

# Enantioselective Synthesis of Tetrahydrofuran Spirooxindoles via Domino Oxa-Michael/Michael Addition Reaction using a Bifunctional Squaramide Catalyst

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## Supplementary Material

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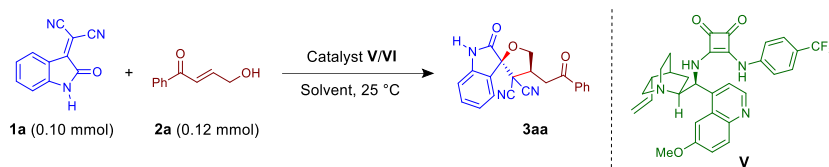
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## General Methods

All reactions were carried out in a closed vial.  $^1\text{H}$  NMR spectra (400 or 500 MHz) and  $^{13}\text{C}$  NMR spectra (100 or 125 MHz) were recorded using acetone- $d_6$  and  $\text{CDCl}_3$  as the solvent, crude was recorded using  $\text{DMSO}-d_6$ , unless specified. TLC was performed with silica gel GF254 precoated on aluminium plates and spots were visualized with UV. Flash column chromatography was performed on silica gel. IR spectra were recorded on an FT-IR spectrometer, and only major peaks were reported in  $\text{cm}^{-1}$ . High-resolution mass spectra (HRMS) were obtained by the ESI-TOF method. Melting points were recorded on a digital melting point apparatus and are uncorrected. The enantiomeric ratio was determined by chiral HPLC analysis with Chiralpak IA3 column. Substrates **1**<sup>1</sup> and **2**<sup>2</sup> were prepared following known procedures. Catalysts **I** was commercially available. Catalysts **II-XII** were synthesized following reported methods.<sup>3</sup> All the other reagents were purchased from commercial sources and used as received unless specified.

## Optimization Table and Experimental Details

**Table S1.** Selected entries for solvent screening<sup>a</sup>



Entry	Solvent	Cat.	Time	Yield <sup>b</sup>	dr <sup>c</sup>	ee <sup>d</sup>
1	Xylene	<b>V</b>	48	85	7:1	64
2	Mesitylene	<b>V</b>	48	83	7:1	64
3	Nitrobenzene	<b>V</b>	12	85	5:1	39
4	Chlorobenzene	<b>V</b>	12	82	7:1	52
5	Trifluorotoluene	<b>V</b>	12	81	7:1	54
6	<i>m</i> -Xylene	<b>V</b>	48	85	7:1	68
7	<i>p</i> -Xylene	<b>V</b>	48	83	6:1	51
8	Anisole	<b>V</b>	40	71	7:1	63

<sup>a</sup>Reaction conditions: **1a** (0.10 mmol), **2a** (0.12 mmol), catalyst (0.01 mmol), solvent (1 mL), 25 °C, unless specified.

<sup>b</sup>Calculated yield using internal standard (major diastereomer).

<sup>c</sup>Determined by  $^1\text{H}$  NMR analysis of the crude reaction mixture.

<sup>d</sup>Determined by chiral HPLC analysis (major diastereomer).

**General procedure for Enantioselective Synthesis of Tetrahydrofuran Spirooxindoles:** To a vial were added the chiral catalyst (0.01 mmol, 10 mol %), and Isatylidene Malononitriles **2** (0.10 mmol) in 1 mL Benzene.  $\gamma$ -Hydroxyenones (0.12 mmol) was then added and the mixture was stirred at 25 °C for the time as specified in Table. Upon the completion of the reaction (monitored by TLC), the diastereomeric ratio was determined by the  $^1\text{H}$  NMR analysis of the crude product. Then the solvent was evaporated off and the crude product **3** was purified by flash column chromatography over silica gel (eluent: EtOAc/hexane = 1:4). Enantiomeric ratio was determined by chiral HPLC analysis.

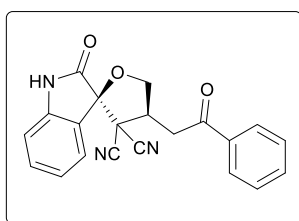
**Procedure for gram-scale reaction:** To a round bottom flask was added the chiral catalyst **VI** (0.05 mmol, 10 mol %), and Isatylidene Malononitriles **2** (0.50 mmol) in 5 mL Benzene.  $\gamma$ -Hydroxyenones (0.60 mmol) was then added and the mixture was stirred at 25 °C overnight. Upon the completion of the reaction (monitored by TLC), the diastereomeric ratio was determined by the  $^1\text{H}$  NMR analysis of the crude product. Then the solvent

was evaporated off and the crude product **3** was purified by flash column chromatography over silica gel (eluent: EtOAc/hexane = 1:4). 84% yield.

**Procedure for Synthetic transformation reaction:** To an oven dried round bottom flask cooled under hydrogen, diastereomeric pure compound **3aa** was taken, dissolved in dry methanol, and was cooled to 0 °C under inert atmosphere. To the solution, Sodium borohydride was added slowly, and the reaction mixture was allowed to stir at 0 °C for 30 mins. After the reaction was completed (monitored by TLC), reaction mixture was quenched with water and organic layer was separated. crude product **4aa** was purified by flash column chromatography over silica gel (eluent: EtOAc/hexane = 1:3)

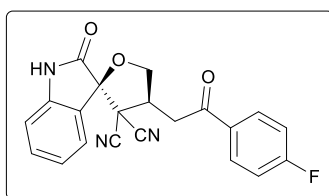
## Characterization Data of Compounds

### **3aa:(2R,4S)-2'-oxo-4-(2-oxo-2-phenylethyl)-4,5-dihydro-3H-spiro[furan-2,3'-indoline]-3,3-dicarbonitrile**



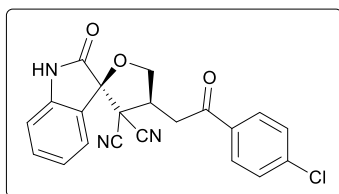
The compound **3aa** was isolated as white solid; in 88% (62.9 mg) yield, 80% ee and 9:1 dr, mp 234-236 °C;  $[\alpha]_D^{25} = -48.4$  (c 0.0025, MeOH). The enantiomeric ratio was determined by chiral HPLC using Daicel Chiralpak IA-3 column, n-hexane/2-propanol (80:20) as eluent, flow rate = 0.9 mL/min,  $\lambda = 254$  nm.  $t_R(\text{major}) = 15.591$  min,  $t_R(\text{minor}) = 44.600$  min.  $^1\text{H NMR}$  (400 MHz, ACETONE- $D_6$ )  $\delta$  10.03 (s, 1H), 8.22 – 8.07 (m, 2H), 7.77 – 7.63 (m, 2H), 7.58 (t,  $J = 7.7$  Hz, 2H), 7.51 (td,  $J = 7.9, 1.0$  Hz, 1H), 7.22 (dd,  $J = 8.0, 7.1$  Hz, 1H), 7.10 (d,  $J = 7.8$  Hz, 1H), 4.99 (t,  $J = 8.8$  Hz, 1H), 4.56 (qd,  $J = 8.6, 5.9$  Hz, 1H), 4.23 (t,  $J = 8.6$  Hz, 1H), 3.98 (dd,  $J = 18.2, 5.7$  Hz, 1H), 3.78 (dd,  $J = 18.3, 8.6$  Hz, 1H).  $^{13}\text{C NMR}$  (500 MHz,  $\delta$ ) 197.27, 174.43, 143.93, 137.11, 134.51, 133.46, 129.66, 129.11, 127.21, 123.86, 122.42, 113.10, 112.39, 111.89, 87.69, 73.51, 47.87, 43.36, 40.10.  $\nu_{\text{max}}$  (neat,  $\text{cm}^{-1}$ ): 3261, 2910, 1743, 1667, 1622, 1595, 1471, 1444, 1402, 1372, 1328, 1279, 1204, 1128, 1081; Exact mass calculated for  $[\text{C}_{21}\text{H}_{15}\text{N}_3\text{O}_3\text{Na}]^+$   $[\text{M}+\text{Na}]^+$ : 380.1006, Found: 380.0998.

### **3ab:(2R,4S)-4-(2-(4-fluorophenyl)-2-oxoethyl)-2'-oxo-4,5-dihydro-3H-spiro[furan-2,3'-indoline]-3,3-dicarbonitrile**



The compound **3ab** was isolated as white solid; in 76% (57.1 mg) yield, 80% ee and 6:1 dr, mp 178-180 °C;  $[\alpha]_D^{25} = -48$  (c 0.005, MeOH). The enantiomeric ratio was determined by chiral HPLC using Daicel Chiralpak IA-3 column, n-hexane/2-propanol (80:20) as eluent, flow rate = 0.9 mL/min,  $\lambda = 254$  nm.  $t_R(\text{major}) = 16.027$  min,  $t_R(\text{minor}) = 59.406$  min.  $^1\text{H NMR}$  (400 MHz, ACETONE- $D_6$ )  $\delta$  10.04 (s, 1H), 8.29 – 8.16 (m, 2H), 7.71 (d,  $J = 7.7$  Hz, 1H), 7.51 (td,  $J = 7.7, 1.0$  Hz, 1H), 7.33 (t,  $J = 8.8$  Hz, 2H), 7.22 (dd,  $J = 11.6, 4.4$  Hz, 1H), 7.10 (d,  $J = 7.9$  Hz, 1H), 4.99 (t,  $J = 8.8$  Hz, 1H), 4.55 (qd,  $J = 8.6, 5.7$  Hz, 1H), 4.23 (t,  $J = 8.6$  Hz, 1H), 3.98 (dd,  $J = 18.2, 5.8$  Hz, 1H), 3.77 (dd,  $J = 18.3, 8.6$  Hz, 1H).  $^{13}\text{C NMR}$  (400 MHz, ACETONE- $D_6$ )  $\delta$  195.86, 174.38, 168.07, 165.55, 143.87, 133.76, 133.45, 132.14, 132.04, 127.17, 123.83, 122.35, 116.66, 116.44, 113.04, 112.32, 111.86, 87.62, 73.44, 47.79, 43.30, 40.01.  $\nu_{\text{max}}$  (neat,  $\text{cm}^{-1}$ ): 2923, 2853, 1737, 1688, 1622, 1598, 1471, 1377, 1275, 1260, 1226, 1158; Exact mass calculated for  $[\text{C}_{21}\text{H}_{14}\text{FN}_3\text{O}_3\text{Na}]^+$   $[\text{M}+\text{Na}]^+$ : 398.0911, Found: 398.0907.

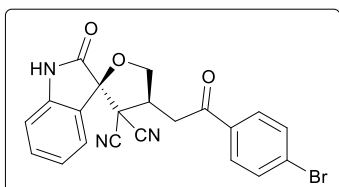
### **3ac:(2R,4S)-4-(2-(4-chlorophenyl)-2-oxoethyl)-2'-oxo-4,5-dihydro-3H-spiro[furan-2,3'-indoline]-3,3-dicarbonitrile**



The compound **3ac** was isolated as white solid; in 74% (58.0 mg) yield, 73% ee and 7:1 dr, mp 210-212 °C;  $[\alpha]_D^{25} = -62$  (c 0.005, MeOH). The enantiomeric ratio was determined by chiral HPLC using Daicel Chiralpak IA-3 column, n-hexane/2-propanol (80:20) as eluent, flow rate = 0.9 mL/min,  $\lambda = 254$  nm.  $t_R(\text{major}) = 16.881$  min,  $t_R(\text{minor}) = 72.205$  min.  $^1\text{H NMR}$  (400 MHz, ACETONE- $D_6$ )  $\delta$  10.05 (s, 1H), 8.20 – 8.10 (m, 2H), 7.71 (d,  $J = 7.7$  Hz, 1H), 7.65 – 7.57 (m, 2H), 7.51 (td,  $J = 7.9, 1.0$  Hz, 1H), 7.22 (t,  $J = 7.6$  Hz, 1H), 7.10 (d,  $J = 7.8$  Hz,

1H), 4.98 (t,  $J = 8.8$  Hz, 1H), 4.55 (qd,  $J = 8.7, 5.7$  Hz, 1H), 4.23 (t,  $J = 8.7$  Hz, 1H), 3.99 (dd,  $J = 18.3, 5.7$  Hz, 1H), 3.78 (dd,  $J = 18.3, 8.6$  Hz, 1H).  $^{13}\text{C}$  NMR (400 MHz, ACETONE- $D_6$ )  $\delta$  196.27, 174.32, 143.81, 140.12, 135.63, 133.40, 130.84, 129.75, 127.11, 123.78, 122.27, 112.96, 112.25, 111.81, 87.56, 73.35, 47.72, 43.21, 40.02.  $\nu_{\text{max}}$  (neat,  $\text{cm}^{-1}$ ): 2920, 1735, 1621, 1471, 1275, 1260, 1216; Exact mass calculated for  $[\text{C}_{21}\text{H}_{14}\text{ClN}_3\text{O}_3\text{Na}]^+$   $[\text{M}+\text{Na}]^+$ : 414.0616, Found: 414.0610

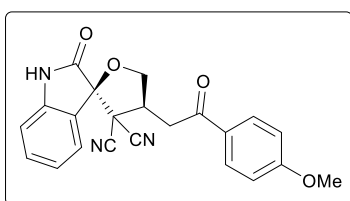
**3ad:(2R,4S)-4-(2-(4-bromophenyl)-2-oxoethyl)-2'-oxo-4,5-dihydro-3H-spiro[furan-2,3'-indoline]-3,3-dicarbonitrile**



The compound **3ad** was isolated as white solid; in 54% (47.1 mg) yield, 81% ee and 6:1 dr, mp 195-197 °C;  $[\alpha]_{\text{D}}^{25} = -52.4$  (c 0.005, MeOH). The enantiomeric ratio was determined by chiral HPLC using Daicel Chiralpak IA-3 column, n-hexane/2-propanol (80:20) as eluent, flow rate = 0.9 mL/min,  $\lambda = 254$  nm.  $t_{\text{R}}$ (major) = 18.024 min,  $t_{\text{R}}$ (minor) = 79.476 min.  $^1\text{H}$  NMR (400 MHz, ACETONE- $D_6$ )  $\delta$  10.05 (s, 1H), 8.12 – 8.02 (m, 2H), 7.83 – 7.74 (m, 2H), 7.70 (d,  $J = 7.7$  Hz, 1H), 7.51 (td,  $J = 7.9, 1.0$  Hz, 1H), 7.22 (dd,  $J = 11.6, 4.5$  Hz, 1H),

7.10 (d,  $J = 7.8$  Hz, 1H), 4.98 (t,  $J = 8.8$  Hz, 1H), 4.55 (qd,  $J = 8.7, 5.6$  Hz, 1H), 4.23 (t,  $J = 8.8$  Hz, 1H), 3.99 (dd,  $J = 18.3, 5.7$  Hz, 1H), 3.77 (dd,  $J = 18.3, 8.8$  Hz, 1H).  $^{13}\text{C}$  NMR (400 MHz, ACETONE- $D_6$ )  $\delta$  196.53, 174.36, 143.87, 136.05, 133.45, 132.83, 130.98, 128.93, 127.16, 123.83, 122.33, 113.01, 112.30, 111.86, 87.60, 73.40, 47.77, 43.25, 40.05.  $\nu_{\text{max}}$  (neat,  $\text{cm}^{-1}$ ): 3300, 2925, 2850, 1734, 1687, 1622, 1585, 1472, 1398, 1326, 1261, 1210, 1070; Exact mass calculated for  $[\text{C}_{21}\text{H}_{14}\text{BrN}_3\text{O}_3\text{Na}]^+$   $[\text{M}+\text{Na}]^+$ : 458.0111 & 460.0090, Found: 458.0107 & 460.0085

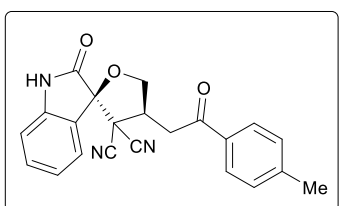
**3ae:(2R,4S)-4-(2-(4-methoxyphenyl)-2-oxoethyl)-2'-oxo-4,5-dihydro-3H-spiro[furan-2,3'-indoline]-3,3-dicarbonitrile**



The compound **3ae** was isolated as white solid; in 65% (50.4 mg) yield, 72% ee and 6:1 dr, mp 166-168 °C;  $[\alpha]_{\text{D}}^{25} = -51.0$  (c 0.005, MeOH). The enantiomeric ratio was determined by chiral HPLC using Daicel Chiralpak IA-3 column, n-hexane/2-propanol (80:20) as eluent, flow rate = 0.9 mL/min,  $\lambda = 254$  nm.  $t_{\text{R}}$ (major) = 19.371 min,  $t_{\text{R}}$ (minor) = 84.501 min.  $^1\text{H}$  NMR (500 MHz, )  $\delta$  10.02 (s), 8.10 (d,  $J = 8.9$  Hz), 7.71 (d,  $J = 7.6$  Hz), 7.50 (td,  $J = 7.7, 0.8$  Hz), 7.21 (t,  $J = 7.6$  Hz), 7.08 (t,  $J = 8.7$  Hz), 4.97 (t,  $J = 8.8$  Hz), 4.53 (qd,  $J = 8.5, 6.2$

Hz), 4.20 (t,  $J = 8.7$  Hz), 3.94 – 3.85 (m), 3.70 (dd,  $J = 18.0, 8.4$  Hz).  $^{13}\text{C}$  NMR (400 MHz, ACETONE- $D_6$ )  $\delta$  195.50, 174.40, 164.97, 143.86, 133.40, 131.40, 130.00, 127.16, 123.80, 122.40, 114.75, 113.10, 112.36, 111.83, 87.65, 73.53, 56.02, 47.85, 43.39, 39.65.  $\nu_{\text{max}}$  (neat,  $\text{cm}^{-1}$ ): 2960, 1733, 1673, 1622, 1600, 1575, 1512, 1472, 1422, 1325, 1275, 1262, 1230, 1174, 1172; Exact mass calculated for  $[\text{C}_{22}\text{H}_{17}\text{N}_3\text{O}_4\text{Na}]^+$   $[\text{M}+\text{Na}]^+$ : 410.1111, Found: 410.1107

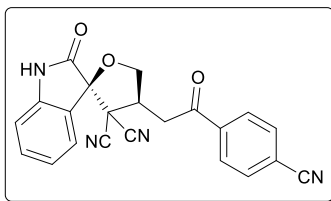
**3af:(2R,4S)-2'-oxo-4-(2-oxo-2-(p-tolyl)ethyl)-4,5-dihydro-3H-spiro[furan-2,3'-indoline]-3,3-dicarbonitrile**



The compound **3af** was isolated as white solid; in 64% (47.5 mg) yield, 75% ee and 6:1 dr, mp 190-192 °C;  $[\alpha]_{\text{D}}^{25} = -40.0$  (c 0.005, MeOH). The enantiomeric ratio was determined by chiral HPLC using Daicel Chiralpak IA-3 column, n-hexane/2-propanol (80:20) as eluent, flow rate = 0.9 mL/min,  $\lambda = 254$  nm.  $t_{\text{R}}$ (major) = 13.826 min,  $t_{\text{R}}$ (minor) = 53.770 min.  $^1\text{H}$  NMR (400 MHz, ACETONE- $D_6$ )  $\delta$  10.03 (s, 1H), 8.02 (d,  $J = 8.3$  Hz, 2H), 7.71 (d,  $J = 7.4$  Hz, 1H), 7.50 (td,  $J = 7.7, 1.0$  Hz, 1H), 7.38 (d,  $J = 8.1$  Hz, 2H), 7.21 (dd,  $J = 11.5, 4.5$  Hz, 1H), 7.09

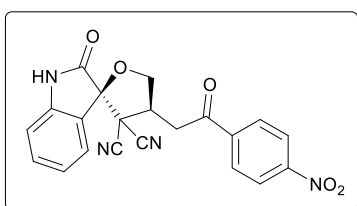
(d,  $J = 7.9$  Hz, 1H), 4.98 (t,  $J = 8.8$  Hz, 1H), 4.54 (qd,  $J = 8.6, 5.9$  Hz, 1H), 4.22 (t,  $J = 8.6$  Hz, 1H), 3.93 (dd,  $J = 18.1, 5.9$  Hz, 1H), 3.73 (dd,  $J = 18.2, 8.5$  Hz, 1H), 2.42 (s, 3H).  $^{13}\text{C}$  NMR (400 MHz, ACETONE- $D_6$ )  $\delta$  196.69, 174.38, 145.35, 143.86, 134.59, 133.41, 130.2, 129.19, 127.15, 123.80, 122.37, 113.07, 112.34, 111.83, 87.64, 73.48, 47.82, 43.32, 39.90, 21.59.  $\nu_{\text{max}}$  (neat,  $\text{cm}^{-1}$ ): 2923, 1733, 1684, 1605, 1472, 1261; Exact mass calculated for  $[\text{C}_{22}\text{H}_{17}\text{N}_3\text{O}_3\text{Na}]^+$   $[\text{M}+\text{Na}]^+$ : 394.1162, Found: 394.1160

**3ag:(2R,4S)-4-(2-(4-cyanophenyl)-2-oxoethyl)-2'-oxo-4,5-dihydro-3H-spiro[furan-2,3'-indoline]-3,3-dicarbonitrile**



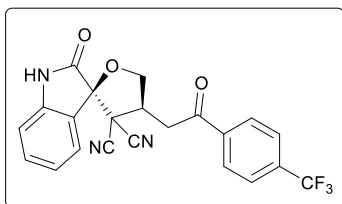
The compound **3ag** was isolated as white solid; in 65% (49.7 mg) yield, 78% ee and 6:1 dr, mp 218-220 °C;  $[\alpha]_D^{25} = -30.6$  (c 0.005, MeOH). The enantiomeric ratio was determined by chiral HPLC using Daicel Chiralpak IA-3 column, n-hexane/2-propanol (80:20) as eluent, flow rate = 0.9 mL/min,  $\lambda = 254$  nm.  $t_R(\text{major}) = 28.372$  min,  $t_R(\text{minor}) = 69.990$  min  $^1\text{H NMR}$  (500 MHz, ACETONE-D<sub>6</sub>)  $\delta$  10.03 (s, 1H), 8.31 (d,  $J = 8.5$  Hz, 2H), 8.00 (d,  $J = 8.5$  Hz, 2H), 7.71 (d,  $J = 7.6$  Hz, 1H), 7.51 (td,  $J = 7.8, 1.1$  Hz, 1H), 7.25 – 7.19 (m, 1H), 7.10 (d,  $J = 7.9$  Hz, 1H), 4.99 (t,  $J = 8.8$  Hz, 1H), 4.58 (qd,  $J = 8.7, 5.4$  Hz, 1H), 4.24 (t,  $J = 8.7$  Hz, 1H), 4.08 (dd,  $J = 18.4, 5.4$  Hz, 1H), 3.85 (dd,  $J = 18.4, 8.8$  Hz, 1H).  $^{13}\text{C NMR}$  (500 MHz, ACETONE-D<sub>6</sub>)  $\delta$  196.63, 174.25, 143.77, 140.00, 133.45, 133.38, 129.66, 127.06, 123.76, 122.21, 118.52, 117.26, 112.86, 112.18, 111.79, 87.50, 73.24, 47.67, 43.13, 40.29.  $\nu_{\text{max}}$  (neat,  $\text{cm}^{-1}$ ): 2923, 1743, 1622, 1463, 1377, 1261 1082; Exact mass calculated for  $[\text{C}_{22}\text{H}_{14}\text{N}_4\text{O}_3\text{Na}]^+$   $[\text{M}+\text{Na}]^+$ : 405.095, Found: 405.0956.

### **3ah:(2R,4S)-4-(2-(4-nitrophenyl)-2-oxoethyl)-2'-oxo-4,5-dihydro-3H-spiro[furan-2,3'-indoline]-3,3-dicarbonitrile**



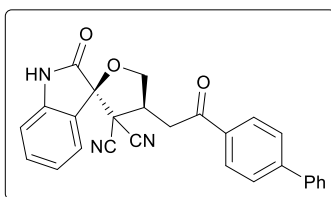
The compound **3ah** was isolated as white solid; in 65% (52.3 mg) yield, 96% ee and 6:1 dr, mp 186-188 °C;  $[\alpha]_D^{25} = -54.0$  (c 0.005, MeOH). The enantiomeric ratio was determined by chiral HPLC using Daicel Chiralpak IA-3 column, n-hexane/2-propanol (80:20) as eluent, flow rate = 0.9 mL/min,  $\lambda = 254$  nm.  $t_R(\text{major}) = 34.368$  min,  $t_R(\text{minor}) = 99.360$  min  $^1\text{H NMR}$  (400 MHz, ACETONE-D<sub>6</sub>)  $\delta$  10.07 (s, 1H), 8.52 – 8.28 (m, 4H), 7.71 (d,  $J = 7.6$  Hz, 1H), 7.51 (dt,  $J = 7.9, 4.0$  Hz, 1H), 7.22 (dd,  $J = 11.5, 4.5$  Hz, 1H), 7.10 (d,  $J = 7.9$  Hz, 1H), 5.00 (t,  $J = 8.8$  Hz, 1H), 4.59 (qd,  $J = 8.8, 5.4$  Hz, 1H), 4.26 (t,  $J = 8.6$  Hz, 1H), 4.13 (dd,  $J = 18.5, 5.3$  Hz, 1H), 3.89 (dd,  $J = 18.5, 8.9$  Hz, 1H).  $^{13}\text{C NMR}$  (400 MHz, ACETONE-D<sub>6</sub>)  $\delta$  196.58, 174.36, 151.60, 143.88, 141.58, 133.49, 130.48, 127.16, 124.67, 123.86, 122.29, 112.96, 112.28, 111.90, 87.58, 73.32, 47.75, 43.22, 40.61.  $\nu_{\text{max}}$  (neat,  $\text{cm}^{-1}$ ): 2925, 2854, 1732, 1695, 1622, 1526, 1472, 1347, 1212; Exact mass calculated for  $[\text{C}_{21}\text{H}_{14}\text{N}_4\text{O}_5\text{Na}]^+$   $[\text{M}+\text{Na}]^+$ : 425.0856, Found: 425.0850.

### **3ai:(2R,4S)-2'-oxo-4-(2-oxo-2-(4-(trifluoromethyl)phenyl)ethyl)-4,5-dihydro-3H-spiro[furan-2,3'-indoline]-3,3-dicarbonitrile**



The compound **3ai** was isolated as white solid; in 61% (51.8 mg) yield, 69% ee and 6:1 dr, mp 132-134 °C;  $[\alpha]_D^{25} = -45.4$  (c 0.005, MeOH). The enantiomeric ratio was determined by chiral HPLC using Daicel Chiralpak IA-3 column, n-hexane/2-propanol (80:20) as eluent, flow rate = 0.9 mL/min,  $\lambda = 254$  nm.  $t_R(\text{major}) = 13.686$  min,  $t_R(\text{minor}) = 49.626$  min  $^1\text{H NMR}$  (400 MHz, ACETONE-D<sub>6</sub>)  $\delta$  10.05 (s, 1H), 8.35 (d,  $J = 8.3$  Hz, 2H), 7.93 (d,  $J = 8.3$  Hz, 2H), 7.71 (d,  $J = 7.7$  Hz, 1H), 7.51 (td,  $J = 7.7, 1.0$  Hz, 1H), 7.22 (dd,  $J = 8.0, 7.1$  Hz, 1H), 7.10 (d,  $J = 7.9$  Hz, 1H), 5.00 (t,  $J = 8.7$  Hz, 1H), 4.59 (qd,  $J = 8.7, 5.4$  Hz, 1H), 4.25 (t,  $J = 8.7$  Hz, 1H), 4.09 (dd,  $J = 18.3, 5.4$  Hz, 1H), 3.86 (dd,  $J = 18.4, 8.7$  Hz, 1H).  $^{13}\text{C NMR}$  (400 MHz, ACETONE-D<sub>6</sub>)  $\delta$  196.81, 174.37, 143.87, 140.11, 135.28, 134.96, 134.63, 134.31, 133.47, 129.86, 127.17, 126.63, 126.60, 123.85, 122.31, 112.99, 112.30, 111.88, 87.60, 73.36, 47.77, 43.23, 40.40.  $\nu_{\text{max}}$  (neat,  $\text{cm}^{-1}$ ): 3283, 2925, 2853, 1734, 1694, 1622, 1512, 1473, 1410, 1377, 1324, 1209, 1170, 1131, 1066; Exact mass calculated for  $[\text{C}_{22}\text{H}_{14}\text{F}_3\text{N}_3\text{O}_3\text{Na}]^+$   $[\text{M}+\text{Na}]^+$ : 448.0879, Found: 448.0875

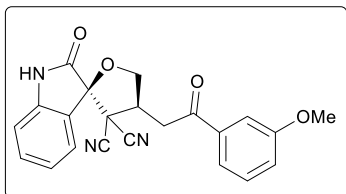
### **3aj:(2R,4S)-4-(2-([1,1'-biphenyl]-4-yl)-2-oxoethyl)-2'-oxo-4,5-dihydro-3H-spiro[furan-2,3'-indoline]-3,3-dicarbonitrile**



The compound **3aj** was isolated as white solid; in 70% (60.6 mg) yield, 85% ee and 6:1 dr, mp 198-200 °C;  $[\alpha]_D^{25} = -72.0$  (c 0.0025, MeOH). The enantiomeric ratio was determined by chiral HPLC using Daicel Chiralpak IA-3 column, n-hexane/2-propanol (80:20) as eluent, flow rate = 0.9 mL/min,  $\lambda = 254$  nm.  $t_R(\text{major}) = 18.163$  min,  $t_R(\text{minor}) = 61.994$  min  $^1\text{H NMR}$  (400 MHz, ACETONE-D<sub>6</sub>)  $\delta$  10.05 (s, 1H), 8.22 (d,  $J = 8.4$  Hz, 2H), 7.94 – 7.82 (m, 2H), 7.82 – 7.66 (m, 3H), 7.52 (ddd,  $J = 7.9, 4.5, 1.8$  Hz, 3H), 7.47 – 7.39 (m, 1H), 7.30 – 7.18 (m, 1H), 7.10 (d,  $J = 7.9$  Hz, 1H), 5.01 (t,  $J = 8.7$  Hz, 1H), 4.58 (qd,  $J = 8.6, 5.9$  Hz, 1H), 4.25 (t,  $J = 8.7$  Hz, 1H), 4.02 (dd,

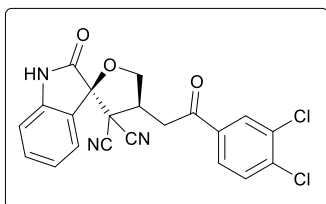
$J = 18.2, 5.8$  Hz, 1H), 3.82 (dd,  $J = 18.2, 8.5$  Hz, 1H).  $^{13}\text{C}$  NMR (101 MHz, ACETONE- $D_6$ )  $\delta$  196.84, 174.44, 146.82, 143.93, 140.48, 135.88, 133.47, 129.97, 129.85, 129.68, 129.30, 128.06, 127.22, 123.87, 122.42, 113.13, 112.41, 111.90, 87.70, 73.53, 47.88, 43.39, 40.14.  $\nu_{\text{max}}$  (neat,  $\text{cm}^{-1}$ ): 2924, 2854, 1732, 1682, 1623, 1604, 1471, 1405, 1263, 1224, 1077; Exact mass calculated for  $[\text{C}_{27}\text{H}_{19}\text{N}_3\text{O}_3\text{Na}]^+$   $[\text{M}+\text{Na}]^+$ : 456.1319, Found: 456.1313

**3ak:(2*R*,4*S*)-4-(2-(3-methoxyphenyl)-2-oxoethyl)-2'-oxo-4,5-dihydro-3H-spiro[furan-2,3'-indoline]-3,3-dicarbonitrile**



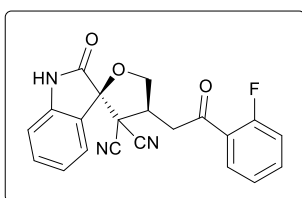
The compound **3ak** was isolated as white solid; in 67% (51.9 mg) yield, 74% ee and 7:1 dr, mp 178-180 °C;  $[\alpha]_{\text{D}}^{25} = -58.8$  (c 0.005, MeOH). The enantiomeric ratio was determined by chiral HPLC using Daicel Chiralpak IA-3 column, n-hexane/2-propanol (80:20) as eluent, flow rate = 0.9 mL/min,  $\lambda = 254$  nm.  $t_{\text{R}}$ (major) = 17.049 min,  $t_{\text{R}}$ (minor) = 26.303 min  $^1\text{H}$  NMR (400 MHz, ACETONE- $D_6$ )  $\delta$  10.03 (s, 1H), 7.72 (t,  $J = 7.8$  Hz, 2H), 7.65 – 7.57 (m, 1H), 7.50 (q,  $J = 8.2$  Hz, 2H), 7.29 – 7.18 (m, 2H), 7.10 (d,  $J = 7.9$  Hz, 1H), 4.98 (t,  $J = 8.8$  Hz, 1H), 4.54 (qd,  $J = 8.5, 6.1$  Hz, 1H), 4.23 (t,  $J = 8.6$  Hz, 1H), 3.97 (dd,  $J = 18.3, 6.0$  Hz, 1H), 3.88 (s, 3H), 3.77 (dd,  $J = 18.3, 8.4$  Hz, 1H).  $^{13}\text{C}$  NMR (400 MHz, ACETONE- $D_6$ )  $\delta$  197.10, 174.38, 160.93, 143.86, 138.39, 133.42, 130.73, 127.16, 123.81, 122.35, 121.60, 120.56, 113.43, 113.07, 112.32, 111.84, 87.68, 73.43, 55.84, 47.78, 43.32, 40.17.  $\nu_{\text{max}}$  (neat,  $\text{cm}^{-1}$ ): 3295, 2960, 2923, 2852, 1737, 1684, 1622, 1598, 1584, 1472, 1431, 1375, 1326, 1260, 1201, 1075, 1019; Exact mass calculated for  $[\text{C}_{22}\text{H}_{17}\text{N}_3\text{O}_4\text{Na}]^+$   $[\text{M}+\text{Na}]^+$ : 410.1111, Found: 410.1117

**3al:(2*R*,4*S*)-4-(2-(3,4-dichlorophenyl)-2-oxoethyl)-2'-oxo-4,5-dihydro-3H-spiro[furan-2,3'-indoline]-3,3-dicarbonitrile**



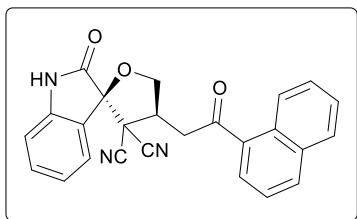
The compound **3al** was isolated as white solid; in 80% (68.2 mg) yield, 62% ee and 6:1 dr, mp 191-193 °C;  $[\alpha]_{\text{D}}^{25} = -40.0$  (c 0.005, MeOH). The enantiomeric ratio was determined by chiral HPLC using Daicel Chiralpak IA-3 column, n-hexane/2-propanol (80:20) as eluent, flow rate = 0.9 mL/min,  $\lambda = 254$  nm.  $t_{\text{R}}$ (major) = 16.201 min,  $t_{\text{R}}$ (minor) = 28.460 min  $^1\text{H}$  NMR (400 MHz, ACETONE- $D_6$ )  $\delta$  10.04 (s, 1H), 8.30 (d,  $J = 2.0$  Hz, 1H), 8.09 (dd,  $J = 8.4, 2.0$  Hz, 1H), 7.79 (d,  $J = 8.4$  Hz, 1H), 7.70 (d,  $J = 7.5$  Hz, 1H), 7.51 (td,  $J = 7.7, 0.9$  Hz, 1H), 7.29 – 7.15 (m, 1H), 7.10 (d,  $J = 7.9$  Hz, 1H), 4.98 (t,  $J = 8.8$  Hz, 1H), 4.55 (qd,  $J = 8.7, 5.5$  Hz, 1H), 4.23 (t,  $J = 8.6$  Hz, 1H), 4.05 (dd,  $J = 18.5, 5.4$  Hz, 1H), 3.80 (dd,  $J = 18.5, 8.7$  Hz, 1H).  $^{13}\text{C}$  NMR (400 MHz, ACETONE- $D_6$ )  $\delta$  195.65, 174.35, 143.85, 138.07, 137.12, 133.45, 131.94, 131.11, 130.88, 128.87, 127.16, 123.84, 122.29, 112.95, 112.24, 111.87, 87.58, 73.33, 47.73, 43.22, 40.15.  $\nu_{\text{max}}$  (neat,  $\text{cm}^{-1}$ ): 2923, 2854, 1731, 1693, 1623, 1586, 1471, 1393, 1326, 1262, 1209, 1075, 1031; Exact mass calculated for  $[\text{C}_{21}\text{H}_{13}\text{Cl}_2\text{N}_3\text{O}_3\text{Na}]^+$   $[\text{M}+\text{Na}]^+$ : 448.0226 & 450.0197, Found 448.0227 & 450.0193

**3am:(2*R*,4*S*)-4-(2-(2-fluorophenyl)-2-oxoethyl)-2'-oxo-4,5-dihydro-3H-spiro[furan-2,3'-indoline]-3,3-dicarbonitrile**



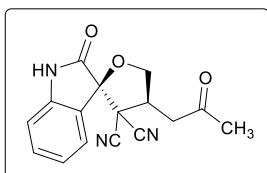
The compound **3am** was isolated as white solid; in 71% (53.3 mg) yield, 66% ee and 7:1 dr, mp 162-164 °C;  $[\alpha]_{\text{D}}^{25} = -33.6$  (c 0.005, MeOH). The enantiomeric ratio was determined by chiral HPLC using Daicel Chiralpak IA-3 column, n-hexane/2-propanol (80:20) as eluent, flow rate = 0.9 mL/min,  $\lambda = 254$  nm.  $t_{\text{R}}$ (major) = 17.874 min,  $t_{\text{R}}$ (minor) = 27.008 min  $^1\text{H}$  NMR (500 MHz, ACETONE- $D_6$ )  $\delta$  10.04 (s, 1H), 7.99 (tt,  $J = 7.6, 2.3$  Hz, 1H), 7.72 (ddt,  $J = 9.2, 5.2, 2.0$  Hz, 2H), 7.51 (td,  $J = 7.8, 1.2$  Hz, 1H), 7.41 – 7.31 (m, 2H), 7.22 (td,  $J = 7.7, 0.9$  Hz, 1H), 7.09 (t,  $J = 8.6$  Hz, 1H), 4.98 (t,  $J = 8.8$  Hz, 1H), 4.64 – 4.52 (m, 1H), 4.24 (t,  $J = 8.7$  Hz, 1H), 3.87 (ddd,  $J = 18.5, 5.5, 2.8$  Hz, 1H), 3.74 (ddd,  $J = 18.6, 8.7, 2.8$  Hz, 1H).  $^{13}\text{C}$  NMR (400 MHz, ACETONE- $D_6$ )  $\delta$  195.14, 195.10, 174.58, 164.59, 162.07, 144.09, 143.97, 136.80, 136.71, 133.69, 133.57, 131.63, 127.94, 127.39, 125.91, 125.88, 125.67, 125.54, 124.08, 122.56, 118.07, 117.83, 113.25, 112.58, 112.10, 87.81, 73.62, 48.03, 44.84, 44.75, 43.49.  $\nu_{\text{max}}$  (neat,  $\text{cm}^{-1}$ ): 3289, 2957, 2923, 2853, 1738, 1682, 1622, 1610, 1472, 1454, 1377, 1326, 1272, 1206, 1077; Exact mass calculated for  $[\text{C}_{22}\text{H}_{14}\text{FN}_3\text{O}_3\text{Na}]^+$   $[\text{M}+\text{Na}]^+$ : 398.0911, Found: 398.0915

### **3an:(2R,4S)-4-(2-(naphthalen-1-yl)-2-oxoethyl)-2'-oxo-4,5-dihydro-3H-spiro[furan-2,3'-indoline]-3,3-dicarbonitrile**



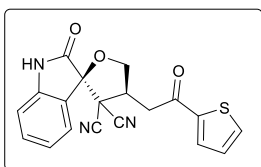
The compound **3an** was isolated as white solid; in 84% (68.5 mg) yield, 60% ee and 6:1 dr, mp 184-186 °C;  $[\alpha]_D^{25} = -52.0$  (c 0.0025, MeOH). The enantiomeric ratio was determined by chiral HPLC using Daicel Chiralpak IA-3 column, n-hexane/2-propanol (80:20) as eluent, flow rate = 0.9 mL/min,  $\lambda = 254$  nm.  $t_R$ (major) = 16.658 min,  $t_R$ (minor) = 35.906 min  $^1\text{H NMR}$  (400 MHz, ACETONE- $D_6$ )  $\delta$  10.08 (s, 1H), 8.84 (s, 1H), 8.19 – 8.09 (m, 2H), 8.02 (dd,  $J = 13.1, 8.3$  Hz, 2H), 7.73 (d,  $J = 7.6$  Hz, 1H), 7.71 – 7.66 (m, 1H), 7.66 – 7.60 (m, 1H), 7.51 (td,  $J = 7.7, 1.0$  Hz, 1H), 7.22 (dd,  $J = 8.0, 7.1$  Hz, 1H), 7.10 (d,  $J = 7.9$  Hz, 1H), 5.04 (t,  $J = 8.8$  Hz, 1H), 4.62 (qd,  $J = 8.7, 5.7$  Hz, 1H), 4.28 (t,  $J = 8.7$  Hz, 1H), 4.13 (dd,  $J = 18.1, 5.7$  Hz, 1H), 3.91 (dd,  $J = 18.2, 8.6$  Hz, 1H).  $^{13}\text{C NMR}$  (400 MHz, ACETONE- $D_6$ )  $\delta$  197.11, 174.36, 143.83, 136.65, 134.32, 133.49, 133.38, 131.22, 130.50, 129.62, 129.27, 128.61, 127.81, 127.12, 124.34, 123.77, 122.33, 113.05, 112.33, 111.80, 87.59, 73.48, 47.82, 43.38, 40.00.  $\nu_{\text{max}}$  (neat,  $\text{cm}^{-1}$ ): 2924, 1735, 1679, 1623, 1471, 1376, 1262, 1187, 1074; Exact mass calculated for  $[\text{C}_{25}\text{H}_{17}\text{N}_3\text{O}_3\text{Na}]^+ [\text{M}+\text{Na}]^+$ : 430.1162 found: 430.1168

### **3ao:(2R,4S)-2'-oxo-4-(2-oxopropyl)-4,5-dihydro-3H-spiro[furan-2,3'-indoline]-3,3-dicarbonitrile**



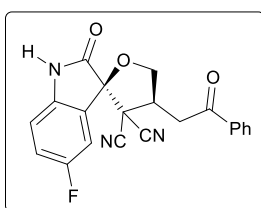
The compound **3ao** was isolated as white solid; in 62% (36.6 mg) yield, 22% ee and 7:1 dr, mp 174-176 °C;  $[\alpha]_D^{25} = -50.0$  (c 0.005, MeOH). The enantiomeric ratio was determined by chiral HPLC using Daicel Chiralpak IA-3 column, n-hexane/2-propanol (80:20) as eluent, flow rate = 0.9 mL/min,  $\lambda = 254$  nm.  $t_R$ (major) = 71.708 min,  $t_R$ (minor) = 88.201 min  $^1\text{H NMR}$  (400 MHz, ACETONE- $D_6$ )  $\delta$  10.01 (s, 1H), 7.67 (d,  $J = 7.6$  Hz, 1H), 7.49 (td,  $J = 7.8, 0.8$  Hz, 1H), 7.20 (t,  $J = 7.6$  Hz, 1H), 7.08 (d,  $J = 7.8$  Hz, 1H), 4.83 (t,  $J = 8.8$  Hz, 1H), 4.33 (qd,  $J = 8.8, 5.4$  Hz, 1H), 4.05 (t,  $J = 8.7$  Hz, 1H), 3.35 (dd,  $J = 18.3, 5.3$  Hz, 1H), 3.19 (dd,  $J = 18.3, 9.1$  Hz, 1H), 2.28 (s, 3H).  $^{13}\text{C NMR}$  (400 MHz, ACETONE- $D_6$ )  $\delta$  205.32, 174.33, 143.80, 133.42, 127.10, 123.82, 122.34, 112.93, 112.21, 111.84, 87.39, 73.32, 47.64, 43.82, 42.90, 30.60.  $\nu_{\text{max}}$  (neat,  $\text{cm}^{-1}$ ): 3280, 2960, 2923, 2853, 1738, 1622, 1604, 1471, 1412, 1377, 1326, 1208, 1175, 1080, 1018; Exact mass calculated for  $[\text{C}_{16}\text{H}_{13}\text{N}_3\text{O}_3\text{Na}]^+ [\text{M}+\text{Na}]^+$ : 394.1162 found: 394.1160

### **3ap: (2R,4S)-2'-oxo-4-(2-oxo-2-(thiophen-2-yl)ethyl)-4,5-dihydro-3H-spiro[furan-2,3'-indoline]-3,3-dicarbonitrile**



The compound **3ap** was isolated as yellow solid; in 50% (36.3 mg) yield and 7:1 dr;  $[\alpha]_D^{25} = -23.6$  (c 0.005, MeOH).  $^1\text{H NMR}$  (500 MHz, ACETONE- $D_6$ )  $\delta$  8.12 (d,  $J = 3.1$  Hz, 1H), 8.01 – 7.93 (m, 1H), 7.71 (d,  $J = 7.6$  Hz, 1H), 7.55 – 7.47 (m, 1H), 7.29 (dd,  $J = 4.7, 4.0$  Hz, 1H), 7.22 (t,  $J = 7.5$  Hz, 1H), 7.10 (d,  $J = 7.9$  Hz, 1H), 4.95 (t,  $J = 8.8$  Hz, 1H), 4.54 (dd,  $J = 8.5, 6.2$  Hz, 1H), 4.23 (t,  $J = 8.7$  Hz, 1H), 3.90 (dd,  $J = 17.8, 6.1$  Hz, 1H), 3.73 (dd,  $J = 17.8, 8.4$  Hz, 1H).  $^{13}\text{C NMR}$  (500 MHz, ACETONE- $D_6$ )  $\delta$  190.76, 175.03, 144.63, 144.56, 136.33, 135.11, 134.13, 130.14, 127.85, 124.52, 123.01, 113.63, 112.93, 112.54, 88.37, 74.08, 48.47, 43.91, 40.77. Exact mass calculated for  $[\text{C}_{19}\text{H}_{13}\text{N}_3\text{O}_3\text{SNa}]^+ [\text{M}+\text{Na}]^+$ : 386.0570 found: 386.0551

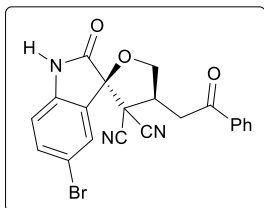
### **3ba:(2R,4S)-5'-fluoro-2'-oxo-4-(2-oxo-2-phenylethyl)-4,5-dihydro-3H-spiro[furan-2,3'-indoline]-3,3-dicarbonitrile**



