Construction of Indeno[1,2-*b*]pyrroles *via* Chemoselective N-Acylation/Cyclization/Wittig Reaction Sequence

Athukuri Edukondalu,[a,‡] Sandip Sambhaji Vagh,[a,‡] Ting-Han Lin[a,] and Wenwei Lin[a,*]

a Department of Chemistry, National Taiwan Normal University, 88, Sec. 4, Tingchow Road, Taipei 11677, Taiwan, R.O.C.
‡ These authors contributed equally.

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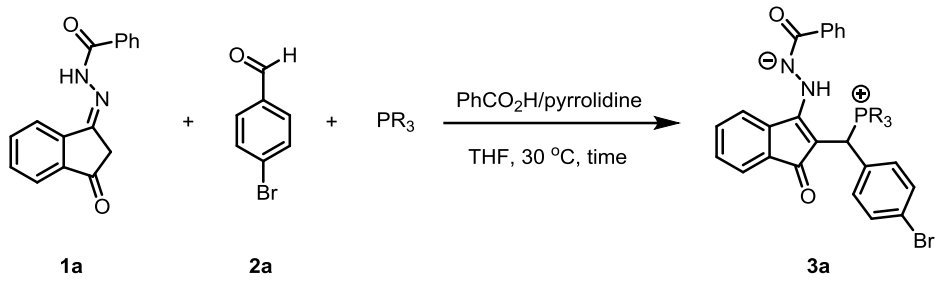
I. General information

All reactions were carried out under argon atmosphere in oven-dried glassware with magnetic stirring. Unless otherwise stated, all reagents were used as purchased from commercial suppliers without further purification. THF was continuously refluxed and freshly distilled from sodium benzophenone ketyl under argon atmosphere. Yields refer to isolated yields of compounds estimated to be >95% pure as determined by ^{1}H NMR. Analytical thin layer chromatography (TLC) was performed on pre coated alumina-backed silica gel plates (Merck 60 F254, 0.2 mm thickness) which were developed using UV irradiation at 254 nm. Flash column chromatography was performed using silica gel (SiliCycle SiliaFlash P60, 230-400 mesh). Melting points were measured on a hostage melting point apparatus and are uncorrected. IR spectra were recorded on a Perkin Elmer 500 spectrometer and only selected peaks are mentioned. ^{1}H NMR spectra were recorded on either an Oxford JEOL 400 MHz spectrometer or a Bruker Ascend 400 MHz spectrometer. ^{13}C NMR spectra at 100 MHz, ^{31}P NMR at 162 MHz and ^{19}F NMR at 376 MHz. Chemical shifts are reported in δ ppm referenced to an internal TMS standard (δ = 0.0 ppm) for ^{1}H NMR, CDCl3 (δ = 77.0 ppm) for ^{13}C NMR, DMSO-d_6 (δ 2.50 ppm for ^{1}H NMR and 39.52 ppm for ^{13}C NMR), H_3PO_4 (δ = 0.0 ppm) for ^{31}P NMR, and C_6H_5F (δ = -113.15 ppm) for ^{19}F NMR. The following abbreviations (or combinations thereof) were used to explain the multiplicities: s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet, dd = doublet of doublet, dt = doublet of triplet, td = triplet of doublet, tt = triplet of triplet, qd = quartet of doublet, br = broad, p = pseudo. High resolution mass spectra were recorded on Waters XeVo G2-S QTof using ESI (TOF analyzer). The X-ray diffraction measurements were carried out at 200 K on either a Bruker D8 Venture or a Bruker KAPPA APEX II CCD area detector system equipped with a graphite monochromator and a Mo-Kα fine-focus sealed tube (k = 0.71073 Å).

II. Reaction optimization for 6aa:

a) Optimization of reaction conditions for the synthesis of zwitterion 3/4[a]



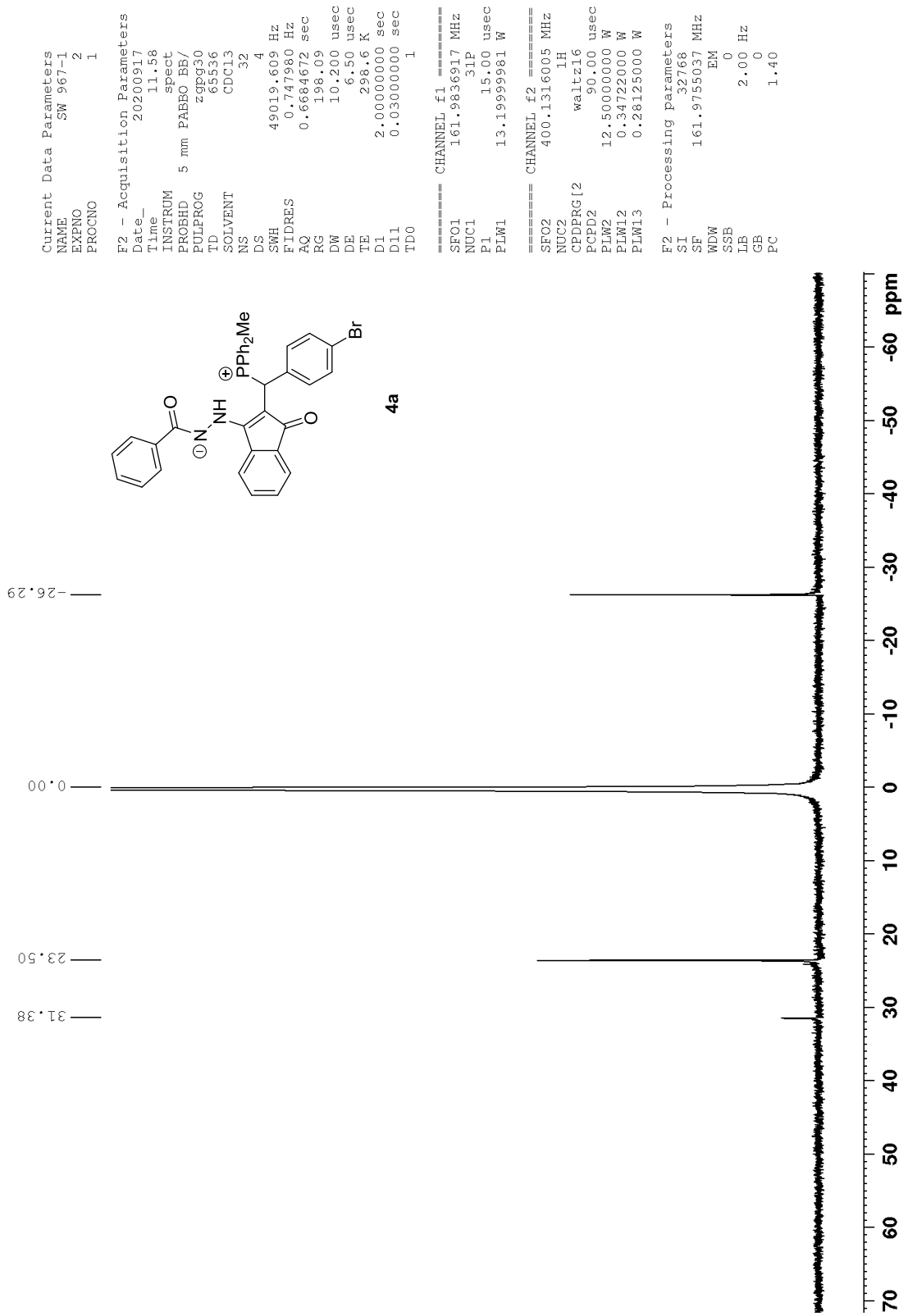
1a 2a 3a

entry	phosphine	*t* (h)	**3/4**[b]
1	PBu_3	5	90
2	PPh_3	16	nr
3	PPh_2Et	12	trace
4	PEt_2Ph	12	trace
5	PPh_2Me	6	75

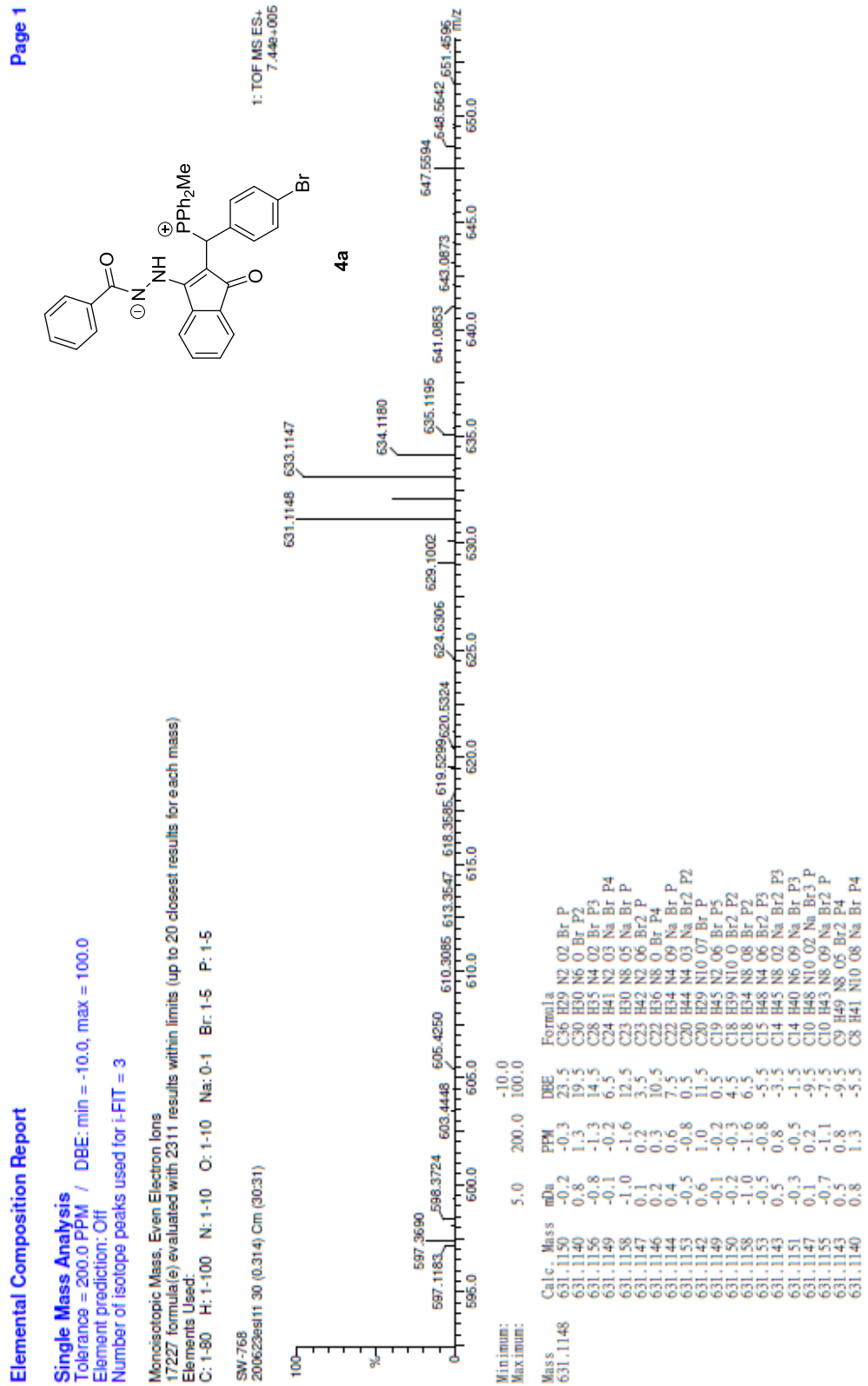
[a] The reactions were carried out with compound **1a** (0.3 mmol), 4-BrPhCHO (**2a**) (1.1 equiv), $PhCO_2H$ (0.1 equiv), PR_3 (1.2 equiv) and pyrrolidine (0.1 equiv) in anhydrous THF (3 mL) under argon at 30 °C. [b] Yield of the zwitterion **3a**/**4a** was determined by NMR analysis of the crude reaction mixture using 1,3,5-trimethoxybenzene as an internal standard. nr = no reaction.

It is noteworthy that the phosphorus zwitterions **3** are very stable and easily isolable and confirmed by the NMR, HRMS and X-ray analysis, further utilized for the desired indeno[1,2-*b*]pyrrole derivatives **6**/**7**. Unfortunately, the phosphorus zwitterions **4** were not able to isolate in pure form but crude reaction mixture was used for the one step reaction of spiro-indene-1,2'-[1,3,4]oxadiazol derivatives **8**. The phosphorus zwitterion **4a** from the crude reaction mixture was confirmed by the ^{31}PNMR and HRMS analysis.

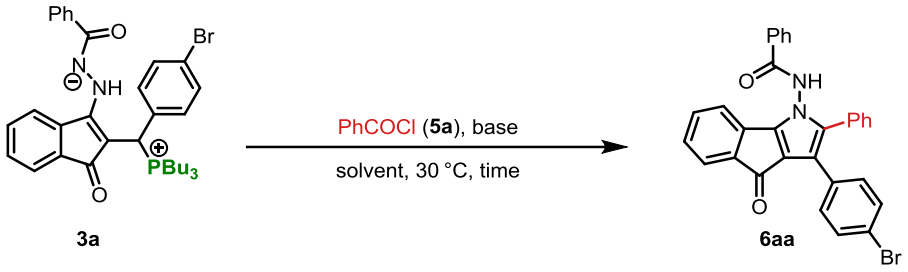
^{31}P NMR Spectrum of **4a** from the crude reaction mixture ($CDCl_3$, 162 MHz)



ESI-HRMS Spectrum of **4a** from the crude reaction mixture



b) Optimization of reaction conditions for the synthesis of compound 6[a]

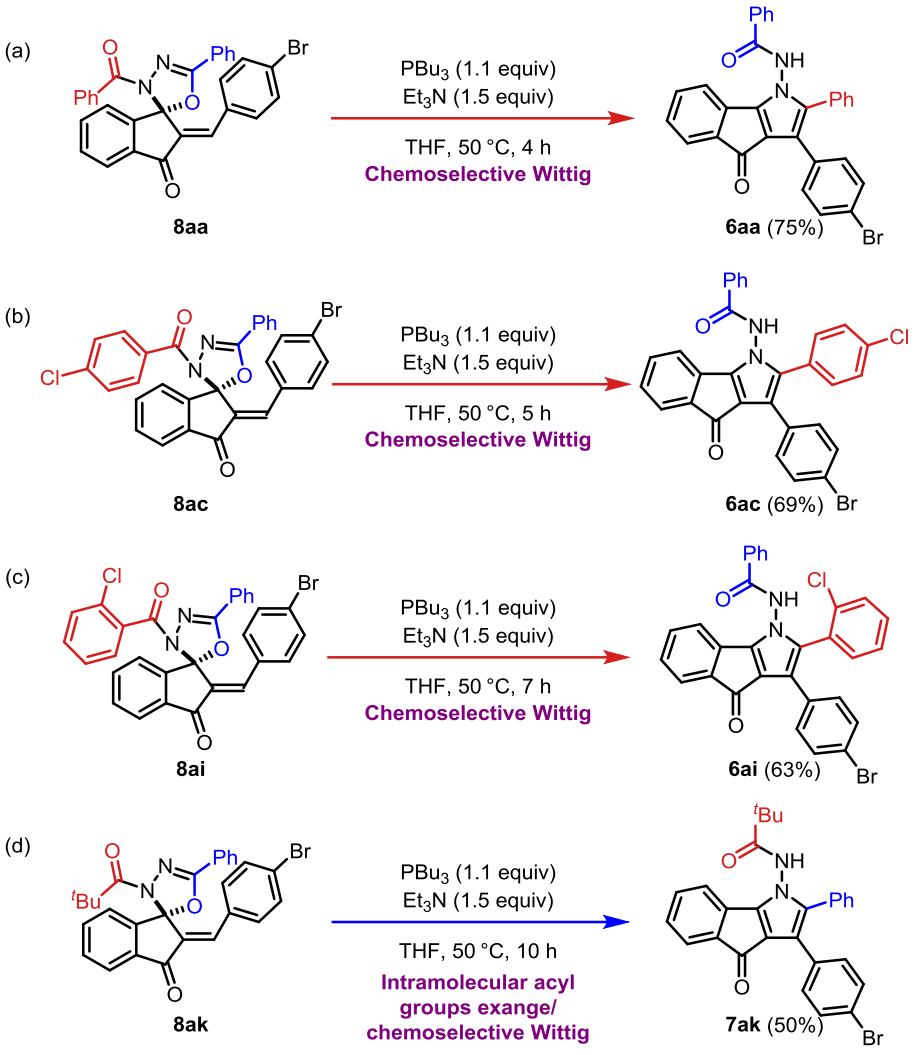


entry	base	solvent	*t* (h)	**6aa**[b]
1	Et_3N	THF	12	85
2	DIPEA	THF	18	60
3	DBU	THF	10	75
4	TMG	THF	10	51
5	TBD	THF	12	84
6	MTBD	THF	12	85
7	Et_3N	CH_2Cl_2	24	25
8	Et_3N	CH_3CN	24	50
9	Et_3N	toluene	48	47
10	Et_3N	Et_2O	24	65
11[c]	Et_3N	THF	4	85
12[d]	Et_3N	THF	4	90
13[d,e]	Et_3N	THF	4	76

[a] The reactions were carried out with compound **3a** (0.1 mmol), PhCOCl (**5a**) (1.1 equiv) and base (1.5 equiv) in dry solvent (1 mL.) under argon at 30 °C. [b] Yield of the product **6aa** was determined by NMR analysis of the crude reaction mixture using 1,3,5-trimethoxybenzene as an internal standard. [c] at 40 °C. [d] at 50 °C. [e] Addition sequence: compound **3a** (0.1 mmol), Et_3N (1.5 equiv) and PhCOCl (**5a**) (1.1 equiv) in dry solvent (1 mL.) under argon at 50 °C.

III. Control experiments:

Scheme S1.

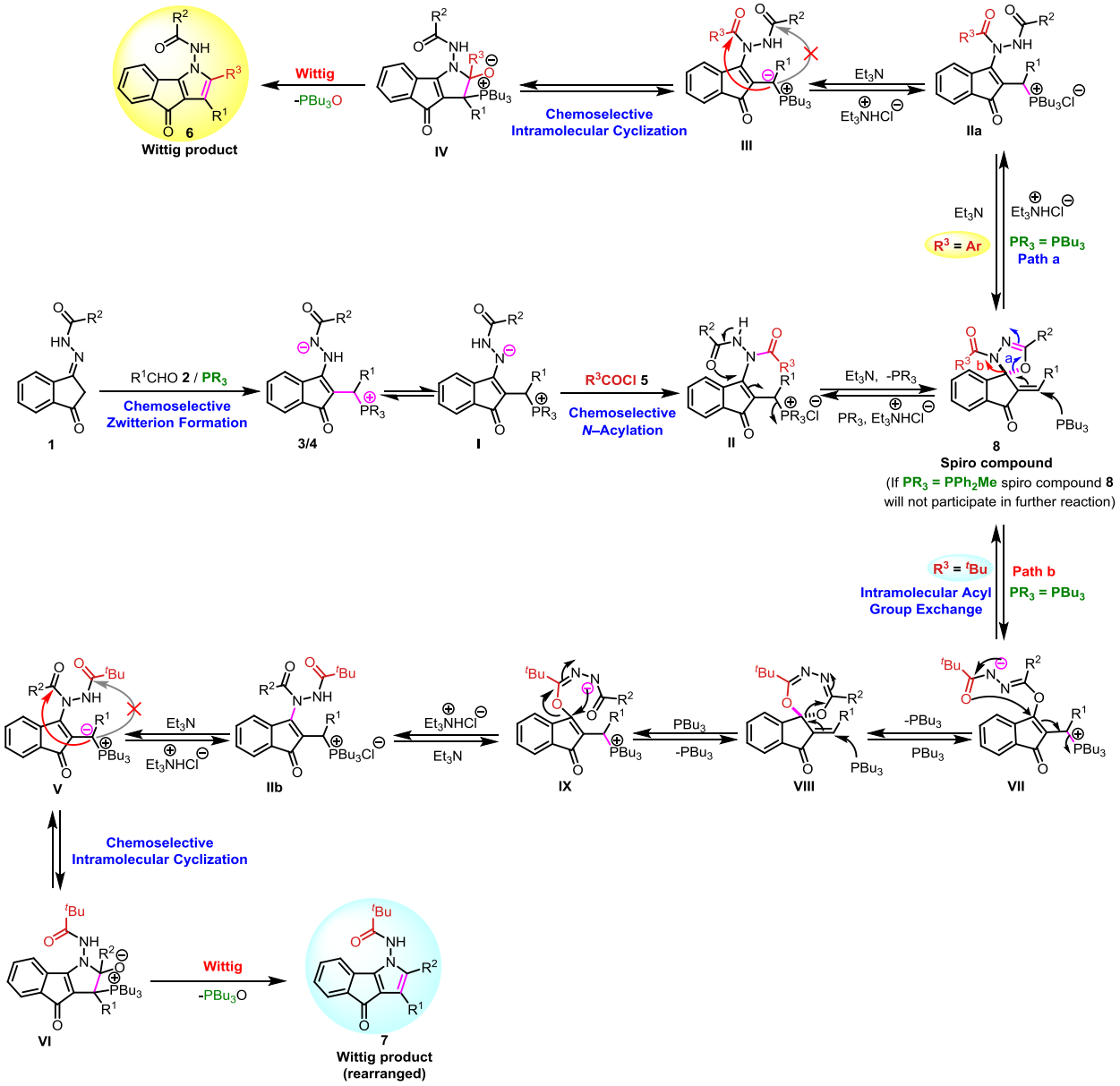


To investigate the mechanism, we have performed control experiments by using different spiro-indene-1,2'-[1,3,4]oxadiazol derivatives, PBu_3 and Et_3N at 50 °C. First, we examined the reaction between **8aa**, PBu_3 (1.1 equiv) in the presence of Et_3N (1.5 equiv) in THF at 50 °C. Interestingly, we have observed the **6aa** in 75% yield within 4 h (Scheme S1a). It could be understood that the spiro-indene-1,2'-[1,3,4]oxadiazol derivative is the key intermediate for the formation of indeno[1,2-*b*]pyrrole in our protocol. Similarly, we have carried out the reactions of *para*- and *ortho*-chloro substituted spiro-indene-1,2'-[1,3,4]oxadiazol derivatives such as **8ac** and **8ai** and PBu_3 (1.1 equiv) in the presence of Et_3N (1.5 equiv) in THF at 50 °C to afford the desired indeno[1,2-*b*]pyrrole derivatives **6ac** and **6ai** in 69% and 63% yields, respectively (Scheme 1b,

and 1c). We have further confirmed the products **6ac** and **6ai** by using EI mass analysis.

Accordingly, pivaloyl group substituted compound **8ak** was also reacted with PBu_3 (1.1 equiv) in the presence of Et_3N (1.5 equiv) in THF at 50 °C, and the rearranged indeno[1,2-*b*]pyrrole **7ak** was obtained in 50 % yield instead of **6ak** in 10 h (Scheme 1d). Further, X-ray and EI mass analysis unambiguously confirmed that the product is rearranged indeno[1,2-*b*]pyrrole **7ak**.

Scheme S2. Plausible Mechanism.

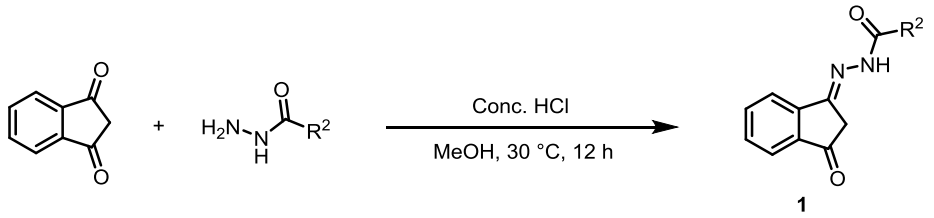


Based on the results and control experiments, a plausible mechanism is depicted in Scheme S2. Initially, a chemoselective tandem three-component reaction of indane-1,3-dione hydrazone **1**,

aldehyde **2**, and phosphine furnished the phosphorus zwitterion **3/4** which could be interchangeable with another possible zwitterion **I**. The chemoselective *N*–acylation of the zwitterion **I** with acyl chloride **5** would generate phosphonium salt **II** that can easily cyclize to give the spiro compound **8** via the allylic substitution with elimination of PR_3. When eliminated PR_3 has less nucleophilic nature such as PPh_2Me, only the spiro compound **8** would be provided. Instead, a more nucleophilic PR_3, such as PBu_3, would further react with **8** to generate the phosphonium salt **IIa** (Path a). The deprotonation of **IIa** by Et_3N generates ylide **III**, and subsequent chemoselective intramolecular Wittig reaction upon **III** would lead to the indeno[1,2-*b*]pyrrole **6** via the formation of a crucial betaine **IV**. On the other hand, the less reactive and hindered pivaloyl group present on the spiro compound **8** would facilitate the intramolecular acyl group exchange to generate the phosphonium salt **IIb** via the sequence of allylic substitution/elimination of PBu_3 and rearrangement reaction with the formation of the intermediates **VII**–**IX** (Path b). Further, deprotonation of **IIb** would provide ylide **V** in the presence of Et_3N, and subsequent chemoselective intramolecular Wittig reaction upon ylide **V** would result in the rearranged indeno[1,2-*b*]pyrrole **7**.

IV. Experimental Procedures:

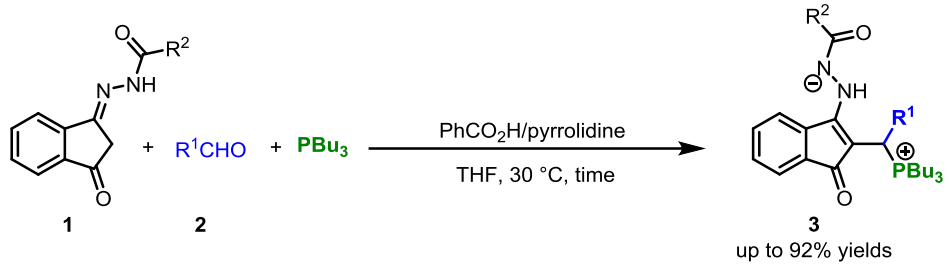
a) Typical procedure (TP-1) for the preparation of indenone-benzohydrazide derivatives 1



1

A 100 mL round bottom flask equipped with a magnetic stir bar and a septum was sequentially charged with 1,3-indandione (5 mmol), benzhydrazide derivative (1.05 equiv) in MeOH (50 mL) and Conc. HCl (2-3 drops) at 30 °C and the reaction mixture was stirred for 12 hours. After completion of reaction, filtered the solid by using Bukner funnel. Then washed with cold MeOH (10 mL), and purified by flash chromatography (MeOH/DCM: 1/100) to furnish the desired products **1** as solid in almost quantitative yields.

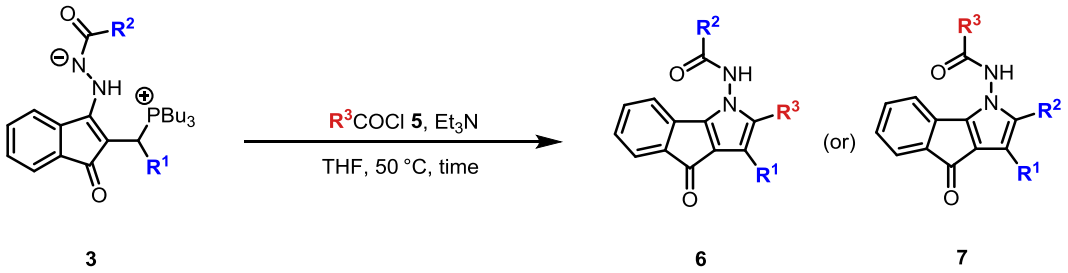
b) Typical procedure (TP-2) for the preparation of phosphorus zwitterion derivatives 3[1]



A flame dried and nitrogen-flushed 25-mL round bottom flask equipped with a magnetic stir bar and a septum was sequentially charged with **1** (0.5 mmol), **2** (1.1 equiv), $PhCO_2H$ (0.1 equiv) and anhydrous THF (5.0 mL). To this stirred reaction mixture, PBu_3 (1.2 equiv) and pyrrolidine (0.1 equiv) were added in sequence. The reaction mixture was stirred for 12 hours at 30 °C. Thereafter, solvent was removed by evaporation in *vacuo*. Purification by flash chromatography (EtOAc/hexanes: 1/3 then MeOH/DCM: 1/100) furnished the desired products **3** in almost quantitative yields.

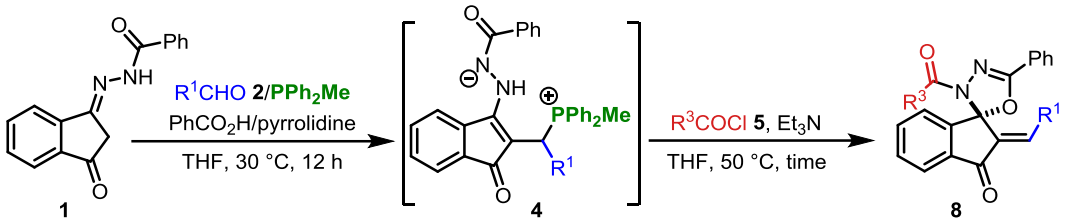
Note: ^{1}H, ^{13}C spectra of compounds **1a, 1i, 1j** and ^{1}H, ^{13}C, ^{31}P NMR spectra of compounds **3a-3j** showed intense broadening and considerable complexity due to their tautomeric and rotameric equilibria.[2]

c) Typical procedure (TP-3) for the preparation of indeno[1,2-*b*]pyrrole derivatives 6/7:



A dry and argon-flushed 10 mL Schlenk flask equipped with a magnetic stir bar and septum was sequentially charged with **3** (0.3 mmol), anhydrous THF (3 mL), acyl chloride **5** (1.1 equiv) and Et_3N (1.5 equiv). The reaction mixture was stirred for 1-8 h at 50 °C. After completion of the reaction, solvent was removed in *vacuo* and the crude residue was subjected to flash column chromatography on silica gel to obtain the product **6/7**.

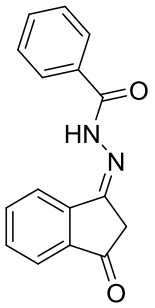
d) Typical procedure (TP-4) for the preparation of spiro-indene-1,2'-[1,3,4]oxadiazol derivatives 8:



A flame dried and nitrogen-flushed 25-mL round bottom flask equipped with a magnetic stir bar and a septum was sequentially charged with **1** (0.5 mmol), **2** (1.1 equiv), $PhCO_2H$ (0.1 equiv) and anhydrous THF (5.0 mL). To this stirred reaction mixture, PPh_2Me (1.2 equiv) and pyrrolidine (0.1 equiv) were added in sequence. The reaction mixture was stirred for 12 hours at 30 °C. Thereafter, solvent with excess volatile substrates were removed by evaporation in *vacuo* and dissolved in anhydrous THF (5 mL), acyl chloride **5** (1.5 equiv) and Et_3N (2.0 equiv). The reaction mixture was stirred for 1-4 h at 50 °C. After completion of the reaction, solvent was removed in *vacuo* and the crude residue was subjected to flash column chromatography on silica gel to obtain the product **8**.

V. Analytical data for all new compounds:

(*Z*)-*N*'-(3-Oxo-2,3-dihydro-1*H*-inden-1-ylidene)benzohydrazide (1a)



Prepared according to TP-1 from 1,3-Indandione (730.8 mg, 5.0 mmol), benzhydrazide (714.8 mg, 1.05 equiv), in MeOH (50 mL) followed by addition of Conc. HCl (3 drops) at 30 °C for 12 h. Thereafter, filtration of the reaction mixture and washed with cold MeOH (10 mL). Futher, purification by flash chromatography (SiO_2, EtOAc/hexanes: 1/2 and then MeOH/DCM: 1/100) furnished the desired product **1a** as green solid (1.21 g, 92%).

R_f = 0.51 (MeOH/DCM: 5/95), mp.: 213.8-214.7 °C.

^{1}H NMR (400 MHz, DMSO-d_6, 25 °C) δ/ppm: 10.91 (s, 1H), 8.13 – 7.98 (m, 1H), 7.99 (d, J = 8.1 Hz, 2H), 7.83 (t, J = 8.1 Hz, 1H), 7.78 (d, J = 7.6 Hz, 1H), 7.66 (t, J = 7.6 Hz, 1H), 7.60 (t, J =

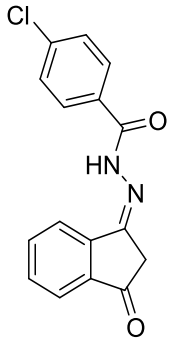
7.3 Hz, 1H), 7.53 (pt, *J* = 7.5 Hz, 2H), 3.69 (s, 2H).

^{13}C NMR (100 MHz, DMSO-d_6, 25 °C) δ/ppm: 198.4, 164.1, 152.0, 146.4, 138.4, 135.5, 133.7, 131.7, 131.3, 128.6, 128.3, 128.1, 127.5, 122.9, 121.9, 38.7.

IR (KBr) $\tilde{\nu}$ (cm^{-1}): 3075, 1725, 1698, 1526, 1375, 790.

HRMS (ESI) *m/z*: $[M+H]^+$ Calcd for $C_{16}H_{13}N_2O_2$ 265.0977; found: 265.0975.

(*Z*)-4-Chloro-*N*'-(3-oxo-2,3-dihydro-1*H*-inden-1-ylidene)benzohydrazide (1i)



Prepared according to TP-1 from 1,3-Indandione (292.3 mg, 2.0 mmol), 4-chloro benzhydrazide (358.2 mg, 1.05 equiv), in MeOH (20 mL) followed by addition of Conc. HCl (1 drop) at 30 °C for 12 h. Thereafter, filtration of the reaction mixture and washed with cold MeOH (5 mL). Futher, purification by flash chromatography (SiO_2, EtOAc/hexanes: 1/2 and then MeOH/DCM: 1/100) furnished the desired product **1i** as white solid (507.8 mg, 85%).

R_f = 0.48 (MeOH/DCM: 5/95), mp.: 254.6-255.7 °C.

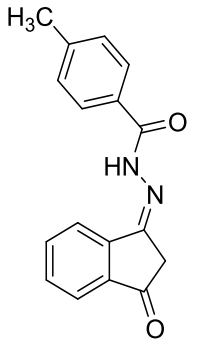
^{1}H NMR (400 MHz, DMSO-d_6, 25 °C) δ/ppm: 10.96 (s, 1H), 8.07 – 7.97 (m, 1H), 7.92 (d, *J* = 8.4 Hz, 2H), 7.83 (t, *J* = 7.5 Hz, 1H), 7.78 (d, *J* = 7.6 Hz, 1H), 7.66 (t, *J* = 7.1 Hz, 1H), 7.60 (d, *J* = 8.2 Hz, 2H), 3.68 (s, 2H).

^{13}C NMR (100 MHz, DMSO-d_6, 25 °C) δ/ppm: 198.3, 163.1, 152.5, 146.3, 138.5, 136.5, 135.5, 132.4, 131.4, 130.0, 128.4, 122.9, 121.9, 38.8.

IR (KBr) $\tilde{\nu}$ (cm^{-1}): 3070, 1724, 1672, 1510, 1370, 750.

HRMS (ESI) *m/z*: $[M-H]^+$ Calcd for $C_{16}H_{10}N_2O_2{}^{35}Cl$ 297.0431; found: 297.0434; $[M-H]^+$ Calcd for $C_{16}H_{10}N_2O_2{}^{37}Cl$ 299.0401; found: 299.0408.

(*Z*)-4-Methyl-*N*'-(3-oxo-2,3-dihydro-1*H*-inden-1-ylidene)benzohydrazide (1j)



Prepared according to TP-1 from 1,3-Indandione (292.3 mg, 2.0 mmol), 4-methyl benzhydrazide (300.4 mg, 1.05 equiv), in MeOH (20 mL) followed by addition of Conc. HCl (1 drop) at 30 °C for 12 h. Thereafter, filtration of the reaction mixture and washed with cold MeOH (10 mL). Futher, purification by flash chromatography (SiO_2, EtOAc/hexanes: 1/2 and then MeOH/DCM: 1/100) furnished the desired product **1j** as white solid (489.8 mg, 88%).

R_f = 0.45 (MeOH/DCM: 5/95), mp.: 218.3-219.3 °C.

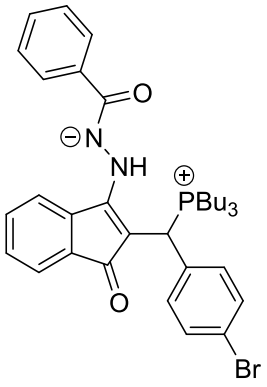
^{1}H NMR (400 MHz, DMSO-d_6, 25 °C) δ/ppm: 10.81 (s, 1H), 8.01 (brs, 1H), 7.86 – 7.80 (m, 3H), 7.78 (d, *J* = 7.8 Hz, 1H), 7.66 (t, *J* = 7.6 Hz, 1H), 7.33 (d, *J* = 8.0 Hz, 2H), 3.68 (s, 2H), 2.38 (s, 3H).

^{13}C NMR (100 MHz, DMSO-d_6, 25 °C) δ/ppm: 198.4, 163.9, 151.7, 146.5, 141.7, 138.4, 135.5, 131.3, 130.8, 129.1, 128.8, 128.1, 127.5, 122.9, 121.8, 38.7, 21.0.

IR (KBr) $\tilde{\nu}$ (cm^{-1}): 3080, 1735, 1680, 1530, 1372, 760.

HRMS (ESI) *m/z*: $[M+H]^+$ Calcd for $C_{17}H_{15}N_2O_2$ 279.1134; found: 279.1133.

1-Benzoyl-2-(2-((4-bromophenyl)(tributylphosphonio)methyl)-1-oxo-1*H*-inden-3-yl)hydrazin-1-ide (3a)



Prepared according to TP-2 from **1** (264.3 mg, 1.0 mmol), 4-bromo benzaldehyde **2a** (203.5 mg, 1.1 equiv), $PhCO_2H$ (12.2 mg, 0.1 equiv), PBu_3 (318.8 µL (94% purity) 1.2 equiv), 1.2 equiv) and

pyrrolidine (8.2 μL, 0.1 equiv) in anhydrous THF (10 mL) at 30 °C for 5 h. Purification by flash chromatography (SiO_2, EtOAc/hexanes: 1/2 and then MeOH/DCM: 1/100) furnished the desired product **3a** as an orange solid (570.2 mg, 90%).

R_f = 0.33 (MeOH/DCM: 20/100), mp.: 136.6-140.0 °C.

^{1}H NMR (400 MHz, $CDCl_3$, 25 °C) δ/ppm: 11.18 (brs, 1H), 8.12 (dd, *J* = 6.9, 3.1 Hz, 2H), 7.58 (dd, *J* = 8.6, 1.8 Hz, 2H), 7.47 (pt, *J* = 7.7 Hz, 4H), 7.44 – 7.39 (m, 4H), 7.36 (dd, *J* = 7.3, 1.3 Hz, 1H), 7.33 (td, *J* = 7.4, 1.9 Hz, 1H), 2.41 – 2.10 (m, 6H), 1.54 – 1.30 (m, 12H), 0.82 (t, J = 7.1 Hz, 9H).

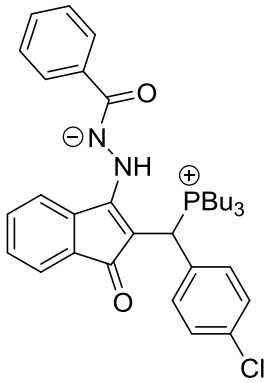
^{13}C NMR (100 MHz, $CDCl_3$, 25 °C) δ/ppm: 188.5, 168.1, 151.1, 137.9, 136.4, 135.7, 135.1, 132.3, 131.52, 131.48, 129.8, 129.5, 129.3, 127.6, 127.1, 122.35, 122.32, 119.6, 117.2, 94.7, 35.9, 35.5, 24.1, 23.91, 23.85, 20.4, 19.9, 13.1.

^{31}P NMR (161 MHz, $CDCl_3$, 25 °C) δ/ppm: 34.8.

IR (KBr) $\tilde{\nu}$ (cm^{-1}): 3450, 2962, 1730, 1644, 1579, 1526, 1379.

HRMS (ESI) *m/z*: $[M+H]^+$ Calcd for $C_{35}H_{43}{}^{79}BrN_2O_2P$ 633.2246; found: 633.2245; . $[M+H]^+$ Calcd for $C_{35}H_{43}{}^{81}BrN_2O_2P$ 635.2225; found: 635.2234.

1-Benzoyl-2-(2-((4-chlorophenyl)(tributylphosphonio)methyl)-1-oxo-1*H*-inden-3-yl)hydrazin-1-ide (3b)



Prepared according to TP-2 from **1** (264.3 mg, 1.0 mmol),4-chloro benzaldehyde **2b** (154.6 mg, 1.1 equiv), $PhCO_2H$ (12.2 mg, 0.1 equiv), PBu_3 (318.8 μL (94% purity), 1.2 equiv) and pyrrolidine (8.2 μL, 0.1 equiv) in anhydrous THF (10 mL) at 30 °C for 4 h. Purification by flash chromatography (SiO_2, EtOAc/hexanes: 1/2 and then MeOH/DCM: 1/100) furnished the desired product **3b** as an orange solid (538.6 mg, 85%).

R_f = 0.3 (MeOH/DCM: 20/100), mp.: 123.4-123.8 °C.

^{1}H NMR (400 MHz, $CDCl_3$, 25 °C) δ/ppm: 11.24 (brs, 1H), 8.13 (dd, *J* = 6.8, 2.4 Hz, 2H), 7.64

(dd, J = 8.7, 2.2 Hz, 2H), 7.46 (t, J = 7.8 Hz, 2H), 7.44 – 7.39 (m, 3H), 7.37 (t, J = 7.3 Hz, 2H), 7.34 – 7.30 (m, 3H), 2.45 – 2.10 (m, 6H), 1.55 – 1.30 (m, 12H), 0.82 (t, J = 7.1 Hz, 9H).

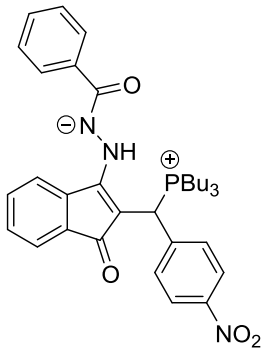
^{13}C NMR (100 MHz, $CDCl_3$, 25 °C) δ/ppm: 188.4, 168.1, 150.9, 138.0, 136.4, 135.7, 134.6, 134.18, 134.15, 131.20, 131.16, 129.8, 129.4, 129.3, 129.2, 127.6, 127.1, 119.6, 117.0, 94.7, 35.9, 35.4, 24.0, 23.89, 23.83, 20.4, 19.9, 13.1.

^{31}P NMR (161 MHz, $CDCl_3$, 25 °C) δ/ppm: 34.4.

IR (KBr) $\tilde{\nu}$ (cm^{-1}): 3441, 3230, 2958, 1666, 1576, 1379, 1294.

HRMS (ESI) *m/z*: $[M+H]^+$ Calcd for $C_{35}H_{43}{}^{35}ClN_2O_2P$ 589.2751; found: 589.2750; $[M+H]^+$ Calcd for $C_{35}H_{43}{}^{37}ClN_2O_2P$ 591.2721; found: 591.2740.

1-Benzoyl-2-(2-((4-nitrophenyl)(tributylphosphonio)methyl)-1-oxo-1*H*-inden-3-yl)hydrazin-1-ide (3c)



Prepared according to TP-2 from **1** (264.3 mg, 1.0 mmol), 4-nitro benzaldehyde **2c** (166.2 mg, 1.1 equiv), $PhCO_2H$ (12.2 mg, 0.1 equiv), PBu_3 (318.8 μL (94% purity), 1.2 equiv) and pyrrolidine (8.2 μL, 0.1 equiv) in anhydrous THF (10 mL) at 30 °C for 6 h. Purification by flash chromatography (SiO_2, EtOAc/hexanes: 1/2 and then MeOH/DCM: 1/100) furnished the desired product **3c** as an orange solid (533.7 mg, 89%).

R_f = 0.23 (MeOH/DCM: =20/100), mp.: 124.6-125 °C.

^{1}H NMR (400 MHz, $CDCl_3$, 25 °C) δ/ppm: 11.22 (brs, 1H), 8.16 (d, J = 8.7 Hz, 2H), 8.08 (d, J = 7.4 Hz, 2H), 7.89 (d, J = 8.4 Hz, 2H), 7.49 (d, J = 7.3 Hz, 2H), 7.45 (d, J = 7.4 Hz, 1H), 7.43 – 7.36 (m, 4H), 7.31 (pt, J = 7.3 Hz, 1H), 2.46 – 2.30 (m, 3H), 2.30 – 2.14 (m, 3H), 1.52 – 1.32 (m, 12H), 0.81 (t, J = 6.8 Hz, 9H).

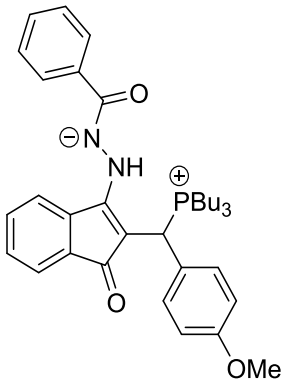
^{13}C NMR (100 MHz, $CDCl_3$, 25 °C) δ/ppm: 188.4, 168.0, 151.1, 147.2, 143.6, 137.5, 136.0, 135.3, 130.72, 130.68, 129.9, 129.5, 129.4, 127.6, 126.9, 124.1, 119.7, 117.2, 93.8, 36.3, 35.9, 23.9, 23.76, 23.71, 20.3, 19.9, 13.0.

^{31}P NMR (161 MHz, $CDCl_3$, 25 °C) δ/ppm: 35.6.

IR (KBr) $\tilde{\nu}$ (cm^{-1}): 3441, 2092, 1638, 1549, 1524, 1346.

HRMS (ESI) *m/z*: $[M+H]^+$ Calcd for $C_{35}H_{43}N_3O_4P$ 600.2991; found: 600.2994.

1-Benzoyl-2-(2-((4-methoxyphenyl)(tributylphosphonio)methyl)-1-oxo-1*H*-inden-3-yl)hydrazin-1-ide (3d)



Prepared according to TP-2 from **1** (264.3 mg, 1.0 mmol), 4-methoxy benzaldehyde **2d** (133.8 μL, 1.1 equiv), $PhCO_2H$ (12.2 mg, 0.1 equiv), PBu_3 (318.8 μL (94% purity), 1.2 equiv) and pyrrolidine (8.2 μL, 0.1 equiv) in anhydrous THF (10 mL) at 30 °C for 4.5 h. Purification by flash chromatography (SiO_2, EtOAc/hexanes: 1/2 and then MeOH/DCM: 1/100) furnished the desired product **3d** as orange solid (538.0 mg, 92%).

R_f = 0.18 (MeOH/DCM: 20/100), mp.: 145.5-145.9 °C.

^{1}H NMR (400 MHz, $CDCl_3$, 25 °C) δ/ppm: 11.15 (brs, 1H), 8.15 (d, *J* = 3.6 Hz, 2H), 7.55 (d, *J* = 7.6 Hz, 2H), 7.46 (pt, *J* = 6.9 Hz, 2H), 7.42 – 7.37 (m, 3H), 7.35 (t, *J* = 7.5 Hz, 1H), 7.33 – 7.26 (m, 2H), 7.14 (d, *J* = 7.8 Hz, 2H), 2.30 (s, 3H), 2.29 – 2.13 (m, 6H), 1.48 – 1.30 (m, 12H), 0.80 (t, *J* = 6.9 Hz, 9H).

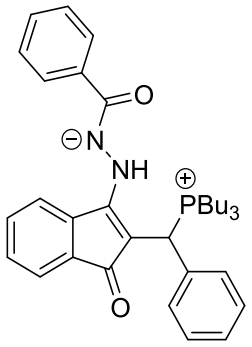
^{13}C NMR (100 MHz, $CDCl_3$, 25 °C) δ/ppm: 188.6, 167.9, 151.2, 138.0, 136.6, 135.9, 132.8, 129.84, 129.82, 129.69, 129.65, 129.3, 129.1, 127.6, 127.2, 119.4, 117.0, 95.5, 35.9, 35.5, 24.1, 23.9, 23.8, 21.0, 20.4, 19.9, 13.1.

^{31}P NMR (161 MHz, $CDCl_3$, 25 °C) δ/ppm: 34.6.

IR (KBr) $\tilde{\nu}$ (cm^{-1}): 3217, 2962, 1650, 1579, 1526, 1381, 1292.

HRMS (ESI) *m/z*: $[M+H]^+$ Calcd for $C_{36}H_{46}N_2O_3P$ 585.3246; found: 585.3245.

1-Benzoyl-2-(1-oxo-2-(phenyl(tributylphosphonio)methyl)-1*H*-inden-3-yl)hydrazin-1-ide (3e)



Prepared according to TP-2 from **1** (264.3 mg, 1.0 mmol), benzaldehyde **2e** (111.8 µL, 1.1 equiv), $PhCO_2H$ (12.2 mg, 0.1 equiv), PBu_3 (318.8 µL (94% purity), 1.2 equiv) and pyrrolidine (8.2 µL, 0.1 equiv) in anhydrous THF (10 mL) at 30 °C for 5 h. Purification by flash chromatography (SiO_2, EtOAc/hexanes: 1/2 and then MeOH/DCM: 1/100) furnished the desired product **3e** as an orange solid (471.5 mg, 85%).

R_f = 0.28 (MeOH/DCM: 20/100), mp.: 113.6-114 °C.

^{1}H NMR (400 MHz, $CDCl_3$, 25 °C) δ/ppm: 11.24 (brs, 1H), 8.15 (d, *J* = 7.3 Hz, 2H), 7.67 (d, *J* = 7.2 Hz, 2H), 7.47 (d, *J* = 7.1 Hz, 1H), 7.44 (d, *J* = 7.2 Hz, 1H), 7.42 – 7.38 (m, 3H), 7.33 (t, *J* = 7.2 Hz, 4H), 7.30 – 7.24 (m, 2H), 2.42 – 2.05 (m, 6H), 1.48 – 1.22 (m, 12H), 0.78 (t, *J* = 6.8 Hz, 9H).

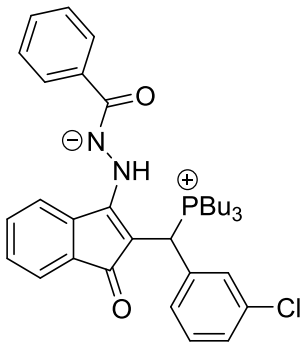
^{13}C NMR (100 MHz, $CDCl_3$, 25 °C) δ/ppm: 188.7, 167.9, 151.4, 137.8, 136.4, 135.9, 129.72, 129.67, 129.3, 129.13, 129.11, 128.1, 127.5, 127.1, 119.5, 117.0, 95.3, 36.3, 35.8, 23.96, 23.81, 23.77, 23.72, 20.3, 19.8, 13.0.

^{31}P NMR (161 MHz, $CDCl_3$, 25 °C) δ/ppm: 34.9.

IR (KBr) $\tilde{\nu}$ (cm^{-1}): 3441, 2962, 1642, 1572, 1524, 1381.

HRMS (ESI) *m/z*: $[M+H]^+$ Calcd for $C_{35}H_{44}N_2O_2P$ 555.3140; found: 555.3141.

1-Benzoyl-2-(2-((3-chlorophenyl)(tributylphosphonio)methyl)-1-oxo-1*H*-inden-3-yl)hydrazin-1-ide (3f)



Prepared according to TP-2 from **1** (264.3 mg, 1.0 mmol), 3-chloro benzaldehyde **2f** (124.6 µL, 1.1 equiv), $PhCO_2H$ (12.2 mg, 0.1 equiv), PBu_3 (318.8 µL (94% purity), 1.2 equiv) and pyrrolidine (8.2 µL, 0.1 equiv) in anhydrous THF (10 mL) at 30 °C for 5 h. Purification by flash chromatography (SiO_2, EtOAc/hexanes: 1/2 and then MeOH/DCM: 1/100) furnished the desired product **3f** as an orange solid (494.9 mg, 84%).

R_f = 0.23 (MeOH/DCM: 20/100), mp.: 110.4-110.8 °C.

^{1}H NMR (400 MHz, $CDCl_3$, 25 °C) δ/ppm: 11.16 (brs, 1H), 8.11 (d, *J* = 6.7 Hz, 2H), 7.69 (s, 1H), 7.58 (s, 1H), 7.47 (d, *J* = 7.2 Hz, 1H), 7.44 (d, *J* = 7.0 Hz, 1H), 7.42 – 7.30 (m, 6H), 7.28 – 7.26 (m, 2H), 2.35 – 2.10 (m, 6H), 1.47 – 1.26 (m, 12H), 0.78 (t, *J* = 6.8 Hz, 9H).

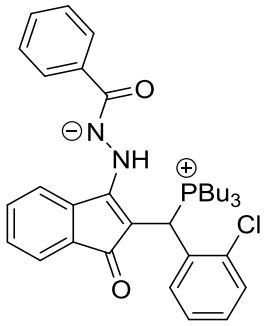
^{13}C NMR (100 MHz, $CDCl_3$, 25 °C) δ/ppm: 188.7, 168.1, 151.3, 138.0, 137.8, 136.2, 135.7, 134.86, 134.84, 130.40, 130.38, 129.8, 129.5, 129.2, 128.3, 128.02, 127.98, 127.6, 127.1, 119.6, 117.1, 94.5, 36.0, 35.6, 23.9, 23.79, 23.74, 20.3, 19.8, 13.0.

^{31}P NMR (161 MHz, $CDCl_3$, 25 °C) δ/ppm: 35.3.

IR (KBr) $\tilde{\nu}$ (cm^{-1}): 3432, 2087, 1640, 1520, 1471, 1384.

HRMS (ESI) *m/z*: $[M+H]^+$ Calcd for $C_{35}H_{43}{}^{35}ClN_2O_2P$ 589.2751; found: 589.2748; $[M+H]^+$ Calcd for $C_{35}H_{43}{}^{37}ClN_2O_2P$ 591.2721; found: 591.2740.

1-Benzoyl-2-(2-((2-chlorophenyl)(tributylphosphonio)methyl)-1-oxo-1*H*-inden-3-yl)hydrazin-1-ide (3g)



Prepared according to TP-2 from **1** (264.3 mg, 1.0 mmol), 2-chloro benzaldehyde **2g** (123.70 µL, 1.1 equiv), $PhCO_2H$ (12.2 mg, 0.1 equiv), PBu_3 (318.8 µL (94% purity), 1.2 equiv) and pyrrolidine (8.2 µL, 0.1 equiv) in anhydrous THF (10 mL) at 30 °C for 5.5 h. Purification by flash chromatography (SiO_2, EtOAc/hexanes: 1/2 and then MeOH/DCM: 1/100) furnished the desired product **3g** as an orange solid (471.3 mg, 80%).

R_f = 0.18 (MeOH/DCM: 20/100), mp.: 136.8-137.2 °C.

^{1}H NMR (400 MHz, $CDCl_3$, 25 °C) δ/ppm: 11.50 (brs, 1H), 8.42 (d, *J* = 8.3 Hz, 1H), 8.21 (d, *J* =

7.7 Hz, 2H), 7.74 (d, *J* = 18.1 Hz, 1H), 7.48 (t, *J* = 7.3 Hz, 2H), 7.42 – 7.30 (m, 6H), 7.26 (pt, *J* = 7.8 Hz, 1H), 7.19 (t, *J* = 7.8 Hz, 1H), 2.45 – 2.25 (m, 6H), 1.50 – 1.30 (m, 12H), 0.79 (t, *J* = 6.7 Hz, 9H).

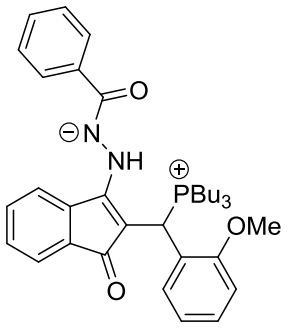
^{13}C NMR (100 MHz, $CDCl_3$, 25 °C) δ/ppm: 188.7, 168.7, 150.4, 137.8, 136.3, 135.8, 134.2, 133.5, 132.78, 132.72, 129.9, 129.7, 129.3, 129.1, 127.6, 127.3, 119.5, 116.9, 94.2, 33.2, 32.8, 24.0, 23.9, 23.77, 23.73, 20.6, 20.2, 13.1.

^{31}P NMR (161 MHz, $CDCl_3$, 25 °C) δ/ppm: 37.9.

IR (KBr) $\tilde{\nu}$ (cm^{-1}): 3446, 2070, 1633, 1576, 1465, 1377.

HRMS (ESI) *m/z*: $[M+H]^+$ Calcd for $C_{35}H_{43}{}^{35}ClN_2O_2P$ 589.2751; found: 589.2748; $[M+H]^+$ Calcd for $C_{35}H_{43}{}^{37}ClN_2O_2P$ 591.2721; found: 591.2733

1-Benzoyl-2-(2-((2-methoxyphenyl)(tributylphosphonio)methyl)-1-oxo-1*H*-inden-3-yl)hydrazin-1-ide (3h)



Prepared according to TP-2 from **1** (264.3 mg, 1.0 mmol), 2-methoxy benzaldehyde **2h** (132.9 µL, 1.1 equiv), $PhCO_2H$ (12.2 mg, 0.1 equiv), PBu_3 (318.8 µL (94% purity), 1.2 equiv) and pyrrolidine (8.2 µL, 0.1 equiv) in anhydrous THF (10 mL) at 30 °C for 6 h. Purification by flash chromatography (SiO_2, EtOAc/hexanes: 1/2 and then MeOH/DCM: 1/100) furnished the desired product **3h** as an orange solid (479.5 mg, 82%).

R_f = 0.18 (MeOH/DCM: 20/100), mp.: 145.5-145.9 °C.

^{1}H NMR (400 MHz, $CDCl_3$, 25 °C) δ/ppm: 11.26 (brs, 1H), 8.25 (d, *J* = 7.5 Hz, 2H), 8.03 (d, *J* = 8.3 Hz, 1H), 7.77 (d, *J* = 19.2 Hz, 1H), 7.48 (t, *J* = 7.3 Hz, 2H), 7.40 – 7.34 (m, 4H), 7.32 (d, *J* = 7.5 Hz, 1H), 7.22 (t, *J* = 7.6 Hz, 1H), 6.93 (t, *J* = 7.5 Hz, 1H), 6.85 (d, *J* = 8.3 Hz, 1H), 3.81 (s, 3H), 2.38 – 2.10 (m, 6H), 1.45 – 1.25 (m, 12H), 0.76 (t, J = 7.0 Hz, 9H).

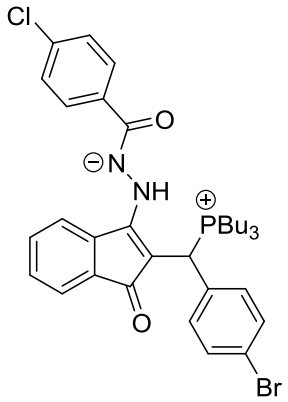
^{13}C NMR (100 MHz, $CDCl_3$, 25 °C) δ/ppm: 189.3, 167.8, 155.72, 155.67, 150.8, 137.9, 136.4, 136.0, 132.72, 132.69, 129.5, 129.19, 129.14, 129.11, 128.98, 127.38, 127.30, 124.0, 121.63, 121.60, 119.3, 116.8, 110.5, 95.5, 55.3, 28.9, 28.4, 34.06, 23.92, 23.73, 23.68, 20.7, 20.3, 13.1.

^{31}P NMR (161 MHz, $CDCl_3$, 25 °C) δ/ppm: 36.5.

IR (KBr) $\tilde{\nu}$ (cm^{-1}): 3428, 2307, 1640, 1580, 1555, 1388.

HRMS (ESI) *m/z*: $[M+H]^+$ Calcd for $C_{36}H_{46}N_2O_3P$ 585.3246; found: 585.3245.

2-(2-((4-Bromophenyl)(tributylphosphonio)methyl)-1-oxo-1*H*-inden-3-yl)-1-(4-chlorobenzoyl)hydrazin-1-ide (3i)



Prepared according to TP-2 from **1b** (298.7 mg, 1.0 mmol), 4-bromo benzaldehyde **2i** (203.5 mg, 1.1 equiv), $PhCO_2H$ (12.2 mg, 0.1 equiv), PBu_3 (318.8 µL (94% purity), 1.2 equiv) and pyrrolidine (8.2 µL, 0.1 equiv) in anhydrous THF (10 mL) at 30 °C for 5 h. Purification by flash chromatography (SiO_2, EtOAc/hexanes: 1/2 and then MeOH/DCM: 1/100) furnished the desired product **3i** as an orange solid (574.5 mg, 86%).

R_f = 0.28 (MeOH/DCM: 20/100), mp.: 116.8-117.2 °C.

^{1}H NMR (400 MHz, $CDCl_3$, 25 °C) δ/ppm: 10.99 (brs, 1H), 8.04 (d, *J* = 7.6 Hz, 2H), 7.53 (d, *J* = 8.6 Hz, 2H), 7.51 – 7.44 (m, 4H), 7.37 (d, *J* = 8.1 Hz, 4H), 7.23 (d, *J* = 17.9 Hz, 1H), 2.38 – 2.13 (m, 6H), 1.50 – 1.35 (m, 12H), 0.83 (t, *J* = 6.8 Hz, 9H).

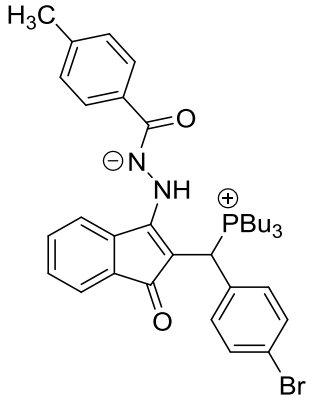
^{13}C NMR (100 MHz, $CDCl_3$, 25 °C) δ/ppm: 188.8, 167.2, 151.3, 136.6, 136.3, 135.7, 135.0, 132.4, 131.45, 131.41, 130.0, 129.7, 128.5, 127.8, 122.49, 122.46, 119.7, 117.2, 94.7, 36.0, 35.6, 24.12, 23.97, 23.92, 20.4, 20.0, 13.2.

^{31}P NMR (161 MHz, $CDCl_3$, 25 °C) δ/ppm: 34.8.

IR (KBr) $\tilde{\nu}$ (cm^{-1}): 3432, 2962, 2360, 1649, 1574, 1458, 1320.

HRMS (ESI) *m/z*: $[M+H]^+$ Calcd for $C_{35}H_{42}{}^{79}Br^{35}ClN_2O_2P$ 667.1856; found: 667.1857; $[M+H]^+$ Calcd for $C_{35}H_{42}{}^{79}Br^{37}ClN_2O_2P$ 669.1835; found: 668.1842; $[M+H]^+$ Calcd for $C_{35}H_{42}{}^{81}Br^{35}ClN_2O_2P$ 669.1835; found: 688.1842 $[M+H]^+$ Calcd for $C_{35}H_{42}{}^{81}Br^{37}ClN_2O_2P$ 671.1806; found: 671.1829.

2-(2-((4-Bromophenyl)(tributylphosphonio)methyl)-1-oxo-1*H*-inden-3-yl)-1-(4-methylbenzoyl)hydrazin-1-ide (3j)



Prepared according to TP-2 from **1c** (278.3 mg, 1.0 mmol), 4-bromo benzaldehyde **2j** (203.5 mg, 1.1 equiv), $PhCO_2H$ (12.2 mg, 0.1 equiv), PBu_3 (318.8 µL (94% purity), 1.2 equiv) and pyrrolidine (8.2 µL, 0.1 equiv) in anhydrous THF (10 mL) at 30 °C for 5 h. Purification by flash chromatography (SiO_2, EtOAc/hexanes: 1/2 and then MeOH/DCM: 1/100) furnished the desired product **3j** as an orange solid (582.6 mg, 90%).

R_f = 0.15 (MeOH/DCM: 20/100), mp.: 139.4-139.8 °C.

^{1}H NMR (400 MHz, $CDCl_3$, 25 °C) δ/ppm: 8.01 (d, *J* = 7.9 Hz, 2H), 7.57 (d, *J* = 8.1 Hz, 2H), 7.46 (d, *J* = 8.1 Hz, 4H), 7.39 – 7.30 (m, 3H), 7.20 (d, *J* = 7.9 Hz, 2H), 2.40 (s, 3H), 2.36 – 2.13 (m, 6H), 1.50 – 1.30 (m, 12H), 0.82 (t, *J* = 6.8 Hz, 9H).

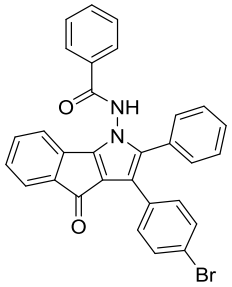
^{13}C NMR (100 MHz, $CDCl_3$, 25 °C) δ/ppm: 188.4, 168.2, 150.9, 139.3, 136.5, 135.7, 135.2, 132.3, 131.58, 131.54, 129.8, 129.5, 128.4, 127.1, 122.4, 119.6, 117.9, 94.7, 36.1, 35.6, 24.1, 23.95, 23.90, 21.4, 20.4, 19.9, 13.2.

^{31}P NMR (161 MHz, $CDCl_3$, 25 °C) δ/ppm: 34.7.

IR (KBr) $\tilde{\nu}$ (cm^{-1}): 3424, 2958, 2325, 1614, 1574 1465.

HRMS (ESI) *m/z*: $[M+H]^+$ Calcd for $C_{36}H_{45}{}^{79}BrN_2O_2P$ 647.2402; found: 647.2404; $[M+H]^+$ Calcd for $C_{36}H_{45}{}^{81}BrN_2O_2P$ 649.2382; found: 649.2393.

***N*-(3-(4-Bromophenyl)-4-oxo-2-phenylindeno[1,2-*b*]pyrrol-1(4*H*)-yl)benzamide (6aa)**



Following the TP-3, **6aa** was obtained from **3a** (190.2 mg, 0.3 mmol), benzoyl chloride **5a** (38.3 μL, 1.1 equiv) and triethylamine (63 μL, 1.5 equiv). The residue was purified by column chromatography (SiO_2, Hexanes/EtOAc= 85:15) to give as an orange solid (137.1 mg, 88% yield). R_f= 0.53 (EtOAc:Hexanes =1:2); mp = 220.3-221.0 °C.

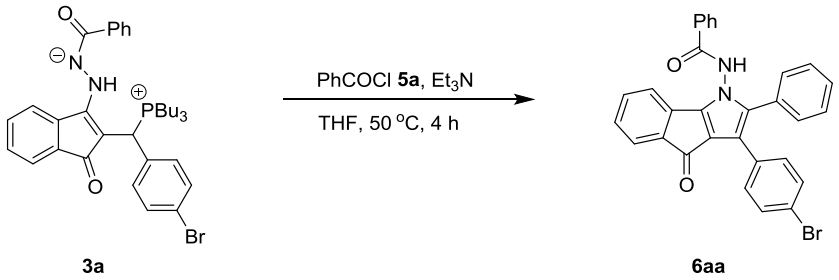
^{1}H NMR (400 MHz, $CDCl_3$, 25 °C) δ/ppm: 9.23 (s, 1H), 7.64 (d, *J* = 7.9 Hz, 2H), 7.55 (t, *J* = 7.3 Hz, 1H), 7.38 (t, *J* = 7.8 Hz, 2H), 7.31 (td, *J* = 7.1, 2.3 Hz, 1H), 7.28 – 7.26 (m, 1H), 7.25 – 7.24 (m ,1H), 7.23 (d, *J* = 2.5 Hz, 4H), 7.22 – 7.19 (m, 3H), 6.99 (t, *J* = 7.4 Hz, 1H), 6.94 (t, *J* = 7.2 Hz, 1H), 6.65 (d, *J* = 7.0 Hz, 1H).

^{13}C NMR (100 MHz, $CDCl_3$, 25 °C) δ/ppm: 186.3, 166.6, 151.4, 139.0, 136.3, 134.0, 133.2, 132.8, 131.2, 131.1, 130.7, 130.5, 130.3, 129.1, 128.9, 128.4, 127.3, 123.4, 120.8, 119.4, 119.2, 117.1.

IR (KBr) $\tilde{\nu}$ (cm^{-1}): 3239, 2923, 1721, 1699, 1675, 1493, 1278, 1072, 893, 755.

HRMS (ESI) *m/z*: $[M+H]^+$ Calcd for $C_{30}H_{20}{}^{79}BrN_2O_2$ 519.0708; found: 519.0706; $[M+H]^+$ Calcd for $C_{30}H_{20}{}^{81}BrN_2O_2$ 521.0688; found: 521.0690.

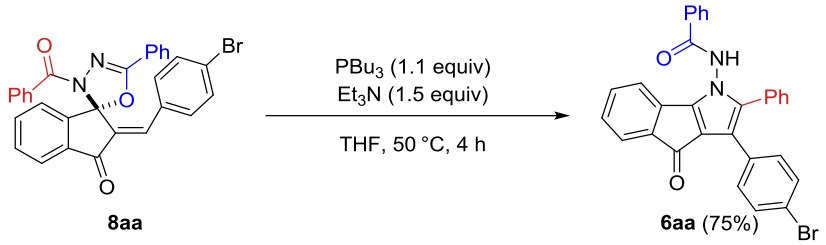
General procedure for the gram-scale preparation of indenopyrrole derivative 6aa:



3a **6aa**

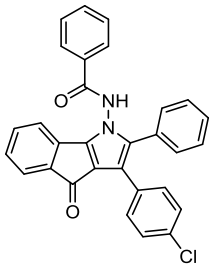
A dry and argon-flushed 100 mL Schlenk flask equipped with a magnetic stir bar and septum was sequentially charged with **3a** (1.267 g, 2 mmol), anhydrous THF (20 mL), benzoyl chloride **5a** (256 μL, 1.1 equiv) and Et_3N (400 μL, 1.5 equiv). The reaction mixture was stirred for 4 h at 50 °C. After completion of the reaction, solvent was removed in *vacuo* and the crude residue was subjected to flash column chromatography (SiO_2, Hexanes/EtOAc= 85:15) to give the product **6aa** in 87% yield (0.903 g).

General procedure for the preparation of indenopyrrole derivative 6aa from spiro-indene-1,2'-[1,3,4]oxadiazol 8aa:



A dry and argon-flushed 10 mL Schlenk flask equipped with a magnetic stir bar and septum was sequentially charged with **8aa** (107.1 mg, 0.2 mmol), anhydrous THF (2 mL), PBu_3 (54.3 µL, 1.1 equiv) and Et_3N (40.0 µL, 1.5 equiv). The reaction mixture was stirred for 4 h at 50 °C. After completion of the reaction, solvent was removed in *vacuo* and the crude residue was subjected to flash column chromatography (SiO_2, Hexanes/EtOAc= 85:15) to give the product **6aa** in 75% yield (78.0 mg).

***N*-(3-(4-Chlorophenyl)-4-oxo-2-phenylindeno[1,2-*b*]pyrrol-1(4*H*)-yl)benzamide (6ba)**



Following the TP-3, **6ba** was obtained from **3b** (176.7 mg, 0.3 mmol), benzoyl chloride **5a** (38.3 µL, 1.1 equiv) and triethylamine (63 µL, 1.5 equiv). The residue was purified by column chromatography (SiO_2, Hexanes/EtOAc= 85:15) to give as an orange solid (133.9 mg, 94% yield). R_f = 0.55 (EtOAc:Hexanes =1:2); mp = 145.9-146.5 °C.

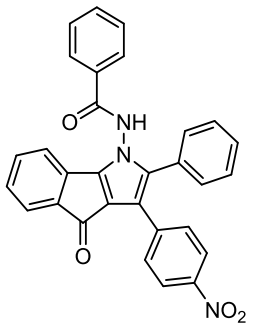
^{1}H NMR (400 MHz, $CDCl_3$, 25 °C) δ/ppm: 9.79 (s, 1H), 7.60 (d, J = 7.9 Hz, 2H), 7.49 (t, J = 7.4 Hz, 1H), 7.31 (d, J = 7.6 Hz, 2H), 7.30-7.14 (m, 7H), 7.09 (d, J = 7.0 Hz, 1H), 7.0 (d, J = 8.6 Hz, 2H), 6.97-6.82 (m, 2H), 6.55 (d, J = 6.80 Hz, 1H).

^{13}C NMR (100 MHz, $CDCl_3$, 25 °C) δ/ppm: 186.4, 166.8, 151.3, 138.9, 136.4, 133.9, 133.1, 132.7, 132.5, 130.7, 130.6, 130.4, 130.0, 129.1, 129.0, 128.8, 128.3, 128.1, 127.3, 123.3, 119.3, 119.1, 117.0.

IR (KBr) $\tilde{\nu}$ (cm^{-1}): 3243, 2914, 1730, 1701, 1670, 1607, 1493, 1092, 850, 740.

HRMS (ESI) *m/z*: $[M+H]^+$ Calcd for $C_{30}H_{20}{}^{35}ClN_2O_2$ 475.1213; found: 475.1213; $[M+H]^+$ Calcd for $C_{30}H_{20}{}^{37}ClN_2O_2$ 477.1184; found: 477.1197.

***N*-(3-(4-Nitrophenyl)-4-oxo-2-phenylindeno[1,2-*b*]pyrrol-1(4*H*)-yl)benzamide (6ca)**



Following the TP-3, **6ca** was obtained from **3c** (179.9 mg, 0.3 mmol), benzoyl chloride **5a** (38.3 μL, 1.1 equiv) and triethylamine (63 μL, 1.5 equiv). The residue was purified by column chromatography (SiO_2, Hexanes/EtOAc= 82:18) to give as an orange solid (126.7 mg, 87% yield). R_f = 0.43 (EtOAc:Hexanes =1:2); mp = 161.4-161.9 °C.

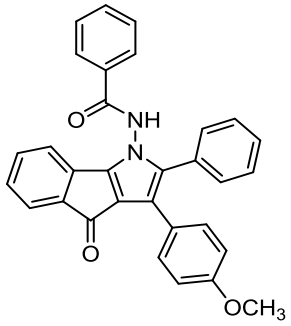
^{1}H NMR (400 MHz, DMSO-d_6, 25 °C) δ/ppm: 12.24 (s, 1H), 8.13 (d, *J* = 8.8 Hz, 2H), 7.80 (d, *J* = 7.5 Hz, 2H), 7.65 (d, *J* = 8.8 Hz, 3H), 7.55 (t, *J* = 7.5 Hz, 2H), 7.48-7.40 (m, 4H), 7.40-7.32 (m, 3H), 7.24 (t, *J* = 7.6 Hz, 1H), 6.97 (d, *J* = 7.2 Hz, 1H).

^{13}C NMR (100 MHz, DMSO-d_6, 25 °C) δ/ppm: 184.9, 166.1, 151.3, 145.8, 139.3, 138.4, 138.1, 133.7, 133.5, 133.0, 130.8, 130.2, 129.4, 129.1, 128.9, 128.4, 127.5, 123.5, 118.0, 117.6, 117.1.

IR (KBr) $\tilde{\nu}$ (cm^{-1}): 2914, 2848, 1735, 1682, 1596, 1342, 1285, 1008, 890, 750.

HRMS (ESI) *m/z*: $[M+H]^+$ Calcd for $C_{30}H_{20}N_3O_4$ 486.1454; found: 486.1454

***N*-(3-(4-Methoxyphenyl)-4-oxo-2-phenylindeno[1,2-*b*]pyrrol-1(4*H*)-yl)benzamide (6da)**



Following the TP-3, **6da** was obtained from **3d** (175.5 mg, 0.3 mmol), benzoyl chloride **5a** (38.3 μL, 1.1 equiv) and triethylamine (63 μL, 1.5 equiv). The residue was purified by column chromatography (SiO_2, Hexanes/EtOAc= 88:12) to give as an orange solid (90.3 mg, 64% yield).

R_f = 0.60 (EtOAc:Hexanes =1:2); mp = 157.6-160.0 °C.

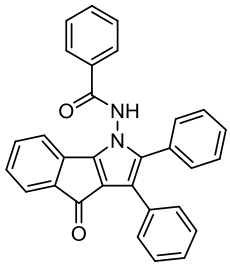
^{1}H NMR (400 MHz, DMSO-d_6, 25 °C) δ/ppm: 12.11 (brs. 1H), 7.79 (d, *J* = 8.3 Hz, 2H), 7.64 (t, *J* = 7.2 Hz, 1H), 7.54 (pt, *J* = 7.6 Hz, 2H), 7.42 – 7.34 (m, 4H), 7.34 – 7.26 (m, 5H), 7.19 (t, *J* = 7.3 Hz, 1H), 7.06 (d, *J* = 7.9 Hz, 2H), 6.90 (d, *J* = 7.3 Hz, 1H), 2.26 (s, 3H).

^{13}C NMR (100 MHz, DMSO-d_6, 25 °C) δ/ppm: 185.0, 166.1, 150.3, 138.5, 136.18, 136.11, 133.8, 133.3, 132.7, 130.3, 129.4, 128.8, 128.7, 128.5, 128.3, 127.5, 123.1, 119.2, 118.0, 117.2, 20.7.

IR (KBr) $\tilde{\nu}$ (cm^{-1}): 3314, 2914, 2848, 1734, 1665, 1471, 1178, 880, 750.

HRMS (ESI) *m/z*: $[M+H]^+$ Calcd for $C_{31}H_{23}N_2O_3$ 471.1709; found: 471.1707.

***N*-(4-Oxo-2,3-diphenylindeno[1,2-*b*]pyrrol-1(4*H*)-yl)benzamide (6ea)**



Following the TP-3, **6ea** was obtained from **3e** (166.2 mg, 0.3 mmol), benzoyl chloride **5a** (38.3 µL, 1.1 equiv) and triethylamine (63 µL, 1.5 equiv). The residue was purified by column chromatography (SiO_2, Hexanes/EtOAc= 85:15) to give as an orange solid (71.4 mg, 54% yield).

R_f = 0.53 (EtOAc:Hexanes =1:2); mp = 268.2-268.6 °C.

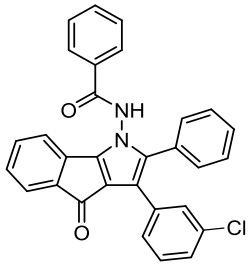
^{1}H NMR (400 MHz, DMSO-d_6, 25 °C) δ/ppm: 12.12 (s, 1H), 7.79 (d, *J* = 7.6 Hz, 2H), 7.65 (t, *J* = 7.5 Hz, 1H), 7.55 (t, *J* = 7.4 Hz, 2H), 7.42 (t, *J* = 1.7 Hz, 1H), 7.41-7.36 (m, 5H), 7.36-7.30 (m, 3H), 7.26 (tt, *J* = 7.5, 1.6 Hz, 2H), 7.20 (t, *J* = 7.7 Hz, 2H), 6.92 (d, *J* = 7.2 Hz, 1H).

^{13}C NMR (100 MHz, DMSO-d_6, 25 °C) δ/ppm: 185.0, 166.0, 150.5, 138.4, 136.5, 133.8, 133.4, 132.8, 132.2, 130.9, 130.3, 129.2, 128.9, 128.8, 128.64, 128.57, 128.3, 128.1, 127.5, 126.9, 123.2, 119.2, 118.0, 117.2.

