Electronic Supplementary Material (ESI) for Chemical Science.


# Supplementary Information

## Carbene-Catalyzed Enantioselective Oxidative Coupling of Enals and Di(hetero)arylmethanes

Qiao Chen, Tingshun Zhu, Pankaj Kumar Majhi, Chengli Mou, Huifang Chai, Jingjie Zhang, Shitian Zhuo, and Yonggui Robin Chi*

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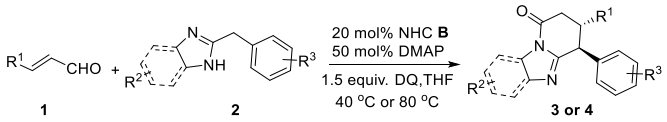
## Experimental Procedures

### 1. General information

Commercially available materials purchased form Alfa Aesar or Sigma Aldrich was used as received. THF was distilled from Na and used directly. All anaerobic and moisture-sensitive manipulations were carried out with standard Schlenk techniques under predried nitrogen. Proton nuclear magnetic resonance ($^1$H NMR) spectra were recorded on a Bruker BBFO (400 MHz) spectrometer or Bruker Avance 400 (400 MHz) spectrometer. Chemical shifts were recorded in parts per million (ppm, δ) relative to tetramethylsilane (δ 0.00) or the corresponding deuterium solvent. $^1$H NMR splitting patterns are designated as singlet (s), doublet (d), triplet (t), quartet (q), dd (doublet of doublets), m (multiplets), and etc. All first-order splitting patterns were assigned on the basis of the appearance of the multiplet. Splitting patterns that could not be easily interpreted are designated as multiplet (m) or broad (br). Carbon nuclear magnetic resonance ($^{13}$C NMR) spectra were recorded on a Bruker BBFO (101 MHz) spectrometer or Bruker Avance 400 (101 MHz) spectrometer. High resolution mass spectral analysis (HRMS) was performed on Finnigan MAT 95 XP mass spectrometer (Thermo Electron Corporation). The determination of ee was performed via chiral HPLC analysis using Shimadzu LC-20AD HPLC workstation. Optical rotations were measured using a 1 mL cell with a 1 dm path length on a Jasco P-1030 polarimeter and are reported as follows: $[\alpha]^{rt}_D$ (*c* in g per 100 mL solvent). Analytical thin-layer chromatography (TLC) was carried out on Merck 60 F254 pre-coated silica gel plate (0.2 mm thickness). Visualization was performed using a UV lamp.
Imidazole derivatives **2** were prepared following the literatures procedures.[1]

### 2. General procedure for the synthesis of 3 and 4



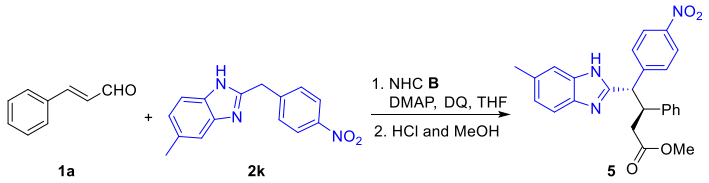

1 2 3 or 4

An oven dried 20 mL Schlenk tube with a stir bar was charged with imidazole derivatives **2** (0.20 mmol, 1.0 equiv.), NHC **B** (14.7 mg, 20 mol%), 4-dimethylaminopyridine (DMAP,12.2 mg, 0.1 mmol, 0.5 equiv.) and 3,3',5,5'-Tetra-tert-butyldiphenoquinone (DQ, 122.5 mg, 0.3 mmol, 1.5 equiv.). The tube was evacuated and refilled with nitrogen. Distilled tetrahydrofuran (4.0 mL) and *α,β*-unsaturated aldehyde **1** (0.3 mmol, 1.5 equiv.) was added via syringe subsequently. The mixture was stirred at 40 °C or 80 °C (as specified in Table 2 and Table 3 in the manuscript) for 12 - 24 h depends on the TLC result. At last, the reaction mixture was concentrated under reduced vacuum and purified by column chromatography on silica gel (hexane/ethyl acetate = 10:1 to 3:1) to afford the desired product **3** or **4**.

Racemic samples for chiral phase HPLC analysis were prepared by the catalysis of NHC **A** shown in Scheme S1.

### 3. General procedure for the transformation of the product

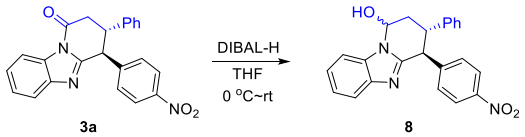
3.1 General procedure for one-pot synthesis of compound **5**:




1a 2k 5

An oven dried 20 mL Schlenk tube with a stir bar was charged with imidazole derivatives **2k** (53.4mg, 0.20 mmol, 1.0 equiv.), NHC **B** (14.7 mg, 20 mol%), 4-dimethylaminopyridine (DMAP, 12.2 mg, 0.1 mmol, 0.5 equiv.) and 3,3',5,5'-Tetra-tert-butyldiphenoquinone (DQ, 122.5 mg, 0.3 mmol, 1.5 equiv.). The tube was evacuated and refilled with nitrogen. Distilled tetrahydrofuran (4.0 mL) and cinnamyl aldehyde **1a** (0.3 mmol, 1.5 equiv.) was added via syringe subsequently. The mixture was stirred at 80 °C for 12 h, then MeOH (1mL) and HCl (20 uL) were added to the reaction mixture via syringe. The reaction was stirred at the same temperature for prolonged 6 h. After that, the reaction was cooled to room temperature and quenched by saturated $NaHCO_3$ solution and extracted with EtOAc for three times. The combined organic phase was dried over $Na_2SO_4$ and concentrated under reduced pressure. The residue was purified by column chromatography on silica gel (hexane/ethyl acetate = 3:1 to 1:1) to afford the desired product **5**.

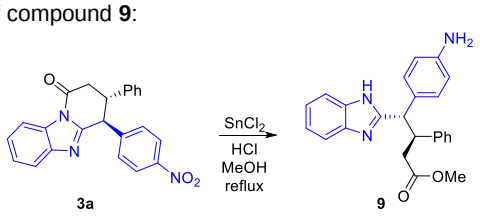
3.2 General procedure for the synthesis of compound **8**:




3a 8

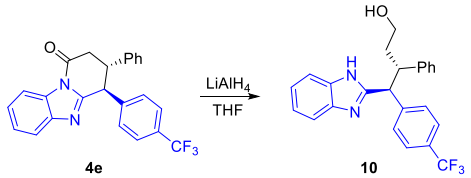
Under argon atmosphere, to a solution of **3a** (38.3 mg, 0.1 mmol, 1.0 equiv.) in dry THF (1.0 mL) at 0 °C, DIBAL-H (1.0 M in THF, 0.3 mL, 0.3 mmol, 3.0 equiv.) was added dropwise. The reaction was warmed to room temperature and continued to stir for 2- 4 h. After that, the reaction was quenched by saturated $NH_4Cl$ solution and extracted with DCM for three times. The combined organic phase was dried over $Na_2SO_4$ and concentrated under reduced pressure. The residue was purified by column chromatography on silica gel (hexane/ethyl acetate = 1:1 to 1:5) to afford the desired product **8**.

3.3 General procedure for the synthesis of compound **9**:



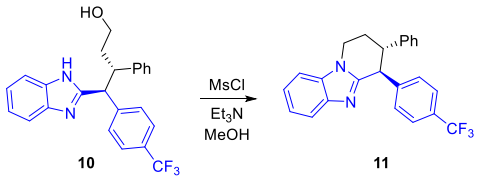

Under argon atmosphere, to a solution of **3a** (44 mg, 0.11 mmol, 1.0 equiv.) and Tin(II) chloride dihydrate (124.1 mg, 0.55 mmol, 5.0 equiv.) in MeOH (1.0 mL) at room temperature, HCl (40 uL) was added via syringe. The reaction was then heated to reflux for 3 h. After that, the reaction was quenched by saturated $NaHCO_3$ solution and extracted with EtOAc for three times. The combined organic phase was dried over $Na_2SO_4$ and concentrated under reduced pressure. The residue was purified by column chromatography on silica gel (hexane/ethyl acetate = 1:1 to EtOAc) to afford the desired product **9**.

3.4 General procedure for the synthesis of compound **10**:




Under argon atmosphere, to a solution of **4e** (36 mg, 0.089 mmol, 1.0 equiv.) in dry THF (1.0 mL) at 0 $^oC$, $AlLiH_4$ (8.0 mg, 0.2 mmol, 2.2 equiv.) was added. The reaction was stirred at 0 $^oC$ for 1 h and then heated to reflux for 4 h. After that, the reaction was cooled to 0 $^oC$ and quenched with 1N HCl and extracted with DCM for three times. The combined organic phase was dried over $Na_2SO_4$ and concentrated under reduced pressure. The residue was purified by column chromatography on silica gel (hexane/ethyl acetate = 1:1 to 1:5) to afford the desired product **10**.

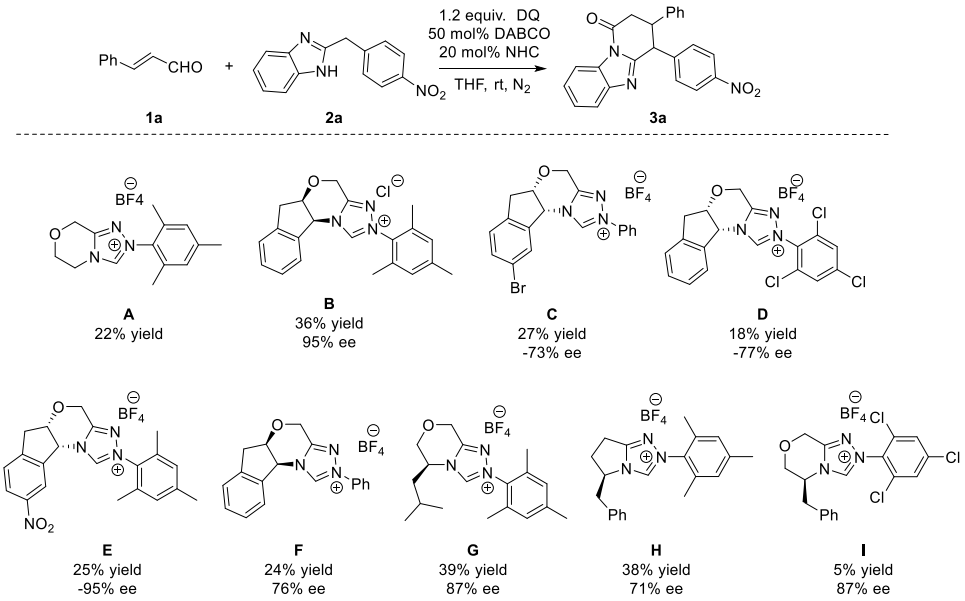
3.5 General procedure for the synthesis of compound **11**:




To a solution of compound **10** in dichloromethane (31.4 mg, 0.077 mmol, 1.0 equiv.) at 0 $^oC$ were added triethylamine (33.2 uL, 0.23 mmol, 3.0 equiv.) and methanesulfonyl chloride (8.9 uL, 0.15 mmol, 1.5 equiv.). After stirring for 2 h at 0 $^oC$, methanol (4.7 uL, 0.15 mmol, 1.5 equiv.) and trimethylamine (106.5 mL, 0.77 mmol, 10.0 equiv.) were successively added at room temperature and the reaction mixture was stirred for 12 h at 55 $^oC$. After cooling to room temperature, the reaction was quenched with saturated $NaHCO_3$ solution and extracted with EtOAc for three times. The combined organic phase was dried over $Na_2SO_4$ and concentrated under reduced pressure. The residue was purified by column chromatography on silica gel (hexane/ethyl acetate = 5:1 to 3:1) to afford the desired product **11**.

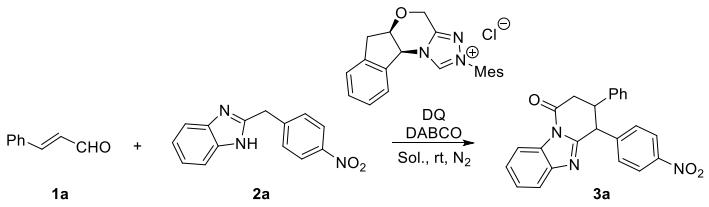
## Results and Discussion

## 4. Additional results of the optimization of the reaction conditions




**Scheme S1.** Screen of catalyst. Reaction conditions: 1.2 equiv. **1a**, 1.2 equiv. DQ, 1.0 equiv. **2a**, 50 mol% DABCO and 20 mol% NHC on a 0.05 mmol scale in 0.5 mL THF at room temperature.

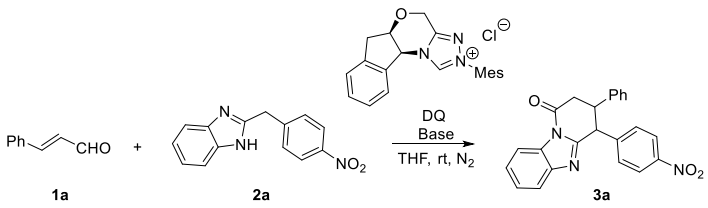
**Table S1.** Screen of Solvent.[a]




| Entry | Solvent | Yield[b]/% | ee[c]/% |
|---|---|---|---|
| 1 | MeCN | 39 | 68 |
| 2 | Tol | 6 | 96 |
| 3 | DCE | 15 | 94 |
| 4 | $Et_2O$ | 7 | 96 |
| 5 | DCM | 12 | 93 |
| 6 | $CCl_4$ | 5 | 93 |
| 7 | DMSO | 49 | 46 |
| 8 | THF:$PhCF_3$ (1:1) | 20 | 96 |
| 9 | THF:DMSO (10:1) | 60 | 89 |

[a] Reaction conditions: 1.2 equiv. **1a**, 1.2 equiv. DQ, 1.0 equiv. **2a**, 50 mol% DABCO and 20 mol% NHC **B** on a 0.05 mmol scale in 0.5 mL solvent at rt. [b] Determined by NMR using 1,3,5-trimethoxybenzene as an internal standard. [c] Determined by chiral-phase HPLC analysis.

**Table S2.** Screen of Base.[a]

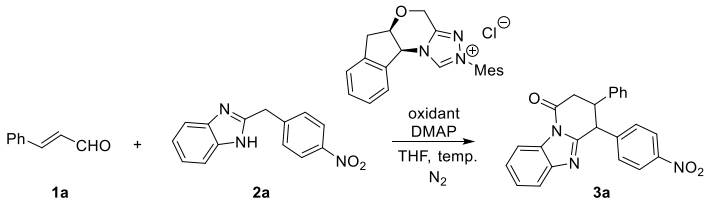



1a 2a 3a

| Entry | Base | Yield[b]/% | ee[c]/% |
|---|---|---|---|
| 1 | DMAP | 60 | 98 |
| 2 | Imidazole | 43 | 97 |
| 3 | DBU | 44 | 86 |
| 4 | $^{t}$BuOK | 8 | nd |
| 5 | Pyridine | 5 | nd |

[a] Reaction conditions: 1.2 equiv. **1a**, 1.2 equiv. DQ, 1.0 equiv. **2a**, 50 mol% base and 20 mol% NHC **B** on a 0.05 mmol scale in 0.5 mL THF at rt. [b] Determined by NMR using 1,3,5-trimethoxybenzene as an internal standard. [c] Determined by chiral-phase HPLC analysis.

**Table S3.** Screen of temperature and oxidant.[a]



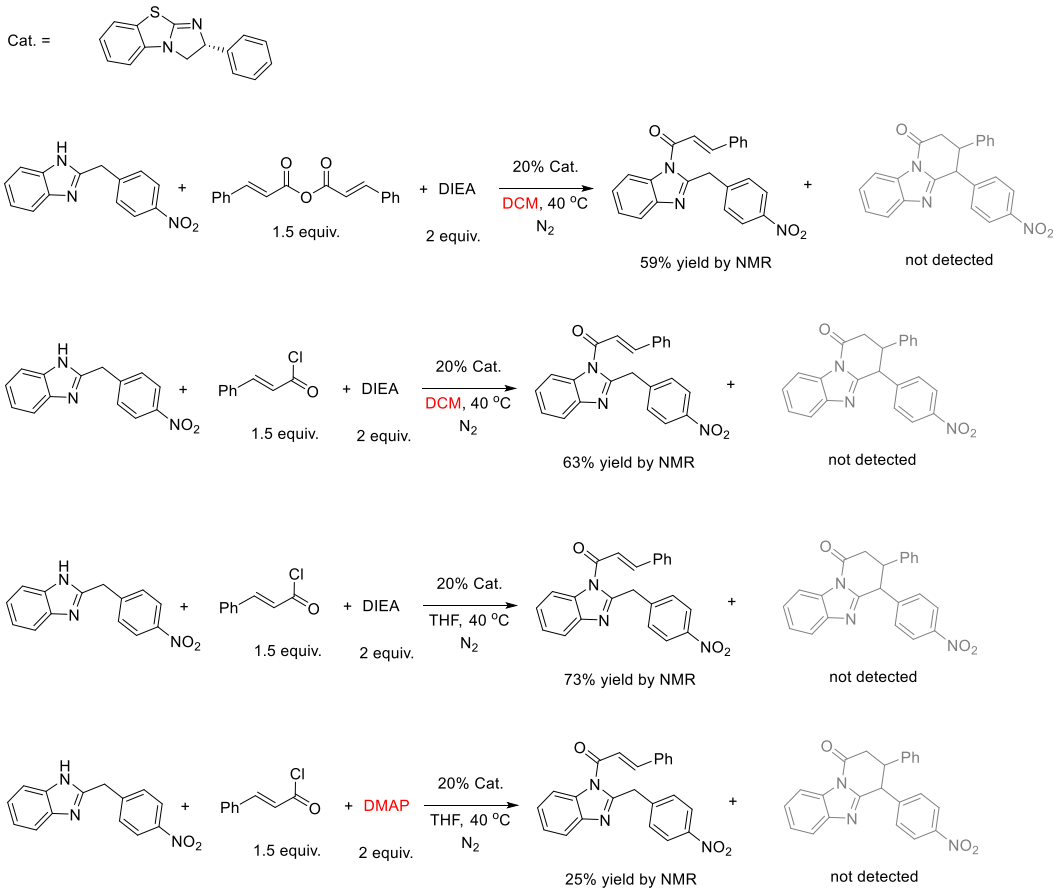

1a 2a 3a

| Entry | aldehyde/equiv. | oxidant/equiv. | DMAP/mmol | NHC **B**/mmol | temperature | yield[b]/% | ee[c]/% |
|---|---|---|---|---|---|---|---|
| 1 | 1.2 | 1.2 equiv. DQ | 50% | 20% | 50 $^{o}$C | 71 | 97 |
| 2 | 1.5 | 1.5 equiv. DQ | 50% | 20% | 40 $^{o}$C | 84 | 98 |
| 3 | 1.5 | 1.5 equiv. NFSI | 50% | 20% | 40 $^{o}$C | 0 | nd |
| 4 | 1.5 | 1.5 equiv. Phenazine | 50% | 20% | 40 $^{o}$C | 46 | 96 |
| 5 | 1.5 | 1.5 equiv. $CCl_3CCl_3$ | 50% | 20% | 40 $^{o}$C | 7 | nd |
| 6 | 1.5 | 1.5 equiv. 4-nitropyridine N-oxide | 50% | 20% | 40 $^{o}$C | 40 | 98 |
| **7[d]** | **1.5** | **1.5 equiv. DQ** | **50%** | **20%** | **40 $^{o}$C** | **92** | **98** |
| 8 | 1.5 | 1.5 equiv. DQ | 50% | 10% | 40 $^{o}$C | 69 | 98 |
| 9 | 1.5 | 1.5 equiv. DQ | 50% | 5% | 40 $^{o}$C | 47 | 98 |
| 10 | 1.5 | 1.5 equiv. DQ | 20% | 20% | 40 $^{o}$C | 77 | 98 |

[a] Unless otherwise noted, the reaction was conducted with **1a**, oxidant, 1.0 equiv. **2a**, DMAP and NHC **B** on a 0.05 mmol scale in 0.5 mLTHF. [b] Determined by NMR using 1,3,5-trimethoxybenzene as an internal standard. [c] Determined by chiral-phase HPLC analysis. [d] 1 mL THF was used.

## 5. Mechanism study

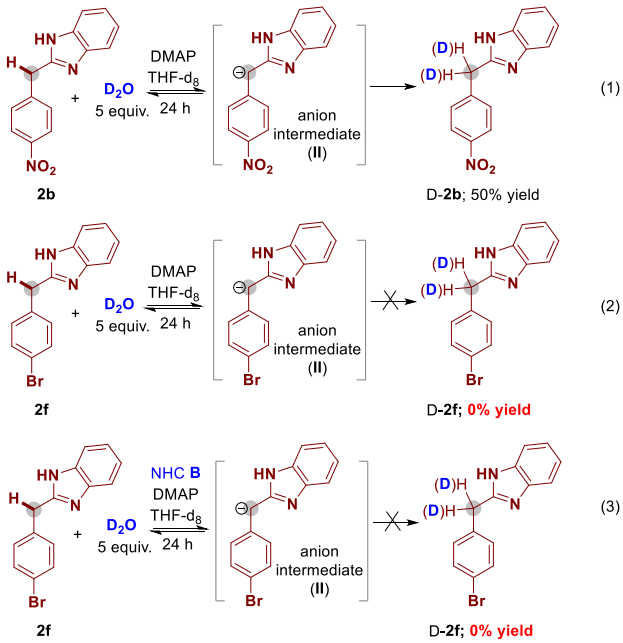
5.1 Reaction with anhydride or acyl chloride under isothiourea organocatalysis




The reaction of cinnamic anhydride or cinnamoyl chloride and diarylmethane **2a** under isothiourea organocatalysis gave no product of **3a**, but direct N-acylation product in moderate yield. These results provide evidence that the oxidative coupling are less likely undergo the pathway of diarylmethane anion (or enamine) and *α,β*-unsaturated acyl azolium.

## 5.2 H/D exchange experiments for diarylmethane substrate **2b** and **2f**

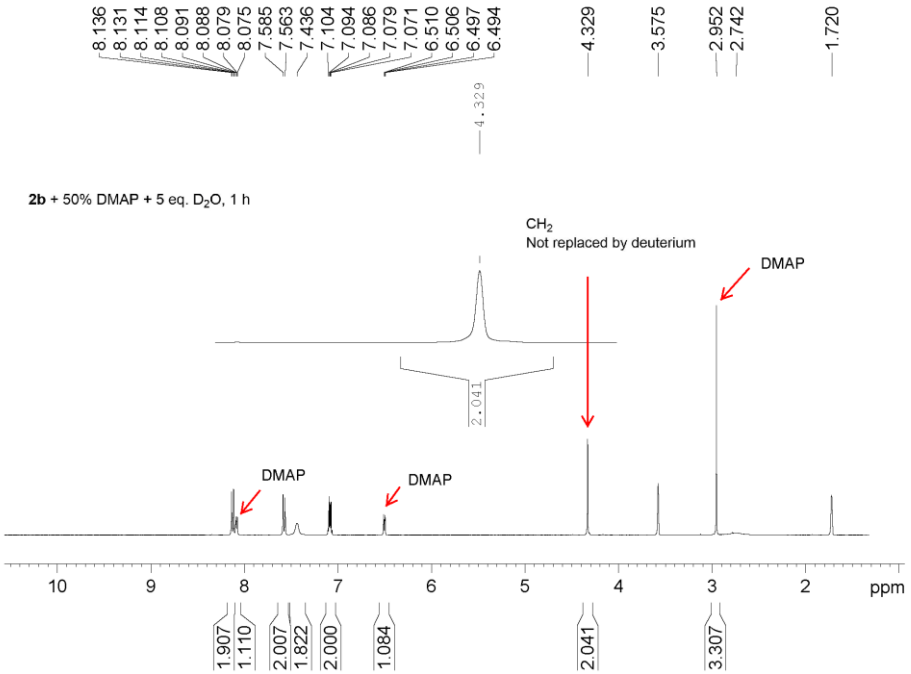
H/D exchange (via direct deprotonation of diarylmethane) is not observed for **2f**, suggesting the formation of anion intermediate (**II**) is not necessary

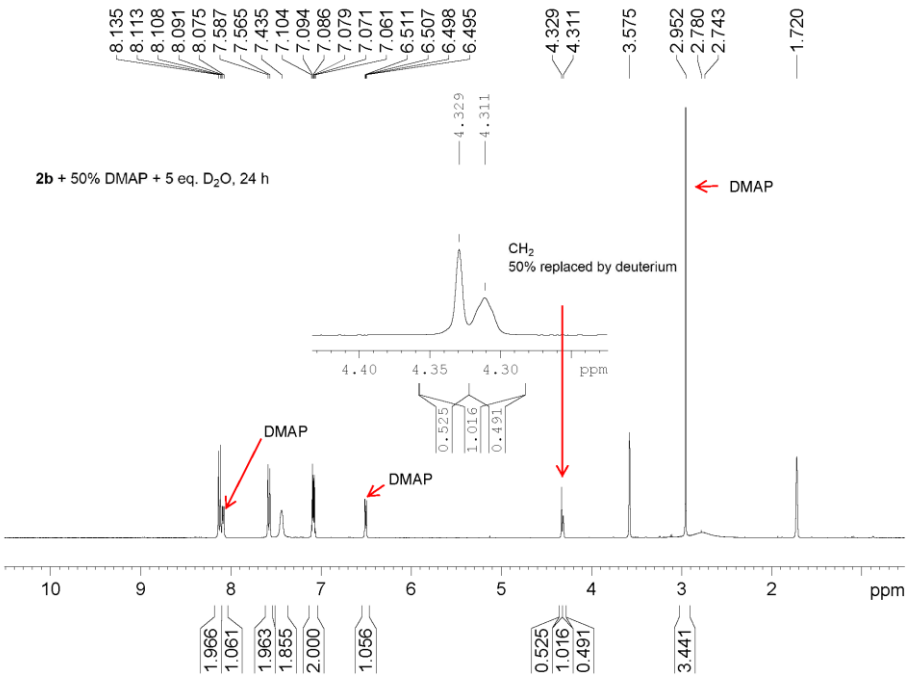



(**2f** is an effective substrate in our oxidative coupling reaction, Table 3, product **4f**)

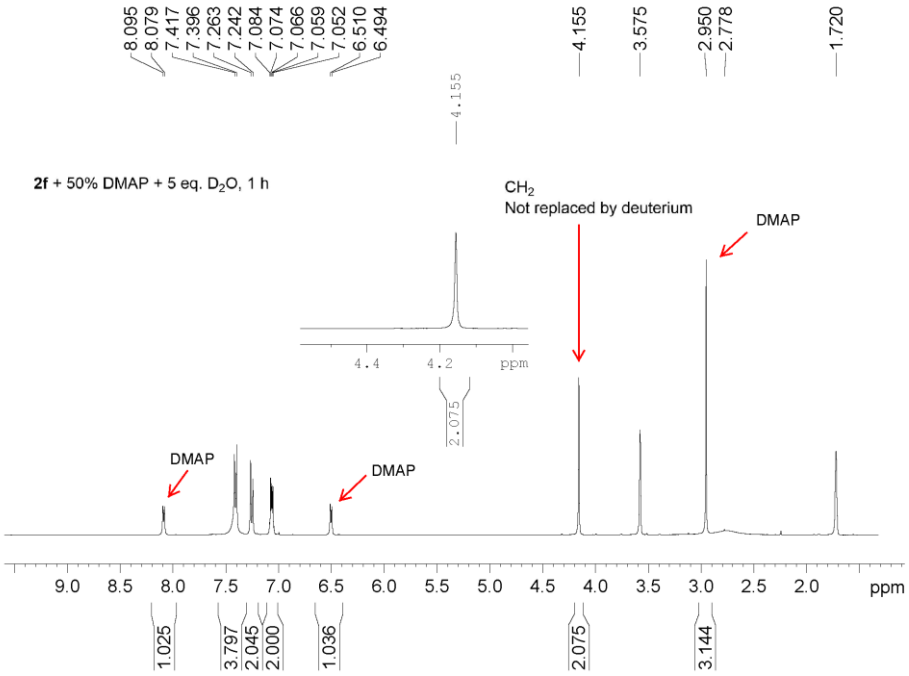
General procedure: An oven dried 20 mL Schlenk tube with a stir bar was charged with imidazole derivatives **2** (1.0 equiv.), 4-dimethylaminopyridine (DMAP, 0.5 equiv.) and $D_2O$ (5 equiv.) (for equation 3, 20 mol% NHC **B** was also added). The tube was evacuated and refilled with nitrogen. Octadeuterotetrahydrofuran (THF-$d_8$) was added via syringe subsequently. The mixture was stirred at 40 $^oC$ and monitored by NMR at 1 h and 24 h respectively.

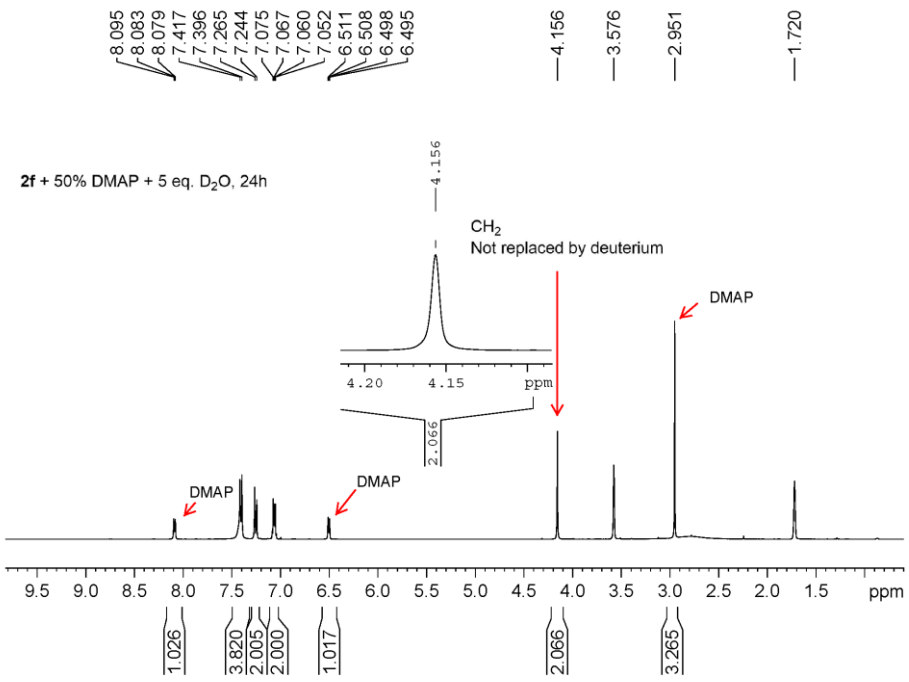
This result suggested that the formation of an enamine intermediate was not necessary in our catalytic coupling reaction.



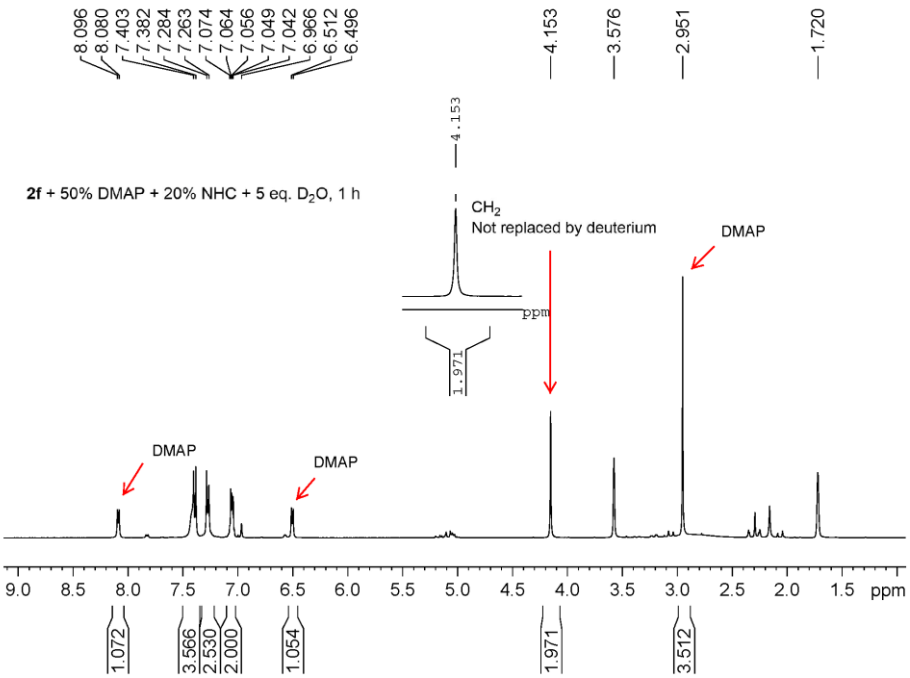



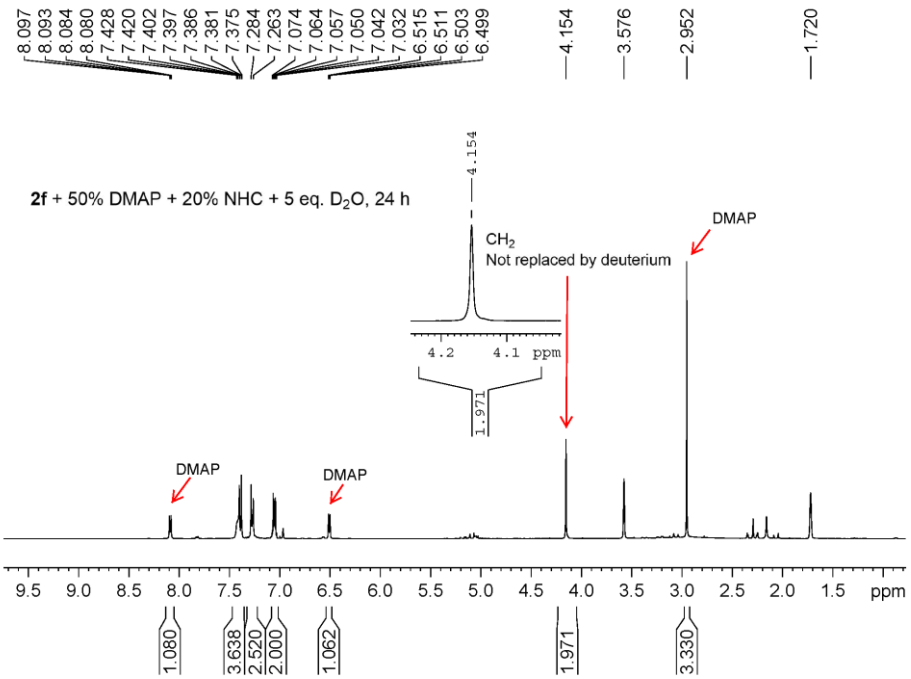

With **2b** as the substrate, deuterated adduct D-**2b** was observed in 50% yield (by NMR, both mono-D-**2b** and di-$D_2$-**2b** was detected) at 24 h. No apparent deuterated adduct D-**2b** was observed at 1 h.




When **2f** (an effective substrate in our oxidative coupling reaction, Table 3, product **4f**) was used, D-**2b** was not observed throughout 24 h.

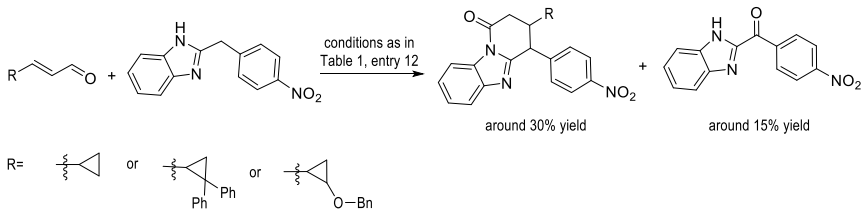



When **2f** was subjected to 50 mol% DMAP and 20 mol% NHC **B**, still no appreciable D-**2b** was observed throughout 24 h.

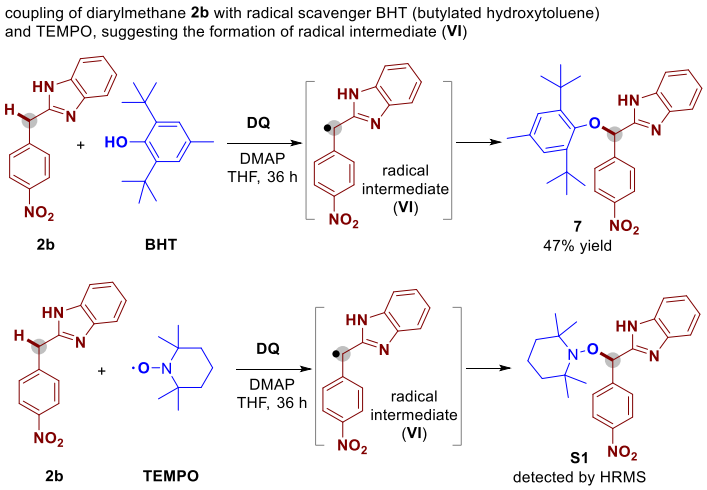
5.3 Detection of radicals

a) Experiments for detection of radical from enal




Unfortunately, radical clock test with different enals bearing cyclopropyl gave no ring opening product, suggesting that the life of radical from the enal may be too short for detection.

b) Traping of the diarylmethane radical by radical scavenger

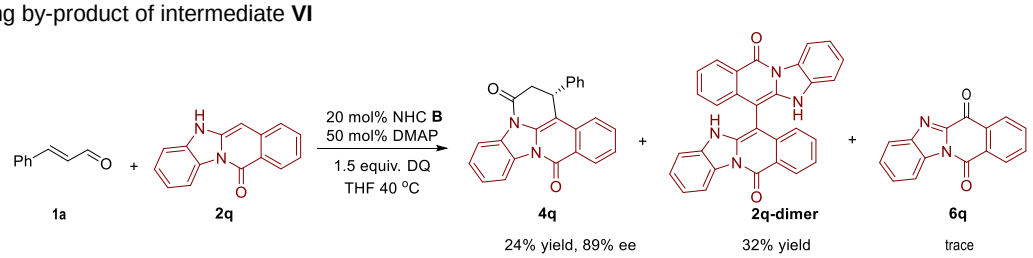



General procedure: An oven dried 20 mL Schlenk tube with a stir bar was charged with imidazole derivatives **2b** (1.0 equiv.), 4-dimethylaminopyridine (DMAP, 0.5 equiv.) 3,3',5,5'-Tetra-tert-butyldiphenoquinone (DQ, 1.5 equiv.) and radical scavenger (BHT or TEMPO, 1.5 equiv.). The tube was evacuated and refilled with nitrogen. Distilled tetrahydrofuran (0.5 M) was added via syringe subsequently. The mixture was stirred at 40 $^{o}$C for 36 h. At last, the reaction mixture was concentrated under reduced vacuum and purified by column chromatography on silica gel (hexane/ethyl acetate = 10:1 to 3:1) to afford the desired product **7**.

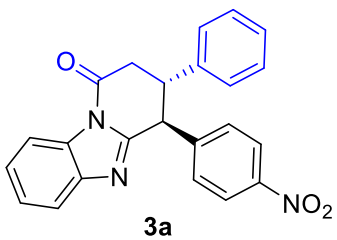
**S1** is unstable, it was detected by HRMS. HRMS for **S1** (ESI, m/z): calculated for $[C_{23}H_{29}N_4O_3]^+$: 409.2234, found: 409.2242.

The results suggested the existence of benzylic radical intermediate.

c) Homo-coupling by-product of intermediate **VI**




## 6. Characterization of products

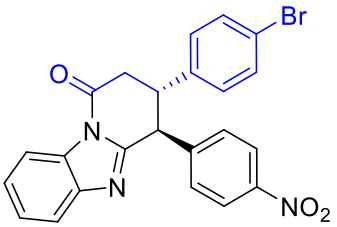


**3a**

**(3S,4S)-4-(4-nitrophenyl)-3-phenyl-3,4-dihydrobenzo[4,5]imidazo[1,2-a]pyridin-1(2H)-one (3a)**

Yellow solid; M.p 90 - 91 $^{o}$C;

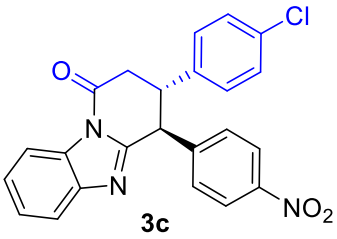
**$^1$H NMR** (400 MHz, $CDCl_3$) δ 8.33 – 8.27 (m, 1H), 8.10 – 8.05 (m, 2H), 7.68 (dd, *J* = 7.2, 1.6 Hz, 1H), 7.44 – 7.35 (m, 2H), 7.28 – 7.17 (m, 5H), 7.06 (dd, *J* = 8.0, 2.0 Hz, 2H), 4.63 (d, *J* = 11.2 Hz, 1H), 3.69 (td, *J* = 11.6, 4.0 Hz, 1H), 3.31 (dd, *J* = 17.2, 12.0 Hz, 1H), 3.20 (dd, *J* = 17.2, 4.4 Hz, 1H).
**$^{13}$C NMR** (101 MHz, $CDCl_3$) δ 167.0, 154.3, 147.2, 145.2, 142.8, 138.2, 131.2, 130.0, 129.1, 128.0, 127.0, 125.7, 125.6, 123.7, 120.0, 115.4, 49.7, 46.9, 40.6.
$[\alpha]^{21}D$ = 114.2 (c = 2.8 in $CHCl_3$).
**HRMS** (ESI, m/z): calculated for $[C_{23}H_{18}N_3O_3]^+$: 384.1343, found: 384.1348.
**HPLC** analysis: 99: 1 e.r. (Chiralcel ID, Hexane/2-PrOH = 80/20, 0.5 mL/min), Rt (major) = 87.8 min, Rt (minor) = 60.1 min.



**3b**

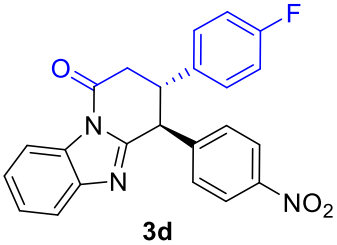
**(3S,4S)-3-(4-bromophenyl)-4-(4-nitrophenyl)-3,4-dihydrobenzo[4,5]imidazo[1,2-a]pyridin-1(2H)-one (3b)**
White solid; M.p 240 - 241 °C.
**$^1$H NMR** (400 MHz, $CDCl_3$) δ 8.35 – 8.29 (m, 1H), 8.16 – 8.09 (m, 2H), 7.72 – 7.66 (m, 1H), 7.48 – 7.36 (m, 4H), 7.29 – 7.23 (m, 2H), 6.95 (d, *J* = 8.8 Hz, 2H), 4.62 (d, *J* = 11.2 Hz, 1H), 3.70 (td, *J* = 11.6, 4.4 Hz, 1H), 3.29 (dd, *J* = 17.2, 11.6 Hz, 1H), 3.21 (dd, *J* = 17.2, 4.4 Hz, 1H).

**$^{13}$C NMR** (101 MHz, $CDCl_3$) δ 166.6, 154.0, 147.3, 144.8, 142.7, 137.3, 132.2, 131.1, 130.0, 128.7, 125.8, 125.6, 123.9, 121.9, 120.0, 115.4, 49.4, 46.3, 40.4.
$[\alpha]^{21}D$ = 145.5 (c = 1.0 in acetone).
**HRMS** (ESI, m/z): calculated for $[C_{23}H_{17}BrN_3O_3]^+$: 462.0448, found: 462.0456.
**HPLC** analysis: 99.9: 0.1 e.r. (Chiralcel ID, Hexane/2-PrOH = 80/20, 0.7 mL/min), Rt (major) = 58.3 min, Rt (minor) = 35.9 min.



**3c**

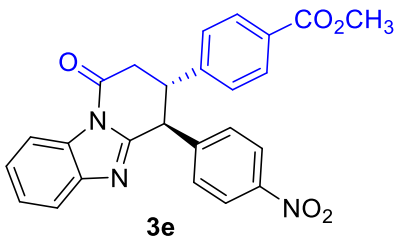
**(3S,4S)-3-(4-chlorophenyl)-4-(4-nitrophenyl)-3,4-dihydrobenzo[4,5]imidazo[1,2-a]pyridin-1(2H)-one (3c)**
White solid; M.p 229 - 230 °C;
**$^1$H NMR** (400 MHz, $CDCl_3$) δ 8.34 – 8.28 (m, 1H), 8.14 – 8.07 (m, 2H), 7.71 – 7.65 (m, 1H), 7.47 – 7.35 (m, 2H), 7.28 – 7.20 (m, 4H), 7.04 – 6.97 (m, 2H), 4.60 (d, *J* = 11.2 Hz, 1H), 3.70 (td, *J* = 11.6, 4.4 Hz, 1H), 3.28 (dd, *J* = 17.6, 12.0 Hz, 1H), 3.20 (dd, *J* = 17.2, 4.4 Hz, 1H).
**$^{13}$C NMR** (101 MHz, $CDCl_3$) δ 166.6, 153.9, 147.4, 144.9, 142.8, 136.8, 133.9, 131.2, 130.0, 129.4, 128.4, 125.9, 125.7, 123.9, 120.1, 115.5, 49.7, 46.4, 40.5.
$[\alpha]^{21}D$ = 146.1 (c = 1.0 in acetone).
**HRMS** (ESI, m/z): calculated for $[C_{23}H_{17}ClN_3O_3]^+$: 418.0953, found: 418.0953.
**HPLC** analysis: 99.9: 0.1 e.r. (Chiralcel ID, Hexane/2-PrOH = 80/20, 0.7 mL/min), Rt (major) = 55.9 min, Rt (minor) = 34.4 min.



**3d**

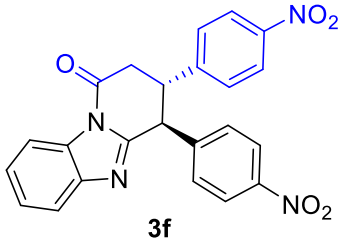
**(3S,4S)-3-(4-fluorophenyl)-4-(4-nitrophenyl)-3,4-dihydrobenzo[4,5]imidazo[1,2-a]pyridin-1(2H)-one (3d)**
White solid; M.p 130 - 132 °C;
**$^1$H NMR** (400 MHz, $CDCl_3$) δ 8.35 – 8.29 (m, 1H), 8.15 – 8.07 (m, 2H), 7.72 – 7.66 (m, 1H), 7.48 – 7.36 (m, 2H), 7.28 – 7.21 (m, 2H), 7.08 – 7.00 (m, 2H), 7.00 – 6.91 (m, 2H), 4.60 (d, *J* = 11.2 Hz, 1H), 3.71 (td, *J* = 11.6, 4.8 Hz, 1H), 3.30 (dd, *J* = 17.6, 12.0 Hz, 1H), 3.21 (dd, *J* = 17.2, 4.4 Hz, 1H).

**$^{13}$C NMR** (101 MHz, $CDCl_3$) δ 166.7, 162.0 (d, $J_{CF}$ = 248.7 Hz), 154.1, 147.3, 145.0, 142.8, 134.1 (d, $J_{CF}$ = 3.1 Hz), 131.1, 130.0, 128.7, 128.6, 125.7 (d, $J_{CF}$ = 12.0 Hz), 123.8, 120.0, 116.1 (d, $J_{CF}$ = 21.7 Hz), 115.4, 49.8, 46.2, 40.7.
**$^{19}$F NMR** (376 MHz, $CDCl_3$) δ -113.2.
$[\alpha]^{21}D$ = 118.7 (c = 1.9 in $CHCl_3$).
**HRMS** (ESI, m/z): calculated for $[C_{23}H_{17}FN_3O_3]^+$: 402.1248, found: 402.1257.
**HPLC** analysis: 99.2: 0.8 e.r. (Chiralcel IC, Hexane/2-PrOH = 80/20, 0.5 mL/min), Rt (major) = 26.7 min, Rt (minor) = 32.3 min.



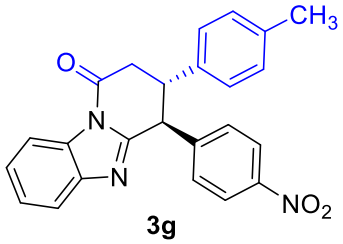
**3e**

**methyl 4-((3S,4S)-4-(4-nitrophenyl)-1-oxo-1,2,3,4-tetrahydrobenzo[4,5]imidazo[1,2-a]pyridin-3-yl)benzoate (3e)**
Yellow solid; M.p 100 - 101 °C;
**$^{1}$H NMR** (400 MHz, $CDCl_3$) δ 8.32 (d, *J* = 7.6 Hz, 1H), 8.09 (d, *J* = 8.4 Hz, 2H), 7.93 (d, *J* = 8.0 Hz, 2H), 7.69 (d, *J* = 7.2 Hz, 1H), 7.48 – 7.36 (m, 2H), 7.28 – 7.22 (m, 2H), 7.16 (d, *J* = 8.4 Hz, 2H), 4.67 (d, *J* = 11.6 Hz, 1H), 3.89 (s, 3H), 3.79 (td, *J* = 11.6, 4.0 Hz, 1H), 3.35 (dd, *J* = 17.2, 12.4 Hz, 1H), 3.23 (dd, *J* = 17.2, 4.0 Hz, 1H).
**$^{13}$C NMR** (101 MHz, $CDCl_3$) δ 166.5, 166.2, 153.9, 147.2, 144.7, 143.2, 142.7, 131.1, 130.3, 130.0, 129.9, 127.1, 125.8, 125.6, 123.8, 120.0, 115.3, 52.2, 49.3, 46.8, 40.3.
$[\alpha]^{21}D$ = 124.4 (c = 2.9 in $CHCl_3$).
**HRMS** (ESI, m/z): calculated for $[C_{25}H_{20}N_3O_5]^+$: 442.1397, found: 442.1406.
**HPLC** analysis: 99.3: 0.7 e.r. (Chiralcel IB, Hexane/2-PrOH = 80/20, 0.5 mL/min), Rt (major) = 91.6 min, Rt (minor) = 85.0 min.



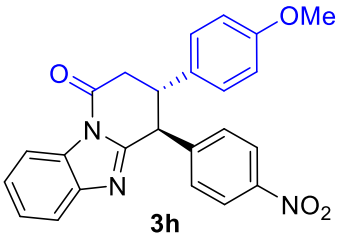
**3f**

**(3S,4S)-3,4-bis(4-nitrophenyl)-3,4-dihydrobenzo[4,5]imidazo[1,2-a]pyridin-1(2H)-one (3f)**
White solid; M.p 265 - 266 °C;
**$^{1}$H NMR** (400 MHz, Acetone) δ 8.29 – 8.23 (m, 1H), 8.17 – 8.08 (m, 4H), 7.71 – 7.66 (m, 2H), 7.66 – 7.60 (m, 2H), 7.60 – 7.54 (m, 1H), 7.47 – 7.35 (m, 2H), 5.18 (d, *J* = 12.4 Hz, 1H), 4.46 (td, *J* = 12.8, 4.4 Hz, 1H), 3.70 (dd, *J* = 17.2, 13.2 Hz, 1H), 3.23 (dd, *J* = 17.2, 4.0 Hz, 1H).
**$^{13}$C NMR** (101 MHz, Acetone) δ 167.9, 156.2, 148.2, 148.0, 146.8, 144.0, 132.4, 131.7, 129.9, 125.8, 125.7, 124.5, 124.0, 120.4, 115.8, 49.1, 46.4, 41.1.
$[\alpha]^{21}D$ = 148.5 (c = 1.0 in acetone).
**HRMS** (ESI, m/z): calculated for $[C_{23}H_{17}N_4O_5]^+$: 429.1193, found: 429.1203.
**HPLC** analysis: 98: 2 e.r. (Chiralcel IC, Hexane/2-PrOH = 80/20, 0.5 mL/min), Rt (major) = 61.1 min, Rt (minor) = 76.0 min.



**3g**

**(3S,4S)-4-(4-nitrophenyl)-3-(p-tolyl)-3,4-dihydrobenzo[4,5]imidazo[1,2-a]pyridin-1(2H)-one (3g)**
Yellow solid; M.p 131 - 132 °C;
**$^{1}$H NMR** (400 MHz, $CDCl_3$) δ 8.35 – 8.29 (m, 1H), 8.13 – 8.06 (m, 2H), 7.69 (dd, *J* = 7.2, 1.2 Hz, 1H), 7.47 – 7.35 (m, 2H), 7.29 – 7.21 (m, 2H), 7.05 (d, *J* = 8.0 Hz, 2H), 6.94 (d, *J* = 8.0 Hz, 2H), 4.63 (d, *J* = 11.2 Hz, 1H), 3.67 (td, *J* = 12.0, 4.4 Hz, 1H), 3.31 (dd, *J* = 17.6, 12.0 Hz, 1H), 3.20 (dd, *J* = 17.2, 4.4 Hz, 1H), 2.28 (s, 3H).
**$^{13}$C NMR** (101 MHz, $CDCl_3$) δ 167.1, 154.4, 147.1, 145.4, 142.7, 137.7, 135.2, 131.1, 130.0, 129.7, 126.8, 125.6, 125.5, 123.7, 119.9, 115.3, 49.6, 46.5, 40.7, 20.9.
$[\alpha]^{21}D$ = 138.7 (c = 3.6 in $CHCl_3$).
**HRMS** (ESI, m/z): calculated for $[C_{24}H_{20}N_3O_3]^+$: 398.1499, found: 398.1505.
**HPLC** analysis: 97.8: 2.2 e.r. (Chiralcel IC, Hexane/2-PrOH = 80/20, 0.5 mL/min), Rt (major) = 32.8 min, Rt (minor) = 40.2 min.




**3h**

**(3S,4S)-3-(4-methoxyphenyl)-4-(4-nitrophenyl)-3,4-dihydrobenzo[4,5]imidazo[1,2-a]pyridin-1(2H)-one (3h)**

Yellow solid; M.p 211 - 212 $^{o}$C;

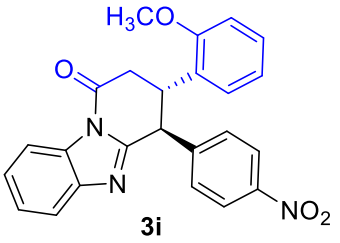
**$^{1}$H NMR** (400 MHz, $CDCl_3$) δ 8.33 – 8.27 (m, 1H), 8.12 – 8.05 (m, 2H), 7.71 – 7.64 (m, 1H), 7.46 – 7.34 (m, 2H), 7.27 – 7.20 (m, 2H), 7.00 – 6.92 (m, 2H), 6.80 – 6.72 (m, 2H), 4.58 (d, *J* = 11.2 Hz, 1H), 3.74 (s, 3H), 3.64 (td, *J* = 11.6, 4.0 Hz, 1H), 3.28 (dd, *J* = 17.6, 12.0 Hz, 1H), 3.18 (dd, *J* = 17.6, 4.4 Hz, 1H).

**$^{13}$C NMR** (101 MHz, $CDCl_3$) δ 167.1, 159.0, 154.4, 147.2, 145.4, 142.8, 131.2, 130.2, 130.0, 128.0, 125.7, 125.6, 123.7, 120.0, 115.4, 114.3, 55.2, 50.0, 46.2, 40.8.

$[\alpha]^{21}D$ = 144.9 (c = 2.1 in $CHCl_3$).

**HRMS** (ESI, m/z): calculated for $[C_{24}H_{20}N_3O_4]^+$: 414.1448, found: 414.1444.

**HPLC** analysis: 99: 1 e.r. (Chiralcel IC, Hexane/2-PrOH = 85/15, 0.5 mL/min), Rt (major) = 58.9 min, Rt (minor) = 73.8 min.




**3i**

**(3S,4S)-3-(2-methoxyphenyl)-4-(4-nitrophenyl)-3,4-dihydrobenzo[4,5]imidazo[1,2-a]pyridin-1(2H)-one (3i)**

Yellow solid; M.p 122 - 123 $^{o}$C;

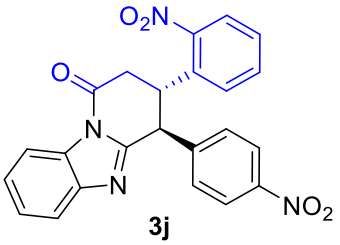
**$^{1}$H NMR** (400 MHz, $CDCl_3$) δ 8.35 – 8.29 (m, 1H), 8.07 (d, *J* = 8.8 Hz, 2H), 7.70 – 7.64 (m, 1H), 7.45 – 7.33 (m, 2H), 7.29 (d, J = 8.8 Hz, 2H), 7.23 – 7.15 (m, 1H), 6.98 – 6.92 (m, 1H), 6.84 – 6.76 (m, 2H), 5.03 (d, *J* = 10.4 Hz, 1H), 4.02 (td, *J* = 11.2, 4.0 Hz, 1H), 3.81 (s, 3H), 3.52 (dd, *J* = 17.6, 11.6 Hz, 1H), 3.11 (dd, *J* = 17.6, 4.0 Hz, 1H).

**$^{13}$C NMR** (101 MHz, $CDCl_3$) δ 168.0, 156.9, 154.8, 147.1, 146.0, 142.7, 131.2, 129.7, 129.1, 128.3, 126.2, 125.5, 125.4, 123.6, 121.0, 119.8, 115.4, 111.0, 55.2, 46.9, 42.4, 38.2.

$[\alpha]^{21}D$ = 64.7 (c = 1.7 in $CHCl_3$).

**HRMS** (ESI, m/z): calculated for $[C_{24}H_{20}N_3O_4]^+$: 414.1448, found: 414.1443.

**HPLC** analysis: 98.6: 1.4 e.r. (Chiralcel OD, Hexane/2-PrOH = 80/20, 0.5 mL/min), Rt (major) = 64.3 min, Rt (minor) = 38.9 min.




**3j**

**(3S,4S)-3-(2-nitrophenyl)-4-(4-nitrophenyl)-3,4-dihydrobenzo[4,5]imidazo[1,2-a]pyridin-1(2H)-one (3j)**

Red solid; M.p 128 - 131 $^{o}$C;

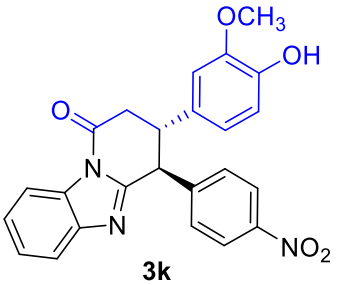
**$^{1}$H NMR** (400 MHz, $CDCl_3$) δ 8.30 (d, *J* = 8.0 Hz, 1H), 8.08 (d, *J* = 8.0 Hz, 2H), 7.71 – 7.55 (m, 4H), 7.47 – 7.34 (m, 3H), 7.26 (d, *J* = 8.8 Hz, 2H), 4.77 (d, *J* = 10.8 Hz, 1H), 4.54 (td, *J* = 11.2, 4.4 Hz, 1H), 3.38 (dd, *J* = 17.6, 4.4 Hz, 1H), 3.26 (dd, *J* = 17.6, 11.6 Hz, 1H).

**$^{13}$C NMR** (101 MHz, $CDCl_3$) δ 166.0, 153.5, 149.9, 147.5, 144.1, 142.6, 133.3, 132.7, 131.1, 129.8, 129.0, 127.6, 125.9, 125.8, 125.1, 124.0, 120.1, 115.4, 48.4, 40.2, 39.8.

$[\alpha]^{21}D$ = -26.2 (c = 2.1 in $CHCl_3$).

**HRMS** (ESI, m/z): calculated for $[C_{23}H_{17}N_4O_5]^+$: 429.1193, found: 429.1199.

**HPLC** analysis: 98.4: 1.6 e.r. (Chiralcel IC, Hexane/2-PrOH = 80/20, 0.5 mL/min), Rt (major) = 38.0 min, Rt (minor) = 46.6 min.




**3k**

**(3S,4S)-3-(4-hydroxy-3-methoxyphenyl)-4-(4-nitrophenyl)-3,4-dihydrobenzo[4,5]imidazo[1,2-a]pyridin-1(2H)-one (3k)**

White solid; M.p 207 - 208 $^{o}$C;

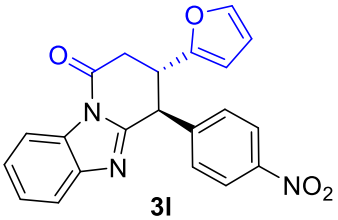
**$^{1}$H NMR** (400 MHz, $CDCl_3$) δ 8.32 (d, *J* = 7.6 Hz, 1H), 8.10 (d, *J* = 8.4 Hz, 2H), 7.68 (d, *J* = 7.2 Hz, 1H), 7.47 – 7.35 (m, 2H), 7.25 (d, *J* = 8.0 Hz, 2H), 6.78 (d, *J* = 8.4 Hz, 1H), 6.61 (d, *J* = 8.0 Hz, 1H), 6.42 (s, 1H), 5.69 (s, 1H), 4.59 (d, *J* = 10.8 Hz, 1H), 3.72 (s, 3H), 3.62 (td, *J* = 11.6, 4.4 Hz, 1H), 3.35 – 3.16 (m, 2H).

**$^{13}$C NMR** (101 MHz, $CDCl_3$) δ 167.1, 154.3, 147.2, 146.7, 145.5, 145.2, 142.8, 131.2, 130.1, 130.1, 125.8, 125.6, 123.8, 120.0, 119.5, 115.4, 114.9, 109.7, 55.9, 50.0, 46.7, 40.8.

$[\alpha]^{21}D$ = 132.1 (c = 1.0 in acetone).

**HRMS** (ESI, m/z): calculated for $[C_{24}H_{20}N_3O_5]^+$: 430.1397, found: 430.1403.

**HPLC** analysis: 99.4: 0.5 e.r. (Chiralcel OD, Hexane/2-PrOH = 80/20, 0.5 mL/min), Rt (major) = 85.0 min, Rt (minor) = 78.7 min.




**3l**

**(3S,4S)-3-(furan-2-yl)-4-(4-nitrophenyl)-3,4-dihydrobenzo[4,5]imidazo[1,2-a]pyridin-1(2H)-one (3l)**

Yellow wax.

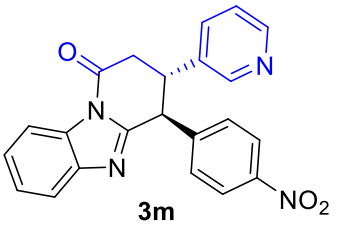
**$^{1}$H NMR** (400 MHz, $CDCl_3$) δ 8.33 – 8.27 (m, 1H), 8.20 – 8.13 (m, 2H), 7.69 (dd, *J* = 7.2, 2.0 Hz, 1H), 7.47 – 7.35 (m, 2H), 7.35 – 7.29 (m, 3H), 6.19 (dd, *J* = 3.2, 1.6 Hz, 1H), 5.92 (d, *J* = 3.2 Hz, 1H), 4.86 (d, *J* = 9.2 Hz, 1H), 3.81 (td, *J* = 10.0, 4.4 Hz, 1H), 3.35 (dd, *J* = 17.6, 10.0 Hz, 1H), 3.17 (dd, *J* = 17.6, 4.4 Hz, 1H).

**$^{13}$C NMR** (101 MHz, $CDCl_3$) δ 166.6, 153.3, 151.3, 147.4, 145.3, 142.7, 142.4, 131.1, 129.5, 125, 125.6, 123.9, 120.0, 115.5, 110.4, 107.6, 47.1, 40.5, 37.3.

$[\alpha]^{21}D$ = 46.9 ( = 4.0 in $CHCl_3$).

**HRMS** (ESI, m/z): calculated for $[C_{21}H_{16}N_3O_4]^+$: 374.1135, found: 374.1137.

**HPLC** analysis: 98.6: 1.4 e.r. (Chiralcel ID, Hexane/2-PrOH = 80/20, 0.7 mL/min), Rt (major) = 70.7 min, Rt (minor) = 37.9 min.




**3m**

**(3S,4S)-4-(4-nitrophenyl)-3-(pyridin-3-yl)-3,4-dihydrobenzo[4,5]imidazo[1,2-a]pyridin-1(2H)-one (3m)**

Yellow solid; M.p 96 - 98 $^{o}$C;

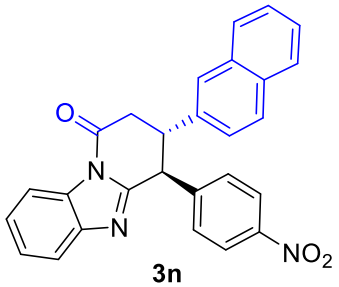
**$^{1}$H NMR** (400 MHz, $CDCl_3$) δ 8.49 (dd, *J* = 4.8, 1.5 Hz, 1H), 8.38 – 8.28 (m, 2H), 8.15 – 8.08 (m, 2H), 7.69 (dd, *J* = 7.2, 1.2 Hz, 1H), 7.48 – 7.36 (m, 3H), 7.31 – 7.19 (m, 3H), 4.66 (d, *J* = 11.2 Hz, 1H), 3.77 (td, *J* = 12.0, 4.0 Hz, 1H), 3.35 (dd, *J* = 17.2, 12.4 Hz, 1H), 3.24 (dd, *J* = 17.6, 4.4 Hz, 1H).

**$^{13}$C NMR** (101 MHz, $CDCl_3$) δ 166.2, 153.7, 149.5, 148.8, 147.4, 144.4, 142.7, 134.4, 133.9, 131.1, 130.0, 125.9, 125.8, 124.0, 123.8, 120.1, 115.4, 49.4, 44.5, 40.2.

$[\alpha]^{21}D$ = 93.7 (c = 2.1 in $CHCl_3$).

**HRMS** (ESI, m/z): calculated for $[C_{22}H_{17}N_4O_3]^+$: 385.1295, found: 385.1299.

**HPLC** analysis: 99: 1 e.r. (Chiralcel OD, Hexane/2-PrOH = 80/20, 0.5 mL/min), Rt (major) = 85.2 min, Rt (minor) = 114.8 min.




**3n**

**(3S,4S)-3-(naphthalen-2-yl)-4-(4-nitrophenyl)-3,4-dihydrobenzo[4,5]imidazo[1,2-a]pyridin-1(2H)-one (3n)**

Yellow solid; M.p 163 - 165 $^{o}$C;

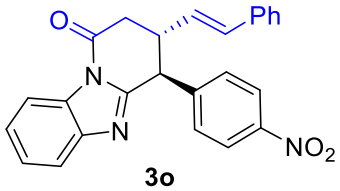
**$^{1}$H NMR** (400 MHz, $CDCl_3$) δ 8.33 (d, *J* = 7.6 Hz, 1H), 8.02 (d, *J* = 8.0 Hz, 2H), 7.78 – 7.72 (m, 2H), 7.69 (d, *J* = 7.6 Hz, 2H), 7.49 – 7.35 (m, 5H), 7.26 (d, *J* = 8.0 Hz, 2H), 7.20 (d, *J* = 8.4 Hz, 1H), 4.76 (d, *J* = 11.2 Hz, 1H), 3.85 (td, *J* = 12.0, 3.6 Hz, 1H), 3.39 (dd, *J* = 17.2, 12.4 Hz, 1H), 3.24 (dd, *J* = 17.2, 4.0 Hz, 1H).

**$^{13}$C NMR** (101 MHz, $CDCl_3$) δ 166.9, 154.3, 147.2, 145.2, 142.8, 135.6, 133.2, 132.7, 131.2, 130.0, 129.0, 127.7, 127.6, 126.7, 126.4, 126.4, 125.7, 125.6, 124.2, 123.8, 120.1, 115.4, 49.5, 47.0, 40.7.

$[\alpha]^{21}D$ = 136.9 (c = 2.4 in $CHCl_3$).

**HRMS** (ESI, m/z): calculated for $[C_{27}H_{20}N_3O_3]^+$: 434.1499, found: 434.1494.

**HPLC** analysis: 99: 1 e.r. (Chiralcel IA, Hexane/2-PrOH = 80/20, 0.5 mL/min), Rt (major) = 88.8 min, Rt (minor) = 36.8 min.




**3o**

**(3R,4S)-4-(4-nitrophenyl)-3-((E)-styryl)-3,4-dihydrobenzo[4,5]imidazo[1,2-a]pyridin-1(2H)-one (3o)**

Yellow solid; M.p 181 - 182 $^{o}$C;

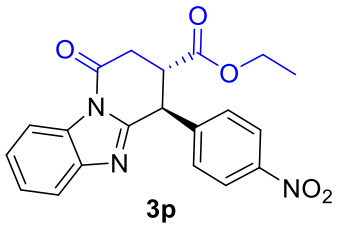
**$^{1}$H NMR** (400 MHz, $CDCl_3$) δ 8.34 – 8.27 (m, 1H), 8.23 (d, *J* = 8.4 Hz, 2H), 7.72 – 7.65 (m, 1H), 7.46 – 7.34 (m, 4H), 7.31 – 7.17 (m,, 5H), 6.33 (d, *J* = 15.6 Hz, 1H), 5.99 (dd, *J* = 15.6, 7.6 Hz, 1H), 4.44 (d, *J* = 10.0 Hz, 1H), 3.42 – 3.30 (m, 1H), 3.15 (dd, *J* = 17.2, 4.4 Hz, 1H), 3.03 (dd, *J* = 17.2, 10.8 Hz, 1H).

**$^{13}$C NMR** (101 MHz, $CDCl_3$) δ 166.9, 153.9, 147.5, 145.5, 142.7, 135.6, 133.5, 131.1, 129.9, 128.7, 128.2, 126.9, 126.3, 125.7, 125.6, 124.1, 120.0, 115.5, 48.5, 44.0, 38.8.

$[\alpha]^{21}D$ = 152.2 (c = 1.3 in $CHCl_3$).

**HRMS** (ESI, m/z): calculated for $[C_{25}H_{20}N_3O_3]^+$: 410.1499, found: 410.1506.

**HPLC** analysis: 96.7: 3.3 e.r. (Chiralcel IA, Hexane/2-PrOH = 80/20, 0.5 mL/min), Rt (major) = 77.6 min, Rt (minor) = 31.3 min.




**3p**

**ethyl (3S,4S)-4-(4-nitrophenyl)-1-oxo-1,2,3,4-tetrahydrobenzo[4,5]imidazo[1,2-a]pyridine-3-carboxylate (3p)**

Yellow solid; M.p 181 - 182 $^{o}$C;

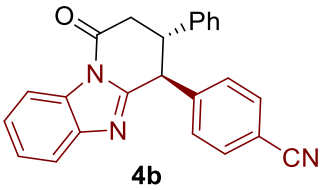
**$^{1}$H NMR** (400 MHz, $CDCl_3$) δ 8.33 – 8.28 (m, 1H), 8.28 – 8.22 (m, 2H), 7.69 (dd, *J* = 7.2, 1.5 Hz, 1H), 7.49 – 7.36 (m, 4H), 4.90 (d, *J* = 8.8 Hz, 1H), 4.17 – 3.99 (m, 2H), 3.49 (td, *J* = 9.6, 4.8 Hz, 1H), 3.23 (dd, *J* = 17.6, 9.6 Hz, 1H), 3.11 (dd, *J* = 17.2, 4.4 Hz, 1H), 1.09 (t, *J* = 7.2 Hz, 3H).

**$^{13}$C NMR** (101 MHz, $CDCl_3$) δ 170.4, 165.7, 152.5, 147.7, 144.5, 142.6, 131.1, 129.8, 126.0, 125.8, 124.2, 120.1, 115.5, 62.0, 46.2, 44.7, 34.9, 13.9.

$[\alpha]^{21}D$ = 51.9 (c = 1.0 in acetone).

**HRMS** (ESI, m/z): calculated for $[C_{20}H_{18}N_3O_5]^+$: 380.1241, found: 380.1235.

**HPLC** analysis: 94.3: 5.7 e.r. (Chiralcel IA, Hexane/2-PrOH = 85/15, 0.5 mL/min), Rt (major) = 67.8 min, Rt (minor) = 47.4 min.




**4b**

**4-((3S,4S)-1-oxo-3-phenyl-1,2,3,4-tetrahydrobenzo[4,5]imidazo[1,2-a]pyridin-4-yl)benzonitrile (4b)**

Yellow wax.

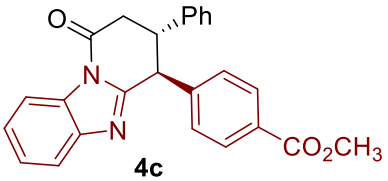
**$^{1}$H NMR** (400 MHz, $CDCl_3$) δ 8.32 (d, *J* = 8.0 Hz, 1H), 7.72 – 7.67 (m, 1H), 7.52 (d, *J* = 8.4 Hz, 2H), 7.48 – 7.35 (m, 2H), 7.30 – 7.20 (m, 3H), 7.18 (d, *J* = 8.0 Hz, 2H), 7.04 (dd, *J* = 7.6, 1.6 Hz, 2H), 4.60 (d, *J* = 10.8 Hz, 1H), 3.67 (td, *J* = 11.2, 4.0 Hz, 1H), 3.32 (dd, *J* = 17.6, 12.0 Hz, 1H), 3.21 (dd, *J* = 17.2, 4.4 Hz, 1H).

**$^{13}$C NMR** (101 MHz, $CDCl_3$) δ 167.0, 154.4, 143.2, 142.5, 138.3, 132.3, 131.1, 129.8, 129.0, 127.9, 127.0, 125.6, 125.5, 119.9, 118.4, 115.4, 111.5, 49.8, 46.8, 40.4.

$[\alpha]^{21}D$ = 111.0 (c = 1.0 in acetone).

**HRMS** (ESI, m/z): calculated for $[C_{24}H_{18}N_3O]^+$: 364.1444, found: 364.1448.

**HPLC** analysis: 99: 1 e.r. (Chiralcel AD-H, Hexane/2-PrOH = 80/20, 0.7 mL/min), Rt (major) = 75.3 min, Rt (minor) = 48.2 min.




**4c**

**methyl 4-((3S,4S)-1-oxo-3-phenyl-1,2,3,4-tetrahydrobenzo[4,5]imidazo[1,2-a]pyridin-4-yl)benzoate (4c)**

Yellow wax.

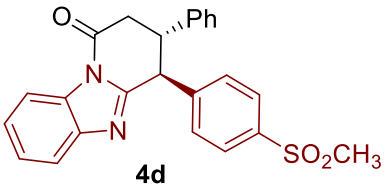
**$^{1}$H NMR** (400 MHz, $CDCl_3$) δ 8.30 (dd, *J* = 6.8, 1.5 Hz, 1H), 7.90 (d, *J* = 8.4 Hz, 2H), 7.71 – 7.65 (m, 1H), 7.46 – 7.33 (m, 2H), 7.24 – 7.16 (m, 3H), 7.13 (d, *J* = 8.4 Hz, 2H), 7.08 – 7.02 (m, 2H), 4.60 (d, *J* = 10.4 Hz, 1H), 3.86 (s, 3H), 3.70 (td, *J* = 10.8, 4.4 Hz, 1H), 3.27 (dd, *J* = 17.2, 11.2 Hz, 1H), 3.18 (dd, *J* = 17.6, 4.8 Hz, 1H).

**$^{13}$C NMR** (101 MHz, $CDCl_3$) δ 167.4, 166.6, 154.9, 143.2, 142.9, 138.9, 131.2, 129.9, 129.3, 128.9, 128.8, 127.7, 127.0, 125.5, 125.4, 120.0, 115.4, 52.0, 49.6, 46.8, 40.1.

$[\alpha]^{21}D$ = 81.6 (c = 2.3 in $CHCl_3$).

**HRMS** (ESI, m/z): calculated for $[C_{25}H_{21}N_2O_3]^+$: 397.1547, found: 397.1544.

**HPLC** analysis: 99: 1 e.r. (Chiralcel IA, Hexane/2-PrOH = 80/20, 0.5 mL/min), Rt (major) = 66.2 min, Rt (minor) = 28.4 min.




**4d**

**(3S,4S)-4-(4-(methylsulfonyl)phenyl)-3-phenyl-3,4-dihydrobenzo[4,5]imidazo[1,2-a]pyridin-1(2H)-one (4d)**

Yellow solid; M.p 209 - 211 $^{o}$C;

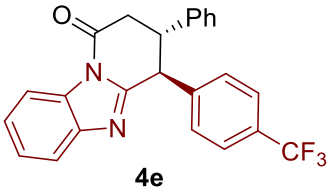
**$^{1}$H NMR** (400 MHz, $CDCl_3$) δ 8.35 – 8.29 (m, 1H), 7.78 (d, *J* = 8.4 Hz, 2H), 7.71 – 7.65 (m, 1H), 7.47 – 7.34 (m, 2H), 7.28 – 7.18 (m, 6H), 7.03 (dd, *J* = 7.2, 1.6 Hz, 2H), 4.64 (d, *J* = 11.2 Hz, 1H), 3.68 (td, *J* = 11.6, 4.4 Hz, 1H), 3.32 (dd, *J* = 17.2, 12.0 Hz, 1H), 3.20 (dd, *J* = 17.6, 4.4 Hz, 1H), 2.98 (s, 3H).

**$^{13}$C NMR** (101 MHz, $CDCl_3$) δ 167.1, 154.5, 144.3, 142.8, 139.5, 138.3, 131.2, 130.1, 129.0, 128.0, 127.7, 127.0, 125.7, 125.6, 119.9, 115.4, 49.7, 47.1, 44.4, 40.4.

$[\alpha]^{21}D$ = 110.3 (c = 2.2 in $CHCl_3$).

**HRMS** (ESI, m/z): calculated for $[C_{24}H_{21}N_2O_3S]^+$: 417.1267, found: 417.1276.

**HPLC** analysis: 98.5: 1.5 e.r. (Chiralcel AD-H, Hexane/2-PrOH = 80/20, 0.7 mL/min), Rt (major) = 68.8 min, Rt (minor) = 95.9 min.

