

The origin for highly enantioselective induction of 1-naphthol to isatin -derived N-Boc ketimines catalyzed by quinine thiourea catalyst: An Experimental and Computational Study

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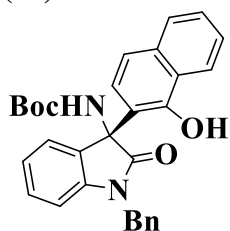
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1. General procedure for the enantioselective Friedel-Crafts reaction of 1-naphthol with ketamine:

To a solution of quinine thiourea **5b** (5 mol%) in 2ml of dichloromethane 1-naphthol or 2-naphthol (3 mmol), ketimine (2 mmol) and 50mg of 4Å MS were added under N₂ atm. The reactions was monitored by TLC until the consumption of ketimine and after the completion of the reaction, solvent was removed under reduced pressure and it was subjected to column chromatography using hexane: ethyl acetate (9.5:5) as eluent to afford desired product **8a-8n** in pure form.

2. Characterization data for products

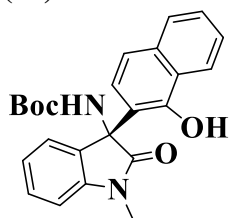
(+)-*tert*-butyl (*R*)-(1-benzyl-3-(1-hydroxynaphthalen-2-yl)-2-oxoindolin-3-yl) carbamate¹ (**8a**)



Enantiomeric excess (99%) was determined by chiral HPLC (Chiralpak IA), hexane-*i*PrOH 80:20, 0.75 mL/min, major enantiomer *t*_r = 40.02 min, minor enantiomer *t*_r = 11.00 min.

mp 104-105 °C; [α]_D²⁰ +358.5 (*c* 0.44, CHCl₃) (99% *ee*); ¹H NMR (500 MHz, CDCl₃) δ 10.62 (s, 1H), 8.51-8.42 (m, 1H), 7.75-7.66 (m, 1H), 7.56-7.46 (m, 2H), 7.42 (m, 1H), 7.30 (m 1H), 7.27-7.15 (m, 7H), 6.81 (d, *J* = 8.8 Hz, 1H), 6.77 (d, *J* = 7.0 Hz, 1H), 5.81 (s, 1H), 5.06 (d, *J* = 15.9 Hz, 1H), 4.83 (d, *J* = 14.4 Hz, 1H), 1.34 (s, 9H).; ¹³C NMR (125 MHz, CDCl₃) δ 179.8, 154.1, 153.75, 142.6, 134.9, 134.8, 129.4, 128.8, 127.6, 127.4, 127.0, 126.9, 125.6, 125.3, 125.0, 123.5, 123.1, 119.5, 114.6, 110.2, 80.7, 66.1, 44.4, 28.1.

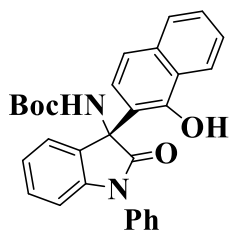
(+)-*tert*-butyl (*R*)-(3-(1-hydroxynaphthalen-2-yl)-1-methyl-2-oxoindolin-3-yl)carbamate¹ (**8b**)



Enantiomeric excess (95%) was determined by chiral HPLC (Chiralpak IA), hexane-*i*PrOH 85:15, 0.75 mL/min, major enantiomer *t*_r = 12.269 min, minor enantiomer *t*_r = 13.779 min.

mp 95-99 °C; $[\alpha]_D^{20} +390.6$ (*c* 0.42, CHCl₃) (95% *ee*); ¹H NMR (500 MHz, CDCl₃) δ 10.86 (s, 1H), 8.45-8.43 (m, 1H), 7.50-7.48 (m, 2H), 7.45-7.41 (m, 2H), 7.29-7.25 (m, 1H), 7.16 (d, *J* = 8.5, 0.9 Hz, 1H), 6.95 (d, *J* = 7.5 Hz, 1H), 6.80 (d, *J* = 9 Hz, 1H), 5.69 (s, 1H), 3.24 (s, 3H), 1.28 (s, 9H); ¹³C NMR (125 MHz, CDCl₃) δ 179.5 , 154.2 , 153.8 , 143.4 , 134.8 , 129.5, 129.25, 127.4 , 126.9 , 125.6 , 125.3 , 125.1 , 123.4 , 123.2 , 119.4 , 114.2 , 109.2 , 80.7, 66.1, 28.0 , 26.8.

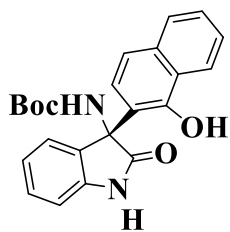
(+) *tert*-butyl (R)-(3-(1-hydroxynaphthalen-2-yl)-1-phenyl-2-oxindolin-3-yl)carbamate (8c)



Enantiomeric excess (95%) was determined by chiral HPLC (Chiralpak IA), hexane-*i*PrOH 70:30, 0.7 mL/min, major enantiomer *t*_r = 30.5 min, minor enantiomer *t*_r = 13.6 min.

mp 115-117 °C; $[\alpha]_D^{20} +381.2$ (*c* 0.45, CHCl₃) (95% *ee*); ¹H NMR (500 MHz, CDCl₃) δ 10.6 (s, 1H), 8.46-8.41 (m, 1H), 7.79-7.70 (m, 1H), 7.52-7.43 (m, 8H), 7.37-7.30 (m, 3H), 7.21 (s, 1H), 6.94 (s, 1H), 6.91-6.88 (m, 1H), 6.81 (d, *J* = 18, 1H), 5.8 (s, 1H), 1.34(s, 9H).; ¹³C NMR (125 MHz, CDCl₃) δ 168.2, 155.9, 152.6, 144.5, 129.6, 128.5, 127.4, 127.0, 127.2, 126.4, 127.2, 125.8, 125.7, 125.8, 118.0, 111.8, 78.5, 55.5, 51.5, 28.4.

(+) *tert*-butyl (R)-(3-(1-hydroxynaphthalen-2-yl)-2-oxindolin-3-yl) carbamate (8d)

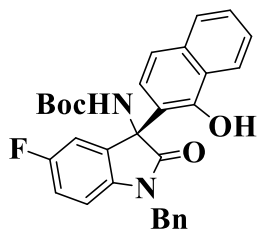


Enantiomeric excess (63%) was determined by chiral HPLC (Chiralpak IA), hexane-*i*PrOH 80:20, 0.7 mL/min, major enantiomer *t*_r = 20.7 min, minor enantiomer *t*_r = 9.40 min.

mp 103-106 °C; $[\alpha]_D^{20} +341.0$ (*c* 0.45, CHCl₃) (63% *ee*); ¹H NMR (200 MHz, CDCl₃) 8.46-8.41 (m, 1H), 7.73-7.68 (m, 1H), 7.52-7.47 (m, 2H), 7.41-7.35 (m, 2H), 7.31-7.17 (m, 3H), 6.91-6.80

(m, 2H), 5.78 (s, 1H), 1.34 (s, 9H); ^{13}C NMR (75.5 MHz, CDCl_3) δ 179.5, 155.5, 152.6, 143.3, 127.8, 127.4, 127.2, 126.4, 125.7, 125.6, 125.0, 124.8, 120.2, 118.0, 78.2, 50.8, 28.

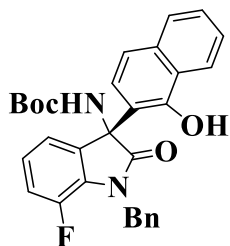
(+)-*tert*-butyl (*R*)-(1-benzyl-5-fluoro-3-(1-hydroxynaphthalen-2-yl)-2-oxoindolin-3-yl) carbamate (8e)



Enantiomeric excess (99%) was determined by chiral HPLC (Chiralpak IA), hexane-*i*PrOH 85:15, 0.7 mL/min, major enantiomer t_r = 45.71 min, minor enantiomer t_r = 16.09 min.

mp 155-157 °C; $[\alpha]_D^{20}$ +382.2 (*c* 0.42, CHCl_3) (96% *ee*); ^1H NMR (500 MHz, CDCl_3) δ 10.7 (s, 1H), 8.46-8.44 (m, 1H), 7.79-7.70 (m, 1H), 7.52-7.50 (m, 2H), 7.46-7.44 (m, 1H), 7.25-7.16 (m, 6H), 6.98-6.95 (m, 1H), 6.77 (d, *J* = 9 Hz, 1H), 6.66-6.64 (m, 1H), 5.92 (d, *J* = 20 Hz, 1H), 5.00 (d, *J* = 15 Hz, 1H), 4.81 (s, 1H), 1.36 (s, 9H); ^{13}C NMR (125 MHz, CDCl_3) δ 179.6, 160.7, 158.7, 154.1, 151.7, 138.4, 134.9, 128.8, 127.7, 127.6, 127.1, 127.0, 120.3, 119.9, 115.9, 115.8, 114.0, 113.5, 113.3, 111.2, 111.1, 108.5, 81.1, 66.3, 44.5, 28.2.

(+)-*tert*-butyl (*R*)-(1-benzyl-7-fluoro-3-(1-hydroxynaphthalen-2-yl)-2-oxoindolin-3-yl) carbamate¹ (8f)

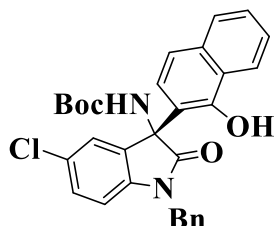


Enantiomeric excess (99%) was determined by chiral HPLC (Chiralpak IA), hexane-*i*PrOH 60:40, 07 mL/min, major enantiomer t_r = 21.67 min, minor enantiomer t_r = 9.12 min.

$[\alpha]_D^{20}$ +405 (*c* 0.35, CHCl_3) (99% *ee*); ^1H NMR (500 MHz, CDCl_3) δ 10.6 (s, 1H), 8.46-8.44 (m, 1H), 7.79-7.77 (m, 2H), 7.70-7.69 (m, 1H), 7.51-7.49 (m, 2H), 7.46-7.44 (m, 1H), 7.40-7.38 (m, 1H), 7.23-7.16 (m, 8H), 7.07-7.03 (m, 1H), 6.74-6.73 (s, 1H), 6.71-6.69 (s, 1H), 6.02-5.90 (d, 1H), 5.14-5.11 (d, 1H), 4.99-4.96 (d, 1H), 1.33 (s, 9H). 1.35; ^{13}C NMR (125 MHz, CDCl_3) δ 178.5,

153.08, 153.0, 150.7, 148.1, 146.1, 135.0, 133.9, 127.5, 126.5, 126.0, 125.3, 124.8, 124.7, 124.0, 123.7, 123.3, 123.2, 122.2, 120.7, 120.1, 119.2, 118.8, 116.8, 113.0, 107.4, 80.1, 65.3, 45.1, 27.1.

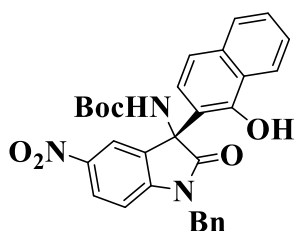
(+)-*tert*-butyl (*R*)-(1-benzyl-6-chloro-3-(1-hydroxynaphthalen-2-yl)-2-oxoindolin-3-yl)carbamate¹ (8g)



Enantiomeric excess (99%) was determined by chiral HPLC (Chiralpak IA), hexane-*i*PrOH 60:40, 0.7 mL/min, major enantiomer $t_r = 33.065$ min, minor enantiomer $t_r = 13.619$ min.

mp 115-118 °C; $[\alpha]_D^{20} +412.8$ (c 0.35, CHCl₃) (99% *ee*); ¹H NMR (500 MHz, CDCl₃) δ 10.68 (s, 1H), 8.45-8.43 (m, 1H), 7.70-7.69 (m, 1H), 7.51-7.49 (m, 2H), 7.33 (s, 1H), 7.25-7.17 (m, 7H), 6.76 (d, $J = 8.5$, Hz, 1H), 6.65 (d, $J = 8.5$, 1H), 5.91 (s, 1H), 4.93 (d, 1H), 1.36 (s, 9H). ¹³C NMR (125 MHz, CDCl₃) δ 178.4, 153.07, 152.94, 140.09, 133.4, 128.4, 128.0, 127.8, 126.6, 126.1, 126.0, 124.8, 124.6, 122.2, 118.9, 112.8, 110.4, 80.11, 65.14, 43.5, 27.20.

(+)-*tert*-butyl (*R*)-(1-benzyl-3-(1-hydroxynaphthalen-2-yl)-5-nitro-2-oxoindolin-3-yl)carbamate¹ (8h)

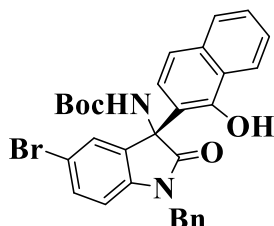


Enantiomeric excess (99%) was determined by chiral HPLC (Chiralpak IA), hexane-*i*PrOH 70:30, 1 mL/min, major enantiomer $t_r = 15.879$ min, minor enantiomer $t_r = 10.205$ min.

mp 145-147 °C; $[\alpha]_D^{20} +499.1$ (c 0.25, CHCl₃) (99% *ee*); ¹H NMR (500 MHz, CDCl₃) δ 10.35 (s, 1H), 8.45-8.43 (m, 1H), 8.31 (d, $J = 5$ Hz, 1H), 8.25 (m, 1H), 7.71-7.69 (m, 1H), 7.55-7.50 (m, 2H), 7.18 (d, $J = 10$, 1H), 6.83 (d, $J = 8.5$, 1H), 6.65 (d, $J = 9$), 6.08 (s, 1H), 4.99 (s, 1H), 1.39 (s, 9H); ¹³C NMR (125 MHz, CDCl₃) δ 179.2, 152.9, 147.0, 143.1, 133.9, 132.7, 129.4, 128.0,

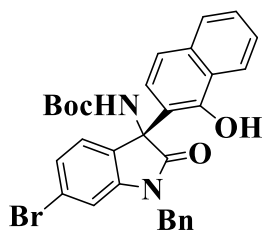
127.08, 126.8, 126.1, 126.0, 125.4, 125.02, 123.13, 122.11, 119.9, 119.3, 111.8, 109.18, 80.49, 64.7, 43.8, 30.5, 27.18, 21.6.

(+)-tert-butyl (R)-(1-benzyl-5-bromo-3-(1-hydroxynaphthalen-2-yl)-2-oxoindolin-3-yl) carbamate¹ (8i)



Enantiomeric excess (97%) was determined by chiral HPLC (Chiralpak IA), hexane-*i*PrOH 85:15, 0.75 mL/min, major enantiomer $t_r = 34.53$ min, minor enantiomer $t_r = 13.66$ min. mp 117-120 °C; $[\alpha]_D^{20} +419.2$ (c 0.27, CHCl₃) (97% *ee*); ¹H NMR (500 MHz, CDCl₃) δ 10.65 (s, 1H), 8.46-8.45 (m, 1H), 7.75-7.73 (m, 1H), 7.53-7.52 (m, 4H), 7.42-7.40 (m, 1H), 7.23-7.22(m, 8H), 6.79(d, $J = 9$, 1H), 6.63 (d, $J = 8$, 1H), 5.82 (s, 1H), 4.98 (d, $J = 12.5$, 1H), 1.37 (s, 9H). ¹³C NMR (125 MHz, CDCl₃) δ 178.3 , 153.0 , 140.5, 133.3, 131.3, 127.8, 127.4, 126.7, 126.0, 125.9, 124.7, 123.6, 122.19, 118.9, 115.3, 112.8, 110.8, 107.6, 80.1, 65.07, 43.5, 27.17.

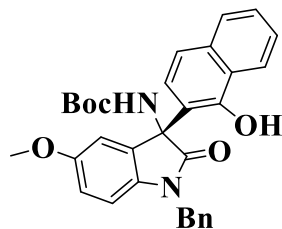
(+)-tert-butyl (R)-(1-benzyl-6-bromo-3-(1-hydroxynaphthalen-2-yl)-2-oxoindolin-3-yl) carbamate¹ (8j)



Enantiomeric excess (97%) was determined by chiral HPLC (Chiralpak IA), hexane-*i*PrOH 60:40, 0.7 mL/min, major enantiomer $t_r = 18.43$ min, minor enantiomer $t_r = 11.52$ min. mp 115-120 °C; $[\alpha]_D^{20} +390$ (c 0.27, CHCl₃) (97% *ee*); ¹H NMR (500 MHz, CDCl₃) δ 10.6 (s, 1H), 8.46-8.44 (m, 1H), 8.18-8.16 (s, 1H), 7.80-7.78 (m, 1H), 7.72-7.71(m, 1H), 7.52-7.50 (m, 2H), 7.48-7.46(m, 1H), 7.40 (d, $J = 10$, 1H), 7.38-7.36 (m, 1H), 7.29-7.21 (m, 2H), 7.24-7.17 (m, 6H), 6.88 (s, 1H), 6.76 (s, 1H), 6.75(d, 1H), 5.02 (d, $J = 15$ Hz, 1H), 4.75 (s, 1H), 1.35 (s, 9H).; ¹³C NMR (125 MHz, CDCl₃) δ 178.7, 153.04, 152.9, 150.5, 142.8, 133.9, 133.7, 133.2, 127.9, 126.8, 126.6, 126.0,

125.9, 125.5, 125.4, 125.3, 124.8, 124.8, 124.14, 123.7, 122.1, 122.0, 120.6, 119.4, 118.9, 112.8, 112.7, 107.5, 80.2, 64.8, 43.5, 27.1.

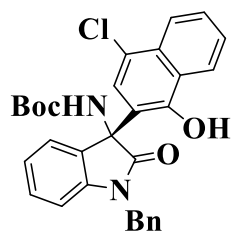
(+)-*tert*-butyl (*R*)-(1-benzyl-3-(1-hydroxynaphthalen-2-yl)-5-methoxy-2-oxindolin-3-yl) carbamate¹ (8k)



Enantiomeric excess (97%) was determined by chiral HPLC (Chiralpak IA), hexane-*i*PrOH 70:30, 0.7 mL/min, major enantiomer t_r = 19.94 min, minor enantiomer t_r = 14.53 min.

mp 100-103 °C; $[\alpha]_D^{20}$ +385.9 (c 0.325, CHCl₃) (97% *ee*); ¹H NMR (500 MHz, CDCl₃) δ 10.9 (s, 1H), 8.46-8.45 (m, 1H), 7.71-7.70 (m, 1H), 7.51-7.49 (m, 2H), 7.24-7.18 (m, 7H), 7.02 (d, J = 2.5 Hz, 1H), 6.85 (d, J = 9 Hz, 1H), 6.81-6.78 (dd, 1H), 6.65 (d, J = 8.5 Hz, 1H), 5.83 (s, 1H), 5.02 (d, J = 15.8 Hz, 1H), 4.85 (d, J = 14.1 Hz, 1H), 3.81 (s, 3H), 1.34 (s, 9H); ¹³C NMR (125 MHz, CDCl₃) δ 179.4, 156.6, 154.1, 135.8, 134.9, 130.6, 128.7, 127.6, 127.4, 127.0, 125.6, 125.0, 123.2, 119.6, 114.6, 113.6, 112.7, 110.8, 80.7, 66.4, 55.8, 44.5, 28.2.

(+)-*tert*-butyl (*R*)-(1-benzyl-3-(4-chloro-1-hydroxynaphthalen-2-yl)-2-oxindolin-3-yl) carbamate¹ (8l)

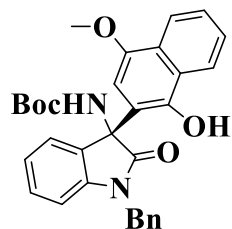


Enantiomeric excess (95%) was determined by chiral HPLC (Chiralpak IA), hexane-*i*PrOH 70:30, 1 mL/min, major enantiomer t_r = 13.38 min, minor enantiomer t_r = 7.66 min.

mp 116-117 °C; $[\alpha]_D^{20}$ +331.1 (c 0.35, CHCl₃) (95% *ee*); ¹H NMR (500 MHz, CDCl₃) δ 11.00 (s, 1H), 8.43 (d, J = 8.5, 1H), 8.19-8.16 (m, 1H), 8.05 (d, J = 13 Hz, 1H), 7.62-7.57 (m, 2H), 7.53-7.50 (m, 1H), 7.43 (d, J = 7, 1H), 7.31-7.18 (m, 8H), 6.89 (s, 1H), 6.76 (d, J = 7.5, 1H), 6.56 (d, J = 5, 1H), 6.02 (s, 1H), 5.04 (d, J = 10, 1H), 4.8 (s, 1H), 1.32 (s, 9H); ¹³C NMR (125 MHz, CDCl₃) δ 178.5, 153.07, 152.2, 150.1, 141.5, 133.6, 130.7, 130.4, 128.8, 127.8, 127.5, 126.9, 126.7, 126.3,

126.0, 125.4, 124.8, 124.6, 124.2, 123.8, 123.2, 122.9, 122.6, 121.8, 121.6, 121.4, 113.6, 109.6, 107, 80.1, 64.8, 43.5, 27.7.

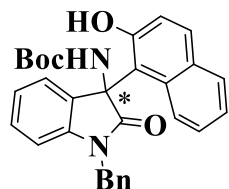
(+)-*tert*-butyl (*R*)-(1-benzyl-3-(4-methoxy-1-hydroxynaphthalen-2-yl)-2-oxoindolin-3-yl) carbamate (8m)



Enantiomeric excess (97%) was determined by chiral HPLC (Chiralpak IA), hexane-*i*PrOH 70:30, 0.7 mL/min, major enantiomer t_r = 18.29 min, minor enantiomer t_r = 13.203 min.

$[\alpha]_D^{20} +301.1$ (c 0.35, CHCl_3) (97% *ee*); $^1\text{H NMR}$ (500 MHz, CDCl_3) δ 10.34 (s, 1H), 8.42-8.41 (m, 1H), 8.21-8.10 (m, 1H), 7.55-7.50 (m, 2H), 7.44 (d, J = 7 Hz, 1H), 7.24-7.20 (m, 7H), 6.78 (d, J = 7.5, 1H), 6.14 (s, 1H), 5.03 (d, J = 15 Hz, 1H), 4.8 (s, 1H), 3.6 (s, 3H), 1.33 (s, 9H). ; $^{13}\text{C NMR}$ (125 MHz, CDCl_3) δ 179.6, 153.9, 148.9, 147.7, 142.6, 134.9, 129.5, 128.7, 127.8, 127.6, 127.0, 126.8, 126.6, 126.3, 125.0, 123.2, 123.0, 121.3, 113.7, 110.4, 103.5, 80.7, 66.2, 55.4, 44.4, 28.1.

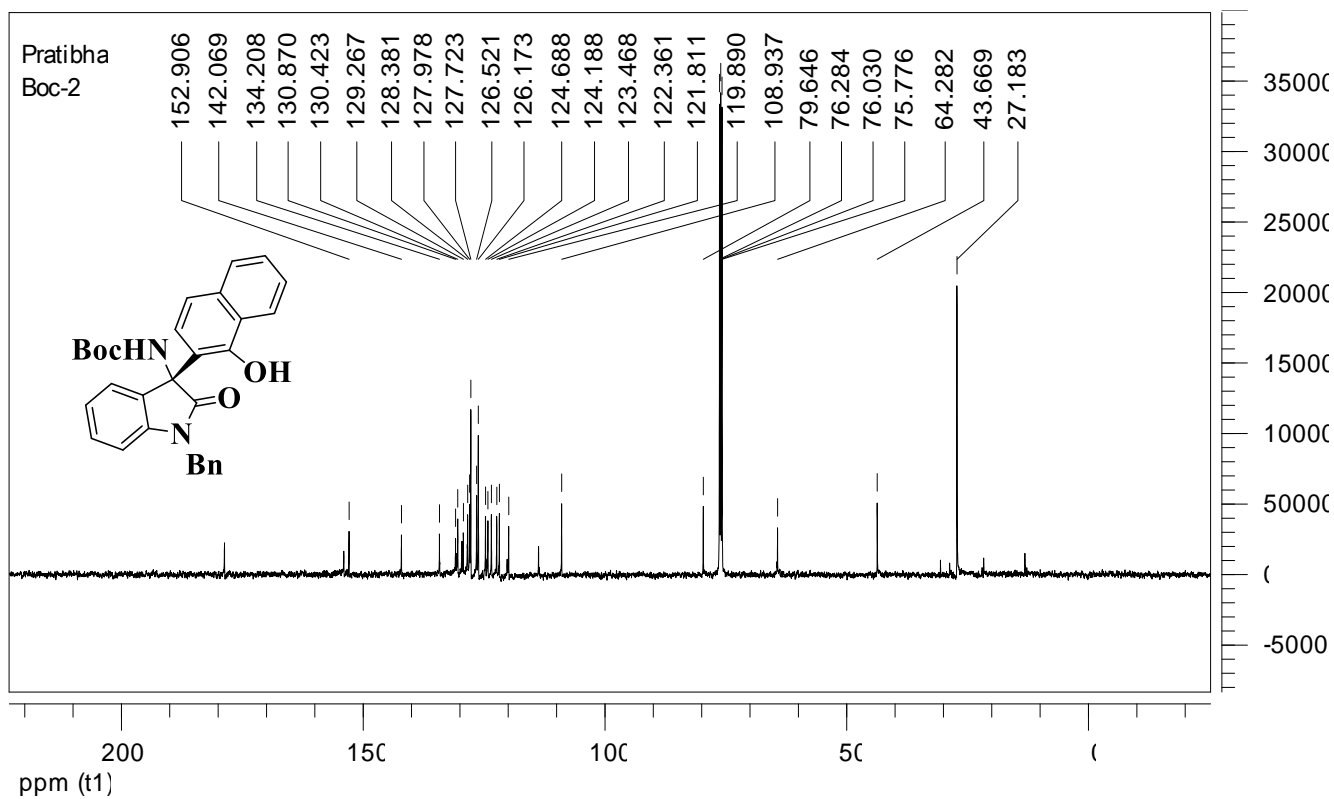
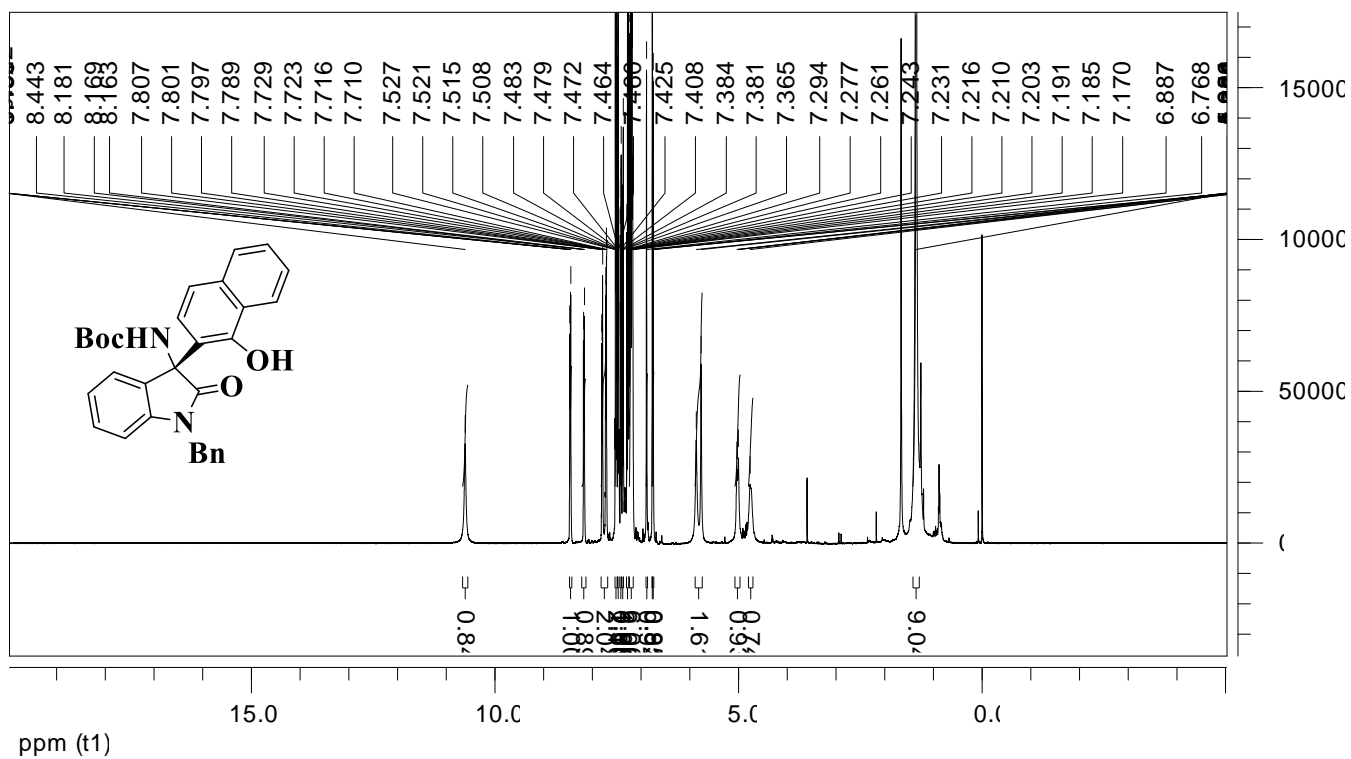
(-)-*tert*-butyl (*R*)-(1-benzyl-3-(2-hydroxynaphthalen-1-yl)-2-oxoindolin-3-yl)carbamate¹ (8n)