IR (KBr) $\tilde{\nu}$ (cm^{-1}): 3340, 2914, 1734, 1699, 1660, 1469, 1053, 890, 740.

HRMS (ESI) *m/z*: $[M+H]^+$ Calcd for $C_{30}H_{21}N_2O_2$ 441.1603; found: 441.1600.

***N*-(3-(3-Chlorophenyl)-4-oxo-2-phenylindeno[1,2-*b*]pyrrol-1(4*H*)-yl)benzamide (6fa)**



Following the TP-3, **6fa** was obtained from **3f** (176.7 mg, 0.3 mmol), benzoyl chloride **5a** (38.3 µL, 1.1 equiv) and triethylamine (63 µL, 1.5 equiv). The residue was purified by column chromatography (SiO_2, Hexanes/EtOAc= 90:10) to give as an orange solid (67.0 mg, 47% yield). R_f = 0.56 (EtOAc:Hexanes =2:8); mp = 125.9-126.5 °C.

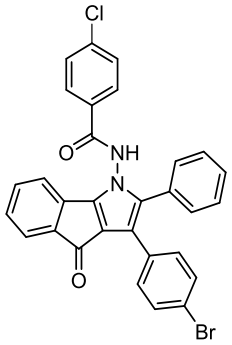
^{1}H NMR (400 MHz, DMSO-d_6, 25 °C) δ/ppm: 12.16 (s, 1H), 7.79 (dd, *J* = 8.1, 1.6 Hz, 2H), 7.65 (tt, *J* = 7.6, 1.5 Hz, 1H), 7.56 (d, *J* = 7.9 Hz, 1H), 7.52 (t, *J* = 1.4 Hz, 2H), 7.42 (td, *J* = 6.8, 2.0 Hz, 4H), 7.38 – 7.32 (m, 3H), 7.31 – 7.25 (m, 3H), 7.23 (t, *J* = 7.8 Hz, 1H), 6.94 (d, *J* = 7.3 Hz, 1H).

^{13}C NMR (100 MHz, DMSO-d_6, 25 °C) δ/ppm: 185.0, 166.0, 150.7, 138.2, 137.2, 134.4, 133.6, 133.5, 132.9, 130.8, 130.3, 129.9, 129.2, 128.9, 128.84, 128.77, 127.9, 127.5, 126.7, 126.6, 123.4, 117.8, 117.6, 117.4.

IR (KBr) $\tilde{\nu}$ (cm^{-1}): 3230, 2914, 2848, 1720, 1701, 1665, 1598, 1465, 1280, 1050, 850, 760.

HRMS (ESI) *m/z*: $[M+H]^+$ Calcd for $C_{30}H_{20}{}^{35}ClN_2O_2$ 475.1213; found: 475.1210; $[M+H]^+$ Calcd for $C_{30}H_{20}{}^{37}ClN_2O_2$ 477.1184; found: 477.1197.

***N*-(3-(4-Bromophenyl)-4-oxo-2-phenylindeno[1,2-*b*]pyrrol-1(4*H*)-yl)-4-chlorobenzamide (6ia)**



Following the TP-3, **6ia** was obtained from **3i** (200.4 mg, 0.3 mmol), benzoyl chloride **5a** (38.3 µL, 1.1 equiv) and triethylamine (63 µL, 1.5 equiv). The residue was purified by column chromatography (SiO_2, Hexanes/EtOAc= 85:15) to give as an orange solid (137.9 mg, 83% yield). R_f = 0.55 (EtOAc:Hexanes =1:2); mp = 173.2-173.8 °C.

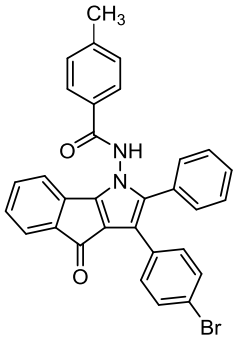
^{1}H NMR (400 MHz, $CDCl_3$, 25 °C) δ/ppm: 9.83 (brs, 1H), 7.54 (d, *J* = 8.2 Hz, 2H), 7.28 (d, *J* = 8.5 Hz, 3H), 7.21 (t, *J* = 7.6 Hz, 2H), 7.17 – 7.11 (m, 6H), 7.07 (d, *J* = 7.0 Hz, 1H), 6.92 (t, *J* = 7.6 Hz, 1H), 6.85 (t, *J* = 7.4 Hz, 1H), 6.54 (d, *J* = 7.1 Hz, 1H).

^{13}C NMR (100 MHz, $CDCl_3$, 25 °C) δ/ppm: 186.6, 165.8, 151.4, 139.6, 138.8, 136.4, 133.8, 132.8, 131.0, 130.4, 130.2, 129.3, 129.1, 128.96, 128.85, 128.79, 128.4, 123.4, 120.8, 119.4, 119.0, 117.0,

IR (KBr) $\tilde{\nu}$ (cm^{-1}): 3239, 2918, 1735, 1704, 1612, 1493, 1298, 1080, 860, 755.

HRMS (ESI) *m/z*: $[M+H]^+$ Calcd for $C_{30}H_{19}{}^{79}Br^{35}ClN_2O_2$ 553.0318; found: 553.0316; $[M+H]^+$ Calcd for $C_{30}H_{19}{}^{81}Br^{35}ClN_2O_2$ 555.0298; found: 555.0297; $[M+H]^+$ Calcd for $C_{30}H_{19}{}^{79}Br^{37}ClN_2O_2$ 555.0298; found: 555.0297; $[M+H]^+$ Calcd for $C_{30}H_{19}{}^{81}Br^{37}ClN_2O_2$ 557.02680; found: 557.0282.

***N*-(3-(4-Bromophenyl)-4-oxo-2-phenylindeno[1,2-*b*]pyrrol-1(4*H*)-yl)-4-methylbenzamide (6ja)**



Following the TP-3, **6ja** was obtained from **3j** (194.1 mg, 0.3 mmol), benzoyl chloride **5a** (38.3 µL, 1.1 equiv) and triethylamine (63 µL, 1.5 equiv). The residue was purified by column chromatography (SiO_2, Hexanes/EtOAc= 85:15) to give as an orange solid (126.4 mg, 79% yield). R_f = 0.55 (EtOAc:Hexanes =1:2); mp = 161.2-161.5 °C.

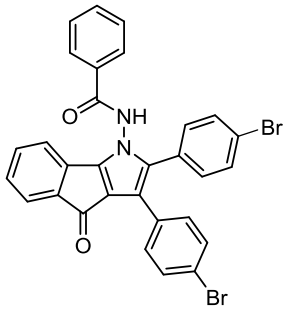
^{1}H NMR (400 MHz, DMSO-d_6, 25 °C) δ/ppm: 9.3 (brs, 1H), 7.53 (d, *J* = 7.9 Hz, 2H), 7.28 (d, *J* = 7.2 Hz, 1H), 7.25 – 7.22 (m, 5H), 7.20 (pt, *J* = 7.4 Hz, 4H), 7.14 (d, *J* = 7.8 Hz, 2H), 6.96 (pt, *J* = 7.4 Hz, 1H), 6.92 (t, *J* = 7.3 Hz, 1H), 6.62 (d, *J* = 6.8 Hz, 1H), 2.35 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$, 25 °C) δ/ppm: 186.3, 166.7, 151.4, 144.0, 139.0, 136.4, 134.0, 132.7, 131.3, 131.0, 130.5, 130.3, 129.6, 129.1, 128.9, 128.8, 128.3, 127.7, 127.4, 123.3, 120.7, 119.3, 119.0, 117.0, 21.5.

IR (KBr) $\tilde{\nu}$ (cm^{-1}): 3248, 2918, 2848, 1735, 1699, 1635, 1498, 1274, 865, 750.

HRMS (ESI) *m/z*: $[M+H]^+$ Calcd for $C_{31}H_{22}{}^{79}BrN_2O_2$ 533.0865; found: 533.0861; $[M+H]^+$ Calcd for $C_{31}H_{22}{}^{81}BrN_2O_2$ 535.0844; found: 535.0839.

***N*-(2,3-Bis(4-bromophenyl)-4-oxoindeno[1,2-*b*]pyrrol-1(4*H*)-yl)benzamide (6ab)**



Following the TP-3, **6ab** was obtained from **3a** (190.2 mg, 0.3 mmol), 4-bromo benzoyl chloride **5b** (72.4 mg, 1.1 equiv) and triethylamine (63 µL, 1.5 equiv). The residue was purified by column chromatography (SiO_2, Hexanes/EtOAc= 88:12) to give as an orange solid (149.0 mg, 83% yield). R_f = 0.60 (EtOAc:Hexanes =1:2); mp = 251.0-251.4 °C.

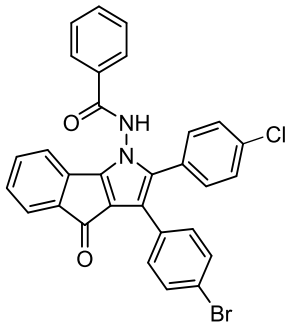
^{1}H NMR (400 MHz, DMSO-d_6, 25 °C) δ/ppm: 12.20 (s, 1H), 7.85 (d, *J* = 7.6 Hz, 2H), 7.67 (t, *J* = 7.2 Hz, 1H), 7.61 (d, *J* = 8.4 Hz, 2H), 7.57 (t, *J* = 7.8 Hz, 2H), 7.50 (d, *J* = 8.6 Hz, 2H), 7.40 (d, *J* = 7.2 Hz, 1H), 7.38-7.31 (m, 3H), 7.28 (d, *J* = 8.4 Hz, 2H), 7.21 (t, *J* = 7.5 Hz, 1H), 6.96 (d, *J* = 7.3 Hz, 1H).

^{13}C NMR (100 MHz, DMSO-d_6, 25 °C) δ/ppm: 184.9, 166.1, 150.8, 138.3, 135.4, 133.6, 133.5, 133.0, 132.2, 131.8, 131.2, 130.7, 130.4, 129.0, 128.9, 128.0, 127.5, 123.3, 122.5, 120.3, 118.3, 118.0, 117.4.

IR (KBr) $\tilde{\nu}$ (cm^{-1}): 3235, 2923, 1725, 1697, 1660, 1493, 1278, 1075, 865, 755.

HRMS (ESI) *m/z*: $[M+H]^+$ Calcd for $C_{30}H_{19}{}^{79}Br_2N_2O_2$ 596.9813; found: 596.9812; $[M+H]^+$ Calcd for $C_{30}H_{19}{}^{79}Br^{81}BrN_2O_2$ 598.9793; found: 598.9794; $[M+H]^+$ Calcd for $C_{30}H_{19}{}^{81}Br_2N_2O_2$ 600.9772; found: 600.9780.

***N*-(3-(4-Bromophenyl)-2-(4-chlorophenyl)-4-oxoindeno[1,2-*b*]pyrrol-1(4*H*)-yl)benzamide (6ac)**



Following the TP-3, **6ac** was obtained from **3a** (190.2 mg, 0.3 mmol), 4-chloro benzoyl chloride **5c** (42.3 µL, 1.1 equiv) and triethylamine (63 µL, 1.5 equiv). The residue was purified by column

chromatography (SiO_2, Hexanes/EtOAc= 85:15) to give as an orange solid (137.9 mg, 83% yield). R_f= 0.55 (EtOAc:Hexanes =1:2); mp = 151.4-151.8 °C.

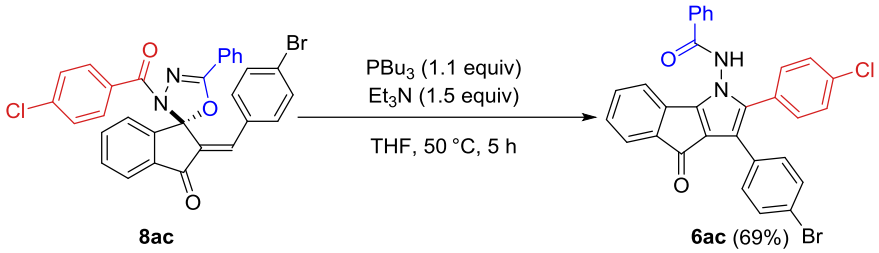
^{1}H NMR (400 MHz, DMSO-d_6, 25 °C) δ/ppm: 12.21 (s, 1H), 7.82 (d, *J* = 7.6 Hz, 2H), 7.67 (t, *J* = 7.2 Hz, 1H), 7.57 (t, *J* = 7.8 Hz, 2H), 7.51 (t, *J* = 1.8 Hz, 1H), 7.49 (t, *J* = 2.2 Hz, 2H), 7.47 (t, *J* = 2.2 Hz, 1H), 7.40 (d, *J* = 7.1 Hz, 1H), 7.37-7.30 (m, 5H), 7.22 (t, *J* = 7.5 Hz, 1H), 6.94 (d, *J* = 7.1 Hz, 1H).

^{13}C NMR (100 MHz, DMSO-d_6, 25 °C) δ/ppm: 184.9, 166.1, 150.8, 138.3, 135.4, 133.8, 133.6, 133.0, 132.0, 131.3, 130.4, 129.01, 128.95, 127.68, 127.56, 123.4, 120.3, 118.4, 118.0, 117.5.

IR (KBr) $\tilde{\nu}$ (cm^{-1}): 3428, 2923, 1760, 1699, 1640, 1493, 1276, 1092, 888, 756.

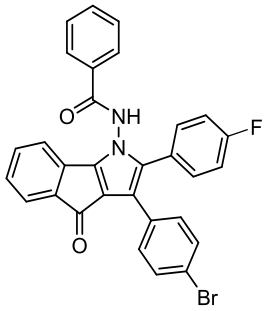
HRMS (ESI) *m/z*: $[M+H]^+$ Calcd for $C_{30}H_{19}{}^{79}Br^{35}ClN_2O_2$ 553.0318; found: 553.0320; $[M+H]^+$ Calcd for $C_{30}H_{19}{}^{79}Br^{37}ClN_2O_2$ 555.0298; found: 555.0301; $[M+H]^+$ Calcd for $C_{30}H_{19}{}^{81}Br^{35}ClN_2O_2$ 555.0298; found: 555.0301; $[M+H]^+$ Calcd for $C_{30}H_{19}{}^{81}Br^{37}ClN_2O_2$ 557.0268; found: 557.0283.

General procedure for the preparation of indenopyrrole derivative 6ac from spiro-indene-1,2'-[1,3,4]oxadiazol 8ac:



A dry and argon-flushed 10 mL Schlenk flask equipped with a magnetic stir bar and septum was sequentially charged with **8ac** (114.0 mg, 0.2 mmol), anhydrous THF (2 mL), PBu_3 (54.3 µL, 1.1 equiv) and Et_3N (40.0 µL, 1.5 equiv). The reaction mixture was stirred for 5 h at 50 °C. After completion of the reaction, solvent was removed in *vacuo* and the crude residue was subjected to flash column chromatography (SiO_2, Hexanes/EtOAc= 85:15) to give the product **6ac** in 69% yield (76.5 mg).

***N*-(3-(4-Bromophenyl)-2-(4-fluorophenyl)-4-oxoindeno[1,2-*b*]pyrrol-1(4*H*)-yl)benzamide (6ad)**



Following the TP-3, **6ad** was obtained from **3a** (190.2 mg, 0.3 mmol), 4-fluoro benzoyl chloride **5d** (39 µL, 1.1 equiv) and triethylamine (63 µL, 1.5 equiv). The residue was purified by column chromatography (SiO_2, Hexanes/EtOAc= 85:15) to give as an orange solid (130.6 mg, 81% yield). R_f= 0.52 (EtOAc:Hexanes =1:2); mp = 138.8-139.2 °C.

^{1}H NMR (400 MHz, $CDCl_3$, 25 °C) δ/ppm: 9.22 (brs, 1H), 7.69 (d, *J* = 7.7 Hz, 2H), 7.59 (t, *J* = 7.6 Hz, 1H), 7.44 (t, *J* = 7.6 Hz, 2H), 7.29-7.14 (m, 7H), 7.02 (t, *J* = 7.68 Hz, 1H), 6.96 (q, *J* = 8.6 Hz, 3H), 6.67 (d, *J* = 7.0 Hz, 1H).

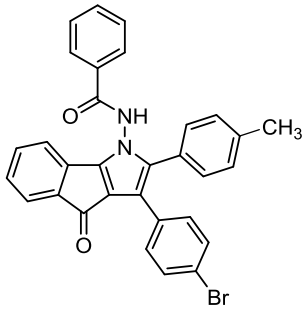
^{13}C NMR (100 MHz, $CDCl_3$, 25 °C) δ/ppm: 186.2, 166.5, 163.0 (d, $^1J_{C\text{-}F}$ = 250.3 Hz), 151.4, 139.0, 135.2, 134.0, 133.3, 132.8, 132.54 (d, $^3J_{C\text{-}F}$ = 8.5 Hz), 131.2, 131.0, 130.6, 130.3, 129.2, 128.5, 127.3, 125.20 (d, $^4J_{C\text{-}F}$ = 3.0 Hz), 123.5, 121.0, 119.7, 119.2, 117.1, 116.15 (d, $^2J_{C\text{-}F}$ = 21.6 Hz).

^{19}F NMR (376 MHz, $CDCl_3$, 25 °C) δ/ppm: -115.31.

IR (KBr) $\tilde{\nu}$ (cm^{-1}): 3243, 2923, 1735, 1689, 1511, 1267, 1158, 852, 760.

HRMS (ESI) *m/z*: $[M+H]^+$ Calcd for $C_{30}H_{19}{}^{79}BrFN_2O_2$ 537.0614; found: 537.0615; $[M+H]^+$ Calcd for $C_{30}H_{19}{}^{81}BrFN_2O_2$ 539.0593; found: 539.0598.

***N*-(3-(4-Bromophenyl)-4-oxo-2-(*p*-tolyl)indeno[1,2-*b*]pyrrol-1(4*H*)-yl)benzamide (6ae)**



Following the TP-3, **6ae** was obtained from **3a** (190.2 mg, 0.3 mmol), 4-methyl benzoyl chloride **5e** (43.6 µL, 1.1 equiv) and triethylamine (63 µL, 1.5 equiv). The residue was purified by column chromatography (SiO_2, Hexanes/EtOAc= 85:15) to give as an orange solid (136.0 mg, 85% yield). R_f= 0.54 (EtOAc:Hexanes =1:2); mp = 255.6-255.9 °C.

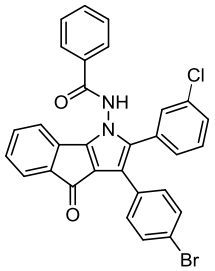
^{1}H NMR (400 MHz, $CDCl_3$, 25 °C) δ/ppm: 9.54 (s, 1H), 7.65 (d, *J* = 7.80 Hz, 2H), 7.52 (t, *J* = 7.2 Hz, 1H), 7.35 (t, *J* = 7.7 Hz, 2H), 7.25-7.16 (m, 4H), 7.13 (d, *J* = 7.1 Hz, 1H), 7.06 (d, *J* = 8.0 Hz, 2H), 7.00 (d, *J* = 8.0 Hz, 2H), 6.94 (t, *J* = 7.7 Hz, 1H), 6.88 (t, *J* = 7.4 Hz, 1H), 6.60 (d, *J* = 7.0 Hz, 1H), 2.28 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$, 25 °C) δ/ppm: 186.4, 166.7, 151.3, 139.0, 136.5, 134.0, 133.1, 132.7, 131.4, 131.0, 130.7, 130.3, 129.6, 129.0, 128.2, 127.4, 126.0, 123.3, 120.6, 119.2, 119.1, 117.0, 21.3.

IR (KBr) $\tilde{\nu}$ (cm^{-1}): 3235, 2918, 2360, 1739, 1699, 1665, 1493, 1278, 865, 750.

HRMS (ESI) *m/z*: $[M+H]^+$ Calcd for $C_{31}H_{22}{}^{79}BrN_2O_2$ 533.0865; found: 533.0870; $[M+H]^+$ Calcd for $C_{31}H_{22}{}^{81}BrN_2O_2$ 535.0844; found: 535.0856.

***N*-(3-(4-Bromophenyl)-2-(3-chlorophenyl)-4-oxoindeno[1,2-*b*]pyrrol-1(4*H*)-yl)benzamide (6af)**



Following the TP-3, **6af** was obtained from **3a** (190.2 mg, 0.3 mmol), 3-chloro benzoyl chloride **5f** (42.2 µL, 1.1 equiv) and triethylamine (63 µL, 1.5 equiv). The residue was purified by column chromatography (SiO_2, Hexanes/EtOAc= 85:15) to give as an orange solid (141.2 mg, 85% yield). R_f = 0.55 (EtOAc:Hexanes =1:2); mp = 234.2-234.6 °C.

^{1}H NMR (400 MHz, $CDCl_3$, 25 °C) δ/ppm: 8.77 (brs, 1H), 7.73 (d, *J* = 7.6 Hz, 2H), 7.62 (t, *J* = 7.8 Hz, 1H), 7.49 (t, *J* = 7.6 Hz, 2H), 7.36 (d, *J* = 6.9 Hz, 1H), 7.35 – 7.29 (m, 6H), 7.23 (d, *J* = 8.6 Hz, 1H), 7.15 (d, *J* = 7.8 Hz, 1H), 7.11 (d, *J* = 7.1 Hz, 1H), 7.07 (pt, *J* = 7.3 Hz, 1H), 6.79 (d, *J* = 7.1 Hz, 1H).

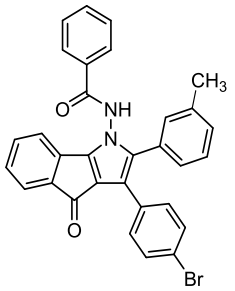
^{13}C NMR (100 MHz, DMSO-d_6, 25 °C) δ/ppm: 184.9, 166.2, 150.9, 138.3, 134.9, 133.55, 133.50, 133.2, 133.0, 131.2, 131.1, 130.80, 130.76, 130.6, 130.4, 129.7, 129.0, 128.94, 128.88, 127.5, 123.4, 120.4, 118.5, 117.9, 117.5.

IR (KBr) $\tilde{\nu}$ (cm^{-1}): 3428, 2918, 2848, 1735, 1638, 1490, 1273, 865, 745.

HRMS (ESI) *m/z*: $[M+H]^+$ Calcd for $C_{30}H_{19}{}^{79}Br^{35}ClN_2O_2$ 553.0318; found: 553.0316; $[M+H]^+$ Calcd for $C_{30}H_{19}{}^{79}Br^{37}ClN_2O_2$ 555.0298; found: 555.0298; $[M+H]^+$ Calcd for $C_{30}H_{19}{}^{81}Br^{35}ClN_2O_2$

555.0298; found: 555.0301; $[M+H]^+$ Calcd for $C_{30}H_{19}{}^{81}Br^{37}ClN_2O_2$ 557.0268; found: 557.0282.

***N*-(3-(4-Bromophenyl)-4-oxo-2-(*m*-tolyl)indeno[1,2-*b*]pyrrol-1(4*H*)-yl)benzamide (6ag)**



Following the TP-3, **6ag** was obtained from **3a** (190.2 mg, 0.3 mmol), 3-methyl benzoyl chloride **5g** (43.6 µL, 1.1 equiv) and triethylamine (63 µL, 1.5 equiv). The residue was purified by column chromatography (SiO_2, Hexanes/EtOAc= 85:15) to give as an orange solid (128.0 mg, 80% yield). R_f= 0.53 (EtOAc:Hexanes =1:2); mp = 151.1-151.5 °C.

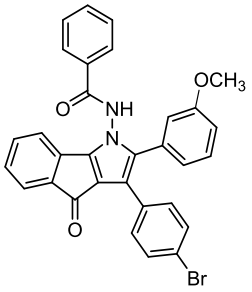
^{1}H NMR (400 MHz, DMSO-d_6, 25 °C) δ/ppm: 12.11 (brs, 1H), 7.79 (dd, *J* = 7.9, 1.7 Hz, 2H), 7.65 (tt, *J* = 7.2, 1.7 Hz, 1H), 7.55 (t, *J* = 7.9 Hz, 2H), 7.47 (dt, *J* = 8.7, 2.2 Hz, 2H), 7.39 (d, *J* = 7.6 Hz, 1H), 7.36 (dt, *J* = 8.5, 2.0 Hz, 2H), 7.31 (d, *J* = 7.5 Hz, 1H), 7.28 (t, *J* = 7.7 Hz, 1H), 7.21 (pt, *J* = 7.3 Hz, 2H), 7.19 – 7.16 (m, 1H), 7.09 (d, *J* = 7.7 Hz, 1H), 6.93 (d, *J* = 7.3 Hz, 1H), 2.23 (s, 3H).

^{13}C NMR (100 MHz, DMSO-d_6, 25 °C) δ/ppm: 185.0, 166.2, 150.7, 138.3, 137.9, 136.8, 133.7, 133.5, 132.8, 131.6, 131.1, 130.5, 130.3, 129.6, 128.89, 128.75, 128.63, 127.5, 127.4, 123.3, 120.0, 117.8, 117.3, 20.9.

IR (KBr) $\tilde{\nu}$ (cm^{-1}): 3428, 2918, 1721, 1642, 1490, 1372, 1076, 896, 754.

HRMS (ESI) *m/z*: $[M+H]^+$ Calcd for $C_{31}H_{22}{}^{79}BrN_2O_2$ 533.0865; found: 533.0861; $[M+H]^+$ Calcd for $C_{31}H_{22}{}^{81}BrN_2O_2$ 535.0844; found: 535.0844.

***N*-(3-(4-Bromophenyl)-2-(3-methoxyphenyl)-4-oxoindeno[1,2-*b*]pyrrol-1(4*H*)-yl)benzamide (6ah)**



Following the TP-3, **6ah** was obtained from **6a** (190.2 mg, 0.3 mmol), 3-methoxy benzoyl chloride

5h (46.4 µL, 1.1 equiv) and triethylamine (63 µL, 1.5 equiv). The residue was purified by column chromatography (SiO_2, Hexanes/EtOAc= 85:15) to give as a yellow solid (110.4 mg, 67% yield). R_f= 0.48 (EtOAc:Hexanes =1:2); mp = 248.3-248.7 °C.

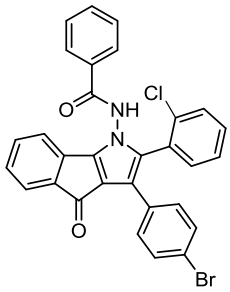
^{1}H NMR (400 MHz, DMSO-d_6, 25 °C) δ/ppm: 8.93 (brs, 1H), 7.70 (d, *J* = 7.6 Hz, 2H), 7.59 (t, *J* = 7.6 Hz, 1H), 7.44 (t, *J* = 7.8 Hz, 2H), 7.36 – 7.30 (m, 3H), 7.30 – 7.27 (m, 2H), 7.21 (t, *J* = 8.5 Hz, 1H), 7.08 (t, *J* = 7.5 Hz, 1H), 7.02 (t, *J* = 7.4 Hz, 1H), 6.87 (dd, *J* = 8.8, 2.1 Hz, 1H), 6.84 (d, *J* = 7.3 Hz, 2H), 6.74 (d, *J* = 7.0 Hz, 1H), 3.63 (s, 3H).

^{13}C NMR (100 MHz, DMSO-d_6, 25 °C) δ/ppm: 186.1, 166.5, 159.9, 151.4, 139.1, 135.9, 134.1, 133.2, 132.8, 131.3, 131.2, 130.8, 130.4, 130.1, 129.2, 128.5, 127.3, 123.6, 122.8, 120.9, 119.6, 119.3, 117.1, 115.5, 115.3, 55.2.

IR (KBr) $\tilde{\nu}$ (cm^{-1}): 3428, 2918, 2852, 2334, 1750, 1644, 1215, 1008, 867, 753.

HRMS (ESI) *m/z*: $[M+H]^+$ Calcd for $C_{31}H_{22}{}^{79}BrN_2O_3$ 549.0814; found: 549.0811; $[M+H]^+$ Calcd for $C_{31}H_{22}{}^{81}BrN_2O_3$ 551.0793; found: 551.0796.

***N*-(3-(4-Bromophenyl)-2-(2-chlorophenyl)-4-oxoindeno[1,2-*b*]pyrrol-1(4*H*)-yl)benzamide (6ai)**



Following the TP-3, **6ai** was obtained from **3a** (190.2 mg, 0.3 mmol), 2-chloro benzoyl chloride **5i** (41.8 µL, 1.1 equiv) and triethylamine (63 µL, 1.5 equiv). The residue was purified by column chromatography (SiO_2, Hexanes/EtOAc= 86:14) to give as an orange solid (124.6 mg, 75% yield). R_f= 0.55 (EtOAc:Hexanes =1:2); mp = 170.3-170.7 °C.

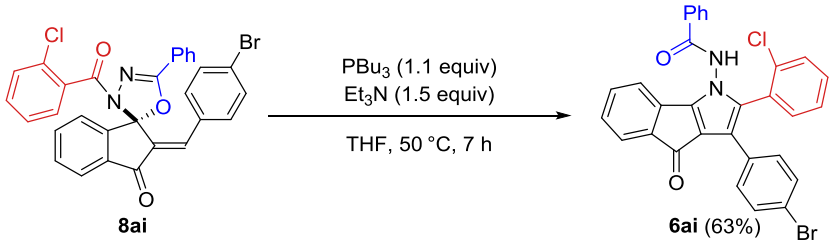
^{1}H NMR (400 MHz, DMSO-d_6, 25 °C) δ/ppm: 9.15 (s, 1H), 7.61 (d, *J* = 7.7 Hz, 2H), 7.53 (t, *J* = 7.5 Hz, 1H), 7.47 (d, *J* = 8.0 Hz, 1H), 7.38 (t, *J* = 7.5 Hz, 2H), 7.35-7.26 (m, 7H), 7.18 (t, *J* = 7.6 Hz, 1H), 7.13 - 6.97 (m, 2H), 6.80 (d, *J* = 6.2 Hz, 1H).

^{13}C NMR (100 MHz, DMSO-d_6, 25 °C) δ/ppm: 186.0, 166.2, 151.6, 139.0, 134.0, 133.1, 132.7, 131.3, 131.1, 130.1, 130.5, 129.9, 129.0, 128.8, 128.6, 127.8, 127.2, 123.6, 121.0, 120.8, 119.2, 117.3.

IR (KBr) $\tilde{\nu}$ (cm^{-1}): 3239, 2918, 1754, 1699, 1665, 1491, 1276, 1213, 852, 743.

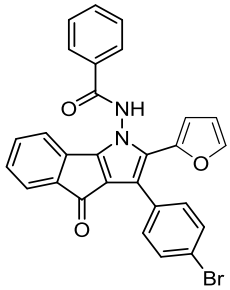
HRMS (ESI) *m/z*: $[M+H]^+$ Calcd for $C_{30}H_{19}{}^{79}Br^{35}ClN_2O_2$ 553.0318; found: 553.0319; $[M+H]^+$ Calcd for $C_{30}H_{19}{}^{79}Br^{37}ClN_2O_2$ 555.0298; found: 555.0301; $[M+H]^+$ Calcd for $C_{30}H_{19}{}^{81}Br^{35}ClN_2O_2$ 555.0298; found: 555.0301; $[M+H]^+$ Calcd for $C_{30}H_{19}{}^{81}Br^{37}ClN_2O_2$ 557.0268; found: 557.0285.

General procedure for the preparation of indenopyrrole derivative 6ai from spiro-indene-1,2'-[1,3,4]oxadiazol 8ai:



A dry and argon-flushed 10 mL Schlenk flask equipped with a magnetic stir bar and septum was sequentially charged with **8ai** (114.0 mg, 0.2 mmol), anhydrous THF (2 mL), PBu_3 (54.3 µL, 1.1 equiv) and Et_3N (40.0 µL, 1.5 equiv). The reaction mixture was stirred for 7 h at 50 °C. After completion of the reaction, solvent was removed in *vacuo* and the crude residue was subjected to flash column chromatography (SiO_2, Hexanes/EtOAc= 86:14) to give the product **6ai** in 63% yield (69.8 mg).

***N*-(3-(4-Bromophenyl)-2-(furan-2-yl)-4-oxoindeno[1,2-*b*]pyrrol-1(4*H*)-yl)benzamide (6aj)**



Following the TP-3, **6aj** was obtained from **3a** (190.2 mg, 0.3 mmol), 2-furoyl chloride **5j** (32.6 µL, 1.5 equiv) and triethylamine (63 µL, 1.5 equiv). The residue was purified by column chromatography (SiO_2, Hexanes/EtOAc= 85:15) to give as an orange solid (110.0 mg, 72% yield). R_f= 0.50 (EtOAc:Hexanes =1:2); mp = 230.1-230.5 °C.

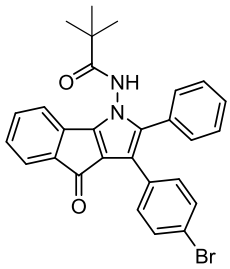
^{1}H NMR (400 MHz, $CDCl_3$, 25 °C) δ/ppm: 9.26 (s, 1H), 7.69 (d, *J* = 7.2 Hz, 2H), 7.58 (t, *J* = 7.6 Hz, 1H), 7.40 (t, *J* = 7.6 Hz, 2H), 7.37-7.29 (m, 4H), 7.22 (d, *J* = 7.1 Hz, 1H), 7.04 (t, *J* = 7.4 Hz, 1H), 6.98 (t, *J* = 7.4 Hz, 1H), 6.73 (d, *J* = 7.2 Hz, 1H), 6.32 (d, *J* = 1.3 Hz, 2H).

^{13}C NMR (100 MHz, $CDCl_3$, 25 °C) δ/ppm: 185.7, 166.5, 151.8, 143.3, 142.6, 139.0, 133.6, 133.2, 132.8, 131.3, 130.8, 130.5, 130.2, 129.1, 128.8, 127.4, 125.6, 123.5, 122.1, 121.5, 119.0, 117.6, 112.4, 111.5.

IR (KBr) $\tilde{\nu}$ (cm^{-1}): 3441, 3243, 2914, 1735, 1699, 1650, 1609, 1491, 1278, 1057, 852, 750.

HRMS (ESI) *m/z*: $[M+H]^+$ Calcd for $C_{28}H_{17}{}^{79}BrN_2O_3$ 509.0501; found: 509.0497; $[M+H]^+$ Calcd for $C_{28}H_{17}{}^{81}BrN_2O_3$ 511.0480; found: 511.0478.

***N*-(3-(4-Bromophenyl)-4-oxo-2-phenylindeno[1,2-*b*]pyrrol-1(4*H*)-yl)pivalamide (7ak)**



Following the TP-3, **7ak** was obtained from **3a** (190.2 mg, 0.3 mmol), pivaloyl chloride **5k** (40.4 µL, 1.1 equiv) and triethylamine (63 µL, 1.5 equiv). The residue was purified by column chromatography (SiO_2, Hexanes/EtOAc= 90:10) to give as an orange solid (89.9 mg, 60% yield) along with zwitterion **3a** (48.1 mg, 25% yield).

R_f= 0.58 (EtOAc:Hexanes =1:2); mp = 300.0 °C.

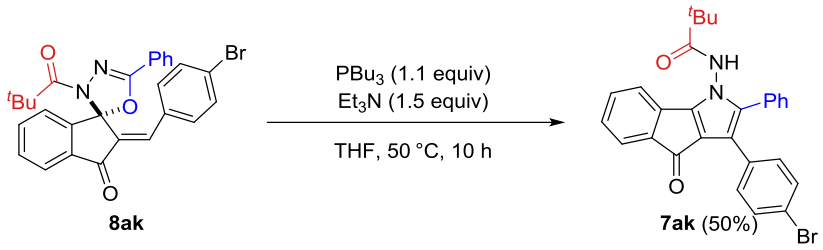
^{1}H NMR (400 MHz, $CDCl_3$, 25 °C) δ/ppm: 8.27 (s, 1H), 7.40 – 7.30 (m, 4H), 7.28 (d, *J* = 2.1 Hz, 4H), 7.20 (dd, *J* = 8.3, 1.7 Hz, 2H), 7.12 (td, *J* = 7.4, 1.4 Hz, 1H), 7.04 (td, *J* = 7.3, 1.2 Hz, 1H), 6.7. (d, *J* = 7.3 Hz, 1H), 1.08 (s, 9H).

^{13}C NMR (100 MHz, $CDCl_3$, 25 °C) δ/ppm: 186.2, 176.7, 151.3, 139.1, 136.3, 134.3, 132.7, 131.3, 131.1, 130.8, 130.2, 129.4, 129.2, 128.8, 128.3, 123.4, 120.8, 119.4, 119.1, 116.9, 38.5, 27.0.

IR (KBr) $\tilde{\nu}$ (cm^{-1}): 3437, 2923, 2360, 1740, 1701, 1493, 1151, 865, 749.

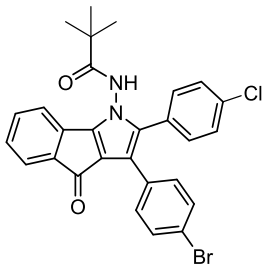
HRMS (ESI) *m/z*: $[M+H]^+$ Calcd for $C_{28}H_{24}{}^{79}BrN_2O_2$ 499.1021; found: 499.1021; $[M+H]^+$ Calcd for $C_{28}H_{24}{}^{81}BrN_2O_2$ 501.1001; found: 501.1004.

General procedure for the preparation of indenopyrrole derivative 7ak from spiro-indene-1,2'-[1,3,4]oxadiazol 8ak:



A dry and argon-flushed 10 mL Schlenk flask equipped with a magnetic stir bar and septum was sequentially charged with **8ak** (103.1 mg, 0.2 mmol), anhydrous THF (2 mL), PBu_3 (54.3 µL, 1.1 equiv) and Et_3N (40.0 µL, 1.5 equiv). The reaction mixture was stirred for 10 h at 50 °C. After completion of the reaction, solvent was removed in *vacuo* and the crude residue was subjected to flash column chromatography (SiO_2, Hexanes/EtOAc= 90:10) to give the product **7ak** in 50% yield (50.0 mg).

_N_-(3-(4-Bromophenyl)-2-(4-chlorophenyl)-4-oxoindeno[1,2-*b*]pyrrol-1(4*H*)-yl)pivalamide (7ik)



Following the TP-3, **7ik** was obtained from **3i** (200.4 mg, 0.3 mmol), pivaloyl chloride **5k** (40.4 µL, 1.1 equiv) and triethylamine (63 µL, 1.5 equiv). The residue was purified by column chromatography (SiO_2, Hexanes/EtOAc= 90:10) to give as an orange solid (64.0 mg, 40% yield) along with zwitterion **3i** (72.0 mg, 36% yield).

R_f= 0.58 (EtOAc:Hexanes =1:2); mp = 265.3-265.7 °C.

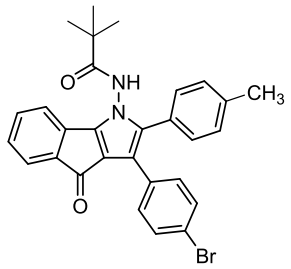
^{1}H NMR (400 MHz, $CDCl_3$, 25 °C) δ/ppm: 8.23 (s, 1H), 7.33 (d, *J* = 7.0 Hz, 1H), 7.33 – 7.30 (m, 2H), 7.29 (d, *J* = 2.5 Hz, 2H), 7.25 (pt, *J* = 2.2 Hz, 1H), 7.23 (t, *J* = 2.2 Hz, 1H), 7.14 (dd, *J* = 7.6, 1.5 Hz, 1H), 7.12 (dt, *J* = 8.4, 1.4 Hz, 2H), 7.06 (td, *J* = 7.5, 1.0 Hz, 1H), 6.72 (d, *J* = 7.4 Hz, 1H), 1.15 (s, 9H).

^{13}C NMR (100 MHz, $CDCl_3$, 25 °C) δ/ppm: 186.1, 176.6, 151.4, 139.1, 135.3, 135.0, 134.1, 132.8, 132.1, 131.3, 130.9, 130.2, 129.1, 128.5, 127.7, 123.6, 121.1, 119.8, 119.2, 117.0, 38.5, 27.1.

IR (KBr) $\tilde{\nu}$ (cm^{-1}): 3430, 2921, 2350, 1735, 1699, 1660, 1495, 1287, 1021, 890, 750.

HRMS (ESI) *m/z*: $[M+H]^+$ Calcd for $C_{28}H_{23}{}^{79}Br^{35}ClN_2O_2$ 533.0631; found: 533.0630; $[M+H]^+$ Calcd for $C_{28}H_{23}{}^{79}Br^{37}ClN_2O_2$ 535.0611; found: 535.0612; $[M+H]^+$ Calcd for $C_{28}H_{23}{}^{81}Br^{35}ClN_2O_2$ 535.0611; found: 535.0612; $[M+H]^+$ Calcd for $C_{28}H_{23}{}^{81}Br^{37}ClN_2O_2$ 537.0581; found: 537.0596.

***N*-(3-(4-Bromophenyl)-4-oxo-2-(*p*-tolyl)indeno[1,2-*b*]pyrrol-1(4*H*)-yl)pivalamide (7jk)**



Following the TP-3, **7jk** was obtained from **3j** (194.3 mg, 0.3 mmol), pivaloyl chloride **5k** (40.4 μL, 1.1 equiv) and triethylamine (63 μL, 1.5 equiv). The residue was purified by column chromatography (SiO_2, Hexanes/EtOAc= 90:10) to give as an orange solid (69.2 mg, 45% yield) along with zwitterion **3j** (60.1 mg, 31% yield).

R_f = 0.58 (EtOAc:Hexanes =1:2); mp = 281.3-281.7 °C.

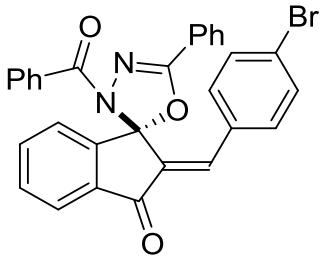
^{1}H NMR (400 MHz, $CDCl_3$, 25 °C) δ/ppm: 8.64 (s, 1H), 7.24 – 7.19 (m, 5H), 7.05 (pt, *J* = 3.6 Hz, 1H), 7.02 (d, *J* = 7.0 Hz, 3H), 7.00 (d, *J* = 6.9 Hz, 1H), 6.95 (t, *J* = 7.2 Hz, 1H), 6.62 (d, *J* = 7.2 Hz, 1H), 2.31 (s, 3H), 1.03 (s, 9H).

^{13}C NMR (100 MHz, $CDCl_3$, 25 °C) δ/ppm: 186.3, 177.0, 151.1, 139.08, 139.04, 136.5, 134.3, 132.6, 131.4, 131.0, 130.5, 130.1, 129.4, 128.1, 126.1, 123.2, 120.6, 119.1, 118.9, 116.8, 38.4, 26.9, 21.3.

IR (KBr) $\tilde{\nu}$ (cm^{-1}): 3428, 2952, 2354, 1735, 1698, 1650, 1492, 1273, 1080, 869, 752.

HRMS (ESI) *m/z*: $[M+H]^+$ Calcd for $C_{29}H_{26}{}^{79}BrN_2O_2$ 513.1178; found: 513.1179; $[M+H]^+$ Calcd for $C_{29}H_{26}{}^{81}BrN_2O_2$ 515.1157; found: 515.1161.

(*E*)-3'-Benzoyl-2-(4-bromobenzylidene)-5'-phenyl-3'*H*-spiro[indene-1,2'-[1,3,4]oxadiazol]-3(2*H*)-one (8aa)



Prepared according to TP-4 from **1a** (132.13 mg, 0.5 mmol), 4-bromo benzaldehyde **2a** (101.76

mg, 1.1 equiv), $PhCO_2H$ (6.1 mg, 0.1 equiv) and anhydrous THF (5.0 mL). To this stirred reaction mixture, PPh_2Me (112.8 µL, 1.2 equiv) and pyrrolidine (4.0 µL, 0.1 equiv) were added in sequence. The reaction mixture was stirred for 12 hours at 30 °C. Thereafter, solvent was removed by evaporation in *vacuo* and dissolved in anhydrous THF (5 mL), benzoyl chloride **5a** (87.1 µL, 1.5 equiv) and Et_3N (133.1 µL, 2.0 equiv.) The residue was purified by column chromatography (SiO_2, Hexanes/EtOAc= 90:10) to give **8aa** as a yellow solid (120.5 mg, 45% yield).

R_f= 0.51 (EtOAc:Hexanes =2:8); mp = 186.9-187.8 °C.

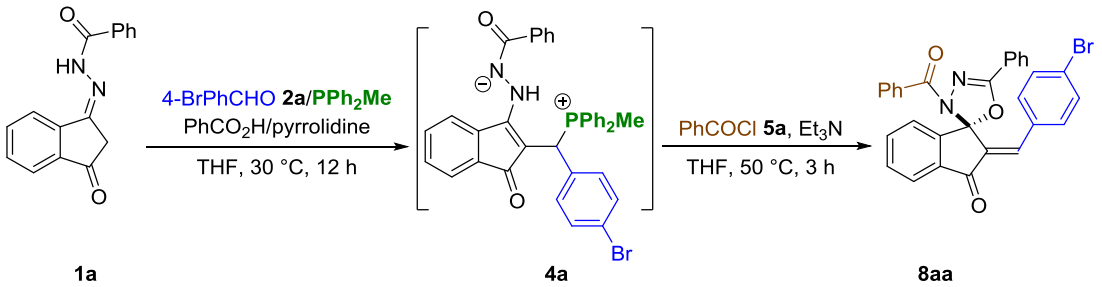
^{1}H NMR (400 MHz, $CDCl_3$, 25 °C) δ/ppm: 8.01 (d, *J* = 7.3 Hz, 1H), 7.93 (s, 1H), 7.80 (dd, *J* = 8.1, 1.5 Hz, 2H), 7.70 (td, *J* = 7.4, 1.3 Hz, 1H), 7.65 (dd, *J* = 7.5, 1.4 Hz, 1H), 7.61 (dt, *J* = 7.7, 1.3 Hz, 3H), 7.55 (tt, *J* = 7.6, 2.2 Hz, 1H), 7.47 (dt, *J* = 7.9, 1.6 Hz, 2H), 7.46 – 7.43 (m, 1H), 7.36 (t, *J* = 7.8 Hz, 2H), 7.29 (dt, *J* = 8.3, 1.4 Hz, 2H), 7.21 (dt, *J* = 8.5, 2.2 Hz, 2H).

^{13}C NMR (100 MHz, $CDCl_3$, 25 °C) δ/ppm: 189.2, 163.0, 154.8, 147.1, 138.3, 137.0, 136.0, 135.0, 133.0, 132.4, 132.0, 131.65, 131.60, 131.56, 130.8, 129.6, 128.9, 127.7, 126.9, 124.1, 123.9, 123.7, 123.2, 98.9.

IR (KBr) $\tilde{\nu}$ (cm^{-1}): 3450, 2910, 1680, 1640, 1490, 1372, 1190, 1076, 754.

HRMS (ESI) *m/z*: $[M+H]^+$ Calcd for $C_{30}H_{20}{}^{79}BrN_2O_3$ 535.0657; found: 535.0653; $[M+H]^+$ Calcd for $C_{30}H_{20}{}^{81}BrN_2O_3$ 537.0637; found: 537.0640.

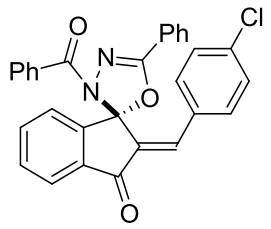
General procedure for the gram-scale preparation of spiro-indene-1,2'-[1,3,4]oxadiazol derivatives 8aa:



A flame dried and nitrogen-flushed 100-mL round bottom flask equipped with a magnetic stir bar and a septum was sequentially charged with **1** (1.057 g, 4 mmol), **2** (814.1 mg, 1.1 equiv), $PhCO_2H$ (48.8 mg, 0.1 equiv) and anhydrous THF (40 mL). To this stirred reaction mixture, PPh_2Me (902.0 µL, 1.2 equiv) and pyrrolidine (32.8 µL, 0.1 equiv) were added in sequence. The reaction mixture was stirred for 12 hours at 30 °C. Thereafter, solvent was removed by evaporation in *vacuo* and

dissolved in anhydrous THF (5 mL), benzoyl chloride **5** (697.0 µL, 1.5 equiv) and Et_3N (1.06 mL, 2.0 equiv). The reaction mixture was stirred for 3 h at 50 °C. After completion of the reaction, solvent was removed in *vacuo* and the crude residue was subjected to flash column chromatography (SiO_2, Hexanes/EtOAc= 90:10) to give the product **8aa** in 43% yield (0.920 g).

(*E*)-3'-Benzoyl-2-(4-chlorobenzylidene)-5'-phenyl-3'*H*-spiro[indene-1,2'-[1,3,4]oxadiazol]-3(2*H*)-one (8ba)



Prepared according to TP-4 from **1a** (132.13 mg, 0.5 mmol), 4-chloro benzaldehyde **2b** (64.4 µL, 1.1 equiv), $PhCO_2H$ (6.1 mg, 0.1 equiv) and anhydrous THF (5.0 mL). To this stirred reaction mixture, PPh_2Me (112.8 µL, 1.2 equiv) and pyrrolidine (4.0 µL, 0.1 equiv) were added in sequence. The reaction mixture was stirred for 12 hours at 30 °C. Thereafter, solvent was removed by evaporation in *vacuo* and dissolved in anhydrous THF (5 mL), benzoyl chloride **5a** (87.1 µL, 1.5 equiv) and Et_3N (133.1 µL, 2.0 equiv.) The residue was purified by column chromatography (SiO_2, Hexanes/EtOAc= 90:10) to give **8ba** as a yellow solid (98.2 mg, 40% yield).

R_f = 0.45 (EtOAc:Hexanes =2:8); mp = 175.3-174.5 °C.

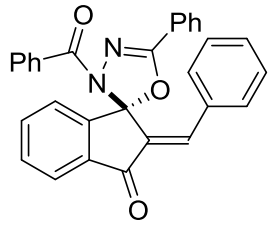
^{1}H NMR (400 MHz, $CDCl_3$, 25 °C) δ/ppm: 8.02 (d, *J* = 7.6 Hz, 1H), 7.96 (s, 1H), 7.81 (dd, *J* = 8.1, 1.7 Hz, 2H), 7.70 (tt, *J* = 7.7, 1.3 Hz, 1H), 7.66 (dd, *J* = 7.4, 1.4 Hz, 1H), 7.64 – 7.60 (m, 3H), 7.55 (tt, *J* = 7.7, 2.2 Hz, 1H), 7.50 – 7.43 (m, 3H), 7.35 (t, *J* = 7.7 Hz, 2H), 7.29 (d, *J* = 8.5 Hz, 2H), 7.14 (dt, *J* = 8.6, 1.8 Hz, 2H).

^{13}C NMR (100 MHz, $CDCl_3$, 25 °C) δ/ppm: 189.2, 163.1, 154.9, 147.1, 138.3, 137.1, 136.0, 135.6, 134.9, 132.51, 132.48, 132.1, 131.62, 131.57, 130.7, 129.7, 128.9, 128.7, 127.7, 127.0, 124.1, 123.7, 123.2, 99.0.

IR (KBr) $\tilde{\nu}$ (cm^{-1}): 3435, 2900, 1682, 1638, 1495, 1372, 1190, 1060, 750.

HRMS (ESI) *m/z*: $[M+H]^+$ Calcd for $C_{30}H_{20}{}^{35}ClN_2O_3$ 491.1162; found: 491.1163; $[M+H]^+$ Calcd for $C_{30}H_{20}{}^{37}ClN_2O_3$ 493.1133; found: 493.1147.

(*E*)-3'-Benzoyl-2-benzylidene-5'-phenyl-3'*H*-spiro[indene-1,2'-[1,3,4]oxadiazol]-3(2*H*)-one (8ea)



Prepared according to TP-4 from **1a** (132.13 mg, 0.5 mmol), benzaldehyde **2e** (55.90 µL, 1.1 equiv), $PhCO_2H$ (6.1 mg, 0.1 equiv) and anhydrous THF (5.0 mL). To this stirred reaction mixture, PPh_2Me (112.8 µL, 1.2 equiv) and pyrrolidine (4.0 µL, 0.1 equiv) were added in sequence. The reaction mixture was stirred for 12 hours at 30 °C. Thereafter, solvent was removed by evaporation in *vacuo* and dissolved in anhydrous THF (5 mL), benzoyl chloride **5a** (87.1 µL, 1.5 equiv) and Et_3N (133.1 µL, 2.0 equiv.) The residue was purified by column chromatography (SiO_2, Hexanes/EtOAc= 90:10) to give **8ea** as a yellow solid (79.9 mg, 35% yield).

R_f = 0.65 (EtOAc:Hexanes =2:8); mp = 163.5-164.2 °C.

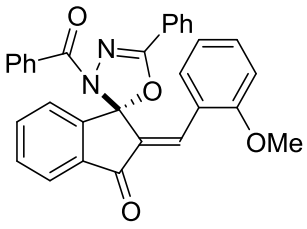
^{1}H NMR (400 MHz, $CDCl_3$, 25 °C) δ/ppm: 8.05 (s, 1H), 8.02 (d, *J* = 7.4 Hz, 1H), 7.80 (dd, *J* = 7.8, 1.7 Hz, 2H), 7.69 (td, *J* = 7.5, 1.6 Hz, 1H), 7.65 (dd, *J* = 7.5, 1.4 Hz, 1H), 7.60 (d, *J* = 8.2 Hz, 1H), 7.57 (d, *J* = 7.9 Hz, 2H), 7.52 (dt, *J* = 7.6, 2.2 Hz, 1H), 7.45 (dd, *J* = 8.0, 1.7 Hz, 2H), 7.42 (dd, *J* = 7.0, 1.4 Hz, 1H), 7.37 (d, *J* = 7.4 Hz, 2H), 7.31 (t, *J* = 7.8 Hz, 2H), 7.23 (dt, *J* = 7.5, 2.3 Hz, 1H), 7.17 (t, *J* = 7.7 Hz, 2H).

^{13}C NMR (100 MHz, $CDCl_3$, 25 °C) δ/ppm: 189.4, 163.1, 154.8, 147.2, 140.0, 137.1, 135.8, 134.3, 134.1, 132.7, 131.8, 131.5, 131.4, 129.7, 129.4, 129.3, 128.7, 128.4, 127.6, 127.0, 124.3, 123.7, 123.2, 99.0.

IR (KBr) $\tilde{\nu}$ (cm^{-1}): 3448, 2912, 1679, 1638, 1492, 1371, 1198, 1075, 751.

HRMS (ESI) *m/z*: $[M+H]^+$ Calcd for $C_{30}H_{21}N_2O_3$ 457.1552; found: 457.1550.

(*E*)-3'-Benzoyl-2-(2-methoxybenzylidene)-5'-phenyl-3'*H*-spiro[indene-1,2'-[1,3,4]oxadiazol]-3(2*H*)-one (8ha)



Prepared according to TP-4 from **1a** (132.13 mg, 0.5 mmol), 2-methoxy benzaldehyde **2h** (66.4 µL, 1.1 equiv), $PhCO_2H$ (6.1 mg, 0.1 equiv) and anhydrous THF (5.0 mL). To this stirred reaction

mixture, PPh_2Me (112.8 µL, 1.2 equiv) and pyrrolidine (4.0 µL, 0.1 equiv) were added in sequence. The reaction mixture was stirred for 12 hours at 30 °C. Thereafter, solvent was removed by evaporation in *vacuo* and dissolved in anhydrous THF (5 mL), benzoyl chloride **5a** (87.1 µL, 1.5 equiv) and Et_3N (133.1 µL, 2.0 equiv.) The residue was purified by column chromatography (SiO_2, Hexanes/EtOAc= 87:13) to give **8ha** as a yellow solid (99.9 mg, 41% yield).

R_f= 0.28 (EtOAc:Hexanes =2:8); mp = 198.1-199.0 °C.

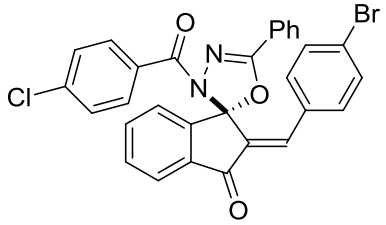
^{1}H NMR (400 MHz, $CDCl_3$, 25 °C) δ/ppm: 8.20 (s, 1H), 8.01 (d, *J* = 7.4 Hz, 1H), 7.74 (dd, *J* = 7.9, 1.5 Hz, 2H), 7.67 (dd, *J* = 7.2, 1.2 Hz, 3H), 7.62 (pt, *J* = 7.5, 1.3 Hz, 1H), 7.59 (d, *J* = 7.5 Hz, 1H), 7.50 (tt, *J* = 7.5, 2.2 Hz, 1H), 7.47 – 7.39 (m, 3H), 7.33 (t, *J* = 7.7 Hz, 2H), 7.22 (d, *J* = 7.6 Hz, 1H), 7.17 (td, *J* = 8.1, 1.7 Hz, 1H), 6.67 (d, *J* = 8.3 Hz, 1H), 6.59 (t, *J* = 7.5 Hz, 1H), 3.59 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$, 25 °C) δ/ppm: 189.4, 162.8, 157.9, 154.6, 147.2, 137.4, 136.9, 135.6, 135.0, 132.8, 131.6, 131.35, 131.29, 130.8, 129.8, 129.7, 128.6, 127.6, 126.9, 124.5, 123.6, 123.3, 120.0, 110.5, 99.1, 55.4.

IR (KBr) $\tilde{\nu}$ (cm^{-1}): 3442, 2918, 1683, 1639, 1498, 1376, 1195, 1072, 759.

HRMS (ESI) *m/z*: $[M+H]^+$ Calcd for $C_{31}H_{23}N_2O_4$ 487.1658; found: 487.1657.

(*E*)-2-Benzylidene-3'-(4-chlorobenzoyl)-5'-phenyl-3'*H*-spiro[indene-1,2'-[1,3,4]oxadiazol]-3(2*H*)-one (8ac)



Prepared according to TP-4 from **1a** (132.13 mg, 0.5 mmol), 4-bromo benzaldehyde **2a** (101.76 mg, 1.1 equiv), $PhCO_2H$ (6.1 mg, 0.1 equiv) and anhydrous THF (5.0 mL). To this stirred reaction mixture, PPh_2Me (112.8 µL, 1.2 equiv) and pyrrolidine (4.0 µL, 0.1 equiv) were added in sequence. The reaction mixture was stirred for 12 hours at 30 °C. Thereafter, solvent was removed by evaporation in *vacuo* and dissolved in anhydrous THF (5 mL), 4-chloro benzoyl chloride **5c** (96.2 µL, 1.5 equiv) and Et_3N (133.1 µL, 2.0 equiv.) The residue was purified by column chromatography (SiO_2, Hexanes/EtOAc= 90:10) to give **8ac** as a yellow solid (108.3 mg, 38% yield).

R_f = 0.54 (EtOAc:Hexanes =2:8); mp = 179.0-180.1 °C.

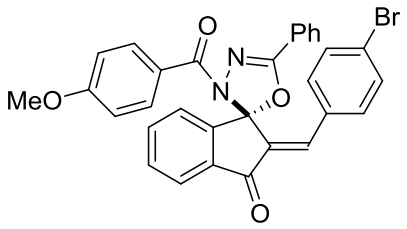
^{1}H NMR (400 MHz, $CDCl_3$, 25 °C) δ/ppm: 8.01 (d, *J* = 7.4 Hz, 1H), 7.93 (s, 1H), 7.79 (dd, *J* = 8.2, 1.6 Hz, 2H), 7.70 (td, *J* = 7.5, 1.4 Hz, 1H), 7.65 (td, *J* = 7.5, 1.4 Hz, 1H), 7.62 – 7.54 (m, 4H), 7.48 (t, *J* = 7.4 Hz, 2H), 7.33 (td, *J* = 8.6, 1.8 Hz, 2H), 7.28 (dt, *J* = 8.4, 1.8 Hz, 2H), 7.18 (d, *J* = 8.4 Hz, 2H).

^{13}C NMR (100 MHz, $CDCl_3$, 25 °C) δ/ppm: 189.0, 161.9, 155.0, 146.9, 138.4, 137.8, 137.0, 136.0, 134.9, 132.9, 132.2, 131.69, 131.64, 131.1, 130.8, 130.6, 128.9, 128.0, 126.9, 123.9, 123.7, 123.2, 98.9.

IR (KBr) $\tilde{\nu}$ (cm^{-1}): 3452, 2912, 1682, 1644, 1492, 1374, 1191, 1070, 748.

HRMS (ESI) *m/z*: $[M+H]^+$ Calcd for $C_{30}H_{19}{}^{79}Br^{35}ClN_2O_3$ 569.0268; found: 569.0266; $[M+H]^+$ Calcd for $C_{30}H_{19}{}^{79}Br^{37}ClN_2O_3$ 571.0238; found: 571.0247; $[M+H]^+$ Calcd for $C_{30}H_{19}{}^{81}Br^{35}ClN_2O_3$ 572.0247; found: 572.0278; $[M+H]^+$ Calcd for $C_{30}H_{19}{}^{81}Br^{37}ClN_2O_3$ 573.0218; found: 573.0235.

(*E*)-2-Benzylidene-3'-(4-methoxybenzoyl)-5'-phenyl-3'*H*-spiro[indene-1,2'-[1,3,4]oxadiazol]-3(2*H*)-one (8al)



Prepared according to TP-4 from **1a** (132.13 mg, 0.5 mmol), 4-bromo benzaldehyde **2a** (101.76 mg, 1.1 equiv), $PhCO_2H$ (6.1 mg, 0.1 equiv) and anhydrous THF (5.0 mL). To this stirred reaction mixture, PPh_2Me (112.8 µL, 1.2 equiv) and pyrrolidine (4.0 µL, 0.1 equiv) were added in sequence. The reaction mixture was stirred for 12 hours at 30 °C. Thereafter, solvent was removed by evaporation in *vacuo* and dissolved in anhydrous THF (5 mL), 4-methoxy benzoyl chloride **5l** (101.5 µL, 1.5 equiv) and Et_3N (133.1 µL, 2.0 equiv.) The residue was purified by column chromatography (SiO_2, Hexanes/EtOAc= 85:15) to give **8al** as a yellow solid (113.1 mg, 40% yield).

R_f = 0.26 (EtOAc:Hexanes =2:8); mp = 187.1-188.0 °C.

^{1}H NMR (400 MHz, $CDCl_3$, 25 °C) δ/ppm: 8.00 (d, *J* = 7.3 Hz, 1H), 7.91 (s, 1H), 7.80 (dd, *J* = 8.3, 1.5 Hz, 2H), 7.72 (dt, *J* = 8.8, 1.8 Hz, 2H), 7.68 (dd, *J* = 7.4, 1.4 Hz, 1H), 7.64 (dd, *J* = 7.5, 1.4 Hz, 1H), 7.60 (d, *J* = 8.2 Hz, 1H), 7.55 (tt, *J* = 7.5, 2.1 Hz, 1H), 7.47 (tt, *J* = 7.4, 1.7 Hz, 2H),

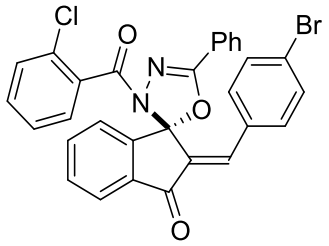
7.27 (d, J = 8.4 Hz, 2H), 7.19 (dt, J = 8.6, 2.2 Hz, 2H), 6.86 (dt, J = 8.1, 2.1 Hz, 2H), 3.85 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$, 25 °C) δ/ppm: 189.3, 162.4, 162.3, 154.7, 147.3, 138.1, 136.9, 135.9, 135.3, 133.0, 131.9, 131.59, 131.52, 130.8, 128.9, 126.9, 124.5, 124.1, 123.8, 123.7, 123.3, 113.0, 99.0, 55.4.

IR (KBr) $\tilde{\nu}$ (cm^{-1}): 3448, 2908, 1672, 1630, 1495, 1365, 1185, 1076, 742.

HRMS (ESI) *m/z*: $[M+H]^+$ Calcd for $C_{31}H_{22}{}^{79}BrN_2O_4$ 565.0763; found: 565.0764; $[M+H]^+$ Calcd for $C_{31}H_{22}{}^{81}BrN_2O_4$ 567.0742; found: 567.0749.

(*E*)-2-Benzylidene-3'-(2-chlorobenzoyl)-5'-phenyl-3'*H*-spiro[indene-1,2'-[1,3,4]oxadiazol]-3(2*H*)-one (8ai)



Prepared according to TP-4 from **1a** (132.13 mg, 0.5 mmol), 4-bromo benzaldehyde **2a** (101.76 mg, 1.1 equiv), $PhCO_2H$ (6.1 mg, 0.1 equiv) and anhydrous THF (5.0 mL). To this stirred reaction mixture, PPh_2Me (112.8 µL, 1.2 equiv) and pyrrolidine (4.0 µL, 0.1 equiv) were added in sequence. The reaction mixture was stirred for 12 hours at 30 °C. Thereafter, solvent was removed by evaporation in *vacuo* and dissolved in anhydrous THF (5 mL), 4-chloro benzoyl chloride **5i** (95.0 µL, 1.5 equiv) and Et_3N (133.1 µL, 2.0 equiv.) The residue was purified by column chromatography (SiO_2, Hexanes/EtOAc= 85:15) to give **8ai** as a yellow solid (105.4 mg, 37% yield).

R_f = 0.40 (EtOAc:Hexanes =2:8); mp = 199.0-200.1 °C.

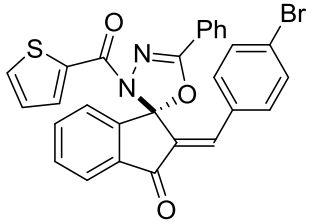
^{1}H NMR (400 MHz, $CDCl_3$, 25 °C) δ/ppm: 8.01 (d, J = 7.7 Hz, 1H), 7.98 (s, 1H), 7.78 – 7.70 (m, 4H), 7.67 (tt, J = 7.3, 2.0 Hz, 1H), 7.52 (tt, J = 7.5, 1.9 Hz, 1H), 7.41 (t, J = 7.5 Hz, 2H), 7.35 (d, J = 8.7 Hz, 3H), 7.31 (d, J = 8.6 Hz, 3H), 7.21 (tt, J = 7.5, 1.9 Hz, 1H), 6.72 (dd, J = 7.8, 1.7 Hz, 1H).

^{13}C NMR (100 MHz, $CDCl_3$, 25 °C) δ/ppm: 189.1, 162.2, 155.0, 146.5, 138.9, 137.2, 136.0, 134.3, 133.9, 132.7, 132.1, 131.8, 131.7, 131.4, 131.1, 130.7, 129.5, 128.8, 128.5, 127.1, 126.4, 124.4, 123.9, 123.68, 123.64, 98.4.

IR (KBr) $\tilde{\nu}$ (cm^{-1}): 3442, 2902, 1678, 1635, 1490, 1350, 1185, 1050, 737.

HRMS (ESI) *m/z*: $[M+H]^+$ Calcd for $C_{30}H_{19}{}^{79}Br^{35}ClN_2O_3$ 569.0268; found: 569.0269; $[M+H]^+$ Calcd for $C_{30}H_{19}{}^{79}Br^{37}ClN_2O_3$ 571.0238; found: 571.0250; $[M+H]^+$ Calcd for $C_{30}H_{19}{}^{81}Br^{35}ClN_2O_3$ 572.0247; found: 572.0279; $[M+H]^+$ Calcd for $C_{30}H_{19}{}^{81}Br^{37}ClN_2O_3$ 573.0218; found: 573.0230.

(*E*)-2-Benzylidene-5'-phenyl-3'-(thiophene-2-carbonyl)-3'*H*-spiro[indene-1,2'-[1,3,4]oxadiazol]-3(2*H*)-one (8am)



Prepared according to TP-4 from **1a** (132.13 mg, 0.5 mmol), 4-bromo benzaldehyde **2a** (101.76 mg, 1.1 equiv), $PhCO_2H$ (6.1 mg, 0.1 equiv) and anhydrous THF (5.0 mL). To this stirred reaction mixture, PPh_2Me (112.8 µL, 1.2 equiv) and pyrrolidine (4.0 µL, 0.1 equiv) were added in sequence. The reaction mixture was stirred for 12 hours at 30 °C. Thereafter, solvent was removed by evaporation in *vacuo* and dissolved in anhydrous THF (5 mL), 2-thiophenecarbonyl chloride **5m** (80.3 µL, 1.5 equiv) and Et_3N (133.1 µL, 2.0 equiv.) The residue was purified by column chromatography (SiO_2, Hexanes/EtOAc= 85:15) to give **8am** as a yellow solid (105.6 mg, 39% yield).

R_f = 0.43 (EtOAc:Hexanes =2:8); mp = 196.5-197.3 °C.

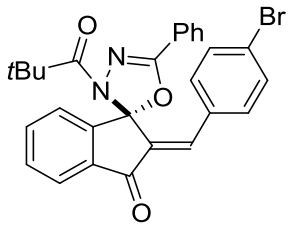
^{1}H NMR (400 MHz, $CDCl_3$, 25 °C) δ/ppm: 8.0 (d, *J* = 7.4 Hz, 1H), 7.97 (d, *J* = 6.5 Hz, 1H), 7.92 (s, 1H), 7.82 (d, *J* = 7.7 Hz, 2H), 7.69 (t, *J* = 7.4 Hz, 1H), 7.64 (d, *J* = 7.3 Hz, 1H), 7.60 (t, *J* = 7.2 Hz, 2H), 7.56 (d, *J* = 7.4 Hz, 1H), 7.49 (t, *J* = 7.6 Hz, 2H), 7.18 (d, *J* = 8.6 Hz, 2H), 7.10 (d, *J* = 8.6 Hz, 2H), 7.08 (d, *J* = 7.0 Hz, 1H).

^{13}C NMR (100 MHz, $CDCl_3$, 25 °C) δ/ppm: 188.9. 156.5, 155.2, 146.6, 138.5, 137.2, 135.9, 135.3, 134.7, 133.9, 133.4, 132.6, 132.1, 131.7, 131.6, 130.5, 128.9, 126.9, 123.9, 123.7, 123.6, 123.5, 98.9.

IR (KBr) $\tilde{\nu}$ (cm^{-1}): 3445, 2900, 1659, 1548, 1472, 1372, 1398, 1308, 1283, 1190, 1075, 750.

HRMS (ESI) *m/z*: $[M+H]^+$ Calcd for $C_{28}H_{18}{}^{79}BrN_2O_3S$ 541.0222; found: 541.0223; $[M+H]^+$ Calcd for $C_{28}H_{18}{}^{81}BrN_2O_3S$ 543.0201; found: 543.0204.

(*E*)-2-Benzylidene-5'-phenyl-3'-pivaloyl-3'*H*-spiro[indene-1,2'-[1,3,4]oxadiazol]-3(2*H*)-one (8ak)



Prepared according to TP-4 from **1a** (132.13 mg, 0.5 mmol), 4-bromo benzaldehyde **2a** (101.76 mg, 1.1 equiv), $PhCO_2H$ (6.1 mg, 0.1 equiv) and anhydrous THF (5.0 mL). To this stirred reaction mixture, PPh_2Me (112.8 µL, 1.2 equiv) and pyrrolidine (4.0 µL, 0.1 equiv) were added in sequence. The reaction mixture was stirred for 12 hours at 30 °C. Thereafter, solvent was removed by evaporation in *vacuo* and dissolved in anhydrous THF (5 mL), Pivaloyl chloride **5k** (91.8 µL, 1.5 equiv) and Et_3N (133.1 µL, 2.0 equiv.) The residue was purified by column chromatography (SiO_2, Hexanes/EtOAc= 85:15) to give **8ak** as a yellow solid (77.3 mg, 30% yield).

R_f = 0.60 (EtOAc:Hexanes =2:8); mp = 201.1-202.0 °C.

^{1}H NMR (400 MHz, $CDCl_3$, 25 °C) δ/ppm: 7.95 (d, *J* = 7.6 Hz, 1H), 7.84 (s, 1H), 7.81 (dd, *J* = 7.7, 1.6 Hz, 2H), 7.67 (td, *J* = 7.4, 1.3 Hz, 1H), 7.60 (td, *J* = 7.5, 1.3 Hz, 1H), 7.55 (tt, *J* = 7.5, 2.3 Hz, 1H), 7.51 (d, *J* = 7.7 Hz, 1H), 7.47 (t, *J* = 7.8 Hz, 2H), 7.31 (dt, *J* = 8.4, 1.8 Hz, 2H), 7.23 (dt, *J* = 8.6, 2.3 Hz, 2H), 1.16 (s, 9H).

^{13}C NMR (100 MHz, $CDCl_3$, 25 °C) δ/ppm: 189.3, 172.9, 153.5, 147.4, 137.6, 137.0, 135.8, 134.8, 132.8, 131.8, 131.5, 131.4, 131.2, 128.9, 126.7, 124.3, 124.0, 123.6, 122.6, 98.9, 39.5, 26.1.

IR (KBr) $\tilde{\nu}$ (cm^{-1}): 3196, 2905, 1692, 1595, 1475, 1442, 1406, 1371, 1306, 1223, 1050, 750.

HRMS (ESI) *m/z*: $[M+H]^+$ Calcd for $C_{28}H_{24}{}^{79}BrN_2O_3$ 515.0970; found: 515.0969; $[M+H]^+$ Calcd for $C_{28}H_{24}{}^{81}BrN_2O_3$ 517.0950; found: 517.0953.

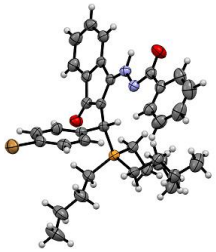
VI. References:

1 C.-J. Lee, Y.-J. Jang, Z.-Z. Wu and W. Lin, *Org. Lett.* 2012, **14**, 1906.

2 R. Saijo, H. Uno, S. Mori and M. Kawase, *Chem. Commun.* 2016, **52**, 8006.

VII. X-Ray crystallographic data for selected compounds:

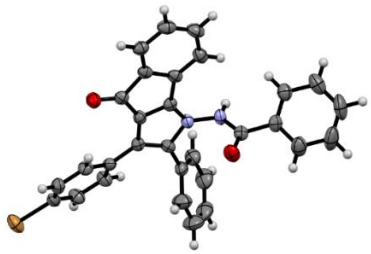
a) **3a** (CCDC no. 2009731): The thermal ellipsoid drawn at 50% probability level.



The purified compound **3a** is dissolved in a mixed solvent of CH_2Cl_2 and hexanes to slowly evaporate. After few days, colorless crystals were obtained.

Empirical formula	$C_{35}\ H_{42}\ Br\ N_2\ O_2\ P$	
Formula weight	633.59	
Temperature	200(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 21/n	
Unit cell dimensions	a = 10.0157(3) Å	α = 90°.
	b = 12.5956(4) Å	β = 91.1220(10)°.
	c = 26.5786(8) Å	γ = 90°.
Volume	3352.35(18) $Å^3$	
Z	4	
Density (calculated)	1.255 Mg/m^3	
Absorption coefficient	1.306 mm^{-1}	
F(000)	1328	
Crystal size	0.22 x 0.17 x 0.07 mm^3	
Theta range for data collection	2.19 to 25.06°.	
Index ranges	-11<=h<=11, -15<=k<=14, -31<=l<=31	
Reflections collected	44500	
Independent reflections	5913 [R(int) = 0.0691]	
Completeness to theta = 25.06°	99.9 %	
Absorption correction	multi-scan	
Max. and min. transmission	0.9142 and 0.7621	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5913 / 0 / 367	
Goodness-of-fit on F^2	1.108	
Final R indices [I>2sigma(I)]	R1 = 0.0461, wR2 = 0.1198	
R indices (all data)	R1 = 0.0657, wR2 = 0.1292	
Largest diff. peak and hole	0.700 and -0.582 $e.Å^{-3}$	

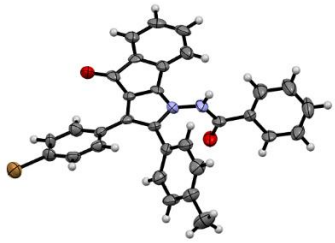
b) **6aa** (CCDC no. 2016707): The thermal ellipsoid drawn at 65% probability level



The purified compound **6aa** is dissolved in a mixed solvent of CH_2Cl_2 and hexanes to slowly evaporate. After few days, colorless crystals were obtained.

Empirical formula	C30 H21 Br N2 O3	
Formula weight	537.40	
Temperature	200(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 21/c	
Unit cell dimensions	a = 7.0854(2) Å	α = 90°.
	b = 18.2878(6) Å	β = 98.9890(10)°.
	c = 19.8064(7) Å	γ = 90°.
Volume	2534.92(14) $Å^3$	
Z	4	
Density (calculated)	1.408 Mg/m^3	
Absorption coefficient	1.656 mm^{-1}	
F(000)	1096	
Crystal size	0.74 x 0.04 x 0.01 mm^3	
Theta range for data collection	2.36 to 25.09°.	
Index ranges	-8<=h<=7, -21<=k<=21, -23<=l<=23	
Reflections collected	33421	
Independent reflections	4498 [R(int) = 0.0654]	
Completeness to theta = 25.09°	99.6 %	
Absorption correction	multi-scan	
Max. and min. transmission	0.9836 and 0.3737	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4498 / 0 / 325	
Goodness-of-fit on F^2	1.017	
Final R indices [I>2sigma(I)]	R1 = 0.0333, wR2 = 0.0703	
R indices (all data)	R1 = 0.0510, wR2 = 0.0786	
Largest diff. peak and hole	0.247 and -0.448 $e.Å^{-3}$	

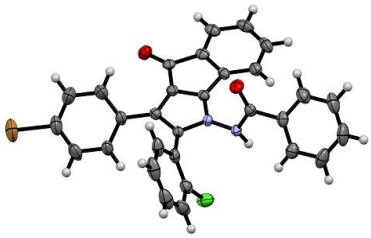
c) **6ae** (CCDC no. 2009642): The thermal ellipsoid drawn at 55% probability level.



The purified compound **6ae** is dissolved in a mixed solvent of CH_2Cl_2 and hexanes to slowly evaporate. After few days, colorless crystals were obtained.

Empirical formula	$C_{62}\ H_{44}\ Br_2\ N_4\ O_5$	
Formula weight	1084.83	
Temperature	200(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P -1	
Unit cell dimensions	a = 11.994(4) Å	α = 96.769(8)°.
	b = 12.841(5) Å	β = 100.451(8)°.
	c = 16.952(6) Å	γ = 97.043(8)°.
Volume	2521.9(15) $Å^3$	
Z	2	
Density (calculated)	1.429 Mg/m^3	
Absorption coefficient	1.664 mm^{-1}	
F(000)	1108	
Crystal size	0.11 x 0.06 x 0.02 mm^3	
Theta range for data collection	2.17 to 25.13°.	
Index ranges	-14<=h<=14, -15<=k<=15, -20<=l<=20	
Reflections collected	81656	
Independent reflections	8981 [R(int) = 0.2092]	
Completeness to theta = 25.13°	99.5 %	
Absorption correction	multi-scan	
Max. and min. transmission	0.9675 and 0.8381	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	8981 / 0 / 660	
Goodness-of-fit on F^2	1.029	
Final R indices [I>2sigma(I)]	R1 = 0.0877, wR2 = 0.1633	
R indices (all data)	R1 = 0.2037, wR2 = 0.2056	
Largest diff. peak and hole	0.645 and -0.662 e.$Å^{-3}$	

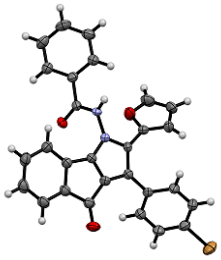
d) **6ai** (CCDC no. 2009644): The thermal ellipsoid drawn at 60% probability level.



