Electronic Supplementary Material (ESI) for Chemical Communications.

Asymmetric [3+2] cycloaddition of 3-amino oxindole-based azomethine ylides with α,β-ynones: a straightforward approach to spirooxindoles incorporating 2,5-dihydropyrroles and pyrroles

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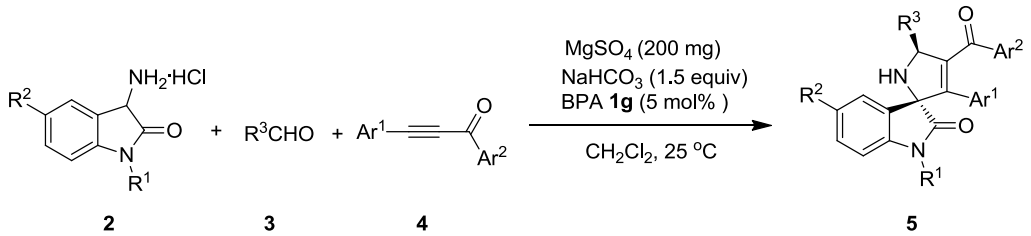
1. General information

All reactions were carried out in Schlenk tube under a dry argon atmosphere. All solvents were purified and dried according to standard methods prior to use. Reactions were monitored by thin layer chromatography (TLC) using silica gel plates. Flash chromatography was carried out utilizing silica gel 200-300 mesh. ^{1}H NMR, ^{19}F NMR spectra were recorded on a Bruker Avance II 400 MHz and Bruker Avance III 471 MHz respectively, ^{13}C NMR spectra were recorded on a Bruker Avance II 101 MHz or Bruker Avance III 126 MHz. The solvent used for NMR spectroscopy was $CDCl_3$, using tetramethylsilane as the internal reference. Data for ^{1}H NMR are recorded as follows: chemical shift (δ, ppm), multiplicity (s = singlet, d = doublet, t = triplet, m = multiplet or unresolved, br = broad singlet, dd = double doublet, coupling constants in Hz, integration). Data for ^{13}C NMR and ^{19}F NMR are reported in terms of chemical shift (δ, ppm). HRMS (ESI) was determined by a HRMS/MS instrument (LTQ Orbitrap XL TM). Enantiomeric excess values were determined by HPLC employing a chiral column on Agilent 1100 series. Optical rotations were reported as follows: $[\alpha]_D^T$(c g/100 mL, solvent). The absolute configuration of **5f** was assigned by the X-ray analysis. All the aldehydes were commercially obtained and recrystallized or distilled prior to use. 3-Amino oxindole hydrochlorides[1] and α,β-ynones[2] were prepared according to literature methods.

2. General procedure for the synthesis of products 5 and 6.

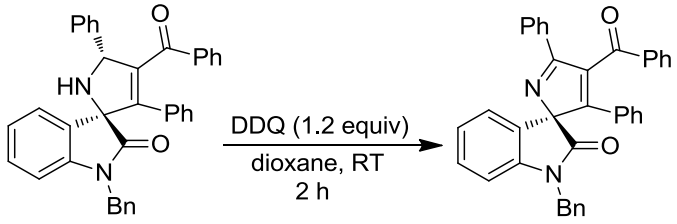
General procedure for the synthesis of spiro[dihydropyrrole-2,3'-oxindoles] (5)



2 **3** **4** **5**

In a Schlenk tube, 3-amino oxindole hydrochloride **2** (0.2 mmol), $NaHCO_3$ (0.3 mmol), α,β-ynone **4** (0.22 mmol), $MgSO_4$ (200 mg) and catalyst (0.02 mmol) were added into CH_2Cl_2 (2 mL) under a dry argon atmosphere at 25 °C. Then, aldehyde **3** (0.24 mmol) was added and the reaction solution was stirred at the same temperature. After the reaction was complete (monitored by TLC), the crude product was purified by column chromatography (ethyl acetate/petroleum ether = 1/20 to 1/4) on silica gel to give the product **5**.

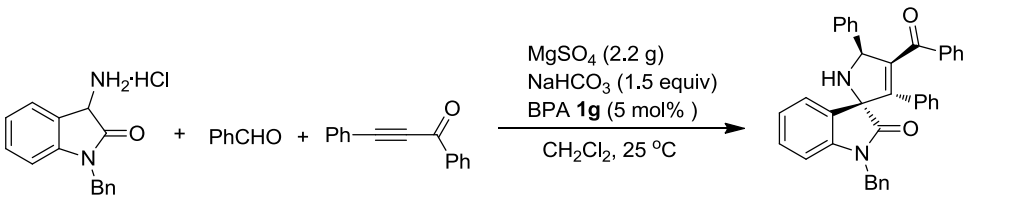
Synthesis of spiro[pyrrole-2,3'-oxindoles] (6)



5 **6**

A reaction tube was charged with **5** (0.1 mmol) and dioxane (1 mL), then DDQ (0.12 mmol) was added at room temperature. After the reaction was stirred for 2 h, the crude product was purified by column chromatography (ethyl acetate/petroleum ether = 1/8) on silica gel to give the product **6**.

Procedure for gram-scale reaction

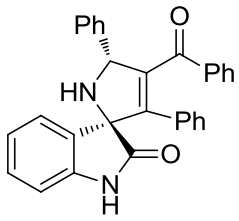


2c **3a** **4a** **5c**

21 h, 0.94 g
88 % yield, > 20 : 1 dr, 99% *ee*

In a Schlenk tube, 3-amino oxindole hydrochloride **2c** (2.2 mmol), BPA **1g** (0.22 mmol), α,β-ynone **4a** (2.42 mmol), $MgSO_4$ (2.2 g) and $NaHCO_3$ (3.3 mmol) were added in CH_2Cl_2 (22 mL) under an argon atmosphere at 25 °C. Then, benzaldehyde **3a** (2.64 mmol) was added and the solution was stirred at the same temperature for 21 h. The crude product was purified by column chromatography (ethyl acetate/petroleum ether = 1/20 to 1/4) on silica gel to give the product **5c**.

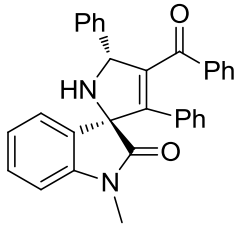
3. Characterization data



5a

(2R,5R)-4-Benzoyl-3,5-diphenyl-1,5-dihydrospiro[pyrrol-2,3'-oxindole]

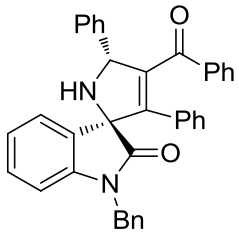
White solid, mp: 88-90 °C, > 99% *ee*. $[\alpha]_D^{22}$ = 170.5 (*c* 0.40, CH_2Cl_2); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.40 (s, 1H), 7.79 (d, *J* = 7.6 Hz, 2H), 7.61 (d, *J* = 7.3 Hz, 1H), 7.54 (d, *J* = 7.4 Hz, 2H), 7.32 (t, *J* = 6.8 Hz, 3H), 7.24 – 7.13 (m, 5H), 6.97 (t, *J* = 7.1 Hz, 1H), 6.89 (t, *J* = 7.4 Hz, 2H), 6.84 (d, *J* = 7.5 Hz, 2H), 6.79 (d, *J* = 7.7 Hz, 1H), 6.10 (s, 1H), 2.92 (br, 1H) ; ^{13}C NMR (101 MHz, $CDCl_3$) δ 194.4, 180.1, 145.0, 144.4, 141.4, 141.3, 136.5, 133.0, 131.8, 130.7, 130.0, 129.4, 128.7, 128.5, 128.3, 128.1, 128.0, 127.8, 125.1, 123.4, 110.6, 79.1, 70.8; HRMS (ESI) for $C_{30}H_{23}N_2O_2$ $[M+H]^+$ calcd 443.1754, found 443.1752. Enantiomeric excess was determined by HPLC with a Chiralpak AD-H column. (n-hexane: i-propanol = 70 : 30, 0.8 mL/min, λ = 254 nm) tR (major) = 22.3 min, tR (minor) = 38.6 min.



5b

(2R,5R)-4-Benzoyl-1'-methyl-3,5-diphenyl-1,5-dihydrospiro[pyrrol-2,3'-oxindole]

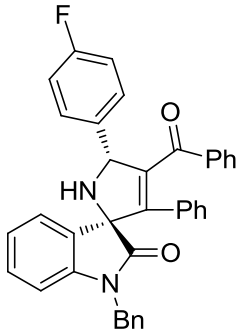
White solid, mp: 71-73 °C, 98% *ee*. $[\alpha]_D^{22}$ = 144.2 (*c* 0.24, CH_2Cl_2); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.84 (d, *J* = 7.7 Hz, 2H), 7.59 (d, *J* = 7.4 Hz, 1H), 7.53 (d, *J* = 7.6 Hz, 2H), 7.39 – 7.30 (m, 4H), 7.30 – 7.23 (m, 3H), 7.16 (t, *J* = 7.4 Hz, 1H), 7.01 – 6.95 (m, 1H), 6.92 (t, *J* = 7.4 Hz, 2H), 6.83 (d, *J* = 7.7 Hz, 2H), 6.74 (d, *J* = 7.8 Hz, 1H), 6.10 (s, 1H), 3.10 (s, 3H), 2.72 (s, 1H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 194.3, 177.8, 145.1, 144.5, 144.1, 141.4, 136.6, 133.1, 131.9, 130.2, 130.0, 129.4, 128.7, 128.3, 128.2, 128.1, 127.9, 127.8, 124.8, 123.4, 108.5, 78.7, 70.9, 26.4; HRMS (ESI) for $C_{31}H_{25}N_2O_2$ $[M+H]^+$ calcd 457.1911, found 457.1901. Enantiomeric excess was determined by HPLC with a Chiralpak AD-H column. (n-hexane: i-propanol = 70 : 30, 0.8 mL/min, λ = 254 nm) tR (major) = 44.9 min, tR (minor) = 22.6 min.



5c

(2R,5R)-4-Benzoyl-1'-benzyl-3,5-diphenyl-1,5-dihydrospiro[pyrrol-2,3'-oxindole]

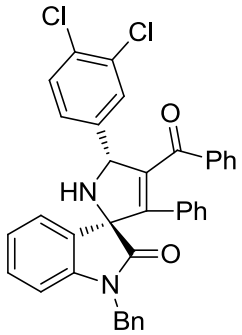
White solid, mp: 86-88 °C, 99% *ee*. $[\alpha]_D^{22}$ = 214.1 (*c* 0.24, CH_2Cl_2); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.80 (d, *J* = 7.8 Hz, 2H), 7.70 (d, *J* = 6.7 Hz, 1H), 7.58 (d, *J* = 7.7 Hz, 2H), 7.34 (t, *J* = 7.2 Hz, 3H), 7.26 – 7.17 (m, 5H), 7.12 (d, *J* = 7.0 Hz, 1H), 7.06 (t, *J* = 7.4 Hz, 3H), 6.92 (t, *J* = 7.5 Hz, 2H), 6.78 (d, *J* = 7.8 Hz, 2H), 6.66 (d, J = 7.5 Hz, 2H), 6.54 (d, *J* = 7.2 Hz, 1H), 6.20 (s, 1H), 5.13 (d, *J* = 16.0 Hz, 1H), 4.43 (d, *J* = 16.0 Hz, 1H), 2.81 (s, 1H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 194.1, 177.9, 145.7, 144.4, 143.3, 141.6, 136.7, 135.0, 133.0, 131.9, 130.3, 130.0, 129.3, 128.7, 128.6, 128.5, 128.3, 128.1, 127.8, 127.3, 126.6, 124.9, 123.4, 109.7, 79.0, 70.7, 43.8; HRMS (ESI) for $C_{37}H_{29}N_2O_2$ $[M+H]^+$ calcd533.2224, found 533.2212. Enantiomeric excess was determined by HPLC with a Chiralpak AD-H column. (n-hexane: i-propanol = 70 : 30, 0.8 mL/min, λ = 254 nm) tR (major) = 31.8 min, tR (minor) = 22.4 min.



5d

(2R,5R)-4-Benzoyl-1'-benzyl-5-(4-fluorophenyl)-3-phenyl-1,5-dihydrospiro[pyrrol-2,3'-oxindole]

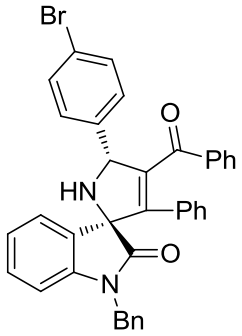
White solid, mp: 80-82 °C, 98% *ee*. $[\alpha]_D^{22}$ = 160.3 (*c* 0.95, CH_2Cl_2); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.77 (d, *J* = 7.5 Hz, 2H), 7.69 (d, *J* = 6.5 Hz, 1H), 7.58 – 7.52 (m, 2H), 7.31 (d, *J* = 7.3 Hz, 1H), 7.24 – 7.17 (m, 4H), 7.10 (d, *J* = 7.2 Hz, 1H), 7.07 – 6.97 (m, 5H), 6.89 (t, *J* = 7.4 Hz, 2H), 6.76 (d, *J* = 7.5 Hz, 2H), 6.64 (d, J = 7.5 Hz, 2H), 6.53 (d, *J* = 6.4 Hz, 1H), 6.21 (s, 1H), 5.11 (d, *J* = 16.0 Hz, 1H), 4.40 (d, *J* = 16.0 Hz, 1H), 2.86 (s, 1H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 194.1, 177.9, 162.5 (*J* = 247.4 Hz), 145.7, 144.2, 143.3, 137.48 (*J* = 3.1 Hz), 136.7, 135.0, 133.1, 131.8, 130.3, 130.1, 129.4 (*J* = 8.1 Hz), 129.3, 128.7, 128.6, 128.3, 128.1, 127.3, 126.6, 124.9, 123.5, 115.6 (*J* = 21.2 Hz), 109.8, 78.9, 69.7, 43.8; ^{19}F NMR (470 MHz, $CDCl_3$) δ -114.33; HRMS (ESI) for $C_{37}H_{28}FN_2O_2$ $[M+H]^+$ calcd 551.2129, found 533.2215. Enantiomeric excess was determined by HPLC with a Chiralpak OD-H column. (n-hexane: i-propanol = 70 : 30, 0.5 mL/min, λ = 254 nm) tR (major) = 17.1 min, tR (minor) = 15.8 min.



5e

(2R,5R)-4-Benzoyl-1'-benzyl-5-(3,4-dichlorophenyl)-3-phenyl-1,5-dihydrospiro[pyrrol-2,3'-oxindole]

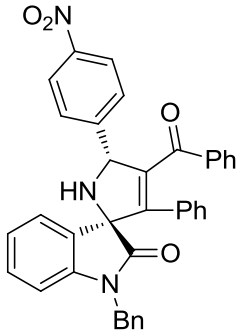
White solid, mp: 91-93 °C, 99% *ee*. $[\alpha]_D^{22}$ = 161.2 (*c* 1.09, CH_2Cl_2); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.71 (d, *J* = 8.9 Hz, 4H), 7.43 – 7.29 (m, 3H), 7.21 (dd, *J* = 14.6, 8.1 Hz, 4H), 7.11 (t, *J* = 7.2 Hz, 1H), 7.04 (t, *J* = 7.2 Hz, 3H), 6.88 (t, *J* = 7.5 Hz, 2H), 6.71 (d, *J* = 7.6 Hz, 2H), 6.60 (d, *J* = 7.5 Hz, 2H), 6.53 (d, *J* = 3.5 Hz, 1H), 6.22 (s, 1H), 5.11 (d, *J* = 16.0 Hz, 1H), 4.38 (d, *J* = 16.0 Hz, 1H), 2.97 (s, 1H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 193.7, 177.8, 146.2, 143.3, 143.2, 142.3, 136.6, 134.9, 133.1, 132.7, 131.8, 131.5, 130.5, 130.2, 130.1, 129.8, 129.3, 128.8, 128.7, 128.3, 128.1, 127.3, 127.1, 126.5, 125.0, 123.6, 109.8, 78.9, 68.9, 43.9; HRMS (ESI) for $C_{37}H_{26}Cl_2N_2NaO_2$ $[M+Na]^+$ calcd 623.1264, found 623.1255. Enantiomeric excess was determined by HPLC with a Chiralpak AD-H column. (n-hexane: i-propanol = 70 : 30, 0.5 mL/min, λ = 254 nm) tR (major) = 51.2 min, tR (minor) = 46.9 min.



5f

(2R,5R)-4-Benzoyl-1'-benzyl-5-(4-bromophenyl)-3-phenyl-1,5-dihydrospiro[pyrrol-2,3'-oxindole]

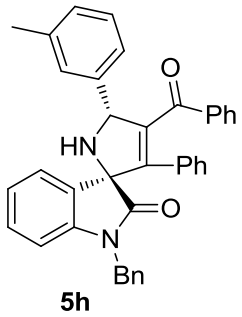
White solid, mp: 84-86 °C, 98% *ee*. $[\alpha]_D^{22}$ = 164.6 (*c* 1.15, CH_2Cl_2); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.75 (d, *J* = 7.5 Hz, 2H), 7.69 (d, *J* = 6.2 Hz, 1H), 7.45 (m, 4H), 7.31 (t, *J* = 7.3 Hz, 1H), 7.22 – 7.18 (m, 4H), 7.14 – 7.08 (m, 1H), 7.04 (t, *J* = 7.5 Hz, 3H), 6.89 (t, *J* = 7.5 Hz, 2H), 6.74 (d, *J* = 7.5 Hz, 2H), 6.63 (d, *J* = 7.4 Hz, 2H), 6.53 (d, *J* = 6.7 Hz, 1H), 6.20 (s, 1H), 5.11 (d, *J* = 16.0 Hz, 1H), 4.39 (d, *J* = 16.0 Hz, 1H), 3.05 (br, 1H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 194.0, 177.8, 146.0, 143.8, 143.2, 140.8, 136.6, 135.0, 133.1, 131.8, 131.7, 130.3, 130.1, 129.5, 129.3, 128.7, 128.6, 128.3, 128.1, 127.3, 126.6, 124.9, 123.5, 122.0, 109.8, 78.9, 69.7, 43.9; HRMS (ESI) for $C_{37}H_{28}BrN_2O_2$ $[M+H]^+$ calcd 613.1314, found 613.1307. Enantiomeric excess was determined by HPLC with a Chiralpak OD-H column. (n-hexane: i-propanol = 70 : 30, 0.5 mL/min, λ = 254 nm) tR (major) = 19.7 min, tR (minor) = 17.4 min.



5g

(2R,5R)-4-Benzoyl-1'-benzyl-5-(4-nitrophenyl)-3-phenyl-1,5-dihydrospiro [pyrrol-2,3'-oxindole]

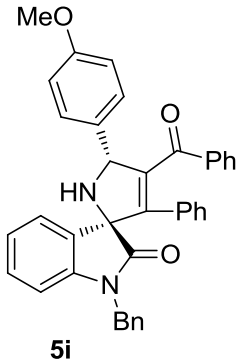
White solid, mp: 104-106 °C, 98% *ee*. $[\alpha]_D^{22}$ = 186.5 (*c* 0.47, CH_2Cl_2); ^1H NMR (400 MHz, $CDCl_3$) δ 8.17 (d, *J* = 8.5 Hz, 2H), 7.81 (d, *J* = 8.5 Hz, 2H), 7.78 – 7.74 (m, 1H), 7.67 (d, *J* = 7.6 Hz, 2H), 7.31 (t, *J* = 7.3 Hz, 1H), 7.25 – 7.23 (m, 2H), 7.18 (t, *J* = 7.6 Hz, 2H), 7.12 (t, *J* = 7.3 Hz, 1H), 7.06 – 7.02 (m, 3H), 6.89 (t, *J* = 7.6 Hz, 2H), 6.70 (d, *J* = 7.7 Hz, 2H), 6.60 (d, *J* = 7.5 Hz, 2H), 6.58 – 6.54 (m, 1H), 6.39 (s, 1H), 5.12 (d, *J* = 16.0 Hz, 1H), 4.39 (d, *J* = 16.0 Hz, 1H), 3.11 (s, 1H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 193.7, 177.7, 149.3, 147.6, 146.5, 143.2, 142.9, 136.5, 134.8, 133.2, 131.3, 130.2, 129.2, 128.9, 128.7, 128.6, 128.3, 128.1, 127.4, 126.5, 125.0, 123.8, 123.6, 109.9, 79.0, 77.4, 69.1, 43.9; HRMS (ESI) for $C_{37}H_{27}N_3NaO_4$ $[M+Na]^+$ calcd 600.1894, found 600.1880. Enantiomeric excess was determined by HPLC with a Chiralpak AD-H column. (n-hexane: i-propanol = 70 : 30, 0.8 mL/min, λ = 254 nm) tR (major) = 68.0 min, tR (minor) = 46.9 min.



5h

(2R,5R)-4-Benzoyl-1'-benzyl-3-phenyl-5-(m-tolyl)-1,5-dihydrospiro[pyrrol-2,3'-oxindole]

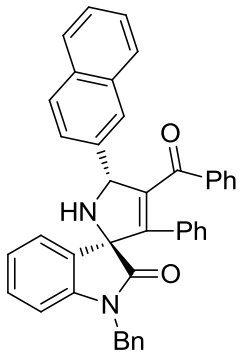
White solid, mp: 80-82 °C, 97% *ee*. $[\alpha]_D^{22}$ = 182.3 (*c* 0.26, CH_2Cl_2); ^1H NMR (400 MHz, $CDCl_3$) δ 7.81 (d, *J* = 7.6 Hz, 2H), 7.68 (d, *J* = 7.0 Hz, 1H), 7.40 – 7.32 (m, 3H), 7.24 (d, *J* = 8.2 Hz, 3H), 7.21 – 7.17 (m, 2H), 7.12 (d, *J* = 7.1 Hz, 1H), 7.06 (t, *J* = 6.4 Hz, 4H), 6.92 (t, *J* = 7.6 Hz, 2H), 6.79 (d, *J* = 7.6 Hz, 2H), 6.66 (d, *J* = 7.5 Hz, 2H), 6.53 (d, *J* = 7.1 Hz, 1H), 6.15 (s, 1H), 5.13 (d, *J* = 16.0 Hz, 1H), 4.42 (d, *J* = 16.0 Hz, 1H), 2.75 (br, 1H), 2.32 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 194.1, 177.9, 145.8, 144.5, 143.3, 141.5, 138.3, 136.8, 135.0, 132.9, 131.9, 130.3, 130.0, 129.4, 128.9, 128.7, 128.6, 128.5, 128.2, 127.3, 126.6, 124.8, 124.7, 123.4, 109.7, 79.1, 70.8, 43.8, 21.5; HRMS (ESI) for $C_{38}H_{31}N_2O_2$ $[M+H]^+$ calcd 547.2380, found 547.2378. Enantiomeric excess was determined by HPLC with a Chiralpak OD-H column. (n-hexane: i-propanol = 90 : 10, 0.8 mL/min, λ = 254 nm) tR (major) = 22.1 min, tR (minor) = 19.1 min.



5i

(2R,5R)-4-Benzoyl-1'-benzyl-5-(4-methoxyphenyl)-3-phenyl-1,5-dihydrospiro[pyrrol-2,3'-oxindole]

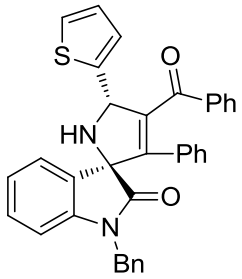
White solid, mp: 92-94 °C, 97% *ee*. $[\alpha]_D^{22}$ = 180.5 (*c* 0.85, CH_2Cl_2); ^1H NMR (400 MHz, $CDCl_3$) δ 7.82 (d, *J* = 7.4 Hz, 2H), 7.67 (d, *J* = 6.5 Hz, 1H), 7.48 (d, *J* = 8.2 Hz, 2H), 7.33 (t, *J* = 7.3 Hz, 1H), 7.22 (d, *J* = 7.7 Hz, 2H), 7.19 – 7.09 (m, 3H), 7.07–7.03 (m, 3H), 6.91 (t, *J* = 7.6 Hz, 2H), 6.86 (d, *J* = 8.2 Hz, 2H), 6.79 (d, *J* = 7.4 Hz, 2H), 6.67 (d, *J* = 7.4 Hz, 2H), 6.53 (d, *J* = 6.8 Hz, 1H), 6.14 (s, 1H), 5.12 (d, *J* = 16.0 Hz, 1H), 4.41 (d, *J* = 16.0 Hz, 1H), 3.72 (s, 3H), 2.73 (s, 1H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 194.3, 178.0, 159.4, 145.5, 144.7, 143.3, 136.7, 135.1, 133.7, 133.0, 132.1, 130.3, 130.0, 129.4, 128.9, 128.7, 128.6, 128.5, 128.3, 128.1, 127.3, 126.6, 124.8, 123.4, 114.2, 109.7, 78.9, 70.3, 55.2, 43.8; HRMS (ESI) for $C_{38}H_{31}N_2O_3$ $[M+H]^+$ calcd 563.2329, found 563.2329. Enantiomeric excess was determined by HPLC with a Chiralpak AD-H column. (n-hexane: i-propanol = 70 : 30, 0.8 mL/min, λ = 254 nm) tR (major) = 58.1 min, tR (minor) = 53.2 min.



5j

(2R,5R)-4-Benzoyl-1'-benzyl-5-(naphthalen-2-yl)-3-phenyl-1,5-dihydrospiro[pyrrol-2,3'-oxindole]

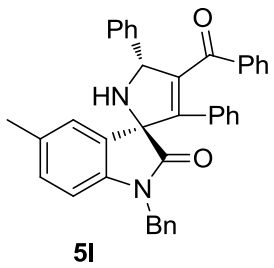
White solid, mp: 75-77 °C, 99% *ee*. $[\alpha]_D^{22}$ = 192.8 (*c* 0.92, CH_2Cl_2); ^1H NMR (400 MHz, $CDCl_3$) δ 7.93 (s, 1H), 7.85–7.76 (m, 7H), 7.46 – 7.37 (m, 2H), 7.30 (t, *J* = 7.2 Hz, 1H), 7.22 – 7.17 (m, 4H), 7.14 – 7.09 (m, 1H), 7.05 (t, *J* = 7.3 Hz, 3H), 6.91 (t, *J* = 7.4 Hz, 2H), 6.81 (d, *J* = 7.6 Hz, 2H), 6.65 (d, *J* = 7.4 Hz, 2H), 6.53 (d, *J* = 6.7 Hz, 1H), 6.38 (s, 1H), 5.13 (d, *J* = 16.0 Hz, 1H), 4.40 (d, *J* = 16.0 Hz, 1H), 2.90 (s, 1H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 194.2, 178.0, 145.9, 144.4, 143.3, 138.9, 136.7, 135.1, 133.4, 133.3, 133.0, 131.9, 130.4, 130.1, 129.4, 128.7, 128.6, 128.3, 128.2, 128.1 127.7, 127.3, 127.2, 126.6, 126.1, 125.3, 125.0, 123.5, 109.8, 79.1, 70.8, 43.9; HRMS (ESI) for $C_{41}H_{31}N_2O_2$ $[M+H]^+$ calcd 583.2380, found 583.2374. Enantiomeric excess was determined by HPLC with a Chiralpak OD-H column. (n-hexane: i-propanol = 90 : 10, 0.8 mL/min, λ = 254 nm) tR (major) = 43.9 min, tR (minor) = 31.8 min.



5k

(2R,5S)-4-Benzoyl-1'-benzyl-3-phenyl-5-(thiophen-2-yl)-1,5-dihydrospiro[pyrrol-2,3'-oxindole]

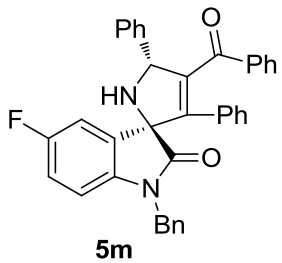
White solid, mp: 58-60 °C, 98% *ee*. $[\alpha]_D^{22}$ = 191.1 (*c* 0.64, CH_2Cl_2); ^1H NMR (400 MHz, $CDCl_3$) δ 7.89 – 7.78 (m, 1H), 7.72 (d, *J* = 7.8 Hz, 2H), 7.27 (t, *J* = 7.4 Hz, 1H), 7.24 – 7.14 (m, 5H), 7.09 (t, *J* = 7.3 Hz, 1H), 7.06 – 6.98 (m, 4H), 6.86 (t, *J* = 7.1 Hz, 3H), 6.67 (d, *J* = 7.8 Hz, 2H), 6.56 (s, 1H), 6.55 – 6.47 (m, 3H), 5.09 (d, *J* = 16.0 Hz, 1H), 4.33 (d, *J* = 16.0 Hz, 1H), 3.09 (s, 1H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 193.7, 177.6, 147.2, 145.6, 143.4, 143.1, 136.8, 135.0, 132.9, 131.6, 130.5, 130.0, 129.3, 128.7, 128.6, 128.1, 128.0, 127.2, 127.2, 126.5, 125.3, 125.3, 125.1, 123.6, 109.7, 79.1, 77.5, 77.1, 76.8, 66.1, 43.9; HRMS (ESI) for $C_{35}H_{27}N_2O_2S$ $[M+H]^+$ calcd 539.1788, found 539.1779. Enantiomeric excess was determined by HPLC with a Chiralpak AD-H column. (n-hexane: i-propanol = 70 : 30, 0.8 mL/min, λ = 254 nm) tR (major) = 36.8 min, tR (minor) = 27.2 min.



5l

(2R,5R)-4-Benzoyl-1'-benzyl-5'-methyl-3,5-diphenyl-1,5-dihydrospiro[pyrrol-2,3'-oxindole]

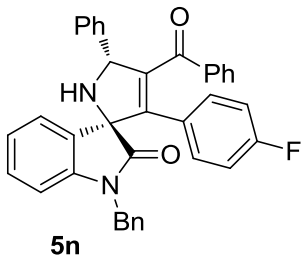
White solid, mp: 91-93 °C, 94% *ee*. $[\alpha]_D^{22}$ = 212.7 (*c* 0.22, CH_2Cl_2); ^1H NMR (400 MHz, $CDCl_3$) δ 7.82 (d, *J* = 7.7 Hz, 2H), 7.57 (d, *J* = 7.6 Hz, 2H), 7.47 (s, 1H), 7.38 – 7.33 (m, 3H), 7.25 (d, *J* = 6.0 Hz, 3H), 7.17 – 7.03 (m, 4H), 7.00 (d, *J* = 7.8 Hz, 1H), 6.93 (t, *J* = 7.6 Hz, 2H), 6.81 (d, *J* = 7.7 Hz, 2H), 6.66 (d, *J* = 7.4 Hz, 2H), 6.43 (d, *J* = 7.9 Hz, 1H), 6.18 (s, 1H), 5.12 (d, *J* = 16.0 Hz, 1H), 4.41 (d, *J* = 16.0 Hz, 1H), 2.79 (s, 1H), 2.40 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 194.2, 177.9, 145.9, 144.4, 141.6, 140.9, 136.7, 135.1, 133.0, 131.9, 130.3, 130.2, 129.4, 128.7, 128.6, 128.5, 128.3, 128.1, 127.8, 127.2, 126.6, 125.5, 109.4, 79.1, 70.8, 43.8, 21.3; HRMS (ESI) for $C_{38}H_{31}N_2O_2$ $[M+H]^+$ calcd 547.2380, found 547.2377. Enantiomeric excess was determined by HPLC with a Chiralpak AD-H column. (n-hexane: i-propanol = 70 : 30, 0.8 mL/min, λ = 254 nm) tR (major) = 26.0min, tR (minor) = 18.7 min.



5m

(2R,5R)-4-Benzoyl-1'-benzyl-5'-fluoro-3,5-diphenyl-1,5-dihydrospiro[pyrrol-2,3'-oxindole]

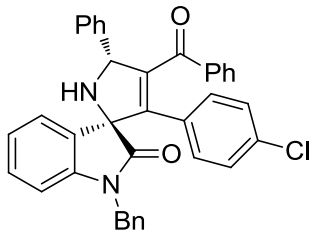
White solid, mp: 74-76 °C, 98% *ee*. $[\alpha]_D^{22}$ = 168.1 (*c* 0.21, CH_2Cl_2); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.77 (d, *J* = 7.8 Hz, 2H), 7.56 (d, *J* = 7.6 Hz, 2H), 7.45 (d, *J* = 5.5 Hz, 1H), 7.34 (t, *J* = 7.4 Hz, 3H), 7.26 – 7.21 (m, 3H), 7.14–7.05 (m, 4H), 6.96 – 6.88 (m, 3H), 6.79 (d, *J* = 7.7 Hz, 2H), 6.63 (d, *J* = 7.6 Hz, 2H), 6.44 (dd, *J* = 8.5, 3.9 Hz, 1H), 6.22 (s, 1H), 5.13 (d, *J* = 16.0 Hz, 1H), 4.40 (d, *J* = 16.0 Hz, 1H), 2.90 (s, 1H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 193.9, 177.8, 159.7 (*J* = 243.4 Hz), 144.8, 144.7, 141.4, 139.1 (*J* = 2.0 Hz), 136.6, 134.7, 133.0, 132.1 (*J* = 7.3 Hz), 131.6, 129.3, 128.8, 128.7, 128.6, 128.3, 128.2, 127.7, 127.4, 126.6, 116.3 (*J* = 23.2 Hz), 112.9 (*J* = 25.3 Hz), 110.4 (d, *J* = 7.8 Hz), 79.1, 70.5, 44.0; ^{19}F NMR (470 MHz, $CDCl_3$) δ -119.07; HRMS (ESI) for $C_{37}H_{28}FN_2O_2$ $[M+H]^+$ calcd 551.2129, found 551.2120. Enantiomeric excess was determined by HPLC with a Chiralpak AD-H column. (n-hexane: i-propanol = 70 : 30, 0.8 mL/min, λ = 254 nm) tR (major) = 26.0min, tR (minor) = 22.0 min.



5n

(2R,5R)-4-Benzoyl-1'-benzyl-3-(4-fluorophenyl)-5-phenyl-1,5-dihyd rospiro[pyrrol-2,3'-oxindole]

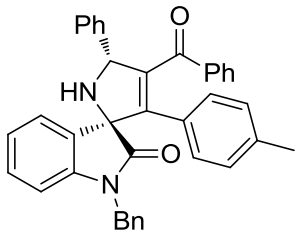
White solid, mp: 81-83 °C, > 99% *ee*. $[\alpha]_D^{22}$ = 197.2 (*c* 0.55, CH_2Cl_2); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.78 (d, *J* = 7.8 Hz, 2H), 7.69 (d, *J* = 6.8 Hz, 1H), 7.57 (d, *J* = 7.7 Hz, 2H), 7.33 (q, *J* = 7.7 Hz, 3H), 7.26 – 7.17 (m, 5H), 7.16 – 7.11 (m, 1H), 7.08 (t, *J* = 7.4 Hz, 2H), 6.73 (dd, *J* = 7.9, 5.7 Hz, 2H), 6.68 (d, *J* = 7.5 Hz, 2H), 6.58 (dd, *J* = 10.7, 7.0 Hz, 3H), 6.20 (s, 1H), 5.11 (d, *J* = 16.0 Hz, 1H), 4.39 (d, *J* = 16.0 Hz, 1H), 2.82 (s, 1H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 194.0, 177.8, 162.8 (*J* = 249.5 Hz), 144.7 (*J* = 14.2 Hz), 143.3, 141.4, 136.6, 135.0, 133.2, 130.6 (*J* = 8.3 Hz), 130.2, 130.1, 129.3, 128.8, 128.6, 128.4, 128.2, 127.9 (*J* = 4.0 Hz), 127.8, 127.5, 126.7, 124.9, 123.5, 115.2 (*J* = 21.2 Hz), 109.8, 79.0, 70.7, 43.8; ^{19}F NMR (470 MHz, $CDCl_3$) δ -112.36; HRMS (ESI) for $C_{37}H_{27}FN_2NaO_2$ $[M+Na]^+$ calcd 573.1949, found 573.1930. Enantiomeric excess was determined by HPLC with a Chiralpak AD-H column. (n-hexane: i-propanol = 70 : 30, 0.8 mL/min, λ = 254 nm) tR (major) = 28.2 min, tR (minor) = 18.9 min.



5o

(2R,5R)-4-Benzoyl-1'-benzyl-3-(4-chlorophenyl)-5-phenyl-1,5-dih ydrospiro[pyrrol-2,3'-oxindole]

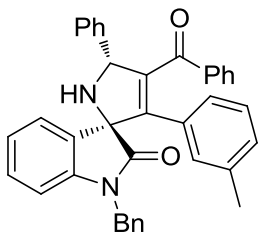
White solid, mp: 85-87 °C, > 99% *ee*. $[\alpha]_D^{22}$ = 195.6 (*c* 0.61, CH_2Cl_2); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.79 (d, *J* = 7.8 Hz, 2H), 7.68 (d, *J* = 6.9 Hz, 1H), 7.55 (d, *J* = 7.7 Hz, 2H), 7.39 – 7.29 (m, 3H), 7.24 (dd, *J* = 16.1, 8.0 Hz, 4H), 7.18 – 7.08 (m, 4H), 6.87 (d, *J* = 8.3 Hz, 2H), 6.68 (t, *J* = 7.0 Hz, 4H), 6.57 (d, *J* = 7.3 Hz, 1H), 6.19 (s, 1H), 5.13 (d, *J* = 16.0 Hz, 1H), 4.39 (d, *J* = 16.0 Hz, 1H), 2.82 (s, 1H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 193.9, 177.7, 145.1, 144.3, 143.2, 141.3, 136.6, 135.0, 134.7, 130.3, 130.0, 129.3, 128.8, 128.7, 128.5, 128.4, 128.2, 127.7, 127.6, 126.7, 124.9, 123.6, 109.8, 78.9, 70.8, 43.9; HRMS (ESI) for $C_{37}H_{28}ClN_2O_2$ $[M+H]^+$ calcd 567.1834, found 567.1827. Enantiomeric excess was determined by HPLC with a Chiralpak AD-H column. (n-hexane: i-propanol = 70 : 30, 0.8 mL/min, λ = 254 nm) tR (major) = 31.0 min, tR (minor) = 17.9 min.



5p

(2R,5R)-4-Benzoyl-1'-benzyl-5-phenyl-3-(p-tolyl)-1,5-dihydrospiro[pyrrol-2,3'-oxindole]

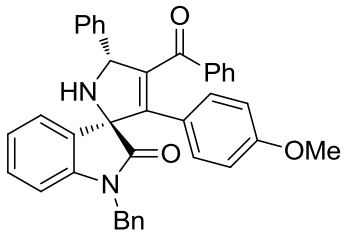
White solid, mp: 86-88 °C, 98 % *ee.* $[\alpha]_D^{22}$ = 168.5 (*c* 0.54, CH_2Cl_2); ^1H NMR (400 MHz, $CDCl_3$) δ 7.82 (d, *J* = 7.8 Hz, 2H), 7.68 (d, *J* = 6.8 Hz, 1H), 7.56 (d, *J* = 7.7 Hz, 2H), 7.34 – 7.29 (m, 3H), 7.22 (t, *J* = 7.6 Hz, 3H), 7.19 – 7.11 (m, 3H), 7.04 (t, *J* = 7.5 Hz, 2H), 6.72 – 6.65 (m, 6H), 6.53 (d, *J* = 7.1 Hz, 1H), 6.18 (s, 1H), 5.13 (d, *J* = 16.0 Hz, 1H), 4.40 (d, *J* = 16.0 Hz, 1H), 2.80 (s, 1H), 2.12 (s, 3H) ^{13}C NMR (101 MHz, $CDCl_3$) δ 194.3, 178.0, 145.8, 144.0, 143.3, 141.7, 138.3, 136.7, 135.1, 133.3, 130.4, 130.0, 129.4, 128.9, 128.8, 128.7, 128.5, 128.3, 128.1, 127.8, 127.3, 126.7, 124.9, 123.4, 109.7, 79.0, 70.8, 43.8, 21.2. HRMS (ESI) for $C_{38}H_{31}N_2O_2$ $[M+H]^+$ calcd 547.2380, found 547.2366. Enantiomeric excess was determined by HPLC with a Chiralpak AD-H column. (n-hexane: i-propanol = 70 : 30, 0.8 mL/min, λ = 254 nm) tR (major) = 25.8 min, tR (minor) = 17.0 min.



5q

(2R,5R)-4-Benzoyl-1'-benzyl-5-phenyl-3-(m-tolyl)-1,5-dihydrospiro[pyrrol-2,3'-oxindole]

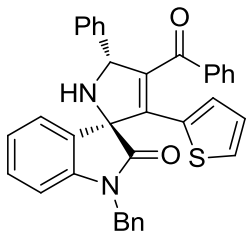
White solid, mp: 68-70 °C, 97 % *ee.* $[\alpha]_D^{22}$ = 166.7 (*c* 0.49, CH_2Cl_2); ^1H NMR (400 MHz, $CDCl_3$) δ 7.78 (d, *J* = 7.5 Hz, 2H), 7.69 (d, *J* = 6.1 Hz, 1H), 7.58 (d, *J* = 7.5 Hz, 2H), 7.33 (t, *J* = 7.4 Hz, 3H), 7.25 – 7.17 (m, 5H), 7.12 (d, *J* = 7.0 Hz, 1H), 7.05 (t, *J* = 7.3 Hz, 2H), 6.86 (d, *J* = 7.6 Hz, 1H), 6.78 (t, *J* = 7.5 Hz, 1H), 6.64 (d, *J* = 7.4 Hz, 2H), 6.57 – 6.52 (m, 3H), 6.19 (s, 1H), 5.15 (d, *J* = 16.0 Hz, 1H), 4.40 (d, *J* = 16.0 Hz, 1H), 2.84 (s, 1H), 1.94 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 194.2, 178.0, 146.1, 144.0, 143.3, 141.7, 137.6, 136.9, 135.1, 132.9, 131.7, 130.5, 129.9, 129.4, 129.3, 128.8, 128.6, 128.2, 128.1, 128.0, 127.8, 127.3, 126.5, 125.6, 124.9, 123.4, 109.6, 79.1, 70.7, 43.8, 21.1; HRMS (ESI) for $C_{38}H_{31}N_2O_2$ $[M+H]^+$ calcd 547.2380, found 547.2366. Enantiomeric excess was determined by HPLC with a Chiralpak AD-H column. (n-hexane: i-propanol = 70 : 30, 0.8 mL/min, λ = 254 nm) tR (major) = 21.3 min, tR (minor) = 18.2 min.



5r

(2R,5R)-4-Benzoyl-1'-benzyl-3-(4-methoxyphenyl)-5-phenyl-1,5-dihydrospiro[pyrrol-2,3'-oxindole]

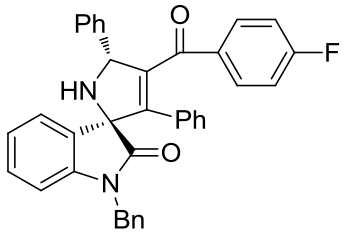
White solid, mp: 77-79 °C, 99 % *ee.* $[\alpha]_D^{22}$ = 203.3 (*c* 0.54, CH_2Cl_2); ^1H NMR (400 MHz, $CDCl_3$) δ 7.79 (d, *J* = 7.9 Hz, 2H), 7.70 (d, *J* = 6.8 Hz, 1H), 7.57 (d, *J* = 7.7 Hz, 2H), 7.31 (t, *J* = 7.3 Hz, 3H), 7.24 – 7.15 (m, 5H), 7.11 (d, *J* = 7.0 Hz, 1H), 7.04 (t, *J* = 7.5 Hz, 2H), 6.67 – 6.64 (m, 4H), 6.54 (d, *J* = 7.2 Hz, 1H), 6.41 (d, *J* = 8.1 Hz, 2H), 6.18 (s, 1H), 5.13 (d, *J* = 16.0 Hz, 1H), 4.37 (d, *J* = 16.0 Hz, 1H), 3.56 (s, 3H), 2.80 (s, 1H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 194.4, 178.0, 159.8, 145.7, 143.6, 143.3, 141.8, 136.8, 135.1, 133.0, 130.5, 130.0, 129.4, 128.7, 128.5, 128.3, 128.1, 127.8, 127.3, 126.7, 124.9, 124.2, 123.4, 113.6, 109.7, 79.0, 70.6, 55.0, 43.8; HRMS (ESI) for $C_{38}H_{31}N_2O_3$ $[M+H]^+$ calcd 563.2329, found 563.2316. Enantiomeric excess was determined by HPLC with a Chiralpak AD-H column. (n-hexane: i-propanol = 70 : 30, 0.8 mL/min, λ = 254 nm) tR (major) = 37.6 min, tR (minor) = 24.8 min.



5s

(2S,5R)-4-Benzoyl-1'-benzyl-5-phenyl-3-(thiophen-2-yl)-1,5-dihydrospiro [pyrrol-2,3'-oxindole]

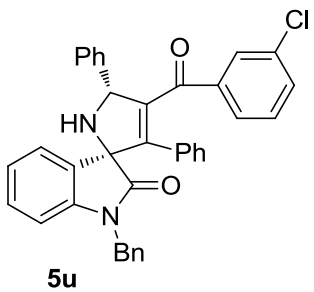
White solid, mp: 92-94 °C, 97 % *ee*. $[\alpha]_D^{22}$ = 199.1 (*c* 0.22, CH_2Cl_2); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.90 (d, *J* = 7.6 Hz, 2H), 7.68 (d, *J* = 7.2 Hz, 1H), 7.52 (d, *J* = 7.4 Hz, 2H), 7.42 (d, *J* = 7.2 Hz, 1H), 7.34 – 7.28 (m, 5H), 7.24 – 7.12 (m, 5H), 6.97 (d, *J* = 4.9 Hz, 1H), 6.91 (d, *J* = 6.4 Hz, 2H), 6.69 (d, *J* = 7.8 Hz, 1H), 6.61 (t, *J* = 4.2 Hz, 1H), 6.53 (d, *J* = 3.1 Hz, 1H), 6.14 (s, 1H), 5.12 (d, *J* = 16.0 Hz, 1H), 4.59 (d, *J* = 16.0 Hz, 1H), 2.77 (s, 1H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 194.4, 177.7, 144.1, 144.0, 140.9, 137.6, 136.4, 135.2, 133.3, 132.2, 130.5, 129.9, 129.3, 129.0, 128.7, 128.5, 128.2, 127.9, 127.5, 127.0, 126.9, 125.2, 123.6, 109.8, 77.9, 71.0, 44.0; HRMS (ESI) for $C_{35}H_{27}N_2O_2S$ $[M+H]^+$ calcd 539.1788, found 539.1784. Enantiomeric excess was determined by HPLC with a Chiralpak AD-H column. (n-hexane: i-propanol = 70 : 30, 0.8 mL/min, λ = 254 nm) tR (major) = 44.1 min, tR (minor) = 37.0 min.



5t

(2R,5R)-1'-Benzyl-4-(4-fluorobenzoyl)-3,5-diphenyl-1,5-dihydros piro[pyrrol-2,3'-oxindole]

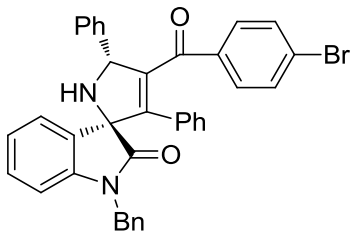
White solid, mp: 85-87 °C, 99 % *ee*. $[\alpha]_D^{22}$ = 172.0 (*c* 1.03, CH_2Cl_2); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.84 – 7.78 (m, 2H), 7.69 (d, *J* = 6.5 Hz, 1H), 7.58 (d, *J* = 7.5 Hz, 2H), 7.33 (t, *J* = 7.4 Hz, 2H), 7.20 – 7.02 (m, 7H), 6.95 – 6.84 (m, 4H), 6.77 (d, *J* = 7.6 Hz, 2H), 6.66 (d, *J* = 7.4 Hz, 2H), 6.54 (d, *J* = 7.2 Hz, 1H), 6.18 (s, 1H), 5.11 (d, *J* = 16.0 Hz, 1H), 4.41 (d, *J* = 16.0 Hz, 1H), 2.83 (s, 1H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 192.6, 177.9 (s), 165.5 (*J* = 255.5 Hz), 145.7, 144.2, 143.3, 141.5, 135.0, 133.1 (*J* = 3.0 Hz), 132.0 (*J* = 10.1 Hz), 131.8, 130.2, 130.1, 128.8, 128.7, 128.6, 128.2, 127.7, 127.3, 126.6, 124.9, 123.5, 115.5 (*J* = 20.2 Hz), 109.7, 79.0, 70.7, 43.9; ^{19}F NMR (470 MHz, $CDCl_3$) δ -104.78; HRMS (ESI) for $C_{37}H_{28}FN_2O_2$ $[M+H]^+$ calcd 551.2129, found 551.2124. Enantiomeric excess was determined by HPLC with a Chiralpak AS-H column. (n-hexane: i-propanol = 90 : 10, 0.8 mL/min, λ = 254 nm) tR (major) = 58.8 min, tR (minor) = 47.1 min.



5u

(2R,5R)-1'-Benzyl-4-(3-chlorobenzoyl)-3,5-diphenyl-1,5-dihydrospi ro[pyrrol-2,3'-oxindole]

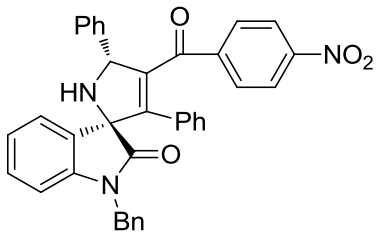
White solid, mp: 78-80 °C, 98 % *ee*. $[\alpha]_D^{22}$ = 171.8 (*c* 1.22, CH_2Cl_2); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.75 7.69 (m, 1H), 7.64 (s, 2H), 7.59 (d, *J* = 7.4 Hz, 2H), 7.33 (t, *J* = 7.3 Hz, 2H), 7.25 – 7.17 (m, 4H), 7.12–7.01 (m, 5H), 6.91 (t, *J* = 7.5 Hz, 2H), 6.74 (d, *J* = 7.6 Hz, 2H), 6.61 (d, *J* = 7.4 Hz, 2H), 6.52 (d, *J* = 5.9 Hz, 1H), 6.21 (s, 1H), 5.10 (d, *J* = 16.0 Hz, 1H), 4.37 (d, *J* = 16.0 Hz, 1H), 2.84 (s, 1H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 192.6, 177.7, 147.1, 143.8, 143.3, 141.6, 138.3, 135.0, 134.4, 132.7, 131.7, 130.1, 129.6, 129.1, 128.8, 128.7, 128.2, 127.7, 127.6, 127.3, 126.6, 124.9, 123.5, 109.8, 79.2, 70.4, 43.8; HRMS (ESI) for $C_{37}H_{28}ClN_2O_2$ $[M+H]^+$ calcd 567.1834, found 567.1825. Enantiomeric excess was determined by HPLC with a Chiralpak AD-H column. (n-hexane: i-propanol = 70 : 30, 0.8 mL/min, λ = 254 nm) tR (major) = 26.1 min, tR (minor) = 20.0 min.



5v

(2R,5R)-1'-Benzyl-4-(4-bromobenzoyl)-3,5-diphenyl-1,5-dihydrospiro[pyrrol-2,3'-oxindole]

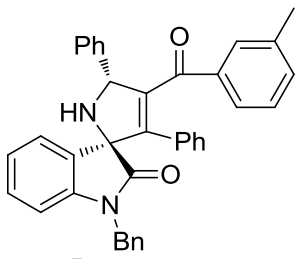
White solid, mp: 90-82 °C, 99 % *ee*. $[\alpha]_D^{22}$ = 150.0 (*c* 1.20, CH_2Cl_2); ^1H NMR (400 MHz, $CDCl_3$) δ 7.69 (d, *J* = 6.6 Hz, 1H), 7.63 (d, *J* = 7.8 Hz, 2H), 7.57 (d, *J* = 7.5 Hz, 2H), 7.33 (t, *J* = 8.4 Hz, 4H), 7.22 – 7.02 (m, 7H), 6.92 (t, *J* = 7.5 Hz, 2H), 6.75 (d, *J* = 7.6 Hz, 2H), 6.66 (d, *J* = 7.4 Hz, 2H), 6.53 (d, *J* = 6.9 Hz, 1H), 6.18 (s, 1H), 5.11 (d, *J* = 16.0 Hz, 1H), 4.40 (d, *J* = 16.0 Hz, 1H), 2.82 (s, 1H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 193.1, 177.8, 146.1, 144.0, 143.3, 141.4, 135.5, 135.0, 131.7, 131.6, 130.8, 130.2, 130.1, 128.8, 128.7, 128.6, 128.2, 127.7, 127.3, 126.6, 124.9, 123.5, 109.8, 79.0, 70.6, 43.9; HRMS (ESI) for $C_{37}H_{28}BrN_2O_2$ $[M+H]^+$ calcd 613.1314, found 613.1323. Enantiomeric excess was determined by HPLC with a Chiralpak AD-H column. (n-hexane: i-propanol = 70 : 30, 0.8 mL/min, λ = 254 nm) tR (major) = 46.1 min, tR (minor) = 44.7 min.



