Supporting Information for

Catalytic Asymmetric Diastereodivergent Synthesis of 2-Alkenylindoles Bearing both Axial and Central Chirality

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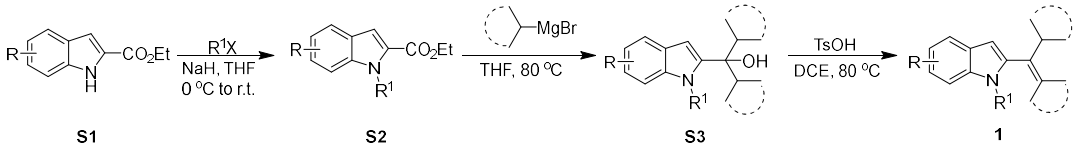
1. General information

^{1}H and ^{13}C NMR spectra were measured at 400 and 100 MHz, respectively. The solvent used for NMR spectroscopy was $CDCl_3$, using tetramethylsilane as the internal reference. HRMS (ESI) was determined by a HRMS/MS instrument. Enantiomeric ratios (*er*) 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 λ = 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 **3aa** and *rac*-**4ak** was GaKα (λ = 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.

2. General procedure for the synthesis of substrates 1

General procedure for the synthesis of substrates 1:



S1 **S2** **S3** **1**

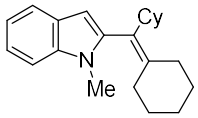
S1 to **S2**: To an ice-bath cooled suspension of NaH (12 mmol, 1.2 equiv.) in THF (10 mL) was added dropwise the corresponding **S1** (10 mmol, 1 equiv.) in THF (20 mL) at 0°C. R^1X (12 mmol, 1.2 equiv.) was added and the mixture was stirred at room temperature for 10 h. After the completion of the reaction indicated by TLC, the reaction mixture was quenched by saturated ammonium chloride solution and extracted by ethyl acetate for three times. The combined organic layers were dried and concentrated under reduced pressure to afford crude product **S2**.

S2 to **S3**: Under argon atmosphere, cyclohexylmagnesium bromide (40 mL, 1 mol/L, 4 equiv.) was added to a Schlenk bottle. Then, the solution of **S2** (10 mmol, 1 equiv.) in anhydrous THF (10 mL) was added dropwise to the Schlenk bottle at 0 °C. Subsequently, the reaction mixture was stirred at 80 °C for 5 h. After the completion of the reaction indicated by TLC, the reaction mixture was quenched by saturated ammonium chloride solution and extracted by ethyl acetate for three times. The combined organic layers were dried and concentrated under reduced pressure to afford crude product **S3**.

S3 to **1**: To the mixture of product **S3** (5 mmol, 1.0 equiv.) in DCE (20 mL) was added TsOH (5 mmol, 1.0 equiv.) at room temperature. Then, the reaction mixture was stirred at 80 °C for 10 h. After the completion of the reaction which was indicated by TLC, the reaction mixture was concentrated and the residue was further purified through flash column chromatography on silica gel (PE) to afford substrates **1** as white solid.

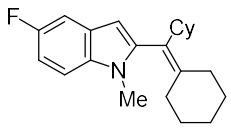
Characterization data of substrates 1:

2-(cyclohexyl(cyclohexylidene)methyl)-1-methyl-1H-indole (1a):



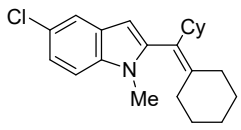
63% yield (0.97 g); white solid; m.p. 106-107 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.61 (d, *J* = 7.7 Hz, 1H), 7.35 – 7.28 (m, 1H), 7.22 – 7.16 (m, 1H), 7.16 – 7.08 (m, 1H), 6.17 (s, 1H), 3.58 (s, 3H), 2.77 – 2.69 (m, 1H), 2.53 – 2.45 (m, 1H), 2.40 – 2.32 (m, 1H), 1.78 – 1.67 (m, 5H), 1.66 – 1.61 (m, 2H), 1.60 – 1.55 (m, 2H), 1.53 – 1.36 (m, 5H), 1.34 – 1.21 (m, 2H), 1.04 – 0.95 (m, 1H), 0.88 – 0.77 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 141.7, 140.3, 136.6, 128.2, 128.1, 120.3, 119.9, 119.2, 109.2, 100.6, 40.3, 33.1, 32.7, 31.0, 30.2, 30.1, 28.6, 27.9, 26.9, 26.7, 26.5, 25.9; IR (KBr): 2925, 2850, 2715, 1638, 1628, 1464, 1447, 1381, 1348, 1230, 1097, 774; ESI FTMS exact mass calcd for $(C_{22}H_{29}N+H)^+$ requires m/z 308.2373, found m/z 308.2379.

2-(cyclohexyl(cyclohexylidene)methyl)-5-fluoro-1-methyl-1H-indole (1b):



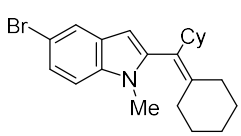
40% yield (0.65 g); white solid; m.p. 74-75 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.25 – 7.15 (m, 2H), 6.95 – 6.87 (m, 1H), 6.11 (s, 1H), 3.55 (s, 3H), 2.75 – 2.67 (m, 1H), 2.51 – 2.43 (m, 1H), 2.37 – 2.29 (m, 1H), 1.78 – 1.66 (m, 5H), 1.62 – 1.53 (m, 5H), 1.49 – 1.35 (m, 4H), 1.33 – 1.19 (m, 2H), 1.02 – 0.93 (m, 1H), 0.84 – 0.73 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ157.9 (d, *J* = 231.8 Hz), 142.0, 141.9, 133.2, 128.1 (d, *J* = 10.0 Hz), 109.6 (d, *J* = 9.8 Hz), 108.3 (d, *J* = 25.9 Hz), 104.6 (d, *J* = 23.0 Hz), 100.6, 100.5, 40.3, 33.1, 32.7, 31.0, 30.3, 30.0, 28.6, 27.9, 26.9, 26.7, 26.5, 25.8; ^{19}F NMR (376 MHz, $CDCl_3$) δ -125.9; IR (KBr): 2925, 2851, 1478, 1447, 1386, 1328, 1253, 1189, 1120, 851; ESI FTMS exact mass calcd for $(C_{22}H_{28}FN+H)^+$ requires m/z 326.2279, found m/z 326.2280.

5-chloro-2-(cyclohexyl(cyclohexylidene)methyl)-1-methyl-1H-indole (1c):



52% yield (0.89 g); white solid; m.p. 105-106 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.53 (s, 1H), 7.22 – 7.16 (m, 1H), 7.14 – 7.07 (m, 1H), 6.10 (s, 1H), 3.54 (s, 3H), 2.75 – 2.66 (m, 1H), 2.51 – 2.43 (m, 1H), 2.37 – 2.29 (m, 1H), 1.79 – 1.66 (m, 5H), 1.62 – 1.56 (m, 4H), 1.53 – 1.41 (m, 3H), 1.39 – 1.22 (m, 4H), 1.01 – 0.93 (m, 1H), 0.82 – 0.71 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 142.1, 141.8, 135.0, 129.0, 127.9, 124.9, 120.4, 119.2, 110.1, 100.2, 40.2, 33.1, 32.7, 31.0, 30.3, 30.0, 28.6, 27.9, 26.9, 26.7, 26.5, 25.8; IR (KBr): 3421, 2926, 2851, 1633, 1606, 1468, 1353, 1265, 1116, 914, 749; ESI FTMS exact mass calcd for $(C_{22}H_{28}ClN+H)^+$ requires m/z 342.1983, found m/z 342.1987.

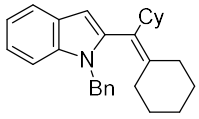
5-bromo-2-(cyclohexyl(cyclohexylidene)methyl)-1-methyl-1H-indole (1d):



57% yield (1.10 g); white solid; m.p. 102-103 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.69 (s, 1H), 7.26 – 7.21 (m, 1H), 7.18 – 7.12 (m, 1H), 6.10 (s, 1H), 3.54 (s, 3H), 2.75 – 2.64 (m, 1H), 2.51 – 2.43 (m, 1H), 2.38 – 2.28 (m, 1H), 1.76 – 1.68 (m, 4H), 1.63 – 1.55 (m, 5H), 1.53 – 1.41 (m, 3H), 1.39 – 1.33 (m, 2H), 1.32 – 1.20 (m, 2H), 1.03 – 0.95 (m, 1H), 0.82 – 0.70 (m, 1H);

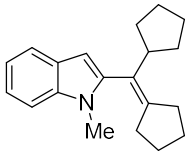
^{13}C NMR (100 MHz, $CDCl_3$) δ 142.1, 141.6, 135.2, 129.6, 127.8, 123.0, 122.3, 112.5, 110.6, 100.1, 40.2, 33.1, 32.7, 30.9, 30.3, 30.0, 28.6, 27.9, 26.9, 26.7, 26.4, 25.8; IR (KBr): 2925, 2851, 1627, 1466, 1447, 1377, 1254, 787; ESI FTMS exact mass calcd for $(C_{22}H_{28}BrN+H)^+$ requires m/z 386.1478, found m/z 386.1473.

1-benzyl-2-(cyclohexyl(cyclohexylidene)methyl)-1H-indole (1e):



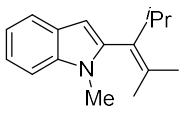
70% yield (1.34 g); white solid; m.p. 98-99 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.62 (d, *J* = 7.7 Hz, 1H), 7.28 – 7.26 (m, 1H), 7.26 – 7.18 (m, 2H), 7.12 – 6.99 (m, 5H), 6.24 (s, 1H), 5.29 – 5.20 (m, 2H), 2.74 – 2.59 (m, 1H), 2.51 – 2.40 (m, 1H), 2.32 – 2.19 (m, 1H), 1.86 – 1.78 (m, 1H), 1.76 – 1.62 (m, 4H), 1.59 – 1.52 (m, 4H), 1.48 – 1.37 (m, 3H), 1.32 – 1.15 (m, 4H), 1.02 – 0.94 (m, 1H), 0.88 – 0.79 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 142.9, 140.7, 137.9, 136.4, 128.5, 128.4, 128.2, 126.9, 126.6, 120.5, 119.9, 119.4, 110.9, 101.4, 47.8, 40.4, 33.5, 33.0, 31.3, 30.2, 28.5, 28.0, 26.8, 26.5, 25.9; IR (KBr): 3420, 2925, 2851, 1708, 1593, 1461, 1352, 1309, 1160, 727; ESI FTMS exact mass calcd for $(C_{28}H_{33}N+H)^+$ requires m/z 384.2686, found m/z 384.2691.

2-(cyclopentyl(cyclopentylidene)methyl)-1-methyl-1H-indole (1f):



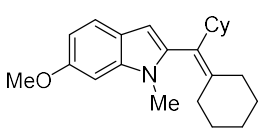
29% yield (0.41 g); colorless oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.61 (d, *J* = 7.8 Hz, 1H), 7.35 – 7.29 (m, 1H), 7.23 – 7.16 (m, 1H), 7.15 – 7.08 (m, 1H), 6.17 (s, 1H), 3.58 (s, 3H), 3.01 – 2.87 (m, 1H), 2.59 – 2.41 (m, 2H), 1.98 – 1.85 (m, 2H), 1.83 – 1.65 (m, 4H), 1.63 – 1.56 (m, 4H), 1.52 – 1.45 (m, 2H), 1.02 – 0.84 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 146.9, 140.5, 136.8, 128.2, 125.9, 120.4, 120.1, 119.2, 109.3, 99.8, 44.8, 32.7, 30.9, 30.3, 30.3, 29.8, 26.6, 26.5, 25.0, 24.7; IR (KBr): 3460, 3053, 2960, 2928, 2868, 1647, 1464, 1310, 1080, 749; ESI FTMS exact mass calcd for $(C_{20}H_{25}N-H)^-$ requires m/z 278.1914, found m/z 278.1931.

2-(2,4-dimethylpent-2-en-3-yl)-1-methyl-1H-indole (1g):



68% yield (0.77 g); colorless oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.66 (d, *J* = 7.8 Hz, 1H), 7.41 – 7.34 (m, 1H), 7.27 – 7.21 (m, 1H), 7.19 – 7.13 (m, 1H), 6.24 (s, 1H), 3.60 (s, 3H), 3.20 – 3.10 (m, 1H), 1.96 (s, 3H), 1.47 (s, 3H), 1.16 (d, *J* = 6.8 Hz, 3H), 0.81 (d, *J* = 6.5 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 139.5, 136.7, 133.3, 131.7, 128.1, 120.4, 120.0, 119.2, 109.2, 100.4, 30.4, 29.9, 22.8, 22.0, 20.6, 19.5; IR (KBr): 3481, 2951, 2866, 1528, 1464, 1365, 1309, 1130, 748; ESI FTMS exact mass calcd for $(C_{16}H_{21}N-H)^-$ requires m/z 221.1601, found m/z 221.1619.

2-(cyclohexyl(cyclohexylidene)methyl)-6-methoxy-1-methyl-1H-indole (1h):

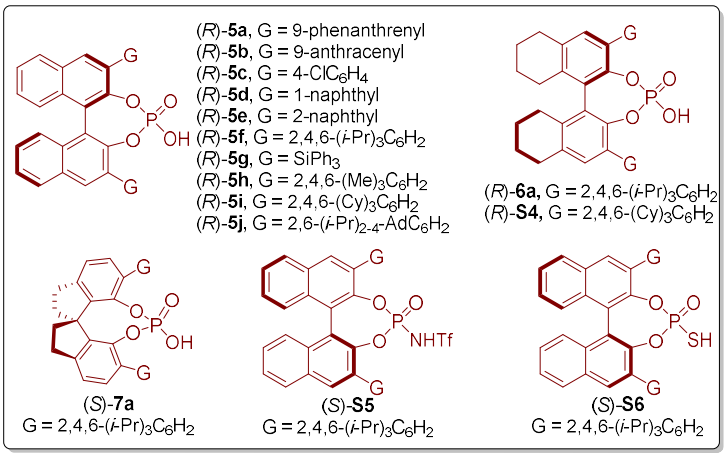


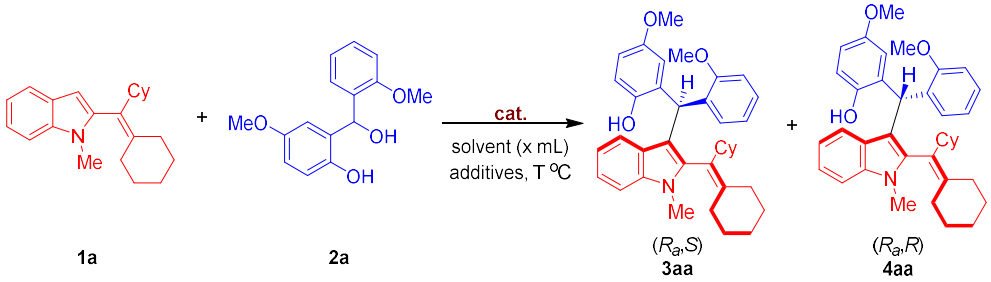
39% yield (0.66 g); white solid; m.p. 89-90 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.47 (d, *J* = 8.8 Hz, 1H), 6.83 – 6.75 (m, 2H), 6.08 (s, 1H), 3.91 (s, 3H), 3.52 (s, 3H), 2.76 – 2.65 (m, 1H), 2.52 – 2.43 (m, 1H), 2.39 – 2.30 (m, 1H), 1.80 – 1.69 (m, 4H), 1.65 – 1.56 (m, 5H), 1.53 – 1.21 (m, 7H), 1.04 – 0.94 (m, 1H), 0.89 – 0.78 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ

155.4, 141.8, 139.2, 137.2, 128.3, 122.4, 120.4, 108.7, 100.2, 93.4, 55.9, 40.3, 33.1, 32.6, 31.0, 30.2, 30.1, 28.6, 27.9, 27.0, 26.7, 26.5, 25.9; IR (KBr): 2924, 2850, 1491, 1447, 1377, 1293, 1241, 1213, 1088, 811; ESI FTMS exact mass calcd for $(C_{23}H_{31}NO+H)^+$ requires m/z 338.2479, found m/z 338.2472.

3. Conditions optimization for the synthesis of 3aa and 4aa

Table S1. Conditions optimization for the synthesis of **3aa**[a]





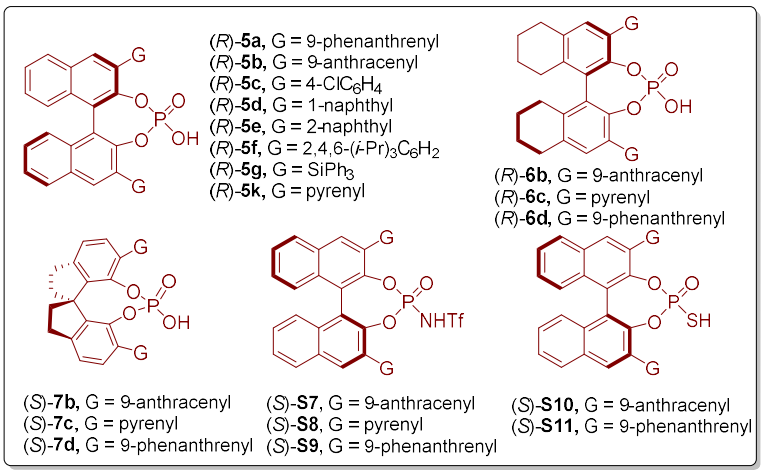
1a 2a

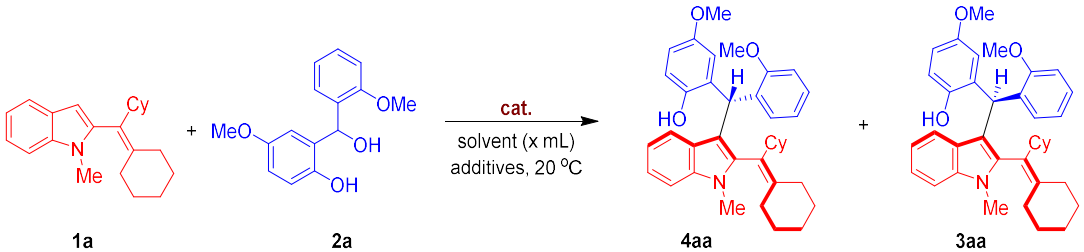
entry	cat.	solvent	T (°C)	additive	**1a**:**2a**	x (mL)	yield (%)[b]	**3aa**:**4aa**[c]	er of **3aa**(**4aa**)[d]
1	(*R*)-**5a**	DCE	20	/	1:1.2	0.5	80	18:82	53:47(64:36)
2	(*R*)-**5b**	DCE	20	/	1:1.2	0.5	58	23:77	62:38(52:48)
3	(*R*)-**5c**	DCE	20	/	1:1.2	0.5	82	31:69	52:48(50:50)
4	(*R*)-**5d**	DCE	20	/	1:1.2	0.5	79	31:69	51:49(52:48)
5	(*R*)-**5e**	DCE	20	/	1:1.2	0.5	79	28:72	53:47(51:49)
6	(*R*)-**5f**	DCE	20	/	1:1.2	0.5	32	72:28	69:31(56:44)
7	(*R*)-**5g**	DCE	20	/	1:1.2	0.5	23	47:53	52:48(68:32)
8	(*R*)-**5f**	DCE	20	5 Å MS	1:1.2	0.5	84	77:23	78:22
9	(*R*)-**5f**	THF	20	5 Å MS	1:1.2	0.5	N.R.	/	/
10	(*R*)-**5f**	toluene	20	5 Å MS	1:1.2	0.5	61	40:60	84:16(69:31)
11	(*R*)-**5f**	CH_3CN	20	5 Å MS	1:1.2	0.5	30	75:25	68:32(52:48)
12	(*R*)-**5f**	EA	20	5 Å MS	1:1.2	0.5	N.R.	/	/
13	(*R*)-**5f**	acetone	20	5 Å MS	1:1.2	0.5	trace	/	/
14	(*R*)-**5h**	DCE	20	5 Å MS	1:1.2	0.5	71	38:62	53:47(48:52)
15	(*S*)-**5i**	DCE	20	5 Å MS	1:1.2	0.5	54	73:27	14:86(52:48)
16	(*R*)-**5j**	DCE	20	5 Å MS	1:1.2	0.5	75	67:33	74:26(52:48)
17	(*S*)-**6a**	DCE	20	5 Å MS	1:1.2	0.5	42	63:27	42:58(61:39)
18	(*R*)-**S4**	DCE	20	5 Å MS	1:1.2	0.5	17	65:35	74:26(48:52)
19	(*S*)-**7a**	DCE	20	5 Å MS	1:1.2	0.5	54	89:11	84:16
20	(*S*)-**S5**	DCE	20	5 Å MS	1:1.2	0.5	48	62:38	45:55(53:47)
21	(*S*)-**S6**	DCE	20	5 Å MS	1:1.2	0.5	44	79:21	26:74
22	(*S*)-**7a**	DCM	20	5 Å MS	1:1.2	0.5	69	74:26	76:24(50:50)
23	(*S*)-**7a**	$CHCl_3$	20	5 Å MS	1:1.2	0.5	15	84:16	80:20
24	(*S*)-**7a**	CCl_4	20	5 Å MS	1:1.2	0.5	23	65:35	75:25(42:58)

25	(*S*)-**7a**	DCE	20	3 Å MS	1:1.2	0.5	36	91:9	85:15
26	(*S*)-**7a**	DCE	20	4 Å MS	1:1.2	0.5	45	91:9	86:14
27	(*S*)-**7a**	DCE	20	Na_2SO_4	1:1.2	0.5	16	89:11	84:16
28	(*S*)-**7a**	DCE	20	$MgSO_4$	1:1.2	0.5	24	89:11	84:16
29	(*S*)-**7a**	DCE	20	4 Å MS	1:1.2	0.25	51	91:9	85:15
30	(*S*)-**7a**	DCE	20	4 Å MS	1:1.2	1	35	92:8	86:14
31	(*S*)-**7a**	DCE	20	4 Å MS	1:1.2	2	28	92:8	87:13
32	(*S*)-**7a**	DCE	0	4 Å MS	1:1.2	2	trace	/	/
33	(*S*)-**7a**	DCE	10	4 Å MS	1:1.2	2	18	94:6	91:9
34	(*S*)-**7a**	DCE	50	4 Å MS	1:1.2	2	40	91:9	82:18
35[e]	(*S*)-**7a**	DCE	0	4 Å MS	1:1.2	2	16	95:5	92:8
36[e]	(*S*)-**7a**	DCE	0	3 Å MS	1:1.2	2	17	95:5	93:7
37[e]	(*S*)-**7a**	DCE	0	5 Å MS	1:1.2	2	31	94:6	91:9
38[e]	(*S*)-**7a**	DCE	0	3 Å MS	1:1.5	2	21	95:5	92:8
39[e]	(*S*)-**7a**	DCE	0	3 Å MS	1:2	2	24	95:5	91:9
40[e]	(*S*)-**7a**	DCE	0	3 Å MS	1.5:1	2	27	95:5	92:8
41[e]	(*S*)-**7a**	DCE	0	3 Å MS	2:1	2	30	95:5	92:8
42[e]	(*S*)-**7a**	DCE	0	3 Å MS	3:1	2	38	95:5	92:8
43[e]	(*S*)-**7a**	DCE	0	3 Å MS	3:1	0.5	45	95:5	91:9
44[e]	(*S*)-**7a**	DCE	0	3 Å MS	3:1	1	43	95:5	92:8
45[e,f]	(*S*)-**7a**	DCE	0	3 Å MS	3:1	1	35	95:5	92:8
46[e,g]	(*S*)-**7a**	DCE	0	3 Å MS	3:1	1	52	95:5	92:8

[a]Unless otherwise indicated, the reaction was carried out on a 0.05 mmol scale with additives (50 mg) at T °C in a solvent for 12 h. [b]Isolated yield. [c]The dr value (**3aa**:**4aa**) was determined by ^{1}H NMR. [d] The er values were determined by HPLC. [e]for 36 h. [f]5 mol% (*S*)-**7a** [g]20 mol% (*S*)-**7a**.

Table S2. Conditions optimization for the synthesis of **4aa**[a]





1a 2a 4aa 3aa

entry	cat.	solvent	**1a**:**2a**	additive	x (mL)	yield (%)[b]	**4aa**:**3aa**[c]	er of **4aa**(**3aa**)[d]
1	(*R*)-**5a**	DCE	1:1.2	/	0.5	80	82:18	64:36(53:47)
2	(*R*)-**5a**	THF	1:1.2	/	0.5	N.R.	/	/
3	(*R*)-**5a**	toluene	1:1.2	/	0.5	47	87:13	78:22
4	(*R*)-**5a**	CH_3CN	1:1.2	/	0.5	61	53:47	52:48(50:50)
5	(*R*)-**5a**	AcOEt	1:1.2	/	0.5	10	85:15	72:28
6	(*R*)-**5a**	acetone	1:1.2	/	0.5	20	79:21	67:33
7	(*R*)-**5k**	toluene	1:1.2	/	0.5	73	71:29	56:44(83:17)
8	(*R*)-**6b**	toluene	1:1.2	/	0.5	37	89:11	77:23
9	(*R*)-**6c**	toluene	1:1.2	/	0.5	70	70:30	54:46(86:14)
10	(*R*)-**6d**	toluene	1:1.2	/	0.5	71	84:16	70:30
11	(*S*)-**7b**	toluene	1:1.2	/	0.5	47	90:10	84:16
12	(*R*)-**7c**	toluene	1:1.2	/	0.5	45	89:11	19:81
13	(*S*)-**7d**	toluene	1:1.2	/	0.5	12	90:10	75:25
14	(*S*)-**S7**	toluene	1:1.2	/	0.5	54	84:16	47:53
15	(*S*)-**S8**	toluene	1:1.2	/	0.5	54	75:25	29:61
16	(*S*)-**S9**	toluene	1:1.2	/	0.5	57	60:40	46:54(56:44)
17	(*S*)-**S10**	toluene	1:1.2	/	0.5	51	89:11	35:65
18	(*S*)-**S11**	toluene	1:1.2	/	0.5	35	88:12	27:73
19	(*S*)-**7b**	*o*-xylene	1:1.2	/	0.5	40	89:11	81:19
20	(*S*)-**7b**	*m*-xylene	1:1.2	/	0.5	48	88:12	81:19
21	(*S*)-**7b**	*p*-xylene	1:1.2	/	0.5	44	89:11	88:12
22	(*S*)-**7b**	PhF	1:1.2	/	0.5	61	90:10	72:28
23	(*S*)-**7b**	PhCl	1:1.2	/	0.5	64	91:9	77:23
24	(*S*)-**7b**	PhBr	1:1.2	/	0.5	49	91:9	75:25
25	(*S*)-**7b**	mesitylene	1:1.2	/	0.5	25	87:13	87:13
26	(*S*)-**7b**	$PhCF_3$	1:1.2	/	0.5	76	91:9	74:26

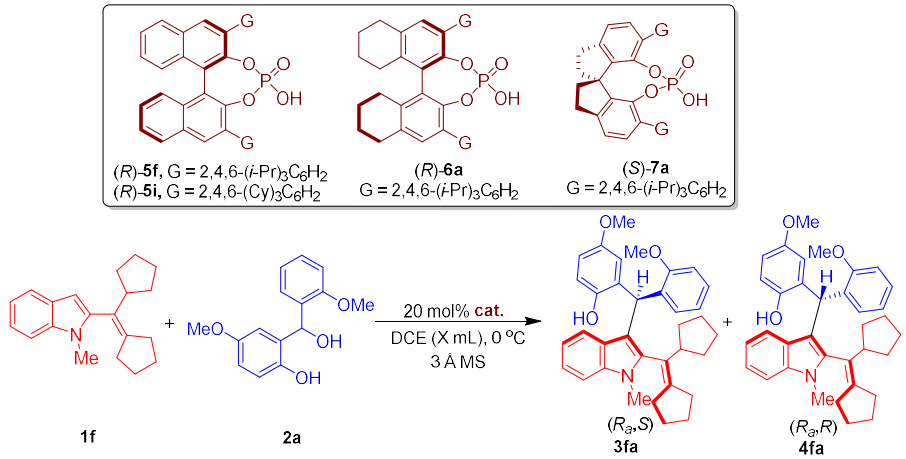
27	(*S*)-**7b**	*p*-xylene	1:2	/	0.5	45	89:11	87:13
28	(*S*)-**7b**	*p*-xylene	1:3	/	0.5	49	89:11	88:12
29	(*S*)-**7b**	*p*-xylene	1.2:1	/	0.5	37	89:11	87:13
30	(*S*)-**7b**	*p*-xylene	2:1	/	0.5	52	89:11	88:12
31	(*S*)-**7b**	*p*-xylene	2:1	3 Å MS	0.5	99	90:10	89:11
32	(*S*)-**7b**	*p*-xylene	2:1	4 Å MS	0.5	99	90:10	90:10
33	(*S*)-**7b**	*p*-xylene	2:1	5 Å MS	0.5	99	90:10	89:11
34	(*S*)-**7b**	*p*-xylene	2:1	Na_2SO_4	0.5	40	89:11	88:16
35	(*S*)-**7b**	*p*-xylene	2:1	$MgSO_4$	0.5	55	89:11	89:11
36	(*S*)-**7b**	*p*-xylene	2:1	4 Å MS	0.25	99	90:10	89:11
37	(*S*)-**7b**	*p*-xylene	2:1	4 Å MS	1	99	91:9	91:9
38	(*S*)-**7b**	*p*-xylene	2:1	4 Å MS	2	99	92:8	93:7
39	(*S*)-**7b**	*p*-xylene	2:1	4 Å MS	3	83	92:8	92:8
40	(*S*)-**7b**	*p*-xylene	2:1	4 Å MS	4	59	92:8	92:8
41[e]	(*S*)-**7b**	*p*-xylene	2:1	4 Å MS	2	87	92:8	92:8
42[f]	(*S*)-**7b**	*p*-xylene	2:1	4 Å MS	2	99	92:8	93:7

[a]Unless otherwise indicated, the reaction was carried out on a 0.05 mmol scale with additives (50 mg) at 20 °C in a solvent for 12 h. [b]Isolated yield. [c]The dr value (**4aa**:**3aa**) was determined by ^{1}H NMR. [d]The er values were determined by HPLC. [e]5 mol% (*S*)-**7b**. [f]20 mol% (*S*)-**7b**.

4. Conditions optimization for the synthesis of 3fa-3ga and 4fa-4ga

In order to improve the enantioselectivity and diastereoselective of products **3fa**, we re-optimized some reaction conditions (**Table S3**). In detail, to improve the stereoselectivity of **3fa**, chiral phosphoric acids (CPAs) **5-7** were re-evaluated (entries 1-4) and it was discovered CPA (*S*)-**5i** could catalyze the reaction to give product **3fa** in a higher enantioselectivity and diastereoselectivity than CPA (*S*)-**7a** (entry 3 vs entry 1). Then, we modulated the volume of solvent and discovered the enantioselectivity could not be significantly improved (entries 5-6). Therefore, 1 mL DCE was still the best solvent volume for this reaction, which was chosen as the optimal reaction conditions for the synthesis of product **3fa** (entry 3).

Table S3. Conditions re-optimization for the synthesis of **3fa**[a]

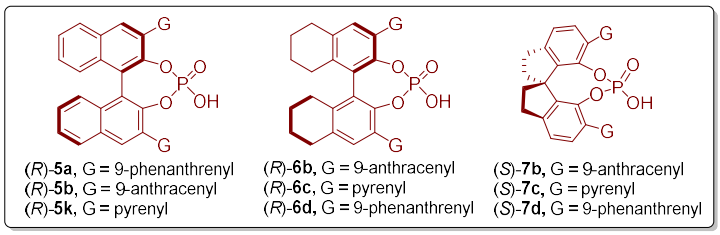


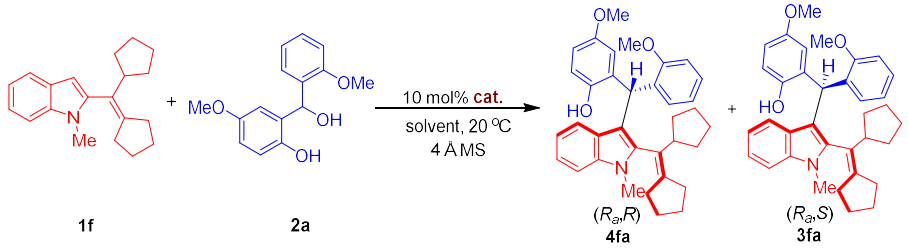
entry	cat.	X	yield (%)[b]	**3fa**:**4fa**[c]	er of **3fa**[d]
1	(*S*)-**7a**	1	47	78:22	85:15
2	(*R*)-**5f**	1	54	81:19	76:24
3	(*S*)-**5i**	1	46	85:15	10:90
4	(*R*)-**6a**	1	39	77:23	55:45
5	(*S*)-**5i**	0.5	49	83:17	11:89
6	(*S*)-**5i**	2	33	85:15	10:90

[a]Unless otherwise indicated, the reaction was carried out on a 0.05 mmol scale with 3 Å MS (50 mg) at 0 °C in DCE for 36 h. [b]Isolated yield. [c]The dr value (**3fa**:**4fa**) was determined by ^{1}H NMR. [d]The er values were determined by HPLC.

In addition, we have re-optimized the reaction conditions for the synthesis of product **4fa** (**Table 2**). To improve the stereoselectivity of **4fa**, we re-evaluated CPAs **5-7** (entries 2-9) and discovered CPA (*R*)-**6b** could catalyze the reaction to give product **4fa** in a higher enantioselectivity than CPA (*R*)-**7b** (entry 5 vs entry 1). Then, different solvents were evaluated under the catalysis of (*R*)-**6b** (entries 10-12), and it was discovered that *p*-xylene was still the best solvent, which was chosen as the optimal reaction conditions for the synthesis of product **4fa** (entry 5).

Table S4. Conditions re-optimization for the synthesis of **4fa**[a]



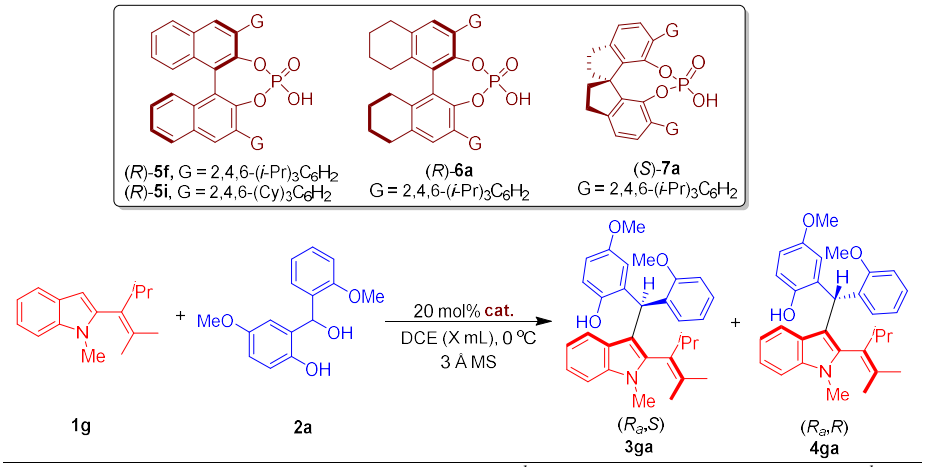


entry	cat.	solvent	yield (%)[b]	4fa:3fa[c]	er of 4fa[d]
1	(*S*)-**7b**	*p*-xylene	62	60:40	73:27
2	(*R*)-**5a**	*p*-xylene	52	67:33	85:15
3	(*R*)-**5b**	*p*-xylene	59	55:45	80:20
4	(*R*)-**5k**	*p*-xylene	66	33:67	60:40
5	(*R*)-**6b**	*p*-xylene	60	75:25	85:15
6	(*R*)-**6c**	*p*-xylene	35	54:46	82:18
7	(*R*)-**6d**	*p*-xylene	76	42:58	72:28
8	(*S*)-**7c**	*p*-xylene	trace	/	/
9	(*S*)-**7d**	*p*-xylene	30	51:49	80:20
10	(*R*)-**6b**	*o*-xylene	49	75:25	83:17
11	(*R*)-**6b**	*m*-xylene	42	75:25	84:16
12	(*R*)-**6b**	mesitylene	53	75:25	84:16

[a]Unless otherwise indicated, the reaction was carried out on a 0.05 mmol scale with 4 Å MS (50 mg) at 20 °C in a solvent (2 mL) for 12 h. [b]Isolated yield. [c]The dr value (**4fa**:**3fa**) was determined by ^{1}H NMR. [d]The er values were determined by HPLC.

As shown in **Table S5**, to improve the stereoselectivity of product **3ga**, the increasing of solvent volume (entries 2-3) discovered that using 2 mL of DCE could slightly increase the enantioselectivity to 86:14 er but with a low yield of 39% (entry 2 vs entry 1). Then, we re-evaluated CPAs **5-7** with 1 mL of DCE (entries 4-6) and discovered CPA (*S*)-**5i** could catalyze the reaction in a higher diastereoselectivity than CPA (*S*)-**7a** (entry 5 vs entry 1). Finally, increasing the solvent volume to 2 mL led to a further increased enantioselectivity of 14:86 er with an acceptable yield of 44% and a good diastereoselectivity of 86:14 dr (entry 7), which was chosen as the optimal reaction conditions for the synthesis of product **3ga**.

Table S5. Conditions re-optimization for the synthesis of **3ga**[a]

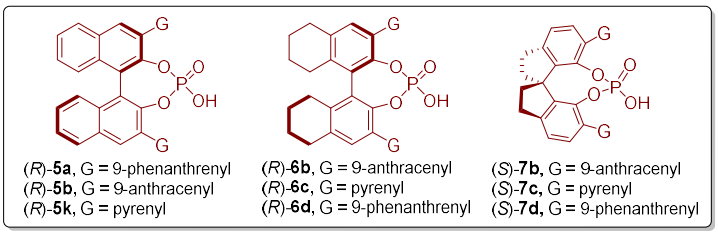


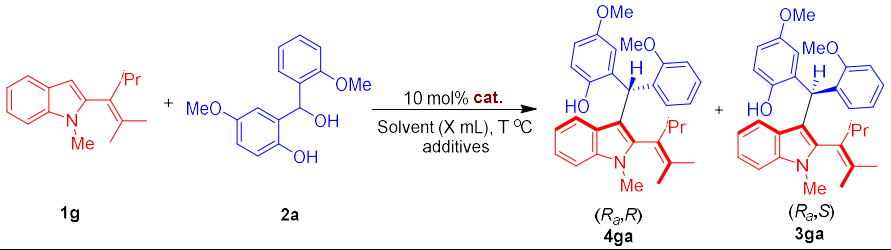
entry	cat.	X	yield (%)[b]	**3ga**:**4ga**[c]	er of **3ga**[d]
1	(*S*)-**7a**	1	48	80:20	85:15
2	(*S*)-**7a**	2	39	80:20	86:14
3	(*S*)-**7a**	3	30	80:20	86:14
4	(*R*)-**5f**	1	51	86:14	70:30
5	(*S*)-**5i**	1	57	86:14	15:85
6	(*S*)-**6a**	1	34	80:20	30:70
7	(*S*)-**5i**	2	44	86:14	14:86

[a]Unless otherwise indicated, the reaction was carried out on a 0.05 mmol scale with 3 Å MS (50 mg) at 0 °C in DCE for 36 h. [b]Isolated yield. [c]The dr value (**3ga**:**4ga**) was determined by ^{1}H NMR. [d]The er values were determined by HPLC.

To improve the enantioselectivity of product **4ga** (**Table S6**), at first, we adjusted the solvent volume, and it was discovered that the enantioselectivity has no significant improvement (entries 1-3). To further increase the enantioselectivity, we re-evaluated CPAs **5-7** (entries 4-11) and discovered CPA (*R*)-**6b** could catalyze the reaction in a higher enantioselectivity than CPA (*R*)-**7b** (entry 7 vs entry 1). Then, different solvents were evaluated under the catalysis of (*R*)-**6b** (entries 12-20), and it was discovered the reaction had similar enantioselectivity when mesitylene was used as the solvent (entry 20 vs entry 7). Because of the lower freezing point, mesitylene was more suitable solvent for modulating reaction temperatures than *p*-xylene. So, the reaction temperature was altered in mesitylene (entries 21-22), which revealed that lowering the reaction temperature to 0 °C could improve the enantioselectivity of **4ga** to 92:8 er albeit with a low yield of 42% (entry 21). Next, modulating the reagent ratio of **1g**:**2a** to 3:1 could slightly increase the yield to 44% (entry 23). To further increase the yield, we screened the additives and it was discovered 4 Å MS was still the best additive for this reaction (entry 21 vs entries 24-25). Finally, the increasing of the catalyst loading discovered that using 20 mol% of (*R*)-**6b** could improve the yield to 53% with a retained enantioselectivity of 92:8 er (entry 26), which was chosen as the optimal reaction conditions for the synthesis of product **4ga**.

Table S6. Conditions optimization for the synthesis of **4ga**[a]

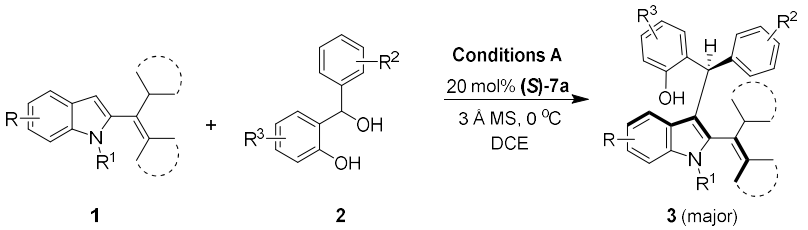




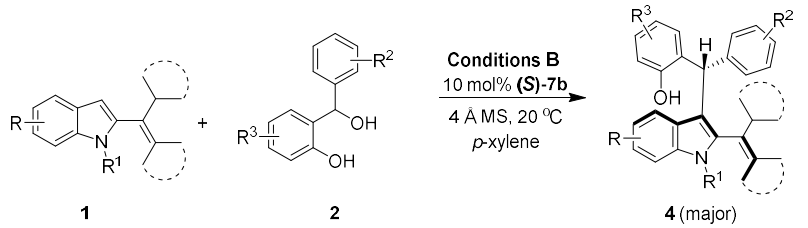
entry	cat.	solvent	additive	T (°C)	**1g**:**2a**	X	yield (%)[b]	**4ga**:**3ga**[c]	er of **4ga**[d]
1	(*S*)-**7b**	*p*-xylene	4 Å MS	20	2:1	1	83	>95:5	78:22
2	(*S*)-**7b**	*p*-xylene	4 Å MS	20	2:1	2	69	>95:5	79:21
3	(*S*)-**7b**	*p*-xylene	4 Å MS	20	2:1	3	60	>95:5	79:21
4	(*R*)-**5a**	*p*-xylene	4 Å MS	20	2:1	2	90	90:10	67:33
5	(*R*)-**5b**	*p*-xylene	4 Å MS	20	2:1	2	82	>95:5	84:16
6	(*R*)-**5k**	*p*-xylene	4 Å MS	20	2:1	2	93	80:20	68:32
7	(*R*)-**6b**	*p*-xylene	4 Å MS	20	2:1	2	60	>95:5	86:14
8	(*R*)-**6c**	*p*-xylene	4 Å MS	20	2:1	2	69	91:9	74:26
9	(*R*)-**6d**	*p*-xylene	4 Å MS	20	2:1	2	99	75:25	81:19
10	(*S*)-**7c**	*p*-xylene	4 Å MS	20	2:1	2	57	94:6	79:21
11	(*S*)-**7d**	*p*-xylene	4 Å MS	20	2:1	2	60	92:8	80:20
12	(*R*)-**6b**	DCE	4 Å MS	20	2:1	2	30	75:25	82:28
13	(*R*)-**6b**	THF	4 Å MS	20	2:1	2	NR	/	/
14	(*R*)-**6b**	toluene	4 Å MS	20	2:1	2	27	80:20	85:15
15	(*R*)-**6b**	CH_3CN	4 Å MS	20	2:1	2	NR	/	/
16	(*R*)-**6b**	AcOEt	4 Å MS	20	2:1	2	NR	/	/
17	(*R*)-**6b**	acetone	4 Å MS	20	2:1	2	NR	/	/
18	(*R*)-**6b**	*o*-xylene	4 Å MS	20	2:1	2	trace	/	/
19	(*R*)-**6b**	*m*-xylene	4 Å MS	20	2:1	2	45	>95:5	85:15
20	(*R*)-**6b**	mesitylene	4 Å MS	20	2:1	2	56	>95:5	86:14
21[e]	(*R*)-**6b**	mesitylene	4 Å MS	0	2:1	2	42	>95:5	92:8
22[e]	(*R*)-**6b**	mesitylene	4 Å MS	-10	2:1	2	27	>95:5	93:7
23[e]	(*R*)-**6b**	mesitylene	4 Å MS	0	3:1	2	44	>95:5	92:8
24[e]	(*R*)-**6b**	mesitylene	3 Å MS	0	3:1	2	40	>95:5	91:9
25[e]	(*R*)-**6b**	mesitylene	5 Å MS	0	3:1	2	45	>95:5	91:9
26[ef]	(*R*)-**6b**	mesitylene	4 Å MS	0	3:1	2	53	>95:5	92:8

[a]Unless otherwise indicated, the reaction was carried out on a 0.05 mmol scale with additives (50 mg) at 20 °C in a solvent for 12 h. [b]Isolated yield. [c]The dr value (**4ga**:**3ga**) was determined by ^{1}H NMR. [d]The er values were determined by HPLC. [e]for 24 h. [f]20 mol%.

5. General procedure for the synthesis of products 3 and 4



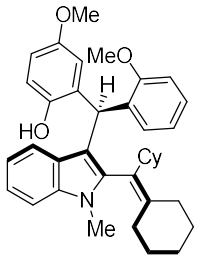
2-Alkenylindoles **1** (0.3 mmol), *o*-hydroxybenzyl alcohols **2** (0.1 mmol), CPA (*S*)-**7a** (0.02 mmol) and 3 Å MS (100 mg) were added to a reaction tube. Then, DCE (2 mL) was added to the reaction mixture, which was stirred at 0 °C for 36 h. After the completion of the reaction indicated by TLC, the reaction mixture was purified through preparative thin layer chromatography on silica gel to afford pure products **3**.



2-Alkenylindoles **1** (0.2 mmol), *o*-hydroxybenzyl alcohols **2** (0.1 mmol), CPA (*S*)-**7b** (0.01 mmol) and 4 Å MS (100 mg) were added to a reaction tube. Then, *p*-xylene (4 mL) was added to the reaction mixture, which was stirred at 20 °C for 12 h. After the completion of the reaction indicated by TLC, the reaction mixture was purified through flash column chromatography on silica gel to afford pure products **4**.

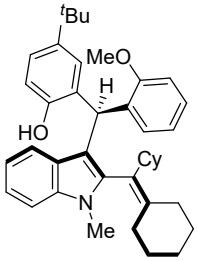
6. Synthetic procedure and characterization data of products 3 and 4

(R_a,*S*)-2-((2-(cyclohexyl(cyclohexylidene)methyl)-1-methyl-1H-indol-3-yl)(2-methoxyphenyl) methyl)-4-methoxyphenol (3aa):



Following the general procedure, 2-alkenylindoles **1a** (92.3 mg, 0.3 mmol), *o*-hydroxybenzyl alcohol **2a** (26.0 mg, 0.1 mmol), CPA (*S*)-**7a** (14.4 mg, 0.02 mmol) and 3 Å MS (100 mg) were added to a reaction tube. Then, DCE (2 mL) was added to the reaction mixture, which was stirred at 0 °C for 36 h. After the completion of the reaction indicated by TLC, the reaction mixture was purified through preparative thin layer chromatography on silica gel (petroleum ether/ethyl acetate = 5:1) to afford pure product **3aa** in 52% yield (28.6 mg) as a white solid; 95:5 dr; m.p. 99-100 °C; $[\alpha]_D^{20}$ = +91.9 (c 0.36, acetone); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.28 – 7.26 (m, 1H), 7.17 – 7.09 (m, 2H), 7.06 – 7.04 (m, 1H), 6.92 – 6.82 (m, 3H), 6.77 – 6.67 (m, 3H), 6.35 (s, 1H), 6.12 (s, 1H), 5.16 (s, 1H), 3.73 (s, 3H), 3.64 (s, 3H), 3.55 (s, 3H), 2.75 – 2.62 (m, 1H), 2.48 – 2.34 (m, 1H), 2.13 – 2.03 (m, 1H), 1.95 – 1.87 (m, 1H), 1.82 – 1.67 (m, 4H), 1.64 – 1.59 (m, 1H), 1.52 – 1.45 (m, 2H), 1.34 – 1.23 (m, 3H), 1.18 – 1.07 (m, 2H), 1.06 – 0.81 (m, 3H), 0.68 – 0.51 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 156.7, 153.4, 149.5, 145.0, 141.2, 136.9, 131.2, 131.1, 127.9, 127.5, 125.7, 121.0, 120.8, 120.0, 119.6, 116.5, 115.9, 111.7, 110.4, 110.0, 109.3, 67.1, 55.6, 41.7, 36.8, 33.6, 32.4, 31.2, 30.8, 30.4, 28.1, 27.3, 27.0, 26.9, 26.5, 25.9; IR (KBr): 3433, 2926, 2850, 1667, 1585, 1489, 1464, 1242, 1047, 740; ESI FTMS exact mass calcd for $(C_{37}H_{43}NO_3+H)^+$ requires m/z 550.3315 , found m/z 550.3344; The enantiomeric ratio: 92:8, determined by HPLC (Daicel Chiralpak AD-3, hexane/ isopropanol = 98/ 2, flow rate 0.8 mL/min, T = 30 °C, 254 nm): t_R = 9.883 (major), t_R = 15.576 (minor).

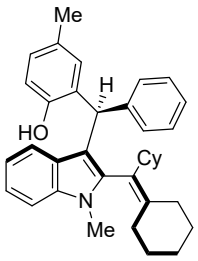
(R_a,*S*)-4-(tert-butyl)-2-((2-(cyclohexyl(cyclohexylidene)methyl)-1-methyl-1H-indol-3-yl)(2-methoxyphenyl)methyl)phenol (3ab):



Following the general procedure, 2-alkenylindoles **1a** (92.3 mg, 0.3 mmol), *o*-hydroxybenzyl alcohol **2b** (28.6 mg, 0.1 mmol), CPA (*S*)-**7a** (14.4 mg, 0.02 mmol) and 3 Å MS (100 mg) were added to a reaction tube. Then, DCE (4 mL) was added to the reaction mixture, which was stirred at 0 °C for 36 h. After the completion of the reaction indicated by TLC, the reaction mixture was purified through preparative thin layer chromatography on silica gel (petroleum ether/ethyl acetate = 5:1) to afford pure product **3ab** in 59% yield (34.0 mg) as colorless oil; 95:5 dr; $[\alpha]_D^{20}$ = +42.4 (c 0.33, acetone); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.28 (s, 1H), 7.19 – 7.09 (m, 3H), 7.07 (d, *J* = 7.6 Hz, 1H), 6.90 – 6.81 (m, 3H), 6.81 – 6.75 (m, 2H), 6.74 – 6.70 (m, 1H), 6.10 (s, 1H), 5.38 (s, 1H), 3.71 (s, 3H), 3.56 (s, 3H), 2.74 – 2.61 (m, 1H), 2.47 – 2.36 (m, 1H), 2.19 – 2.09 (m, 1H), 1.89 – 1.81 (m, 1H), 1.72 – 1.48 (m, 9H), 1.44 – 1.38 (m, 1H), 1.26 – 1.23 (m, 2H), 1.15 (s, 9H), 1.11 – 1.04 (m, 1H), 1.00 – 0.91 (m, 2H), 0.87 – 0.78 (m, 1H), 0.71 – 0.58 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 156.9, 153.0, 144.8, 142.6, 140.9, 136.9, 131.4, 131.0, 128.8, 128.0, 127.4, 126.5, 125.9, 124.2, 120.9, 120.7,

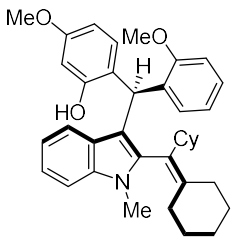
120.0, 119.5, 115.4, 110.3, 109.2, 41.6, 37.2, 34.1, 33.5, 32.5, 31.5, 31.2, 30.7, 30.5, 28.1, 27.2, 27.1, 26.9, 26.6, 25.9; IR (KBr): 3421, 2927, 2851, 1594, 1489, 1383, 1351, 1243, 1121, 741; ESI FTMS exact mass calcd for $(C_{40}H_{49}NO_2\text{-}H)^-$ requires m/z 574.3690, found m/z 574.3689; The enantiomeric ratio: 92:8, determined by HPLC (Daicel Chiralpak ID, hexane/ isopropanol = 98/ 2, flow rate 1.0 mL/min, T = 30 °C, 254 nm): t_R = 4.679 (major), t_R = 6.253 (minor).

(R_a,*S*)-2-((2-(cyclohexyl(cyclohexylidene)methyl)-1-methyl-1H-indol-3-yl)(phenyl)methyl)-4-methylphenol (3ac):



Following the general procedure, 2-alkenylindoles **1a** (92.3 mg, 0.3 mmol), *o*-hydroxybenzyl alcohol **2c** (21.4 mg, 0.1 mmol), CPA (*S*)-**7a** (7.2 mg, 0.02 mmol) and 3 Å MS (100 mg) were added to a reaction tube. Then, DCE (2 mL) was added to the reaction mixture, which was stirred at 0 °C for 36 h. After the completion of the reaction indicated by TLC, the reaction mixture was purified through preparative thin layer chromatography on silica gel (petroleum ether/ethyl acetate = 5:1) to afford pure product **3ac** in 70% yield (35.3 mg) as colorless oil; 83:17 dr; $[\alpha]_D^{20}$ = -97.3 (c 0.22, acetone); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.31 – 7.27 (m, 1H), 7.24 – 7.19 (m, 2H), 7.18 – 7.09 (m, 4H), 6.99 – 6.92 (m, 2H), 6.89 – 6.82 (m, 1H), 6.79 (s, 1H), 6.74 (d, *J* = 8.0 Hz, 1H), 5.56 (s, 1H), 4.79 (s, 1H), 3.58 (s, 3H), 2.64 – 2.55 (m, 1H), 2.50 – 2.42 (m, 1H), 2.31 – 2.23 (m, 1H), 2.13 (s, 3H), 1.67 – 1.58 (m, 4H), 1.51 – 1.39 (m, 6H), 1.31 – 1.22 (m, 4H), 1.12 – 1.01 (m, 2H), 0.83 – 0.76 (m, 1H), 0.66 – 0.56 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 151.9, 144.3, 142.9, 140.0, 136.9, 131.0, 129.7, 129.6, 129.1, 128.4, 128.3, 127.6, 126.7, 126.3, 120.7, 120.4, 119.2, 115.8, 111.6, 109.2, 43.9, 41.1, 33.0, 32.8, 30.7, 30.6, 30.4, 28.2, 27.8, 26.9, 26.7, 25.7, 20.9. IR (KBr): 3446, 2926, 2853, 1732, 1632, 1601, 1362, 1262, 1122, 741; ESI FTMS exact mass calcd for $(C_{36}H_{41}NO+H)^+$ requires m/z 504.3261, found m/z 504.3247; The enantiomeric ratio: 90:10, determined by HPLC (Daicel Chiralpak AD-3, hexane/ isopropanol = 98/ 2, flow rate 1.0 mL/min, T = 30 °C, 254 nm): t_R = 6.786 (major), t_R = 12.833 (minor).

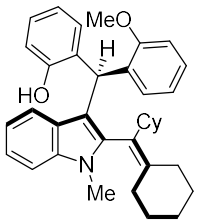
(R_a,*S*)-2-((2-(cyclohexyl(cyclohexylidene)methyl)-1-methyl-1H-indol-3-yl)(2-methoxyphenyl) methyl)-5-methoxyphenol (3ad):



Following the general procedure, 2-alkenylindoles **1a** (92.3 mg, 0.3 mmol), *o*-hydroxybenzyl alcohol **2d** (26.0 mg, 0.1 mmol), CPA (*S*)-**7a** (14.4 mg, 0.02 mmol) and 3 Å MS (100 mg) were added to a reaction tube. Then, DCE (2 mL) was added to the reaction mixture, which was stirred at 0 °C for 36 h. After the completion of the reaction indicated by TLC, the reaction mixture was purified through preparative thin layer chromatography on silica gel (petroleum ether/ethyl acetate = 5:1) to afford pure product **3ad** in 88% yield (48.5 mg) as colorless oil; 90:10 dr; $[\alpha]_D^{20}$ = +74.7 (c 0.94, acetone); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.31 – 7.27 (m, 1H), 7.18 – 7.13 (m, 2H), 7.07 (d, *J* = 7.7 Hz, 1H), 6.96 – 6.85 (m, 3H), 6.78 – 6.72 (m, 1H), 6.60 (d, *J* = 8.4 Hz, 1H), 6.44 – 6.37 (m, 2H), 6.08 (s, 1H), 5.65 (s, 1H), 3.76 (s, 3H), 3.74 (s, 3H), 3.56

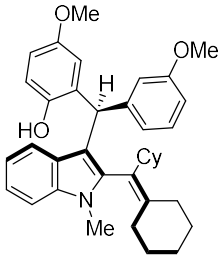
(s, 3H), 2.76 – 2.65 (m, 1H), 2.46 – 2.37 (m, 1H), 2.15 – 2.06 (m, 1H), 1.96 – 1.88 (m, 1H), 1.80 – 1.67 (m, 4H), 1.66 – 1.58 (m, 2H), 1.52 – 1.46 (m, 2H), 1.36 – 1.25 (m, 3H), 1.18 – 1.08 (m, 2H), 1.04 – 0.97 (m, 1H), 0.91 – 0.85 (m, 1H), 0.73 – 0.63 (m, 1H), 0.60 – 0.51 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.5, 156.7, 156.2, 145.0, 141.1, 137.0, 131.7, 131.1, 129.5, 128.1, 127.3, 125.7, 122.0, 121.0, 120.8, 120.1, 119.6, 110.4, 110.3, 109.3, 105.9, 101.9, 55.7, 55.3, 41.6, 36.0, 33.7, 32.4, 31.3, 30.8, 30.4, 28.1, 27.3, 27.0, 26.9, 26.5, 25.9; IR (KBr): 2927, 2851, 1582, 1504, 1464, 1364, 1242, 1033, 741; ESI FTMS exact mass calcd for $(C_{37}H_{43}NO_3\text{-}H)^-$ requires m/z 548.3170, found m/z 548.3198; The enantiomeric ratio: 90:10, determined by HPLC (Daicel Chiralpak AD-3, hexane/ isopropanol = 98/ 2, flow rate 0.8 mL/min, T = 30 °C, 254 nm): t_R = 11.769 (major), t_R = 22.193 (minor).

(*R*$_a$,*S*)-2-((2-(cyclohexyl(cyclohexylidene)methyl)-1-methyl-1H-indol-3-yl)(2-methoxyphenyl) methyl)phenol (3ae):



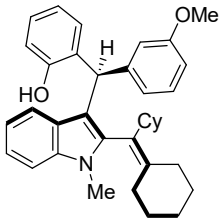
Following the general procedure, 2-alkenylindoles **1a** (92.3 mg, 0.3 mmol), *o*-hydroxybenzyl alcohol **2e** (23.0 mg, 0.1 mmol), CPA (*S*)-**7a** (14.4 mg, 0.02 mmol) and 3 Å MS (100 mg) were added to a reaction tube. Then, DCE (2 mL) was added to the reaction mixture, which was stirred at 0 °C for 36 h. After the completion of the reaction indicated by TLC, the reaction mixture was purified through preparative thin layer chromatography on silica gel (petroleum ether/ethyl acetate = 5:1) to afford pure product **3ae** in 50% yield (25.8 mg) as colorless oil; 95:5 dr; $[\alpha]_D^{20}$ = +88.0 (c 0.29, acetone); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.32 – 7.26 (m, 1H), 7.20 – 7.11 (m, 3H), 7.07 (d, *J* = 7.6 Hz, 1H), 6.91 – 6.84 (m, 3H), 6.83 – 6.78 (m, 2H), 6.78 – 6.70 (m, 2H), 6.14 (s, 1H), 5.56 (s, 1H), 3.73 (s, 3H), 3.56 (s, 3H), 2.75 – 2.63 (m, 1H), 2.47 – 2.37 (m, 1H), 2.15 – 2.04 (m, 1H), 1.93 – 1.86 (m, 1H), 1.79 – 1.66 (m, 4H), 1.62 – 1.59 (m, 1H), 1.53 – 1.46 (m, 2H), 1.34 – 1.27 (m, 2H), 1.25 – 1.24 (m, 1H), 1.18 – 1.10 (m, 2H), 1.07 – 0.82 (m, 3H), 0.73 – 0.64 (m, 1H), 0.63 – 0.53 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 156.8, 155.4, 145.0, 141.1, 136.9, 131.4, 131.1, 129.7, 129.1, 128.0, 127.7, 127.4, 125.8, 121.0, 120.8, 120.2, 120.0, 119.6, 116.1, 110.4, 110.1, 109.3, 55.7, 41.7, 36.6, 33.7, 32.5, 31.2, 30.8, 30.4, 28.1, 27.2, 27.0, 26.9, 26.5, 25.9; IR (KBr): 3420, 2927, 2851, 1597, 1462, 1350, 1242, 1106, 751; ESI FTMS exact mass calcd for $(C_{36}H_{41}NO_2\text{-}H)^-$ requires m/z 518.3064, found m/z 518.3093; The enantiomeric ratio: 93:7, determined by HPLC (Daicel Chiralpak OD-3, hexane/ isopropanol = 95/ 5, flow rate 0.8 mL/min, T = 30 °C, 254 nm): t_R = 4.876 (major), t_R = 5.546 (minor).

(*R*$_a$,*S*)-2-((2-(cyclohexyl(cyclohexylidene)methyl)-1-methyl-1H-indol-3-yl)(3-methoxyphenyl) methyl)-4-methoxyphenol (3af):



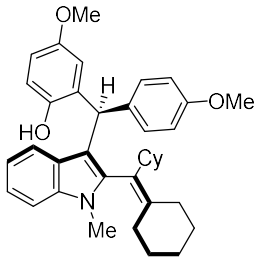
Following the general procedure, 2-alkenylindoles **1a** (92.3 mg, 0.3 mmol), *o*-hydroxybenzyl alcohol **2f** (26.0 mg, 0.1 mmol), CPA (*S*)-**7a** (21.6 mg, 0.03 mmol) and 5 Å MS (100 mg) were added to a reaction tube. Then, DCE (1 mL) was added to the reaction mixture, which was stirred at 0 °C for 48 h. After the completion of the reaction indicated by TLC, the reaction mixture was purified through preparative thin layer chromatography on silica gel (petroleum ether/ethyl acetate = 5:1) to afford pure product **3af** in 52% yield (28.6 mg) as colorless oil; 85:15 dr; $[\alpha]_D^{20}$ = -122.1 (c 0.18, acetone); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.26 – 7.23 (m, 1H), 7.15 – 7.08 (m, 2H), 7.03 (d, *J* = 8.0 Hz, 1H), 6.88 – 6.84 (m, 1H), 6.79 – 6.76 (m, 2H), 6.74 – 6.68 (m, 3H), 6.67 (s, 1H), 5.53 (s, 1H), 4.61 (s, 1H), 3.67 (s, 3H), 3.57 (s, 3H), 3.55 (s, 3H), 2.64 – 2.56 (m, 1H), 2.50 – 2.43 (m, 1H), 2.33 – 2.25 (m, 1H), 1.72 – 1.59 (m, 5H), 1.51 – 1.41 (m, 5H), 1.17 – 1.02 (m, 4H), 0.91 – 0.81 (m, 2H), 0.80 – 0.71 (m, 1H), 0.64 – 0.54 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.7, 153.8, 148.1, 144.4, 144.3, 139.8, 136.9, 131.2, 129.3, 127.5, 126.8, 121.5, 120.7, 120.3, 119.3, 116.8, 116.7, 115.0, 112.6, 111.6, 111.4, 109.1, 55.7, 55.1, 44.1, 41.1, 33.1, 32.8, 30.6, 30.4, 29.7, 28.2, 27.8, 26.9, 26.7, 26.6, 25.7; IR (KBr): 3424, 2924, 2851, 1673, 1589, 1388, 1359, 1122, 796; ESI FTMS exact mass calcd for $(C_{37}H_{43}NO_3+H)^+$ requires m/z 550.3316, found m/z 550.3312; The enantiomeric ratio: 91:9, determined by HPLC (Daicel Chiralpak AD-3, hexane/ isopropanol = 95/ 5, flow rate 1.0 mL/min, T = 30 °C, 254 nm): t_R = 9.426 (major), t_R = 13.639 (minor).

(*R*$_a$,*S*)-2-((2-(cyclohexyl(cyclohexylidene)methyl)-1-methyl-1H-indol-3-yl)(3-methoxyphenyl) methyl)phenol (3ag):



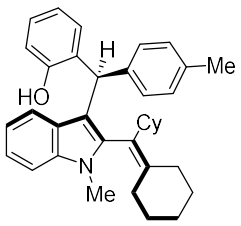
Following the general procedure, 2-alkenylindoles **1a** (92.3 mg, 0.3 mmol), *o*-hydroxybenzyl alcohol **2g** (23.0 mg, 0.1 mmol), CPA (*S*)-**7a** (21.6 mg, 0.03 mmol) and 3 Å MS (100 mg) were added to a reaction tube. Then, DCE (1 mL) was added to the reaction mixture, which was stirred at 0 °C for 48 h. After the completion of the reaction indicated by TLC, the reaction mixture was purified through preparative thin layer chromatography on silica gel (petroleum ether/ethyl acetate = 5:1) to afford pure product **3ag** in 57% yield (29.7 mg) as colorless oil; 95:5 dr; $[\alpha]_D^{20}$ = -121.1 (c 0.28, acetone); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.31 – 7.27 (m, 1H), 7.19 – 7.09 (m, 3H), 7.08 – 7.00 (m, 2H), 6.89 – 6.76 (m, 4H), 6.76 – 6.68 (m, 2H), 5.56 (s, 1H), 4.93 (s, 1H), 3.68 (s, 3H), 3.58 (s, 3H), 2.63 – 2.53 (m, 1H), 2.52 – 2.42 (m, 1H), 2.36 – 2.25 (m, 1H), 1.76 – 1.59 (m, 5H), 1.54 – 1.38 (m, 5H), 1.37 – 1.24 (m, 3H), 1.17 – 0.98 (m, 3H), 0.79 – 0.67 (m, 1H), 0.58 – 0.45 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.7, 154.0, 144.6, 144.2, 139.8, 136.9, 130.7, 129.7, 129.3, 127.9, 127.6, 126.8, 121.5, 120.7, 120.5, 119.2, 115.9, 115.1, 111.7, 111.5, 109.2, 55.1, 43.7, 41.1, 33.2, 32.8, 30.6, 30.5, 30.4, 28.3, 27.9, 26.8, 26.7, 26.6, 25.6; IR (KBr): 2929, 2813, 2715, 1632, 1382, 1349, 1119, 776; ESI FTMS exact mass calcd for $(C_{36}H_{41}NO_2-H)^-$ requires m/z 518.3064, found m/z 518.3089; The enantiomeric ratio: 90:10, determined by HPLC (Daicel Chiralpak AD-3, hexane/ isopropanol = 98/ 2, flow rate 1.0 mL/min, T = 30 °C, 254 nm): t_R = 12.449 (major), t_R = 25.949 (minor).

(R_a,*S*)-2-((2-(cyclohexyl(cyclohexylidene)methyl)-1-methyl-1H-indol-3-yl)(4-methoxyphenyl) methyl)-4-methoxyphenol (3ah):



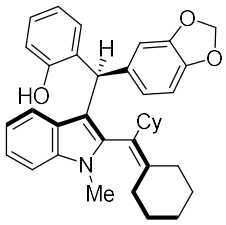
Following the general procedure, 2-alkenylindoles **1a** (92.3 mg, 0.3 mmol), *o*-hydroxybenzyl alcohol **2h** (26.0 mg, 0.1 mmol), CPA (*S*)-**7a** (14.4 mg, 0.02 mmol) and 3 Å MS (100 mg) were added to a reaction tube. Then, DCE (2 mL) was added to the reaction mixture, which was stirred at 0 °C for 36 h. After the completion of the reaction indicated by TLC, the reaction mixture was purified through preparative thin layer chromatography on silica gel (petroleum ether/ethyl acetate = 5:1) to afford pure product **3ah** in 65% yield (35.5 mg) as colorless oil; 80:20 dr; $[\alpha]_D^{20}$ = -115.7 (c 0.18, acetone); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.26 – 7.23 (m, 1H), 7.14 – 7.04 (m, 3H), 6.98 (d, *J* = 8.0 Hz, 1H), 6.88 – 6.83 (m, 1H), 6.80 – 6.68 (m, 4H), 6.64 (s, 1H), 5.49 (s, 1H), 4.63 (s, 1H), 3.74 (s, 3H), 3.57 (s, 3H), 3.55 (s, 3H), 2.64 – 2.54 (m, 1H), 2.51 – 2.43 (m, 1H), 2.33 – 2.23 (m, 1H), 1.74 – 1.61 (m, 4H), 1.55 – 1.49 (m, 3H), 1.48 – 1.39 (m, 4H), 1.20 – 1.01 (m, 4H), 1.00 – 0.91 (m, 1H), 0.80 – 0.72 (m, 1H), 0.65 – 0.55 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.1, 153.7, 148.1, 144.2, 139.7, 136.9, 134.7, 131.5, 129.9, 127.4, 126.7, 120.7, 120.4, 119.2, 116.7, 116.6, 113.9, 112.4, 111.7, 109.2, 55.7, 55.3, 43.3, 41.1, 33.1, 32.8, 30.6, 30.4, 28.3, 27.8, 26.9, 26.7, 26.6, 25.7; IR (KBr): 3445, 2916, 2849, 1673, 1574, 1261, 1020, 799; ESI FTMS exact mass calcd for $(C_{37}H_{43}NO_3\text{-}H)^-$ requires m/z 548.3170, found m/z 548.3186; The enantiomeric ratio: 90:10, determined by HPLC (Daicel Chiralpak IF, hexane/ isopropanol = 98/ 2, flow rate 0.5 mL/min, T = 30 °C, 254 nm): t_R = 20.283 (major), t_R = 23.513 (minor).

(R_a,*S*)-2-((2-(cyclohexyl(cyclohexylidene)methyl)-1-methyl-1H-indol-3-yl)(p-tolyl)methyl) phenol (3ai):



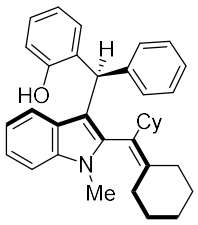
Following the general procedure, 2-alkenylindoles **1a** (92.3 mg, 0.3 mmol), *o*-hydroxybenzyl alcohol **2i** (21.4 mg, 0.1 mmol), CPA (*S*)-**7a** (21.6 mg, 0.03 mmol) and 3 Å MS (100 mg) were added to a reaction tube. Then, DCE (1 mL) was added to the reaction mixture, which was stirred at 0 °C for 48 h. After the completion of the reaction indicated by TLC, the reaction mixture was purified through preparative thin layer chromatography on silica gel (petroleum ether/ethyl acetate = 5:1) to afford pure product **3ai** in 56% yield (28.4 mg) as colorless oil; 83:17 dr; $[\alpha]_D^{20}$ = -78.7 (c 0.14, acetone); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.30 – 7.26 (m, 1H), 7.17 – 7.09 (m, 2H), 7.08 – 6.97 (m, 6H), 6.89 – 6.77 (m, 3H), 5.53 (s, 1H), 4.90 (s, 1H), 3.57 (s, 3H), 2.63 – 2.52 (m, 1H), 2.50 – 2.42 (m, 1H), 2.37 – 2.30 (m, 1H), 2.27 (s, 3H), 1.77 – 1.60 (m, 5H), 1.51 – 1.28 (m, 8H), 1.14 – 1.05 (m, 2H), 1.00 – 0.94 (m, 1H), 0.78 – 0.66 (m, 1H), 0.56 – 0.44 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 154.0, 144.2, 139.7, 139.6, 136.9, 135.8, 130.7, 129.9, 129.1, 128.8, 127.8, 127.6, 126.9, 120.7, 120.6, 120.5, 119.1, 115.9, 112.0, 109.2, 43.3, 41.1, 33.2, 32.7, 30.6, 30.4, 28.3, 27.8, 26.8, 26.7, 26.6, 25.6, 21.1; IR (KBr): 3443, 2928, 2100, 1662, 1584, 1388, 1332, 781; ESI FTMS exact mass calcd for $(C_{36}H_{41}NO\text{-}H)^-$ requires m/z 502.3115, found m/z 502.3140; The enantiomeric ratio: 91:9, determined by HPLC (Daicel Chiralpak AD-3, hexane/ isopropanol = 98/ 2, flow rate 1.0 mL/min, T = 30 °C, 254 nm): t_R = 7.196 (major), t_R = 13.443 (minor).

(R_a,*S*)-2-(benzo[d][1,3]dioxol-5-yl(2-(cyclohexyl(cyclohexylidene)methyl)-1-methyl-1H-indol-3-yl)methyl)phenol (3aj):



Following the general procedure, 2-alkenylindoles **1a** (92.3 mg, 0.3 mmol), *o*-hydroxybenzyl alcohol **2j** (24.4 mg, 0.1 mmol), CPA (*S*)-**7a** (14.4 mg, 0.02 mmol) and 3 Å MS (100 mg) were added to a reaction tube. Then, DCE (2 mL) was added to the reaction mixture, which was stirred at 0 °C for 36 h. After the completion of the reaction indicated by TLC, the reaction mixture was purified through preparative thin layer chromatography on silica gel (petroleum ether/ethyl acetate = 5:1) to afford pure product **3aj** in 69% yield (37.0 mg) as colorless oil; 82:18 dr; $[\alpha]_D^{20}$ = -130.3 (c 0.10, acetone); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.31 – 7.27 (m, 1H), 7.19 – 7.10 (m, 2H), 7.09 – 7.01 (m, 2H), 6.92 – 6.86 (m, 1H), 6.85 – 6.78 (m, 2H), 6.70 – 6.60 (m, 3H), 5.87 (d, *J* = 10.4 Hz, 2H), 5.49 (s, 1H), 4.92 (s, 1H), 3.57 (s, 3H), 2.61 – 2.52 (m, 1H), 2.50 – 2.43 (m, 1H), 2.34 – 2.26 (m, 1H), 1.77 – 1.61 (m, 4H), 1.61 – 1.59 (m, 1H), 1.56 – 1.42 (m, 3H), 1.41 – 1.31 (m, 5H), 1.15 – 1.05 (m, 2H), 1.01 – 0.93 (m, 1H), 0.75 – 0.65 (m, 1H), 0.54 – 0.43 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 153.9, 147.8, 146.0, 144.2, 139.7, 136.9, 130.6, 129.9, 127.9, 127.5, 126.8, 121.6, 120.7, 120.4, 119.2, 115.9, 111.8, 109.8, 109.2, 108.0, 100.8, 43.3, 41.1, 33.3, 32.7, 30.6, 30.5, 30.4, 28.3, 27.9, 26.8, 26.7, 26.6, 25.6; IR (KBr): 3420, 2925, 2851, 1594, 1383, 1351, 1121, 767; ESI FTMS exact mass calcd for $(C_{36}H_{39}NO_3\text{-}H)^-$ requires m/z 532.2857, found m/z 532.2867; The enantiomeric ratio: 91:9, determined by HPLC (Daicel Chiralpak IB, hexane/ isopropanol = 99/ 1, flow rate 0.5 mL/min, T = 30 °C, 254 nm): t_R = 23.439 (major), t_R = 31.393 (minor).

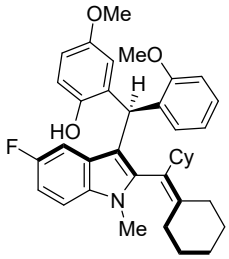
(R_a,*S*)-2-((2-(cyclohexyl(cyclohexylidene)methyl)-1-methyl-1H-indol-3-yl)(phenyl)methyl) phenol (3ak):



Following the general procedure, 2-alkenylindoles **1a** (92.3 mg, 0.3 mmol), *o*-hydroxybenzyl alcohol **2k** (20 mg, 0.1 mmol), CPA (*S*)-**7a** (14.4 mg, 0.02 mmol) and 3 Å MS (100 mg) were added to a reaction tube. Then, DCE (2 mL) was added to the reaction mixture, which was stirred at 0 °C for 36 h. After the completion of the reaction indicated by TLC, the reaction mixture was purified through preparative thin layer chromatography on silica gel (petroleum ether/ethyl acetate = 5:1) to afford pure product **3ak** in 50% yield (24.5 mg) as a white solid; m.p. 102-103 °C; 80:20 dr; $[\alpha]_D^{20}$ = -131.6 (c 0.14, acetone); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.32 – 7.27 (m, 1H), 7.26 – 7.08 (m, 7H), 7.07 – 7.00 (m, 1H), 6.98 – 6.93 (m, 1H), 6.91 – 6.75 (m, 3H), 5.59 (s, 1H), 4.95 (s, 1H), 3.58 (s, 3H), 2.64 – 2.54 (m, 1H), 2.52 – 2.42 (m, 1H), 2.34 – 2.23 (m, 1H), 1.77 – 1.58 (m, 5H), 1.53 – 1.35 (m, 6H), 1.34 – 1.27 (m, 2H), 1.17 – 1.02 (m, 3H), 0.80 – 0.70 (m, 1H), 0.61 – 0.49 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 154.1, 144.3, 142.9, 140.0, 136.9, 130.6, 129.8, 129.0, 128.4, 127.9, 127.6, 126.7, 126.3, 120.7, 120.4, 119.2, 115.9, 111.7, 109.2, 43.7, 41.1, 33.1, 32.8, 30.6, 30.4, 29.7, 28.2, 27.8, 26.9, 26.7, 26.6, 25.6; IR (KBr): 3444, 2924, 2853, 1673, 1580, 1455, 1261, 1076, 741; ESI FTMS exact mass calcd for $(C_{35}H_{39}NO\text{-}H)^-$ requires m/z 488.2959, found m/z 488.2970; The enantiomeric ratio: 90:10, determined by HPLC (Daicel

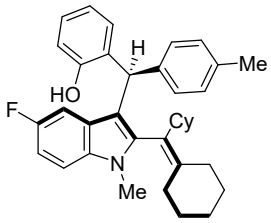
Chiralpak OD-3, hexane/ isopropanol = 98/ 2, flow rate 0.8 mL/min, T = 30 °C, 254 nm): t_R = 5.926 (major), t_R = 7.326 (minor).

(R_a,*S*)-2-((2-(cyclohexyl(cyclohexylidene)methyl)-5-fluoro-1-methyl-1H-indol-3-yl)(2-meth oxyphenyl)methyl)-4-methoxyphenol (3ba):



Following the general procedure, 2-alkenylindoles **1b** (97.6 mg, 0.3 mmol), *o*-hydroxybenzyl alcohol **2a** (26.0 mg, 0.1 mmol), CPA (*S*)-**7a** (21.6 mg, 0.03 mmol) and 3 Å MS (100 mg) were added to a reaction tube. Then, DCE (1 mL) was added to the reaction mixture, which was stirred at 0 °C for 48 h. After the completion of the reaction indicated by TLC, the reaction mixture was purified through preparative thin layer chromatography on silica gel (petroleum ether/ethyl acetate = 5:1) to afford pure product **3ba** in 53% yield (30.1 mg) as colorless oil; 89:11 dr; $[\alpha]_D^{20}$ = +105.3 (c 0.4, acetone); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.19 – 7.12 (m, 2H), 7.03 – 6.97 (m, 1H), 6.90 – 6.82 (m, 2H), 6.79 – 6.70 (m, 3H), 6.54 – 6.45 (m, 1H), 6.34 (s, 1H), 6.07 (s, 1H), 5.05 (s, 1H), 3.72 (s, 3H), 3.64 (s, 3H), 3.53 (s, 3H), 2.72 – 2.61 (m, 1H), 2.45 – 2.35 (m, 1H), 2.15 – 2.02 (m, 1H), 1.93 – 1.83 (m, 1H), 1.79 – 1.60 (m, 5H), 1.53 – 1.28 (m, 5H), 1.17 – 0.81 (m, 5H), 0.73 – 0.57 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 157.7 (d, *J* = 232.2 Hz), 156.7, 149.2, 145.1, 142.8, 133.5, 130.9, 130.8, 130.7, 128.0 (d, *J* = 10.2 Hz), 127.6, 125.7, 120.8, 116.5, 115.9, 111.9, 110.5, 110.2, 109.8, (d, *J* = 9.8 Hz), 109.2 (d, *J* = 26.4 Hz) 104.8 (d, *J* = 24.1 Hz), 55.6, 41.6, 36.8, 33.5, 32.5, 31.2, 30.9, 30.4, 28.0, 27.2, 27.0, 26.9, 26.5, 25.9; ^{19}F NMR (376 MHz, $CDCl_3$) δ -124.16; IR (KBr): 3446, 2926, 2851, 1660, 1577, 1489, 1242, 793, 573; ESI FTMS exact mass calcd for ($C_{37}H_{42}FNO_3$-H)$^-$ requires m/z 566.3076, found m/z 566.3084; The enantiomeric ratio: 92:8, determined by HPLC (Daicel Chiralpak OD-3, hexane/ isopropanol = 98/ 2, flow rate 0.8 mL/min, T = 30 °C, 254 nm): t_R = 5.393 (major), t_R = 6.473 (minor).

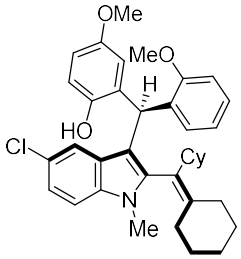
(R_a,*S*)-2-((2-(cyclohexyl(cyclohexylidene)methyl)-5-fluoro-1-methyl-1H-indol-3-yl)(p-tolyl) methyl)phenol (3bi):



Following the general procedure, 2-alkenylindoles **1b** (97.6 mg, 0.3 mmol), *o*-hydroxybenzyl alcohol **2i** (21.4 mg, 0.1 mmol), CPA (*S*)-**7a** (14.4 mg, 0.02 mmol) and 3 Å MS (100 mg) were added to a reaction tube. Then, DCE (2 mL) was added to the reaction mixture, which was stirred at 0 °C for 36 h. After the completion of the reaction indicated by TLC, the reaction mixture was purified through preparative thin layer chromatography on silica gel (petroleum ether/ethyl acetate = 5:1) to afford pure product **3bi** in 43% yield (22.4 mg) as colorless oil; 80:20 dr; $[\alpha]_D^{20}$ = -132.3 (c 0.17, acetone); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.19 – 7.12 (m, 2H), 7.08 – 6.96 (m, 5H), 6.89 – 6.77 (m, 3H), 6.63 (d, *J* = 10.4 Hz, 1H), 5.51 (s, 1H), 4.81 (s, 1H), 3.55 (s, 3H), 2.60 – 2.51 (m, 1H), 2.49 – 2.41 (m, 1H), 2.37 – 2.30 (m, 1H), 2.28 (s, 3H), 1.73 – 1.61 (m, 4H), 1.53 – 1.43 (m, 2H), 1.42 – 1.28 (m, 6H), 1.15 – 1.03 (m, 2H), 1.02 – 0.77 (m, 2H), 0.76 – 0.64 (m, 1H), 0.54 – 0.41 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 157.4 (d, *J* = 231.6 Hz), 153.8, 144.3, 141.4, 139.3, 136.0, 133.5,

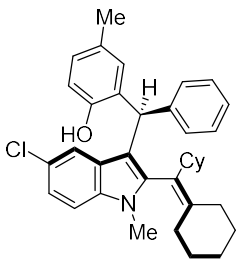
130.6, 129.6, 129.2, 128.7, 128.0, 127.8 (d, J = 10.1 Hz), 126.8, 120.8, 115.9, 112.3, 112.2, 109.6 (d, J = 9.8 Hz), 108.8 (d, J = 26.3 Hz), 105.3 (d, J = 23.8 Hz), 43.1, 41.0, 33.2, 32.6, 30.8, 30.5, 30.4, 28.2, 27.9, 26.8, 26.7, 26.6, 25.6, 21.1; ^{19}F NMR (376 MHz, $CDCl_3$) δ -124.7; IR (KBr): 2926, 2852, 1632, 1456, 1353, 1126, 786; ESI FTMS exact mass calcd for $(C_{36}H_{40}FNO\text{-}H)^-$ requires m/z 520.3021, found m/z 520.3031; The enantiomeric ratio: 91:9, determined by HPLC (Daicel Chiralpak OD-3, hexane/ isopropanol = 98/ 2, flow rate 1.0 mL/min, T = 30 °C, 254 nm): t_R = 5.019 (major), t_R = 7.873 (minor).

(R_a,*S*)-2-((5-chloro-2-(cyclohexyl(cyclohexylidene)methyl)-1-methyl-1H-indol-3-yl)(2-methoxyphenyl)methyl)-4-methoxyphenol (3ca):



Following the general procedure, 2-alkenylindoles **1c** (102.6 mg, 0.3 mmol), *o*-hydroxybenzyl alcohol **2a** (26.0 mg, 0.1 mmol), CPA (*S*)-**7a** (14.4 mg, 0.02 mmol) and 3 Å MS (100 mg) were added to a reaction tube. Then, DCE (2 mL) was added to the reaction mixture, which was stirred at 0 °C for 36 h. After the completion of the reaction indicated by TLC, the reaction mixture was purified through preparative thin layer chromatography on silica gel (petroleum ether/ethyl acetate = 5:1) to afford pure product **3ca** in 50% yield (29.2 mg) as colorless oil; 91:9 dr; $[\alpha]_D^{20}$ = +67.0 (c 0.19, acetone); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.19 – 7.13 (m, 2H), 7.08 – 7.04 (m, 1H), 6.99 (d, J = 7.6 Hz, 1H), 6.84 (d, J = 8.2 Hz, 1H), 6.80 – 6.69 (m, 4H), 6.34 (s, 1H), 6.06 (s, 1H), 4.95 (s, 1H), 3.71 (s, 3H), 3.65 (s, 3H), 3.52 (s, 3H), 2.70 – 2.59 (m, 1H), 2.45 – 2.36 (m, 1H), 2.11 – 2.03 (m, 1H), 1.89 – 1.81 (m, 1H), 1.70 – 1.54 (m, 6H), 1.52 – 1.36 (m, 4H), 1.17 – 1.07 (m, 2H), 0.99 – 0.84 (m, 3H), 0.75 – 0.61 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 156.7, 153.5, 149.1, 145.2, 142.4, 135.2, 130.9, 130.7, 130.6, 128.8, 127.7, 125.6, 125.1, 121.2, 120.9, 119.3, 116.6, 116.1, 112.0, 110.5, 110.3, 110.1, 55.7, 55.6, 41.6, 36.8, 33.5, 32.5, 31.1, 30.9, 30.4, 29.7, 28.0, 27.2, 27.1, 26.9, 26.5, 25.9; IR (KBr): 3451, 2927, 2851, 1667, 1489, 1242, 1031, 753; ESI FTMS exact mass calcd for $(C_{37}H_{42}ClNO_3\text{-}H)^-$ requires m/z 582.2780, found m/z 582.2800; The enantiomeric ratio: 92:8, determined by HPLC (Daicel Chiralpak AD-3, hexane/ isopropanol = 95/ 5, flow rate 1.0 mL/min, T = 30 °C, 254 nm): t_R = 5.566 (major), t_R = 9.849 (minor).

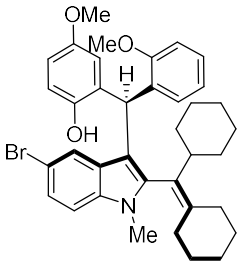
(R_a,*S*)-2-((5-chloro-2-(cyclohexyl(cyclohexylidene)methyl)-1-methyl-1H-indol-3-yl)(phenyl) methyl)-4-methylphenol (3cc):



Following the general procedure, 2-alkenylindoles **1c** (102.6 mg, 0.3 mmol), *o*-hydroxybenzyl alcohol **2c** (21.4 mg, 0.1 mmol), CPA (*S*)-**7a** (14.4 mg, 0.02 mmol) and 3 Å MS (100 mg) were added to a reaction tube. Then, DCE (1 mL) was added to the reaction mixture, which was stirred at 0 °C for 36 h. After the completion of the reaction indicated by TLC, the reaction mixture was purified through preparative thin layer chromatography on silica gel (petroleum ether/ethyl acetate = 5:1) to afford pure product **3cc** in 42% yield (22.6 mg) as colorless oil; 80:20 dr; $[\alpha]_D^{20}$ = -28.8 (c 0.39, acetone); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.26 – 7.10 (m, 6H), 7.05 (d, J = 8.6 Hz, 1H), 6.97 (d, J = 7.9 Hz, 1H), 6.86 (s, 1H), 6.81 – 6.69 (m,

2H), 5.53 (s, 1H), 4.63 (s, 1H), 3.55 (s, 3H), 2.59 – 2.50 (m, 1H), 2.48 – 2.40 (m, 1H), 2.33 – 2.25 (m, 1H), 2.14 (s, 3H), 1.65 – 1.59 (m, 3H), 1.54 – 1.45 (m, 3H), 1.43 – 1.36 (m, 3H), 1.34 – 1.30 (m, 2H), 1.15 – 1.05 (m, 2H), 1.02 – 0.80 (m, 3H), 0.78 – 0.67 (m, 1H), 0.59 – 0.47 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 151.6, 144.5, 142.5, 141.2, 135.3, 131.0, 129.9, 129.2, 128.9, 128.6, 128.5, 128.4, 126.6, 126.5, 124.8, 120.9, 119.6, 115.8, 111.9, 110.1, 43.5, 41.0, 33.1, 32.6, 30.7, 30.5, 30.4, 29.7, 28.2, 27.9, 26.8, 26.7, 26.6, 25.6, 20.9; IR (KBr): 2925, 2852, 1748, 1631, 1489, 1362, 1261, 1110, 811; ESI FTMS exact mass calcd for $(C_{36}H_{40}ClNO\text{-}H)^-$ requires m/z 536.2725, found m/z 536.2747; The enantiomeric ratio: 91:9, determined by HPLC (Daicel Chiralpak OD-3, hexane/ isopropanol = 98/ 2, flow rate 1.0 mL/min, T = 30 °C, 254 nm): t_R = 5.226 (major), t_R = 6.199 (minor).

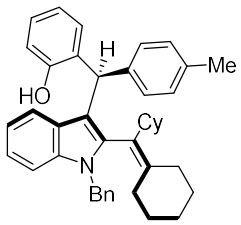
(*R*$_a$,*S*)-2-((5-bromo-2-(cyclohexyl(cyclohexylidene)methyl)-1-methyl-1H-indol-3-yl)(2-meth oxyphenyl)methyl)-4-methoxyphenol (3da):



Following the general procedure, 2-alkenylindoles **1d** (115.1 mg, 0.3 mmol), *o*-hydroxybenzyl alcohol **2a** (21.4 mg, 0.1 mmol), CPA (*S*)-**7a** (14.4 mg, 0.02 mmol) and 3 Å MS (100 mg) were added to a reaction tube. Then, DCE (1 mL) was added to the reaction mixture, which was stirred at 0 °C for 36 h. After the completion of the reaction indicated by TLC, the reaction mixture was purified through preparative thin layer chromatography on silica gel (petroleum ether/ethyl acetate = 5:1) to afford pure product **3da** in 55% yield (34.6 mg) as colorless oil; 91:9 dr; $[\alpha]_D^{20}$ = -102.2 (c 0.11, acetone) ;^{1}H NMR (400 MHz, $CDCl_3$) δ 7.22 – 7.10 (m, 3H), 6.99 (d, *J* = 7.6 Hz, 1H), 6.93 (s, 1H), 6.84 (d, *J* = 8.2 Hz, 1H), 6.80 – 6.70 (m, 3H), 6.35 (s, 1H), 6.06 (s, 1H), 4.93 (s, 1H), 3.71 (s, 3H), 3.65 (s, 3H), 3.52 (s, 3H), 2.69 – 2.60 (m, 1H), 2.45 – 2.37 (m, 1H), 2.12 – 2.03 (m, 1H), 1.90 – 1.82 (m, 1H), 1.78 – 1.53 (m, 7H), 1.49 – 1.38 (m, 2H), 1.33 – 1.29 (m, 1H), 1.23 – 1.05 (m, 3H), 0.98 – 0.88 (m, 2H), 0.77 – 0.58 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 156.7, 153.5, 149.1, 145.2, 142.3, 135.4, 130.9, 130.6, 130.6, 129.4, 127.7, 125.5, 123.7, 122.3, 120.9, 116.6, 116.1, 112.9, 112.0, 110.7, 110.5, 110.1, 55.7, 55.6, 41.6, 36.8, 33.5, 32.5, 31.1, 30.8, 30.4, 28.0, 27.2, 27.1, 26.8, 26.5, 25.9; IR (KBr): 3447, 2920, 2763, 1673, 1569, 1275, 795, 750; ESI FTMS exact mass calcd for $(C_{37}H_{42}BrNO_3\text{-}H)^-$ requires m/z 626.2275, found m/z 626.2301; The enantiomeric ratio: 92:8, determined by HPLC (Daicel Chiralpak ID, hexane/ isopropanol = 98/ 2, flow rate 1.0 mL/min, T = 30 °C, 254 nm): t_R = 7.766 (major), t_R = 9.309 (minor).

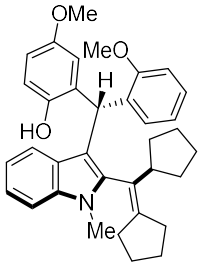
(*R*$_a$,*S*)-2-((1-benzyl-2-(cyclohexyl(cyclohexylidene)methyl)-1H-indol-3-yl)(p-tolyl)methyl) phenol (3ei):

Following the general procedure, 2-alkenylindoles **1e** (115.1 mg, 0.3 mmol), *o*-hydroxybenzyl alcohol **2i** (21.4 mg, 0.1 mmol), CPA (*S*)-**7a** (14.4 mg, 0.02 mmol) and 3 Å MS (100 mg) were added to a reaction tube. Then, DCE (1 mL) was added to the reaction mixture, which was stirred at 0 °C for 36 h. After the completion of the reaction indicated by TLC, the reaction mixture was purified through preparative thin layer chromatography on silica gel (petroleum ether/ethyl acetate = 5:1) to afford pure product **3ei** in 44% yield (25.5 mg) as colorless oil;



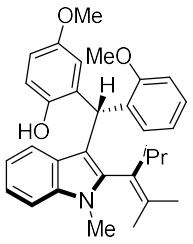
75:25 dr; $[\alpha]_D^{20}$ = -102.2 (c 0.11, acetone); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.31 – 7.26 (m, 2H), 7.26 – 7.20 (m, 2H), 7.19 – 7.13 (m, 1H), 7.12 – 7.02 (m, 7H), 7.02 – 6.94 (m, 2H), 6.89 – 6.77 (m, 3H), 5.58 (s, 1H), 5.31 – 5.15 (m, 2H), 4.87 (s, 1H), 2.50 – 2.41 (m, 1H), 2.37 – 2.31 (m, 2H), 2.29 (s, 3H), 1.73 – 1.67 (m, 1H), 1.60 – 1.51 (m, 5H), 1.47 – 1.41 (m, 2H), 1.37 – 1.30 (m, 4H), 1.00 – 0.83 (m, 4H), 0.79 – 0.70 (m, 1H), 0.52 – 0.40 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 153.9, 145.1, 140.2, 139.5, 137.8, 136.7, 135.9, 130.7, 129.9, 129.2, 128.8, 128.5, 128.0, 127.9, 127.0, 126.7, 126.6, 120.8, 120.7, 120.6, 119.3, 115.9, 112.6, 110.8, 48.1, 43.2, 41.4, 33.6, 32.6, 30.7, 30.6, 29.7, 28.2, 28.0, 26.9, 26.6, 25.6, 21.1; IR (KBr): 3420, 2925, 2815, 1594, 1383, 1351, 1122, 766, 617; ESI FTMS exact mass calcd for $(C_{42}H_{45}NO+Na)^+$ requires m/z 602.3393, found m/z 602.3399; The enantiomeric ratio: 91:9, determined by HPLC (Daicel Chiralpak OD-3, hexane/ isopropanol = 98/ 2, flow rate 1.0 mL/min, T = 30 °C, 254 nm): t_R = 10.023 (major), t_R = 12.343 (minor).

(*S*$_a$,*R*)-2-((2-(cyclopentyl(cyclopentylidene)methyl)-1-methyl-1H-indol-3-yl)(2-methoxyphenyl)methyl)-4-methoxyphenol (3fa):



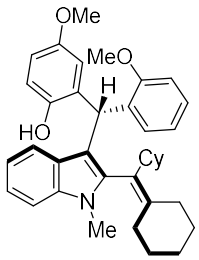
Following the general procedure, 2-alkenylindoles **1f** (83.8 mg, 0.3 mmol), *o*-hydroxybenzyl alcohol **2a** (26.0 mg, 0.1 mmol), CPA (*S*)-5i (20mg, 0.02 mmol) and 3 Å MS (100 mg) were added to a reaction tube. Then, DCE (2 mL) was added to the reaction mixture, which was stirred at 0 °C for 36 h. After the completion of the reaction indicated by TLC, the reaction mixture was purified through preparative thin layer chromatography on silica gel (petroleum ether/ethyl acetate = 5:1) to afford pure product **3fa** in 46% yield (24.0 mg) as colorless oil; 85:15 dr; $[\alpha]_D^{20}$ = -48.6 (c 0.35, acetone); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.32 – 7.26 (m, 1H), 7.20 – 7.09 (m, 3H), 6.96 – 6.81 (m, 3H), 6.80 – 6.67 (m, 3H), 6.42 (s, 1H), 6.10 (s, 1H), 5.09 (s, 1H), 3.74 (s, 3H), 3.65 (s, 3H), 3.53 (s, 3H), 2.96 – 2.85 (m, 1H), 2.46 – 2.36 (m, 1H), 2.32 – 2.21 (m, 1H), 1.90 – 1.80 (m, 1H), 1.75 – 1.57 (m, 4H), 1.54 – 1.41 (m, 3H), 1.27 – 1.08 (m, 4H), 0.95 – 0.86 (m, 1H), 0.81 – 0.71 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 156.6, 153.3, 150.2, 149.5, 141.4, 136.9, 131.2, 131.1, 127.7, 127.5, 123.7, 121.0, 120.9, 120.0, 119.5, 116.5, 115.8, 111.6, 110.6, 109.5, 109.3, 55.6, 55.5, 45.4, 36.6, 31.9, 31.6, 30.8, 30.6, 30.1, 26.4, 26.0, 24.9, 24.7. IR (KBr):3436, 2929, 2866, 1598, 1489, 1465, 1399, 1243, 1030, 752; ESI FTMS exact mass calcd for $(C_{35}H_{39}NO_3-H)^-$ requires m/z 520.2857, found m/z 520.2878; The enantiomeric ratio: 90:10, determined by HPLC (Daicel Chiralpak AD-3, hexane/ isopropanol = 98/ 2, flow rate 1.0 mL/min, T = 30 °C, 254 nm): t_R = 11.252 (minor), t_R = 23.098 (major).

(*S*$_a$,*R*)-2-((2-(2,4-dimethylpent-2-en-3-yl)-1-methyl-1H-indol-3-yl)(2-methoxyphenyl)methyl)-4-methoxyphenol (3ga):



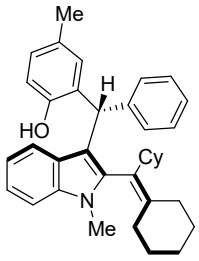
Following the general procedure, 2-alkenylindoles **1g** (68.2 mg, 0.3 mmol), *o*-hydroxybenzyl alcohol **2a** (26.0 mg, 0.1 mmol), CPA (*S*)-**5i** (20.0 mg, 0.02 mmol) and 3 Å MS (100 mg) were added to a reaction tube. Then, DCE (4 mL) was added to the reaction mixture, which was stirred at 0 °C for 36 h. After the completion of the reaction indicated by TLC, the reaction mixture was purified through preparative thin layer chromatography on silica gel (petroleum ether/ethyl acetate = 5:1) to afford pure product **3ga** in 44% yield (20.7 mg) as colorless oil; 86:14 dr; $[\alpha]_D^{20}$ = -21.2 (c 0.58, acetone); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.31 – 7.27 (m, 1H), 7.18 – 7.10 (m, 3H), 7.01 – 6.96 (m, 1H), 6.94 – 6.88 (m, 1H), 6.84 (d, *J* = 8.4 Hz, 1H), 6.78 – 6.69 (m, 3H), 6.44 (s, 1H), 6.13 (s, 1H), 5.21 (s, 1H), 3.74 (s, 3H), 3.65 (s, 3H), 3.52 (s, 3H), 3.14 – 3.02 (m, 1H), 1.77 (s, 3H), 1.34 (d, *J* = 8.8 Hz, 3H), 0.95 (d, *J* = 6.9 Hz, 3H), 0.55 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 156.5, 153.4, 149.4, 140.9, 137.4, 137.0, 131.3, 131.1, 129.1, 127.7, 127.4, 121.1, 120.8, 120.0, 119.6, 116.5, 115.8, 111.6, 110.4, 110.3, 109.4, 55.6, 36.6, 31.4, 30.4, 23.0, 22.0, 20.9, 19.7; IR (KBr):3433, 2927, 1598, 1490, 1464, 1364, 1243, 1208, 1031, 742; ESI FTMS exact mass calcd for $(C_{31}H_{35}NO_3\text{-}H)^-$ requires m/z 468.2544, found m/z 468.2557; The enantiomeric ratio: 86:14, determined by HPLC (Daicel Chiralpak AD-3, hexane/ isopropanol = 98/ 2, flow rate 1.0 mL/min, T = 30 °C, 254 nm): t_R = 11.329 (minor), t_R = 14.323 (major).

(*R*$_a$,*R*)-2-((2-(cyclohexyl(cyclohexylidene)methyl)-1-methyl-1H-indol-3-yl)(2-methoxyphenyl) methyl)-4-methoxyphenol (4aa):



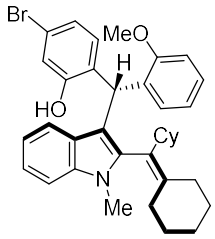
Following the general procedure, 2-alkenylindoles **1a** (61.5 mg, 0.2 mmol), *o*-hydroxybenzyl alcohol **2a** (26.0 mg, 0.1 mmol), CPA (*S*)-**7b** (6.6 mg, 0.01 mmol) and 4 Å MS (100 mg) were added to a reaction tube. Then, *p*-xylene (4 mL) was added to the reaction mixture, which was stirred at 20 °C for 12 h. After the completion of the reaction indicated by TLC, the reaction mixture was purified through flash column chromatography on silica gel (petroleum ether/ethyl acetate = 5:1) to afford pure product **4aa** in 99% yield (54.4 mg) as white solid; 92:8 dr; m.p. 100-101 °C; $[\alpha]_D^{20}$ = -29.8 (c 0.24, acetone); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.36 – 7.32 (m, 1H), 7.30 – 7.24 (m, 1H), 7.22 – 7.16 (m, 2H), 7.05 (d, *J* = 8.0 Hz, 1H), 6.96 – 6.89 (m, 2H), 6.88 – 6.83 (m, 1H), 6.71 (s, 2H), 6.48 (s, 1H), 5.81 (s, 1H), 5.08 (s, 1H), 3.75 (s, 3H), 3.71 (s, 3H), 3.64 (s, 3H), 2.64 – 2.56 (m, 1H), 2.50 – 2.41 (m, 1H), 2.39 – 2.29 (m, 1H), 1.93 – 1.83 (m, 2H), 1.81 – 1.75 (m, 1H), 1.71 – 1.59 (m, 5H), 1.43 – 1.27 (m, 4H), 1.26 – 1.20 (m, 1H), 1.14 – 1.00 (m, 2H), 0.99 – 0.90 (m, 1H), 0.73 – 0.62 (m, 1H), 0.31 – 0.17 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 156.9, 153.2, 149.0, 144.4, 140.1, 136.8, 131.0, 131.0, 130.8, 128.1, 128.0, 126.9, 121.1, 120.6, 120.5, 119.5, 116.2, 115.6, 111.8, 110.4, 109.6, 109.3, 55.6, 55.4, 41.4, 38.2, 33.2, 31.8, 30.6, 30.5, 29.8, 28.1, 27.7, 26.8, 26.6, 26.4, 25.3; IR (KBr): 2927, 2852, 2769, 1489, 1464, 1372, 1243, 1030, 804; ESI FTMS exact mass calcd for $(C_{37}H_{43}NO_3\text{+Na})^+$ requires m/z 572.3135, found m/z 572.3143; The enantiomeric ratio: 93:7, determined by HPLC (Daicel Chiralpak AD-3, hexane/ isopropanol = 98/ 2, flow rate 0.8 mL/min, T = 30 °C, 254 nm): t_R = 7.766 (minor), t_R = 9.309 (major).

(R_a,*R*)-2-((2-(cyclohexyl(cyclohexylidene)methyl)-1-methyl-1H-indol-3-yl)(phenyl)methyl)-4-methylphenol (4ac):



Following the general procedure, 2-alkenylindoles **1a** (61.5 mg, 0.2 mmol), *o*-hydroxybenzyl alcohol **2c** (21.4 mg, 0.1 mmol), CPA (*S*)-**7b** (6.6 mg, 0.01 mmol) and 4 Å MS (100 mg) were added to a reaction tube. Then, *p*-xylene (4 mL) was added to the reaction mixture, which was stirred at 20 °C for 12 h. After the completion of the reaction indicated by TLC, the reaction mixture was purified through flash column chromatography on silica gel (petroleum ether/ethyl acetate = 5:1) to afford pure product **4ac** in 99% yield (49.8 mg) as colorless oil; 83:17 dr; $[\alpha]_D^{20}$ = +113 (c 0.13, acetone) ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.34 – 7.26 (m, 3H), 7.25 – 7.19 (m, 3H), 7.17 – 7.10 (m, 1H), 6.94 – 6.83 (m, 3H), 6.73 (s, 1H), 6.67 (d, *J* = 8.1 Hz, 1H), 5.68 (s, 1H), 4.97 (s, 1H), 3.62 (s, 3H), 2.63 – 2.54 (m, 1H), 2.50 – 2.41 (m, 1H), 2.34 – 2.26 (m, 1H), 2.15 (s, 3H), 1.79 – 1.71 (m, 1H), 1.66 – 1.60 (m, 2H), 1.55 – 1.38 (m, 7H), 1.33 – 1.05 (m, 6H), 0.94 – 0.84 (m, 1H), 0.70 – 0.56 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 152.0, 145.0, 142.9, 140.1, 137.0, 131.1, 129.8, 129.5, 129.4, 128.3, 128.2, 127.4, 126.5, 126.3, 120.8, 120.5, 119.4, 115.8, 111.2, 109.3, 43.4, 41.3, 33.1, 33.0, 31.1, 30.7, 30.5, 28.2, 27.4, 26.8, 26.6, 26.5, 25.8, 20.8; IR (KBr): 3420, 2814, 2716, 1632, 1597, 1382, 1351, 1123, 776, 618; ESI FTMS exact mass calcd for $(C_{36}H_{41}NO\text{-}H)^-$ requires m/z 502.3115, found m/z 502.3121; The enantiomeric ratio: 92:8, determined by HPLC (Daicel Chiralpak AD-3, hexane/ isopropanol = 98/ 2, flow rate 0.8 mL/min, T = 30 °C, 254 nm): t_R = 7.396 (minor), t_R = 12.299 (major).

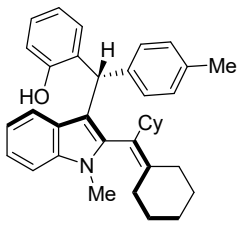
(R_a,*R*)-5-bromo-2-((2-(cyclohexyl(cyclohexylidene)methyl)-1-methyl-1H-indol-3-yl)(2-methoxyphenyl)methyl)phenol (4al):



Following the general procedure, 2-alkenylindoles **1a** (61.5 mg, 0.2 mmol), *o*-hydroxybenzyl alcohol **2l** (30.9 mg, 0.1 mmol), CPA (*S*)-**7b** (6.6 mg, 0.01 mmol) and 4 Å MS (100 mg) were added to a reaction tube. Then, *p*-xylene (4 mL) was added to the reaction mixture, which was stirred at 20 °C for 12 h. After the completion of the reaction indicated by TLC, the reaction mixture was purified through flash column chromatography on silica gel (petroleum ether/ethyl acetate = 5:1) to afford pure product **4al** in 99% yield (59.5 mg) as colorless oil; >95:5 dr; $[\alpha]_D^{20}$ = +17.9 (c 0.22, acetone); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.32 – 7.28 (m, 1H), 7.26 – 7.21 (m, 1H), 7.19 – 7.08 (m, 2H), 6.99 – 6.85 (m, 5H), 6.85 – 6.78 (m, 1H), 6.65 (d, *J* = 8.2 Hz, 1H), 5.68 (s, 1H), 5.50 (s, 1H), 3.70 (s, 3H), 3.59 (s, 3H), 2.58 – 2.48 (m, 1H), 2.44 – 2.35 (m, 1H), 2.35 – 2.26 (m, 1H), 1.87 – 1.71 (m, 3H), 1.68 – 1.58 (m, 4H), 1.50 – 1.42 (m, 1H), 1.38 – 1.20 (m, 4H), 1.19 – 1.12 (m, 1H), 1.08 – 0.98 (m, 1H), 0.96 – 0.80 (m, 2H), 0.65 – 0.53 (m, 1H), 0.23 – 0.09 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 156.8, 155.6, 144.5, 140.2, 136.9, 130.8, 130.7, 130.3, 128.9, 128.2, 127.9, 126.9, 123.0, 121.3, 120.6, 120.4, 119.7, 119.1, 110.4, 109.4, 108.9, 41.4, 37.7, 33.3, 31.8, 30.6, 30.5, 29.8, 28.1, 27.7, 26.8, 26.6, 26.4, 25.3; IR (KBr): 3446, 2925, 2851, 1586, 1464, 1384, 1350, 1243, 1121, 741; ESI FTMS exact mass calcd for $(C_{36}H_{40}BrNO_2\text{-}H)^-$

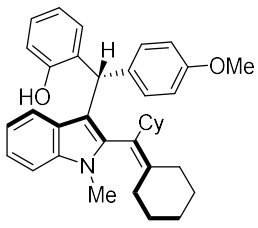
requires m/z 596.2169, found m/z 596.2205; The enantiomeric ratio: 93:7, determined by HPLC (Daicel Chiralpak AD-3, hexane/ isopropanol = 95/ 5, flow rate 0.8 mL/min, T = 30 °C, 254 nm): t_R = 5.219 (minor), t_R = 6.636 (major).

(R_a,*R*)-2-((2-(cyclohexyl(cyclohexylidene)methyl)-1-methyl-1H-indol-3-yl)(p-tolyl)methyl) phenol (4ai):



Following the general procedure, 2-alkenylindoles **1a** (61.5 mg, 0.2 mmol), *o*-hydroxybenzyl alcohol **2i** (21.4 mg, 0.1 mmol), CPA (*S*)-**7c** (7.1 mg, 0.01 mmol) and 4 Å MS (100 mg) were added to a reaction tube. Then, *p*-xylene (4 mL) was added to the reaction mixture, which was stirred at 20 °C for 12 h. After the completion of the reaction indicated by TLC, the reaction mixture was purified through flash column chromatography on silica gel (petroleum ether/ethyl acetate = 5:1) to afford pure product **4ai** in 64% yield (32.0 mg) as colorless oil; 67:33 dr; $[\alpha]_D^{20}$ = +99.5 (c 0.38, acetone); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.32 – 7.27 (m, 1H), 7.16 – 7.06 (m, 6H), 6.97 (d, *J* = 7.7 Hz, 1H), 6.94 – 6.90 (m, 1H), 6.90 – 6.84 (m, 1H), 6.81 – 6.74 (m, 2H), 5.69 (s, 1H), 5.11 (s, 1H), 3.58 (s, 3H), 2.65 – 2.55 (m, 1H), 2.49 – 2.41 (m, 1H), 2.33 (s, 3H), 2.32 – 2.25 (m, 1H), 1.77 – 1.71 (m, 1H), 1.66 – 1.57 (m, 4H), 1.53 – 1.38 (m, 6H), 1.34 – 1.28 (m, 1H), 1.24 – 1.16 (m, 2H), 1.14 – 1.02 (m, 2H), 0.96 – 0.87 (m, 1H), 0.74 – 0.60 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 154.2, 145.0, 139.9, 139.7, 137.0, 135.7, 130.6, 130.3, 129.2, 129.0, 127.6, 127.5, 126.5, 120.8, 120.6, 120.5, 119.3, 115.8, 111.5, 109.3, 42.6, 41.2, 33.1, 33.0, 31.0, 30.7, 30.5, 28.2, 27.4, 26.8, 26.6, 26.5, 25.7, 21.1; IR (KBr): 3420, 2927, 2851, 1631, 1594, 1384, 1351, 1122, 740; ESI FTMS exact mass calcd for $(C_{36}H_{41}NO\text{-}H)^-$ requires m/z 502.3115, found m/z 502.3145; The enantiomeric ratio: 91:9, determined by HPLC (Daicel Chiralpak IB, hexane/ isopropanol = 98/ 2, flow rate 0.8 mL/min, T = 30 °C, 254 nm): t_R = 6.006 (major), t_R = 7.619 (minor).

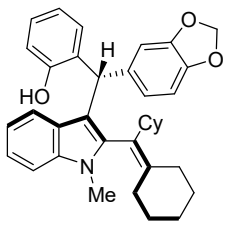
(R_a,*R*)-2-((2-(cyclohexyl(cyclohexylidene)methyl)-1-methyl-1H-indol-3-yl)(4-methoxyphenyl) methyl)phenol (4am):



Following the general procedure, 2-alkenylindoles **1a** (61.5 mg, 0.2 mmol), *o*-hydroxybenzyl alcohol **2m** (23.0 mg, 0.1 mmol), CPA (*S*)-**7b** (6.6 mg, 0.01 mmol) and 4 Å MS (100 mg) were added to a reaction tube. Then, *p*-xylene (4 mL) was added to the reaction mixture, which was stirred at 20 °C for 12 h. After the completion of the reaction indicated by TLC, the reaction mixture was purified through flash column chromatography on silica gel (petroleum ether/ethyl acetate = 5:1) to afford pure product **4am** in 92% yield (47.8 mg) as colorless oil; 95:5 dr; $[\alpha]_D^{20}$ = +144.4 (c 0.45, acetone); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.29 (d, *J* = 8.2 Hz, 1H), 7.17 – 7.05 (m, 4H), 6.96 (d, *J* = 7.7 Hz, 1H), 6.94 – 6.85 (m, 2H), 6.85 – 6.72 (m, 4H), 5.67 (s, 1H), 5.11 (s, 1H), 3.79 (s, 3H), 3.58 (s, 3H), 2.65 – 2.55 (m, 1H), 2.49 – 2.39 (m, 1H), 2.35 – 2.26 (m, 1H), 1.78 – 1.72 (m, 1H), 1.66 – 1.59 (m, 2H), 1.51 – 1.39 (m, 5H), 1.31 – 1.26 (m, 2H), 1.25 – 1.14 (m, 3H), 1.14 – 1.02 (m, 2H), 0.97 – 0.83 (m, 2H), 0.75 – 0.63 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.1, 154.1, 145.0, 139.9, 137.0, 134.9, 130.5, 130.4, 130.3, 127.6, 127.5, 126.4, 120.8, 120.6, 120.5, 119.3, 115.8, 113.7, 111.5, 109.3,

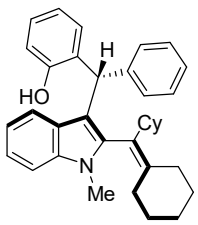
55.4, 42.3, 41.2, 33.1, 33.0, 31.1, 30.7, 30.5, 29.8, 28.2, 27.4, 26.8, 26.7, 26.6, 25.8; IR (KBr): 3446, 2927, 2851, 1585, 1508, 1464, 1351, 1246, 1177, 1038, 741; ESI FTMS exact mass calcd for $(C_{36}H_{41}NO_2\text{-}H)^-$ requires m/z 518.3064, found m/z 518.3086; The enantiomeric ratio: 90:10, determined by HPLC (Daicel Chiralpak AD-3, hexane/ isopropanol = 98/ 2, flow rate 1.0 mL/min, T = 30 °C, 254 nm): t_R = 10.843 (major), t_R = 18.006 (minor).

(*R*$_a$,*R*)-2-(benzo[d][1,3]dioxol-5-yl(2-(cyclohexyl(cyclohexylidene)methyl)-1-methyl-1H-indol-3-yl)methyl)phenol (4aj):



Following the general procedure, 2-alkenylindoles **1a** (61.5 mg, 0.2 mmol), *o*-hydroxybenzyl alcohol **2j** (24.4 mg, 0.1 mmol), CPA (*S*)-**7b** (6.6 mg, 0.01 mmol) and 4 Å MS (100 mg) were added to a reaction tube. Then, *p*-xylene (4 mL) was added to the reaction mixture, which was stirred at 20 °C for 12 h. After the completion of the reaction indicated by TLC, the reaction mixture was purified through flash column chromatography on silica gel (petroleum ether/ethyl acetate = 5:1) to afford pure product **4aj** in 75% yield (40.0 mg) as colorless oil; >95:5 dr; $[\alpha]_D^{20}$ = +95.1 (c 0.32, acetone); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.30 (d, *J* = 8.2 Hz, 1H), 7.17 – 7.08 (m, 2H), 7.02 – 6.95 (m, 2H), 6.93 – 6.87 (m, 1H), 6.82 – 6.75 (m, 3H), 6.74 – 6.67 (m, 2H), 5.94 – 5.89 (m, 2H), 5.66 (s, 1H), 5.09 (s, 1H), 3.59 (s, 3H), 2.67 – 2.57 (m, 1H), 2.49 – 2.39 (m, 1H), 2.36 – 2.27 (m, 1H), 1.82 – 1.75 (m, 1H), 1.60 – 1.46 (m, 6H), 1.45 – 1.31 (m, 3H), 1.29 – 1.09 (m, 4H), 1.04 – 0.91 (m, 2H), 0.83 – 0.73 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 154.1, 147.8, 146.0, 145.1, 140.0, 137.1, 130.6, 130.2, 127.8, 127.5, 126.4, 122.3, 120.9, 120.8, 120.7, 120.6, 119.4, 115.9, 111.6, 110.1, 109.4, 108.0, 100.9, 42.6, 41.3, 33.2, 33.1, 31.3, 30.7, 30.6, 28.3, 27.4, 26.9, 26.8, 26.6, 26.0; IR (KBr): 3443, 2926, 2851, 1647, 1569, 1486, 1465, 1366, 1229, 1040; ESI FTMS exact mass calcd for $(C_{36}H_{39}NO_3\text{-}H)^-$ requires m/z 532.2857, found m/z 532.2888; The enantiomeric ratio: 90:10, determined by HPLC (Daicel Chiralpak IB, hexane/ isopropanol = 99/ 1, flow rate 1.0 mL/min, T = 30 °C, 254 nm): t_R = 10.366 (major), t_R = 17.443 (minor).