The purified compound **6ai** is dissolved in a mixed solvent of CH_2Cl_2 and hexanes to slowly evaporate. After few days, colorless crystals were obtained.

Empirical formula	$C_{30}H_{20}BrClN_2O_3$	
Formula weight	571.84	
Temperature	200(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	C 2/c	
Unit cell dimensions	a = 30.7223(10) Å	α = 90°.
	b = 6.9755(2) Å	β = 115.5280(10)°.
	c = 27.9045(9) Å	γ = 90°.
Volume	5396.2(3) $Å^3$	
Z	8	
Density (calculated)	1.408 Mg/m^3	
Absorption coefficient	1.656 mm^{-1}	
F(000)	2320	
Crystal size	0.16 x 0.09 x 0.02 mm^3	
Theta range for data collection	2.61 to 25.04°.	
Index ranges	-35<=h<=36, -8<=k<=8, -32<=l<=32	
Reflections collected	36745	
Independent reflections	4758 [R(int) = 0.0582]	
Completeness to theta = 25.04°	99.5 %	
Absorption correction	multi-scan	
Max. and min. transmission	0.9676 and 0.7775	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4758 / 0 / 335	
Goodness-of-fit on F^2	0.994	
Final R indices [I>2sigma(I)]	R1 = 0.0702, wR2 = 0.1844	
R indices (all data)	R1 = 0.0909, wR2 = 0.1973	
Largest diff. peak and hole	2.155 and -1.374 e.$Å^{-3}$	

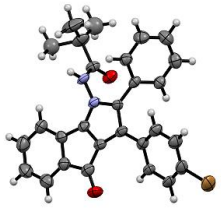
e) **6aj** (CCDC no. 2009643): The thermal ellipsoid drawn at 60% probability level.



The purified compound **6aj** is dissolved in a mixed solvent of Ethyl acetate and hexanes to slowly evaporate. After few days, colorless crystals were obtained.

Empirical formula	C_{28} H_{17} Br N_2 O_3	
Formula weight	509.35	
Temperature	200(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 21/n	
Unit cell dimensions	a = 9.9178(2) Å	α = 90°.
	b = 25.0870(5) Å	β = 99.6680(10)°.
	c = 18.0566(4) Å	γ = 90°.
Volume	4428.82(16) $Å^3$	
Z	8	
Density (calculated)	1.528 Mg/m^3	
Absorption coefficient	1.891 mm^{-1}	
F(000)	2064	
Crystal size	0.32 x 0.30 x 0.04 mm^3	
Theta range for data collection	2.20 to 25.03°.	
Index ranges	-11<=h<=11, -29<=k<=29, -21<=l<=19	
Reflections collected	77253	
Independent reflections	7805 [R(int) = 0.0549]	
Completeness to theta = 25.03°	99.7 %	
Absorption correction	multi-scan	
Max. and min. transmission	0.9282 and 0.5829	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	7805 / 0 / 613	
Goodness-of-fit on F^2	0.994	
Final R indices [I>2sigma(I)]	R1 = 0.0326, wR2 = 0.0822	
R indices (all data)	R1 = 0.0465, wR2 = 0.0900	
Largest diff. peak and hole	0.312 and -0.461 $e.Å^{-3}$	

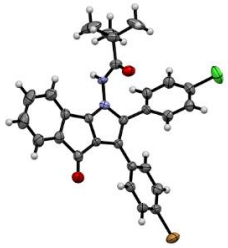
f) **7ak** (CCDC no. 2009645): The thermal ellipsoid drawn at 60% probability level.



The purified compound **7ak** is dissolved in a mixed solvent of CH_2Cl_2 and hexanes to slowly evaporate. After few days, colorless crystals were obtained.

Empirical formula	$C_{28}\ H_{23}\ Br\ N_2\ O_2$	
Formula weight	499.39	
Temperature	200(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	C c	
Unit cell dimensions	a = 17.2881(7) Å	α = 90°.
	b = 16.3136(7) Å	β = 113.2390(10)°.
	c = 9.3609(4) Å	γ = 90°.
Volume	2425.87(18) $Å^3$	
Z	4	
Density (calculated)	1.367 Mg/m^3	
Absorption coefficient	1.722 mm^{-1}	
F(000)	1024	
Crystal size	0.23 x 0.04 x 0.02 mm^3	
Theta range for data collection	2.50 to 25.07°.	
Index ranges	-19<=h<=20, -19<=k<=19, -11<=l<=11	
Reflections collected	16214	
Independent reflections	4042 [R(int) = 0.0537]	
Completeness to theta = 25.07°	99.8 %	
Absorption correction	multi-scan	
Max. and min. transmission	0.9664 and 0.6929	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4042 / 2 / 299	
Goodness-of-fit on F^2	0.996	
Final R indices [I>2sigma(I)]	R1 = 0.0405, wR2 = 0.0834	
R indices (all data)	R1 = 0.0674, wR2 = 0.0949	
Absolute structure parameter	0.001(10)	
Largest diff. peak and hole	0.370 and -0.322 $e.Å^{-3}$	

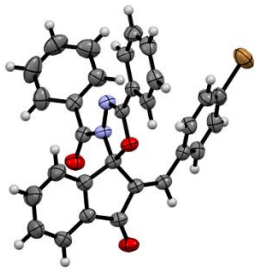
g) **7ik** (CCDC no. 2009646): The thermal ellipsoid drawn at 60% probability level.



The purified compound **7ik** is dissolved in a mixed solvent of CH_2Cl_2 and hexanes to slowly evaporate. After few days, colorless crystals were obtained.

Empirical formula	C_{28} H_{22} Br Cl N_2 O_2	
Formula weight	533.84	
Temperature	200(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	C c	
Unit cell dimensions	a = 17.544(5) Å	α = 90°.
	b = 16.528(4) Å	β = 113.870(7)°.
	c = 9.324(3) Å	γ = 90°.
Volume	2472.5(11) $Å^3$	
Z	4	
Density (calculated)	1.434 Mg/m^3	
Absorption coefficient	1.799 mm^{-1}	
F(000)	1088	
Crystal size	0.15 x 0.06 x 0.03 mm^3	
Theta range for data collection	2.46 to 25.43°.	
Index ranges	-21<=h<=21, -19<=k<=19, -11<=l<=11	
Reflections collected	19037	
Independent reflections	4472 [R(int) = 0.0796]	
Completeness to theta = 25.43°	99.6 %	
Absorption correction	multi-scan	
Max. and min. transmission	0.9480 and 0.7742	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4472 / 2 / 310	
Goodness-of-fit on F^2	0.994	
Final R indices [I>2sigma(I)]	R1 = 0.0434, wR2 = 0.0899	
R indices (all data)	R1 = 0.0751, wR2 = 0.1008	
Absolute structure parameter	0.015(9)	
Largest diff. peak and hole	0.435 and -0.378 $e.Å^{-3}$	

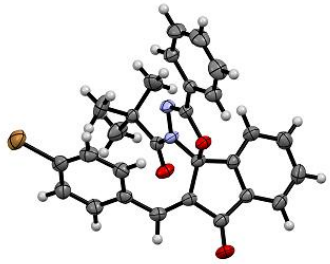
h) **8aa** (CCDC no. 2009650): The thermal ellipsoid drawn at 60% probability level.



The purified compound **8aa** is dissolved in a mixed solvent of CH_2Cl_2 and hexanes to slowly evaporate. After few days, colorless crystals were obtained.

Empirical formula	$C_{30}\ H_{19}\ Br\ N_2\ O_3$	
Formula weight	535.38	
Temperature	200(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P -1	
Unit cell dimensions	a = 8.3291(7) Å	α = 79.558(2)°.
	b = 9.2178(7) Å	β = 87.777(3)°.
	c = 16.6899(15) Å	γ = 74.713(2)°.
Volume	1215.52(18) $Å^3$	
Z	2	
Density (calculated)	1.463 Mg/m^3	
Absorption coefficient	1.727 mm^{-1}	
F(000)	544	
Crystal size	0.77 x 0.58 x 0.17 mm^3	
Theta range for data collection	2.44 to 25.09°.	
Index ranges	-9<=h<=9, -10<=k<=10, -19<=l<=19	
Reflections collected	35541	
Independent reflections	4276 [R(int) = 0.0797]	
Completeness to theta = 25.09°	99.2 %	
Absorption correction	multi-scan	
Max. and min. transmission	0.7579 and 0.3499	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4276 / 0 / 325	
Goodness-of-fit on F^2	1.001	
Final R indices [I>2sigma(I)]	R1 = 0.0378, wR2 = 0.0978	
R indices (all data)	R1 = 0.0450, wR2 = 0.1037	
Largest diff. peak and hole	0.489 and -0.638 $e.Å^{-3}$	

i) **8ak** (CCDC no. 2019535): The thermal ellipsoid drawn at 60% probability level.

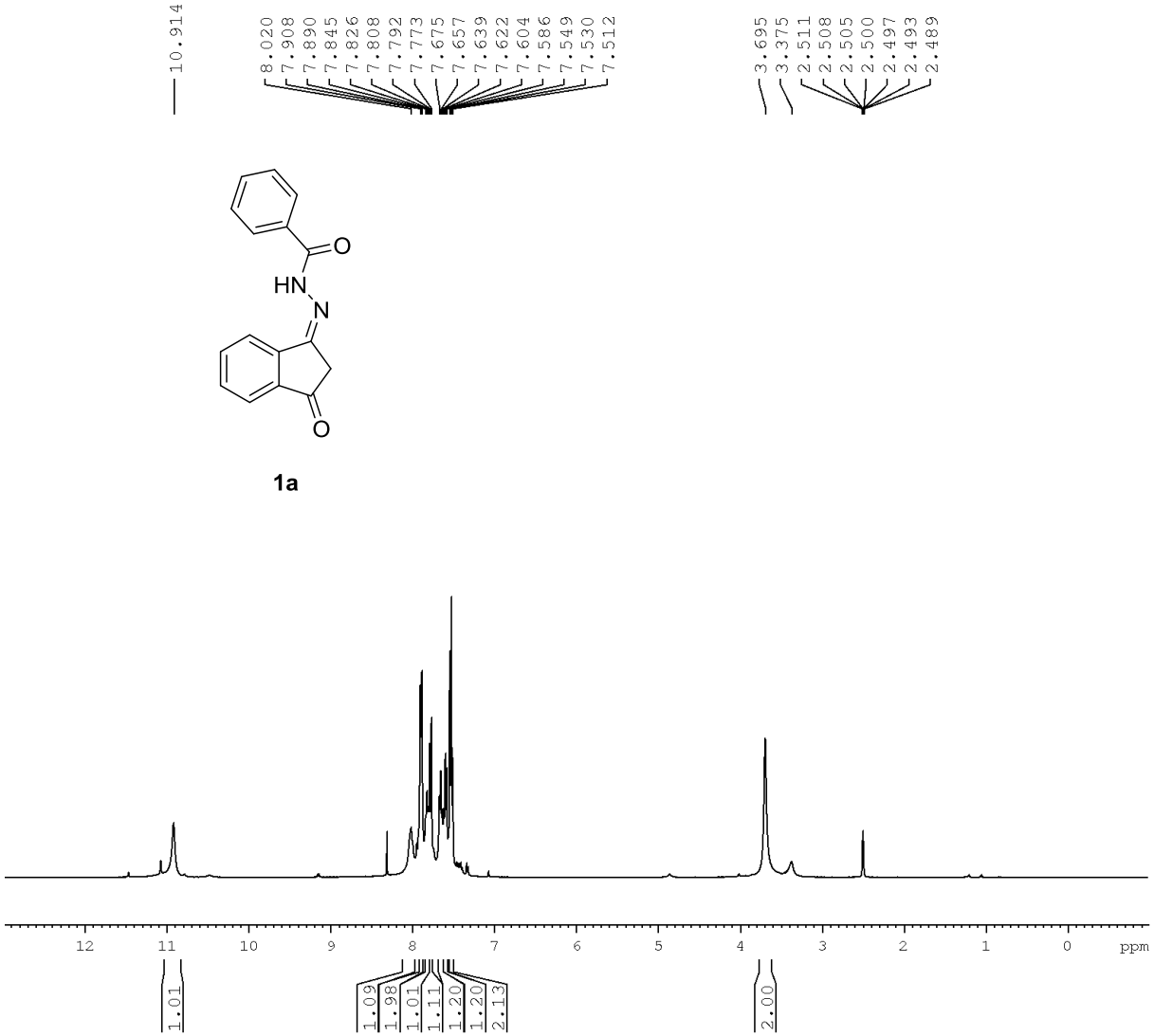


The purified compound **8ak** is dissolved in a mixed solvent of CH_2Cl_2 and hexanes to slowly evaporate. After few days, colorless crystals were obtained.

Empirical formula	C28 H23 Br N2 O3	
Formula weight	515.39	
Temperature	200(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P -1	
Unit cell dimensions	a = 9.7575(13) Å	α = 70.686(3)°.
	b = 10.9781(14) Å	β = 73.323(3)°.
	c = 12.4931(14) Å	γ = 72.669(3)°.
Volume	1178.9(3) $Å^3$	
Z	2	
Density (calculated)	1.452 Mg/m^3	
Absorption coefficient	1.777 mm^{-1}	
F(000)	528	
Crystal size	0.44 x 0.38 x 0.19 mm^3	
Theta range for data collection	2.24 to 25.20°.	
Index ranges	-11<=h<=11, -13<=k<=13, -14<=l<=14	
Reflections collected	33847	
Independent reflections	4196 [R(int) = 0.0471]	
Completeness to theta = 25.20°	98.9 %	
Absorption correction	multi-scan	
Max. and min. transmission	0.7289 and 0.5086	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4196 / 0 / 310	
Goodness-of-fit on F^2	1.004	
Final R indices [I>2sigma(I)]	R1 = 0.0305, wR2 = 0.0797	
R indices (all data)	R1 = 0.0375, wR2 = 0.0841	
Largest diff. peak and hole	0.340 and -0.535 $e.Å^{-3}$	

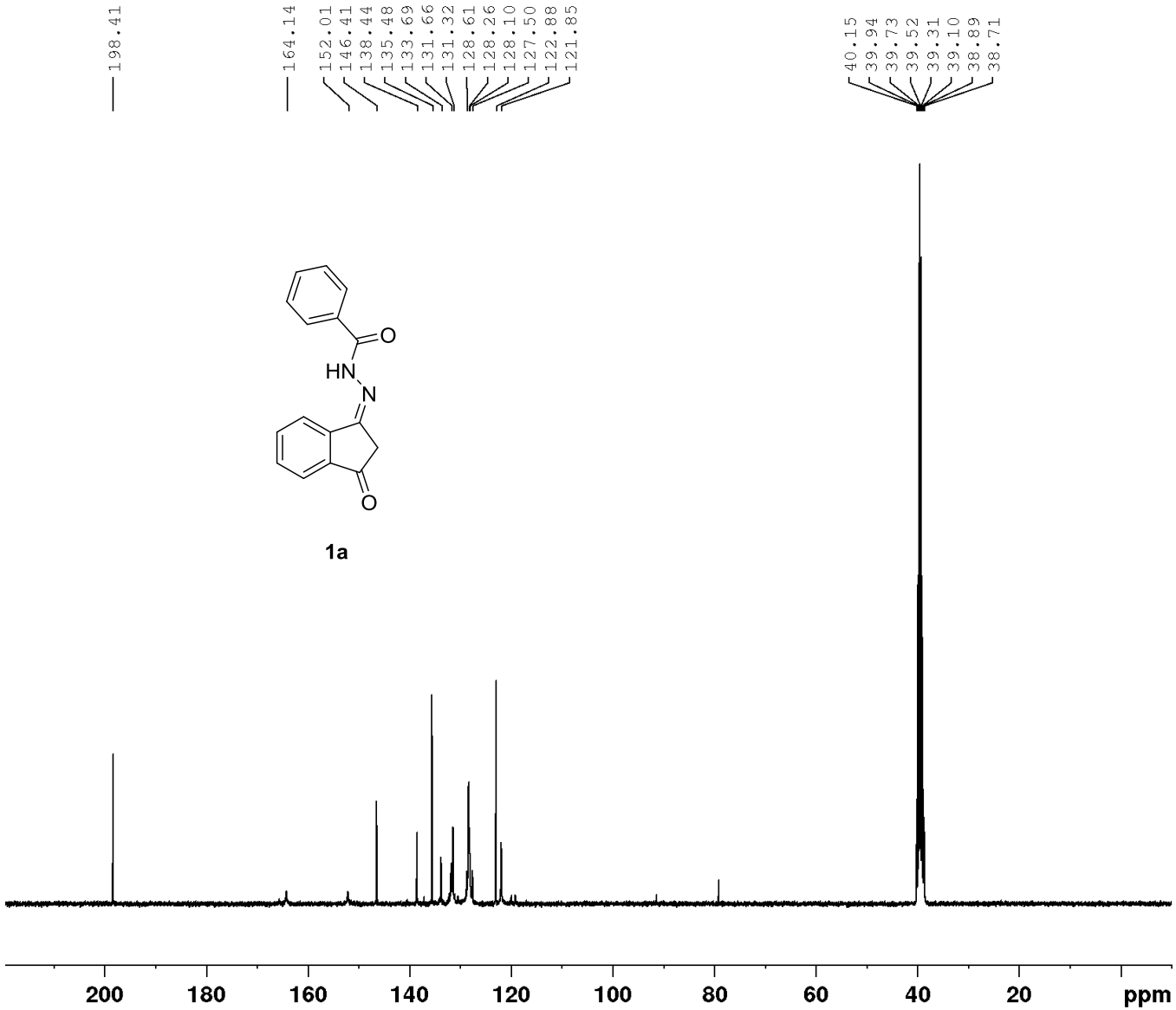
VIII. ^{1}H NMR, ^{13}C NMR, ^{31}P NMR and ^{19}F NMR spectra of all new compounds:

^{1}H NMR Spectrum of **1a** (DMSO-d_6, 400 MHz)



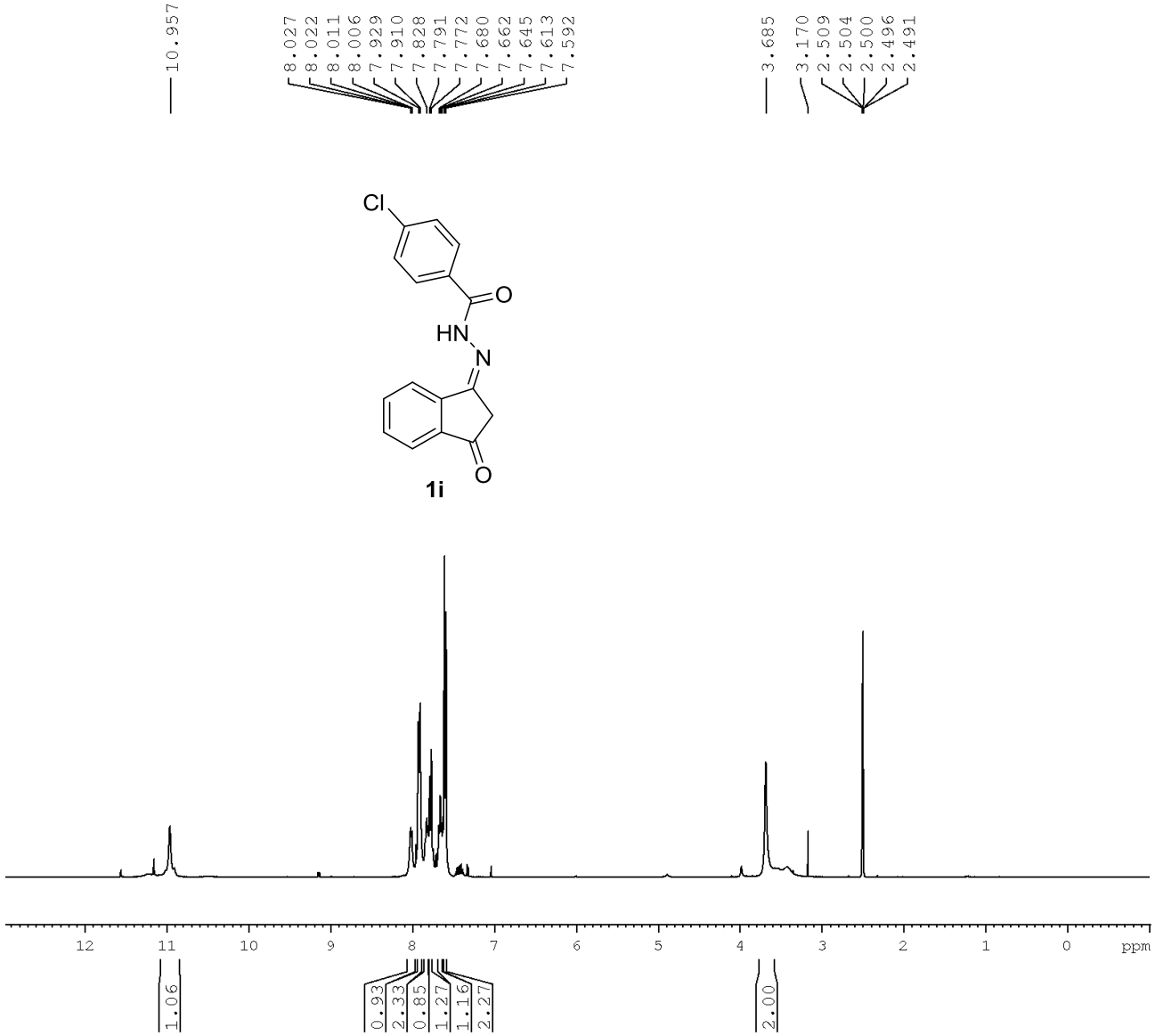

```
Current Data Parameters
NAME                  SW 909-1
EXPNO                        1
PROCNO                       1

F2 - Acquisition Parameters
Date_                 20200616
Time                     10.24
INSTRUM                  spect
PROBHD    5 mm PABBO BB/
PULPROG                  zg30
TD                      32768
SOLVENT                  DMSO
NS                         64
DS                          0
SWH                  7211.539 Hz
FIDRES               0.220079 Hz
AQ                   2.2719147 sec
RG                       63.58
DW                      69.333 usec
DE                       10.06 usec
TE                       298.5 K
D1                2.00000000 sec
TD0                          1

======== CHANNEL f1 ========
SFO1              400.1324008 MHz
NUC1                        1H
P1                       15.00 usec
PLW1              11.39999962 W

F2 - Processing parameters
SI                       16384
SF                400.1300032 MHz
WDW                        EM
SSB                         0
LB                          0 Hz
GB                          0
PC                       1.00
```

^{13}C NMR Spectrum of **1a** (DMSO-d_6, 100 MHz)



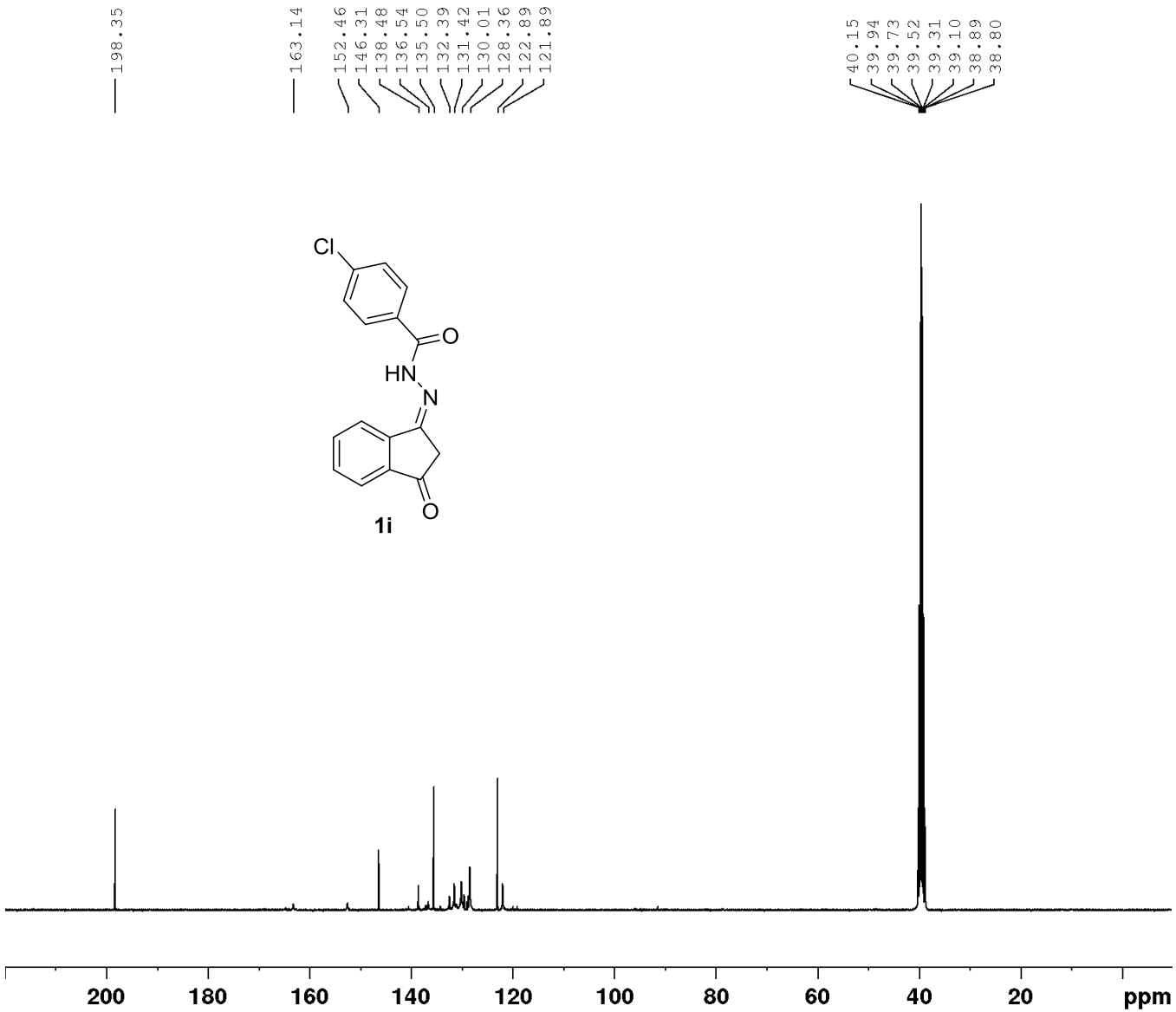

```
Current Data Parameters
NAME                 SW 909
EXPNO                     3
PROCNO                    1

F2 - Acquisition Parameters
Date_              20200615
Time                  22.10
INSTRUM               spect
PROBHD    5 mm BBO BB-1H
PULPROG              zgpg30
TD                    32768
SOLVENT                DMSO
NS                     3252
DS                        0
SWH              24038.461 Hz
FIDRES            0.733596 Hz
AQ               0.6815744 sec
RG                  5792.6
DW                 20.800 usec
DE                  6.50 usec
TE                  297.9 K
D1              2.00000000 sec
D11             0.03000000 sec
TD0                       1

======== CHANNEL f1 ========
NUC1                    13C
P1                   10.00 usec
PL1                   3.80 dB
SFO1           100.6233325 MHz

======== CHANNEL f2 ========
CPDPRG[2           waltz16
NUC2                    1H
PCPD2                90.00 usec
PL2                  10.20 dB
PL12                 26.00 dB
PL13                 29.00 dB
SFO2           400.1316005 MHz

F2 - Processing parameters
SI                    32768
SF             100.6128214 MHz
WDW                      EM
SSB                       0
LB                   1.00 Hz
GB                        0
PC                   1.00
```

^{1}H NMR Spectrum of **1i** (DMSO-d_6, 400 MHz)



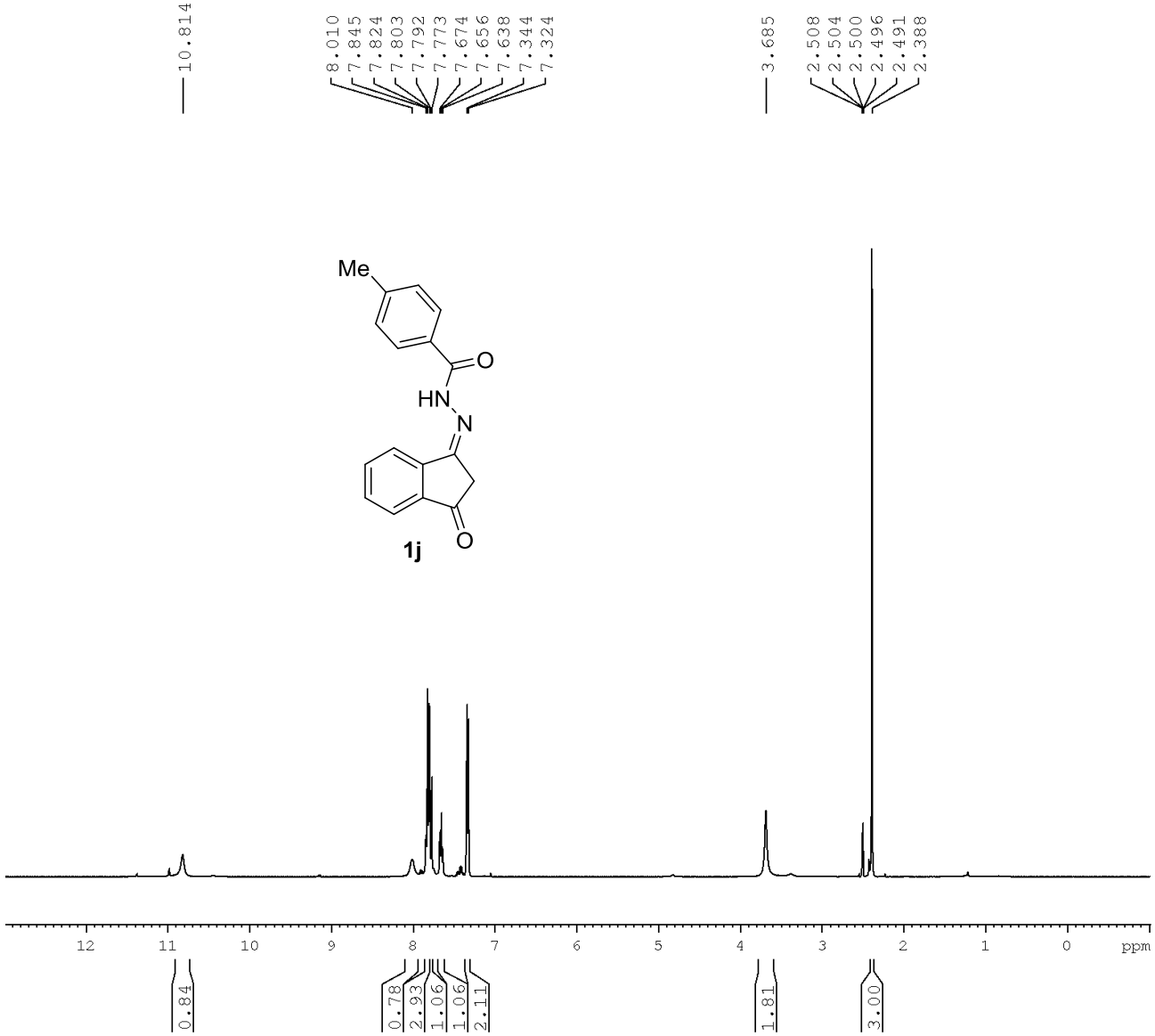

```
Current Data Parameters
NAME            SW 916-1
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20200721
Time               11.33
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG             zg30
TD                 32768
SOLVENT             DMSO
NS                    32
DS                     0
SWH             7211.539 Hz
FIDRES          0.220079 Hz
AQ              2.2719147 sec
RG                 78.51
DW                69.333 usec
DE                10.06 usec
TE                295.9 K
D1             2.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         400.1324008 MHz
NUC1                   1H
P1                 15.00 usec
PLW1         11.39999962 W

F2 - Processing parameters
SI                 16384
SF           400.1300028 MHz
WDW                   EM
SSB                    0
LB                     0 Hz
GB                     0
PC                  1.00
```

^{13}C NMR Spectrum of **1i** (DMSO-d_6, 100 MHz)



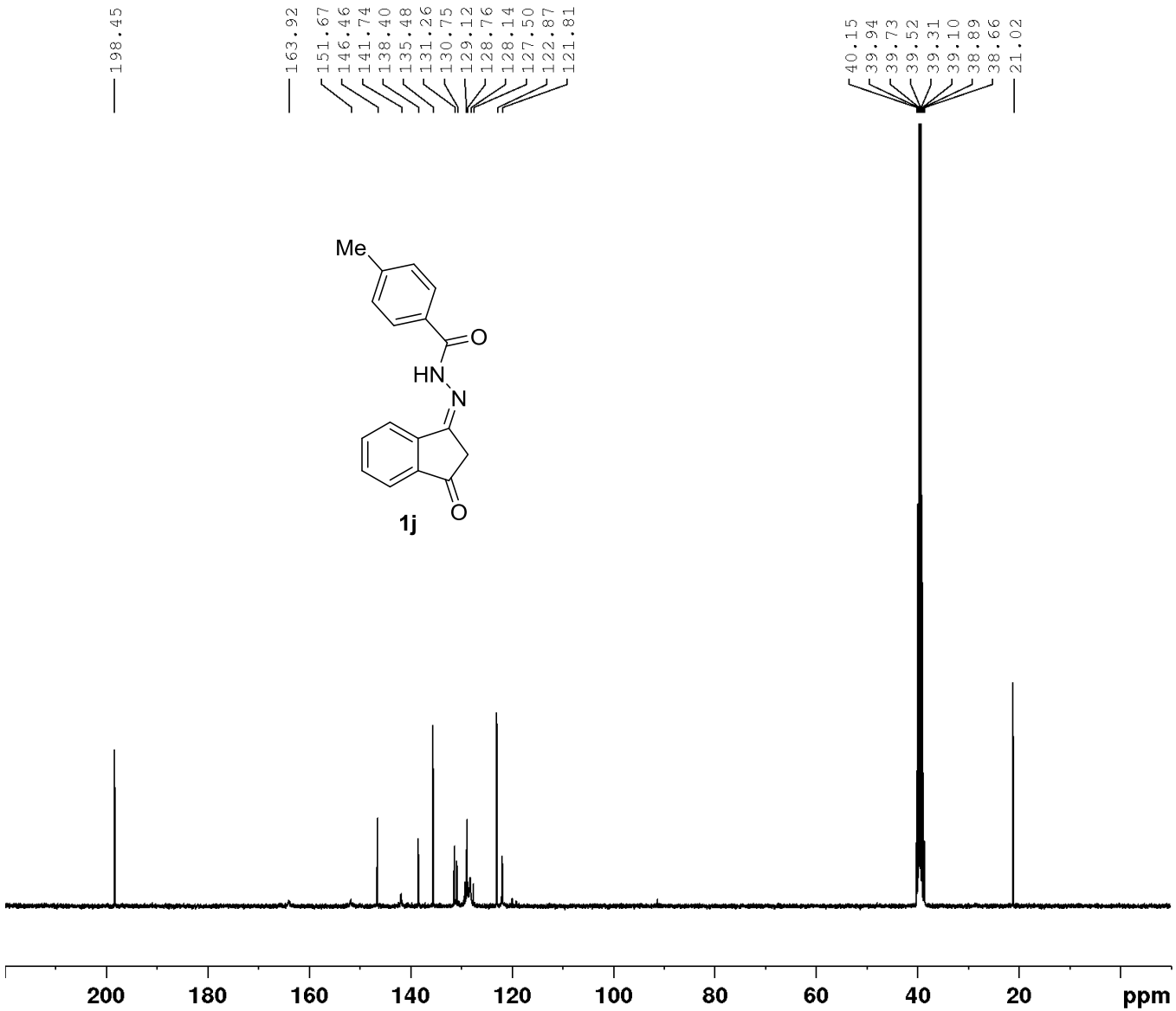

```
Current Data Parameters
NAME                 SW 916
EXPNO                     3
PROCNO                    1

F2 - Acquisition Parameters
Date_              20200720
Time                 23.18
INSTRUM              spect
PROBHD    5 mm BBO BB-1H
PULPROG             zgpg30
TD                   32768
SOLVENT               DMSO
NS                   12000
DS                       0
SWH              24038.461 Hz
FIDRES            0.733596 Hz
AQ               0.6815744 sec
RG                    4096
DW                  20.800 usec
DE                   6.50 usec
TE                  297.5 K
D1               2.00000000 sec
D11              0.03000000 sec
TD0                       1

======== CHANNEL f1 ========
NUC1                    13C
P1                    10.00 usec
PL1                    3.80 dB
SFO1           100.6233325 MHz

======== CHANNEL f2 ========
CPDPRG[2           waltz16
NUC2                    1H
PCPD2                90.00 usec
PL2                  10.20 dB
PL12                 26.00 dB
PL13                 29.00 dB
SFO2           400.1316005 MHz

F2 - Processing parameters
SI                    32768
SF             100.6128195 MHz
WDW                     EM
SSB                      0
LB                    1.00 Hz
GB                       0
PC                    1.00
```

^{1}H NMR Spectrum of **1j** (DMSO-d_6, 400 MHz)



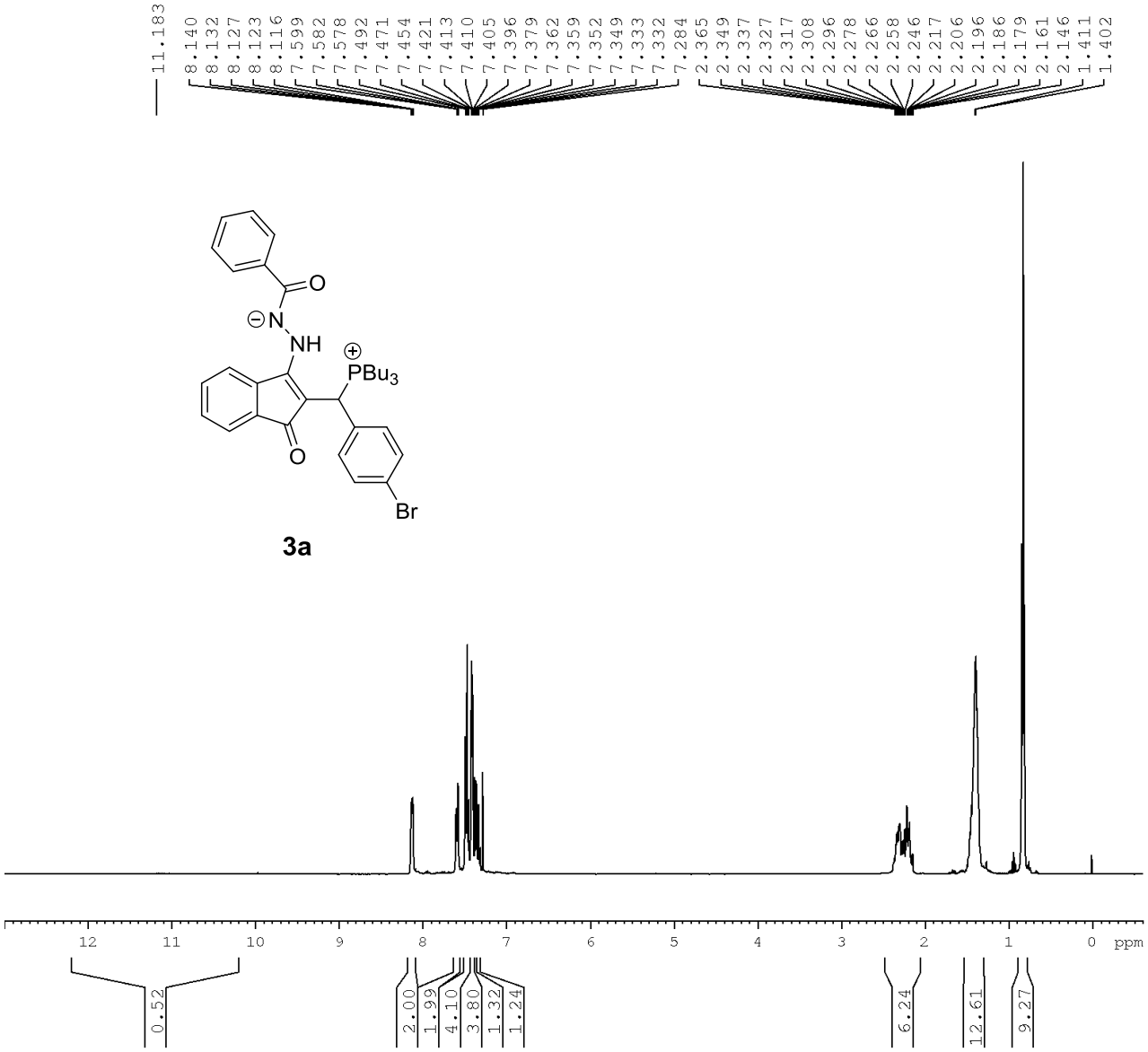

```
Current Data Parameters
NAME                  485
EXPNO                   3
PROCNO                  1

F2 - Acquisition Parameters
Date_            20200614
Time                17.13
INSTRUM             spect
PROBHD   5 mm BBO BB-1H
PULPROG              zg30
TD                  32768
SOLVENT              DMSO
NS                     16
DS                      0
SWH              7246.377 Hz
FIDRES           0.221142 Hz
AQ               2.2609921 sec
RG                    114
DW                 69.000 usec
DE                  6.50 usec
TE                 297.6 K
D1              2.00000000 sec
TD0                     1

======== CHANNEL f1 ========
NUC1                   1H
P1                 15.00 usec
PL1                11.10 dB
SFO1         400.1324008 MHz

F2 - Processing parameters
SI                  16384
SF           400.1300062 MHz
WDW                    EM
SSB                     0
LB                      0 Hz
GB                      0
PC                   1.00
```

^{13}C NMR Spectrum of **1j** (DMSO-d_6, 100 MHz)



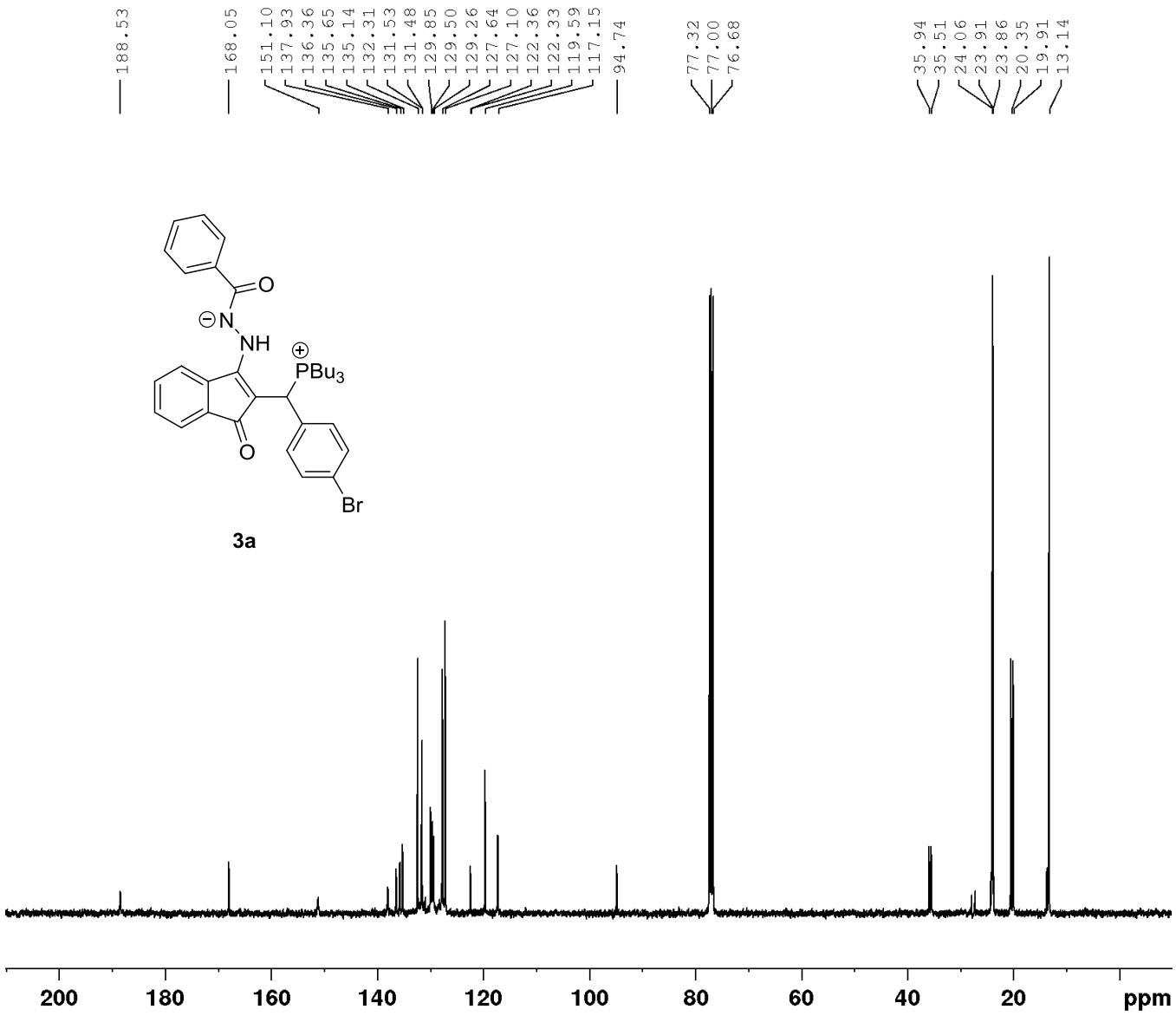

```
Current Data Parameters
NAME                  485
EXPNO                   4
PROCNO                  1

F2 - Acquisition Parameters
Date_            20200614
Time                17.17
INSTRUM             spect
PROBHD    5 mm BBO BB-1H
PULPROG           zgpg30
TD                 32768
SOLVENT             DMSO
NS                  3990
DS                     0
SWH            24038.461 Hz
FIDRES          0.733596 Hz
AQ             0.6815744 sec
RG                  8192
DW                20.800 usec
DE                 6.50 usec
TE                297.7 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  13C
P1                 10.00 usec
PL1                 3.80 dB
SFO1         100.6233325 MHz

======== CHANNEL f2 ========
CPDPRG[2          waltz16
NUC2                  1H
PCPD2              90.00 usec
PL2                10.20 dB
PL12               26.00 dB
PL13               29.00 dB
SFO2         400.1316005 MHz

F2 - Processing parameters
SI                 32768
SF           100.6128205 MHz
WDW                   EM
SSB                    0
LB                 1.00 Hz
GB                     0
PC                 1.00
```

^{1}H NMR Spectrum of **3a** ($CDCl_3$, 400 MHz)



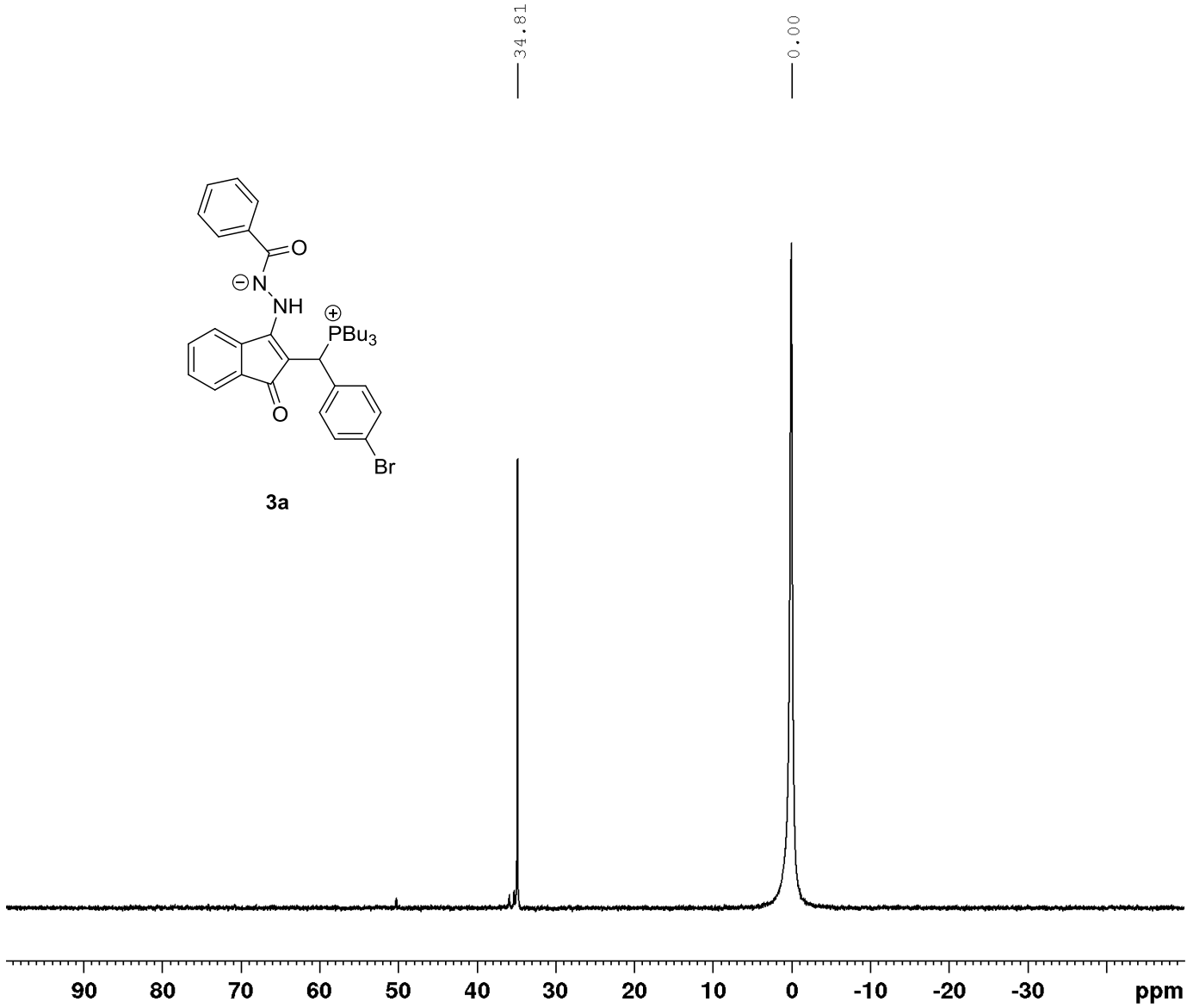

```
Current Data Parameters
NAME                  SW 747-1
EXPNO                        2
PROCNO                       1

F2 - Acquisition Parameters
Date_                 20200526
Time                     19.59
INSTRUM                  spect
PROBHD    5 mm PABBO BB/
PULPROG                  zg30
TD                      32768
SOLVENT                 CDCl3
NS                         32
DS                          0
SWH                  7211.539 Hz
FIDRES               0.220079 Hz
AQ                   2.2719147 sec
RG                       57.42
DW                     69.333 usec
DE                     10.06 usec
TE                     297.9 K
D1                2.00000000 sec
TD0                         1

======== CHANNEL f1 ========
SFO1             400.1324008 MHz
NUC1                       1H
P1                      15.00 usec
PLW1             11.39999962 W

F2 - Processing parameters
SI                      16384
SF               400.1300000 MHz
WDW                        EM
SSB                         0
LB                          0 Hz
GB                          0
PC                       1.00
```

^{13}C NMR Spectrum of **3a** ($CDCl_3$, 100 MHz)



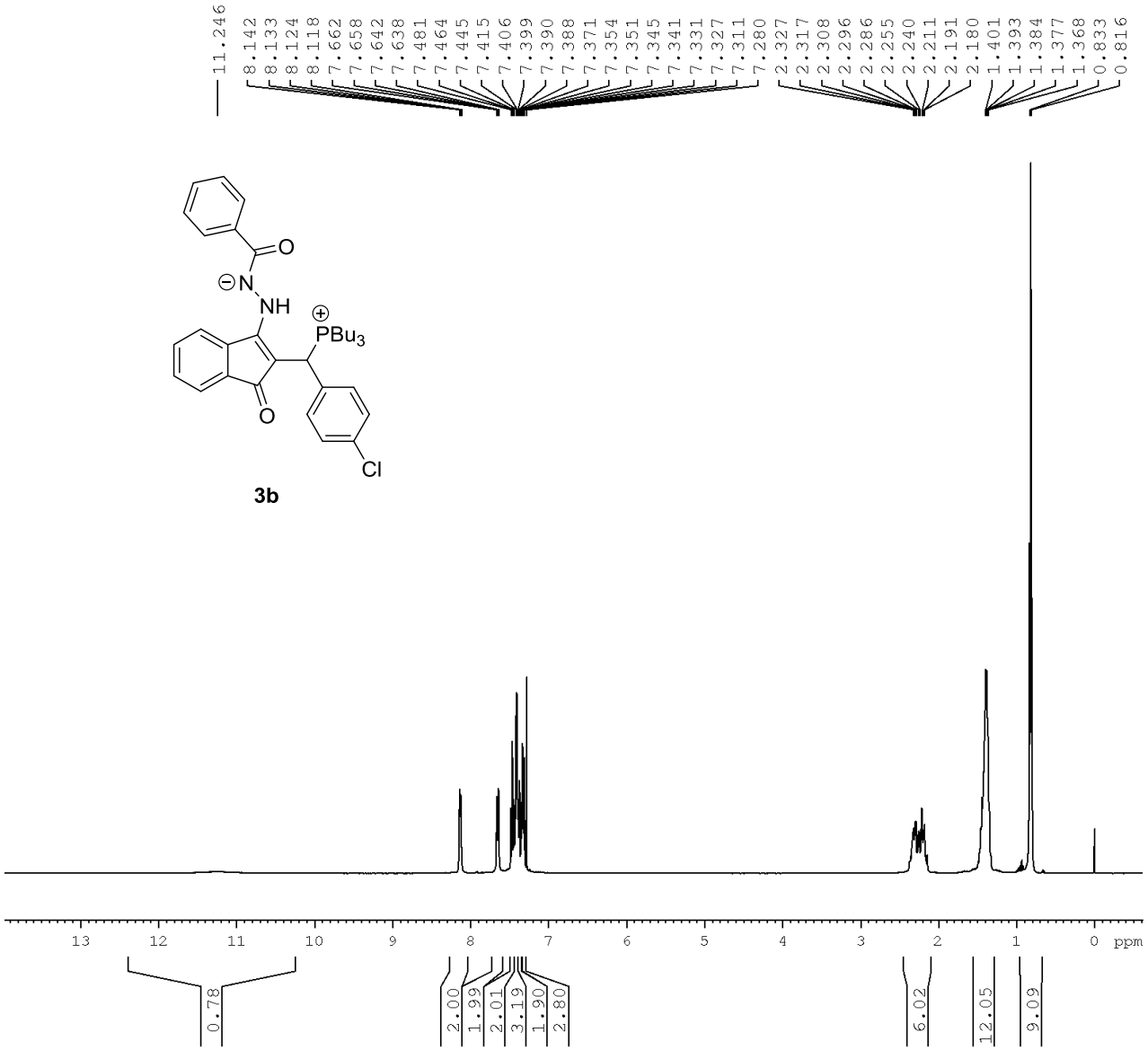

```
Current Data Parameters
NAME            SW 747-1
EXPNO                  4
PROCNO                 1

F2 - Acquisition Parameters
Date_           20200527
Time               23.26
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                 32768
SOLVENT            CDCl3
NS                  1660
DS                     0
SWH           24038.461 Hz
FIDRES         0.733596 Hz
AQ            0.6815744 sec
RG               198.09
DW               20.800 usec
DE                6.50 usec
TE                298.5 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1        100.6228298 MHz
NUC1                13C
P1                10.00 usec
PLW1        49.50000000 W

======== CHANNEL f2 ========
SFO2        400.1316005 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2             90.00 usec
PLW2        12.50000000 W
PLW12        0.34722000 W
PLW13        0.28125000 W

F2 - Processing parameters
SI                 32768
SF          100.6127760 MHz
WDW                  EM
SSB                   0
LB                 2.00 Hz
GB                    0
PC                 1.00
```

^{31}P NMR Spectrum of **3a** ($CDCl_3$, 162 MHz)



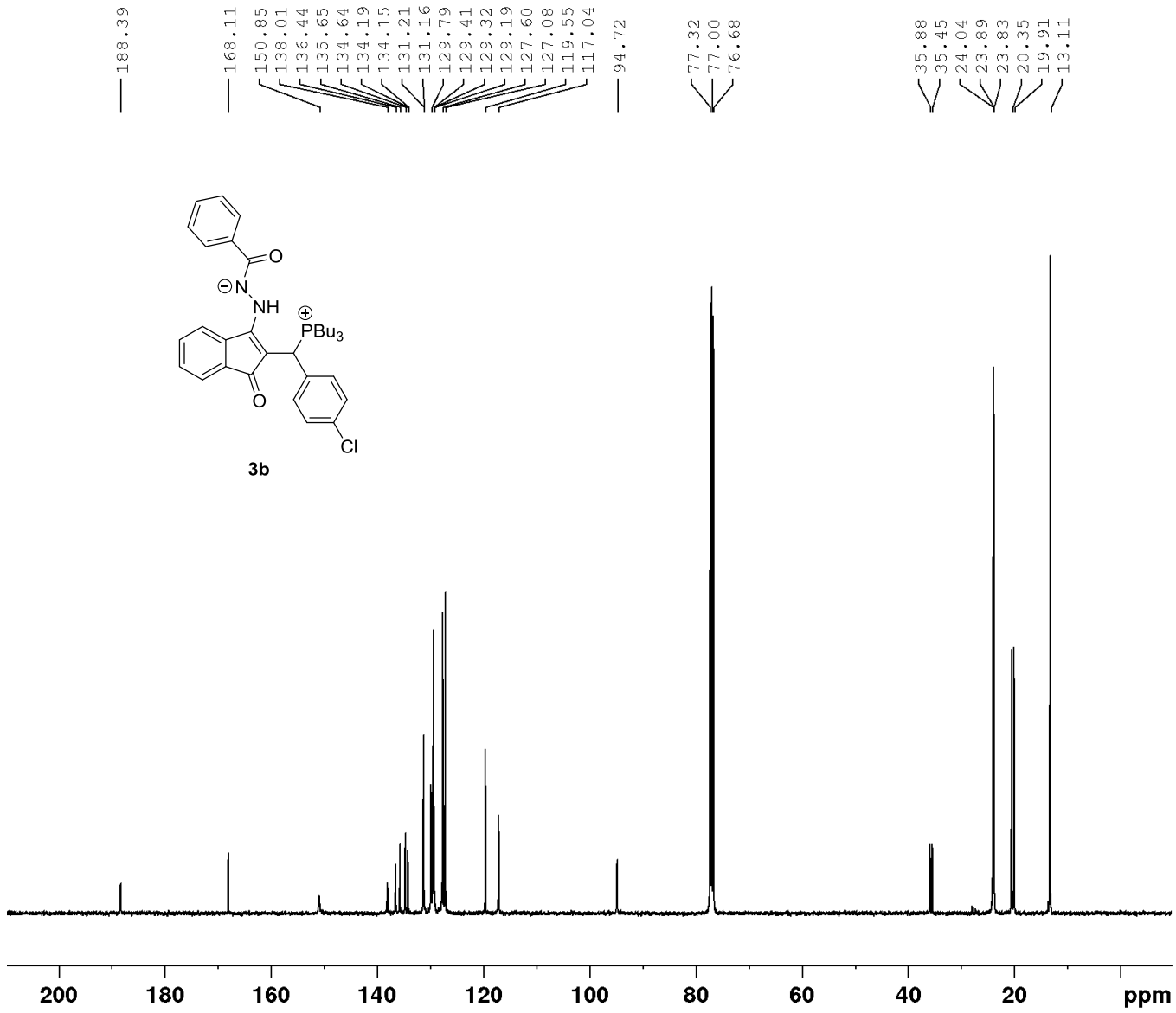

```
Current Data Parameters
NAME            SW 747-1
EXPNO                  5
PROCNO                 1

F2 - Acquisition Parameters
Date_           20200615
Time               11.46
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     4
SWH            49019.609 Hz
FIDRES          0.747980 Hz
AQ             0.6684672 sec
RG                198.09
DW                10.200 usec
DE                 6.50 usec
TE                296.5 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         161.9836917 MHz
NUC1                31P
P1                15.00 usec
PLW1         13.19999981 W

======== CHANNEL f2 ========
SFO2         400.1316005 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2             90.00 usec
PLW2         12.50000000 W
PLW12         0.34722000 W
PLW13         0.28125000 W

F2 - Processing parameters
SI                 32768
SF           161.9755119 MHz
WDW                   EM
SSB                    0
LB                 2.00 Hz
GB                     0
PC                 1.40
```

^{1}H NMR Spectrum of **3b** ($CDCl_3$, 400 MHz)



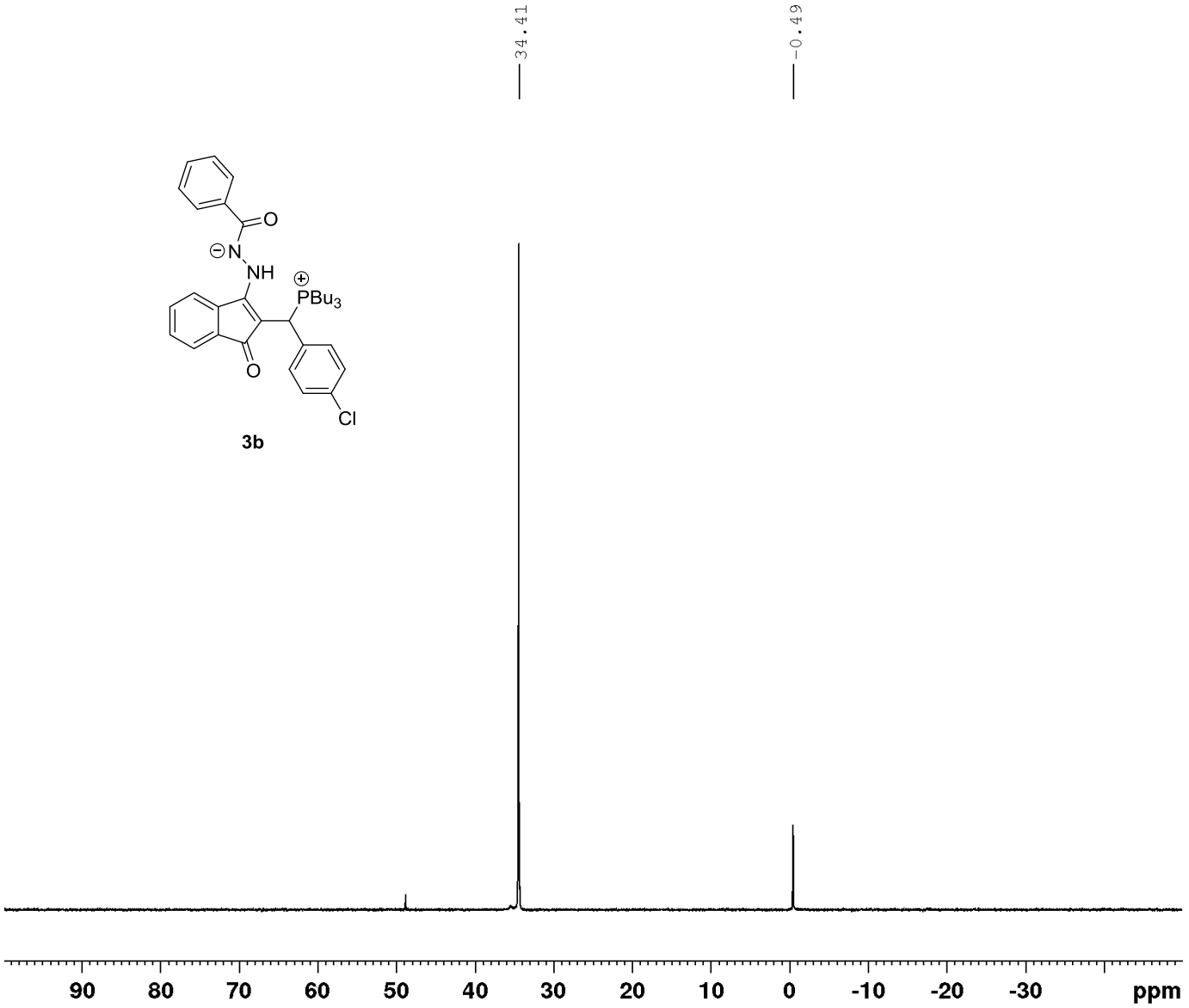

```
Current Data Parameters
NAME            SW 893-1
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20200531
Time               22.03
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG             zg30
TD                 32768
SOLVENT            CDCl3
NS                    32
DS                     0
SWH             7211.539 Hz
FIDRES          0.220079 Hz
AQ             2.2719147 sec
RG                 45.15
DW                69.333 usec
DE                10.06 usec
TE                298.1 K
D1            2.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         400.1324008 MHz
NUC1                   1H
P1                 15.00 usec
PLW1         11.39999962 W

F2 - Processing parameters
SI                 16384
SF           400.1300017 MHz
WDW                   EM
SSB                    0
LB                     0 Hz
GB                     0
PC                  1.00
```

^{13}C NMR Spectrum of **3b** ($CDCl_3$, 100 MHz)



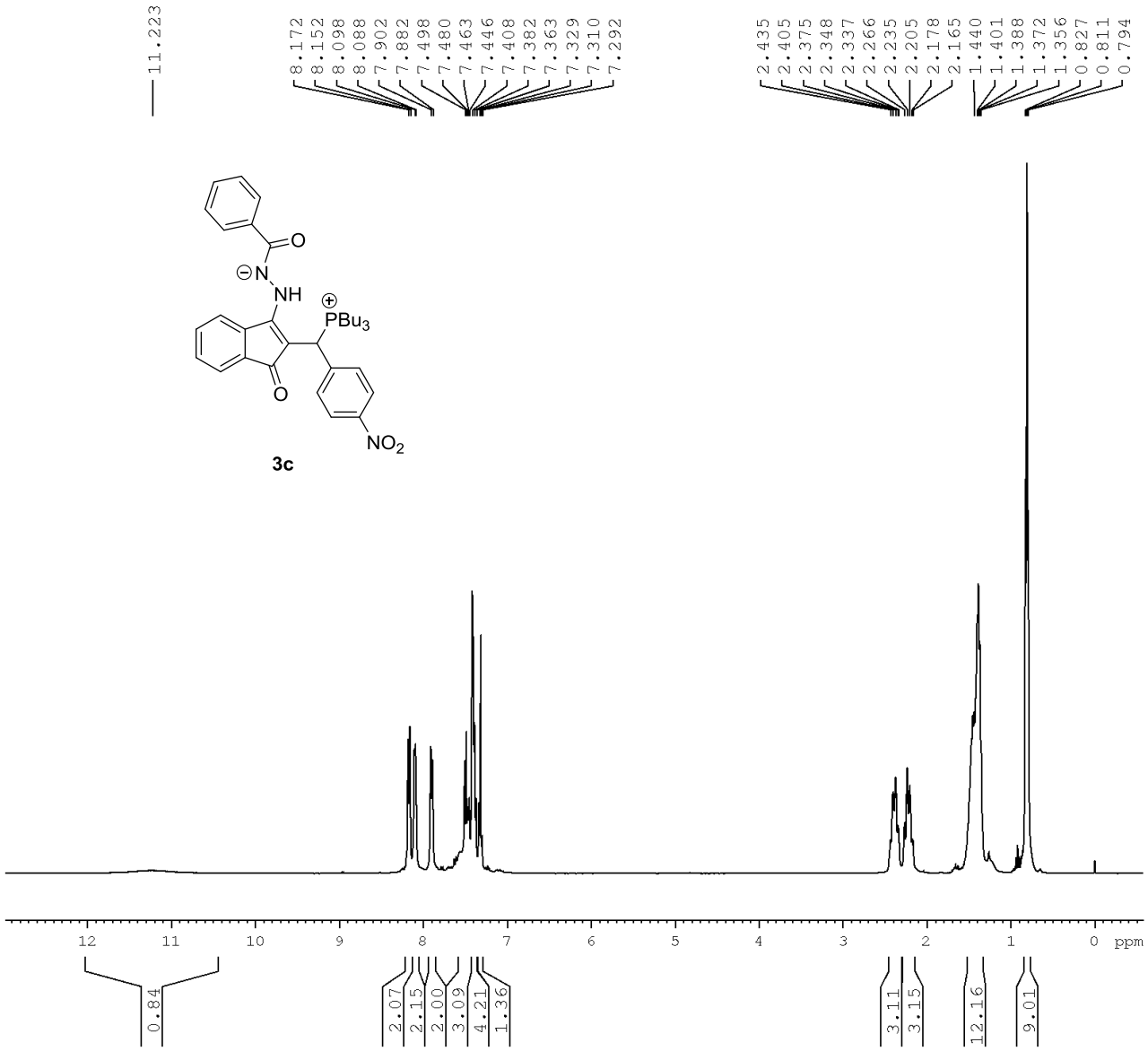

```
Current Data Parameters
NAME            SW 893-1
EXPNO                  3
PROCNO                 1

F2 - Acquisition Parameters
Date_           20200531
Time               22.05
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                 32768
SOLVENT            CDCl3
NS                  3327
DS                     0
SWH           24038.461 Hz
FIDRES         0.733596 Hz
AQ            0.6815744 sec
RG                198.09
DW               20.800 usec
DE                6.50 usec
TE                298.2 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1        100.6228298 MHz
NUC1                  13C
P1                10.00 usec
PLW1         49.50000000 W

======== CHANNEL f2 ========
SFO2        400.1316005 MHz
NUC2                  1H
CPDPRG[2         waltz16
PCPD2             90.00 usec
PLW2         12.50000000 W
PLW12         0.34722000 W
PLW13         0.28125000 W

F2 - Processing parameters
SI                 32768
SF          100.6127774 MHz
WDW                   EM
SSB                    0
LB                 2.00 Hz
GB                     0
PC                  1.00
```

^{31}P NMR Spectrum of **3b** ($CDCl_3$, 162 MHz)



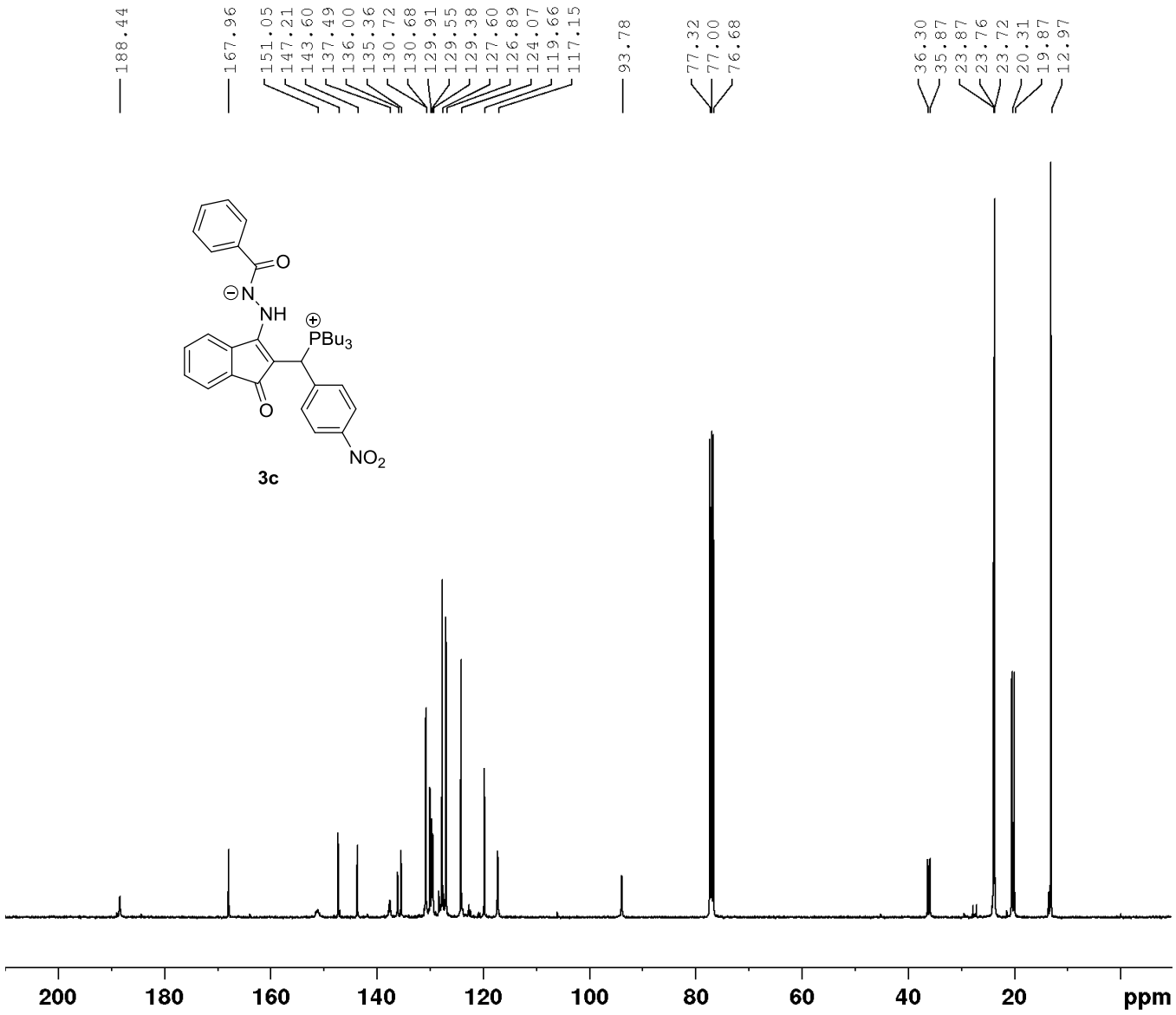

```
Current Data Parameters
NAME            SW 893-1
EXPNO                  4
PROCNO                 1

F2 - Acquisition Parameters
Date_           20200601
Time               11.44
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     4
SWH            49019.609 Hz
FIDRES          0.747980 Hz
AQ             0.6684672 sec
RG                198.09
DW                10.200 usec
DE                 6.50 usec
TE                293.4 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         161.9836917 MHz
NUC1                 31P
P1                15.00 usec
PLW1         13.19999981 W

======== CHANNEL f2 ========
SFO2         400.1316005 MHz
NUC2                 1H
CPDPRG[2          waltz16
PCPD2             90.00 usec
PLW2         12.50000000 W
PLW12         0.34722000 W
PLW13         0.28125000 W

F2 - Processing parameters
SI                 32768
SF           161.9755930 MHz
WDW                   EM
SSB                    0
LB                  2.00 Hz
GB                     0
PC                  1.40
```

^{1}H NMR Spectrum of **3c** ($CDCl_3$, 400 MHz)



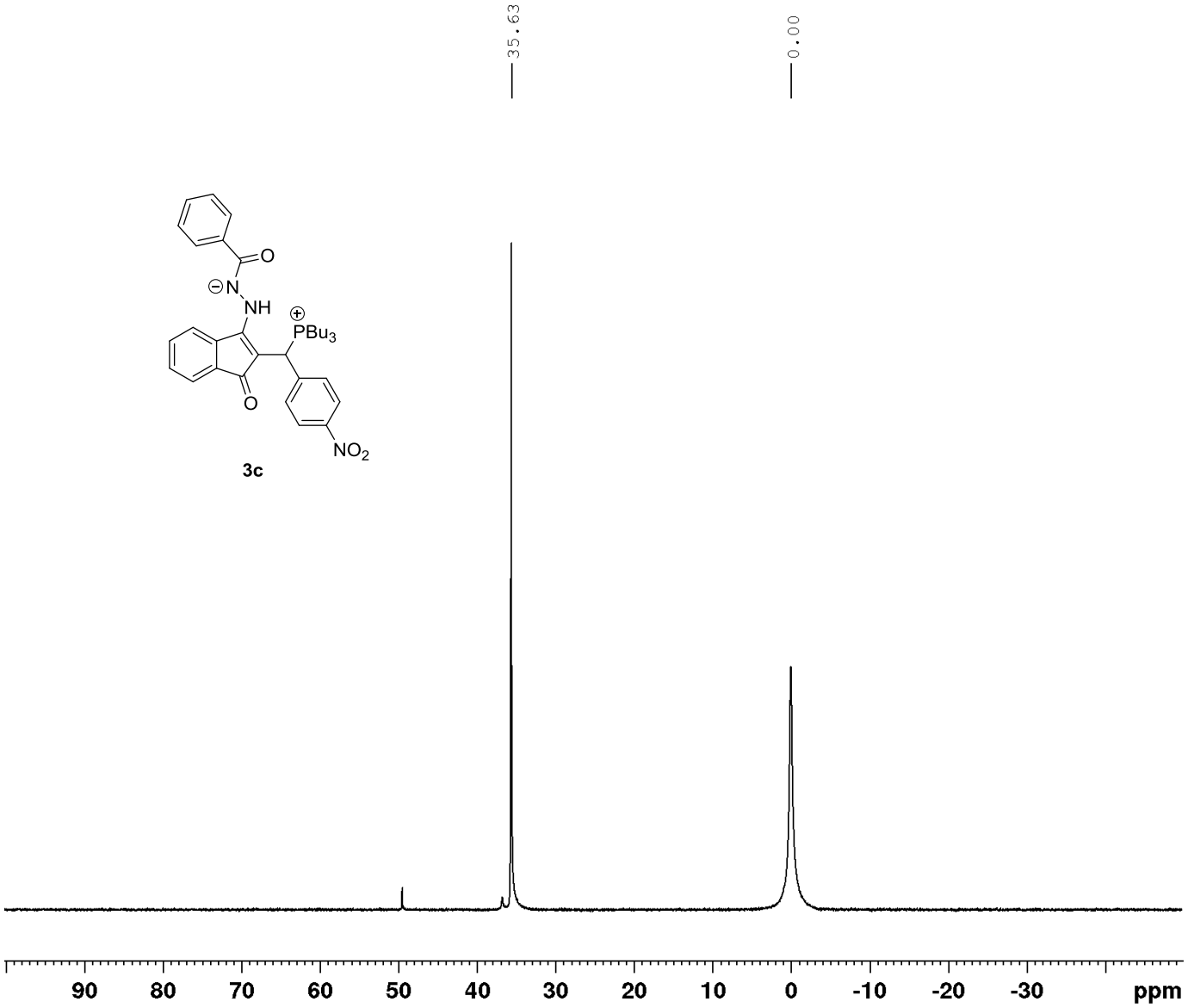

```
Current Data Parameters
NAME         SW ZW 4-NO2
EXPNO                  3
PROCNO                 1

F2 - Acquisition Parameters
Date_           20200613
Time               23.42
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG             zg30
TD                 32768
SOLVENT            CDCl3
NS                    32
DS                     0
SWH             7211.539 Hz
FIDRES          0.220079 Hz
AQ             2.2719147 sec
RG                 24.54
DW                69.333 usec
DE                10.06 usec
TE                298.0 K
D1             2.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         400.1324008 MHz
NUC1                   1H
P1                 15.00 usec
PLW1         11.39999962 W

F2 - Processing parameters
SI                 16384
SF           400.1299895 MHz
WDW                   EM
SSB                    0
LB                     0 Hz
GB                     0
PC                  1.00
```

