Supporting Information

Synthesis of a class of chiral-bridged phosphoramidite ligands and their applications in the first iridium-catalyzed asymmetric addition of arylboronic acids to isatins

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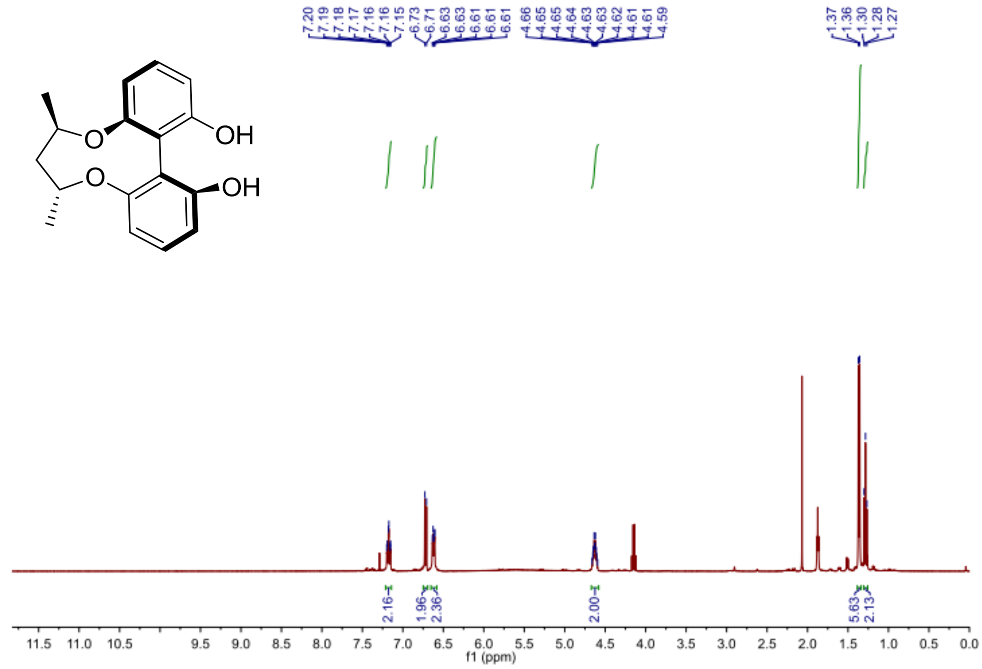
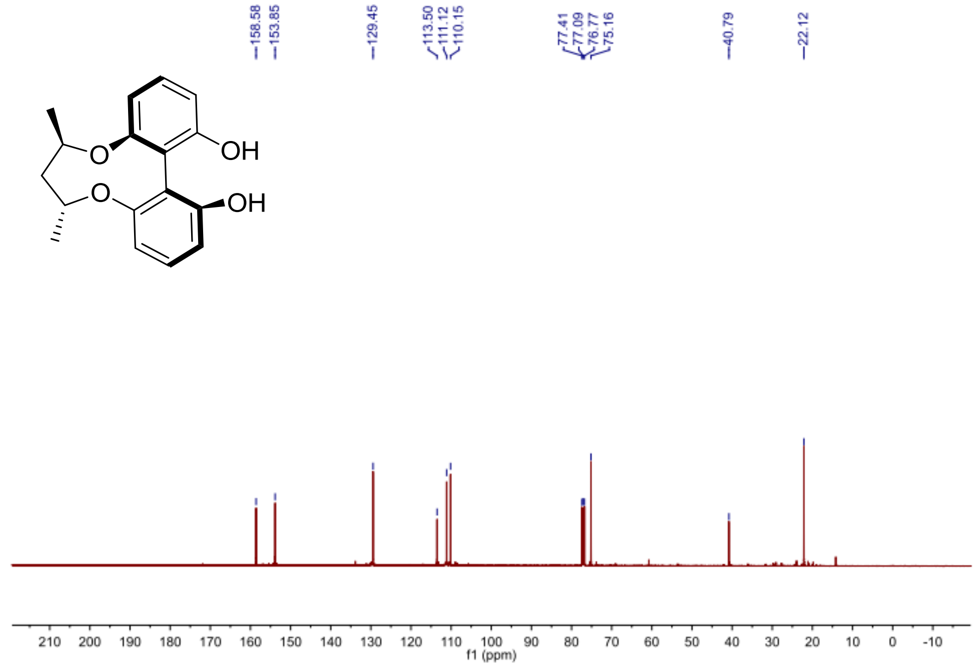
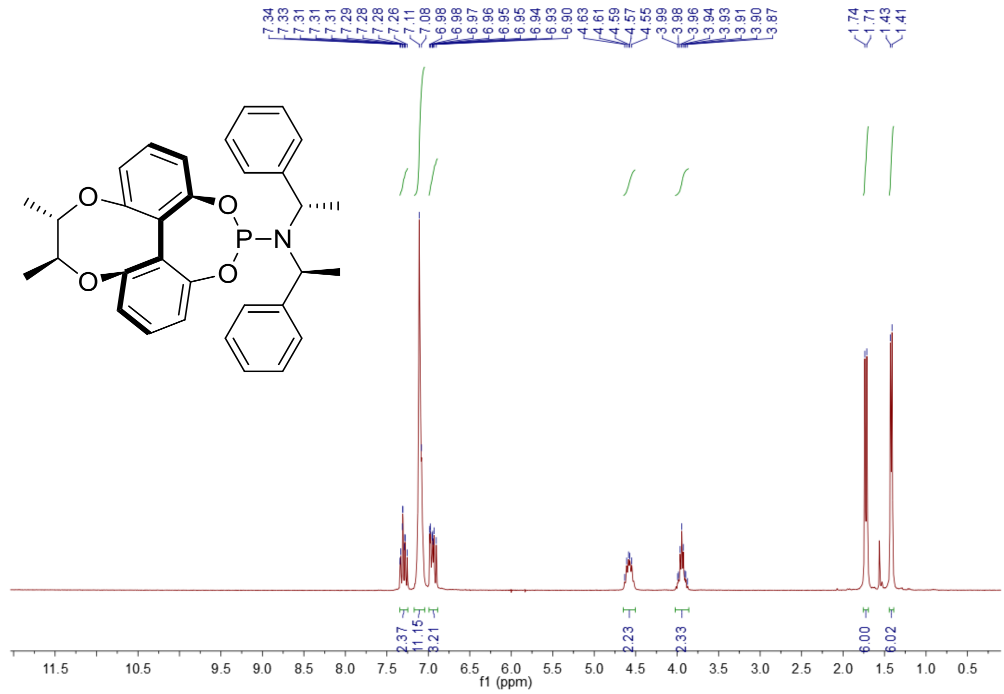
[1]H and [13]C NMR spectra of compounds (*R*,*R*,*S*$_a$)-3c, 4 and 7

(*R*,*R*,*S*$_a$)-3c





(*S*,*S*,*R*$_a$,*S*,*S*)-4a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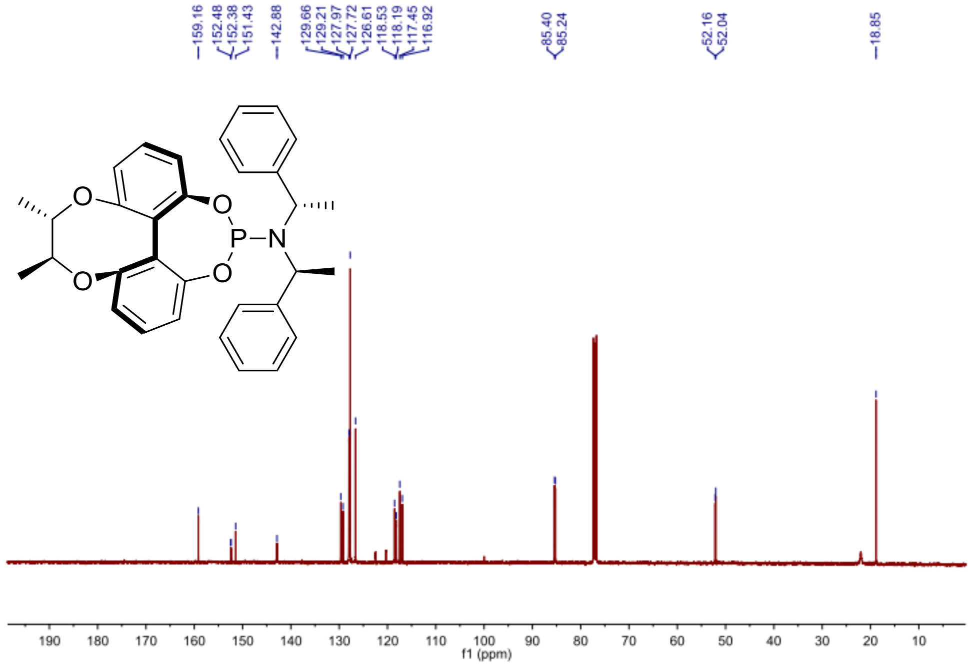
O
P
N
O
O
O
2.37 11.15 3.21 2.23 2.33 6.00 6.02
11.5 10.5 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (ppm)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N
O
O
O
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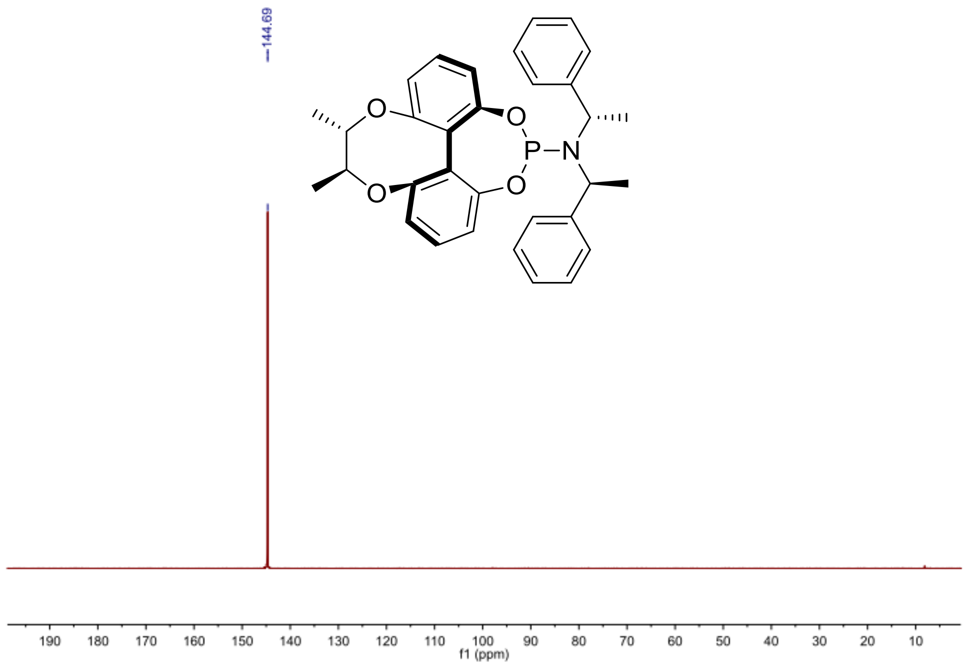
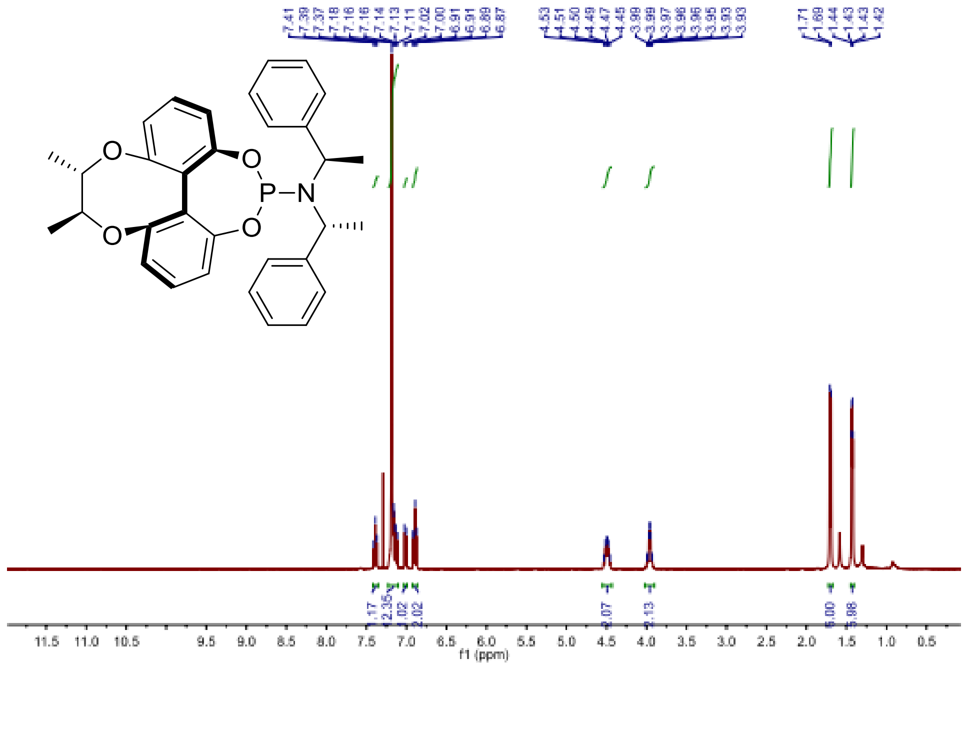
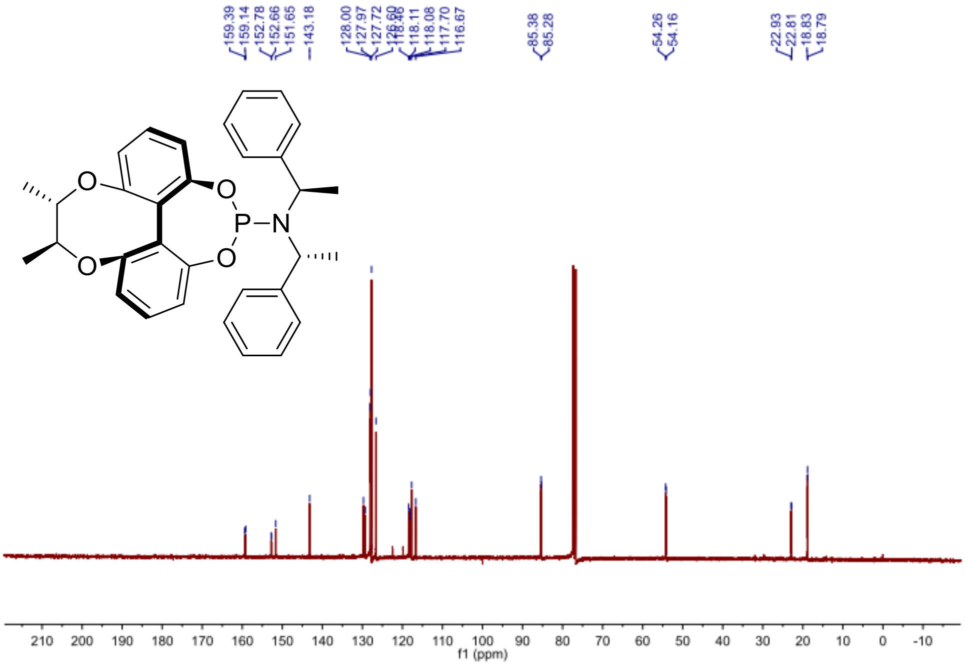
f1 (ppm)



(*S*,*S*,*R*$_a$,*R*,*R*)-4b

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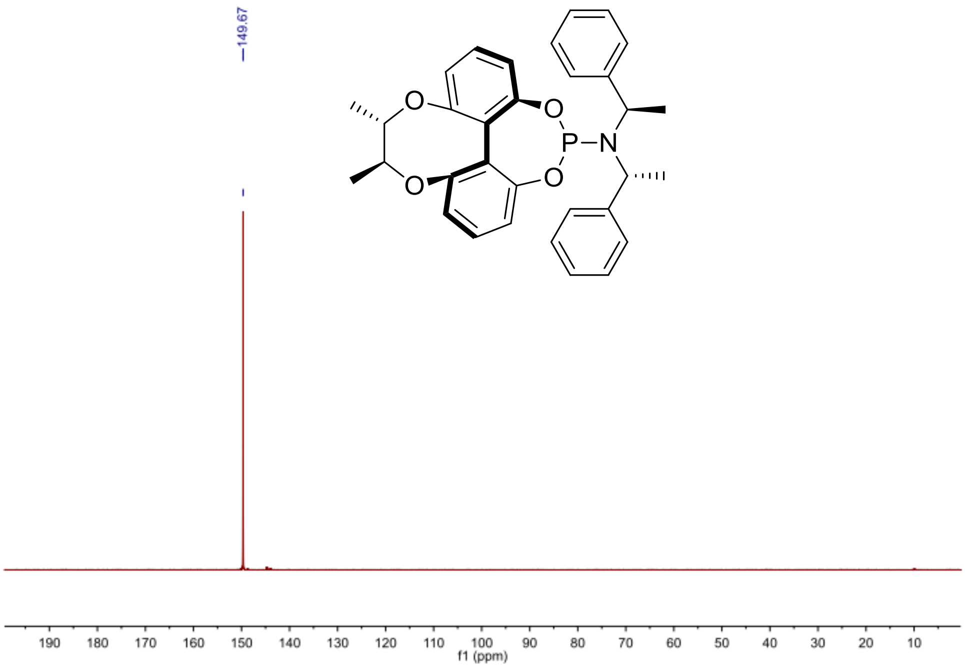
116.67
85.38
85.28
54.26
54.16
22.93
22.81
18.83
18.79
O
O
P
N
O
O
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