5w

(2R,5R)-1'-Benzyl-4-(4-nitrobenzoyl)-3,5-diphenyl-1,5-dihydrospiro[pyrrol-2,3'-oxindole]

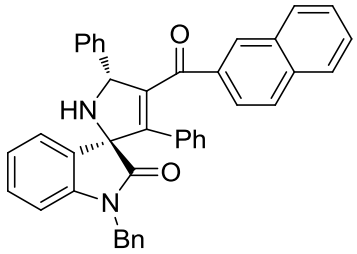
Pale yellow solid, mp: 99-101 °C, 92 % *ee*. $[\alpha]_D^{22}$ = 171.8 (*c* 1.22, CH_2Cl_2); ^1H NMR (400 MHz, $CDCl_3$) δ 7.97 (d, *J* = 8.2 Hz, 2H), 7.80–7.74 (m, 3H), 7.61 (d, *J* = 7.6 Hz, 2H), 7.35 (t, *J* = 7.4 Hz, 2H), 7.24–7.20 (m, 3H), 7.14 – 7.01 (m, 4H), 6.89 (t, *J* = 7.5 Hz, 2H), 6.70 (d, *J* = 7.7 Hz, 2H), 6.61 (d, *J* = 7.5 Hz, 2H), 6.54 (d, *J* = 7.2 Hz, 1H), 6.23 (s, 1H), 5.10 (d, *J* = 16.0 Hz, 1H), 4.38 (d, *J* = 16.0 Hz, 1H), 2.91 (s, 1H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 192.4, 177.6, 149.8, 148.4, 143.6, 143.3, 141.6, 141.5, 134.9, 131.4, 130.3, 130.0, 129.1, 128.8, 128.7, 128.3, 127.7, 127.3, 126.5, 124.9, 123.5, 123.3, 109.9, 79.1, 70.1, 43.8; HRMS (ESI) for $C_{37}H_{28}N_3O_4$ $[M+H]^+$ calcd 578.2074, found 578.2054. Enantiomeric excess was determined by HPLC with a Chiralpak AD-H column. (n-hexane: i-propanol = 70 : 30, 0.8 mL/min, λ = 254 nm) tR (major) = 44.5 min, tR (minor) = 35.6 min.



5x

(2R,5R)-1'-Benzyl-4-(3-methylbenzoyl)-3,5-diphenyl-1,5-dihydrospiro[pyrrol-2,3'-oxindole]

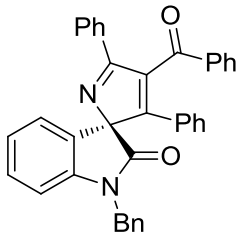
White solid, mp: 79-81 °C, 97 % *ee*. $[\alpha]_D^{22}$ = 166.1 (*c* 1.03, CH_2Cl_2); ^1H NMR (400 MHz, $CDCl_3$) δ 7.71 – 7.63 (m, 2H), 7.57 (d, *J* = 6.5 Hz, 3H), 7.32 (t, *J* = 7.2 Hz, 2H), 7.21–7.10 (m, 6H), 7.05 (t, *J* = 7.5 Hz, 3H), 6.91 (t, *J* = 7.4 Hz, 2H), 6.78 (d, *J* = 7.7 Hz, 2H), 6.65 (d, *J* = 7.4 Hz, 2H), 6.52 (d, *J* = 6.6 Hz, 1H), 6.20 (s, 1H), 5.12 (d, *J* = 16.0 Hz, 1H), 4.40 (d, *J* = 16.0 Hz, 1H), 2.80 (s, 1H), 2.22 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 194.2, 177.9, 145.6, 144.5, 143.3, 141.7, 138.0, 136.6, 135.1, 133.8, 132.0, 130.4 130.0, 128.7, 128.6, 128.0, 128.2, 128.1, 128.0, 127.8, 127.3, 127.0, 126.6, 124.9, 123.4, 109.7, 79.1, 70.9, 43.8, 21.2; HRMS (ESI) for $C_{38}H_{31}N_2O_2$ $[M+H]^+$ calcd 547.2380, found 547.2373. Enantiomeric excess was determined by HPLC with a Chiralpak AD-H column. (n-hexane: i-propanol = 90 : 10, 0.8 mL/min, λ = 254 nm) tR (major) = 75.8 min, tR (minor) = 55.9 min.



5y

(2R,5R)-4-(2-Naphthoyl)-1'-benzyl-3,5-diphenyl-1,5-dihydrospiro[pyrrol-2,3'-oxindole]

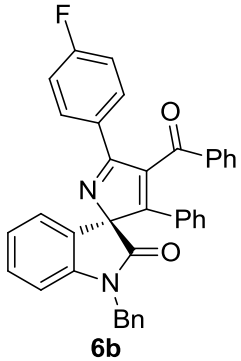
White solid, mp: 95-97 °C, 99 % *ee*. $[\alpha]_D^{22}$ = 173.5 (*c* 1.06, CH_2Cl_2); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.49 (s, 1H), 7.90–7.84 (m, 2H), 7.72–7.66 (m, 3H), 7.59 (d, *J* = 7.5 Hz, 2H), 7.51 – 7.42 (m, 2H), 7.31 (t, *J* = 7.3 Hz, 2H), 7.21 – 7.03 (m, 6H), 6.98 – 6.93 (m, 1H), 6.88–6.85 (m, 4H), 6.71 (d, *J* = 7.4 Hz, 2H), 6.55 (d, *J* = 6.5 Hz, 1H), 6.27 (s, 1H), 5.15 (d, *J* = 16.0 Hz, 1H), 4.46 (d, *J* = 16.0 Hz, 1H), 2.85 (s, 1H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 194.1, 178.0, 145.3, 144.7, 143.4, 141.5, 135.6, 135.1, 133.9, 132.4, 132.2, 132.0, 130.3, 123.0, 128.7, 128.7, 128.5, 128.3, 128.1, 127.8, 127.7, 127.3, 126.7, 126.6, 124.9 124.5, 123.5, 109.7, 79.0, 71.1, 43.9; HRMS (ESI) for $C_{38}H_{31}N_2O_2$ $[M+H]^+$ calcd 547.2380, found 547.2373. Enantiomeric excess was determined by HPLC with a Chiralpak AD-H column. (n-hexane: i-propanol = 70 : 30, 0.8 mL/min, λ = 254 nm) tR (major) = 53.8 min, tR (minor) = 31.1 min.



6a

(R)-4-Benzoyl-1'-benzyl-3,5-diphenylspiro[pyrrol-2,3'-oxindole]

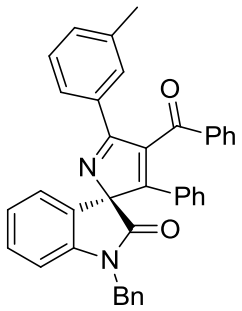
White solid, mp: 113-135 °C, 97 % *ee*. $[\alpha]_D^{22}$ = 115.9 (*c* 0.49, CH_2Cl_2); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.07 (d, *J* = 7.7 Hz, 2H), 7.74 (d, *J* = 7.5 Hz, 2H), 7.46 (t, *J* = 7.3 Hz, 1H), 7.38–7.34 (m, 3H), 7.31–7.26 (m, 3H), 7.25–7.22 (m, 3H), 7.15–7.12 (m, 4H), 7.04–6.97 (m, 5H), 6.81 (d, *J* = 7.9 Hz, 1H), 5.27 (d, *J* = 16.0 Hz, 1H), 4.75 (d, *J* = 16.0 Hz, 1H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 194.6, 175.6, 170.6, 162.7, 144.0, 140.6, 136.3, 135.1, 134.1, 133.1, 131.1, 130.8, 123.0, 129.9, 129.3, 128.9, 128.8, 128.6, 128.5, 128.4, 127.7, 127.3, 124.8, 124.4, 123.6, 110.1, 89.4, 44.8; HRMS (ESI) for $C_{37}H_{27}N_2O2$ $[M+H]^+$ calcd 531.2067, found 531.2063. Enantiomeric excess was determined by HPLC with a Chiralpak AD-H column. (n-hexane: i-propanol = 70 : 30, 0.8 mL/min, λ = 254 nm) tR (major) = 28.1 min, tR (minor) = 26.2 min.



6b

(R)-4'-Benzoyl-1-benzyl-5'-(4-fluorophenyl)-3'-phenylspiro[pyrrol-2,3'-oxindole]

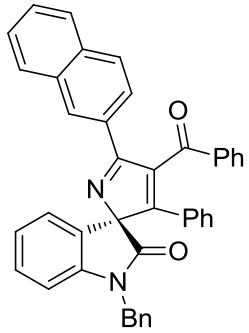
White solid, mp: 129-131 °C, 96 % *ee*. $[\alpha]_D^{22}$ = 103.0 (*c* 0.24, CH_2Cl_2); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.06 (d, *J* = 8.0 Hz, 2H), 7.75 (dd, *J* = 8.4, 5.5 Hz, 2H), 7.48 (t, *J* = 7.4 Hz, 1H), 7.37 (t, *J* = 7.7 Hz, 2H), 7.26 (s, 1H), 7.25–7.22 (m, 3H), 7.15 – 7.11 (m, 4H), 7.05 – 6.94 (m, 7H), 6.82 (d, *J* = 7.9 Hz, 1H), 5.26 (d, *J* = 16.0 Hz, 1H), 4.77 (d, *J* = 15.7 Hz, 1H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 194.6, 174.4, 170.5, 164.3 (*J* = 252.5 Hz), 162.9, 144.0, 140.3, 136.2, 135.0, 134.3, 131.1, 130.7 (*J* = 8.8 Hz), 130.1, 129.9, 129.4, 129.3 (*J* = 3.3 Hz) 129.0, 128.8, 128.6, 127.8, 127.7, 127.3, 124.8, 124.3, 123.7, 115.6 (*J* = 21.2 Hz), 110.2, 89.4, 44.8; ^{19}F NMR (470 MHz, $CDCl_3$) δ -108.91; HRMS (ESI) for $C_{37}H_{26}FN_2O_2$ $[M+H]^+$ calcd 549.1973, found 549.1968. Enantiomeric excess was determined by HPLC with a Chiralpak AD-H column. (n-hexane: i-propanol = 70 : 30, 0.8 mL/min, λ = 254 nm) tR (major) = 26.1 min, tR (minor) = 32.8 min.



6c

(R)-4-Benzoyl-1'-benzyl-3-phenyl-5-(m-tolyl)spiro[pyrrol-2,3'-oxindole]

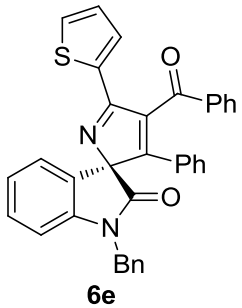
White solid, mp: 78-80 °C, 95 % *ee*. $[\alpha]_D^{22}$ = 92.8 (*c* 0.65, CH_2Cl_2); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.07 (d, *J* = 7.7 Hz, 2H), 7.66 (s, 1H), 7.45 (t, *J* = 7.1 Hz, 2H), 7.35 (t, *J* = 7.6 Hz, 2H), 7.24– 7.20 (m, 4H), 7.15 – 7.11 (m, 6H), 7.03 – 7.97 (m, 5H), 6.80 (d, *J* = 7.9 Hz, 1H), 5.27 (d, *J* = 16.0 Hz, 1H), 4.73 (d, *J* = 15.7 Hz, 1H), 2.26 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 194.7, 175.8, 170.6, 162.6, 144.0, 140.8, 138.3, 136.4, 135.1, 134.1, 132.9, 131.7, 131.1, 130.0, 129.8, 129.3, 129.2, 128.9, 128.8, 128.6, 128.2, 127.7, 127.3, 125.6, 124.8, 124.4, 123.6, 110.1, 89.4, 44.8, 21.3; HRMS (ESI) for $C_{38}H_{29}N_2O_2$ $[M+H]^+$ calcd 545.2224, found 545.2215. Enantiomeric excess was determined by HPLC with a Chiralpak AD-H column. (n-hexane: i-propanol = 70 : 30, 0.8 mL/min, λ = 254 nm) tR (major) = 15.4 min, tR (minor) = 13.5 min.



6d

(R)-4-Benzoyl-1'-benzyl-5-(naphthalen-2-yl)-3-phenylspiro[pyrrol-2,3'-oxindole]

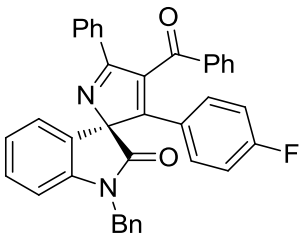
White solid, mp: 92-94 °C, 98 % *ee*. $[\alpha]_D^{22}$ = 92.8 (*c* 0.65, CH_2Cl_2); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.24 (s, 1H), 8.13 (d, *J* = 7.5 Hz, 2H), 7.89 (d, *J* = 8.5 Hz, 1H), 7.75 (d, *J* = 8.7 Hz, 3H), 7.49 – 7.38 (m, 3H), 7.34 (t, *J* = 7.5 Hz, 2H), 7.24–7.21(m, 4H), 7.17 – 7.14 (m, 4H), 7.06 – 6.99 (m, 5H), 6.81 (d, *J* = 7.9 Hz, 1H), 5.29 (d, *J* = 16.0 Hz, 1H), 4.76 (d, *J* = 15.7 Hz, 1H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 194.9, 175.5, 170.6, 162.7, 144.0, 140.8, 136.4, 135.1, 134.4, 134.2, 132.8, 131.1, 130.5, 130.1, 129.9, 129.4, 129.1, 129.0, 128.9, 128.6, 128.3, 127.7, 127.4, 127.3, 126.5, 125.3, 124.9, 124.4, 123.7, 110.2, 89.6, 44.8; HRMS (ESI) for $C_{41}H_{29}N_2O_2$ $[M+H]^+$ calcd 581.2224, found 581.2219. Enantiomeric excess was determined by HPLC with a Chiralpak AD-H column. (n-hexane: i-propanol = 70 : 30, 0.8 mL/min, λ = 254 nm) tR (major) = 43.8 min, tR (minor) = 32.4 min.



6e

(R)-4-Benzoyl-1'-benzyl-3-phenyl-5-(thiophen-2-yl)spiro[pyrrol-2,3'-oxindole]

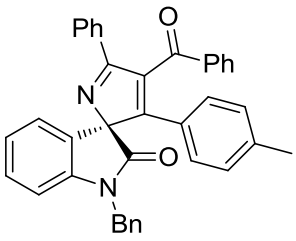
White solid, mp: 146-148 °C, 95 % *ee*. $[\alpha]_D^{22}$ = 113.9 (*c* 0.74, CH_2Cl_2); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.14 (d, *J* = 7.8 Hz, 2H), 7.50 (t, *J* = 7.3 Hz, 1H), 7.39 (dd, *J* = 15.2, 6.5 Hz, 3H), 7.30 (d, *J* = 3.7 Hz, 1H), 7.24 – 7.18 (m, 4H), 7.17 – 7.07 (m, 4H), 7.03 – 6.94 (m, 5H), 6.91 (t, *J* = 4.4 Hz, 1H), 6.79 (d, *J* = 7.9 Hz, 1H), 5.27 (d, *J* = 15.7 Hz, 1H), 4.71 (d, *J* = 15.7 Hz, 1H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 194.7, 170.6, 168.3, 162.1, 144.0, 139.4, 136.6, 136.3, 135.1, 134.5, 130.9, 130.5, 130.2, 130.1, 130.0, 129.4, 129.1, 128.8, 128.6, 127.8, 127.7, 127.4, 124.9, 124.5, 123.6, 110.1, 89.1, 44.8; HRMS (ESI) for $C_{35}H_{25}N_2O_2S$ $[M+H]^+$ calcd 537.1631, found 537.1625. Enantiomeric excess was determined by HPLC with a Chiralpak AD-H column. (n-hexane: i-propanol = 70 : 30, 0.8 mL/min, λ = 254 nm) tR (major) = 41.3 min, tR (minor) = 44.8 min.



6f

(R)-4-Benzoyl-1'-benzyl-3-(4-fluorophenyl)-5-phenylspiro[pyrrol-2, 3'-oxindole]

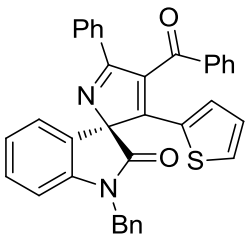
White solid, mp: 146-148 °C, 98 % *ee*. $[\alpha]_D^{22}$ = 113.9 (*c* 0.74, CH_2Cl_2); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.06 (d, *J* = 7.7 Hz, 2H), 7.74 (d, *J* = 7.5 Hz, 2H), 7.46 (t, *J* = 7.4 Hz, 1H), 7.35 (dd, *J* = 15.3, 7.5 Hz, 3H), 7.28–7.22 (m, 6H), 7.16 – 7.10 (m, 3H), 7.02 (t, *J* = 7.5 Hz, 1H), 6.95 (dd, *J* = 8.6, 5.4 Hz, 2H), 6.84 (d, *J* = 7.9 Hz, 1H), 6.68 (t, *J* = 8.6 Hz, 2H), 5.25 (d, *J* = 15.7 Hz, 1H), 4.73 (d, *J* = 15.7 Hz, 1H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 194.5, 175.6, 170.4, 164.3, 161.1 (*J* = 251.6 Hz), 161.6, 144.0, 140.7, 136.2, 135.0, 134.3, 133.0, 130.9, 130.2, 129.8, 129.7, 129.0, 128.8, 128.5, 127.9, 127.4, 127.3 (*J* = 34.3 Hz), 124.8, 124.1, 123.7, 115.8 (*J* = 22.2 Hz), 115.7, 110.2, 89.5, 44.8; HRMS (ESI) for $C_{37}H_{26}FN_2O_2$ $[M+H]^+$ calcd 549.1973, found 549.1972. Enantiomeric excess was determined by HPLC with a Chiralpak AD-H column. (n-hexane: i-propanol = 70 : 30, 0.8 mL/min, λ = 254 nm) tR (major) = 35.5 min, tR (minor) = 22.3 min



6g

(R)-4-Benzoyl-1'-benzyl-5-phenyl-3-(p-tolyl)spiro[pyrrol-2,3'-oxindole]

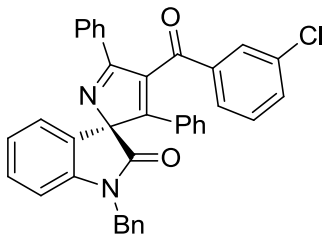
White solid, mp: 141-143 °C, 97 % *ee*. $[\alpha]_D^{22}$ = 114.4 (*c* 0.32, CH_2Cl_2); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.09 (d, *J* = 7.8 Hz, 2H), 7.73 (d, *J* = 7.7 Hz, 2H), 7.46 (t, *J* = 7.3 Hz, 1H), 7.35 (dd, *J* = 15.9, 7.8 Hz, 3H), 7.31 – 7.25 (m, 4H), 7.25–7.21 (m, 2H), 7.19–7.17 (m, 2H), 7.11 (d, *J* = 7.4 Hz, 1H), 7.01 (t, *J* = 7.5 Hz, 1H), 6.87 (d, *J* = 7.8 Hz, 2H), 6.83–6.80 (m, 3H), 5.27 (d, *J* = 15.7 Hz, 1H), 4.76 (d, *J* = 15.7 Hz, 1H), 2.16 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 194.9, 175.7, 170.7, 162.7, 144.0, 140.0, 139.5, 136.4, 135.1, 134.1, 133.2, 130.7, 123.0, 129.9, 129.3, 128.9, 128.8, 128.5, 128.4, 128.2, 127.7, 127.6, 127.4, 124.8, 124.7, 123.6, 110.1, 89.3, 44.8, 21.2; HRMS (ESI) for $C_{38}H_{29}N_2O_2$ $[M+H]^+$ calcd 545.2224, found 545.2222. Enantiomeric excess was determined by HPLC with a Chiralpak AD-H column. (n-hexane: i-propanol = 70 : 30, 0.8 mL/min, λ = 254 nm) tR (major) = 24.0 min, tR (minor) = 18.8 min



6h

(S)-4-Benzoyl-1'-benzyl-5-phenyl-3-(thiophen-2-yl)spiro[pyrrol-2,3'-oxindole]

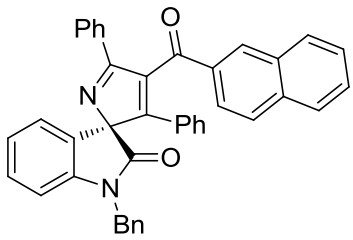
White solid, mp: 132-135 °C, 97 % *ee*. $[\alpha]_D^{22}$ = 84.7 (*c* 0.32, CH_2Cl_2); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.17 (d, *J* = 7.9 Hz, 2H), 7.74 (d, *J* = 7.9 Hz, 2H), 7.52 (t, *J* = 7.3 Hz, 1H), 7.42 (t, *J* = 7.6 Hz, 2H), 7.35–7.26 (m, 9H), 7.18 – 7.11 (m, 2H), 7.05 (t, *J* = 7.5 Hz, 1H), 6.93 (d, *J* = 7.9 Hz, 1H), 6.71 (t, *J* = 4.4 Hz, 1H), 6.67 (d, *J* = 3.7 Hz, 1H), 5.19 (d, *J* = 15.6 Hz, 1H), 4.89 (d, *J* = 15.6 Hz, 1H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 195.2, 175.2, 170.6, 154.4, 144.3, 138.1, 136.2, 135.2, 134.4, 133.1, 132.5, 130.8, 130.4, 129.9, 129.3, 129.1, 128.8, 128.5, 128.4, 127.9, 127.8, 125.5, 125.3, 123.8, 110.2, 88.6, 45.0; HRMS (ESI) for $C_{35}H_{25}N_2O_2S$ $[M+H]^+$ calcd 537.1631, found 537.1628. Enantiomeric excess was determined by HPLC with a Chiralpak AD-H column. (n-hexane: i-propanol = 70 : 30, 0.8 mL/min, λ = 254 nm) tR (major) = 56.7 min, tR (minor) = 53.8 min.



6i

(R)-1'-Benzyl-4-(3-chlorobenzoyl)-3,5-diphenylspiro[pyrrol-2,3'-oxindole]

White solid, mp: 89-91 °C, 97 % *ee*. $[\alpha]_D^{22}$ = 109.7 (*c* 0.74, CH_2Cl_2); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.06 (s, 1H), 7.93 (d, *J* = 7.7 Hz, 1H), 7.73 (d, *J* = 7.9 Hz, 2H), 7.41–7.28 (m, 4H), 7.26 – 7.20 (m, 5H), 7.16 – 7.10 (m, 4H), 7.06 – 6.98 (m, 3H), 6.96 (d, *J* = 8.0 Hz, 2H), 6.81 (d, *J* = 7.9 Hz, 1H), 5.26 (d, *J* = 15.6 Hz, 1H), 4.75 (d, *J* = 16.0 Hz, 1H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 193.2, 175.4, 170.4, 163.6, 144.0, 139.9, 137.8, 135.2, 135.0, 134.1, 132.9, 131.0, 130.3, 130.1, 129.5, 129.0, 128.9, 128.7, 128.6, 128.5, 127.8, 127.6, 127.3, 124.8, 124.2, 123.7, 110.2, 89.6, 44.8; HRMS (ESI) for $C_{37}H_{26}ClN_2O_2$ $[M+H]^+$ calcd 565.1677, found 565.1673. Enantiomeric excess was determined by HPLC with a Chiralpak AD-H column. (n-hexane: i-propanol = 70 : 30, 0.8 mL/min, λ = 254 nm) tR (major) = 20.8 min, tR (minor) = 30.5 min.

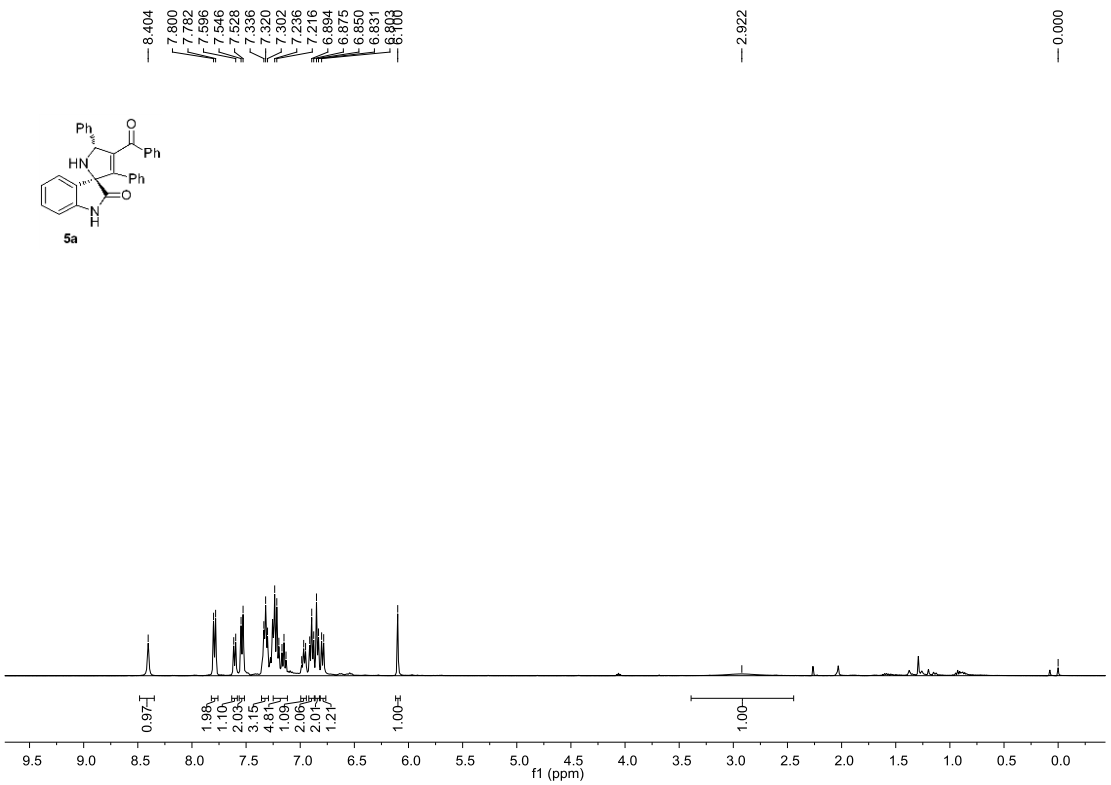


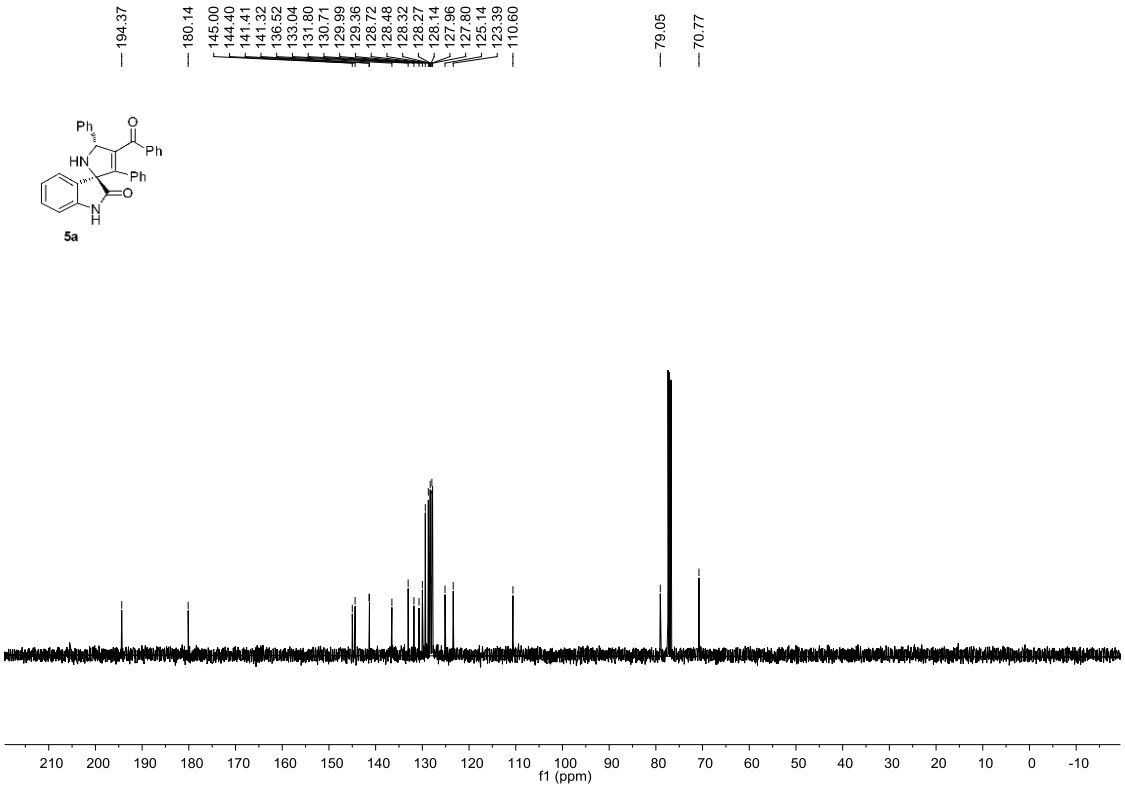
6j

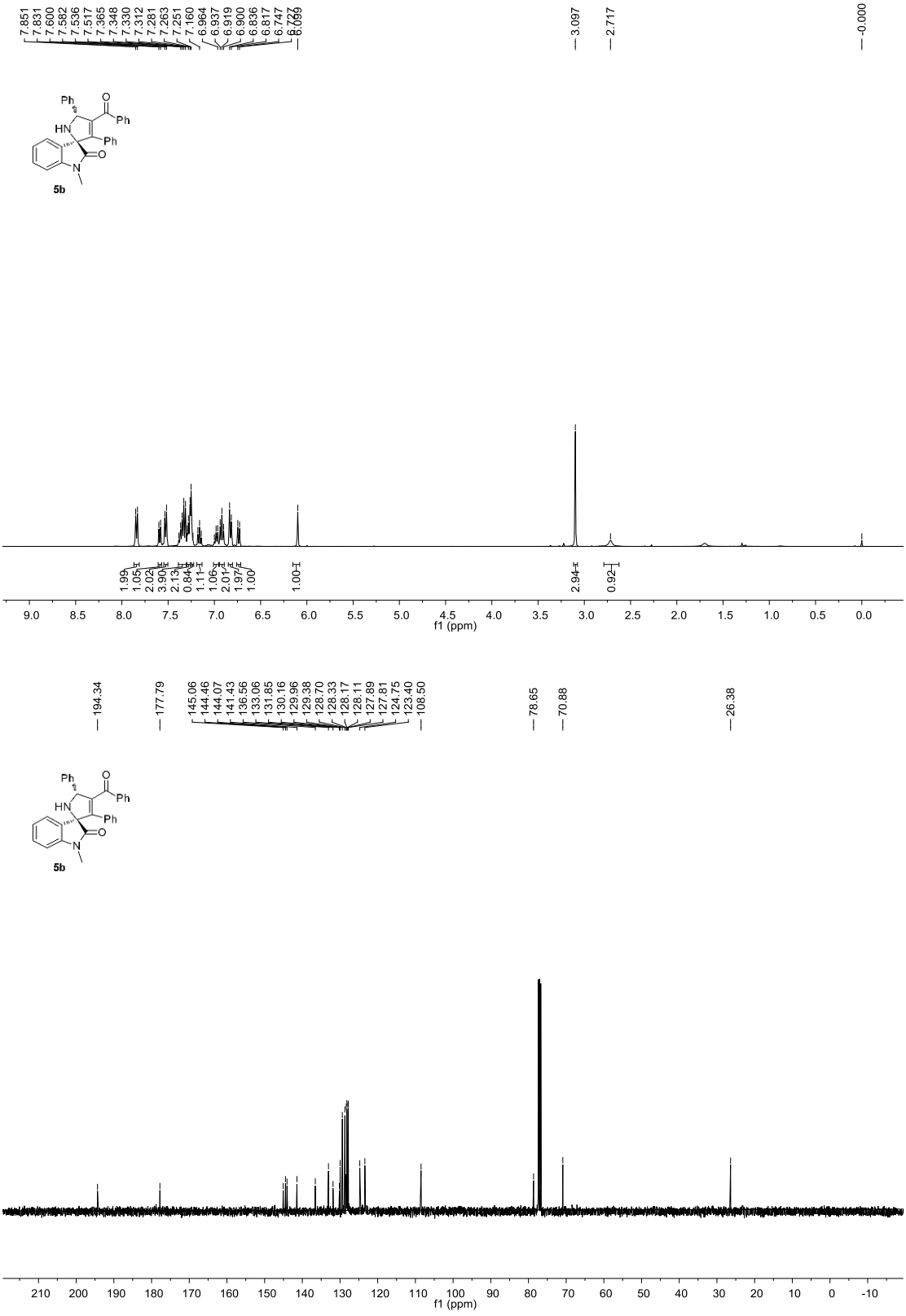
(R)-4-(2-naphthoyl)-1'-Benzyl-3,5-diphenylspiro[pyrrol-2,3'-oxindole]

White solid, mp: 106-108 °C, 96 % *ee*. $[\alpha]_D^{22}$ = 109.7 (*c* 0.74, CH_2Cl_2); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.71 (s, 1H), 8.14 (d, *J* = 8.6 Hz, 1H), 7.94 (d, *J* = 8.1 Hz, 1H), 7.86 – 7.73 (m, 4H), 7.53 (t, *J* = 7.5 Hz, 1H), 7.46 (t, *J* = 7.5 Hz, 1H), 7.32–7.23 (m, 7H), 7.21 – 7.14 (m, 3H), 7.09 – 6.94 (m, 6H), 6.82 (d, *J* = 7.9 Hz, 1H), 5.30 (d, *J* = 15.7 Hz, 1H), 4.79 (d, *J* = 15.7 Hz, 1H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 194.7, 175.6, 170.7, 162.5, 144.0, 140.7, 136.1, 135.1, 133.8, 133.5, 133.1, 132.6, 131.2, 130.9, 130.3, 130.1, 129.3, 129.1, 128.9, 128.6, 128.5, 127.8, 127.7, 127.4, 126.8, 124.9, 124.5, 124.2, 123.7, 110.2, 89.5, 44.8; HRMS (ESI) for $C_{41}H_{29}N_2O_2$ $[M+H]^+$ calcd 581.2224, found 581.2226. Enantiomeric excess was determined by HPLC with a Chiralpak AD-H column. (n-hexane: i-propanol = 70 : 30, 0.8 mL/min, λ = 254 nm) tR (major) = 39.0 min, tR (minor) = 44.0 min.