^{13}C NMR Spectrum of **3c** ($CDCl_3$, 100 MHz)



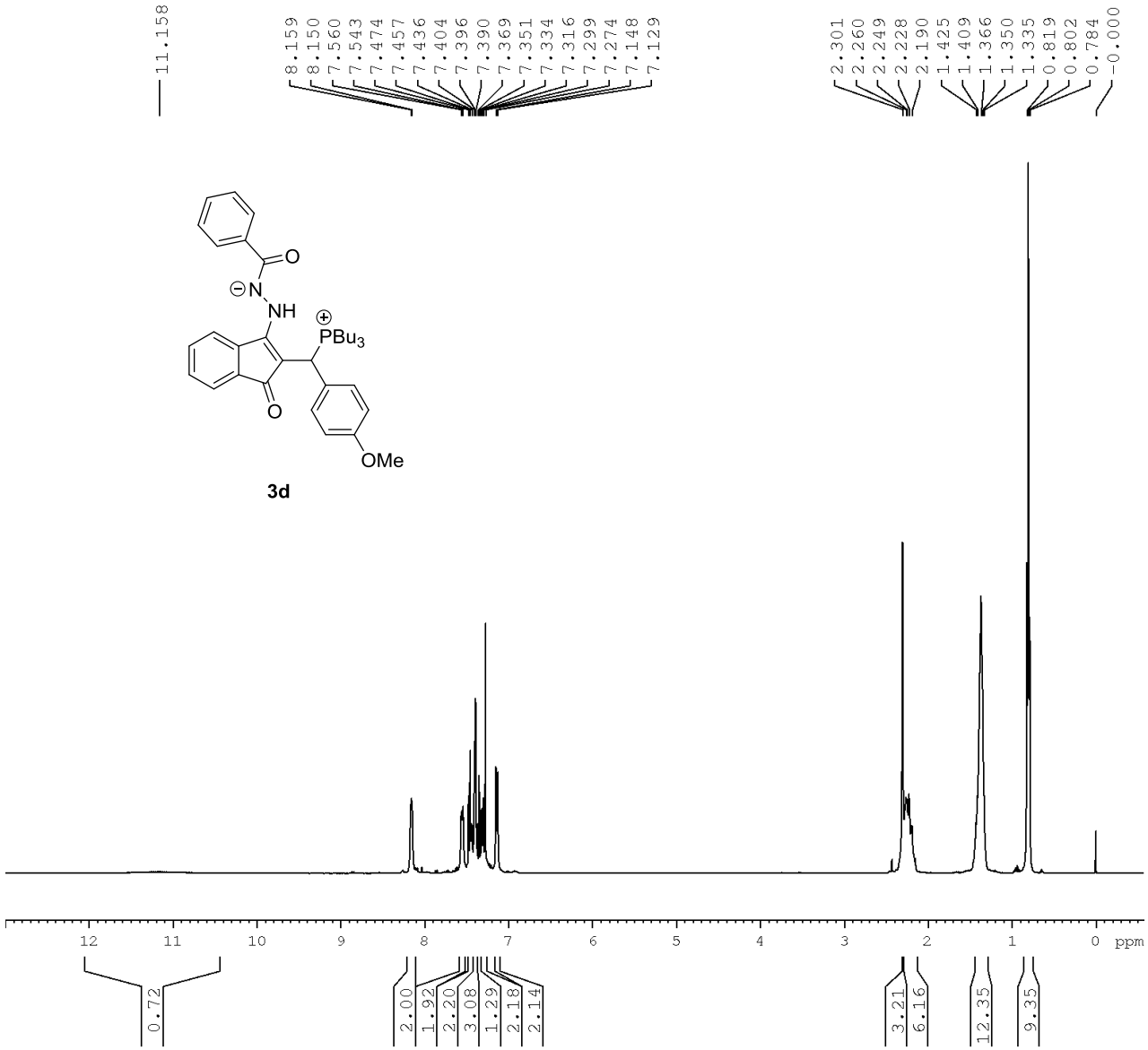

```
Current Data Parameters
NAME         SW ZW 4-NO2
EXPNO                  4
PROCNO                 1

F2 - Acquisition Parameters
Date_           20200613
Time               23.45
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                32768
SOLVENT           CDCl3
NS                 9950
DS                    0
SWH           24038.461 Hz
FIDRES         0.733596 Hz
AQ            0.6815744 sec
RG               198.09
DW               20.800 usec
DE                6.50 usec
TE                297.9 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1        100.6228298 MHz
NUC1                13C
P1                10.00 usec
PLW1        49.50000000 W

======== CHANNEL f2 ========
SFO2        400.1316005 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2             90.00 usec
PLW2        12.50000000 W
PLW12        0.34722000 W
PLW13        0.28125000 W

F2 - Processing parameters
SI                 32768
SF          100.6127887 MHz
WDW                  EM
SSB                   0
LB                 2.00 Hz
GB                    0
PC                 1.00
```

^{31}P NMR Spectrum of **3c** ($CDCl_3$, 162 MHz)



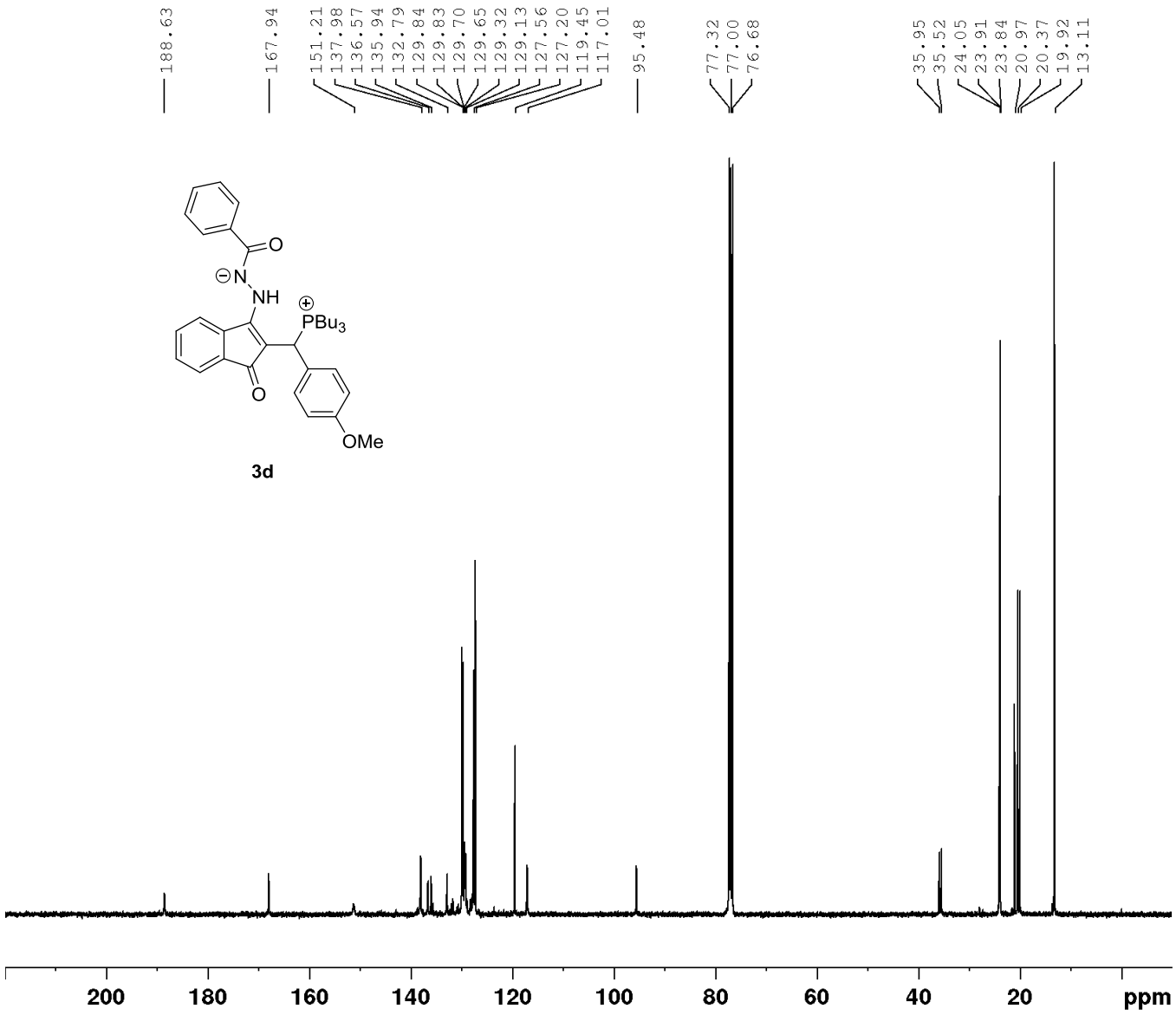

```
Current Data Parameters
NAME         SW ZW 4-NO2
EXPNO                  5
PROCNO                 1

F2 - Acquisition Parameters
Date_           20200614
Time               11.08
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                 65536
SOLVENT            CDCl3
NS                    32
DS                     4
SWH            49019.609 Hz
FIDRES          0.747980 Hz
AQ             0.6684672 sec
RG                198.09
DW                10.200 usec
DE                 6.50 usec
TE                294.5 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         161.9836917 MHz
NUC1                 31P
P1                15.00 usec
PLW1         13.19999981 W

======== CHANNEL f2 ========
SFO2         400.1316005 MHz
NUC2                 1H
CPDPRG[2          waltz16
PCPD2             90.00 usec
PLW2         12.50000000 W
PLW12         0.34722000 W
PLW13         0.28125000 W

F2 - Processing parameters
SI                  32768
SF           161.9755107 MHz
WDW                    EM
SSB                     0
LB                   2.00 Hz
GB                      0
PC                   1.40
```

^{1}H NMR Spectrum of **3d** ($CDCl_3$, 400 MHz)



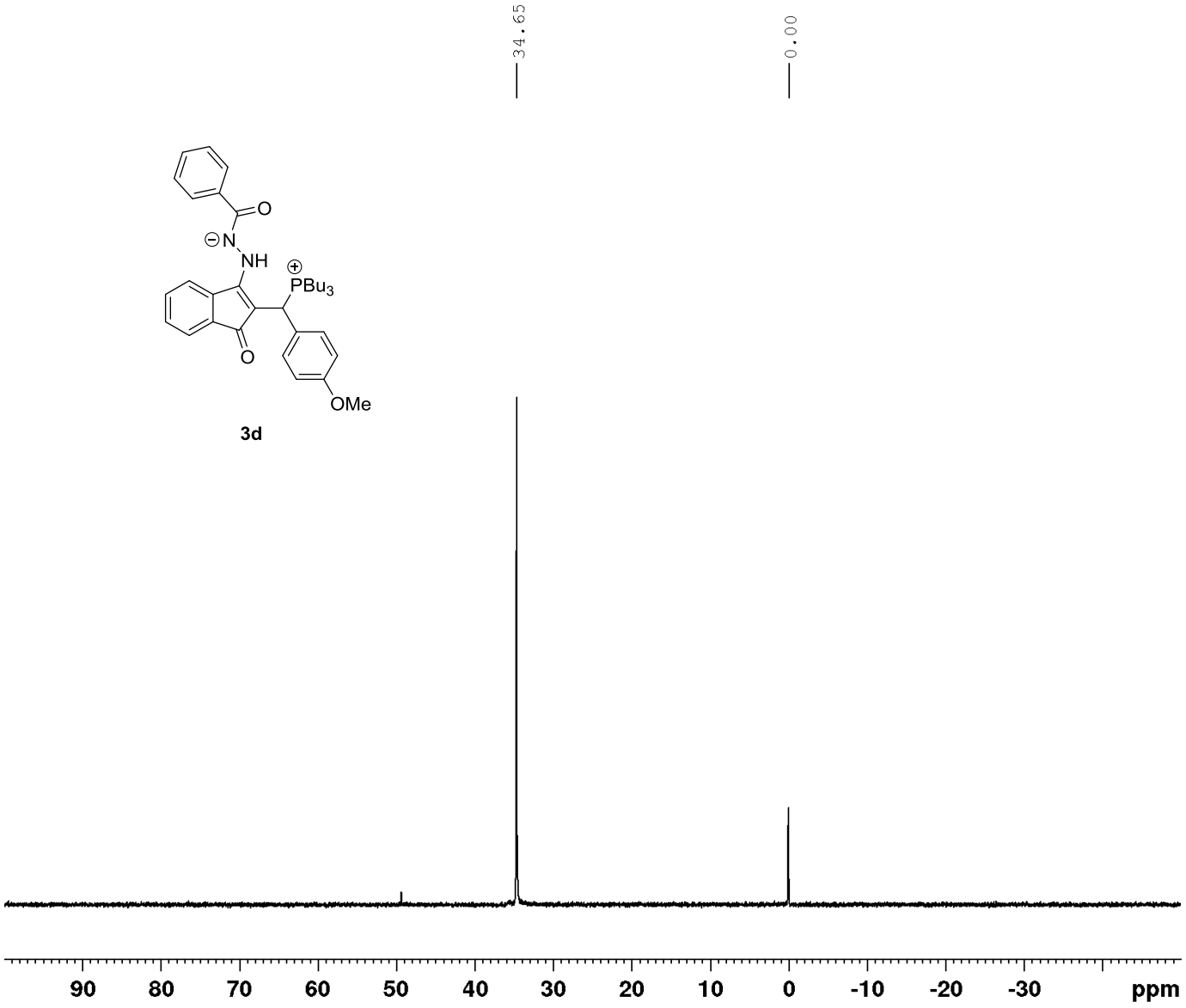

```
Current Data Parameters
NAME                  SW 894
EXPNO                      4
PROCNO                     1

F2 - Acquisition Parameters
Date_               20200530
Time                   23.54
INSTRUM                spect
PROBHD   5 mm BBO BB-1H
PULPROG                zg30
TD                    32768
SOLVENT               CDCl3
NS                        32
DS                         0
SWH                 7246.377 Hz
FIDRES              0.221142 Hz
AQ                2.2609921 sec
RG                        57
DW                   69.000 usec
DE                    6.50 usec
TE                    299.6 K
D1                2.00000000 sec
TD0                        1

======== CHANNEL f1 ========
NUC1                      1H
P1                    15.00 usec
PL1                   11.10 dB
SFO1          400.1324008 MHz

F2 - Processing parameters
SI                        16384
SF            400.1300062 MHz
WDW                       EM
SSB                        0
LB                         0 Hz
GB                         0
PC                      1.00
```

^{13}C NMR Spectrum of **3d** ($CDCl_3$, 100 MHz)



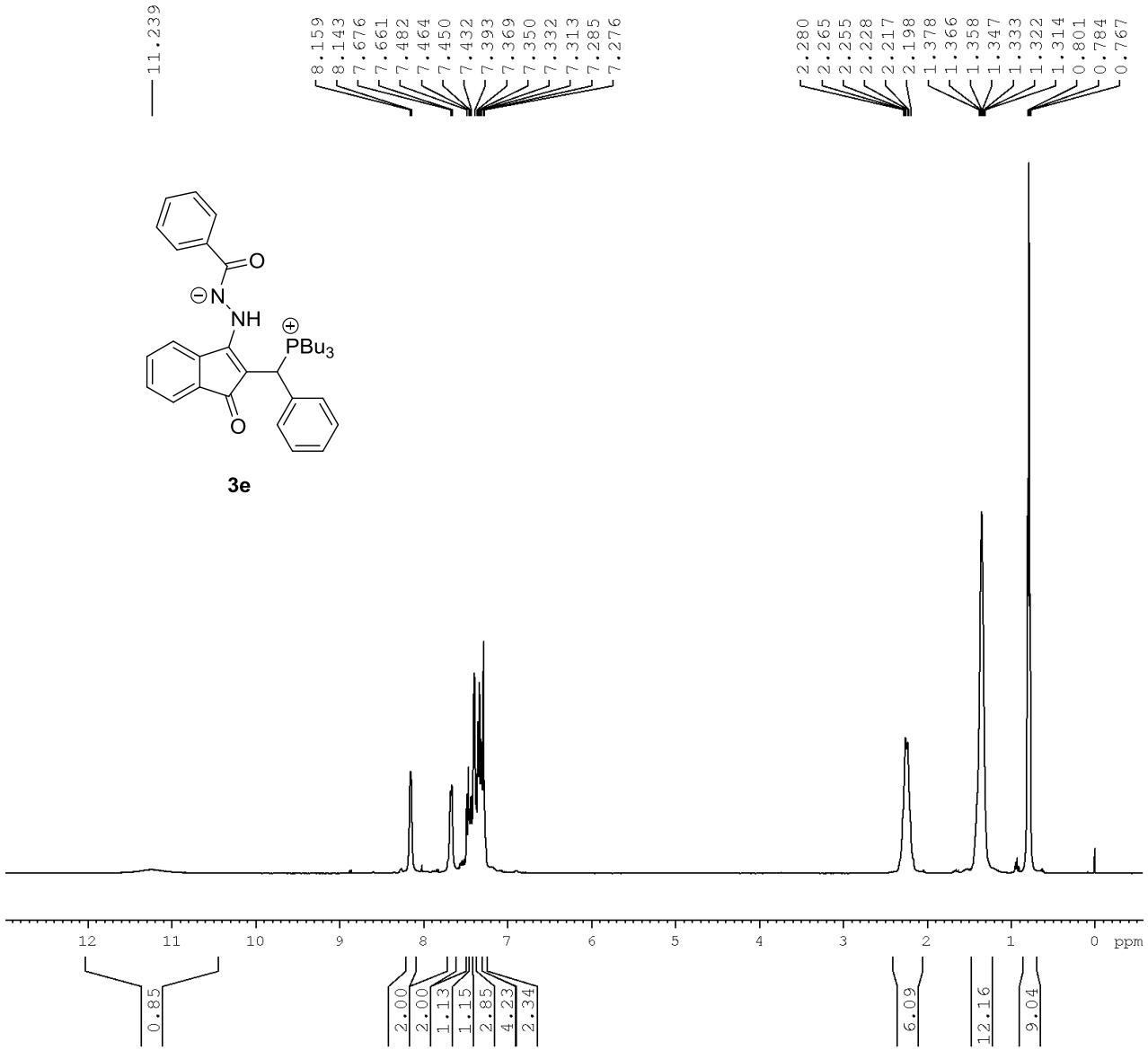

```
Current Data Parameters
NAME                  SW 894
EXPNO                      5
PROCNO                     1

F2 - Acquisition Parameters
Date_              20200530
Time                  23.57
INSTRUM               spect
PROBHD    5 mm BBO BB-1H
PULPROG             zgpg30
TD                    32768
SOLVENT               CDCl3
NS                    10000
DS                        0
SWH              24038.461 Hz
FIDRES            0.733596 Hz
AQ               0.6815744 sec
RG                     4096
DW                  20.800 usec
DE                   6.50 usec
TE                  299.6 K
D1               2.00000000 sec
D11              0.03000000 sec
TD0                       1

======== CHANNEL f1 ========
NUC1                    13C
P1                   10.00 usec
PL1                   3.80 dB
SFO1           100.6233325 MHz

======== CHANNEL f2 ========
CPDPRG[2           waltz16
NUC2                    1H
PCPD2                90.00 usec
PL2                  10.20 dB
PL12                 26.00 dB
PL13                 29.00 dB
SFO2           400.1316005 MHz

F2 - Processing parameters
SI                    32768
SF             100.6127763 MHz
WDW                      EM
SSB                       0
LB                    1.00 Hz
GB                        0
PC                    1.00
```

^{31}P NMR Spectrum of **3d** ($CDCl_3$, 162 MHz)



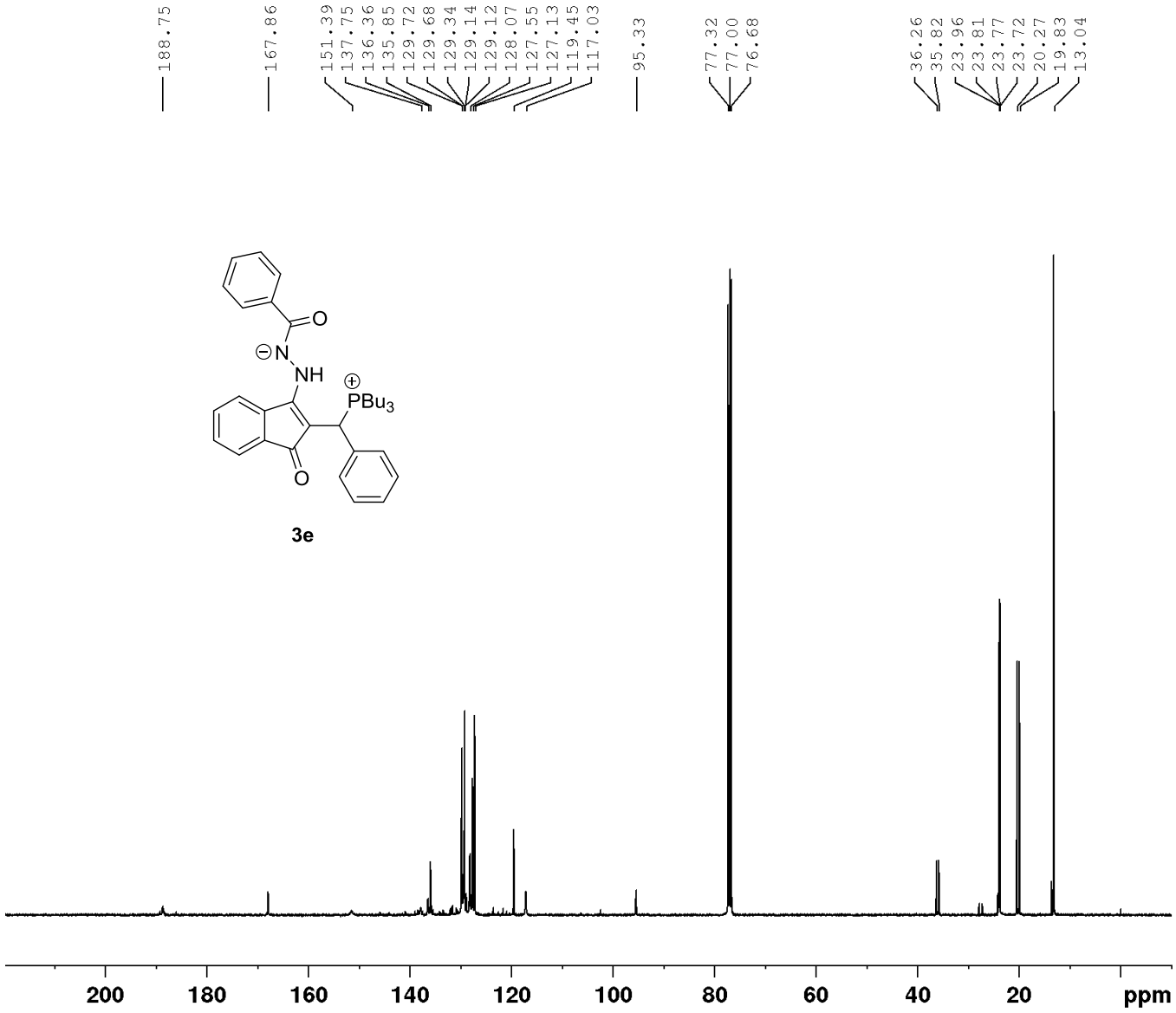

```
Current Data Parameters
NAME                 SW 894
EXPNO                     6
PROCNO                    1

F2 - Acquisition Parameters
Date_              20200601
Time                  11.56
INSTRUM               spect
PROBHD    5 mm BBO BB-1H
PULPROG              zgpg30
TD                    65536
SOLVENT               CDCl3
NS                       16
DS                        0
SWH               64724.918 Hz
FIDRES             0.987624 Hz
AQ                0.5062656 sec
RG                  11585.2
DW                    7.725 usec
DE                    6.50 usec
TE                   296.8 K
D1               2.00000000 sec
D11              0.03000000 sec
TD0                       1

======== CHANNEL f1 ========
NUC1                    31P
P1                    15.40 usec
PL1                   10.90 dB
SFO1           161.9674942 MHz

======== CHANNEL f2 ========
CPDPRG[2             waltz16
NUC2                    1H
PCPD2                 90.00 usec
PL2                   10.20 dB
PL12                  26.00 dB
PL13                  29.00 dB
SFO2           400.1316005 MHz

F2 - Processing parameters
SI                    32768
SF             161.9755116 MHz
WDW                      EM
SSB                       0
LB                    1.00 Hz
GB                        0
PC                    1.00
```

^{1}H NMR Spectrum of **3e** ($CDCl_3$, 400 MHz)



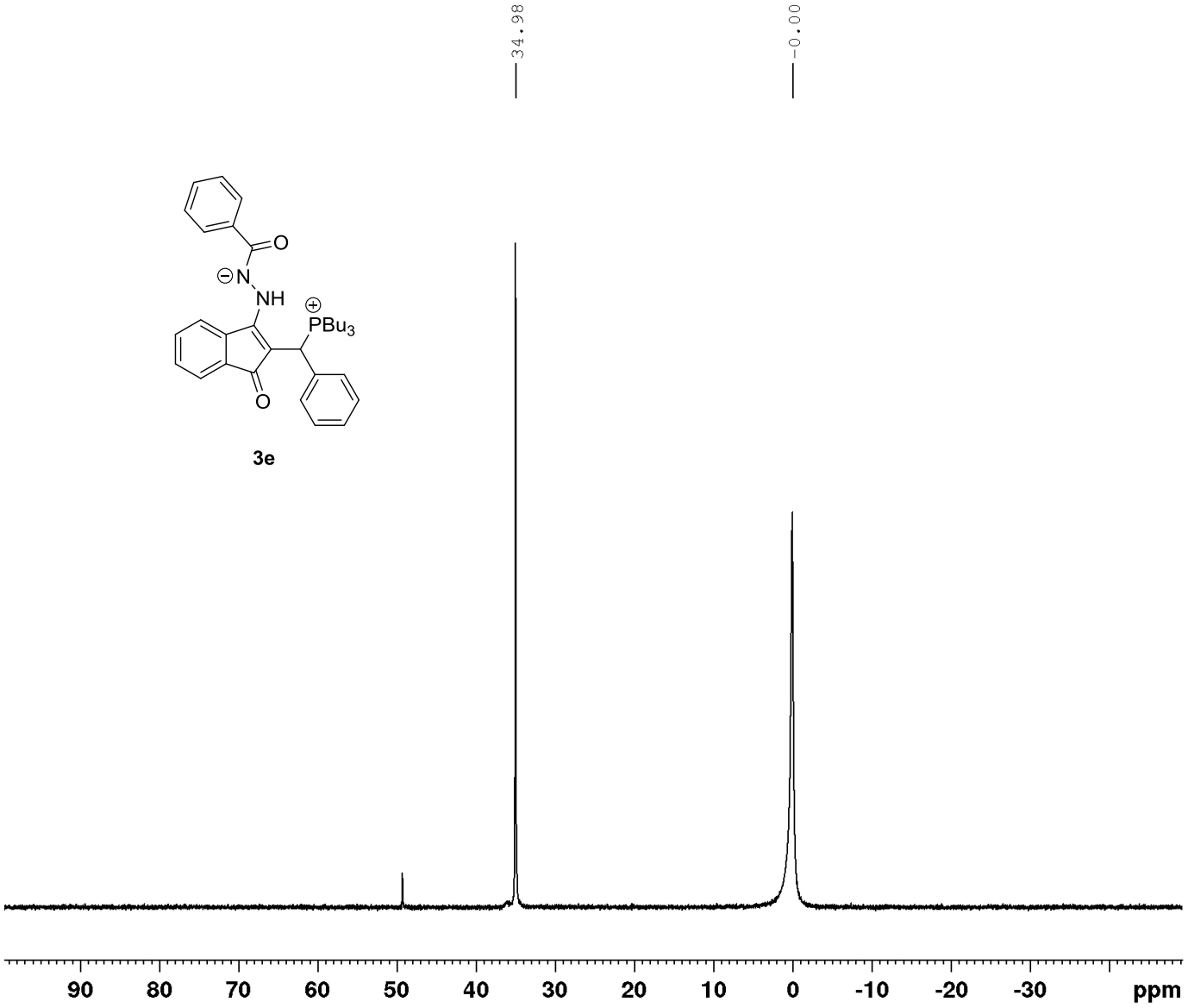

```
Current Data Parameters
NAME            SW ZW ns
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20200611
Time               22.00
INSTRUM            spect
PROBHD   5 mm BBO BB-1H
PULPROG             zg30
TD                 32768
SOLVENT            CDCl3
NS                    32
DS                     0
SWH             7246.377 Hz
FIDRES          0.221142 Hz
AQ             2.2609921 sec
RG                  35.9
DW                69.000 usec
DE                 6.50 usec
TE                297.9 K
D1            2.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                15.00 usec
PL1               11.10 dB
SFO1         400.1324008 MHz

F2 - Processing parameters
SI                 16384
SF           400.1300019 MHz
WDW                   EM
SSB                    0
LB                     0 Hz
GB                     0
PC                  1.00
```

^{13}C NMR Spectrum of **3e** ($CDCl_3$, 100 MHz)



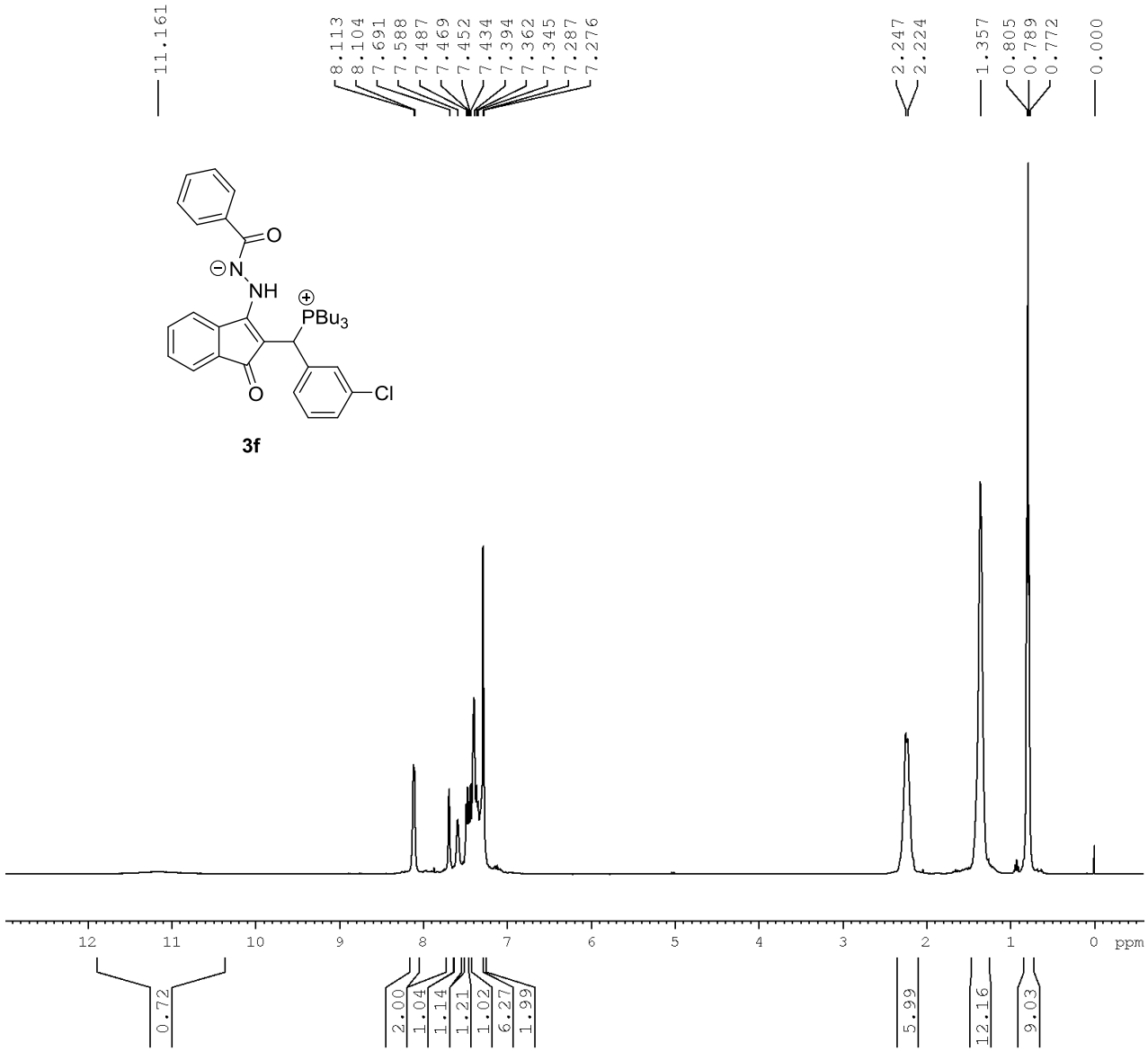

```
Current Data Parameters
NAME                  SW ZW ns
EXPNO                        2
PROCNO                       1

F2 - Acquisition Parameters
Date_                 20200611
Time                     22.03
INSTRUM                  spect
PROBHD    5 mm BBO BB-1H
PULPROG                zgpg30
TD                       32768
SOLVENT                  CDCl3
NS                       15000
DS                           0
SWH                 24038.461 Hz
FIDRES               0.733596 Hz
AQ                  0.6815744 sec
RG                        4096
DW                      20.800 usec
DE                       6.50 usec
TE                      297.8 K
D1                 2.00000000 sec
D11                0.03000000 sec
TD0                          1

======== CHANNEL f1 ========
NUC1                       13C
P1                      10.00 usec
PL1                      3.80 dB
SFO1               100.6233325 MHz

======== CHANNEL f2 ========
CPDPRG[2               waltz16
NUC2                       1H
PCPD2                   90.00 usec
PL2                     10.20 dB
PL12                    26.00 dB
PL13                    29.00 dB
SFO2               400.1316005 MHz

F2 - Processing parameters
SI                       32768
SF                 100.6127817 MHz
WDW                         EM
SSB                          0
LB                      1.00 Hz
GB                           0
PC                      1.00
```

^{31}P NMR Spectrum of **3e** ($CDCl_3$, 162 MHz)



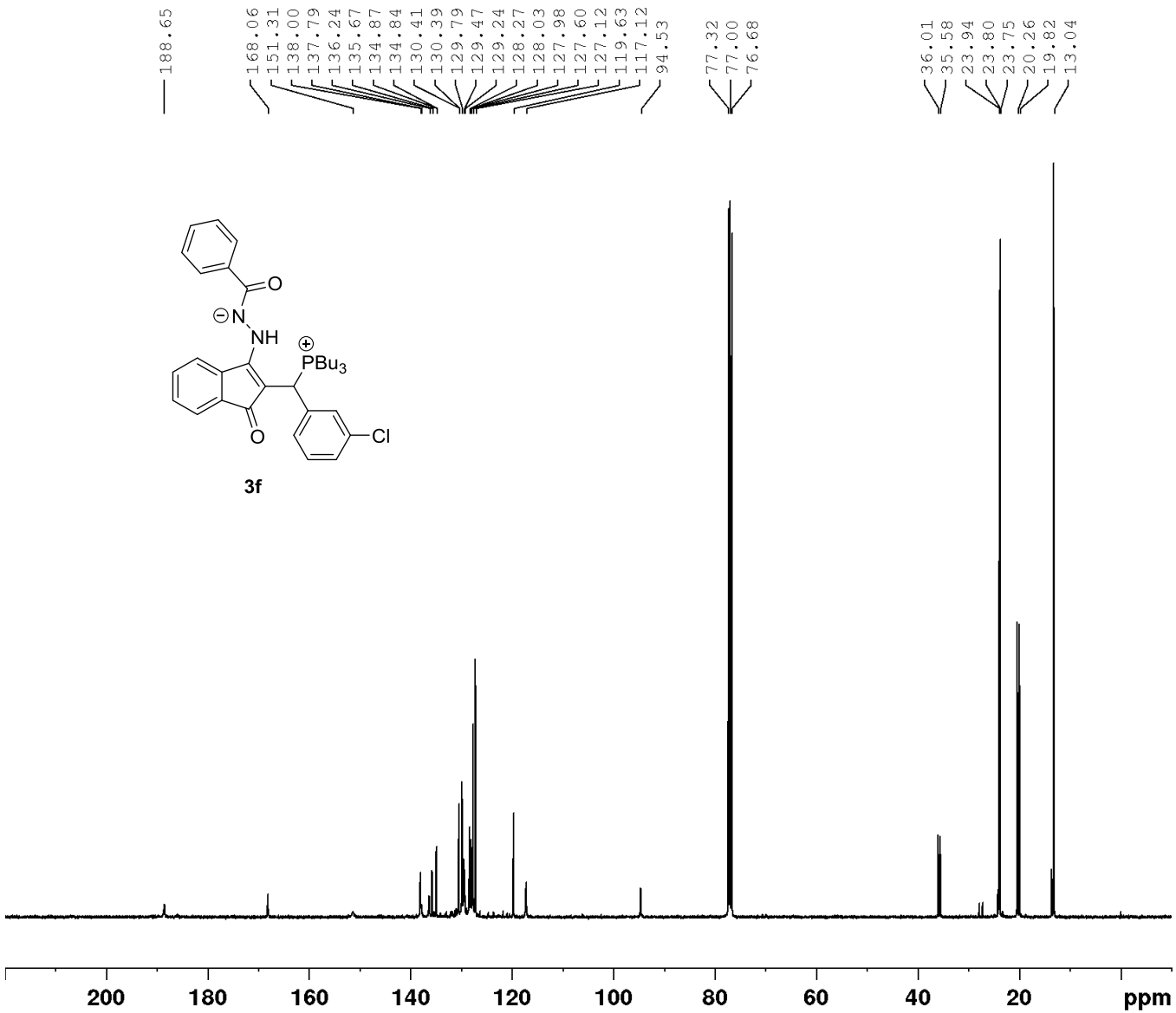

```
Current Data Parameters
NAME            SW ZW ns
EXPNO                  3
PROCNO                 1

F2 - Acquisition Parameters
Date_           20200612
Time               10.03
INSTRUM            spect
PROBHD   5 mm BBO BB-1H
PULPROG          zgpg30
TD                 65536
SOLVENT            CDCl3
NS                    32
DS                     0
SWH            64724.918 Hz
FIDRES          0.987624 Hz
AQ             0.5062656 sec
RG                3649.1
DW                 7.725 usec
DE                 6.50 usec
TE                297.7 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                 31P
P1                15.40 usec
PL1               10.90 dB
SFO1         161.9674942 MHz

======== CHANNEL f2 ========
CPDPRG[2          waltz16
NUC2                 1H
PCPD2             90.00 usec
PL2               10.20 dB
PL12              26.00 dB
PL13              29.00 dB
SFO2         400.1316005 MHz

F2 - Processing parameters
SI                 32768
SF           161.9755139 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.00
```

^{1}H NMR Spectrum of **3f** ($CDCl_3$, 400 MHz)



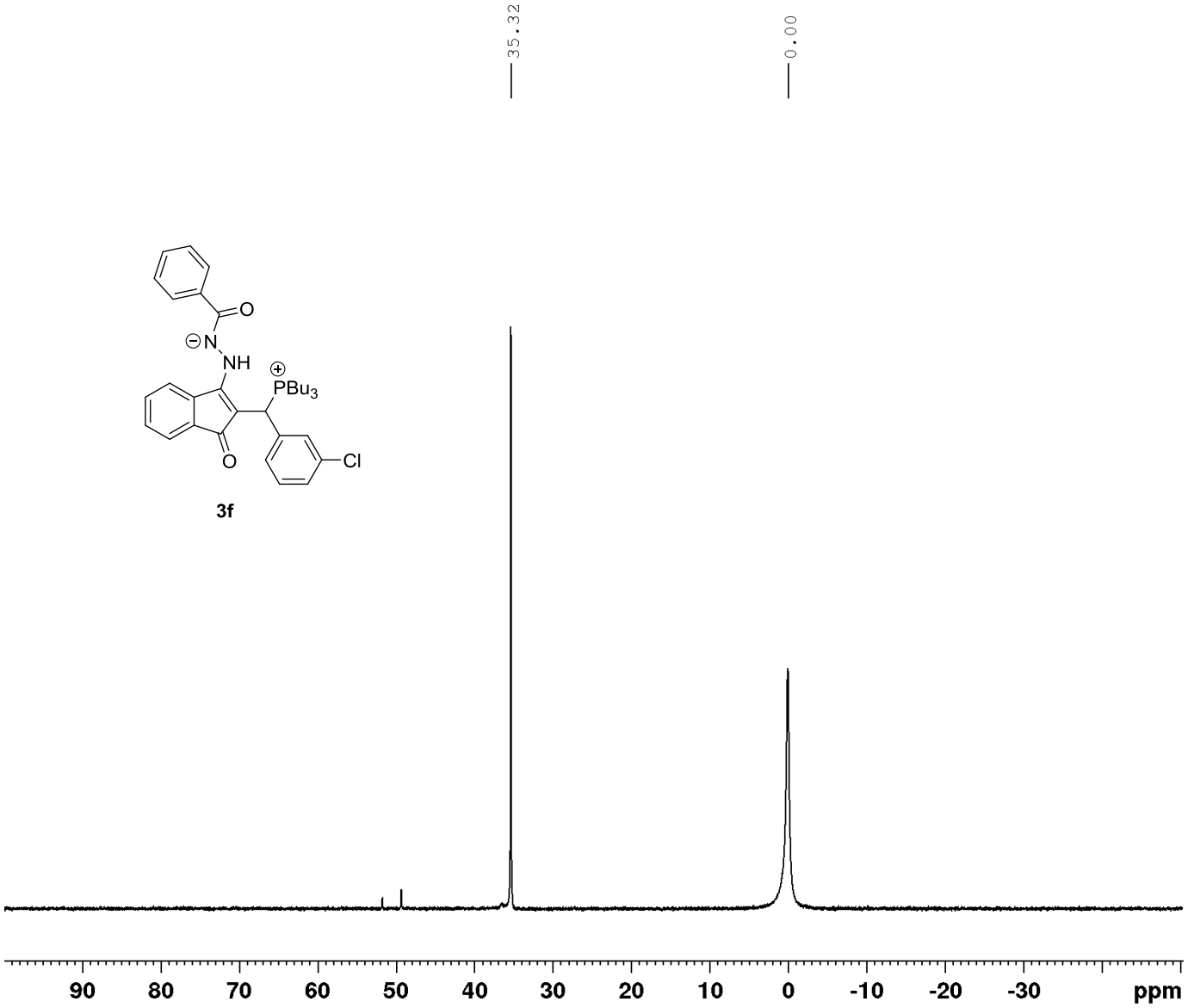

```
Current Data Parameters
NAME          SW ZW 3-Cl
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20200610
Time               22.04
INSTRUM            spect
PROBHD   5 mm BBO BB-1H
PULPROG             zg30
TD                 32768
SOLVENT            CDCl3
NS                    32
DS                     0
SWH             7246.377 Hz
FIDRES          0.221142 Hz
AQ             2.2609921 sec
RG                  35.9
DW                69.000 usec
DE                 6.50 usec
TE                297.7 K
D1           2.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                15.00 usec
PL1               11.10 dB
SFO1        400.1324008 MHz

F2 - Processing parameters
SI                 16384
SF          400.1300011 MHz
WDW                   EM
SSB                    0
LB                     0 Hz
GB                     0
PC                  1.00
```

^{13}C NMR Spectrum of **3f** ($CDCl_3$, 100 MHz)



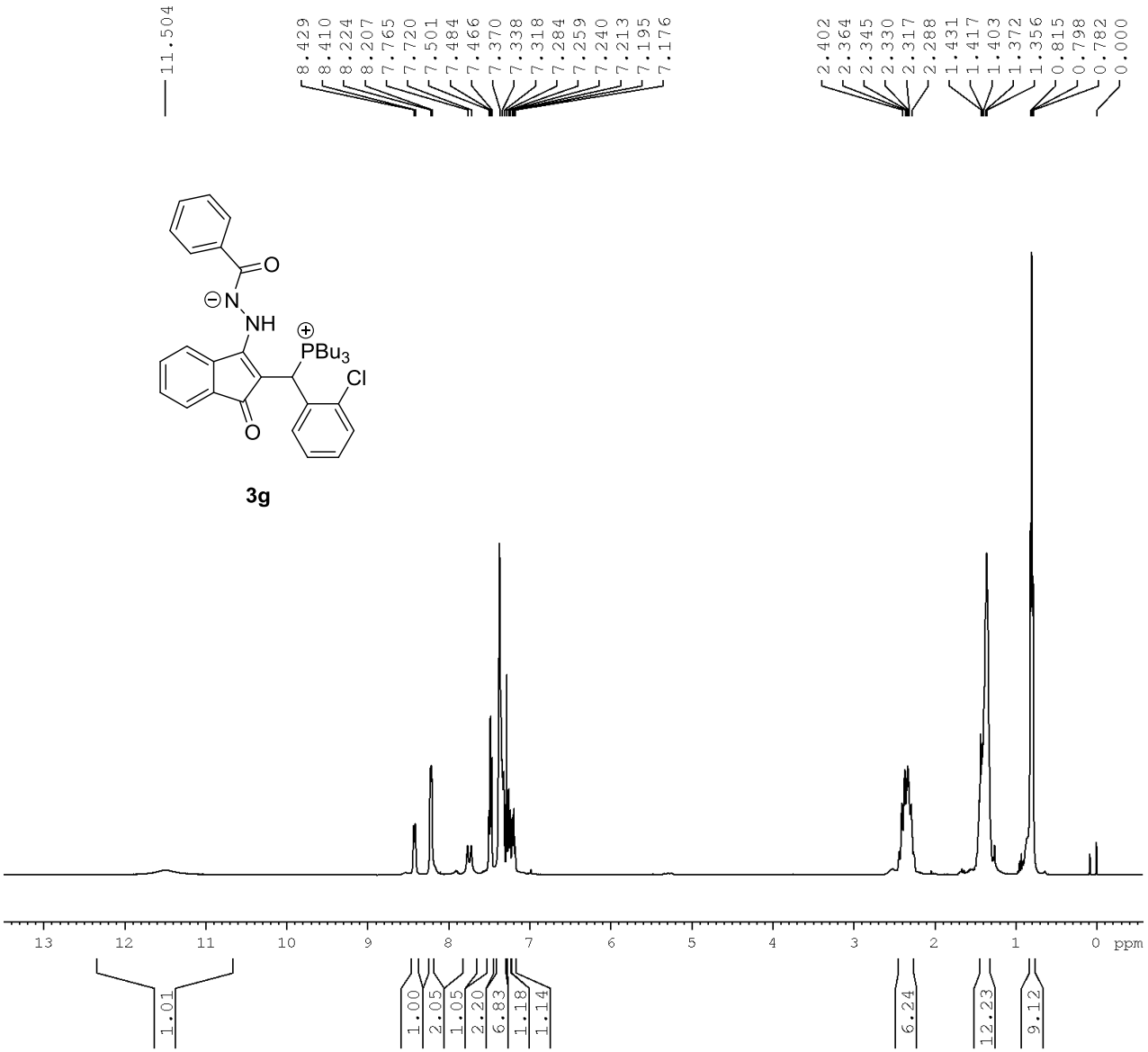

```
Current Data Parameters
NAME          SW ZW 3-Cl
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20200610
Time               22.07
INSTRUM            spect
PROBHD   5 mm BBO BB-1H
PULPROG          zgpg30
TD                 32768
SOLVENT            CDCl3
NS                 13449
DS                     0
SWH           24038.461 Hz
FIDRES         0.733596 Hz
AQ            0.6815744 sec
RG                  4096
DW                20.800 usec
DE                 6.50 usec
TE                297.7 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                 13C
P1                10.00 usec
PL1                3.80 dB
SFO1        100.6233325 MHz

======== CHANNEL f2 ========
CPDPRG[2         waltz16
NUC2                 1H
PCPD2             90.00 usec
PL2               10.20 dB
PL12              26.00 dB
PL13              29.00 dB
SFO2        400.1316005 MHz

F2 - Processing parameters
SI                 32768
SF          100.6127806 MHz
WDW                 EM
SSB                    0
LB                 1.00 Hz
GB                     0
PC                 1.00
```

^{31}P NMR Spectrum of **3f** ($CDCl_3$, 162 MHz)



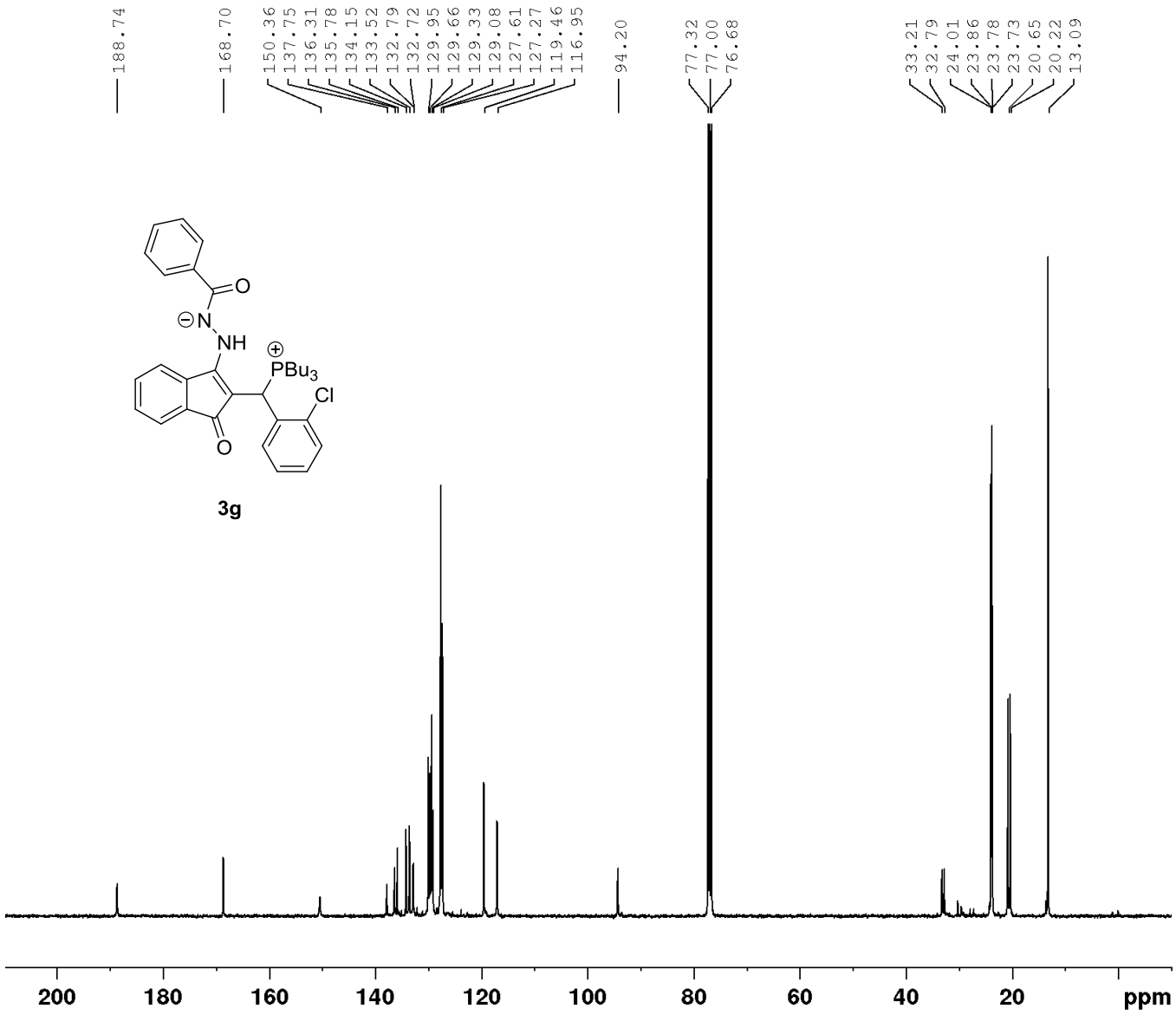

```
Current Data Parameters
NAME          SW ZW 3-Cl
EXPNO                  3
PROCNO                 1

F2 - Acquisition Parameters
Date_           20200611
Time               10.38
INSTRUM            spect
PROBHD   5 mm BBO BB-1H
PULPROG          zgpg30
TD                 65536
SOLVENT            CDCl3
NS                    32
DS                     0
SWH            64724.918 Hz
FIDRES          0.987624 Hz
AQ             0.5062656 sec
RG                  4096
DW                 7.725 usec
DE                 6.50 usec
TE                 297.4 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                 31P
P1                15.40 usec
PL1               10.90 dB
SFO1         161.9674942 MHz

======== CHANNEL f2 ========
CPDPRG[2          waltz16
NUC2                 1H
PCPD2             90.00 usec
PL2               10.20 dB
PL12              26.00 dB
PL13              29.00 dB
SFO2         400.1316005 MHz

F2 - Processing parameters
SI                 32768
SF           161.9755150 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.00
```

^{1}H NMR Spectrum of **3g** ($CDCl_3$, 400 MHz)



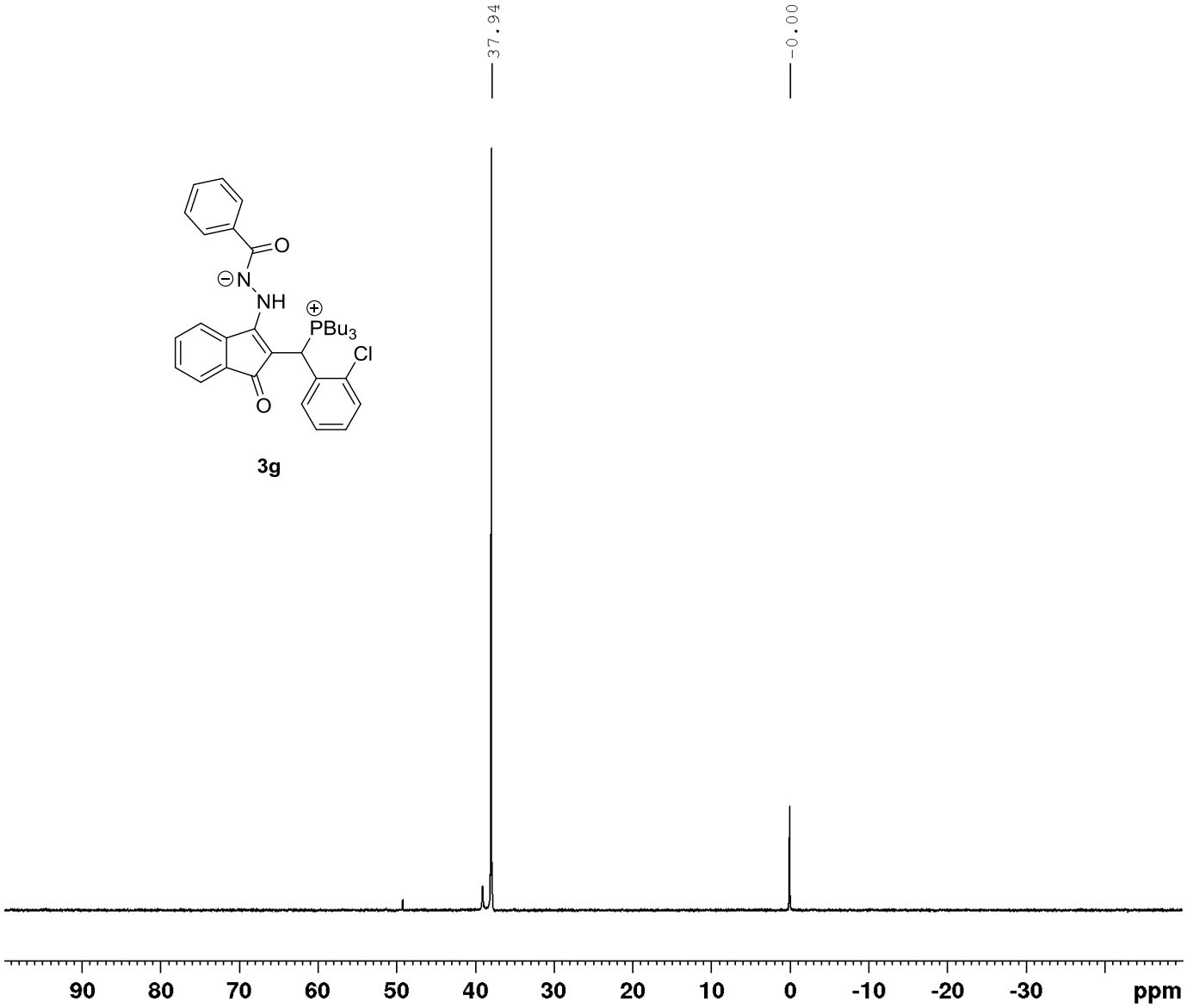

```
Current Data Parameters
NAME                  SW 895-1
EXPNO                        3
PROCNO                       1

F2 - Acquisition Parameters
Date_                 20200601
Time                      0.42
INSTRUM                  spect
PROBHD   5 mm PABBO BB/
PULPROG                  zg30
TD                      32768
SOLVENT                 CDCl3
NS                         32
DS                          0
SWH                  7211.539 Hz
FIDRES               0.220079 Hz
AQ                 2.2719147 sec
RG                      38.89
DW                     69.333 usec
DE                      10.06 usec
TE                      295.2 K
D1                 2.00000000 sec
TD0                         1

======== CHANNEL f1 ========
SFO1            400.1324008 MHz
NUC1                       1H
P1                      15.00 usec
PLW1            11.39999962 W

F2 - Processing parameters
SI                      16384
SF              400.1300000 MHz
WDW                        EM
SSB                         0
LB                          0 Hz
GB                          0
PC                       1.00
```

^{13}C NMR Spectrum of **3g** ($CDCl_3$, 100 MHz)



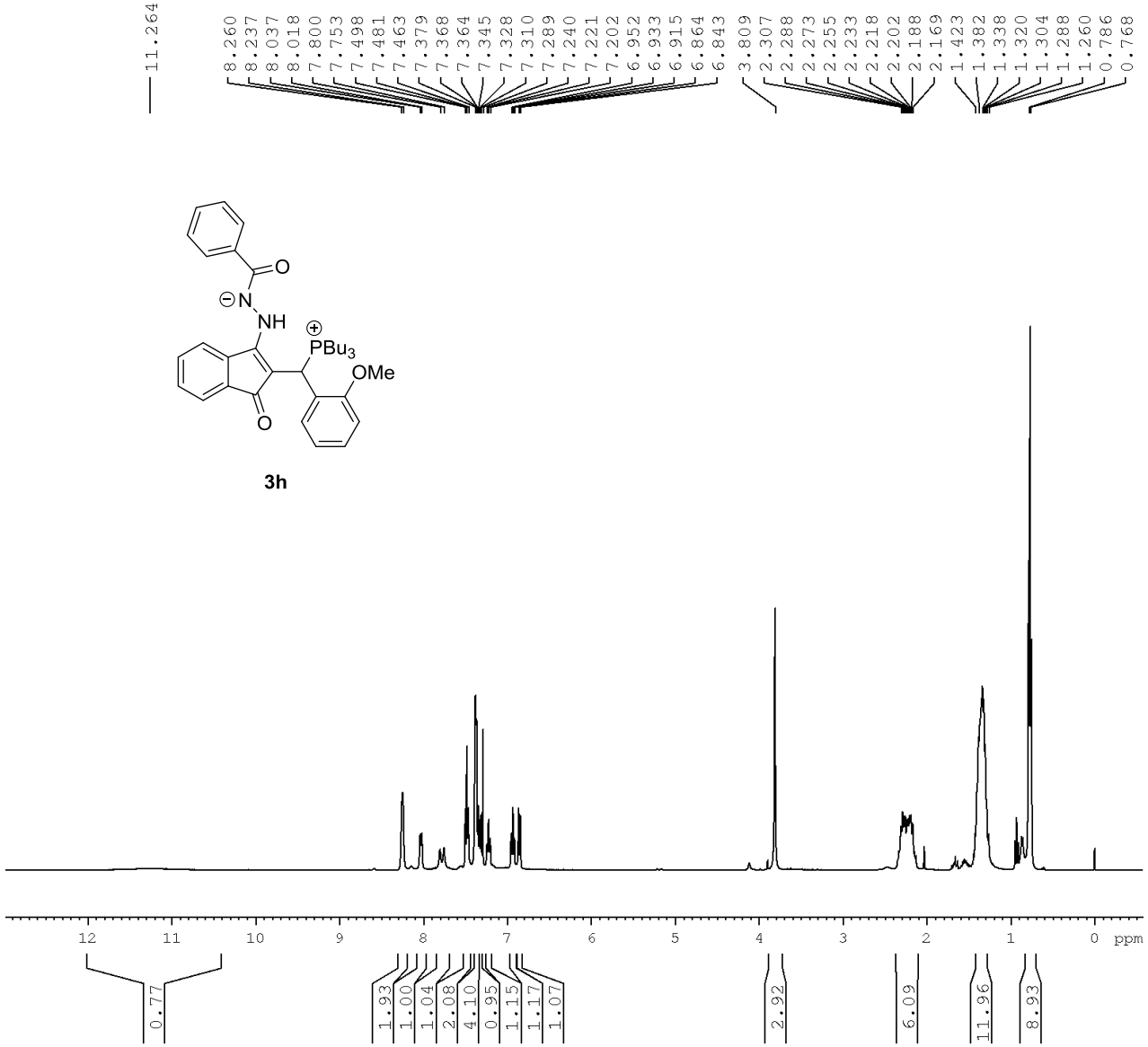

```
Current Data Parameters
NAME            SW 895-1
EXPNO                  4
PROCNO                 1

F2 - Acquisition Parameters
Date_           20200601
Time                0.45
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                32768
SOLVENT           CDCl3
NS                 8000
DS                    0
SWH           24038.461 Hz
FIDRES         0.733596 Hz
AQ            0.6815744 sec
RG               198.09
DW              20.800 usec
DE               6.50 usec
TE              295.0 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1        100.6228298 MHz
NUC1               13C
P1               10.00 usec
PLW1        49.50000000 W

======== CHANNEL f2 ========
SFO2        400.1316005 MHz
NUC2               1H
CPDPRG[2         waltz16
PCPD2            90.00 usec
PLW2        12.50000000 W
PLW12        0.34722000 W
PLW13        0.28125000 W

F2 - Processing parameters
SI                32768
SF          100.6127795 MHz
WDW                EM
SSB                 0
LB               2.00 Hz
GB                  0
PC               1.00
```

^{31}P NMR Spectrum of **3g** ($CDCl_3$, 162 MHz)




```
Current Data Parameters
NAME            SW 895-1
EXPNO                  5
PROCNO                 1

F2 - Acquisition Parameters
Date_           20200601
Time               11.26
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     4
SWH            49019.609 Hz
FIDRES          0.747980 Hz
AQ             0.6684672 sec
RG                198.09
DW                10.200 usec
DE                 6.50 usec
TE                293.5 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         161.9836917 MHz
NUC1                31P
P1                15.00 usec
PLW1         13.19999981 W

======== CHANNEL f2 ========
SFO2         400.1316005 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2             90.00 usec
PLW2         12.50000000 W
PLW12         0.34722000 W
PLW13         0.28125000 W

F2 - Processing parameters
SI                 32768
SF           161.9755116 MHz
WDW                   EM
SSB                    0
LB                  2.00 Hz
GB                     0
PC                  1.40
```

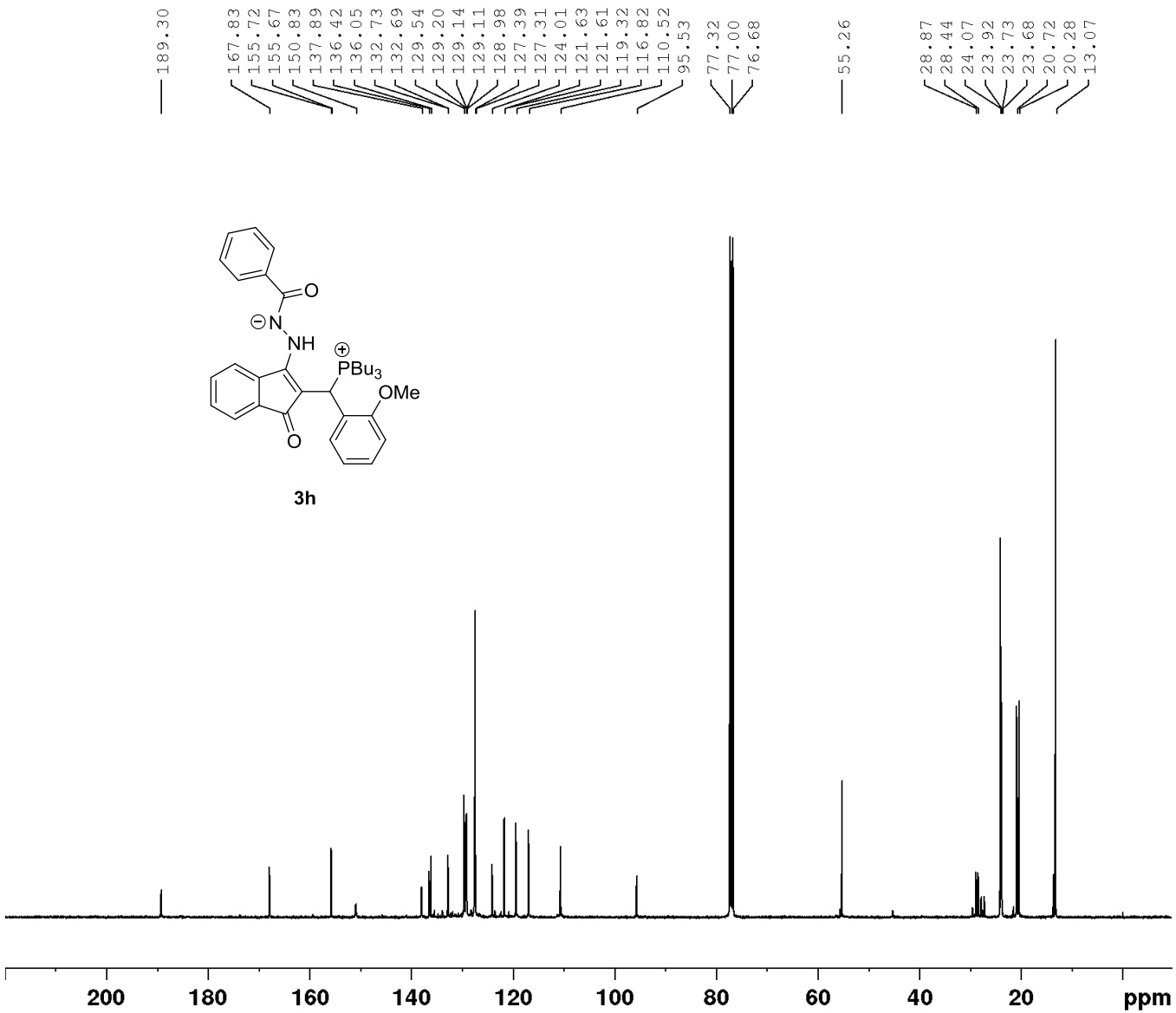
^{1}H NMR Spectrum of **3h** ($CDCl_3$, 400 MHz)



3h

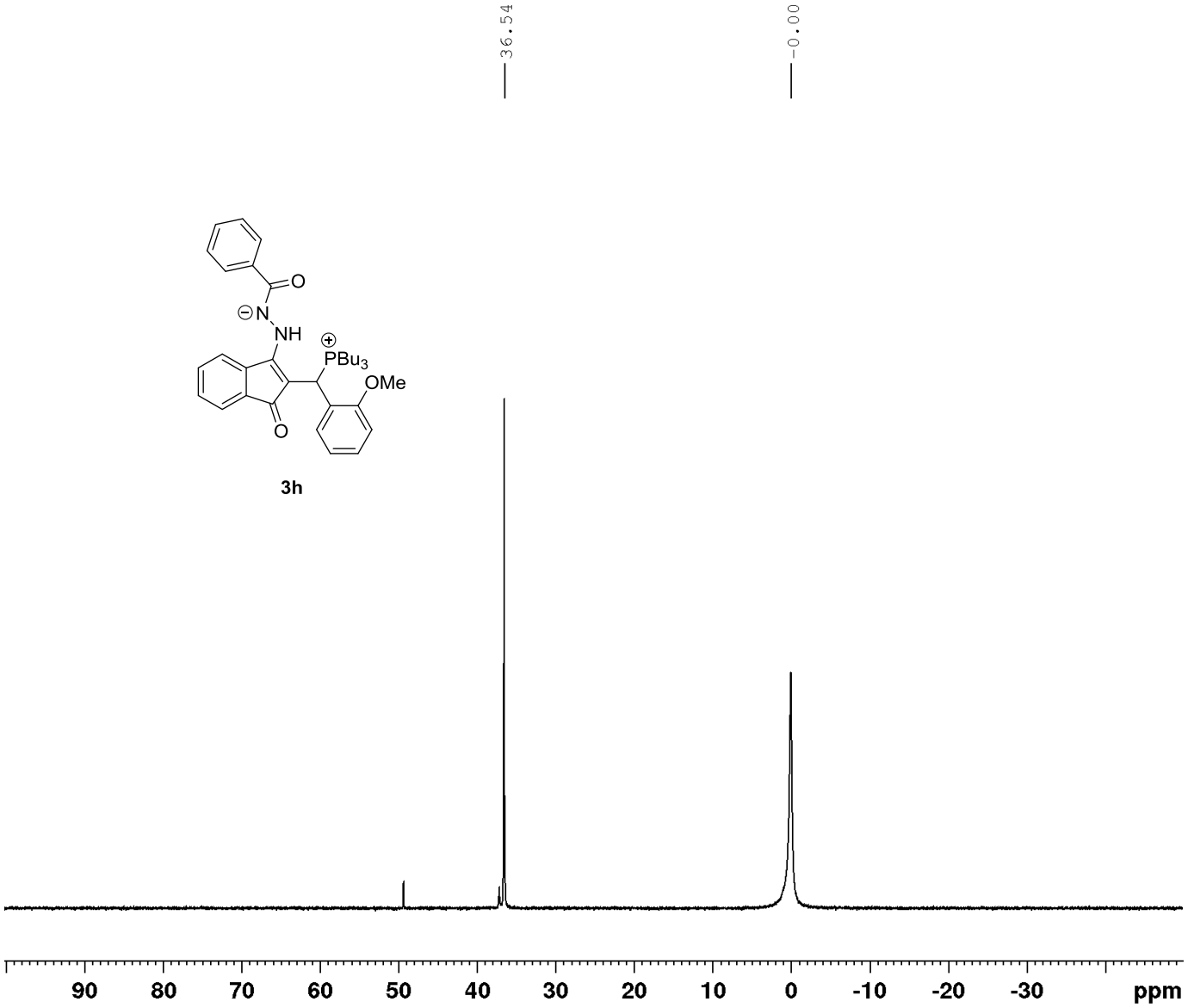
```
Current Data Parameters
NAME          SW ZW 2 OMe
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_            20200613
Time                23.26
INSTRUM             spect
PROBHD   5 mm BBO BB-1H
PULPROG              zg30
TD                  32768
SOLVENT             CDCl3
NS                     32
DS                      0
SWH              7246.377 Hz
FIDRES           0.221142 Hz
AQ             2.2609921 sec
RG                   35.9
DW                 69.000 usec
DE                  6.50 usec
TE                 297.7 K
D1             2.00000000 sec
TD0                     1

======== CHANNEL f1 ========
NUC1                   1H
P1                 15.00 usec
PL1                11.10 dB
SFO1         400.1324008 MHz

F2 - Processing parameters
SI                  16384
SF           400.1300000 MHz
WDW                    EM
SSB                     0
LB                      0 Hz
GB                      0
PC                   1.00
```

^{13}C NMR Spectrum of **3h** ($CDCl_3$, 100 MHz)



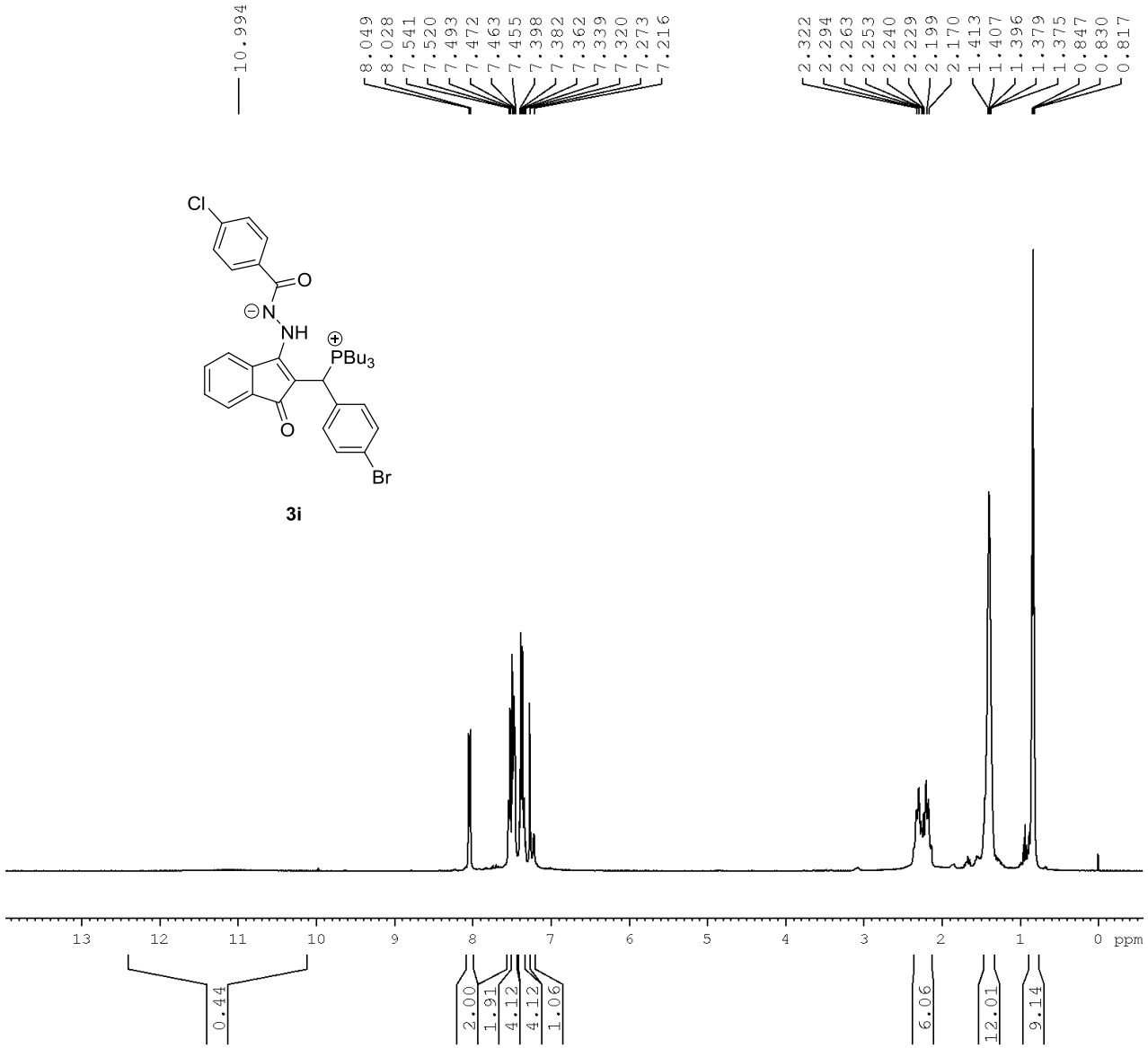

```
Current Data Parameters
NAME         SW ZW 2 OMe
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20200613
Time               23.29
INSTRUM            spect
PROBHD   5 mm BBO BB-1H
PULPROG          zgpg30
TD                 32768
SOLVENT            CDCl3
NS                 14590
DS                     0
SWH           24038.461 Hz
FIDRES         0.733596 Hz
AQ            0.6815744 sec
RG                  4096
DW                20.800 usec
DE                 6.50 usec
TE                297.7 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                 13C
P1                10.00 usec
PL1                3.80 dB
SFO1        100.6233325 MHz

======== CHANNEL f2 ========
CPDPRG[2         waltz16
NUC2                 1H
PCPD2             90.00 usec
PL2               10.20 dB
PL12              26.00 dB
PL13              29.00 dB
SFO2        400.1316005 MHz

F2 - Processing parameters
SI                 32768
SF          100.6127815 MHz
WDW                 EM
SSB                    0
LB                 1.00 Hz
GB                     0
PC                 1.00
```

^{31}P NMR Spectrum of **3h** ($CDCl_3$, 162 MHz)



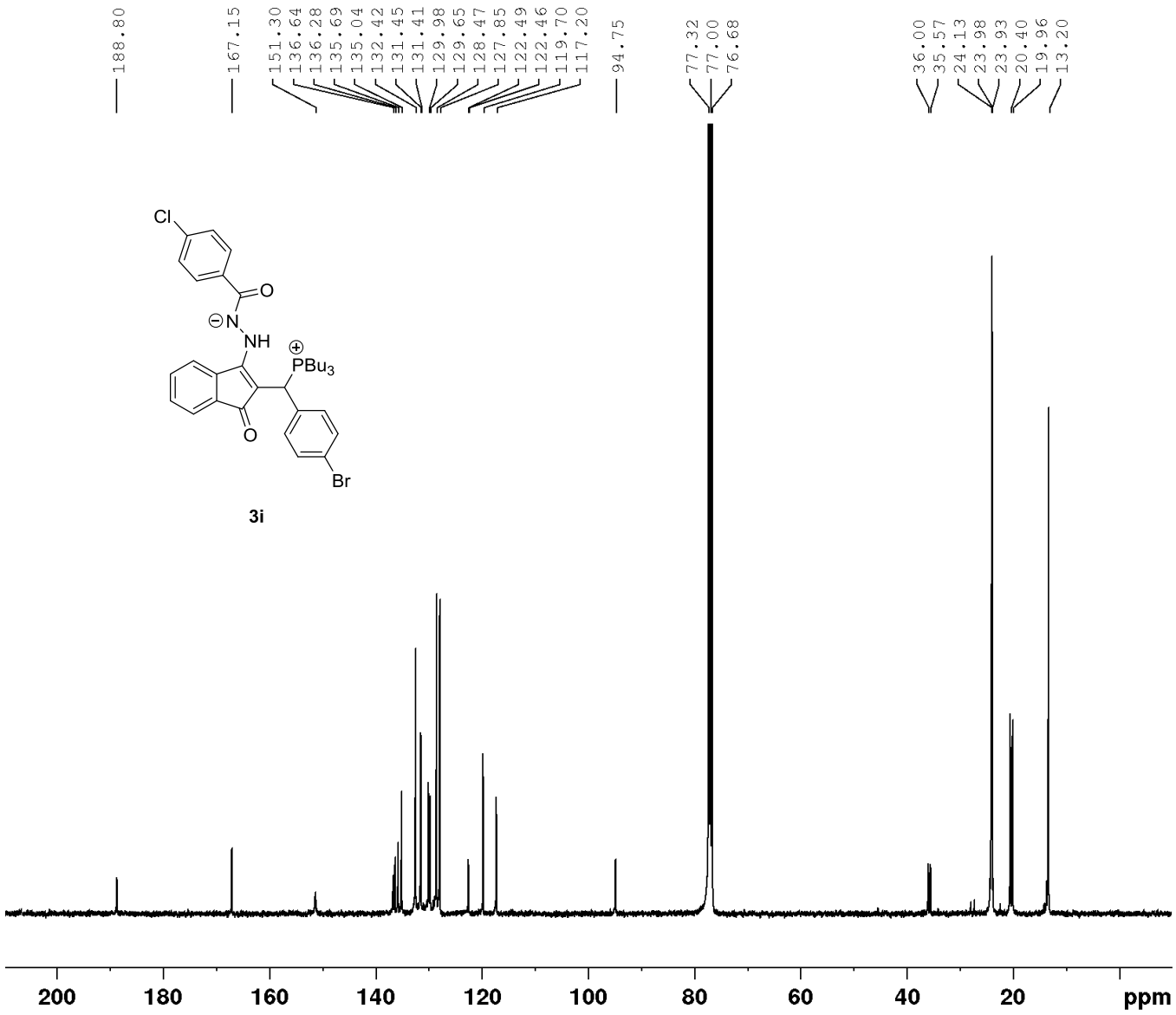

```
Current Data Parameters
NAME         SW ZW 2 OMe
EXPNO                  3
PROCNO                 1

F2 - Acquisition Parameters
Date_           20200614
Time               10.51
INSTRUM            spect
PROBHD   5 mm BBO BB-1H
PULPROG          zgpg30
TD                 65536
SOLVENT            CDCl3
NS                    32
DS                     0
SWH            64724.918 Hz
FIDRES          0.987624 Hz
AQ             0.5062656 sec
RG                  4096
DW                 7.725 usec
DE                 6.50 usec
TE                 298.1 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                 31P
P1                15.40 usec
PL1               10.90 dB
SFO1         161.9674942 MHz

======== CHANNEL f2 ========
CPDPRG[2          waltz16
NUC2                 1H
PCPD2             90.00 usec
PL2               10.20 dB
PL12              26.00 dB
PL13              29.00 dB
SFO2         400.1316005 MHz

F2 - Processing parameters
SI                 32768
SF           161.9755140 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.00
```