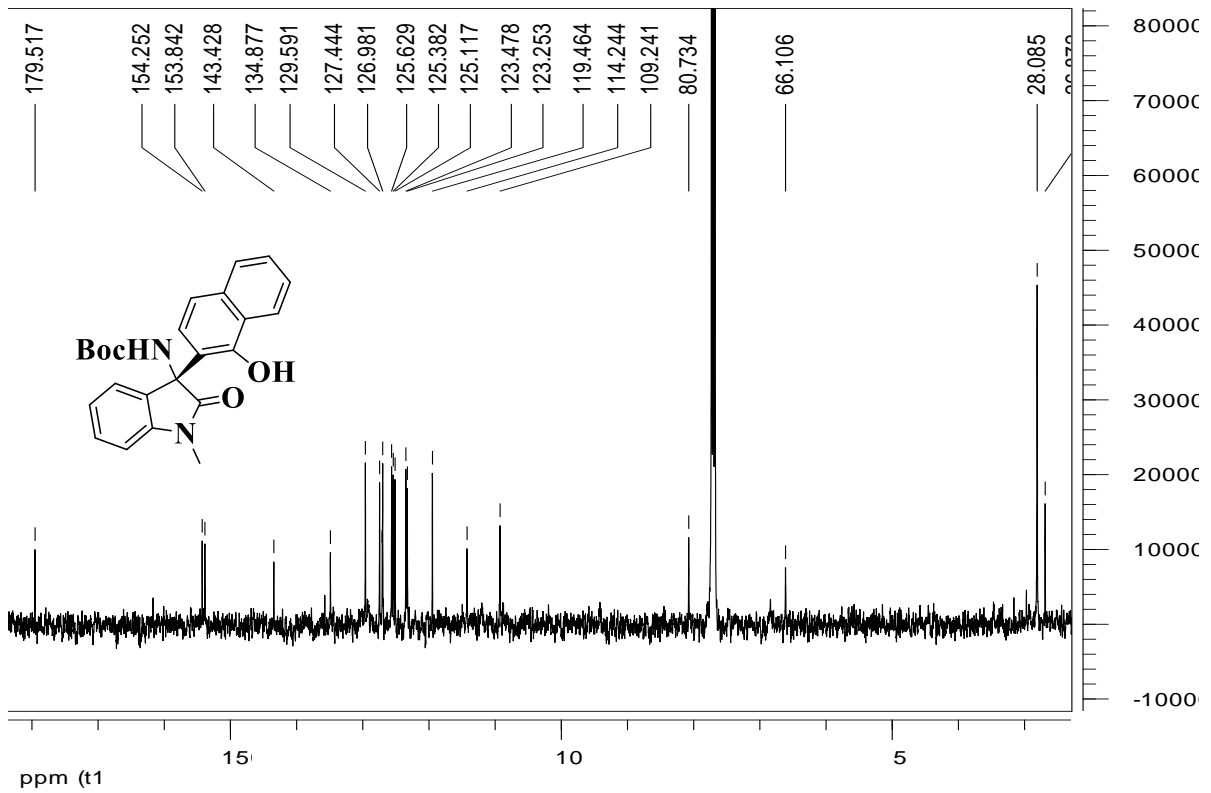
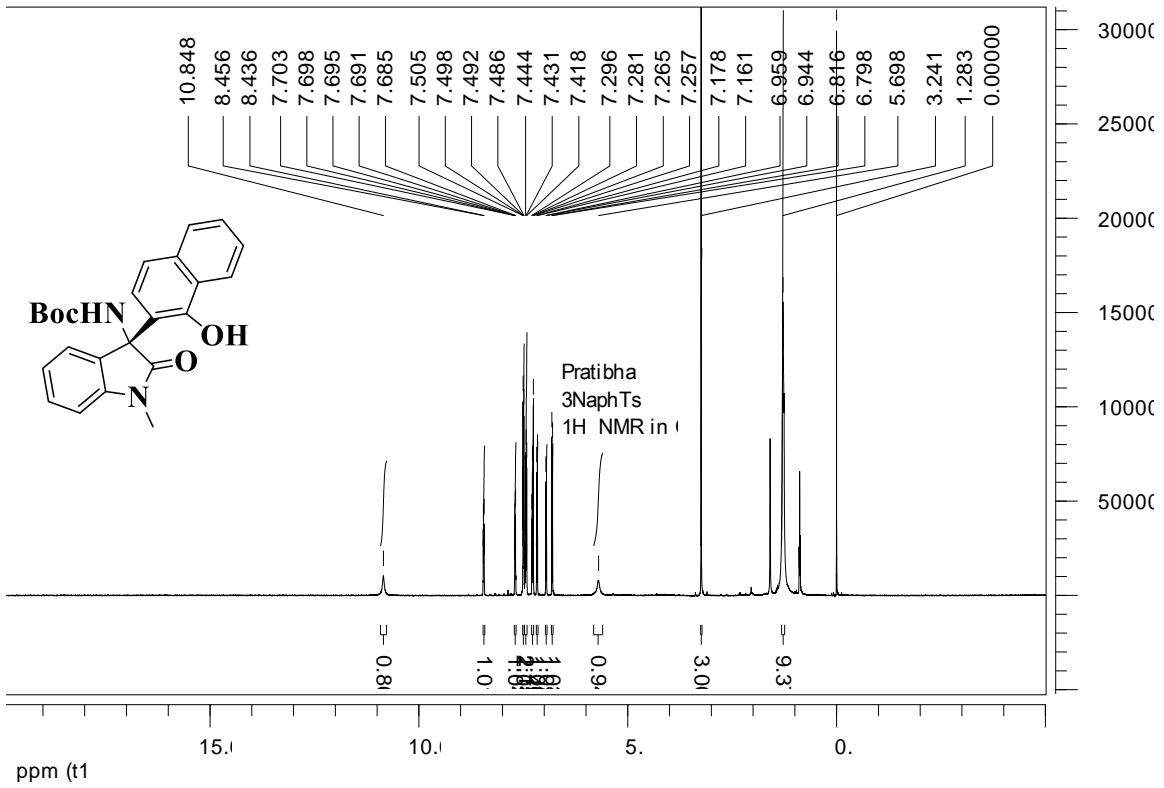


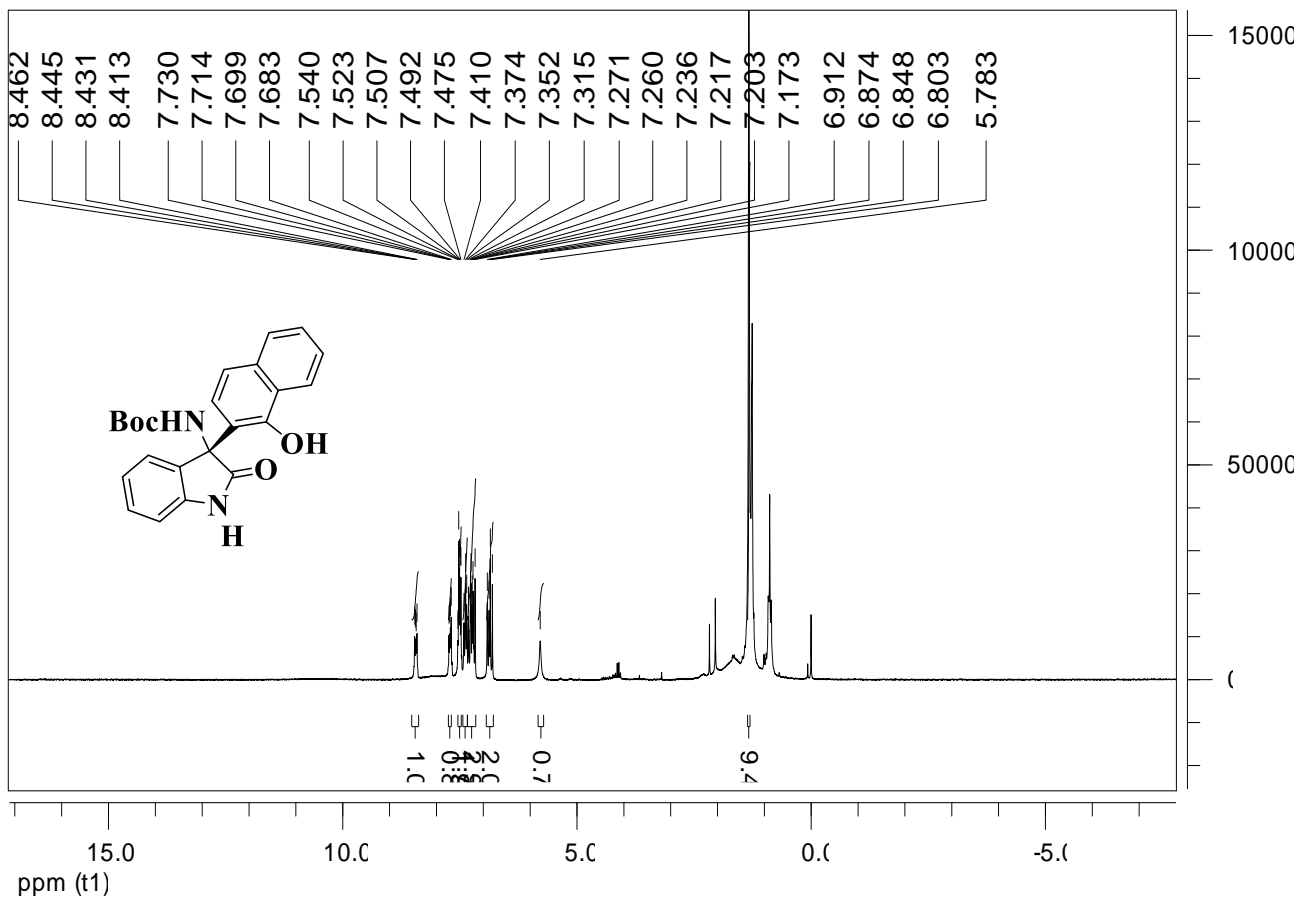
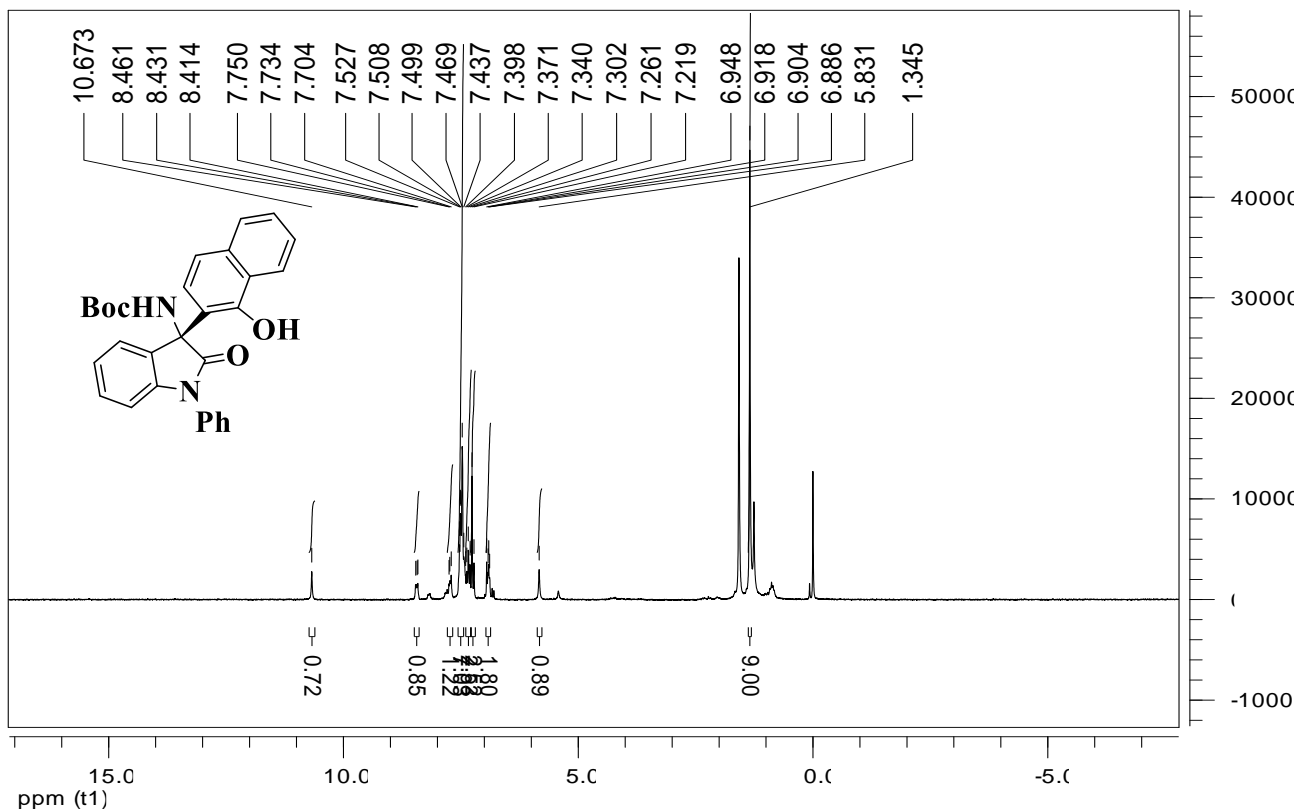
Enantiomeric excess (92%) was determined by chiral HPLC (Chiralpak IA), hexane-*i*PrOH 80:20, 1 mL/min, major enantiomer t_r = 26.062 min, minor enantiomer t_r = 16.269 min.

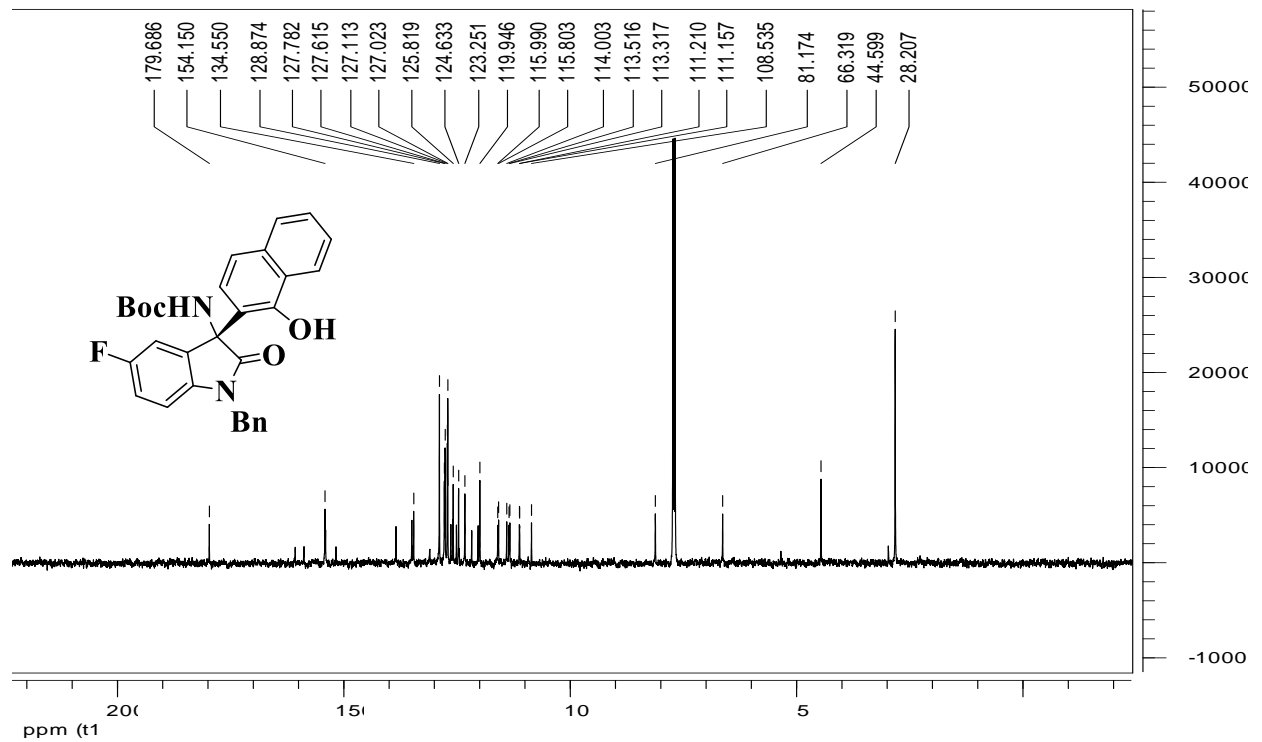
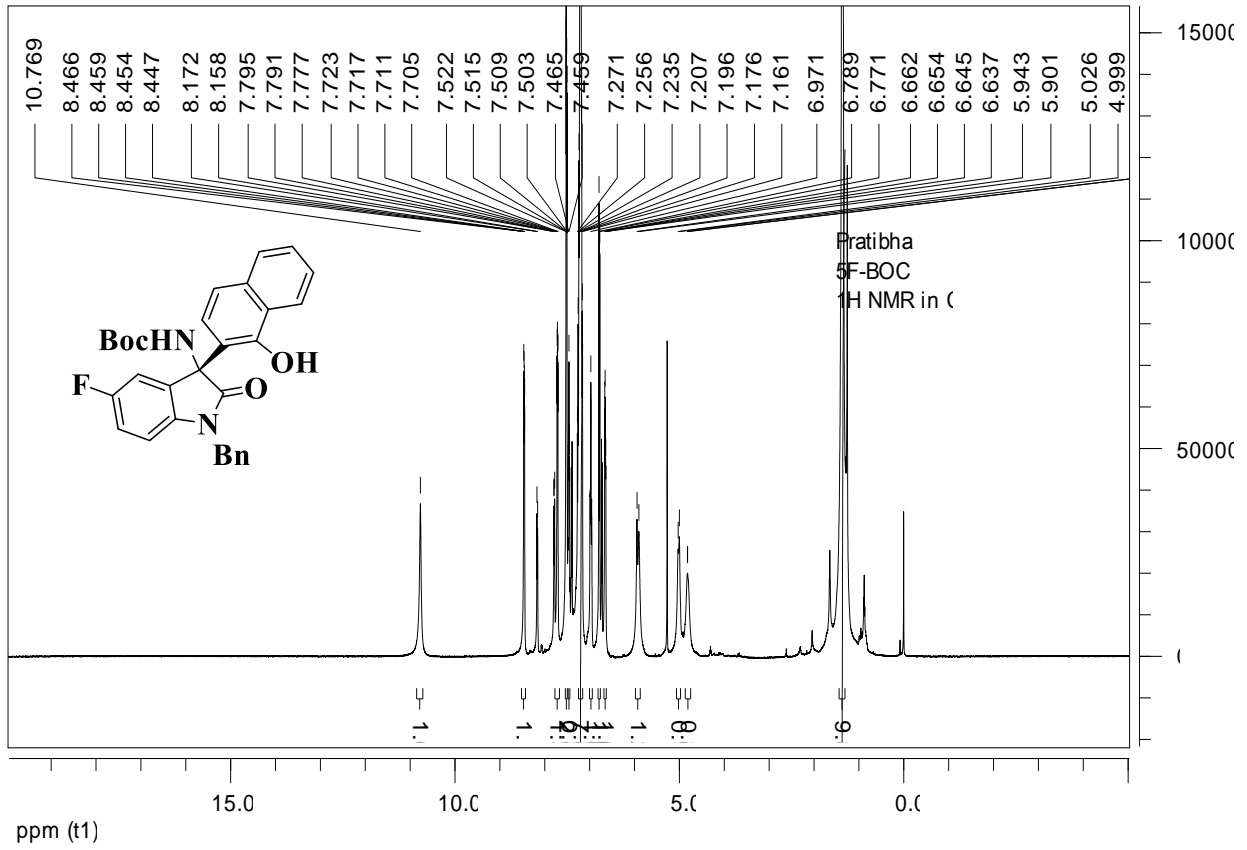
mp 140-142 °C; $[\alpha]_D^{20} -15$ (c 0.28, CHCl_3) (92% *ee*); $^1\text{H NMR}$ (500 MHz, CDCl_3) δ 9.7 (s, 1H), 7.66 (m, 1H), 7.50 (d, J = 8.5, 1H), 7.35-7.33 (m, 3H), 7.24-7.19 (m, 5H), 7.06 (d, J = 8.5, 1H), 7.00-6.97 (m, 1H), 6.75 (d, J = 7.5, 1H), 5.89 (s, 1H), 5.08 (d, J = 15, 1H), 4.88-4.84 (m, 1H), 1.30 (s, 9H).; $^{13}\text{C NMR}$ (125 MHz, CDCl_3) δ 178.6, 153.9, 152.9, 142.06, 134.2, 130.8, 129.2, 128.3, 127.9, 127.7, 126.5, 126.2, 124.6, 124.1, 123.4, 122.3, 121.3, 119.8, 113.7, 108.9, 79.6, 64.2, 43.6, 27.1.

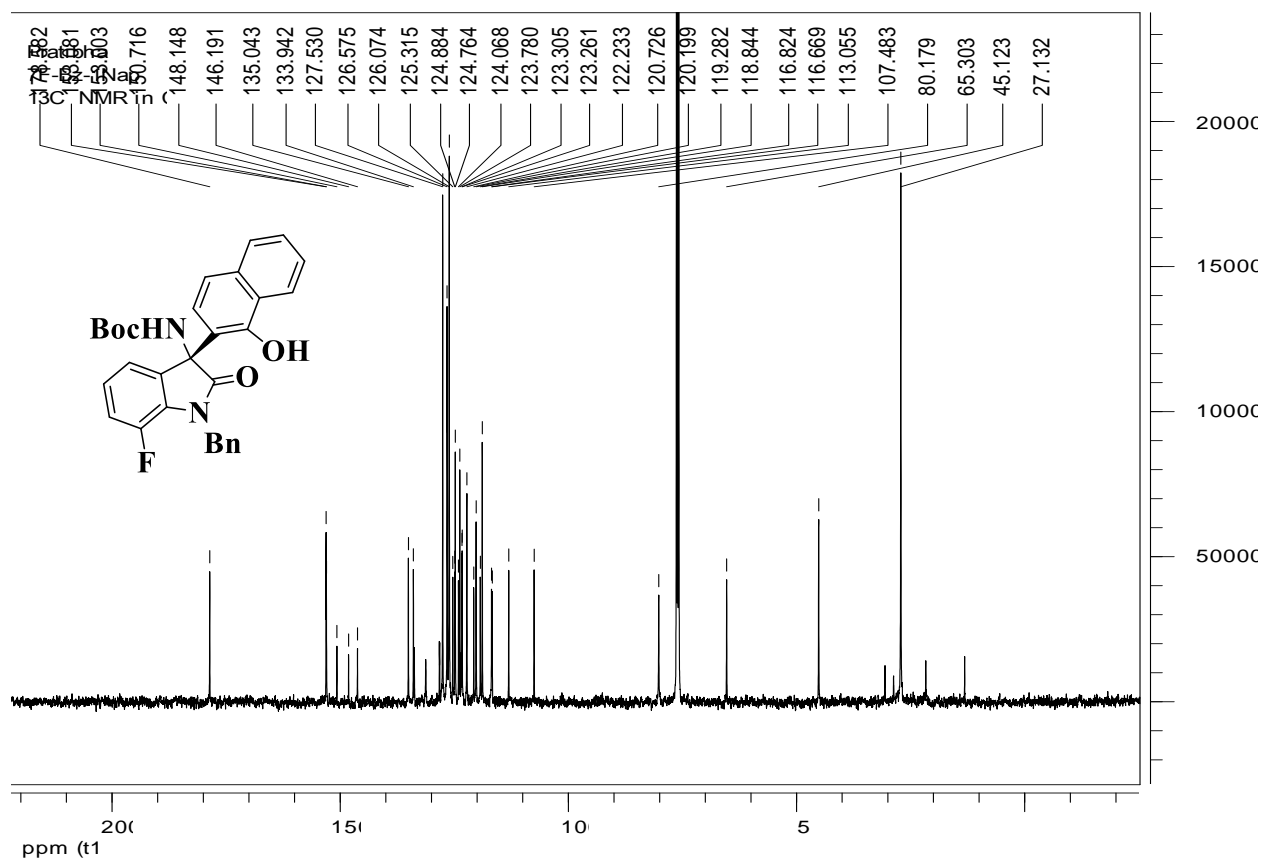
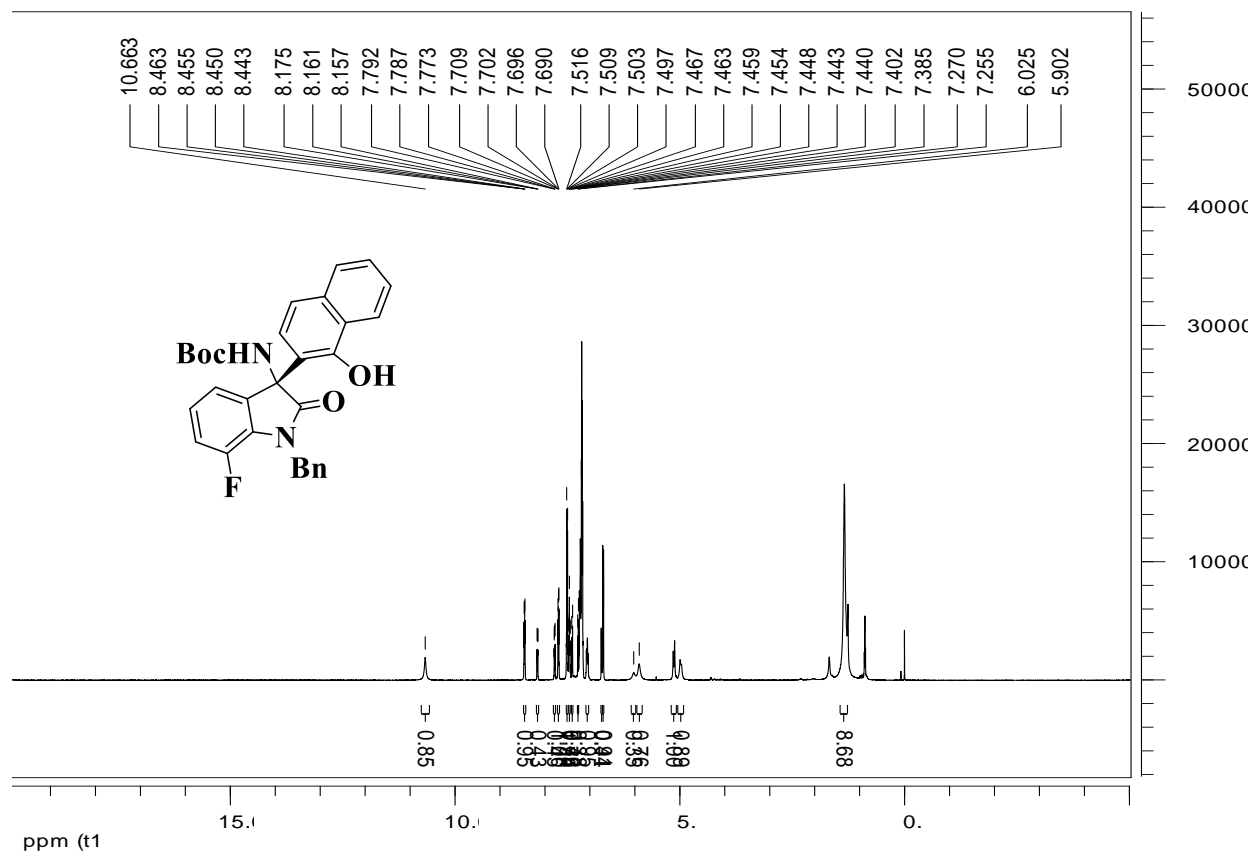
¹H NMR and ¹³C NMR spectra of products:

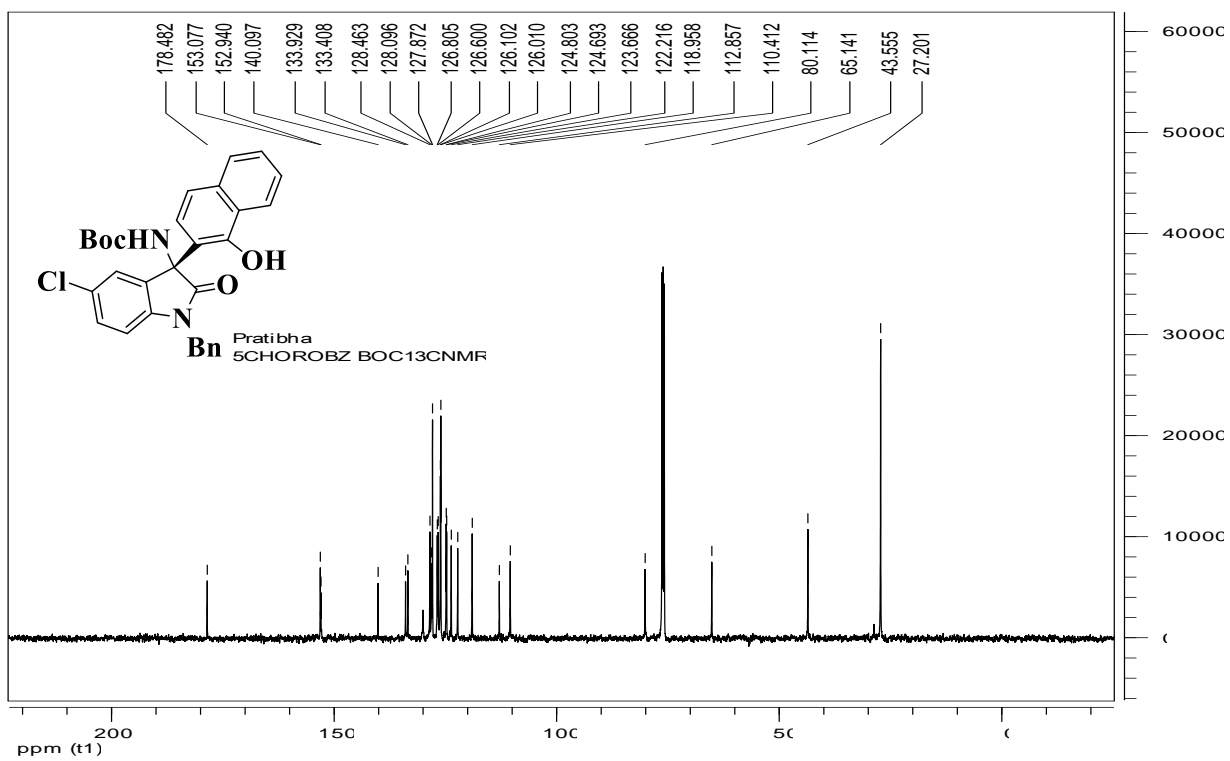
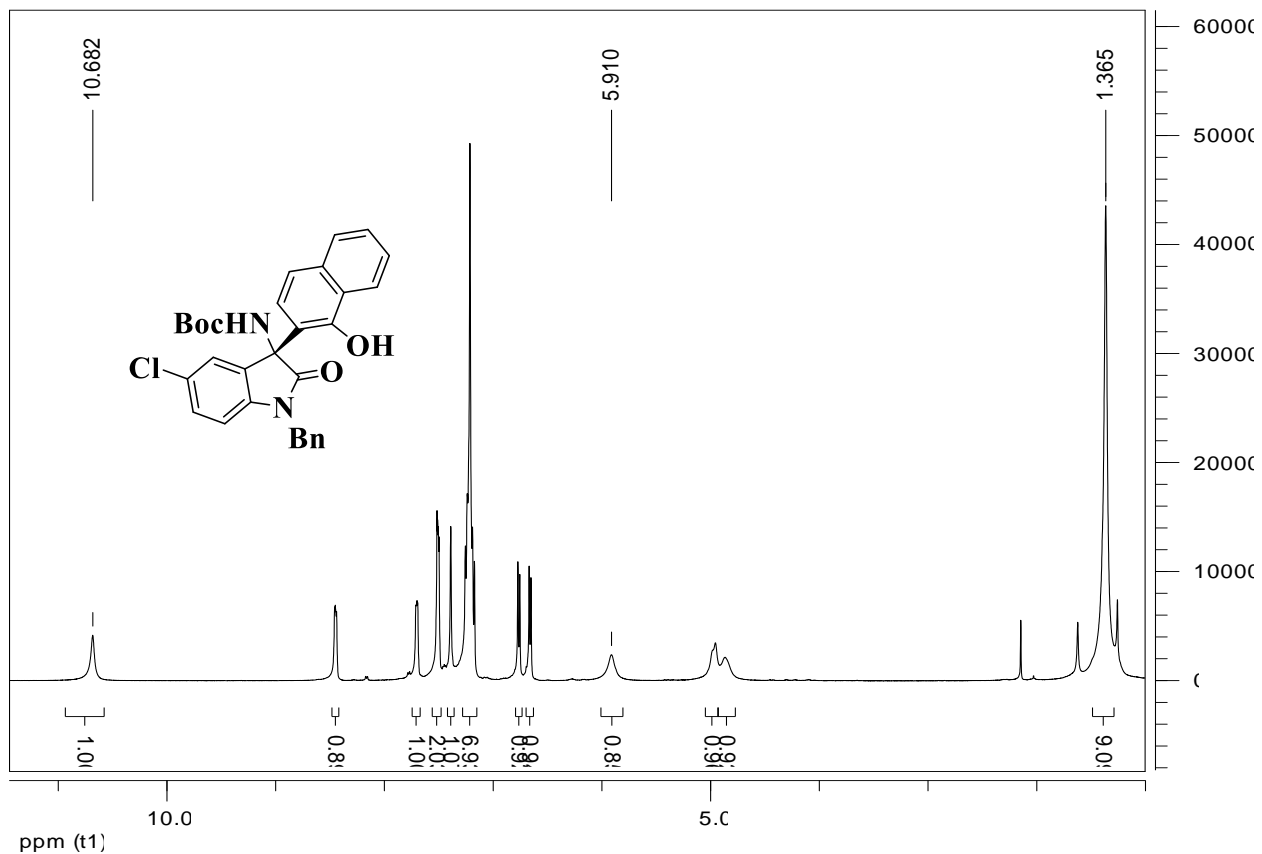


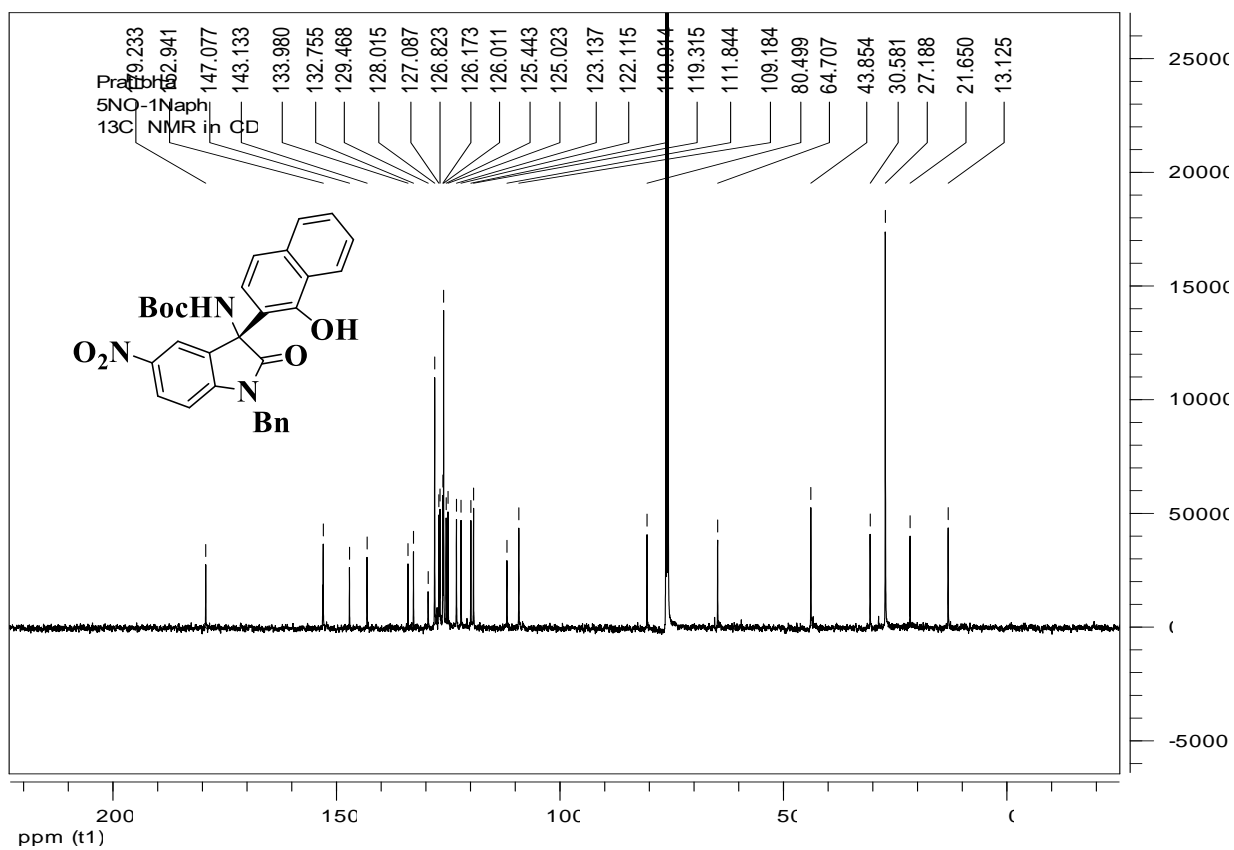
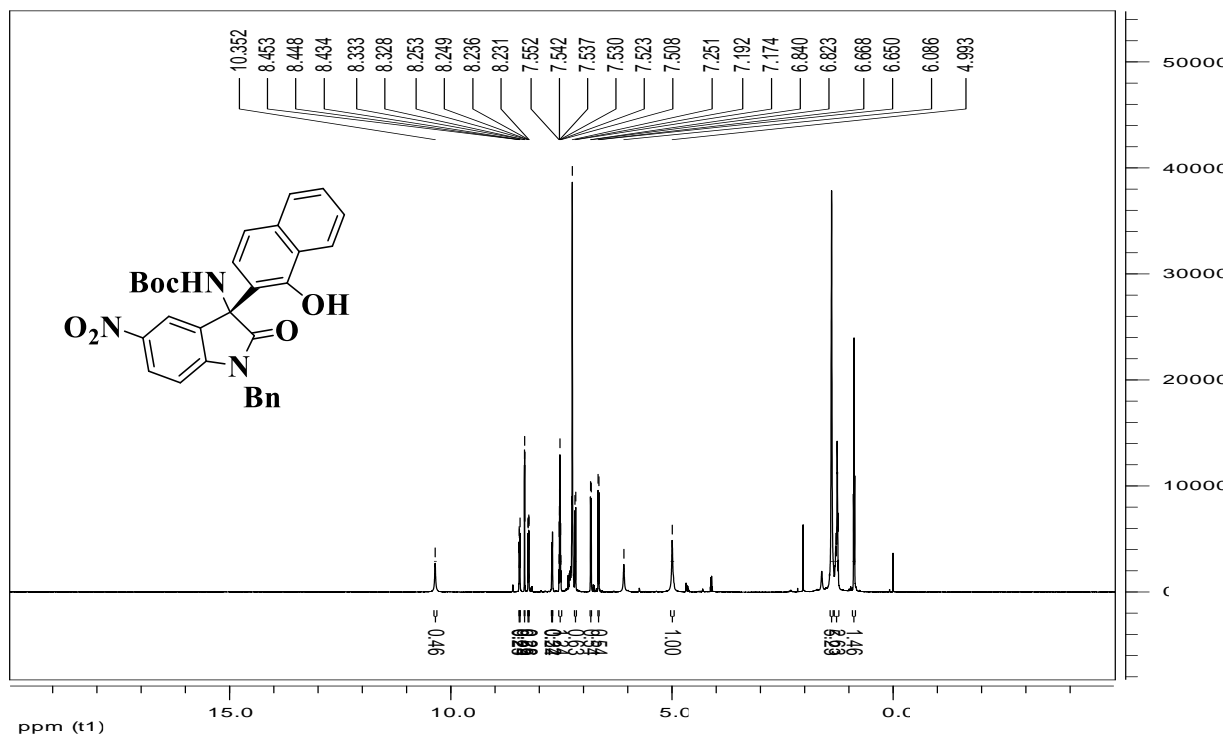


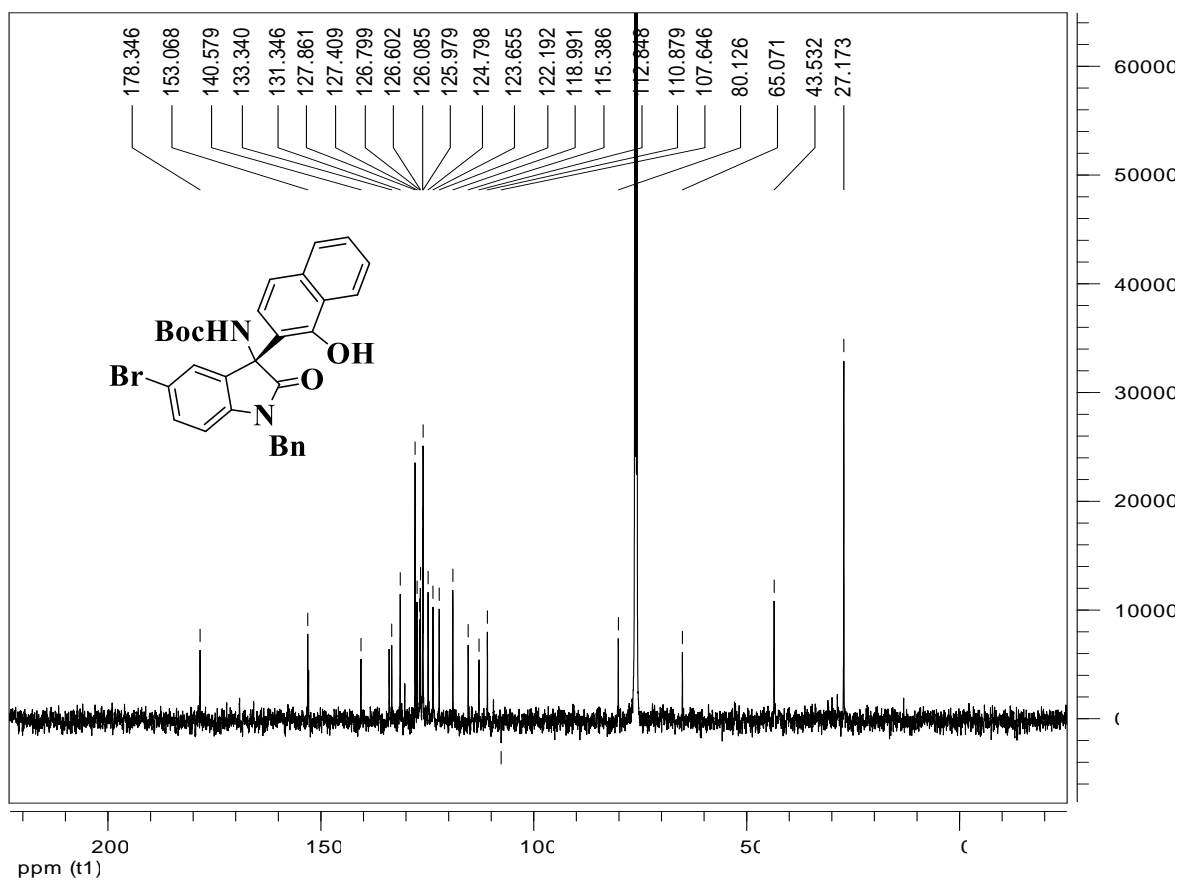
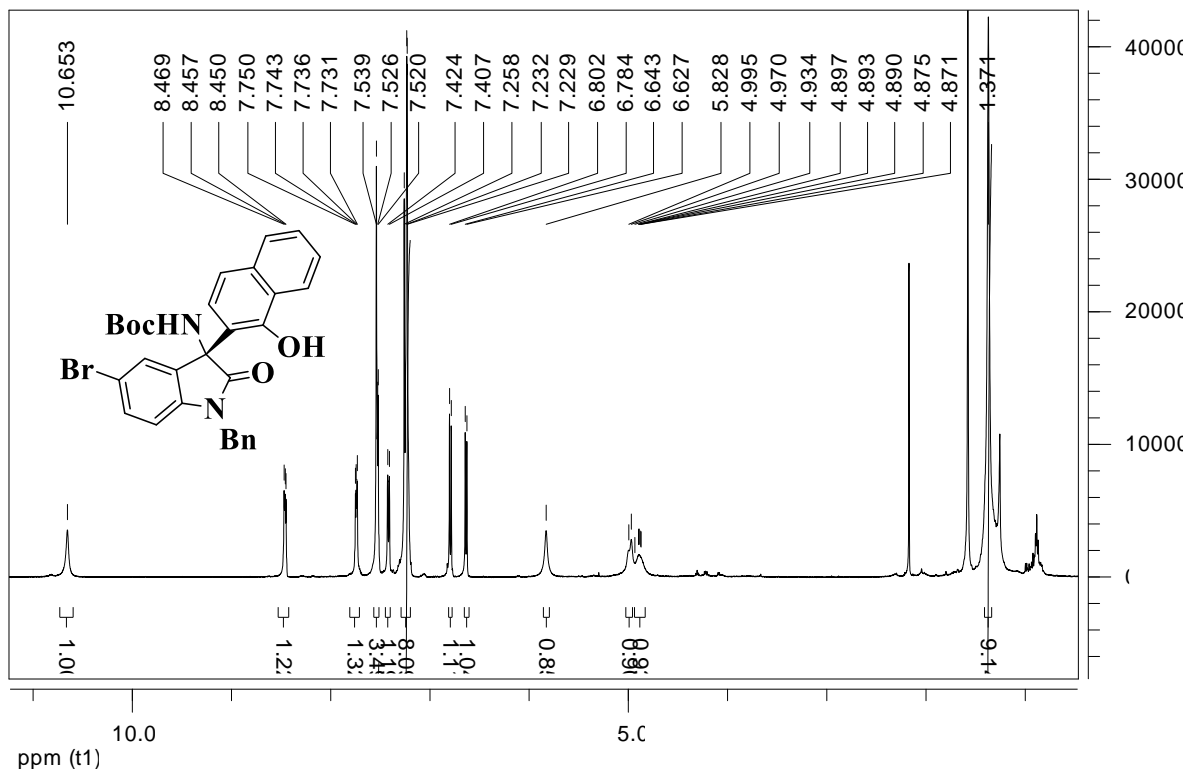


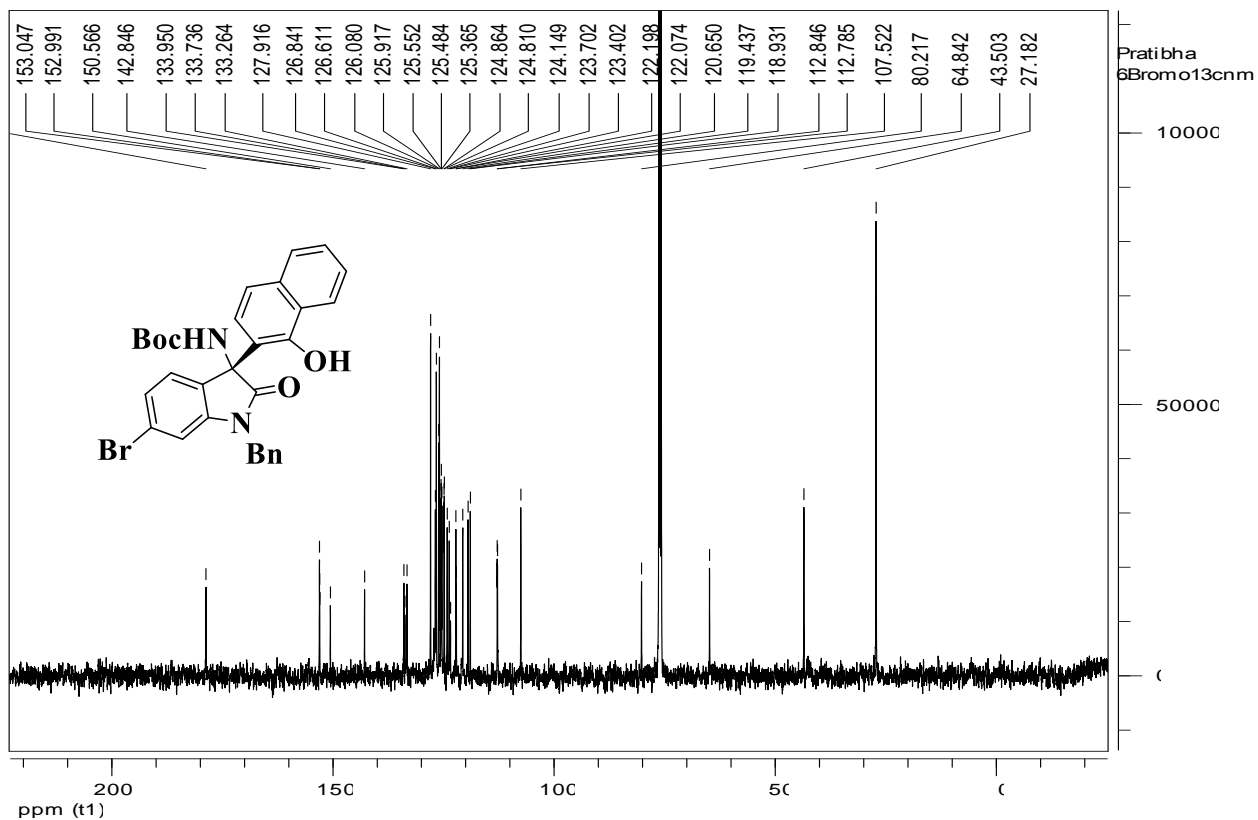
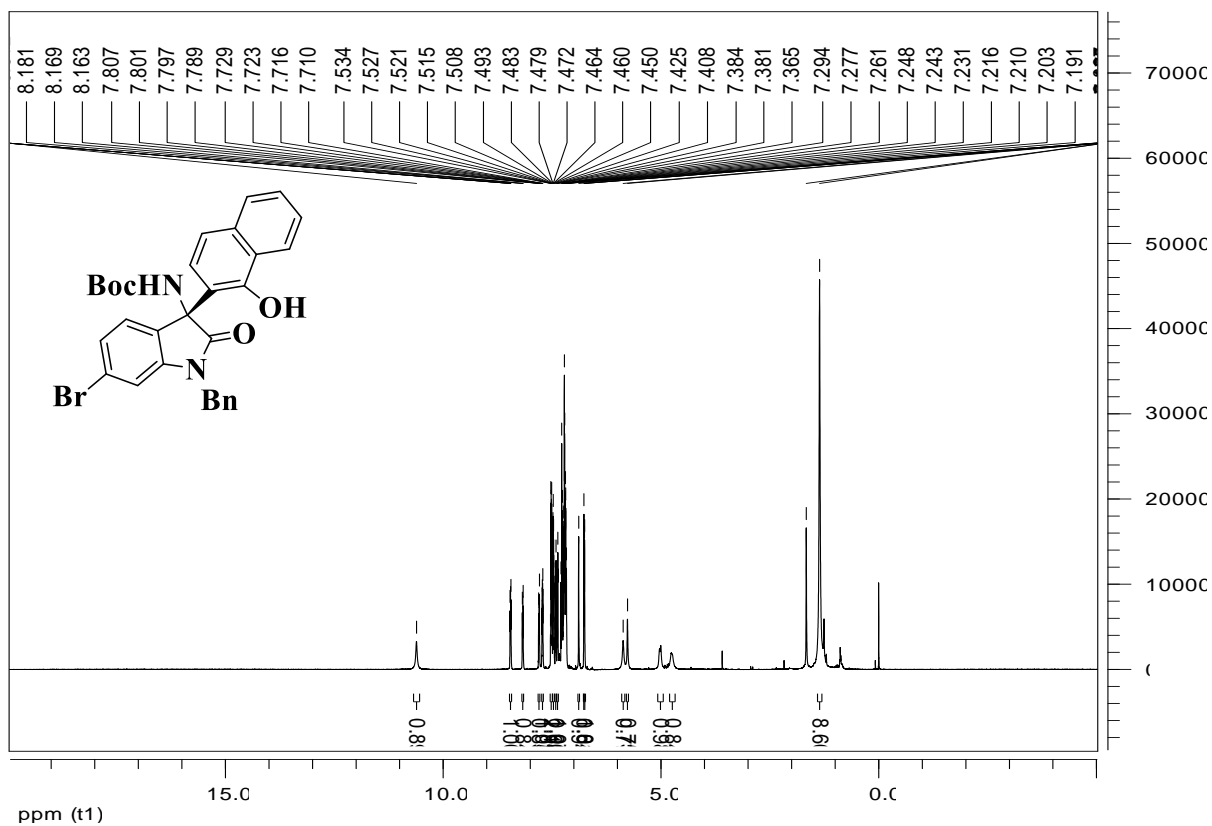


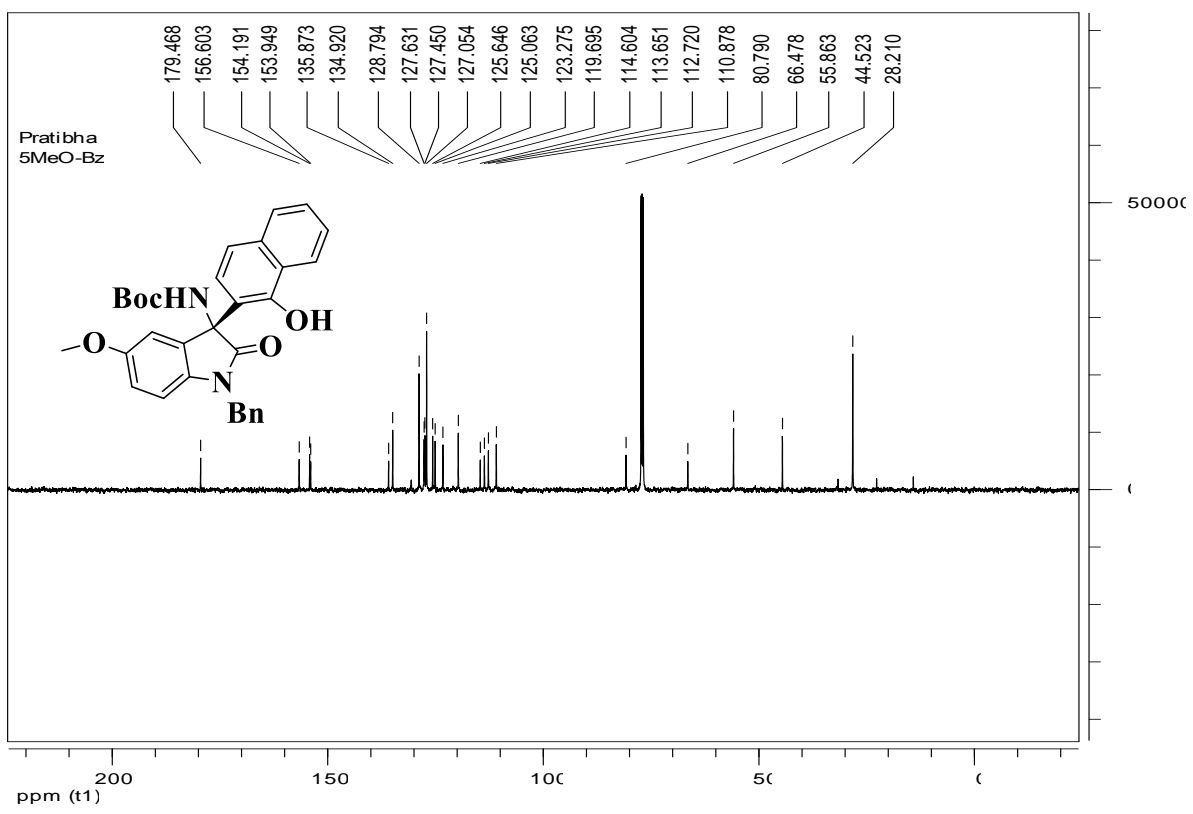
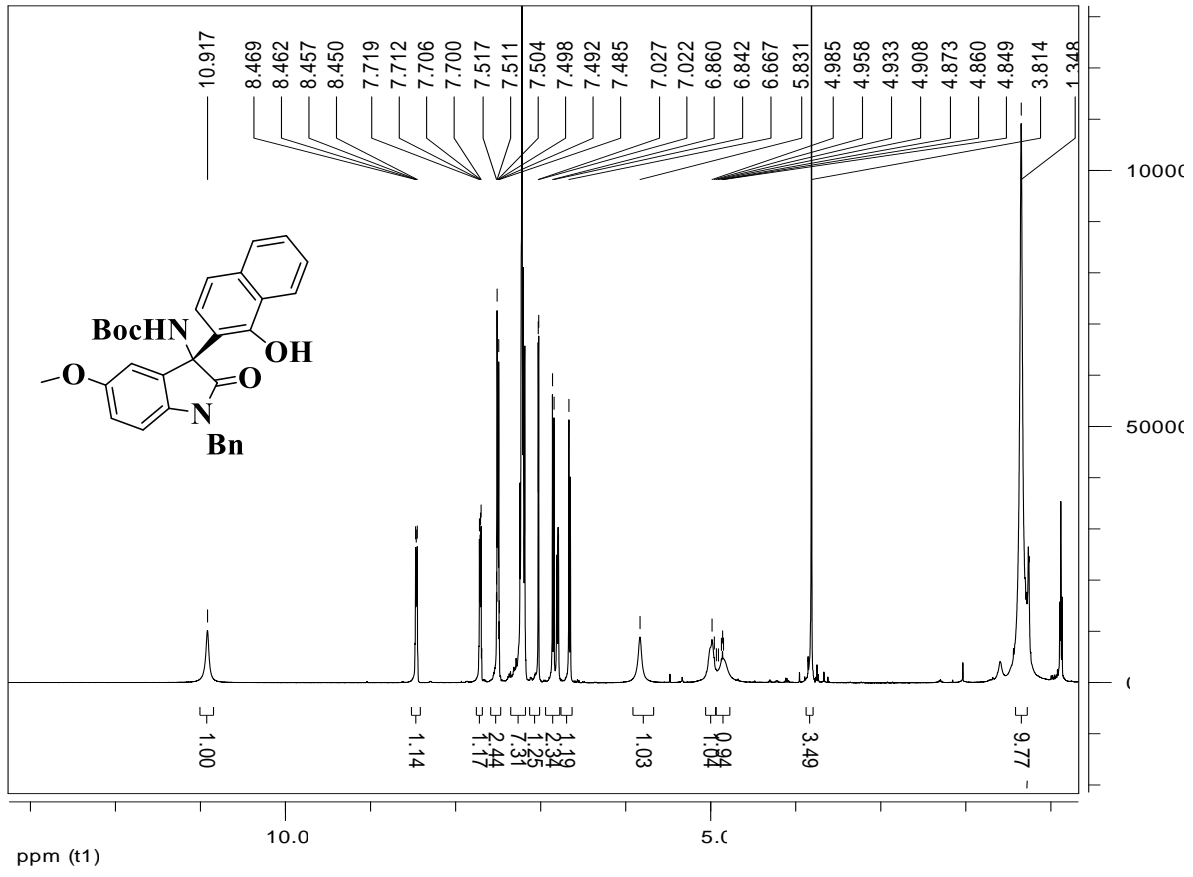