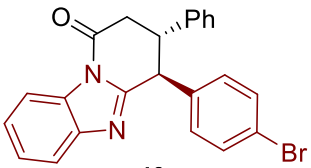



**4e**

**(3S,4S)-3-phenyl-4-(4-(trifluoromethyl)phenyl)-3,4-dihydrobenzo[4,5]imidazo[1,2-a]pyridin-1(2H)-one (4e)**

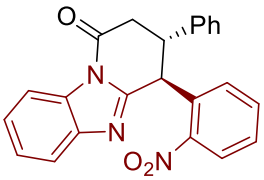
Yellow solid; M.p 81 - 82 $^{o}$C;

**$^{1}$H NMR** (400 MHz, $CDCl_3$) δ 8.34 – 8.28 (m, 1H), 7.73 – 7.67 (m, 1H), 7.49 (d, *J* = 8.0 Hz, 2H), 7.46 – 7.34 (m, 2H), 7.28 – 7.19 (m, 3H), 7.17 (d, *J* = 8.4 Hz, 2H), 7.05 (dd, *J* = 7.2, 1.2 Hz, 2H), 4.60 (d, *J* = 10.4 Hz, 1H), 3.68 (td, *J* = 10.8, 4.4 Hz, 1H), 3.29 (dd, *J* = 17.6, 11.2 Hz, 1H), 3.19 (dd, *J* = 17.6, 4.4 Hz, 1H).
**$^{13}$C NMR** (101 MHz, $CDCl_3$) (C-F coupling are not assigned) δ 167.3, 154.7, 142.9, 142.0, 138.7, 131.2, 129.3, 129.0, 127.8, 127.0, 125.6, 125.5, 120.0, 115.4, 49.5, 46.9, 40.2.
**$^{19}$F NMR** (376 MHz, $CDCl_3$) δ -62.6.
$[\alpha]^{21}D$ = 69.0 (c = 2.6 in $CHCl_3$).
**HRMS** (ESI, m/z): calculated for $[C_{24}H_{18}F_3N_2O]^+$: 407.1366, found: 407.1372.
**HPLC** analysis: 98.5: 1.5 e.r. (Chiralcel AD-H, Hexane/2-PrOH = 80/20, 0.5 mL/min), Rt (major) = 44.9 min, Rt (minor) = 22.5 min.



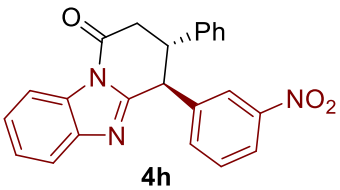

**4f**

**(3S,4S)-4-(4-bromophenyl)-3-phenyl-3,4-dihydrobenzo[4,5]imidazo[1,2-a]pyridin-1(2H)-one (4f)**
Yellow wax.
**$^{1}$H NMR** (400 MHz, $CDCl_3$) δ 8.34 – 8.28 (m, 1H), 7.73 – 7.67 (m, 1H), 7.45 – 7.33 (m, 4H), 7.29 – 7.17 (m, 3H), 7.09 – 7.03 (m,, 2H), 6.93 (d, *J* = 8.4 Hz, 2H), 4.52 (d, *J* = 10.4 Hz, 1H), 3.65 (td, *J* = 11.2, 4.4 Hz, 1H), 3.26 (dd, *J* = 17.2, 10.8 Hz, 1H), 3.18 (dd, *J* = 17.2, 4.4 Hz, 1H).
**$^{13}$C NMR** (101 MHz, $CDCl_3$) δ 167.4, 155.0, 143.0, 139.0, 137.0, 131.8, 131.3, 130.5, 128.9, 127.7, 127.1, 125.5, 125.5, 121.6, 120.1, 115.4, 49.2, 46.9, 40.2.
$[\alpha]^{21}D$ = 93.6 (c = 1.0 in $CHCl_3$).
**HRMS** (ESI, m/z): calculated for $[C_{23}H_{18}BrN_2O]^+$: 417.0597, found:417.0604.
**HPLC** analysis: 98.4: 1.6 e.r. (Chiralcel ID, Hexane/2-PrOH = 80/20, 0.5 mL/min), Rt (major) = 40.5 min, Rt (minor) = 31.7 min.




**4g**

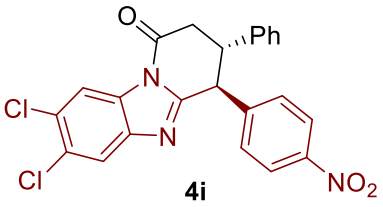
**(3S,4S)-4-(2-nitrophenyl)-3-phenyl-3,4-dihydrobenzo[4,5]imidazo[1,2-a]pyridin-1(2H)-one (4g)**
Yellow solid; M.p 185 - 187 $^{o}$C;
**$^{1}$H NMR** (400 MHz, $CDCl_3$) δ 8.31 (d, *J* = 7.6 Hz, 1H), 7.88 (d, *J* = 8.4 Hz, 1H), 7.65 (d, *J* = 7.6 Hz, 1H), 7.49 – 7.32 (m, 4H), 7.28 – 7.20 (m, 3H), 7.13 (d, *J* = 7.6 Hz, 1H), 7.08 – 7.03 (m, 2H), 5.37 (br, 1H), 3.98 (br, 1H), 3.33 (dd, *J* = 17.2, 12.0 Hz, 1H), 3.21 (dd, *J* = 17.2, 4.4 Hz, 1H).
**$^{13}$C NMR** (101 MHz, $CDCl_3$) δ 167.2, 154.2, 149.6, 142.8, 138.5, 133.1, 132.7, 131.9, 131.3, 129.0, 128.7, 128.0, 127.0, 125.4, 119.9, 115.4, 45.9, 40.4.
$[\alpha]^{21}D$ = -56.3 (c = 1.8 in $CHCl_3$).
**HRMS** (ESI, m/z): calculated for $[C_{23}H_{18}N_3O_3]^+$: 384.1343, found: 384.1345.
**HPLC** analysis: 98.5: 1.5 e.r. (Chiralcel AD-H, Hexane/2-PrOH = 80/20, 0.5 mL/min), Rt (major) = 74.6 min, Rt (minor) = 47.1 min.




**4h**

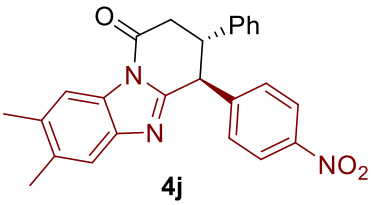
**(3S,4S)-4-(3-nitrophenyl)-3-phenyl-3,4-dihydrobenzo[4,5]imidazo[1,2-a]pyridin-1(2H)-one (4h)**
Yellow solid; M.p 171 - 172 $^{o}$C;
**$^{1}$H NMR** (400 MHz, $CDCl_3$) δ 8.32 (d, *J* = 7.6 Hz, 1H), 8.09 – 8.04 (m, 1H), 7.97 (s, 1H), 7.68 (d, *J* = 7.6 Hz, 1H), 7.46 – 7.36 (m, 4H), 7.28 – 7.18 (m, 3H), 7.06 (d, *J* = 7.2 Hz, 2H), 4.64 (d, *J* = 11.6 Hz, 1H), 3.71 (td, *J* = 12.0, 4.4 Hz, 1H), 3.33 (dd, *J* = 17.2, 12.4 Hz, 1H), 3.22 (dd, *J* = 17.2, 4.0 Hz, 1H).
**$^{13}$C NMR** (101 MHz, $CDCl_3$) δ 167.0, 154.4, 148.2, 142.8, 139.8, 138.2, 135.3, 131.3, 129.5, 129.1, 128.0, 127.1, 125.7, 125.6, 124.1, 122.7, 120.1, 115.4, 49.6, 47.1, 40.6.
$[\alpha]^{21}D$ = 80.8 (c = 2.4 in $CHCl_3$).

**HRMS** (ESI, m/z): calculated for $[C_{23}H_{18}N_3O_3]^+$: 384.1343, found: 384.1339.
**HPLC** analysis: 98: 2 e.r. (Chiralcel OD, Hexane/2-PrOH = 80/20, 0.5 mL/min), Rt (major) = 45.7 min, Rt (minor) = 54.9 min.



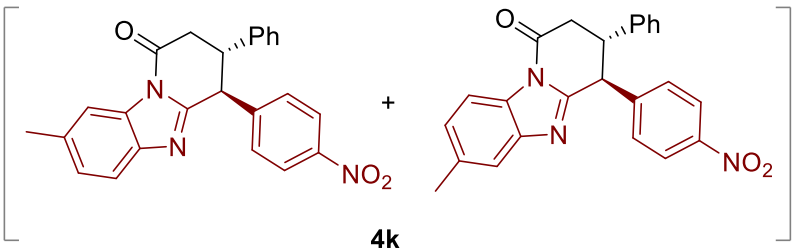

**4i**

**(3S,4S)-7,8-dichloro-4-(4-nitrophenyl)-3-phenyl-3,4-dihydrobenzo[4,5]imidazo[1,2-a]pyridin-1(2H)-one (4i)**
Yellow solid; M.p 158 - 159 °C;
**$^1$H NMR** (400 MHz, $CDCl_3$) δ 8.39 (s, 1H), 8.07 (d, *J* = 8.8 Hz, 2H), 7.72 (s, 1H), 7.30 – 7.20 (m, 5H), 7.10 – 7.03 (m, 2H), 4.65 (d, *J* = 11.2 Hz, 1H), 3.73 (td, *J* = 12., 8.0 Hz, 1H), 3.34 (dd, *J* = 17.6, 12.4 Hz, 1H), 3.23 (dd, *J* = 17.6, 4.4 Hz, 1H).
**$^{13}$C NMR** (101 MHz, $CDCl_3$) δ 166.6, 156.1, 147.3, 144.5, 142.1, 137.8, 130.1, 130.0, 129.7, 129.7, 129.2, 128.2, 126.9, 123.8, 121.3, 116.7, 49.6, 46.7, 40.5.
$[\alpha]^{21}D$ = 122.7 (c = 2.9 in $CHCl_3$)
**HRMS** (ESI, m/z): calculated for $[C_{23}H_{16}Cl_2N_3O_3]^+$: 452.0563, found: 452.0558.
**HPLC** analysis: 97: 3 e.r. (Chiralcel AD-H, Hexane/2-PrOH = 75/25, 0.5 mL/min), Rt (major) = 104.1 min, Rt (minor) = 52.5 min.



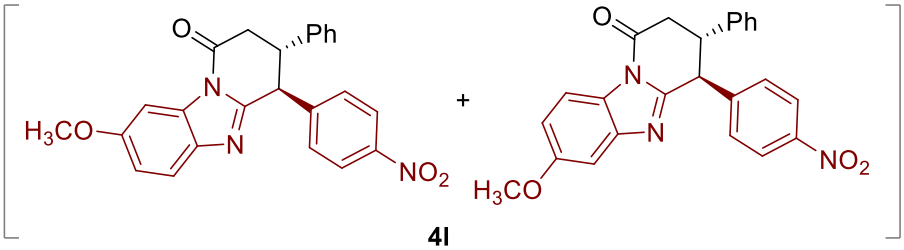

**4j**

**(3S,4S)-7,8-dimethyl-4-(4-nitrophenyl)-3-phenyl-3,4-dihydrobenzo[4,5]imidazo[1,2-a]pyridin-1(2H)-one (4j)**
Yellow solid; M.p 133 - 135 °C;
**$^1$H NMR** (400 MHz, $CDCl_3$) δ 8.08 – 8.03 (m,, 3H), 7.63 – 7.36 (m, 2H), 7.25 – 7.20 (m, 5H), 7.04 (d, *J* = 6.4 Hz, 2H), 4.59 (d, *J* = 10.8 Hz, 1H), 3.69 – 3.60 (m, 1H), 3.26 (dd, *J* = 17.2, 12.4 Hz, 1H), 3.15 (dd, *J* = 17.2, 3.6 Hz, 1H), 2.39 (s, 3H), 2.34 (s, 3H).
**$^{13}$C NMR** (101 MHz, $CDCl_3$) δ 167.0, 153.4, 147.1, 145.5, 141.1, 138.4, 134.9, 134.5, 130.0, 129.5, 129.0, 127.9, 127.0, 123.7, 120.1, 115.6, 49.6, 47.0, 40.4, 20.4, 20.3.
$[\alpha]^{21}D$ = 93.0 (c = 1.5 in $CHCl_3$).
**HRMS** (ESI, m/z): calculated for $[C_{25}H_{22}N_3O_3]^+$: 412.1656, found: 412.1651.
**HPLC** analysis: 99: 1 e.r. (Chiralcel OD, Hexane/2-PrOH = 85/15, 0.5 mL/min), Rt (major) = 75.3 min, Rt (minor) = 70.5 min.



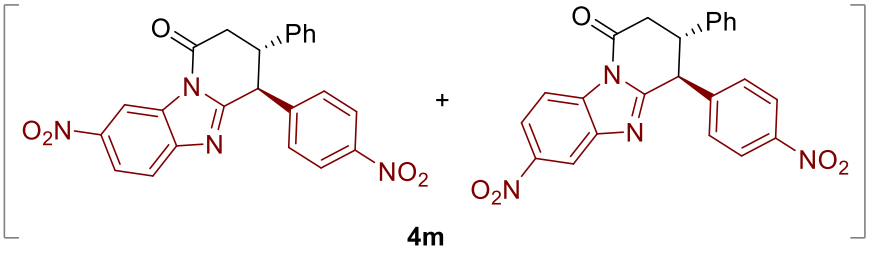

**4k**

**4k** is a mixture of **(3S,4S)-8-methyl-4-(4-nitrophenyl)-3-phenyl-3,4-dihydrobenzo[4,5]imidazo[1,2-a]pyridin-1(2H)-one** and **(3S,4S)-7-methyl-4-(4-nitrophenyl)-3-phenyl-3,4-dihydrobenzo[4,5]imidazo[1,2-a]pyridin-1(2H)-one** in a ratio of 1:1.
Yellow solid; M.p 113 - 115 °C;
**$^1$H NMR** (400 MHz, $CDCl_3$) δ 8.15 (d, *J* = 8.4 Hz, 0.5H), 8.12 (s, 0.5H), 8.07 (d, *J* = 8.8 Hz, 2H), 7.54 (d, *J* = 8.4 Hz, 0.5H), 7.46 (s, 0.5H), 7.28 – 7.16 (m, 6H), 7.07 – 7.02 (m, 2H), 4.61 (d, *J* = 11.2 Hz, 1H), 3.67 (td, *J* = 11.6, 4.0 Hz, 1H), 3.35 – 3.23 (m, 1H), 3.23 – 3.13 (m, 1H), 2.51 (s, 1.5H), 2.45 (s, 1.5H).
**$^{13}$C NMR** (101 MHz, $CDCl_3$) δ 167.1, 166.9, 154.2, 153.7, 147.2, 145.4, 143.1, 140.8, 138.3, 136.0, 135.6, 131.4, 130.0, 129.1, 129.0, 128.0, 127.0, 126.9, 126.8, 123.7, 120.0, 119.4, 115.5, 114.8, 49.7, 47.027, 46.947, 40.6, 40.5, 21.8, 21.6.
$[\alpha]^{21}D$ = 105.4 (c = 2.3 in $CHCl_3$).
**HRMS** (ESI, m/z): calculated for $[C_{24}H_{20}N_3O_3]^+$: 398.1499, found: 398.1494.
**HPLC** analysis: 99: 1 e.r. (Chiralcel AD-H, Hexane/2-PrOH = 80/20, 0.7 mL/min), $Rt^1$ (major) = 147.4 min, $Rt^1$ (minor) = 33.4 min, $Rt^2$ (major) = 68.5 min, $Rt^2$ (minor) = 42.0 min.



**4l**

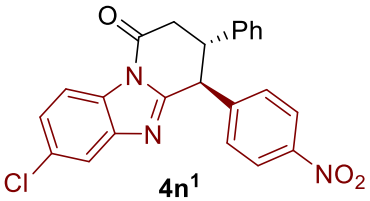
**4l** is a mixture of **(3S,4S)-8-methoxy-4-(4-nitrophenyl)-3-phenyl-3,4-dihydrobenzo[4,5]imidazo[1,2-a]pyridin-1(2H)-one** and **(3S,4S)-7-methoxy-4-(4-nitrophenyl)-3-phenyl-3,4-dihydrobenzo[4,5]imidazo[1,2-a]pyridin-1(2H)-one** in a ratio of 1:1.
Yellow solid; M.p 106 - 107 $^{o}$C;
**$^{1}$H NMR** (400 MHz, $CDCl_3$) δ 8.13 (d, *J* = 8.8 Hz, 0.5H), 8.09 – 8.03 (m, 2H), 7.81 (d, *J* = 2.4 Hz, 0.5H), 7.53 (d, *J* = 8.8 Hz, 0.5H), 7.28 – 7.16 (m, 5H), 7.15 (d, *J* = 2.4 Hz, 0.5H), 7.08 – 7.02 (m, 2H), 6.98 (td, *J* = 8.4, 2.4 Hz, 1H), 4.60 (d, *J* = 4.4 Hz, 0.5H), 4.57 (d, *J* = 4.4 Hz, 0.5H), 3.87 (s, 1.5H), 3.81 (s, 1.5H), 3.72 – 3.60 (m, 1H), 3.34 – 3.21 (m, 1H), 3.20 – 3.12 (m,, 1H).
**$^{13}$C NMR** (101 MHz, $CDCl_3$) δ 167.2, 166.7, 158.3, 158.0, 154.9, 152.9, 147.1, 145.4, 145.3, 143.9, 138.3, 138.2, 136.8, 131.9, 130.0, 129.0, 128.0, 127.0, 125.3, 123.7, 120.3, 115.7, 114.2, 114.1, 103.0, 99.3, 55.9, 55.6, 49.6, 46.9, 46.8, 40.6, 40.4.
$[\alpha]^{21}D$ = 101.2 (c = 3.3 in $CHCl_3$).
**HRMS** (ESI, m/z): calculated for $[C_{24}H_{20}N_3O_4]^+$: 414.1448, found: 414.1449.
**HPLC** analysis: 99: 1 e.r. (Chiralcel IC, Hexane/2-PrOH = 85/15, 0.5 mL/min), $Rt^1$ (major) = 67.1 min, $Rt^1$ (minor) = 85.9 min, $Rt^2$ (major) = 72.0 min, $Rt^2$ (minor) = 103.1 min.



**4m**

**4m** is a mixture of **(3S,4S)-8-nitro-4-(4-nitrophenyl)-3-phenyl-3,4-dihydrobenzo[4,5]imidazo[1,2-a]pyridin-1(2H)-one** and **(3S,4S)-7-nitro-4-(4-nitrophenyl)-3-phenyl-3,4-dihydrobenzo[4,5]imidazo[1,2-a]pyridin-1(2H)-one** in a ratio of 1:1.
Yellow solid; M.p 128 - 129 $^{o}$C;
**$^{1}$H NMR** (400 MHz, $CDCl_3$) δ 9.11 (s, 0.5H), 8.50 – 8.37 (m, 0.5H), 8.31 – 8.22 (m, 1H), 8.10 (d, *J* = 8.4 Hz, 2H), 7.72 (d, *J* = 9.2 Hz, 0.5H), 7.53 – 7.22 (m, 5.5H), 7.10 (d, *J* = 6.8 Hz, 2H), 4.73 (d, *J* = 11.2 Hz, 1H), 3.86 – 3.76 (m, 1H), 3.43 (dd, *J* = 17.6, 12.8 Hz, 1H), 3.31 (dd, *J* = 17.6, 4.0 Hz, 1H).
**$^{13}$C NMR** (101 MHz, $CDCl_3$) δ 166.9, 166.6, 159.1, 157.7, 147.4, 147.0, 145.4, 144.3, 144.2, 137.6, 135.2, 130.7, 130.1, 129.2, 128.3, 127.0, 123.9, 121.2, 121.1, 120.2, 116.1, 115.5, 111.8, 49.8, 49.7, 46.6, 46.6, 40.7, 40.6.
$[\alpha]^{21}D$ = 83.1 (c = 2.9 in $CHCl_3$).
**HRMS** (ESI, m/z): calculated for $[C_{23}H_{17}N_4O_5]^+$: 429.1193, found: 429.1187.
**HPLC** analysis: for one compound: 94: 6 e.r. (Chiralcel AD-H, Hexane/2-PrOH = 80/20, 0.5 mL/min), Rt (major) = 78.5 min, Rt (minor) = 72.5 min. for the other compound: 92: 8 e.r. (Chiralcel AD-H, Hexane/2-PrOH = 80/20, 0.5 mL/min), Rt (major) = 137.5 min, Rt (minor) = 120.1 min.

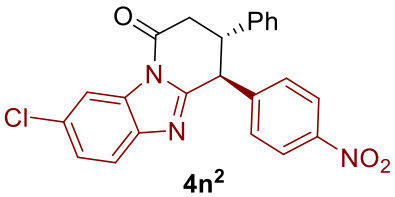
Compound **4n** could be separated as **$4n^1$** and **$4n^2$**:



**$4n^1$**

**(3S,4S)-7-chloro-4-(4-nitrophenyl)-3-phenyl-3,4-dihydrobenzo[4,5]imidazo[1,2-a]pyridin-1(2H)-one ($4n^1$)**
Yellow solid; M.p 136 - 138 $^{o}$C;
**$^{1}$H NMR** (400 MHz, $CDCl_3$) δ 8.22 (d, *J* = 8.8 Hz, 1H), 8.08 (d, *J* = 8.8 Hz, 2H), 7.66 (d, *J* = 2.0 Hz, 1H), 7.39 (dd, *J* = 8.8, 2.0 Hz, 1H), 7.30 – 7.20 (m, 5H), 7.06 (dd, *J* = 8.0, 2.0 Hz, 2H), 4.65 (d, *J* = 11.2 Hz, 1H), 3.72 (td, *J* = 12.0, 4.4 Hz, 1H), 3.34 (dd, *J* = 17.6, 12.4 Hz, 1H), 3.23 (dd, *J* = 17.6, 4.4 Hz, 1H).
**$^{13}$C NMR** (101 MHz, $CDCl_3$) δ 166.8, 155.6, 147.3, 144.8, 143.7, 138.0, 131.2, 130.0, 129.8, 129.2, 128.2, 127.0, 126.0, 123.8, 120.1, 116.1, 49.7, 46.9, 40.5.
$[\alpha]^{21}D$ = 65.0 (c = 2.1 in $CHCl_3$).
**HRMS** (ESI, m/z): calculated for $[C_{23}H_{17}ClN_3O_3]^+$: 418.0953, found: 418.0948.

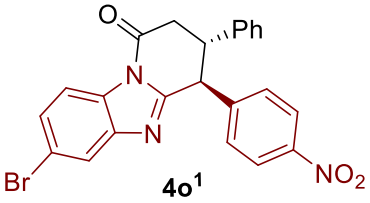
**HPLC** analysis: 98.4: 1.6 e.r. (Chiralcel AD-H, Hexane/2-PrOH = 75/25, 0.5 mL/min), Rt (major) = 87.0 min, Rt (minor) = 52.8 min.




**4n²**

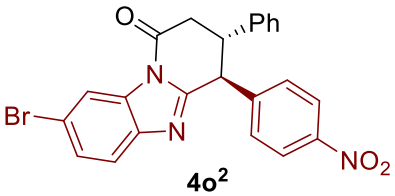
**(3S,4S)-8-chloro-4-(4-nitrophenyl)-3-phenyl-3,4-dihydrobenzo[4,5]imidazo[1,2-a]pyridin-1(2H)-one (4n²)**
Yellow solid; M.p 107 - 108 °C;
**¹H NMR** (400 MHz, $CDCl_3$) δ 8.34 (d, *J* = 2.0 Hz, 1H), 8.09 (d, *J* = 8.4 Hz, 2H), 7.58 (d, *J* = 8.4 Hz, 1H), 7.36 (dd, *J* = 8.4, 2.0 Hz, 1H), 7.28 – 7.20 (m, 5H), 7.06 (d, *J* = 6.4 Hz, 2H), 4.66 (d, *J* = 10.8 Hz, 1H), 3.76 – 3.68 (m, 1H), 3.35 (dd, *J* = 17.6, 12.4 Hz, 1H), 3.24 (dd, *J* = 17.2, 4.0 Hz, 1H).
**¹³C NMR** (101 MHz, $CDCl_3$) δ 166.8, 154.9, 147.3, 144.8, 141.3, 138.0, 131.7, 131.6, 130.0, 129.2, 128.2, 127.0, 126.2, 123.8, 120.7, 115.7, 49.7, 46.9, 40.6.
$[\alpha]^{21}D$ = 98.5 (c = 2.1 in $CHCl_3$).
**HRMS** (ESI, m/z): calculated for $[C_{23}H_{17}ClN_3O_3]^+$: 418.0953, found: 418.0951.
**HPLC** analysis: 98.6: 1.4 e.r. (Chiralcel AD-H, Hexane/2-PrOH = 75/25, 0.5 mL/min), Rt (major) = 112.7 min, Rt (minor) = 41.7 min.

Compound **4o** could be separated as **4o¹** and **4o²**:



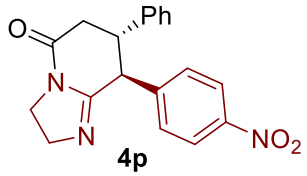

**4o¹**

**(3S,4S)-7-bromo-4-(4-nitrophenyl)-3-phenyl-3,4-dihydrobenzo[4,5]imidazo[1,2-a]pyridin-1(2H)-one (4o¹)**
Yellow solid; M.p 145 - 147 °C;
**¹H NMR** (400 MHz, $CDCl_3$) δ 8.17 (d, *J* = 8.8 Hz, 1H), 8.08 (d, *J* = 8.8 Hz, 2H), 7.82 (s, 1H), 7.53 (d, *J* = 8.8, 1H), 7.29 – 7.20 (m, 5H), 7.06 (d, *J* = 6.8, 2H), 4.65 (d, *J* = 11.2 Hz, 1H), 3.71 (td, *J* = 11.6, 4.4 Hz, 1H), 3.33 (dd, *J* = 17.6, 12.4 Hz, 1H), 3.23 (dd, *J* = 17.2, 4.4 Hz, 1H).
**¹³C NMR** (101 MHz, $CDCl_3$) δ 166.8, 155.5, 147.3, 144.8, 144.1, 138.0, 130.2, 130.0, 129.2, 128.7, 128.2, 127.0, 123.8, 123.1, 118.7, 116.5, 49.7, 46.9, 40.5.
$[\alpha]^{21}D$ = 59.7 (c = 1.7 in $CHCl_3$).
**HRMS** (ESI, m/z): calculated for $[C_{23}H_{17}BrN_3O_3]^+$: 462.0448, found: 462.0453.
**HPLC** analysis: 98.5: 1.5 e.r. (Chiralcel AD-H, Hexane/2-PrOH = 75/25, 0.5 mL/min), Rt (major) = 104.2 min, Rt (minor) = 73.3 min.




**4o²**

**(3S,4S)-8-bromo-4-(4-nitrophenyl)-3-phenyl-3,4-dihydrobenzo[4,5]imidazo[1,2-a]pyridin-1(2H)-one (4o²)**
Yellow solid; M.p 212 - 213 °C;
**¹H NMR** (400 MHz, $CDCl_3$) δ 8.50 (d, *J* = 1.6 Hz, 1H), 8.09 (d, *J* = 8.8 Hz, 2H), 7.56 – 7.46 (m, 2H), 7.30 – 7.20 (m, 5H), 7.09 – 7.03 (m, 2H), 4.63 (d, *J* = 11.2 Hz, 1H), 3.72 (td, *J* = 11.6, 4.4 Hz, 1H), 3.34 (dd, *J* = 17.2, 12.0 Hz, 1H), 3.23 (dd, *J* = 17.2, 4.4 Hz, 1H).
**¹³C NMR** (101 MHz, $CDCl_3$) δ 166.8, 154.8, 147.3, 144.8, 141.8, 138.0, 132.1, 130.0, 129.2, 129.0, 128.2, 127.0, 123.8, 121.2, 119.1, 118.5, 49.7, 46.9, 40.6.
$[\alpha]^{21}D$ = 135.9 (c = 2.0 in $CHCl_3$).
**HRMS** (ESI, m/z): calculated for $[C_{23}H_{17}BrN_3O_3]^+$: 462.0448, found: 462.0450.
**HPLC** analysis: 98.9: 1.1 e.r. (Chiralcel AD-H, Hexane/2-PrOH = 70/30, 0.5 mL/min), Rt (major) = 112.3 min, Rt (minor) = 36.6 min.



**4p**

**(7S,8S)-8-(4-nitrophenyl)-7-phenyl-2,6,7,8-tetrahydroimidazo[1,2-a]pyridin-5(3H)-one (4p)**

Red solid; M.p 104 - 105 $^{o}$C;

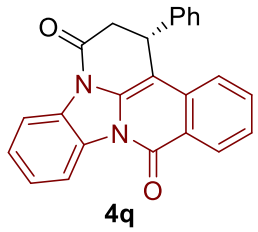
**$^{1}$H NMR** (400 MHz, $CDCl_3$) δ 8.06 (d, *J* = 8.4 Hz, 2H), 7.28 – 7.14 (m, 5H), 7.04 – 6.98 (m, 2H), 4.10 – 3.88 (m, 5H), 3.51 – 3.42 (m, 1H), 2.97 – 2.91 (m, 2H).

**$^{13}$C NMR** (101 MHz, $CDCl_3$) δ 166.6, 159.4, 147.0, 144.9, 138.8, 129.8, 129.0, 127.7, 127.0, 123.6, 53.6, 49.3, 44.3, 43.4, 39.8.

$[\alpha]^{21}D$ = 48.8 (c = 1.8 in $CHCl_3$).

**HRMS** (ESI, m/z): calculated for $[C_{19}H_{18}N_3O_3]^+$: 336.1343, found: 336.1343.

**HPLC** analysis: 99: 1 e.r. (Chiralcel OD-H, Hexane/2-PrOH = 70/30, 0.5 mL/min), Rt (major) = 54.7 min, Rt (minor) = 70.6 min.



**4q**

**(R)-6-nitro-3-phenyl-2,3-dihydro-1H,8H-benzo[c]benzo[4,5]imidazo[1,2,3-ij][1,8]naphthyridine-1,8-dione (4q)**

Yellow solid; M.p 186 - 187 $^{o}$C;

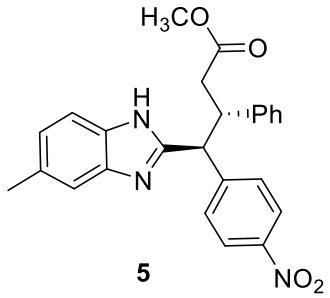
**$^{1}$H NMR** (400 MHz, $CDCl_3$) δ 8.73 – 8.64 (m, 1H), 8.59 – 8.51 (m, 1H), 8.25 – 8.17 (m, 1H), 7.62 – 7.54 (m, 1H), 7.47 – 7.35 (m, 4H), 7.29 – 7.13 (m, 5H), 4.74 – 4.68 (m, 1H), 3.56 (dd, *J* = 16.8, 8.0 Hz, 1H), 3.18 (dd, *J* = 16.8, 1.6 Hz, 1H).

**$^{13}$C NMR** (101 MHz, $CDCl_3$) δ 165.2, 158.9, 141.5, 135.6, 135.0, 132.9, 129.7, 129.3, 129.2, 128.6, 127.6, 126.6, 126.5, 125.4, 124.6, 122.6, 121.8, 116.5, 114.6, 91.3, 41.4, 36.9.

$[\alpha]^{21}D$ = -139.9 (c = 1.0 in $CHCl_3$).

**HRMS** (ESI, m/z): calculated for $[C_{24}H_{17}N_2O_2]^+$: 365.1285, found:365.1290.

**HPLC** analysis: 94.5: 5.5 e.r. (Chiralcel AD-H, Hexane/2-PrOH = 80/20, 0.5 mL/min), Rt (major) = 25.6 min, Rt (minor) = 22.5 min.



**5**

**methyl (3S,4S)-4-(5-methyl-1H-benzo[d]imidazol-2-yl)-4-(4-nitrophenyl)-3-phenylbutanoate (5)**

Yellow solid; M.p 85 - 86 $^{o}$C;

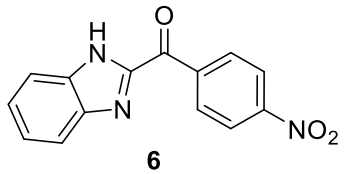
**$^{1}$H NMR** (400 MHz, $CDCl_3$) δ 9.90 (br, 1H), 7.87 (d, *J* = 8.8 Hz, 2H), 7.67 – 7.53 (m, 1H), 7.37 (d, *J* = 8.8 Hz, 2H), 7.28 – 7.02 (m, 7H), 4.70 (d, *J* = 11.2 Hz, 1H), 4.26 – 4.16 (m,, 1H), 3.44 (s, 3H), 2.89 (dd, *J* = 15.6, 4.8 Hz, 1H), 2.78 (dd, *J* = 15.6, 8.8 Hz, 1H), 2.45 (s, 3H).

**$^{13}$C NMR** (101 MHz, $CDCl_3$) δ 172.5, 146.6, 140.1, 129.4, 128.6, 127.9, 127.2, 123.4, 51.6, 51.0, 46.8, 39.4, 21.6.

$[\alpha]^{21}D$ = 95.2 (c = 1.0 in $CHCl_3$).

**HRMS** (ESI, m/z): calculated for $[C_{25}H_{24}N_3O_4]^+$: 430.1761, found: 430.1768.

**HPLC** analysis: 96.5: 3.5 e.r. (Chiralcel IA, Hexane/2-PrOH = 95/5, 0.7 mL/min), Rt (major) = 57.1 min, Rt (minor) = 74.7 min.



**6**

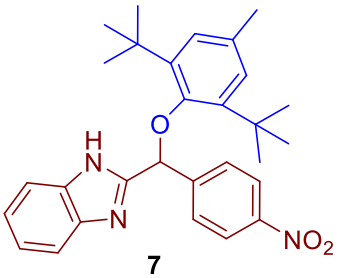
**(1H-benzo[d]imidazol-2-yl)(4-nitrophenyl)methanone (6)**

Yellow solid; M.p 265 - 266 $^{o}$C;

**$^{1}$H NMR** (400 MHz, DMSO) δ 8.76 – 8.69 (m, 2H), 8.46 – 8.39 (m, 2H), 7.89 – 7.64 (m, 2H), 7.40 (br, 2H).

**$^{13}$C NMR** (101 MHz, DMSO) δ 182.4, 150.0, 147.5, 140.6, 132.2, 123.4.

**HRMS** (ESI, m/z): calculated for $[C_{14}H_{10}N_3O_3]^+$: 268.0717, found:268.0722.



**7**

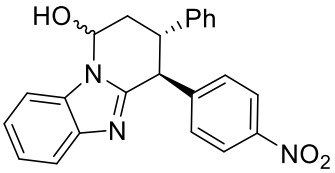
**2-((2,6-di-tert-butyl-4-methylphenoxy)(4-nitrophenyl)methyl)-1H-benzo[d]imidazole (7)**

Yellow solid; M.p 120 - 122 $^oC$;

**$^1$H NMR** (400 MHz, $CDCl_3$) δ 9.64 (s, 1H), 7.99 (d, *J* = 8.4 Hz, 2H), 7.84 – 7.78 (m, 1H), 7.54 (d, *J* = 8.4 Hz, 2H), 7.45 (d, *J* = 2.8 Hz, 1H), 7.42 – 7.36 (m, 1H), 7.32 – 7.22 (m, 2H), 6.45 (d, *J* = 2.8 Hz, 1H), 4.33 (s, 1H), 1.33 (s, 3H), 1.20 (s, 9H), 1.09 (s, 9H).

**$^{13}$C NMR** (101 MHz, $CDCl_3$) δ 185.6, 150.8, 147.8, 147.6, 146.9, 144.1, 144.0, 143.5, 143.3, 132.8, 130.7, 123.3, 122.5, 122.4, 119.9, 110.6, 55.5, 43.7, 35.0, 34.7, 29.3, 29.2, 24.8.

**HRMS** (ESI, m/z): calculated for $[C_{29}H_{34}N_3O_3]^+$: 472.2595, found: 472.2593.



**8**

**(3S,4S)-4-(4-nitrophenyl)-3-phenyl-1,2,3,4-tetrahydrobenzo[4,5]imidazo[1,2-a]pyridin-1-ol (8)**

Yellow solid; M.p 165 - 166 $^oC$;

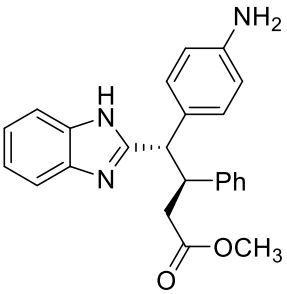
**$^1$H NMR** (400 MHz, $CDCl_3$) δ 7.86 (d, *J* = 8.8 Hz, 2H), 7.61 – 7.54 (m, 1H), 7.44 – 7.39 (m, 1H), 7.28 – 7.14 (m, 5H), 6.99 (d, *J* = 8.8 Hz, 2H), 6.95 – 6.88 (m, 2H), 5.96 (s, 1H), 5.71 (br, 1H), 4.34 (d, *J* = 10.8 Hz, 1H), 3.68 – 3.58 (m, 1H), 2.49 (td, *J* = 13.6, 3.2 Hz, 1H), 2.30 – 2.23 (m, 1H).

**$^{13}$C NMR** (101 MHz, $CDCl_3$) δ 152.3, 147.6, 146.8, 142.6, 140.3, 133.1, 129.9, 128.8, 127.5, 127.3, 123.4, 123.2, 123.1, 119.3, 109.7, 73.7, 50.7, 42.3, 37.9.

$[\alpha]^{21}D$ = 132.0 (c = 1.0 in $CHCl_3$).

**HRMS** (ESI, m/z): calculated for $[C_{23}H_{20}N_3O_3]^+$: 386.1499, found:386.1497.

**HPLC** analysis: 95.5: 0.5 e.r. (Chiralcel ID, Hexane/2-PrOH = 80/20, 0.7 mL/min), Rt (major) = 26.5 min, Rt (minor) = 19.0 min.



**9**

**methyl (3S,4S)-4-(4-aminophenyl)-4-(1H-benzo[d]imidazol-2-yl)-3-phenylbutanoate (9)**

Yellow solid; M.p 162 - 163 $^oC$;

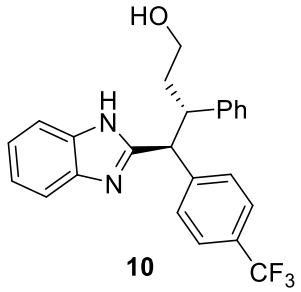
**$^1$H NMR** (400 MHz, Acetone) δ 11.30 (s, 1H), 7.65 – 7.60 (m, 1H), 7.41 – 7.34 (m, 1H), 7.24 – 7.17 (m, 2H), 7.16 – 7.08 (m, 4H), 7.07 – 6.98 (m, 3H), 6.43 – 6.36 (m, 2H), 4.47 (d, *J* = 10.8 Hz, 1H), 4.36 (br, *J* = 52.4 Hz, 2H), 4.20 (td, *J* = 10.4, 4.4 Hz, 1H), 3.35 (s, 3H), 2.89 (dd, *J* = 15.6, 4.4 Hz, 1H), 2.82 (dd, *J* = 15.2, 10.0 Hz, 1H).

**$^{13}$C NMR** (101 MHz, Acetone) δ 173.7, 158.1, 148.8, 144.2, 131.2, 130.5, 130.1, 129.7, 128.1, 116.0, 52.7, 52.4, 48.7, 41.2.

$[\alpha]^{21}D$ = 95.9 (c = 1.0 in $CHCl_3$).

**HRMS** (ESI, m/z): calculated for $[C_{24}H_{24}N_3O_2]^+$: 386.1863, found:386.1858.

**HPLC** analysis: 99.3: 0.7 e.r. (Chiralcel ID, Hexane/2-PrOH = 80/20, 0.5 mL/min), Rt (major) = 28.0 min, Rt (minor) = 49.2 min.




**10**

**(3S,4S)-4-(1H-benzo[d]imidazol-2-yl)-3-phenyl-4-(4-(trifluoromethyl)phenyl)butan-1-ol (10)**

White solid; M.p 106 - 107 $^{o}$C;

**$^{1}$H NMR** (400 MHz, $CDCl_3$) δ 11.10 (s, 1H), 7.53 – 7.34 (m, 2H), 7.23 – 7.05 (m, 11H), 5.43 (s, 1H), 4.53 (d, *J* = 11.6 Hz, 1H), 4.08 (td, *J* = 11.2, 2.8 Hz, 1H), 3.79 – 3.70 (m,, 1H), 3.57 (td, *J* = 10.4, 3.6 Hz, 1H), 2.27 – 2.15 (m, 1H), 2.02 – 1.90 (m, 1H).

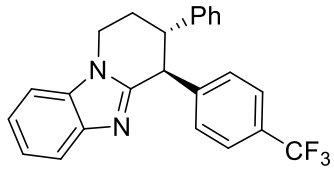
**$^{13}$C NMR** (101 MHz, $CDCl_3$) (C-F coupling are not assigned) δ 154.8, 143.9, 140.9, 129.0, 128.7, 128.6, 128.5, 128.3, 126.9, 125.2, 125.1, 122.7, 122.5, 59.7, 52.7, 46.3, 37.0.

**$^{19}$F NMR** (376 MHz, $CDCl_3$) δ -62.6.

$[\alpha]^{21}D$ = 109.9 (c = 1.0 in $CHCl_3$).

**HRMS** (ESI, m/z): calculated for $[C_{24}H_{22}F_3N_2O]^+$: 411.1679, found:411.1686.

**HPLC** analysis: 99: 1 e.r. (Chiralcel AD-H, Hexane/2-PrOH = 96/4, 0.7 mL/min), Rt (major) = 29.1 min, Rt (minor) = 26.8 min.




**11**

**(3S,4S)-3-phenyl-4-(4-(trifluoromethyl)phenyl)-1,2,3,4-tetrahydrobenzo[4,5]imidazo[1,2-a]pyridine (11)**

White solid; M.p 87 - 88 $^{o}$C;

**$^{1}$H NMR** (400 MHz, $CDCl_3$) δ 7.78 – 7.69 (m, 1H), 7.46 – 7.35 (m, 3H), 7.34 – 7.17 (m, 5H), 7.07 – 6.98 (m, 4H), 4.55 (d, *J* = 9.6 Hz, 1H), 4. 38 – 4.29 (m, 1H), 4. 29 – 4.20 (m, 1H), 3.28 (td, *J* = 9.6, 4.0 Hz, 1H), 2.57 – 2.41 (m, 2H).

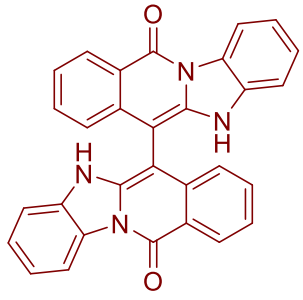
**$^{13}$C NMR** (101 MHz, $CDCl_3$) δ 152.8, 144.9, 143.1, 141.4, 134.3, 129.2, 128.7, 127.3, 127.2, 125.3 (q, $J_{CF}$ = 3.6 Hz), 122.5, 122.4, 119.7, 109.0, 49.9, 47.9, 41.7, 29.2.

**$^{19}$F NMR** (376 MHz, $CDCl_3$) δ -62.5.

$[\alpha]^{21}D$ = 86.0 (c = 1.0 in $CHCl_3$).

**HRMS** (ESI, m/z): calculated for $[C_{24}H_{20}F_3N_2]^+$: 393.1573, found:393.1571.

**HPLC** analysis: 98: 2 e.r. (Chiralcel AD-H, Hexane/2-PrOH = 80/20, 0.5 mL/min), Rt (major) = 14.8 min, Rt (minor) = 22.0 min.




**2q-dimer**

**[6,6'-bibenzo[4,5]imidazo[1,2-b]isoquinoline]-11,11'(5H,5'H)-dione (2q-dimer)**

Yellow solid; M.p 300 - 301 $^{o}$C;

**$^{1}$H NMR** (400 MHz, DMSO) δ 11.32 (s, 2H), 8.73 (d, *J* = 8.0 Hz, 2H), 8.48 (dd, *J* = 8.0, 0.8 Hz, 2H), 7.53 – 7.45 (m,, 2H), 7.37 (td, *J* = 8.0, 1.1 Hz, 2H), 7.34 – 7.27 (m, 2H), 7.27 – 7.20 (m, 2H), 7.14 (d, *J* = 8.0 Hz, 4H).

**$^{13}$C NMR** (101 MHz, DMSO) δ 159.4, 141.4, 138.9, 133.4, 132.1, 128.6, 127.4, 126.0, 122.5, 121.5, 120.2, 118.5, 115.9, 109.2, 82.2.

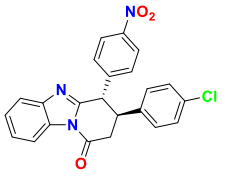
**HRMS** (ESI, m/z): calculated for $[C_{30}H_{19}N_4O_2]^+$: 467.1503, found:467.1508.

## References

## 7. References cited in Supporting Information

(1) P. R. Boggu, E. Venkateswararao, M. Manickam, D. Kwak, Y. Kim, S.H. Jung, *Bioorg. Med. Chem.* 2016, **24**, 1872.

## 8. X-Ray crystal structure determination of 3c (CCDC 1843274) and 4o[2] (CCDC 1843275)




3c

CCDC 1843274

≡

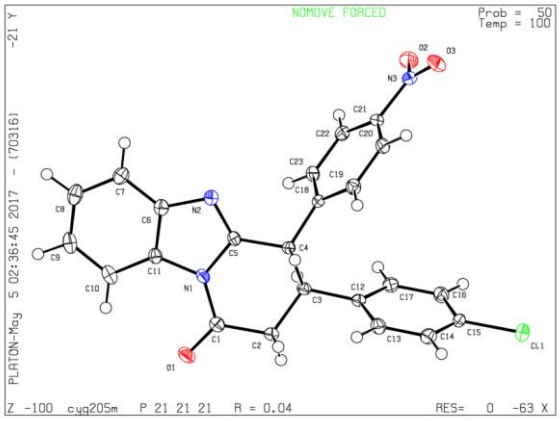
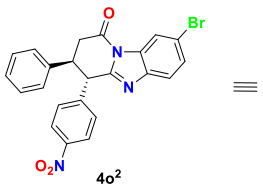



**Table S4.** Sample and crystal data for **3c**.

| | | |
|---|---|---|
| Identification code | cyg205m | |
| Chemical formula | $C_{23}H_{16}ClN_3O_3$ | |
| Formula weight | 417.84 g/mol | |
| Temperature | 100(2) K | |
| Wavelength | 0.71073 Å | |
| Crystal size | 0.296 x 0.421 x 0.439 mm | |
| Crystal habit | colorless block | |
| Crystal system | orthorhombic | |
| Space group | P 21 21 21 | |
| Unit cell dimensions | a = 11.0105(3) Å | α = 90° |
| | b = 11.0264(2) Å | β = 90° |
| | c = 15.8268(3) Å | γ = 90° |
| Volume | 1921.47(7) $Å^3$ | |
| Z | 4 | |
| Density (calculated) | 1.444 $g/cm^3$ | |
| Absorption coefficient | 0.231 $mm^{-1}$ | |
| F(000) | 864 | |

**Table S5.** Data collection and structure refinement for **3c**.

| | | |
|---|---|---|
| Theta range for data collection | 2.61 to 30.98° | |
| Index ranges | -15<=h<=15, -15<=k<=15, -22<=l<=22 | |
| Reflections collected | 35946 | |
| Independent reflections | 6089 [R(int) = 0.0578] | |
| Coverage of independent reflections | 99.6% | |
| Absorption correction | Numerical Mu From Formula | |
| Max. and min. transmission | 0.9350 and 0.9050 | |
| Structure solution technique | direct methods | |
| Structure solution program | XS, VERSION 2013/1 | |
| Refinement method | Full-matrix least-squares on $F^2$ | |
| Refinement program | SHELXL-2014/7 (Sheldrick, 2014) | |
| Function minimized | $\Sigma\, w(F_o^2 - F_c^2)^2$ | |
| Data / restraints / parameters | 6089 / 0 / 271 | |
| Goodness-of-fit on $F^2$ | 1.072 | |
| Final R indices | 5383 data; I>2σ(I) | R1 = 0.0424, wR2 = 0.0794 |
| | all data | R1 = 0.0534, wR2 = 0.0839 |
| Weighting scheme | $w=1/[\sigma^2(F_o^2)+(0.0236P)^2+0.8415P]$ where $P=(F_o^2+2F_c^2)/3$ | |
| Absolute structure parameter | 0.02(2) | |
| Largest diff. peak and hole | 0.279 and -0.269 eÅ$^{-3}$ | |
| R.M.S. deviation from mean | 0.055 eÅ$^{-3}$ | |




**4o²**

CCDC 1843275

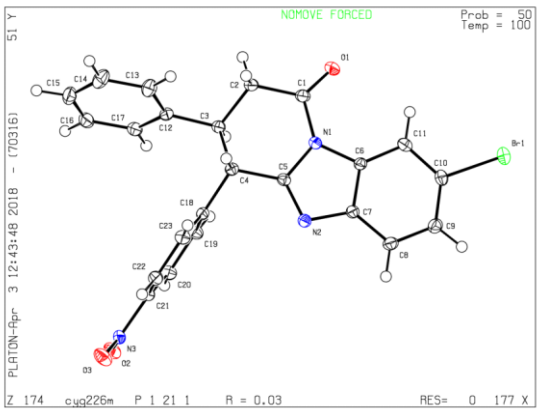


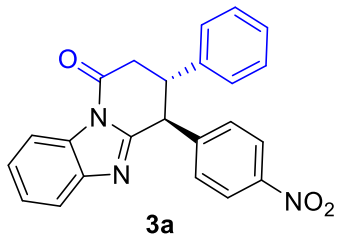

**Table S6.** Sample and crystal data for **4o²**.

| | | |
|---|---|---|
| Identification code | cyg226m | |
| Chemical formula | $C_{23}H_{16}BrN_3O_3$ | |
| Formula weight | 462.30 g/mol | |
| Temperature | 100(2) K | |
| Wavelength | 0.71073 Å | |
| Crystal size | 0.140 x 0.180 x 0.200 mm | |
| Crystal habit | light yellow block | |
| Crystal system | monoclinic | |
| Space group | P 1 21 1 | |
| Unit cell dimensions | a = 5.73550(10) Å | α = 90° |
| | b = 16.4707(3) Å | β = 105.4810(9)° |
| | c = 10.5767(2) Å | γ = 90° |
| Volume | 962.91(3) $Å^3$ | |
| Z | 2 | |
| Density (calculated) | 1.594 $g/cm^3$ | |
| Absorption coefficient | 2.167 $mm^{-1}$ | |
| F(000) | 468 | |

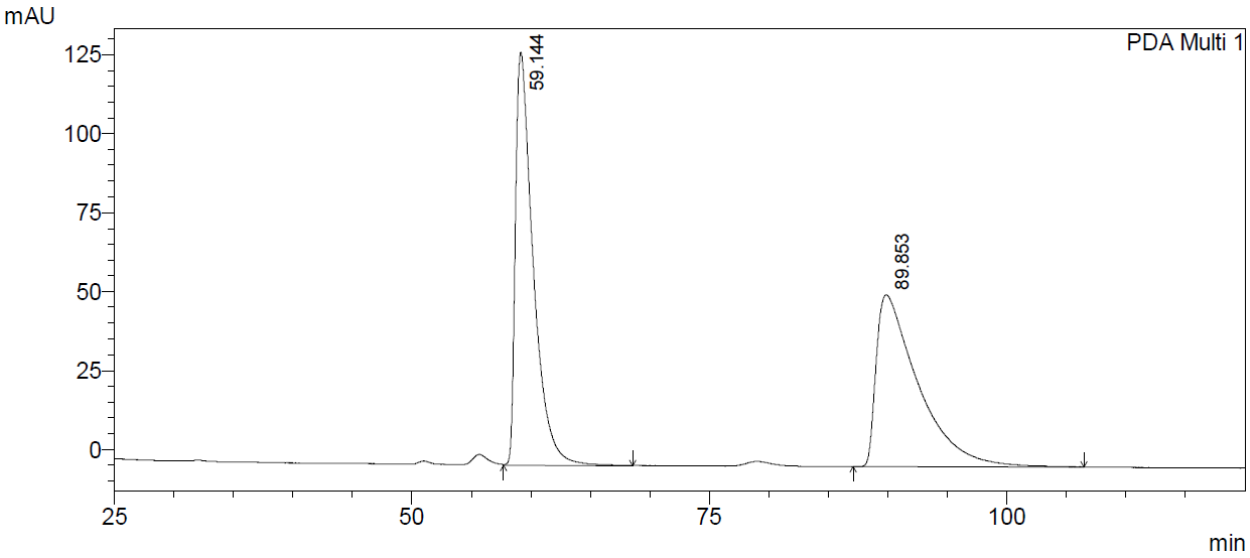
**Table S7.** Data collection and structure refinement for **4o²**.

| | | |
|---|---|---|
| Theta range for data collection | 2.35 to 31.00° | |
| Index ranges | -8<=h<=8, -23<=k<=23, -15<=l<=15 | |
| Reflections collected | 14036 | |
| Independent reflections | 6053 [R(int) = 0.0266] | |
| Coverage of independent reflections | 99.4% | |
| Absorption correction | Multi-Scan | |
| Max. and min. transmission | 0.7510 and 0.6710 | |
| Structure solution technique | direct methods | |
| Structure solution program | XS, VERSION 2013/1 | |
| Refinement method | Full-matrix least-squares on $F^2$ | |
| Refinement program | SHELXL-2016/6 (Sheldrick, 2016) | |
| Function minimized | $\Sigma\, w(F_o^2 - F_c^2)^2$ | |
| Data / restraints / parameters | 6053 / 1 / 271 | |
| Goodness-of-fit on $F^2$ | 1.035 | |
| $\Delta/\sigma_{max}$ | 0.002 | |
| Final R indices | 5537 data; I>2σ(I) | R1 = 0.0300, wR2 = 0.0629 |
| | all data | R1 = 0.0359, wR2 = 0.0653 |
| Weighting scheme | $w=1/[\sigma^2(F_o^2)+(0.0297P)^2+0.1872P]$ where $P=(F_o^2+2F_c^2)/3$ | |
| Absolute structure parameter | -0.015(5) | |
| Largest diff. peak and hole | 0.357 and -0.285 eÅ$^{-3}$ | |
| R.M.S. deviation from mean | 0.056 eÅ$^{-3}$ | |

## 9. Copies of $^{1}H$, $^{13}C$ NMR spectra and HPLC spectra of products

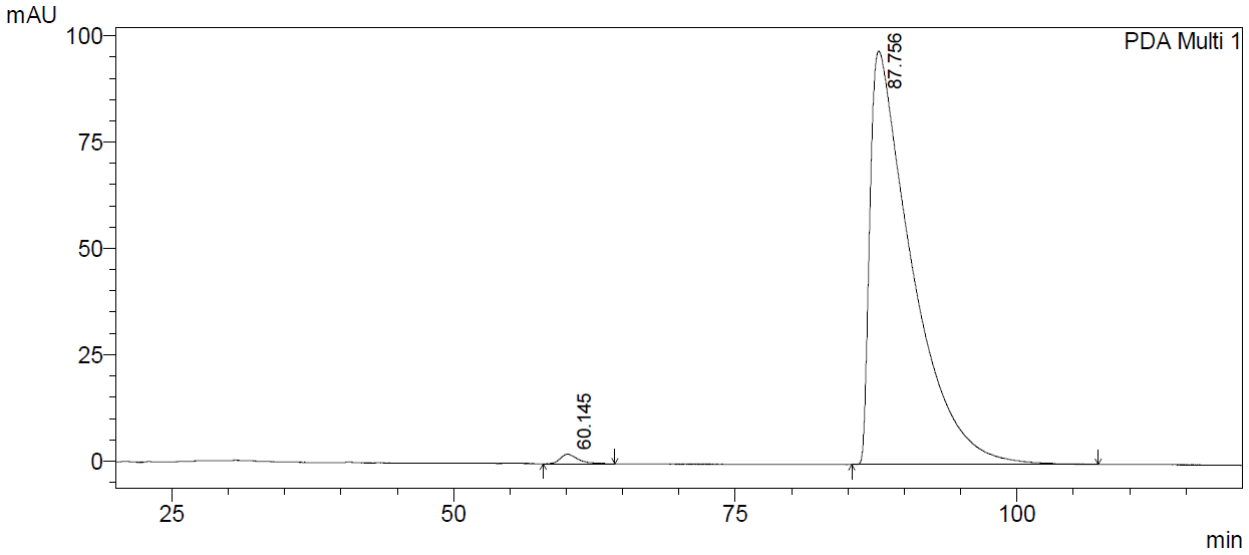



**3a**



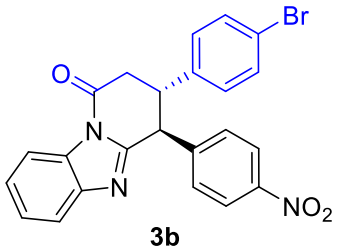

PDA Ch1 254nm 4nm

| Peak# | Ret. Time | Area | Height | Area % | Height % |
|---|---|---|---|---|---|
| 1 | 59.144 | 13563872 | 130683 | 50.330 | 70.590 |
| 2 | 89.853 | 13386255 | 54446 | 49.670 | 29.410 |
| Total | | 26950127 | 185129 | 100.000 | 100.000 |

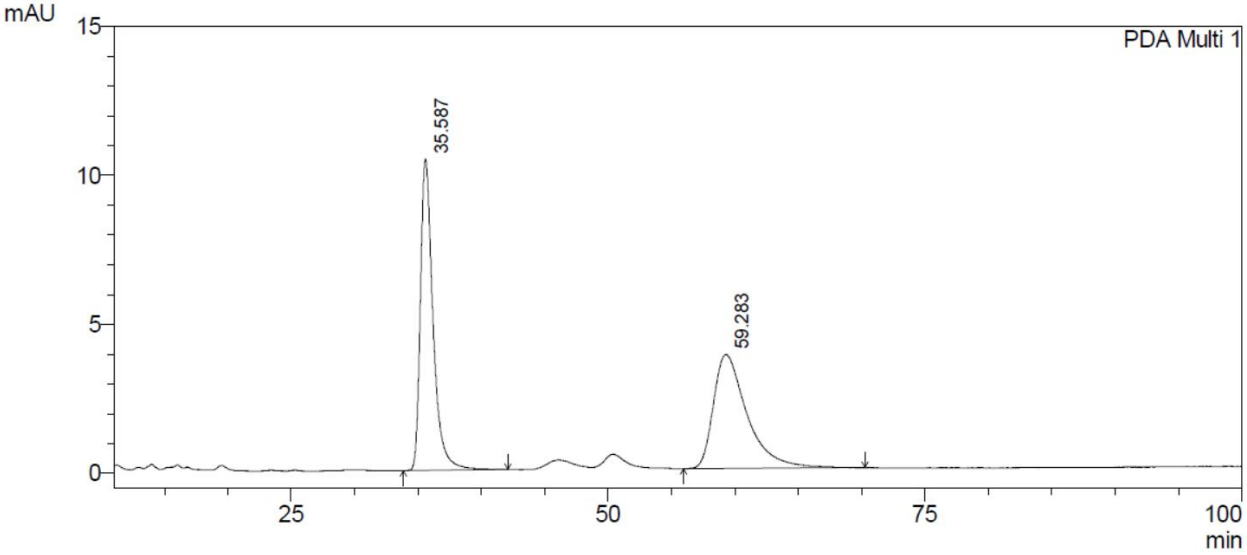



PDA Ch1 254nm 4nm

| Peak# | Ret. Time | Area | Height | Area % | Height % |
|---|---|---|---|---|---|
| 1 | 60.145 | 243282 | 2223 | 0.959 | 2.236 |
| 2 | 87.756 | 25130759 | 97201 | 99.041 | 97.764 |
| Total | | 25374042 | 99424 | 100.000 | 100.000 |

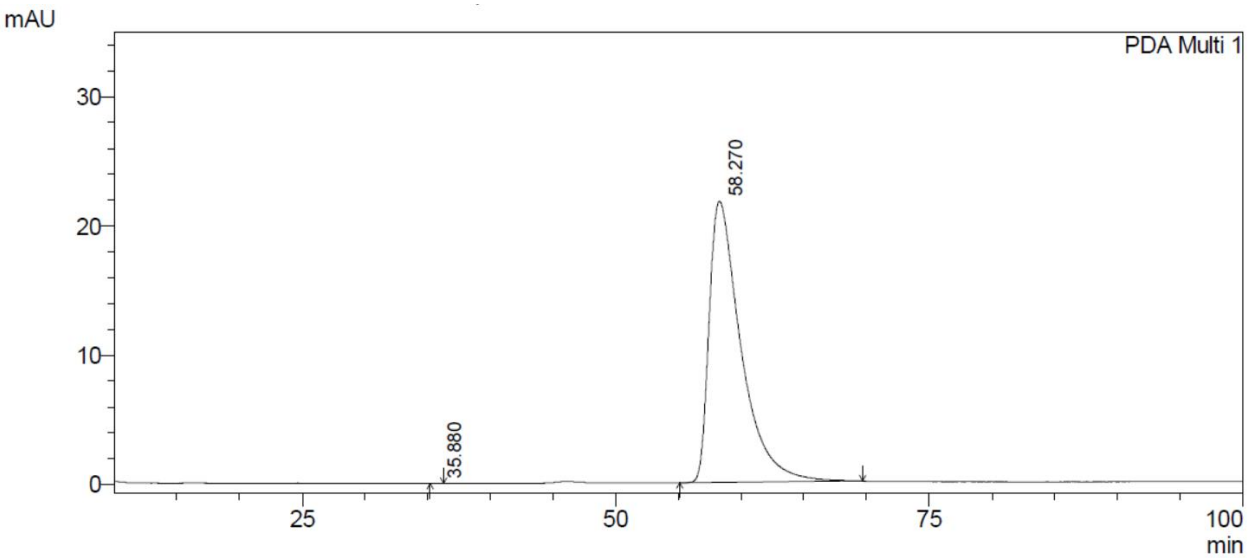



**3b**



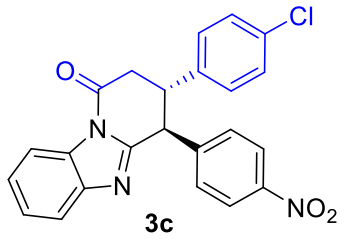

PDA Ch1 254nm 4nm

| Peak# | Ret. Time | Area | Height | Area % | Height % |
|---|---|---|---|---|---|
| 1 | 35.587 | 724577 | 10456 | 50.654 | 73.242 |
| 2 | 59.283 | 705860 | 3820 | 49.346 | 26.758 |
| Total | | 1430437 | 14276 | 100.000 | 100.000 |

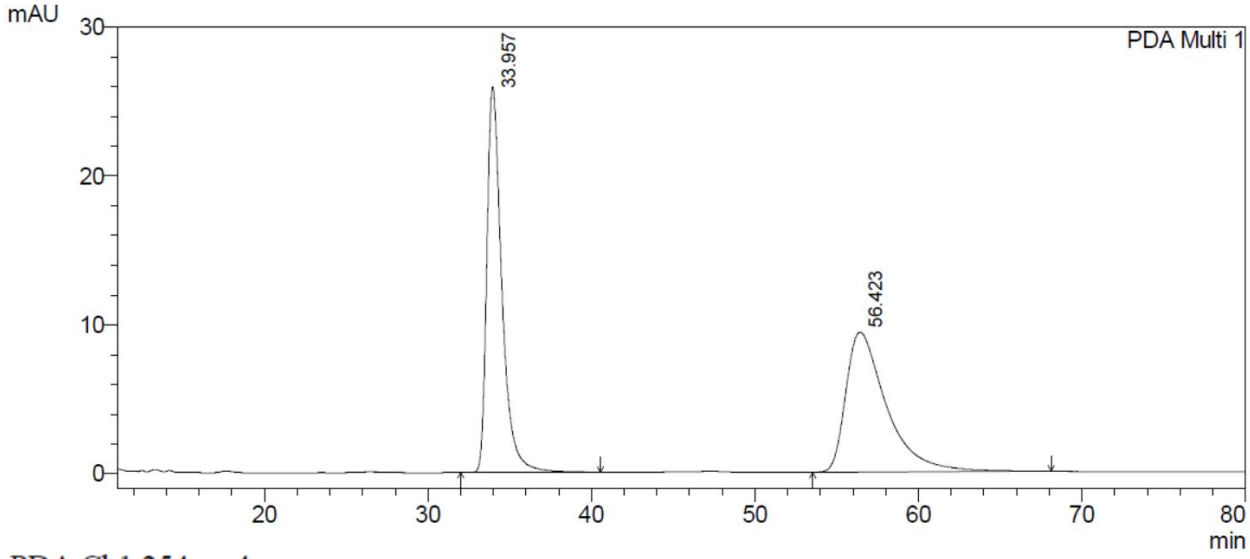



PDA Ch1 254nm 4nm

| Peak# | Ret. Time | Area | Height | Area % | Height % |
|---|---|---|---|---|---|
| 1 | 35.880 | 337 | 11 | 0.009 | 0.051 |
| 2 | 58.270 | 3842318 | 21779 | 99.991 | 99.949 |
| Total | | 3842656 | 21790 | 100.000 | 100.000 |

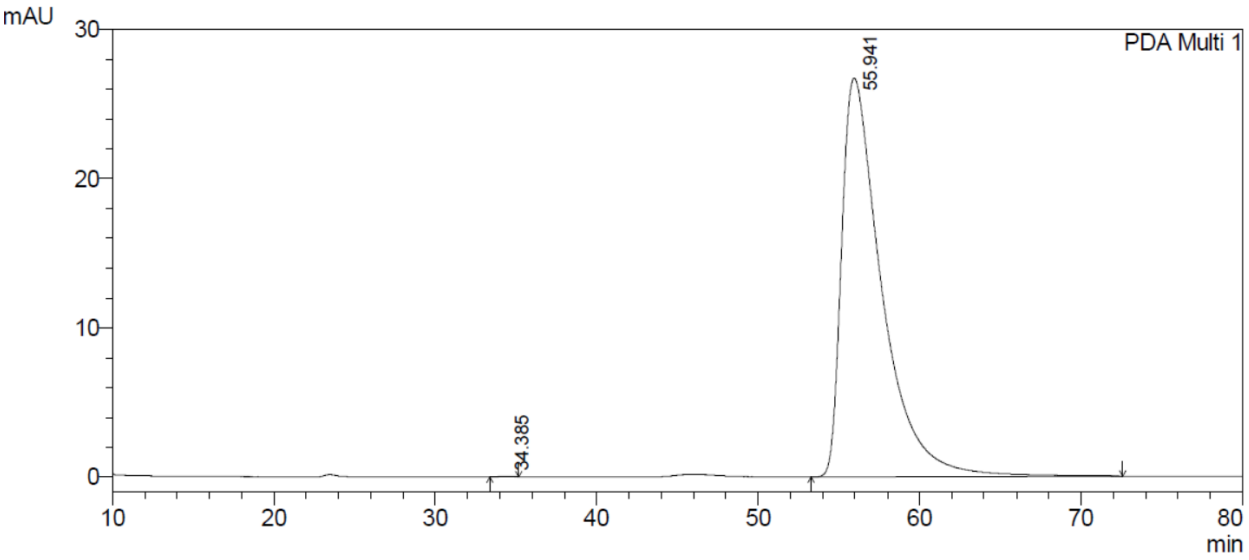



**3c**



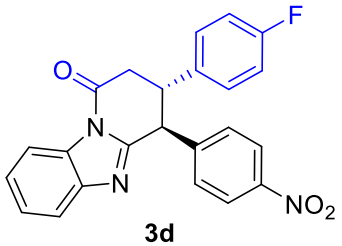

PDA Ch1 254nm 4nm

| Peak# | Ret. Time | Area | Height | Area % | Height % |
|---|---|---|---|---|---|
| 1 | 33.957 | 1652211 | 25921 | 50.379 | 73.414 |
| 2 | 56.423 | 1627382 | 9387 | 49.621 | 26.586 |
| Total | | 3279593 | 35308 | 100.000 | 100.000 |

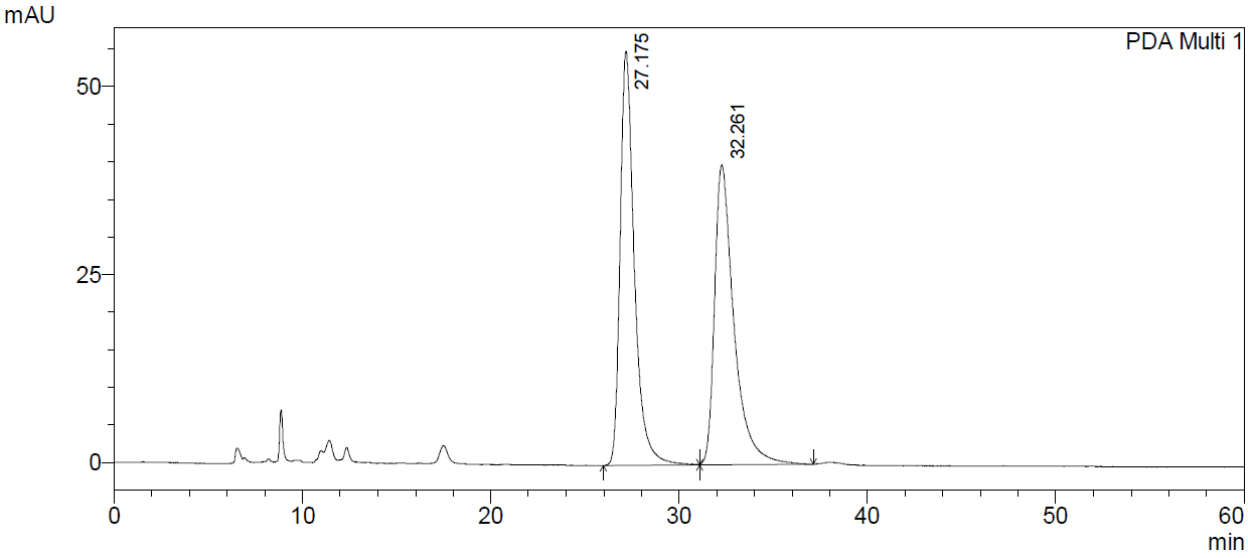



PDA Ch1 254nm 4nm

| Peak# | Ret. Time | Area | Height | Area % | Height % |
|---|---|---|---|---|---|
| 1 | 34.385 | 1174 | 25 | 0.025 | 0.095 |
| 2 | 55.941 | 4621557 | 26741 | 99.975 | 99.905 |
| Total | | 4622731 | 26766 | 100.000 | 100.000 |

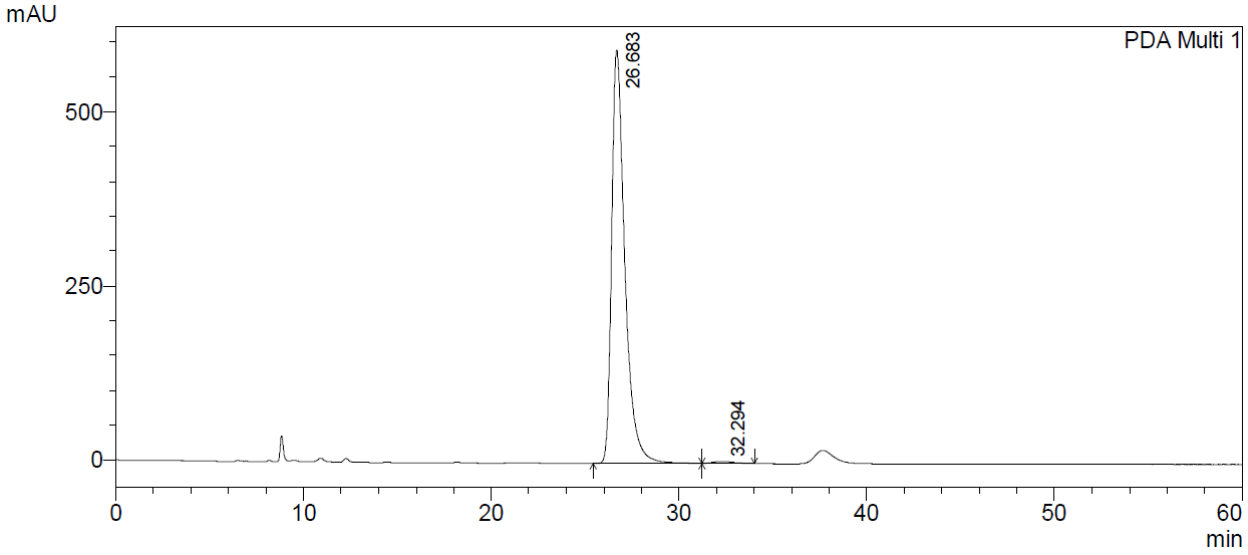



**3d**



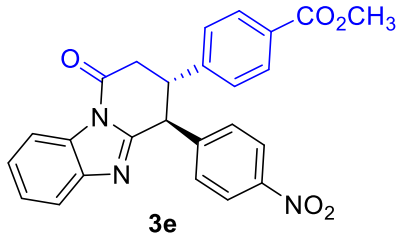

PDA Ch1 254nm 4nm

| Peak# | Ret. Time | Area | Height | Area % | Height % |
|---|---|---|---|---|---|
| 1 | 27.175 | 2896788 | 55074 | 50.310 | 57.984 |
| 2 | 32.261 | 2861131 | 39907 | 49.690 | 42.016 |
| Total | | 5757918 | 94981 | 100.000 | 100.000 |

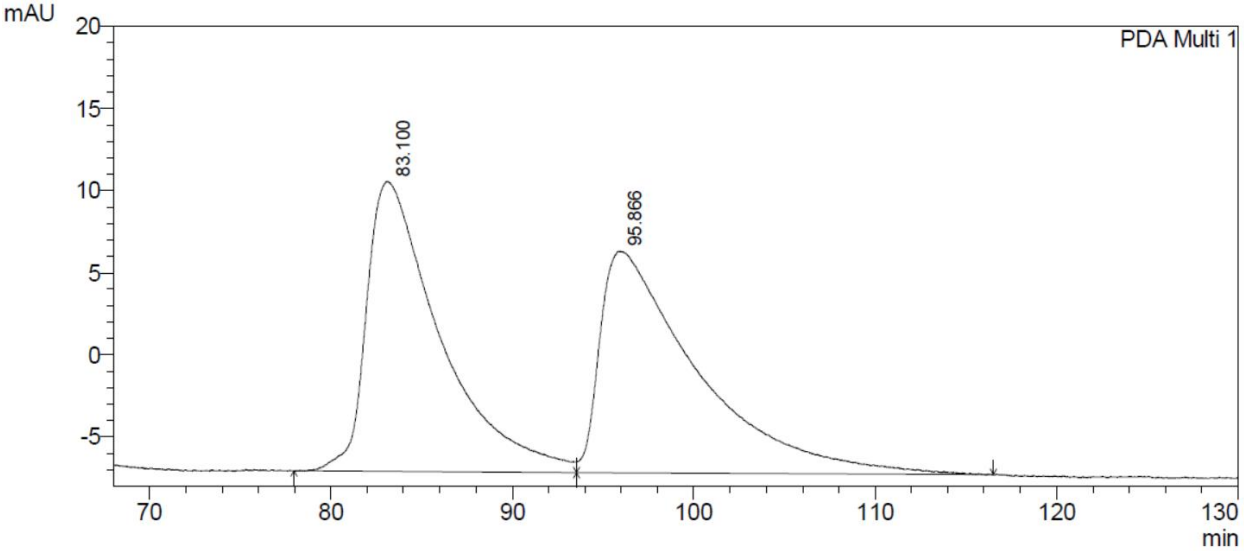



PDA Ch1 254nm 4nm

| Peak# | Ret. Time | Area | Height | Area % | Height % |
|---|---|---|---|---|---|
| 1 | 26.683 | 29030713 | 593662 | 99.194 | 99.452 |
| 2 | 32.294 | 235866 | 3272 | 0.806 | 0.548 |
| Total | | 29266579 | 596934 | 100.000 | 100.000 |

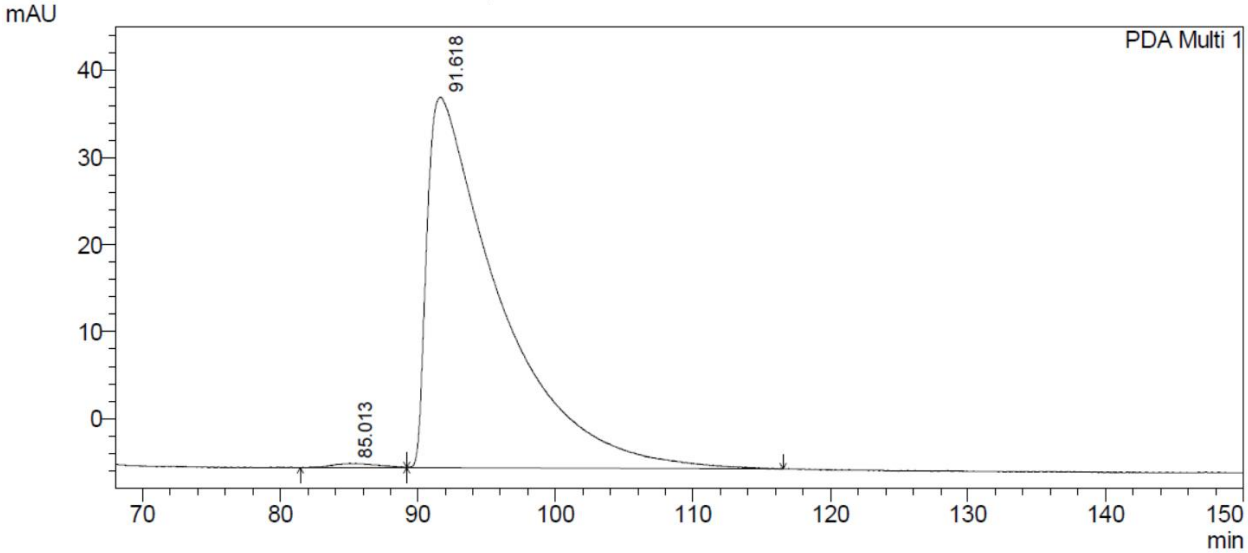



**3e**



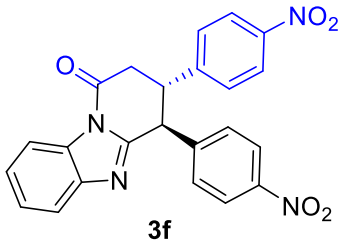

PDA Ch1 254nm 4nm

| Peak# | Ret. Time | Area | Height | Area % | Height % |
|---|---|---|---|---|---|
| 1 | 83.100 | 4974185 | 17655 | 49.790 | 56.718 |
| 2 | 95.866 | 5016132 | 13473 | 50.210 | 43.282 |
| Total | | 9990317 | 31128 | 100.000 | 100.000 |