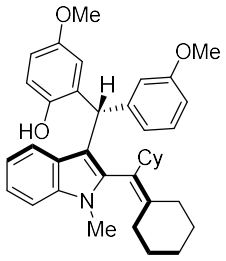
(*R*$_a$,*R*)-2-((2-(cyclohexyl(cyclohexylidene)methyl)-1-methyl-1H-indol-3-yl)(phenyl)methyl) phenol (4ak):



Following the general procedure, 2-alkenylindoles **1a** (61.5 mg, 0.2 mmol), *o*-hydroxybenzyl alcohol **2k** (20 mg, 0.1 mmol), CPA (*S*)-**7c** (7.1 mg, 0.01 mmol) and 4 Å MS (100 mg) were added to a reaction tube. Then, *p*-xylene (4 mL) was added to the reaction mixture, which was stirred at 20 °C for 12 h. After the completion of the reaction indicated by TLC, the reaction mixture was purified through flash column chromatography on silica gel (petroleum ether/ethyl acetate = 5:1) to afford pure product **4ak** in 96% yield (47.0 mg) as white solid; m.p. 97-98 °C; >95:5 dr; $[\alpha]_D^{20}$ = +143.2 (c 0.49, acetone); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.38 – 7.32 (m, 2H), 7.31 – 7.25 (m, 4H), 7.22 – 7.12 (m, 2H), 7.00 (d, *J* = 7.7 Hz, 1H), 6.97 – 6.88 (m, 2H), 6.87 – 6.79 (m, 2H), 5.78 (s, 1H), 5.14 (s, 1H), 3.64 (s, 3H), 2.70 – 2.59 (m, 1H), 2.56 – 2.47 (m, 1H), 2.39 – 2.31 (m, 1H), 1.85 – 1.76 (m, 1H), 1.70 – 1.62 (m, 3H), 1.62 – 1.55 (m, 3H), 1.54 – 1.44 (m, 4H), 1.34 – 1.23 (m, 3H), 1.22 – 1.14 (m, 2H), 1.00 – 0.91 (m, 1H), 0.77 – 0.61 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 154.2, 145.0, 142.9, 140.1, 137.0,

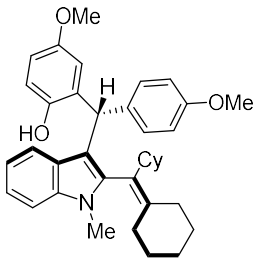
130.6, 130.1, 129.3, 128.3, 127.7, 127.5, 126.5, 126.3, 120.9, 120.6, 119.4, 115.9, 111.2, 109.3, 43.1, 41.3, 33.1, 33.0, 31.0, 30.7, 30.5, 28.2, 27.4, 26.8, 26.6, 25.8; IR (KBr): 3444, 2926, 2851, 1668, 1583, 1466, 1388, 1265, 741; ESI FTMS exact mass calcd for $(C_{35}H_{39}NO\text{-}H)^-$ requires m/z 488.2959, found m/z 488.2987; The enantiomeric ratio: 90:10, determined by HPLC (Daicel Chiralpak OD-3, hexane/ isopropanol = 98/ 2, flow rate 0.8 mL/min, T = 30 °C, 254 nm): t_R = 5.839 (minor), t_R = 10.556 (major).

(*R*$_a$,*R*)-2-((2-(cyclohexyl(cyclohexylidene)methyl)-1-methyl-1H-indol-3-yl)(3-methoxyphenyl) methyl)-4-methoxyphenol (4af):



Following the general procedure, 2-alkenylindoles **1a** (61.5 mg, 0.2 mmol), *o*-hydroxybenzyl alcohol **2f** (26.0 mg, 0.1 mmol), CPA (*S*)-**7b** (6.6 mg, 0.01 mmol) and 4 Å MS (100 mg) were added to a reaction tube. Then, *p*-xylene (4 mL) was added to the reaction mixture, which was stirred at 20 °C for 12 h. After the completion of the reaction indicated by TLC, the reaction mixture was purified through flash column chromatography on silica gel (petroleum ether/ethyl acetate = 5:1) to afford pure product **4af** in 95% yield (52.2 mg) as colorless oil; 86:14 dr; $[\alpha]_D^{20}$ = +135.7 (c 0.58, acetone); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.32 – 7.26 (m, 1H), 7.21 – 7.15 (m, 1H), 7.14 – 7.10 (m, 1H), 6.97 (d, *J* = 8.0 Hz, 1H), 6.89 – 6.82 (m, 2H), 6.81 – 6.75 (m, 2H), 6.72 – 6.64 (m, 2H), 6.58 (s, 1H), 5.65 (s, 1H), 4.76 (s, 1H), 3.68 (s, 3H), 3.59 (s, 3H), 3.57 (s, 3H), 2.63 – 2.55 (m, 1H), 2.48 – 2.41 (m, 1H), 2.36 – 2.28 (m, 1H), 1.78 – 1.71 (m, 1H), 1.66 – 1.60 (m, 2H), 1.57 – 1.39 (m, 8H), 1.25 – 1.04 (m, 5H), 0.94 – 0.87 (m, 1H), 0.74 – 0.61 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.8, 153.6, 148.2, 145.0, 144.4, 140.0, 137.0, 131.3, 129.3, 127.4, 126.5, 121.9, 120.9, 120.5, 119.4, 116.6, 116.5, 115.2, 112.3, 111.7, 111.1, 109.3, 55.6, 55.2, 43.3, 41.3, 33.1, 33.0, 31.0, 30.7, 30.5, 28.2, 27.4, 26.8, 26.6, 25.8; IR (KBr): 3482, 2926, 2851, 1659, 1488, 1466, 1365, 1264, 1203, 1045, 742; ESI FTMS exact mass calcd for $(C_{37}H_{43}NO_3\text{-}H)^-$ requires m/z 548.3170, found m/z 548.3189; The enantiomeric ratio: 93:7, determined by HPLC (Daicel Chiralpak AD-3, hexane/ isopropanol = 95/ 5, flow rate 1.0 mL/min, T = 30 °C, 254 nm): t_R = 6.516 (minor), t_R = 8.979 (major).

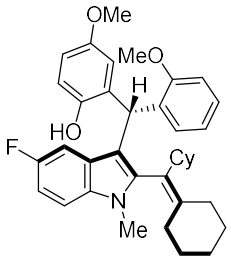
(*R*$_a$,*R*)-2-((2-(cyclohexyl(cyclohexylidene)methyl)-1-methyl-1H-indol-3-yl)(4-methoxyphenyl) methyl)-4-methoxyphenol (4ah):



Following the general procedure, 2-alkenylindoles **1a** (61.5 mg, 0.2 mmol), *o*-hydroxybenzyl alcohol **2h** (26.0 mg, 0.1 mmol), CPA (*S*)-**7b** (6.6 mg, 0.01 mmol) and 4 Å MS (100 mg) were added to a reaction tube. Then, *p*-xylene (4 mL) was added to the reaction mixture, which was stirred at 20 °C for 12 h. After the completion of the reaction indicated by TLC, the reaction mixture was purified through flash column chromatography on silica gel (petroleum ether/ethyl acetate = 5:1) to afford pure product **4ah** in 92% yield (50.6 mg) as colorless oil; 91:9 dr; $[\alpha]_D^{20}$ = +152.1 (c 0.36, acetone); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.26 – 7.23 (m, 1H), 7.13 – 7.04 (m, 3H), 6.98 (d, *J* = 8.0 Hz, 1H), 6.88 – 6.83 (m, 1H), 6.80 –

6.69 (m, 4H), 6.67 – 6.61 (m, 1H), 5.49 (s, 1H), 4.63 (s, 1H), 3.74 (s, 3H), 3.57 (s, 3H), 3.55 (s, 3H), 2.64 – 2.54 (m, 1H), 2.51 – 2.42 (m, 1H), 2.32 – 2.23 (m, 1H), 1.72 – 1.61 (m, 4H), 1.55 – 1.51 (m, 2H), 1.47 – 1.37 (m, 4H), 1.33 – 1.27 (m, 2H), 1.16 – 1.08 (m, 2H), 1.07 – 1.00 (m, 1H), 0.91 – 0.81 (m, 1H), 0.80 – 0.73 (m, 1H), 0.65 – 0.56 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.1, 153.7, 148.1, 144.2, 139.7, 136.9, 134.7, 131.5, 129.9, 127.4, 126.7, 120.7, 120.4, 119.2, 116.7, 116.6, 113.9, 112.4, 111.7, 109.2, 55.7, 55.3, 43.3, 41.1, 33.1, 32.8, 30.6, 30.4, 28.3, 27.8, 26.9, 26.7, 26.6, 25.7; IR (KBr): 2927, 2852, 2769, 1489, 1464, 1372, 1243, 1030, 804, 740; ESI FTMS exact mass calcd for $(C_{37}H_{43}NO_3\text{-}H)^-$ requires m/z 548.3170, found m/z 548.3178; The enantiomeric ratio: 90:10, determined by HPLC (Daicel Chiralpak AD-3, hexane/ isopropanol = 98/ 2, flow rate 1.0 mL/min, T = 30 °C, 254 nm): t_R = 10.633 (minor), t_R = 17.606 (major).

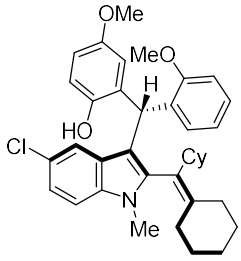
(*R*$_a$,*R*)-2-((2-(cyclohexyl(cyclohexylidene)methyl)-5-fluoro-1-methyl-1H-indol-3-yl)(2-meth oxyphenyl)methyl)-4-methoxyphenol (4ba):



Following the general procedure, 2-alkenylindoles **1b** (65.1 mg, 0.2 mmol), *o*-hydroxybenzyl alcohol **2a** (26.0 mg, 0.1 mmol), CPA (*S*)-**7b** (6.6 mg, 0.01 mmol) and 4 Å MS (100 mg) were added to a reaction tube. Then, *p*-xylene (4 mL) was added to the reaction mixture, which was stirred at 20 °C for 12 h. After the completion of the reaction indicated by TLC, the reaction mixture was purified through flash column chromatography on silica gel (petroleum ether/ethyl acetate = 5:1) to afford pure product **4ba** in 73% yield (41.4 mg) as colorless oil; >95:5 dr; $[\alpha]_D^{20}$ = +15.4 (c 0.26, acetone); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.23 (d, *J* = 7.9 Hz, 1H), 7.19 – 7.13 (m, 1H), 7.07 (d, *J* = 7.6 Hz, 1H), 6.89 – 6.79 (m, 3H), 6.70 – 6.62 (m, 2H), 6.59 (d, *J* = 10.4 Hz, 1H), 6.38 (s, 1H), 5.72 (s, 1H), 4.92 (s, 1H), 3.69 (s, 3H), 3.65 (s, 3H), 3.56 (s, 3H), 2.56 – 2.46 (m, 1H), 2.43 – 2.34 (m, 1H), 2.32 – 2.24 (m, 1H), 1.80 – 1.69 (m, 3H), 1.57 – 1.48 (m, 3H), 1.45 – 1.40 (m, 1H), 1.37 – 1.24 (m, 4H), 1.22 – 1.16 (m, 1H), 1.11 – 0.81 (m, 4H), 0.69 – 0.58 (m, 1H), 0.29 – 0.15 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 157.6 (d, *J* = 232.2 Hz), 156.9, 153.3, 148.8, 144.6, 141.9, 133.4, 130.7, 130.6, 130.5, 128.2, 128.1, 126.8, 120.6, 116.3, 115.6, 112.1, 110.5, 109.8, 109.7, 109.3 (d, *J* = 26.4 Hz), 105.3 (d, *J* = 24.3 Hz), 55.6, 55.4, 41.4, 38.0, 33.2, 31.8, 30.7, 30.6, 29.9, 28.0, 27.7, 26.8, 26.6, 26.4, 25.3; ^{19}F NMR (376 MHz, $CDCl_3$) δ -124.0; IR (KBr): 2854, 2603, 1596, 1489, 1369, 1242, 933; ESI FTMS exact mass calcd for $(C_{37}H_{42}FNO_3\text{-}H)^-$ requires m/z 566.3076, found m/z 566.3104; The enantiomeric ratio: 94:6, determined by HPLC (Daicel Chiralpak OD-3, hexane/ isopropanol = 98/ 2, flow rate 0.8 mL/min, T = 30 °C, 254 nm): t_R = 7.479 (minor), t_R = 11.263 (major).

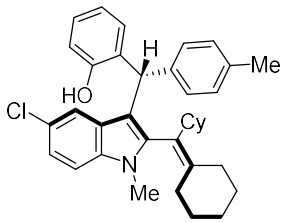
(*R*$_a$,*R*)-2-((5-chloro-2-(cyclohexyl(cyclohexylidene)methyl)-1-methyl-1H-indol-3-yl)(2-meth oxyphenyl)methyl)-4-methoxyphenol (4ca):

Following the general procedure, 2-alkenylindoles **1c** (68.4 mg, 0.2 mmol), *o*-hydroxybenzyl alcohol **2a** (26.0 mg, 0.1 mmol), CPA (*S*)-**7b** (6.6 mg, 0.01 mmol) and 4 Å MS (100 mg) were added to a reaction tube. Then, *p*-xylene (4 mL) was added to the reaction mixture, which was stirred at 20 °C for 12 h. After the completion of



the reaction indicated by TLC, the reaction mixture was purified through flash column chromatography on silica gel (petroleum ether/ethyl acetate = 5:1) to afford pure product **4ca** in 84% yield (49.2 mg) as colorless oil; >95:5 dr; $[\alpha]_D^{20}$ = +10.6 (c 0.21, acetone); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.26 – 7.21 (m, 1H), 7.20 – 7.14 (m, 1H), 7.06 (d, *J* = 8.8 Hz, 2H), 6.90 – 6.81 (m, 3H), 6.72 – 6.64 (m, 2H), 6.40 (s, 1H), 5.73 (s, 1H), 4.85 (s, 1H), 3.68 (s, 3H), 3.65 (s, 3H), 3.55 (s, 3H), 2.56 – 2.47 (m, 1H), 2.43 – 2.35 (m, 1H), 2.32 – 2.24 (m, 1H), 1.78 – 1.68 (m, 3H), 1.57 – 1.49 (m, 3H), 1.41 – 1.24 (m, 5H), 1.21 – 1.16 (m, 1H), 1.10 – 0.84 (m, 4H), 0.70 – 0.59 (m, 1H), 0.31 – 0.19 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 156.9, 153.4, 148.7, 144.7, 141.5, 135.2, 130.6, 130.4, 128.9, 128.2, 126.6, 125.1, 121.3, 120.7, 119.6, 116.3, 115.7, 112.4, 110.5, 110.3, 109.7, 55.8, 55.4, 41.4, 38.0, 33.2, 31.9, 30.6, 30.6, 29.9, 28.0, 27.7, 26.8, 26.6, 26.4, 25.4; IR (KBr): 3456, 2926, 1652, 1578, 1383, 1350, 1266, 1119, 741; ESI FTMS exact mass calcd for $(C_{37}H_{42}ClNO_3\text{-}H)^-$ requires m/z 582.2780, found m/z 582.2796; The enantiomeric ratio: 91:9, determined by HPLC (Daicel Chiralpak AD-3, hexane/ isopropanol = 98/ 2, flow rate 1.0 mL/min, T = 30 °C, 254 nm): t_R = 16.223 (minor), t_R = 18.173 (major).

(*R*$_a$,*R*)-2-((5-chloro-2-(cyclohexyl(cyclohexylidene)methyl)-1-methyl-1H-indol-3-yl)(p-tolyl) methyl)phenol (4ci):



Following the general procedure, 2-alkenylindoles **1c** (68.4 mg, 0.2 mmol), *o*-hydroxybenzyl alcohol **2i** (21.4 mg, 0.1 mmol), CPA (*S*)-**7c** (7.1 mg, 0.01 mmol) and 4 Å MS (100 mg) were added to a reaction tube. Then, mesitylene (4 mL) was added to the reaction mixture, which was stirred at -30 °C for 12 h. After the completion of the reaction indicated by TLC, the reaction mixture was purified through flash column chromatography on silica gel (petroleum ether/ethyl acetate = 5:1) to afford pure product **4ci** in 60% yield (32.3 mg) as colorless oil; 93:7 dr; $[\alpha]_D^{20}$ = +147.9 (c 0.33, acetone); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.21 – 7.16 (m, 1H), 7.15 – 7.01 (m, 6H), 6.95 – 6.89 (m, 1H), 6.85 (s, 1H), 6.82 – 6.73 (m, 2H), 5.67 (s, 1H), 4.89 (s, 1H), 3.55 (s, 3H), 2.62 – 2.56 (m, 1H), 2.45 – 2.37 (m, 1H), 2.34 (s, 3H), 2.31 – 2.27 (m, 1H), 1.79 – 1.70 (m, 1H), 1.64 – 1.53 (m, 5H), 1.49 – 1.39 (m, 4H), 1.31 – 1.23 (m, 2H), 1.22 – 1.07 (m, 3H), 1.01 – 0.86 (m, 2H), 0.76 – 0.65 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 153.8, 145.3, 141.3, 139.3, 136.0, 135.3, 130.5, 129.9, 129.1, 129.0, 128.6, 127.8, 126.2, 124.9, 121.0, 120.7, 119.9, 115.8, 111.8, 110.2, 42.1, 41.2, 33.1, 31.0, 30.8, 30.5, 28.2, 27.3, 26.8, 26.6, 26.5, 25.7, 21.1; IR (KBr): 3436, 2927, 2852, 1699, 1586, 1455, 1389, 1265, 751; ESI FTMS exact mass calcd for $(C_{36}H_{40}ClNO+Na)^+$ requires m/z 560.2691 found m/z 560.2701; The enantiomeric ratio: 95:5, determined by HPLC (Daicel Chiralpak OD-3, hexane/ isopropanol = 98/ 2, flow rate 1.0 mL/min, T = 30 °C, 254 nm): t_R = 5.236 (minor), t_R = 8.196 (major).

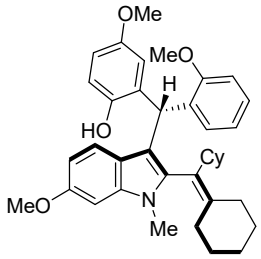
(*R*$_a$,*R*)-2-((5-bromo-2-(cyclohexyl(cyclohexylidene)methyl)-1-methyl-1H-indol-3-yl)(2-meth oxyphenyl)methyl)-4-methoxyphenol (4da):

Following the general procedure, 2-alkenylindoles **1d** (77.3 mg, 0.2 mmol), *o*-hydroxybenzyl alcohol **2a** (26.0 mg, 0.1 mmol), CPA (*S*)-**7b** (6.6 mg, 0.01 mmol) and 4 Å MS (100 mg) were added to a reaction tube. Then, *p*-xylene (4 mL) was added to the reaction mixture, which was stirred at 20 °C for 12 h. After the completion of the reaction indicated by TLC, the reaction mixture was purified through flash column chromatography on silica gel (petroleum ether/ethyl acetate = 5:1) to afford pure product **4da** in 99% yield (62.4 mg) as colorless oil; >95:5 dr; $[\alpha]_D^{20}$ = +18.5 (c 1.14, acetone); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.26 – 7.22 (m, 1H), 7.21 – 7.18 (m, 1H), 7.14 – 7.12 (m, 1H), 7.08 – 7.02 (m, 2H), 6.90 – 6.82 (m, 2H), 6.68 (s, 2H), 6.41 (s, 1H), 5.74 (s, 1H), 4.84 (s, 1H), 3.68 (s, 3H), 3.66 (s, 3H), 3.55 (s, 3H), 2.54 – 2.48 (m, 1H), 2.43 – 2.37 (m, 1H), 2.32 – 2.25 (m, 1H), 1.77 – 1.69 (m, 3H), 1.57 – 1.47 (m, 3H), 1.41 – 1.15 (m, 6H), 1.12 – 0.85 (m, 4H), 0.70 – 0.61 (m, 1H), 0.31 – 0.21 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 156.9, 153.4, 148.7, 144.8, 141.4, 135.4, 130.6, 130.4, 129.6, 128.2, 126.6, 123.9, 122.7, 120.7, 116.4, 115.8, 112.8, 112.5, 110.8, 110.5, 109.8, 55.9, 55.4, 41.4, 38.0, 33.2, 31.9, 30.6, 29.9, 28.0, 27.7, 26.8, 26.6, 26.4, 25.4; IR (KBr): 2962, 2921, 2850, 1770, 1759, 1654, 1470, 1377, 1246, 1096, 1050, 801; ESI FTMS exact mass calcd for $(C_{37}H_{42}BrNO_3\text{-}H)^-$ requires m/z 626.2275, found m/z 626.2307; The enantiomeric ratio: 91:9, determined by HPLC (Daicel Chiralpak AD-3, hexane/ isopropanol = 98/ 2, flow rate 1.0 mL/min, T = 30 °C, 254 nm): t_R = 8.229 (minor), t_R = 9.969 (major).

(R_a,*R*)-2-((5-bromo-2-(cyclohexyl(cyclohexylidene)methyl)-1-methyl-1H-indol-3-yl)(p-tolyl) methyl)phenol (4di):

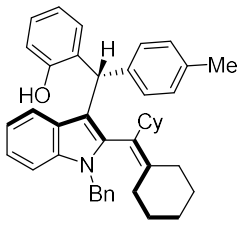
Following the general procedure, 2-alkenylindoles **1d** (77.3 mg, 0.2 mmol), *o*-hydroxybenzyl alcohol **2i** (21.4 mg, 0.1 mmol), CPA (*S*)-**7c** (7.1 mg, 0.01 mmol) and 4 Å MS (100 mg) were added to a reaction tube. Then, mesitylene (4 mL) was added to the reaction mixture, which was stirred at -30 °C for 12 h. After the completion of the reaction indicated by TLC, the reaction mixture was purified through flash column chromatography on silica gel (petroleum ether/ethyl acetate = 5:1) to afford pure product **4di** in 52% yield (30.3 mg) as colorless oil; 93:7 dr; $[\alpha]_D^{20}$ = +16.8 (c 0.43, acetone); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.23 – 7.18 (m, 1H), 7.17 – 7.04 (m, 6H), 7.01 (s, 1H), 6.95 – 6.90 (m, 1H), 6.84 – 6.74 (m, 2H), 5.68 (s, 1H), 4.89 (s, 1H), 3.55 (s, 3H), 2.61 – 2.56 (m, 1H), 2.45 – 2.37 (m, 1H), 2.37 – 2.33 (m, 3H), 2.31 – 2.27 (m, 1H), 1.78 – 1.71 (m, 1H), 1.63 – 1.55 (m, 5H), 1.49 – 1.39 (m, 4H), 1.31 – 1.24 (m, 2H), 1.22 – 1.08 (m, 3H), 1.00 – 0.85 (m, 2H), 0.78 – 0.66 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 153.8, 145.3, 141.1, 139.2, 136.0, 135.6, 130.5, 129.8, 129.2, 129.1, 129.0, 127.8, 126.1, 123.6, 122.9, 120.7, 115.8, 112.6, 111.7, 110.7, 42.1, 41.2, 33.1, 31.0, 30.8, 30.5, 28.2, 27.3, 26.8, 26.6, 26.5, 25.7, 21.1; IR (KBr): 2926, 2851, 1631, 1508, 1456, 1382, 1351, 1264, 1120, 826; ESI FTMS exact mass calcd for $(C_{36}H_{40}BrNO\text{-}H)^-$ requires m/z 580.2220, found m/z 580.2229; The enantiomeric ratio: 95:5, determined by HPLC (Daicel Chiralpak OD-3, hexane/ isopropanol = 98/ 2, flow rate 1.0 mL/min, T = 30 °C, 254 nm): t_R = 5.316 (minor), t_R = 7.983 (major).

(R_a,*R*)-2-((2-(cyclohexyl(cyclohexylidene)methyl)-6-methoxy-1-methyl-1H-indol-3-yl)(2-methoxyphenyl)methyl)-4-methoxyphenol (4ha):



Following the general procedure, 2-alkenylindoles **1f** (67.5 mg, 0.2 mmol), *o*-hydroxybenzyl alcohol **2a** (26.0 mg, 0.1 mmol), CPA (*S*)-**7b** (6.6 mg, 0.01 mmol) and 4 Å MS (100 mg) were added to a reaction tube. Then, *p*-xylene (4 mL) was added to the reaction mixture, which was stirred at 20 °C for 12 h. After the completion of the reaction indicated by TLC, the reaction mixture was purified through flash column chromatography on silica gel (petroleum ether/ethyl acetate = 5:1) to afford pure product **4ha** in 53% yield (30.7 mg) as colorless oil; 94:6 dr; $[\alpha]_D^{20}$ = +65.3 (c 0.17, acetone)**;** ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.16 – 7.11 (m, 1H), 7.04 (d, *J* = 7.6 Hz, 1H), 6.84 (d, *J* = 8.3 Hz, 1H), 6.77 – 6.69 (m, 5H), 6.55 (d, *J* = 8.7 Hz, 1H), 6.33 (s, 1H), 6.08 (s, 1H), 5.24 (s, 1H), 3.84 (s, 3H), 3.73 (s, 3H), 3.64 (s, 3H), 3.49 (s, 3H), 2.72 – 2.64 (m, 1H), 2.43 – 2.36 (m, 1H), 2.11 – 2.04 (m, 1H), 1.91 – 1.85 (m, 1H), 1.81 – 1.65 (m, 5H), 1.50 – 1.45 (m, 2H), 1.40 – 1.28 (m, 3H), 1.16 – 1.09 (m, 2H), 1.03 – 0.97 (m, 1H), 0.89 – 0.84 (m, 1H), 0.71 – 0.62 (m, 1H), 0.59 – 0.51 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 156.7, 155.8, 153.3, 149.6, 145.0, 139.9, 137.6, 131.2, 131.1, 131.0, 127.4, 125.8, 122.2, 120.8, 120.7, 116.4, 115.8, 111.6, 110.4, 109.8, 109.0, 93.2, 55.6, 55.5, 55.4, 41.7, 36.8, 33.7, 32.4, 31.2, 30.8, 30.4, 28.1, 27.3, 27.0, 26.9, 26.5, 25.9; IR (KBr): 3420, 2926, 2851, 2715, 1628, 1489, 1382, 1350, 1243, 1117, 1043, 785; ESI FTMS exact mass calcd for $(C_{38}H_{45}NO_4\text{-}H)^-$ requires m/z 578.3276, found m/z 578.3315; The enantiomeric ratio: 93:7, determined by HPLC (Daicel Chiralpak OD-3, hexane/ isopropanol = 98/ 2, flow rate 1.0 mL/min, T = 30 °C, 254 nm): t_R = 16.396 (minor), t_R = 20.039 (major).

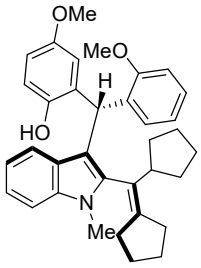
(R_a,*R*)-2-((1-benzyl-2-(cyclohexyl(cyclohexylidene)methyl)-1H-indol-3-yl)(p-tolyl) methyl)phenol (4ei):



Following the general procedure, 2-alkenylindoles **1e** (76.7 mg, 0.2 mmol), *o*-hydroxybenzyl alcohol **2i** (21.4 mg, 0.1 mmol), CPA (*S*)-**7c** (7.1 mg, 0.01 mmol) and 4 Å MS (100 mg) were added to a reaction tube. Then, *p*-xylene (4 mL) was added to the reaction mixture, which was stirred at 20 °C for 12 h. After the completion of the reaction indicated by TLC, the reaction mixture was purified through flash column chromatography on silica gel (petroleum ether/ethyl acetate = 5:1) to afford pure product **4ei** in 58% yield (33.6 mg) as colorless oil; 67:33 dr; $[\alpha]_D^{20}$ = +100.1 (c 0.25, acetone); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.32 – 7.27 (m, 1H), 7.26 – 7.19 (m, 2H), 7.18 – 6.96 (m, 10H), 6.95 – 6.90 (m, 1H), 6.88 – 6.75 (m, 3H), 5.70 (s, 1H), 5.33 – 5.17 (m, 2H), 5.07 (s, 1H), 2.55 – 2.46 (m, 1H), 2.33 (s, 3H), 2.32 – 2.19 (m, 2H), 1.70 – 1.63 (m, 1H), 1.54 – 1.40 (m, 7H), 1.36 – 1.31 (m, 2H), 1.28 – 1.24 (m, 1H), 1.18 – 0.90 (m, 4H), 0.88 – 0.80 (m, 2H), 0.76 – 0.67 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 154.1, 146.0, 140.5, 139.6, 137.8, 136.7, 135.8, 130.6, 130.0, 129.1, 128.5, 127.9, 127.7, 127.0, 126.5, 126.2, 120.9, 120.7, 120.6, 119.4, 115.9, 112.3, 110.9, 48.1, 42.7, 41.5, 33.4, 32.9, 31.4, 30.7, 28.1, 27.4, 26.9, 26.7, 26.4, 25.8, 21.1; IR (KBr): 2924, 2853, 1748, 1508, 1456, 1363, 1262, 741; ESI FTMS exact mass calcd for $(C_{42}H_{45}NO+Na)^+$ requires m/z 602.3393, found m/z

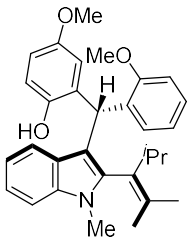
602.3404; The enantiomeric ratio: 95:5, determined by HPLC (Daicel Chiralpak OD-3, hexane/ isopropanol = 98/ 2, flow rate 1.0 mL/min, T = 30 °C, 254 nm): t_R = 5.336 (minor), t_R = 6.133 (major).

(R_a,*R*)-2-((2-(cyclopentyl(cyclopentylidene)methyl)-1-methyl-1H-indol-3-yl)(2-methoxyphenyl)methyl)-4-methoxyphenol (4fa):



Following the general procedure, 2-alkenylindoles **1f** (55.9 mg, 0.2 mmol), *o*-hydroxybenzyl alcohol **2a** (26.0 mg, 0.1 mmol), CPA (*R*)-**6b** (7.1 mg, 0.01 mmol) and 4 Å MS (100 mg) were added to a reaction tube. Then, *p*-xylene (4 mL) was added to the reaction mixture, which was stirred at 20 °C for 12 h. After the completion of the reaction indicated by TLC, the reaction mixture was purified through flash column chromatography on silica gel (petroleum ether/ethyl acetate = 5:1) to afford pure product **4fa** in 60% yield (31.3 mg) as colorless oil; 75:25 dr; $[\alpha]_D^{20}$ = +4.9 (c 0.35, acetone); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.32 – 7.26 (m, 1H), 7.23 – 7.16 (m, 1H), 7.16 – 7.08 (m, 2H), 6.95 – 6.90 (m, 1H), 6.89 – 6.82 (m, 2H), 6.81 – 6.75 (m, 1H), 6.70 – 6.61 (m, 2H), 6.41 (s, 1H), 5.79 (s, 1H), 3.69 (s, 3H), 3.65 (s, 3H), 3.54 (s, 3H), 2.74 – 2.62 (m, 1H), 2.53 – 2.39 (m, 2H), 2.03 – 1.95 (m, 1H), 1.84 – 1.61 (m, 5H), 1.51 – 1.39 (m, 2H), 1.24 – 1.16 (m, 2H), 1.09 – 0.97 (m, 2H), 0.91 – 0.84 (m, 1H), 0.82 – 0.69 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 156.9, 153.2, 149.3, 149.0, 140.9, 136.8, 131.1, 131.0, 130.6, 127.9, 127.8, 124.9, 121.1, 120.6, 120.3, 119.5, 116.4, 115.6, 111.9, 110.5, 109.3, 55.6, 55.4, 45.0, 38.2, 32.8, 30.7, 30.6, 30.0, 29.8, 26.5, 26.2, 24.6, 24.3. IR (KBr): 3648, 2935, 2866, 1598, 1489, 1465, 1243, 1206, 1030, 741; ESI FTMS exact mass calcd for $(C_{35}H_{39}NO_3\text{-}H)^-$ requires m/z 520.2857, found m/z 520.2881; The enantiomeric ratio: 85:15, determined by HPLC (Daicel Chiralpak AD-3, hexane/ isopropanol = 98/ 2, flow rate 1.0 mL/min, T = 30 °C, 254 nm): t_R = 17.805 (major), t_R = 21.058 (minor).

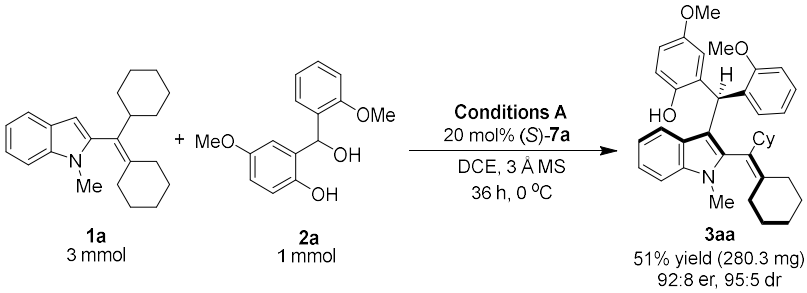
(R_a,*R*)-2-((2-(2,4-dimethylpent-2-en-3-yl)-1-methyl-1H-indol-3-yl)(2-methoxyphenyl)methyl)-4-methoxyphenol (4ga):



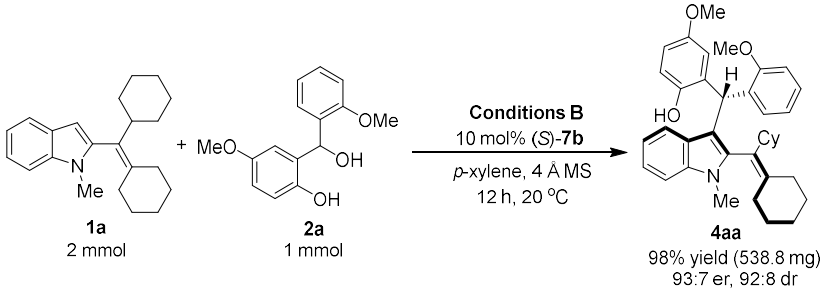
Following the general procedure, 2-alkenylindoles **1g** (68.2 mg, 0.3 mmol), *o*-hydroxybenzyl alcohol **2a** (26.0 mg, 0.1 mmol), CPA (*R*)-**6b** (7.1 mg, 0.01 mmol) and 4 Å MS (100 mg) were added to a reaction tube. Then, mesitylene (4 mL) was added to the reaction mixture, which was stirred at 0 °C for 24 h. After the completion of the reaction indicated by TLC, the reaction mixture was purified through flash column chromatography on silica gel (petroleum ether/ethyl acetate = 5:1) to afford pure product **4ga** in 53% yield (24.9 mg) as colorless oil; >95:5 dr; $[\alpha]_D^{20}$ = +74.5 (c 0.36, acetone); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.32 – 7.27 (m, 1H), 7.26 – 7.21 (m, 1H), 7.21 – 7.12 (m, 2H), 7.04 (d, *J* = 8.0 Hz, 1H), 6.91 – 6.80 (m, 3H), 6.70 – 6.62 (m, 2H), 6.46 (s, 1H), 5.78 (s, 1H), 5.01 (s, 1H), 3.67 (s, 3H), 3.65 (s, 3H), 3.54 (s, 3H), 2.91 – 2.79 (m, 1H), 1.93 (s, 3H), 1.41 (s, 3H), 0.88 (d, *J* = 6.8 Hz, 3H), 0.60 (d, *J* = 6.7 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 157.0, 153.2, 148.8, 139.8, 137.1, 136.9, 131.1, 130.9, 130.5, 130.4, 127.9, 127.8, 121.1, 120.5, 119.5, 116.3, 115.6, 111.9, 110.5, 110.1, 109.3, 55.6, 55.3, 38.5, 31.4, 30.1, 23.1, 21.6, 20.2, 20.1. IR (KBr): 3451, 2922, 2852, 1633, 1468, 1263, 1097,

743; ESI FTMS exact mass calcd for $(C_{31}H_{35}NO_3\text{-}H)^-$ requires m/z 468.2544, found m/z 468.2538; The enantiomeric ratio: 92:8, determined by HPLC (Daicel Chiralpak AD-3, hexane/ isopropanol = 98/ 2, flow rate 1.0 mL/min, T = 30 °C, 254 nm): t_R = 9.836 (minor), t_R = 11.179 (major).

7. Procedure for one-mmol-scale synthesis of product 3aa and 4aa

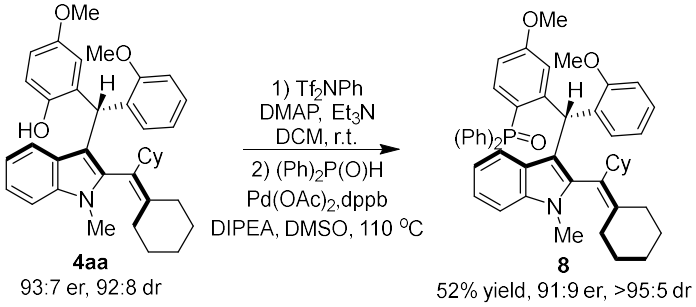


2-Alkenylindoles **1a** (3 mmol), *o*-hydroxybenzyl alcohols **2a** (1 mmol), CPA (*S*)-**7a** (0.2 mmol) and 3 Å MS (1.0 g) were added to a reaction bottle. Then, DCE (20 mL) was added to the reaction mixture, which was stirred at 0 °C for 36 h. After the completion of the reaction indicated by TLC, the reaction mixture was purified through flash column chromatography on silica gel to afford pure product **3aa**.



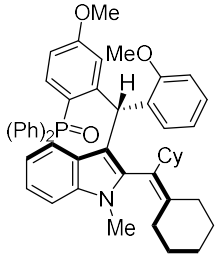
2-Alkenylindoles **1a** (2 mmol), *o*-hydroxybenzyl alcohols **2a** (1 mmol), CPA (*S*)-**7b** (0.1 mmol) and 4 Å MS (1.0 g) were added to a reaction bottle. Then, *p*-xylene (40 mL) was added to the reaction mixture, which was stirred at 20 °C for 12 h. After the completion of the reaction indicated by TLC, the reaction mixture was purified through flash column chromatography on silica gel to afford pure product **4aa**.

8. Procedure for the synthesis of 8-10, 13 and characterization data

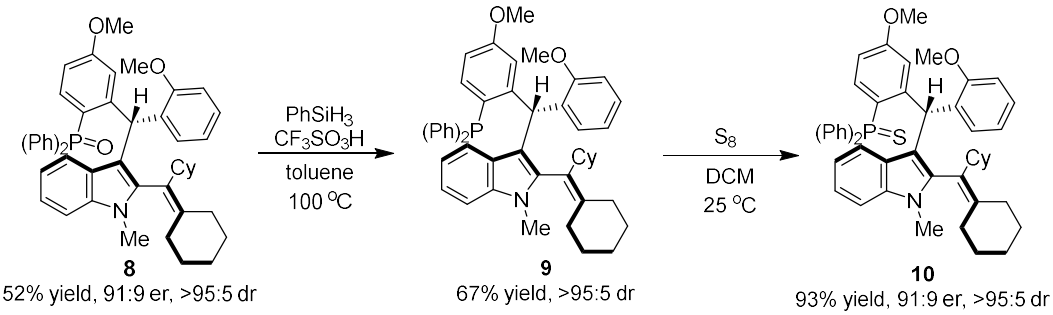


4aa (164.8 mg, 0.3 mmol) was dissolved in DCM (3 mL), which was added DMAP (73.6 mg, 0.6 mmol) and Et_3N (0.13 mL, 0.9 mmol). Then, Tf_2NPh (160.8 mg, 0.45 mmol) in DCM (1 mL) was added to the reaction mixture, which was further stirred at 25 °C for 1 h. After the completion of the reaction indicated by TLC, the reaction mixture was concentrated under reduced pressure to afford crude product. Under argon atmosphere, DMSO (3 mL) was added to the mixture of previous crude product, $Ph_2P(O)H$ (42.5 mg, 0.21 mmol), $Pd(OAc)_2$ (13.5 mg, 0.06 mmol) and dppb (25.5 mg, 0.06 mmol). Then, DIPEA (2.6 mL, 1.5 mmol) was added to the reaction mixture, which was stirred at 110 °C for 24 h. After the completion of the reaction which was indicated by TLC, the reaction mixture was diluted with DCM and quenched with hydrochloric acid (1 M). The resultant mixture was extracted with DCM, 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 through flash column chromatography (petroleum ether/ethyl acetate = 4:1) on silica gel to afford pure products **8** as single configuration.

(*R*$_a$,*S*)-(2-((2-(cyclohexyl(cyclohexylidene)methyl)-1-methyl-1H-indol-3-yl)(2-methoxyphenyl) methyl)-4-methoxyphenyl)diphenylphosphine oxide (8):

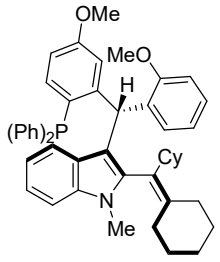


Yield: 52% (114.5 mg); white solid; m.p. 156.2-157.4 °C; >95:5 dr; $[\alpha]_D^{20}$ = +100.1 (c 0.25, acetone); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.64 – 7.57 (m, 2H), 7.50 – 7.45 (m, 1H), 7.43 – 7.37 (m, 2H), 7.26 – 7.22 (m, 2H), 7.20 – 7.13 (m, 2H), 7.06 – 6.94 (m, 5H), 6.88 – 6.81 (m, 2H), 6.67 – 6.52 (m, 4H), 6.48 – 6.40 (m, 2H), 3.54 (s, 3H), 3.51 (s, 3H), 3.42 (s, 3H), 2.96 – 2.87 (m, 1H), 2.54 – 2.46 (m, 1H), 2.34 – 2.28 (m, 1H), 2.23 – 2.16 (m, 1H), 1.81 – 1.67 (m, 4H), 1.51 – 1.37 (m, 5H), 1.33 – 1.28 (m, 2H), 1.23 – 1.10 (m, 3H), 0.98 – 0.76 (m, 3H), 0.71 – 0.62 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 157.9, 143.4, 136.4, 132.1, 132.0, 131.8, 131.5, 131.4, 130.8, 129.0, 128.3, 128.2, 127.3, 127.2, 127.1, 119.8, 119.4, 118.9, 118.4, 113.4, 110.3, 108.6, 55.0, 54.8, 41.3, 33.2, 33.0, 31.4, 30.8, 29.7, 28.0, 27.3, 27.3, 26.7, 26.4; ^{31}P NMR (162 MHz, $CDCl_3$) δ 29.36; IR (KBr): 3390, 2929, 2813, 2715, 1632, 1597, 1382, 1350, 1116, 776; ESI FTMS exact mass calcd for $(C_{49}H_{52}NO_3P+Na)^+$ requires m/z 756.3577, found m/z 756.3581; The enantiomeric ratio: 91:9, determined by HPLC (Daicel Chiralpak IG, hexane/ isopropanol = 98/ 2, flow rate 1.0 mL/min, T = 30 °C, 254 nm): t_R = 17.076 (minor), t_R = 21.163 (major).



Under argon atmosphere, compound **8** (73.4 mg, 0.1 mmol) was dissolved in anhydrous toluene (1 mL), which was added $PhSiH_3$ (49 μL, 0.4 mmol) and CF_3SO_3H (1.6 μL, 0.02 mmol). Then, the reaction mixture was heated to 100 °C for 12 h. After the completion of the reaction which was indicated by TLC, the reaction mixture was quenched with saturated $NaHCO_3$ aqueous solution. The organic layer was dried over anhydrous Na_2SO_4 and concentrated in vacuo to give a residue, which was further purified by preparative thin layer chromatography on silica gel (petroleum ether/ethyl acetate = 10:1) to afford compound **9**.

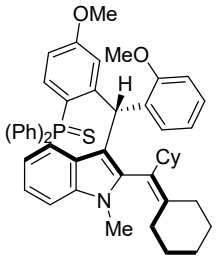
(R_a,*S*)-2-(cyclohexyl(cyclohexylidene)methyl)-3-((2-(diphenylphosphaneyl)-5-methoxyphenyl) (2-methoxyphenyl)methyl)-1-methyl-1H-indole (9):



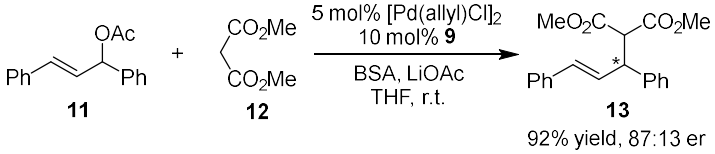
Yield: 67% (48.2 mg); colorless oil; >95:5 dr; $[\alpha]_D^{20}$ = +118.7 (c 0.20, acetone); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.33 – 7.27 (m, 3H), 7.25 – 7.15 (m, 3H), 7.11 – 6.98 (m, 6H), 6.91 – 6.84 (m, 2H), 6.76 (d, *J* = 7.4 Hz, 1H), 6.73 – 6.58 (m, 7H), 3.56 (s, 3H), 3.52 (s, 3H), 3.51 (s, 3H), 2.63 – 2.55 (m, 1H), 2.36 – 2.26 (m, 1H), 2.06 – 1.99 (m, 1H), 1.85 – 1.75 (m, 2H), 1.72 – 1.60 (m, 4H), 1.50 – 1.41 (m, 3H), 1.34 – 1.29 (m, 3H), 1.24 – 1.15 (m, 2H), 1.03 – 0.84 (m, 3H), 0.74 – 0.64 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.1, 157.8, 152.5, 143.8, 139.5, 139.2, 138.2, 136.7, 136.4, 133.6, 133.4, 133.4, 133.2, 132.5, 131.7, 128.8, 128.1, 127.7, 127.6, 127.2, 126.7, 126.5, 120.0, 119.6, 119.4, 118.5, 117.3, 113.1, 111.3, 110.5, 108.6, 55.2, 54.9, 42.2, 42.0, 41.8, 33.2, 33.0, 31.0, 30.5, 29.7, 27.9, 27.4, 27.3, 27.1, 26.6, 26.1; ^{31}P NMR (162 MHz, $CDCl_3$) δ -20.13; IR (KBr): 3421, 2926, 2849, 1632, 1598, 1382, 1352, 1116, 910, 746, 618. ESI FTMS exact mass calcd for $(C_{49}H_{52}NO_2P+H)^+$ requires m/z 718.3809, found m/z 718.3812.

To the solution of **9** (71.8 mg, 0.1 mmol) in DCM (1 mL) was added sulfur (4.8 mg, 0.15 mmol). Then, the reaction mixture was stirred at 25 °C for 10 min. After the completion of the reaction which was indicated by TLC, the reaction mixture was purified through preparative thin layer chromatography on silica gel (petroleum ether/ethyl acetate = 5:1) to afford pure product **10**.

(R_a,*S*)-(2-((2-(cyclohexyl(cyclohexylidene)methyl)-1-methyl-1H-indol-3-yl)(2-methoxyphenyl) methyl)-4-methoxyphenyl)diphenylphosphine sulfide (10):

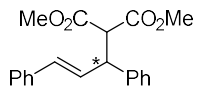


Yield: 93% (69.7 mg); colorless oil; >95:5 dr; $[\alpha]_D^{20}$ = +104.7 (c 0.22, acetone); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.78 – 7.68 (m, 2H), 7.52 – 7.44 (m, 2H), 7.44 – 7.33 (m, 3H), 7.16 (d, *J* = 8.1 Hz, 1H), 7.13 – 7.07 (m, 1H), 7.06 – 6.89 (m, 6H), 6.87 – 6.81 (m, 1H), 6.70 (d, *J* = 7.6 Hz, 1H), 6.64 – 6.53 (m, 3H), 6.33 – 6.23 (m, 2H), 3.54 (s, 3H), 3.50 (s, 3H), 3.29 (s, 3H), 3.08 – 2.99 (m, 1H), 2.59 – 2.49 (m, 2H), 2.25 – 2.17 (m, 1H), 1.89 – 1.72 (m, 4H), 1.70 – 1.65 (m, 1H), 1.52 – 1.39 (m, 4H), 1.36 – 1.30 (m, 1H), 1.26 – 1.17 (m, 3H), 1.13 – 1.05 (m, 1H), 0.89 – 0.79 (m, 2H), 0.65 – 0.56 (m, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 157.8, 143.3, 139.7, 136.4, 135.9, 135.7, 132.3, 132.2, 131.2, 131.0, 130.6, 130.4, 129.1, 128.3, 128.1, 127.3, 127.1, 127.0, 126.9, 119.8, 119.4, 118.8, 118.4, 113.8, 110.2, 110.1, 109.9, 108.6, 55.0, 54.5, 41.6, 40.5, 34.5, 33.2, 31.1, 31.0, 30.9, 28.0, 27.6, 27.4, 26.7, 26.6; ^{31}P NMR (162 MHz, $CDCl_3$) δ 41.12; IR (KBr): 3432, 2920, 1667, 1589, 1388, 1265, 1116, 912, 747; ESI FTMS exact mass calcd for $(C_{49}H_{52}NO_2PS+Na)^+$ requires m/z 772.3348, found m/z 772.3325; The enantiomeric ratio: 91:9, determined by HPLC (Daicel Chiralpak AD-3, hexane/ isopropanol = 98/ 2, flow rate 0.3 mL/min, T = 30 °C, 254 nm): t_R = 21.923 (minor), t_R = 27.363 (major).



Under argon atmosphere, to the mixture of chiral phosphine ligand **9** (7.8 mg, 0.01 mmol), $[Pd(allyl)Cl]_2$ (18.3 mg, 0.005 mmol) and LiOAc (2.6 mg, 0.04 mmol) in THF (1 mL) were added allylic ester **11** (25.2 mg, 0.1 mmol), which was stirred at room temperature for 30 min. Then, dimethyl malonate **12** (39.6 mg, 0.3 mmol) and *N*,*O*-bis(trimethylsilyl)acetamide (BSA, 61.0 mg, 0.3 mmol) was added and the reaction mixture was stirred at 25 °C for 12 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 preparative thin layer chromatography on silica gel (petroleum ether/ethyl acetate = 4:1) to afford product **13**.

dimethyl (E)-2-(1,3-diphenylallyl)malonate (13):

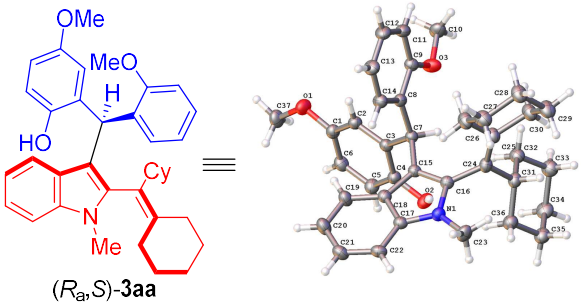


Yield: 92% (29.8 mg); colorless oil; $[\alpha]_D^{20}$ = -13.6 (c 0.26, acetone); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.37 – 7.27 (m, 7H), 7.27 – 7.18 (m, 3H), 6.49 (d, *J* = 15.7 Hz, 1H), 6.39 – 6.27 (m, 1H), 4.34 – 4.22 (m, 1H), 3.96 (d, *J* = 12.3 Hz, 1H), 3.71 (s, 3H), 3.52 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 168.2, 167.8, 140.2, 136.9, 131.9, 129.2, 128.8, 128.5, 127.9, 127.6, 127.2, 126.4, 57.7, 52.7, 52.5, 49.2; IR (KBr): 3396, 2921, 2754, 1736, 1596, 1389, 1265, 1115, 745; ESI FTMS exact mass calcd for $(C_{20}H_{20}O_4+Na)^+$ requires m/z 347.1254, found m/z 347.1242; The enantiomeric ratio: 87:13, determined by HPLC (Daicel Chiralpak ID, hexane/ isopropanol = 70/ 30, flow rate 1.0 mL/min, T = 30 °C, 254 nm): t_R = 8.676(major), t_R = 18.413 (minor).

9. Determination of the absolute configurations of products 3 and 4

Determination of the absolute configuration of products 3:

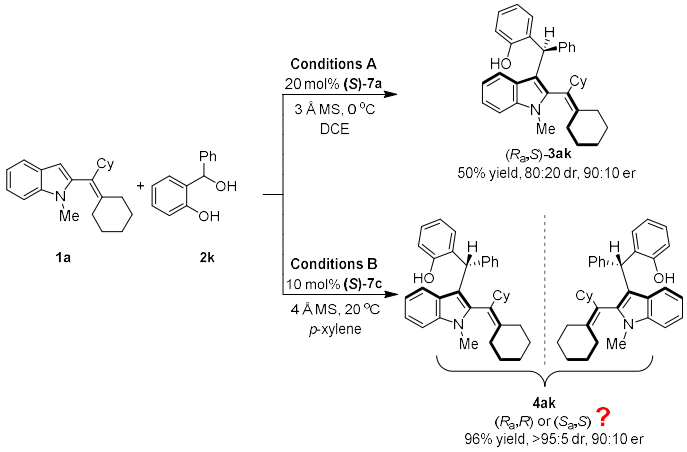
The absolute configuration of **3aa** was determined to be (*R*a,*S*) by single-crystal X-ray diffraction analysis. Products **3** were synthesized in the presence of the same chiral phosphoric acid (*S*)-**7a**, so the absolute configurations of products **3** were deduced to be (*R*a,*S*) by analogy with **3aa**.



Determination of the absolute configuration of products 4:

The absolute configuration of **4ak** was determined as (R_a,*R*) by comparison its HPLC trace with that of a known chiral compound.

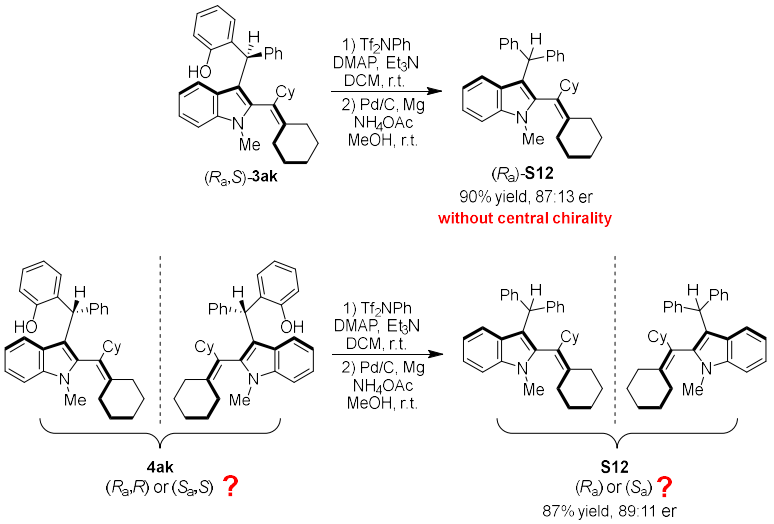
The details are as follows:



According to the general procedure **A**, we utilized the reaction of C3-unsubstituted 2-alkenylindole **1a** and *o*-hydroxybenzyl alcohol **2k** under the catalysis of (*S*)-**7a** to synthesize (R_a,*S*)-**3ak** in 50% yield with 80:20 dr and 90:10 er. According to the general procedure **B**, we utilized the reaction of C3-unsubstituted 2-alkenylindole **1a** and *o*-hydroxybenzyl alcohol **2k** under the catalysis of (*S*)-**7c** to synthesize **4ak** in 96% yield with >95:5 dr and 90:10 er. Product **4ak** was the diastereoisomer of product (R_a,*S*)-**3ak**, so the absolute configuration of **4ak** was deduced to be (R_a,*R*) or (S_a,*S*).

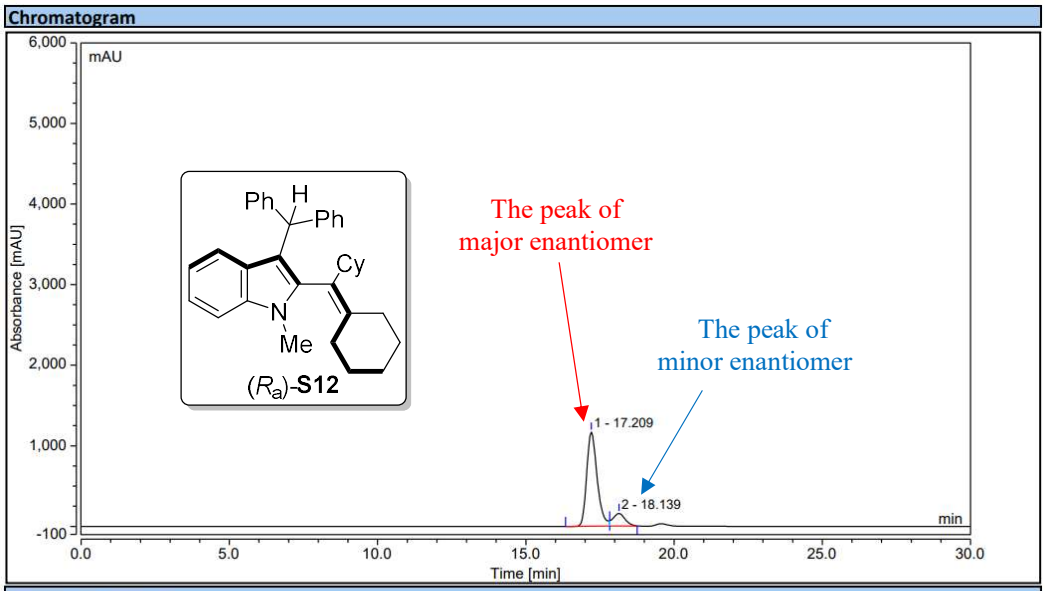
Compound (R_a,*S*)-**3ak** bearing axial and central chirality could be easily transformed into compound (R_a)-**S12** only bearing axial chirality in 90% yield with 87:13 er. In addition, compound **4ak** could be transformed

into compound **S12** in 87% yield with 89:11 er.



Then, we compared the HPLC trace of compound (R_a)-**S12** with that of compound **S12**. Obviously, in the two cases, the retention time for the peak of the major enantiomer and that of the minor enantiomer are similar. As shown below, in the HPLC trace of compound (R_a)-**S12**, the retention time for the peak of the major enantiomer is around 17.2 min, and that of the minor enantiomer is around 18.1 min (**Figure S1**). Similarly, in the HPLC trace of compound **S13**, the retention time for the peak of the major enantiomer is around 16.8 min, and that of the minor enantiomer is around 17.6 min (**Figure S2**).

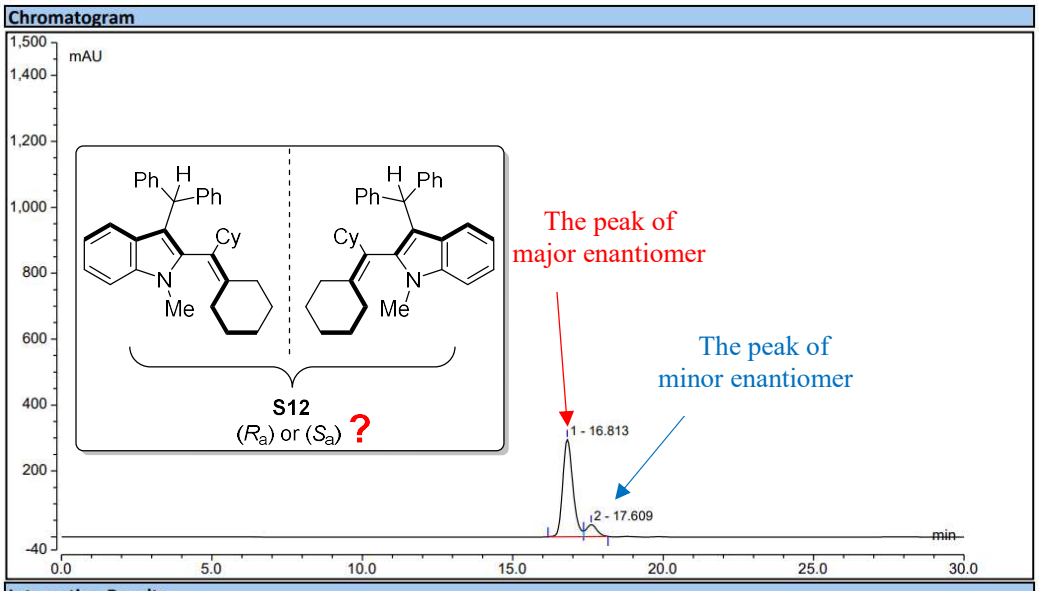
This result demonstrates that compound (R_a)-**S12** and compound **S12** have the same absolute configuration. Therefore, the absolute configuration of compound **S12** was determined to be (R_a), and the absolute configuration of **4ak** was deduced to be (R_a,*R*) by analogy with **S12**. Products **4** were synthesized in the presence of the same type of chiral phosphoric acid (*S*)-**7b** or (*S*)-**7c**, so the absolute configurations of products **4** were deduced to be (*R*a,*R*) by analogy with **4ak**.



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		17.209	478.069	1169.619	86.78	88.21	n.a.
2		18.139	72.854	156.292	13.22	11.79	n.a.
Total:			**550.923**	**1325.911**	**100.00**	**100.00**	

Figure S1. HPLC trace of (R_a)-**S12**

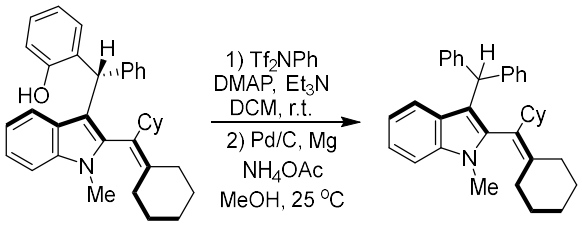


Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
n.a.		16.813	115.370	295.712	88.70	89.13	n.a.
n.a.		17.609	14.699	36.050	11.30	10.87	n.a.
Total:			**130.069**	**331.762**	**100.00**	**100.00**	

Figure S2. HPLC trace of **12**

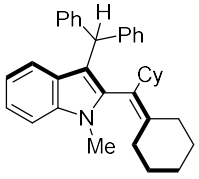
10. Synthetic procedure and characterization data of products S12



4ak **S12**
87% yield, 89:11 er

4ak (49.0 mg, 0.1 mmol) was dissolved in DCM (1 mL), which was added DMAP (24.5mg, 0.2 mmol) and Et_3N (43 μL, 0.3 mmol). Then, Tf_2NPh (53.6 mg, 0.15 mmol) in DCM (1 mL) was added to the reaction mixture, which was further stirred at 25 °C for 1 h. After the completion of the reaction indicated by TLC, the reaction mixture was concentrated under reduced pressure to afford crude product. Under argon atmosphere, methanol (2 mL) was added to the mixture of crude product, Mg (24 mg, 1 mmol), Pd/C (63.6 mg, 0.6 mmol), and ammonium acetate (154 mg, 2 mmol). After the mixture had been stirred at room temperature overnight and the completion of the reaction indicated by TLC, the reaction mixture was filtered, and the filtrate was concentrated under the reduced pressure to give the residue, which was then added to water (5 mL), extracted by ethyl acetate, and dried by anhydrous Na_2SO_4. The resultant organic layer was again concentrated under reduced pressure to give pure products **S12**.

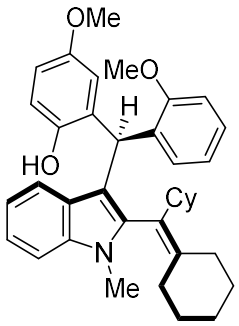
(R_a)-3-benzhydryl-2-(cyclohexyl(cyclohexylidene)methyl)-1-methyl-1H-indole (S12):



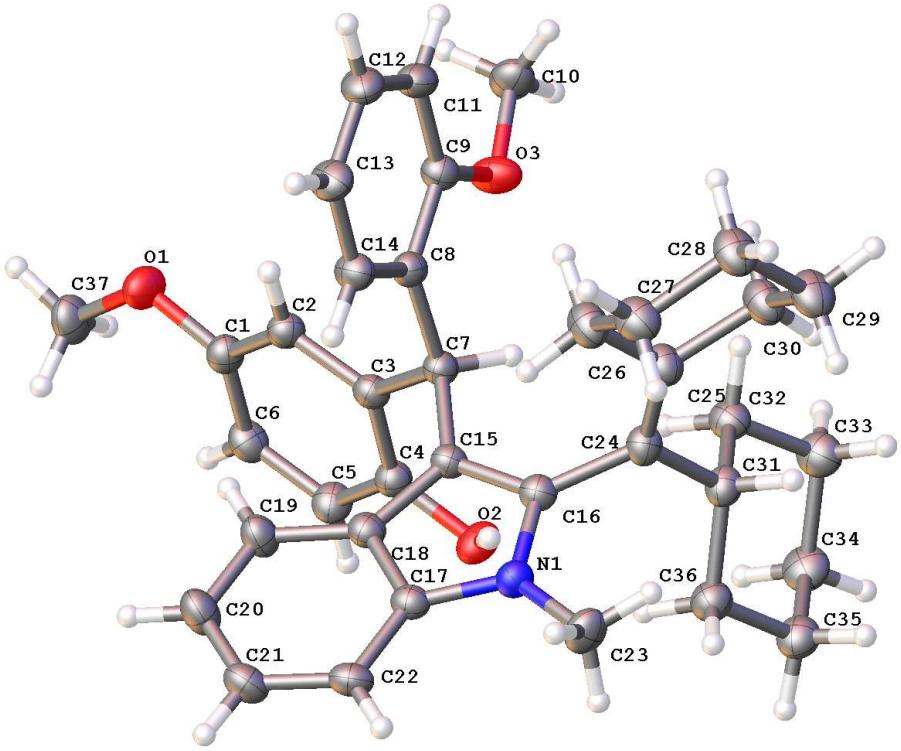
Yield: 87% (41.2 mg); colorless oil; $[\alpha]_D^{20}$ = -7.1 (c 0.56, acetone); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.31 – 7.27 (m, 1H), 7.26 – 7.22 (m, 4H), 7.22 – 7.08 (m, 7H), 6.97 – 6.91 (m, 1H), 6.90 – 6.83 (m, 1H), 5.59 (s, 1H), 3.58 (s, 3H), 2.71 – 2.59 (m, 1H), 2.52 – 2.42 (m, 1H), 2.38 – 2.28 (m, 1H), 1.72 – 1.56 (m, 5H), 1.54 – 1.41 (m, 6H), 1.25 – 1.08 (m, 5H), 0.94 – 0.85 (m, 1H), 0.74 – 0.59 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 145.0, 144.3, 139.5, 136.9, 129.5, 129.4, 128.0, 127.5, 126.8, 125.8, 125.7, 121.0, 120.3, 118.8, 114.0, 109.1, 48.5, 40.9, 33.2, 33.1, 31.3, 30.7, 30.4, 28.4, 27.6, 26.8, 26.7, 25.9; IR (KBr): 3447, 2925, 2851, 2085, 1636, 1466, 1263, 741; ESI FTMS exact mass calcd for $(C_{35}H_{39}N+H)^+$ requires m/z 474.3156, found m/z 474.3162; The enantiomeric ratio: 89:11, determined by HPLC (Daicel Chiralpak AD-3, hexane/ isopropanol = 99.8/0.2, flow rate 0.2 mL/min, T = 30 °C, 254 nm): t_R = 16.813 (major), t_R = 17.609 (minor).

11. X-ray single crystal data for compounds 3aa and *rac*-4ak

X-ray single crystal data for compound 3aa:



(R_a,*S*)-**3aa**

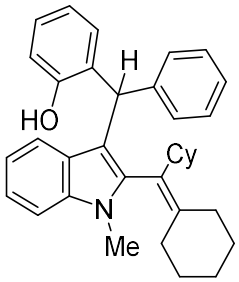


The X-ray source used for the single crystal X-ray diffraction analysis of compound **3aa** was GaKα (λ = 1.34139), and the thermal ellipsoid was drawn at the 30% probability level.

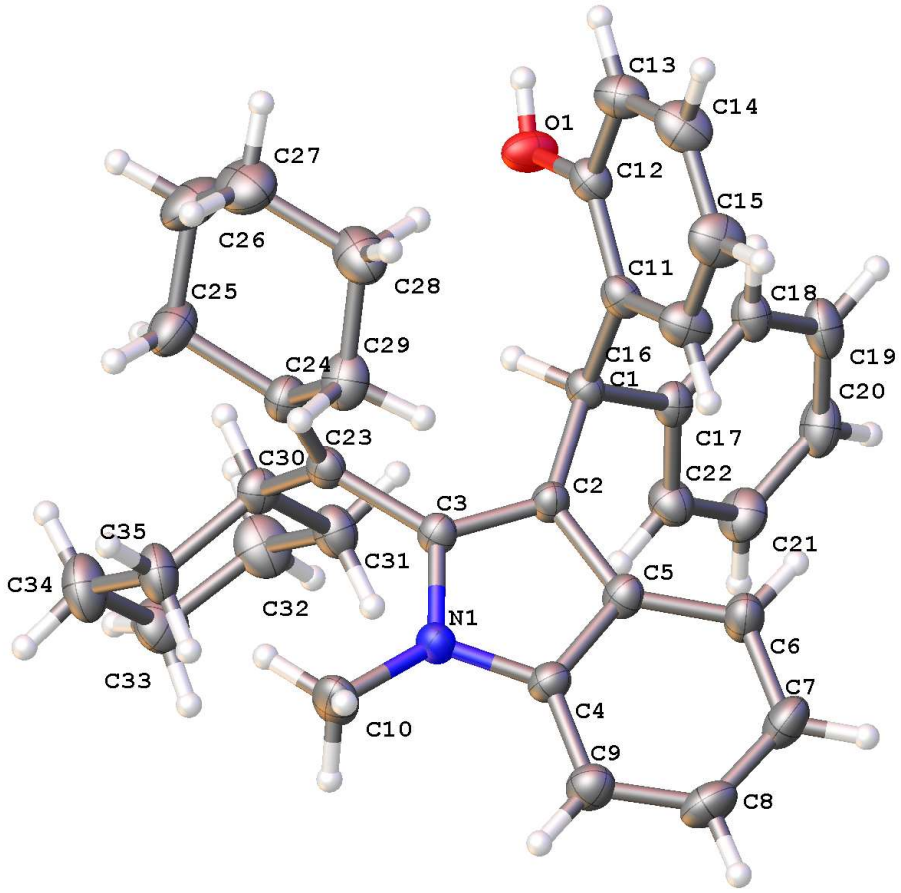
Empirical formula	$C_{37}H_{43}NO_3$
Formula weight	549.72
Temperature/K	213.00
Crystal system	orthorhombic

Space group	$P2_12_12_1$
a/Å	8.6573(3)
b/Å	15.4579(5)
c/Å	22.6451(8)
α/°	90
β/°	90
γ/°	90
Volume/Å^3	3030.45(18)
Z	4
ρ_{calc}g/cm^3	1.205
μ/mm^{-1}	0.373
F(000)	1184.0
Crystal size/mm^3	0.07 × 0.07 × 0.05
Radiation	GaKα (λ = 1.34139)
2Θ range for data collection/°	6.022 to 109.784
Index ranges	$-10 \leqslant h \leqslant 10, -18 \leqslant k \leqslant 18, -25 \leqslant l \leqslant 27$
Reflections collected	32877
Independent reflections	5766 [R_{int} = 0.0593, R_{sigma} = 0.0394]
Data/restraints/parameters	5766/1/377
Goodness-of-fit on F^2	1.098
Final R indexes [I>=2σ (I)]	R_1 = 0.0526, wR_2 = 0.1377
Final R indexes [all data]	R_1 = 0.0627, wR_2 = 0.1479
Largest diff. peak/hole / e Å^{-3}	0.30/-0.23
Flack parameter	0.08(13)

X-ray single crystal data for compound *rac*-4ak:



***rac*-4ak**



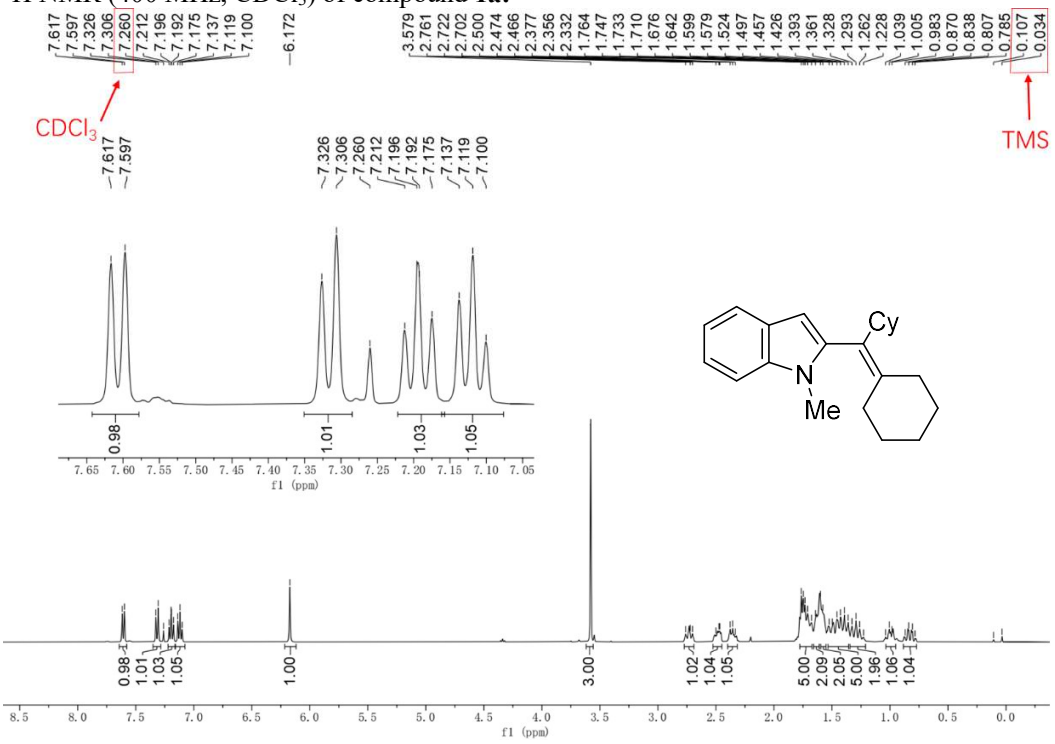
The X-ray source used for the single crystal X-ray diffraction analysis of compound ***rac*-4ak** was GaKα (λ = 1.34139), and the thermal ellipsoid was drawn at the 30% probability level.

Empirical formula	$C_{35}H_{39}NO$
Formula weight	489.30
Temperature/K	213.00
Crystal system	monoclinic

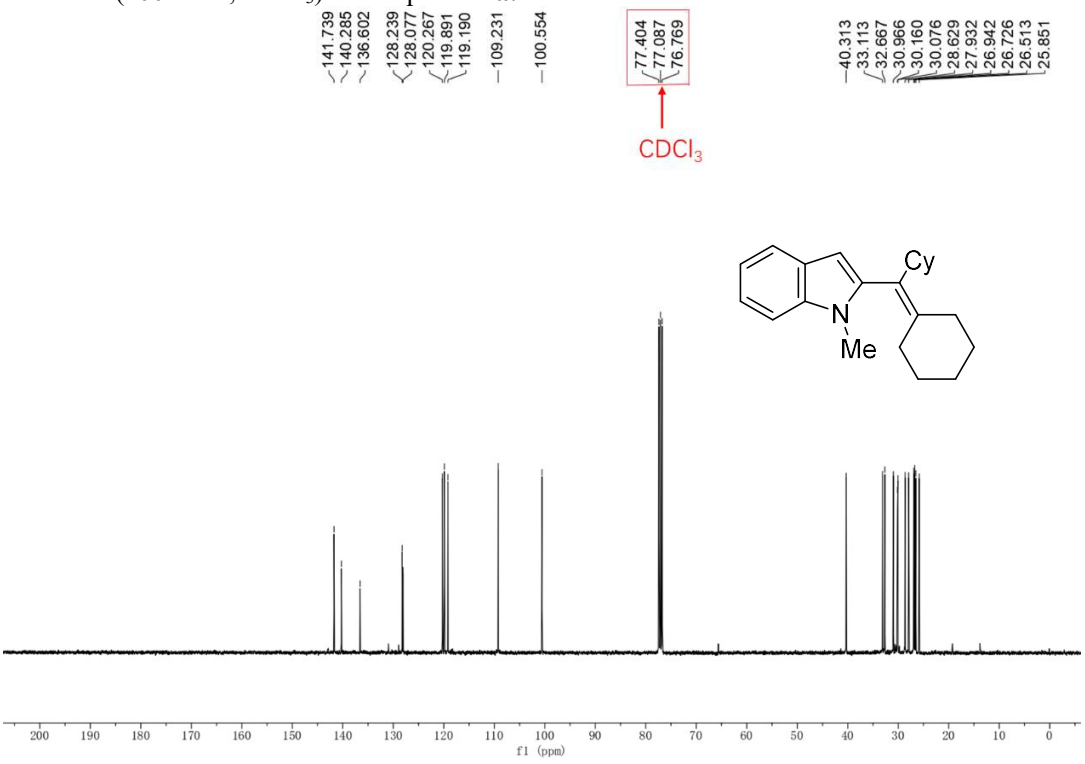
Space group	$P2_1/c$
a/Å	23.0178(8)
b/Å	14.5823(5)
c/Å	23.1103(8)
α/°	90
β/°	117.911(2)
γ/°	90
Volume/Å^3	6854.7(4)
Z	8
ρ_{calc}g/cm^3	1.007
μ/mm^{-1}	0.293
F(000)	2248.0
Crystal size/mm^3	0.07 × 0.07 × 0.05
Radiation	GaKα (λ = 1.34139)
2Θ range for data collection/°	5.272 to 109.93
Index ranges	$-28 \leq h \leq 28$, $-13 \leq k \leq 17$, $-28 \leq l \leq 28$
Reflections collected	56358
Independent reflections	13259 [R_{int} = 0.0815, R_{sigma} = 0.0743]
Data/restraints/parameters	13259/157/757
Goodness-of-fit on F^2	1.134
Final R indexes [I>=2σ (I)]	R_1 = 0.0993, wR_2 = 0.2842
Final R indexes [all data]	R_1 = 0.1465, wR_2 = 0.3249
Largest diff. peak/hole / e Å^{-3}	0.79/-0.45

12. NMR spectra of substrates 1

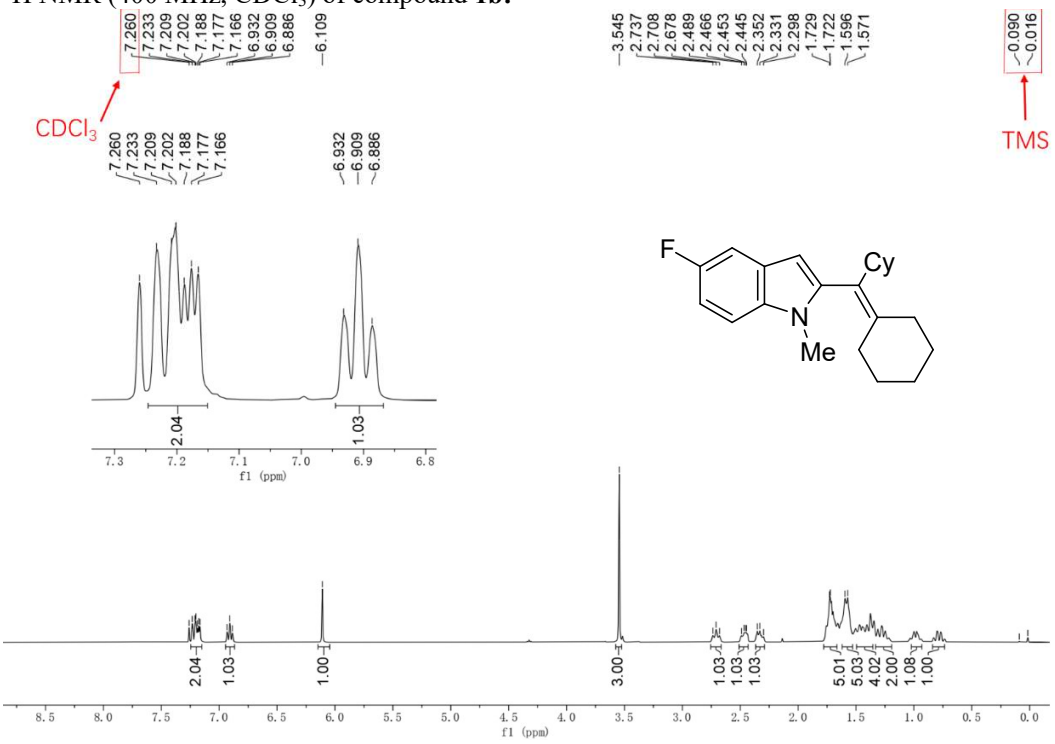
^{1}H NMR (400 MHz, $CDCl_3$) of compound **1a:**



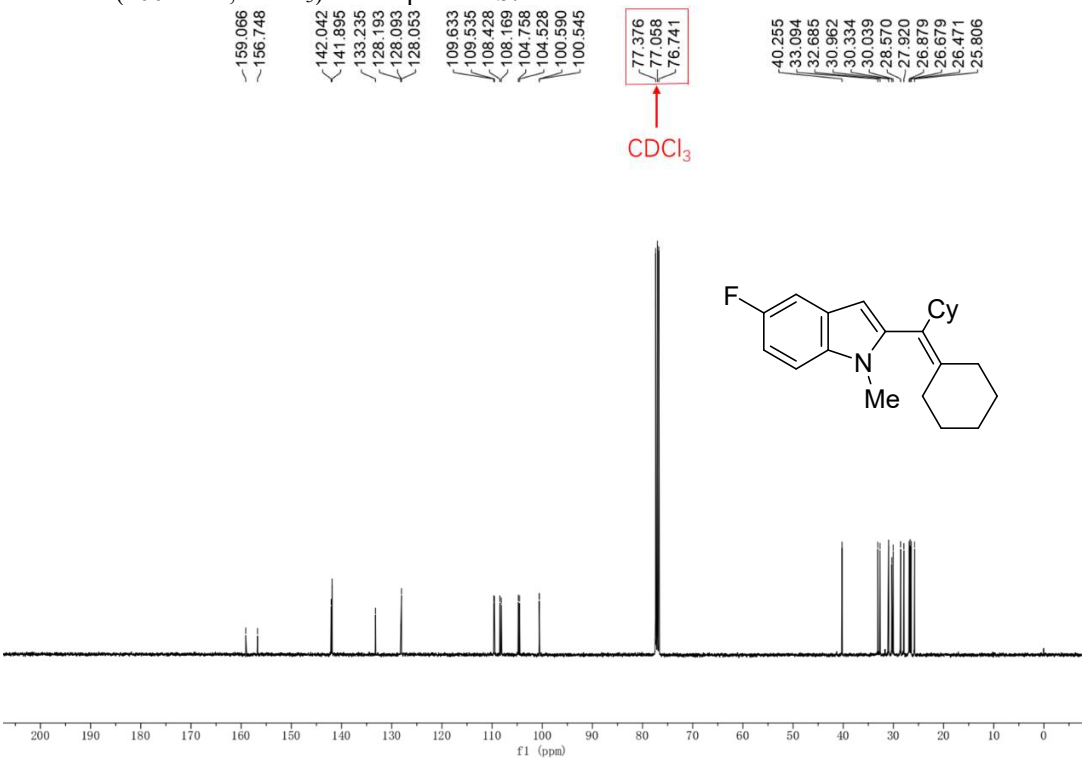
^{13}C NMR (100 MHz, $CDCl_3$) of compound **1a:**



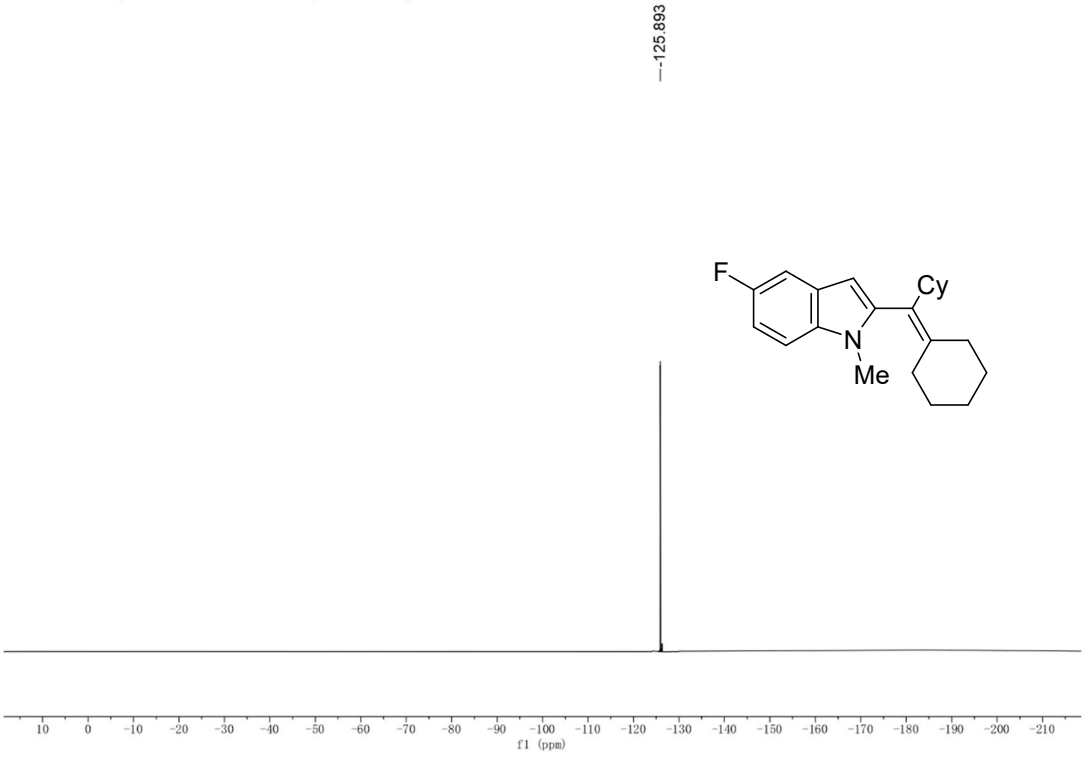
^{1}H NMR (400 MHz, $CDCl_3$) of compound **1b:**



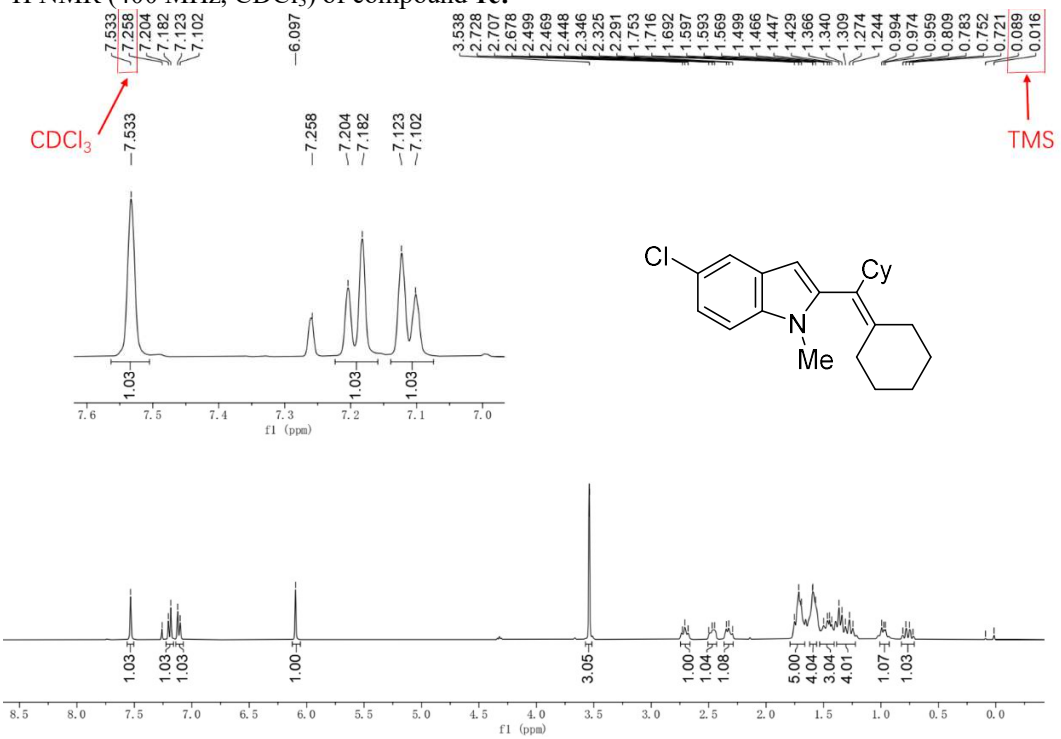
^{13}C NMR (100 MHz, $CDCl_3$) of compound **1b:**



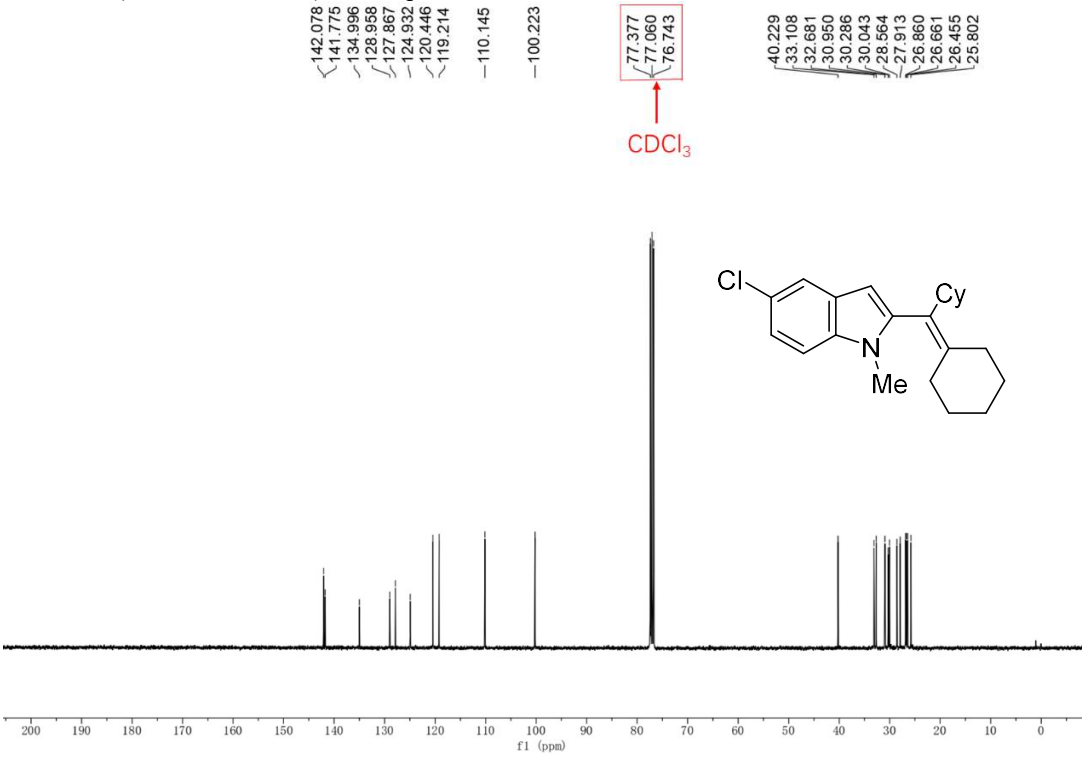
^{19}F NMR (376 MHz, $CDCl_3$) of compound **1b:**



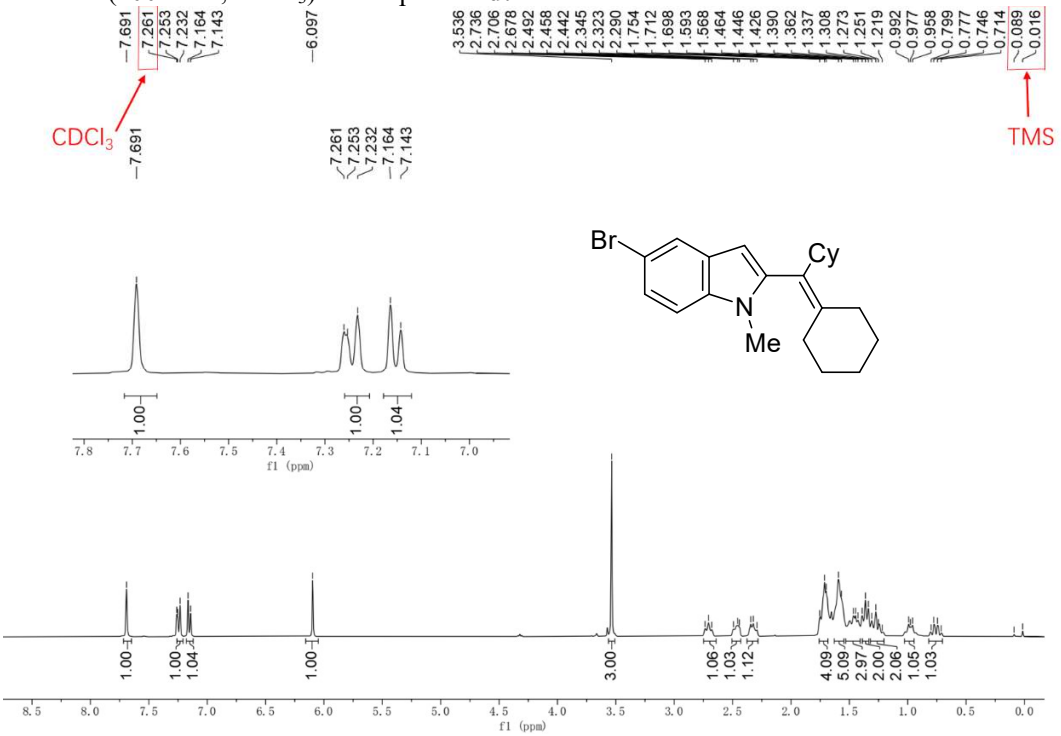
^{1}H NMR (400 MHz, $CDCl_3$) of compound **1c:**



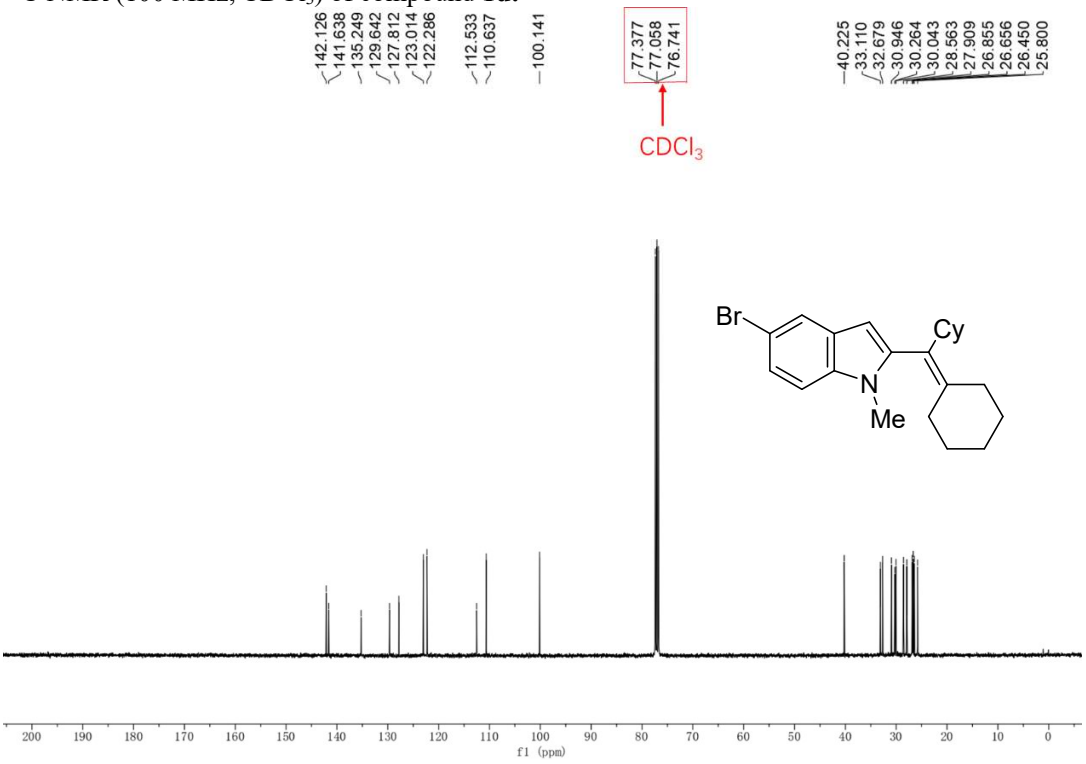
^{13}C NMR (100 MHz, $CDCl_3$) of compound **1c:**



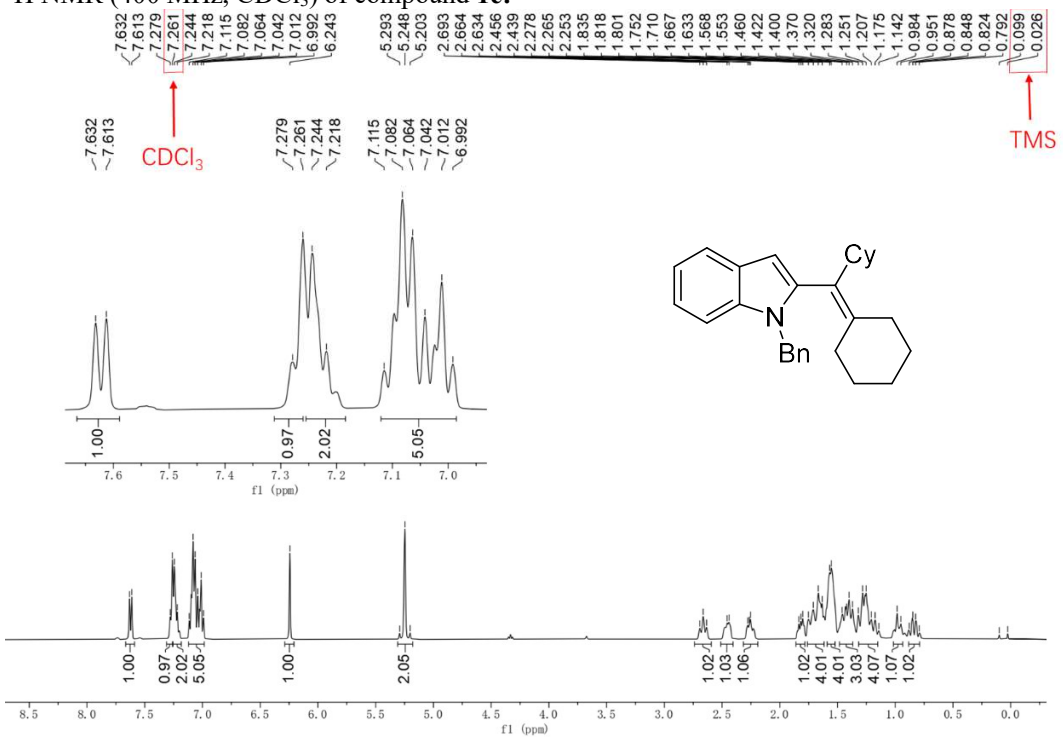
^{1}H NMR (400 MHz, $CDCl_3$) of compound **1d:**



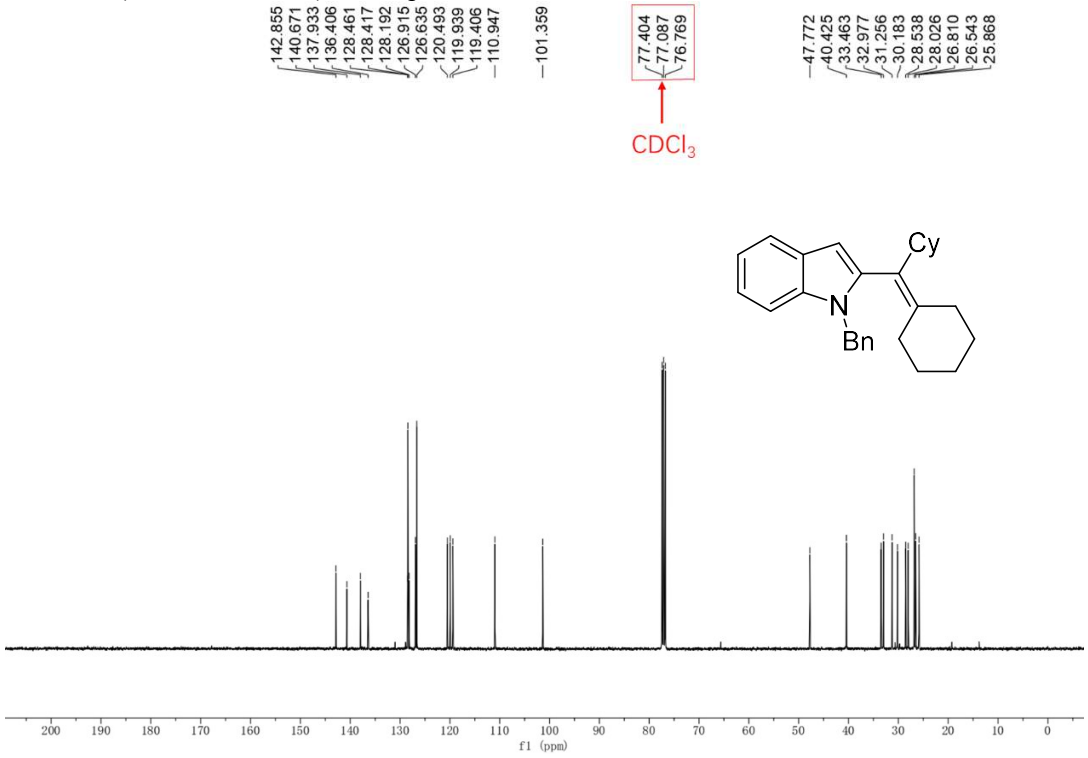
^{13}C NMR (100 MHz, $CDCl_3$) of compound **1d:**



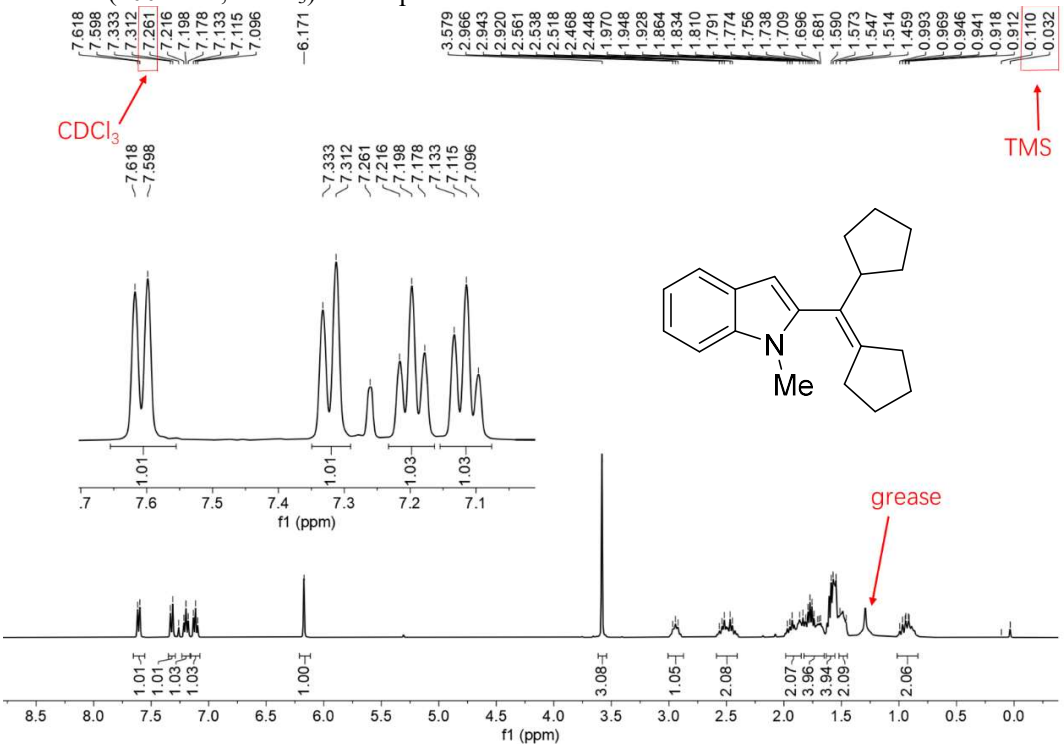
^{1}H NMR (400 MHz, $CDCl_3$) of compound **1e:**



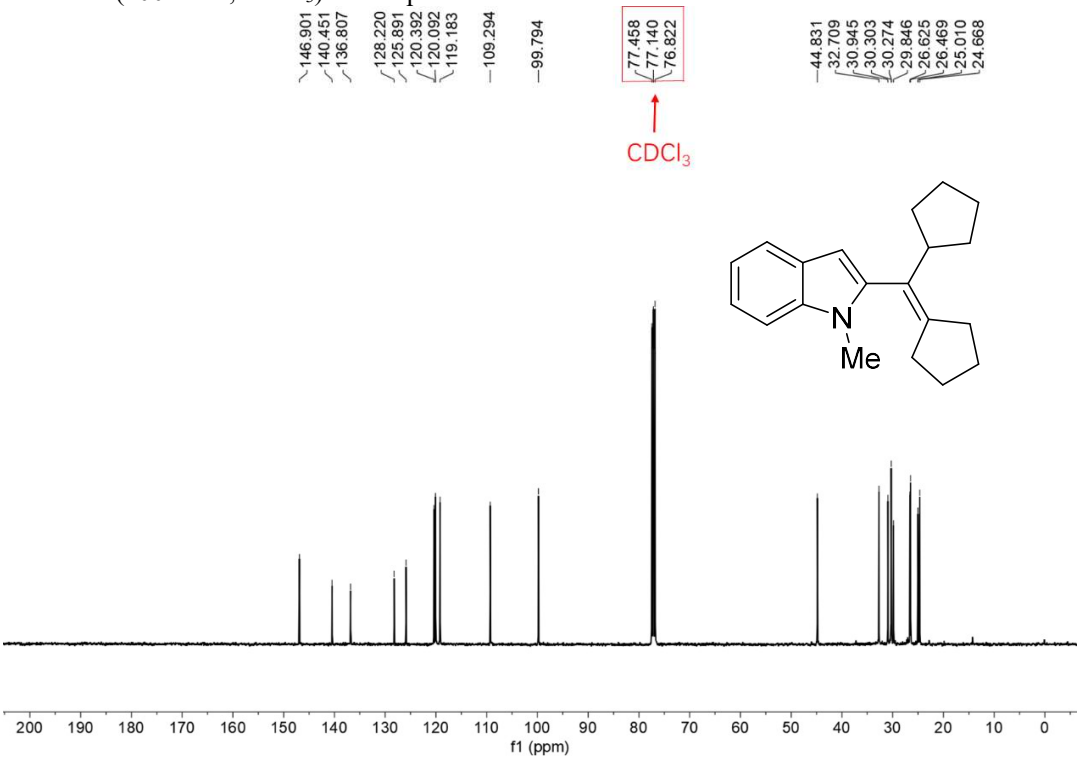
^{13}C NMR (100 MHz, $CDCl_3$) of compound **1e:**



^{1}H NMR (400 MHz, $CDCl_3$) of compound **1f**:

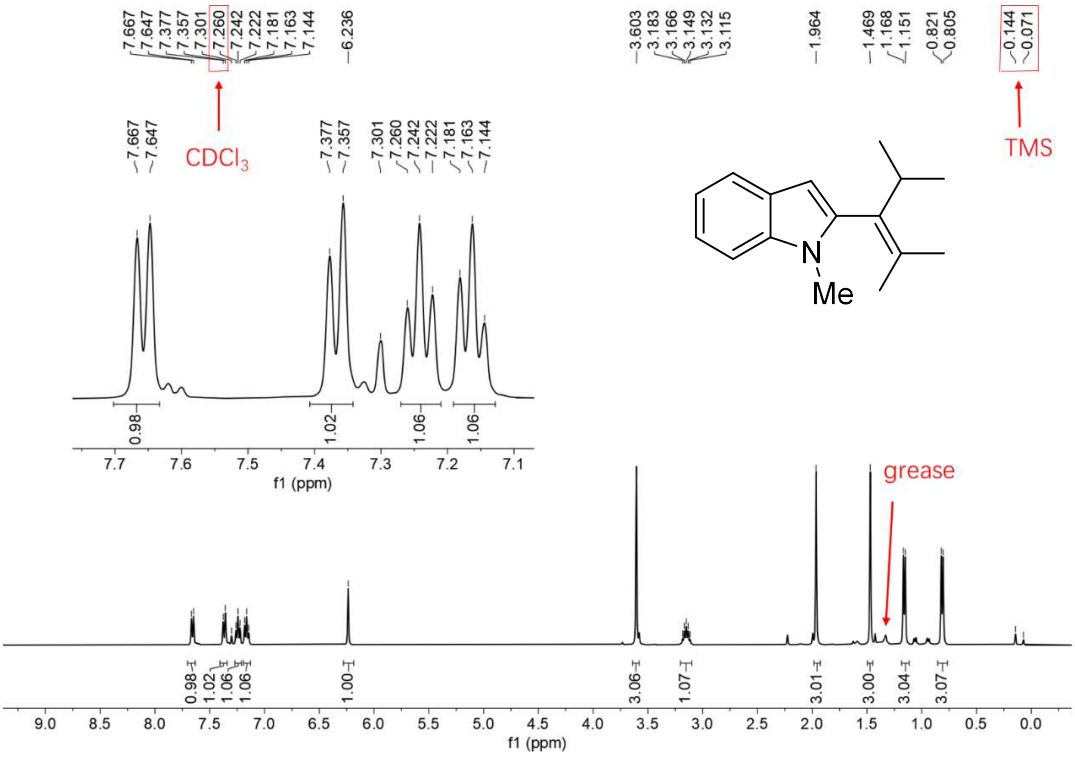


^{13}C NMR (100 MHz, $CDCl_3$) of compound **1f**:

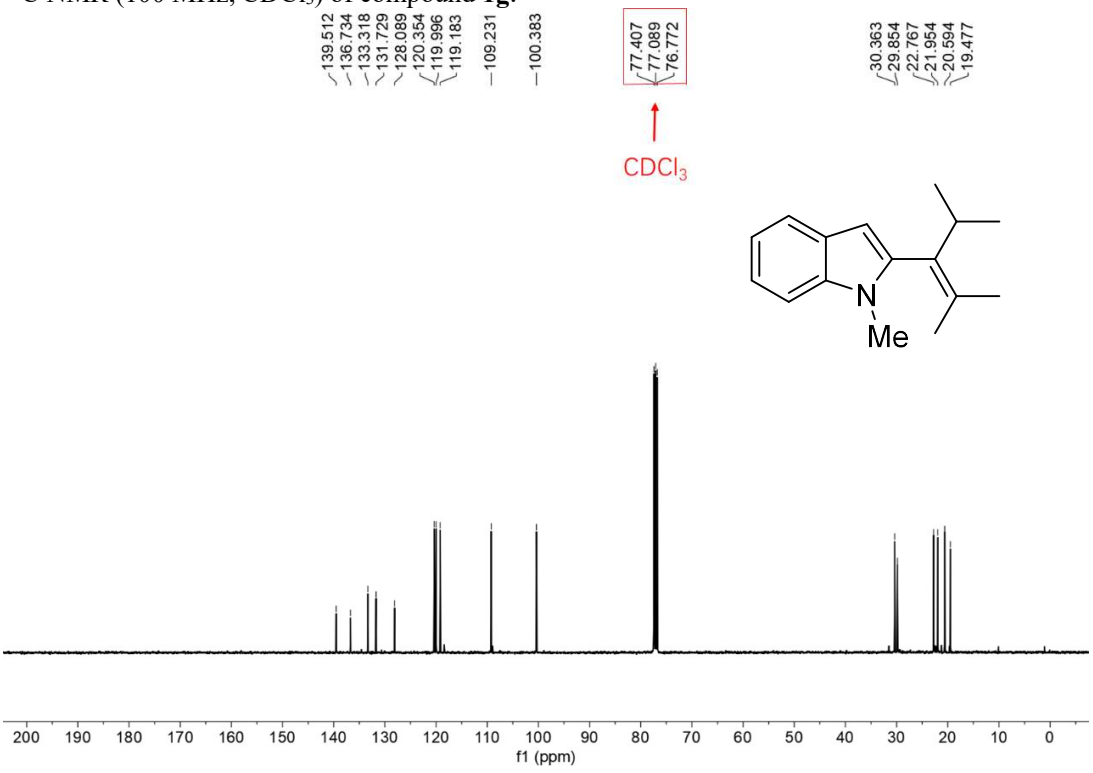


^{1}H NMR (400 MHz, $CDCl_3$) of compound **1g**:

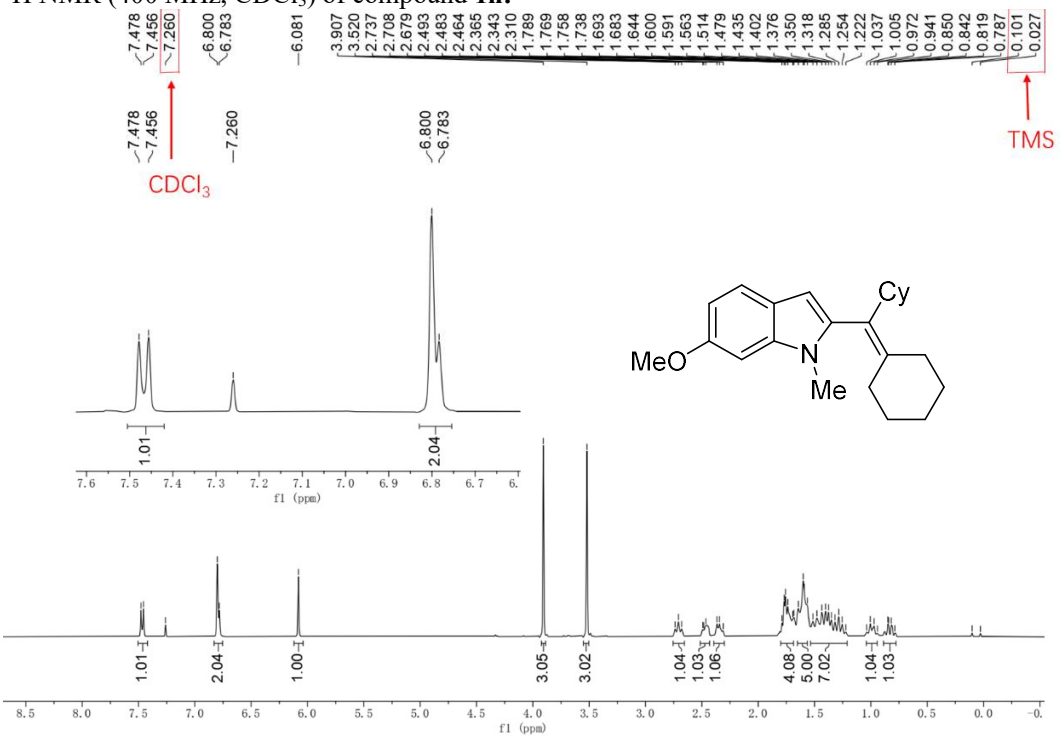
A



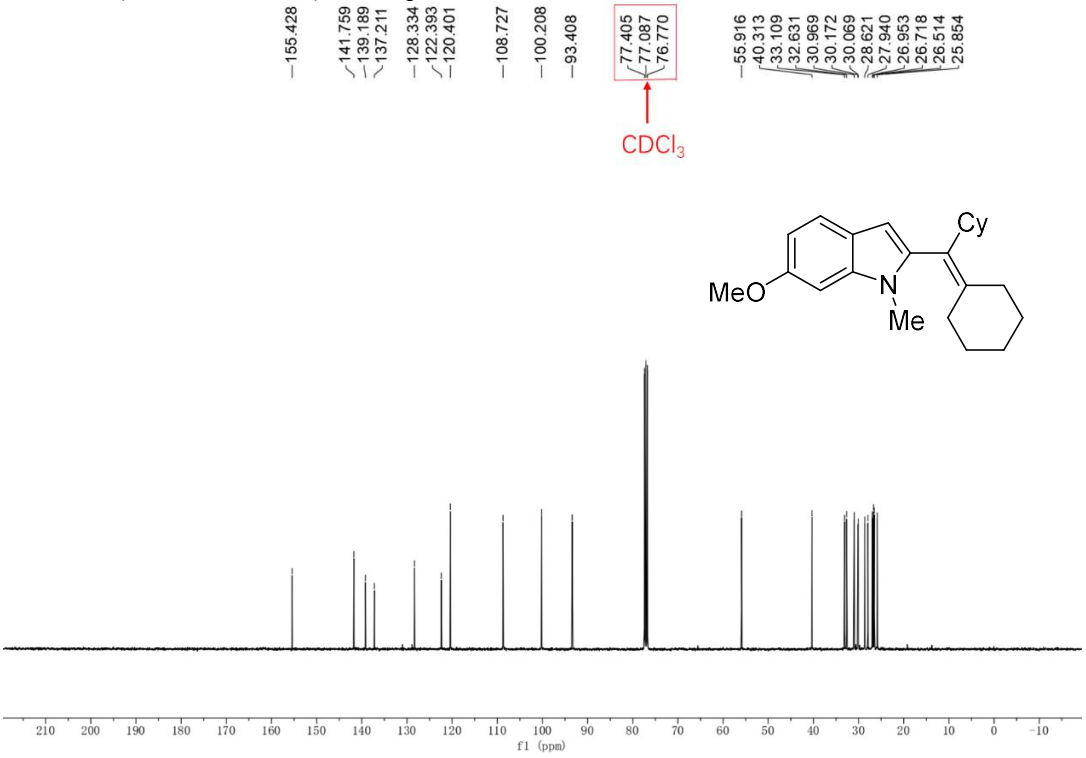
^{13}C NMR (100 MHz, $CDCl_3$) of compound **1g**:



^{1}H NMR (400 MHz, $CDCl_3$) of compound **1h:**

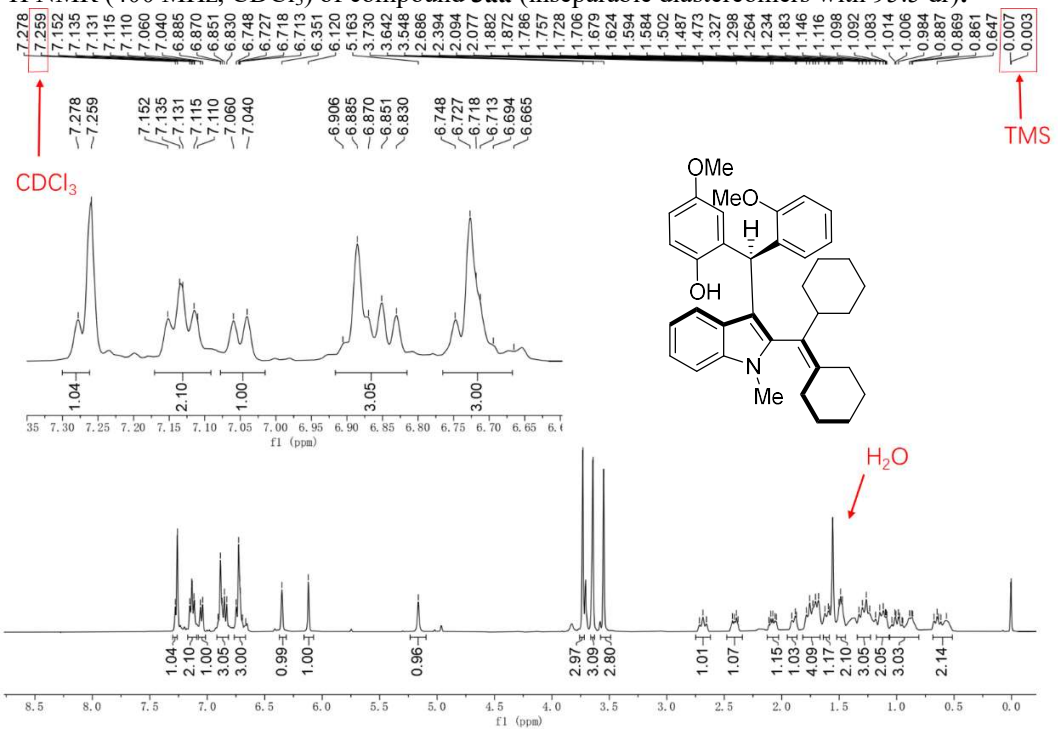


^{13}C NMR (100 MHz, $CDCl_3$) of compound **1h:**

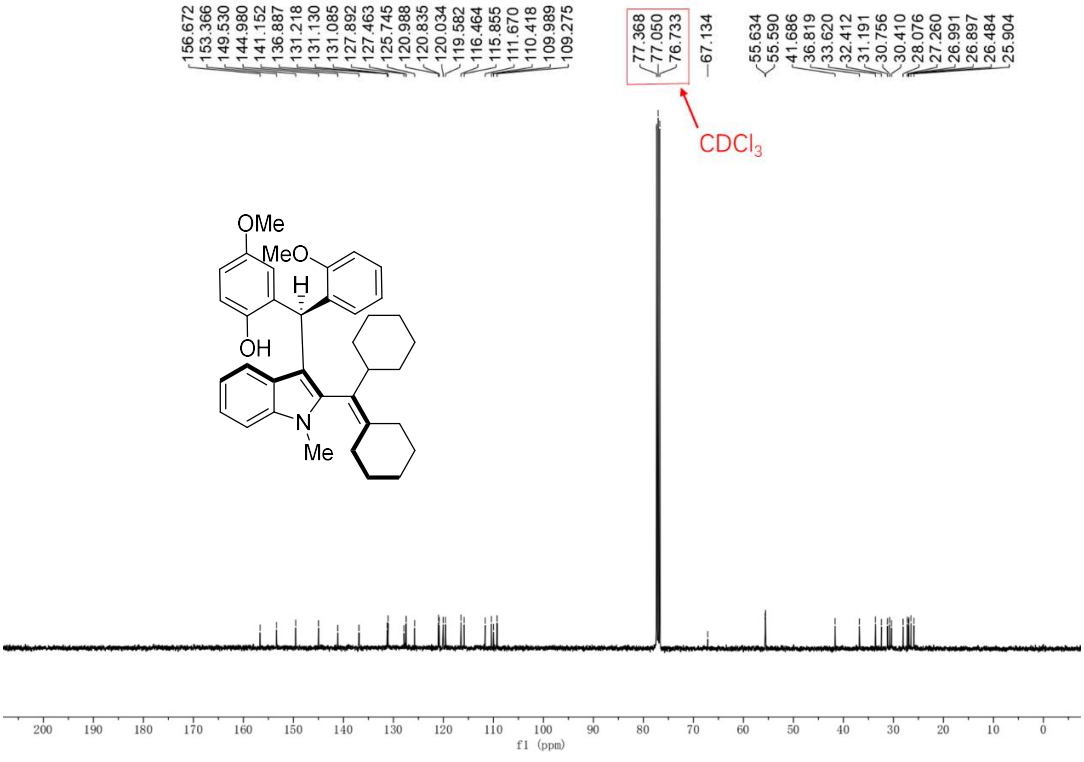


13. NMR spectra of compounds 3, 4, 8-10, 13 and S12

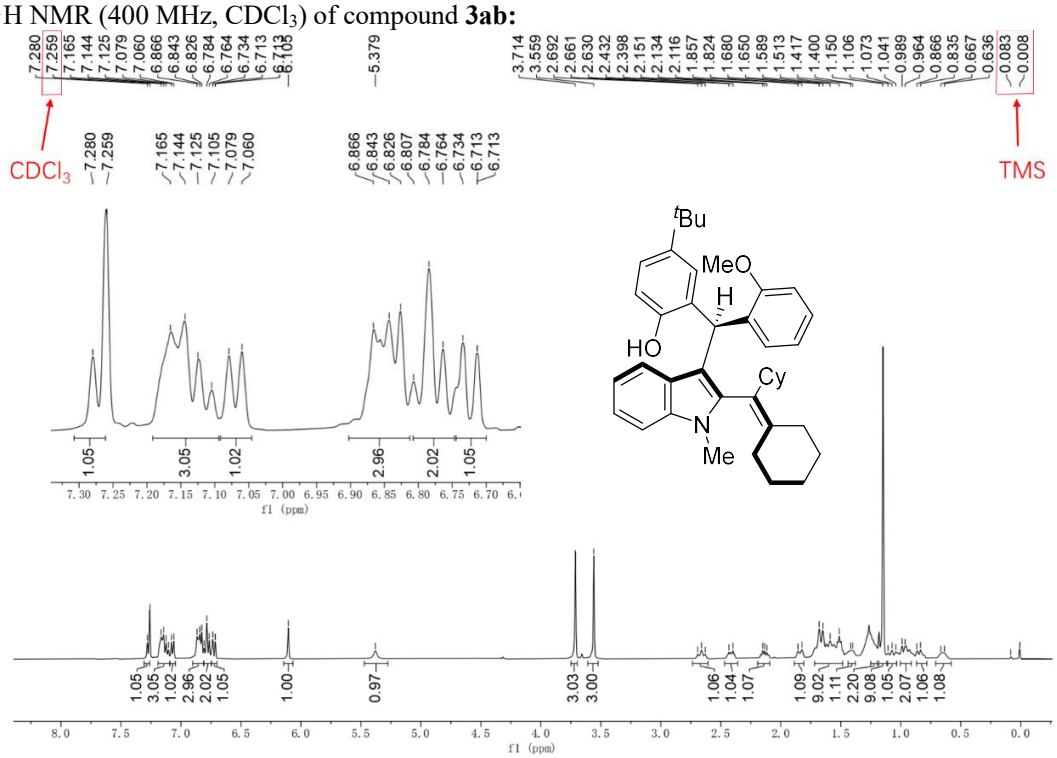
^{1}H NMR (400 MHz, $CDCl_3$) of compound **3aa** (inseparable diastereomers with 95:5 dr)**:**



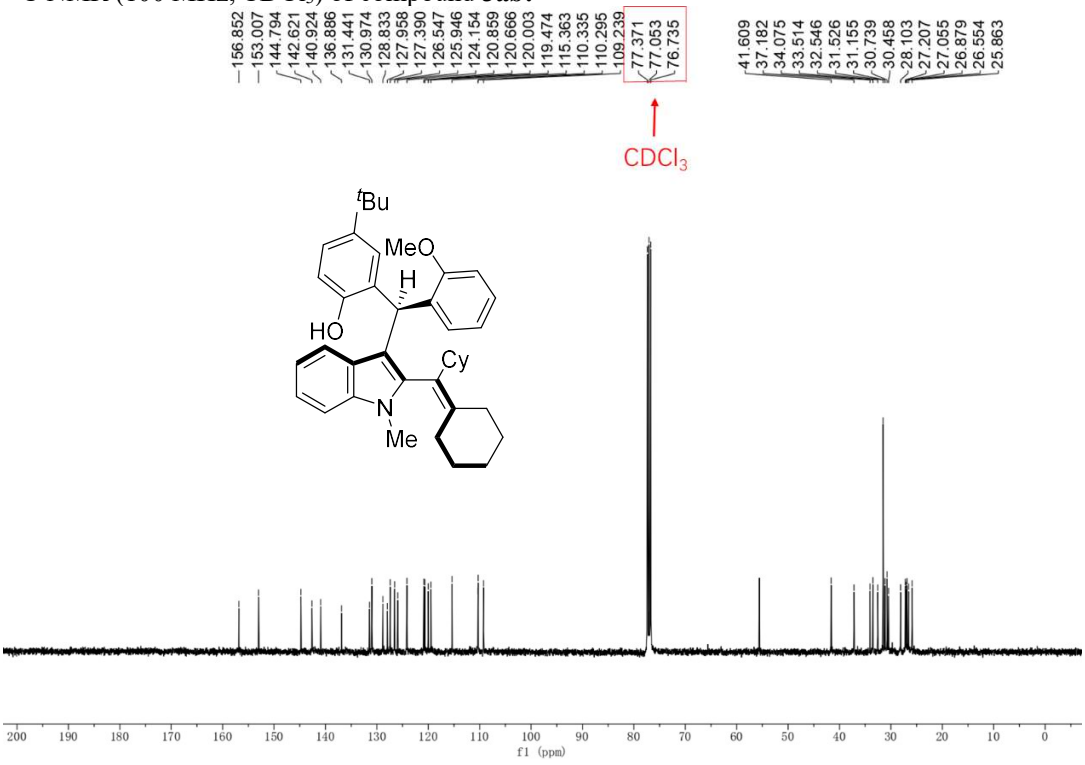
^{13}C NMR (100 MHz, $CDCl_3$) of compound **3aa:**



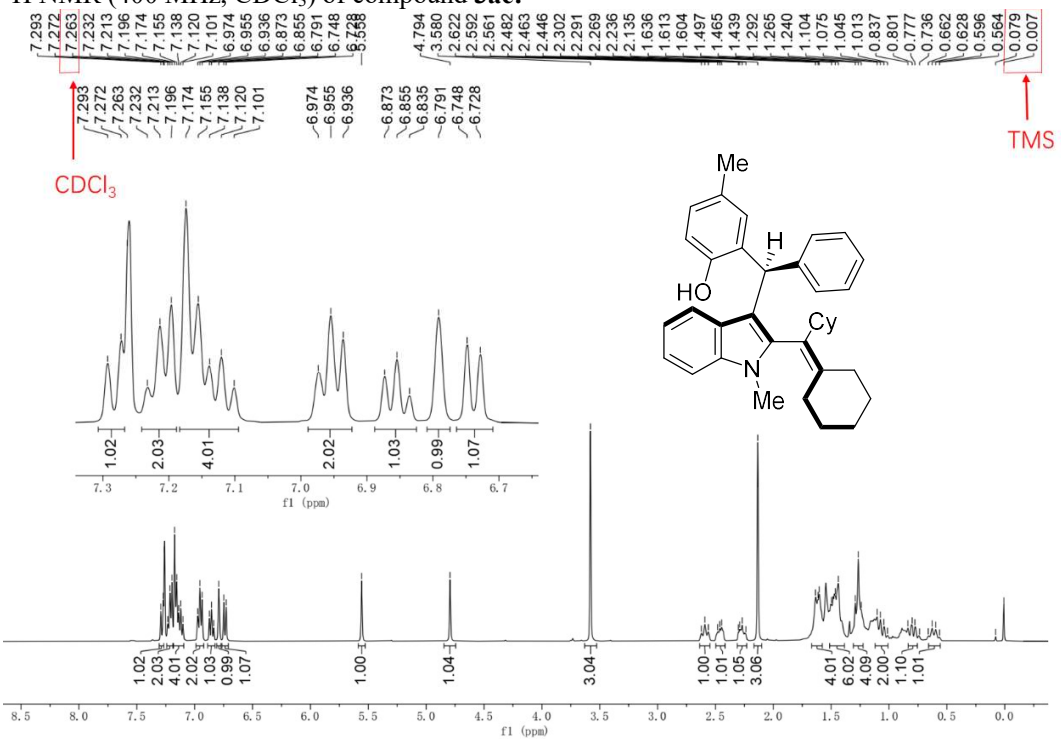
^{1}H NMR (400 MHz, $CDCl_3$) of compound **3ab:**



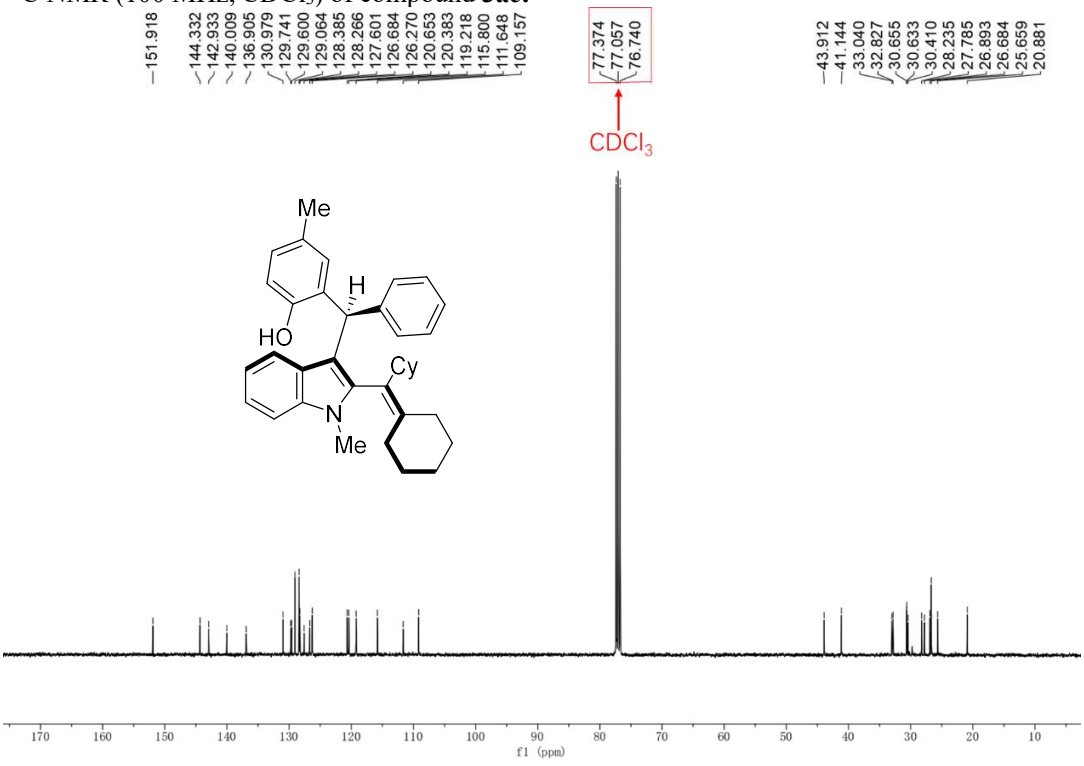
^{13}C NMR (100 MHz, $CDCl_3$) of compound **3ab:**



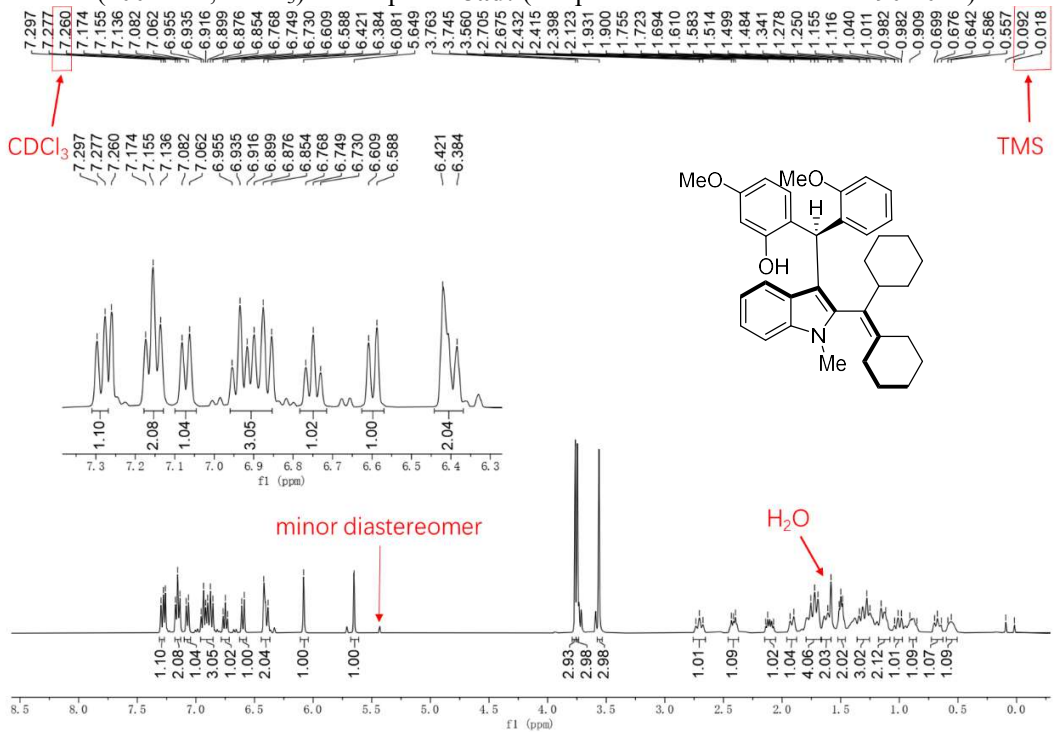
^{1}H NMR (400 MHz, $CDCl_3$) of compound **3ac:**



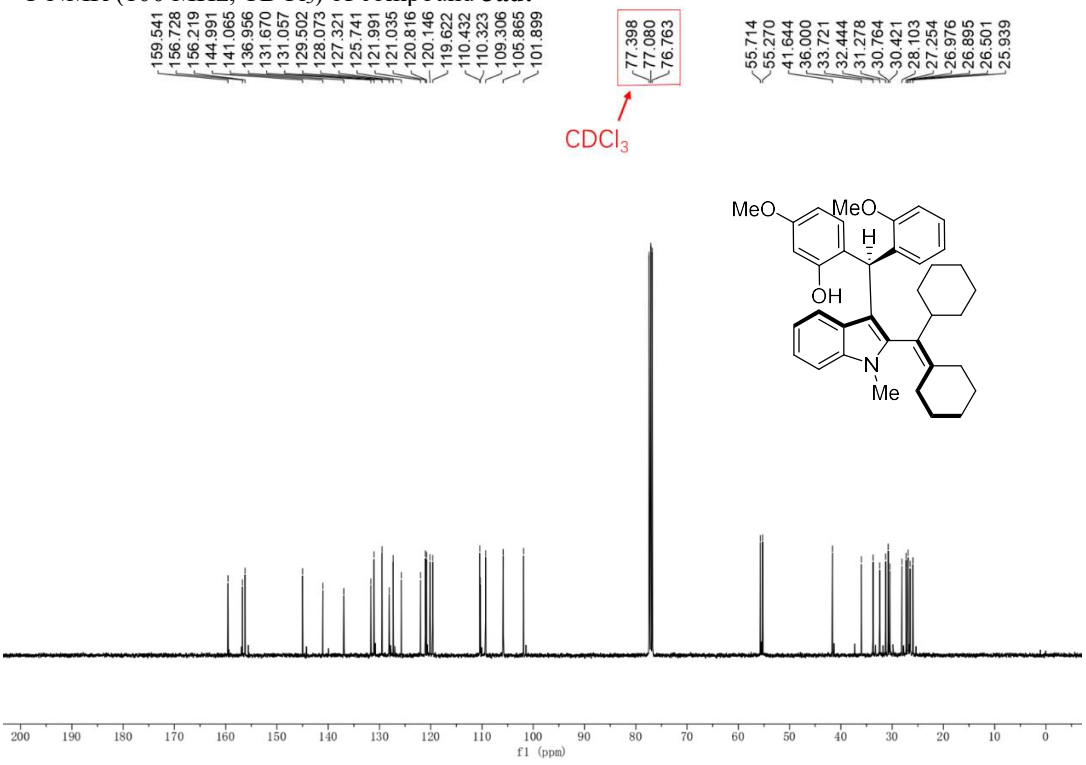
^{13}C NMR (100 MHz, $CDCl_3$) of compound **3ac:**



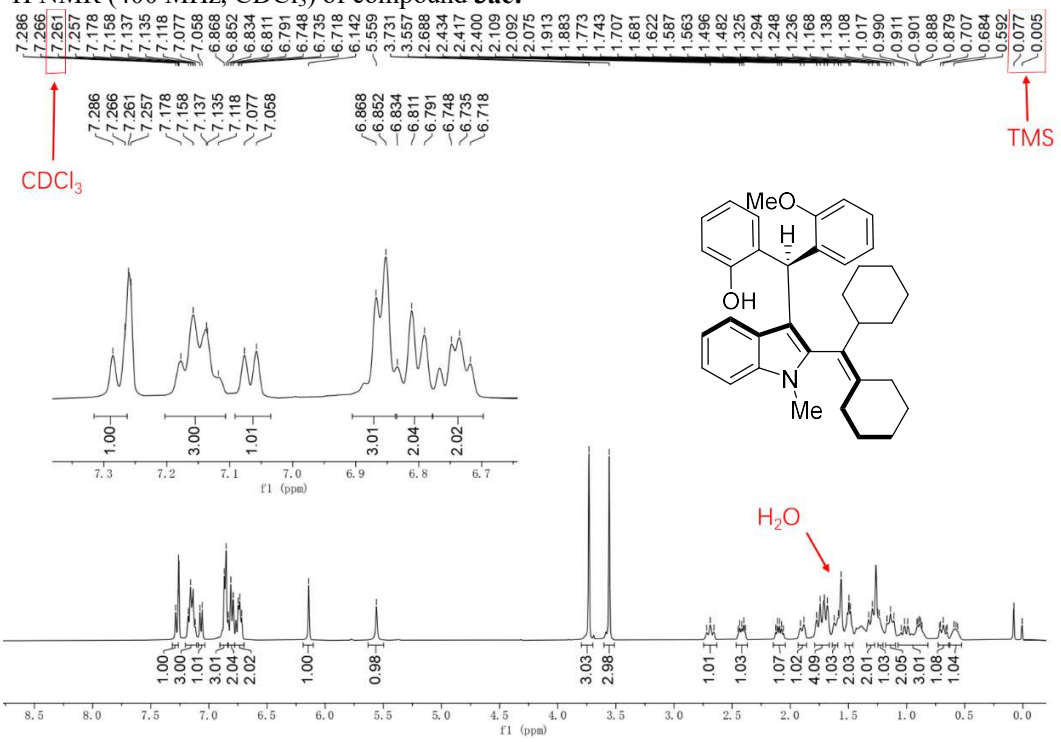
^{1}H NMR (400 MHz, $CDCl_3$) of compound **3ad:** (inseparable diastereomers with 90:10 dr)



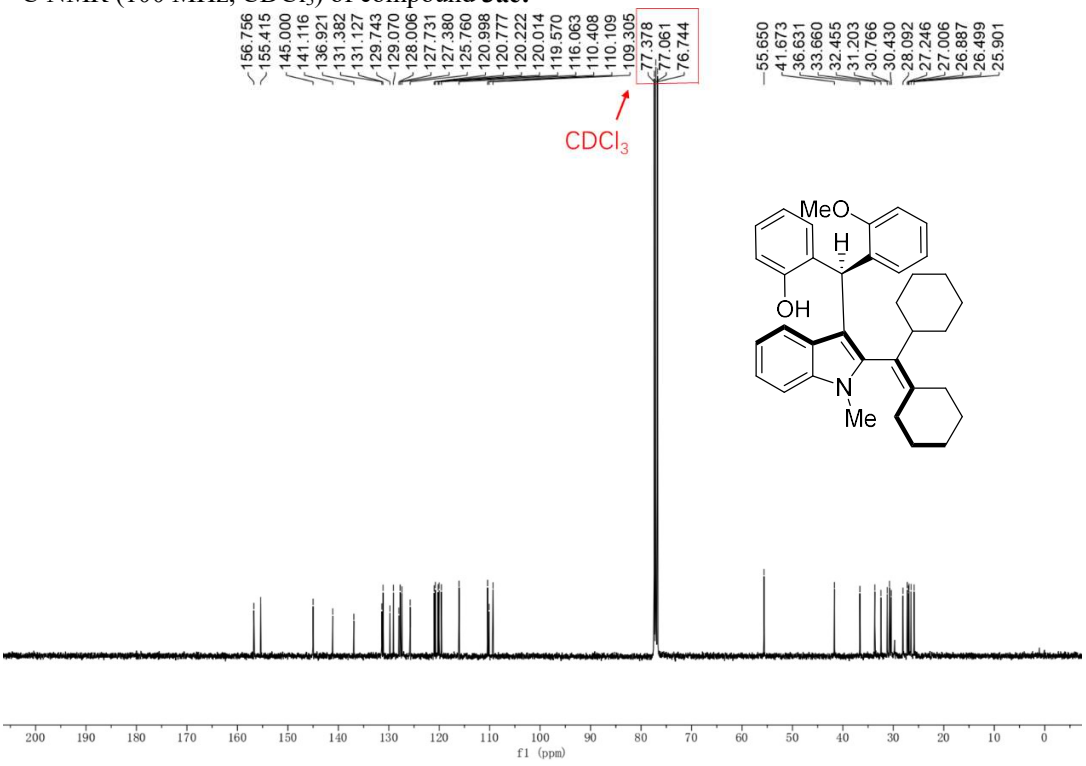
^{13}C NMR (100 MHz, $CDCl_3$) of compound **3ad:**



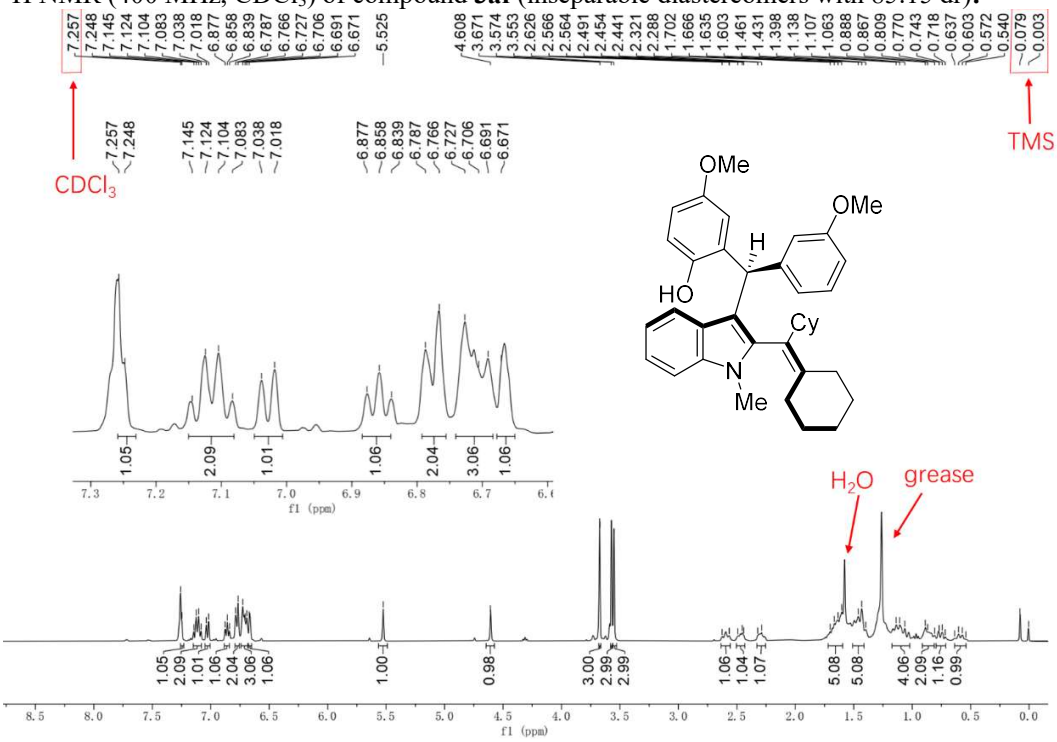
^{1}H NMR (400 MHz, $CDCl_3$) of compound **3ae:**



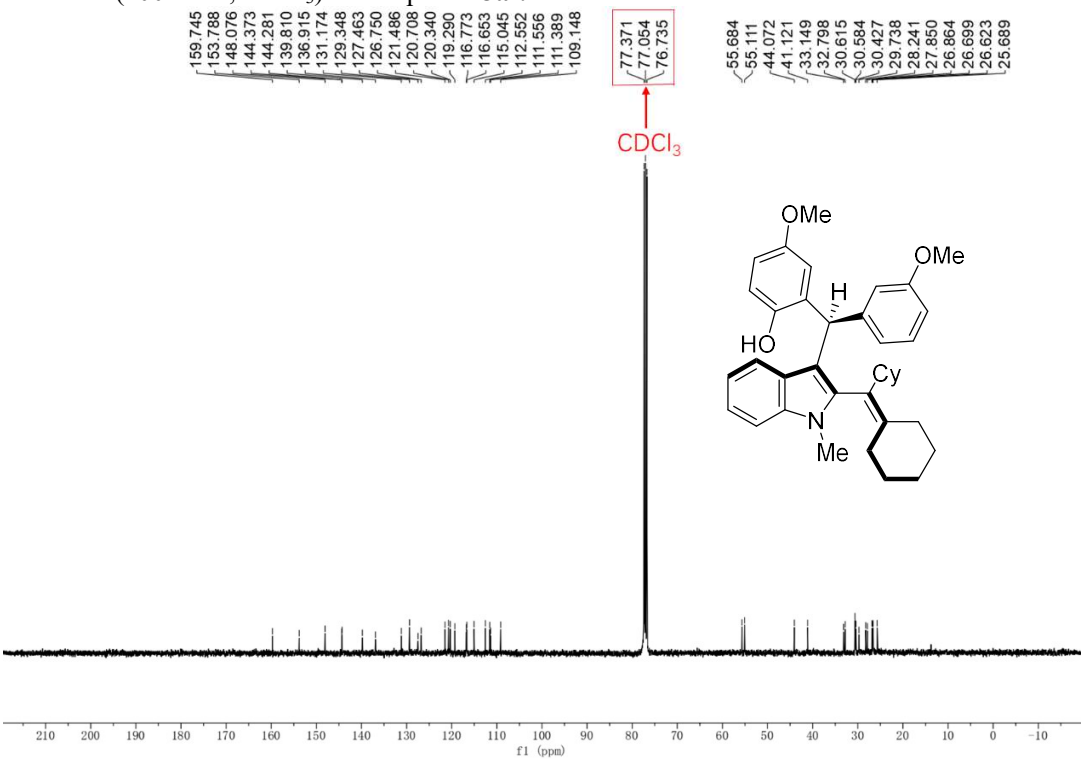
^{13}C NMR (100 MHz, $CDCl_3$) of compound **3ae:**



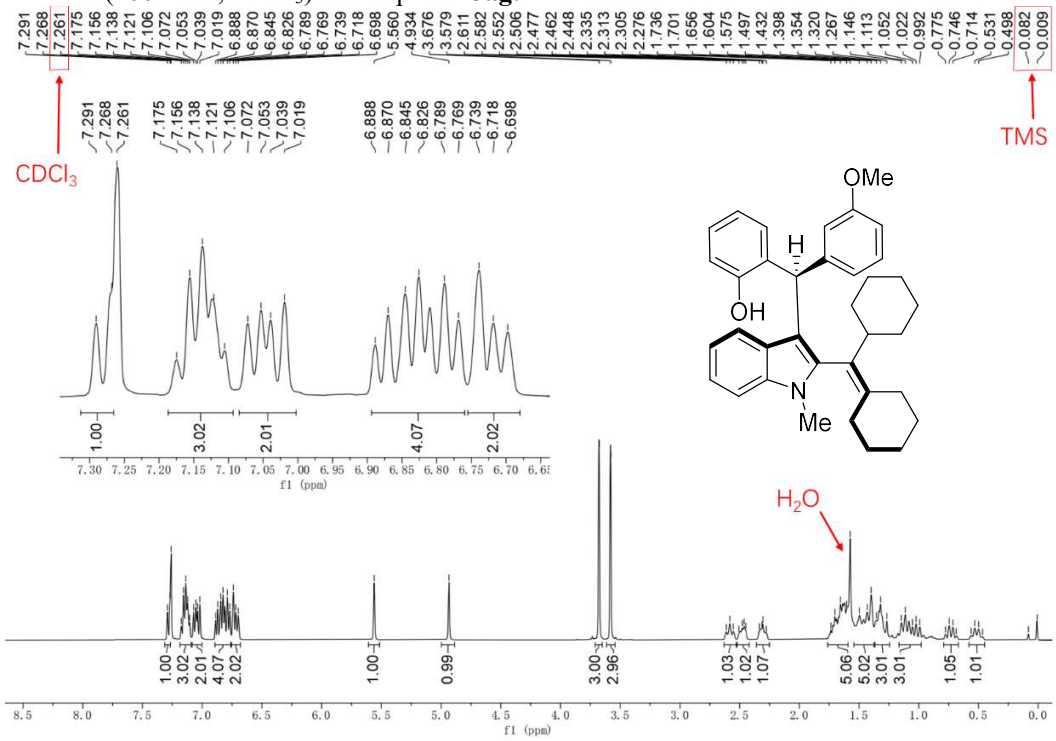
^{1}H NMR (400 MHz, $CDCl_3$) of compound **3af** (inseparable diastereomers with 85:15 dr)**:**



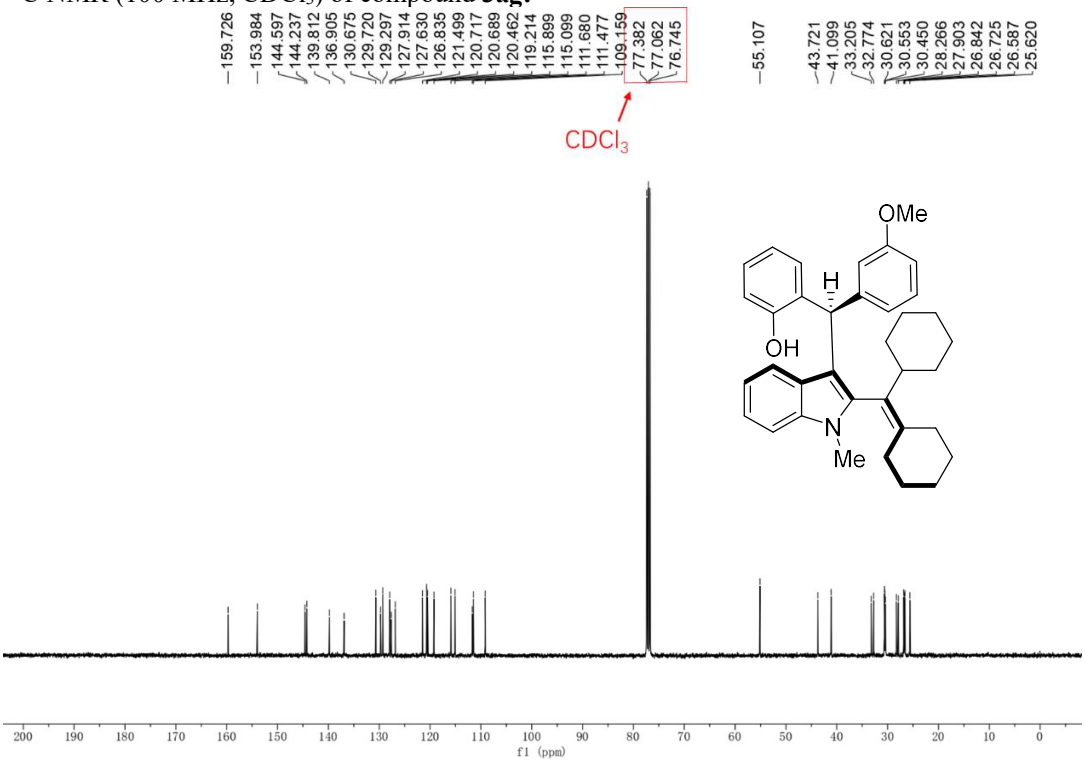
^{13}C NMR (100 MHz, $CDCl_3$) of compound **3af:**



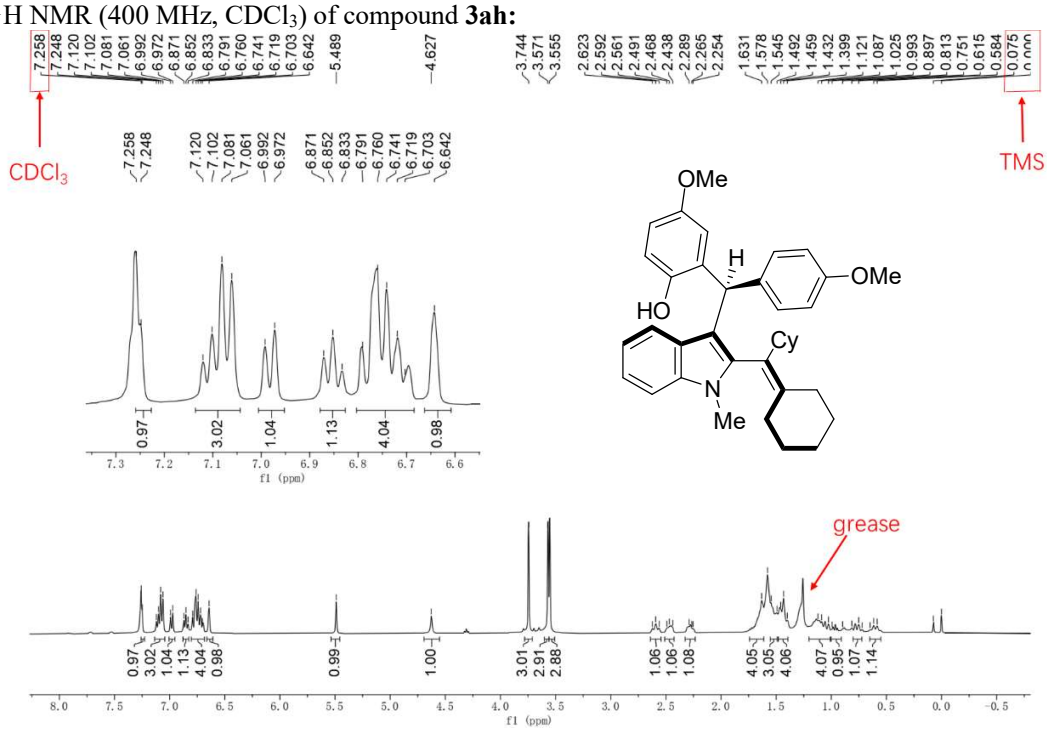
^{1}H NMR (400 MHz, $CDCl_3$) of compound **3ag:**



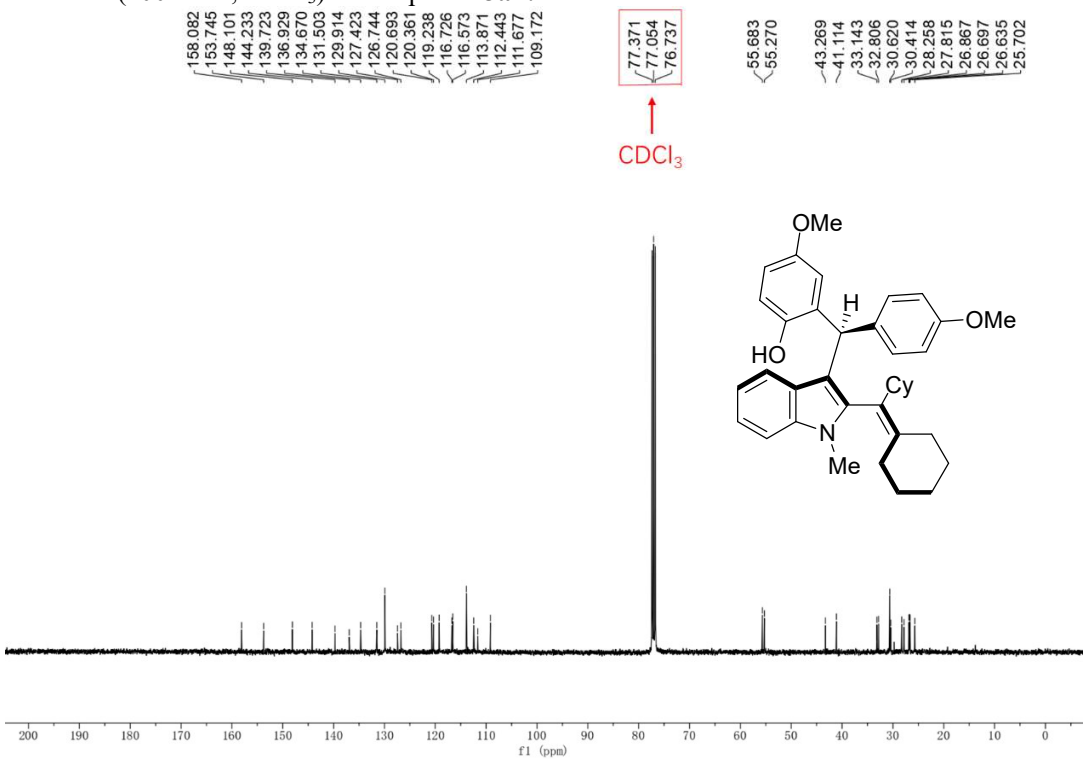
^{13}C NMR (100 MHz, $CDCl_3$) of compound **3ag:**



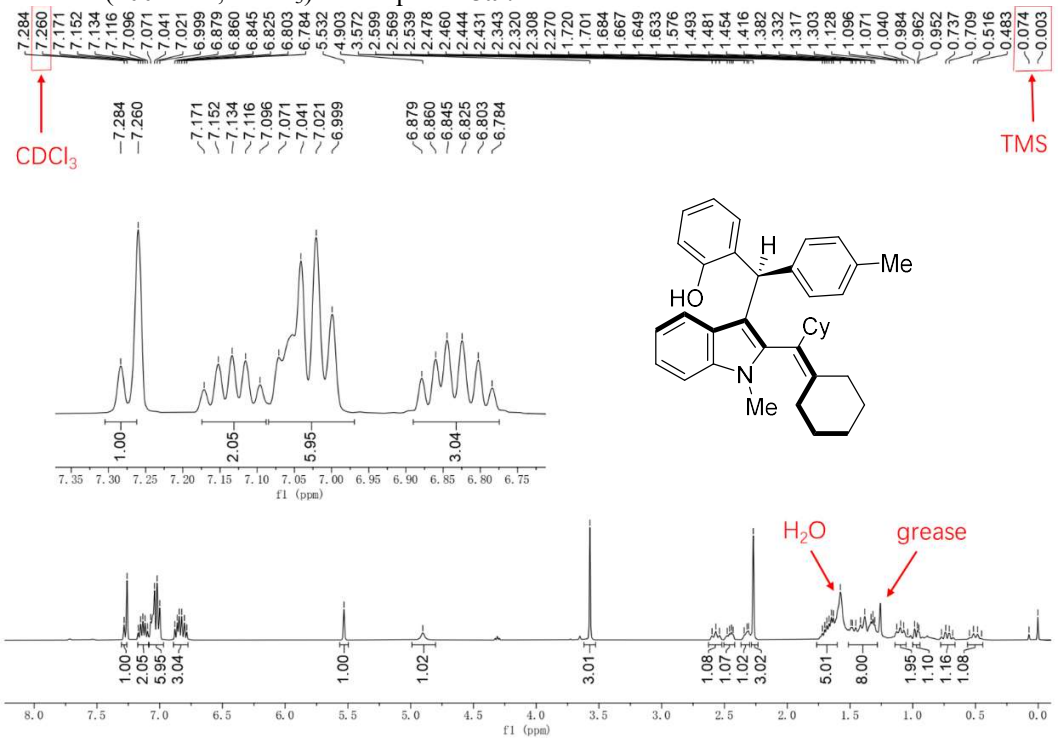
^{1}H NMR (400 MHz, $CDCl_3$) of compound **3ah:**



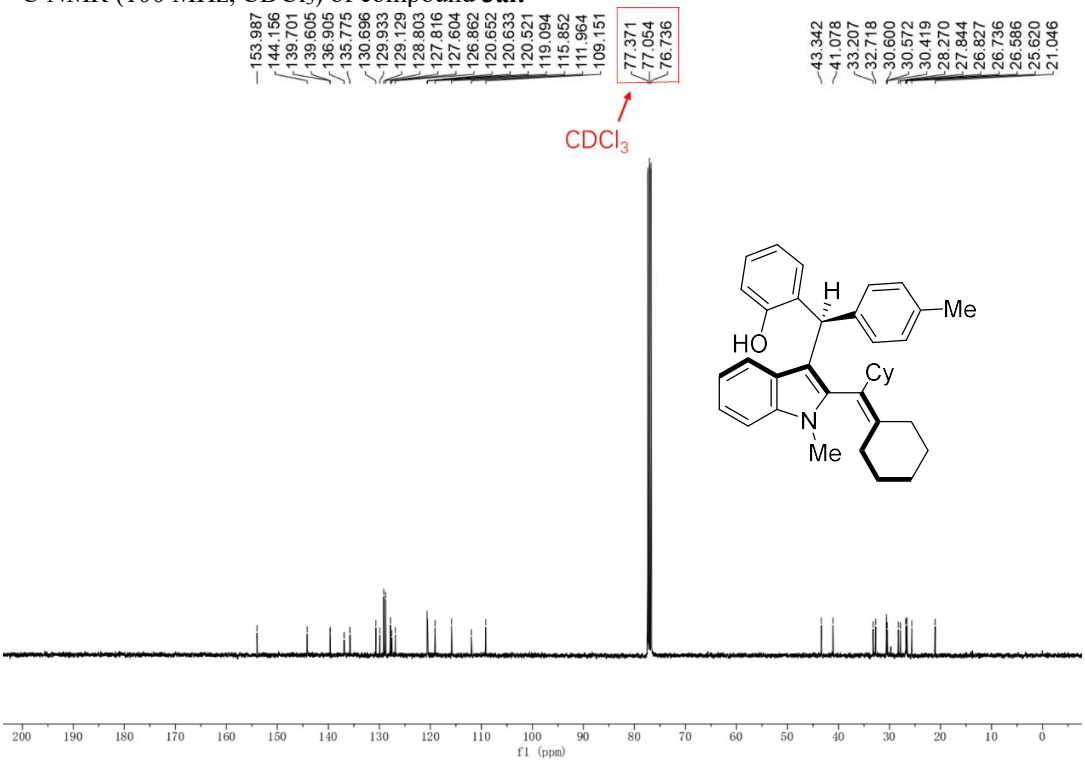
^{13}C NMR (100 MHz, $CDCl_3$) of compound **3ah:**



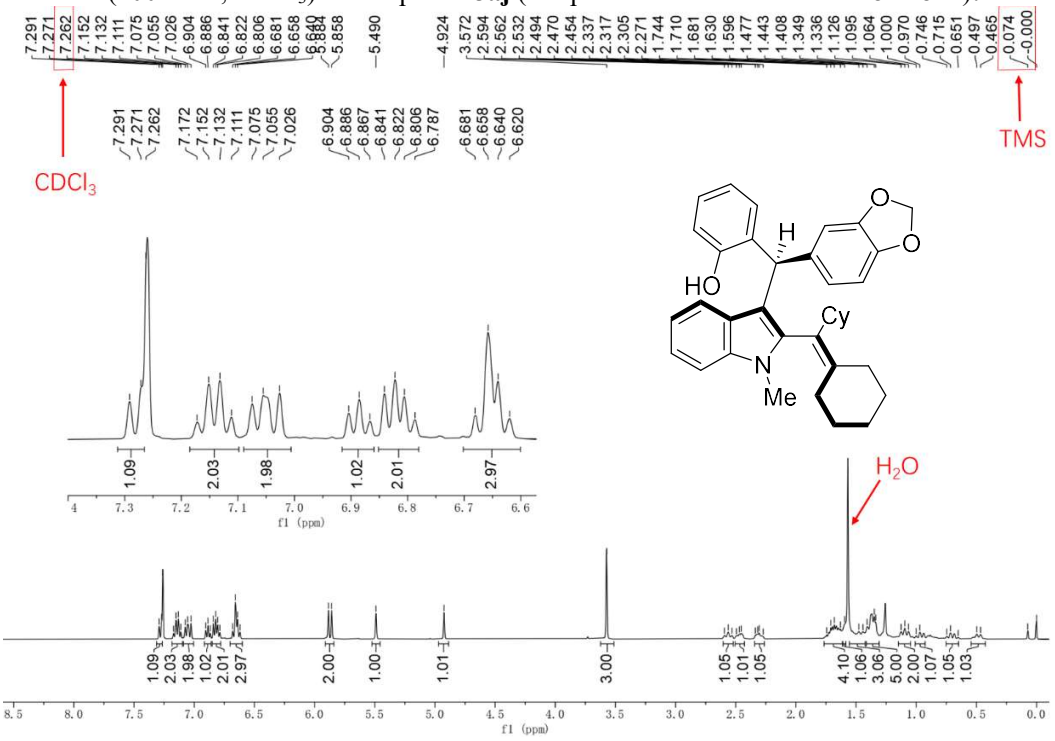
^{1}H NMR (400 MHz, $CDCl_3$) of compound **3ai:**



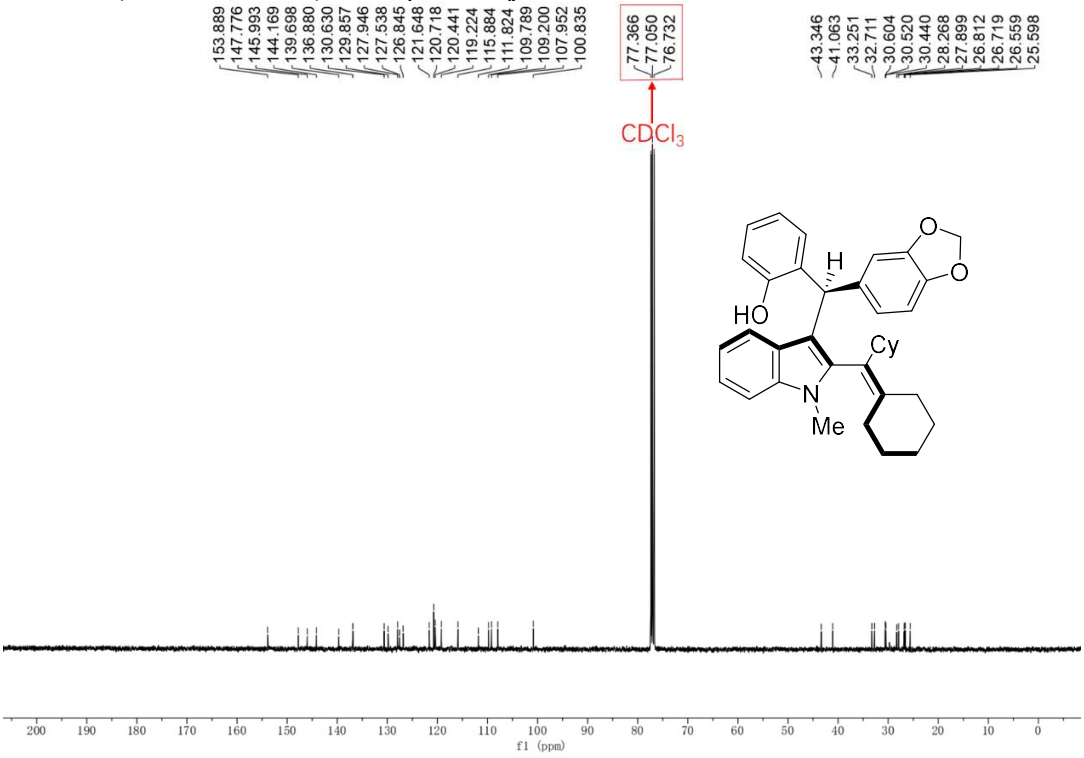
^{13}C NMR (100 MHz, $CDCl_3$) of compound **3ai:**



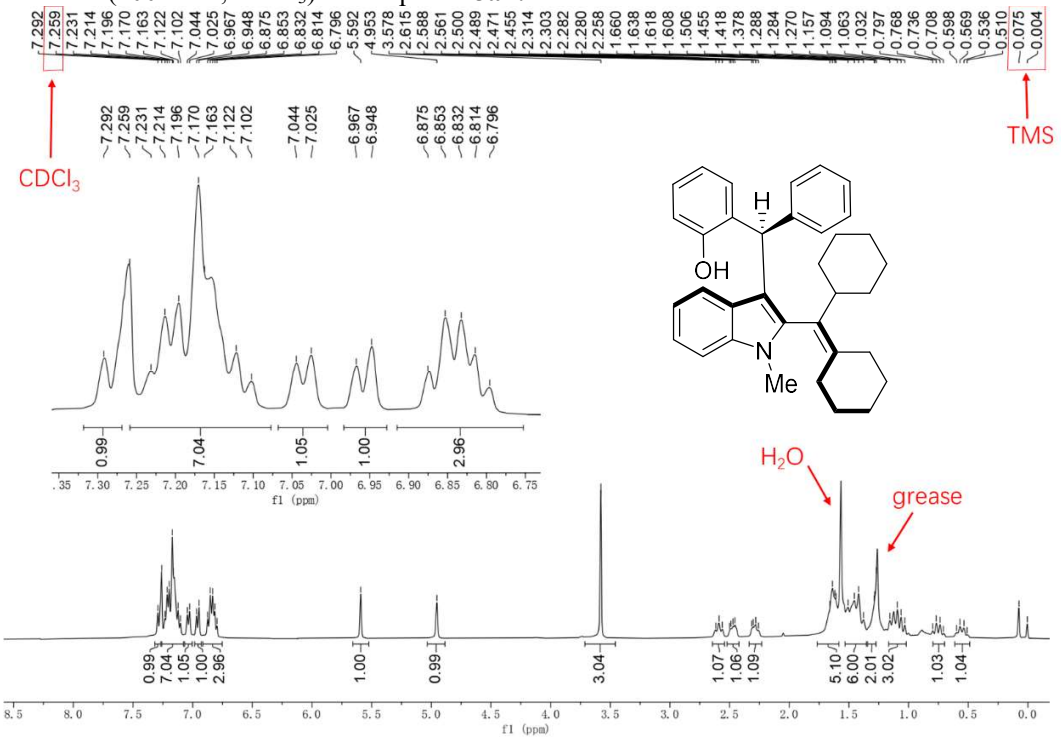
^{1}H NMR (400 MHz, $CDCl_3$) of compound **3aj** (inseparable diastereomers with 82:18 dr)**:**



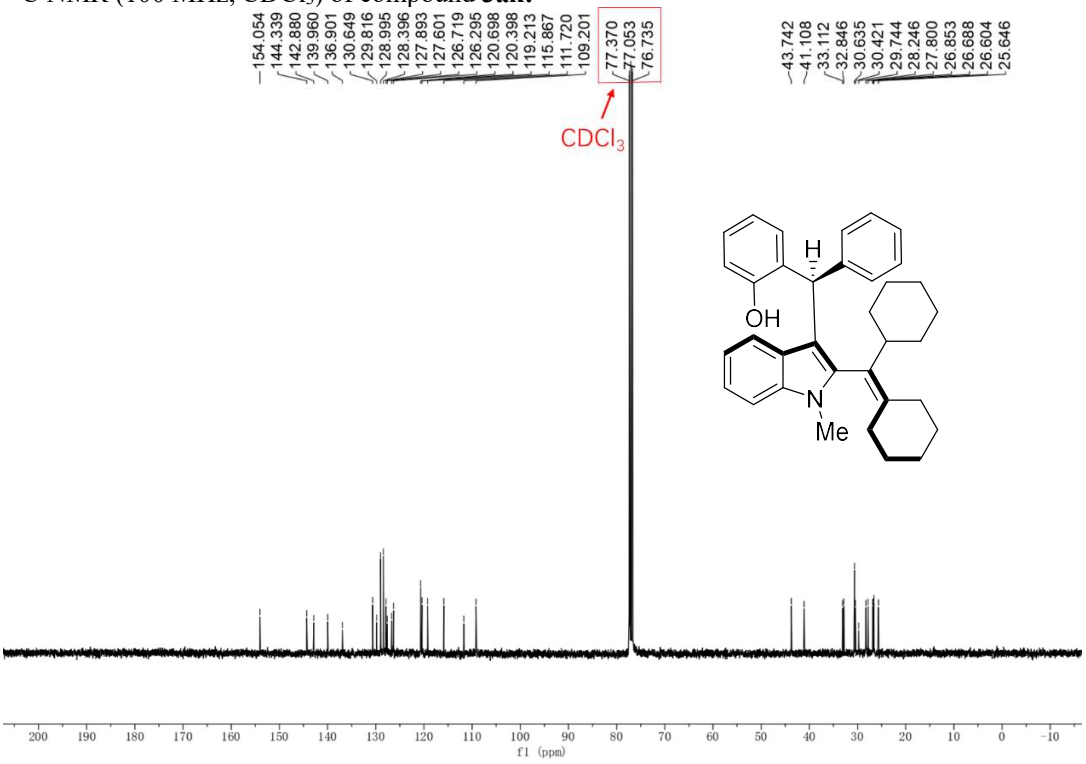
^{13}C NMR (100 MHz, $CDCl_3$) of compound **3aj:**



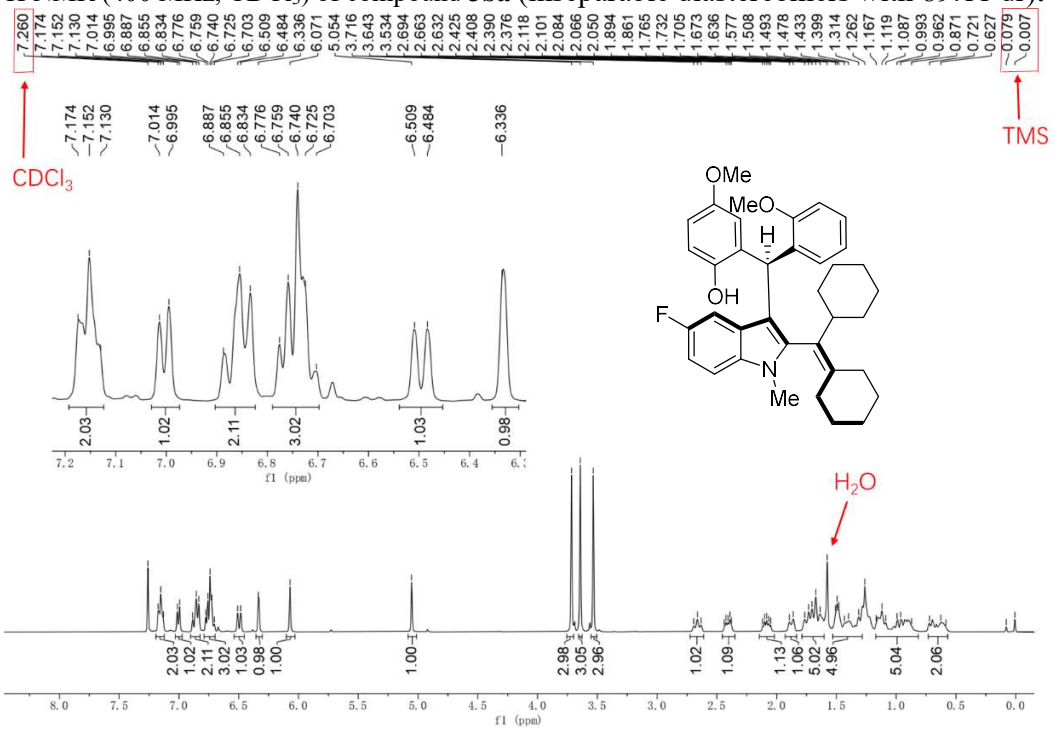
^{1}H NMR (400 MHz, $CDCl_3$) of compound **3ak:**



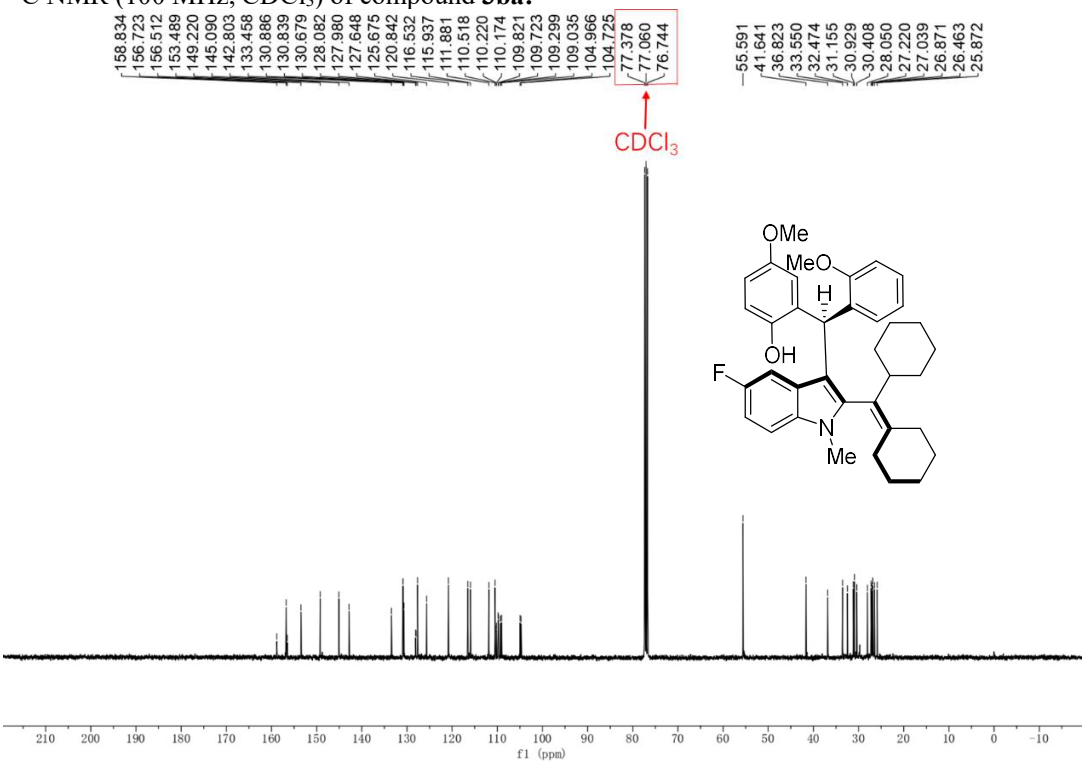
^{13}C NMR (100 MHz, $CDCl_3$) of compound **3ak:**



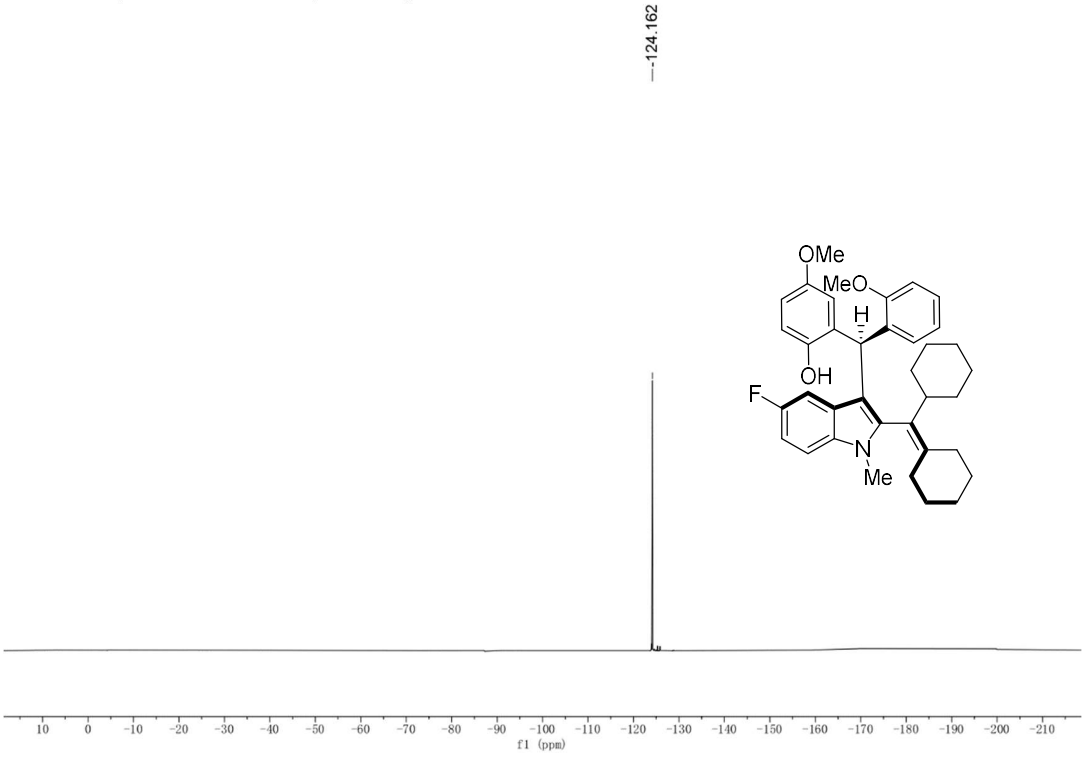
^{1}H NMR (400 MHz, $CDCl_3$) of compound **3ba** (inseparable diastereomers with 89:11 dr)**:**



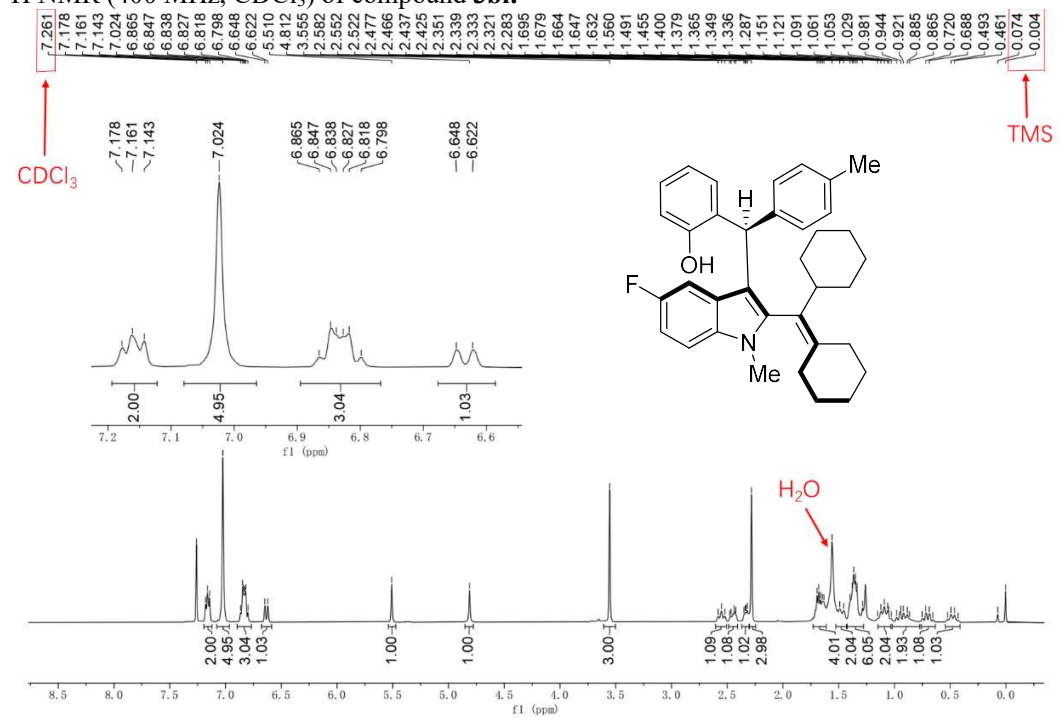
^{13}C NMR (100 MHz, $CDCl_3$) of compound **3ba:**



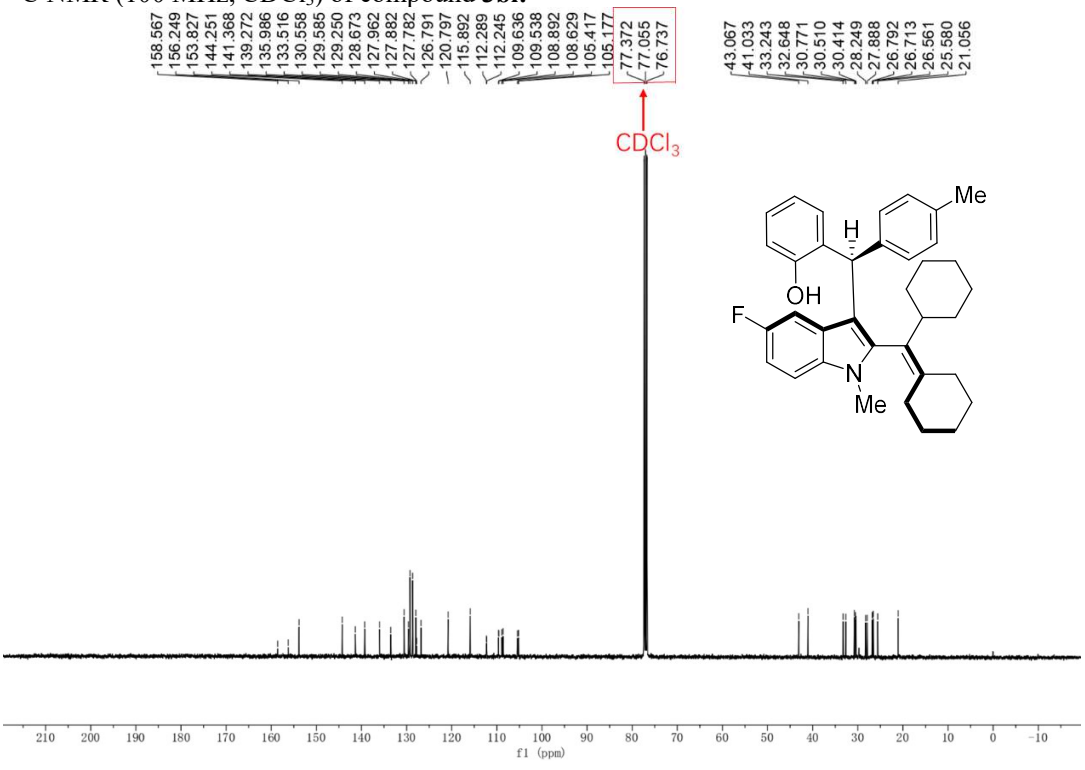
^{19}F NMR (376 MHz, $CDCl_3$) of compound **3ba:**



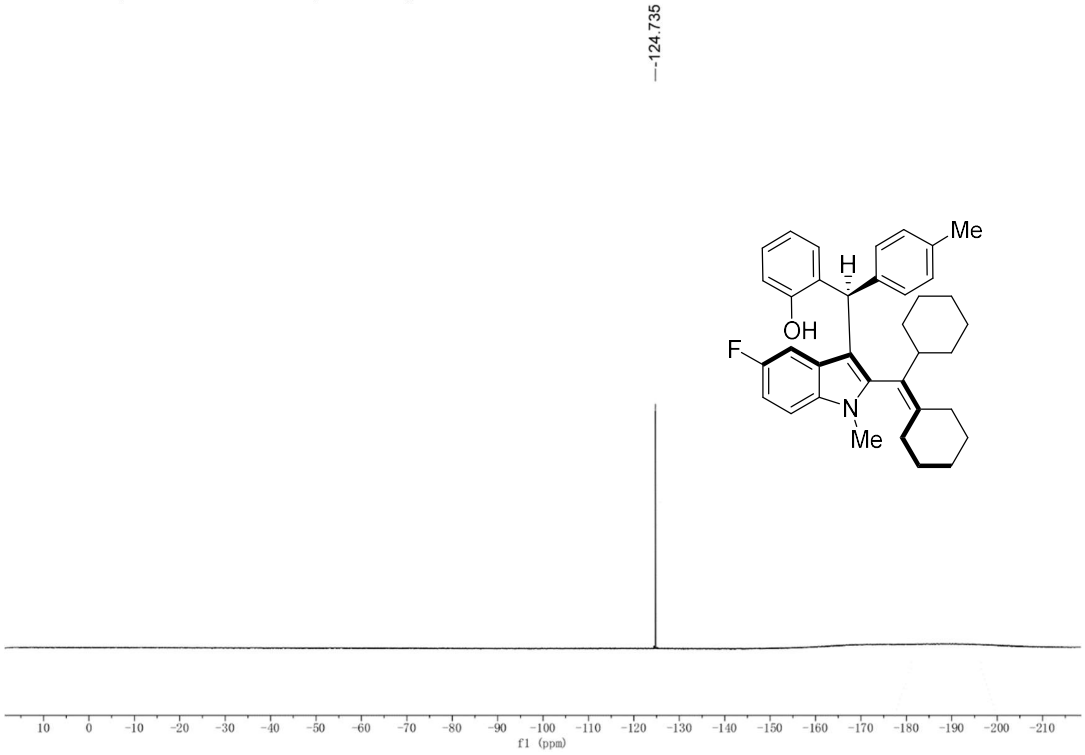
^{1}H NMR (400 MHz, $CDCl_3$) of compound **3bi:**



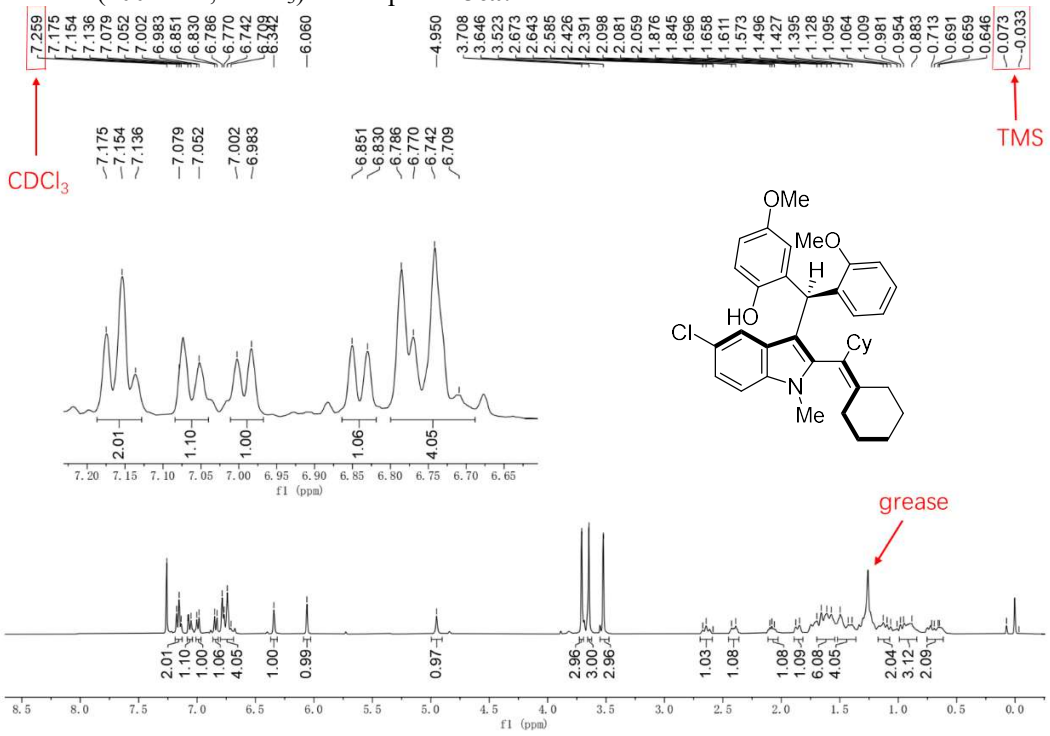
^{13}C NMR (100 MHz, $CDCl_3$) of compound **3bi:**



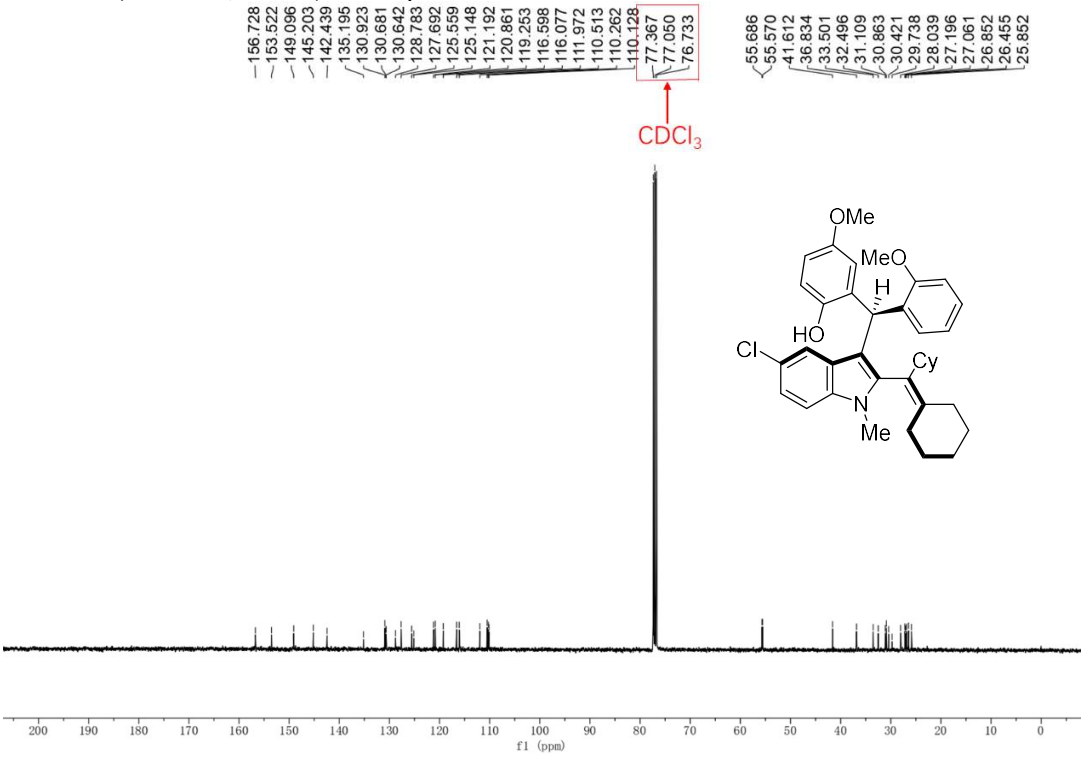
^{19}F NMR (376 MHz, $CDCl_3$) of compound **3bi:**



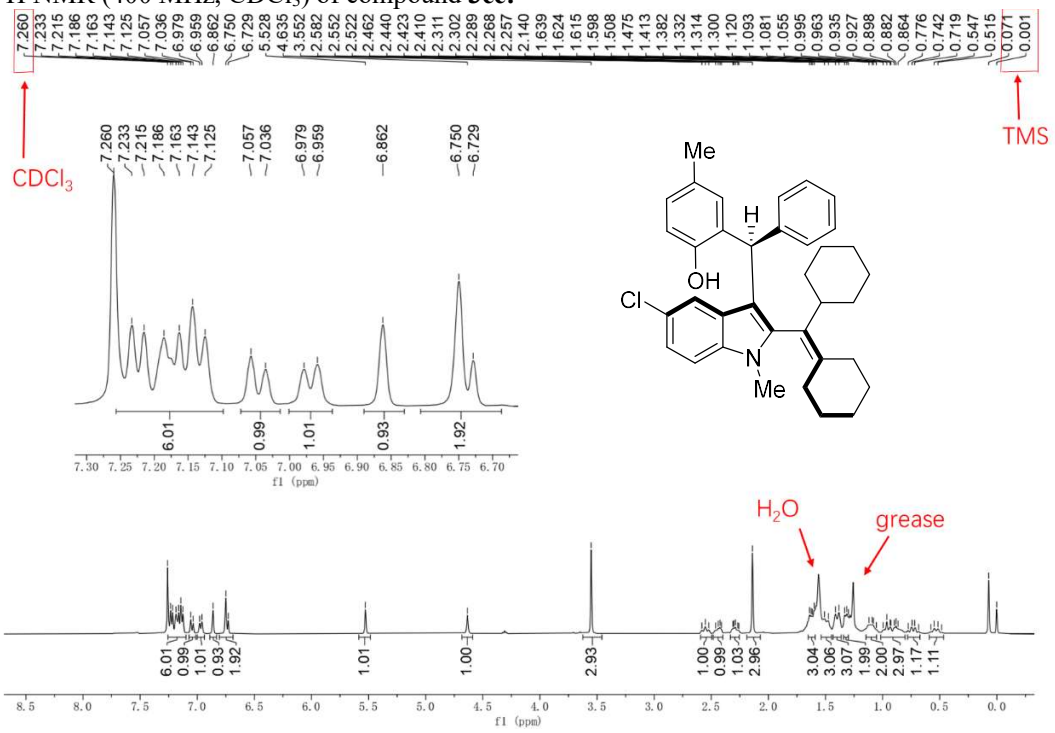
^{1}H NMR (400 MHz, $CDCl_3$) of compound **3ca:**



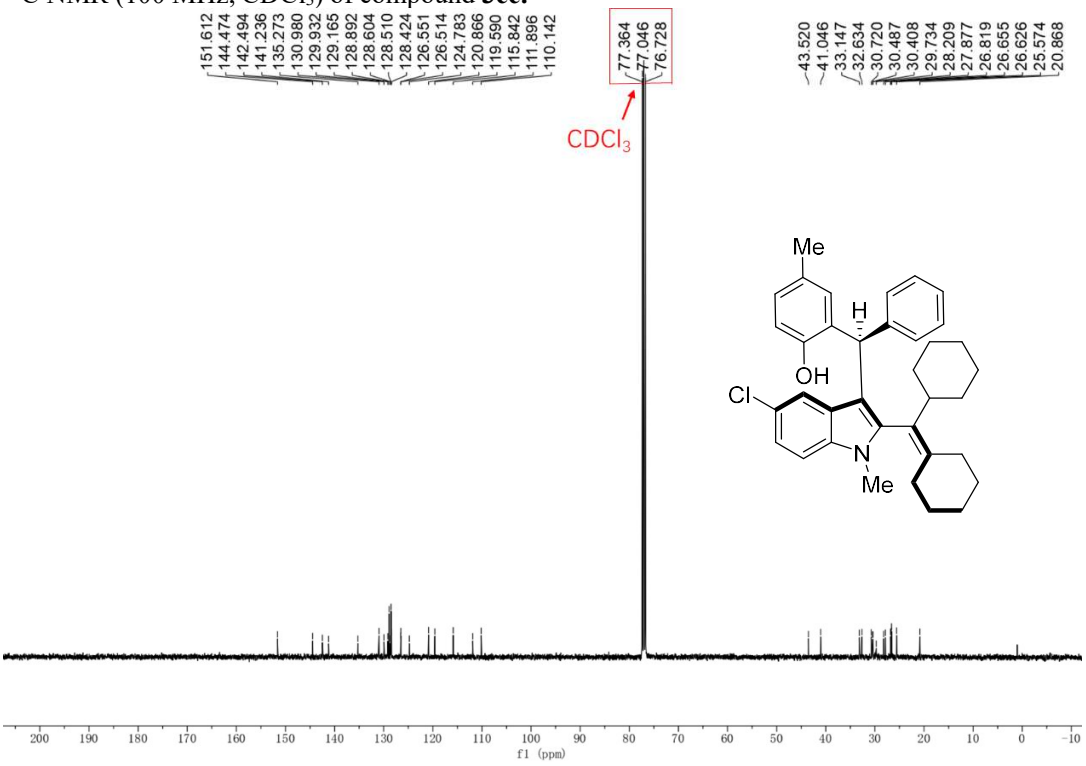
^{13}C NMR (100 MHz, $CDCl_3$) of compound **3ca:**



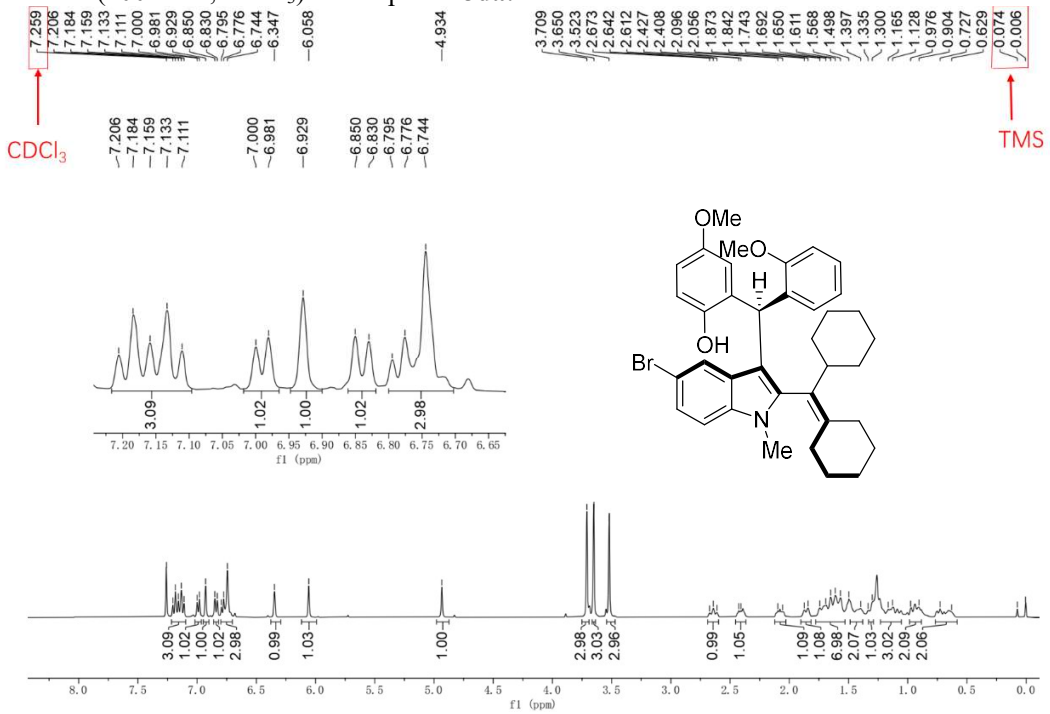
^{1}H NMR (400 MHz, $CDCl_3$) of compound **3cc:**



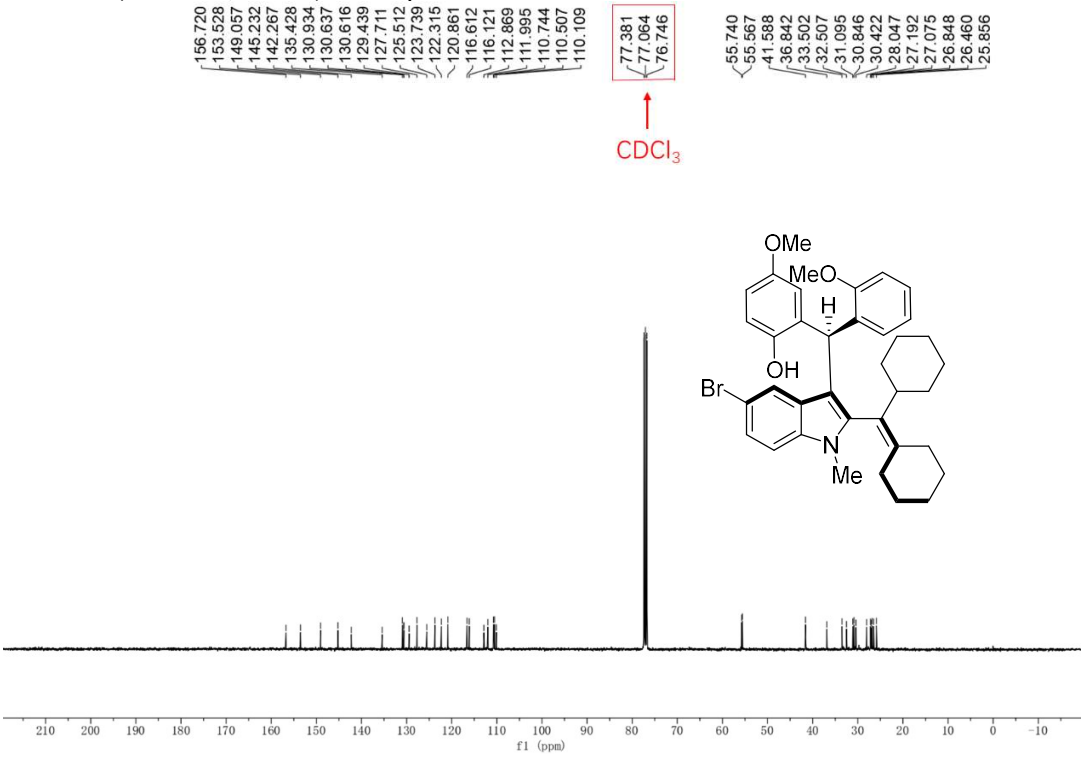
^{13}C NMR (100 MHz, $CDCl_3$) of compound **3cc:**



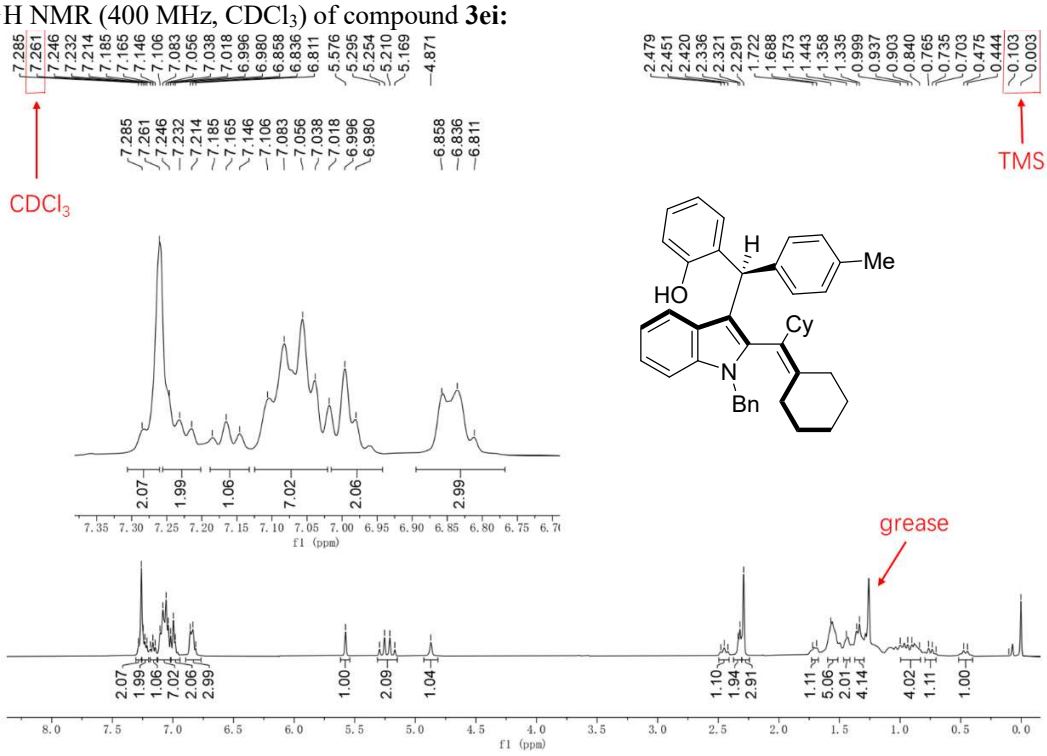
^{1}H NMR (400 MHz, $CDCl_3$) of compound **3da:**



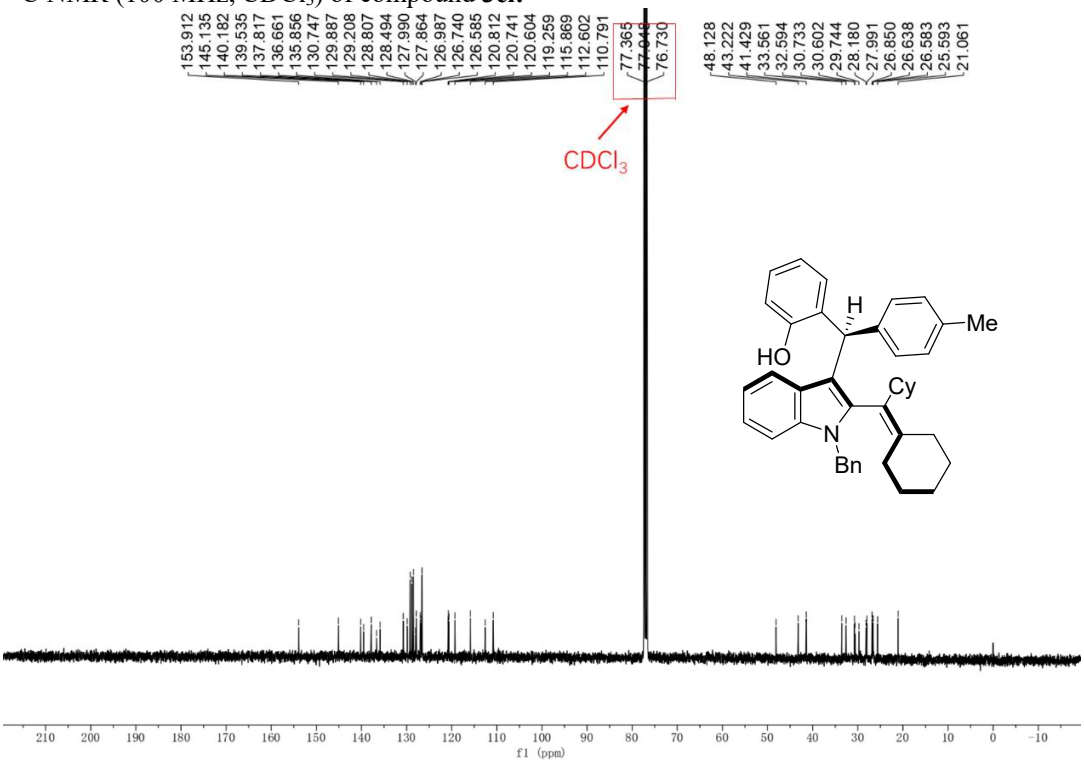
^{13}C NMR (100 MHz, $CDCl_3$) of compound **3da:**



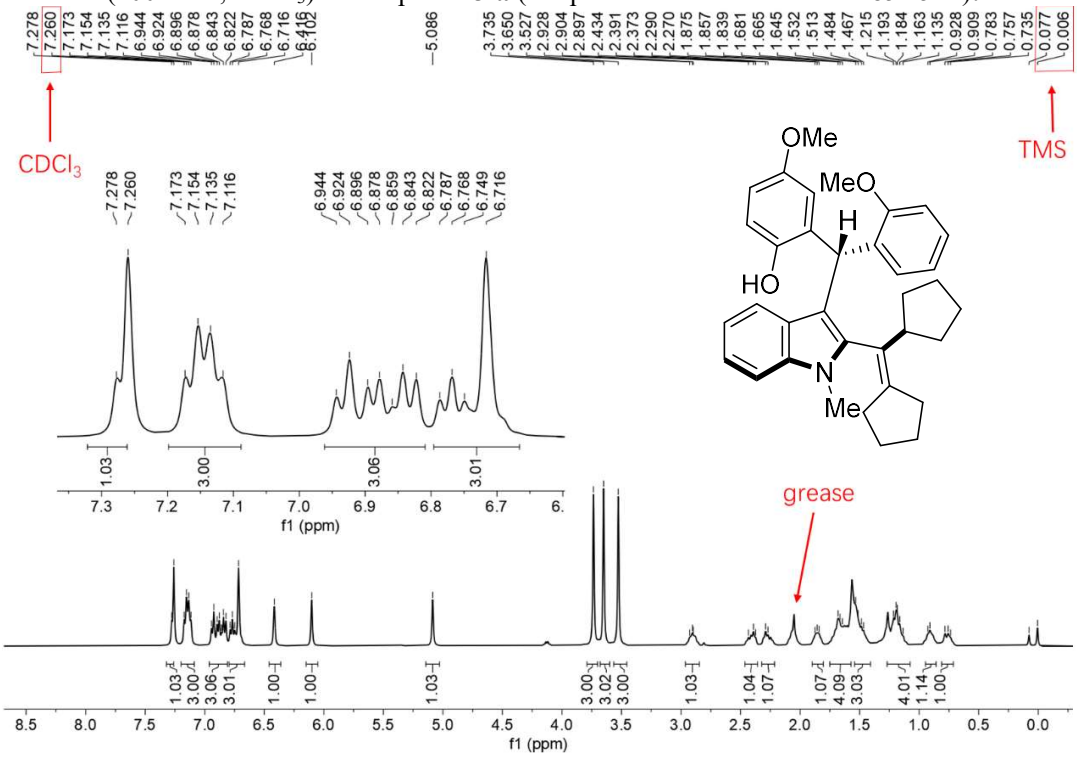
^{1}H NMR (400 MHz, $CDCl_3$) of compound **3ei:**



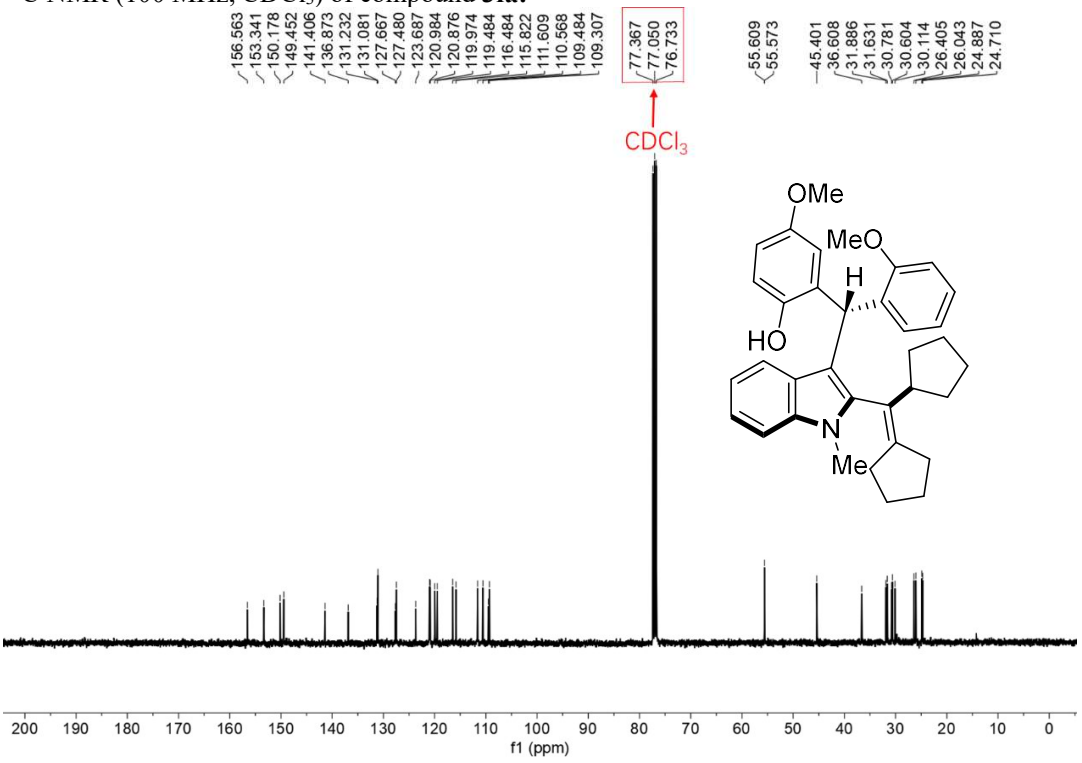
^{13}C NMR (100 MHz, $CDCl_3$) of compound **3ei:**



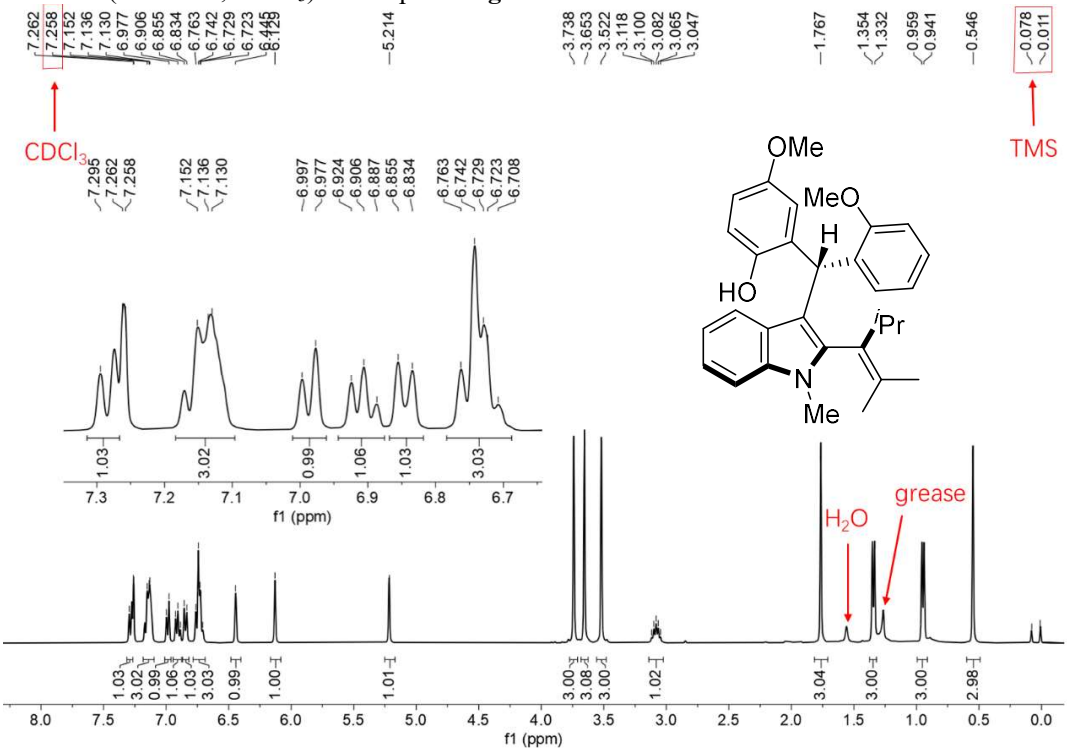
^{1}H NMR (400 MHz, $CDCl_3$) of compound **3fa** (inseparable diastereomers with 85:15 dr)**:**



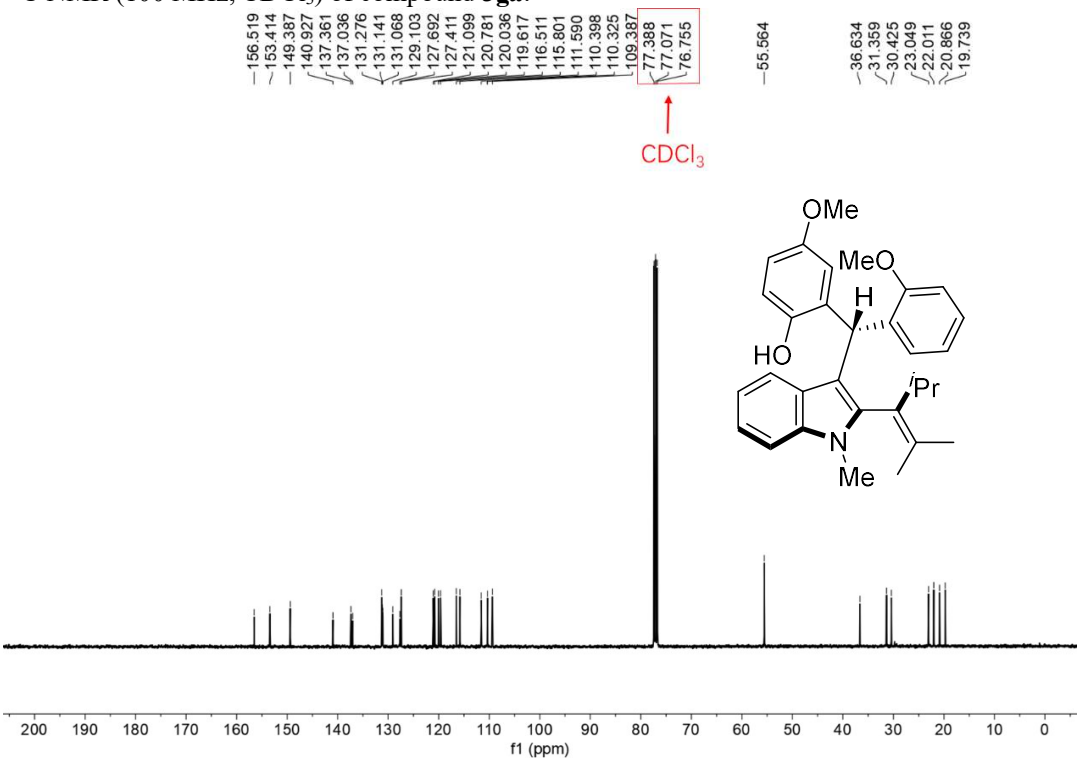
^{13}C NMR (100 MHz, $CDCl_3$) of compound **3fa:**



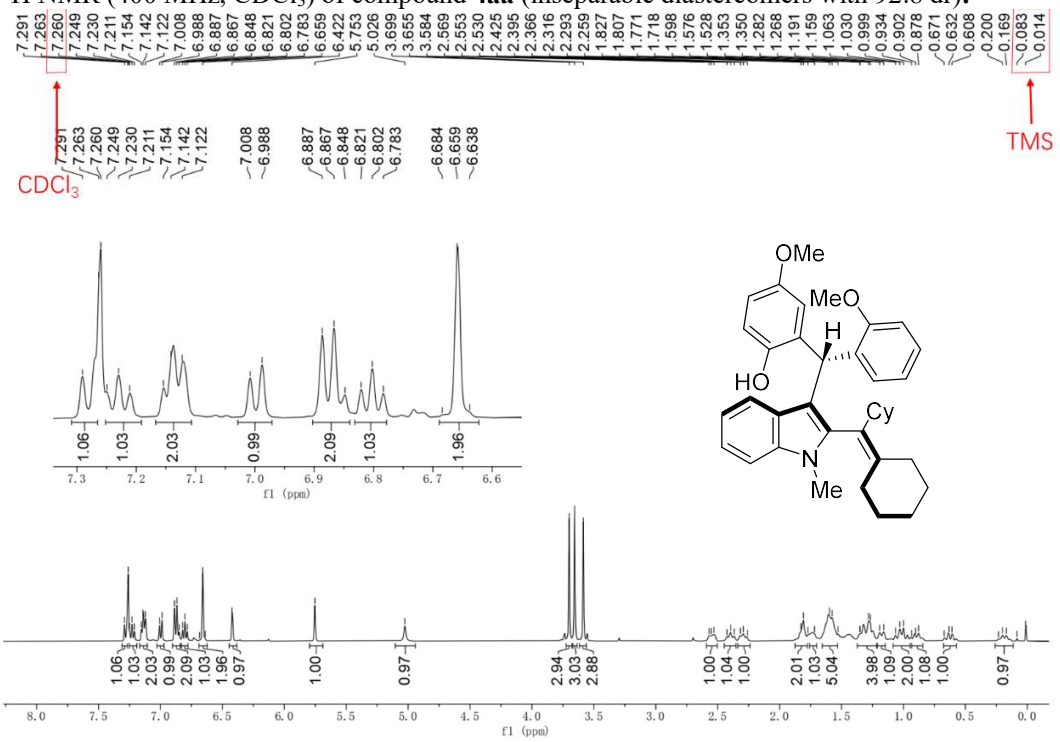
^{1}H NMR (400 MHz, $CDCl_3$) of compound **3ga**:



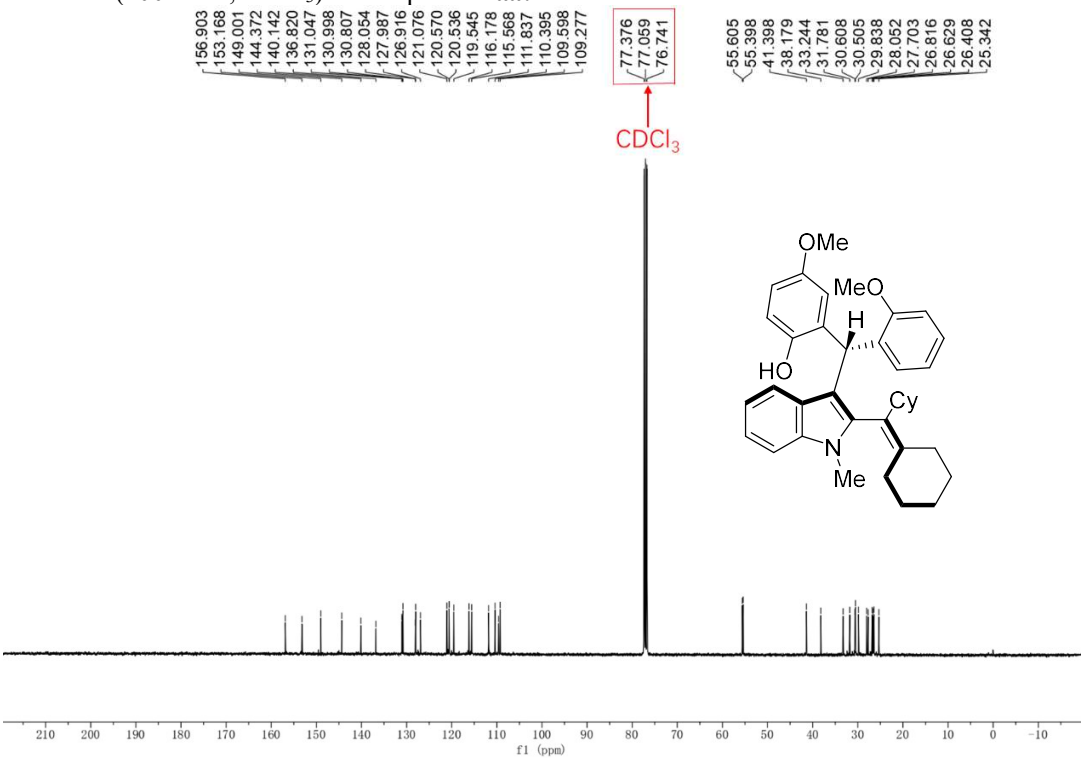
^{13}C NMR (100 MHz, $CDCl_3$) of compound **3ga**:



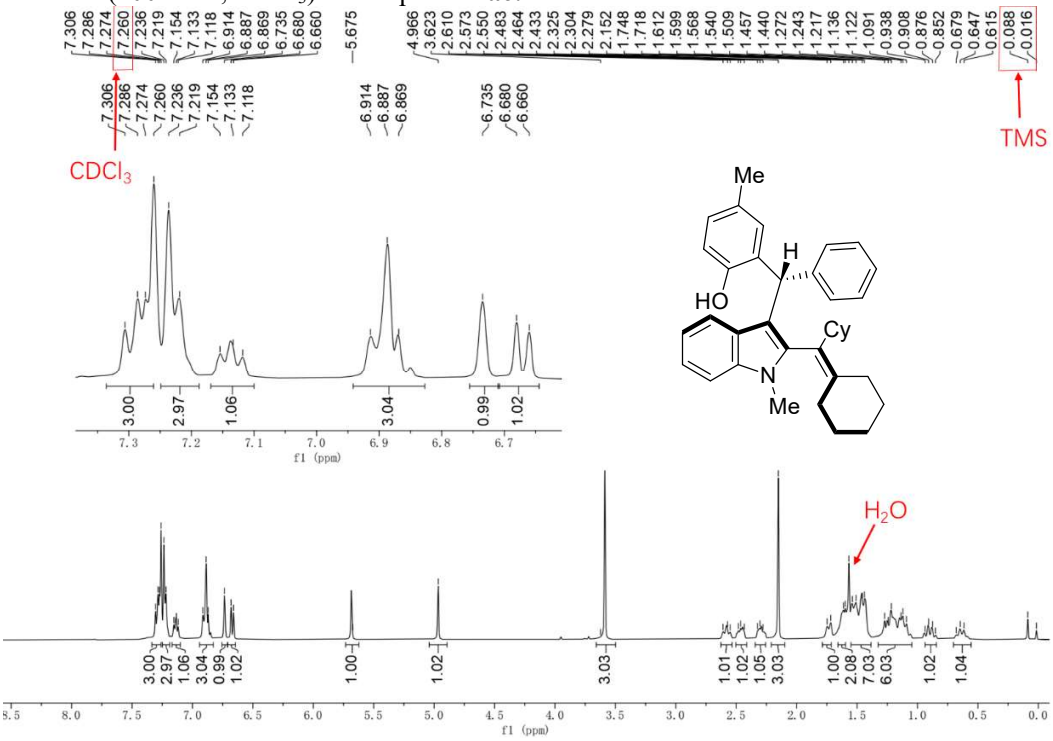
^{1}H NMR (400 MHz, $CDCl_3$) of compound **4aa** (inseparable diastereomers with 92:8 dr)**:**



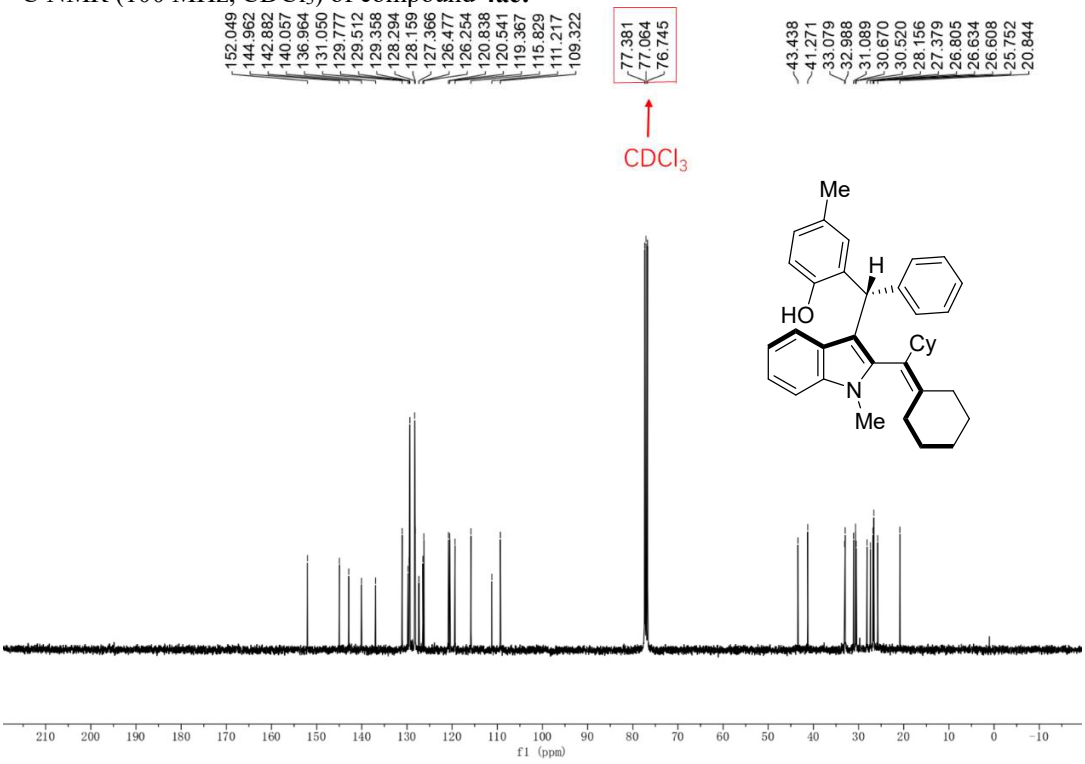
^{13}C NMR (100 MHz, $CDCl_3$) of compound **4aa:**



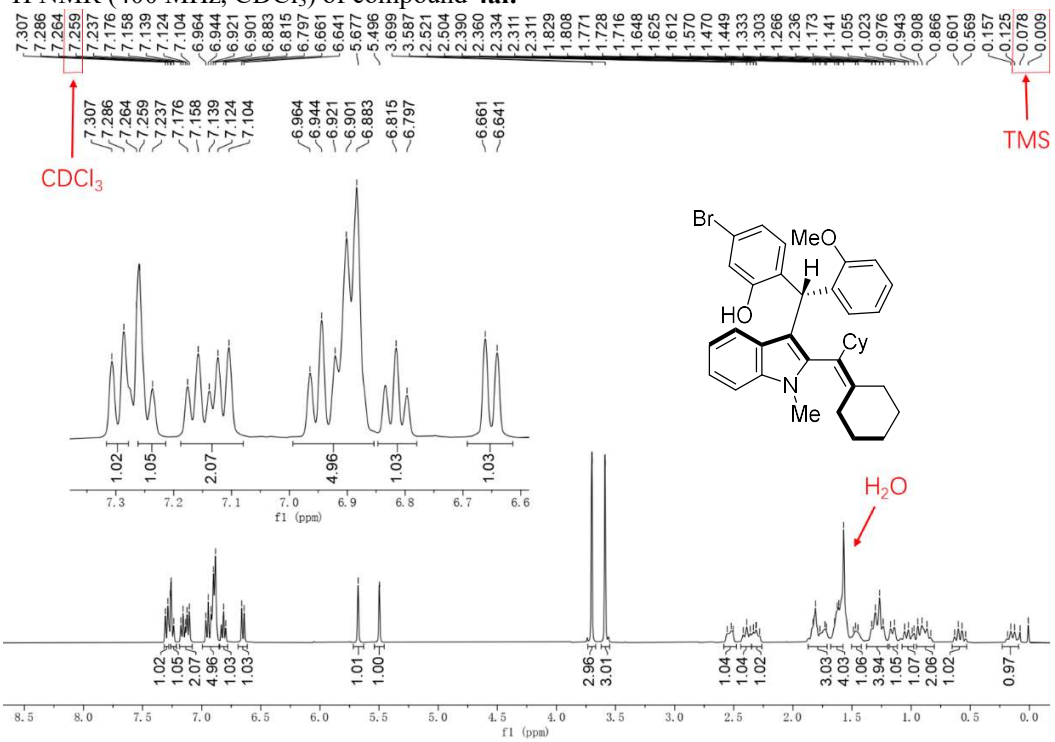
^{1}H NMR (400 MHz, $CDCl_3$) of compound **4ac:**



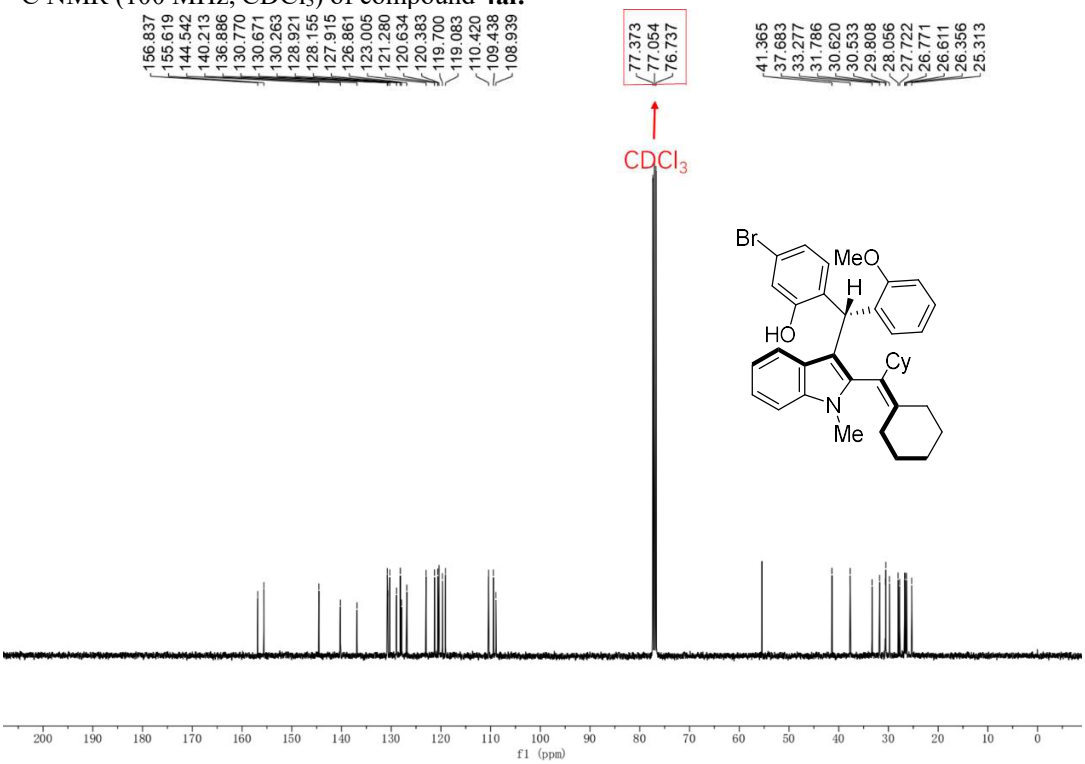
^{13}C NMR (100 MHz, $CDCl_3$) of compound **4ac:**



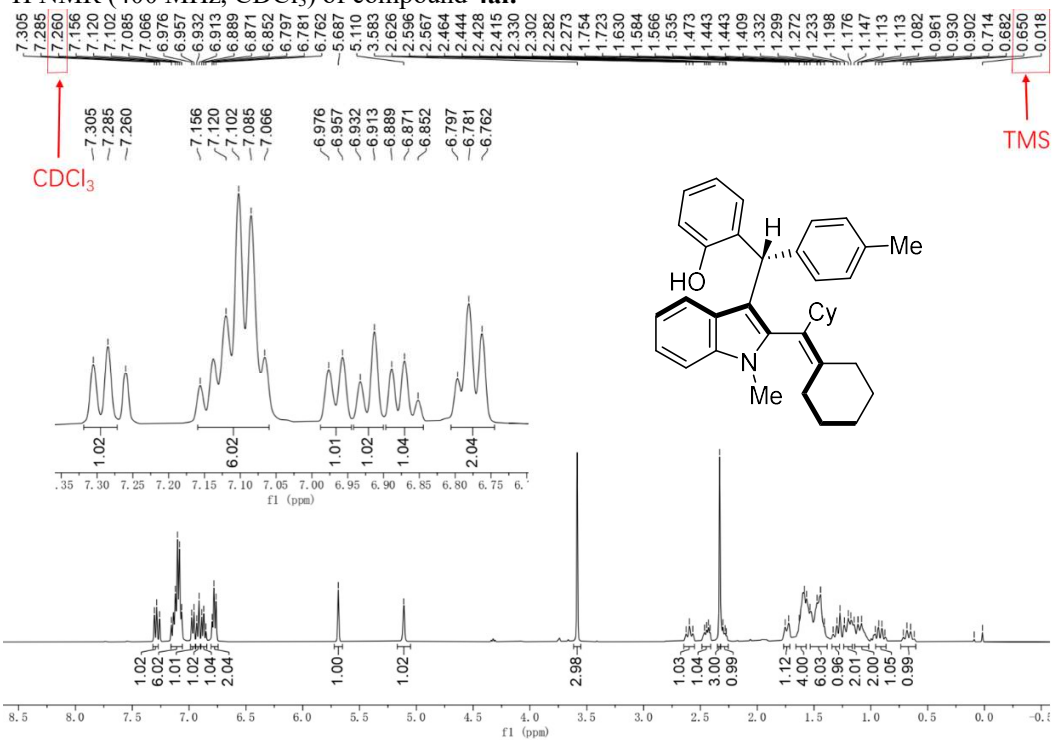
^{1}H NMR (400 MHz, $CDCl_3$) of compound **4al:**