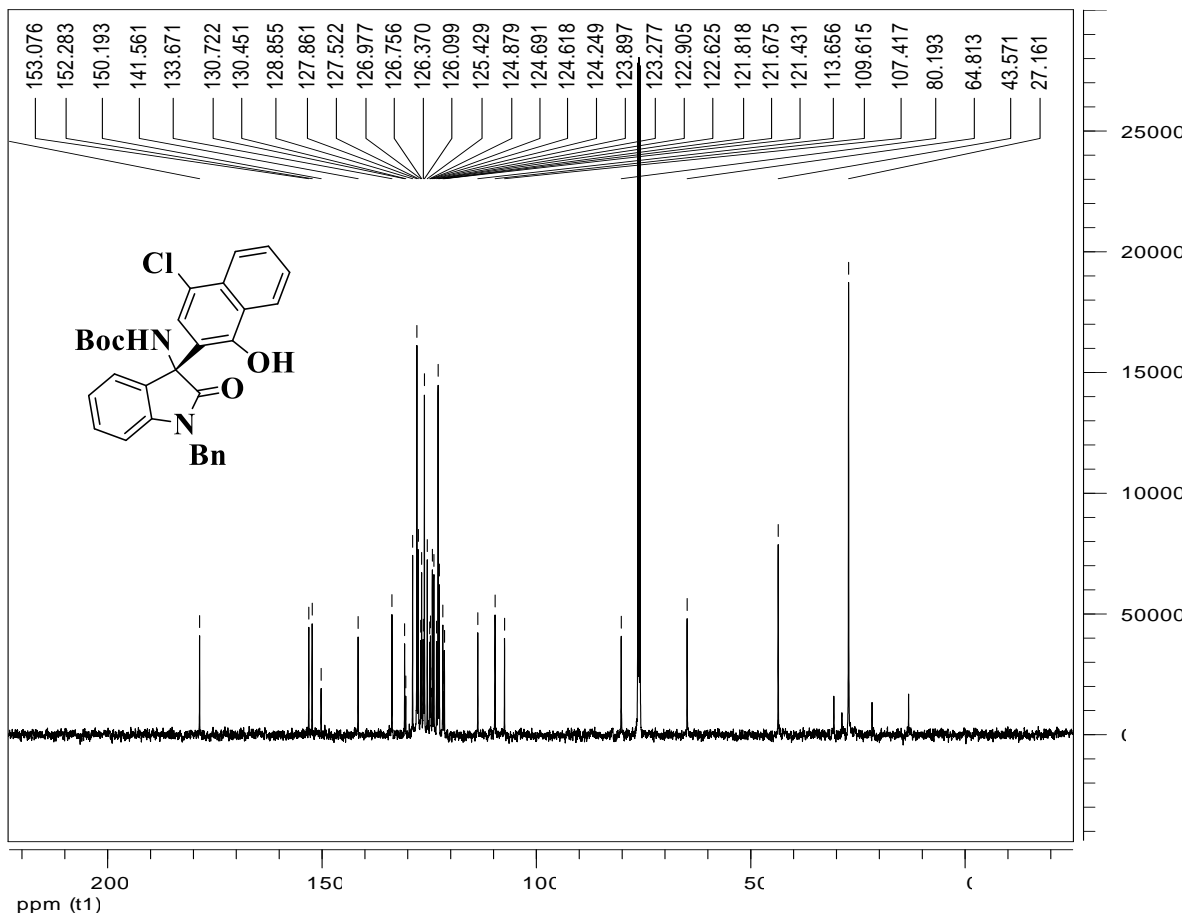
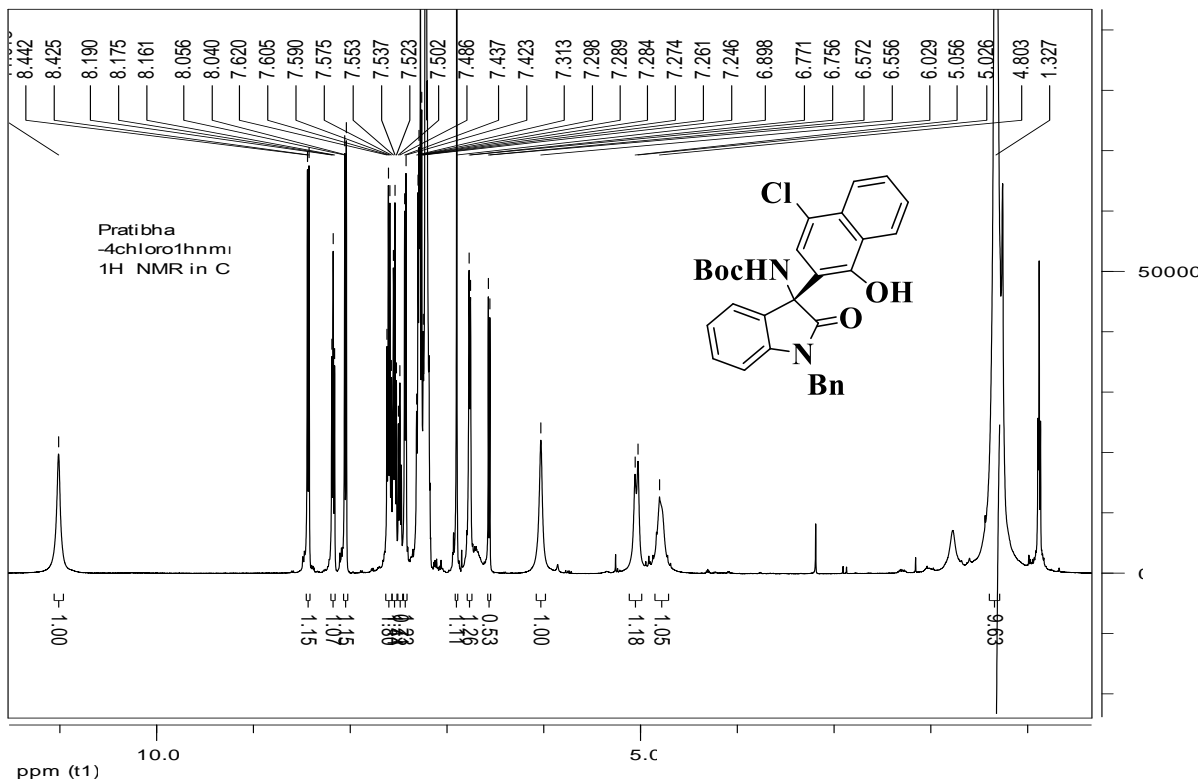


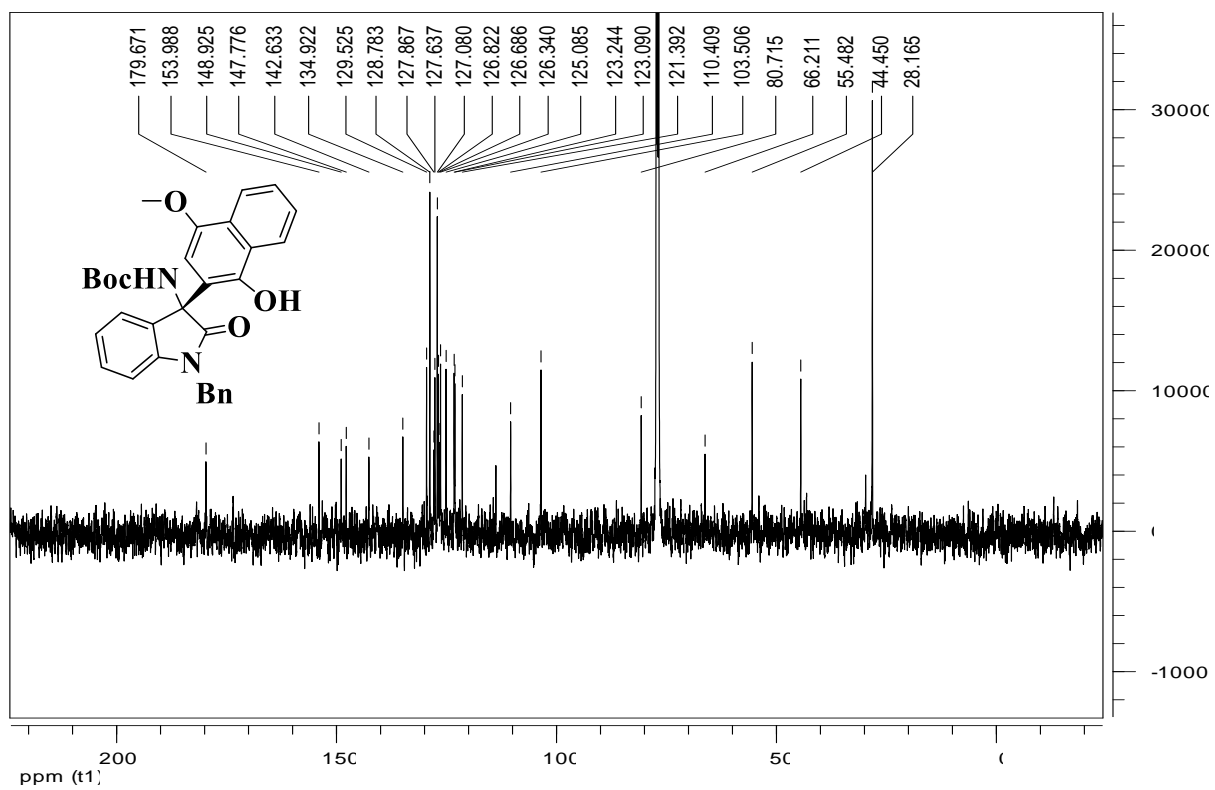
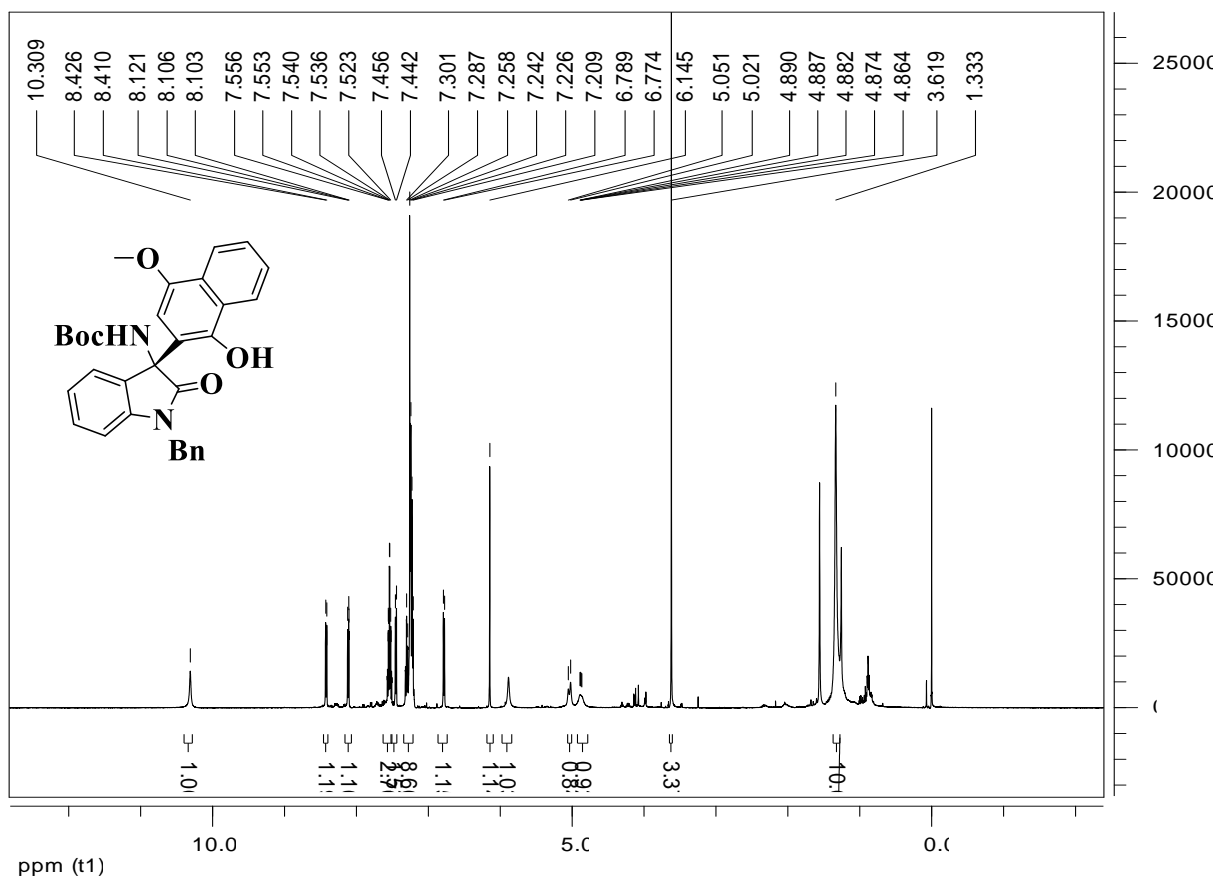


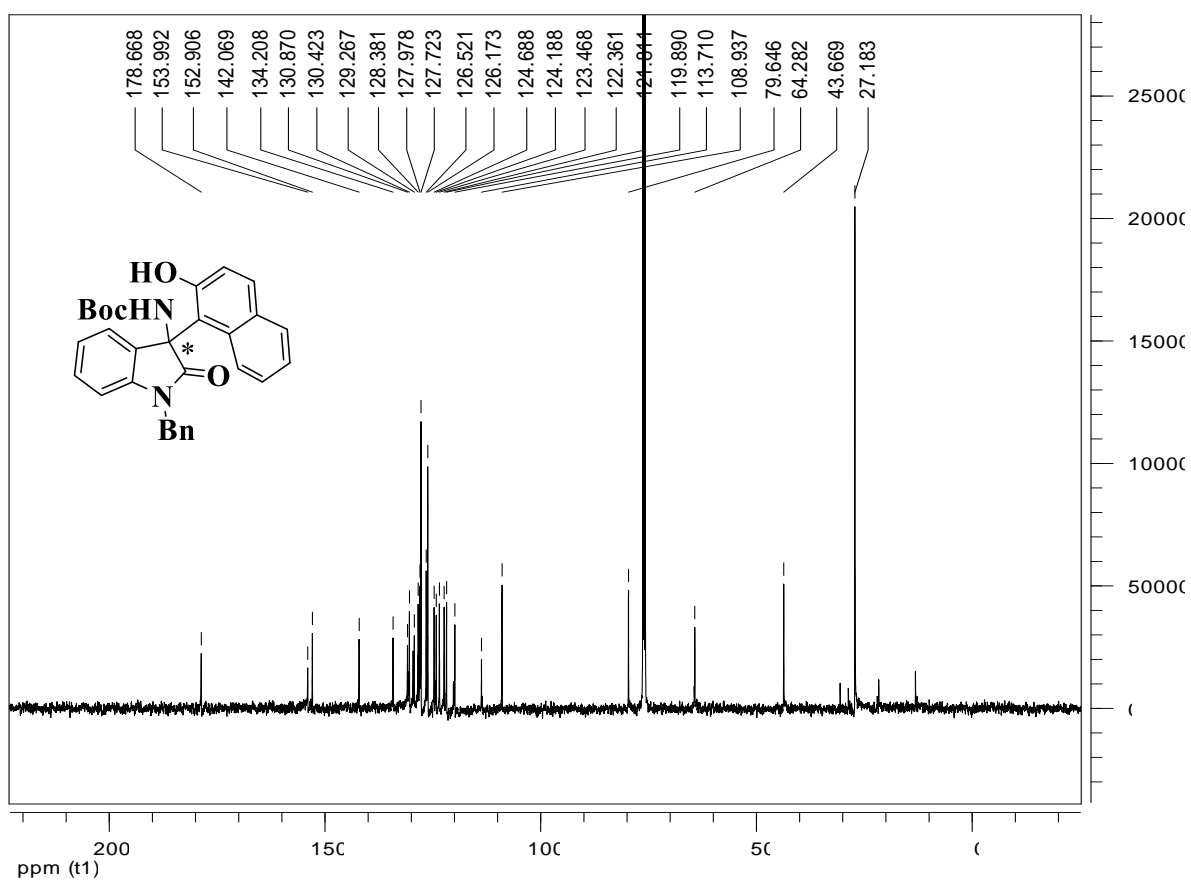
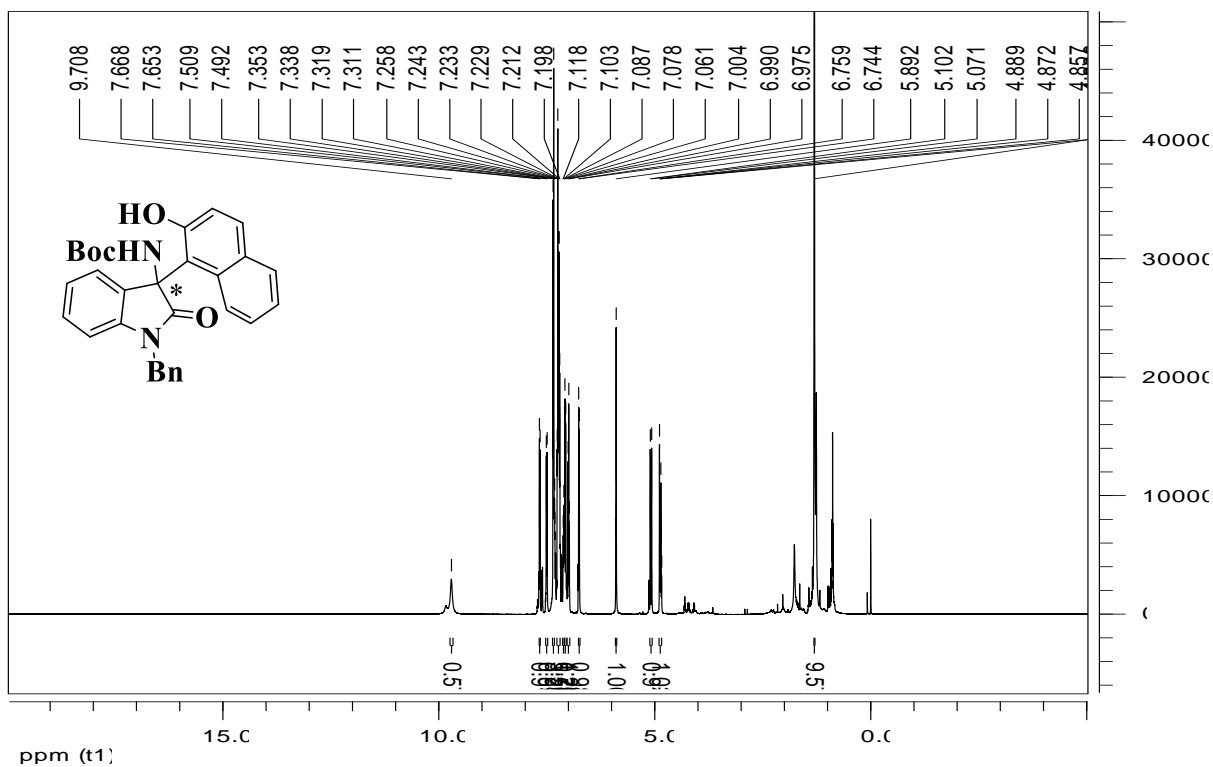




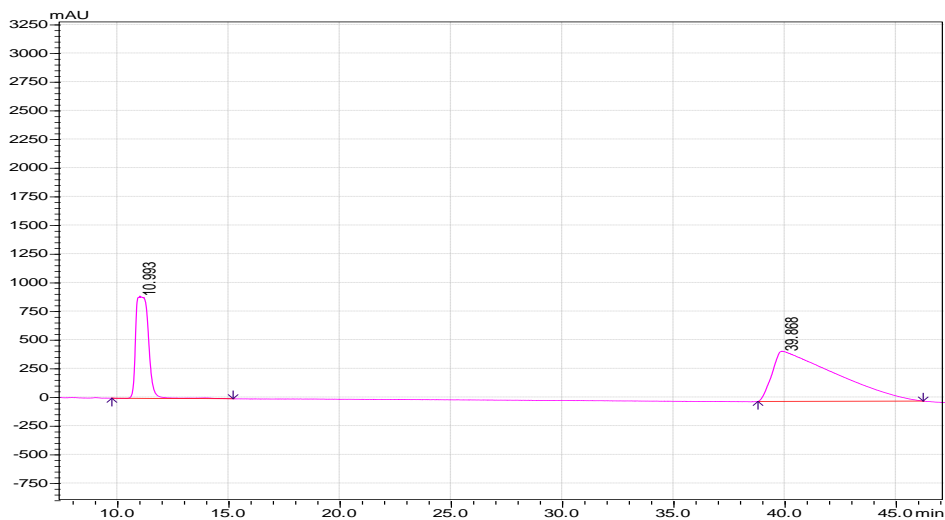
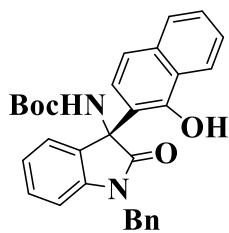




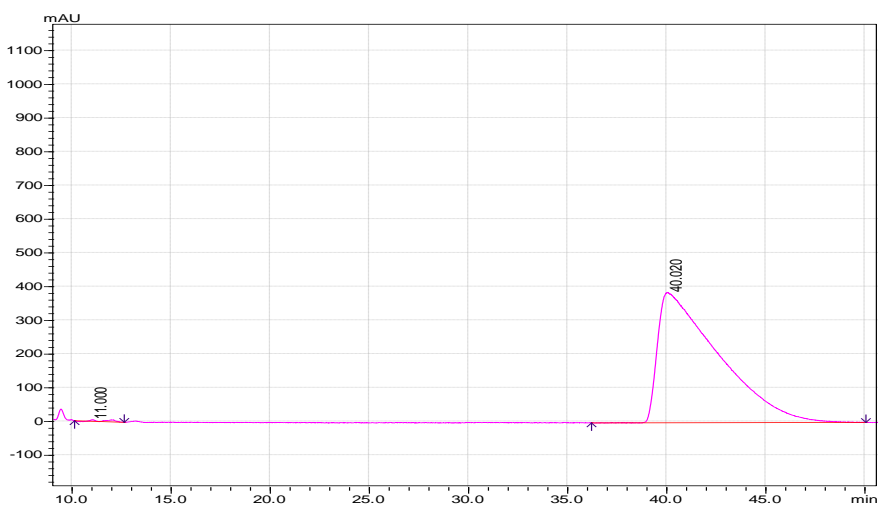




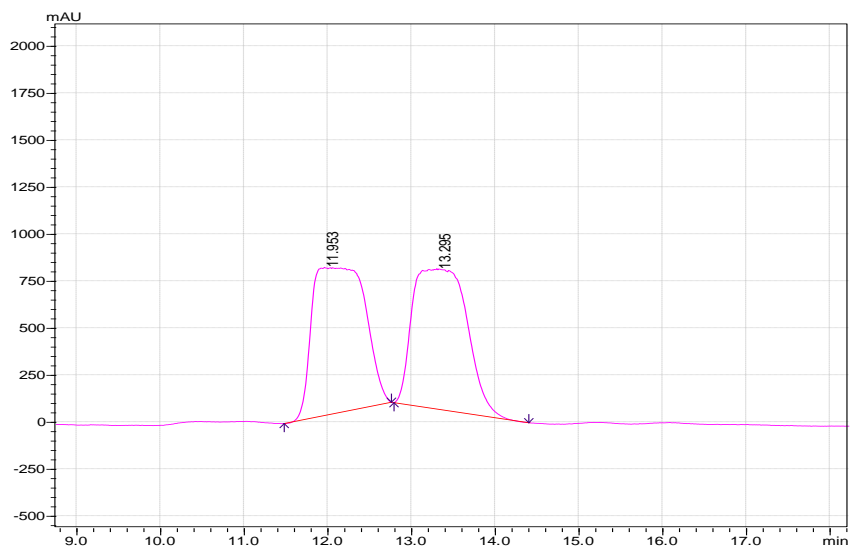
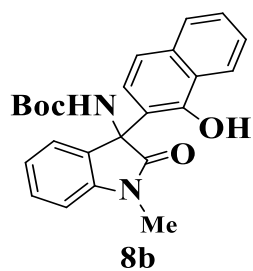
HPLC chromatogram of racemic and chiral compounds



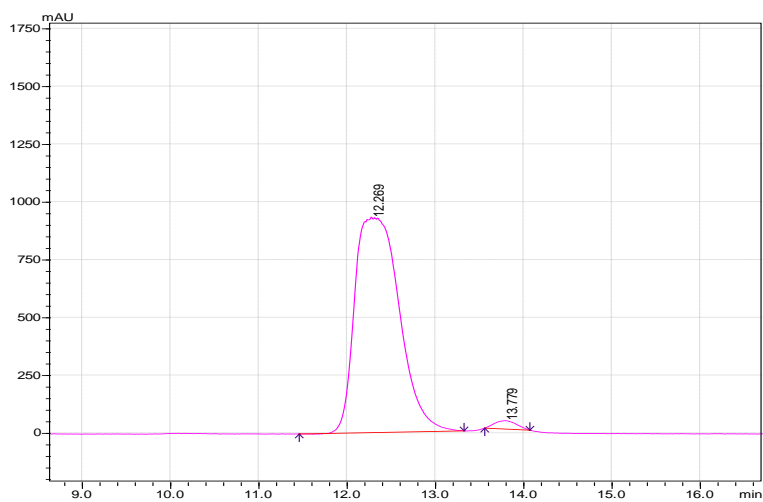
Peak#	Ret. Time	Peak Start	Peak End	Area%
1	10.993	9.739	15.189	49.8962
2	39.868	38.784	46.208	50.1038



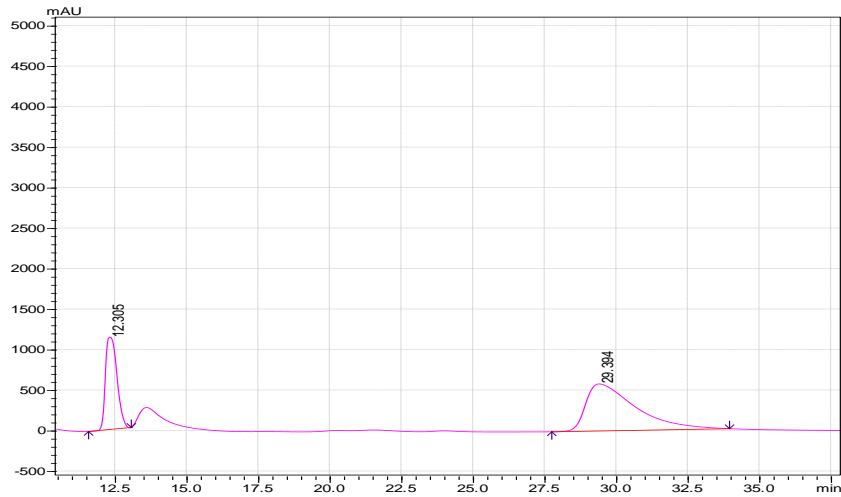
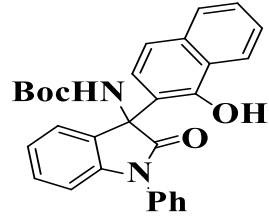
Peak#	Ret. Time	Peak Start	Peak End	Area%
1	11.000	10.123	12.629	0.2725
2	40.020	36.203	50.048	99.7275



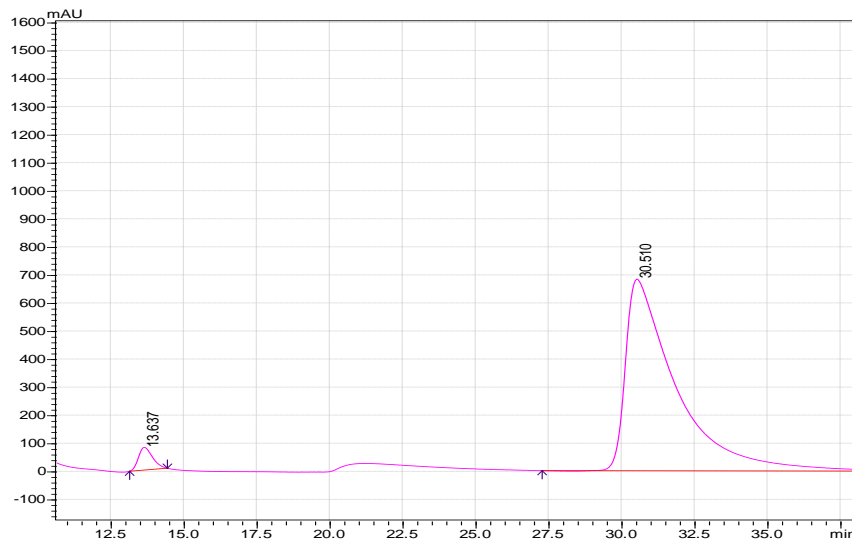
Peak#	Ret. Time	Peak Start	Peak End	Area%
1	11.953	11.521	12.655	49.8962
2	13.296	12.823	14.457	50.1038



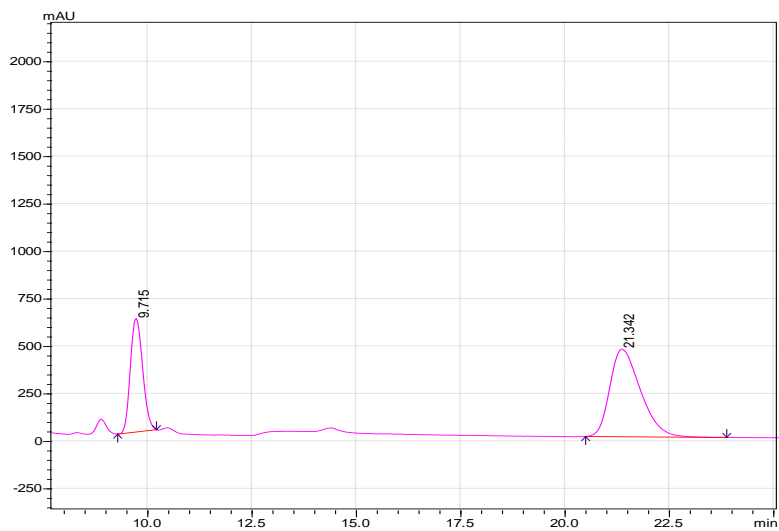
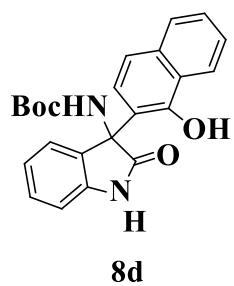
Peak#	Ret. Time	Peak Start	Peak End	Area%
1	12.269	11.521	12.655	97.2345
2	13.779	12.823	14.457	2.7655