The compound **3ba** was isolated as white solid; in 76% (57.1 mg) yield, 64% ee and 7:1 dr, mp 175-177 °C;  $[\alpha]_D^{25} = -54.0$  (c 0.005, MeOH). The enantiomeric ratio was determined by chiral HPLC using Daicel Chiralpak IA-3 column, n-hexane/2-propanol (80:20) as eluent, flow rate = 0.9 mL/min,  $\lambda = 254$  nm.  $t_R$ (major) = 13.295 min,  $t_R$ (minor) = 35.689 min  $^1\text{H NMR}$  (400 MHz, ACETONE- $D_6$ )  $\delta$  10.12 (s, 1H), 8.20 – 8.06 (m, 2H), 7.68 (t,  $J = 7.5$  Hz, 1H), 7.57 (t,  $J = 7.7$  Hz, 2H), 7.47 (dd,  $J = 8.1, 2.6$  Hz, 1H), 7.37 – 7.26 (m, 1H), 7.14 (dd,  $J = 8.7, 4.3$  Hz, 1H), 5.00 (t,  $J = 8.8$  Hz, 1H), 4.54 (qd,  $J = 8.6, 5.8$  Hz, 1H), 4.26 (t,  $J = 8.7$  Hz, 1H), 3.99 (dd,  $J = 18.3, 5.7$  Hz, 1H), 3.79 (dd,  $J = 18.2, 8.5$  Hz, 1H).  $^{13}\text{C NMR}$  (400 MHz, ACETONE- $D_6$ )  $\delta$  197.12, 174.25, 160.76, 158.36, 139.97, 136.93, 134.43, 129.55, 129.00, 123.85, 123.77, 120.01, 119.78, 114.81, 114.55, 113.09, 113.01, 112.73, 112.11, 87.44, 73.59, 47.75, 43.28, 39.88.  $\nu_{\text{max}}$  (neat,  $\text{cm}^{-1}$ ): 3282, 2960, 2924, 2853, 1738, 1684, 1629, 1596, 1580, 1490, 1463, 1449, 1414, 1372, 1303,

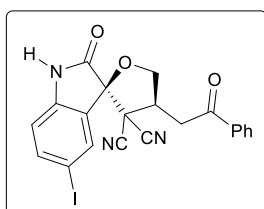
1278, 1261, 1221, 1205, 1181, 1068; Exact mass calculated for  $[C_{21}H_{14}FN_3O_3Na]^+$   $[M+Na]^+$ : 398.0911 found: 398.0904

### **3ca:(2R,4S)-5'-bromo-2'-oxo-4-(2-oxo-2-phenylethyl)-4,5-dihydro-3H-spiro[furan-2,3'-indoline]-3,3-dicarbonitrile**



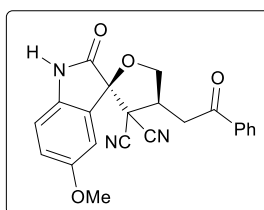
The compound **3ca** was isolated as white solid; in 50% (43.6 mg) yield, 77% ee and 8:1 dr, mp 207-208 °C;  $[\alpha]_D^{25} = +10$  (c 0.005, MeOH). The enantiomeric ratio was determined by chiral HPLC using Daicel Chiralpak IA-3 column, n-hexane/2-propanol (80:20) as eluent, flow rate = 0.9 mL/min,  $\lambda = 254$  nm.  $t_R(\text{major}) = 13.329$  min,  $t_R(\text{minor}) = 36.244$  min  $^1H$  NMR (400 MHz, ACETONE- $D_6$ )  $\delta$  10.22 (s, 1H), 8.13 (dd,  $J = 8.3, 1.1$  Hz, 2H), 7.81 (d,  $J = 2.0$  Hz, 1H), 7.73 – 7.65 (m, 2H), 7.57 (t,  $J = 7.7$  Hz, 2H), 7.10 (d,  $J = 8.4$  Hz, 1H), 4.99 (t,  $J = 8.7$  Hz, 1H), 4.53 (qd,  $J = 8.6, 5.8$  Hz, 1H), 4.27 (t,  $J = 8.8$  Hz, 1H), 3.99 (dd,  $J = 18.2, 5.9$  Hz, 1H), 3.79 (dd,  $J = 18.2, 8.5$  Hz, 1H).  $^{13}C$  NMR (400 MHz, ACETONE- $D_6$ )  $\delta$  197.16, 173.89, 143.17, 136.98, 136.28, 134.49, 130.02, 129.61, 129.06, 124.56, 115.57, 113.85, 112.74, 112.15, 87.21, 73.68, 47.83, 43.35, 39.91.  $\nu_{\text{max}}$  (neat,  $cm^{-1}$ ): 1737, 1260, 750; Exact mass calculated for  $[C_{21}H_{14}BrN_3O_3Na]^+$   $[M+Na]^+$ : 458.0111 & 460.0090 found: 458.0099 & 460.0086

### **3da:(2R,4S)-5'-iodo-2'-oxo-4-(2-oxo-2-phenylethyl)-4,5-dihydro-3H-spiro[furan-2,3'-indoline]-3,3-dicarbonitrile**



The compound **3da** was isolated as white solid; in 50% (48.3 mg) yield, 84% ee and 6:1 dr, mp 196-198 °C;  $[\alpha]_D^{25} = -39.3$  (c 0.005, MeOH). The enantiomeric ratio was determined by chiral HPLC using Daicel Chiralpak IA-3 column, n-hexane/2-propanol (80:20) as eluent, flow rate = 0.9 mL/min,  $\lambda = 254$  nm.  $t_R(\text{major}) = 14.303$  min,  $t_R(\text{minor}) = 44.828$  min  $^1H$  NMR (400 MHz, ACETONE- $D_6$ )  $\delta$  10.24 (s, 1H), 8.13 (dd,  $J = 8.2, 1.1$  Hz, 2H), 7.97 (d,  $J = 1.7$  Hz, 1H), 7.87 (dd,  $J = 8.1, 1.8$  Hz, 1H), 7.69 (t,  $J = 7.3$  Hz, 1H), 7.58 (t,  $J = 7.7$  Hz, 2H), 6.98 (d,  $J = 8.2$  Hz, 1H), 4.98 (t,  $J = 8.7$  Hz, 1H), 4.52 (qd,  $J = 8.6, 5.9$  Hz, 1H), 4.26 (t,  $J = 8.6$  Hz, 1H), 3.99 (dd,  $J = 18.2, 5.9$  Hz, 1H), 3.78 (dd,  $J = 18.3, 8.5$  Hz, 1H).  $^{13}C$  NMR (400 MHz, ACETONE- $D_6$ )  $\delta$  197.15, 173.66, 143.70, 142.19, 136.96, 135.72, 134.46, 129.58, 129.04, 124.79, 114.17, 112.74, 112.14, 87.00, 85.12, 73.62, 47.81, 43.31, 39.89.  $\nu_{\text{max}}$  (neat,  $cm^{-1}$ ): 2959, 2922, 2852, 1739, 1687, 1617, 1470, 1368, 1275, 1260, 1207, 1081, 1020; Exact mass calculated for  $[C_{21}H_{14}IN_3O_3Na]^+$   $[M+Na]^+$ : 505.9972 found: 505.9977

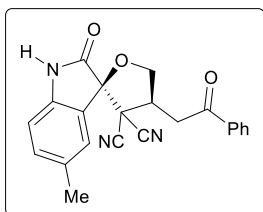
### **3ea:(2R,4S)-5'-methoxy-2'-oxo-4-(2-oxo-2-phenylethyl)-4,5-dihydro-3H-spiro[furan-2,3'-indoline]-3,3-dicarbonitrile**



The compound **3ea** was isolated as white solid; in 85% (65.8 mg) yield, 74% ee and 7:1 dr, mp 176-178 °C;  $[\alpha]_D^{25} = -33.0$  (c 0.005, MeOH). The enantiomeric ratio was determined by chiral HPLC using Daicel Chiralpak IA-3 column, n-hexane/2-propanol (80:20) as eluent, flow rate = 0.9 mL/min,  $\lambda = 254$  nm.  $t_R(\text{major}) = 16.591$  min,  $t_R(\text{minor}) = 48.726$  min  $^1H$  NMR (400 MHz, ACETONE- $D_6$ )  $\delta$  9.88 (s, 1H), 8.13 (d,  $J = 7.4$  Hz, 2H), 7.68 (t,  $J = 7.4$  Hz, 1H), 7.57 (t,  $J = 7.7$  Hz, 2H), 7.31 (d,  $J = 2.5$  Hz, 1H), 7.07 (dd,  $J = 8.6, 2.5$  Hz, 1H), 7.02 (d,  $J = 8.5$  Hz, 1H), 4.99 (t,  $J = 8.8$  Hz, 1H), 4.56 (qd,  $J = 8.6, 5.7$  Hz, 1H), 4.23 (t,  $J = 8.6$  Hz, 1H), 3.98 (dd,  $J = 18.2, 5.6$  Hz, 1H), 3.85 – 3.72 (m, 4H).  $^{13}C$  NMR (400 MHz, ACETONE- $D_6$ )  $\delta$  197.22, 174.34, 156.91, 137.05, 136.72, 134.47, 129.62, 129.07, 123.40, 118.14, 113.76, 113.02, 112.46, 112.38, 87.86, 73.54, 56.13, 47.92, 43.31, 40.05.  $\nu_{\text{max}}$  (neat,  $cm^{-1}$ ): 2959, 2923, 2852, 1733, 1495, 1466, 1377, 1261, 1210, 1022, 801, 751; Exact mass calculated for  $[C_{22}H_{17}N_3O_4Na]^+$   $[M+Na]^+$ : 410.1111 found: 410.1111

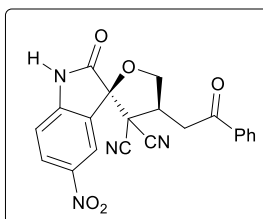
### **3fa:(2R,4S)-5'-methyl-2'-oxo-4-(2-oxo-2-phenylethyl)-4,5-dihydro-3H-spiro[furan-2,3'-indoline]-3,3-dicarbonitrile**





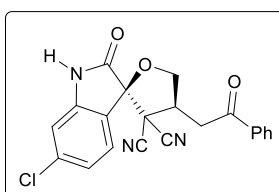
The compound **3fa** was isolated as white solid; in 75% (55.7 mg) yield, 70% ee and 7:1 dr, mp 194-196 °C;  $[\alpha]_D^{25} = -31.0$  (c 0.01, MeOH). The enantiomeric ratio was determined by chiral HPLC using Daicel Chiralpak IA-3 column, n-hexane/2-propanol (80:20) as eluent, flow rate = 0.9 mL/min,  $\lambda = 254$  nm.  $t_R(\text{major}) = 13.000$  min,  $t_R(\text{minor}) = 42.459$  min  $^1\text{H NMR}$  (400 MHz, ACETONE- $D_6$ )  $\delta$  9.94 (s, 1H), 8.13 (dd,  $J = 5.1, 3.5$  Hz, 2H), 7.68 (t,  $J = 7.5$  Hz, 1H), 7.58 (t,  $J = 7.7$  Hz, 2H), 7.52 (s, 1H), 7.31 (d,  $J = 7.9$  Hz, 1H), 6.98 (d,  $J = 8.0$  Hz, 1H), 4.98 (t,  $J = 8.8$  Hz, 1H), 4.56 (qd,  $J = 8.7, 5.7$  Hz, 1H), 4.22 (t,  $J = 8.6$  Hz, 1H), 3.98 (dd,  $J = 18.3, 5.6$  Hz, 1H), 3.77 (dd,  $J = 18.2, 8.6$  Hz, 1H), 2.36 (s, 3H).  $^{13}\text{C NMR}$  (400 MHz, ACETONE- $D_6$ )  $\delta$  197.25, 174.43, 141.40, 137.09, 134.50, 133.72, 133.39, 129.65, 129.10, 127.72, 122.43, 113.12, 112.38, 111.61, 87.73, 73.47, 47.87, 43.32, 40.08, 21.09.  $\nu_{\text{max}}$  (neat,  $\text{cm}^{-1}$ ): 2922, 1737, 1366, 1275, 1260, 1217, 1021, 800, 750; Exact mass calculated for  $[\text{C}_{22}\text{H}_{17}\text{N}_3\text{O}_3\text{Na}]^+ [\text{M}+\text{Na}]^+$ : 394.1162 found: 394.1162

### **3ga:(2R,4S)-5'-nitro-2'-oxo-4-(2-oxo-2-phenylethyl)-4,5-dihydro-3H-spiro[furan-2,3'-indoline]-3,3-dicarbonitrile**



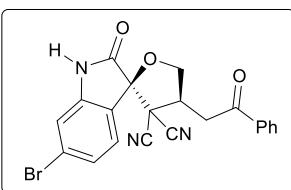
The compound **3ga** was isolated as white solid; in 72% (57.9 mg) yield, 79% ee and 10:1 dr, mp 233-235 °C;  $[\alpha]_D^{25} = -36.0$  (c 0.005, MeOH). The enantiomeric ratio was determined by chiral HPLC using Daicel Chiralpak IA-3 column, n-hexane/2-propanol (80:20) as eluent, flow rate = 0.9 mL/min,  $\lambda = 254$  nm.  $t_R(\text{major}) = 14.411$  min,  $t_R(\text{minor}) = 39.220$  min  $^1\text{H NMR}$  (500 MHz, Acetone- $d_6$ )  $\delta$  10.67 (s, 1H), 8.63 – 8.38 (m, 2H), 8.14 (dd,  $J = 8.4, 1.1$  Hz, 2H), 7.73 – 7.63 (m, 1H), 7.58 (t,  $J = 7.7$  Hz, 2H), 7.37 (d,  $J = 8.7$  Hz, 1H), 5.03 (t,  $J = 8.8$  Hz, 1H), 4.53 (qd,  $J = 8.6, 5.8$  Hz, 1H), 4.36 (t,  $J = 8.8$  Hz, 1H), 4.03 (dd,  $J = 18.3, 5.8$  Hz, 1H), 3.83 (dd,  $J = 18.3, 8.5$  Hz, 1H).  $^{13}\text{C NMR}$  (101 MHz, ACETONE- $D_6$ )  $\delta$  197.20, 174.49, 149.75, 144.57, 136.99, 134.56, 130.08, 129.65, 129.11, 123.29, 122.88, 112.57, 112.47, 112.02, 86.87, 73.90, 47.84, 43.54, 39.90.  $\nu_{\text{max}}$  (neat,  $\text{cm}^{-1}$ ): 2959, 2924, 2854, 1746, 1682, 1630, 1579, 1529, 1449, 1342, 1278, 1261, 1206, 1132, 1104, 1003; Exact mass calculated for  $[\text{C}_{21}\text{H}_{14}\text{N}_4\text{O}_5\text{Na}]^+ [\text{M}+\text{Na}]^+$ : 425.0856 found: 425.0858

### **3ha:(2R,4S)-6'-chloro-2'-oxo-4-(2-oxo-2-phenylethyl)-4,5-dihydro-3H-spiro[furan-2,3'-indoline]-3,3-dicarbonitrile**



The compound **3ha** was isolated as white solid; in 65% (50.9 mg) yield, 79% ee and 7:1 dr, mp 212-214 °C;  $[\alpha]_D^{25} = -68$  (c 0.005, MeOH). The enantiomeric ratio was determined by chiral HPLC using Daicel Chiralpak IA-3 column, n-hexane/2-propanol (80:20) as eluent, flow rate = 0.9 mL/min,  $\lambda = 254$  nm.  $t_R(\text{major}) = 12.415$  min,  $t_R(\text{minor}) = 47.738$  min  $^1\text{H NMR}$  (400 MHz, ACETONE- $D_6$ )  $\delta$  10.21 (s, 1H), 8.13 (d,  $J = 7.4$  Hz, 2H), 7.68 (t,  $J = 6.7$  Hz, 2H), 7.57 (t,  $J = 7.7$  Hz, 2H), 7.27 (dd,  $J = 8.3, 1.9$  Hz, 1H), 7.15 (d,  $J = 1.9$  Hz, 1H), 4.98 (t,  $J = 8.8$  Hz, 1H), 4.52 (qd,  $J = 8.6, 5.8$  Hz, 1H), 4.25 (t,  $J = 8.7$  Hz, 1H), 3.98 (dd,  $J = 18.2, 5.8$  Hz, 1H), 3.78 (dd,  $J = 18.2, 8.5$  Hz, 1H).  $^{13}\text{C NMR}$  (101 MHz, ACETONE- $D_6$ )  $\delta$  197.24, 174.30, 145.34, 138.77, 137.07, 134.55, 129.67, 129.13, 128.61, 123.87, 121.15, 112.90, 112.38, 112.25, 87.27, 73.62, 47.82, 43.39, 40.04.  $\nu_{\text{max}}$  (neat,  $\text{cm}^{-1}$ ): 3275, 2958, 2920, 1753, 1736, 1688, 1597, 1580, 1487, 1448, 1416, 1355, 1320, 1221, 1203, 1139; Exact mass calculated for  $[\text{C}_{21}\text{H}_{14}\text{ClN}_3\text{O}_3\text{Na}]^+ [\text{M}+\text{Na}]^+$ : 414.0616 found: 414.0612

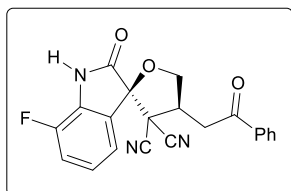
### **3ia:(2R,4S)-6'-bromo-2'-oxo-4-(2-oxo-2-phenylethyl)-4,5-dihydro-3H-spiro[furan-2,3'-indoline]-3,3-dicarbonitrile**



The compound **3ia** was isolated as white solid; in 60% (52.4 mg) yield, 84% ee and 7:1 dr, mp 201-203 °C;  $[\alpha]_D^{25} = -39.6$  (c 0.005, MeOH). The enantiomeric ratio was determined by chiral HPLC using Daicel Chiralpak IA-3 column, n-hexane/2-propanol (80:20) as eluent, flow rate = 0.9 mL/min,  $\lambda = 254$  nm.  $t_R(\text{major}) = 12.323$  min,  $t_R(\text{minor}) = 47.573$  min  $^1\text{H NMR}$  (400 MHz, ACETONE- $D_6$ )  $\delta$  10.21 (s, 1H), 8.16 – 8.09 (m, 2H), 7.68 (t,  $J = 7.4$  Hz, 1H), 7.65 – 7.54 (m, 3H), 7.43 (dd,  $J = 8.0, 1.8$  Hz, 1H), 7.30 (d,  $J = 1.7$  Hz, 1H), 4.98 (t,  $J = 8.7$  Hz, 1H), 4.52 (qd,  $J = 8.6, 5.9$  Hz, 1H), 4.25 (t,  $J = 8.6$  Hz, 1H), 3.98 (dd,  $J = 18.3, 5.7$  Hz, 1H), 3.78 (dd,  $J = 18.3, 8.5$  Hz, 1H).  $^{13}\text{C NMR}$  (400 MHz, ACETONE- $D_6$ )  $\delta$  197.23, 174.19, 145.37, 137.05, 134.53, 129.66, 129.12, 128.81, 126.86, 121.62, 115.22, 115.18, 112.88, 112.23, 87.33, 73.63, 47.75, 43.38, 40.01.  $\nu_{\text{max}}$  (neat,  $\text{cm}^{-1}$ ): 2960, 2923, 2852, 1739, 1688, 1614, 1377, 1322,

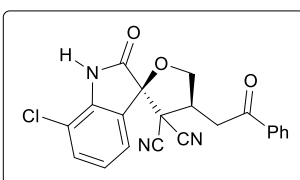
1262, 1221, 1080; Exact mass calculated for  $[C_{21}H_{14}BrN_3O_3Na]^+$   $[M+Na]^+$ : 458.0111 & 460.0090 found: 458.0100 460.0079

### 3ja:(2R,4S)-7'-fluoro-2'-oxo-4-(2-oxo-2-phenylethyl)-4,5-dihydro-3H-spiro[furan-2,3'-indoline]-3,3-dicarbonitrile



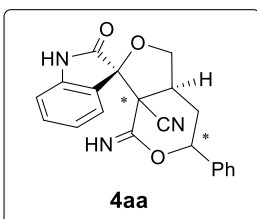
The compound **3ja** was isolated as white solid; in 55% (41.3 mg) yield, 68% ee and 6:1 dr, mp 173-175 °C;  $[\alpha]_D^{25} = -60$  (c 0.005, MeOH). The enantiomeric ratio was determined by chiral HPLC using Daicel Chiralpak IA-3 column, n-hexane/2-propanol (80:20) as eluent, flow rate = 0.9 mL/min,  $\lambda = 254$  nm.  $t_R$ (major) = 19.898 min,  $t_R$ (minor) = 42.046 min  $^1H$  NMR (500 MHz, ACETONE- $D_6$ )  $\delta$  8.20 – 8.08 (m, 2H), 7.68 (tt,  $J = 6.9, 1.2$  Hz, 1H), 7.64 – 7.49 (m, 3H), 7.40 (ddd,  $J = 10.0, 8.5, 0.9$  Hz, 1H), 7.27 (ddd,  $J = 8.5, 7.7, 4.8$  Hz, 1H), 5.00 (t,  $J = 8.8$  Hz, 1H), 4.55 (qd,  $J = 8.6, 5.9$  Hz, 1H), 4.27 (t,  $J = 8.7$  Hz, 1H), 3.99 (dd,  $J = 18.2, 5.8$  Hz, 1H), 3.79 (dd,  $J = 18.2, 8.5$  Hz, 1H).  $^{13}C$  NMR (400 MHz, ACETONE- $D_6$ )  $\delta$  197.14, 174.01, 149.08, 146.65, 136.95, 134.44, 131.11, 130.98, 129.56, 129.01, 124.88, 124.83, 123.11, 123.07, 120.44, 120.27, 112.78, 112.04, 87.52, 73.58, 47.83, 43.22, 39.90.  $\nu_{max}$  (neat,  $cm^{-1}$ ): 2917, 2849, 1742, 1686, 1646, 1598, 1493, 1470, 1449, 1364, 1322, 1259, 1217, 1141, 1025; Exact mass calculated for  $[C_{21}H_{14}FN_3O_3Na]^+$   $[M+Na]^+$ : 398.0911 found: 398.0903

### 3ka:(2R,4S)-7'-chloro-2'-oxo-4-(2-oxo-2-phenylethyl)-4,5-dihydro-3H-spiro[furan-2,3'-indoline]-3,3-dicarbonitrile



The compound **3ka** was isolated as white solid; in 78% (61.1 mg) yield, 70% ee and 7:1 dr, mp 86-88 °C;  $[\alpha]_D^{25} = -74.0$  (c 0.005, MeOH). The enantiomeric ratio was determined by chiral HPLC using Daicel Chiralpak IA-3 column, n-hexane/2-propanol (80:20) as eluent, flow rate = 0.9 mL/min,  $\lambda = 254$  nm.  $t_R$ (major) = 36.163 min,  $t_R$ (minor) = 54.271 min  $^1H$  NMR (500 MHz, )  $\delta$  10.43 (s, 1H), 8.22 – 8.07 (m, 2H), 7.76 – 7.63 (m, 2H), 7.62 – 7.47 (m, 3H), 7.27 (t,  $J = 7.9$  Hz, 1H), 5.00 (t,  $J = 8.8$  Hz, 1H), 4.53 (qd,  $J = 8.6, 5.9$  Hz, 1H), 4.26 (t,  $J = 8.8$  Hz, 1H), 3.98 (dd,  $J = 18.2, 5.8$  Hz, 1H), 3.79 (dd,  $J = 18.2, 8.5$  Hz, 1H).  $^{13}C$  NMR (400 MHz, ACETONE- $D_6$ )  $\delta$  197.18, 174.12, 141.51, 137.00, 134.51, 133.40, 129.63, 129.08, 125.77, 125.10, 124.13, 116.54, 112.83, 112.08, 87.99, 73.69, 47.89, 43.35, 39.94.  $\nu_{max}$  (neat,  $cm^{-1}$ ): 3283, 2919, 2850, 1743, 1687, 1622, 1597, 1476, 1450, 1372, 1319, 1261, 1222, 1182, 1147, 1094, 1020; Exact mass calculated for  $[C_{21}H_{14}ClN_3O_3Na]^+$   $[M+Na]^+$ : 414.0616 found: 414.0616

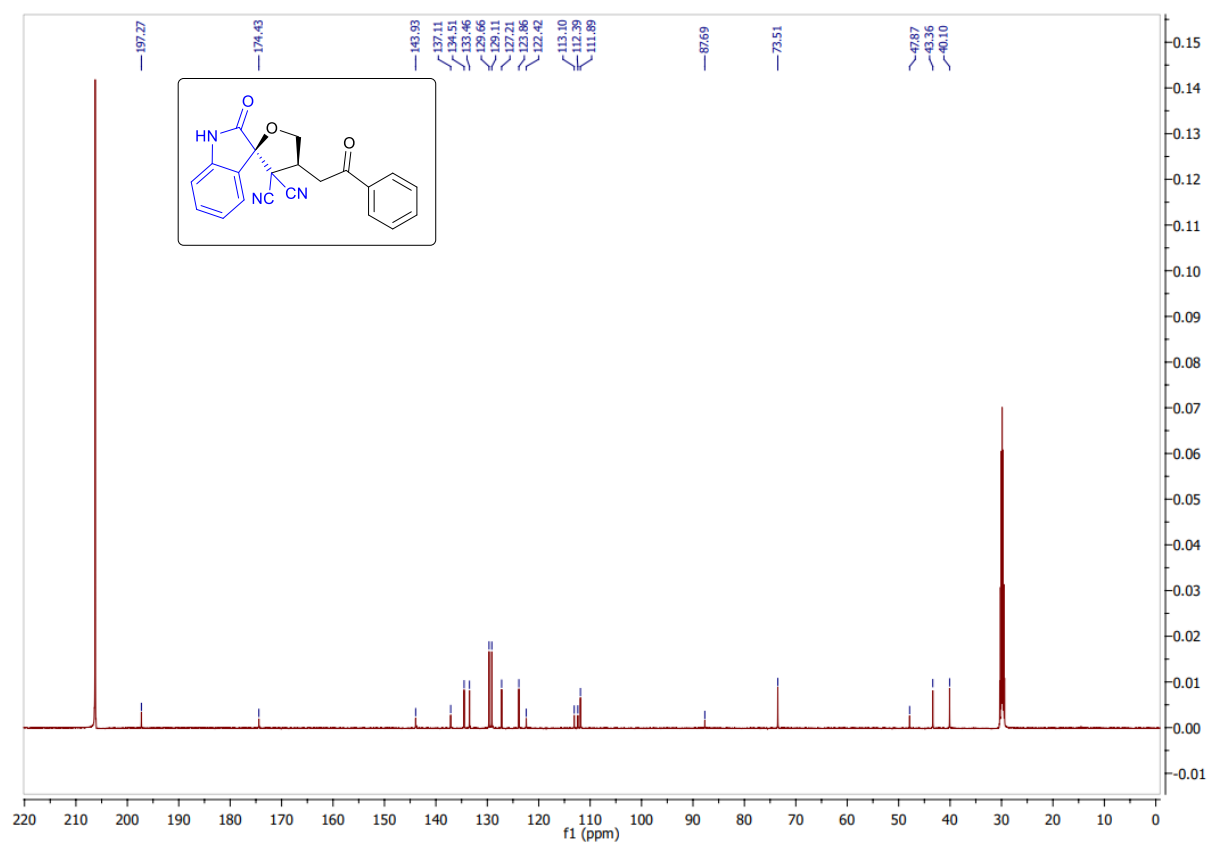
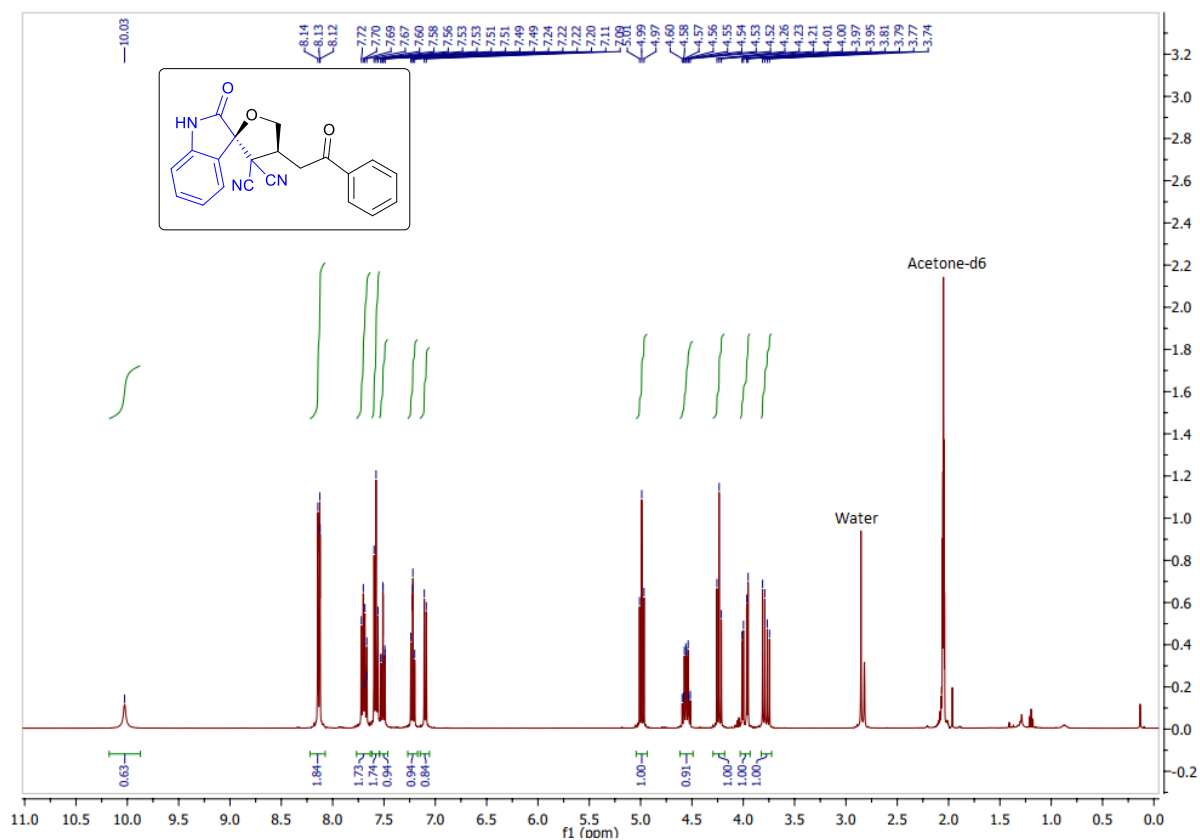
### 4aa:(3R,3aS,7aS)-4-imino-2'-oxo-6-phenyl-1,6,7,7a-tetrahydrospiro[furo[3,4-c]pyran-3,3'-indoline]-3a(4H)-carbonitrile



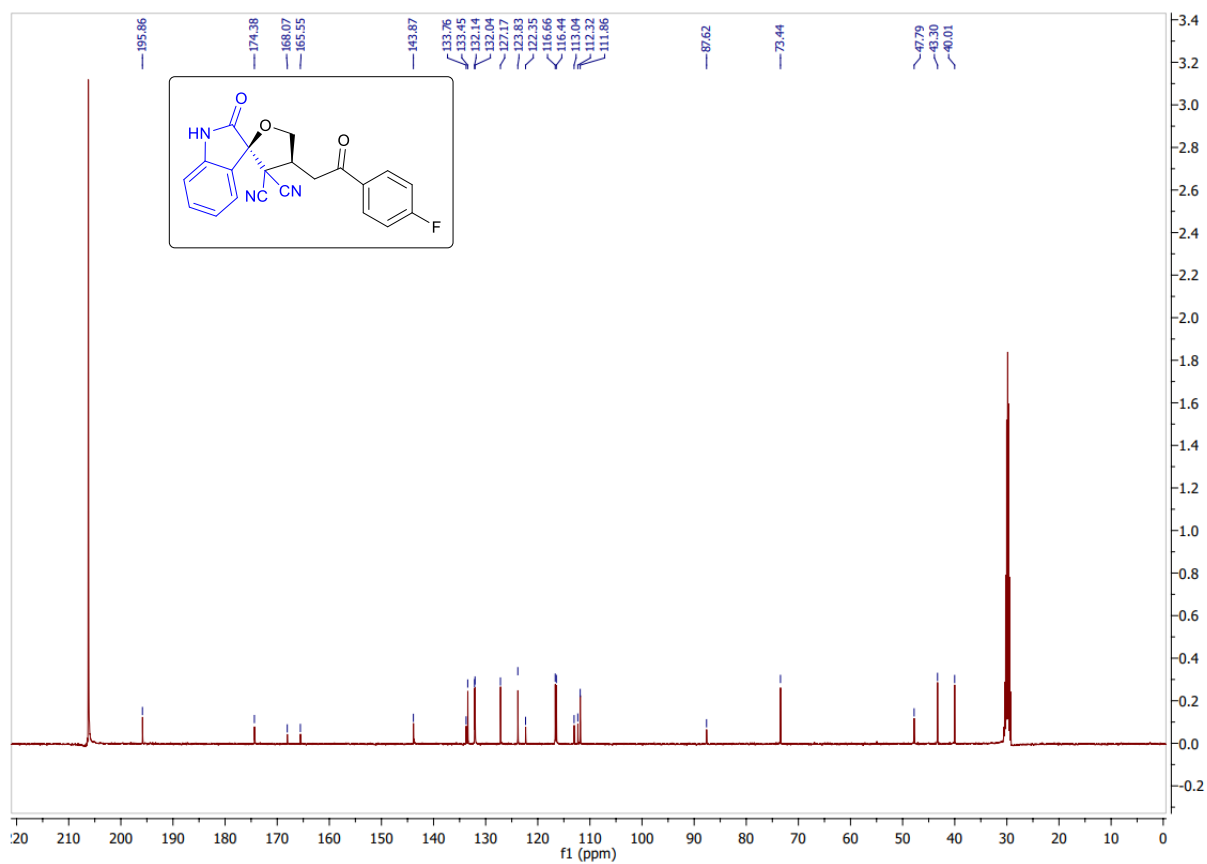
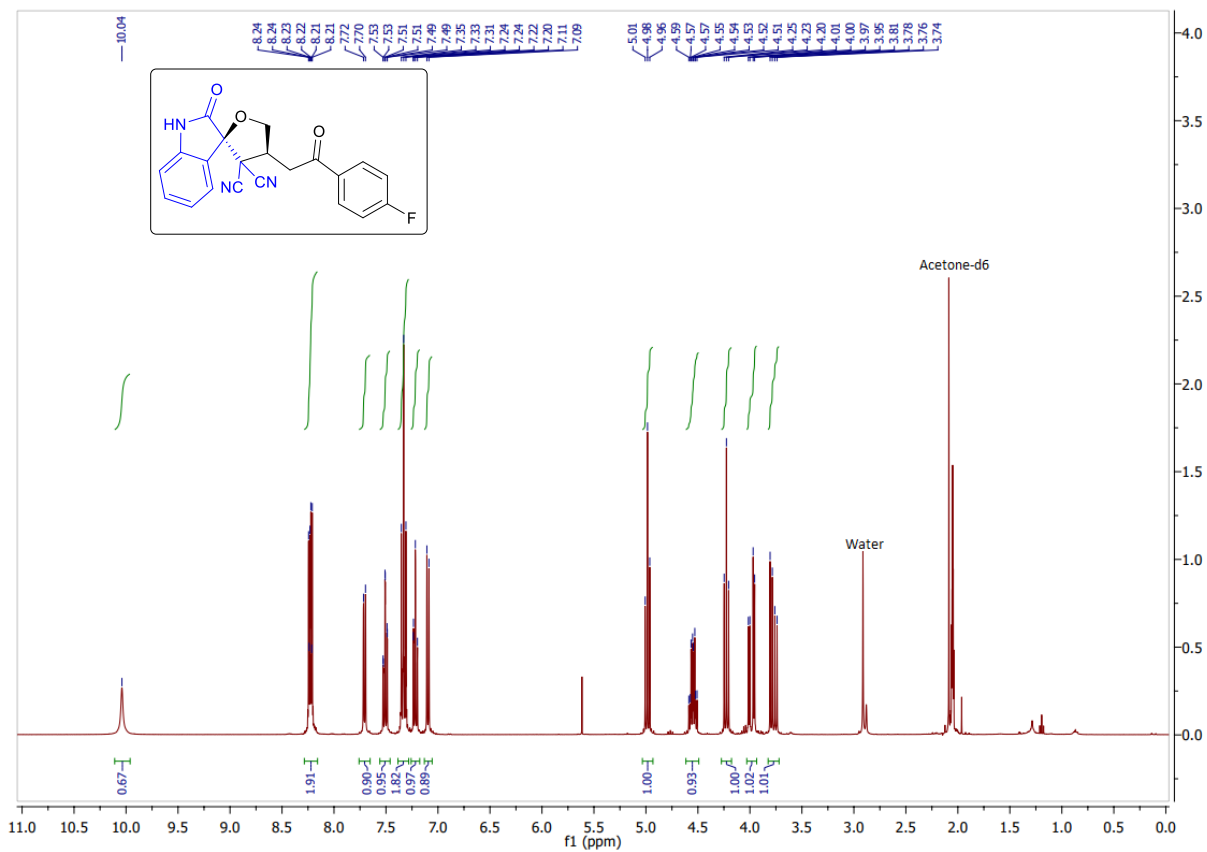
The compound **4aa** was isolated as white solid; in 68% (48.8 mg) yield, 80% ee 1:1 dr, mp 158-160;  $[\alpha]_D^{25} = -39.4$  (c 0.0037, MeOH).  $^1H$  NMR (500 MHz, )  $\delta$  7.88 (d,  $J = 11.5$  Hz, 2H), 7.66 (t,  $J = 7.4$  Hz, 2H), 7.39 – 7.29 (m, 11H), 7.28 – 7.23 (m, 2H), 7.10 (td,  $J = 7.7, 1.0$  Hz, 2H), 6.83 (dd,  $J = 7.8, 4.2$  Hz, 2H), 4.88 (dd,  $J = 9.6, 3.2$  Hz, 1H), 4.78 (dd,  $J = 9.0, 3.7$  Hz, 1H), 4.68 (t,  $J = 8.8$  Hz, 1H), 4.60 (t,  $J = 8.6$  Hz, 1H), 4.28 – 4.19 (m, 1H), 4.19 – 4.10 (m, 1H), 4.06 (t,  $J = 9.3$  Hz, 1H), 3.95 (t,  $J = 9.0$  Hz, 1H), 2.29 (ddd,  $J = 14.3, 9.0, 7.0$  Hz, 2H), 2.22 (ddd,  $J = 14.2, 5.8, 3.3$  Hz, 1H), 2.17 – 2.11 (m, 1H), 2.11 – 2.03 (m, 2H).  $^{13}C$  NMR (500 MHz, )  $\delta$  174.25, 174.20, 143.62, 143.52, 141.36, 141.32, 132.51, 129.00, 128.98, 128.48, 128.36, 126.94, 126.83, 125.77, 125.60, 123.97, 121.69, 121.61, 112.41, 112.26, 111.03, 111.00, 110.89, 87.39, 86.68, 73.74, 73.14, 72.79, 72.66, 47.98, 47.68, 44.95, 44.71, 38.99, 38.70.  $\nu_{max}$  (neat,  $cm^{-1}$ ): 3507, 2964, 1738, 1625, 1474, 1262, 1024; Exact mass calculated for  $[C_{21}H_{17}N_3O_3Na]^+$   $[M+Na]^+$ : 382.1162 found: 382.1164

## References

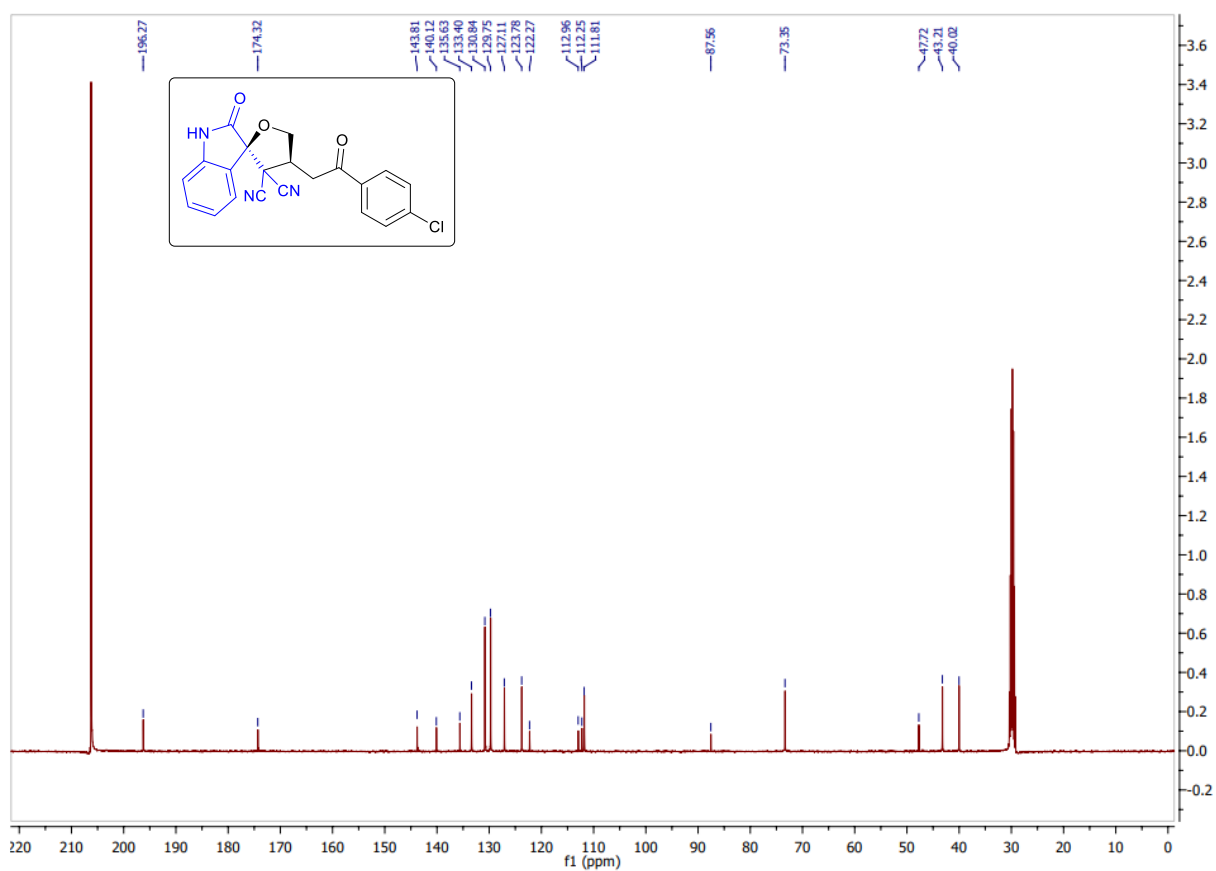
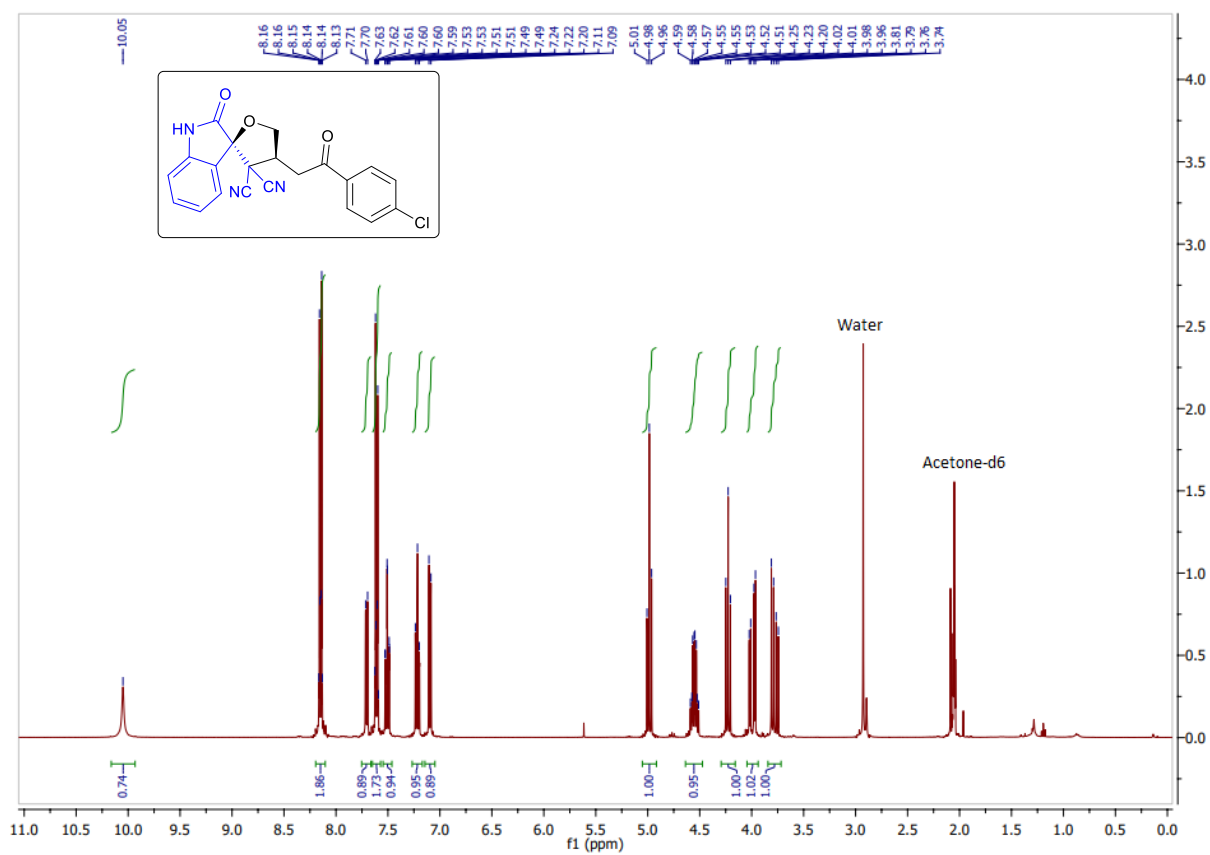
1. Y. Lin, B.-L. Zhao, D.-M. Du, *J. Org. Chem.*, 2019, **84**, 10209–10220.
2. S.-H. Huang, Y.-W. Shih, W.-T. Huang, D.-H. Li, T.-F. Yang, *RSC Adv.*, 2016, **6**, 91870–91874.
3. (a) Y. Flukata, K. Asano, S. Matsubara, *J. Am. Chem. Soc.*, 2013, **135**, 12160;  
(b) R. Miyaji, K. Asano, S. Matsubara, *Org. Lett.*, 2013, **15**, 3658;  
(c) J. Xu, Y. Hu, D. Huang, K.-H. Wang, C. Xu, T. Niu, *Adv. Synth. Catal.*, 2012, **354**, 515;  
(d) S. Meninno, A. Vidal-Albalat, A. Lattanzi, *Org. Lett.*, 2015, **17**, 4348;  
(e) Y.-L. Zhao, Q.-X. Lou, L.-S. Wang, W.-H. Hu, J.-L. Zhao, *Angew. Chem. Int. Ed.*, 2017, **129**, 344;  
(f) F. Manoni, S. J. Connon, *Angew. Chem.*, 2014, **126**, 2666.