^{1}H NMR Spectrum of **3i** ($CDCl_3$, 400 MHz)



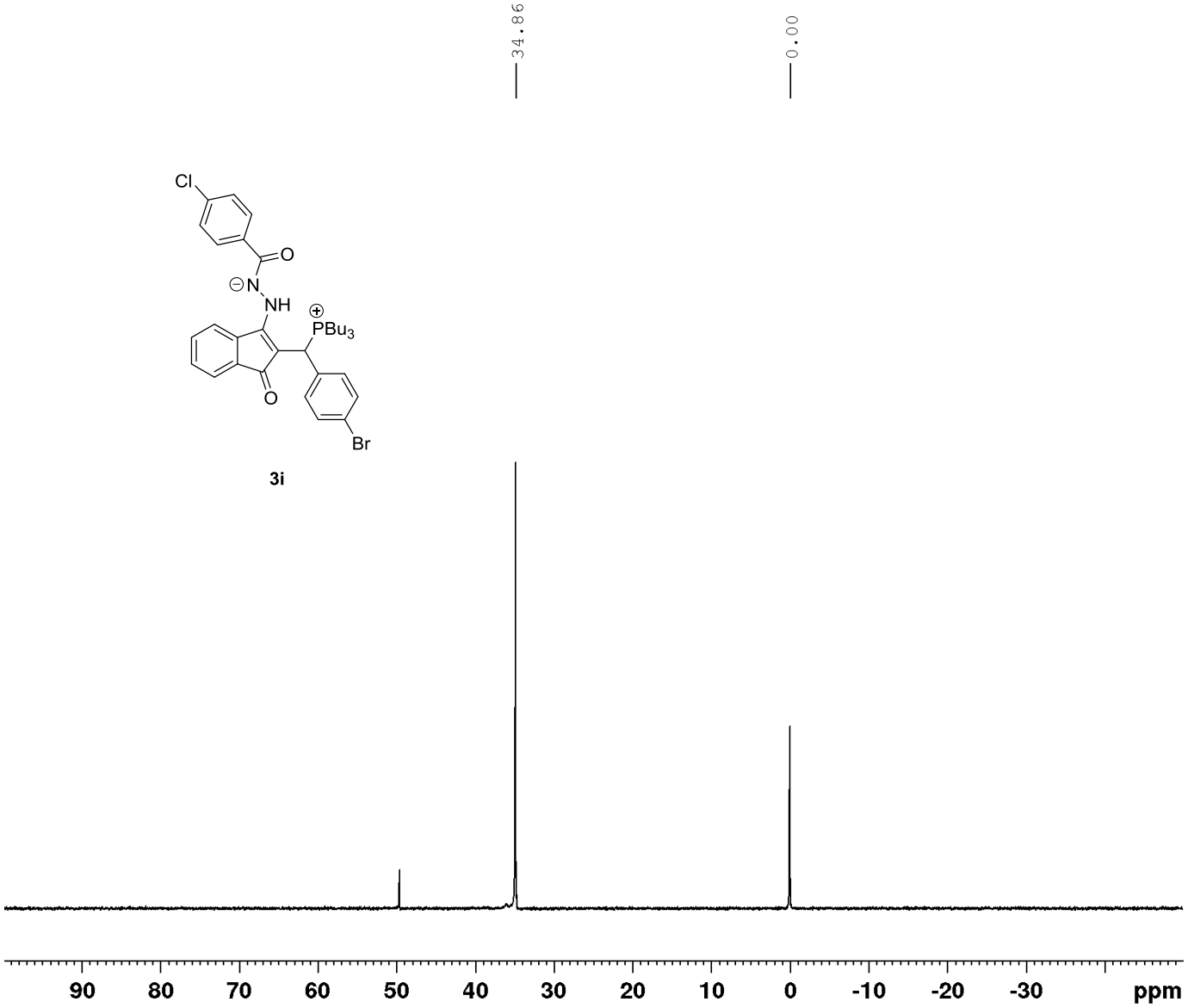

```
Current Data Parameters
NAME         SW ZW hy Cl
EXPNO                 1
PROCNO                1

F2 - Acquisition Parameters
Date_          20200531
Time               1.32
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG            zg30
TD                32768
SOLVENT           CDCl3
NS                   64
DS                    0
SWH            7211.539 Hz
FIDRES        0.220079 Hz
AQ            2.2719147 sec
RG                71.42
DW               69.333 usec
DE                10.06 usec
TE                293.9 K
D1            2.00000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1        400.1324008 MHz
NUC1                1H
P1                15.00 usec
PLW1        11.39999962 W

F2 - Processing parameters
SI                16384
SF          400.1300045 MHz
WDW                EM
SSB                 0
LB                  0 Hz
GB                  0
PC                1.00
```

^{13}C NMR Spectrum of **3i** ($CDCl_3$, 100 MHz)



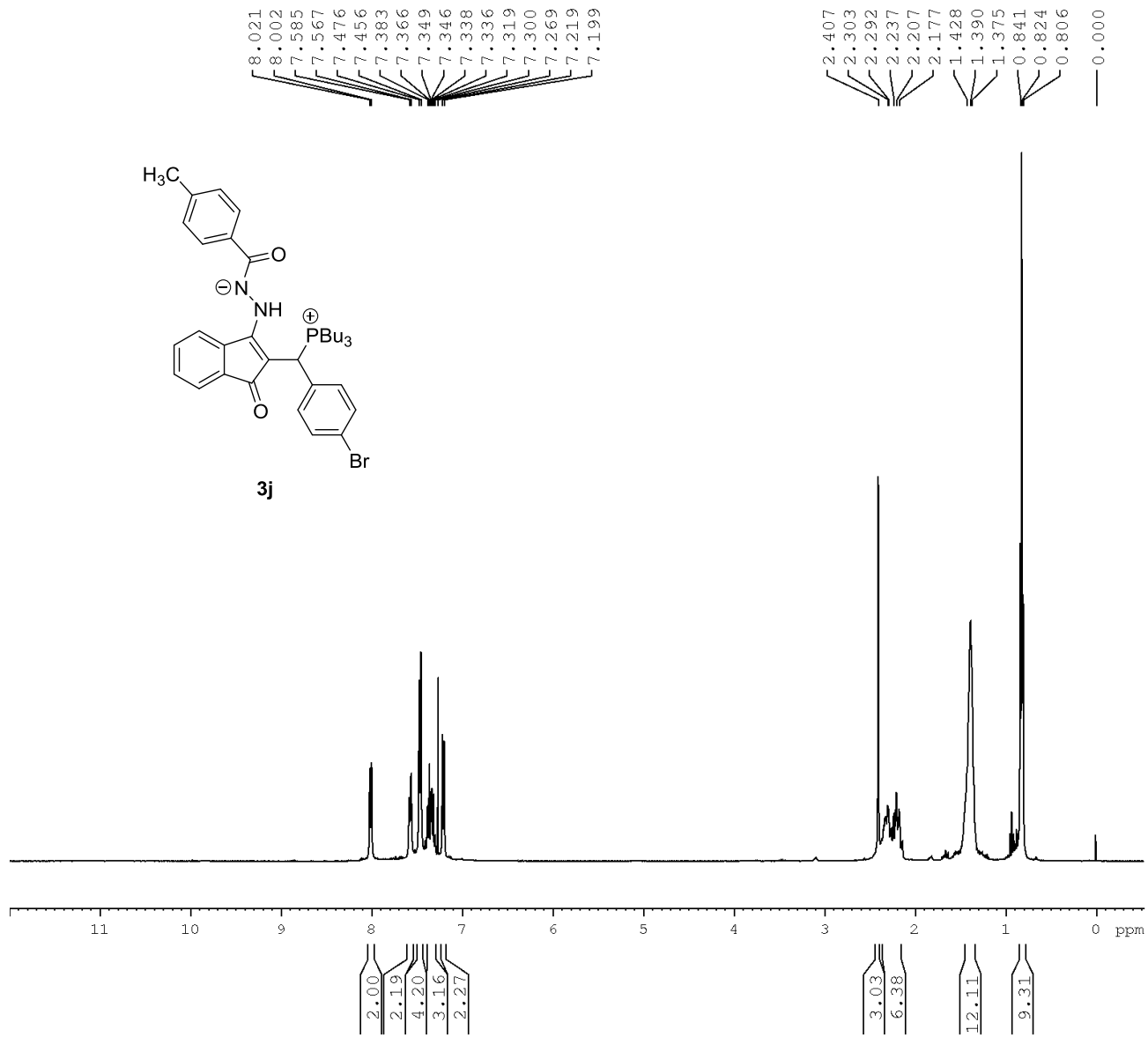

```
Current Data Parameters
NAME         SW ZW hy Cl
EXPNO                 2
PROCNO                1

F2 - Acquisition Parameters
Date_          20200531
Time               1.37
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG         zgpg30
TD                32768
SOLVENT           CDCl3
NS                15000
DS                    0
SWH           24038.461 Hz
FIDRES         0.733596 Hz
AQ            0.6815744 sec
RG               198.09
DW               20.800 usec
DE                6.50 usec
TE                293.8 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1        100.6228298 MHz
NUC1                13C
P1                10.00 usec
PLW1        49.50000000 W

======== CHANNEL f2 ========
SFO2        400.1316005 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2             90.00 usec
PLW2        12.50000000 W
PLW12        0.34722000 W
PLW13        0.28125000 W

F2 - Processing parameters
SI                32768
SF          100.6127723 MHz
WDW                  EM
SSB                   0
LB                 2.00 Hz
GB                    0
PC                 1.00
```

^{31}P NMR Spectrum of **3i** ($CDCl_3$, 162 MHz)



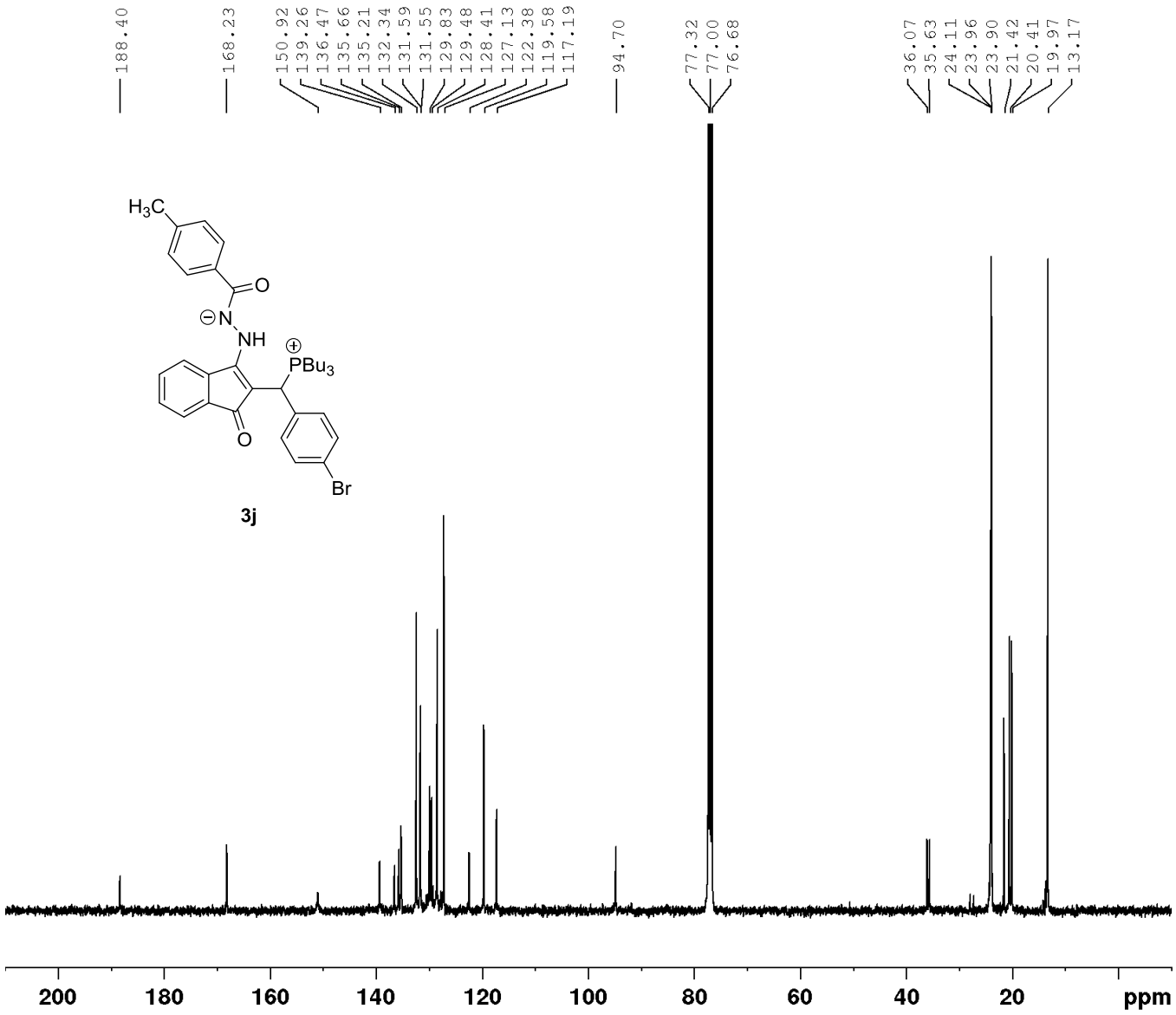

```
Current Data Parameters
NAME         SW ZW hy Cl
EXPNO                 3
PROCNO                1

F2 - Acquisition Parameters
Date_          20200601
Time              15.23
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG         zgpg30
TD                65536
SOLVENT           CDCl3
NS                   32
DS                    4
SWH           49019.609 Hz
FIDRES         0.747980 Hz
AQ            0.6684672 sec
RG               198.09
DW               10.200 usec
DE                6.50 usec
TE               292.7 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1        161.9836917 MHz
NUC1                31P
P1                15.00 usec
PLW1        13.19999981 W

======== CHANNEL f2 ========
SFO2        400.1316005 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2             90.00 usec
PLW2        12.50000000 W
PLW12        0.34722000 W
PLW13        0.28125000 W

F2 - Processing parameters
SI                32768
SF          161.9755132 MHz
WDW                  EM
SSB                   0
LB                 2.00 Hz
GB                    0
PC                 1.40
```

^{1}H NMR Spectrum of **3j** ($CDCl_3$, 400 MHz)



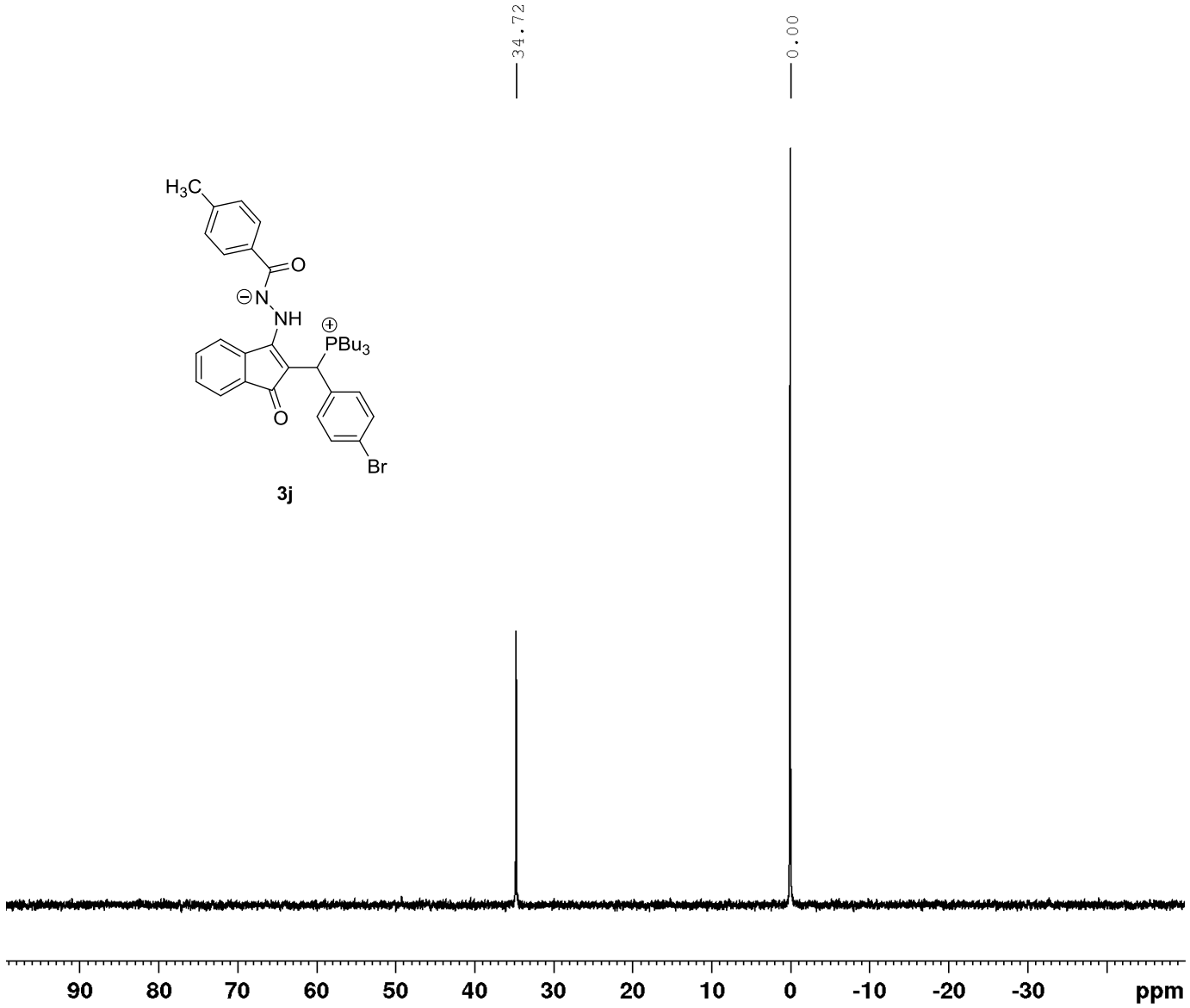

```
Current Data Parameters
NAME        SW ZW hy CH3
EXPNO                 1
PROCNO                1

F2 - Acquisition Parameters
Date_          20200530
Time              21.26
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG            zg30
TD                32768
SOLVENT           CDCl3
NS                   32
DS                    0
SWH            7211.539 Hz
FIDRES         0.220079 Hz
AQ            2.2719147 sec
RG                71.42
DW               69.333 usec
DE                10.06 usec
TE                298.0 K
D1           2.00000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1        400.1324008 MHz
NUC1                1H
P1                15.00 usec
PLW1        11.39999962 W

F2 - Processing parameters
SI                16384
SF          400.1300061 MHz
WDW                 EM
SSB                  0
LB                   0 Hz
GB                   0
PC                1.00
```

^{13}C NMR Spectrum of **3j** ($CDCl_3$, 100 MHz)



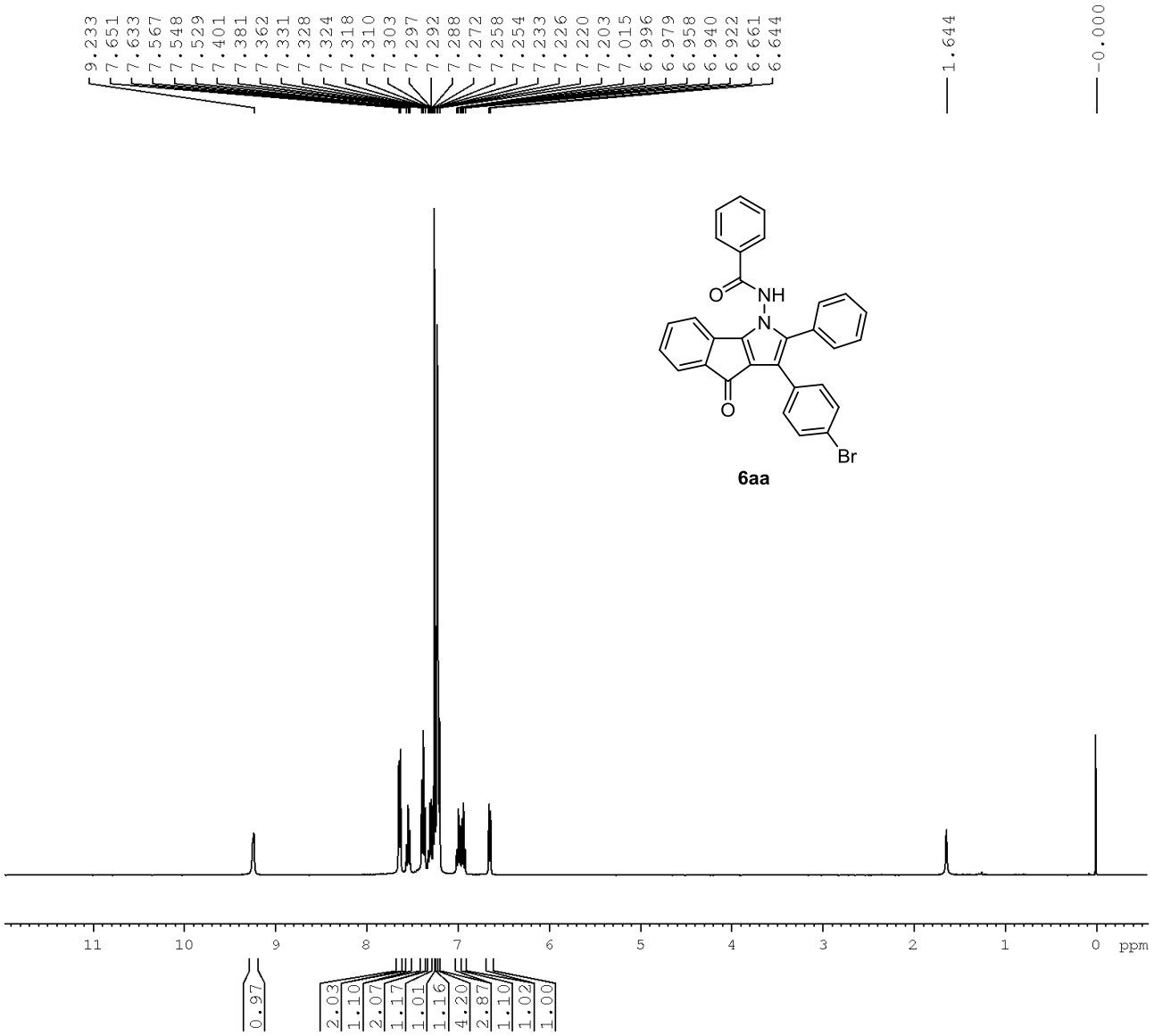

```
Current Data Parameters
NAME        SW ZW hy CH3
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20200530
Time               21.29
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                32768
SOLVENT           CDCl3
NS                 5199
DS                    0
SWH           24038.461 Hz
FIDRES         0.733596 Hz
AQ            0.6815744 sec
RG               198.09
DW               20.800 usec
DE                6.50 usec
TE                298.1 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1         100.6228298 MHz
NUC1                13C
P1                10.00 usec
PLW1         49.50000000 W

======== CHANNEL f2 ========
SFO2         400.1316005 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2             90.00 usec
PLW2         12.50000000 W
PLW12         0.34722000 W
PLW13         0.28125000 W

F2 - Processing parameters
SI                 32768
SF           100.6127727 MHz
WDW                  EM
SSB                   0
LB                 2.00 Hz
GB                    0
PC                 1.00
```

^{31}P NMR Spectrum of **3j** ($CDCl_3$, 162 MHz)



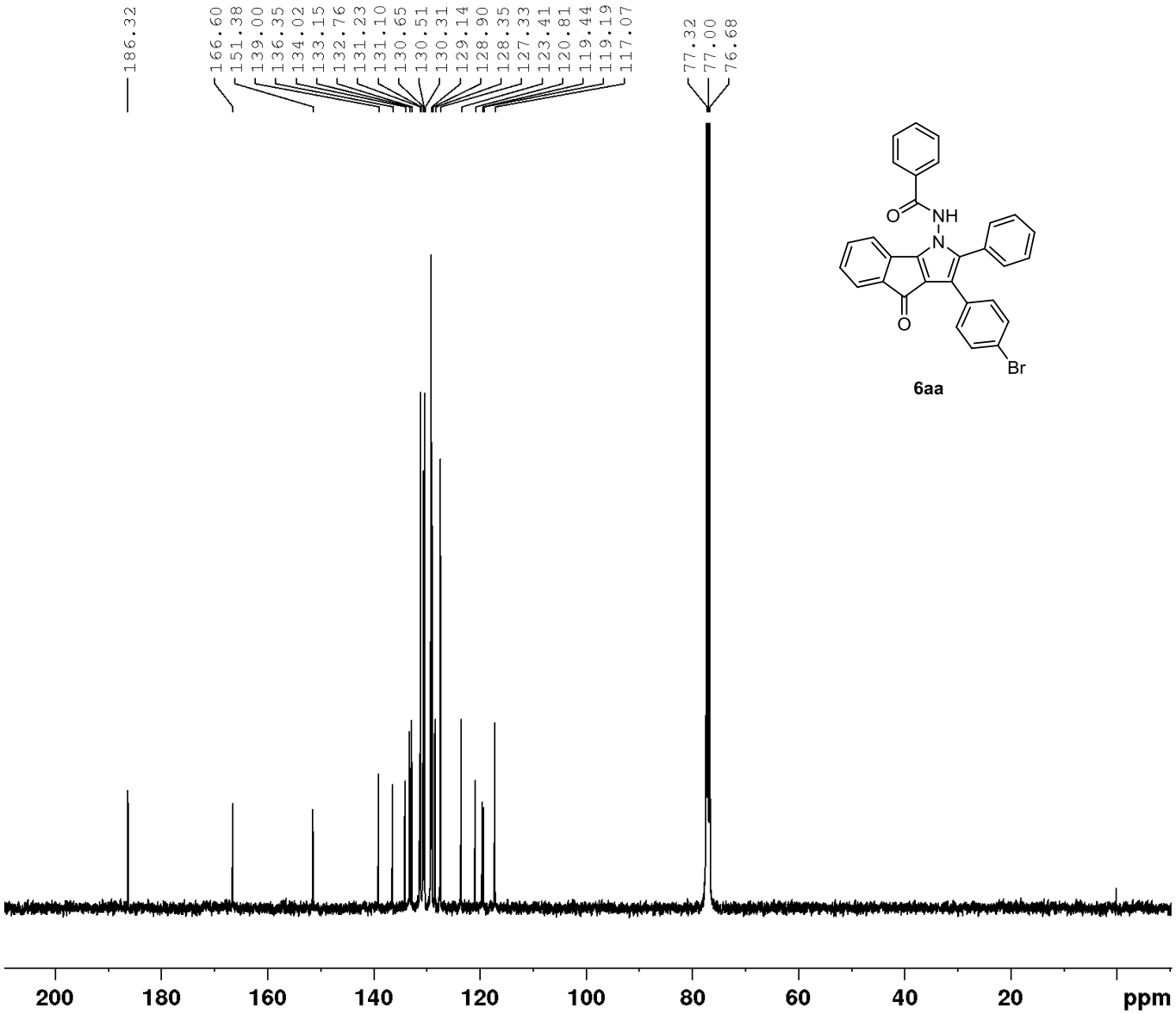

```
Current Data Parameters
NAME        SW ZW hy CH3
EXPNO                 5
PROCNO                1

F2 - Acquisition Parameters
Date_          20200601
Time              16.59
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG         zgpg30
TD                65536
SOLVENT           CDCl3
NS                   32
DS                    4
SWH           49019.609 Hz
FIDRES         0.747980 Hz
AQ            0.6684672 sec
RG               198.09
DW               10.200 usec
DE                6.50 usec
TE               296.2 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1        161.9836917 MHz
NUC1                31P
P1                15.00 usec
PLW1        13.19999981 W

======== CHANNEL f2 ========
SFO2        400.1316005 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2             90.00 usec
PLW2        12.50000000 W
PLW12        0.34722000 W
PLW13        0.28125000 W

F2 - Processing parameters
SI                32768
SF          161.9755126 MHz
WDW                  EM
SSB                   0
LB                 2.00 Hz
GB                    0
PC                 1.40
```

^{1}H NMR Spectrum of **6aa** ($CDCl_3$, 400 MHz)




```
Current Data Parameters
NAME      SW-bc Ph Zi 4Br
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20200523
Time               18.20
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG             zg30
TD                 32768
SOLVENT            CDCl3
NS                    32
DS                     0
SWH             7211.539 Hz
FIDRES          0.220079 Hz
AQ             2.2719147 sec
RG                177.16
DW                69.333 usec
DE                10.06 usec
TE                298.0 K
D1           2.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         400.1324008 MHz
NUC1                   1H
P1                 15.00 usec
PLW1         11.39999962 W

F2 - Processing parameters
SI                 16384
SF           400.1300105 MHz
WDW                   EM
SSB                    0
LB                     0 Hz
GB                     0
PC                  1.00
```

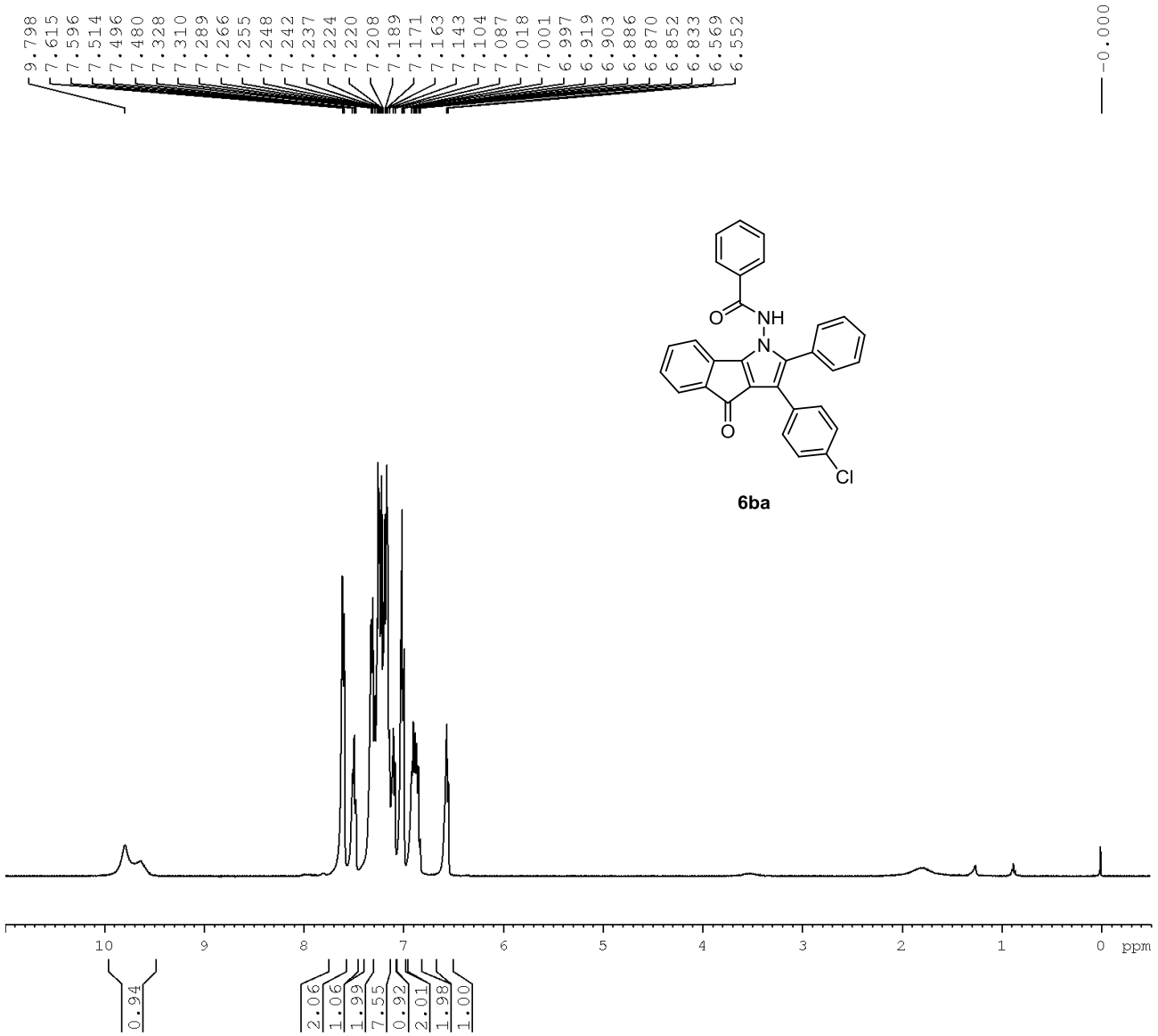
^{13}C NMR Spectrum of **6aa** ($CDCl_3$, 100 MHz)



6aa

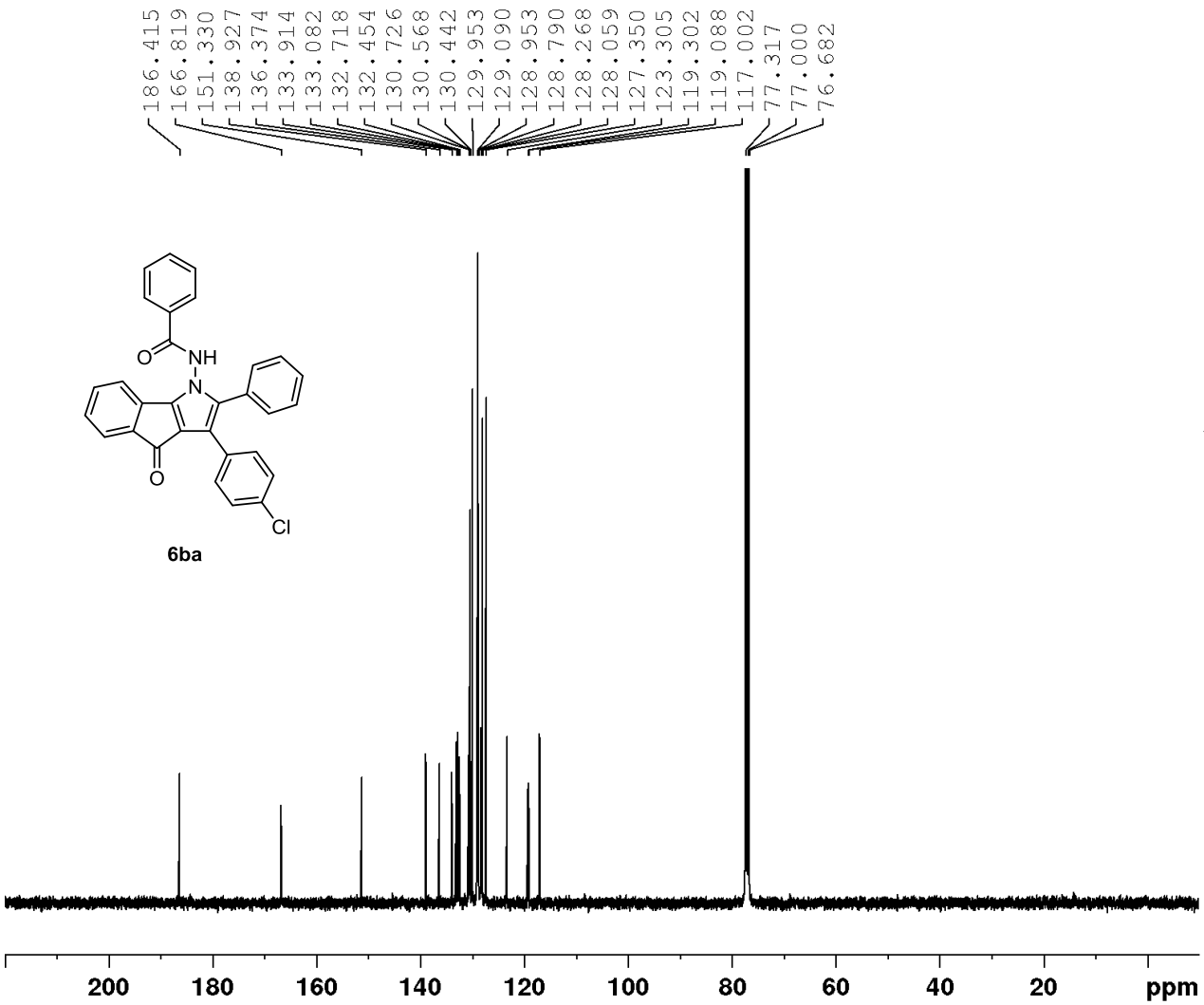
```
Current Data Parameters
NAME      SW-bc Ph Zi 4Br
EXPNO                  3
PROCNO                 1

F2 - Acquisition Parameters
Date_           20200523
Time              18.23
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG         zgpg30
TD              32768
SOLVENT          CDCl3
NS                4171
DS                   0
SWH          24038.461 Hz
FIDRES        0.733596 Hz
AQ           0.6815744 sec
RG              198.09
DW              20.800 usec
DE               6.50 usec
TE              298.0 K
D1          2.00000000 sec
D11         0.03000000 sec
TD0                  1

======== CHANNEL f1 ========
SFO1        100.6228298 MHz
NUC1               13C
P1               10.00 usec
PLW1        49.50000000 W

======== CHANNEL f2 ========
SFO2        400.1316005 MHz
NUC2               1H
CPDPRG[2        waltz16
PCPD2            90.00 usec
PLW2        12.50000000 W
PLW12        0.34722000 W
PLW13        0.28125000 W

F2 - Processing parameters
SI                32768
SF          100.6127708 MHz
WDW                EM
SSB                 0
LB               2.00 Hz
GB                  0
PC               1.00
```

^{1}H NMR Spectrum of **6ba** ($CDCl_3$, 400 MHz)



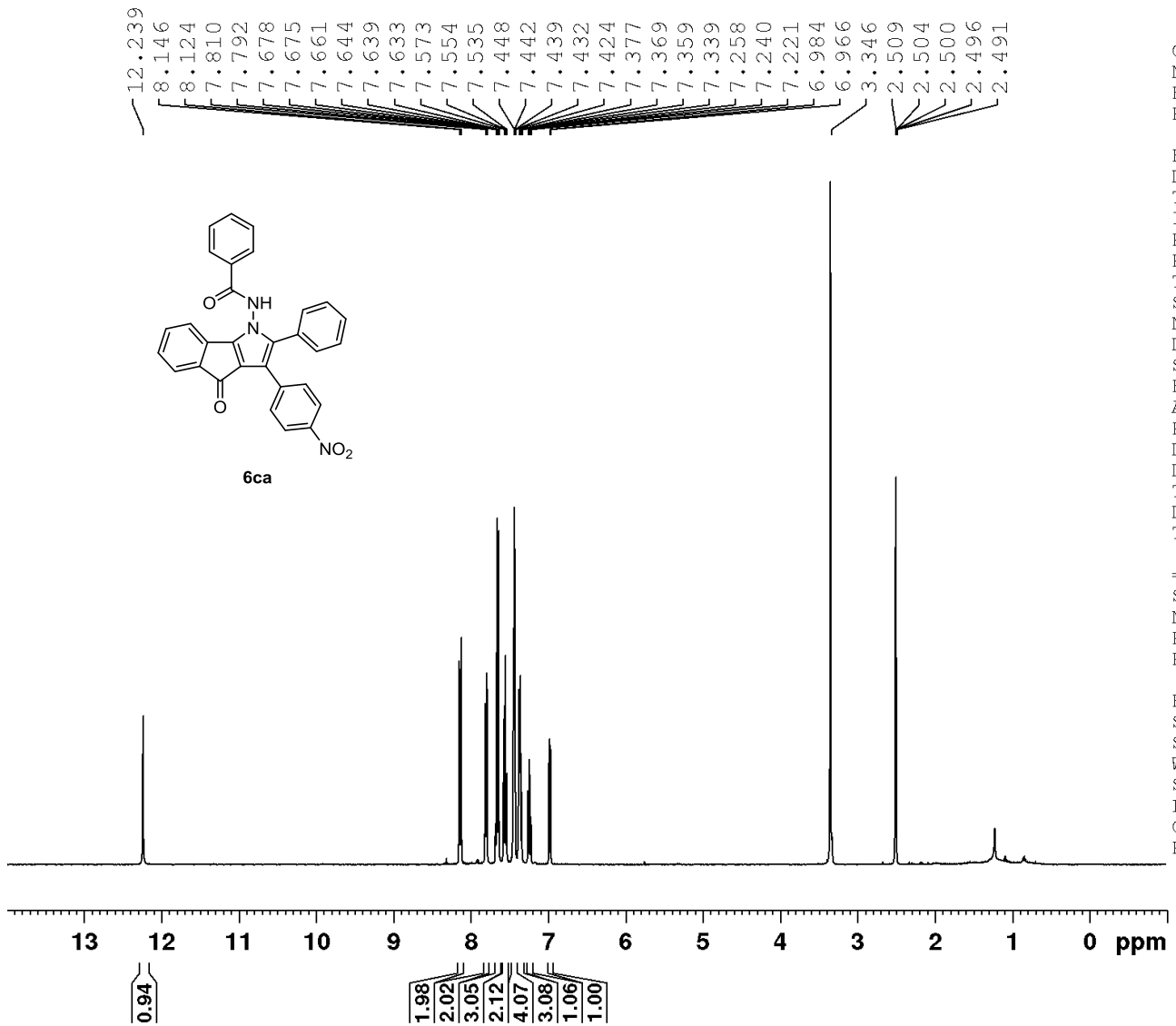

```
Current Data Parameters
NAME          SW Zi 4-Cl
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20200325
Time               21.55
INSTRUM            spect
PROBHD   5 mm BBO BB-1H
PULPROG             zg30
TD                 32768
SOLVENT            CDCl3
NS                    32
DS                     0
SWH             7246.377 Hz
FIDRES          0.221142 Hz
AQ              2.2609921 sec
RG                   114
DW                69.000 usec
DE                 6.50 usec
TE                295.6 K
D1             2.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                15.00 usec
PL1               11.10 dB
SFO1         400.1324008 MHz

F2 - Processing parameters
SI                 16384
SF           400.1300106 MHz
WDW                   EM
SSB                    0
LB                     0 Hz
GB                     0
PC                  1.00
```

^{13}C NMR Spectrum of **6ba** ($CDCl_3$, 100 MHz)



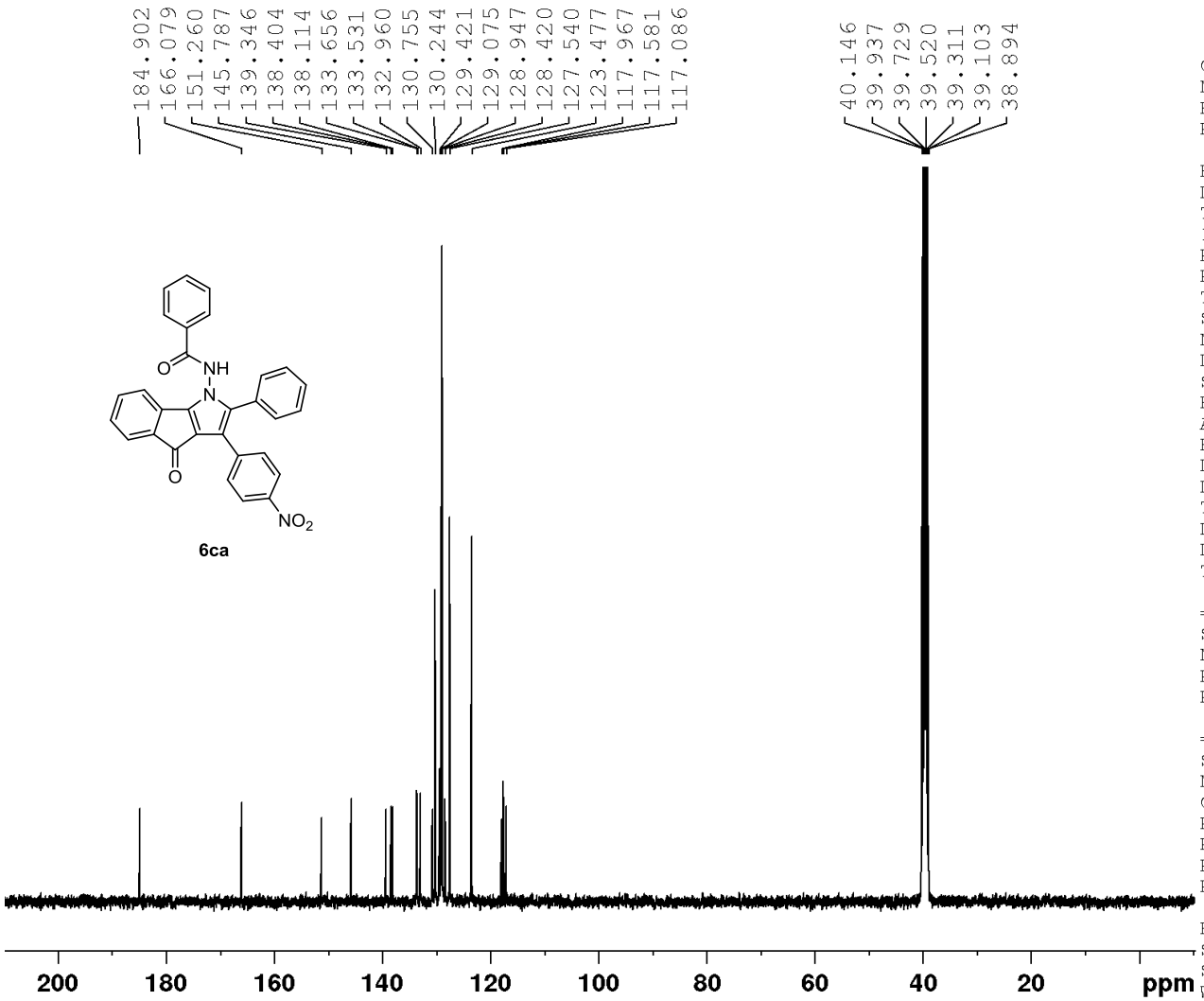

```
Current Data Parameters
NAME          SW Zi 4-Cl
EXPNO                  3
PROCNO                 1

F2 - Acquisition Parameters
Date_           20200325
Time               21.58
INSTRUM            spect
PROBHD   5 mm BBO BB-1H
PULPROG          zgpg30
TD                32768
SOLVENT           CDCl3
NS                 3483
DS                    0
SWH           24038.461 Hz
FIDRES         0.733596 Hz
AQ            0.6815744 sec
RG               5792.6
DW                20.800 usec
DE                 6.50 usec
TE                295.5 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 13C
P1                10.00 usec
PL1                3.80 dB
SFO1        100.6233325 MHz

======== CHANNEL f2 ========
CPDPRG[2         waltz16
NUC2                 1H
PCPD2             90.00 usec
PL2               10.20 dB
PL12              26.00 dB
PL13              29.00 dB
SFO2        400.1316005 MHz

F2 - Processing parameters
SI                32768
SF          100.6127728 MHz
WDW                  EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.00
```

^{1}H NMR Spectrum of **6ca** (DMSO-d_6, 400 MHz)



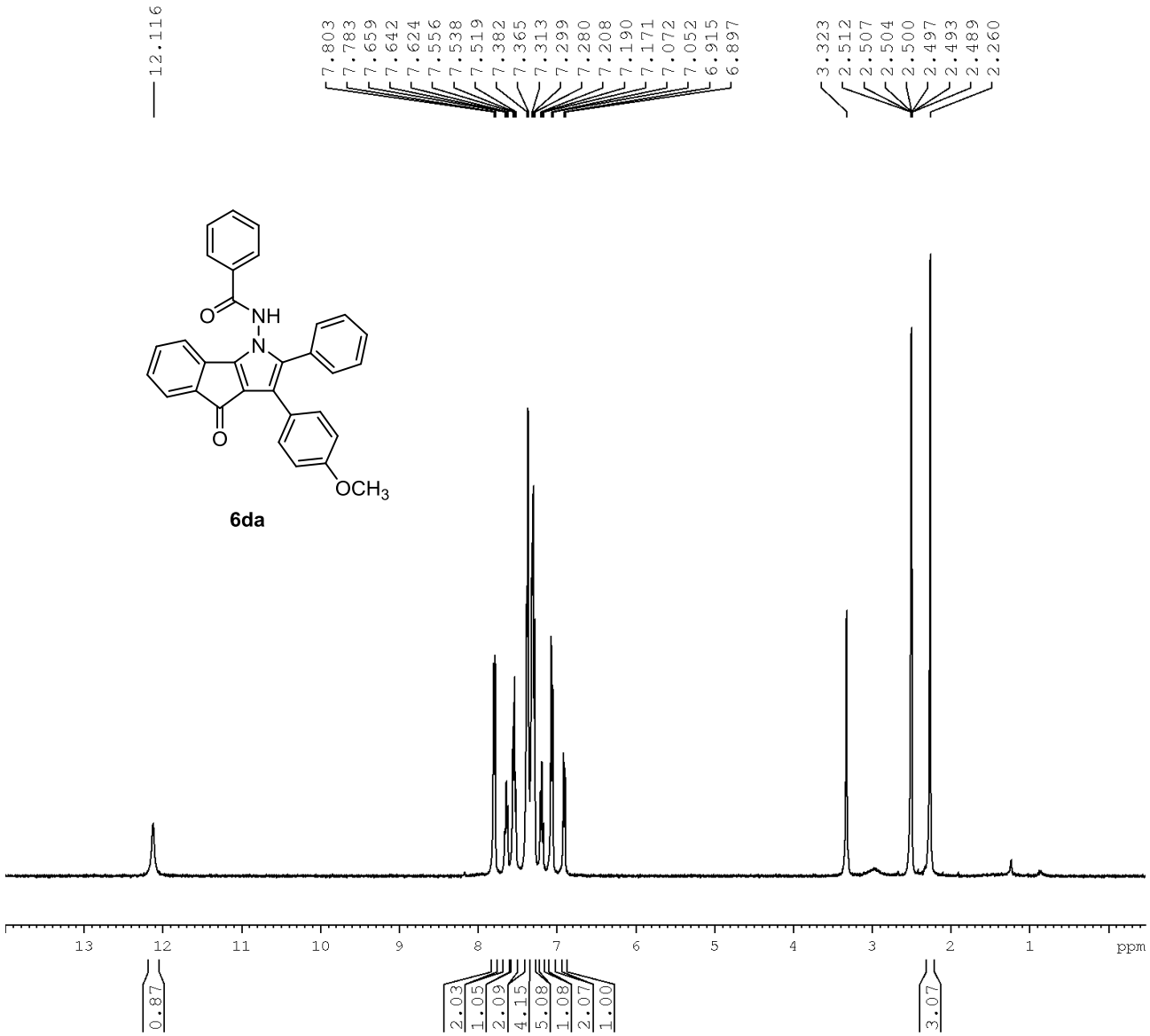

```
Current Data Parameters
NAME            zi 4-NO2
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20200222
Time               16.11
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG             zg30
TD                 32768
SOLVENT             DMSO
NS                    16
DS                     0
SWH             7211.539 Hz
FIDRES          0.220079 Hz
AQ             2.2719147 sec
RG                 89.08
DW                69.333 usec
DE                10.06 usec
TE                296.2 K
D1             2.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         400.1324008 MHz
NUC1                   1H
P1                 15.00 usec
PLW1         11.39999962 W

F2 - Processing parameters
SI                 16384
SF           400.1300031 MHz
WDW                   EM
SSB       0
LB        0 Hz
GB        0
PC                  1.00
```

^{13}C NMR Spectrum of **6ca** (DMSO-d_6, 100 MHz)



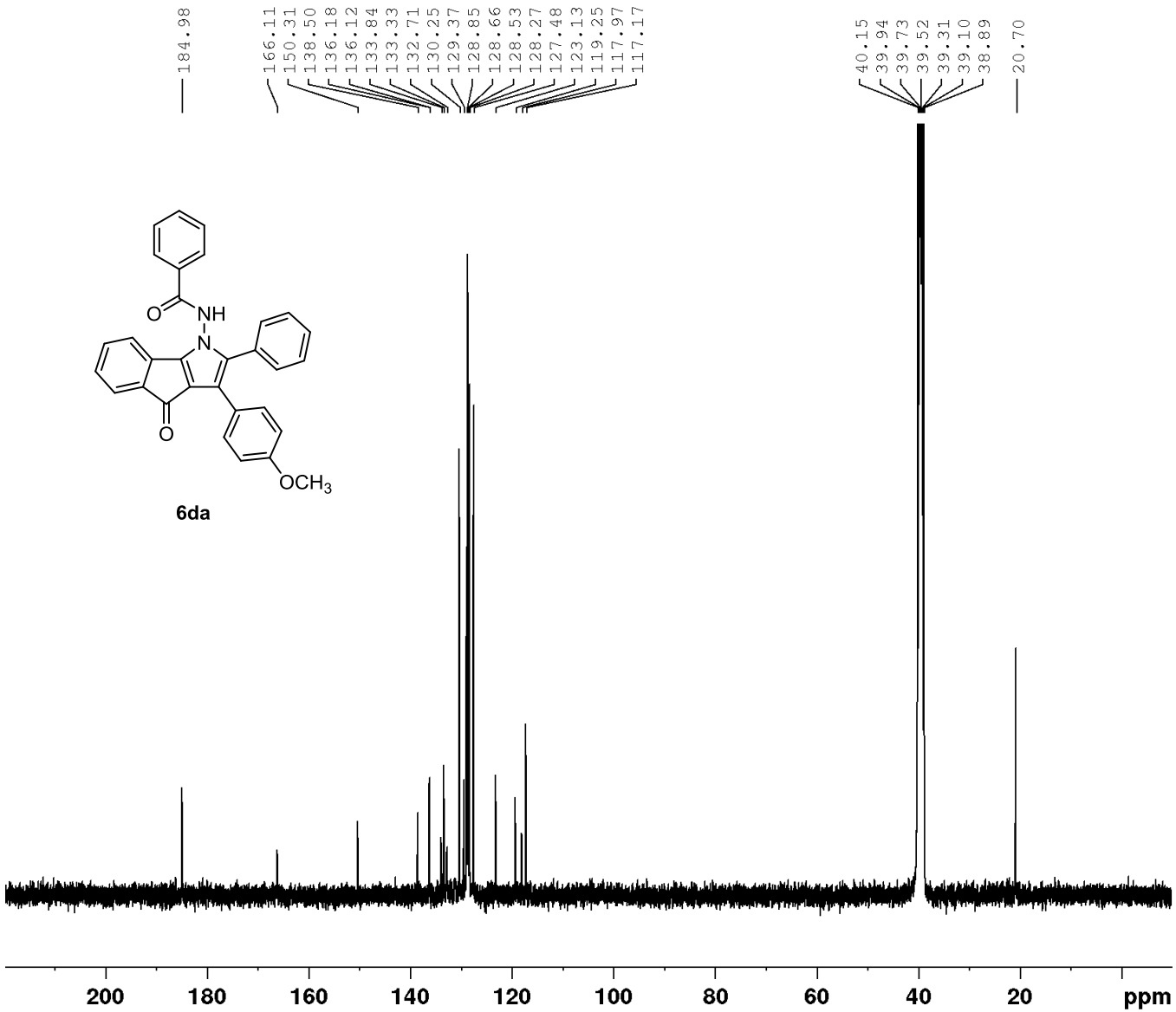

```
Current Data Parameters
NAME            zi 4-NO2
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20200222
Time               16.12
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                 32768
SOLVENT             DMSO
NS                  1174
DS                     0
SWH           24038.461 Hz
FIDRES         0.733596 Hz
AQ            0.6815744 sec
RG               198.09
DW               20.800 usec
DE                6.50 usec
TE               296.6 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1        100.6228298 MHz
NUC1                13C
P1                10.00 usec
PLW1         49.50000000 W

======== CHANNEL f2 ========
SFO2        400.1316005 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2             90.00 usec
PLW2         12.50000000 W
PLW12         0.34722000 W
PLW13         0.28125000 W

F2 - Processing parameters
SI                 32768
SF          100.6128172 MHz
WDW                   EM
SSB       0
LB                 2.00 Hz
GB        0
PC                 1.00
```

^{1}H NMR Spectrum of **6da** (DMSO-d_6, 400 MHz)



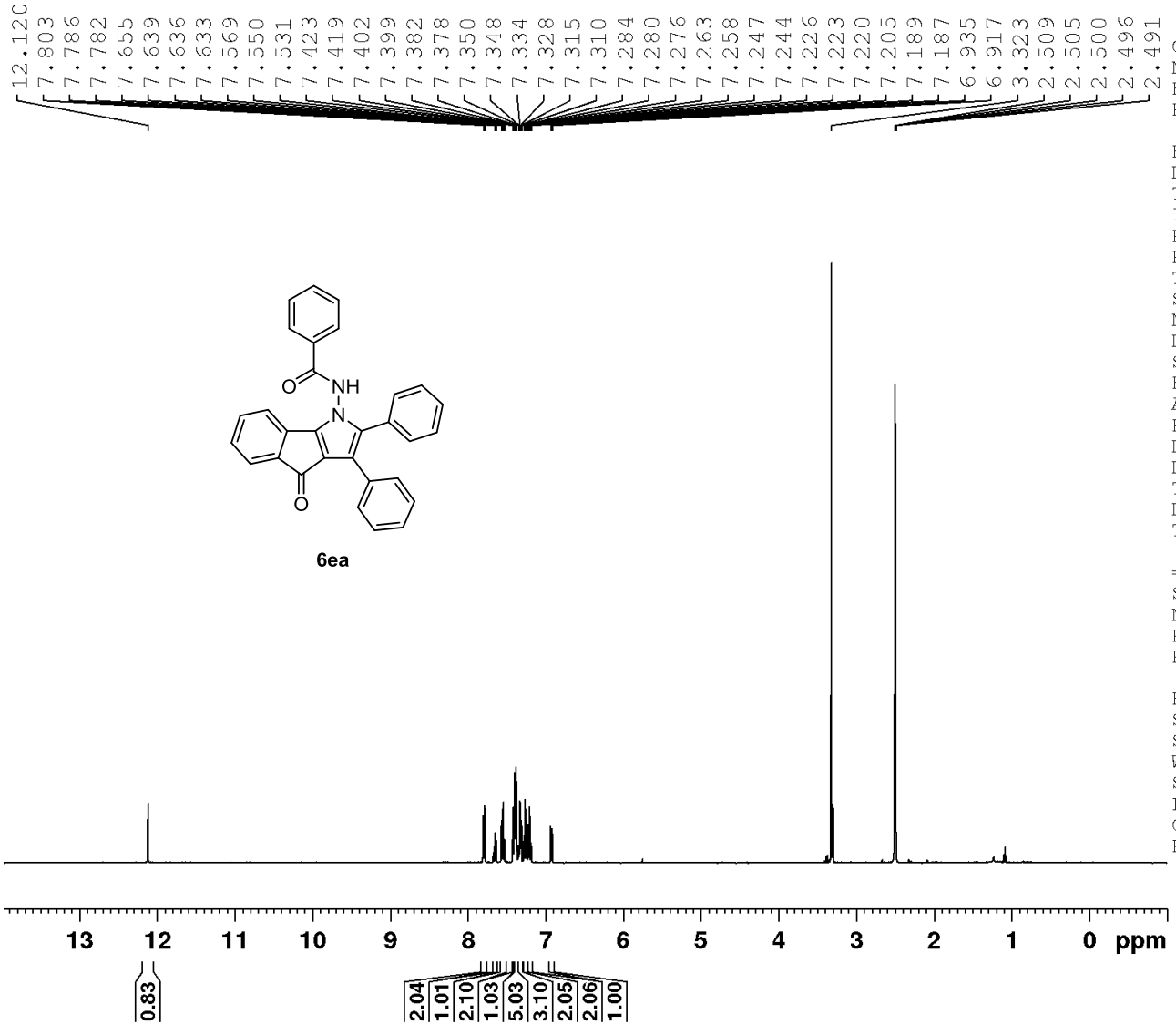

```
Current Data Parameters
NAME         SW Zi 4-OMe
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20200502
Time               22.09
INSTRUM            spect
PROBHD   5 mm BBO BB-1H
PULPROG             zg30
TD                 32768
SOLVENT             DMSO
NS                    32
DS                     0
SWH             7246.377 Hz
FIDRES          0.221142 Hz
AQ             2.2609921 sec
RG                   362
DW                69.000 usec
DE                 6.50 usec
TE                296.8 K
D1           2.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                15.00 usec
PL1               11.10 dB
SFO1         400.1324008 MHz

F2 - Processing parameters
SI                 16384
SF           400.1300067 MHz
WDW                   EM
SSB                    0
LB                     0 Hz
GB                     0
PC                  1.00
```

^{13}C NMR Spectrum of **6da** (DMSO-d_6, 100 MHz)



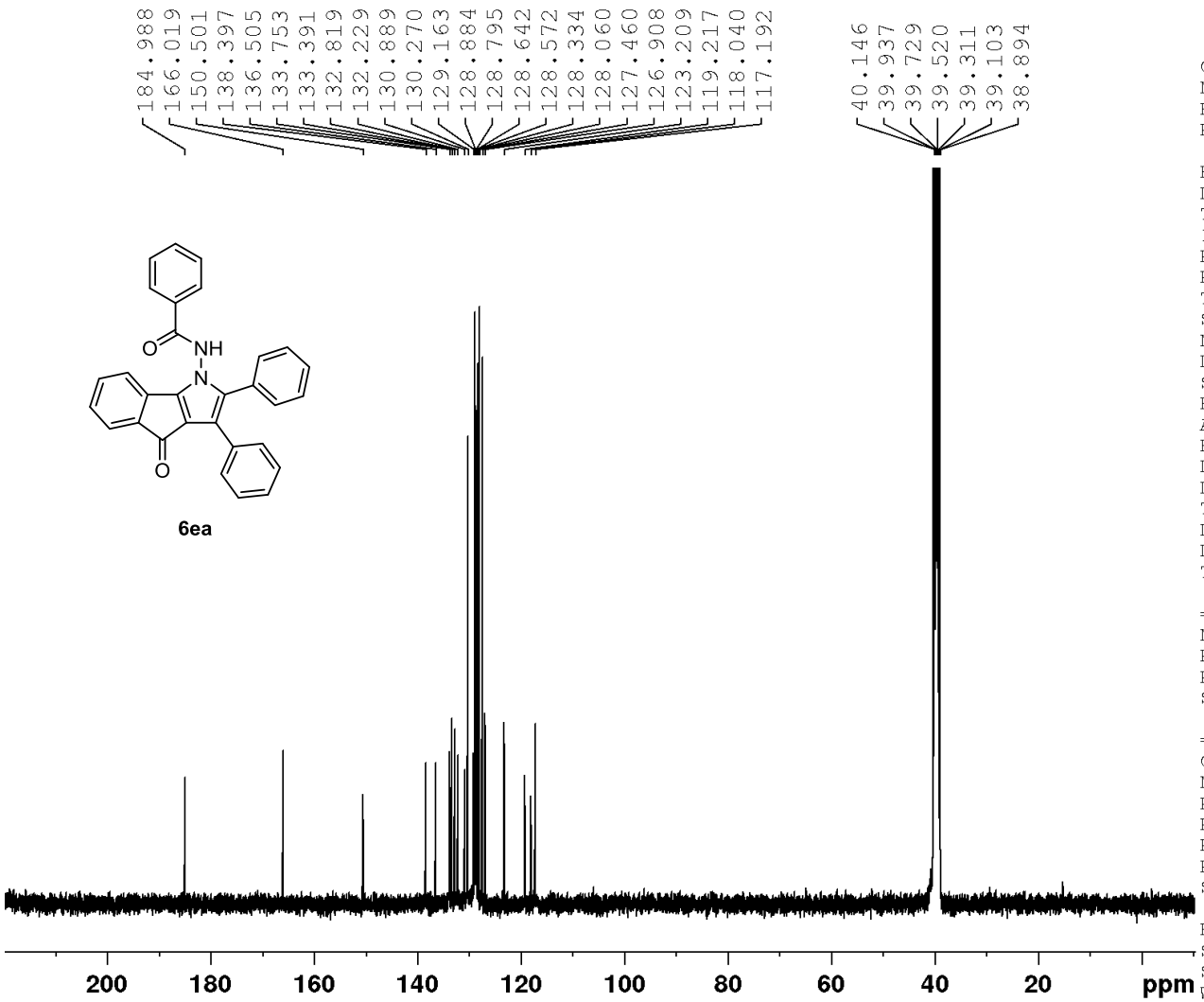

```
Current Data Parameters
NAME         SW Zi 4-OMe
EXPNO                  3
PROCNO                 1

F2 - Acquisition Parameters
Date_           20200502
Time               22.12
INSTRUM            spect
PROBHD   5 mm BBO BB-1H
PULPROG          zgpg30
TD                 32768
SOLVENT             DMSO
NS                 23910
DS                     0
SWH           24038.461 Hz
FIDRES         0.733596 Hz
AQ            0.6815744 sec
RG               9195.2
DW                20.800 usec
DE                 6.50 usec
TE                296.7 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  13C
P1                 10.00 usec
PL1                 3.80 dB
SFO1         100.6233325 MHz

======== CHANNEL f2 ========
CPDPRG[2          waltz16
NUC2                  1H
PCPD2              90.00 usec
PL2                10.20 dB
PL12               26.00 dB
PL13               29.00 dB
SFO2         400.1316005 MHz

F2 - Processing parameters
SI                 32768
SF           100.6128205 MHz
WDW                   EM
SSB                    0
LB                 1.00 Hz
GB                     0
PC                 1.00
```

^{1}H NMR Spectrum of **6ea** (DMSO-d_6, 400 MHz)



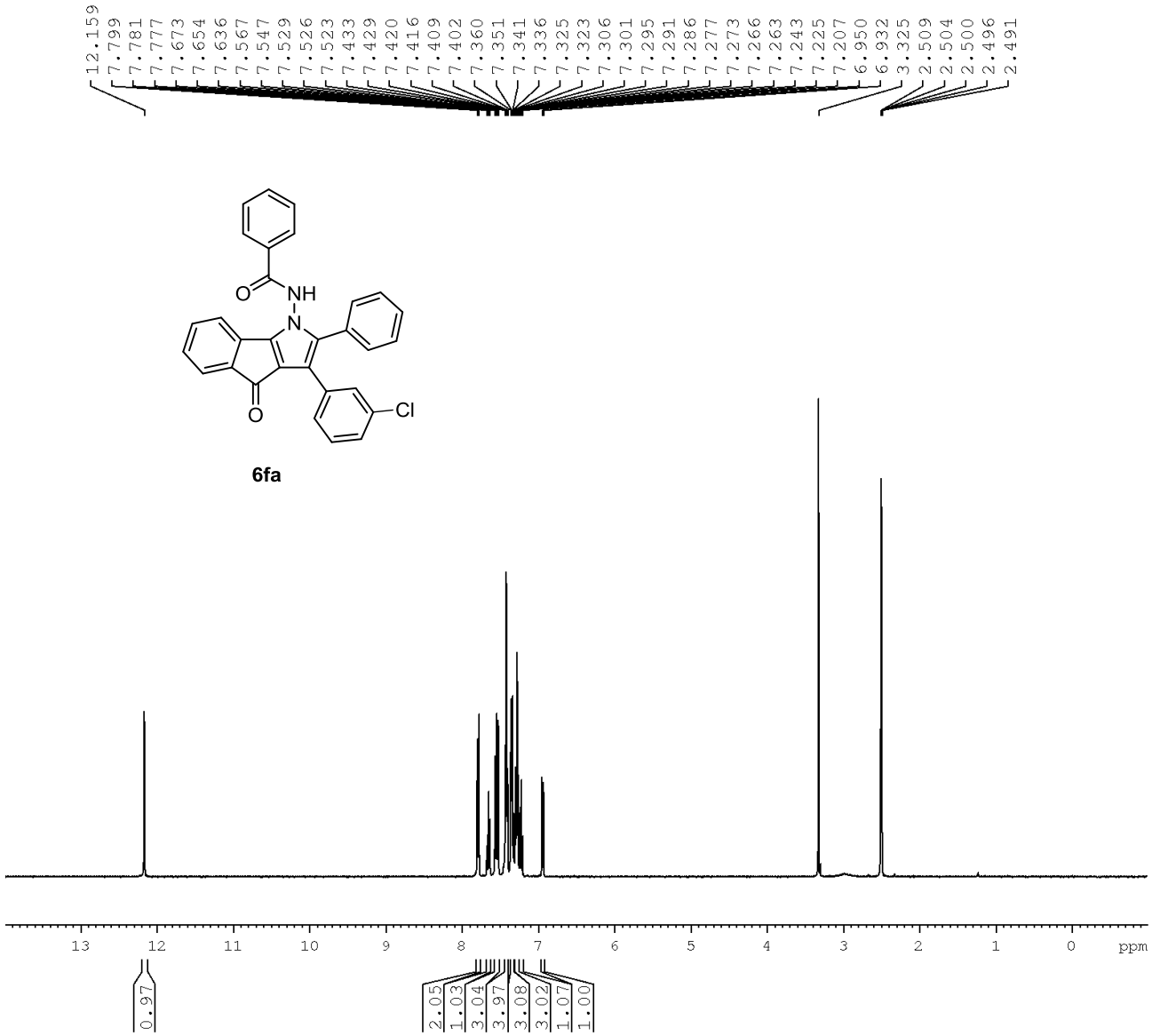

```
Current Data Parameters
NAME      Zi Non sub iso
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20200221
Time               21.10
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG             zg30
TD                 32768
SOLVENT             DMSO
NS                    16
DS                     0
SWH             7211.539 Hz
FIDRES          0.220079 Hz
AQ             2.2719147 sec
RG                198.09
DW                69.333 usec
DE                10.06 usec
TE                297.5 K
D1           2.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         400.1324008 MHz
NUC1                   1H
P1                 15.00 usec
PLW1         11.39999962 W

F2 - Processing parameters
SI                 16384
SF           400.1300031 MHz
WDW                   EM
SSB       0
LB        0 Hz
GB        0
PC                  1.00
```

^{13}C NMR Spectrum of **6ea** (DMSO-d_6, 100 MHz)



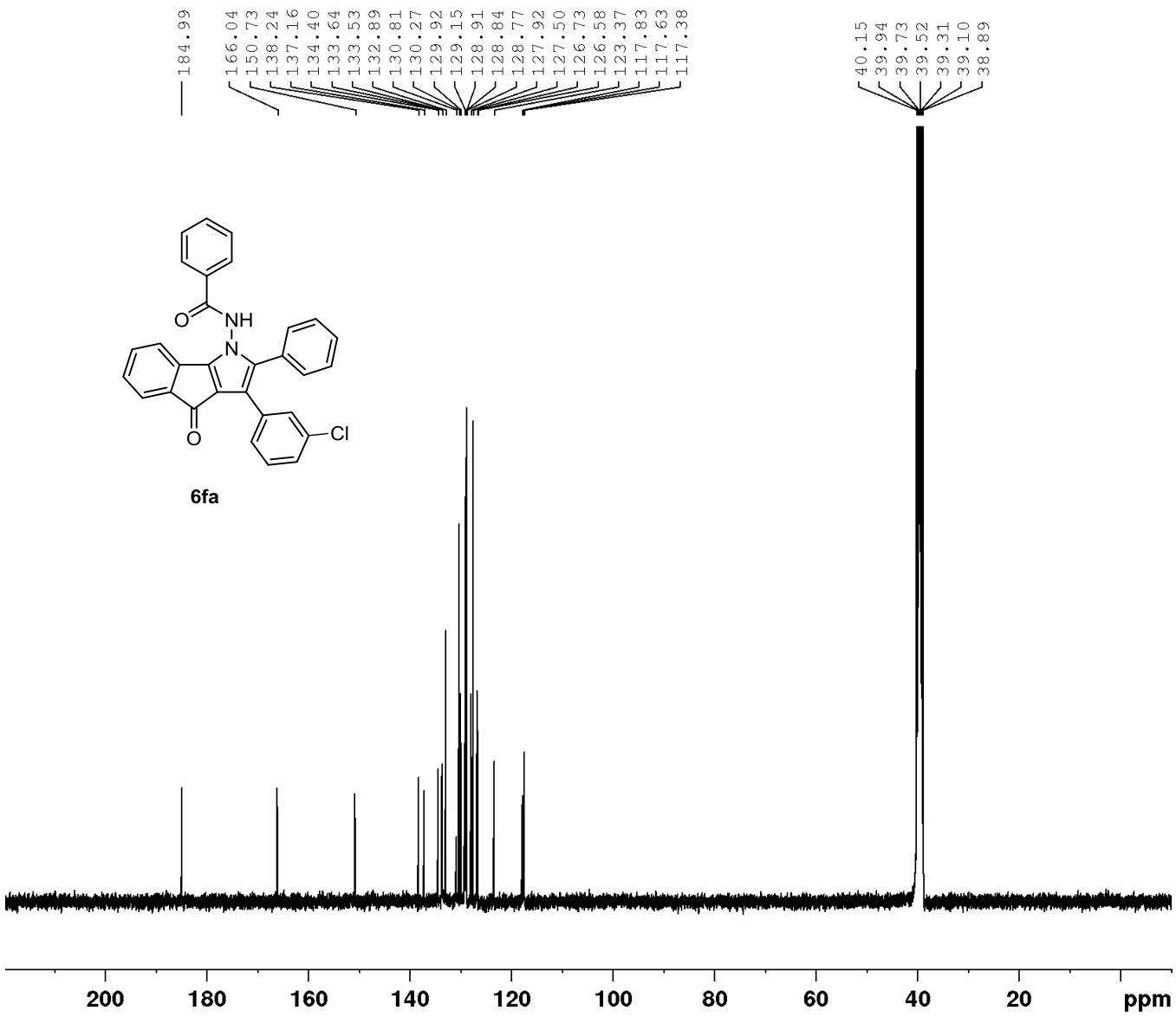

```
Current Data Parameters
NAME       SW Zi non sbu
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20200302
Time               23.22
INSTRUM            spect
PROBHD   5 mm BBO BB-1H
PULPROG          zgpg30
TD                32768
SOLVENT            DMSO
NS                12000
DS                    0
SWH           24038.461 Hz
FIDRES         0.733596 Hz
AQ             0.6815744 sec
RG                 8192
DW                20.800 usec
DE                 6.50 usec
TE                299.9 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 13C
P1                10.00 usec
PL1                3.80 dB
SFO1        100.6233325 MHz

======== CHANNEL f2 ========
CPDPRG[2         waltz16
NUC2                 1H
PCPD2             90.00 usec
PL2               10.20 dB
PL12              26.00 dB
PL13              29.00 dB
SFO2        400.1316005 MHz

F2 - Processing parameters
SI                32768
SF          100.6128208 MHz
WDW                  EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.00
```

^{1}H NMR Spectrum of **6fa** (DMSO-d_6, 400 MHz)



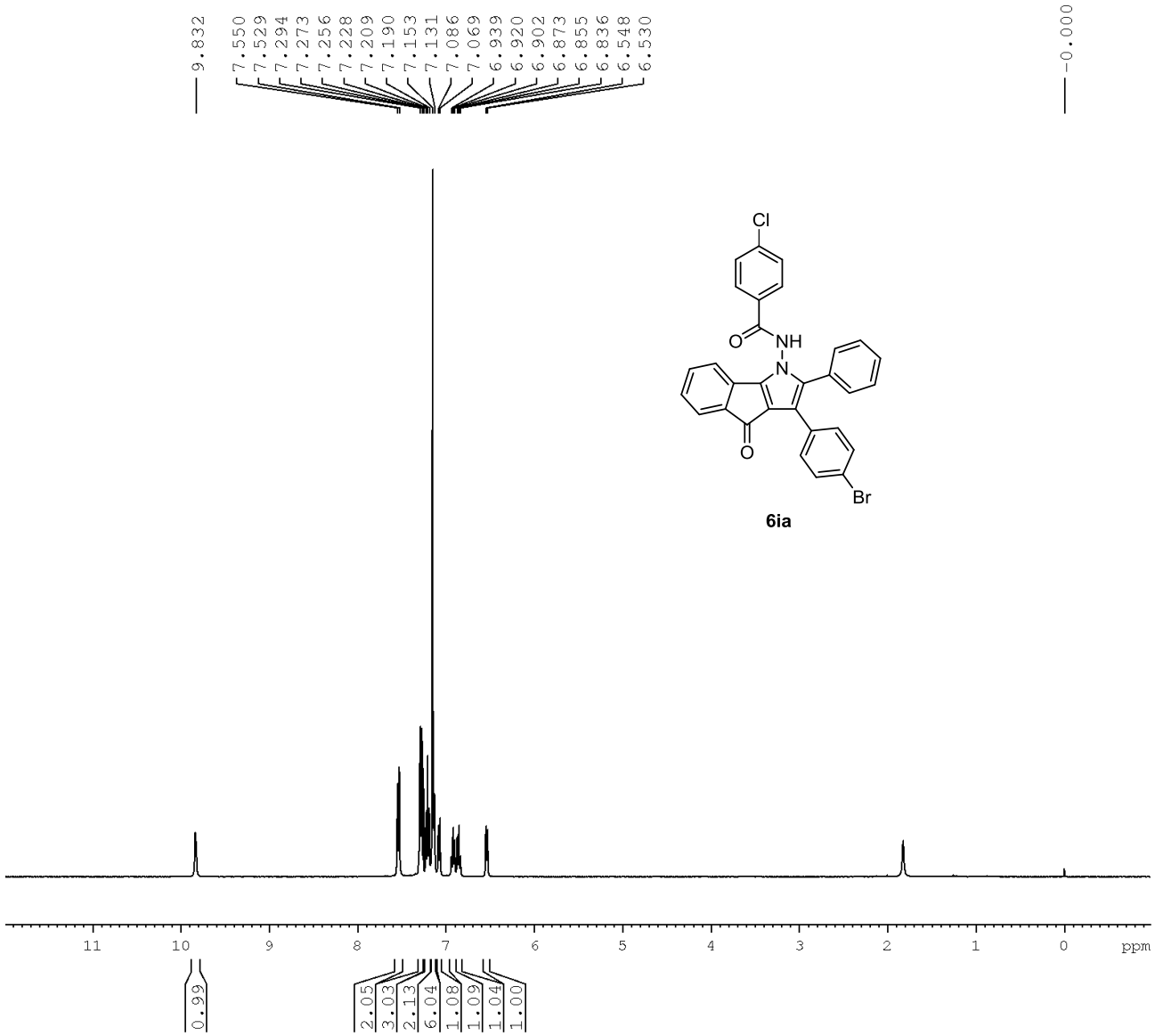

```
Current Data Parameters
NAME          SW Zi 3-Cl
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20200608
Time               23.13
INSTRUM            spect
PROBHD   5 mm BBO BB-1H
PULPROG             zg30
TD                 32768
SOLVENT             DMSO
NS                    32
DS                     0
SWH             7246.377 Hz
FIDRES          0.221142 Hz
AQ              2.2609921 sec
RG                   362
DW                69.000 usec
DE                 6.50 usec
TE                296.3 K
D1             2.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                 15.00 usec
PL1                11.10 dB
SFO1         400.1324008 MHz

F2 - Processing parameters
SI                 16384
SF           400.1300058 MHz
WDW                   EM
SSB                    0
LB                     0 Hz
GB                     0
PC                  1.00
```