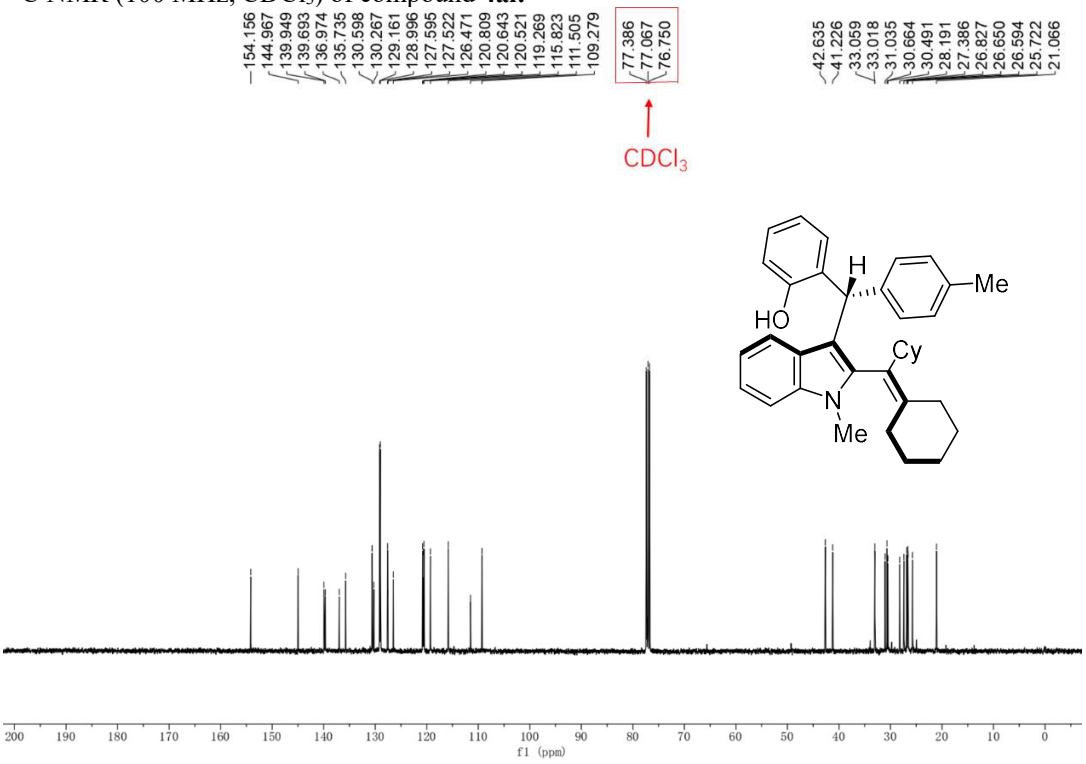
^{13}C NMR (100 MHz, $CDCl_3$) of compound **4al:**



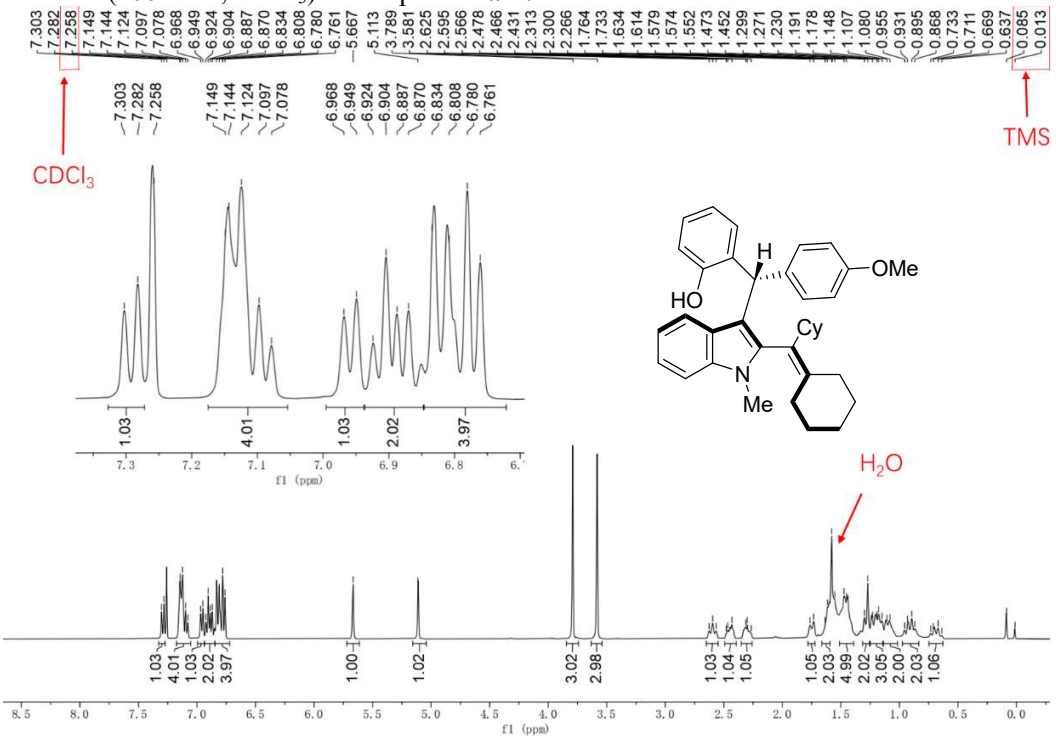
^{1}H NMR (400 MHz, $CDCl_3$) of compound **4ai:**



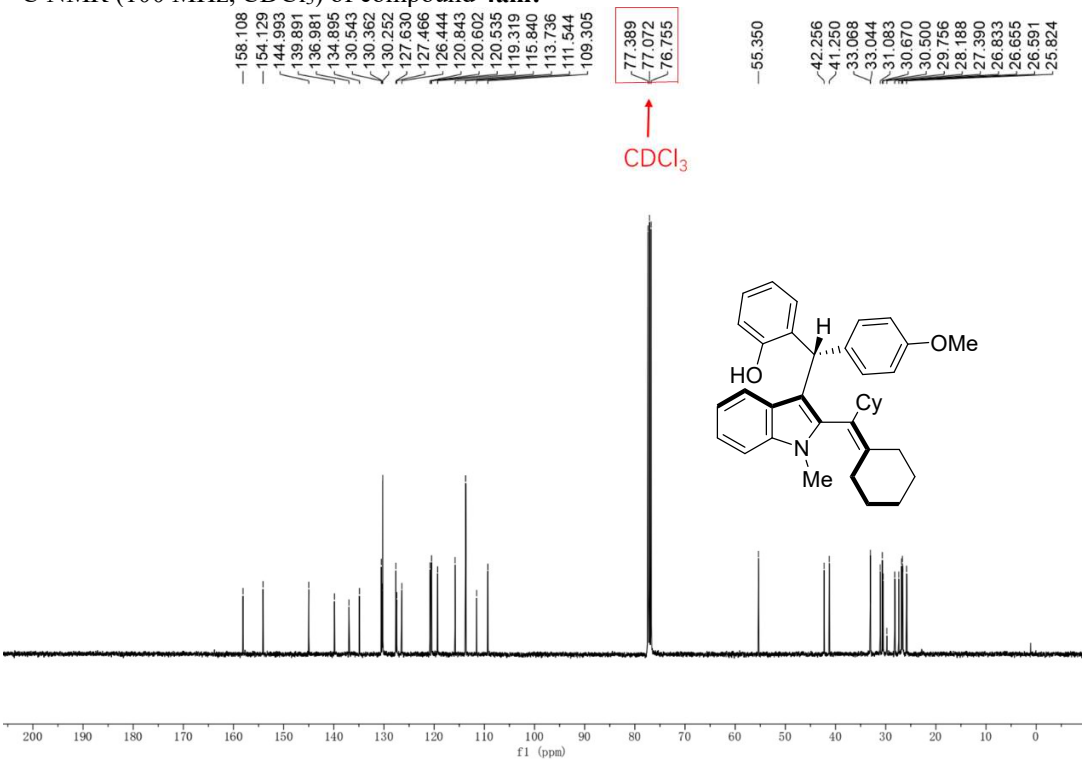
^{13}C NMR (100 MHz, $CDCl_3$) of compound **4ai:**



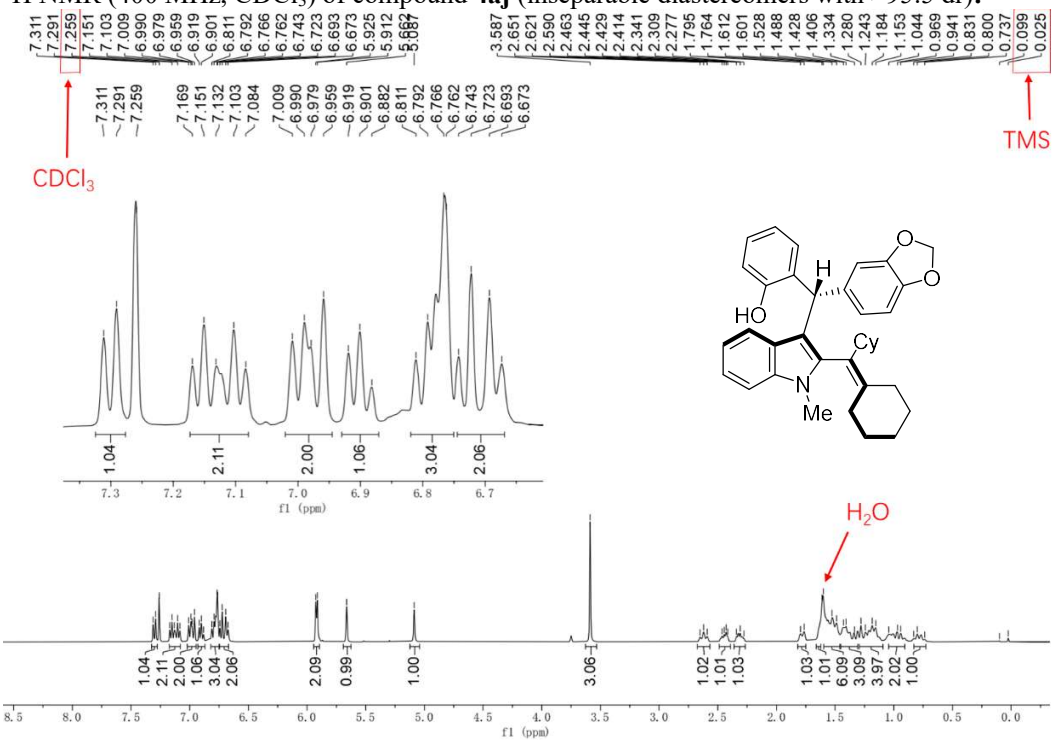
^{1}H NMR (400 MHz, $CDCl_3$) of compound **4am:**



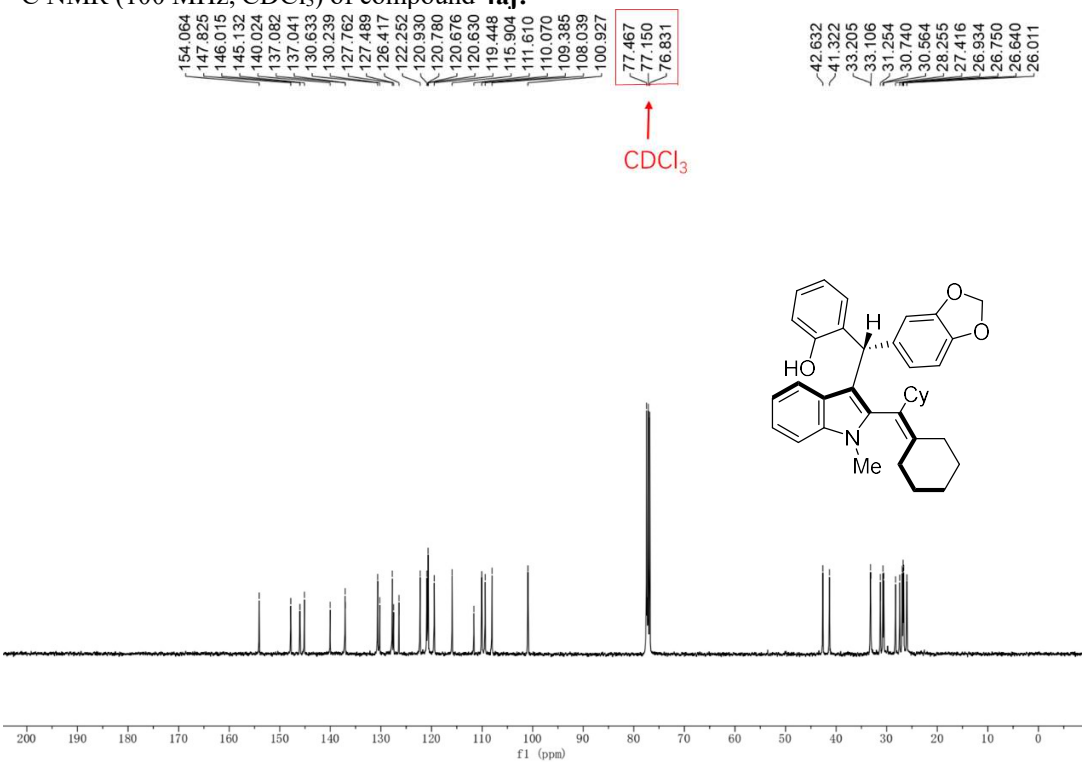
^{13}C NMR (100 MHz, $CDCl_3$) of compound **4am:**



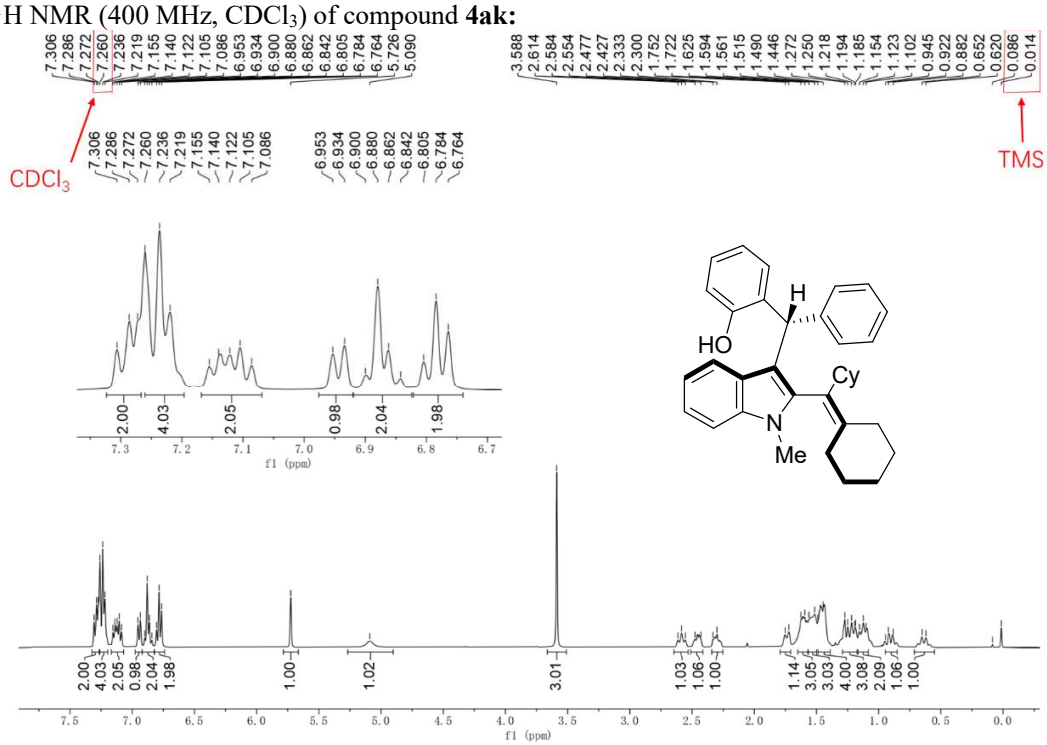
^{1}H NMR (400 MHz, $CDCl_3$) of compound **4aj** (inseparable diastereomers with >95:5 dr)**:**



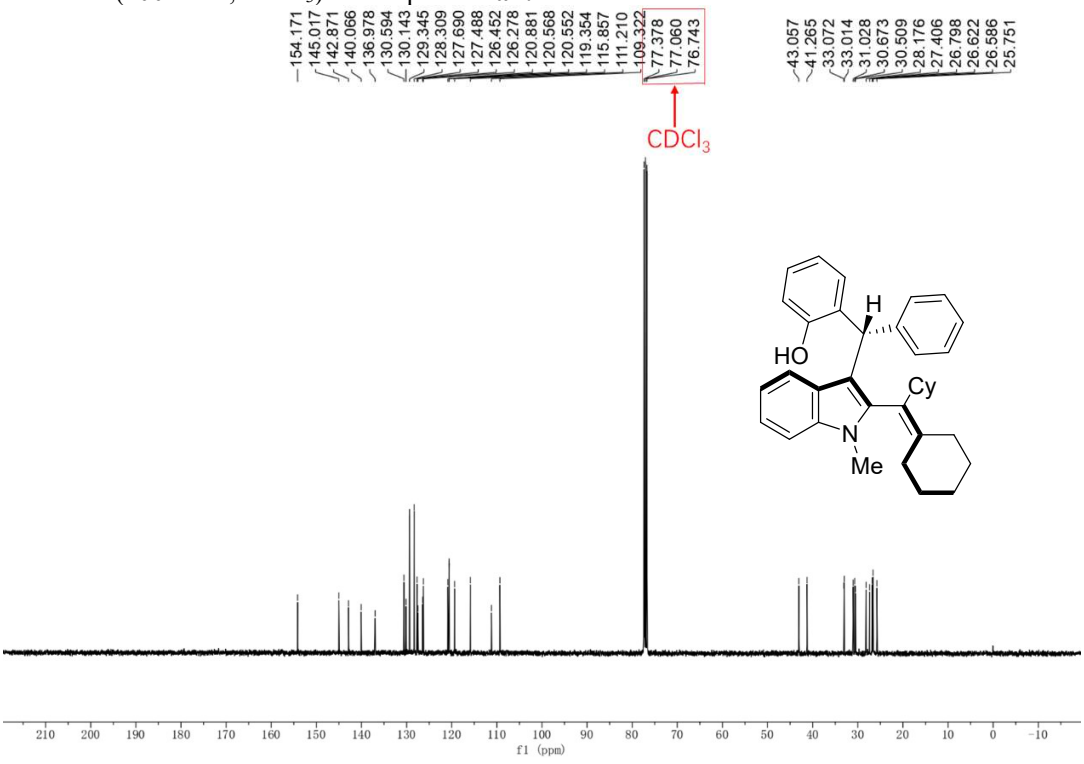
^{13}C NMR (100 MHz, $CDCl_3$) of compound **4aj:**



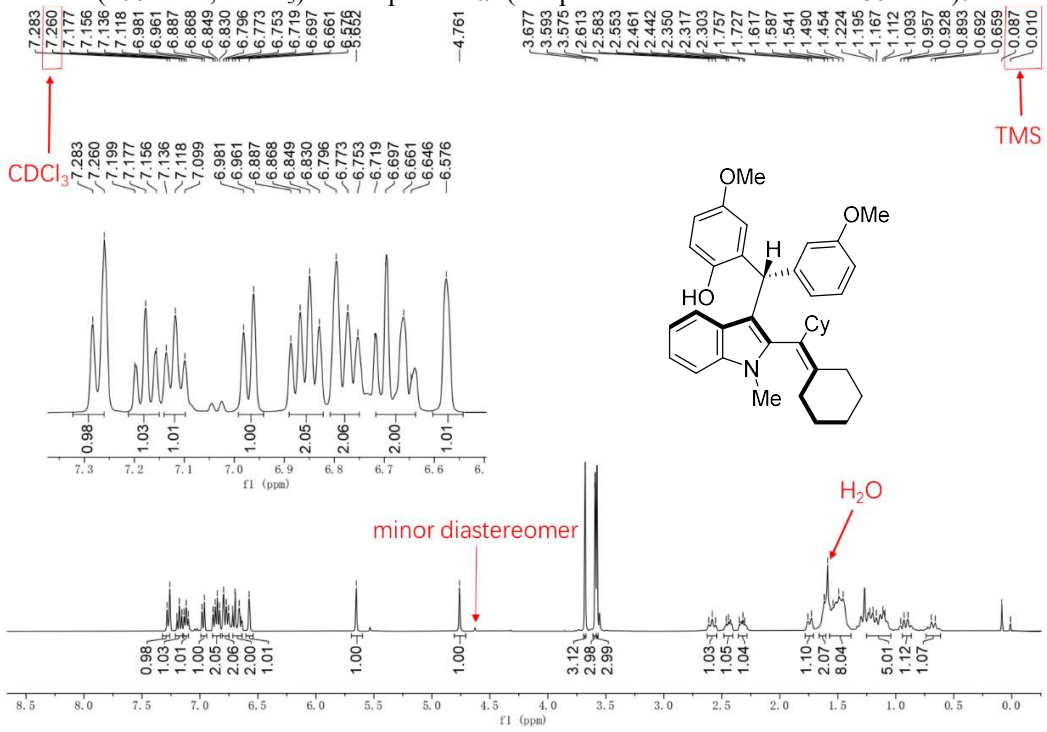
^{1}H NMR (400 MHz, $CDCl_3$) of compound **4ak:**



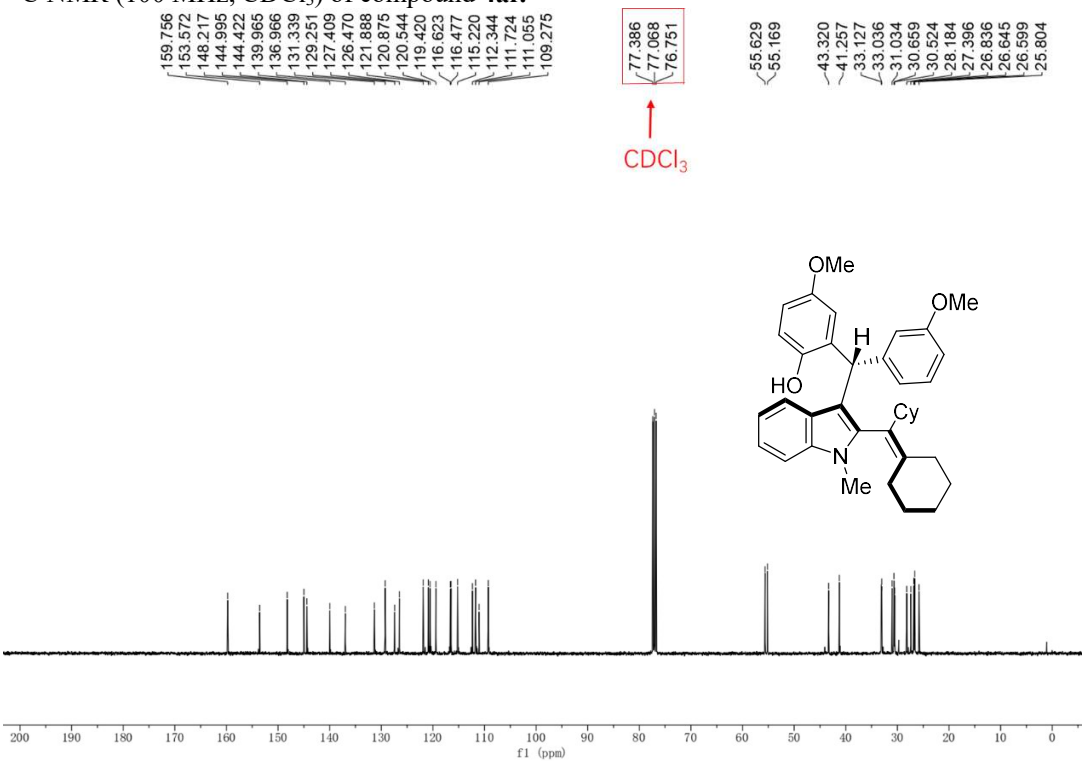
^{13}C NMR (100 MHz, $CDCl_3$) of compound **4ak:**



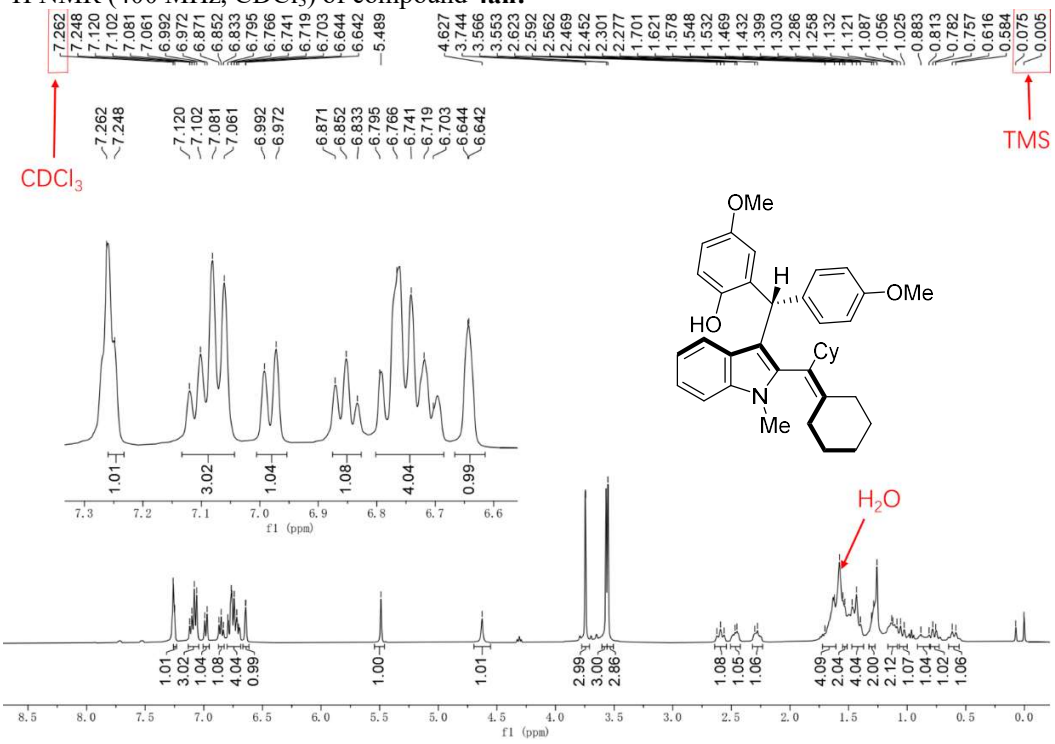
^{1}H NMR (400 MHz, $CDCl_3$) of compound **4af** (inseparable diastereomers with 86:14 dr)**:**



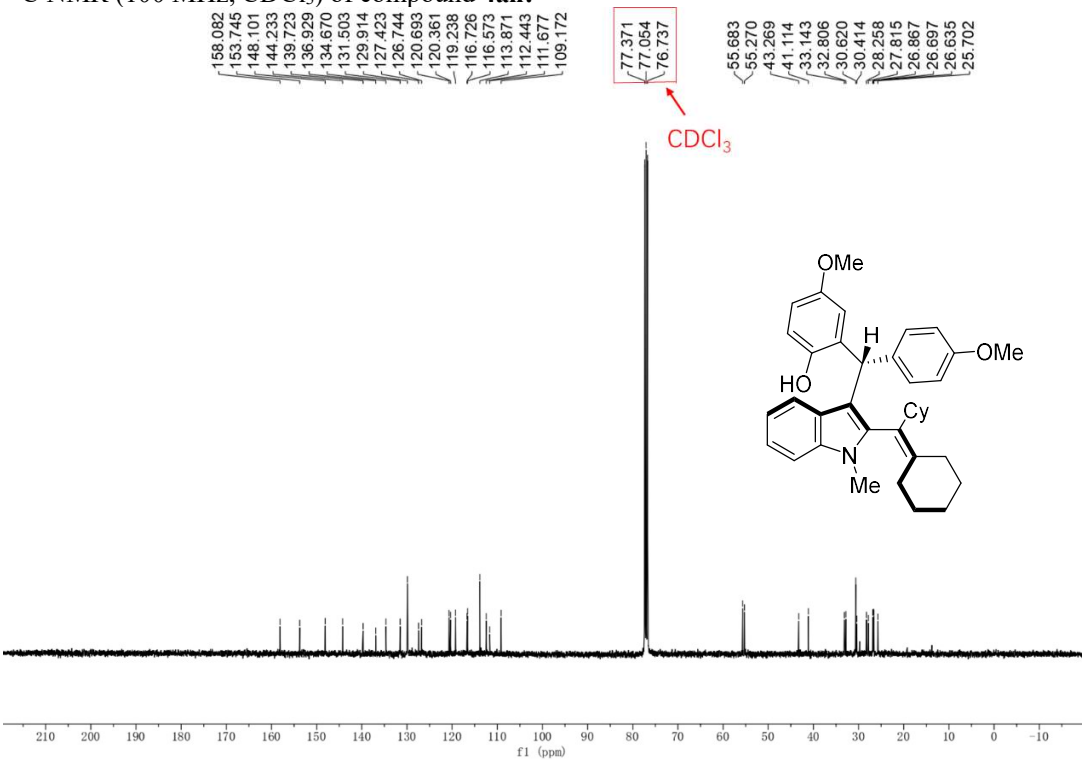
^{13}C NMR (100 MHz, $CDCl_3$) of compound **4af:**



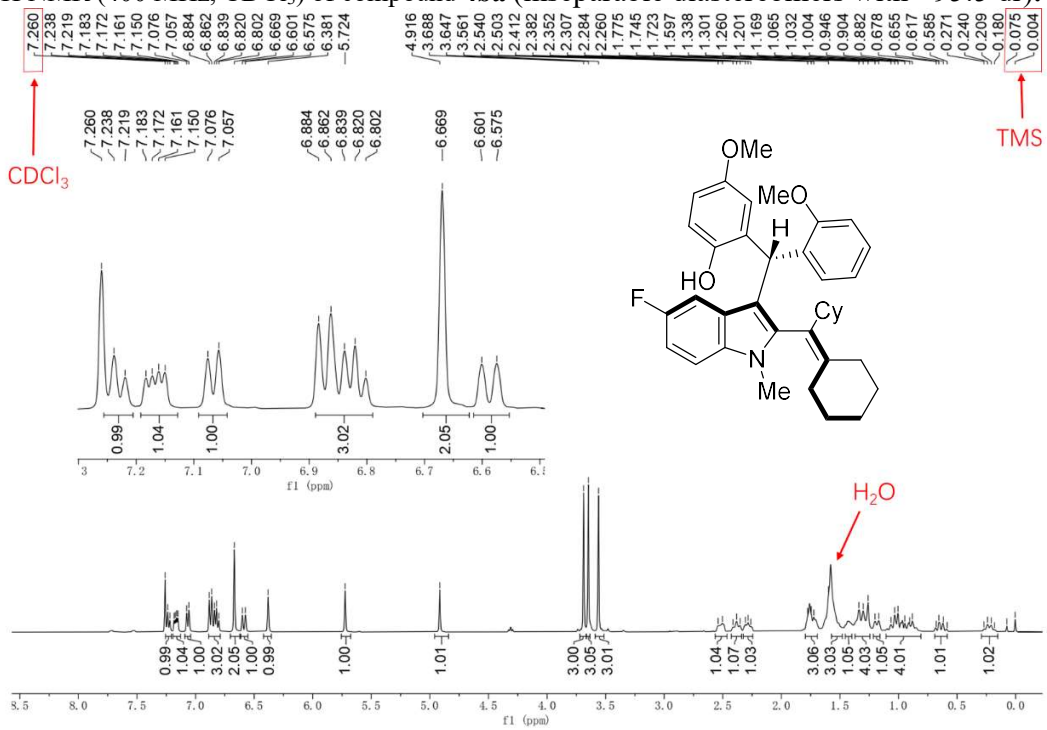
^{1}H NMR (400 MHz, $CDCl_3$) of compound **4ah:**



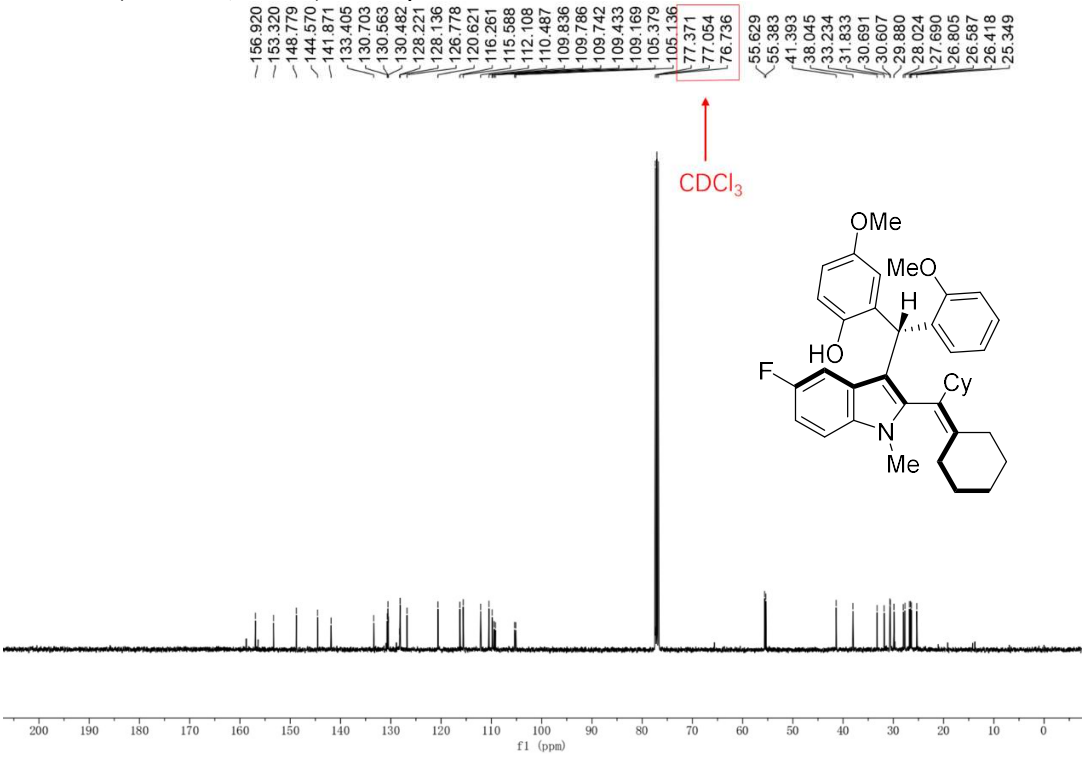
^{13}C NMR (100 MHz, $CDCl_3$) of compound **4ah:**



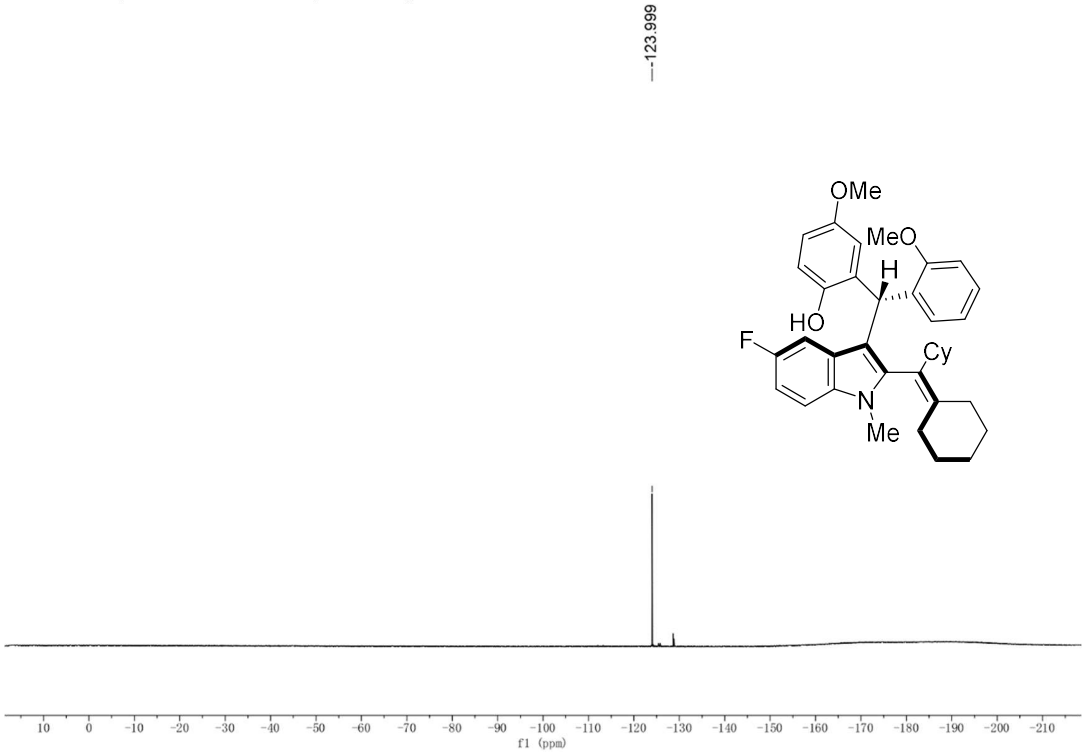
^{1}H NMR (400 MHz, $CDCl_3$) of compound **4ba** (inseparable diastereomers with >95:5 dr)**:**



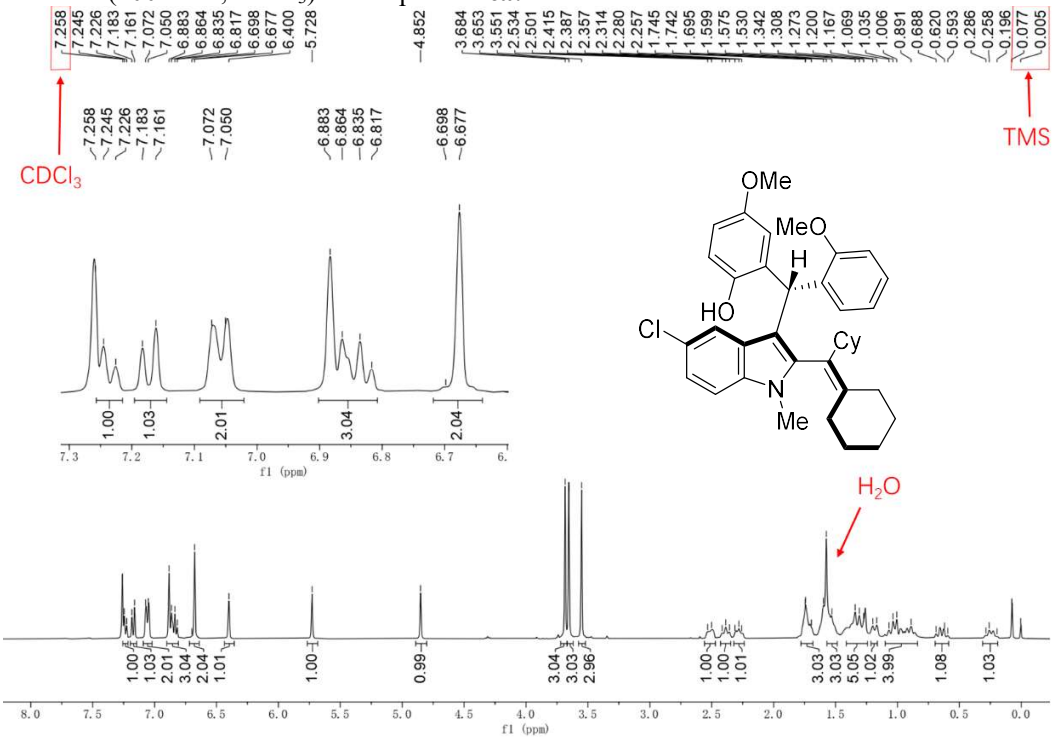
^{13}C NMR (100 MHz, $CDCl_3$) of compound **4ba:**



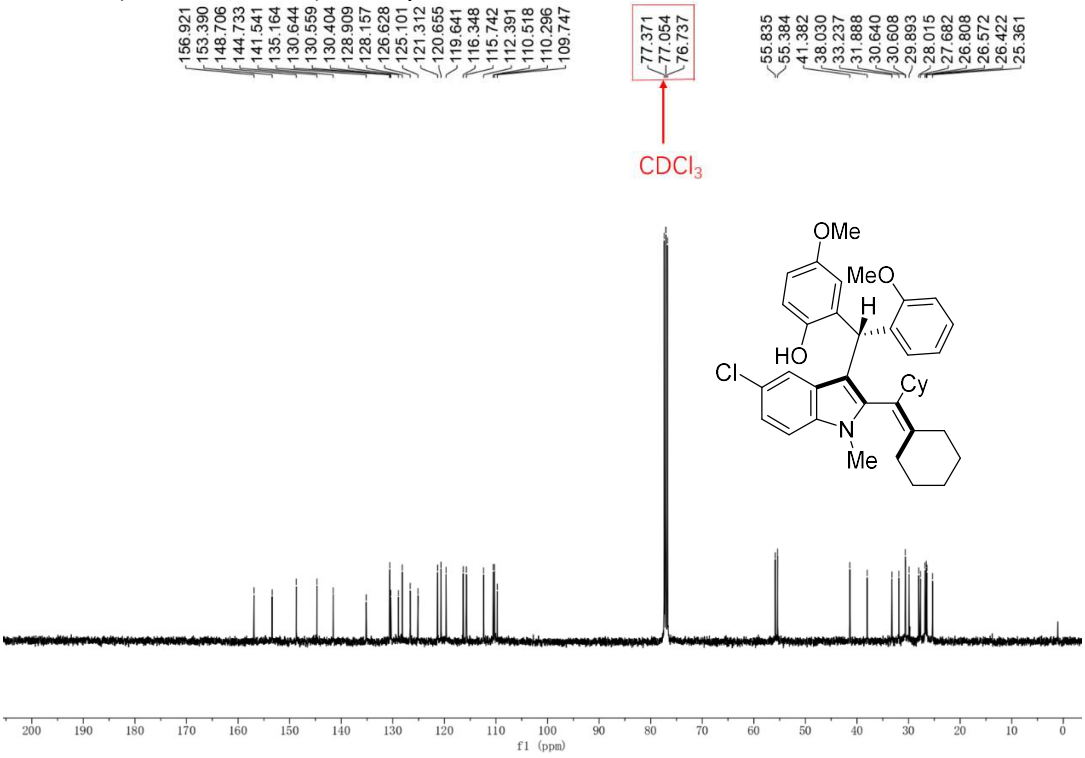
^{19}F NMR (376 MHz, $CDCl_3$) of compound **4ba:**



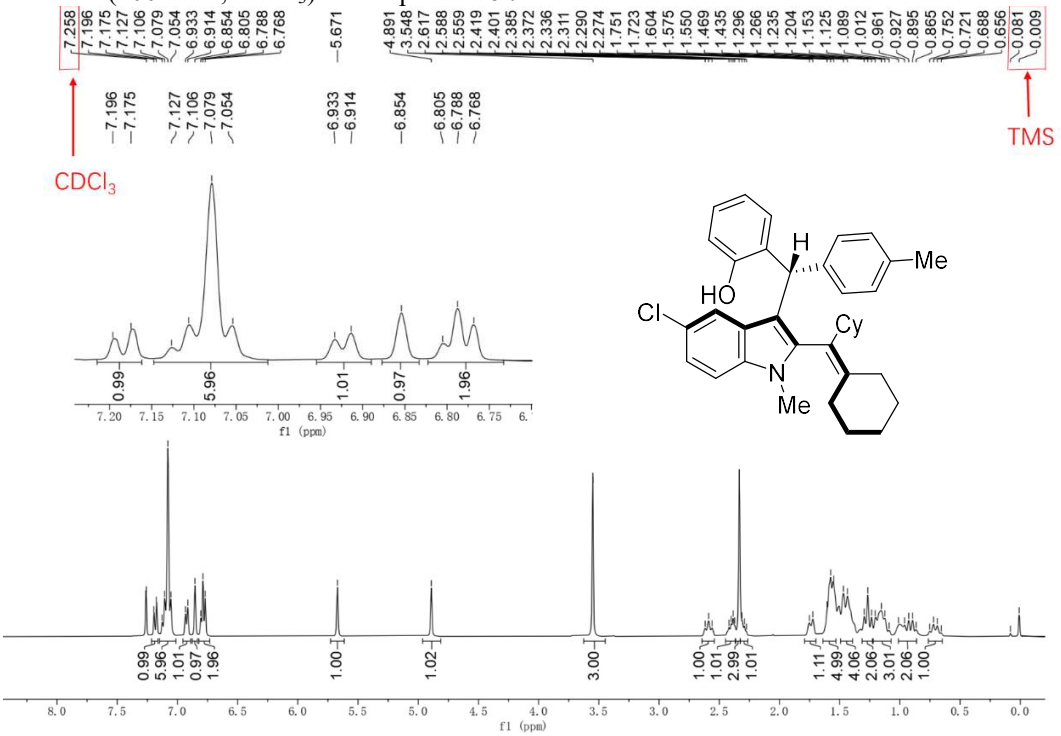
^{1}H NMR (400 MHz, $CDCl_3$) of compound **4ca:**



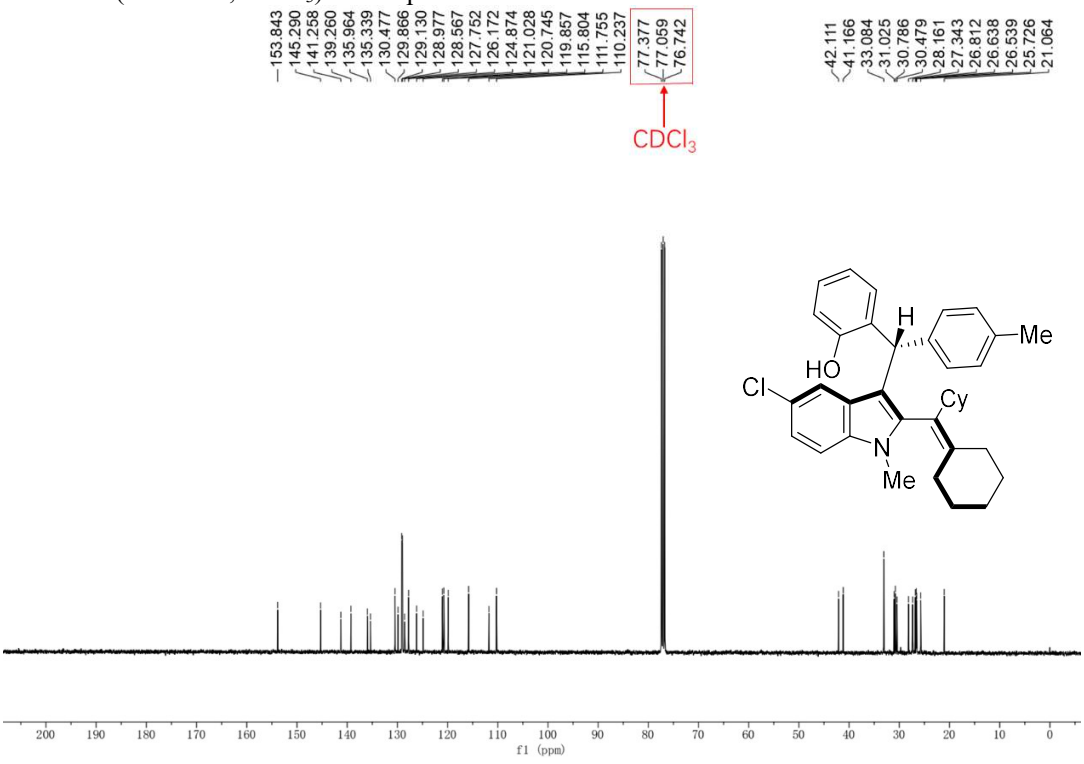
^{13}C NMR (100 MHz, $CDCl_3$) of compound **4ca:**



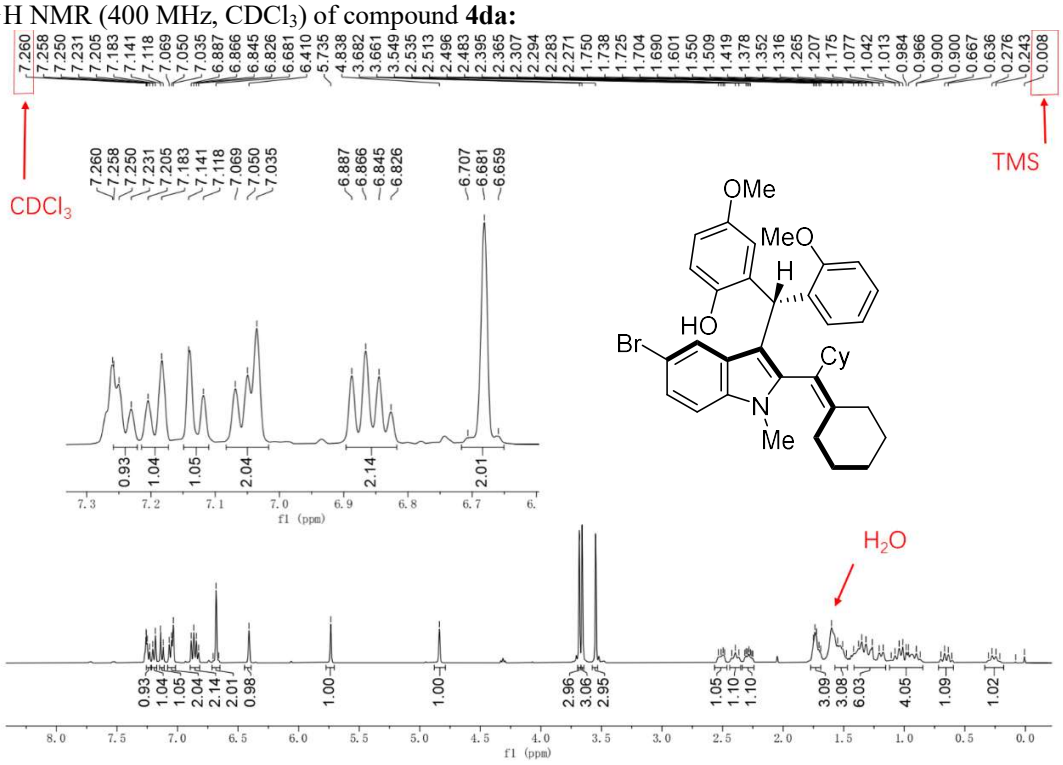
^{1}H NMR (400 MHz, $CDCl_3$) of compound **4ci:**



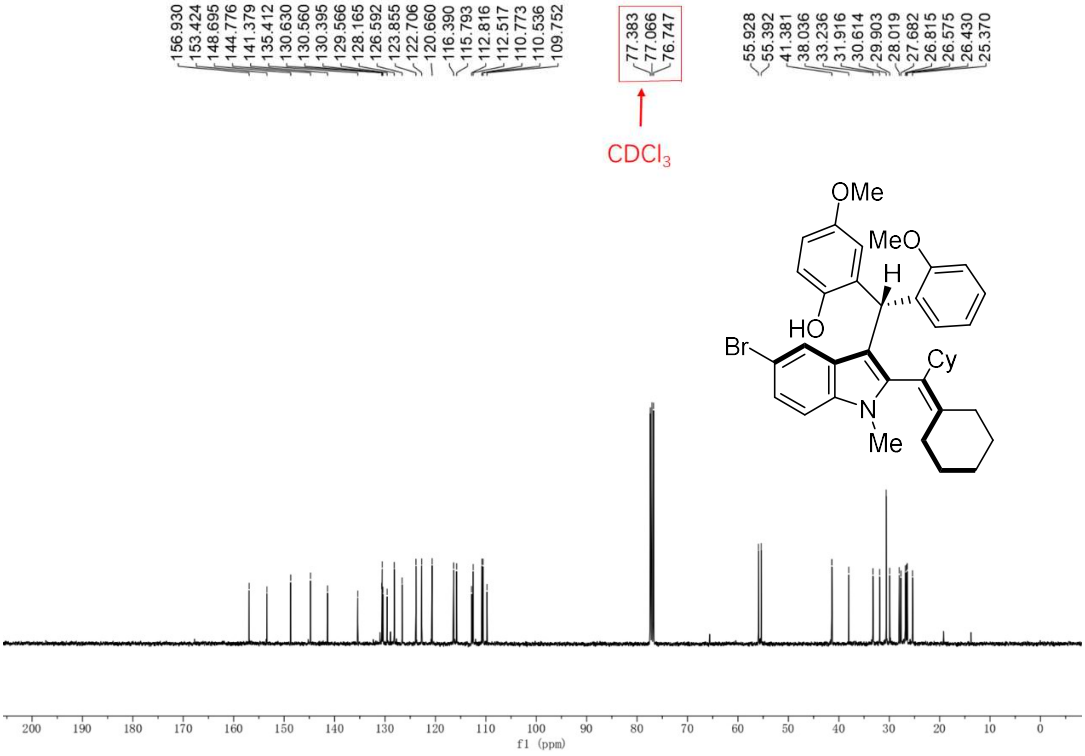
^{13}C NMR (100 MHz, $CDCl_3$) of compound **4ci:**



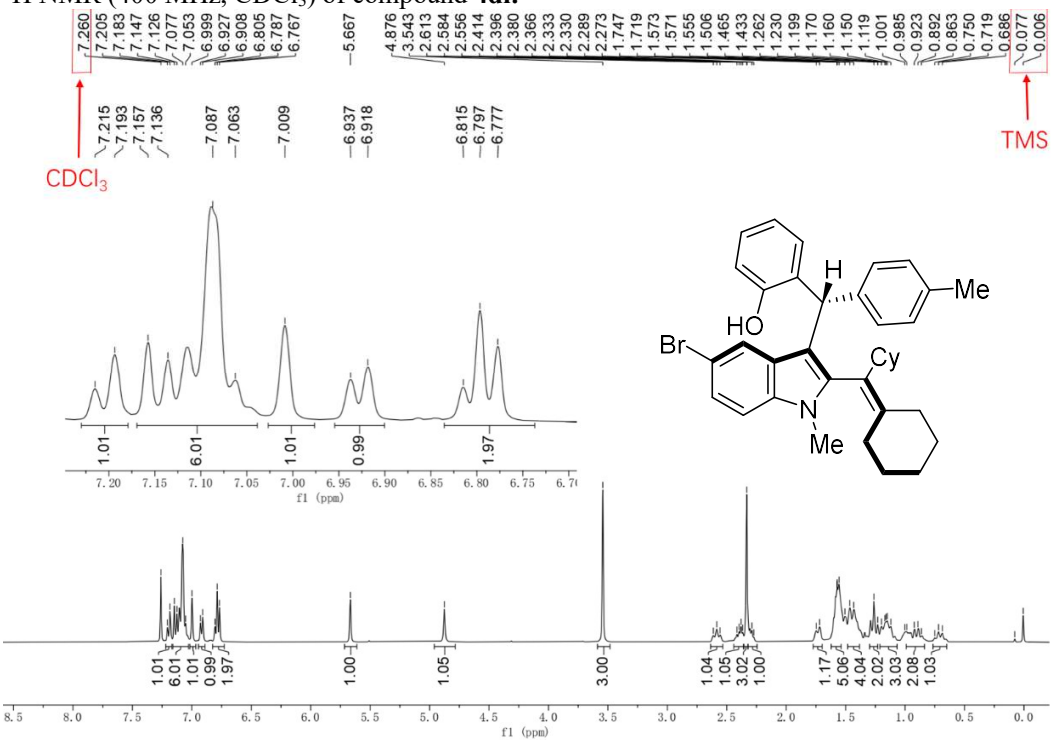
^{1}H NMR (400 MHz, $CDCl_3$) of compound **4da:**



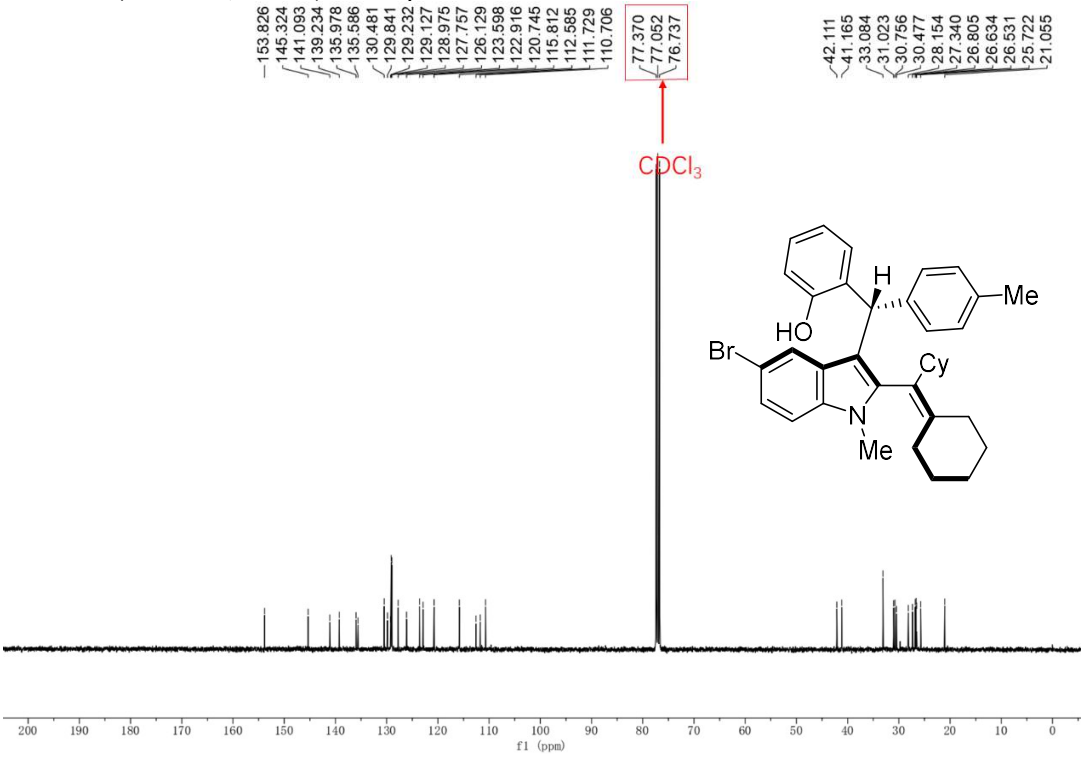
^{13}C NMR (100 MHz, $CDCl_3$) of compound **4da:**



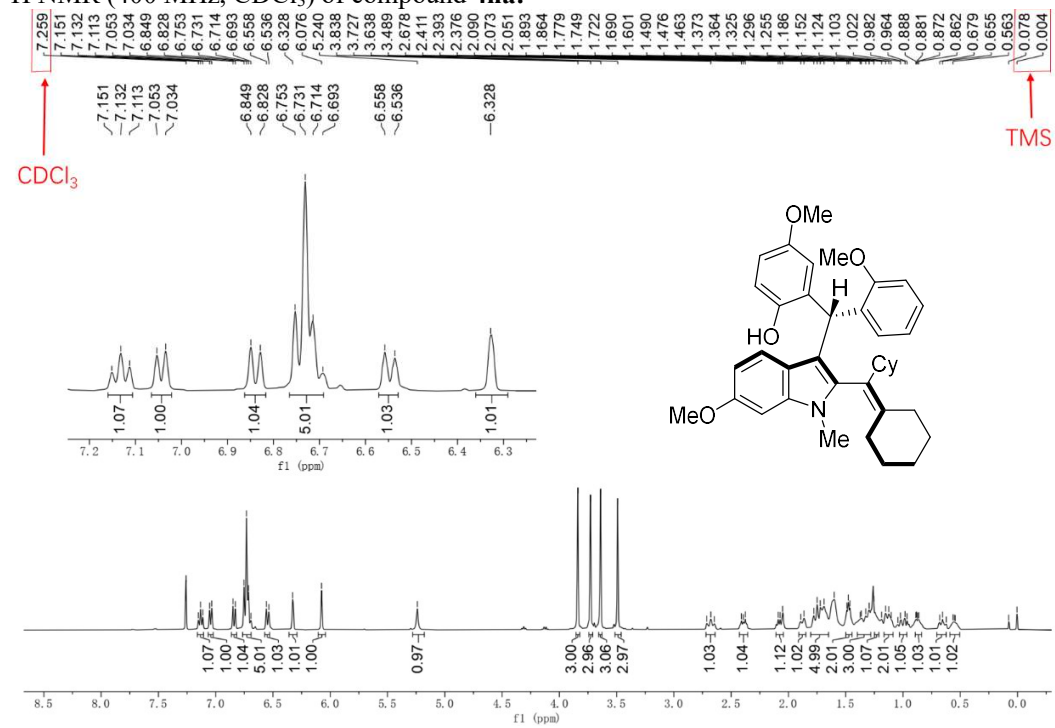
^{1}H NMR (400 MHz, $CDCl_3$) of compound **4di:**



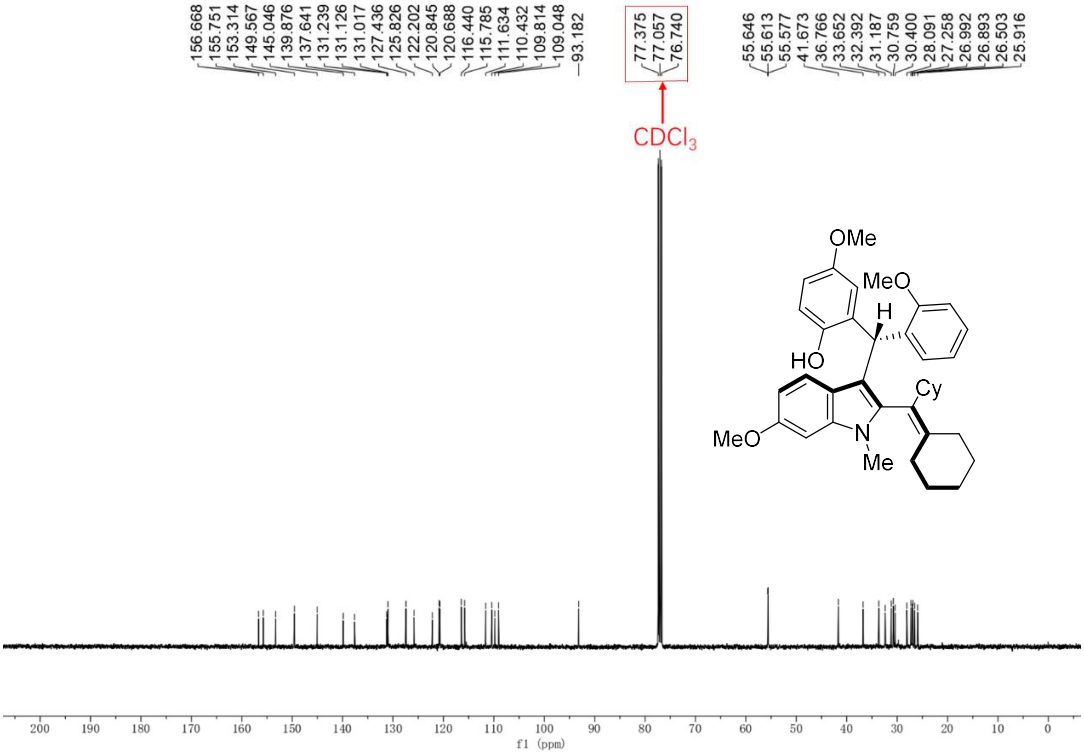
^{13}C NMR (100 MHz, $CDCl_3$) of compound **4di:**



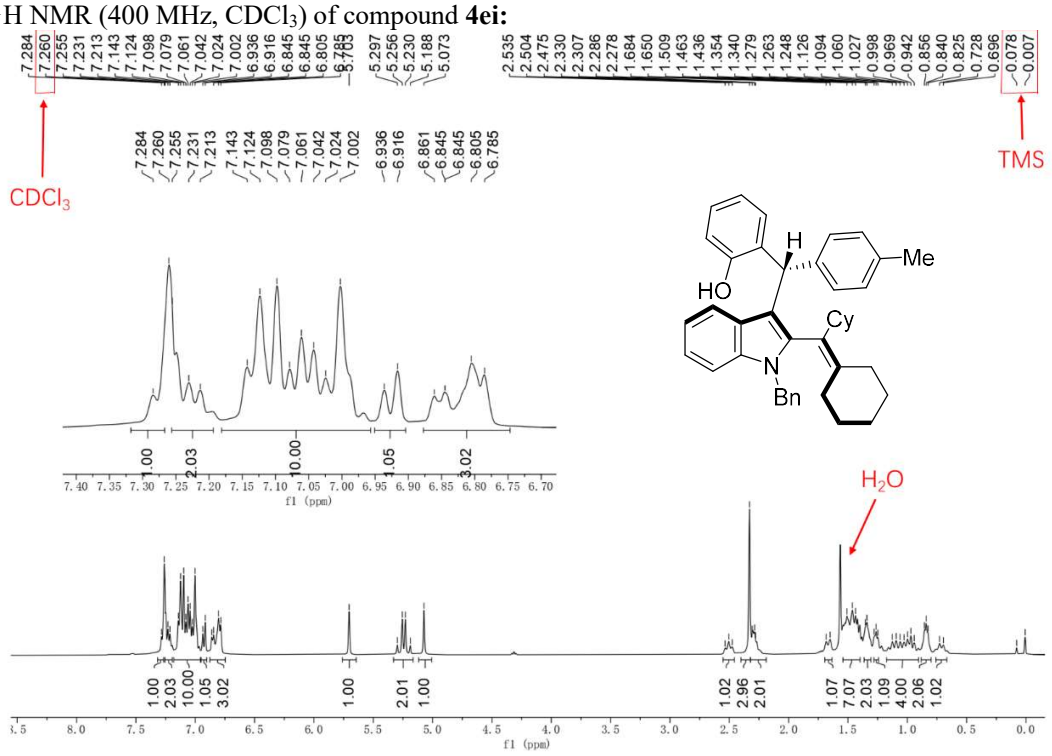
^{1}H NMR (400 MHz, $CDCl_3$) of compound **4ha:**



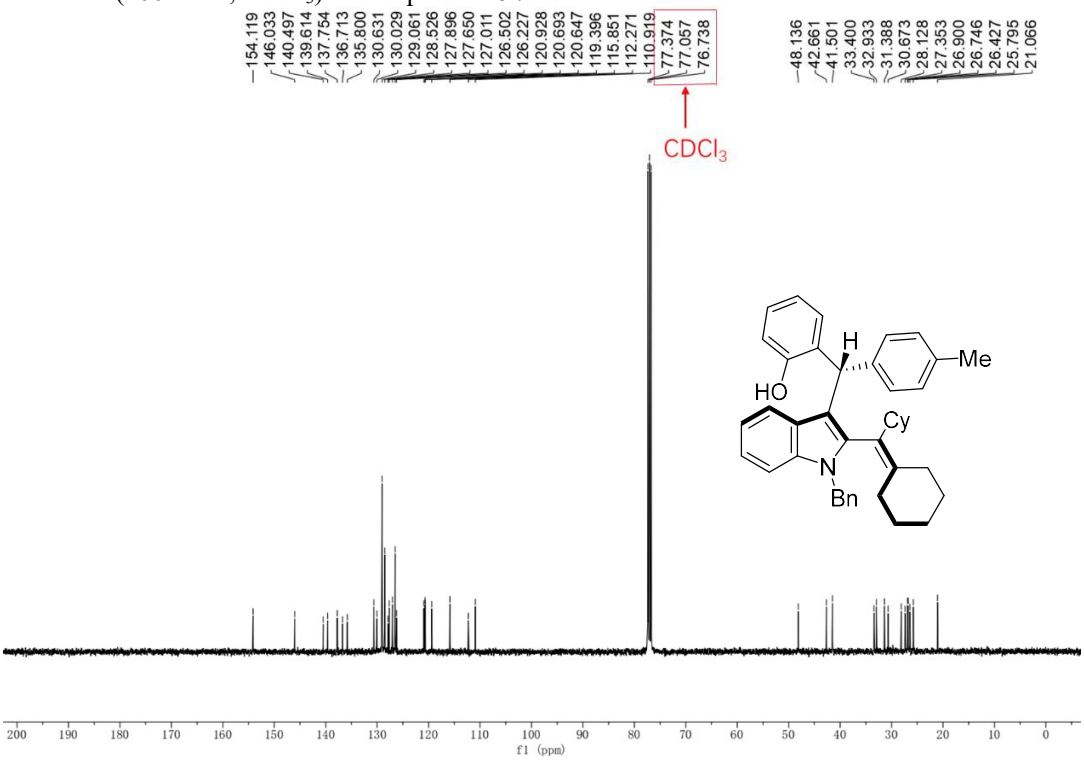
^{13}C NMR (100 MHz, $CDCl_3$) of compound **4ha:**



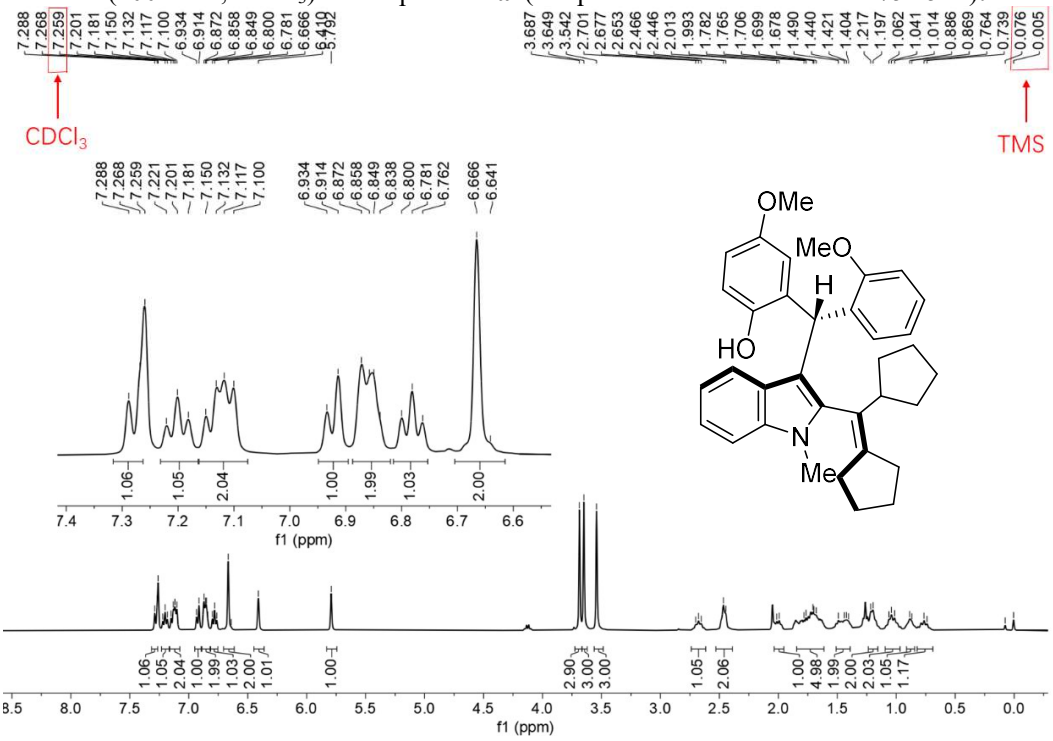
^{1}H NMR (400 MHz, $CDCl_3$) of compound **4ei:**



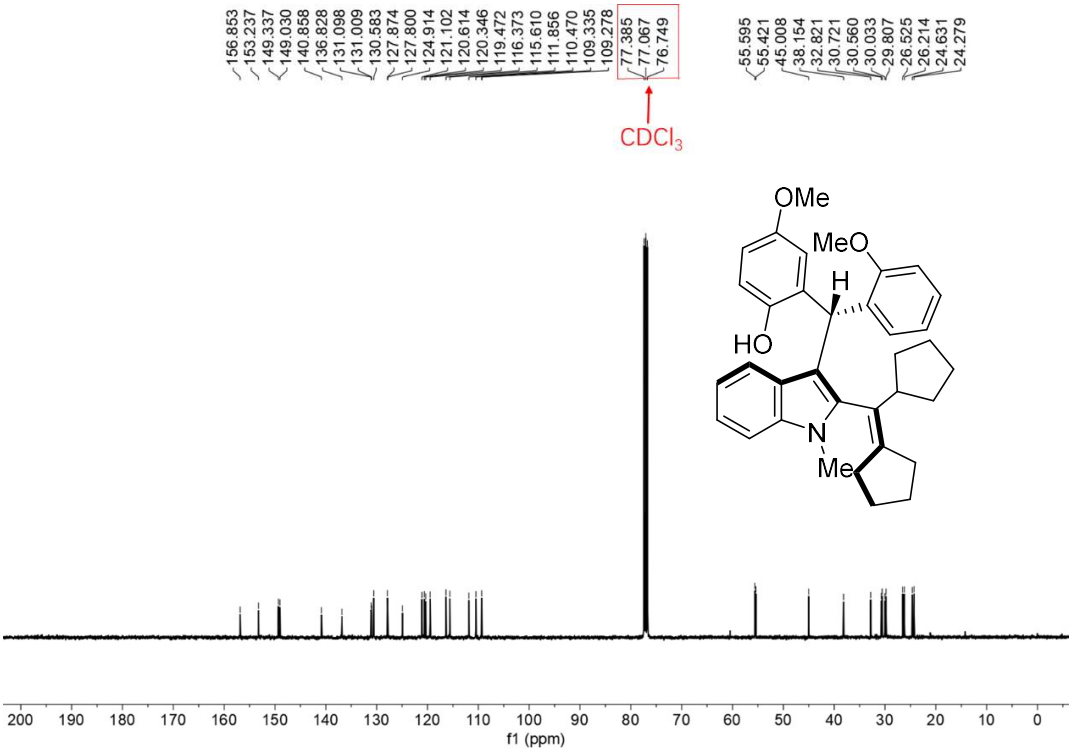
^{13}C NMR (100 MHz, $CDCl_3$) of compound **4ei:**



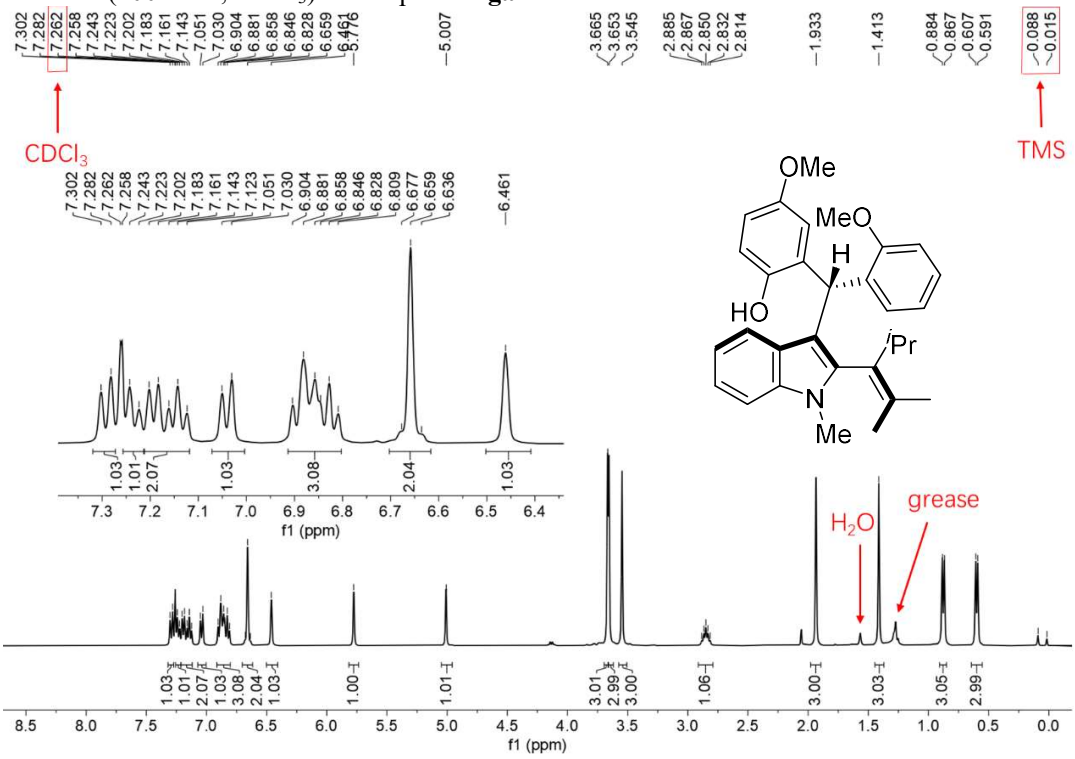
^{1}H NMR (400 MHz, $CDCl_3$) of compound **4fa** (inseparable diastereomers with 75:25 dr)**:**



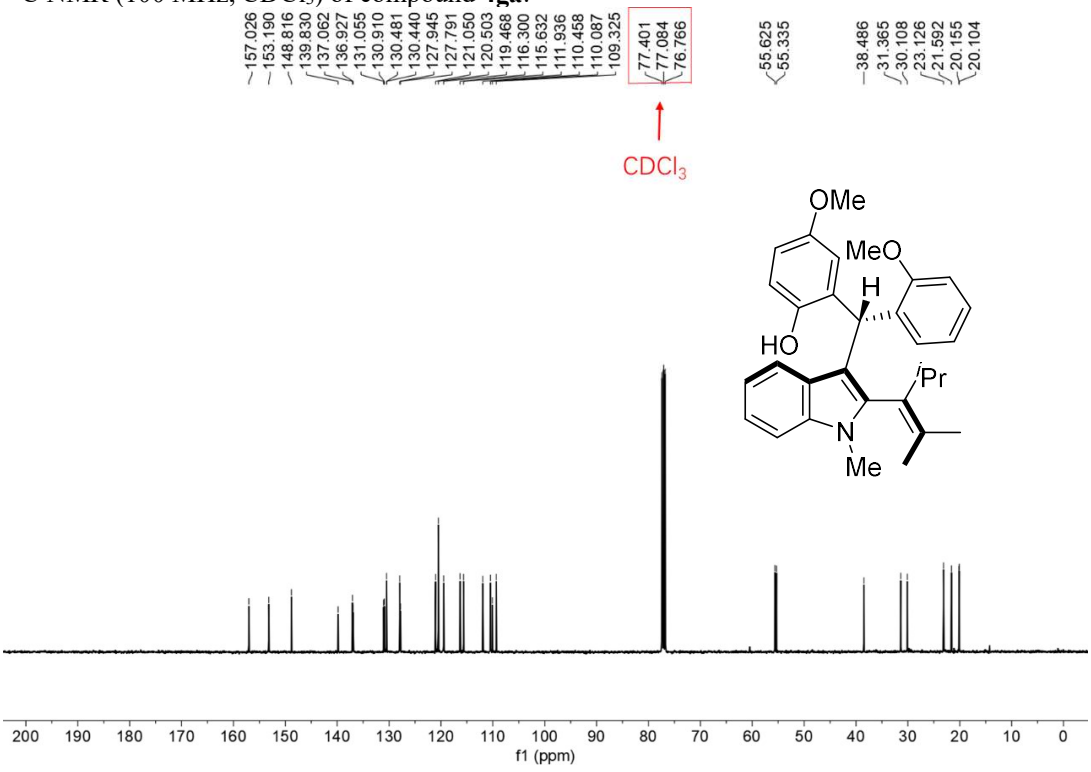
^{13}C NMR (100 MHz, $CDCl_3$) of compound **4fa:**



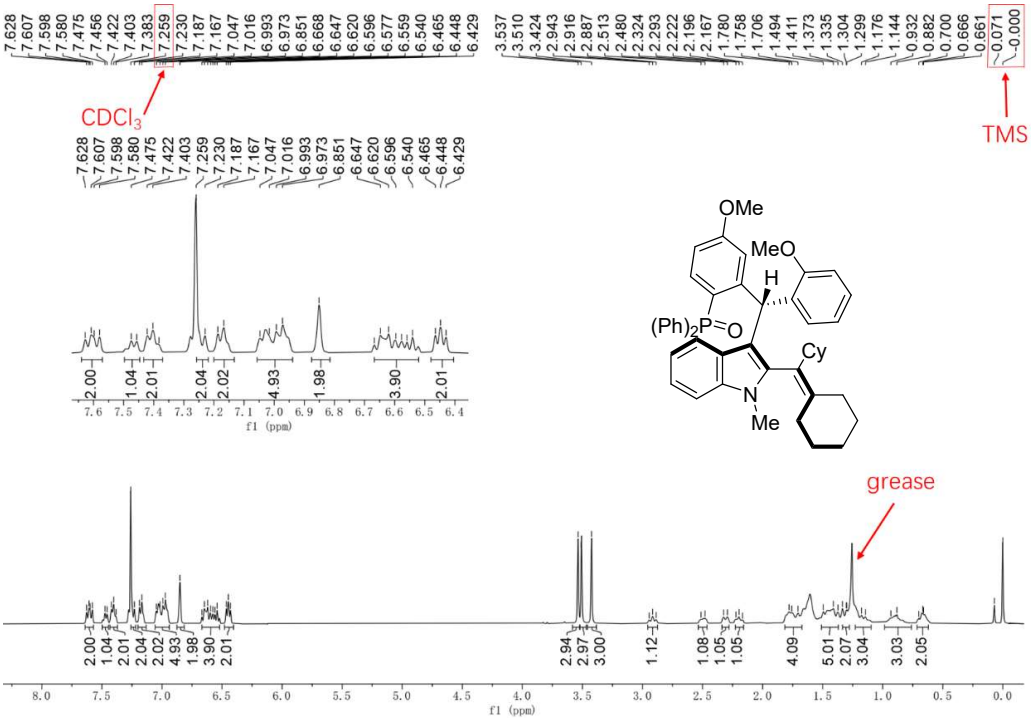
^{1}H NMR (400 MHz, $CDCl_3$) of compound **4ga**:



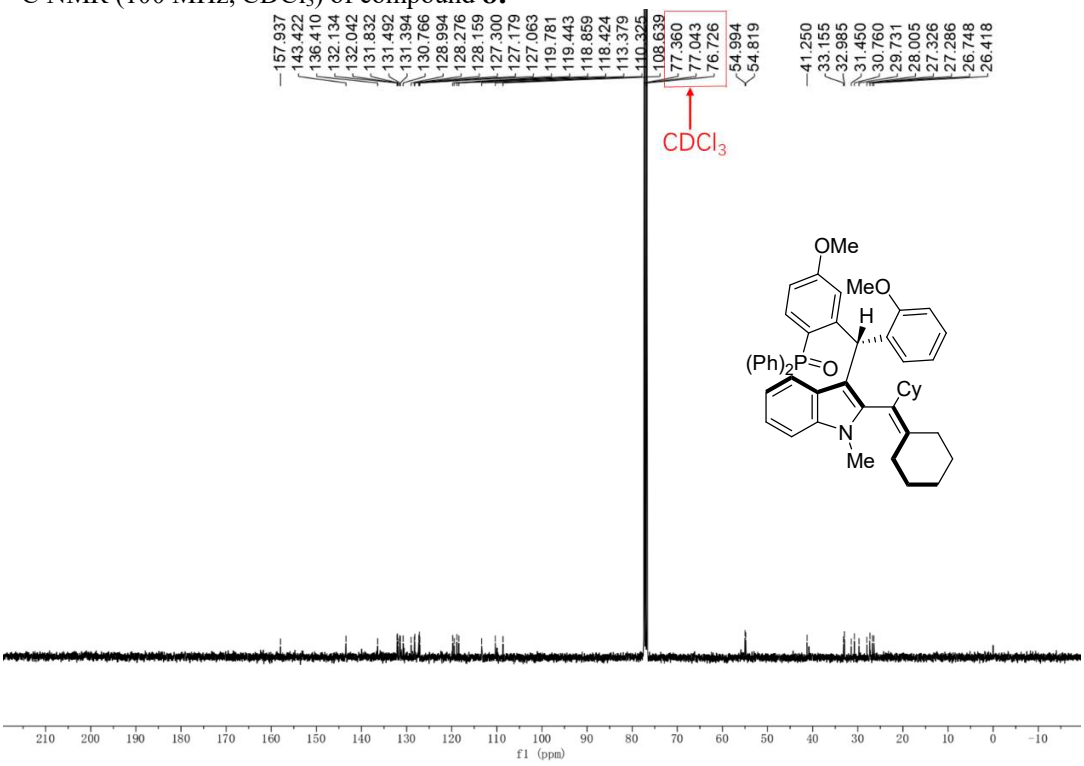
^{13}C NMR (100 MHz, $CDCl_3$) of compound **4ga**:



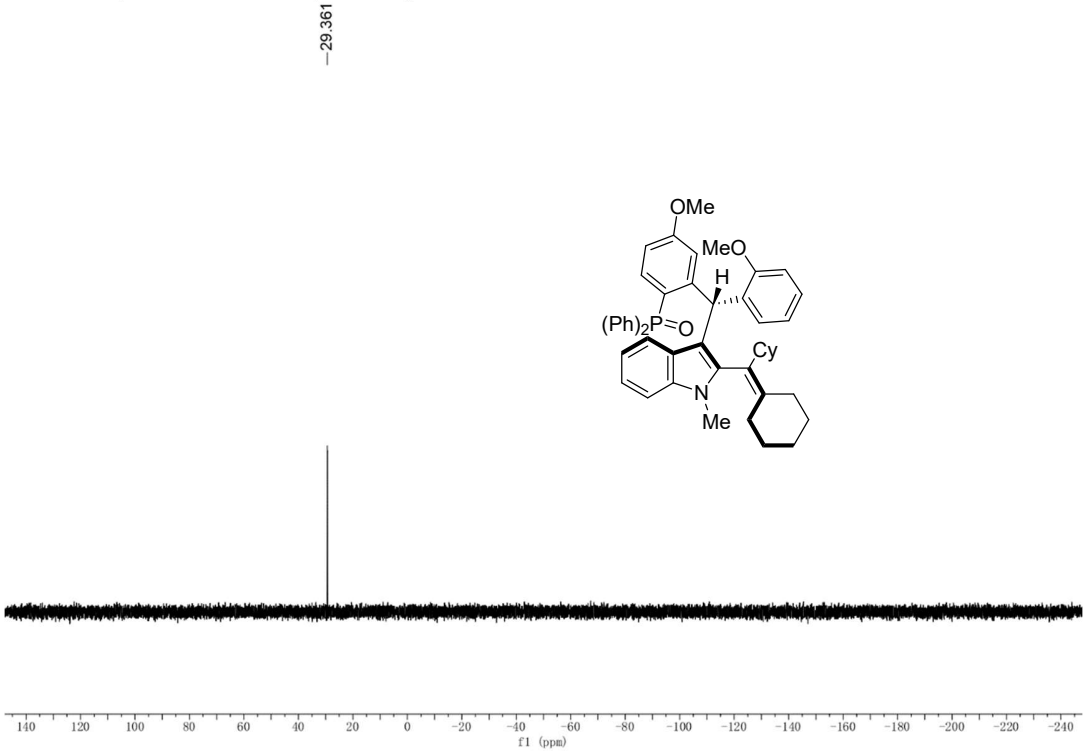
^{1}H NMR (400 MHz, $CDCl_3$) of compound **8:**



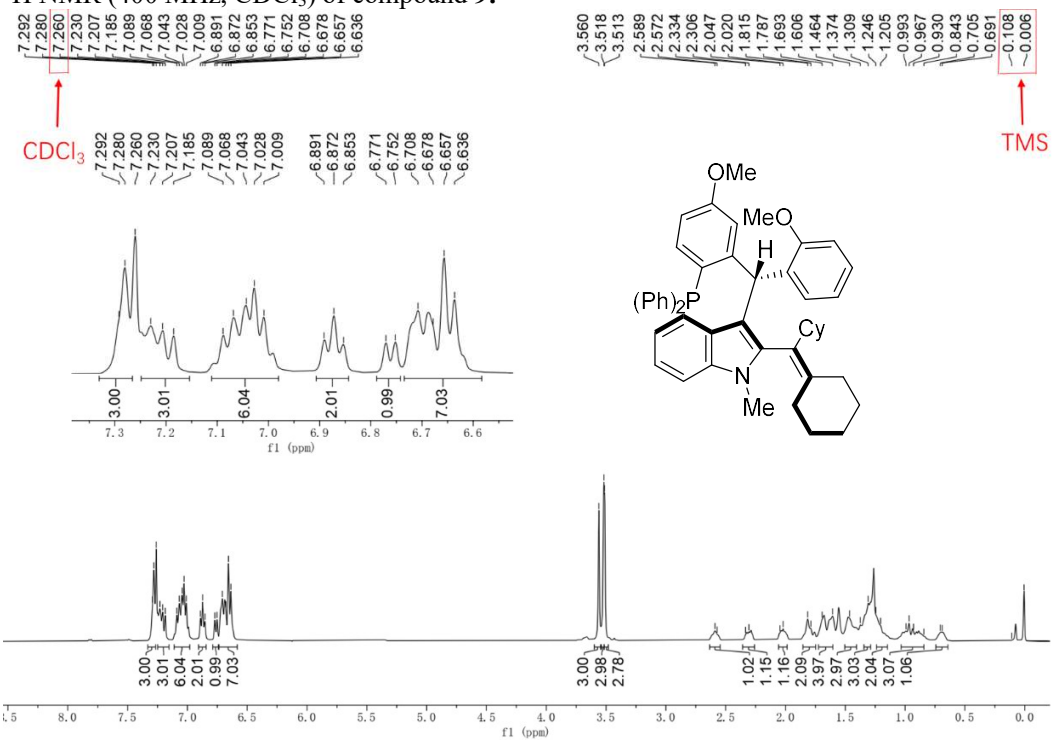
^{13}C NMR (100 MHz, $CDCl_3$) of compound **8:**



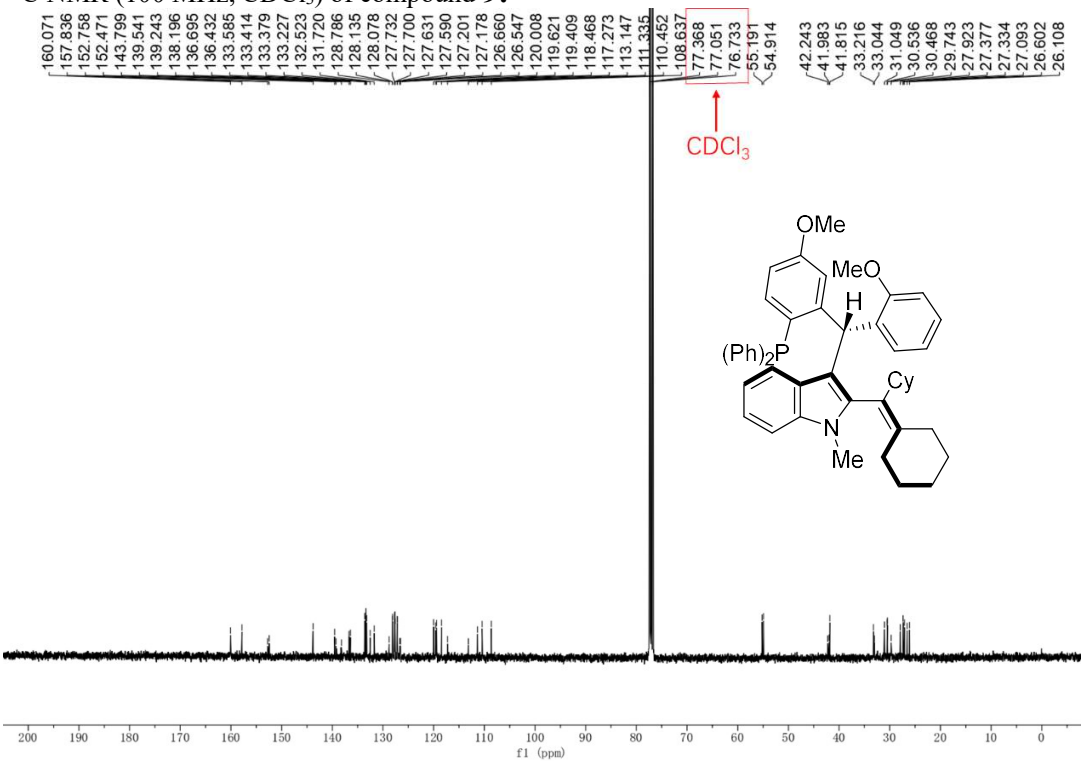
^{31}P NMR (162 MHz, $CDCl_3$) of compound **8:**



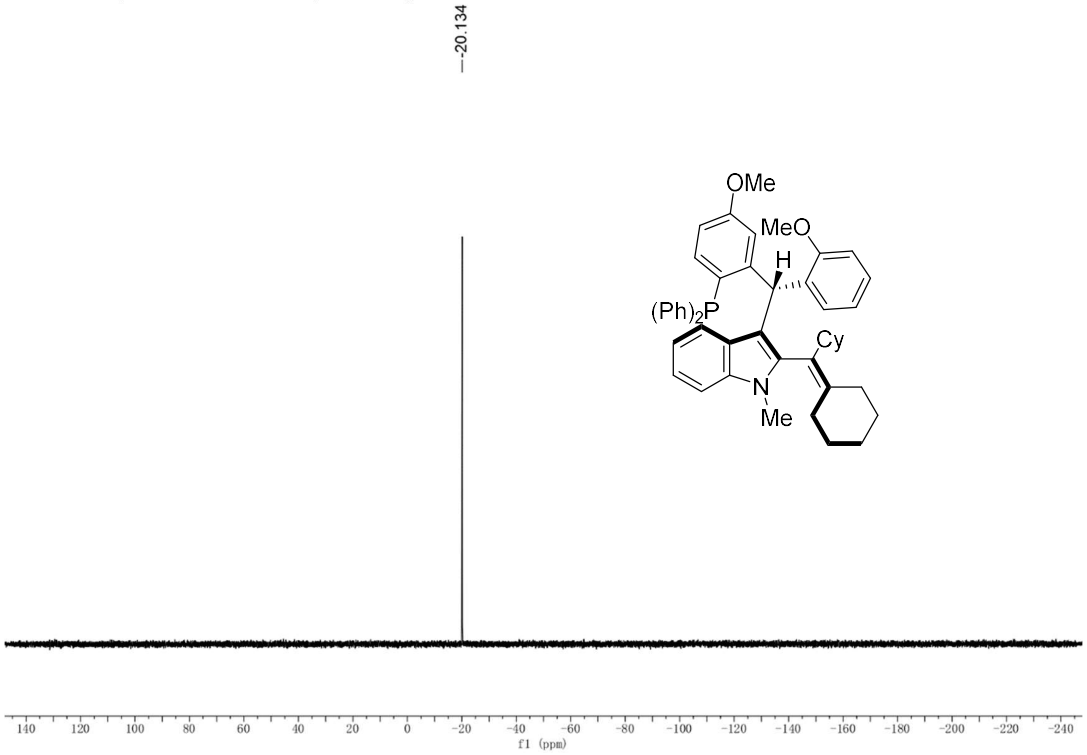
^{1}H NMR (400 MHz, $CDCl_3$) of compound **9:**



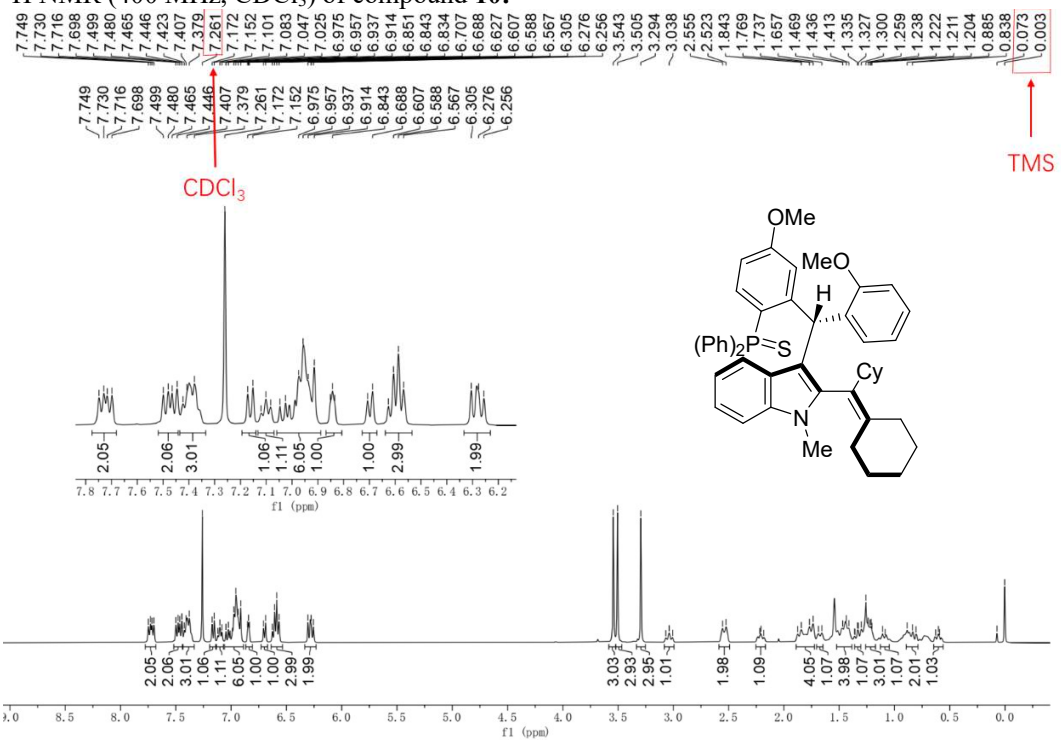
^{13}C NMR (100 MHz, $CDCl_3$) of compound **9:**



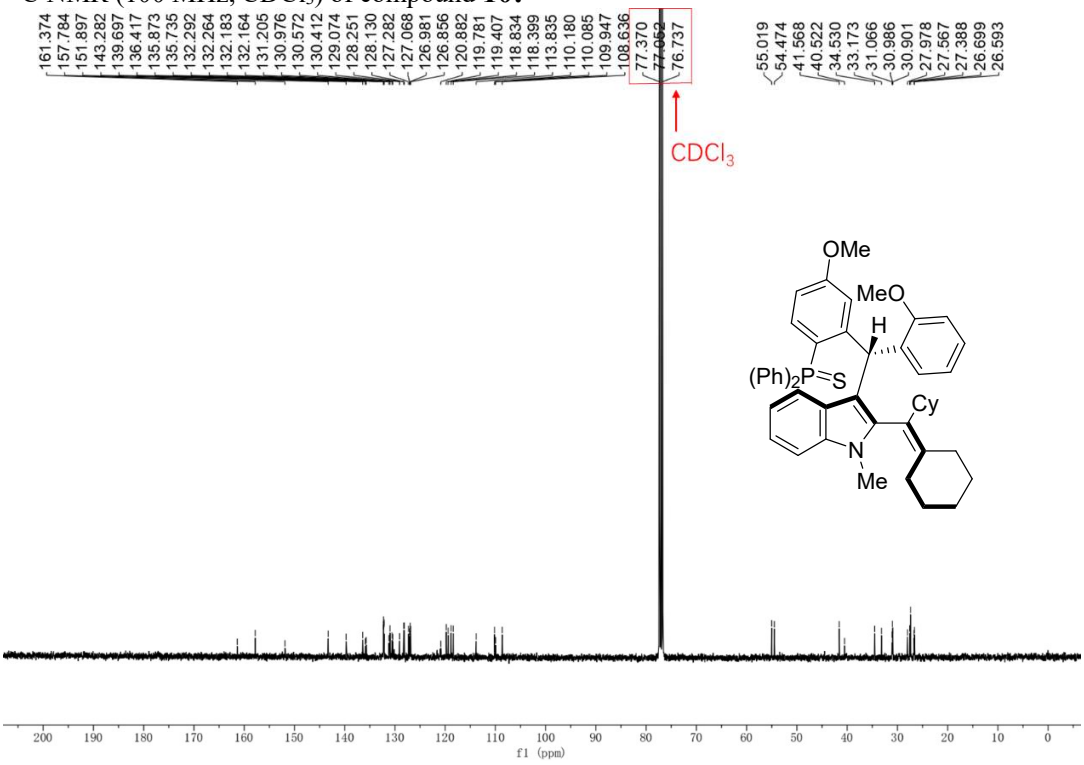
^{31}P NMR (162 MHz, $CDCl_3$) of compound **9:**



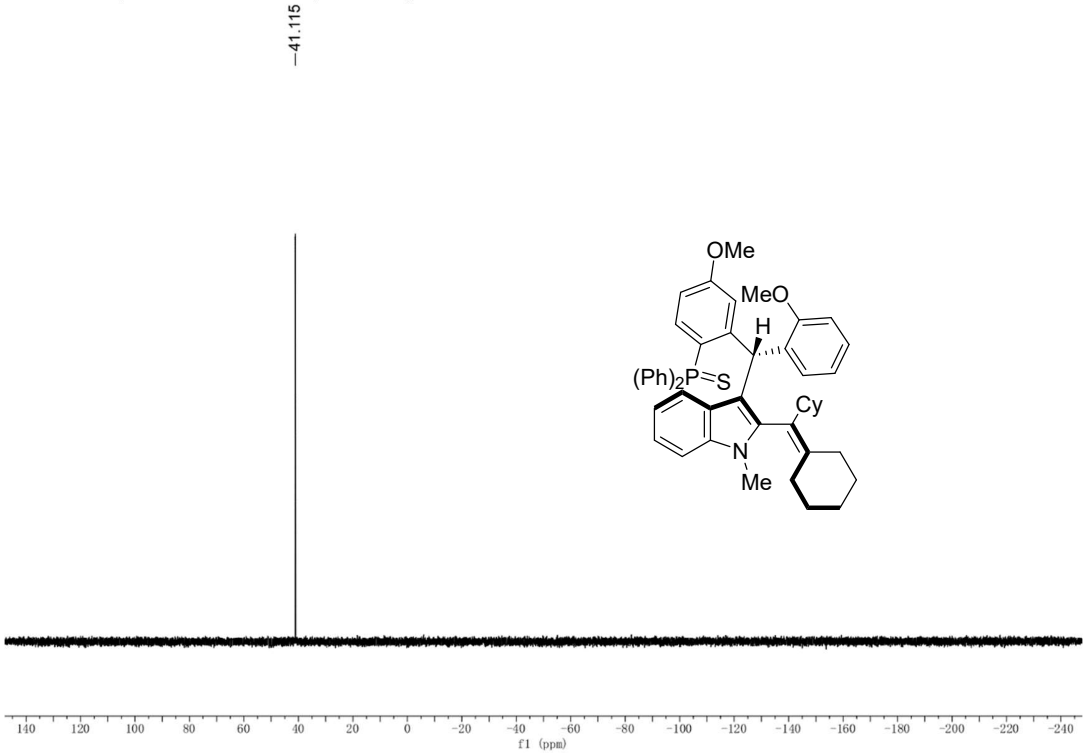
^{1}H NMR (400 MHz, $CDCl_3$) of compound **10:**



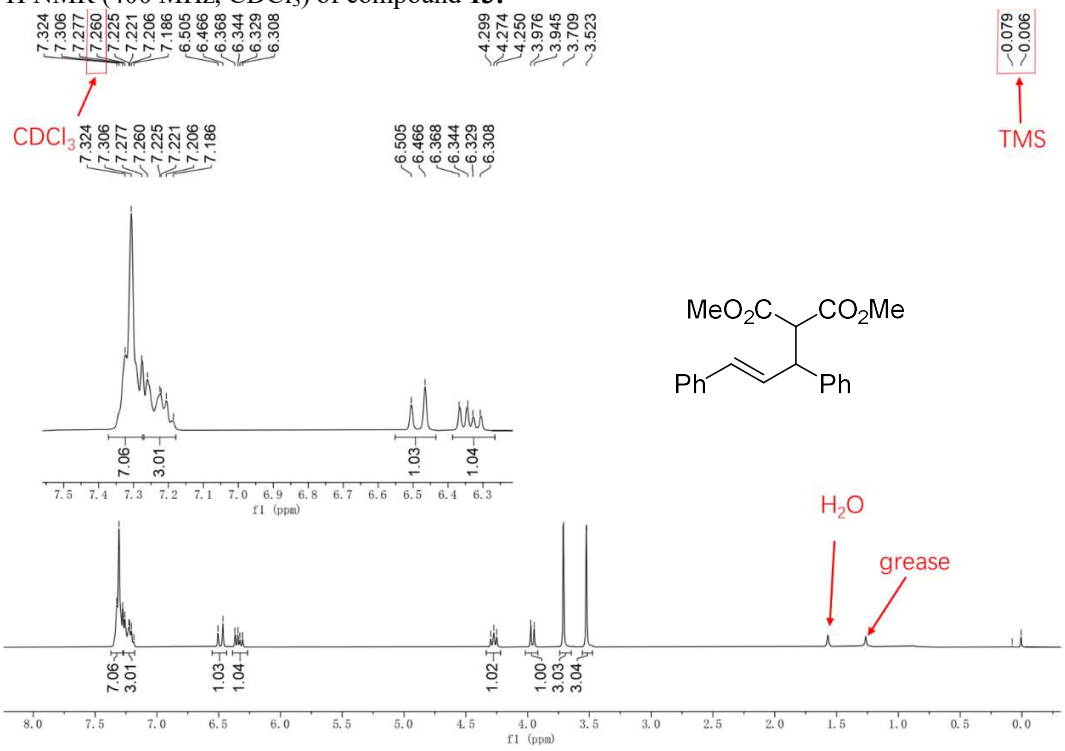
^{13}C NMR (100 MHz, $CDCl_3$) of compound **10:**



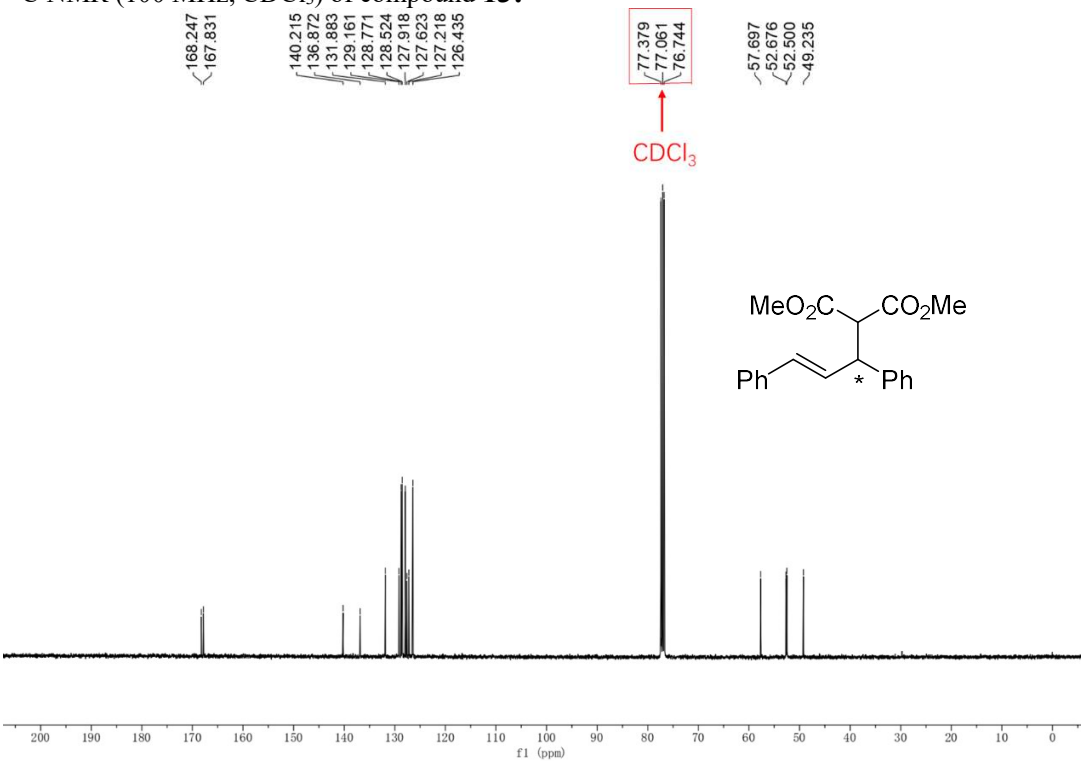
^{31}P NMR (162 MHz, $CDCl_3$) of compound **10:**



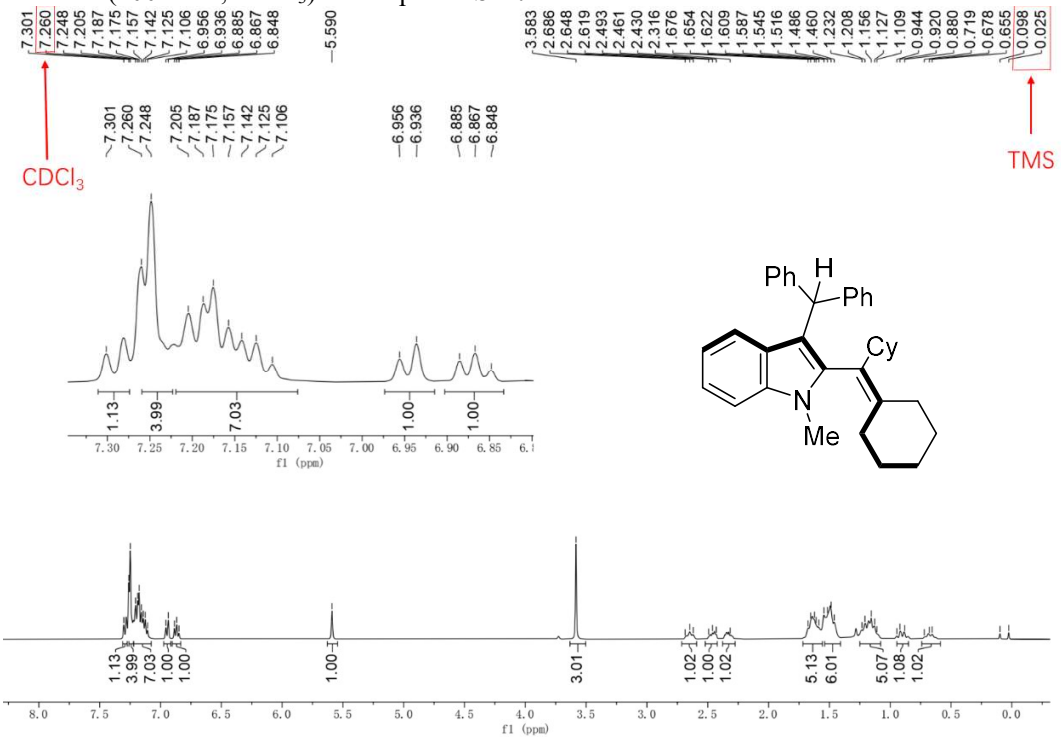
^{1}H NMR (400 MHz, $CDCl_3$) of compound **13:**



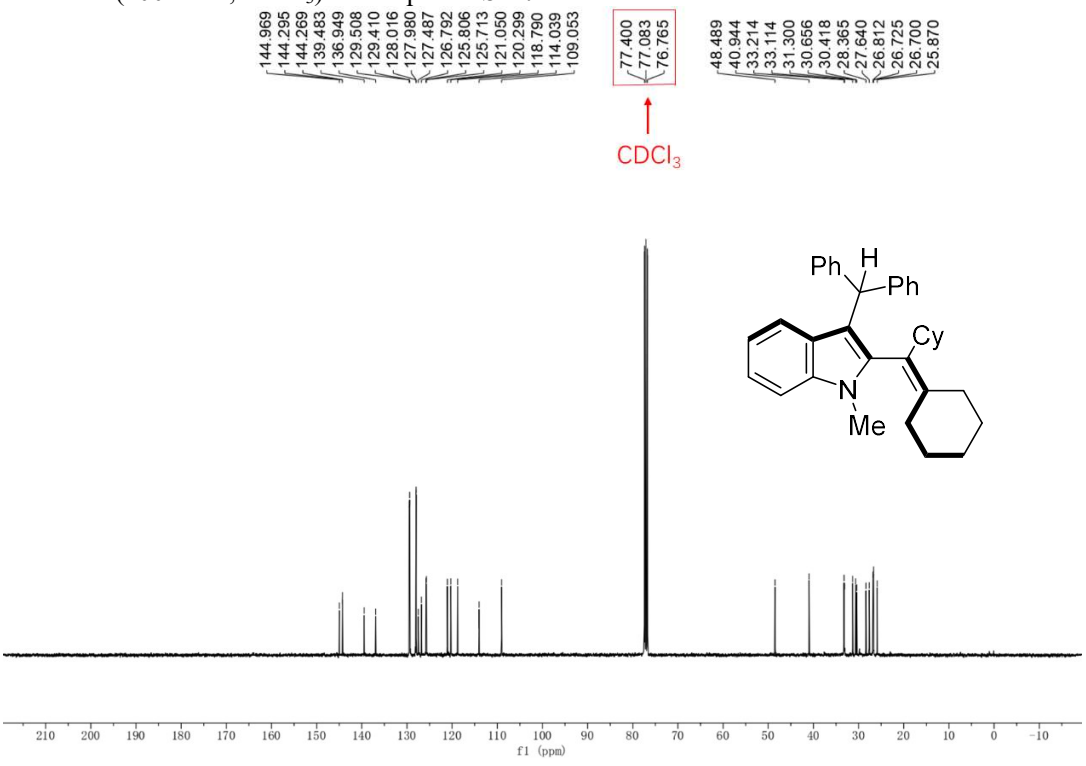
^{13}C NMR (100 MHz, $CDCl_3$) of compound **13:**



^{1}H NMR (400 MHz, $CDCl_3$) of compound **S12:**



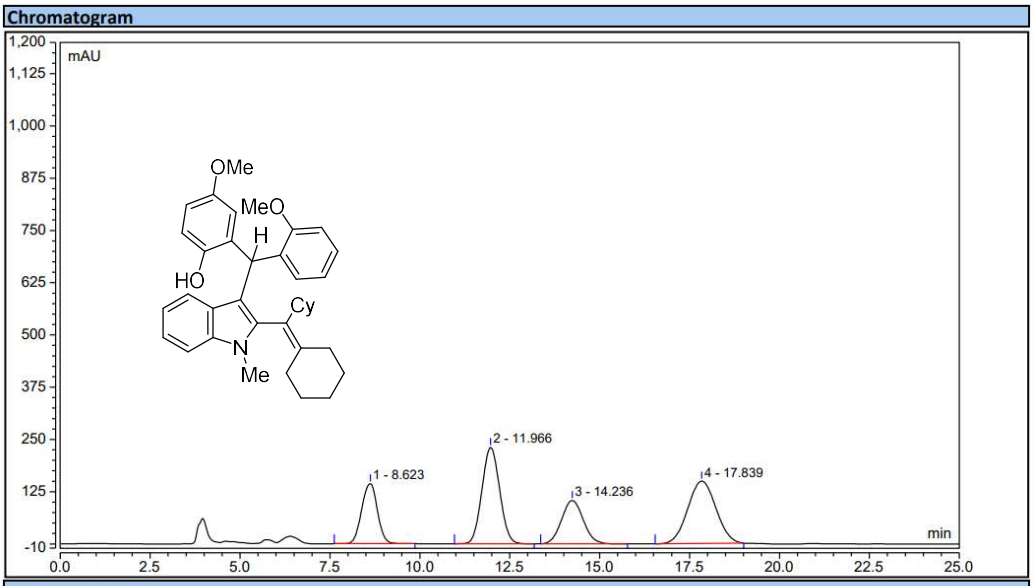
^{13}C NMR (100 MHz, $CDCl_3$) of compound **S12:**



14. HPLC traces of compounds 3, 4, 8, 10, 13 and S12

3aa

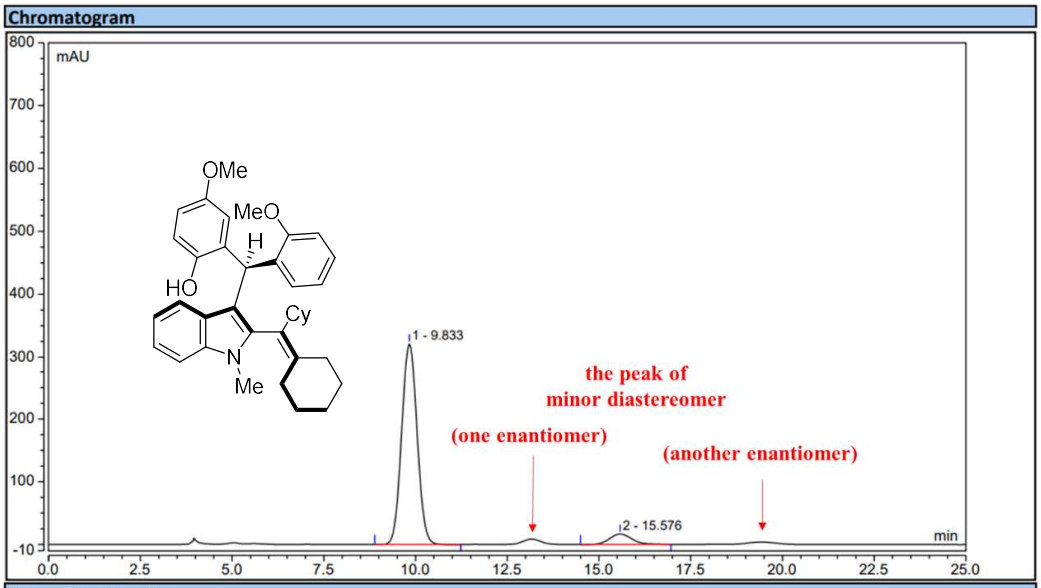
Racemic:



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		8.623	72.804	143.434	17.61	22.88	n.a.
2		11.966	132.314	230.426	32.01	36.75	n.a.
3		14.236	72.532	103.783	17.55	16.55	n.a.
4		17.839	135.734	149.328	32.83	23.82	n.a.
Total:			**413.384**	**626.971**	**100.00**	**100.00**	

Enantioselective (inseparable diastereomers with 95:5 dr):

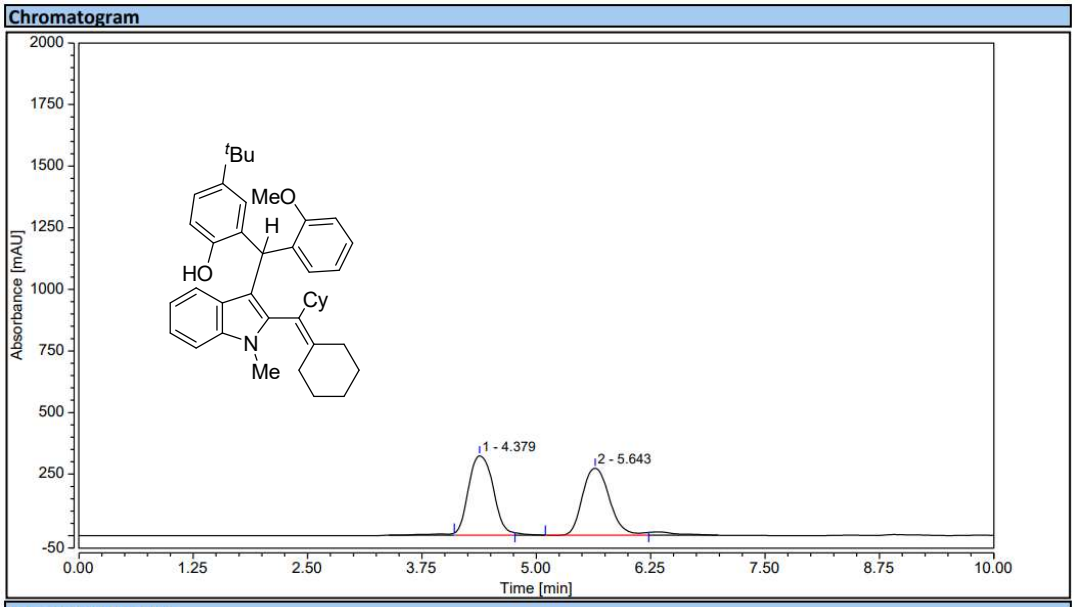


Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		9.833	156.475	321.079	92.92	95.03	n.a.
2		15.576	11.922	16.795	7.08	4.97	n.a.
Total:			**168.397**	**337.875**	**100.00**	**100.00**	