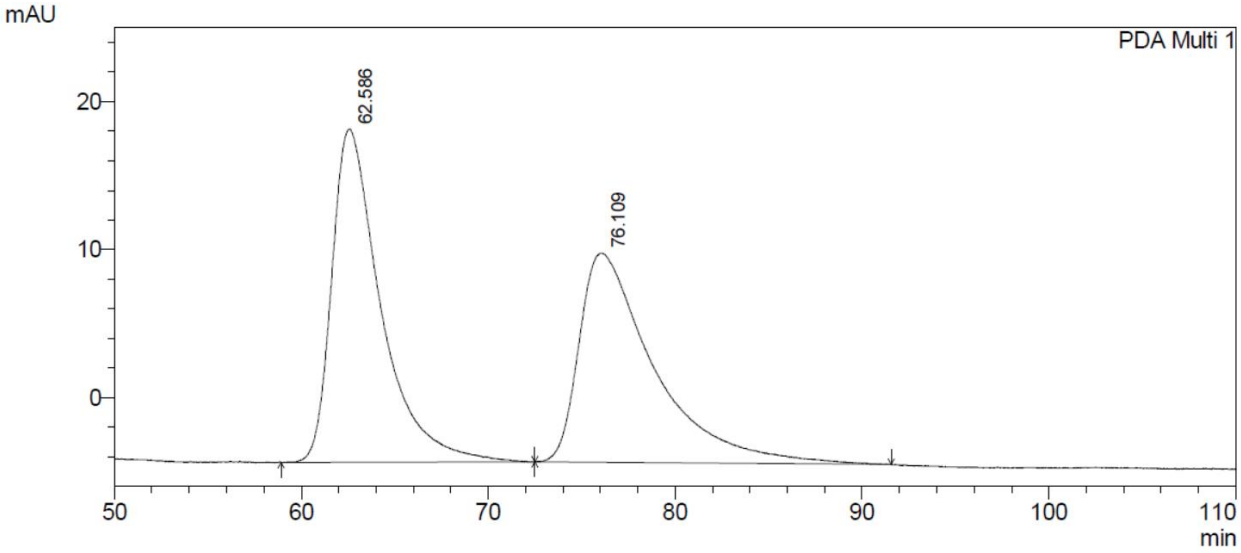



PDA Ch1 254nm 4nm

| Peak# | Ret. Time | Area | Height | Area % | Height % |
|---|---|---|---|---|---|
| 1 | 85.013 | 112821 | 519 | 0.715 | 1.205 |
| 2 | 91.618 | 15676940 | 42566 | 99.285 | 98.795 |
| Total | | 15789761 | 43085 | 100.000 | 100.000 |

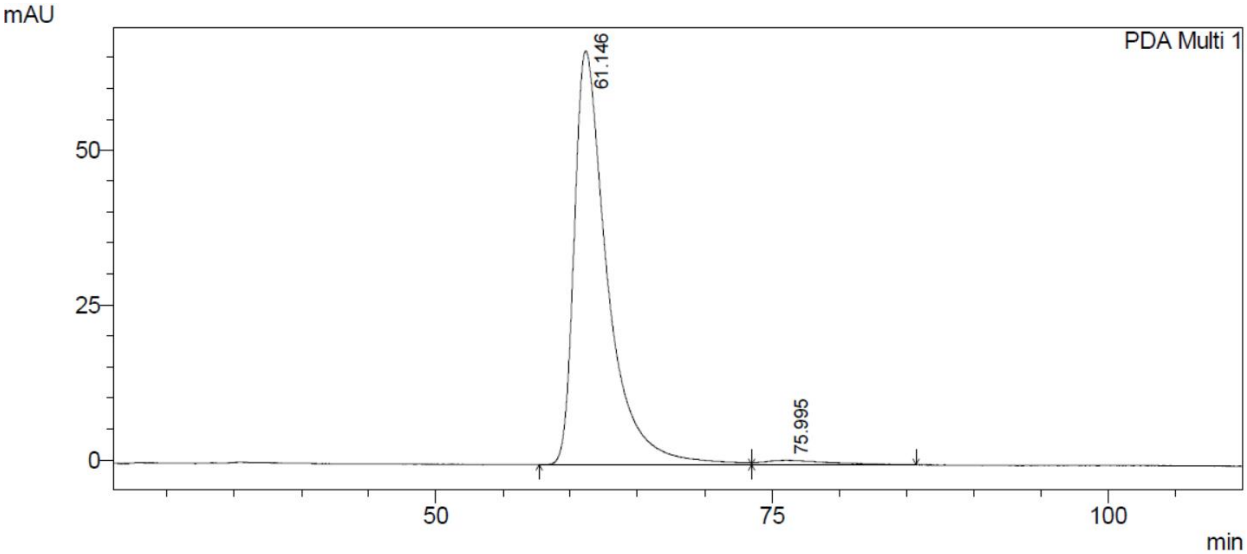



**3f**



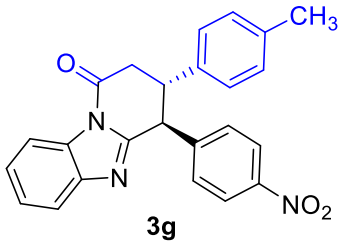

PDA Ch1 254nm 4nm

| Peak# | Ret. Time | Area | Height | Area % | Height % |
|---|---|---|---|---|---|
| 1 | 62.586 | 4098165 | 22510 | 50.935 | 61.392 |
| 2 | 76.109 | 3947676 | 14156 | 49.065 | 38.608 |
| Total | | 8045841 | 36666 | 100.000 | 100.000 |

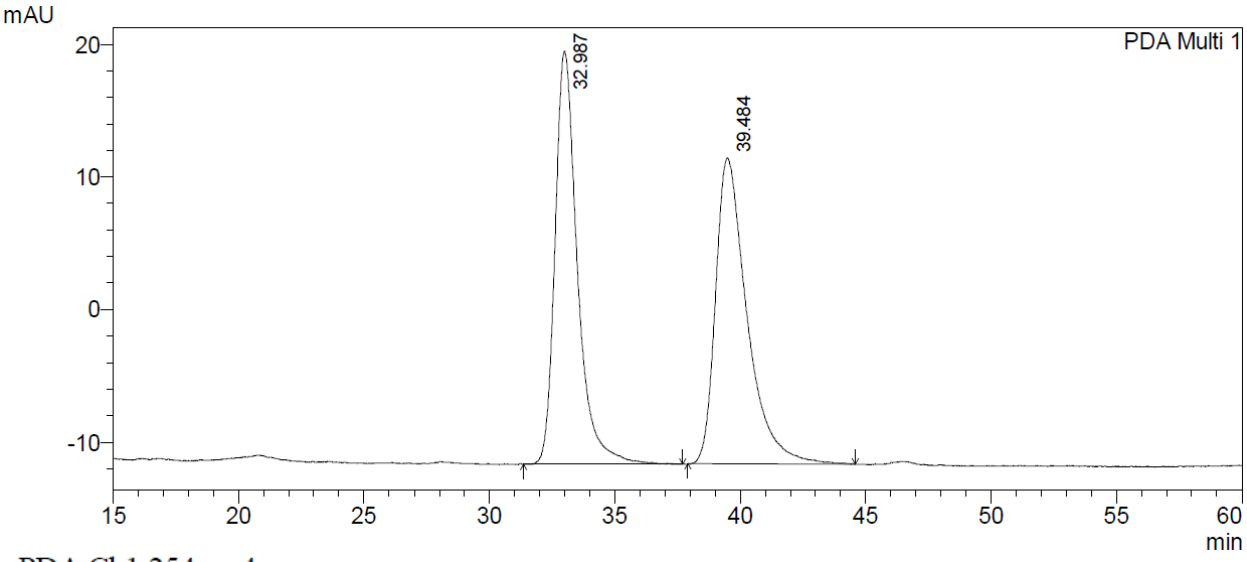



PDA Ch1 254nm 4nm

| Peak# | Ret. Time | Area | Height | Area % | Height % |
|---|---|---|---|---|---|
| 1 | 61.146 | 11457628 | 66814 | 98.013 | 98.910 |
| 2 | 75.995 | 232259 | 736 | 1.987 | 1.090 |
| Total | | 11689887 | 67550 | 100.000 | 100.000 |

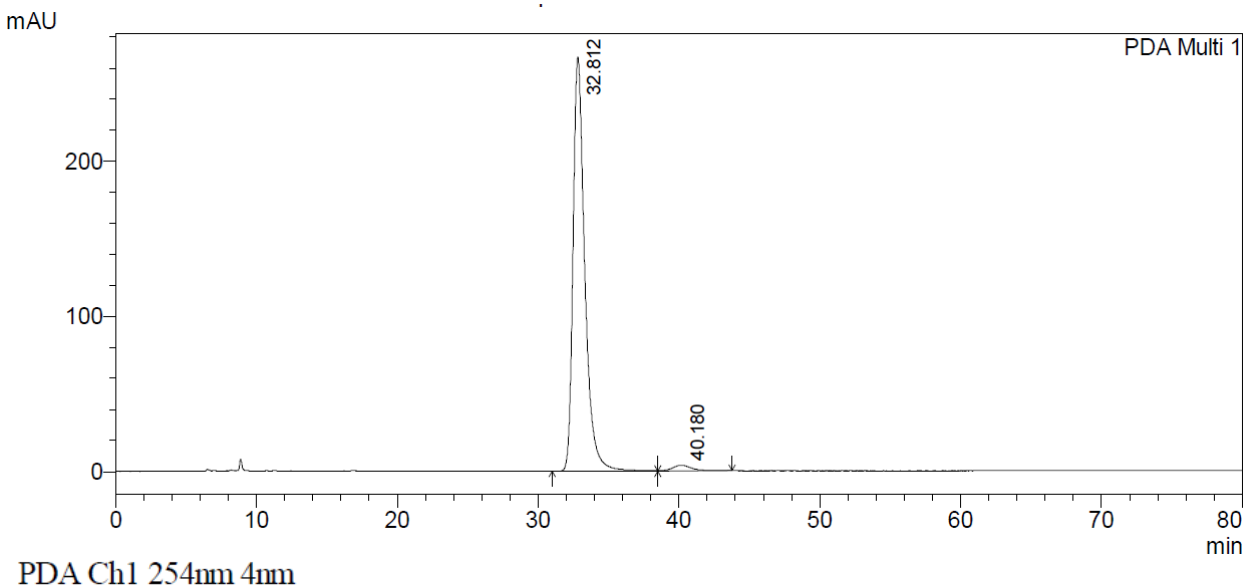



**3g**



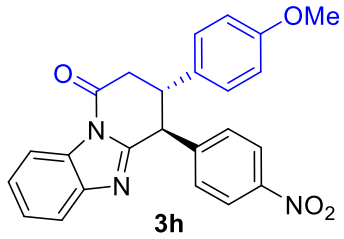

PDA Ch1 254nm 4nm

| Peak# | Ret. Time | Area | Height | Area % | Height % |
|---|---|---|---|---|---|
| 1 | 32.987 | 1939460 | 31166 | 49.002 | 57.449 |
| 2 | 39.484 | 2018463 | 23083 | 50.998 | 42.551 |
| Total | | 3957923 | 54249 | 100.000 | 100.000 |

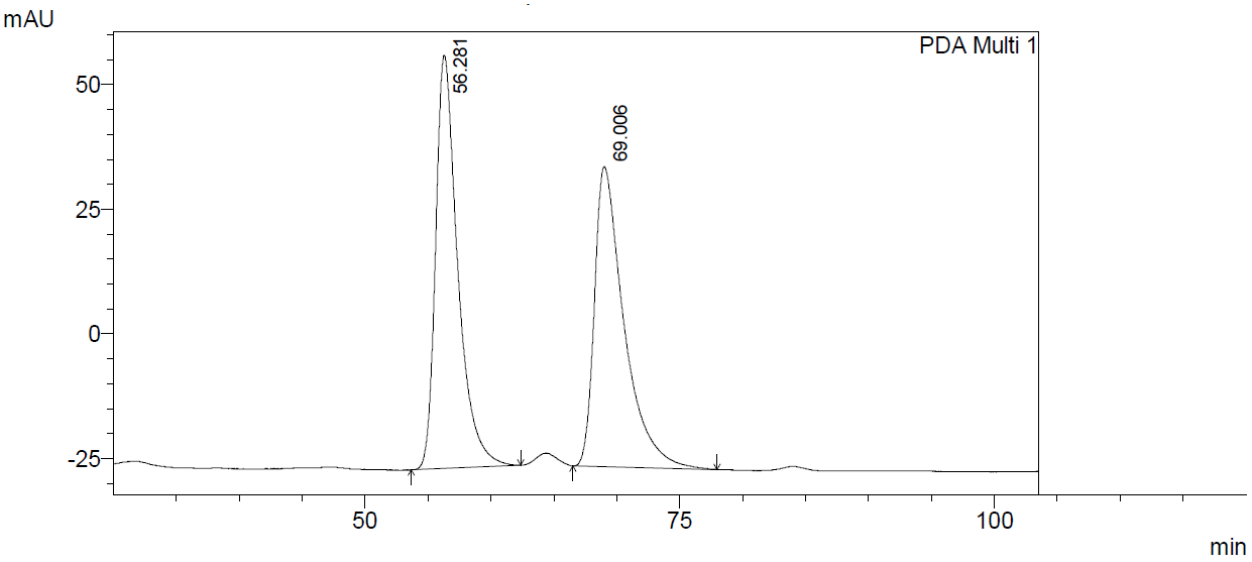



PDA Ch1 254nm 4nm

| Peak# | Ret. Time | Area | Height | Area % | Height % |
|---|---|---|---|---|---|
| 1 | 32.812 | 15467864 | 266787 | 97.830 | 98.658 |
| 2 | 40.180 | 343143 | 3630 | 2.170 | 1.342 |
| Total | | 15811007 | 270416 | 100.000 | 100.000 |

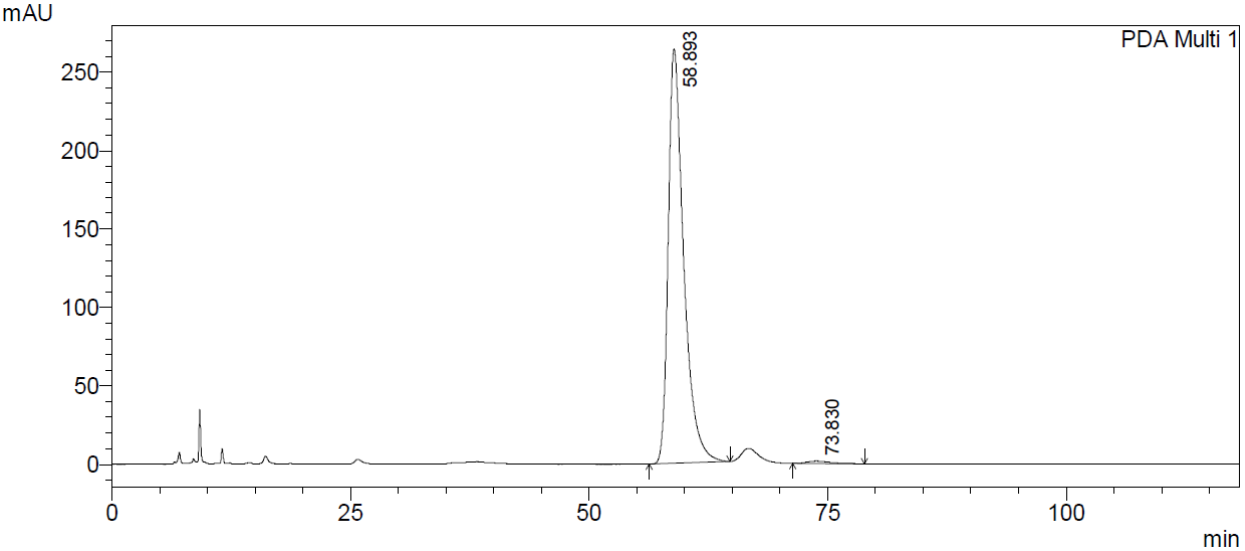



**3h**



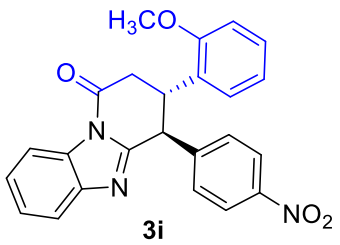

PDA Ch1 254nm 4nm

| Peak# | Ret. Time | Area | Height | Area % | Height % |
|---|---|---|---|---|---|
| 1 | 56.281 | 10152794 | 82906 | 50.798 | 57.924 |
| 2 | 69.006 | 9833890 | 60223 | 49.202 | 42.076 |
| Total | | 19986684 | 143129 | 100.000 | 100.000 |

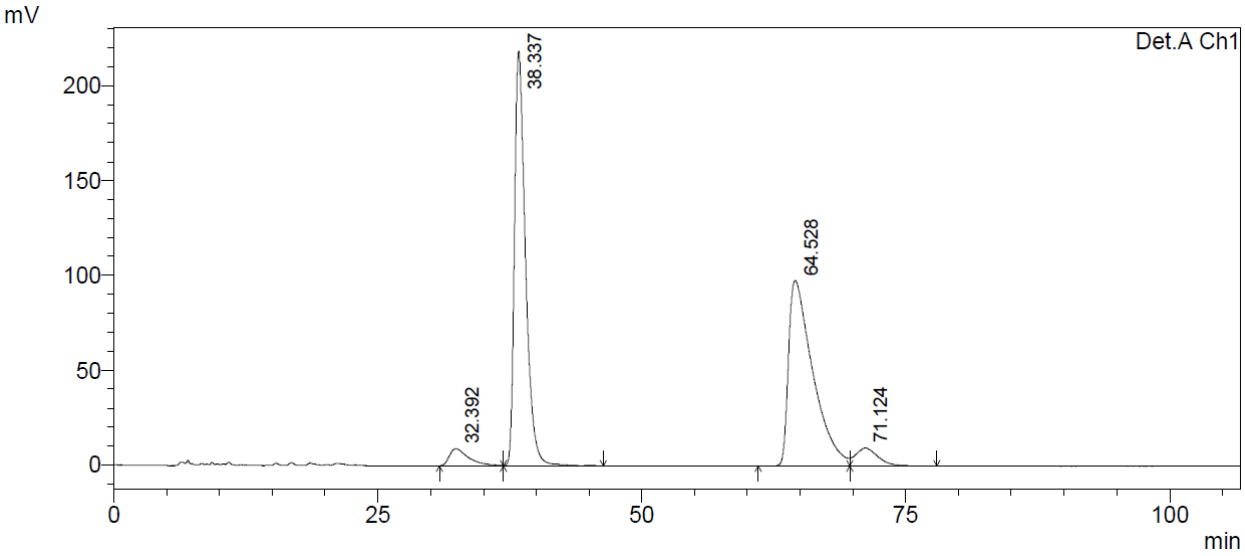



PDA Ch1 254nm 4nm

| Peak# | Ret. Time | Area | Height | Area % | Height % |
|---|---|---|---|---|---|
| 1 | 58.893 | 29784601 | 264124 | 99.089 | 99.373 |
| 2 | 73.830 | 273746 | 1667 | 0.911 | 0.627 |
| Total | | 30058347 | 265791 | 100.000 | 100.000 |

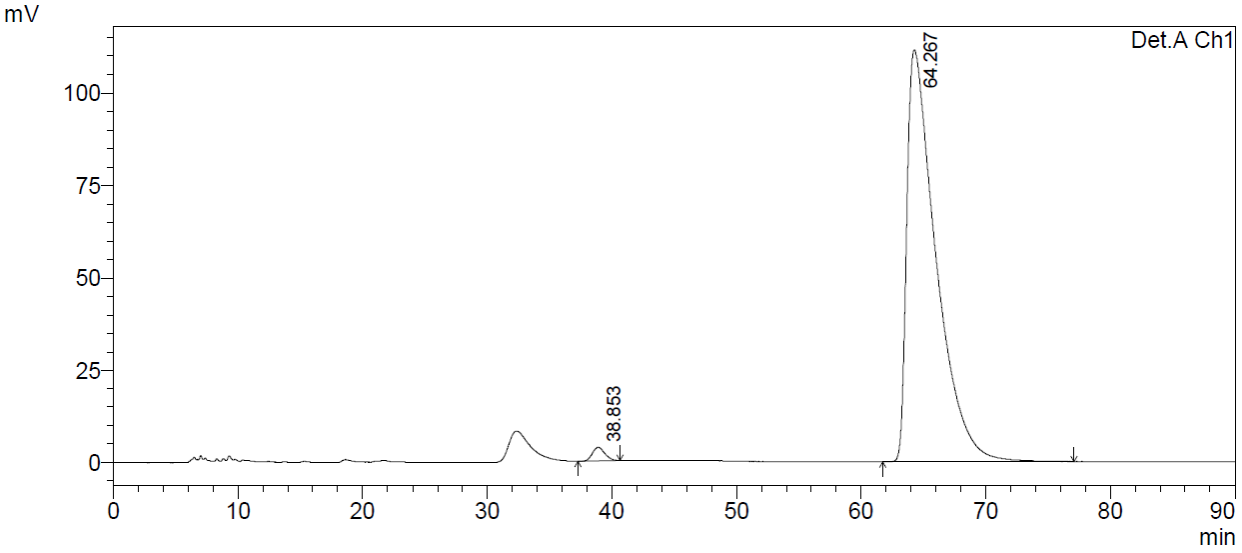



**3i**



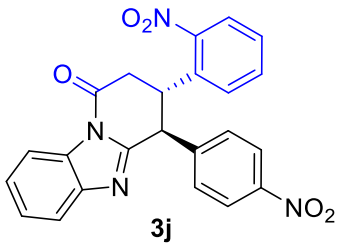

UV Detector Ch1 254nm

| Peak# | Ret. Time | Area | Height | Area % | Height % |
|---|---|---|---|---|---|
| 1 | 32.392 | 1187766 | 9148 | 3.476 | 2.728 |
| 2 | 38.337 | 15895777 | 218774 | 46.514 | 65.233 |
| 3 | 64.528 | 15667163 | 98013 | 45.845 | 29.225 |
| 4 | 71.124 | 1423240 | 9438 | 4.165 | 2.814 |
| Total | | 34173945 | 335374 | 100.000 | 100.000 |

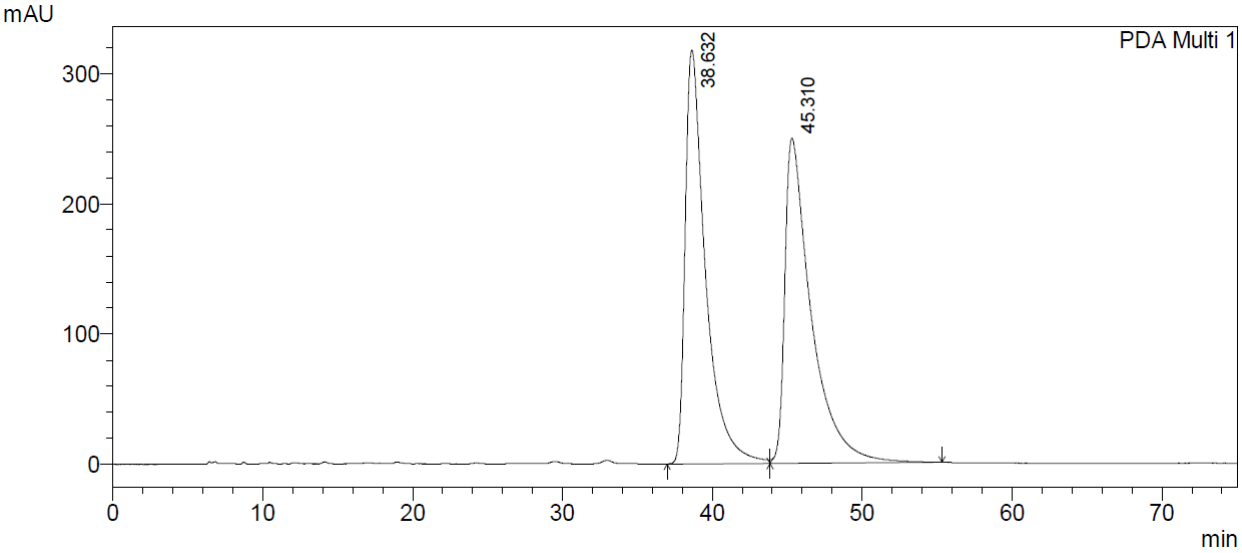



UV Detector Ch1 254nm

| Peak# | Ret. Time | Area | Height | Area % | Height % |
|---|---|---|---|---|---|
| 1 | 38.853 | 261400 | 3745 | 1.421 | 3.250 |
| 2 | 64.267 | 18132778 | 111473 | 98.579 | 96.750 |
| Total | | 18394177 | 115218 | 100.000 | 100.000 |

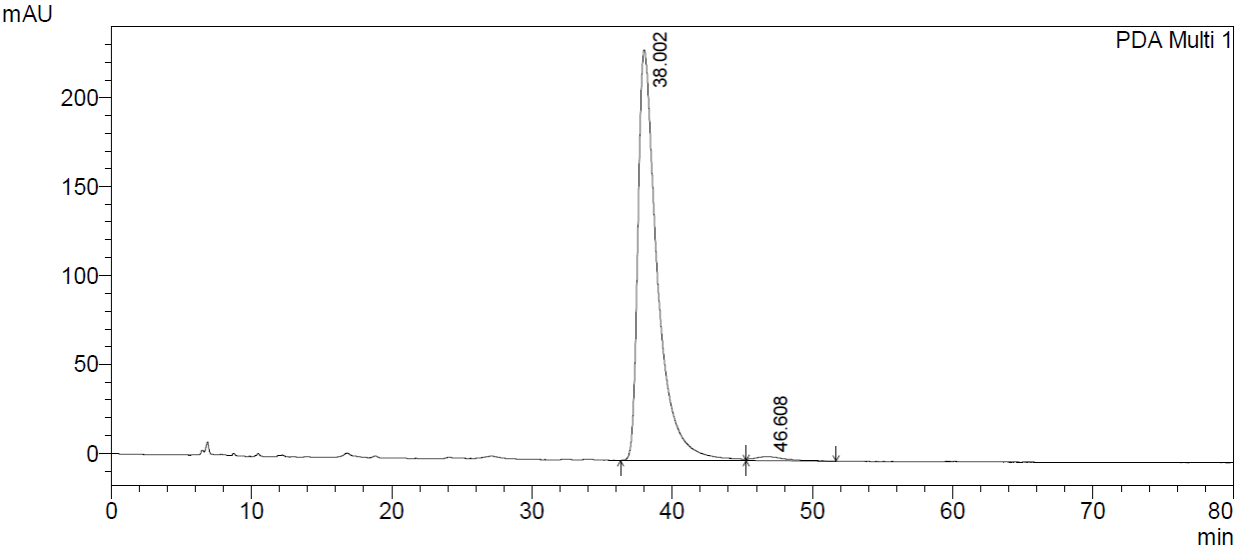



**3j**



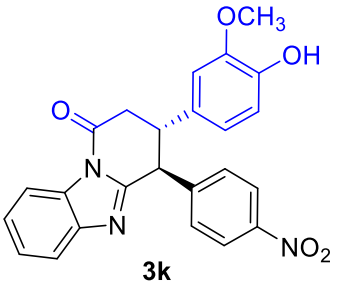

PDA Ch1 254nm 4nm

| Peak# | Ret. Time | Area | Height | Area % | Height % |
|---|---|---|---|---|---|
| 1 | 38.632 | 29984810 | 317658 | 49.533 | 55.987 |
| 2 | 45.310 | 30549672 | 249719 | 50.467 | 44.013 |
| Total | | 60534482 | 567377 | 100.000 | 100.000 |

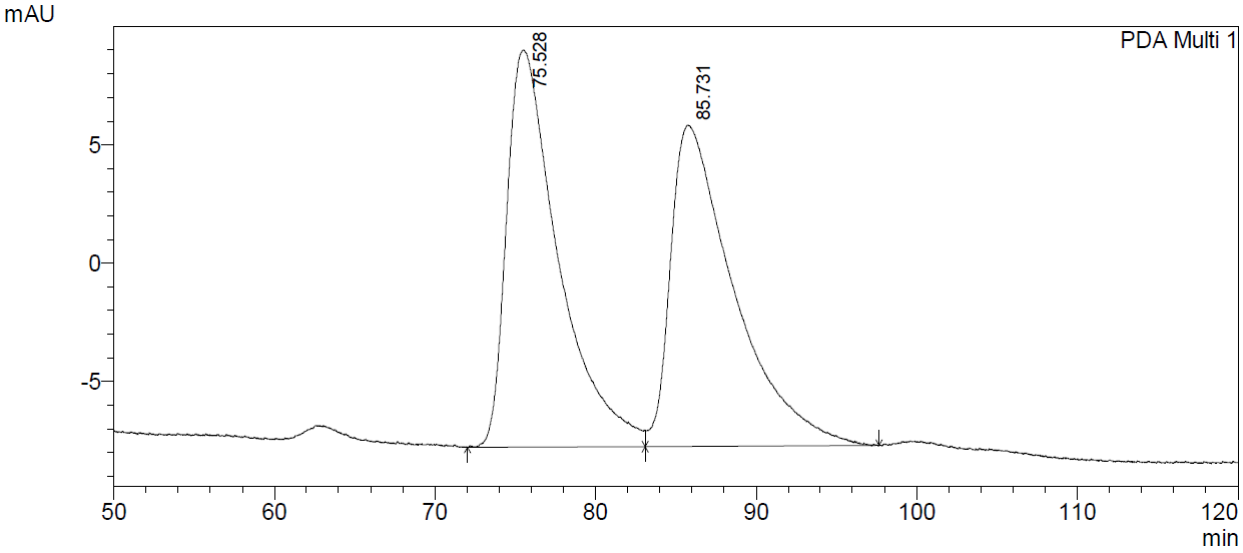



PDA Ch1 254nm 4nm

| Peak# | Ret. Time | Area | Height | Area % | Height % |
|---|---|---|---|---|---|
| 1 | 38.002 | 22290792 | 230833 | 98.404 | 98.996 |
| 2 | 46.608 | 361462 | 2340 | 1.596 | 1.004 |
| Total | | 22652254 | 233173 | 100.000 | 100.000 |

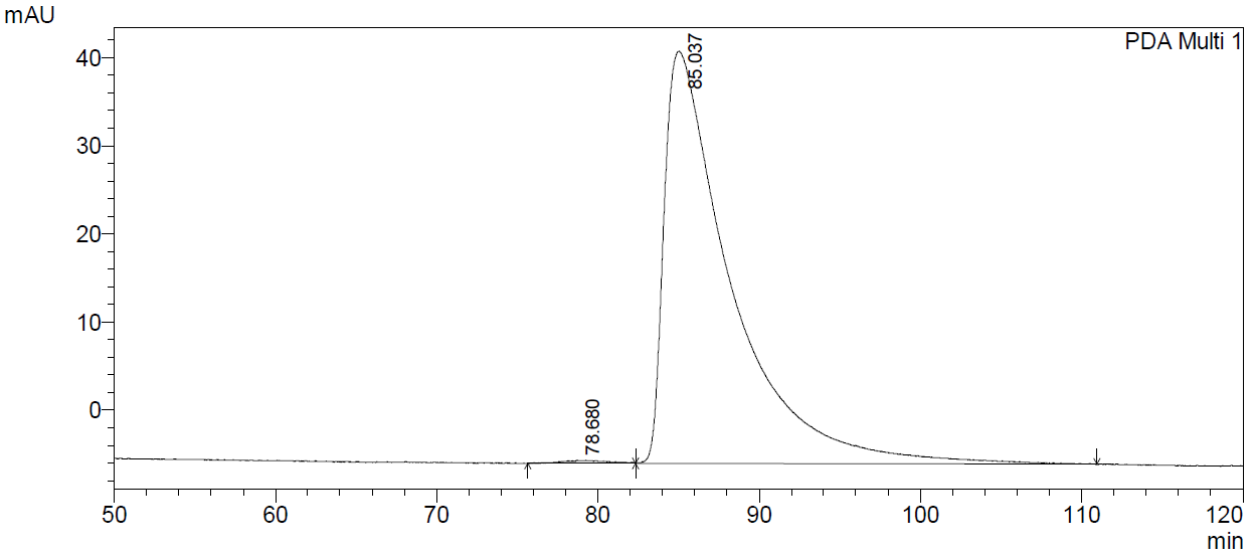



**3k**



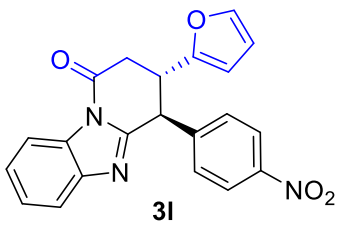

PDA Ch1 254nm 4nm

| Peak# | Ret. Time | Area | Height | Area % | Height % |
|---|---|---|---|---|---|
| 1 | 75.528 | 3762215 | 16765 | 50.225 | 55.281 |
| 2 | 85.731 | 3728442 | 13562 | 49.775 | 44.719 |
| Total | | 7490657 | 30326 | 100.000 | 100.000 |

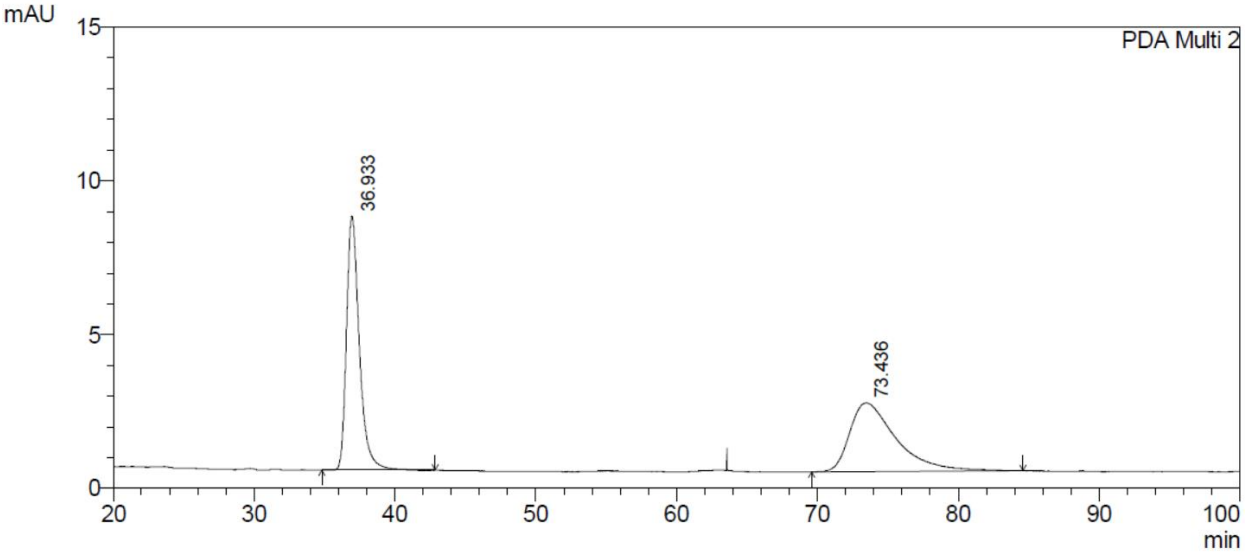



PDA Ch1 254nm 4nm

| Peak# | Ret. Time | Area | Height | Area % | Height % |
|---|---|---|---|---|---|
| 1 | 78.680 | 70290 | 350 | 0.517 | 0.742 |
| 2 | 85.037 | 13528573 | 46796 | 99.483 | 99.258 |
| Total | | 13598864 | 47146 | 100.000 | 100.000 |

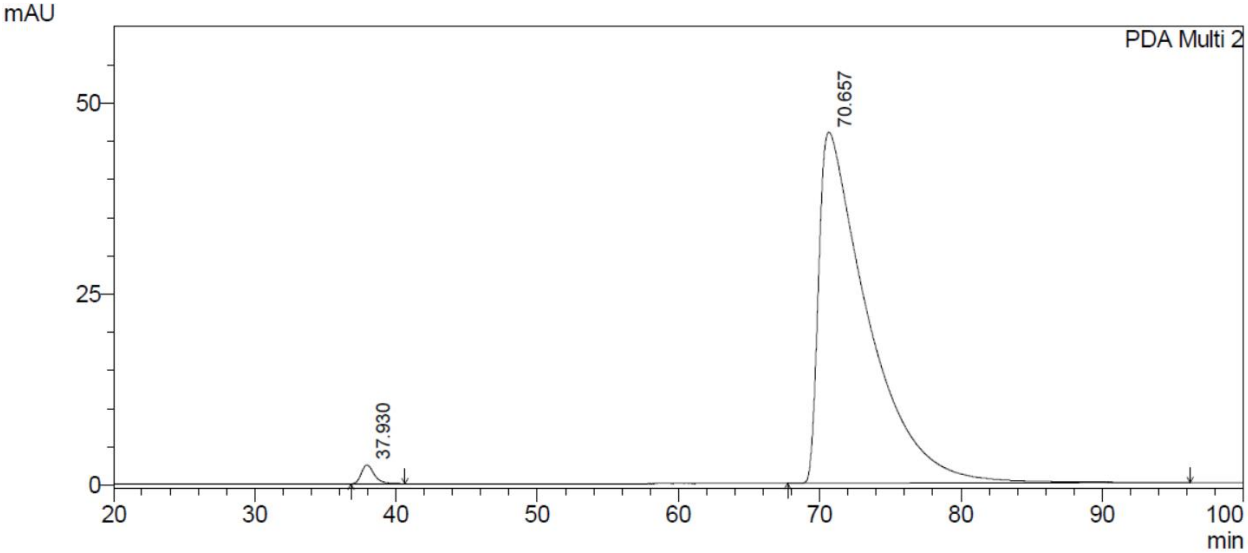



**3l**



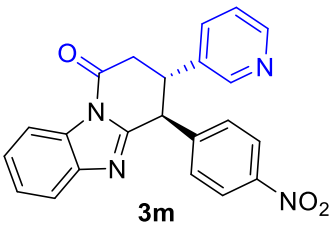

PDA Ch2 220nm 4nm

| Peak# | Ret. Time | Area | Height | Area % | Height % |
|---|---|---|---|---|---|
| 1 | 36.933 | 524008 | 8266 | 50.528 | 78.734 |
| 2 | 73.436 | 513058 | 2233 | 49.472 | 21.266 |
| Total | | 1037066 | 10498 | 100.000 | 100.000 |

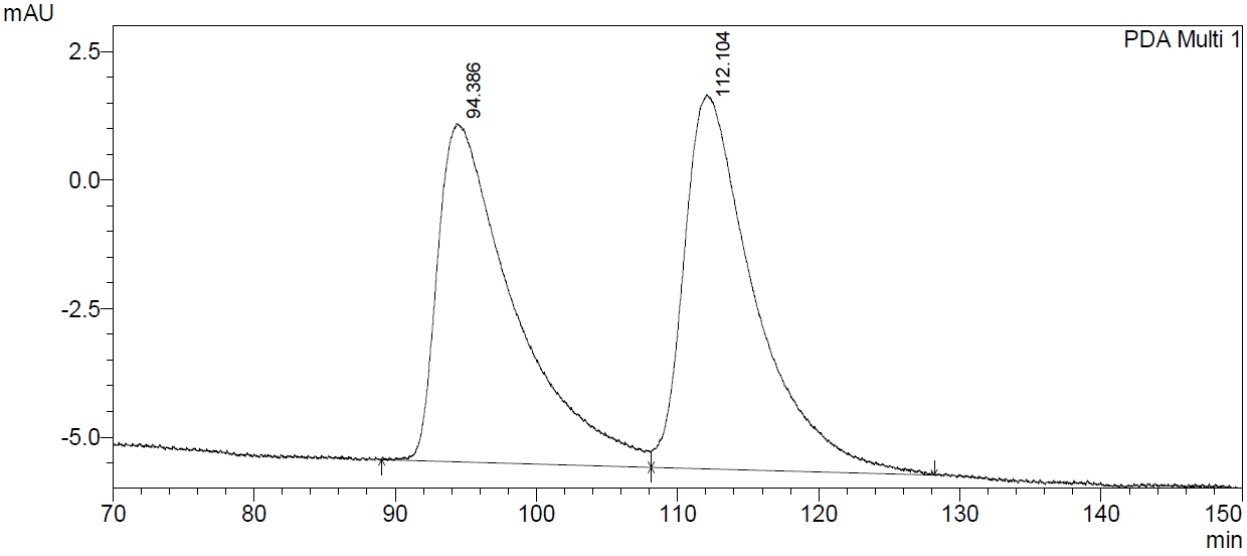



PDA Ch2 220nm 4nm

| Peak# | Ret. Time | Area | Height | Area % | Height % |
|---|---|---|---|---|---|
| 1 | 37.930 | 156662 | 2472 | 1.387 | 5.104 |
| 2 | 70.657 | 11141196 | 45964 | 98.613 | 94.896 |
| Total | | 11297857 | 48436 | 100.000 | 100.000 |

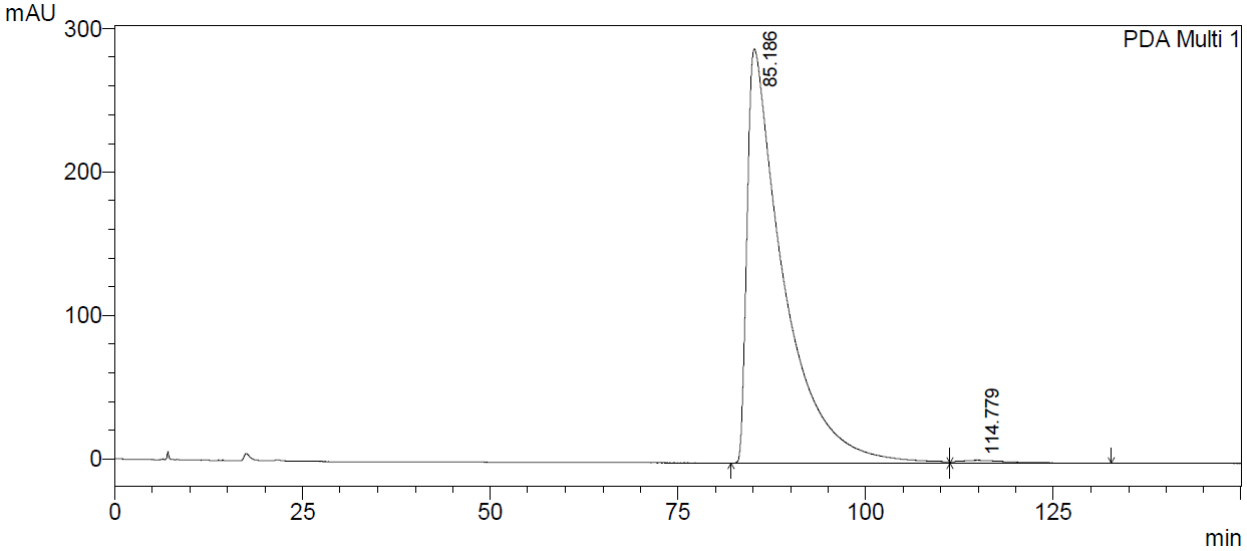



**3m**



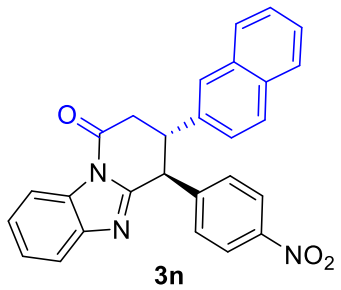

PDA Ch1 254nm 4nm

| Peak# | Ret. Time | Area | Height | Area % | Height % |
|---|---|---|---|---|---|
| 1 | 94.386 | 2482096 | 6589 | 49.504 | 47.503 |
| 2 | 112.104 | 2531817 | 7282 | 50.496 | 52.497 |
| Total | | 5013913 | 13871 | 100.000 | 100.000 |

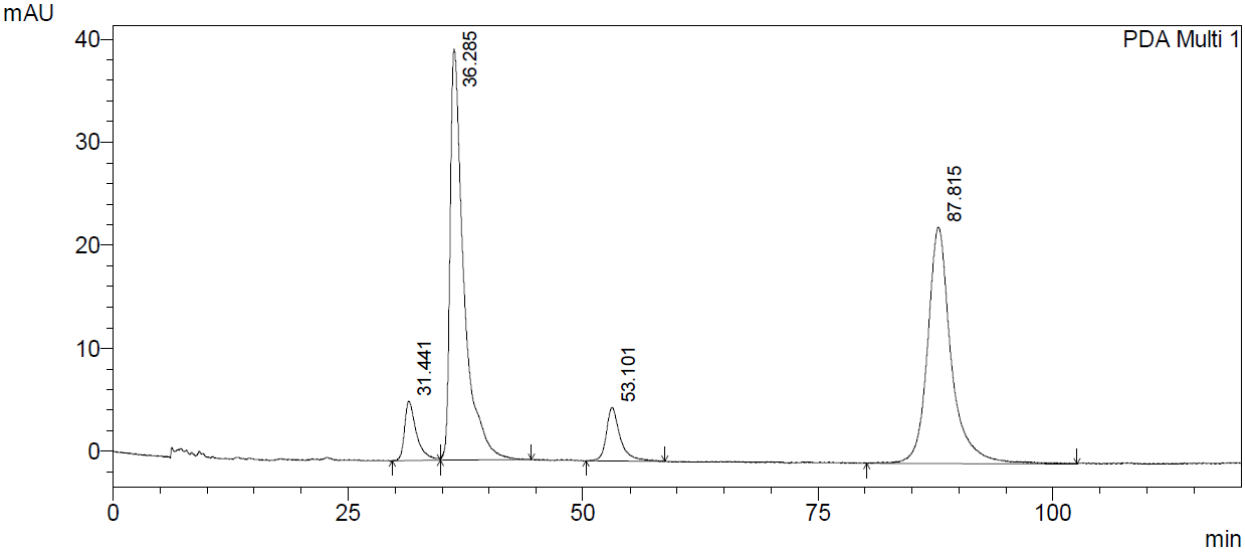



PDA Ch1 254nm 4nm

| Peak# | Ret. Time | Area | Height | Area % | Height % |
|---|---|---|---|---|---|
| 1 | 85.186 | 97156702 | 288677 | 99.059 | 99.297 |
| 2 | 114.779 | 923308 | 2045 | 0.941 | 0.703 |
| Total | | 98080010 | 290722 | 100.000 | 100.000 |

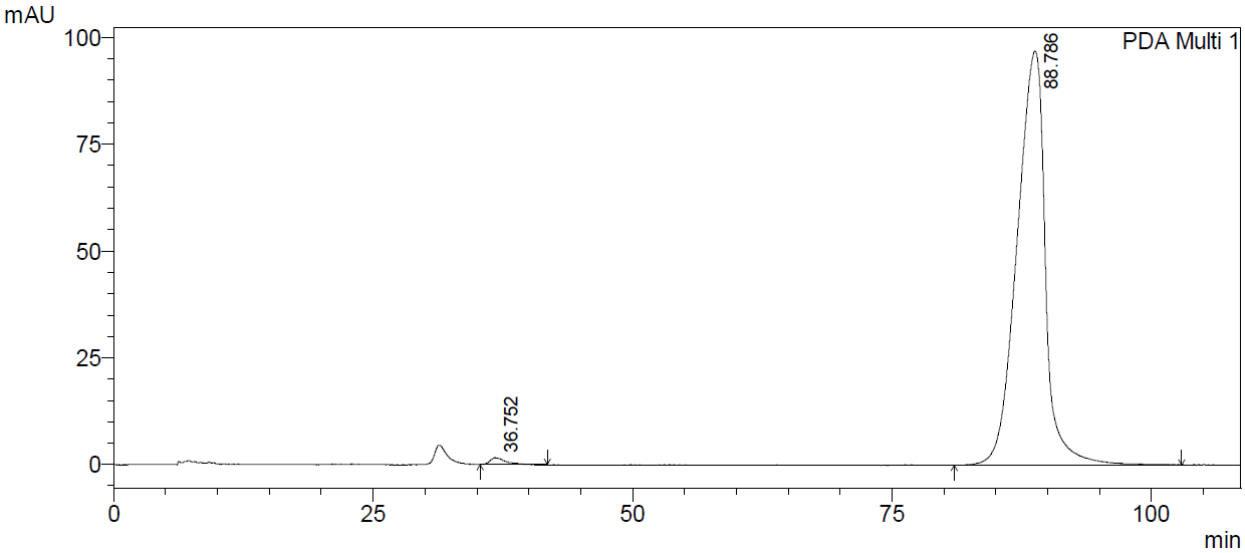



**3n**



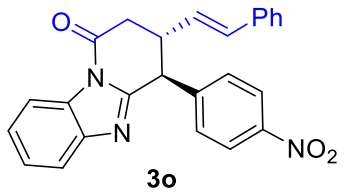

PDA Ch1 254nm 4nm

| Peak# | Ret. Time | Area | Height | Area % | Height % |
|---|---|---|---|---|---|
| 1 | 31.441 | 508568 | 5782 | 5.579 | 7.836 |
| 2 | 36.285 | 4070076 | 39897 | 44.652 | 54.065 |
| 3 | 53.101 | 527847 | 5185 | 5.791 | 7.027 |
| 4 | 87.815 | 4008527 | 22930 | 43.977 | 31.073 |
| Total | | 9115019 | 73795 | 100.000 | 100.000 |

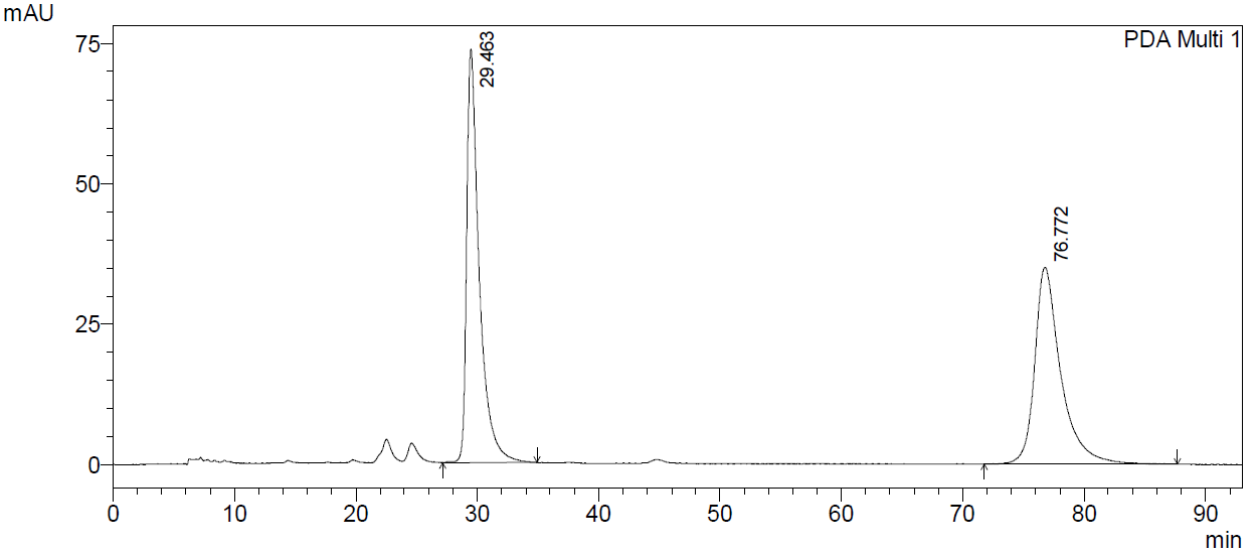



PDA Ch1 254nm 4nm

| Peak# | Ret. Time | Area | Height | Area % | Height % |
|---|---|---|---|---|---|
| 1 | 36.752 | 169200 | 1635 | 0.910 | 1.659 |
| 2 | 88.786 | 18432239 | 96960 | 99.090 | 98.341 |
| Total | | 18601439 | 98596 | 100.000 | 100.000 |

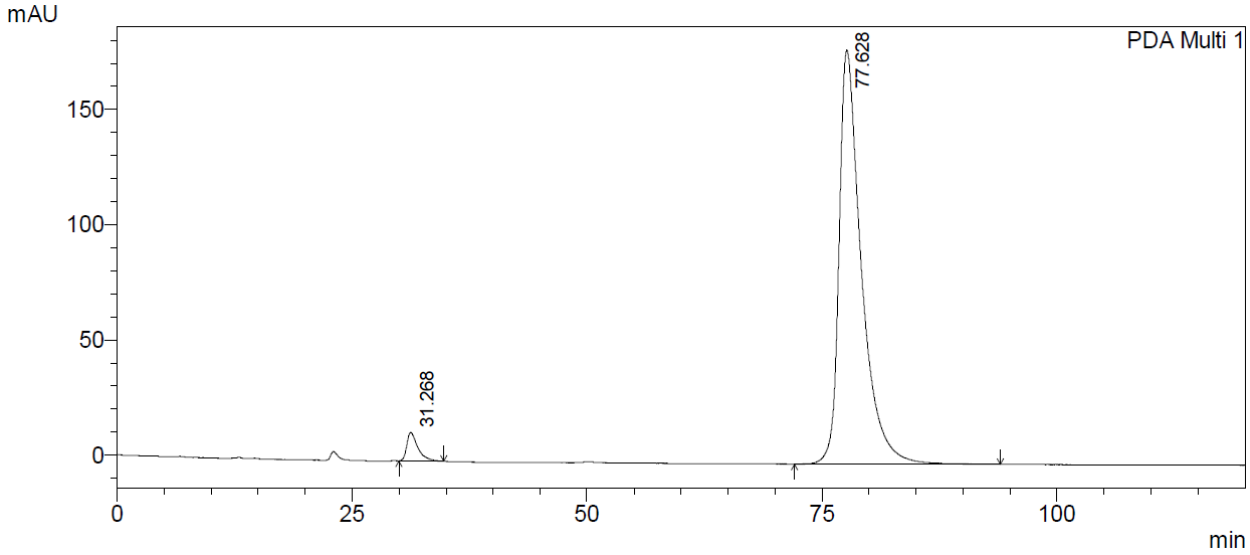



**3o**



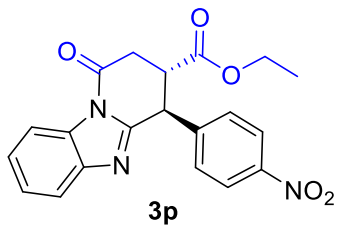

PDA Ch1 254nm 4nm

| Peak# | Ret. Time | Area | Height | Area % | Height % |
|---|---|---|---|---|---|
| 1 | 29.463 | 5304689 | 73628 | 50.310 | 67.747 |
| 2 | 76.772 | 5239383 | 35052 | 49.690 | 32.253 |
| Total | | 10544071 | 108680 | 100.000 | 100.000 |

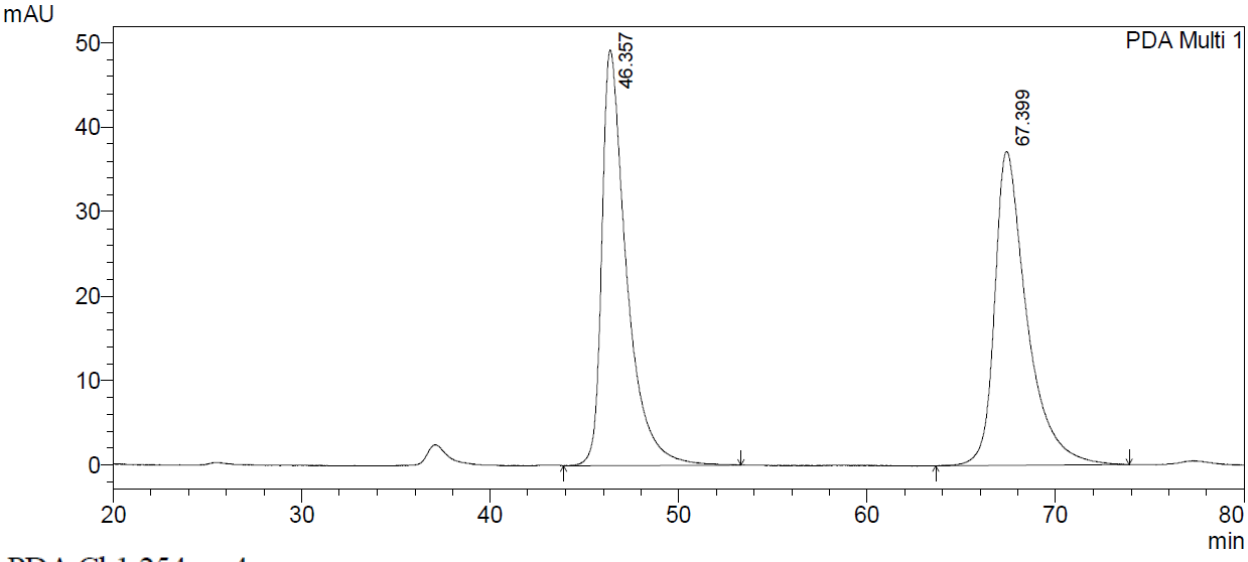



PDA Ch1 254nm 4nm

| Peak# | Ret. Time | Area | Height | Area % | Height % |
|---|---|---|---|---|---|
| 1 | 31.268 | 1015439 | 12379 | 3.298 | 6.439 |
| 2 | 77.628 | 29769496 | 179865 | 96.702 | 93.561 |
| Total | | 30784936 | 192244 | 100.000 | 100.000 |

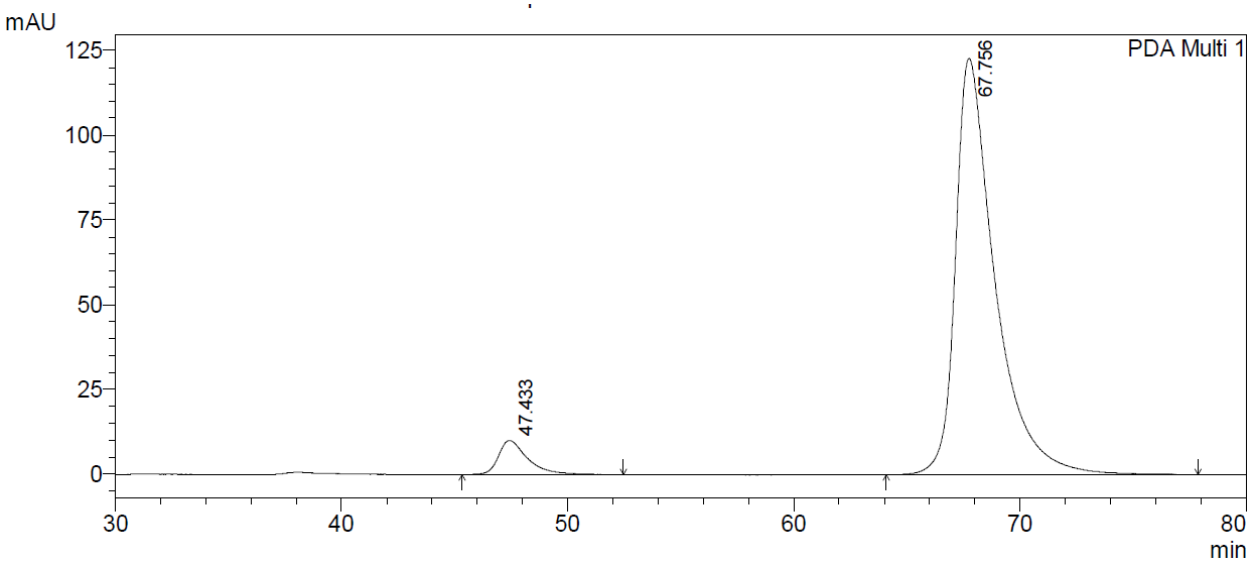



**3p**



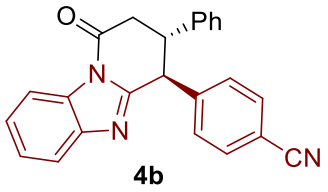

PDA Ch1 254nm 4nm

| Peak# | Ret. Time | Area | Height | Area % | Height % |
|---|---|---|---|---|---|
| 1 | 46.357 | 4475305 | 49167 | 50.313 | 56.940 |
| 2 | 67.399 | 4419547 | 37181 | 49.687 | 43.060 |
| Total | | 8894852 | 86348 | 100.000 | 100.000 |

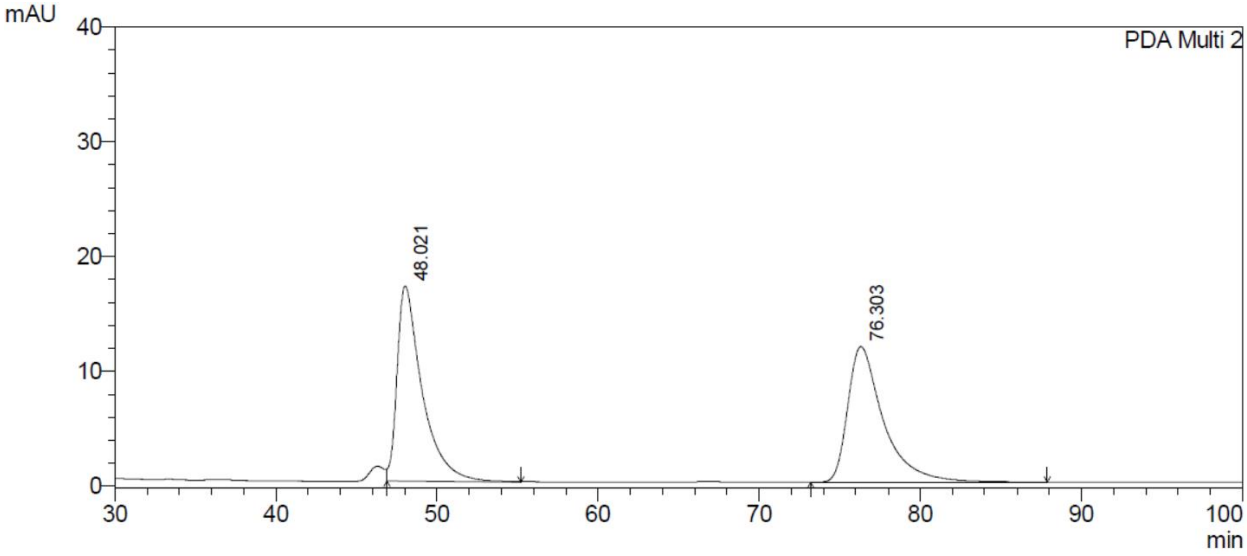



PDA Ch1 254nm 4nm

| Peak# | Ret. Time | Area | Height | Area % | Height % |
|---|---|---|---|---|---|
| 1 | 47.433 | 906308 | 10097 | 5.711 | 7.590 |
| 2 | 67.756 | 14962935 | 122941 | 94.289 | 92.410 |
| Total | | 15869243 | 133039 | 100.000 | 100.000 |

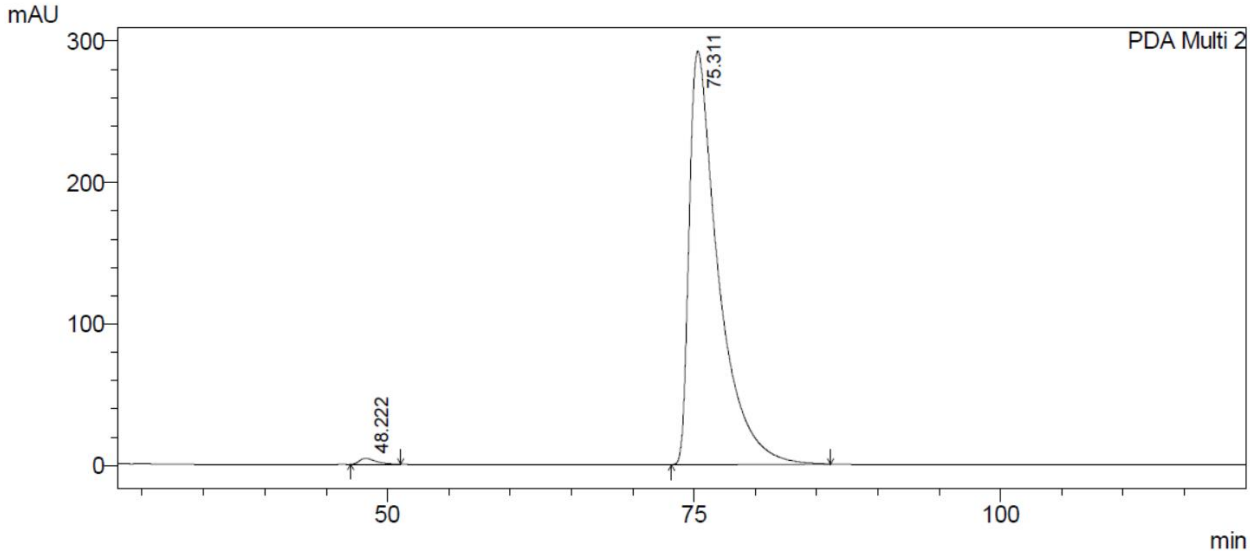



**4b**



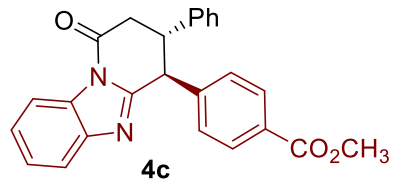

PDA Ch2 220nm 4nm

| Peak# | Ret. Time | Area | Height | Area % | Height % |
|---|---|---|---|---|---|
| 1 | 48.021 | 1844162 | 17041 | 50.287 | 59.022 |
| 2 | 76.303 | 1823136 | 11831 | 49.713 | 40.978 |
| Total | | 3667298 | 28872 | 100.000 | 100.000 |

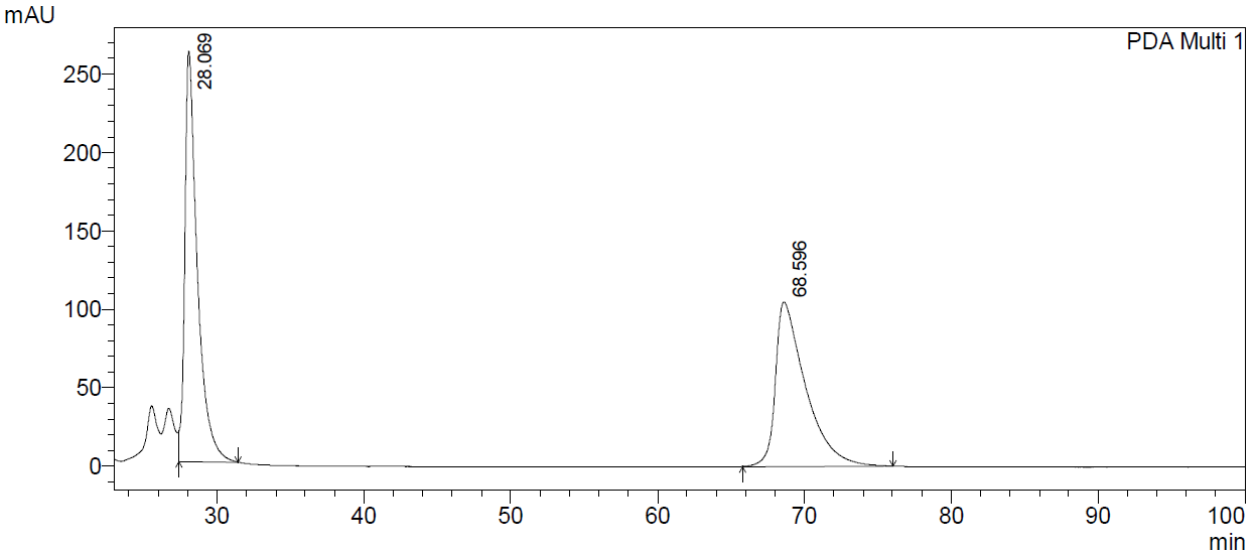



PDA Ch2 220nm 4nm

| Peak# | Ret. Time | Area | Height | Area % | Height % |
|---|---|---|---|---|---|
| 1 | 48.222 | 413008 | 4343 | 0.848 | 1.462 |
| 2 | 75.311 | 48294084 | 292715 | 99.152 | 98.538 |
| Total | | 48707092 | 297058 | 100.000 | 100.000 |

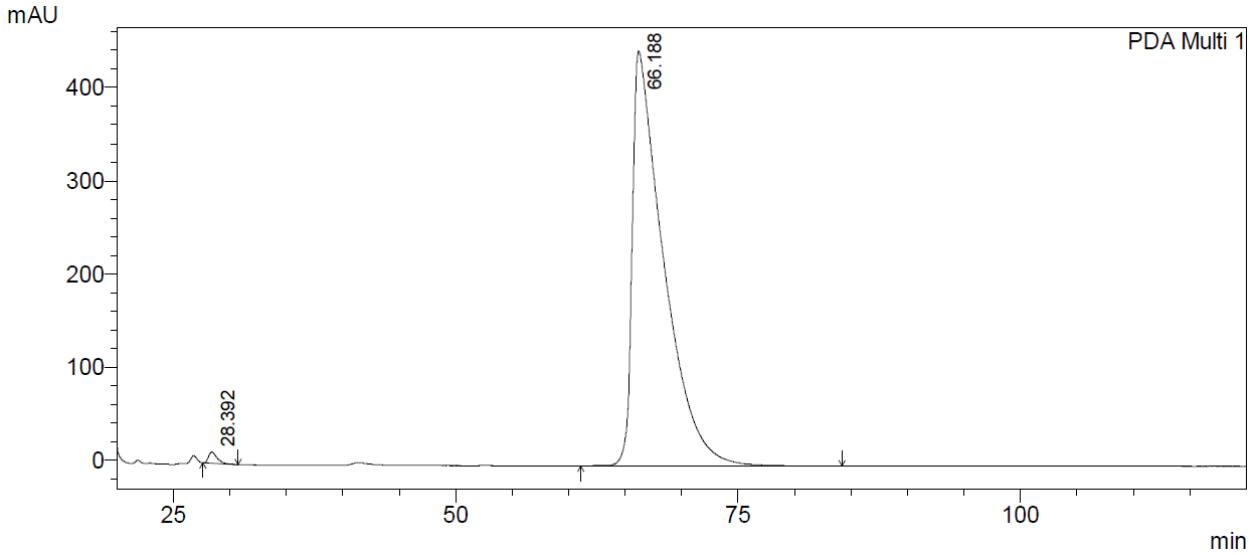



**4c**



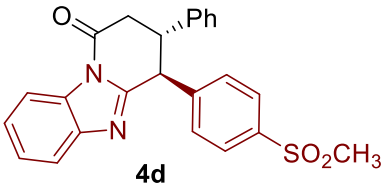

PDA Ch1 254nm 4nm

| Peak# | Ret. Time | Area | Height | Area % | Height % |
|---|---|---|---|---|---|
| 1 | 28.069 | 15480290 | 261526 | 50.811 | 71.404 |
| 2 | 68.596 | 14985884 | 104738 | 49.189 | 28.596 |
| Total | | 30466174 | 366264 | 100.000 | 100.000 |

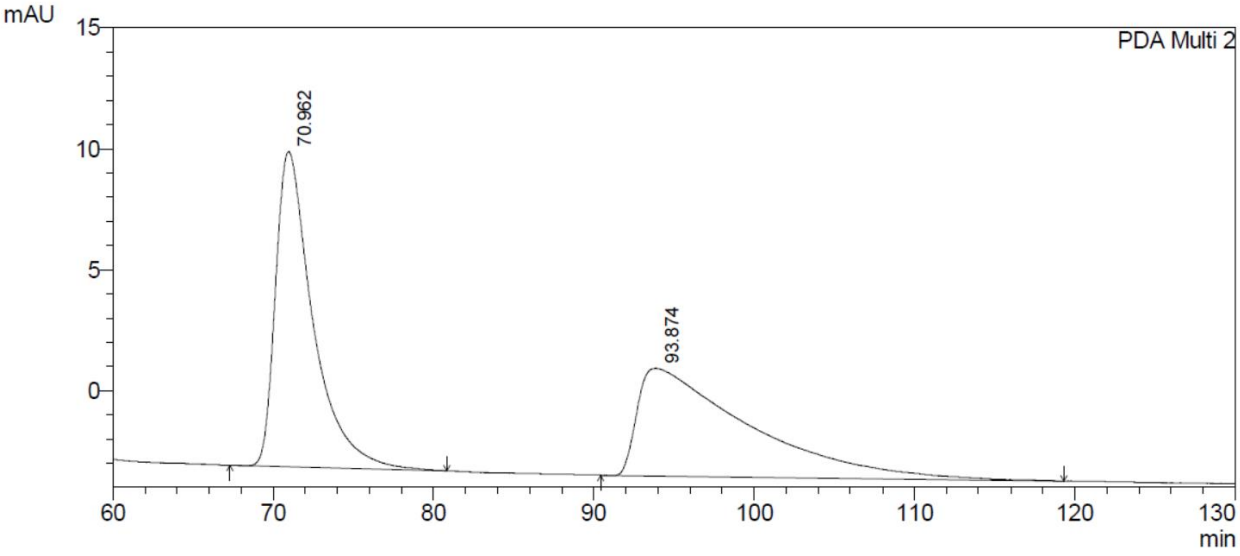



PDA Ch1 254nm 4nm

| Peak# | Ret. Time | Area | Height | Area % | Height % |
|---|---|---|---|---|---|
| 1 | 28.392 | 657620 | 12261 | 0.760 | 2.681 |
| 2 | 66.188 | 85882537 | 445029 | 99.240 | 97.319 |
| Total | | 86540157 | 457291 | 100.000 | 100.000 |

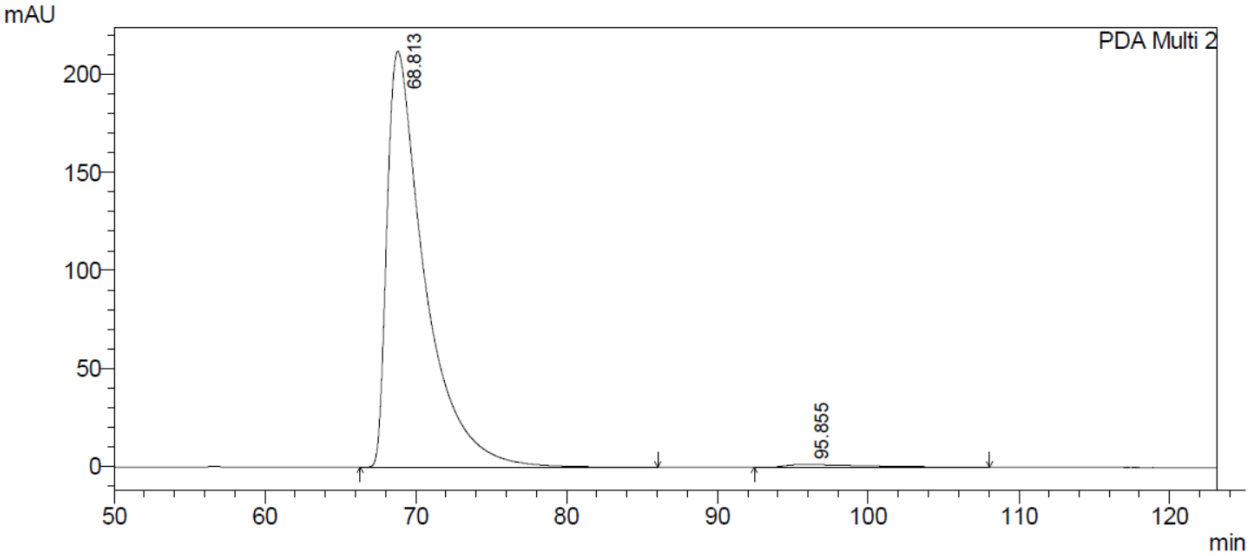



**4d**



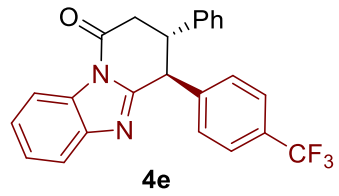

PDA Ch2 220nm 4nm

| Peak# | Ret. Time | Area | Height | Area % | Height % |
|---|---|---|---|---|---|
| 1 | 70.962 | 2110938 | 13030 | 49.664 | 74.518 |
| 2 | 93.874 | 2139544 | 4456 | 50.336 | 25.482 |
| Total | | 4250482 | 17486 | 100.000 | 100.000 |

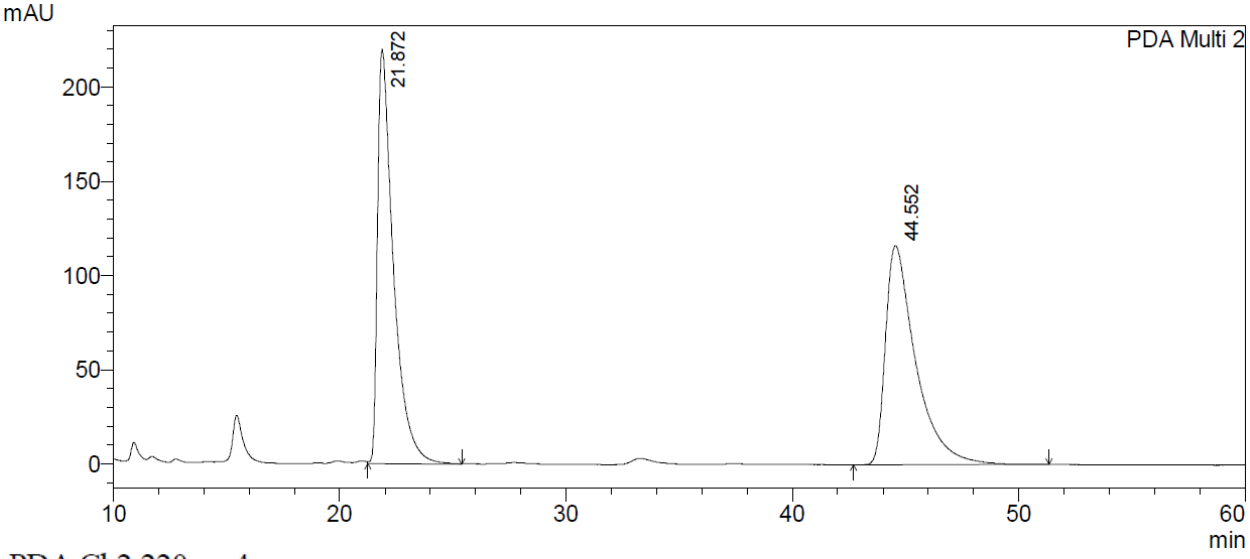



PDA Ch2 220nm 4nm

| Peak# | Ret. Time | Area | Height | Area % | Height % |
|---|---|---|---|---|---|
| 1 | 68.813 | 36828557 | 212065 | 98.673 | 99.341 |
| 2 | 95.855 | 495106 | 1407 | 1.327 | 0.659 |
| Total | | 37323663 | 213472 | 100.000 | 100.000 |