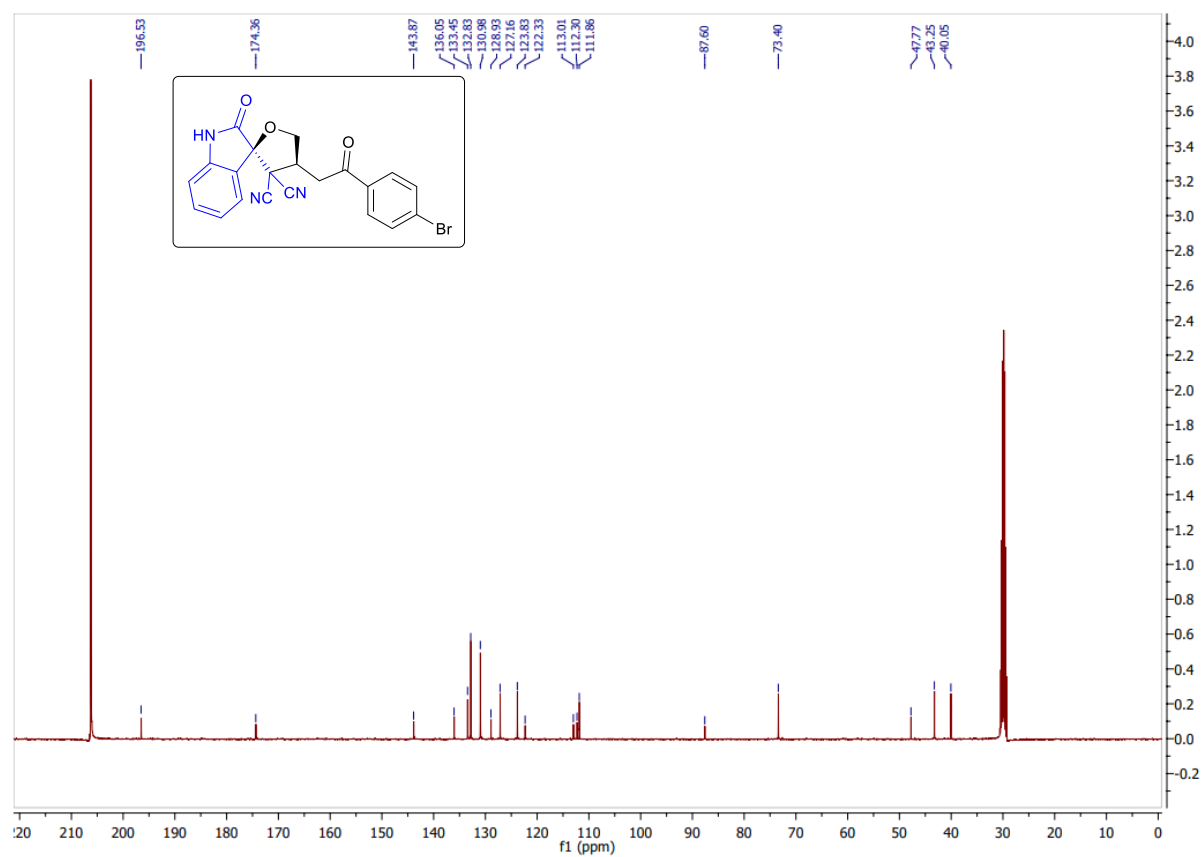
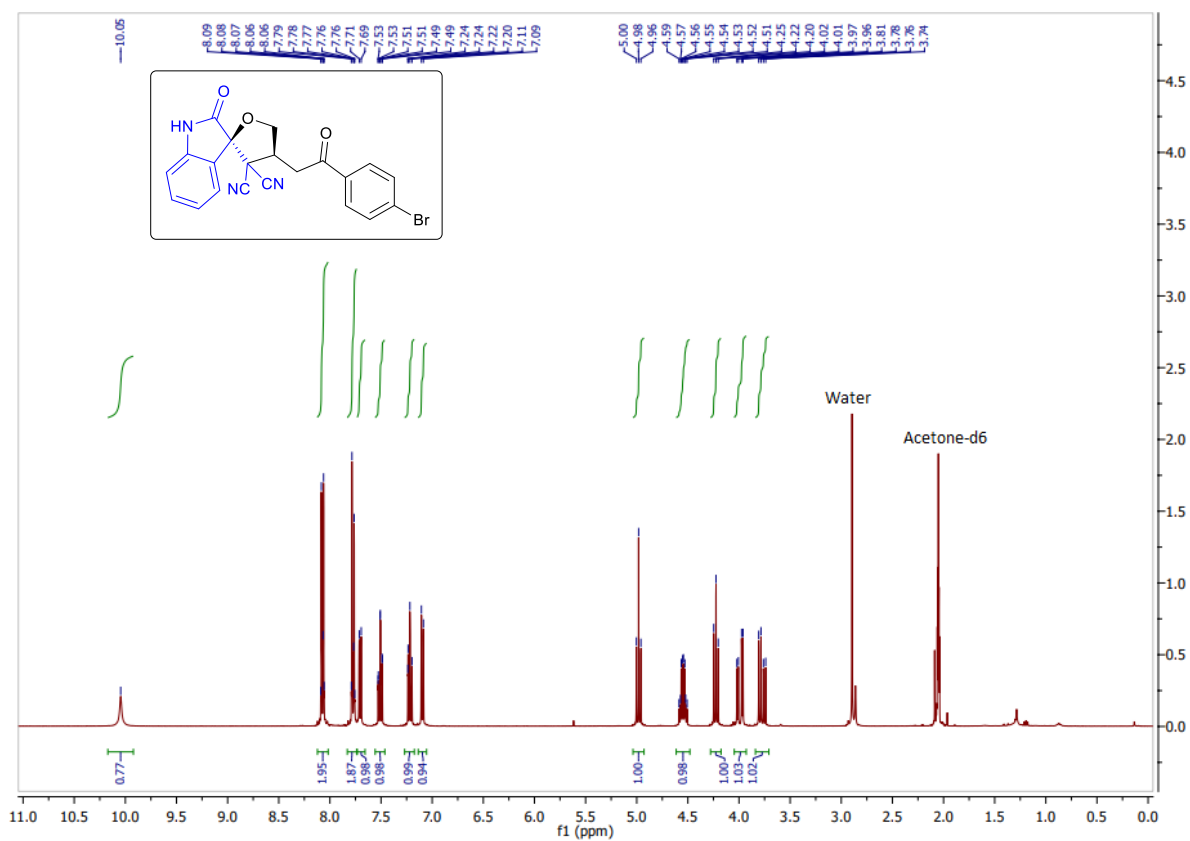
400 MHz <sup>1</sup>H NMR and 500 MHz <sup>13</sup>C NMR (Acetone-d<sub>6</sub>) Spectra of 3aa



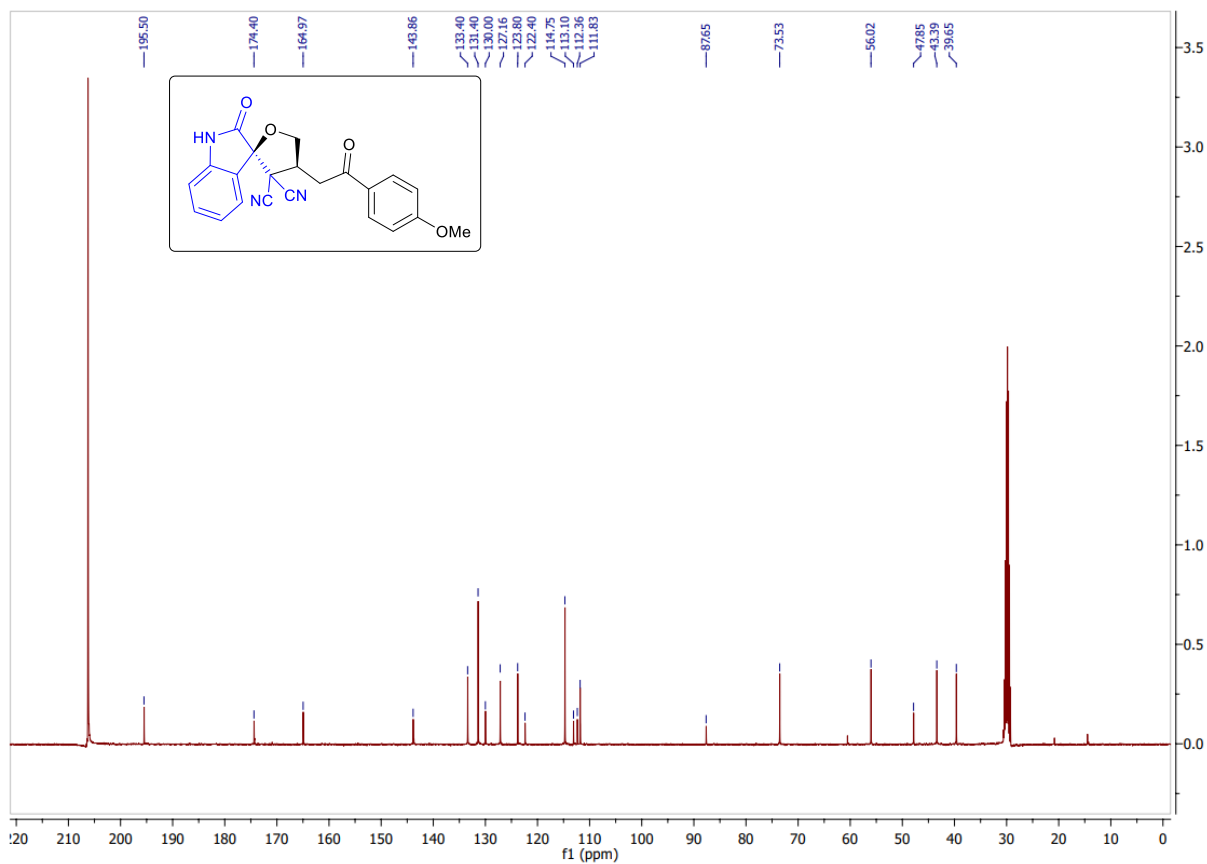
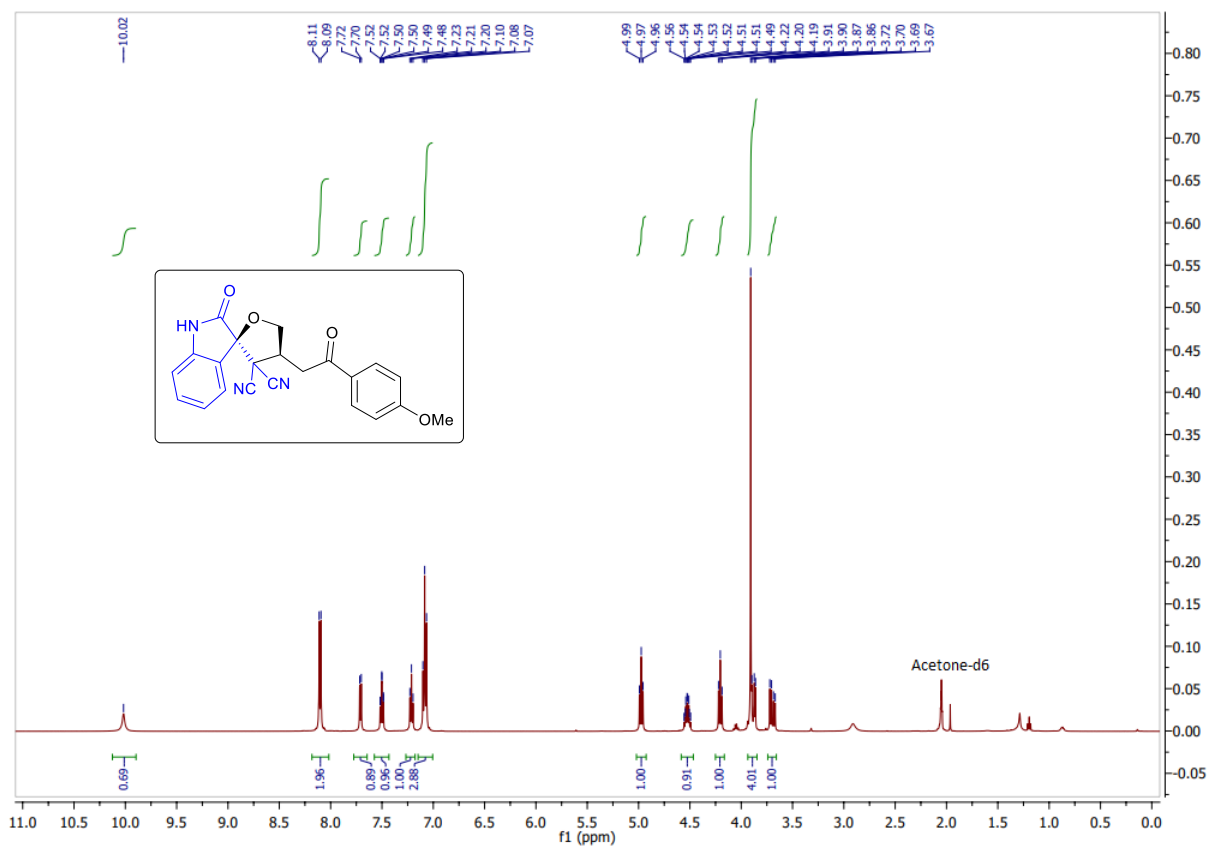
400 MHz <sup>1</sup>H NMR and 400 MHz <sup>13</sup>C NMR (Acetone-d<sub>6</sub>) Spectra of 3ab



400 MHz <sup>1</sup>H NMR and 400 MHz <sup>13</sup>C NMR (Acetone-d<sub>6</sub>) Spectra of 3ac

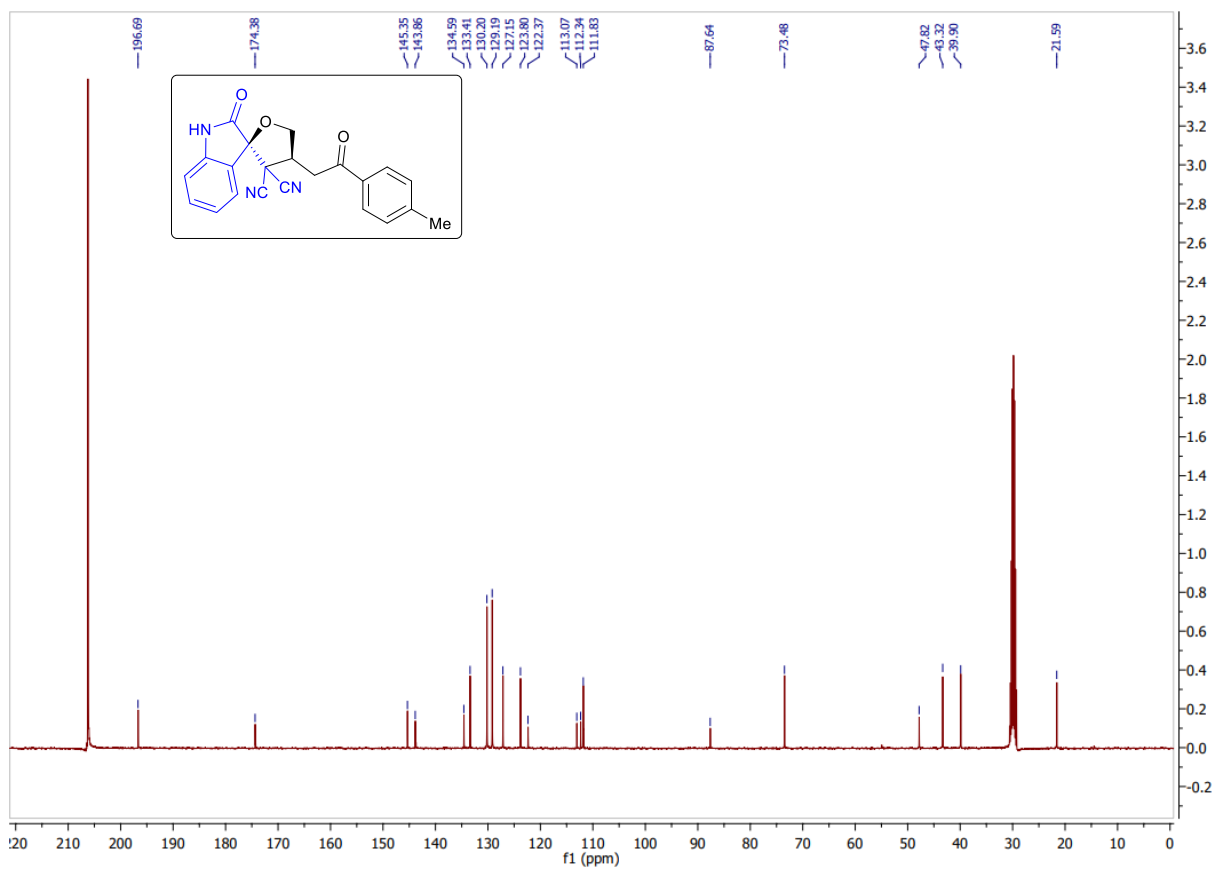
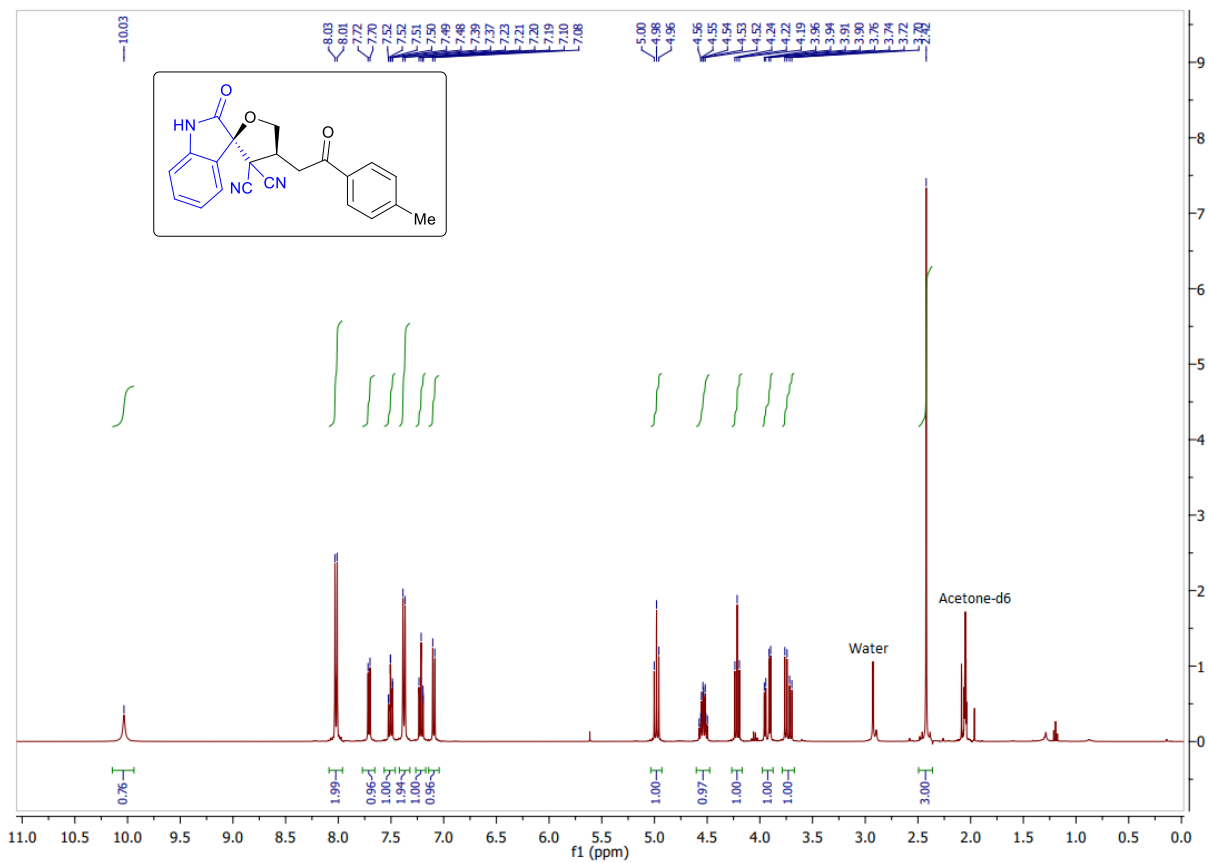


400 MHz  $^1\text{H}$  NMR and 400 MHz  $^{13}\text{C}$  NMR (Acetone- $d_6$ ) Spectra of 3ad

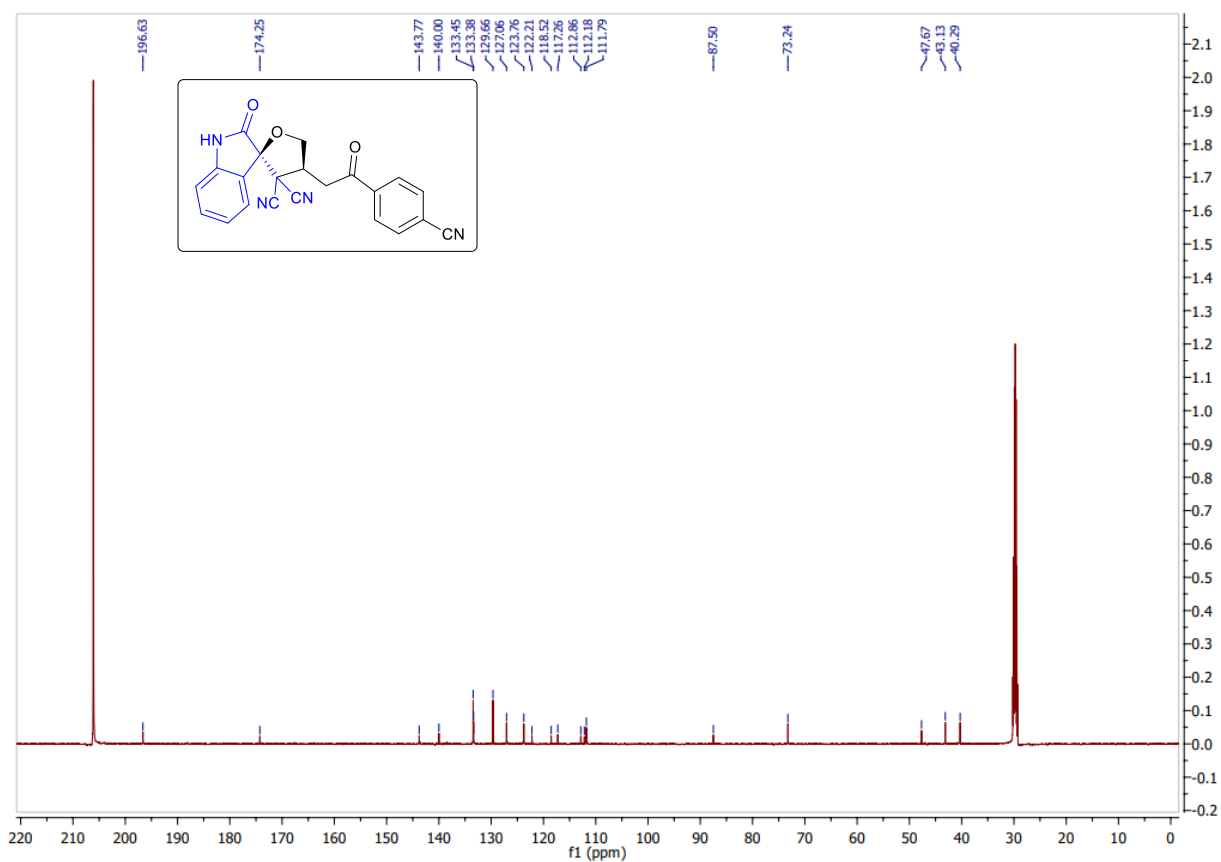
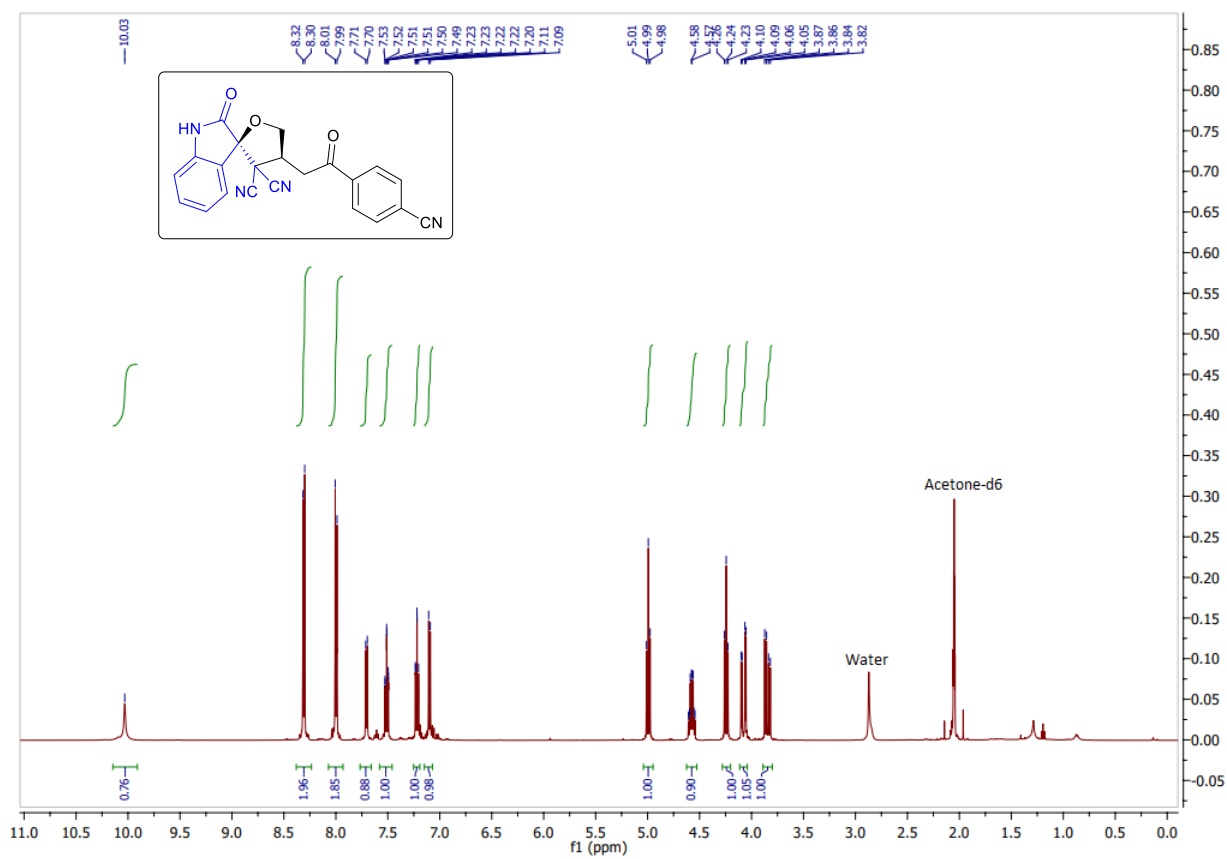


500 MHz  $^1\text{H}$  NMR and 400 MHz  $^{13}\text{C}$  NMR (Acetone- $d_6$ ) Spectra of 3ae

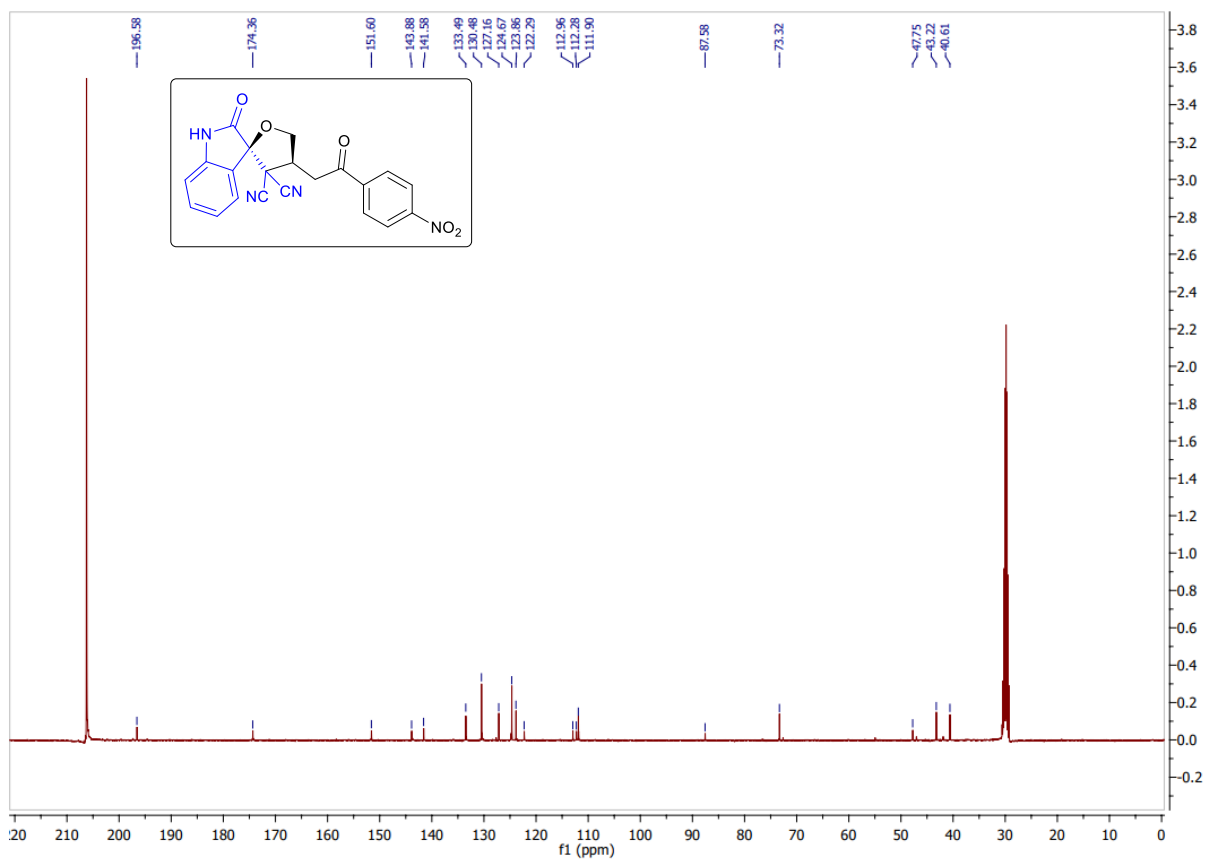
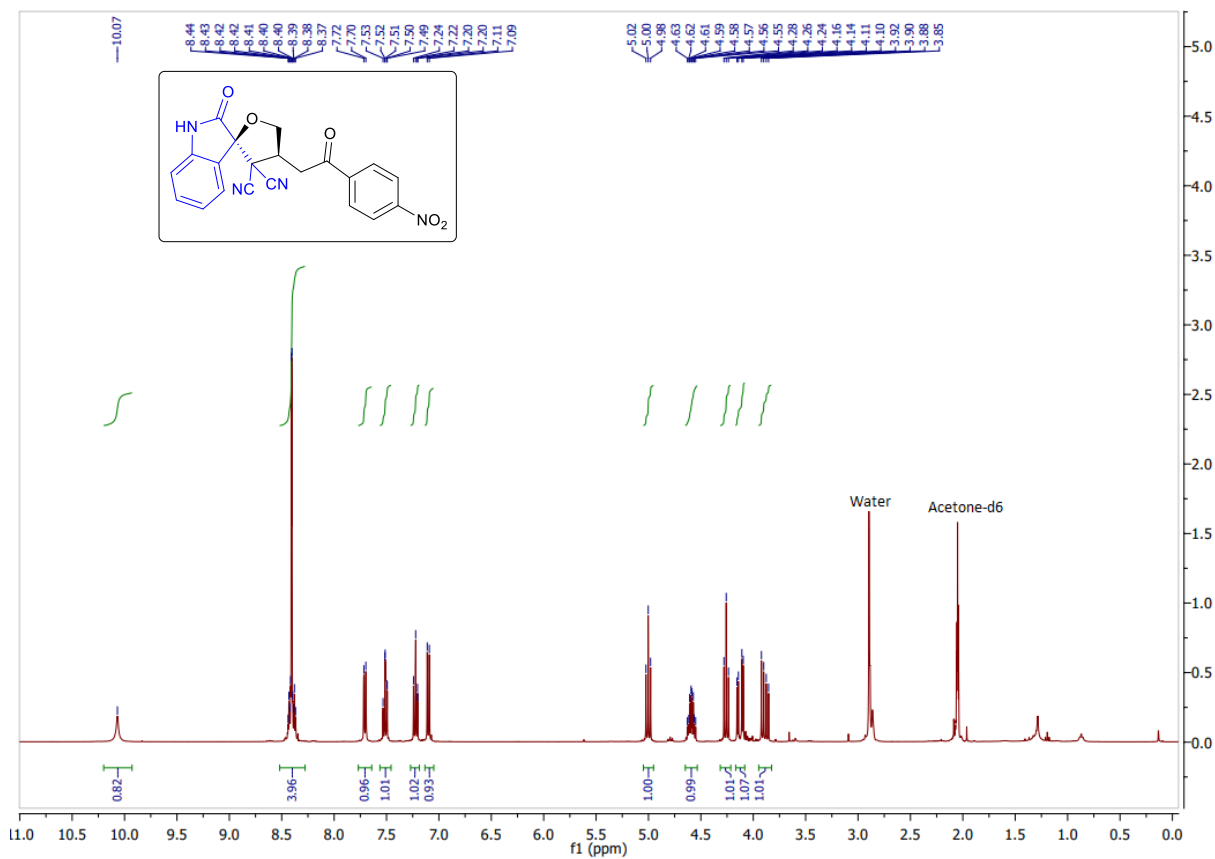




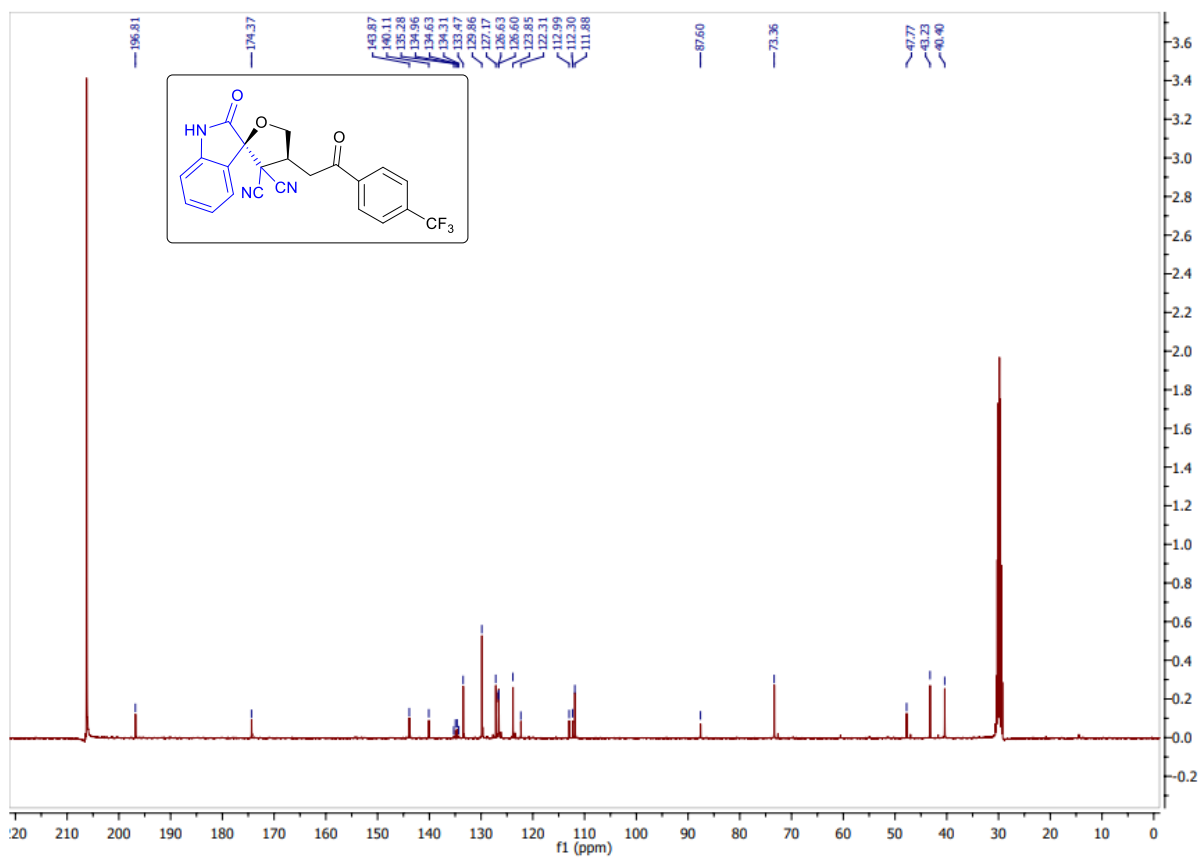
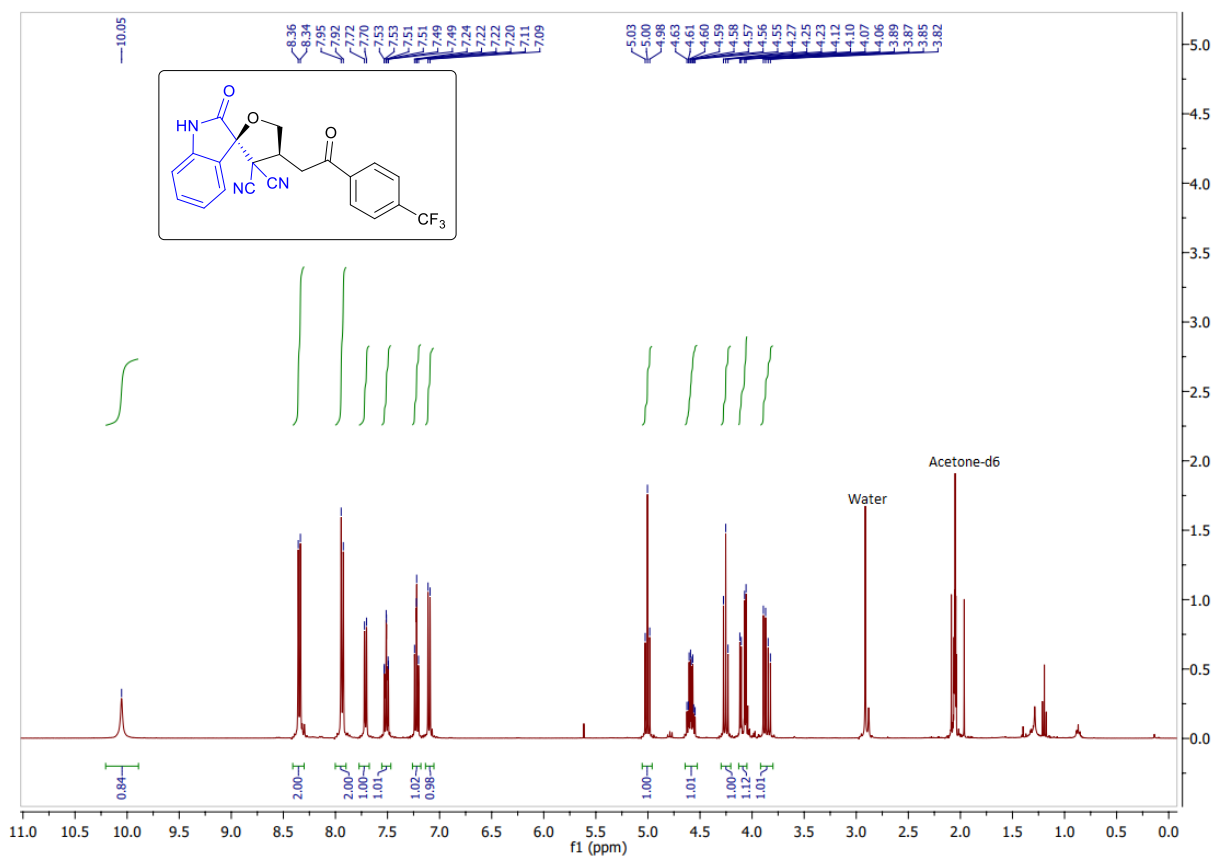
400 MHz  $^1\text{H}$  NMR and 400 MHz  $^{13}\text{C}$  NMR (Acetone- $d_6$ ) Spectra of 3af