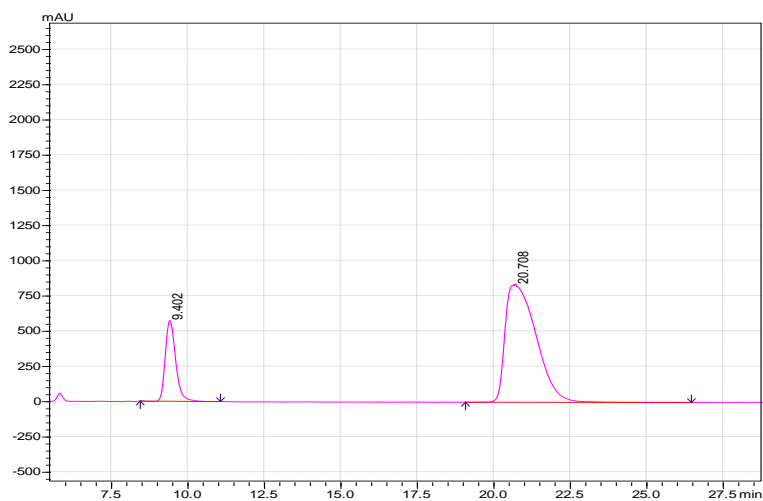
Peak#	Ret. Time	Peak Start	Peak End	Area%
1	13.662	12.821	15.669	44.2722
2	36.238	34.859	39.829	55.7278



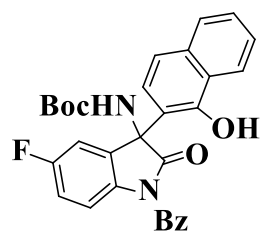
Peak#	Ret. Time	Peak Start	Peak End	Area%
1	13.637	12.821	15.669	2.5984
2	30.510	34.859	39.829	97.4016



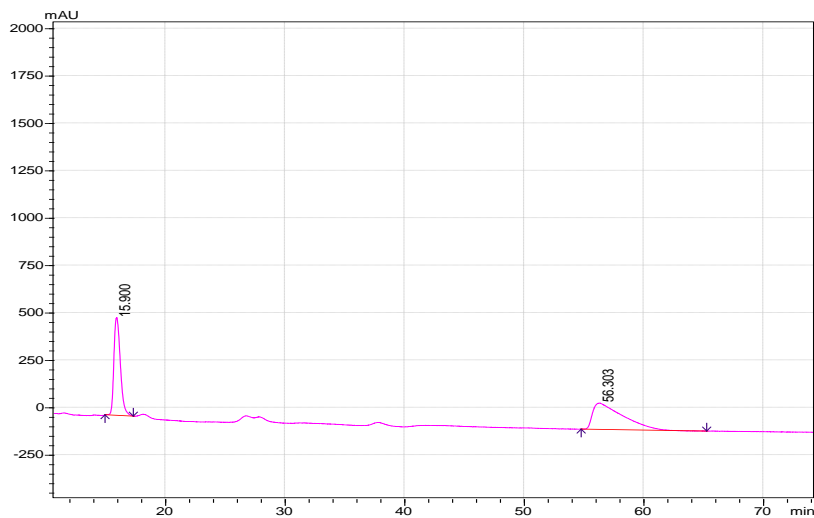
Peak#	Ret. Time	Peak Start	Peak End	Area%
1	9.715	9.280	10.208	50.330
2	21.342	20.491	23.872	49.670



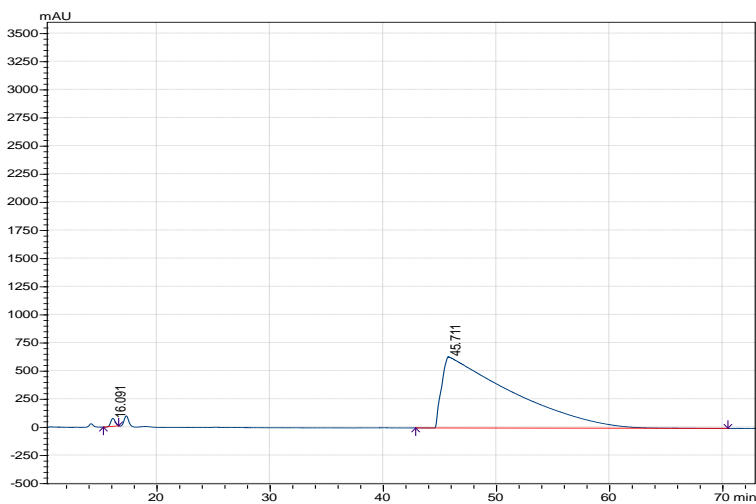
Peak#	Ret. Time	Peak Start	Peak End	Area%
1	9.402	8.437	11.061	18.5792
2	20.708	19.072	26.453	81.4208



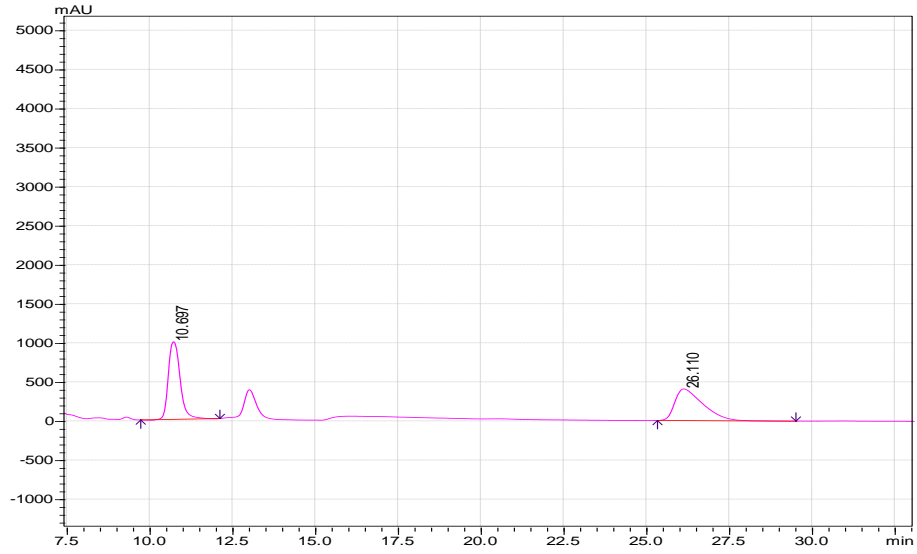
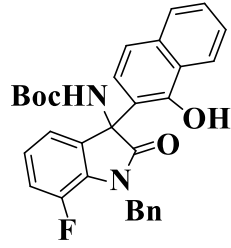
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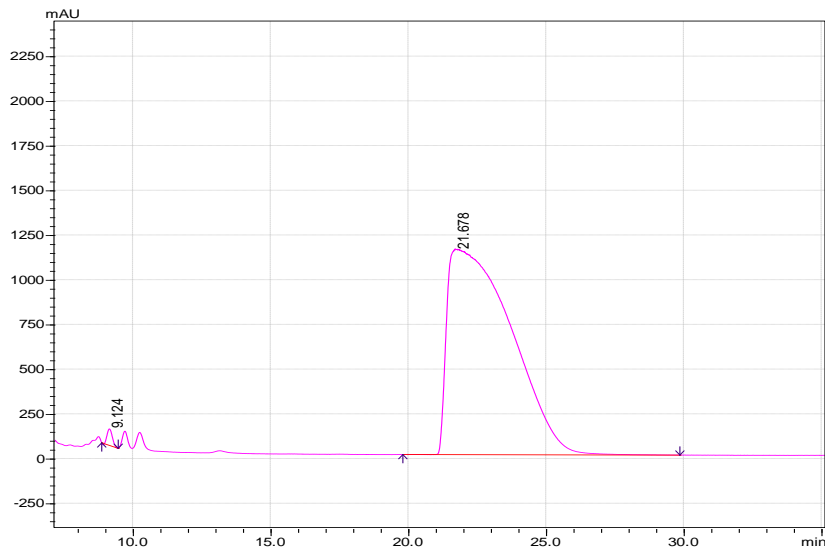
Peak#	Ret. Time	Peak Start	Peak End	Area%
1	15.900	14.933	17.301	50.0005
2	56.303	54.752	65.248	49.9995



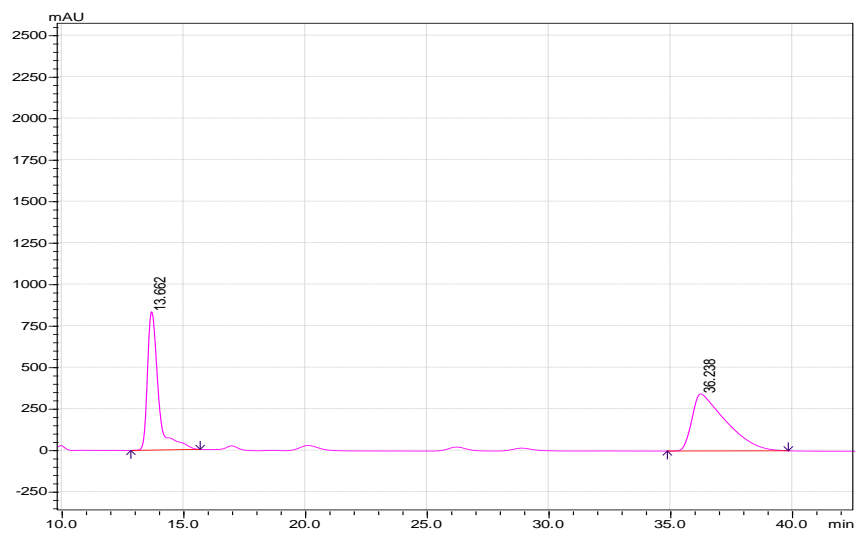
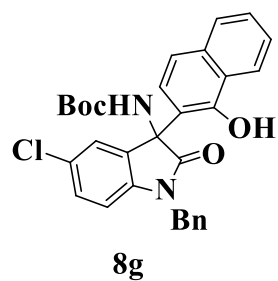
Peak#	Ret. Time	Peak Start	Peak End	Area%
1	16.091	15.264	16.608	0.6996
2	45.711	42.859	70.453	99.3004



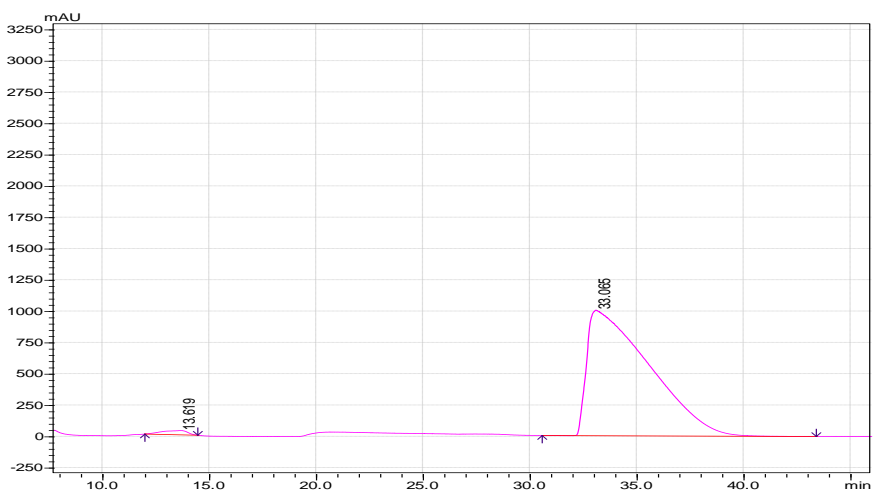
Peak#	Ret. Time	Peak Start	Peak End	Area%
1	10.687	8.853	11.451	50.0005
2	26.110	19.787	29.845	49.9995



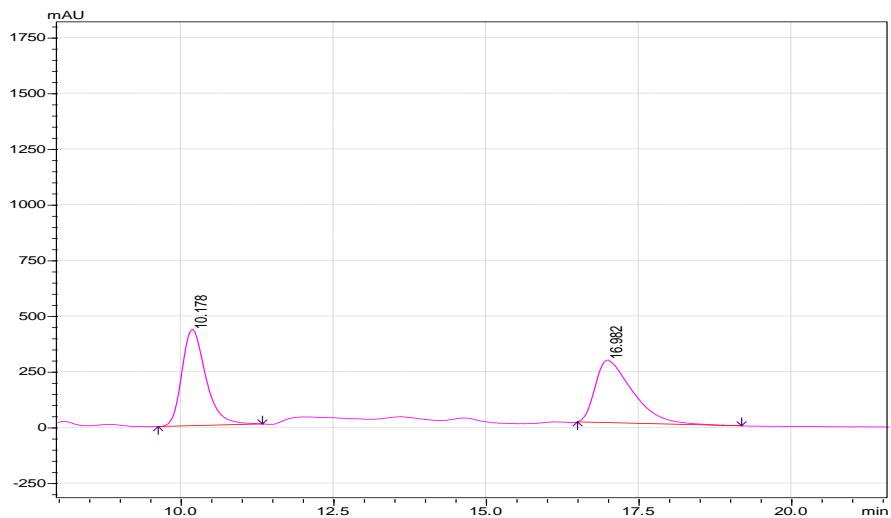
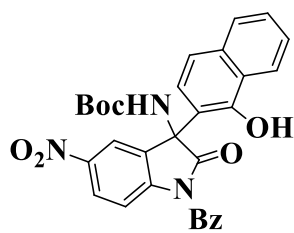
Peak#	Ret. Time	Peak Start	Peak End	Area%
1	9.124	8.853	9.451	0.6238
2	21.678	19.787	29.845	99.3762



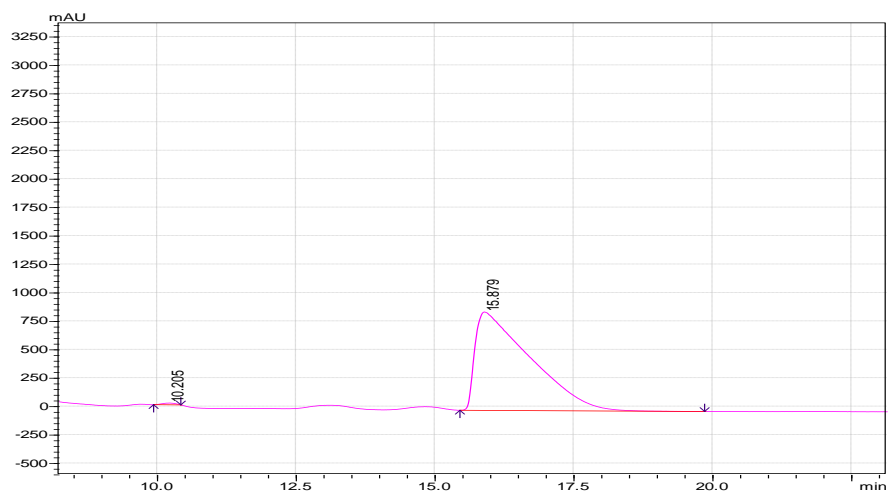
Peak#	Ret. Time	Peak Start	Peak End	Area%
1	13.662	12.821	15.669	44.2722
2	36.238	34.859	39.829	55.7278



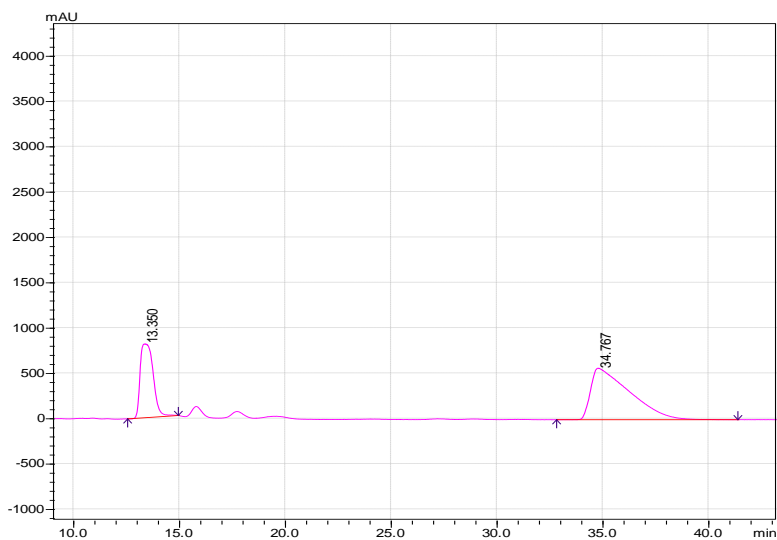
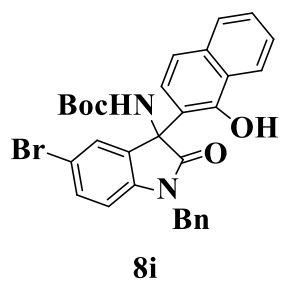
Peak#	Ret. Time	Peak Start	Peak End	Area%
1	13.619	11.968	14.443	1.3680
2	33.065	30.560	43.381	98.6320



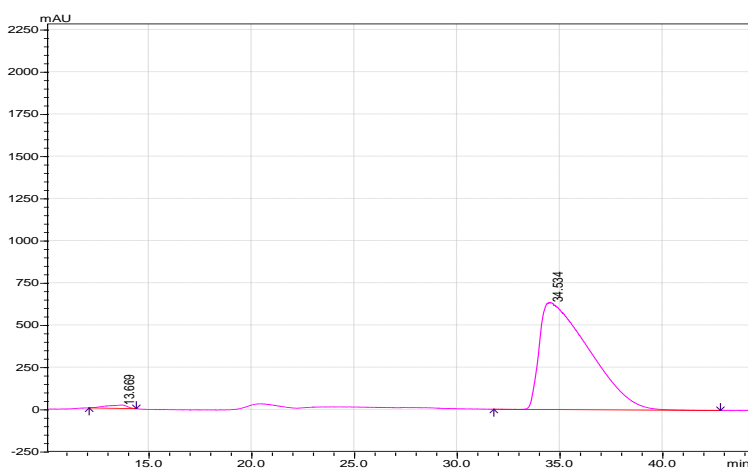
Peak#	Ret. Time	Peak Start	Peak End	Area%
1	10.178	9.621	11.328	49.7249
2	16.982	16.491	19.179	50.2751



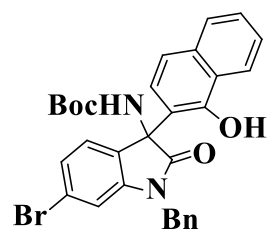
Peak#	Ret. Time	Peak Start	Peak End	Area%
1	10.205	9.931	10.421	0.4318
2	15.879	15.445	19.851	99.5682



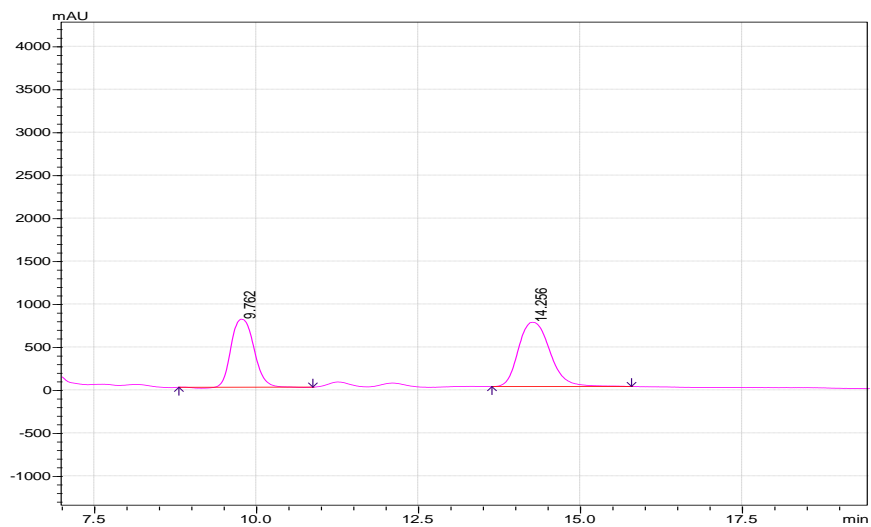
Peak#	Ret. Time	Peak Start	Peak End	Area%
1	13.350	12.544	14.944	32.4339
2	34.767	32.811	41.376	67.5661



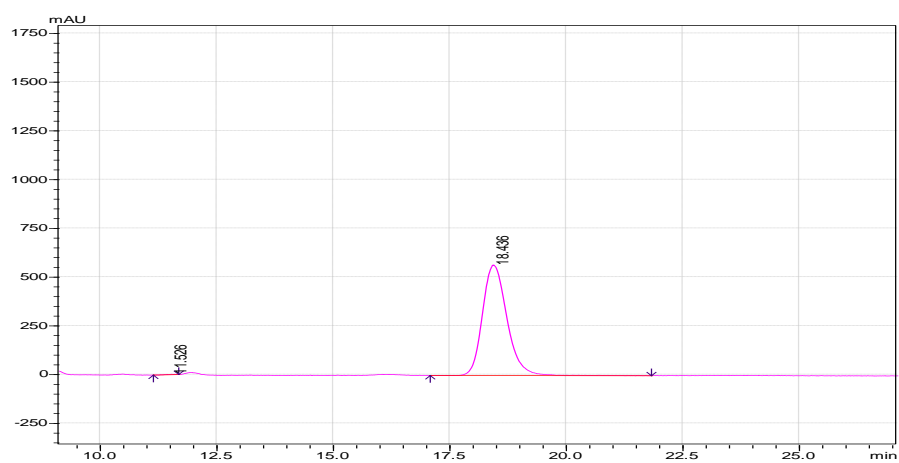
Peak#	Ret. Time	Peak Start	Peak End	Area%
1	13.669	12.085	14.379	1.2917
2	34.534	31.776	42.805	98.7083



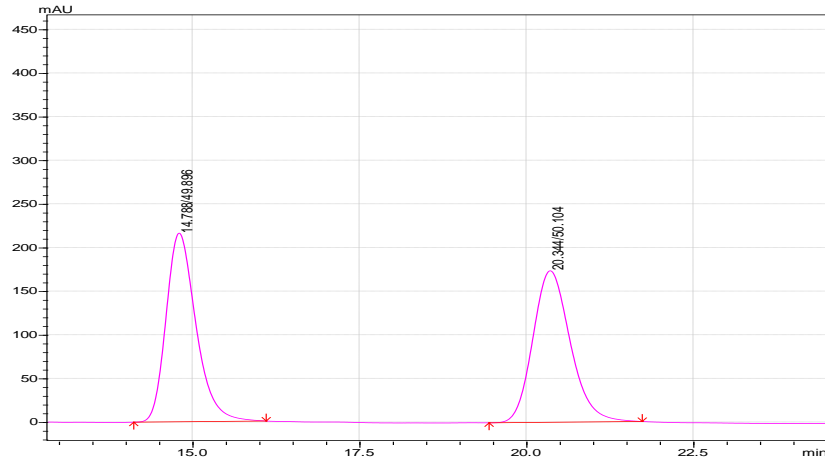
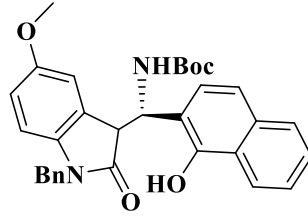
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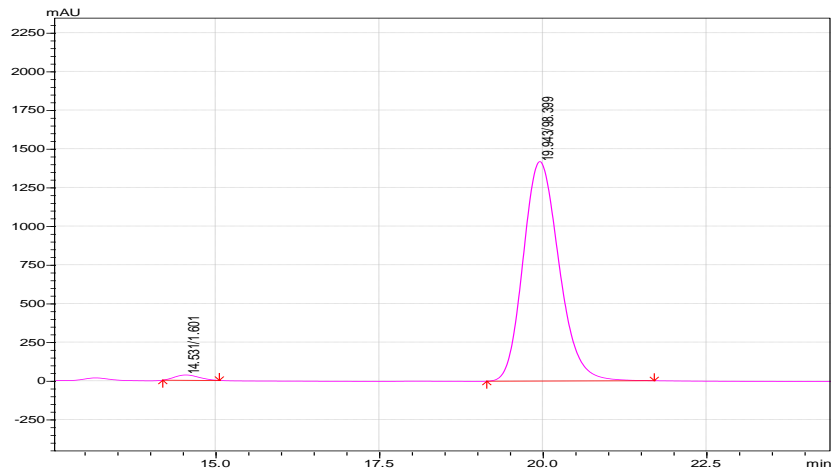
Peak#	Ret. Time	Peak Start	Peak End	Area%
1	9.762	8.800	10.869	43.1674
2	14.256	13.632	15.787	56.8326



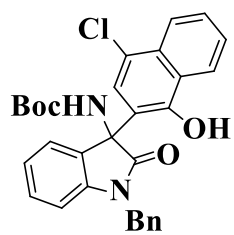
Peak#	Ret. Time	Peak Start	Peak End	Area%
1	11.526	11.136	11.680	0.1535
2	18.436	17.077	21.824	99.8465



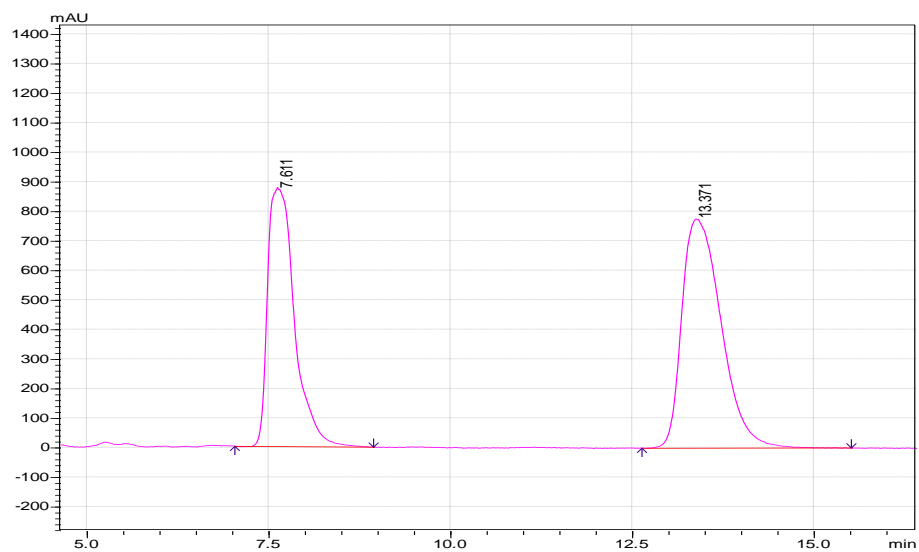
Peak	Ret. Time	Peak Start	Peak End	Area%
1	14.788	14.112	16.096	49.8962
2	20.344	19.435	21.728	50.1038



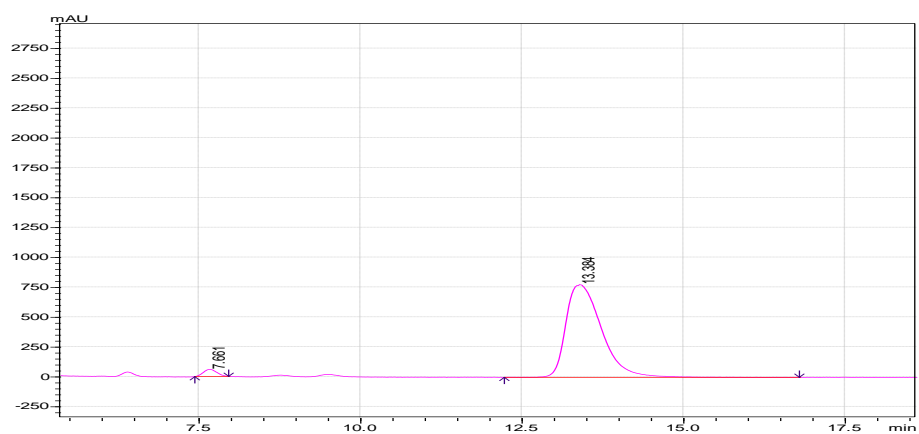
Peak#	Ret. Time	Peak Start	Peak End	Area%
1	14.531	14.187	15.051	1.6013
2	19.943	19.136	21.696	98.3987