4. Copies of ^{1}H NMR and ^{13}C NMR spectra



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7.517
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7.251
7.160
6.964
6.937
6.919
6.900
6.836
6.817
6.747
6.727
6.099
3.097
2.717
-0.000
5b
1.99
1.05
2.02
3.90
2.13
0.84
1.11
1.06
2.01
1.97
1.00
1.00
2.94
0.92
f1 (ppm)
194.34
177.79
145.06
144.46
144.07
141.43
136.56
133.06
131.85
130.16
129.96
129.38
128.70
128.33
128.17
128.11
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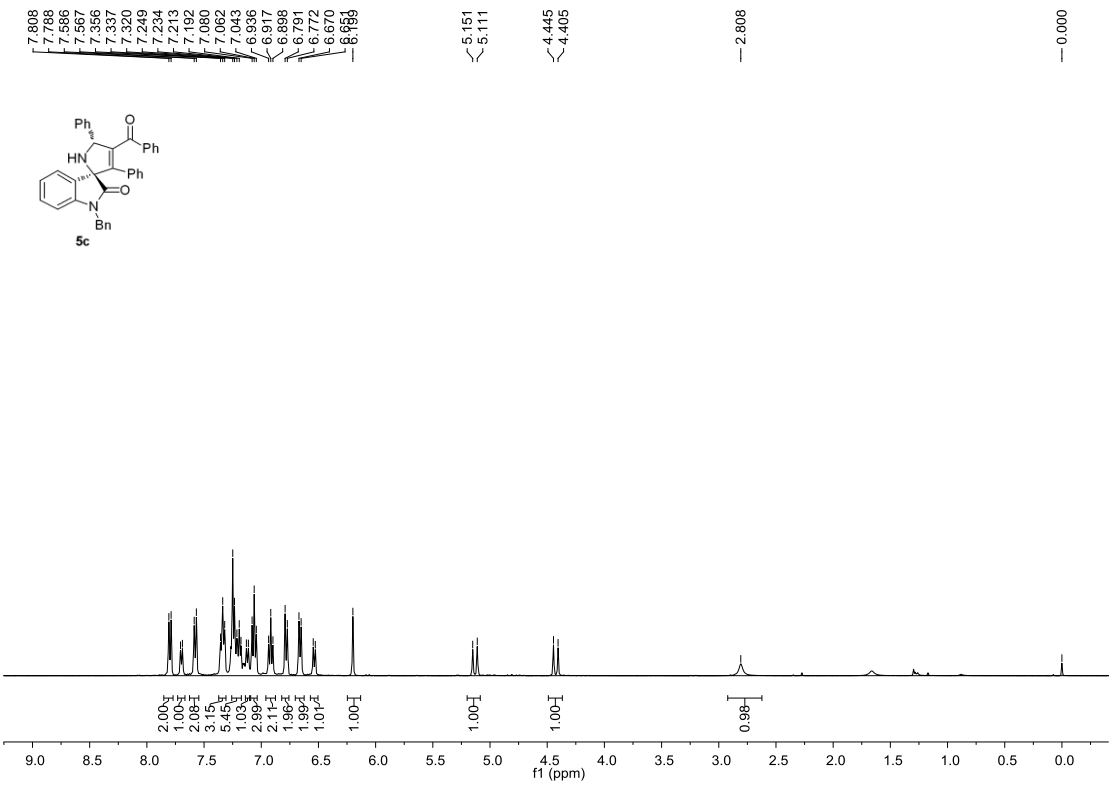
127.81
124.75
123.40
108.50
78.65
70.88
26.38
5b
f1 (ppm)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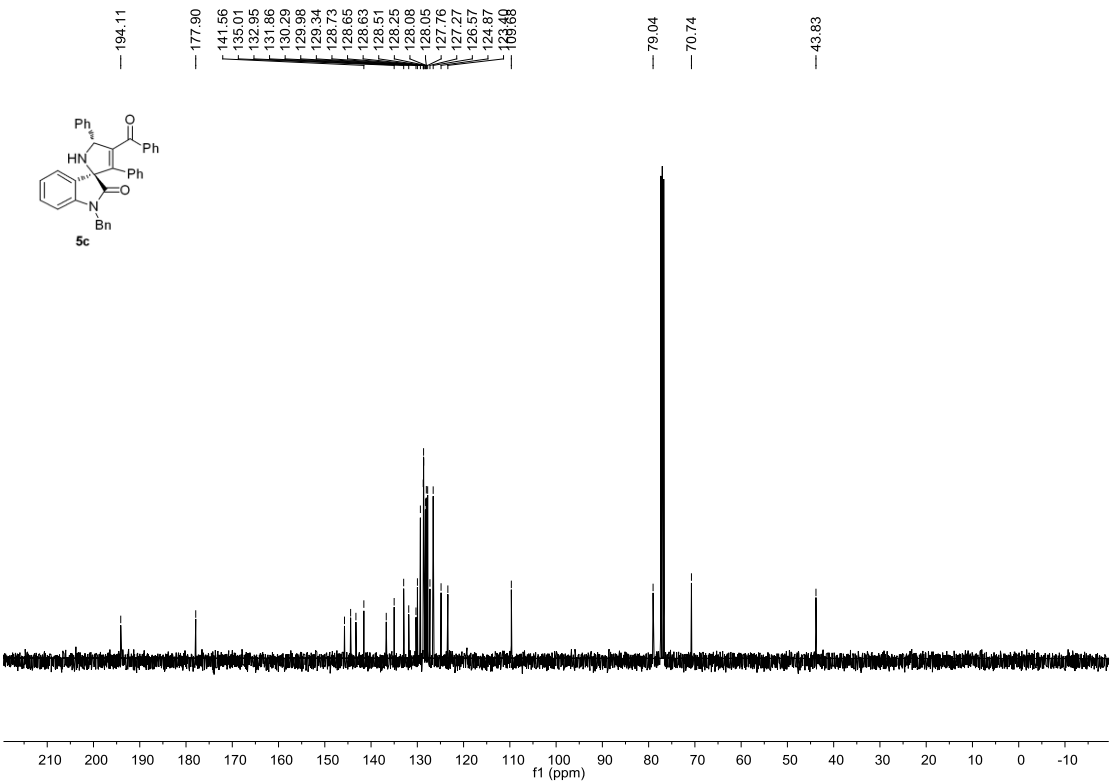
7.586
7.567
7.356
7.337
7.320
7.249
7.234
7.213
7.192
7.080
7.062
7.043
6.936
6.917
6.898
6.791
6.772
6.670
6.651
6.199
5.151
5.111
4.445
4.405
2.808
0.000
Ph
O
Ph
HN
Ph
O
N
Bn
5c
2.00
1.00
2.08
3.15
5.45
1.03
2.99
2.11
1.96
1.99
1.01
1.00
1.00
1.00
0.98
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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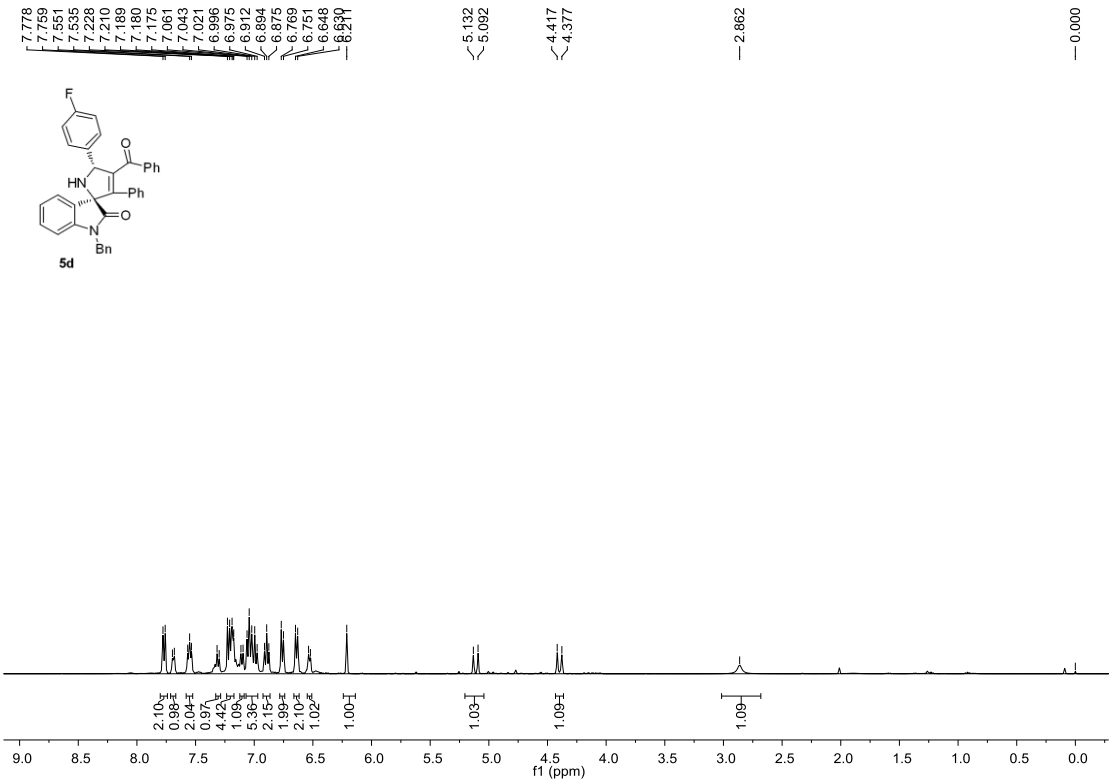
177.90
141.56
135.01
132.95
131.86
130.29
129.98
129.34
128.73
128.65
128.63
128.51
128.25
128.08
128.05
127.76
127.27
126.57
124.87
123.40
79.04
70.74
43.83
Ph
O
Ph
HN
Ph
O
N
Bn
5c
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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7.180
7.175
7.061
7.043
7.021
6.996
6.975
6.912
6.894
6.875
6.769
6.751
6.648
5.132
5.092
4.417
4.377
2.862
0.000
F
O
Ph
HN
Ph
O
N
Bn
5d
2.10
0.98
2.04
0.97
4.42
1.09
5.36
2.15
1.99
2.10
1.02
1.00
1.03
1.09
1.09
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
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3.0
2.5
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1.0
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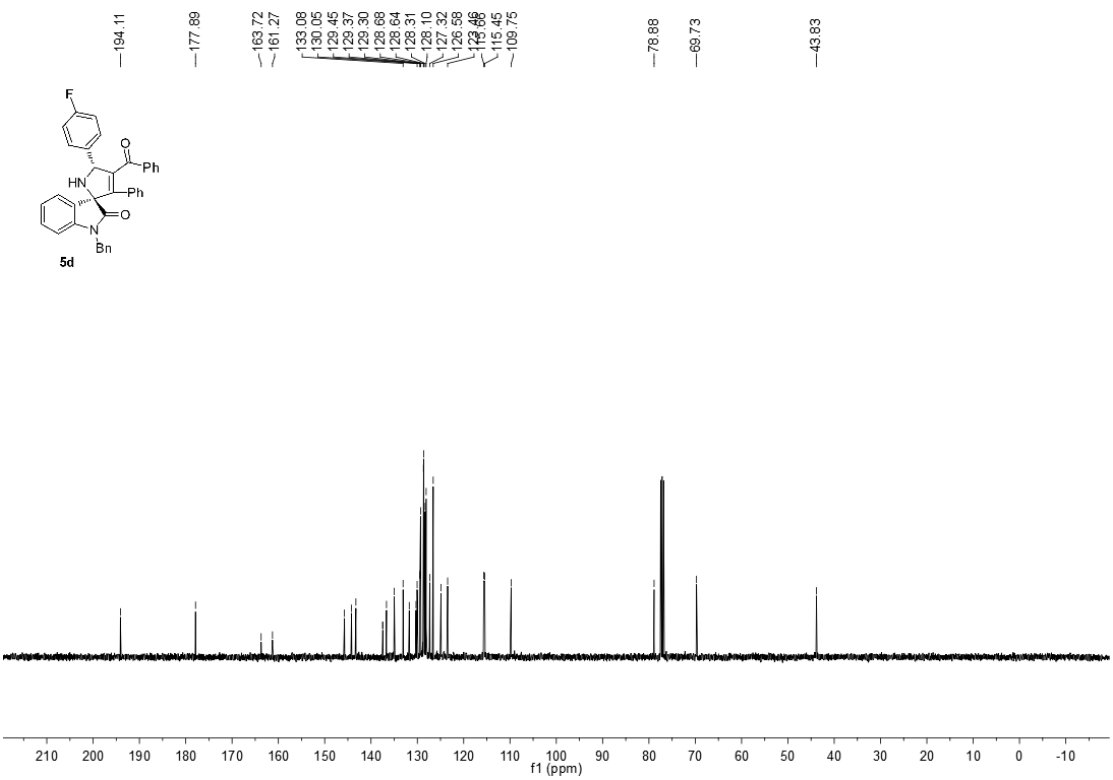
0.0
f1 (ppm)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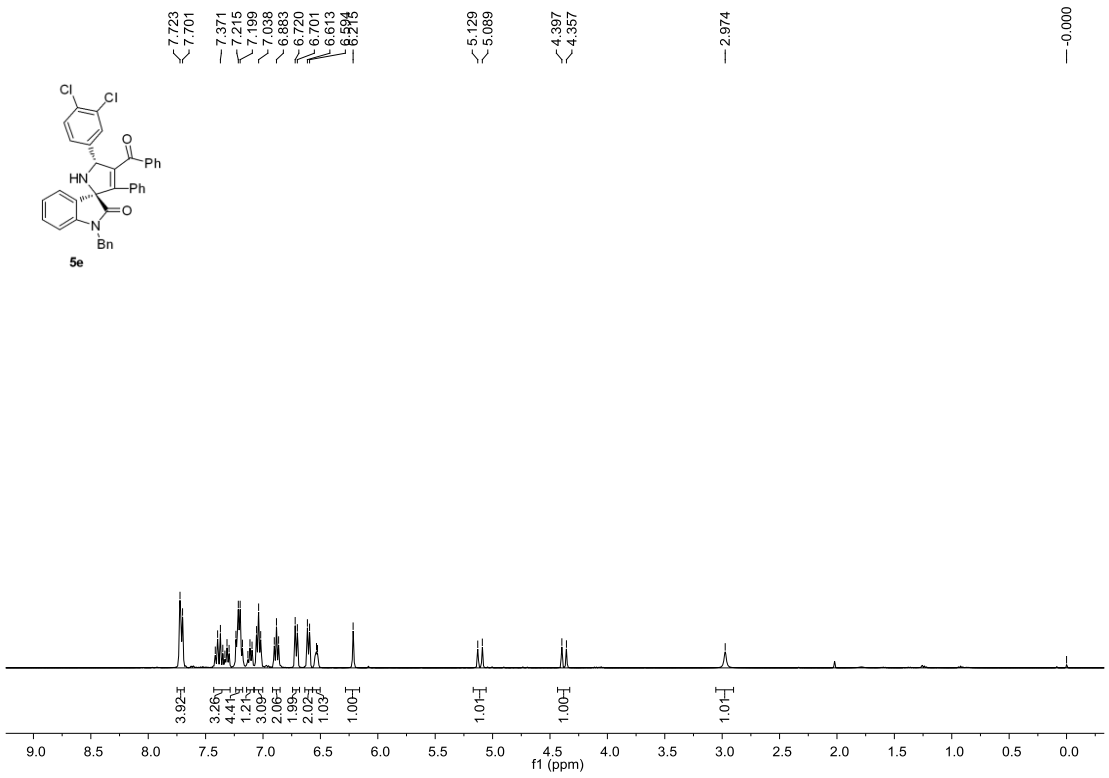
133.08
130.05
129.45
129.37
129.30
128.88
128.64
128.31
128.10
127.32
126.58
115.45
109.75
78.88
69.73
43.83
F
O
Ph
HN
Ph
O
N
Bn
5d
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)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7.038
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6.720
6.701
6.613
5.129
5.089
4.397
4.357
2.974
-0.000
Cl
Cl
O
Ph
HN
Ph
O
N
Bn
5e
3.92
3.26
4.41
1.21
3.09
2.06
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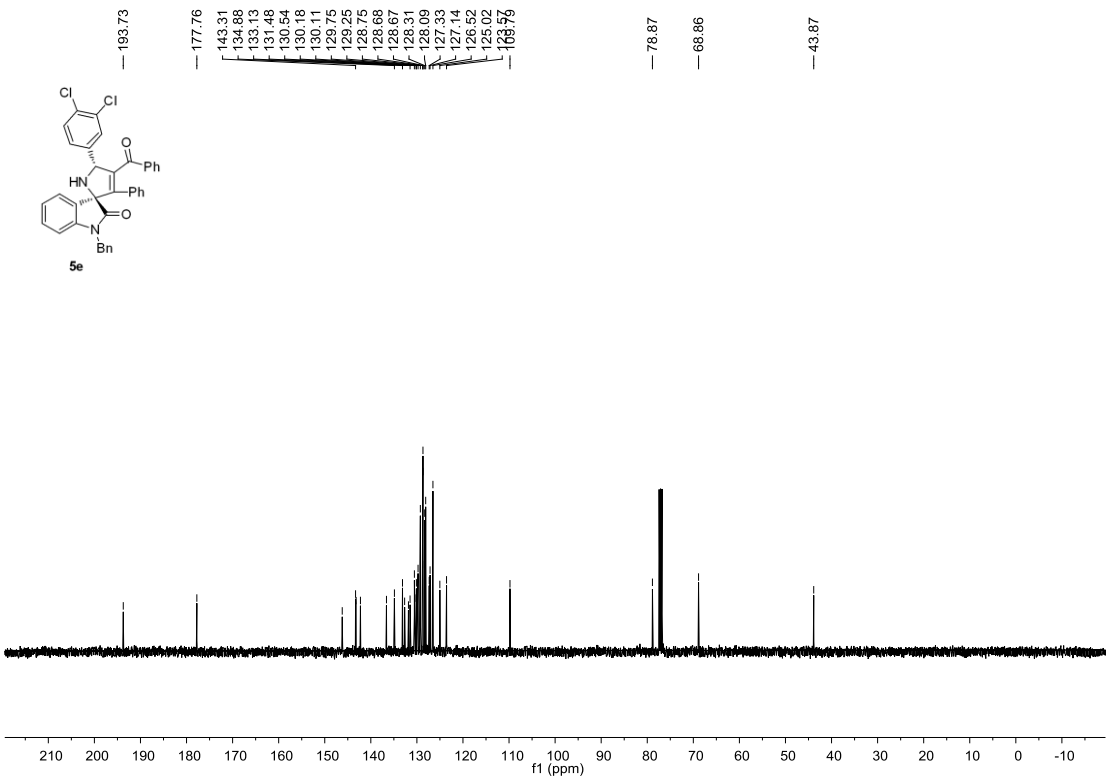
1.00
1.01
1.00
1.01
f1 (ppm)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130.18
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129.75
129.25
128.75
128.68
128.67
128.31
128.09
127.33
127.14
126.52
125.02
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43.87
Cl
Cl
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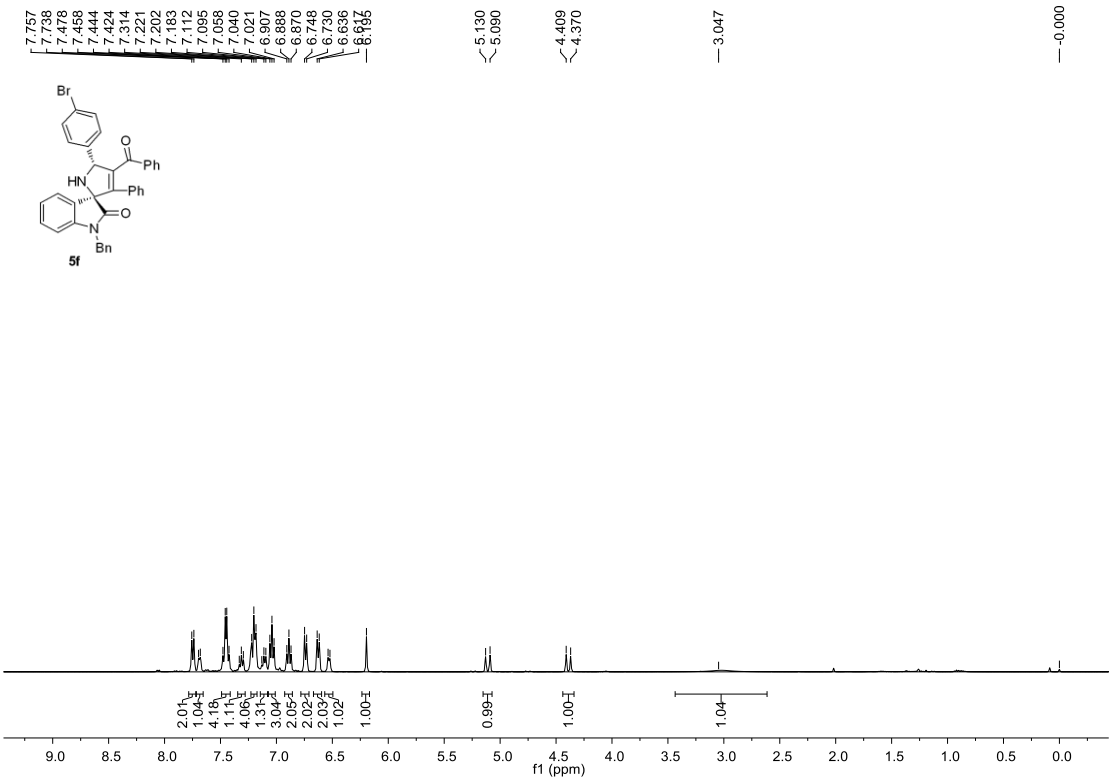
Ph
HN
Ph
O
N
Bn
5e
f1 (ppm)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7.202
7.183
7.112
7.095
7.058
7.040
7.021
6.907
6.888
6.870
6.748
6.730
6.636
6.617
6.195
5.130
5.090
4.409
4.370
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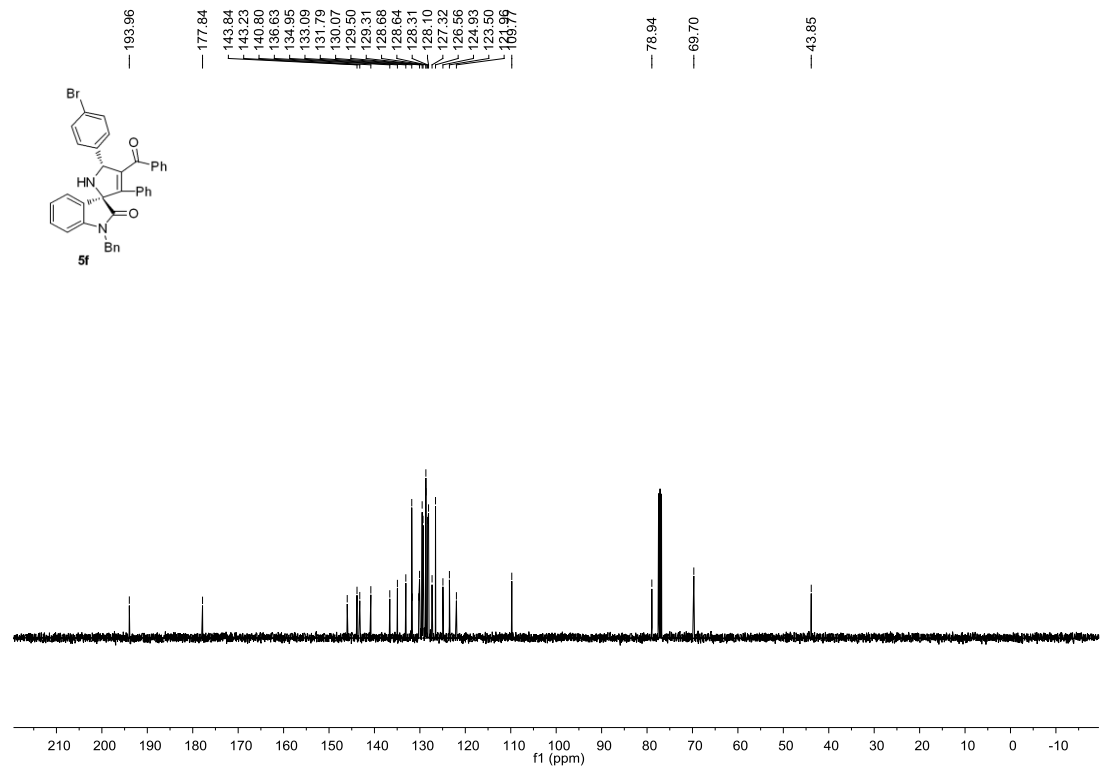
O
Ph
HN
Ph
O
N
Bn
5f
2.01
1.04
4.18
1.11
4.06
1.31
3.04
2.05
2.02
2.03
1.02
1.00
0.99
1.00
1.04
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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133.09
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129.31
128.68
128.64
128.31
128.10
127.32
126.56
124.93
123.50
78.94
69.70
43.85
Br
O
Ph
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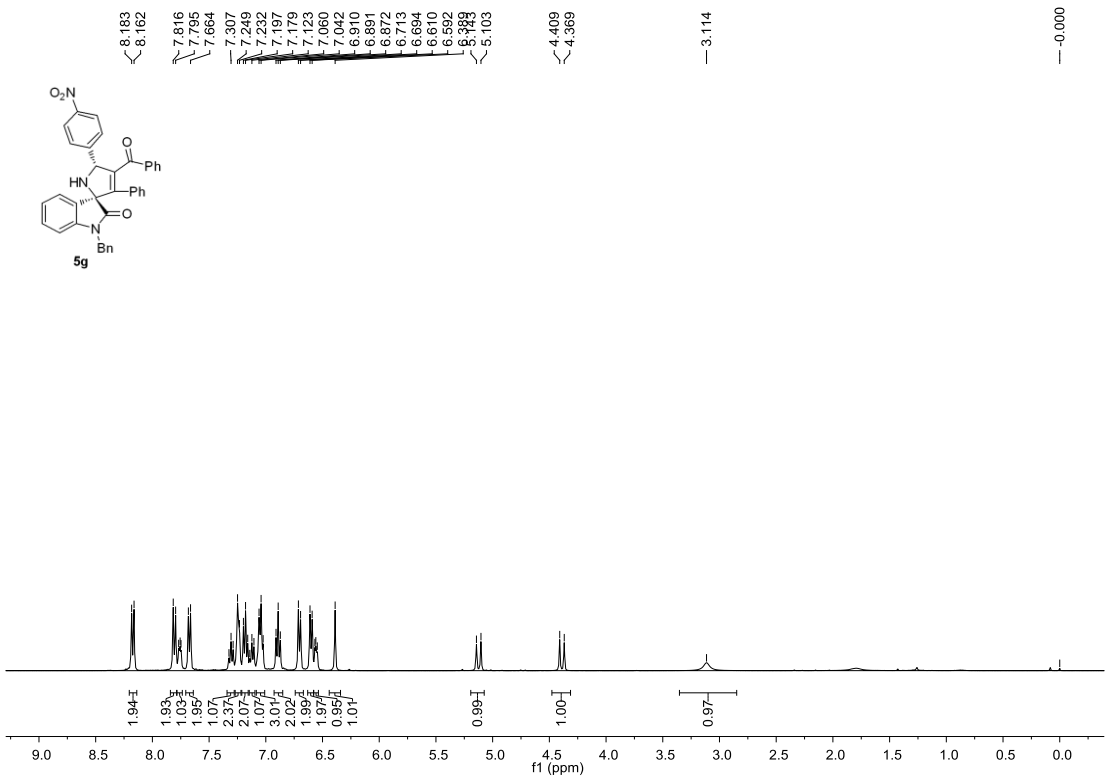
Ph
O
N
Bn
5f
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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7.232
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7.042
6.910
6.891
6.872
6.713
6.694
6.610
6.592
5.103
4.409
4.369
3.114
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O
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HN
Ph
O
N
Bn
5g
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1.93
1.03
1.95
1.07
2.37
2.07
1.07
3.01
2.02
1.99
1.97
0.95
1.01
0.99
1.00
0.97
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
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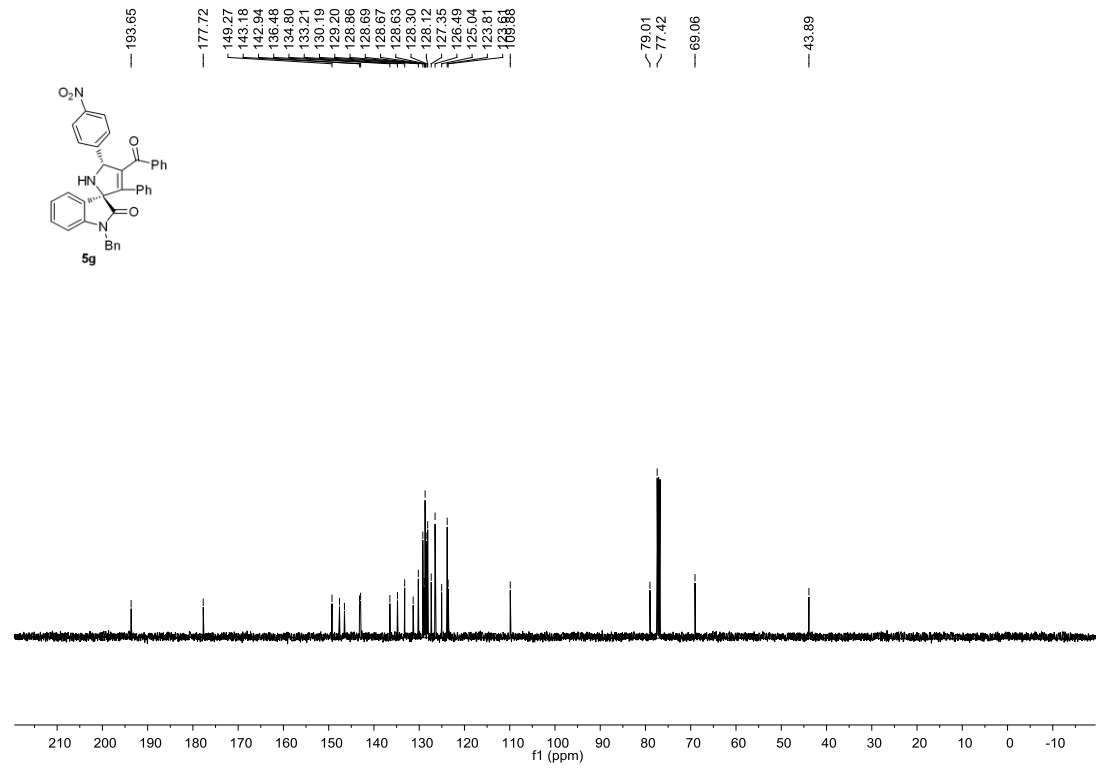
f1 (ppm)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136.48
134.80
133.21
130.19
129.20
128.86
128.69
128.67
128.63
128.30
128.12
127.35
126.49
125.04
123.81
79.01
77.42
69.06
43.89
O2N
O
Ph
HN
Ph
O
N
Bn
5g
210
200
190
180
170
160
150
140
130
120
110
100
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80
70
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50
40
30
20
10
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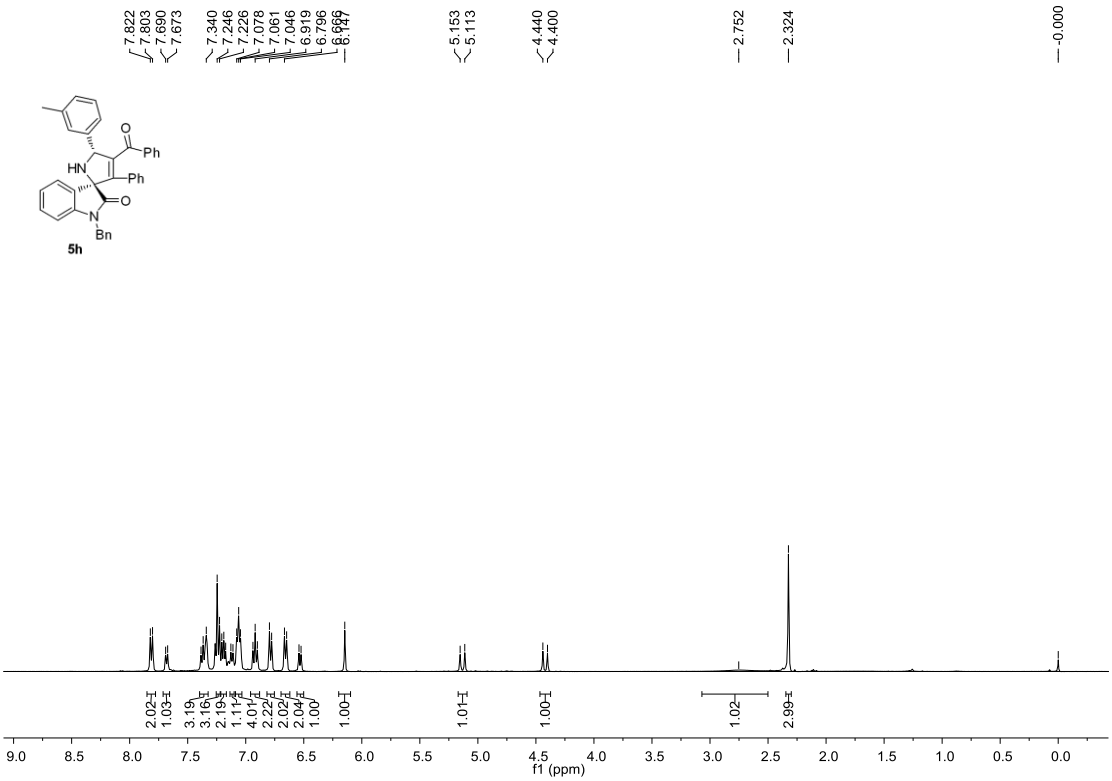
f1 (ppm)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5.153
5.113
4.440
4.400
2.752
2.324
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O
Ph
HN
Ph
O
N
Bn
5h
2.02
1.03
3.19
3.16
2.19
1.11
4.01
2.22
2.02
2.04
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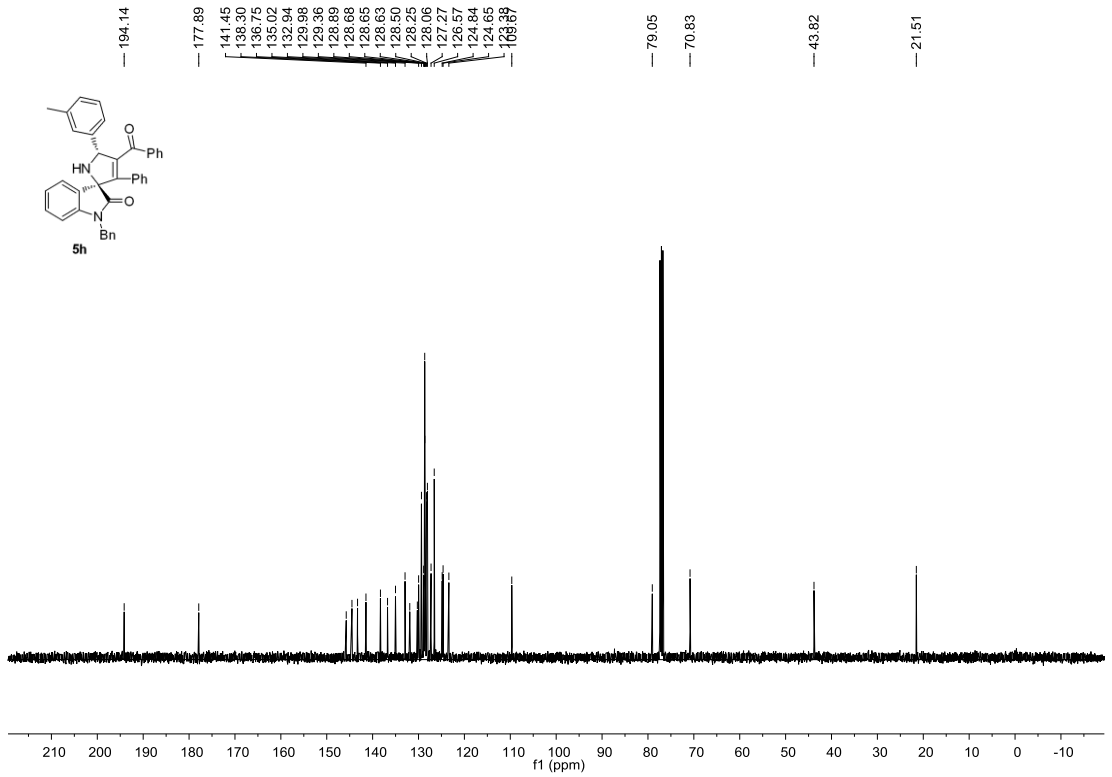
1.00
1.02
2.99
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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128.06
127.27
126.57
124.84
124.65
123.38
123.87
79.05
70.83
43.82
21.51
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Ph
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5h
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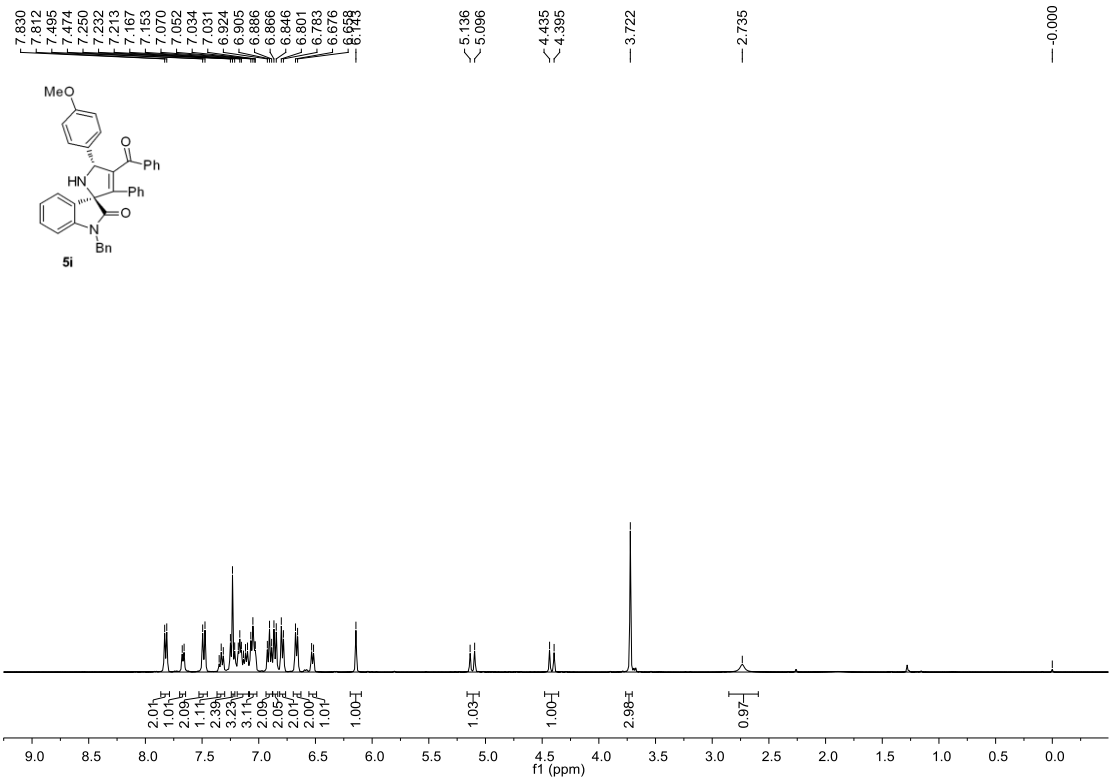
f1 (ppm)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6.846
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6.783
6.676
6.658
6.143
5.136
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4.435
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3.722
2.735
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Ph
HN
Ph
O
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Bn
5i
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2.09
1.11
2.39
3.23
3.11
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2.05
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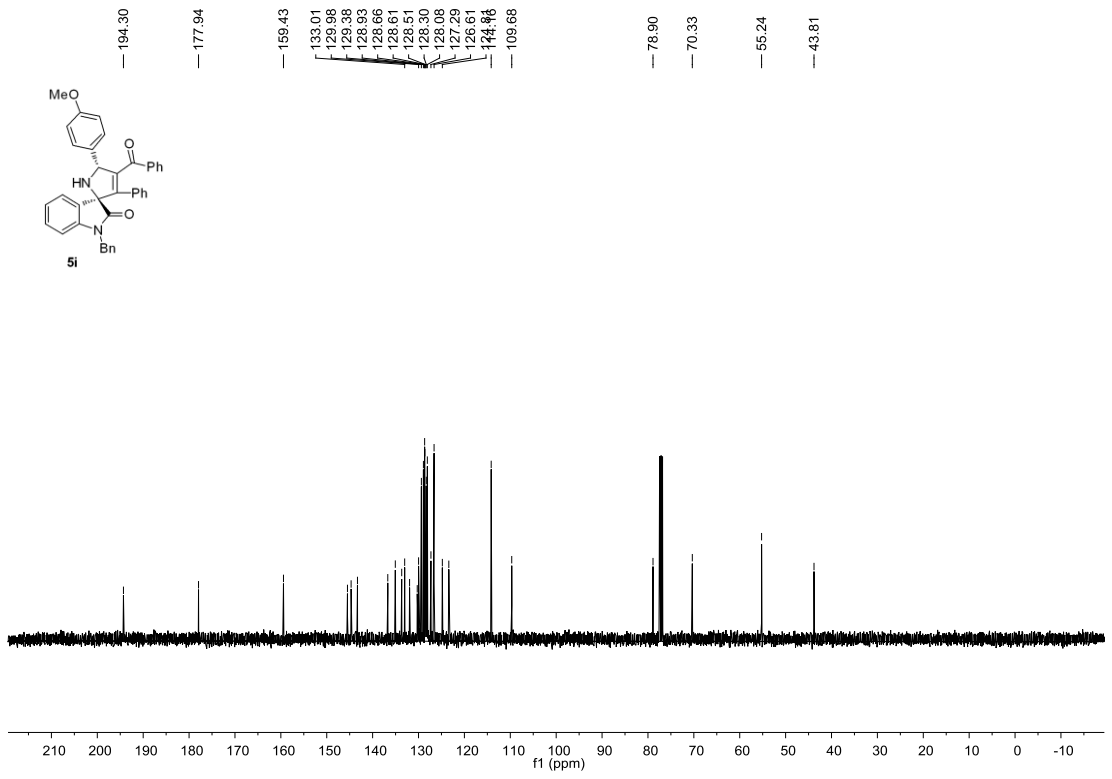
2.00
1.01
1.00
1.03
1.00
2.98
0.97
f1 (ppm)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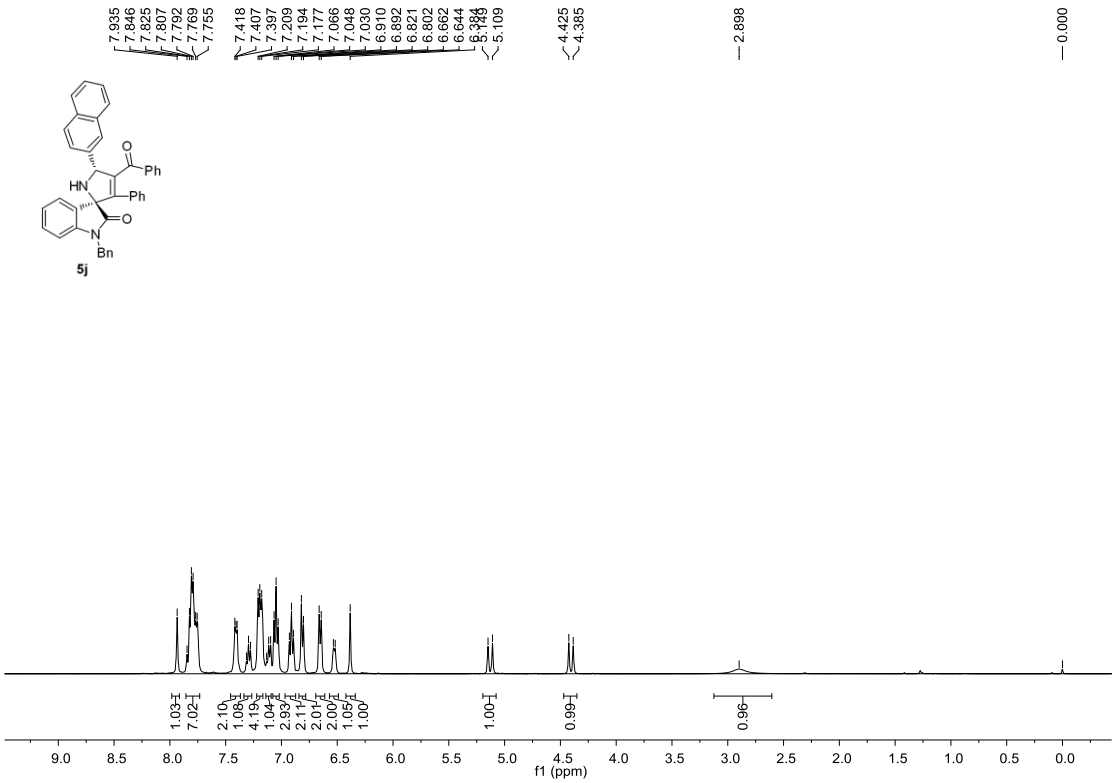
177.94
159.43
133.01
129.98
129.38
128.93
128.66
128.61
128.51
128.30
128.08
127.29
126.61
114.18
109.68
78.90
70.33
55.24
43.81
MeO
O
Ph
HN
Ph
O
N
Bn
5i
f1 (ppm)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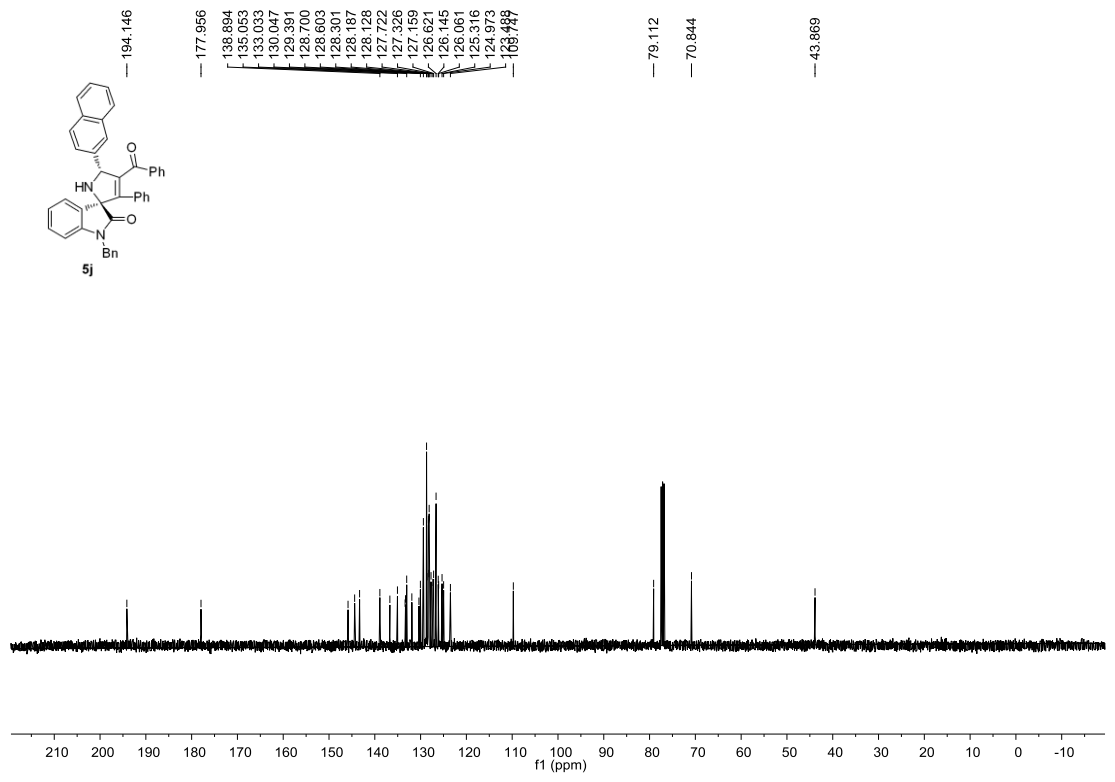
7.846
7.825
7.807
7.792
7.769
7.755
7.418
7.407
7.397
7.209
7.194
7.177
7.066
7.048
7.030
6.910
6.892
6.821
6.802
6.662
6.644
6.384
6.369
5.149
5.109
4.425
4.385
2.898
0.000
Ph
HN
Ph
O
N
Bn
5j
1.03
7.02
2.10
1.08
4.19
1.04
2.93
2.11
2.01
2.00
1.05
1.00
1.00
0.99
0.96
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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130.047
129.391
128.700
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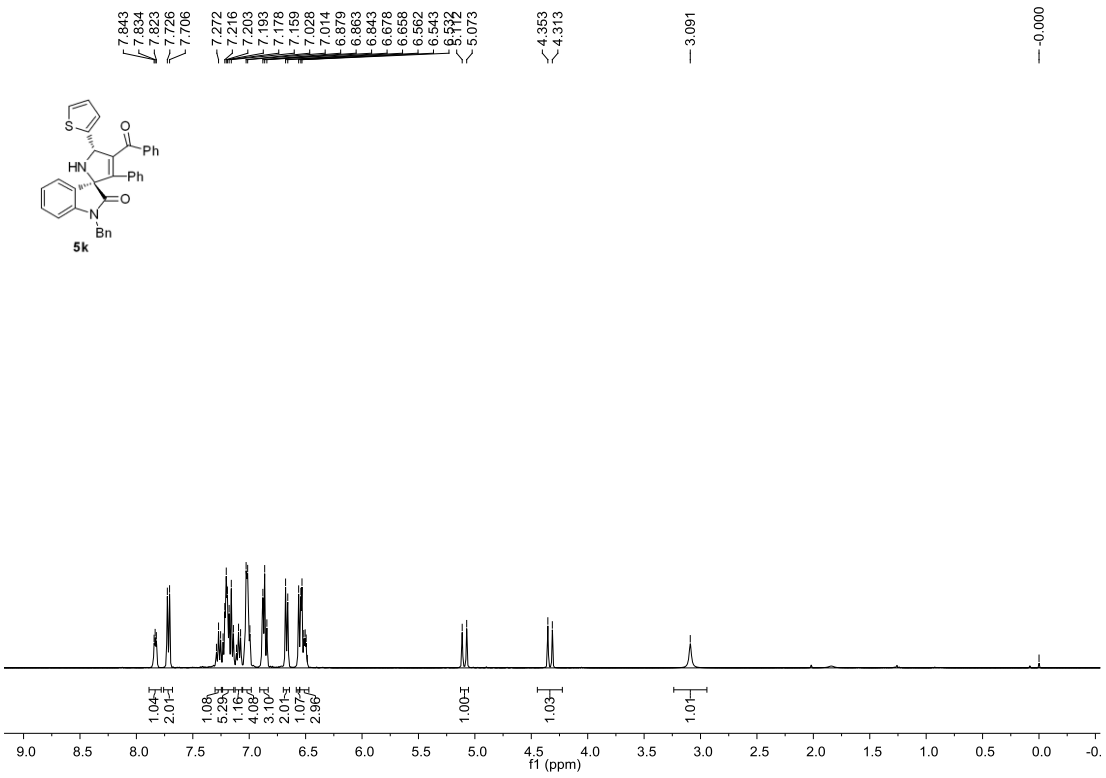
128.301
128.187
128.128
127.722
127.326
127.159
126.621
126.145
126.061
125.316
124.973
79.112
70.844
43.869
Ph
HN
Ph
O
N
Bn
5j
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)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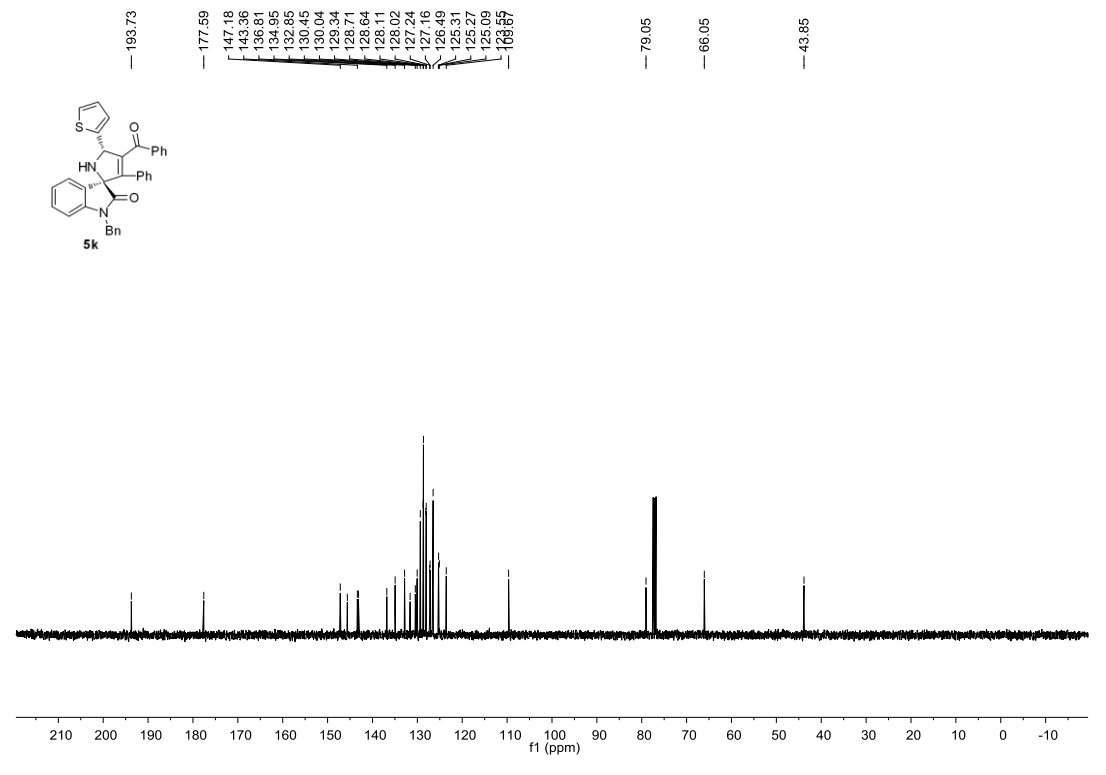
7.834
7.823
7.726
7.706
7.272
7.216
7.203
7.193
7.178
7.159
7.028
7.014
6.879
6.863
6.843
6.678
6.658
6.562
6.543
6.532
6.512
5.073
4.353
4.313
3.091
0.000
S
HN
O
Ph
Ph
O
N
Bn
5k
1.04
2.01
1.08
5.29
1.16
4.08
3.10
2.01
1.07
2.96
1.00
1.03
1.01
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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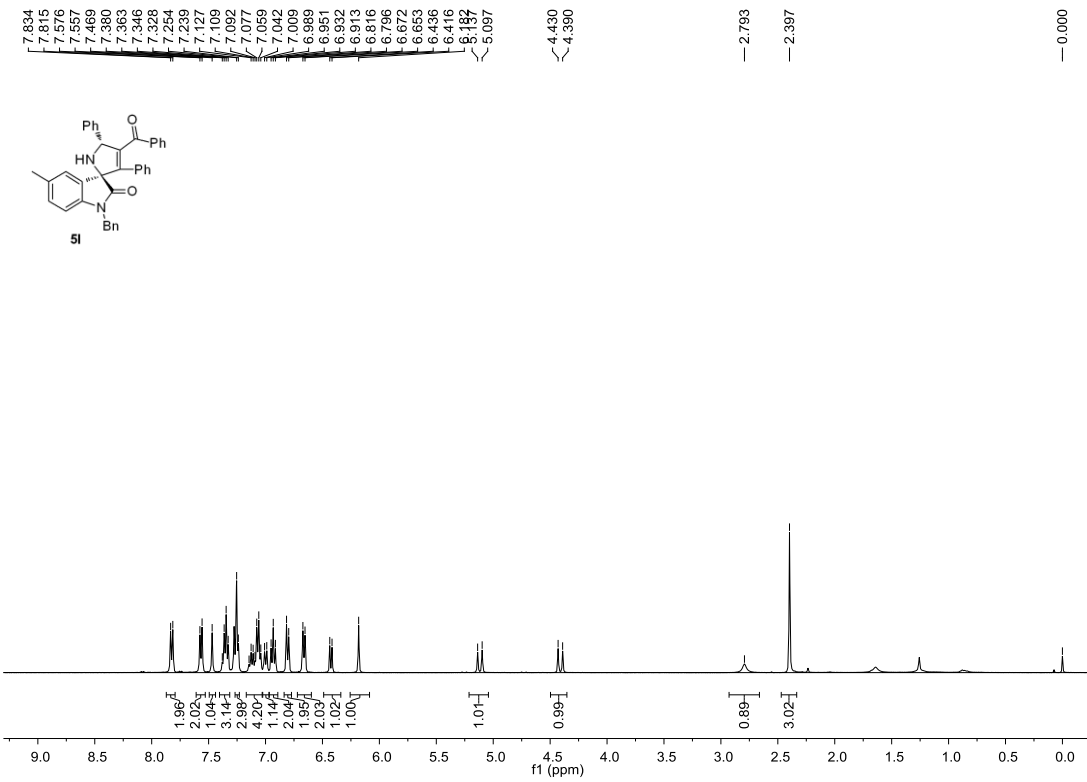
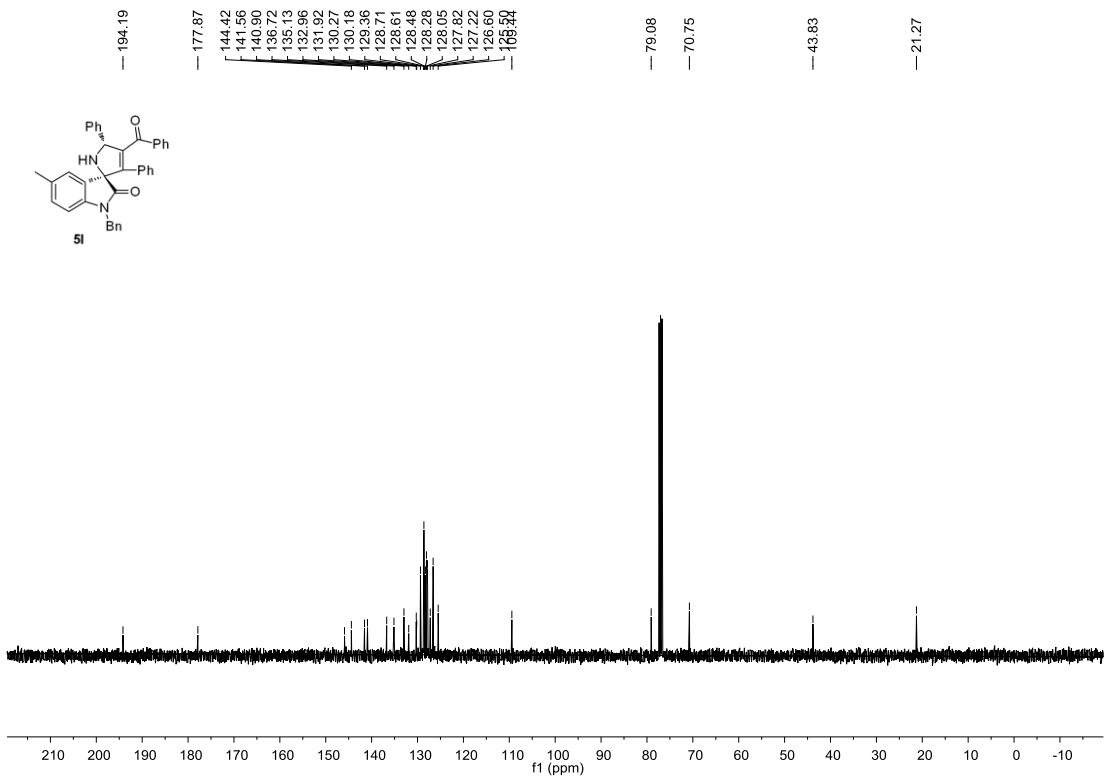
177.59
147.18
143.36
136.81
134.95
132.85
130.45
130.04
129.34
128.71
128.64
128.11
128.02
127.24
127.16
126.49
125.31
125.27
125.09
79.05
66.05
43.85
S
HN
O
Ph
Ph
O
N
Bn
5k
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


7.834
7.815
7.576
7.557
7.469
7.380
7.363
7.346
7.328
7.254
7.239
7.127
7.109
7.092
7.077
7.059
7.042
7.009
6.989
6.951
6.932
6.913
6.816
6.796
6.672
6.653
6.436
6.416
5.182
5.097
4.430
4.390
2.793
2.397
0.000
Ph
O
Ph
HN
Ph
O
N
Bn
5l
1.96
2.02
1.04
3.14
2.98
4.20
1.14
2.04
1.95
2.03
1.02
1.00
1.01
0.99
0.89
3.02
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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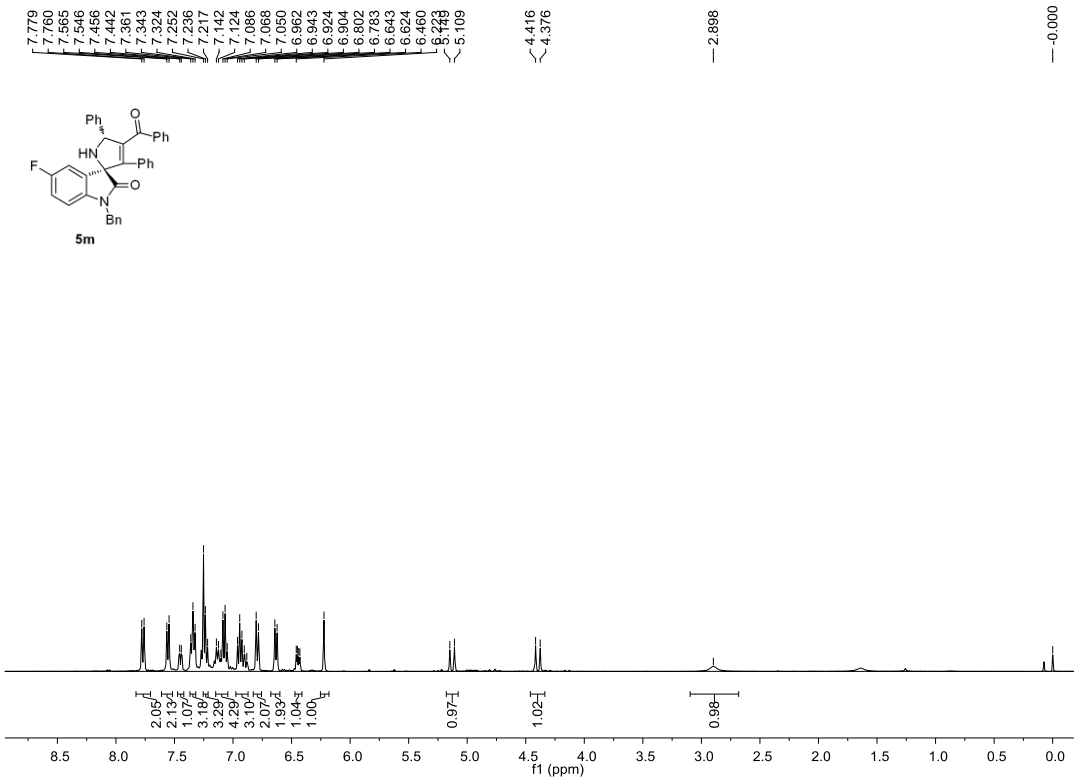
177.87
144.42
141.56
140.90
136.72
135.13
132.96
131.92
130.27
130.18
129.36
128.71
128.61
128.48
128.28
128.05
127.82
127.22
126.60
79.08
70.75
43.83
21.27
Ph
O
Ph
HN
Ph
O
N
Bn
5l
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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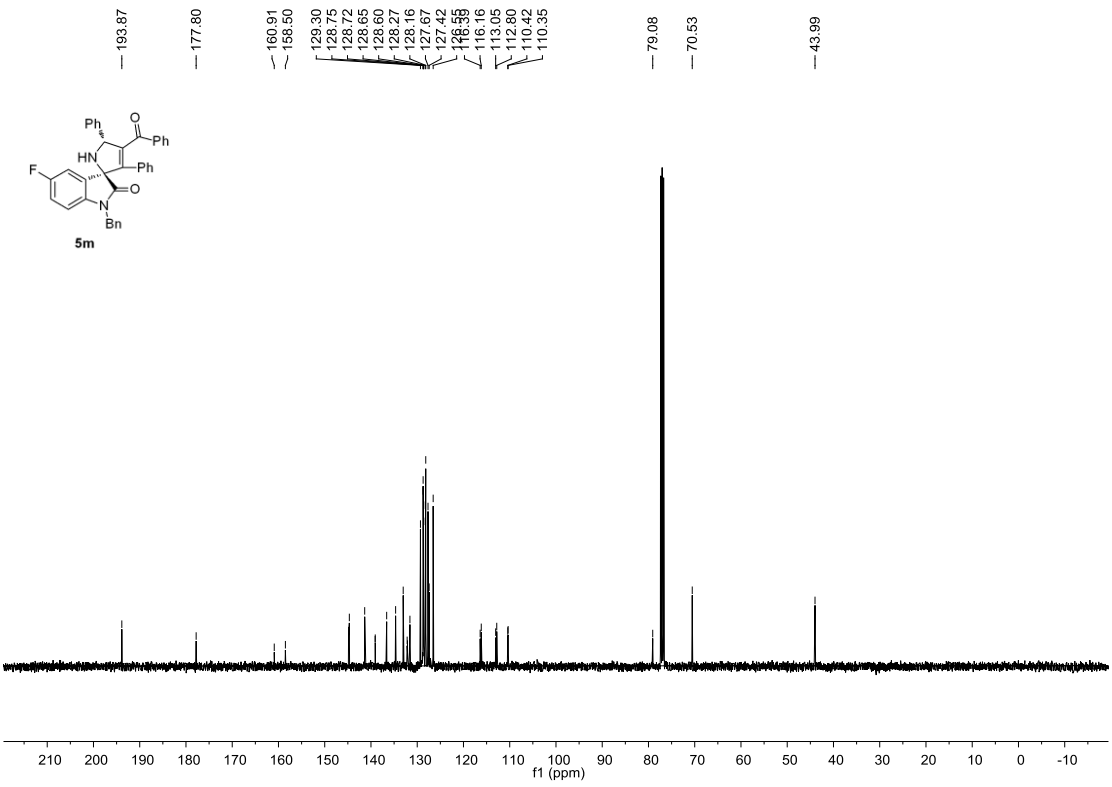
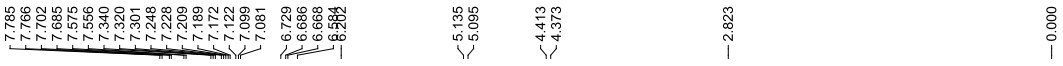
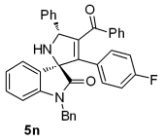
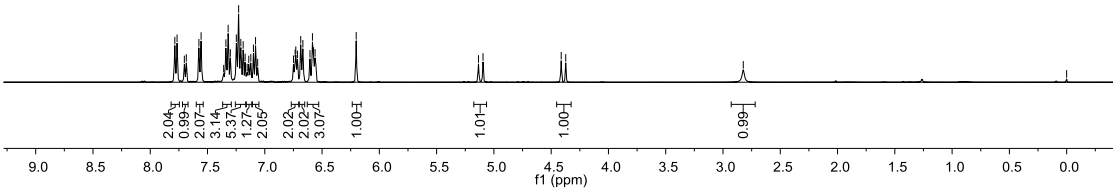
7.760
7.565
7.546
7.456
7.442
7.361
7.343
7.324
7.252
7.236
7.217
7.142
7.124
7.086
7.068
7.050
6.962
6.943
6.924
6.904
6.802
6.783
6.643
6.624
6.460
5.148
5.109
4.416
4.376
2.898
-0.000
Ph
O
Ph
HN
F
Ph
O
N
Bn
5m
2.05
2.13
1.07
3.18
3.29
4.29
3.10
2.07
1.93
1.04
1.00
0.97
1.02
0.98
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


193.87
177.80
160.91
158.50
129.30
128.75
128.72
128.65
128.60
128.27
128.16
127.67
127.42
116.16
113.05
112.80
110.42
110.35
79.08
70.53
43.99
Ph
O
Ph
HN
F
Ph
O
N
Bn
5m
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


7.785
7.766
7.702
7.685
7.575
7.556
7.340
7.320
7.301
7.248
7.228
7.209
7.189
7.172
7.122
7.099
7.081
6.729
6.686
6.668
6.584
6.262
5.135
5.095
4.413
4.373
2.823
0.000


Ph
O
Ph
HN
O
F
N
Bn

5n


2.04
0.99
2.07
3.14
5.37
1.27
2.05
2.02
2.02
3.07
1.00
1.01
1.00
0.99
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