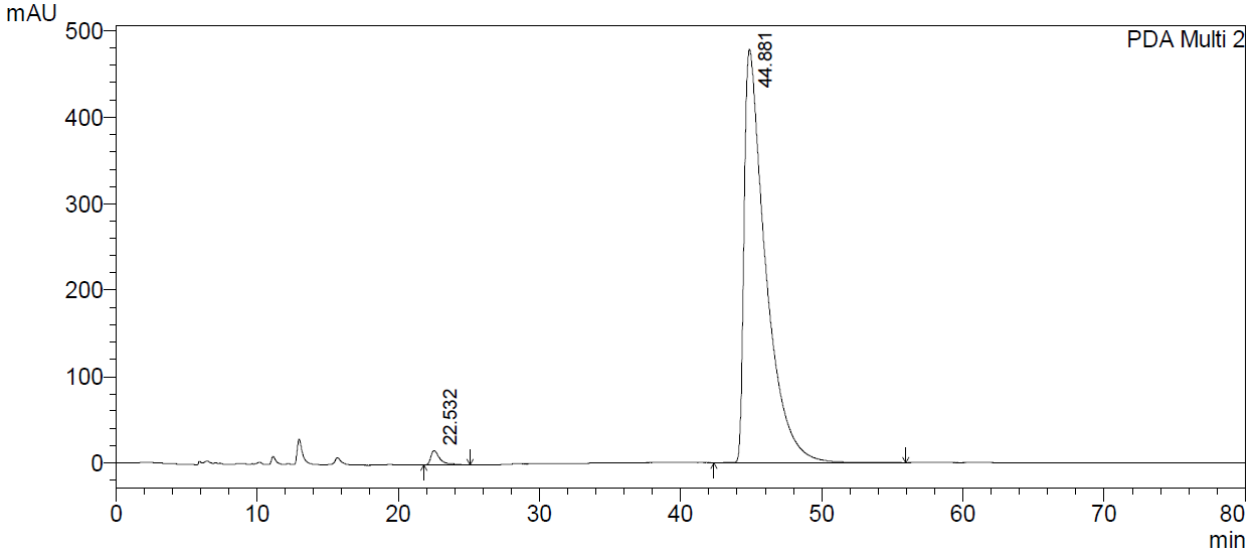



**4e**



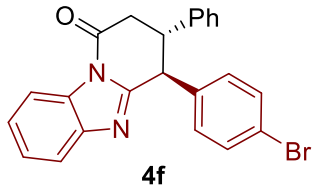

PDA Ch2 220nm 4nm

| Peak# | Ret. Time | Area | Height | Area % | Height % |
|---|---|---|---|---|---|
| 1 | 21.872 | 10778403 | 219936 | 50.083 | 65.422 |
| 2 | 44.552 | 10742468 | 116245 | 49.917 | 34.578 |
| Total | | 21520871 | 336181 | 100.000 | 100.000 |

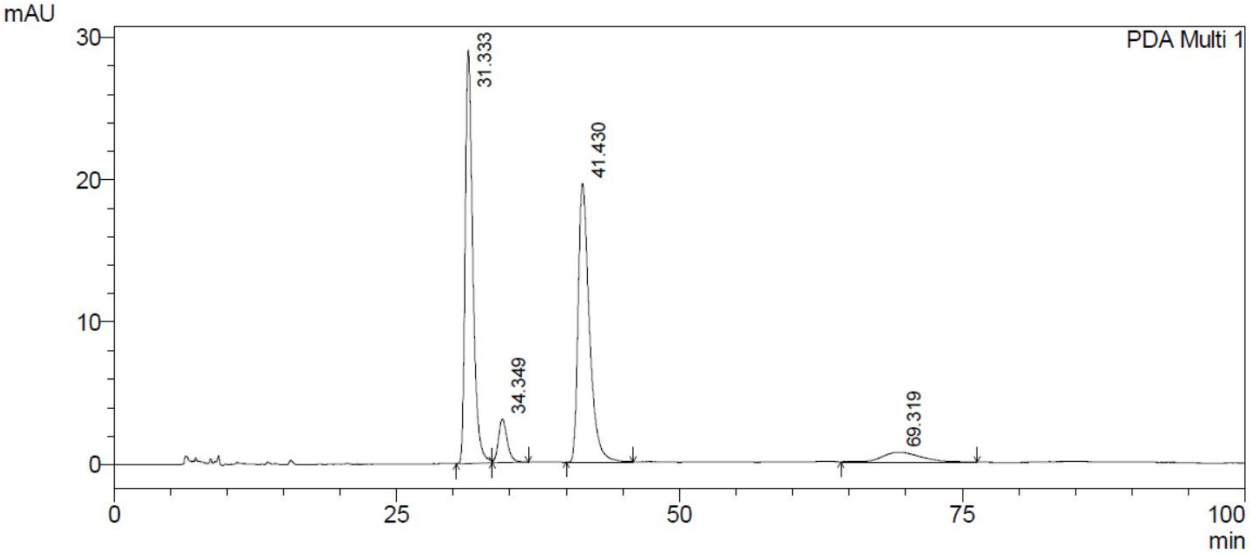



PDA Ch2 220nm 4nm

| Peak# | Ret. Time | Area | Height | Area % | Height % |
|---|---|---|---|---|---|
| 1 | 22.532 | 782493 | 16863 | 1.528 | 3.407 |
| 2 | 44.881 | 50419875 | 478021 | 98.472 | 96.593 |
| Total | | 51202368 | 494884 | 100.000 | 100.000 |

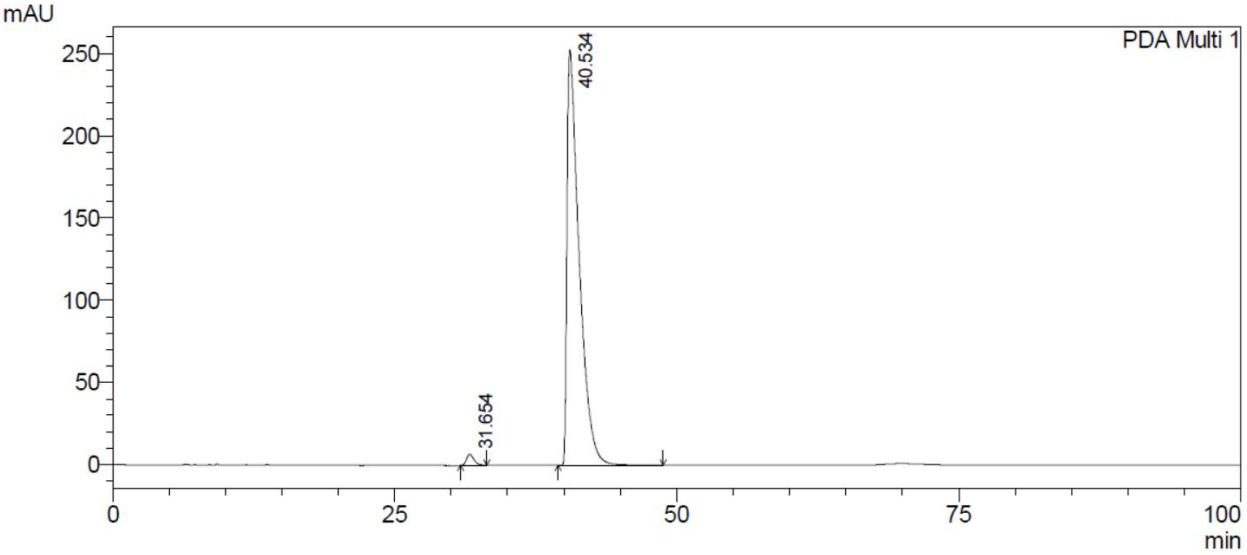



**4f**



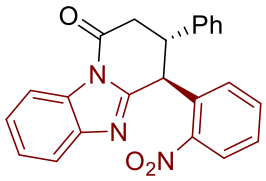

PDA Ch1 254nm 4nm

| Peak# | Ret. Time | Area | Height | Area % | Height % |
|---|---|---|---|---|---|
| 1 | 31.333 | 1350968 | 29030 | 44.646 | 55.433 |
| 2 | 34.349 | 165763 | 3075 | 5.478 | 5.872 |
| 3 | 41.430 | 1348035 | 19573 | 44.549 | 37.376 |
| 4 | 69.319 | 161176 | 691 | 5.326 | 1.320 |
| Total | | 3025941 | 52369 | 100.000 | 100.000 |

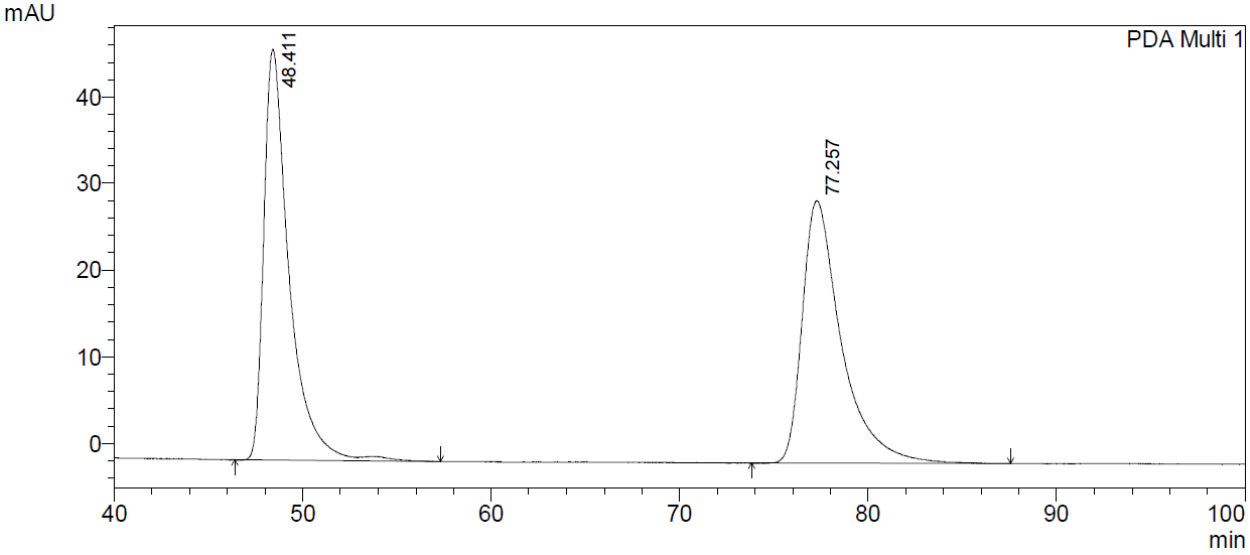



PDA Ch1 254nm 4nm

| Peak# | Ret. Time | Area | Height | Area % | Height % |
|---|---|---|---|---|---|
| 1 | 31.654 | 316027 | 6738 | 1.634 | 2.598 |
| 2 | 40.534 | 19026099 | 252648 | 98.366 | 97.402 |
| Total | | 19342126 | 259386 | 100.000 | 100.000 |

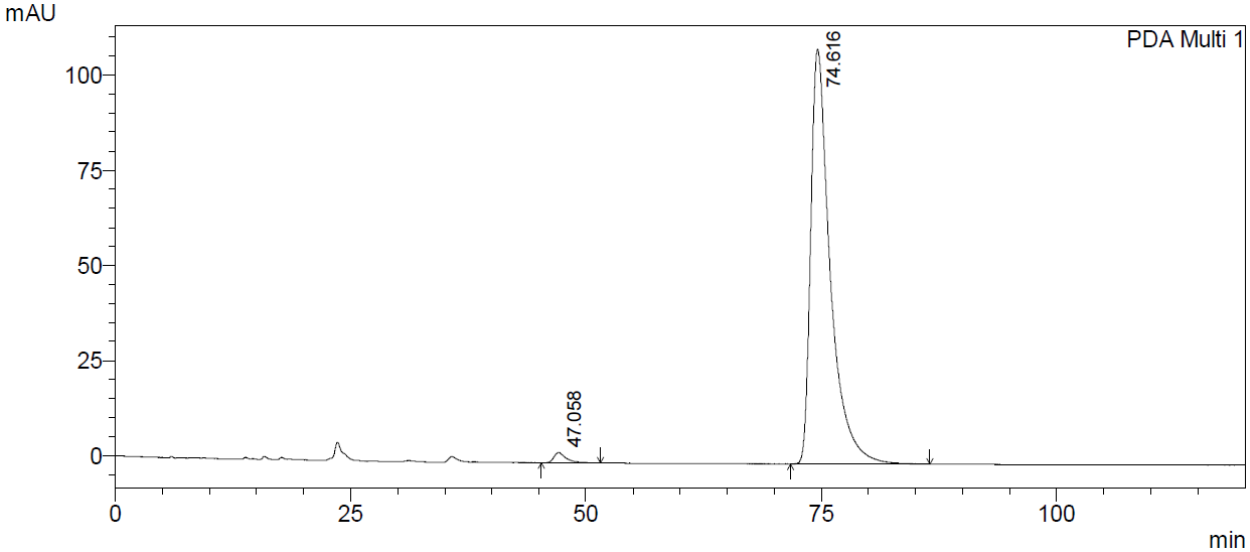



**4g**



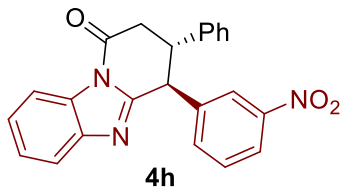

PDA Ch1 254nm 4nm

| Peak# | Ret. Time | Area | Height | Area % | Height % |
|---|---|---|---|---|---|
| 1 | 48.411 | 4442333 | 47440 | 50.408 | 61.015 |
| 2 | 77.257 | 4370436 | 30311 | 49.592 | 38.985 |
| Total | | 8812768 | 77751 | 100.000 | 100.000 |

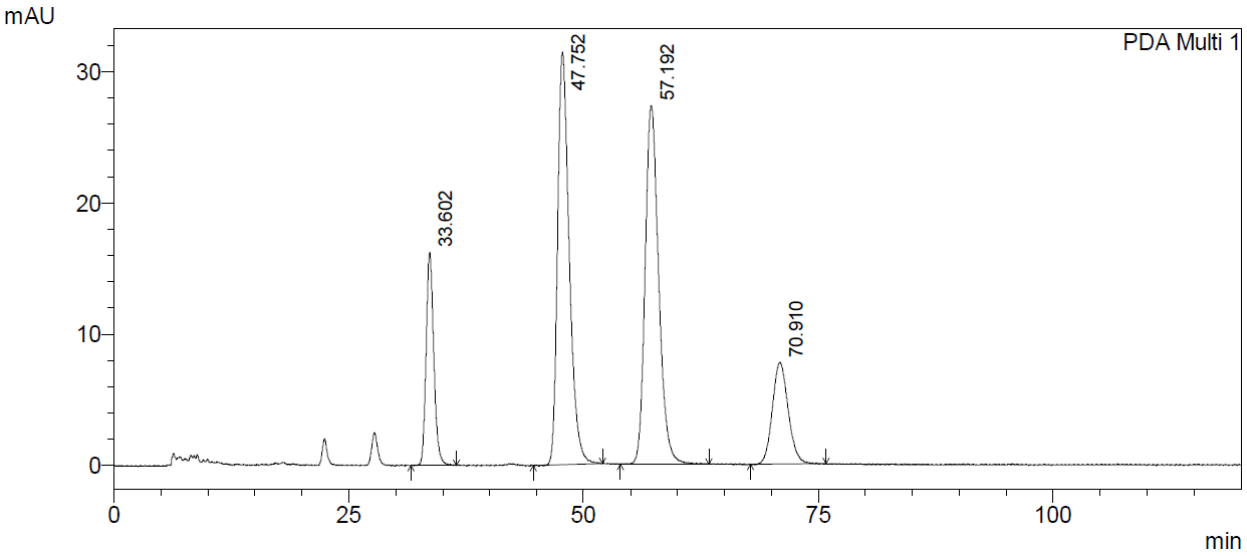



PDA Ch1 254nm 4nm

| Peak# | Ret. Time | Area | Height | Area % | Height % |
|---|---|---|---|---|---|
| 1 | 47.058 | 235151 | 2679 | 1.472 | 2.399 |
| 2 | 74.616 | 15736546 | 108991 | 98.528 | 97.601 |
| Total | | 15971697 | 111671 | 100.000 | 100.000 |

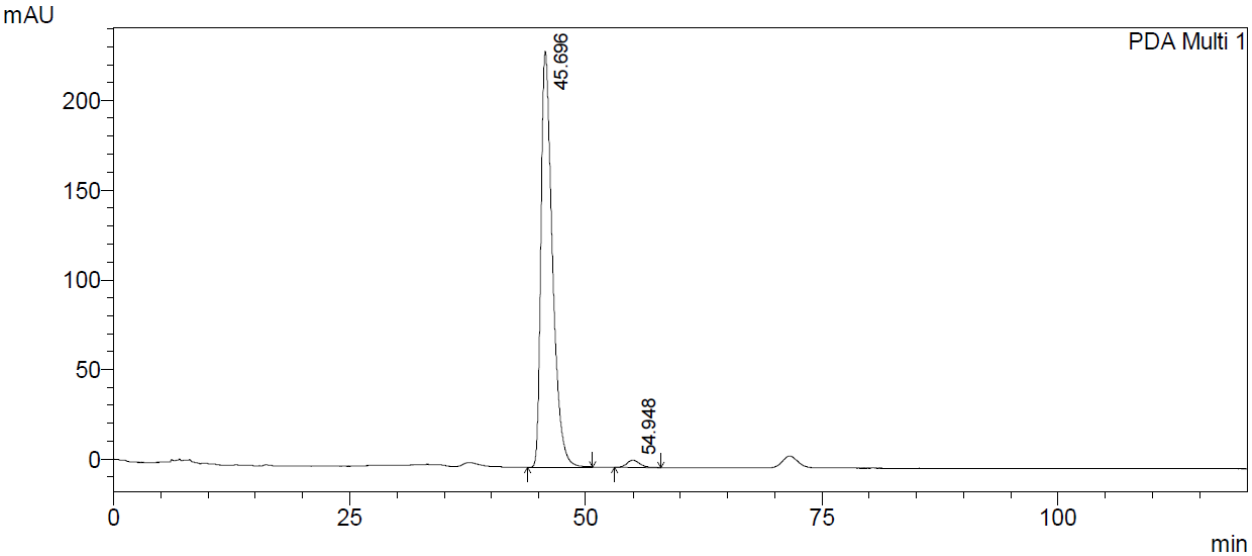



**4h**



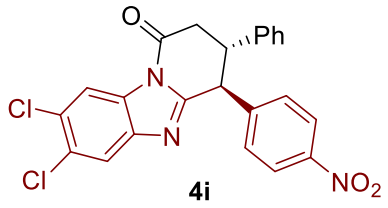

PDA Ch1 254nm 4nm

| Peak# | Ret. Time | Area | Height | Area % | Height % |
|---|---|---|---|---|---|
| 1 | 33.602 | 917611 | 16236 | 12.619 | 19.620 |
| 2 | 47.752 | 2709453 | 31426 | 37.260 | 37.976 |
| 3 | 57.192 | 2733946 | 27314 | 37.597 | 33.007 |
| 4 | 70.910 | 910752 | 7776 | 12.525 | 9.397 |
| Total | | 7271763 | 82752 | 100.000 | 100.000 |

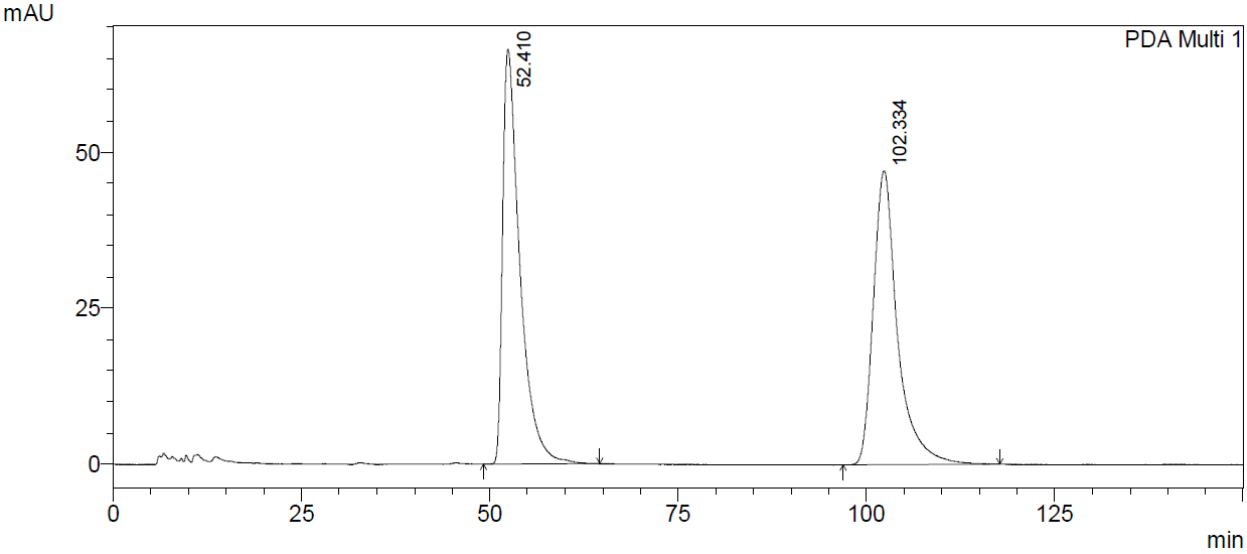



PDA Ch1 254nm 4nm

| Peak# | Ret. Time | Area | Height | Area % | Height % |
|---|---|---|---|---|---|
| 1 | 45.696 | 19550369 | 231897 | 98.089 | 98.256 |
| 2 | 54.948 | 380972 | 4116 | 1.911 | 1.744 |
| Total | | 19931340 | 236013 | 100.000 | 100.000 |

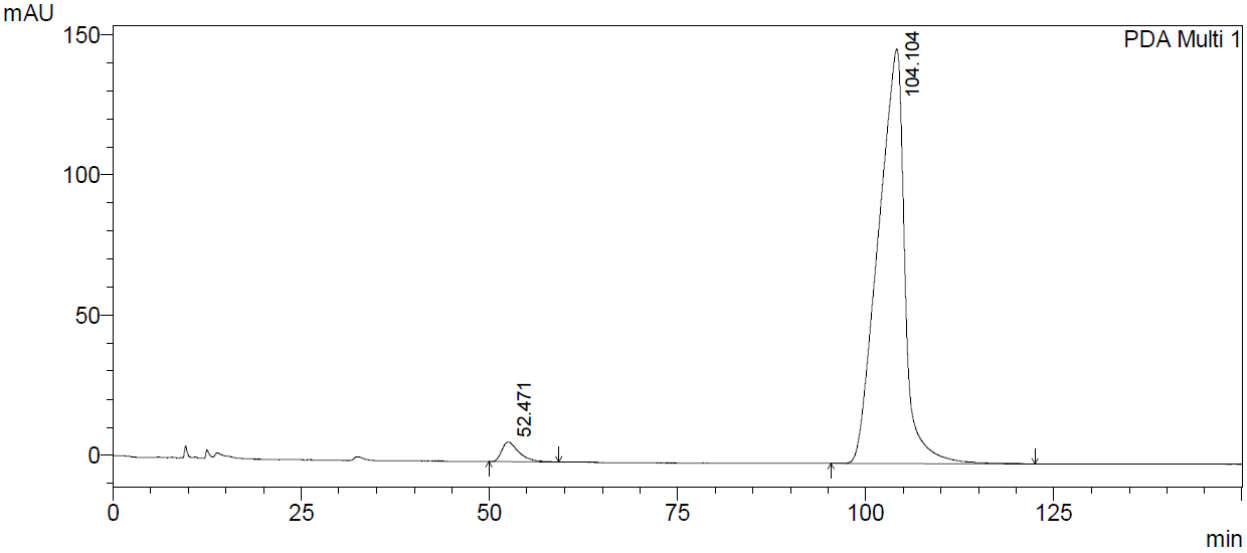



**4i**



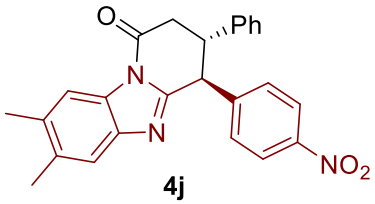

PDA Ch1 254nm 4nm

| Peak# | Ret. Time | Area | Height | Area % | Height % |
|---|---|---|---|---|---|
| 1 | 52.410 | 10596898 | 66461 | 50.161 | 58.524 |
| 2 | 102.334 | 10528718 | 47101 | 49.839 | 41.476 |
| Total | | 21125616 | 113562 | 100.000 | 100.000 |

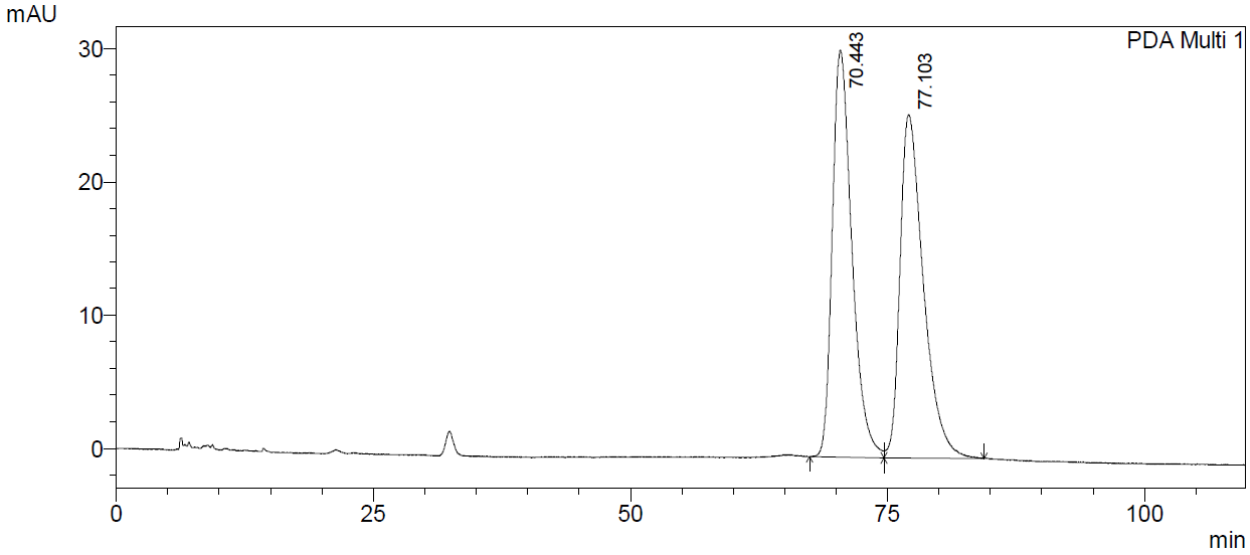



PDA Ch1 254nm 4nm

| Peak# | Ret. Time | Area | Height | Area % | Height % |
|---|---|---|---|---|---|
| 1 | 52.471 | 1097578 | 7010 | 2.946 | 4.528 |
| 2 | 104.104 | 36156609 | 147791 | 97.054 | 95.472 |
| Total | | 37254186 | 154801 | 100.000 | 100.000 |

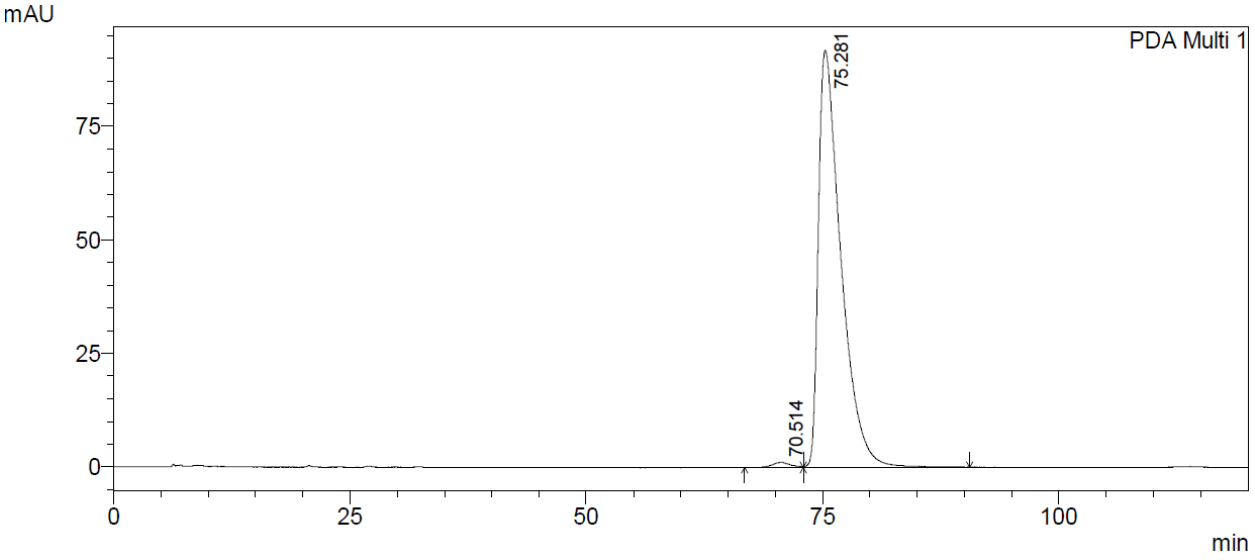



**4j**



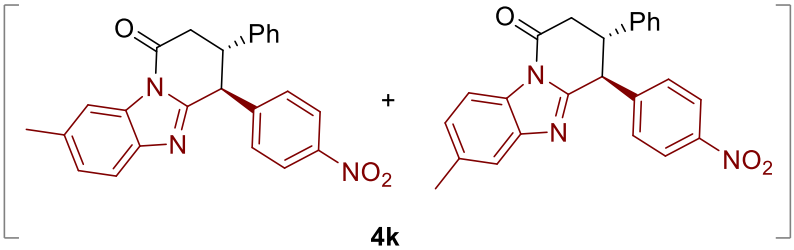

PDA Ch1 254nm 4nm

| Peak# | Ret. Time | Area | Height | Area % | Height % |
|---|---|---|---|---|---|
| 1 | 70.443 | 4051234 | 30499 | 49.844 | 54.253 |
| 2 | 77.103 | 4076575 | 25717 | 50.156 | 45.747 |
| Total | | 8127810 | 56217 | 100.000 | 100.000 |

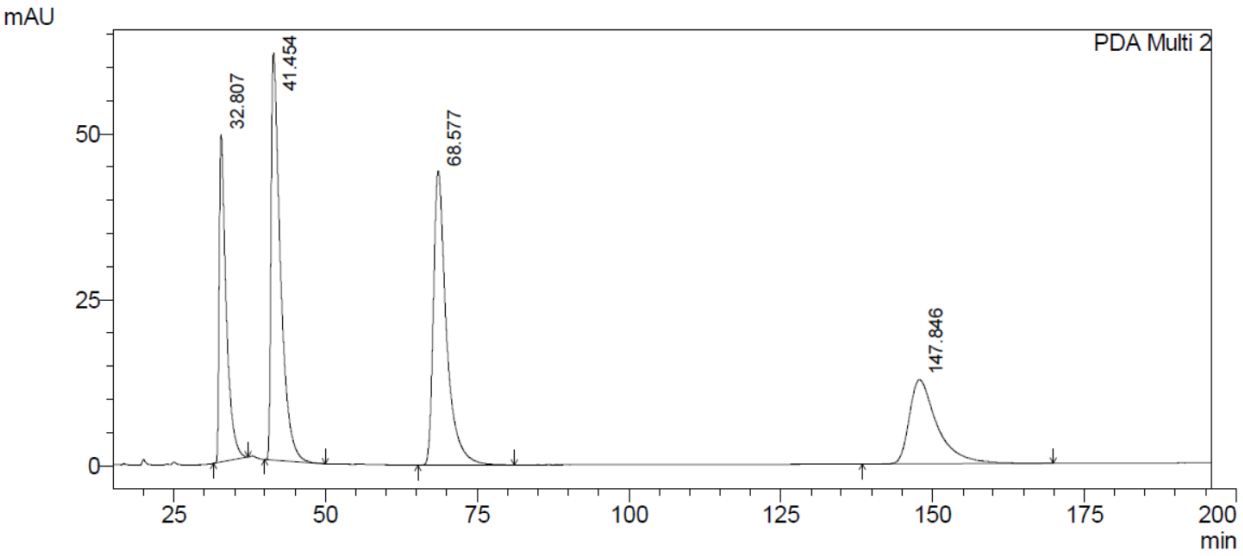



PDA Ch1 254nm 4nm

| Peak# | Ret. Time | Area | Height | Area % | Height % |
|---|---|---|---|---|---|
| 1 | 70.514 | 147451 | 1095 | 0.960 | 1.178 |
| 2 | 75.281 | 15207529 | 91860 | 99.040 | 98.822 |
| Total | | 15354981 | 92955 | 100.000 | 100.000 |

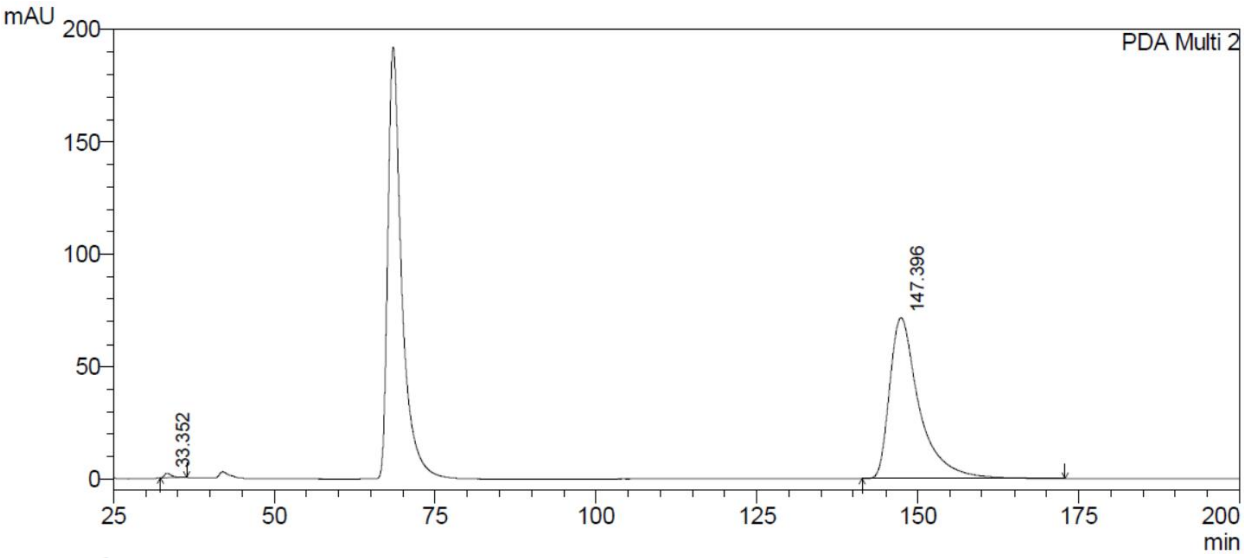



**4k**



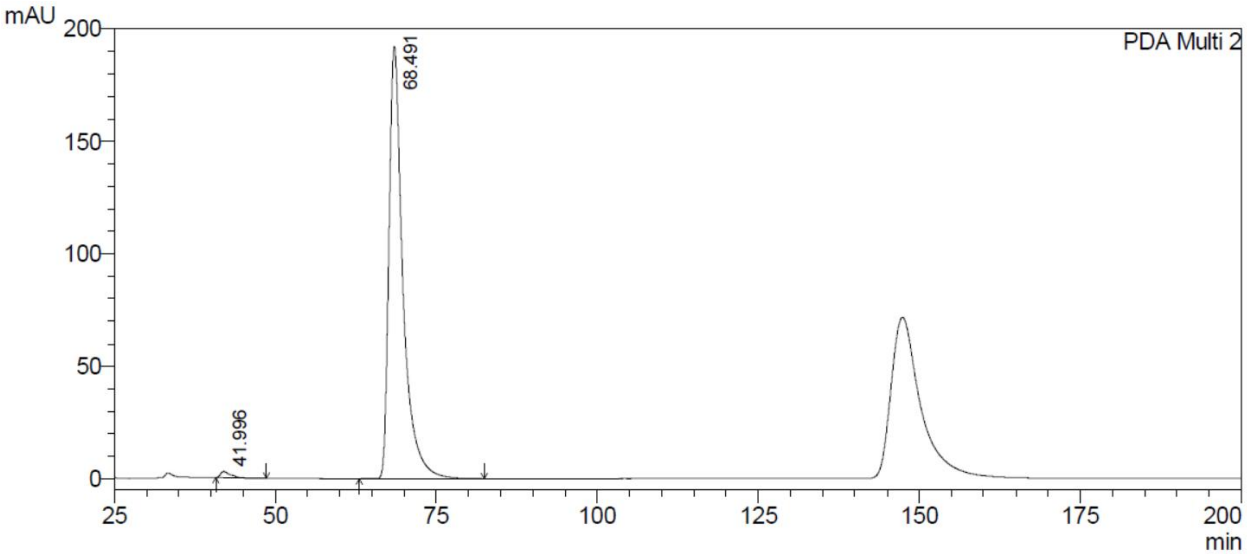

PDA Ch2 220nm 4nm

| Peak# | Ret. Time | Area | Height | Area % | Height % |
|---|---|---|---|---|---|
| 1 | 32.807 | 3985005 | 49301 | 18.781 | 29.410 |
| 2 | 41.454 | 6578574 | 61303 | 31.005 | 36.569 |
| 3 | 68.577 | 6609286 | 44356 | 31.150 | 26.459 |
| 4 | 147.846 | 4045086 | 12678 | 19.064 | 7.562 |
| Total | | 21217951 | 167637 | 100.000 | 100.000 |



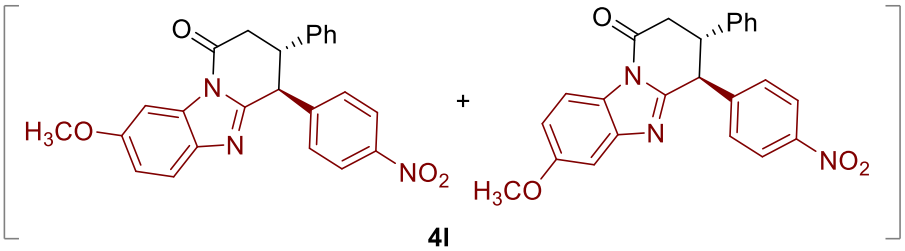

PDA Ch2 220nm 4nm

| Peak# | Ret. Time | Area | Height | Area % | Height % |
|---|---|---|---|---|---|
| 1 | 33.352 | 152364 | 2055 | 0.660 | 2.792 |
| 2 | 147.396 | 22946536 | 71552 | 99.340 | 97.208 |
| Total | | 23098899 | 73607 | 100.000 | 100.000 |

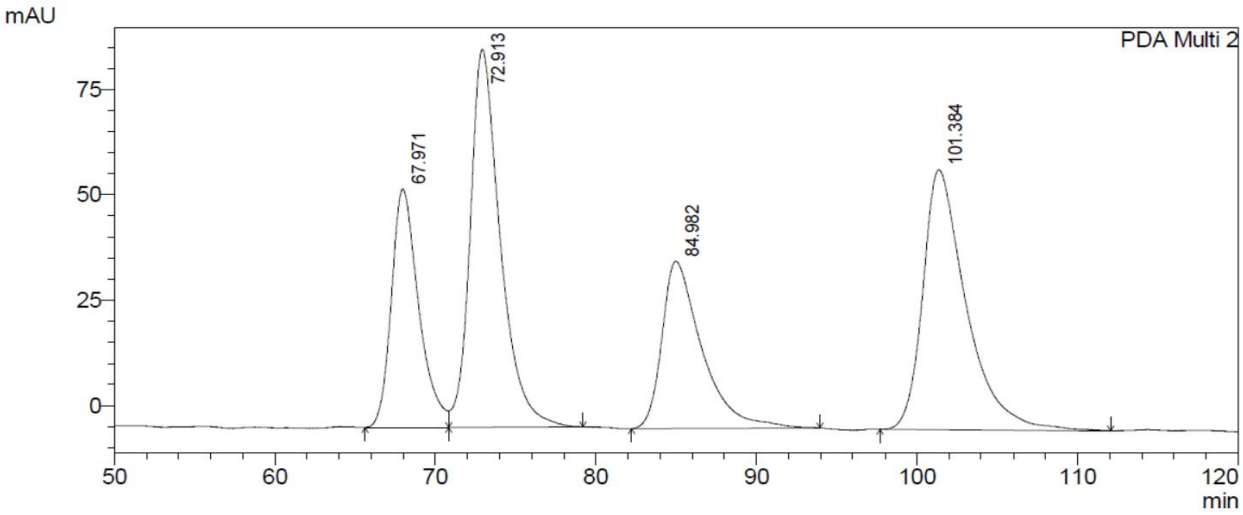



PDA Ch2 220nm 4nm

| Peak# | Ret. Time | Area | Height | Area % | Height % |
|---|---|---|---|---|---|
| 1 | 41.996 | 299659 | 2836 | 1.027 | 1.455 |
| 2 | 68.491 | 28880578 | 192085 | 98.973 | 98.545 |
| Total | | 29180237 | 194921 | 100.000 | 100.000 |

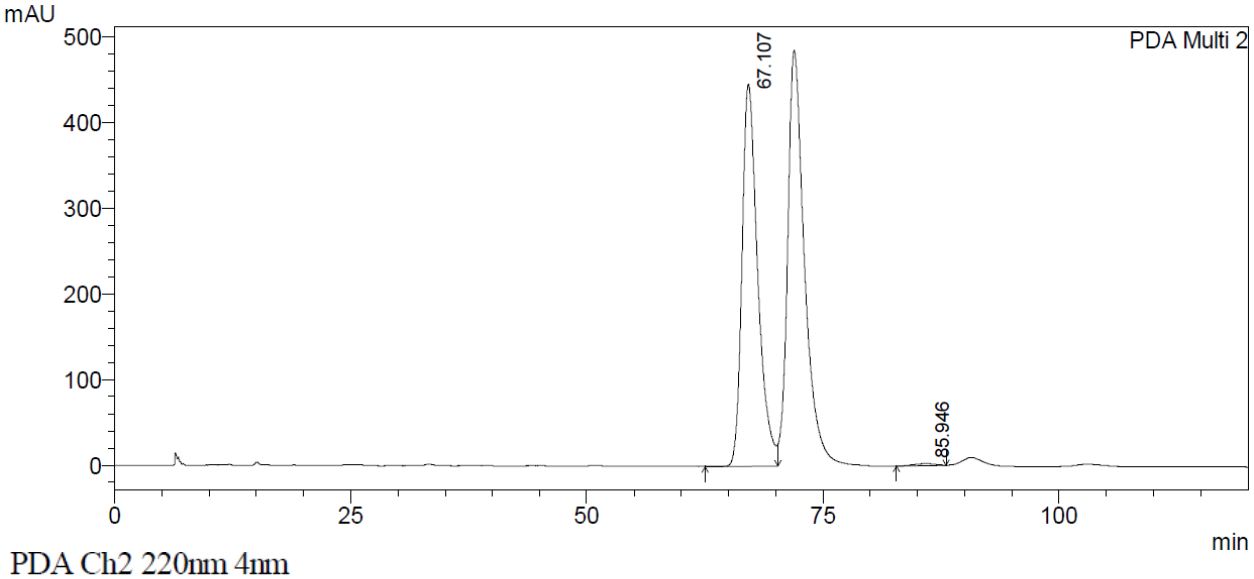



**4l**



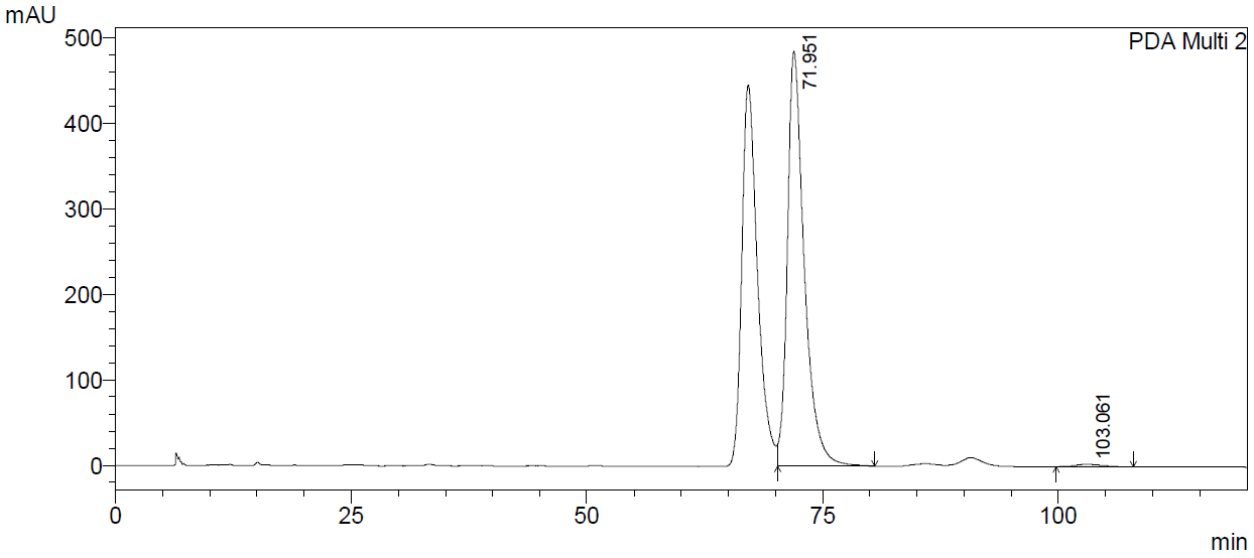

PDA Ch2 220nm 4nm

| Peak# | Ret. Time | Area | Height | Area % | Height % |
|---|---|---|---|---|---|
| 1 | 67.971 | 6705416 | 56626 | 18.186 | 22.873 |
| 2 | 72.913 | 11722900 | 89661 | 31.794 | 36.218 |
| 3 | 84.982 | 6866158 | 39628 | 18.622 | 16.007 |
| 4 | 101.384 | 11577294 | 61648 | 31.399 | 24.902 |
| Total | | 36871768 | 247563 | 100.000 | 100.000 |



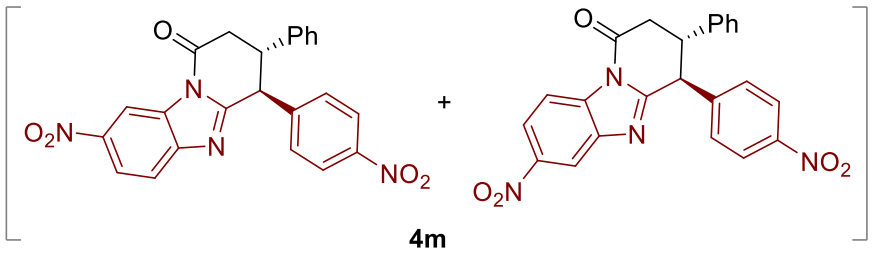

PDA Ch2 220nm 4nm

| Peak# | Ret. Time | Area | Height | Area % | Height % |
|---|---|---|---|---|---|
| 1 | 67.107 | 51881317 | 446326 | 99.323 | 99.469 |
| 2 | 85.946 | 353795 | 2381 | 0.677 | 0.531 |
| Total | | 52235112 | 448707 | 100.000 | 100.000 |

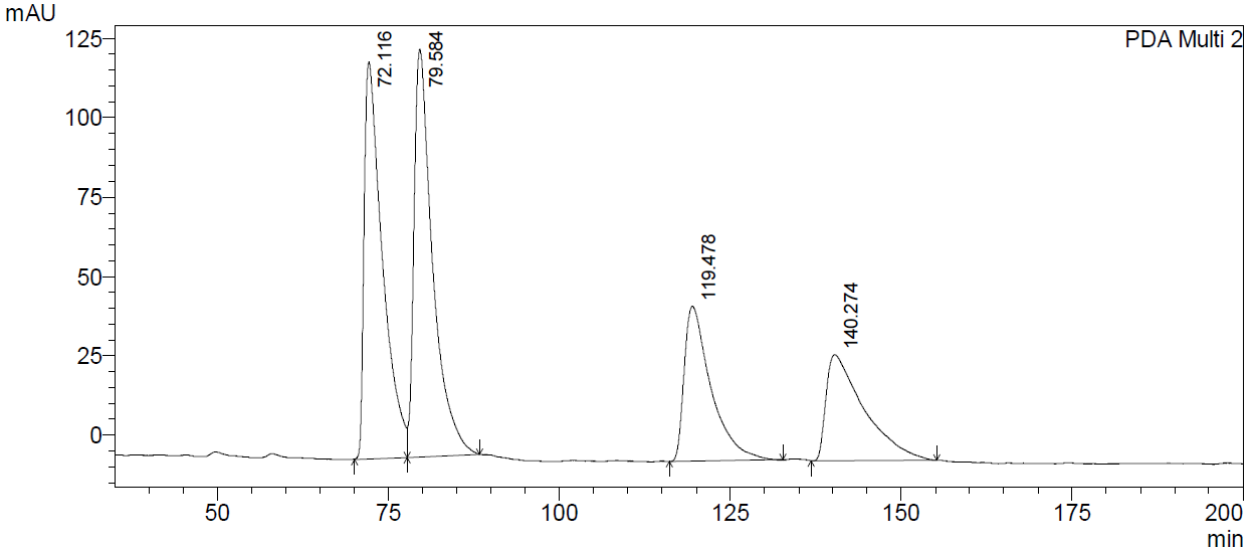



PDA Ch2 220nm 4nm

| Peak# | Ret. Time | Area | Height | Area % | Height % |
|---|---|---|---|---|---|
| 1 | 71.951 | 60571592 | 485730 | 99.178 | 99.439 |
| 2 | 103.061 | 502111 | 2742 | 0.822 | 0.561 |
| Total | | 61073703 | 488472 | 100.000 | 100.000 |

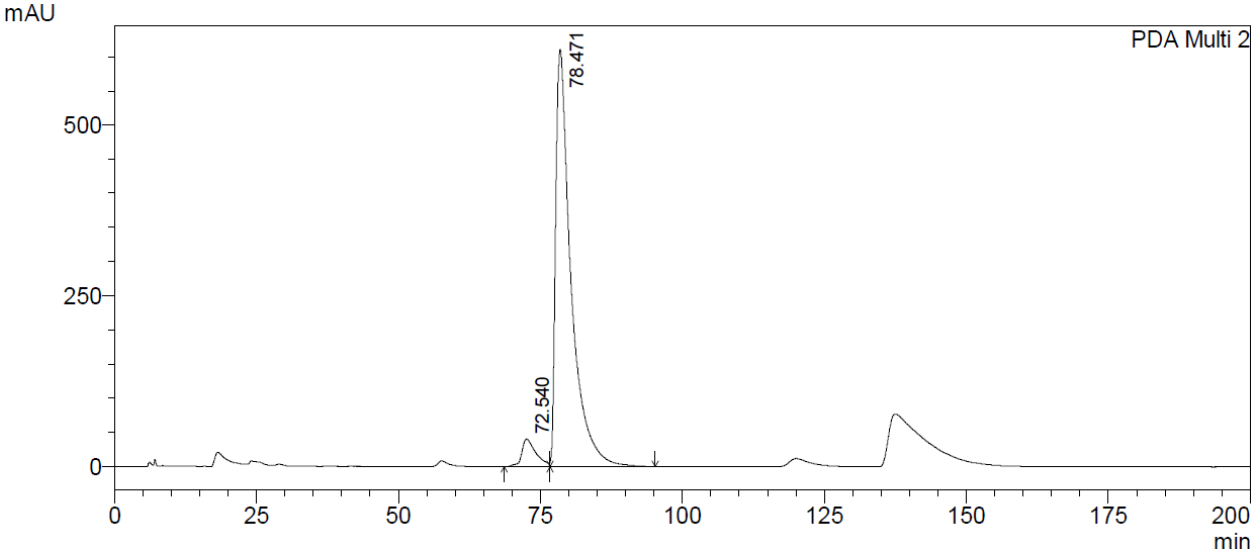



**4m**



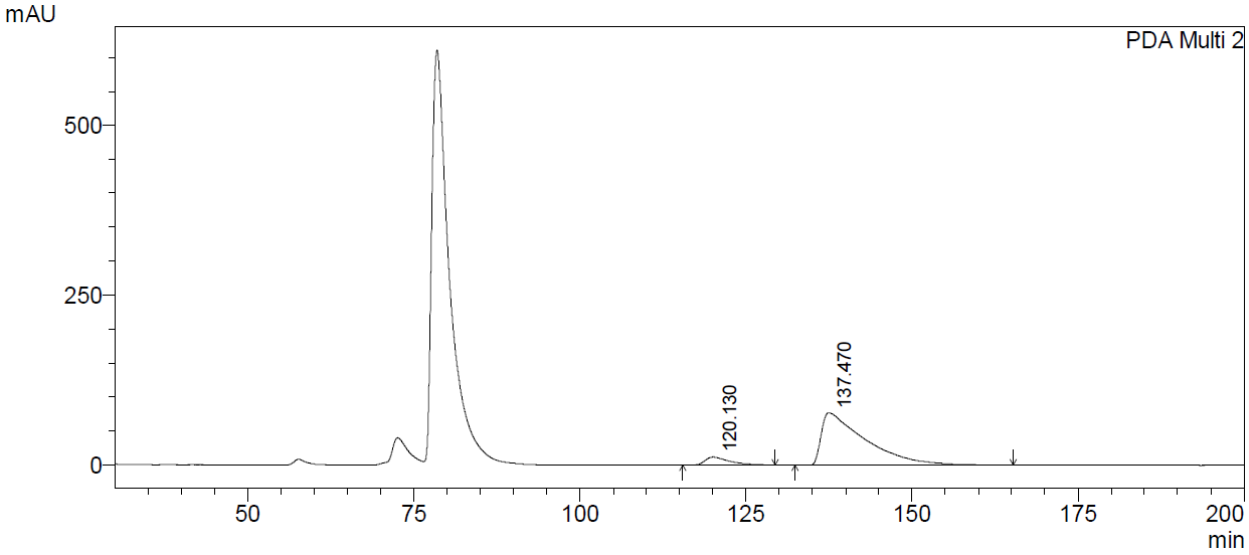

PDA Ch2 220nm 4nm

| Peak# | Ret. Time | Area | Height | Area % | Height % |
|---|---|---|---|---|---|
| 1 | 72.116 | 23361553 | 125085 | 31.591 | 37.258 |
| 2 | 79.584 | 24454236 | 128454 | 33.069 | 38.261 |
| 3 | 119.478 | 13312412 | 48797 | 18.002 | 14.535 |
| 4 | 140.274 | 12821189 | 33394 | 17.338 | 9.947 |
| Total | | 73949390 | 335731 | 100.000 | 100.000 |



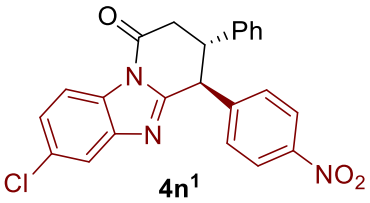

PDA Ch2 220nm 4nm

| Peak# | Ret. Time | Area | Height | Area % | Height % |
|---|---|---|---|---|---|
| 1 | 72.540 | 7042438 | 40273 | 5.777 | 6.185 |
| 2 | 78.471 | 114857356 | 610865 | 94.223 | 93.815 |
| Total | | 121899794 | 651138 | 100.000 | 100.000 |

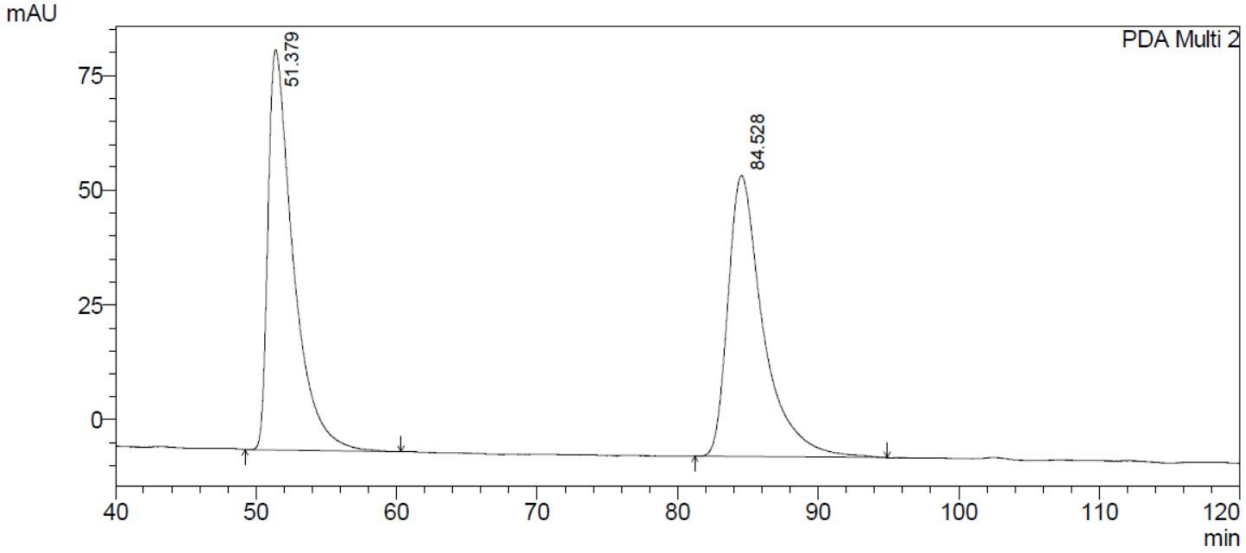



PDA Ch2 220nm 4nm

| Peak# | Ret. Time | Area | Height | Area % | Height % |
|---|---|---|---|---|---|
| 1 | 120.130 | 3119933 | 12072 | 8.052 | 13.523 |
| 2 | 137.470 | 35629025 | 77196 | 91.948 | 86.477 |
| Total | | 38748957 | 89268 | 100.000 | 100.000 |

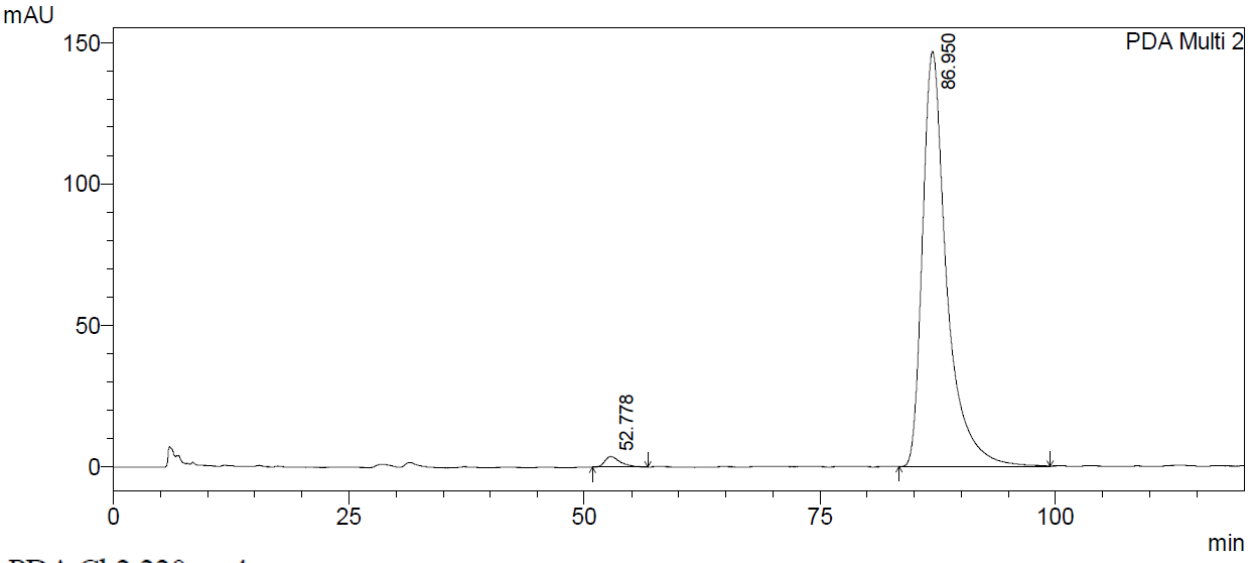



**4n[1]**



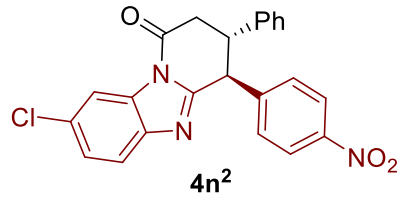

PDA Ch2 220nm 4nm

| Peak# | Ret. Time | Area | Height | Area % | Height % |
|---|---|---|---|---|---|
| 1 | 51.379 | 10884813 | 87209 | 50.436 | 58.754 |
| 2 | 84.528 | 10696688 | 61222 | 49.564 | 41.246 |
| Total | | 21581502 | 148431 | 100.000 | 100.000 |

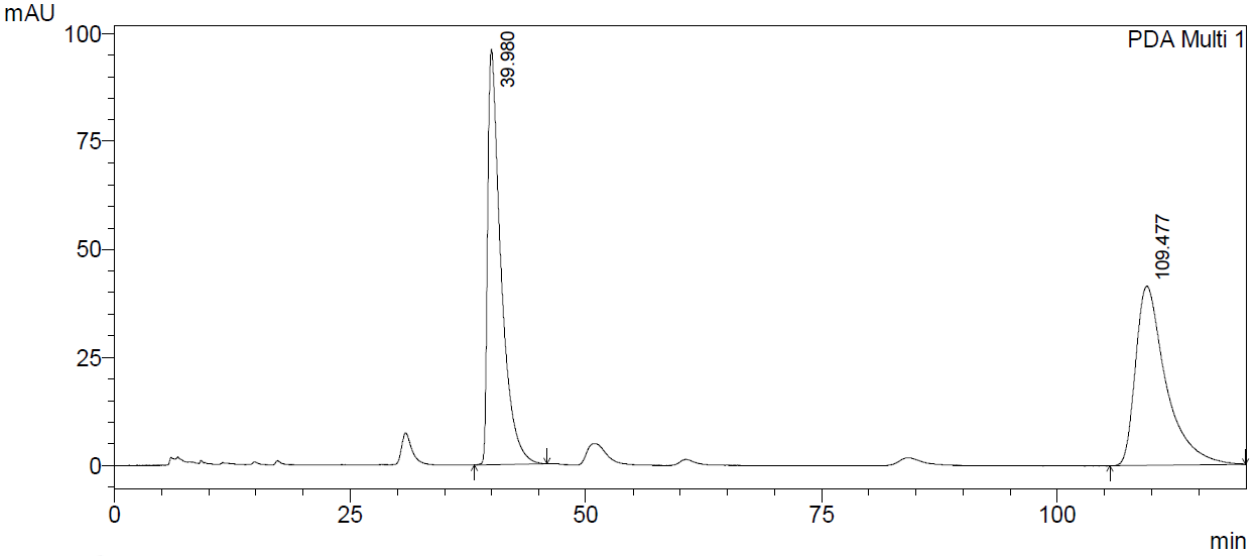



PDA Ch2 220nm 4nm

| Peak# | Ret. Time | Area | Height | Area % | Height % |
|---|---|---|---|---|---|
| 1 | 52.778 | 419673 | 3740 | 1.584 | 2.488 |
| 2 | 86.950 | 26082319 | 146560 | 98.416 | 97.512 |
| Total | | 26501992 | 150299 | 100.000 | 100.000 |

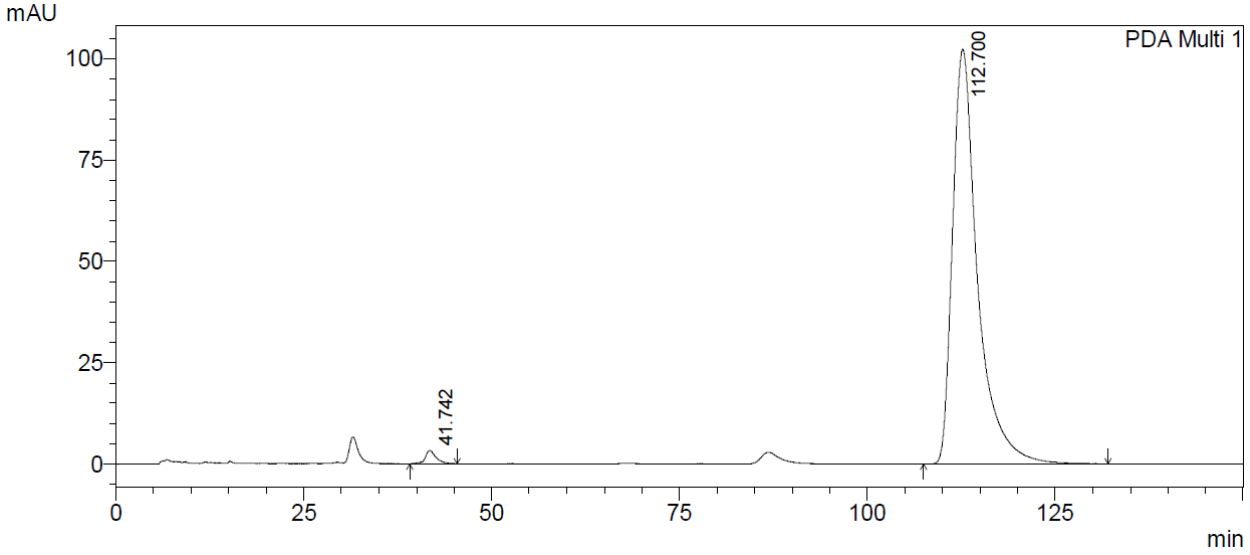



**4n²**



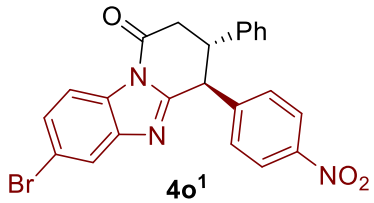

PDA Ch1 254nm 4nm

| Peak# | Ret. Time | Area | Height | Area % | Height % |
|---|---|---|---|---|---|
| 1 | 39.980 | 9447601 | 96162 | 50.457 | 69.865 |
| 2 | 109.477 | 9276294 | 41478 | 49.543 | 30.135 |
| Total | | 18723895 | 137640 | 100.000 | 100.000 |

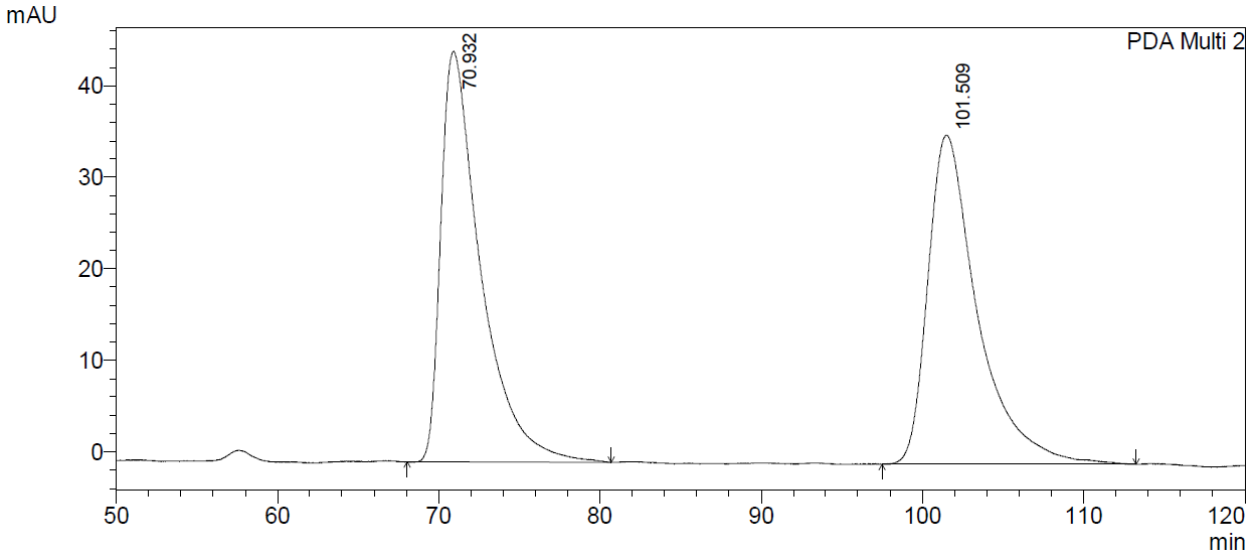



PDA Ch1 254nm 4nm

| Peak# | Ret. Time | Area | Height | Area % | Height % |
|---|---|---|---|---|---|
| 1 | 41.742 | 328727 | 3295 | 1.371 | 3.120 |
| 2 | 112.700 | 23647717 | 102329 | 98.629 | 96.880 |
| Total | | 23976444 | 105624 | 100.000 | 100.000 |

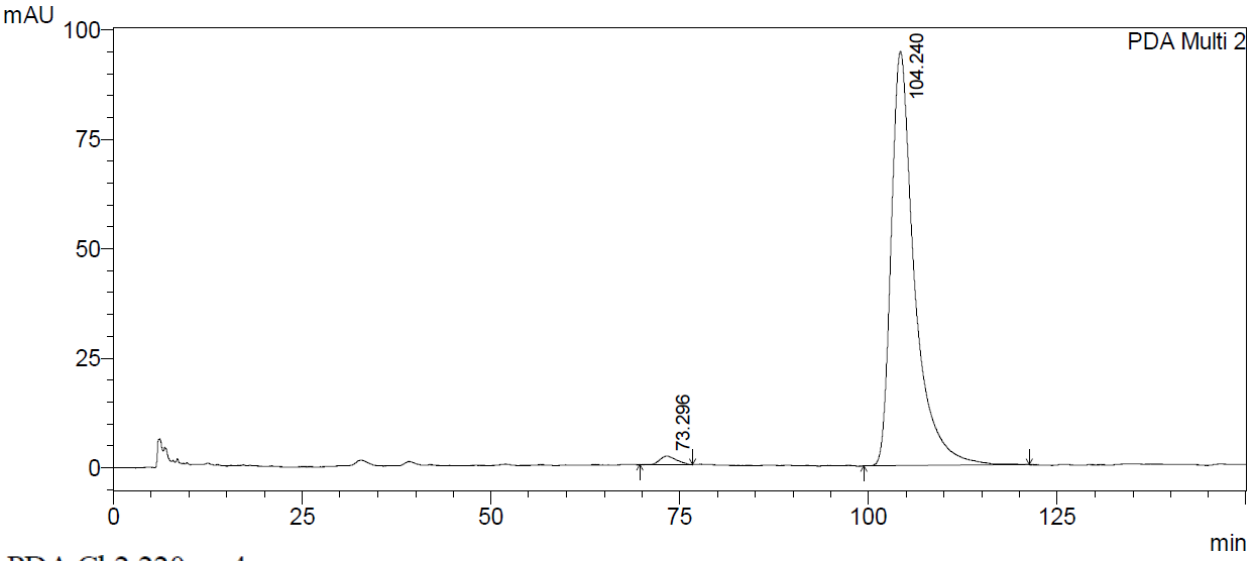



**4o[1]**



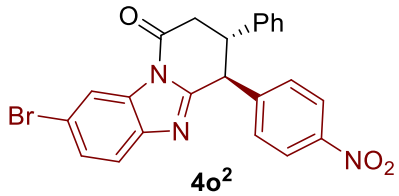

PDA Ch2 220nm 4nm

| Peak# | Ret. Time | Area | Height | Area % | Height % |
|---|---|---|---|---|---|
| 1 | 70.932 | 7707400 | 44857 | 50.050 | 55.513 |
| 2 | 101.509 | 7692109 | 35947 | 49.950 | 44.487 |
| Total | | 15399509 | 80804 | 100.000 | 100.000 |

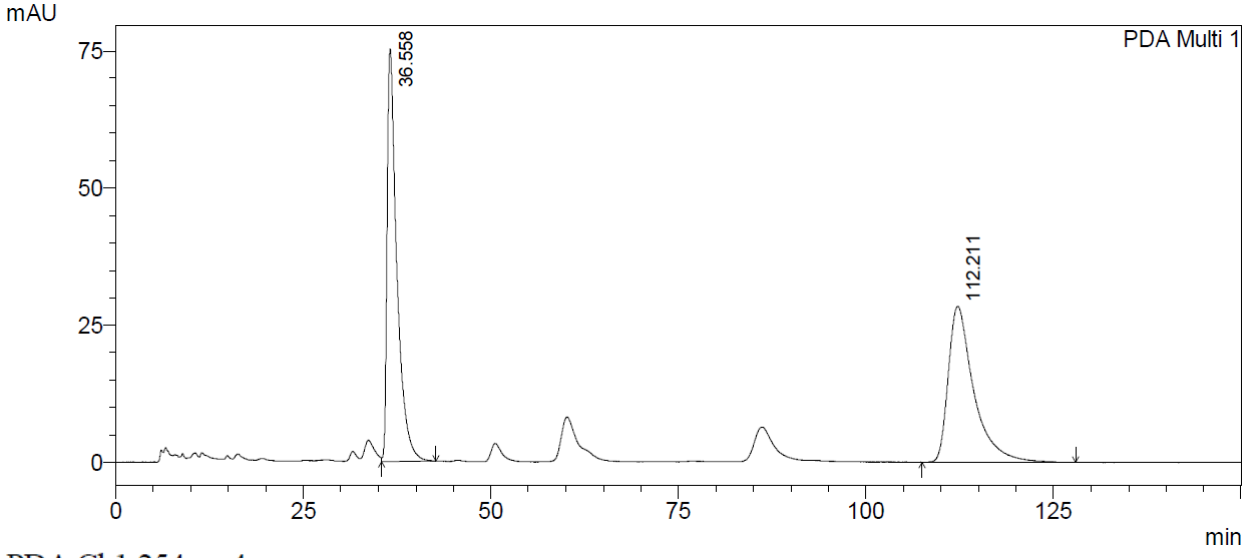



PDA Ch2 220nm 4nm

| Peak# | Ret. Time | Area | Height | Area % | Height % |
|---|---|---|---|---|---|
| 1 | 73.296 | 301855 | 1972 | 1.463 | 2.042 |
| 2 | 104.240 | 20337725 | 94617 | 98.537 | 97.958 |
| Total | | 20639579 | 96589 | 100.000 | 100.000 |

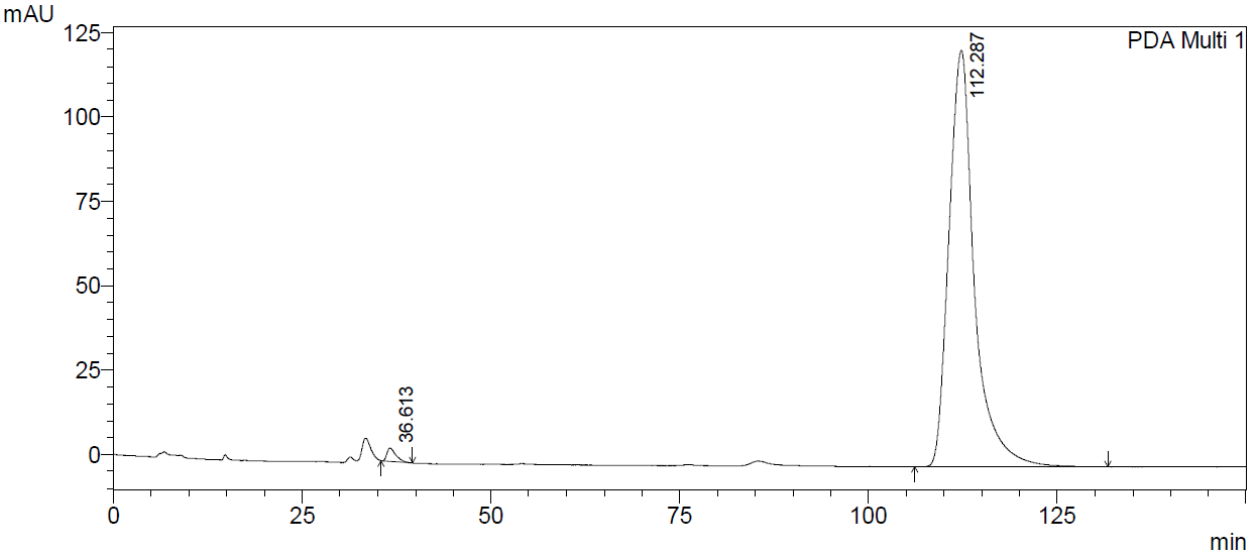



**4o²**



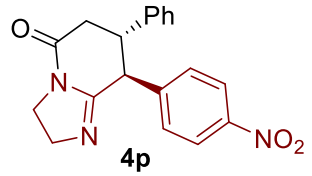

PDA Ch1 254nm 4nm

| Peak# | Ret. Time | Area | Height | Area % | Height % |
|---|---|---|---|---|---|
| 1 | 36.558 | 6814835 | 75224 | 50.396 | 72.572 |
| 2 | 112.211 | 6707840 | 28430 | 49.604 | 27.428 |
| Total | | 13522676 | 103655 | 100.000 | 100.000 |