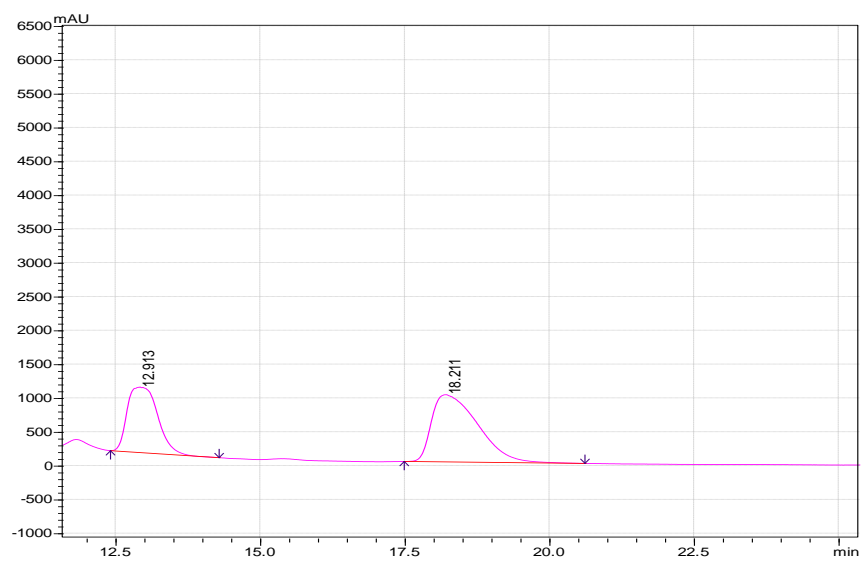
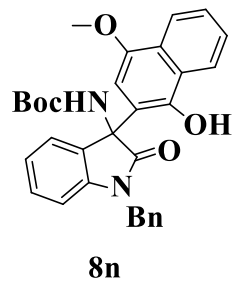
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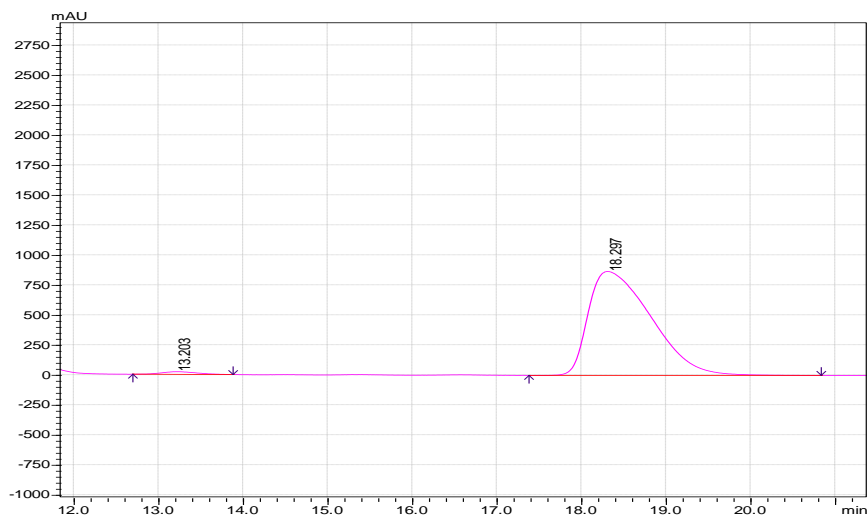
Peak#	Ret. Time	Peak Start	Peak End	Area%
1	7.611	7.029	8.939	43.5749
2	13.371	12.629	15.509	56.4251



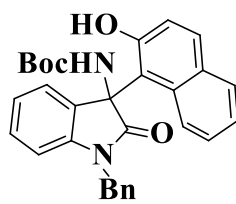
Peak#	Ret. Time	Peak Start	Peak End	Area%
1	7.661	7.435	7.957	2.8295
2	13.384	12.224	16.789	97.1705



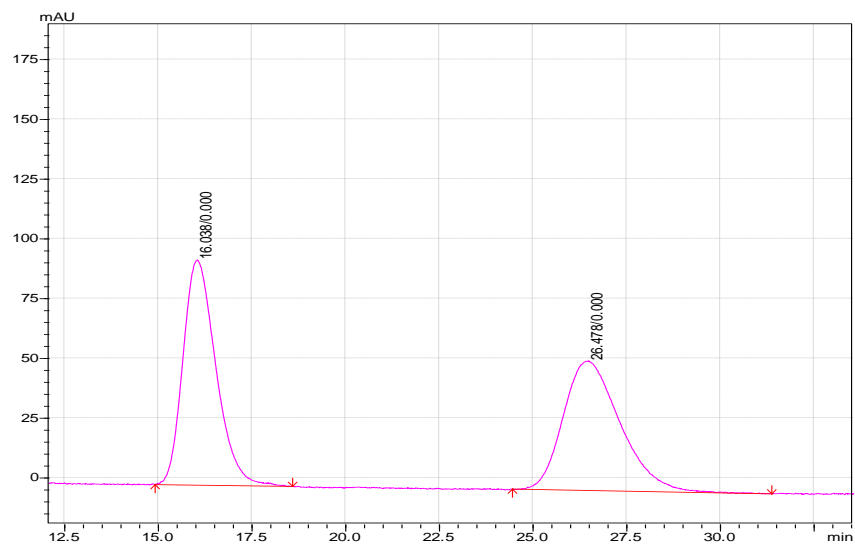
Peak#	Ret. Time	Peak Start	Peak End	Area%
1	12.913	12.405	14.283	39.1803
2	18.211	17.483	20.608	60.8197



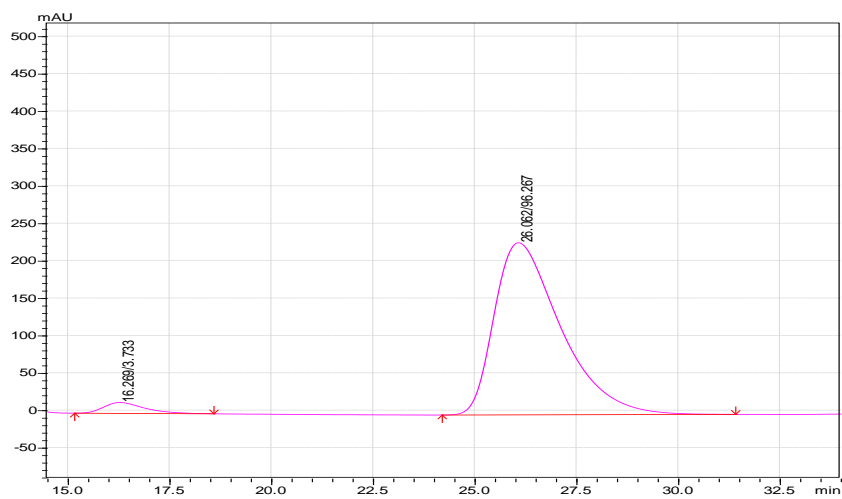
Peak#	Ret. Time	Peak Start	Peak End	Area%
1	13.203	12.693	13.877	1.3931
2	18.297	17.376	20.832	98.6069



80



Peak#	Ret. Time	Peak Start	Peak End	Area%
1	16.038	14.912	18.581	50.1661
2	26.478	24.448	31.371	49.8339



Peak#	Ret. Time	Peak Start	Peak End	Area %
1	16.269	15.157	18.581	3.7328
2	26.062	24.192	31.403	96.2672

Computational Study:

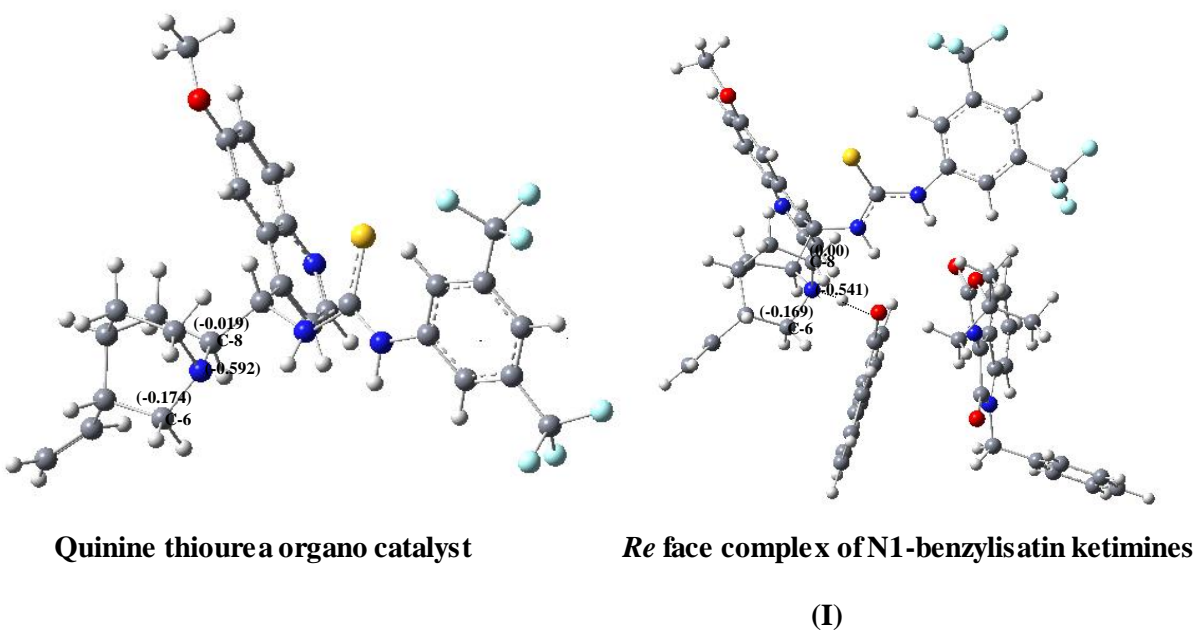
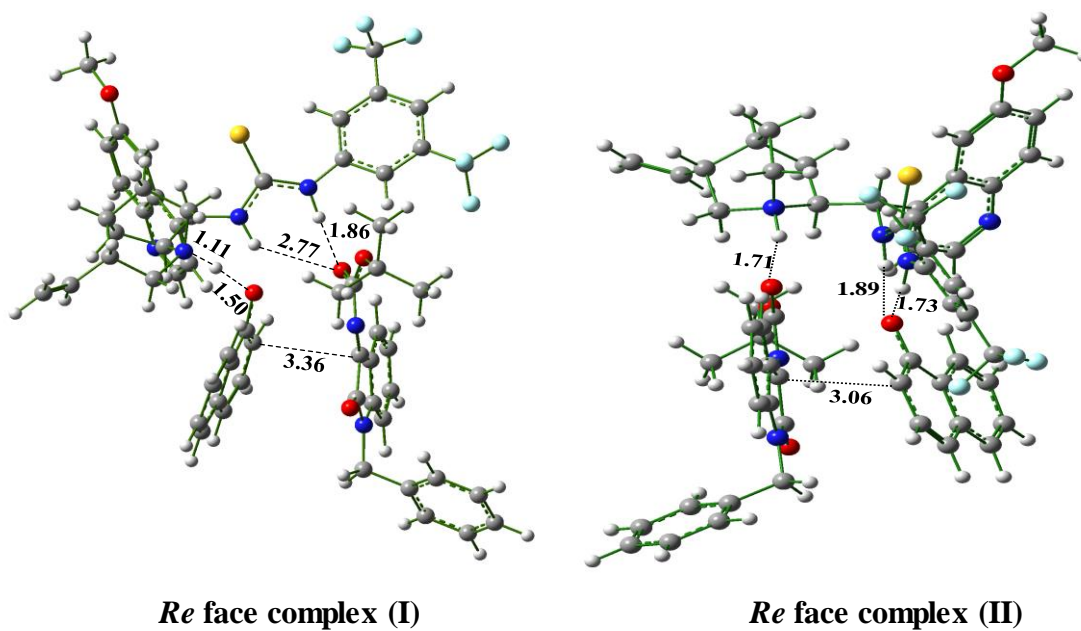


Figure S1: Calculated NBO charges for Quinine thiourea organo catalyst and the *Re* face complex of N1-benzylisatin ketimines with **Cat** and **Nu**.



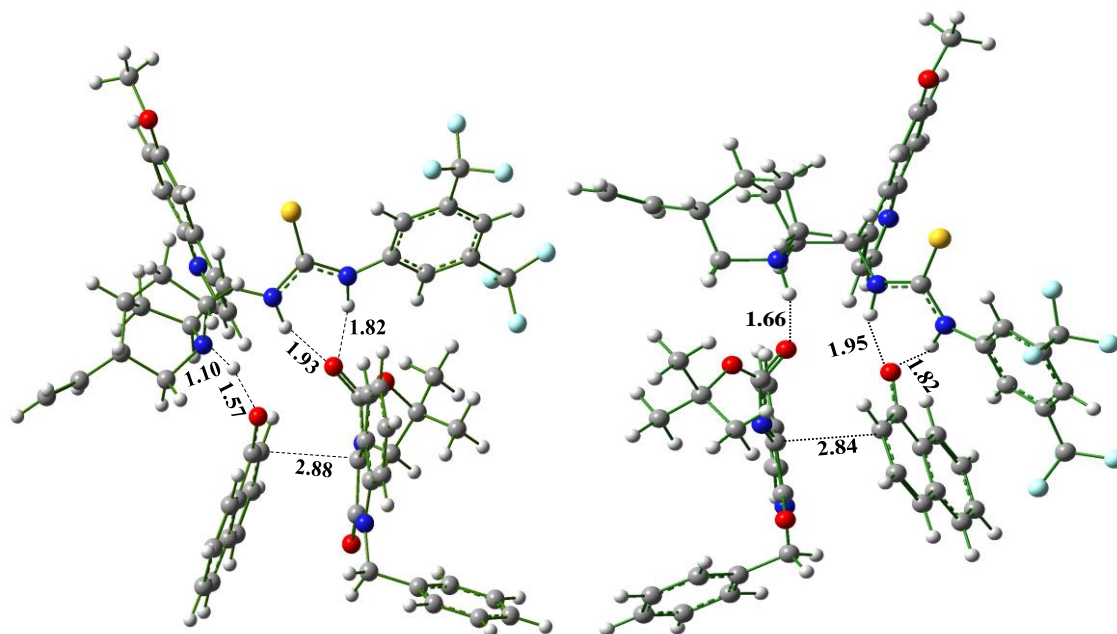
M06-2X /6-311+G(d,p)//B3LYP/6-31G(d)

ΔE (kcal/mol)

[0.0]

[2.6]

Figure S2: *Re* face Complex structures of 1-naphthol and *N*-benzylisatinas with chiral quinine thiourea organocatalyst of both the former (I) and later case (II) calculated with B3LYP/6-31G(d) level of theory. Single point energy calculated at M06-2X /6-311+G(d,p)//B3LYP/6-31G(d) level of theory. The distances are given in Å.



***Si* face complex (I)**

***Si* face complex (II)**

M06-2X /6-311+G(d,p)//B3LYP/6-31G(d)

$\Delta E(\text{kcal/mol})$

[0.0]

[1.6]

Figure S3: *Si* face Complex structures of 1-naphthol and N1-benzyl isatin with chiral quinine thiourea organocatalyst of both the former (I) and later case (II) calculated with B3LYP/6-31G(d) level of theory. Single point energy calculated at M06-2X /6-311+G(d,p)//B3LYP/6-31G(d) level of theory. The distances are given in Å.

Co-ordinates of the catalyst, complexes and transition states

Quinine thiourea organo catalyst

B3LYP/6-31G(d) level of theory:

Charge: 0

Spin Multiplicity: 1

Electronic Energy (au): -2413.3992323

C	-2.69527000	-1.66448900	0.05818400	H	-0.36172400	-1.80400800	0.00036300
C	-4.48690000	-2.41170300	1.65047700	C	0.63083100	-0.01757000	-0.12023900
C	-4.15261000	-1.39961600	0.53429500	S	0.52915600	1.62022600	0.19454400
H	-2.71936800	-2.14972200	-0.92507000	N	1.80390800	-0.74186800	-0.27119300
H	-4.26436800	-0.38399800	0.93003200	H	1.68492300	-1.62526900	-0.75324700
H	-4.85287100	-1.48194600	-0.30290300	C	3.14865500	-0.36601800	-0.10890100
C	-2.09055900	-2.21597600	2.36419300	C	4.10304200	-1.06632200	-0.85937600
H	-1.52374900	-2.94562900	2.95226300	C	3.57920400	0.61136400	0.80018000
H	-1.56922200	-1.25919600	2.46467300	C	5.46152900	-0.79513400	-0.70889000
C	-3.56751300	-2.11575400	2.85152700	H	3.78513200	-1.82038700	-1.57392900
H	-3.76228700	-2.82897000	3.66157400	C	4.94114800	0.88030300	0.92574100
H	-3.78049800	-1.11597100	3.24806100	H	2.85936100	1.15396600	1.39491200
H	-5.53786000	-2.31316100	1.94195000	C	5.89488200	0.18585100	0.18061800
C	-4.21399300	-3.87151000	1.18573300	H	6.95007200	0.40272700	0.29255500
C	-2.68993200	-3.94405700	0.80199500	C	5.39041600	1.98060500	1.85433200
H	-2.16586200	-4.66859400	1.43473300	C	6.46289600	-1.61499600	-1.47905400
H	-2.56791300	-4.27449200	-0.23580600	F	6.61154900	1.72325300	2.37552100
N	-2.01698400	-2.64072000	0.94857100	F	5.47932500	3.16521800	1.21060000
C	-1.83620700	-0.37733700	-0.11372900	F	4.53643000	2.15083100	2.88536600
C	-2.35053000	0.43745700	-1.29883800	F	6.75718300	-2.76966200	-0.83647400
C	-4.29563700	3.32419700	0.16996100	F	5.99320800	-1.95842200	-2.70007400
H	-3.11186600	1.80259400	1.03275100	F	7.62504000	-0.95459400	-1.65881500
C	-4.48438400	3.37032100	-2.23691000	C	-2.08330600	0.00797400	-2.58127400
H	-2.39727500	0.34340700	-4.70135500	C	-3.49662100	2.19598900	0.09984600
C	-4.80225700	3.91710100	-1.01488600	C	-3.66514200	2.21905500	-2.34484500
H	-4.84928400	3.80890600	-3.16022200	C	-2.61831900	0.69682100	-3.69446400
H	-5.42880600	4.80031400	-0.96753100	C	-3.16544900	1.60684600	-1.14353300
N	-3.39162100	1.75697400	-3.59914800	H	-1.44976800	-0.85907100	-2.74449600
N	-0.45696000	-0.82930400	-0.29693500	H	-1.88499400	0.23075100	0.79459900

O	-4.54641900	3.80205500	1.42415700	C	-5.10988500	-4.32706300	0.06589100
C	-5.31162000	4.98944700	1.56267800	H	-4.99796400	-3.80609500	-0.88687600
H	-5.35730600	5.18908500	2.63481900	C	-6.00393500	-5.31314200	0.15538300
H	-4.83563600	5.83987800	1.05755200	H	-6.15067500	-5.87006500	1.07902400
H	-6.33180400	4.86361400	1.17648600	H	-6.62430300	-5.60259200	-0.68850200
H	-4.39743100	-4.52719000	2.04686900				

Re face complex for N1-benzylisatin ketimine of former case

B3LYP/6-31G(d) level of theory:

Charge: 0

Spin Multiplicity: 1

Electronic Energy (au): -3983.90120115

Electronic Energy (au): -3983.51569232 at M06-2X/6-311+G(d,p)// B3LYP/6-31G(d) level of theory

C	1.81891600	-3.32330600	-0.60096800	C	0.61764000	-4.09469400	-2.60122400
C	3.02877300	-4.66112200	-2.37597800	H	-0.01334700	-3.72915400	-3.41227400
C	2.76643600	-4.52968300	-0.86066500	H	-0.04331800	-4.56005700	-1.86658200
H	0.94476200	-3.62913800	-0.02329200	N	1.23603100	-2.89297000	-1.93242600
H	3.71097800	-4.38373800	-0.32833300	C	2.56213000	-2.18599800	0.15640100
H	2.32932400	-5.45222300	-0.46601200	C	2.65894200	-2.58799100	1.63808000
C	2.28002600	-2.30183000	-2.83826200	C	6.33921500	-3.02847500	2.37841500
H	1.78987000	-2.12985800	-3.80038100	H	5.28861400	-2.36737600	0.66679800
				C	5.05449000	-3.54527100	4.35668700
H	2.59003800	-1.33976900	-2.43203100	H	0.64200400	-3.21327400	4.30791000
C	3.46429100	-3.29441300	-2.94365900	C	6.27677400	-3.44247500	3.73385400
H	3.77091300	-3.39900000	-3.98991300	H	4.97652900	-3.85120900	5.39511700
H	4.32767900	-2.90414300	-2.39456300	H	7.18199800	-3.67014500	4.28490000
H	3.80321500	-5.41256700	-2.55744500	N	2.68473500	-3.38189600	4.37496900
C	1.71757100	-5.06778300	-3.10188000	N	1.98795700	-0.85344100	-0.01863200

H	0.96330600	-0.76976400	-0.01267000	O	7.50524300	-2.88856000	1.68432600
C	2.77314900	0.25293000	-0.22887300	C	8.73489300	-3.08456200	2.36546600
S	4.39637700	0.14018300	-0.71721600	H	9.51590700	-2.88148500	1.63061700
N	2.10589900	1.43080000	-0.05487800	H	8.84512600	-2.39179900	3.20975400
H	1.09585600	1.36594500	0.12900400	H	8.84064400	-4.11609400	2.72713000
C	2.55945000	2.75996400	-0.20969900	C	-4.30687200	-4.60851500	-2.56855300
C	1.59867600	3.71281700	-0.57557700	C	-4.36981200	-4.57814900	-1.19285200
C	3.86923600	3.18681400	0.05794300	C	-3.52568100	-3.72401000	-0.43091000
C	1.94371200	5.05726600	-0.69737300	C	-2.56300300	-2.91893500	-1.12717600
H	0.58376600	3.39469900	-0.77472000	C	-2.55174000	-2.94536800	-2.54398300
				C	-3.40029500	-3.76813000	-3.25571900
C	4.19864200	4.53546500	-0.08147200	H	-4.35810100	-4.25090900	1.50446000
H	4.61942000	2.47688100	0.37235400	H	-4.96885400	-5.26337200	-3.12982200
C	3.24864200	5.48428900	-0.46090100	H	-5.08579800	-5.20427900	-0.66417500
H	3.51587200	6.52998700	-0.55236700	C	-3.62906800	-3.63514700	0.98372300
C	5.62387800	4.97251300	0.13774300	C	-1.64542600	-2.07219700	-0.38332000
C	0.89468000	6.03152800	-1.15891500	H	-1.87343300	-2.27134800	-3.05773100
F	6.27674300	4.16716400	1.00187400	H	-3.38718200	-3.76120900	-4.34281900
F	6.32881100	4.96775200	-1.01761100	C	-1.85254000	-1.97219000	1.00130300
F	5.69011500	6.23249800	0.62787300	C	-2.82357900	-2.75016600	1.66782600
F	1.19266500	7.30331500	-0.82151300	H	-1.23911500	-1.27013300	1.55830300
F	0.75018500	6.00846600	-2.51069200	H	-2.92282300	-2.65068400	2.74703700
F	-0.32410700	5.74700000	-0.64327300	O	-0.67343300	-1.41459100	-0.99018800
C	1.50399100	-2.72471900	2.37983500	C	-4.87370400	0.67719600	2.18602700
C	5.17951900	-2.73674600	1.67962600	C	-3.60423800	1.11648900	1.72511300
C	3.84751200	-3.25579900	3.67352300	C	-2.70600100	1.70273600	2.62334300
C	1.56528000	-3.11336000	3.73824300	C	-3.08109300	1.85127600	3.95957000
C	3.90867600	-2.84751200	2.29394700	C	-4.33675100	1.41521000	4.39353300
H	0.52961100	-2.54169000	1.93680900	C	-5.25163400	0.82275800	3.51449400
H	3.56514600	-2.10700300	-0.25804000	C	-4.91955500	0.19176500	-0.04724700

C	-3.56140700	0.83359400	0.29196200	H	-9.36219100	3.05212300	-0.76318700
H	-1.73034600	2.01586200	2.27639200	H	-10.56606400	1.85367800	3.18927000
H	-2.39141900	2.30369800	4.66524800	H	-10.85433700	3.32831600	1.20778100
H	-4.61530100	1.53679800	5.43694500	C	-2.05501500	0.89105000	-3.59515400
H	-6.22783500	0.50430100	3.86201100	H	-2.89639300	0.45904900	-3.05336500
N	-5.61944000	0.11411300	1.14206500	H	-2.34199900	1.04085500	-4.64241500
C	-6.96812300	-0.43857600	1.23232300	H	-1.21971000	0.18434300	-3.56165200
H	-7.06937900	-1.09537200	0.36333300	C	-0.49952200	2.85562600	-3.84213800
H	-7.02791400	-1.06117000	2.13131400	H	-0.16718900	3.80861900	-3.42143900
O	-5.31829000	-0.15046900	-1.14217000	H	0.36003700	2.17974000	-3.89279600
N	-2.77361400	1.03402400	-0.70148100	H	-0.85703900	3.03641400	-4.86118400
C	-1.46835400	1.48305500	-0.59289800	C	-2.78115000	3.22226100	-2.84123900
O	-0.74438900	1.37384100	0.39663700	H	-2.43555600	4.13279500	-2.33909900
O	-0.95162700	2.04262400	-1.69046700	H	-3.16487900	3.50220600	-3.82865500
C	-1.62342000	2.23579500	-3.00581100	H	-3.60051100	2.78066400	-2.26985400
C	-8.06170600	0.61533400	1.23400100	H	1.87127100	-4.90881500	-4.17682800
C	-8.23704700	1.44419100	0.11629900	C	1.31454200	-6.50550300	-2.90771600
C	-8.91076200	0.77140200	2.33352500	H	1.08649400	-6.81335100	-1.88630500
C	-9.23542400	2.41633200	0.10903800	C	1.21833800	-7.40058200	-3.89115800
H	-7.59047100	1.31710700	-0.74802300	H	1.42390000	-7.13850500	-4.92723100
C	-9.91432100	1.74351300	2.32661700	H	0.92849800	-8.42981700	-3.69985300
H	-8.79297200	0.12481500	3.20115800	H	0.40708900	-2.20078100	-1.67690400
C	-10.07589100	2.57014900	1.21534300				

Si face complex for N1-benzylisatin ketimine of former case

B3LYP/6-31G(d) level of theory:

Charge: 0

Spin Multiplicity: 1

Electronic Energy (au): -3983.89335284

Electronic Energy (au): -3983.50656717 at M06-2X/6-311+G(d,p)// B3LYP/6-31G(d) level of theory

C	2.52986500	-2.82744800	-0.11608600	H	7.33805000	-1.04602900	4.29299300
C	3.70230700	-4.44701800	-1.67678900	H	8.99540700	-1.02276300	2.45342700
C	3.67869600	-3.87163700	-0.24501100	N	4.79511600	-1.13085100	4.08692700
H	1.88295600	-3.05338700	0.73616400	N	2.10519200	-0.35671800	-0.17826500
H	4.63818300	-3.39977500	-0.01819500	H	1.31310800	-0.34211800	0.46184200
H	3.54993400	-4.67359500	0.48824500	C	2.41498400	0.85133400	-0.76865400
C	2.31290200	-2.55227600	-2.58877900	S	3.66329900	1.02654900	-1.88871300
H	1.63149800	-2.80413700	-3.40491800	N	1.58078300	1.84227100	-0.33205700
H	2.42587500	-1.46762900	-2.56097600	H	0.99198900	1.57014900	0.46233400
C	3.67229900	-3.28879600	-2.69640000	C	1.40666800	3.18393600	-0.70860200
H	3.80676900	-3.67500800	-3.71229700	C	0.68465900	3.97648300	0.19895400
H	4.49749800	-2.59279300	-2.51027000	C	1.85134100	3.75523100	-1.90961400
H	4.60131500	-5.05453500	-1.81883100	C	0.41594800	5.31238100	-0.08775900
C	2.43418100	-5.30965700	-1.91150100	H	0.33993000	3.54419100	1.13443300
C	1.23442300	-4.45053000	-1.44993500	C	1.57706300	5.09687200	-2.17291300
H	0.38658200	-4.47791900	-2.13338600	H	2.40519400	3.16106300	-2.62152100
H	0.86135100	-4.75277400	-0.46816700	C	0.86046400	5.88946900	-1.27598200
N	1.62821500	-2.99352800	-1.32487600	H	0.65255300	6.92847800	-1.49844200
C	3.10442900	-1.39320800	0.04814500	C	2.11797400	5.71995100	-3.43441200
C	3.74470900	-1.27302700	1.44211600				
C	7.48135000	-1.09485800	0.88548200	C	-0.39817000	6.11017300	0.89560300
H	5.83414700	-1.12495600	-0.43780800	F	1.30688400	6.70001400	-3.89314000
				F	3.33195400	6.27935200	-3.22927800
C	7.02039500	-1.07962600	3.25577100	F	2.26086700	4.81420400	-4.42479500
H	2.84647600	-1.16058000	4.72489700	F	-0.35589000	7.43265100	0.64301400
C	7.93591300	-1.06575700	2.22929400	F	-1.70413900	5.74152700	0.87819200

F	0.03412700	5.92602600	2.16699600	H	-0.63814800	-1.80751100	1.27617100
C	2.93535500	-1.25527200	2.55995400	H	-1.80067800	-2.80049700	3.22622800
C	6.12549400	-1.15201900	0.60573900	O	-0.92084200	-2.56618200	-1.21743500
C	5.62628600	-1.13425900	3.00617200	C	-4.05670000	-0.52131300	-1.03416000
C	3.50121800	-1.17601300	3.85462800	C	-2.85783800	-0.00919500	-0.47085400
C	5.16344300	-1.18631700	1.64412400	C	-1.90477100	0.58605200	-1.30173100
H	1.85252300	-1.28912200	2.47123800	C	-2.17506800	0.71710000	-2.66394600
H	3.86316900	-1.22827200	-0.71453400	C	-3.38220100	0.24879400	-3.19147000
O	8.31267600	-1.06902900	-0.19432100	C	-4.33790400	-0.38393600	-2.38665300
C	9.71024400	-0.92897000	0.01834600	C	-4.24797700	-0.99014000	1.19606700
H	10.15822200	-0.89476700	-0.97617800	C	-2.94559800	-0.21777300	0.96505900
H	9.94670500	-0.00023100	0.55308200	H	-0.96737300	0.93351400	-0.88915200
H	10.12471300	-1.78234300	0.57087300	H	-1.44321300	1.18365300	-3.31602600
C	-4.36255200	-6.25217700	-0.71508000	H	-3.58576200	0.36901000	-4.25224200
C	-4.09000400	-5.78399900	0.55434400	H	-5.27102300	-0.74097500	-2.80788600
C	-3.19070600	-4.70614000	0.76479000	N	-4.84602900	-1.12127400	-0.04750500
C	-2.55575200	-4.11520800	-0.37651000	C	-6.16253700	-1.71727800	-0.23450100
C	-2.87167600	-4.59934000	-1.66549100	H	-6.12719200	-2.38793300	-1.09962300
C	-3.75655500	-5.64858900	-1.83882100	H	-6.33053600	-2.33237800	0.65471800
H	-3.40727800	-4.66277800	2.92798700	O	-4.70698000	-1.36733900	2.25690100
H	-5.04957400	-7.08398900	-0.85195200	N	-2.37125400	0.29359500	2.01061200
H	-4.56316300	-6.24174100	1.42065400	C	-1.14922800	0.87881900	2.03687300
C	-2.90313700	-4.22000100	2.07354600	O	-0.15783500	0.50308400	1.38519500
C	-1.56570700	-3.05117900	-0.20050000	O	-0.94430100	1.87285500	2.90865600
H	-2.39657300	-4.11763400	-2.51504900	C	-1.95516000	2.42745600	3.84747000
H	-3.98582100	-6.01243300	-2.83753800	C	-7.26930500	-0.68661100	-0.39086400
C	-1.35177100	-2.60890200	1.12530000	C	-7.45044800	0.30348500	0.58568200
C	-2.00325700	-3.19259900	2.23242100	C	-8.12729700	-0.71194900	-1.49413600