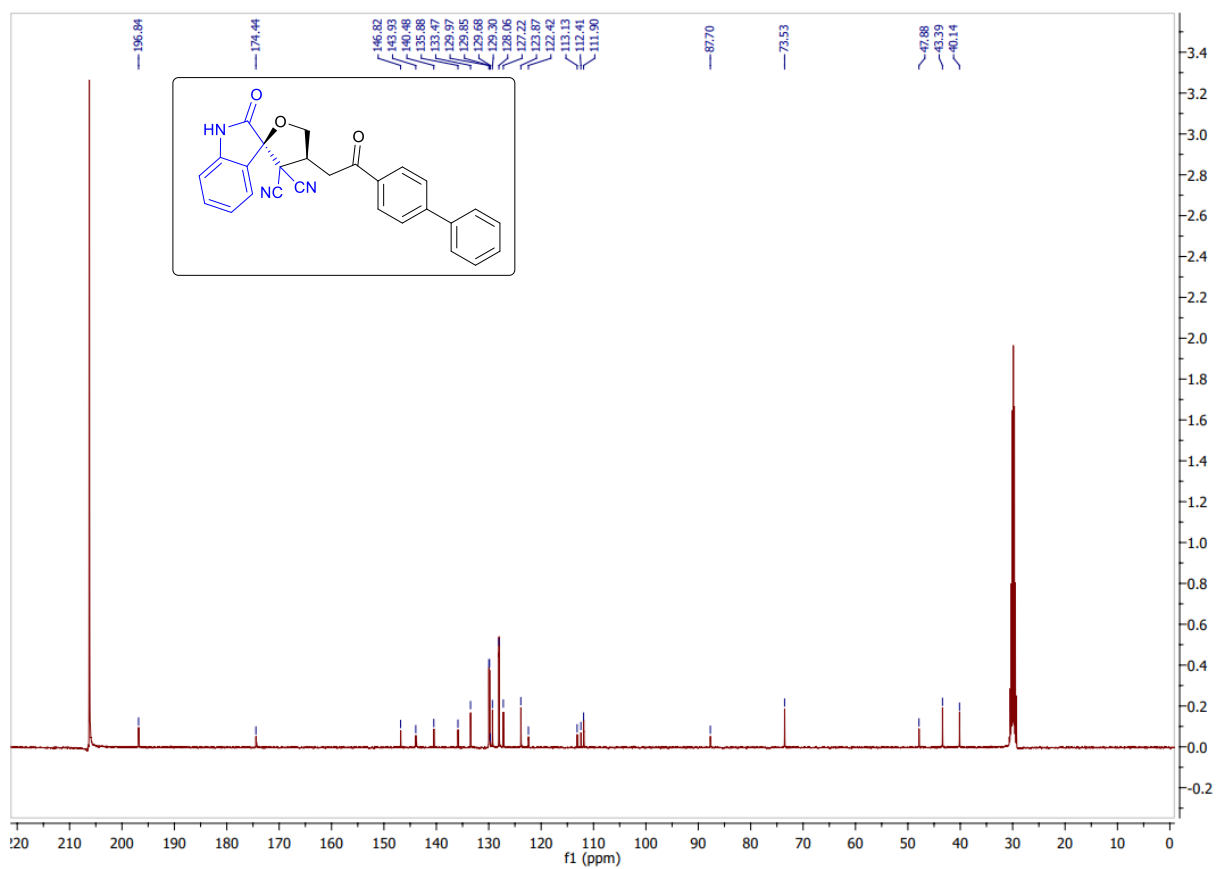
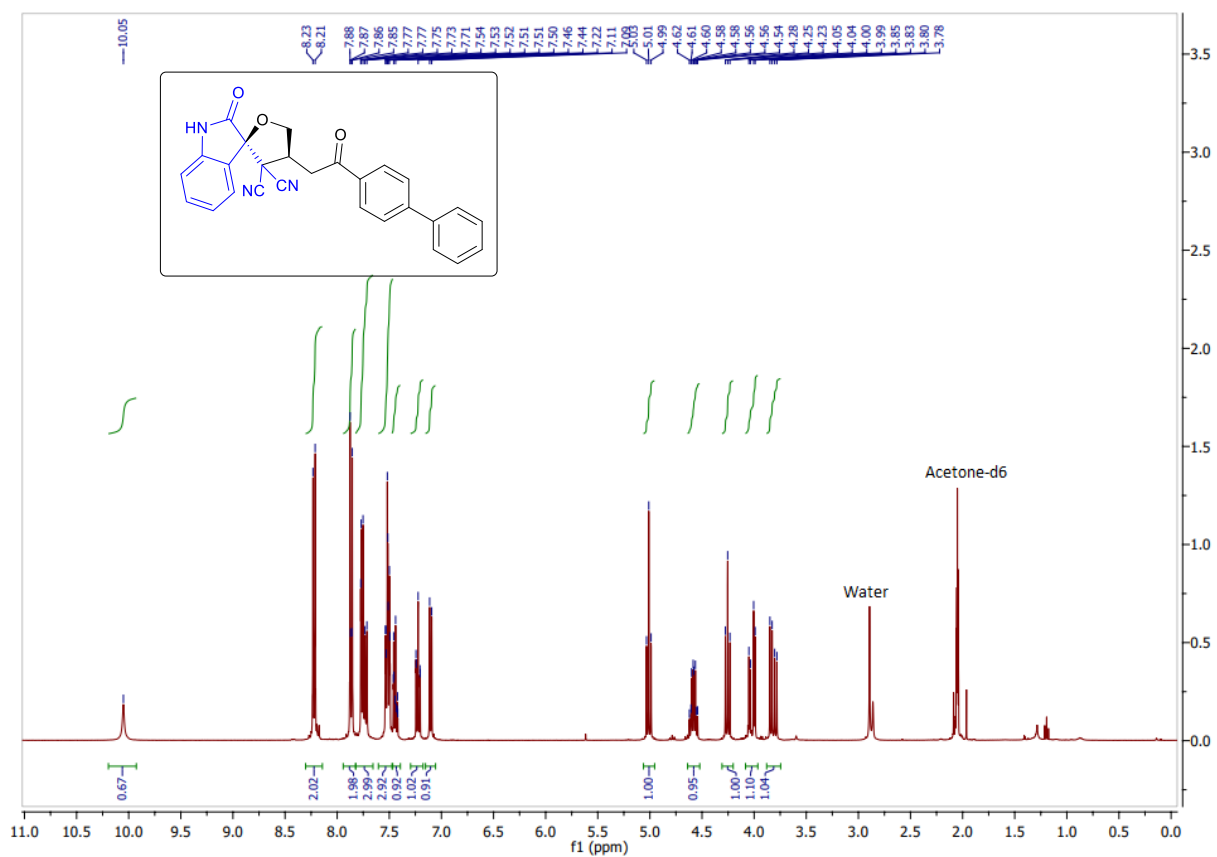
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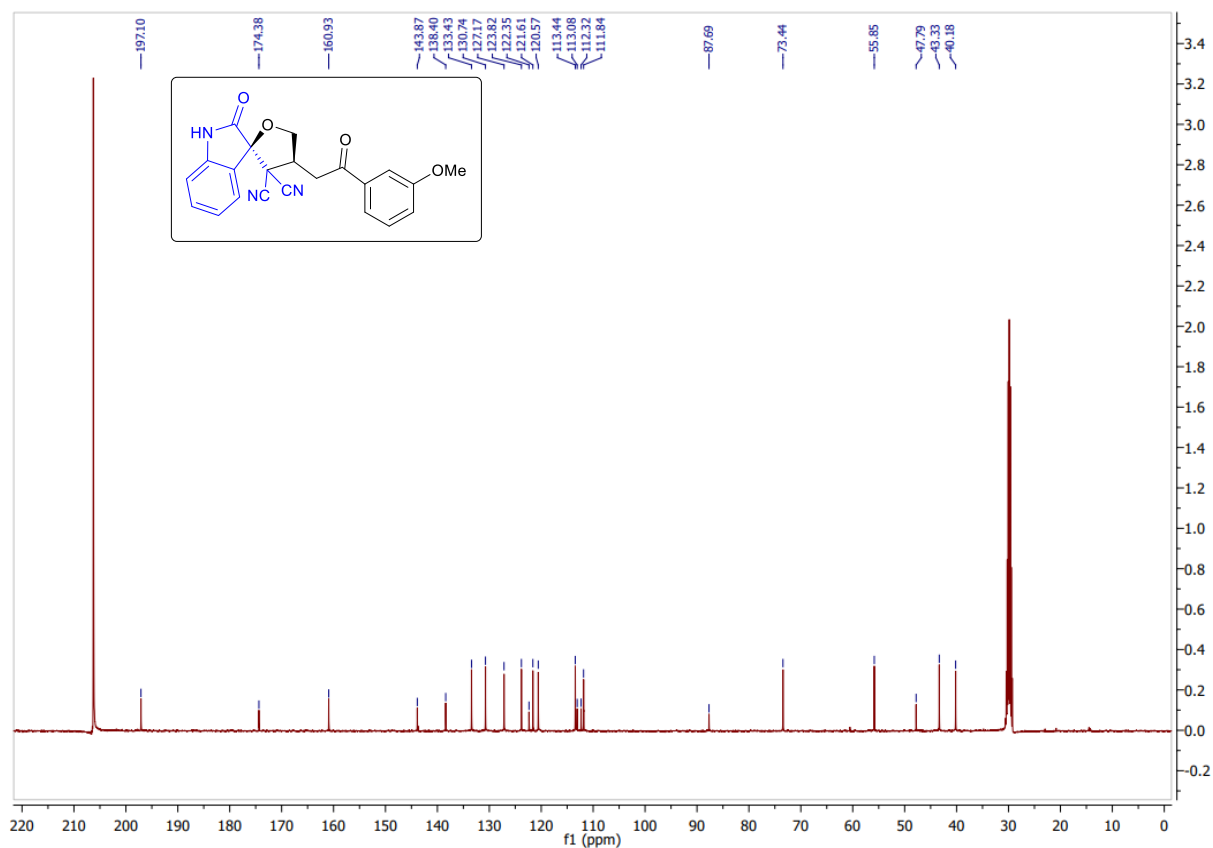
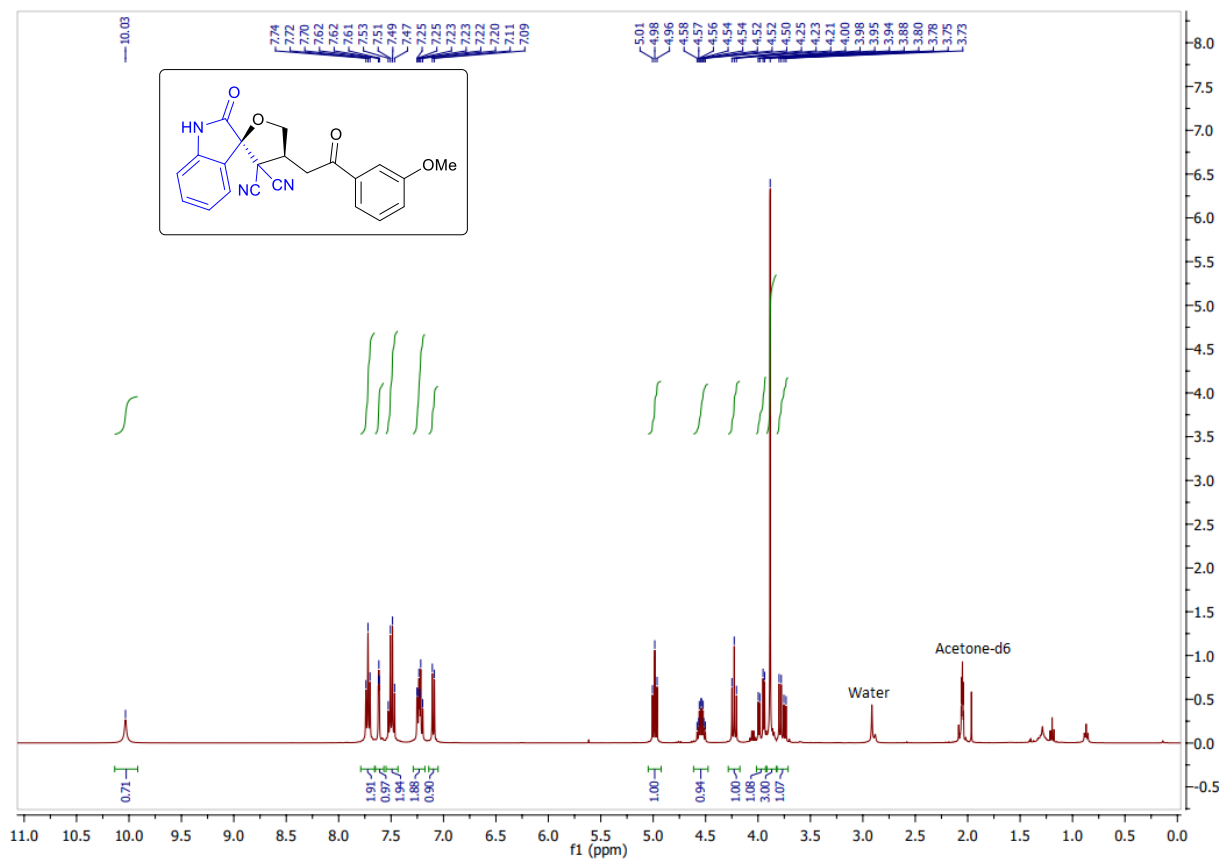
400 MHz  $^1\text{H}$  NMR and 400 MHz  $^{13}\text{C}$  NMR (Acetone- $d_6$ ) Spectra of 3ah



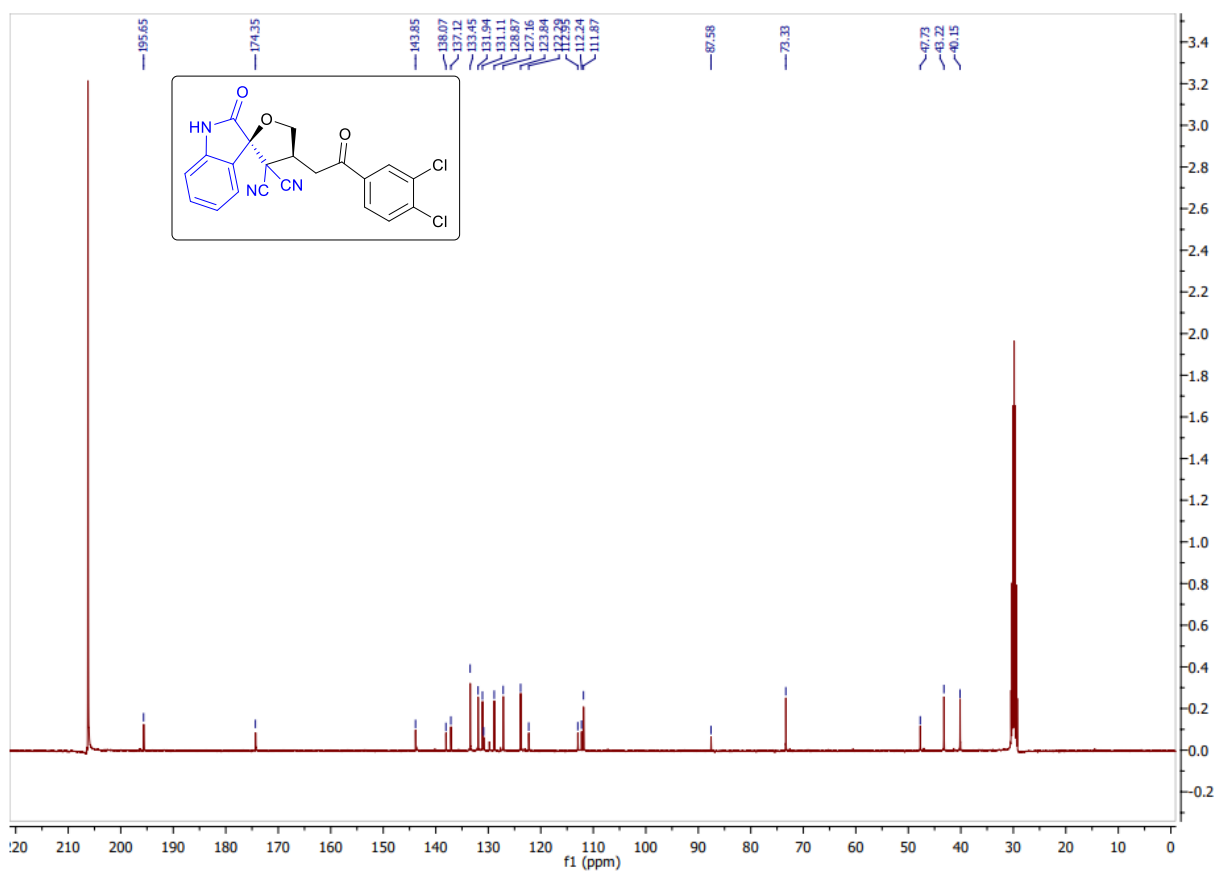
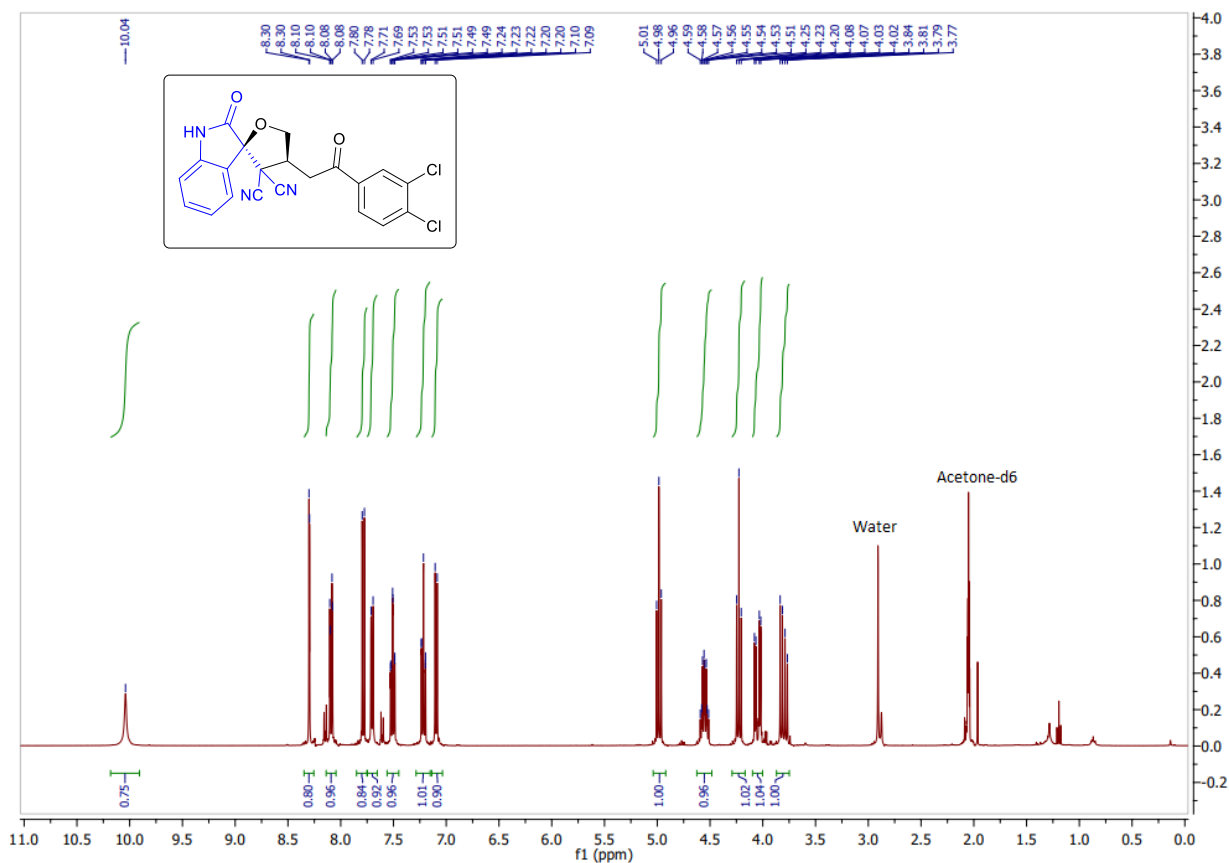
400 MHz <sup>1</sup>H NMR and 400 MHz <sup>13</sup>C NMR (Acetone-d<sub>6</sub>) Spectra of 3ai



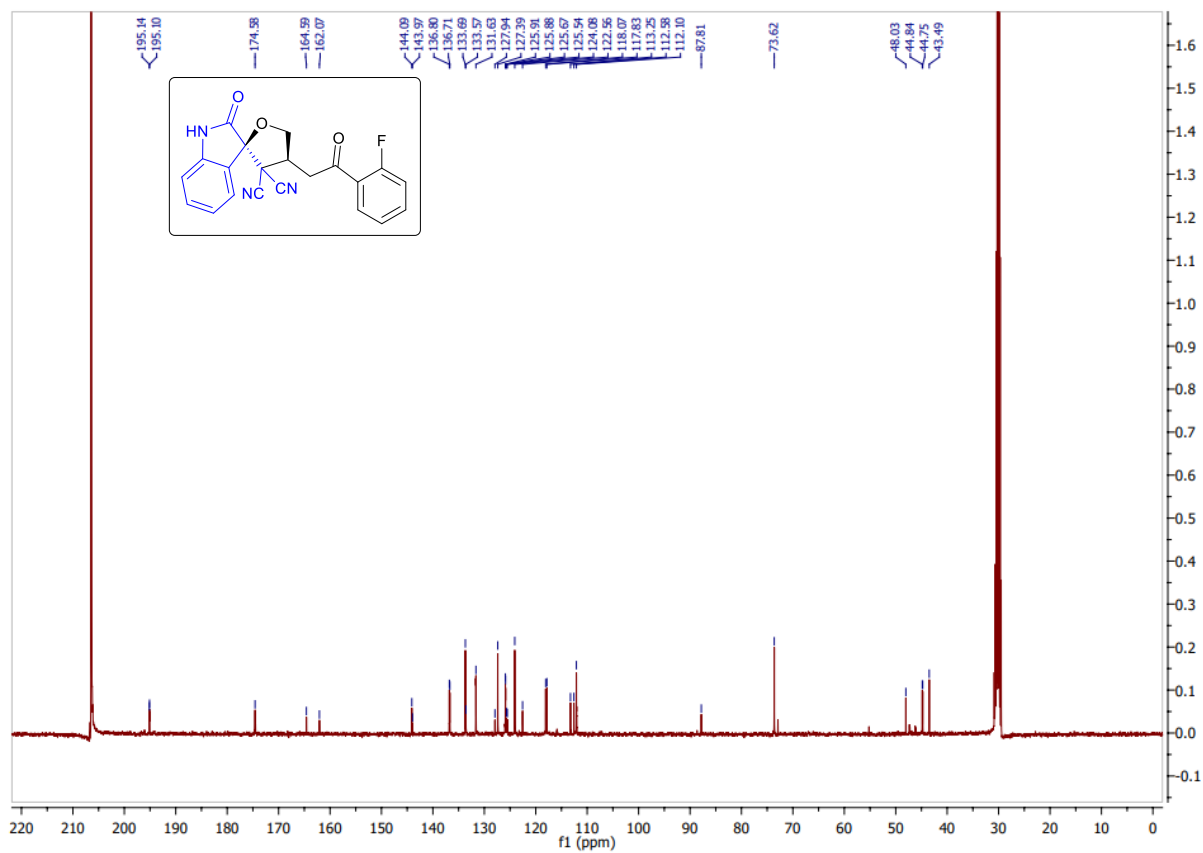
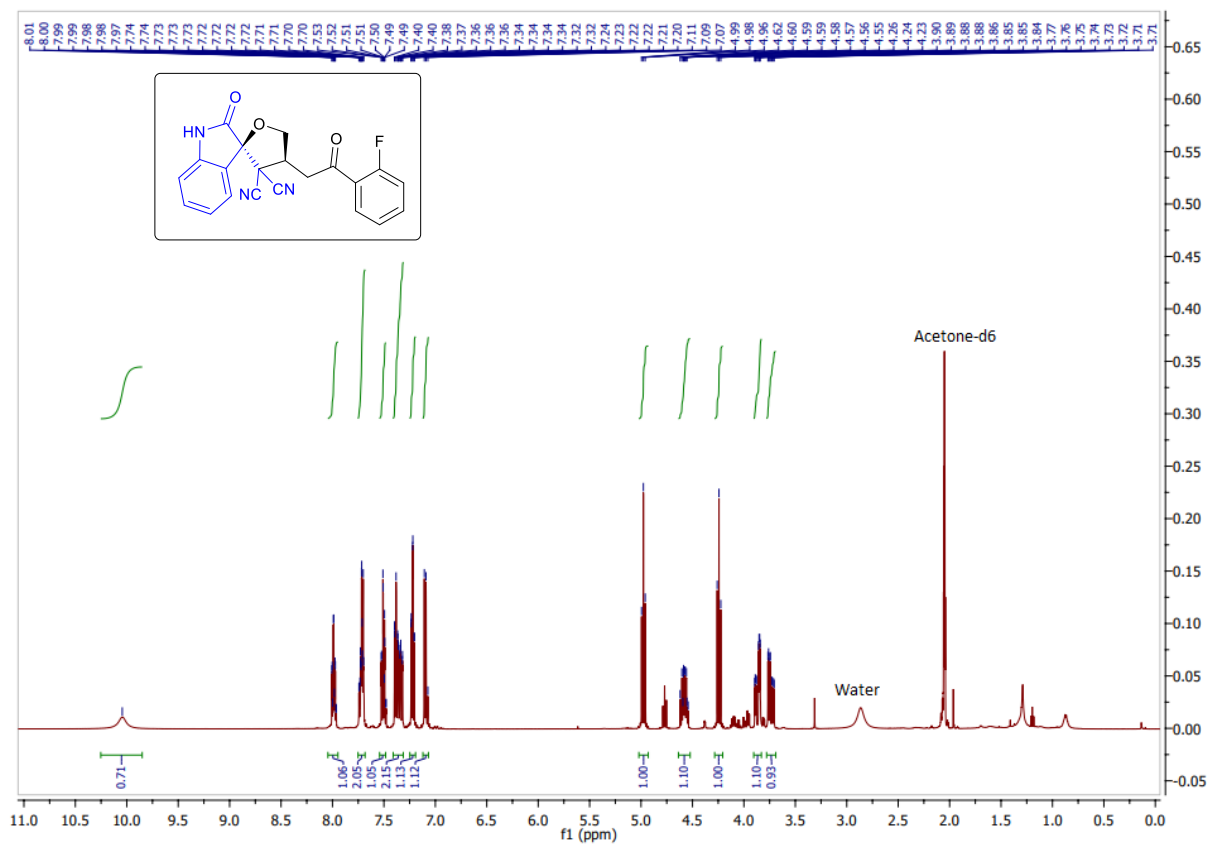
400 MHz  $^1\text{H}$  NMR and 400 MHz  $^{13}\text{C}$  NMR (Acetone- $d_6$ ) Spectra of 3aj



400 MHz  $^1\text{H}$  NMR and 400 MHz  $^{13}\text{C}$  NMR (Acetone- $d_6$ ) Spectra of 3ak

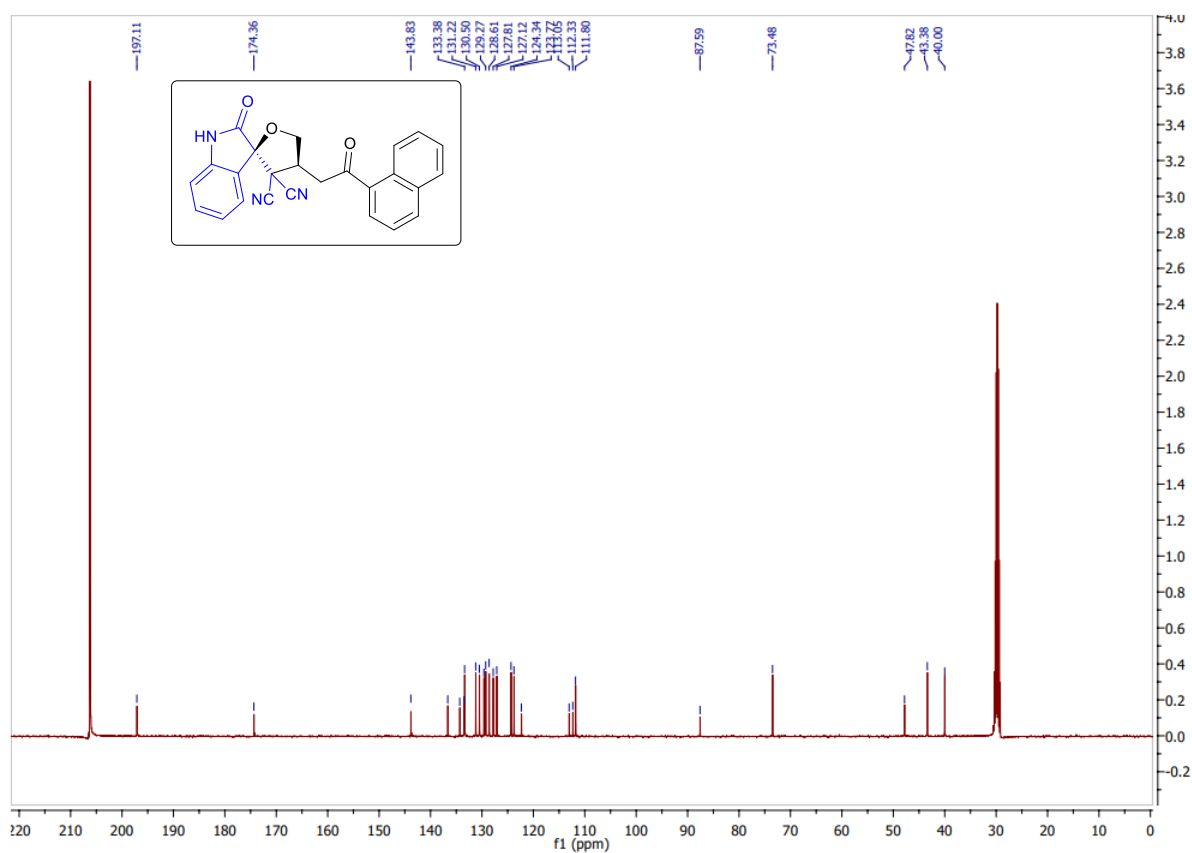
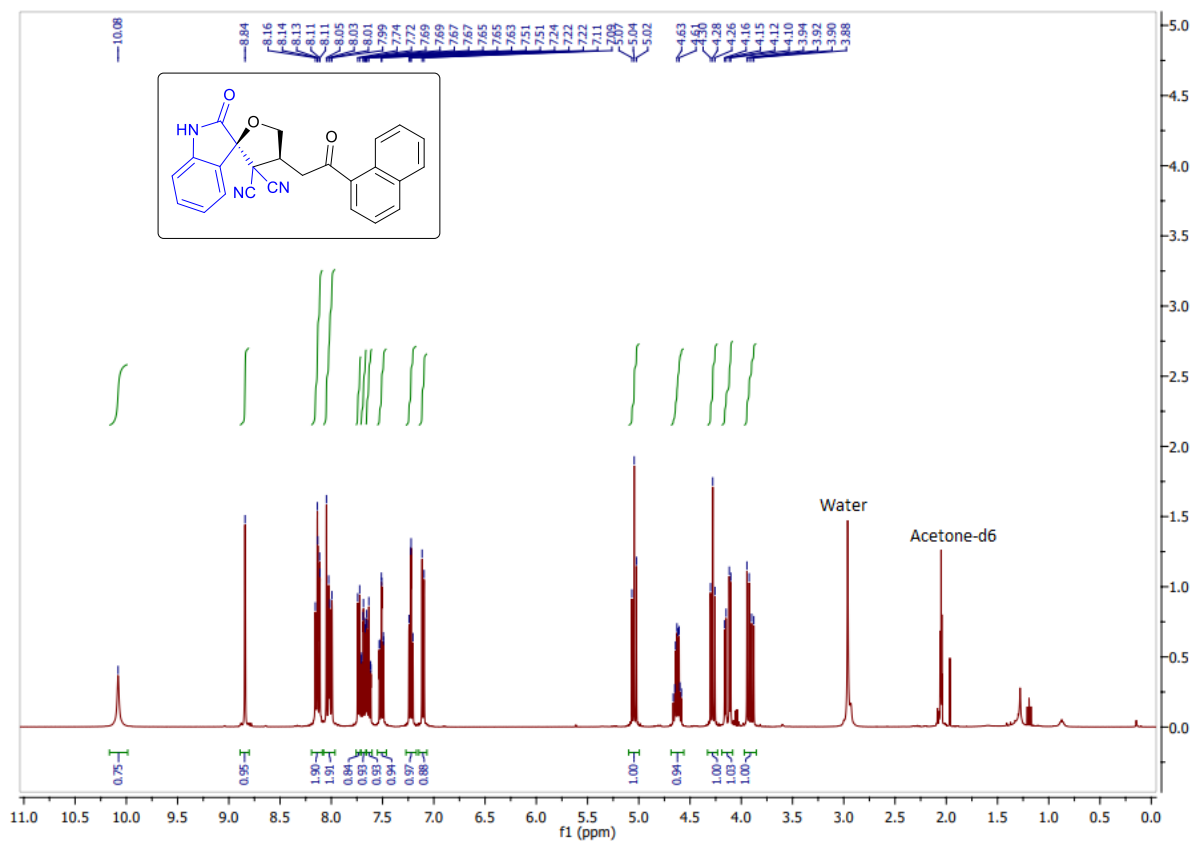


400 MHz <sup>1</sup>H NMR and 400 MHz <sup>13</sup>C NMR (Acetone-d<sub>6</sub>) Spectra of 3aI

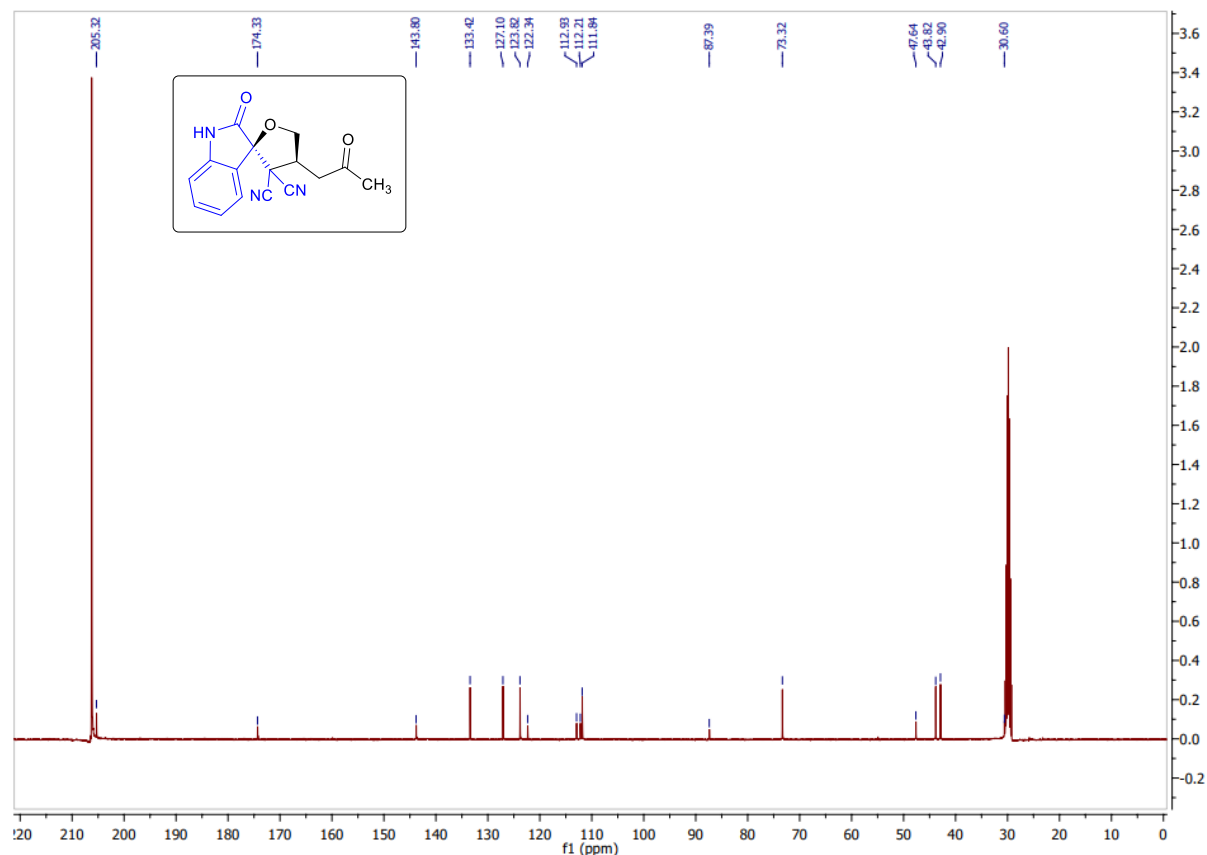
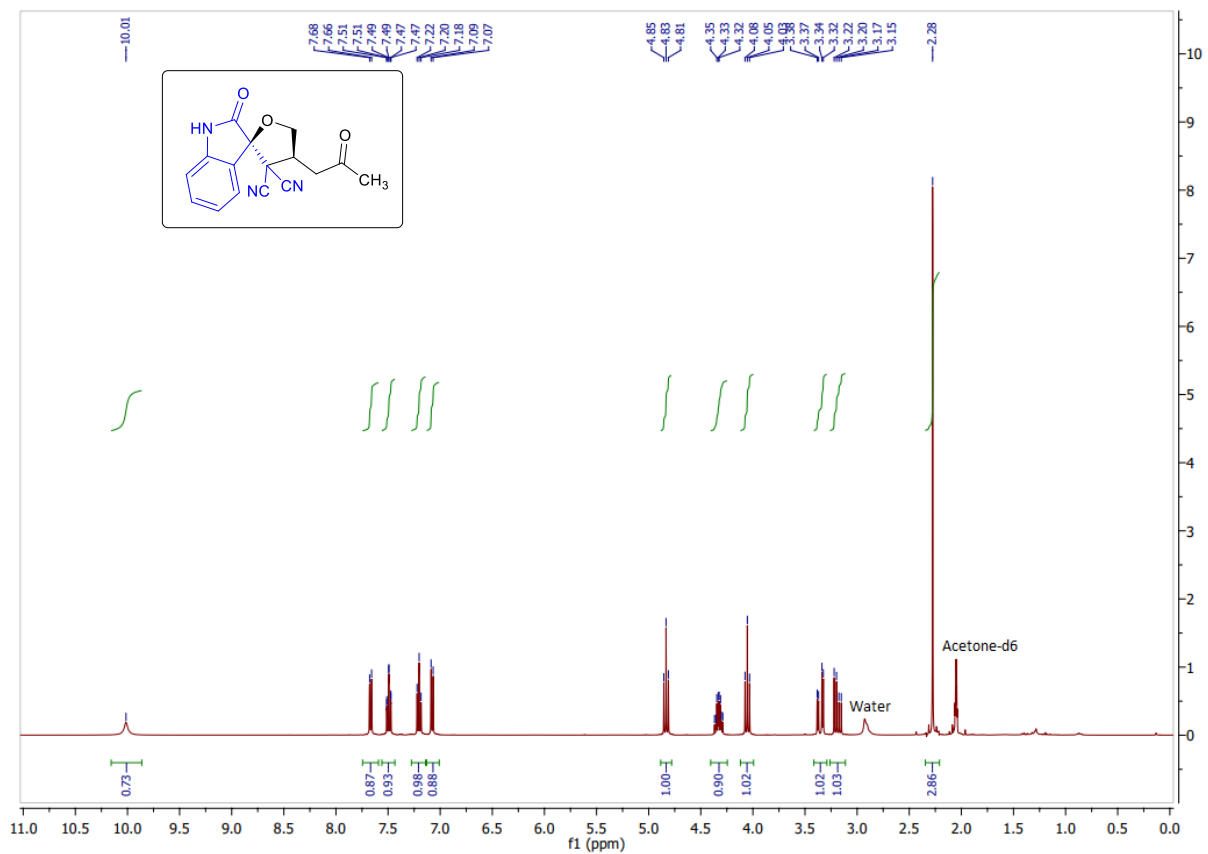


500 MHz  $^1\text{H}$  NMR and 400 MHz  $^{13}\text{C}$  NMR (Acetone- $\text{d}_6$ ) Spectra of 3am

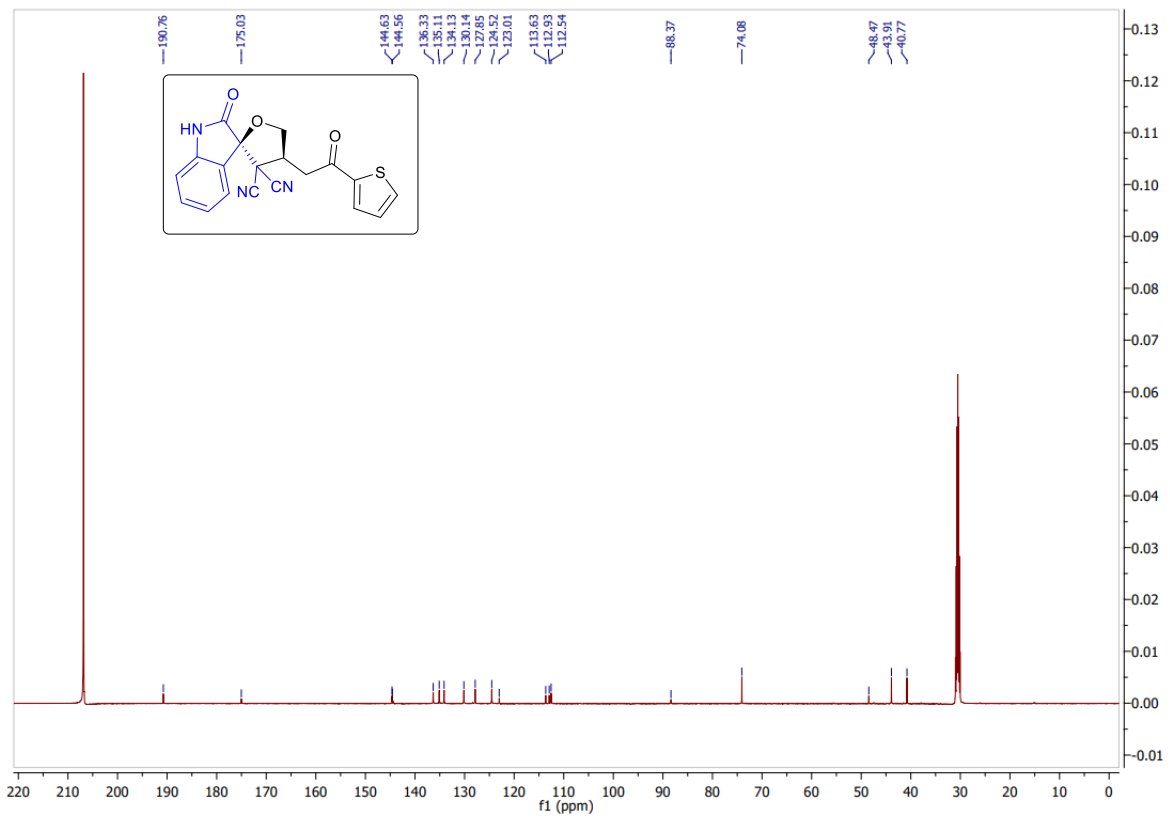
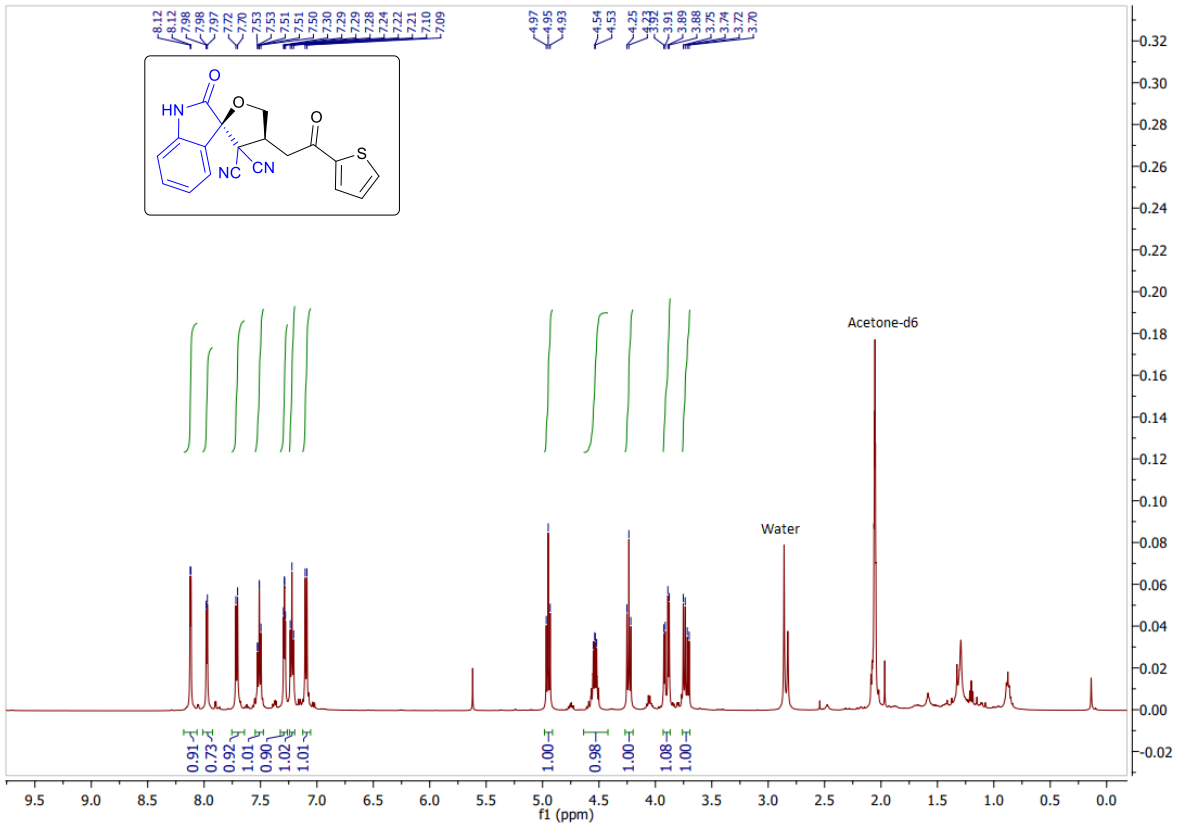




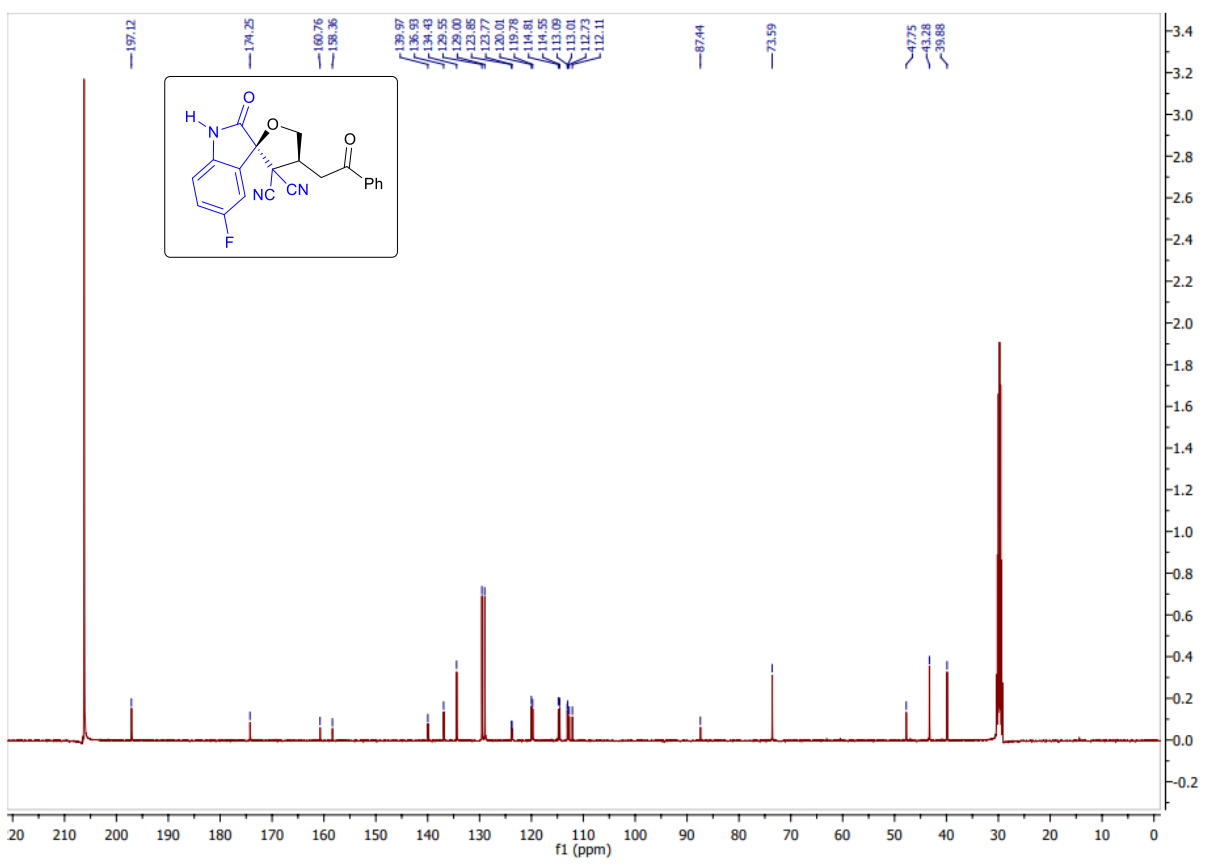
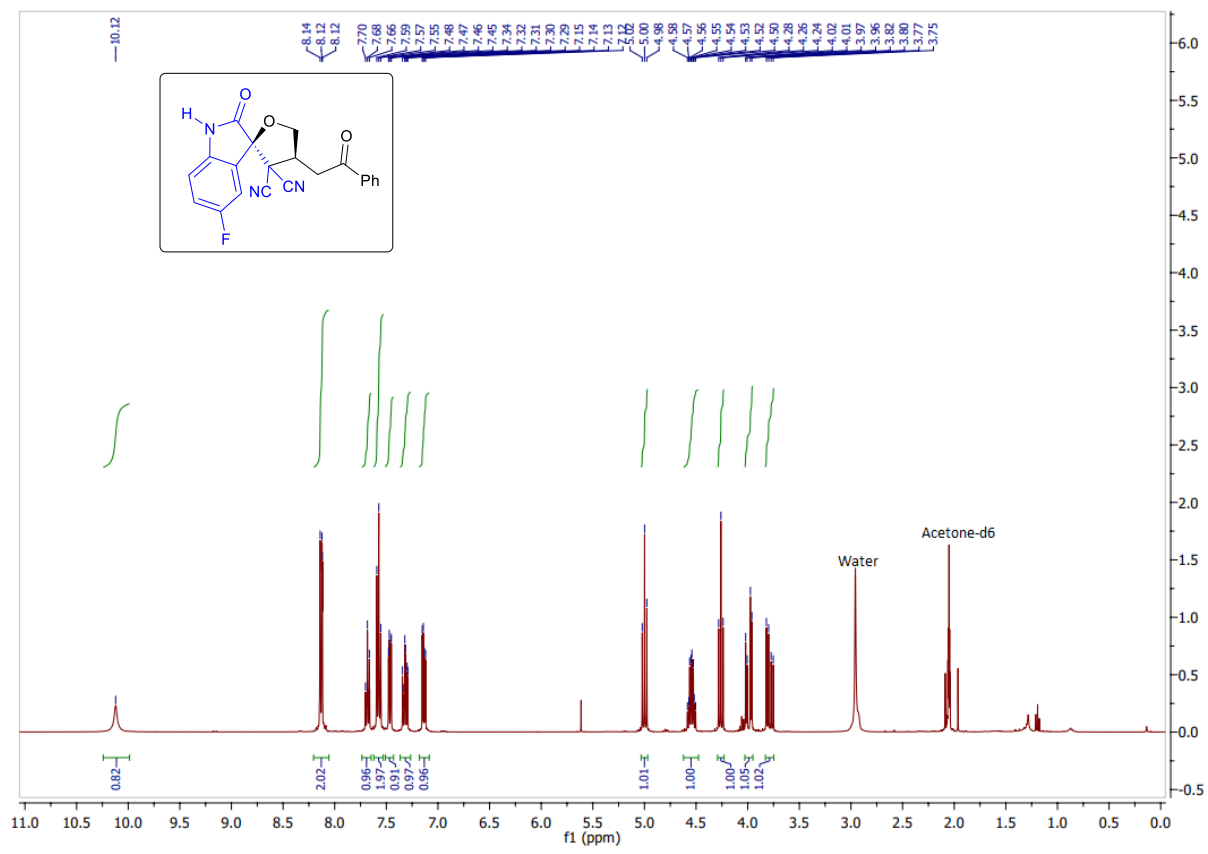
400 MHz  $^1\text{H}$  NMR and 400 MHz  $^{13}\text{C}$  NMR (Acetone- $d_6$ ) Spectra of 3an