194.00
177.77
164.02
161.55
130.60
130.52
130.15
129.30
128.77
128.62
128.38
128.16
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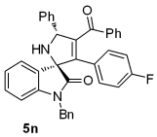
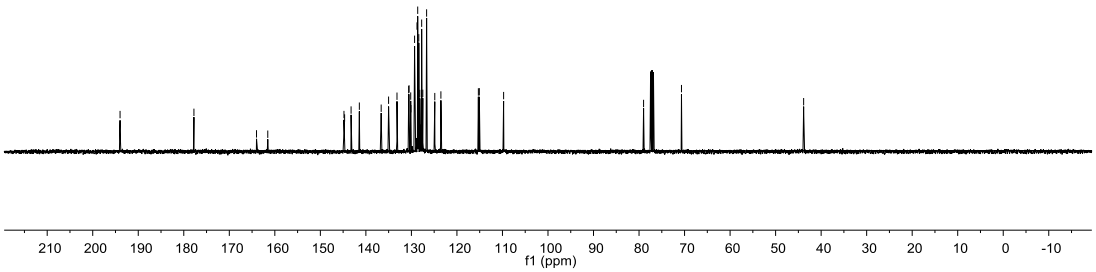
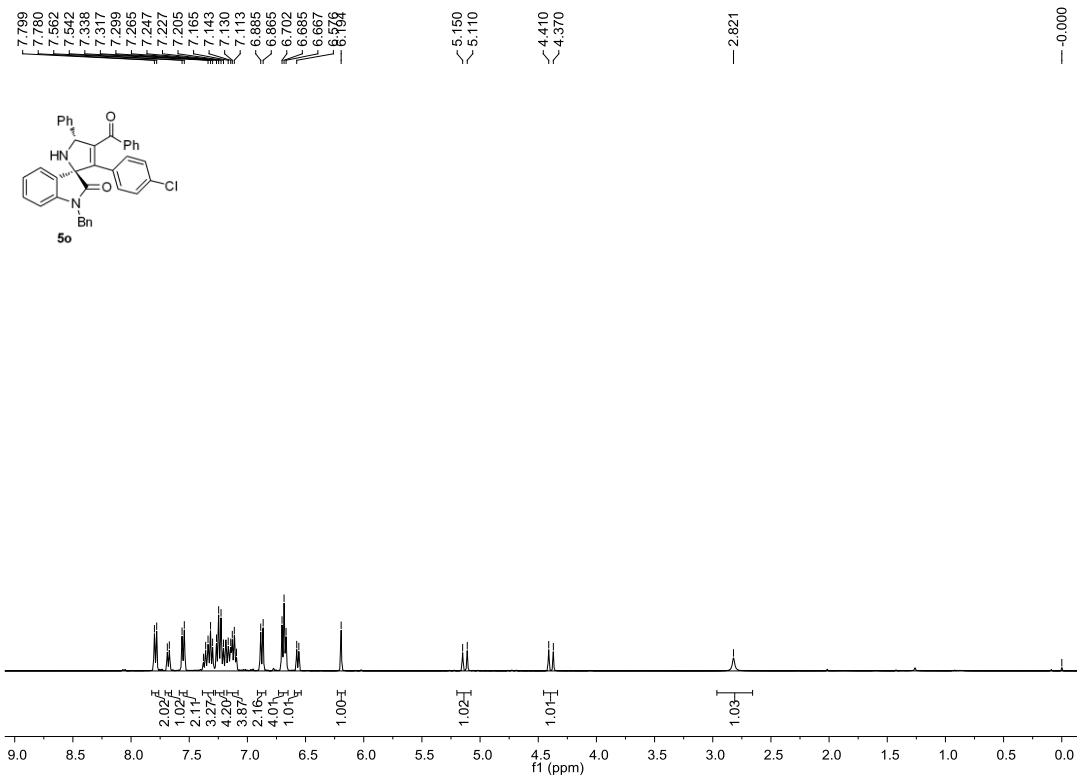
127.50
126.66
115.08
109.75
79.00
70.68
43.84


Ph
O
Ph
HN
O
F
N
Bn

5n


210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


7.799
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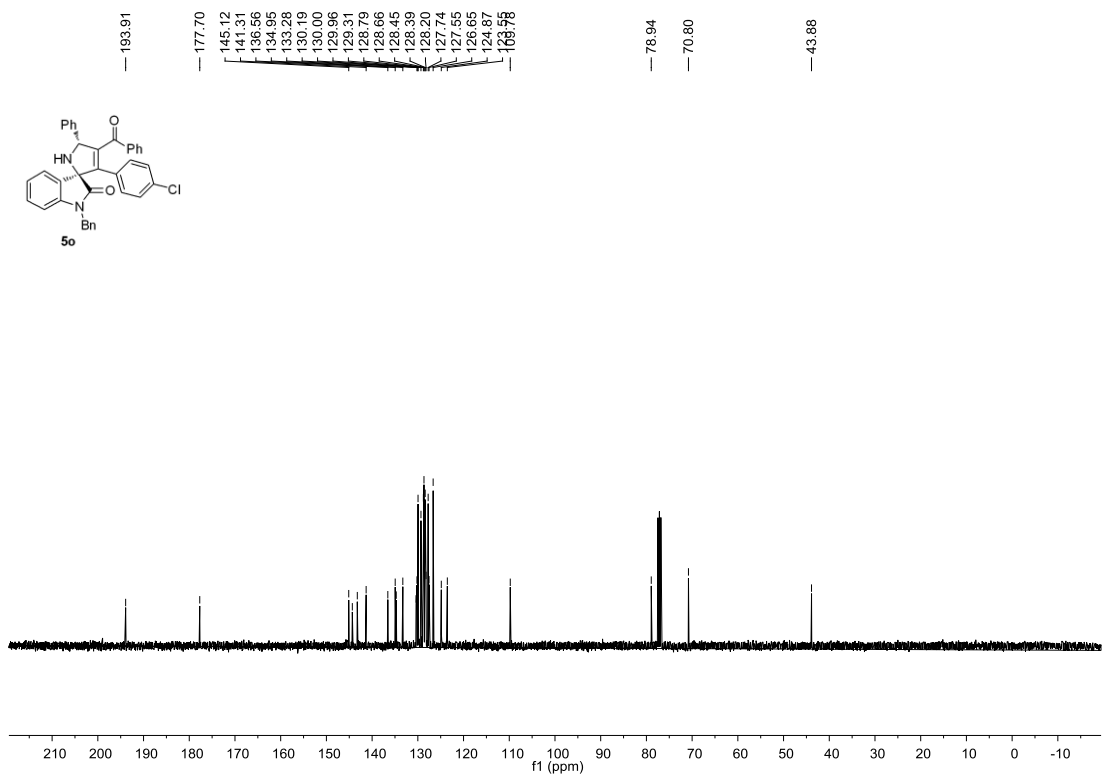
7.562
7.542
7.338
7.317
7.299
7.265
7.247
7.227
7.205
7.165
7.143
7.130
7.113
6.885
6.865
6.702
6.685
6.667
6.576
6.194
5.150
5.110
4.410
4.370
2.821
-0.000
Ph
O
Ph
HN
O
Cl
N
Bn
5o
2.02
1.02
2.11
3.27
4.20
3.87
2.16
4.01
1.01
1.00
1.02
1.01
1.03
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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145.12
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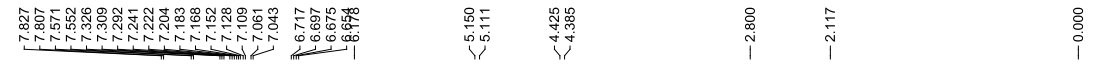
136.56
134.95
133.28
130.19
130.00
129.96
129.31
128.79
128.66
128.45
128.39
128.20
127.74
127.55
126.65
124.87
123.55
109.78
78.94
70.80
43.88
Ph
O
Ph
HN
O
Cl
N
Bn
5o
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)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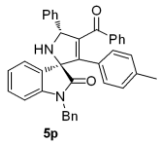
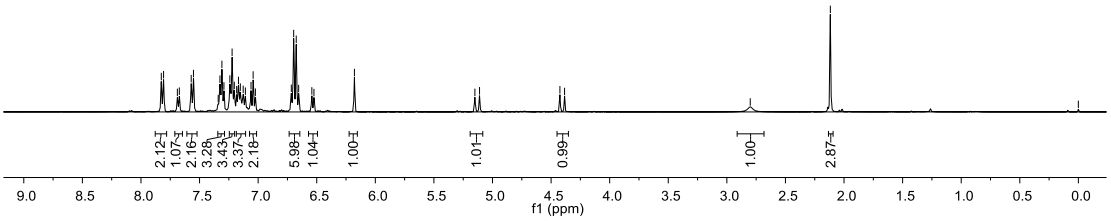
7.571
7.552
7.326
7.309
7.292
7.241
7.222
7.204
7.183
7.168
7.152
7.128
7.109
7.061
7.043
6.717
6.697
6.675
6.654
6.178
5.150
5.111
4.425
4.385
2.800
2.117
0.000


Ph
O
Ph
HN
O
N
Bn

5p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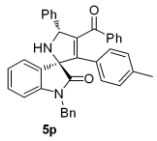
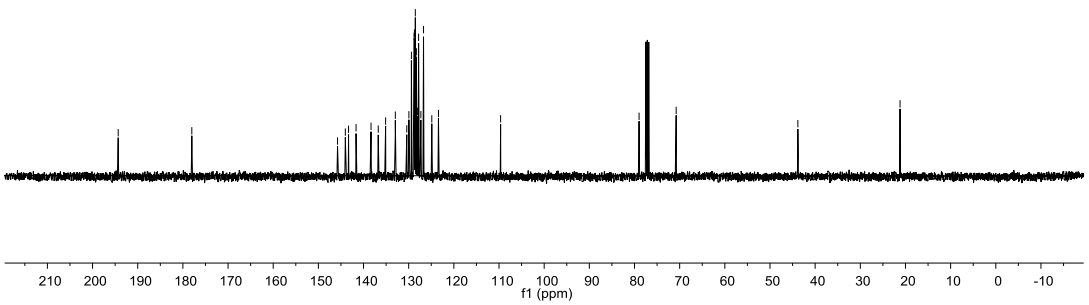
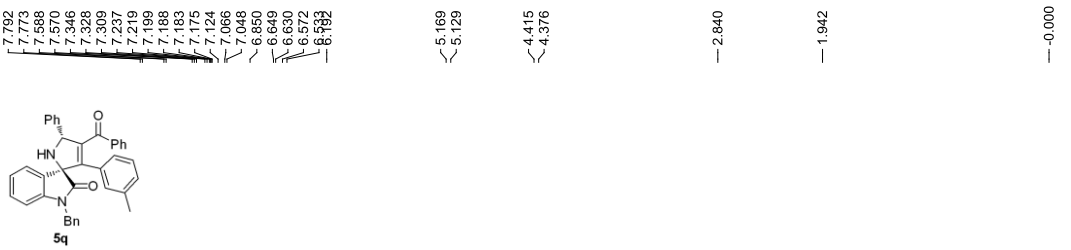
1.07
2.16
3.28
3.43
3.37
2.18
5.98
1.04
1.00
1.01
0.99
1.00
2.87
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


194.32
178.02
141.66
138.34
135.11
132.96
130.42
129.96
129.40
128.92
128.81
128.73
128.53
128.49
128.30
128.08
127.81
127.30
126.71
124.88
78.99
70.77
43.83
21.20


Ph
O
Ph
HN
O
N
Bn

5p


210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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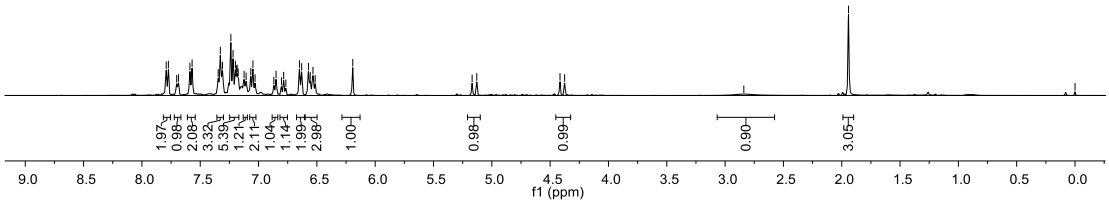
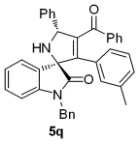
7.570
7.346
7.328
7.309
7.237
7.219
7.199
7.188
7.183
7.175
7.124
7.066
7.048
6.850
6.649
6.630
6.572
6.533
6.192
5.169
5.129
4.415
4.376
2.840
1.942
-0.000

Ph
O
Ph
HN
O
N
Bn

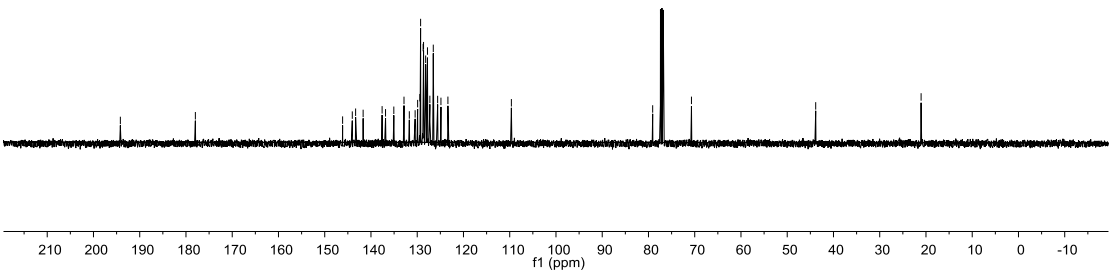
5q

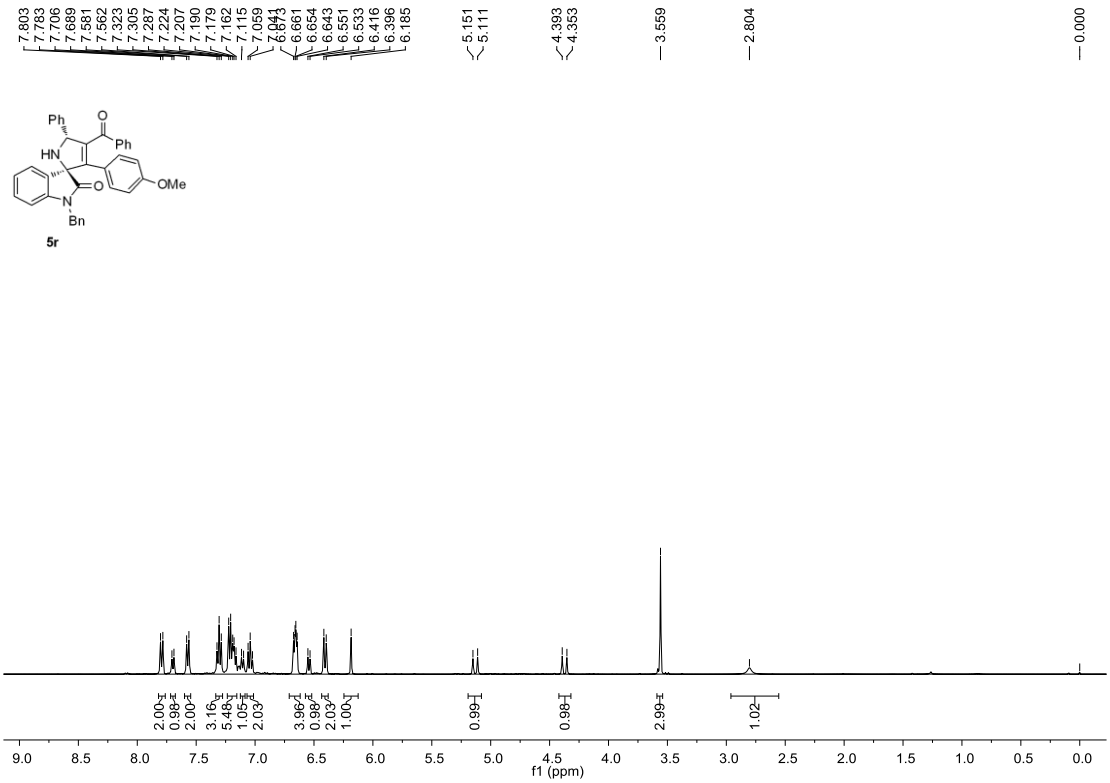

1.97
0.98
2.08
3.32
5.39
1.21
2.11
1.04
1.14
1.99
2.98
1.00
0.98
0.99
0.90
3.05
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

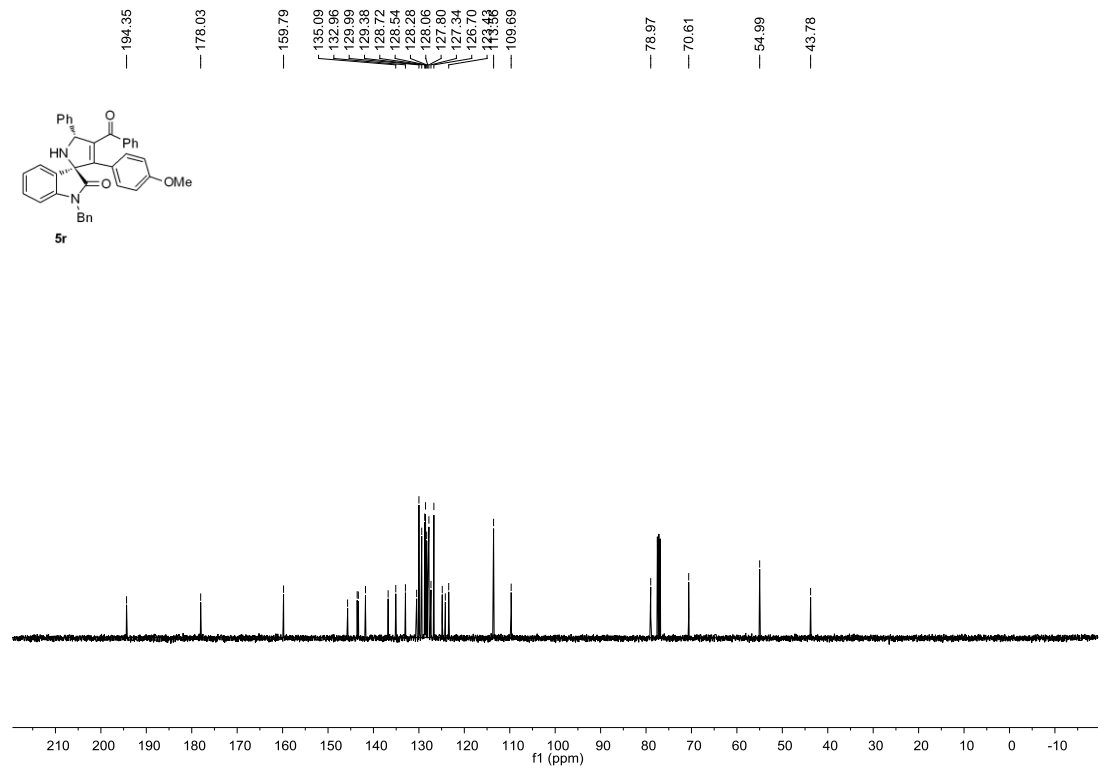

194.19
177.97
143.32
137.59
136.85
135.06
132.86
129.91
129.44
129.27
128.72
128.63
128.18
128.06
127.92
127.78
127.26
126.53
125.58
124.87
123.37
79.09
70.70
43.84
21.05