3ab

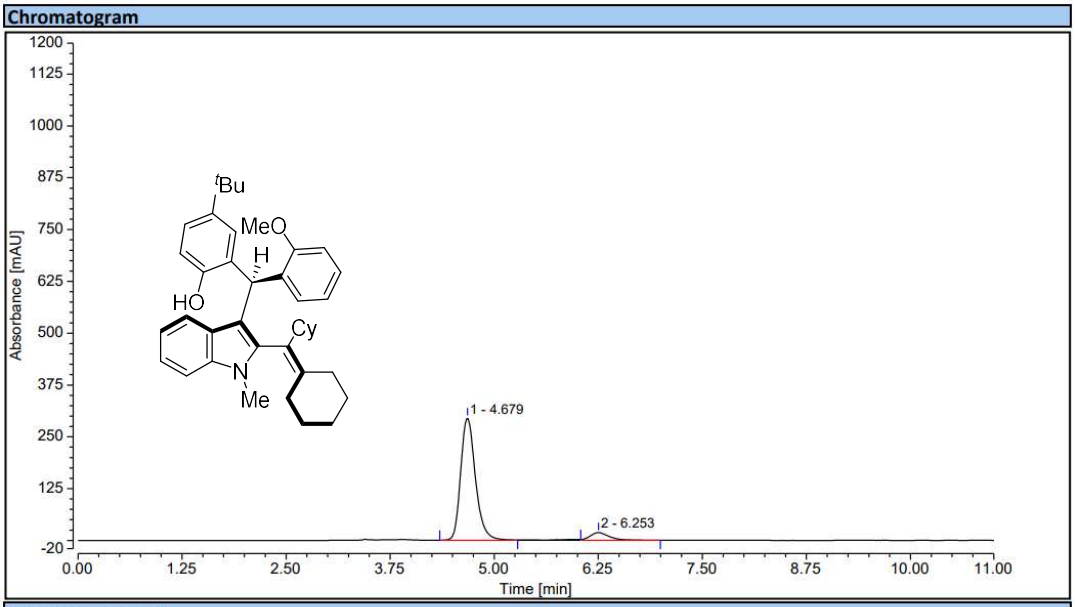
Racemic:



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		4.379	100.939	322.084	51.88	54.23	n.a.
2		5.643	93.607	271.847	48.12	45.77	n.a.
Total:			**194.546**	**593.931**	**100.00**	**100.00**	

Enantioselective:



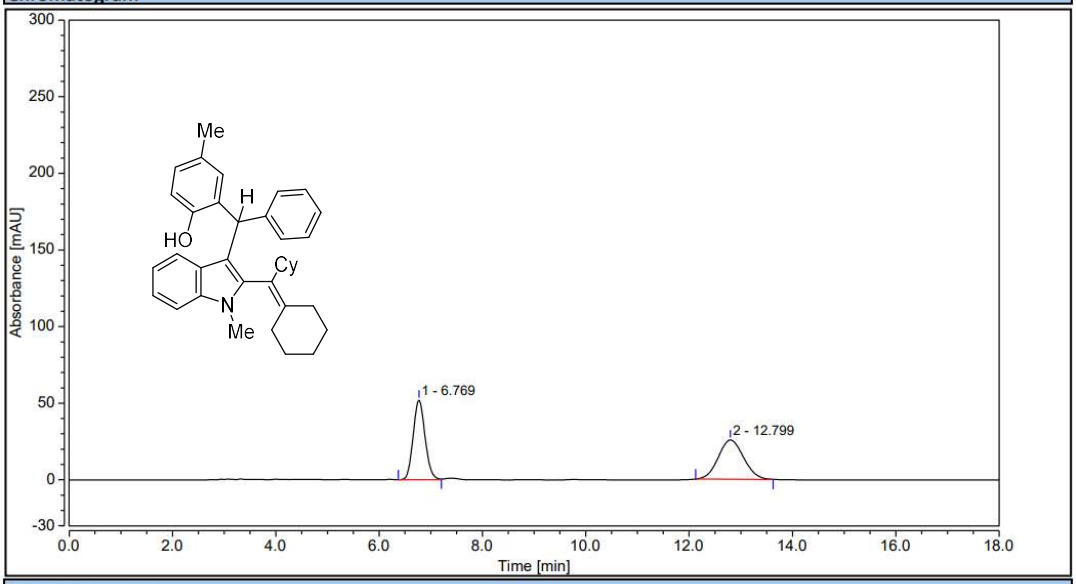
Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
n.a.		4.679	60.851	295.175	92.43	94.11	n.a.
n.a.		6.253	4.986	18.473	7.57	5.89	n.a.
Total:			**65.837**	**313.648**	**100.00**	**100.00**	

3ac

Racemic:

Chromatogram

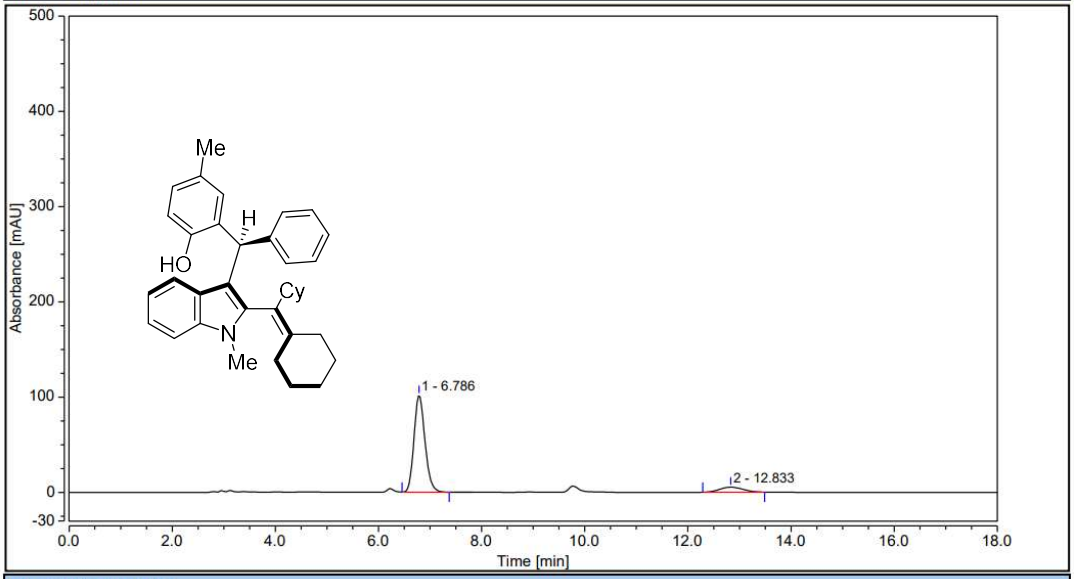


Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		6.769	13.947	52.053	48.96	67.03	n.a.
2		12.799	14.540	25.600	51.04	32.97	n.a.
Total:			**28.487**	**77.654**	**100.00**	**100.00**	

Enantioselective:

Chromatogram

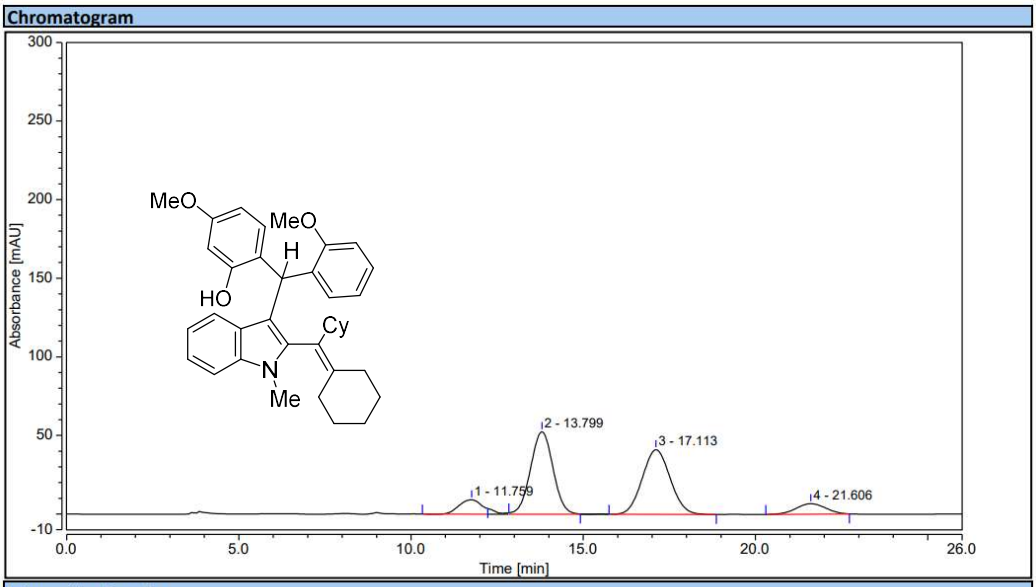


Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		6.786	25.215	101.661	90.01	95.01	n.a.
2		12.833	2.800	5.339	9.99	4.99	n.a.
Total:			**28.015**	**107.001**	**100.00**	**100.00**	

3ad

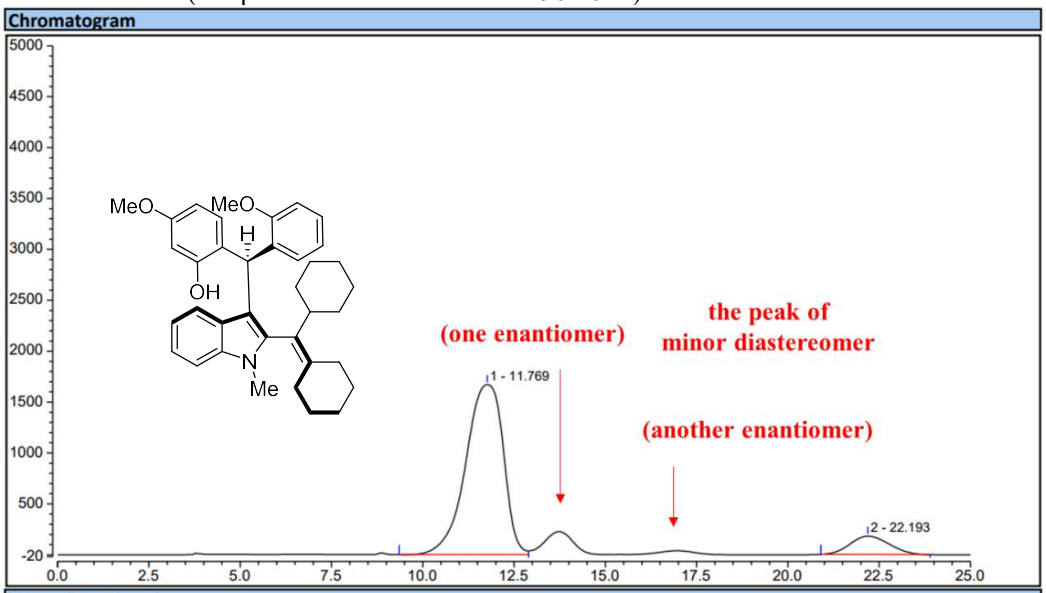
Racemic:



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		11.759	6.835	9.140	7.41	8.35	n.a.
2		13.799	39.913	52.525	43.26	47.96	n.a.
3		17.113	38.806	41.168	42.06	37.59	n.a.
4		21.606	6.700	6.681	7.26	6.10	n.a.
Total:			**92.254**	**109.515**	**100.00**	**100.00**	

Enantioselective (inseparable diastereomers with 90:10 dr):

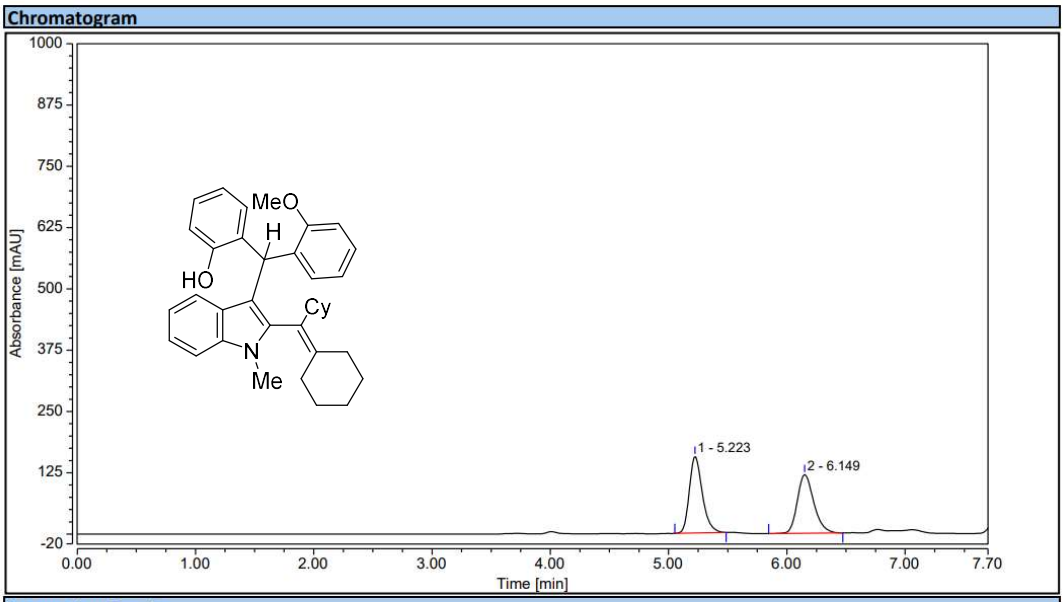


Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		11.769	2001.141	1671.487	89.96	90.28	n.a.
2		22.193	223.245	179.863	10.04	9.72	n.a.
Total:			**2224.387**	**1851.350**	**100.00**	**100.00**	

3ae

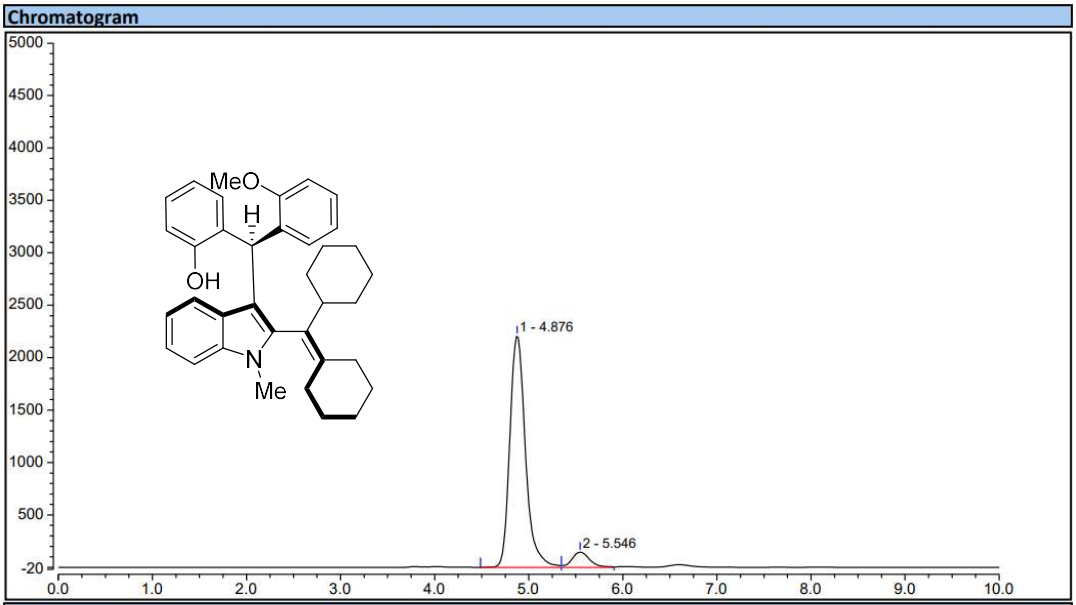
Racemic:



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		5.223	20.050	156.399	50.80	56.64	n.a.
2		6.149	19.417	119.738	49.20	43.36	n.a.
Total:			**39.467**	**276.138**	**100.00**	**100.00**	

Enantioselective:

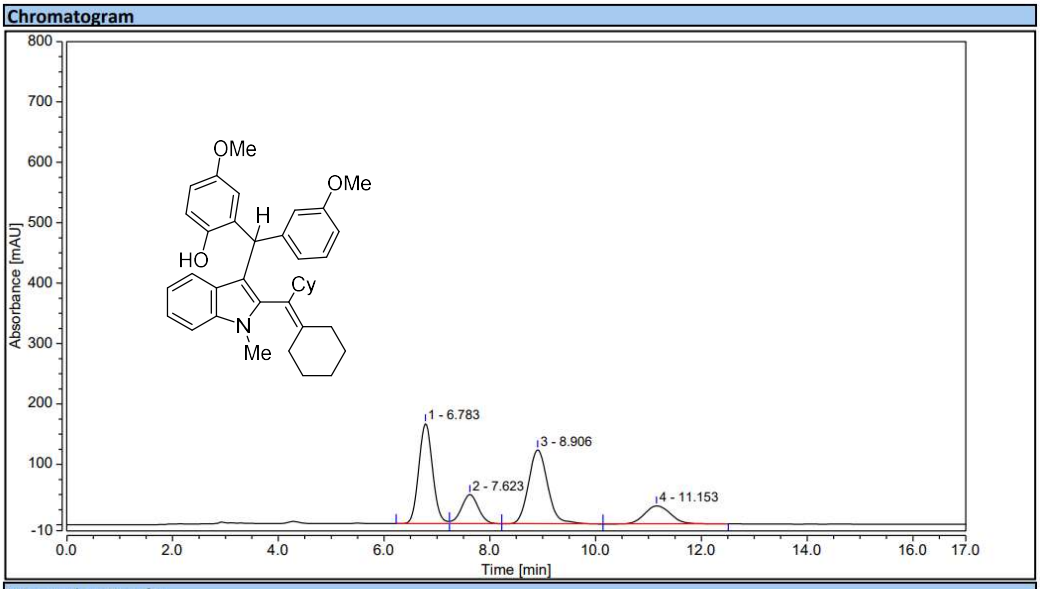


Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		4.876	426.212	2210.708	93.02	93.84	n.a.
2		5.546	31.983	145.169	6.98	6.16	n.a.
Total:			**458.195**	**2355.877**	**100.00**	**100.00**	

3af

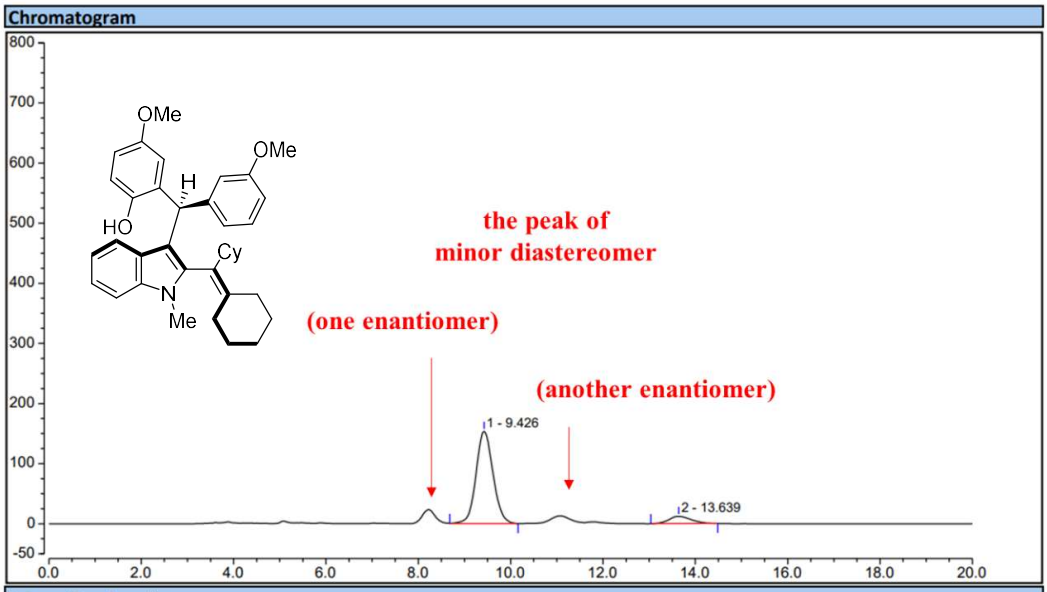
Racemic:



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		6.783	50.231	165.317	37.14	45.29	n.a.
2		7.623	17.619	48.002	13.03	13.15	n.a.
3		8.906	50.942	122.119	37.67	33.46	n.a.
4		11.153	16.445	29.548	12.16	8.10	n.a.
Total:			**135.237**	**364.986**	**100.00**	**100.00**	

Enantioselective (inseparable diastereomers with 85:15 dr):

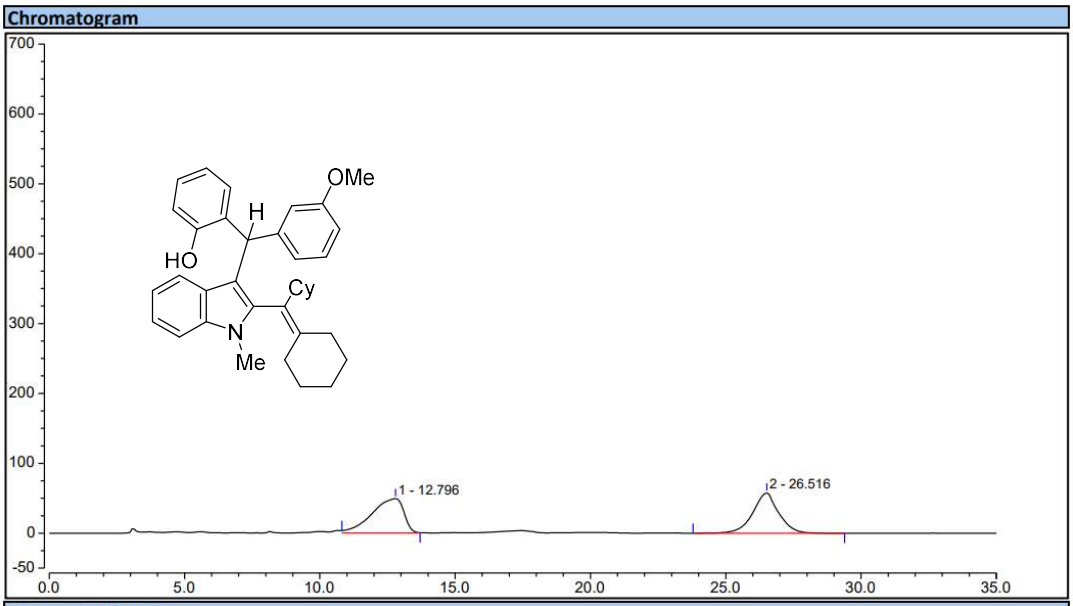


Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
n.a.		9.426	65.691	153.658	90.71	92.75	n.a.
n.a.		13.639	6.725	12.004	9.29	7.25	n.a.
Total:			**72.417**	**165.662**	**100.00**	**100.00**	

3ag

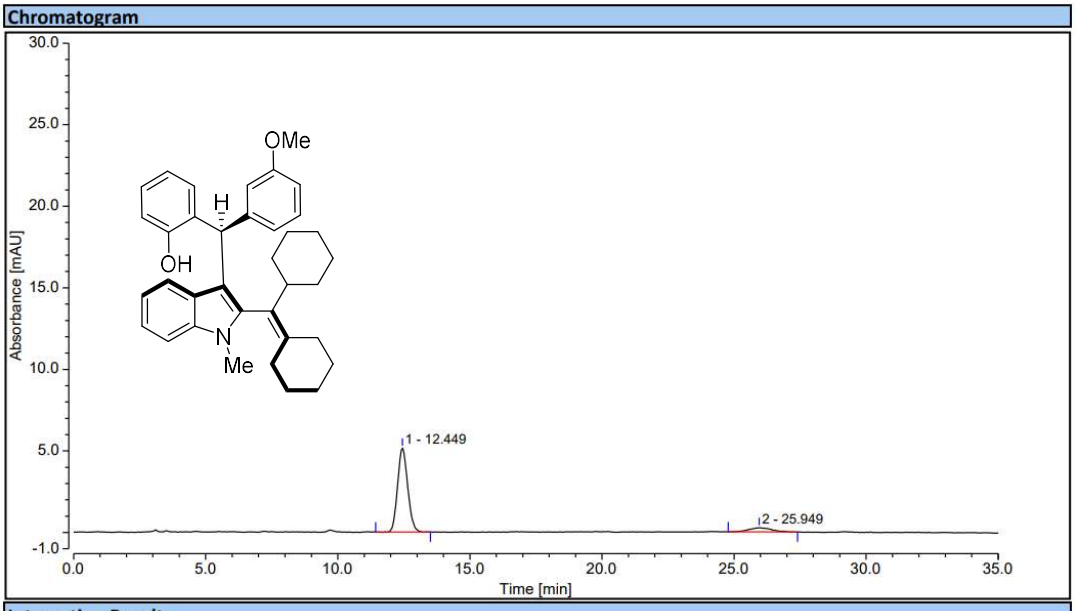
Racemic:



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
n.a.		12.796	67.634	49.271	51.24	46.09	n.a.
n.a.		26.516	64.352	57.627	48.76	53.91	n.a.
Total:			**131.986**	**106.898**	**100.00**	**100.00**	

Enantioselective:

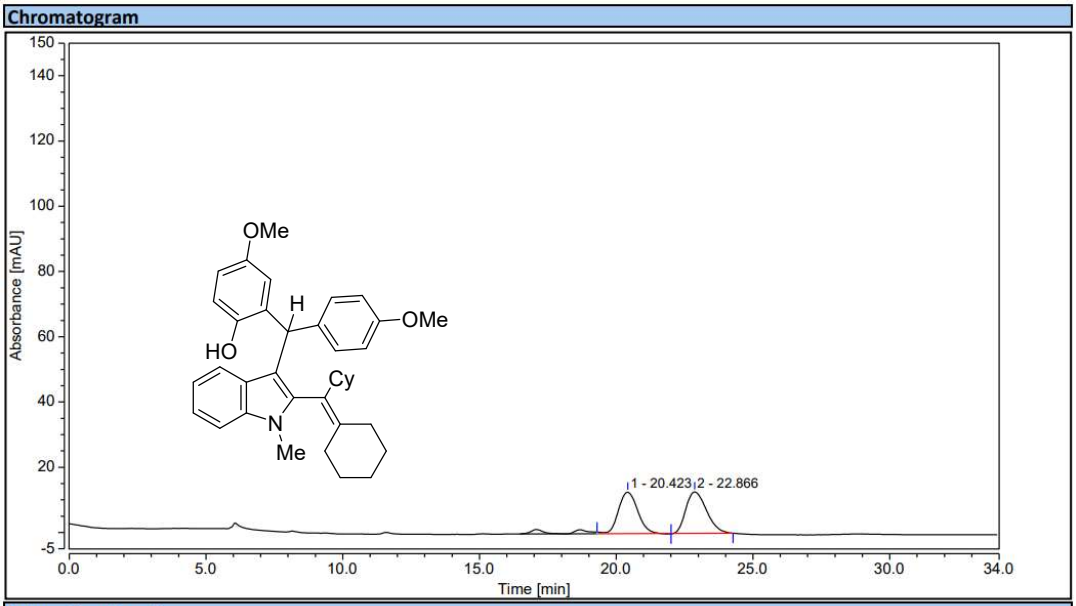


Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
n.a.		12.449	2.281	5.143	90.06	95.14	n.a.
n.a.		25.949	0.252	0.263	9.94	4.86	n.a.
Total:			**2.533**	**5.406**	**100.00**	**100.00**	

3ah

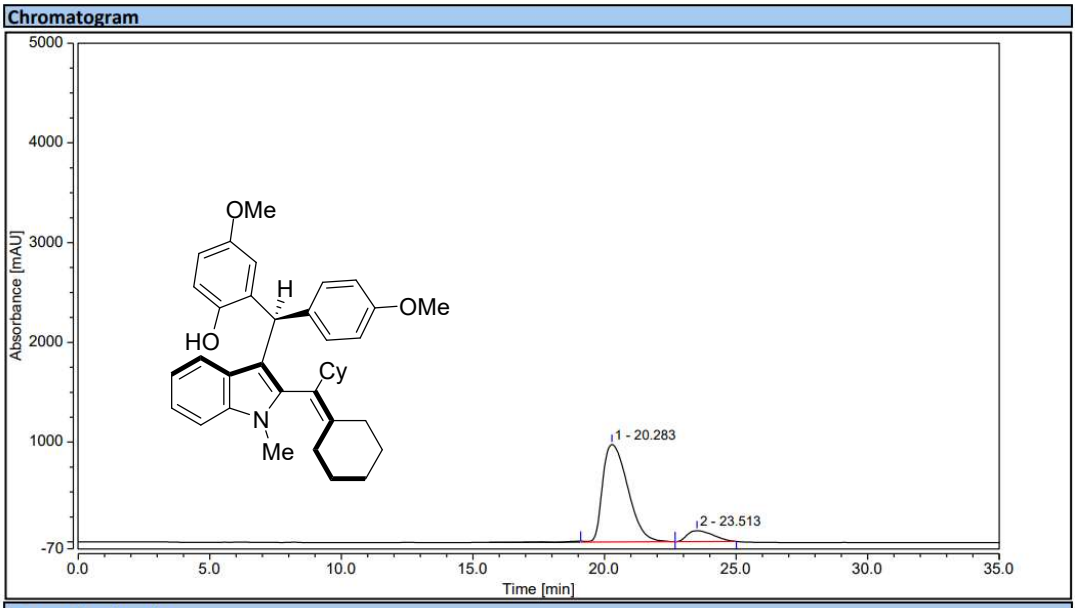
Racemic:



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		20.423	10.337	12.689	48.08	49.94	n.a.
2		22.866	11.162	12.718	51.92	50.06	n.a.
Total:			**21.498**	**25.407**	**100.00**	**100.00**	

Enantioselective:

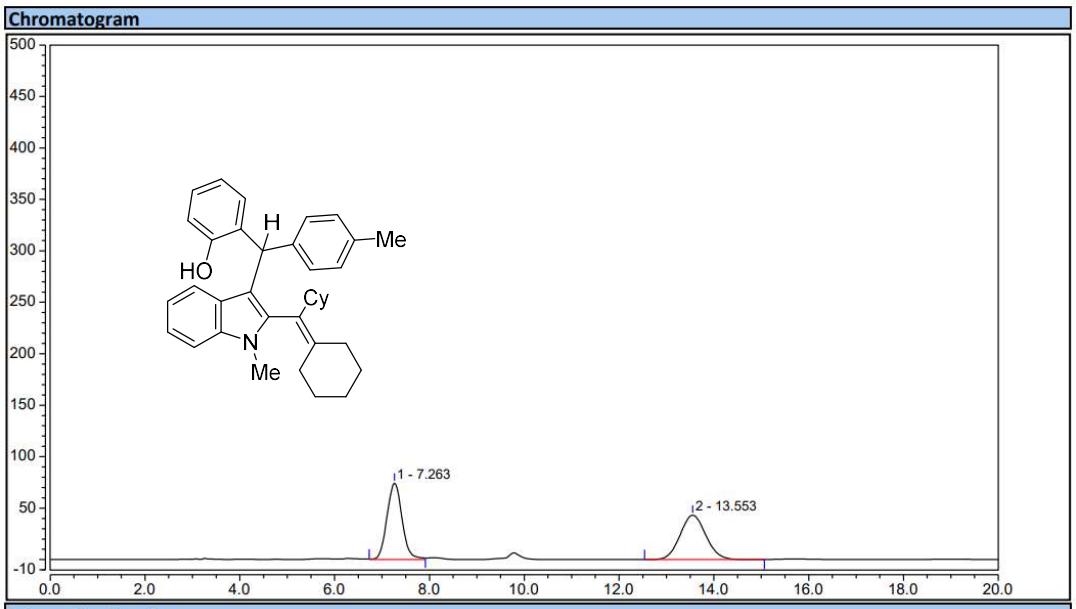


Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		20.283	1083.156	977.135	89.64	89.91	n.a.
2		23.513	125.238	109.629	10.36	10.09	n.a.
Total:			**1208.394**	**1086.764**	**100.00**	**100.00**	

3ai

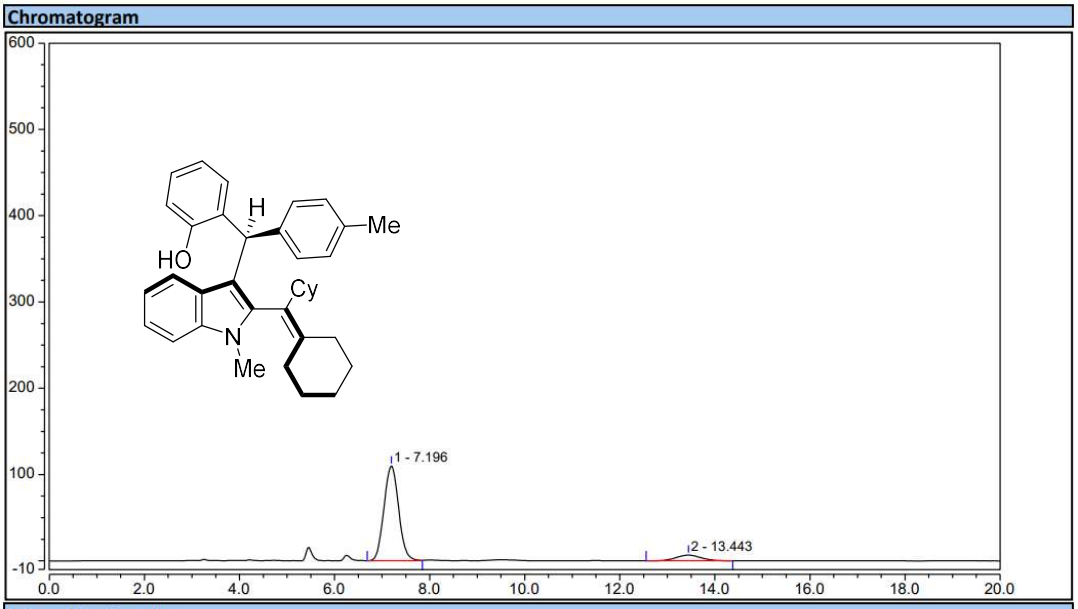
Racemic:



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		7.263	27.454	74.231	50.34	63.27	n.a.
2		13.553	27.086	43.090	49.66	36.73	n.a.
Total:			**54.541**	**117.321**	**100.00**	**100.00**	

Enantioselective:

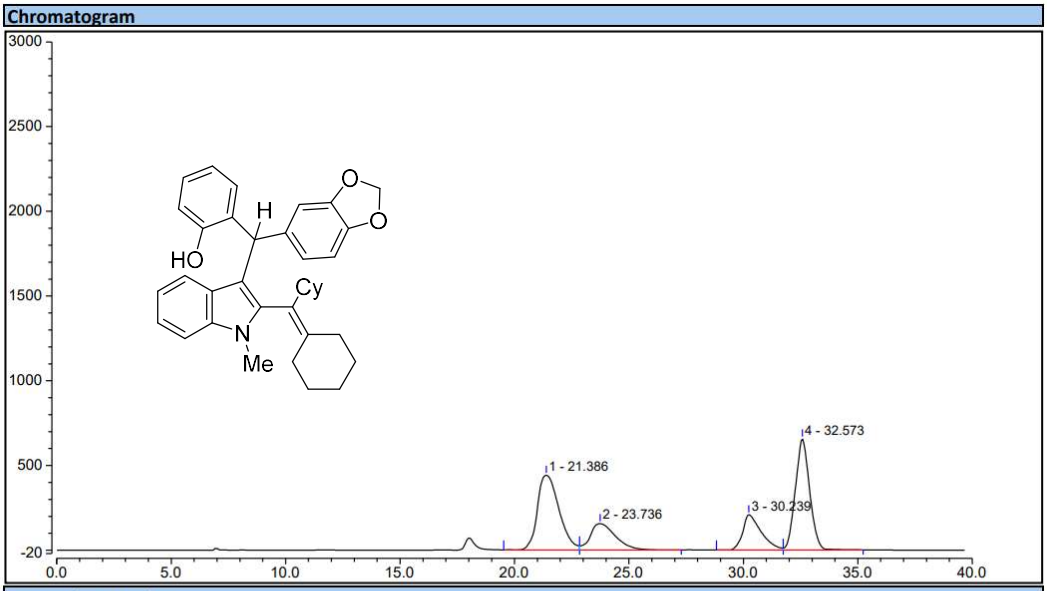


Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		7.196	39.475	109.917	90.96	94.42	n.a.
2		13.443	3.925	6.494	9.04	5.58	n.a.
Total:			**43.400**	**116.411**	**100.00**	**100.00**	

3aj

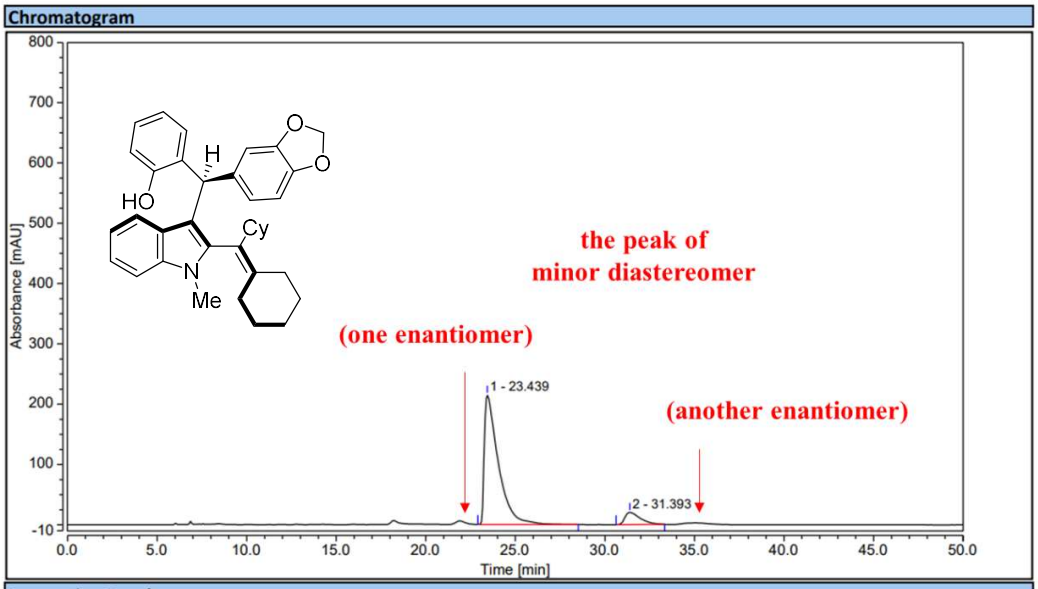
Racemic:



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		21.386	480.339	440.462	35.73	30.20	n.a.
2		23.736	196.081	154.967	14.58	10.62	n.a.
3		30.239	193.517	208.389	14.39	14.29	n.a.
4		32.573	474.565	654.720	35.30	44.89	n.a.
Total:			**1344.501**	**1458.538**	**100.00**	**100.00**	

Enantioselective (inseparable diastereomers with 82:18 dr):

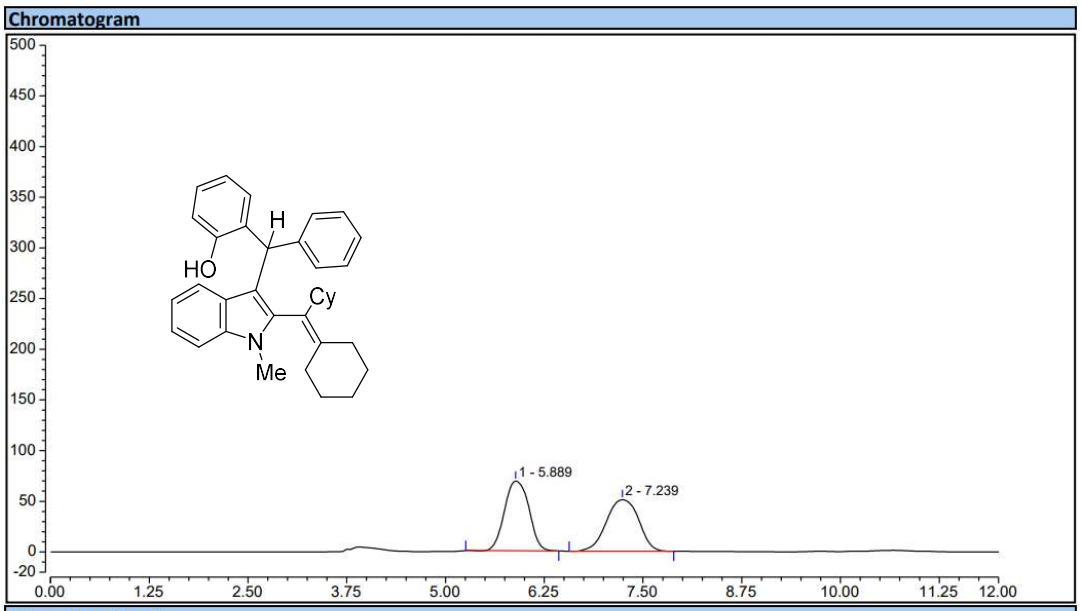


Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		23.439	195.070	214.523	90.69	91.34	n.a.
2		31.393	20.022	20.332	9.31	8.66	n.a.
Total:			**215.092**	**234.855**	**100.00**	**100.00**	

3ak

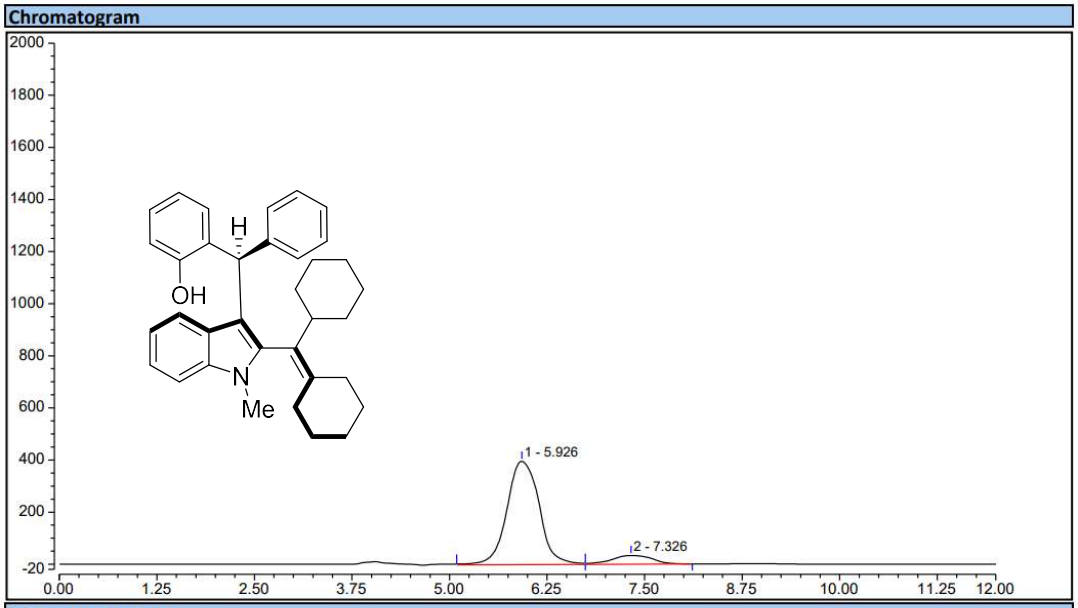
Racemic:



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		5.889	24.646	68.746	50.49	57.46	n.a.
2		7.239	24.170	50.886	49.51	42.54	n.a.
Total:			**48.816**	**119.632**	**100.00**	**100.00**	

Enantioselective:

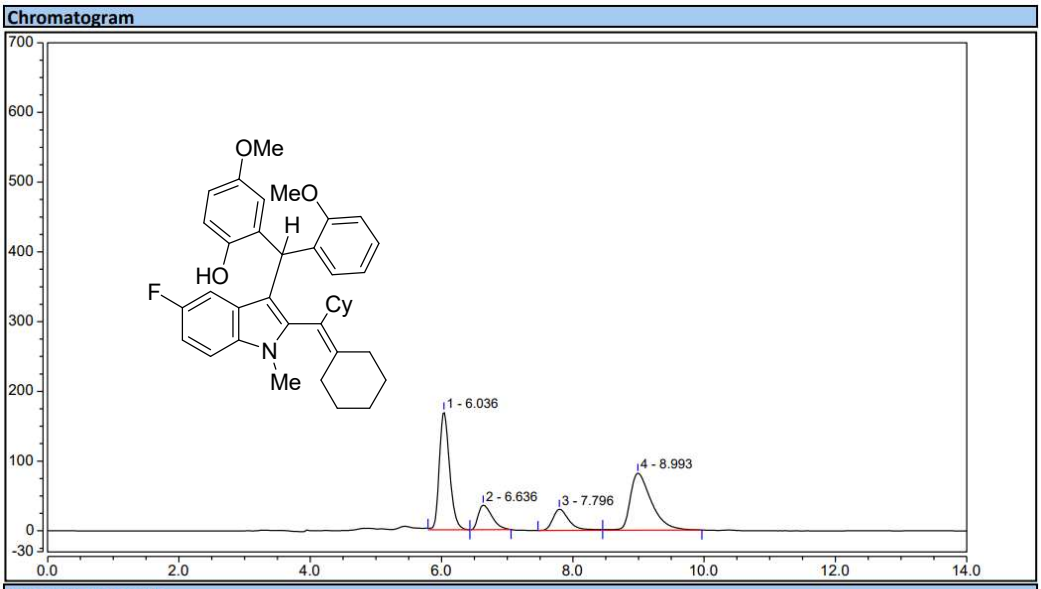


Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		5.926	191.461	396.895	90.28	92.18	n.a.
2		7.326	20.602	33.652	9.72	7.82	n.a.
Total:			**212.064**	**430.547**	**100.00**	**100.00**	

3ba

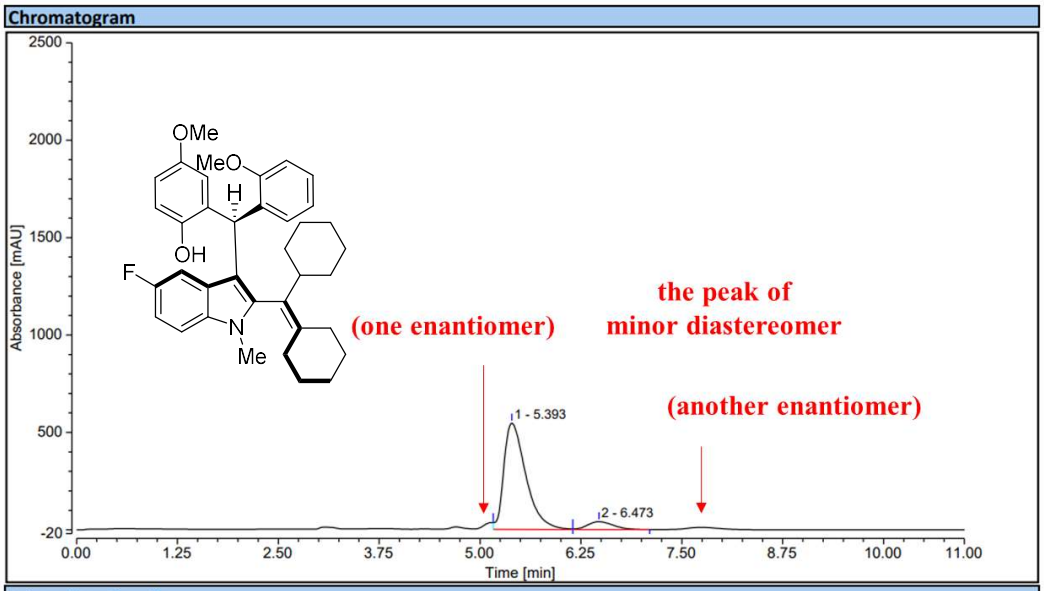
Racemic:



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		6.036	30.471	168.993	38.98	53.47	n.a.
2		6.636	8.556	35.211	10.95	11.14	n.a.
3		7.796	8.628	30.255	11.04	9.57	n.a.
4		8.993	30.505	81.601	39.03	25.82	n.a.
Total:			**78.160**	**316.060**	**100.00**	**100.00**	

Enantioselective (inseparable diastereomers with 89:11 dr):

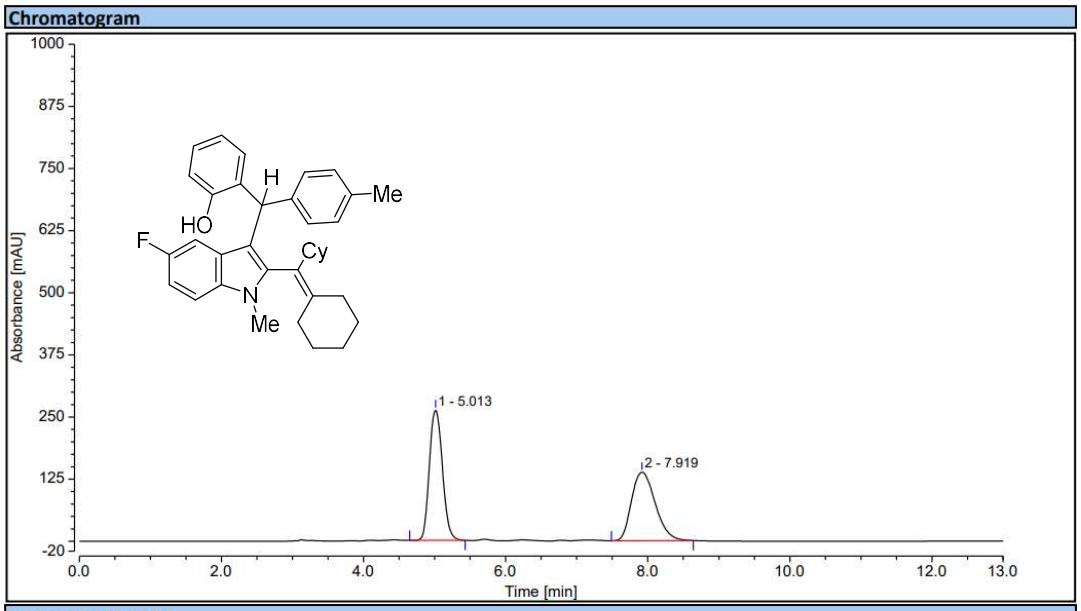


Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
n.a.		5.393	172.931	545.481	92.03	93.12	n.a.
n.a.		6.473	14.970	40.273	7.97	6.88	n.a.
Total:			**187.901**	**585.754**	**100.00**	**100.00**	

3bi

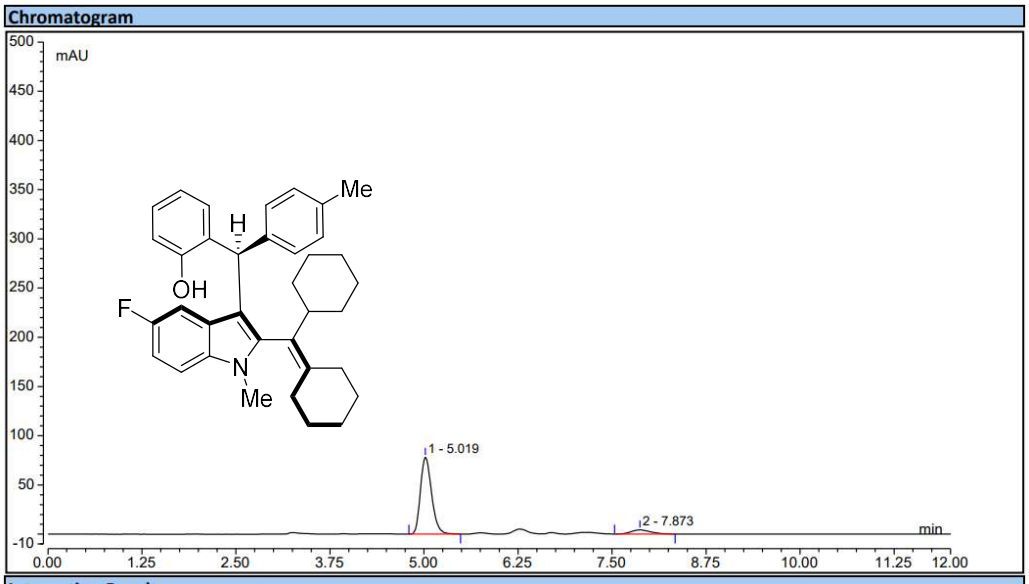
Racemic:



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
n.a.		5.013	55.917	262.215	51.15	65.52	n.a.
n.a.		7.919	53.412	137.982	48.85	34.48	n.a.
Total:			**109.329**	**400.197**	**100.00**	**100.00**	

Enantioselective:

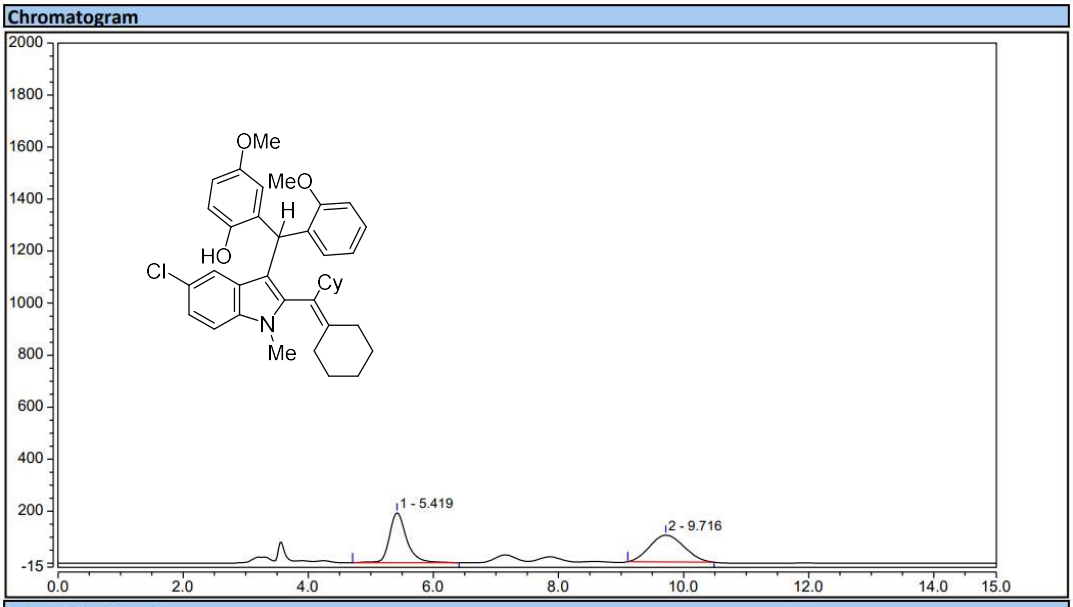


Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
n.a.		5.019	13.422	77.948	91.22	94.86	n.a.
n.a.		7.873	1.293	4.228	8.78	5.14	n.a.
Total:			**14.715**	**82.176**	**100.00**	**100.00**	

3ca

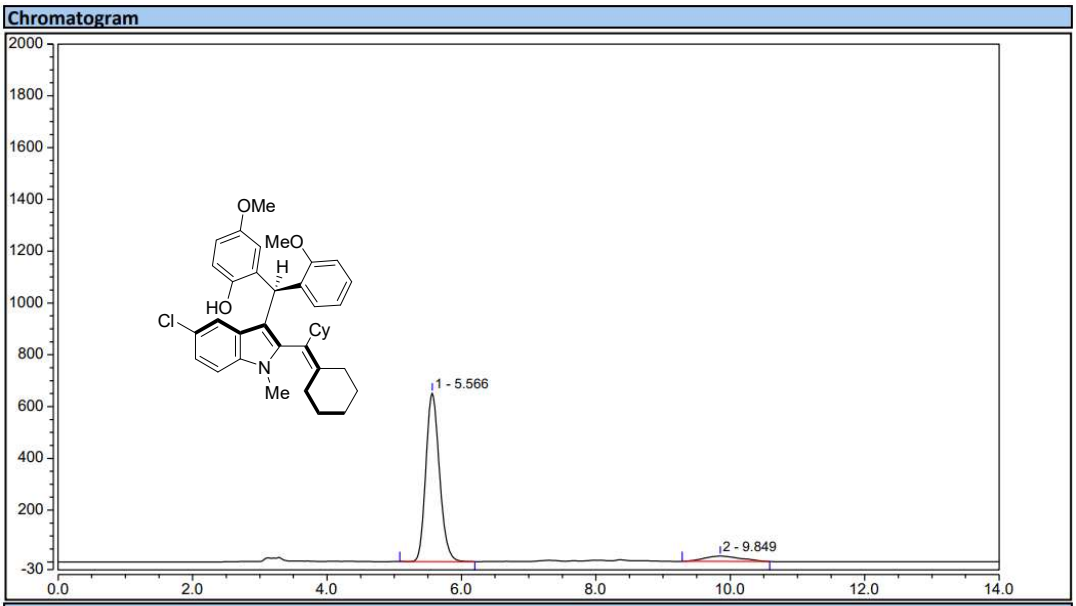
Racemic:



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		5.419	60.991	191.786	48.16	65.00	n.a.
2		9.716	65.650	103.253	51.84	35.00	n.a.
Total:			**126.642**	**295.040**	**100.00**	**100.00**	

Enantioselective:

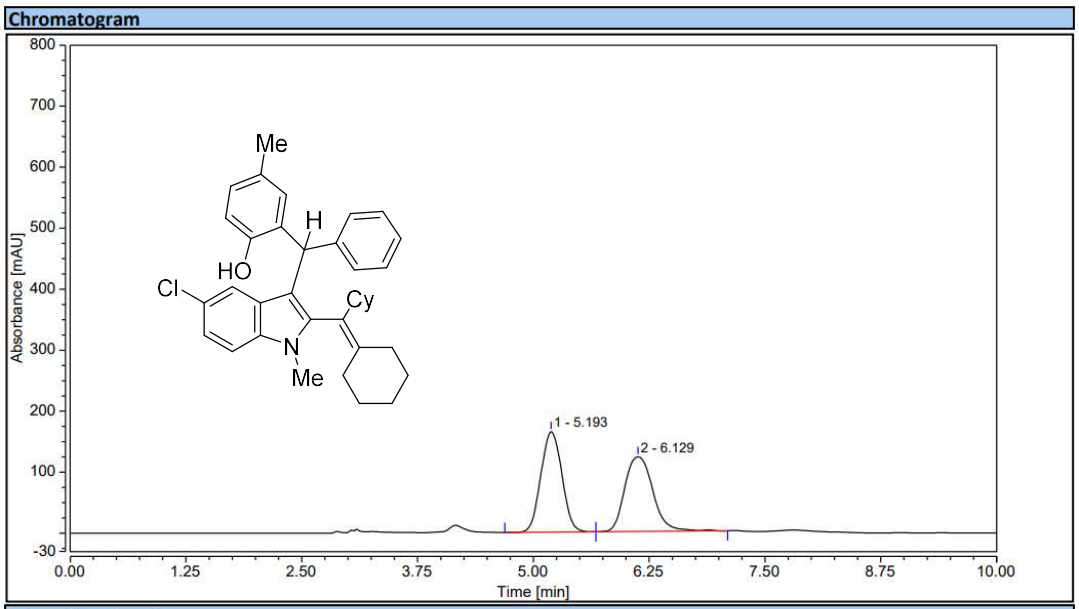


Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		5.566	153.123	651.189	92.13	96.96	n.a.
2		9.849	13.072	20.420	7.87	3.04	n.a.
Total:			**166.196**	**671.609**	**100.00**	**100.00**	

3cc

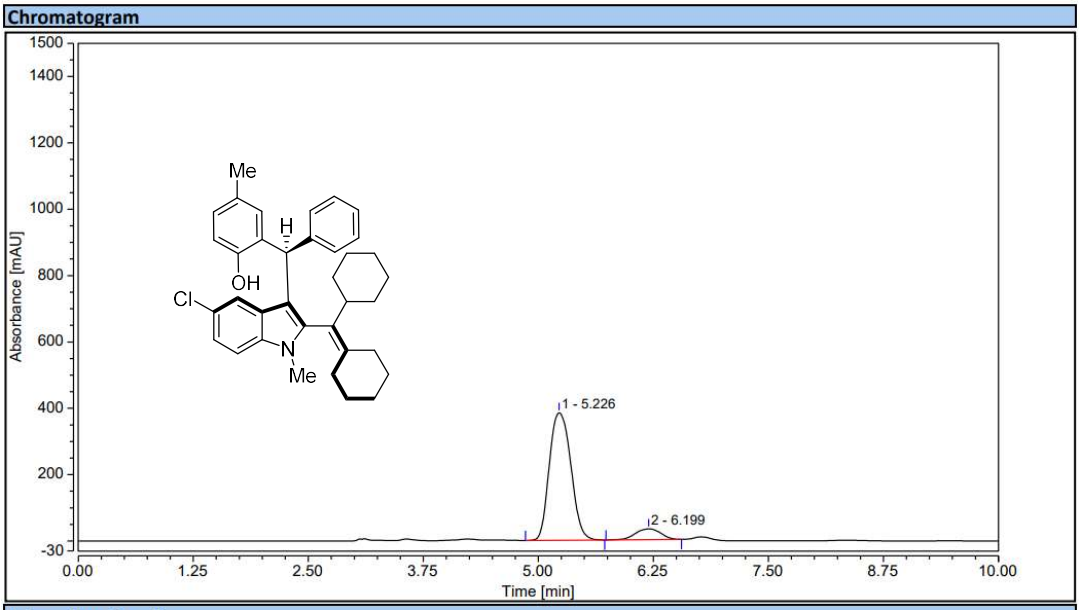
Racemic:



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		5.193	43.409	164.901	50.19	57.38	n.a.
2		6.129	43.088	122.504	49.81	42.62	n.a.
Total:			**86.497**	**287.405**	**100.00**	**100.00**	

Enantioselective:

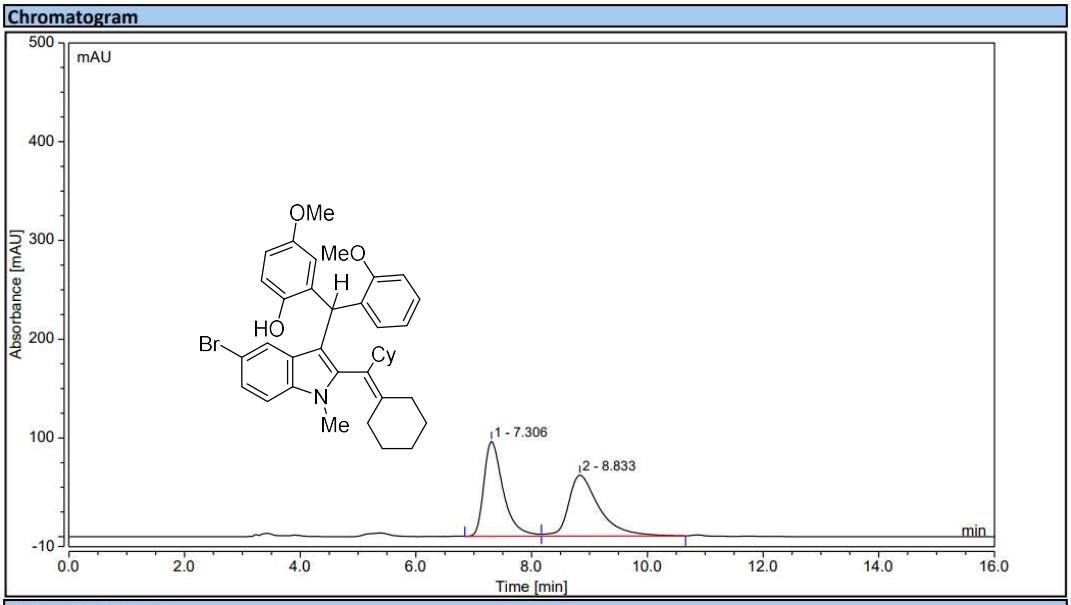


Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		5.226	104.369	384.370	91.08	92.29	n.a.
2		6.199	10.222	32.106	8.92	7.71	n.a.
Total:			**114.591**	**416.476**	**100.00**	**100.00**	

3da

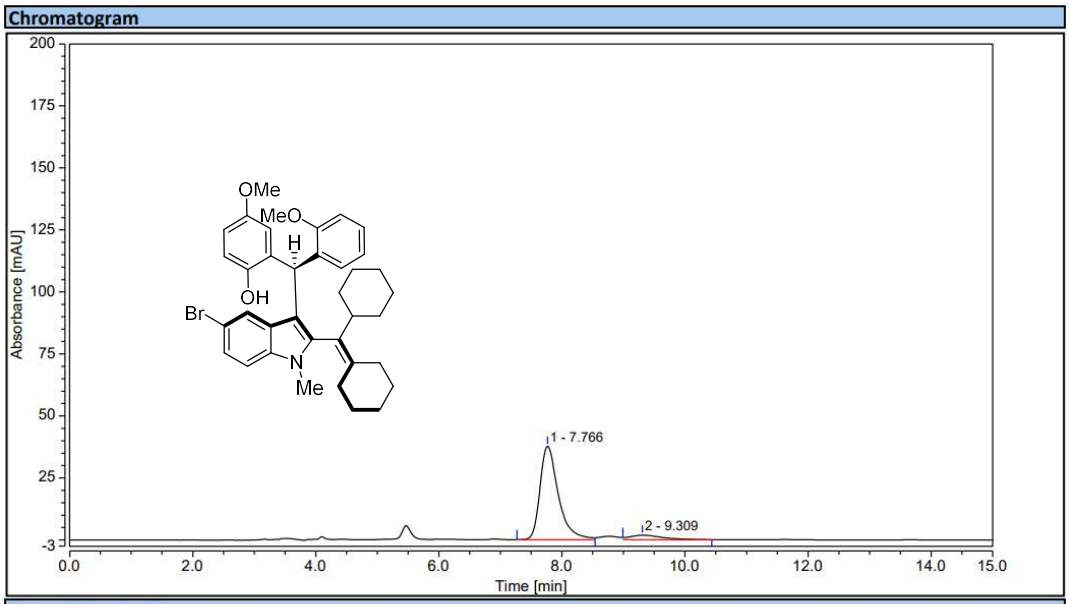
Racemic:



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		7.306	37.516	96.220	49.71	60.91	n.a.
2		8.833	37.951	61.755	50.29	39.09	n.a.
Total:			**75.467**	**157.976**	**100.00**	**100.00**	

Enantioselective:



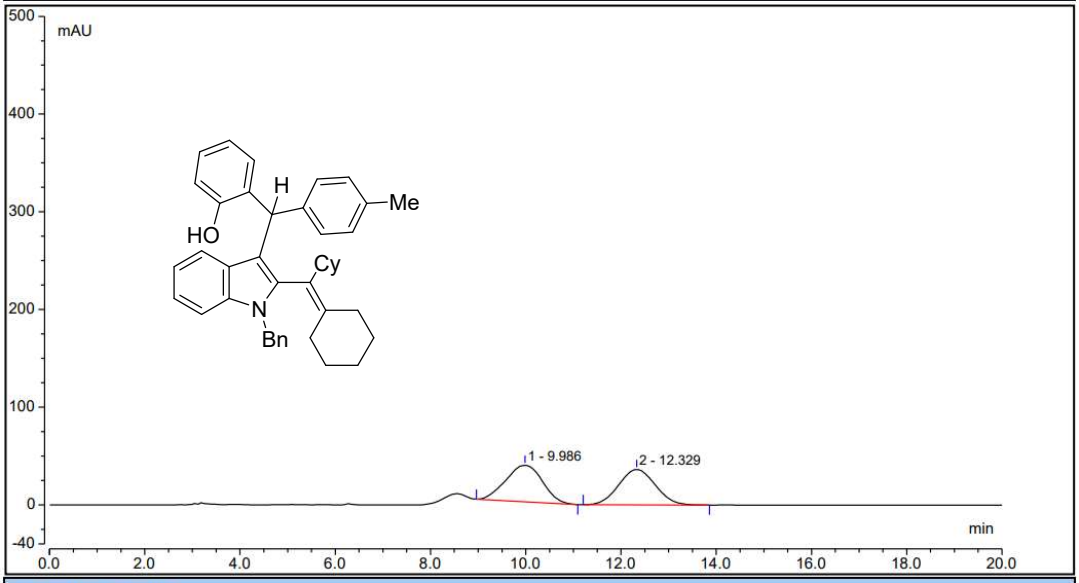
Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		7.766	13.110	37.758	91.86	95.32	n.a.
2		9.309	1.161	1.854	8.14	4.68	n.a.
Total:			**14.271**	**39.612**	**100.00**	**100.00**	

3ei

Racemic:

Chromatogram

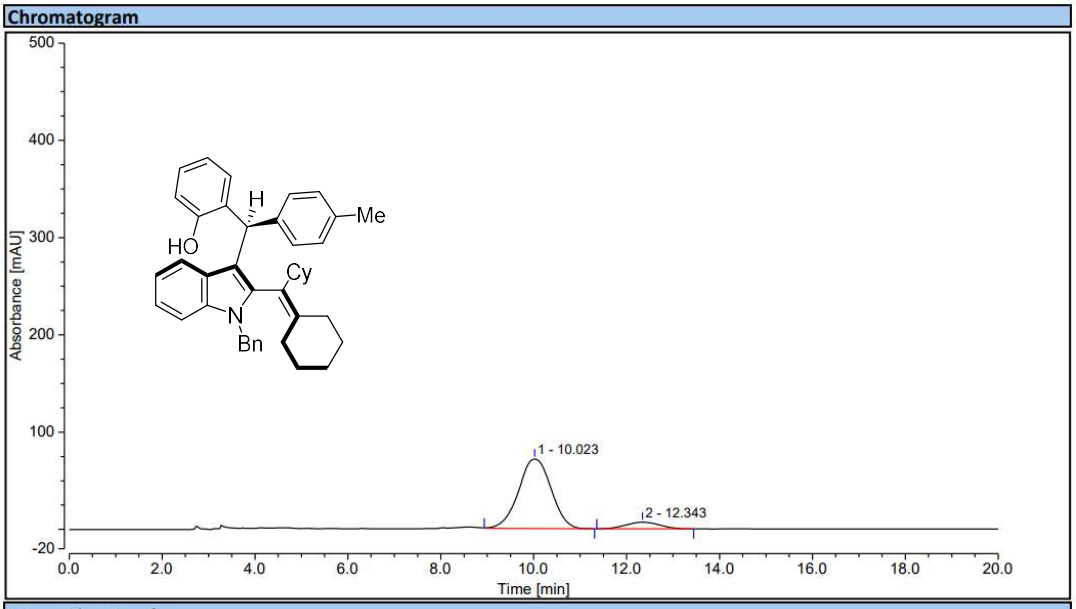


Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
n.a.		9.986	33.346	37.280	50.81	50.74	n.a.
n.a.		12.329	32.279	36.198	49.19	49.26	n.a.
Total:			**65.625**	**73.478**	**100.00**	**100.00**	

Enantioselective:

Chromatogram

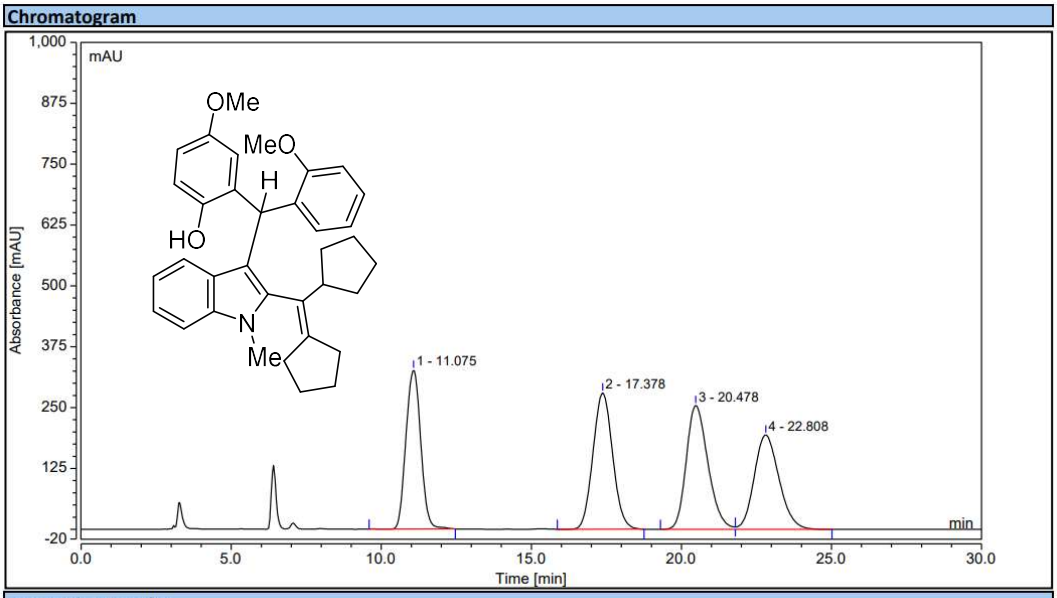


Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
n.a.		10.023	57.918	71.429	90.96	91.32	n.a.
n.a.		12.343	5.757	6.788	9.04	8.68	n.a.
Total:			**63.675**	**78.217**	**100.00**	**100.00**	

3fa

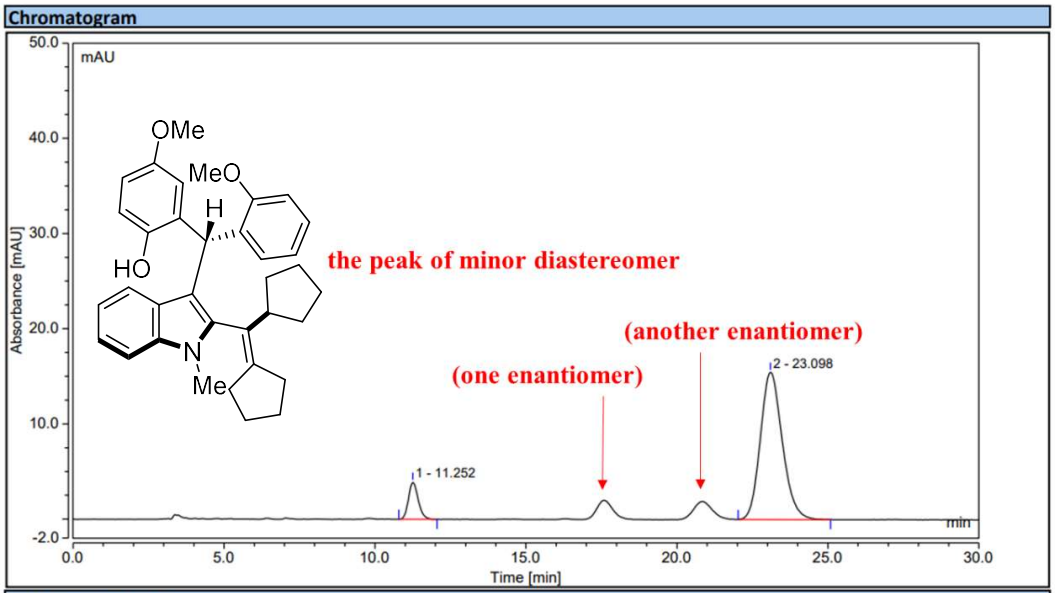
Racemic:



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		11.075	186.348	326.108	23.33	30.93	n.a.
2		17.378	212.831	279.805	26.64	26.54	n.a.
3		20.478	213.439	254.299	26.72	24.12	n.a.
4		22.808	186.236	193.992	23.31	18.40	n.a.
Total:			**798.853**	**1054.203**	**100.00**	**100.00**	

Enantioselective: (inseparable diastereomers with 85:15 dr):

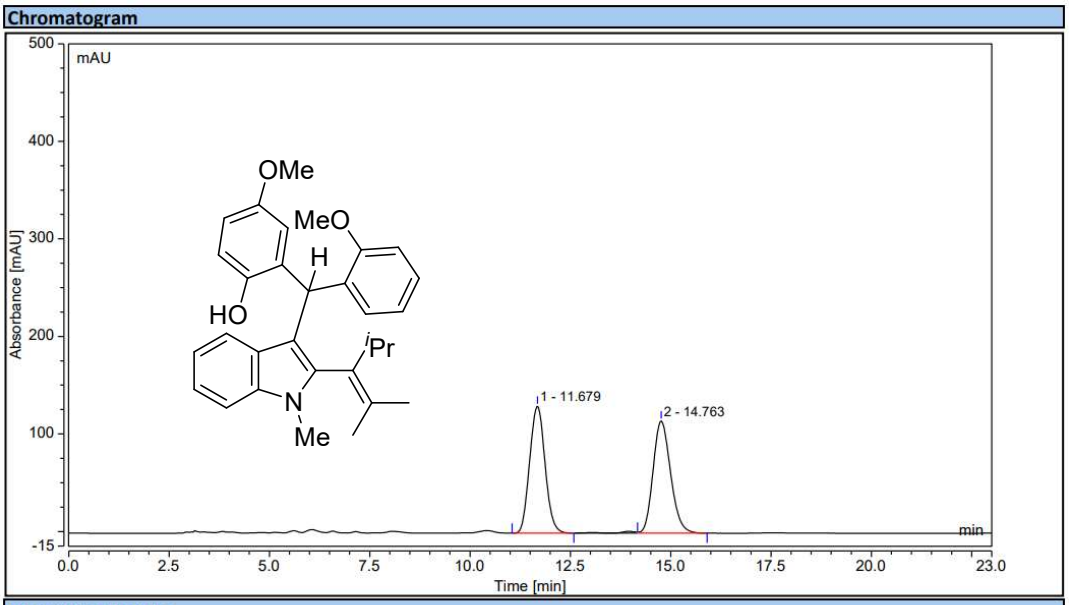


Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		11.252	1.450	3.893	10.02	20.09	n.a.
2		23.098	13.019	15.484	89.98	79.91	n.a.
Total:			**14.468**	**19.377**	**100.00**	**100.00**	

3ga

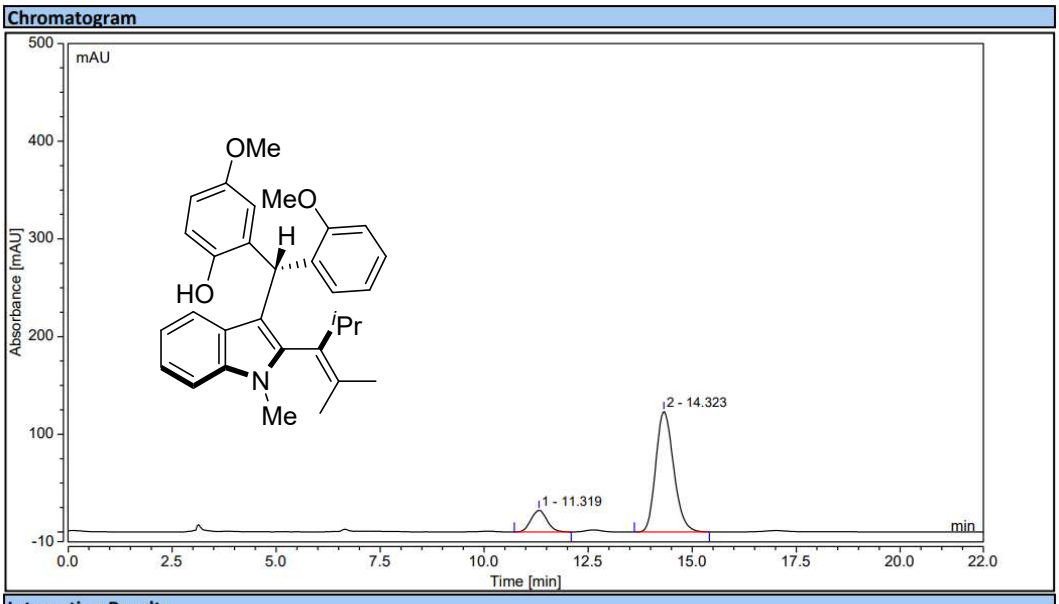
Racemic:



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		11.679	58.197	130.264	50.01	53.12	n.a.
2		14.763	58.174	114.943	49.99	46.88	n.a.
Total:			**116.371**	**245.207**	**100.00**	**100.00**	

Enantioselective:

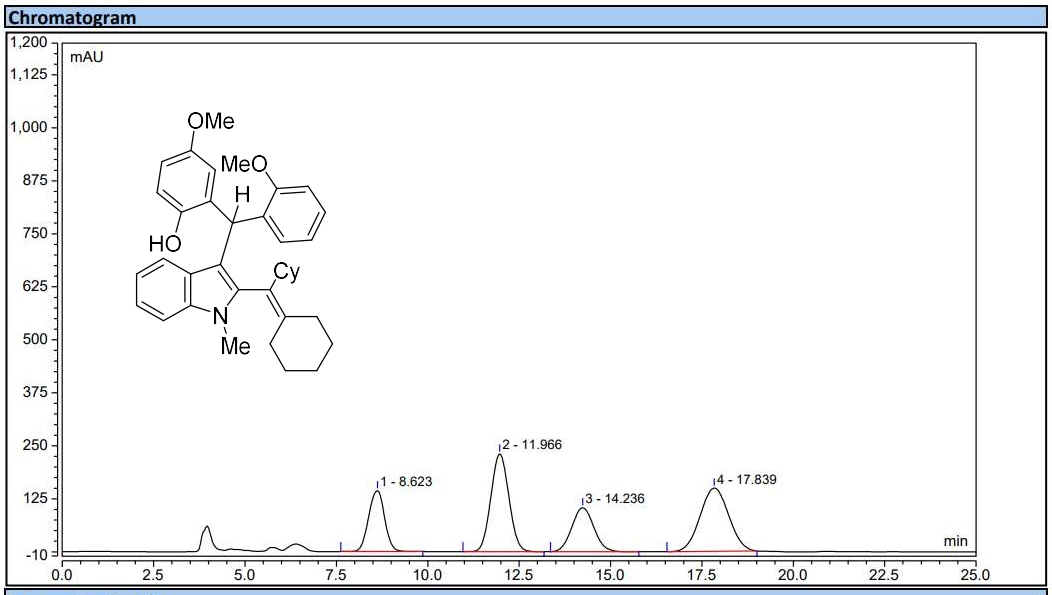


Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		11.319	9.847	22.047	13.80	15.17	n.a.
2		14.323	61.529	123.283	86.20	84.83	n.a.
Total:			**71.376**	**145.329**	**100.00**	**100.00**	

4aa

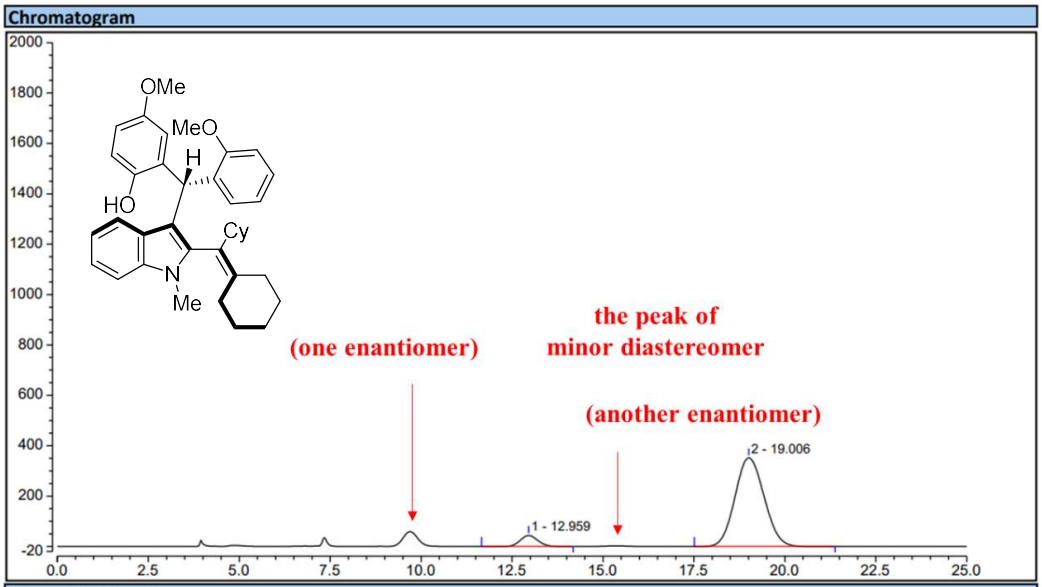
Racemic:



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		8.623	72.804	143.434	17.61	22.88	n.a.
2		11.966	132.314	230.426	32.01	36.75	n.a.
3		14.236	72.532	103.783	17.55	16.55	n.a.
4		17.839	135.734	149.328	32.83	23.82	n.a.
Total:			**413.384**	**626.971**	**100.00**	**100.00**	

Enantioselective (inseparable diastereomers with 92:8 dr):

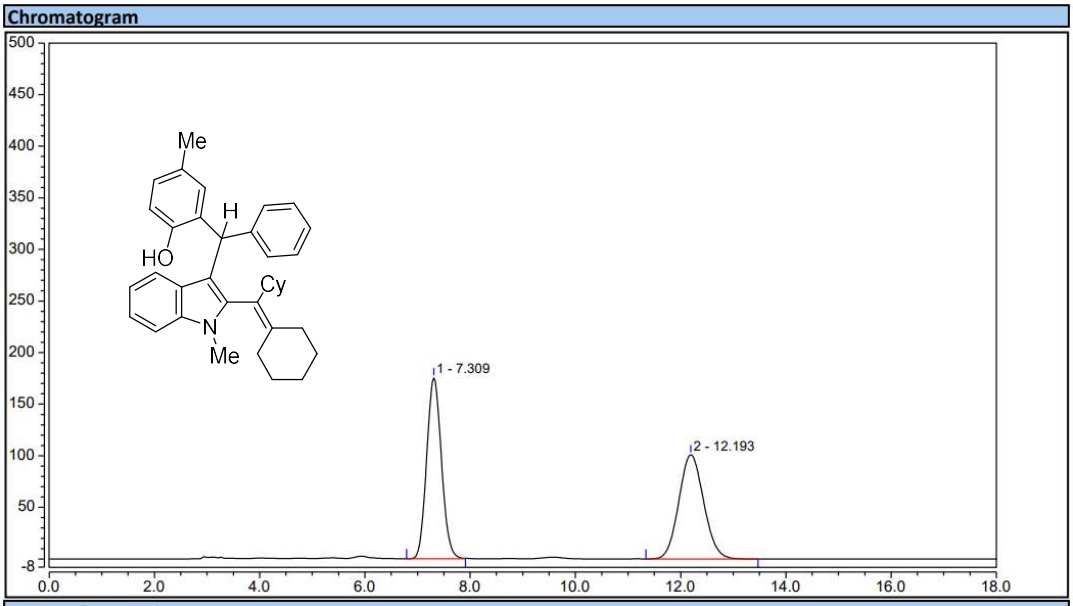


Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		12.959	24.623	43.637	6.99	11.03	n.a.
2		19.006	327.458	352.108	93.01	88.97	n.a.
Total:			**352.081**	**395.745**	**100.00**	**100.00**	

4ac

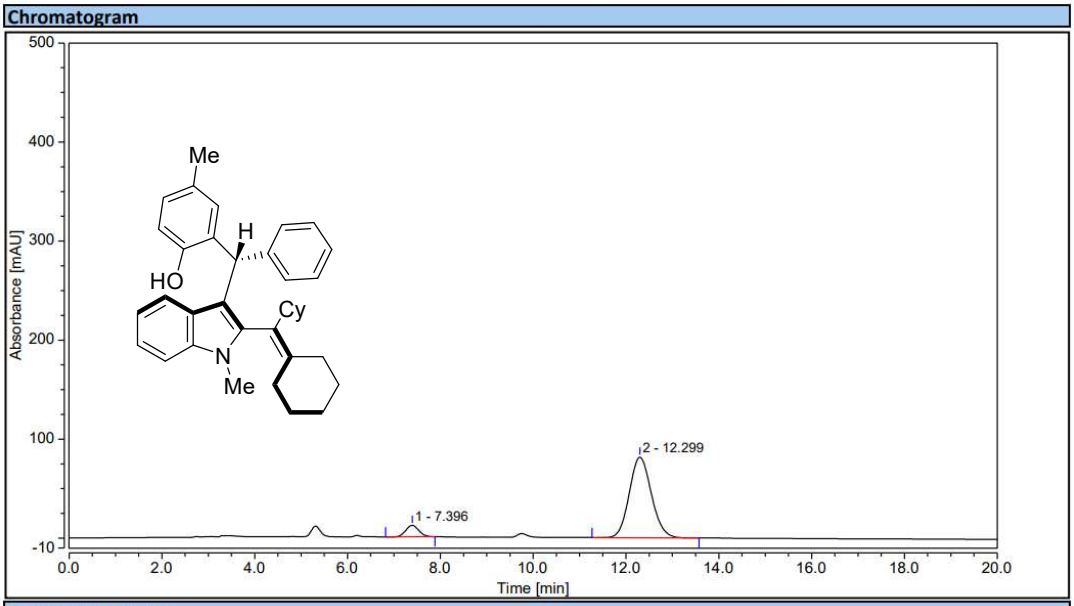
Racemic:



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		7.309	57.195	175.521	50.85	63.47	n.a.
2		12.193	55.278	101.003	49.15	36.53	n.a.
Total:			**112.473**	**276.524**	**100.00**	**100.00**	

Enantioselective:

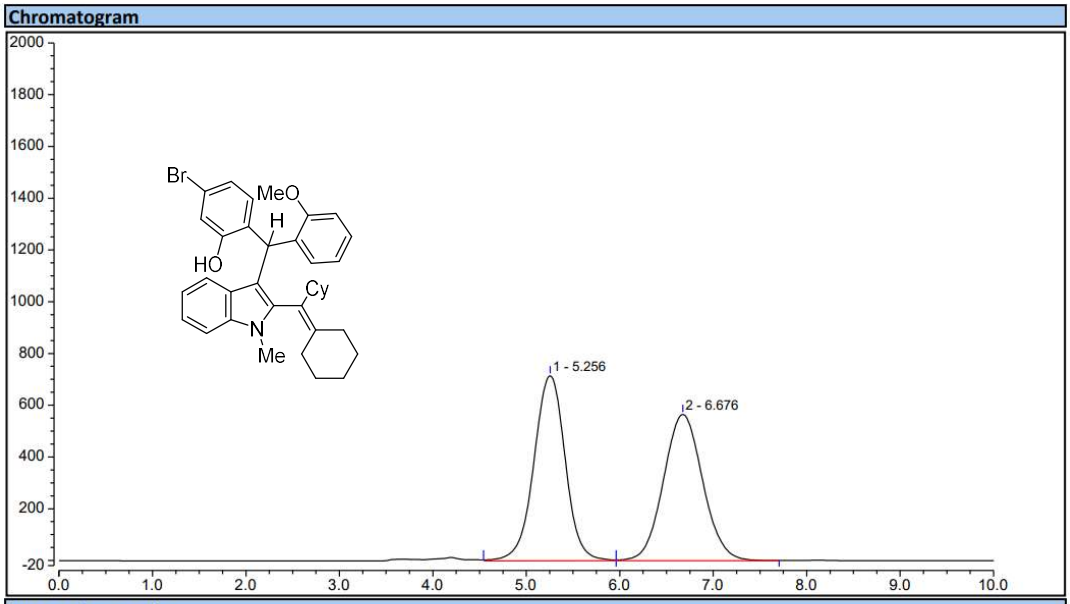


Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		7.396	3.826	11.712	7.85	12.58	n.a.
2		12.299	44.934	81.383	92.15	87.42	n.a.
Total:			**48.760**	**93.095**	**100.00**	**100.00**	

4al

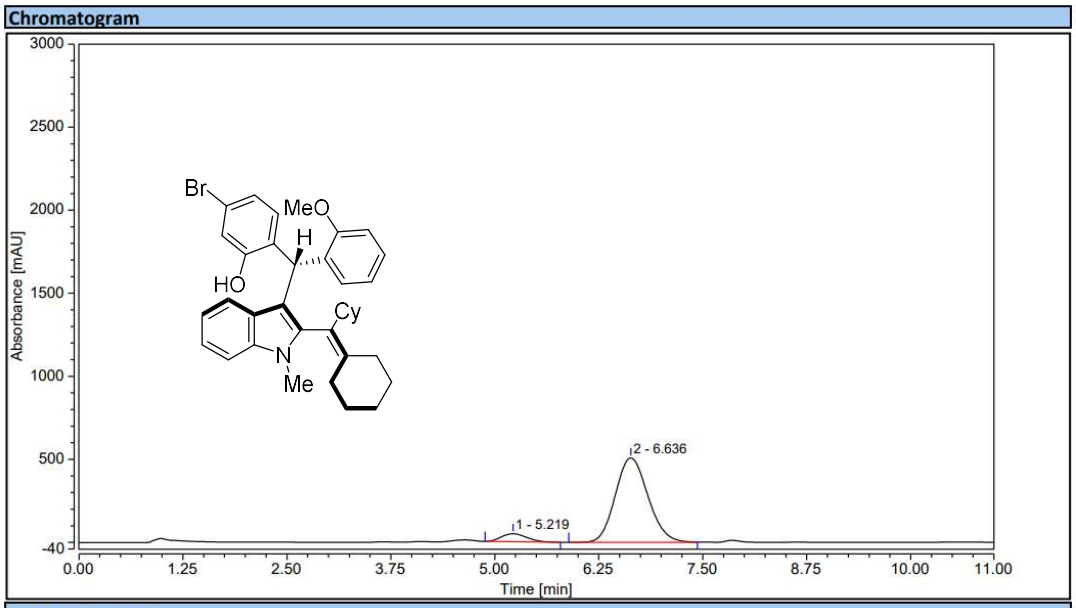
Racemic:



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		5.256	278.915	715.127	50.24	55.84	n.a.
2		6.676	276.304	565.567	49.76	44.16	n.a.
Total:			**555.219**	**1280.694**	**100.00**	**100.00**	

Enantioselective:

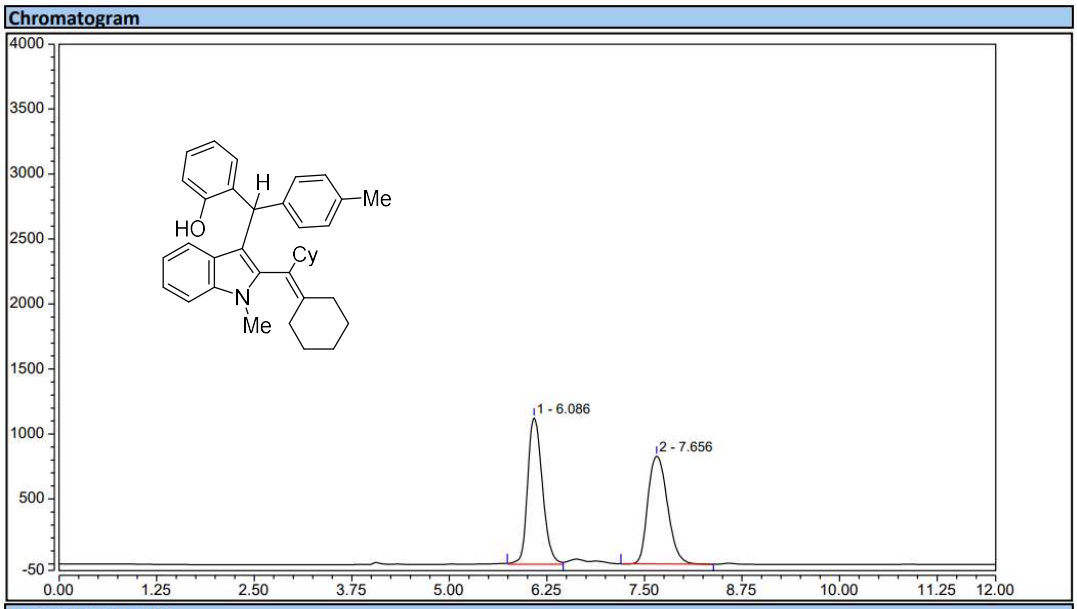


Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		5.219	17.076	48.201	6.87	8.66	n.a.
2		6.636	231.507	508.180	93.13	91.34	n.a.
Total:			**248.583**	**556.381**	**100.00**	**100.00**	

4ai

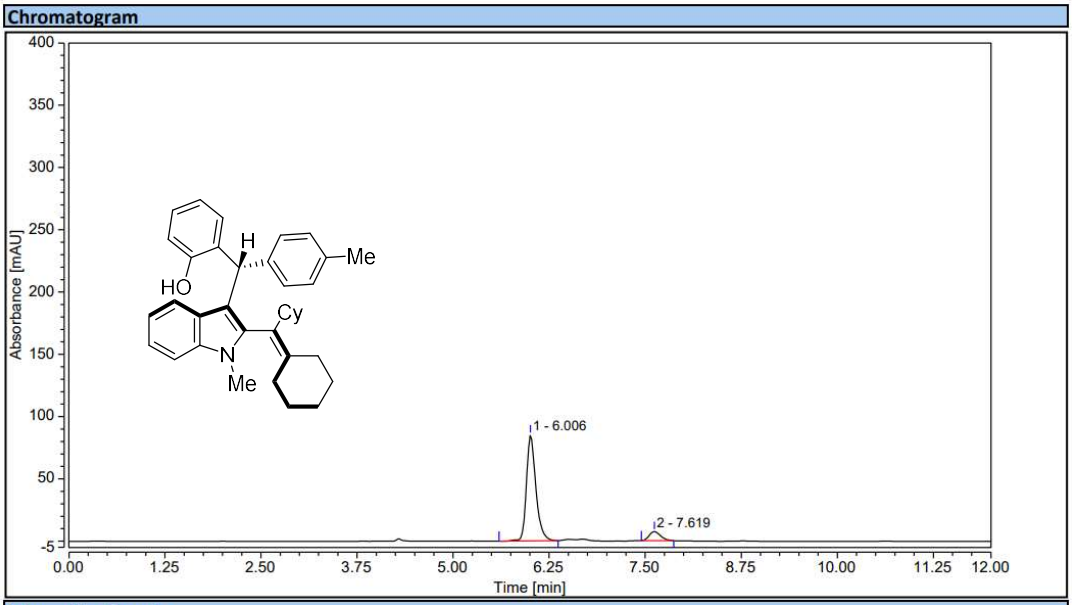
Racemic:



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		6.086	247.851	1125.782	50.60	57.58	n.a.
2		7.656	241.963	829.456	49.40	42.42	n.a.
Total:			**489.814**	**1955.238**	**100.00**	**100.00**	

Enantioselective:

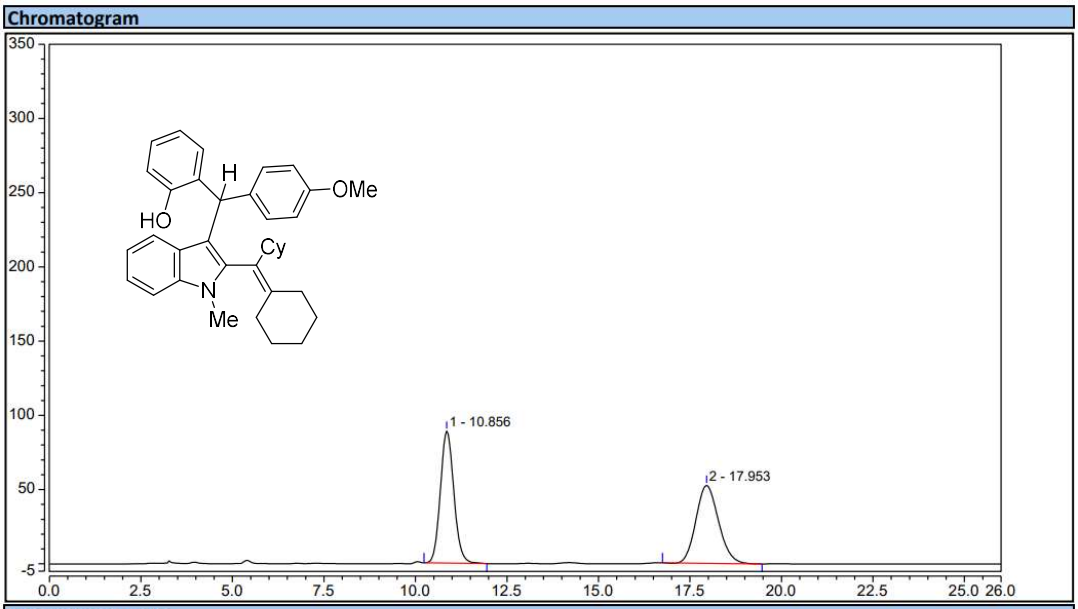


Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		6.006	12.112	84.999	90.74	92.05	n.a.
2		7.619	1.236	7.337	9.26	7.95	n.a.
Total:			**13.349**	**92.336**	**100.00**	**100.00**	

4am

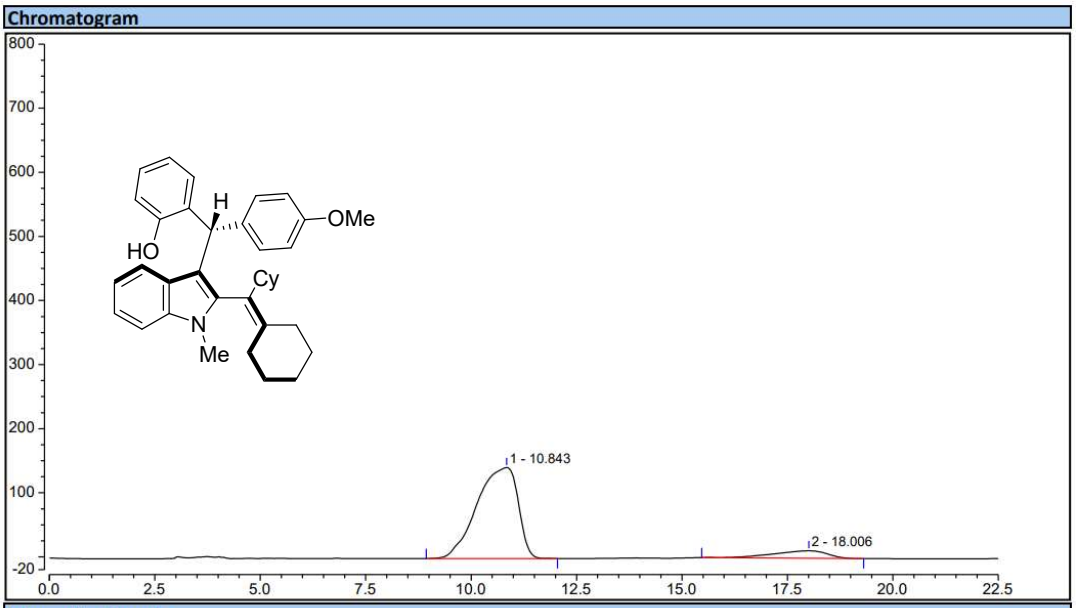
Racemic:



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		10.856	38.109	88.822	50.44	62.85	n.a.
2		17.953	37.450	52.496	49.56	37.15	n.a.
Total:			**75.558**	**141.318**	**100.00**	**100.00**	

Enantioselective:

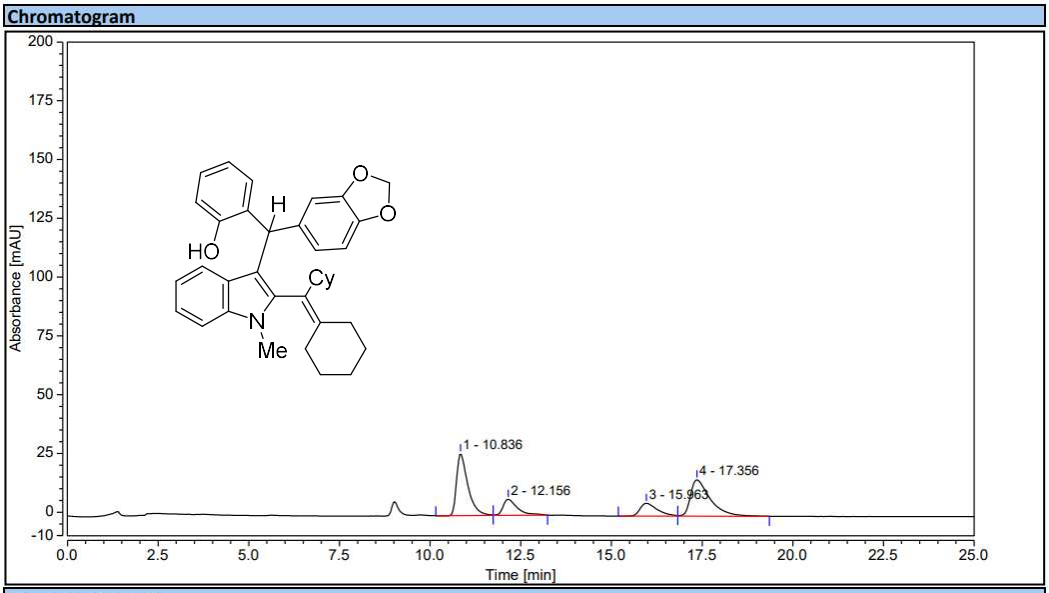


Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
n.a.		10.843	160.776	141.986	90.34	92.42	n.a.
n.a.		18.006	17.185	11.642	9.66	7.58	n.a.
Total:			**177.961**	**153.628**	**100.00**	**100.00**	

4aj

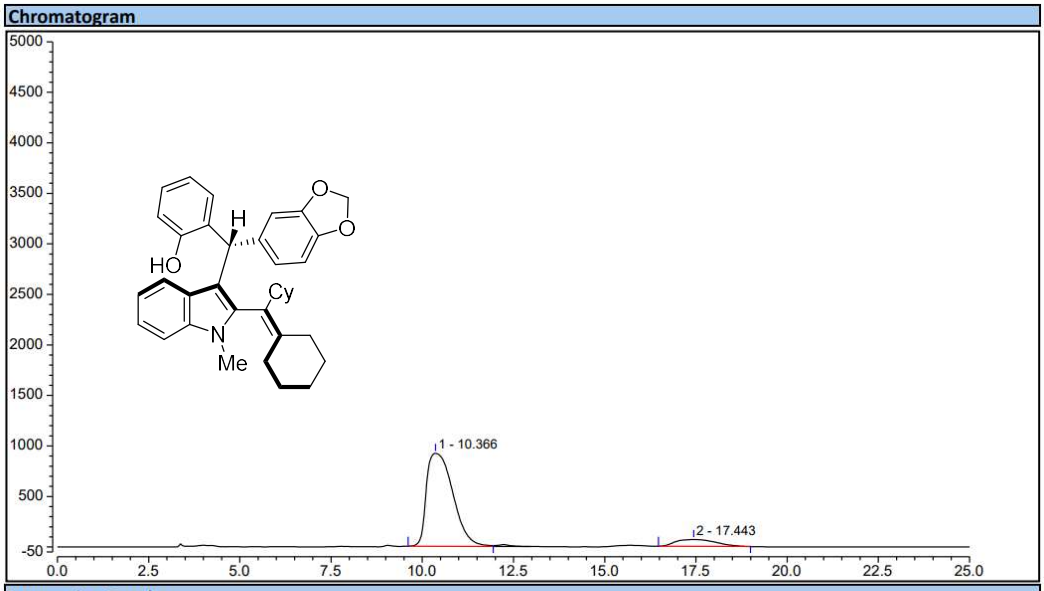
Racemic:



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		10.836	9.503	26.327	37.35	48.70	n.a.
2		12.156	3.131	6.795	12.30	12.57	n.a.
3		15.963	3.040	5.451	11.95	10.08	n.a.
4		17.356	9.771	15.491	38.40	28.65	n.a.
Total:			**25.444**	**54.063**	**100.00**	**100.00**	

Enantioselective (inseparable diastereomers with >95:5 dr):

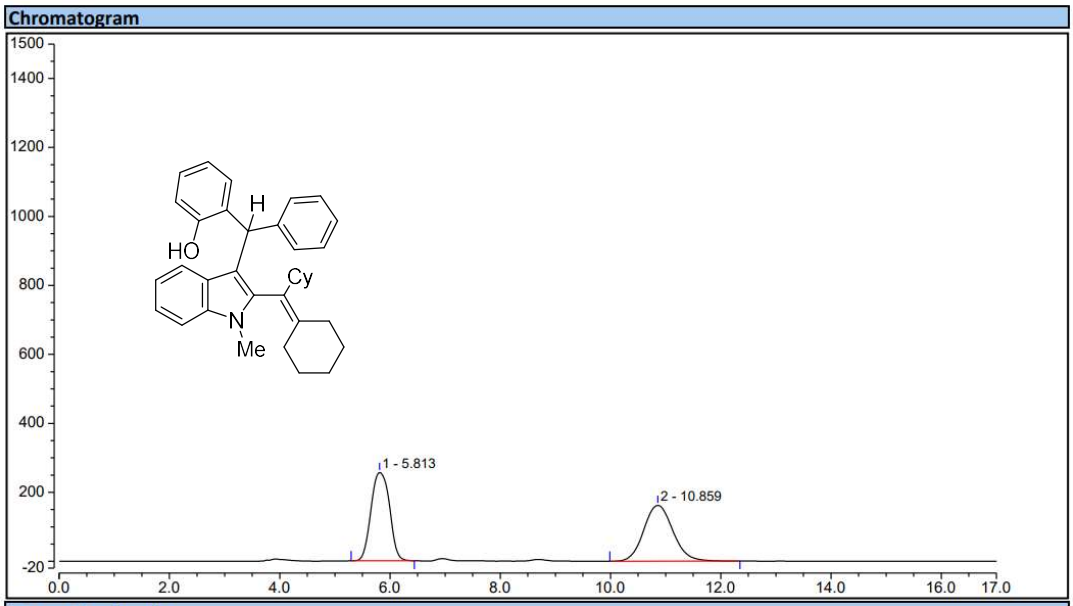


Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
n.a.		10.366	773.247	920.229	89.85	93.20	n.a.
n.a.		17.443	87.318	67.162	10.15	6.80	n.a.
Total:			**860.565**	**987.390**	**100.00**	**100.00**	

4ak

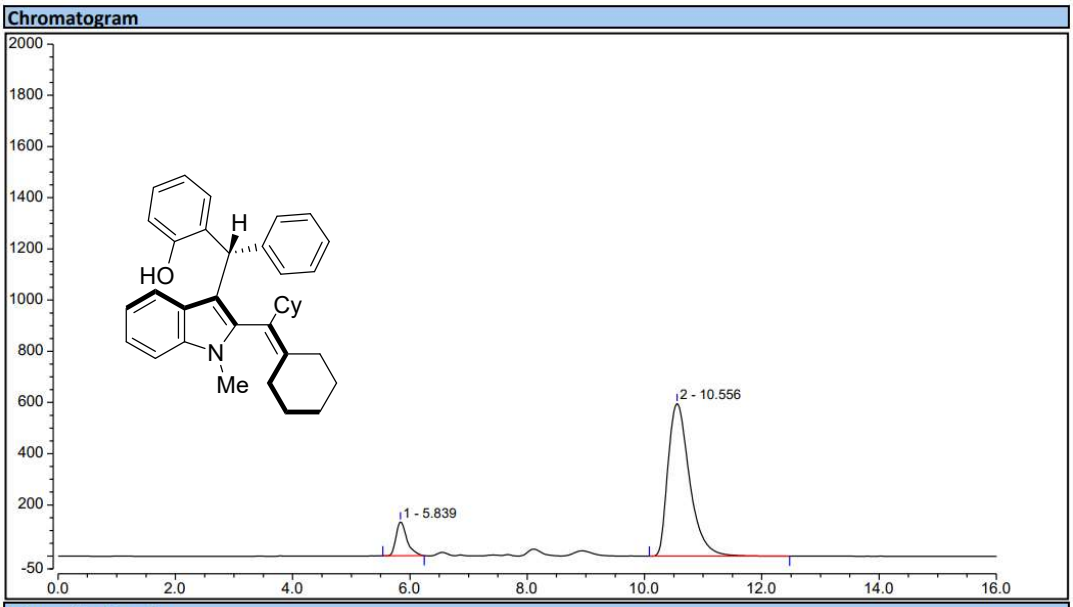
Racemic:



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		5.813	99.788	255.947	50.17	61.27	n.a.
2		10.859	99.128	161.799	49.83	38.73	n.a.
Total:			**198.916**	**417.746**	**100.00**	**100.00**	

Enantioselective:

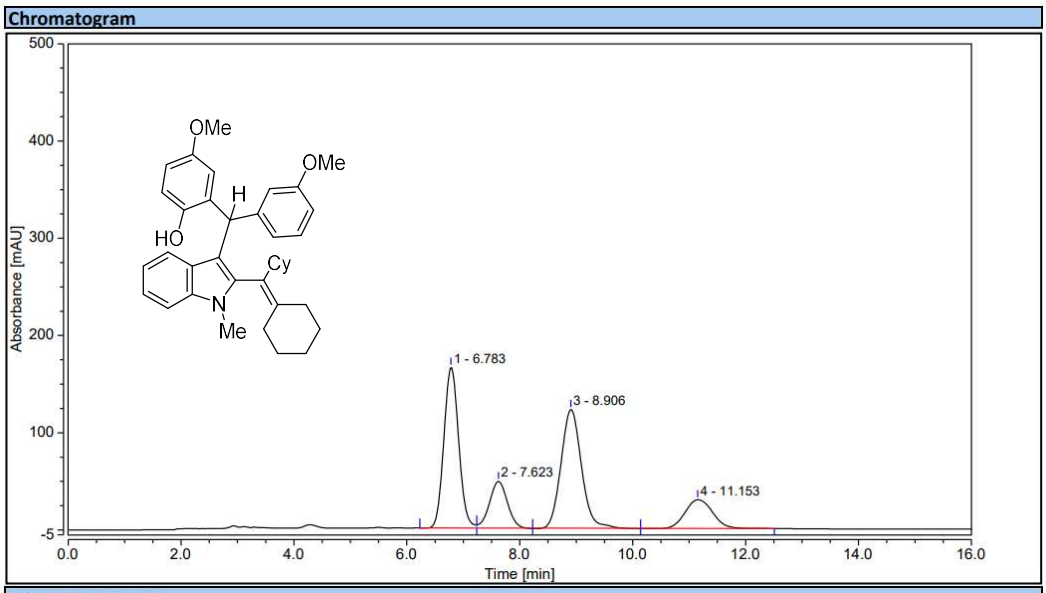


Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
n.a.		5.839	28.550	132.724	10.08	18.21	n.a.
n.a.		10.556	254.796	596.136	89.92	81.79	n.a.
Total:			**283.346**	**728.860**	**100.00**	**100.00**	

4af

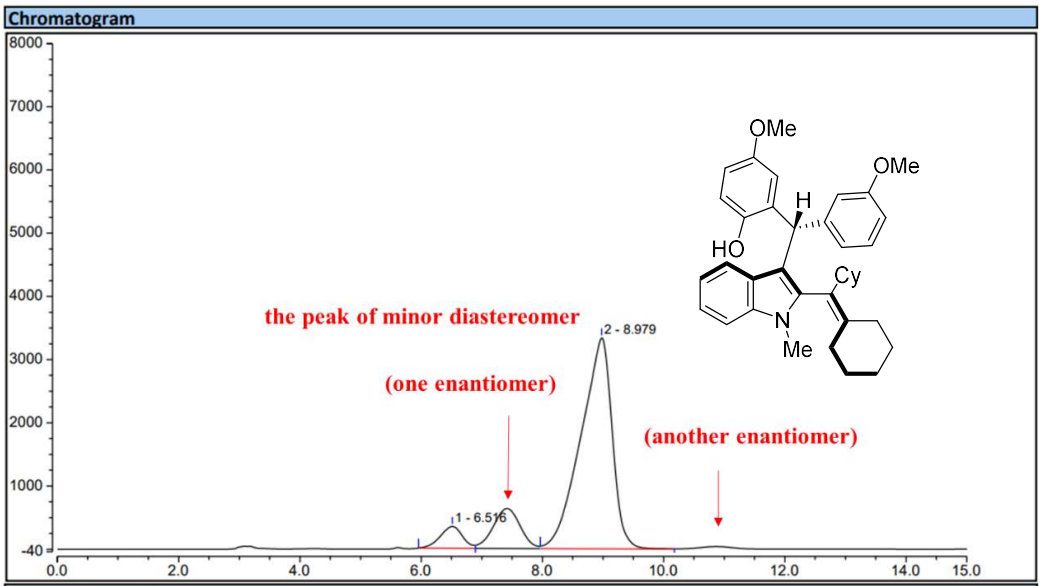
Racemic:



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		6.783	50.231	165.317	37.14	45.29	n.a.
2		7.623	17.619	48.002	13.03	13.15	n.a.
3		8.906	50.942	122.119	37.67	33.46	n.a.
4		11.153	16.445	29.548	12.16	8.10	n.a.
Total:			**135.237**	**364.986**	**100.00**	**100.00**	

Enantioselective (inseparable diastereomers with 86:14 dr):

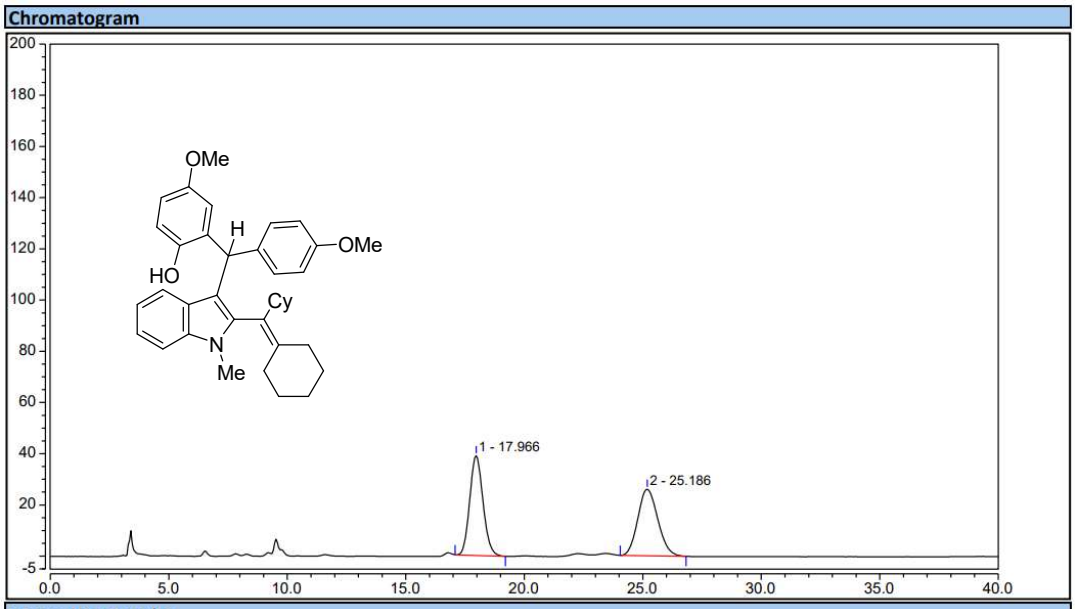


Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		6.516	146.859	343.593	6.84	9.33	n.a.
2		8.979	1999.177	3338.620	93.16	90.67	n.a.
Total:			**2146.036**	**3682.214**	**100.00**	**100.00**	