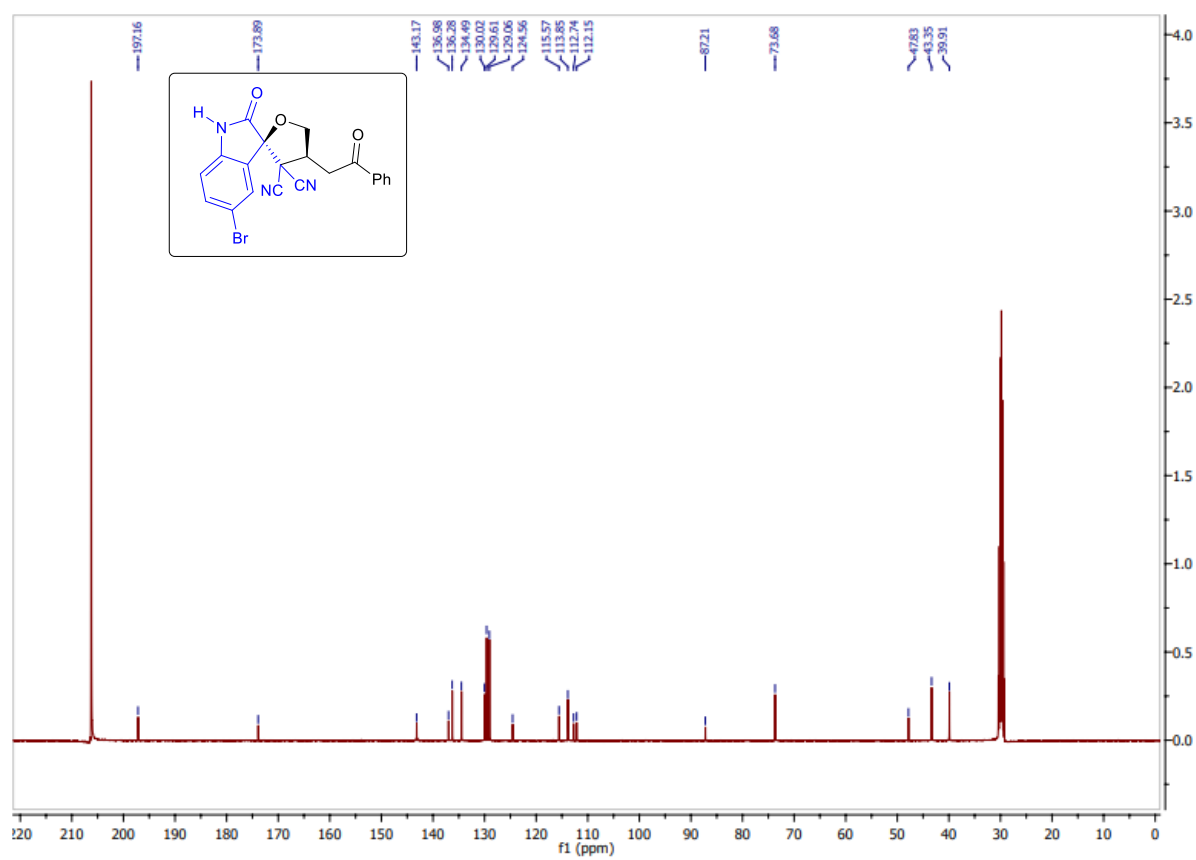
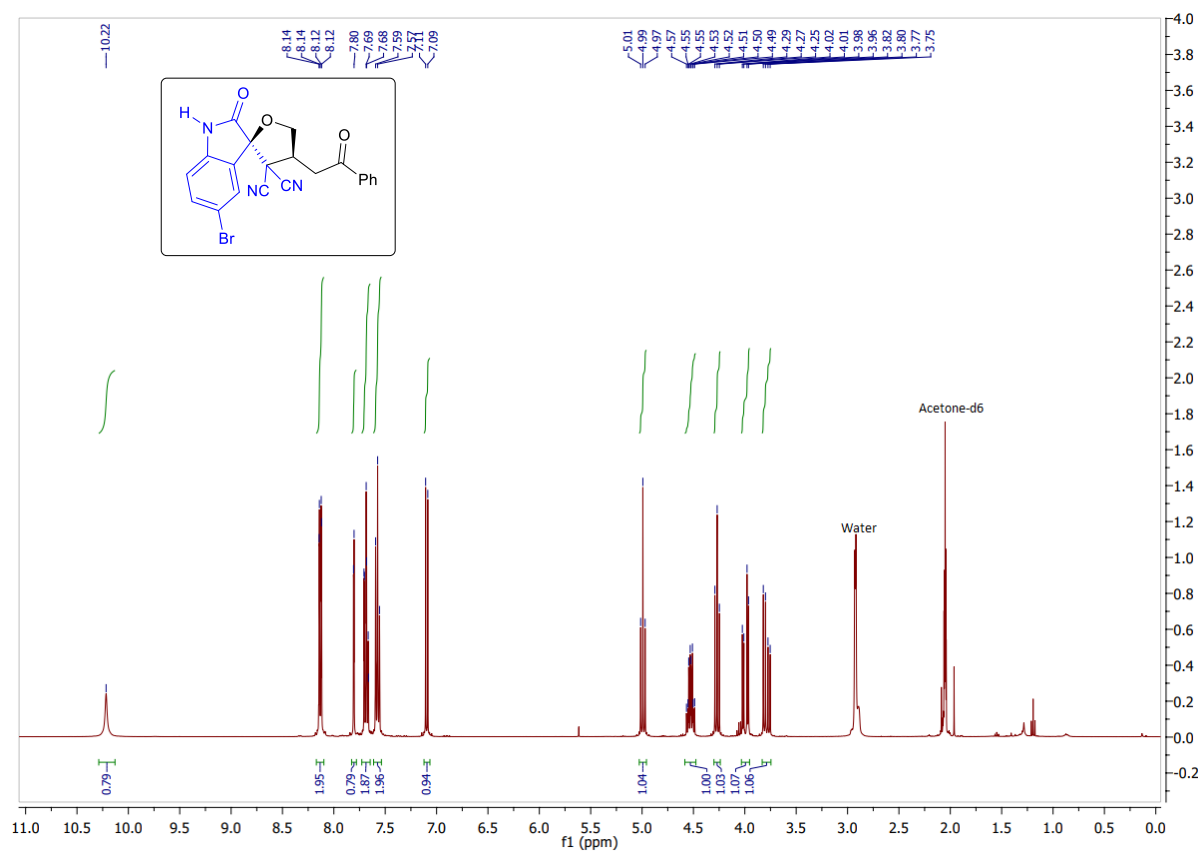
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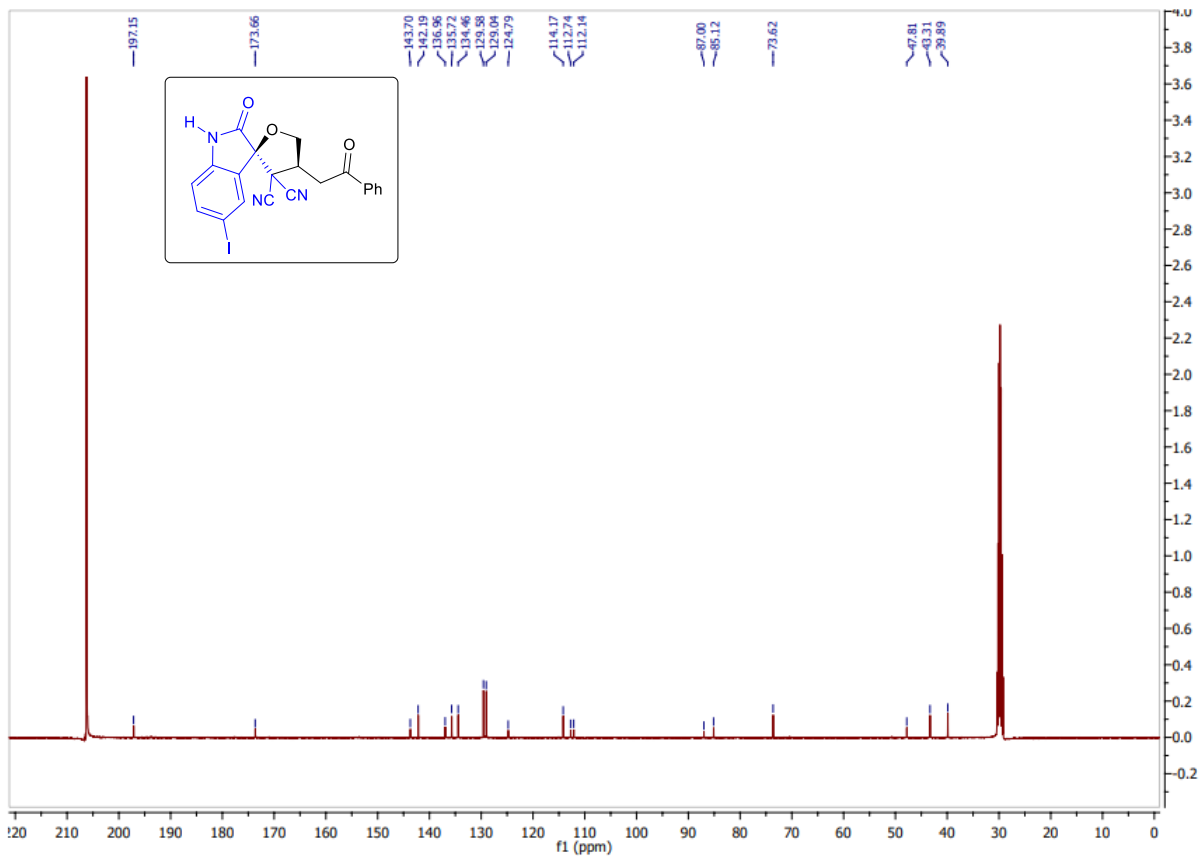
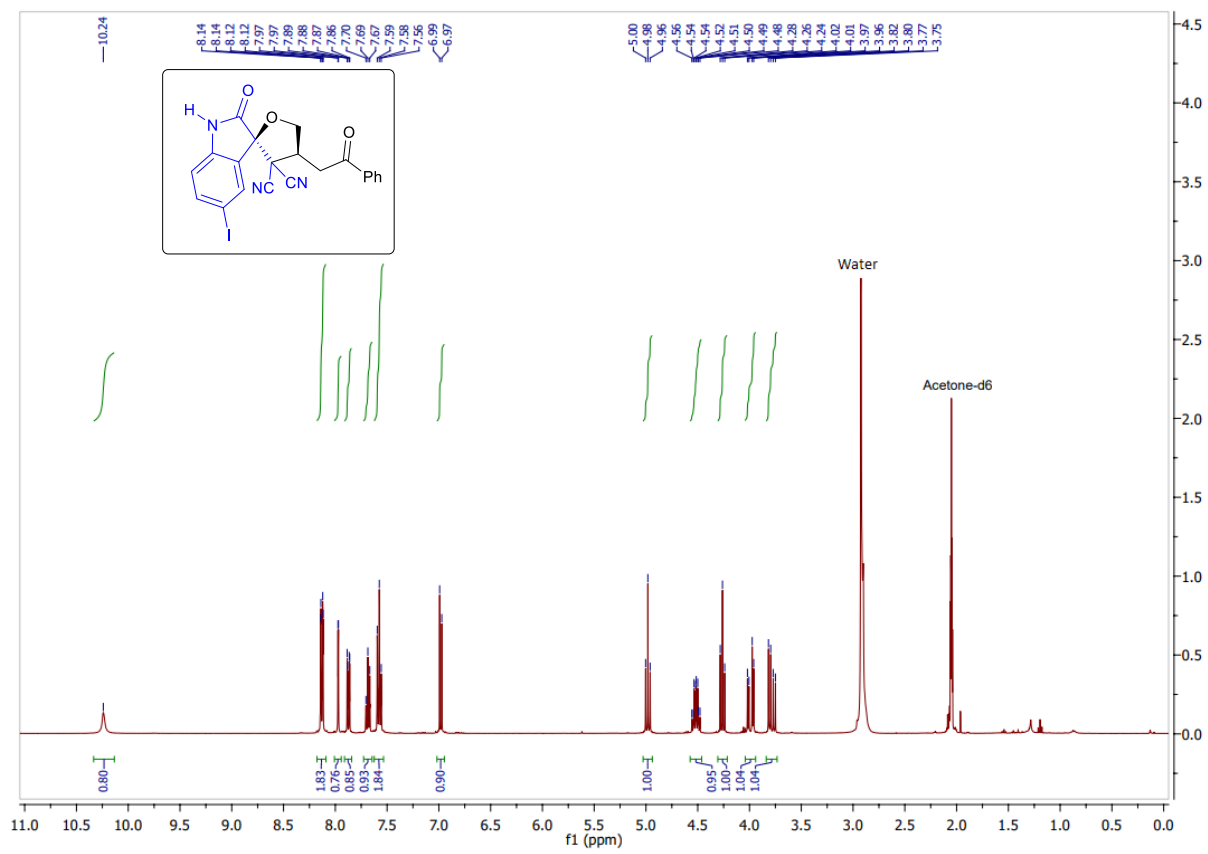
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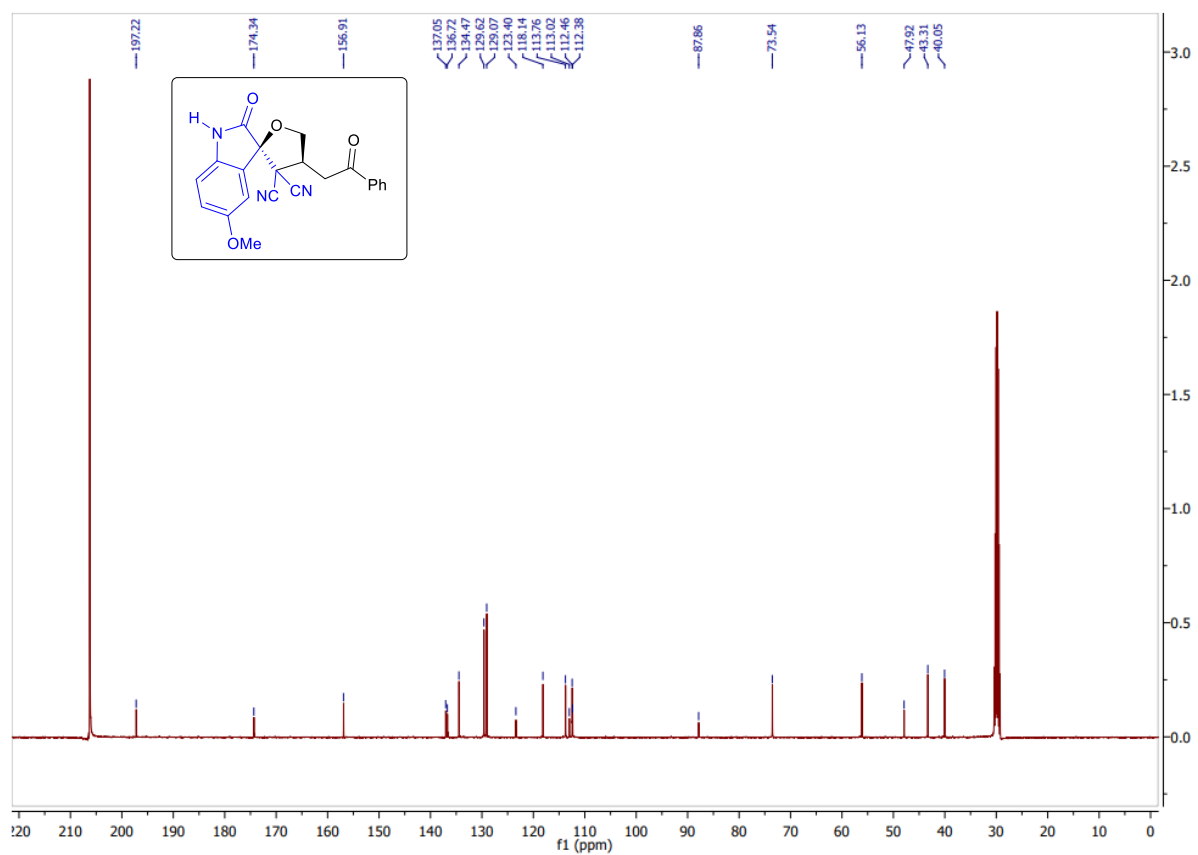
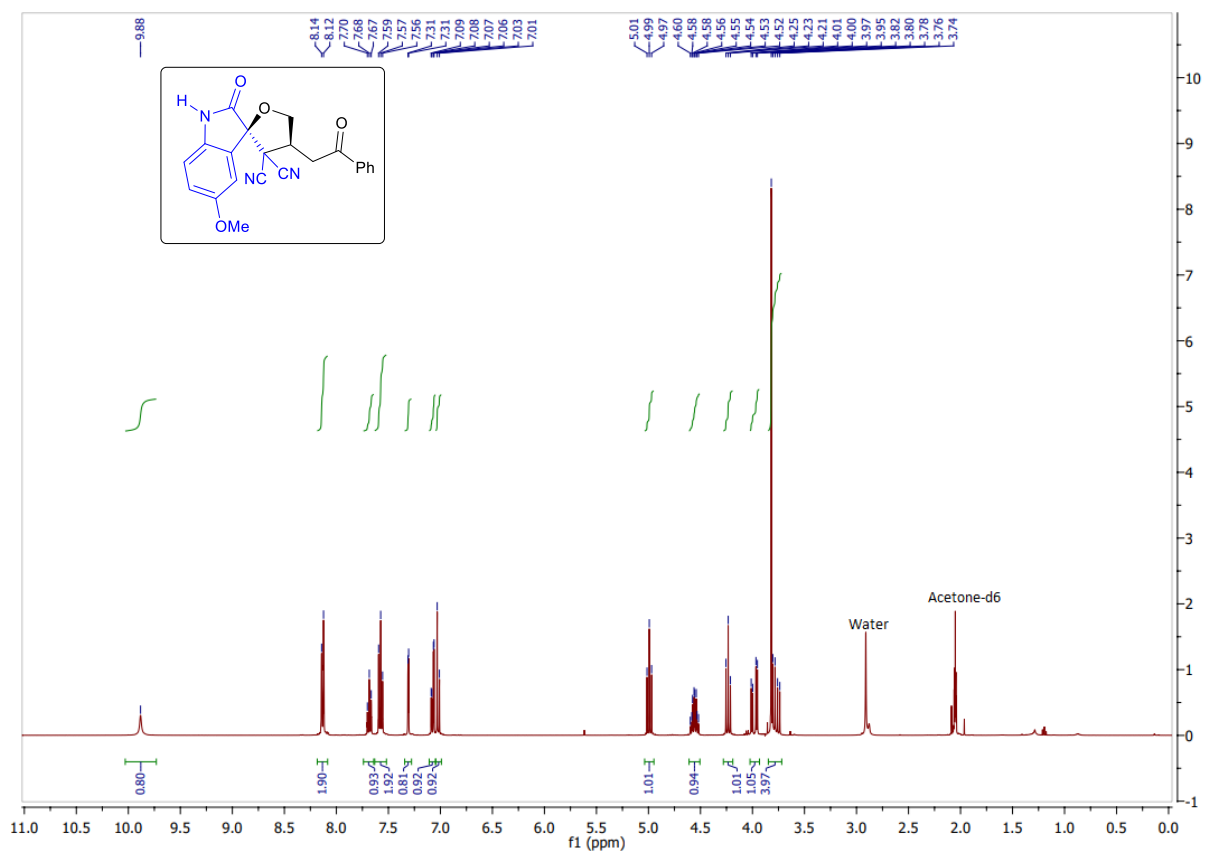
400 MHz <sup>1</sup>H NMR and 400 MHz <sup>13</sup>C NMR (Acetone-d<sub>6</sub>) Spectra of 3ba



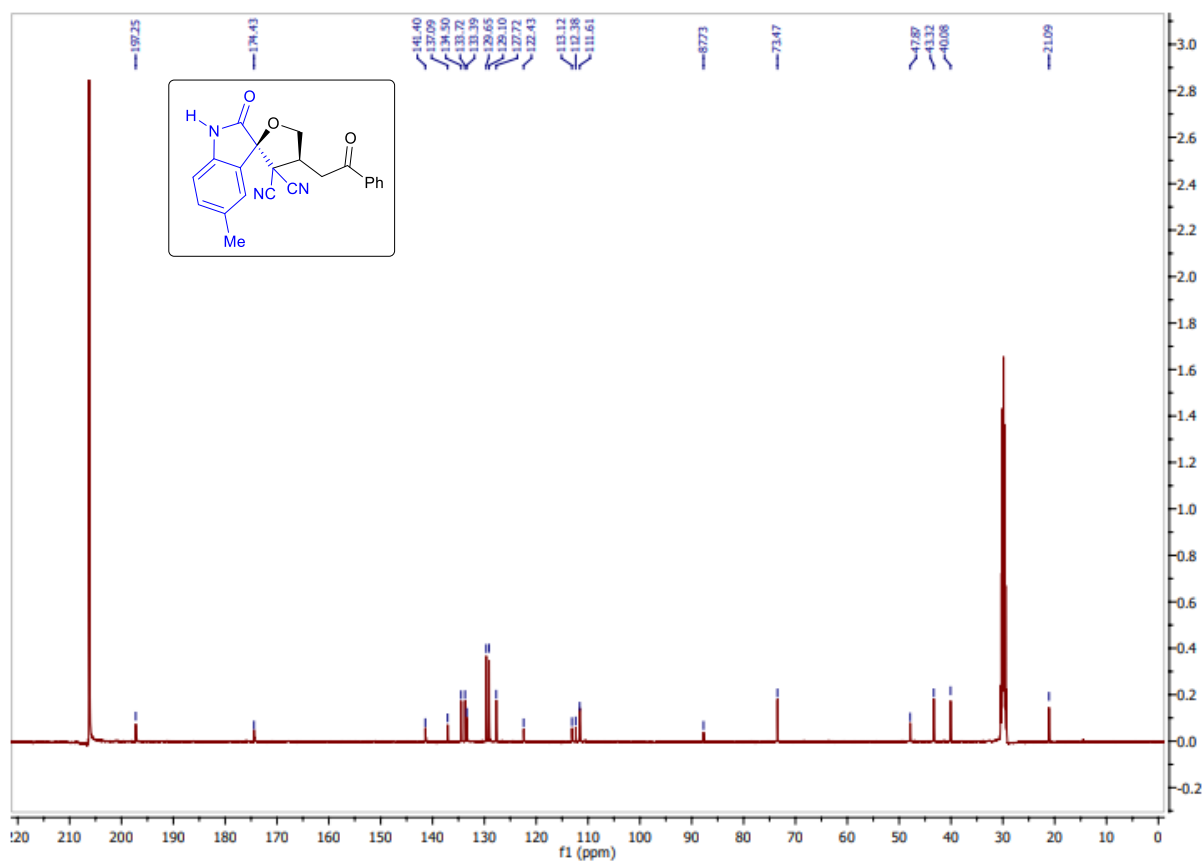
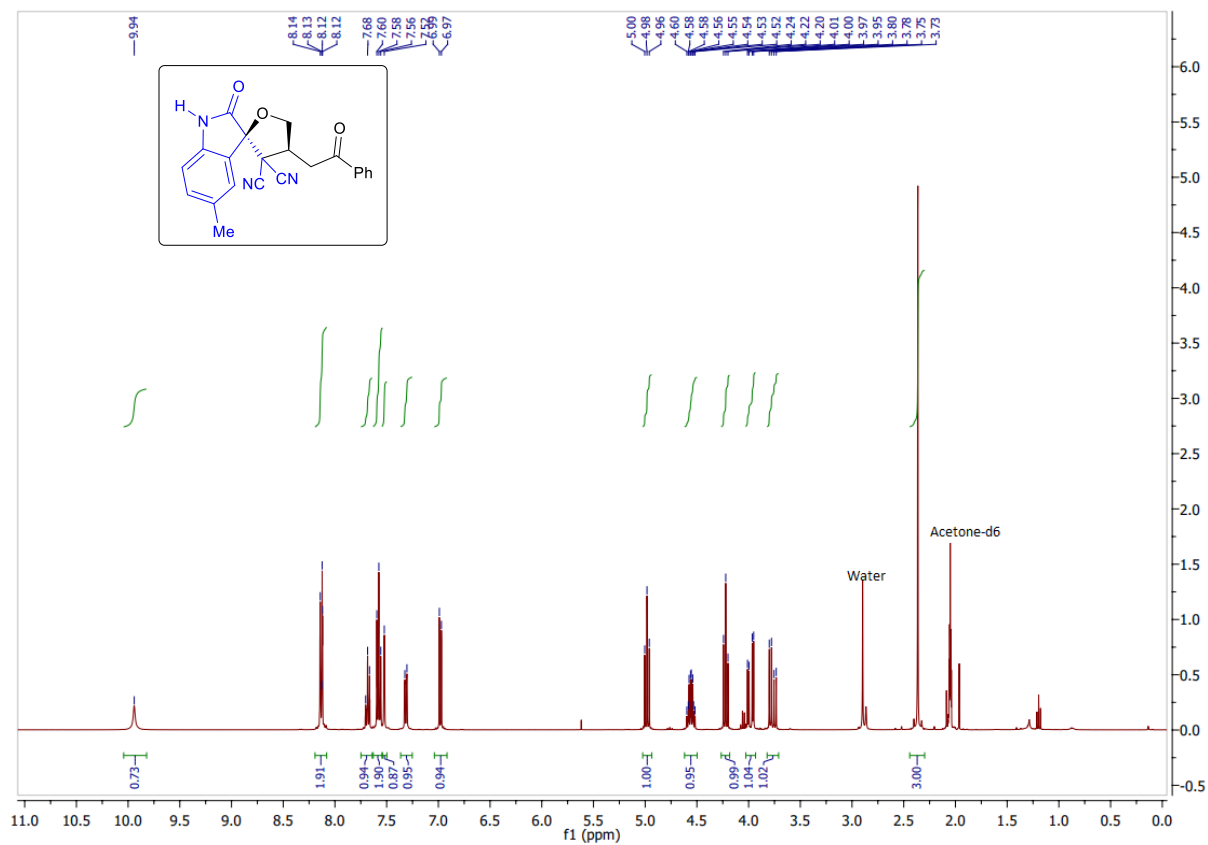
400 MHz <sup>1</sup>H NMR and 400 MHz <sup>13</sup>C NMR (Acetone-d<sub>6</sub>) Spectra of 3ca



400 MHz <sup>1</sup>H NMR and 400 MHz <sup>13</sup>C NMR (Acetone-d6) Spectra of 3da

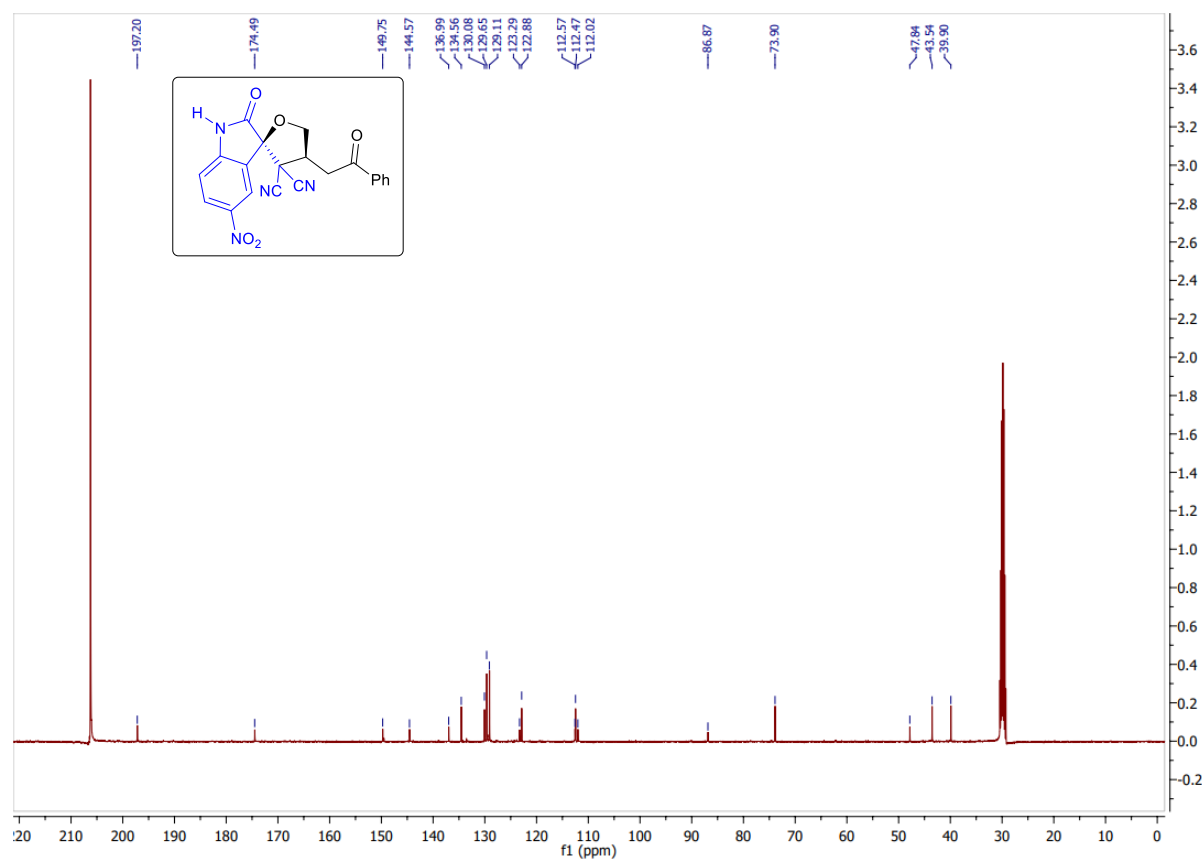
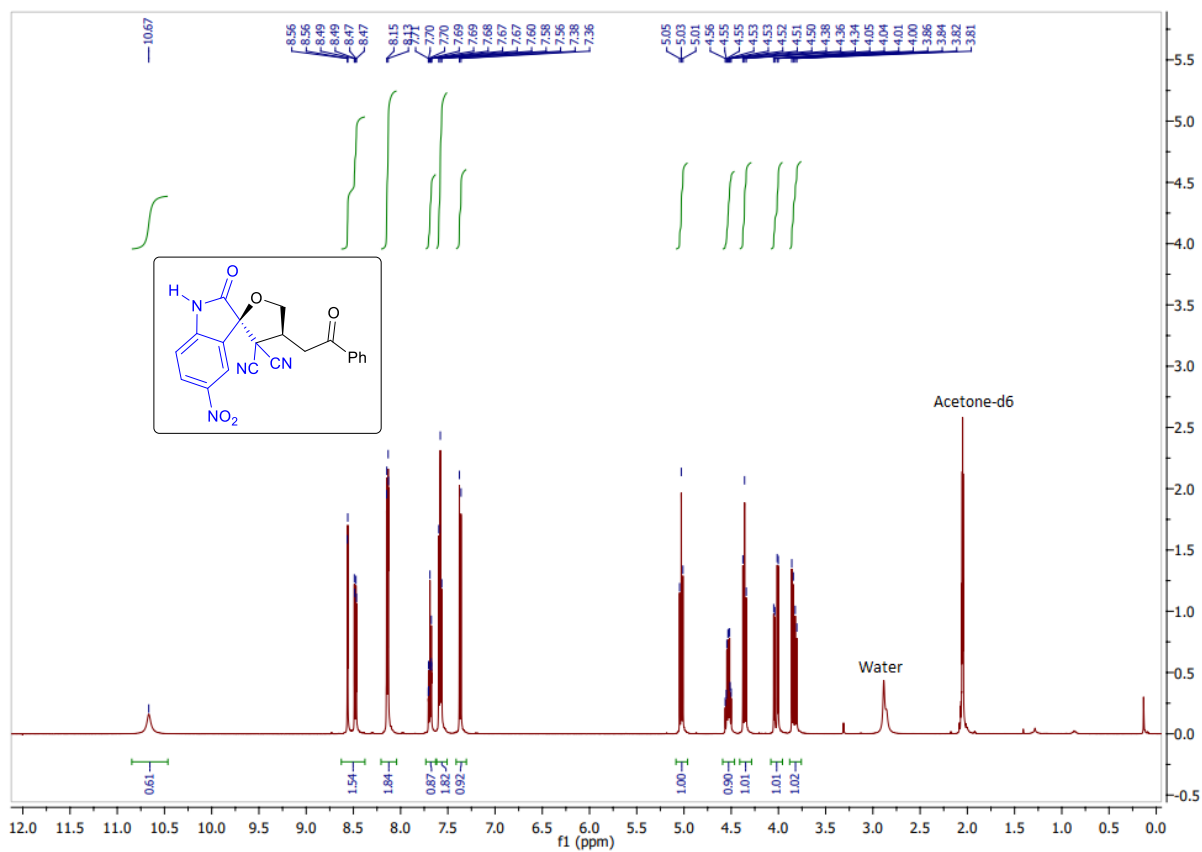


400 MHz  $^1\text{H}$  NMR and 400 MHz  $^{13}\text{C}$  NMR (Acetone- $d_6$ ) Spectra of 3ea

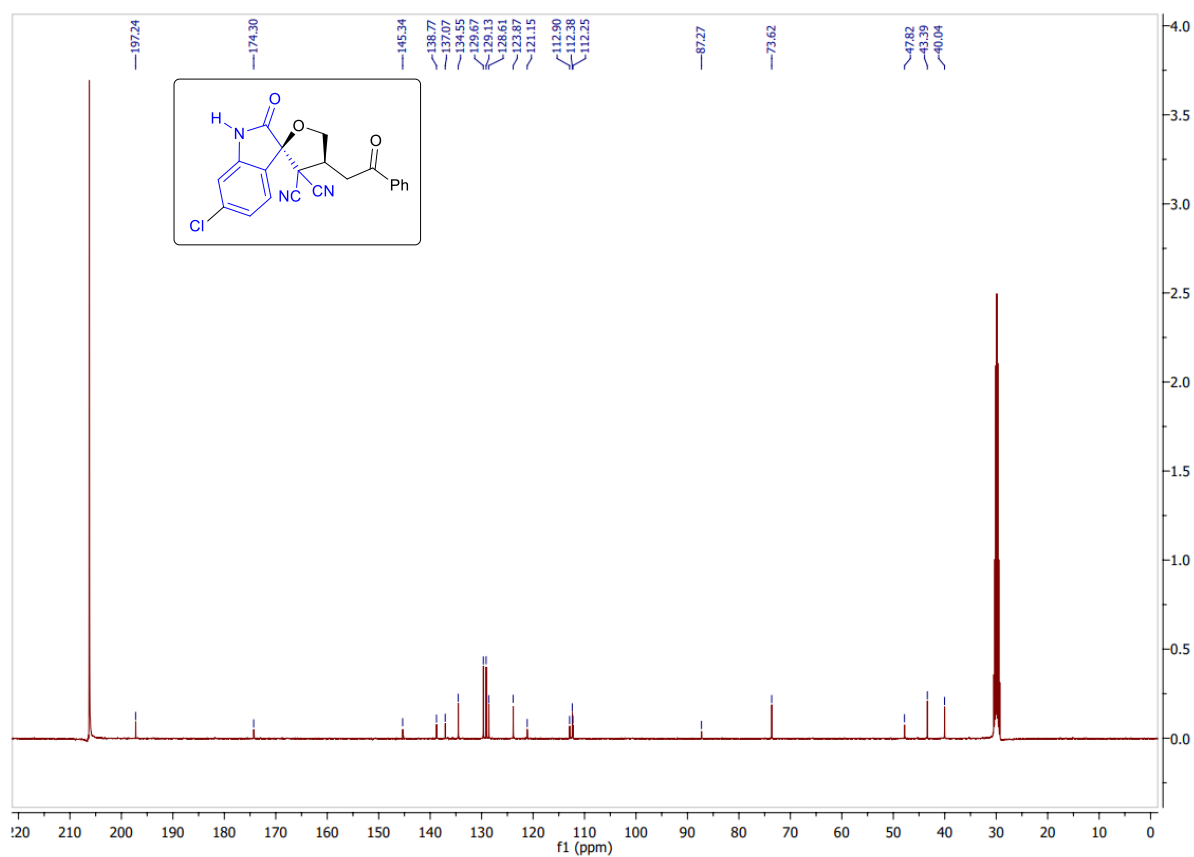
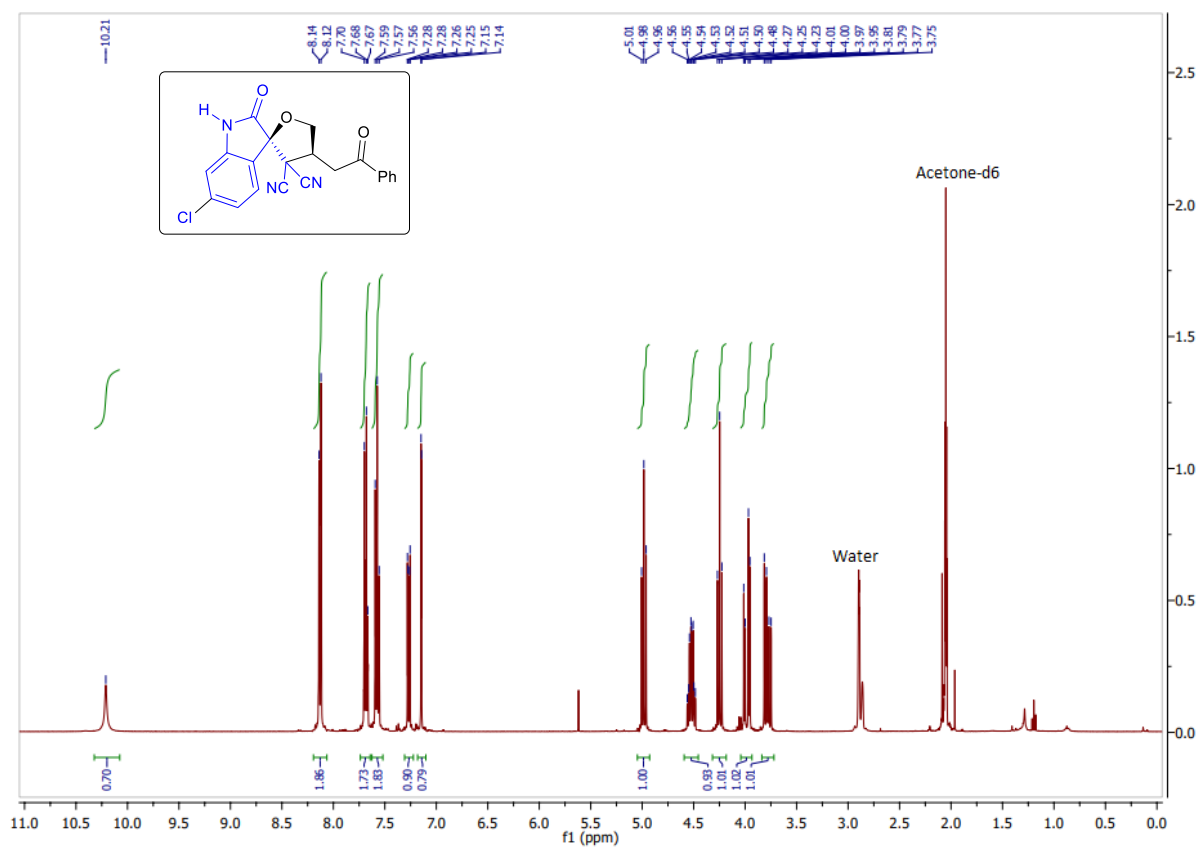


400 MHz  $^1\text{H}$  NMR and 400 MHz  $^{13}\text{C}$  NMR (Acetone- $\text{d}_6$ ) Spectra of 3fa

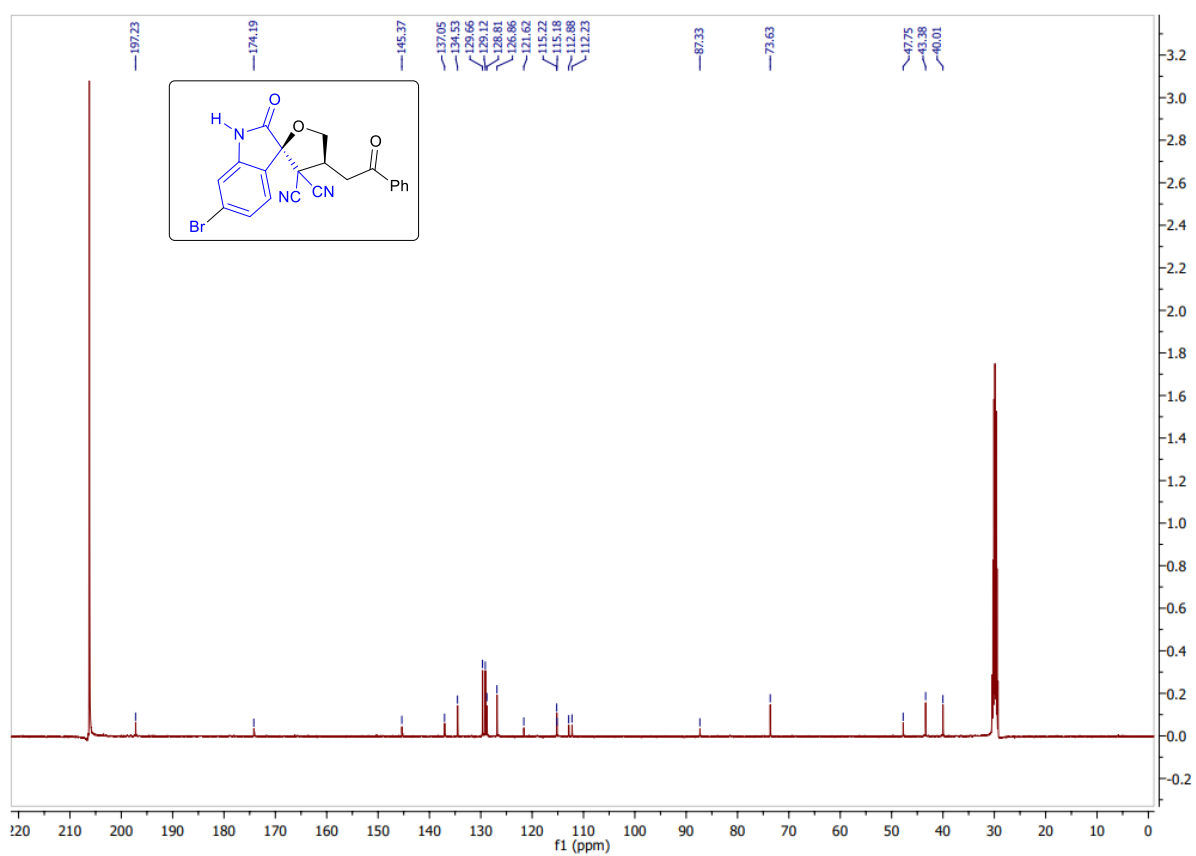
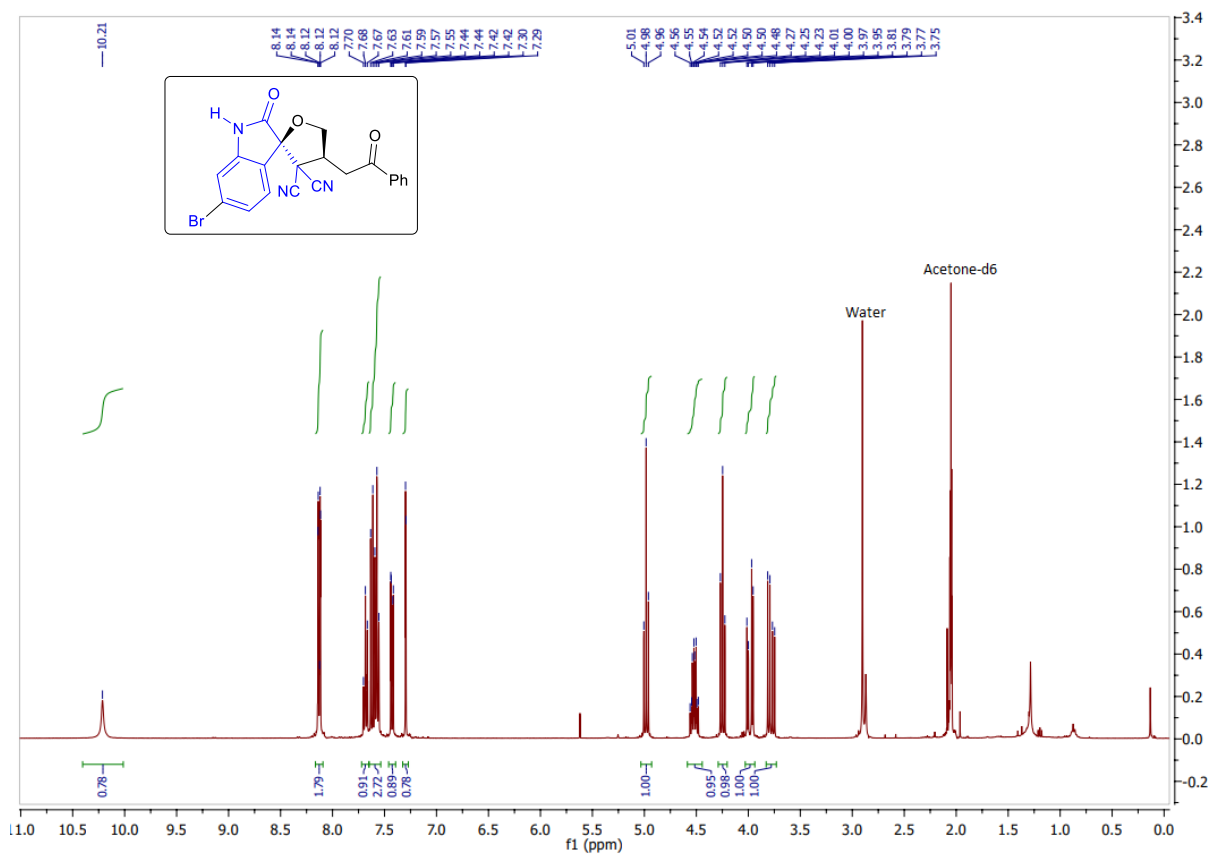