Ph
O
Ph
HN
O
N
Bn

5q


210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


7.803
7.783
7.706
7.689
7.581
7.562
7.323
7.305
7.287
7.224
7.207
7.190
7.179
7.162
7.115
7.059
7.041
6.673
6.661
6.654
6.643
6.551
6.533
6.416
6.396
6.185
5.151
5.111
4.393
4.353
3.559
2.804
0.000
Ph
O
Ph
HN
OMe
O
N
Bn
5r
2.00
0.98
2.00
3.16
5.48
1.05
2.03
3.96
0.98
2.03
1.00
0.99
0.98
2.99
1.02
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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159.79
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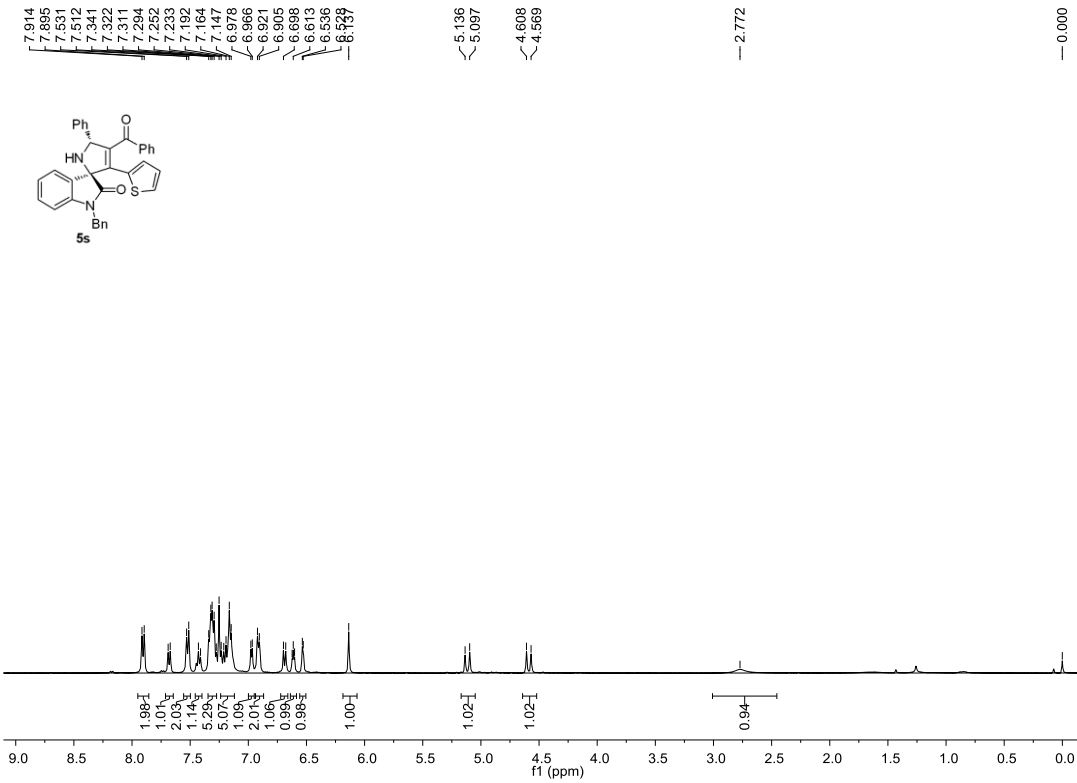
129.99
129.38
128.72
128.54
128.28
128.06
127.80
127.34
126.70
123.43
113.98
109.69
78.97
70.61
54.99
43.78
Ph
O
Ph
HN
OMe
O
N
Bn
5r
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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7.322
7.311
7.294
7.252
7.233
7.192
7.164
7.147
6.978
6.966
6.921
6.905
6.698
6.613
6.536
6.528
6.137
5.136
5.097
4.608
4.569
2.772
0.000
Ph
HN
O
Ph
O
S
N
Bn
5s
1.98
1.01
2.03
1.14
5.29
5.07
1.09
2.01
1.06
0.99
0.98
1.00
1.02
1.02
0.94
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
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3.5
3.0
2.5
2.0
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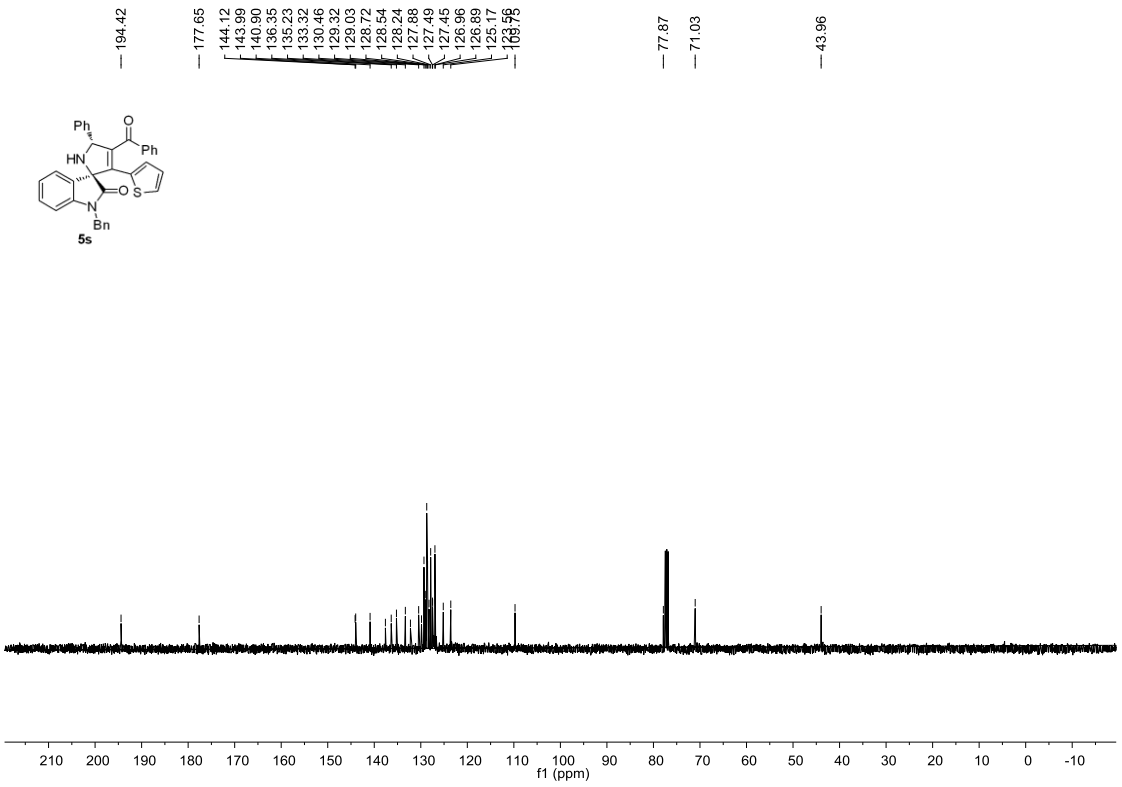
1.0
0.5
0.0
f1 (ppm)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133.32
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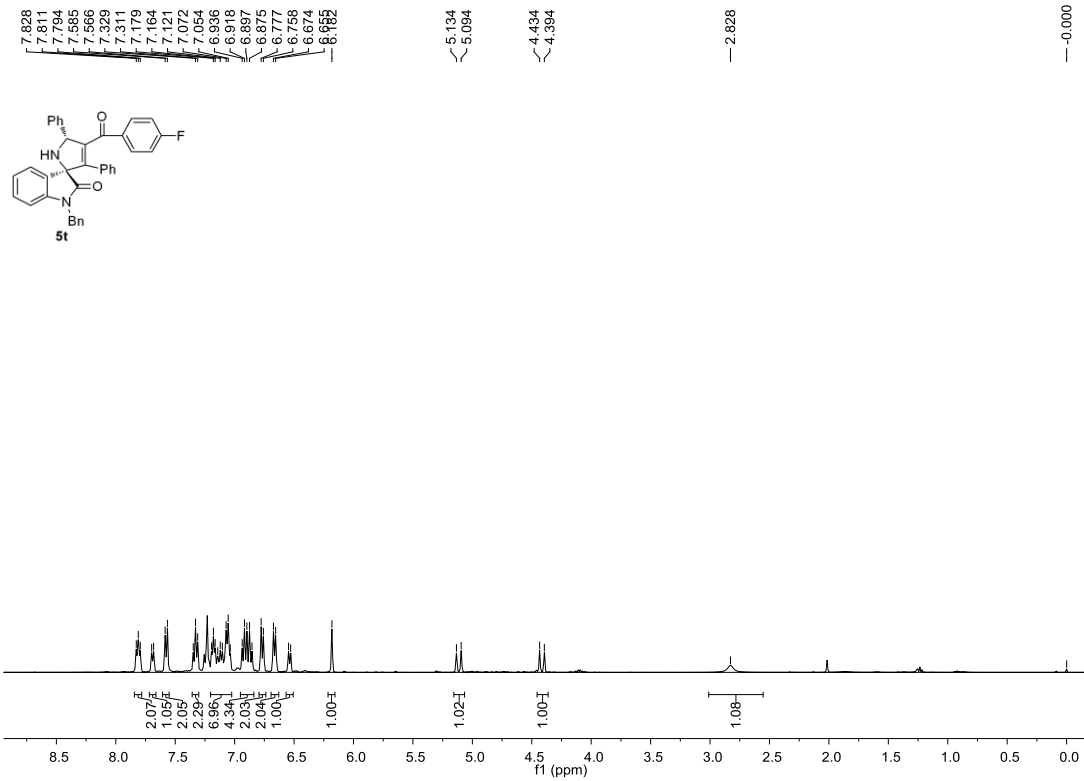
129.03
128.72
128.54
128.24
127.88
127.49
127.45
126.96
126.89
125.17
77.87
71.03
43.96
Ph
HN
O
Ph
O
S
N
Bn
5s
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)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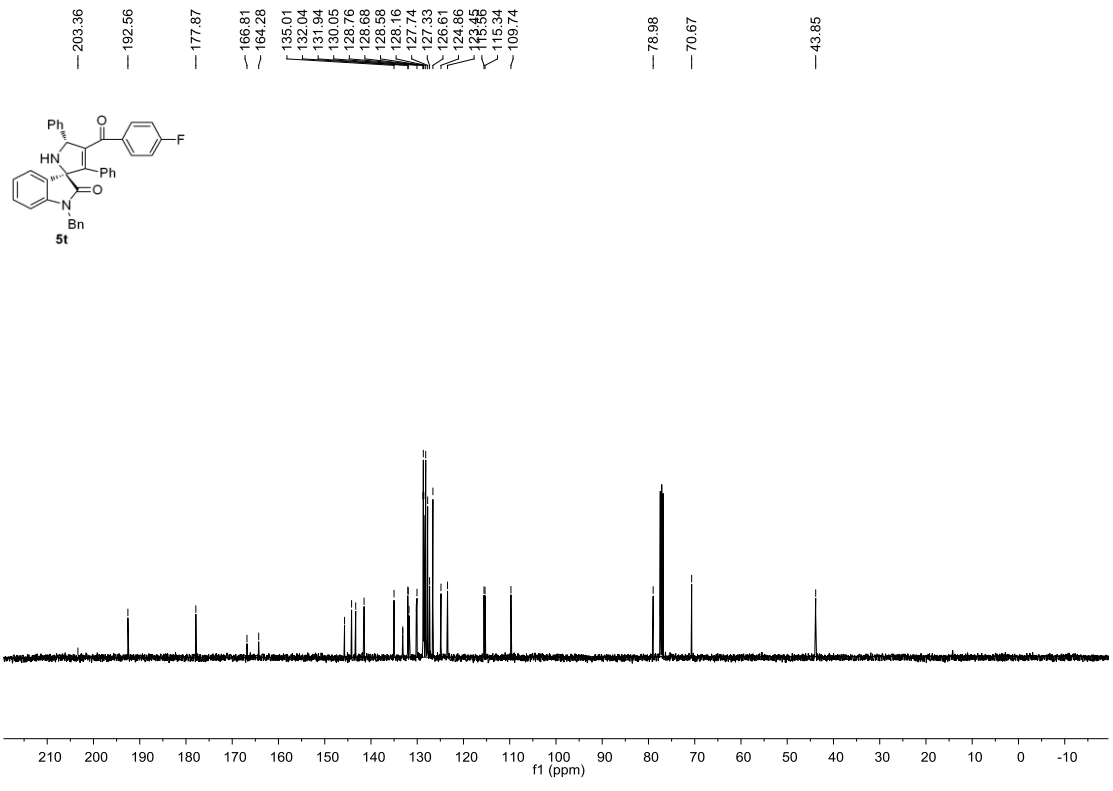
7.811
7.794
7.585
7.566
7.329
7.311
7.179
7.164
7.121
7.072
7.054
6.936
6.918
6.897
6.875
6.777
6.758
6.674
5.134
5.094
4.434
4.394
2.828
-0.000
Ph
O
F
HN
Ph
O
N
Bn
5t
2.07
1.05
2.05
2.29
6.96
4.34
2.03
2.04
1.00
1.00
1.02
1.00
1.08
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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131.94
130.05
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128.68
128.58
128.16
127.74
127.33
126.61
124.86
123.45
115.56
115.34
109.74
78.98
70.67
43.85
Ph
O
F
HN
Ph
O
N
Bn
5t
210
200
190
180
170
160
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140
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120
110
100
90
80
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60
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40
30
20
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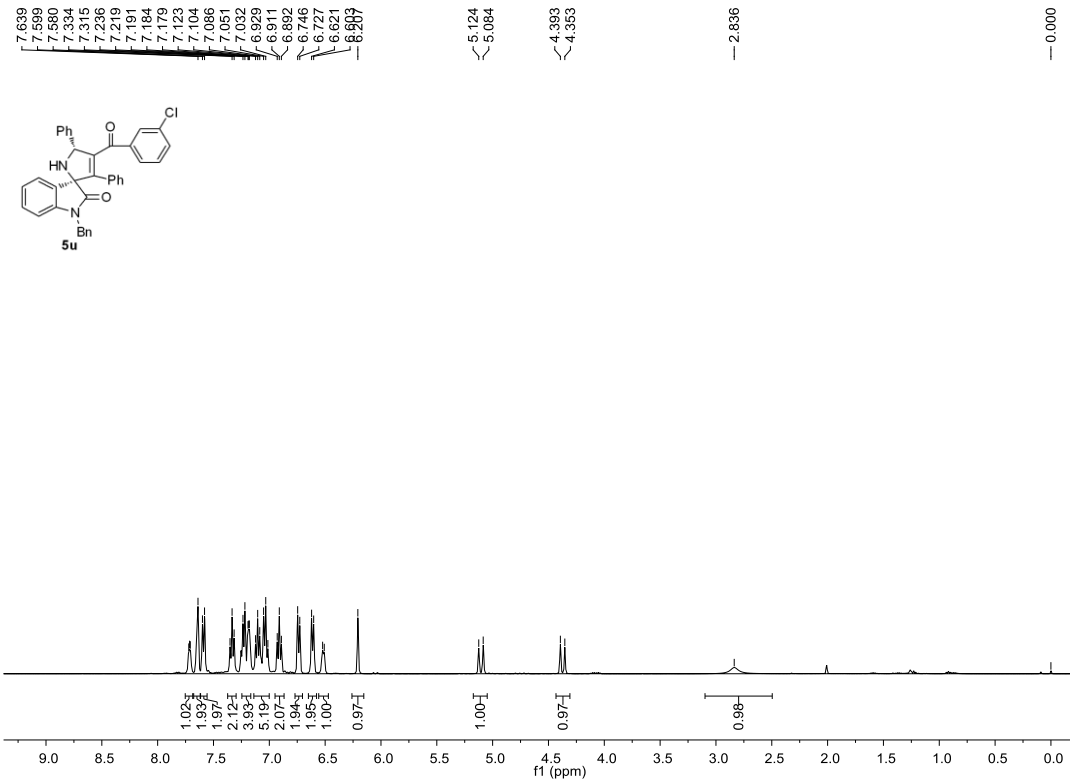
0
-10
f1 (ppm)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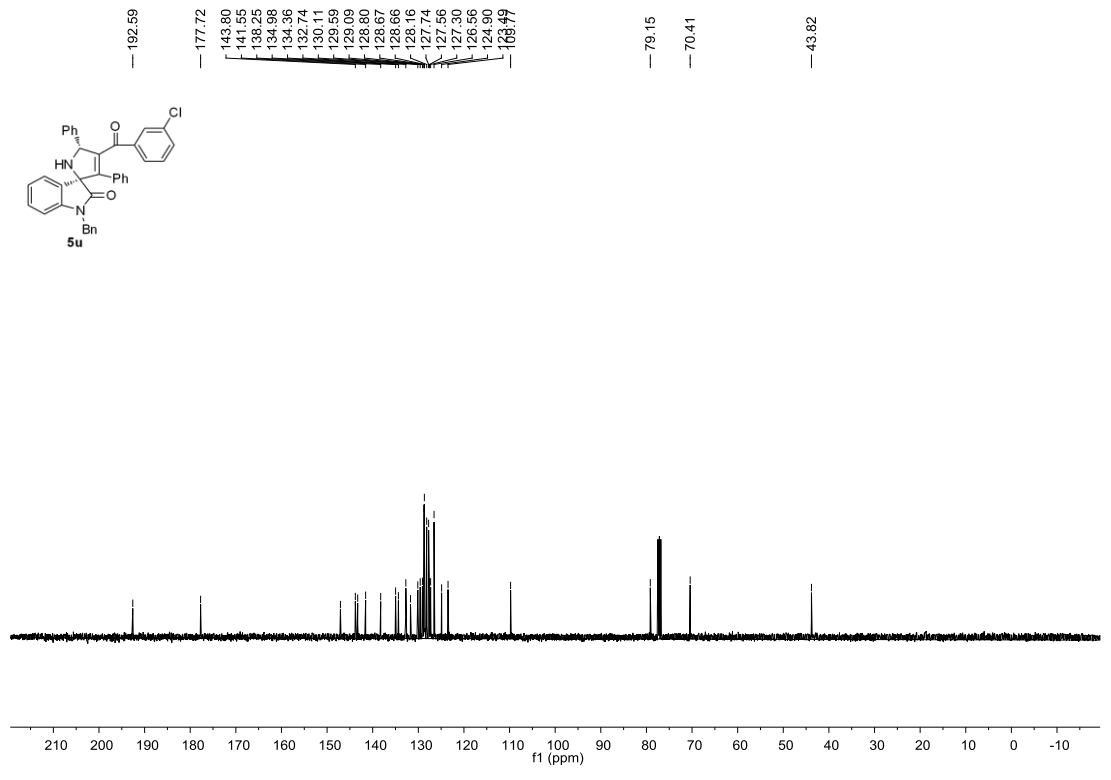
7.599
7.580
7.334
7.315
7.236
7.219
7.191
7.184
7.179
7.123
7.104
7.086
7.051
7.032
6.929
6.911
6.892
6.746
6.727
6.621
6.603
6.007
5.124
5.084
4.393
4.353
2.836
0.000
Ph
O
Cl
HN
Ph
O
N
Bn
5u
1.02
1.93
1.97
2.12
3.93
5.19
2.07
1.94
1.95
1.00
0.97
1.00
0.97
0.98
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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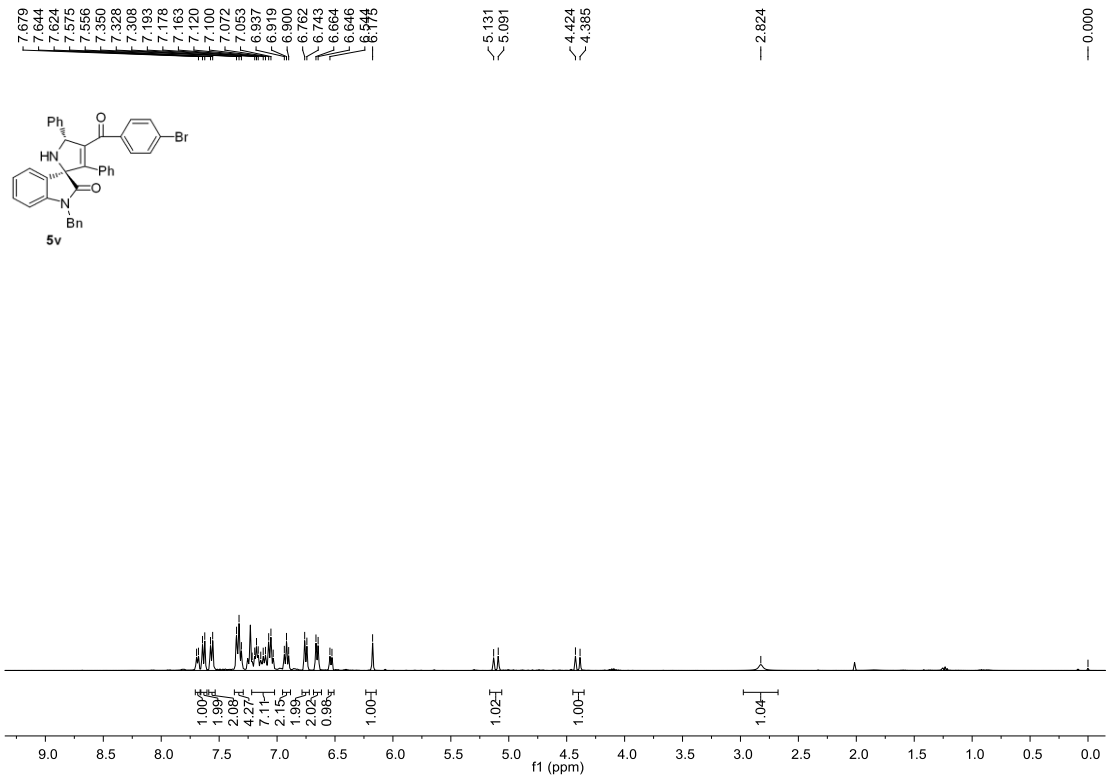
134.98
134.36
132.74
130.11
129.59
129.09
128.80
128.67
128.66
128.16
127.74
127.56
127.30
126.56
124.90
123.49
79.15
70.41
43.82
Ph
O
Cl
HN
Ph
O
N
Bn
5u
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)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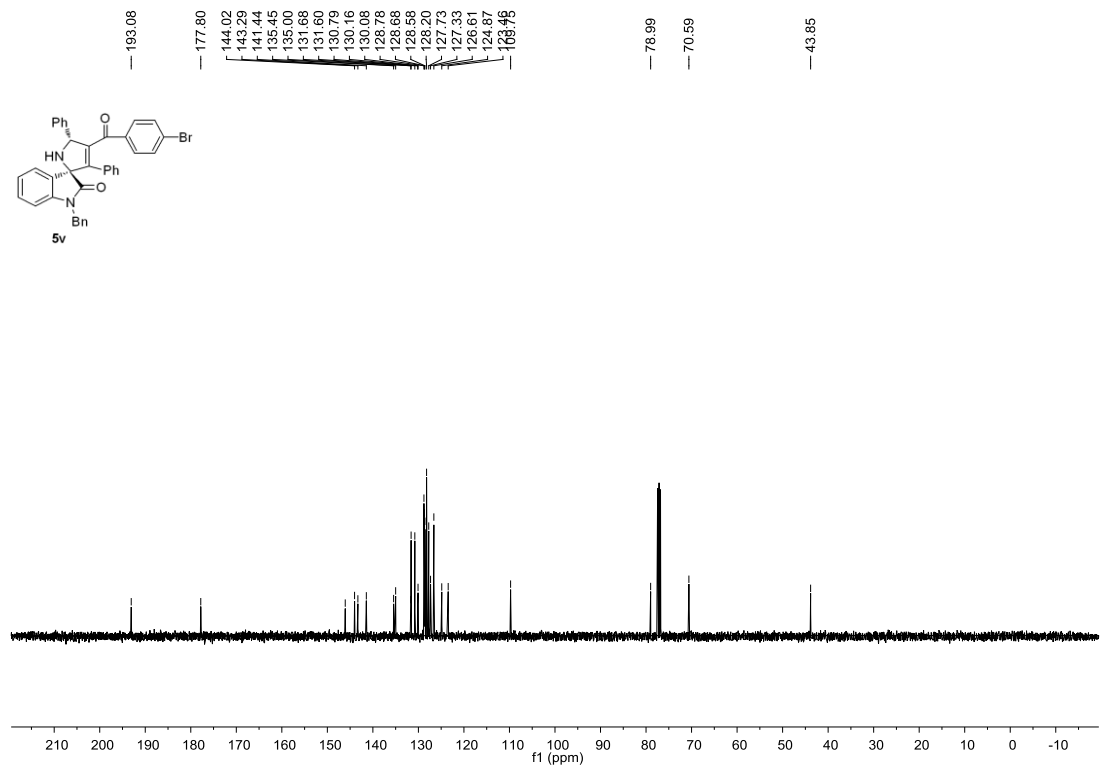
7.624
7.575
7.556
7.350
7.328
7.308
7.193
7.178
7.163
7.120
7.100
7.072
7.053
6.937
6.919
6.900
6.762
6.743
6.664
6.646
6.175
5.131
5.091
4.424
4.385
2.824
0.000
Ph
HN
O
Br
Ph
O
N
Bn
5v
1.00
1.99
2.08
4.27
7.11
2.15
1.99
2.02
0.98
1.00
1.02
1.00
1.04
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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135.45
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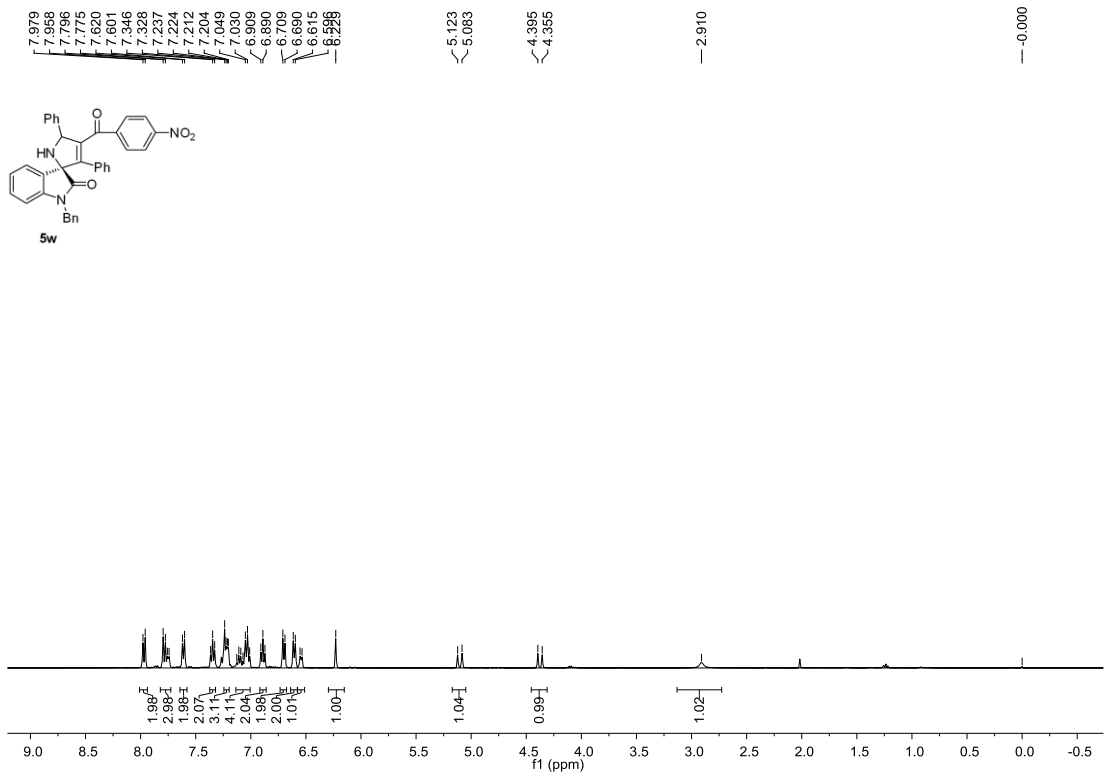
131.68
131.60
130.79
130.16
130.08
128.78
128.68
128.58
128.20
127.73
127.33
126.61
124.87
78.99
70.59
43.85
Ph
HN
O
Br
Ph
O
N
Bn
5v
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)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7.601
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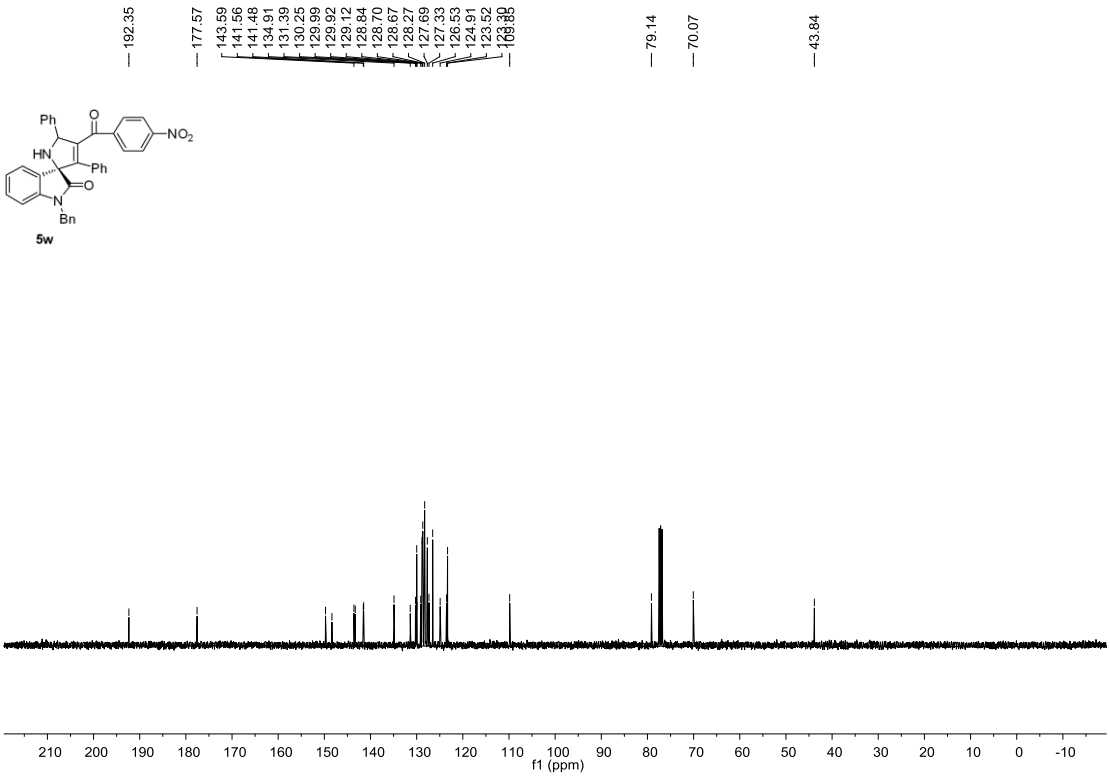
7.328
7.237
7.224
7.212
7.204
7.049
7.030
6.909
6.890
6.709
6.690
6.615
6.596
6.229
5.123
5.083
4.395
4.355
2.910
-0.000
Ph
HN
O
NO2
Ph
O
N
Bn
5w
1.98
2.98
1.98
2.07
3.11
4.04
1.98
2.00
1.01
1.00
1.04
0.99
1.02
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)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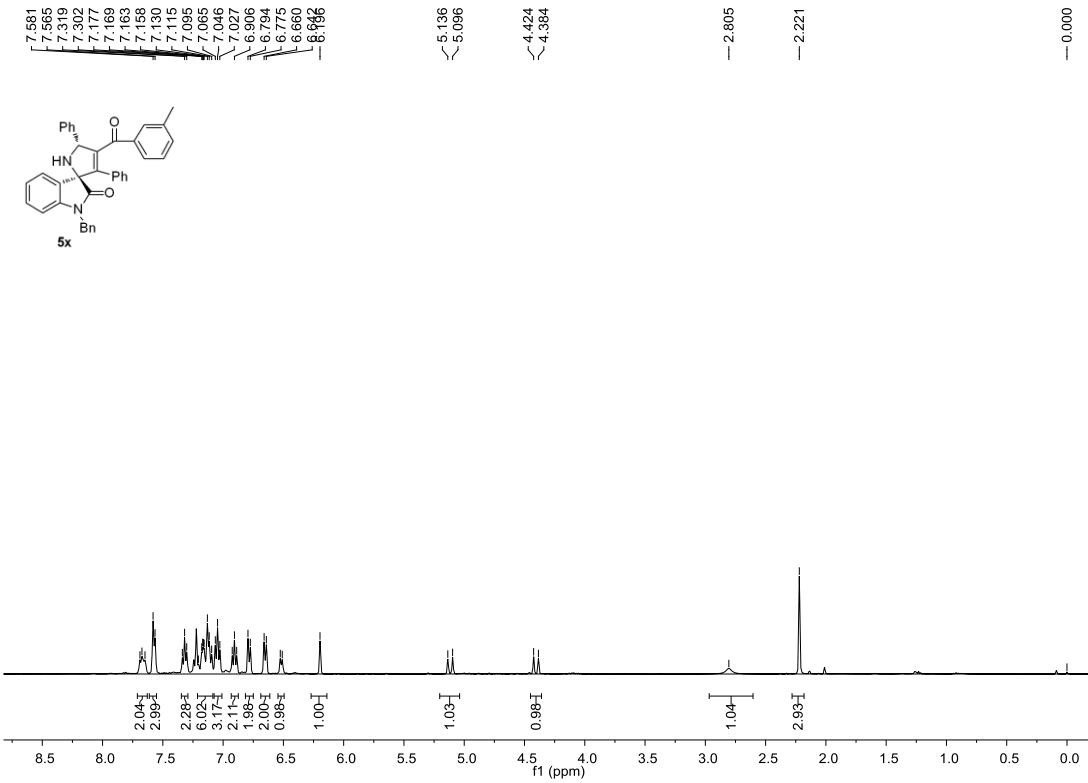
128.84
128.70
128.67
128.27
127.69
127.33
126.53
124.91
123.52
123.30
79.14
70.07
43.84
Ph
HN
O
NO2
Ph
O
N
Bn
5w
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)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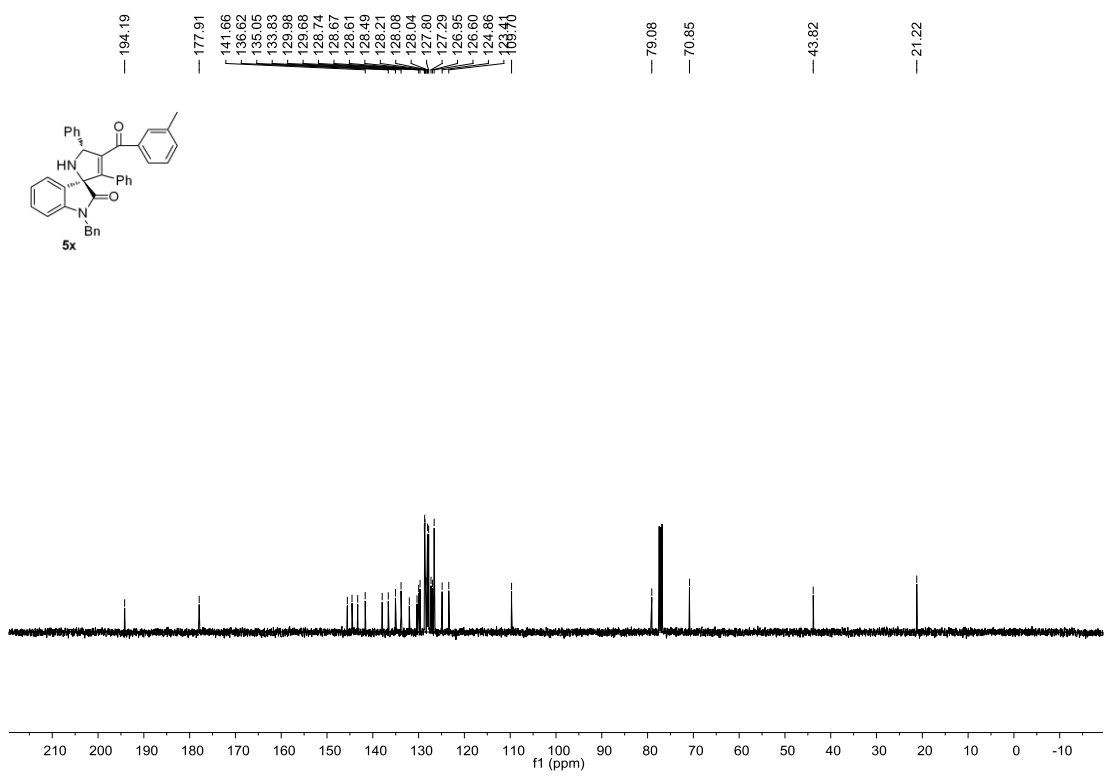
7.319
7.302
7.177
7.169
7.163
7.158
7.130
7.115
7.095
7.065
7.046
7.027
6.906
6.794
6.775
6.660
5.136
5.096
4.424
4.384
2.805
2.221
0.000
Ph
HN
O
Ph
O
N
Bn
5x
2.04
2.99
2.28
6.02
3.17
2.11
1.98
2.00
0.98
1.00
1.03
0.98
1.04
2.93
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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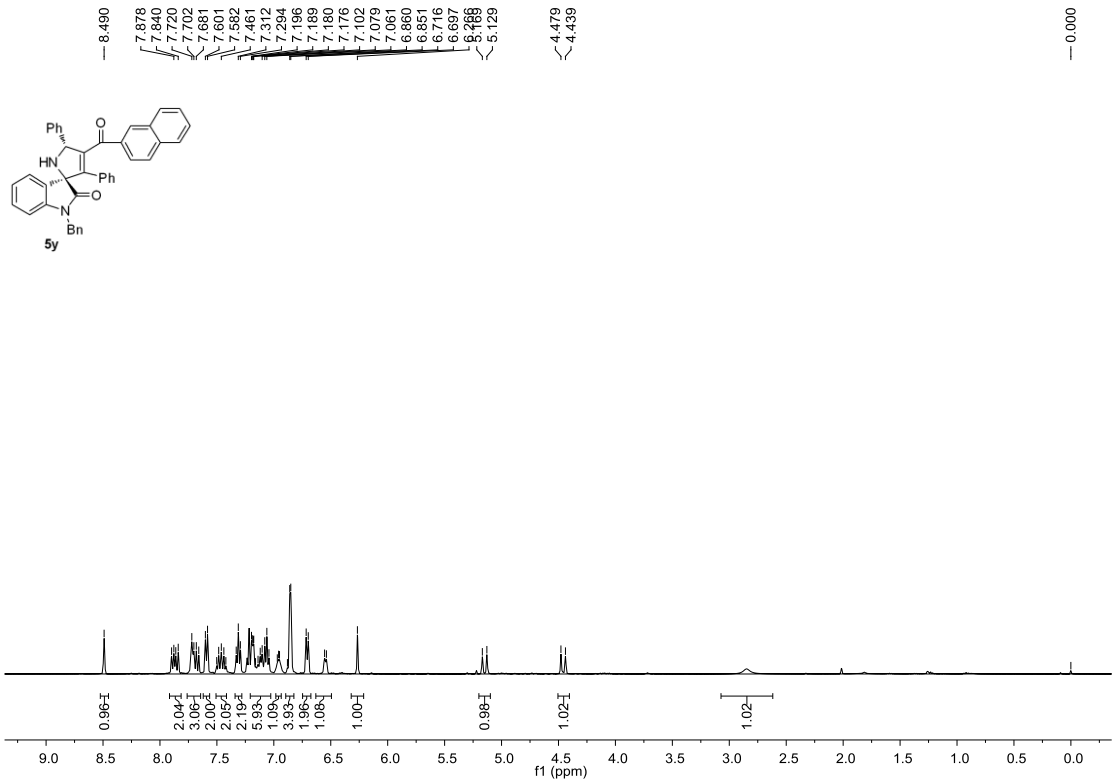
128.21
128.08
128.04
127.80
127.29
126.95
126.60
124.86
123.41
79.08
70.85
43.82
21.22
Ph
HN
O
Ph
O
N
Bn
5x
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)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7.582
7.461
7.312
7.294
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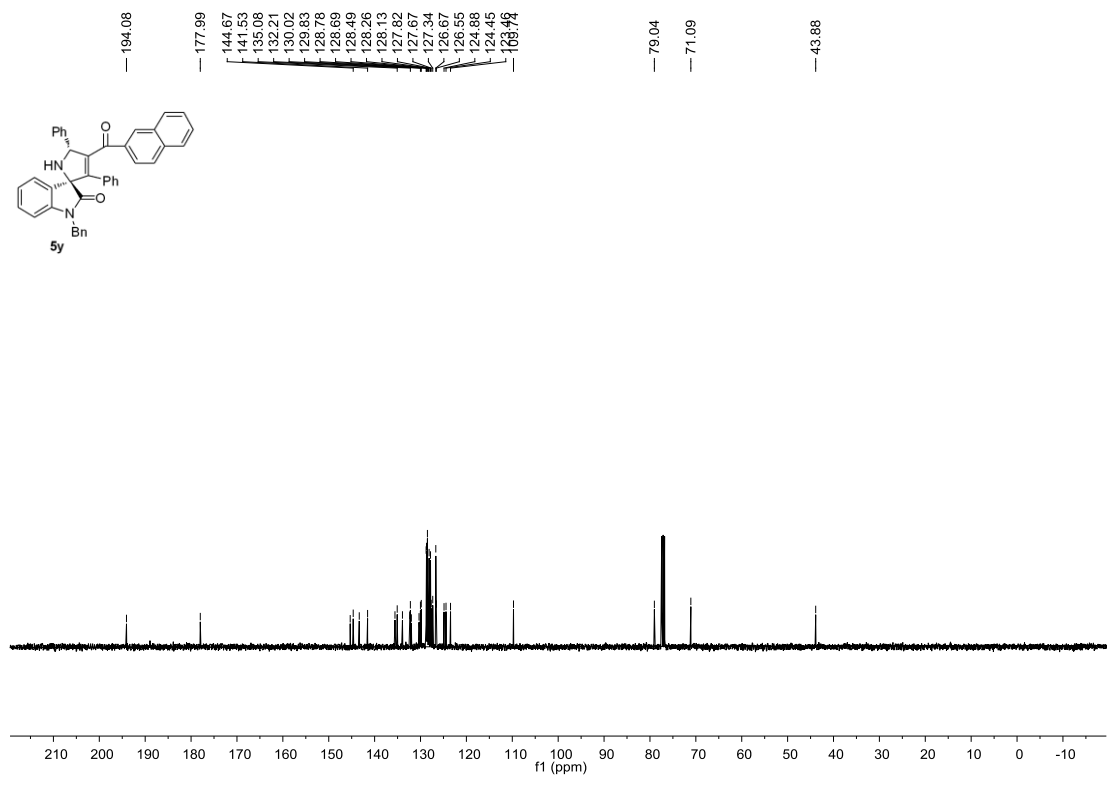
7.189
7.180
7.176
7.102
7.079
7.061
6.860
6.851
6.716
6.697
5.129
4.479
4.439
0.000
Ph
HN
O
Ph
O
N
Bn
5y
0.96
2.04
3.06
2.00
2.05
2.19
5.93
1.09
3.93
1.96
1.08
1.00
0.98
1.02
1.02
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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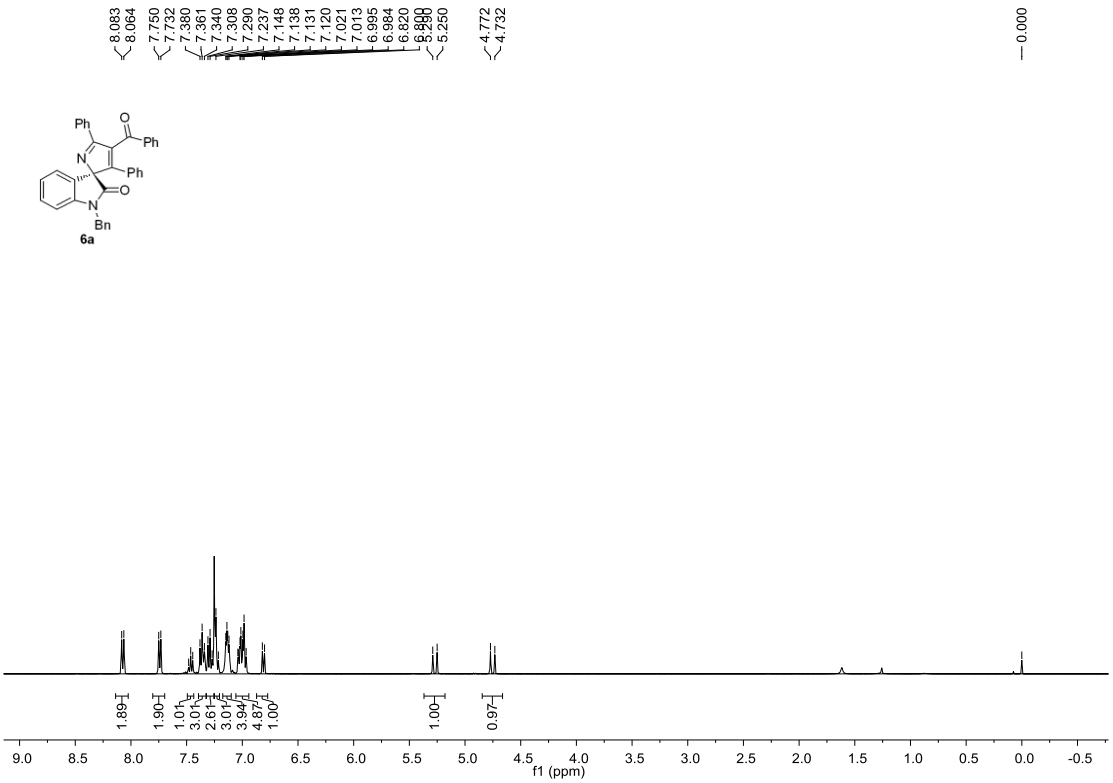
141.53
135.08
132.21
130.02
129.83
128.78
128.69
128.49
128.26
128.13
127.82
127.67
127.34
126.67
126.55
124.88
124.45
79.04
71.09
43.88
Ph
HN
O
Ph
O
N
Bn
5y
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)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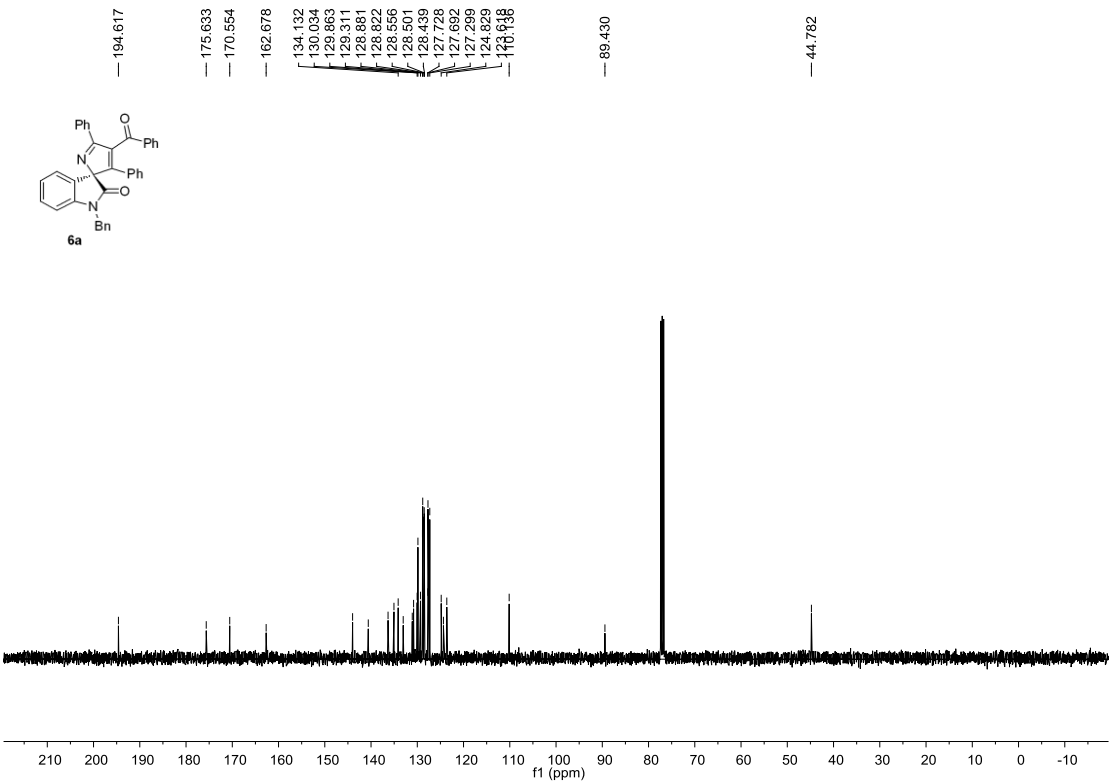
7.308
7.290
7.237
7.148
7.138
7.131
7.120
7.021
7.013
6.995
6.984
6.820
5.250
4.772
4.732
0.000
Ph
O
Ph
N
Ph
O
N
Bn
6a
1.89
1.90
1.01
3.01
2.61
3.01
3.94
4.87
1.00
1.00
0.97
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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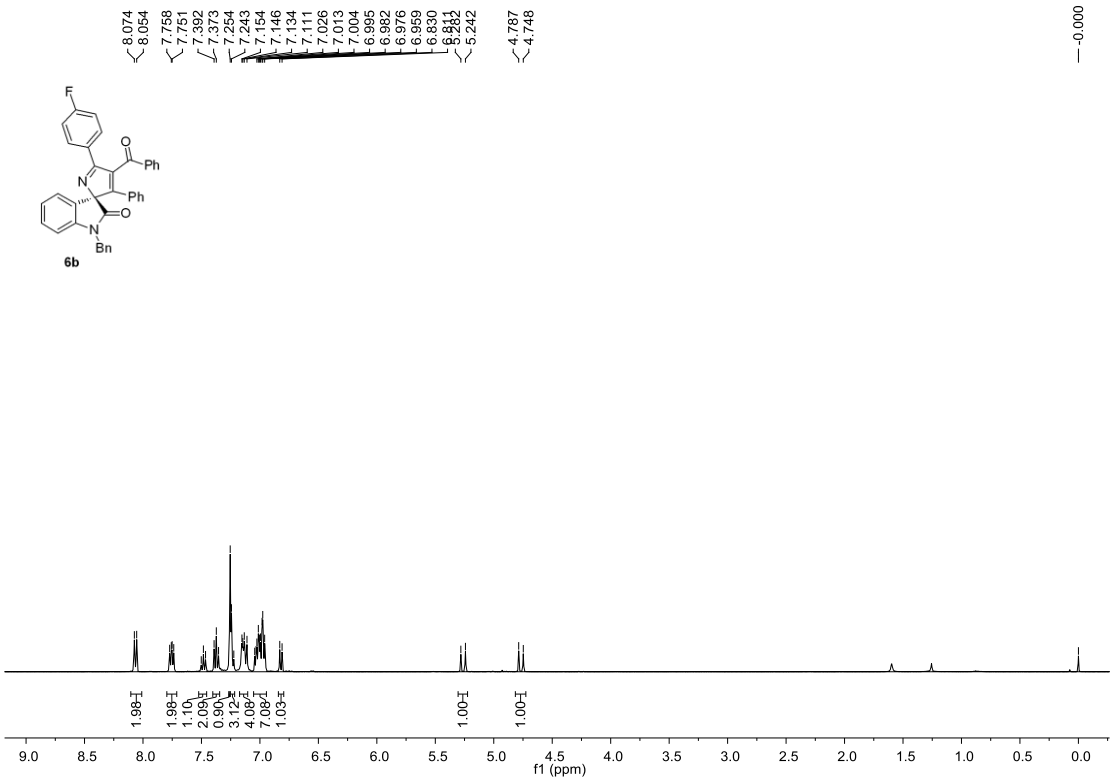
128.822
128.556
128.501
128.439
127.728
127.692
127.299
124.829
123.618
110.138
89.430
44.782
Ph
O
Ph
N
Ph
O
N
Bn
6a
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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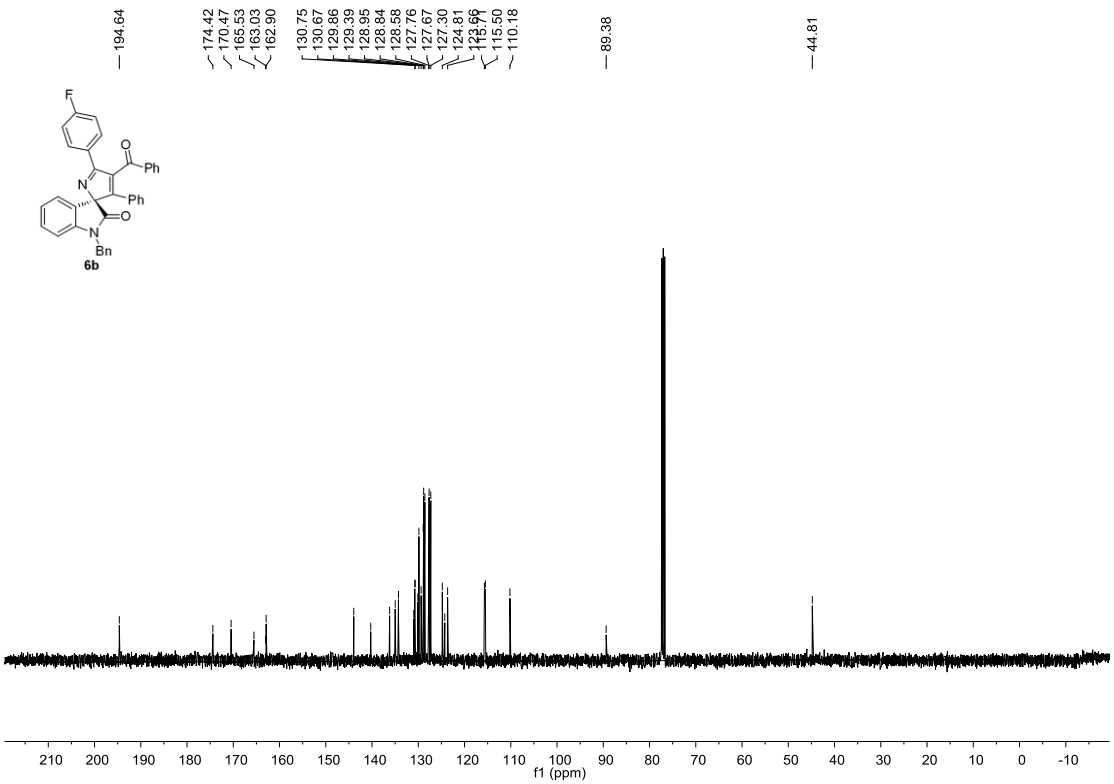
7.154
7.146
7.134
7.111
7.026
7.013
7.004
6.995
6.982
6.976
6.959
6.830
6.811
5.282
5.242
4.787
4.748
-0.000
F
O
Ph
N
Ph
O
N
Bn
6b
1.98
1.98
1.10
2.09
0.90
3.12
4.08
7.08
1.03
1.00
1.00
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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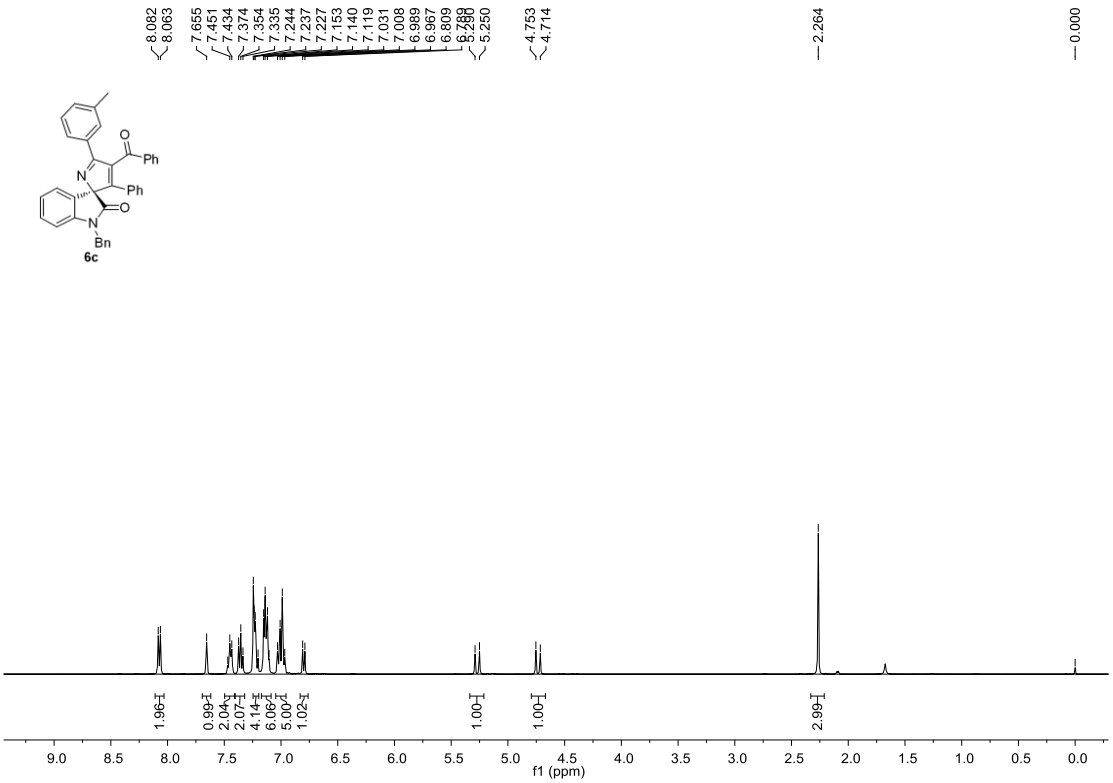
128.58
127.76
127.67
127.30
124.81
123.66
115.71
115.50
110.18
89.38
44.81
F
O
Ph
N
Ph
O
N
Bn
6b
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)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7.374
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7.335
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7.237
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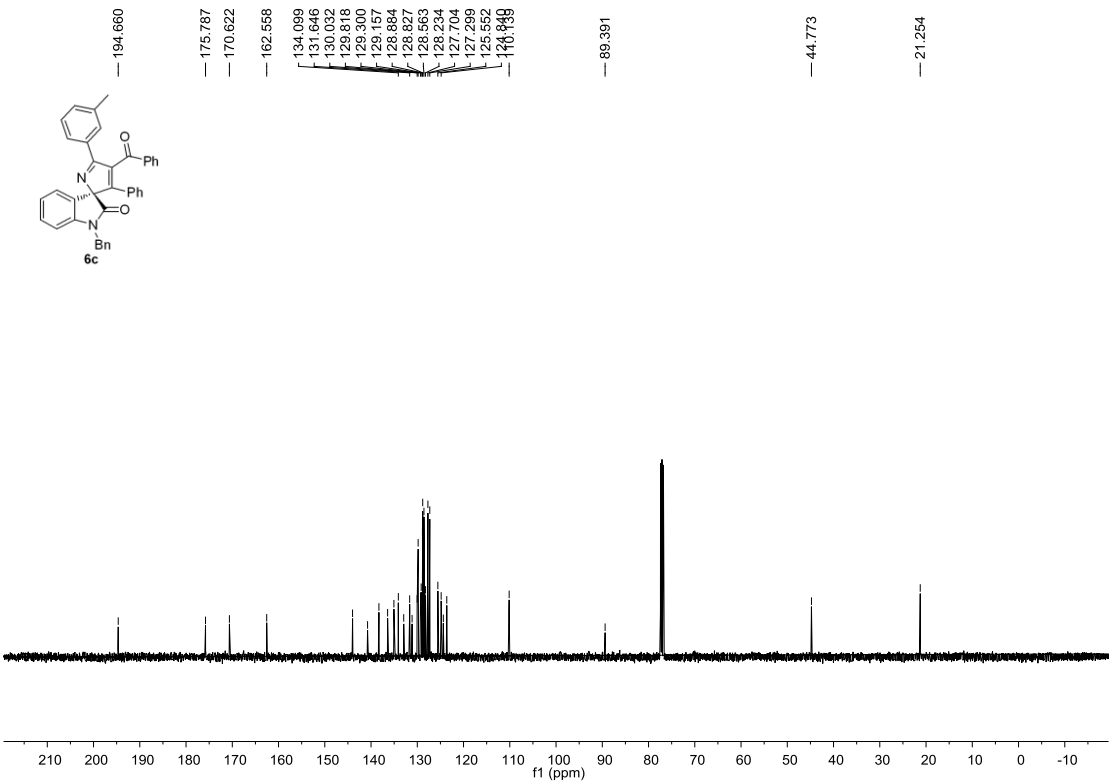
7.153
7.140
7.119
7.031
7.008
6.989
6.967
6.809
6.788
5.290
5.250
4.753
4.714
2.264
0.000
O
Ph
N
Ph
O
N
Bn
6c
1.96
0.99
2.04
2.07
4.14
6.06
5.00
1.02
1.00
1.00
2.99
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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162.558
134.099
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129.157
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128.563
128.234
127.704
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125.552
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110.139
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44.773
21.254
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Ph
N
Ph
O
N
Bn
6c
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200
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180
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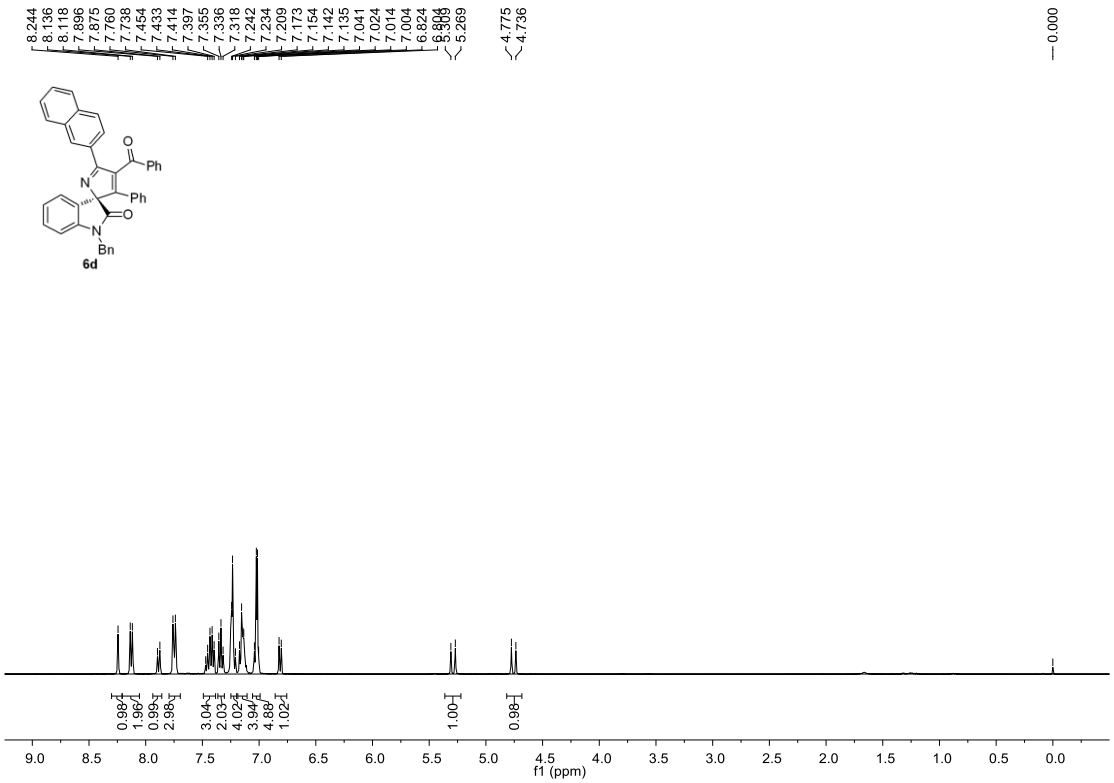
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7.004
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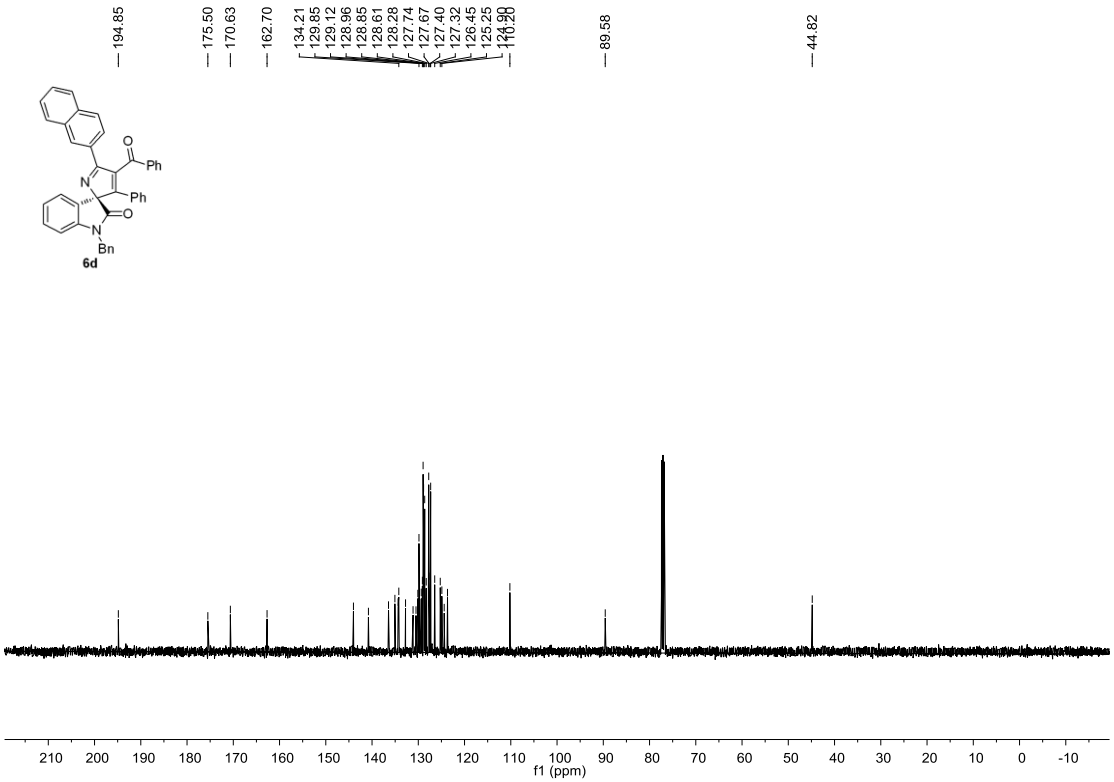
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127.40
127.32
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44.82
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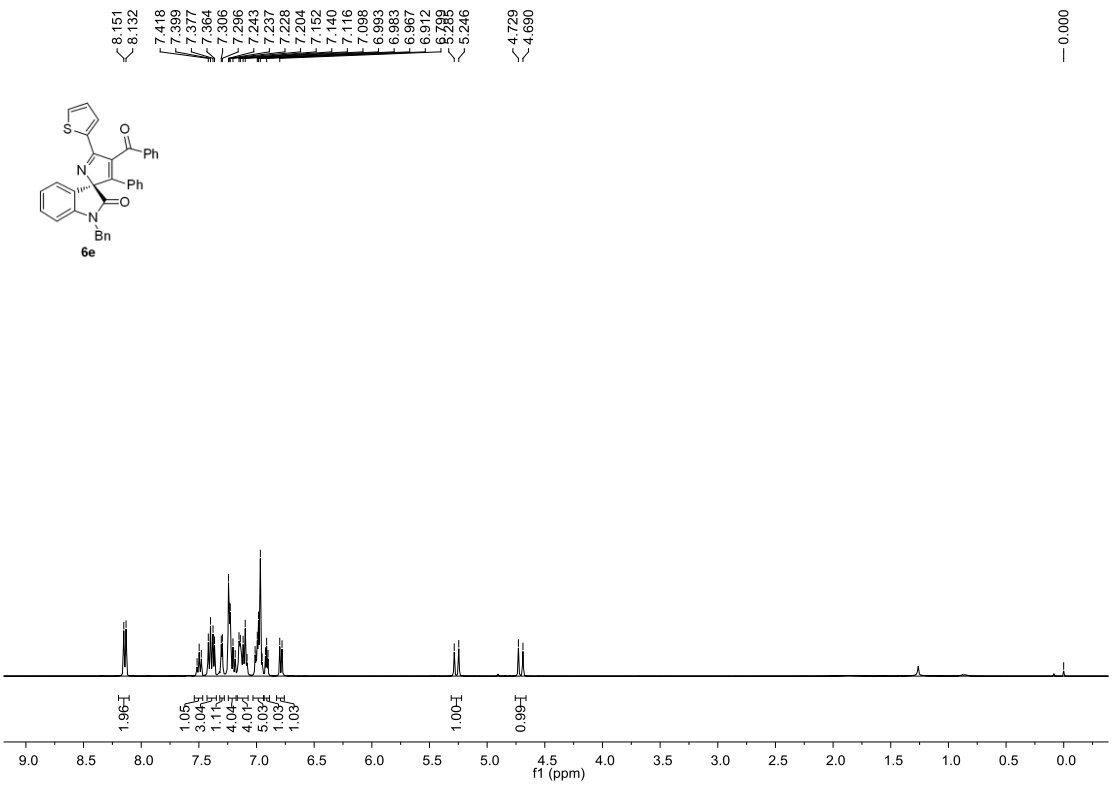
Ph
N
Ph
O
N
Bn
6d
f1 (ppm)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7.237
7.228
7.204
7.152
7.140
7.116
7.098
6.993
6.983
6.967
6.912
5.285
5.246
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4.690
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Ph
Bn
6e
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1.03
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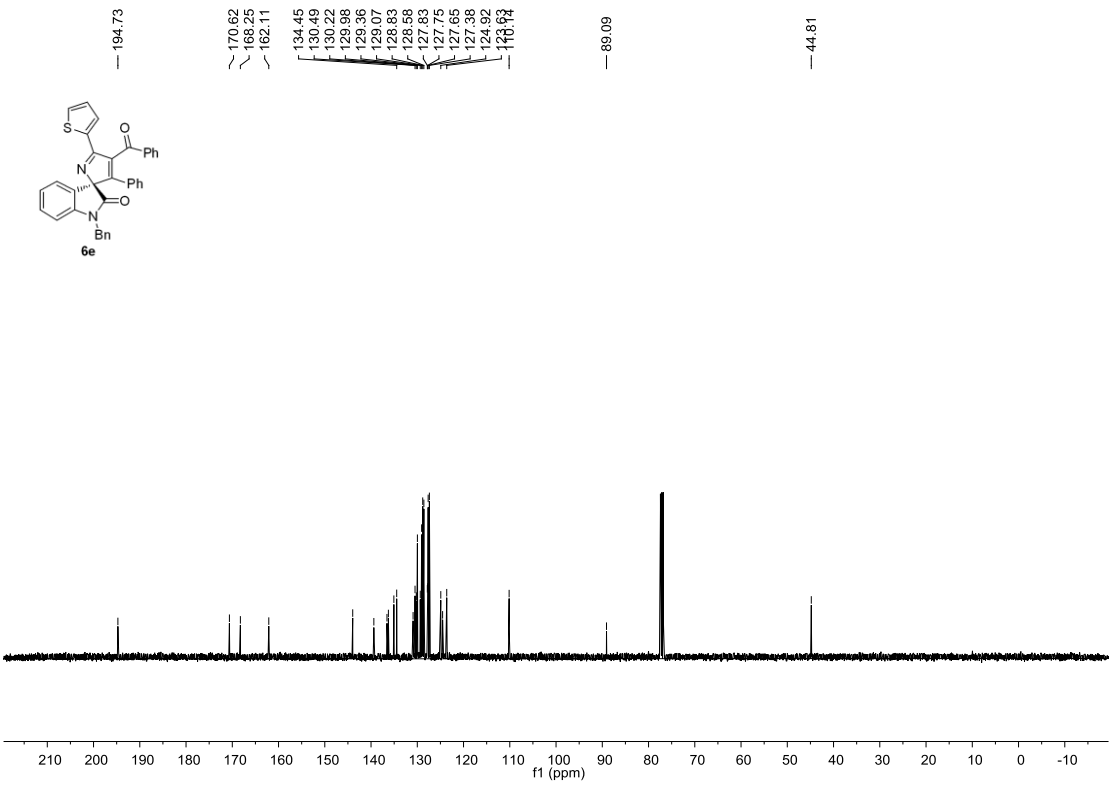
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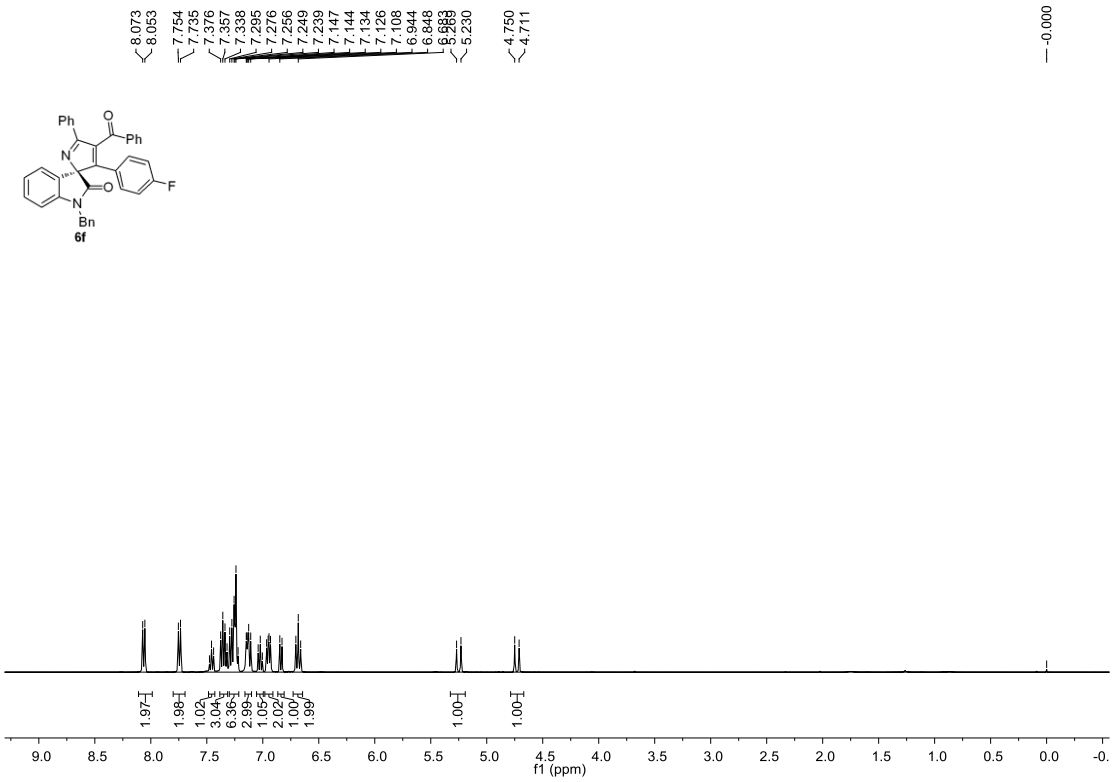
6e
f1 (ppm)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7.134
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5.289
5.230
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4.711
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O
Ph
N
O
F
N
Bn
6f
1.97
1.98
1.02
3.04
6.36
2.99
1.05
2.02
1.00
1.99
1.00
1.00
9.0
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8.0
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7.0
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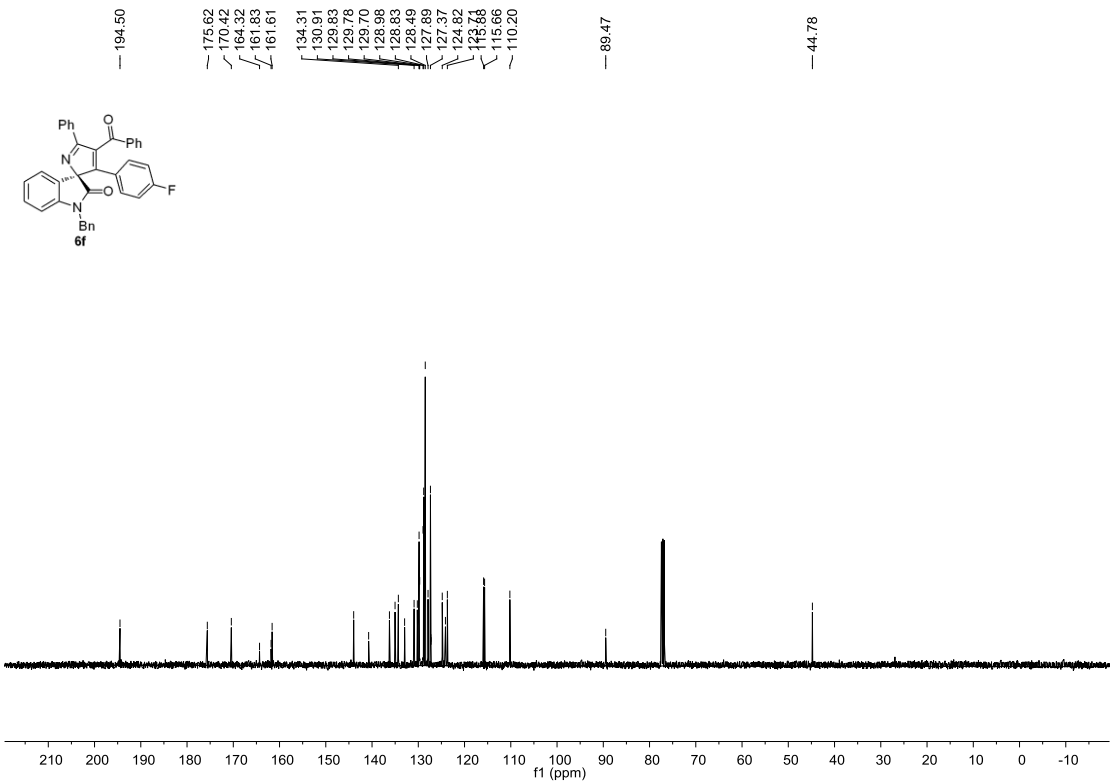
f1 (ppm)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128.49
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127.37
124.82
123.71
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115.66
110.20
89.47
44.78
Ph
O
Ph
N
O
F
N
Bn
6f
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200
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180
170
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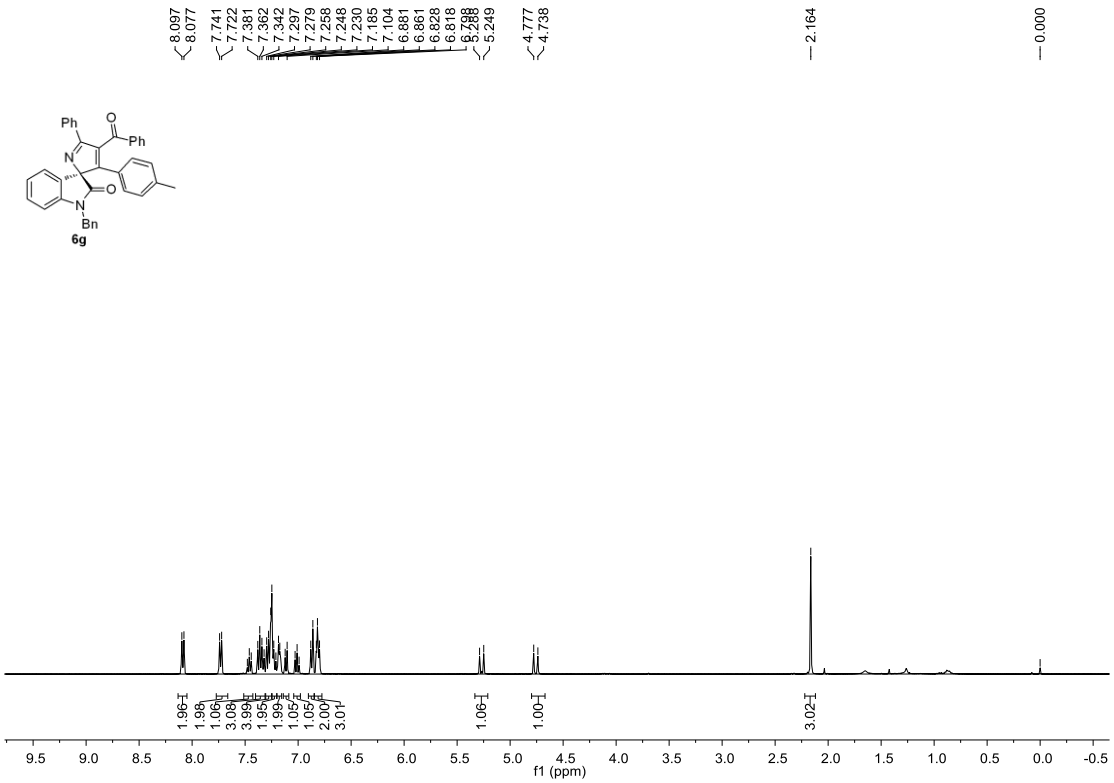
f1 (ppm)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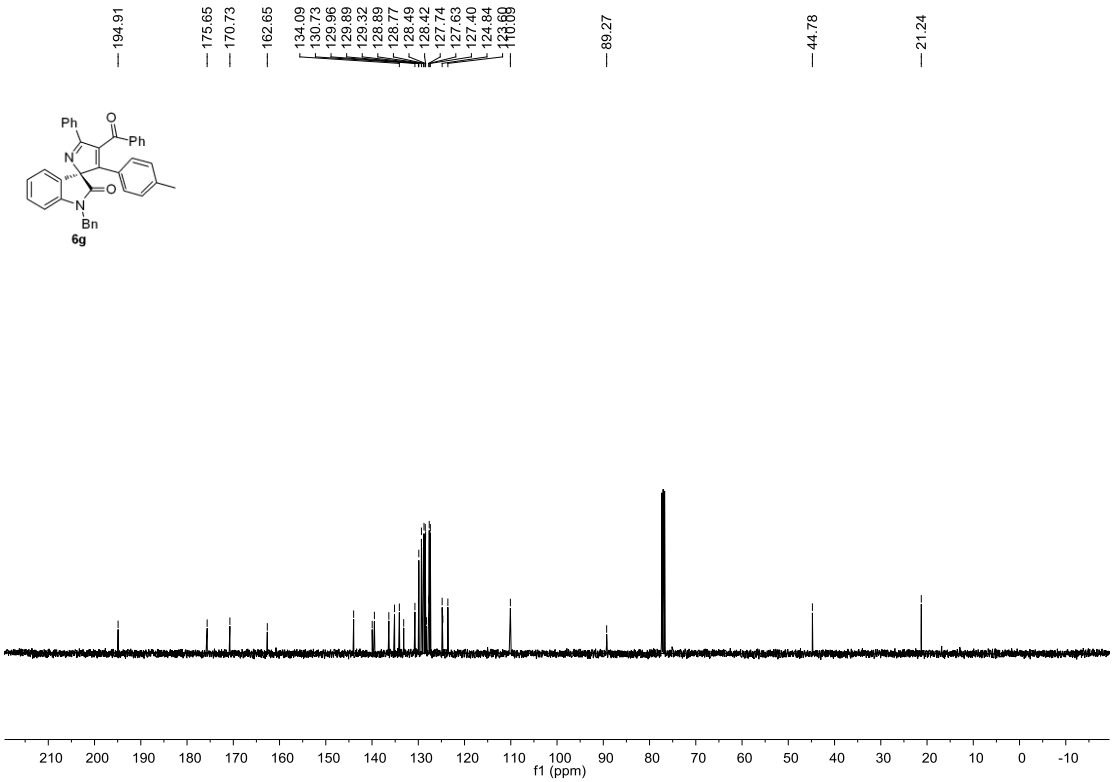
6.818
5.288
5.249
4.777
4.738
2.164
0.000
Ph
O
Ph
N
O
N
Bn
6g
1.96
1.96
1.06
3.08
3.99
1.95
1.99
1.05
1.05
2.00
3.01
1.06
1.00
3.02
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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128.42
127.74
127.63
127.40
124.84
123.60
110.09
89.27
44.78
21.24
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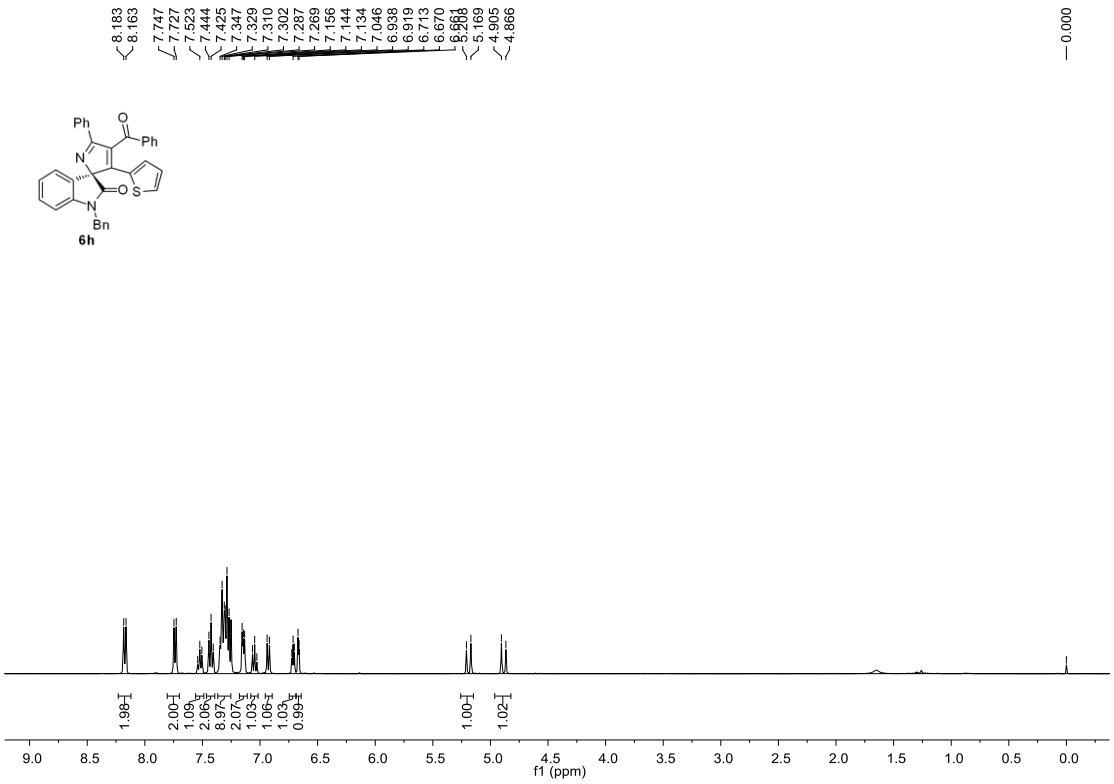
Ph
N
O
N
Bn
6g
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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4.905
4.866
0.000
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Ph
N
O
S
N
Bn
6h
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2.00
1.09
2.06
8.97
2.07
1.03
1.06
1.05
0.99
1.00
1.02
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
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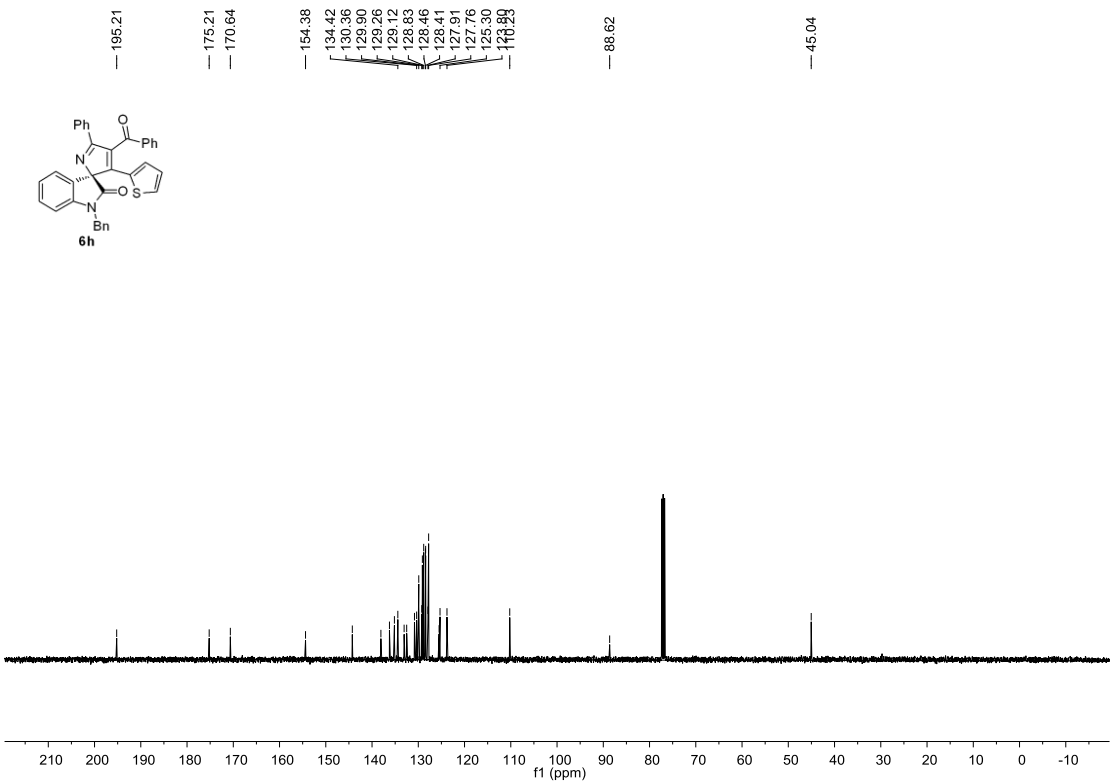
f1 (ppm)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125.30
123.80
110.23
88.62
45.04
Ph
O
Ph
N
O
S
N
Bn
6h
210
200
190
180
170
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120
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100
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80
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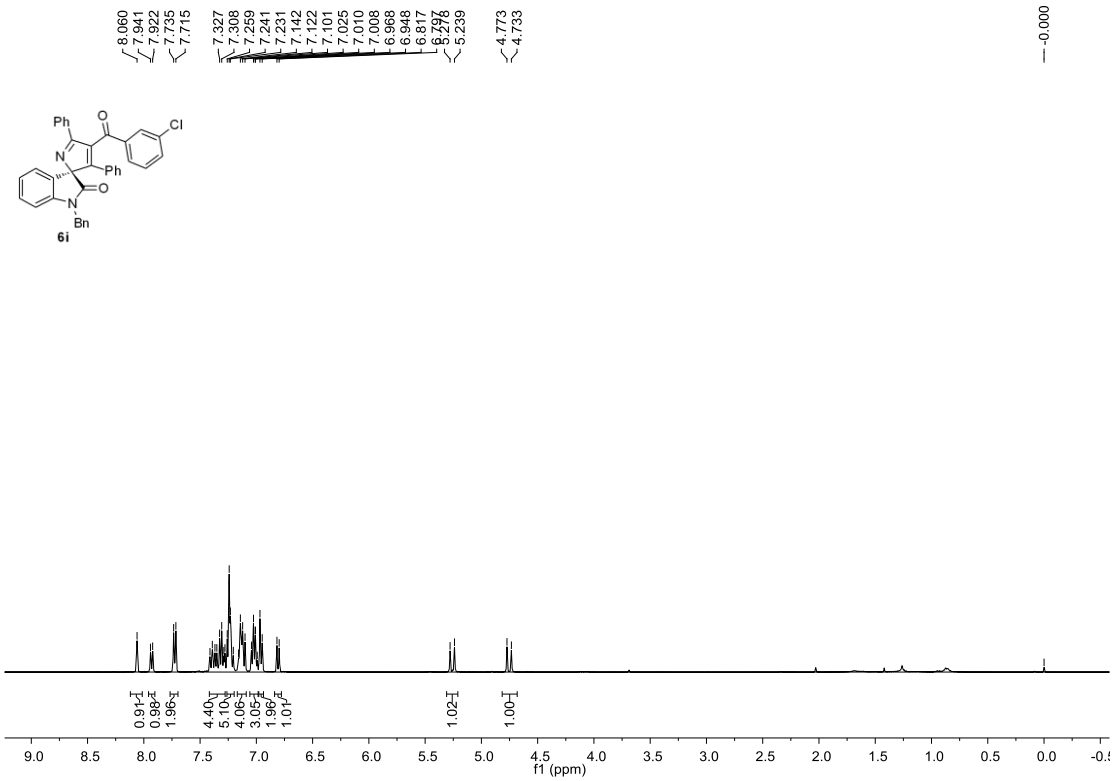
f1 (ppm)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6.948
6.817
5.239
4.773
4.733
-0.000
Ph
O
Cl
N
Ph
O
N
Bn
6i
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0.98
1.96
4.40
5.10
4.06
3.05
1.96
1.01
1.02
1.00
9.0
8.5
8.0
7.5
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6.0
5.5
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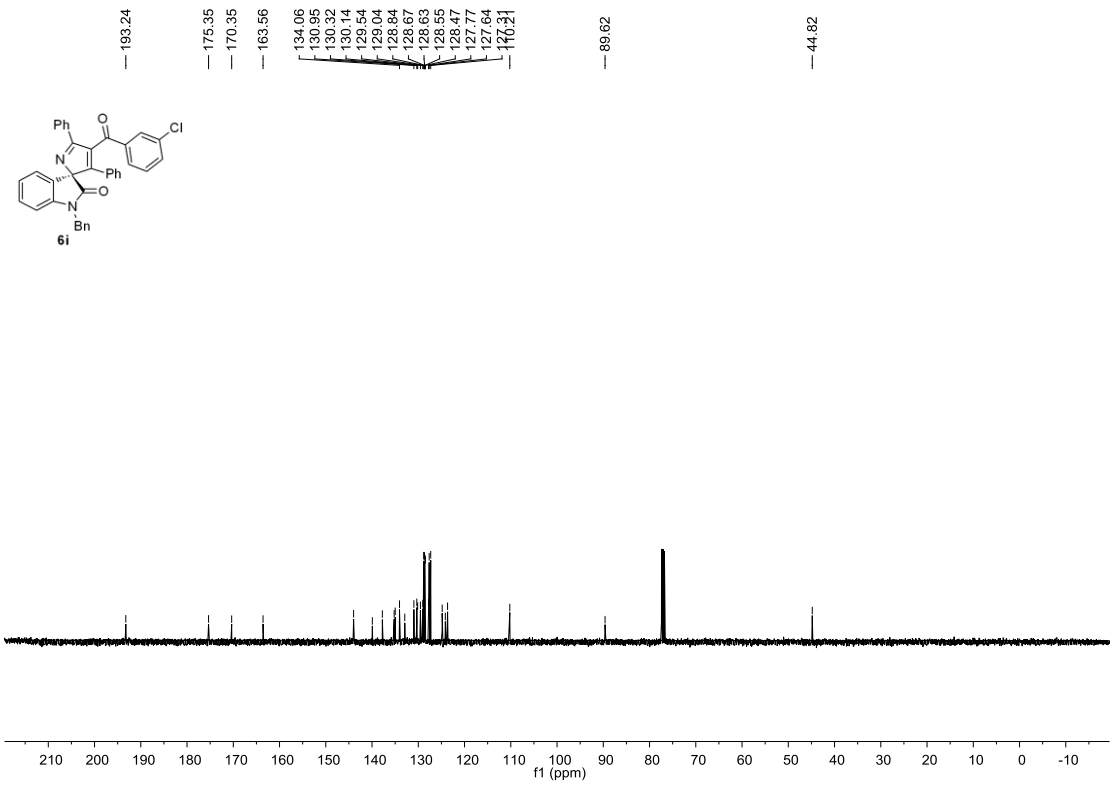
f1 (ppm)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128.55
128.47
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127.64
127.31
127.21
89.62
44.82
Ph
O
Cl
N
Ph
O
N
Bn
6i
210
200
190
180
170
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100
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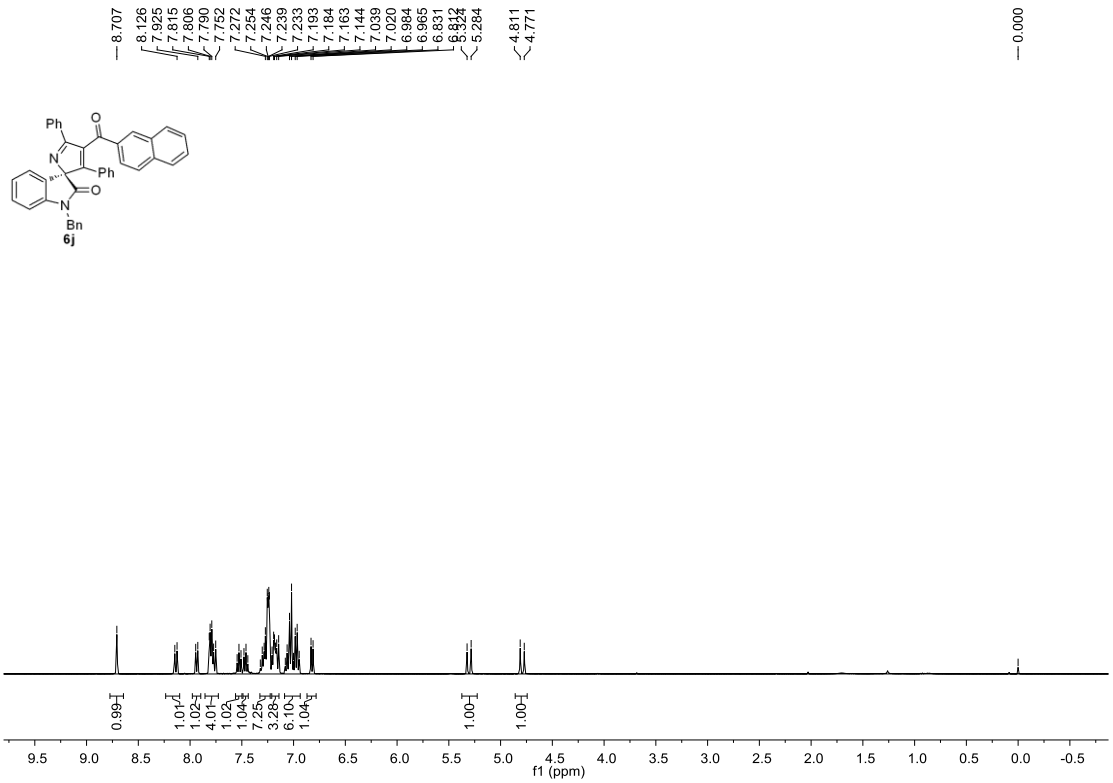
f1 (ppm)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4.811
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Ph
O
N
Bn
6j
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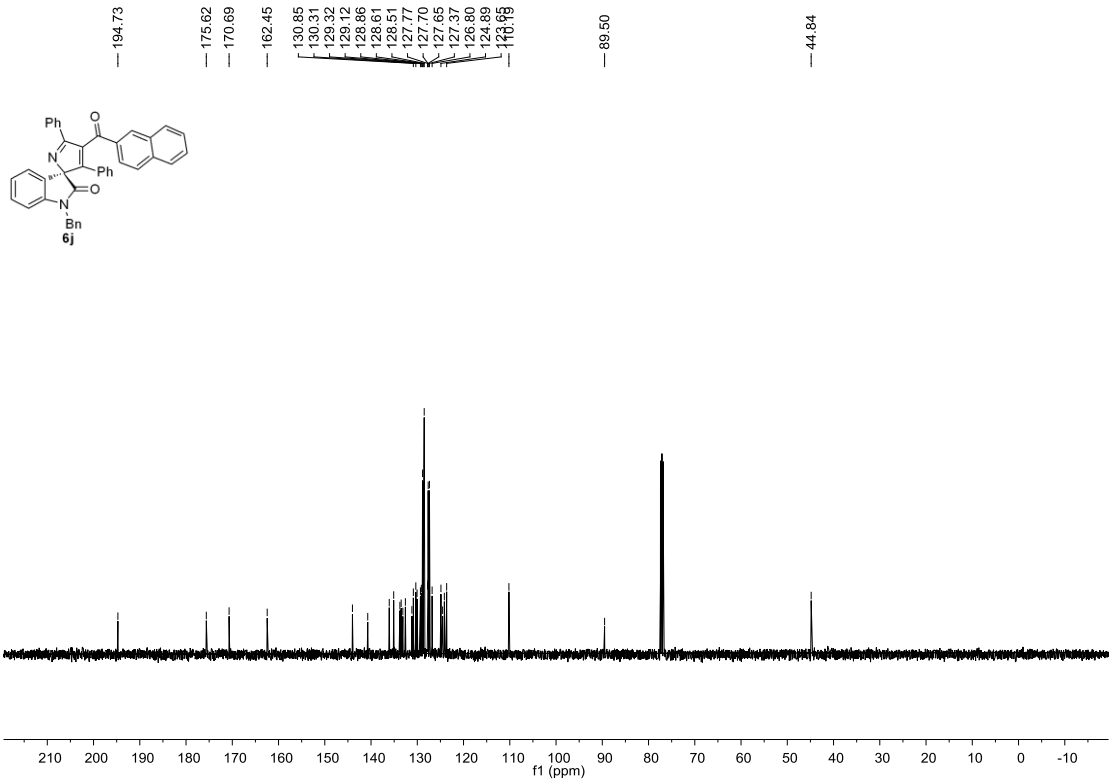
1.01
1.02
4.01
1.02
1.04
7.25
3.28
6.10
1.04
1.00
1.00
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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127.37
126.80
124.89
123.65
110.19
89.50
44.84
Ph
O
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Ph
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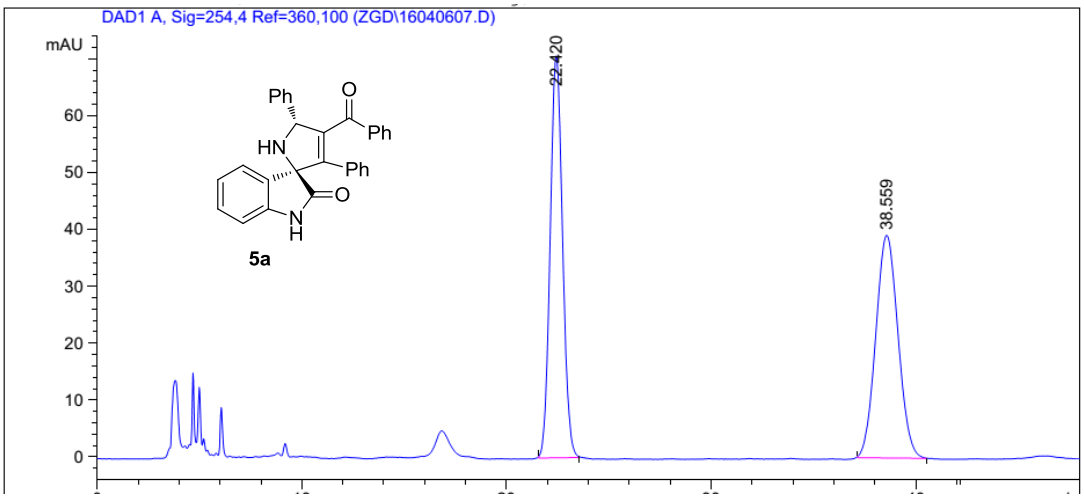
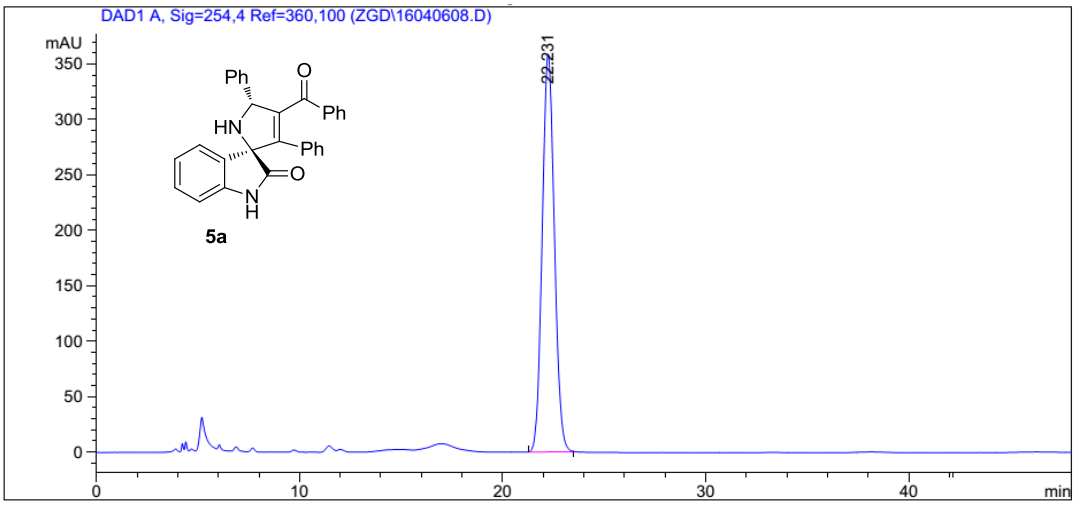
N
Bn
6j
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