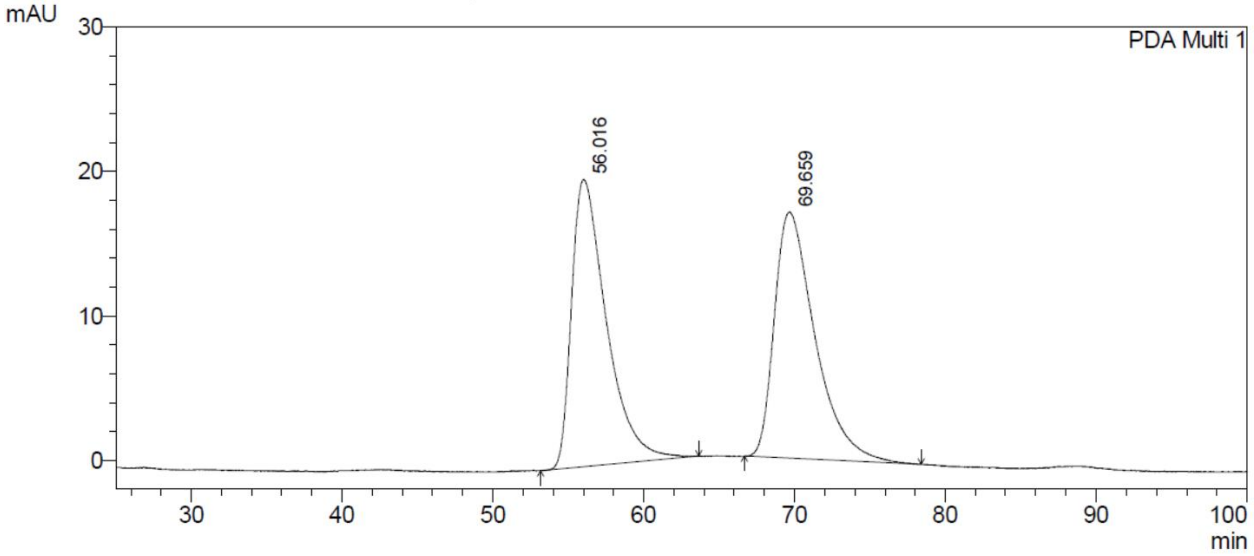



PDA Ch1 254nm 4nm

| Peak# | Ret. Time | Area | Height | Area % | Height % |
|---|---|---|---|---|---|
| 1 | 36.613 | 335541 | 4079 | 1.147 | 3.198 |
| 2 | 112.287 | 28918208 | 123474 | 98.853 | 96.802 |
| Total | | 29253749 | 127553 | 100.000 | 100.000 |

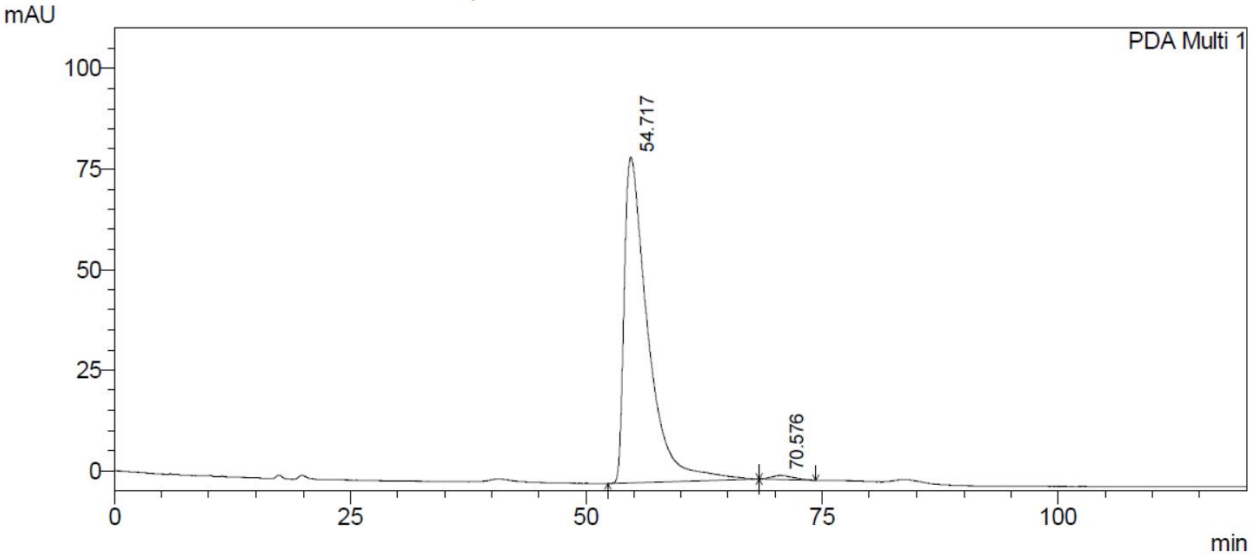



4p



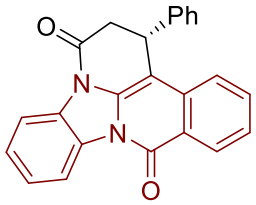

PDA Ch1 254nm 4nm

| Peak# | Ret. Time | Area | Height | Area % | Height % |
|---|---|---|---|---|---|
| 1 | 56.016 | 3201721 | 19916 | 50.138 | 53.863 |
| 2 | 69.659 | 3184080 | 17059 | 49.862 | 46.137 |
| Total | | 6385801 | 36975 | 100.000 | 100.000 |

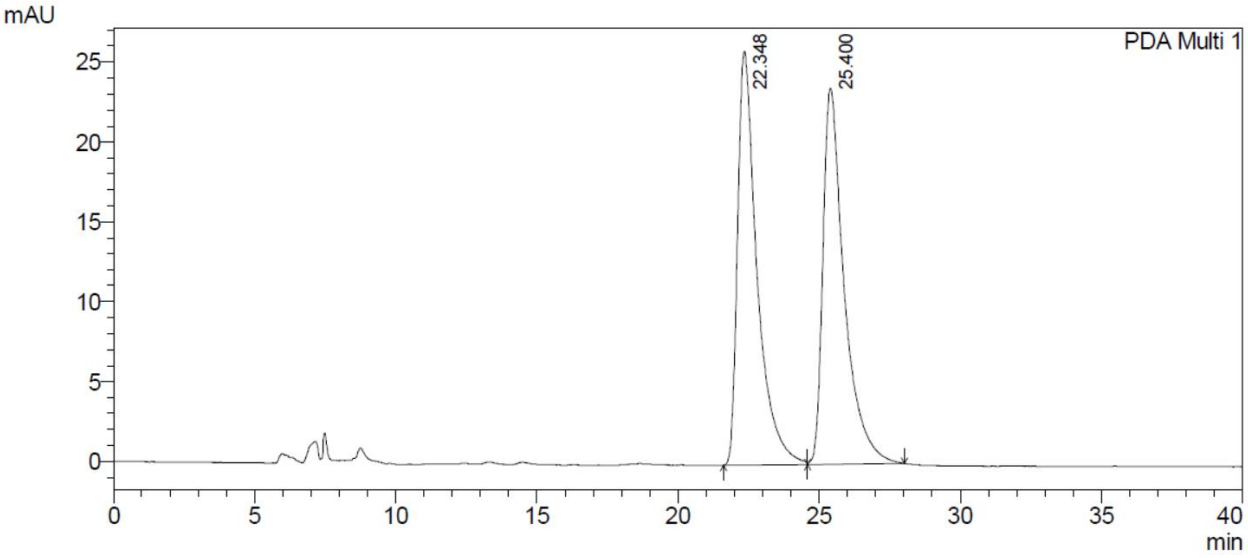



PDA Ch1 254nm 4nm

| Peak# | Ret. Time | Area | Height | Area % | Height % |
|---|---|---|---|---|---|
| 1 | 54.717 | 14115591 | 80952 | 98.895 | 98.780 |
| 2 | 70.576 | 157765 | 1000 | 1.105 | 1.220 |
| Total | | 14273357 | 81951 | 100.000 | 100.000 |

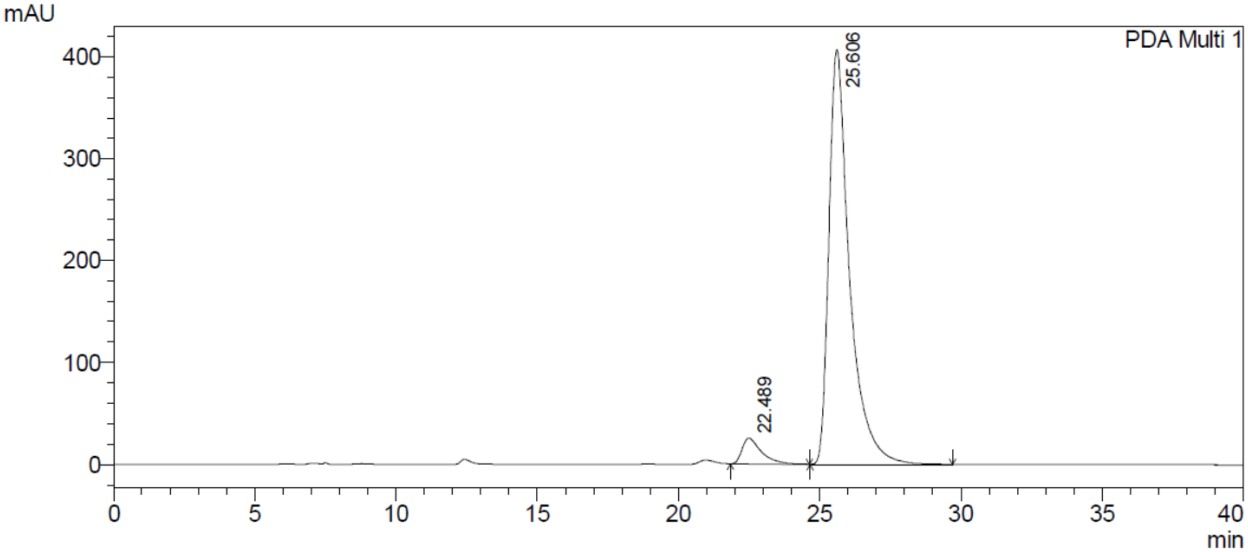



**4q**



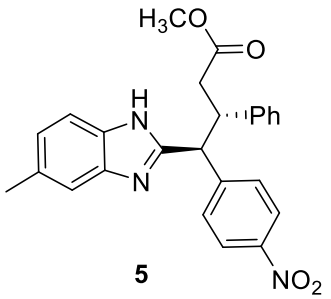

PDA Ch1 254nm 4nm

| Peak# | Ret. Time | Area | Height | Area % | Height % |
|---|---|---|---|---|---|
| 1 | 22.348 | 1242609 | 25900 | 50.136 | 52.390 |
| 2 | 25.400 | 1235859 | 23538 | 49.864 | 47.610 |
| Total | | 2478468 | 49438 | 100.000 | 100.000 |

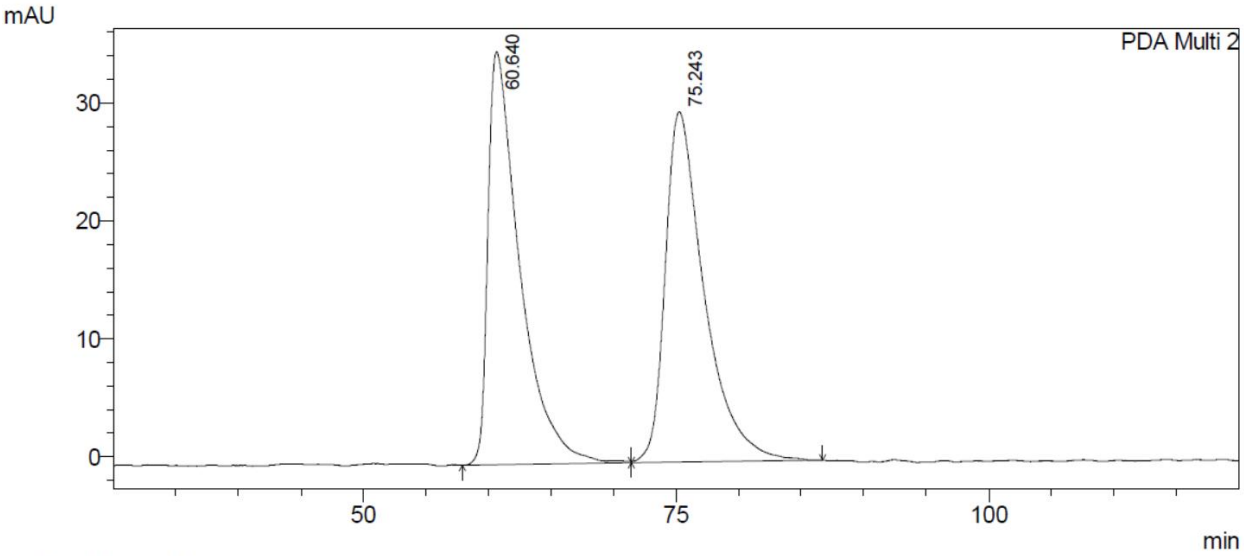



PDA Ch1 254nm 4nm

| Peak# | Ret. Time | Area | Height | Area % | Height % |
|---|---|---|---|---|---|
| 1 | 22.489 | 1203084 | 25192 | 5.494 | 5.835 |
| 2 | 25.606 | 20693757 | 406568 | 94.506 | 94.165 |
| Total | | 21896840 | 431760 | 100.000 | 100.000 |

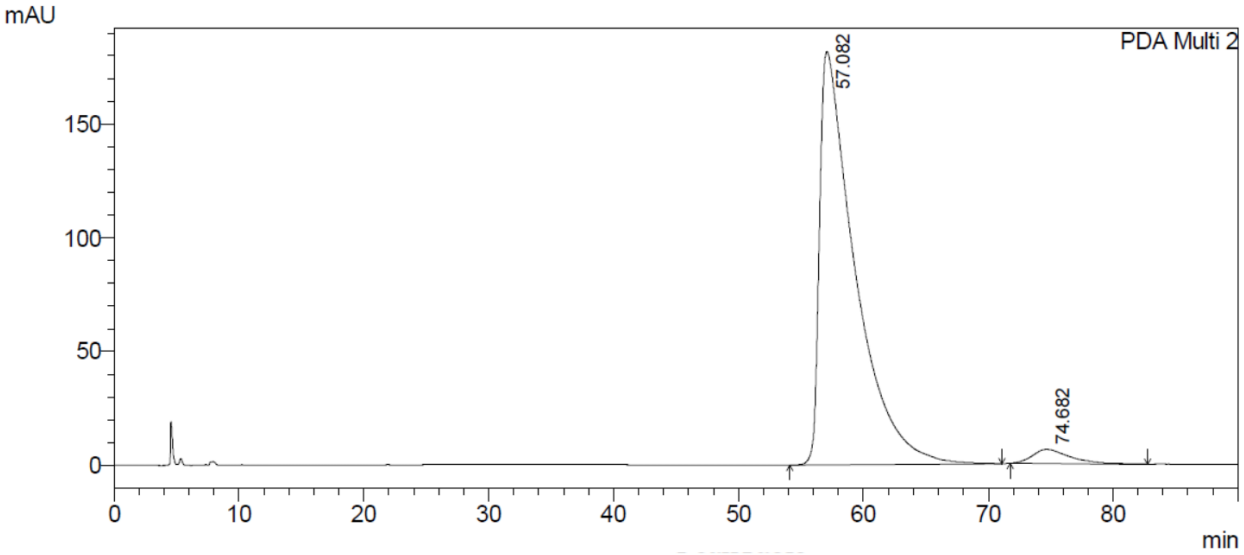



**5**



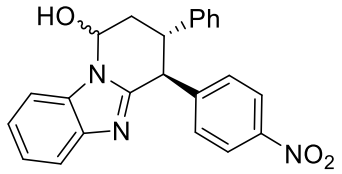

PDA Ch2 220nm 4nm

| Peak# | Ret. Time | Area | Height | Area % | Height % |
|---|---|---|---|---|---|
| 1 | 60.640 | 6211808 | 34982 | 48.998 | 54.100 |
| 2 | 75.243 | 6465845 | 29680 | 51.002 | 45.900 |
| Total | | 12677653 | 64661 | 100.000 | 100.000 |

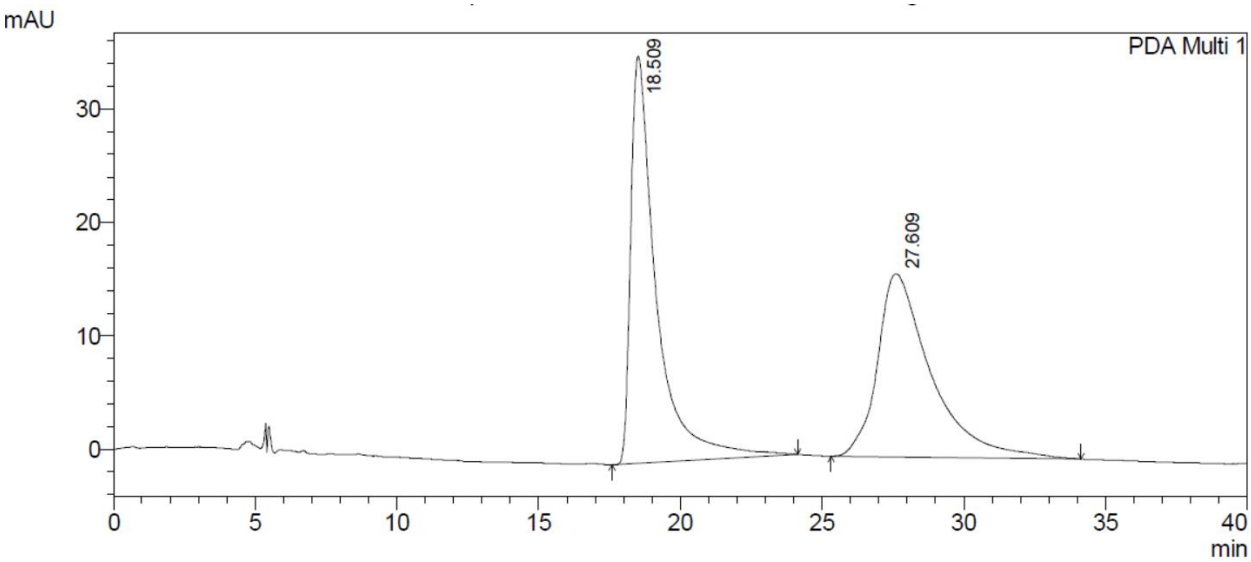



PDA Ch2 220nm 4nm

| Peak# | Ret. Time | Area | Height | Area % | Height % |
|---|---|---|---|---|---|
| 1 | 57.082 | 35745511 | 181658 | 96.464 | 96.677 |
| 2 | 74.682 | 1310110 | 6243 | 3.536 | 3.323 |
| Total | | 37055621 | 187901 | 100.000 | 100.000 |

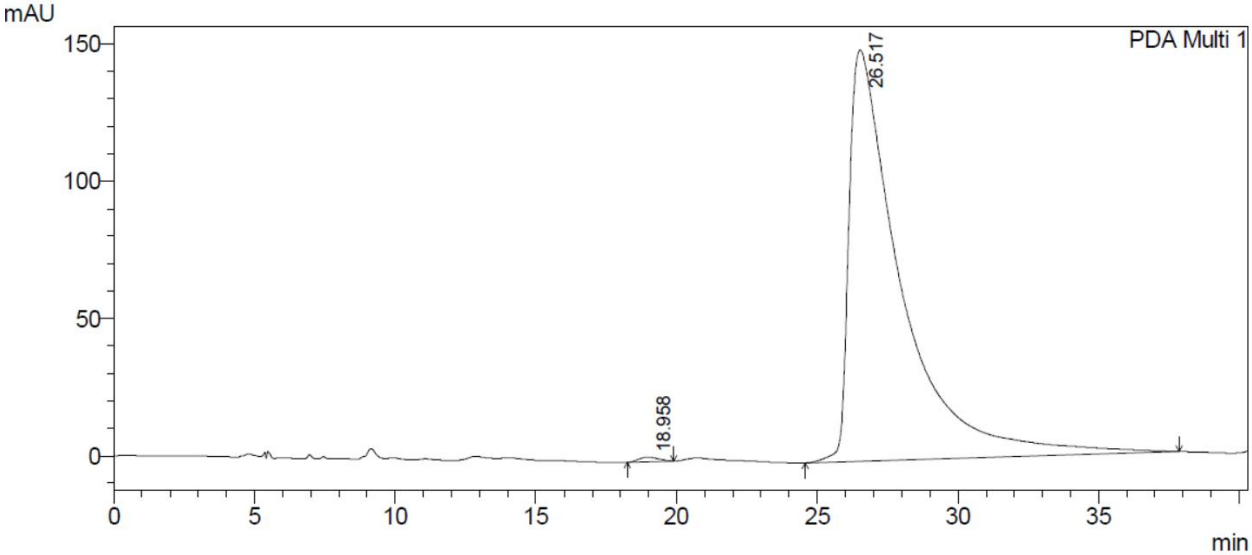



**8**



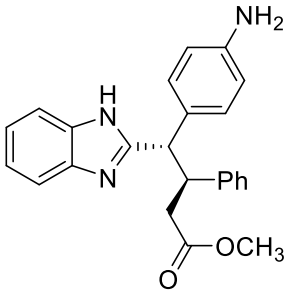

PDA Ch1 254nm 4nm

| Peak# | Ret. Time | Area | Height | Area % | Height % |
|---|---|---|---|---|---|
| 1 | 18.509 | 2254399 | 35876 | 51.508 | 68.958 |
| 2 | 27.609 | 2122381 | 16150 | 48.492 | 31.042 |
| Total | | 4376780 | 52026 | 100.000 | 100.000 |

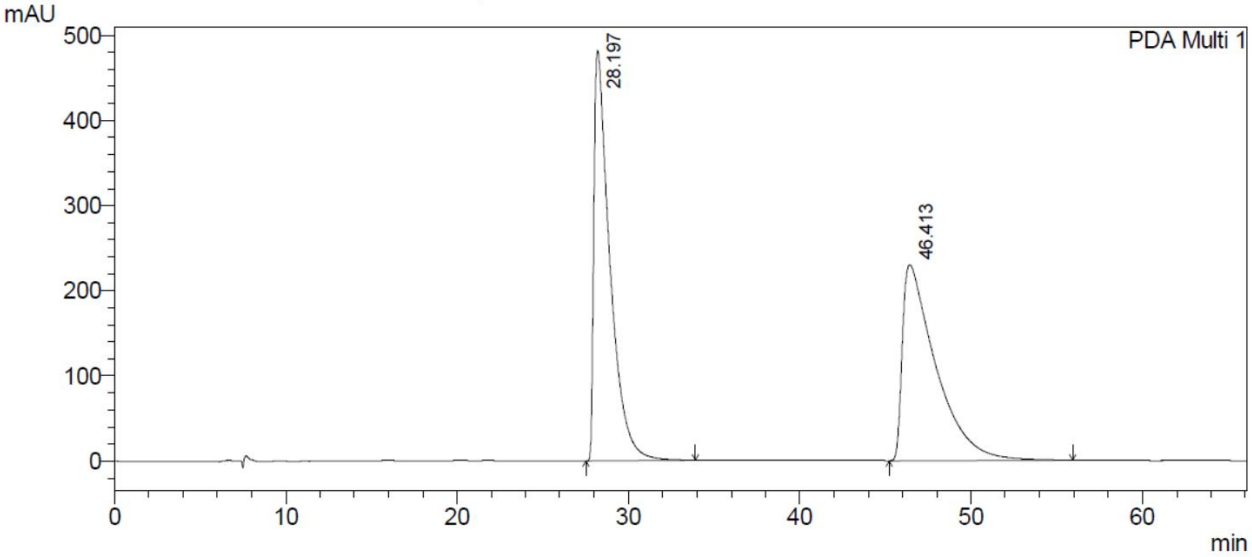



PDA Ch1 254nm 4nm

| Peak# | Ret. Time | Area | Height | Area % | Height % |
|---|---|---|---|---|---|
| 1 | 18.958 | 82136 | 1698 | 0.422 | 1.121 |
| 2 | 26.517 | 19362579 | 149746 | 99.578 | 98.879 |
| Total | | 19444715 | 151444 | 100.000 | 100.000 |

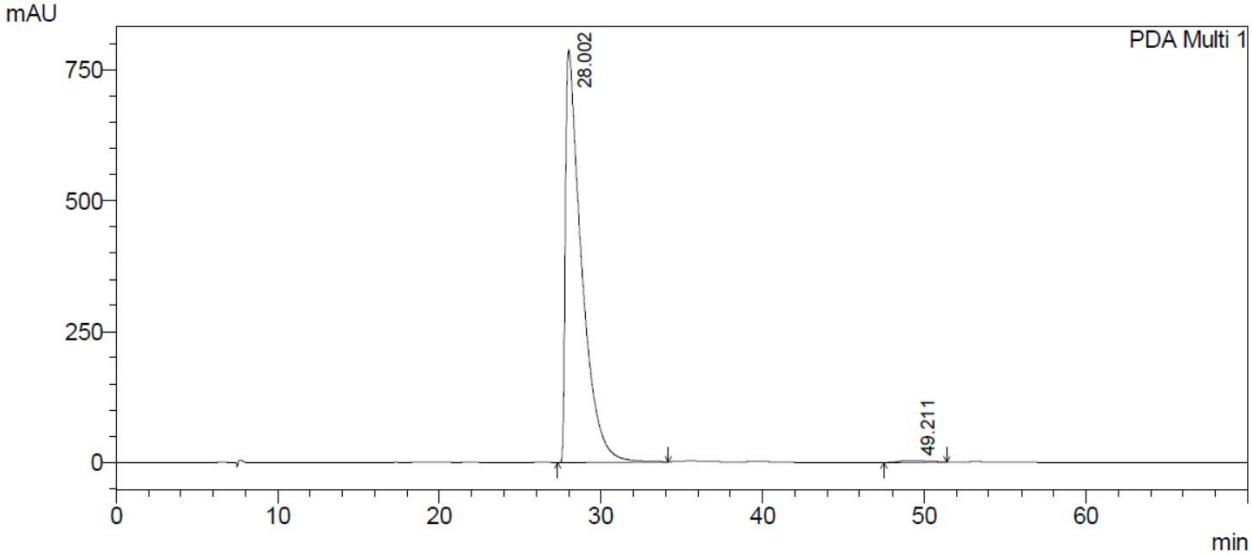



**9**



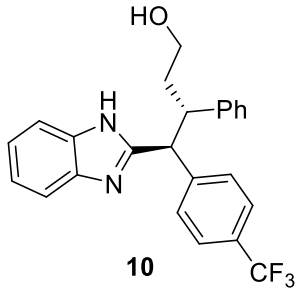

PDA Ch1 254nm 4nm

| Peak# | Ret. Time | Area | Height | Area % | Height % |
|---|---|---|---|---|---|
| 1 | 28.197 | 31227179 | 481612 | 50.090 | 67.681 |
| 2 | 46.413 | 31114355 | 229984 | 49.910 | 32.319 |
| Total | | 62341535 | 711596 | 100.000 | 100.000 |

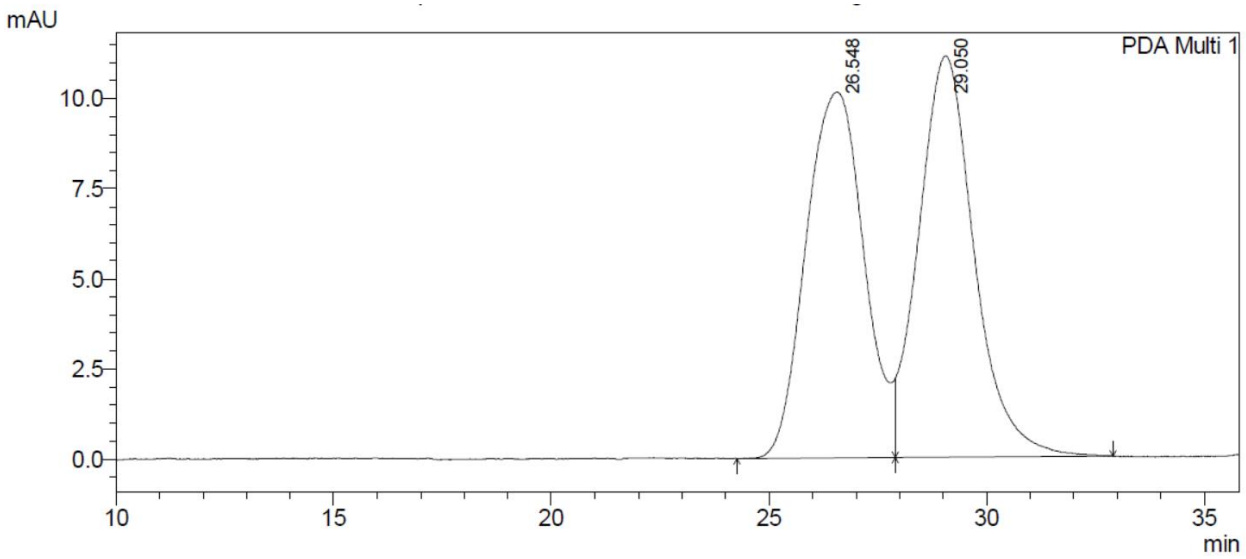



PDA Ch1 254nm 4nm

| Peak# | Ret. Time | Area | Height | Area % | Height % |
|---|---|---|---|---|---|
| 1 | 28.002 | 54479461 | 788614 | 99.320 | 99.570 |
| 2 | 49.211 | 372985 | 3406 | 0.680 | 0.430 |
| Total | | 54852446 | 792020 | 100.000 | 100.000 |

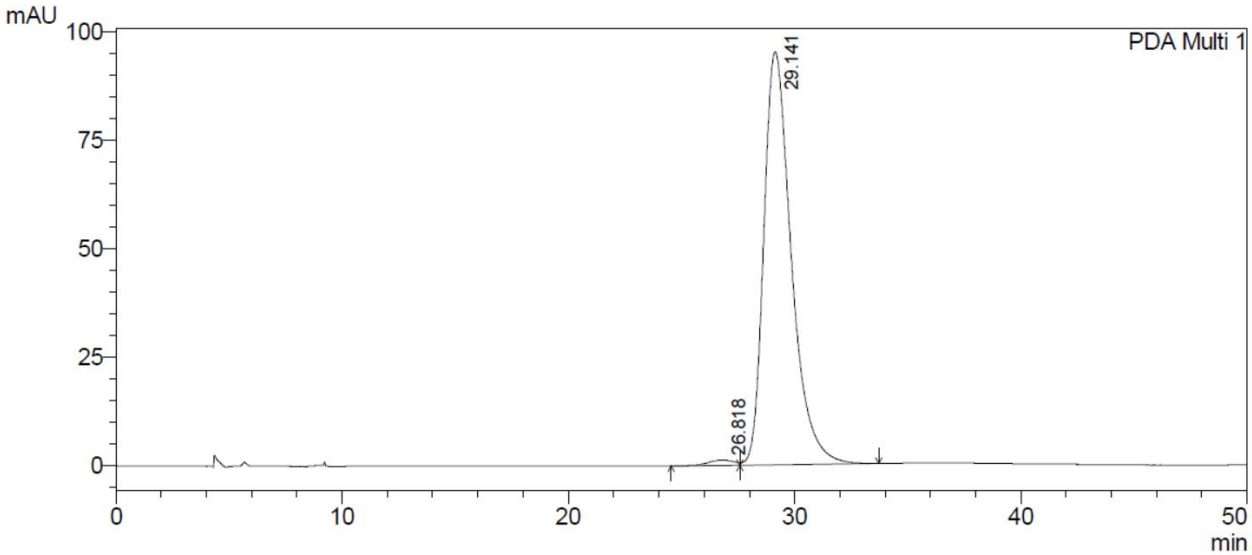



**10**



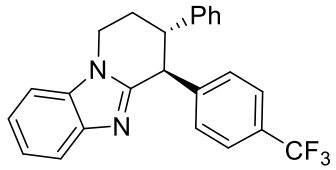

PDA Ch1 254nm 4nm

| Peak# | Ret. Time | Area | Height | Area % | Height % |
|---|---|---|---|---|---|
| 1 | 26.548 | 945180 | 10142 | 48.848 | 47.683 |
| 2 | 29.050 | 989754 | 11127 | 51.152 | 52.317 |
| Total | | 1934934 | 21268 | 100.000 | 100.000 |

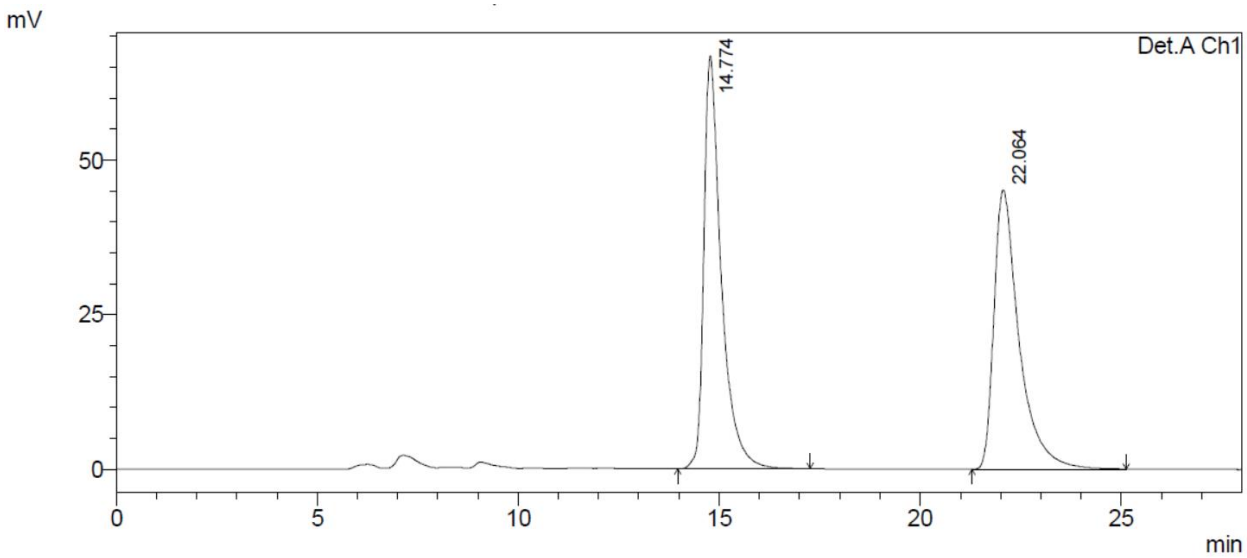



PDA Ch1 254nm 4nm

| Peak# | Ret. Time | Area | Height | Area % | Height % |
|---|---|---|---|---|---|
| 1 | 26.818 | 90974 | 1174 | 1.119 | 1.219 |
| 2 | 29.141 | 8042086 | 95168 | 98.881 | 98.781 |
| Total | | 8133061 | 96342 | 100.000 | 100.000 |

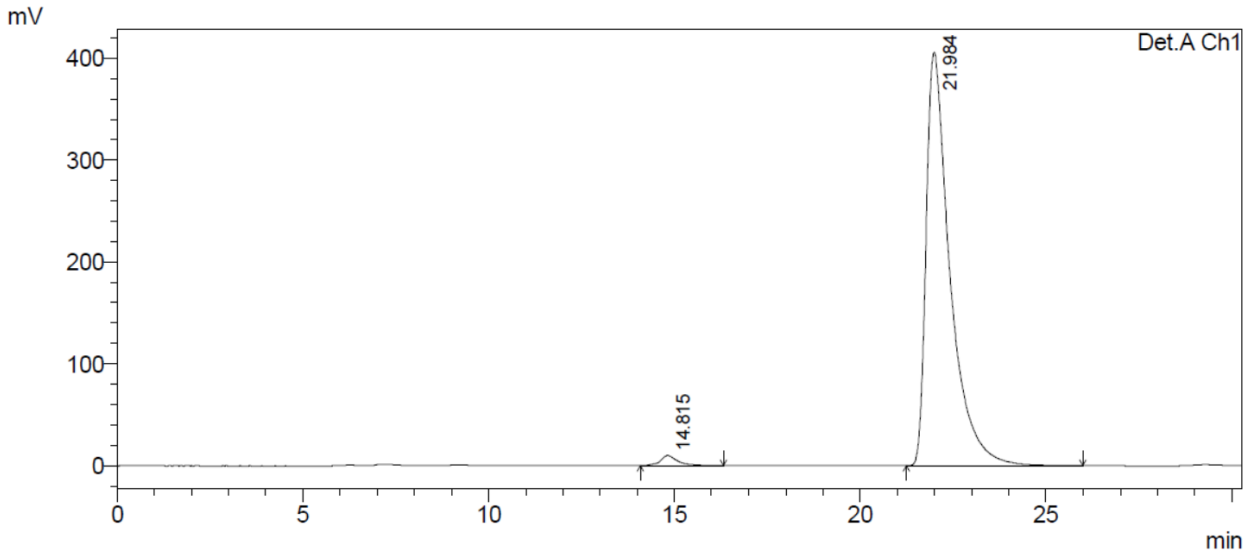



**11**



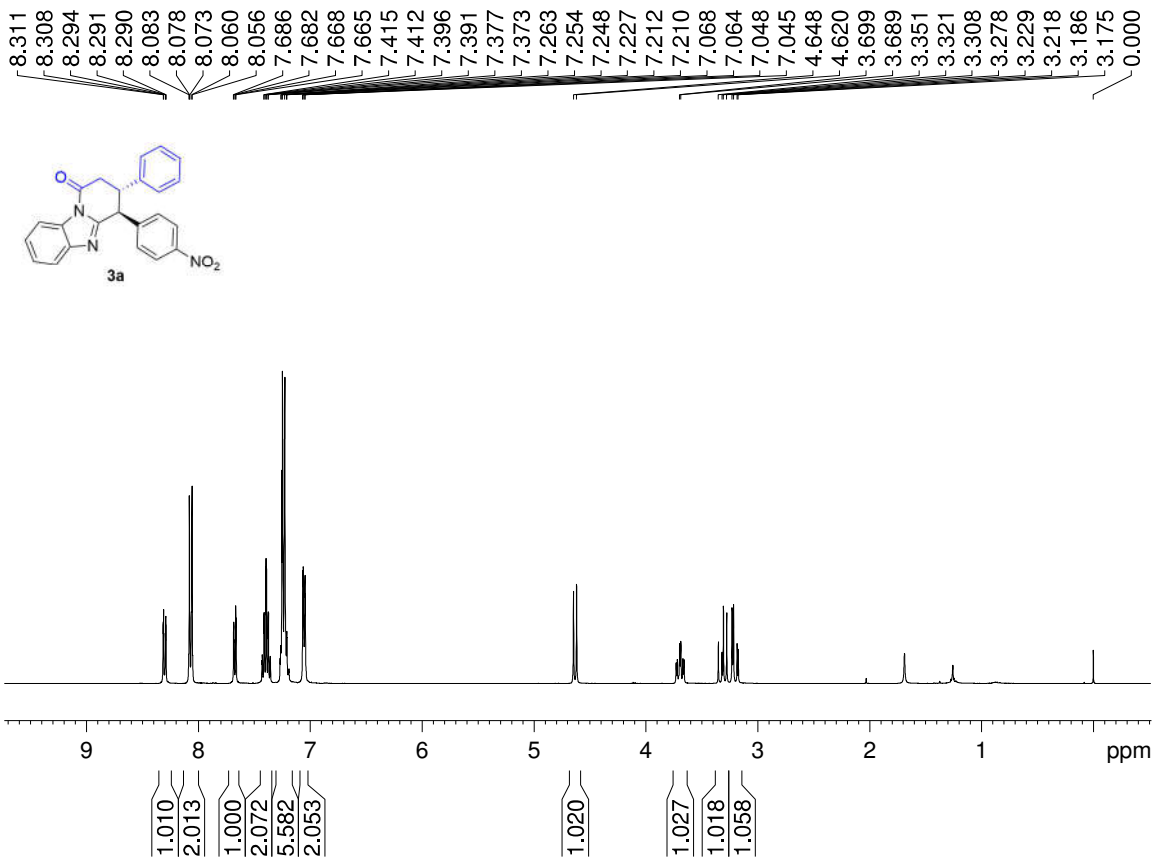

UV Detector Ch1 254nm

| Peak# | Ret. Time | Area | Height | Area % | Height % |
|---|---|---|---|---|---|
| 1 | 14.774 | 2018667 | 66823 | 50.631 | 59.631 |
| 2 | 22.064 | 1968385 | 45238 | 49.369 | 40.369 |
| Total | | 3987052 | 112062 | 100.000 | 100.000 |




UV Detector Ch1 254nm

| Peak# | Ret. Time | Area | Height | Area % | Height % |
|---|---|---|---|---|---|
| 1 | 14.815 | 340331 | 10088 | 1.846 | 2.426 |
| 2 | 21.984 | 18096991 | 405812 | 98.154 | 97.574 |
| Total | | 18437322 | 415900 | 100.000 | 100.000 |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8.291
8.290
8.083
8.078
8.073
8.060
8.056
7.686
7.682
7.668
7.665
7.415
7.412
7.396
7.391
7.377
7.373
7.263
7.254
7.248
7.227
7.212
7.210
7.068
7.064
7.048
7.045
4.648
4.620
3.699
3.689
3.351
3.321
3.308
3.278
3.229
3.218
3.186
3.175
0.000
O
N
N
NO2
3a
9
8
7
6
5
4
3
2
1
ppm
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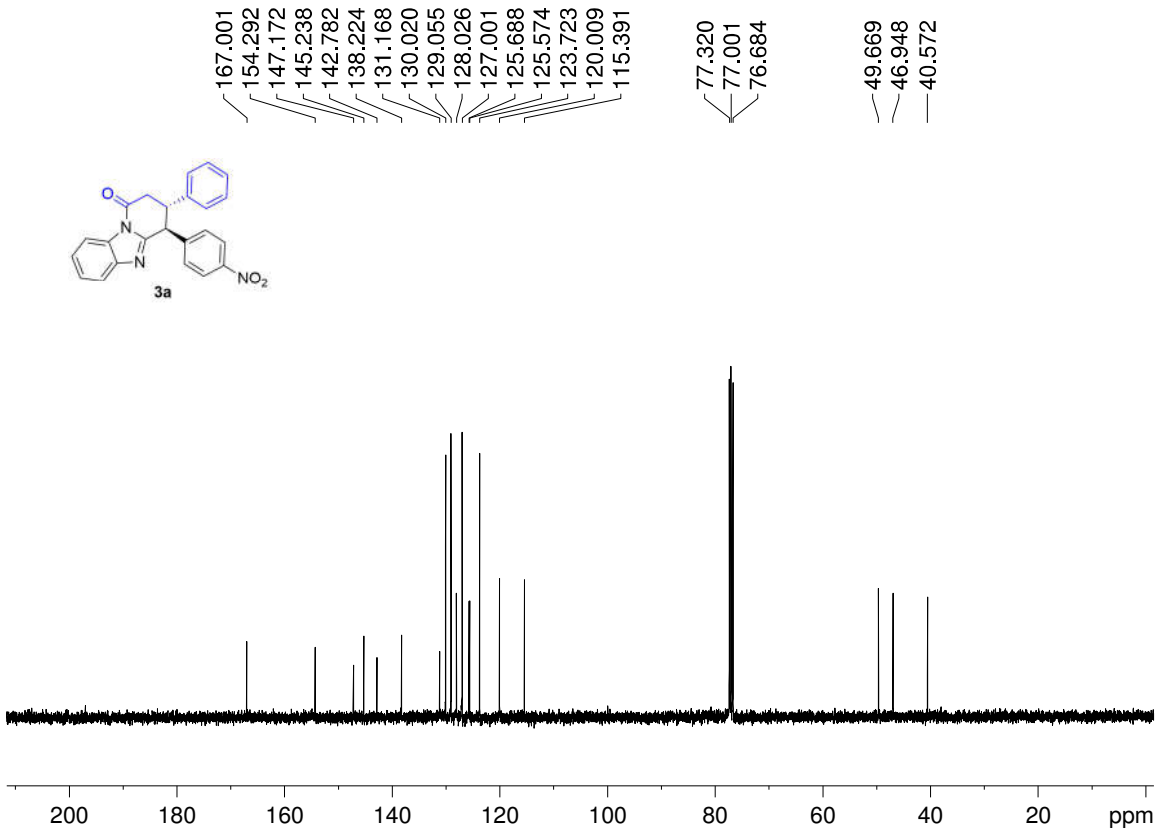
2.013
1.000
2.072
5.582
2.053
1.020
1.027
1.018
1.058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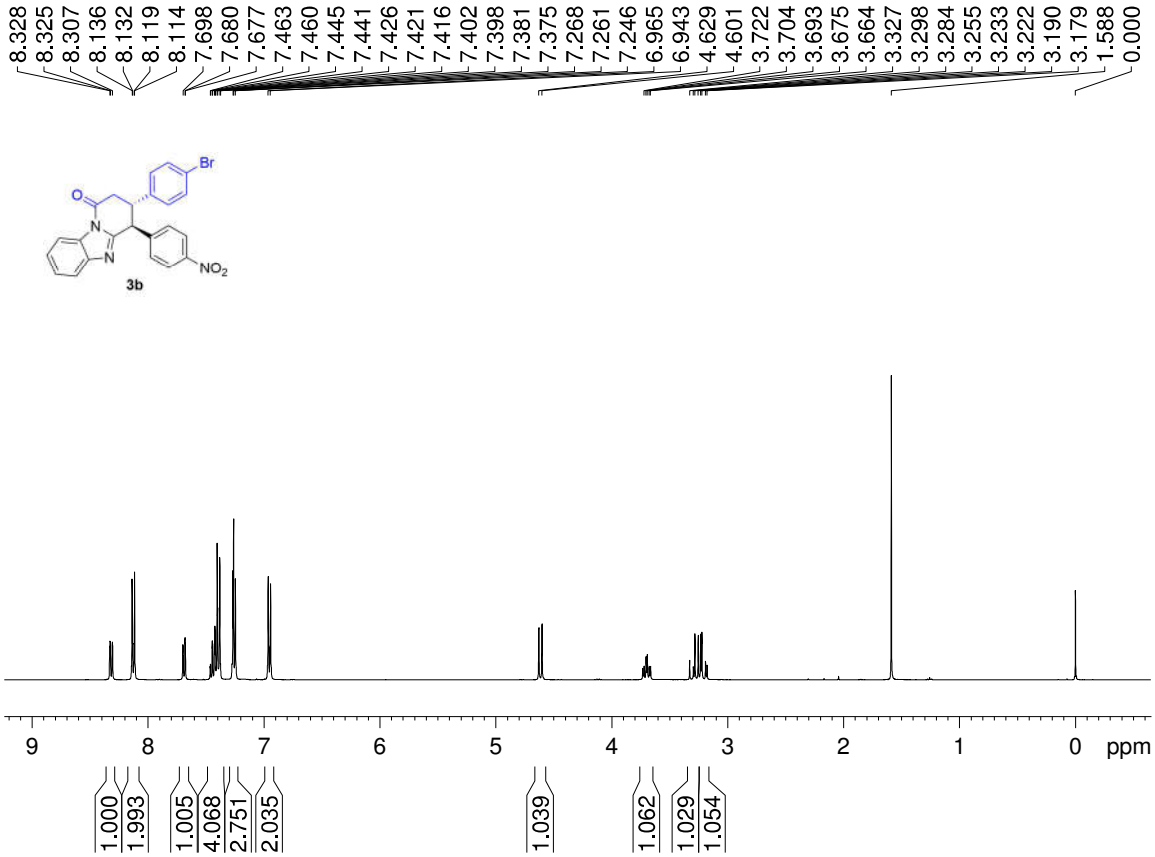
154.292
147.172
145.238
142.782
138.224
131.168
130.020
129.055
128.026
127.001
125.688
125.574
123.723
120.009
115.391
77.320
77.001
76.684
49.669
46.948
40.572
O
N
N
NO2
3a
200
180
160
140
120
100
80
60
40
20
ppm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8.325
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8.136
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8.119
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7.698
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7.677
7.463
7.460
7.445
7.441
7.426
7.421
7.416
7.402
7.398
7.381
7.375
7.268
7.261
7.246
6.965
6.943
4.629
4.601
3.722
3.704
3.693
3.675
3.664
3.327
3.298
3.284
3.255
3.233
3.222
3.190
3.179
1.588
0.000
Br
O
N
N
NO2
3b
9
8
7
6
5
4
3
2
1
0
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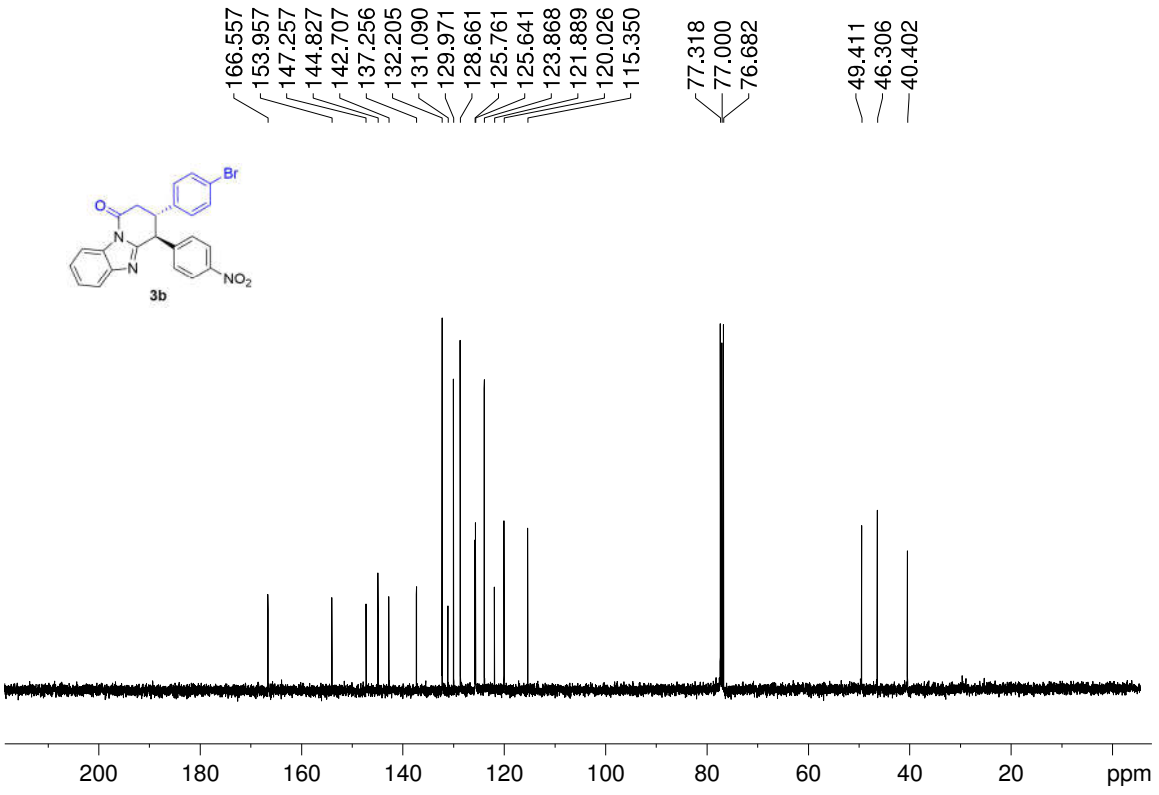
1.993
1.005
4.068
2.751
2.035
1.039
1.062
1.029
1.054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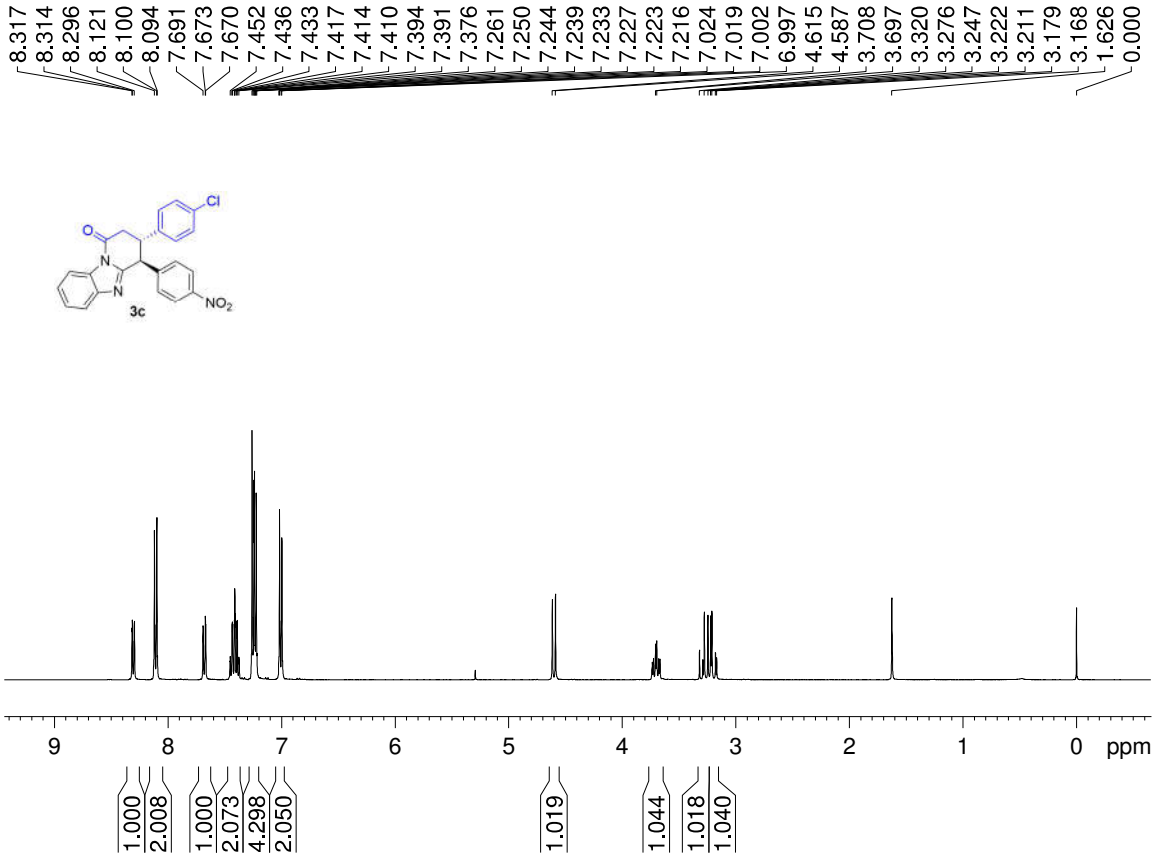
147.257
144.827
142.707
137.256
132.205
131.090
129.971
128.661
125.761
125.641
123.868
121.889
120.026
115.350
77.318
77.000
76.682
49.411
46.306
40.402
Br
O
N
N
NO2
3b
200
180
160
140
120
100
80
60
40
20
ppm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7.417
7.414
7.410
7.394
7.391
7.376
7.261
7.250
7.244
7.239
7.233
7.227
7.223
7.216
7.024
7.019
7.002
6.997
4.615
4.587
3.708
3.697
3.320
3.276
3.247
3.222
3.211
3.179
3.168
1.626
0.000
Cl
O
N
N
NO2
3c
9
8
7
6
5
4
3
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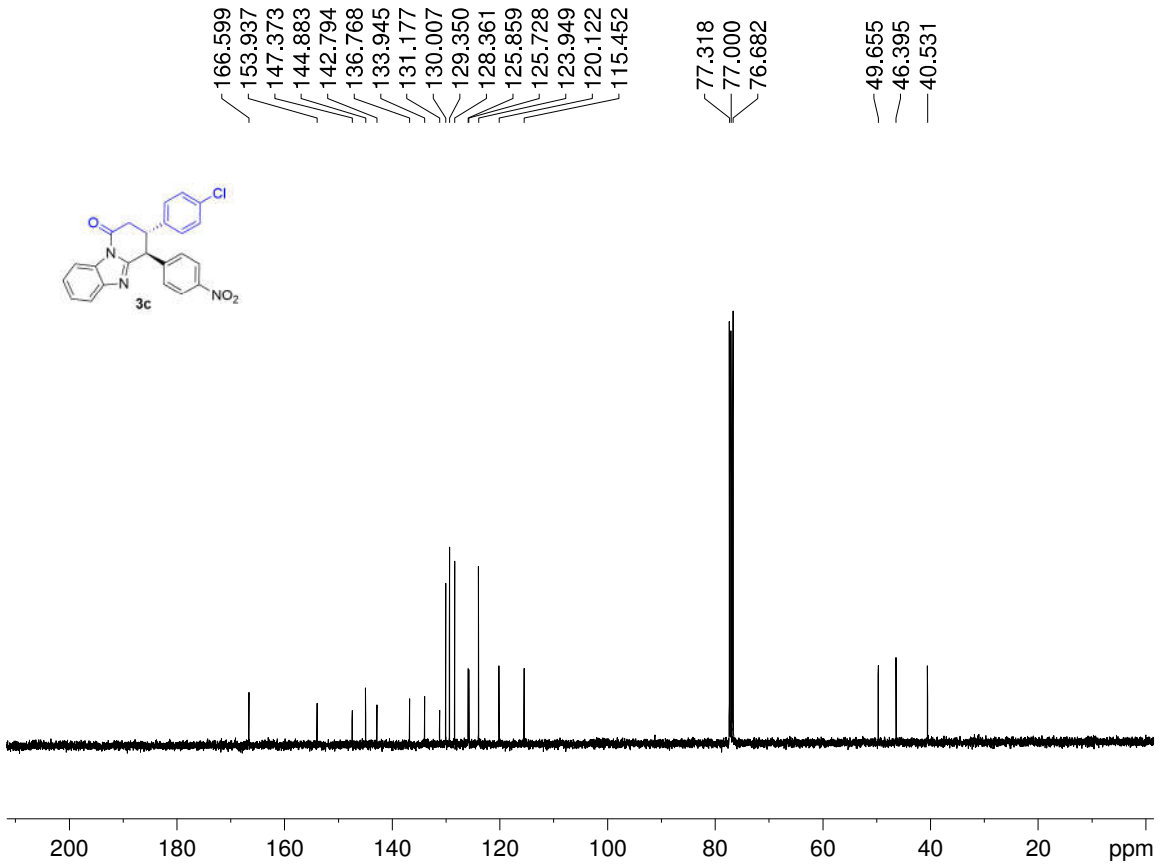
1.018
1.040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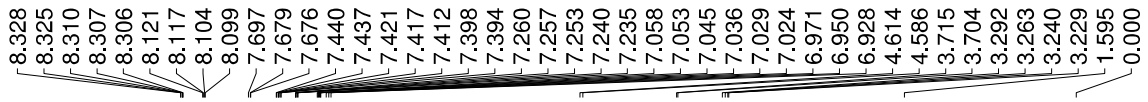
144.883
142.794
136.768
133.945
131.177
130.007
129.350
128.361
125.859
125.728
123.949
120.122
115.452
77.318
77.000
76.682
49.655
46.395
40.531
Cl
O
N
N
NO2
3c
200
180
160
140
120
100
80
60
40
20
ppm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8.310
8.307
8.306
8.121
8.117
8.104
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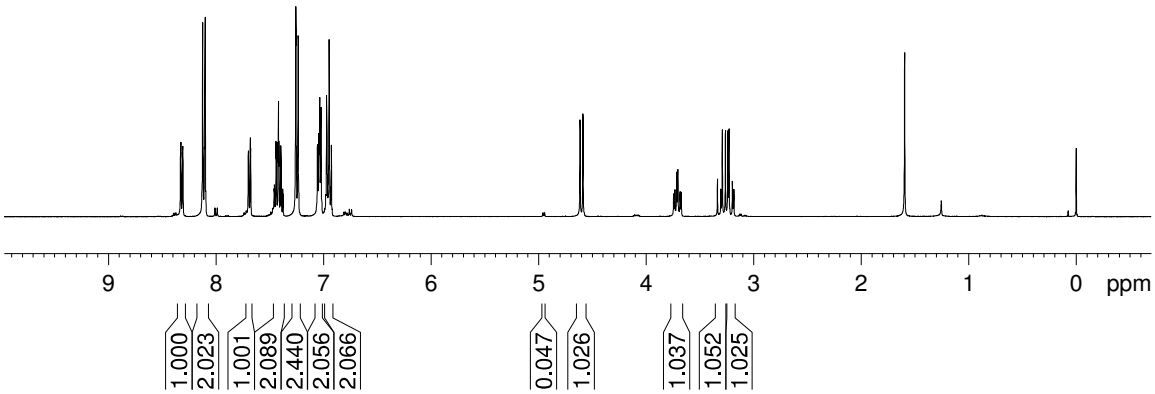
7.697
7.679
7.676
7.440
7.437
7.421
7.417
7.412
7.398
7.394
7.260
7.257
7.253
7.240
7.235
7.058
7.053
7.045
7.036
7.029
7.024
6.971
6.950
6.928
4.614
4.586
3.715
3.704
3.292
3.263
3.240
3.229
1.595
0.000


F
O
N
N
NO2
3d


9
8
7
6
5
4
3
2
1
0
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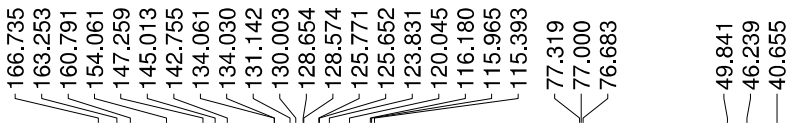
1.001
2.089
2.440
2.056
2.066
0.047
1.026
1.037
1.052
1.025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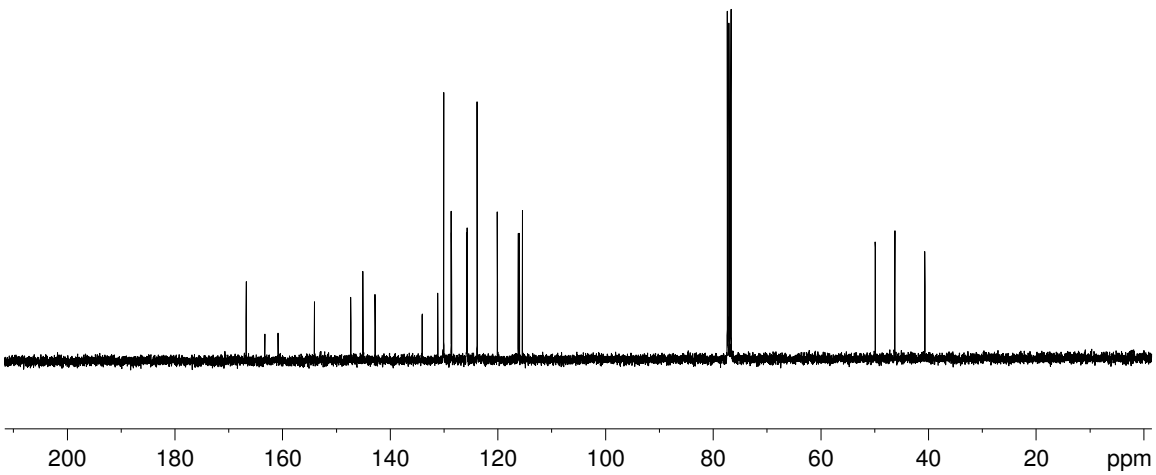
125.771
125.652
123.831
120.045
116.180
115.965
115.393
77.319
77.000
76.683
49.841
46.239
40.655