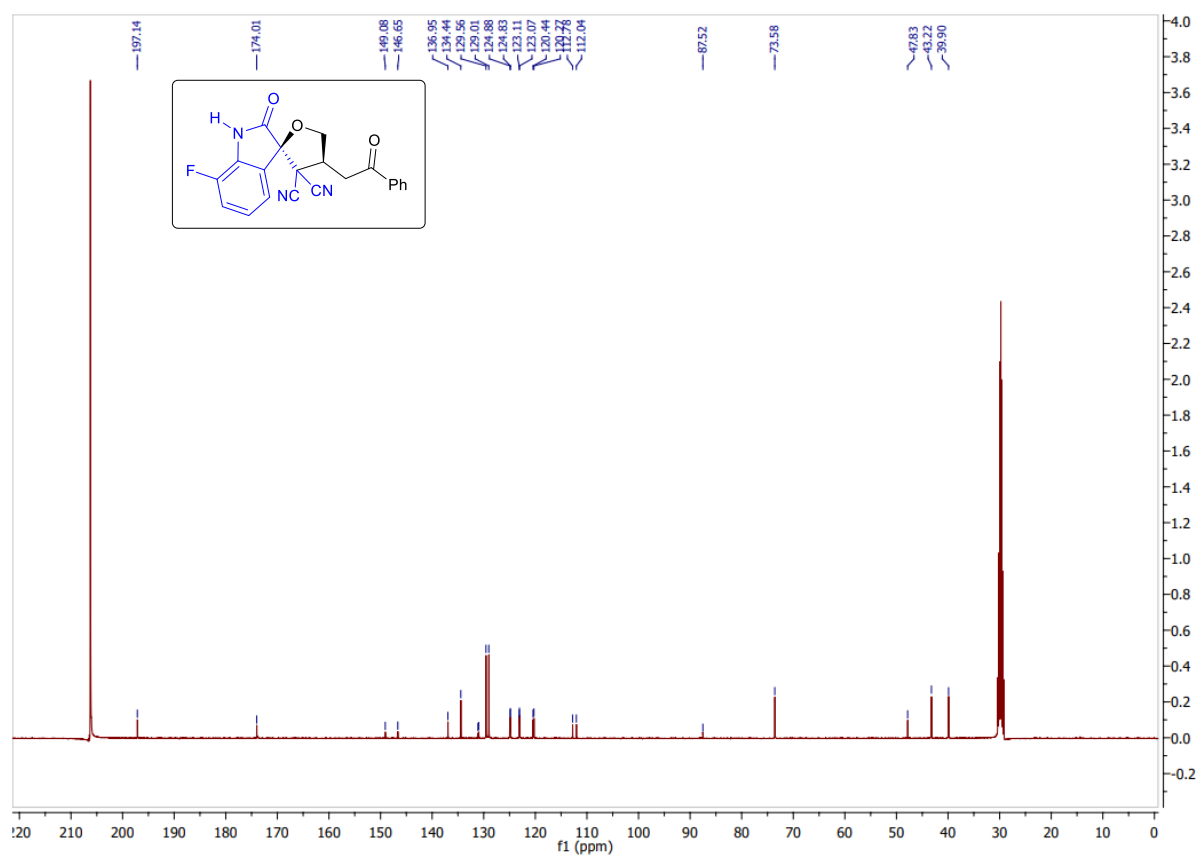
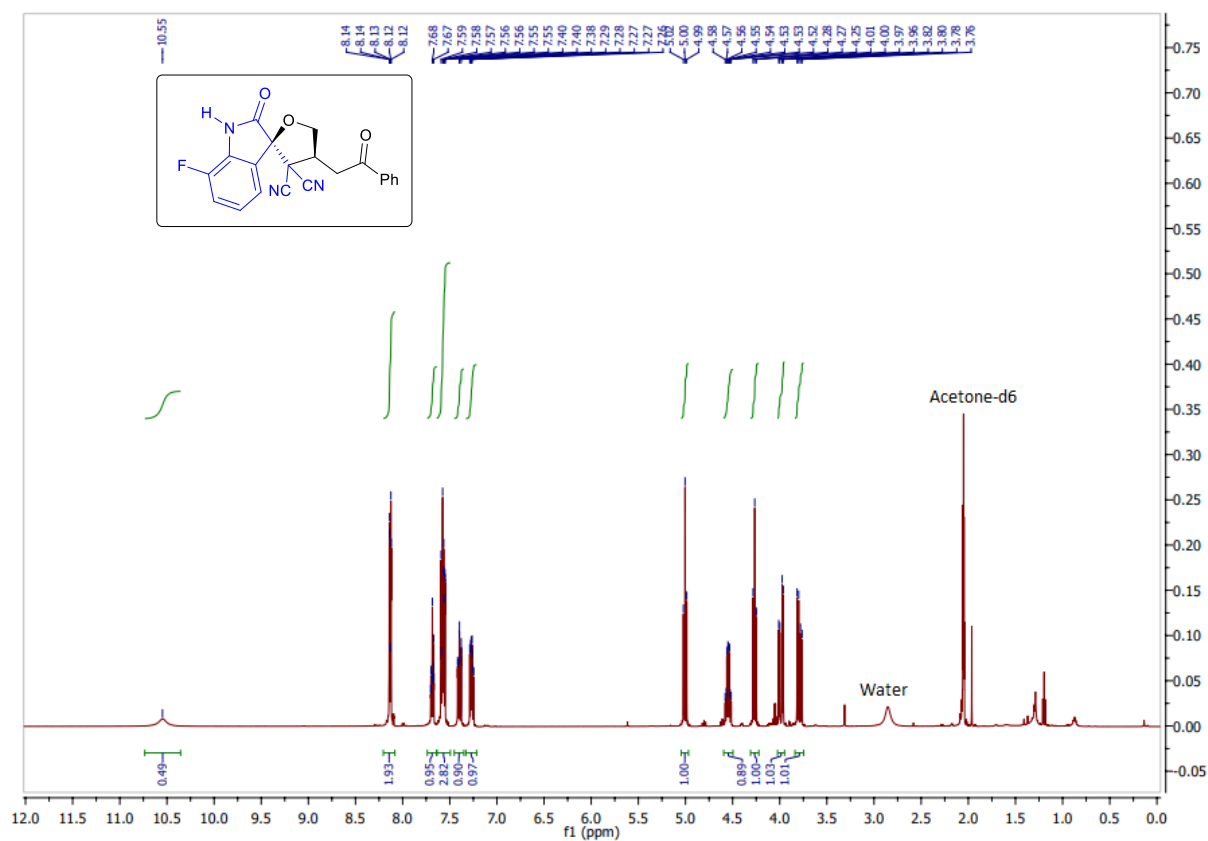
500 MHz  $^1\text{H}$  NMR and 400 MHz  $^{13}\text{C}$  NMR (Acetone- $d_6$ ) Spectra of 3ga



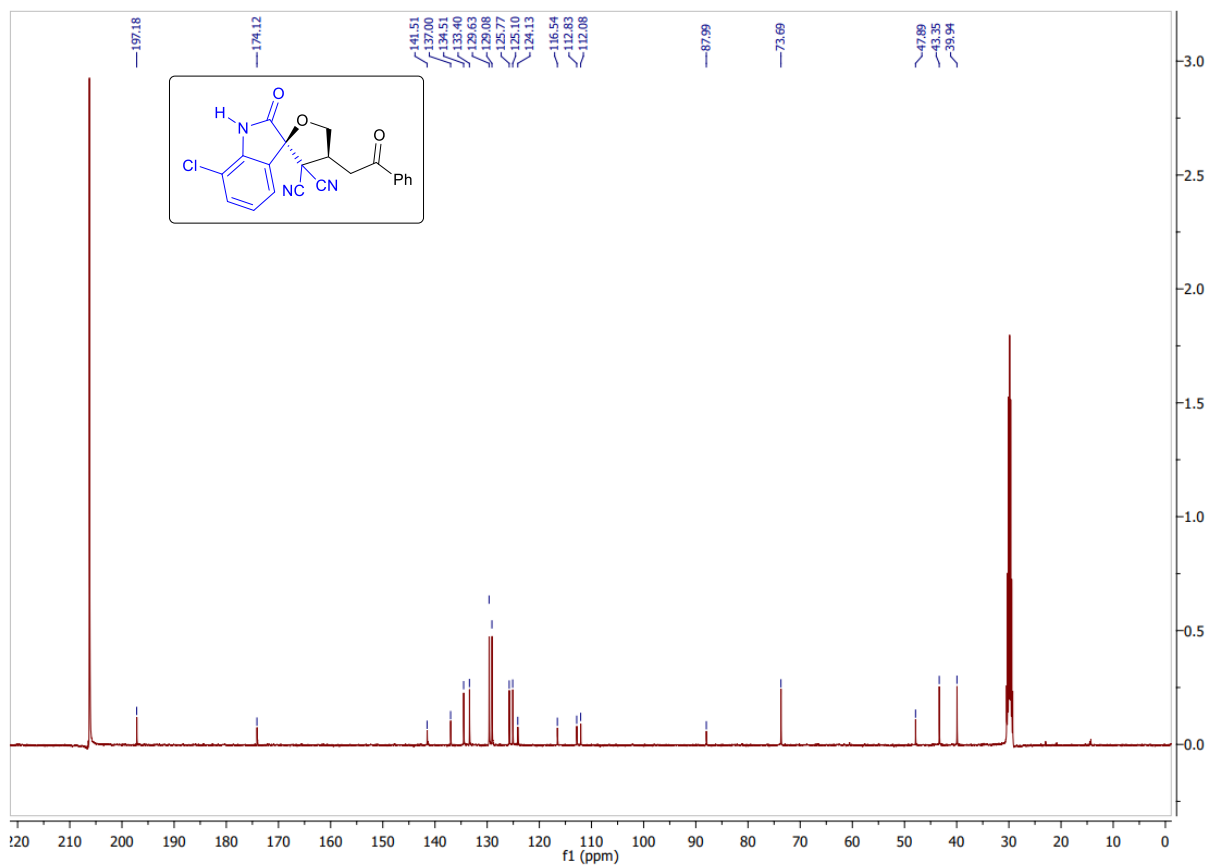
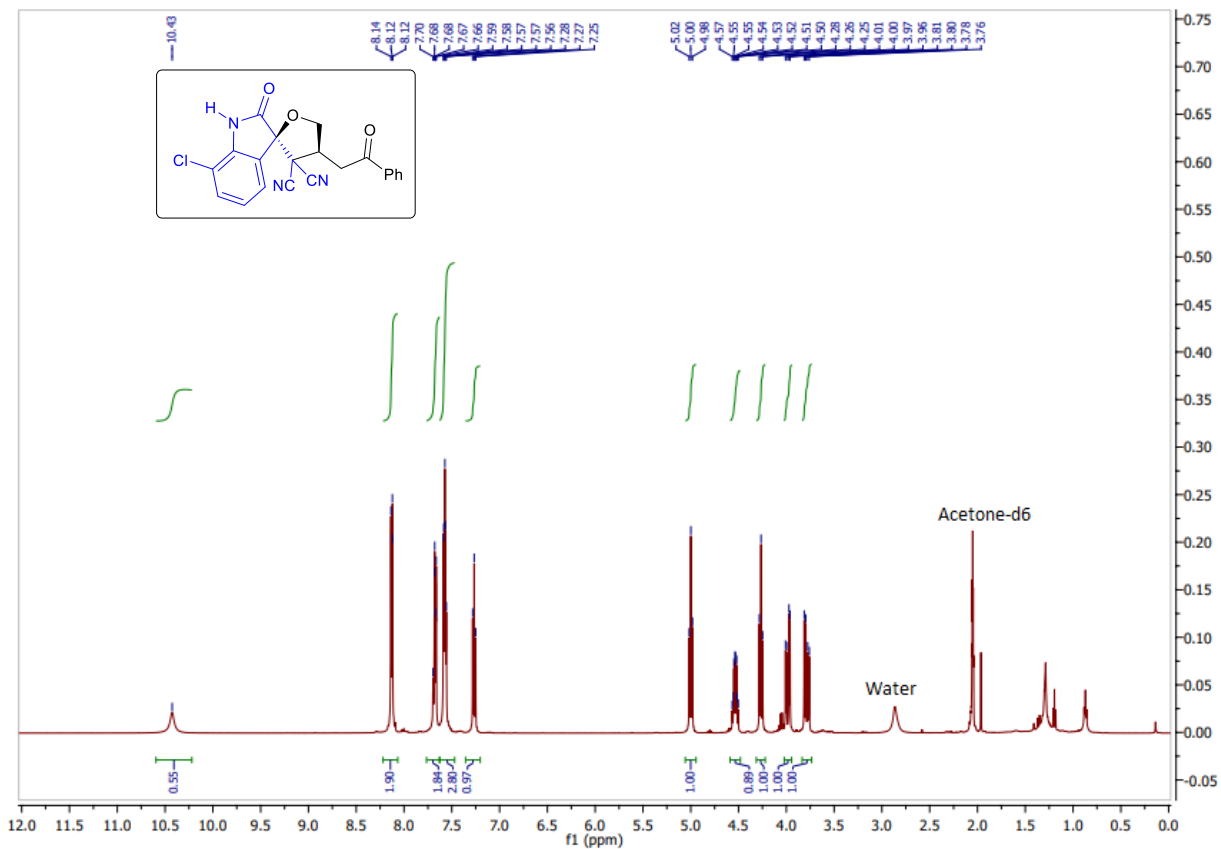
400 MHz <sup>1</sup>H NMR and 400 MHz <sup>13</sup>C NMR (Acetone-d<sub>6</sub>) Spectra of 3ha



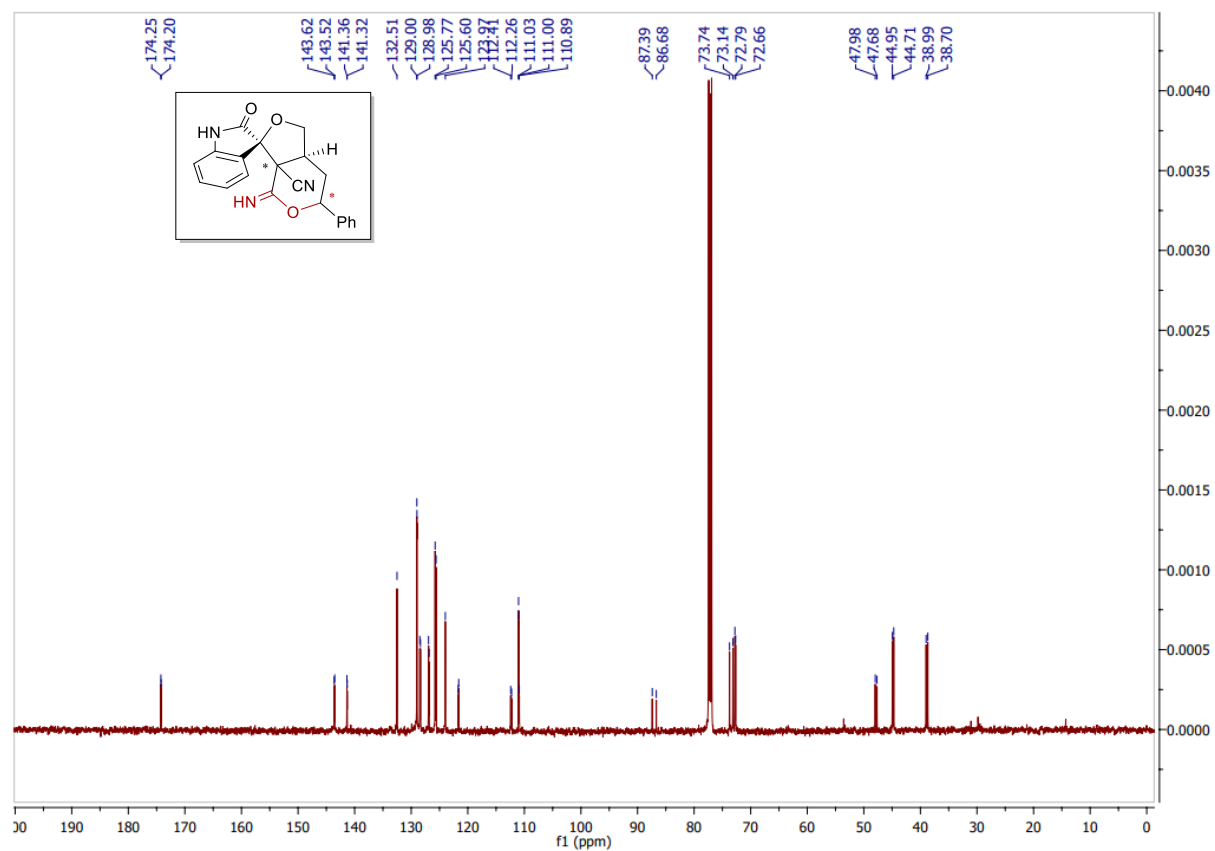
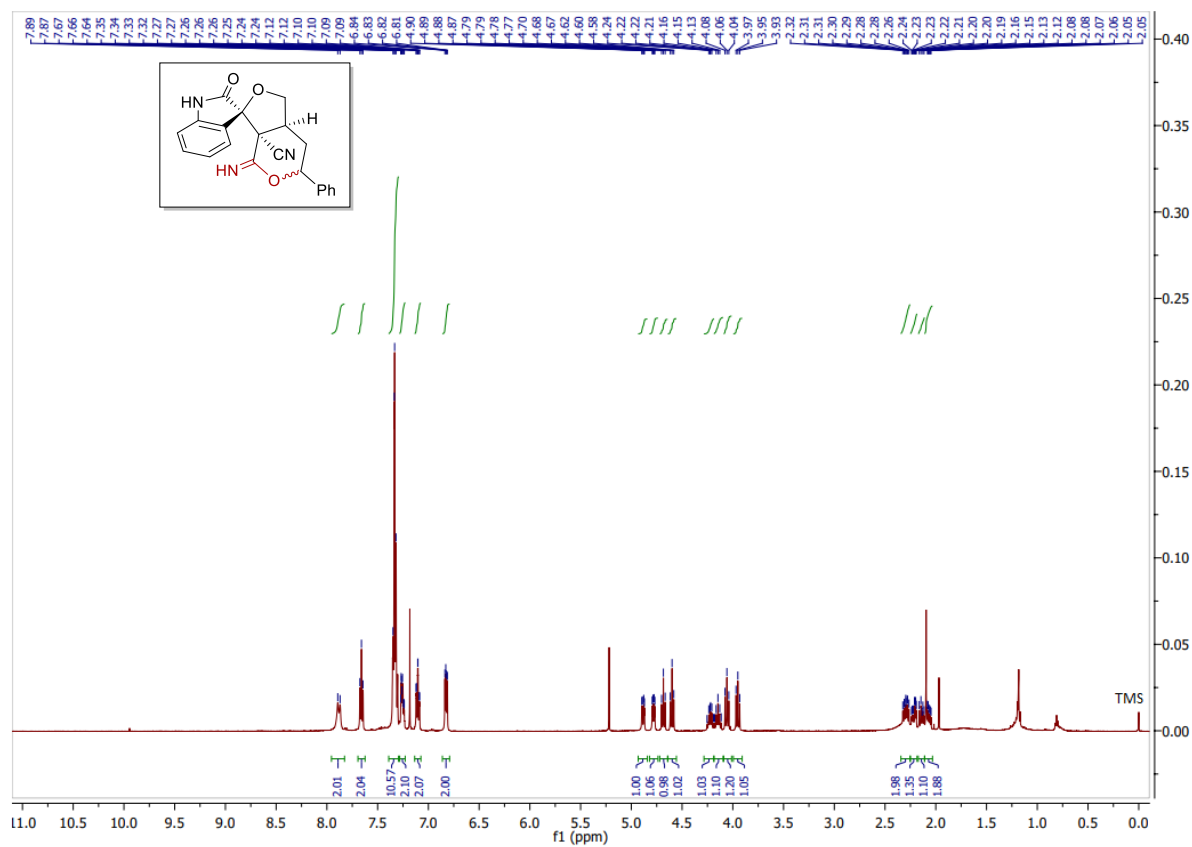
400 MHz <sup>1</sup>H NMR and 400 MHz <sup>13</sup>C NMR (Acetone-d<sub>6</sub>) Spectra of 3ia



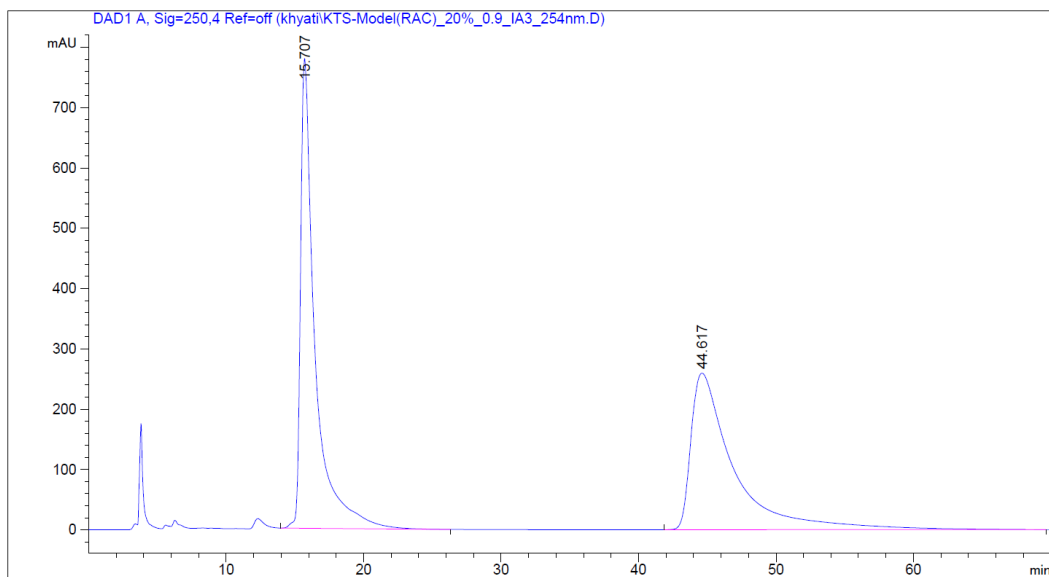
500 MHz  $^1\text{H}$  NMR and 400 MHz  $^{13}\text{C}$  NMR (Acetone- $d_6$ ) Spectra of 3ja



500 MHz <sup>1</sup>H NMR and 400 MHz <sup>13</sup>C NMR (Acetone-d<sub>6</sub>) Spectra of 3ka



500 MHz <sup>1</sup>H NMR and 500 MHz <sup>13</sup>C NMR (CDCl<sub>3</sub>) Spectra of 4aa

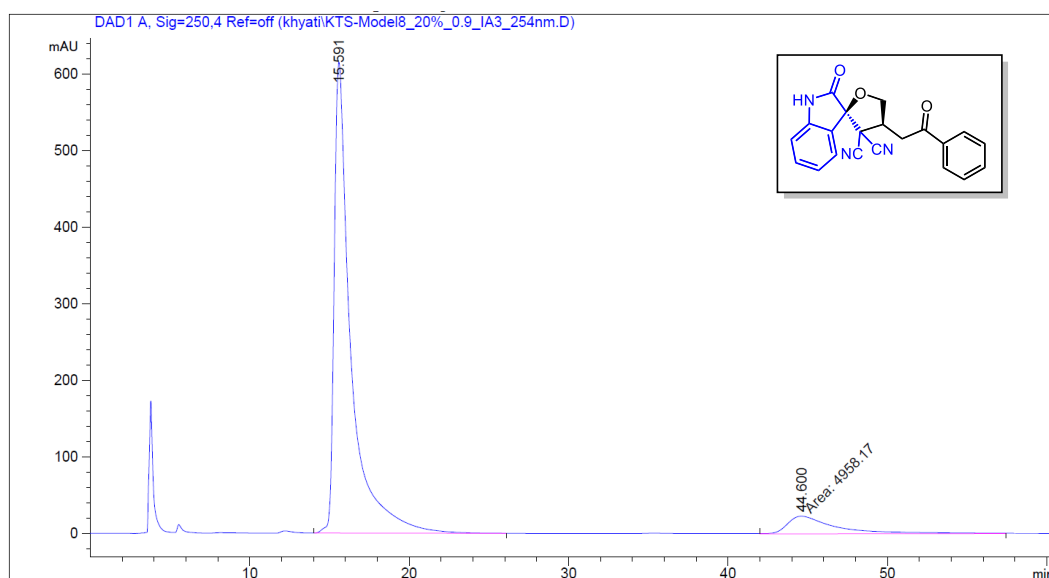


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 Area Percent Report  
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Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	15.707	BB	1.0324	5.68932e4	778.68622	50.3059
2	44.617	BB	3.0051	5.62014e4	259.45819	49.6941

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 \*\*\* End of Report \*\*\*

### HPLC graph of racemic 3aa

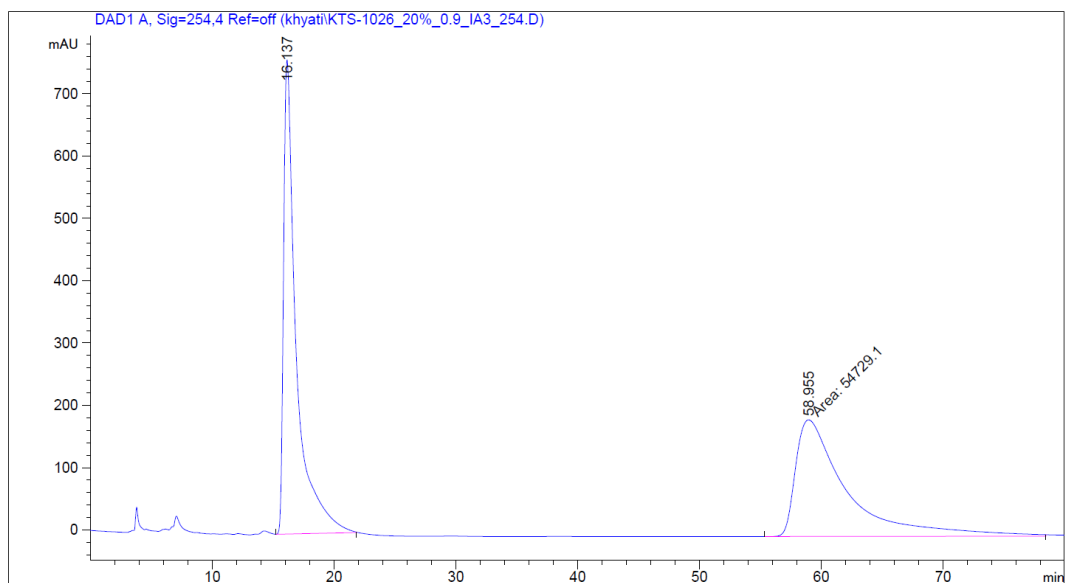


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 Area Percent Report  
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Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	15.591	BB	1.0282	4.48167e4	614.97888	90.0388
2	44.600	MM	3.5835	4958.16797	23.06004	9.9612

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 \*\*\* End of Report \*\*\*

### HPLC graph of enantioenriched 3aa

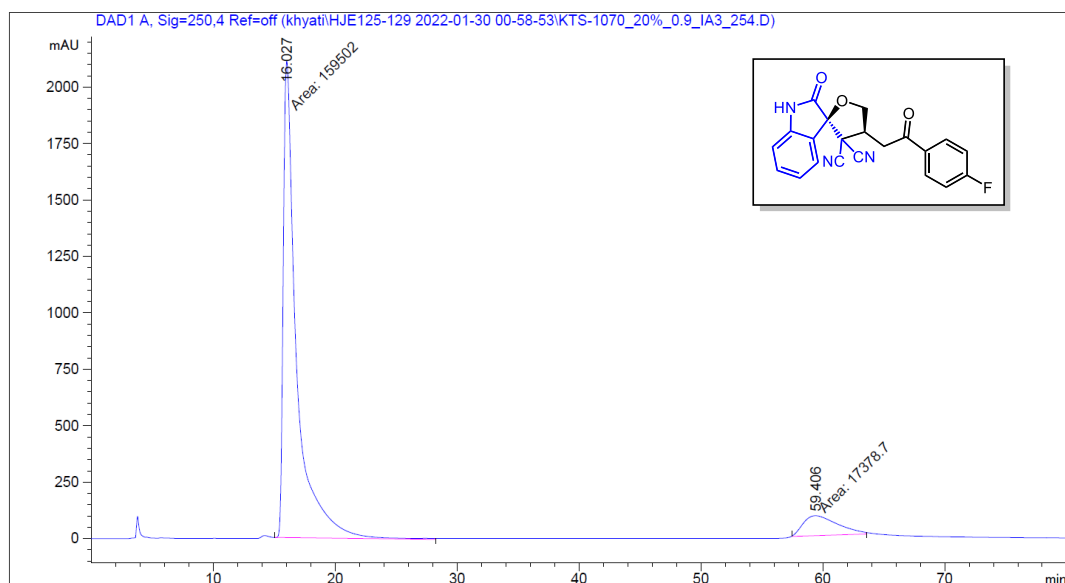


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 Area Percent Report  
 =====

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	16.137	VB	1.0266	5.50822e4	760.88824	50.1607
2	58.955	MM	4.8745	5.47291e4	187.12692	49.8393

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 \*\*\* End of Report \*\*\*

HPLC graph of racemic **3ab**



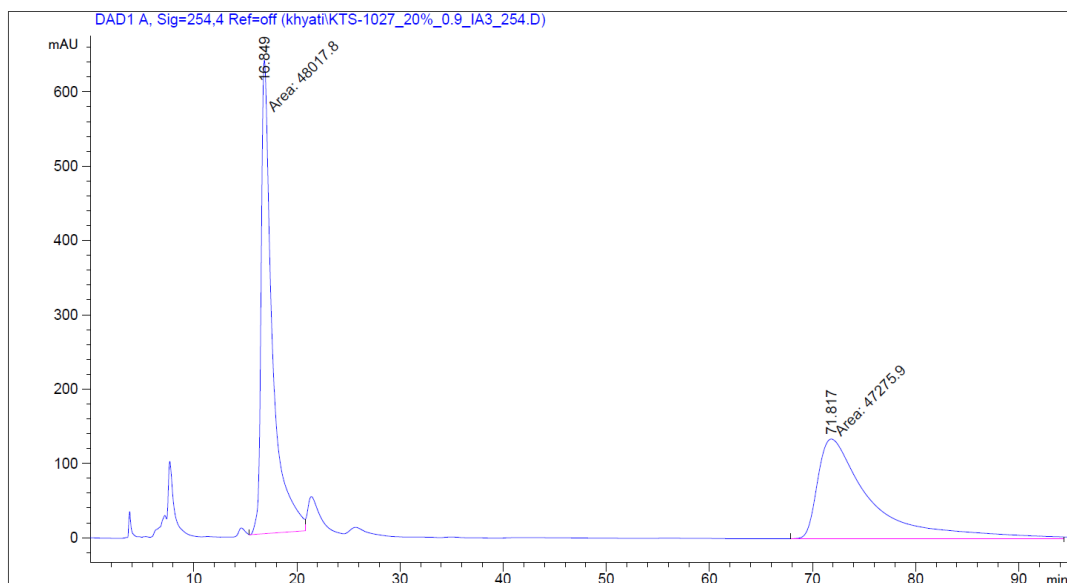
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 Area Percent Report  
 =====

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	16.027	MM	1.2596	1.59502e5	2110.52344	90.1749
2	59.406	MM	3.2807	1.73787e4	88.28668	9.8251

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 \*\*\* End of Report \*\*\*

HPLC graph of enantioenriched **3ab**



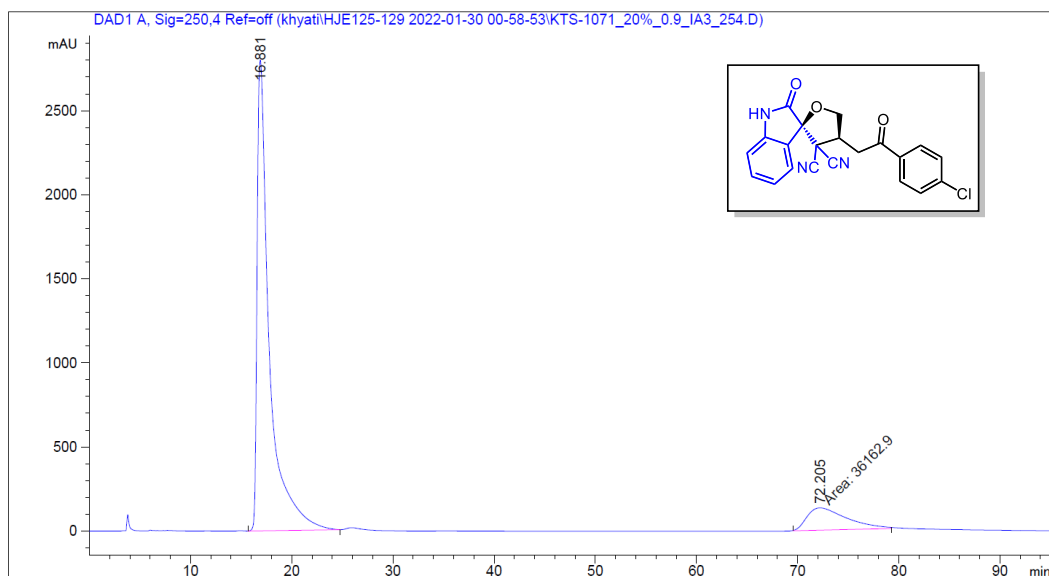


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 Area Percent Report  
 =====

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	16.849	MM	1.2558	4.80178e4	637.29138	50.3892
2	71.817	MM	5.8889	4.72759e4	133.79961	49.6108

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 \*\*\* End of Report \*\*\*

HPLC graph of racemic **3ac**

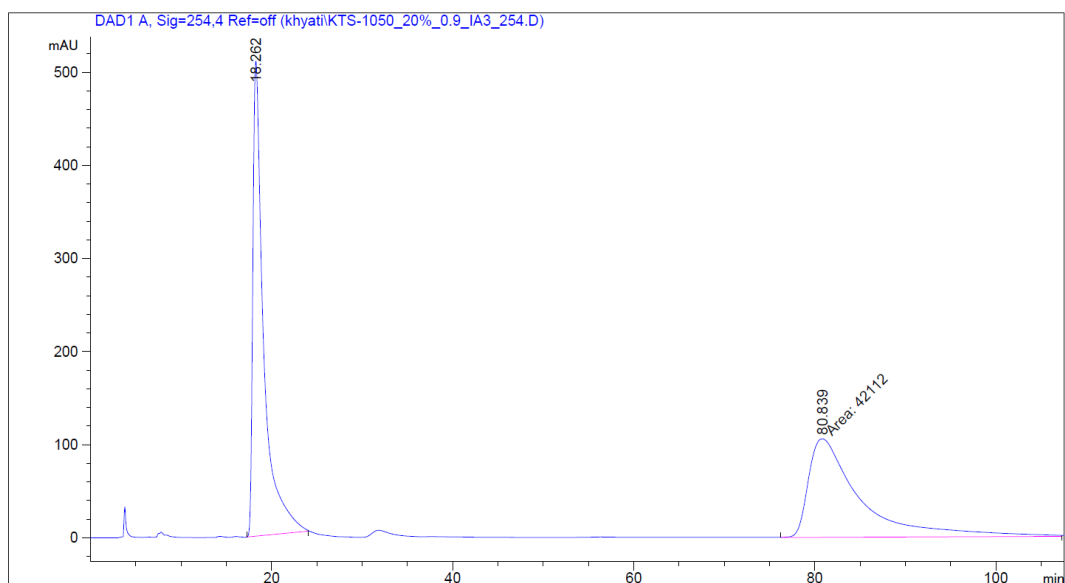


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 Area Percent Report  
 =====

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	16.881	BB	1.1748	2.34598e5	2801.99390	86.6440
2	72.205	MM	4.5398	3.61629e4	132.76340	13.3560

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 \*\*\* End of Report \*\*\*

HPLC graph of enantioenriched **3ac**

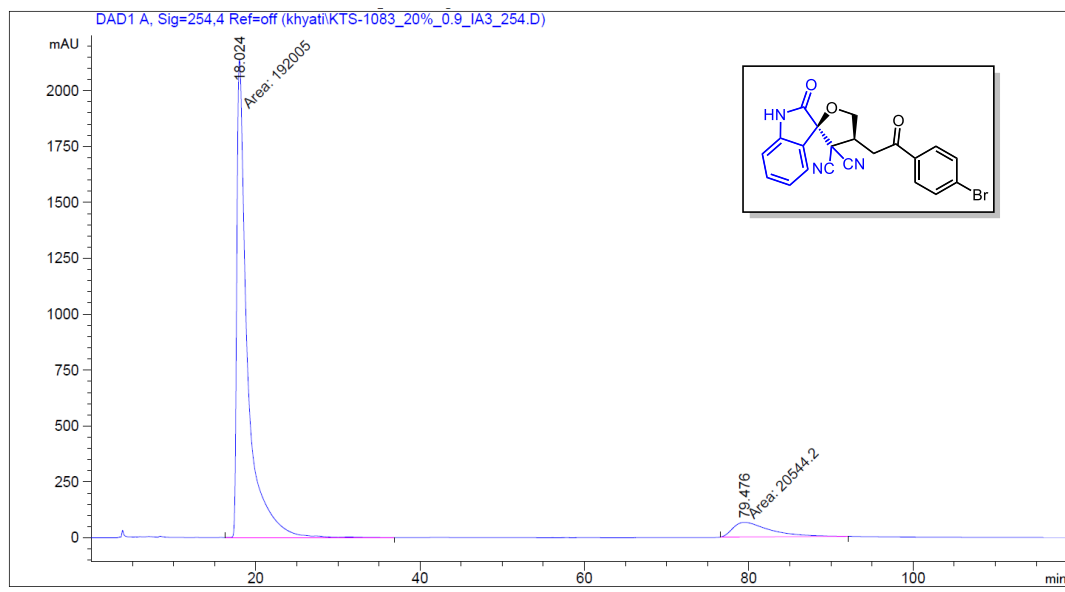


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 Area Percent Report  
 =====

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	18.262	BB	1.1828	4.23641e4	510.15558	50.1492
2	80.839	MM	6.6263	4.21120e4	105.92084	49.8508

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 \*\*\* End of Report \*\*\*

HPLC graph of racemic **3ad**

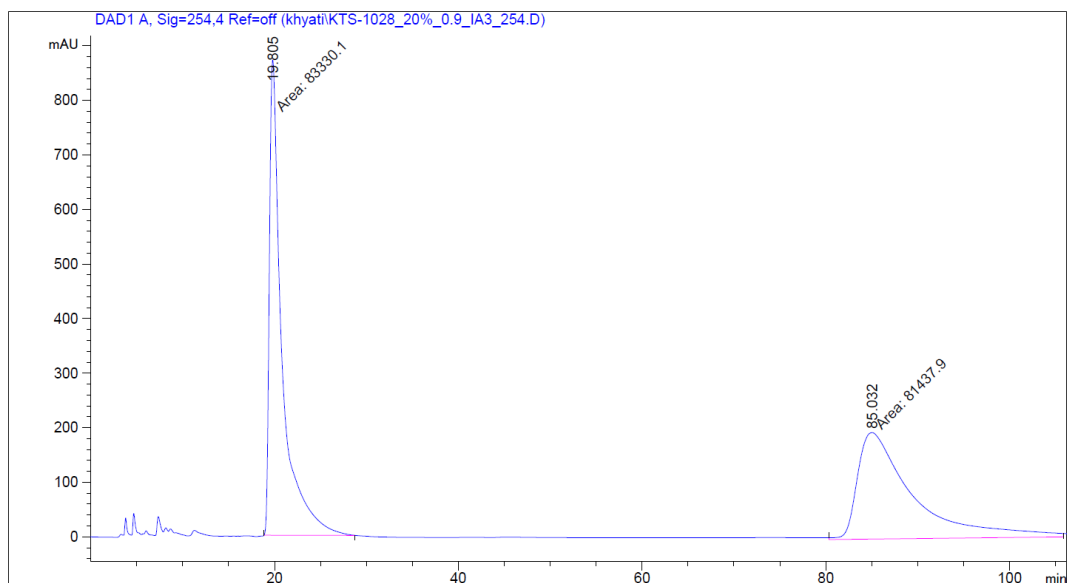


=====  
 Area Percent Report  
 =====

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	18.024	MM	1.4973	1.92005e5	2137.30103	90.3344
2	79.476	MM	5.2373	2.05442e4	65.37817	9.6656

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 \*\*\* End of Report \*\*\*

HPLC graph of enantioenriched **3ad**

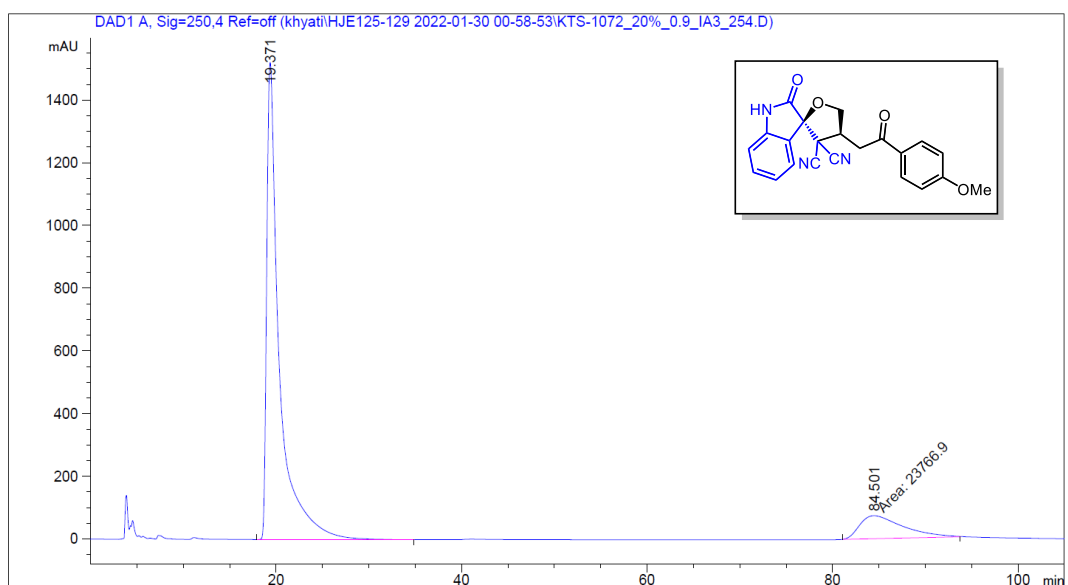


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 Area Percent Report  
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Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	19.805	MM	1.5947	8.33301e4	870.88110	50.5742
2	85.032	MM	6.9586	8.14379e4	195.05414	49.4258

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 \*\*\* End of Report \*\*\*

HPLC graph of racemic **3ae**

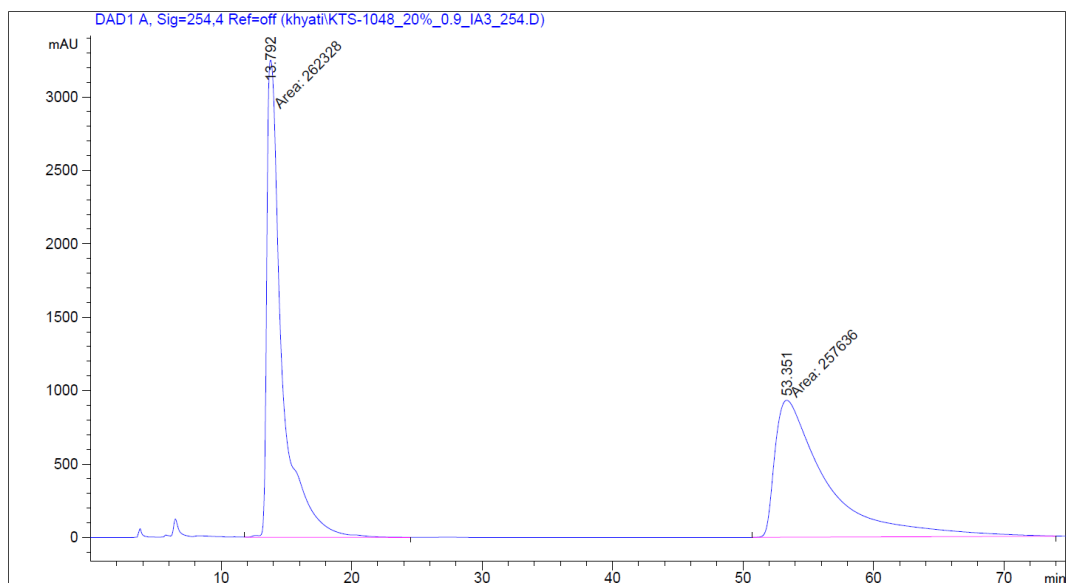


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 Area Percent Report  
 =====

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	19.371	BB	1.3309	1.43620e5	1521.95081	85.8012
2	84.501	MM	5.4029	2.37669e4	73.31554	14.1988

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 \*\*\* End of Report \*\*\*

HPLC graph of enantioenriched **3ae**

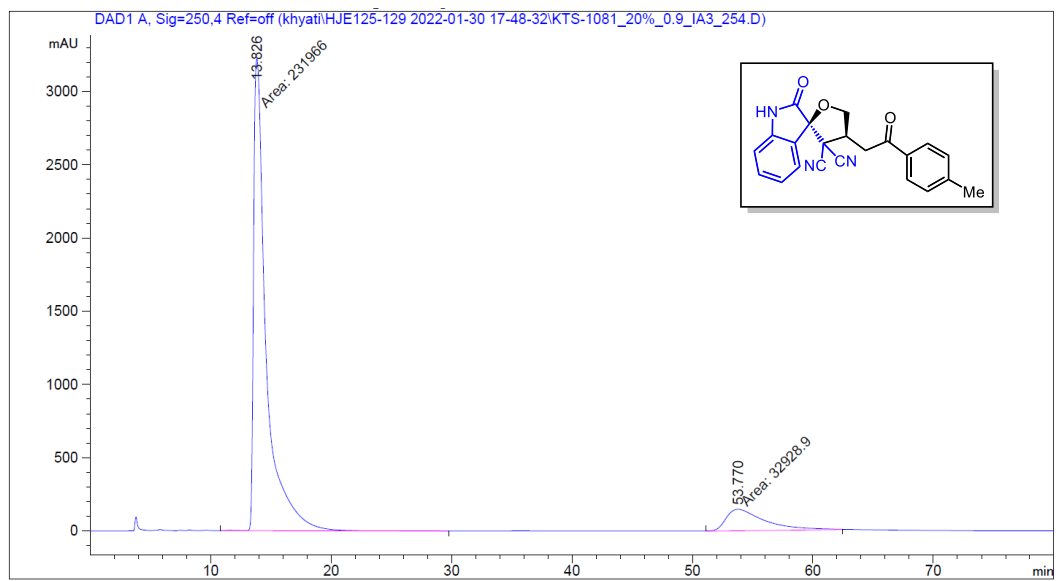


=====  
 Area Percent Report  
 =====

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	13.792	MM	1.3450	2.62328e5	3250.70288	50.4512
2	53.351	MM	4.6015	2.57636e5	933.15717	49.5488