149.67
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O
O
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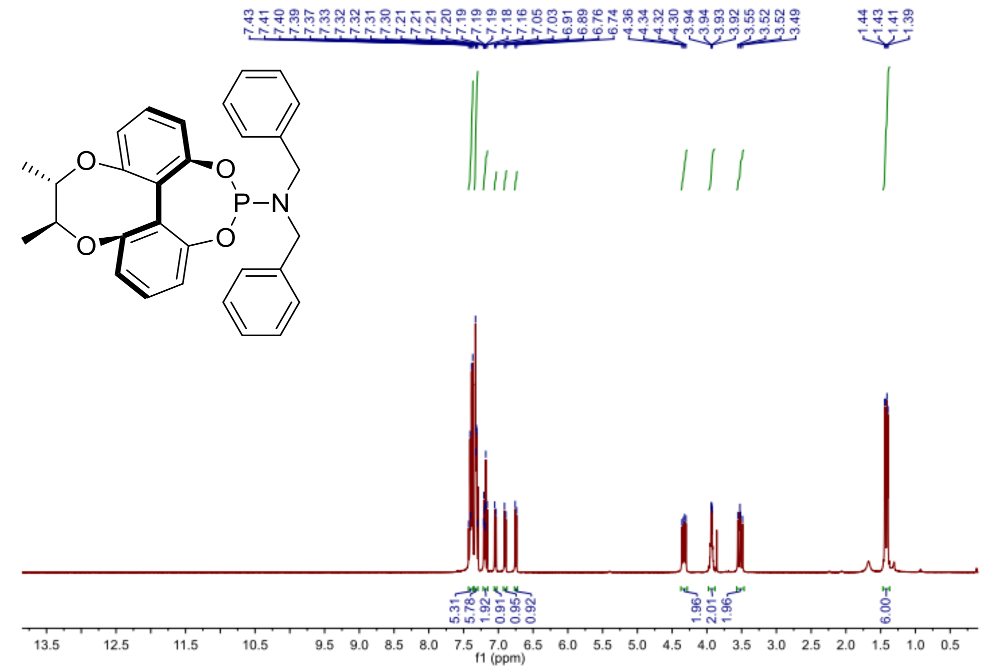
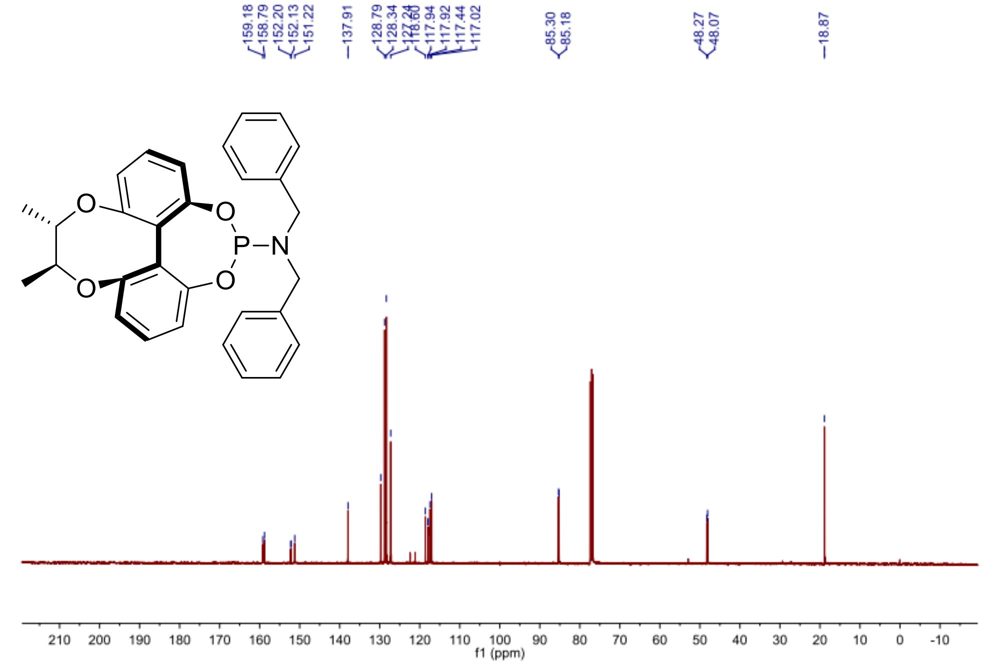
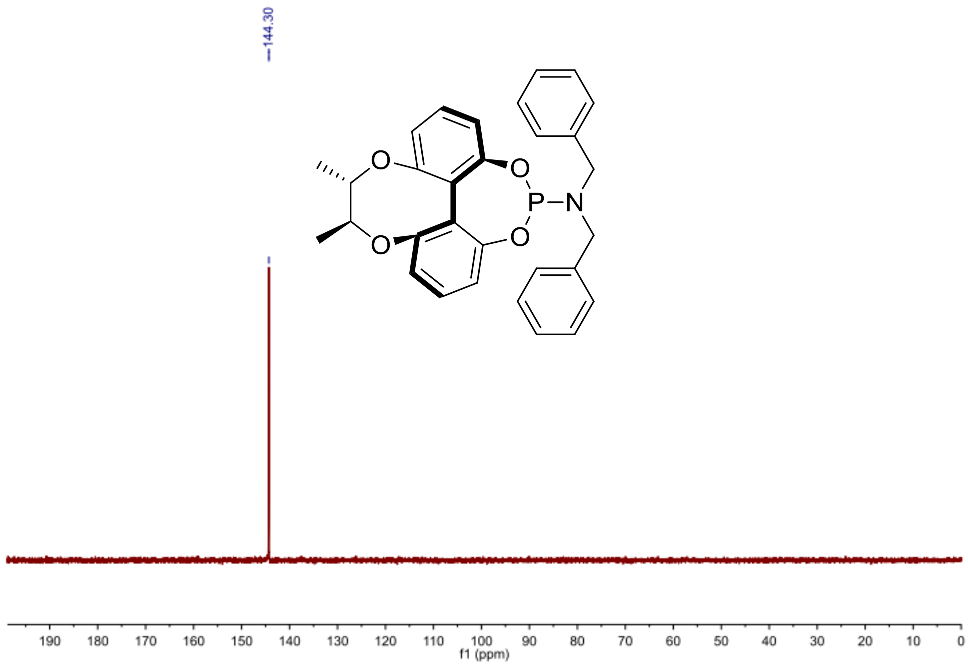
f1 (ppm)

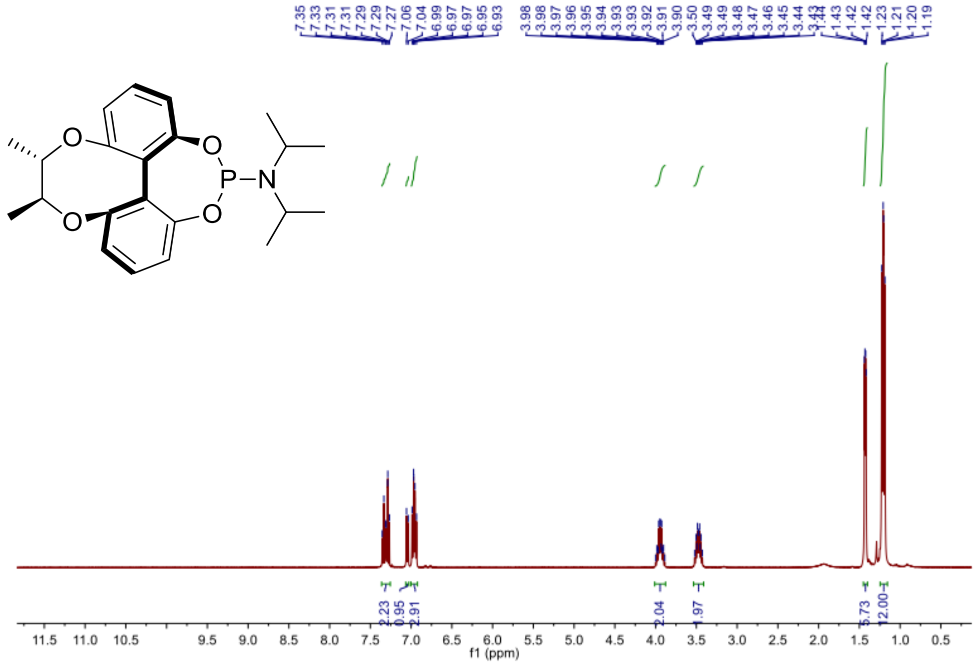
***(S,S,R_a)*-4c**

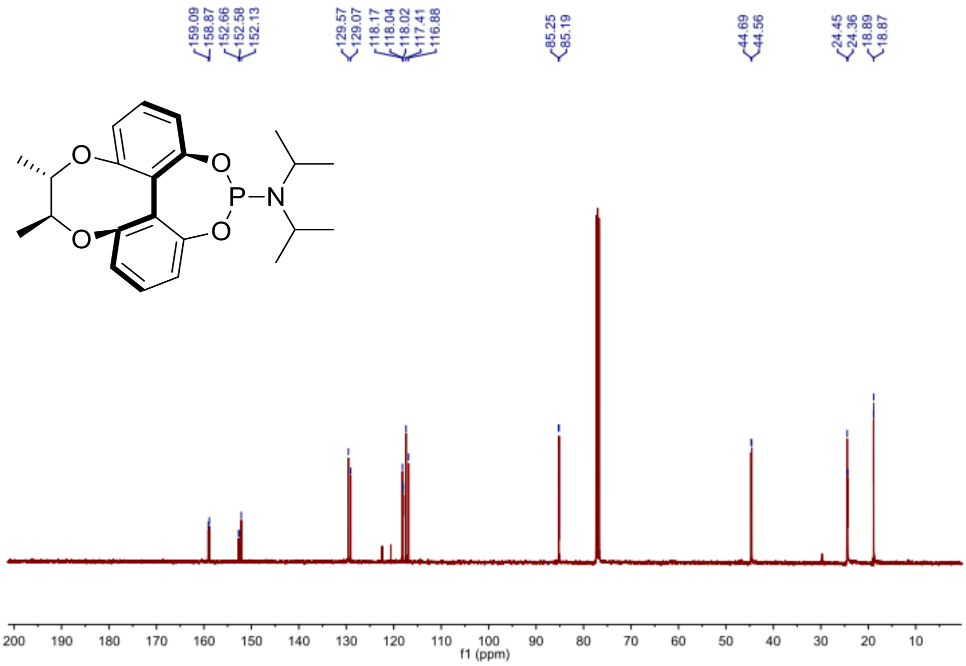






***(S,S,R$_a$)*-4d**





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118.02
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85.25
85.19
44.69
44.56
24.45
24.36
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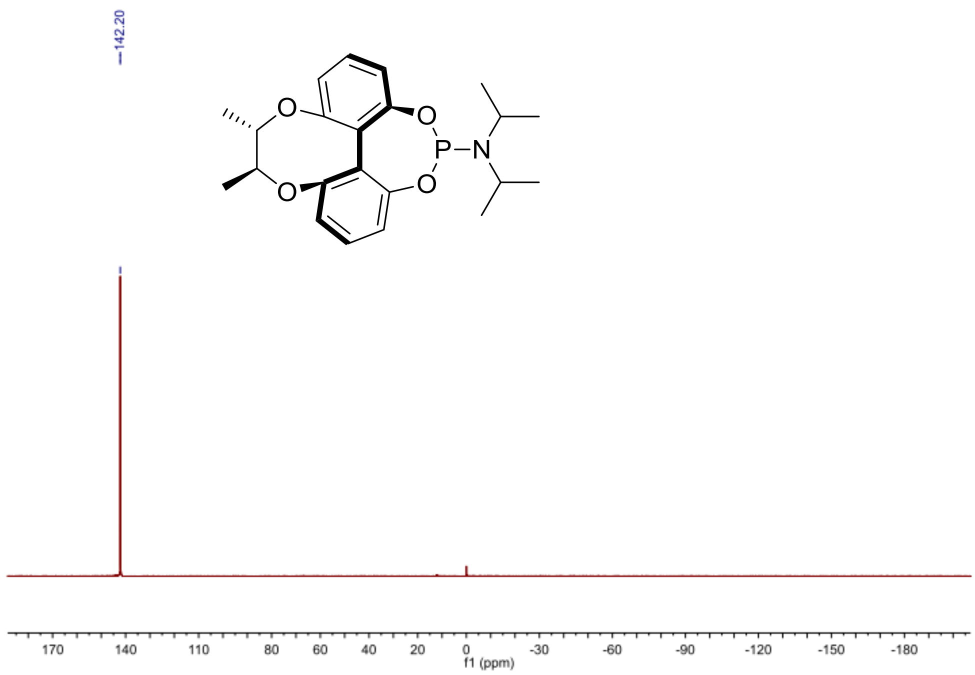
O
P
N
O
O
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)



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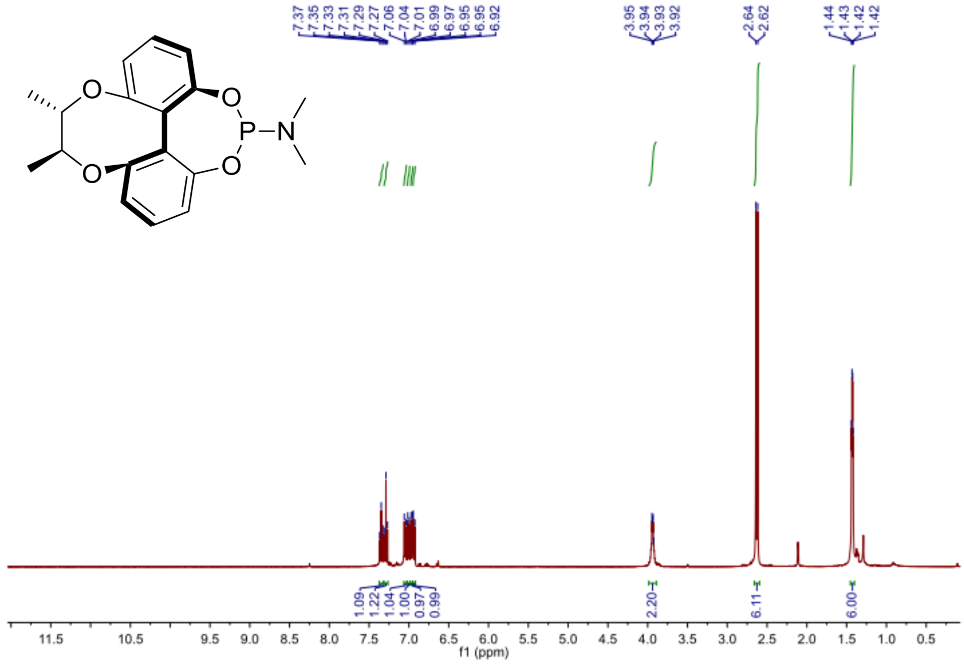
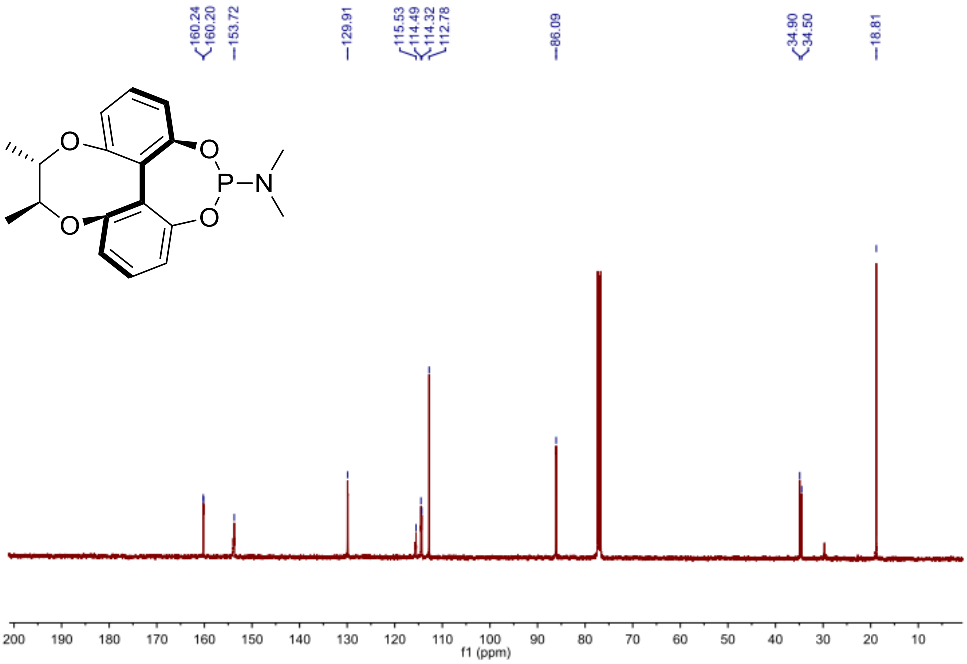
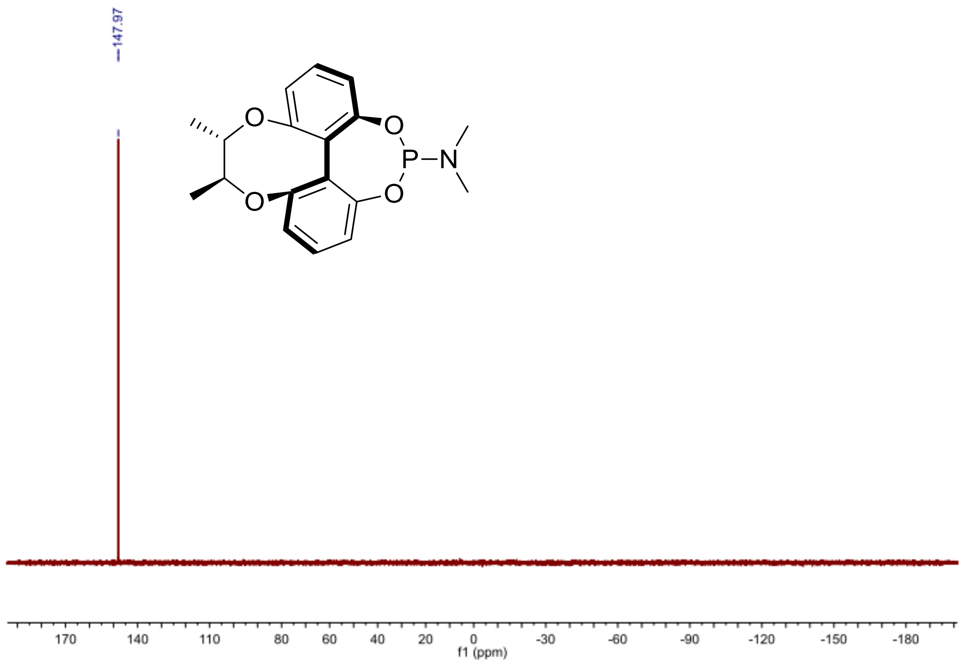
f1 (ppm)