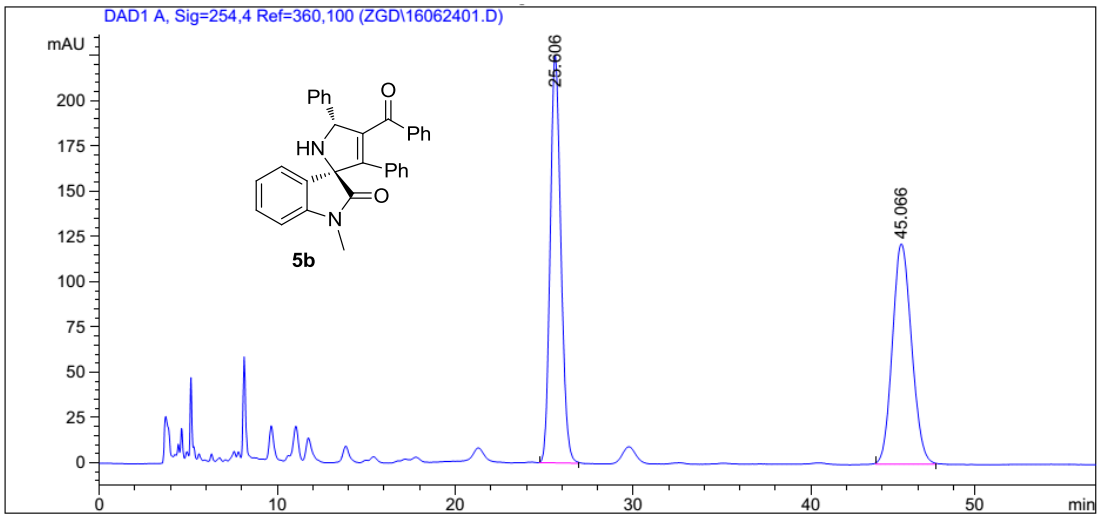
5. Copies of HPLC chromatographs



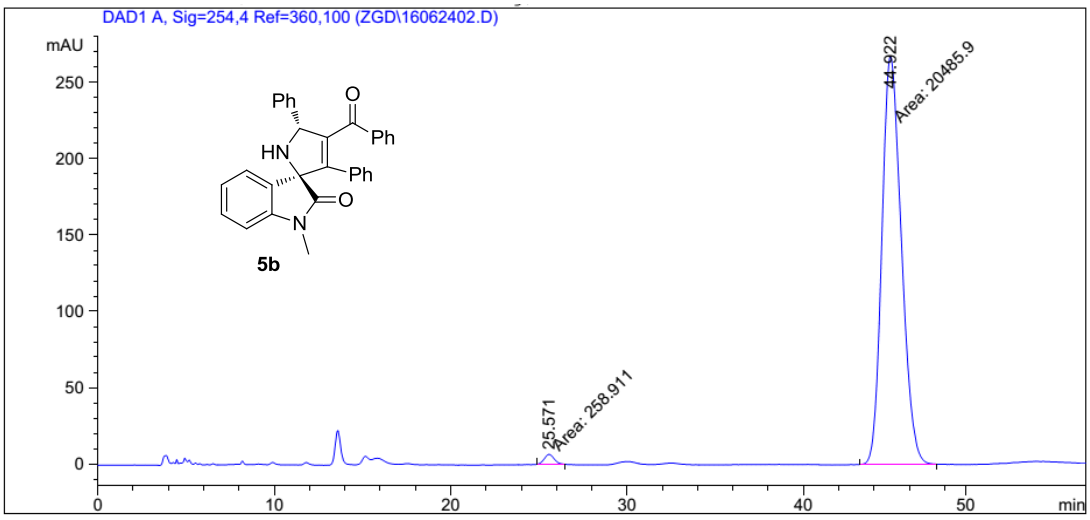
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	22.420	BB	0.6399	2954.66382	70.65221	50.0387
2	38.559	BB	0.9654	2950.09863	39.13935	49.9613



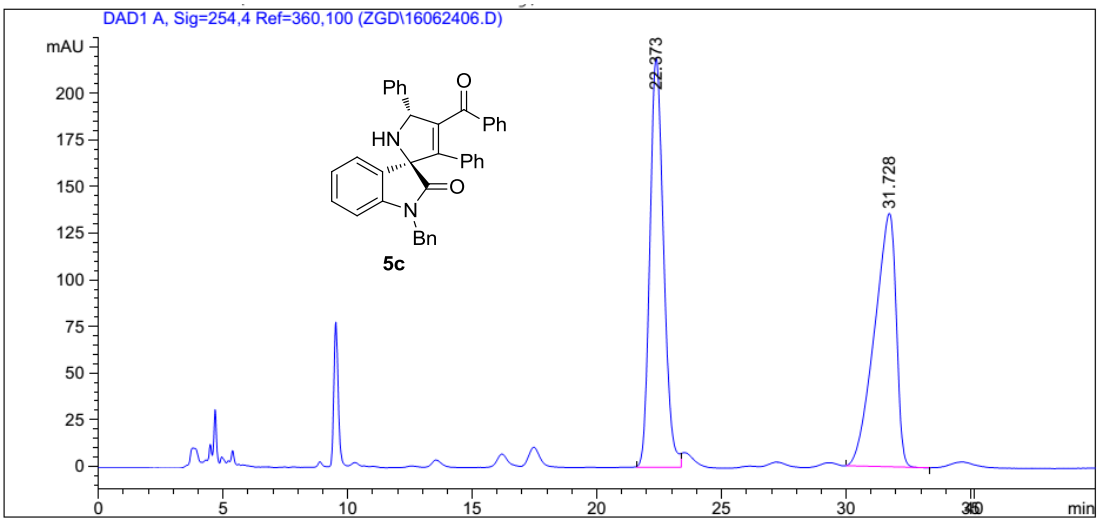
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	22.231	BB	0.6440	1.48937e4	359.01648	100.0000



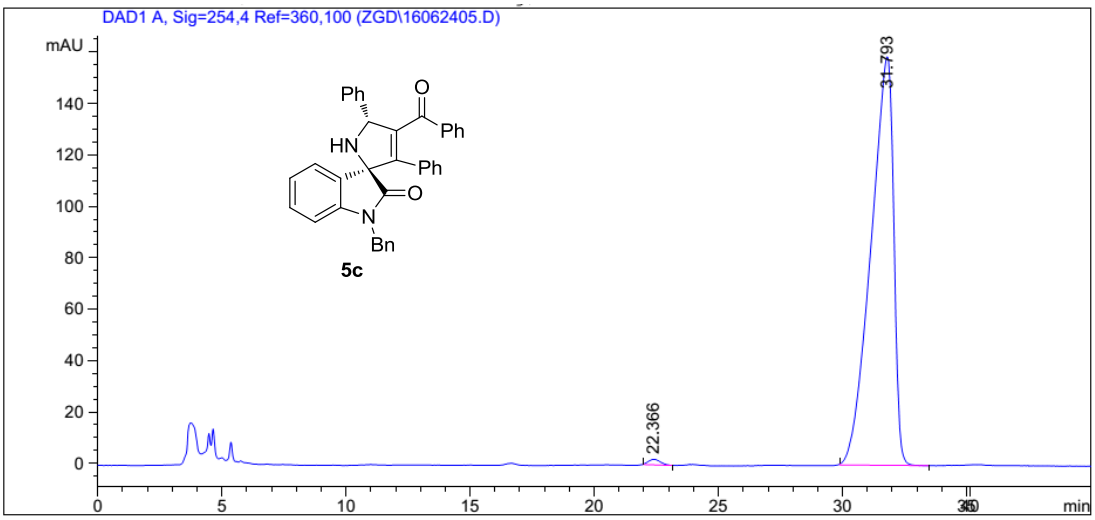
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	25.606	BB	0.6398	9328.46582	224.94127	50.5344
2	45.066	BB	1.1670	9131.18652	121.75535	49.4656



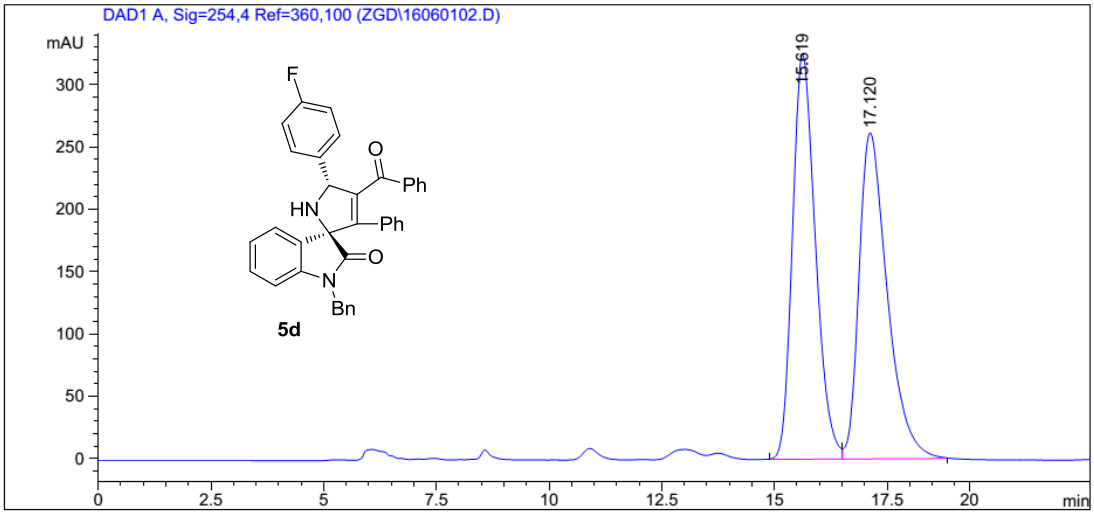
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	25.571	MM	0.6607	258.91119	6.53130	1.2481
2	44.922	MM	1.2774	2.04859e4	267.28900	98.7519



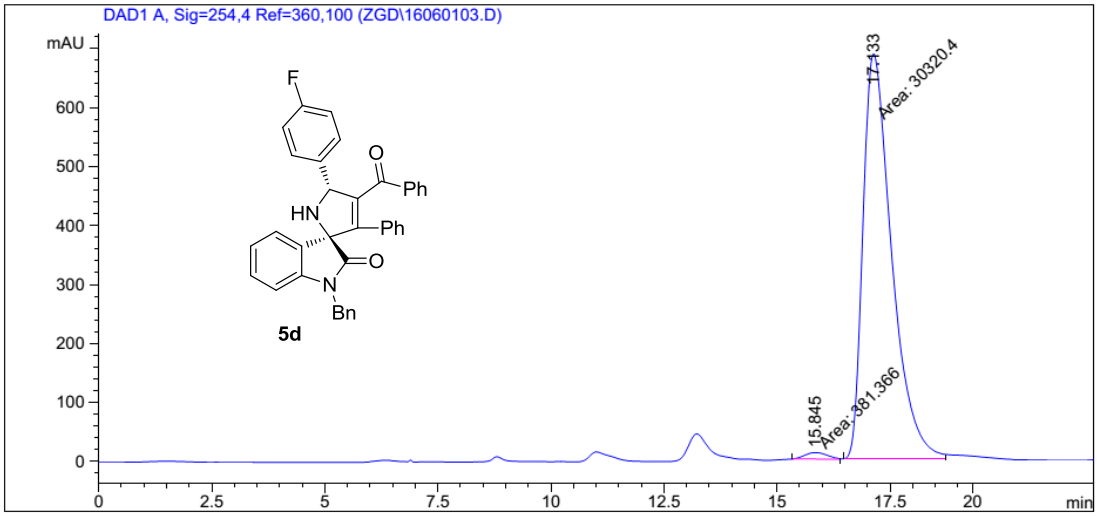
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	22.373	BB	0.5939	8385.82715	219.40019	50.5327
2	31.728	BP	0.8627	8209.02051	135.90546	49.4673



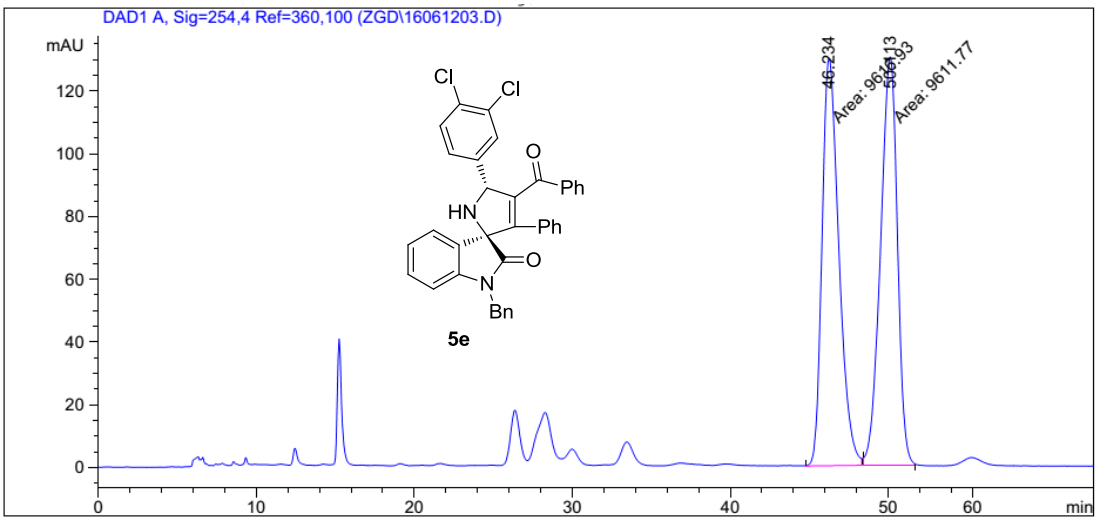
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	22.366	BP	0.4123	73.55579	2.13317	0.7245
2	31.793	BB	0.9077	1.00792e4	158.97536	99.2755



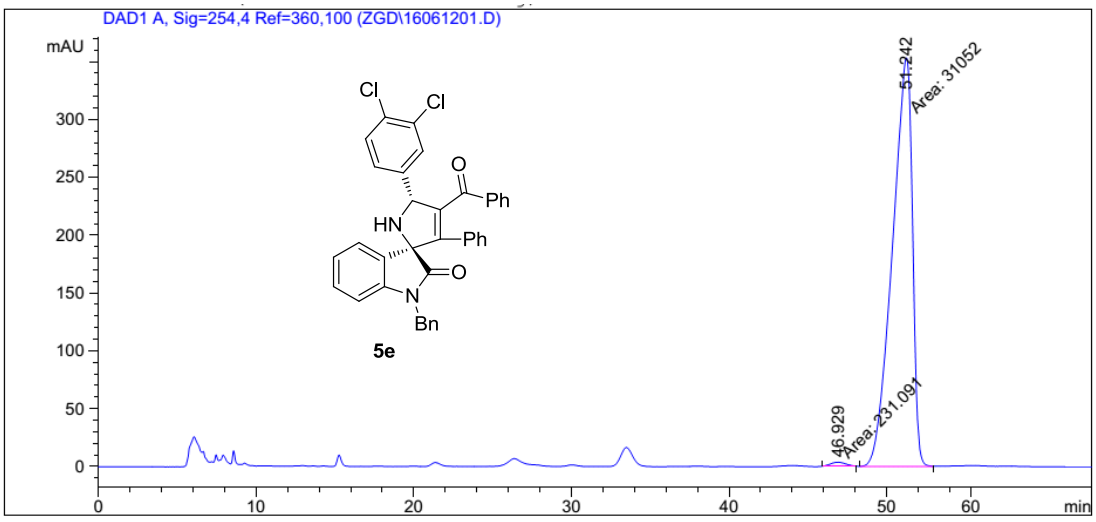
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	15.619	BV	0.5436	1.14814e4	325.47134	50.2049
2	17.120	VB	0.6498	1.13877e4	261.64728	49.7951



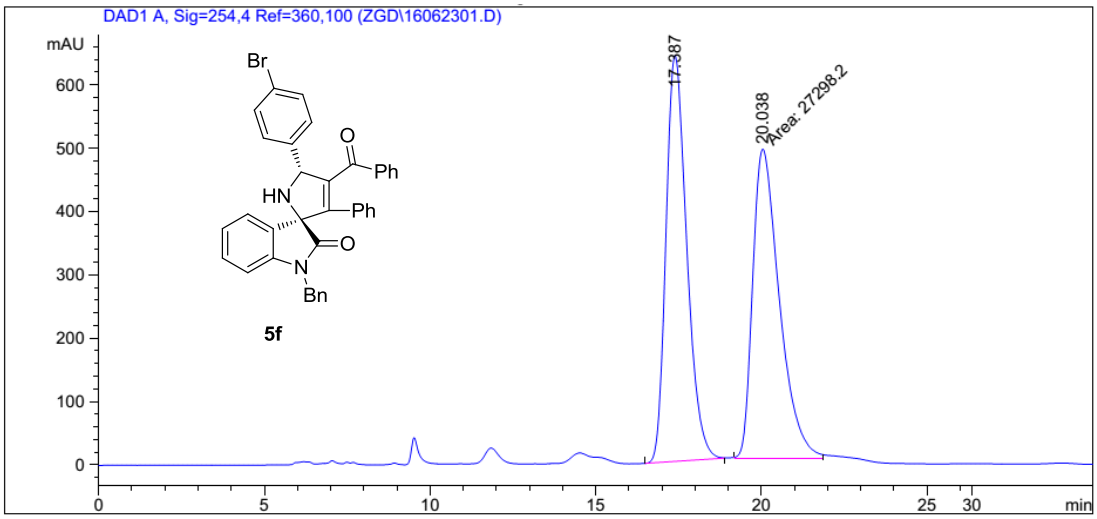
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	15.845	MM	0.5707	381.36603	11.13768	1.2422
2	17.133	MM	0.7352	3.03204e4	687.35046	98.7578



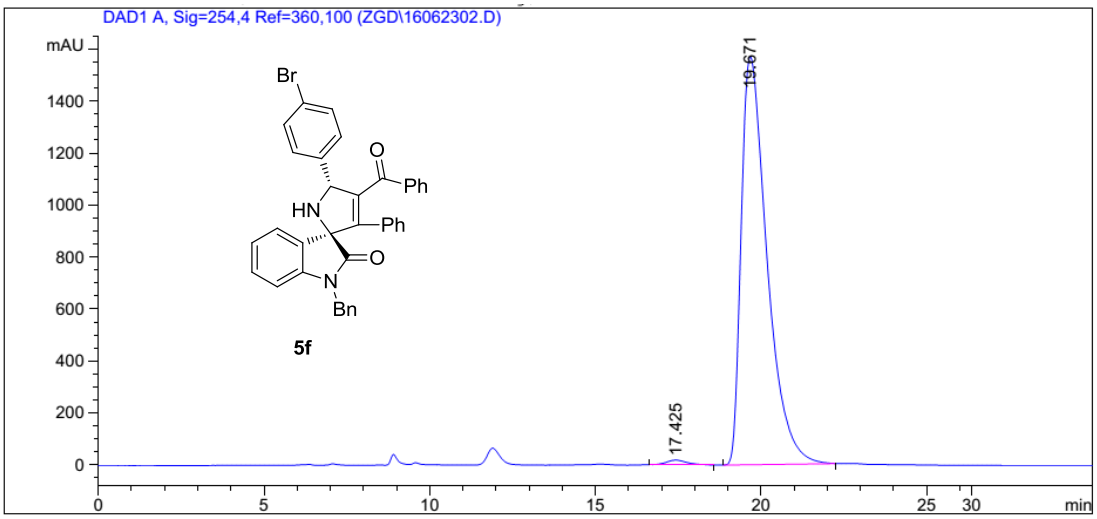
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	46.234	MM	1.2347	9616.93066	129.81737	50.0134
2	50.113	MM	1.2306	9611.76563	130.17908	49.9866



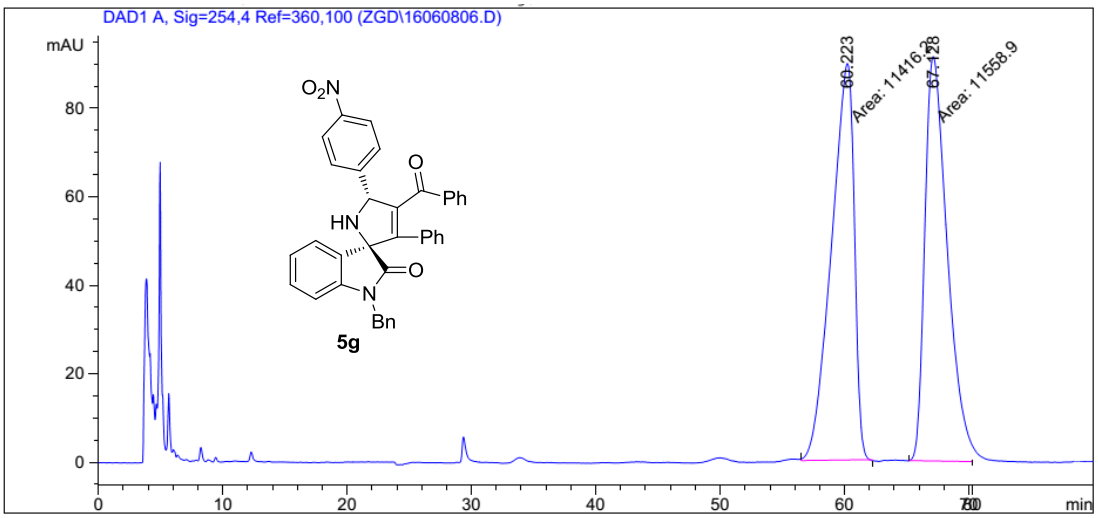
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	46.929	MM	1.1155	231.09125	3.45269	0.7387
2	51.242	MM	1.4654	3.10520e4	353.17957	99.2613



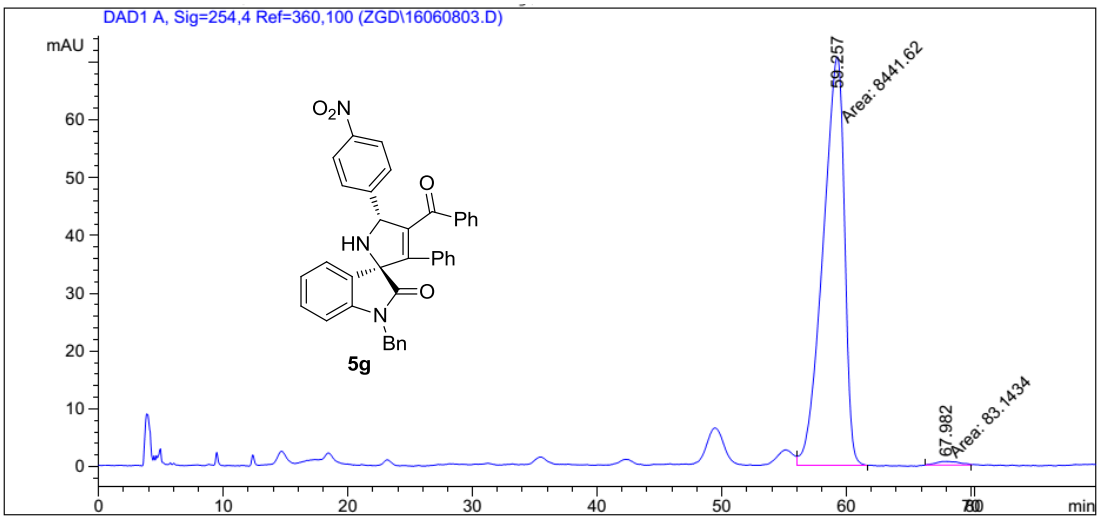
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	17.387	PB	0.6654	2.78693e4	640.81335	50.5176
2	20.038	MM	0.9311	2.72982e4	488.62137	49.4824



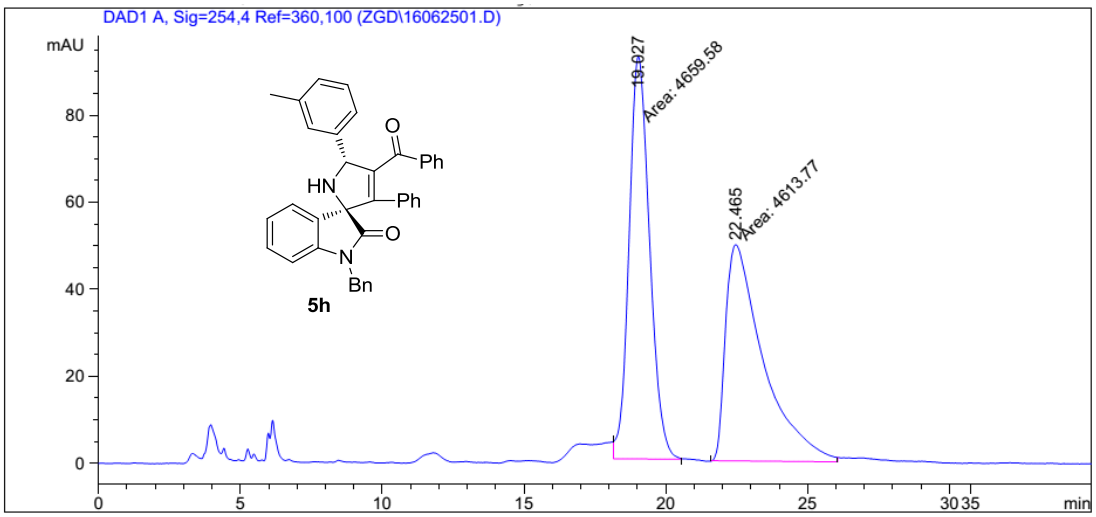
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	17.425	BB	0.6613	891.28723	19.06773	1.0392
2	19.671	PB	0.7986	8.48726e4	1570.22412	98.9608



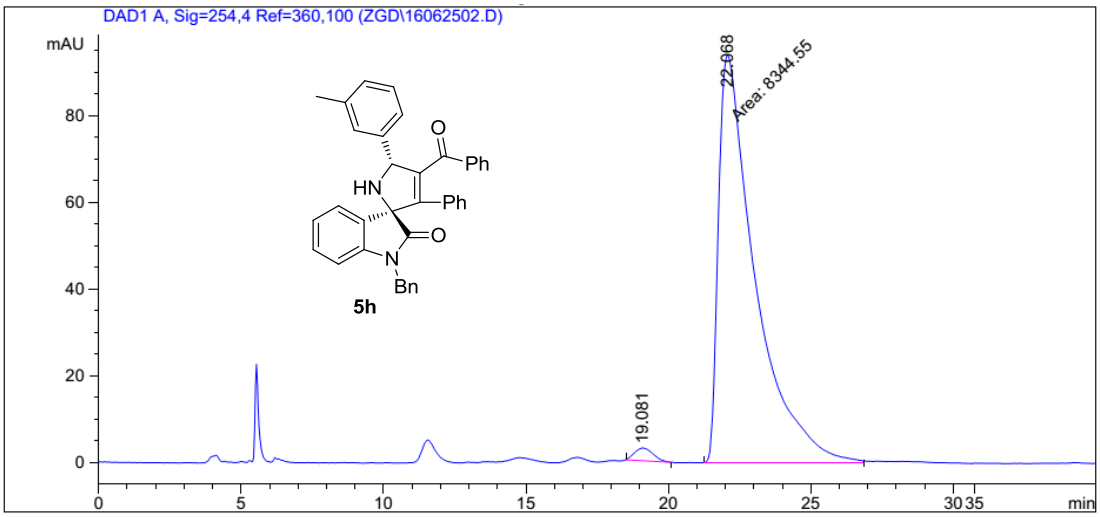
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	60.223	MM	2.1226	1.14162e4	89.63847	49.6896
2	67.128	MM	2.1082	1.15589e4	91.37935	50.3104



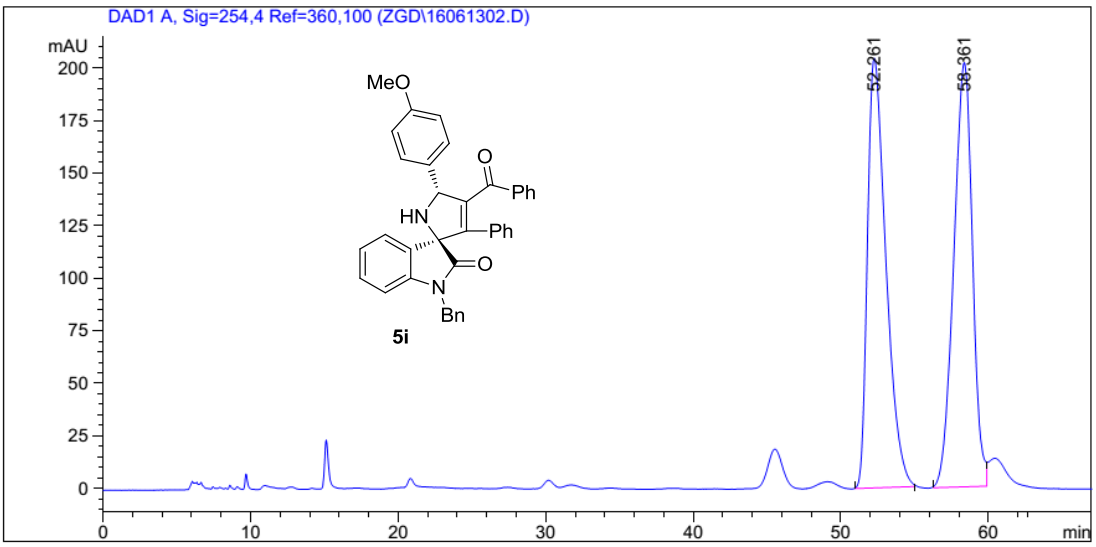
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	59.257	MM	1.9920	8441.62012	70.62825	99.0247
2	67.982	MM	2.1655	83.14337	6.39906e-1	0.9753



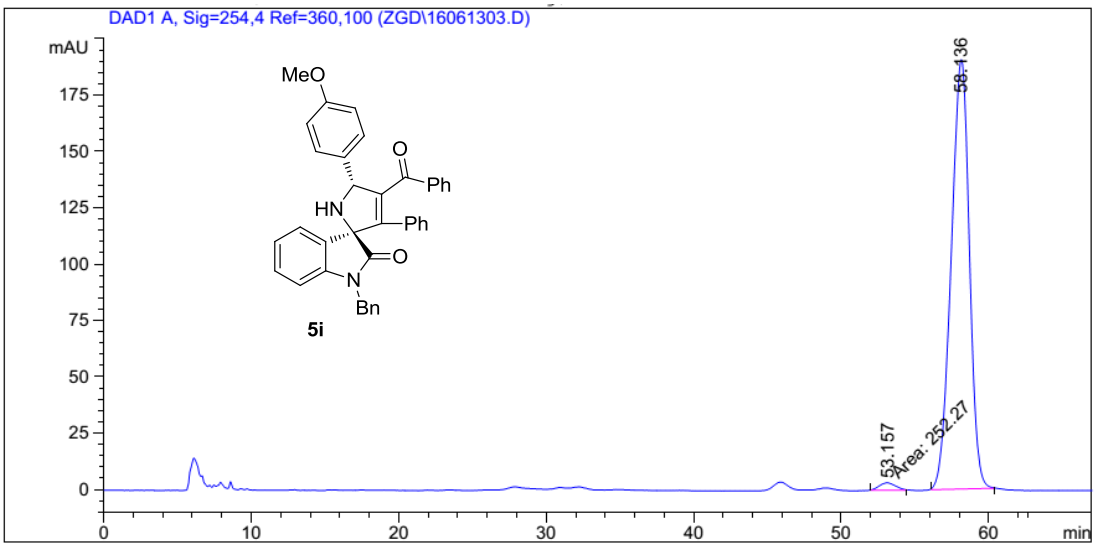
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	19.027	MM	0.8397	4659.57959	92.48219	50.2470
2	22.465	MM	1.5464	4613.76709	49.72622	49.7530



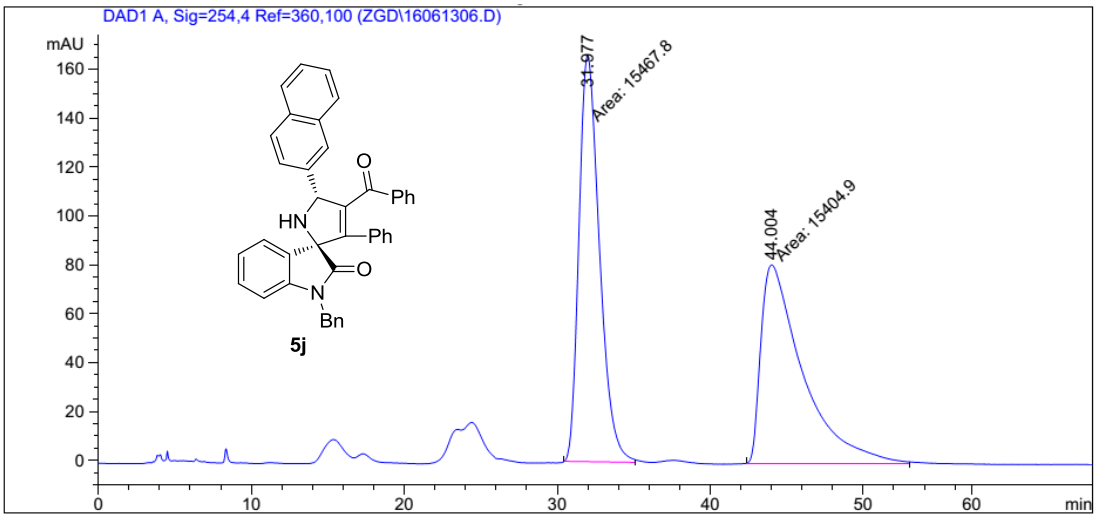
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	19.081	BB	0.5422	132.67552	2.91943	1.5651
2	22.068	MM	1.4807	8344.54785	93.92825	98.4349