4ah

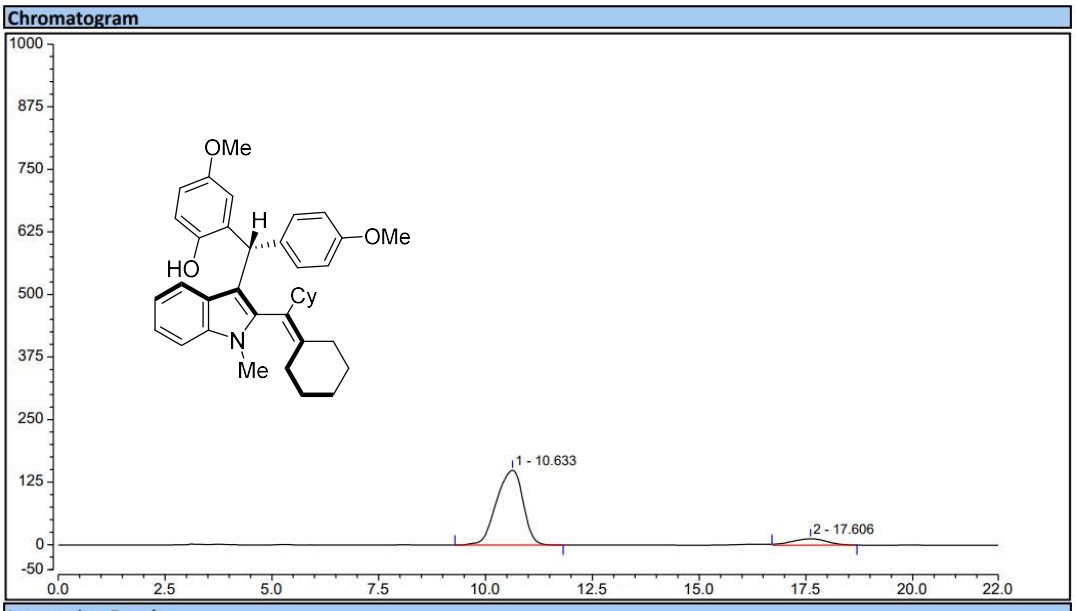
Racemic:



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		17.966	25.336	38.944	49.95	60.01	n.a.
2		25.186	25.388	25.951	50.05	39.99	n.a.
Total:			**50.724**	**64.895**	**100.00**	**100.00**	

Enantioselective:

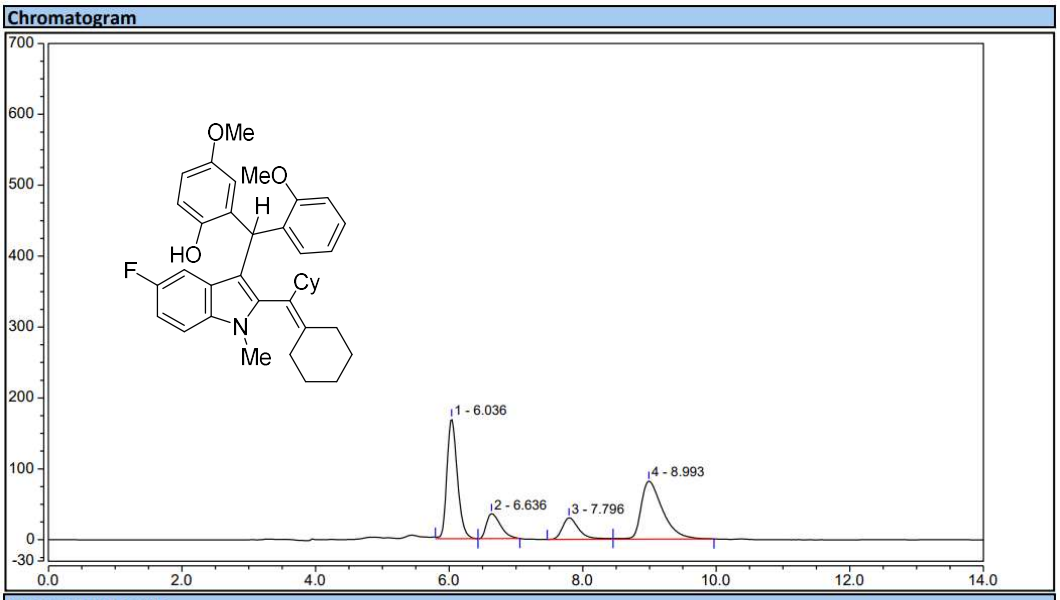


Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
n.a.		10.633	108.025	149.478	89.92	92.17	n.a.
n.a.		17.606	12.104	12.703	10.08	7.83	n.a.
Total:			**120.129**	**162.181**	**100.00**	**100.00**	

4ba

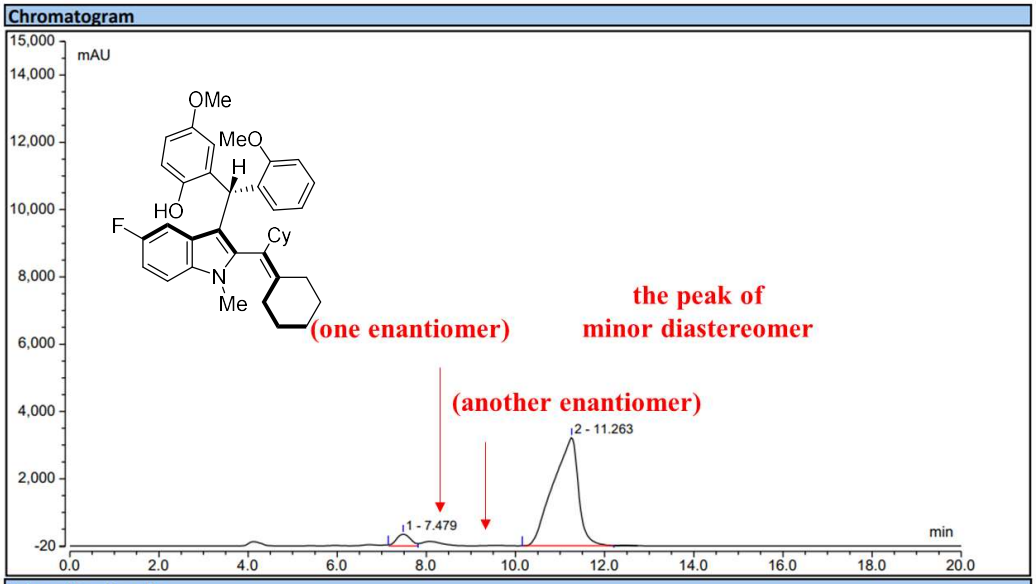
Racemic:



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		6.036	30.471	168.993	38.98	53.47	n.a.
2		6.636	8.556	35.211	10.95	11.14	n.a.
3		7.796	8.628	30.255	11.04	9.57	n.a.
4		8.993	30.505	81.601	39.03	25.82	n.a.
Total:			**78.160**	**316.060**	**100.00**	**100.00**	

Enantioselective (inseparable diastereomers with >95:5 dr):

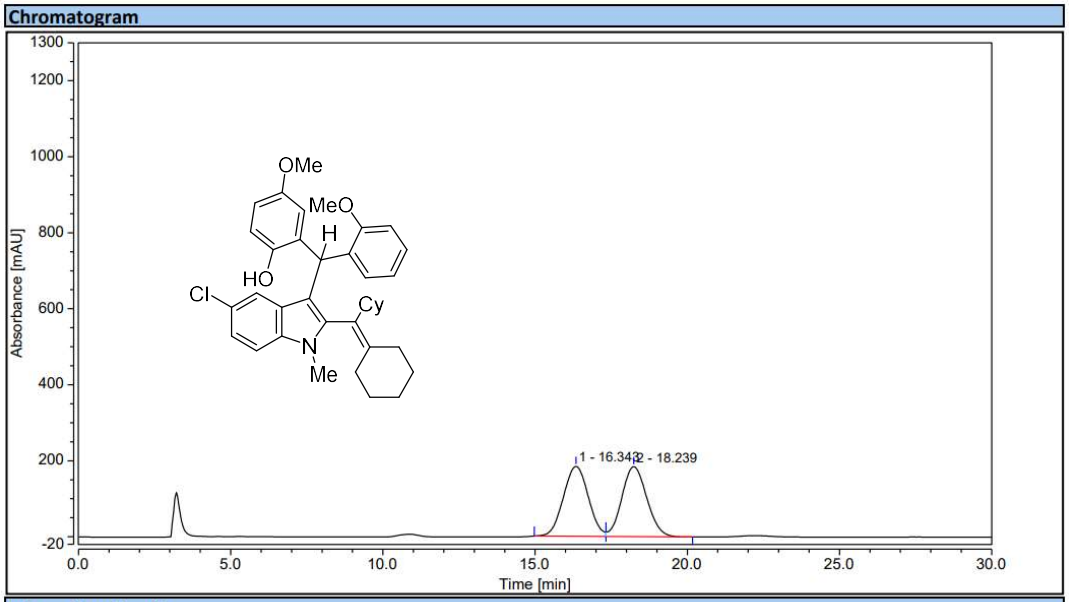


Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
n.a.		7.479	127.323	342.703	5.67	9.63	n.a.
n.a.		11.263	2118.058	3216.941	94.33	90.37	n.a.
Total:			**2245.381**	**3559.644**	**100.00**	**100.00**	

4ca

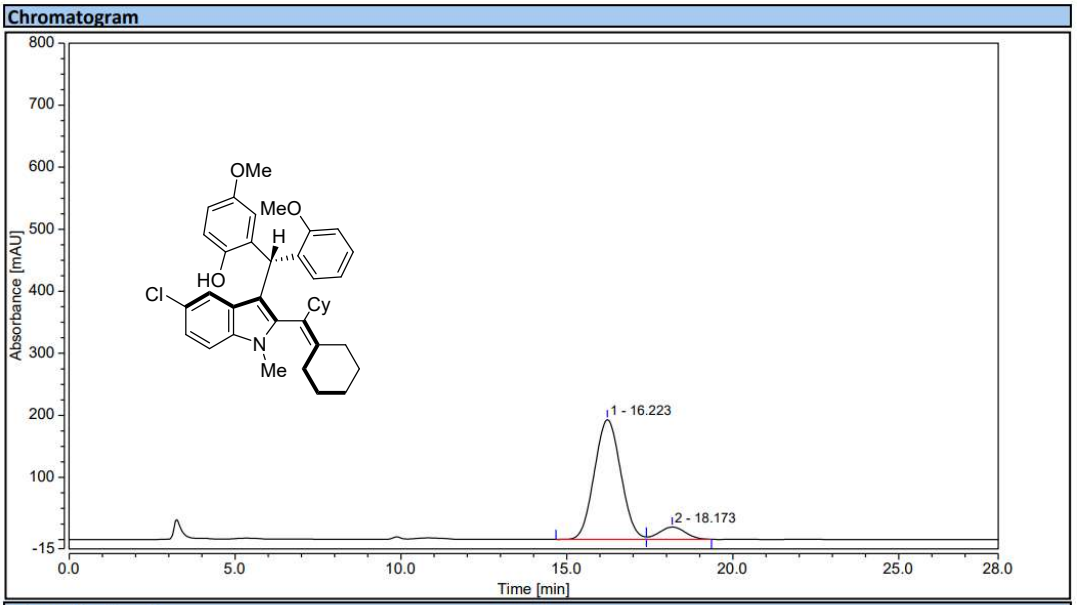
Racemic:



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		16.343	174.989	183.997	49.97	49.98	n.a.
2		18.239	175.210	184.128	50.03	50.02	n.a.
Total:			**350.199**	**368.126**	**100.00**	**100.00**	

Enantioselective:

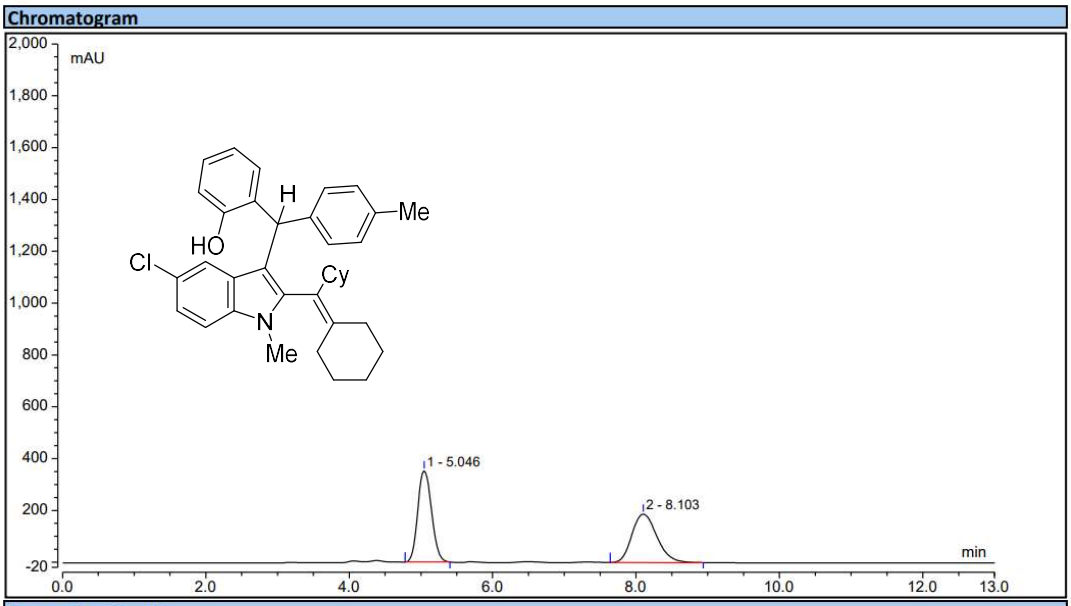


Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		16.223	178.198	192.893	90.71	90.66	n.a.
2		18.173	18.244	19.864	9.29	9.34	n.a.
Total:			**196.442**	**212.757**	**100.00**	**100.00**	

4ci

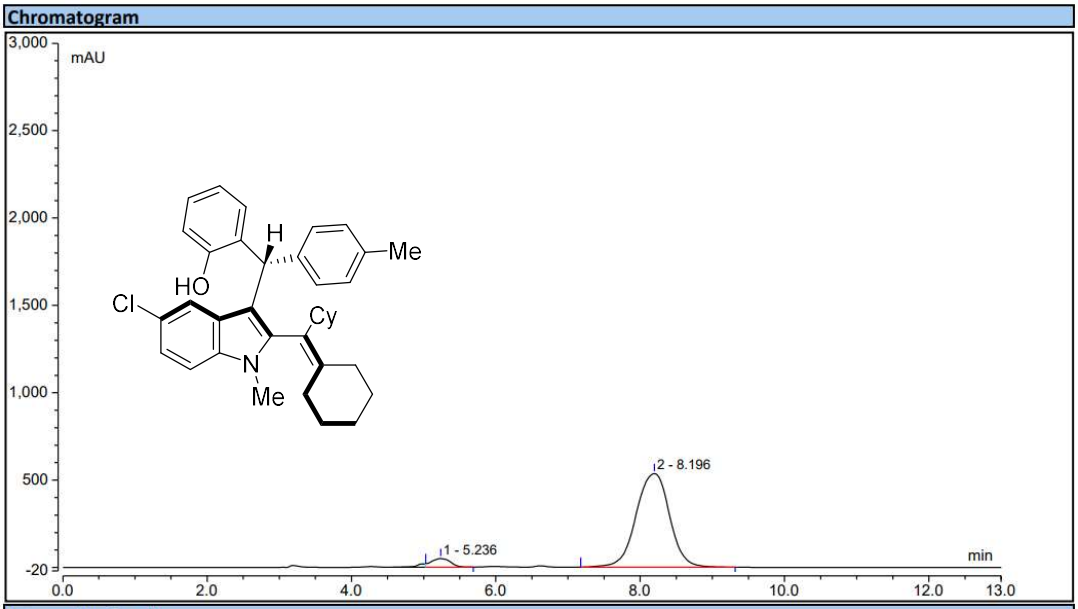
Racemic:



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
n.a.		5.046	78.652	351.885	51.00	65.33	n.a.
n.a.		8.103	75.560	186.768	49.00	34.67	n.a.
Total:			**154.211**	**538.654**	**100.00**	**100.00**	

Enantioselective:

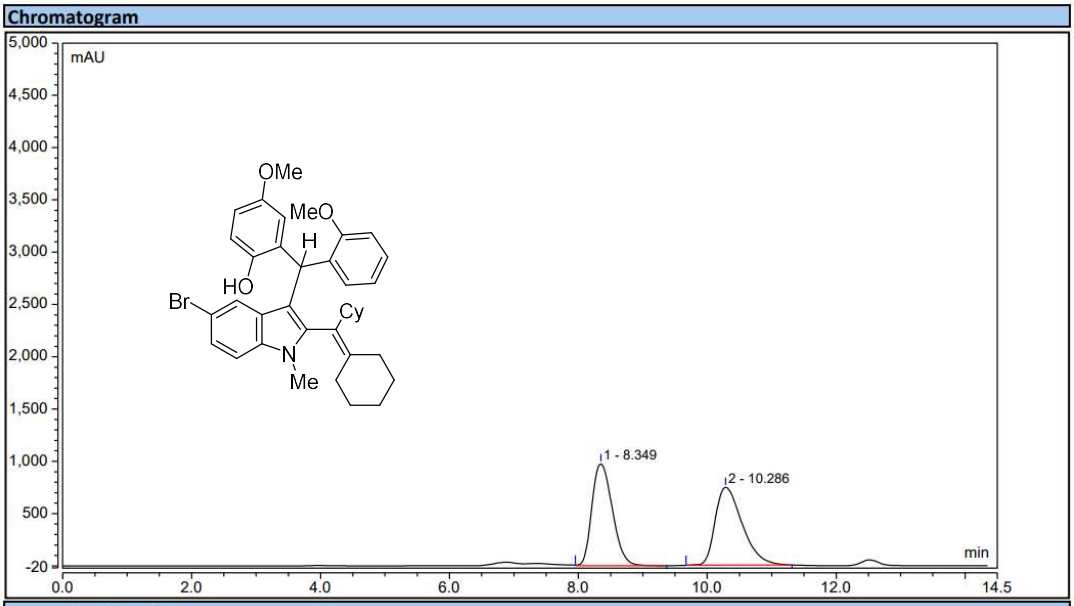


Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
n.a.		5.236	15.280	48.775	5.03	8.34	n.a.
n.a.		8.196	288.239	535.717	94.97	91.66	n.a.
Total:			**303.519**	**584.492**	**100.00**	**100.00**	

4da

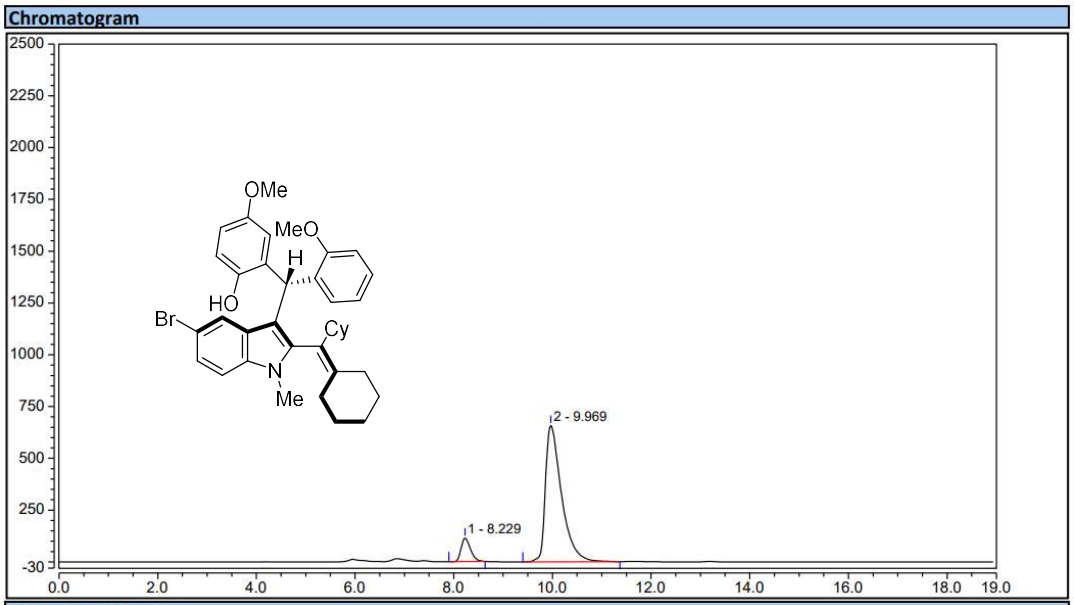
Racemic:



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		8.349	358.521	973.645	49.68	56.64	n.a.
2		10.286	363.170	745.278	50.32	43.36	n.a.
Total:			**721.690**	**1718.923**	**100.00**	**100.00**	

Enantioselective:



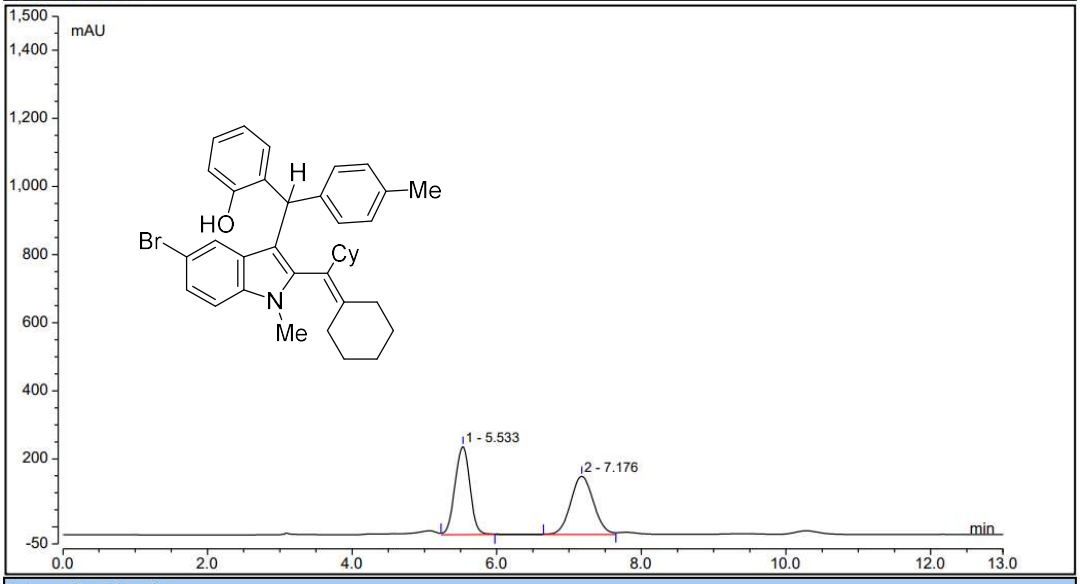
Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		8.229	25.015	113.388	9.14	14.69	n.a.
2		9.969	248.666	658.741	90.86	85.31	n.a.
Total:			**273.682**	**772.129**	**100.00**	**100.00**	

4di

Racemic:

Chromatogram

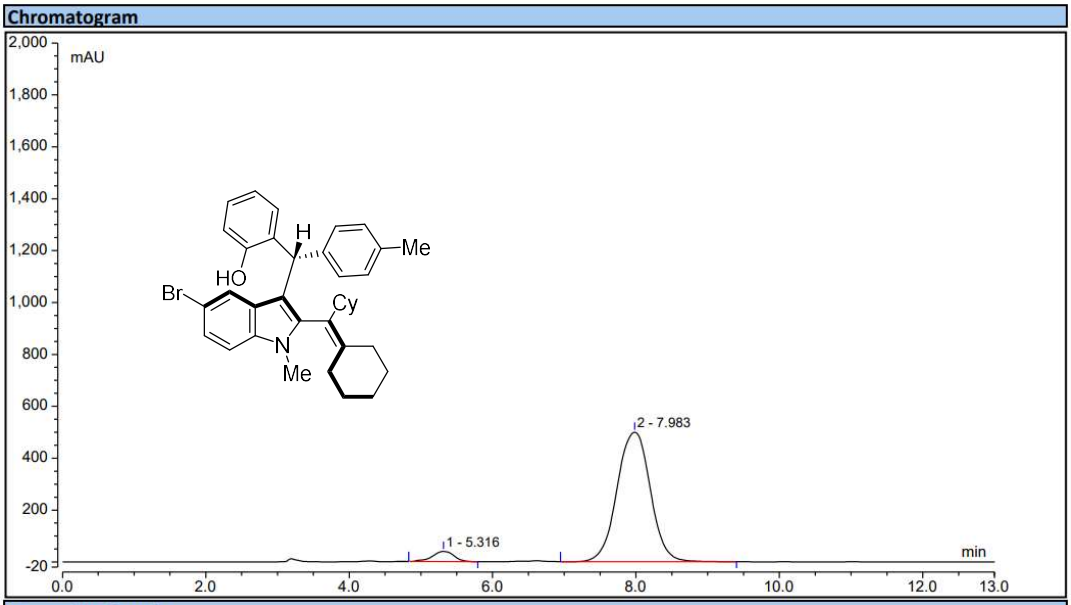


Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
n.a.		5.533	62.322	259.332	49.79	60.29	n.a.
n.a.		7.176	62.856	170.796	50.21	39.71	n.a.
Total:			**125.178**	**430.128**	**100.00**	**100.00**	

Enantioselective:

Chromatogram

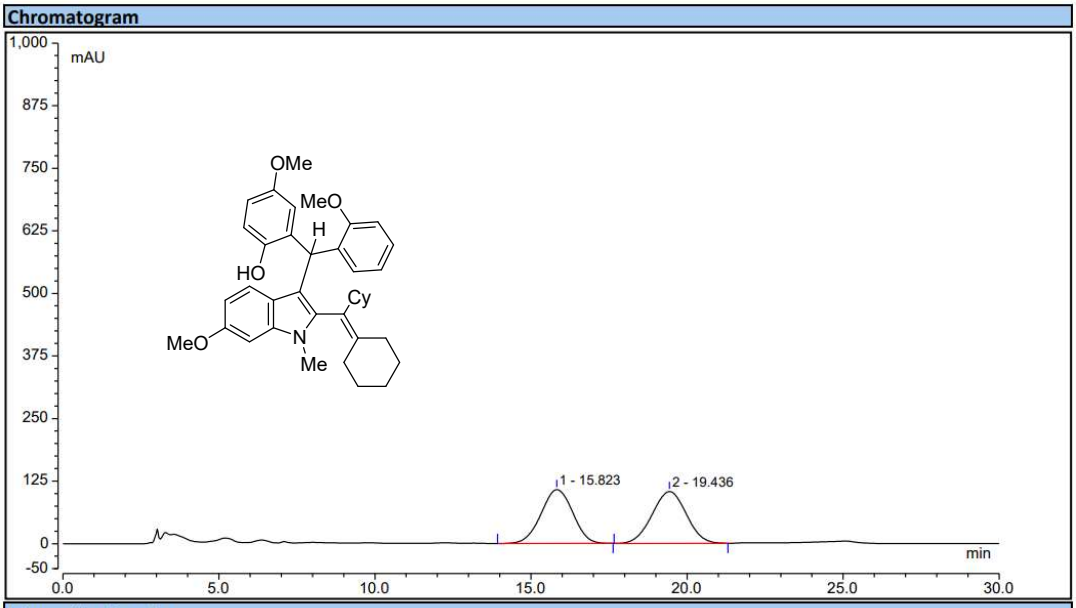


Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
n.a.		5.316	13.817	39.161	4.89	7.28	n.a.
n.a.		7.983	268.954	498.987	95.11	92.72	n.a.
Total:			**282.771**	**538.148**	**100.00**	**100.00**	

4ha

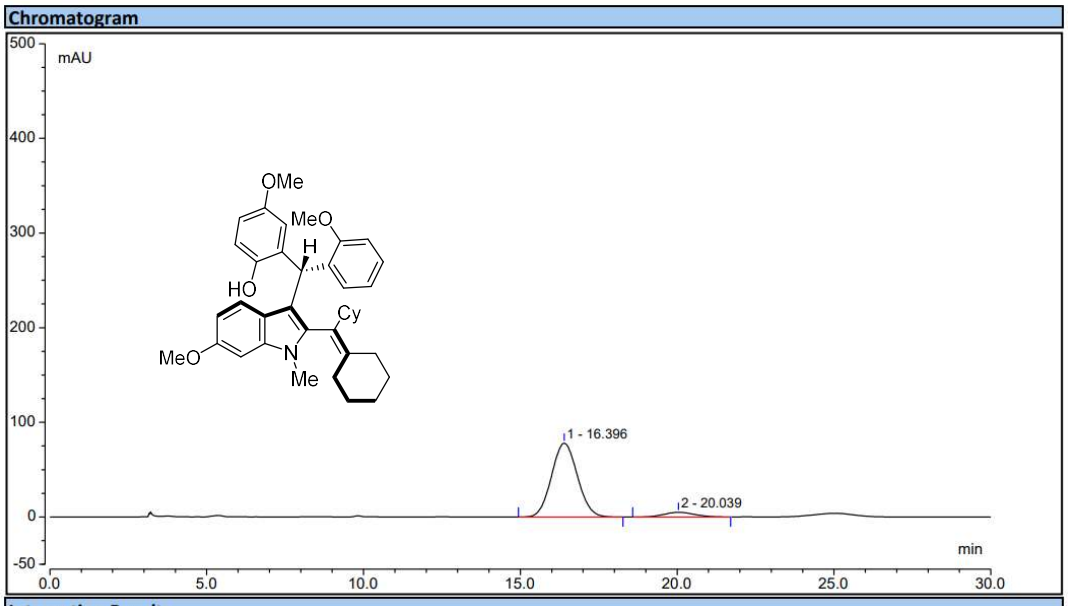
Racemic:



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
n.a.		15.823	126.969	107.599	49.13	50.97	n.a.
n.a.		19.436	131.482	103.503	50.87	49.03	n.a.
Total:			**258.452**	**211.101**	**100.00**	**100.00**	

Enantioselective:

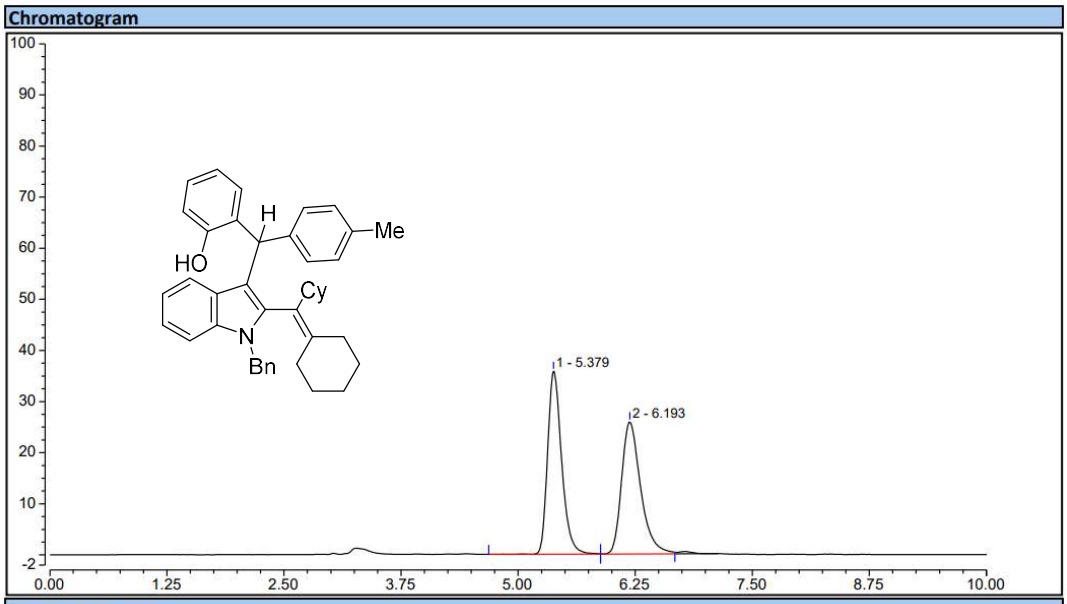


Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
n.a.		16.396	74.746	78.012	92.91	94.03	n.a.
n.a.		20.039	5.701	4.955	7.09	5.97	n.a.
Total:			**80.448**	**82.968**	**100.00**	**100.00**	

4ei

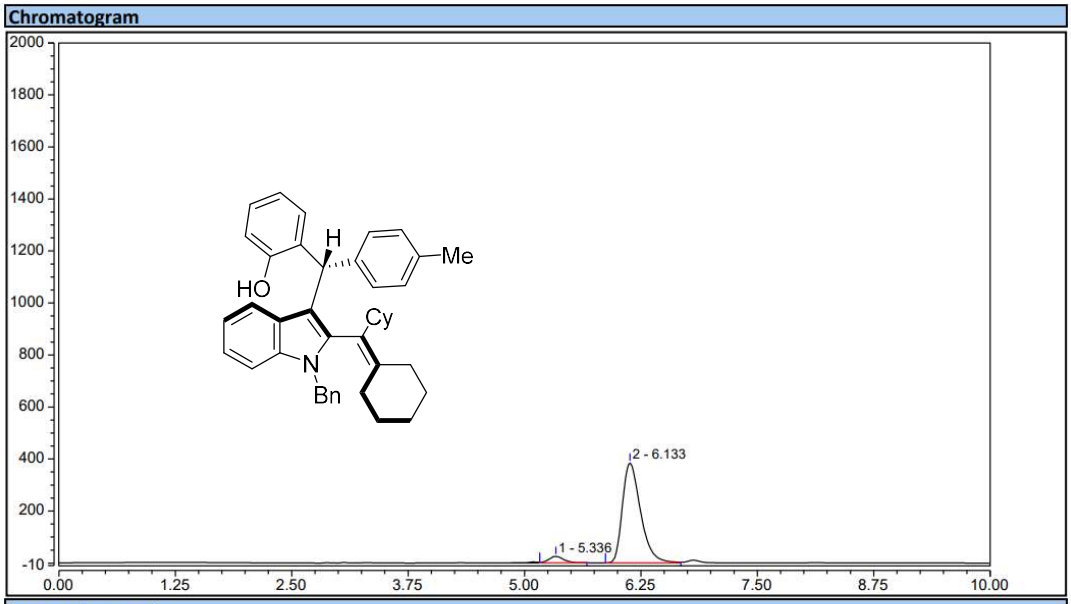
Racemic:



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
n.a.		5.379	6.215	35.785	50.53	58.08	n.a.
n.a.		6.193	6.084	25.830	49.47	41.92	n.a.
Total:			**12.298**	**61.615**	**100.00**	**100.00**	

Enantioselective:

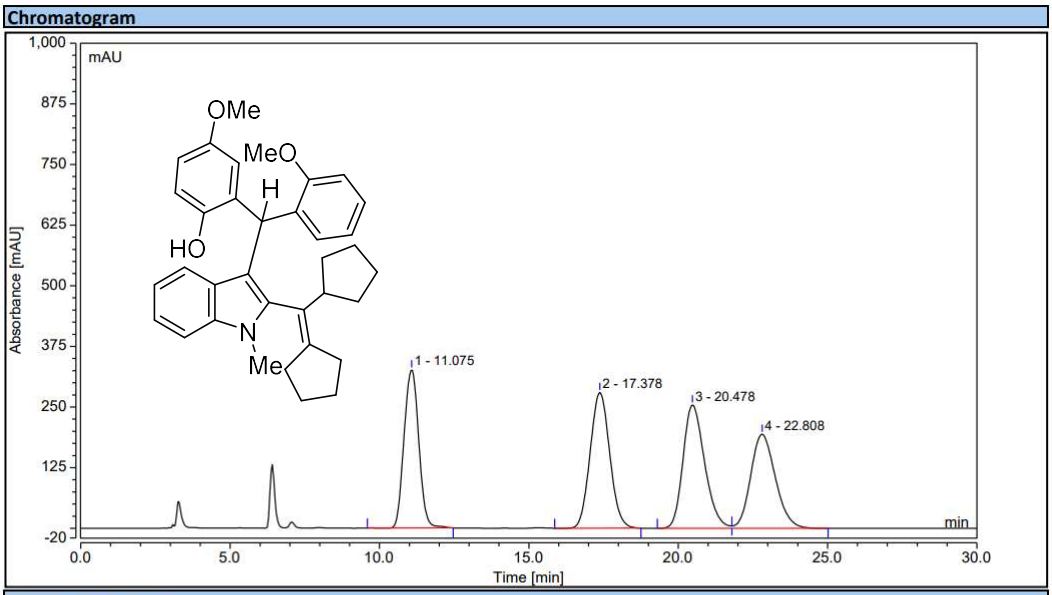


Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		5.336	4.474	24.513	4.89	6.00	n.a.
2		6.133	86.950	383.861	95.11	94.00	n.a.
Total:			**91.423**	**408.375**	**100.00**	**100.00**	

4fa

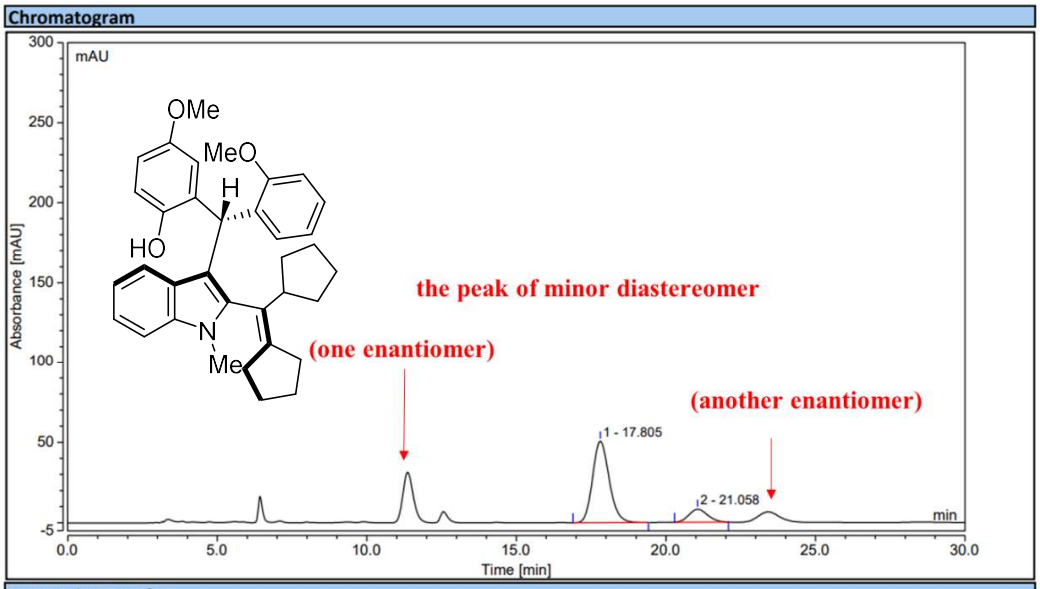
Racemic:



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		11.075	186.348	326.108	23.33	30.93	n.a.
2		17.378	212.831	279.805	26.64	26.54	n.a.
3		20.478	213.439	254.299	26.72	24.12	n.a.
4		22.808	186.236	193.992	23.31	18.40	n.a.
Total:			**798.853**	**1054.203**	**100.00**	**100.00**	

Enantioselective:

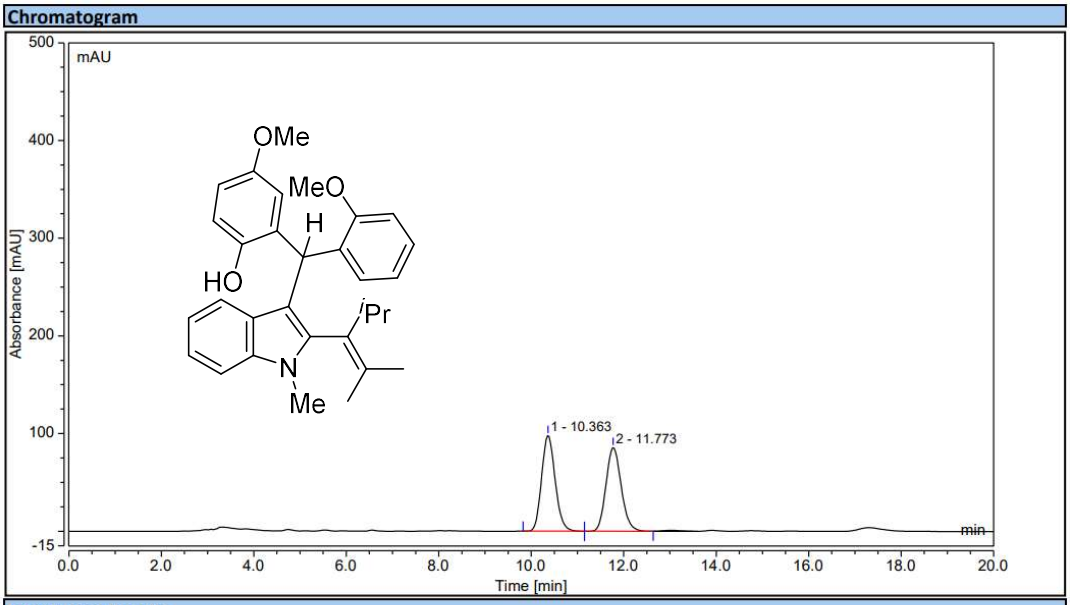


Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		17.805	32.719	50.749	84.76	86.24	n.a.
2		21.058	5.882	8.098	15.24	13.76	n.a.
Total:			**38.601**	**58.847**	**100.00**	**100.00**	

4ga

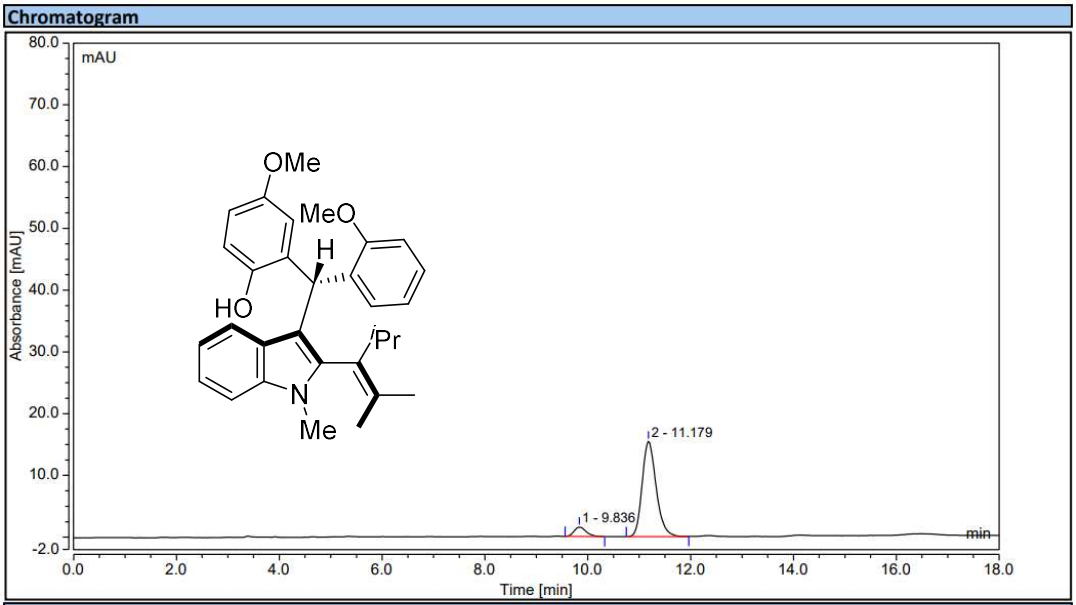
Racemic:



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		10.363	33.274	97.965	50.58	53.34	n.a.
2		11.773	32.511	85.691	49.42	46.66	n.a.
Total:			**65.785**	**183.655**	**100.00**	**100.00**	

Enantioselective:

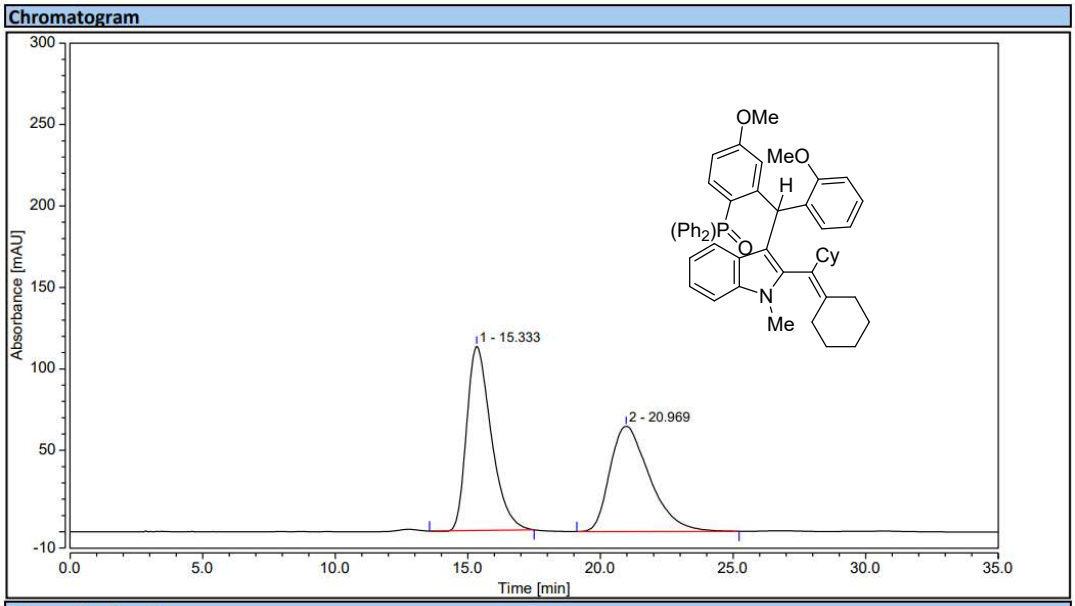


Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		9.836	0.418	1.520	7.92	8.96	n.a.
2		11.179	4.860	15.445	92.08	91.04	n.a.
Total:			**5.278**	**16.965**	**100.00**	**100.00**	

8

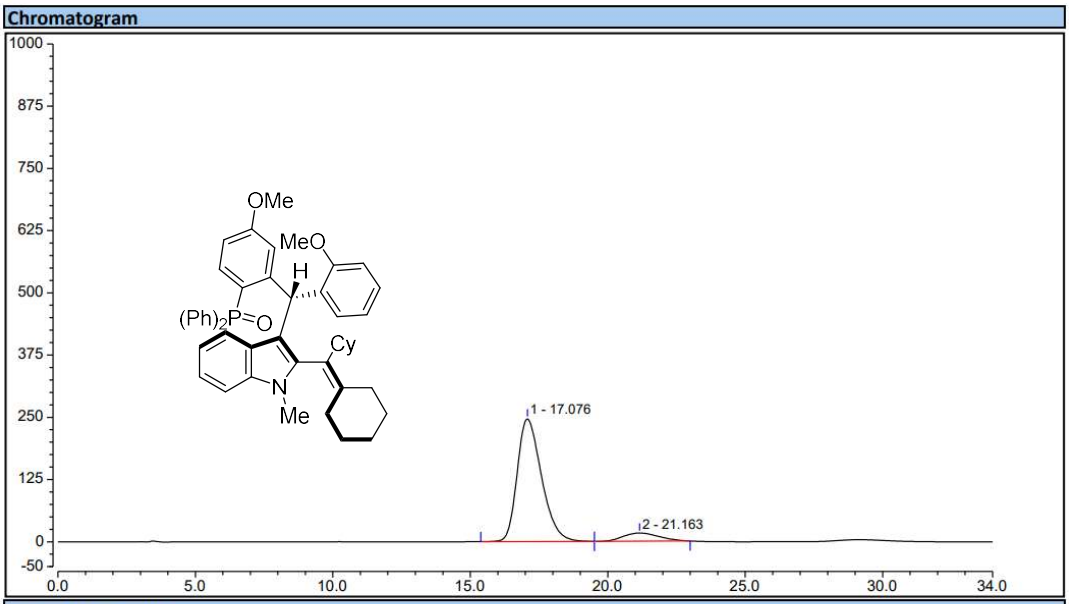
Racemic:



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		15.333	121.279	113.091	51.92	63.68	n.a.
2		20.969	112.318	64.508	48.08	36.32	n.a.
Total:			**233.597**	**177.599**	**100.00**	**100.00**	

Enantioselective:

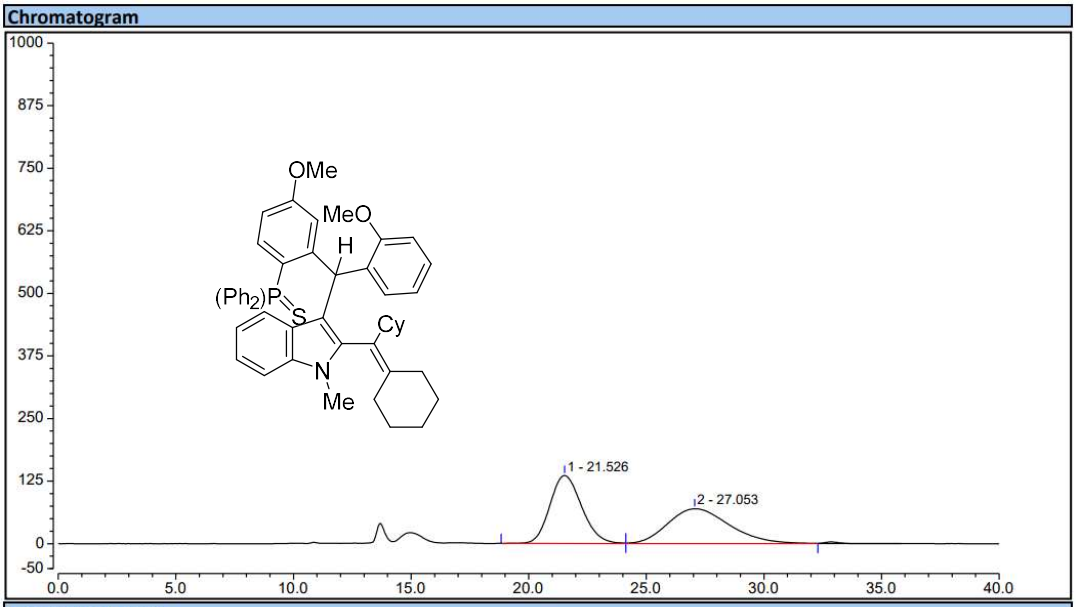


Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
n.a.		17.076	252.815	246.432	91.12	93.73	n.a.
n.a.		21.163	24.634	16.477	8.88	6.27	n.a.
Total:			**277.449**	**262.909**	**100.00**	**100.00**	

10

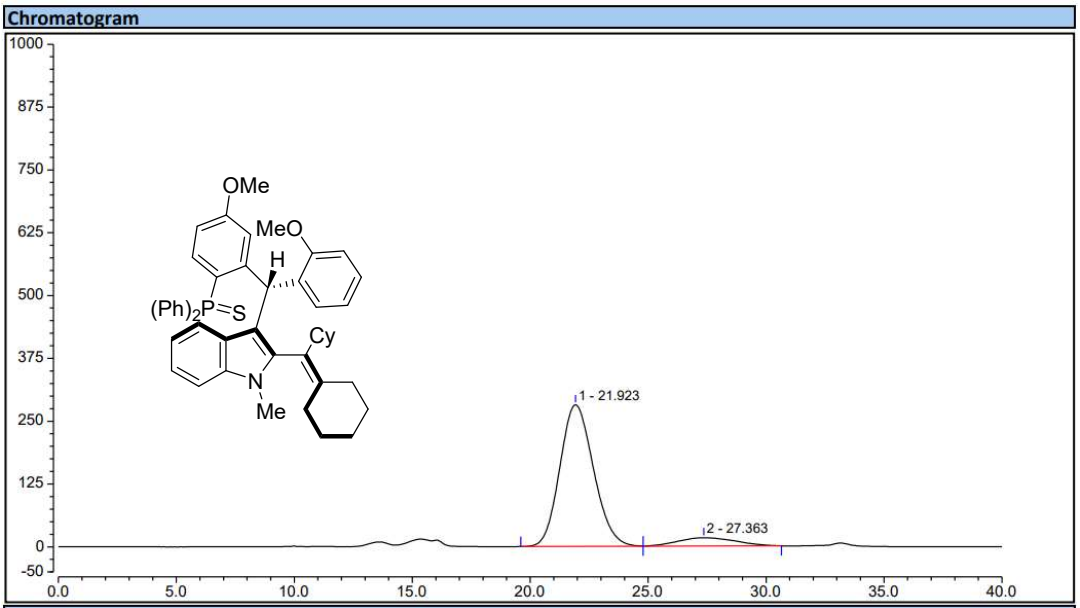
Racemic:



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
n.a.		21.526	212.749	135.719	50.18	66.14	n.a.
n.a.		27.053	211.247	69.465	49.82	33.86	n.a.
Total:			**423.996**	**205.184**	**100.00**	**100.00**	

Enantioselective:

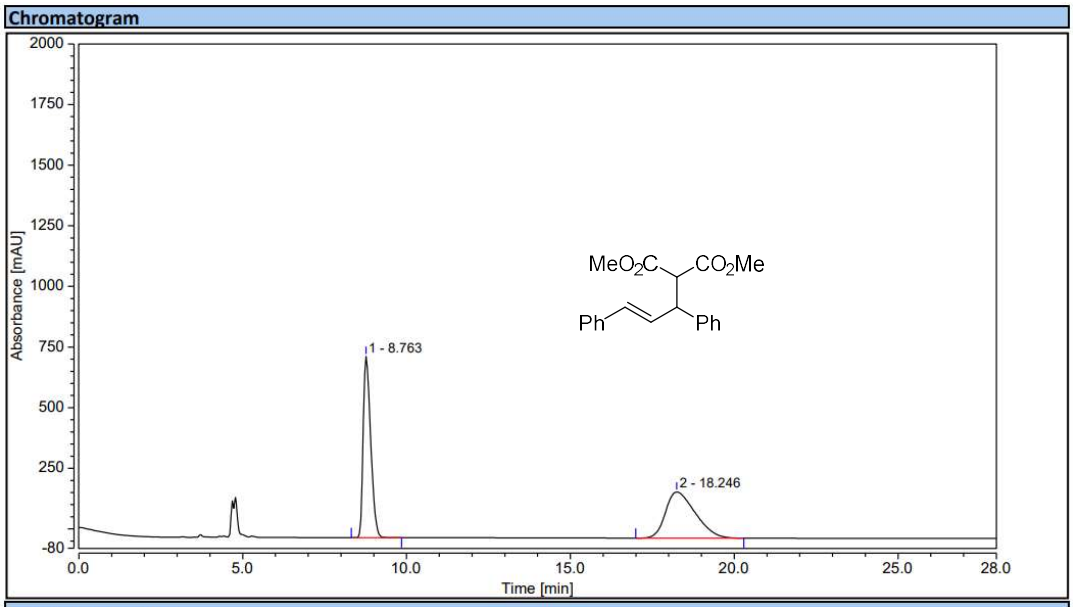


Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
n.a.		21.923	465.749	281.798	90.84	94.44	n.a.
n.a.		27.363	46.950	16.584	9.16	5.56	n.a.
Total:			**512.698**	**298.382**	**100.00**	**100.00**	

13

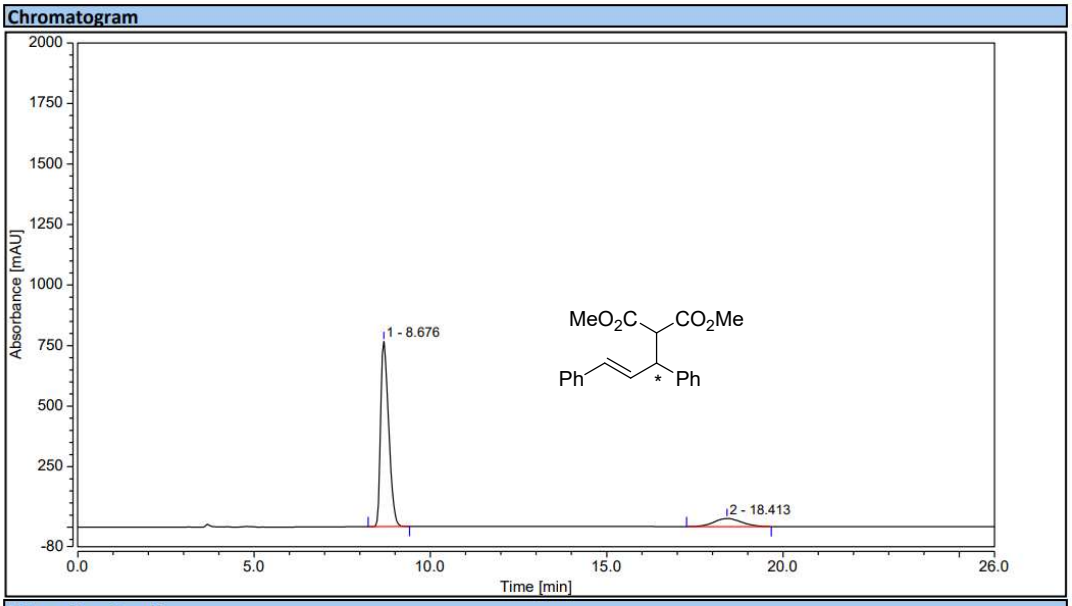
Racemic:



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		8.763	199.714	746.931	50.01	79.69	n.a.
2		18.246	199.635	190.323	49.99	20.31	n.a.
Total:			**399.349**	**937.254**	**100.00**	**100.00**	

Enantioselective:

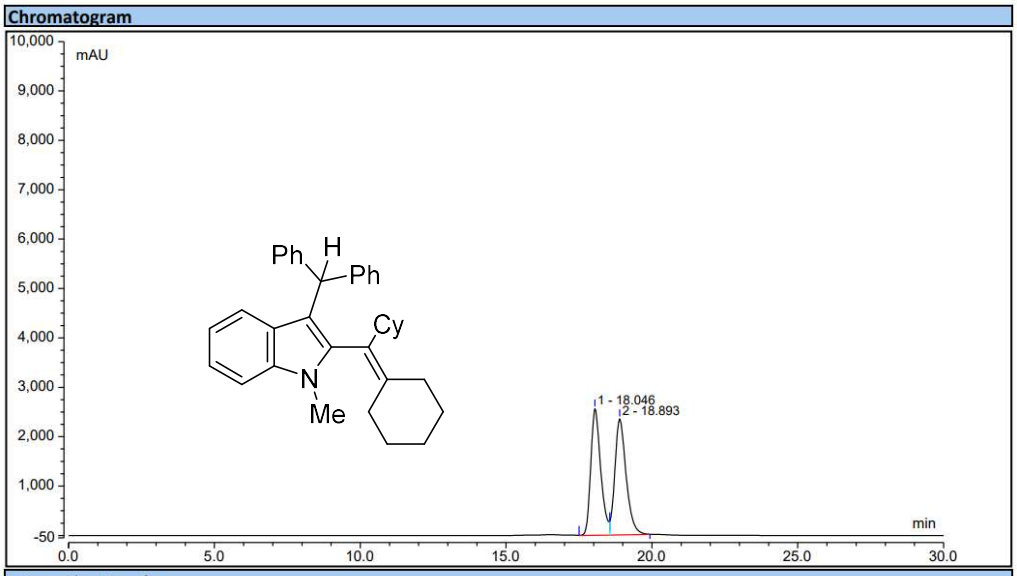


Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		8.676	202.211	764.377	87.09	95.82	n.a.
2		18.413	29.979	33.320	12.91	4.18	n.a.
Total:			**232.190**	**797.697**	**100.00**	**100.00**	

S12

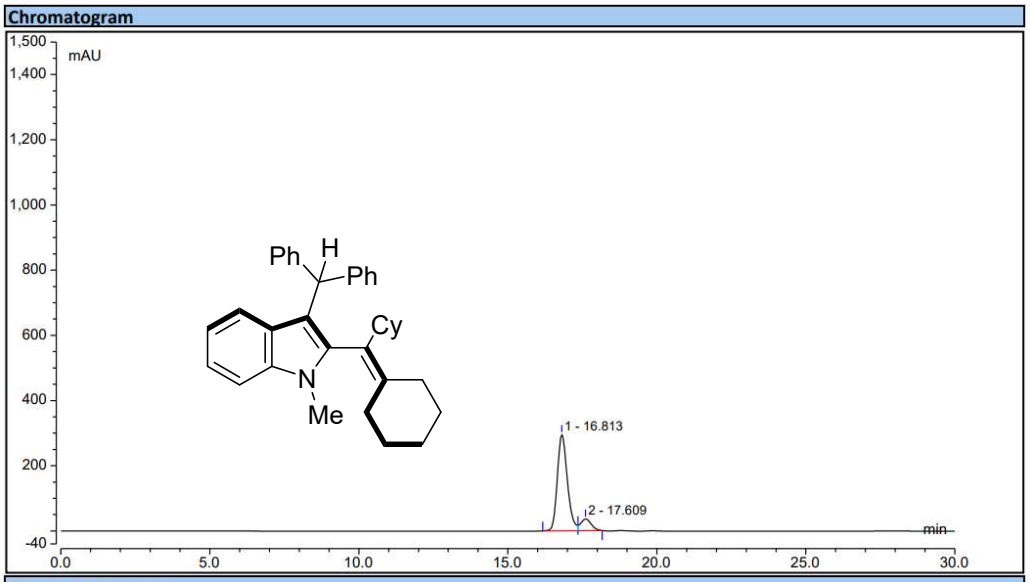
Racemic:



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
n.a.		18.046	1010.807	2557.697	49.08	52.13	n.a.
n.a.		18.893	1048.600	2349.027	50.92	47.87	n.a.
Total:			**2059.407**	**4906.723**	**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.
n.a.		16.813	115.370	295.712	88.70	89.13	n.a.
n.a.		17.609	14.699	36.050	11.30	10.87	n.a.
Total:			**130.069**	**331.762**	**100.00**	**100.00**	

15. Biological evaluation of selected compounds 3 and 4

Procedure for determination of Hep G2 cell viability by Cell Counting Kit-8 (CCK8) assay:

Human liver cancer cell lines (HepG2) were seeded in 96-well plates at the density of 5000 cells per well with 100 μL of complete culture medium. After adhesion for 24 hours, the medium was changed to DMEM supplemented without FBS. The selected products **3ak**, **3af, 3ah** and **4ak** were added to the medium with final concentrations ranging from 6.25 μg/mL to 100 μg/mL. Besides. the selected products **4af** and **4ah** were added to the medium with final concentrations ranging from 12.5 μg/mL to 200 μg/mL. The cells were then cultured for another 24 h. Cells that did not exposed to products **3** or **4** were used as controls, and the wells to which only culture medium was added served as blanks. At the end of compounds stimulation, the supernatant was removed, and 100 μL of DMEM containing 10 μL of CCK8 was added to each well for another 1 h at 37 °C. The culture plates were then shaken for 5s and the optical density (OD) values were read at 450 nm. Then, the IC_{50} values of tested products **3** to HepG2 cell line were calculated by GraphPad software.

Table S7. Cytotoxicity of selected products **3** and **4** on HepG2 cancer cell line

Compound	Viability rate of HepG2 cancer cell line (%)					IC_{50} (μg/mL)[a]
	6.25 (μg/mL)	12.5 (μg/mL)	25 (μg/mL)	50 (μg/mL)	100 (μg/mL)	
3af	77.20±0.03	62.81±0.04	33.26±0.03	11.86±0.03	7.00±0.01	20.0
3ah	85.93±0.07	80.47±0.10	58.23±0.10	42.30±0.06	31.14±0.05	25.6
3ak	92.69±0.10	80.31±0.07	52.57±0.03	35.09±0.02	10.38±0.01	37.1
4ak	91.20±0.13	81.60±0.13	53.71±0.06	36.44±0.07	15.39±0.04	31.7

[a]The IC_{50} value corresponded to the compound concentration causing 50% mortality in cancer cells.

Table S8. Cytotoxicity of selected products **4** on HepG2 cancer cell line

Compound	Viability rate of Hep G2 cancer cell line (%)					IC_{50} (μg/mL)[a]
	12.5 (μg/mL)	25 (μg/mL)	50 (μg/mL)	100 (μg/mL)	200 (μg/mL)	
4af	92.58±0.06	79.70±0.09	57.62±0.04	36.20±0.01	22.53±0.01	50.4
4ah	80.08±0.08	54.74±0.06	42.18±0.06	11.65±0.02	8.88±0.05	41.6

[a]The IC_{50} value corresponded to the compound concentration causing 50% mortality in cancer cells.

Procedure for determination of PC-3 cell viability by MTT assay:

Human prostate cancer cells (PC-3) were seeded in 96-well plates at the density of 4000 cells per well with 100 μL of complete culture medium. After adhesion for 48 hours, selected products 3 were added to the medium with five concentrations ranging from 15.625 μg/mL to 250 μg/mL. The cells were then cultured for another 24 h. Cells that did not exposed to products 3 were used as controls, and the wells to which only culture medium was added served as blanks. At the end of stimulation, 20 μL MTT (5 mg/mL) was added to the medium, and the cells were cultured for another 4 h. Then, the supernatant was removed, and 150 μL of DMSO was added to each well for another 15 min at 37 °C. The culture plates were then shaken for 2 min and the optical density (OD) values were read at a wave-length of 490 nm in a microplate reader (BioTek ELx800, USA).

Table S9. Cytotoxicity of selected products **3** and **4** on PC-3 cancer cell line

Compound	Viability rate of PC-3 cancer cell line (%)					IC_{50} (μg/mL)[a]
	15.625 (μg/mL)	31.25 (μg/mL)	62.5 (μg/mL)	125 (μg/mL)	250 (μg/mL)	
3ac	50.47±0.34	34.89± 2.72	16.48± 1.01	9.09± 1.26	1.73± 0.11	16.7
3ak	85.48±2.1	71.73 ±1.7	61.94±3.65	38.16±4.06	13.79±1.75	78.0
4ai	71.38±1.03	62.62±1.29	45.64±0.96	34.67±1.04	20.93±3.59	53.1
4ak	72.75±1.33	66.03±1.92	57.32±3.85	41.55±4.36	21.82±3.88	71.5

[a]The IC_{50} value corresponded to the compound concentration causing 50% mortality in cancer cells.

16. Theoretical calculations

Computational details:

All calculations were performed using Gaussian 16, Revision A.03 package.[1] All of the reactants, intermediates, transition states, products were optimized by the DFT with the M06-2X functional.[2] For geometry optimizations and frequency calculations, BS-I basis set system was employed. In BS-I, we employed 6-31G(d) basis sets for H, C, O, N, and P. All the stationary structures were characterized with no imaginary frequency and the transition state structures (TSs) were characterized with a single imaginary frequency. Intrinsic reaction coordinate (IRC) calculations were performed on the TSs. The solvent effect of dichloroethane or *p*-xylene was evaluated through the SMD method,[3] in which a better basis system BS-II was used. In BS-II, we employed 6-311++G(d,p) basis sets for all atoms. All reported energies are free energies at a concentration of 1 M and a temperature of 298.15 K. The NCI plot was prepared by Multiwfn 3.8.[4]

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[1] Gaussian 16, Revision A.03, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Petersson, G. A.; Nakatsuji, H.; Li, X.; Caricato, M.; Marenich, A. V.; Bloino, J.; Janesko, B. G.; Gomperts, R.; Mennucci, B.; Hratchian, H. P.; Ortiz, J. V.; Izmaylov, A. F.; Sonnenberg, J. L.; Williams-Young; D.; Ding, F.; Lipparini, F.; Egidi, F.; Goings, J.; Peng, B.; Petrone, A.; Henderson, T.; Ranasinghe, D.; Zakrzewski, V. G.; Gao, J.; Rega, N.; Zheng, G.; Liang, W.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Throssell, K.; Montgomery, J. A.; Jr., Peralta, J. E.; Ogliaro, F.; Bearpark, M. J.; Heyd, J. J.; Brothers, E. N.; Kudin, K. N.; Staroverov, V. N.; Keith, T. A.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A. P.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Millam, J. M.; Klene, M.; Adamo, C.; Cammi, R.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Farkas, O.; Foresman, J. B.; Fox, D. J.; Gaussian.; Inc., Wallingford CT, **2016**.

[2] Zhao, Y.; Truhlar, D. G. The M06 suite of density functionals for main group thermochemistry, thermochemical kinetics, noncovalent interactions, excited states, and transition elements: two new functionals and systematic testing of four M06-class functionals and 12 other functionals. *Theor Chem Account*., **2008**, *120*, 215-241.

[3] Marenich, A. V.; Cramer, C. J.; Truhlar, D. G. Universal Solvation Model Based on Solute Electron Density and on a Continuum Model of the Solvent Defined by the Bulk Dielectric Constant and Atomic Surface Tensions. *J. Phys. Chem. B.,* **2009**, *113*, 6378-6396.

[4] Lu, T.; Chen, F. W. Multiwfn: A multifunctional wavefunction analyzer. *J. Comput. Chem*. **2012**, *33*, 580-592.

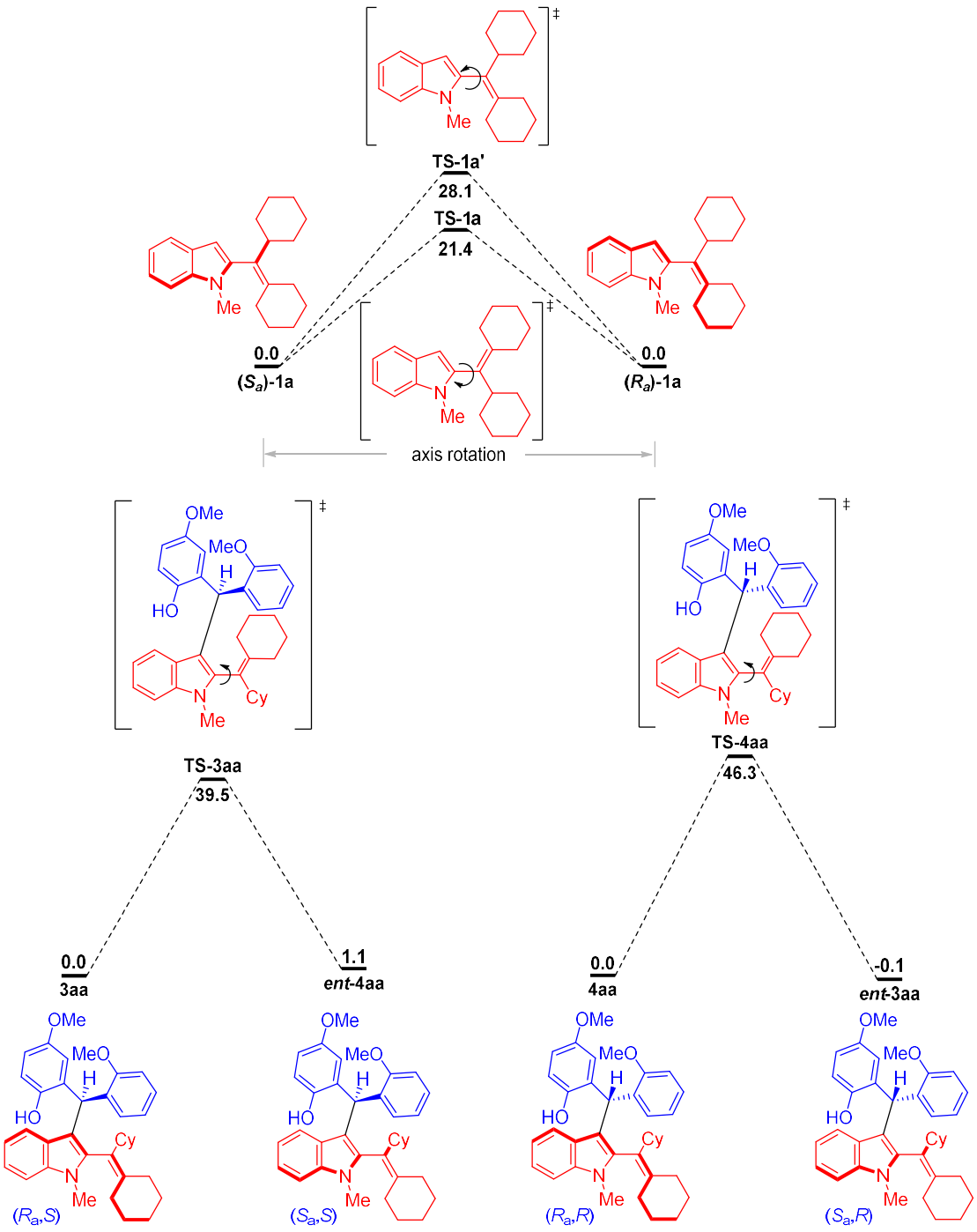

Figure S3. Calculated rotational barriers of the substrate **1a** and products **3aa**, **4aa** (kcal·mol^{-1})

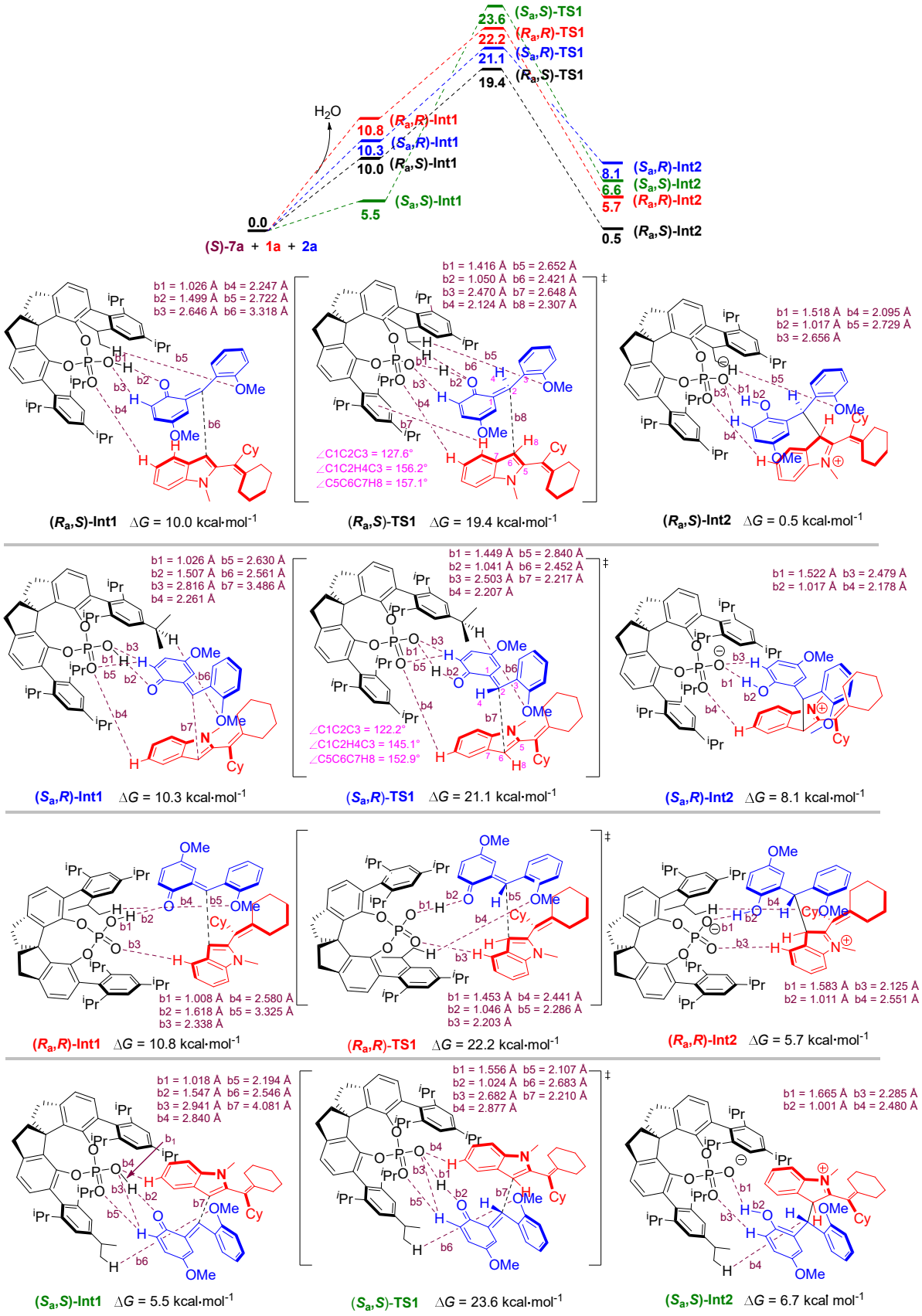

Figure S4. The calculated key reaction pathway for the synthesis of product **3aa**

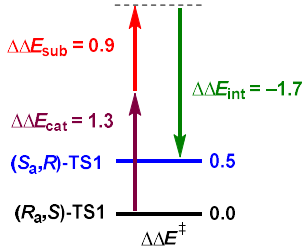

Figure S5. Energy decomposition analysis for **(*R*$_a$,*S*)-TS1** and **(*S*$_a$,*R*)-TS1**

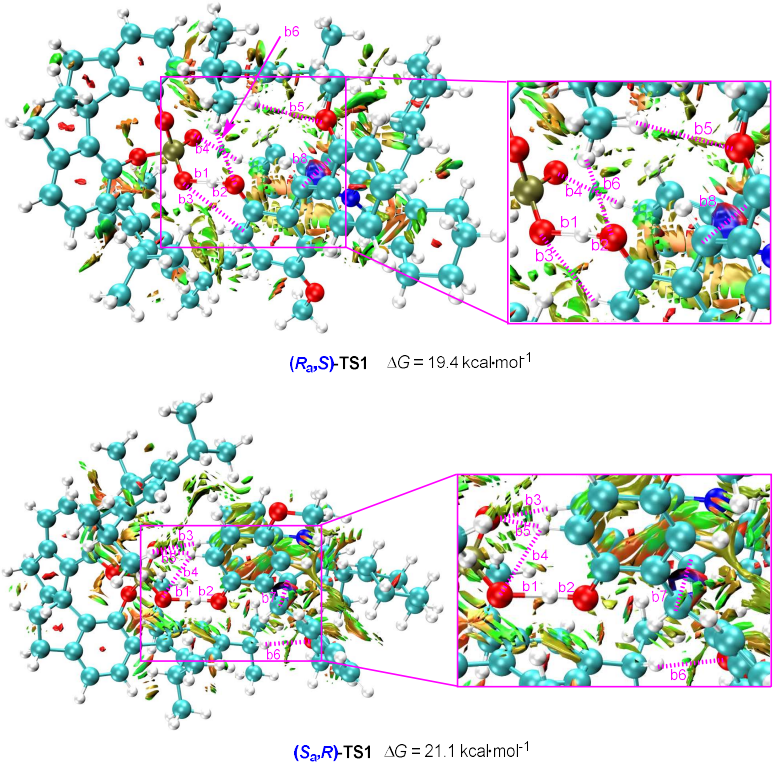

Figure S6. Visualization of noncovalent interactions in **(*R*$_a$,*S*)-TS1** and **(*S*$_a$,*R*)-TS1**

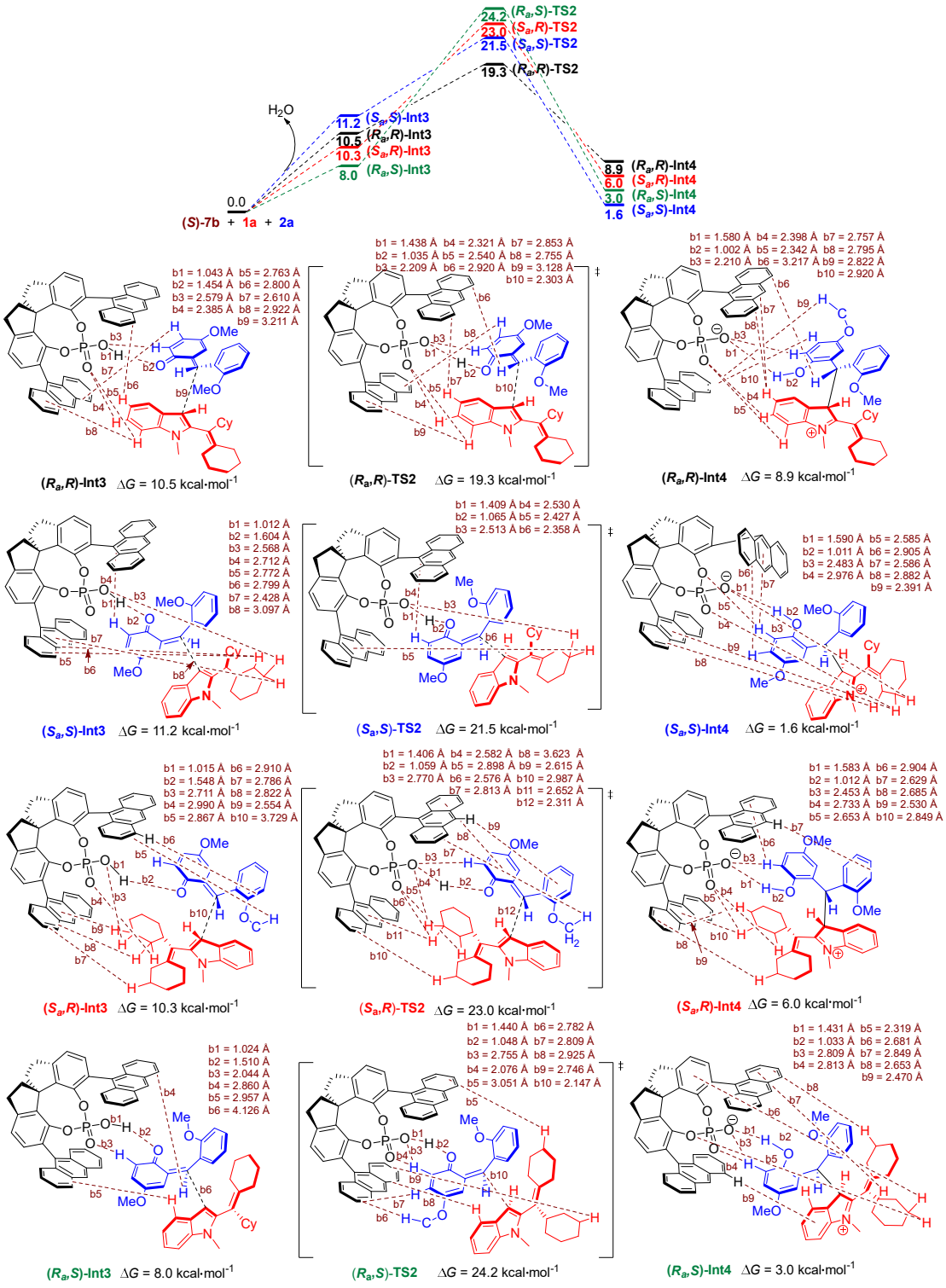

Figure S7. The calculated key reaction pathway for the synthesis of product **4aa**

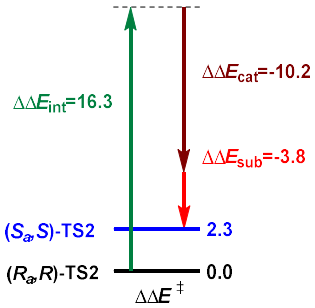

Figure S8. Energy decomposition analysis for (***R***$_a$,***R***)-TS2 and (***S***$_a$,***S***)-TS2

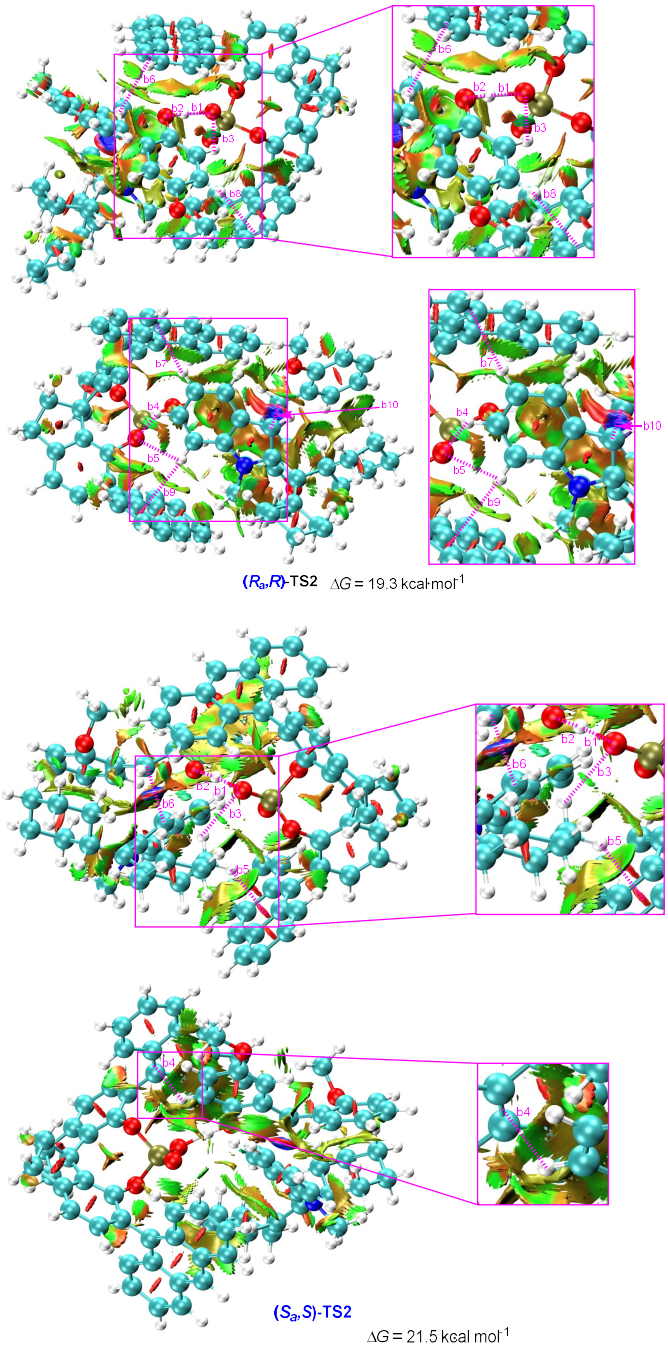

Figure S9. Visualization of noncovalent interactions in (***R***$_a$,***R***)-TS2 and (***S***$_a$,***S***)-TS2

Cartesian coordinates of the optimized structures:

(S_a)-1a

E = -910.158267744 a.u.

0 1

C	-1.41594400	-1.73385600	0.37413000
C	-2.62895500	-2.36427900	0.74172800
C	-3.68408800	-1.57159500	1.21845400
C	-3.50718200	-0.20154400	1.31346900
C	-2.29102300	0.40329600	0.94216400
C	-1.22975100	-0.35129900	0.46901200
C	-1.16956800	-3.94288000	0.03571000
C	-2.44215400	-3.76808600	0.51626200
H	-4.62567800	-2.02899100	1.50780300
H	-4.31763800	0.42059000	1.67987300
H	-2.18360000	1.48002100	1.02728300
H	-0.29228600	0.11453600	0.18003000
H	-3.15310800	-4.56204500	0.69679700
N	-0.54215900	-2.70797100	-0.05205800
C	0.81551000	-2.45201300	-0.47188300
H	0.83541700	-1.85612600	-1.39112200
H	1.35948000	-1.91284600	0.31095900
H	1.31188500	-3.40644600	-0.65309800
C	-0.50047300	-5.19593100	-0.40092200
C	-0.82706000	-5.65335600	-1.81549200
C	-2.13665000	-6.46099300	-1.84046000
C	-0.91355300	-4.48507300	-2.81131000
H	-0.02332800	-6.31243200	-2.16849800
C	-2.47412100	-6.94937900	-3.25092400
H	-2.94696900	-5.81730100	-1.46986100
H	-2.05609000	-7.30664400	-1.14625900
C	-1.23682000	-4.98121800	-4.22273000
H	-1.69785500	-3.78955700	-2.48292200
H	0.02999500	-3.92488000	-2.81360300
C	-2.54024800	-5.78251100	-4.23846700
H	-3.42184200	-7.49895200	-3.24286400
H	-1.70009100	-7.65649800	-3.58148000
H	-1.30220700	-4.13248900	-4.91219200
H	-0.41696900	-5.61943400	-4.58161300
H	-2.75173800	-6.14903600	-5.24894700
H	-3.37105100	-5.12059500	-3.95787200
C	0.27561900	-5.87748100	0.46083500
C	0.88916300	-7.22984600	0.18243700
C	0.54118600	-5.40508900	1.87234000

C	0.35871300	-8.26374400	1.19218900
H	1.98072500	-7.15939500	0.29930500
H	0.69400700	-7.57433100	-0.83519700
C	0.01110100	-6.42975000	2.88786500
H	1.62865500	-5.30647700	2.01140100
H	0.09544500	-4.42398000	2.05423100
C	0.60914200	-7.81401500	2.63266100
H	0.82648800	-9.23660600	1.00603300
H	-0.72078500	-8.38811200	1.03377000
H	0.23433800	-6.09586000	3.90679300
H	-1.08181200	-6.47768800	2.79473300
H	0.19535500	-8.54523500	3.33557700
H	1.69270700	-7.77651800	2.81345400

TS-1a

E = -910.124440494 a.u.

0 1

C	0.07324800	-1.84161600	0.09550400
C	-1.29621400	-1.73437400	-0.20633300
C	-1.84588500	-0.47880100	-0.50920200
C	-1.02102000	0.63142600	-0.49849400
C	0.34741100	0.50871300	-0.19069800
C	0.91197600	-0.72004400	0.11182500
C	-0.81421800	-3.93722400	0.19394400
C	-1.83006900	-3.05068200	-0.11610100
H	-2.90156600	-0.38571600	-0.74690900
H	-1.42794400	1.61009400	-0.73181400
H	0.97636300	1.39334100	-0.19791700
H	1.97299800	-0.80095800	0.32484800
H	-2.86942700	-3.27233200	-0.26385600
N	0.36465000	-3.16565500	0.36253600
C	1.57645100	-3.44387800	1.12400900
H	2.40960300	-3.76271900	0.48844700
H	1.86780500	-2.52681500	1.63977900
H	1.39665400	-4.19741300	1.88707800
C	-0.85978000	-5.42497700	0.31056300
C	0.47880500	-6.15732300	0.47664100
C	0.81527100	-6.65463300	1.89654200
C	0.72710900	-7.26469500	-0.56959000
H	1.25239900	-5.43438600	0.21804500
C	2.26572700	-7.14021600	1.96624600
H	0.15420200	-7.48138600	2.18018000
H	0.62905000	-5.86660000	2.63595400
C	2.17707800	-7.75322400	-0.48378000

H	0.05694000	-8.11886300	-0.43239800
H	0.51866000	-6.86031200	-1.56612600
C	2.52190700	-8.23573200	0.92772900
H	2.49691000	-7.50539000	2.97290000
H	2.94175700	-6.29432400	1.77159900
H	2.34834800	-8.55366600	-1.21185300
H	2.85295100	-6.92959600	-0.75523600
H	3.56497200	-8.56725700	0.97343900
H	1.89988300	-9.10896100	1.17060200
C	-2.00654900	-6.14554700	0.19092500
C	-3.36349500	-5.67175600	-0.27532400
C	-2.17352500	-7.55702700	0.71845900
C	-4.29082600	-5.47883100	0.93517800
H	-3.78668000	-6.48165500	-0.88687900
H	-3.31711800	-4.80842500	-0.93132100
C	-3.09256400	-7.47269100	1.95911700
H	-2.64842400	-8.19481600	-0.03996000
H	-1.24446000	-8.03818800	1.00892100
C	-4.44649300	-6.82544600	1.65136500
H	-5.27008300	-5.10057300	0.62119900
H	-3.85135700	-4.73506200	1.61222000
H	-3.24243800	-8.47637100	2.37321000
H	-2.57060500	-6.88130300	2.72315800
H	-5.02296200	-6.70699300	2.57533700
H	-5.02222900	-7.49978700	1.00240000

TS-1a’

E = -910.112969074 a.u.

0 1

C	-0.28640400	-1.62527500	-0.39439900
C	0.89879100	-1.93275100	0.31348900
C	1.92214700	-0.97569500	0.42902900
C	1.74499400	0.26857100	-0.15636200
C	0.55885800	0.56683600	-0.85704300
C	-0.46525600	-0.36559800	-0.98502300
C	-0.47784300	-3.78545100	0.36630000
C	0.75116600	-3.26428600	0.77541300
H	2.83404800	-1.21382300	0.97013300
H	2.52369300	1.02182800	-0.07883900
H	0.44041500	1.54514100	-1.31411600
H	-1.35712600	-0.10532300	-1.54528700
H	1.52679300	-3.78745300	1.30631400
N	-1.11652900	-2.74178100	-0.36451400
C	-2.47076700	-2.60469100	-0.86666600

H	-2.66468200	-3.25403300	-1.72212300
H	-3.20963400	-2.78916400	-0.08200500
H	-2.60745400	-1.57560800	-1.19367300
C	-0.79230100	-5.24373800	0.52914800
C	0.24118500	-5.91048400	1.47348600
C	-0.31937600	-6.92750800	2.49278900
C	1.51942000	-6.45031900	0.79537600
H	0.57127400	-5.10574100	2.13216800
C	0.75138600	-7.25145500	3.54593800
H	-0.62592400	-7.86548100	2.02503800
H	-1.21344900	-6.50640400	2.96843500
C	2.58128000	-6.80982800	1.84444200
H	1.28755300	-7.34205600	0.19996100
H	1.90952800	-5.70497400	0.09409300
C	2.03046000	-7.79036700	2.88922300
H	0.35972500	-7.97954200	4.26737900
H	0.99244100	-6.34217300	4.11588000
H	3.46906900	-7.23117800	1.35633500
H	2.91034500	-5.89109800	2.35312700
H	2.79107800	-8.00112000	3.65134600
H	1.80392900	-8.74829700	2.39780200
C	-1.74200300	-6.02607900	-0.06602600
C	-3.07833800	-5.61816500	-0.64353800
C	-1.54900500	-7.52342700	-0.26878800
C	-4.22610800	-6.47390600	-0.05715600
H	-3.08349200	-5.72899000	-1.74019500
H	-3.31871800	-4.59380900	-0.41284100
C	-2.67845700	-8.40867700	0.28592100
H	-1.53527900	-7.66414200	-1.36332000
H	-0.58183700	-7.87357800	0.07760000
C	-4.02800400	-7.97148900	-0.28554400
H	-5.17458700	-6.13646900	-0.49374200
H	-4.28523200	-6.27768500	1.02264500
H	-2.47524300	-9.45968100	0.04442300
H	-2.70254600	-8.32968300	1.38030000
H	-4.84768100	-8.54209200	0.16849900
H	-4.05310500	-8.18247400	-1.36472600

(R_a)-1a

E = -910.158240461 a.u.

0 1

C	1.31123000	-2.64176200	0.12779000
C	0.13514400	-1.85664300	0.19446100
C	0.25809100	-0.45935500	0.23332100

C	1.52167600	0.10635100	0.20623200
C	2.67740600	-0.69530200	0.13943200
C	2.59016700	-2.07735900	0.09847100
C	-0.44729800	-4.04260100	0.13850300
C	-0.96659900	-2.77465500	0.19940800
H	-0.62735600	0.16748100	0.28420100
H	1.62756800	1.18614200	0.23718100
H	3.65389700	-0.22175400	0.12072300
H	3.48088500	-2.69666300	0.04935200
H	-2.02010900	-2.53481900	0.23143000
N	0.93781300	-3.96590000	0.09500700
C	1.86544200	-5.06711700	-0.01382500
H	2.50367100	-4.94042800	-0.89479000
H	2.50037900	-5.13313500	0.87664000
H	1.29870300	-5.99333500	-0.11889500
C	-1.15833500	-5.34708200	0.16855000
C	-1.55415700	-5.84538000	1.55133600
C	-0.47851200	-5.56693300	2.61393400
C	-2.89520700	-5.23138000	1.99032800
H	-1.68507600	-6.93451200	1.51026100
C	-0.90795000	-6.08775000	3.98768600
H	-0.30426200	-4.48405500	2.67455300
H	0.47152000	-6.02741000	2.31465100
C	-3.32518800	-5.73698800	3.36917500
H	-2.78258200	-4.13823000	2.01719000
H	-3.66192700	-5.45627200	1.23860400
C	-2.24182200	-5.47278400	4.41677900
H	-0.13167300	-5.87123500	4.72963300
H	-1.01202400	-7.18126200	3.94678700
H	-4.26876300	-5.26607300	3.66611500
H	-3.51419600	-6.81841300	3.31259900
H	-2.54885100	-5.86732800	5.39156100
H	-2.11423400	-4.38811200	4.53651000
C	-1.46599300	-5.97120100	-0.98259900
C	-1.08692400	-5.42111600	-2.33890400
C	-2.30156700	-7.22593200	-1.08408300
C	-2.34621600	-5.13726000	-3.17323400
H	-0.48115100	-6.17359800	-2.86665600
H	-0.48088100	-4.51644100	-2.24592900
C	-3.56827600	-6.94760100	-1.91339000
H	-1.71700000	-8.00517400	-1.59525900
H	-2.58096300	-7.62089600	-0.10517400
C	-3.21787300	-6.38821200	-3.29323200
H	-2.06209200	-4.76927300	-4.16488600

H	-2.91561800	-4.33746500	-2.68175400
H	-4.15724700	-7.86626700	-2.00885200
H	-4.18905000	-6.21980900	-1.37408900
H	-4.13125400	-6.16584800	-3.85562100
H	-2.67194000	-7.15379000	-3.86252600

3aa

E = -1715.50808024 a.u.

0 1

C	0.35053400	-2.30812000	-1.69053800
C	-0.89869800	-1.84472800	-1.20423600
C	-1.23604700	-0.49381900	-1.40592100
C	-0.34121300	0.33224400	-2.06569200
C	0.89433800	-0.15182800	-2.53564500
C	1.25723100	-1.47615300	-2.35444700
C	-0.68994900	-4.04527000	-0.72398000
C	-1.54109700	-2.97567400	-0.59135500
H	-2.18198500	-0.10276800	-1.04505700
H	-0.59538000	1.37578400	-2.22324000
H	1.57257700	0.52273900	-3.04882700
H	2.20799800	-1.85496600	-2.71787300
N	0.45974600	-3.64485500	-1.39089600
C	1.60192000	-4.45853300	-1.73369200
H	1.44763100	-5.46473200	-1.34259700
H	1.72282900	-4.51592800	-2.82140700
H	2.51577400	-4.03971300	-1.29873300
C	-0.88823200	-5.43266600	-0.23092900
C	-0.83053800	-5.55187500	1.29120200
C	-2.03112900	-6.24628900	1.96100600
C	0.49534700	-6.14658200	1.79801000
H	-0.85483500	-4.51679500	1.65994500
C	-1.93479100	-6.09046700	3.48102000
H	-2.05611100	-7.31600600	1.72120100
H	-2.96675900	-5.81643700	1.58506300
C	0.58795700	-6.04260200	3.32351600
H	0.57344200	-7.19929900	1.49260100
H	1.33679000	-5.61837200	1.33227500
C	-0.62390000	-6.68368900	4.00540600
H	-2.79090700	-6.57102000	3.96847400
H	-1.98172700	-5.02099400	3.73001600
H	1.51576200	-6.50336900	3.68098800
H	0.63268200	-4.98008400	3.60096300
H	-0.55412900	-6.56245100	5.09228000
H	-0.61750400	-7.76482400	3.80585800

C	-1.08451400	-6.43052700	-1.11316900
C	-1.29903100	-6.18196400	-2.59007800
C	-1.23638900	-7.89218900	-0.76549200
C	-2.70507500	-6.66902600	-2.98516600
H	-0.54818700	-6.73909000	-3.17138500
H	-1.19499200	-5.12210900	-2.83877400
C	-2.64601600	-8.38098200	-1.13605500
H	-0.50843700	-8.46090200	-1.36394500
H	-1.00857800	-8.09782500	0.28007400
C	-2.92016800	-8.13872100	-2.62220700
H	-2.86790900	-6.50710100	-4.05659900
H	-3.44110800	-6.05498300	-2.45261700
H	-2.75498300	-9.44311800	-0.88963400
H	-3.37925900	-7.82543400	-0.53460600
H	-3.94199900	-8.44313300	-2.87504200
H	-2.24294200	-8.76806100	-3.21725000
C	-2.92450400	-3.10911100	-0.00231800
H	-2.86010800	-3.87131100	0.78150400
C	-3.38130300	-1.83734000	0.69601200
C	-4.39978000	-1.02941600	0.21650200
C	-2.71725000	-1.44914200	1.87316600
C	-4.75304600	0.16274600	0.86190200
H	-4.94014200	-1.30204900	-0.68453400
C	-3.05886100	-0.26890500	2.51291700
C	-4.07474700	0.55047400	2.01171000
H	-2.53402200	0.02504000	3.41922700
H	-4.31885100	1.46822500	2.53276600
C	-3.92846100	-3.61564300	-1.02525700
C	-4.97887300	-4.45379400	-0.60849700
C	-3.85252600	-3.27163100	-2.37142800
C	-5.90531900	-4.94677400	-1.52833100
C	-4.78657700	-3.73986100	-3.29683600
H	-3.03856900	-2.62820800	-2.69556000
C	-5.80555600	-4.58126300	-2.87138100
H	-6.70670300	-5.60326100	-1.21032600
H	-4.70781400	-3.45484300	-4.34065700
H	-6.53357300	-4.96402700	-3.57991400
O	-5.01702100	-4.73317000	0.72469800
C	-5.98302400	-5.65165900	1.17953800
H	-5.87438400	-6.62316200	0.68115200
H	-5.80642100	-5.77034100	2.24890000
H	-6.99992900	-5.27430300	1.01805400
O	-1.74373700	-2.28805000	2.34652400
H	-1.32283400	-1.87780900	3.11488100

O	-5.76788900	0.86853100	0.28465700
C	-6.13812600	2.07659300	0.90210100
H	-5.30280300	2.78841400	0.92414000
H	-6.94918400	2.49075000	0.30286200
H	-6.49237600	1.91118600	1.92782200

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E = -1715.44894162 a.u.

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C	0.03326600	-2.03414900	0.13143100
C	-1.19153400	-1.90001900	-0.53472100
C	-1.47494700	-0.68899300	-1.19039500
C	-0.55723500	0.34619300	-1.11817100
C	0.64097900	0.20530400	-0.39665100
C	0.95123500	-0.98613100	0.23973400
C	-1.04269100	-4.04790700	0.24914900
C	-1.90346400	-3.15043400	-0.38363900
H	-2.39343500	-0.56274800	-1.75167000
H	-0.76733600	1.28250600	-1.62519400
H	1.34081300	1.03396900	-0.35182000
H	1.88922100	-1.11126800	0.77230700
N	0.11830100	-3.31227900	0.63807700
C	0.75144400	-3.46199300	1.94750800
H	1.74462000	-3.91939200	1.89842300
H	0.84588600	-2.47343800	2.40250400
H	0.11323900	-4.06445800	2.59328100
C	-0.98232200	-5.53768700	0.49818100
C	0.45496600	-6.09109600	0.72532100
C	0.87261600	-6.63716200	2.11034000
C	0.84798800	-7.10000900	-0.37754700
H	1.12919500	-5.25720600	0.52680100
C	2.38122100	-6.90811000	2.14159400
H	0.36413800	-7.57806700	2.34034200
H	0.59490300	-5.94947000	2.91326200
C	2.35020900	-7.39637500	-0.33235000
H	0.29392500	-8.03978200	-0.27395100
H	0.57475700	-6.67969400	-1.35140400
C	2.78053700	-7.90001900	1.04681500
H	2.67373400	-7.28824000	3.12687500
H	2.92809500	-5.96602800	1.98989600
H	2.61237700	-8.12853800	-1.10431000
H	2.90524200	-6.47715600	-0.56692300
H	3.86113900	-8.07952600	1.06909500
H	2.29336800	-8.86510300	1.24625200

C	-1.98052200	-6.44790900	0.33458900
C	-3.32569800	-6.28929100	-0.32613800
C	-1.94404100	-7.85060600	0.91460900
C	-4.44890500	-6.27388400	0.72291800
H	-3.46913700	-7.18784300	-0.94442400
H	-3.35565300	-5.46600000	-1.02678300
C	-3.01758000	-7.91803400	2.02360200
H	-2.19128800	-8.58547400	0.13575500
H	-0.98750500	-8.14036900	1.33323000
C	-4.42009400	-7.59522500	1.49862800
H	-5.42066800	-6.12762700	0.23906900
H	-4.29449300	-5.42784400	1.40587700
H	-3.00778200	-8.91281000	2.48394800
H	-2.74198500	-7.19676500	2.80434000
H	-5.13622800	-7.57381700	2.32777500
H	-4.73820000	-8.40389000	0.82586400
C	-3.38485800	-3.20859600	-0.71505100
H	-3.82512900	-4.01432000	-0.13325400
C	-4.11691300	-1.98284700	-0.15863000
C	-4.78253600	-1.06091400	-0.95001700
C	-4.16763300	-1.81700700	1.23674300
C	-5.45912500	0.03221800	-0.39691200
H	-4.78611900	-1.16507300	-2.03125200
C	-4.83358400	-0.73510000	1.79083400
C	-5.48148400	0.20212500	0.98227500
H	-4.85790200	-0.61525900	2.87189100
H	-5.99266500	1.03774100	1.44460600
C	-3.69838200	-3.45039200	-2.18103100
C	-4.98268200	-3.91407100	-2.52932400
C	-2.77669900	-3.23881600	-3.19945200
C	-5.32623600	-4.13570400	-3.86081700
C	-3.11012800	-3.45561700	-4.53843800
H	-1.77878100	-2.90087400	-2.93720000
C	-4.38300100	-3.89967100	-4.86271700
H	-6.31453200	-4.49076800	-4.12776300
H	-2.37410700	-3.27911600	-5.31549000
H	-4.65677800	-4.07250800	-5.89891500
O	-5.82495300	-4.12782400	-1.48129900
C	-7.13227000	-4.56726000	-1.76713800
H	-7.12495500	-5.54093900	-2.27268700
H	-7.63647300	-4.66148100	-0.80524800
H	-7.66746200	-3.84051200	-2.38989500
O	-3.55521600	-2.76994300	2.00634100
H	-3.69095100	-2.54804300	2.93810900

O	-6.06187400	0.86830200	-1.29234700
C	-6.73351100	1.98680400	-0.76801100
H	-6.05023200	2.64001000	-0.21005000
H	-7.13574900	2.53139800	-1.62253100
H	-7.55802800	1.68752900	-0.10782200

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C	-0.43604100	-1.92984500	1.61506800
C	-1.50688200	-1.62576000	0.73762400
C	-1.78236900	-0.27173100	0.46962000
C	-1.00750100	0.70660000	1.07047100
C	0.04673500	0.37638600	1.94184500
C	0.34715000	-0.94530100	2.22523300
C	-1.33789700	-3.87380100	0.94140800
C	-2.07061000	-2.88742900	0.32605400
H	-2.58968300	0.00763700	-0.19860000
H	-1.21644500	1.75166300	0.86397600
H	0.63618700	1.16792400	2.39401800
H	1.16695200	-1.20687200	2.88769100
N	-0.34972100	-3.29692900	1.72739600
C	0.55797700	-3.98187200	2.61650100
H	1.57822300	-4.00492600	2.21563100
H	0.57267300	-3.47857100	3.58837100
H	0.20627000	-5.00521900	2.75860500
C	-1.43652300	-5.35288500	0.80287400
C	-0.46921600	-5.95324000	-0.22416500
C	0.61256100	-6.86794900	0.38508300
C	-1.15611600	-6.64809600	-1.41603600
H	0.06879000	-5.09686500	-0.65894700
C	1.62641100	-7.30884600	-0.67527600
H	0.14833500	-7.75696800	0.83124800
H	1.13026200	-6.34634600	1.19763100
C	-0.12651800	-7.07081300	-2.46607500
H	-1.70416600	-7.53569900	-1.07682500
H	-1.89099700	-5.97232200	-1.86109400
C	0.93692900	-7.98842400	-1.86009100
H	2.37031000	-7.97750600	-0.22753500
H	2.17049900	-6.42536600	-1.03756800
H	-0.63048900	-7.56205700	-3.30620900
H	0.35537800	-6.17059100	-2.87222500
H	1.67628800	-8.27506400	-2.61630200
H	0.45885000	-8.91629500	-1.51439800

C	-2.32061200	-6.02735100	1.56248800
C	-3.20574500	-5.34336000	2.58215000
C	-2.50107900	-7.52795500	1.57554100
C	-2.92933400	-5.89273600	3.99109500
H	-4.25636100	-5.54745500	2.32580000
H	-3.08230400	-4.25882800	2.55149900
C	-2.20741700	-8.08494400	2.97896000
H	-3.54689700	-7.75600500	1.32132500
H	-1.87767600	-8.03065900	0.83753000
C	-3.08551500	-7.41345000	4.03582800
H	-3.60019200	-5.41717800	4.71514800
H	-1.90439100	-5.62469800	4.28320900
H	-2.35696600	-9.17022300	2.98749300
H	-1.14924900	-7.90290100	3.21422100
H	-2.84206900	-7.79590100	5.03330300
H	-4.13625200	-7.67163000	3.84295900
C	-3.22615300	-3.16206500	-0.60824000
H	-3.76102300	-4.03200200	-0.20204300
C	-4.22647900	-2.01467600	-0.61829800
C	-4.43224500	-1.20408700	-1.72294400
C	-4.94045400	-1.73248700	0.55906900
C	-5.30993700	-0.11374000	-1.67886300
H	-3.89816000	-1.39140400	-2.64919400
C	-5.80450000	-0.65035600	0.61151600
C	-5.99444800	0.17171500	-0.50290100
H	-6.34345000	-0.43549700	1.53164000
H	-6.67533500	1.01117900	-0.43120900
C	-2.77119000	-3.55018000	-2.00544600
C	-3.66479000	-4.24880500	-2.84053900
C	-1.49529600	-3.27822500	-2.48415900
C	-3.26426600	-4.69100000	-4.10078000
C	-1.08557700	-3.70799600	-3.74847600
H	-0.80787800	-2.73368200	-1.84303000
C	-1.96853500	-4.42213700	-4.54588200
H	-3.94465700	-5.24416500	-4.73728800
H	-0.08222000	-3.48857200	-4.09869600
H	-1.66155100	-4.77360700	-5.52613400
O	-4.90188300	-4.46425700	-2.31825400
C	-5.83962200	-5.15093100	-3.11316100
H	-5.49786100	-6.16688000	-3.34703900
H	-6.75521000	-5.20270600	-2.52431500
H	-6.03778200	-4.61338700	-4.04833000
O	-4.73966500	-2.56519700	1.62533500
H	-5.23429300	-2.22639300	2.38447000

O	-5.41974700	0.60430900	-2.83430800
C	-6.27352800	1.72134300	-2.81304700
H	-5.94879300	2.46057100	-2.06934600
H	-6.22333500	2.16451500	-3.80782000
H	-7.30995800	1.43103600	-2.59702700

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C	-0.99307000	14.81870600	-9.16806500
C	0.27693900	14.58836700	-8.69693500
N	-1.70379500	13.62775600	-9.18798000
C	-3.09318300	13.47146300	-9.54334200
H	-3.58289600	14.44537000	-9.48024100
H	-3.21365800	13.07574800	-10.55939600
H	-3.57895800	12.78934500	-8.83939000
C	-1.55940900	16.10404600	-9.65207900
C	-1.93156000	17.04404400	-8.76044400
C	-2.37310400	18.43986900	-9.14433200
C	-1.96761500	16.79497300	-7.26750200
C	-1.63644500	19.51402600	-8.32688100
H	-3.45265200	18.53631300	-8.94819000
H	-2.22852600	18.62882200	-10.21100800
C	-1.23806700	17.88525600	-6.47057800
H	-3.02485800	16.79737000	-6.95525600
H	-1.55293900	15.81185700	-7.03345000
C	-1.77369100	19.27132900	-6.82497800
H	-0.57223400	19.48636800	-8.58989100
H	-1.34589300	17.68969000	-5.39687400
H	-0.16490700	17.83987700	-6.69288600
H	-1.23900600	20.04602000	-6.26440200
H	-2.83291700	19.34074500	-6.53803400
C	-1.62744300	16.33077900	-11.16676700
C	-0.90615800	15.26034400	-11.99902500
C	-3.07565600	16.45565400	-11.68085500
H	-1.11770100	17.28551400	-11.37685500
C	-0.91727600	15.62558400	-13.48460700
H	-1.41012800	14.29211200	-11.85857100
H	0.12125600	15.12910900	-11.65303000
C	-3.10808700	16.83003400	-13.16494800
H	-3.57916200	15.48780700	-11.54676200
H	-3.63835300	17.18501200	-11.08899300
C	-2.34352500	15.80658100	-14.00778700
H	-0.39017300	14.85722400	-14.06200300

H	-0.35591800	16.56134200	-13.62077000
H	-4.14405500	16.91520000	-13.51194200
H	-2.64812500	17.82054600	-13.29336900
H	-2.33458000	16.10814900	-15.06127600
H	-2.86789800	14.84182500	-13.95755900
C	0.37545800	13.18057900	-8.41907100
C	-0.88723600	12.61784100	-8.73813200
C	1.38434900	12.32926000	-7.93089500
C	-1.16518700	11.25641300	-8.58287000
C	1.11120900	10.97993100	-7.77688800
H	2.36523800	12.72051700	-7.67838800
C	-0.15128700	10.44717500	-8.09740000
H	-2.13577600	10.84501500	-8.84375500
H	1.88647000	10.31832700	-7.40333700
H	-0.33170700	9.38450100	-7.96859500
C	1.90002300	15.94481100	-9.96495600
C	2.50163700	14.92695800	-10.69771800
C	2.91180800	15.11352200	-12.01995800
C	2.69886300	16.34639700	-12.63447000
C	2.09608600	17.37345200	-11.90836600
C	1.70790000	17.18767200	-10.58635700
H	2.62505700	13.94156600	-10.25482500
H	2.98626900	16.52441000	-13.66365000
H	1.92426500	18.33474400	-12.38854300
O	3.49018700	14.03804700	-12.62432800
O	1.10287200	18.18657700	-9.86821200
C	3.83101200	14.17301200	-13.98265200
H	4.58547600	14.95600200	-14.13255200
H	4.24341200	13.21235600	-14.29106100
H	2.94926600	14.40428300	-14.59442700
C	2.37650000	15.37067400	-7.51633700
C	1.93944600	15.18843900	-6.18786500
C	3.73772600	15.25579000	-7.77310500
C	2.83645200	14.84907200	-5.17806700
C	4.64877600	14.92687300	-6.76596400
H	4.09830800	15.41594500	-8.78321400
C	4.19343000	14.71346400	-5.47462400
H	2.49174600	14.69279600	-4.16290900
H	5.70411100	14.83648200	-7.00063000
H	4.88660600	14.44736900	-4.68270000
O	0.60754000	15.36795200	-5.97776000
C	0.08747600	15.04634800	-4.70959900
H	0.48924600	15.70696700	-3.93117300
H	-0.99186600	15.18934900	-4.78123000

H	0.30135400	14.00274900	-4.44979400
C	1.33120200	15.67269000	-8.58250300
H	0.80641000	16.58051100	-8.26673200
H	1.03638300	18.97381900	-10.42683700
H	-2.02009100	20.50426800	-8.59736800

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C	-0.69605300	14.98671700	-9.69351800
C	0.39699600	14.70050500	-8.87231300
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C	-1.23701100	13.71306800	-11.78769200
H	-1.02073200	14.69085500	-12.21499800
H	-0.50787800	13.00496700	-12.19117400
H	-2.23641700	13.39632600	-12.09955200
C	-1.56503200	16.17443100	-9.98433000
C	-1.41640000	17.43573200	-9.48392600
C	-2.09188500	18.64959900	-10.10653300
C	-0.66649400	17.90002400	-8.26395500
C	-1.00032200	19.66546200	-10.50640000
H	-2.76956700	19.12413400	-9.38067400
H	-2.67753500	18.42183700	-10.99680300
C	0.46945700	18.87370800	-8.61781700
H	-1.40418600	18.47438400	-7.67977300
H	-0.38429200	17.07694200	-7.61613600
C	-0.12732100	20.09186900	-9.32519100
H	-0.36756700	19.20012600	-11.27378400
H	1.01951700	19.16882700	-7.71809600
H	1.18780500	18.37728600	-9.28323800
H	0.66385400	20.76817400	-9.66778100
H	-0.74187800	20.65601600	-8.60971600
C	-2.94602600	15.98616600	-10.69810400
C	-3.11457500	16.18618300	-12.22173900
C	-3.79240800	14.79652200	-10.19400600
H	-3.51793200	16.82324200	-10.28826600
C	-4.59215300	16.45301700	-12.53125300
H	-2.81474500	15.31081300	-12.79950000
H	-2.48816000	17.01825100	-12.56528600
C	-5.26706500	15.04367300	-10.53709400
H	-3.48370000	13.84324700	-10.62674400
H	-3.66429000	14.69873200	-9.10975900
C	-5.46085500	15.29257600	-12.03595700

H	-4.73289400	16.60032000	-13.60785700
H	-4.91062300	17.38286700	-12.03793300
H	-5.87394900	14.18986700	-10.21521000
H	-5.63003800	15.91814700	-9.97898300
H	-6.51682600	15.48443700	-12.25657400
H	-5.18228200	14.38286800	-12.58750100
C	0.56161700	13.25539000	-8.86382200
C	-0.36124200	12.73261000	-9.78192500
C	1.42777100	12.35700600	-8.21113700
C	-0.42894000	11.37719000	-10.10808600
C	1.34474500	11.00380200	-8.50275200
H	2.15558400	12.69905600	-7.48752300
C	0.42957600	10.51320500	-9.44699900
H	-1.14608600	11.01411800	-10.83826300
H	2.00721500	10.31130900	-7.99309300
H	0.39004700	9.44909300	-9.65790700
C	2.64211400	15.75684900	-9.27287000
C	2.83490300	14.96837600	-10.39684900
C	3.88883400	15.20522600	-11.28869000
C	4.77202300	16.25233500	-11.05510600
C	4.58948900	17.05364900	-9.92490000
C	3.54500300	16.81535200	-9.04603800
H	2.16521300	14.14388000	-10.61522800
H	5.59545300	16.46303800	-11.72661300
H	5.27604400	17.87571200	-9.73458200
O	3.95803100	14.35673900	-12.35470300
O	3.34334900	17.57462600	-7.92538000
C	5.01390100	14.55456400	-13.26210800
H	5.98994800	14.44652700	-12.77163200
H	4.90807500	13.78559200	-14.02754300
H	4.95931500	15.54489700	-13.73266900
C	1.97222100	15.09122300	-6.90917700
C	1.02990300	14.95811300	-5.87275800
C	3.29348900	14.76016400	-6.63108100
C	1.40093200	14.46773600	-4.62203800
C	3.68135500	14.27895700	-5.37979400
H	4.03369700	14.85037000	-7.42006600
C	2.73113700	14.12638700	-4.38068400
H	0.66568900	14.35268900	-3.83444500
H	4.71898900	14.01971200	-5.19738200
H	3.01421900	13.74567000	-3.40429600
O	-0.24104700	15.33397500	-6.18248600
C	-1.25976400	15.08870100	-5.24212000
H	-1.10933600	15.67224400	-4.32542400

H	-2.18952300	15.39769800	-5.72058700
H	-1.31494700	14.02345900	-4.98883800
C	1.49239700	15.57341000	-8.28150900
H	1.13738700	16.58234500	-8.11627400
H	4.00506700	18.27982300	-7.89897500
H	-1.47342800	20.54036200	-10.96651900

***ent*-3aa**

E = -1715.50576803 a.u.