^{13}C NMR Spectrum of **6fa** (DMSO-d_6, 100 MHz)



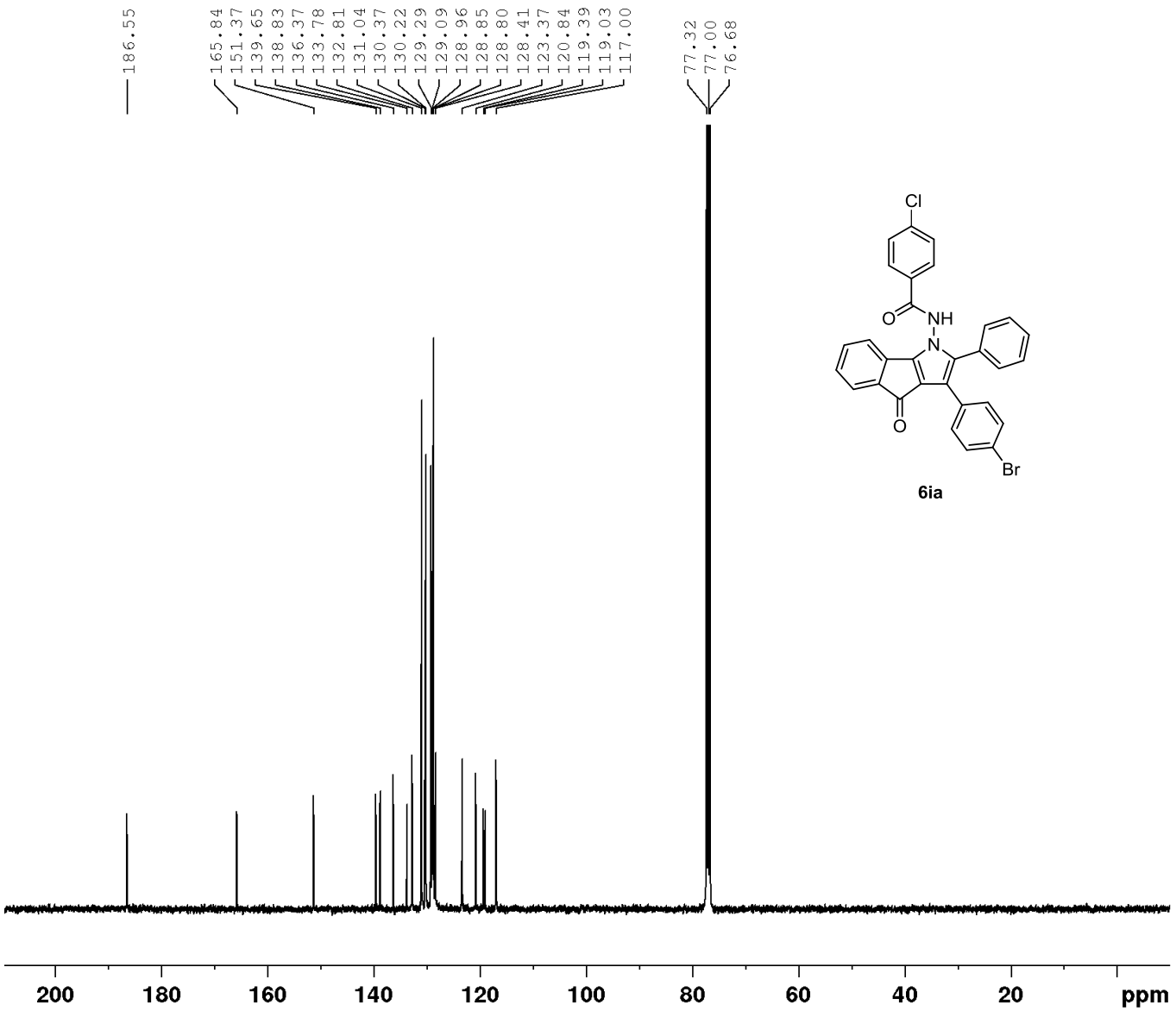

```
Current Data Parameters
NAME          SW Zi 3-Cl
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20200608
Time               23.16
INSTRUM            spect
PROBHD   5 mm BBO BB-1H
PULPROG          zgpg30
TD                 32768
SOLVENT             DMSO
NS                 22301
DS                     0
SWH           24038.461 Hz
FIDRES         0.733596 Hz
AQ            0.6815744 sec
RG                  8192
DW                20.800 usec
DE                 6.50 usec
TE                296.1 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                 13C
P1                10.00 usec
PL1                3.80 dB
SFO1        100.6233325 MHz

======== CHANNEL f2 ========
CPDPRG[2         waltz16
NUC2                 1H
PCPD2             90.00 usec
PL2               10.20 dB
PL12              26.00 dB
PL13              29.00 dB
SFO2        400.1316005 MHz

F2 - Processing parameters
SI                 32768
SF          100.6128196 MHz
WDW                 EM
SSB                    0
LB                 1.00 Hz
GB                     0
PC                 1.00
```

^{1}H NMR Spectrum of **6ia** ($CDCl_3$, 400 MHz)




```
Current Data Parameters
NAME            SW-hy Cl
EXPNO                  3
PROCNO                 1

F2 - Acquisition Parameters
Date_           20200424
Time               22.18
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG             zg30
TD                 32768
SOLVENT            CDCl3
NS                    32
DS                     0
SWH             7211.539 Hz
FIDRES          0.220079 Hz
AQ              2.2719147 sec
RG                 89.08
DW                69.333 usec
DE                10.06 usec
TE                298.2 K
D1             2.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         400.1324008 MHz
NUC1                   1H
P1                 15.00 usec
PLW1         11.39999962 W

F2 - Processing parameters
SI                 16384
SF           400.1300110 MHz
WDW                   EM
SSB                    0
LB                     0 Hz
GB                     0
PC                  1.00
```

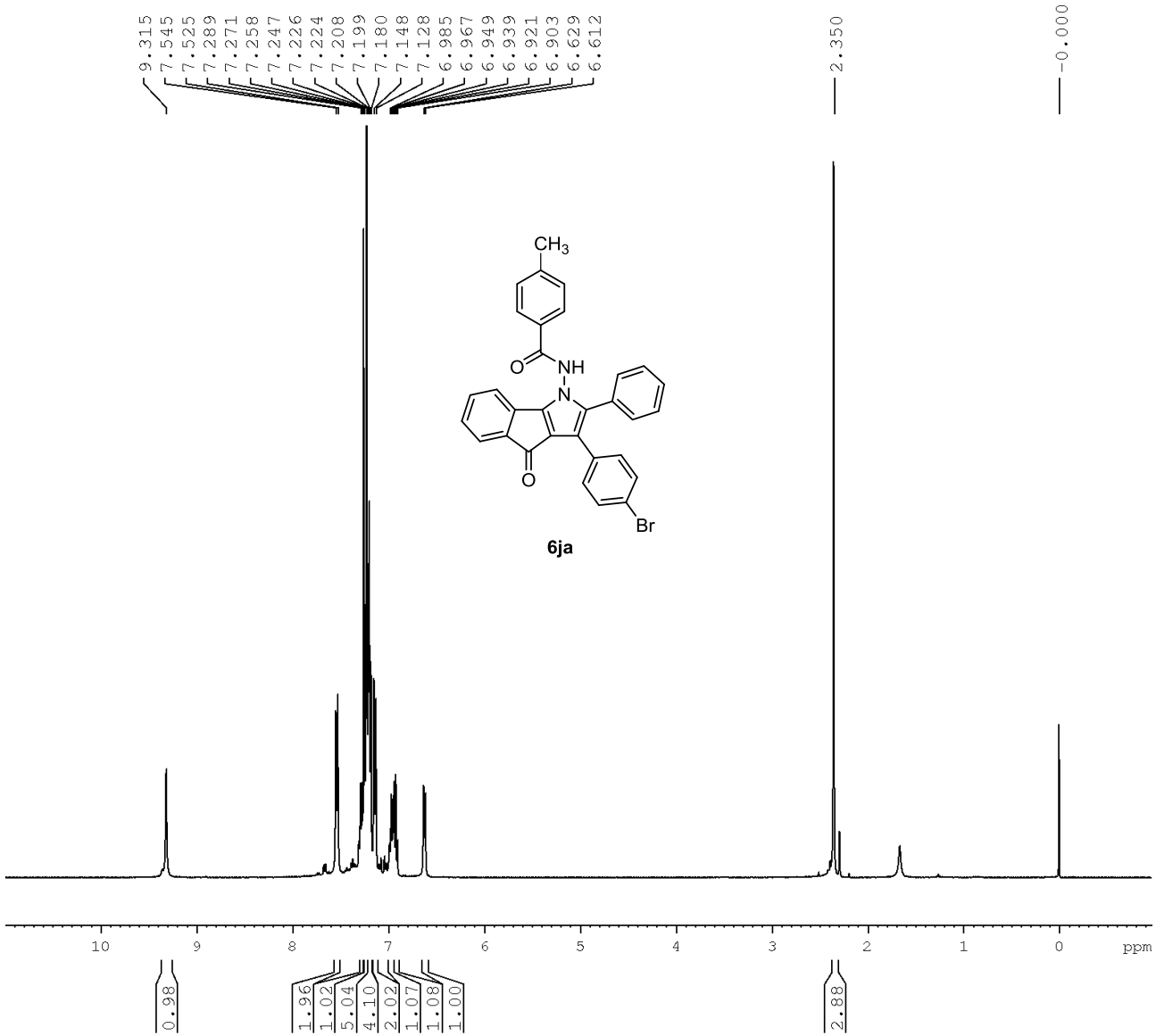
^{13}C NMR Spectrum of **6ia** ($CDCl_3$, 100 MHz)



6ia

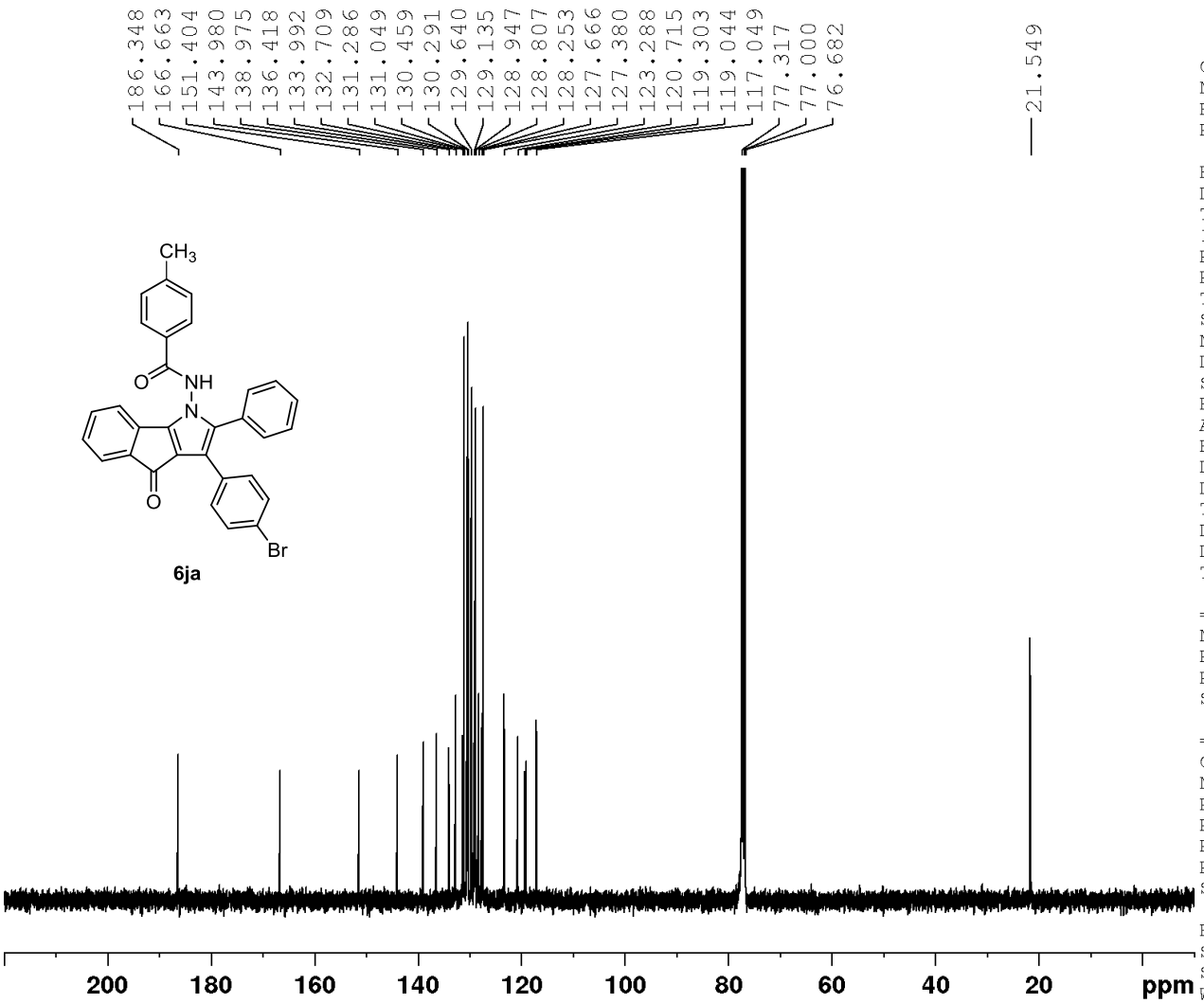
```
Current Data Parameters
NAME            SW-hy Cl
EXPNO                  4
PROCNO                 1

F2 - Acquisition Parameters
Date_           20200424
Time               22.22
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                32768
SOLVENT           CDCl3
NS                 2759
DS                    0
SWH           24038.461 Hz
FIDRES         0.733596 Hz
AQ            0.6815744 sec
RG               198.09
DW               20.800 usec
DE                6.50 usec
TE               299.0 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1         100.6228298 MHz
NUC1                13C
P1                10.00 usec
PLW1         49.50000000 W

======== CHANNEL f2 ========
SFO2         400.1316005 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2             90.00 usec
PLW2         12.50000000 W
PLW12         0.34722000 W
PLW13         0.28125000 W

F2 - Processing parameters
SI                 32768
SF           100.6127727 MHz
WDW                   EM
SSB                    0
LB                 2.00 Hz
GB                     0
PC                 1.00
```

^{1}H NMR Spectrum of **6ja** ($CDCl_3$, 400 MHz)



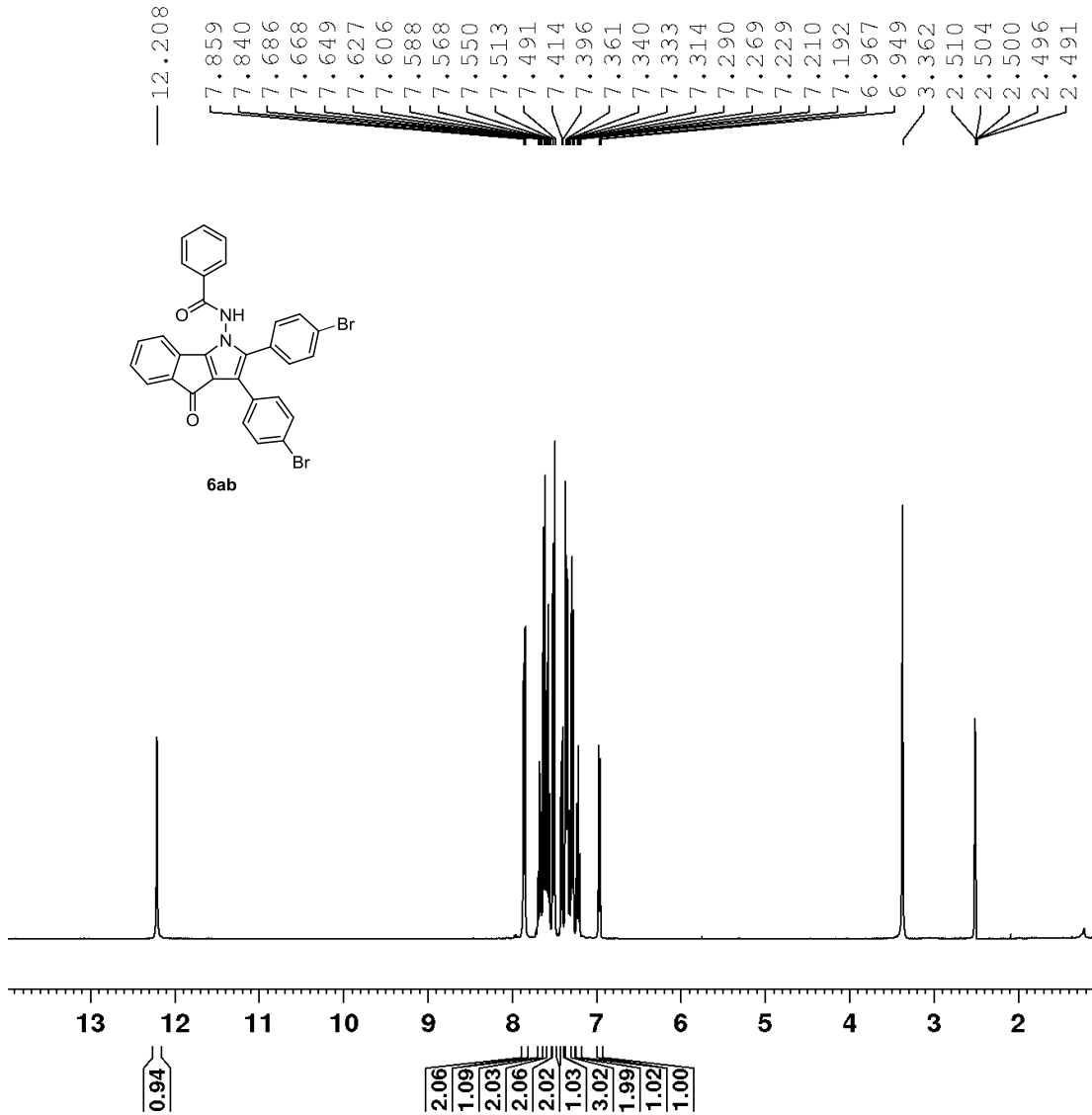

```
Current Data Parameters
NAME          SW-hy Me-1
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20200520
Time               15.00
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG             zg30
TD                 32768
SOLVENT            CDCl3
NS                    32
DS                     0
SWH             7211.539 Hz
FIDRES          0.220079 Hz
AQ              2.2719147 sec
RG                 113.31
DW                 69.333 usec
DE                 10.06 usec
TE                 296.3 K
D1             2.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         400.1324008 MHz
NUC1                   1H
P1                 15.00 usec
PLW1         11.39999962 W

F2 - Processing parameters
SI                 16384
SF           400.1300106 MHz
WDW                   EM
SSB                    0
LB                     0 Hz
GB                     0
PC                  1.00
```

^{13}C NMR Spectrum of **6ja** ($CDCl_3$, 100 MHz)



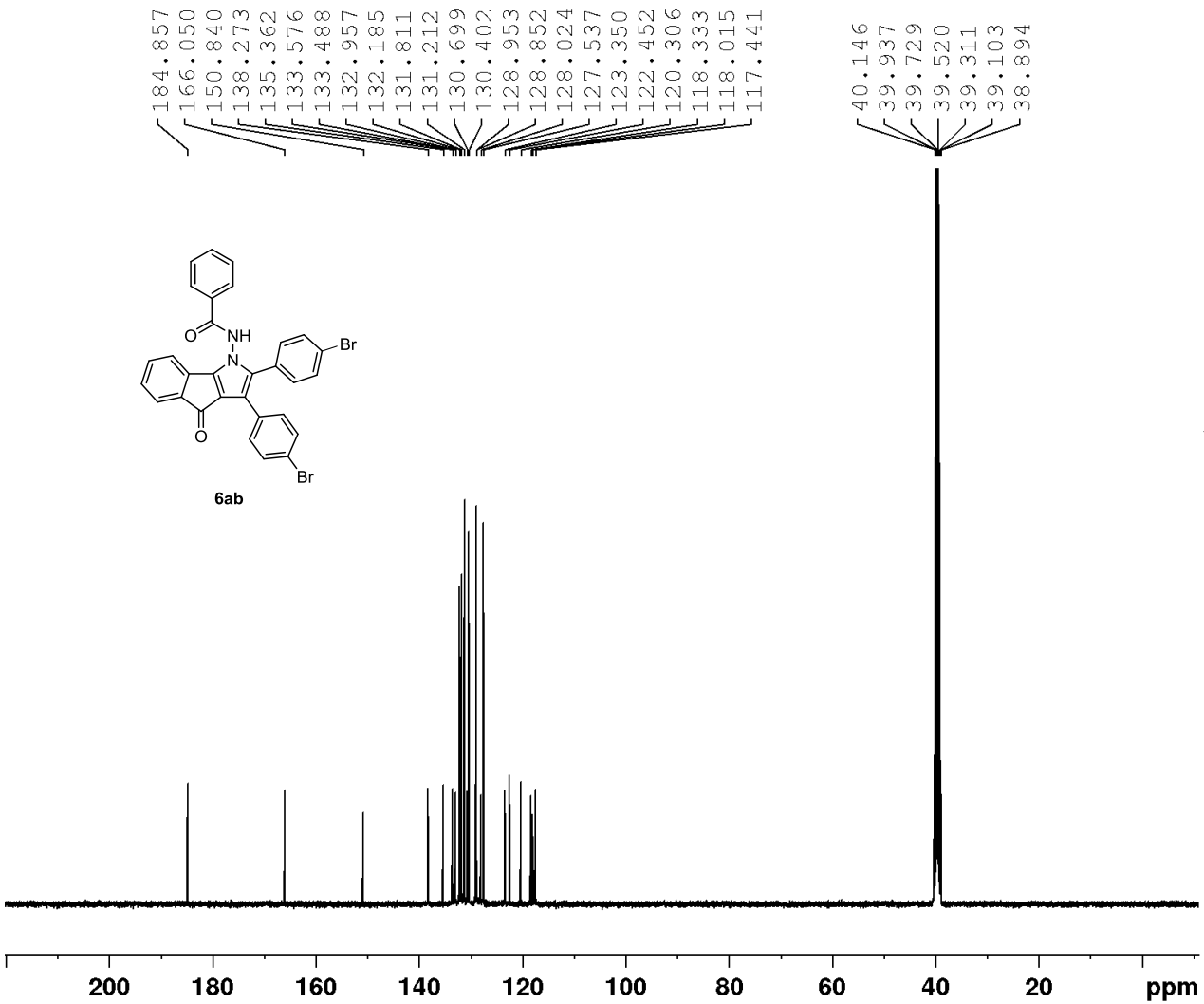

```
Current Data Parameters
NAME            SW-hyCH3
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20200321
Time                2.05
INSTRUM            spect
PROBHD   5 mm BBO BB-1H
PULPROG          zgpg30
TD                 32768
SOLVENT            CDCl3
NS                  2660
DS                     0
SWH           24038.461 Hz
FIDRES         0.733596 Hz
AQ            0.6815744 sec
RG                  8192
DW                20.800 usec
DE                 6.50 usec
TE                296.5 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                13C
P1                10.00 usec
PL1                3.80 dB
SFO1        100.6233325 MHz

======== CHANNEL f2 ========
CPDPRG[2         waltz16
NUC2                1H
PCPD2              90.00 usec
PL2                10.20 dB
PL12               26.00 dB
PL13               29.00 dB
SFO2        400.1316005 MHz

F2 - Processing parameters
SI                 32768
SF          100.6127721 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.00
```

^{1}H NMR Spectrum of **6ab** (DMSO-d_6, 400 MHz)



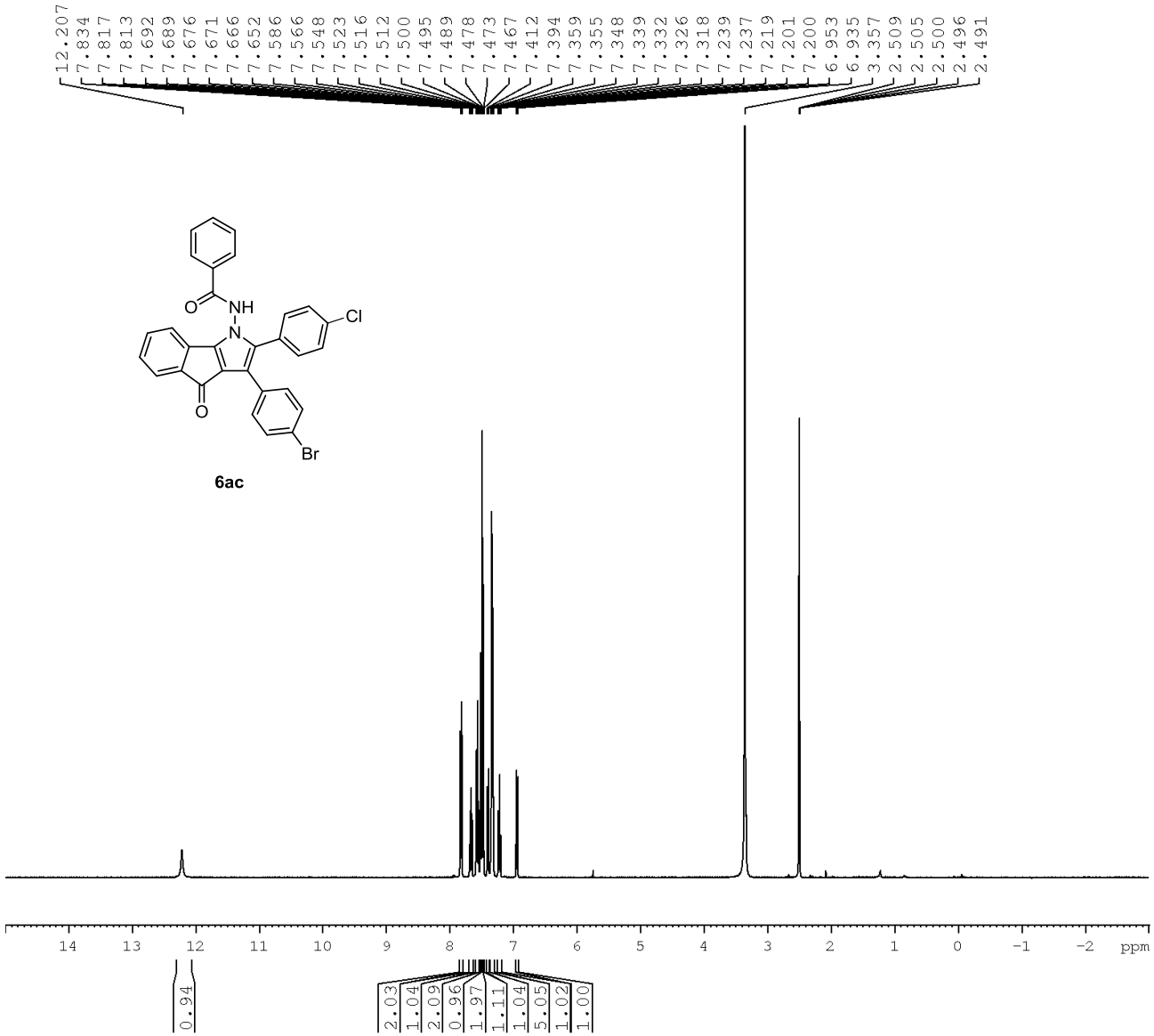

```
Current Data Parameters
NAME          SW bc 4-Br
EXPNO                  3
PROCNO                 1

F2 - Acquisition Parameters
Date_           20200304
Time               23.25
INSTRUM            spect
PROBHD   5 mm BBO BB-1H
PULPROG             zg30
TD                 32768
SOLVENT             DMSO
NS                    32
DS                     0
SWH             7246.377 Hz
FIDRES          0.221142 Hz
AQ              2.2609921 sec
RG                   114
DW                69.000 usec
DE                 6.50 usec
TE                298.8 K
D1             2.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                 15.00 usec
PL1                11.10 dB
SFO1         400.1324008 MHz

F2 - Processing parameters
SI                 16384
SF           400.1300028 MHz
WDW                   EM
SSB       0
LB        0 Hz
GB        0
PC                  1.00
```

^{13}C NMR Spectrum of **6ab** (DMSO-d_6, 100 MHz)



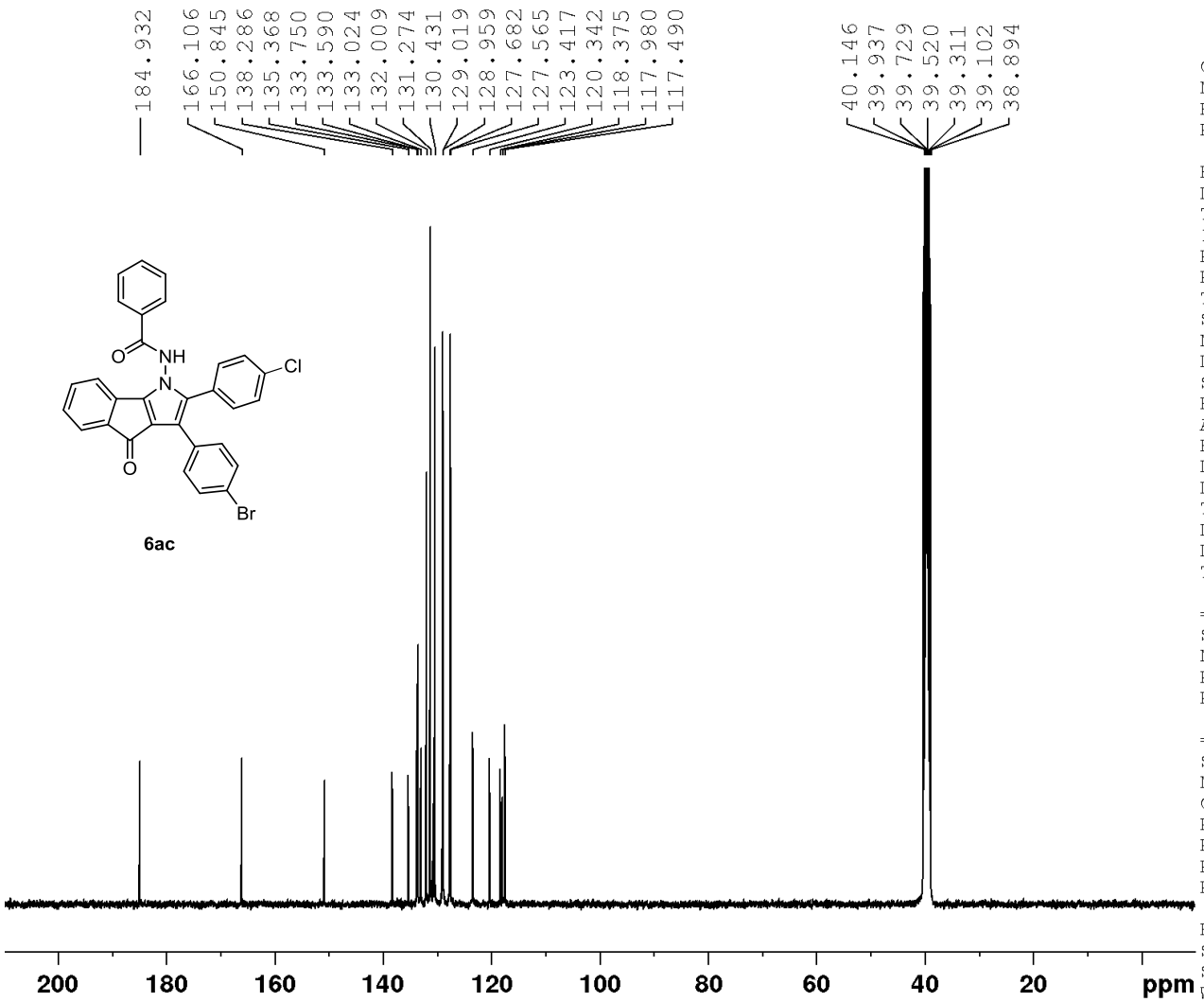

```
Current Data Parameters
NAME          SW bc 4-Br
EXPNO                  4
PROCNO                 1

F2 - Acquisition Parameters
Date_           20200304
Time               23.28
INSTRUM            spect
PROBHD   5 mm BBO BB-1H
PULPROG          zgpg30
TD                32768
SOLVENT             DMSO
NS                 1963
DS                    0
SWH           24038.461 Hz
FIDRES         0.733596 Hz
AQ             0.6815744 sec
RG                 4096
DW                20.800 usec
DE                 6.50 usec
TE                298.8 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                13C
P1                10.00 usec
PL1                3.80 dB
SFO1        100.6233325 MHz

======== CHANNEL f2 ========
CPDPRG[2         waltz16
NUC2                1H
PCPD2             90.00 usec
PL2               10.20 dB
PL12              26.00 dB
PL13              29.00 dB
SFO2        400.1316005 MHz

F2 - Processing parameters
SI                32768
SF          100.6128210 MHz
WDW                 EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.00
```

^{1}H NMR Spectrum of **6ac** (DMSO-d_6, 400 MHz)



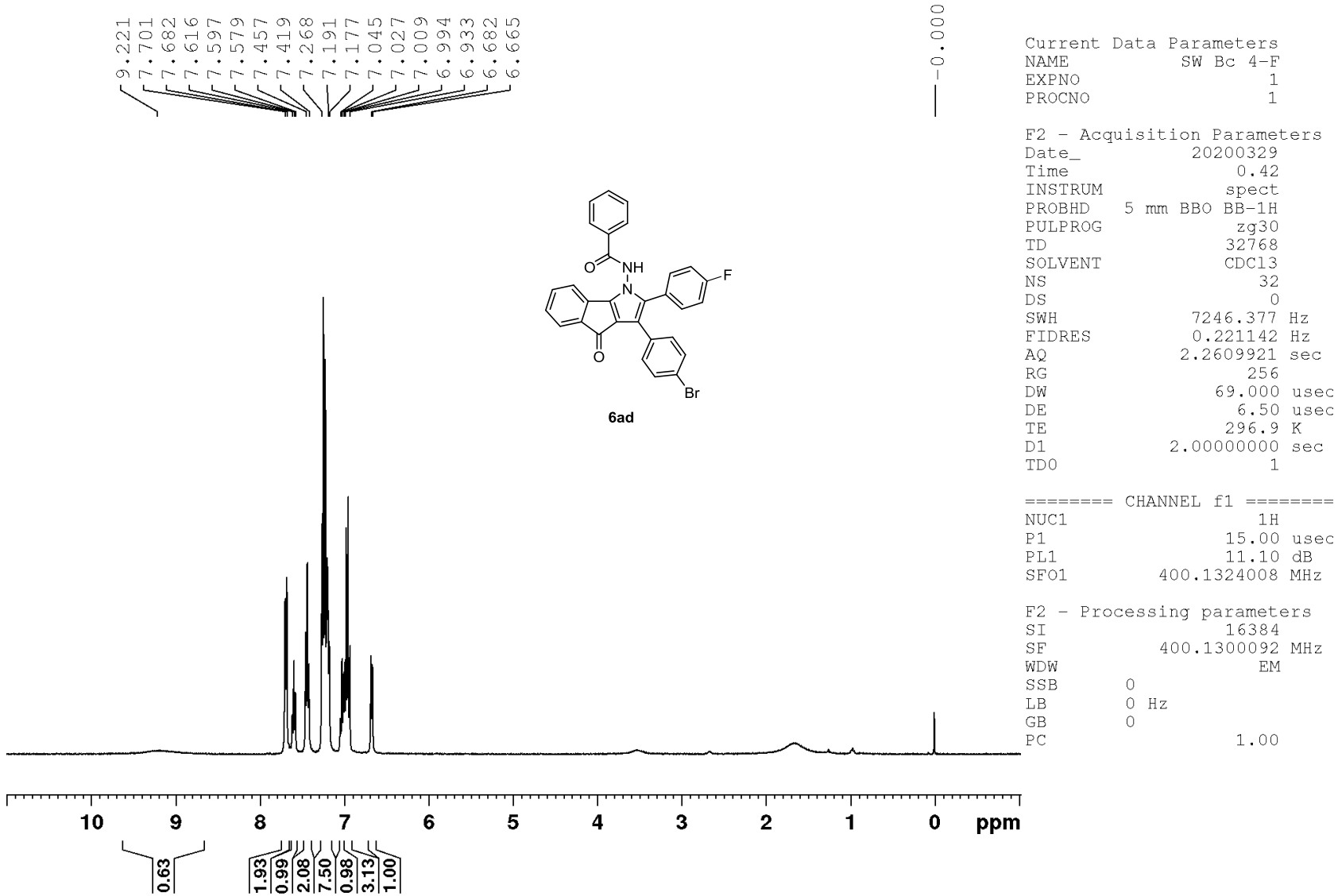

```
Current Data Parameters
NAME                  bc 4-Cl
EXPNO                       1
PROCNO                      1

F2 - Acquisition Parameters
Date_               20200321
Time                   22.15
INSTRUM                spect
PROBHD    5 mm PABBO BB/
PULPROG                 zg30
TD                     32768
SOLVENT                 DMSO
NS                        16
DS                         0
SWH                 7211.539 Hz
FIDRES              0.220079 Hz
AQ                2.2719147 sec
RG                        89.08
DW                     69.333 usec
DE                     10.06 usec
TE                     297.9 K
D1               2.00000000 sec
TD0                         1

======== CHANNEL f1 ========
SFO1            400.1324008 MHz
NUC1                       1H
P1                     15.00 usec
PLW1            11.39999962 W

F2 - Processing parameters
SI                      16384
SF              400.1300031 MHz
WDW                        EM
SSB                         0
LB                          0 Hz
GB                          0
PC                       1.00
```

^{13}C NMR Spectrum of **6ac** (DMSO-d_6, 100 MHz)



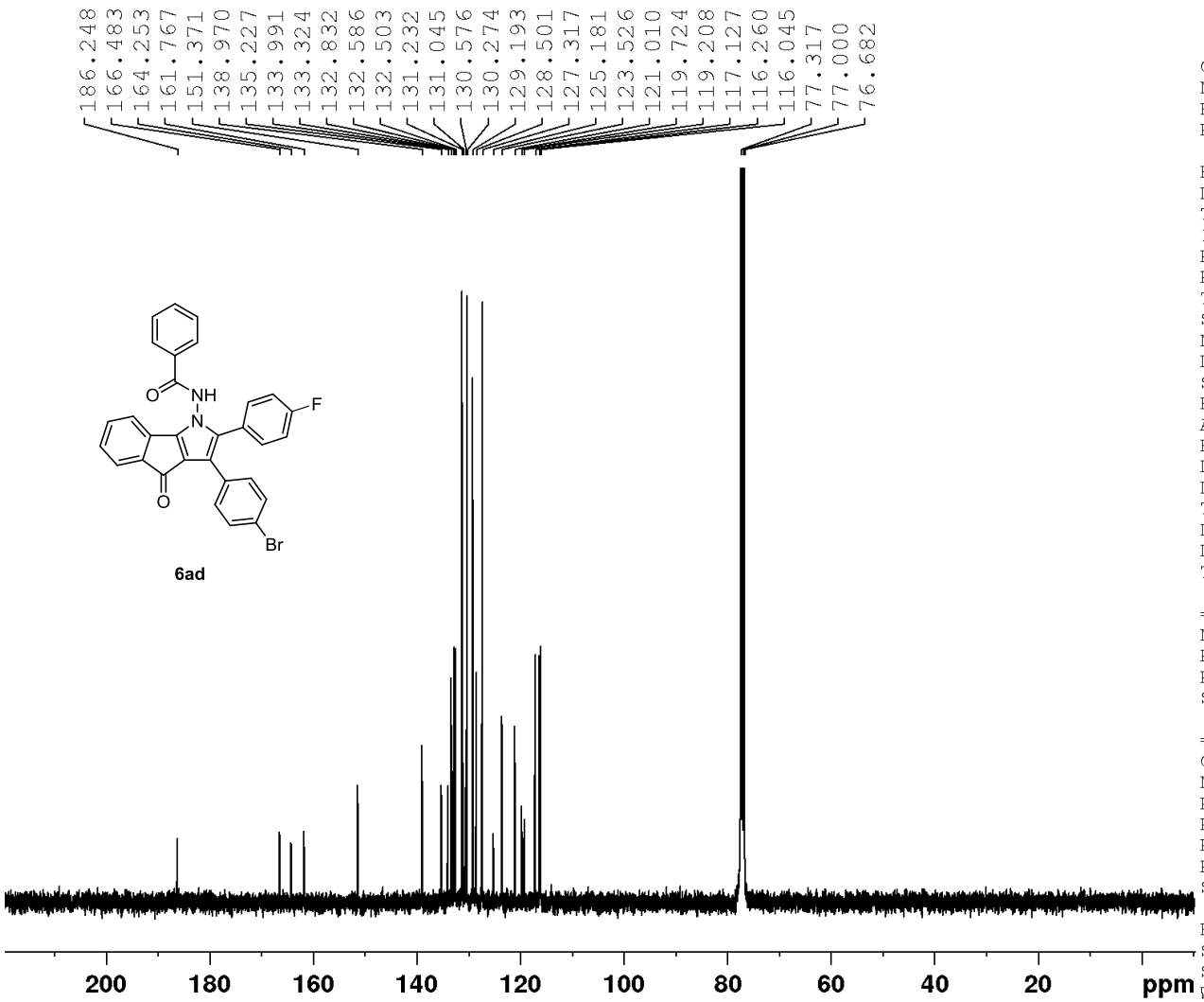

```
Current Data Parameters
NAME              bc 4-Cl
EXPNO                   2
PROCNO                  1

F2 - Acquisition Parameters
Date_            20200321
Time                22.25
INSTRUM             spect
PROBHD   5 mm PABBO BB/
PULPROG            zgpg30
TD                  32768
SOLVENT              DMSO
NS                  13451
DS                      0
SWH             24038.461 Hz
FIDRES           0.733596 Hz
AQ               0.6815744 sec
RG                 198.09
DW                 20.800 usec
DE                  6.50 usec
TE                 298.7 K
D1              2.00000000 sec
D11             0.03000000 sec
TD0                     1

======== CHANNEL f1 ========
SFO1          100.6228298 MHz
NUC1                  13C
P1                 10.00 usec
PLW1          49.50000000 W

======== CHANNEL f2 ========
SFO2          400.1316005 MHz
NUC2                  1H
CPDPRG[2          waltz16
PCPD2               90.00 usec
PLW2          12.50000000 W
PLW12          0.34722000 W
PLW13          0.28125000 W

F2 - Processing parameters
SI                  32768
SF            100.6128155 MHz
WDW                   EM
SSB       0
LB                 2.00 Hz
GB        0
PC                 1.00
```

^{1}H NMR Spectrum of **6ad** ($CDCl_3$, 400 MHz)



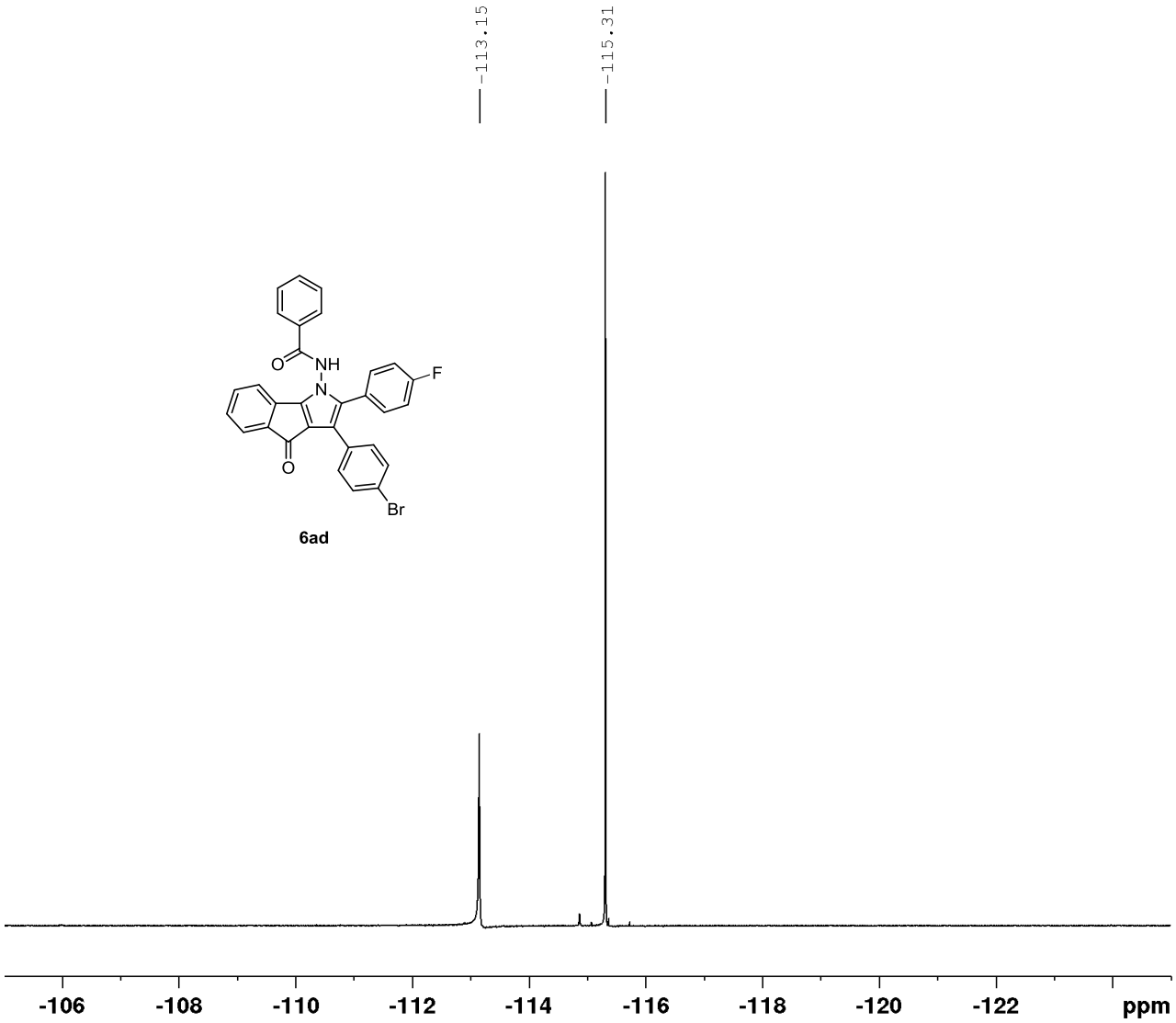

```
Current Data Parameters
NAME          SW Bc 4-F
EXPNO                 1
PROCNO                1

F2 - Acquisition Parameters
Date_          20200329
Time               0.42
INSTRUM           spect
PROBHD   5 mm BBO BB-1H
PULPROG             zg30
TD                 32768
SOLVENT            CDCl3
NS                    32
DS                     0
SWH             7246.377 Hz
FIDRES          0.221142 Hz
AQ             2.2609921 sec
RG                   256
DW                69.000 usec
DE                 6.50 usec
TE                296.9 K
D1           2.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                15.00 usec
PL1               11.10 dB
SFO1        400.1324008 MHz

F2 - Processing parameters
SI                 16384
SF          400.1300092 MHz
WDW                   EM
SSB       0
LB        0 Hz
GB        0
PC                  1.00
```

^{13}C NMR Spectrum of **6ad** ($CDCl_3$, 100 MHz)



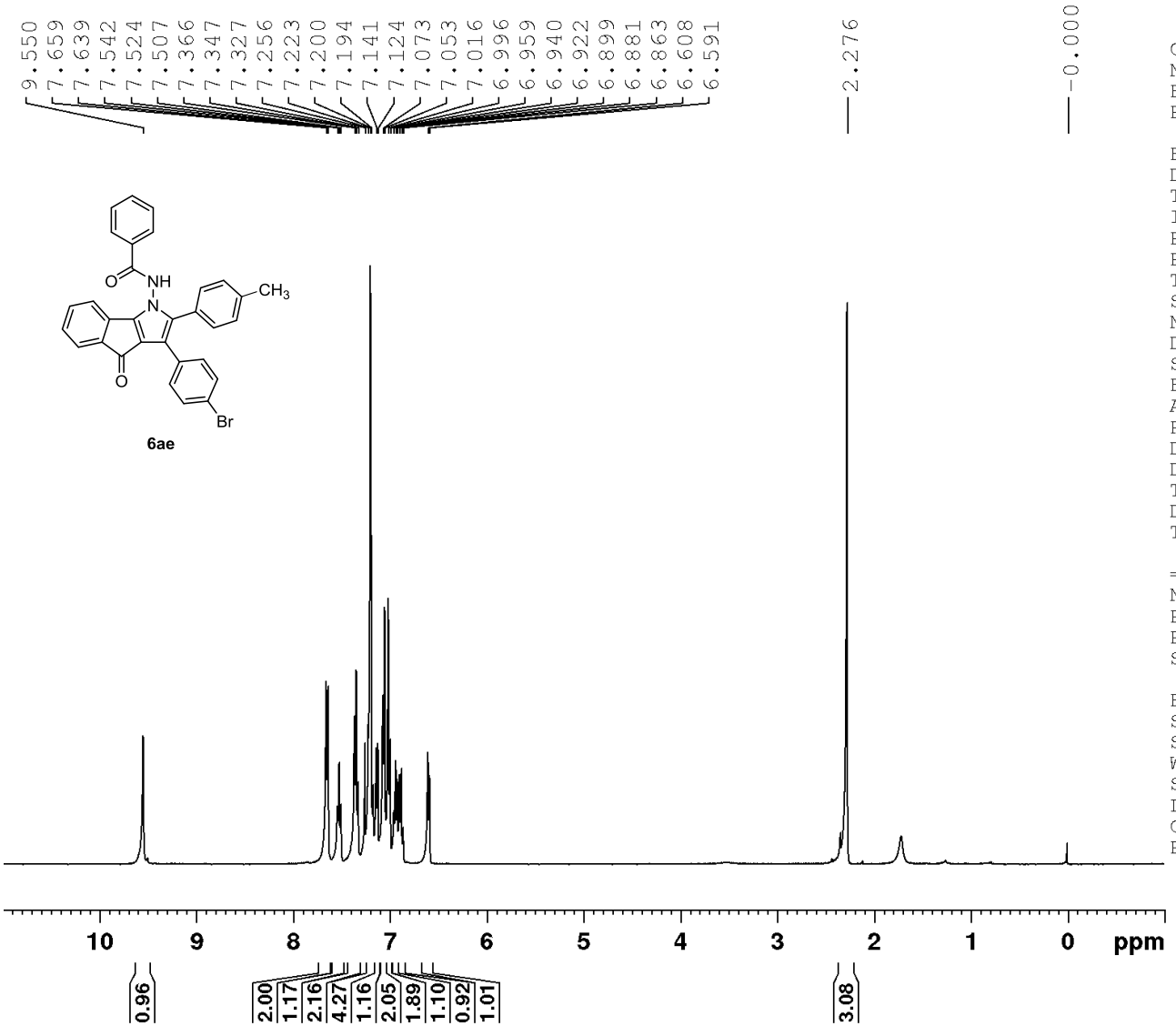

```
Current Data Parameters
NAME           SW Bc 4-F
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20200329
Time                0.45
INSTRUM            spect
PROBHD   5 mm BBO BB-1H
PULPROG           zgpg30
TD                 32768
SOLVENT            CDCl3
NS                 15000
DS                     0
SWH            24038.461 Hz
FIDRES          0.733596 Hz
AQ              0.6815744 sec
RG                 9195.2
DW                20.800 usec
DE                 6.50 usec
TE                296.8 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  13C
P1                 10.00 usec
PL1                 3.80 dB
SFO1         100.6233325 MHz

======== CHANNEL f2 ========
CPDPRG[2          waltz16
NUC2                  1H
PCPD2              90.00 usec
PL2                10.20 dB
PL12               26.00 dB
PL13               29.00 dB
SFO2         400.1316005 MHz

F2 - Processing parameters
SI                 32768
SF           100.6127693 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.00
```

^{19}F NMR Spectrum of **6ad** ($CDCl_3$, 376 MHz)



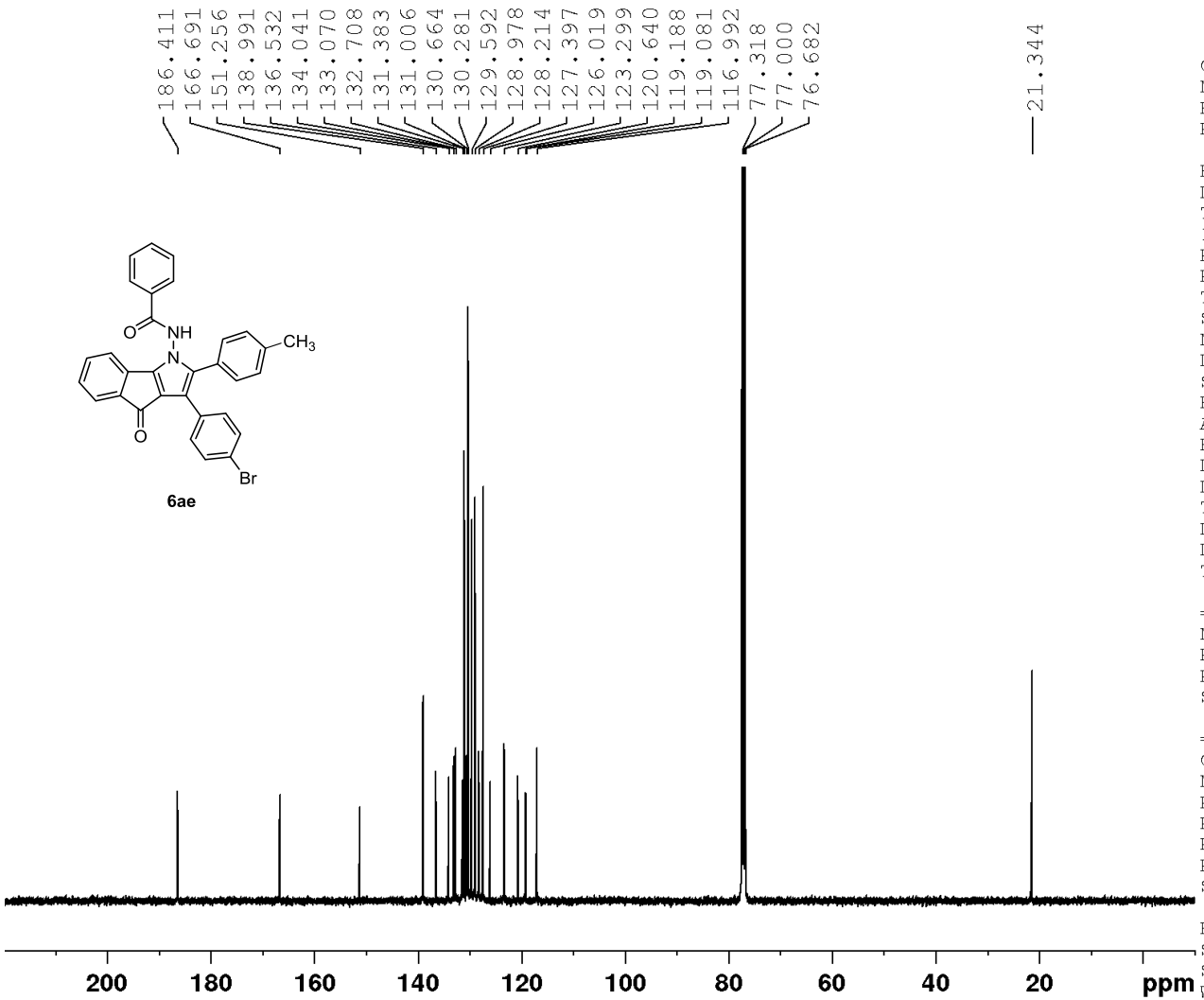

```
Current Data Parameters
NAME       SW Bc 4F - 1
EXPNO                1
PROCNO               1

F2 - Acquisition Parameters
Date_          20200612
Time              20.23
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG            zgig
TD               131072
SOLVENT            CDCl3
NS                    32
DS                     0
SWH            89285.711 Hz
FIDRES          0.681196 Hz
AQ             0.7340032 sec
RG                198.09
DW                 5.600 usec
DE                 6.50 usec
TE                298.3 K
D1           1.00000000 sec
D11          0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         376.4607168 MHz
NUC1                19F
P1                15.00 usec
PLW1         18.00000000 W

======== CHANNEL f2 ========
SFO2         400.1316005 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2             90.00 usec
PLW2         12.50000000 W
PLW12         0.34722000 W

F2 - Processing parameters
SI                 65536
SF           376.4992047 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.00
```

^{1}H NMR Spectrum of **6ae** ($CDCl_3$, 400 MHz)



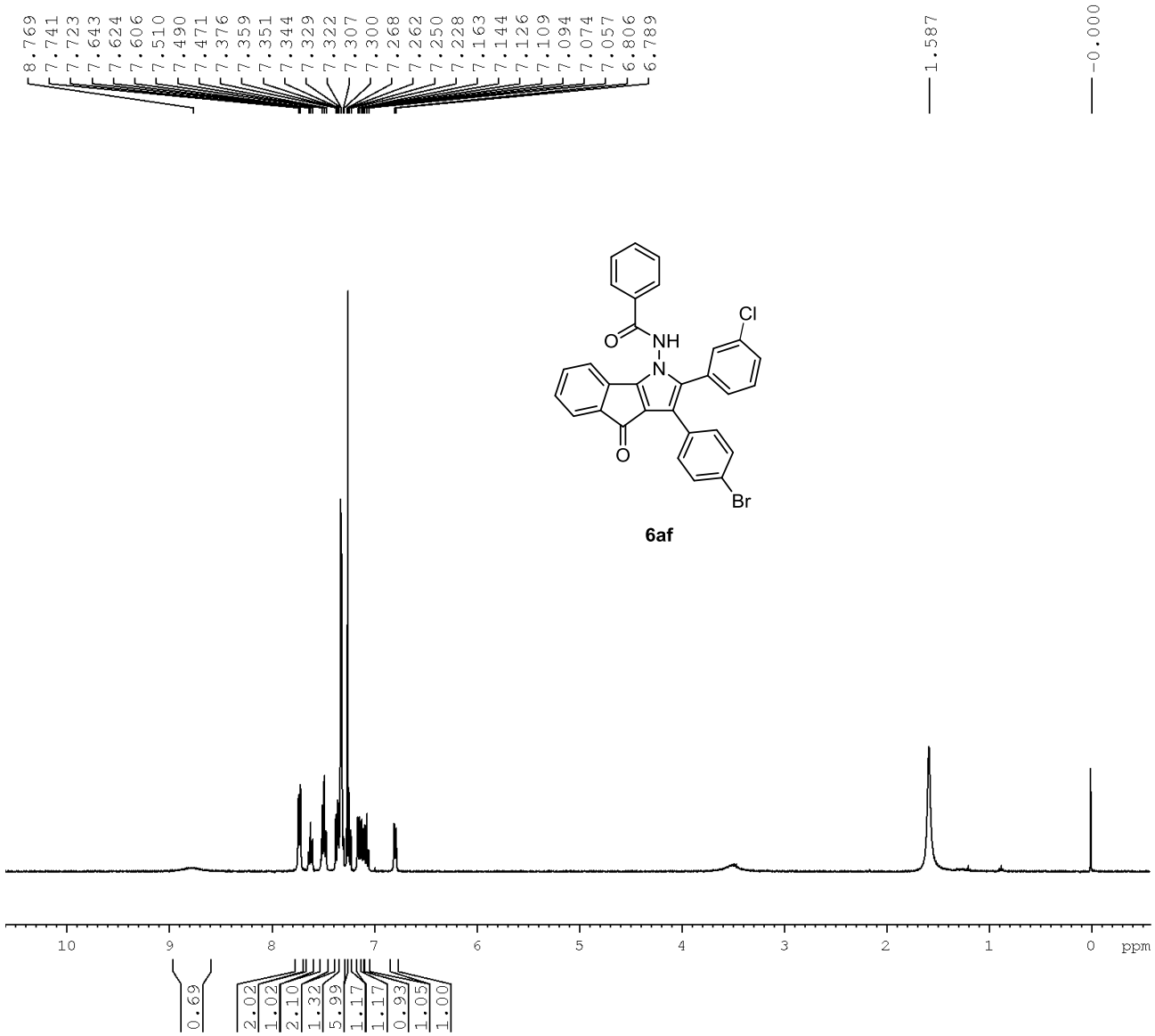

```
Current Data Parameters
NAME          SW Bc 4-Me
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20200326
Time                0.43
INSTRUM            spect
PROBHD   5 mm BBO BB-1H
PULPROG             zg30
TD                 32768
SOLVENT            CDCl3
NS                    32
DS                     0
SWH             7246.377 Hz
FIDRES          0.221142 Hz
AQ              2.2609921 sec
RG                 161.3
DW                69.000 usec
DE                 6.50 usec
TE                296.2 K
D1             2.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                 15.00 usec
PL1                11.10 dB
SFO1         400.1324008 MHz

F2 - Processing parameters
SI                 16384
SF           400.1300102 MHz
WDW                   EM
SSB       0
LB        0 Hz
GB        0
PC                  1.00
```

^{13}C NMR Spectrum of **6ae** ($CDCl_3$, 100 MHz)



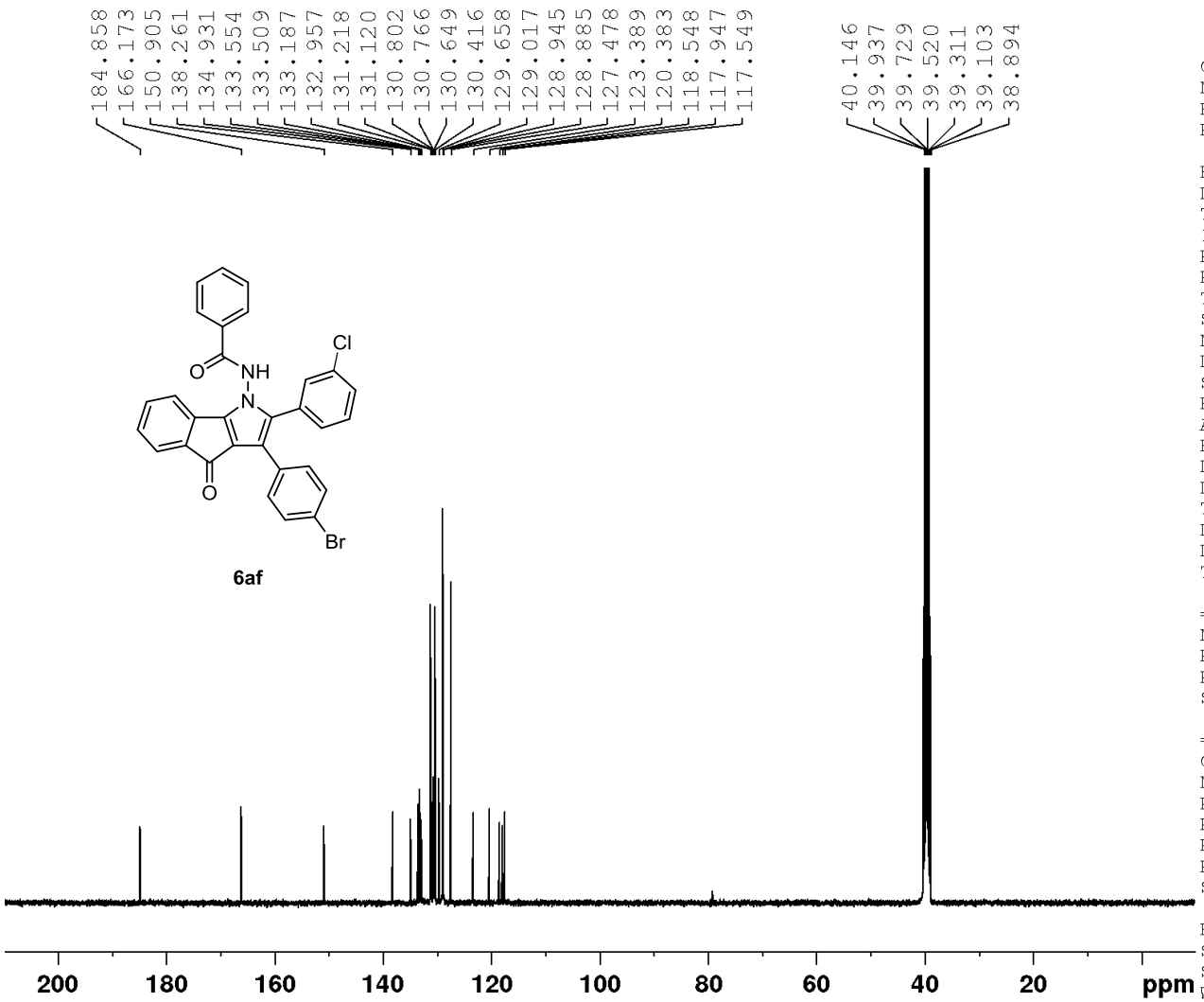

```
Current Data Parameters
NAME          SW Bc 4-Me
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20200326
Time                0.48
INSTRUM            spect
PROBHD   5 mm BBO BB-1H
PULPROG          zgpg30
TD                32768
SOLVENT           CDCl3
NS                11452
DS                    0
SWH           24038.461 Hz
FIDRES         0.733596 Hz
AQ            0.6815744 sec
RG                 8192
DW               20.800 usec
DE                6.50 usec
TE               296.0 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 13C
P1                10.00 usec
PL1                3.80 dB
SFO1        100.6233325 MHz

======== CHANNEL f2 ========
CPDPRG[2         waltz16
NUC2                 1H
PCPD2             90.00 usec
PL2               10.20 dB
PL12              26.00 dB
PL13              29.00 dB
SFO2        400.1316005 MHz

F2 - Processing parameters
SI                32768
SF          100.6127717 MHz
WDW                  EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.00
```

^{1}H NMR Spectrum of **6af** ($CDCl_3$, 400 MHz)



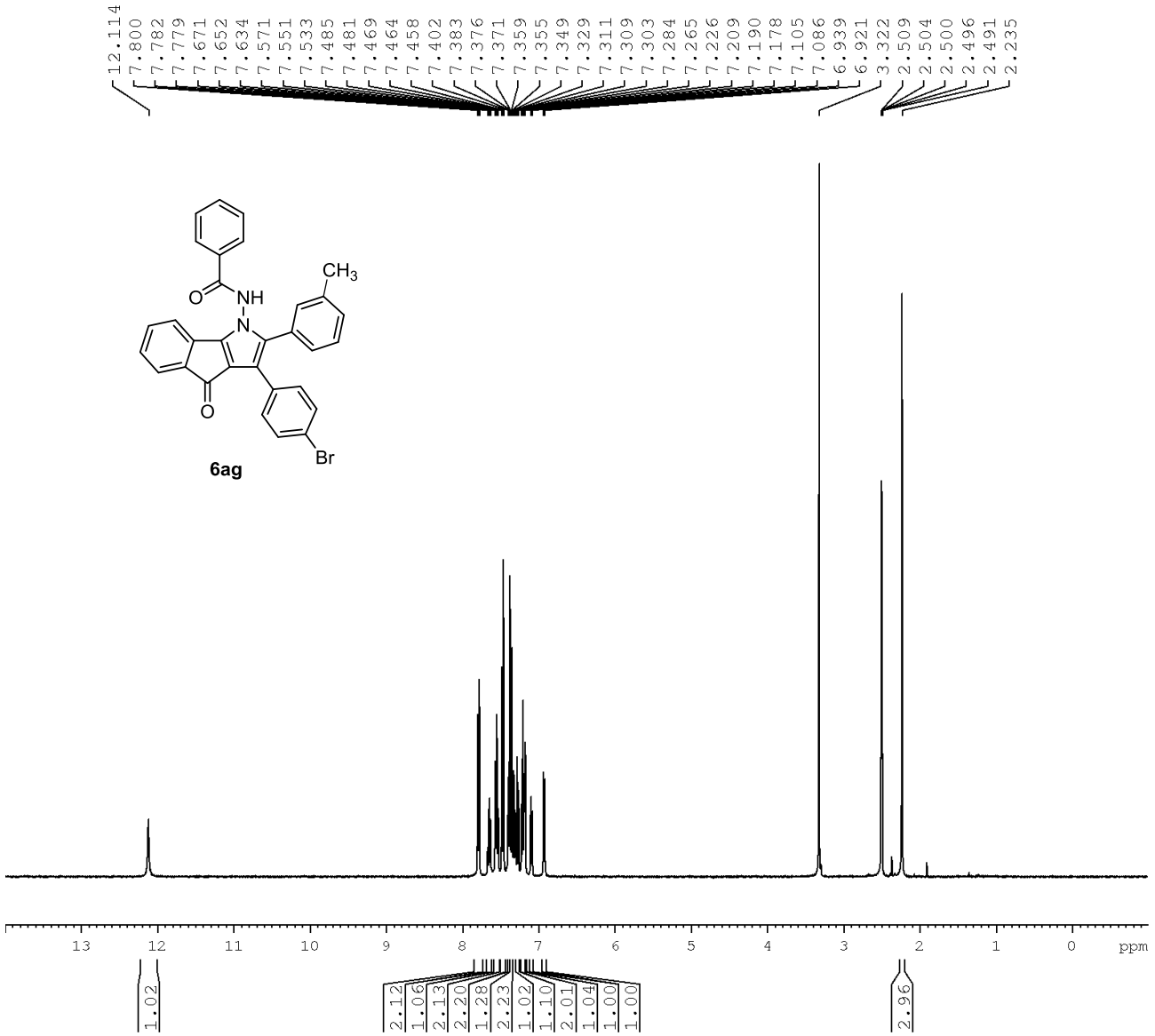

```
Current Data Parameters
NAME                  454
EXPNO                   4
PROCNO                  1

F2 - Acquisition Parameters
Date_            20200425
Time                11.52
INSTRUM             spect
PROBHD   5 mm BBO BB-1H
PULPROG              zg30
TD                  32768
SOLVENT             CDCl3
NS                     32
DS                      0
SWH              7246.377 Hz
FIDRES           0.221142 Hz
AQ               2.2609921 sec
RG                    362
DW                 69.000 usec
DE                  6.50 usec
TE                 296.4 K
D1              2.00000000 sec
TD0                     1

======== CHANNEL f1 ========
NUC1                   1H
P1                  15.00 usec
PL1                 11.10 dB
SFO1         400.1324008 MHz

F2 - Processing parameters
SI                  16384
SF           400.1300101 MHz
WDW                    EM
SSB                     0
LB                      0 Hz
GB                      0
PC                   1.00
```

^{13}C NMR Spectrum of **6af** (DMSO-d_6, 100 MHz)



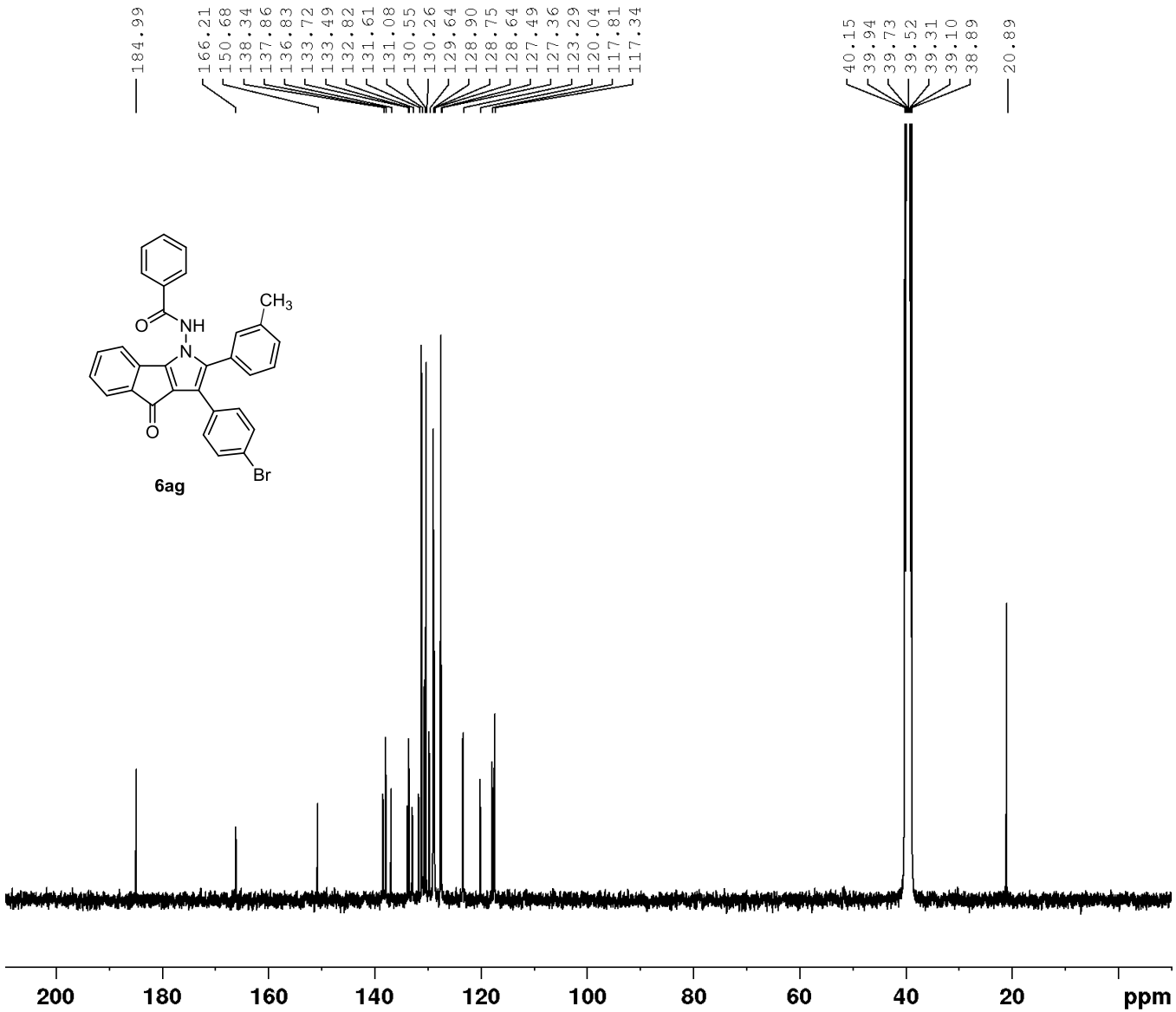

```
Current Data Parameters
NAME          SW Bc 3-Cl
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20200305
Time                1.08
INSTRUM            spect
PROBHD   5 mm BBO BB-1H
PULPROG           zgpg30
TD                 32768
SOLVENT             DMSO
NS                  5000
DS                     0
SWH           24038.461 Hz
FIDRES         0.733596 Hz
AQ             0.6815744 sec
RG                  4096
DW                20.800 usec
DE                 6.50 usec
TE                299.1 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                13C
P1                10.00 usec
PL1                3.80 dB
SFO1        100.6233325 MHz

======== CHANNEL f2 ========
CPDPRG[2         waltz16
NUC2                1H
PCPD2             90.00 usec
PL2               10.20 dB
PL12              26.00 dB
PL13              29.00 dB
SFO2        400.1316005 MHz

F2 - Processing parameters
SI                 32768
SF          100.6128200 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.00
```

^{1}H NMR Spectrum of **6ag** (DMSO-d_6, 400 MHz)



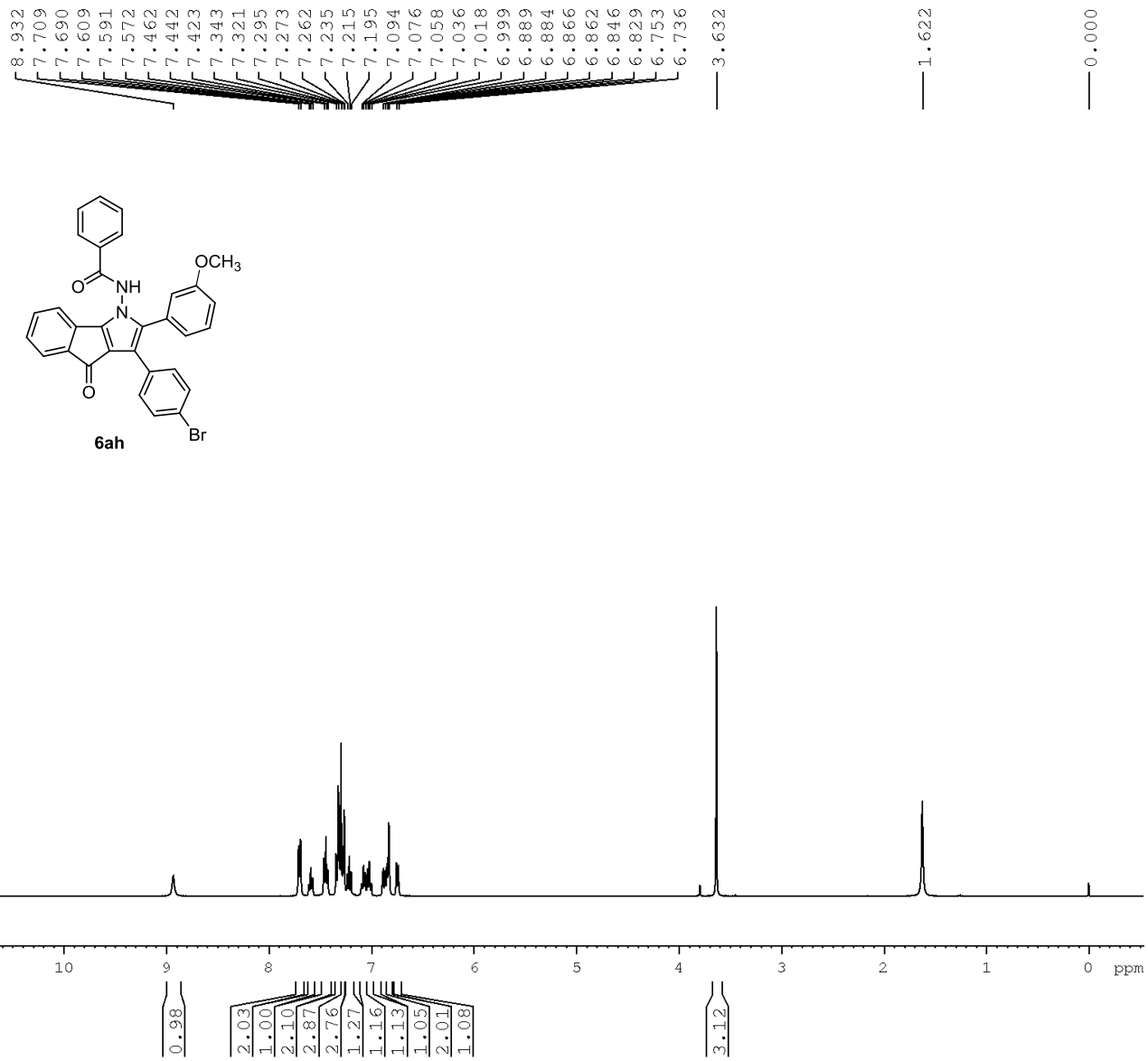

```
Current Data Parameters
NAME                  18
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20200426
Time               22.21
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG             zg30
TD                 32768
SOLVENT             DMSO
NS                    16
DS                     0
SWH             7211.539 Hz
FIDRES          0.220079 Hz
AQ              2.2719147 sec
RG                198.09
DW                69.333 usec
DE                10.06 usec
TE                297.7 K
D1             2.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         400.1324008 MHz
NUC1                   1H
P1                 15.00 usec
PLW1        11.39999962 W

F2 - Processing parameters
SI                 16384
SF           400.1300031 MHz
WDW                   EM
SSB                    0
LB                     0 Hz
GB                     0
PC                  1.00
```