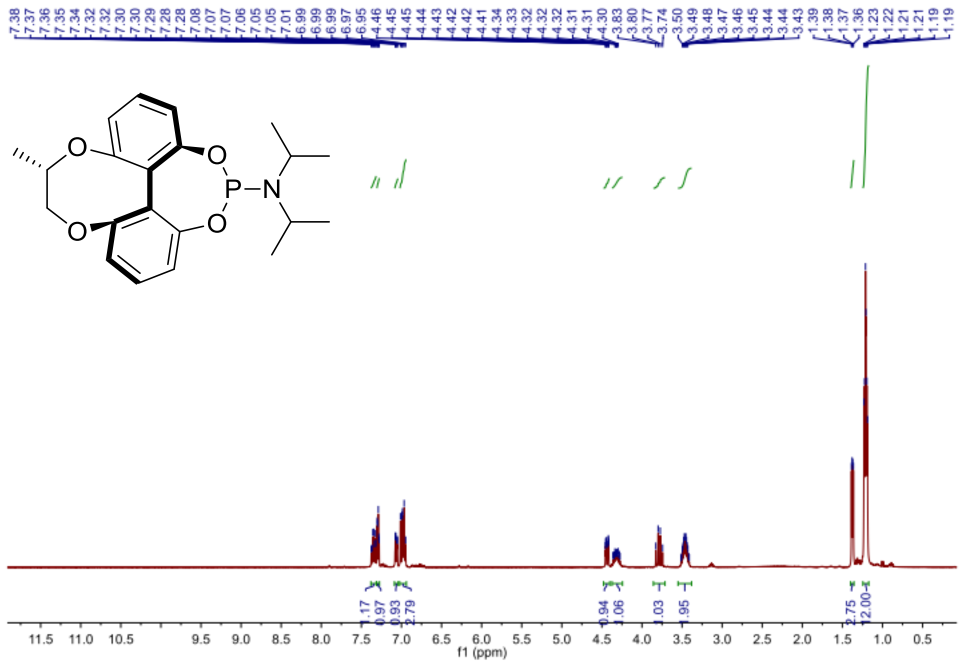
***(S,S,R$_a$)*-4e**

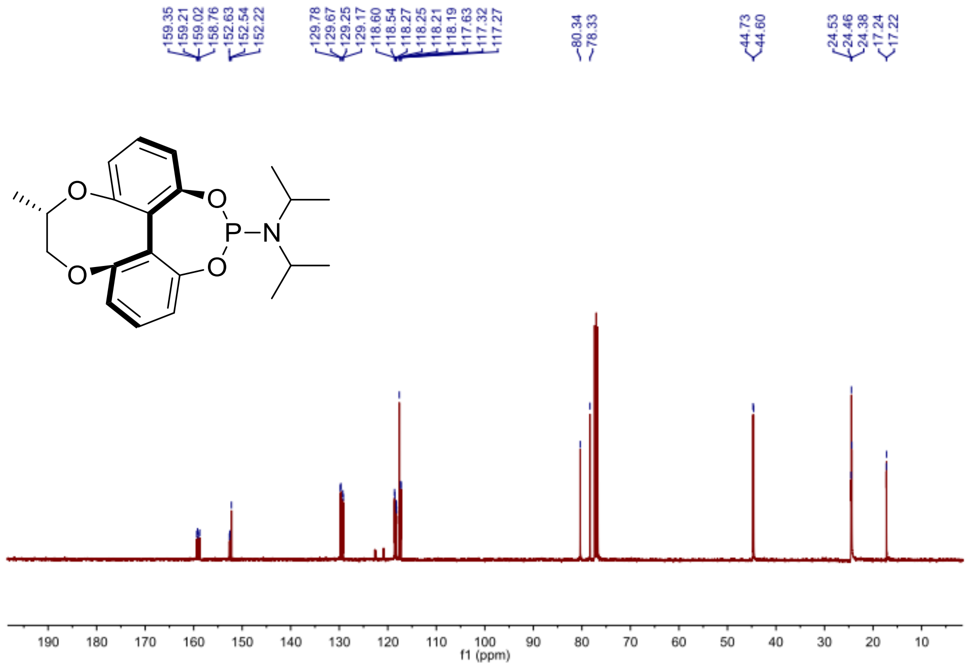






***(S,R_a)*-4f**

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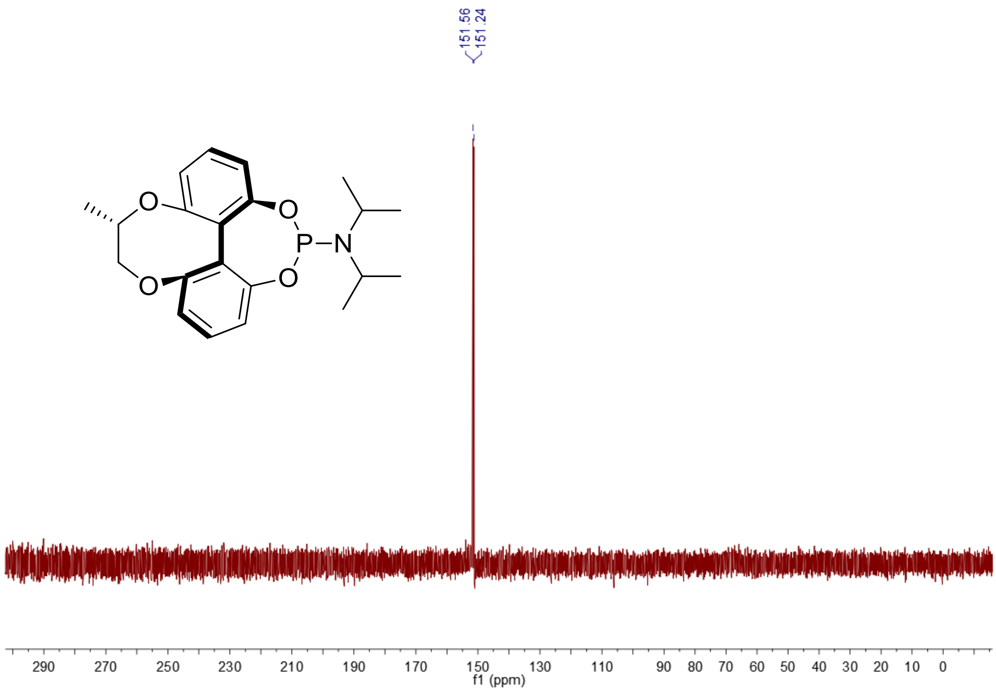
118.25
118.21
118.19
117.63
117.32
117.27
80.34
78.33
44.73
44.60
24.53
24.46
24.38
17.24
17.22
O
O
P
N
O
O
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)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151.24
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O
P
N
O
O
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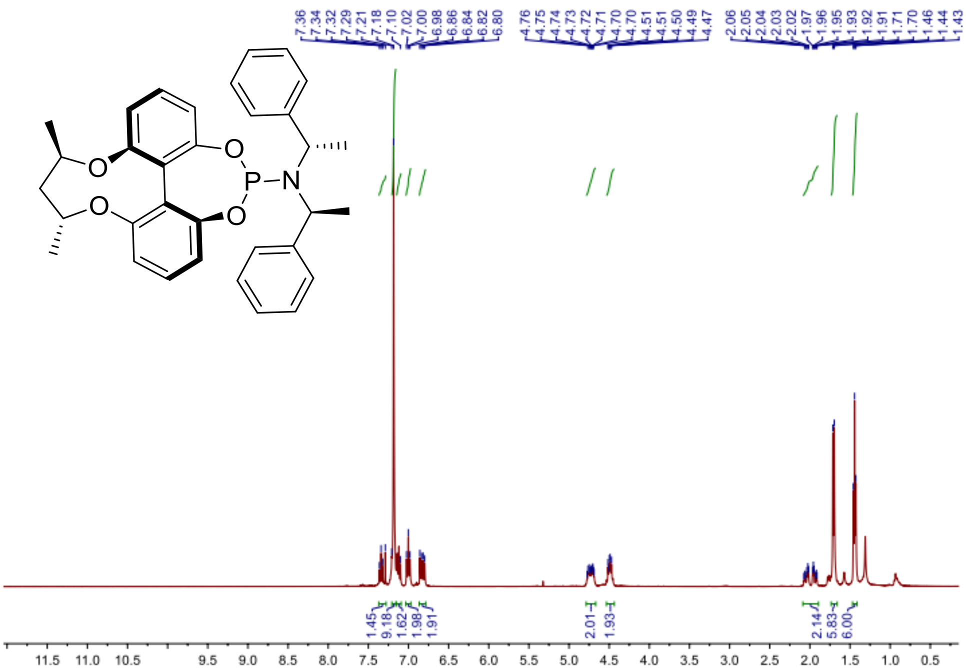
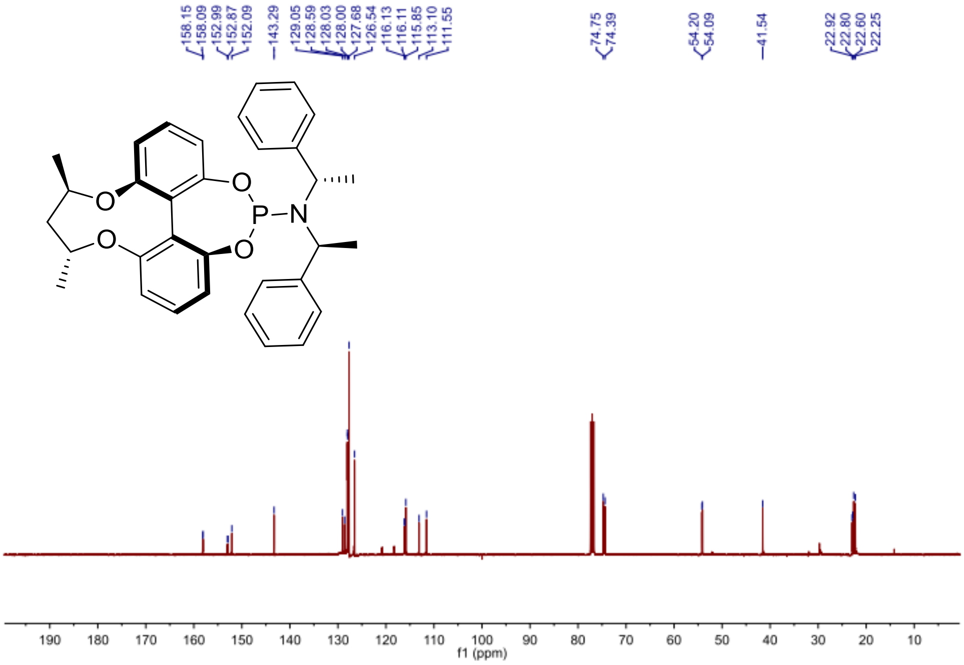
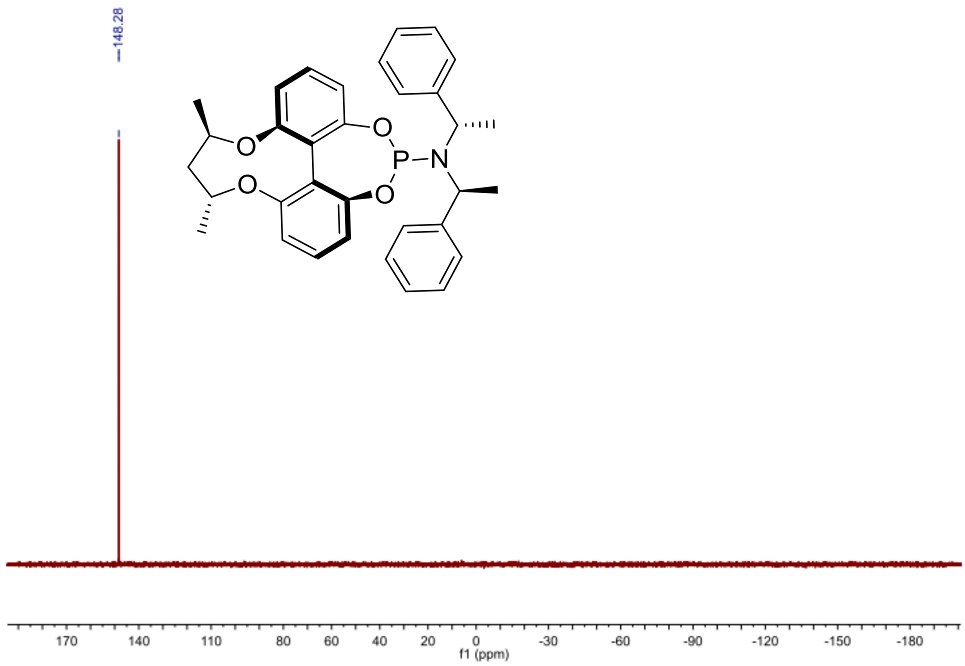
f1 (ppm)

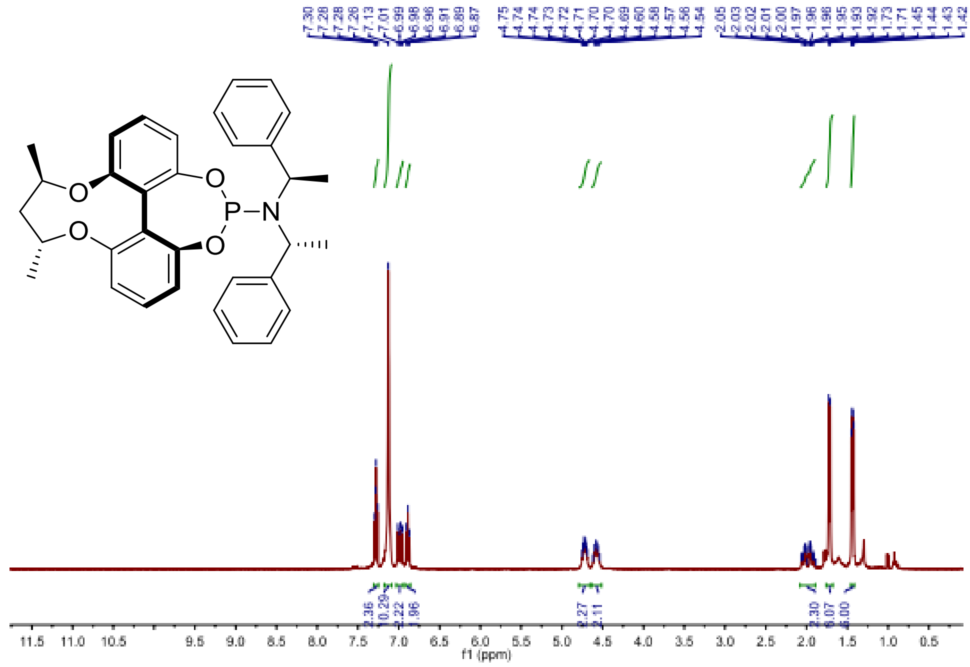
***(R,R,S$_a$,S,S)*-4g**

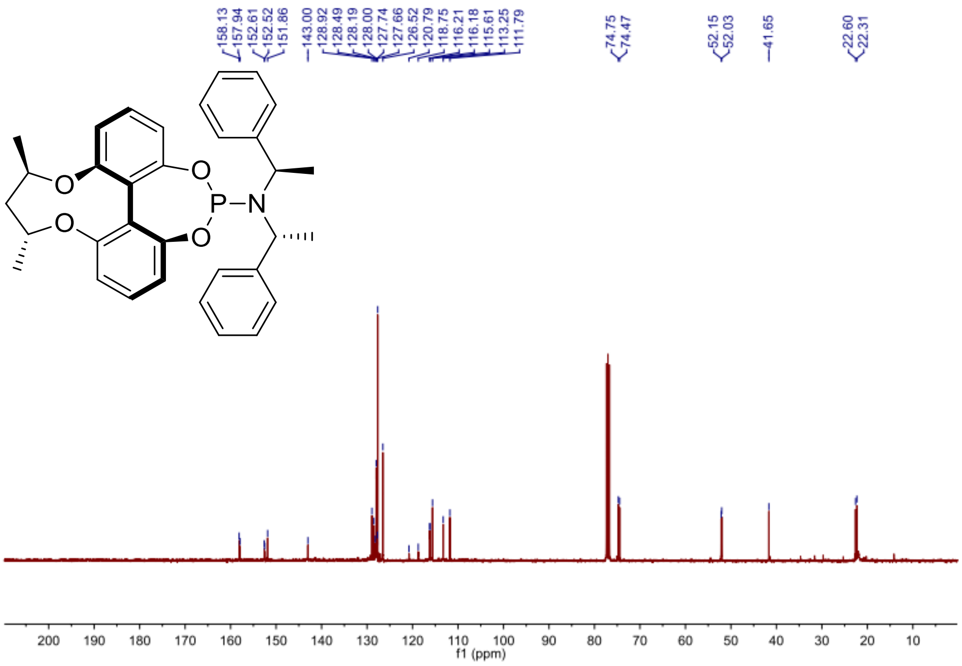






***(R,R,S$_a$,R,R)*-4h**

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120.79
118.75
116.21
116.18
115.61
113.25
111.79
74.75
74.47
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52.03
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22.31
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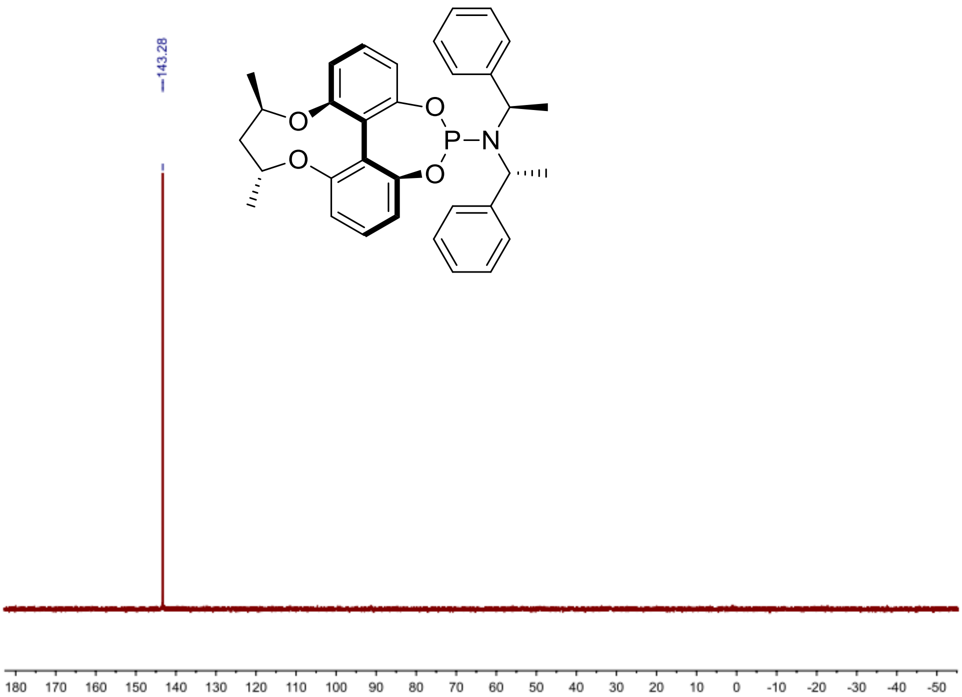
f1 (ppm)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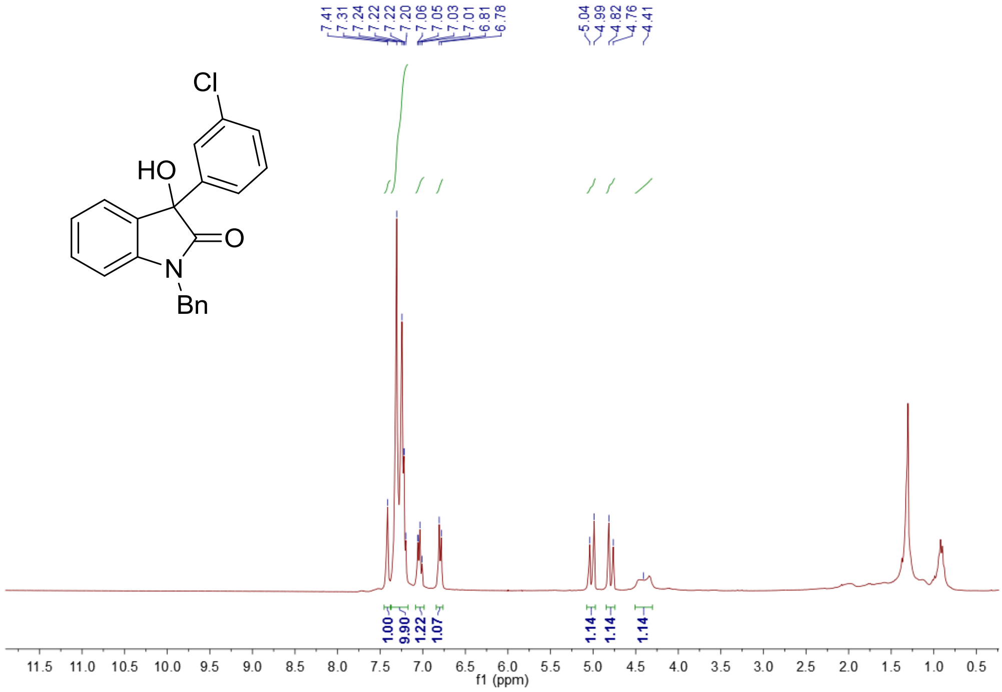
7e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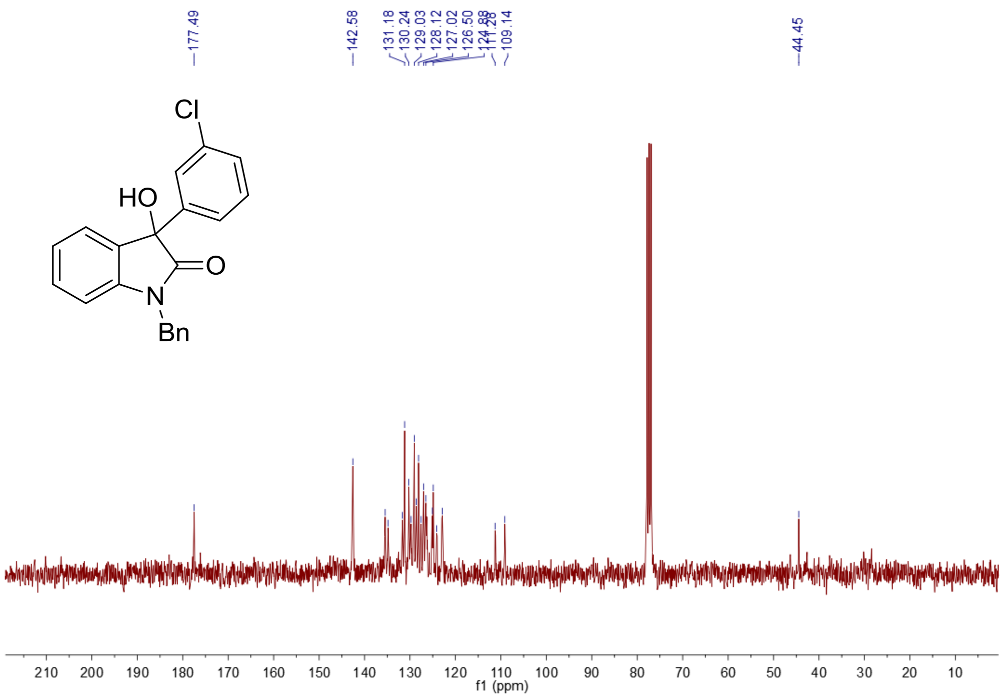
7.22
7.22
7.20
7.06
7.05
7.03
7.01
6.81
6.78
5.04
4.99
4.82
4.76
4.41
Cl
HO
O
N
Bn
1.00
9.90
1.22
1.07
1.14
1.14
1.14
f1 (ppm)