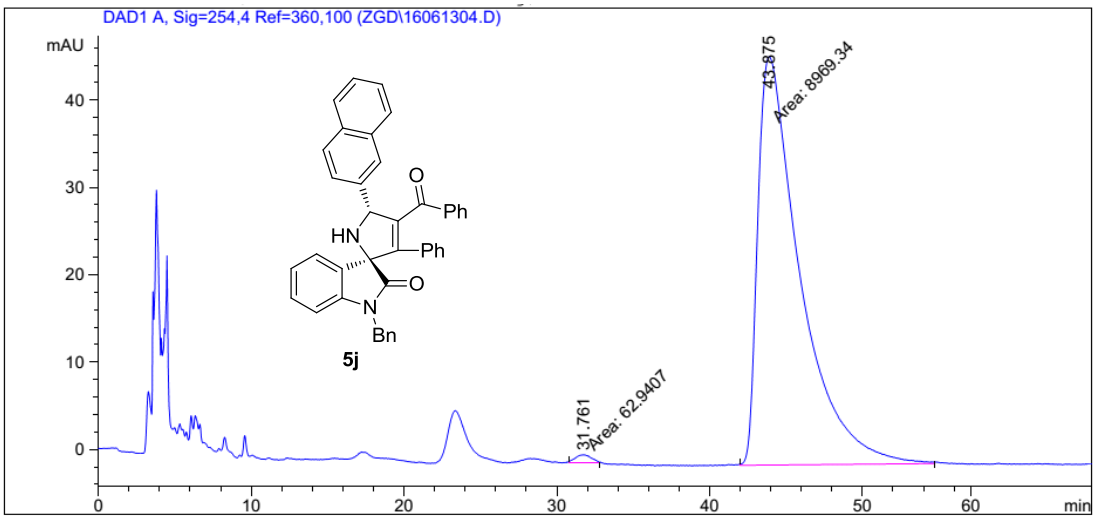
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	52.261	BB	1.2653	1.77524e4	204.39128	50.0371
2	58.361	BV	1.2829	1.77261e4	201.77988	49.9629



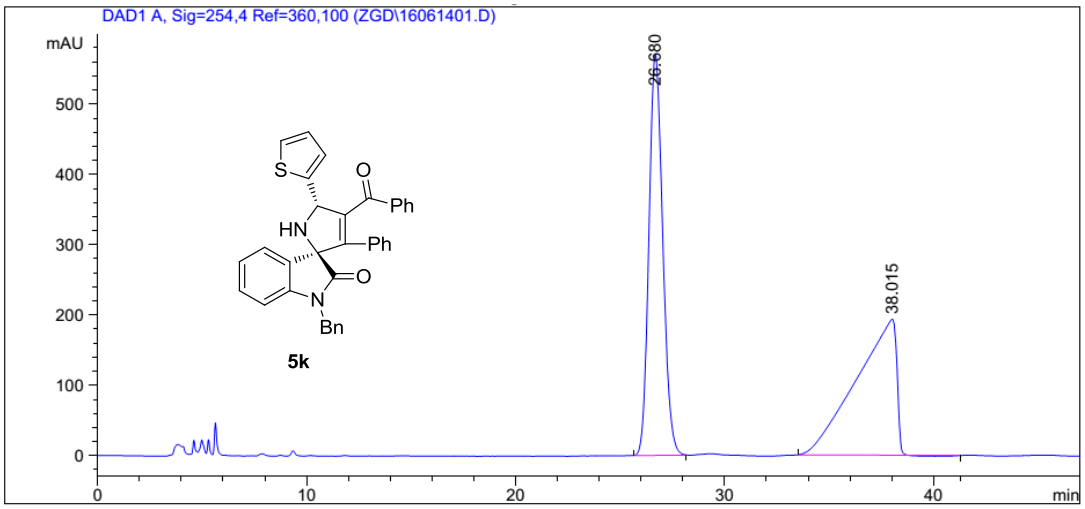
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	53.157	MM	1.2951	252.26978	3.24641	1.5243
2	58.136	BB	1.2200	1.62981e4	190.52280	98.4757



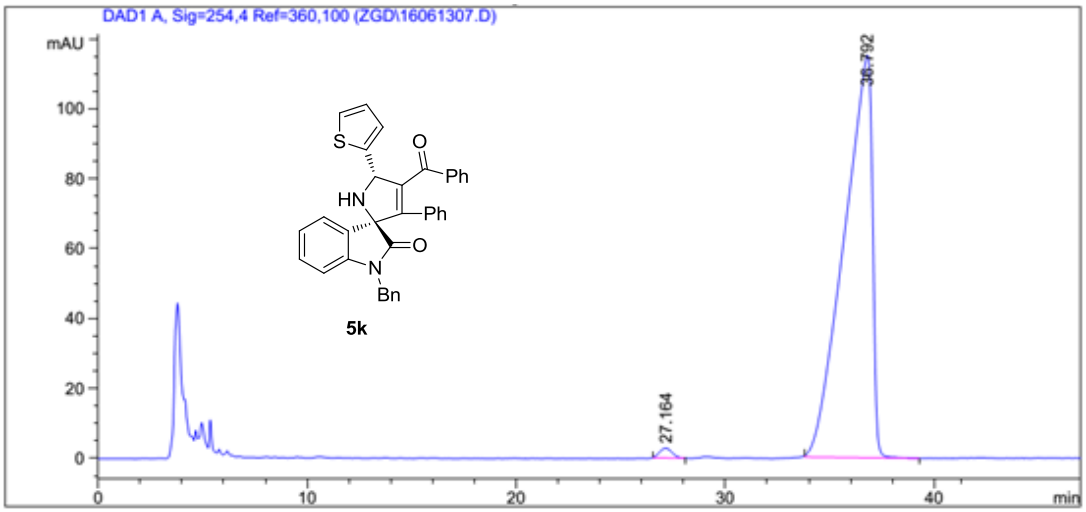
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	31.977	MM	1.5511	1.54678e4	166.20383	50.1018
2	44.004	MM	3.1601	1.54049e4	81.24774	49.8982



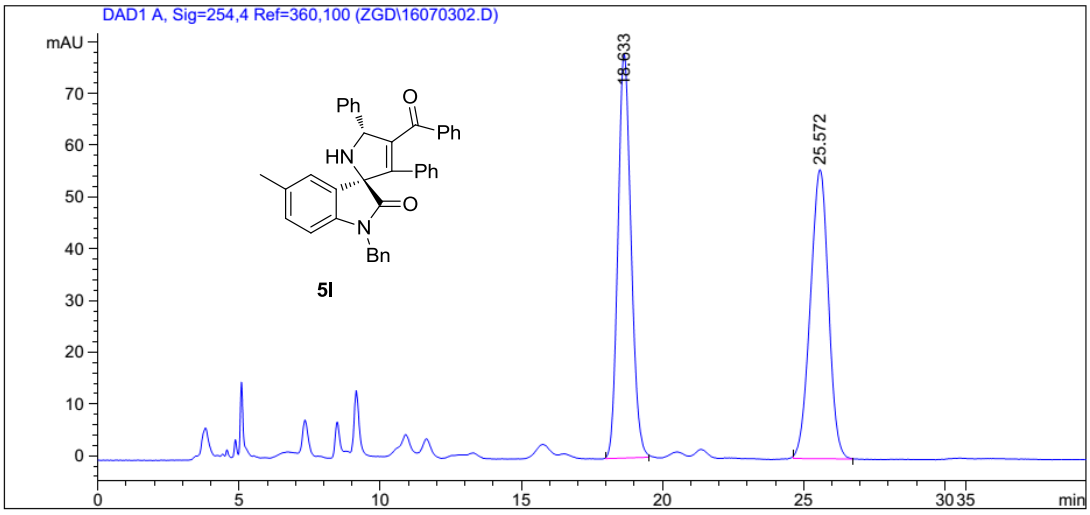
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	31.761	MM	1.1889	62.94069	8.82326e-1	0.6968
2	43.875	MM	3.1967	8969.33691	46.76393	99.3032



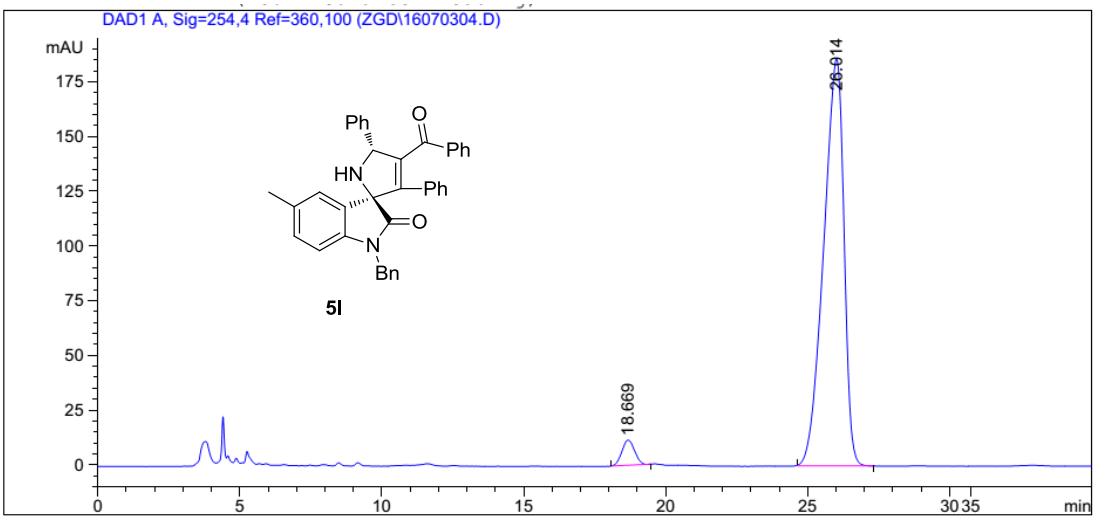
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	26.680	BB	0.7143	2.61147e4	570.18359	50.2254
2	38.015	BP	1.6803	2.58803e4	193.51527	49.7746



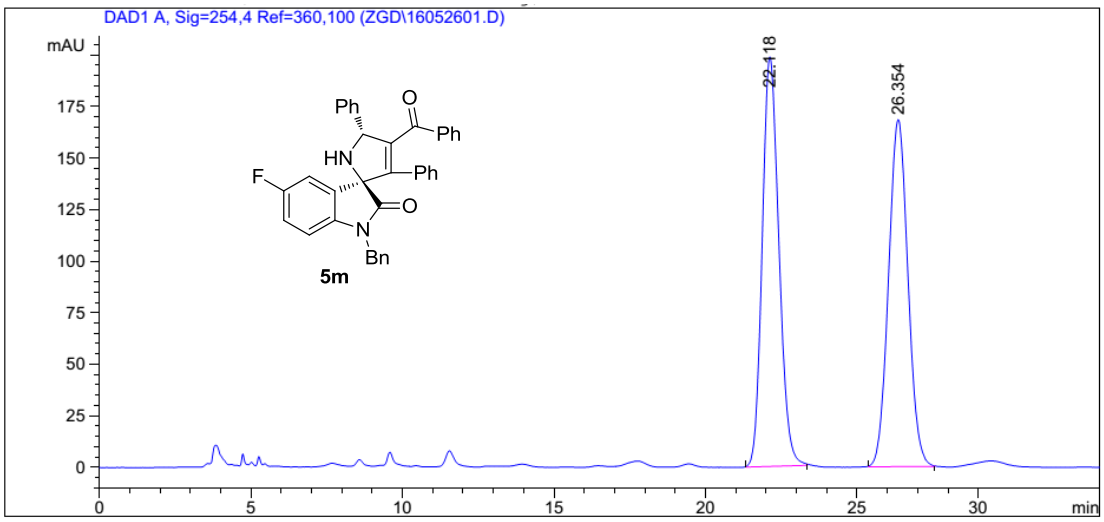
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	27.164	BB	0.5040	115.75916	2.77887	1.0593
2	36.792	BP	1.2106	1.08118e4	115.23243	98.9407



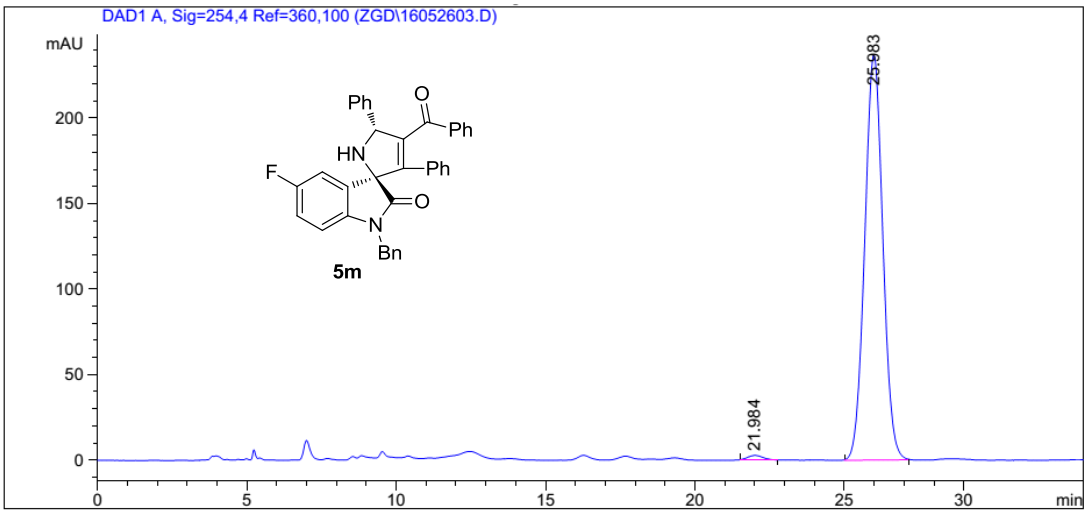
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	18.633	BB	0.4996	2526.13965	78.05955	50.3078
2	25.572	BB	0.6850	2495.22974	55.87595	49.6922



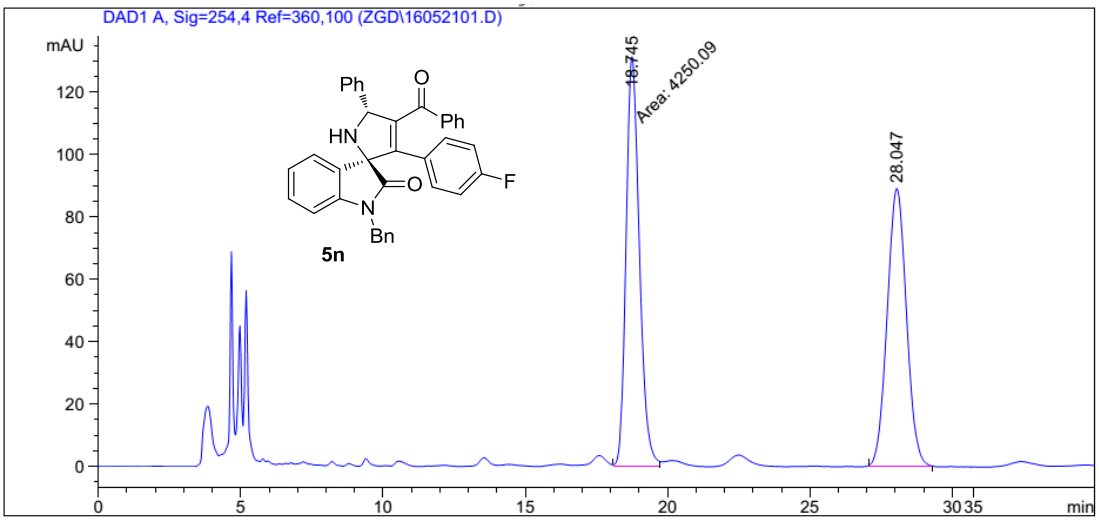
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	18.669	BP	0.4631	356.85767	11.52873	3.7257
2	26.014	BB	0.7543	9221.41895	186.02074	96.2743



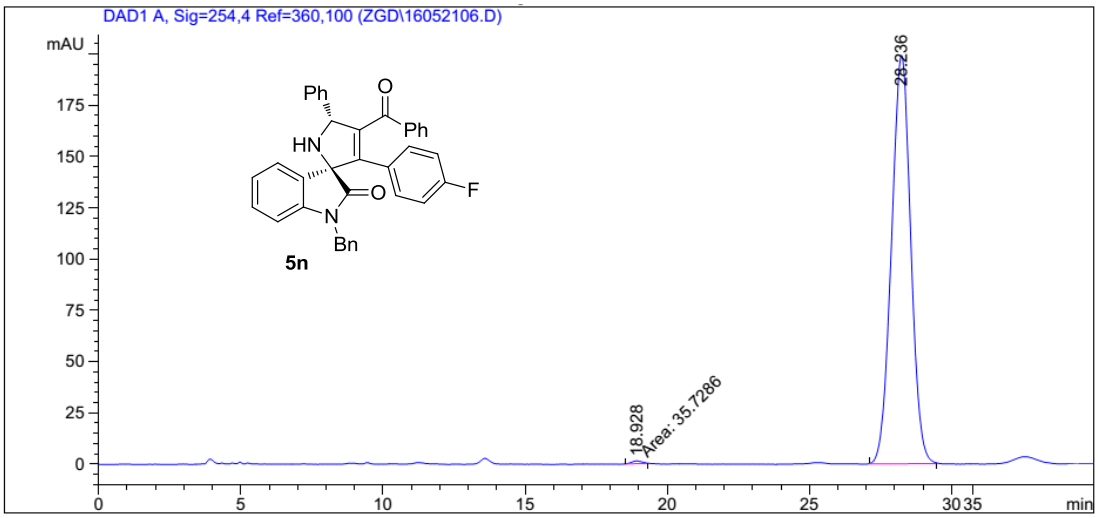
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	22.118	BB	0.5882	7560.90186	198.58777	50.3405
2	26.354	BB	0.6870	7458.62988	168.29939	49.6595



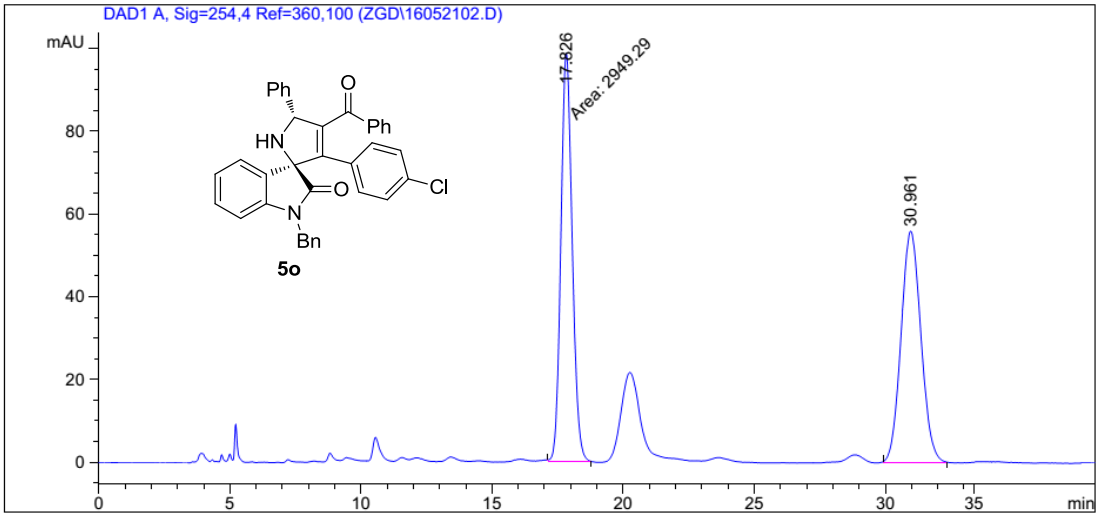
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	21.984	BP	0.4294	93.85864	2.61072	0.9343
2	25.983	BB	0.6541	9951.53418	236.88171	99.0657



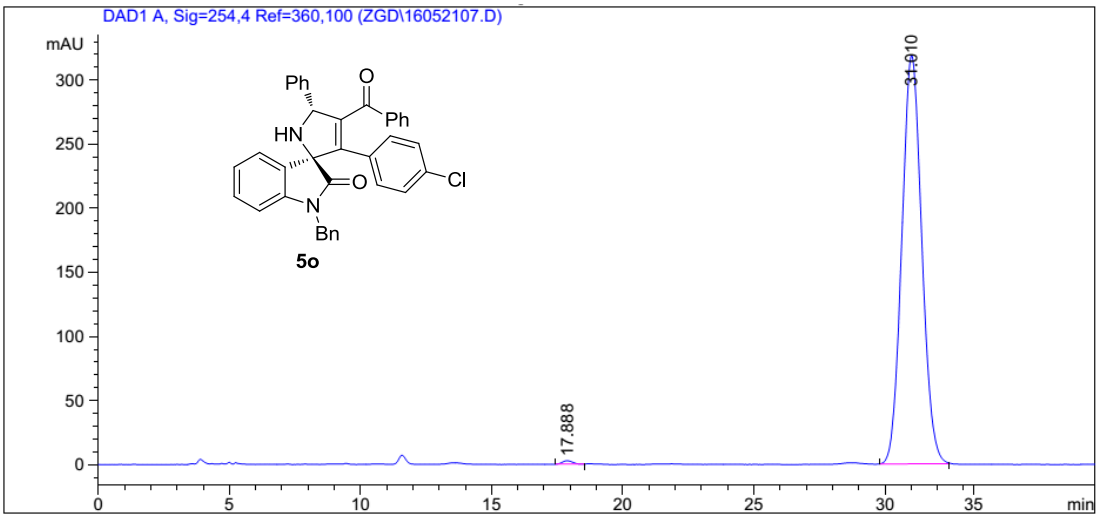
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	18.745	MM	0.5396	4250.09082	131.27013	50.3317
2	28.047	BB	0.7305	4194.08008	89.21189	49.6683



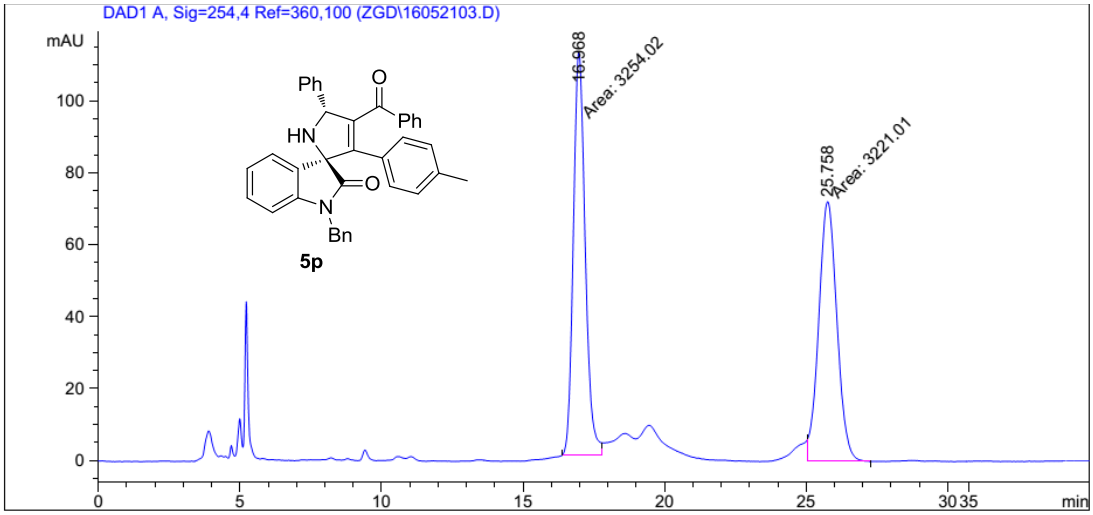
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	18.928	MM	0.4412	35.72859	1.34958	0.3804
2	28.236	BB	0.7240	9356.35449	199.19664	99.6196



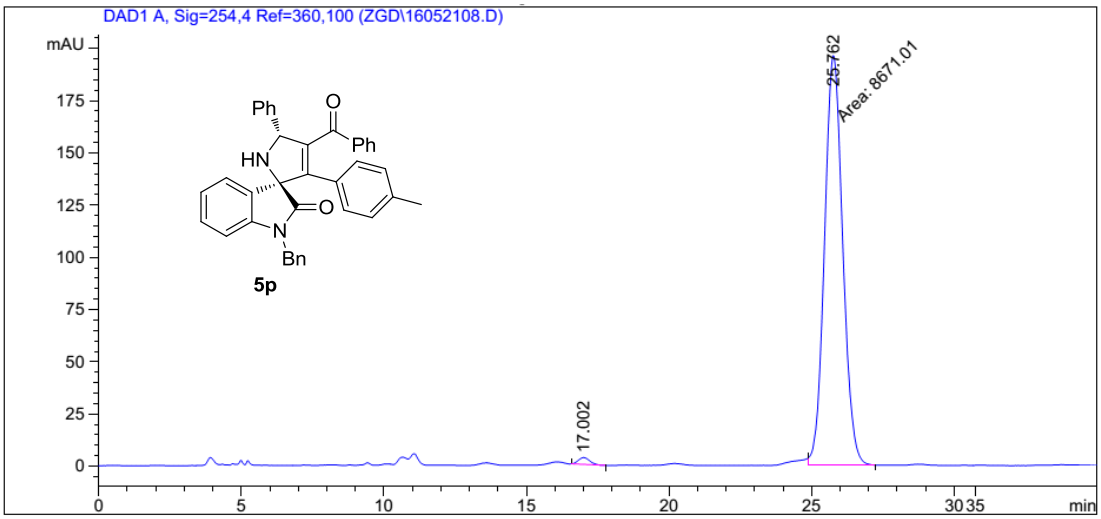
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	17.826	MM	0.4983	2949.29150	98.64017	50.0309
2	30.961	BB	0.7840	2945.64746	55.96914	49.9691



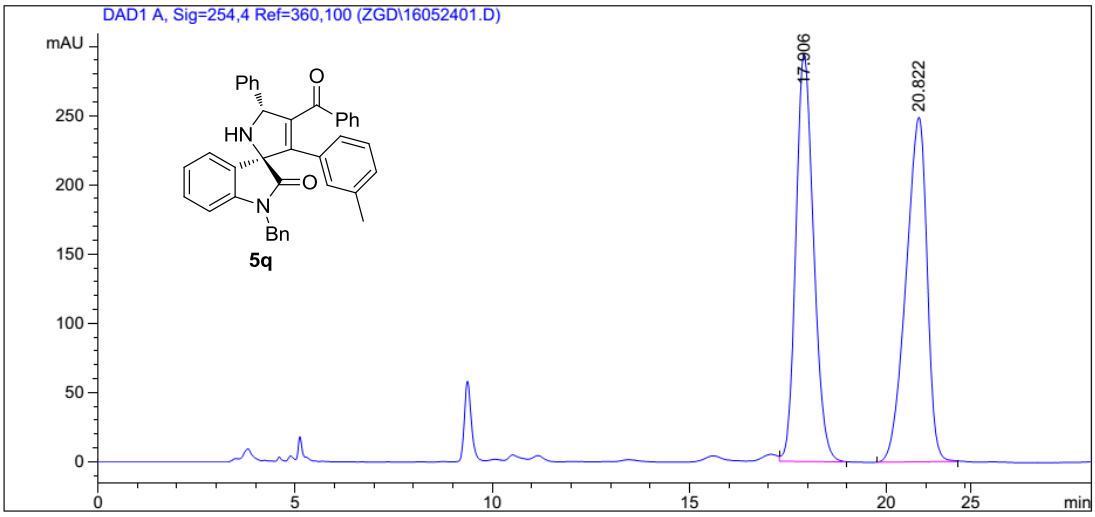
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	17.888	BP	0.3448	69.81161	2.67241	0.4123
2	31.010	BB	0.8313	1.68620e4	318.66595	99.5877



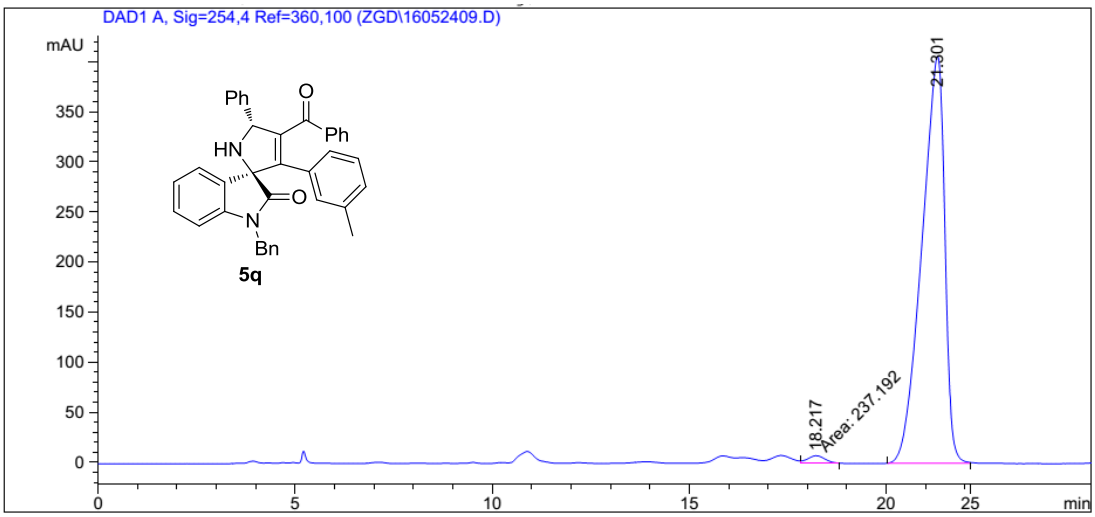
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	16.968	MM	0.4835	3254.02124	112.16496	50.2549
2	25.758	MM	0.7432	3221.01245	72.23598	49.7451



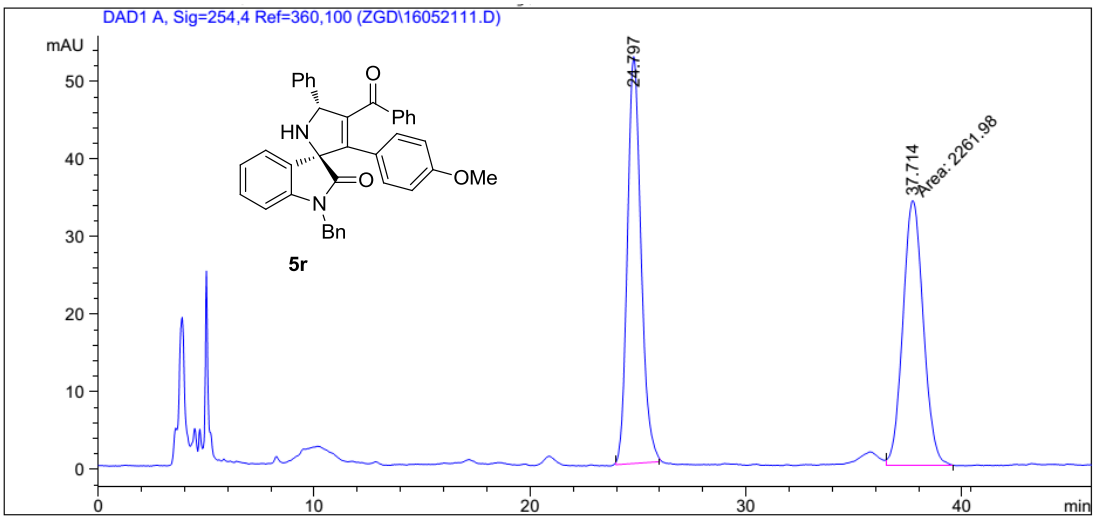
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	17.002	PP	0.3834	89.56337	3.25111	1.0223
2	25.762	MM	0.7376	8671.00977	195.93837	98.9777



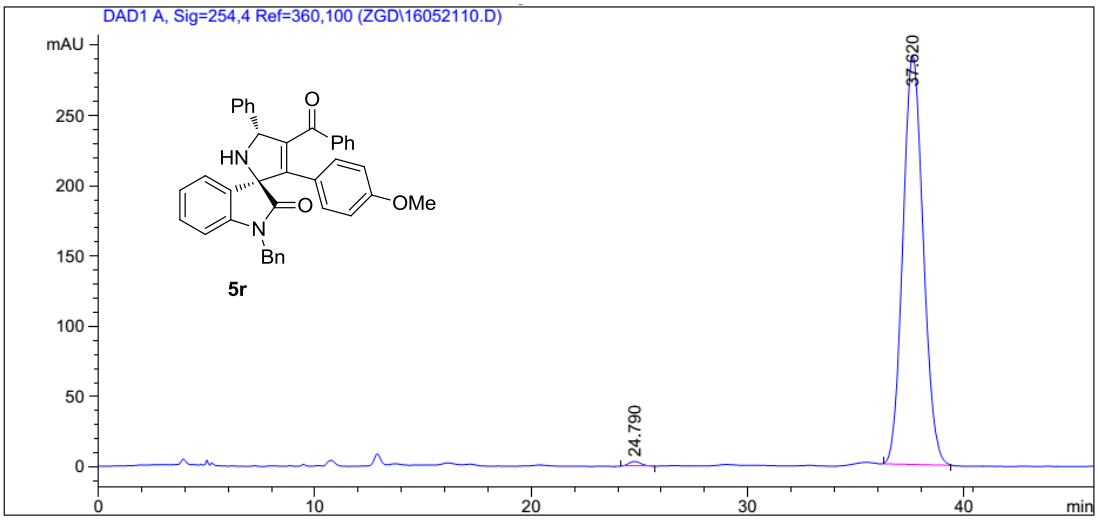
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	17.906	VB	0.4832	9205.14453	294.10449	49.9707
2	20.822	BB	0.5723	9215.92871	248.74269	50.0293



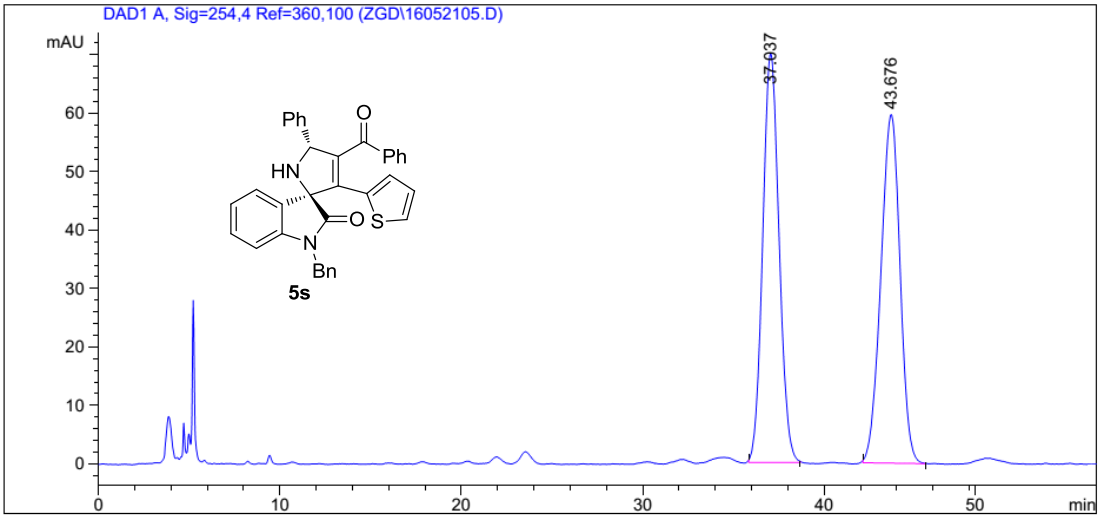
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	18.217	MM	0.5187	237.19234	7.62122	1.4291
2	21.301	BB	0.5978	1.63604e4	406.30286	98.5709



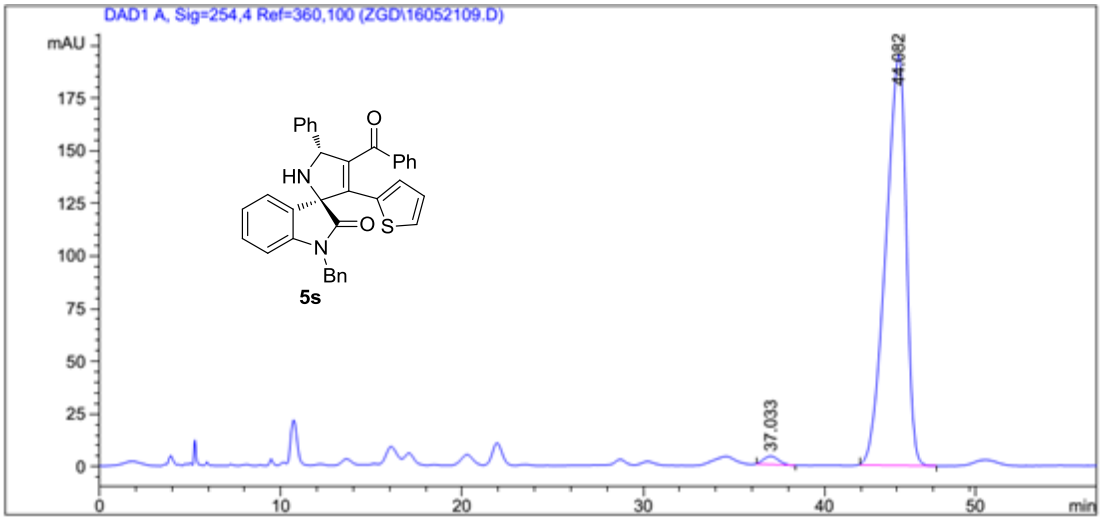
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	24.797	BB	0.6539	2291.73169	52.44054	50.3267
2	37.714	MM	1.1018	2261.97998	34.21627	49.6733



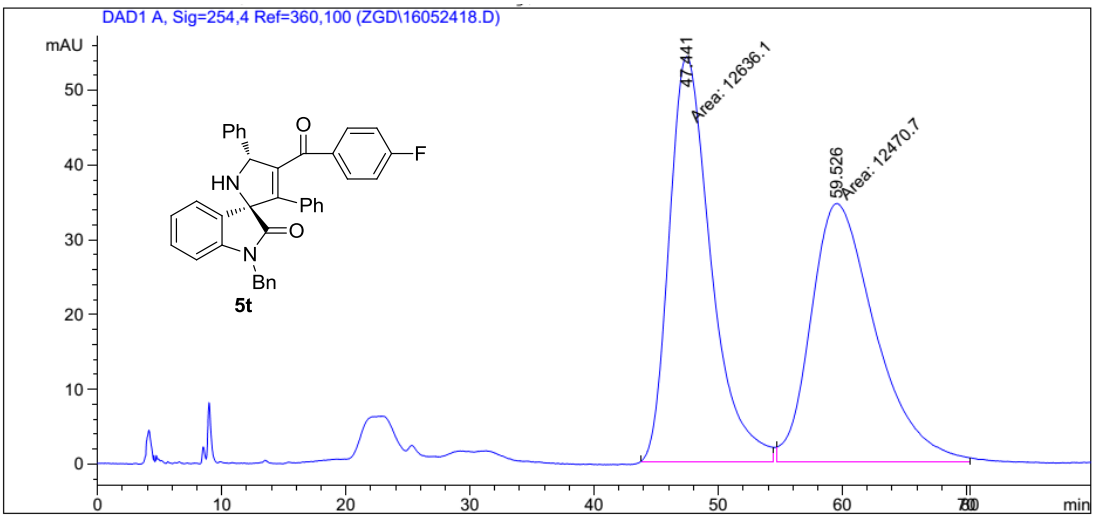
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	24.790	BP	0.4816	134.86891	3.35092	0.7053
2	37.620	BB	1.0035	1.89871e4	290.91376	99.2947



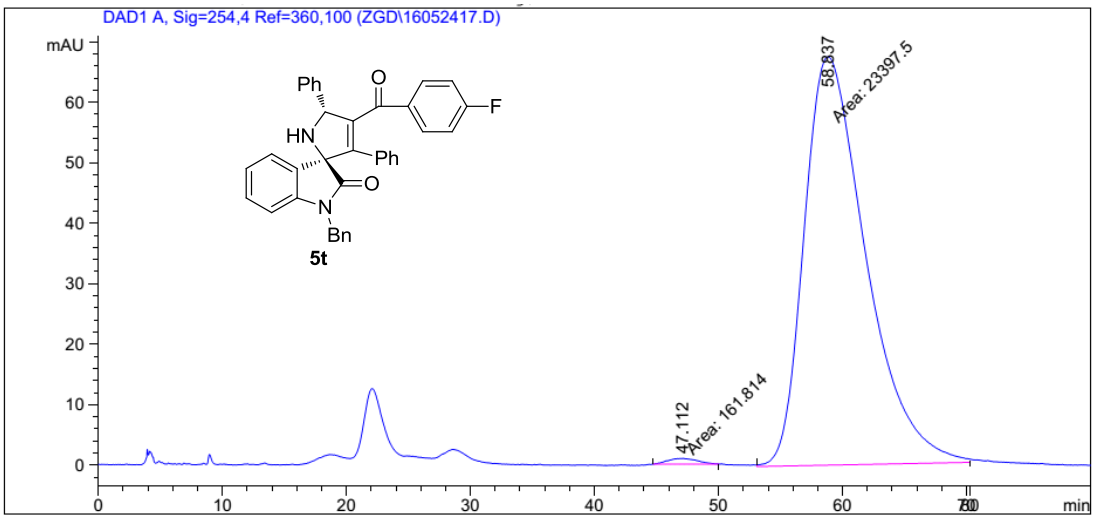
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	37.037	BB	0.9237	4364.42773	69.97485	49.9776
2	43.676	BB	1.0104	4368.34668	59.64691	50.0224



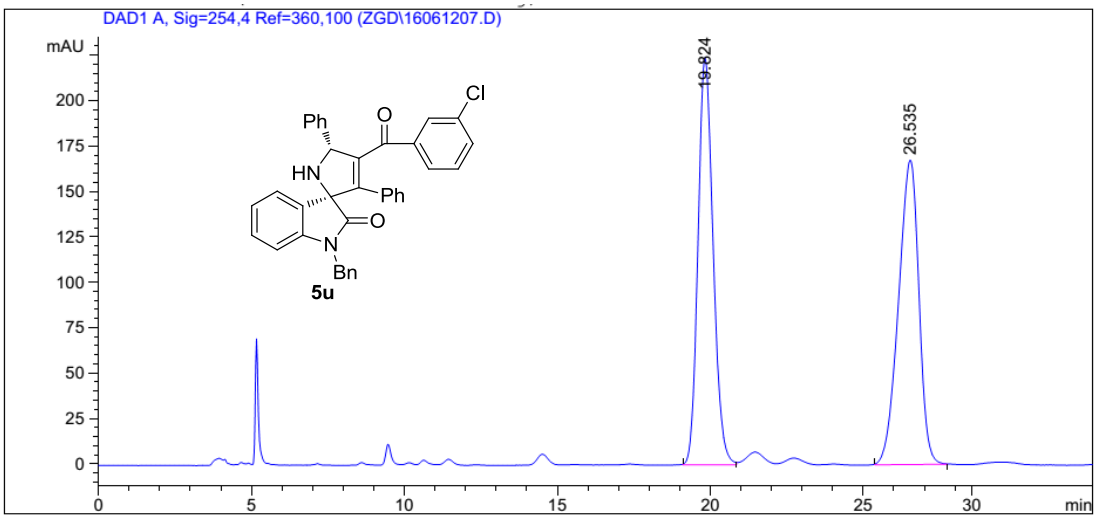
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	37.033	BP	0.6812	227.29326	3.98616	1.4700
2	44.082	BB	1.1270	1.52347e4	195.09560	98.5300



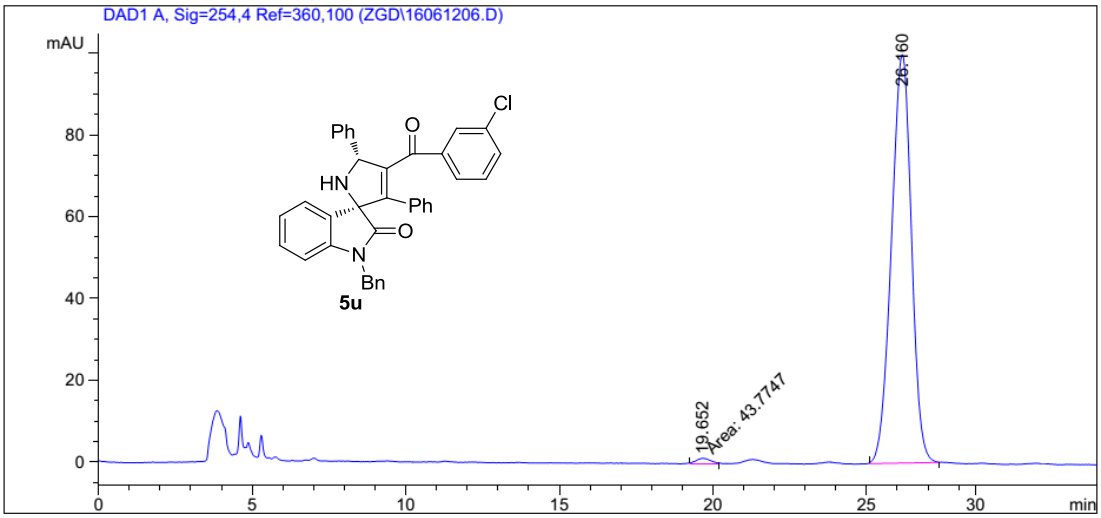
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	47.441	MM	3.8848	1.26361e4	54.21203	50.3293
2	59.526	MM	6.0135	1.24707e4	34.56304	49.6707



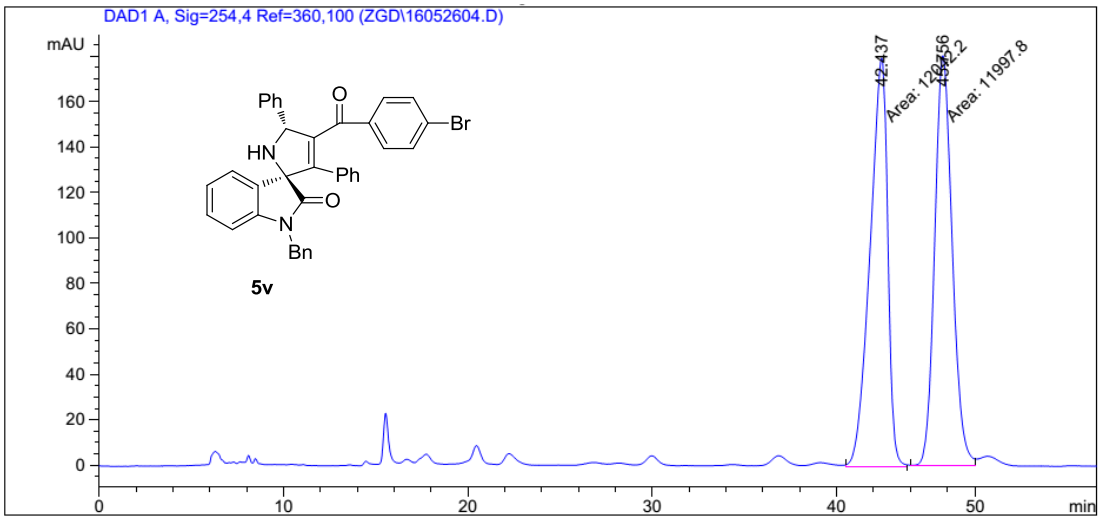
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	47.112	MM	2.7893	161.81415	9.66864e-1	0.6868
2	58.837	MM	5.7714	2.33975e4	67.56709	99.3132



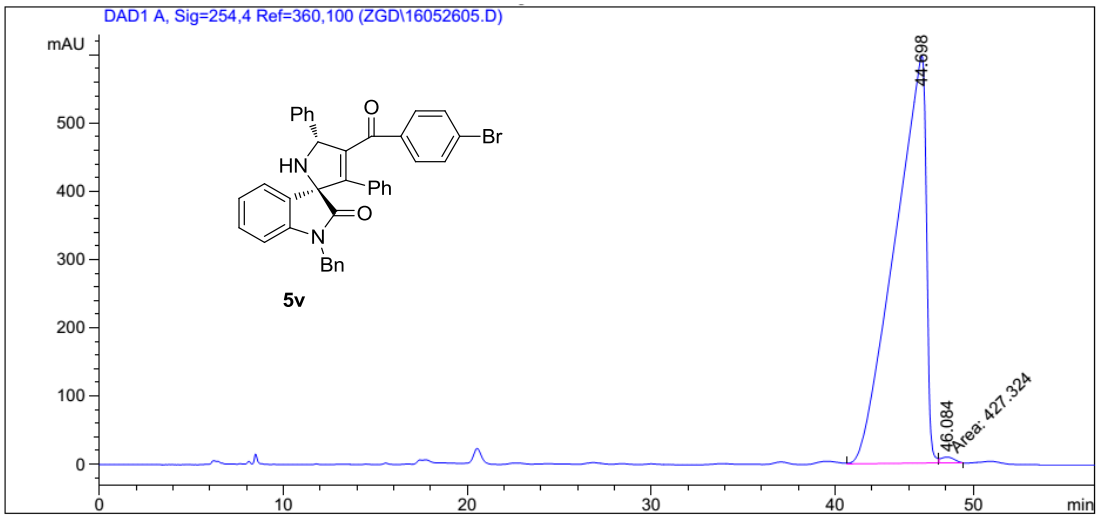
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	19.824	BB	0.5301	7690.78516	224.25137	49.7929
2	26.535	BB	0.7095	7754.76709	167.70964	50.2071



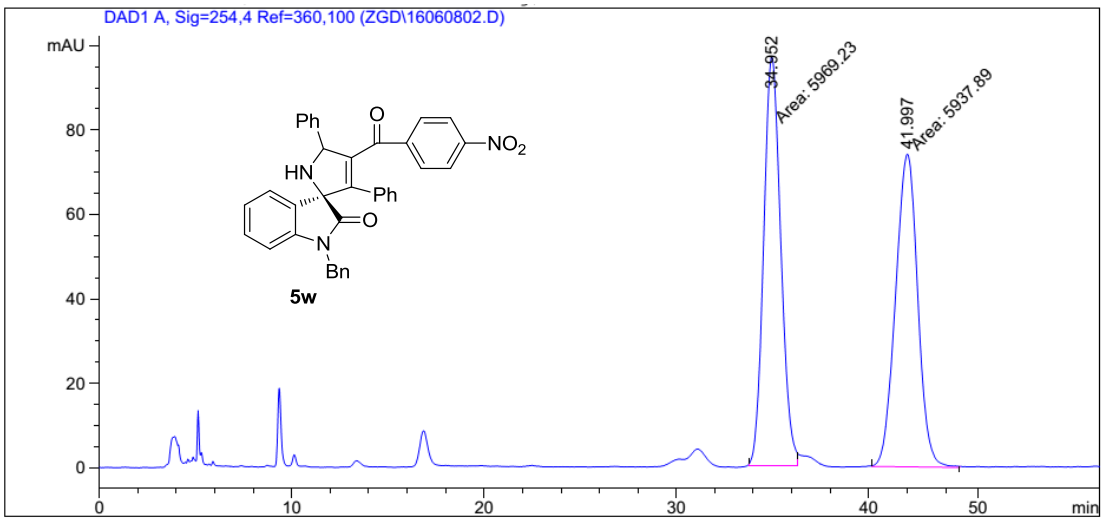
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	19.652	MM	0.5468	43.77467	1.33415	0.9627
2	26.160	BB	0.6880	4503.36230	99.88251	99.0373



