2.40865900
H	-7.44176100	-0.61828200	-3.85305000
H	-7.31635500	-2.31608600	-3.40451900
C	-6.07487600	-1.20919400	0.90428500
C	-6.81637900	-2.50024200	0.60042600
C	-6.63105800	-0.25811500	1.77532400
C	-8.32520800	-2.40487100	0.83355600
H	-6.40343100	-3.27641400	1.26111000
H	-6.60336900	-2.84493000	-0.41299800
C	-8.05356300	-0.38300800	2.29163700
C	-8.60934000	-1.80649300	2.21249600
H	-8.77865200	-3.39743800	0.73628800
H	-8.78136600	-1.77022300	0.06086300
H	-8.10294600	-0.00918000	3.32045800
H	-8.70040400	0.28093600	1.69890800
H	-9.68378100	-1.80132800	2.42653600

H	-8.13353800	-2.43220400	2.97896700
C	-0.86409400	-3.57172800	-1.40464500
C	-0.27733000	-3.97949400	-0.21920900
C	-0.03086000	-3.44918800	-2.55806600
C	1.11596500	-4.21698200	-0.12456300
H	-0.87710000	-4.06934300	0.67615400
C	1.31448900	-3.71662600	-2.50944900
H	-0.46818100	-3.09386100	-3.48470600
C	1.93421100	-4.10002700	-1.29253800
C	1.73936200	-4.51619300	1.11691700
H	1.92945300	-3.59722600	-3.39717500
C	3.33333300	-4.30771400	-1.17874400
C	3.10344600	-4.67299400	1.20722800
H	1.12158700	-4.58361400	2.00576100
C	3.90883900	-4.57496500	0.04509100
H	3.94559300	-4.22488300	-2.07196200
H	3.56409900	-4.86066500	2.17112800
H	4.98290900	-4.71958100	0.12185900
C	-3.76029700	2.21079700	2.19445600
C	-2.46959300	2.10007400	2.67982600
C	-4.33554300	3.50804900	2.07250100
C	-1.69268900	3.24604200	2.97090000
H	-2.02873000	1.12100500	2.83043700
C	-3.61656900	4.63835600	2.38830500
H	-5.35210300	3.59718500	1.70075500
C	-2.26396300	4.54746400	2.81280300
C	-0.32995800	3.13011400	3.35602700
H	-4.07000200	5.62149900	2.28722500
C	-1.44758900	5.68663100	3.03711500
C	0.43972100	4.25262400	3.54885700
H	0.09445200	2.13559900	3.45754200
C	-0.12466800	5.54228200	3.38794000
H	-1.87870500	6.67575700	2.90663800
H	1.48764300	4.15519300	3.81479500
H	0.49563200	6.42094000	3.53731300
H	0.98886300	-0.24628600	-0.75454300
H	2.90657800	-1.76485900	-0.32274400

TS-1a-trans

O	-0.48393100	2.42227700	0.82800700
H	-0.30825300	3.37161400	0.80441100
N	-1.99287200	-2.26618900	-0.00706100
C	-0.70725200	-1.81221900	0.10731600
C	-0.66453100	-0.42483800	0.18864800

C	-2.07610300	-0.00736200	0.03865700
C	-2.78856800	1.20051100	-0.11915700
H	-2.27025900	2.14300400	-0.10929400
C	-4.16648900	1.18822900	-0.29409900
H	-4.68748600	2.13398000	-0.40949800
C	-4.90021800	-0.00953600	-0.33181900
H	-5.97722400	0.01468100	-0.46509600
C	-4.24270500	-1.22397500	-0.21938900
H	-4.77598000	-2.16869700	-0.27325700
C	-2.85578600	-1.19763200	-0.05666000
C	0.58946200	0.36724700	0.23049400
C	0.60648100	1.76361300	0.33184800
C	1.72148400	2.54294800	-0.05973500
H	1.62026800	3.62660900	-0.05665100
C	2.88683100	1.95482500	-0.46495600
H	3.72213200	2.55033900	-0.81932500
C	3.02960000	0.55232200	-0.33436800
C	4.28890100	-0.05706800	-0.56697800
H	5.09493300	0.56695800	-0.94362700
C	4.50764900	-1.38378000	-0.28151500
H	5.47964300	-1.83550600	-0.45146500
C	3.46611400	-2.12705000	0.30901200
H	3.65166200	-3.14123700	0.65012100
C	2.21836800	-1.57018100	0.49678700
H	1.49104500	-2.14085500	1.05234600
C	1.91131900	-0.23513900	0.10970100
H	-2.25488500	-3.23247100	-0.10749200
H	0.08861800	-2.52879700	0.05148100

TS-1a-cis

O	0.78523700	3.13935900	0.60737700
H	1.45293800	3.81749500	0.76958200
N	-2.71369300	1.82497800	-0.44944400
C	-1.36743300	1.96875000	-0.30930800
C	-0.74994600	0.77015500	0.03212100
C	-1.86480000	-0.21331600	0.07287100
C	-2.07987100	-1.59665800	0.28487500
H	-1.27791400	-2.29211000	0.45433800
C	-3.35423200	-2.14947400	0.24577700
H	-3.45965000	-3.21646400	0.41583300
C	-4.49451700	-1.37568900	-0.01467000
H	-5.47721700	-1.83526200	-0.03793600
C	-4.34910700	-0.02035100	-0.25571400
H	-5.20183700	0.61522900	-0.47684900

C	-3.06253300	0.51849700	-0.21524300
C	0.74392100	0.75588300	0.15884100
C	1.44330200	1.97147800	0.28572900
C	2.83318000	2.08581600	0.05244300
H	3.28128200	3.07687800	0.09635000
C	3.59690800	0.99747700	-0.26539700
H	4.65344400	1.10022400	-0.49175600
C	3.00511800	-0.28418900	-0.23279600
C	3.80170200	-1.44400500	-0.42033100
H	4.84830000	-1.30620000	-0.67837200
C	3.28593200	-2.70476400	-0.24102900
H	3.90847900	-3.58324400	-0.37768900
C	1.94851900	-2.83440800	0.18828200
H	1.54853500	-3.81450900	0.43056600
C	1.15009400	-1.72198500	0.33311200
H	0.17597900	-1.83356100	0.76155400
C	1.60276400	-0.40902200	0.06208700
H	-3.35457400	2.56749000	-0.67419300
H	-0.91781600	2.92913900	-0.47423900