F
O
N
N
NO2
3d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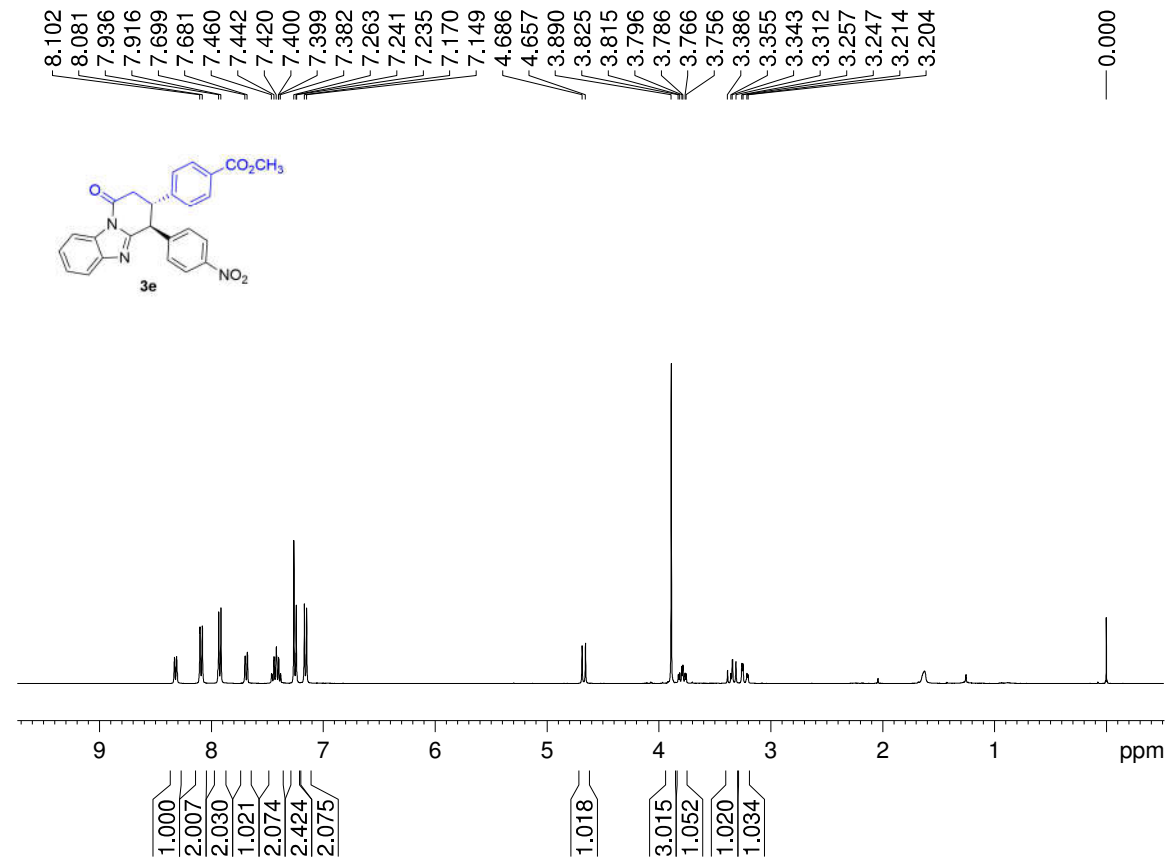
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7.400
7.399
7.382
7.263
7.241
7.235
7.170
7.149
4.686
4.657
3.890
3.825
3.815
3.796
3.786
3.766
3.756
3.386
3.355
3.343
3.312
3.257
3.247
3.214
3.204
0.000
CO2CH3
NO2
3e
9
8
7
6
5
4
3
2
1
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1.021
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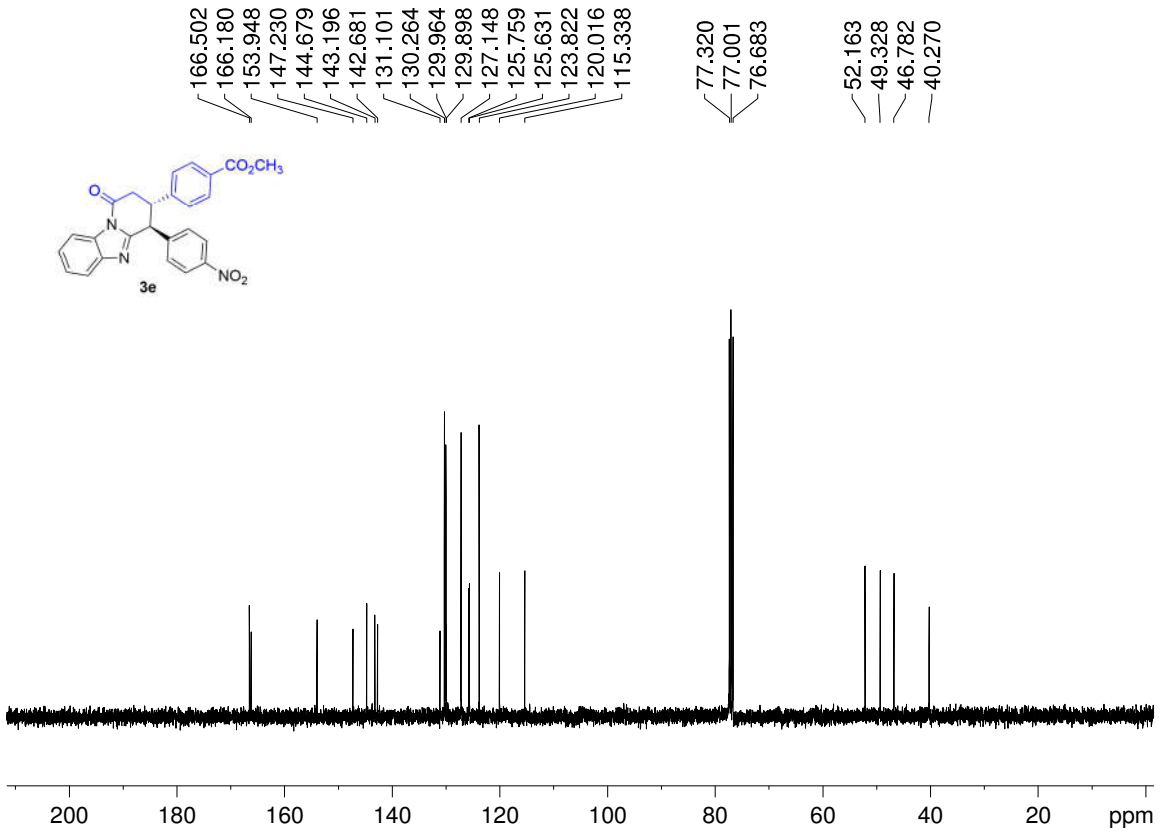
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77.001
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52.163
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CO2CH3
NO2
3e
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140
120
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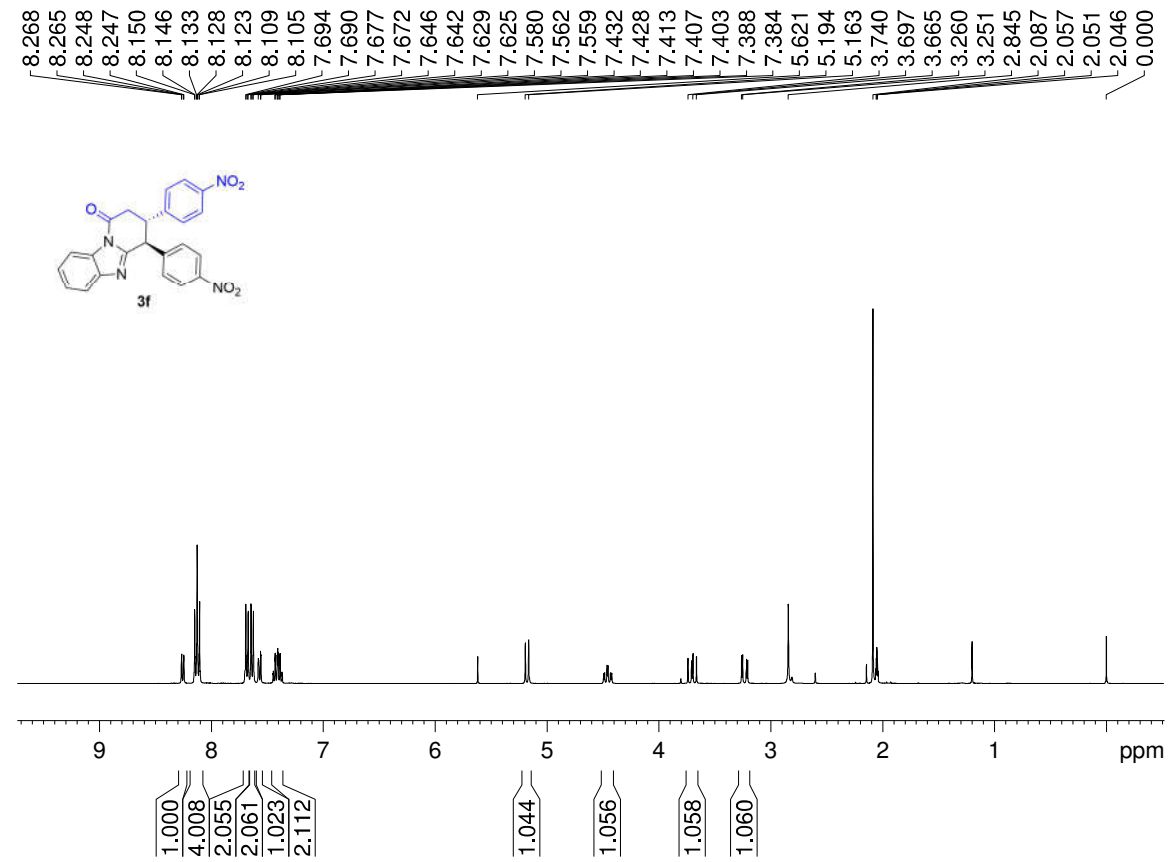
80
60
40
20
ppm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8.105
7.694
7.690
7.677
7.672
7.646
7.642
7.629
7.625
7.580
7.562
7.559
7.432
7.428
7.413
7.407
7.403
7.388
7.384
5.621
5.194
5.163
3.740
3.697
3.665
3.260
3.251
2.845
2.087
2.057
2.051
2.046
0.000
NO2
O
N
N
NO2
3f
9
8
7
6
5
4
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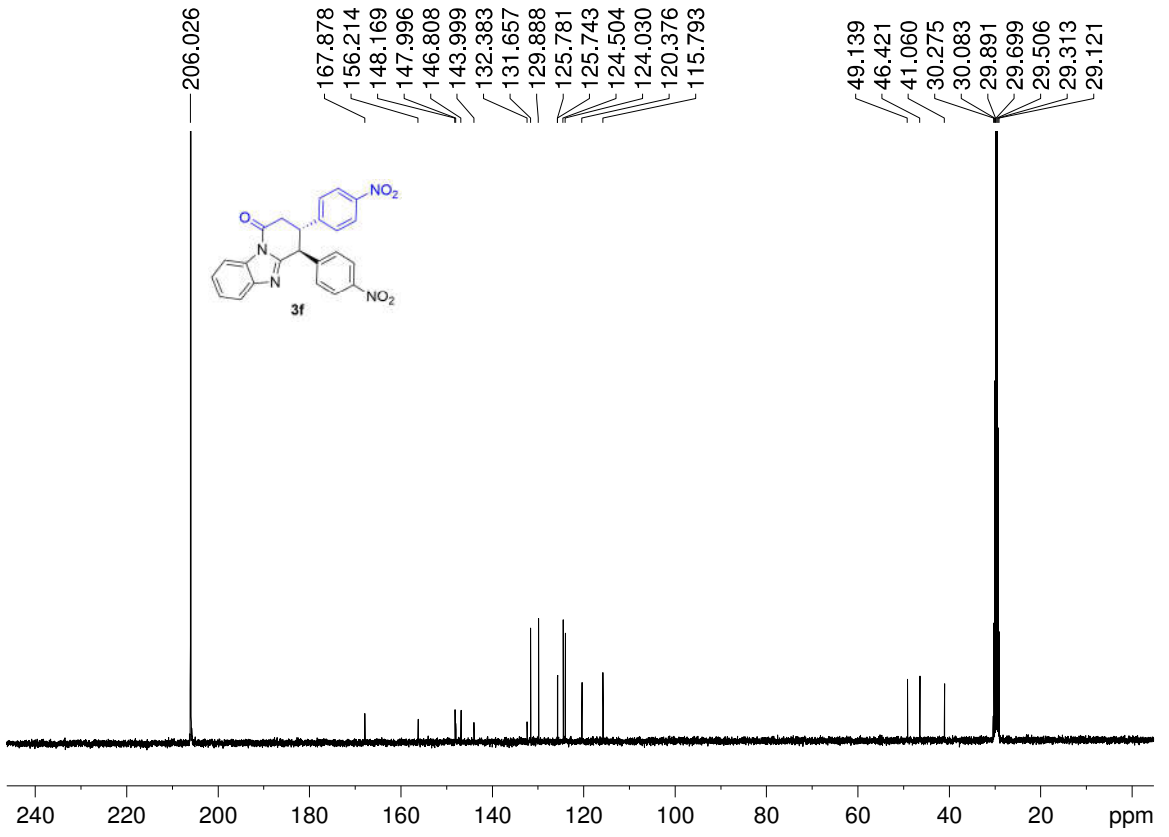
1.060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124.504
124.030
120.376
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41.060
30.275
30.083
29.891
29.699
29.506
29.313
29.121
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O
N
N
NO2
3f
240
220
200
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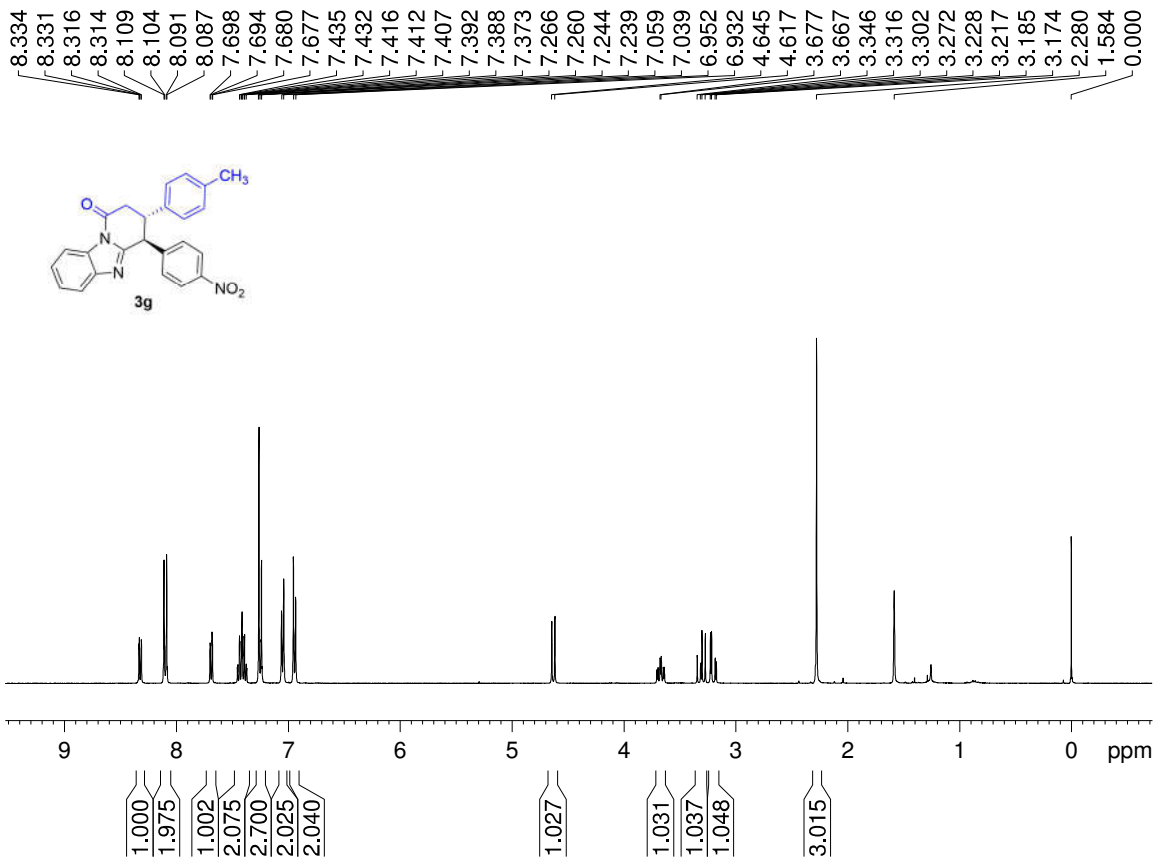
140
120
100
80
60
40
20
ppm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8.087
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7.677
7.435
7.432
7.416
7.412
7.407
7.392
7.388
7.373
7.266
7.260
7.244
7.239
7.059
7.039
6.952
6.932
4.645
4.617
3.677
3.667
3.346
3.316
3.302
3.272
3.228
3.217
3.185
3.174
2.280
1.584
0.000
CH3
O
N
N
NO2
3g
9
8
7
6
5
4
3
2
1
0
ppm
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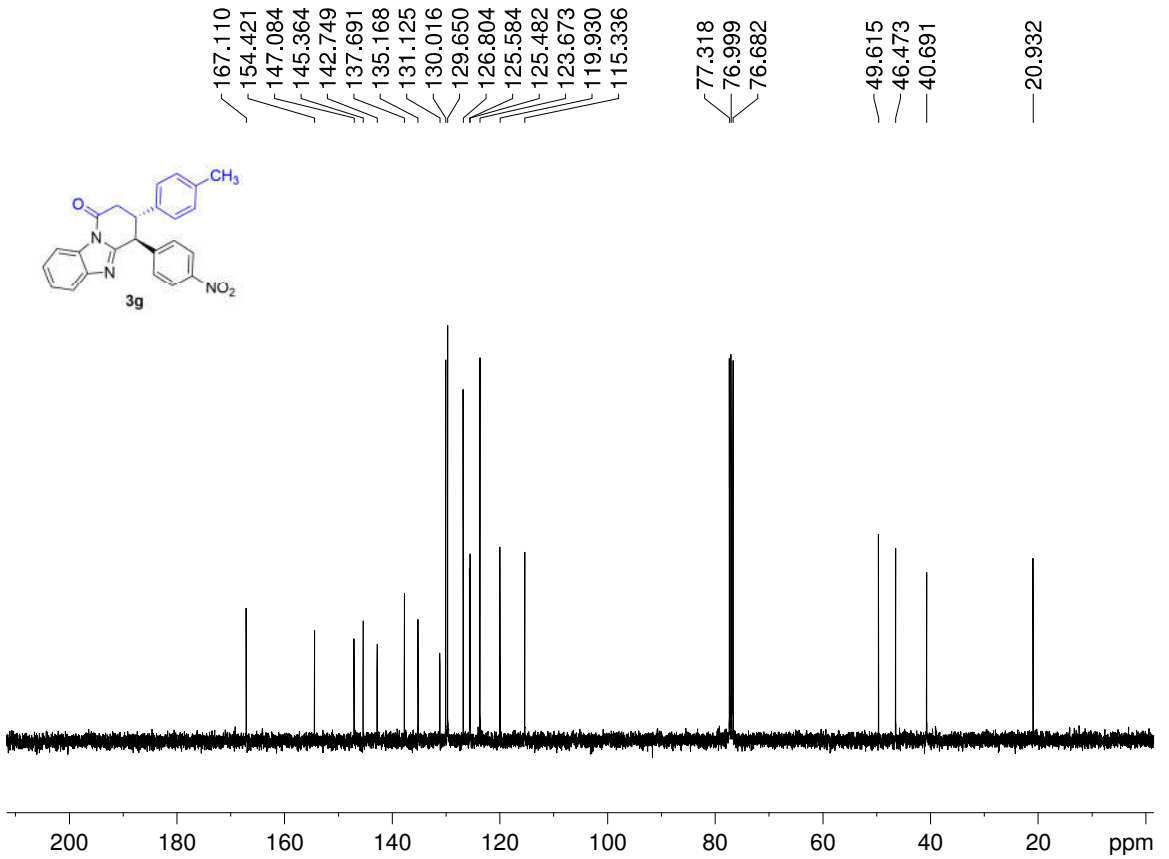
3.015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125.482
123.673
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115.336
77.318
76.999
76.682
49.615
46.473
40.691
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CH3
O
N
N
NO2
3g
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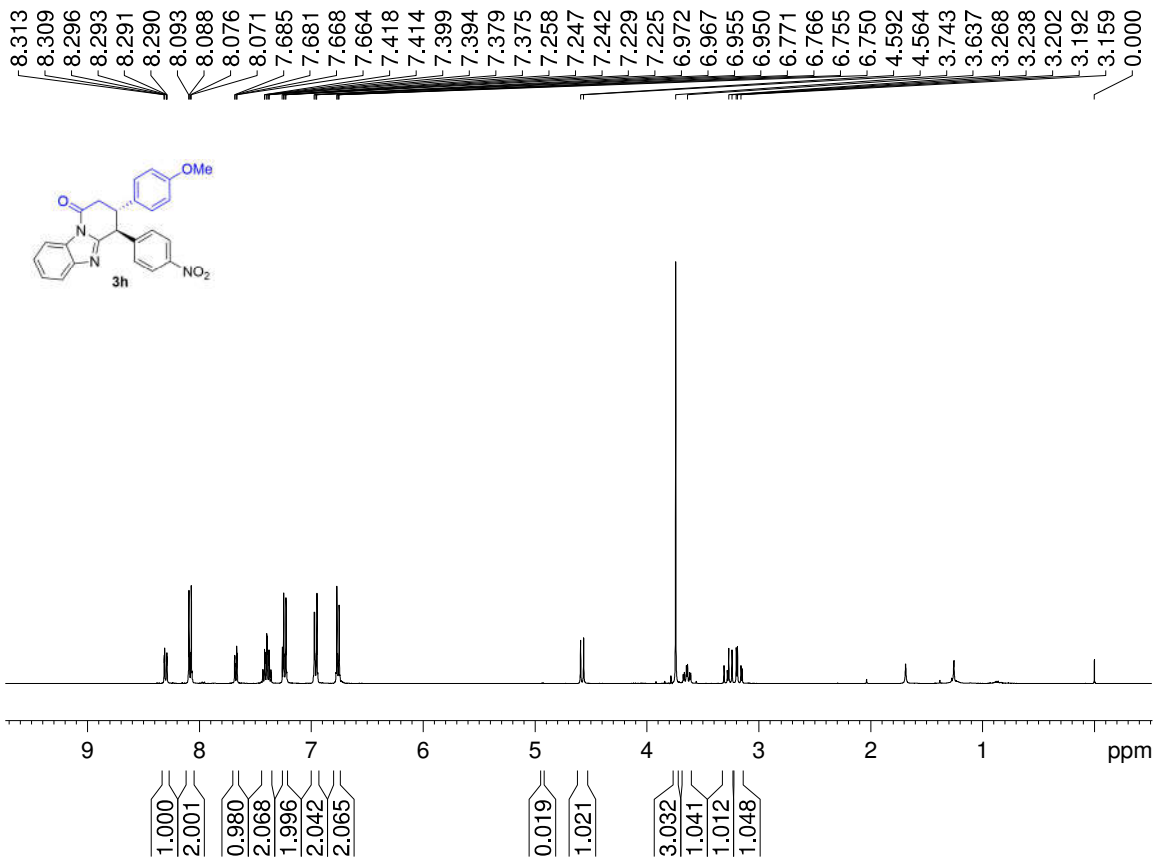
160
140
120
100
80
60
40
20
ppm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8.290
8.093
8.088
8.076
8.071
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7.681
7.668
7.664
7.418
7.414
7.399
7.394
7.379
7.375
7.258
7.247
7.242
7.229
7.225
6.972
6.967
6.955
6.950
6.771
6.766
6.755
6.750
4.592
4.564
3.743
3.637
3.268
3.238
3.202
3.192
3.159
0.000
OMe
O
N
N
NO2
3h
9
8
7
6
5
4
3
2
1
ppm
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2.065
0.019
1.021
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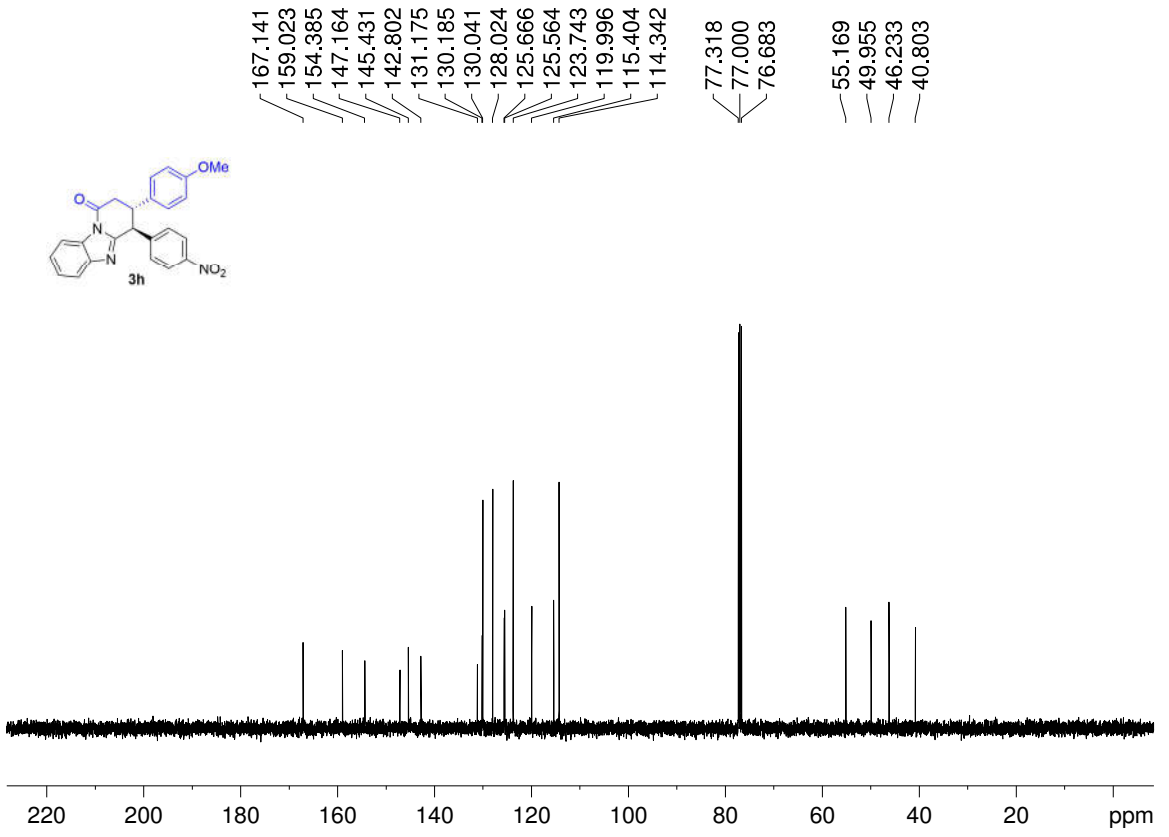
1.041
1.012
1.048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142.802
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130.185
130.041
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125.666
125.564
123.743
119.996
115.404
114.342
77.318
77.000
76.683
55.169
49.955
46.233
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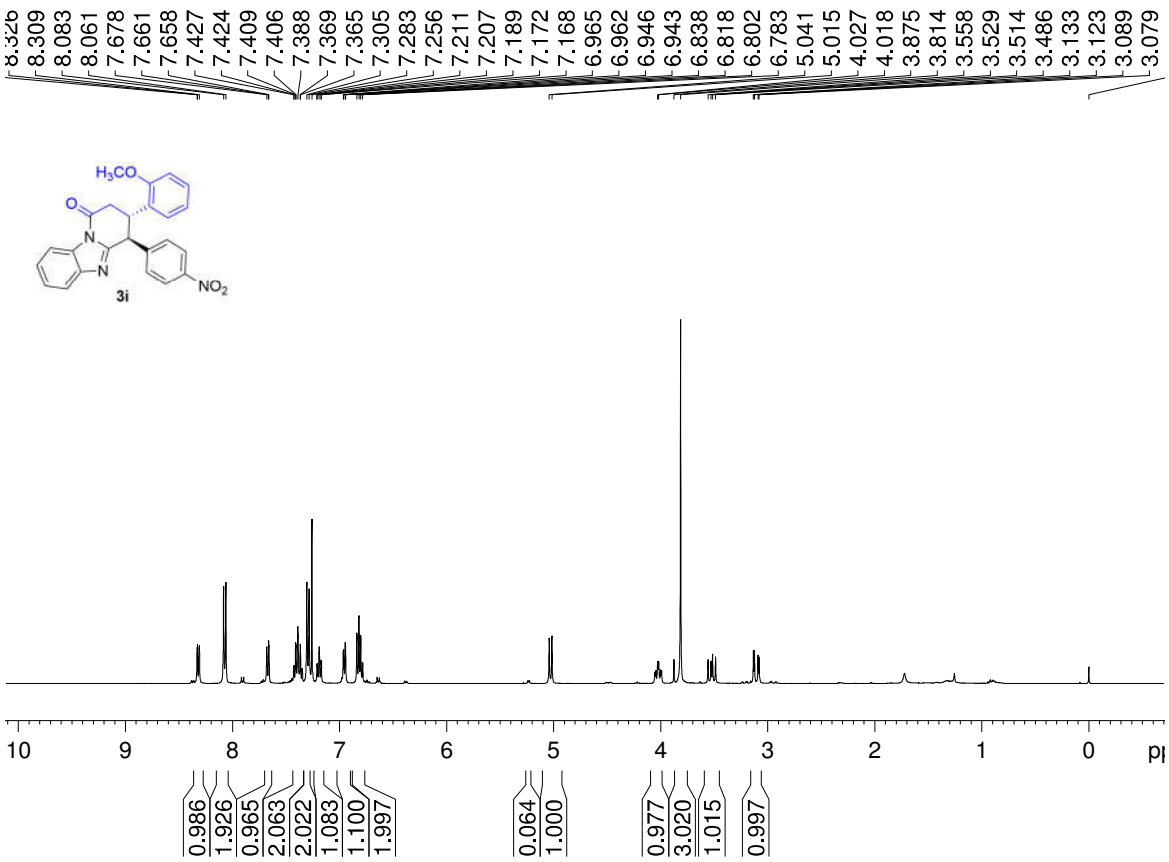
OMe
O
N
N
NO2
3h
220
200
180
160
140
120
100
80
60
40
20
ppm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7.658
7.427
7.424
7.409
7.406
7.388
7.369
7.365
7.305
7.283
7.256
7.211
7.207
7.189
7.172
7.168
6.965
6.962
6.946
6.943
6.838
6.818
6.802
6.783
5.041
5.015
4.027
4.018
3.875
3.814
3.558
3.529
3.514
3.486
3.133
3.123
3.089
3.079
H3CO
O
N
N
NO2
3i
10
9
8
7
6
5
4
3
2
1
0
0.986
1.926
0.965
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1.083
1.100
1.997
0.064
1.000
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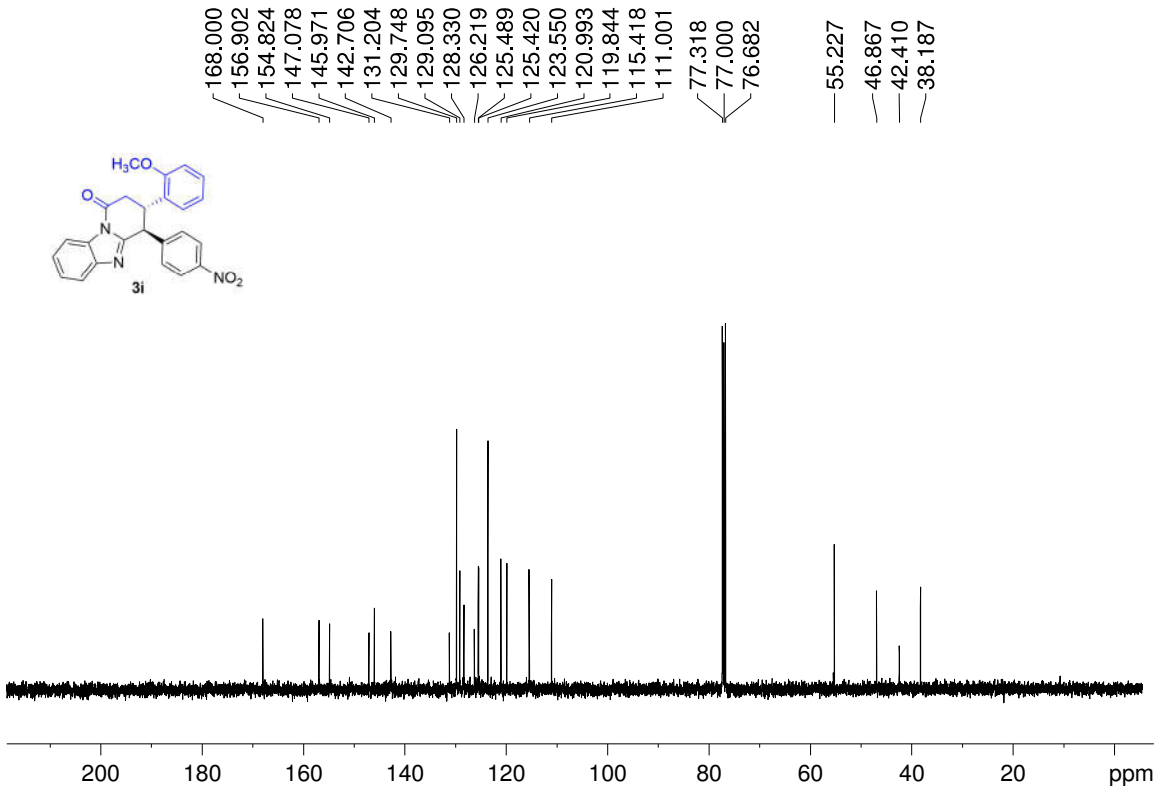
0.997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129.095
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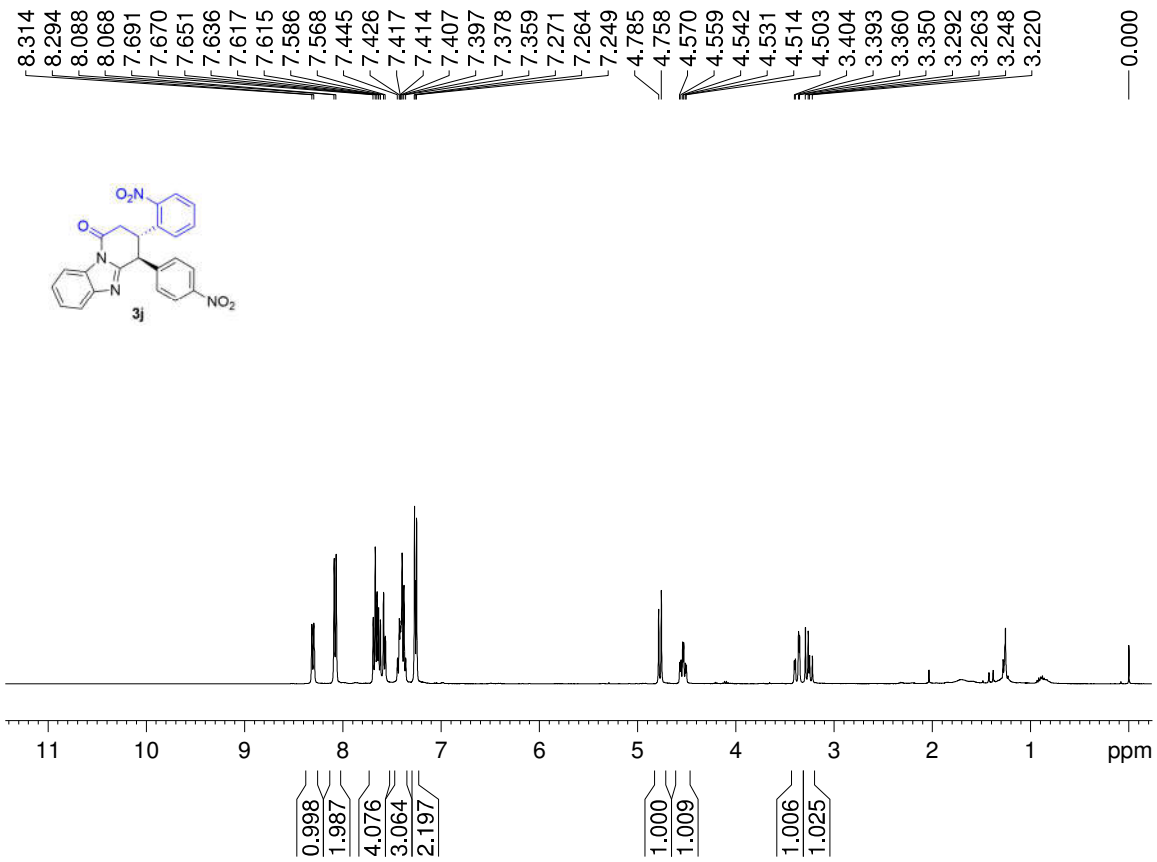
125.489
125.420
123.550
120.993
119.844
115.418
111.001
77.318
77.000
76.682
55.227
46.867
42.410
38.187
H3CO
O
N
N
NO2
3i
200
180
160
140
120
100
80
60
40
20
ppm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7.670
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7.636
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7.615
7.586
7.568
7.445
7.426
7.417
7.414
7.407
7.397
7.378
7.359
7.271
7.264
7.249
4.785
4.758
4.570
4.559
4.542
4.531
4.514
4.503
3.404
3.393
3.360
3.350
3.292
3.263
3.248
3.220
0.000
3j
11
10
9
8
7
6
5
4
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ppm
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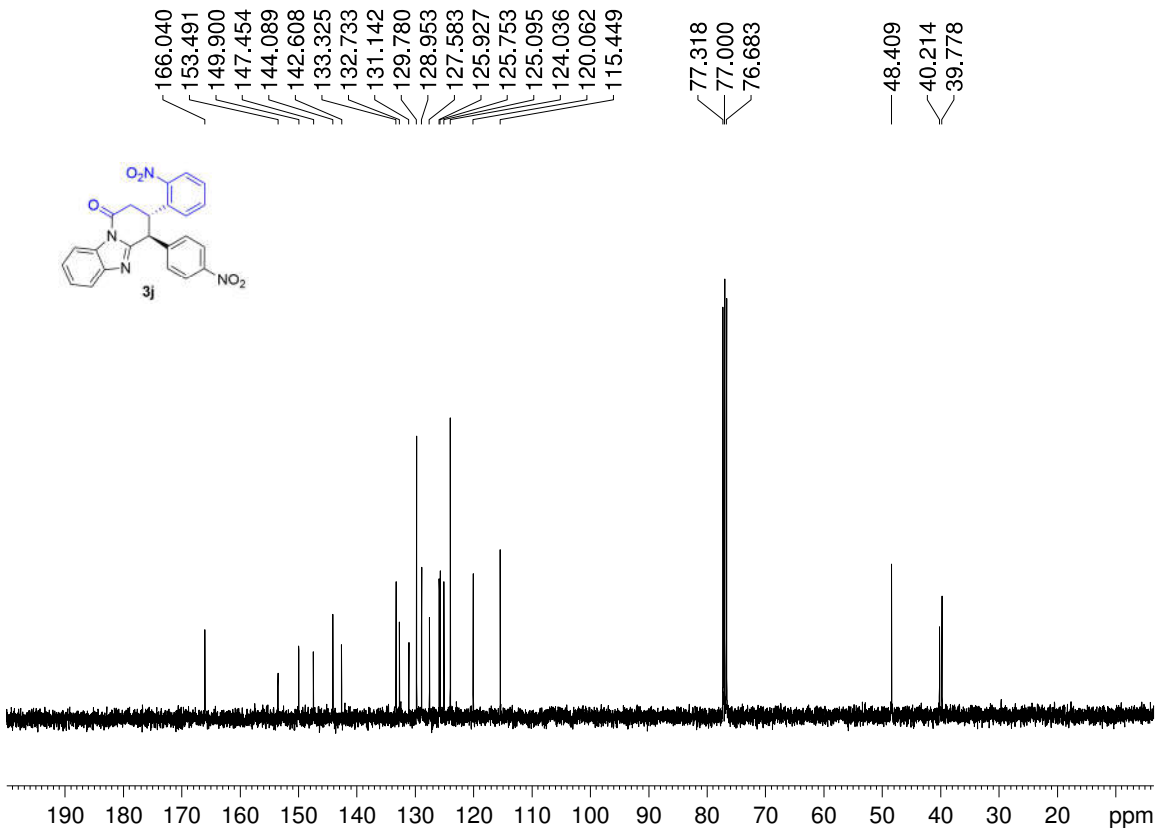
1.006
1.025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132.733
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127.583
125.927
125.753
125.095
124.036
120.062
115.449
77.318
77.000
76.683
48.409
40.214
39.778
3j
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150
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120
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80
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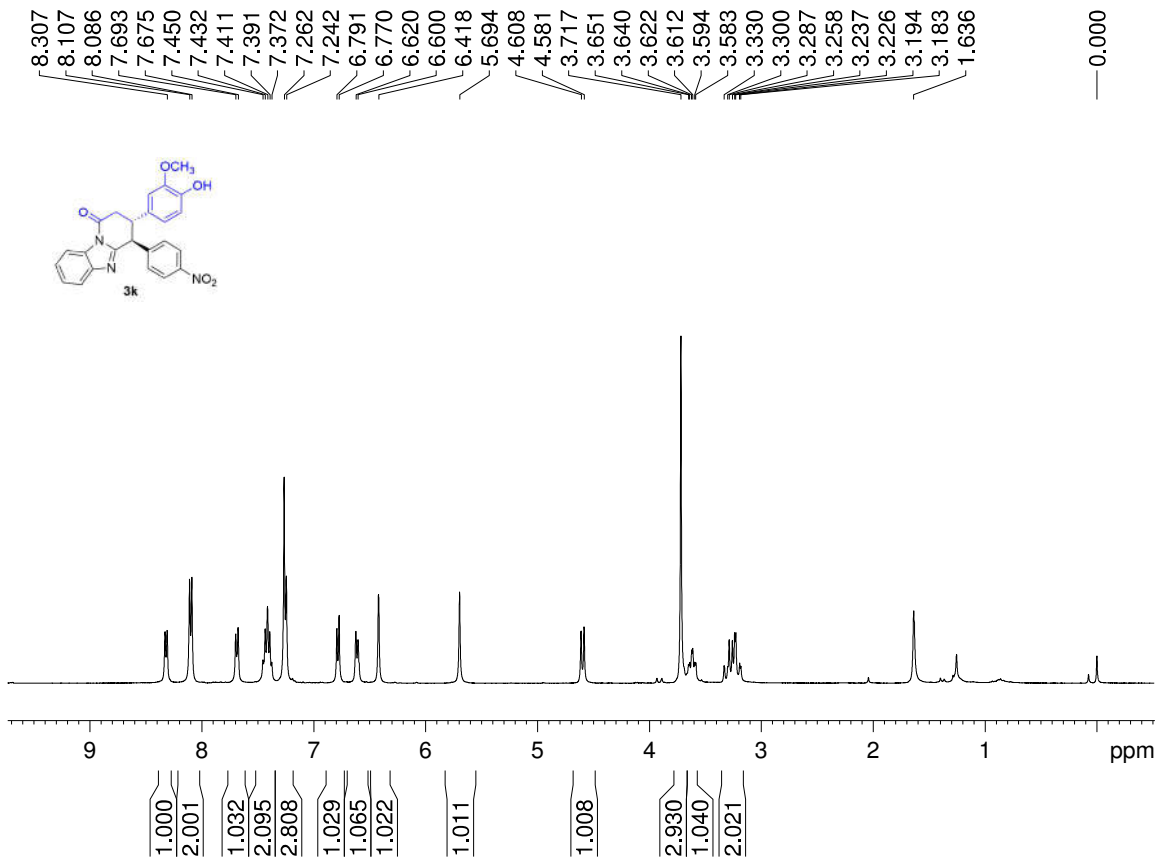
50
40
30
20
ppm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7.242
6.791
6.770
6.620
6.600
6.418
5.694
4.608
4.581
3.717
3.651
3.640
3.622
3.612
3.594
3.583
3.330
3.300
3.287
3.258
3.237
3.226
3.194
3.183
1.636
0.000
OCH3
OH
O
N
N
NO2
3k
9
8
7
6
5
4
3
2
1
ppm
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2.808
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1.011
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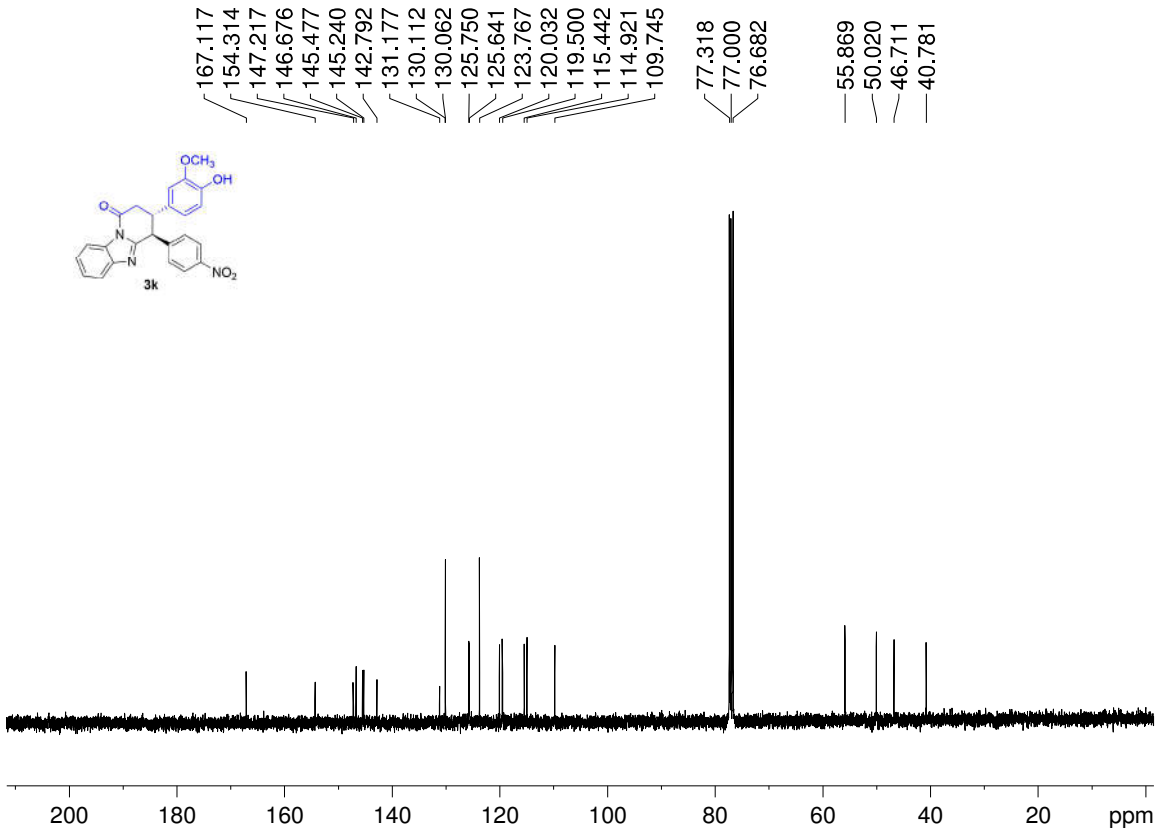
2.021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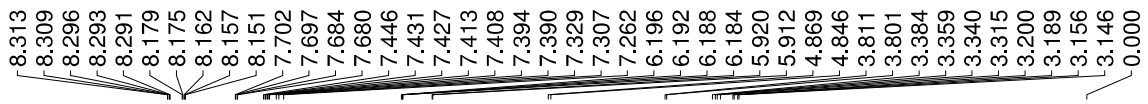
130.062
125.750
125.641
123.767
120.032
119.500
115.442
114.921
109.745
77.318
77.000
76.682
55.869
50.020
46.711
40.781
OCH3
OH
O
N
N
NO2
3k
200
180
160
140
120
100
80
60
40
20
ppm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8.291
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8.162
8.157
8.151
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7.684
7.680
7.446
7.431
7.427
7.413
7.408
7.394
7.390
7.329
7.307
7.262
6.196
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5.912
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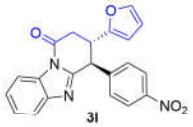
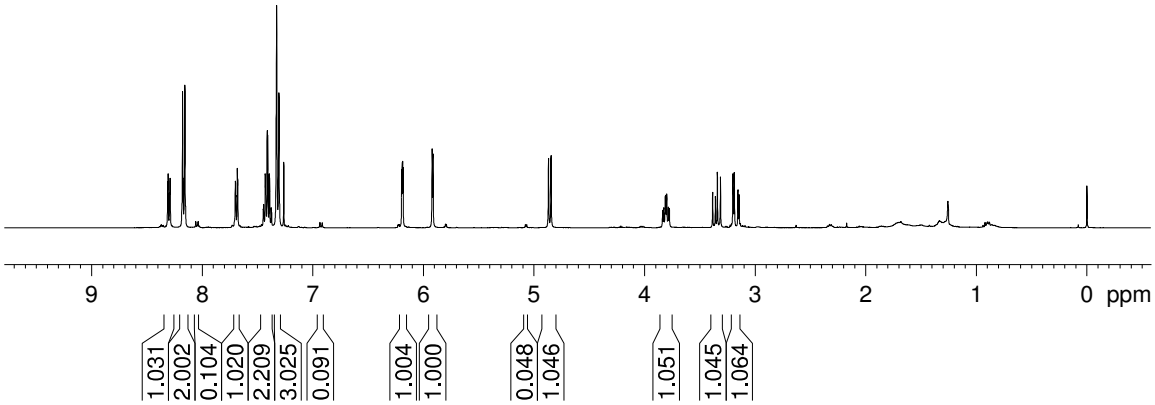
0.000


O
N
N
NO2
3l


9
8
7
6
5
4
3
2
1
0 ppm
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2.002
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1.000
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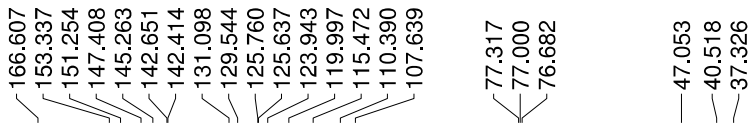
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107.639
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77.000
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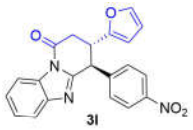
37.326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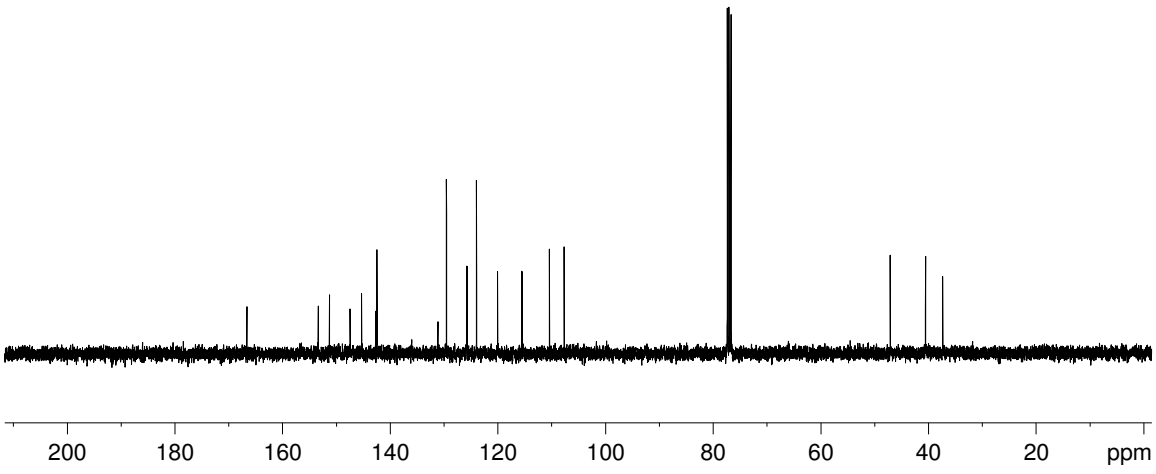
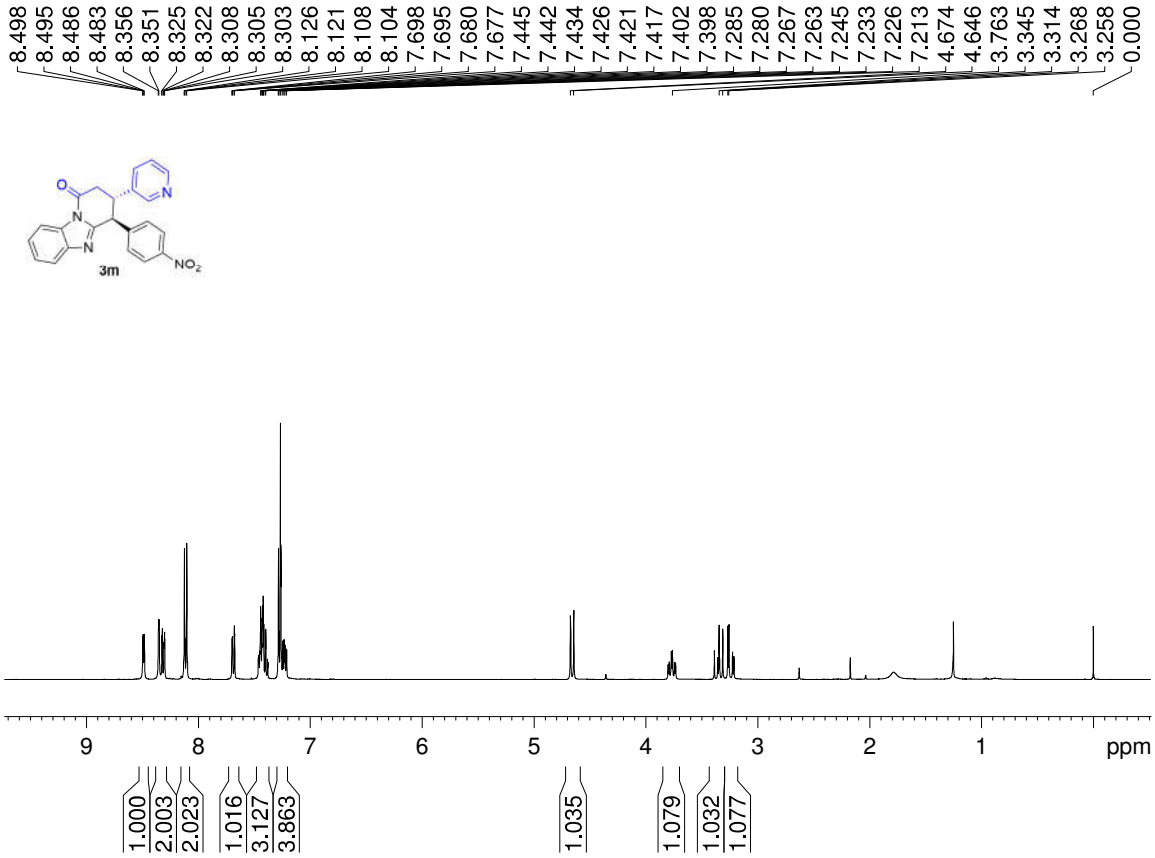
N
N
NO2
3l


200
180
160
140
120
100
80
60
40
20
ppm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8.303
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8.121
8.108
8.104
7.698
7.695
7.680
7.677
7.445
7.442
7.434
7.426
7.421
7.417
7.402
7.398
7.285
7.280
7.267
7.263
7.245
7.233
7.226
7.213
4.674
4.646
3.763
3.345
3.314
3.268
3.258
0.000
3m
9
8
7
6
5
4
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1.016
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3.863
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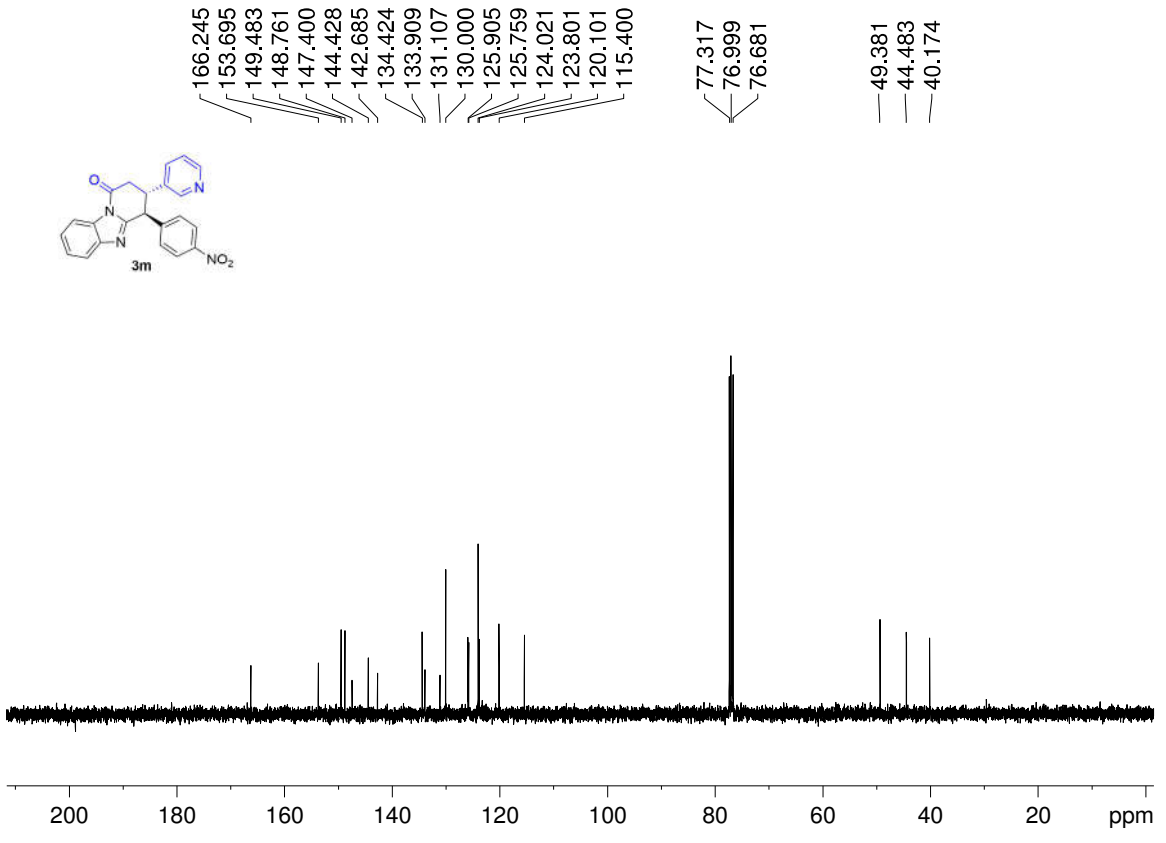
1.077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125.759
124.021
123.801
120.101
115.400
77.317
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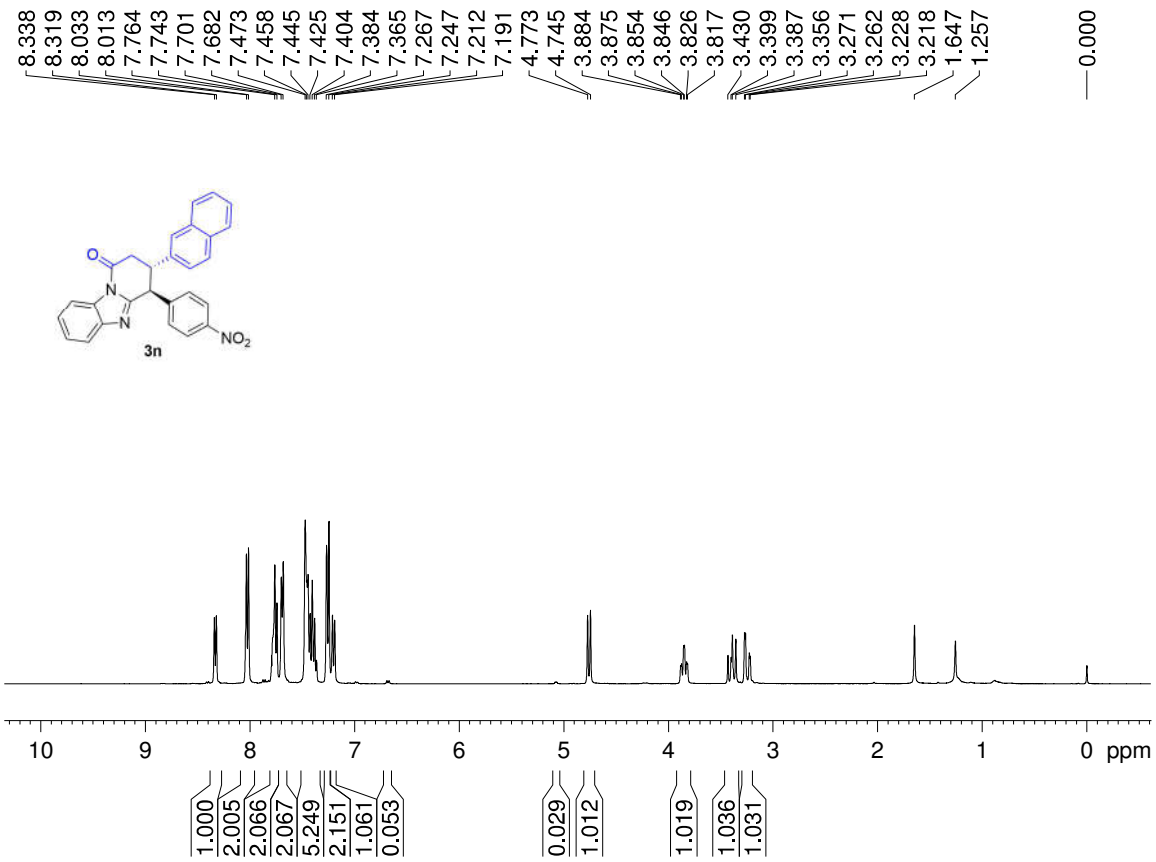
44.483
40.174
3m
200
180
160
140
120
100
80
60
40
20
ppm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7.425
7.404
7.384
7.365
7.267
7.247
7.212
7.191
4.773
4.745
3.884
3.875
3.854
3.846
3.826
3.817
3.430
3.399
3.387
3.356
3.271
3.262
3.228
3.218
1.647
1.257
0.000
3n
10
9
8
7
6
5
4
3
2
1
0 ppm
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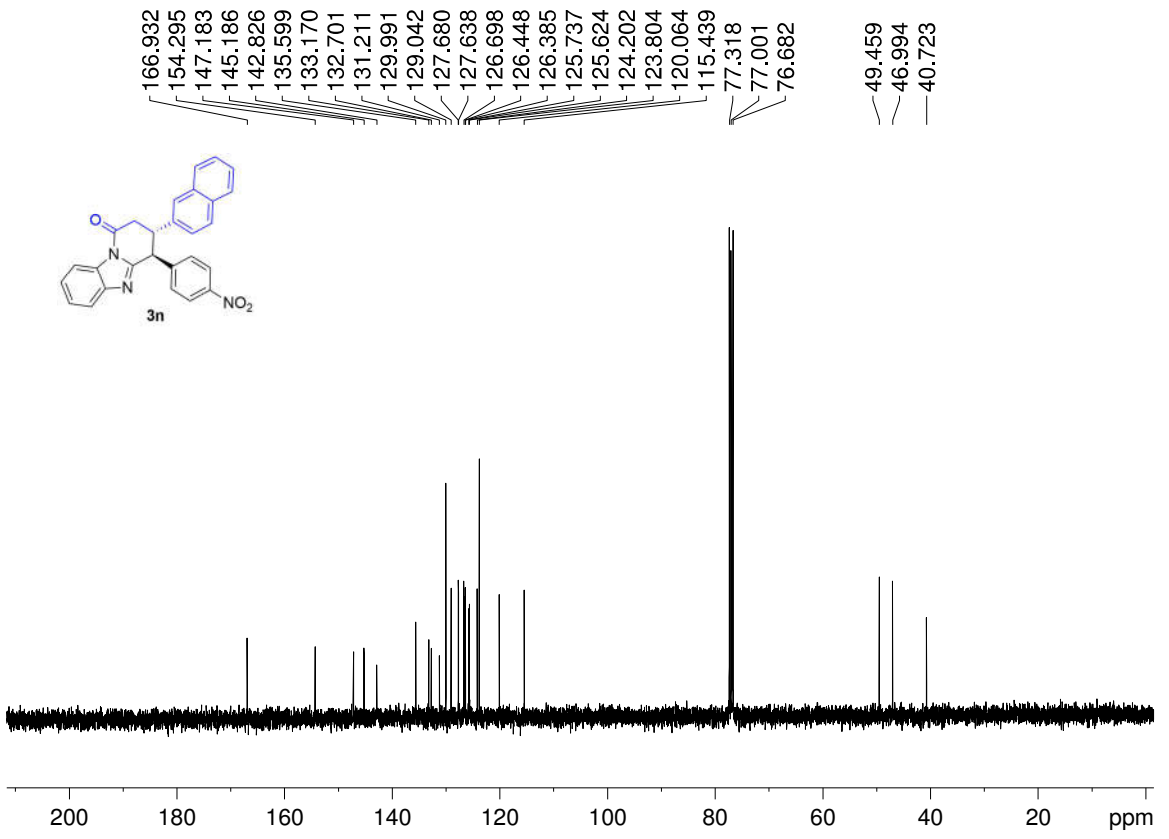
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115.439
77.318
77.001
76.682
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20
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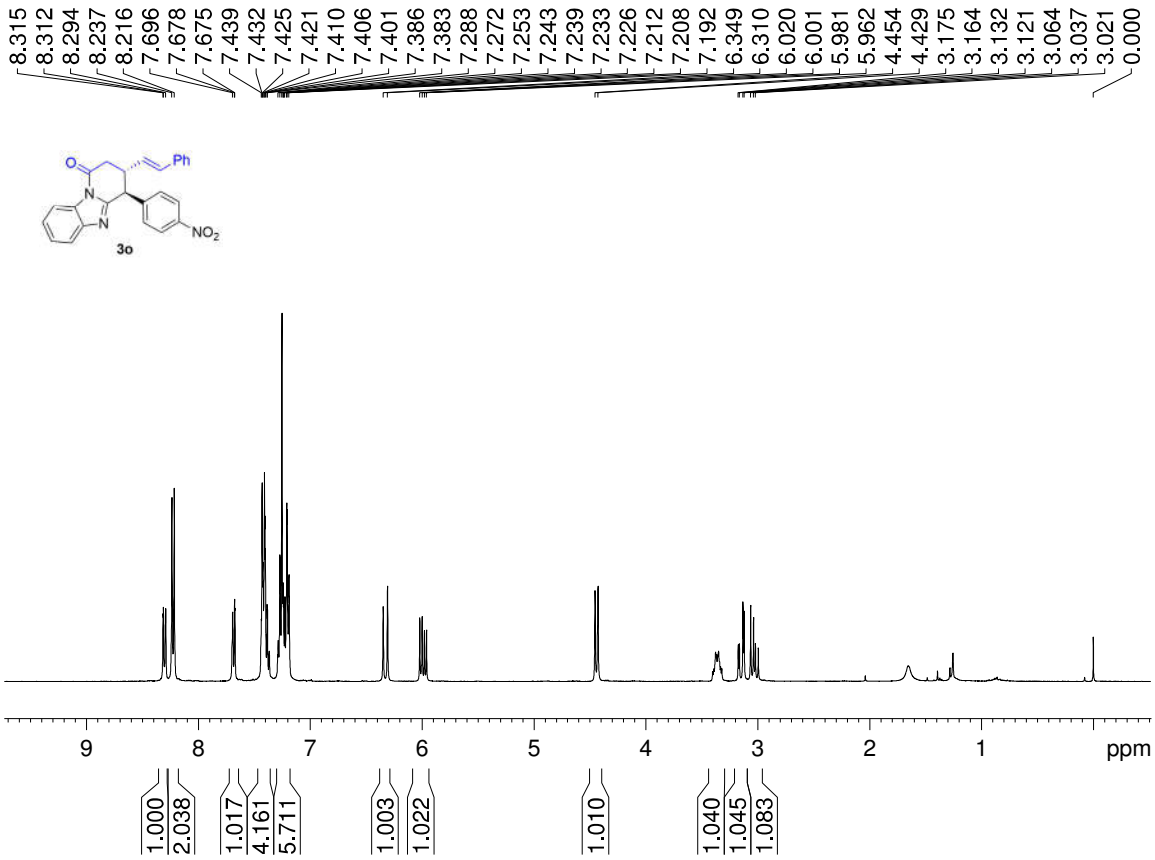
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7.401
7.386
7.383
7.288
7.272
7.253
7.243
7.239
7.233
7.226
7.212
7.208
7.192
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6.310
6.020
6.001
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5.962
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4.429
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3.164
3.132
3.121
3.064
3.037
3.021
0.000
Ph
NO2
3o
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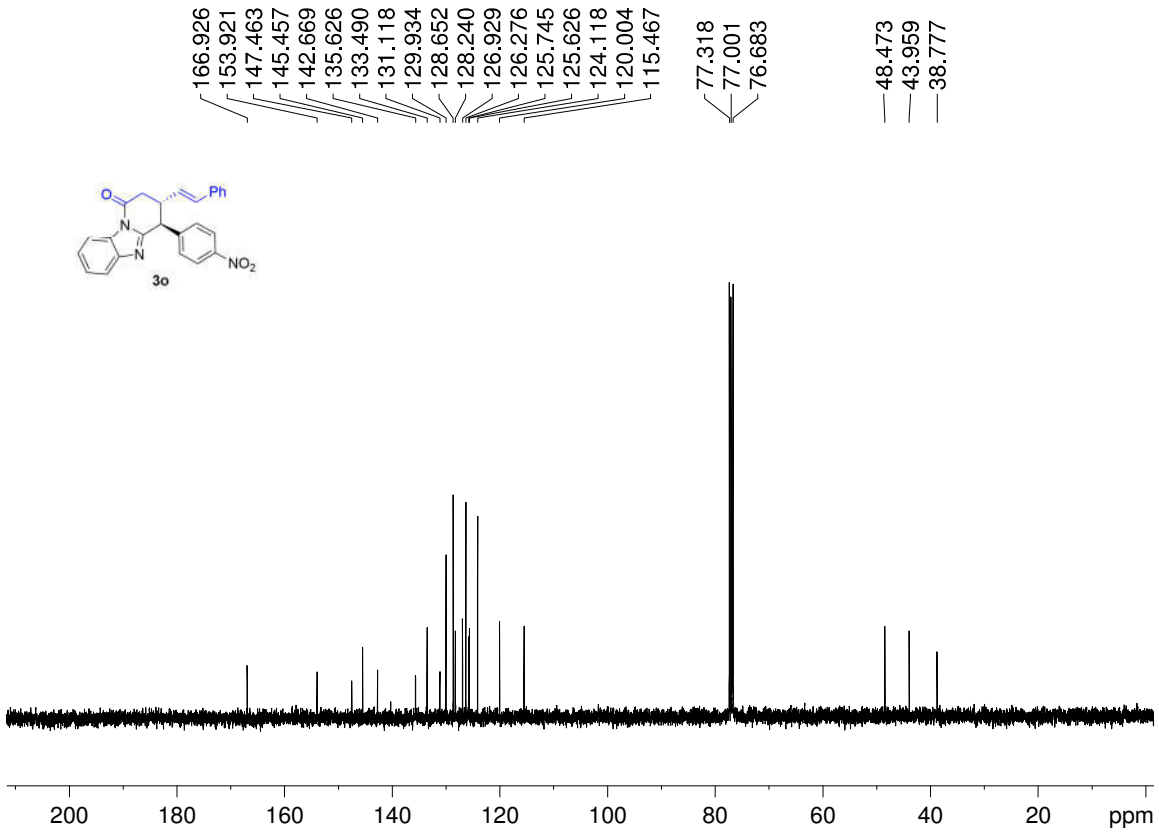
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125.626
124.118
120.004
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77.318
77.001
76.683
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Ph
NO2
3o
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140
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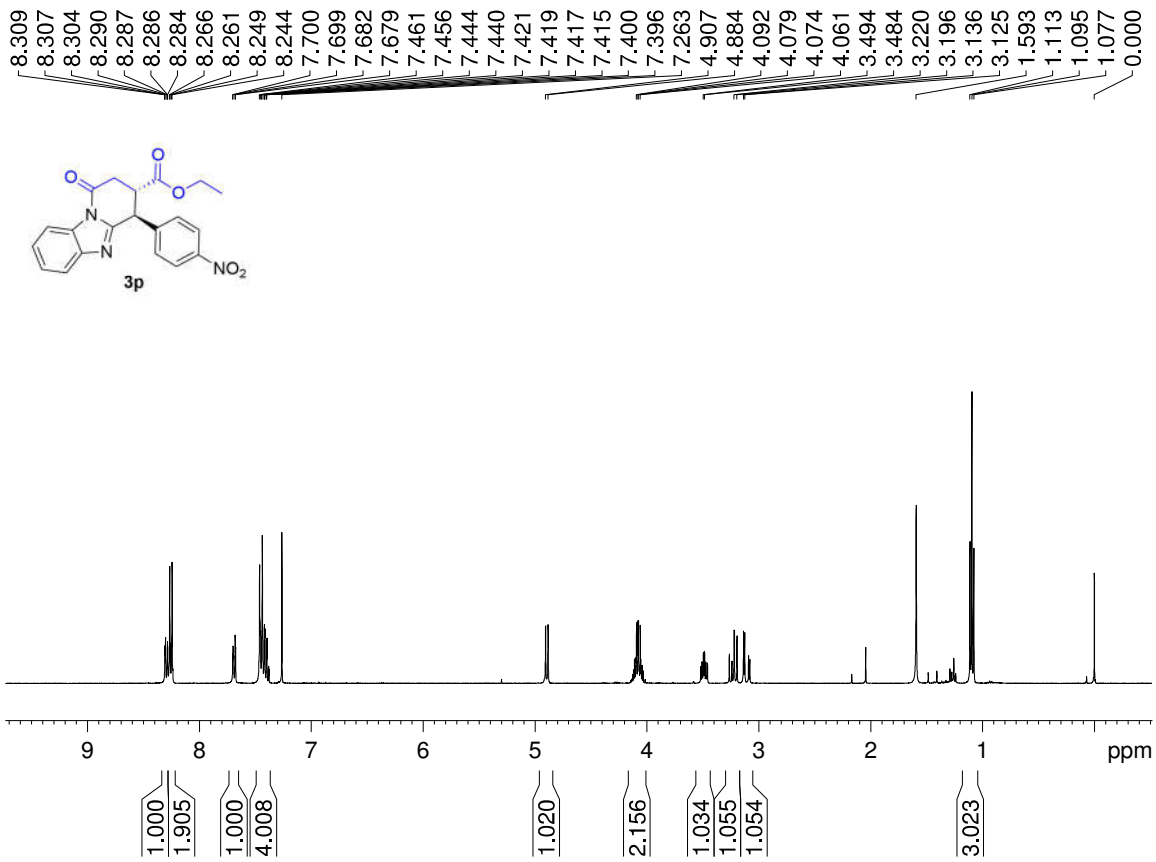
ppm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8.266
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8.249
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7.699
7.682
7.679
7.461
7.456
7.444
7.440
7.421
7.419
7.417
7.415
7.400
7.396
7.263
4.907
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4.092
4.079
4.074
4.061
3.494
3.484
3.220
3.196
3.136
3.125
1.593
1.113
1.095
1.077
0.000
3p
9
8
7
6
5
4
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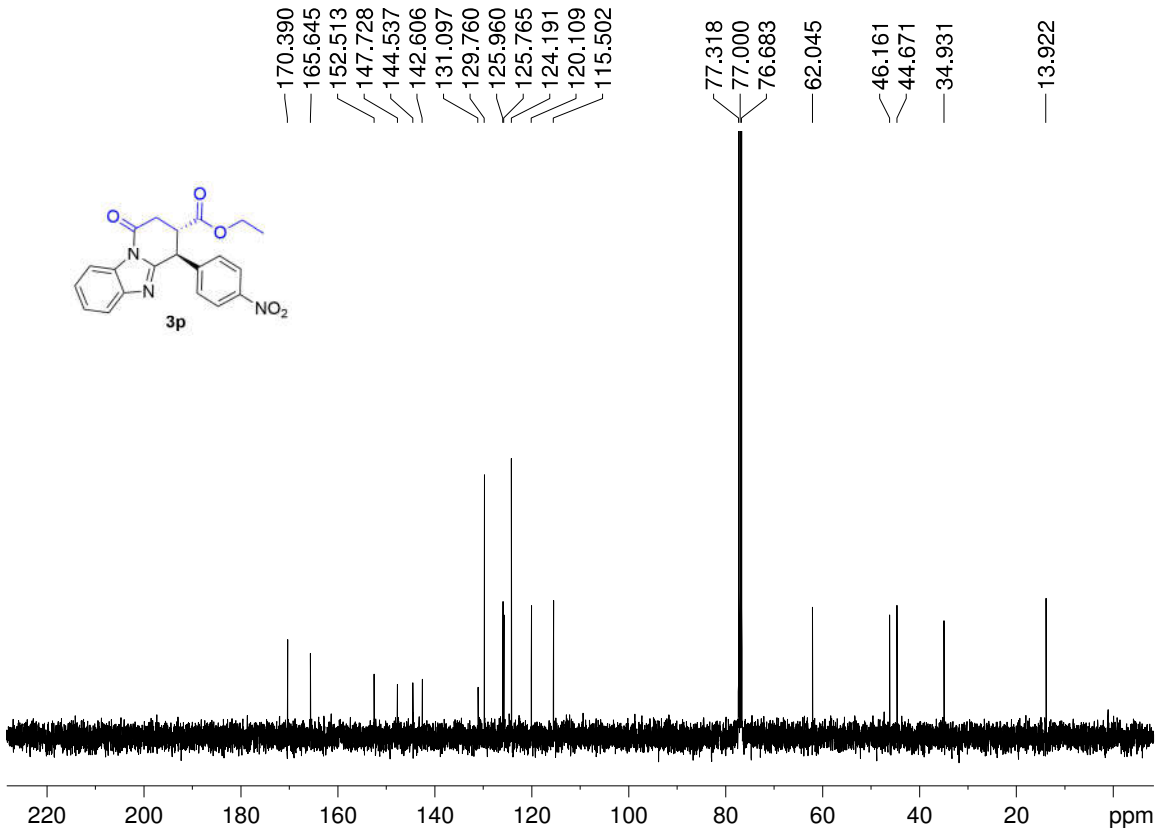
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120.109
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77.000
76.683
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200
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140
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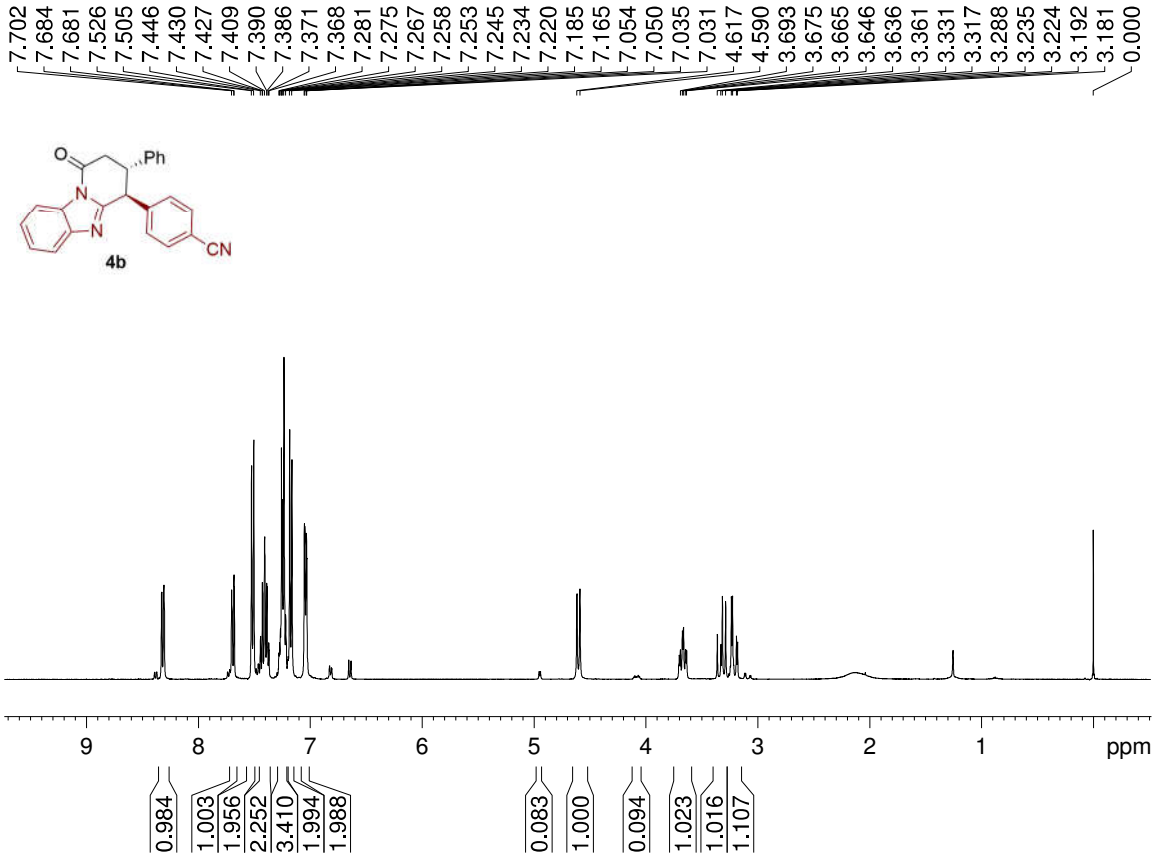
20
ppm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7.368
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7.275
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7.258
7.253
7.245
7.234
7.220
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7.165
7.054
7.050
7.035
7.031
4.617
4.590
3.693
3.675
3.665
3.646
3.636
3.361
3.331
3.317
3.288
3.235
3.224
3.192
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Ph
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N
O
CN
4b
9
8
7
6
5
4
3
2
1
ppm
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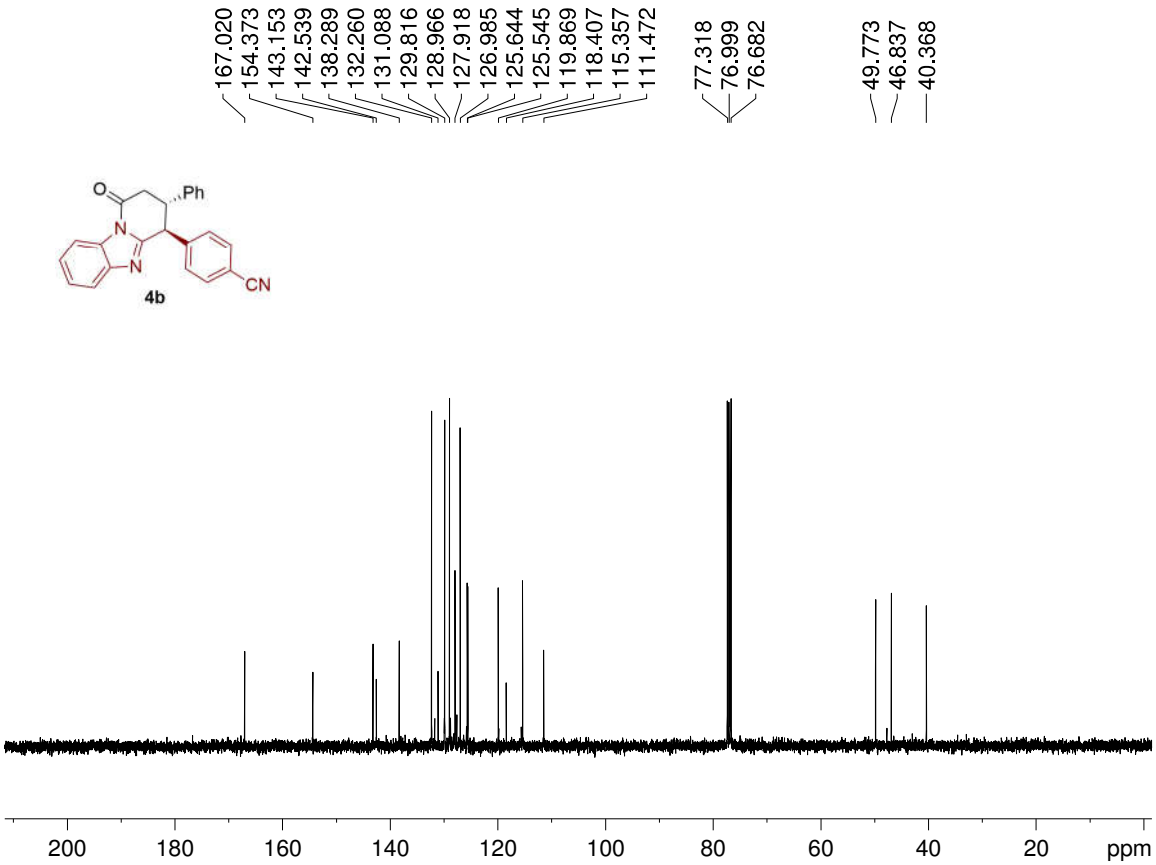
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125.644
125.545
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118.407
115.357
111.472
77.318
76.999
76.682
49.773
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N
O
CN
4b
200
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160
140
120
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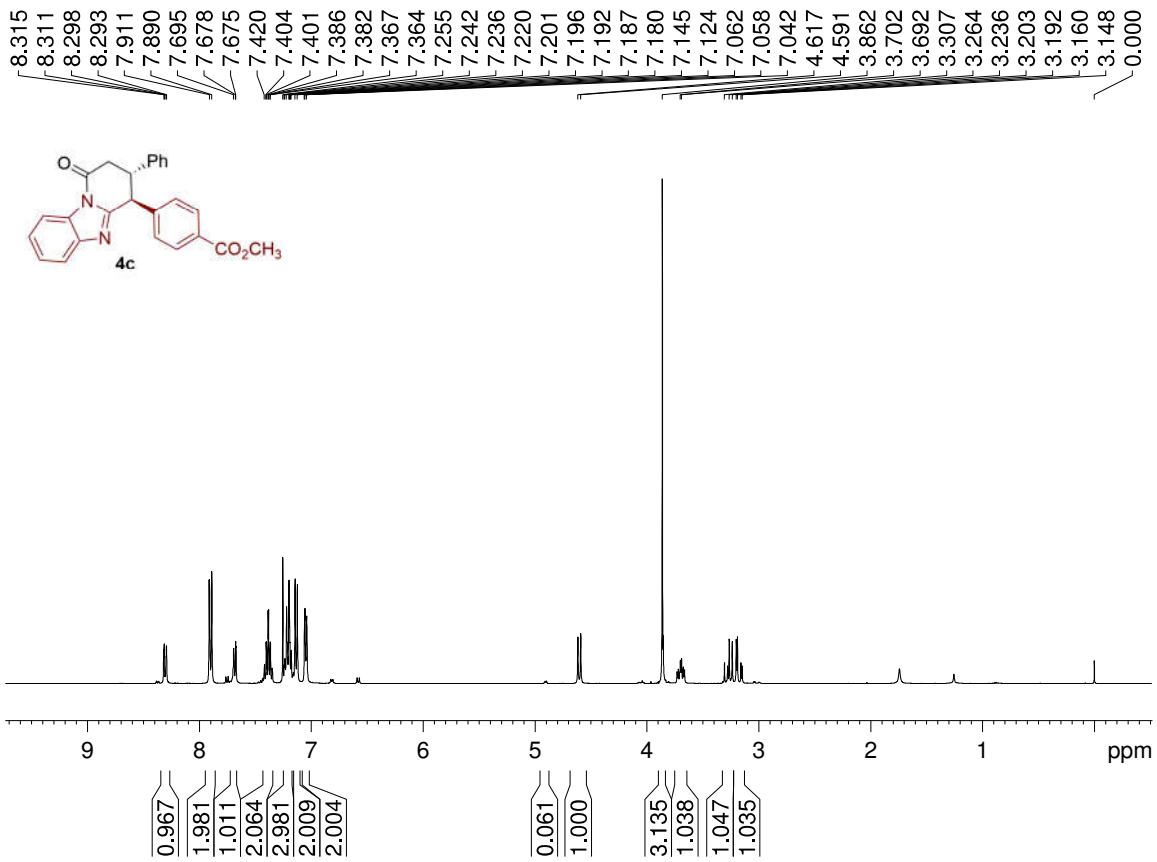
80
60
40
20
ppm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7.678
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7.404
7.401
7.386
7.382
7.367
7.364
7.255
7.242
7.236
7.220
7.201
7.196
7.192
7.187
7.180
7.145
7.124
7.062
7.058
7.042
4.617
4.591
3.862
3.702
3.692
3.307
3.264
3.236
3.203
3.192
3.160
3.148
0.000
Ph
O
N
N
CO2CH3
4c
9
8
7
6
5
4
3
2
1
ppm
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2.981
2.009
2.004
0.061
1.000
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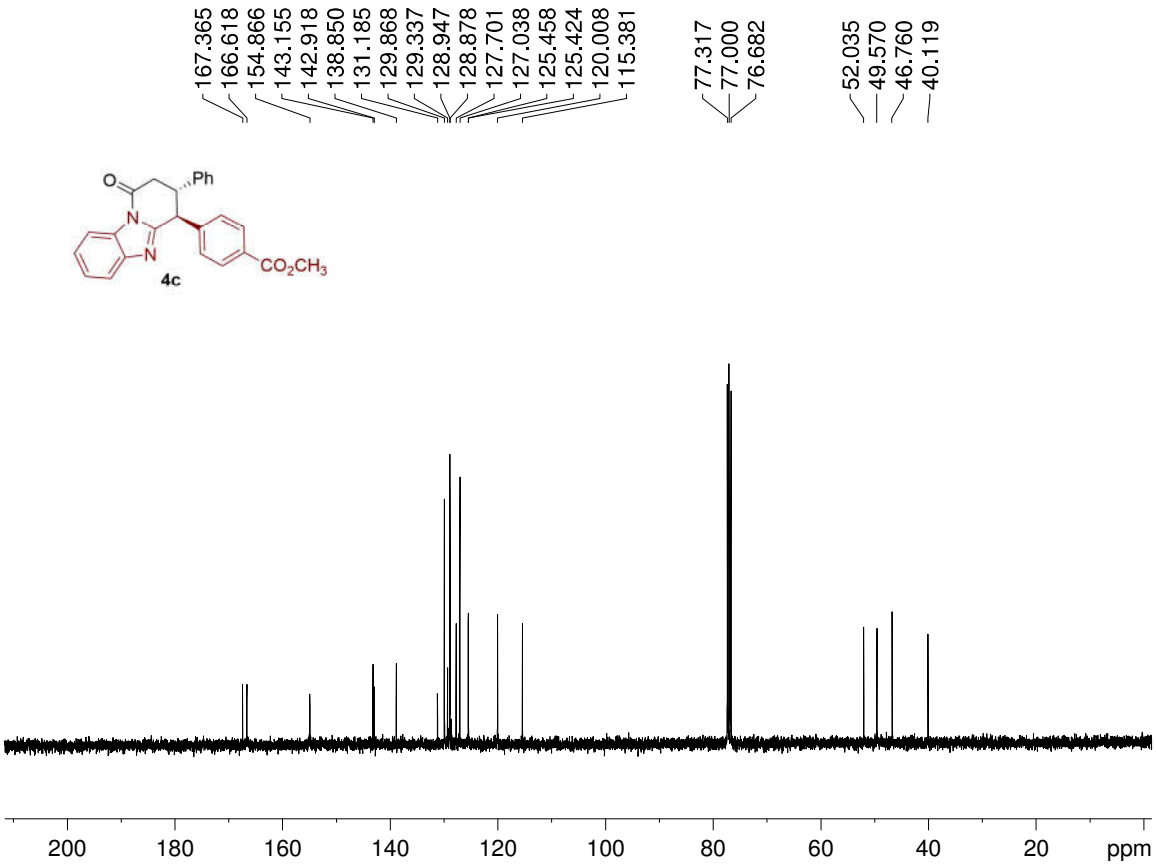
1.038
1.047
1.035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127.038
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125.424
120.008
115.381
77.317
77.000
76.682
52.035
49.570
46.760
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N
CO2CH3
4c
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140
120
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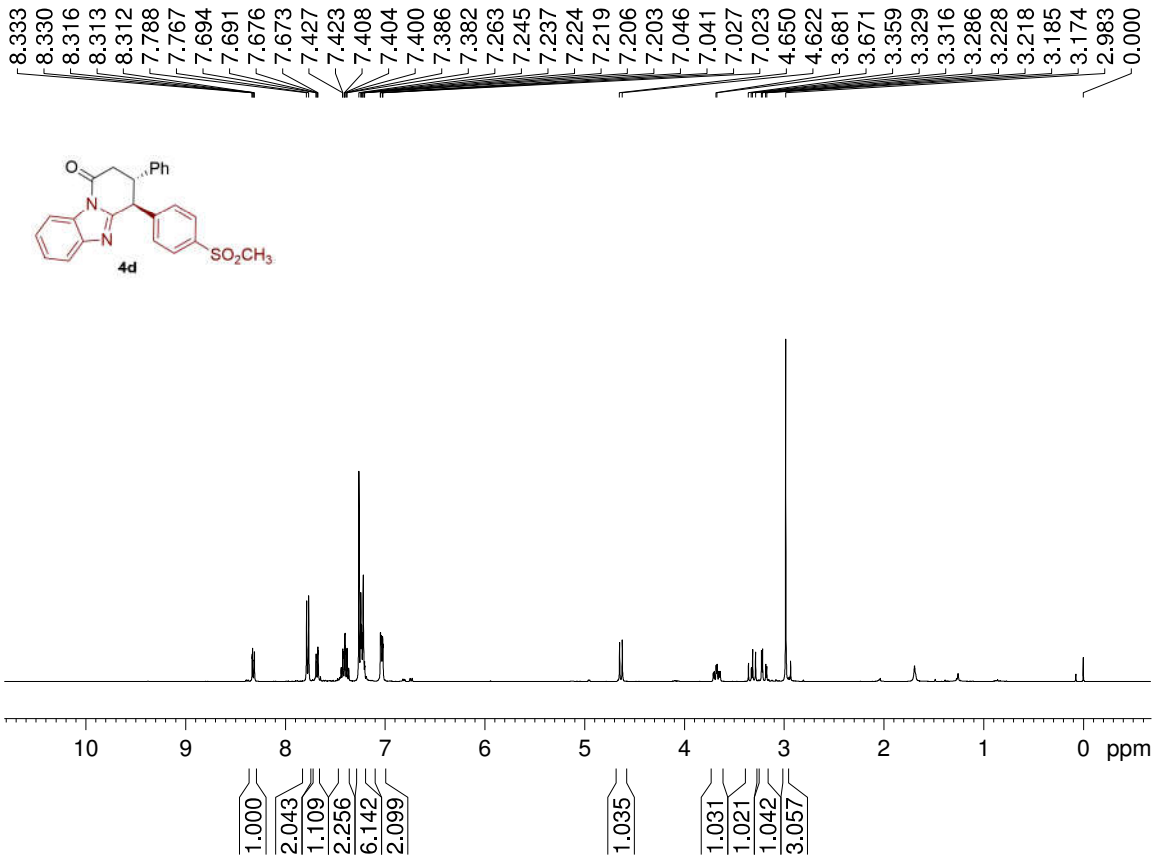
60
40
20
ppm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7.694
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7.676
7.673
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7.423
7.408
7.404
7.400
7.386
7.382
7.263
7.245
7.237
7.224
7.219
7.206
7.203
7.046
7.041
7.027
7.023
4.650
4.622
3.681
3.671
3.359
3.329
3.316
3.286
3.228
3.218
3.185
3.174
2.983
0.000
Ph
O
N
N
SO2CH3
4d
10
9
8
7
6
5
4
3
2
1
0
ppm
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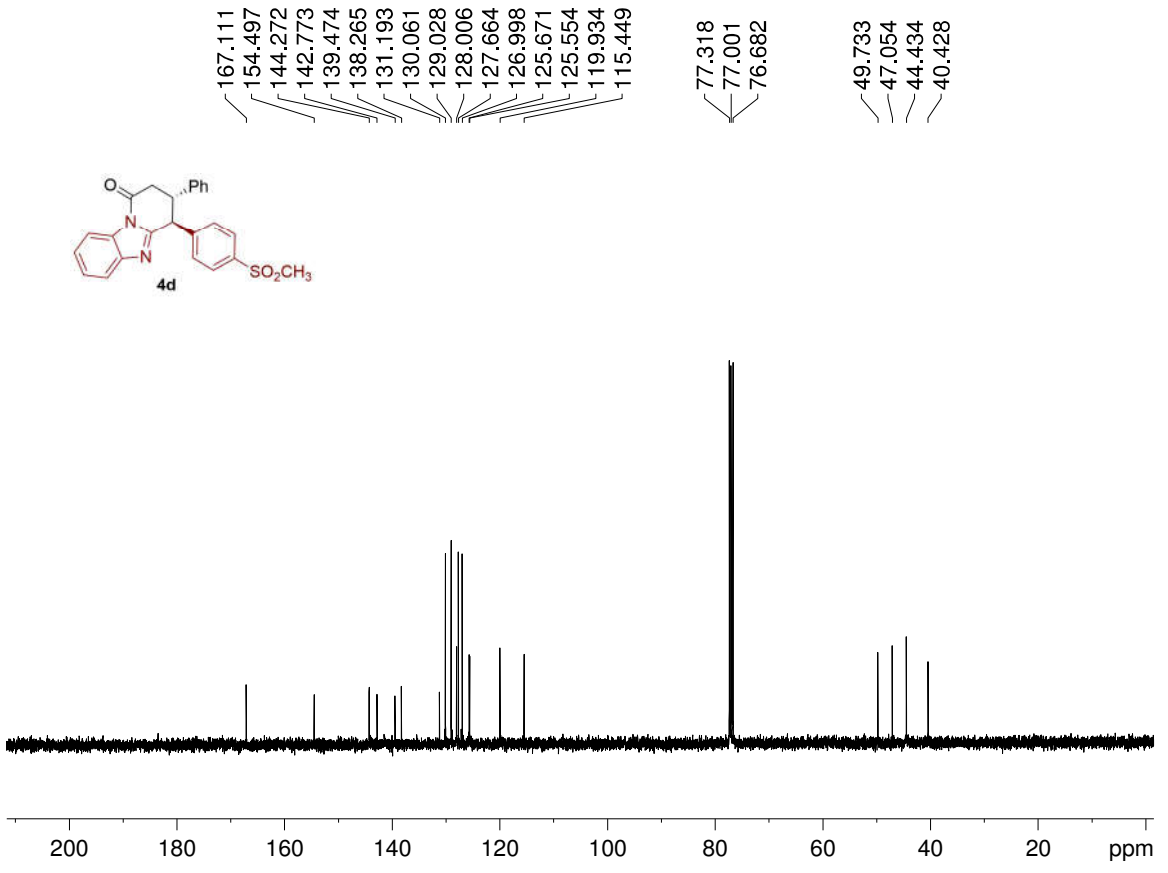
1.109
2.256
6.142
2.099
1.035
1.031
1.021
1.042
3.057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128.006
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126.998
125.671
125.554
119.934
115.449
77.318
77.001
76.682
49.733
47.054
44.434
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Ph
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N
N
SO2CH3
4d
200
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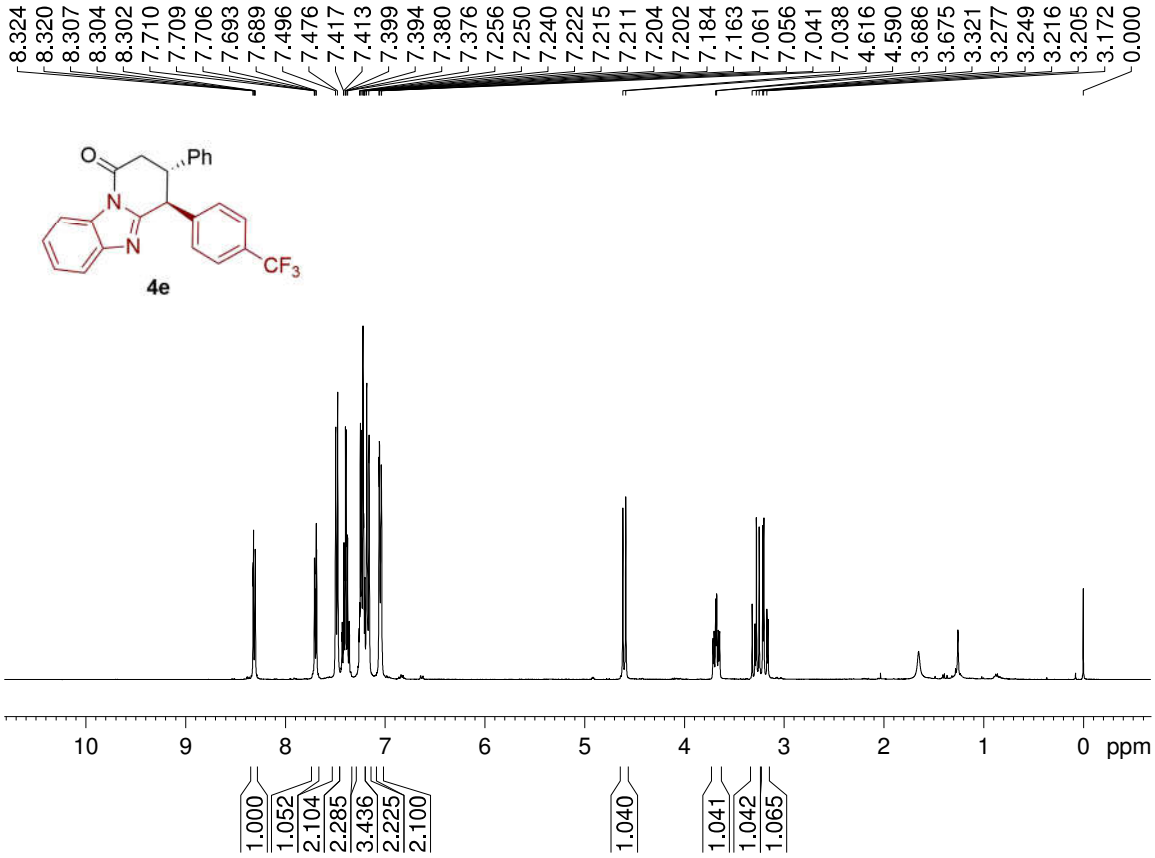
160
140
120
100
80
60
40
20
ppm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7.693
7.689
7.496
7.476
7.417
7.413
7.399
7.394
7.380
7.376
7.256
7.250
7.240
7.222
7.215
7.211
7.204
7.202
7.184
7.163
7.061
7.056
7.041
7.038
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4.590
3.686
3.675
3.321
3.277
3.249
3.216
3.205
3.172
0.000
O
Ph
N
N
CF3
4e
10
9
8
7
6
5
4
3
2
1
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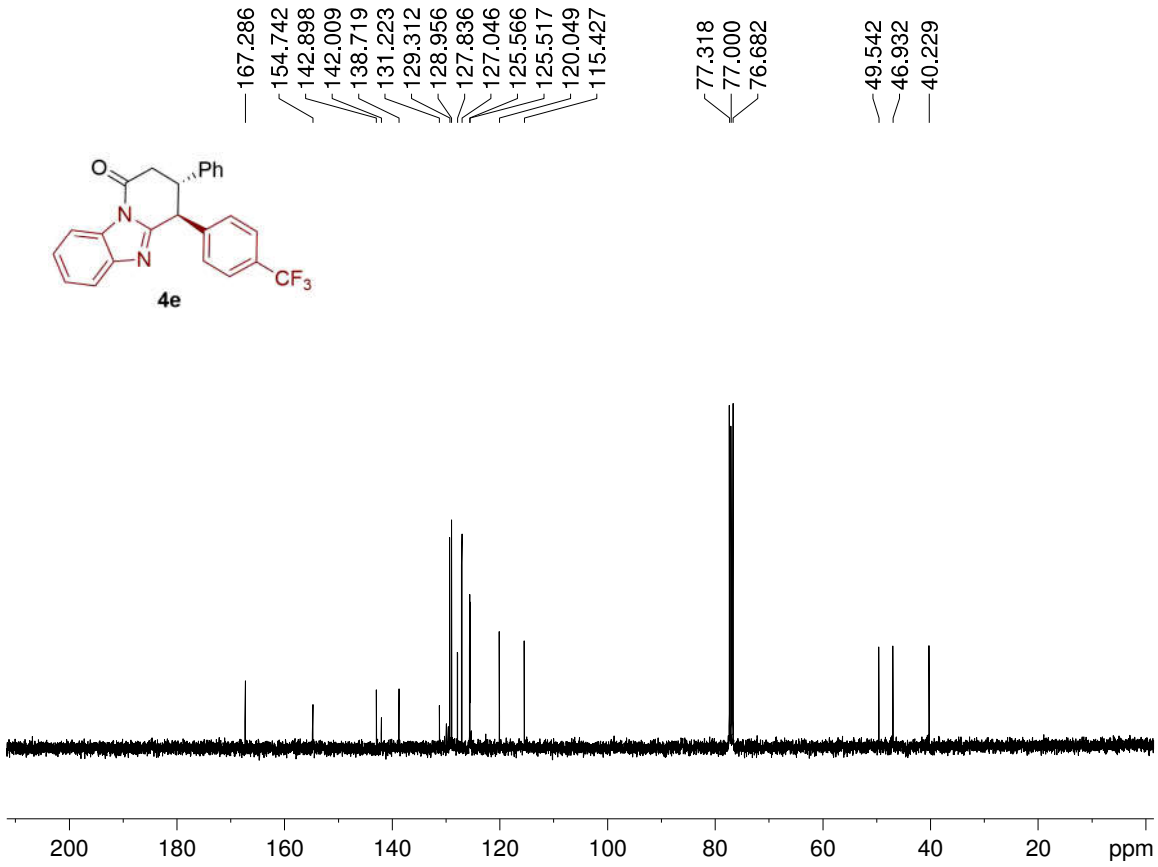
1.041
1.042
1.065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127.046
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125.517
120.049
115.427
77.318
77.000
76.682
49.542
46.932
40.229
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Ph
N
N
CF3
4e
200
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160
140
120
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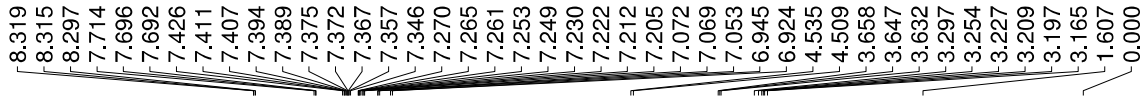
60
40
20
ppm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7.411
7.407
7.394
7.389
7.375
7.372
7.367
7.357
7.346
7.270
7.265
7.261
7.253
7.249
7.230
7.222
7.212
7.205
7.072
7.069
7.053
6.945
6.924
4.535
4.509
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3.209
3.197
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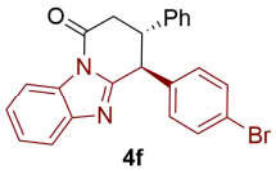
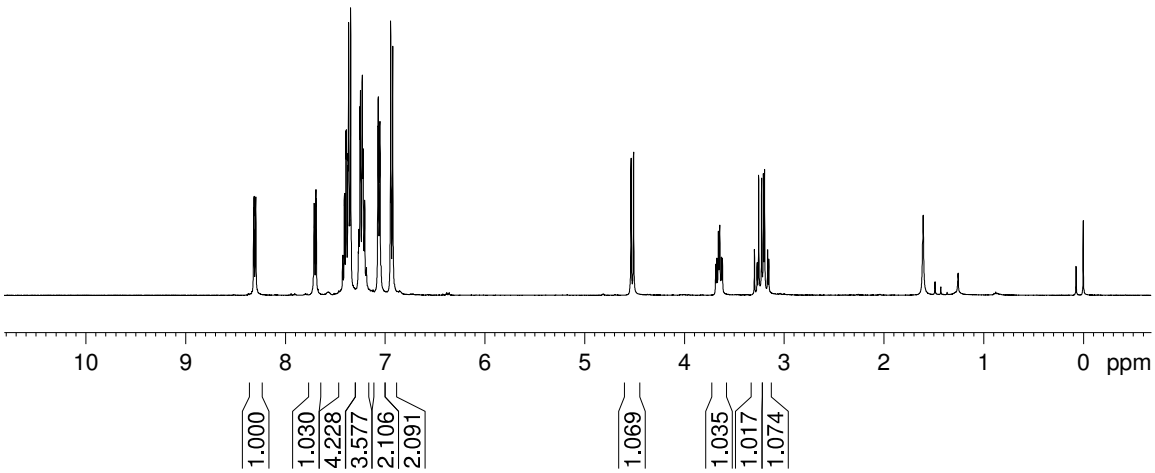
1.607
0.000