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 \*\*\* End of Report \*\*\*

### HPLC graph of racemic **3af**

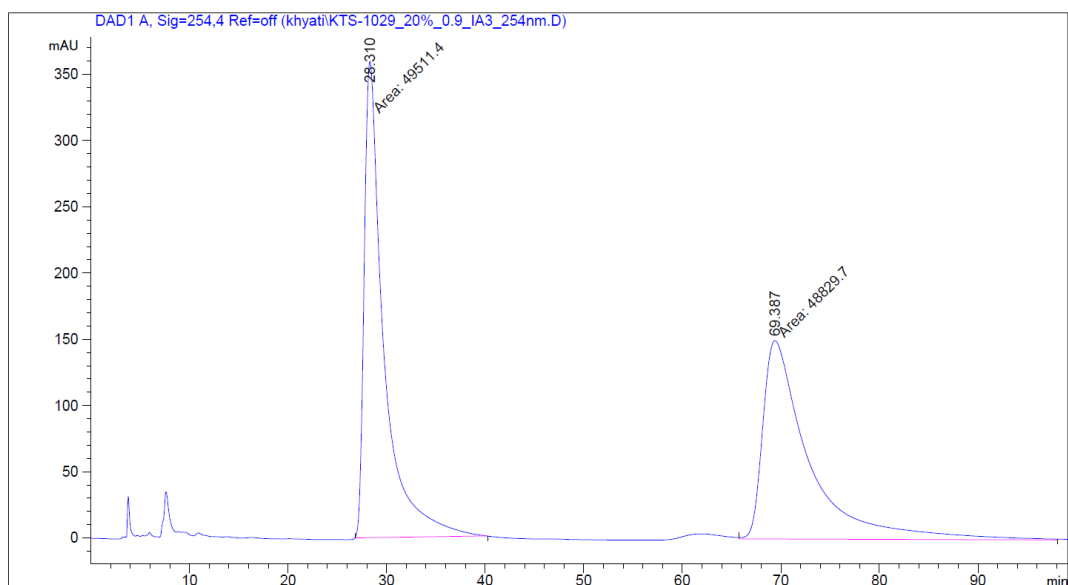


=====  
 Area Percent Report  
 =====

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	13.826	MM	1.2013	2.31966e5	3218.25610	87.5691
2	53.770	MM	3.7337	3.29239e4	146.98755	12.4309

=====  
 \*\*\* End of Report \*\*\*

### HPLC graph of enantioenriched **3af**

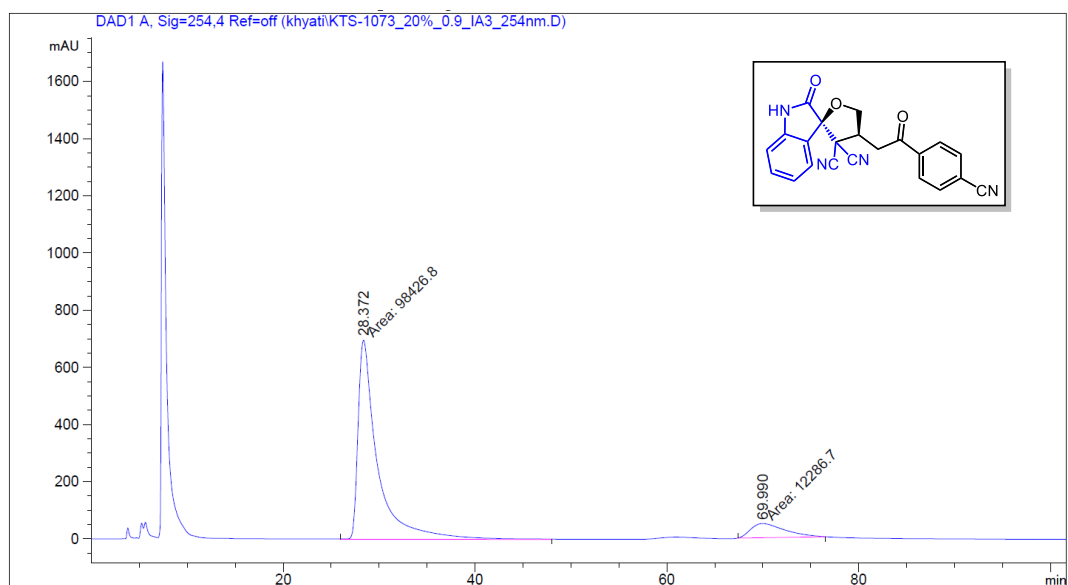


=====  
 Area Percent Report  
 =====

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	28.310	MM	2.2951	4.95114e4	359.54770	50.3466
2	69.387	MM	5.4306	4.88297e4	149.85948	49.6534

=====  
 \*\*\* End of Report \*\*\*

HPLC graph of racemic **3ag**

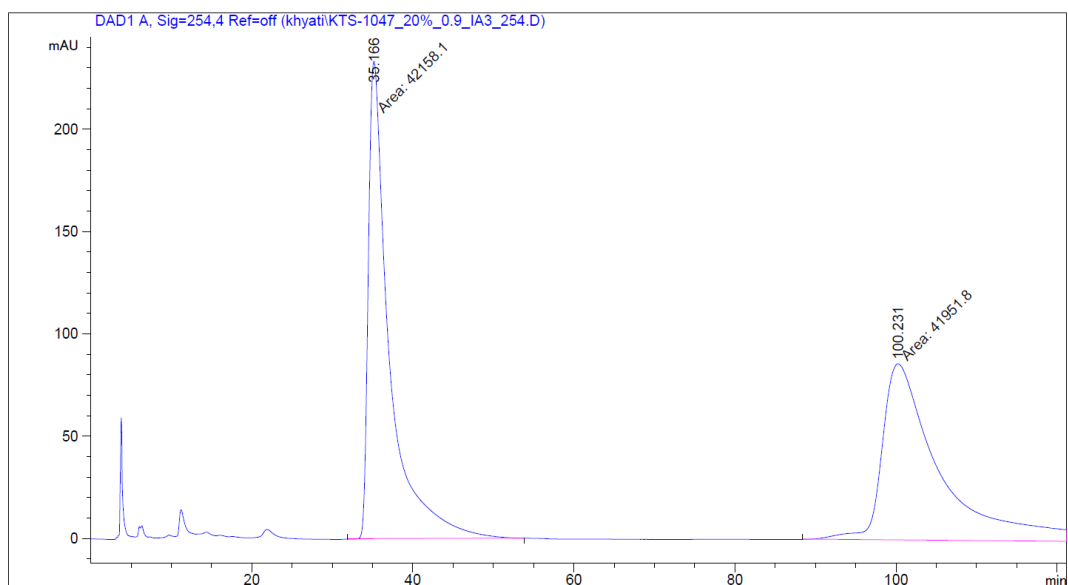


=====  
 Area Percent Report  
 =====

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	28.372	MM	2.3559	9.84267e4	696.30963	88.9023
2	69.990	MM	4.1167	1.22867e4	49.74283	11.0977

=====  
 \*\*\* End of Report \*\*\*

HPLC graph of enantioenriched **3ag**

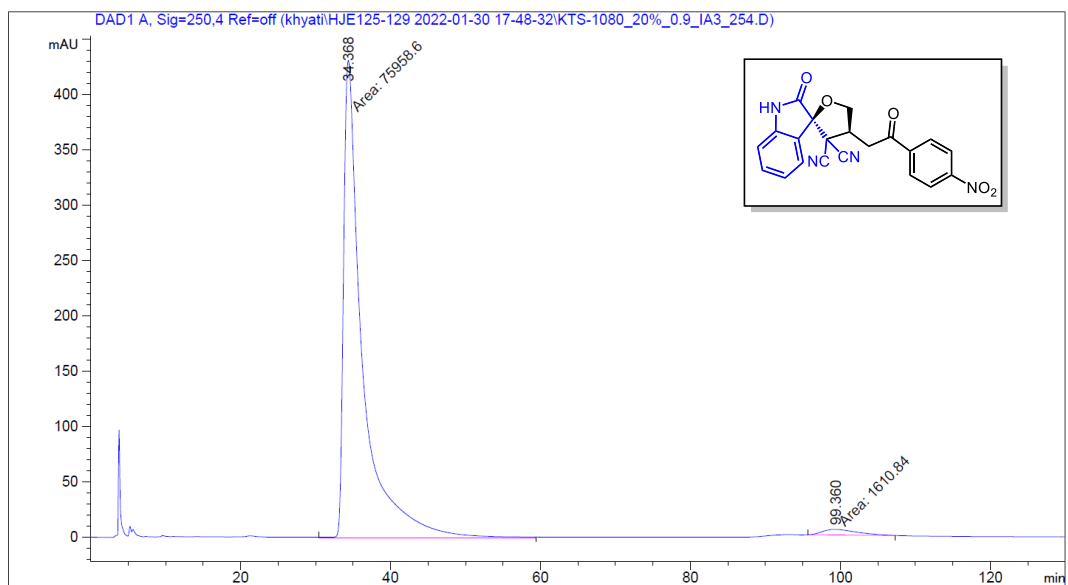


=====  
 Area Percent Report  
 =====

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	35.166	MM	3.0129	4.21581e4	233.20970	50.1226
2	100.231	MM	8.1280	4.19518e4	86.02268	49.8774

=====  
 \*\*\* End of Report \*\*\*

### HPLC graph of racemic 3ah

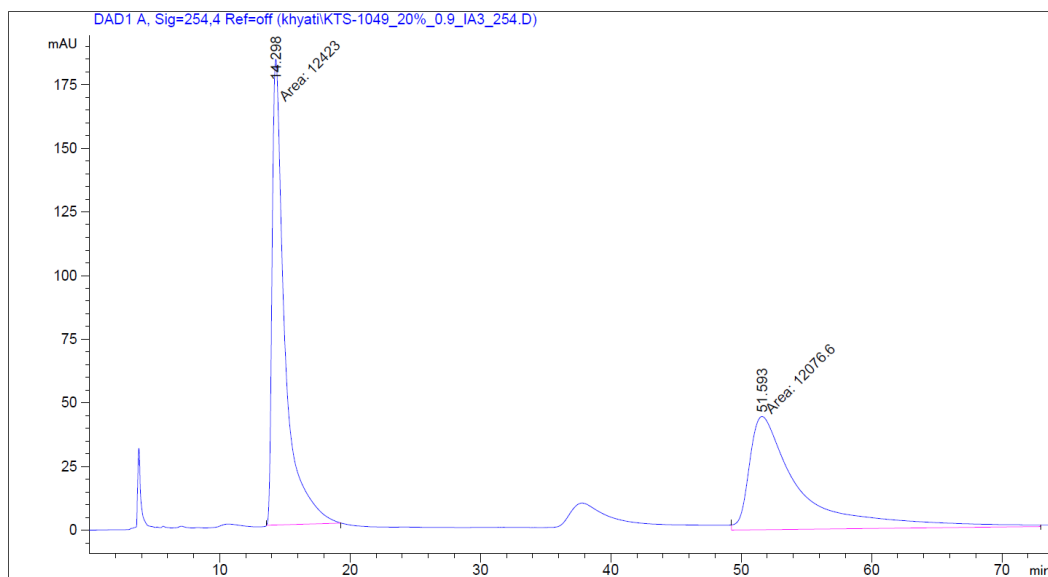


=====  
 Area Percent Report  
 =====

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	34.368	MM	2.9338	7.59586e4	431.51273	97.9234
2	99.360	MM	5.3447	1610.84436	5.02320	2.0766

=====  
 \*\*\* End of Report \*\*\*

### HPLC graph of enantioenriched 3ah

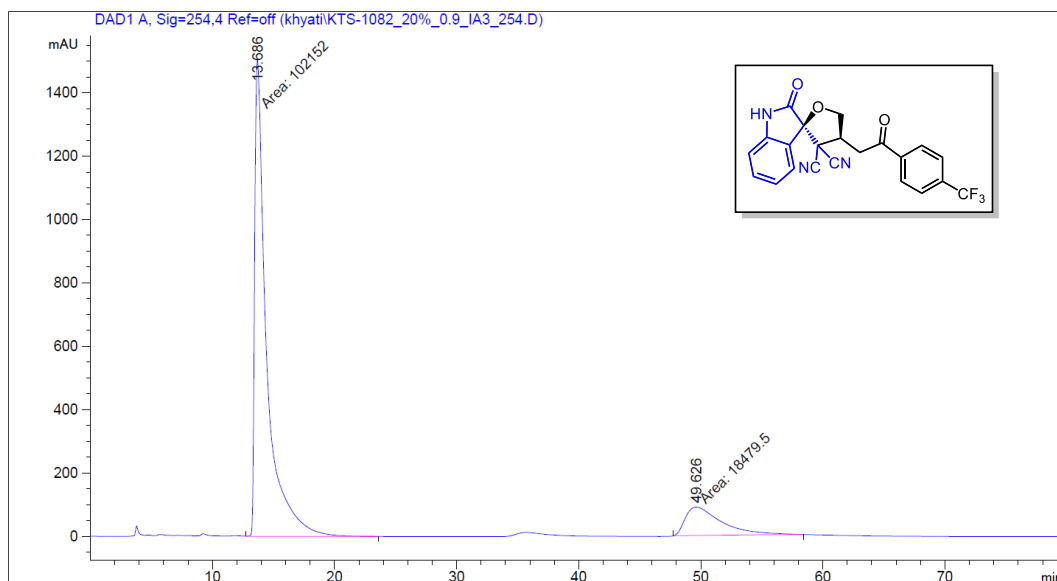


=====  
 Area Percent Report  
 =====

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	14.298	MM	1.1319	1.24230e4	182.91446	50.7070
2	51.593	MM	4.5276	1.20766e4	44.45565	49.2930

=====  
 \*\*\* End of Report \*\*\*

### HPLC graph of racemic 3ai

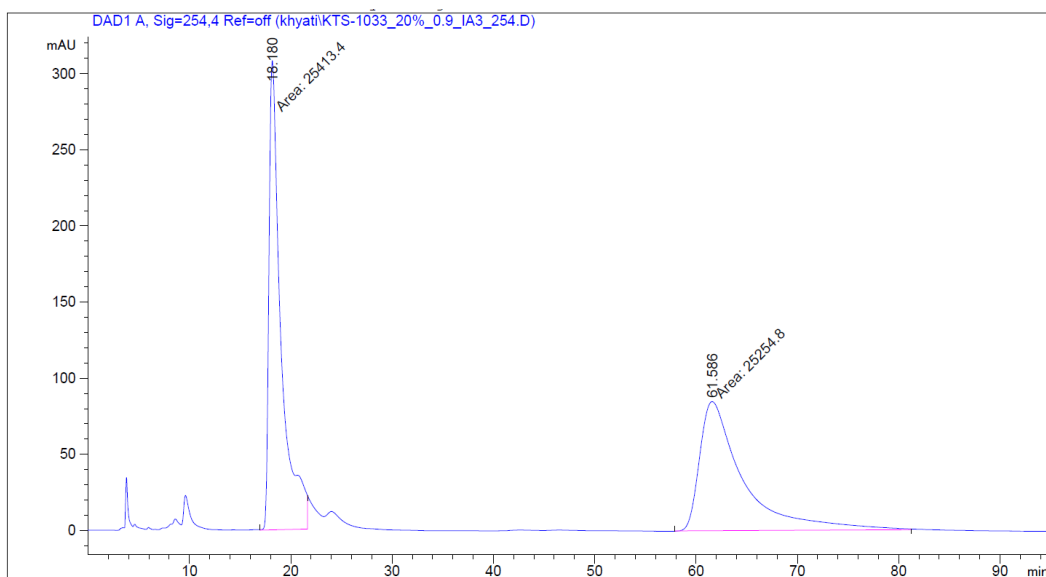


=====  
 Area Percent Report  
 =====

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	13.686	MM	1.1319	1.02152e5	1504.17163	84.6811
2	49.626	MM	3.4317	1.84795e4	89.74892	15.3189

=====  
 \*\*\* End of Report \*\*\*

### HPLC graph of enantioenriched 3ai

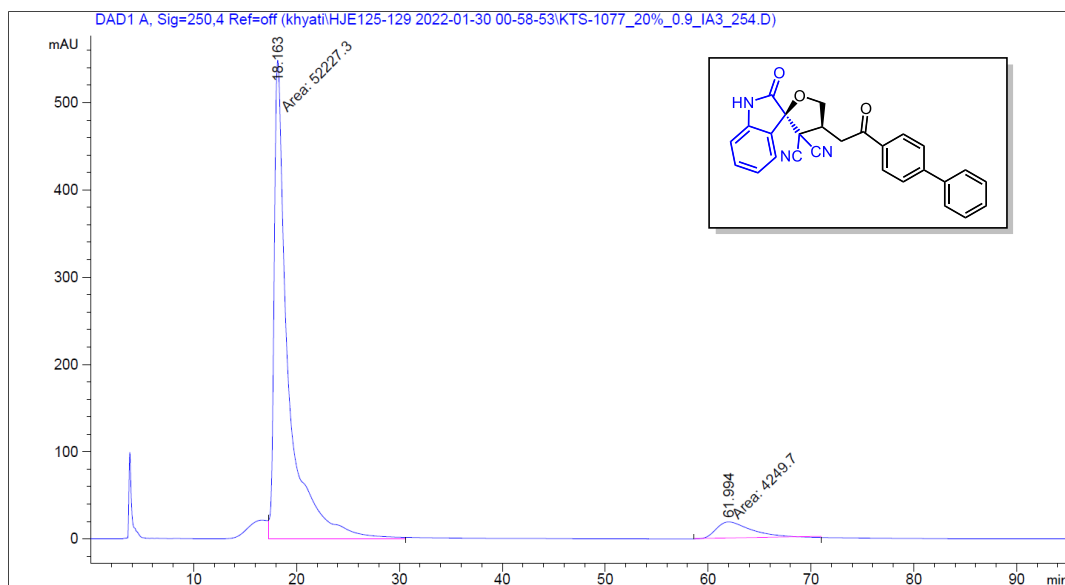


=====  
 Area Percent Report  
 =====

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	18.180	MM	1.3746	2.54134e4	308.12198	50.1564
2	61.586	MM	4.9633	2.52548e4	84.80476	49.8436

=====  
 \*\*\* End of Report \*\*\*

### HPLC graph of racemic 3aj



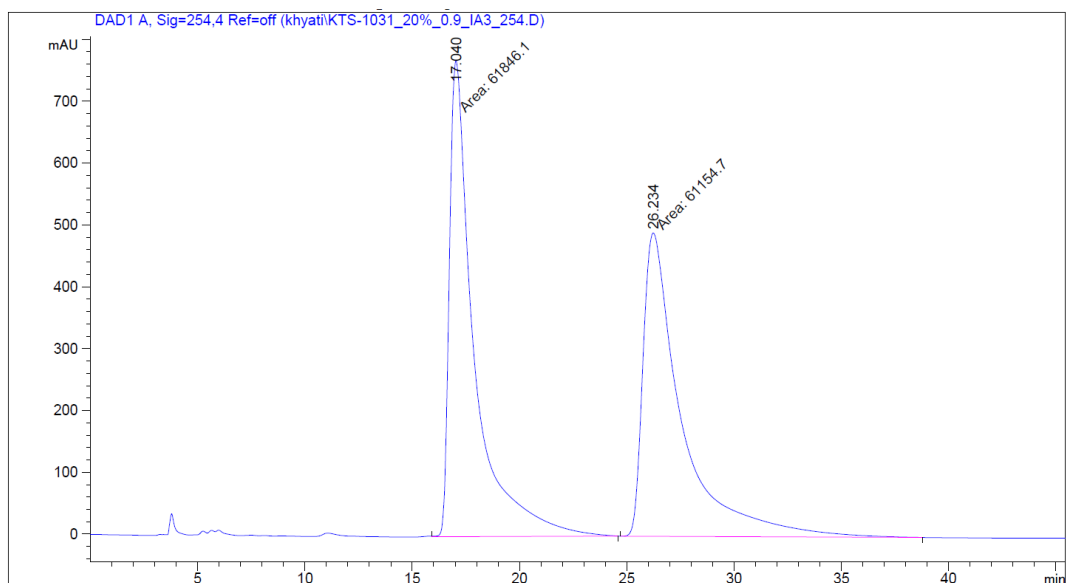
=====  
 Area Percent Report  
 =====

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	18.163	MM	1.5874	5.22273e4	548.33545	92.4754
2	61.994	MM	3.8472	4249.69629	18.41032	7.5246

=====  
 \*\*\* End of Report \*\*\*

### HPLC graph of enantioenriched 3aj



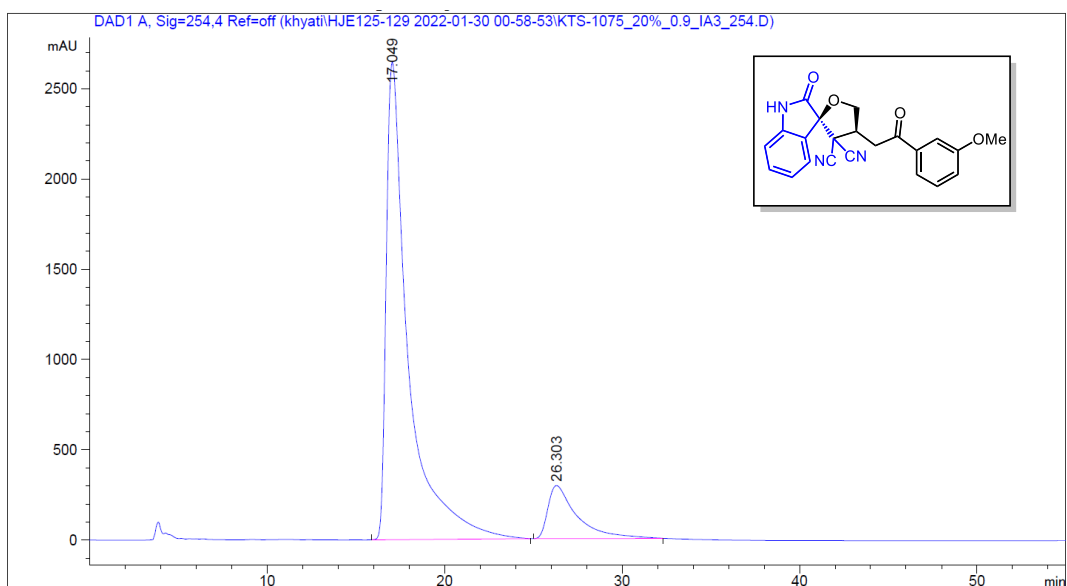


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 Area Percent Report  
 =====

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	17.040	MM	1.3392	6.18461e4	769.68719	50.2810
2	26.234	MM	2.0775	6.11547e4	490.60025	49.7190

=====  
 \*\*\* End of Report \*\*\*

### HPLC graph of racemic **3ak**

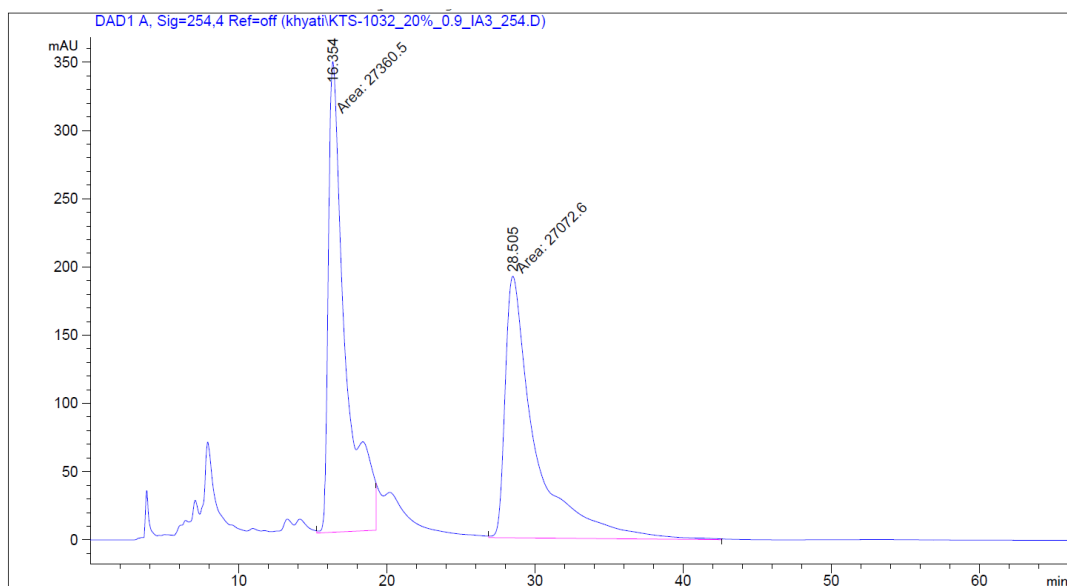


=====  
 Area Percent Report  
 =====

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	17.049	BB	1.1971	2.26657e5	2646.68945	87.1375
2	26.303	BB	1.6284	3.34572e4	293.84677	12.8625

=====  
 \*\*\* End of Report \*\*\*

### HPLC graph of enantioenriched **3ak**

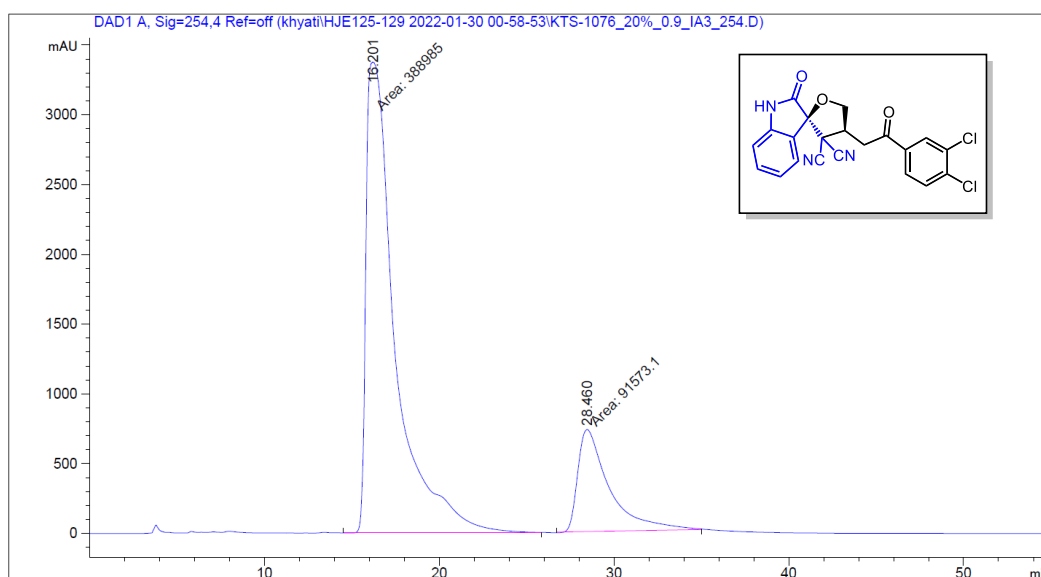


=====  
 Area Percent Report  
 =====

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	16.354	MM	1.3222	2.73605e4	344.89081	50.2645
2	28.505	MM	2.3541	2.70726e4	191.67010	49.7355

=====  
 \*\*\* End of Report \*\*\*

### HPLC graph of racemic **3a**

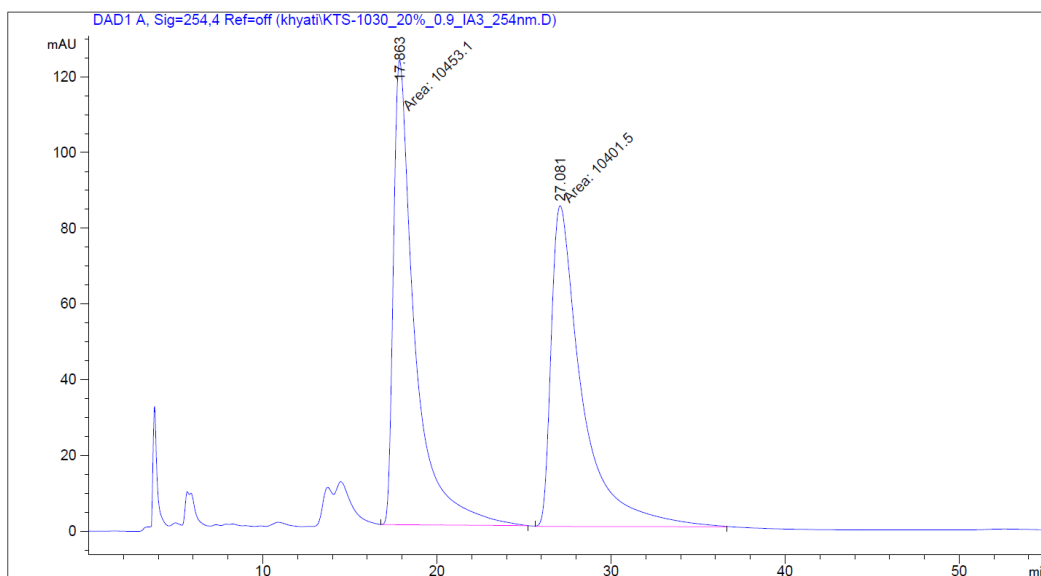


=====  
 Area Percent Report  
 =====

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	16.201	MM	1.9217	3.88985e5	3373.69116	80.9444
2	28.460	MM	2.0878	9.15731e4	731.00385	19.0556

=====  
 \*\*\* End of Report \*\*\*

### HPLC graph of enantioenriched **3a**

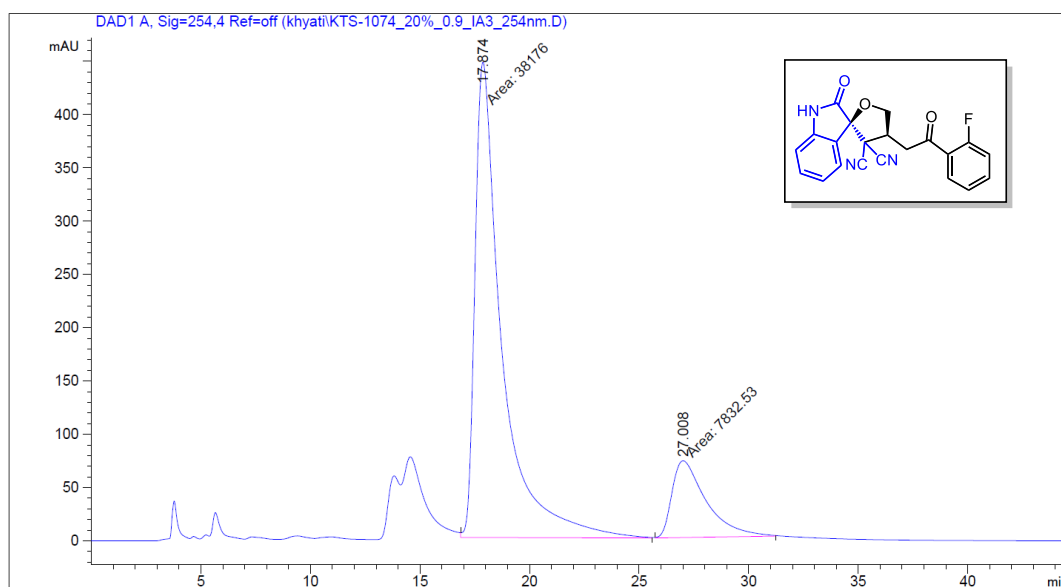


=====  
 Area Percent Report  
 =====

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	17.863	MM	1.4193	1.04531e4	122.75302	50.1237
2	27.081	MM	2.0461	1.04015e4	84.72681	49.8763

=====  
 \*\*\* End of Report \*\*\*

### HPLC graph of racemic **3am**

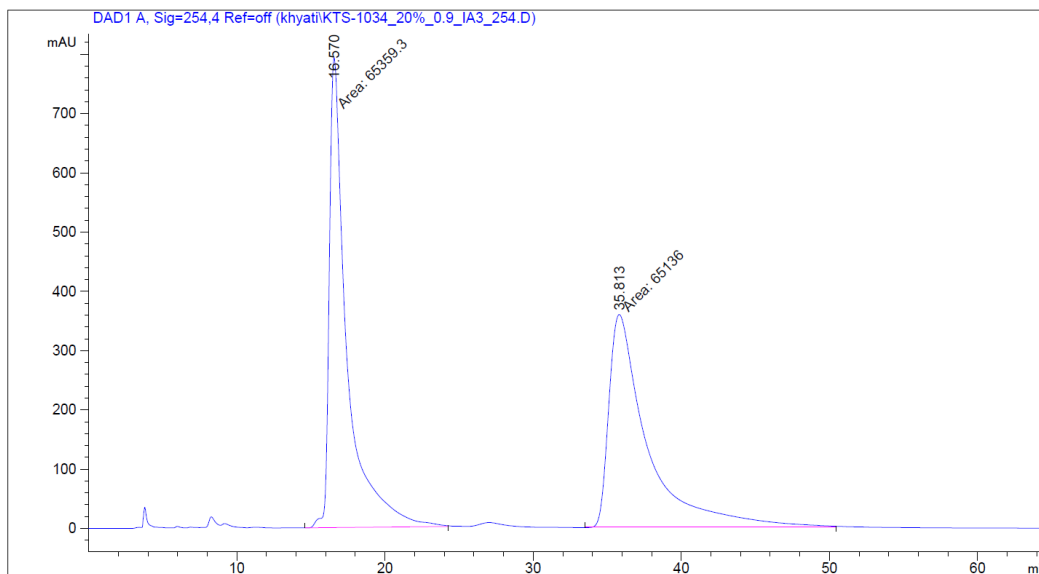


=====  
 Area Percent Report  
 =====

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	17.874	MM	1.4267	3.81760e4	445.98090	82.9759
2	27.008	MM	1.8121	7832.52881	72.03979	17.0241

=====  
 \*\*\* End of Report \*\*\*

### HPLC graph of enantioenriched **3am**

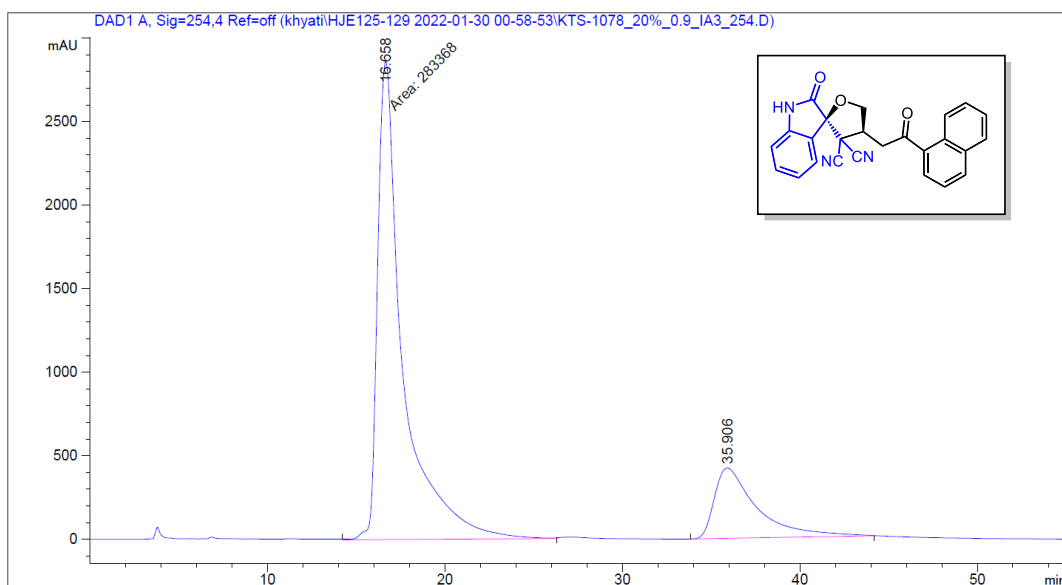


=====  
 Area Percent Report  
 =====

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	16.570	MM	1.3741	6.53593e4	792.77563	50.0856
2	35.813	MM	3.0242	6.51360e4	358.96573	49.9144

=====  
 \*\*\* End of Report \*\*\*

### HPLC graph of racemic **3an**

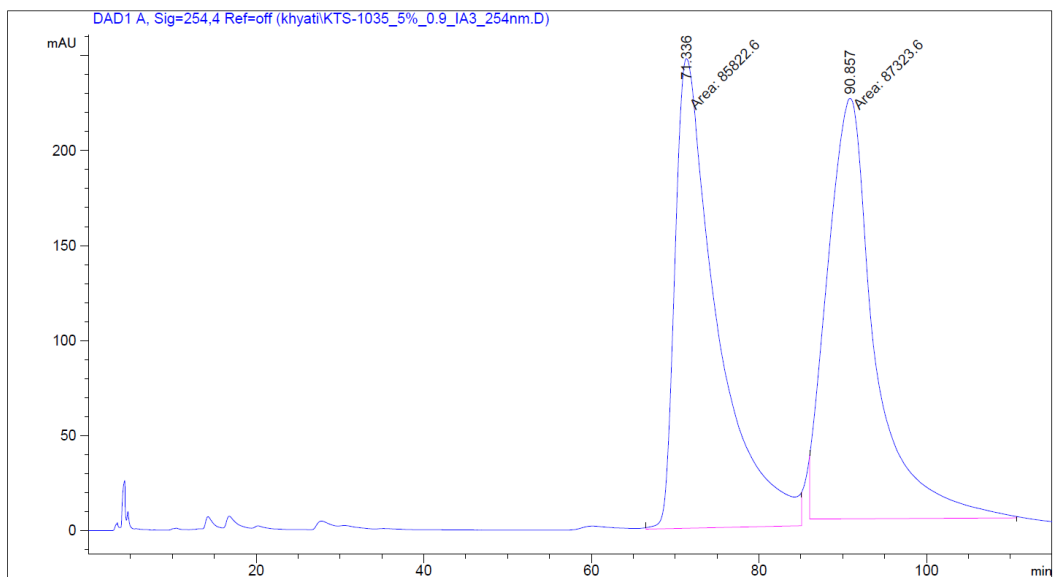


=====  
 Area Percent Report  
 =====

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	16.658	MM	1.6499	2.83368e5	2862.55249	80.1865
2	35.906	BB	2.3699	7.00180e4	421.09830	19.8135

=====  
 \*\*\* End of Report \*\*\*

### HPLC graph of enantioenriched **3an**

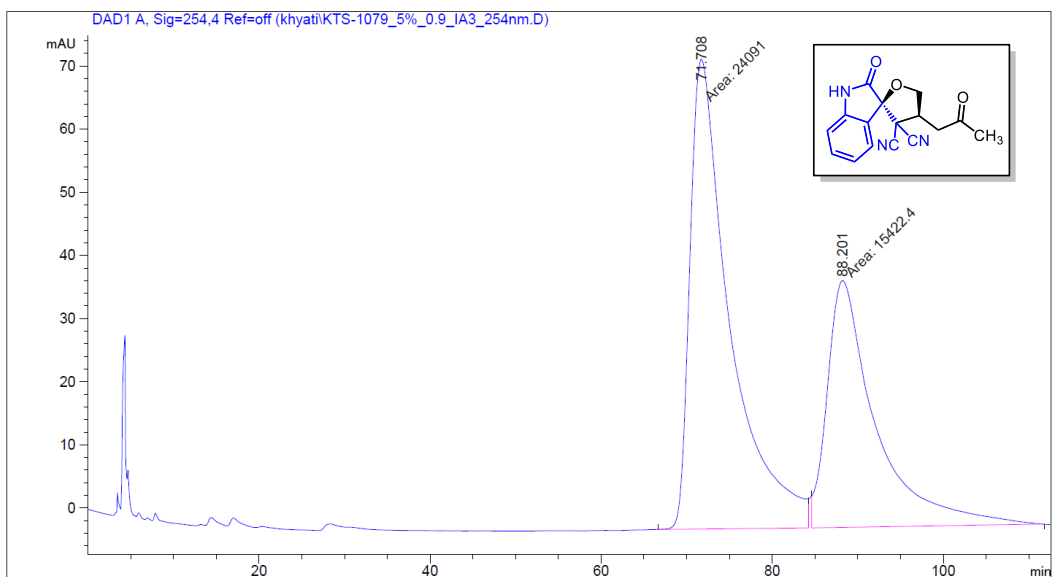


=====  
 Area Percent Report  
 =====

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	71.336	MM	5.7904	8.58226e4	247.02734	49.5666
2	90.857	MM	6.5822	8.73236e4	221.10945	50.4334

=====  
 \*\*\* End of Report \*\*\*

HPLC graph of racemic **3ao**

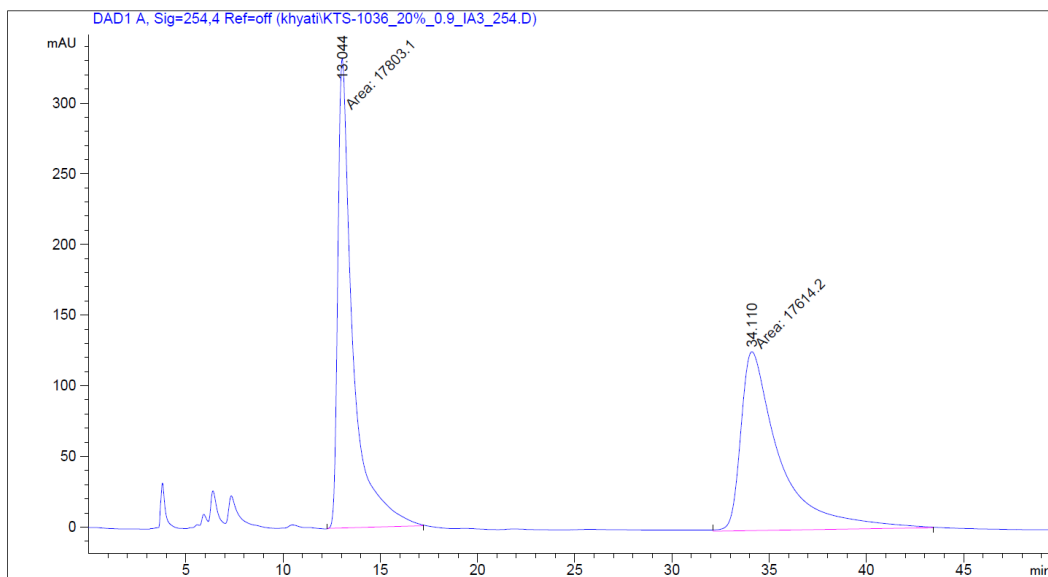


=====  
 Area Percent Report  
 =====

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	71.708	MM	5.3967	2.40910e4	74.40009	60.9692
2	88.201	MM	6.5781	1.54224e4	39.07525	39.0308

=====  
 \*\*\* End of Report \*\*\*

HPLC graph of enantioenriched **3ao**

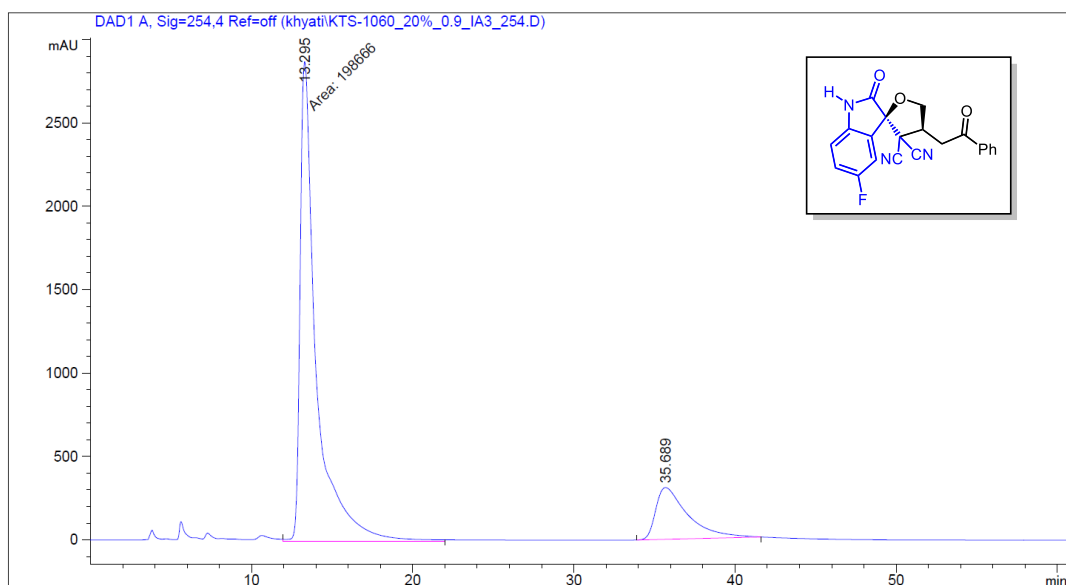


=====  
Area Percent Report  
=====

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	13.044	MM	0.8936	1.78031e4	332.06311	50.2667
2	34.110	MM	2.3203	1.76142e4	126.52483	49.7333