177.49
142.58
131.18
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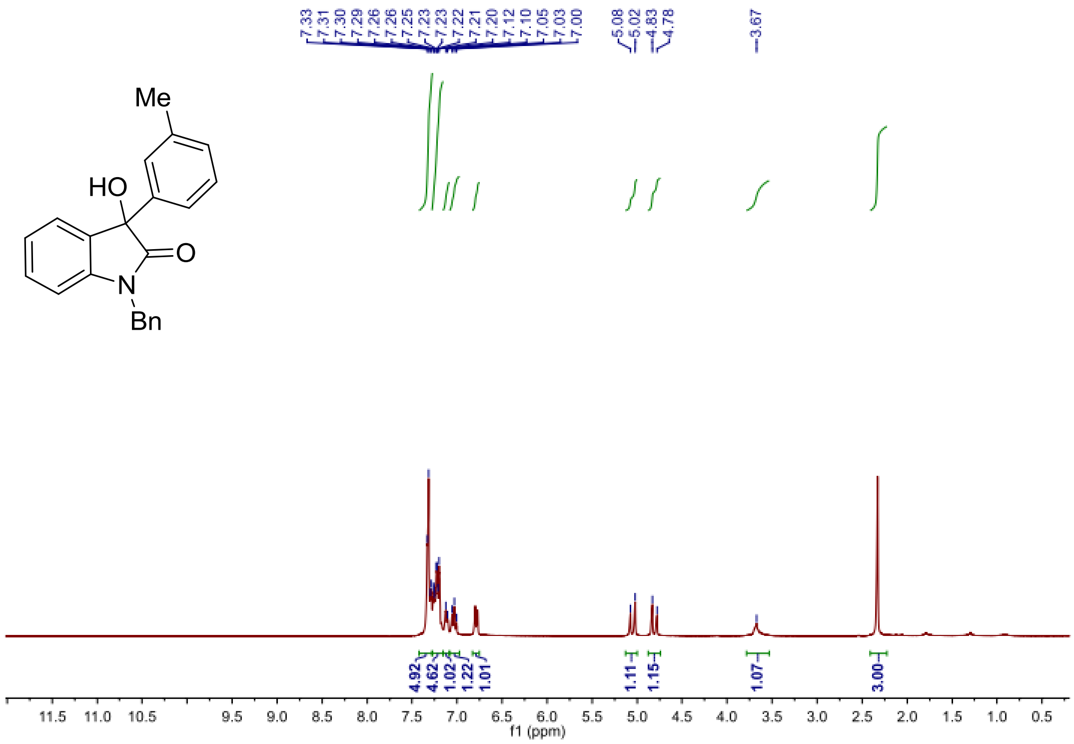
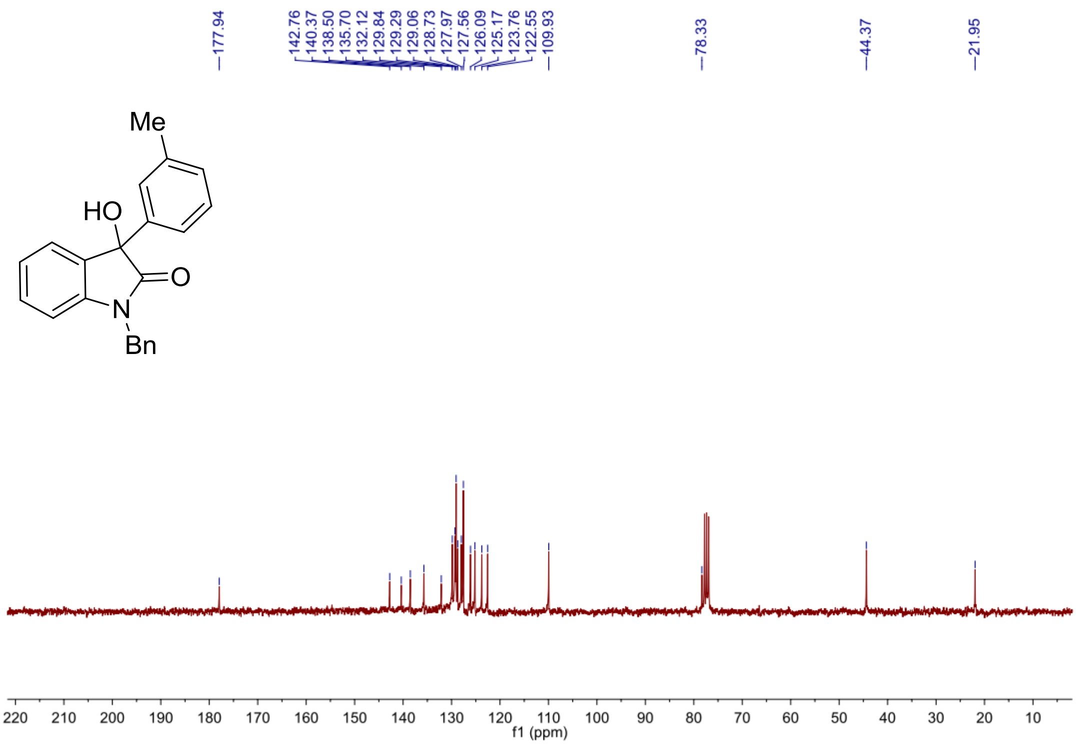
127.02
126.50
109.14
44.45
Cl
HO
O
N
Bn
f1 (ppm)

7f





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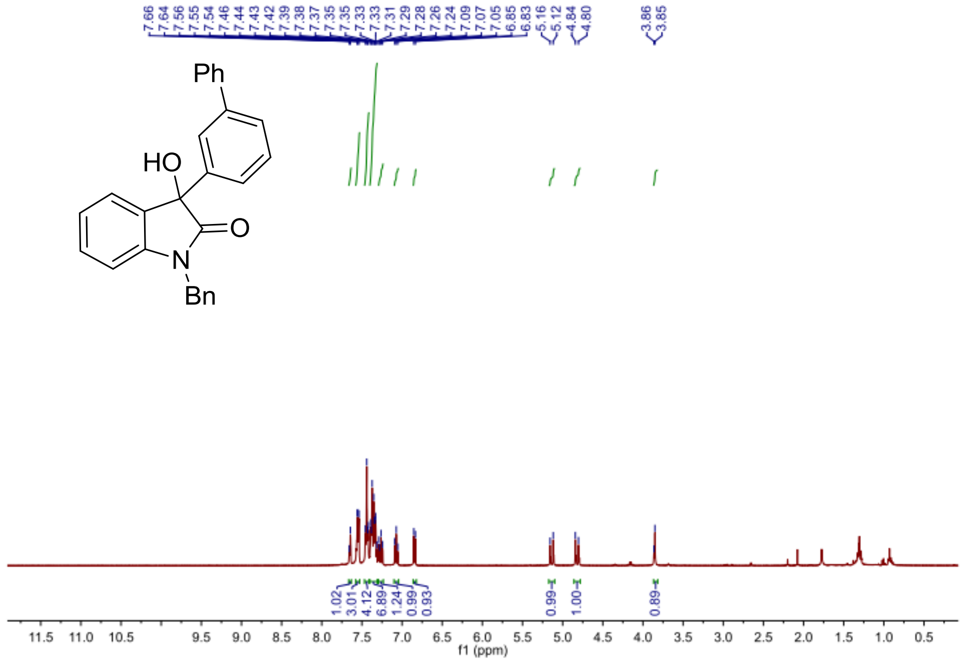

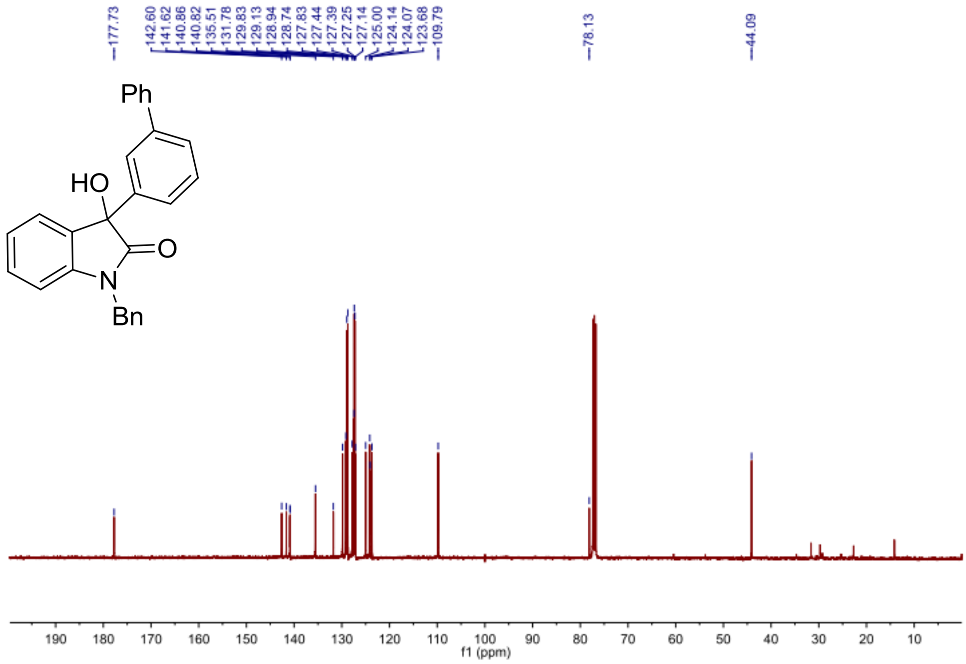

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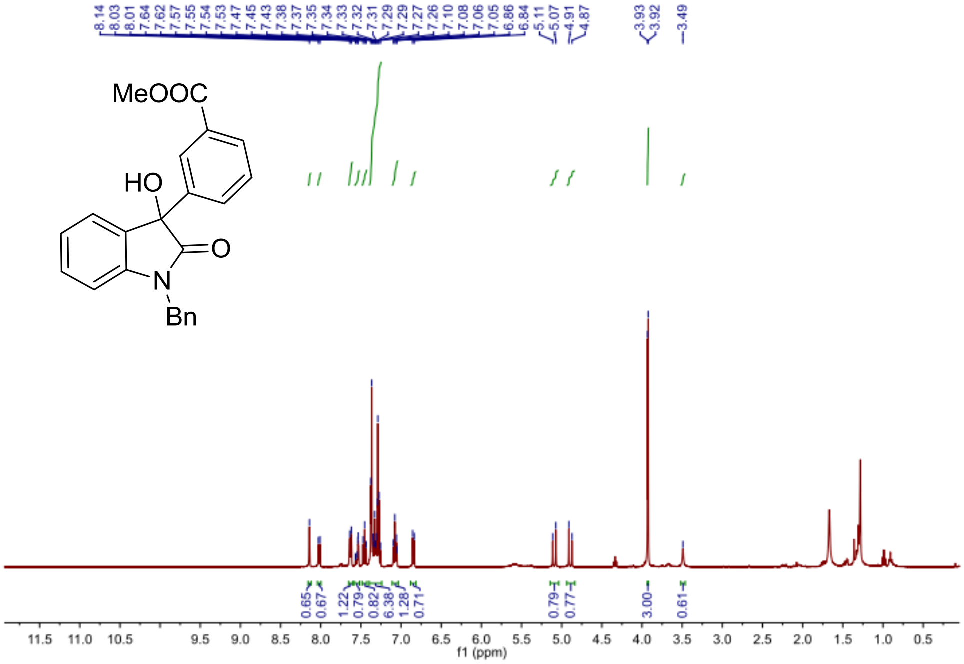

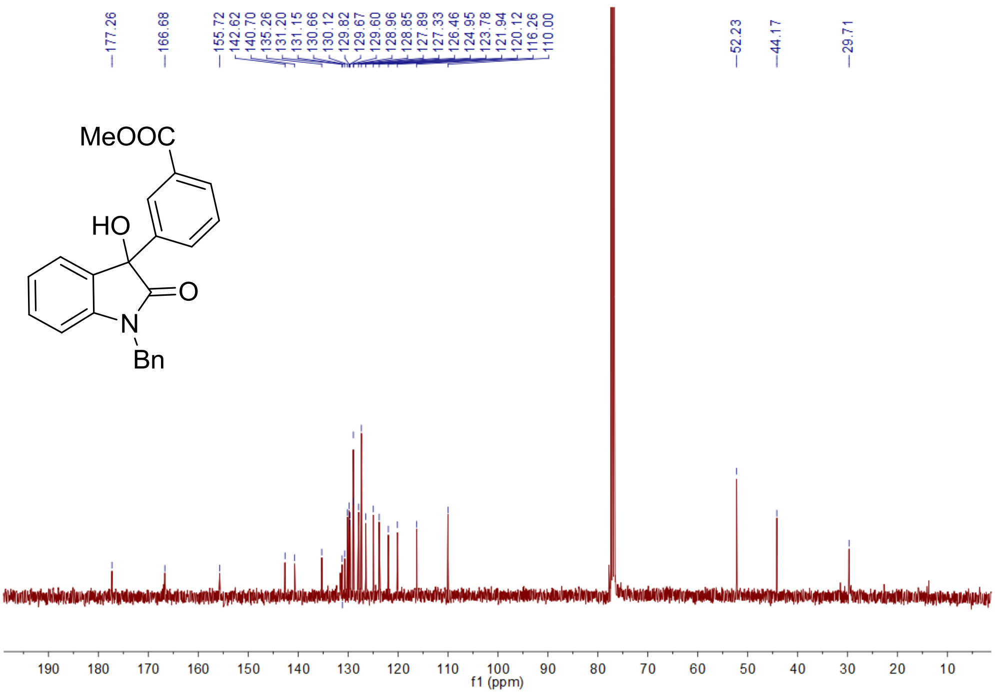

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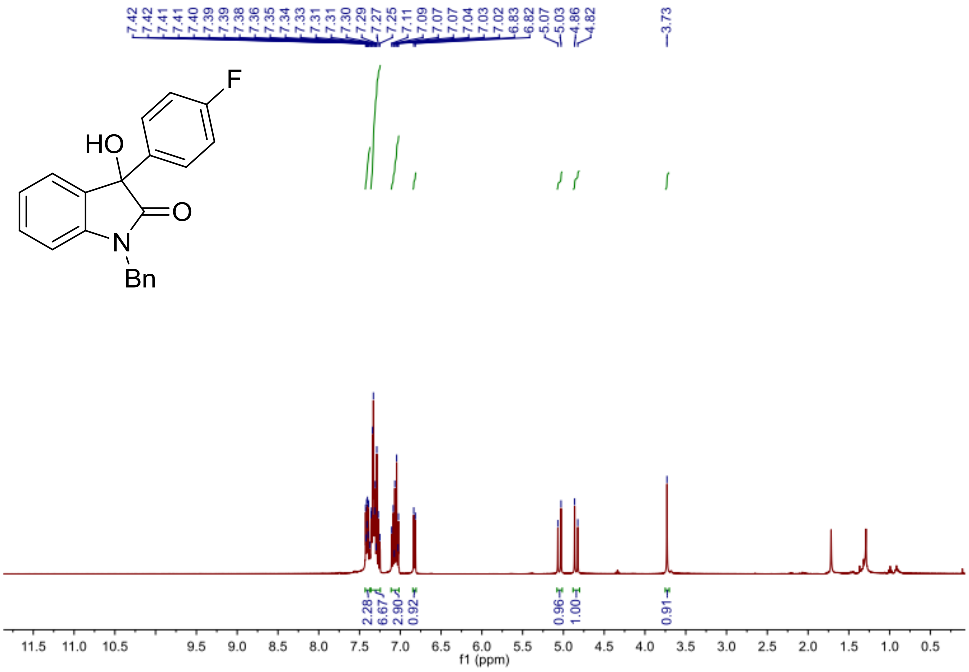

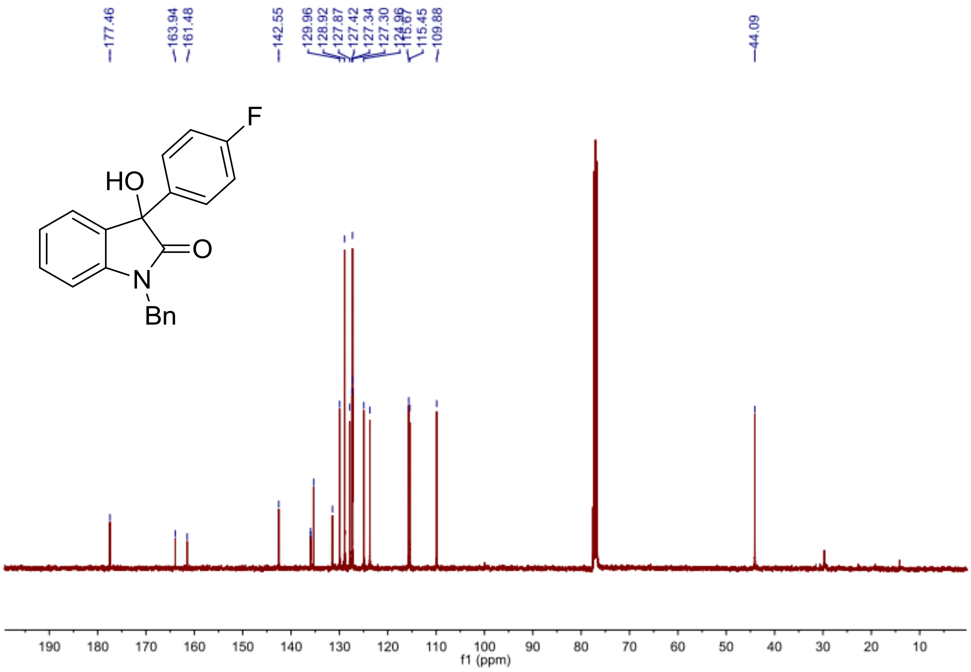

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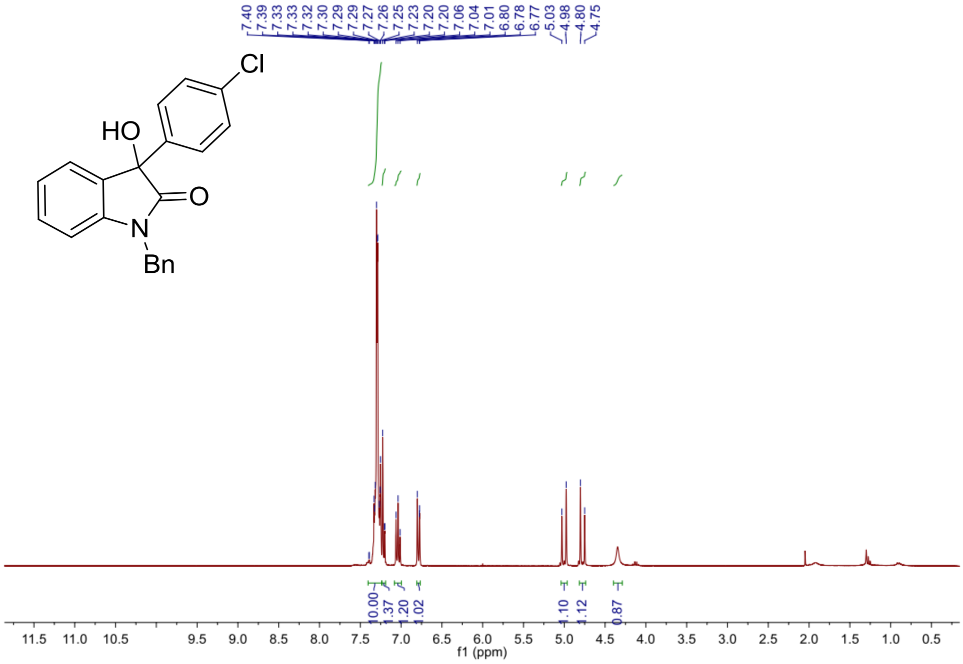