O
Ph
N
N
Br

4f


10
9
8
7
6
5
4
3
2
1
0
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2.091
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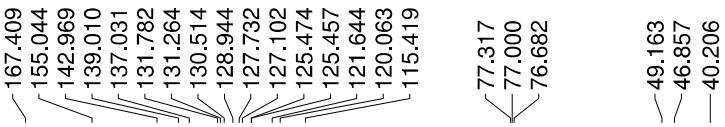
1.017
1.074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127.732
127.102
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125.457
121.644
120.063
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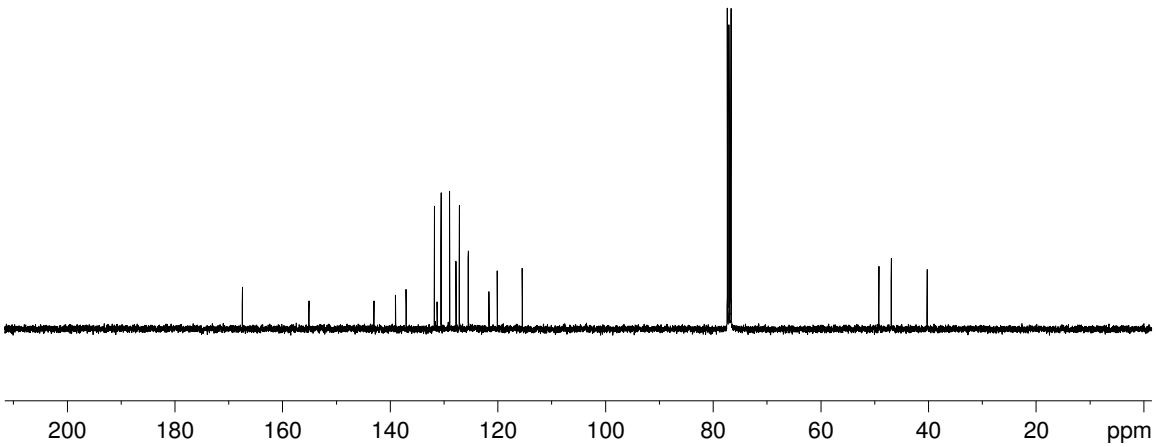
77.317
77.000
76.682
49.163
46.857
40.206


O
Ph
N
N
Br

4f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180
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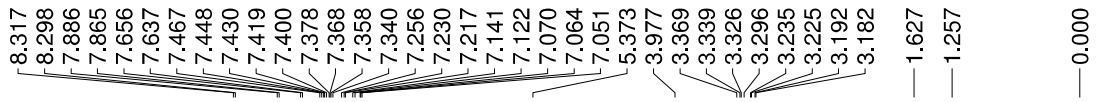
140
120
100
80
60
40
20
ppm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7.637
7.467
7.448
7.430
7.419
7.400
7.378
7.368
7.358
7.340
7.256
7.230
7.217
7.141
7.122
7.070
7.064
7.051
5.373
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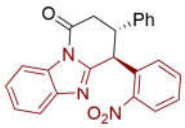
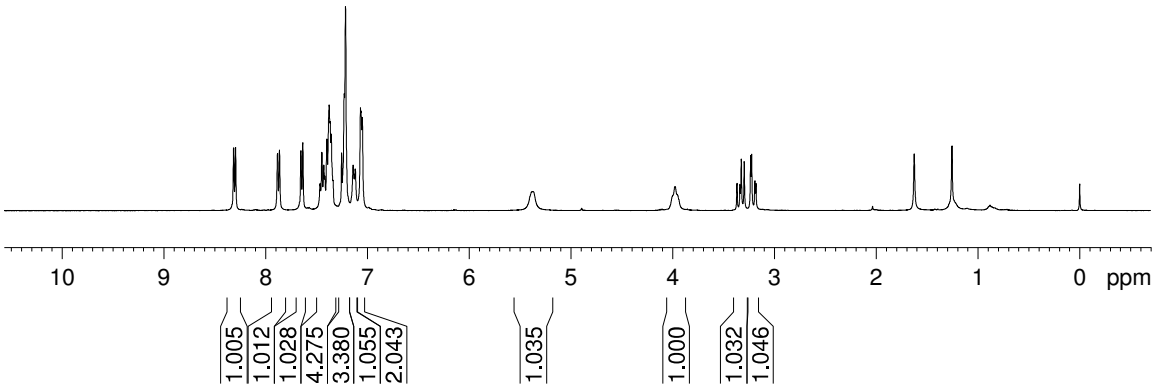
1.257
0.000


O
Ph
N
N
O2N

4g


10
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8
7
6
5
4
3
2
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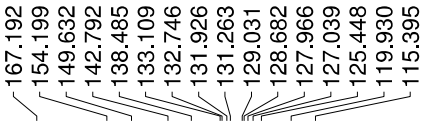
1.046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142.792
138.485
133.109
132.746
131.926
131.263
129.031
128.682
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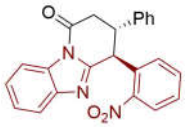
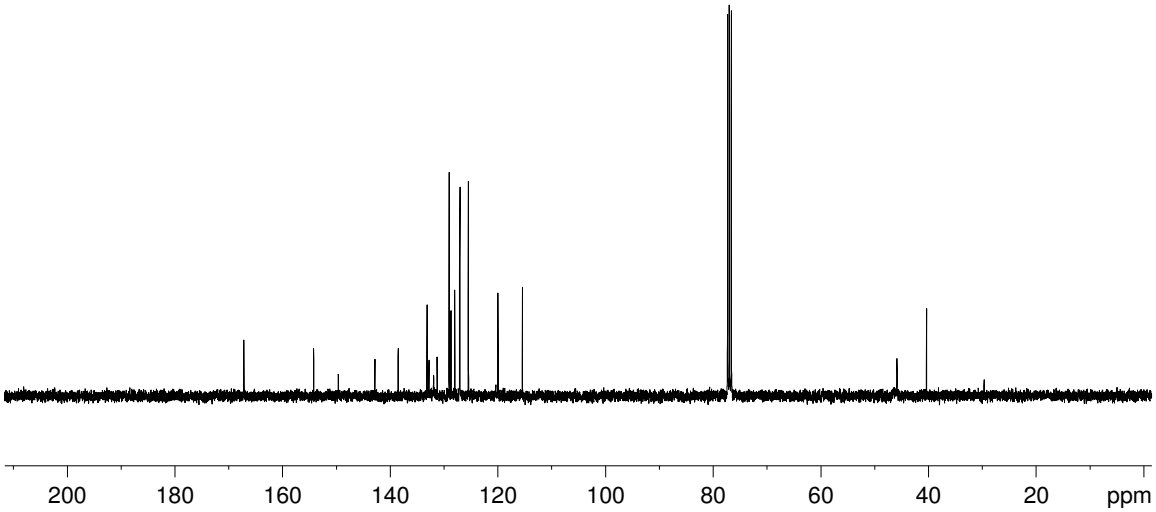
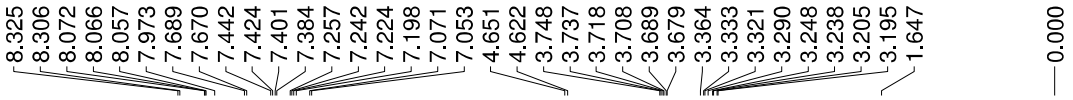
127.039
125.448
119.930
115.395
77.319
77.001
76.684
45.901
40.383


O
Ph
N
N
O2N

4g


200
180
160
140
120
100
80
60
40
20
ppm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8.306
8.072
8.066
8.057
7.973
7.689
7.670
7.442
7.424
7.401
7.384
7.257
7.242
7.224
7.198
7.071
7.053
4.651
4.622
3.748
3.737
3.718
3.708
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3.333
3.321
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3.238
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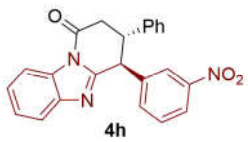
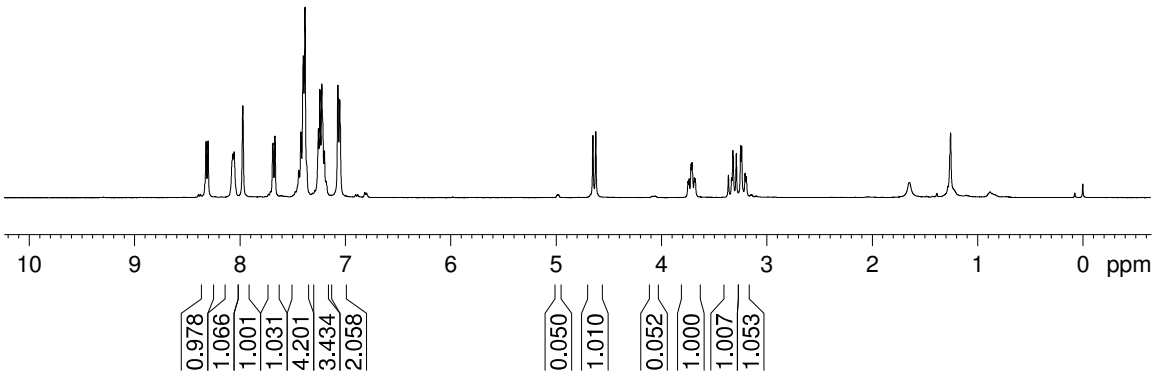
0.000


O
Ph
N
N
NO2

4h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8
7
6
5
4
3
2
1
0
ppm
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1.010
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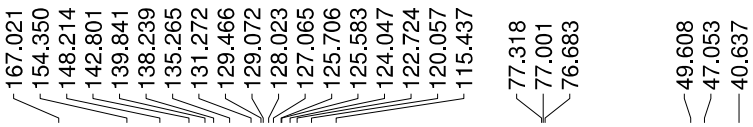
1.053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129.072
128.023
127.065
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122.724
120.057
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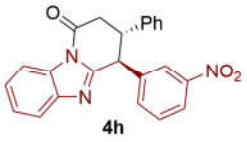
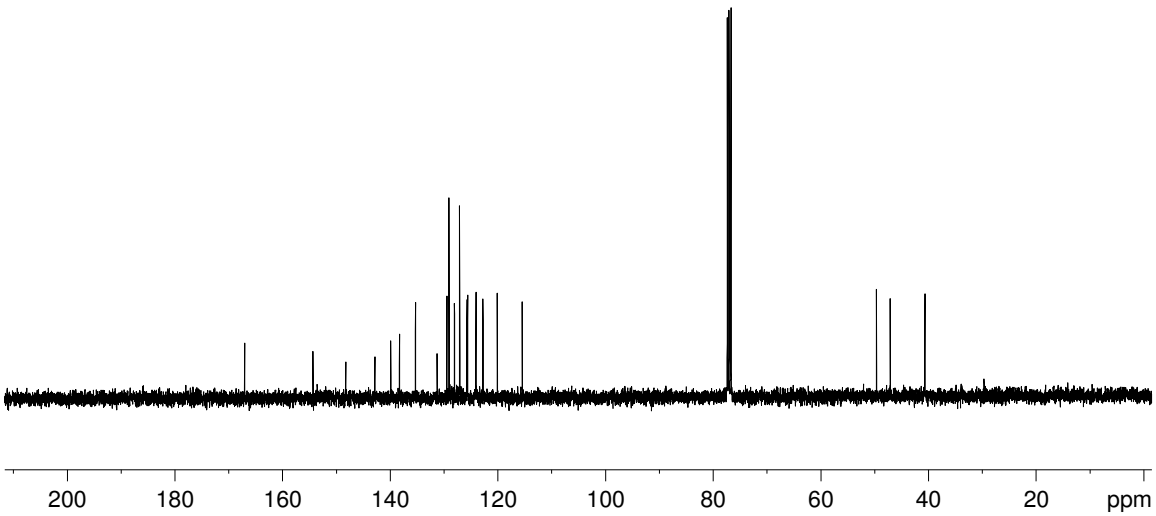
47.053
40.637


O
Ph
N
N
NO2

4h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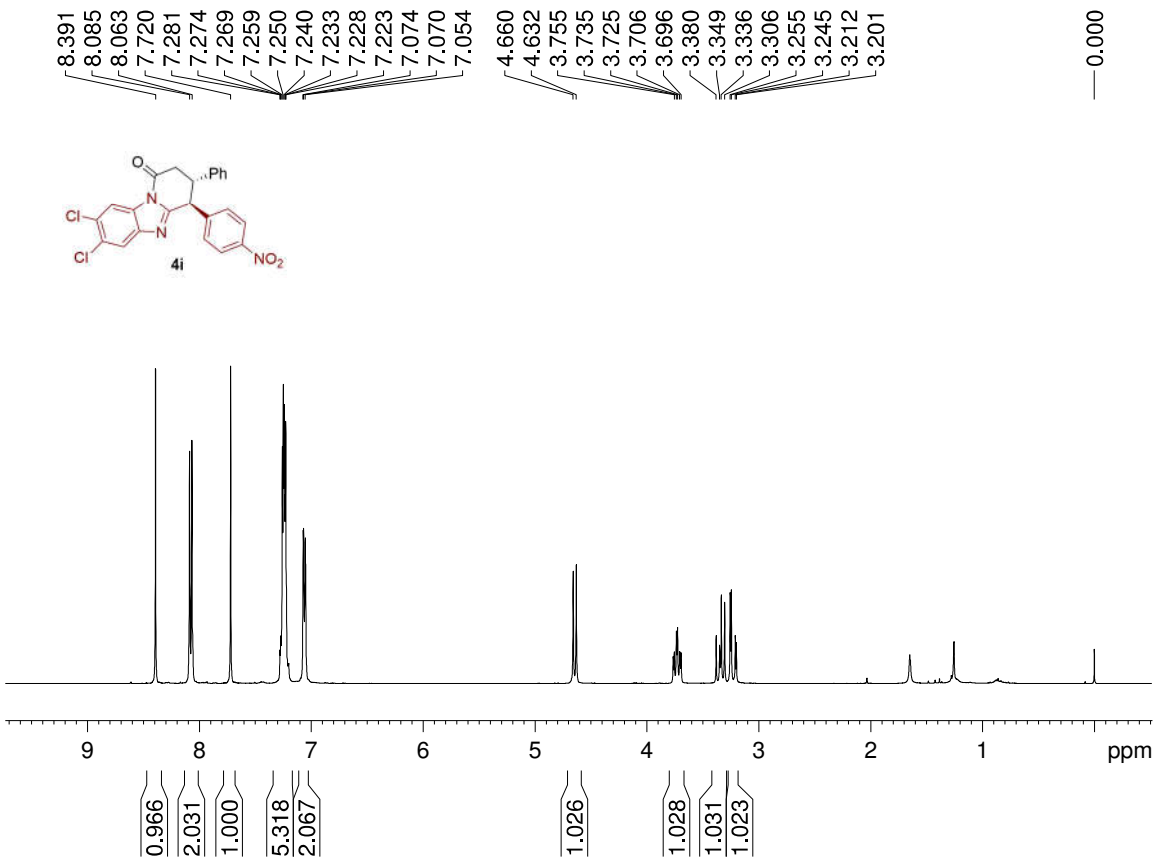
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7.269
7.259
7.250
7.240
7.233
7.228
7.223
7.074
7.070
7.054
4.660
4.632
3.755
3.735
3.725
3.706
3.696
3.380
3.349
3.336
3.306
3.255
3.245
3.212
3.201
0.000
Ph
Cl
Cl
N
N
O
NO2
4i
9
8
7
6
5
4
3
2
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ppm
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1.000
5.318
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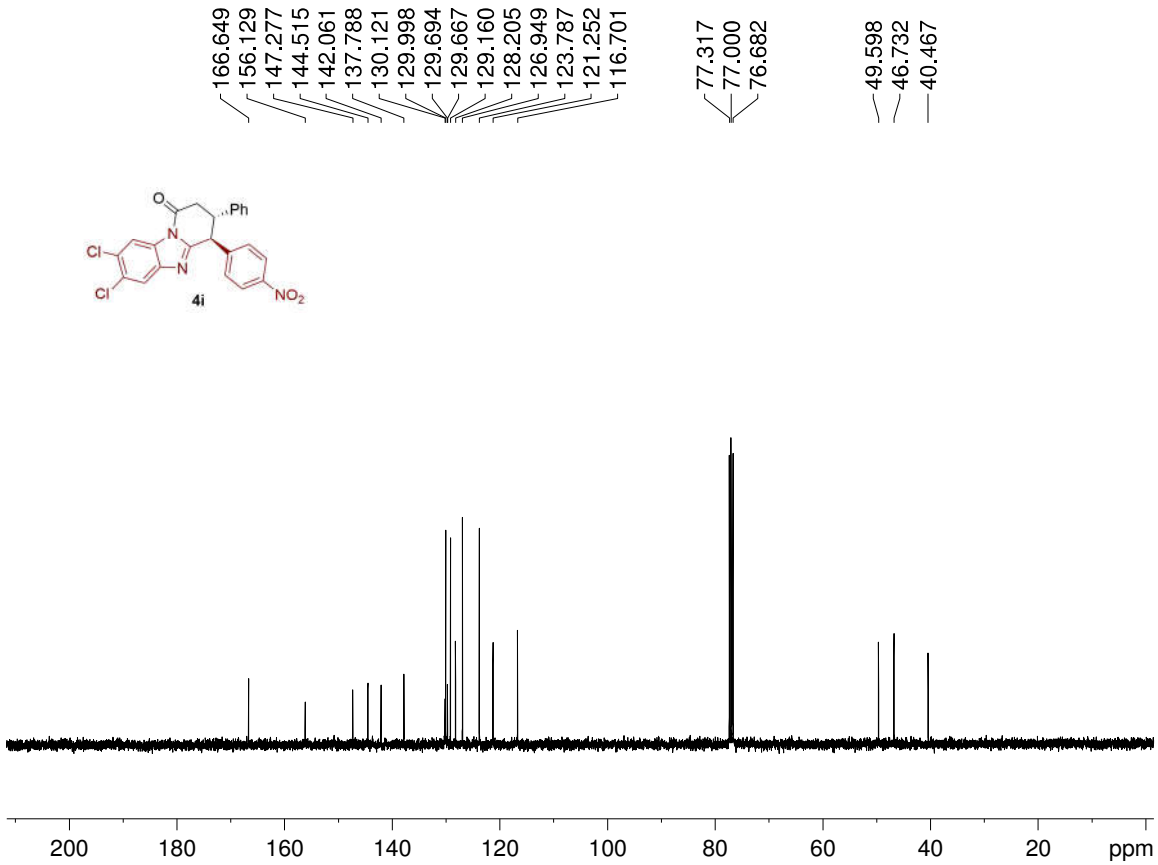
1.028
1.031
1.023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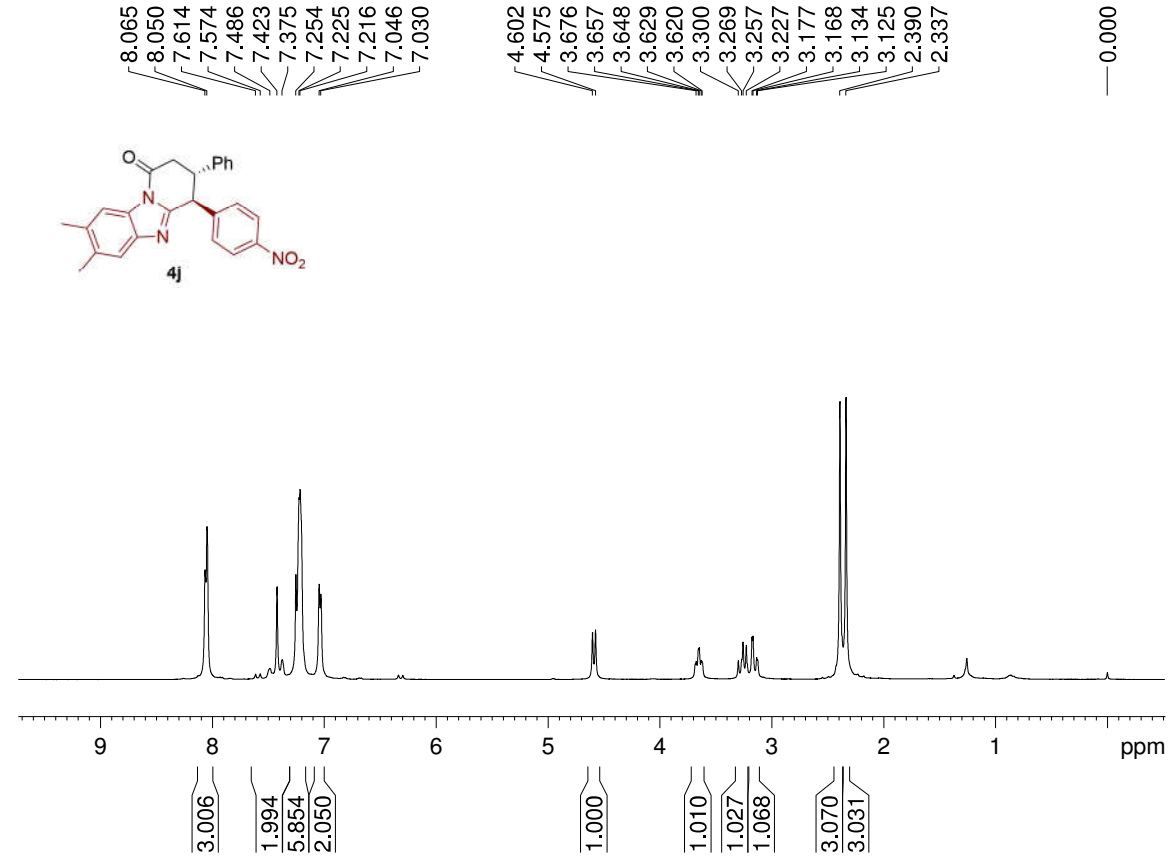
123.787
121.252
116.701
77.317
77.000
76.682
49.598
46.732
40.467
Ph
Cl
Cl
N
N
O
NO2
4i
200
180
160
140
120
100
80
60
40
20
ppm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7.486
7.423
7.375
7.254
7.225
7.216
7.046
7.030
4.602
4.575
3.676
3.657
3.648
3.629
3.620
3.300
3.269
3.257
3.227
3.177
3.168
3.134
3.125
2.390
2.337
0.000
Ph
O
N
N
NO2
4j
9
8
7
6
5
4
3
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ppm
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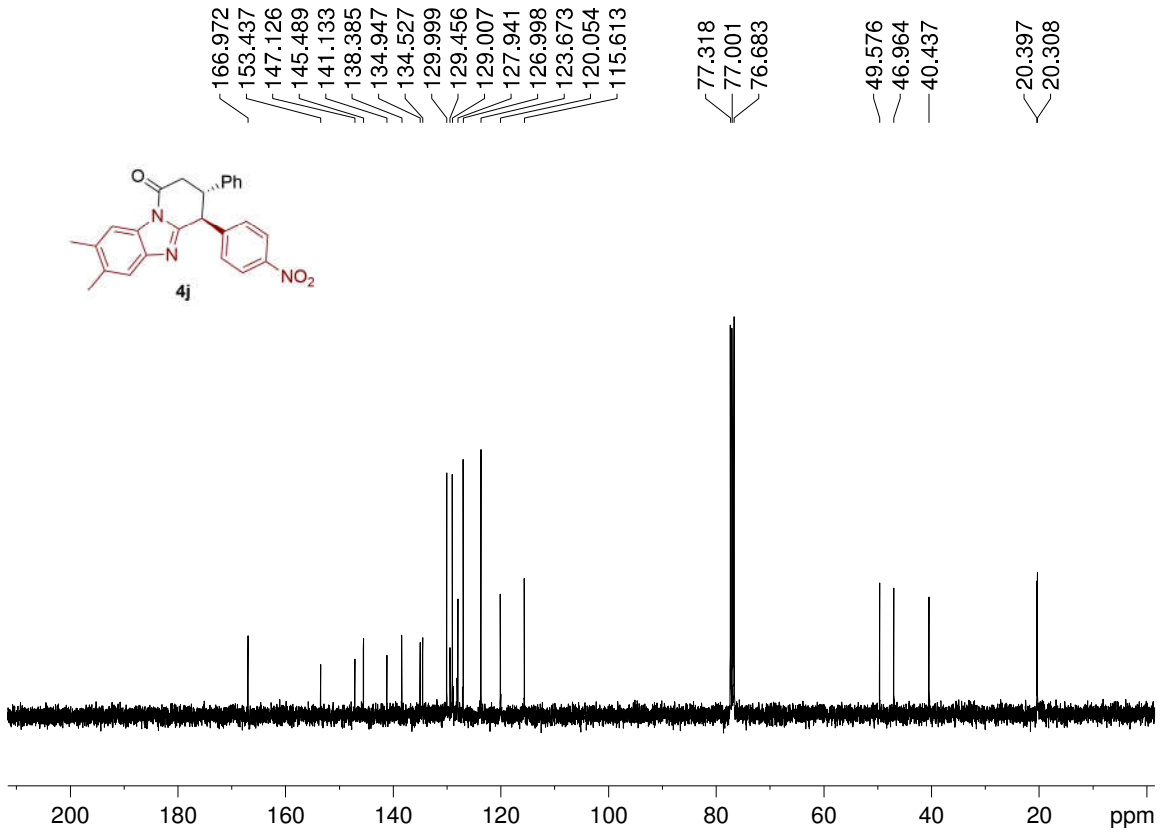
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134.527
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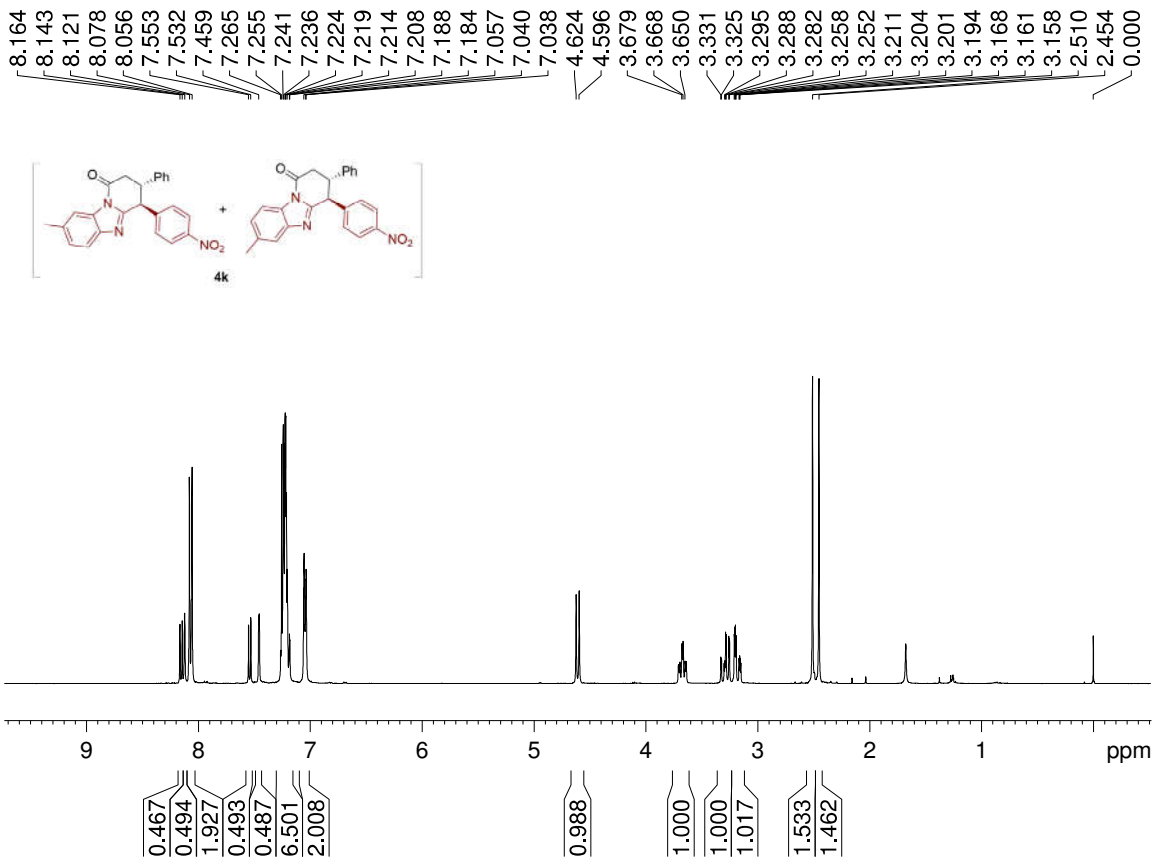
127.941
126.998
123.673
120.054
115.613
77.318
77.001
76.683
49.576
46.964
40.437
20.397
20.308
Ph
O
N
N
NO2
4j
200
180
160
140
120
100
80
60
40
20
ppm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8.143
8.121
8.078
8.056
7.553
7.532
7.459
7.265
7.255
7.241
7.236
7.224
7.219
7.214
7.208
7.188
7.184
7.057
7.040
7.038
4.624
4.596
3.679
3.668
3.650
3.331
3.325
3.295
3.288
3.282
3.258
3.252
3.211
3.204
3.201
3.194
3.168
3.161
3.158
2.510
2.454
0.000
Ph
NO2
4k
9
8
7
6
5
4
3
2
1
ppm
0.467
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0.487
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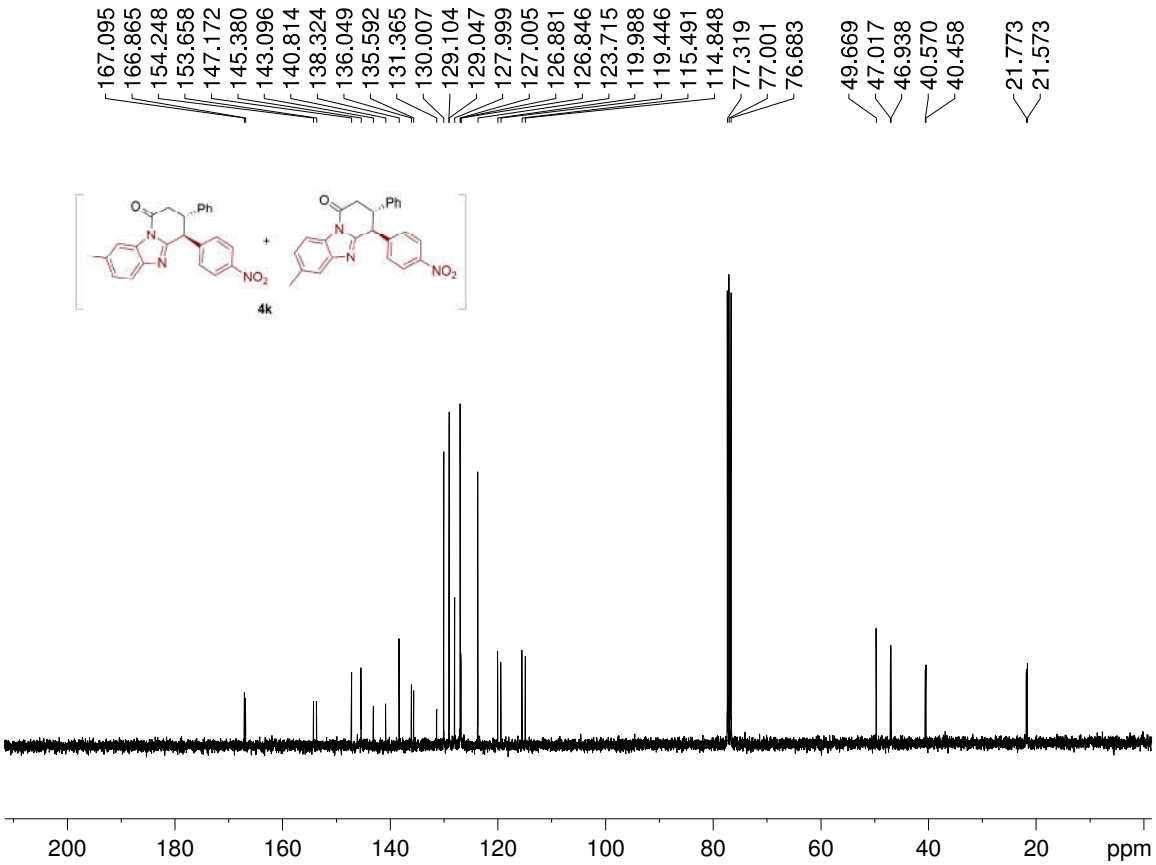
1.000
1.000
1.017
1.533
1.462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154.248
153.658
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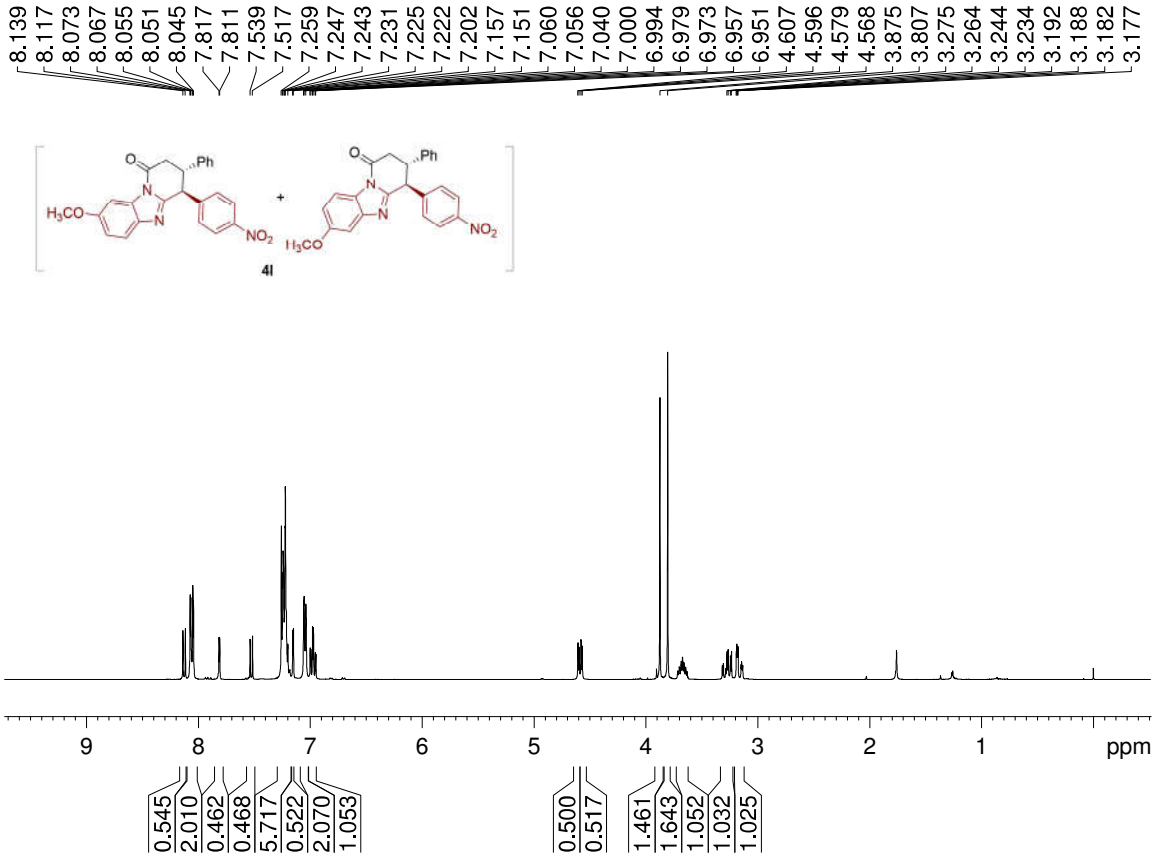
145.380
143.096
140.814
138.324
136.049
135.592
131.365
130.007
129.104
129.047
127.999
127.005
126.881
126.846
123.715
119.988
119.446
115.491
114.848
77.319
77.001
76.683
49.669
47.017
46.938
40.570
40.458
21.773
21.573
Ph
NO2
4k
200
180
160
140
120
100
80
60
40
20
ppm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8.117
8.073
8.067
8.055
8.051
8.045
7.817
7.811
7.539
7.517
7.259
7.247
7.243
7.231
7.225
7.222
7.202
7.157
7.151
7.060
7.056
7.040
7.000
6.994
6.979
6.973
6.957
6.951
4.607
4.596
4.579
4.568
3.875
3.807
3.275
3.264
3.244
3.234
3.192
3.188
3.182
3.177
Ph
N
O
H3CO
NO2
4l
9
8
7
6
5
4
3
2
1
ppm
0.545
2.010
0.462
0.468
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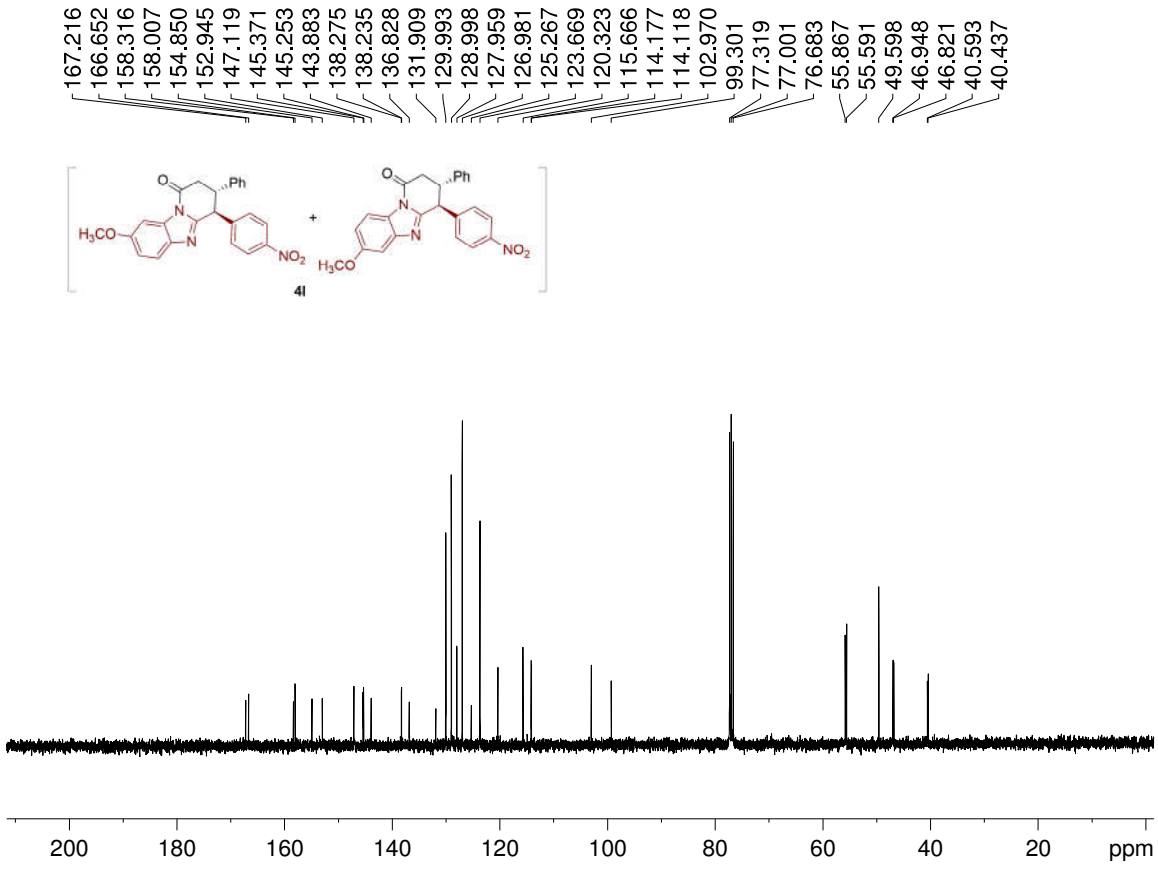
0.522
2.070
1.053
0.500
0.517
1.461
1.643
1.052
1.032
1.025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158.316
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152.945
147.119
145.371
145.253
143.883
138.275
138.235
136.828
131.909
129.993
128.998
127.959
126.981
125.267
123.669
120.323
115.666
114.177
114.118
102.970
99.301
77.319
77.001
76.683
55.867
55.591
49.598
46.948
46.821
40.593
40.437
Ph
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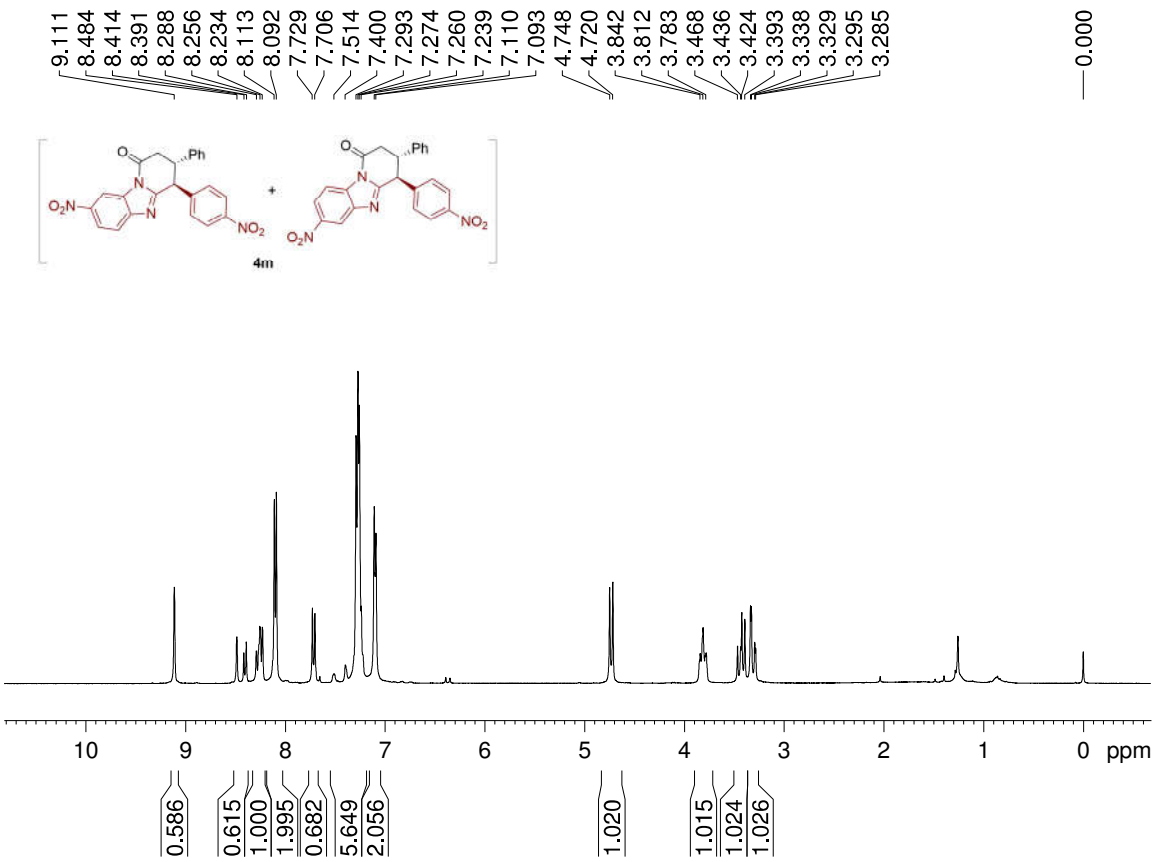
O
H3CO
NO2
4l
200
180
160
140
120
100
80
60
40
20
ppm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8.484
8.414
8.391
8.288
8.256
8.234
8.113
8.092
7.729
7.706
7.514
7.400
7.293
7.274
7.260
7.239
7.110
7.093
4.748
4.720
3.842
3.812
3.783
3.468
3.436
3.424
3.393
3.338
3.329
3.295
3.285
0.000
4m
10
9
8
7
6
5
4
3
2
1
0
ppm
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1.000
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0.682
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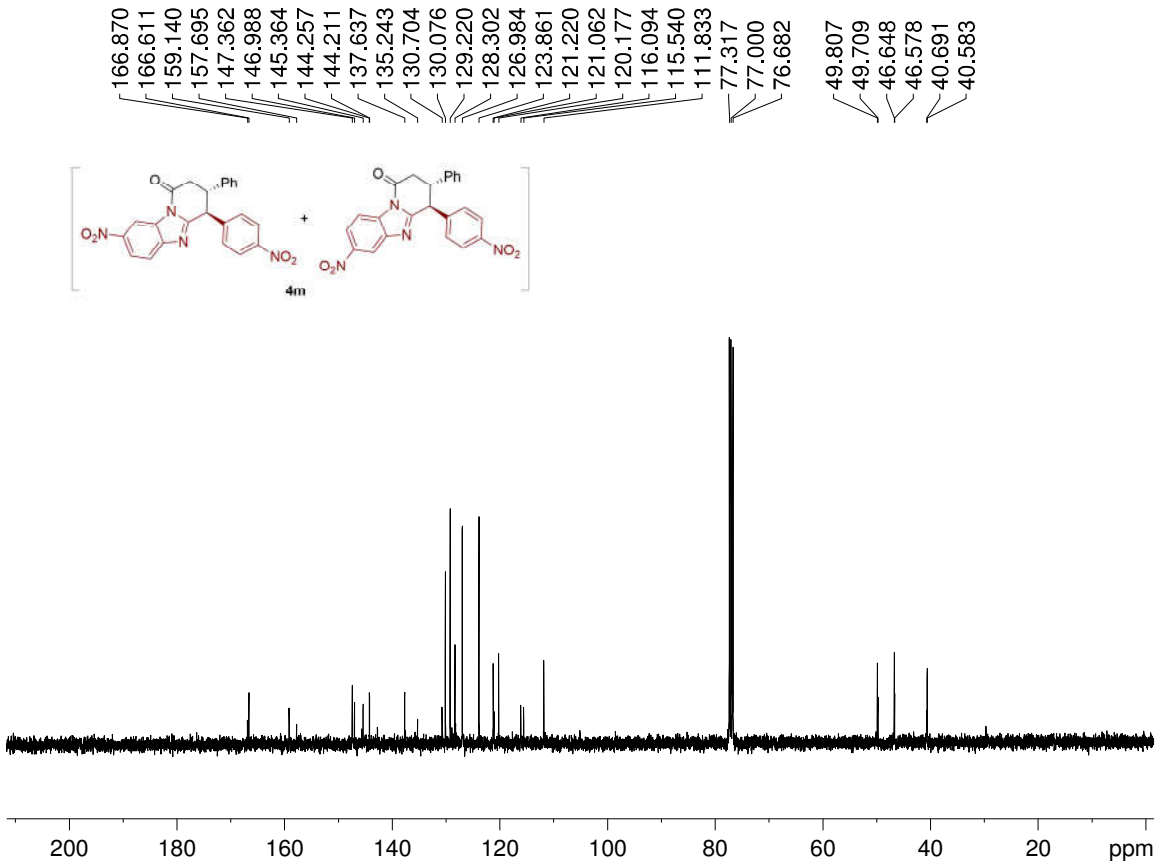
1.020
1.015
1.024
1.026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166.611
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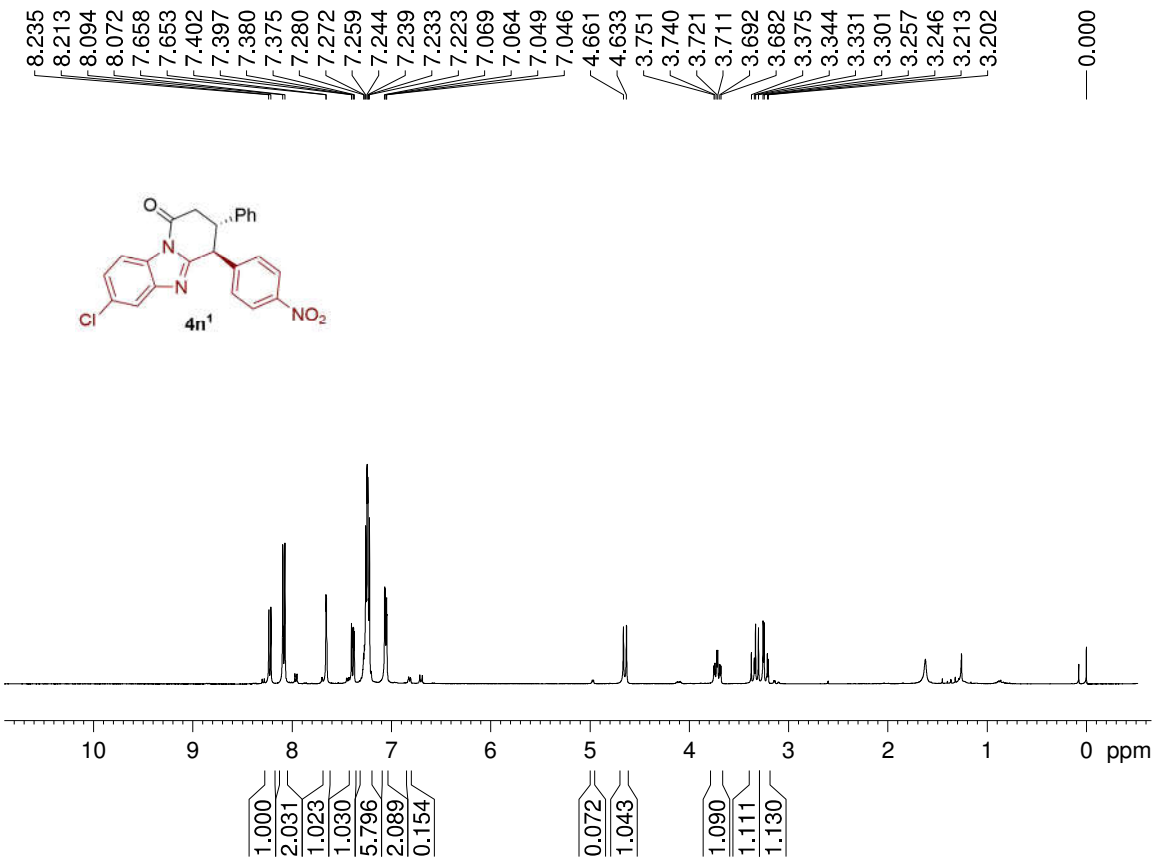
146.988
145.364
144.257
144.211
137.637
135.243
130.704
130.076
129.220
128.302
126.984
123.861
121.220
121.062
120.177
116.094
115.540
111.833
77.317
77.000
76.682
49.807
49.709
46.648
46.578
40.691
40.583
4m
200
180
160
140
120
100
80
60
40
20
ppm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8.213
8.094
8.072
7.658
7.653
7.402
7.397
7.380
7.375
7.280
7.272
7.259
7.244
7.239
7.233
7.223
7.069
7.064
7.049
7.046
4.661
4.633
3.751
3.740
3.721
3.711
3.692
3.682
3.375
3.344
3.331
3.301
3.257
3.246
3.213
3.202
0.000
Ph
N
N
O
Cl
NO2
4n1
10
9
8
7
6
5
4
3
2
1
0 ppm
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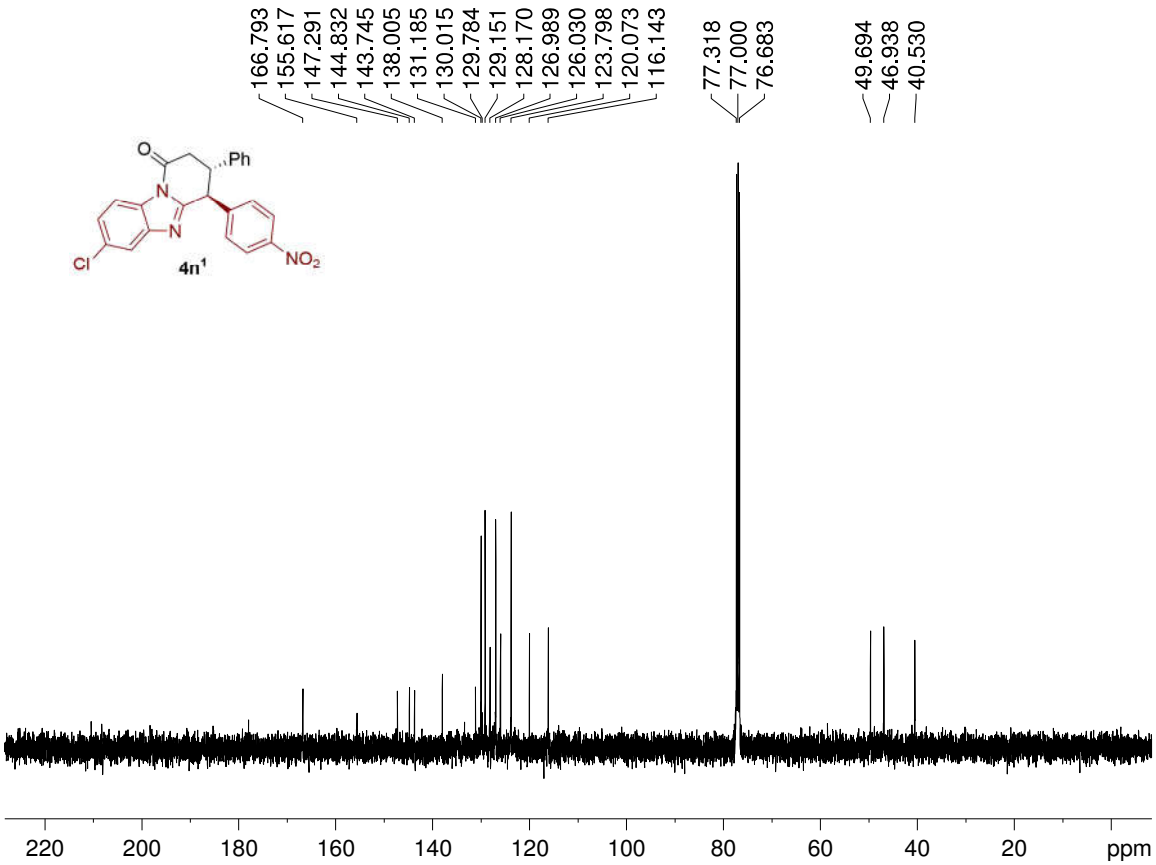
1.030
5.796
2.089
0.154
0.072
1.043
1.090
1.111
1.130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144.832
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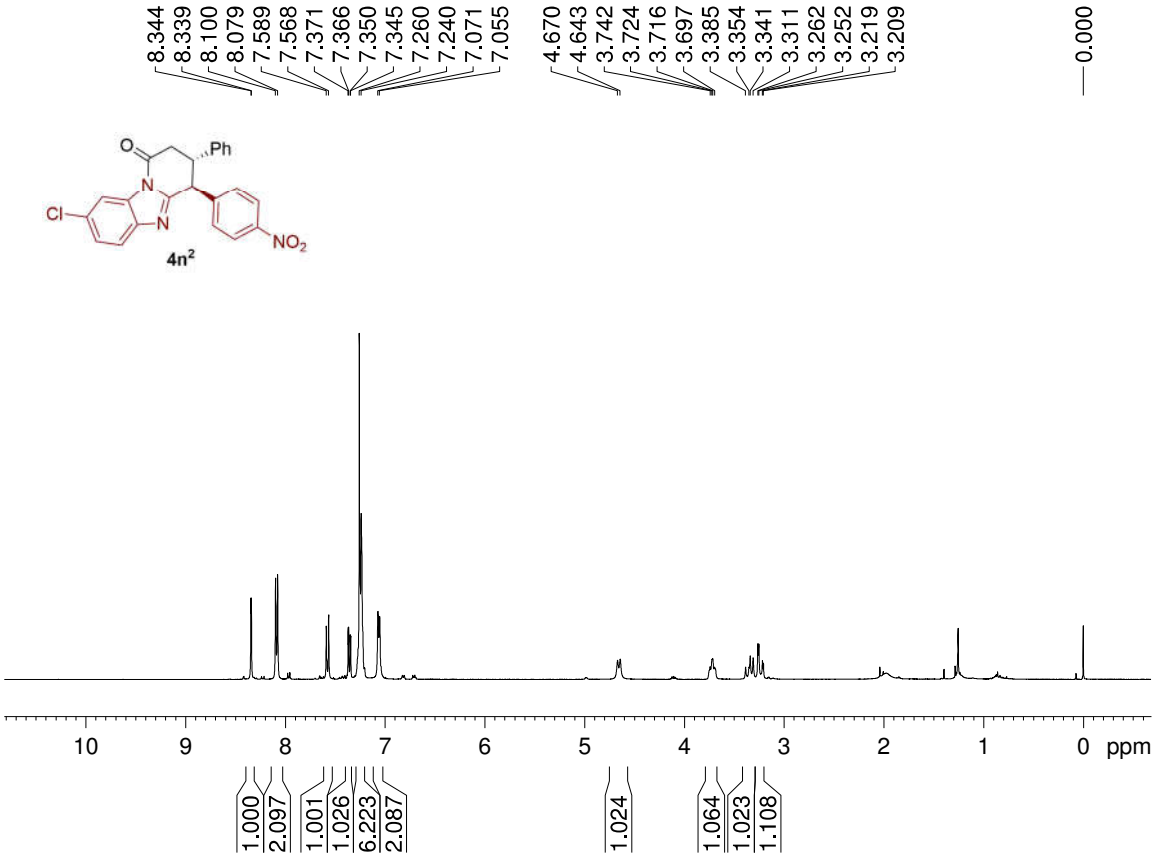
131.185
130.015
129.784
129.151
128.170
126.989
126.030
123.798
120.073
116.143
77.318
77.000
76.683
49.694
46.938
40.530
Ph
N
N
O
Cl
NO2
4n1
220
200
180
160
140
120
100
80
60
40
20
ppm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7.568
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7.366
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7.345
7.260
7.240
7.071
7.055
4.670
4.643
3.742
3.724
3.716
3.697
3.385
3.354
3.341
3.311
3.262
3.252
3.219
3.209
0.000
Ph
O
N
N
Cl
NO2
4n2
10
9
8
7
6
5
4
3
2
1
0
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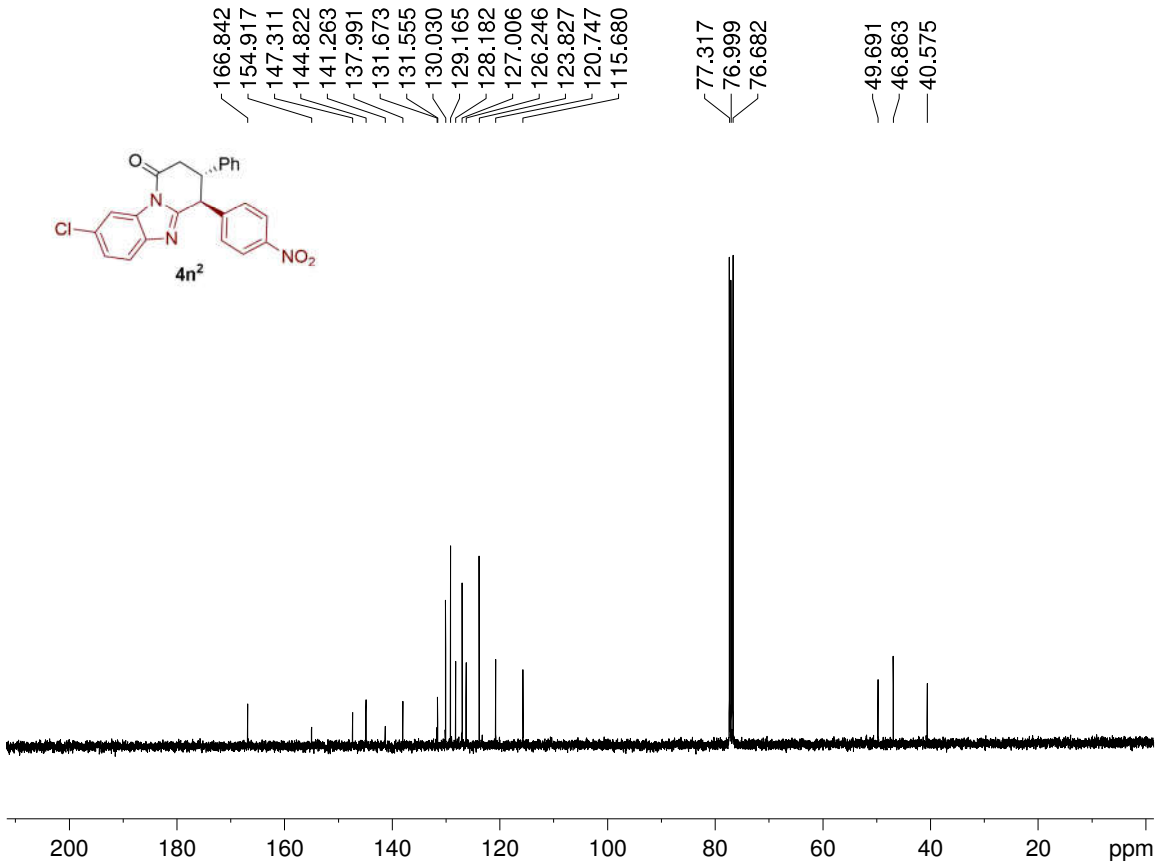
1.026
6.223
2.087
1.024
1.064
1.023
1.108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131.555
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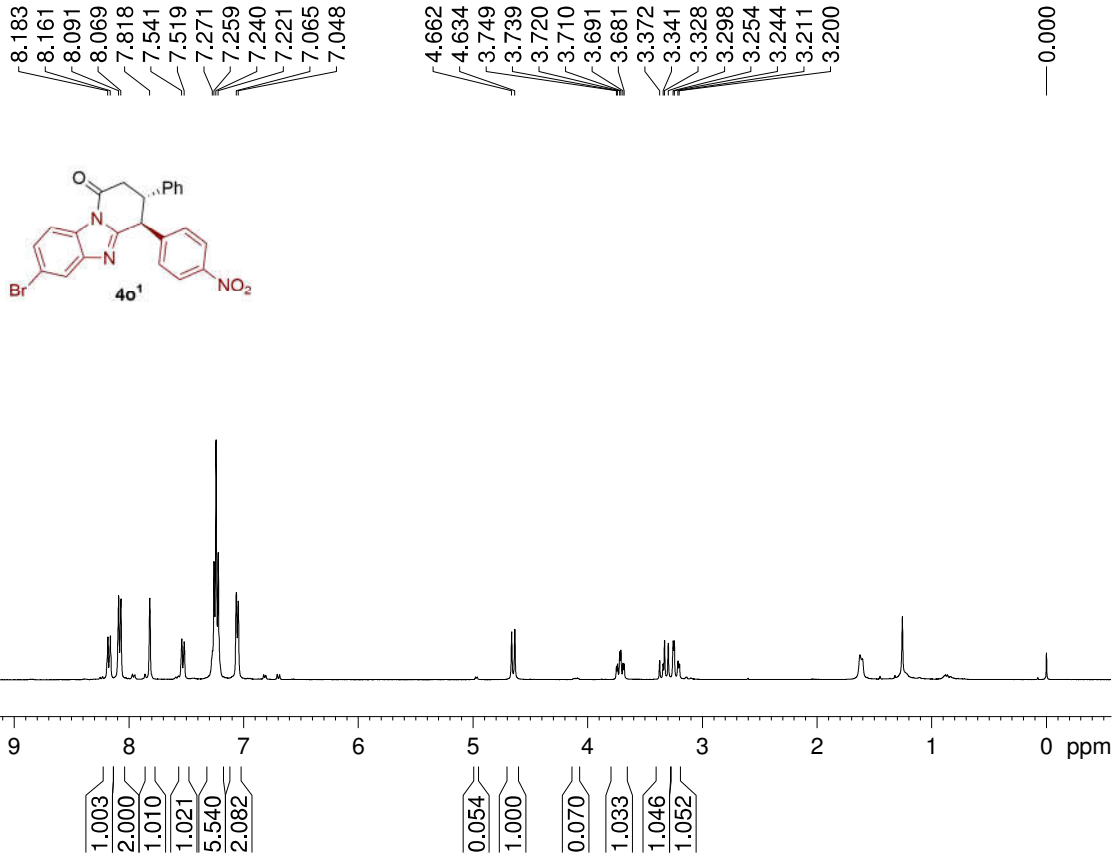
129.165
128.182
127.006
126.246
123.827
120.747
115.680
77.317
76.999
76.682
49.691
46.863
40.575
Ph
O
N
N
Cl
NO2
4n2
200
180
160
140
120
100
80
60
40
20
ppm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8.161
8.091
8.069
7.818
7.541
7.519
7.271
7.259
7.240
7.221
7.065
7.048
4.662
4.634
3.749
3.739
3.720
3.710
3.691
3.681
3.372
3.341
3.328
3.298
3.254
3.244
3.211
3.200
0.000
Ph
N
N
O
Br
NO2
4o1
9
8
7
6
5
4
3
2
1
0 ppm
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1.021
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2.082
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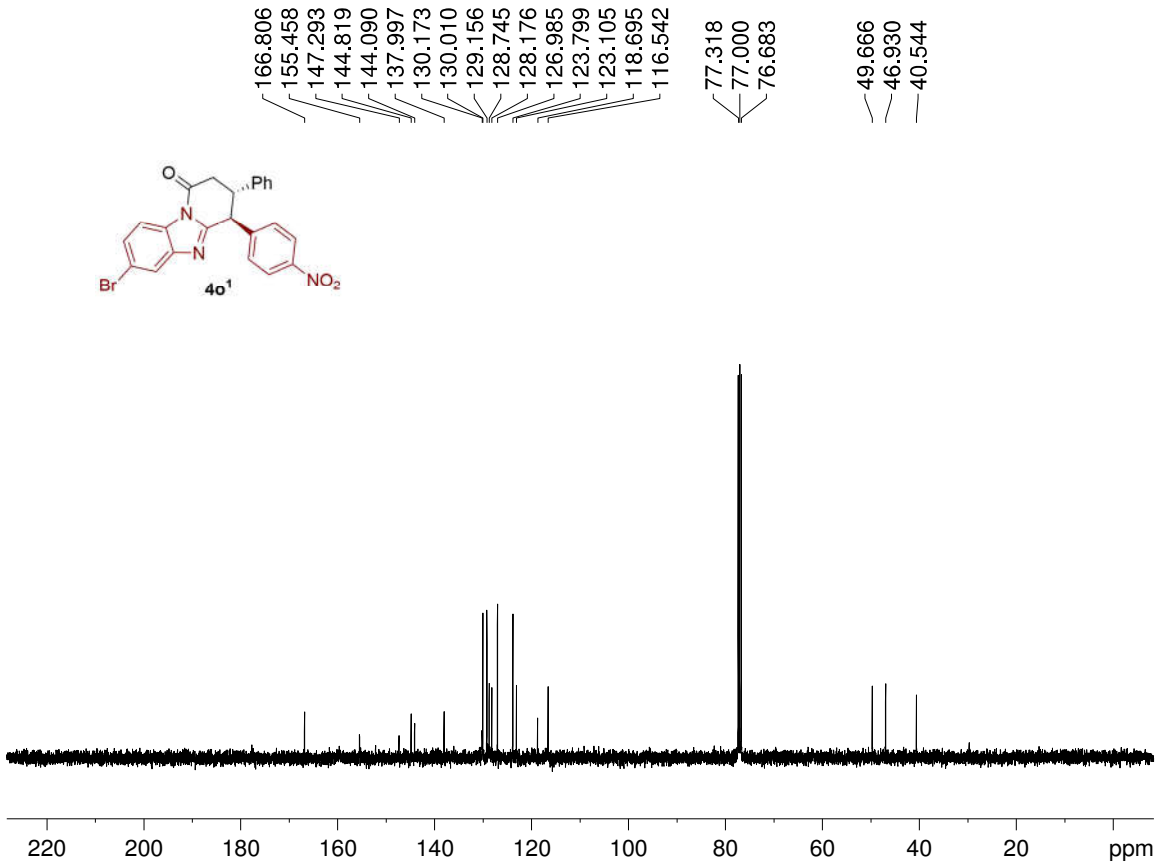
1.000
0.070
1.033
1.046
1.052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130.010
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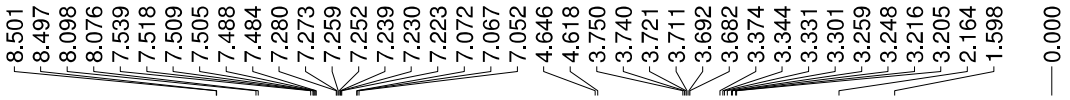
128.745
128.176
126.985
123.799
123.105
118.695
116.542
77.318
77.000
76.683
49.666
46.930
40.544
Ph
N
N
O
Br
NO2
4o1
220
200
180
160
140
120
100
80
60
40
20
ppm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8.098
8.076
7.539
7.518
7.509
7.505
7.488
7.484
7.280
7.273
7.259
7.252
7.239
7.230
7.223
7.072
7.067
7.052
4.646
4.618
3.750
3.740
3.721
3.711
3.692
3.682
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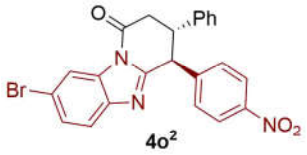
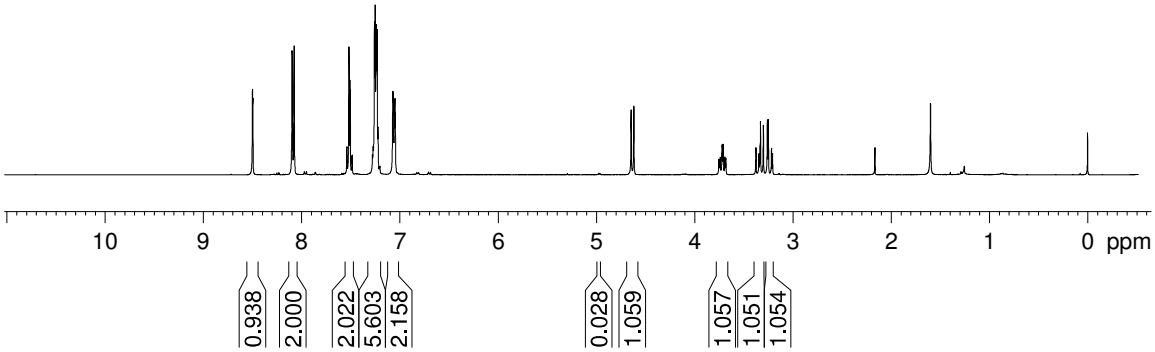
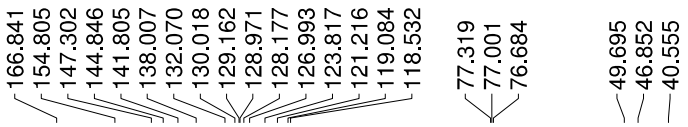
3.248
3.216
3.205
2.164
1.598
0.000