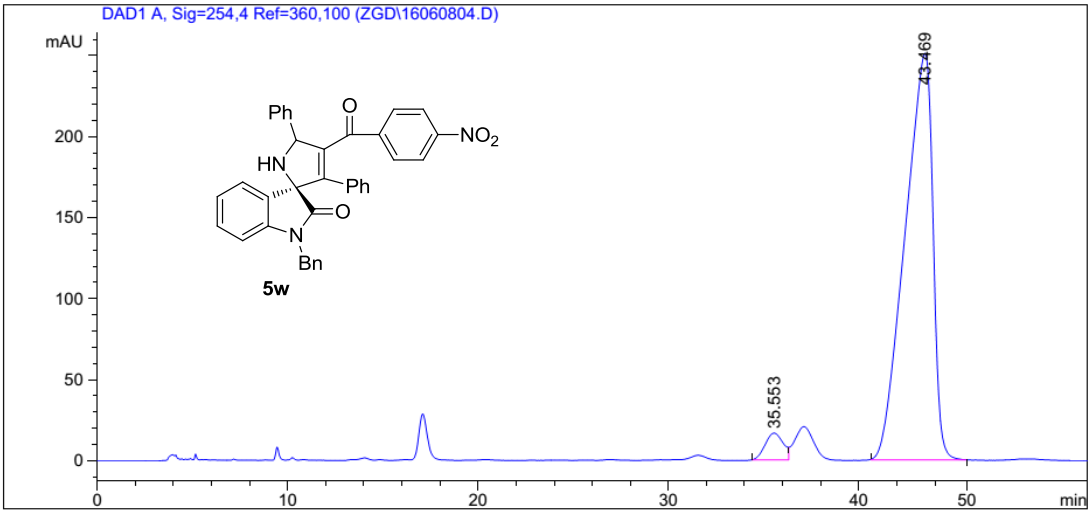
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	42.437	MM	1.1148	1.20422e4	180.04362	50.0924
2	45.756	MM	1.1069	1.19978e4	180.65005	49.9076



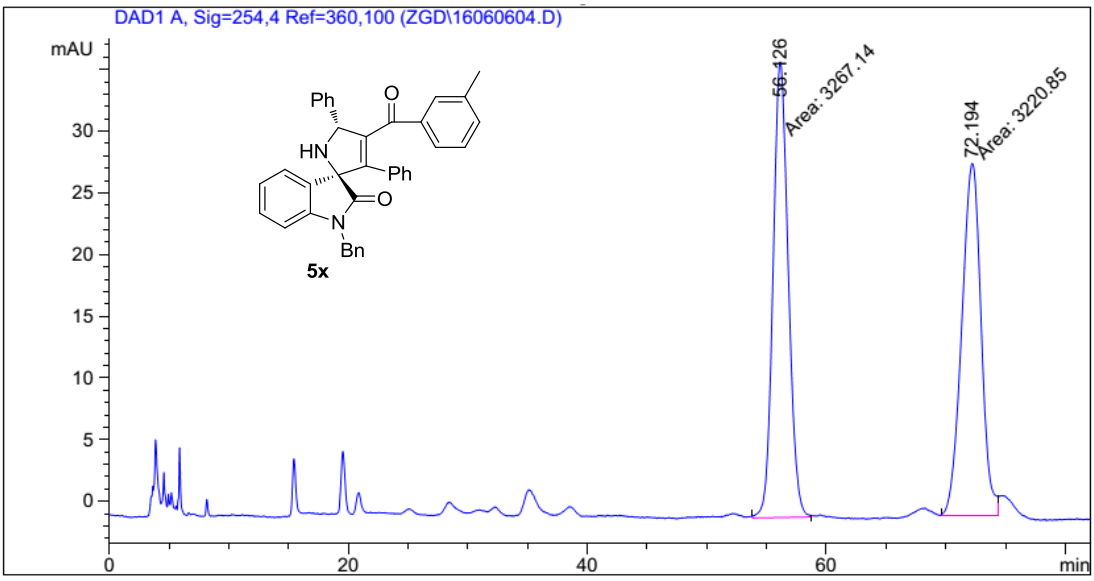
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	44.698	VV	1.4906	7.01787e4	597.35236	99.3948
2	46.084	MM	0.8419	427.32391	8.45924	0.6052



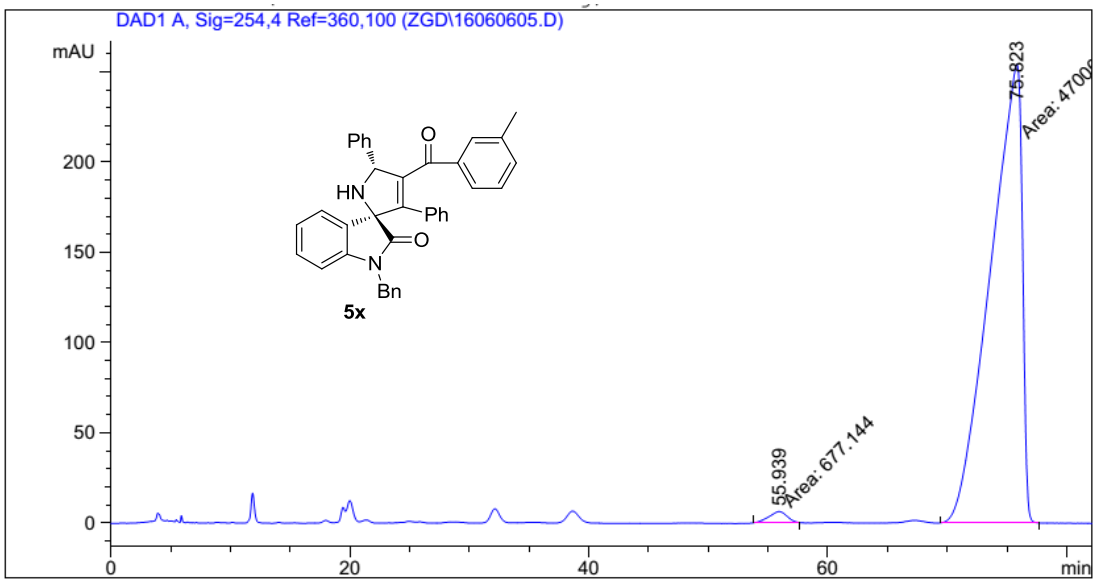
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	34.952	MM	1.0274	5969.23438	96.83535	50.1316
2	41.997	MM	1.3361	5937.89111	74.07263	49.8684



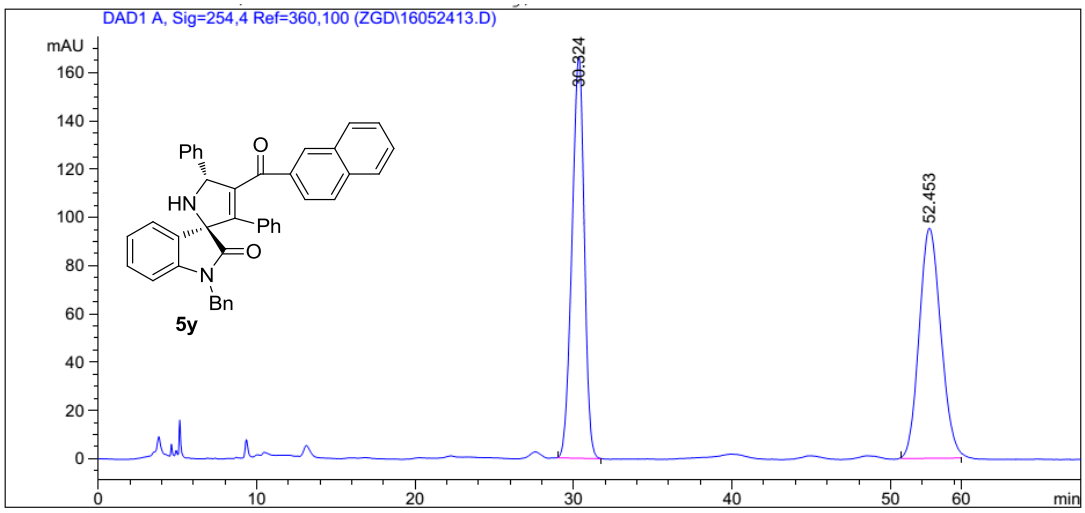
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	35.553	BV	0.8133	1102.25159	16.62933	4.1497
2	43.469	BB	1.3791	2.54602e4	251.06267	95.8503



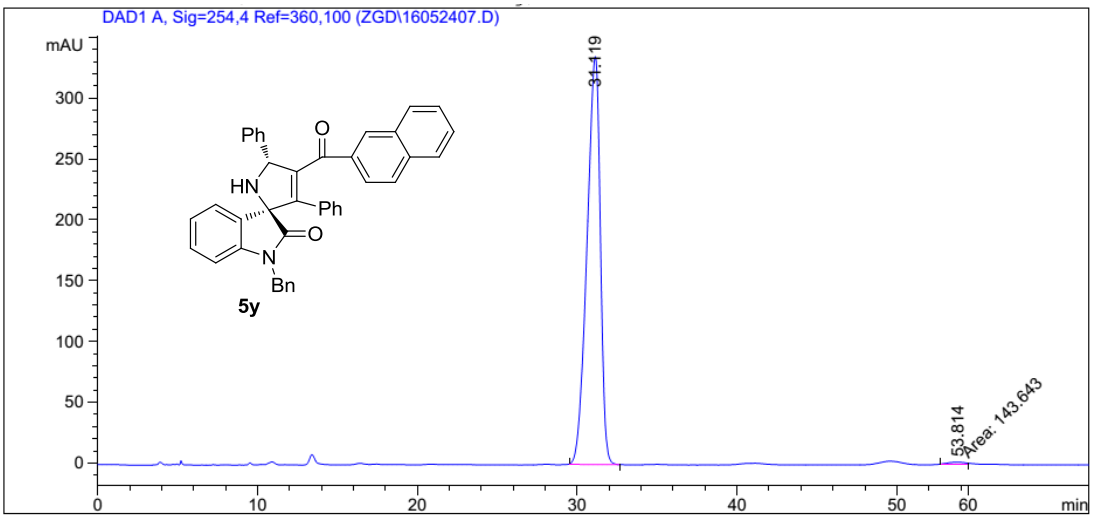
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	56.126	MM	1.4736	3267.13696	36.95299	50.3567
2	72.194	MM	1.8787	3220.85229	28.57343	49.6433



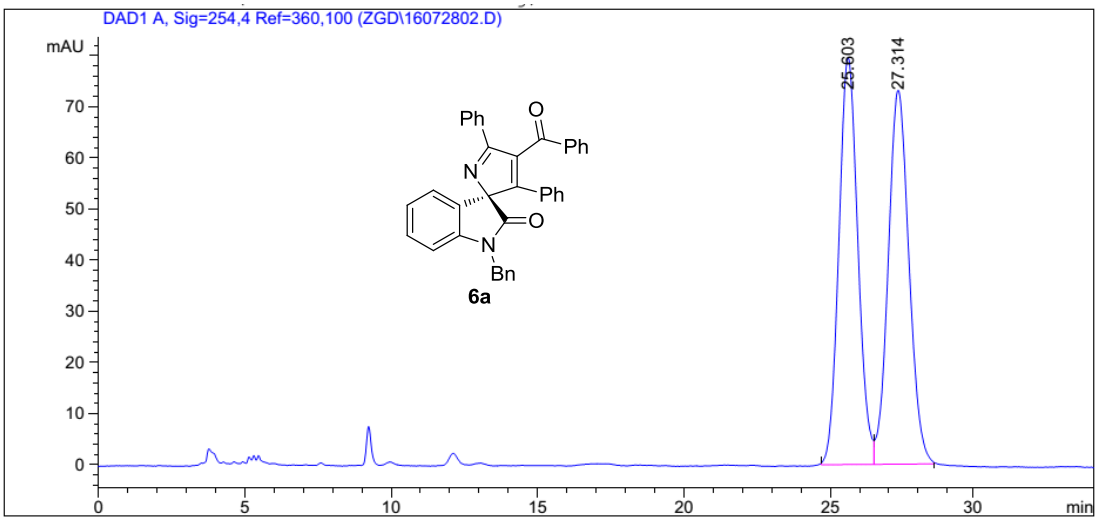
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	55.939	MM	1.7980	677.14441	6.27676	1.4203
2	75.823	MM	3.0823	4.70002e4	254.14299	98.5797



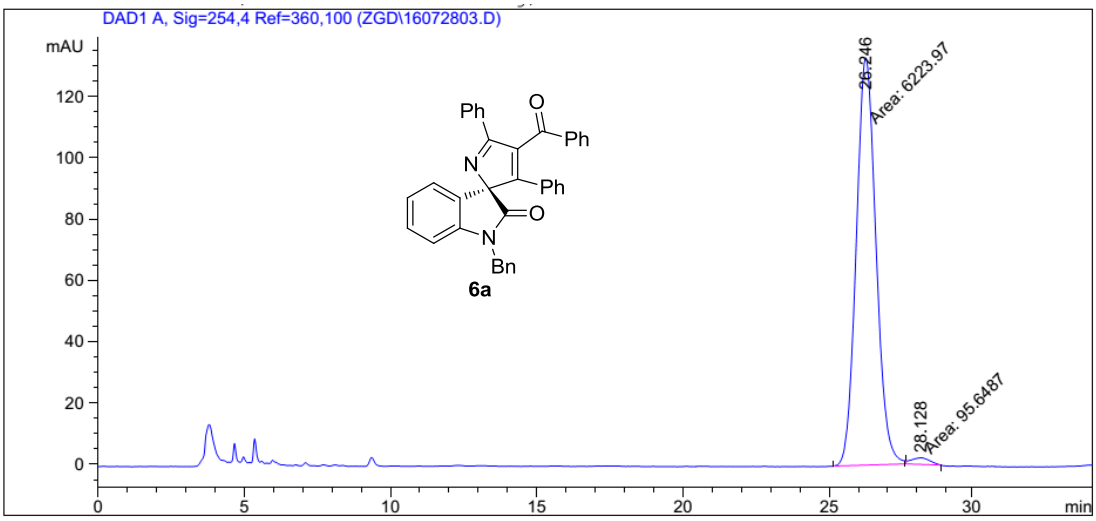
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	30.324	BB	0.8407	8960.79883	166.29689	49.7054
2	52.453	BB	1.3851	9067.02539	95.37458	50.2946



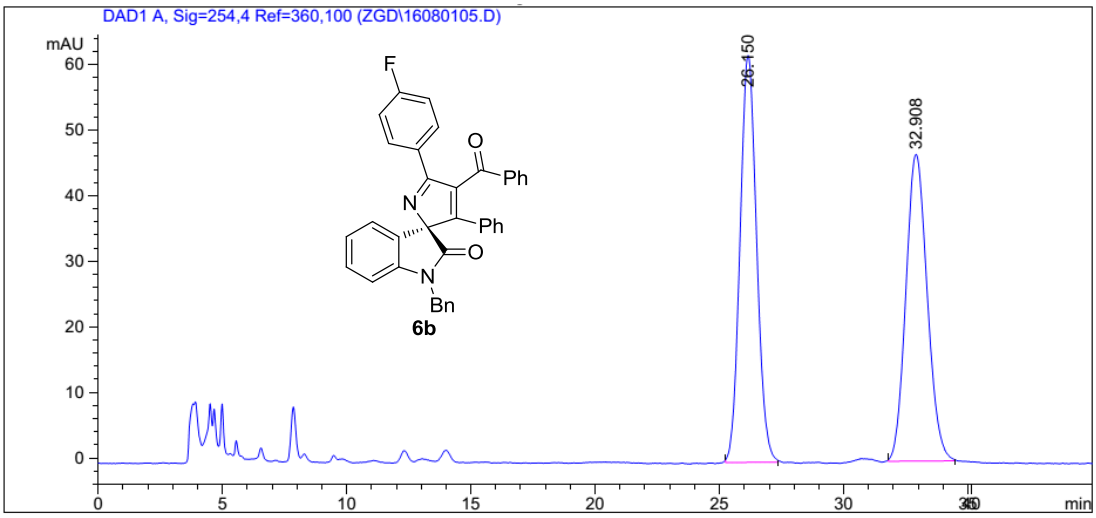
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	31.119	BB	0.8976	1.94144e4	335.25970	99.2656
2	53.814	MM	1.2999	143.64293	1.84173	0.7344



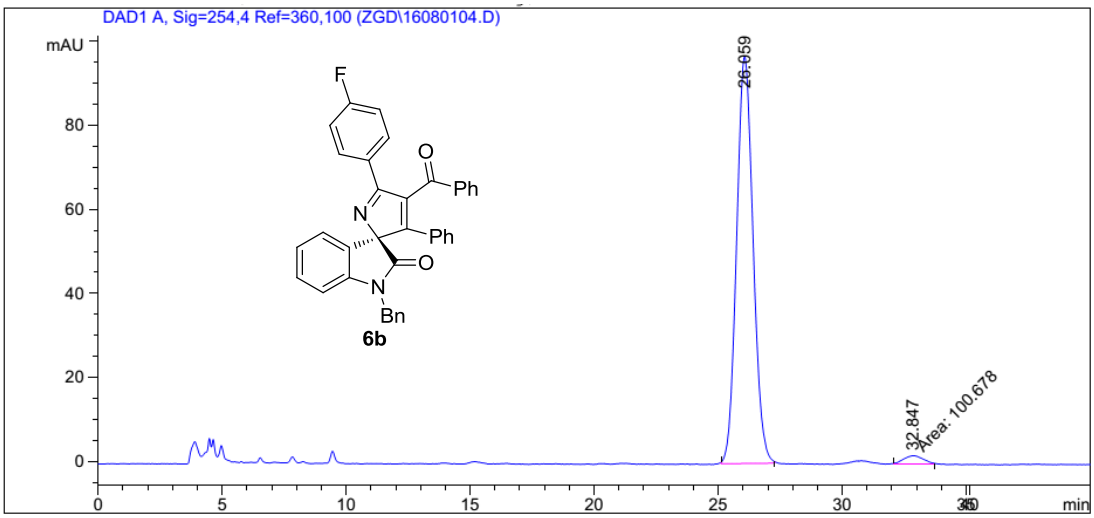
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	25.603	BV	0.6903	3587.66479	79.53097	49.9494
2	27.314	VB	0.7414	3594.93481	73.13801	50.0506



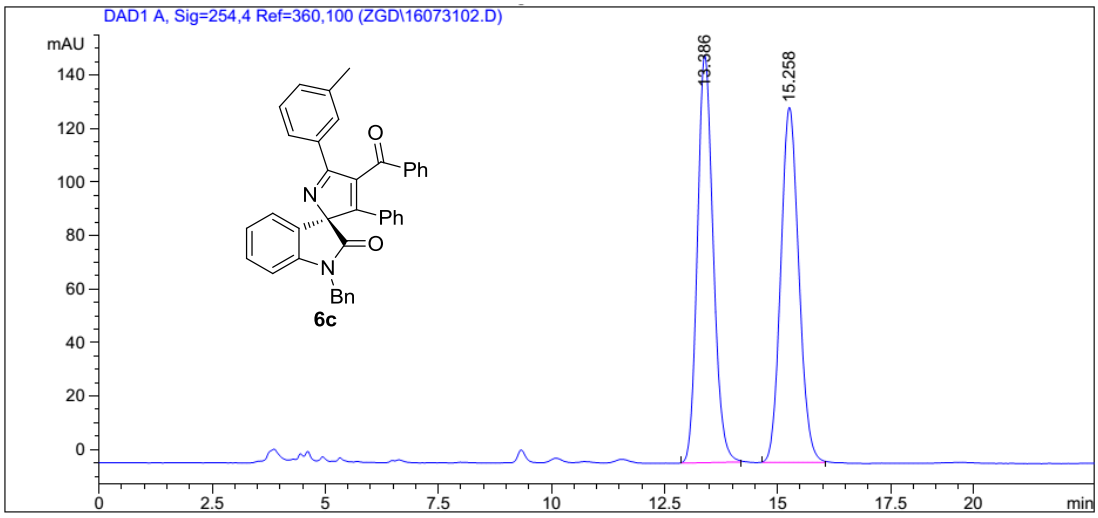
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	26.246	MM	0.7808	6223.97412	132.85262	98.4865
2	28.128	MM	0.7308	95.64865	2.18122	1.5135



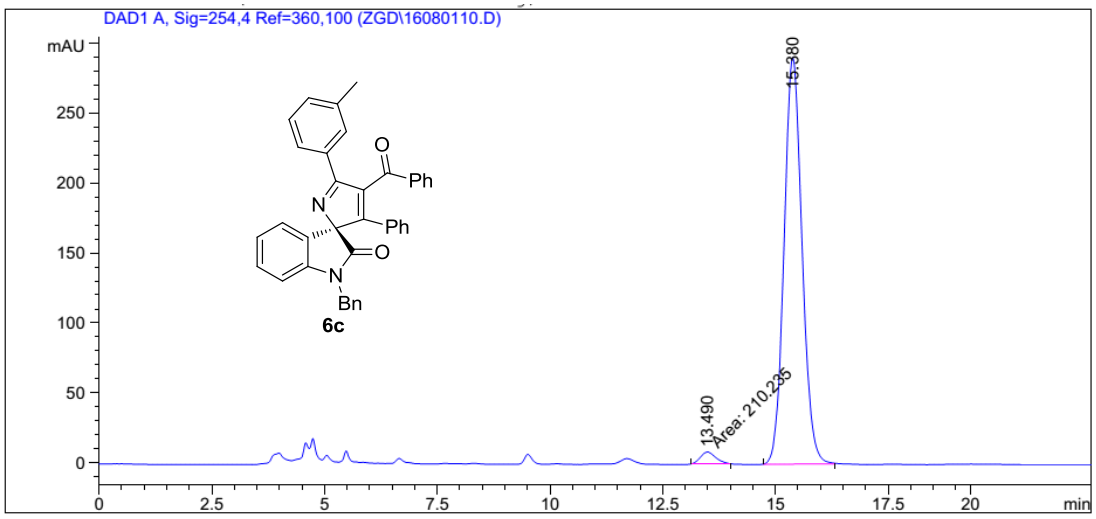
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	26.150	BB	0.7078	2870.55713	62.04610	50.6728
2	32.908	BB	0.8807	2794.32690	46.78971	49.3272



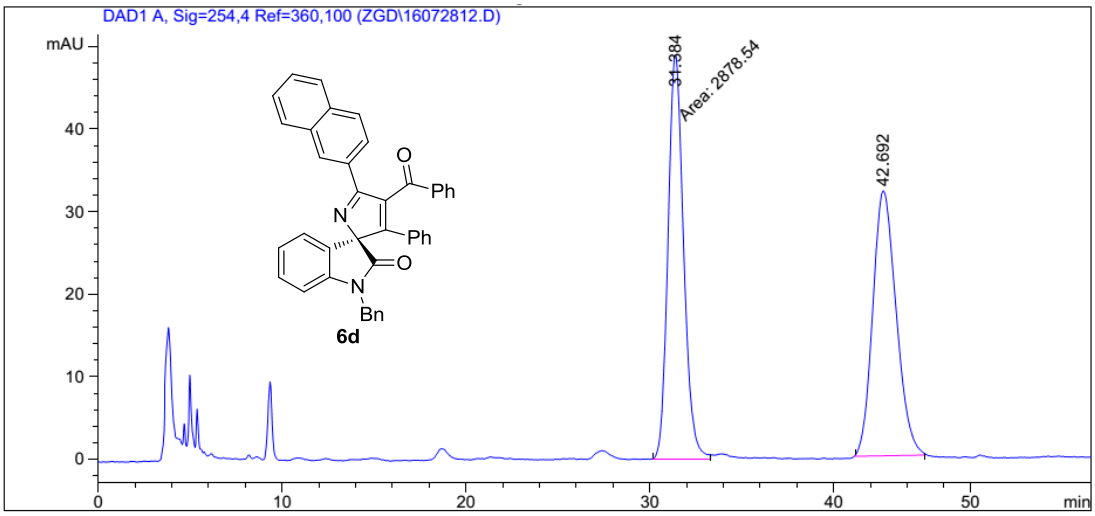
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	26.059	BB	0.7113	4460.30615	96.85553	97.7926
2	32.847	MM	0.8796	100.67838	1.90776	2.2074



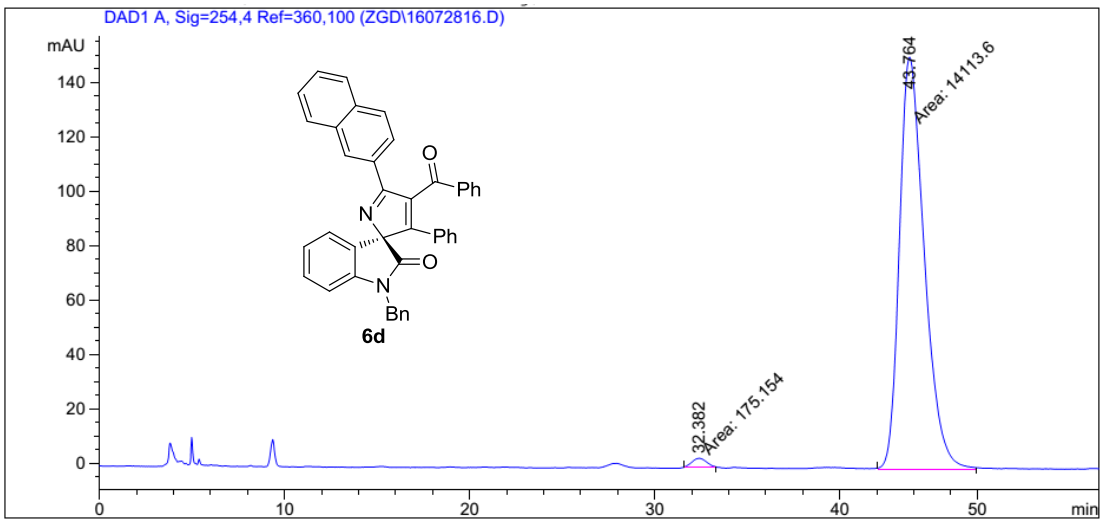
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	13.386	BB	0.3765	3686.38501	152.22832	50.0361
2	15.258	BB	0.4315	3681.05884	132.74548	49.9639



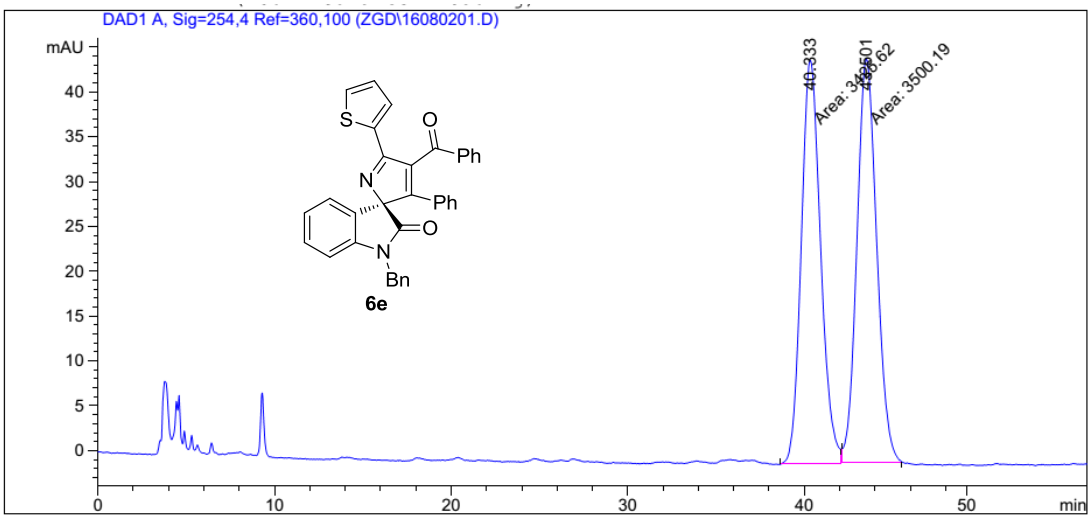
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	13.490	MM	0.4043	210.23512	8.66722	2.5475
2	15.380	BB	0.4287	8042.28223	290.75464	97.4525



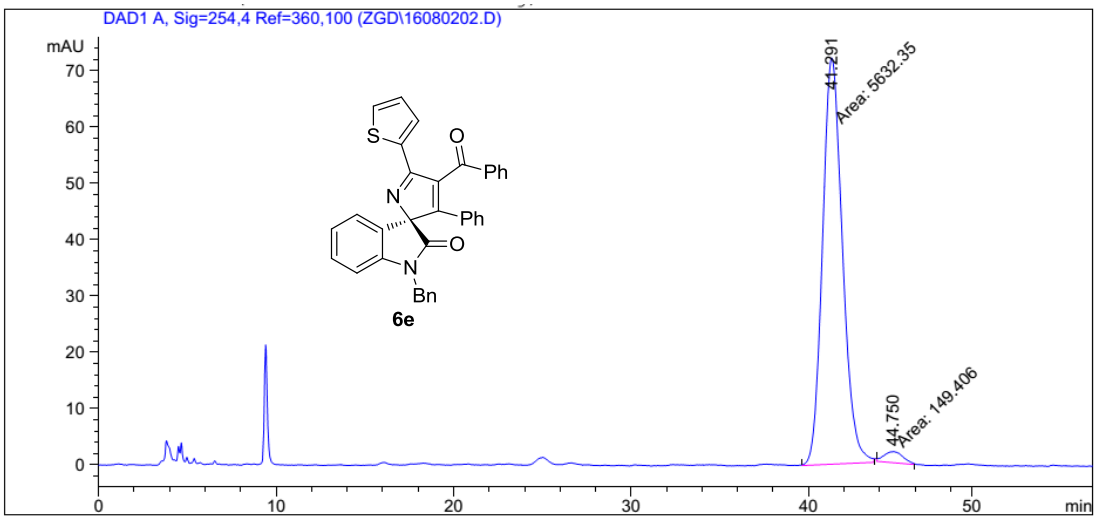
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	31.384	MM	0.9803	2878.53711	48.94133	50.3338
2	42.692	BB	1.0435	2840.35522	32.12421	49.6662



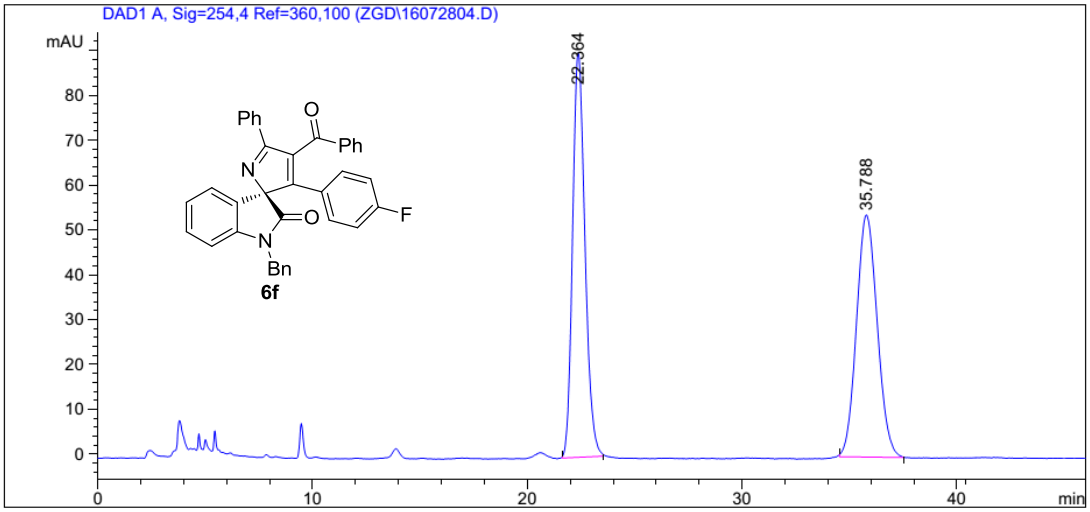
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	32.382	MM	0.8941	175.15419	3.26497	1.2258
2	43.764	MM	1.5543	1.41136e4	151.34146	98.7742



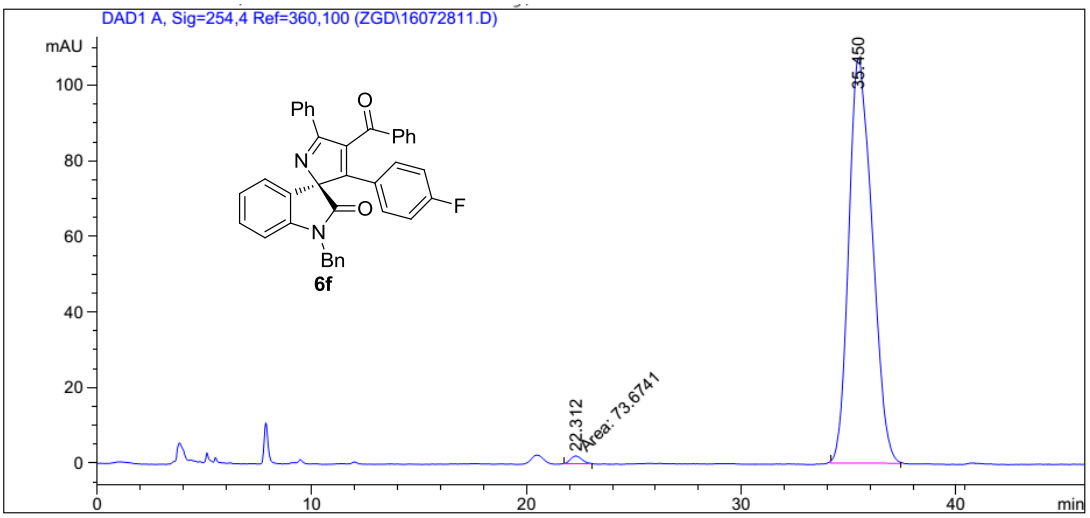
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	40.333	MM	1.2685	3425.61841	45.00711	49.4616
2	43.501	MM	1.2949	3500.19141	45.05029	50.5384



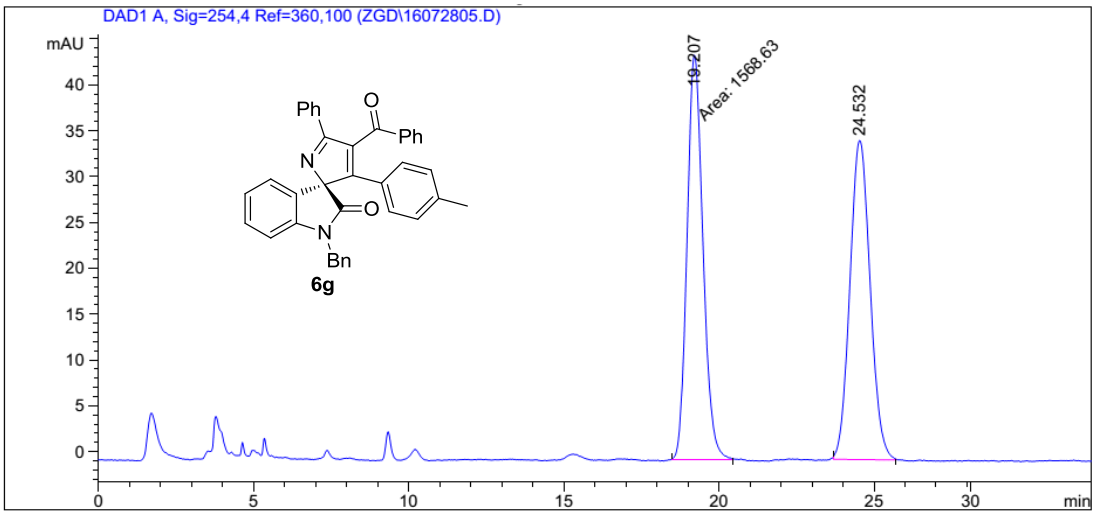
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	41.291	MM	1.3002	5632.34521	72.19974	97.4159
2	44.750	MM	1.2489	149.40550	1.99389	2.5841



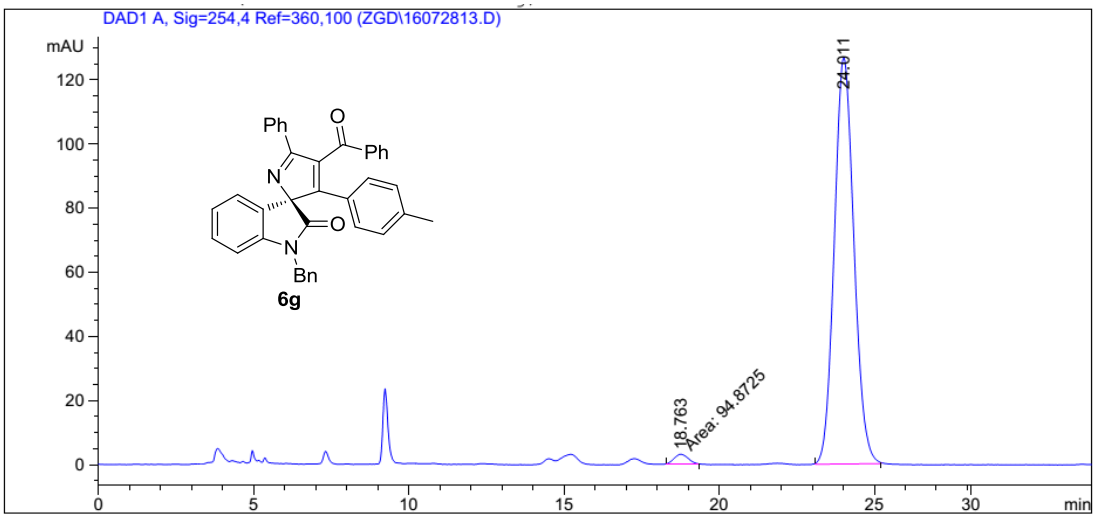
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	22.364	BB	0.6142	3603.20117	90.16087	49.8542
2	35.788	BB	0.9793	3624.28149	53.97836	50.1458



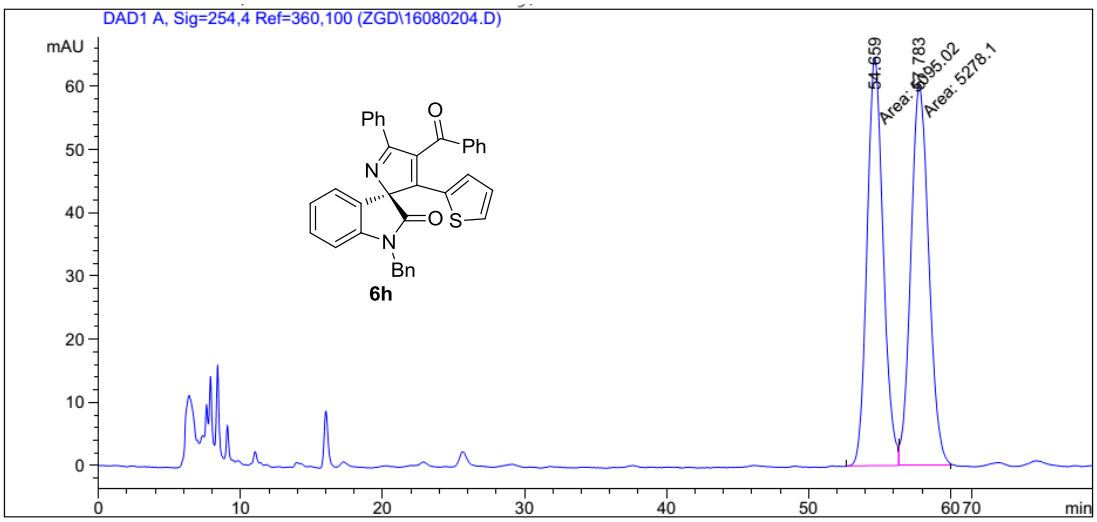
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	22.312	MM	0.5997	73.67406	2.04741	0.8987
2	35.450	BB	1.0590	8124.40918	107.34961	99.1013



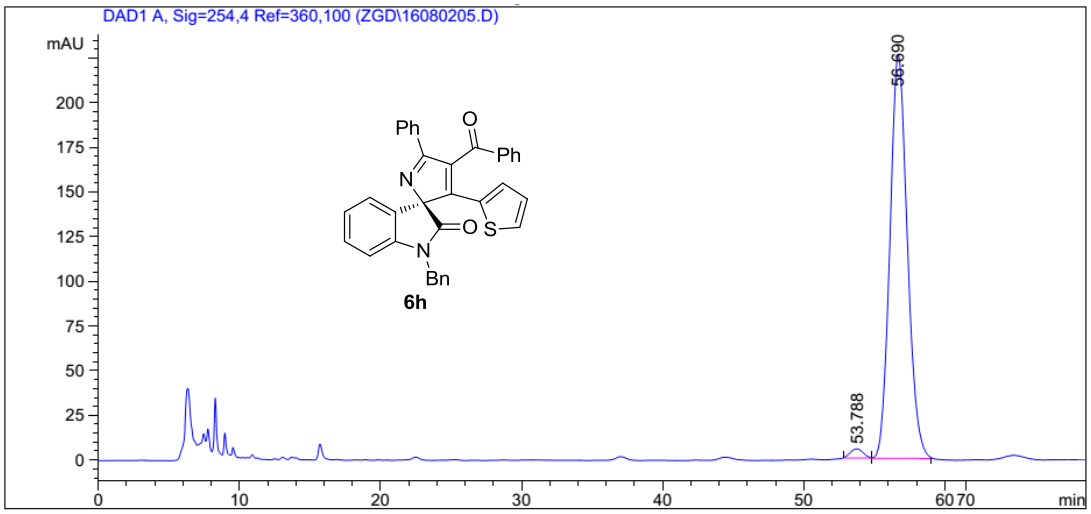
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	19.207	MM	0.5928	1568.62817	44.10250	49.9080
2	24.532	BB	0.6758	1574.41345	34.80036	50.0920



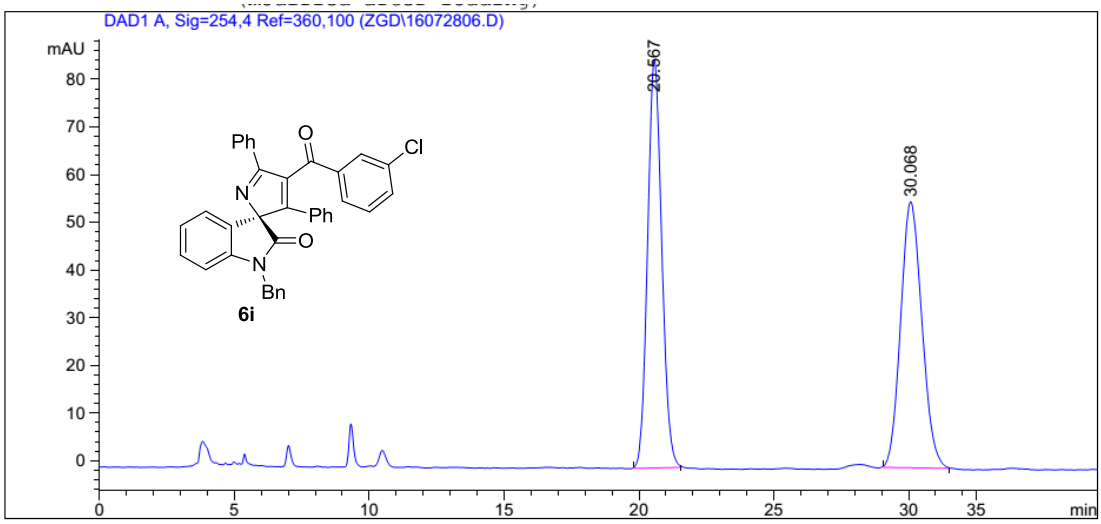
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	18.763	MM	0.5194	94.87246	3.04411	1.6751
2	24.011	BB	0.6870	5568.74316	126.63853	98.3249



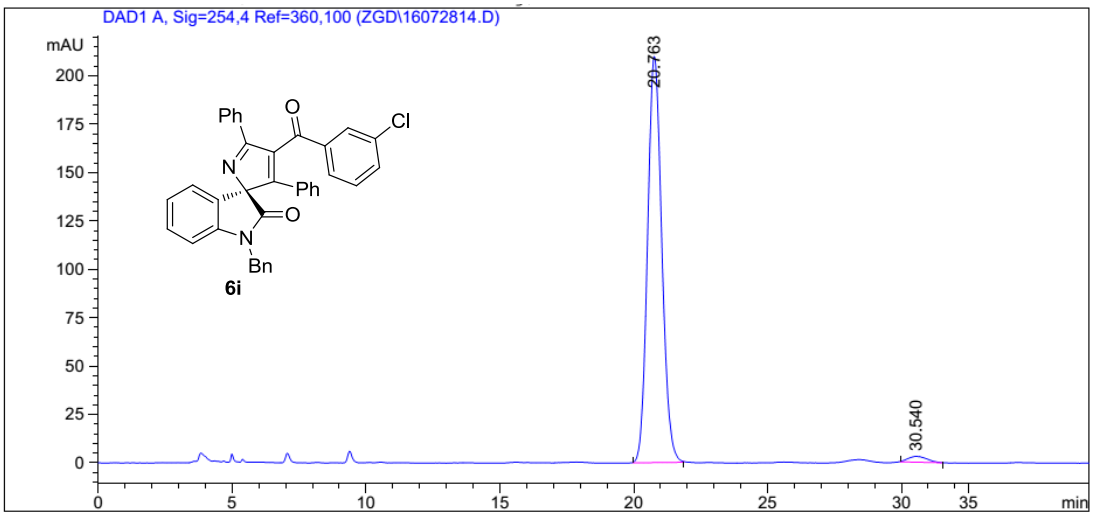
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	54.659	MM	1.3162	5095.01611	64.51736	49.1175
2	57.783	MM	1.4631	5278.10059	60.12587	50.8825



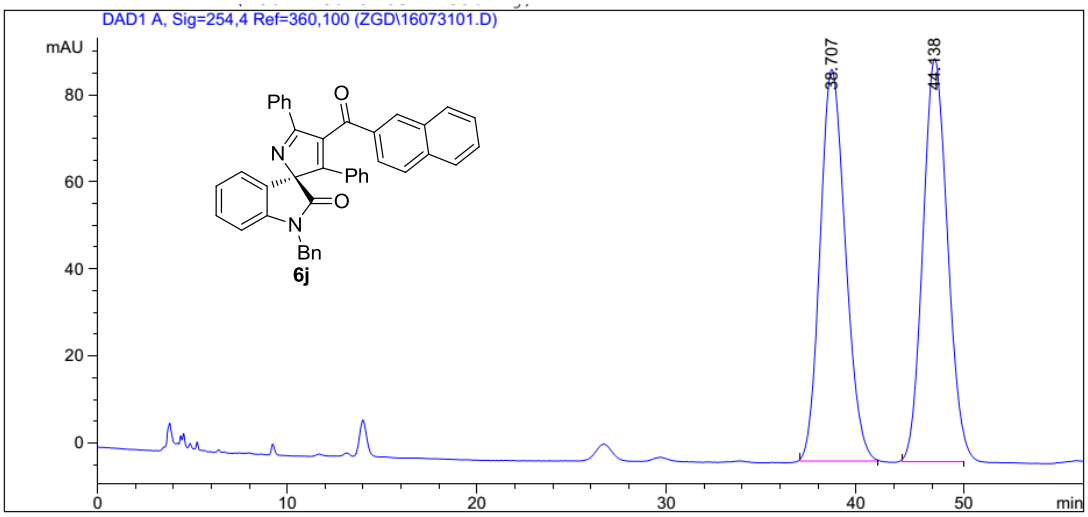
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	53.788	BV	0.7577	329.70859	5.15825	1.6712
2	56.690	VB	1.1843	1.93989e4	225.79892	98.3288



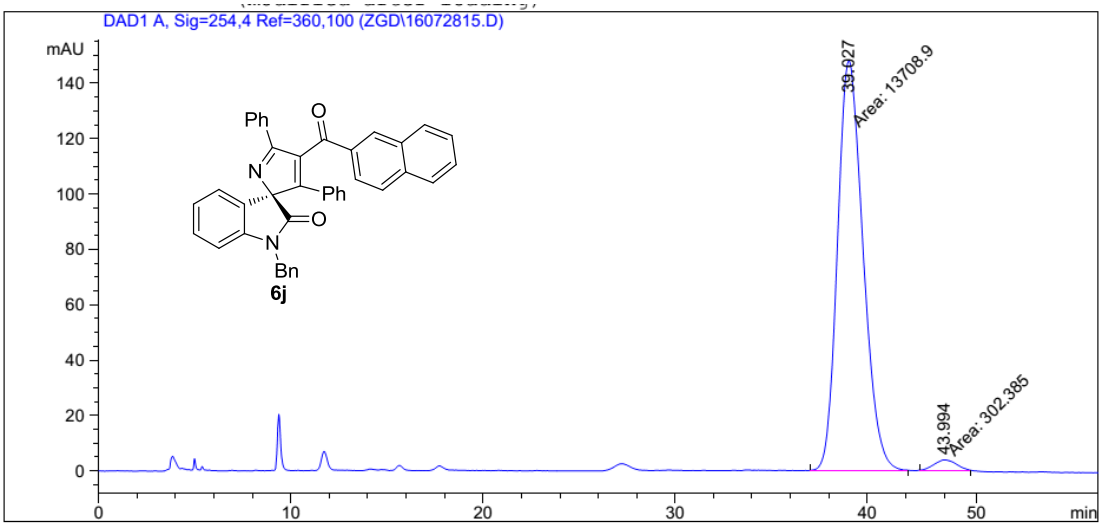
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	20.567	BB	0.5681	3108.70630	85.50920	50.4378
2	30.068	BB	0.7845	3054.73926	55.81464	49.5622



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	20.763	BB	0.5739	7736.89648	209.97536	98.0869
2	30.540	BB	0.5948	150.90189	3.03109	1.9131



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	38.707	BB	1.2399	8347.71387	90.01738	49.9396
2	44.138	BB	1.1644	8367.89844	92.59071	50.0604



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	39.027	MM	1.5411	1.37089e4	148.25916	97.8418
2	43.994	MM	1.3447	302.38461	3.74787	2.1582

6. Crystal data of 5f

Empirical formula C37 H27 Br N2 O2

Formula weight 611.52

Temperature (K) 297(2)

Crystal system Monoclinic

Space group P2(1)

a (Å) 17.9007(6)

b (Å) 13.4705(4)

c (Å) 18.9244(7)

α(°) 90.00

β(°) 98.1603(16)

γ(°) 90.00

Volume ($Å^3$) 4517.1(3)

Z 6

Dcalcd (g cm^3) = 1.349

μ(mm^{-1}) =1.401

F (000) = 1884

Theta range for data collection 2.11 to 25.00

Index ranges -21<=h<=21, -16<=k<=16, -20<=l<=22

Reflections collected 101610

Independent reflections 15834 [R(int) = 0.0434]

Data/restraints/parameters 15834/1/1135

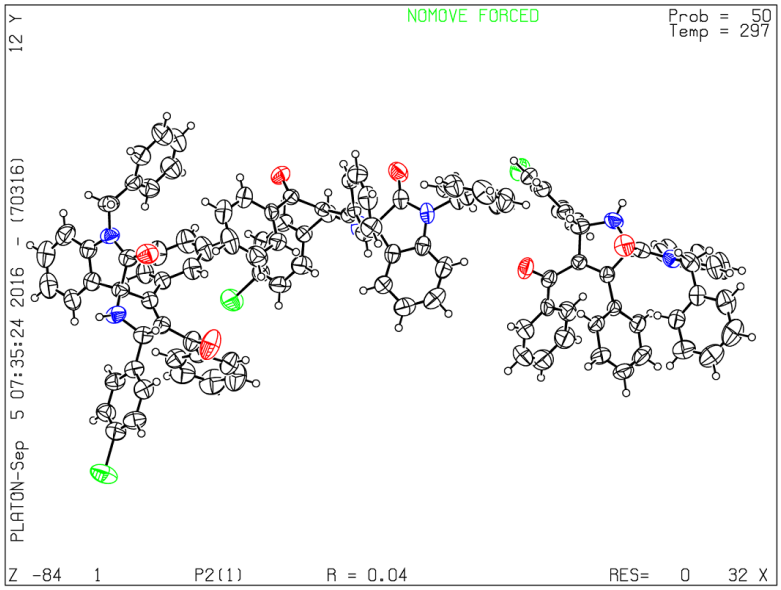
GOF (on F^2) 0.988

Final R indexes [I>=2σ (I)] R1 = 0.0391, wR2 = 0.0839

Final R indexes [all data] R1 = 0.0736, wR2 = 0.0923

Largest diff. peak and hole (e $Å^{-3}$) 0.273/-0.391

Flack parameter 0.009(4)



7. References

1. For the synthesis of 3-amino oxindole hydrochloride, see: W.-B. Chen, Z.-J. Wu, J. Hu., L.-F. Cun, X.-M. Zhang, W.-C. Yuan, *Org. Lett.* **2011**, *13*, 2472.
2. For the synthesis of α,β-ynones, see: J. P. Waldo, R. C. Larock, *J. Org. Chem.* **2007**, *72*, 9643.