C	-8.46052400	1.25379600	0.45103000				
H	-6.80086300	0.32020400	1.45677700	H	-3.68426800	2.34049700	2.52189600
C	-9.14541100	0.23607400	-1.62778000	H	-3.75351700	3.61282900	3.75158300
H	-8.00152400	-1.47959700	-2.25531800	C	-1.13586100	3.48137000	4.59704400
C	-9.31094400	1.22397800	-0.65776900	H	-0.75747100	4.24493900	3.91134200
H	-8.58859900	2.01624500	1.21495300	H	-1.76235400	3.97227400	5.34889900
H	-9.80299300	0.20392500	-2.49256400	H	-0.28512500	3.01685200	5.10570100
H	-10.09849000	1.96552400	-0.76197000	H	2.35005000	-5.49652900	-2.98970100
C	-2.44671300	1.34099500	4.80891900	C	2.44619300	-6.64468900	-1.21536800
H	-1.59568600	0.85862700	5.30247400	H	2.50219200	-6.62350000	-0.12614200
H	-3.06432600	1.80800200	5.58456100	C	2.37629100	-7.82161900	-1.83723800
H	-3.03822100	0.58051200	4.29773800	H	2.30316000	-7.89429900	-2.92057300
C	-3.09041500	3.08306400	3.05838200	H	2.38522200	-8.75868500	-1.28794300
H	-2.69586400	3.81407300	2.34530000	H	0.64623300	-2.52362800	-1.19283700

***Re*-face complex for N1-benzylisatin ketimine of later case**

B3LYP/6-31G(d) level of theory:

Charge: 0

Spin Multiplicity: 1

Electronic Energy (au): -3983.89669929

Electronic Energy (au): -3983.51144281 at M06-2X/6-311+G(d,p)// B3LYP/6-31G(d) level of theory

				H	4.96068900	-3.20938500	-1.40172000
C	3.39387700	-1.68814800	-1.26007700	C	3.04252800	-0.35828400	-3.37574800
C	4.81973700	-2.14144800	-3.30434000				
C	4.77284700	-2.19437400	-1.76408300	H	2.37405100	-0.33067700	-4.24034200
H	2.85765800	-2.46911100	-0.71894100	H	2.96289400	0.59494600	-2.84874000
H	5.57132800	-1.56722000	-1.35492000	C	4.50053500	-0.70298800	-3.76012000

H	4.63564800	-0.60534300	-4.84235800	C	-0.52715900	5.22257700	-1.18307700
H	5.18927300	0.00427300	-3.28526900	H	0.96223300	3.85961200	-1.92468900
H	5.81306500	-2.43705600	-3.65536200	C	-1.48237200	5.49608700	-0.20249600
C	3.75077700	-3.08882100	-3.91783100	H	-2.08650900	6.39319800	-0.25323400
				C	-0.30242700	6.21872300	-2.29001400
C	2.39123900	-2.73019700	-3.25922900	C	-2.71192900	4.79529600	1.88295000
H	1.59629800	-2.57686000	-3.99263800	F	-1.44144900	6.87620400	-2.61033600
H	2.04693400	-3.48666500	-2.55300800	F	0.60580200	7.15899000	-1.94389100
N	2.51473800	-1.44590100	-2.47680000	F	0.15215200	5.62923000	-3.41858800
C	3.50693300	-0.43325900	-0.34944200	F	-3.74363900	3.93190200	1.71625100
C	4.16512700	-0.85677900	0.96730800	F	-2.23570100	4.59511500	3.12988700
C	7.41476800	1.05824800	1.16553100	F	-3.22958500	6.04273600	1.83995200
H	5.79869400	1.11310200	-0.19748400	C	3.53545900	-1.78058400	1.77647000
C	7.22975200	-0.41298500	3.07361600	C	6.18372000	0.63144800	0.69428600
H	3.63339600	-2.93907200	3.60840500	C	5.96682200	-0.87123800	2.62359100
C	7.94748600	0.52472800	2.36784700	C	4.14474400	-2.21185400	2.97890600
H	7.60821500	-0.82887300	4.00187500	C	5.43370700	-0.34324700	1.39528800
H	8.90992300	0.85595200	2.74048000	H	2.56104800	-2.18288800	1.51138000
N	5.32148700	-1.79427700	3.39247800	H	4.12887300	0.30763400	-0.85014900
N	2.22175900	0.21421100	-0.14751500	O	8.04998000	1.99755700	0.40971100
H	1.53542200	-0.24545400	0.46210200	C	9.27688800	2.53971300	0.87637700
C	1.98193100	1.54396500	-0.40996500	H	9.56878200	3.28815400	0.13775300
S	3.11767500	2.55833700	-1.16608600	H	9.15926900	3.02410000	1.85409400
N	0.74334000	1.91510900	0.00625200	H	10.06073300	1.77365200	0.94219600
H	0.21427000	1.15848600	0.49659500	C	-0.83089400	-2.02654900	6.02095000
C	0.07838100	3.15207500	-0.08894300	C	-2.02203700	-1.45001400	5.62808800
C	-0.86990800	3.43048600	0.90552200	C	-2.16230700	-0.84650600	4.35146200
C	0.24379300	4.06172200	-1.14413600	C	-1.04368900	-0.87264100	3.46054000
C	-1.64885500	4.58470200	0.83734000	C	0.16780600	-1.45086400	3.89670100
H	-1.00954600	2.73333500	1.72518800	C	0.28121200	-2.01820800	5.15208000

H	-4.20253700	-0.16167900	4.65212700	C	-0.52215300	-2.23802300	-0.95168900
H	-0.74417900	-2.47651000	7.00702100	O	-0.11724100	-1.35893900	-1.72833400
H	-2.87417600	-1.44047300	6.30444200	O	0.34009000	-3.25243300	-0.69598700
C	-3.36667100	-0.19235100	3.95809300	C	0.01067400	-4.50487500	0.04549300
C	-1.14833500	-0.27554300	2.13218100	C	-7.41262400	-1.73639900	-0.32890500
H	1.01642100	-1.41510000	3.22219500	C	-7.28869200	-3.08854800	-0.67825000
H	1.22537800	-2.44900400	5.47654000				
C	-2.36720200	0.37449200	1.81592700	C	-8.54771400	-1.03156300	-0.74023200
C	-3.44040600	0.42638800	2.73060700	C	-8.27852500	-3.71573700	-1.43253200
H	-2.43702000	0.89556300	0.86742500	H	-6.41626100	-3.64558200	-0.34623900
H	-4.33879200	0.97336100	2.45206400	C	-9.54294900	-1.65950100	-1.49363000
O	-0.16831200	-0.33823200	1.28697200	H	-8.65958600	0.01547300	-0.46483000
C	-4.54604300	-0.22438100	-1.10216400	C	-9.40841400	-3.00250600	-1.84367200
C	-3.17238000	-0.47557500	-1.38183700	H	-8.17243800	-4.76501600	-1.69547400
C	-2.51688000	0.29933500	-2.34749900	H	-10.41937200	-1.09803400	-1.80646200
C	-3.22553300	1.29483900	-3.02094900	H	-10.18003400	-3.49368900	-2.43052000
C	-4.57712800	1.51823900	-2.73755900	C	-0.32877800	-4.21774000	1.50823700
C	-5.25641400	0.76172800	-1.77561800	H	0.44546800	-3.60392300	1.97725500
C	-4.00420700	-1.94237200	0.30380500	H	-1.28451600	-3.70390400	1.60414200
C	-2.76228700	-1.57205500	-0.51240500	H	-0.38144600	-5.16866200	2.05139000
H	-1.46936300	0.11980500	-2.54516000	C	1.32583300	-5.28549500	-0.05794900
H	-2.72269500	1.90358600	-3.76626800	H	1.58822300	-5.48395000	-1.10360600
H	-5.11653100	2.29549600	-3.27229100	H	2.14702700	-4.73550800	0.41503300
H	-6.30762900	0.93459400	-1.57373500	H	1.22771400	-6.24804900	0.45388000
N	-5.01270800	-1.07818500	-0.10212100	C	-1.11229300	-5.25909100	-0.67284100
C	-6.33726800	-1.06445100	0.50683600	H	-0.88503500	-5.37260900	-1.73930900
H	-6.21828200	-1.58148700	1.46397500	H	-1.20657300	-6.26093200	-0.23906500
H	-6.61238400	-0.02533400	0.72060200	H	-2.06677400	-4.74398300	-0.55662800
O	-4.12626200	-2.84866400	1.10644400	H	3.69500200	-2.86838800	-4.99107000
N	-1.73502900	-2.34619700	-0.33976400	C	4.06775700	-4.55424000	-3.76684600

H	4.12424100	-4.93631800	-2.74657800	H	4.50901100	-6.43862500	-4.62341800
C	4.27519500	-5.39016400	-4.78456400	H	1.54150700	-1.23009500	-2.13359
H	4.22046600	-5.05861200	-5.81963000				

Si-face complex for N1-benzylisatin ketimine of later case

B3LYP/6-31G(d) level of theory:

Charge: 0

Spin Multiplicity: 1

Electronic Energy (au): -3983.89014087

Electronic Energy (au): -3983.50403940 at M06-2X/6-311+G(d,p)// B3LYP/6-31G(d) level of theory

C	-2.63256400	-2.77051700	0.21852700	H	-1.43174000	-2.03940700	-4.74315000
C	-4.14654400	-4.25019600	1.61902500	C	-7.03170700	-1.82422000	-3.87923000
C	-3.74277600	-3.85987100	0.18115500	H	-5.85737500	-2.17687800	-5.64369100
H	-1.73349200	-3.11008500	-0.30317000	H	-7.97911000	-1.88816800	-4.40196000
H	-4.61827000	-3.48196000	-0.35363800	N	-3.48171500	-2.05431300	-4.70539700
H	-3.39601000	-4.73569500	-0.37588900	N	-2.14477800	-0.34110500	-0.06740300
C	-3.26970000	-2.08622700	2.55602000	H	-1.19371200	-0.36870500	-0.46397300
H	-2.86362300	-2.11106700	3.57053800	C	-2.57839600	0.91473100	0.30282400
H	-3.44873600	-1.04392900	2.28074100	S	-4.11041900	1.19622800	0.97370100
C	-4.52728600	-2.97138300	2.39395400	N	-1.62266100	1.85135100	0.05960300
H	-4.93472200	-3.22630100	3.37783500	H	-0.84857100	1.49458700	-0.52695000
H	-5.30816300	-2.42175700	1.85703800	C	-1.48556800	3.19293000	0.45682600
H	-4.99365200	-4.94202100	1.58999800	C	-0.48082300	3.92514000	-0.19880700
C	-2.95261100	-4.91647100	2.35867000	C	-2.22739400	3.81480400	1.47088200
C	-1.73249900	-3.97868400	2.17065800	C	-0.21725900	5.24274700	0.16066300
H	-1.17643700	-3.79982100	3.09196500	H	0.09766200	3.46078400	-0.98954700
H	-1.02595600	-4.36485100	1.43163700	C	-1.95621900	5.14193100	1.80702000
N	-2.18691300	-2.63209400	1.66400900	H	-3.01441500	3.27589300	1.97736400
C	-3.07103100	-1.41397200	-0.39516300	C	-0.95533100	5.86899400	1.16487600
C	-3.25490300	-1.59484600	-1.90676600	H	-0.76323700	6.90155100	1.43002400
C	-6.99036800	-1.55934400	-2.48594100	C	-2.71822800	5.78463000	2.93628000
H	-5.80174300	-1.22084900	-0.77276300	C	0.92017100	5.97625100	-0.50184100
C	-5.85585100	-1.98701400	-4.57508600	F	-2.06654900	5.64881700	4.11699000

F	-2.88469200	7.11201500	2.73618300	C	1.81071800	1.22349300	0.32646600
F	-3.94303300	5.24262300	3.10127700	C	2.84885000	2.10609800	0.69935500
F	0.70094600	7.31180900	-0.53170300	H	1.18751200	0.76198900	1.08255900
F	2.08541100	5.78725000	0.15928400	H	3.07209900	2.23438500	1.75494800
F	1.11538700	5.56763800	-1.77207200	O	0.35120300	0.41436800	-1.37297800
C	-2.14830000	-1.71644200	-2.72282500	H	-3.20656300	-4.95884600	3.42521600
C	-5.77558000	-1.47911700	-1.82521100	C	-2.64360400	-6.31955900	1.90564300
C	-4.59525600	-1.90387600	-3.93261800	H	-2.35573100	-6.43977600	0.86009900
C	-2.31324100	-1.94237300	-4.11069300	C	-2.69595700	-7.39549800	2.69125800
C	-4.55217600	-1.65634200	-2.51649700	H	-2.96935300	-7.32571500	3.74226600
H	-1.13918100	-1.60814900	-2.33253600	H	-2.46914400	-8.38870400	2.31446700
H	-4.01823200	-1.11794700	0.05448000	H	-1.32390200	-2.02576200	1.67958700
O	-8.10074900	-1.36913100	-1.71755400	C	4.00423300	-1.63822500	-1.28898600
C	-9.37392100	-1.34315600	-2.34643400	C	2.82246600	-1.88227300	-0.53656600
H	-10.09200200	-1.13393500	-1.55168300	C	1.77777300	-2.60967700	-1.11516700
H	-9.43393800	-0.55226500	-3.10483500	C	1.93003000	-3.11347800	-2.40899800
H	-9.61909400	-2.30870700	-2.80820000	C	3.10822200	-2.87987900	-3.12338100
C	3.78000700	3.05836600	-3.97903800	C	4.16151300	-2.13577700	-2.57424200
C	4.06269400	3.24645300	-2.63965200	C	4.41461600	-0.65128300	0.73197800
C	3.31345900	2.58691100	-1.63287700	C	3.03664100	-1.30496000	0.78104500
C	2.24708900	1.72184900	-2.03654800	H	0.86686400	-2.76722400	-0.55392800
C	1.97428800	1.55340000	-3.41042400	H	1.12570200	-3.68281500	-2.86583500
C	2.72949300	2.20239100	-4.37112300	H	3.21455400	-3.27769900	-4.12903000
H	4.38534800	3.45710800	0.04903100	H	5.07349700	-1.96867600	-3.13638400
H	4.36546100	3.57711900	-4.73451700	N	4.91065500	-0.88082900	-0.54110400
H	4.86678900	3.91423400	-2.33776000	C	6.24389200	-0.46208000	-0.95658200
C	3.58913000	2.77848600	-0.24410300	H	6.18393000	-0.05636100	-1.97181100
C	1.41753900	1.05727000	-1.02933500	H	6.51078500	0.35975400	-0.28555600
H	1.15208200	0.89965900	-3.68369900	O	5.00006000	-0.08256700	1.63574500
H	2.51108000	2.06150200	-5.42668400	N	2.50788500	-1.46151800	1.96635700

C	1.23246600	-1.83693400	2.18905300	H	9.91045300	-4.43441100	-0.63341300
O	0.27741500	-1.67921100	1.40447500	C	2.48815100	-1.19120400	4.95320500
O	0.93023300	-2.34155300	3.40376300	H	1.68793200	-0.47957900	5.18497100
C	1.89522500	-2.53337500	4.51379400	H	3.07899700	-1.34282400	5.86382700
C	7.27621000	-1.57507200	-0.87550800	H	3.13120900	-0.76582800	4.18198400
C	7.50612800	-2.23028500	0.34323600	C	2.96773500	-3.54782100	4.10806200
C	8.01513000	-1.95773200	-1.99866900	H	2.50450900	-4.46483500	3.72636000
C	8.44623100	-3.25522200	0.42837600	H	3.63136800	-3.13786800	3.34511800
H	6.95026100	-1.92457800	1.22551000	H	3.57059900	-3.81222600	4.98405300
C	8.96287800	-2.98140500	-1.91374700	C	0.99760400	-3.11000000	5.61292300
H	7.85262700	-1.45033300	-2.94766800	H	0.55168900	-4.05955400	5.29613900
C	9.17672400	-3.63555900	-0.70104600	H	1.58417400	-3.29373400	6.51866700
H	8.61488500	-3.75442200	1.37908000	H	0.19304100	-2.40984100	5.86053800
H	9.52863300	-3.26807600	-2.79638000				

Transition State - 1 (TS-1, *Re* face) for *NI*-benzylisatin ketimine

B3LYP/6-31G(d) level of theory:

Charge: 0

Spin Multiplicity: 1

Imaginary frequency: -281.92 cm⁻¹

Electronic Energy (au): -3983.88353843

Electronic Energy (au): -3983.50557539 at M06-2X/6-311+G(d,p)// B3LYP/6-31G(d) level of theory

				C	2.56465800	-1.96261100	-2.91926900
C	1.81939000	-2.98840300	-0.73983900	H	2.16118500	-1.70668900	-3.90224100
C	2.99645700	-4.40563200	-2.47418400	H	2.95524800	-1.05708200	-2.45441500
C	2.66954000	-4.26679200	-0.97276900	C	3.62247600	-3.08926200	-2.98028200
H	0.86909700	-3.22212700	-0.25884800	H	3.97804100	-3.20729300	-4.00899800
H	3.59739400	-4.20307000	-0.39594400	H	4.48990700	-2.81548200	-2.37031900
H	2.13793500	-5.15109100	-0.60873100	H	3.68900900	-5.23823300	-2.62860900

C	1.69483200	-4.65247300	-3.28651700	C	3.30004900	5.75430100	-0.42363800
C	0.68172900	-3.55800100	-2.86227800	H	3.54026400	6.80634000	-0.51640800
H	0.19133000	-3.08473100	-3.71502900	C	5.70691900	5.29132300	0.09275100
H	-0.10134100	-3.93305100	-2.20341400	C	0.91361400	6.25390100	-1.05174600
N	1.39605000	-2.46116800	-2.10387800	F	6.39180400	4.50937500	0.95465200
				F	6.38659100	5.27816700	-1.07738100
C	2.57820200	-1.92305300	0.09732200	F	5.76290500	6.55884400	0.56225700
C	2.57362500	-2.36747000	1.56592400	F	1.19888900	7.53274900	-0.72952700
C	6.19185100	-2.96356500	2.47960800	F	0.73244500	6.21706500	-2.39714300
H	5.25757200	-2.22057700	0.73489200	F	-0.28139300	5.94825600	-0.49687500
C	4.78697100	-3.48496800	4.37437900	C	1.37626600	-2.47365200	2.24300800
H	0.39737800	-2.97295600	4.11285600	C	5.08094500	-2.61120300	1.73045500
C	6.04293300	-3.41101300	3.81795300	C	3.62856200	-3.13236600	3.63860500
H	4.64418600	-3.81454500	5.39850900	C	1.35115600	-2.89870500	3.59231700
H	6.90917900	-3.68655200	4.40834500	C	3.77733100	-2.69130500	2.27635800
N	2.42611600	-3.22980300	4.27435300	H	0.43384900	-2.23483000	1.75766700
N	2.06443400	-0.57175900	-0.08959200	H	3.60440300	-1.87609300	-0.26326100
H	1.10980600	-0.35961700	0.21883300	O	7.39533900	-2.84864500	1.85062700
C	2.90003600	0.51963900	-0.24790500	C	8.58258000	-3.10269200	2.58762600
S	4.51019400	0.36944400	-0.76002200	H	9.40560600	-2.90665700	1.89834300
N	2.25427500	1.68850100	-0.00776500	H	8.67082200	-2.43536900	3.45437600
H	1.23420500	1.58486000	0.15602300	H	8.63643500	-4.14608000	2.92532500
C	2.68161400	3.02062700	-0.16665100	C	-4.66384200	-5.24765600	-1.88585700
C	1.68369300	3.95146700	-0.48770500	C	-4.68070400	-4.86685900	-0.55235300
C	3.99226900	3.46779100	0.04957100	C	-3.85938700	-3.81966300	-0.08571500
C	1.99575700	5.30199600	-0.61890700	C	-2.98839100	-3.17791000	-1.00825500
H	0.67007800	3.60266000	-0.65049300	C	-2.99316500	-3.57107900	-2.35737500
C	4.28513000	4.82561400	-0.08612300	C	-3.82421400	-4.58971400	-2.79997400
H	4.76810000	2.76842200	0.32504700	H	-4.52126400	-3.93255900	1.99080500
				H	-5.31126400	-6.05167300	-2.22658600

H	-5.34135400	-5.37022100	0.14986700	O	-0.66708000	1.84235800	-1.57689000
C	-3.88076100	-3.39505300	1.29580700	C	-1.40641700	2.23164000	-2.79286600
C	-2.05908400	-2.13794500	-0.53320200	C	-7.73674800	0.76749000	1.12772400
H	-2.35431700	-3.03161000	-3.04891500	C	-7.67652400	1.64919000	0.03982200
H	-3.83538000	-4.87137300	-3.84941600	C	-8.73127100	0.95024900	2.09325700
C	-2.29118400	-1.58847900	0.79864000	C	-8.58996600	2.69598900	-0.07110500
C	-3.12698300	-2.34626000	1.71326100	H	-6.91454900	1.50485600	-0.72169900
H	-1.42849200	-1.07681500	1.21636400	C	-9.65078200	1.99623500	1.98165900
H	-3.16423700	-2.02613600	2.75134900	H	-8.79046700	0.26765100	2.93905300
O	-1.10511200	-1.73776000	-1.25132600	C	-9.57978900	2.87328300	0.89991000
C	-4.61954300	0.59673400	2.21851100	H	-8.53238200	3.37347000	-0.91903800
C	-3.27408600	0.76726700	1.82896100	H	-10.41678100	2.12621100	2.74178900
C	-2.37286800	1.35545800	2.71072000	H	-10.29081200	3.69043700	0.81159400
C	-2.82176700	1.76396300	3.97430700	C	-1.96973200	1.00094300	-3.51393600
C	-4.15457100	1.58253800	4.34580700	H	-2.75275900	0.51886700	-2.92908600
C	-5.07704900	0.99645100	3.46894100	H	-2.37680800	1.30920800	-4.48431000
C	-4.56476700	-0.19822900	0.06099900	H	-1.17082300	0.27263600	-3.69705100
C	-3.13517000	0.23187000	0.43397600	C	-0.31586100	2.88753800	-3.64878900
H	-1.33987500	1.48608200	2.41122400	H	0.08500500	3.78654100	-3.17194300
H	-2.12475300	2.22638100	4.66733400	H	0.51042800	2.18922600	-3.82042600
H	-4.49107800	1.90625300	5.32725700	H	-0.73032100	3.17689700	-4.62055100
H	-6.11856000	0.88433400	3.75106400	C	-2.49297300	3.25300400	-2.44086700
N	-5.35569600	0.00492600	1.17994900	H	-2.05722300	4.10331500	-1.90405300
C	-6.75608000	-0.38785000	1.23209000	H	-2.95365200	3.63251300	-3.36042400
H	-6.89078600	-1.07597300	0.39133400	H	-3.26873700	2.79840900	-1.82253200
H	-6.93001800	-0.94926700	2.15789300	H	1.94083400	-4.51919400	-4.34735800
O	-4.95978700	-0.62628400	-1.00826100	C	1.11303500	-6.03250400	-3.12098900
N	-2.47708700	0.81597200	-0.59535800	H	0.75659400	-6.29396400	-2.12390900
C	-1.20409600	1.16741000	-0.52031400	C	1.01072700	-6.92827500	-4.10294000
O	-0.37914900	0.92928100	0.41058000	H	1.34066300	-6.70913200	-5.11657200

H 0.59212400 -7.91584400 -3.93217800 H 0.68930700 -1.72881100 -1.91716000

Transition State-2 (TS-2, Si face) for N1-benzylisatin ketimine

B3LYP/6-31G(d) level of theory:

Charge: 0

Spin Multiplicity: 1

Imaginary frequency: -282.30 cm-1

Electronic Energy (au): -3983.88001671

Electronic Energy (au): -3983.49851599 at M06-2X/6-311+G(d,p)// B3LYP/6-31G(d) level of theory

				C	3.75971100	-1.16064200	1.43563800
C	2.57999200	-2.71730700	-0.13675100	C	7.49458700	-1.00451400	0.87253100
C	3.72912500	-4.35638400	-1.69444800	H	5.84584300	-1.02324400	-0.44764500
C	3.71805100	-3.76938400	-0.26718100	C	7.03717700	-0.99424600	3.24403800
H	1.91837100	-2.95272100	0.70209600	H	2.86257400	-1.03955300	4.71654200
H	4.68103900	-3.29938300	-0.05180100	C	7.95099800	-0.97883500	2.21581400
H	3.58980700	-4.56376000	0.47424500	H	7.35700800	-0.96264800	4.28064800
C	2.39693700	-2.43426500	-2.62662300	H	9.01085600	-0.93655100	2.43839500
H	1.71345200	-2.67053300	-3.44562300	N	4.81122000	-1.03853500	4.07747600
H	2.53408700	-1.35198300	-2.59144500	N	2.10016700	-0.27158700	-0.18978600
C	3.73557200	-3.20398500	-2.72001300	H	1.33839800	-0.23257400	0.49194400
H	3.86735200	-3.59650200	-3.73351600	C	2.40092600	0.94551500	-0.78220200
H	4.57454900	-2.52652800	-2.52849300	S	3.65263800	1.11652800	-1.90518400
H	4.61238300	-4.98775500	-1.82859700	N	1.56024500	1.92371400	-0.35080100
C	2.44246600	-5.19313000	-1.93225000	H	0.93556400	1.63147300	0.42043100
C	1.25174200	-4.30808200	-1.48875200	C	1.39521300	3.26939800	-0.72420200
H	0.41340700	-4.31945800	-2.18440100	C	0.67244900	4.06111900	0.18295200
H	0.86336900	-4.59830400	-0.50956700	C	1.84954400	3.84084700	-1.92164200
N	1.69169000	-2.86309900	-1.36347000	C	0.41679600	5.40041000	-0.10152200
C	3.12770700	-1.27753500	0.04121100	H	0.31313100	3.62250700	1.11046500

C	1.58415300	5.18456500	-2.18427400	H	-3.27397200	-4.52937000	2.94449800
H	2.40058800	3.24503700	-2.63414700	H	-4.92967500	-7.06337800	-0.77085900
C	0.87050000	5.97796800	-1.28612100	H	-4.42157000	-6.17547400	1.47911600
H	0.66915400	7.01890800	-1.50561500	C	-2.88128000	-4.01692600	2.07053000
C	2.12568900	5.80771400	-3.44528900	C	-1.71085400	-2.81445400	-0.24993700
C	-0.39404500	6.20466600	0.87979600	H	-2.50191000	-3.97342700	-2.53886400
F	1.31484900	6.78785200	-3.90490500	H	-3.99052300	-5.96439200	-2.79872400
F	3.34007600	6.36841700	-3.24229100	C	-1.69047400	-2.12613600	1.04090800
F	2.26931600	4.90252100	-4.43679400	C	-2.17101600	-2.87109000	2.19955800
F	-0.34387400	7.52740200	0.62118100	H	-0.78992400	-1.53289800	1.18115400
F	-1.70001900	5.84390200	0.86220800	H	-2.00638600	-2.43648100	3.18094700
F	0.03995700	6.02472600	2.15010600	O	-0.97161500	-2.46183800	-1.20592700
C	2.94804200	-1.12981400	2.55147100	C	-4.02531800	-0.46417900	-1.05856800
C	6.13839400	-1.05870000	0.59532900	C	-2.78006300	-0.08139600	-0.51804200
C	5.64246200	-1.04443500	2.99685700	C	-1.85050800	0.55352400	-1.33256500
C	3.51647500	-1.06405000	3.84605600	C	-2.17133900	0.81192600	-2.67163300
C	5.17861600	-1.09058700	1.63584600	C	-3.40753000	0.42506800	-3.18893900
H	1.86456200	-1.12617800	2.46247600	C	-4.35633800	-0.22216500	-2.38663800
H	3.88586100	-1.09310900	-0.71829800	C	-4.18631700	-1.02016800	1.16520900
O	8.32311600	-0.97786200	-0.20929700	C	-2.76240000	-0.47434000	0.92930600
C	9.72068600	-0.83097200	-0.00018800	H	-0.88575400	0.83213800	-0.93113300
H	10.16589700	-0.79368900	-0.99583100	H	-1.45011800	1.31639200	-3.30833700
H	9.95356600	0.09849500	0.53464700	H	-3.64819400	0.63369800	-4.22818600
H	10.14075900	-1.68272500	0.55058800	H	-5.32835600	-0.49441800	-2.78381100
C	-4.28813300	-6.19195000	-0.66658300	N	-4.81784900	-1.06474700	-0.06810300
C	-4.00391600	-5.69477800	0.59771900	C	-6.15450400	-1.61348100	-0.24705100
C	-3.18367300	-4.55963800	0.76343600	H	-6.14304900	-2.28689800	-1.11212900
C	-2.63878100	-3.94810300	-0.39977700	H	-6.33679200	-2.21871000	0.64656700
C	-2.92746000	-4.47066900	-1.67244500	O	-4.69295900	-1.34555200	2.22281200
C	-3.75456700	-5.57622400	-1.81161200	N	-2.35889700	0.35830100	1.94217900