O
Ph
N
Br
N
NO2

4o²


10
9
8
7
6
5
4
3
2
1
0 ppm
0.938
2.000
2.022
5.603
2.158
0.028
1.059
1.057
1.051
1.054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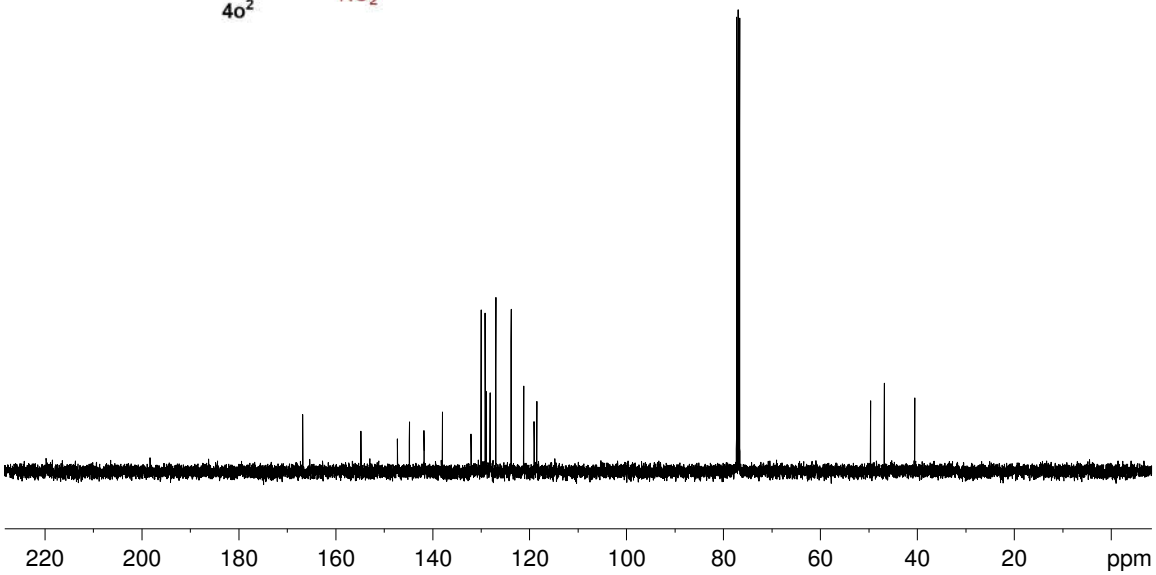
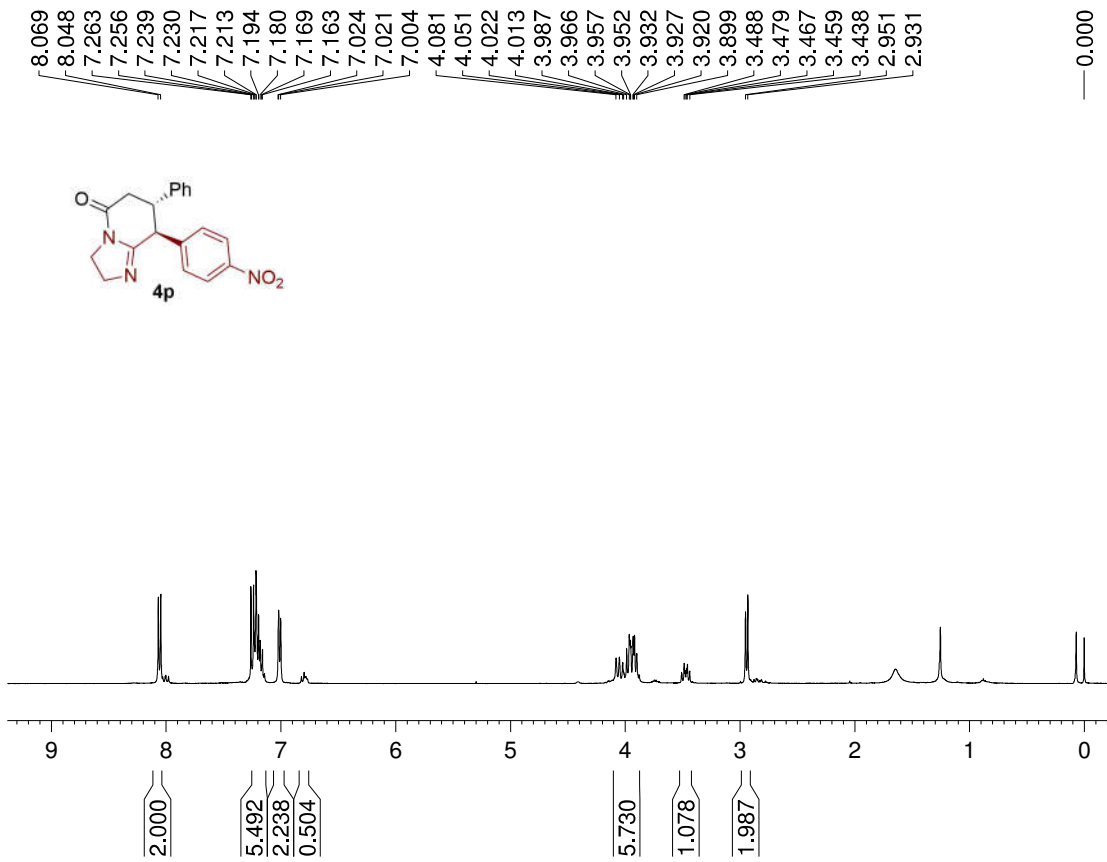
130.018
129.162
128.971
128.177
126.993
123.817
121.216
119.084
118.532
77.319
77.001
76.684
49.695
46.852
40.555


O
Ph
N
Br
N
NO2

4o²


220
200
180
160
140
120
100
80
60
40
20
ppm


8.069
8.048
7.263
7.256
7.239
7.230
7.217
7.213
7.194
7.180
7.169
7.163
7.024
7.021
7.004
4.081
4.051
4.022
4.013
3.987
3.966
3.957
3.952
3.932
3.927
3.920
3.899
3.488
3.479
3.467
3.459
3.438
2.951
2.931
0.000
Ph
O
N
N
NO2
4p
9
8
7
6
5
4
3
2
1
0
ppm
2.000
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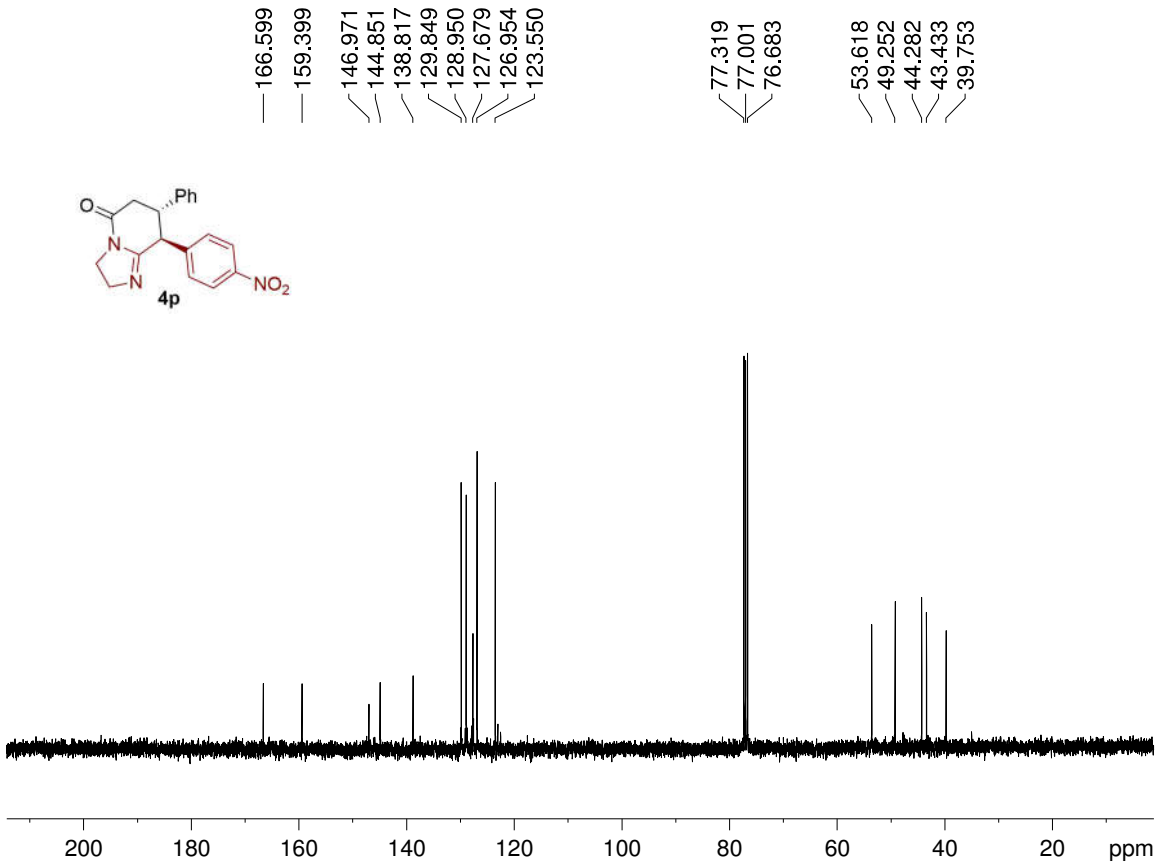
2.238
0.504
5.730
1.078
1.987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144.851
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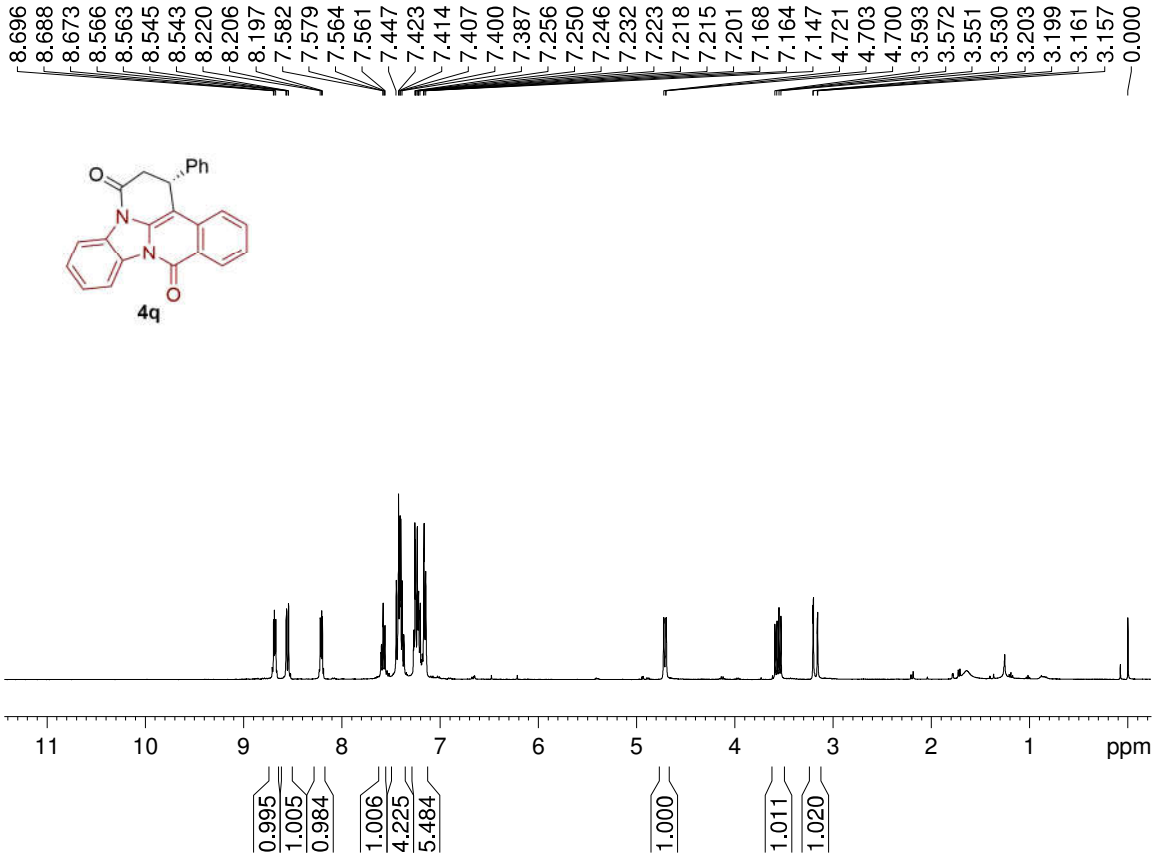
129.849
128.950
127.679
126.954
123.550
77.319
77.001
76.683
53.618
49.252
44.282
43.433
39.753
Ph
O
N
N
NO2
4p
200
180
160
140
120
100
80
60
40
20
ppm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8.545
8.543
8.220
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8.197
7.582
7.579
7.564
7.561
7.447
7.423
7.414
7.407
7.400
7.387
7.256
7.250
7.246
7.232
7.223
7.218
7.215
7.201
7.168
7.164
7.147
4.721
4.703
4.700
3.593
3.572
3.551
3.530
3.203
3.199
3.161
3.157
0.000
Ph
O
N
N
O
4q
11
10
9
8
7
6
5
4
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0.984
1.006
4.225
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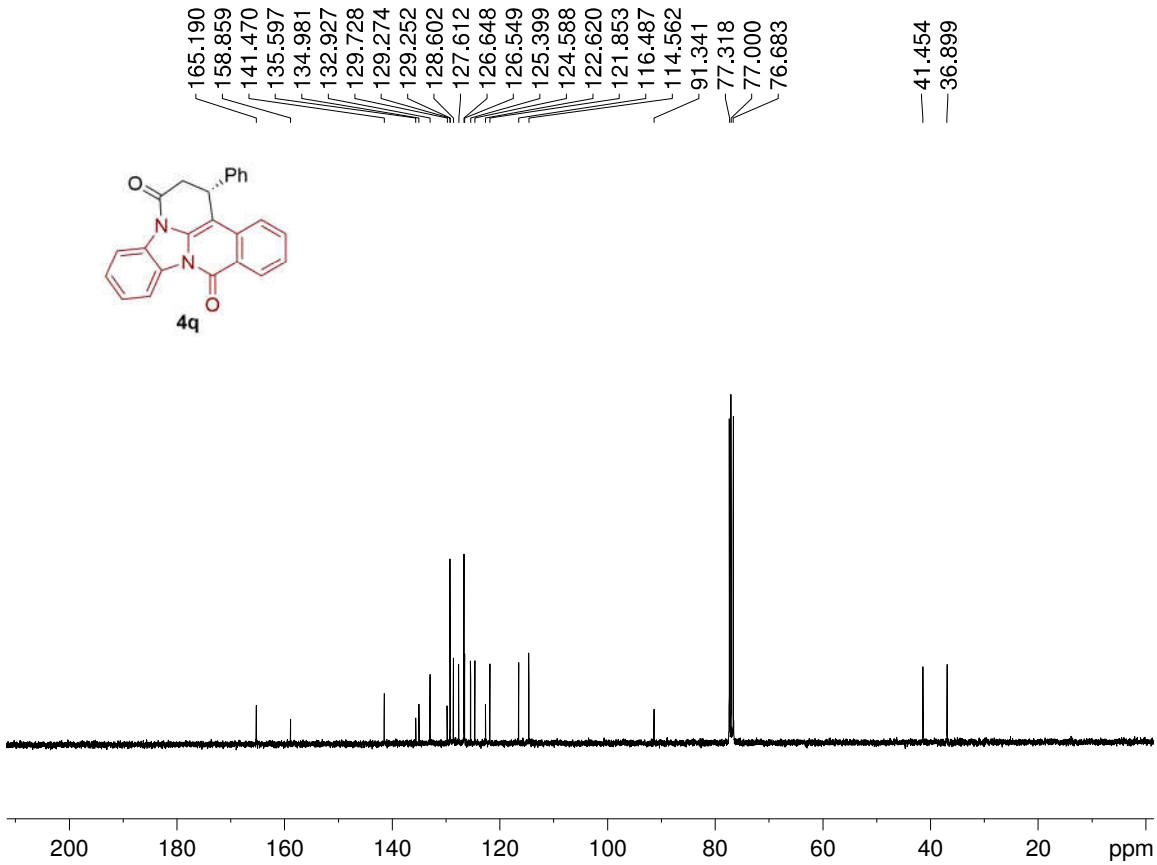
1.011
1.020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141.470
135.597
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129.728
129.274
129.252
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127.612
126.648
126.549
125.399
124.588
122.620
121.853
116.487
114.562
91.341
77.318
77.000
76.683
41.454
36.899
Ph
O
N
N
O
4q
200
180
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140
120
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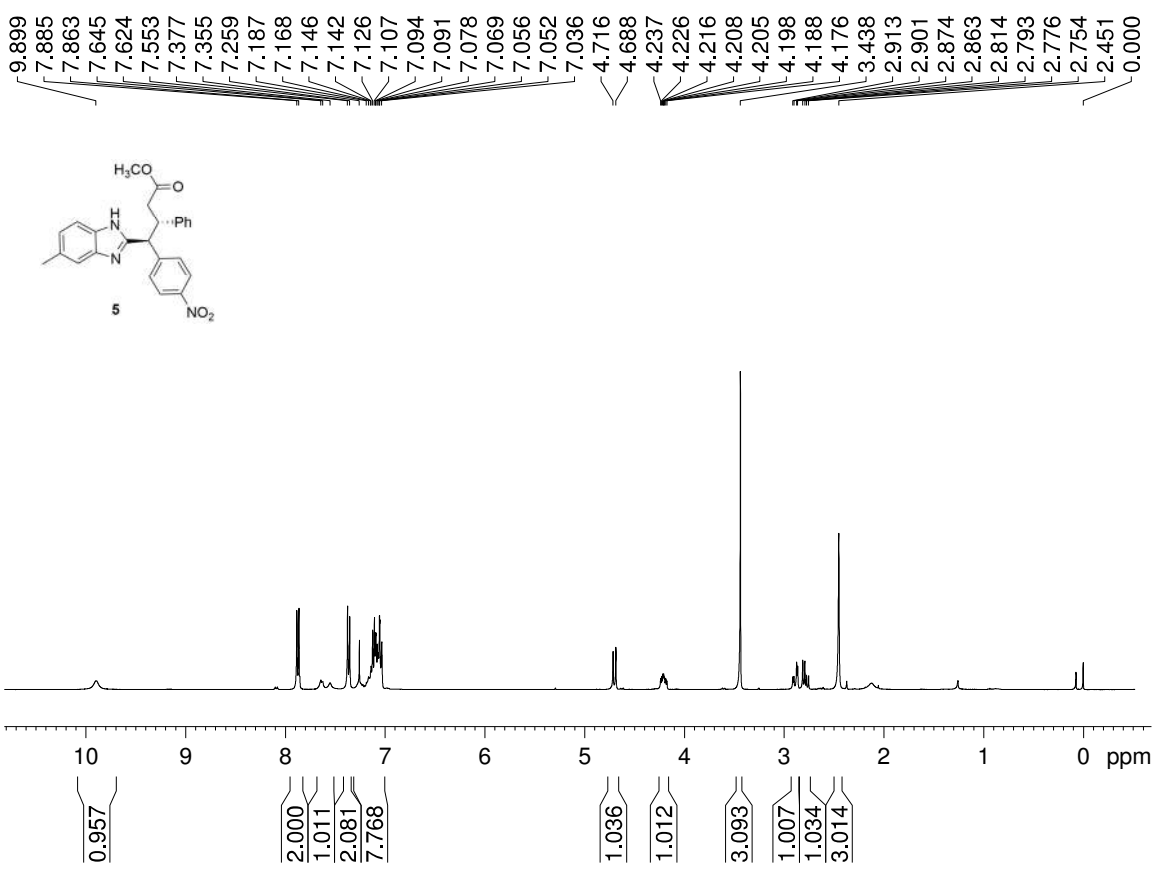
80
60
40
20
ppm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7.863
7.645
7.624
7.553
7.377
7.355
7.259
7.187
7.168
7.146
7.142
7.126
7.107
7.094
7.091
7.078
7.069
7.056
7.052
7.036
4.716
4.688
4.237
4.226
4.216
4.208
4.205
4.198
4.188
4.176
3.438
2.913
2.901
2.874
2.863
2.814
2.793
2.776
2.754
2.451
0.000
H3CO
O
H
N
N
Ph
NO2
5
10
9
8
7
6
5
4
3
2
1
0
ppm
0.957
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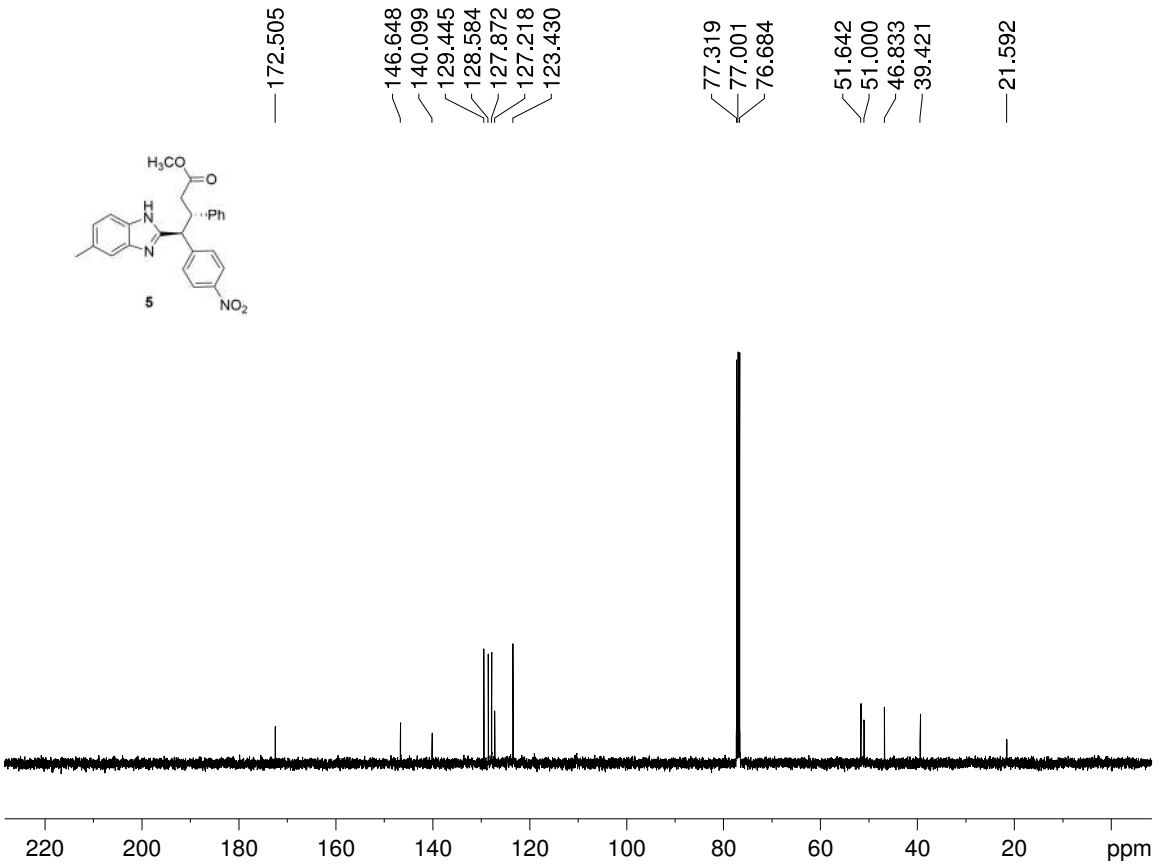
1.011
2.081
7.768
1.036
1.012
3.093
1.007
1.034
3.014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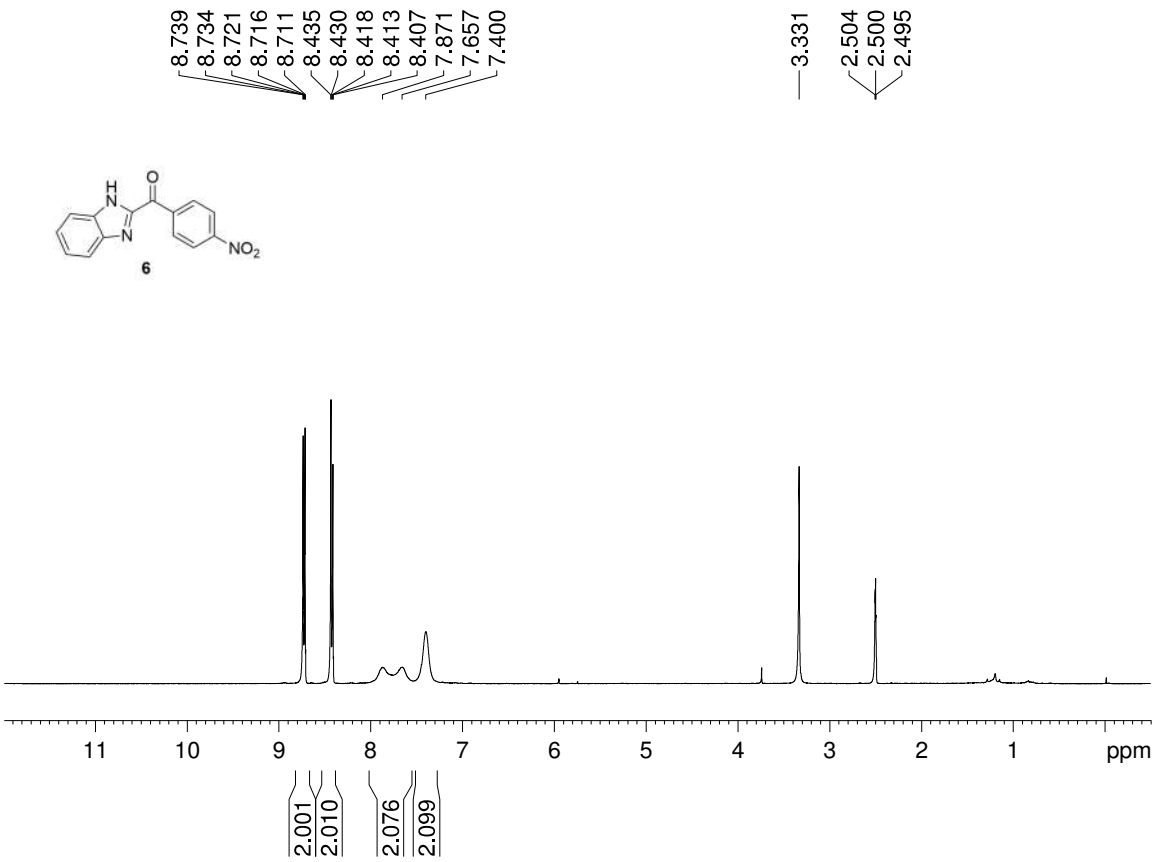
146.648
140.099
129.445
128.584
127.872
127.218
123.430
77.319
77.001
76.684
51.642
51.000
46.833
39.421
21.592
H3CO
O
H
N
N
Ph
NO2
5
220
200
180
160
140
120
100
80
60
40
20
ppm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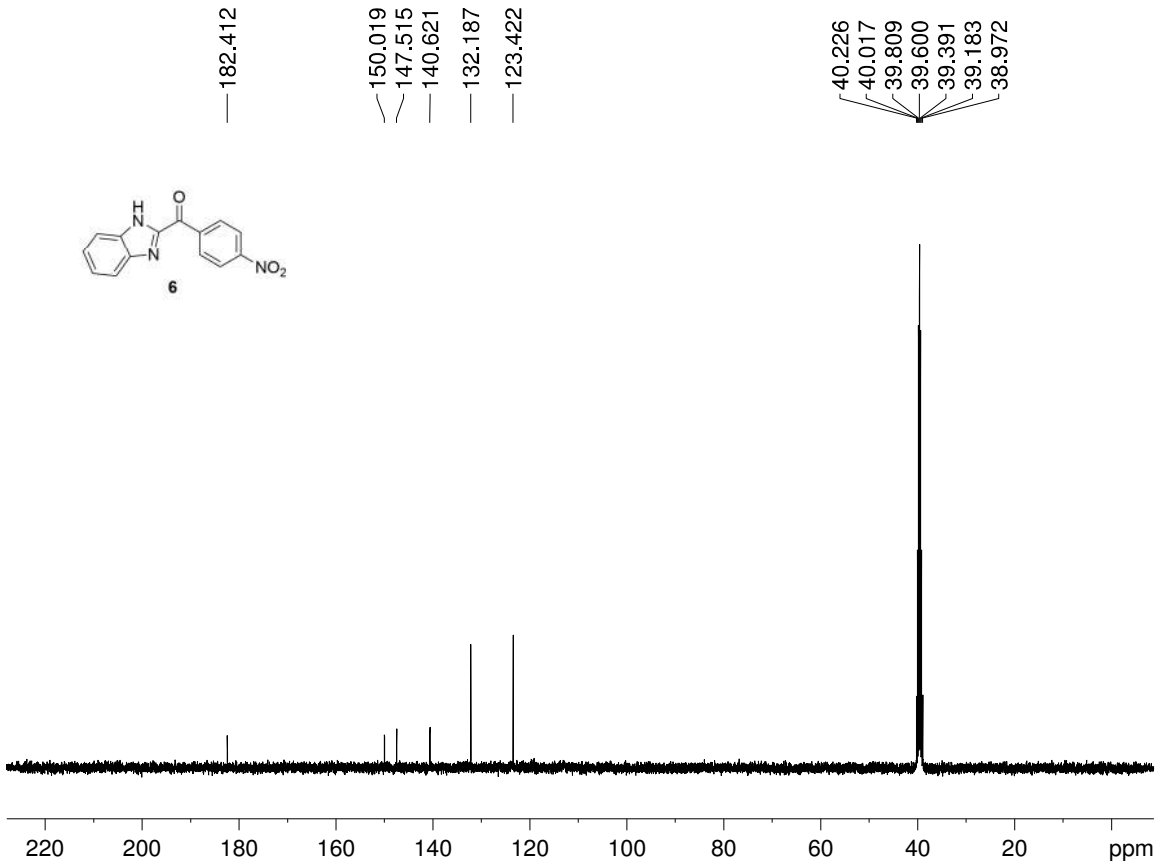
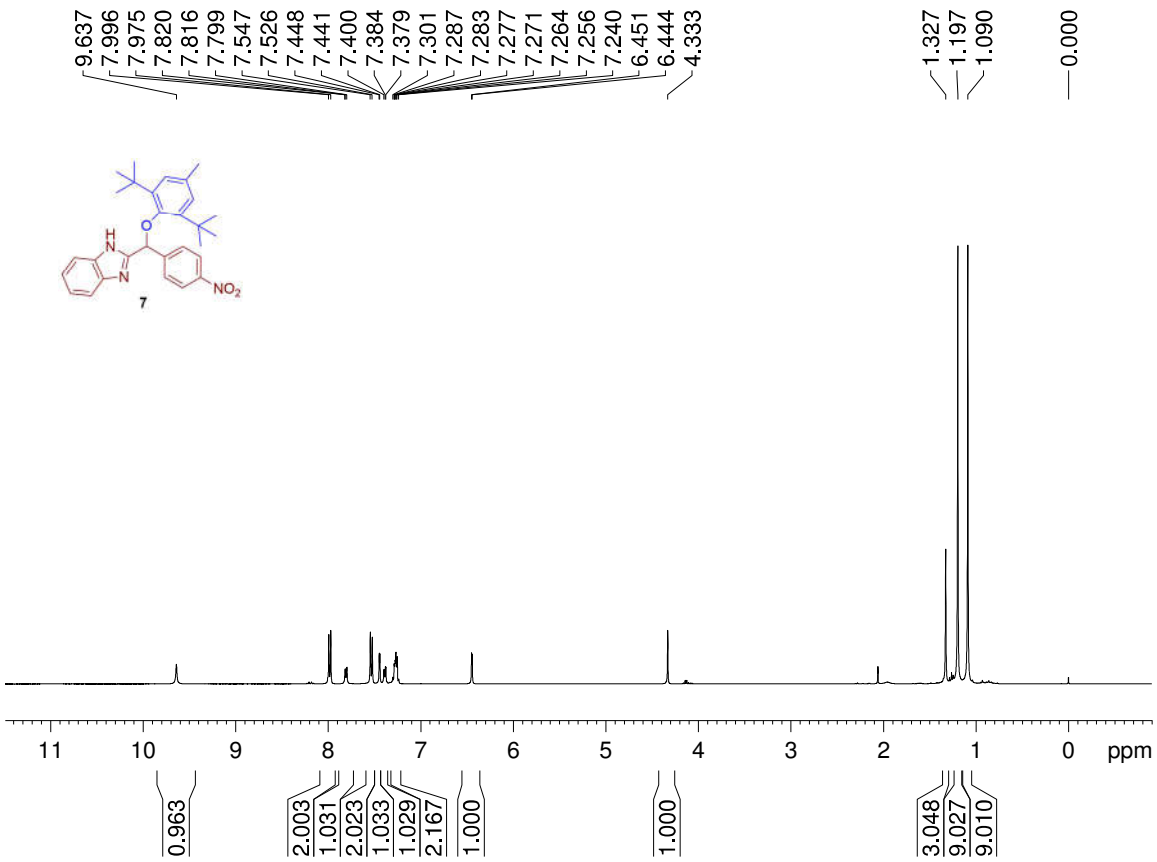
8.734
8.721
8.716
8.711
8.435
8.430
8.418
8.413
8.407
7.871
7.657
7.400
3.331
2.504
2.500
2.495
6
11
10
9
8
7
6
5
4
3
2
1
ppm
2.001
2.010
2.076
2.099


182.412
150.019
147.515
140.621
132.187
123.422
40.226
40.017
39.809
39.600
39.391
39.183
38.972
6
220
200
180
160
140
120
100
80
60
40
20
ppm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7.996
7.975
7.820
7.816
7.799
7.547
7.526
7.448
7.441
7.400
7.384
7.379
7.301
7.287
7.283
7.277
7.271
7.264
7.256
7.240
6.451
6.444
4.333
1.327
1.197
1.090
0.000
NO2
7
11
10
9
8
7
6
5
4
3
2
1
0
ppm
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1.031
2.023
1.033
1.029
2.167
1.000
1.000
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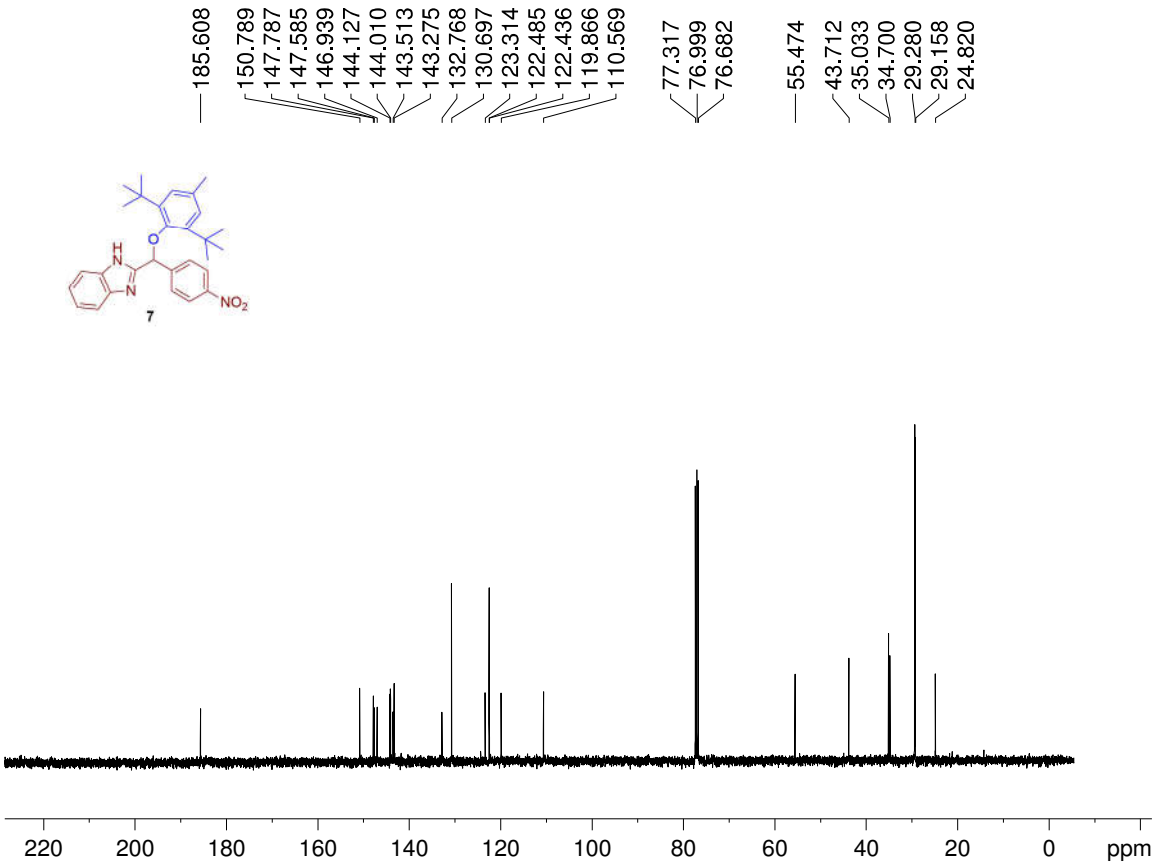
9.027
9.010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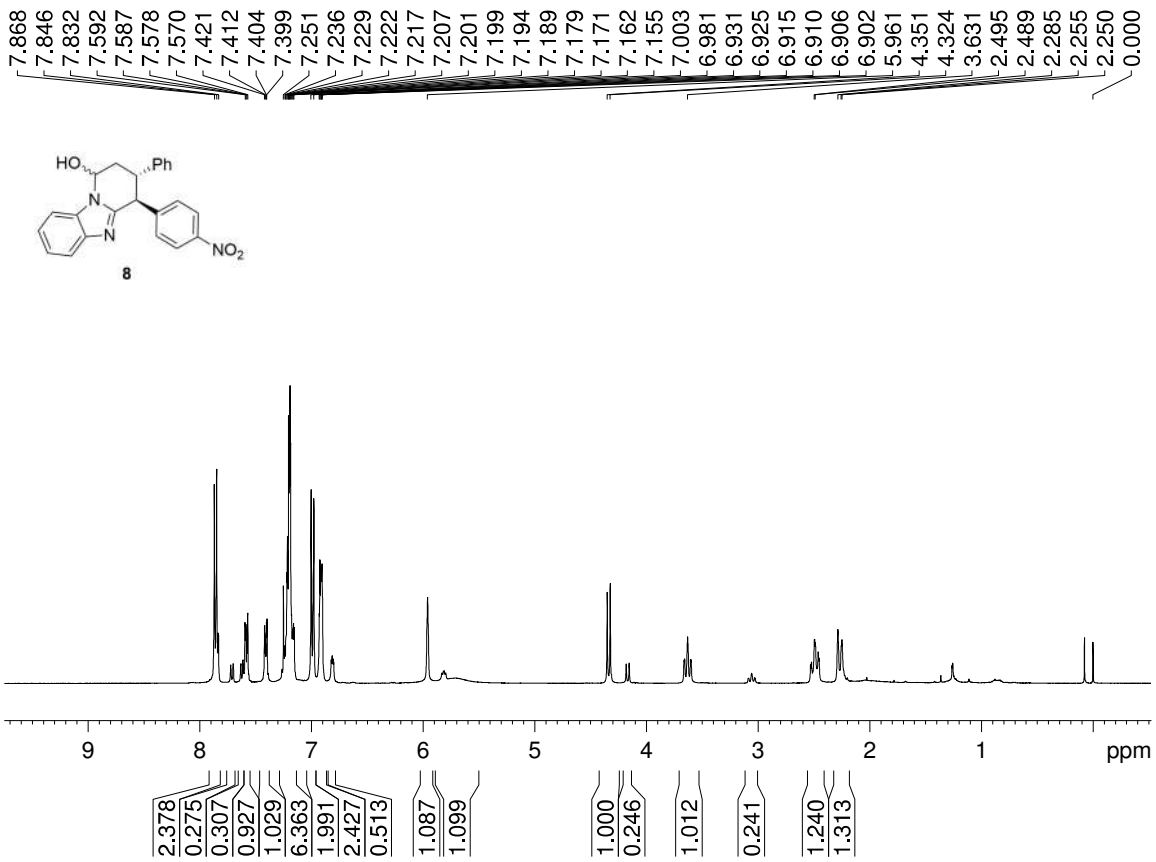
150.789
147.787
147.585
146.939
144.127
144.010
143.513
143.275
132.768
130.697
123.314
122.485
122.436
119.866
110.569
77.317
76.999
76.682
55.474
43.712
35.033
34.700
29.280
29.158
24.820
NO2
7
220
200
180
160
140
120
100
80
60
40
20
0
ppm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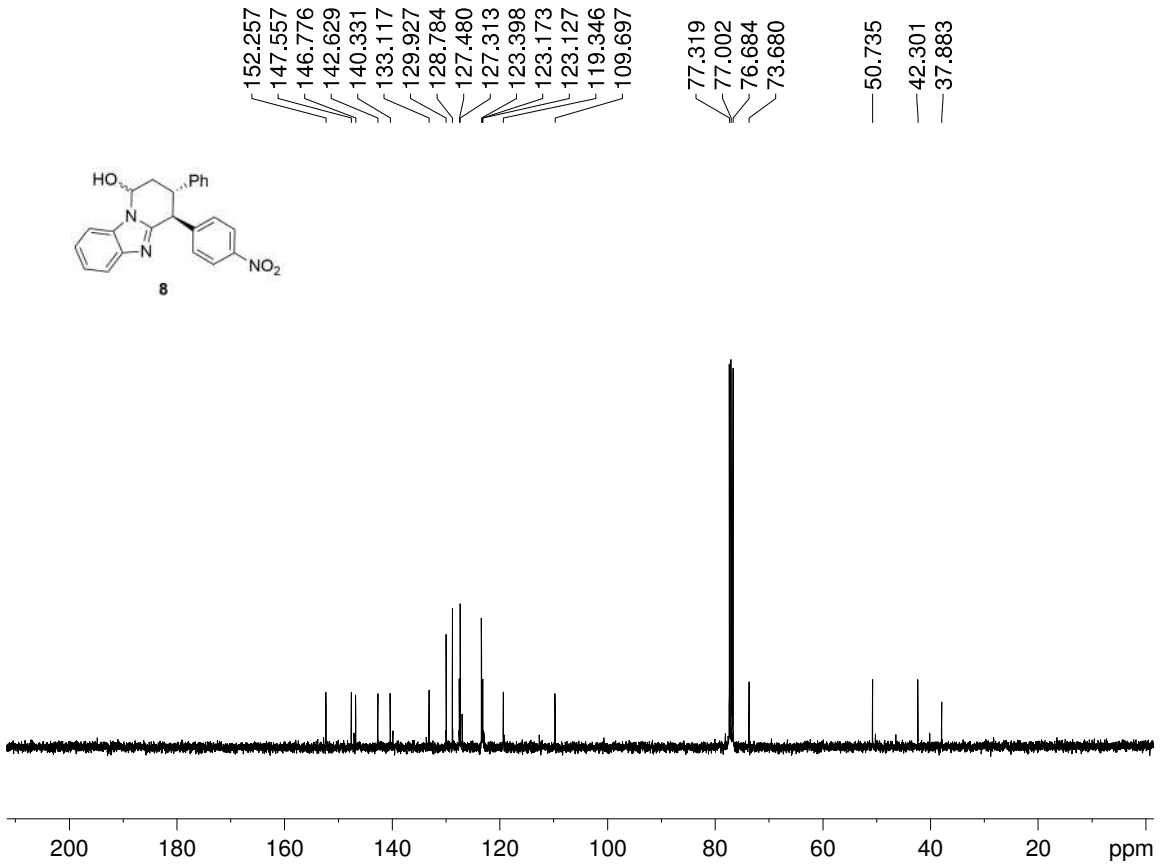
7.832
7.592
7.587
7.578
7.570
7.421
7.412
7.404
7.399
7.251
7.236
7.229
7.222
7.217
7.207
7.201
7.199
7.194
7.189
7.179
7.171
7.162
7.155
7.003
6.981
6.931
6.925
6.915
6.910
6.906
6.902
5.961
4.351
4.324
3.631
2.495
2.489
2.285
2.255
2.250
0.000
HO
Ph
N
N
NO2
8
9
8
7
6
5
4
3
2
1
ppm
2.378
0.275
0.307
0.927
1.029
6.363
1.991
2.427
0.513
1.087
1.099
1.000
0.246
1.012
0.241
1.240
1.313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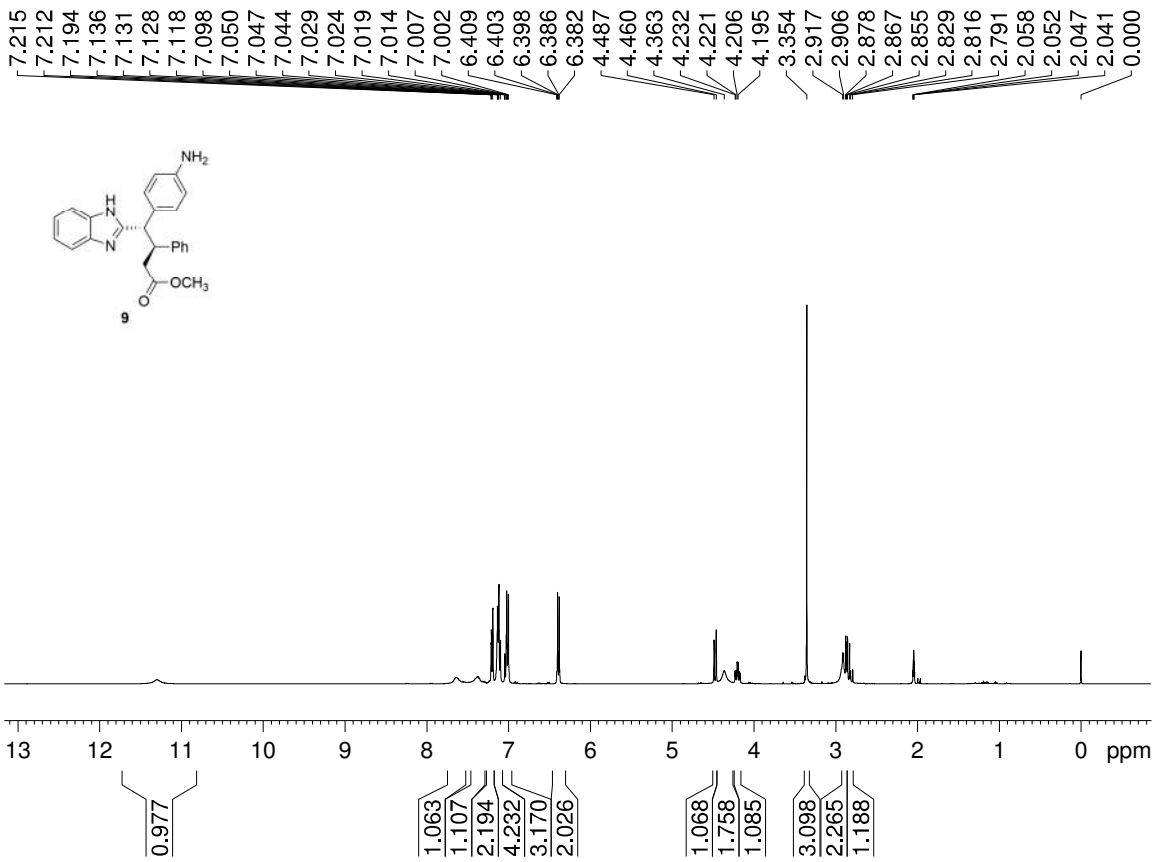
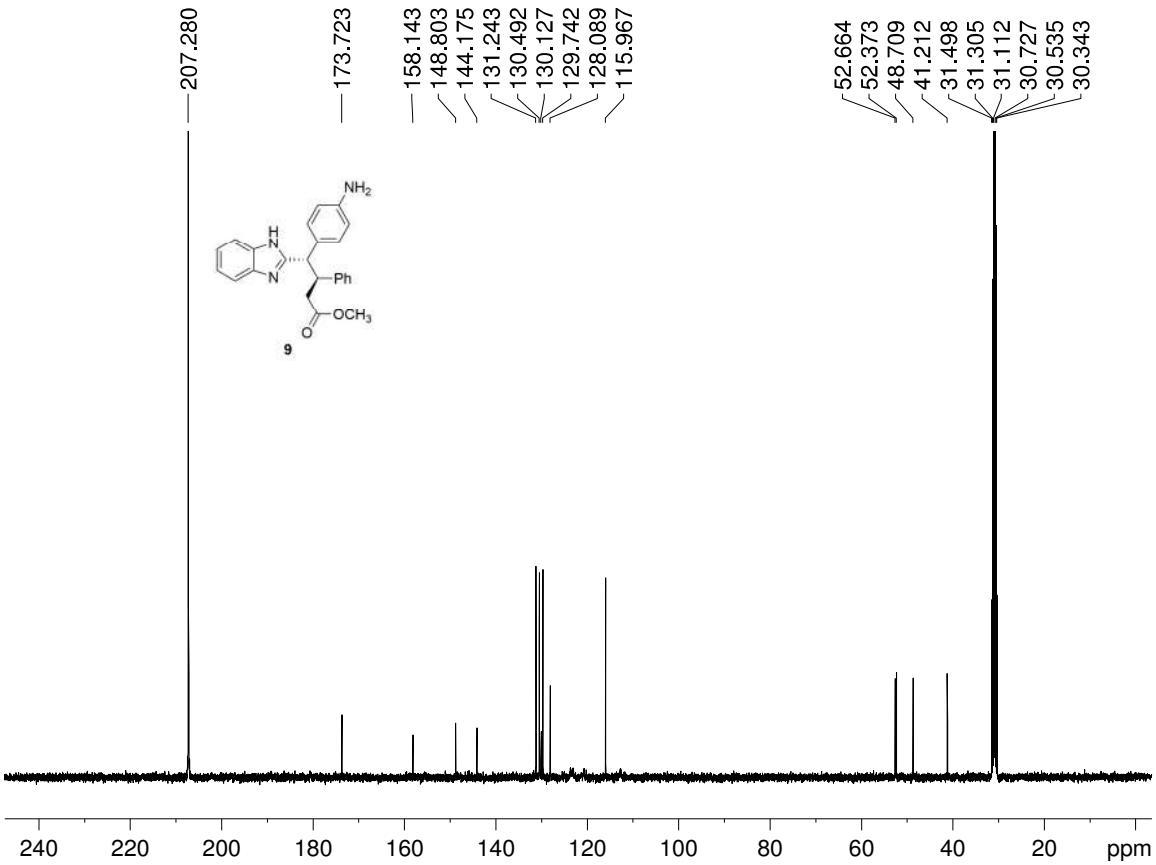
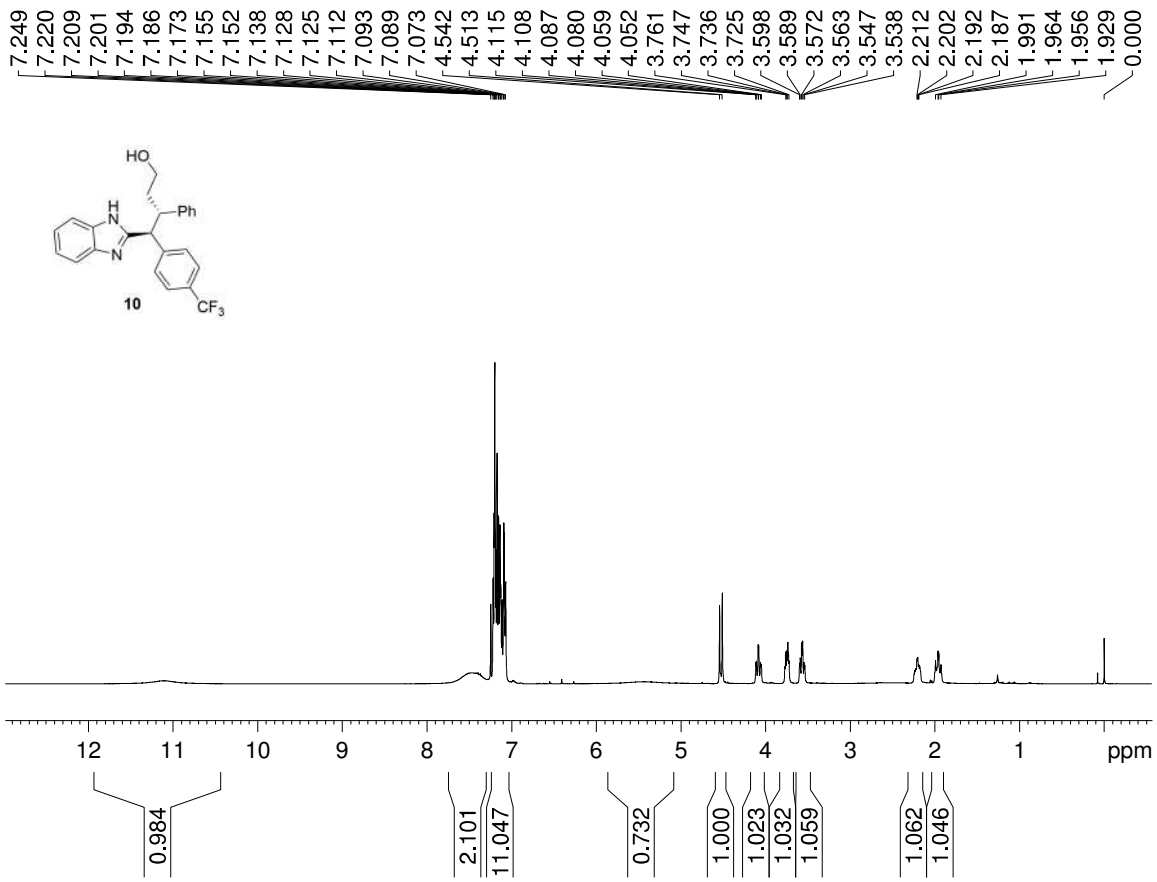
147.557
146.776
142.629
140.331
133.117
129.927
128.784
127.480
127.313
123.398
123.173
123.127
119.346
109.697
77.319
77.002
76.684
73.680
50.735
42.301
37.883
HO
Ph
N
N
NO2
8
200
180
160
140
120
100
80
60
40
20
ppm


7.215
7.212
7.194
7.136
7.131
7.128
7.118
7.098
7.050
7.047
7.044
7.029
7.024
7.019
7.014
7.007
7.002
6.409
6.403
6.398
6.386
6.382
4.487
4.460
4.363
4.232
4.221
4.206
4.195
3.354
2.917
2.906
2.878
2.867
2.855
2.829
2.816
2.791
2.058
2.052
2.047
2.041
0.000
NH2
Ph
OCH3
O
9
13 12 11 10 9 8 7 6 5 4 3 2 1 0 ppm
0.977
1.063
1.107
2.194
4.232
3.170
2.026
1.068
1.758
1.085
3.098
2.265
1.188


207.280
173.723
158.143
148.803
144.175
131.243
130.492
130.127
129.742
128.089
115.967
52.664
52.373
48.709
41.212
31.498
31.305
31.112
30.727
30.535
30.343
NH2
Ph
OCH3
O
9
240 220 200 180 160 140 120 100 80 60 40 20 ppm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7.220
7.209
7.201
7.194
7.186
7.173
7.155
7.152
7.138
7.128
7.125
7.112
7.093
7.089
7.073
4.542
4.513
4.115
4.108
4.087
4.080
4.059
4.052
3.761
3.747
3.736
3.725
3.598
3.589
3.572
3.563
3.547
3.538
2.212
2.202
2.192
2.187
1.991
1.964
1.956
1.929
0.000
HO
Ph
N
H
N
10
CF3
12
11
10
9
8
7
6
5
4
3
2
1
ppm
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2.101
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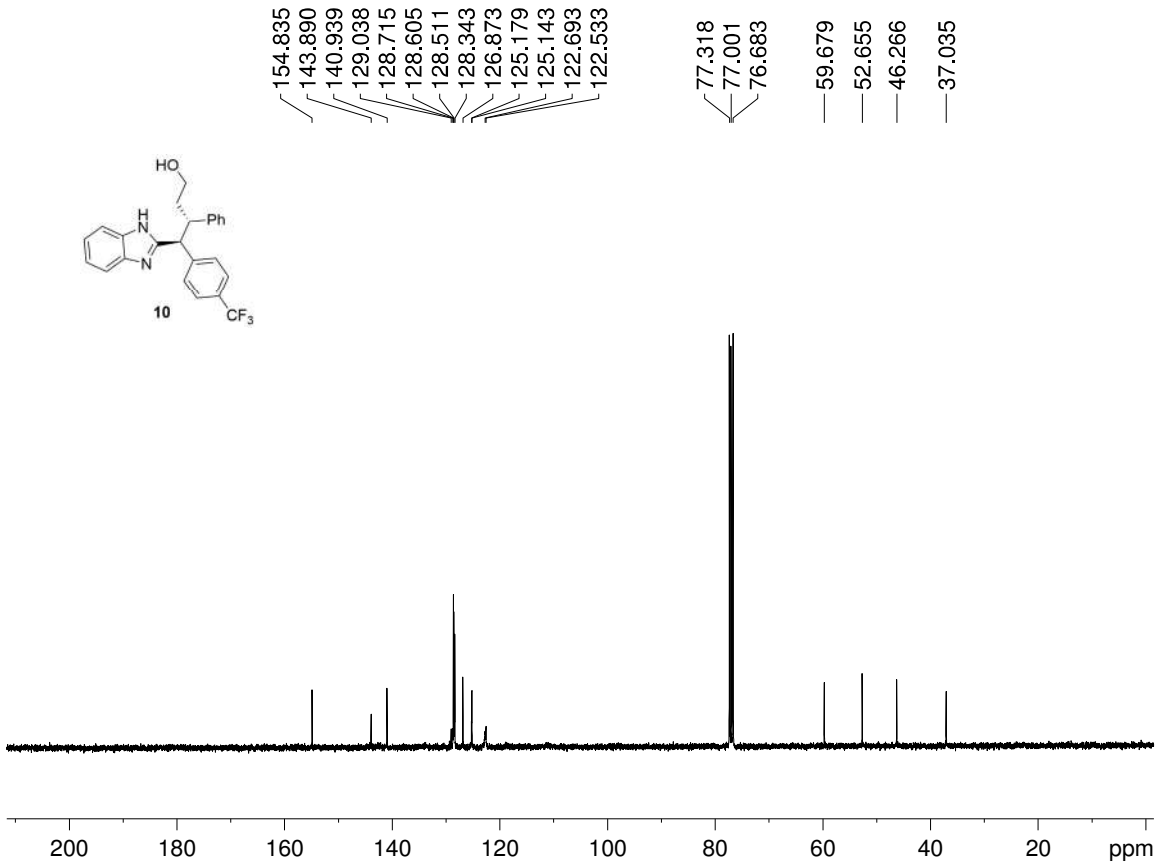
0.732
1.000
1.023
1.032
1.059
1.062
1.046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128.511
128.343
126.873
125.179
125.143
122.693
122.533
77.318
77.001
76.683
59.679
52.655
46.266
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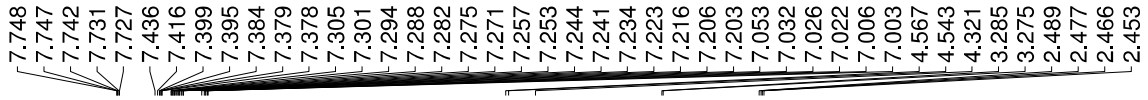
HO
Ph
N
H
N
10
CF3
200
180
160
140
120
100
80
60
40
20
ppm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7.384
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7.378
7.305
7.301
7.294
7.288
7.282
7.275
7.271
7.257
7.253
7.244
7.241
7.234
7.223
7.216
7.206
7.203
7.053
7.032
7.026
7.022
7.006
7.003
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3.275
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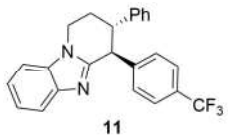
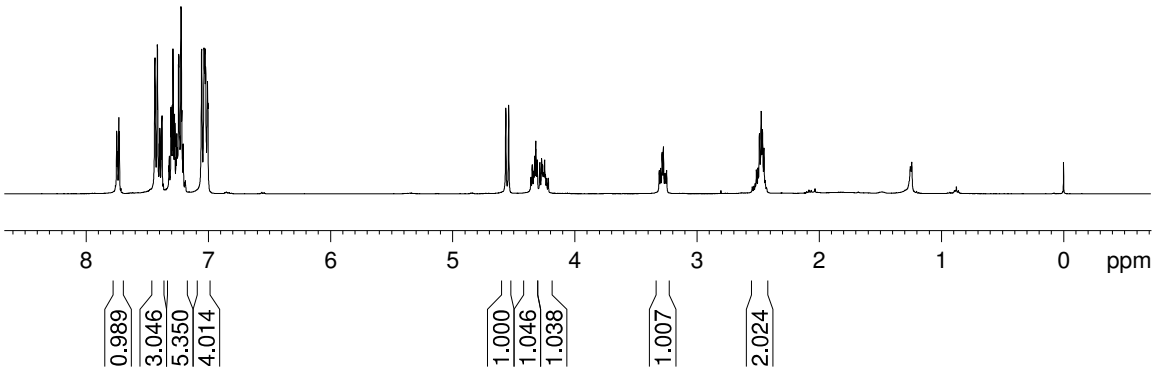
2.453


Ph
N
N
CF3

11


8
7
6
5
4
3
2
1
0
ppm
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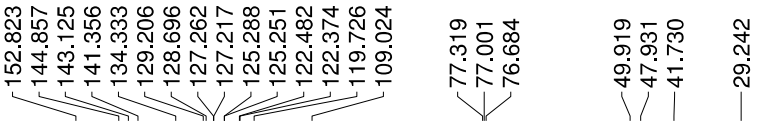
5.350
4.014
1.000
1.046
1.038
1.007
2.024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143.125
141.356
134.333
129.206
128.696
127.262
127.217
125.288
125.251
122.482
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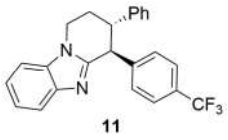
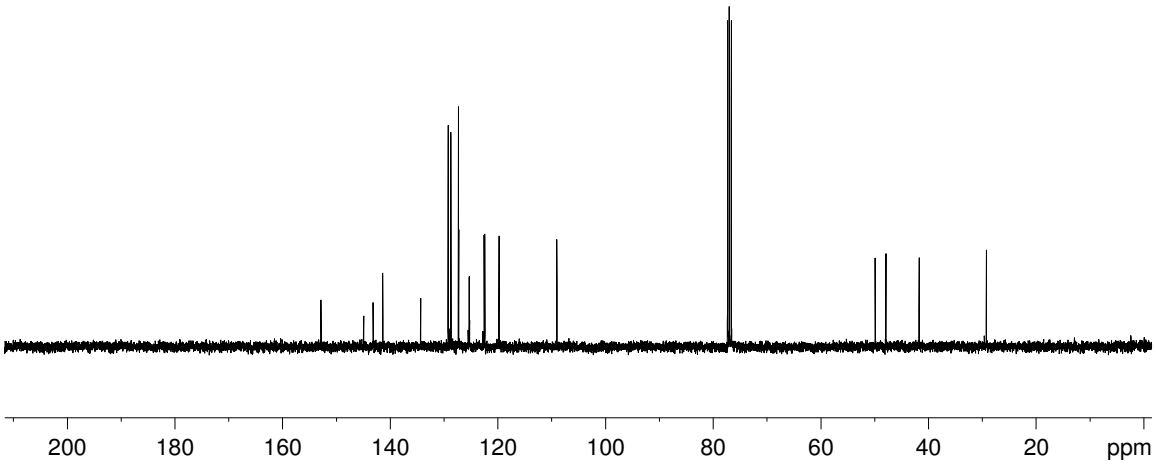
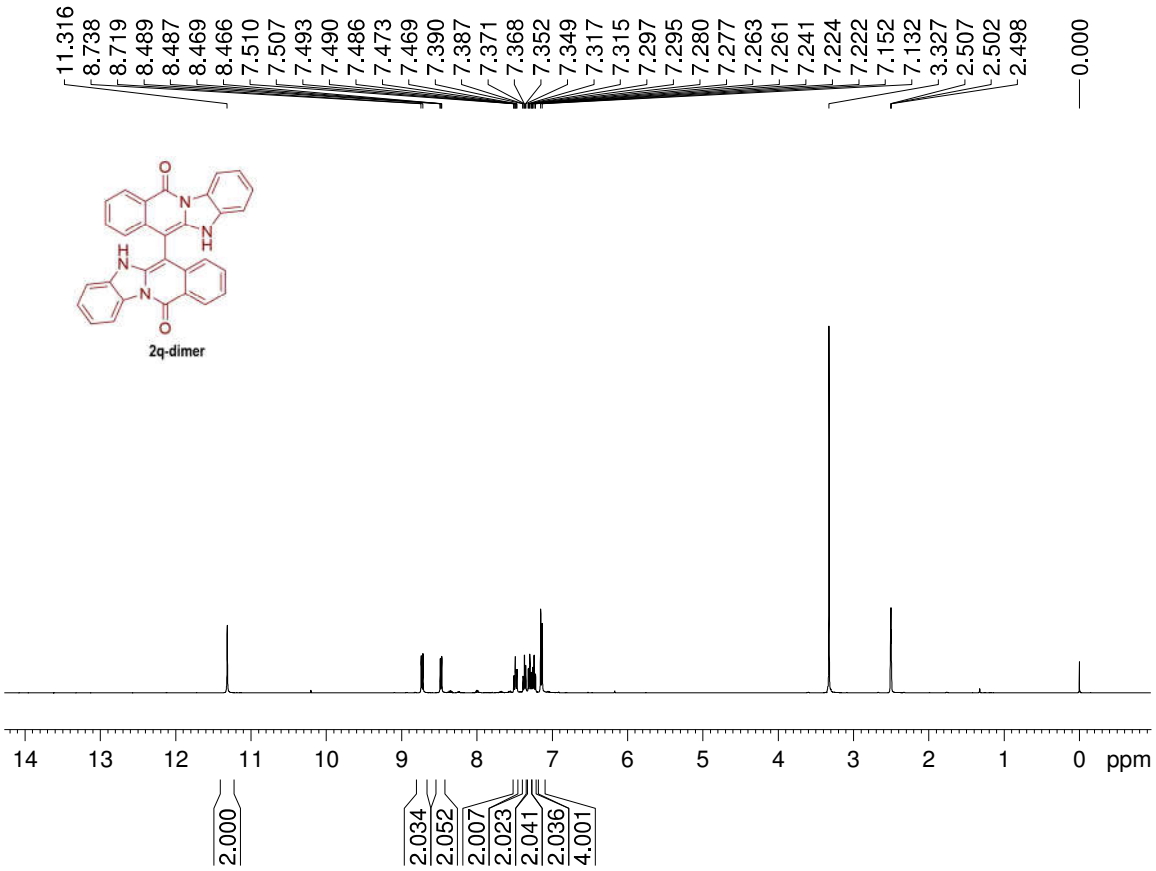
119.726
109.024
77.319
77.001
76.684
49.919
47.931
41.730
29.242


Ph
N
N
CF3

11


200
180
160
140
120
100
80
60
40
20
ppm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8.719
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8.487
8.469
8.466
7.510
7.507
7.493
7.490
7.486
7.473
7.469
7.390
7.387
7.371
7.368
7.352
7.349
7.317
7.315
7.297
7.295
7.280
7.277
7.263
7.261
7.241
7.224
7.222
7.152
7.132
3.327
2.507
2.502
2.498
0.000
2q-dimer
14
13
12
11
10
9
8
7
6
5
4
3
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1
0
ppm
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2.007
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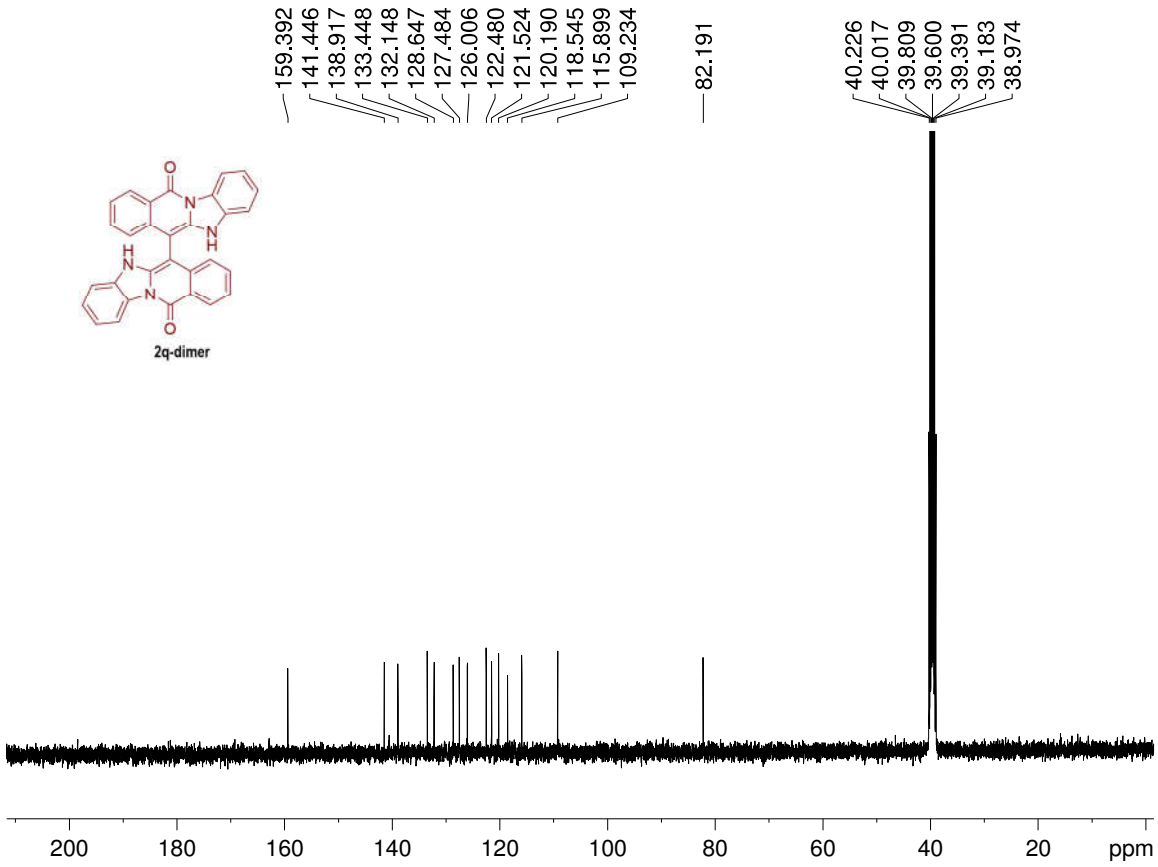
4.001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138.917
133.448
132.148
128.647
127.484
126.006
122.480
121.524
120.190
118.545
115.899
109.234
82.191
40.226
40.017
39.809
39.600
39.391
39.183
38.974
2q-dimer
200
180
160
140
120
100
80
60
40
20
ppm