0 1

C	-0.51951300	14.95753700	-10.26463900
C	0.52086000	14.49304700	-9.48756900
N	-0.87233400	13.98988800	-11.19516400
C	-1.76866100	14.17067400	-12.31212000
H	-1.32401500	13.73124900	-13.20982100
H	-2.74668000	13.70493700	-12.13830900
H	-1.90903200	15.24029000	-12.48108800
C	-1.29742300	16.20914500	-10.10387700
C	-0.70951900	17.40562800	-10.30412400
C	-1.36135700	18.73502900	-9.99561400
C	0.67275700	17.57334700	-10.89154500
C	-1.42360800	19.62683900	-11.24595700
H	-0.73745300	19.24284700	-9.24427300
H	-2.35438100	18.62310100	-9.55546900
C	0.61835100	18.46021100	-12.14669600
H	1.32574700	18.05358100	-10.14606700
H	1.12340300	16.60741000	-11.12897200
C	-0.03130900	19.81237600	-11.85163100
H	-2.08165700	19.15630400	-11.98939600
H	1.62963800	18.59733900	-12.54410300
H	0.03624100	17.94071500	-12.92031200
H	-0.08963300	20.41757800	-12.76309500
H	0.59762200	20.36587100	-11.14035200
C	-2.73676300	16.08223800	-9.58388400
C	-3.79168000	16.54156300	-10.61020400
C	-3.10856800	14.68135500	-9.07155300
H	-2.81860700	16.75742800	-8.71704900
C	-5.19629200	16.54461200	-10.00239500
H	-3.78033000	15.85376100	-11.46583400
H	-3.54054500	17.53233900	-11.00390200
C	-4.51326100	14.67318800	-8.46141700
H	-3.08615400	13.96511900	-9.90362000
H	-2.36020600	14.34149900	-8.34916900
C	-5.56111800	15.15938300	-9.46489700

H	-5.93005400	16.87292000	-10.74695000
H	-5.23113200	17.27308400	-9.17944400
H	-4.76123700	13.66626000	-8.10742600
H	-4.53638600	15.33132600	-7.58108900
H	-6.55583900	15.17479700	-9.00588200
H	-5.60849700	14.45166600	-10.30473900
C	0.80712600	13.15378100	-9.93915000
C	-0.07752400	12.88367800	-11.01042400
C	1.72902700	12.16047300	-9.56698400
C	-0.06408800	11.67492800	-11.71305000
C	1.74414400	10.95915400	-10.25544100
H	2.41894200	12.33109500	-8.74781000
C	0.85688100	10.71782200	-11.32058600
H	-0.75715700	11.48719800	-12.52762500
H	2.45214800	10.18790200	-9.96932400
H	0.89116500	9.76515200	-11.83970000
C	2.60018000	15.78288200	-8.78746400
C	3.35463000	15.25541700	-9.82340400
C	4.63187000	15.74932800	-10.12374800
C	5.16363000	16.79203500	-9.37482400
C	4.40721700	17.33508000	-8.33146200
C	3.14612000	16.84272400	-8.03793000
H	2.96551100	14.44728000	-10.43399500
H	6.14694700	17.19657500	-9.58187300
H	4.81444400	18.15789400	-7.74781800
O	5.26742100	15.14192700	-11.16684000
O	2.36691100	17.35800500	-7.03866700
C	6.55311300	15.60899700	-11.49189300
H	7.24954900	15.48497000	-10.65244400
H	6.89359400	15.00727800	-12.33474300
H	6.53412500	16.66677400	-11.78506200
C	1.23496100	14.56365400	-7.06715400
C	0.09094000	14.60729200	-6.25083800
C	2.34355300	13.86584600	-6.60390500
C	0.05772000	13.93476900	-5.03073100
C	2.32463400	13.18750800	-5.38403300
H	3.24717300	13.86457300	-7.20821300
C	1.17785900	13.21974800	-4.60507400
H	-0.82783900	13.96094100	-4.40687800
H	3.20284700	12.64490100	-5.05014900
H	1.14346800	12.69637700	-3.65458900
O	-0.94690400	15.35271400	-6.72914300
C	-2.06789900	15.52190400	-5.89497200
H	-1.78133800	15.94775500	-4.92568700

H	-2.72998000	16.21625200	-6.41404800
H	-2.59613200	14.57327400	-5.73295400
C	1.20993300	15.29177600	-8.40811100
H	0.60089100	16.18964800	-8.25306500
H	2.86590500	18.04416800	-6.57427500
H	-1.86610100	20.59618000	-10.99134500

1a

E = -910.158267744 a.u.

0 1

C	-1.41594400	-1.73385600	0.37413000
C	-2.62895500	-2.36427900	0.74172800
C	-3.68408800	-1.57159500	1.21845400
C	-3.50718200	-0.20154400	1.31346900
C	-2.29102300	0.40329600	0.94216400
C	-1.22975100	-0.35129900	0.46901200
C	-1.16956800	-3.94288000	0.03571000
C	-2.44215400	-3.76808600	0.51626200
H	-4.62567800	-2.02899100	1.50780300
H	-4.31763800	0.42059000	1.67987300
H	-2.18360000	1.48002100	1.02728300
H	-0.29228600	0.11453600	0.18003000
H	-3.15310800	-4.56204500	0.69679700
N	-0.54215900	-2.70797100	-0.05205800
C	0.81551000	-2.45201300	-0.47188300
H	0.83541700	-1.85612600	-1.39112200
H	1.35948000	-1.91284600	0.31095900
H	1.31188500	-3.40644600	-0.65309800
C	-0.50047300	-5.19593100	-0.40092200
C	-0.82706000	-5.65335600	-1.81549200
C	-2.13665000	-6.46099300	-1.84046000
C	-0.91355300	-4.48507300	-2.81131000
H	-0.02332800	-6.31243200	-2.16849800
C	-2.47412100	-6.94937900	-3.25092400
H	-2.94696900	-5.81730100	-1.46986100
H	-2.05609000	-7.30664400	-1.14625900
C	-1.23682000	-4.98121800	-4.22273000
H	-1.69785500	-3.78955700	-2.48292200
H	0.02999500	-3.92488000	-2.81360300
C	-2.54024800	-5.78251100	-4.23846700
H	-3.42184200	-7.49895200	-3.24286400
H	-1.70009100	-7.65649800	-3.58148000
H	-1.30220700	-4.13248900	-4.91219200
H	-0.41696900	-5.61943400	-4.58161300

H	-2.75173800	-6.14903600	-5.24894700
H	-3.37105100	-5.12059500	-3.95787200
C	0.27561900	-5.87748100	0.46083500
C	0.88916300	-7.22984600	0.18243700
C	0.54118600	-5.40508900	1.87234000
C	0.35871300	-8.26374400	1.19218900
H	1.98072500	-7.15939500	0.29930500
H	0.69400700	-7.57433100	-0.83519700
C	0.01110100	-6.42975000	2.88786500
H	1.62865500	-5.30647700	2.01140100
H	0.09544500	-4.42398000	2.05423100
C	0.60914200	-7.81401500	2.63266100
H	0.82648800	-9.23660600	1.00603300
H	-0.72078500	-8.38811200	1.03377000
H	0.23433800	-6.09586000	3.90679300
H	-1.08181200	-6.47768800	2.79473300
H	0.19535500	-8.54523500	3.33557700
H	1.69270700	-7.77651800	2.81345400

2a

E = -881.702855497 a.u.

0 1

C	-0.07949600	-0.24517500	0.52573100
C	1.18647400	-0.19781000	-0.09006400
C	1.63399400	1.01662900	-0.59137700
C	0.85074900	2.16918800	-0.51177900
C	-0.40089600	2.10253000	0.08119500
C	-0.87194600	0.89902000	0.60641100
H	2.61500800	1.06639700	-1.05104300
H	1.22100200	3.10668600	-0.91277800
H	-1.02408400	2.98912900	0.14806000
H	-1.84748800	0.86648200	1.07634200
O	-0.44124300	-1.44984600	1.04136800
C	-1.70282700	-1.54716800	1.65777600
H	-2.50947800	-1.31472000	0.95215500
H	-1.79938000	-2.58131000	1.98842900
H	-1.77961700	-0.87886200	2.52465500
C	1.98341500	-1.48665000	-0.15588500
H	1.94597100	-1.92880500	0.85179300
C	3.45120000	-1.31443600	-0.50330600
C	4.40739300	-1.49194400	0.48603900
C	3.88576500	-1.01985500	-1.81020500
C	5.77678500	-1.37796100	0.22504300
H	4.10159300	-1.72770500	1.50153500

C	5.24535200	-0.91364700	-2.07412500
C	6.19838700	-1.09047800	-1.06835600
H	5.57620100	-0.68575900	-3.08514200
H	7.24946900	-1.00108900	-1.31528400
O	1.31815300	-2.34468200	-1.06796200
H	1.78957500	-3.19037000	-1.06098300
O	2.94229600	-0.82600400	-2.77412100
H	3.38585600	-0.59256800	-3.60191700
O	6.60496500	-1.57376600	1.28997700
C	7.98770500	-1.46487200	1.05249800
H	8.25448600	-0.46334900	0.69156500
H	8.47772300	-1.64602500	2.00911700
H	8.32880200	-2.21030800	0.32259600

H_2O

E = -76.3722218542 a.u.

0 1

O	-0.51818400	-0.87003500	0.00000000
H	0.44639500	-0.82736300	0.00000000
H	-0.79994300	0.05346200	0.00000000

(*S*)-7a

E = -2467.97465468 a.u.

0 1

P	-0.64869900	-0.65695400	0.83873500
O	0.15376700	-0.24908800	1.99298000
O	-0.69917600	-2.20270000	0.40390600
O	-2.20644200	-0.28625200	1.06660000
O	-0.24329800	-0.07233500	-0.58837300
H	-0.13530600	0.89702100	-0.55248500
C	-3.10959000	-4.26283400	2.26160800
C	-2.58586200	-3.37649300	1.31190700
C	-1.22201000	-3.12085500	1.31577400
C	-0.35082300	-3.77559600	2.20215500
C	-0.89713900	-4.75481200	3.03735700
C	-2.26996300	-4.98358200	3.09731900
C	-4.62012900	-4.25800700	2.21062800
C	-4.90953200	-2.99024100	1.38750300
H	-0.22664300	-5.31678100	3.67989900
H	-2.67502700	-5.70386700	3.80220400
H	-5.00617500	-5.15558500	1.71144600
H	-5.87034200	-3.01458700	0.86516700
H	-4.89919900	-2.11240700	2.04304400
C	-3.70611200	-2.88970900	0.40718200

C	-3.69030700	-1.55872100	-0.32170300
C	-3.94400500	-3.85112600	-0.79239900
C	-4.48327500	-1.64195900	-1.47249900
C	-3.06747200	-0.35890700	-0.02104100
C	-4.90204100	-3.07419600	-1.71520400
H	-2.98873400	-4.01521800	-1.30305000
H	-4.33247100	-4.82316100	-0.47518600
C	-4.74758600	-0.51233000	-2.23256400
C	-3.26564100	0.79134600	-0.80133800
H	-4.80453800	-3.36059400	-2.76635900
C	-4.15562500	0.69825100	-1.87508500
H	-5.38451900	-0.57053800	-3.11032300
H	-4.34567600	1.58731500	-2.46801100
H	-5.94939400	-3.23701500	-1.43202000
H	-5.06711800	-4.22715200	3.20847900
C	-2.47907400	2.03594400	-0.53677400
C	-1.58313200	2.52699900	-1.52332000
C	-2.58241800	2.70111700	0.70164500
C	-0.82076100	3.66002200	-1.23602100
C	-1.79737500	3.83449200	0.93166700
C	-0.90906600	4.32927000	-0.01477500
H	-0.13716600	4.03642600	-1.99374500
H	-1.88171000	4.34733700	1.88739200
C	-1.42209600	1.88918300	-2.90152100
H	-1.89212300	0.90257600	-2.88309900
C	-3.54899700	2.27332200	1.79583700
H	-4.02779800	1.33890300	1.49418200
C	-0.05868500	5.55183400	0.26830300
H	-0.30933600	5.89614800	1.27958000
C	1.08518200	-3.37504200	2.29164200
C	1.57868600	-2.80843600	3.49200200
C	1.92556700	-3.50557300	1.16987000
C	2.89443300	-2.34601700	3.50623800
C	3.23735400	-3.03711500	1.24676800
C	3.73437300	-2.43794800	2.39841600
H	3.29157500	-1.89156700	4.40814000
H	3.88634300	-3.14659300	0.38000900
C	0.72375200	-2.68303600	4.75631900
H	0.21359200	-3.63845700	4.90914900
C	1.48851700	-4.20747300	-0.10818300
H	0.41628800	-4.41214800	-0.04835600
C	5.15332400	-1.90605400	2.45230300
H	5.31079200	-1.49394000	3.45730400
C	-2.12615500	2.74915800	-3.96183300

H	-1.63836900	3.72747900	-4.04039100
H	-2.07815900	2.26695200	-4.94365600
H	-3.17665800	2.92703200	-3.71558700
C	0.04157300	1.68106500	-3.31472400
H	0.07629000	1.18204100	-4.28830900
H	0.57717200	2.63015800	-3.41793300
H	0.58615300	1.05165700	-2.60607800
C	1.43459800	5.20611700	0.24290700
H	1.73863000	4.87067100	-0.75492700
H	2.03766000	6.08326700	0.49860000
H	1.66694200	4.40696600	0.95255000
C	-0.37151900	6.68934300	-0.71033200
H	-1.43329300	6.95083400	-0.68606800
H	0.21145800	7.58201700	-0.46185700
H	-0.11901700	6.40058400	-1.73662200
C	-4.65915800	3.32017200	1.95979900
H	-5.19882300	3.47413500	1.02021400
H	-5.37674500	2.99842500	2.72169600
H	-4.24584600	4.28499400	2.27363000
C	-2.83030100	2.02309100	3.12748300
H	-2.00365800	1.31747700	3.00744800
H	-2.43096100	2.95519700	3.54243600
H	-3.53348400	1.61355100	3.86019400
C	-0.36114600	-1.60291400	4.64128100
H	0.08994600	-0.62670600	4.44781900
H	-1.06001400	-1.80326600	3.82488400
H	-0.93073200	-1.55619100	5.57642300
C	1.54584400	-2.43264500	6.02430200
H	0.89428300	-2.51203000	6.89979200
H	2.35889500	-3.15668900	6.13637200
H	1.97779700	-1.42617200	6.03100700
C	6.18107000	-3.02190500	2.23339900
H	7.20059800	-2.63243100	2.32334000
H	6.05143200	-3.82627000	2.96330000
H	6.07593800	-3.45590200	1.23290600
C	5.35683400	-0.77307500	1.44006300
H	6.36649900	-0.35681700	1.52206200
H	5.22715200	-1.14166300	0.41645500
H	4.63295000	0.03078200	1.60072100
C	1.72664300	-3.35055900	-1.35604600
H	1.24100100	-2.37574000	-1.26304700
H	2.79602200	-3.18867700	-1.53012900
H	1.32369500	-3.85480800	-2.24088600
C	2.20277300	-5.56031300	-0.23172000

H	3.28760000	-5.42256000	-0.30065300
H	1.99948100	-6.19215200	0.63849500
H	1.87126100	-6.09133500	-1.13053200

(R_a,S)-Int1

E = -4183.49104263 a.u.

0 1

H	0.53284800	-1.12133700	-0.93028700
C	-0.52747000	1.87020700	1.84933900
C	-1.30041000	1.69769200	0.74077200
C	-2.54607900	2.38588400	0.49190100
C	-0.88505600	0.61699600	-0.18378900
C	-3.32360600	2.04915300	-0.56169000
H	-2.91508500	3.10601000	1.21102500
C	-1.75265000	0.32846800	-1.31715300
C	-2.90193100	1.01765100	-1.49144600
H	-1.44636200	-0.45707100	-2.00414300
H	-3.53478100	0.78310300	-2.34228600
C	-0.66351200	2.89840400	2.87297300
C	-0.35291800	2.57362800	4.21348900
C	-0.99905800	4.22380600	2.57092000
C	-0.38402500	3.55260300	5.20527500
C	-1.04478500	5.20147700	3.55891500
H	-1.18460600	4.48904000	1.53454000
C	-0.73668400	4.85944600	4.87233600
H	-0.16008900	3.30361800	6.23595700
H	-1.30177300	6.22374700	3.30165600
H	-0.76497300	5.61355100	5.65274900
O	-0.07448400	1.26640000	4.45022100
C	0.33069600	0.89956400	5.75588600
H	0.56403600	-0.16451900	5.71201100
H	-0.47640000	1.06586500	6.47959400
H	1.22215000	1.45844900	6.06171500
O	-4.50231100	2.71254700	-0.73587900
C	-5.54515000	2.02668400	-1.40437500
H	-5.40620600	2.04138000	-2.49213500
H	-6.46328300	2.56445600	-1.16097600
H	-5.62047400	0.98835700	-1.05992400
O	0.18159800	0.00083100	-0.00032100
C	-4.73905800	-0.48170900	1.44013200
C	-3.40078800	-0.56468600	1.89316800
C	-2.53328000	-1.48996400	1.28809200
C	-3.01674000	-2.31176600	0.27953100
C	-4.35399200	-2.21325100	-0.14987500

C	-5.23263600	-1.29900500	0.41662600
C	-4.49390200	0.99631500	3.12317100
H	-1.49900700	-1.57806900	1.61292100
H	-2.34582000	-3.03010000	-0.18209500
H	-4.70849400	-2.87271500	-0.93665500
H	-6.26840900	-1.23755100	0.09249900
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C	-6.80841200	0.72251400	2.10899600
H	-7.35888500	-0.22328400	2.14414900
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H	-7.10946700	1.34248100	2.95401900
C	-4.89429600	2.01040100	4.12958700
C	-5.36748700	3.21919100	3.76121500
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C	-5.75743800	4.31381400	4.73170900
H	-5.18467100	2.87901700	1.62467900
H	-5.61673300	4.01848400	5.77285700
C	-4.68257500	1.62782000	5.59272100
C	-3.31534600	2.11999800	6.09416100
C	-4.83466100	0.12856800	5.88668400
H	-5.45223800	2.13437200	6.18965700
C	-3.12195700	1.82889800	7.58309100
H	-2.53235800	1.60708100	5.51611100
H	-3.20512400	3.19094800	5.88295200
C	-4.66283700	-0.15687700	7.38051100
H	-4.07379400	-0.42929100	5.32801600
H	-5.81004700	-0.22789300	5.53079500
C	-3.30161100	0.33781700	7.87759800
H	-2.13261800	2.17181100	7.91337800
H	-3.85959200	2.40329600	8.16130800
H	-4.76916100	-1.23133400	7.57036500
H	-5.45866200	0.34478400	7.94915000
H	-3.18823200	0.14065000	8.94923700
H	-2.51028100	-0.22724400	7.36257500
H	0.27025600	1.14380100	1.99660400
C	-3.27674700	0.38178300	2.96081400
H	-2.37815300	0.59804700	3.52471400
H	-6.58144600	3.84243700	2.11438300
H	-6.82908400	4.53032700	4.60114800
C	-4.74046500	4.95348500	2.04855200
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H	-3.66876200	4.76285500	2.19385300
C	-4.97221000	5.60683100	4.45494200
H	-5.29138600	6.38739000	5.15431500

H	-3.90484700	5.41942100	4.63860300
C	-5.15768800	6.06569400	3.00863800
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H	-6.21333200	6.32170000	2.84038900
P	0.84237600	-3.31040400	-1.17066600
O	0.79044000	-1.82084700	-1.63545900
O	1.40221300	-4.10652300	-2.45553600
O	2.10804700	-3.29216800	-0.15273200
O	-0.36295200	-3.97491800	-0.65374500
C	4.84341500	-3.31562600	-3.43224700
C	3.76220300	-3.89746700	-2.76093100
C	2.47348700	-3.58994400	-3.16649300
C	2.22373000	-2.77001200	-4.27987600
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C	4.63701000	-2.55132000	-4.57148600
C	6.13575300	-3.62900700	-2.71186600
C	5.63148600	-4.15081100	-1.35227400
H	3.15763600	-1.69999900	-5.88033500
H	5.47631900	-2.12388300	-5.11255400
H	6.71487800	-4.39436100	-3.24357800
H	6.33189000	-4.82950200	-0.85647200
H	5.43799000	-3.30807300	-0.67959600
C	4.27727100	-4.83865400	-1.68499300
C	3.50070600	-5.21921000	-0.43188400
C	4.55480800	-6.25333400	-2.27098400
C	3.89422500	-6.49465500	-0.00967200
C	2.54331200	-4.53054400	0.30434200
C	4.79990100	-7.13559700	-1.03527900
H	3.65521900	-6.59370000	-2.79572500
H	5.38487800	-6.25201400	-2.98354100
C	3.42587300	-7.02360600	1.18377800
C	2.00132100	-5.06500500	1.48283200
H	4.55268300	-8.18723800	-1.20732400
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H	3.75141100	-8.00309000	1.52222700
H	2.11610900	-6.69559700	2.85836200
H	5.85030100	-7.09766600	-0.71978200
H	6.77865700	-2.74904400	-2.61578000
C	0.87776500	-4.41538100	2.22767900
C	-0.37785000	-5.05776200	2.27475500
C	1.06616300	-3.19595000	2.90685200
C	-1.39728400	-4.49307300	3.04314700
C	0.00701500	-2.66242000	3.64212700
C	-1.22940500	-3.29960000	3.73720900

H	-2.35969600	-4.99418600	3.07498800
H	0.13917500	-1.70623500	4.14792900
C	-0.68184500	-6.34955400	1.52535000
H	0.12256400	-6.52420900	0.80519100
C	2.40666900	-2.47814000	2.92891200
H	3.06508900	-2.95101200	2.19525800
C	-2.32882400	-2.68808600	4.58758500
H	-2.28916400	-1.60103500	4.42727800
C	0.82973100	-2.32968100	-4.59375200
C	0.50261100	-0.95637100	-4.53628000
C	-0.18558000	-3.27798600	-4.84312200
C	-0.83084100	-0.57471900	-4.69857800
C	-1.50339000	-2.84409900	-4.98403800
C	-1.85225100	-1.49890500	-4.89224900
H	-1.08946500	0.48130900	-4.64430800
H	-2.28122200	-3.58405900	-5.16147400
C	1.52977900	0.14614200	-4.30764000
H	2.46576500	-0.31228500	-3.98197700
C	0.09774000	-4.76272000	-5.02058400
H	1.14060300	-4.95366600	-4.75627100
C	-3.29978200	-1.05530400	-4.97253000
H	-3.31136100	0.03772600	-4.85520900
C	-0.74440700	-7.53982900	2.49342400
H	-0.94412900	-8.46810700	1.94731700
H	0.18514400	-7.66765900	3.05515800
H	-1.55292200	-7.39600100	3.21963000
C	-1.98951700	-6.27135400	0.72722500
H	-2.10852900	-7.18322300	0.13161500
H	-2.86258900	-6.19581000	1.38478600
H	-1.97473200	-5.41360500	0.05456800
C	-2.05438500	-2.95239000	6.07466500
H	-2.83107300	-2.49592800	6.70008000
H	-2.04647300	-4.03003700	6.27299200
H	-1.08253400	-2.54964300	6.38037100
C	-3.73342900	-3.16450000	4.21618700
H	-3.92264400	-3.05752800	3.14359800
H	-3.87620200	-4.21605900	4.49152300
H	-4.48443600	-2.57998000	4.75847400
C	3.06257100	-2.63738300	4.30663100
H	2.44177700	-2.17670200	5.08466500
H	3.18813600	-3.69437800	4.56184100
H	4.04634100	-2.15607500	4.32758900
C	2.28586900	-1.00032500	2.54630600
H	1.80809200	-0.88386700	1.56968300

H	1.69507200	-0.43965500	3.28172600
H	3.27893500	-0.53978700	2.50377900
C	1.12519300	1.13425300	-3.20878300
H	0.20046000	1.66950500	-3.45020200
H	0.99071100	0.62297900	-2.25398700
H	1.91285400	1.88467300	-3.08109200
C	1.79001200	0.90063400	-5.61941800
H	2.57293000	1.65457800	-5.48429600
H	2.09594200	0.22482600	-6.42416700
H	0.87998700	1.41370000	-5.95141100
C	-4.12319100	-1.66687500	-3.83142100
H	-4.19142700	-2.75465000	-3.94540900
H	-3.66917700	-1.47136100	-2.85398900
H	-5.14398700	-1.26626800	-3.82766700
C	-3.92325700	-1.38885700	-6.33196800
H	-4.95670300	-1.03011800	-6.38479300
H	-3.35528100	-0.93328000	-7.14811900
H	-3.93592600	-2.47206100	-6.49471500
C	-0.78082900	-5.63675300	-4.11789000
H	-0.45844600	-6.68150400	-4.18115800
H	-0.72120400	-5.31647000	-3.07435800
H	-1.83032200	-5.60130300	-4.43140500
C	-0.07645500	-5.15306400	-6.49481100
H	-1.10827500	-4.98348000	-6.82270700
H	0.58242800	-4.56294100	-7.13948800
H	0.15469700	-6.21359300	-6.64149200

(R_a,*S*)-TS1

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C	-1.34479300	1.53691600	1.91839100
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C	-2.93094900	2.30992800	0.13492600
C	-1.30336100	0.52325000	-0.27199800
C	-3.53516100	2.04965600	-1.07473600
H	-3.35286500	3.07624700	0.77206800
C	-1.93414800	0.26873000	-1.50543100
C	-3.02782600	1.01593700	-1.89384200
H	-1.54497700	-0.52631300	-2.13695500
H	-3.49209900	0.78993000	-2.84782800
C	-1.13805100	2.68754700	2.78684100
C	-0.55245900	2.48981400	4.06368700
C	-1.32242900	4.00669700	2.34933000

C	-0.25228600	3.57812200	4.88271800
C	-1.01860600	5.09319800	3.15931400
H	-1.65814500	4.17304200	1.33233900
C	-0.49858800	4.87242900	4.43149900
H	0.17894100	3.42702700	5.86453500
H	-1.16691300	6.10326900	2.79194600
H	-0.25584500	5.71185000	5.07548800
O	-0.31021000	1.20487600	4.41918900
C	0.39365900	0.96718000	5.62643100
H	0.52928200	-0.11220100	5.68934800
H	-0.18475700	1.31288400	6.49159800
H	1.37115100	1.46033300	5.60873800
O	-4.63728500	2.80081900	-1.38389900
C	-5.30573000	2.49163000	-2.58626100
H	-4.66104600	2.65158100	-3.45931000
H	-6.15939500	3.16739400	-2.64247100
H	-5.66081000	1.45248600	-2.59147800
O	-0.22485000	-0.11412000	0.12694800
C	-4.39052400	-0.48457700	1.35847900
C	-3.13823200	-0.75113600	1.93917200
C	-2.35249800	-1.77551900	1.39706600
C	-2.84820600	-2.50003900	0.31694700
C	-4.10496200	-2.21068900	-0.23553200
C	-4.89932000	-1.18835500	0.26995800
C	-4.14922100	0.99493800	3.04680500
H	-1.36174100	-1.99528800	1.78388200
H	-2.22331800	-3.27638400	-0.11504200
H	-4.45792300	-2.79088300	-1.08240700
H	-5.86392400	-0.94898500	-0.16730800
N	-4.98598100	0.56038400	2.06674800
C	-6.38113900	0.90086000	1.86705300
H	-6.95762400	-0.02593000	1.80469000
H	-6.51111100	1.46919300	0.94028800
H	-6.73294200	1.49130700	2.71203800
C	-4.55408600	1.97773600	4.08256700
C	-5.03810300	3.20897200	3.79443200
C	-5.33984900	3.73201500	2.40713900
C	-5.37507500	4.23371900	4.85892900
H	-5.05718000	3.02111400	1.63207400
H	-5.11307600	3.89650300	5.86199500
C	-4.43591600	1.49025000	5.53064200
C	-3.09603000	1.86213300	6.18060000
C	-4.71730500	-0.01107600	5.69748900
H	-5.22429900	1.99790700	6.09975700

C	-3.05722100	1.45270600	7.65424300
H	-2.29497100	1.34083200	5.64187500
H	-2.90987100	2.93706800	6.06097400
C	-4.67074700	-0.41977500	7.17196500
H	-3.97198200	-0.59395800	5.14716800
H	-5.69299300	-0.25839700	5.25878100
C	-3.32849600	-0.04509300	7.80503800
H	-2.08880900	1.71616000	8.09670500
H	-3.81937900	2.01847500	8.20881000
H	-4.84735400	-1.49763700	7.26524300
H	-5.48053500	0.08171500	7.72044700
H	-3.30802900	-0.33698800	8.86050100
H	-2.52587900	-0.60595400	7.30306500
H	-0.68343800	0.70037100	2.13575200
C	-2.94476800	0.24930600	2.96953400
H	-2.23078900	0.19082700	3.78040400
H	-6.43394800	3.84831600	2.33928900
H	-6.46244400	4.40573400	4.84866700
C	-4.70840400	5.10098900	2.11852900
H	-5.03566600	5.44473700	1.13147300
H	-3.62017100	4.98834800	2.07837300
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C	-5.05224400	6.11875500	3.20356700
H	-4.53797500	7.06674300	3.01192000
H	-6.13051400	6.33018700	3.18407000
P	0.66767700	-3.32905700	-1.08410100
O	0.40121200	-1.88957500	-1.46254100
O	1.33216700	-4.09277100	-2.37262800
O	1.96358300	-3.23939400	-0.06418300
O	-0.37925900	-4.23492100	-0.55493800
C	4.73764000	-3.13897600	-3.31228000
C	3.67337300	-3.76157200	-2.65294700
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C	3.20202100	-2.17712000	-4.87580400
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C	5.54189600	-3.96107500	-1.23535800
H	3.00730500	-1.56632900	-5.75314300
H	5.34020100	-1.91946600	-4.98626300
H	6.64363900	-4.15656300	-3.12086900
H	6.26198900	-4.61796900	-0.73791500

H	5.31407400	-3.12926900	-0.55969100
C	4.21321000	-4.69126100	-1.58132400
C	3.44601800	-5.10020100	-0.33257400
C	4.54206900	-6.09300500	-2.16981500
C	3.89288100	-6.35687500	0.09272300
C	2.45900200	-4.44098700	0.39524200
C	4.81813600	-6.96696100	-0.93471100
H	3.65457300	-6.46341600	-2.69464300
H	5.37193900	-6.06145000	-2.88225800
C	3.45623500	-6.89941700	1.29157900
C	1.96087400	-4.99449100	1.58641900
H	4.60535800	-8.02651200	-1.10582100
C	2.51352900	-6.19787800	2.03740700
H	3.82313000	-7.86303800	1.63354300
H	2.15754900	-6.60332600	2.97944500
H	5.86757900	-6.89481800	-0.62124800
H	6.65002300	-2.51374800	-2.48291000
C	0.84209300	-4.38559100	2.37199900
C	-0.37847800	-5.08709100	2.49234200
C	1.01778400	-3.17124900	3.06228300
C	-1.36246800	-4.59136200	3.34896400
C	-0.00797800	-2.70792600	3.89048500
C	-1.19765400	-3.40976500	4.06622100
H	-2.29072500	-5.14704000	3.44287800
H	0.12173500	-1.76065600	4.41318600
C	-0.67071500	-6.38162200	1.74304000
H	0.10214400	-6.51365800	0.98180200
C	2.30626100	-2.36740800	2.98616500
H	2.97448800	-2.85439300	2.27156100
C	-2.24752100	-2.90169400	5.03796700
H	-2.17403100	-1.80234500	5.04458500
C	0.71284300	-2.26195300	-4.49925700
C	0.37310600	-0.89163400	-4.45629900
C	-0.27977900	-3.21707500	-4.80338700
C	-0.94800000	-0.51553100	-4.71081200
C	-1.58772400	-2.78983200	-5.03146900
C	-1.94746300	-1.44522200	-4.97905500
H	-1.21297500	0.54070000	-4.67200300
H	-2.34734200	-3.53518000	-5.26033600
C	1.37418500	0.21610100	-4.14738500
H	2.31620300	-0.24132600	-3.84190100
C	0.02090100	-4.70116200	-4.95411300
H	1.05934800	-4.87655500	-4.66473800
C	-3.38368600	-1.01074200	-5.20118700

H	-3.41509500	0.08334400	-5.09044800
C	-0.64675400	-7.58376200	2.69815300
H	-0.83302300	-8.51189000	2.14719400
H	0.31000900	-7.68337600	3.21803700
H	-1.42929800	-7.48324300	3.45976300
C	-2.01614300	-6.33910700	1.00884900
H	-2.14768600	-7.26397900	0.43645000
H	-2.85936000	-6.26317000	1.70501900
H	-2.03871000	-5.49797400	0.31655500
C	-1.93488100	-3.39652300	6.45706100
H	-2.67434800	-3.02405400	7.17639000
H	-1.95324600	-4.49162400	6.48414700
H	-0.94042900	-3.07098900	6.77942800
C	-3.67596800	-3.28162400	4.64447000
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H	-3.82684100	-4.36385100	4.71596700
H	-4.39668200	-2.81249000	5.32280300
C	3.01514500	-2.35638500	4.34623200
H	2.40024800	-1.85722000	5.10531000
H	3.21420100	-3.37447000	4.69503700
H	3.96807900	-1.82037100	4.28042700
C	2.05613600	-0.94372200	2.48117600
H	1.58682600	-0.95626600	1.49476200
H	1.40071500	-0.38578000	3.16325400
H	3.00160100	-0.39499700	2.40674500
C	0.93427400	1.10928800	-2.98394400
H	-0.00822600	1.62765100	-3.19340300
H	0.81334700	0.51754100	-2.07437600
H	1.69700000	1.87373700	-2.79746700
C	1.63661800	1.06256500	-5.40039300
H	2.39983700	1.82240000	-5.20013700
H	1.97380900	0.44831300	-6.24156500
H	0.72261900	1.57885800	-5.71636000
C	-4.31984700	-1.62602900	-4.15292600
H	-4.35192800	-2.71598700	-4.25973000
H	-3.98094300	-1.40670800	-3.13465800
H	-5.34213500	-1.24791500	-4.27321900
C	-3.86286700	-1.34880600	-6.61736300
H	-4.88748900	-0.99632800	-6.77854400
H	-3.21479500	-0.89116200	-7.37015000
H	-3.85075900	-2.43222700	-6.77835400
C	-0.86664100	-5.56555700	-4.05123000
H	-0.55784700	-6.61444400	-4.11823900
H	-0.79689600	-5.25046000	-3.00671400

H	-1.91643100	-5.51418200	-4.36348200
C	-0.12106100	-5.11963100	-6.42400400
H	-1.14939800	-4.97579500	-6.77490200
H	0.53906900	-4.52961300	-7.06769800
H	0.13141600	-6.17836200	-6.54739800

(R_a,*S*)-Int2

E = -4183.49613519 a.u.

0 1

H	0.08065200	-0.70728900	-0.45231700
C	-1.73918300	1.22391200	2.17506400
C	-2.10713100	1.35128800	0.71644800
C	-3.24552000	2.02642300	0.29558800
C	-1.36900200	0.59765700	-0.21496800
C	-3.68904900	1.96331200	-1.02314800
H	-3.80964000	2.62275400	1.00084000
C	-1.83889500	0.49573900	-1.52739800
C	-2.98087600	1.18147600	-1.93604900
H	-1.30336100	-0.14128400	-2.22643100
H	-3.30217700	1.08596100	-2.96758800
C	-1.29684400	2.47515800	2.90548500
C	-0.48528700	2.32747800	4.04825100
C	-1.57017900	3.76655300	2.46653500
C	0.00039200	3.43794400	4.73571900
C	-1.10224400	4.88815900	3.15330000
H	-2.12029100	3.89702000	1.54159000
C	-0.32085600	4.71920100	4.28789100
H	0.62770300	3.31872800	5.61082500
H	-1.32795900	5.88285300	2.78233600
H	0.06185600	5.58087500	4.82560200
O	-0.24741600	1.03958300	4.43915700
C	0.55656300	0.83717500	5.58390600
H	0.60376000	-0.24119500	5.73752100
H	0.10845600	1.31090400	6.46715100
H	1.56829300	1.22781400	5.42891400
O	-4.82968100	2.67209500	-1.30802400
C	-5.29114100	2.60465600	-2.63716300
H	-4.54750900	3.00165800	-3.33955500
H	-6.19295000	3.21638400	-2.68215500
H	-5.53412200	1.57355000	-2.92595500
O	-0.26126000	-0.02075400	0.21583400
C	-4.50933200	-0.94184100	1.93007900
C	-3.13841800	-0.87558300	2.14980300
C	-2.31435100	-1.82482800	1.56281900

C	-2.90735400	-2.83120700	0.79645600
C	-4.29309600	-2.89008400	0.62312400
C	-5.13361600	-1.93073600	1.18685900
C	-4.22746100	0.94814400	3.15657100
H	-1.23379000	-1.78730700	1.65807700
H	-2.24947400	-3.54428600	0.30904200
H	-4.72072400	-3.68426600	0.01998000
H	-6.20700100	-1.95215700	1.03005300
N	-5.11362400	0.16643700	2.58821200
C	-6.56365500	0.28488500	2.65258300
H	-6.96788400	-0.68008000	2.96552500
H	-6.94525100	0.53816700	1.66020100
H	-6.83114600	1.06055000	3.36736300
C	-4.61115900	2.03520800	4.08517400
C	-5.25976700	3.14920600	3.68258600
C	-5.79315700	3.40316400	2.29031000
C	-5.53789100	4.31101300	4.61112400
H	-5.60861000	2.57342200	1.60530700
H	-5.11596500	4.15676800	5.60523900
C	-4.33641300	1.71510800	5.56026400
C	-2.95746900	2.14871100	6.06686700
C	-4.59126800	0.23232200	5.89434500
H	-5.08699000	2.27615200	6.13047600
C	-2.82670700	1.90604400	7.57164600
H	-2.19205800	1.55444300	5.55720600
H	-2.77182100	3.19777800	5.80596500
C	-4.42993400	-0.02975900	7.39417000
H	-3.88243600	-0.41013900	5.35405600
H	-5.59726200	-0.06118000	5.56471800
C	-3.05745800	0.42792900	7.89352100
H	-1.83702100	2.22653800	7.91652200
H	-3.56282200	2.51820500	8.11172400
H	-4.57742900	-1.09615900	7.59903300
H	-5.21302300	0.51107400	7.94335900
H	-2.96578100	0.24583900	8.96925000
H	-2.27767200	-0.17149900	7.39980600
H	-0.88344100	0.54172400	2.21056100
C	-2.83908900	0.37867600	2.92865900
H	-2.41357200	0.16812300	3.91981700
H	-6.88764500	3.48936000	2.38745100
H	-6.62648100	4.42062200	4.72691400
C	-5.27071800	4.71877700	1.69162900
H	-5.72109300	4.86919400	0.70603900
H	-4.18837500	4.64055200	1.53681000

C	-4.97237500	5.61340200	4.01602500
H	-5.18446600	6.44188200	4.69948800
H	-3.88059800	5.51799700	3.94547200
C	-5.55180100	5.89119800	2.62944900
H	-5.12876000	6.81371800	2.21891500
H	-6.63670800	6.04597500	2.71201400
P	0.74282600	-3.20512700	-1.06878600
O	0.65072800	-1.74141900	-1.40569500
O	1.32665500	-4.01770100	-2.37380300
O	2.04553800	-3.30333100	-0.05126000
O	-0.39642500	-4.00604700	-0.55202700
C	4.78631700	-3.26849200	-3.31065000
C	3.68612100	-3.84546100	-2.66865300
C	2.39913900	-3.48954800	-3.05182100
C	2.18939600	-2.61374400	-4.13093600
C	3.31173100	-2.15457900	-4.82920900
C	4.60897000	-2.44926300	-4.41598000
C	6.06762900	-3.65190600	-2.60474600
C	5.54388700	-4.21682100	-1.27077900
H	3.15322000	-1.50367900	-5.68441000
H	5.46167400	-2.02382400	-4.93762100
H	6.62502300	-4.41130800	-3.16798900
H	6.22261500	-4.93585400	-0.80165000
H	5.37054700	-3.39796600	-0.56385800
C	4.17063200	-4.84754600	-1.63687500
C	3.38366000	-5.25300300	-0.40088700
C	4.40782200	-6.24427100	-2.27902100
C	3.74936900	-6.54992700	-0.02435900
C	2.44540000	-4.55376300	0.35434600
C	4.62973000	-7.18020800	-1.07873300
H	3.49736500	-6.53699600	-2.81360200
H	5.23659200	-6.23925900	-2.99344000
C	3.28349700	-7.10596400	1.15781600
C	1.91826800	-5.11738800	1.52872900
H	4.34801000	-8.21671900	-1.28783600
C	2.39137500	-6.37143600	1.93236300
H	3.58781000	-8.10307000	1.46326200
H	2.00380200	-6.79130200	2.85633300
H	5.68249200	-7.18841400	-0.76825000
H	6.73718500	-2.79688900	-2.46986900
C	0.83776300	-4.46966100	2.33373400
C	-0.39783000	-5.13734600	2.48967400
C	1.05346200	-3.24429200	2.99586100
C	-1.35853600	-4.59933500	3.34926400

C	0.04901600	-2.73674300	3.82223400
C	-1.15479100	-3.40435300	4.03137400
H	-2.30150900	-5.12753600	3.46442400
H	0.20304900	-1.77342500	4.30791700
C	-0.74190600	-6.44108100	1.77661300
H	0.07122900	-6.68329300	1.08939100
C	2.35405500	-2.46330000	2.88806500
H	3.02504600	-2.99958200	2.21314500
C	-2.18123200	-2.81788600	4.98423300
H	-2.13903800	-1.72420900	4.85798400
C	0.82449600	-2.11310100	-4.47528600
C	0.55724900	-0.72726100	-4.40878900
C	-0.20378900	-3.00453500	-4.84494700
C	-0.72557700	-0.27216500	-4.72398400
C	-1.47181600	-2.49931300	-5.13247400
C	-1.75791100	-1.13805400	-5.07220700
H	-0.93406600	0.79622100	-4.67284800
H	-2.25815400	-3.19637900	-5.41681500
C	1.60334000	0.31270700	-4.02130900
H	2.49848000	-0.20881100	-3.67859100
C	0.01376000	-4.50302900	-4.99695700
H	1.03390200	-4.74027800	-4.68779600
C	-3.14819300	-0.61795100	-5.38457600
H	-3.14088900	0.46652700	-5.20195300
C	-0.88249500	-7.58920700	2.78603300
H	-1.05706000	-8.53679100	2.26552900
H	0.01160700	-7.69932900	3.40754100
H	-1.73165700	-7.41556700	3.45744800
C	-2.01256300	-6.32513000	0.92522000
H	-2.26290000	-7.30456200	0.50204100
H	-2.87250200	-5.99053700	1.51840400
H	-1.84330000	-5.62492200	0.10562800
C	-1.79856600	-3.12099900	6.43920400
H	-2.51667500	-2.67265500	7.13720500
H	-1.78802600	-4.20335300	6.60743200
H	-0.80019500	-2.73742700	6.67317300
C	-3.61271900	-3.27895100	4.70539400
H	-3.87772000	-3.16053500	3.64926100
H	-3.73770500	-4.33518600	4.96835700
H	-4.32466500	-2.70937400	5.31487700
C	3.04927300	-2.37772800	4.25295500
H	2.44051200	-1.81602600	4.97187100
H	3.22625300	-3.37371900	4.67084800
H	4.01276400	-1.86530200	4.16004300

C	2.12174500	-1.06883000	2.29813200
H	1.68080800	-1.13464100	1.30101400
H	1.45032300	-0.47253500	2.93039300
H	3.07141800	-0.52826600	2.21731500
C	1.15956400	1.21370200	-2.86426000
H	0.25456000	1.78263500	-3.10588300
H	0.97247400	0.62403200	-1.96485500
H	1.95199400	1.93672300	-2.64010400
C	1.97823400	1.16845100	-5.23967400
H	2.77921000	1.87116900	-4.98557300
H	2.31224700	0.55536400	-6.08280900
H	1.11500300	1.75214800	-5.58036500
C	-4.20577400	-1.25048600	-4.47168000
H	-4.29002400	-2.32516100	-4.66603400
H	-3.94815300	-1.12496200	-3.41517200
H	-5.19042500	-0.80259500	-4.65133600
C	-3.50644500	-0.83930900	-6.85879500
H	-4.49714100	-0.43097900	-7.08732200
H	-2.77347000	-0.36316100	-7.51631900
H	-3.52041800	-1.90965600	-7.09209500
C	-0.94066700	-5.31011100	-4.10896300
H	-0.70142000	-6.37725100	-4.17469100
H	-0.86193900	-5.00061900	-3.06339800
H	-1.98042000	-5.18612800	-4.43446800
C	-0.12468800	-4.91539600	-6.46862800
H	-1.13619800	-4.71557100	-6.84027200
H	0.57975500	-4.36471900	-7.10004300
H	0.07042300	-5.98689200	-6.58637100

(S_a,*R*)-Int1

E = -4183.49323565 a.u.

0 1

P	2.28755000	0.10546200	4.67137400
O	2.77559900	1.55459000	4.99331400
O	3.47805100	-0.67666100	3.90870200
O	2.36470200	-0.51628200	6.16297700
O	1.02121200	-0.06714900	3.94124000
H	2.28699900	2.28212600	4.46042900
C	6.59959700	-0.81558700	5.82420000
C	5.32818100	-1.15477800	5.34902200
C	4.78098600	-0.42043500	4.30934200
C	5.50158400	0.59092900	3.65464600
C	6.81573000	0.81512000	4.07784900
C	7.35984500	0.14563800	5.17392700

C	6.91381200	-1.60046000	7.07867200
C	5.53243300	-2.16690300	7.46482900
H	7.40246800	1.57068800	3.56430100
H	8.35871900	0.39218700	5.52233700
H	7.63334200	-2.40432400	6.87898000
H	5.58636600	-3.09124400	8.04783700
H	4.97695700	-1.42533500	8.04918900
C	4.81022100	-2.36738900	6.10353200
C	3.33455100	-2.70205600	6.25864400
C	5.31623400	-3.68548400	5.44685100
C	3.17238900	-4.08773100	6.36443400
C	2.20952900	-1.88779300	6.29767100
C	4.48728800	-4.79119000	6.12224500
H	5.08283000	-3.65167900	4.37680800
H	6.39691300	-3.81545600	5.55578700
C	1.92307100	-4.64020600	6.60886600
C	0.92335900	-2.41927300	6.46655200
H	4.37378600	-5.68126600	5.49660500
C	0.81537900	-3.79945700	6.67235500
H	1.80278400	-5.71450700	6.71466800
H	-0.17398200	-4.21655000	6.83480300
H	4.94649500	-5.11413900	7.06522400
H	7.34583200	-0.97035200	7.86171300
C	-0.31480500	-1.58880300	6.34158900
C	-1.21340100	-1.85967800	5.28483100
C	-0.61064000	-0.56985900	7.26623500
C	-2.41426600	-1.15190700	5.21916000
C	-1.82409200	0.11435300	7.15196300
C	-2.75282700	-0.17647500	6.15441400
H	-3.10971000	-1.38278400	4.41564300
H	-2.06885100	0.88348600	7.88427000
C	-0.94424800	-2.90466700	4.20766100
H	0.07777900	-3.27219800	4.32855000
C	0.30969600	-0.21592600	8.42502700
H	1.19999200	-0.84761800	8.36669300
C	-4.11856900	0.49019500	6.16790100
H	-4.01050900	1.45661200	6.68106900
C	4.84749800	1.42932500	2.60161200
C	4.72521100	2.82965700	2.78169800
C	4.30689200	0.82842600	1.44599800
C	4.06511900	3.57662700	1.80625300
C	3.65369100	1.62488400	0.50251300
C	3.51559600	2.99886900	0.66250600
H	3.96293800	4.65322300	1.94131700

H	3.24263900	1.14695900	-0.38230800
C	5.33339400	3.57504500	3.96610300
H	5.64520800	2.84247600	4.71392700
C	4.44764800	-0.65412000	1.12980500
H	4.90786800	-1.15542400	1.98406500
C	2.86040600	3.87746500	-0.38905900
H	2.32539500	4.67773700	0.14508800
C	0.56194300	5.83049600	2.96703200
C	-0.26978600	4.89741500	3.49621100
C	-1.71464500	5.02107200	3.55382800
C	0.37547000	3.66995200	4.03574600
C	-2.43536700	4.08731400	4.21731700
H	-2.17793600	5.82026300	2.98349700
C	-0.45023700	2.79435000	4.85829000
C	-1.77683800	3.01094000	4.93698400
H	0.00365700	1.92520700	5.32420100
H	-2.41013300	2.33713200	5.50404100
C	0.22106600	7.21517500	2.64572100
C	0.82593300	7.84831900	1.53887200
C	-0.56632700	7.98873000	3.50711500
C	0.60952500	9.20396800	1.29408300
C	-0.76415700	9.34788600	3.28257300
H	-0.99066100	7.51125000	4.38521100
C	-0.18338600	9.94655900	2.16985200
H	1.06210600	9.68898400	0.43697800
H	-1.36515700	9.93230300	3.97107400
H	-0.33556100	11.00411400	1.97587500
O	1.61545200	7.05908200	0.76636900
C	2.50034800	7.70155000	-0.13328200
H	3.13496000	6.91578600	-0.54153900
H	1.95733700	8.18742000	-0.95092600
H	3.11439900	8.44255300	0.39126400
O	-3.78596100	4.01261700	4.28207500
C	-4.49990800	4.83583300	3.38646000
H	-4.17556100	4.64016800	2.35574700
H	-5.55244700	4.57822900	3.50522000
H	-4.35479600	5.89941700	3.61666700
O	1.57592800	3.44353300	3.81539000
C	-2.64926200	3.16607700	0.47371800
C	-1.27135500	3.39616400	0.69229300
C	-0.53409700	2.45790000	1.43329700
C	-1.18519400	1.35391300	1.96059800
C	-2.56402400	1.16213000	1.75216400
C	-3.31626200	2.05679900	1.00295300

C	-2.11033400	5.11253500	-0.52465700
H	0.53239400	2.59663000	1.59933400
H	-0.62821200	0.65093500	2.57178800
H	-3.04711000	0.29097800	2.18519700
H	-4.37881000	1.90030800	0.83776200
N	-3.14066400	4.20830800	-0.28462500
C	-4.49094300	4.26097200	-0.79280700
H	-4.72876000	3.33564000	-1.32744300
H	-5.21512900	4.39163000	0.02131400
H	-4.57968200	5.10452900	-1.47813700
C	-2.30536900	6.34340600	-1.33138800
C	-3.13225300	7.31887000	-0.90634400
C	-3.87420500	7.24986200	0.40861700
C	-3.30275900	8.66541600	-1.57211600
H	-3.76129400	6.27117300	0.87974500
H	-2.79460600	8.72715900	-2.53612600
C	-1.47564400	6.44303700	-2.60307800
C	-0.06778100	6.99647400	-2.32157800
C	-1.37743200	5.11624200	-3.37077200
H	-1.96879900	7.15368100	-3.27844900
C	0.72900900	7.17490200	-3.61611800
H	0.46611100	6.30126900	-1.65700100
H	-0.15845000	7.94759800	-1.77810700
C	-0.59114600	5.29706000	-4.67194300
H	-0.88091500	4.36783600	-2.74028700
H	-2.38465800	4.73459500	-3.58099300
C	0.80561200	5.86348600	-4.40226800
H	1.73850700	7.54398700	-3.39529900
H	0.24139900	7.93981200	-4.23694400
H	-0.51572800	4.34140200	-5.20171600
H	-1.13583200	5.98491300	-5.33426200
H	1.34345800	6.01675200	-5.34429100
H	1.38407200	5.13055500	-3.82291400
H	1.60039000	5.53470000	2.82370600
C	-0.95983700	4.64463800	0.06415400
H	-0.00636000	5.15683000	0.08419000
C	-1.90210600	-4.09533200	4.35238400
H	-1.67467300	-4.86317800	3.60539600
H	-1.84098100	-4.55292700	5.34454800
H	-2.93946000	-3.77592900	4.19998000
C	-1.03915000	-2.32084700	2.79351900
H	-0.80361800	-3.09639100	2.05634900
H	-2.04876200	-1.95624300	2.57209200
H	-0.33303000	-1.49772900	2.67354400

C	-5.09301300	-0.36104200	6.99496300
H	-6.07488500	0.12020800	7.05837200
H	-5.22178600	-1.34376800	6.52779000
H	-4.71539300	-0.51837400	8.00962900
C	-4.69562400	0.75994300	4.77646400
H	-4.00303700	1.32537800	4.14602000
H	-4.93994300	-0.17722800	4.26324500
H	-5.62193700	1.33733400	4.86249100
C	-0.36907100	-0.50685000	9.76987000
H	-1.25297600	0.12435700	9.91269000
H	-0.68869000	-1.55172100	9.83033000
H	0.32060500	-0.30823600	10.59698500
C	0.77126500	1.24393800	8.34856700
H	1.32327700	1.43306600	7.42349500
H	-0.08171400	1.93117300	8.39158600
H	1.43120500	1.47850400	9.19070100
C	4.36522700	4.53154900	4.67077100
H	3.96386300	5.28870600	3.98862500
H	3.52526900	3.99509300	5.11288300
H	4.89566500	5.05788600	5.47194700
C	6.57417700	4.35266600	3.50030700
H	7.08096000	4.82063200	4.35112800
H	7.29080000	3.70831800	2.98168000
H	6.28454000	5.14597600	2.80120500
C	1.85697400	3.14183300	-1.27842700
H	2.36767000	2.45118100	-1.95939600
H	1.12645400	2.57389500	-0.69571300
H	1.30591200	3.86202400	-1.89294700
C	3.94493900	4.52406700	-1.26459400
H	3.49799500	5.18011100	-2.02278900
H	4.65233800	5.10732600	-0.66526900
H	4.51518200	3.74717700	-1.78593800
C	3.08802200	-1.31622500	0.87387300
H	3.21120200	-2.39973800	0.77063400
H	2.39293600	-1.12021200	1.69448100
H	2.63665700	-0.94775900	-0.05404800
C	5.38661900	-0.85355600	-0.06784900
H	4.97946100	-0.38034200	-0.96824300
H	6.37119700	-0.41652400	0.12626800
H	5.51736900	-1.92046300	-0.27845800
H	-4.94836000	7.41522900	0.23362100
H	-4.37278200	8.84021900	-1.75816800
C	-3.33158000	8.33731100	1.34526000
H	-3.83598600	8.29508100	2.31890000

H	-2.27073100	8.12261100	1.51751900
C	-2.78318700	9.77742100	-0.64106400
H	-2.93197800	10.75528200	-1.11241900
H	-1.70222500	9.64094200	-0.50025700
C	-3.46847500	9.72664600	0.72492100
H	-3.03835900	10.48238600	1.39244600
H	-4.53377100	9.97109300	0.60724300

(S_a,*R*)-TS1

E = -4183.47039278 a.u.

0 1

P	2.09043600	-0.01196100	4.41603100
O	2.30453300	1.47184000	4.59966400
O	3.44616400	-0.69867200	3.79016900
O	2.15639800	-0.57098100	5.95959300
O	0.94843900	-0.56654400	3.65073100
H	1.73646100	2.46437700	3.71020700
C	6.37654000	-0.66425800	5.98346700
C	5.17383900	-1.06546000	5.39384800
C	4.65851800	-0.33766700	4.32743300
C	5.36001100	0.75459000	3.79113300
C	6.61403100	1.05510400	4.33520500
C	7.12000300	0.37347900	5.43939300
C	6.64753600	-1.47561700	7.23009500
C	5.27398700	-2.11732500	7.49958900
H	7.17683300	1.87903800	3.90577700
H	8.06805300	0.66936900	5.87960300
H	7.41603100	-2.23867100	7.05171100
H	5.32912600	-3.05153900	8.06678300
H	4.64087100	-1.41666500	8.05498700
C	4.66003700	-2.31851400	6.08476400
C	3.19297700	-2.70926300	6.15693600
C	5.25174600	-3.61020900	5.45170800
C	3.08113500	-4.09801700	6.27437000
C	2.04299900	-1.92899000	6.14072900
C	4.43044400	-4.75178800	6.07940100
H	5.07455100	-3.57820700	4.37099400
H	6.32948100	-3.70072200	5.61873800
C	1.84663700	-4.69163400	6.49708900
C	0.77386700	-2.50753000	6.30137500
H	4.37382800	-5.63677600	5.43840200
C	0.71042600	-3.88645800	6.53129500
H	1.75990200	-5.76797300	6.61595800
H	-0.26518600	-4.33601500	6.69058800

H	4.86171300	-5.07358200	7.03602000
H	6.99740600	-0.85498200	8.06060000
C	-0.48497500	-1.71361400	6.14989900
C	-1.39014800	-2.05051000	5.11567600
C	-0.79021900	-0.64949500	7.01855800
C	-2.59393000	-1.35529200	5.01447200
C	-2.00668900	0.02515400	6.86580600
C	-2.92860400	-0.31641200	5.88164600
H	-3.29438900	-1.63910400	4.23103200
H	-2.25086700	0.83382700	7.55407900
C	-1.11279200	-3.14032100	4.08701400
H	-0.07362500	-3.45841300	4.19604600
C	0.12452200	-0.21526700	8.15406900
H	1.02518800	-0.83307600	8.13029600
C	-4.27583900	0.37827500	5.79825800
H	-4.22570600	1.27619900	6.43029800
C	4.77822700	1.62834100	2.72454100
C	4.57656000	3.00572700	2.98935800
C	4.44879800	1.11211500	1.45643800
C	4.10703300	3.82480600	1.96488400
C	3.97602300	1.97893500	0.46388100
C	3.81371900	3.34087700	0.69070800
H	3.95929200	4.88623200	2.16532200
H	3.74563800	1.56584800	-0.51529600
C	4.87771200	3.65687500	4.33595600
H	5.13490300	2.87157000	5.04946500
C	4.62877800	-0.35124700	1.07938100
H	5.00641100	-0.89208900	1.94937600
C	3.43091400	4.32217700	-0.40445900
H	2.78514000	5.08582200	0.05407800
C	0.19721200	5.48202900	2.14662700
C	-0.52575700	4.71857800	3.11907800
C	-1.83645300	5.05363400	3.55953200
C	0.09845400	3.53268700	3.59945800
C	-2.50764700	4.22775200	4.43079600
H	-2.28890800	5.96808600	3.19713600
C	-0.61984400	2.69172600	4.48394800
C	-1.88463700	3.04236800	4.88551600
H	-0.17078000	1.76435700	4.82528600
H	-2.43158700	2.40467800	5.57275300
C	0.21648700	6.96256900	2.16102200
C	0.85465500	7.70565900	1.14039700
C	-0.13757800	7.64976900	3.33319500
C	1.07878500	9.07565400	1.28720100

C	0.10661400	9.00988800	3.49365600
H	-0.54871200	7.08427200	4.16080100
C	0.70833200	9.72238700	2.46469400
H	1.56904700	9.63772300	0.50200700
H	-0.15698800	9.49937600	4.42468400
H	0.90932800	10.78343600	2.57315800
O	1.26367600	7.00912100	0.05110900
C	2.17084100	7.63748200	-0.83577000
H	2.44590600	6.88002000	-1.57072500
H	1.70480100	8.48493600	-1.35051300
H	3.06608200	7.97339000	-0.30030500
O	-3.76539300	4.45217800	4.91571100
C	-4.34040300	5.70021800	4.62471100
H	-4.52016800	5.82715800	3.54699400
H	-5.29402500	5.73323000	5.15163200
H	-3.70033100	6.52405100	4.96845200
O	1.32866200	3.28191500	3.21120600
C	-2.06977500	3.15722400	0.89598700
C	-0.69338300	3.23940500	0.63569900
C	0.11430900	2.13368900	0.90977100
C	-0.47744400	0.99898100	1.45284400
C	-1.84978900	0.96208900	1.74447100
C	-2.67880300	2.04188700	1.46222900
C	-1.71135000	5.20249700	0.01206100
H	1.19048900	2.17355500	0.76372200
H	0.14456800	0.15456800	1.72564200
H	-2.26221900	0.07906500	2.22412500
H	-3.73953200	2.01875000	1.69191500
N	-2.65640500	4.36499800	0.49446400
C	-4.08908800	4.56673000	0.51581100
H	-4.57858200	3.67504000	0.11570800
H	-4.42916800	4.72814200	1.54491200
H	-4.34181700	5.42977300	-0.09913800
C	-2.04478200	6.34523300	-0.87817700
C	-2.68486700	7.45651000	-0.46716500
C	-3.15939700	7.66114000	0.95165000
C	-3.03642100	8.61102200	-1.38073900
H	-2.80060800	6.84979000	1.59000200
H	-2.60678300	8.49220300	-2.37650100
C	-1.71273800	6.06110300	-2.34663200
C	-0.28530200	6.46647300	-2.73807400
C	-1.98604600	4.59832200	-2.74354900
H	-2.39756700	6.66459600	-2.95467600
C	-0.01923700	6.22803000	-4.22650700

H	0.42624100	5.87763800	-2.14590000
H	-0.12492500	7.51946800	-2.47412800
C	-1.73730200	4.38416200	-4.23807600
H	-1.33038100	3.92425100	-2.17569700
H	-3.01868600	4.33069900	-2.48469800
C	-0.30661700	4.77540100	-4.61317000
H	1.01741800	6.49104200	-4.46729000
H	-0.66114300	6.89365000	-4.82064100
H	-1.92872700	3.33869900	-4.50073900
H	-2.44401700	4.99355300	-4.81877900
H	-0.13734500	4.62690800	-5.68481100
H	0.39497600	4.11520700	-4.08419100
H	1.15592500	5.04266700	1.87291000
C	-0.43849500	4.60395400	0.21257300
H	0.44491500	4.94619500	-0.30365700
C	-2.02529000	-4.35407700	4.30927600
H	-1.79559400	-5.14477300	3.58681100
H	-1.92109200	-4.76955400	5.31595100
H	-3.07677400	-4.07313100	4.17646200
C	-1.26540900	-2.62656500	2.65113400
H	-0.96435800	-3.40615000	1.94268000
H	-2.30549200	-2.36381900	2.42239600
H	-0.62703800	-1.75340800	2.50686600
C	-5.37765500	-0.52831600	6.36181600
H	-6.34936700	-0.02271100	6.34368400
H	-5.45761100	-1.44328300	5.76411700
H	-5.15557000	-0.82008200	7.39235600
C	-4.62474400	0.82888100	4.37631000
H	-3.82822400	1.44918300	3.95482400
H	-4.77009700	-0.03311900	3.71451200
H	-5.55366000	1.40940000	4.37661100
C	-0.54928800	-0.44116700	9.51392000
H	-1.44716800	0.17778700	9.62019800
H	-0.84570900	-1.48753500	9.63712200
H	0.13541800	-0.17836400	10.32738600
C	0.55880600	1.24647800	7.99120400
H	1.07838900	1.39816300	7.04082800
H	-0.30528200	1.92098600	8.02951900
H	1.23789600	1.53165100	8.80226500
C	3.67799500	4.40722000	4.92774000
H	3.28605800	5.16580300	4.24045500
H	2.87380300	3.71170900	5.16855000
H	3.98680800	4.91645900	5.84780500
C	6.07774100	4.60703000	4.20792600

H	6.35321600	5.01256200	5.18730400
H	6.95387100	4.10633800	3.78410200
H	5.83323100	5.45147400	3.55255700
C	2.67252400	3.70206000	-1.57962700
H	3.31218000	3.01517000	-2.14437000
H	1.78438200	3.14739900	-1.25727000
H	2.35123600	4.48636800	-2.27771100
C	4.70060800	5.02161800	-0.91537400
H	4.47312500	5.74395300	-1.70853600
H	5.21588700	5.54520300	-0.10447600
H	5.39273900	4.27805600	-1.32534400
C	3.29261800	-0.98903700	0.67906100
H	3.43332800	-2.05183700	0.45381300
H	2.56130400	-0.90414400	1.48788600
H	2.88201000	-0.51204900	-0.21931500
C	5.66940400	-0.50447600	-0.03786300
H	5.33919000	-0.01467700	-0.96081200
H	6.62754500	-0.06264600	0.25332700
H	5.83249400	-1.56373300	-0.26335500
H	-4.26100500	7.60967000	0.94980600
H	-4.13037300	8.63855300	-1.50123400
C	-2.73749300	9.01947600	1.52146700
H	-3.14545200	9.14006000	2.53151200
H	-1.64860000	9.03464900	1.60923600
C	-2.58386800	9.95430100	-0.78692700
H	-2.87511900	10.76609600	-1.46141400
H	-1.48692700	9.96146900	-0.72110800
C	-3.16776300	10.16456700	0.60852100
H	-2.83449100	11.12251400	1.02154700
H	-4.26424200	10.20559600	0.54440400

(S_a,*R*)-Int2

E = -4183.48644319 a.u.

0 1

P	2.06083400	-0.00518800	4.46751600
O	2.27939600	1.46834600	4.68688900
O	3.41821500	-0.68843800	3.82908100
O	2.12612600	-0.60411500	5.99859600
O	0.92908000	-0.55692100	3.68179700
H	1.71075900	2.53885100	3.76720300
C	6.34734400	-0.69214900	6.02211600
C	5.14503300	-1.08410300	5.42565900
C	4.62982500	-0.33913500	4.37049200
C	5.33443600	0.75890500	3.84950400

C	6.58752200	1.05153100	4.39980300
C	7.09137600	0.35402200	5.49506700
C	6.61768000	-1.52254500	7.25633400
C	5.24415700	-2.16870800	7.51487000
H	7.15179900	1.88082400	3.98278100
H	8.03861400	0.64347300	5.94131800
H	7.38654300	-2.28264900	7.06689400
H	5.29916900	-3.11136400	8.06804200
H	4.61024700	-1.47668300	8.08008000
C	4.63117200	-2.34856000	6.09669600
C	3.16465100	-2.74230300	6.16285400
C	5.22370400	-3.63067600	5.44501700
C	3.05329200	-4.13250000	6.26130800
C	2.01450900	-1.96248700	6.15745800
C	4.40327300	-4.78218000	6.05616200
H	5.04623800	-3.58301900	4.36490000
H	6.30156800	-3.72309200	5.61047900
C	1.81901300	-4.72955400	6.47717000
C	0.74557000	-2.54381000	6.31215400
H	4.34734800	-5.65775800	5.40218800
C	0.68193100	-3.92545200	6.52335500
H	1.73289900	-5.80751000	6.58131600
H	-0.29357300	-4.37826700	6.67541600
H	4.83539500	-5.11771800	7.00769200
H	6.96672400	-0.91462900	8.09657400
C	-0.50487300	-1.73712000	6.16236900
C	-1.40352100	-2.04864800	5.11483700
C	-0.79587600	-0.66887200	7.03078400
C	-2.58309100	-1.31678100	4.99365700
C	-1.98687900	0.04455900	6.85636200
C	-2.89793800	-0.26472700	5.85275600
H	-3.27998400	-1.57865500	4.19875000
H	-2.21934100	0.85830000	7.54241800
C	-1.14252000	-3.15004700	4.09424600
H	-0.11524700	-3.49828500	4.22000600
C	0.10471500	-0.27419300	8.19203100
H	0.99276000	-0.91045000	8.17448200
C	-4.21182900	0.48403100	5.72836700
H	-4.16994500	1.34238400	6.41283000
C	4.75878600	1.64317900	2.78750900
C	4.55787400	3.01852900	3.06102800
C	4.44014100	1.13821400	1.51139600
C	4.09976100	3.84784100	2.03869200
C	3.97951800	2.01427500	0.52156300

C	3.81720000	3.37539500	0.75818900
H	3.94949300	4.90694100	2.24791000
H	3.75909700	1.60993900	-0.46393600
C	4.85026100	3.65744300	4.41526900
H	5.09938100	2.86473900	5.12346200
C	4.62026300	-0.32282800	1.12470300
H	4.99633500	-0.86938700	1.99183500
C	3.44425900	4.36420400	-0.33419400
H	2.83526500	5.15317800	0.12998300
C	0.15029700	5.36227100	1.84940700
C	-0.54565000	4.71642600	3.03373100
C	-1.83451500	5.08465300	3.45179600
C	0.09951400	3.64023900	3.66055100
C	-2.48767700	4.38122700	4.45531600
H	-2.29545900	5.95903100	3.00985900
C	-0.57749100	2.91775800	4.66260200
C	-1.84813300	3.28963100	5.05477200
H	-0.08908100	2.06103400	5.11694700
H	-2.36708500	2.74027100	5.83446400
C	0.29042500	6.88156300	1.95063000
C	0.88668300	7.64908700	0.92822200
C	0.04102000	7.53646700	3.16081200
C	1.14002800	9.01144100	1.09553500
C	0.31763700	8.89074300	3.35026100
H	-0.34630300	6.96157000	3.99262900
C	0.85364500	9.63304000	2.30991000
H	1.59092700	9.58617600	0.29554900
H	0.11726400	9.34990400	4.31229500
H	1.07144100	10.68903100	2.43421300
O	1.24415500	6.98137500	-0.20724000
C	2.14439200	7.61829500	-1.09083400
H	2.41422100	6.87199500	-1.83982300
H	1.67950600	8.47630400	-1.59125000
H	3.04574000	7.94444800	-0.55948900
O	-3.74388200	4.68025100	4.91999900
C	-4.32119500	5.87340100	4.46405500
H	-4.52893800	5.84409800	3.38287300
H	-5.26316800	5.98930700	5.00114600
H	-3.67510300	6.73922500	4.66571600
O	1.32719500	3.32078700	3.24169900
C	-2.02589300	3.09666300	0.90883100
C	-0.65567900	3.26651500	0.72220300
C	0.19802600	2.20613500	0.97954500
C	-0.35919800	1.01918500	1.46581400

C	-1.72938400	0.90484100	1.71102800
C	-2.60734700	1.94766500	1.41190300
C	-1.80722000	5.21184600	0.13316300
H	1.27499200	2.30537600	0.88553500
H	0.29445400	0.19897600	1.74070300
H	-2.11149100	-0.00684100	2.15897500
H	-3.67383800	1.86280800	1.59371000
N	-2.67205300	4.30423400	0.51100300
C	-4.12125100	4.39932000	0.46249400
H	-4.51185100	3.54793100	-0.09961100
H	-4.49674800	4.35953900	1.48952600
H	-4.40537800	5.33678100	-0.01323000
C	-2.15277400	6.32152700	-0.78873900
C	-2.76975300	7.45996700	-0.43011500
C	-3.23820400	7.75386600	0.97123700
C	-3.04447300	8.59465700	-1.38910800
H	-2.99128000	6.92779800	1.64179800
H	-2.67088800	8.38891900	-2.39385700
C	-1.82512000	5.95926700	-2.24816900
C	-0.46001100	6.46947200	-2.72869400
C	-1.96027500	4.45499000	-2.55204200
H	-2.59264300	6.45572100	-2.85624700
C	-0.26416000	6.20207500	-4.22266200
H	0.32825200	5.95589900	-2.16667100
H	-0.36461400	7.53807800	-2.49879100
C	-1.76688400	4.18641500	-4.04667500
H	-1.20867400	3.88070200	-1.98947300
H	-2.94475800	4.09026700	-2.23116700
C	-0.41482700	4.71137100	-4.53312900
H	0.72174200	6.56139600	-4.53839400
H	-1.00867900	6.77150300	-4.79676000
H	-1.85457600	3.11330400	-4.24359400
H	-2.57146900	4.68104700	-4.60844500
H	-0.30130900	4.53095400	-5.60694000
H	0.38806400	4.15545300	-4.02919400
H	1.17152900	4.95935800	1.84130200
C	-0.42170800	4.73436000	0.46720500
H	0.28683300	4.98648100	-0.32093100
C	-2.09230000	-4.33564700	4.31123300
H	-1.87552600	-5.13893300	3.59858100
H	-2.01356300	-4.74459900	5.32304000
H	-3.13352000	-4.02578700	4.16227700
C	-1.25568000	-2.64180000	2.65303900
H	-0.96804700	-3.43504600	1.95408300

H	-2.28413300	-2.34986900	2.40625600
H	-0.58724100	-1.78950200	2.51562200
C	-5.38434300	-0.40471400	6.16116100
H	-6.33162400	0.14335300	6.10948500
H	-5.46121500	-1.27976100	5.50592000
H	-5.24596600	-0.76490400	7.18465200
C	-4.43816000	1.02887800	4.31458300
H	-3.58868800	1.63989400	3.99633700
H	-4.56032700	0.20875100	3.59567900
H	-5.34444900	1.64425900	4.28024300
C	-0.60447700	-0.51506700	9.53143600
H	-1.49271400	0.11913900	9.62901400
H	-0.92380400	-1.55774200	9.62592300
H	0.06571700	-0.28223500	10.36592600
C	0.57335600	1.18098800	8.07268400
H	1.12120700	1.34134700	7.13980600
H	-0.27608800	1.87418400	8.10511800
H	1.23690900	1.43307800	8.90735200
C	3.64988000	4.40824400	5.00540000
H	3.26232600	5.17135000	4.32104600
H	2.84226000	3.71436700	5.23903200
H	3.95747400	4.91069600	5.92967200
C	6.05494400	4.60396700	4.30302300
H	6.32596200	4.99900300	5.28791600
H	6.93195600	4.10431700	3.87956200
H	5.81712000	5.45574900	3.65471800
C	2.63497600	3.76387600	-1.48641100
H	3.23686600	3.06017800	-2.07173200
H	1.74426700	3.23015000	-1.13650400
H	2.31147500	4.55646300	-2.17427400
C	4.72419600	5.01560400	-0.88079800
H	4.50091300	5.74727300	-1.66656400
H	5.27849700	5.51958100	-0.08355600
H	5.37814300	4.24782500	-1.30874600
C	3.28426300	-0.95791200	0.71993300
H	3.42665800	-2.01601100	0.47411500
H	2.55965400	-0.89081800	1.53639800
H	2.86690800	-0.46514800	-0.16703500
C	5.66173700	-0.47034000	0.00751700
H	5.33168000	0.02199500	-0.91419900
H	6.61882700	-0.02782500	0.30098100
H	5.82693900	-1.52854000	-0.22155200
H	-4.33715000	7.83388700	0.94748300
H	-4.13266200	8.73603900	-1.46586000

C	-2.65527700	9.07134900	1.49811600
H	-3.05080700	9.27737700	2.49858000
H	-1.57336400	8.95419500	1.59497600
C	-2.42013800	9.89656900	-0.85650700
H	-2.62853700	10.71257400	-1.55587800
H	-1.32923600	9.77187200	-0.81095600
C	-2.94416200	10.22614700	0.54093300
H	-2.47793500	11.14440800	0.91287600
H	-4.02613500	10.41240700	0.48977900

(R_a,*R*)-Int1

E = -4183.49112746 a.u.

0 1

P	-0.14360400	-0.94344000	0.64545700
O	0.57958900	-0.29668400	1.74941500
O	-0.37916600	-2.53875700	0.76594500
O	-1.65098700	-0.34320900	0.54847600
O	0.45766300	-0.88217100	-0.80685100
H	0.78099400	0.05877700	-0.96926000
C	-2.73549300	-3.15119600	3.51405400
C	-2.24272600	-2.91221200	2.22768600
C	-0.87516700	-2.94071200	2.00574200
C	0.01857500	-3.34072300	3.00620100
C	-0.51853200	-3.67619100	4.25394800
C	-1.87838000	-3.54642100	4.53071900
C	-4.22659000	-2.89713800	3.55642000
C	-4.47668500	-2.16651100	2.22111800
H	0.16145000	-4.01320500	5.02957300
H	-2.25547100	-3.75214800	5.52838700
H	-4.78940800	-3.83754000	3.60844400
H	-5.49170100	-2.29802700	1.83384300
H	-4.29302400	-1.09326900	2.34354300
C	-3.39913100	-2.74591600	1.26441100
C	-3.29382600	-1.98454800	-0.04342400
C	-3.86357300	-4.13630500	0.73904300
C	-4.15764000	-2.54715800	-0.98907000
C	-2.52792600	-0.87749000	-0.38814000
C	-4.78411900	-3.81031600	-0.44754400
H	-2.98293300	-4.68244500	0.38236800
H	-4.34227900	-4.73548000	1.51910900
C	-4.32427900	-1.96139200	-2.23466000
C	-2.65051200	-0.28092600	-1.65114500
H	-4.82128800	-4.61113600	-1.19180400
C	-3.58437900	-0.82444100	-2.54202100

H	-5.00923800	-2.38609000	-2.96277600
H	-3.70689000	-0.34190200	-3.50669900
H	-5.81419400	-3.62836600	-0.11518200
H	-4.51936300	-2.30033000	4.42536900
C	-1.85533700	0.90397800	-2.09706700
C	-0.99107300	0.79093600	-3.20813200
C	-2.06510600	2.16233400	-1.49871300
C	-0.40642100	1.94709500	-3.73187400
C	-1.45996900	3.28588400	-2.06174800
C	-0.64789800	3.20658500	-3.18997100
H	0.23935300	1.85773500	-4.60237700
H	-1.64204400	4.26608200	-1.62011100
C	-0.69107400	-0.53754400	-3.89474600
H	-1.12039400	-1.34232100	-3.29145700
C	-2.96424800	2.36143500	-0.28876700
H	-3.32230100	1.38668000	0.04814100
C	-0.12895600	4.48077200	-3.82614400
H	-0.04658200	5.22382800	-3.02246600
C	1.48931300	-3.41306300	2.76217700
C	2.36809000	-2.61856500	3.52581900
C	2.00459300	-4.30466300	1.79638400
C	3.74381900	-2.76477400	3.33105700
C	3.38514700	-4.39261300	1.62563000
C	4.27412800	-3.63388500	2.38387800
H	4.42916300	-2.16637700	3.92840100
H	3.77707300	-5.08195000	0.87994200
C	1.89121000	-1.58988300	4.54226800
H	0.81643500	-1.44064200	4.40568200
C	1.12613900	-5.21146400	0.94570400
H	0.07810900	-5.01241700	1.18292500
C	5.77188700	-3.74733400	2.18013600
H	6.24623600	-2.99899800	2.82923300
C	0.17062600	8.44848400	0.27010000
C	0.77617100	8.04608500	-0.91779700
C	1.10572100	6.70807700	-1.09105100
C	0.83202300	5.75460100	-0.09801600
C	0.18903800	6.17940000	1.09094200
C	-0.12439800	7.52855600	1.27351600
H	-0.08543200	9.49263600	0.42173300
H	0.98250000	8.76528200	-1.70241800
H	1.55573300	6.37545400	-2.02183100
H	-0.59628500	7.86250800	2.18948700
C	1.09085100	4.33726800	-0.28796200
H	0.36855300	3.64912700	0.14583100

C	2.11813700	3.77417300	-0.98990100
C	2.01384200	2.32158600	-1.27194200
C	3.30295800	4.48685200	-1.41539300
C	3.01920200	1.75428700	-2.16716400
C	4.25791300	3.86457600	-2.14156900
C	4.08141600	2.49164400	-2.56703800
H	2.89595300	0.71699100	-2.46102900
H	4.84311600	2.06169700	-3.21298800
O	5.41716100	4.51406600	-2.47907300
C	6.53992500	4.03018000	-1.75603400
H	6.72788600	2.96958000	-1.96765100
H	7.39890300	4.62213000	-2.07444200
H	6.38180000	4.15184500	-0.67601000
O	-0.05784800	5.21611900	1.99618900
C	-0.83515900	5.53976300	3.13675900
H	-1.03483200	4.59492700	3.64180200
H	-0.27751700	6.20376600	3.80790000
H	-1.77750800	6.01488000	2.83914700
O	1.10336000	1.63396500	-0.78862000
C	2.89330500	3.62040100	2.98354900
C	1.89344400	2.78565000	2.54113300
N	2.56910100	4.06155300	4.27085000
H	1.83611100	2.28324800	1.58544700
C	3.40321600	4.79260700	5.19607500
H	4.39044000	4.93507900	4.75686600
H	2.97151500	5.77429400	5.42457000
H	3.50771100	4.22781200	6.12870900
C	4.19513000	4.00019000	2.37094500
C	4.52247200	5.29746200	2.18181300
C	3.56708400	6.43589200	2.48608700
C	5.89207400	5.79496600	1.76258400
C	3.54035900	7.50381200	1.38426900
H	3.89782500	6.92278900	3.41850800
H	2.55494300	6.05677200	2.66210500
C	5.83461500	6.83609900	0.63636400
H	6.34715900	6.28169600	2.64080700
H	6.56483300	4.98368300	1.48267200
C	4.93810700	8.00735300	1.03312400
H	2.89361500	8.33160600	1.69576900
H	3.08229300	7.07568700	0.48676300
H	6.84892600	7.18397500	0.40978400
H	5.44877600	6.36677100	-0.27964600
H	4.88485100	8.74444200	0.22441900
H	5.37723800	8.51672100	1.90291400

C	5.14234500	2.83527000	2.12873300
C	5.38427000	2.03120200	3.41630600
C	4.67533500	1.89765200	1.00547500
H	6.11491800	3.22950000	1.81215800
C	6.38105800	0.89209700	3.18362800
H	4.42509900	1.62332700	3.75772200
H	5.75204000	2.69770200	4.20752500
C	5.71606700	0.80785800	0.74501900
H	3.72888300	1.41866800	1.28648100
H	4.49127000	2.48757200	0.10214300
C	5.96282900	-0.00733900	2.01662800
H	6.48809900	0.29669400	4.09850500
H	7.37126500	1.31934000	2.96857000
H	5.38034200	0.15438100	-0.06915400
H	6.65915400	1.27158100	0.41723200
H	6.73046900	-0.77038700	1.84044900
H	5.03628800	-0.53926400	2.27629400
C	0.90893100	2.69742000	3.57759600
C	1.36426600	3.51332900	4.63888300
C	-0.29235000	1.98614400	3.73278900
C	0.64856600	3.66445300	5.83236100
C	-1.00899100	2.13721200	4.91059000
H	-0.62268000	1.30486100	2.95614900
C	-0.54746400	2.97280100	5.94778400
H	1.01261800	4.29796700	6.63599700
H	-1.93624900	1.58884200	5.04591900
H	-1.13116400	3.06583400	6.85863100
H	3.46194800	5.50896500	-1.08882800
C	-4.19541000	3.20123900	-0.64899700
H	-4.77101500	2.72868100	-1.45112800
H	-4.84867800	3.31647500	0.22250600
H	-3.90493100	4.20231700	-0.98638300
C	-2.17861200	2.99010300	0.86617300
H	-1.26053300	2.42636800	1.06283800
H	-1.90037700	4.02613600	0.63727700
H	-2.77384100	3.00176400	1.78649600
C	-1.15357200	5.00770900	-4.84088500
H	-0.81661700	5.95206700	-5.28208800
H	-1.28978500	4.28077400	-5.64944900
H	-2.12667800	5.17199400	-4.36878300
C	1.24303500	4.33054900	-4.48382700
H	1.18184900	3.71856300	-5.39071000
H	1.63253300	5.31030600	-4.78049900
H	1.96566200	3.86284600	-3.80905000

C	-1.32254600	-0.58429400	-5.29360100
H	-2.40111200	-0.40740800	-5.26204600
H	-0.88090300	0.18206300	-5.94075600
H	-1.14918200	-1.55953200	-5.76048500
C	0.81398600	-0.81278600	-4.00727400
H	0.97947100	-1.76429800	-4.52367400
H	1.32697200	-0.03227000	-4.58035000
H	1.27399000	-0.88753700	-3.01979700
C	2.56107500	-0.23043800	4.32003000
H	3.63438800	-0.27890800	4.54230100
H	2.42009300	0.10373800	3.28843000
H	2.11801300	0.52214000	4.98255600
C	2.15336900	-2.06409300	5.97825100
H	1.78683800	-1.32309400	6.69649800
H	1.67057500	-3.02106800	6.19696300
H	3.22919000	-2.19267200	6.14608100
C	6.28611300	-5.13055300	2.59544300
H	7.37336700	-5.19330600	2.47889000
H	6.03560400	-5.34650100	3.63808200
H	5.83467700	-5.91140900	1.97320000
C	6.16602900	-3.43515000	0.73225600
H	7.25589600	-3.42602500	0.62141100
H	5.76745400	-4.19223800	0.04797800
H	5.77550900	-2.46206500	0.41872400
C	1.32138200	-4.93912100	-0.55056000
H	1.13995600	-3.88637200	-0.78198600
H	2.33914300	-5.19336500	-0.86748300
H	0.62886200	-5.54967200	-1.14024000
C	1.38911300	-6.68677200	1.27439900
H	2.42192200	-6.96565000	1.03832800
H	1.22140100	-6.88834700	2.33687200
H	0.72543000	-7.33364700	0.69063600

(R_a,*R*)-TS1

E = -4183.46963055 a.u.

0 1

P	-0.33000700	-1.05960000	0.62880400
O	0.17254500	-0.48499600	1.90165600
O	-0.44494100	-2.69758400	0.65613100
O	-1.92371200	-0.63743900	0.55484100
O	0.32725300	-0.75239800	-0.70010100
H	0.61766000	0.66871400	-0.61469800
C	-2.83975500	-3.71608700	3.23433300
C	-2.32268800	-3.34646200	1.98865000

C	-0.95086500	-3.20970600	1.83301900
C	-0.06630400	-3.56658800	2.86080700
C	-0.61249500	-4.02082900	4.06487800
C	-1.99083700	-4.06352600	4.27539600
C	-4.35062500	-3.63450600	3.21589200
C	-4.62103800	-2.83349700	1.92644500
H	0.06591500	-4.32347300	4.85684900
H	-2.38839500	-4.36503200	5.24047300
H	-4.80233100	-4.63353900	3.16574700
H	-5.60066300	-3.03609600	1.48204400
H	-4.55485300	-1.76004300	2.13579000
C	-3.45043900	-3.22136100	0.98105800
C	-3.37924200	-2.33787700	-0.25131300
C	-3.75531200	-4.59453300	0.31421700
C	-4.15556600	-2.88326500	-1.27681100
C	-2.70655500	-1.13851800	-0.45606000
C	-4.66410300	-4.25000500	-0.87923400
H	-2.81239400	-5.01692400	-0.05130700
H	-4.19944700	-5.30838200	1.01482500
C	-4.34292500	-2.19142700	-2.46558000
C	-2.84839800	-0.43382600	-1.66202100
H	-4.59091600	-4.97697200	-1.69373500
C	-3.70348700	-0.96631400	-2.63481300
H	-4.96139300	-2.60259000	-3.25837500
H	-3.83376000	-0.41183000	-3.56000400
H	-5.71872700	-4.20793700	-0.57740300
H	-4.75137100	-3.14632600	4.10956600
C	-2.09909000	0.82786900	-1.95305700
C	-1.17856000	0.85790800	-3.02370200
C	-2.33666200	2.00101100	-1.20914900
C	-0.55385300	2.06425600	-3.35120200
C	-1.67918400	3.17817000	-1.57006500
C	-0.79749800	3.23972300	-2.64634700
H	0.14572500	2.07638600	-4.18339400
H	-1.86214100	4.08658900	-0.99384200
C	-0.84810400	-0.36693300	-3.86965000
H	-1.34336600	-1.23477000	-3.42862800
C	-3.29426500	2.04707200	-0.02823600
H	-3.76599100	1.06646300	0.07621600
C	-0.18222200	4.57309600	-3.03133600
H	0.05554800	5.09783900	-2.09598600
C	1.41459100	-3.49576600	2.66896000
C	2.19932300	-2.64249600	3.47032900
C	2.03944700	-4.32601900	1.71265700

C	3.59055400	-2.68724400	3.34299300
C	3.42965400	-4.31594500	1.60995300
C	4.22670900	-3.51628700	2.42572700
H	4.20225000	-2.04573200	3.97609800
H	3.90415900	-4.96130900	0.87256700
C	1.59868100	-1.65534000	4.46103200
H	0.52532200	-1.59010500	4.26473500
C	1.26935300	-5.25627300	0.78605900
H	0.20209300	-5.15996100	0.99791300
C	5.73766200	-3.54024900	2.30618300
H	6.13441700	-2.84315400	3.05630700
C	0.36115900	8.34834900	0.72184000
C	1.24599700	7.91310700	-0.26110900
C	1.54765600	6.56244400	-0.35545000
C	0.99073000	5.61096800	0.51730900
C	-0.00117200	6.06783700	1.42881700
C	-0.27472400	7.43344900	1.55356900
H	0.12926600	9.40430000	0.82039500
H	1.68892700	8.61663000	-0.95754600
H	2.18508300	6.22176300	-1.16132700
H	-1.00355200	7.77954900	2.27541400
C	1.24581600	4.17814600	0.39888300
H	0.40158500	3.55144600	0.67800500
C	2.15016700	3.55941800	-0.53100500
C	1.83217600	2.21451900	-0.89248700
C	3.36758100	4.11465200	-0.97887400
C	2.69336300	1.52171100	-1.76616100
C	4.20746700	3.41423100	-1.82031700
C	3.85592100	2.11276600	-2.22718700
H	2.44018900	0.50299200	-2.03904700
H	4.50591900	1.54379600	-2.88277200
O	5.38118800	4.03355800	-2.15541300
C	6.33917200	3.27062100	-2.85420700
H	5.97881400	2.98665000	-3.85031400
H	7.21673800	3.90870800	-2.95942200
H	6.61116600	2.36512800	-2.29654500
O	-0.66320400	5.12335100	2.11503200
C	-1.79600900	5.50702300	2.87509800
H	-2.22687200	4.57723200	3.24215400
H	-1.50094300	6.13175800	3.72490800
H	-2.51938600	6.03857400	2.24573800
O	0.76842400	1.67170400	-0.35825400
C	3.07715900	4.23626600	2.69394300
C	2.15134000	3.24956400	2.28188400

N	2.55864800	4.88365000	3.77584000
H	2.40142700	2.40339100	1.65987700
C	3.20026900	5.91008600	4.57170200
H	4.27025600	5.90574100	4.36332900
H	2.78922300	6.89878100	4.34440100
H	3.03875200	5.68428600	5.62836600
C	4.48902800	4.38627100	2.27081700
C	5.03119400	5.55489500	1.86153700
C	4.26186300	6.85769300	1.76875100
C	6.49985800	5.69938600	1.51290600
C	4.55407900	7.65896200	0.48957000
H	4.57198600	7.48692200	2.61902500
H	3.18360300	6.68982200	1.87005100
C	6.72800800	6.47508600	0.20860500
H	6.98709000	6.25272400	2.33188100
H	6.99707400	4.73183700	1.44341500
C	6.05172800	7.84161200	0.26349000
H	4.03853300	8.62340600	0.55224000
H	4.13527100	7.13928600	-0.37978600
H	7.80490400	6.57980100	0.03908200
H	6.32135100	5.89386200	-0.62996200
H	6.22891100	8.39861700	-0.66244700
H	6.48345200	8.43352700	1.08298300
C	5.31477400	3.10253800	2.42046800
C	4.89061400	2.21971000	3.60756400
C	5.37456000	2.28827800	1.11791300
H	6.34140200	3.41255600	2.65096200
C	5.83613400	1.02497900	3.75034100
H	3.87247800	1.83995400	3.46524100
H	4.88105900	2.81749900	4.52884100
C	6.27727300	1.06155600	1.26781500
H	4.36251200	1.96594100	0.83211100
H	5.73280300	2.93518200	0.30675800
C	5.86564000	0.19897000	2.46285900
H	5.52302100	0.40163600	4.59566700
H	6.85075800	1.38253400	3.97819100
H	6.25648000	0.47107100	0.34427200
H	7.31533500	1.39681000	1.40856800
H	6.55637900	-0.64489900	2.56991800
H	4.86783600	-0.22897800	2.28454800
C	1.11261500	3.21087400	3.28300900
C	1.36053100	4.27573600	4.16292700
C	0.03443500	2.34962100	3.49961400
C	0.52574600	4.56412000	5.24031300

C	-0.78636800	2.61076600	4.59126500
H	-0.11047000	1.47482800	2.86614100
C	-0.55240700	3.70708400	5.43951600
H	0.70977800	5.40030100	5.90780800
H	-1.61865100	1.94555700	4.79941700
H	-1.21812900	3.88295600	6.27905000
H	3.71385400	5.07038200	-0.60565600
C	-4.41180700	3.07332000	-0.25114000
H	-4.95451600	2.87238500	-1.17987000
H	-5.12634900	3.04412900	0.57869300
H	-4.01132900	4.09199400	-0.30971100
C	-2.52847500	2.33778400	1.26598800
H	-1.77047300	1.57123100	1.43846200
H	-2.02768500	3.31172000	1.21174800
H	-3.20985200	2.35143200	2.12660800
C	-1.20851200	5.42686800	-3.78947300
H	-0.79486500	6.41210500	-4.03240000
H	-1.49048500	4.93193500	-4.72546000
H	-2.11813700	5.56891200	-3.19843600
C	1.10682300	4.45028000	-3.84342000
H	0.89969800	4.08399100	-4.85553300
H	1.58647200	5.43020600	-3.94351700
H	1.81729300	3.76334900	-3.37320300
C	-1.36887000	-0.19049400	-5.30274300
H	-2.44163800	0.02535200	-5.32220800
H	-0.85653600	0.63997100	-5.80220200
H	-1.19012000	-1.09707400	-5.89072300
C	0.65206400	-0.68124800	-3.88559800
H	0.84396100	-1.54336800	-4.53420400
H	1.23928500	0.16069300	-4.27199100
H	0.98713300	-0.92554400	-2.87529100
C	2.17432200	-0.24749800	4.26488800
H	3.23683600	-0.20856400	4.53611900
H	2.05126400	0.06370800	3.22352100
H	1.64614200	0.46849600	4.90486400
C	1.82453500	-2.11065600	5.90873300
H	1.37833300	-1.39685500	6.60998300
H	1.39015200	-3.09561000	6.10255700
H	2.89705100	-2.17294500	6.12866400
C	6.30519900	-4.93081000	2.61204100
H	7.39959100	-4.92344800	2.56523500
H	6.00228700	-5.26818700	3.60743000
H	5.94309300	-5.66555800	1.88463100
C	6.19320500	-3.06201600	0.92282700

H	7.28633900	-3.00505500	0.86969900
H	5.85387400	-3.75470700	0.14472100
H	5.77968800	-2.07517600	0.69230300
C	1.48574300	-4.87256300	-0.68302500
H	1.21552600	-3.82721500	-0.85339100
H	2.53259900	-5.01624200	-0.97526600
H	0.86975100	-5.50315600	-1.33376300
C	1.64763000	-6.72173400	1.03569800
H	2.70491200	-6.90314200	0.81272300
H	1.47148600	-7.00111200	2.07913300
H	1.05362200	-7.38350200	0.39614600

(R_a,*R*)-Int2

E = -4183.48853223 a.u.

0 1

P	-0.31159200	-1.10086300	0.56886500
O	0.20695200	-0.51574200	1.83412600
O	-0.46152100	-2.74024200	0.65995300
O	-1.90703700	-0.65977400	0.52228600
O	0.32877200	-0.85196200	-0.76957600
H	0.75019500	0.67236600	-0.69848200
C	-2.86187000	-3.66025600	3.26562100
C	-2.34018400	-3.32881400	2.01144400
C	-0.96756900	-3.20216900	1.85269100
C	-0.08682700	-3.52566100	2.89595400
C	-0.63727700	-3.94092200	4.11208700
C	-2.01655500	-3.97754100	4.31941100
C	-4.37257400	-3.57757300	3.23858800
C	-4.63555800	-2.80681300	1.92936600
H	0.03787300	-4.22044400	4.91538900
H	-2.41734200	-4.25104500	5.29155300
H	-4.82445900	-4.57741800	3.20859400
H	-5.61456300	-3.01604300	1.48663100
H	-4.56620700	-1.72881000	2.11344900
C	-3.46305800	-3.22011700	0.99660400
C	-3.38294400	-2.35836400	-0.25077500
C	-3.77362700	-4.60267500	0.35316500
C	-4.16100800	-2.91571000	-1.26864000
C	-2.70354600	-1.16627900	-0.47394700
C	-4.67640700	-4.27386400	-0.84971700
H	-2.83174500	-5.03644000	-0.00148000
H	-4.22459300	-5.30182000	1.06440300
C	-4.34316000	-2.24161400	-2.46831800
C	-2.84786900	-0.47534800	-1.68784900

H	-4.60286100	-5.01491400	-1.65146100
C	-3.70209300	-1.01899300	-2.65427000
H	-4.96072000	-2.66340200	-3.25630100
H	-3.83312300	-0.47623500	-3.58618600
H	-5.73211200	-4.22316600	-0.55271400
H	-4.77814900	-3.06923900	4.11888700
C	-2.10263900	0.78994900	-1.97062400
C	-1.15860600	0.82955800	-3.01894100
C	-2.35994600	1.95654200	-1.22231900
C	-0.51852200	2.03658700	-3.31441700
C	-1.67764700	3.12974800	-1.54190700
C	-0.76320500	3.19956600	-2.59087800
H	0.20113900	2.05710300	-4.12882300
H	-1.86698600	4.03096100	-0.95637200
C	-0.82657400	-0.38502400	-3.87803900
H	-1.31009200	-1.25987700	-3.43711900
C	-3.39102400	2.00867900	-0.10356100
H	-3.87856300	1.03208700	-0.03444700
C	-0.11070100	4.53274600	-2.91071900
H	0.19097500	4.97293400	-1.95135600
C	1.39475600	-3.45712900	2.70627100
C	2.17652000	-2.57888600	3.48374600
C	2.02446700	-4.30807000	1.77162300
C	3.56764500	-2.61826300	3.35551400
C	3.41465900	-4.29122700	1.66564100
C	4.20804600	-3.46523900	2.45782700
H	4.17737300	-1.95799700	3.97125300
H	3.89148200	-4.95115600	0.94283300
C	1.57264700	-1.56907600	4.44998100
H	0.50009600	-1.50787900	4.24754500
C	1.26021300	-5.26724600	0.87015300
H	0.19238500	-5.16988200	1.07781100
C	5.71858500	-3.47564700	2.33075800
H	6.11229300	-2.76708700	3.07218100
C	0.27790200	8.23680800	0.59457400
C	1.21436600	7.78328800	-0.32000900
C	1.59139200	6.43931400	-0.31367700
C	1.07088800	5.51687900	0.59498300
C	0.02708000	5.98449100	1.43009800
C	-0.33142100	7.33300200	1.46187800
H	-0.01618200	9.28139700	0.61666700
H	1.65367600	8.45918100	-1.04635700
H	2.28072100	6.09873700	-1.07399400
H	-1.11038200	7.67427600	2.13256200

C	1.43169700	4.03316700	0.59759000
H	0.48370500	3.48714600	0.52788500
C	2.30728200	3.50404200	-0.52048700
C	1.97964200	2.19801600	-0.95989200
C	3.48601900	4.08514600	-0.97510200
C	2.80498400	1.55776500	-1.88578400
C	4.30873900	3.44012900	-1.89948400
C	3.96357400	2.17425800	-2.36267300
H	2.54290700	0.55636100	-2.21110900
H	4.58673200	1.64357400	-3.07338700
O	5.45902900	4.11315700	-2.22908300
C	6.35653700	3.44857400	-3.08651600
H	5.90163400	3.24739000	-4.06424200
H	7.20918100	4.11574400	-3.21610100
H	6.69712000	2.50063300	-2.64958100
O	-0.62224500	5.04059400	2.15165800
C	-1.74522600	5.41817500	2.91854300
H	-2.14027600	4.49202900	3.33514500
H	-1.45719800	6.09401300	3.73357700
H	-2.50649700	5.89696400	2.29121100
O	0.91428800	1.62456200	-0.39936000
C	3.06436500	4.31372100	2.62180500
C	2.05394400	3.42207900	1.95372500
N	2.59162800	4.70327600	3.78382000
H	2.52112200	2.48576000	1.63306400
C	3.25317900	5.57265900	4.74526700
H	4.28175300	5.73659900	4.42863300
H	2.71854300	6.52476700	4.79313900
H	3.23019500	5.08641900	5.72264500
C	4.47705800	4.50465400	2.23279600
C	5.01129000	5.69613000	1.90264400
C	4.22464700	6.98910600	1.86931400
C	6.47579000	5.86251000	1.55897500
C	4.48631000	7.80992100	0.59549200
H	4.54996600	7.59569200	2.73066600
H	3.14870600	6.81027800	1.98237400
C	6.67735300	6.66048200	0.26264600
H	6.95507900	6.41418700	2.38298300
H	6.98377100	4.90105900	1.47569400
C	5.97833500	8.01486000	0.34824100
H	3.95552600	8.76444200	0.67306400
H	4.05983700	7.28474100	-0.26579500
H	7.75045900	6.78559200	0.08519800
H	6.27440800	6.08326200	-0.58055100

H	6.13047800	8.58437800	-0.57421800
H	6.41696500	8.60418600	1.16596800
C	5.28435400	3.20363800	2.37954200
C	4.80958800	2.32360800	3.55326000
C	5.39472300	2.39128900	1.07895600
H	6.30090700	3.51576400	2.64981200
C	5.73908600	1.12041400	3.72792600
H	3.79070800	1.94874300	3.38256100
H	4.78091900	2.91756200	4.47755600
C	6.28790700	1.16316000	1.27102300
H	4.40068100	2.06513300	0.74295400
H	5.78824800	3.03612100	0.28401300
C	5.81451300	0.29803700	2.44078700
H	5.39135700	0.50066100	4.56153700
H	6.74479200	1.47629500	3.99390500
H	6.30603600	0.57919400	0.34427900
H	7.31975600	1.49218700	1.46224100
H	6.49113800	-0.55266900	2.57695500
H	4.82166100	-0.12054200	2.21846100
C	1.07800000	3.17101400	3.05855500
C	1.37551500	4.02436400	4.11081400
C	0.04211500	2.25993400	3.16071700
C	0.63385900	4.08433000	5.28000300
C	-0.71164000	2.28296300	4.33710100
H	-0.12084900	1.50905300	2.38917000
C	-0.43528700	3.18904100	5.36747600
H	0.87002300	4.76381400	6.09237700
H	-1.51680900	1.56462200	4.45682900
H	-1.04339000	3.18140600	6.26619100
H	3.84400300	5.02825600	-0.57739600
C	-4.48120700	3.04430800	-0.40812300
H	-4.94817400	2.85176900	-1.37879600
H	-5.26043100	3.01606700	0.36147400
H	-4.06954000	4.05988800	-0.42951400
C	-2.72584600	2.29129500	1.24700200
H	-2.05520300	1.46993100	1.50507700
H	-2.14210600	3.21991300	1.21344500
H	-3.48127400	2.38891800	2.03778100
C	-1.13100300	5.48500500	-3.55015900
H	-0.68675800	6.47201200	-3.72202000
H	-1.46715700	5.08604400	-4.51384900
H	-2.01192600	5.60993800	-2.91344600
C	1.13532400	4.42739700	-3.78764700
H	0.87345900	4.11679400	-4.80611400

H	1.62719400	5.40395900	-3.85939500
H	1.85423300	3.70797700	-3.38423300
C	-1.36620100	-0.19677200	-5.30284200
H	-2.44124500	0.00835800	-5.30825200
H	-0.86786800	0.64647700	-5.79525100
H	-1.18423500	-1.09329500	-5.90536100
C	0.67491000	-0.68901700	-3.91882800
H	0.85971500	-1.55620000	-4.56292700
H	1.24909400	0.15209600	-4.32564900
H	1.03001100	-0.92102000	-2.91270800
C	2.14941600	-0.16651200	4.22183500
H	3.21464800	-0.12726500	4.48077200
H	2.01335700	0.12033100	3.17477000
H	1.63141400	0.56298800	4.85623600
C	1.79540200	-1.98949100	5.90861500
H	1.34557900	-1.26120900	6.59288900
H	1.36302800	-2.97062700	6.12378800
H	2.86759700	-2.04462000	6.13253900
C	6.30373000	-4.85649700	2.64675500
H	7.39773800	-4.83684000	2.59457000
H	6.00929600	-5.18843100	3.64652400
H	5.94730600	-5.60209800	1.92776400
C	6.16067500	-3.00587400	0.93994500
H	7.25296100	-2.94105100	0.87792000
H	5.82054900	-3.70810400	0.17091400
H	5.73702900	-2.02497400	0.70232500
C	1.47741800	-4.92358600	-0.60871400
H	1.20750300	-3.88334100	-0.80797300
H	2.52421300	-5.07630100	-0.89678600
H	0.86128900	-5.57177300	-1.24176800
C	1.64536300	-6.72316500	1.16192900
H	2.70419900	-6.90544000	0.94685400
H	1.46753100	-6.97456600	2.21224700
H	1.05656300	-7.40540000	0.53931500

(S_a,*S*)-Int1

E = -4183.49348136 a.u.

0 1

C	-7.83671000	1.26537200	-5.22874800
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C	-8.26726600	3.17524800	-6.62440500
C	-8.59753500	3.94398300	-5.50473800
C	-8.53664400	3.34014600	-4.22903900
C	-8.14320500	2.01123700	-4.08976300

H	-7.54710600	0.22489500	-5.11581900
H	-7.67417600	1.24658200	-7.37569600
H	-8.35605200	3.62846200	-7.60784600
H	-8.08530700	1.54821100	-3.11200200
C	-9.15220500	5.28845800	-5.61086200
H	-9.99146800	5.50971600	-4.95323100
C	-8.76394400	6.30433500	-6.42237000
C	-9.62604400	7.51489900	-6.36898600
C	-7.52681200	6.34429000	-7.17847000
C	-9.21156800	8.67790000	-7.14059800
C	-7.18575800	7.47917300	-7.83547100
H	-6.85489400	5.49563200	-7.10405000
C	-8.06505800	8.63735200	-7.84565400
H	-9.85167700	9.55597200	-7.12678900
H	-7.74008000	9.49752900	-8.42401500
O	-6.03269900	7.69891000	-8.51058100
C	-5.03773400	6.70748300	-8.39218300
H	-5.37184600	5.75394300	-8.82348300
H	-4.17120200	7.07258900	-8.94492600
H	-4.77825700	6.55218200	-7.33765000
O	-8.87318300	4.14944900	-3.19337500
C	-8.85994600	3.60823200	-1.88847500
H	-7.84980000	3.28988900	-1.60499200
H	-9.18732200	4.41241300	-1.22922700
H	-9.54840500	2.75940900	-1.80495700
O	-10.67170400	7.51737600	-5.69644600
C	-4.93798800	7.25482500	-4.74818600
C	-5.96489800	6.52864000	-4.10219800
C	-7.17314900	7.18087900	-3.80914700
C	-7.33609900	8.50028200	-4.19635400
C	-6.31187400	9.19233200	-4.87502900
C	-5.09608800	8.58565200	-5.15145700
C	-4.16912100	5.17355100	-4.36876200
C	-5.45362300	5.20455300	-3.88773300
H	-7.97548100	6.64153300	-3.31190100
H	-8.27277700	9.01429500	-3.99352100
H	-6.48986900	10.21746700	-5.19209900
H	-4.30434800	9.11652200	-5.67413200
N	-3.85133300	6.41935800	-4.89698500
C	-2.56078700	6.85420800	-5.37850500
H	-2.59614800	7.09695100	-6.44747700
H	-2.23409900	7.74315700	-4.82890800
H	-1.83787900	6.05273000	-5.21855000
C	-3.20570100	4.04168600	-4.39139100

C	-3.28400200	3.13029000	-5.60731400
C	-4.42823200	2.11384700	-5.45071100
C	-3.47368600	3.90632600	-6.91921800
H	-2.34310900	2.57299500	-5.69740700
C	-4.51560100	1.17279700	-6.65434400
H	-5.37207400	2.66933900	-5.34664300
H	-4.28831400	1.54382000	-4.52332200
C	-3.53179600	2.96576100	-8.12402800
H	-4.41808100	4.46384400	-6.85264000
H	-2.67073900	4.64304000	-7.04898700
C	-4.66646600	1.95407200	-7.96107700
H	-5.35246800	0.47684400	-6.52635300
H	-3.60231800	0.56281800	-6.70461200
H	-3.66306900	3.54279100	-9.04694400
H	-2.57551100	2.43248100	-8.21824700
H	-4.70018100	1.27020100	-8.81661900
H	-5.62148400	2.49832500	-7.94254800
C	-2.39589100	3.83487100	-3.33688600
C	-1.48945500	2.63781000	-3.16716900
C	-2.37667900	4.74145700	-2.12700500
C	-1.90153500	1.84497600	-1.91336100
H	-0.45523300	2.98719000	-3.03247900
H	-1.49759100	1.97930900	-4.03794900
C	-2.79180500	3.96162300	-0.86924500
H	-1.35070500	5.11282600	-1.98318400
H	-3.02551600	5.60906100	-2.26853400
C	-1.90263300	2.73343500	-0.66827900
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H	-2.90980400	1.43908300	-2.07072300
H	-2.74844100	4.61593600	0.00794800
H	-3.83699200	3.64518500	-0.98617500
H	-2.23120300	2.16105500	0.20610000
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P	-11.61252700	10.91453100	-5.19741800
O	-11.42966300	11.00546400	-6.65467500
O	-10.98989900	12.11640200	-4.31264100
O	-13.19153300	10.96680000	-4.85164100
O	-10.99518600	9.70217900	-4.42106200
H	-10.99409500	8.84324600	-4.96831400
C	-12.96411800	15.14752100	-4.90229900
C	-12.52716400	13.94989700	-4.32897100
C	-11.34383700	13.38092400	-4.77244200
C	-10.51149200	14.02779600	-5.69365700
C	-10.93678200	15.26972700	-6.17859100

C	-12.16759700	15.81810000	-5.82001700
C	-14.34510000	15.49471000	-4.39186800
C	-14.79718800	14.17243700	-3.74006000
H	-10.29205600	15.79710200	-6.87475500
H	-12.49559700	16.75599300	-6.25888600
H	-14.30276700	16.30781600	-3.65618200
H	-15.53273900	14.30724300	-2.94112500
H	-15.23381800	13.51497500	-4.50003300
C	-13.48002100	13.52650400	-3.22665900
C	-13.66846300	12.08309900	-2.79500300
C	-13.07935100	14.16831800	-1.86627100
C	-14.00706700	12.02795900	-1.43986900
C	-13.57867700	10.90405700	-3.52058500
C	-13.90852800	13.40258700	-0.81966000
H	-12.01238500	13.98395400	-1.69697400
H	-13.24413900	15.24990300	-1.85344200
C	-14.34188900	10.81960900	-0.84536700
C	-13.88010500	9.66102400	-2.94604700
H	-13.43534900	13.38390200	0.16646200
C	-14.29586500	9.65579900	-1.60929000
H	-14.62352700	10.77553100	0.20276000
H	-14.56306600	8.70395900	-1.16086200
H	-14.90234100	13.85085400	-0.69339600
H	-15.01410900	15.82102900	-5.19351000
C	-13.76159900	8.37664800	-3.70375600
C	-12.88372200	7.36387000	-3.24759600
C	-14.55840700	8.14632900	-4.84287700
C	-12.86305300	6.13775000	-3.91075800
C	-14.47937200	6.90751800	-5.48337600
C	-13.65238700	5.88635700	-5.03121100
H	-12.19420000	5.35800700	-3.54852400
H	-15.09858000	6.72773000	-6.36028800
C	-11.94729600	7.54491000	-2.05728000
H	-11.95859800	8.59866500	-1.76559000
C	-15.55190000	9.16282300	-5.38785300
H	-15.48906900	10.07411500	-4.78894200
C	-13.64396400	4.53512000	-5.71937700
H	-14.21518400	4.64204400	-6.65051300
C	-9.20462400	13.44493100	-6.12988500
C	-8.96944900	13.15619100	-7.49445300
C	-8.17014600	13.25638900	-5.19395700
C	-7.69133500	12.76240400	-7.88883100
C	-6.90979300	12.84748700	-5.64223000
C	-6.63623000	12.61684600	-6.98615300

H	-7.50350200	12.58151300	-8.94602600
H	-6.11915900	12.73184200	-4.90639300
C	-10.04850200	13.27067400	-8.56361200
H	-11.00894900	13.42471400	-8.06428300
C	-8.32820100	13.50908900	-3.70103700
H	-9.34677200	13.85255600	-3.50539300
C	-5.25154600	12.23840900	-7.49470800
H	-4.98190900	12.97963900	-8.26050400
H	-5.96362000	4.36928400	-3.42628400
C	-16.98814300	8.63833200	-5.25853800
H	-17.13526500	7.73491100	-5.86030300
H	-17.22486400	8.39229400	-4.21865600
H	-17.70244000	9.39221400	-5.60631000
C	-15.23397700	9.53853700	-6.83995700
H	-14.21213100	9.91476400	-6.93653700
H	-15.34899300	8.67462600	-7.50415700
H	-15.92261000	10.31646800	-7.18701100
C	-14.34602100	3.48359600	-4.85140100
H	-14.37325900	2.51306000	-5.35846000
H	-13.81217400	3.35585300	-3.90273000
H	-15.37215500	3.78442200	-4.62055200
C	-12.22991400	4.07576100	-6.08525400
H	-11.69702800	4.85085100	-6.64501800
H	-11.64580900	3.84844400	-5.18512000
H	-12.26372100	3.16328200	-6.69003400
C	-10.49530600	7.18543200	-2.39919700
H	-9.84320200	7.40869100	-1.54631700
H	-10.38522800	6.12008500	-2.63408500
H	-10.13606500	7.75300800	-3.25964900
C	-12.40849500	6.69969400	-0.86153500
H	-11.75467000	6.86435900	0.00199400
H	-13.43469900	6.93182800	-0.56281000
H	-12.37363900	5.63308300	-1.11400300
C	-10.17596200	11.98374400	-9.38814200
H	-9.26025700	11.77321200	-9.95276400
H	-10.40476000	11.13642000	-8.73999800
H	-10.99039000	12.08810000	-10.11303800
C	-9.77597900	14.45947100	-9.49565600
H	-10.57829400	14.55895000	-10.23435900
H	-9.69623000	15.40340400	-8.94843600
H	-8.83528600	14.31385100	-10.03929200
C	-5.26478500	10.85980300	-8.16652200
H	-5.57638900	10.08516000	-7.45821400
H	-5.95112300	10.82765500	-9.01827700

H	-4.26669000	10.59862100	-8.53670100
C	-4.17186300	12.27796700	-6.41357200
H	-3.19416300	12.05608500	-6.85245400
H	-4.11351900	13.25850200	-5.93129900
H	-4.36538200	11.52964100	-5.63507100
C	-8.11271500	12.21673500	-2.90325500
H	-8.81219500	11.44130400	-3.22743500
H	-7.09219800	11.83674100	-3.03056300
H	-8.26969300	12.39810400	-1.83434900
C	-7.38289000	14.61818100	-3.22135500
H	-7.54443000	15.54294100	-3.78381200
H	-7.54987000	14.82649700	-2.15926400
H	-6.33342400	14.32878300	-3.34222600

(S_a,*S*)-TS1

E = -4183.46175681 a.u.

0 1

C	-8.37121800	1.30683900	-6.41655000
C	-8.16658400	2.27657300	-7.39302700
C	-7.94836200	3.59717200	-7.01540600
C	-7.92833800	3.97953800	-5.66782900
C	-8.18976100	2.98330700	-4.69462600
C	-8.39159200	1.65539800	-5.06770800
H	-8.54326500	0.27329500	-6.69990900
H	-8.20156700	2.01267900	-8.44454400
H	-7.85049200	4.36363100	-7.77681100
H	-8.58558700	0.89618800	-4.32001000
C	-7.90658900	5.38523000	-5.24574100
H	-8.52348500	5.56269900	-4.36651200
C	-7.85005400	6.51909500	-6.11995800
C	-8.71406000	7.61044400	-5.81452300
C	-6.92751600	6.63484900	-7.19779300
C	-8.61225100	8.79654800	-6.57716300
C	-6.86064600	7.79420700	-7.93430600
H	-6.24301100	5.81890800	-7.38651500
C	-7.71028400	8.87630100	-7.60824000
H	-9.27774200	9.63154500	-6.37336500
H	-7.64682400	9.78375000	-8.20094500
O	-6.01862900	8.00588000	-8.98851800
C	-5.28985000	6.89866200	-9.45231300
H	-5.95235700	6.05287600	-9.68280800
H	-4.77746900	7.22137800	-10.35875200
H	-4.54442700	6.56457400	-8.71680700
O	-8.27049300	3.41288700	-3.41182700

C	-8.82450200	2.53570900	-2.44757100
H	-8.16039000	1.68526900	-2.25706200
H	-8.93308900	3.12393700	-1.53695500
H	-9.80603800	2.17450100	-2.77442700
O	-9.61847300	7.45842200	-4.86089700
C	-5.35524300	7.61922900	-4.51242500
C	-6.33017800	7.02109200	-3.70203900
C	-7.27011100	7.82919200	-3.06451700
C	-7.23307700	9.19945200	-3.29038400
C	-6.26488500	9.77111200	-4.13195300
C	-5.29436200	8.98974400	-4.74712900
C	-4.98106900	5.39732600	-4.59825600
C	-6.18617100	5.58668800	-3.87444600
H	-8.04138700	7.39222700	-2.44138100
H	-7.98948200	9.83291400	-2.83904700
H	-6.29449000	10.83873700	-4.32742500
H	-4.54275900	9.42683800	-5.39646900
N	-4.53502400	6.60378400	-5.01628500
C	-3.30895000	6.89619600	-5.72882300
H	-3.53505800	7.24418100	-6.74291200
H	-2.77059300	7.68522800	-5.19708500
H	-2.68957100	5.99989500	-5.76673300
C	-4.11815000	4.17926500	-4.62135400
C	-3.94488600	3.30012800	-5.85826000
C	-4.71634400	1.97251800	-5.73575200
C	-4.32502000	3.95023000	-7.19166100
H	-2.87481600	3.05443600	-5.92801800
C	-4.37236000	1.02781100	-6.88979400
H	-5.79055200	2.19472300	-5.74377000
H	-4.50122400	1.49384100	-4.77406800
C	-3.94749100	3.03935900	-8.36359700
H	-5.40975800	4.11088300	-7.20060100
H	-3.84630200	4.92764600	-7.31070300
C	-4.63869500	1.67920100	-8.24893800
H	-4.94867800	0.10044800	-6.79710400
H	-3.31049300	0.75036600	-6.82046200
H	-4.21221700	3.52056200	-9.31226100
H	-2.85742200	2.90032800	-8.37261100
H	-4.31436700	1.01767600	-9.05939200
H	-5.72001700	1.82315500	-8.36360200
C	-3.46402100	3.90909200	-3.47117500
C	-2.57626500	2.70124900	-3.26706400
C	-3.56184500	4.73490800	-2.20682600
C	-3.13905100	1.82697800	-2.13080200

H	-1.57642100	3.05040100	-2.97153400
H	-2.45342900	2.10526900	-4.17292500
C	-4.13689900	3.88397000	-1.06185100
H	-2.54522500	5.04730600	-1.92623600
H	-4.15082500	5.64475700	-2.33998400
C	-3.29223200	2.62882200	-0.83706200
H	-2.48512800	0.96292100	-1.97301100
H	-4.12030600	1.43901900	-2.43583000
H	-4.18975300	4.48215700	-0.14657200
H	-5.16525400	3.59474600	-1.31920000
H	-3.73574700	2.00424700	-0.05442900
H	-2.29689900	2.92670900	-0.47979400
P	-11.25099000	10.74022400	-4.90529800
O	-11.03468400	10.79450000	-6.37217400
O	-10.85009300	12.16883900	-4.17533400
O	-12.88384500	10.75175200	-4.69479400
O	-10.59931700	9.68943100	-4.04032500
H	-10.07472100	8.34126500	-4.61347400
C	-13.04965100	14.90223700	-5.23857100
C	-12.54306300	13.82387600	-4.50568000
C	-11.29816300	13.29791500	-4.82630600
C	-10.49964000	13.89977700	-5.81141900
C	-10.99819800	15.03281100	-6.46187000
C	-12.27742200	15.52352400	-6.20843500
C	-14.47548400	15.19210800	-4.82747600
C	-14.85441700	13.91466000	-4.05605400
H	-10.36906500	15.51911800	-7.20110900
H	-12.66187400	16.37116000	-6.76863300
H	-14.53106100	16.07830400	-4.18202000
H	-15.64662200	14.06573200	-3.31617700
H	-15.18576600	13.14285300	-4.75977600
C	-13.52024400	13.44561000	-3.40846900
C	-13.64290600	12.04573600	-2.83887500
C	-13.26904500	14.25142100	-2.10261100
C	-14.12070600	12.10928400	-1.52701500
C	-13.41207500	10.80959600	-3.42935900
C	-14.13723800	13.54294100	-1.04516300
H	-12.21022100	14.15693900	-1.83634900
H	-13.49858800	15.31528600	-2.21803800
C	-14.48531100	10.95308900	-0.85071900
C	-13.75551200	9.62333800	-2.76265500
H	-13.73948000	13.64578300	-0.03086500
C	-14.32624900	9.72490200	-1.48890600
H	-14.87965100	10.99984400	0.16050000

H	-14.61281400	8.80866400	-0.97936500
H	-15.15794000	13.94643500	-1.03299800
H	-15.12648100	15.37863200	-5.68694700
C	-13.48068200	8.29144300	-3.37682300
C	-12.61321300	7.38796100	-2.72361800
C	-14.07406200	7.92666100	-4.60124200
C	-12.37211800	6.14383400	-3.30203200
C	-13.78942400	6.67133600	-5.14422000
C	-12.94292700	5.76711200	-4.51532900
H	-11.69910800	5.45327200	-2.79588500
H	-14.24530400	6.39022500	-6.09179200
C	-11.90632300	7.70854000	-1.41282400
H	-12.11373900	8.74735200	-1.14884000
C	-15.05424800	8.81751600	-5.35043700
H	-15.13964300	9.76803100	-4.81921100
C	-12.63190400	4.41913600	-5.13393600
H	-13.16051100	4.36504200	-6.09428100
C	-9.13906900	13.38860000	-6.16199800
C	-8.86811600	12.92421200	-7.47006700
C	-8.09603400	13.45725400	-5.22218400
C	-7.55488100	12.60502800	-7.81170400
C	-6.79806100	13.10361200	-5.60997900
C	-6.49617000	12.69221400	-6.90440500
H	-7.34602200	12.29372700	-8.83405700
H	-6.00456300	13.18689000	-4.87175900
C	-9.94809100	12.78276400	-8.53523800
H	-10.91909800	12.89263800	-8.04609400
C	-8.30472000	13.94224000	-3.79471200
H	-9.34980300	14.23871600	-3.67963800
C	-5.07803300	12.37697200	-7.36562600
H	-4.82967900	13.10017900	-8.15588700
H	-6.56758900	4.82249700	-3.21037400
C	-16.45033500	8.18057800	-5.36879900
H	-16.44147200	7.22621900	-5.90723600
H	-16.81061400	7.99031400	-4.35279400
H	-17.16526700	8.84156200	-5.87065500
C	-14.57165200	9.12176100	-6.77371300
H	-13.57235600	9.56454700	-6.76529600
H	-14.54742100	8.21138800	-7.38400400
H	-15.25778400	9.82454200	-7.25920000
C	-13.12832900	3.26736600	-4.25296200
H	-12.91937500	2.29896200	-4.72144700
H	-12.62766700	3.28703400	-3.27755100
H	-14.20491200	3.34161200	-4.07454300

C	-11.13170400	4.28056600	-5.40557500
H	-10.76171400	5.11050300	-6.01672000
H	-10.57582800	4.30035400	-4.45913600
H	-10.90229500	3.33521300	-5.91349400
C	-10.38676000	7.59062800	-1.55413000
H	-9.89577600	7.84120700	-0.60586600
H	-10.08732500	6.57117900	-1.83038500
H	-10.04118500	8.27917400	-2.32830100
C	-12.41908400	6.81270400	-0.27858100
H	-11.93821600	7.07624000	0.66983900
H	-13.50257700	6.90306000	-0.15147800
H	-12.19956800	5.75869800	-0.48635300
C	-9.93755200	11.39569000	-9.18790200
H	-9.00954400	11.21576800	-9.74525300
H	-10.07133200	10.62156000	-8.43033600
H	-10.76420100	11.31984200	-9.90282900
C	-9.79861000	13.86343800	-9.61521000
H	-10.60055300	13.77654600	-10.35617500
H	-9.82912000	14.87375600	-9.19745700
H	-8.84279700	13.75213700	-10.14115000
C	-4.98845400	10.97447800	-7.98104100
H	-5.31843100	10.21912900	-7.26002200
H	-5.61892600	10.86773900	-8.86781000
H	-3.95838700	10.74687300	-8.27929300
C	-4.02988000	12.52980100	-6.26363300
H	-3.03229700	12.31688400	-6.66043300
H	-4.01883200	13.54165500	-5.84798000
H	-4.21926400	11.83118500	-5.43857000
C	-8.03510100	12.81982800	-2.78657800
H	-8.67320600	11.95910000	-3.00545500
H	-6.98365100	12.50643400	-2.81519700
H	-8.25037300	13.16002100	-1.76761300
C	-7.44839300	15.17765300	-3.49053500
H	-7.65254900	15.98203900	-4.20384800
H	-7.66098800	15.54866500	-2.48222000
H	-6.37853600	14.94650200	-3.54021900

(S_a,*S*)-Int2

E = -4183.48475283 a.u.