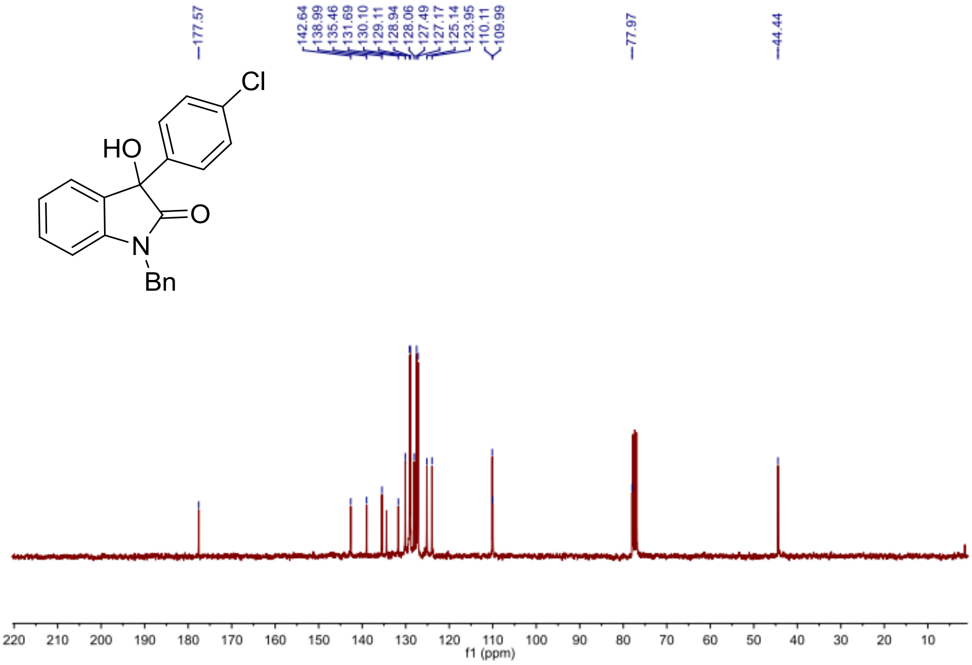

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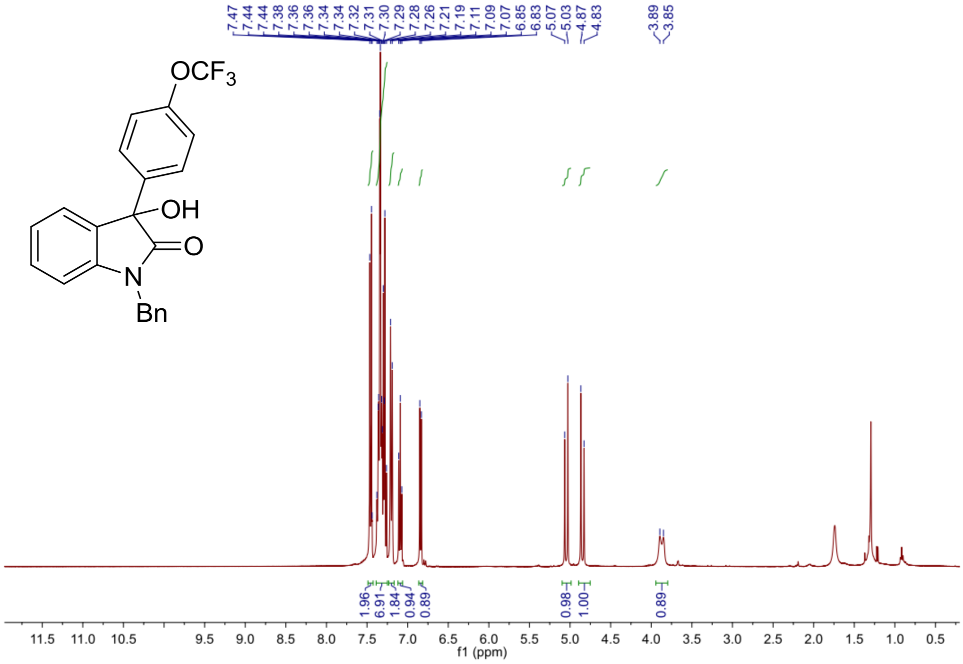

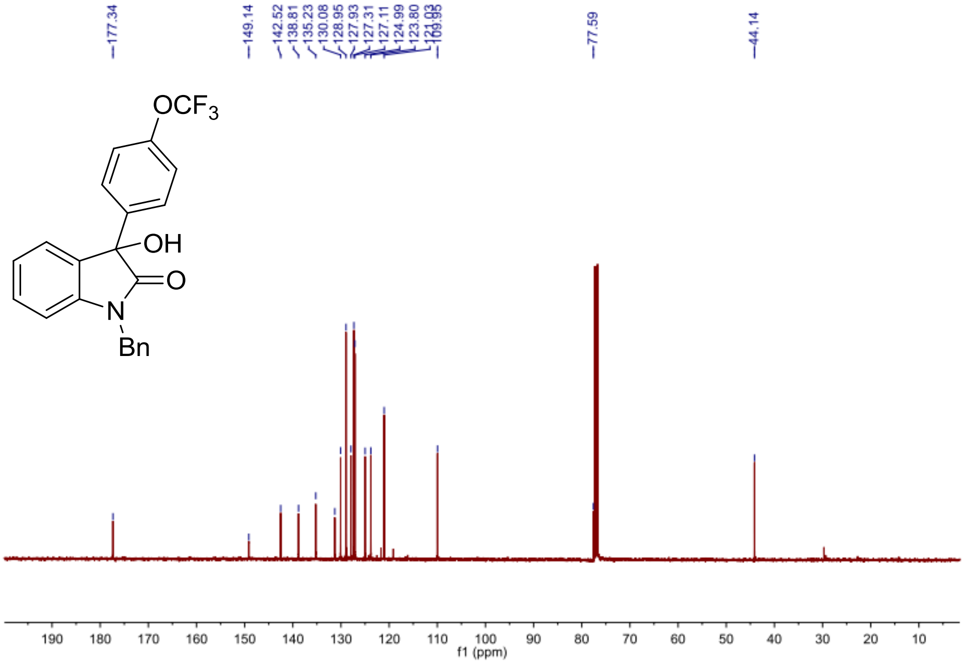

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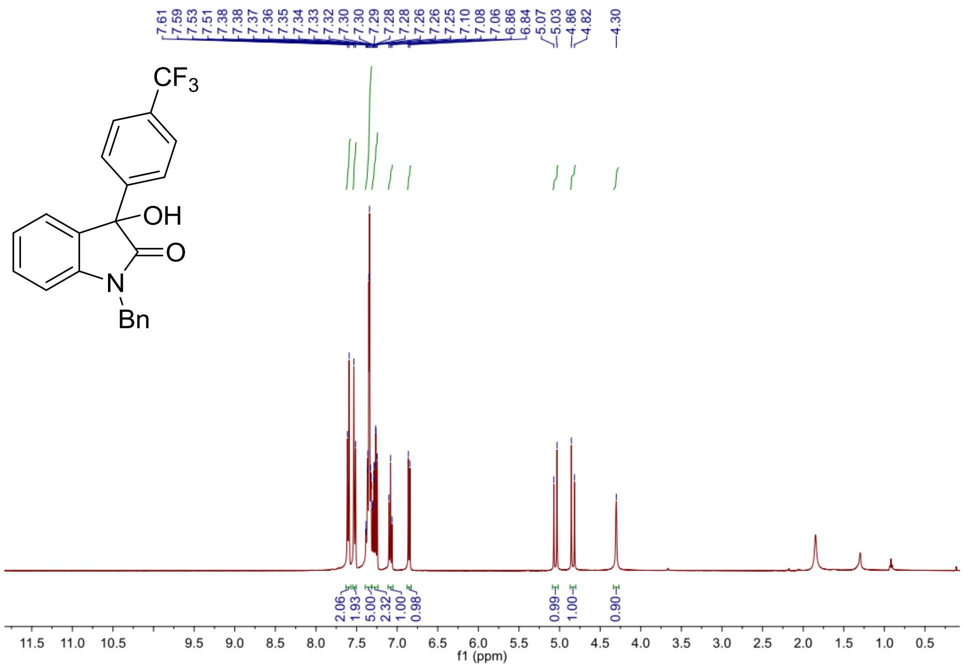

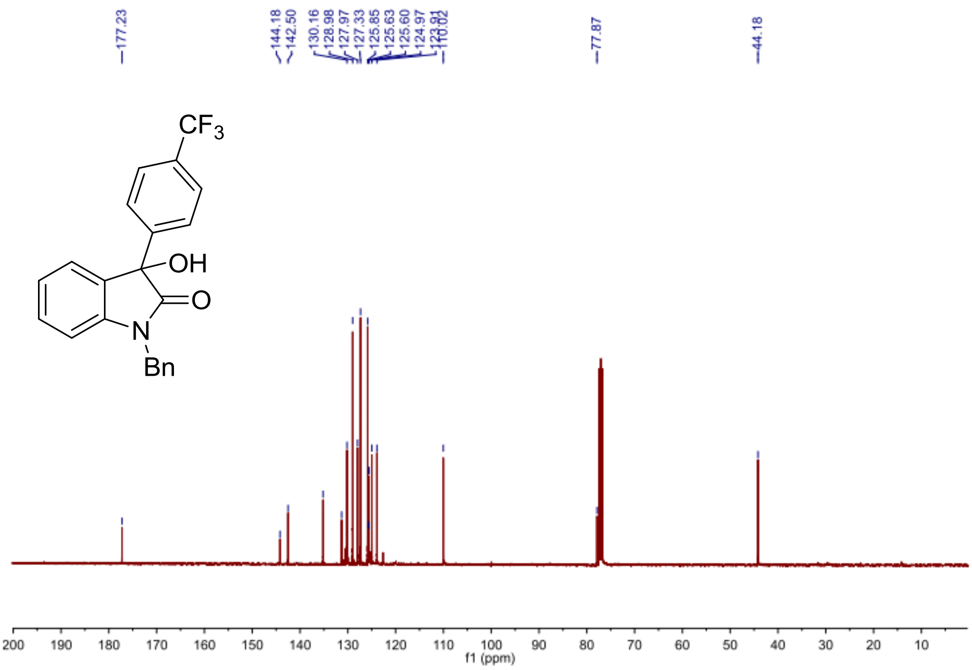

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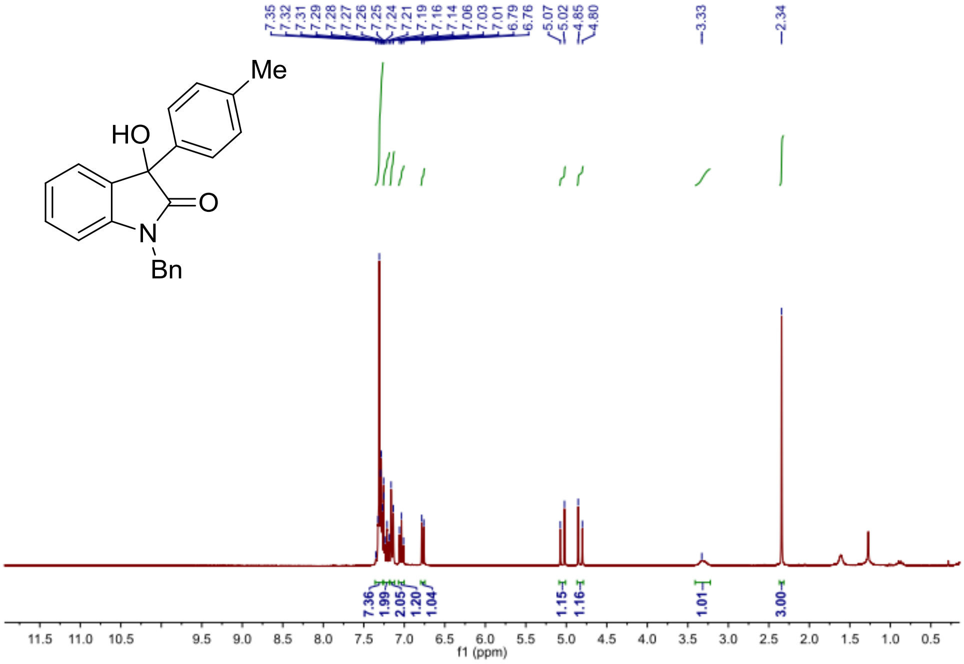

7.35
7.32
7.31
7.29
7.28
7.27
7.26
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7.21
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7.14
7.06
7.03
7.01
6.79
6.76
5.07
5.02
4.85
4.80
3.33
2.34
Me
HO
O
N
Bn
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1.20
1.04
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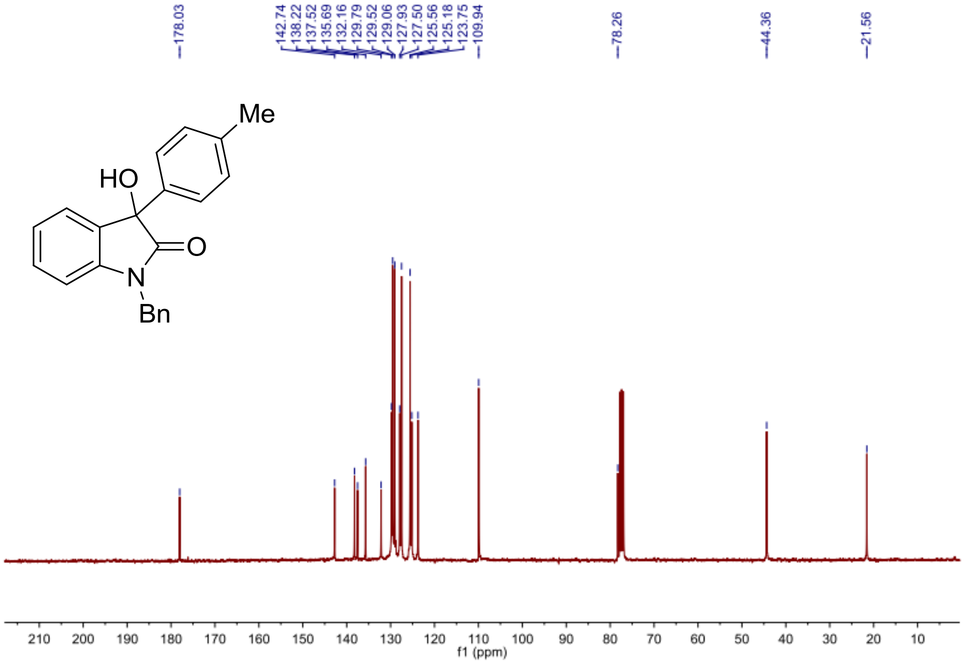
1.16
1.01
3.00
f1 (ppm)



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132.16
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129.52
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127.50
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109.94
78.26
44.36
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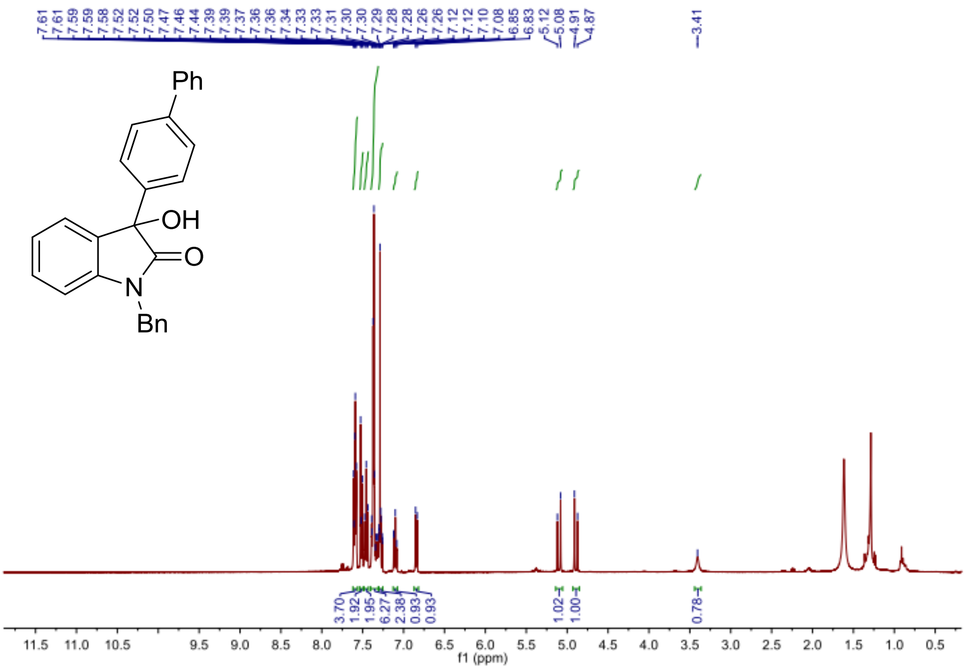
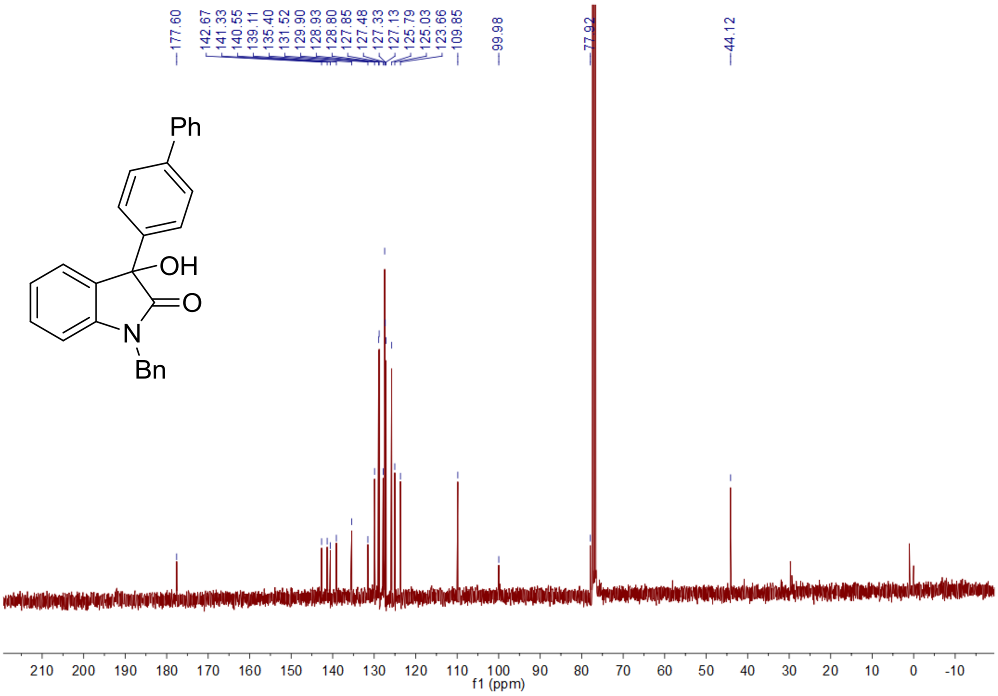
Me
HO
O
N
Bn
f1 (ppm)