C	-1.15125100	0.88313300	1.99764600	C	-3.05095700	3.13313300	2.99812600
O	-0.11775700	0.53082900	1.34624200	H	-2.64929900	3.87341400	2.29833200
O	-0.91479200	1.89354400	2.87619500	H	-3.62668100	2.39119300	2.44305600
C	-1.92000900	2.46705700	3.78903800	H	-3.72256500	3.65396800	3.69093300
C	-7.24834800	-0.57112600	-0.40552300	C	-1.10441900	3.52161200	4.54568800
C	-7.42500800	0.42201200	0.56779700	H	-0.71518400	4.28123600	3.86120800
C	-8.11368200	-0.60497000	-1.50325400	H	-1.73479500	4.01992800	5.29002600
C	-8.44252000	1.36537500	0.43610400	H	-0.25948000	3.05565800	5.06356700
H	-6.76515300	0.44547200	1.43107700	H	2.36288600	-5.38383900	-3.00984000
C	-9.13734300	0.33674900	-1.63460700	C	2.42900800	-6.52551300	-1.22927400
H	-7.98880500	-1.37575700	-2.26163900	H	2.46812200	-6.50017400	-0.13938800
C	-9.30168000	1.32618200	-0.66582100	C	2.36983000	-7.70432500	-1.84892900
H	-8.56845700	2.13120900	1.19697500	H	2.31743400	-7.78080100	-2.93316700
H	-9.80043700	0.29831700	-2.49504100	H	2.36984400	-8.63946900	-1.29644600
H	-10.09428100	2.06294300	-0.76636600	H	0.80182200	-2.32352600	-1.23386700
C	-2.43985300	1.39937100	4.75898700				
H	-1.60073600	0.91475700	5.27187100				
H	-3.06944800	1.87615100	5.51953800				
H	-3.02464700	0.64115100	4.23655500				

Transition State (*Re* face) for N1-phenylisatin ketimine

B3LYP/6-31G(d) level of theory:

Charge: 0

Spin Multiplicity: 1

Imaginary frequency: -277.90 cm⁻¹

Electronic Energy (au): -3944.56759875

Electronic Energy (au): -3944.19942896 at M06-2X/6-311+G(d,p)// B3LYP/6-31G(d) level of theory

C	0.85627200	-3.12357200	-0.83026700	C	2.84885100	-0.06450500	-0.22727300
C	1.60724100	-4.76388200	-2.60530200	S	4.36356500	-0.63067100	-0.74051600
C	1.31587100	-4.58152800	-1.10127100	N	2.54066600	1.22987600	0.03836100
H	-0.12701300	-3.09204000	-0.36042100	H	1.52957300	1.40178000	0.19996700
H	2.21829900	-4.79776900	-0.52115100	C	3.31225200	2.40076700	-0.08818700
H	0.55382300	-5.29112200	-0.76555900	C	2.60317100	3.57283000	-0.38793700
C	1.88756400	-2.28668900	-2.97414600	C	4.69284800	2.47494500	0.14104900
H	1.58493400	-1.89863400	-3.95002700	C	3.26670300	4.79273800	-0.48454200
H	2.51116000	-1.54155600	-2.47912200	H	1.53445600	3.51297700	-0.56089600
C	2.58489600	-3.66352400	-3.06785300	C	5.34032000	3.70754600	0.03911300
H	2.90515100	-3.84652400	-4.09863400	H	5.25013500	1.58700500	0.40213600
H	3.48680600	-3.66552600	-2.44642400	C	4.64317900	4.87384700	-0.27642700
H	2.03932600	-5.75311400	-2.78262700	H	5.15764700	5.82459200	-0.34190600
C	0.29864700	-4.61150200	-3.42916200	C	6.83322600	3.76757800	0.23409600
C	-0.37013100	-3.28836000	-2.97434100	C	2.48380200	6.01176100	-0.89139400
H	-0.69663700	-2.67182300	-3.81413600	F	7.23211200	4.98014000	0.68146300
H	-1.23516600	-3.44554900	-2.33005000	F	7.26421400	2.84626400	1.12258800
N	0.61546700	-2.45939400	-2.17997000	F	7.49736700	3.53945600	-0.92262100
C	1.87450600	-2.33844000	0.03946800	F	3.09583800	7.15690900	-0.52438100
C	1.74638500	-2.82231300	1.48984800	F	2.31783400	6.06726900	-2.23795700
C	5.07253300	-4.39808200	2.34651900	F	1.24303400	6.01969500	-0.35266300
H	4.37740000	-3.35190600	0.64640700	C	0.56204700	-2.63372000	2.17215300
C	3.57136200	-4.61581900	4.22666900	C	4.09842800	-3.72896400	1.62352500
H	-0.52052700	-2.93721700	4.02695800	C	2.55180900	-3.93322300	3.51780700
C	4.80413800	-4.85255200	3.66356100	C	0.42008100	-3.09705800	3.50165600
H	3.34202600	-4.94288200	5.23576700	C	2.81792300	-3.48580300	2.17581900
H	5.56373300	-5.37600500	4.23270100	H	-0.28149100	-2.13179600	1.70564600
N	1.36451300	-3.73484600	4.15864300	H	2.87519300	-2.56048100	-0.32744900
N	1.74935700	-0.89293400	-0.09463200	O	6.26631300	-4.57686800	1.71378900
H	0.88322100	-0.43995600	0.21535800	C	7.33995000	-5.17156200	2.42836700

H	8.18895500	-5.16795500	1.74272200	H	-1.50515400	2.92796100	4.68573400
H	7.59763600	-4.59391600	3.32526800	H	-3.86685700	3.27328800	5.35795700
H	7.11333200	-6.20681800	2.71561100	H	-5.71999900	2.70245300	3.80795400
C	-5.97918000	-3.45712000	-2.07093600	N	-5.25395200	1.64920400	1.22450200
C	-5.91573500	-3.13596000	-0.72337100	O	-5.01094400	0.99700600	-0.99567700
C	-4.84247100	-2.38111600	-0.20693800	N	-2.24816800	1.69171800	-0.55011800
C	-3.80705400	-1.97763100	-1.09398200	C	-0.92744600	1.67813700	-0.47469600
C	-3.89480500	-2.30382100	-2.45821100	O	-0.20007200	1.20322500	0.44641400
C	-4.96945800	-3.03010300	-2.94947100	O	-0.22534900	2.20452800	-1.51887800
H	-5.55432500	-2.37617500	1.85536400	C	-0.82823400	2.81171700	-2.72064100
H	-6.82025300	-4.03171900	-2.45050400	C	-1.71080600	1.80290100	-3.46586000
H	-6.70697500	-3.45445000	-0.04882100	H	-2.59821600	1.54541400	-2.88817300
C	-4.77241200	-2.01861800	1.19025800	H	-2.01402200	2.23373400	-4.42749200
C	-2.63444700	-1.25750000	-0.56890300	H	-1.14623400	0.88490700	-3.66764900
H	-3.11691500	-1.94069500	-3.12182400	C	0.40091000	3.16141500	-3.56829700
H	-5.03810000	-3.25858000	-4.00963000	H	1.03637300	3.89942200	-3.07045800
C	-2.73214900	-0.71294200	0.78118700	H	1.00019600	2.26595700	-3.76552200
C	-3.76417900	-1.23890200	1.65691500	H	0.08257600	3.58212000	-4.52823100
H	-1.77163800	-0.46891400	1.22643700	C	-1.59055700	4.08476200	-2.33802200
H	-3.73090800	-0.95933600	2.70688900	H	-0.93641400	4.77050000	-1.78766600
O	-1.59196000	-1.11233400	-1.26112600	H	-1.93201500	4.59666300	-3.24527100
C	-4.37160300	1.99958500	2.27124700	H	-2.45976000	3.84725400	-1.72253300
C	-3.03369400	1.80719600	1.87093300	H	0.58479600	-4.52220400	-4.48454500
C	-1.99860400	2.14119200	2.74086700	C	-0.65019500	-5.77575100	-3.30907400
C	-2.30723900	2.66573800	4.00181300	H	-1.07138800	-5.96102300	-2.32023500
C	-3.63688300	2.85727400	4.38055600	C	-0.99753900	-6.56968200	-4.32204700
C	-4.68973900	2.52960800	3.51778500	H	-0.61405200	-6.41665900	-5.32895500
C	-4.53338300	1.27212800	0.08505200	H	-1.68000200	-7.40339600	-4.18472600
C	-3.04393000	1.28650600	0.46708900	H	0.14191300	-1.56382400	-1.97264800
H	-0.97198100	1.99255400	2.42884800	C	-6.67434800	1.62971500	1.30076900

C	-7.43848400	2.21314800	0.28307200	H	-6.71624800	0.52884300	3.15233100
C	-7.31204400	1.00675900	2.38141200	C	-9.46899100	1.57348400	1.44188900
C	-8.83023700	2.17624200	0.35654200	H	-9.41718400	2.62860300	-0.43821200
H	-6.94057000	2.67712600	-0.55944000	H	-9.19074900	0.50888900	3.29816400
C	-8.70454800	0.98996700	2.45357100	H	-10.55394800	1.55536900	1.49709000

Transition State (*Si* face) for N1-phenylisatin ketimine

B3LYP/6-31G(d) level of theory:

Charge: 0

Spin Multiplicity: 1

Imaginary frequency: -283.32 cm⁻¹

Electronic Energy (au): -3944.56369980

Electronic Energy (au): -3944.19250544 at M06-2X/6-311+G(d,p)// B3LYP/6-31G(d) level of theory

				H	-1.12825400	-3.94408900	-2.32061900
C	1.39929500	-3.23851000	-0.18197400	H	-0.85988300	-4.36940400	-0.63744800
C	1.94416100	-5.15006100	-1.74863600	N	0.55311200	-3.04588500	-1.43394900
C	2.08851200	-4.62636700	-0.30549700	C	2.41523500	-2.08698500	0.03384600
H	0.67239900	-3.22978500	0.63549000	C	3.00364300	-2.20489400	1.44688400
H	3.14471400	-4.54023300	-0.03846600	C	6.55833400	-3.40747300	0.99054900
H	1.63935400	-5.33908800	0.39291000	H	5.05304700	-2.83445500	-0.37588300
C	1.40106600	-2.87357800	-2.66931400				
H	0.70349100	-2.84416500	-3.50977500	C	6.06604400	-3.22683800	3.34828900
H	1.90810600	-1.90924200	-2.60559700	H	2.11299500	-1.76413400	4.70194600
C	2.38578500	-4.06253300	-2.74886000	C	6.95358000	-3.54477200	2.34638500
H	2.39932400	-4.46467500	-3.76724000	H	6.34531600	-3.31019200	4.39370200
H	3.40368400	-3.72582900	-2.52597200	H	7.95029600	-3.88717300	2.59963200
H	2.55496300	-6.04948300	-1.87765000	N	3.94992400	-2.46439700	4.11815900
C	0.45074600	-5.47776600	-2.02072600	N	1.81753400	-0.78143000	-0.21343200
C	-0.36599000	-4.23894000	-1.60064500	H	1.09188400	-0.47941000	0.44129000

C	2.54880000	0.25288100	-0.77723600	H	9.17885200	-4.18324900	-0.79912500
S	3.82448400	-0.02957800	-1.85052300	H	9.25902300	-3.27253000	0.73302000
N	2.08659600	1.46462900	-0.36650200	H	8.78613600	-5.00000100	0.73756300
H	1.36248000	1.40951300	0.37024000	C	-6.15656600	-4.20999900	-0.88046700
C	2.42154700	2.78343300	-0.72240300	C	-5.77814600	-3.82647100	0.39827500
C	1.93902300	3.78055500	0.14189300	C	-4.64047400	-3.01959800	0.60750100
C	3.15405900	3.15886200	-1.85777900	C	-3.88009600	-2.62242000	-0.52720200
C	2.19169600	5.12401200	-0.12408500	C	-4.27096200	-3.02850100	-1.81561900
H	1.37399100	3.49731900	1.02656000	C	-5.40510500	-3.80714700	-1.99798300
C	3.39438000	4.51077800	-2.10413500	H	-4.80270600	-2.95671600	2.78332100
H	3.54297300	2.40471000	-2.52606100	H	-7.04251100	-4.82466100	-1.01815900
C	2.92263700	5.50522300	-1.24829100	H	-6.36658600	-4.13897600	1.25744700
H	3.12732200	6.54949800	-1.44636500	C	-4.22887900	-2.60374000	1.93089400
C	4.12663800	4.90087700	-3.36248500	C	-2.64321300	-1.84794600	-0.33188100
C	1.64503000	6.15928600	0.82294700	H	-3.67261300	-2.69889400	-2.65970600
F	5.05774700	3.98818400	-3.71015400	H	-5.71280400	-4.10370200	-2.99709800
F	3.27881700	5.01673000	-4.41241300	C	-2.44073300	-1.21333600	0.97084800
F	4.75254100	6.09181500	-3.23139300	C	-3.18422500	-1.75823700	2.10077700
F	0.29184300	6.21061100	0.77727300	H	-1.39809400	-0.95927400	1.14559500
F	1.97803300	5.88456200	2.10709900	H	-2.92246600	-1.40397800	3.09315200
F	2.10043000	7.39805500	0.54676100	O	-1.80128600	-1.74445600	-1.26202000
C	2.22449600	-1.88271900	2.53943700	C	-4.08021700	1.16731400	-1.11726000
C	5.28280800	-2.96921400	0.67476700	C	-2.77716000	1.08638500	-0.58757000
C	4.75487100	-2.77160800	3.06150200	C	-1.68805900	1.37941000	-1.40128800
C	2.73984700	-2.02345700	3.85004800	C	-1.90503600	1.76422300	-2.72953800
C	4.34584200	-2.65066600	1.68752400	C	-3.20267900	1.84813500	-3.23490600
H	1.21795400	-1.49028000	2.41932600	C	-4.31188300	1.55119500	-2.43353400
H	3.21412400	-2.17984300	-0.69969000	C	-4.40106200	0.69973700	1.11944500
O	7.37219100	-3.68454200	-0.06723200	C	-2.88085600	0.711129500	0.85766300
C	8.72073100	-4.05475200	0.18298900	H	-0.68587100	1.30141000	-1.00201900

H	-1.05724500	1.99888300	-3.36679100	H	0.34659400	-5.61489500	-3.10784200
H	-3.36366200	2.15548000	-4.26499200	C	0.01159200	-6.77377900	-1.37915100
H	-5.32021600	1.63966400	-2.82250000	H	0.64077300	-7.62347400	-1.64887500
N	-5.03442700	0.88237400	-0.11449100	C	-1.03057200	-6.99026500	-0.57545300
O	-4.95905900	0.57049500	2.18841700	H	-1.72890800	-6.21521000	-0.27123200
N	-2.20449500	1.35437300	1.86303400	H	-1.23853900	-7.98631100	-0.19555700
C	-0.88934600	1.43019500	1.90844100	H	-0.09206100	-2.23020500	-1.30653200
O	-0.04671200	0.74699700	1.24576000	C	-6.44656500	0.85646800	-0.29255000
O	-0.31330300	2.29358100	2.78683200	C	-7.00717400	0.08085700	-1.31503300
C	-1.05387900	3.16308000	3.72004000	C	-7.27638800	1.59150400	0.56233700
C	-1.89420600	2.32231200	4.68812800	C	-8.38995600	0.06366100	-1.49544900
H	-1.26310500	1.57656200	5.18572400	H	-6.36176700	-0.51816000	-1.94942200
H	-2.31794700	2.97487400	5.46050300	C	-8.65864600	1.55324500	0.38391600
H	-2.70581000	1.81272900	4.16731600	H	-6.83696600	2.17430000	1.36276900
C	-1.89933300	4.18276200	2.94984300	C	-9.22046200	0.79850300	-0.64768100
H	-1.27646100	4.74872000	2.24941200	H	-8.81766300	-0.53756300	-2.29340100
H	-2.69847200	3.68644900	2.39744000	H	-9.29799600	2.12366200	1.05226400
H	-2.34662300	4.89363700	3.65461300	H	-10.29798100	0.77916100	-0.78647400
C	0.08057000	3.86759400	4.47240900				
H	0.69785900	4.45611300	3.78731300				
H	-0.33320700	4.54301600	5.22898800				
H	0.72135100	3.13570800	4.97528900				

Transition State (Re face) for N1-methylisatin ketimine

B3LYP/6-31G(d) level of theory:

Charge: 0

Spin Multiplicity: 1

Imaginary frequency: -277.40 cm⁻¹

Electronic Energy (au): -3752.83267660

Electronic Energy (au): -3752.49179172 at M06-2X/6-311+G(d,p)// B3LYP/6-31G(d) level of theory

C	0.71356300	2.94544700	-0.83594000	H	-3.33538200	6.82772300	3.77219100
C	0.64159100	4.62880900	-2.72453000	N	0.06985700	3.88880900	4.08379000
C	0.74586600	4.45593100	-1.19461700	N	-0.89766100	1.14351200	-0.13605900
H	1.59846000	2.64759400	-0.27263400	H	-0.25427200	0.45526500	0.26759900
H	-0.08846800	4.96833000	-0.70588500	C	-2.19491700	0.70626000	-0.33835800
H	1.66078200	4.92025500	-0.81468100	S	-3.40112400	1.70011000	-0.99775900
C	-0.34175200	2.33111700	-3.04285300	N	-2.34493300	-0.60101900	-0.00822900
H	-0.08840100	1.81768100	-3.97387500	H	-1.45926100	-1.08222100	0.24100700
H	-1.19914700	1.83313600	-2.59022800	C	-3.44753700	-1.46316800	-0.16238200
C	-0.58328500	3.84557500	-3.24122400	C	-3.14517200	-2.81440600	-0.38123300
H	-0.75165700	4.05717600	-4.30205800	C	-4.78723300	-1.07230500	-0.03213300
H	-1.48880700	4.14949000	-2.70528400	C	-4.16529700	-3.75496500	-0.49485800
H	0.54508800	5.68976000	-2.97307400	H	-2.10770500	-3.11345600	-0.47918300
C	1.90317000	4.04282200	-3.41790200	C	-5.79574900	-2.02993600	-0.14944900
C	2.10345400	2.61182800	-2.85508100	H	-5.03655900	-0.04007400	0.16584800
H	2.30010700	1.87491500	-3.63606600	C	-5.50179700	-3.37347800	-0.38452900
H	2.91770900	2.54750700	-2.13342100	H	-6.29467000	-4.10709900	-0.46376400
N	0.85153800	2.16228400	-2.13445100	C	-7.23596900	-1.59580600	-0.06232500
C	-0.56275300	2.55871800	-0.04025500	C	-3.80241400	-5.17947400	-0.81681600
C	-0.39200600	3.03804700	1.40742400	F	-7.39194500	-0.51073200	0.72613800
C	-3.05823200	5.66050200	1.95100600	F	-7.73463700	-1.27470800	-1.27869000
H	-2.62610800	4.36998300	0.33365200	F	-8.02401900	-2.57610300	0.43587700
C	-1.71674000	5.45080800	3.94899400	F	-4.77517900	-6.04604200	-0.46525400
H	1.58878400	2.51093600	4.12543000	F	-3.58758300	-5.34629200	-2.14717000
C	-2.75358200	6.05776600	3.27868400	F	-2.66520000	-5.56546500	-0.19441900
H	-1.46787000	5.72736200	4.96852600	C	0.60903600	2.50102800	2.19050000

C	-2.31220100	4.67497700	1.32527400	C	2.60917700	-2.90149100	2.22642200
C	-0.93265600	4.43922100	3.34097100	C	1.48861300	-2.84175300	3.04825500
C	0.79635500	2.94840500	3.51973900	C	1.55835600	-3.38434900	4.33960900
C	-1.23093800	4.04649300	1.98855000	C	2.73718700	-3.97213200	4.79989000
H	1.27160500	1.73071400	1.80474600	C	3.87496300	-4.04392500	3.98463400
H	-1.41135800	3.06901200	-0.49249700	C	4.31524100	-2.91893600	0.54490100
O	-4.07229200	6.19696100	1.21527200	C	2.87638700	-2.44446000	0.82257600
C	-4.93531300	7.14654400	1.82396500	H	0.58086100	-2.37700100	2.68251000
H	-5.68263600	7.39340400	1.06798400	H	0.68625600	-3.34318800	4.98587300
H	-5.43803400	6.72915400	2.70571200	H	2.77887900	-4.38550800	5.80423000
H	-4.39764600	8.06002200	2.11042000	H	4.78792600	-4.51055400	4.34169000
C	7.40370100	1.07894100	-1.37067900	N	4.78212500	-3.49420400	1.71656800
C	7.11323500	0.81903600	-0.03982600	C	6.11218000	-4.04440800	1.85345200
C	5.81286900	0.44805900	0.36095400	H	6.62100900	-3.89843900	0.89906400
C	4.79335300	0.37306700	-0.62762700	H	6.66974500	-3.53154700	2.64644500
C	5.11035400	0.62916600	-1.97259700	O	4.94000100	-2.83149400	-0.49479000
C	6.40049400	0.97268700	-2.34843100	N	2.05806600	-2.59537400	-0.24401000
H	6.28536700	0.25917400	2.48293400	C	0.80761100	-2.16326500	-0.25213800
H	8.41462100	1.35545500	-1.65936500	O	0.22034300	-1.44905600	0.61275000
H	7.89529600	0.88980200	0.71274600	O	0.03391000	-2.47596500	-1.33096500
C	5.49875800	0.15222500	1.73999700	C	0.48012100	-3.28300500	-2.48299700
C	3.40810000	0.07011500	-0.22775400	C	1.67116000	-2.62294400	-3.18806300
H	4.32523900	0.51623000	-2.71285300	H	2.55692700	-2.61807200	-2.55322000
H	6.63870400	1.14826500	-3.39402000	H	1.88891500	-3.16958100	-4.11329300
C	3.19759000	-0.44388300	1.12056800	H	1.42507300	-1.58831000	-3.45569800
C	4.25516900	-0.25810000	2.09737500	C	-0.74994200	-3.26435400	-3.39879500
H	2.17193700	-0.35898000	1.46877500	H	-1.60681800	-3.75988000	-2.93314600
H	4.03558400	-0.49312400	3.13569000	H	-1.03514000	-2.23471900	-3.64025100
O	2.44593500	0.24432700	-1.02253400	H	-0.52400600	-3.78798000	-4.33388400
C	3.78979000	-3.50914600	2.70426700	C	0.78540200	-4.71562600	-2.03294000

H	-0.07494400	-5.13842600	-1.50157500	C	3.79759000	5.46540500	-4.25506500
H	0.98356300	-5.34280600	-2.90993100	H	3.46580700	5.37215100	-5.28732000
H	1.65873200	-4.74061400	-1.37935100	H	4.68785900	6.06366800	-4.08417800
H	1.68681600	3.97754000	-4.49151600	H	1.01520100	1.17898700	-1.85592200
C	3.14773000	4.87562600	-3.25157500	H	6.07223200	-5.11586300	2.08448200
H	3.52663900	4.98698400	-2.23492300				

Transition State (*Si* face) for N1-methylisatin ketimine

B3LYP/6-31G(d) level of theory:

Charge: 0

Spin Multiplicity: 1

Imaginary frequency: -281.33 cm⁻¹

Electronic Energy (au): -3752.82839035

Electronic Energy (au): -3752.48472009 at M06-2X/6-311+G(d,p)// B3LYP/6-31G(d) level of theory

C	1.28539300	3.03019100	-0.22363300	C	3.29283400	4.27066600	-2.16014600
C	1.93039400	4.91421100	-1.78516000	C	3.21229300	2.78388300	-1.75929400
C	1.59097000	4.55077100	-0.32504600	H	3.59868200	2.09821000	-2.51224500
H	1.89482500	2.55486100	0.55030900	H	3.73526100	2.57204000	-0.82651700
H	0.72666900	5.12525900	0.01751900	N	1.76724700	2.39104500	-1.52034000
H	2.42949500	4.81662200	0.32600700	C	-0.21283800	2.74950500	0.06599800
C	0.92258800	2.80024600	-2.70064100	C	-0.52156700	3.16500800	1.51124700
H	1.41148500	2.37718300	-3.58153700	C	-2.60991900	6.30666000	1.26287000
H	-0.06177000	2.34116500	-2.59574800	H	-1.85024100	4.97292700	-0.18805900
C	0.85721100	4.34456300	-2.73434100	C	-2.20267900	5.79248800	3.58726900
H	1.02595800	4.69968100	-3.75632500	H	0.09613200	2.17988900	4.71013900
H	-0.14041900	4.68617500	-2.43902300	C	-2.76284300	6.61677300	2.63898700
H	1.98746100	6.00246200	-1.89116100	H	-2.31333700	5.99859800	4.64703700

H	-3.32415500	7.49024700	2.94992500	H	0.50920400	1.48349300	2.38034000
N	-0.95846800	3.87280700	4.23309600	H	-0.81798500	3.34140200	-0.61841700
N	-0.57892300	1.36485500	-0.20474300	O	-3.13868300	7.05597900	0.25446200
H	-0.18225500	0.65691100	0.41812300	C	-3.96270000	8.16550100	0.58316100
C	-1.82302000	1.03766600	-0.72524300	H	-4.29852300	8.57672000	-0.37028800
S	-2.67855300	2.09128500	-1.73470900	H	-4.83649400	7.85933300	1.17218500
N	-2.21291100	-0.20432000	-0.33120600	H	-3.40615000	8.93656300	1.13188800
H	-1.58558800	-0.63878300	0.36803000	C	7.83534400	-0.80013600	-0.91324500
C	-3.31263700	-1.01258600	-0.67053800	C	7.27092600	-0.89087600	0.35138000
C	-3.50602000	-2.13833500	0.14814400	C	5.87295600	-0.83205500	0.52853200
C	-4.18375600	-0.79422600	-1.74762500	C	5.05561600	-0.65859300	-0.62321200
C	-4.55305700	-3.02082100	-0.10550000	C	5.64408300	-0.55891300	-1.89630200
H	-2.83893000	-2.31307500	0.98876500	C	7.02107900	-0.63949500	-2.04753400
C	-5.22522100	-1.69215600	-1.98248100	H	5.91187800	-1.02312500	2.70257400
H	-4.05793300	0.07307600	-2.37878600	H	8.91511900	-0.85593400	-1.02656500
C	-5.42553000	-2.80855400	-1.17195200	H	7.90663900	-1.01779200	1.22437500
H	-6.24528100	-3.48981800	-1.36003000	C	5.26235700	-0.93318600	1.83618500
C	-6.11182800	-1.47481900	-3.18186200	C	3.59937000	-0.51233100	-0.45819400
C	-4.71983800	-4.21510500	0.79644700	H	4.99028800	-0.43935500	-2.75495600
F	-6.30879100	-0.16368200	-3.43390300	H	7.46900700	-0.58121900	-3.03582200
F	-5.57121700	-2.01262600	-4.30133200	C	3.02142100	-0.91693700	0.82256600
F	-7.32643700	-2.04537900	-3.02000300	C	3.91529600	-0.96741100	1.97300600
F	-3.66613100	-5.06149200	0.70254200	H	2.03527300	-0.48908800	0.98639700
F	-4.80520700	-3.84770500	2.09780100	H	3.46765200	-1.11022200	2.95194600
F	-5.82895500	-4.92532100	0.50709200	O	2.89202000	-0.05637300	-1.39458400
C	-0.04150200	2.40380000	2.55741500	C	2.82185700	-3.69179700	-1.38842000
C	-1.89108000	5.18837800	0.87339300	C	1.84296500	-2.87030300	-0.79071500
C	-1.46407300	4.63850300	3.22477800	C	0.78819800	-2.40048200	-1.56363600
C	-0.28817100	2.79235200	3.89583700	C	0.71225200	-2.75818000	-2.91671700
C	-1.29269900	4.33232800	1.82950600	C	1.69282900	-3.56681300	-3.49118400

C	2.76837900	-4.04587400	-2.73153000	H	5.60118200	3.48122100	-0.61667400
C	3.43360800	-3.62418600	0.82501800	H	6.29118700	5.18451100	-0.53317900
C	2.20208100	-2.70765900	0.65606900	H	1.79289100	1.34929500	-1.41315700
H	0.03987600	-1.75891000	-1.11828300	C	4.89049700	-4.96885200	-0.68608900
H	-0.11640500	-2.39901900	-3.52037100	H	4.55037800	-5.93455900	-1.08007900
H	1.62476700	-3.83627100	-4.54203400	H	5.59168700	-4.52018200	-1.39960300
H	3.52531500	-4.68412100	-3.17695000	H	5.39429000	-5.12641700	0.26909000
N	3.77183700	-4.08631900	-0.43906600				
O	4.01057500	-3.91081200	1.85555300				
N	1.30999400	-2.85106800	1.68818200				
C	0.22023900	-2.11615000	1.78983800				
O	-0.05358800	-1.04143400	1.16817700				
O	-0.73580000	-2.47962000	2.68505000				
C	-0.65145200	-3.64930500	3.57896600				
C	0.55474300	-3.52594400	4.51728200				
H	0.52437700	-2.56660800	5.04725200				
H	0.51396300	-4.32599600	5.26568100				
H	1.49339400	-3.60107400	3.96670200				
C	-0.62593100	-4.94814900	2.76651300				
H	-1.48261500	-4.99167300	2.08602700				
H	0.29606000	-5.02853200	2.18891900				
H	-0.69055300	-5.80557400	3.44669100				
C	-1.95788600	-3.54124200	4.37342400				
H	-2.82595300	-3.61075200	3.71112100				
H	-2.01891500	-4.35242700	5.10702200				
H	-2.00498000	-2.58667200	4.90804100				
H	3.38562900	4.33468100	-3.25508300				
C	4.47271800	5.01756300	-1.58243400				
H	4.46625500	6.08356400	-1.81519000				
C	5.49342400	4.53132300	-0.87469000				

References

1. M. Montesinos-Magraner, C. Vila, R. Canton, G. Blay, I. Fernandez, M. C. Munoz, J. R. Pedro, *Angew. Chem. Int. Ed.*, 2015, **54**, 632