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C	-7.88311900	3.64101900	-6.77022800
C	-7.87003700	4.17662900	-5.48379500

C	-8.17349800	3.31636700	-4.40978800
C	-8.44436100	1.96601900	-4.62240000
H	-8.66065900	0.40771500	-6.08313300
H	-8.17932000	1.90589700	-8.01126700
H	-7.72028000	4.30797200	-7.61159300
H	-8.68385300	1.31383900	-3.79046400
C	-7.78312900	5.66913400	-5.23272500
H	-8.66142600	5.90030100	-4.61895600
C	-7.92607400	6.55078000	-6.45009800
C	-9.10168000	7.29929700	-6.55649800
C	-6.86031400	6.79992600	-7.32451200
C	-9.19132700	8.31336900	-7.52215700
C	-6.96008600	7.79701000	-8.28739900
H	-5.93749200	6.24070300	-7.20536700
C	-8.12967600	8.56297400	-8.37298300
H	-10.08597800	8.93086100	-7.54020600
H	-8.18070100	9.36167100	-9.10684300
O	-5.96263200	8.10509000	-9.17266800
C	-4.70080000	7.54863900	-8.92159100
H	-4.70594400	6.45460000	-9.03512800
H	-4.01844900	7.98272000	-9.65345000
H	-4.35424700	7.79749300	-7.90584100
O	-8.23281000	3.90202200	-3.17753000
C	-8.92065500	3.21156100	-2.15102100
H	-8.34528700	2.34762800	-1.79464000
H	-9.04704700	3.92656200	-1.33632600
H	-9.90504500	2.87863200	-2.50048400
O	-10.10813400	7.05459300	-5.68269200
C	-5.13539300	7.97236000	-4.65038900
C	-6.46095700	7.66590500	-4.37204700
C	-7.40652600	8.68219000	-4.38740000
C	-6.97668500	9.97954000	-4.65807100
C	-5.62571600	10.26466000	-4.88083300
C	-4.66565100	9.25544000	-4.89181500
C	-5.17695100	5.70820600	-4.50076600
C	-6.60322800	6.16758700	-4.30385500
H	-8.46707300	8.50367000	-4.25723500
H	-7.71682200	10.77349900	-4.71897500
H	-5.33162800	11.28742500	-5.08557900
H	-3.62278200	9.46744500	-5.10660000
N	-4.40461300	6.75050200	-4.68526100
C	-2.95204000	6.75212100	-4.79527500
H	-2.67264700	7.16649200	-5.76715100
H	-2.54739100	7.38499800	-4.00195600

H	-2.57674900	5.73570200	-4.69345900
C	-4.58504900	4.37186600	-4.21455000
C	-4.14915600	3.44762700	-5.35517900
C	-4.94679800	2.13123200	-5.40296600
C	-4.21191200	4.11130700	-6.73942300
H	-3.09388700	3.19072700	-5.16509600
C	-4.40508400	1.19055400	-6.48093900
H	-5.98796700	2.36913800	-5.62378500
H	-4.94124400	1.63553900	-4.42781500
C	-3.65767100	3.18538700	-7.82466100
H	-5.26229600	4.33586200	-6.96796900
H	-3.66736300	5.06536500	-6.75250100
C	-4.42200800	1.86116200	-7.85534300
H	-5.00510200	0.27429700	-6.49850100
H	-3.37585500	0.89454500	-6.23086200
H	-3.71299000	3.68276300	-8.79903400
H	-2.59425500	2.99118300	-7.62556100
H	-3.99966400	1.19502800	-8.61480000
H	-5.46419900	2.05814500	-8.14008300
C	-4.33675500	4.12132900	-2.91357600
C	-3.74541600	2.82858100	-2.40733300
C	-4.68093300	5.04704200	-1.76655300
C	-4.80518800	2.11568800	-1.54568500
H	-2.88052600	3.06426000	-1.77158000
H	-3.38860900	2.18238700	-3.21044300
C	-5.71924600	4.37490700	-0.85122200
H	-3.76205800	5.22497600	-1.18975600
H	-5.03907800	6.02854700	-2.09098300
C	-5.23412400	3.00363000	-0.37404300
H	-4.40999200	1.16217400	-1.18074700
H	-5.67602300	1.89118900	-2.17786000
H	-5.93615100	5.02496400	0.00239100
H	-6.64672900	4.25980300	-1.42343600
H	-6.02041700	2.50963100	0.20692200
H	-4.37883900	3.13808700	0.30222900
P	-11.12598500	10.49553500	-5.08867300
O	-11.15957200	10.69317800	-6.55834800
O	-10.54991900	11.84082800	-4.30400900
O	-12.70026300	10.50269400	-4.59632100
O	-10.40445800	9.34632200	-4.43571200
H	-10.43058400	7.91609100	-5.28867500
C	-12.88472000	14.65709100	-4.61608100
C	-12.26798800	13.50217200	-4.12110700
C	-11.09467800	13.04116200	-4.70981000

C	-10.46370600	13.79632300	-5.71209900
C	-11.06075600	14.99116700	-6.12378700
C	-12.28496400	15.41353200	-5.61095300
C	-14.21639200	14.87857600	-3.93552100
C	-14.46511400	13.51787200	-3.26195200
H	-10.55148600	15.58900600	-6.87345000
H	-12.75716000	16.31754100	-5.98503500
H	-14.15373400	15.68533000	-3.19367900
H	-15.11224600	13.57346900	-2.38104600
H	-14.92241100	12.82764000	-3.97965200
C	-13.04267000	12.99197500	-2.91883400
C	-13.08610800	11.53865900	-2.49463500
C	-12.55258200	13.64830200	-1.59689000
C	-13.32591600	11.45183000	-1.12156700
C	-12.99030800	10.38469900	-3.26089100
C	-13.22942300	12.82126000	-0.48639300
H	-11.46452300	13.53071500	-1.53631600
H	-12.78360100	14.71714300	-1.55060400
C	-13.59713700	10.22451000	-0.53280000
C	-13.23456800	9.12541200	-2.68714800
H	-12.65392000	12.80951100	0.44444600
C	-13.57838400	9.08214400	-1.32997400
H	-13.81450900	10.14999300	0.52905900
H	-13.79916800	8.11354500	-0.88898500
H	-14.22372800	13.21833400	-0.24462300
H	-15.00407700	15.15321300	-4.64365800
C	-13.10258100	7.86300000	-3.47385300
C	-12.19315700	6.86396500	-3.05251900
C	-13.88608200	7.64462500	-4.62455100
C	-12.09164700	5.68487800	-3.78734300
C	-13.74119300	6.44470000	-5.32585500
C	-12.85248600	5.45334900	-4.93066600
H	-11.36712500	4.93261500	-3.47429800
H	-14.34756000	6.27788000	-6.21421100
C	-11.29638500	7.00605400	-1.82741600
H	-11.43023400	8.00421700	-1.40688500
C	-14.93796500	8.62776600	-5.11853000
H	-14.91321100	9.51662300	-4.48486600
C	-12.69627200	4.17642900	-5.73191000
H	-13.44305900	4.20115700	-6.53621600
C	-9.14452000	13.39623400	-6.29094500
C	-9.04932500	12.94434800	-7.62562700
C	-7.97801500	13.57439700	-5.52592900
C	-7.78779800	12.66704800	-8.14670100

C	-6.73287900	13.28412500	-6.09854000
C	-6.61415300	12.82669800	-7.40767900
H	-7.70815600	12.33887500	-9.18169900
H	-5.83804100	13.45963100	-5.50514400
C	-10.26398700	12.83162800	-8.53574700
H	-11.15520800	12.81783600	-7.90410700
C	-8.01439900	14.13834400	-4.11068600
H	-9.04309300	14.43649100	-3.89055100
C	-5.28193400	12.52610800	-8.08032800
H	-5.27348300	13.09062400	-9.02356400
H	-6.87329700	5.80597500	-3.29941300
C	-16.34099800	8.01905800	-4.98914500
H	-16.44638800	7.13017000	-5.62107000
H	-16.54887800	7.72361800	-3.95575500
H	-17.10133200	8.74343700	-5.30087100
C	-14.66623900	9.07573100	-6.55953800
H	-13.66675000	9.50707500	-6.65863200
H	-14.75622400	8.23421900	-7.25631000
H	-15.39957500	9.83206300	-6.86061700
C	-12.96323200	2.93169700	-4.87881600
H	-12.90368200	2.02401300	-5.48917300
H	-12.21546400	2.84331100	-4.08121700
H	-13.95088700	2.97274000	-4.41005500
C	-11.30514400	4.09973000	-6.36791400
H	-11.09631100	4.98392300	-6.97613700
H	-10.53932600	4.05652700	-5.58528600
H	-11.20510500	3.19991600	-6.98610800
C	-9.81543000	6.88724300	-2.19728100
H	-9.18611400	7.01997100	-1.30777000
H	-9.58343300	5.90988500	-2.63623000
H	-9.57161400	7.66528800	-2.92136800
C	-11.67003100	5.97809400	-0.75255600
H	-11.04136200	6.10021500	0.13712700
H	-12.71721300	6.07340800	-0.44823600
H	-11.53290500	4.95667500	-1.12853200
C	-10.27554800	11.53568900	-9.35037300
H	-9.46873000	11.51173800	-10.09340300
H	-10.18954300	10.67856700	-8.68305100
H	-11.22190900	11.45074600	-9.89450600
C	-10.33018900	14.03613000	-9.48620800
H	-11.21596800	13.96767800	-10.12700200
H	-10.37371600	14.98622400	-8.94682000
H	-9.44562900	14.06129300	-10.13401200
C	-5.17881300	11.03770600	-8.44118600

H	-5.24401900	10.41337700	-7.54242300
H	-5.98713500	10.72468500	-9.10565000
H	-4.22772100	10.82530500	-8.94484100
C	-4.05949100	12.97299600	-7.27971900
H	-3.15039200	12.82618900	-7.87134500
H	-4.11938400	14.02990600	-7.00277500
H	-3.94586900	12.38863300	-6.35840500
C	-7.61006300	13.09179600	-3.06661500
H	-8.30873700	12.25034400	-3.07062000
H	-6.59989000	12.70930400	-3.26254400
H	-7.60982000	13.53403700	-2.06390700
C	-7.14488000	15.39615900	-3.98921400
H	-7.42490100	16.14115900	-4.74015900
H	-7.26379100	15.84442500	-2.99712800
H	-6.08187100	15.16626000	-4.12235700

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P	-0.56208200	-0.50295500	0.95629100
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O	-2.13997200	-0.14311700	1.06615700
O	-0.03888000	0.18872200	-0.37865700
H	0.13344200	1.13989200	-0.27277200
C	-2.95371100	-4.04417900	2.28291100
C	-2.41698200	-3.21683400	1.29240800
C	-1.05612400	-2.95012400	1.29667500
C	-0.19198800	-3.56760800	2.20860200
C	-0.75321500	-4.43792600	3.15055700
C	-2.12706700	-4.66164400	3.21202000
C	-4.46073700	-4.08396700	2.16751900
C	-4.75047500	-2.87904000	1.25224500
H	-0.08885800	-4.91882600	3.86253500
H	-2.54199000	-5.30560400	3.98187900
H	-4.79531600	-5.02277400	1.70826100
H	-5.68195500	-2.97193100	0.68560500
H	-4.80568500	-1.96481100	1.85376000
C	-3.50407200	-2.78641800	0.32684400
C	-3.45997900	-1.47337800	-0.43075400
C	-3.65128600	-3.78472300	-0.85678000
C	-4.13507400	-1.59768000	-1.64925900
C	-2.90931600	-0.24932100	-0.08363400
C	-4.52592200	-3.03936100	-1.88240600

H	-2.65852200	-3.96754400	-1.28301800
H	-4.06850800	-4.74498900	-0.53919000
C	-4.33233300	-0.49343800	-2.46735100
C	-3.09778200	0.88574000	-0.88381500
H	-4.34094400	-3.36073600	-2.91140000
C	-3.83192700	0.74370400	-2.06629400
H	-4.86106500	-0.58967200	-3.41106300
H	-3.98123200	1.62153300	-2.68846500
H	-5.59386900	-3.19326500	-1.68256800
H	-4.95630000	-4.00618900	3.13947400
C	1.27982400	-3.33376500	2.17979100
C	1.91492900	-2.71804600	3.27654700
C	2.03522800	-3.78714800	1.07843100
C	1.18784300	-2.18496000	4.39087900
C	3.34505500	-2.58935400	3.28413500
C	3.46219500	-3.62729100	1.08743300
C	1.44362700	-4.42919500	-0.05814300
C	1.83663300	-1.61668700	5.44614800
H	0.10456200	-2.20841500	4.36631700
C	3.98759400	-1.99084300	4.41426700
C	4.08174700	-3.04381100	2.19191700
C	4.22537100	-4.08560400	-0.03273100
H	0.36967400	-4.58097400	-0.07649400
C	2.20549700	-4.85428700	-1.10617600
C	3.26017900	-1.52754400	5.46776200
H	1.26530500	-1.20823500	6.27362400
H	5.07152800	-1.91253200	4.40584500
H	5.16474900	-2.93914900	2.19999200
C	3.62030700	-4.67717600	-1.09982100
H	5.30338400	-3.94965000	-0.00760300
H	1.73312600	-5.33611100	-1.95654600
H	3.75601100	-1.07345500	6.32001400
H	4.20833900	-5.02075700	-1.94496100
C	-2.53374400	2.21008200	-0.49405500
C	-1.54910100	2.82153200	-1.30112800
C	-3.01492900	2.86693000	0.65837300
C	-0.98526300	2.18066000	-2.45661900
C	-1.05143900	4.12396800	-0.94971500
C	-2.49994000	4.16227100	1.00382000
C	-4.02390200	2.30171100	1.50449800
C	-0.02915300	2.79845500	-3.20861400
H	-1.31303900	1.17850700	-2.70955600
C	-0.05667900	4.74005800	-1.77442200
C	-1.53805600	4.76031800	0.19100300

C	-2.99036300	4.82250100	2.17480200
H	-4.43891500	1.33237300	1.25137500
C	-4.46769500	2.96387000	2.61042400
C	0.43767800	4.10367900	-2.87225000
H	0.38904500	2.28889900	-4.07078100
H	0.29812100	5.72855500	-1.49555400
H	-1.15616500	5.74422900	0.45456200
C	-3.94189100	4.24320400	2.95751200
H	-2.58257500	5.79896300	2.42149800
H	-5.23145900	2.51507300	3.23744700
H	1.19476600	4.57795500	-3.48827500
H	-4.30715500	4.75029100	3.84474100

(R_a,*R*)-Int3

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0 1

C	-3.16153400	-0.80260100	1.68179400
C	-2.93741700	0.49333800	2.27514700
C	-3.06656900	0.68282000	3.61152700
C	-3.45717100	-0.41495300	4.46991800
C	-3.70437600	-1.65015700	3.97771500
C	-3.51046700	-1.94101200	2.56203900
H	-2.71307400	1.34790500	1.64831000
H	-3.58770100	-0.24889500	5.53411400
H	-4.05177000	-2.44728700	4.62799800
O	-2.86244300	1.94131100	4.09859200
O	-3.57327300	-3.09894600	2.11168800
C	-3.03698400	2.15978500	5.48082900
H	-4.06584000	1.94190300	5.79806500
H	-2.82833600	3.21696800	5.64490100
H	-2.34302600	1.55487500	6.07721700
C	-2.58544500	-0.25197500	-0.72801700
C	-3.09680600	-0.41865900	-2.03888100
C	-1.50335100	0.62170100	-0.54839700
C	-2.56832600	0.31322000	-3.10264300
C	-0.96457100	1.34174900	-1.60891900
H	-1.05399700	0.69529800	0.43654800
C	-1.50677300	1.18940400	-2.88083800
H	-2.96728300	0.20089900	-4.10321900
H	-0.12278300	2.00554800	-1.44417700
H	-1.10076500	1.74883800	-3.71783300
O	-4.10156500	-1.31551400	-2.16980500
C	-4.67240700	-1.49221600	-3.44946100
H	-5.11040600	-0.55682200	-3.81700900

H	-5.45855600	-2.23673400	-3.32742800
H	-3.93037500	-1.85627900	-4.16952100
C	-3.11354900	-1.08119700	0.34534700
H	-3.49907600	-2.05711100	0.05777000
H	-3.38960100	-4.11944300	3.13104700
C	-6.31251700	0.62264700	1.02016300
C	-6.19235700	-0.25030200	-0.03393300
N	-6.47674400	-0.10209900	2.19162100
H	-6.05656100	0.03807700	-1.06760400
C	-6.65118100	0.42952300	3.52318000
H	-6.12563300	-0.20735000	4.24066800
H	-7.71074700	0.46738200	3.80476700
H	-6.23332000	1.43890000	3.55975000
C	-6.31766600	2.10643700	0.96225800
C	-7.42269900	2.79195500	1.32047800
C	-7.57345700	4.29646300	1.26971300
C	-8.71793200	2.11485700	1.71946800
C	-8.70179900	4.70674200	0.30930900
H	-7.83464600	4.65143200	2.27859100
H	-6.64826900	4.79748800	0.99022100
C	-9.84955600	2.51605300	0.75753300
H	-8.99549600	2.42999000	2.73747400
H	-8.61925700	1.02750300	1.72521700
C	-10.01947200	4.03303600	0.69104800
H	-8.81100800	5.79698700	0.30961900
H	-8.42292400	4.40853800	-0.71041300
H	-10.78385400	2.03632900	1.06880800
H	-9.60687300	2.13135900	-0.24156800
H	-10.80661100	4.29983400	-0.02275800
H	-10.34144300	4.40422700	1.67436000
C	-5.04889200	2.70902200	0.36071100
C	-4.24369400	3.61524100	1.30999900
C	-5.28331900	3.39467000	-0.99747300
H	-4.39376500	1.85259400	0.14231000
C	-2.91858100	4.02998500	0.66307000
H	-4.81098700	4.52075600	1.55518500
H	-4.06279200	3.09587500	2.25792200
C	-3.95151900	3.80472000	-1.62875700
H	-5.91841700	4.28176300	-0.87614600
H	-5.82642900	2.70912300	-1.65975100
C	-3.14810000	4.70850300	-0.69008700
H	-2.35986200	4.68926600	1.33665600
H	-2.29523300	3.13844800	0.50077600
H	-4.12323000	4.30654200	-2.58808700

H	-3.36692800	2.89888600	-1.83997100
H	-2.18860500	4.97406700	-1.14877800
H	-3.69770600	5.64803900	-0.53419300
C	-6.33614300	-1.57723400	0.48271800
C	-6.52443900	-1.44927100	1.87998900
C	-6.32909600	-2.86153000	-0.08585600
C	-6.71987000	-2.55519200	2.71634900
C	-6.53712300	-3.95697700	0.73243200
H	-6.16877300	-2.98523800	-1.15399800
C	-6.72868500	-3.80525000	2.11960500
H	-6.84491100	-2.45864200	3.79281200
H	-6.54748800	-4.95616700	0.30874800
H	-6.86180200	-4.67862600	2.74684800
P	-4.24420900	-5.32489700	4.77987400
O	-3.09422700	-4.73485300	3.92012100
O	-4.33627100	-6.91147200	4.43807400
O	-3.51579400	-5.31224900	6.23806000
O	-5.58168000	-4.71769200	4.75891300
C	-1.34462100	-8.73420700	5.51404800
C	-2.61122900	-8.14354300	5.54309300
C	-3.13231900	-7.59571100	4.37961900
C	-2.44939600	-7.69257200	3.15787000
C	-1.21000100	-8.34172300	3.15164300
C	-0.64236800	-8.84465300	4.32134400
C	-0.92681000	-9.13826200	6.90984900
C	-1.91142200	-8.34278200	7.78771600
H	-0.67647000	-8.42077100	2.20867100
H	0.34094600	-9.30535500	4.29752500
H	-1.04560000	-10.21920400	7.05829400
H	-2.08988200	-8.79480600	8.76831500
H	-1.52739600	-7.32838000	7.94325100
C	-3.20918800	-8.25239300	6.93540900
C	-4.18085600	-7.22854900	7.49357900
C	-4.04769600	-9.55078700	7.11015000
C	-5.05227400	-7.82995200	8.40505300
C	-4.29202300	-5.86948700	7.23983400
C	-4.84166900	-9.32730200	8.41207500
H	-4.74161000	-9.63175200	6.26608700
H	-3.42275600	-10.44899500	7.12625700
C	-5.97286400	-7.06598500	9.11078100
C	-5.21307200	-5.07098600	7.93171900
H	-5.78400800	-9.88223700	8.43488900
C	-6.03173600	-5.69211700	8.88218800
H	-6.65153100	-7.53055300	9.82014500

H	-6.74950100	-5.08064400	9.42156100
H	-4.26171100	-9.63818900	9.29039600
H	0.11919100	-8.89705600	7.12035400
C	-3.02095200	-7.12454000	1.90118400
C	-2.38000700	-6.04978800	1.24922400
C	-4.19652900	-7.68406500	1.35733100
C	-1.20775100	-5.41228800	1.77531700
C	-2.93313500	-5.52631900	0.03095400
C	-4.73453900	-7.15556100	0.13599100
C	-4.88335800	-8.78393100	1.96734200
C	-0.63141200	-4.35579500	1.13404000
H	-0.80505600	-5.76126200	2.71933400
C	-2.29468300	-4.41960100	-0.61319300
C	-4.09042700	-6.09319700	-0.49670700
C	-5.93129800	-7.72299900	-0.40565000
H	-4.48240600	-9.21088700	2.88024700
C	-6.02059500	-9.29965900	1.41913200
C	-1.17688200	-3.85020900	-0.08327100
H	0.24692500	-3.88147100	1.56089800
H	-2.74280700	-4.02819400	-1.52407300
H	-4.51060900	-5.68659300	-1.41488600
C	-6.56071000	-8.75926400	0.21543900
H	-6.32590100	-7.30220000	-1.32727000
H	-6.52368800	-10.13146400	1.90209200
H	-0.70845700	-3.00019300	-0.57172300
H	-7.46992300	-9.18019200	-0.20197400
C	-5.33816600	-3.60536900	7.67344800
C	-6.53300200	-3.08538500	7.13280300
C	-4.28084100	-2.73729000	8.01908000
C	-7.60738700	-3.92475600	6.68918800
C	-6.68455400	-1.66581600	6.97612100
C	-4.44502700	-1.31891600	7.85785700
C	-3.03576200	-3.20712800	8.55159000
C	-8.74816100	-3.39244700	6.16662500
H	-7.47800700	-4.99930200	6.73434700
C	-7.90663700	-1.14527700	6.44120300
C	-5.64195200	-0.81741400	7.34667700
C	-3.37562900	-0.44360700	8.23254700
H	-2.89657700	-4.27346500	8.69174200
C	-2.03344000	-2.34250100	8.87978100
C	-8.90947200	-1.97950900	6.05005400
H	-9.53849900	-4.04830000	5.81651800
H	-8.00968900	-0.06633500	6.35370400
H	-5.76840000	0.25965600	7.24040600

C	-2.20210700	-0.93551200	8.71970000
H	-3.53172400	0.62829600	8.12883400
H	-1.09749200	-2.72480500	9.27417100
H	-9.82930000	-1.57674900	5.63747400
H	-1.39757900	-0.26274600	9.00008700

(R_a,*R*)-TS2

E = -4090.486432 a.u.

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C	-3.14871100	-0.76089300	1.58982500
C	-2.78221200	0.47117200	2.18549700
C	-2.54432000	0.57879800	3.53551100
C	-2.65828600	-0.57158500	4.35372600
C	-3.01613300	-1.78531200	3.81109800
C	-3.29082400	-1.91150100	2.42338300
H	-2.70349600	1.37023500	1.58822500
H	-2.48266700	-0.51560900	5.42379300
H	-3.10789300	-2.66511400	4.43843900
O	-2.21771500	1.82017600	4.00377600
O	-3.66376100	-3.04004000	1.87770300
C	-1.91854800	1.93402600	5.37719100
H	-2.77641900	1.65386600	5.99998500
H	-1.67014700	2.98179100	5.54705700
H	-1.06244200	1.30628700	5.65471700
C	-2.87806900	-0.17411900	-0.90386800
C	-3.34654400	-0.41272800	-2.22095900
C	-1.73643400	0.62808100	-0.75869900
C	-2.74459200	0.20629200	-3.31642100
C	-1.12151600	1.23240400	-1.84983400
H	-1.29490300	0.73657900	0.22448800
C	-1.63899800	1.03240100	-3.12456500
H	-3.11725900	0.03732800	-4.31904700
H	-0.23657000	1.84197300	-1.70278100
H	-1.17380900	1.50241300	-3.98523200
O	-4.38812700	-1.27177100	-2.33241400
C	-4.84378900	-1.60673200	-3.62873600
H	-5.23804500	-0.72668000	-4.14903500
H	-5.64425500	-2.33236100	-3.48722300
H	-4.04114900	-2.05608500	-4.22372000
C	-3.48850500	-0.91037800	0.21058200
H	-3.80793000	-1.91338900	-0.05554600
H	-3.73901100	-3.78477200	2.59199400
C	-5.91915600	0.47907000	1.23348600
C	-5.72210700	-0.35975600	0.10937600

N	-6.13196300	-0.29926500	2.31606300
H	-5.74628100	0.01465600	-0.90441400
C	-6.16514300	0.10813400	3.70896900
H	-5.41447600	-0.46139000	4.26587300
H	-7.15187000	-0.09832500	4.13644400
H	-5.94233000	1.17391500	3.77047500
C	-6.00090600	1.95543900	1.22712700
C	-7.10630900	2.57047000	1.70957000
C	-7.31931200	4.06858000	1.69253700
C	-8.33044100	1.84571100	2.23353800
C	-8.56296500	4.45494900	0.87582300
H	-7.47406000	4.39856800	2.73118700
H	-6.45042100	4.60499800	1.31912200
C	-9.57974700	2.22987400	1.41997000
H	-8.49373600	2.13101900	3.28430800
H	-8.21658300	0.76190600	2.20479800
C	-9.80566000	3.73944000	1.40117400
H	-8.69777300	5.54146900	0.90588800
H	-8.39824700	4.17750300	-0.17406600
H	-10.45116800	1.71165200	1.83354400
H	-9.44937200	1.86832700	0.39167700
H	-10.67957300	3.98794000	0.78962600
H	-10.01933400	4.08815200	2.42114400
C	-4.86311100	2.64134200	0.47511700
C	-4.00051700	3.60968700	1.30816100
C	-5.30024000	3.29600300	-0.84826900
H	-4.18327900	1.83489200	0.17086800
C	-2.77224700	4.04143900	0.50096200
H	-4.57076800	4.50537400	1.57797600
H	-3.70040000	3.13876400	2.25105400
C	-4.07058300	3.72790600	-1.65074700
H	-5.93870400	4.16782800	-0.65498300
H	-5.90500000	2.58577700	-1.42582400
C	-3.17832500	4.66902700	-0.83602600
H	-2.16610800	4.74218200	1.08510200
H	-2.13985300	3.16434900	0.30177600
H	-4.37772900	4.21024600	-2.58553400
H	-3.49592400	2.83231600	-1.92589200
H	-2.28685100	4.93774700	-1.41376100
H	-3.72445200	5.60325200	-0.64180200
C	-6.12237300	-1.69166200	0.52718500
C	-6.30095000	-1.63520300	1.91969100
C	-6.25266200	-2.91655100	-0.13020500
C	-6.57729100	-2.75605800	2.69743200

C	-6.56973700	-4.03739900	0.62451900
H	-6.10167000	-2.98516900	-1.20341600
C	-6.71529700	-3.96216700	2.01835600
H	-6.66317200	-2.72968500	3.78125000
H	-6.68774900	-5.00023600	0.13728600
H	-6.91725000	-4.85330700	2.60086300
P	-4.60488500	-5.33346700	4.64836000
O	-3.62799400	-4.68398100	3.70876200
O	-4.49962600	-6.96582500	4.44057400
O	-3.84438800	-5.15517100	6.11055300
O	-6.04199100	-4.99540600	4.74568500
C	-1.34710300	-8.39856100	5.61158600
C	-2.66385000	-7.93259600	5.59965500
C	-3.22797900	-7.48580600	4.41044100
C	-2.50111700	-7.53504000	3.20806300
C	-1.20454300	-8.06240700	3.24379600
C	-0.61546800	-8.48291700	4.43430500
C	-0.91481300	-8.70390700	7.02756400
C	-1.97184000	-7.95027600	7.85536500
H	-0.64267200	-8.10592300	2.31479000
H	0.40672400	-8.85039400	4.43985400
H	-0.95050400	-9.78300300	7.22613900
H	-2.12018400	-8.36097200	8.85908000
H	-1.67606500	-6.89989900	7.95626600
C	-3.26586800	-8.01383200	6.99312700
C	-4.31332200	-7.03570600	7.49797600
C	-4.00140900	-9.35903200	7.24787200
C	-5.12016200	-7.64645800	8.46090100
C	-4.53411400	-5.70628900	7.16150100
C	-4.80049600	-9.12264500	8.54507400
H	-4.69289200	-9.53736700	6.41705500
H	-3.31058100	-10.20608800	7.30701700
C	-6.08082400	-6.91404300	9.14704900
C	-5.49518800	-4.94197700	7.83991900
H	-5.70051100	-9.74158900	8.60750200
C	-6.24400200	-5.56247400	8.84621800
H	-6.70854400	-7.38639200	9.89718200
H	-6.99231400	-4.97496600	9.37112700
H	-4.19359300	-9.34502700	9.43225100
H	0.10625000	-8.37104000	7.23668500
C	-3.05941500	-7.01786900	1.92316500
C	-2.44213800	-5.92345600	1.27690500
C	-4.18909200	-7.63109300	1.34321700
C	-1.33772600	-5.20891000	1.84943800

C	-2.95908500	-5.45061000	0.02323900
C	-4.70031800	-7.14491300	0.09221600
C	-4.85520300	-8.74709900	1.94732900
C	-0.77081000	-4.14755500	1.20686000
H	-0.98199600	-5.50507800	2.82934200
C	-2.33605800	-4.33291600	-0.61943500
C	-4.07078900	-6.07363300	-0.53958900
C	-5.85282500	-7.76941500	-0.48257400
H	-4.47336900	-9.13782500	2.88386500
C	-5.95073700	-9.31612900	1.36841600
C	-1.26930600	-3.70269000	-0.05360800
H	0.05544700	-3.61661200	1.66984200
H	-2.75095400	-3.99010800	-1.56558200
H	-4.46429000	-5.70758100	-1.48673300
C	-6.46504900	-8.81794200	0.13516500
H	-6.22578700	-7.38446100	-1.42897500
H	-6.44047700	-10.15713300	1.84897900
H	-0.80980700	-2.84905600	-0.54501500
H	-7.34040700	-9.28230900	-0.30838300
C	-5.73410200	-3.50746300	7.50054000
C	-6.98876400	-3.10318500	6.99600100
C	-4.72940900	-2.54400300	7.73599300
C	-8.00904700	-4.04483600	6.63766200
C	-7.26109500	-1.70799500	6.78847800
C	-5.01294100	-1.15157000	7.52134000
C	-3.41991200	-2.89026800	8.20597400
C	-9.21224600	-3.62797000	6.15085500
H	-7.78306100	-5.10125400	6.71091700
C	-8.54465300	-1.31053500	6.29220800
C	-6.27293000	-0.76497700	7.06727600
C	-4.00165600	-0.17875700	7.80325200
H	-3.18663100	-3.93536400	8.37550600
C	-2.47242500	-1.93626200	8.43813100
C	-9.49279300	-2.23933800	5.98574100
H	-9.96095800	-4.35956000	5.86512100
H	-8.74164900	-0.24760000	6.16927300
H	-6.48859300	0.29358300	6.92730500
C	-2.76653900	-0.55383700	8.24249200
H	-4.25352300	0.87114600	7.66994800
H	-1.48714000	-2.22736500	8.78781500
H	-10.46136400	-1.92918900	5.60545800
H	-2.00793700	0.19366000	8.45796500

(R_a,*R*)-Int4

E = -4090.50352 a.u.

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C	-3.11296300	-0.70627000	1.49842400
C	-2.74873200	0.48804500	2.12362000
C	-2.38442500	0.54313700	3.46617000
C	-2.38480400	-0.62988200	4.22302100
C	-2.73155500	-1.83295600	3.61778500
C	-3.10324400	-1.89232600	2.26322900
H	-2.72198700	1.42105000	1.57628500
H	-2.12822800	-0.62849500	5.27750800
H	-2.74747400	-2.75143400	4.19518200
O	-2.05472000	1.78568500	3.94074700
O	-3.48421400	-3.03116900	1.67394400
C	-1.60595100	1.85244400	5.27417300
H	-2.38082400	1.51968900	5.97538700
H	-1.36371400	2.89863700	5.46427900
H	-0.71049500	1.23593300	5.42489800
C	-2.99679500	0.01134000	-1.00465800
C	-3.47973300	-0.11293900	-2.32777100
C	-1.80510600	0.71366500	-0.82888200
C	-2.85106500	0.53229700	-3.39137200
C	-1.15652500	1.34976300	-1.88931800
H	-1.35364600	0.74494000	0.15502500
C	-1.69166200	1.27394900	-3.16576200
H	-3.24139400	0.44525600	-4.39802400
H	-0.23380900	1.89080300	-1.70803400
H	-1.20567400	1.76959100	-4.00006300
O	-4.56562400	-0.92392100	-2.49228300
C	-5.03322100	-1.15368900	-3.80437100
H	-5.38599300	-0.22627100	-4.27054600
H	-5.86636600	-1.85013800	-3.70919600
H	-4.25162900	-1.59980500	-4.42966300
C	-3.70216900	-0.75877400	0.10172000
H	-3.66310700	-1.80835700	-0.20646000
H	-3.60212400	-3.74650500	2.36509300
C	-5.72325900	0.36725300	1.35096600
C	-5.31286400	-0.47659500	0.16682900
N	-6.02133600	-0.43098500	2.35004600
H	-5.64873500	-0.04667500	-0.77516100
C	-6.11548500	-0.09977800	3.76555900
H	-5.36814900	-0.70547700	4.28847400
H	-7.10979700	-0.35045400	4.14469500
H	-5.90012200	0.95989300	3.89885500
C	-5.91036300	1.82124600	1.34958900

C	-7.07514500	2.34401100	1.82132100
C	-7.36787000	3.82851500	1.81970500
C	-8.26974800	1.55098600	2.31298100
C	-8.62441600	4.17831700	1.00752400
H	-7.54477200	4.12014000	2.86637300
H	-6.52063400	4.41222700	1.47139200
C	-9.53377900	1.90317600	1.50473100
H	-8.44650900	1.79506200	3.37163100
H	-8.12045900	0.47398800	2.25169100
C	-9.83298300	3.39883300	1.51811800
H	-8.80224800	5.25716000	1.06272200
H	-8.44795200	3.93267400	-0.04805700
H	-10.37677900	1.33193700	1.90622200
H	-9.38714900	1.57106000	0.46876300
H	-10.71692500	3.61595000	0.90965400
H	-10.06380500	3.71682500	2.54405600
C	-4.84942100	2.60118700	0.57640900
C	-4.02675600	3.60766900	1.40569100
C	-5.36430000	3.24026900	-0.72684900
H	-4.12469600	1.85501300	0.23413700
C	-2.84964300	4.12153700	0.57075600
H	-4.64154300	4.46437200	1.70397700
H	-3.67177100	3.14104000	2.33121400
C	-4.18347600	3.76227800	-1.55006600
H	-6.05569500	4.06521700	-0.51260600
H	-5.92930300	2.49485200	-1.30143000
C	-3.33353900	4.74626500	-0.74116400
H	-2.26917100	4.84672800	1.15067100
H	-2.17504700	3.28490900	0.33916800
H	-4.54663100	4.23789500	-2.46790000
H	-3.55942100	2.91134000	-1.85523500
H	-2.47823200	5.08131700	-1.33787800
H	-3.93272400	5.63986700	-0.51379600
C	-5.91308900	-1.80645700	0.53870100
C	-6.17972600	-1.77903500	1.90414200
C	-6.01628400	-2.99809100	-0.15416900
C	-6.52421800	-2.89245900	2.64799900
C	-6.41681700	-4.13326000	0.55519900
H	-5.76662700	-3.04956600	-1.20998300
C	-6.64269800	-4.08639800	1.93147800
H	-6.66556900	-2.89282000	3.72525600
H	-6.52371600	-5.08086800	0.03769200
H	-6.89025600	-4.98561000	2.48370400
P	-4.65122600	-5.27848000	4.61770500

O	-3.69306700	-4.67094400	3.64291700
O	-4.59076100	-6.92348200	4.45635300
O	-3.88099800	-5.09240600	6.07994100
O	-6.08555900	-4.92102100	4.74197900
C	-1.49161500	-8.42811600	5.68147900
C	-2.79125400	-7.91817200	5.64932800
C	-3.33724100	-7.48322900	4.44650000
C	-2.60685800	-7.59373300	3.25118800
C	-1.32844800	-8.16347000	3.30779800
C	-0.75766300	-8.56988800	4.51118600
C	-1.07664400	-8.71206500	7.10697100
C	-2.11345100	-7.90535900	7.90951800
H	-0.76564200	-8.25167600	2.38257700
H	0.25140200	-8.97154500	4.53172200
H	-1.14730000	-9.78429200	7.33176300
H	-2.28165000	-8.28726000	8.92147800
H	-1.78426500	-6.86301800	7.98809600
C	-3.40291200	-7.94691900	7.03924300
C	-4.41877000	-6.92252300	7.51267800
C	-4.18413500	-9.26056100	7.32010600
C	-5.24965200	-7.48277900	8.48602100
C	-4.58940500	-5.59441100	7.14173600
C	-4.98196100	-8.96676500	8.60605100
H	-4.87631500	-9.43486000	6.48899000
H	-3.52241000	-10.12859100	7.40343200
C	-6.18581600	-6.70262900	9.15235100
C	-5.52092000	-4.78239200	7.80630300
H	-5.90349100	-9.55232500	8.67712900
C	-6.29595700	-5.35291500	8.82255200
H	-6.83245400	-7.13528100	9.91031600
H	-7.02066100	-4.72540000	9.33416500
H	-4.38831900	-9.18936600	9.50212300
H	-0.04659300	-8.40652300	7.31393300
C	-3.13348700	-7.10650100	1.94243800
C	-2.45480900	-6.07443200	1.25715600
C	-4.27217300	-7.70512100	1.36519100
C	-1.34038000	-5.37269800	1.82576900
C	-2.90571000	-5.66418600	-0.04295600
C	-4.72152600	-7.27716300	0.06966800
C	-5.00435700	-8.75354900	2.01250300
C	-0.69981300	-4.38620200	1.13572000
H	-1.03717900	-5.61617500	2.83732800
C	-2.20384600	-4.62607100	-0.73535600
C	-4.02252400	-6.27827700	-0.60674800

C	-5.88268800	-7.88702000	-0.50403600
H	-4.66904300	-9.10136000	2.98298500
C	-6.10698300	-9.30936400	1.43393500
C	-1.12795400	-4.01092000	-0.17179500
H	0.13032700	-3.85884500	1.59555600
H	-2.56072800	-4.33602600	-1.72129200
H	-4.36186200	-5.96536300	-1.59329400
C	-6.56062800	-8.86706000	0.15635100
H	-6.20758200	-7.54832900	-1.48533100
H	-6.64821600	-10.09711500	1.94833200
H	-0.60858100	-3.21708100	-0.70094700
H	-7.44155900	-9.32068400	-0.28747100
C	-5.70201000	-3.34234000	7.45901600
C	-6.94837700	-2.88671800	6.97811900
C	-4.65876000	-2.41865500	7.68717100
C	-8.00230400	-3.78886100	6.61356300
C	-7.17895400	-1.47923900	6.80814800
C	-4.89488400	-1.01435600	7.49380100
C	-3.35667100	-2.81915400	8.13324000
C	-9.20003400	-3.32380700	6.15648700
H	-7.80421200	-4.85260500	6.65504400
C	-8.45962400	-1.03106200	6.34788800
C	-6.15262600	-0.57562600	7.08085600
C	-3.83986000	-0.08392600	7.75660100
H	-3.16115800	-3.87337700	8.29156500
C	-2.36959700	-1.90391900	8.35489200
C	-9.44083600	-1.92309600	6.03361400
H	-9.97527700	-4.02483900	5.86502100
H	-8.62660600	0.04061000	6.25681100
H	-6.33464400	0.49243300	6.96724600
C	-2.61267100	-0.51064400	8.16912900
H	-4.04925900	0.97571500	7.62808800
H	-1.39036400	-2.23482400	8.68561000
H	-10.40726400	-1.57382300	5.68223400
H	-1.81975500	0.20495500	8.36855600

(S_a,*S*)-Int3

E = -4090.495131 a.u.

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C	2.23531000	2.39190400	1.13283300
C	2.51611800	2.91123300	2.45132600
C	1.51373500	3.12731000	3.33877500
C	0.15025300	2.79012300	2.98709700
C	-0.17544200	2.28738400	1.77368800

C	0.83839500	2.05703200	0.75879200
H	3.53090600	3.18586500	2.71816600
H	-0.64787700	2.96209100	3.70177900
H	-1.20606700	2.05720600	1.53466200
O	1.83405700	3.67066100	4.54584700
O	0.57802500	1.56970900	-0.35561700
C	0.78424500	4.04163700	5.41266100
H	0.23193300	3.16778100	5.77861800
H	1.25776500	4.54191000	6.25752200
H	0.08341600	4.73230400	4.92652500
C	4.62748200	2.15455600	0.35132400
C	5.45213100	2.67187000	-0.66241600
C	5.23175200	1.50868100	1.44218900
C	6.83517500	2.55709500	-0.59250200
C	6.61428300	1.37113900	1.50152400
H	4.60468500	1.07119900	2.21429900
C	7.41491200	1.89280400	0.48668400
H	7.43672300	2.97894300	-1.39158900
H	7.06108000	0.84121600	2.33615500
H	8.49406800	1.78500200	0.53325300
O	4.87810700	3.29110300	-1.74642900
C	4.47093800	4.62541900	-1.48409200
H	5.33632500	5.25174100	-1.23607900
H	3.99949800	4.99489200	-2.39643500
H	3.75096000	4.65999400	-0.65707300
C	3.17920600	2.17775400	0.17353900
H	2.80837700	1.97512000	-0.83043400
P	-2.22024500	-0.19357000	0.24252400
O	-1.33809100	-0.52451200	1.36723500
O	-3.15775500	-1.38134900	-0.33466900
O	-3.28037500	0.96161400	0.71757000
O	-1.59623800	0.33313100	-1.09660000
H	-0.75990900	0.86406300	-0.88941400
C	-5.95785700	-1.91845400	1.97474600
C	-5.20117800	-1.42300400	0.90921300
C	-3.96259100	-1.98332000	0.63071800
C	-3.51443900	-3.12047400	1.31571000
C	-4.31216300	-3.61759100	2.35231600
C	-5.51392000	-3.00923800	2.70930500
C	-7.21226900	-1.09332000	2.15228500
C	-6.90047400	0.16256900	1.31743600
H	-3.96351500	-4.49604400	2.88739400
H	-6.09609800	-3.39255900	3.54223600
H	-8.08816800	-1.62528500	1.75958500

H	-7.79183100	0.66844600	0.93381100
H	-6.33673400	0.87826600	1.92665400
C	-5.97423300	-0.34543400	0.17564800
C	-5.30570000	0.80862300	-0.54282000
C	-6.82810900	-0.93827200	-0.98064500
C	-6.09966700	1.23801200	-1.60980600
C	-4.12975600	1.48136700	-0.24717700
C	-7.25716300	0.28612400	-1.81227400
H	-6.18688200	-1.58892200	-1.58587800
H	-7.66842000	-1.53425900	-0.61157000
C	-5.76658900	2.38241800	-2.32157500
C	-3.79490500	2.66849800	-0.91465100
H	-7.42109200	0.04558600	-2.86669900
C	-4.63439200	3.10335200	-1.94623500
H	-6.37922700	2.71888600	-3.15277900
H	-4.37238900	4.01917800	-2.46841200
H	-8.19045000	0.71987600	-1.43131900
H	-7.41868400	-0.86417200	3.20182300
C	-2.29085500	-3.87005300	0.90390800
C	-1.10941700	-3.81517800	1.66628900
C	-2.36971800	-4.69412800	-0.23980600
C	-0.97295100	-2.97613200	2.82035600
C	0.02274300	-4.60756700	1.27130500
C	-1.23892000	-5.49825200	-0.60902100
C	-3.53735900	-4.76491900	-1.06752700
C	0.21084500	-2.89592600	3.48962700
H	-1.81494800	-2.36284600	3.11854600
C	1.24898300	-4.48938700	2.00177100
C	-0.07890600	-5.44580000	0.16378900
C	-1.31291800	-6.31531900	-1.78056000
H	-4.40787700	-4.17542500	-0.79920600
C	-3.56864200	-5.55491800	-2.17972600
C	1.34787500	-3.64909700	3.06807200
H	0.30904100	-2.22668700	4.33861000
H	2.10477600	-5.06994600	1.66526400
H	0.78071400	-6.04647100	-0.12757900
C	-2.43904800	-6.34235000	-2.54807800
H	-0.44261800	-6.91080300	-2.04507300
H	-4.46310700	-5.58714100	-2.79400400
H	2.29199600	-3.52820000	3.59215200
H	-2.48328900	-6.96178300	-3.43834900
C	-2.61839000	3.49754800	-0.51854600
C	-1.50122600	3.60913100	-1.36765400
C	-2.65599600	4.20915600	0.70251700

C	-1.38187500	2.86186800	-2.58697400
C	-0.40185700	4.45401200	-0.98735700
C	-1.56215500	5.06776400	1.05763500
C	-3.73981600	4.09128000	1.63174000
C	-0.24067200	2.91071000	-3.33081200
H	-2.19965300	2.21362500	-2.88129600
C	0.76672800	4.49590000	-1.81259000
C	-0.46506400	5.17430300	0.20218200
C	-1.58547800	5.75211700	2.31216000
H	-4.58347200	3.45919100	1.37572200
C	-3.72226300	4.75164800	2.82649800
C	0.85683100	3.73552700	-2.93796500
H	-0.15875400	2.31155900	-4.23221300
H	1.58438700	5.14163800	-1.50433700
H	0.37592100	5.80198400	0.49100000
C	-2.62811400	5.59512200	3.17778100
H	-0.74402000	6.39409500	2.56157700
H	-4.55181000	4.63948000	3.51741300
H	1.75940500	3.74926100	-3.54233900
H	-2.63594800	6.11664000	4.13021400
C	3.53144900	-1.60390100	-0.53354800
C	2.62708400	-0.86974600	0.19176200
N	4.47484400	-2.14822300	0.33231000
H	1.77813500	-0.34543800	-0.22442700
C	5.43052400	-3.18594600	0.02234200
H	5.25830000	-3.52509400	-1.00069900
H	6.46094000	-2.82553100	0.11377900
H	5.29023000	-4.03378000	0.70168700
C	3.49022900	-1.84635800	-1.99746700
C	2.45354400	-2.55891600	-2.48393900
C	2.06803200	-2.63797500	-3.94307700
C	1.42249700	-3.22724700	-1.60966800
C	0.69708500	-1.95117000	-4.14007100
H	1.97278500	-3.69351500	-4.23528700
H	2.80917800	-2.18187600	-4.60489600
C	0.08685700	-2.48372900	-1.75176400
H	1.27903700	-4.26091500	-1.96034700
H	1.73294000	-3.26852700	-0.56428500
C	-0.37902700	-2.51651200	-3.20636200
H	0.38966600	-2.04466500	-5.18808200
H	0.81153800	-0.87886400	-3.93096600
H	-0.67027300	-2.91657300	-1.09147300
H	0.22687400	-1.44346600	-1.43531300
H	-1.30838600	-1.94675100	-3.31534500

H	-0.60268900	-3.55669000	-3.48552400
C	4.47100500	-1.10751100	-2.90235200
C	3.87778800	0.22797000	-3.38758800
C	5.84965800	-0.83001800	-2.28593400
H	4.64309800	-1.73274600	-3.79050400
C	4.77402200	0.88122300	-4.44117300
H	3.77644600	0.89715700	-2.52075400
H	2.86973500	0.06770800	-3.78601200
C	6.78123300	-0.17345800	-3.31137600
H	5.73255100	-0.17652500	-1.40820300
H	6.31067400	-1.75865800	-1.93517200
C	6.18856600	1.10625800	-3.90454200
H	4.34203000	1.83458700	-4.76678100
H	4.81338500	0.22910900	-5.32608600
H	7.75040600	0.04292700	-2.84599400
H	6.97328800	-0.89200500	-4.12115100
H	6.84058100	1.48917000	-4.69862100
H	6.14040600	1.87832200	-3.13044900
C	2.99885400	-0.96122900	1.56845400
C	4.17135000	-1.75490400	1.61676000
C	2.46618400	-0.45224500	2.76172500
C	4.83620500	-2.02773600	2.81605400
C	3.13182400	-0.70454200	3.95273000
H	1.53496800	0.10922500	2.74802700
C	4.30797100	-1.48064800	3.97847200
H	5.73918500	-2.63117200	2.83923400
H	2.73864600	-0.30488700	4.88285800
H	4.80587700	-1.66204400	4.92616900

(S_a,*S*)-TS2

E = -4090.482802 a.u.

0 1

C	2.20578100	2.07818500	1.02783900
C	2.47406600	2.64996800	2.30112200
C	1.44331300	3.03824400	3.12508500
C	0.10796200	2.81535200	2.71235200
C	-0.18168800	2.25657700	1.48702300
C	0.84834200	1.90814400	0.59466500
H	3.49511200	2.82772500	2.61962400
H	-0.72439400	3.10470100	3.34571900
H	-1.21442800	2.11785200	1.19789700
O	1.78040300	3.62564700	4.30806600
O	0.64176700	1.40308300	-0.59812000
C	0.72578900	4.06495200	5.13582400

H	0.11032700	3.22550600	5.48238300
H	1.19647100	4.54416000	5.99437700
H	0.08261500	4.78788800	4.61810100
C	4.65353200	1.75271600	0.40644000
C	5.45043300	2.38452000	-0.56751300
C	5.28084900	1.26321000	1.56276200
C	6.82970100	2.47506600	-0.41823100
C	6.66223600	1.33730100	1.70394700
H	4.68117100	0.80146300	2.34035200
C	7.43798500	1.93140900	0.71013900
H	7.40438600	2.97145500	-1.19377900
H	7.13003200	0.92931800	2.59375500
H	8.51616600	1.98932500	0.82078700
O	4.86681400	2.92260000	-1.68578400
C	4.23643800	4.17912100	-1.46293900
H	4.96829800	4.91693300	-1.11428400
H	3.82378300	4.49008800	-2.42341400
H	3.42603200	4.09104200	-0.72949600
C	3.21498200	1.63146800	0.14753900
H	2.92501800	1.56589800	-0.89765000
P	-2.21644200	-0.15414400	0.23388800
O	-1.39743000	-0.58457800	1.38709300
O	-3.20707200	-1.34393500	-0.33121500
O	-3.31955400	0.96089400	0.79787900
O	-1.59820100	0.44980400	-1.00974200
H	-0.35173500	1.06336200	-0.77342500
C	-5.90727000	-1.95988200	2.06964300
C	-5.19707900	-1.43386900	0.98756900
C	-3.96149200	-1.96716600	0.64319300
C	-3.48296900	-3.11551300	1.29042600
C	-4.23352500	-3.64798200	2.34461200
C	-5.42719300	-3.06300500	2.76184000
C	-7.15900900	-1.14792100	2.31694300
C	-6.88874400	0.12917600	1.49948800
H	-3.85387000	-4.53301500	2.84742700
H	-5.97297200	-3.47145400	3.60748600
H	-8.04749300	-1.67624600	1.94768300
H	-7.79826200	0.63793400	1.16457400
H	-6.30378000	0.83378100	2.10148600
C	-6.00619300	-0.34648300	0.31108300
C	-5.36918700	0.82204100	-0.41194700
C	-6.90175500	-0.92389400	-0.82130100
C	-6.19762800	1.25826500	-1.44864000
C	-4.17913300	1.48573100	-0.14134600

C	-7.36386000	0.31073200	-1.61807800
H	-6.28018600	-1.56164400	-1.45999700
H	-7.72591800	-1.52966100	-0.43156800
C	-5.88530300	2.40297400	-2.16888900
C	-3.86610100	2.67144000	-0.82595300
H	-7.57163100	0.08506000	-2.66829100
C	-4.73557100	3.11274800	-1.83015200
H	-6.52367800	2.74517100	-2.97824000
H	-4.48295900	4.02638900	-2.36117100
H	-8.28054000	0.73913900	-1.19255900
H	-7.32420300	-0.94486700	3.37931600
C	-2.25875200	-3.83472300	0.83348900
C	-1.09249300	-3.84832700	1.62162000
C	-2.31502700	-4.57449700	-0.36828600
C	-0.96678900	-3.06759800	2.81758000
C	0.02951900	-4.64834400	1.21489600
C	-1.19064600	-5.37824200	-0.75844500
C	-3.45680600	-4.56060100	-1.23367500
C	0.19027700	-3.07390900	3.53685700
H	-1.79221200	-2.42810300	3.10525000
C	1.22849500	-4.62121600	1.99837400
C	-0.05697600	-5.41264200	0.05368200
C	-1.24772600	-6.11649400	-1.98261700
H	-4.31976100	-3.96721400	-0.95151900
C	-3.47104500	-5.27252300	-2.39758900
C	1.31083300	-3.85410900	3.12020200
H	0.27825700	-2.45545300	4.42479400
H	2.07348700	-5.21909300	1.66439000
H	0.79176200	-6.02607700	-0.24408900
C	-2.34980900	-6.06386100	-2.78294900
H	-0.38475900	-6.71740600	-2.25938800
H	-4.34535700	-5.23942100	-3.04005600
H	2.23141900	-3.81632200	3.69577300
H	-2.38141300	-6.62340500	-3.71271800
C	-2.67831100	3.50902700	-0.48578500
C	-1.60041200	3.62217400	-1.38594800
C	-2.67259200	4.24743200	0.71888300
C	-1.52574200	2.84996100	-2.59280400
C	-0.50988800	4.50842200	-1.08382400
C	-1.58332100	5.13954200	1.00209700
C	-3.70942100	4.12676700	1.70041200
C	-0.44576000	2.94320700	-3.41908700
H	-2.32360800	2.14909500	-2.80677400
C	0.59621400	4.58893900	-1.98925800

C	-0.53451300	5.25685200	0.09070200
C	-1.57321600	5.86329700	2.23584000
H	-4.54229800	3.46130000	1.50031800
C	-3.65826900	4.82334100	2.87336300
C	0.63342900	3.82697800	-3.11704600
H	-0.39765600	2.33140300	-4.31434700
H	1.40126300	5.27946100	-1.74978000
H	0.29523700	5.92400800	0.31659400
C	-2.57440800	5.70817900	3.14919800
H	-0.74063400	6.53573300	2.42896000
H	-4.45225900	4.70880000	3.60451500
H	1.48010000	3.88716900	-3.79527100
H	-2.55631600	6.26086600	4.08391400
C	3.65108100	-1.40693800	-0.48907500
C	2.70395300	-0.66901000	0.24153000
N	4.51902500	-1.99456600	0.38277900
H	1.77084600	-0.34416900	-0.19861100
C	5.52640200	-2.98756900	0.07220500
H	5.36821900	-3.33936600	-0.94792000
H	6.53454900	-2.57365400	0.16837300
H	5.41381800	-3.82965200	0.76069400
C	3.58919300	-1.67650300	-1.94877900
C	2.51476000	-2.37896500	-2.37033000
C	2.11140500	-2.54351100	-3.81681200
C	1.48912900	-2.99265900	-1.45028200
C	0.74232300	-1.85680300	-4.03388600
H	2.00175700	-3.61440300	-4.03780100
H	2.84908800	-2.13899300	-4.51439600
C	0.14277000	-2.27428200	-1.62482000
H	1.35518300	-4.04264200	-1.74848800
H	1.79826600	-2.99419300	-0.40199300
C	-0.32949200	-2.38221200	-3.07237400
H	0.43304400	-1.99324800	-5.07623600
H	0.86287600	-0.77727900	-3.86922700
H	-0.59993000	-2.68876300	-0.93752500
H	0.25028400	-1.21559000	-1.36422400
H	-1.25858300	-1.81646500	-3.19666300
H	-0.55291000	-3.43420500	-3.30355900
C	4.59046800	-1.04671700	-2.91375000
C	4.03103000	0.25901300	-3.50720600
C	5.98254000	-0.78379600	-2.32191800
H	4.73212100	-1.75130600	-3.74587500
C	4.96397100	0.84122000	-4.57048700
H	3.91039800	0.99096800	-2.69927100

H	3.03460300	0.07846800	-3.92517800
C	6.92914900	-0.18218600	-3.36647300
H	5.89534300	-0.10566000	-1.46042400
H	6.42286100	-1.71475000	-1.95344700
C	6.36295400	1.08727100	-4.00305800
H	4.54545600	1.77424100	-4.96424400
H	5.02916300	0.13972000	-5.41511400
H	7.90162600	0.02486000	-2.90461400
H	7.10564700	-0.93080100	-4.15204300
H	7.03695700	1.44524600	-4.78975500
H	6.29777900	1.87801400	-3.24716400
C	2.95783500	-0.92697600	1.63243600
C	4.13104200	-1.70443400	1.69004800
C	2.33029600	-0.53132900	2.81843600
C	4.73859000	-2.05906500	2.89220300
C	2.93452000	-0.87079600	4.02388300
H	1.38129900	-0.00208700	2.78682200
C	4.12646700	-1.61529500	4.06052300
H	5.65465400	-2.64098000	2.92241100
H	2.47136400	-0.56713400	4.95756700
H	4.57077000	-1.86268100	5.01948200

(S_a,*S*)-Int4

E = -4090.512006 a.u.

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C	2.26625900	1.86962200	1.00543300
C	2.53598600	2.55266900	2.18723600
C	1.49956400	3.14463400	2.91317600
C	0.18654700	3.02262000	2.45835900
C	-0.07968600	2.36030600	1.26306300
C	0.95073400	1.80992700	0.50842800
H	3.54884300	2.62919800	2.57210700
H	-0.64678600	3.45199600	3.00409100
H	-1.10149600	2.28133300	0.91152200
O	1.86586200	3.80642800	4.05360200
O	0.77478200	1.19790900	-0.68155200
C	0.83058000	4.41995300	4.78439700
H	0.11248300	3.68078000	5.16252000
H	1.30742400	4.92456700	5.62554300
H	0.28714600	5.15308900	4.17427300
C	4.73612500	1.51358400	0.48026900
C	5.31308200	2.45070800	-0.39662200
C	5.53094600	1.05903700	1.53988600
C	6.63284500	2.86969800	-0.24700000

C	6.85144700	1.47661300	1.69482000
H	5.11527000	0.37962000	2.27463600
C	7.41100000	2.37647900	0.79440300
H	7.02850100	3.57915800	-0.96744700
H	7.43699300	1.09880500	2.52674300
H	8.44032600	2.70169300	0.90623000
O	4.61128200	2.92782300	-1.47598300
C	3.78300800	4.05573900	-1.20414000
H	4.38480600	4.88152100	-0.80617600
H	3.34203300	4.34169000	-2.15918800
H	2.98584800	3.80483400	-0.49622100
C	3.30486700	1.08353700	0.23088800
H	3.09050900	1.23927800	-0.83057400
P	-2.22972400	-0.15206600	0.14783600
O	-1.39120700	-0.61425000	1.27744500
O	-3.26333000	-1.35053300	-0.36335900
O	-3.31802500	0.96089900	0.75030600
O	-1.65842600	0.42444000	-1.11914500
H	-0.19852500	1.00360500	-0.87168200
C	-5.80432600	-1.96354100	2.20346000
C	-5.16759900	-1.44351100	1.07426100
C	-3.95394300	-1.97060200	0.65133400
C	-3.43481900	-3.11606600	1.27243300
C	-4.11368400	-3.64748800	2.37508000
C	-5.27857500	-3.06339900	2.86765500
C	-7.03597900	-1.14763600	2.52815000
C	-6.82256000	0.12248800	1.68191400
H	-3.70014800	-4.52938800	2.85657600
H	-5.76638400	-3.46921600	3.74923500
H	-7.94813900	-1.67852500	2.22617300
H	-7.75357000	0.62673100	1.40376300
H	-6.19940500	0.83333900	2.23618500
C	-6.02114900	-0.36473000	0.44264300
C	-5.43123700	0.78920300	-0.34081000
C	-6.98883100	-0.96220300	-0.61834500
C	-6.31987400	1.20080800	-1.33653800
C	-4.22617000	1.45781500	-0.15474900
C	-7.49844100	0.25636200	-1.40930000
H	-6.40969300	-1.61356800	-1.28281200
H	-7.78681600	-1.55891300	-0.16507400
C	-6.04899300	2.32286700	-2.10704800
C	-3.95602600	2.62412300	-0.88892600
H	-7.77631300	0.00928700	-2.43840000
C	-4.88054300	3.03745800	-1.85559100

H	-6.73366400	2.64422200	-2.88664300
H	-4.65808600	3.93603900	-2.42445900
H	-8.38347200	0.69815600	-0.93308600
H	-7.12732000	-0.93464500	3.59752600
C	-2.23566200	-3.82971800	0.75061900
C	-1.06001600	-3.91002500	1.52291400
C	-2.31672000	-4.50485000	-0.48747900
C	-0.88827500	-3.15291300	2.72815600
C	0.02240700	-4.74741600	1.08649700
C	-1.21843100	-5.32155100	-0.92409700
C	-3.46153900	-4.41488200	-1.34447800
C	0.26027700	-3.25036000	3.45626600
H	-1.66910800	-2.45882700	3.01429700
C	1.20725500	-4.82813900	1.88656800
C	-0.09144000	-5.44867300	-0.11234400
C	-1.30028200	-5.99139000	-2.18611200
H	-4.30679800	-3.81516600	-1.02646800
C	-3.49882400	-5.06093200	-2.54530700
C	1.32102300	-4.10849000	3.03817600
H	0.38279600	-2.65506400	4.35582000
H	2.00868500	-5.48423600	1.55225700
H	0.72702700	-6.09035500	-0.43544700
C	-2.40143900	-5.86134500	-2.97821900
H	-0.45788500	-6.60459200	-2.49717200
H	-4.37365000	-4.96829300	-3.18096500
H	2.22108800	-4.17709100	3.64138200
H	-2.45192000	-6.36850800	-3.93678300
C	-2.76658700	3.48761900	-0.63100000
C	-1.73998000	3.60006900	-1.58908300
C	-2.72787000	4.27415700	0.54169700
C	-1.70152700	2.78514600	-2.76874100
C	-0.67594100	4.54337200	-1.38462900
C	-1.65958900	5.21463200	0.73284900
C	-3.71535100	4.16675300	1.57472800
C	-0.68924100	2.90976100	-3.67345500
H	-2.46988600	2.03298500	-2.89983600
C	0.35551800	4.65570900	-2.37034300
C	-0.66571700	5.33369000	-0.23742000
C	-1.62346200	6.00057000	1.92763900
H	-4.53070000	3.46314100	1.44627300
C	-3.63936800	4.92364500	2.70797700
C	0.35302900	3.86513100	-3.47899400
H	-0.66857200	2.27051500	-4.55063200
H	1.13543700	5.39618800	-2.20986900

H	0.14354100	6.04546300	-0.08620600
C	-2.57834100	5.85908300	2.89075400
H	-0.80754000	6.70900300	2.04988600
H	-4.39566900	4.81805000	3.47944600
H	1.14262300	3.95541300	-4.21966000
H	-2.53967700	6.45828000	3.79568800
C	3.76489400	-1.40327200	-0.36746800
C	2.97273100	-0.44227600	0.46848900
N	4.41172300	-2.23525700	0.41063200
H	1.92470400	-0.52639600	0.13609500
C	5.17505300	-3.40002200	-0.01397900
H	5.09866300	-3.49247000	-1.09626000
H	6.21817700	-3.28198500	0.28766000
H	4.74578500	-4.28171000	0.46846400
C	3.65435800	-1.55428500	-1.83779700
C	2.55670600	-2.22602000	-2.24285600
C	2.12613500	-2.34298300	-3.68318500
C	1.54919500	-2.85134000	-1.31023600
C	0.77357100	-1.61004800	-3.84586800
H	1.97821500	-3.40479500	-3.92378700
H	2.87030000	-1.94677200	-4.37831400
C	0.19678800	-2.13781900	-1.45397300
H	1.42570300	-3.90175900	-1.60886500
H	1.86513700	-2.86634500	-0.26015600
C	-0.29022400	-2.17525700	-2.89910200
H	0.45005800	-1.68359200	-4.88983200
H	0.91940400	-0.54487900	-3.61967700
H	-0.53592000	-2.58707900	-0.77983000
H	0.30578500	-1.09492100	-1.14362500
H	-1.21300600	-1.59176400	-2.97256500
H	-0.52669700	-3.21206400	-3.18182400
C	4.69880400	-0.94821700	-2.77071800
C	4.20091100	0.34947600	-3.43143300
C	6.05691900	-0.71401000	-2.08991000
H	4.86527400	-1.68191400	-3.57401600
C	5.22825700	0.89528300	-4.42457800
H	4.02428700	1.10638200	-2.66095600
H	3.24006100	0.16889900	-3.92496000
C	7.08328600	-0.14260500	-3.07204400
H	5.93423300	-0.01243700	-1.25359700
H	6.44057600	-1.65145200	-1.66651800
C	6.57233800	1.13715600	-3.73628600
H	4.85501500	1.82504000	-4.86654100
H	5.36142200	0.17917800	-5.24875600

H	8.02565500	0.04827400	-2.54700800
H	7.29496500	-0.89292500	-3.84715400
H	7.31154800	1.50847200	-4.45461100
H	6.43987100	1.91492000	-2.97337700
C	3.18072000	-0.97050000	1.85574100
C	4.11531100	-2.00115600	1.78615000
C	2.65919200	-0.60878900	3.09145100
C	4.63225700	-2.65520300	2.89178600
C	3.16009800	-1.25350700	4.22500600
H	1.88717300	0.14934800	3.16684500
C	4.14326800	-2.24299200	4.13177100
H	5.37331900	-3.44333400	2.80802100
H	2.77533400	-0.98006200	5.20206100
H	4.51625100	-2.71612700	5.03413200

(S_a,*R*)-Int3

E = -4090.497009 a.u.

0 1

C	-1.13684200	15.04595700	-9.47143700
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N	-0.28892900	14.01662700	-9.85257600
H	-1.79435800	15.79466200	-7.53300900
C	-0.02217700	13.64131500	-11.22224300
H	-0.94549000	13.34232900	-11.72995200
H	0.42690200	14.47936000	-11.76607100
H	0.68839800	12.81357800	-11.23589300
C	-1.87392700	15.86331500	-10.46807900
C	-3.20285300	15.66805500	-10.58895000
C	-4.15279000	16.54143500	-11.38002400
C	-3.94462700	14.55147000	-9.88203900
C	-5.23180300	17.10952300	-10.43995400
H	-4.64099800	15.93658200	-12.15910900
H	-3.64608300	17.36826900	-11.87715700
C	-5.02007900	15.10311800	-8.93650100
H	-4.44828000	13.94729600	-10.65310100
H	-3.26254400	13.89167000	-9.34343400
C	-5.98845200	16.00830600	-9.69769500
H	-4.73523300	17.76650000	-9.71467000
H	-5.55843000	14.27761300	-8.45790800
H	-4.52839400	15.67588100	-8.13916900
H	-6.72414000	16.44795400	-9.01475000
H	-6.54966200	15.40294300	-10.42361700
C	-1.03444000	16.87311300	-11.24930600
C	-1.15295700	16.71956100	-12.77901800

C	-1.25642600	18.33251600	-10.79957000
H	0.01699700	16.64577700	-11.00683800
C	-0.22280600	17.68894800	-13.51092000
H	-2.18113700	16.91023700	-13.10548900
H	-0.93353700	15.68291700	-13.06331400
C	-0.36145800	19.30056500	-11.57551200
H	-2.30726600	18.61612100	-10.94664000
H	-1.05392600	18.42517300	-9.72643200
C	-0.51152600	19.12951800	-13.08719100
H	-0.33866600	17.57291200	-14.59518700
H	0.81971700	17.43798700	-13.27160100
H	-0.58618600	20.32966600	-11.27368100
H	0.68394800	19.11865700	-11.29142300
H	0.13820600	19.83534900	-13.61800200
H	-1.54302600	19.37751600	-13.37566800
C	-0.41682000	14.00562400	-7.59881500
C	0.14539200	13.35402100	-8.72576300
C	-0.14860000	13.49855700	-6.31739700
C	0.96916600	12.22853500	-8.59492300
C	0.66478300	12.38788700	-6.18412500
H	-0.57475700	13.98195000	-5.44161700
C	1.22267600	11.76130400	-7.31567800
H	1.40193400	11.73623200	-9.46149400
H	0.88779300	11.99726800	-5.19614200
H	1.86148300	10.89349300	-7.18306900
C	2.59126900	15.96393200	-9.15874200
C	2.88840700	14.73343000	-9.84411500
C	3.09526500	14.70504300	-11.18568800
C	3.06985500	15.92970800	-11.95199700
C	2.81358800	17.12394900	-11.36435200
C	2.54084000	17.22066800	-9.93691500
H	2.84775000	13.79372100	-9.30670700
H	3.25341000	15.89928100	-13.02140100
H	2.80142100	18.04841000	-11.93397700
O	3.28742100	13.48190800	-11.76614200
O	2.31540700	18.31126400	-9.38727600
C	3.30050200	13.40576100	-13.17407400
H	4.16572000	13.92569700	-13.60299400
H	3.37004100	12.34535800	-13.41701300
H	2.38025700	13.81635700	-13.60981700
C	2.65147600	15.20522300	-6.71642400
C	2.05827400	15.49960600	-5.46059500
C	3.61598700	14.18826900	-6.76769600
C	2.44111500	14.80487700	-4.31300900

C	3.98828900	13.48450900	-5.62878400
H	4.12176400	13.98892300	-7.70571400
C	3.40248600	13.80064900	-4.40646000
H	1.99252400	15.03352900	-3.35373000
H	4.74548100	12.71075100	-5.69115100
H	3.69543800	13.26513200	-3.50849200
O	1.12289000	16.46847900	-5.47418600
C	0.55795300	16.87930200	-4.24674100
H	1.33120200	17.24119600	-3.55976000
H	-0.11957900	17.69615300	-4.49113200
H	-0.00155700	16.06009600	-3.77923400
C	2.36501600	16.10430900	-7.81442000
H	1.98837000	17.08038600	-7.51714000
P	1.43733700	21.57498700	-9.18927900
O	0.17381000	20.97135900	-8.75305600
O	1.31233900	22.90378000	-10.11986600
O	2.27071100	22.12174900	-7.89671400
O	2.45325700	20.77022100	-10.07031200
H	2.41900000	19.77232500	-9.88916500
C	0.39686600	25.82474700	-8.09862600
C	1.16954500	24.86980900	-8.76440100
C	0.54952500	23.92085900	-9.56513000
C	-0.83119300	23.96420600	-9.79362600
C	-1.57244600	24.96748300	-9.15637700
C	-0.97635000	25.88296700	-8.29326700
C	1.26940700	26.66101100	-7.19056700
C	2.55605600	25.81857800	-7.10994500
H	-2.64407300	24.99977200	-9.33023300
H	-1.58036500	26.62433000	-7.77831900
H	1.46548900	27.64645300	-7.63214000
H	3.45327800	26.40524800	-6.89020100
H	2.44749600	25.05533600	-6.33111400
C	2.64012400	25.10466800	-8.48937500
C	3.66288700	23.98632100	-8.47579100
C	3.27983800	26.05786500	-9.53759800
C	4.91760300	24.48456100	-8.83829700
C	3.52986900	22.64886200	-8.12706600
C	4.79618000	25.91648500	-9.30813500
H	3.02283500	25.69456400	-10.53894700
H	2.91456300	27.08501200	-9.44254300
C	6.04691800	23.68102500	-8.76515000
C	4.65602100	21.82212400	-8.01677600
H	5.38232700	26.11035200	-10.21124000
C	5.90833900	22.36635800	-8.32835900

H	7.02335400	24.06650500	-9.04365200
H	6.78053400	21.72419300	-8.24619700
H	5.14956500	26.61404400	-8.53811800
H	0.81174100	26.83201100	-6.21179300
C	-1.52921300	23.00835700	-10.69837100
C	-2.52813900	22.16245500	-10.17647300
C	-1.26634200	23.02921700	-12.08453500
C	-2.77173900	22.03808700	-8.76928800
C	-3.33108200	21.37768000	-11.07085200
C	-2.05140500	22.20964400	-12.96421400
C	-0.25461500	23.85794600	-12.67049600
C	-3.77652000	21.24703200	-8.29791400
H	-2.11581600	22.55827100	-8.08129100
C	-4.38034800	20.56468000	-10.53583200
C	-3.07637000	21.42191700	-12.44017000
C	-1.77490500	22.22446400	-14.36798200
H	0.33408100	24.50268600	-12.02736800
C	-0.02157900	23.84501300	-14.01401100
C	-4.60770200	20.51126800	-9.19372600
H	-3.93722400	21.15815700	-7.22826600
H	-4.98860500	19.98872700	-11.22939200
H	-3.68574100	20.82300200	-13.11491600
C	-0.78806300	23.01118000	-14.88035900
H	-2.37324000	21.58689800	-15.01407600
H	0.75549000	24.47661300	-14.43297800
H	-5.41055100	19.89535500	-8.79908500
H	-0.58391800	23.01282200	-15.94648200
C	4.57439700	20.40535300	-7.56095000
C	5.01534100	19.37407500	-8.41407800
C	4.16163500	20.10501500	-6.24379200
C	5.33162200	19.59939200	-9.79596200
C	5.12928800	18.03372500	-7.91121700
C	4.24415500	18.75309700	-5.76669600
C	3.68868700	21.10303000	-5.33142300
C	5.74974400	18.57755500	-10.59700100
H	5.19438800	20.59424300	-10.20492100
C	5.59990700	16.99659300	-8.77676300
C	4.75700800	17.75701000	-6.59747300
C	3.82721800	18.44964500	-4.43238000
H	3.64090100	22.13516800	-5.65945400
C	3.29903400	20.77656300	-4.06547200
C	5.89889300	17.25463000	-10.08022000
H	5.96338900	18.76631700	-11.64475200
H	5.68460200	15.99091800	-8.37115600

H	4.85881000	16.74413000	-6.21343900
C	3.36254600	19.42870800	-3.60559300
H	3.89915200	17.41618500	-4.09840300
H	2.93908200	21.55123100	-3.39581400
H	6.22964300	16.45491400	-10.73609300
H	3.05238000	19.19264500	-2.59168300
H	-5.93007600	17.73111600	-11.01360200

(S_a,*R*)-TS2

E = -4090.475907 a.u.

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C	-0.71335500	14.81961300	-9.63757900
C	-0.38160100	14.65996600	-8.27432500
N	-0.18595300	13.78580600	-10.33543000
H	-0.85455400	15.22914000	-7.48382600
C	-0.22315500	13.62983300	-11.77538200
H	-1.20903900	13.92216000	-12.13882800
H	0.54720500	14.25103500	-12.24608700
H	-0.04777300	12.58303600	-12.02219000
C	-1.58698900	15.83336100	-10.28787500
C	-2.91245000	15.70663600	-10.06973700
C	-3.97895000	16.64227500	-10.59243700
C	-3.52345800	14.61236500	-9.21722600
C	-4.74891000	17.26632000	-9.41511100
H	-4.68211200	16.05740800	-11.20403400
H	-3.57587300	17.43064500	-11.22556900
C	-4.27376900	15.21855500	-8.02103600
H	-4.25026800	14.06662900	-9.83730800
H	-2.78540400	13.88273900	-8.87647000
C	-5.34627500	16.19800200	-8.49843500
H	-4.05957400	17.90563500	-8.84886100
H	-4.71987200	14.42023900	-7.41806400
H	-3.55326800	15.74597700	-7.38142900
H	-5.84352000	16.66759100	-7.64272000
H	-6.11764100	15.64027200	-9.04801700
C	-0.89978300	16.87130300	-11.17797400
C	-1.29570300	16.77503100	-12.66706300
C	-1.04934700	18.32320300	-10.66293000
H	0.17724800	16.64343000	-11.14532500
C	-0.45073400	17.73290900	-13.50765200
H	-2.35483800	17.03036800	-12.79546900
H	-1.17996900	15.75144200	-13.03468000
C	-0.32055000	19.32661000	-11.56166500
H	-2.11057400	18.59991200	-10.61528600

H	-0.65877000	18.40861100	-9.64347700
C	-0.67849000	19.16691700	-13.03816600
H	-0.70356300	17.62308100	-14.56884400
H	0.61129600	17.46651400	-13.39762200
H	-0.54885000	20.33866100	-11.21099700
H	0.76188500	19.20231900	-11.43899100
H	-0.10832200	19.88080600	-13.64354900
H	-1.73934400	19.41029500	-13.18507500
C	0.21367600	13.34705100	-8.15297300
C	0.38225100	12.85815800	-9.46206600
C	0.67607600	12.58122900	-7.07808500
C	1.02753100	11.65590100	-9.74075000
C	1.30006700	11.36817100	-7.34098900
H	0.55842000	12.93221700	-6.05662900
C	1.48137500	10.91492900	-8.65596500
H	1.19169000	11.31262200	-10.75644000
H	1.66272100	10.76460800	-6.51528100
H	1.98537500	9.97049000	-8.83195100
C	2.20768100	15.97730000	-9.31530700
C	2.73033200	14.87508600	-10.01815500
C	3.26700800	15.03506600	-11.28369800
C	3.33577100	16.32171300	-11.85193700
C	2.88290700	17.42893100	-11.15604200
C	2.30879100	17.28739900	-9.87824300
H	2.67340600	13.87115100	-9.61280000
H	3.76026300	16.46616300	-12.83960200
H	2.97081200	18.42779800	-11.57307700
O	3.68206600	13.89124300	-11.91250800
O	1.87667100	18.29605600	-9.16270000
C	4.32700400	14.03951500	-13.15522400
H	5.21707400	14.67619700	-13.07267400
H	4.62797000	13.03833300	-13.46449000
H	3.65459500	14.46372600	-13.91225000
C	2.01984000	15.29306900	-6.83852100
C	1.39964000	15.64856700	-5.61208500
C	3.12006100	14.42396200	-6.80456000
C	1.90148800	15.16307300	-4.40316300
C	3.61676300	13.93654400	-5.60322200
H	3.60907300	14.16389200	-7.73620700
C	3.00661200	14.31380800	-4.40825900
H	1.44230400	15.44655300	-3.46360300
H	4.47674500	13.27628600	-5.59644100
H	3.39186300	13.94603900	-3.46223300
O	0.32094100	16.44811900	-5.70768000

C	-0.18739200	17.05278200	-4.52854900
H	0.59988400	17.61615700	-4.01749000
H	-0.96588700	17.73684000	-4.86236200
H	-0.61773700	16.30087000	-3.85769700
C	1.53533200	15.92982500	-8.04467800
H	0.93949800	16.81777300	-7.85112400
P	1.38018100	21.51723700	-9.25275900
O	0.03156600	21.09913500	-8.81874900
O	1.33977400	22.83576000	-10.25166700
O	2.14158400	22.17028900	-7.93239900
O	2.35314800	20.58080100	-9.94399300
H	2.09123200	19.25523200	-9.55562400
C	0.54207300	25.92524500	-8.44647500
C	1.27383300	24.88493700	-9.02478300
C	0.62348800	23.90824200	-9.77197400
C	-0.75416900	24.00906400	-10.01406200
C	-1.45425500	25.08868700	-9.46119100
C	-0.82403800	26.03884300	-8.66340100
C	1.44039200	26.78295800	-7.58528200
C	2.66789300	25.87430900	-7.39797400
H	-2.52195500	25.15688100	-9.64988800
H	-1.39507000	26.84593500	-8.21349700
H	1.70946200	27.71332100	-8.10227000
H	3.59387400	26.41980500	-7.19067600
H	2.48689000	25.18087600	-6.56890600
C	2.74848600	25.05044000	-8.71546900
C	3.69067800	23.87405900	-8.56400800
C	3.49693600	25.87051700	-9.80233400
C	4.99216200	24.26043500	-8.89126400
C	3.43740200	22.58093600	-8.12294500
C	4.98954500	25.65150100	-9.48560900
H	3.26077400	25.44188300	-10.78265800
H	3.19982500	26.92405500	-9.80826400
C	6.05872100	23.39649700	-8.68174800
C	4.49957800	21.69621600	-7.88474500
H	5.62688400	25.72724800	-10.37184400
C	5.80330000	22.13393600	-8.15273100
H	7.07443600	23.69362800	-8.92668300
H	6.62413900	21.44677400	-7.96718300
H	5.35558000	26.39087300	-8.76157800
H	0.96990700	27.06474900	-6.63847100
C	-1.50559800	23.03623500	-10.85680700
C	-2.52955000	22.26003500	-10.27859900
C	-1.28085000	22.98871400	-12.24846600

C	-2.74064600	22.20990500	-8.86187400
C	-3.39167000	21.47775500	-11.11877400
C	-2.14120300	22.19279000	-13.07749100
C	-0.23337700	23.72926000	-12.88723900
C	-3.76714300	21.48767400	-8.33069200
H	-2.03928900	22.72677900	-8.21827900
C	-4.45752100	20.73067200	-10.52121600
C	-3.18626800	21.47423100	-12.49718400
C	-1.91235100	22.15521100	-14.48947100
H	0.41901800	24.34390700	-12.27721700
C	-0.04371300	23.66341500	-14.23606100
C	-4.65073200	20.74896600	-9.17235300
H	-3.90533900	21.45552600	-7.25460900
H	-5.11368300	20.15855000	-11.17385000
H	-3.84888200	20.89081500	-13.13445200
C	-0.89412200	22.86234200	-15.05412000
H	-2.56992300	21.53978500	-15.09872100
H	0.76262800	24.22584200	-14.69626700
H	-5.46947700	20.18939400	-8.72875600
H	-0.72616100	22.82285900	-16.12602800
C	4.29069000	20.32211000	-7.34676500
C	4.75965500	19.21188300	-8.08014100
C	3.74230100	20.13194900	-6.05953500
C	5.25044700	19.33336800	-9.42263400
C	4.75541700	17.90556100	-7.48368500
C	3.70624400	18.81325200	-5.49126500
C	3.25218900	21.21413900	-5.25778400
C	5.76778700	18.25726600	-10.08233000
H	5.16973300	20.29489200	-9.91646100
C	5.31496600	16.80486200	-8.20892300
C	4.22964400	17.73547500	-6.20426100
C	3.17901100	18.63167400	-4.17316600
H	3.28573600	22.22002400	-5.65914500
C	2.74586200	21.00062400	-4.00944300
C	5.81944000	16.97315800	-9.46287600
H	6.12203400	18.36984300	-11.10292700
H	5.33445100	15.83236800	-7.72346700
H	4.24461100	16.74897300	-5.74331300
C	2.70584300	19.68841900	-3.45344000
H	3.18558300	17.62605800	-3.75775200
H	2.37548800	21.83805600	-3.42678400
H	6.23715100	16.12973400	-10.00513000
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H	-5.53733500	17.91970100	-9.80432000

(S_a,*R*)-Int4

E = -4090.503618 a.u.

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C	-0.75783700	14.70567300	-9.53489600
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N	-0.84249200	13.55776700	-10.16168600
H	-0.54299900	14.74058100	-7.44613600
C	-1.67966100	13.24588600	-11.31369800
H	-2.40084200	14.04875900	-11.45012300
H	-1.05269400	13.13997300	-12.20190500
H	-2.19841000	12.30711400	-11.11027000
C	-1.52641900	15.90723500	-9.94220600
C	-2.72882900	16.04150200	-9.34770600
C	-3.70407700	17.17053500	-9.56748100
C	-3.20525200	15.13767400	-8.22775400
C	-3.77084600	18.02447800	-8.28687600
H	-4.69468100	16.72855100	-9.74901700
H	-3.46281900	17.78776200	-10.43195400
C	-3.20625900	15.95478200	-6.92204800
H	-4.23239200	14.81330200	-8.44246000
H	-2.60994700	14.22584700	-8.11420600
C	-4.12018400	17.17472100	-7.06116800
H	-2.80524400	18.52750600	-8.14831800
H	-3.52814000	15.32434100	-6.08565800
H	-2.17751800	16.28132800	-6.71351200
H	-4.07105300	17.78770700	-6.15512800
H	-5.15810700	16.82444900	-7.15134700
C	-0.87392700	16.79174900	-11.01490700
C	-1.50034900	16.56642100	-12.40524500
C	-0.80578800	18.29497900	-10.65562700
H	0.16845200	16.45748200	-11.10605800
C	-0.72272500	17.34316400	-13.46762400
H	-2.55031100	16.89423100	-12.39774700
H	-1.49637300	15.50128100	-12.66010300
C	-0.12649700	19.10566700	-11.76581400
H	-1.80680100	18.71463400	-10.50353500
H	-0.26351400	18.43718200	-9.71456300
C	-0.74413900	18.83124900	-13.13676200
H	-1.15318200	17.15349500	-14.45803700
H	0.31407200	16.97572500	-13.48642900
H	-0.20744900	20.16718100	-11.50883900
H	0.94339300	18.86962400	-11.79247300
H	-0.23138700	19.41582900	-13.90902000

H	-1.78994700	19.16127500	-13.13225100
C	0.48505600	13.09109500	-8.36462800
C	-0.08899400	12.54040500	-9.50756000
C	1.20739200	12.26126000	-7.51393500
C	0.05262800	11.21687900	-9.88995900
C	1.36325500	10.92012000	-7.87076200
H	1.64020600	12.63895200	-6.59452700
C	0.80719900	10.40635800	-9.04325400
H	-0.38978200	10.82486200	-10.79920800
H	1.93199000	10.26366100	-7.22082800
H	0.95484200	9.36250600	-9.29778500
C	2.01190800	15.88769000	-9.44860500
C	2.31436900	14.90865600	-10.39301800
C	2.92321400	15.24216100	-11.60386400
C	3.24145900	16.57585500	-11.86446500
C	2.96563000	17.55723200	-10.91552500
C	2.36131100	17.23030000	-9.69771200
H	2.09136600	13.85953200	-10.21594200
H	3.70598000	16.86878800	-12.79921800
H	3.20190900	18.59982200	-11.10624500
O	3.15653900	14.19979200	-12.46188400
O	2.05785700	18.13902900	-8.76362200
C	3.77165400	14.51507000	-13.68719500
H	4.76049100	14.96625000	-13.53643700
H	3.88381400	13.57359000	-14.22612800
H	3.15540600	15.20273700	-14.28124400
C	2.09976100	15.22314900	-6.99094200
C	1.57702400	15.38973200	-5.69557300
C	3.33535700	14.60421200	-7.13961400
C	2.28327600	14.93197100	-4.58260400
C	4.04792200	14.13721100	-6.03386600
H	3.73959000	14.48931600	-8.14122900
C	3.51649300	14.30129100	-4.76018800
H	1.88362500	15.06134300	-3.58327500
H	5.01113400	13.65629800	-6.17010900
H	4.05946000	13.94684600	-3.88956200
O	0.34673300	15.96812700	-5.62692900
C	-0.11403000	16.39836100	-4.35922300
H	0.61004900	17.07774400	-3.89723500
H	-1.04507500	16.93413100	-4.54406700
H	-0.30953800	15.54598200	-3.69759600
C	1.24567900	15.62084500	-8.17697200
H	0.73476700	16.55396100	-7.91750600
P	1.27721300	21.44778100	-9.28130100

O	-0.13225300	21.07627100	-9.01809800
O	1.36186500	22.77528900	-10.28372000
O	1.88159100	22.11551900	-7.88121300
O	2.30481900	20.48999700	-9.82578100
H	2.19404800	19.07263500	-9.12872400
C	0.09251800	25.75588800	-8.56081400
C	0.97557300	24.78639900	-9.04296200
C	0.52993300	23.80993200	-9.92778600
C	-0.77530600	23.87853500	-10.43556200
C	-1.62576100	24.89271100	-9.97814300
C	-1.21479900	25.81677300	-9.02205600
C	0.77303000	26.61187200	-7.51627400
C	2.02450600	25.78048900	-7.17848500
H	-2.63708200	24.93034700	-10.37348600
H	-1.90505100	26.56803700	-8.64905600
H	1.04561700	27.59255800	-7.92751700
H	2.86290100	26.37777000	-6.80604000
H	1.77447800	25.02984100	-6.42031400
C	2.36582900	25.04188600	-8.50256000
C	3.37301100	23.93365500	-8.28768100
C	3.17601800	25.98383900	-9.43766900
C	4.66914200	24.42807300	-8.44561200
C	3.16329400	22.60385000	-7.93697100
C	4.62972700	25.85344400	-8.94798500
H	3.09809400	25.60233300	-10.46202300
H	2.79677700	27.01064000	-9.42555000
C	5.76927900	23.62644900	-8.17476300
C	4.26045300	21.78188500	-7.63921700
H	5.36346000	26.03993300	-9.73814400
C	5.55033800	22.31957700	-7.75158500
H	6.78051800	24.00551300	-8.29181300
H	6.39376700	21.67481700	-7.52105700
H	4.84156900	26.56257700	-8.13705800
H	0.13556700	26.79442000	-6.64572300
C	-1.28651700	22.95114900	-11.48173300
C	-2.39102600	22.12299500	-11.19942500
C	-0.76298500	23.00824700	-12.79021500
C	-2.89312000	21.95701400	-9.86772300
C	-3.04296900	21.41580900	-12.26409900
C	-1.40786300	22.27474100	-13.84359600
C	0.38135800	23.80074300	-13.13156400
C	-3.99222300	21.18725300	-9.62638600
H	-2.35228600	22.42083500	-9.05172400
C	-4.18195700	20.60109700	-11.96568600

C	-2.55061200	21.52789000	-13.56343900
C	-0.87212400	22.33670500	-15.16954000
H	0.87122500	24.37437700	-12.35314900
C	0.86308400	23.83249200	-14.40672600
C	-4.65207600	20.50019700	-10.68955000
H	-4.35882000	21.08071000	-8.61018500
H	-4.66661400	20.07436300	-12.78453800
H	-3.04901000	20.99513500	-14.37150200
C	0.23188100	23.08523800	-15.44472700
H	-1.37054200	21.76761600	-15.95038100
H	1.73818800	24.43142900	-14.63840600
H	-5.52586900	19.88933200	-10.47556200
H	0.63347000	23.12189600	-16.45277100
C	4.12842600	20.37229700	-7.17718900
C	4.75480400	19.34486300	-7.91375100
C	3.52441200	20.08061200	-5.93649600
C	5.29374800	19.56587900	-9.22380900
C	4.85522900	18.02562000	-7.35905700
C	3.60472000	18.74800200	-5.40768500
C	2.86725700	21.07550100	-5.14037500
C	5.93686700	18.56827900	-9.89738400
H	5.14210600	20.53422700	-9.68717700
C	5.55341400	17.01318800	-8.09138700
C	4.28408000	17.75870900	-6.11605900
C	3.02939600	18.46837000	-4.12715000
H	2.80581200	22.08990700	-5.51621000
C	2.31802400	20.76690300	-3.93079100
C	6.08681200	17.27454000	-9.31779100
H	6.32145400	18.75259400	-10.89624000
H	5.65177000	16.03164200	-7.63601400
H	4.37524100	16.76435300	-5.68496500
C	2.39983800	19.44172300	-3.41002900
H	3.12813800	17.45757500	-3.73771700
H	1.81969300	21.53799400	-3.35170100
H	6.60899500	16.49690100	-9.86726700
H	1.97432500	19.22041000	-2.43494600
H	-4.52102800	18.80864300	-8.41734800

(R_a,*S*)-Int3

E = -4090.497684 a.u.

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C	8.26788400	-1.84097900	1.60047500
C	9.36436000	-2.67689400	1.16995800
C	9.72427900	-3.76986500	1.88314800

C	9.00597200	-4.11695000	3.09271100
C	7.99820700	-3.35414200	3.57860400
C	7.59922000	-2.13244800	2.89520900
H	9.91621900	-2.42928600	0.27031100
H	9.27812600	-5.01190900	3.64235100
H	7.48374700	-3.62381000	4.49715600
O	10.76584600	-4.51724700	1.42056700
O	6.71710800	-1.37582600	3.33552400
C	11.06330700	-5.72935900	2.07755500
H	11.40719500	-5.56274100	3.10562400
H	11.86631500	-6.19137100	1.50303200
H	10.19562200	-6.40145700	2.09397900
C	8.00941400	-0.49107100	-0.51419600
C	7.94421100	0.85474700	-0.94156000
C	8.17419000	-1.49511000	-1.47682800
C	8.02858100	1.17142500	-2.29539900
C	8.26454700	-1.18107800	-2.82974100
H	8.17573600	-2.53380000	-1.15907400
C	8.18833800	0.14798400	-3.23185000
H	7.97611300	2.20050200	-2.62990600
H	8.38423700	-1.97784000	-3.55709400
H	8.25295400	0.40460300	-4.28487600
O	7.79977900	1.77376300	0.04830800
C	7.61202900	3.12279900	-0.32552500
H	8.49205900	3.51489700	-0.84794100
H	7.46385000	3.67458900	0.60311600
H	6.72676700	3.23596300	-0.96468300
C	7.74819800	-0.80617200	0.88247100
H	7.01974900	-0.17877300	1.39635700
H	5.64479400	-1.69747800	4.34892000
C	4.32370800	-2.90096700	-1.61406700
C	4.78595900	-3.37117800	-0.41062300
N	5.15843300	-3.34216200	-2.63196500
H	4.33631600	-3.17929000	0.55454400
C	5.09418500	-2.96673800	-4.02468300
H	4.22965300	-2.31817900	-4.17249200
H	4.99415800	-3.85170700	-4.66218200
H	5.99788000	-2.41681300	-4.31185800
C	3.12993900	-2.06394100	-1.89642600
C	3.25570300	-0.72536500	-1.91359700
C	2.09901300	0.24271600	-1.99481900
C	4.57919700	-0.02574400	-1.71380300
C	2.04747800	1.09010000	-0.70845300
H	2.24872600	0.91744700	-2.85046900

H	1.14182200	-0.26289100	-2.14223500
C	4.53811700	0.80590000	-0.42435600
H	4.75494600	0.65336200	-2.56274300
H	5.41316700	-0.73267900	-1.68605200
C	3.37831600	1.80258800	-0.45627500
H	1.22857800	1.81469700	-0.77430600
H	1.82778200	0.42755900	0.13956700
H	5.49049200	1.32674800	-0.29004100
H	4.42621400	0.12680100	0.43326200
H	3.33248500	2.37344900	0.47926700
H	3.55341900	2.53056100	-1.26211500
C	1.81150900	-2.80226800	-2.07548000
C	1.09744300	-2.99522900	-0.72695800
C	1.98096400	-4.15978100	-2.77614100
H	1.15690300	-2.19430100	-2.71513900
C	-0.24663000	-3.70546300	-0.90313800
H	1.74794400	-3.58600600	-0.06558400
H	0.95819100	-2.02041900	-0.24372100
C	0.63333500	-4.86046200	-2.96131900
H	2.64152900	-4.79574000	-2.17025900
H	2.47360800	-4.02512100	-3.74725300
C	-0.07536200	-5.04775400	-1.61843400
H	-0.73367900	-3.84189300	0.06940900
H	-0.91500200	-3.06769800	-1.49921600
H	0.77728700	-5.82768300	-3.45496600
H	-0.00302800	-4.25686400	-3.62382000
H	-1.04708300	-5.53305200	-1.76133400
H	0.52804800	-5.72121500	-0.99245600
C	5.97440800	-4.12843100	-0.67802200
C	6.17248600	-4.08867700	-2.08148100
C	6.92394100	-4.78552200	0.11954600
C	7.26842300	-4.69421400	-2.70372100
C	8.01730800	-5.38152200	-0.49198700
H	6.81598000	-4.80441600	1.20222600
C	8.18763900	-5.33951700	-1.88901600
H	7.40011700	-4.65496600	-3.78146700
H	8.77402000	-5.86672200	0.11825600
H	9.05590000	-5.81442800	-2.33463100
P	5.00149400	-2.94459100	6.04704600
O	6.13736900	-3.87777000	6.01345300
O	3.52539200	-3.61922200	6.00102800
O	5.00159900	-2.16937800	7.47316100
O	4.81917400	-1.88377100	4.92550600
C	3.03404700	-5.44208600	9.13066900

C	2.99041600	-4.41494800	8.18433200
C	3.39819300	-4.67503400	6.88798900
C	3.75187700	-5.96489300	6.46730600
C	3.72175100	-6.98729800	7.42038500
C	3.39341600	-6.73011300	8.75360400
C	2.69727900	-4.89108400	10.49941200
C	2.83461300	-3.36814000	10.28742300
H	3.99191000	-7.99282500	7.11043200
H	3.42822500	-7.53159200	9.48582500
H	1.67458400	-5.16102000	10.79192800
H	2.22382100	-2.77499700	10.97519900
H	3.88151700	-3.07154000	10.41524300
C	2.43608800	-3.14416000	8.80156400
C	2.79586200	-1.75715600	8.29060900
C	0.88564000	-3.08990000	8.67159700
C	1.72256800	-0.87913200	8.46655200
C	3.96870600	-1.28311900	7.71887700
C	0.51772700	-1.62872100	8.98705800
H	0.61728400	-3.31865900	7.63402600
H	0.39003800	-3.81832700	9.32069200
C	1.84267000	0.46456800	8.13590700
C	4.12251300	0.06732400	7.37200400
H	-0.41354900	-1.31228100	8.50837700
C	3.04562000	0.92906800	7.60636800
H	1.00761900	1.14519400	8.27427200
H	3.15720600	1.97656200	7.34098200
H	0.39640800	-1.47359600	10.06687300
H	3.36531700	-5.27039300	11.27812000
C	4.12240500	-6.19697700	5.03950000
C	5.42551200	-6.59777200	4.68200500
C	3.14885100	-5.98382100	4.03938300
C	6.46501500	-6.79583300	5.64916300
C	5.75290900	-6.79440900	3.29611400
C	3.50054000	-6.14401300	2.65640700
C	1.79739300	-5.61768300	4.34536600
C	7.70229100	-7.22970200	5.27460500
H	6.25732600	-6.56735300	6.68797100
C	7.06635100	-7.24393900	2.94135200
C	4.79115000	-6.54847800	2.31665000
C	2.51439400	-5.89796300	1.64805300
H	1.50346500	-5.51580400	5.38433900
C	0.88014100	-5.41079500	3.35857900
C	8.00459400	-7.47925000	3.90182400
H	8.47223800	-7.37728200	6.02548900

H	7.28498100	-7.40172200	1.88708900
H	5.05185800	-6.67556300	1.26753900
C	1.24272900	-5.54438300	1.98669000
H	2.80933300	-6.00093800	0.60554500
H	-0.13902800	-5.13953500	3.61574500
H	8.98959300	-7.84996900	3.63031000
H	0.49732100	-5.36913600	1.21736800
C	5.39726400	0.56829200	6.77628900
C	5.43021100	1.02301500	5.44134000
C	6.56929000	0.58627900	7.56046300
C	4.28105600	0.98484000	4.58401700
C	6.66601700	1.49755600	4.88259600
C	7.79719000	1.06628400	6.99133600
C	6.59100700	0.15170100	8.92601600
C	4.35209900	1.40838100	3.29013900
H	3.35562700	0.57581500	4.97325400
C	6.69870600	1.93176900	3.51849600
C	7.81598700	1.50884300	5.66935900
C	8.98176100	1.08111900	7.79389900
H	5.67061200	-0.20259300	9.37755100
C	7.74013800	0.18339300	9.65907500
C	5.57674100	1.89964900	2.74771800
H	3.47125200	1.35369800	2.65609700
H	7.64735400	2.26844600	3.10662300
H	8.75075500	1.86390000	5.24050500
C	8.95895000	0.65242800	9.08627500
H	9.90139200	1.44415400	7.34260000
H	7.73137500	-0.15147700	10.69157200
H	5.61459500	2.22377300	1.71162400
H	9.86331200	0.66673400	9.68637300

(R_a,*S*)-TS2

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C	7.48844200	-2.82122900	1.01089300
C	8.67418000	-3.54659200	0.75041800
C	9.27816100	-4.28499000	1.74599400
C	8.69579700	-4.31755900	3.03030500
C	7.53335400	-3.62417800	3.31183900
C	6.90383400	-2.86269900	2.31156300
H	9.15502400	-3.49767500	-0.21952800
H	9.14731200	-4.89466600	3.83113200
H	7.12567300	-3.66772100	4.31864700
O	10.42869800	-4.94043400	1.41162700

O	5.77649000	-2.19700000	2.49261500
C	11.18094700	-5.49660700	2.46777100
H	11.44533600	-4.73544000	3.21249900
H	12.09052900	-5.89267300	2.01500400
H	10.63879900	-6.30741100	2.96804200
C	7.53438600	-1.61138800	-1.21851500
C	7.90092300	-0.25250400	-1.36515700
C	7.94529800	-2.51117100	-2.20601200
C	8.57548300	0.18514900	-2.50377200
C	8.60786300	-2.07622000	-3.35204500
H	7.76286500	-3.57022200	-2.07225000
C	8.90947100	-0.72821600	-3.50167800
H	8.85122100	1.22751200	-2.61065900
H	8.90276400	-2.79623800	-4.10777400
H	9.43236200	-0.37890400	-4.38652300
O	7.58292300	0.55552900	-0.32586300
C	8.20076600	1.82364100	-0.24596300
H	9.29112200	1.72602400	-0.29333900
H	7.90585500	2.23263900	0.72078800
H	7.86015700	2.49174500	-1.04627100
C	6.84933400	-1.98200000	0.04154200
H	6.25375900	-1.18851500	0.48412000
H	5.53584800	-2.06545400	3.50388100
C	4.31634600	-2.42032600	-1.34343300
C	5.05808700	-3.10120900	-0.34231200
N	4.57073200	-2.99402700	-2.54491300
H	4.79117000	-3.03274500	0.70752900
C	4.21767500	-2.47646700	-3.85350400
H	3.57551300	-1.60534800	-3.72622300
H	3.68859400	-3.24097100	-4.42872800
H	5.13105800	-2.18709600	-4.38308600
C	3.17154200	-1.48307200	-1.18829600
C	3.25554400	-0.15378200	-1.35930700
C	2.06859200	0.77944500	-1.28782100
C	4.54965700	0.58600600	-1.57761700
C	2.25289400	1.77955800	-0.13679800
H	2.02395600	1.34057500	-2.23317000
H	1.11847800	0.25189100	-1.19189500
C	4.76038900	1.62110100	-0.45740500
H	4.49901200	1.11326100	-2.54250600
H	5.39580500	-0.10542000	-1.62885400
C	3.55812900	2.55626800	-0.30711700
H	1.40009600	2.46507000	-0.09670000
H	2.26630000	1.22383500	0.80952400

H	5.65916100	2.20718900	-0.66871300
H	4.94334300	1.08815200	0.48443200
H	3.71213600	3.23102500	0.54325400
H	3.47889300	3.18898200	-1.20256700
C	1.83179800	-2.19644400	-0.96412500
C	1.90766400	-3.51919800	-0.18536300
C	1.11320200	-2.42766000	-2.30746200
H	1.20585400	-1.52732000	-0.36084400
C	0.50056800	-4.08632300	0.02827900
H	2.51293700	-4.25052000	-0.74199300
H	2.40329200	-3.37264300	0.78085800
C	-0.28792800	-3.00702100	-2.10527400
H	1.70979900	-3.13241000	-2.90599000
H	1.06497100	-1.48747200	-2.87120600
C	-0.22874200	-4.30397600	-1.29812200
H	0.55735000	-5.02658300	0.58439200
H	-0.07705000	-3.38883500	0.65074000
H	-0.76977800	-3.17531000	-3.07454900
H	-0.90351700	-2.27278000	-1.56699700
H	-1.23803700	-4.69023100	-1.12081500
H	0.30659800	-5.06669300	-1.88117800
C	5.61826200	-4.26862600	-0.99689900
C	5.35049300	-4.13836700	-2.36956900
C	6.40466000	-5.33311900	-0.54778000
C	5.85159700	-5.01577200	-3.32740800
C	6.90169700	-6.22552300	-1.49142700
H	6.61787600	-5.45313600	0.51053100
C	6.63307900	-6.06724700	-2.86190400
H	5.65240800	-4.88531600	-4.38627000
H	7.51433700	-7.06000800	-1.16510000
H	7.04070300	-6.78106400	-3.57012100
P	5.27206600	-2.75087300	5.99475100
O	6.43989000	-3.61650800	6.27710500
O	3.90966800	-3.66859000	5.74166400
O	4.87631500	-1.99599900	7.40395200
O	5.23262100	-1.74455000	4.87415400
C	3.05097100	-5.43129400	8.82682900
C	3.06960900	-4.45768800	7.82580200
C	3.76451500	-4.69035900	6.64687200
C	4.35918900	-5.93704700	6.40233100
C	4.27373800	-6.91716900	7.39848700
C	3.64797300	-6.66772900	8.61881800
C	2.36554500	-4.89129000	10.06248700
C	2.34471100	-3.37405100	9.78909900

H	4.73752200	-7.88208700	7.21317700
H	3.63752000	-7.42871900	9.39381800
H	1.34799700	-5.29240900	10.15617100
H	1.53408200	-2.84694400	10.30234100
H	3.29587300	-2.93064200	10.10392200
C	2.23934600	-3.25892700	8.24239000
C	2.52053600	-1.85145100	7.74772800
C	0.75589300	-3.41699700	7.80140200
C	1.33372600	-1.11812300	7.67642800
C	3.72666800	-1.24656000	7.41135700
C	0.14924700	-2.01161500	7.96710300
H	0.73967900	-3.70048200	6.74287300
H	0.23313600	-4.19231700	8.37037300
C	1.35138900	0.23028200	7.34422100
C	3.77308200	0.11582400	7.07989200
H	-0.69160100	-1.82836000	7.29118900
C	2.57368100	0.83816600	7.06812100
H	0.42951500	0.80262200	7.29241600
H	2.61189300	1.89315400	6.81087400
H	-0.21868700	-1.85570800	8.98957400
H	2.89883900	-5.14891300	10.98244700
C	5.04555100	-6.25290000	5.11551700
C	6.40370100	-6.63690500	5.11599100
C	4.30936100	-6.28503800	3.91126800
C	7.23192600	-6.51148100	6.27984900
C	7.00025700	-7.15666700	3.91775000
C	4.93425800	-6.75469900	2.70484000
C	2.92971000	-5.90348500	3.84004100
C	8.52573300	-6.94471100	6.27082500
H	6.82004600	-6.01728400	7.15150800
C	8.35175100	-7.62617600	3.95754600
C	6.25559200	-7.19921300	2.74029800
C	4.17091200	-6.80855700	1.49473400
H	2.43272400	-5.56630600	4.74200000
C	2.23715600	-5.96259400	2.66692000
C	9.08906400	-7.53744300	5.10114000
H	9.14025700	-6.82713900	7.15750900
H	8.77424200	-8.05078500	3.04947600
H	6.70911800	-7.59998300	1.83463600
C	2.86525800	-6.42166700	1.47124200
H	4.65705800	-7.17903300	0.59594200
H	1.19169700	-5.66940200	2.64721400
H	10.11291900	-7.90076300	5.12310700
H	2.29582200	-6.48104800	0.54768200

C	5.05500800	0.80488100	6.75512400
C	5.24395500	1.36477900	5.47556400
C	6.04384200	0.96419600	7.74741900
C	4.30210000	1.17812000	4.41196600
C	6.42062600	2.13986900	5.20124900
C	7.23358400	1.71267700	7.45102800
C	5.90507600	0.42579100	9.06826900
C	4.48280700	1.77324100	3.19897500
H	3.45221700	0.52784800	4.58284300
C	6.57296400	2.74885900	3.91395700
C	7.38828200	2.29247300	6.19264400
C	8.23160900	1.86979100	8.46452900
H	5.00736400	-0.12975300	9.31498100
C	6.87775400	0.59916800	10.00747400
C	5.62820400	2.58528100	2.94589300
H	3.75225300	1.62053000	2.41034000
H	7.46050500	3.35105400	3.73464400
H	8.28178200	2.87676300	5.98196400
C	8.06456200	1.32899100	9.70296900
H	9.12748200	2.43380000	8.21804100
H	6.75207900	0.17668000	10.99940100
H	5.74379500	3.06397900	1.97587500
H	8.82900500	1.45200400	10.46393800

(R_a,*S*)-Int4

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0 1

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C	9.88637300	-3.71586100	1.58258700
C	9.46507500	-3.78426300	2.91137800
C	8.20229700	-3.32068200	3.27514600
C	7.36057000	-2.77213900	2.30784900
H	9.39770300	-3.10833100	-0.41228000
H	10.09757700	-4.21420100	3.67866200
H	7.86676200	-3.39114100	4.30796400
O	11.10084400	-4.16379900	1.13084300
O	6.12053500	-2.32281100	2.55425300
C	11.94272800	-4.76671200	2.08198300
H	12.23309300	-4.06014400	2.87013100
H	12.83349300	-5.09121200	1.54260300
H	11.46041900	-5.63577100	2.54968100
C	7.41358900	-1.61661300	-1.28388100
C	8.20880900	-0.45457000	-1.15287800

C	7.32712500	-2.20182800	-2.54243300
C	8.89485400	0.07476400	-2.24273700
C	7.99381100	-1.66567300	-3.64855100
H	6.73175700	-3.09761800	-2.68224300
C	8.78224400	-0.53645500	-3.49233500
H	9.50648300	0.96199700	-2.12939800
H	7.90414700	-2.14568700	-4.61716100
H	9.31768200	-0.11883800	-4.33913900
O	8.21457100	0.09929800	0.08398600
C	9.10637100	1.16160900	0.34405300
H	10.13900000	0.86871400	0.12315300
H	9.00344300	1.37911400	1.40712800
H	8.84523600	2.05230700	-0.24193800
C	6.76988900	-2.11649100	-0.00679200
H	6.32804400	-1.25340900	0.50771700
H	5.94209000	-2.16785100	3.56022100
C	4.27702500	-2.65801300	-0.64743500
C	5.59886100	-3.14182800	-0.12816200
N	3.81130200	-3.52218500	-1.52050300
H	5.37272800	-3.38832400	0.92996200
C	2.54877900	-3.44526300	-2.24380800
H	2.06523200	-2.49788300	-2.01355700
H	1.91266300	-4.28001300	-1.93937100
H	2.75892200	-3.51117100	-3.31378800
C	3.50198100	-1.47112800	-0.20447100
C	3.55723700	-0.34389500	-0.94170700
C	2.76401900	0.90483800	-0.62125700
C	4.40862000	-0.19813400	-2.17901200
C	3.63260600	2.17570200	-0.61129500
H	2.00153700	1.01163500	-1.40882400
H	2.22797100	0.81847200	0.32615200
C	5.32936100	1.02467300	-2.05177600
H	3.74474900	-0.04387000	-3.04412400
H	5.00031600	-1.09455200	-2.38059400
C	4.49878500	2.29308900	-1.86526000
H	2.97913500	3.04795500	-0.50779600
H	4.27719000	2.15877200	0.27471300
H	5.98043200	1.08748900	-2.93025900
H	5.97992900	0.88695300	-1.17712700
H	5.14973500	3.17027000	-1.78835100
H	3.86036800	2.44485500	-2.74713100
C	2.59529800	-1.63524100	1.02353200
C	2.97418800	-2.76209200	1.99563500
C	1.12628800	-1.80366600	0.58526000

H	2.66531300	-0.69661400	1.59019400
C	2.01999300	-2.78917200	3.19421500
H	2.92986300	-3.73436400	1.47625600
H	3.99508600	-2.62880000	2.36371800
C	0.18728800	-1.78030900	1.79282000
H	1.01979500	-2.77392200	0.07570400
H	0.85042600	-1.02645000	-0.13861400
C	0.55569900	-2.89104900	2.77582500
H	2.29992700	-3.61890100	3.84684600
H	2.16336100	-1.87764000	3.79331900
H	-0.85260200	-1.87635600	1.46099800
H	0.27654600	-0.80776300	2.29759600
H	-0.09161400	-2.84625900	3.65938700
H	0.38040700	-3.86598100	2.29715100
C	5.81929500	-4.40452600	-0.90202200
C	4.71165600	-4.60609700	-1.72061700
C	6.87051300	-5.31297100	-0.94620500
C	4.57447500	-5.67979500	-2.58796700
C	6.76812700	-6.39355800	-1.82306600
H	7.74360300	-5.17482500	-0.31748900
C	5.63809700	-6.58002200	-2.62675900
H	3.69432700	-5.81890000	-3.20686700
H	7.58097100	-7.11034200	-1.87865400
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P	5.30282000	-2.84914600	5.97318600
O	6.32263500	-3.68226800	6.64100900
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O	5.60852600	-1.83293100	4.91066000
C	2.70018700	-5.73253600	8.03832700
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C	4.16209500	-7.14002000	6.75699700
C	3.36704500	-6.94192300	7.88883400
C	1.78990000	-5.25694900	9.15257800
C	1.67830100	-3.73941900	8.87798000
H	4.64710900	-8.09793200	6.59052600
H	3.26383900	-7.73022800	8.62893700
H	0.80836500	-5.74508200	9.09873100
H	0.74139300	-3.30106900	9.23725600
H	2.51216500	-3.21348800	9.35489700
C	1.83753700	-3.61910400	7.33958900
C	2.05294900	-2.20913500	6.82254700

C	0.48791300	-3.97009900	6.63886100
C	0.84760700	-1.64749600	6.39508500
C	3.23914600	-1.48743900	6.71770400
C	-0.27767700	-2.63987200	6.57003200
H	0.70565100	-4.31397200	5.61968900
H	-0.05413700	-4.76750800	7.15662100
C	0.81097400	-0.36386900	5.86571100
C	3.22607500	-0.18292700	6.19457400
H	-1.01347700	-2.60635000	5.76035300
C	2.00141200	0.35416400	5.77521300
H	-0.12369500	0.07238200	5.52389300
H	1.99994800	1.36164900	5.36795400
H	-0.81927400	-2.44748700	7.50574000
H	2.20131500	-5.47410600	10.14289200
C	5.13023100	-6.33057300	4.56692700
C	6.52598000	-6.50207400	4.55635200
C	4.39646800	-6.40541000	3.36133600
C	7.31450300	-6.37842300	5.74752800
C	7.19577800	-6.80754300	3.32112200
C	5.08063500	-6.67080000	2.12732600
C	2.96970200	-6.26617500	3.31554800
C	8.65913000	-6.60431000	5.71604200
H	6.82639300	-6.05085100	6.65795900
C	8.60653300	-7.04662800	3.33710700
C	6.46170700	-6.87642900	2.13818500
C	4.32360400	-6.75988500	0.91506800
H	2.43135800	-6.10251700	4.24323600
C	2.28142000	-6.35237100	2.13929300
C	9.31272200	-6.96498100	4.49947100
H	9.24447000	-6.49623400	6.62345200
H	9.09882300	-7.28797000	2.39786500
H	6.97079900	-7.11869000	1.20773300
C	2.96950600	-6.59494200	0.91410500
H	4.85411300	-6.98872800	-0.00528300
H	1.19988000	-6.25324400	2.13807800
H	10.38285300	-7.15468900	4.50371600
H	2.40912600	-6.68219900	-0.01383900
C	4.44815900	0.66965300	6.10068400
C	4.97298800	1.01536400	4.84007700
C	5.02833500	1.18958100	7.27373500
C	4.48823900	0.43109500	3.62518000
C	6.07753200	1.92646800	4.75165500
C	6.13553200	2.09975100	7.17511800
C	4.54624300	0.85899700	8.58230800

C	5.04960400	0.73632600	2.42189100
H	3.70827900	-0.31992700	3.69331100
C	6.61340300	2.25357700	3.46361000
C	6.62449500	2.45666600	5.91937000
C	6.71161300	2.62932300	8.37333400
H	3.70972400	0.17482800	8.67292100
C	5.12423800	1.38322400	9.70012800
C	6.11941900	1.67645000	2.33265700
H	4.70999700	0.23337100	1.52027800
H	7.43823600	2.96092500	3.41686800
H	7.46059400	3.14977500	5.85110800
C	6.22611400	2.28326400	9.59773300
H	7.55061700	3.31394800	8.27931000
H	4.74665000	1.11325200	10.68136400
H	6.54370100	1.90858900	1.35860600
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