^{13}C NMR Spectrum of **6ag** (DMSO-d_6, 100 MHz)



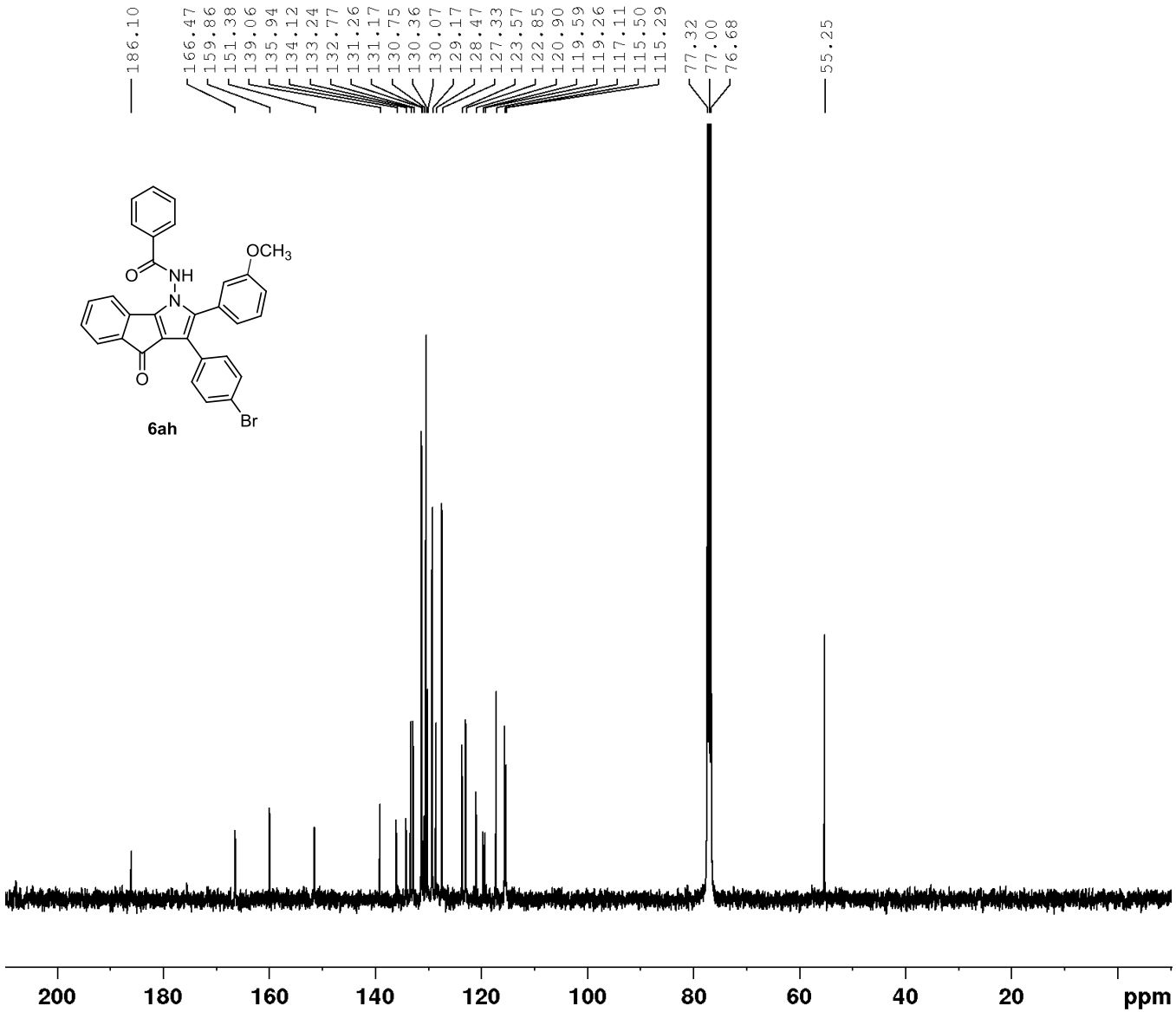

```
Current Data Parameters
NAME                   18
EXPNO                   2
PROCNO                  1

F2 - Acquisition Parameters
Date_           20200426
Time               22.24
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                32768
SOLVENT             DMSO
NS                15233
DS                    0
SWH           24038.461 Hz
FIDRES         0.733596 Hz
AQ            0.6815744 sec
RG               198.09
DW               20.800 usec
DE                6.50 usec
TE                298.0 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1        100.6228298 MHz
NUC1               13C
P1                10.00 usec
PLW1        47.50000000 W

======== CHANNEL f2 ========
SFO2        400.1316005 MHz
NUC2               1H
CPDPRG[2         waltz16
PCPD2             90.00 usec
PLW2        15.00000000 W
PLW12        0.33750001 W
PLW13        0.27338001 W

F2 - Processing parameters
SI                32768
SF          100.6128180 MHz
WDW                EM
SSB                   0
LB                2.00 Hz
GB                    0
PC                1.00
```

^{1}H NMR Spectrum of **6ah** ($CDCl_3$, 400 MHz)



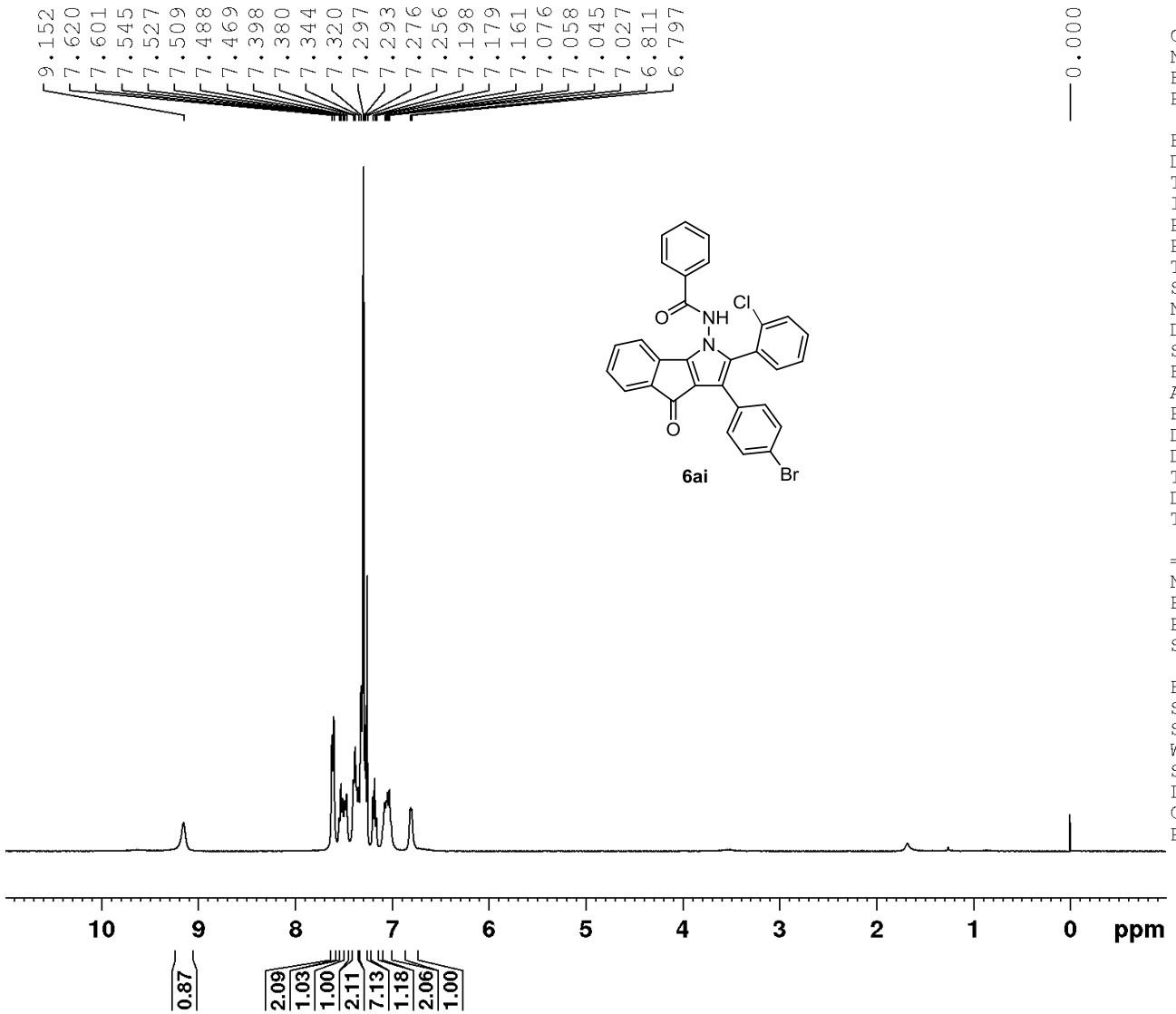

```
Current Data Parameters
NAME                  16
EXPNO                  3
PROCNO                 1

F2 - Acquisition Parameters
Date_           20200421
Time                1.05
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG             zg30
TD                 32768
SOLVENT            CDCl3
NS                    32
DS                     0
SWH             7211.539 Hz
FIDRES          0.220079 Hz
AQ             2.2719147 sec
RG                198.09
DW                69.333 usec
DE                10.06 usec
TE                294.9 K
D1           2.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         400.1324008 MHz
NUC1                   1H
P1                 15.00 usec
PLW1         11.39999962 W

F2 - Processing parameters
SI                 16384
SF           400.1300088 MHz
WDW                   EM
SSB                    0
LB                     0 Hz
GB                     0
PC                  1.00
```

^{13}C NMR Spectrum of **6ah** ($CDCl_3$, 100 MHz)



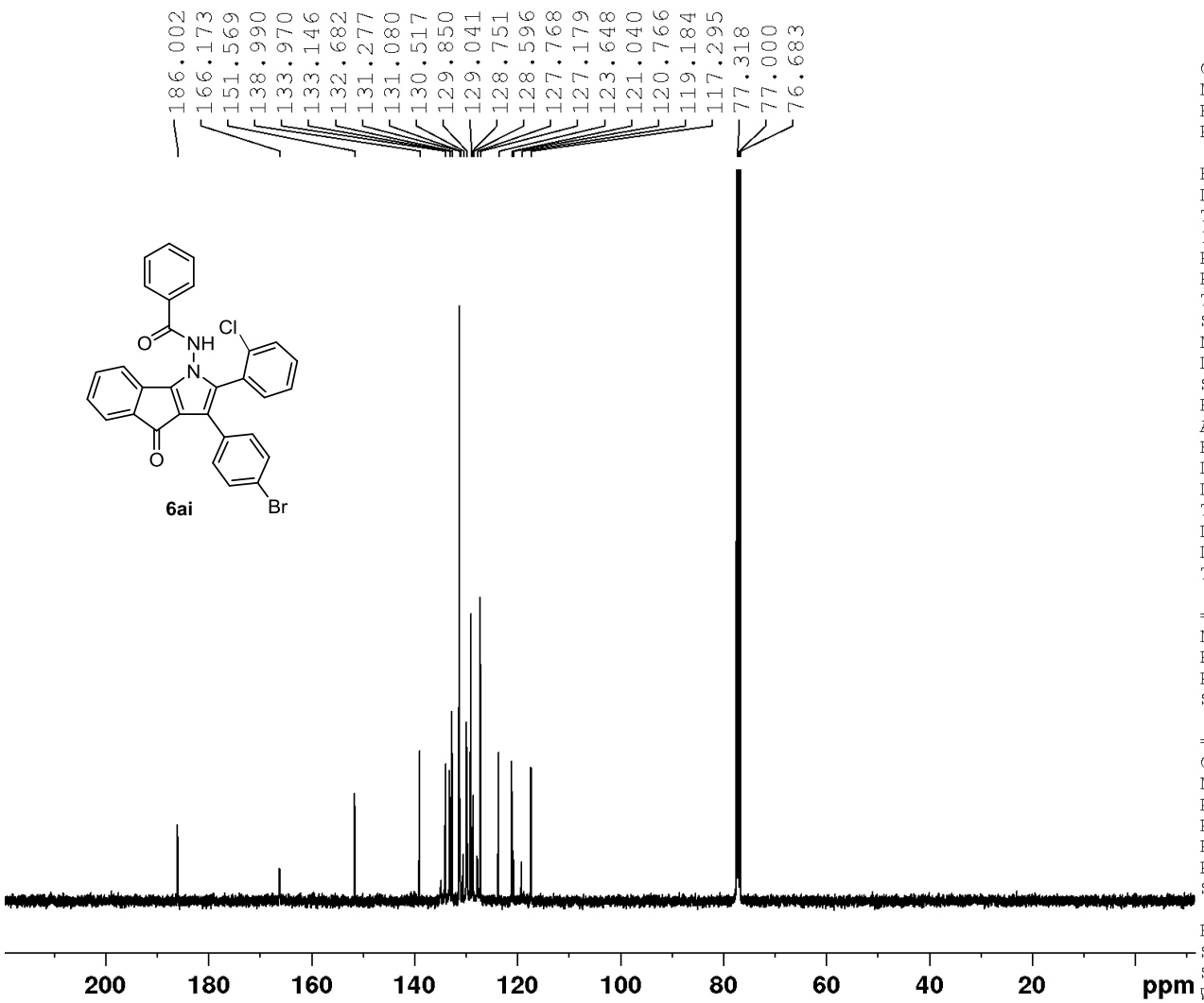

```
Current Data Parameters
NAME                   16
EXPNO                   4
PROCNO                  1

F2 - Acquisition Parameters
Date_           20200421
Time                1.11
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                32768
SOLVENT           CDCl3
NS                12512
DS                    0
SWH           24038.461 Hz
FIDRES         0.733596 Hz
AQ            0.6815744 sec
RG                198.09
DW               20.800 usec
DE                6.50 usec
TE                295.8 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1        100.6228298 MHz
NUC1                13C
P1                10.00 usec
PLW1        49.50000000 W

======== CHANNEL f2 ========
SFO2        400.1316005 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2             90.00 usec
PLW2        12.50000000 W
PLW12        0.34722000 W
PLW13        0.28125000 W

F2 - Processing parameters
SI                32768
SF          100.6127698 MHz
WDW                EM
SSB                   0
LB                2.00 Hz
GB                    0
PC                1.00
```

^{1}H NMR Spectrum of **6ai** ($CDCl_3$, 400 MHz)



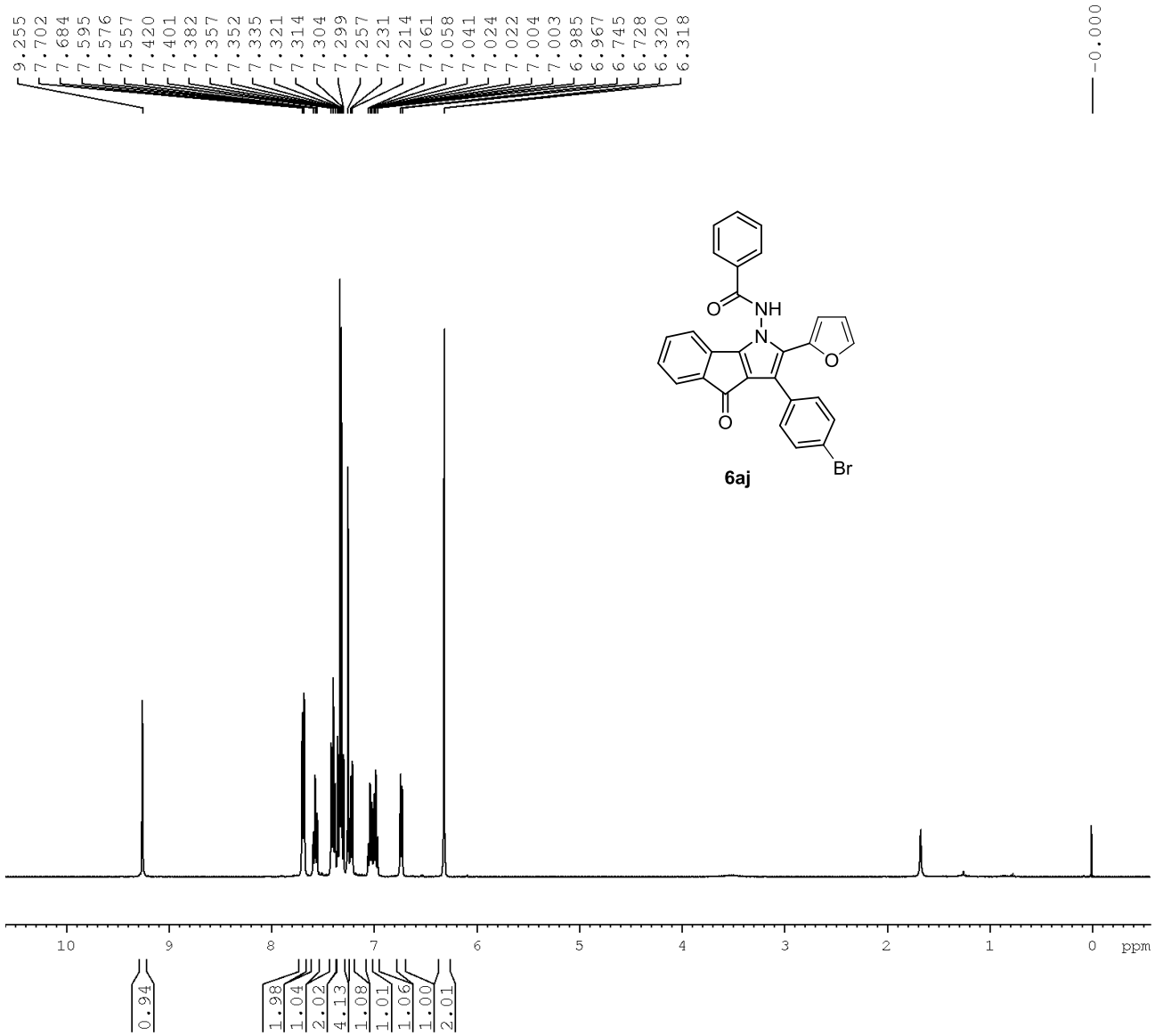

```
Current Data Parameters
NAME                  bc 2-Cl
EXPNO                       1
PROCNO                      1

F2 - Acquisition Parameters
Date_               20200317
Time                   11.56
INSTRUM                spect
PROBHD   5 mm BBO BB-1H
PULPROG                 zg30
TD                     32768
SOLVENT                CDCl3
NS                        16
DS                         0
SWH                 7246.377 Hz
FIDRES              0.221142 Hz
AQ                  2.2609921 sec
RG                      161.3
DW                     69.000 usec
DE                      6.50 usec
TE                     296.2 K
D1                  2.00000000 sec
TD0                         1

======== CHANNEL f1 ========
NUC1                       1H
P1                     15.00 usec
PL1                    11.10 dB
SFO1             400.1324008 MHz

F2 - Processing parameters
SI                      16384
SF                400.1300112 MHz
WDW                        EM
SSB          0
LB           0 Hz
GB           0
PC                      1.00
```

^{13}C NMR Spectrum of **6ai** ($CDCl_3$, 100 MHz)



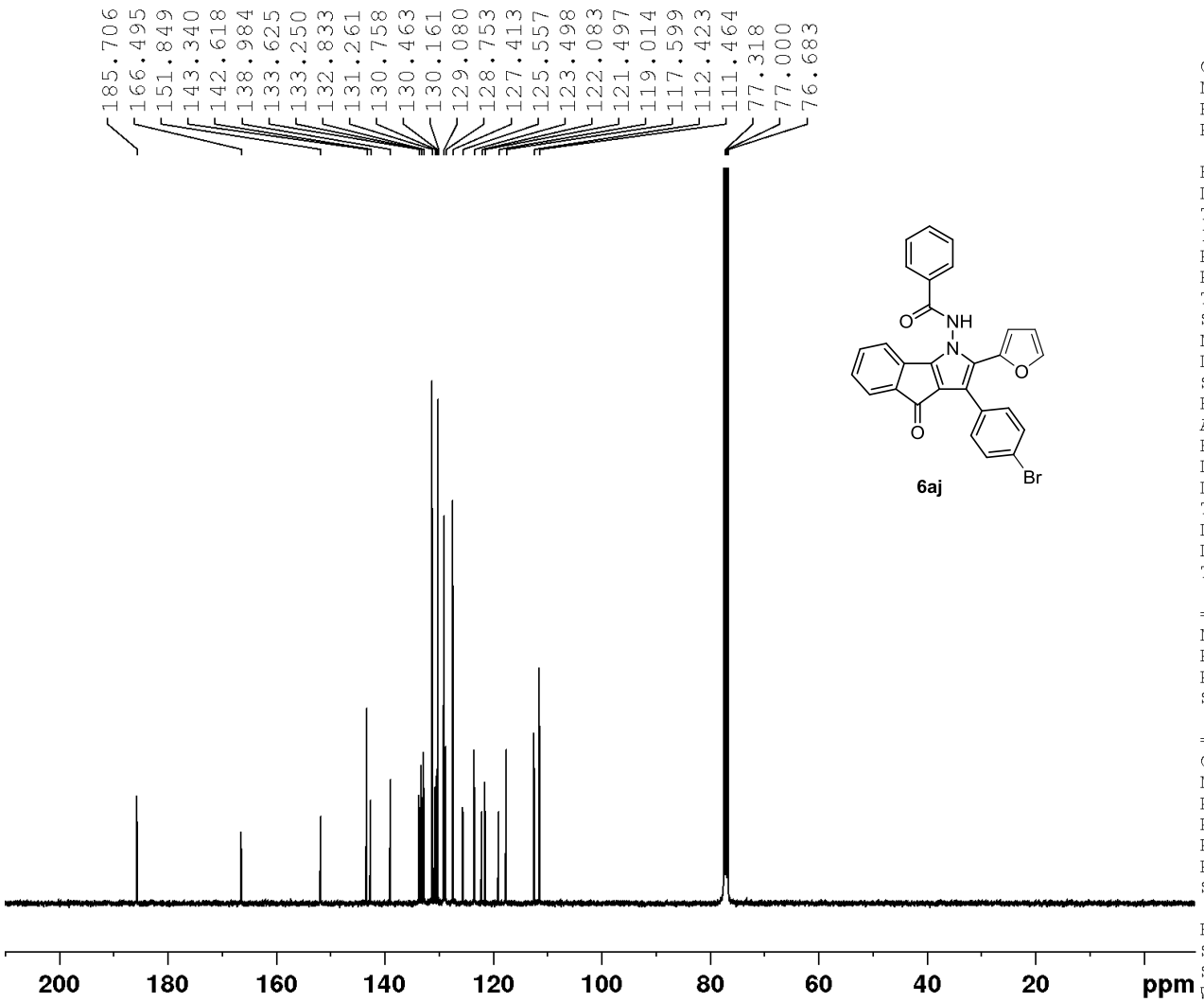

```
Current Data Parameters
NAME              bc 2-Cl
EXPNO                   2
PROCNO                  1

F2 - Acquisition Parameters
Date_           20200317
Time               11.59
INSTRUM             spect
PROBHD   5 mm BBO BB-1H
PULPROG           zgpg30
TD                 32768
SOLVENT            CDCl3
NS                  2085
DS                     0
SWH           24038.461 Hz
FIDRES         0.733596 Hz
AQ             0.6815744 sec
RG                5792.6
DW                20.800 usec
DE                 6.50 usec
TE                296.1 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                 13C
P1                10.00 usec
PL1                3.80 dB
SFO1        100.6233325 MHz

======== CHANNEL f2 ========
CPDPRG[2          waltz16
NUC2                 1H
PCPD2             90.00 usec
PL2               10.20 dB
PL12              26.00 dB
PL13              29.00 dB
SFO2        400.1316005 MHz

F2 - Processing parameters
SI                 32768
SF          100.6127724 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.00
```

^{1}H NMR Spectrum of **6aj** ($CDCl_3$, 400 MHz)




```
Current Data Parameters
NAME            Bc Furyl
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20200303
Time               21.54
INSTRUM            spect
PROBHD   5 mm BBO BB-1H
PULPROG             zg30
TD                 32768
SOLVENT            CDCl3
NS                    16
DS                     0
SWH             7246.377 Hz
FIDRES          0.221142 Hz
AQ              2.2609921 sec
RG                   181
DW                69.000 usec
DE                 6.50 usec
TE                296.4 K
D1             2.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                15.00 usec
PL1               11.10 dB
SFO1         400.1324008 MHz

F2 - Processing parameters
SI                 16384
SF           400.1300105 MHz
WDW                   EM
SSB                    0
LB                     0 Hz
GB                     0
PC                  1.00
```

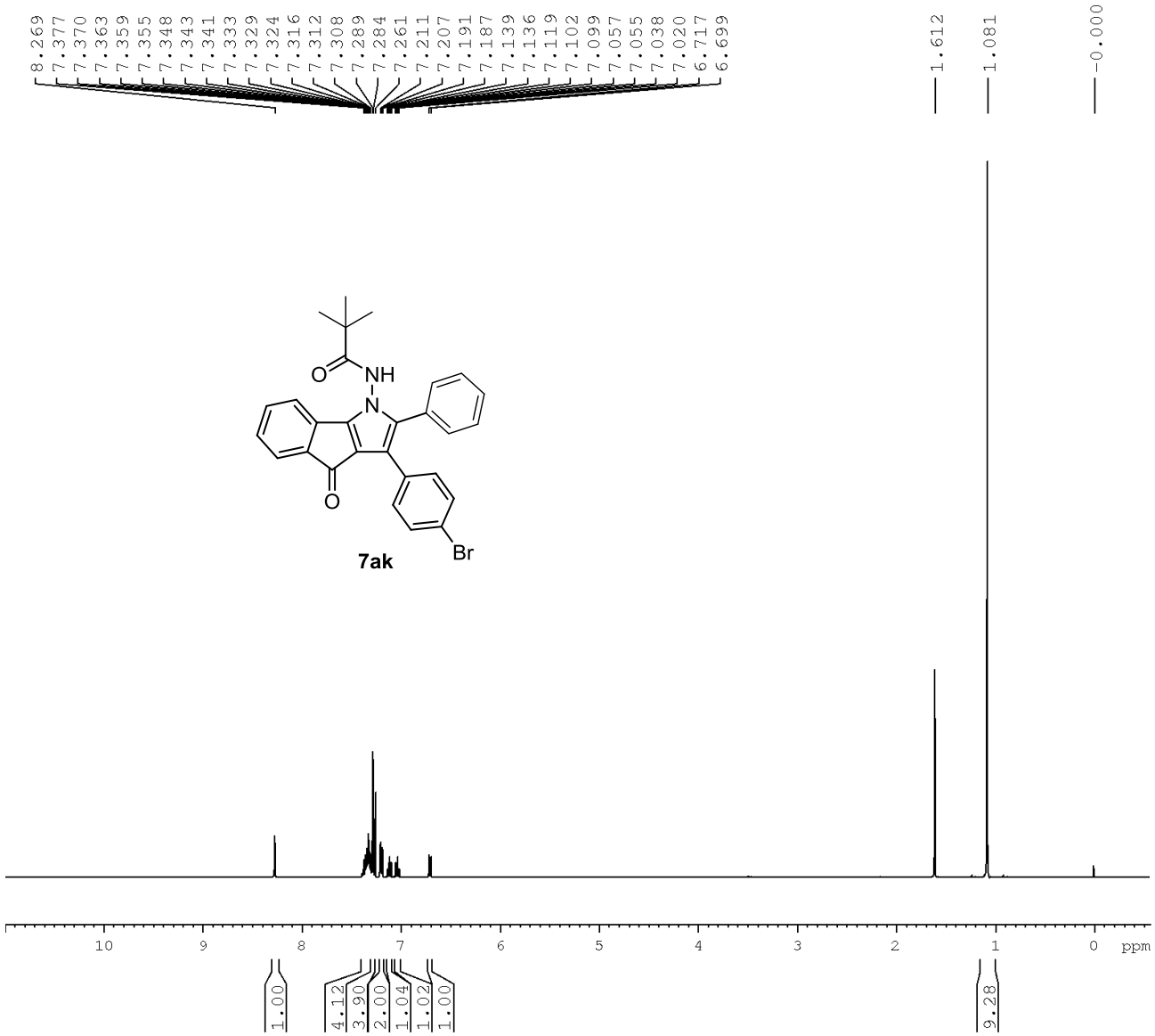
^{13}C NMR Spectrum of **6aj** ($CDCl_3$, 100 MHz)



6aj

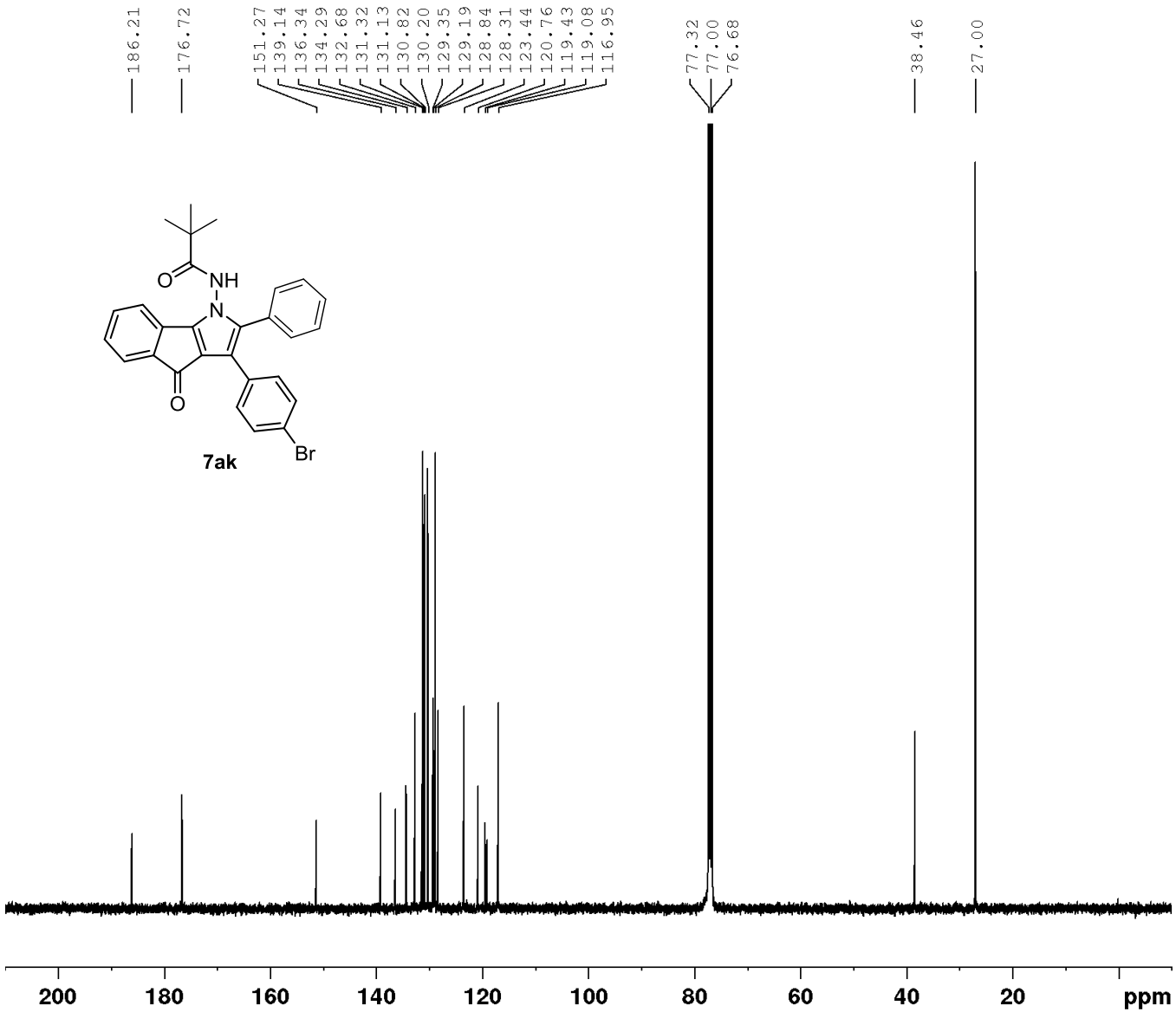
```
Current Data Parameters
NAME            Bc Furyl
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20200303
Time               21.56
INSTRUM            spect
PROBHD   5 mm BBO BB-1H
PULPROG          zgpg30
TD                 32768
SOLVENT            CDCl3
NS                 15000
DS                     0
SWH           24038.461 Hz
FIDRES         0.733596 Hz
AQ            0.6815744 sec
RG                  8192
DW                20.800 usec
DE                 6.50 usec
TE                296.4 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                13C
P1                10.00 usec
PL1                3.80 dB
SFO1        100.6233325 MHz

======== CHANNEL f2 ========
CPDPRG[2         waltz16
NUC2                1H
PCPD2              90.00 usec
PL2                10.20 dB
PL12               26.00 dB
PL13               29.00 dB
SFO2        400.1316005 MHz

F2 - Processing parameters
SI                 32768
SF          100.6127710 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.00
```

^{1}H NMR Spectrum of **7ak** ($CDCl_3$, 400 MHz)



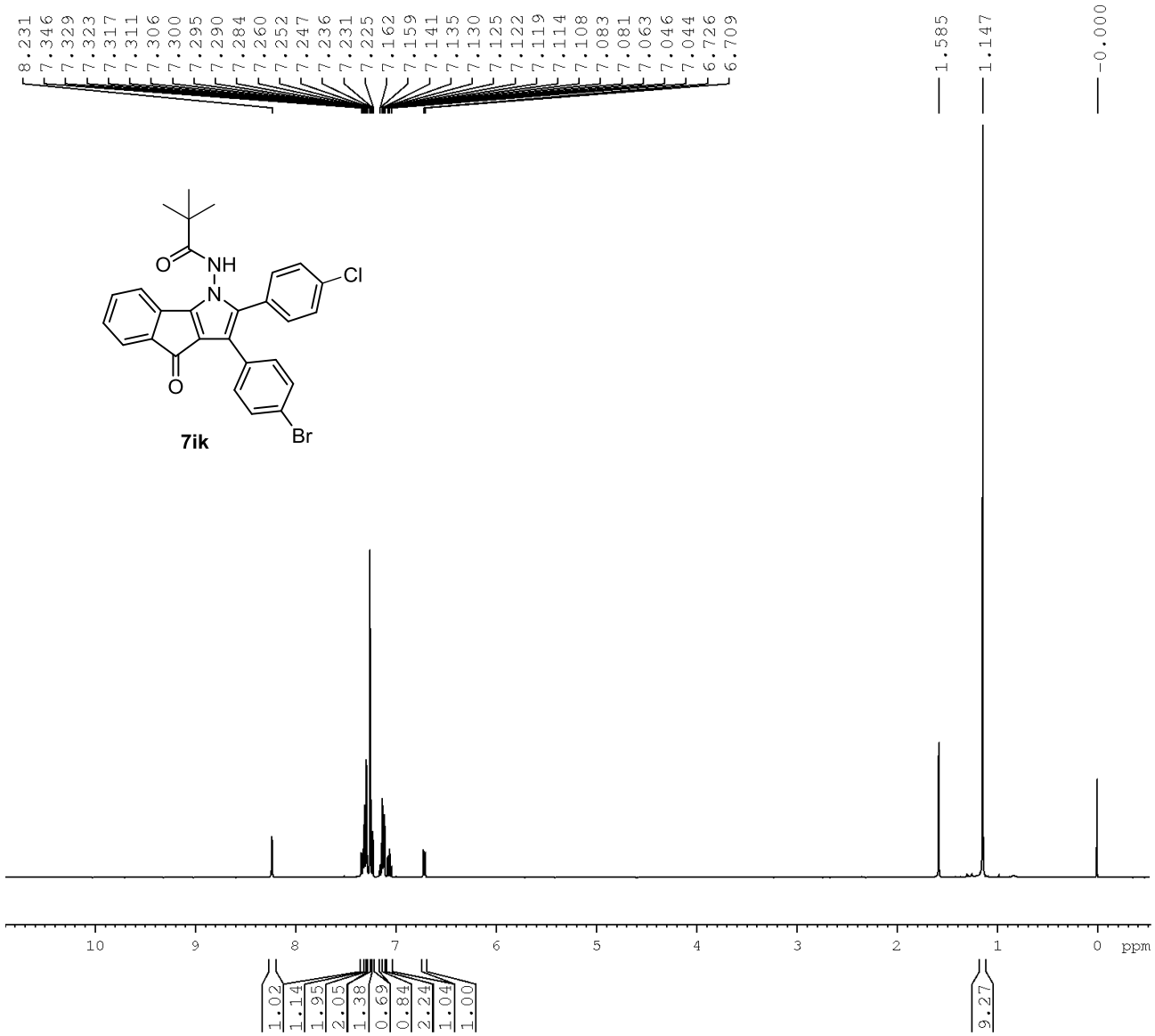

```
Current Data Parameters
NAME                  452
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_            20200422
Time                22.15
INSTRUM             spect
PROBHD   5 mm BBO BB-1H
PULPROG              zg30
TD                  32768
SOLVENT             CDCl3
NS                     32
DS                      0
SWH              7246.377 Hz
FIDRES           0.221142 Hz
AQ               2.2609921 sec
RG                    256
DW                 69.000 usec
DE                  6.50 usec
TE                 296.6 K
D1              2.00000000 sec
TD0                     1

======== CHANNEL f1 ========
NUC1                   1H
P1                 15.00 usec
PL1                11.10 dB
SFO1         400.1324008 MHz

F2 - Processing parameters
SI                  16384
SF           400.1300101 MHz
WDW                    EM
SSB                     0
LB                      0 Hz
GB                      0
PC                   1.00
```

^{13}C NMR Spectrum of **7ak** ($CDCl_3$, 100 MHz)



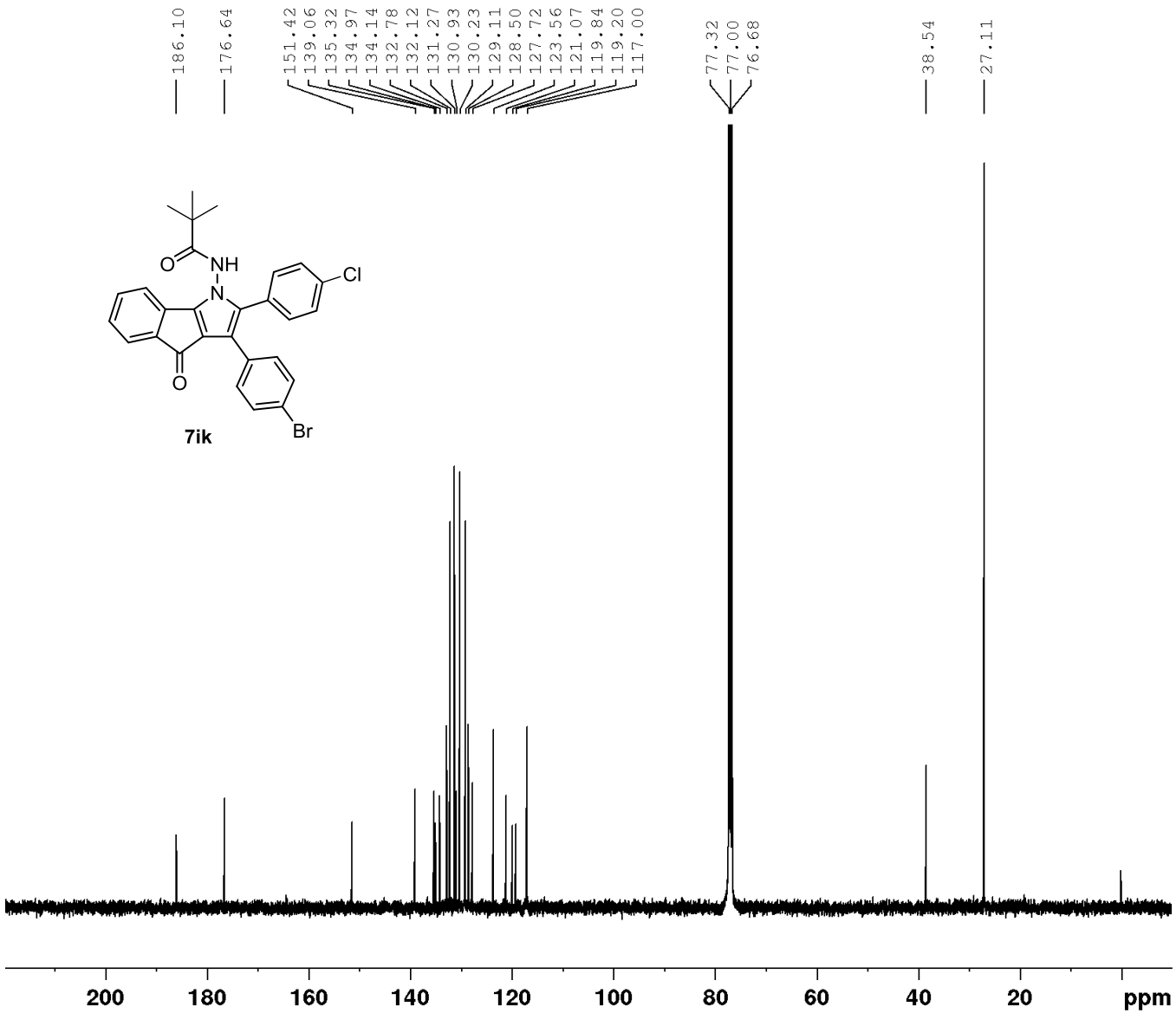

```
Current Data Parameters
NAME                  452
EXPNO                   2
PROCNO                  1

F2 - Acquisition Parameters
Date_           20200422
Time               22.18
INSTRUM            spect
PROBHD   5 mm BBO BB-1H
PULPROG          zgpg30
TD                32768
SOLVENT           CDCl3
NS                14849
DS                    0
SWH           24038.461 Hz
FIDRES         0.733596 Hz
AQ            0.6815744 sec
RG               9195.2
DW               20.800 usec
DE                6.50 usec
TE                296.6 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 13C
P1                10.00 usec
PL1                3.80 dB
SFO1        100.6233325 MHz

======== CHANNEL f2 ========
CPDPRG[2         waltz16
NUC2                 1H
PCPD2             90.00 usec
PL2               10.20 dB
PL12              26.00 dB
PL13              29.00 dB
SFO2        400.1316005 MHz

F2 - Processing parameters
SI                32768
SF          100.6127696 MHz
WDW                  EM
SSB                   0
LB                1.00 Hz
GB                    0
PC                1.00
```

^{1}H NMR Spectrum of **7ik** ($CDCl_3$, 400 MHz)



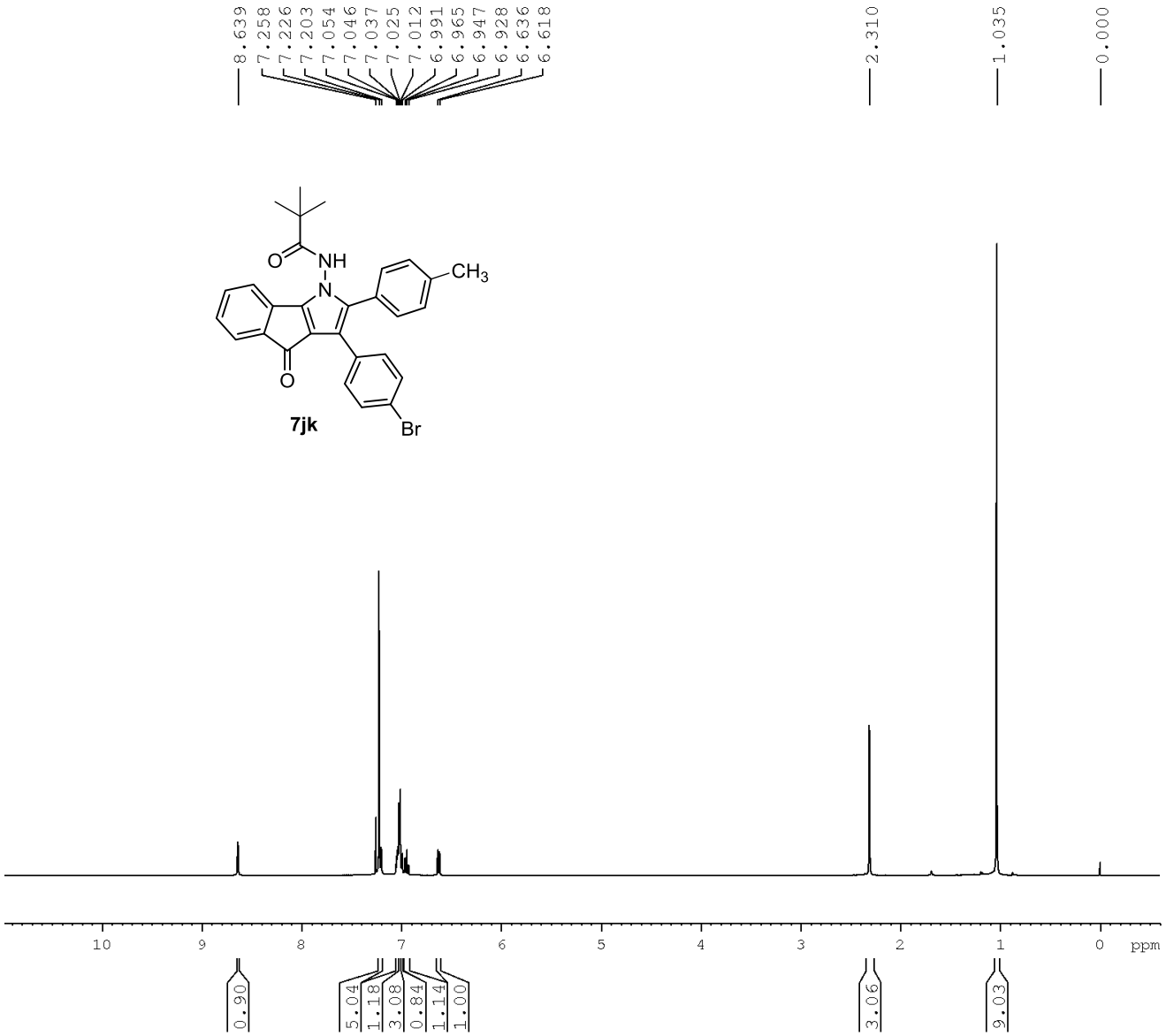

```
Current Data Parameters
NAME            SW 876-1
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20200520
Time               10.09
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG             zg30
TD                 32768
SOLVENT            CDCl3
NS                    64
DS                     0
SWH             7211.539 Hz
FIDRES          0.220079 Hz
AQ              2.2719147 sec
RG                198.09
DW                69.333 usec
DE                10.06 usec
TE                298.1 K
D1             2.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         400.1324008 MHz
NUC1                   1H
P1                 15.00 usec
PLW1         11.39999962 W

F2 - Processing parameters
SI                 16384
SF           400.1300092 MHz
WDW                   EM
SSB                    0
LB                     0 Hz
GB                     0
PC                  1.00
```

^{13}C NMR Spectrum of **7ik** ($CDCl_3$, 100 MHz)



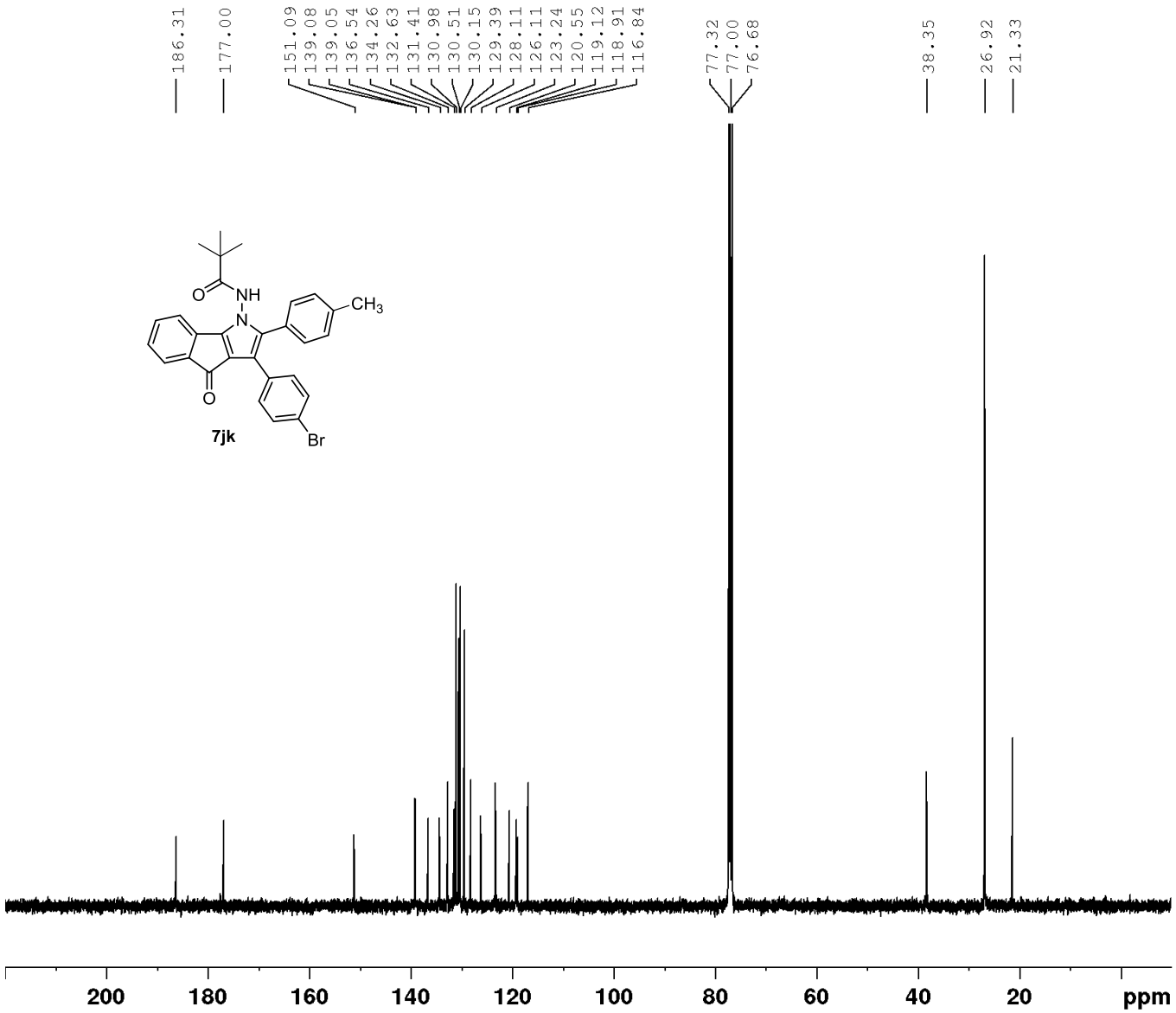

```
Current Data Parameters
NAME                  SW 876
EXPNO                      2
PROCNO                     1

F2 - Acquisition Parameters
Date_              20200519
Time                  23.47
INSTRUM               spect
PROBHD    5 mm BBO BB-1H
PULPROG             zgpg30
TD                    32768
SOLVENT               CDCl3
NS                    13144
DS                        0
SWH              24038.461 Hz
FIDRES            0.733596 Hz
AQ               0.6815744 sec
RG                  9195.2
DW                 20.800 usec
DE                  6.50 usec
TE                 296.6 K
D1              2.00000000 sec
D11             0.03000000 sec
TD0                       1

======== CHANNEL f1 ========
NUC1                    13C
P1                  10.00 usec
PL1                  3.80 dB
SFO1          100.6233325 MHz

======== CHANNEL f2 ========
CPDPRG[2           waltz16
NUC2                    1H
PCPD2               90.00 usec
PL2                 10.20 dB
PL12                26.00 dB
PL13                29.00 dB
SFO2          400.1316005 MHz

F2 - Processing parameters
SI                    32768
SF            100.6127700 MHz
WDW                      EM
SSB                       0
LB                   1.00 Hz
GB                        0
PC                   1.00
```

^{1}H NMR Spectrum of **7jk** ($CDCl_3$, 400 MHz)



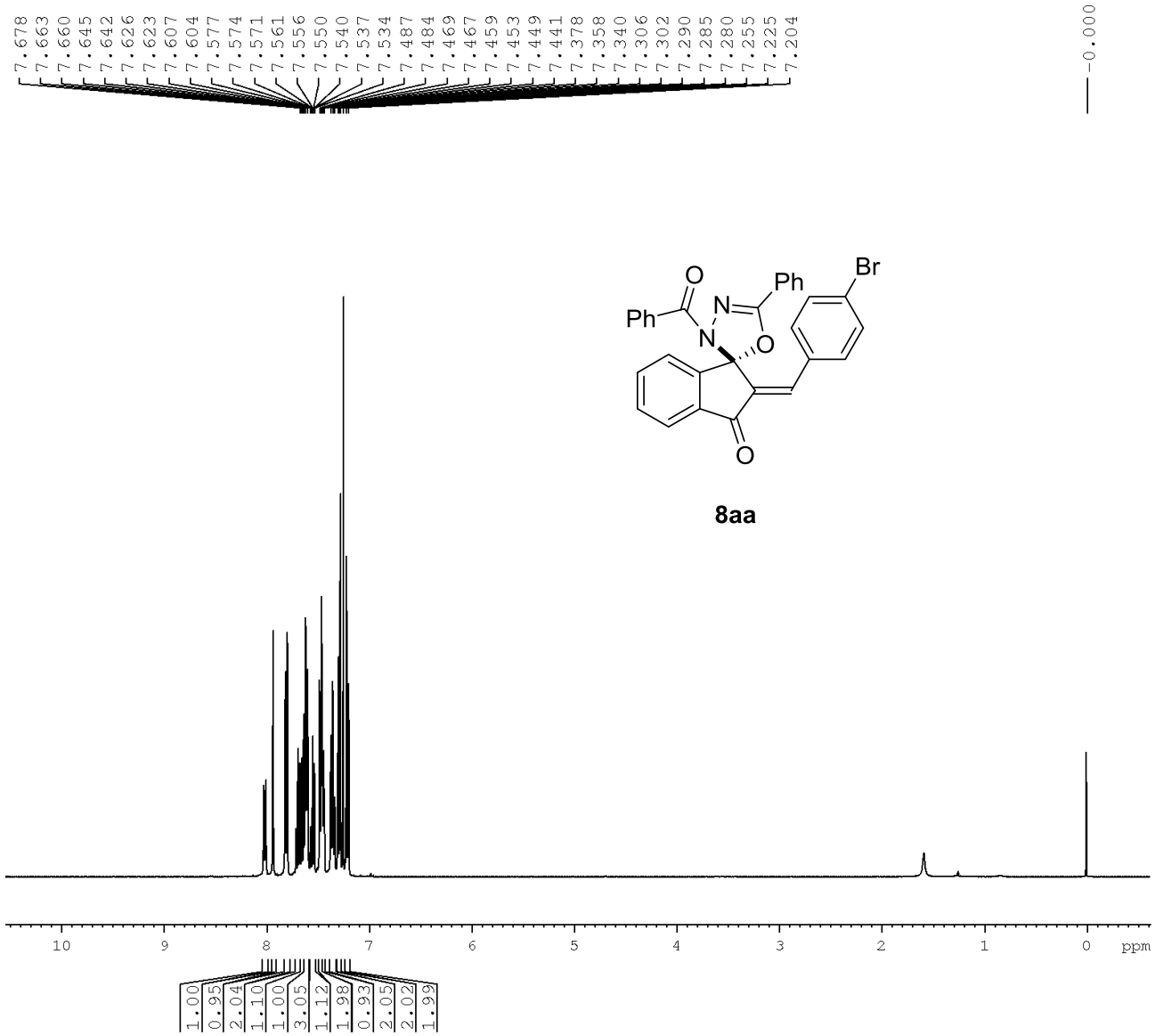

```
Current Data Parameters
NAME            SW 875-1
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20200520
Time               10.03
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG             zg30
TD                 32768
SOLVENT            CDCl3
NS                    32
DS                     0
SWH             7211.539 Hz
FIDRES          0.220079 Hz
AQ              2.2719147 sec
RG                 71.42
DW                69.333 usec
DE                10.06 usec
TE                299.1 K
D1           2.000000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         400.1324008 MHz
NUC1                   1H
P1                 15.00 usec
PLW1         11.39999962 W

F2 - Processing parameters
SI                 16384
SF           400.1300102 MHz
WDW                   EM
SSB                    0
LB                     0 Hz
GB                     0
PC                  1.00
```

^{13}C NMR Spectrum of **7jk** ($CDCl_3$, 100 MHz)




```
Current Data Parameters
NAME                  SW 875
EXPNO                      3
PROCNO                     1

F2 - Acquisition Parameters
Date_              20200519
Time                  22.17
INSTRUM               spect
PROBHD    5 mm BBO BB-1H
PULPROG             zgpg30
TD                    32768
SOLVENT               CDCl3
NS                     1749
DS                        0
SWH              24038.461 Hz
FIDRES            0.733596 Hz
AQ               0.6815744 sec
RG                     4096
DW                  20.800 usec
DE                   6.50 usec
TE                  296.0 K
D1              2.00000000 sec
D11             0.03000000 sec
TD0                       1

======== CHANNEL f1 ========
NUC1                    13C
P1                   10.00 usec
PL1                   3.80 dB
SFO1           100.6233325 MHz

======== CHANNEL f2 ========
CPDPRG[2           waltz16
NUC2                    1H
PCPD2                90.00 usec
PL2                  10.20 dB
PL12                 26.00 dB
PL13                 29.00 dB
SFO2           400.1316005 MHz

F2 - Processing parameters
SI                    32768
SF             100.6127730 MHz
WDW                      EM
SSB                       0
LB                    1.00 Hz
GB                        0
PC                    1.00
```

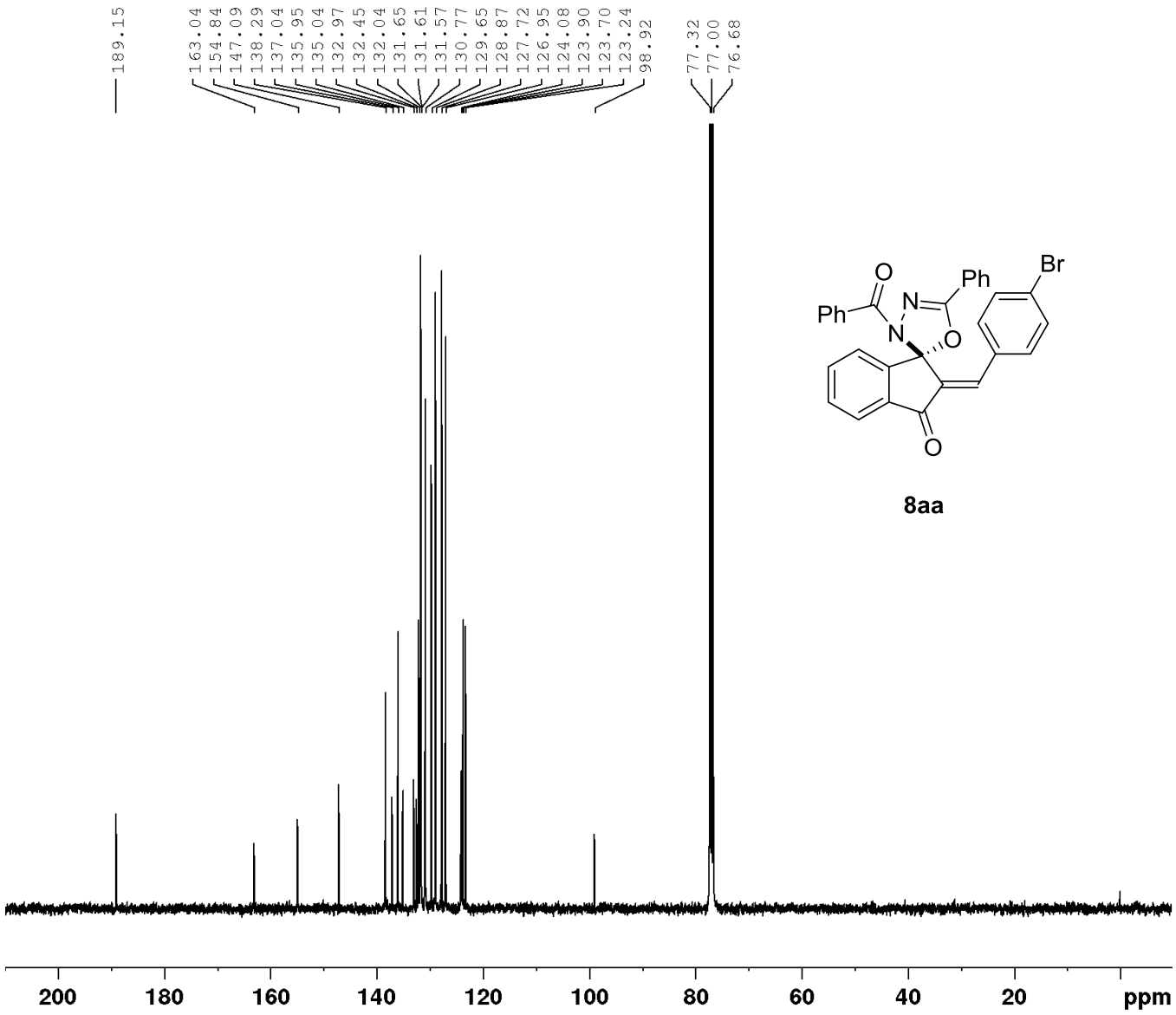
^{1}H NMR Spectrum of **8aa** ($CDCl_3$, 400 MHz)



8aa

```
Current Data Parameters
NAME            SW 852-1
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20200520
Time               21.56
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG             zg30
TD                 32768
SOLVENT            CDCl3
NS                    32
DS                     0
SWH              7211.539 Hz
FIDRES           0.220079 Hz
AQ               2.2719147 sec
RG                 99.72
DW                69.333 usec
DE                10.06 usec
TE                298.3 K
D1             2.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         400.1324008 MHz
NUC1                   1H
P1                 15.00 usec
PLW1         11.39999962 W

F2 - Processing parameters
SI                 16384
SF           400.1300115 MHz
WDW                   EM
SSB                    0
LB                     0 Hz
GB                     0
PC                  1.00
```

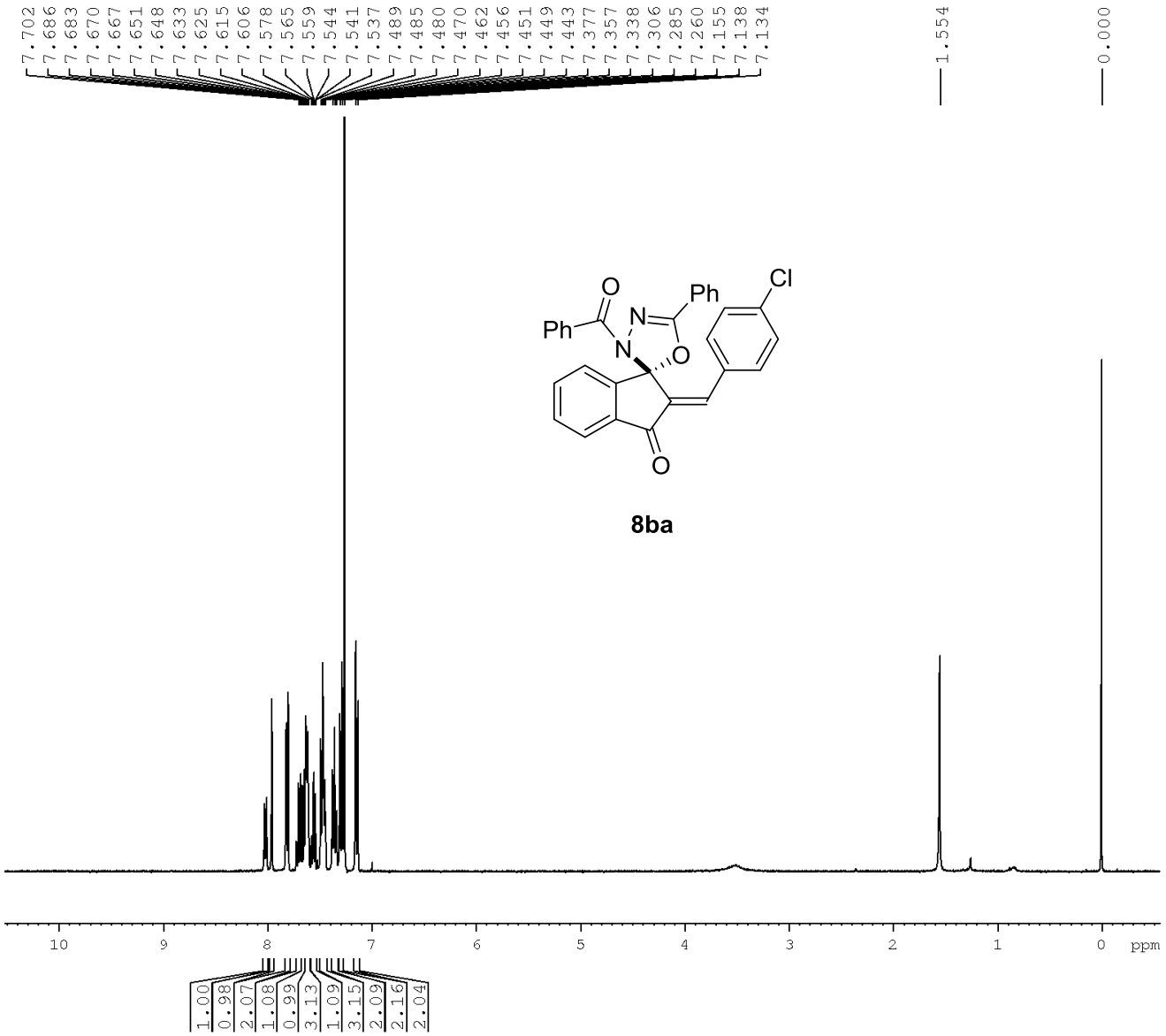
^{13}C NMR Spectrum of **8aa** ($CDCl_3$, 100 MHz)



8aa

```
Current Data Parameters
NAME            SW 852-1
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20200520
Time               21.59
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG         zgpg30
TD                 32768
SOLVENT            CDCl3
NS                  2377
DS                     0
SWH           24038.461 Hz
FIDRES         0.733596 Hz
AQ            0.6815744 sec
RG                198.09
DW               20.800 usec
DE                6.50 usec
TE                298.3 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1        100.6228298 MHz
NUC1                13C
P1                10.00 usec
PLW1         49.50000000 W

======== CHANNEL f2 ========
SFO2        400.1316005 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2             90.00 usec
PLW2         12.50000000 W
PLW12         0.34722000 W
PLW13         0.28125000 W

F2 - Processing parameters
SI                 32768
SF          100.6127717 MHz
WDW                  EM
SSB                   0
LB                 2.00 Hz
GB                    0
PC                 1.00
```

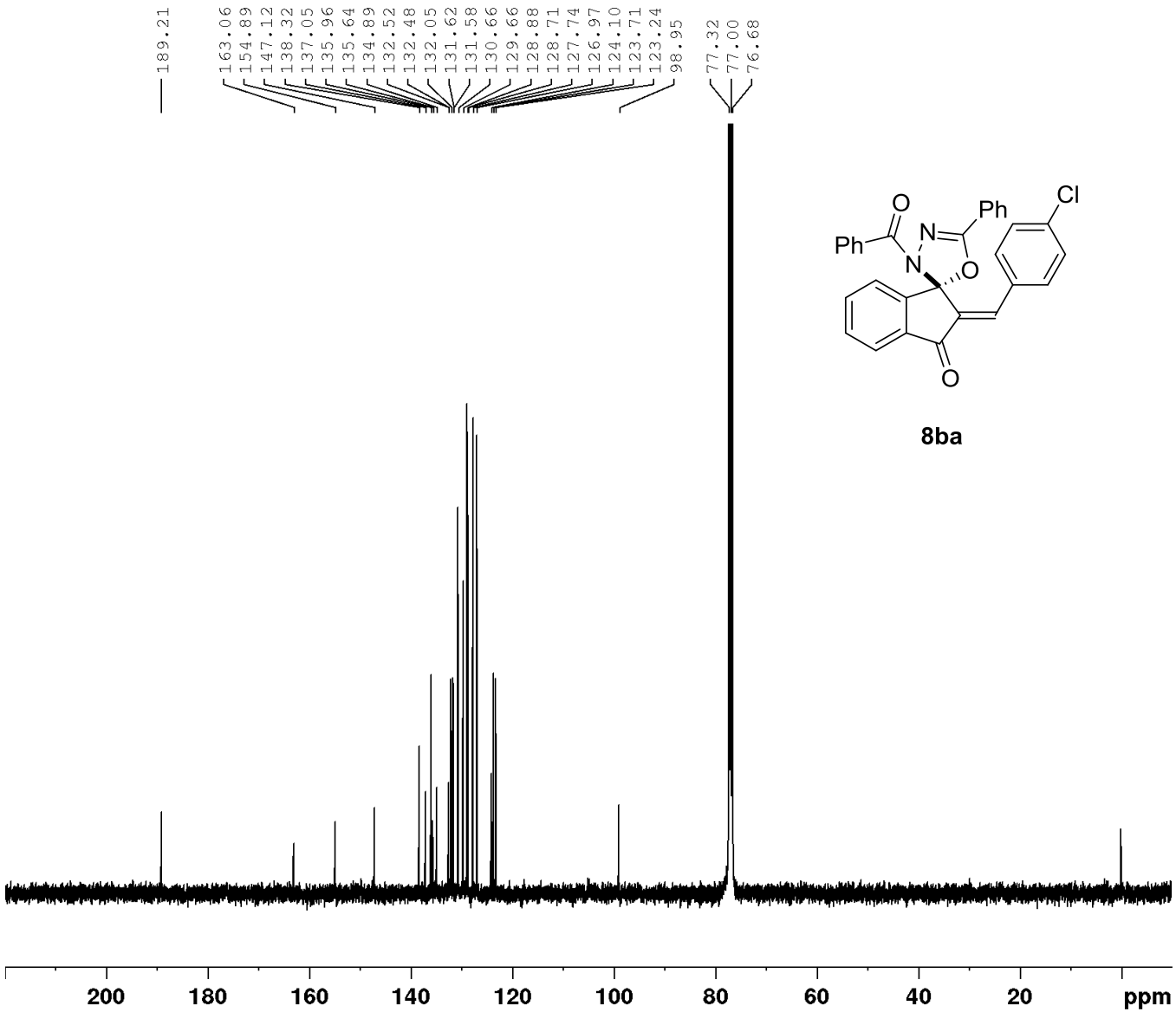
^{1}H NMR Spectrum of **8ba** ($CDCl_3$, 400 MHz)



8ba

```
Current Data Parameters
NAME                 SW 819
EXPNO                     4
PROCNO                    1

F2 - Acquisition Parameters
Date_              20200523
Time                 21.07
INSTRUM              spect
PROBHD    5 mm BBO BB-1H
PULPROG               zg30
TD                   32768
SOLVENT              CDCl3
NS                      32
DS                       0
SWH               7246.377 Hz
FIDRES            0.221142 Hz
AQ                2.2609921 sec
RG                     362
DW                  69.000 usec
DE                   6.50 usec
TE                  295.8 K
D1              2.00000000 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                    1H
P1                   15.00 usec
PL1                  11.10 dB
SFO1          400.1324008 MHz

F2 - Processing parameters
SI                   16384
SF            400.1300106 MHz
WDW                     EM
SSB                      0
LB                       0 Hz
GB                       0
PC                    1.00
```

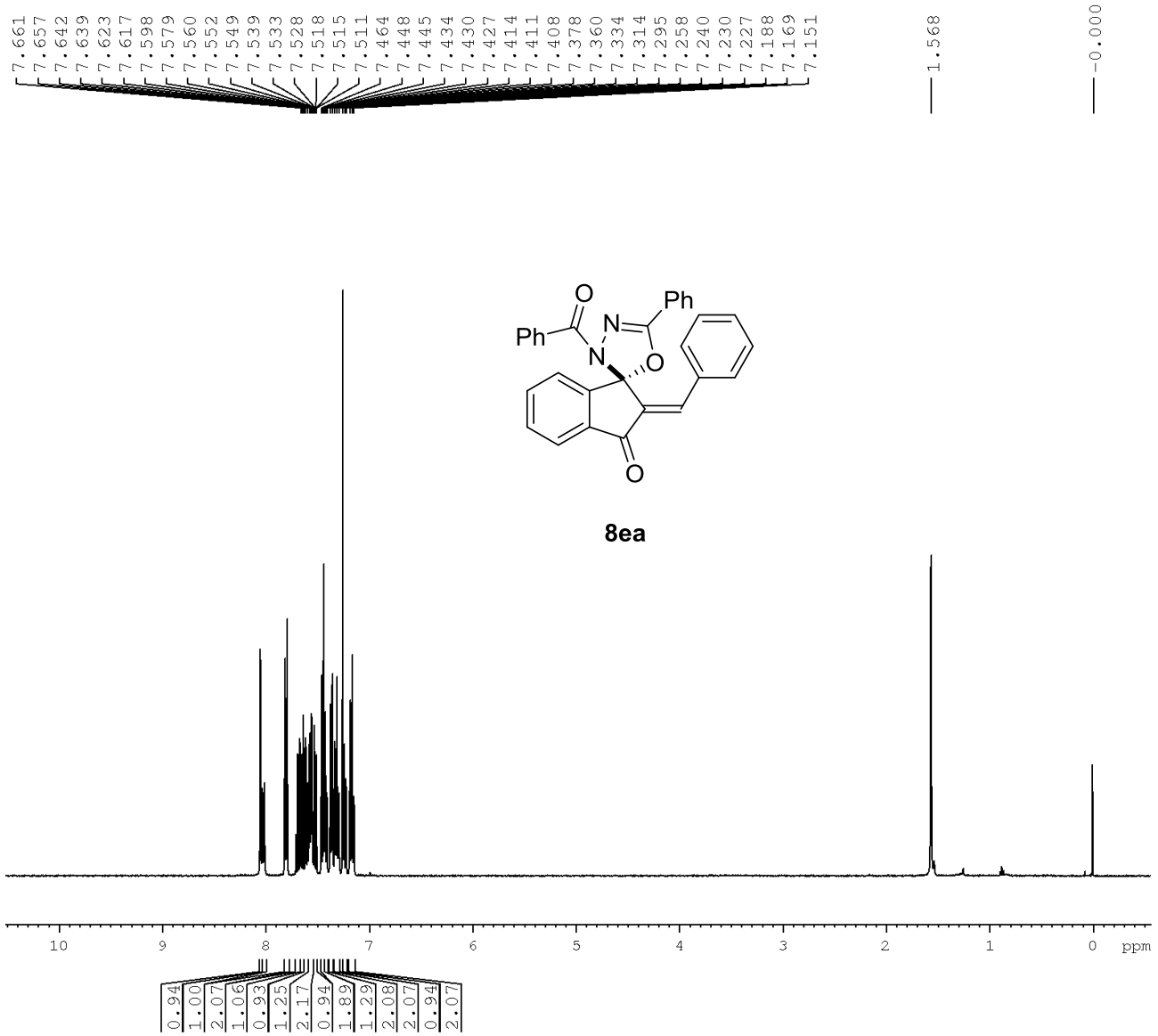
^{13}C NMR Spectrum of **8ba** ($CDCl_3$, 100 MHz)



8ba

```
Current Data Parameters
NAME                 SW 819
EXPNO                     5
PROCNO                    1

F2 - Acquisition Parameters
Date_              20200523
Time                 21.11
INSTRUM              spect
PROBHD    5 mm BBO BB-1H
PULPROG             zgpg30
TD                   32768
SOLVENT              CDCl3
NS                   18238
DS                       0
SWH             24038.461 Hz
FIDRES           0.733596 Hz
AQ              0.6815744 sec
RG                 9195.2
DW                20.800 usec
DE                 6.50 usec
TE                 295.8 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                   13C
P1                  10.00 usec
PL1                  3.80 dB
SFO1          100.6233325 MHz

======== CHANNEL f2 ========
CPDPRG[2           waltz16
NUC2                   1H
PCPD2               90.00 usec
PL2                 10.20 dB
PL12                26.00 dB
PL13                29.00 dB
SFO2          400.1316005 MHz

F2 - Processing parameters
SI                   32768
SF            100.6127694 MHz
WDW                    EM
SSB                     0
LB                   1.00 Hz
GB                      0
PC                   1.00
```