7o





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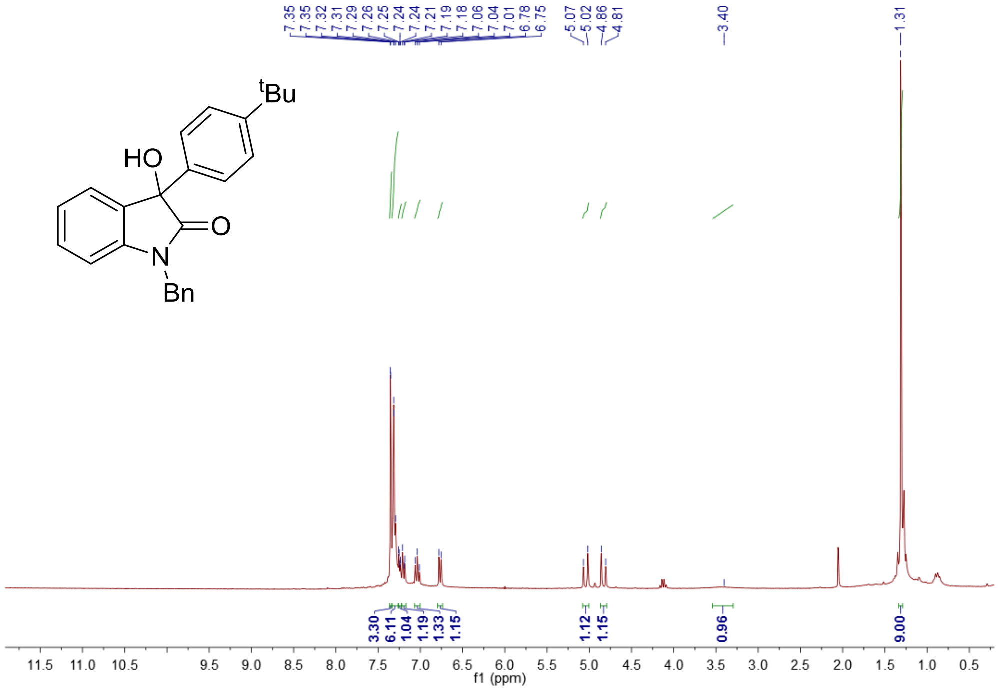

7.35
7.35
7.32
7.31
7.29
7.26
7.25
7.24
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7.04
7.01
6.78
6.75
5.07
5.02
4.86
4.81
3.40
1.31
tBu
HO
O
N
Bn
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1.04
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1.33
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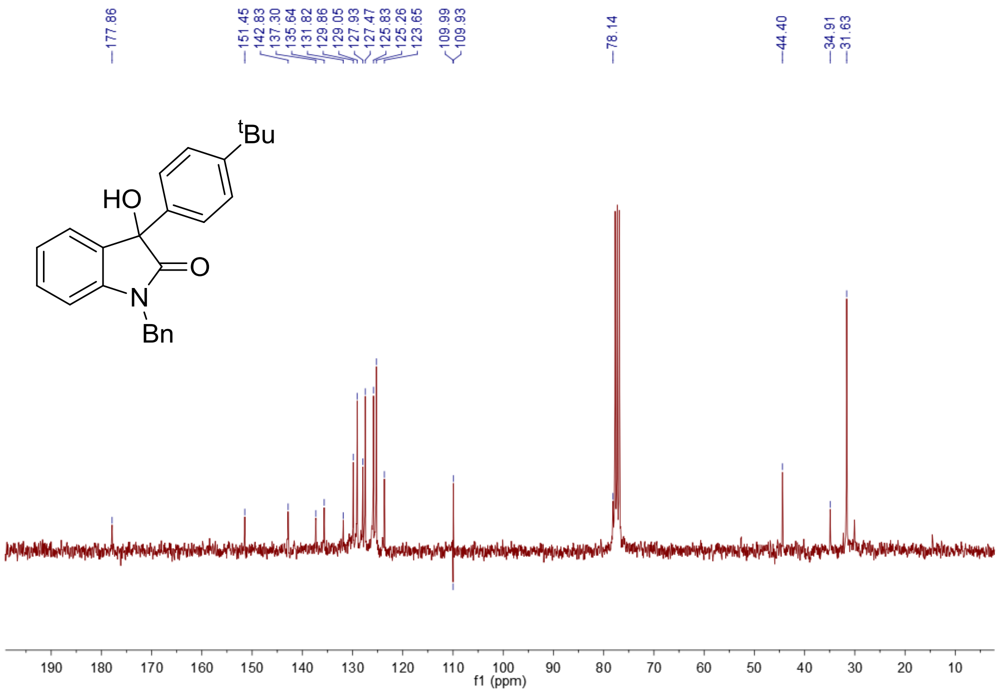
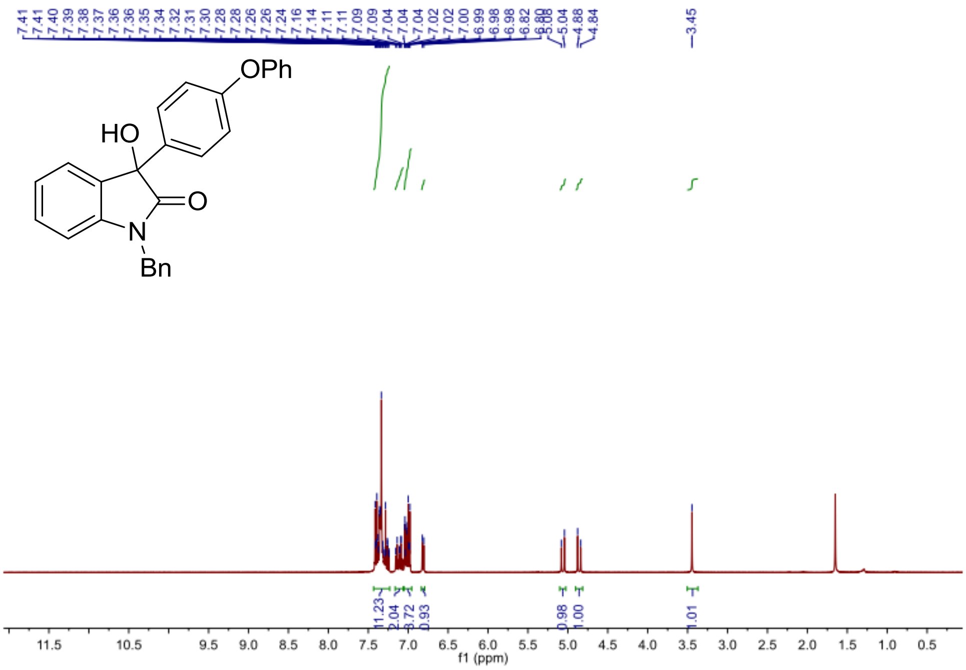
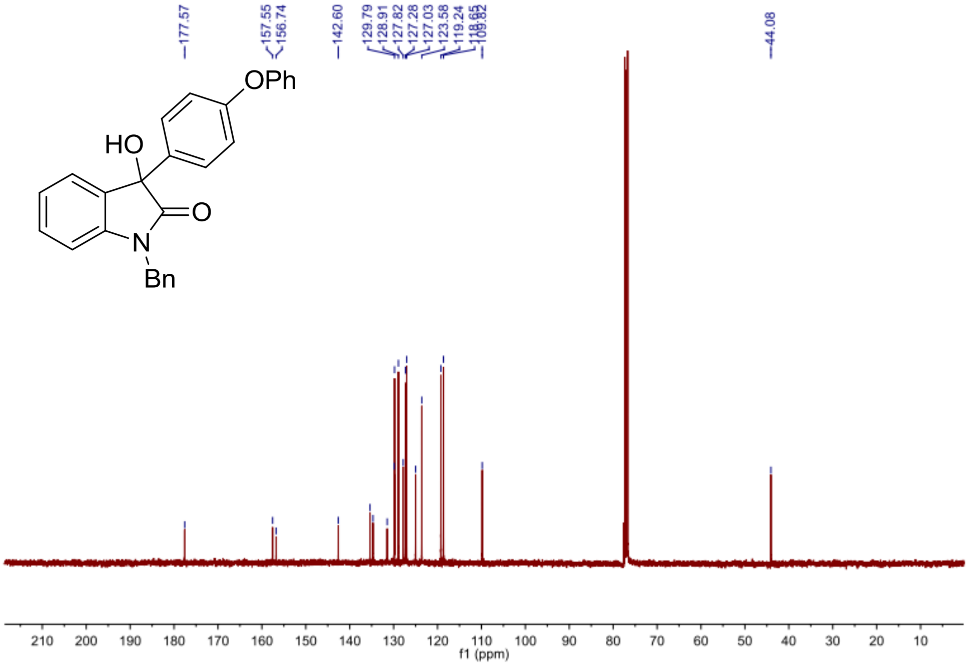
0.96
9.00
f1 (ppm)



177.86
151.45
142.83
137.30
135.64
131.82
129.86
129.05
127.93
127.47
125.83
125.26
123.65
109.99
109.93
78.14
44.40
34.91
31.63
tBu
HO
O
N
Bn
f1 (ppm)

7q





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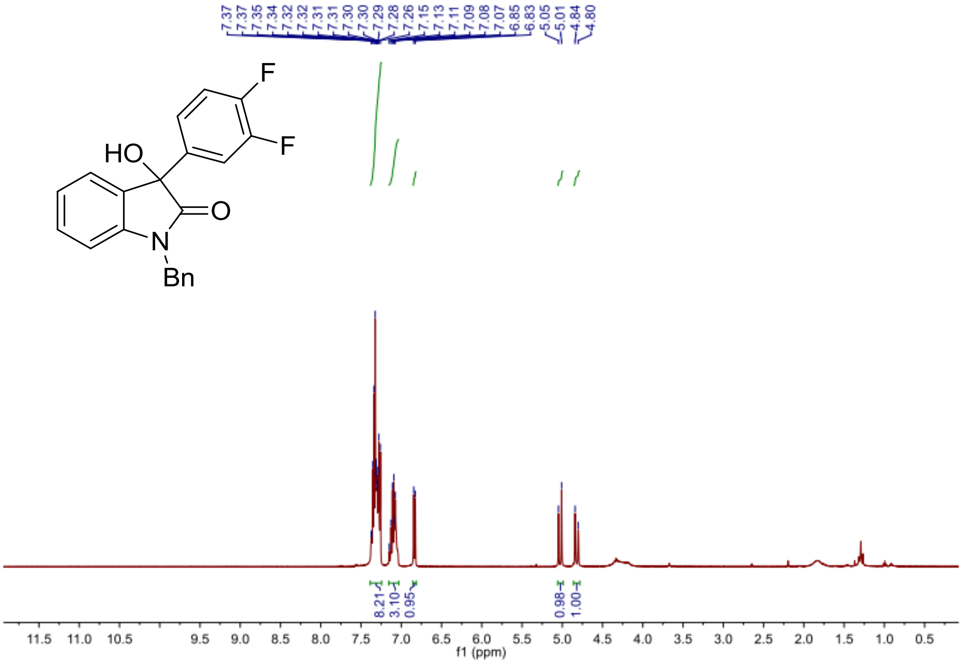
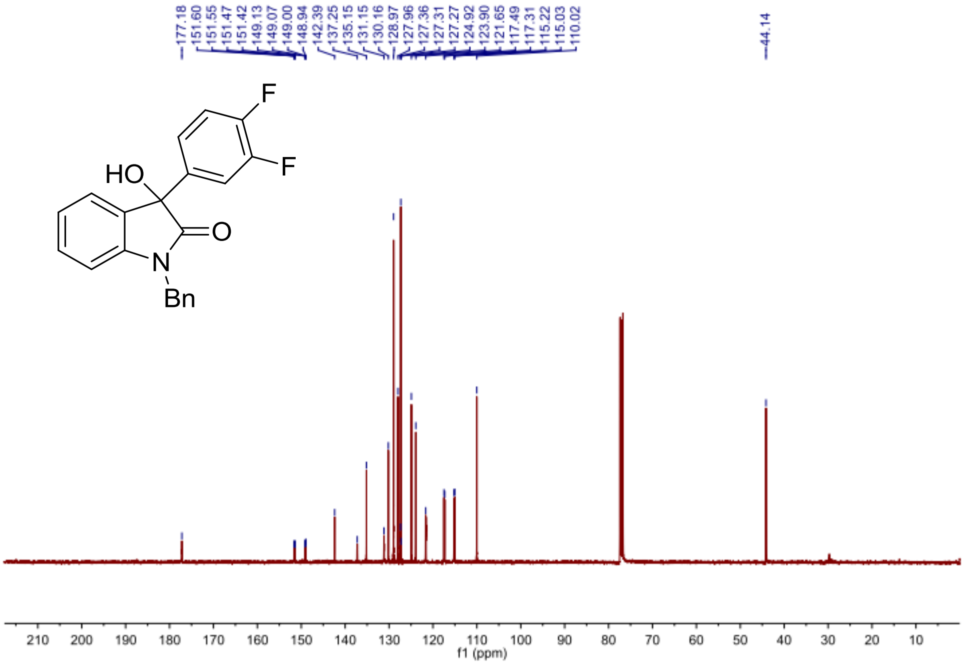
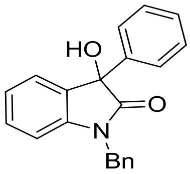


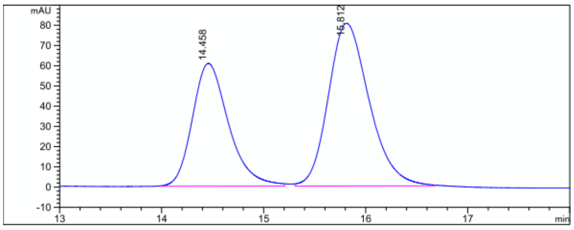


HPLC spectra.

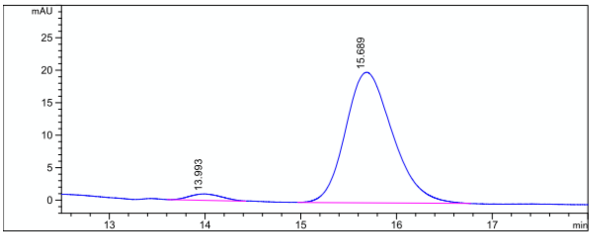


7a

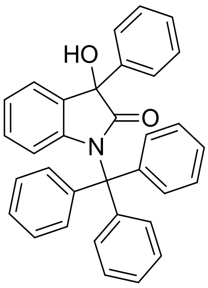
(The top one is racemic, the bottom one is chiral catalyzed by Ir-(S,S,R_a,S,S)-**4a** complex. Conditions: column, OD-H, flow rate 0.5 mL/min, 20% *i*-PrOH, 80% hexane, λ = 227 nm)



Entry #	RetTime [min]	Area [mAU*s]	Height [mAU]	Width [min]	Area %
1	14.46	1498.136	60.714	0.371	40.08
2	15.81	2238.854	80.422	0.419	59.91

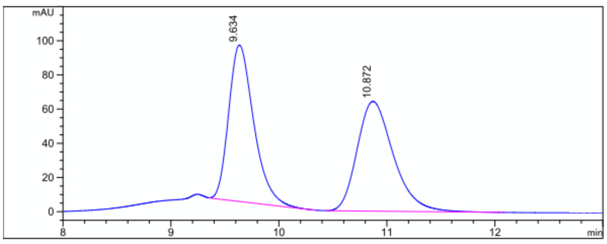


Entry #	RetTime [min]	Area [mAU*s]	Height [mAU]	Width [min]	Area %
1	13.99	23.043	0.991	0.387	3.24
2	15.69	687.330	20.086	0.570	96.75

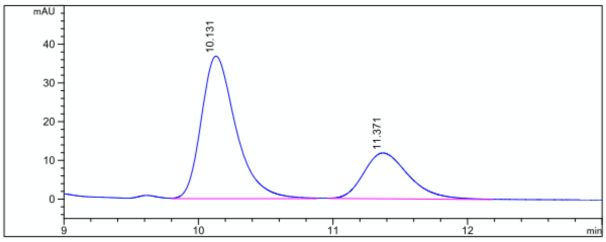


7b

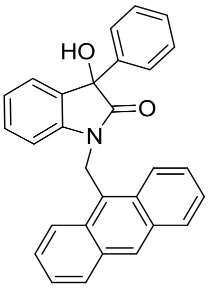
(The top one is racemic, the bottom one is chiral catalyzed by Ir-(S,S,R_a,S,S)-**4a** complex. Conditions: column, OD-H, flow rate 0.5 mL/min, 20% *i*-PrOH, 80% hexane, λ = 227 nm)



Entry #	RetTime [min]	Area [mAU*s]	Height [mAU]	Width [min]	Area %
1	9.63	1479.236	91.505	0.269	49.66
2	10.87	1499.175	64.155	0.361	50.33

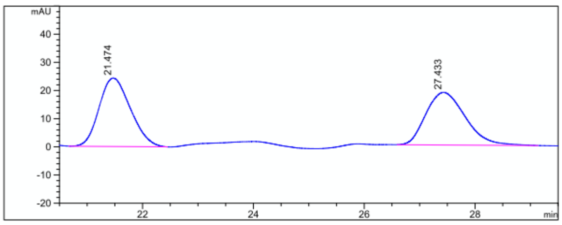


Entry #	RetTime [min]	Area [mAU*s]	Height [mAU]	Width [min]	Area %
1	10.13	658.217	36.802	0.298	70.51
2	11.37	275.263	11.837	0.388	29.48

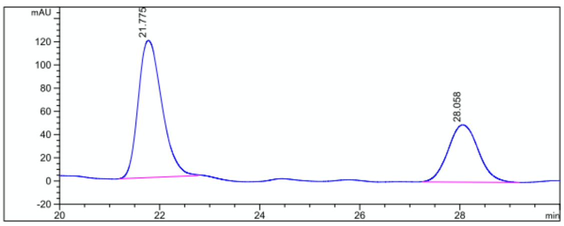


7c

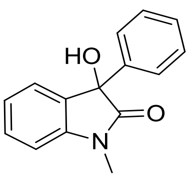
The top one is racemic, the bottom one is chiral catalyzed by Ir-*(S,S,R_a,S,S)*-**4a** complex. Conditions: column, IC-3, flow rate 0.7 mL/min, 15% *i*-PrOH, 85% hexane, λ = 227 nm.



Entry #	RetTime [min]	Area [mAU*s]	Height [mAU]	Width [min]	Area %
1	21.47	957.464	24.289	0.657	50.85
2	27.43	925.459	18.696	0.825	49.15



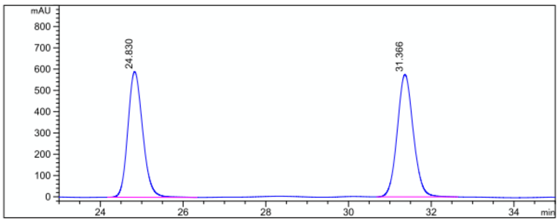
Entry #	RetTime [min]	Area [mAU*s]	Height [mAU]	Width [min]	Area %
1	21.77	3882.745	118.146	0.483	65.12
2	28.06	2079.016	49.360	0.647	34.87



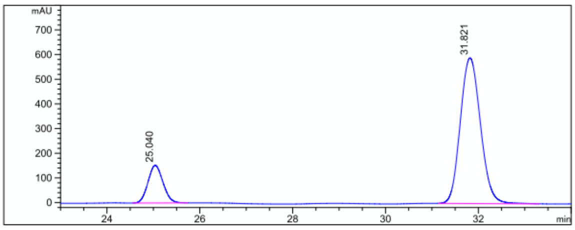
7d

The top one is racemic, the bottom one is chiral catalyzed by Ir-*(S,S,R_a,S,S)*-**4a** complex.