=====  
\*\*\* End of Report \*\*\*

### HPLC graph of racemic **3ba**

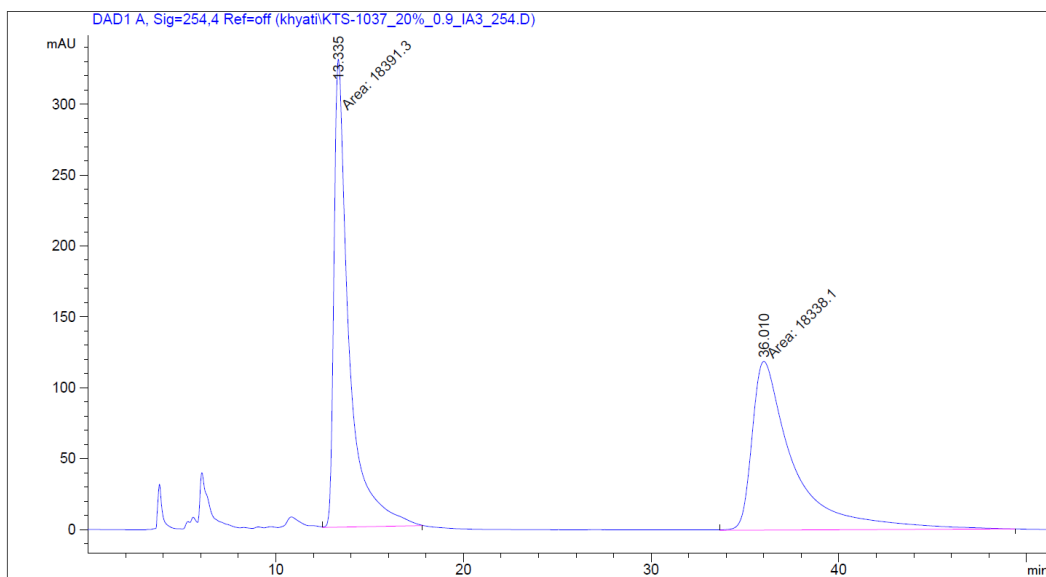


=====  
Area Percent Report  
=====

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	13.295	MM	1.1520	1.98666e5	2874.13843	82.1714
2	35.689	BB	1.9994	4.31042e4	310.54001	17.8286

=====  
\*\*\* End of Report \*\*\*

### HPLC graph of enantioenriched **3ba**

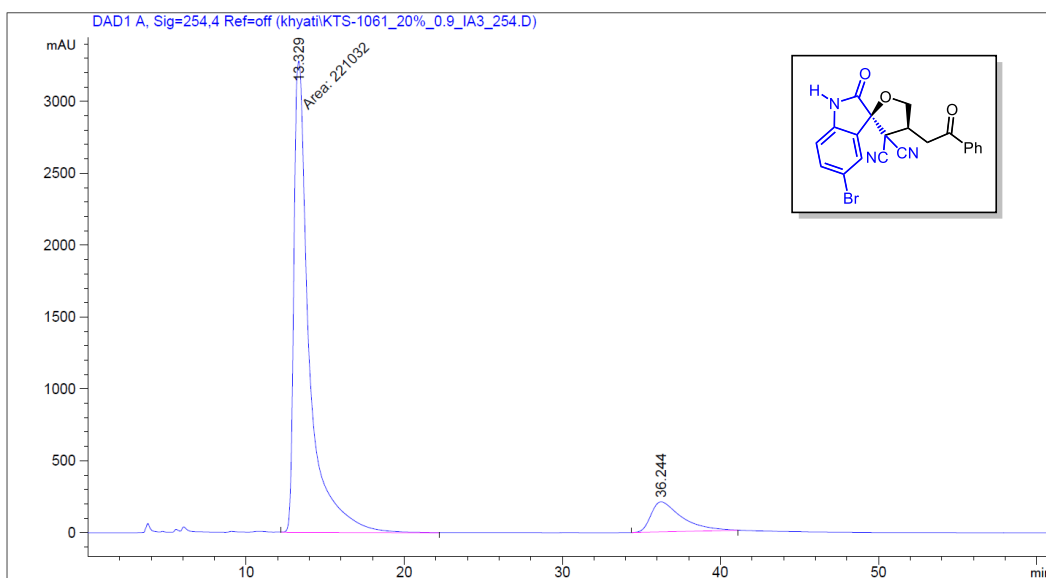


=====  
 Area Percent Report  
 =====

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	13.335	MM	0.9287	1.83913e4	330.06714	50.0724
2	36.010	MM	2.5687	1.83381e4	118.98417	49.9276

=====  
 \*\*\* End of Report \*\*\*

### HPLC graph of racemic **3ca**

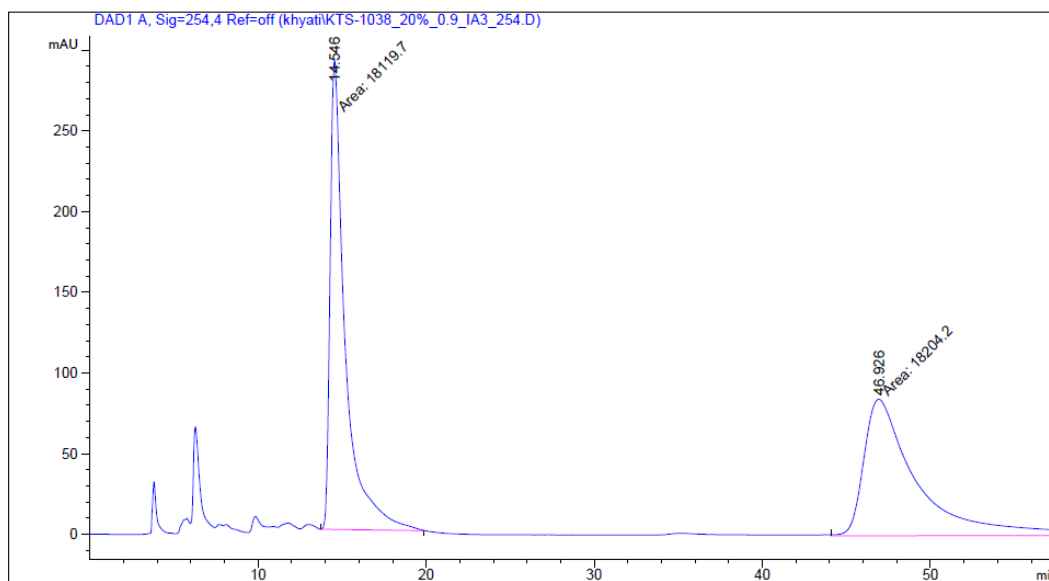


=====  
 Area Percent Report  
 =====

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	13.329	MM	1.1234	2.21032e5	3279.14307	88.6286
2	36.244	BB	1.9702	2.83592e4	209.11510	11.3714

=====  
 \*\*\* End of Report \*\*\*

### HPLC graph of enantioenriched **3ca**

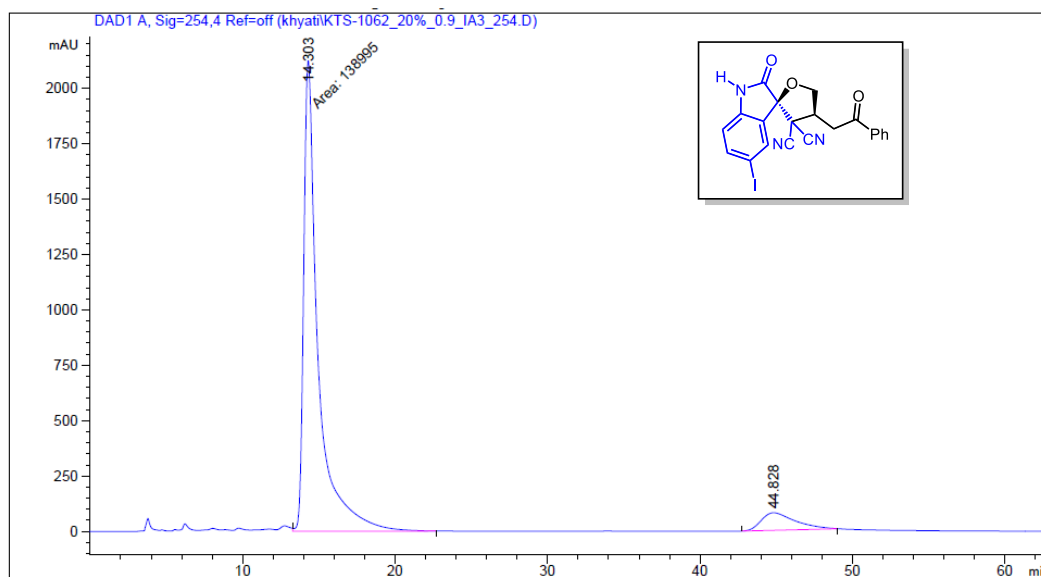


=====  
 Area Percent Report  
 =====

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	14.546	MM	1.0383	1.81197e4	290.84421	49.8836
2	46.926	MM	3.5849	1.82042e4	84.63439	50.1164

=====  
 \*\*\* End of Report \*\*\*

HPLC graph of racemic **3da**



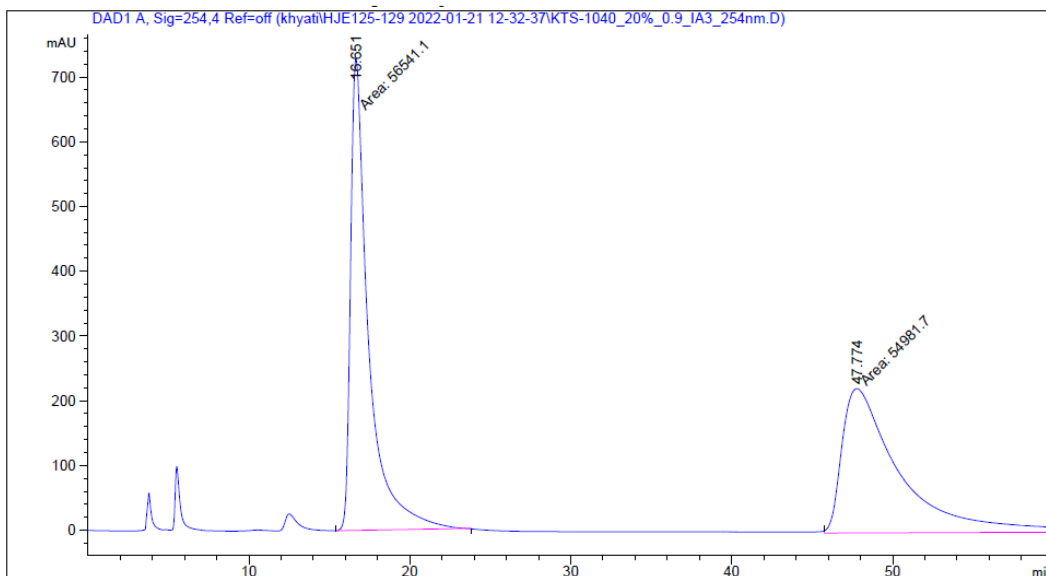
=====  
 Area Percent Report  
 =====

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	14.303	MM	1.0906	1.38995e5	2124.12036	91.8873
2	44.828	BB	2.1579	1.22719e4	79.19316	8.1127

=====  
 \*\*\* End of Report \*\*\*

HPLC graph of enantioenriched **3da**



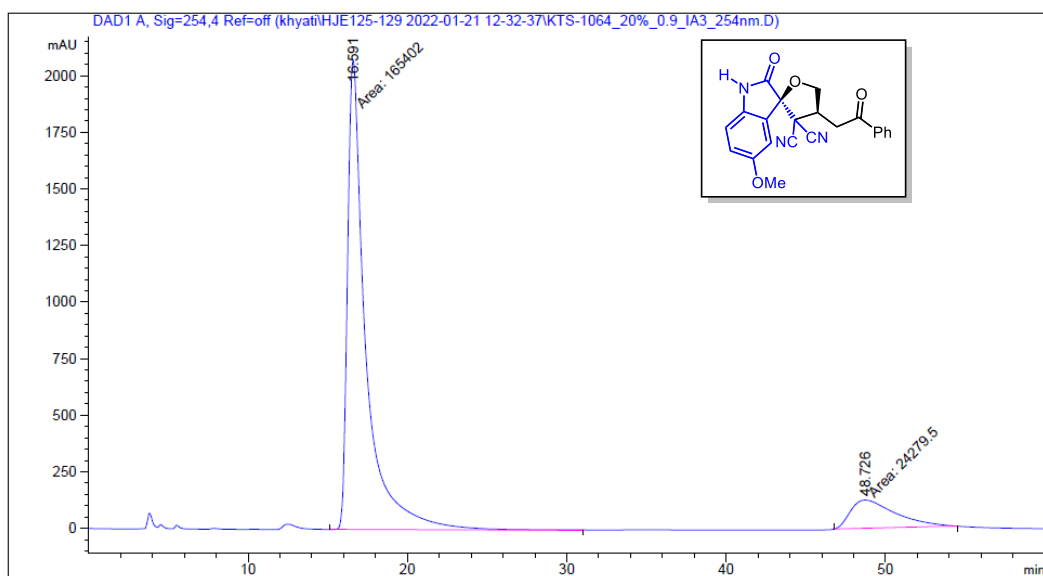


=====  
 Area Percent Report  
 =====

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	16.651	MM	1.2936	5.65411e4	728.49792	50.6992
2	47.774	MM	4.1130	5.49817e4	222.79768	49.3008

=====  
 \*\*\* End of Report \*\*\*

HPLC graph of racemic **3ea**

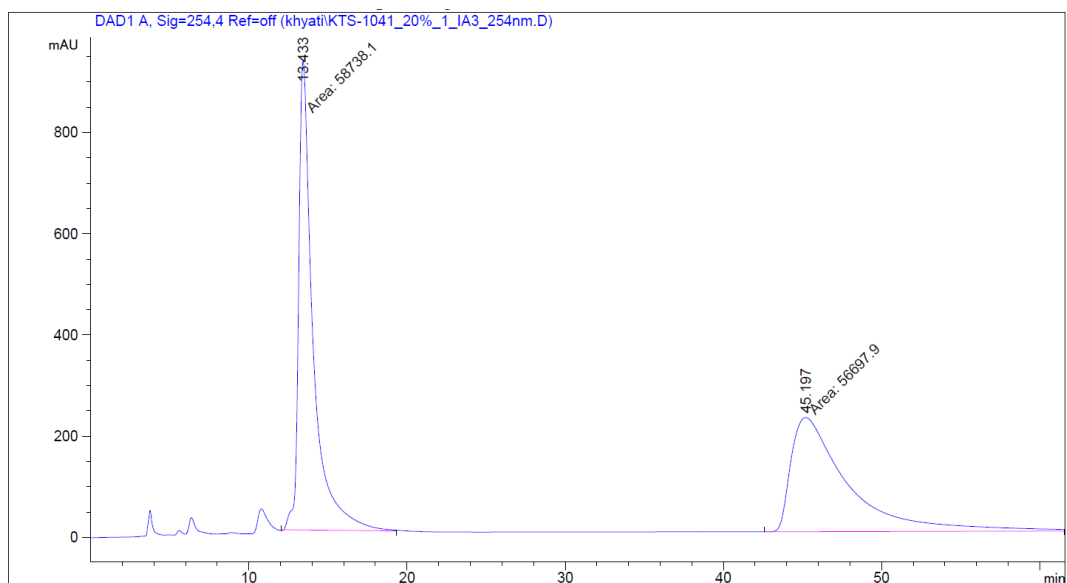


=====  
 Area Percent Report  
 =====

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	16.591	MM	1.3309	1.65402e5	2071.26880	87.1999
2	48.726	MM	3.2515	2.42795e4	124.45325	12.8001

=====  
 \*\*\* End of Report \*\*\*

HPLC graph of enantioenriched **3ea**

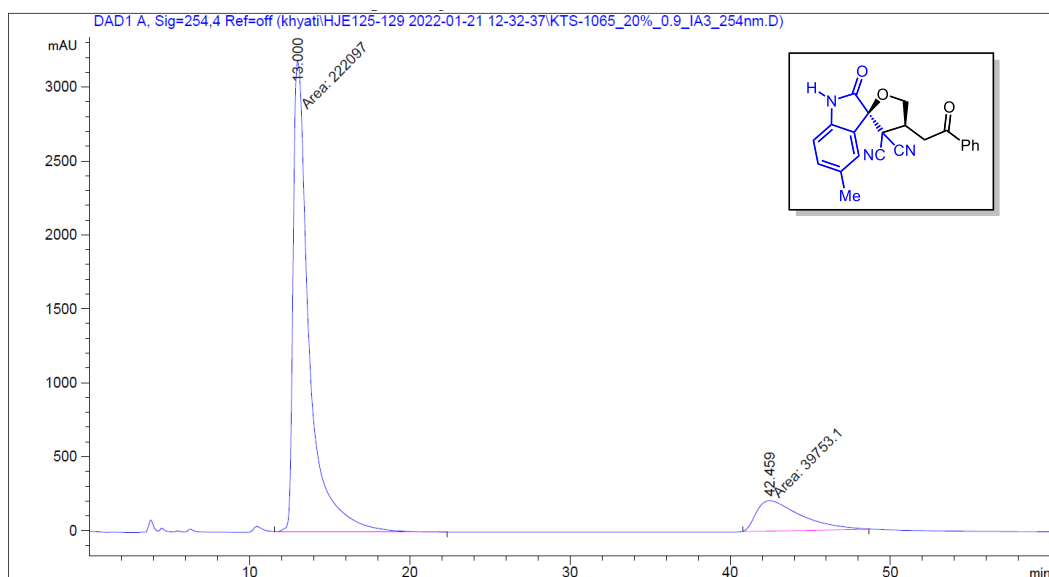


=====  
 Area Percent Report  
 =====

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	13.433	MM	1.0562	5.87381e4	926.86224	50.8837
2	45.197	MM	4.1859	5.66979e4	225.75166	49.1163

=====  
 \*\*\* End of Report \*\*\*

### HPLC graph of racemic **3fa**

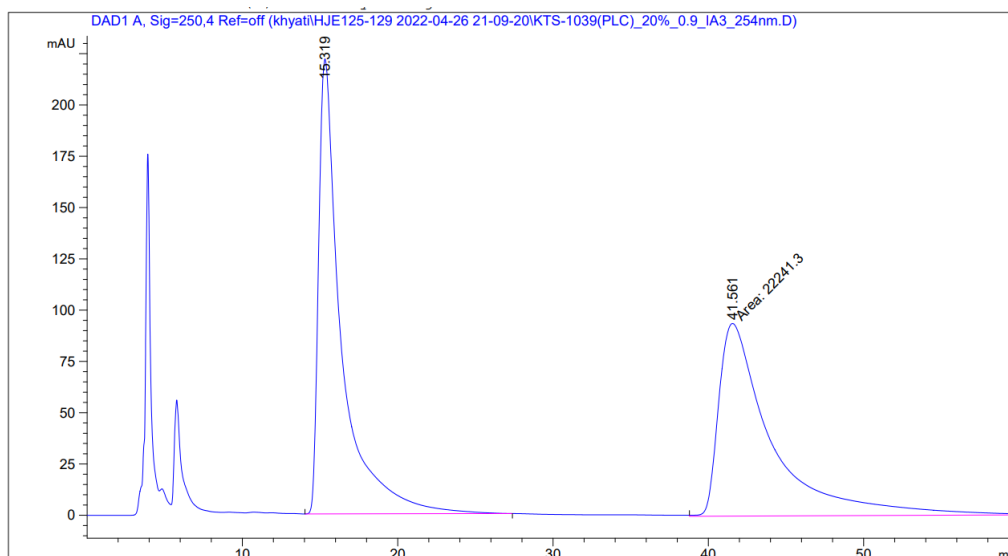


=====  
 Area Percent Report  
 =====

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	13.000	MM	1.1620	2.22097e5	3185.56787	84.8184
2	42.459	MM	3.2154	3.97531e4	206.05502	15.1816

=====  
 \*\*\* End of Report \*\*\*

### HPLC graph of enantioenriched **3fa**

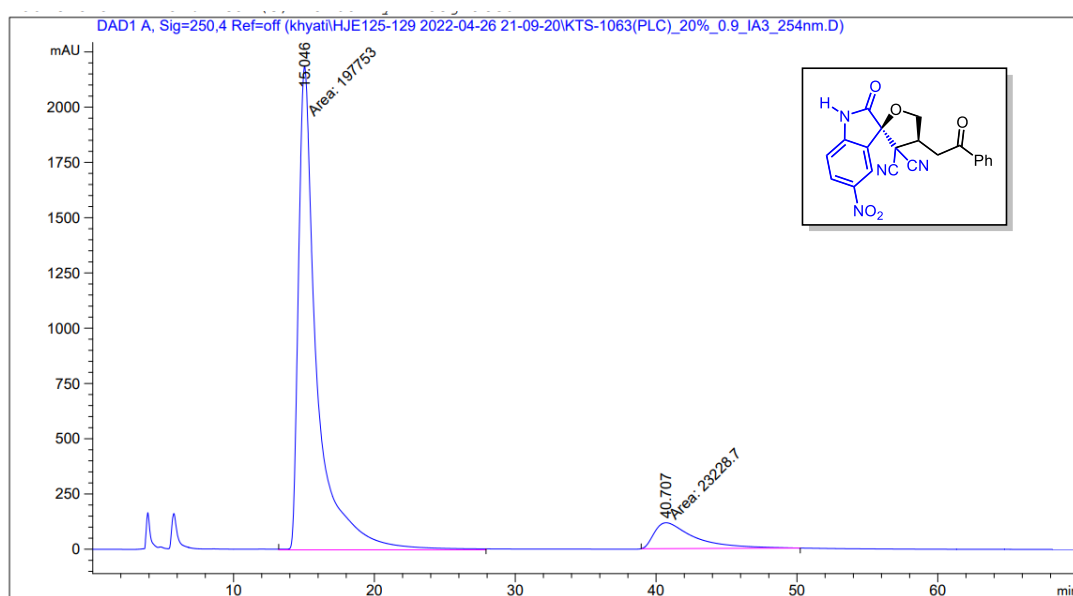


=====  
Area Percent Report  
=====

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	15.319	BB	1.4384	2.26683e4	221.78676	50.4754
2	41.561	MM	3.9491	2.22413e4	93.86544	49.5246

=====  
\*\*\* End of Report \*\*\*

**HPLC graph of racemic 3ga**

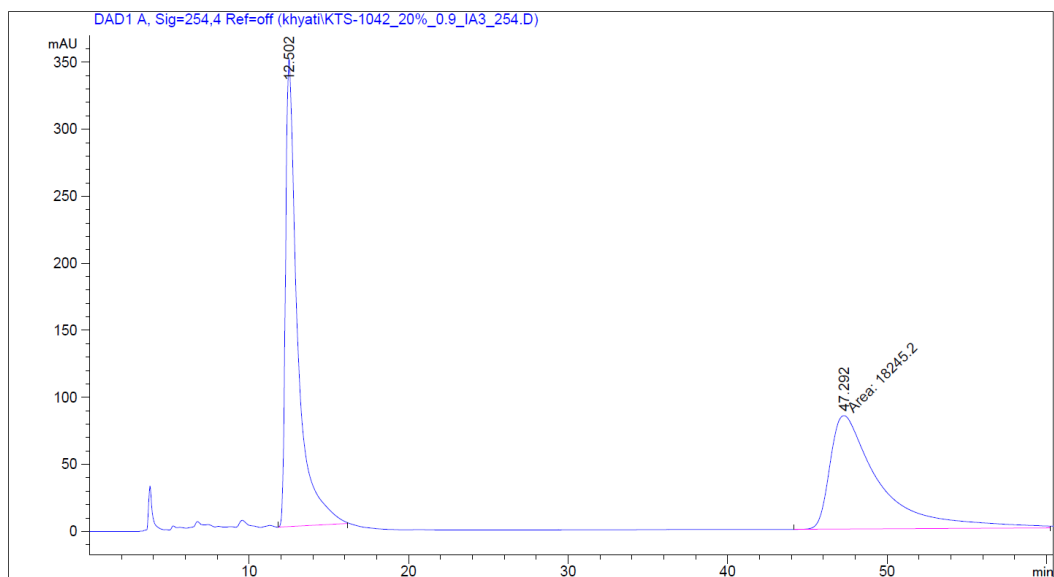


=====  
Area Percent Report  
=====

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	15.046	MM	1.5075	1.97753e5	2186.27441	89.4884
2	40.707	MM	3.3052	2.32287e4	117.13207	10.5116

=====  
\*\*\* End of Report \*\*\*

**HPLC graph of enantioenriched 3ga**

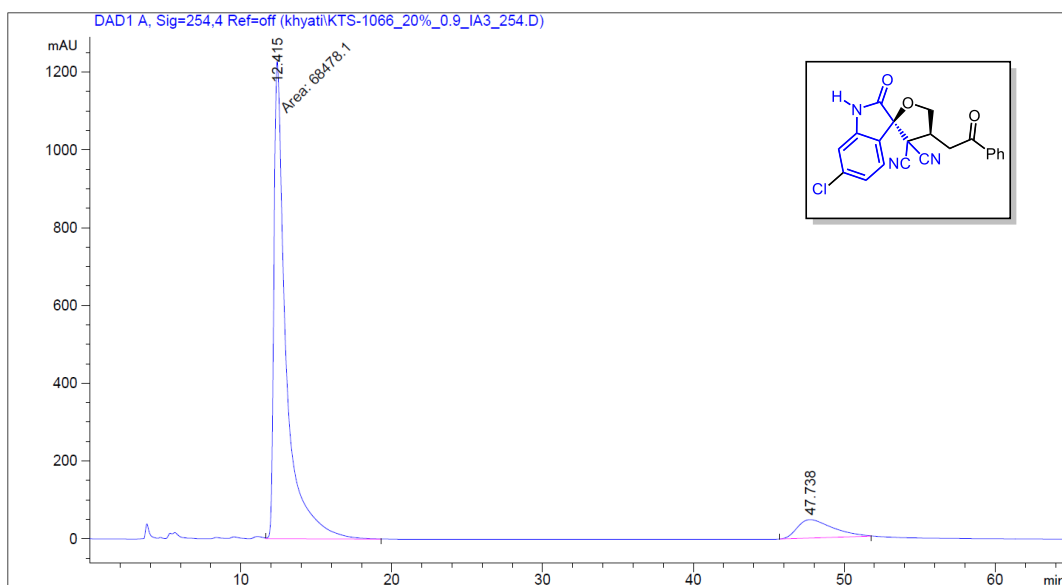


=====  
 Area Percent Report  
 =====

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	12.502	BB	0.7527	1.83626e4	348.50198	50.1604
2	47.292	MM	3.5960	1.82452e4	84.56358	49.8396

=====  
 \*\*\* End of Report \*\*\*

### HPLC graph of racemic **3ha**

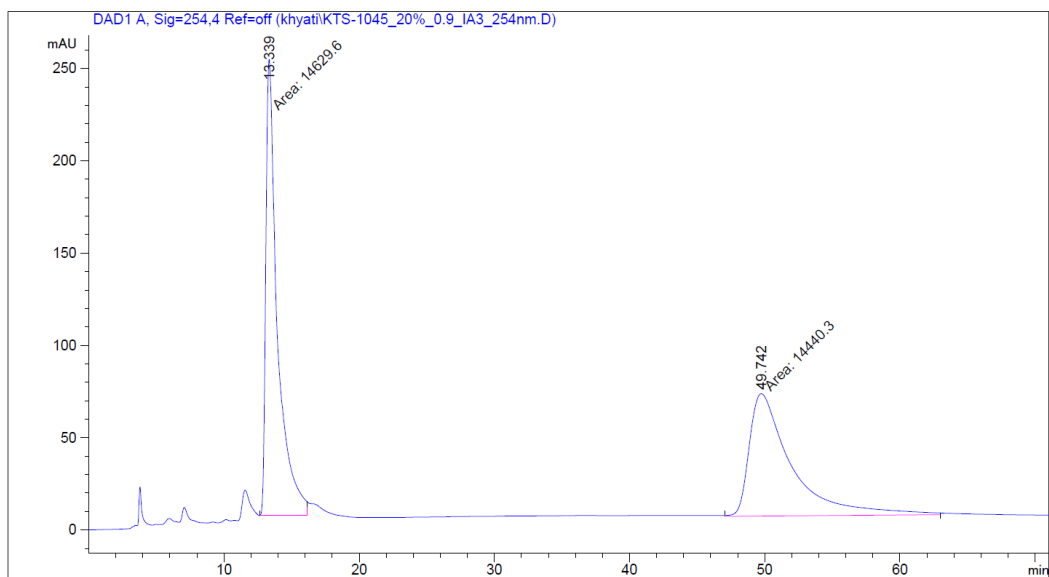


=====  
 Area Percent Report  
 =====

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	12.415	MM	0.9298	6.84781e4	1227.52515	89.9264
2	47.738	BB	2.1778	7670.96094	47.35542	10.0736

=====  
 \*\*\* End of Report \*\*\*

### HPLC graph of enantioenriched **3ha**

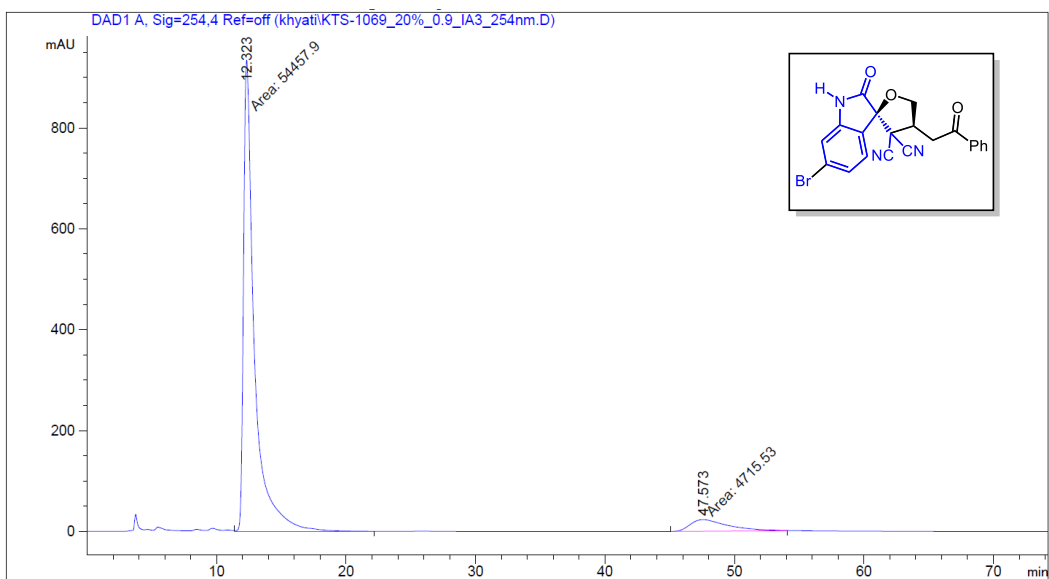


=====  
 Area Percent Report  
 =====

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	13.339	MM	0.9864	1.46296e4	247.19460	50.3256
2	49.742	MM	3.6296	1.44403e4	66.30856	49.6744

=====  
 \*\*\* End of Report \*\*\*

### HPLC graph of racemic **3ia**

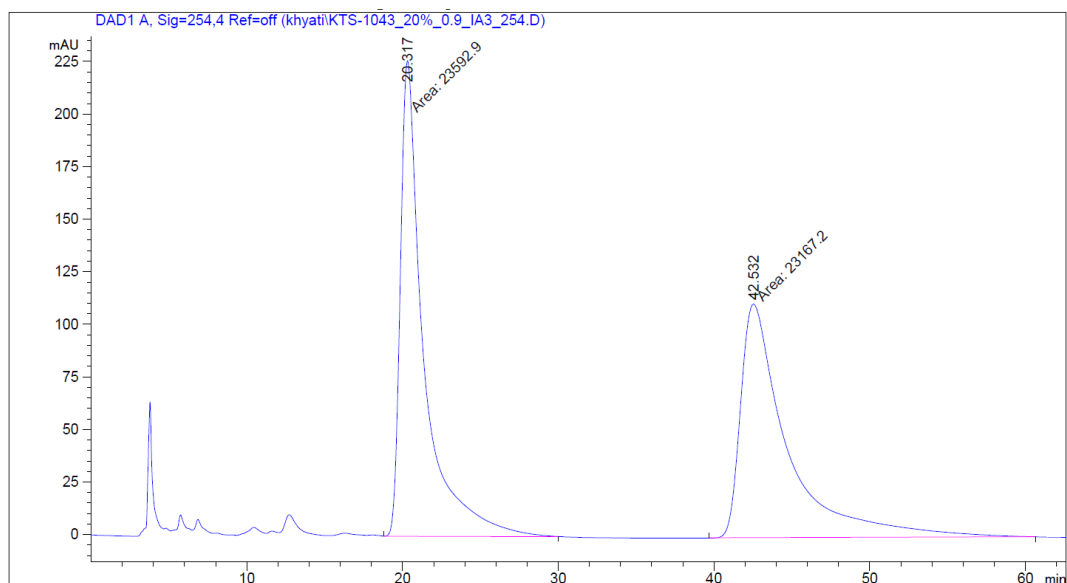


=====  
 Area Percent Report  
 =====

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	12.323	MM	0.9708	5.44579e4	934.94073	92.0310
2	47.573	MM	3.3986	4715.52734	23.12482	7.9690

=====  
 \*\*\* End of Report \*\*\*

### HPLC graph of enantioenriched **3ia**

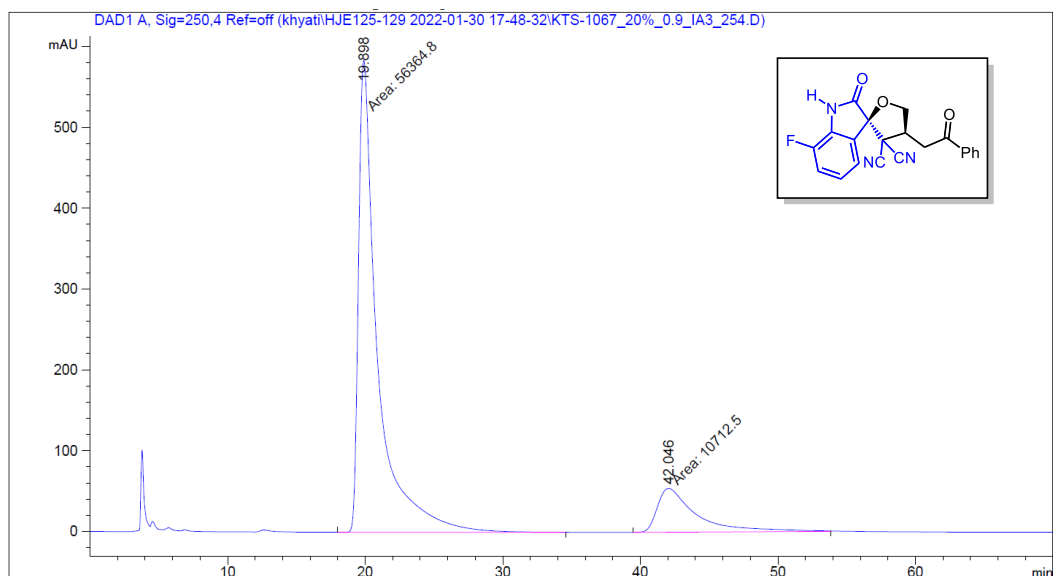


=====  
 Area Percent Report  
 =====

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	20.317	MM	1.7386	2.35929e4	226.17363	50.4552
2	42.532	MM	3.4763	2.31672e4	111.07204	49.5448

=====  
 \*\*\* End of Report \*\*\*

### HPLC graph of racemic **3ja**

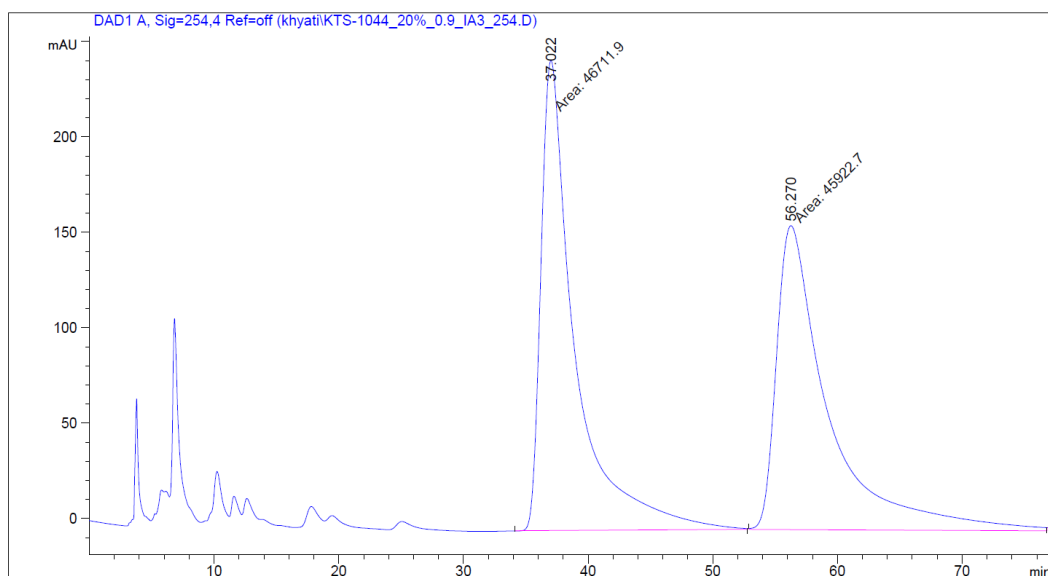


=====  
 Area Percent Report  
 =====

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	19.898	MM	1.6084	5.63648e4	584.05432	84.0296
2	42.046	MM	3.2883	1.07125e4	54.29554	15.9704

=====  
 \*\*\* End of Report \*\*\*

### HPLC graph of enantioenriched **3ja**

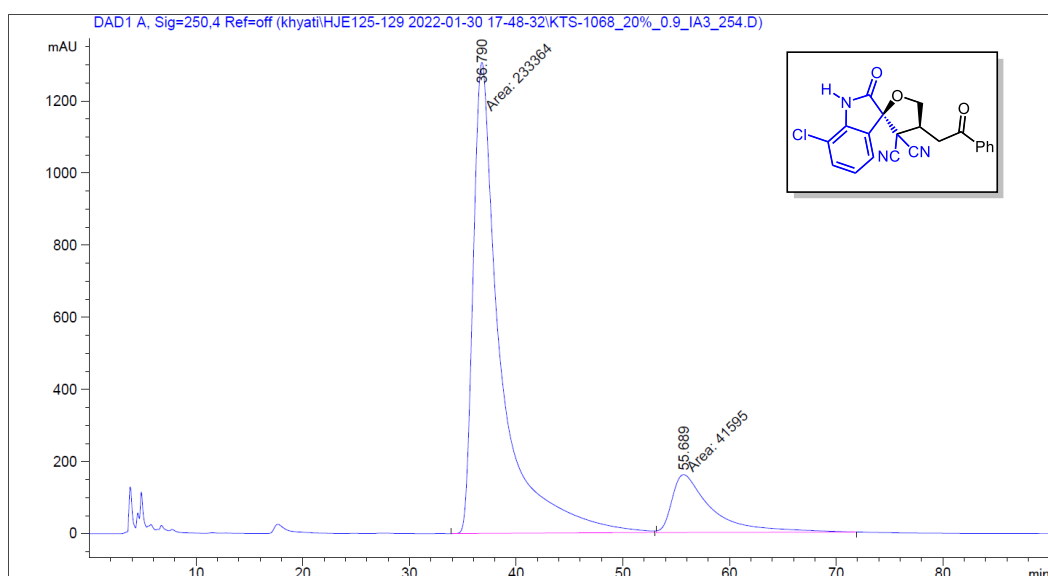


=====  
 Area Percent Report  
 =====

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	37.022	MM	3.1619	4.67119e4	246.22227	50.4260
2	56.270	MM	4.8062	4.59227e4	159.24709	49.5740

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 \*\*\* End of Report \*\*\*

### HPLC graph of racemic 3ka

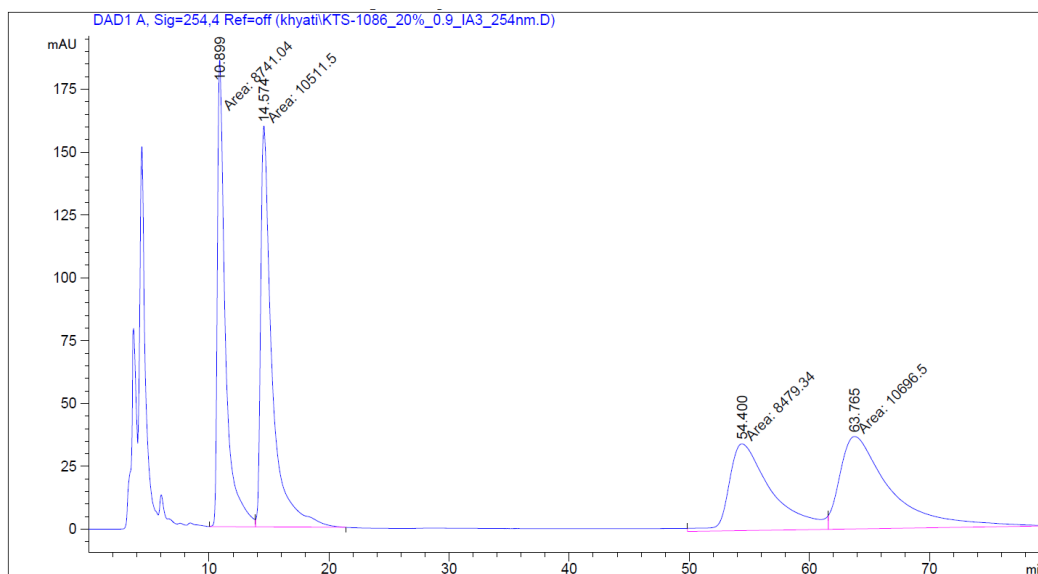


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 Area Percent Report  
 =====

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	36.790	MM	2.9778	2.33364e5	1306.13989	84.8723
2	55.689	MM	4.3195	4.15950e4	160.49490	15.1277

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 \*\*\* End of Report \*\*\*

### HPLC graph of enantioenriched 3ka

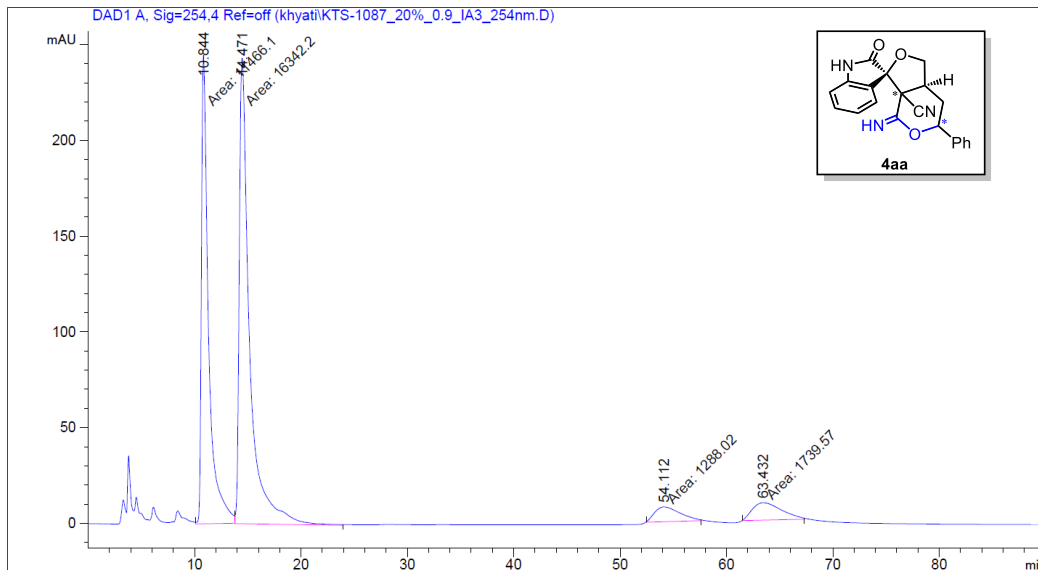


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 Area Percent Report  
 =====

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	10.899	MF	0.7845	8741.03613	185.70013	22.7463
2	14.574	FM	1.0988	1.05115e4	159.44200	27.3536
3	54.400	MF	4.0926	8479.33594	34.53119	22.0653
4	63.765	FM	4.8533	1.06965e4	36.73270	27.8348

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 \*\*\* End of Report \*\*\*

HPLC graph of racemic **4aa**



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 Area Percent Report  
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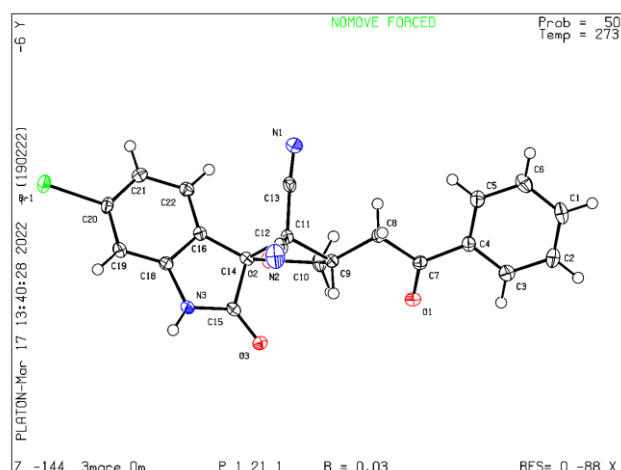
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	10.844	MM	0.7809	1.14661e4	244.72032	37.1844
2	14.471	MM	1.1201	1.63422e4	243.16748	52.9972
3	54.112	MM	1.9712	1288.01892	7.73442	4.1770
4	63.432	MM	3.1739	1739.57397	9.13471	5.6414

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 \*\*\* End of Report \*\*\*

HPLC graph of enantioenriched **4aa**



**Table 1 Crystal data and structure refinement for 3ia.**



Identification code	3mare_0m
Empirical formula	C <sub>21</sub> H <sub>14</sub> BrN <sub>3</sub> O <sub>3</sub>
Formula weight	436.26
Temperature/K	273.15
Crystal system	monoclinic
Space group	P2 <sub>1</sub>
a/Å	10.769(3)
b/Å	7.643(2)
c/Å	11.587(4)
α/°	90
β/°	99.015(8)
γ/°	90
Volume/Å <sup>3</sup>	941.9(5)
Z	2
ρ <sub>calc</sub> /cm <sup>3</sup>	1.538
μ/mm <sup>-1</sup>	2.210
F(000)	440.0
Crystal size/mm <sup>3</sup>	0.026 × 0.023 × 0.02
Radiation	MoKα (λ = 0.71073)
2θ range for data collection/°	6.564 to 56.82
Index ranges	-14 ≤ h ≤ 14, -10 ≤ k ≤ 10, -15 ≤ l ≤ 15
Reflections collected	14049
Independent reflections	4657 [R <sub>int</sub> = 0.0449, R <sub>sigma</sub> = 0.0571]
Data/restraints/parameters	4657/1/253
Goodness-of-fit on F <sup>2</sup>	1.005
Final R indexes [I ≥ 2σ (I)]	R <sub>1</sub> = 0.0270, wR <sub>2</sub> = 0.0618
Final R indexes [all data]	R <sub>1</sub> = 0.0283, wR <sub>2</sub> = 0.0623
Largest diff. peak/hole / e Å <sup>-3</sup>	0.32/-0.26
Flack parameter	0.039(5)