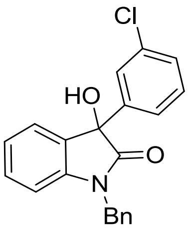
Conditions: column, OD-H, flow rate 0.5 mL/min, 15% *i*-PrOH, 85% hexane, λ = 227 nm.



Entry #	RetTime [min]	Area [mAU*s]	Height [mAU]	Width [min]	Area %
1	24.83	14709.694	589.962	0.416	48.65
2	31.37	15525.848	575.133	0.450	51.35

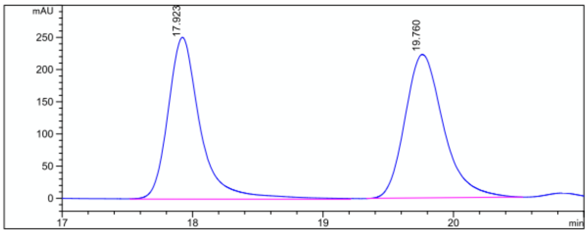


Entry #	RetTime [min]	Area [mAU*s]	Height [mAU]	Width [min]	Area %
1	25.04	3428.429	153.125	0.327	16.12
2	31.82	17830.508	590.586	0.472	83.87

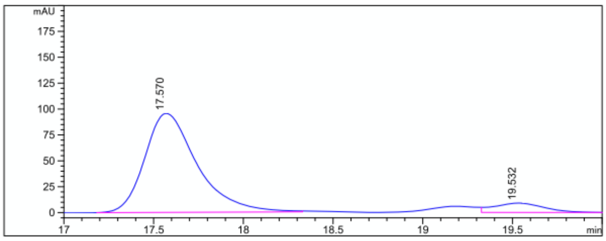


7e

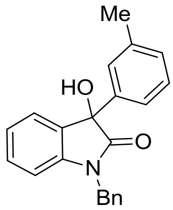
The top one is racemic, the bottom one is chiral catalyzed by Ir-*(S,S,R$_a$,S,S)*-**4a** complex. Conditions: column, IA-3, flow rate 0.5 mL/min, 20% *i*-PrOH, 80% hexane, λ = 227 nm.



Entry #	RetTime [min]	Area [mAU*s]	Height [mAU]	Width [min]	Area %
1	17.92	4332.998	251.185	0.288	48.77
2	19.76	4551.419	222.767	0.341	51.22

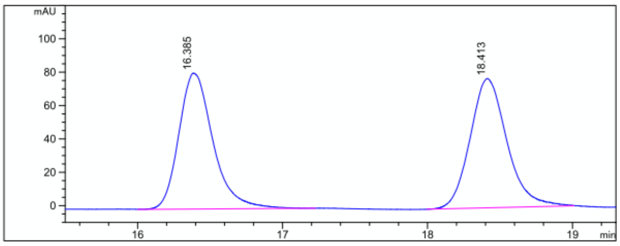


Entry #	RetTime [min]	Area [mAU*s]	Height [mAU]	Width [min]	Area %
1	17.57	1941.710	95.624	0.301	91.68
2	19.53	176.114	9.069	0.289	8.31

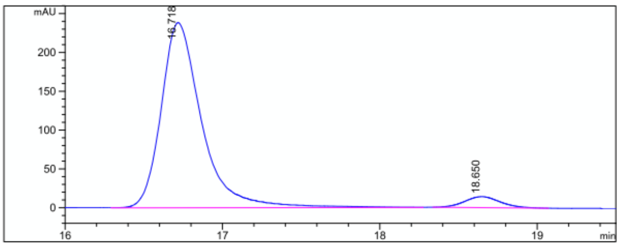


7f

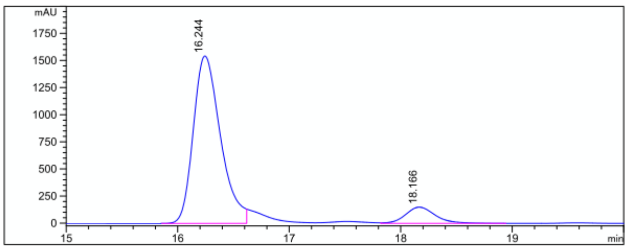
The top one is racemic, the middle one is chiral catalyzed by Ir-*(S,S,R_a,S,S)*-**4a** complex, the bottom one is chiral catalyzed by Ir-(*R_a,S,S*)-**6** complex. Conditions: column, IA-3, flow rate 0.7mL/min, 15% *i*-PrOH, 85% hexane, λ = 227 nm.



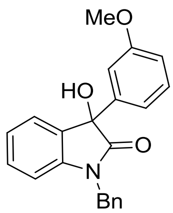
Entry #	RetTime [min]	Area [mAU*s]	Height [mAU]	Width [min]	Area %
1	16.39	1336.193	81.458	0.273	49.40
2	18.41	1368.156	77.450	0.294	50.59



Entry #	RetTime [min]	Area [mAU*s]	Height [mAU]	Width [min]	Area %
1	16.72	4274.561	238.563	0.299	95.00
2	18.65	224.802	14.188	0.264	4.99

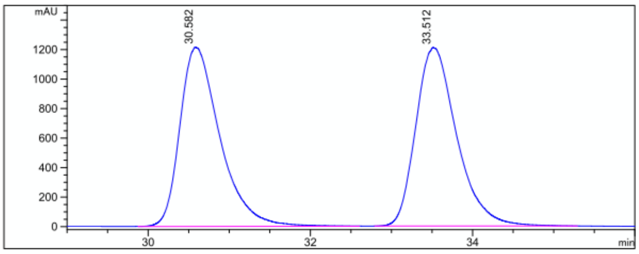


Entry #	RetTime [min]	Area [mAU*s]	Height [mAU]	Width [min]	Area %
1	16.24	26186.973	1543.664	0.283	90.31
2	18.17	2809.231	149.888	0.282	9.68

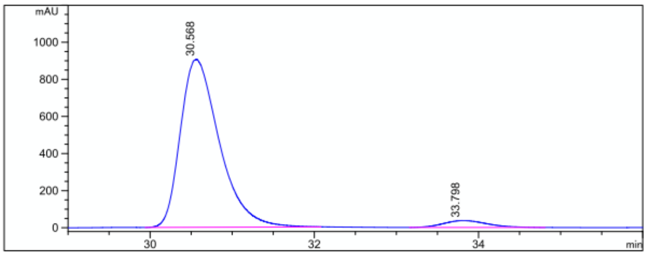


7g

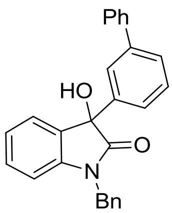
The top one is racemic, the bottom one is chiral catalyzed by Ir-(S,S,R_a,S,S)-**4a** complex. Conditions: column, IA-3, flow rate 0.7 mL/min, 10% *i*-PrOH, 90% hexane, λ = 227 nm.



Entry #	RetTime [min]	Area [mAU*s]	Height [mAU]	Width [min]	Area %
1	30.58	41699.250	1215.226	0.572	49.61
2	33.51	42340.965	1209.868	0.583	50.38

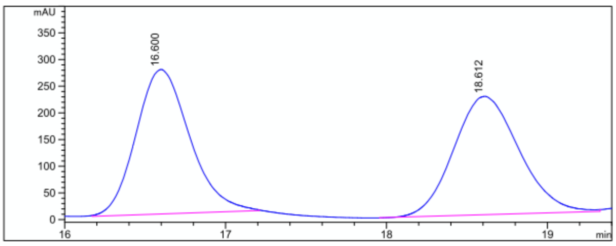


Entry #	RetTime [min]	Area [mAU*s]	Height [mAU]	Width [min]	Area %
1	30.57	29869.383	905.184	0.396	95.54
2	33.80	1391.960	37.036	0.448	4.45

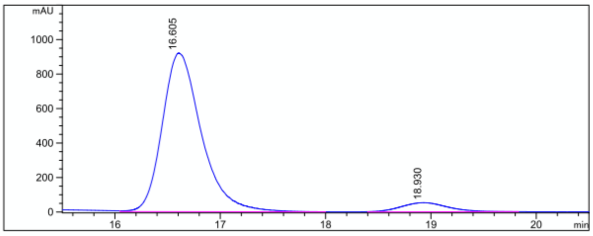


7h

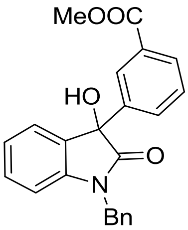
The top one is racemic, the bottom one is chiral catalyzed by Ir-(S,S,R_a,S,S)-**4a** complex. Conditions: column, IC-3, flow rate 0.7 mL/min, 20% *i*-PrOH, 80% hexane, λ = 227 nm.



Entry #	RetTime [min]	Area [mAU*s]	Height [mAU]	Width [min]	Area %
1	16.60	6291.261	270.955	0.387	50.06
2	18.61	6275.166	221.838	0.471	49.93

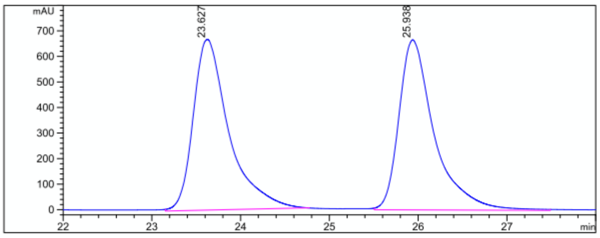


Entry #	RetTime [min]	Area [mAU*s]	Height [mAU]	Width [min]	Area %
1	16.60	23747.844	919.999	0.386	93.58
2	18.93	1626.761	52.904	0.512	6.41

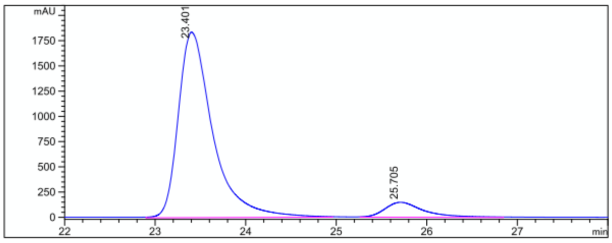


7i

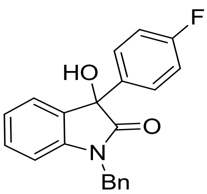
The top one is racemic, the bottom one is chiral catalyzed by Ir-*(S,S,R$_a$,S,S)*-**4a** complex. Conditions: column, IA-3, flow rate 0.5 mL/min, 20% *i*-PrOH, 80% hexane, λ = 227 nm.



Entry #	RetTime [min]	Area [mAU*s]	Height [mAU]	Width [min]	Area %
1	23.63	18635.271	667.949	0.465	50.31
2	25.94	18404.029	665.900	0.461	49.68

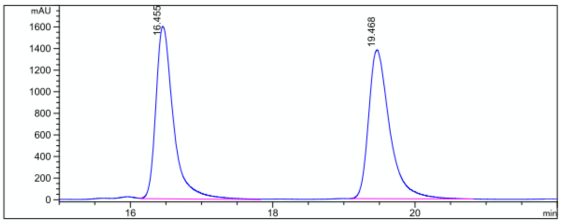


Entry #	RetTime [min]	Area [mAU*s]	Height [mAU]	Width [min]	Area %
1	23.40	48623.676	1839.012	0.441	91.51
2	25.71	4505.723	148.004	0.507	8.48

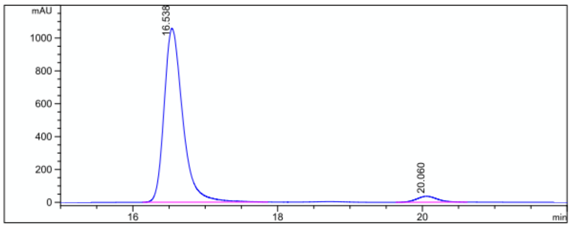


7j

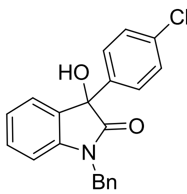
The top one is racemic, the bottom one is chiral catalyzed by Ir-*(S,S,R$_a$,S,S)*-**4a** complex. Conditions: column, IA-3, flow rate 0.7 mL/min, 15% *i*-PrOH, 85% hexane, λ = 227 nm.



Entry #	RetTime [min]	Area [mAU*s]	Height [mAU]	Width [min]	Area %
1	16.45	27404.764	1595.938	0.286	49.21
2	19.47	28282.770	1377.442	0.342	50.78

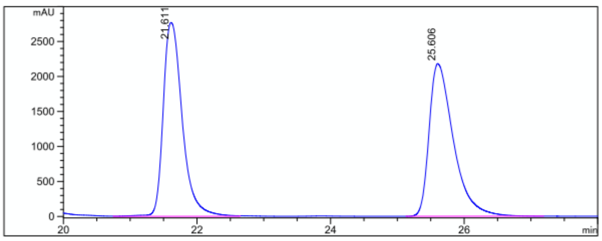


Entry #	RetTime [min]	Area [mAU*s]	Height [mAU]	Width [min]	Area %
1	16.54	18887.459	1058.317	0.297	96.28
2	20.06	728.846	36.387	0.287	3.71

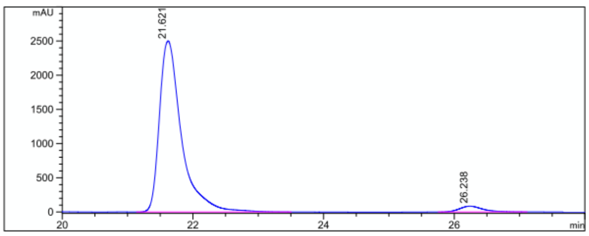


7k

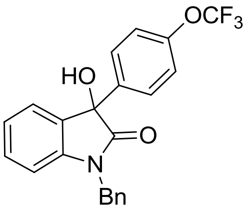
The top one is racemic, the bottom one is chiral catalyzed by Ir-*(S,S,R_a,S,S)*-**4a** complex. Conditions: column, IA-3, flow rate 0.5 mL/min, 20% *i*-PrOH, 80% hexane, λ = 227 nm.



Entry #	RetTime [min]	Area [mAU*s]	Height [mAU]	Width [min]	Area %
1	21.61	54973.117	2768.580	0.302	49.94
2	25.61	55092.555	2179.900	0.379	50.05

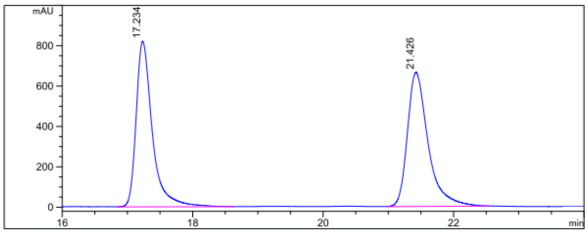


Entry #	RetTime [min]	Area [mAU*s]	Height [mAU]	Width [min]	Area %
1	21.62	58514.613	2501.745	0.340	96.55
2	26.24	2089.391	84.081	0.358	3.44

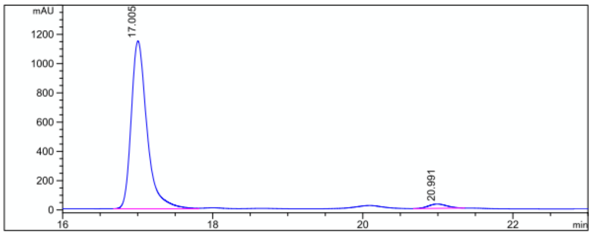


7l

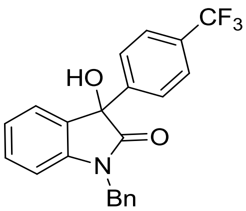
The top one is racemic, the bottom one is chiral catalyzed by Ir-*(S,S,R_a,S,S)*-**4a** complex. Conditions: column, IA-3, flow rate 0. 5 mL/min, 20% *i*-PrOH, 80% hexane, λ = 227 nm.



Entry #	RetTime [min]	Area [mAU*s]	Height [mAU]	Width [min]	Area %
1	17.23	14120.916	820.630	0.287	49.06
2	21.43	14660.250	665.329	0.367	50.93

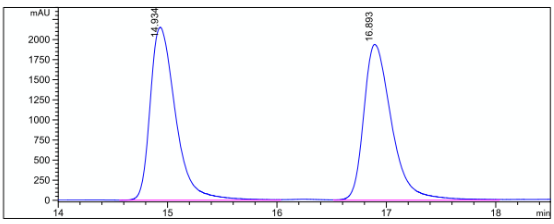


Entry #	RetTime [min]	Area [mAU*s]	Height [mAU]	Width [min]	Area %
1	17.00	16742.480	1146.761	0.222	97.01
2	20.99	515.700	29.717	0.289	2.98

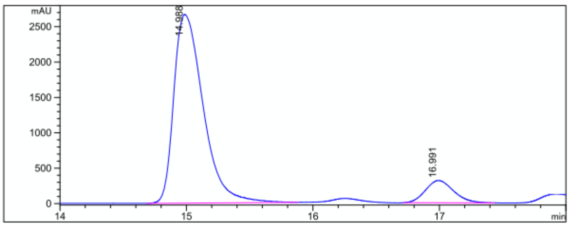


7m

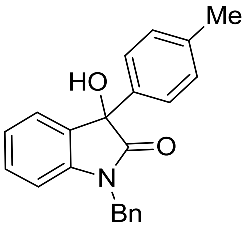
The top one is racemic, the bottom one is chiral catalyzed by Ir-*(S,S,R_a,S,S)*-**4a** complex. Conditions: column, IA-3, flow rate 0.5 mL/min, 20% *i*-PrOH, 80% hexane, λ = 227 nm.



Entry #	RetTime [min]	Area [mAU*s]	Height [mAU]	Width [min]	Area %
1	14.93	34689.813	2151.023	0.250	50.21
2	16.89	34390.914	1937.849	0.269	49.78

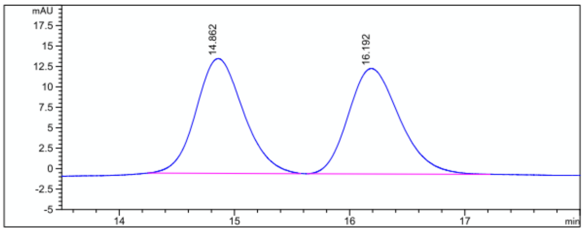


Entry #	RetTime [min]	Area [mAU*s]	Height [mAU]	Width [min]	Area %
1	14.99	43018.766	2666.494	0.269	89.81
2	16.99	4877.725	314.462	0.259	10.18

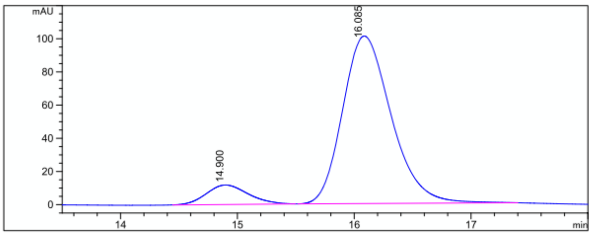


7n

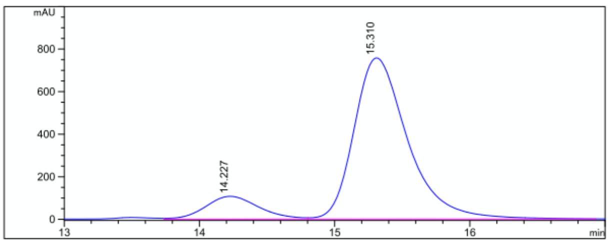
The top one is racemic, the middle one is chiral catalyzed by Ir-*(S,S,R_a,S,S)*-**4a** complex, the bottom one is chiral catalyzed by Ir-(*R_a,S,S*)-**6** complex. Conditions: column, OD-H, flow rate 0.5mL/min, 20% *i*-PrOH, 80% hexane, λ = 227 nm.



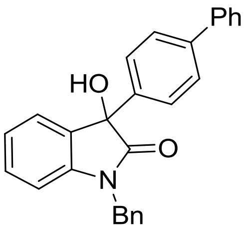
Entry #	RetTime [min]	Area [mAU*s]	Height [mAU]	Width [min]	Area %
1	14.86	402.406	14.047	0.477	50.24
2	16.19	398.506	12.907	0.515	49.75



Entry #	RetTime [min]	Area [mAU*s]	Height [mAU]	Width [min]	Area %
1	14.90	293.153	11.771	0.325	9.10
2	16.09	2925.685	100.987	0.483	90.89

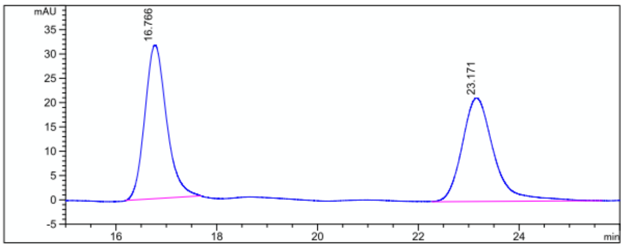


Entry #	RetTime [min]	Area [mAU*s]	Height [mAU]	Width [min]	Area %
1	14.23	2930.485	107.004	0.420	12.28
2	15.31	20927.299	756.778	0.423	87.71

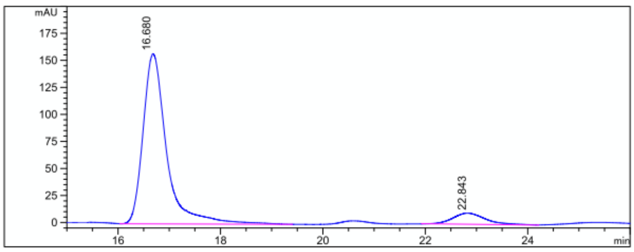


7o

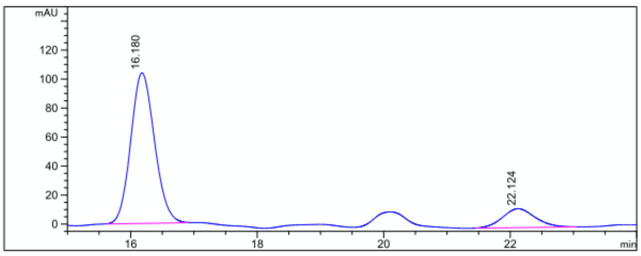
The top one is racemic, the middle one is chiral catalyzed by Ir-*(S,S,R$_a$,S,S)*-**4a** complex, the bottom one is chiral catalyzed by Ir-(*R$_a$,S,S*)-**6** complex. Conditions: column, IC-3, flow rate 0.7mL/min, 20% *i*-PrOH, 80% hexane, λ = 227 nm.



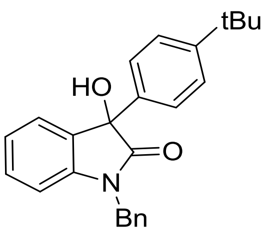
Entry #	RetTime [min]	Area [mAU*s]	Height [mAU]	Width [min]	Area %
1	16.77	946.638	31.616	0.499	50.41
2	23.17	931.017	21.281	0.729	49.58



Entry #	RetTime [min]	Area [mAU*s]	Height [mAU]	Width [min]	Area %
1	16.68	5019.521	157.369	0.532	91.72
2	22.84	452.833	10.213	0.739	8.27

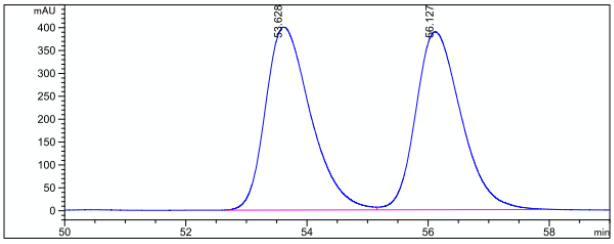


Entry #	RetTime [min]	Area [mAU*s]	Height [mAU]	Width [min]	Area %
1	16.18	2713.305	103.858	0.402	85.16
2	22.12	472.482	13.078	0.453	14.83

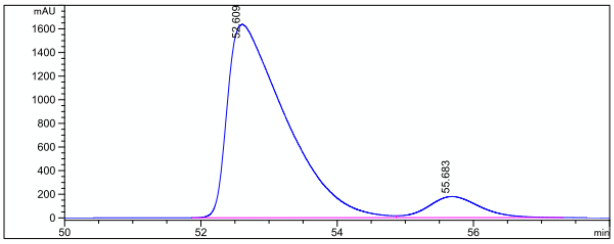


7p

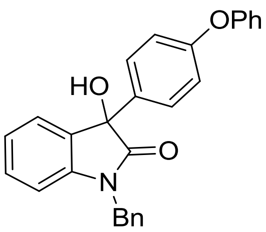
The top one is racemic, the bottom one is chiral catalyzed by Ir-(S,S,R_a,S,S)-**4a** complex. Conditions: column, IC-3, flow rate 0.7 mL/min, 20% *i*-PrOH, 80% hexane, λ = 227 nm.



Entry #	RetTime [min]	Area [mAU*s]	Height [mAU]	Width [min]	Area %
1	53.63	20719.506	399.357	0.651	50.59
2	56.13	20232.227	388.797	0.621	49.40

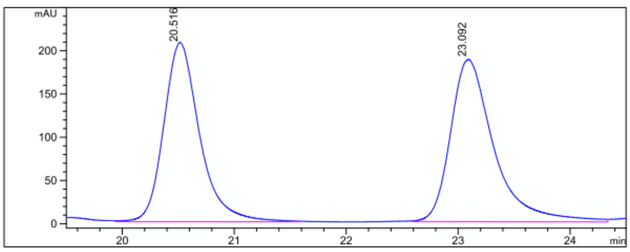


Entry #	RetTime [min]	Area [mAU*s]	Height [mAU]	Width [min]	Area %
1	52.61	96813.523	1638.070	0.703	91.16
2	55.68	9377.453	178.593	0.645	8.83

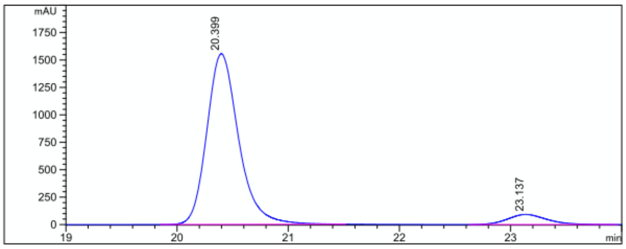


7q

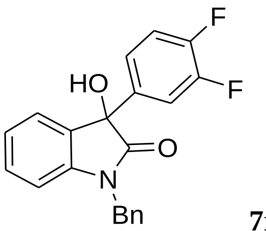
The top one is racemic, the bottom one is chiral catalyzed by Ir-(S,S,R_a,S,S)-**4a** complex. Conditions: column, IC-3, flow rate 0.5 mL/min, 20% *i*-PrOH, 80% hexane, λ = 227 nm.



Entry #	RetTime [min]	Area [mAU*s]	Height [mAU]	Width [min]	Area %
1	20.52	4608.993	207.170	0.328	47.74
2	23.09	5043.935	187.328	0.400	52.25

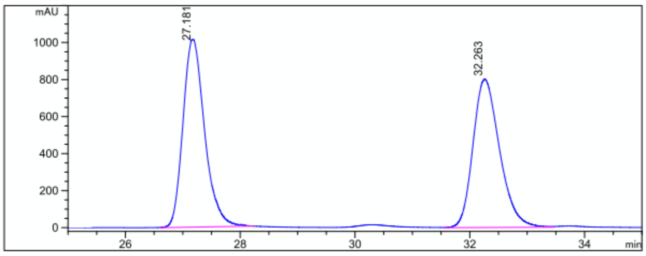


Entry #	RetTime [min]	Area [mAU*s]	Height [mAU]	Width [min]	Area %
1	20.40	30933.707	1556.197	0.301	93.18
2	23.14	2263.567	91.731	0.369	6.81

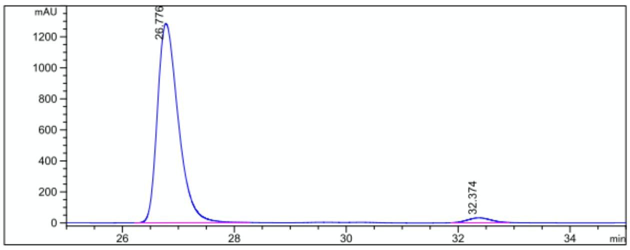


7r

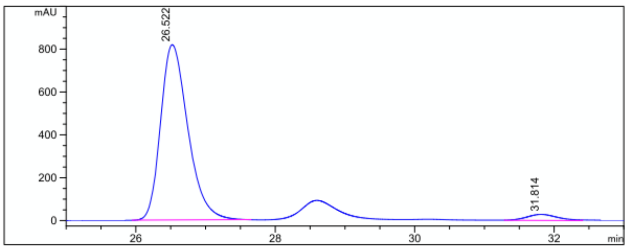
The top one is racemic, the middle one is chiral catalyzed by Ir-(S,S,Ra,S,S)-4a complex, the bottom one is chiral catalyzed by Ir-(R_a,S,S)-**6** complex. Conditions: column, IA-3, flow rate 0.5mL/min, 10% i-PrOH, 90% hexane, $\lambda = 227$ nm.



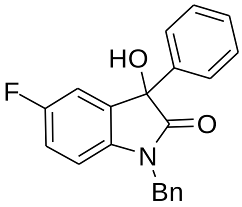
Entry #	RetTime [min]	Area [mAU*s]	Height [mAU]	Width [min]	Area %
1	27.18	26600.008	1013.746	0.437	50.72
2	32.26	25837.791	801.573	0.537	49.27



Entry #	RetTime [min]	Area [mAU*s]	Height [mAU]	Width [min]	Area %
1	26.78	33307.730	1285.625	0.432	97.29
2	32.37	927.849	31.744	0.487	2.71

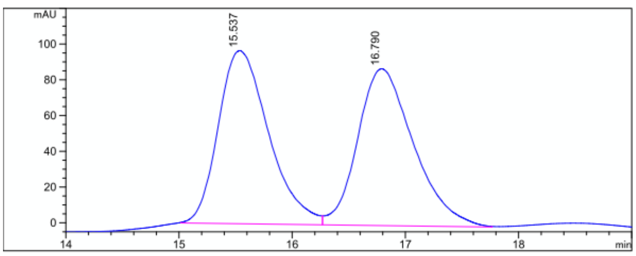


Entry #	RetTime [min]	Area [mAU*s]	Height [mAU]	Width [min]	Area %
1	26.52	22247.670	817.476	0.454	96.23
2	31.81	869.906	28.207	0.514	3.76

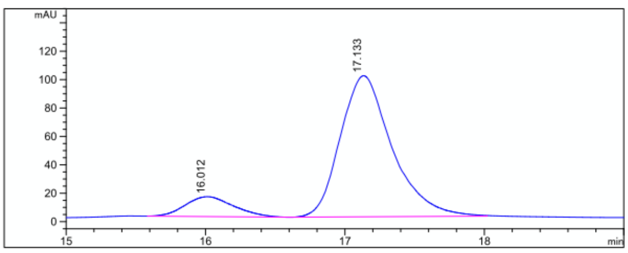


7s

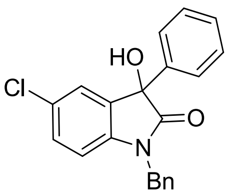
The top one is racemic, the bottom one is chiral catalyzed by Ir-*(S,S,R_a,S,S)*-**4a** complex. Conditions: column, IA-3, flow rate 0.5 mL/min, 15% *i*-PrOH, 85% hexane, λ = 227 nm.



Entry #	RetTime [min]	Area [mAU*s]	Height [mAU]	Width [min]	Area %
1	15.54	3001.387	96.843	0.517	49.89
2	16.79	3013.903	87.743	0.572	50.10

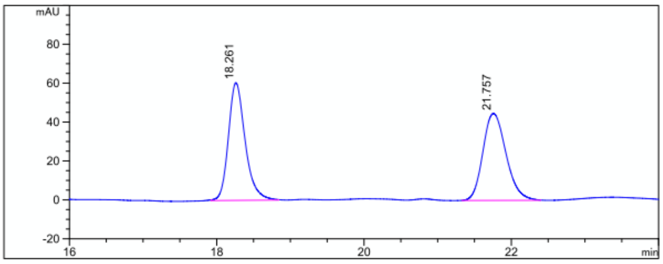


Entry #	RetTime [min]	Area [mAU*s]	Height [mAU]	Width [min]	Area %
1	16.01	337.700	13.994	0.311	11.63
2	17.13	2563.703	99.358	0.366	88.36

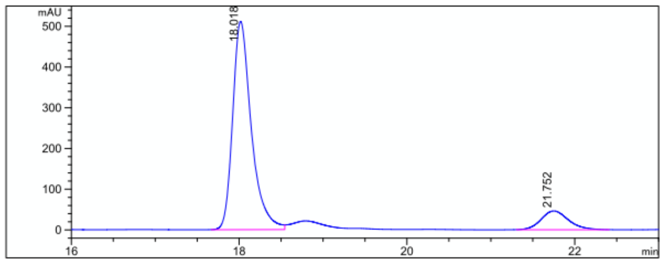


7t

The top one is racemic, the bottom one is chiral catalyzed by Ir-*(S,S,R_a,S,S)*-**4a** complex. Conditions: column, IA-3, flow rate 0.5 mL/min, 20% *i*-PrOH, 80% hexane, λ = 227 nm.



Entry #	RetTime [min]	Area [mAU*s]	Height [mAU]	Width [min]	Area %
1	18.26	958.534	60.482	0.240	49.53
2	21.76	976.601	44.675	0.338	50.46



Entry #	RetTime [min]	Area [mAU*s]	Height [mAU]	Width [min]	Area %
1	18.02	7906.521	511.231	0.233	88.27
2	21.75	1050.011	46.068	0.349	11.72

X-ray data of ligand (*S*,*S*,*R*$_a$,*S*,*S*)-4a

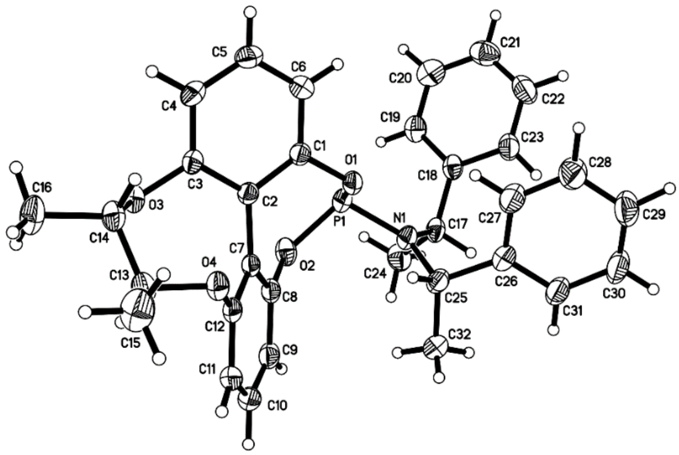


Table 1. Crystal data and structure refinement for (*S*,*S*,*R*$_a$,*S*,*S*)-**4a**

Empirical formula	C_{32} H_{32} N O_4 P
Formula weight	525.56
Temperature	296(2) K
Wavelength	0.71073 Å
Crystal system	Orthorhombic

Space group	P2(1)2(1)2(1)	
Unit cell dimensions	a = 8.4161(2) Å	□= 90°.
	b = 13.3624(3) Å	□= 90°.
	c = 24.8701(5) Å	□ = 90°.
Volume	2796.87(11) Å^3	
Z	4	
Density (calculated)	1.248 Mg/m^3	
Absorption coefficient	0.136 mm^{-1}	
F(000)	1112	
Crystal size	0.46 x 0.44 x 0.40 mm^3	
Theta range for data collection	1.64 to 27.41°.	
Index ranges	-10<=h<=10, -17<=k<=17, -31<=l<=32	
Reflections collected	34196	
Independent reflections	6351 [R(int) = 0.0365]	
Completeness to theta = 27.41°	99.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7456 and 0.6658	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	6351 / 1 / 416	
Goodness-of-fit on F^2	1.002	
Final R indices [I>2sigma(I)]	R1 = 0.0377, wR2 = 0.0797	
R indices (all data)	R1 = 0.0613, wR2 = 0.0906	
Absolute structure parameter	0.04(8)	
Largest diff. peak and hole	0.125 and -0.174 e.Å^{-3}	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3) for (*S*,*S*,*R*$_a$,*S*,*S*)-**4a**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

x

P(1)	4272(1)	6336(1)	1562(1)	48(1)
O(1)	5625(1)	6295(1)	1077(1)	45(1)
O(2)	5252(1)	7092(1)	1981(1)	55(1)

O(3)	8117(1)	9517(1)	1068(1)	48(1)
O(4)	10275(1)	8068(1)	1229(1)	52(1)
N(1)	4500(2)	5173(1)	1776(1)	50(1)
C(1)	5965(2)	7195(1)	819(1)	43(1)
C(2)	6979(2)	7871(1)	1071(1)	40(1)
C(3)	7289(2)	8771(1)	800(1)	44(1)
C(4)	6695(2)	8943(1)	293(1)	54(1)
C(5)	5762(2)	8231(1)	47(1)	60(1)
C(6)	5369(2)	7358(1)	310(1)	55(1)
C(7)	7738(2)	7633(1)	1591(1)	40(1)
C(8)	6877(2)	7239(1)	2023(1)	47(1)
C(9)	7600(2)	7078(1)	2519(1)	59(1)
C(10)	9188(3)	7283(1)	2582(1)	64(1)
C(11)	10081(2)	7626(1)	2156(1)	59(1)
C(12)	9362(2)	7792(1)	1665(1)	45(1)
C(13)	10848(2)	9090(1)	1230(1)	57(1)
C(14)	9722(2)	9706(1)	891(1)	53(1)
C(15)	12532(2)	9072(2)	1014(1)	94(1)
C(16)	10007(3)	10827(1)	947(1)	84(1)
C(17)	3048(2)	4628(1)	1965(1)	51(1)
C(18)	1823(2)	4509(1)	1524(1)	50(1)
C(19)	649(2)	5210(1)	1428(1)	60(1)
C(20)	-409(2)	5107(2)	1011(1)	75(1)
C(21)	-315(3)	4284(2)	686(1)	81(1)
C(22)	814(3)	3567(2)	778(1)	83(1)
C(23)	1869(2)	3673(1)	1196(1)	64(1)
C(24)	2390(3)	5070(1)	2485(1)	70(1)
C(25)	6029(2)	4629(1)	1816(1)	56(1)
C(26)	5988(2)	3698(1)	1468(1)	55(1)
C(27)	5719(3)	3798(1)	921(1)	74(1)
C(28)	5630(3)	2984(2)	592(1)	89(1)
C(29)	5817(3)	2028(2)	796(1)	92(1)
C(30)	6068(3)	1913(1)	1330(1)	89(1)
C(31)	6162(2)	2736(1)	1665(1)	71(1)
C(32)	6495(3)	4433(2)	2401(1)	80(1)