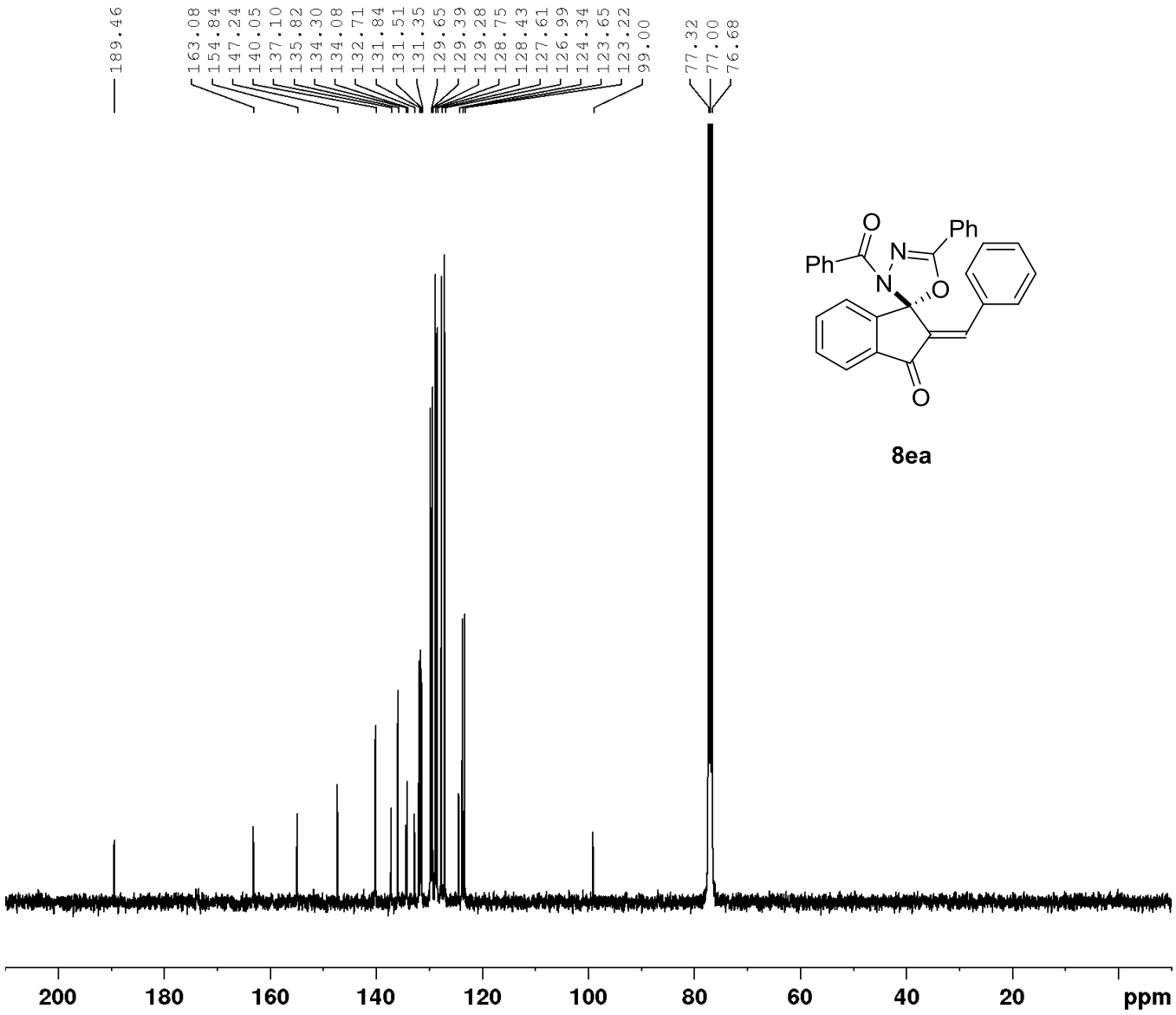
^{1}H NMR Spectrum of **8ea** ($CDCl_3$, 400 MHz)



8ea

```
Current Data Parameters
NAME            SW 861-1
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20200510
Time               21.50
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG             zg30
TD                 32768
SOLVENT            CDCl3
NS                    32
DS                     0
SWH             7211.539 Hz
FIDRES          0.220079 Hz
AQ              2.2719147 sec
RG                198.09
DW                69.333 usec
DE                10.06 usec
TE                298.6 K
D1             2.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         400.1324008 MHz
NUC1                   1H
P1                 15.00 usec
PLW1         11.39999962 W

F2 - Processing parameters
SI                 16384
SF           400.1300104 MHz
WDW                   EM
SSB                    0
LB                     0 Hz
GB                     0
PC                  1.00
```

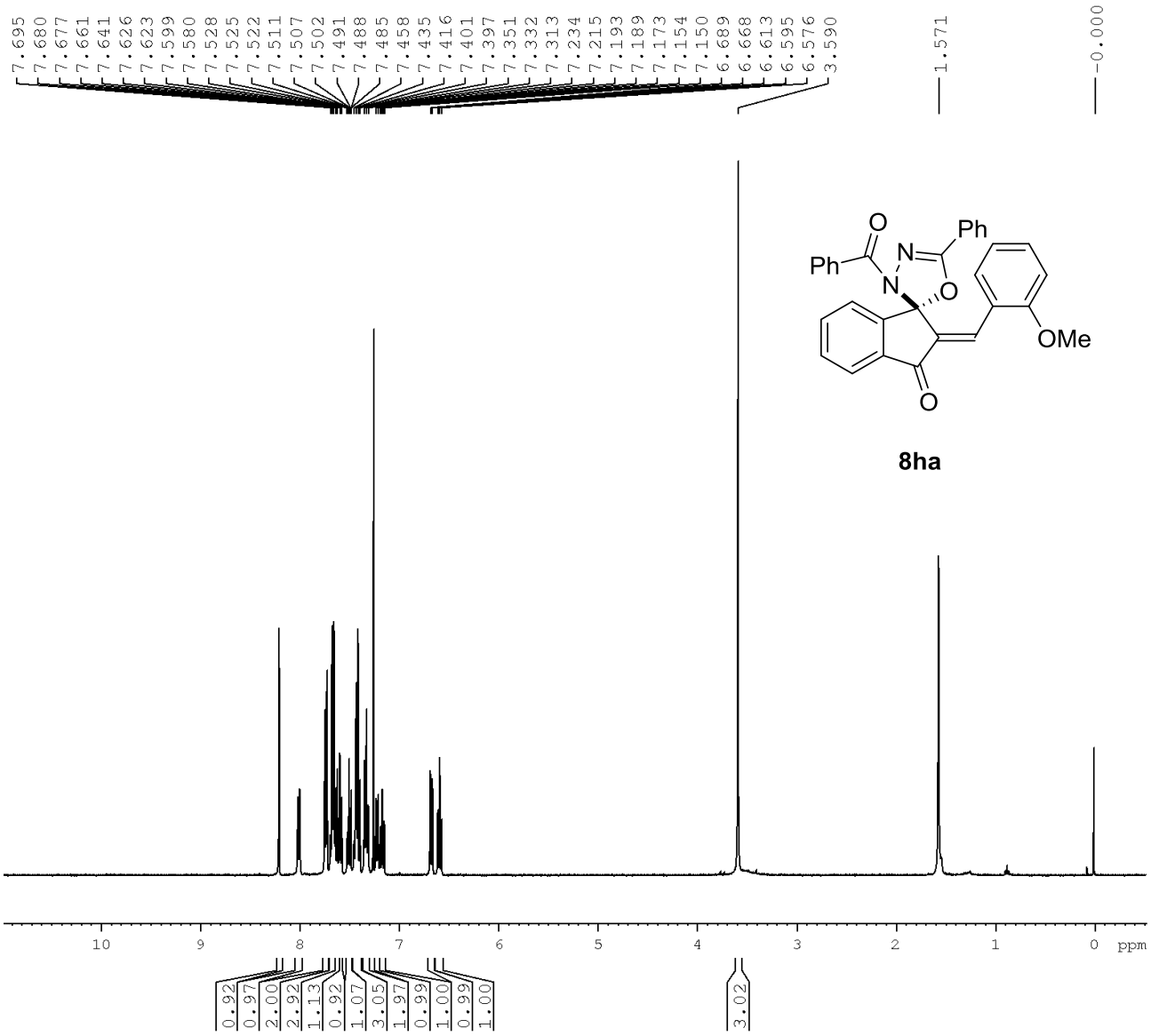
^{13}C NMR Spectrum of **8ea** ($CDCl_3$, 100 MHz)



8ea

```
Current Data Parameters
NAME            SW 861-1
EXPNO                  3
PROCNO                 1

F2 - Acquisition Parameters
Date_           20200510
Time               21.53
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                 32768
SOLVENT            CDCl3
NS                 10000
DS                     0
SWH           24038.461 Hz
FIDRES         0.733596 Hz
AQ            0.6815744 sec
RG                198.09
DW               20.800 usec
DE                6.50 usec
TE                298.6 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         100.6228298 MHz
NUC1                13C
P1                10.00 usec
PLW1         49.50000000 W

======== CHANNEL f2 ========
SFO2         400.1316005 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2             90.00 usec
PLW2         12.50000000 W
PLW12         0.34722000 W
PLW13         0.28125000 W

F2 - Processing parameters
SI                 32768
SF           100.6127708 MHz
WDW                  EM
SSB                   0
LB                 2.00 Hz
GB                    0
PC                 1.00
```

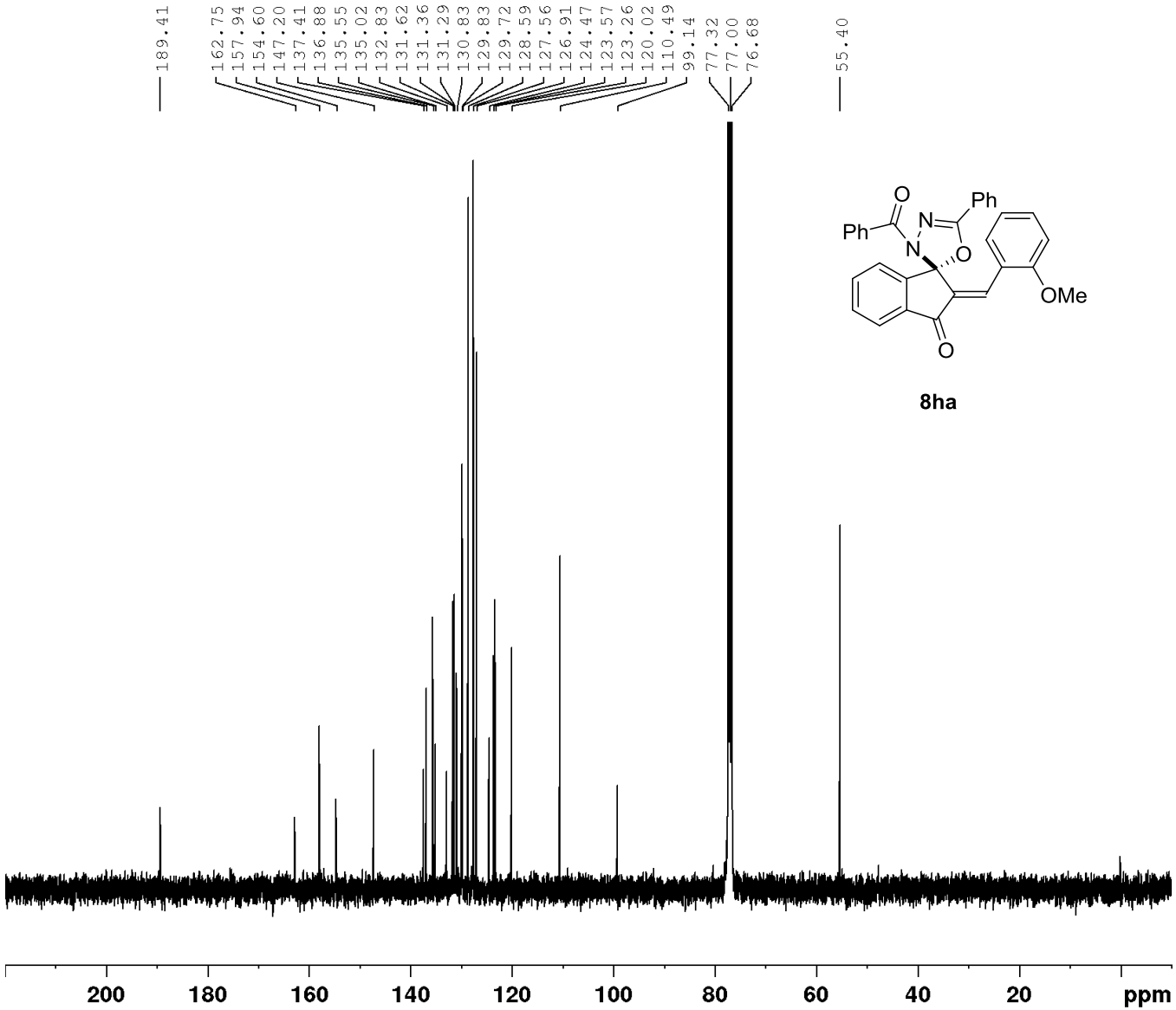
^{1}H NMR Spectrum of **8ha** ($CDCl_3$, 400 MHz)



8ha

```
Current Data Parameters
NAME                 SW 853
EXPNO                     3
PROCNO                    1

F2 - Acquisition Parameters
Date_              20200509
Time                   0.36
INSTRUM               spect
PROBHD    5 mm BBO BB-1H
PULPROG                zg30
TD                    32768
SOLVENT               CDCl3
NS                       32
DS                        0
SWH                7246.377 Hz
FIDRES            0.221142 Hz
AQ                2.2609921 sec
RG                    322.5
DW                   69.000 usec
DE                    6.50 usec
TE                   296.9 K
D1              2.00000000 sec
TD0                       1

======== CHANNEL f1 ========
NUC1                     1H
P1                   15.00 usec
PL1                  11.10 dB
SFO1           400.1324008 MHz

F2 - Processing parameters
SI                    16384
SF             400.1300110 MHz
WDW                      EM
SSB                       0
LB                        0 Hz
GB                        0
PC                     1.00
```

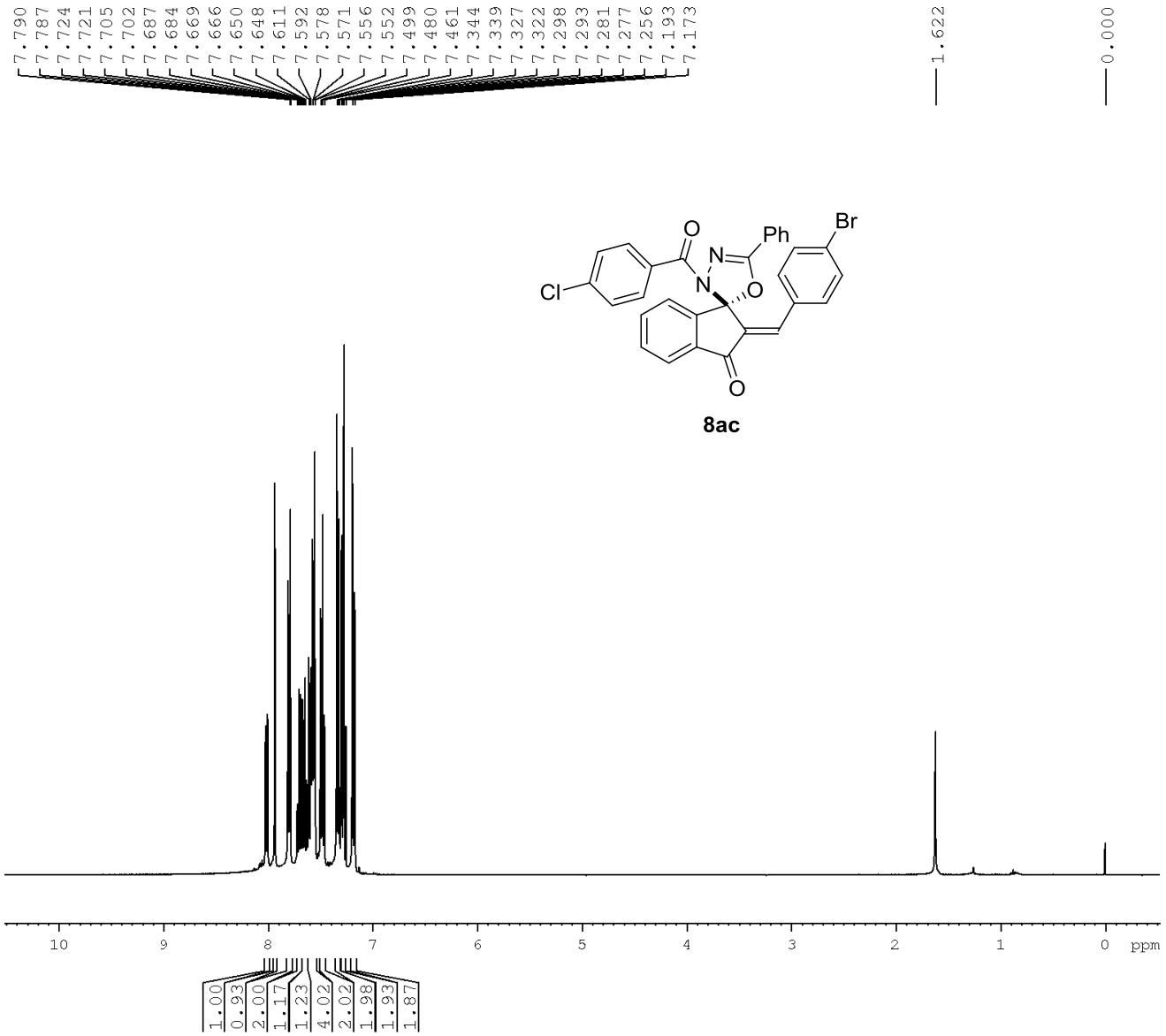
^{13}C NMR Spectrum of **8ha** ($CDCl_3$, 100 MHz)



8ha

```
Current Data Parameters
NAME                 SW 853
EXPNO                     4
PROCNO                    1

F2 - Acquisition Parameters
Date_              20200509
Time                   0.39
INSTRUM               spect
PROBHD    5 mm BBO BB-1H
PULPROG              zgpg30
TD                    32768
SOLVENT               CDCl3
NS                     9945
DS                        0
SWH              24038.461 Hz
FIDRES            0.733596 Hz
AQ               0.6815744 sec
RG                     8192
DW                  20.800 usec
DE                   6.50 usec
TE                   296.8 K
D1              2.00000000 sec
D11             0.03000000 sec
TD0                       1

======== CHANNEL f1 ========
NUC1                    13C
P1                   10.00 usec
PL1                   3.80 dB
SFO1          100.6233325 MHz

======== CHANNEL f2 ========
CPDPRG[2           waltz16
NUC2                    1H
PCPD2                90.00 usec
PL2                  10.20 dB
PL12                 26.00 dB
PL13                 29.00 dB
SFO2          400.1316005 MHz

F2 - Processing parameters
SI                    32768
SF            100.6127701 MHz
WDW                      EM
SSB                       0
LB                    1.00 Hz
GB                        0
PC                    1.00
```

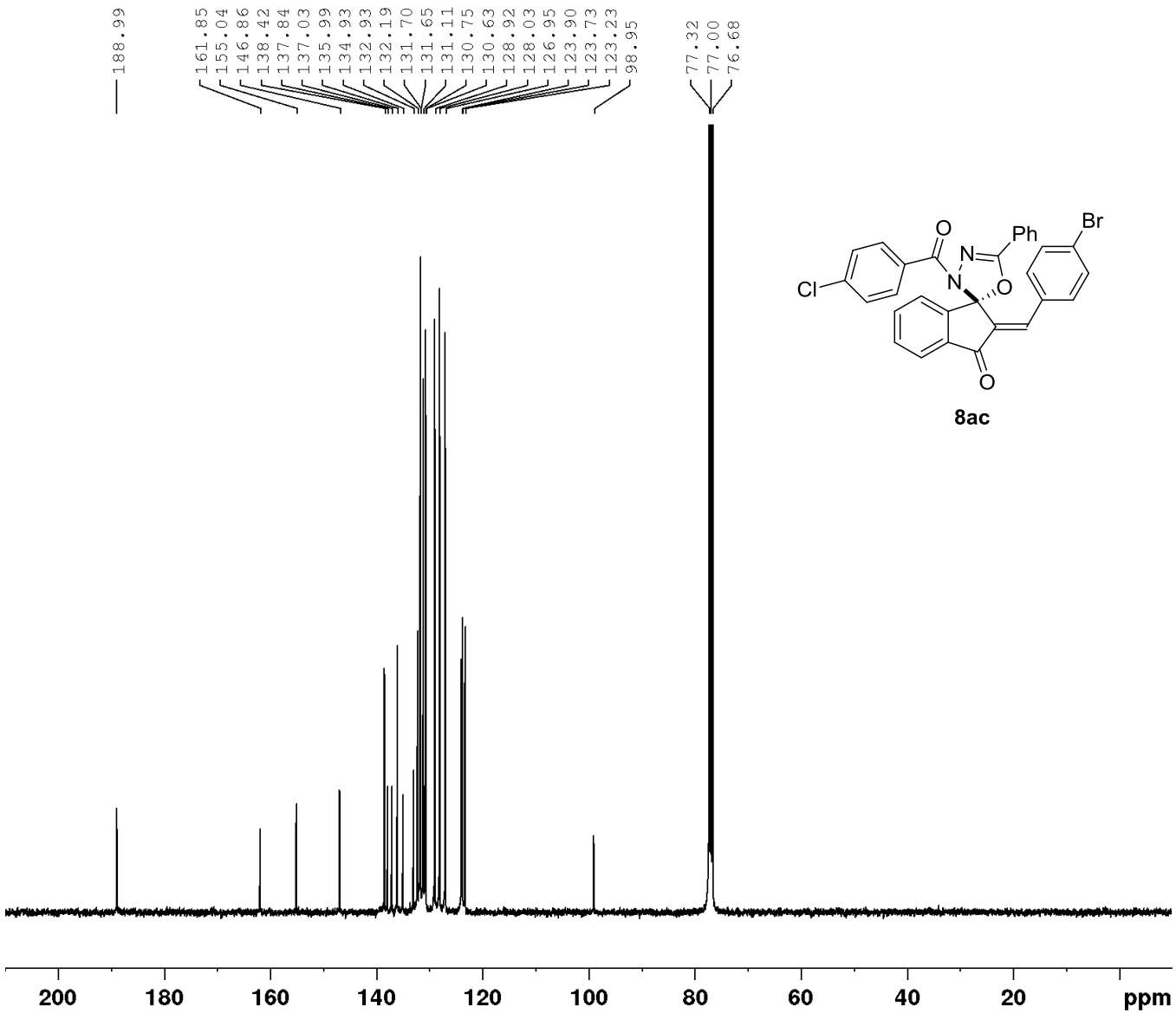
^{1}H NMR Spectrum of **8ac** ($CDCl_3$, 400 MHz)



8ac

```
Current Data Parameters
NAME            SW 856-1
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20200509
Time               18.08
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG             zg30
TD                 32768
SOLVENT            CDCl3
NS                    32
DS                     0
SWH             7211.539 Hz
FIDRES          0.220079 Hz
AQ             2.2719147 sec
RG                 89.08
DW                69.333 usec
DE                10.06 usec
TE                297.7 K
D1            2.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         400.1324008 MHz
NUC1                   1H
P1                 15.00 usec
PLW1         11.39999962 W

F2 - Processing parameters
SI                 16384
SF           400.1300111 MHz
WDW                   EM
SSB                    0
LB                     0 Hz
GB                     0
PC                  1.00
```

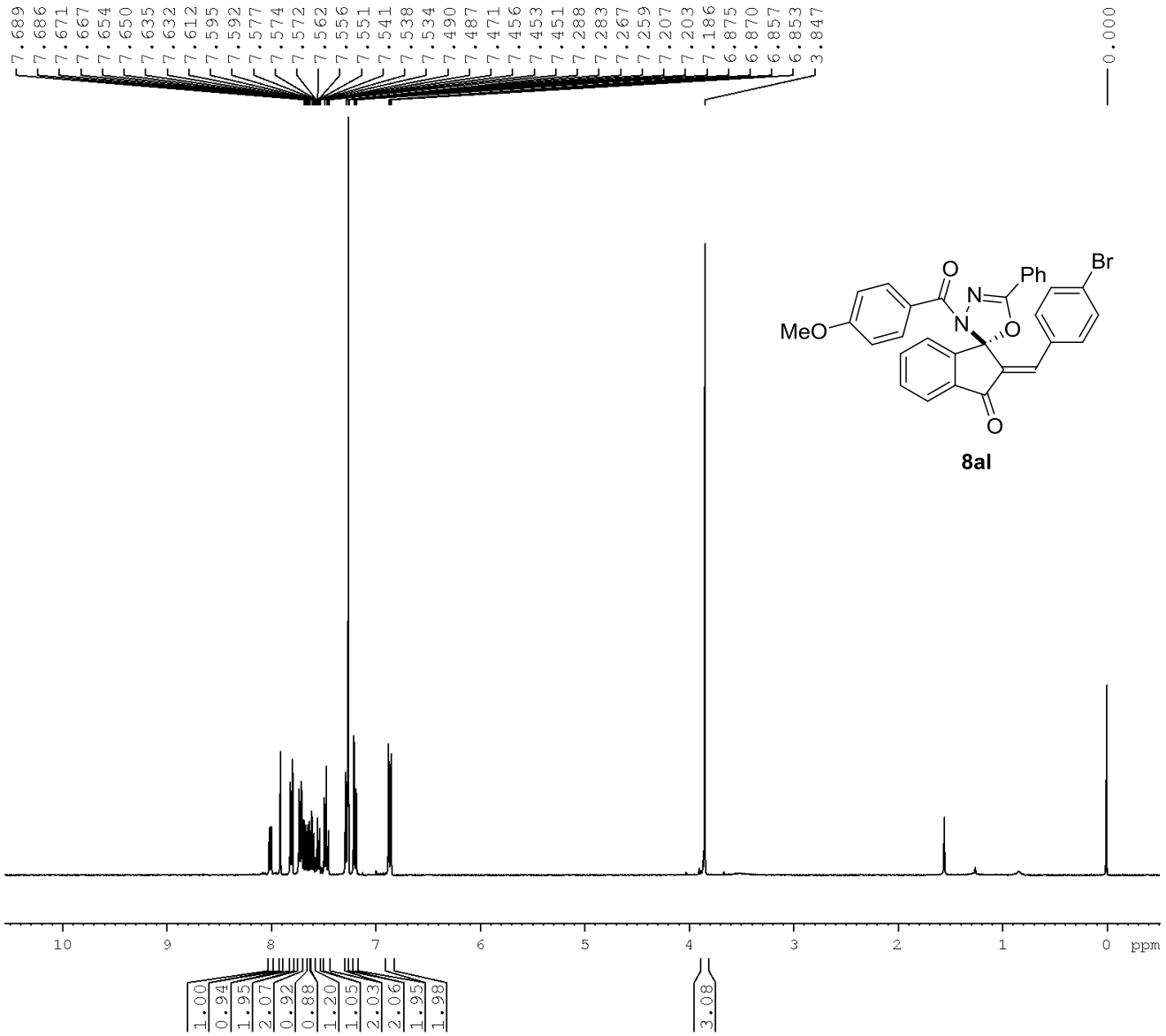
^{13}C NMR Spectrum of **8ac** ($CDCl_3$, 100 MHz)



8ac

```
Current Data Parameters
NAME            SW 856-1
EXPNO                  3
PROCNO                 1

F2 - Acquisition Parameters
Date_           20200509
Time               18.11
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG         zgpg30
TD                32768
SOLVENT           CDCl3
NS                 4222
DS                    0
SWH           24038.461 Hz
FIDRES         0.733596 Hz
AQ            0.6815744 sec
RG                198.09
DW               20.800 usec
DE                6.50 usec
TE                297.9 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1        100.6228298 MHz
NUC1                13C
P1                10.00 usec
PLW1        49.50000000 W

======== CHANNEL f2 ========
SFO2        400.1316005 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2             90.00 usec
PLW2        12.50000000 W
PLW12        0.34722000 W
PLW13        0.28125000 W

F2 - Processing parameters
SI                32768
SF          100.6127727 MHz
WDW                EM
SSB                 0
LB                2.00 Hz
GB                  0
PC                1.00
```

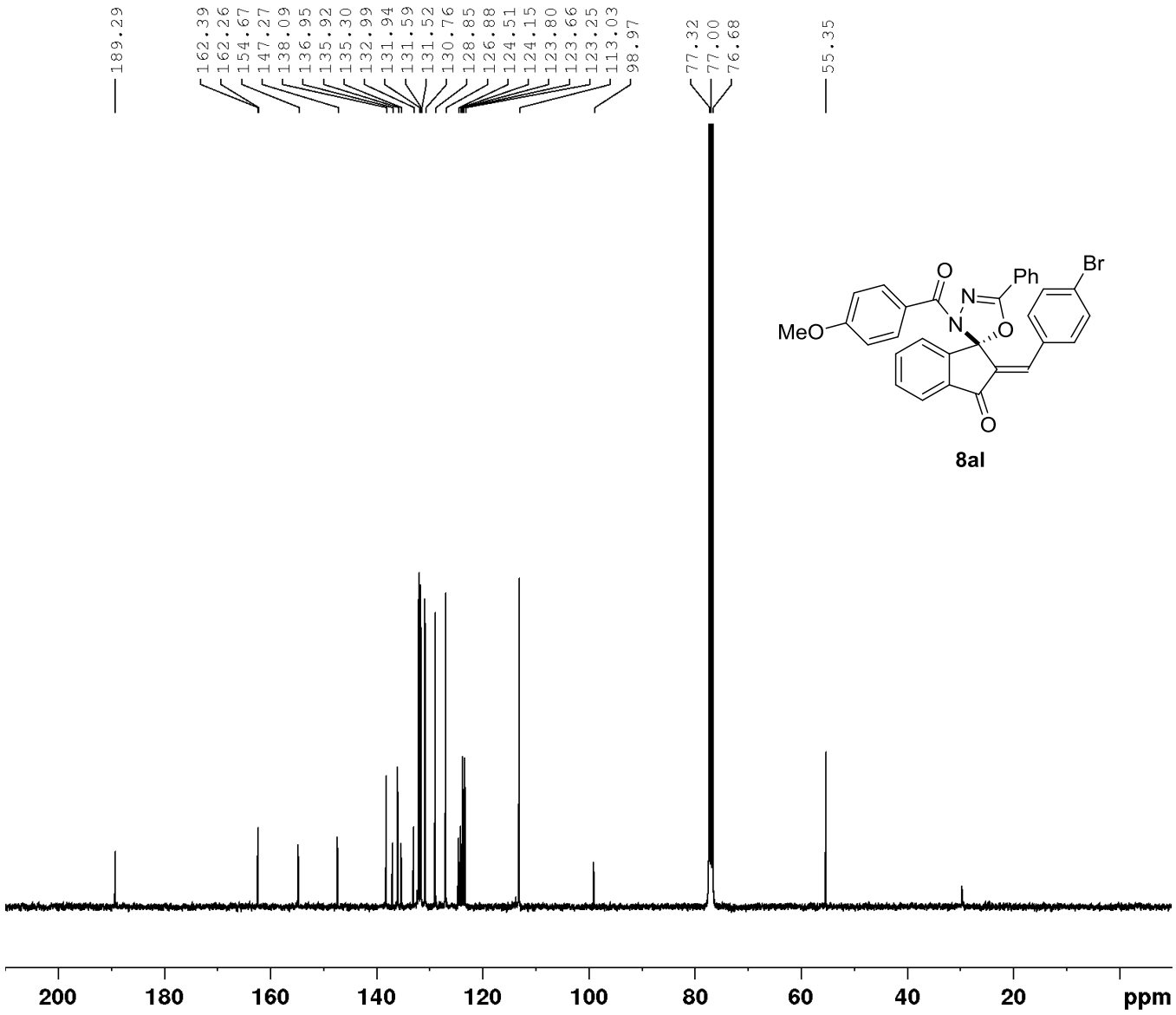
^{1}H NMR Spectrum of **8al** ($CDCl_3$, 400 MHz)



8al

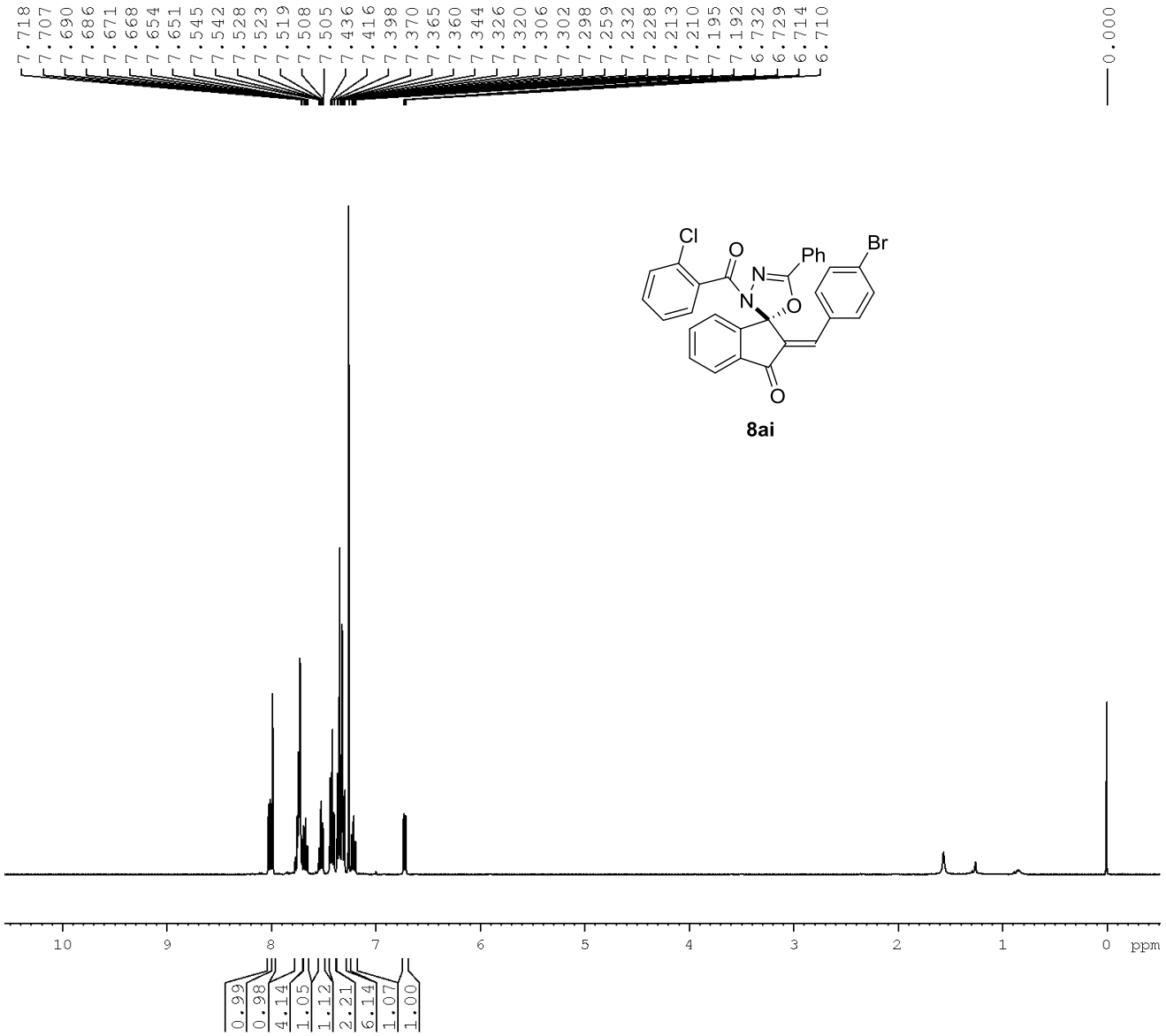
```
Current Data Parameters
NAME                 SW 831
EXPNO                     9
PROCNO                    1

F2 - Acquisition Parameters
Date_             20200524
Time                 19.48
INSTRUM              spect
PROBHD    5 mm BBO BB-1H
PULPROG               zg30
TD                   32768
SOLVENT              CDCl3
NS                      32
DS                       0
SWH                7246.377 Hz
FIDRES            0.221142 Hz
AQ                2.2609921 sec
RG                   322.5
DW                  69.000 usec
DE                   6.50 usec
TE                  297.3 K
D1               2.00000000 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                    1H
P1                   15.00 usec
PL1                  11.10 dB
SFO1           400.1324008 MHz

F2 - Processing parameters
SI                   16384
SF             400.1300113 MHz
WDW                     EM
SSB                      0
LB                       0 Hz
GB                       0
PC                    1.00
```

^{13}C NMR Spectrum of **8al** ($CDCl_3$, 100 MHz)




```
Current Data Parameters
NAME            SW 831-1
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20200425
Time                0.36
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                 32768
SOLVENT            CDCl3
NS                  5000
DS                     0
SWH           24038.461 Hz
FIDRES         0.733596 Hz
AQ            0.6815744 sec
RG                198.09
DW              20.800 usec
DE                6.50 usec
TE                294.2 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1        100.6228298 MHz
NUC1                13C
P1                10.00 usec
PLW1        49.50000000 W

======== CHANNEL f2 ========
SFO2        400.1316005 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2             90.00 usec
PLW2        12.50000000 W
PLW12        0.34722000 W
PLW13        0.28125000 W

F2 - Processing parameters
SI                 32768
SF          100.6127720 MHz
WDW                   EM
SSB                    0
LB                  2.00 Hz
GB                     0
PC                  1.00
```

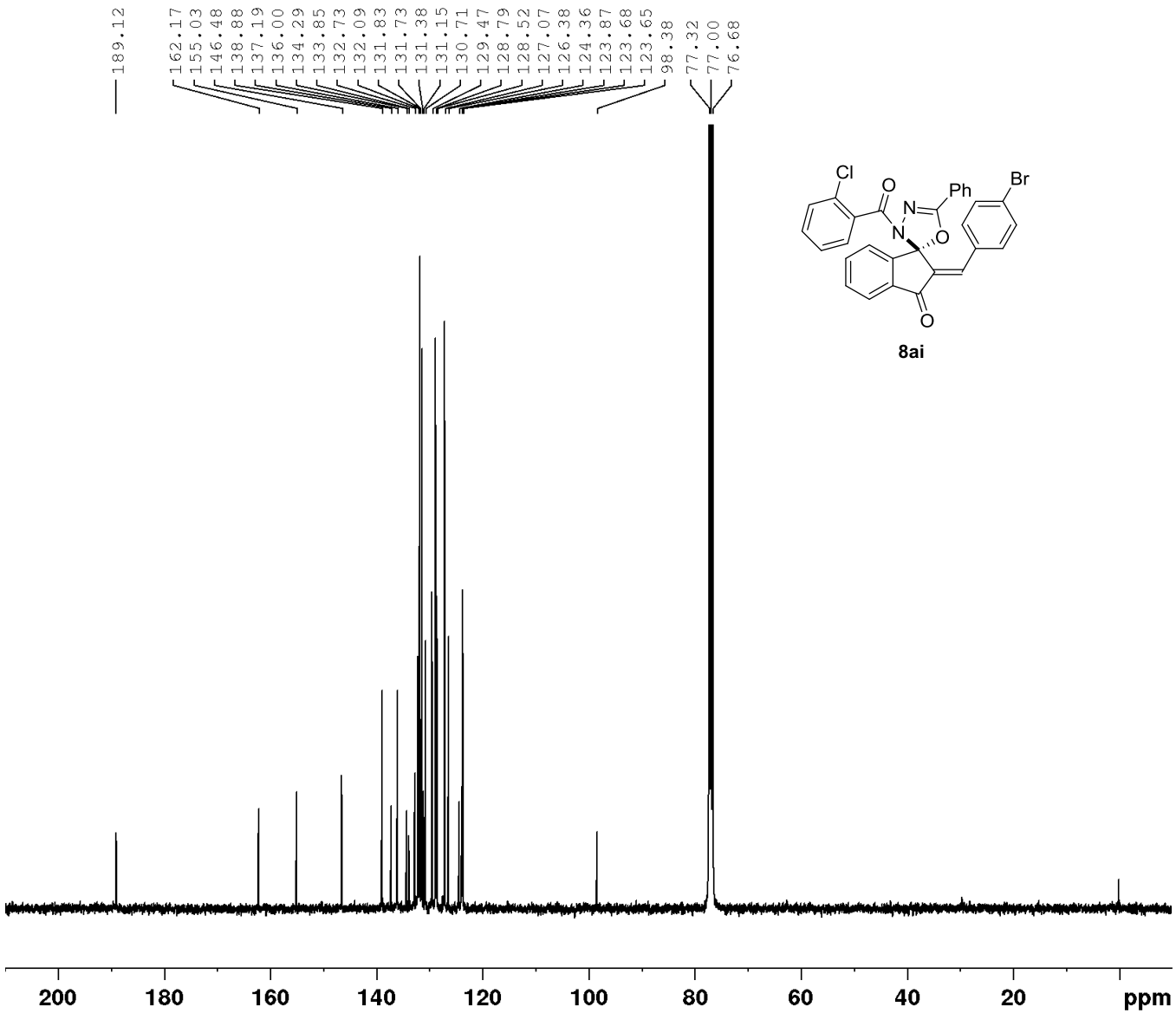
^{1}H NMR Spectrum of **8ai** ($CDCl_3$, 400 MHz)



8ai

```
Current Data Parameters
NAME            SW 832-1
EXPNO                  3
PROCNO                 1

F2 - Acquisition Parameters
Date_           20200520
Time               23.52
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG             zg30
TD                 32768
SOLVENT            CDCl3
NS                    32
DS                     0
SWH             7211.539 Hz
FIDRES          0.220079 Hz
AQ             2.2719147 sec
RG                198.09
DW                69.333 usec
DE                10.06 usec
TE                297.1 K
D1            2.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         400.1324008 MHz
NUC1                   1H
P1                 15.00 usec
PLW1         11.39999962 W

F2 - Processing parameters
SI                 16384
SF           400.1300100 MHz
WDW                   EM
SSB                    0
LB                     0 Hz
GB                     0
PC                  1.00
```

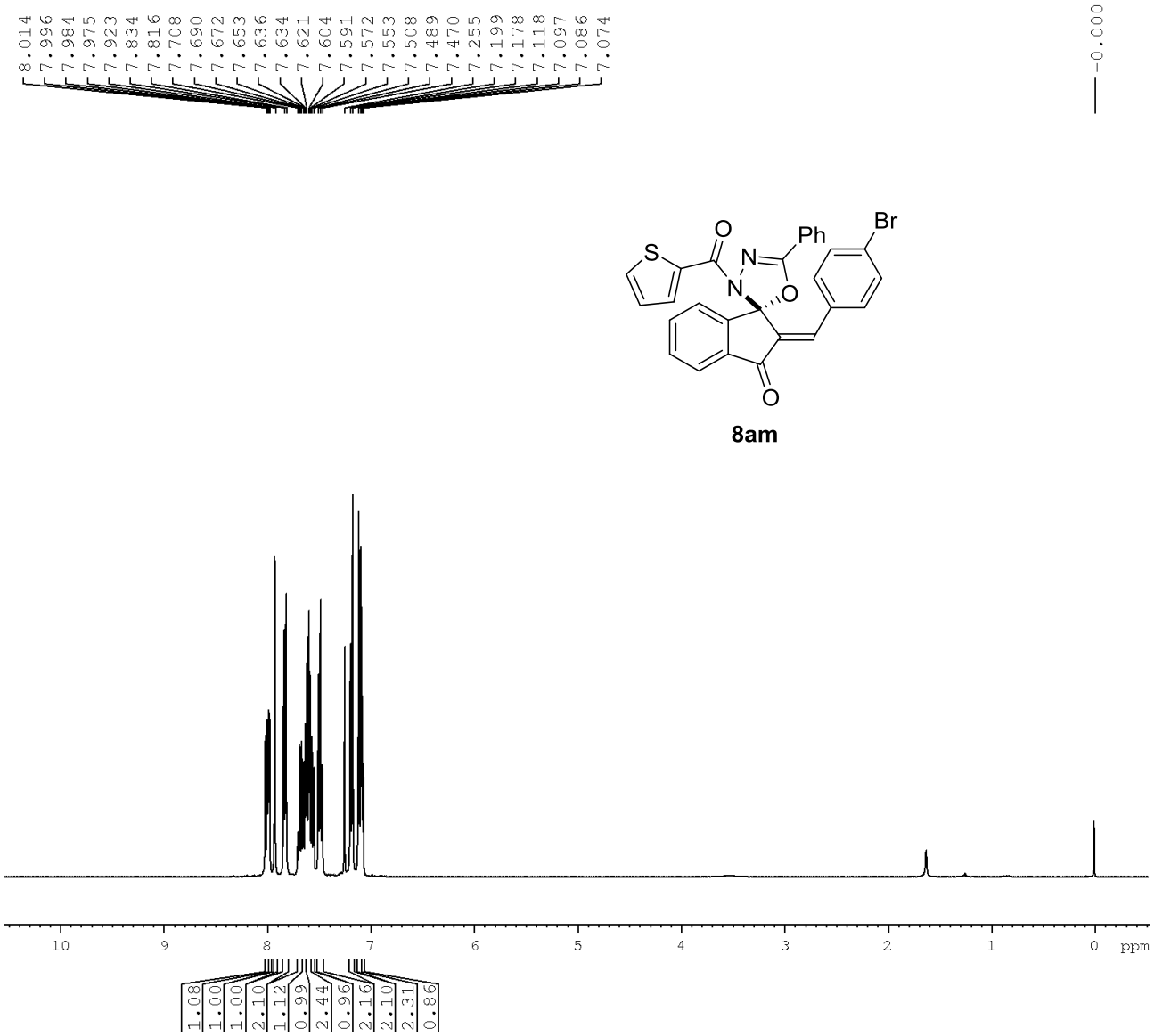
^{13}C NMR Spectrum of **8ai** ($CDCl_3$, 100 MHz)



8ai

```
Current Data Parameters
NAME                  SW 832-1
EXPNO                        4
PROCNO                       1

F2 - Acquisition Parameters
Date_                 20200520
Time                     23.56
INSTRUM                  spect
PROBHD    5 mm PABBO BB/
PULPROG                zgpg30
TD                      32768
SOLVENT                 CDCl3
NS                      13073
DS                          0
SWH                24038.461 Hz
FIDRES              0.733596 Hz
AQ                  0.6815744 sec
RG                     198.09
DW                     20.800 usec
DE                      6.50 usec
TE                     296.8 K
D1                 2.00000000 sec
D11                0.03000000 sec
TD0                         1

======== CHANNEL f1 ========
SFO1               100.6228298 MHz
NUC1                       13C
P1                      10.00 usec
PLW1               49.50000000 W

======== CHANNEL f2 ========
SFO2               400.1316005 MHz
NUC2                       1H
CPDPRG[2                waltz16
PCPD2                   90.00 usec
PLW2               12.50000000 W
PLW12               0.34722000 W
PLW13               0.28125000 W

F2 - Processing parameters
SI                      32768
SF                 100.6127707 MHz
WDW                        EM
SSB                         0
LB                       2.00 Hz
GB                          0
PC                       1.00
```

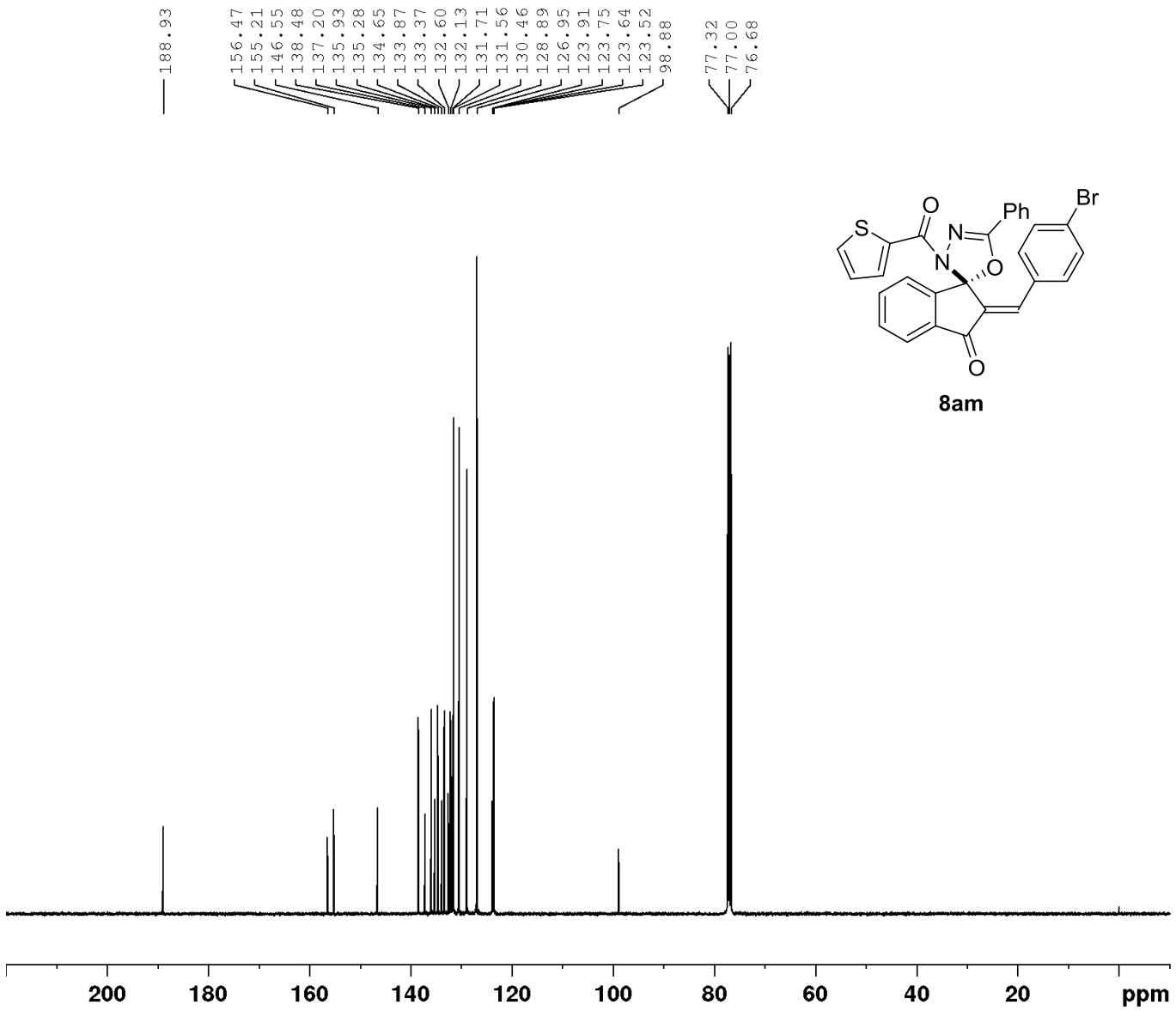
^{1}H NMR Spectrum of **8am** ($CDCl_3$, 400 MHz)



8am

```
Current Data Parameters
NAME                  SW 862
EXPNO                      1
PROCNO                     1

F2 - Acquisition Parameters
Date_               20200517
Time                   22.38
INSTRUM                spect
PROBHD   5 mm BBO BB-1H
PULPROG                zg30
TD                    32768
SOLVENT               CDCl3
NS                       32
DS                        0
SWH                7246.377 Hz
FIDRES            0.221142 Hz
AQ                2.2609921 sec
RG                      114
DW                 69.000 usec
DE                  6.50 usec
TE                  296.4 K
D1               2.00000000 sec
TD0                        1

======== CHANNEL f1 ========
NUC1                      1H
P1                    15.00 usec
PL1                   11.10 dB
SFO1           400.1324008 MHz

F2 - Processing parameters
SI                     16384
SF             400.1300134 MHz
WDW                       EM
SSB                        0
LB                         0 Hz
GB                         0
PC                      1.00
```

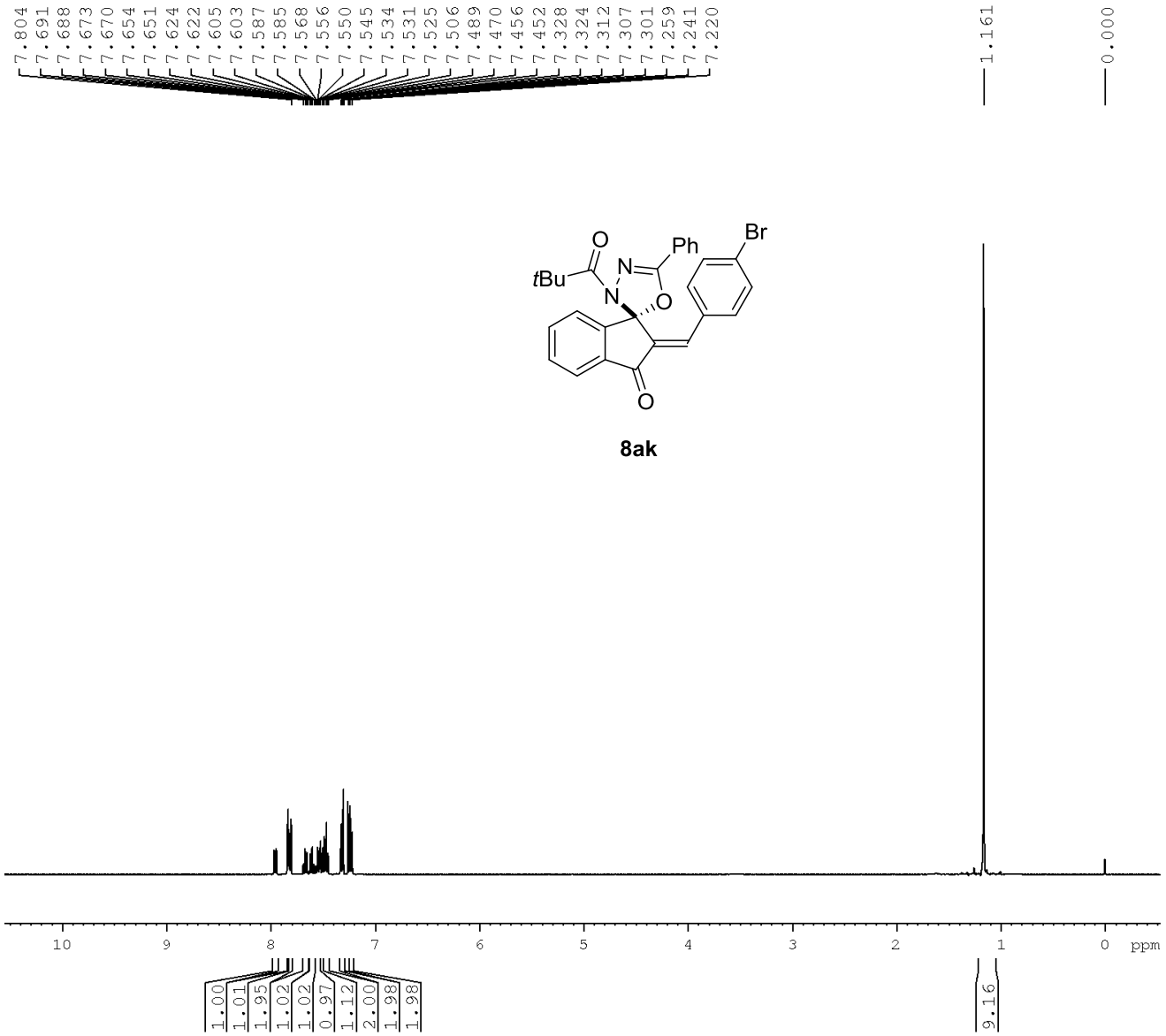
^{13}C NMR Spectrum of **8am** ($CDCl_3$, 100 MHz)



8am

```
Current Data Parameters
NAME                 SW 862
EXPNO                     2
PROCNO                    1

F2 - Acquisition Parameters
Date_              20200517
Time                  22.43
INSTRUM               spect
PROBHD    5 mm BBO BB-1H
PULPROG              zgpg30
TD                    32768
SOLVENT               CDCl3
NS                    12000
DS                        0
SWH              24038.461 Hz
FIDRES            0.733596 Hz
AQ               0.6815744 sec
RG                     8192
DW                  20.800 usec
DE                   6.50 usec
TE                   296.4 K
D1              2.00000000 sec
D11             0.03000000 sec
TD0                       1

======== CHANNEL f1 ========
NUC1                    13C
P1                   10.00 usec
PL1                   3.80 dB
SFO1           100.6233325 MHz

======== CHANNEL f2 ========
CPDPRG[2           waltz16
NUC2                    1H
PCPD2                90.00 usec
PL2                  10.20 dB
PL12                 26.00 dB
PL13                 29.00 dB
SFO2           400.1316005 MHz

F2 - Processing parameters
SI                    32768
SF             100.6127735 MHz
WDW                      EM
SSB                       0
LB                    1.00 Hz
GB                        0
PC                    1.00
```

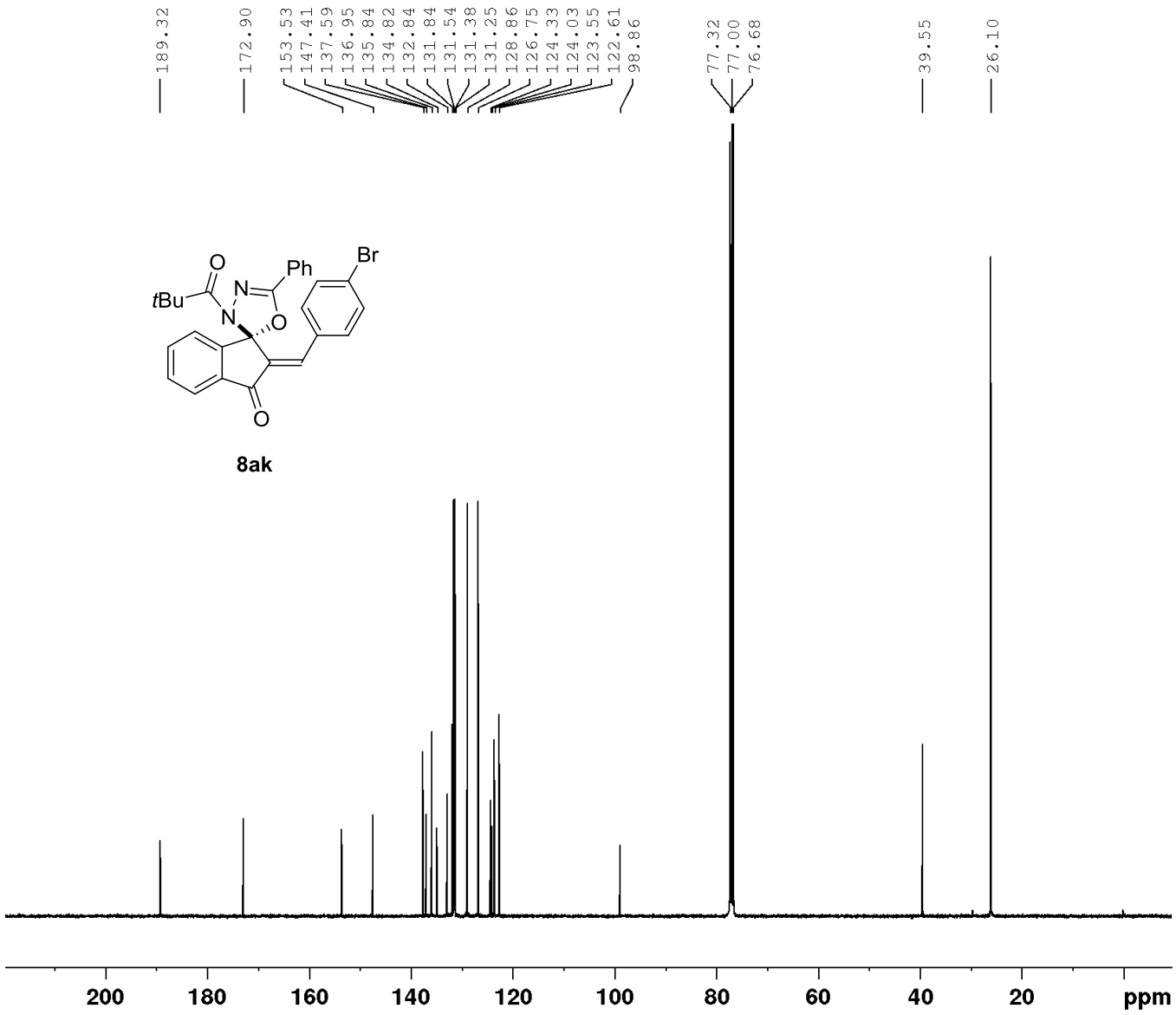
^{1}H NMR Spectrum of **8ak** ($CDCl_3$, 400 MHz)



8ak

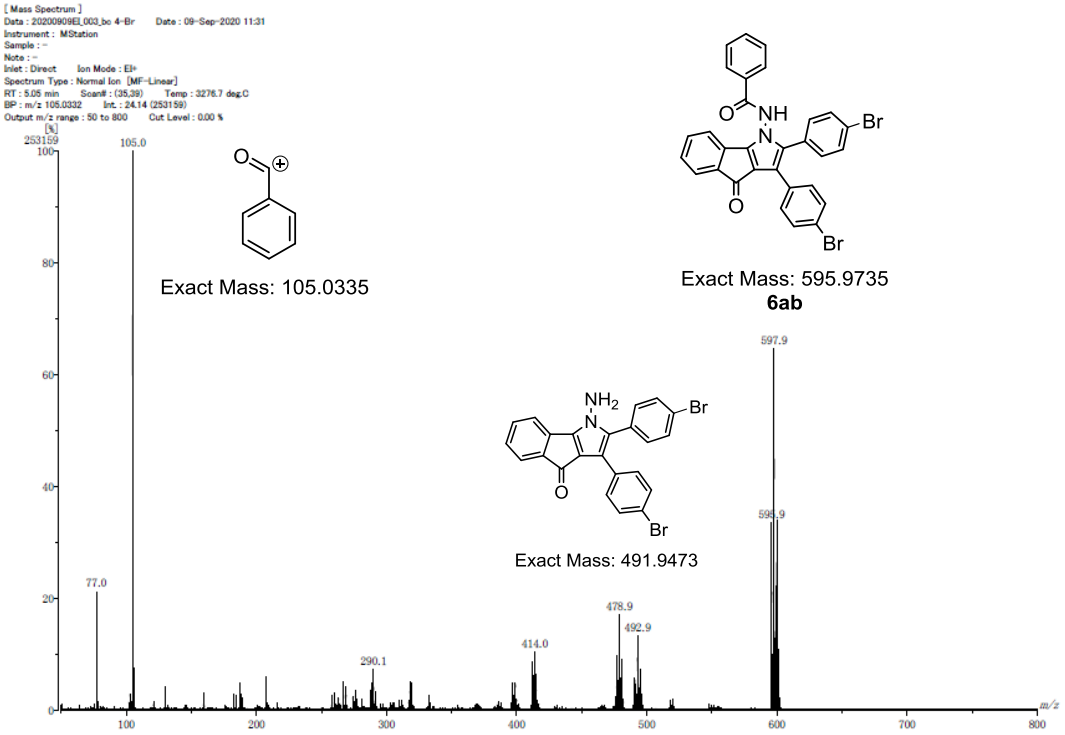
```
Current Data Parameters
NAME                 SW 836
EXPNO                     5
PROCNO                    1

F2 - Acquisition Parameters
Date_             20200524
Time                 20.02
INSTRUM              spect
PROBHD    5 mm BBO BB-1H
PULPROG               zg30
TD                   32768
SOLVENT              CDCl3
NS                       1
DS                       0
SWH               7246.377 Hz
FIDRES            0.221142 Hz
AQ                2.2609921 sec
RG                     114
DW                  69.000 usec
DE                   6.50 usec
TE                  296.7 K
D1              2.00000000 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                    1H
P1                   15.00 usec
PL1                  11.10 dB
SFO1          400.1324008 MHz

F2 - Processing parameters
SI                   16384
SF            400.1300116 MHz
WDW                     EM
SSB                      0
LB                       0 Hz
GB                       0
PC                    1.00
```

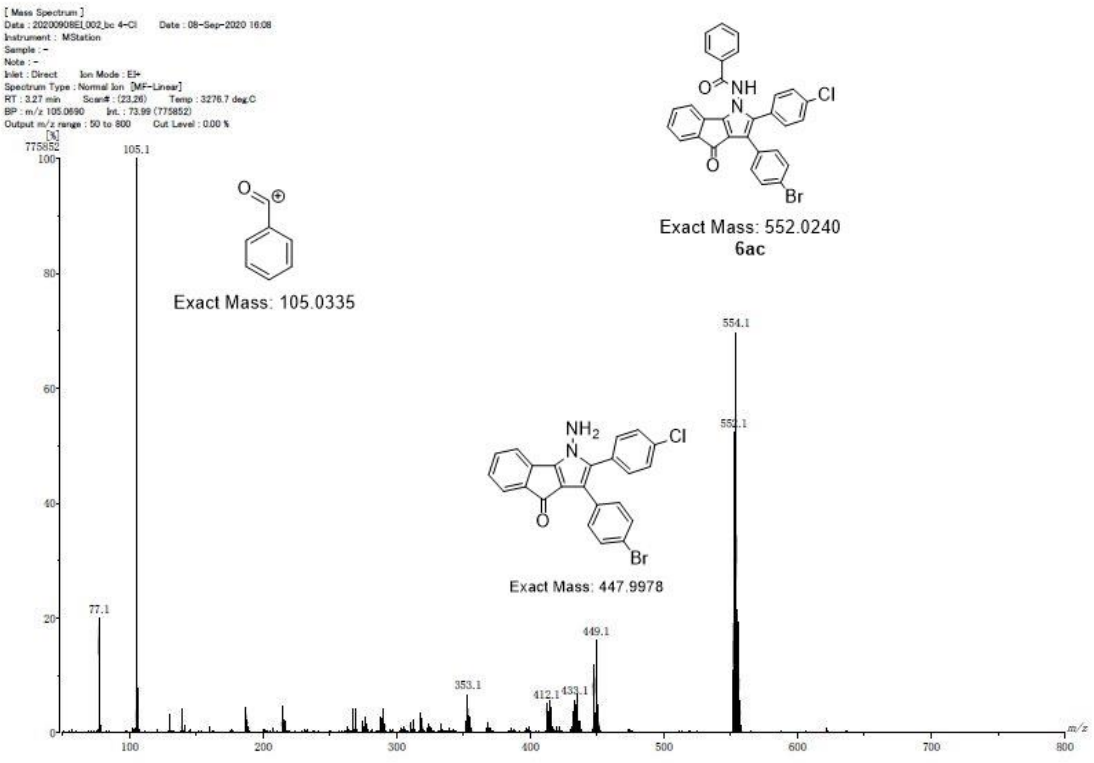
^{13}C NMR Spectrum of **8ak** ($CDCl_3$, 100 MHz)

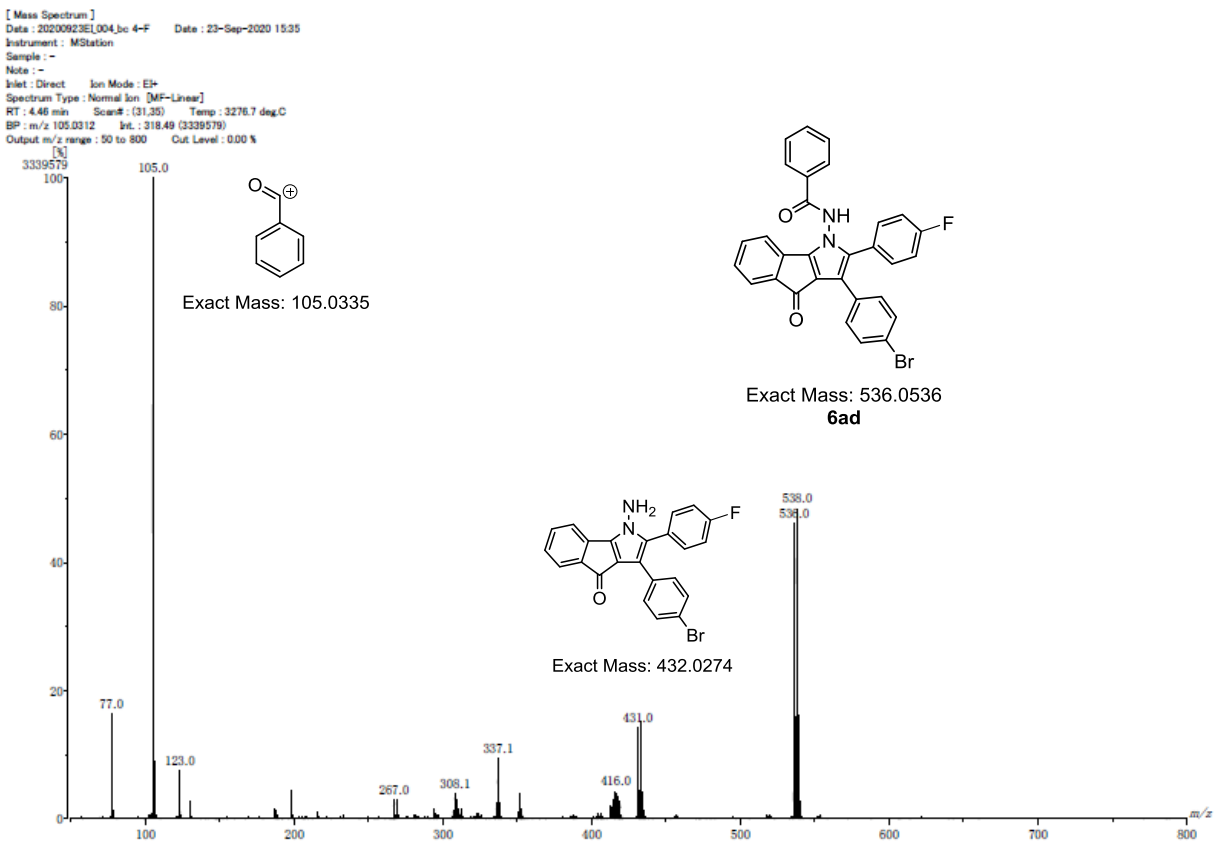


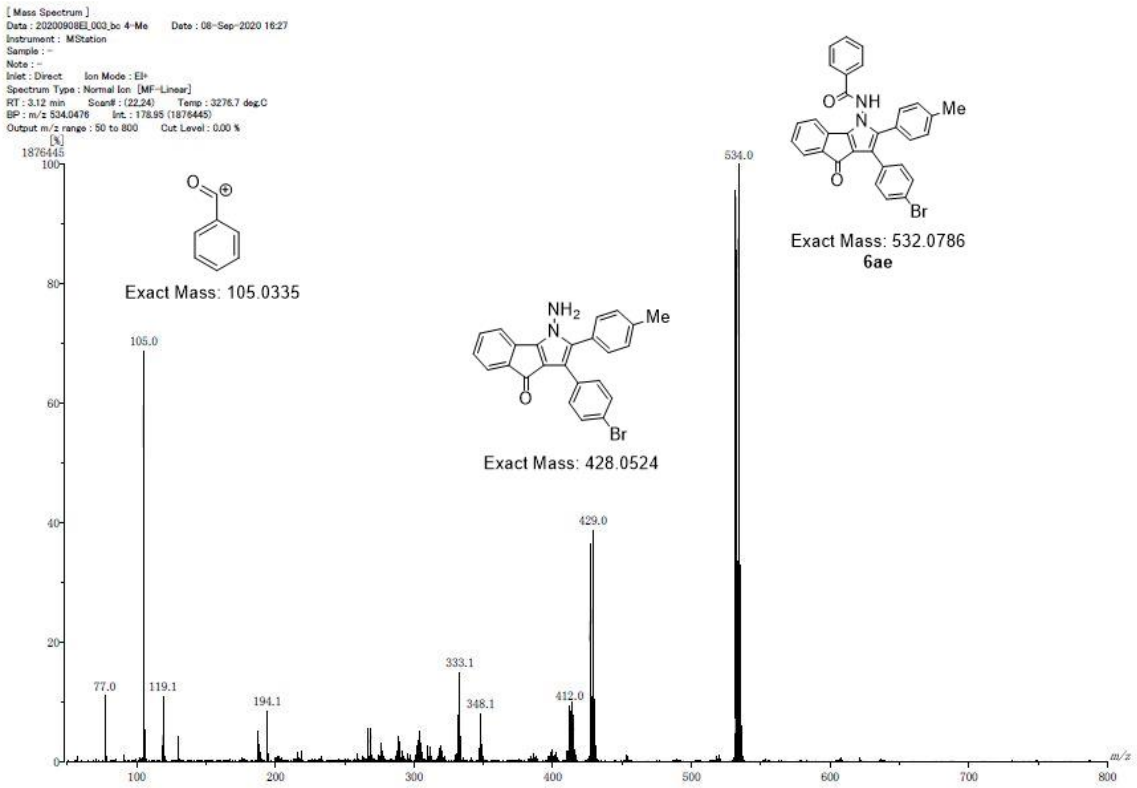

```
Current Data Parameters
NAME                 SW 836
EXPNO                     6
PROCNO                    1

F2 - Acquisition Parameters
Date_              20200524
Time                  20.03
INSTRUM               spect
PROBHD    5 mm BBO BB-1H
PULPROG              zgpg30
TD                    32768
SOLVENT               CDCl3
NS                    10000
DS                        0
SWH              24038.461 Hz
FIDRES            0.733596 Hz
AQ               0.6815744 sec
RG                  5792.6
DW                 20.800 usec
DE                  6.50 usec
TE                  296.6 K
D1              2.00000000 sec
D11             0.03000000 sec
TD0                       1

======== CHANNEL f1 ========
NUC1                    13C
P1                   10.00 usec
PL1                   3.80 dB
SFO1           100.6233325 MHz

======== CHANNEL f2 ========
CPDPRG[2           waltz16
NUC2                    1H
PCPD2                90.00 usec
PL2                  10.20 dB
PL12                 26.00 dB
PL13                 29.00 dB
SFO2           400.1316005 MHz

F2 - Processing parameters
SI                    32768
SF             100.6127730 MHz
WDW                      EM
SSB                       0
LB                    1.00 Hz
GB                        0
PC                    1.00
```

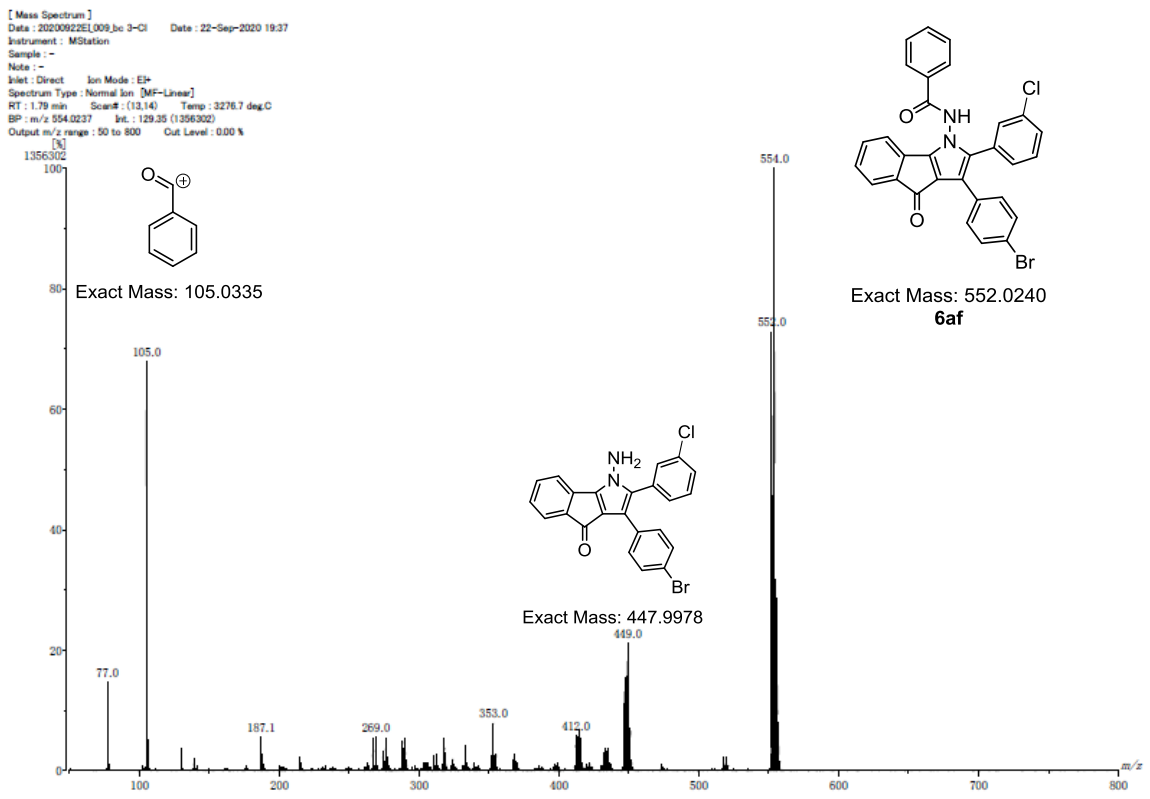
IX. Scanned copies of EI Mass Spectra for selected compounds 6/7

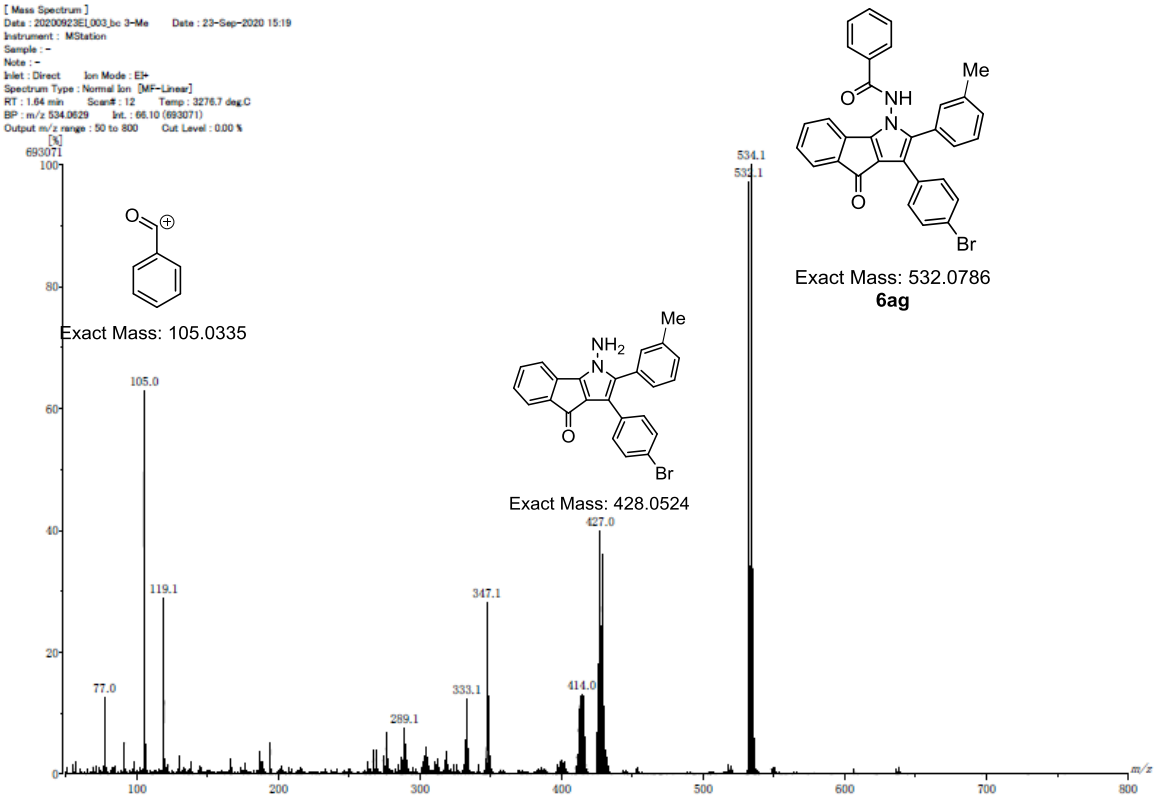


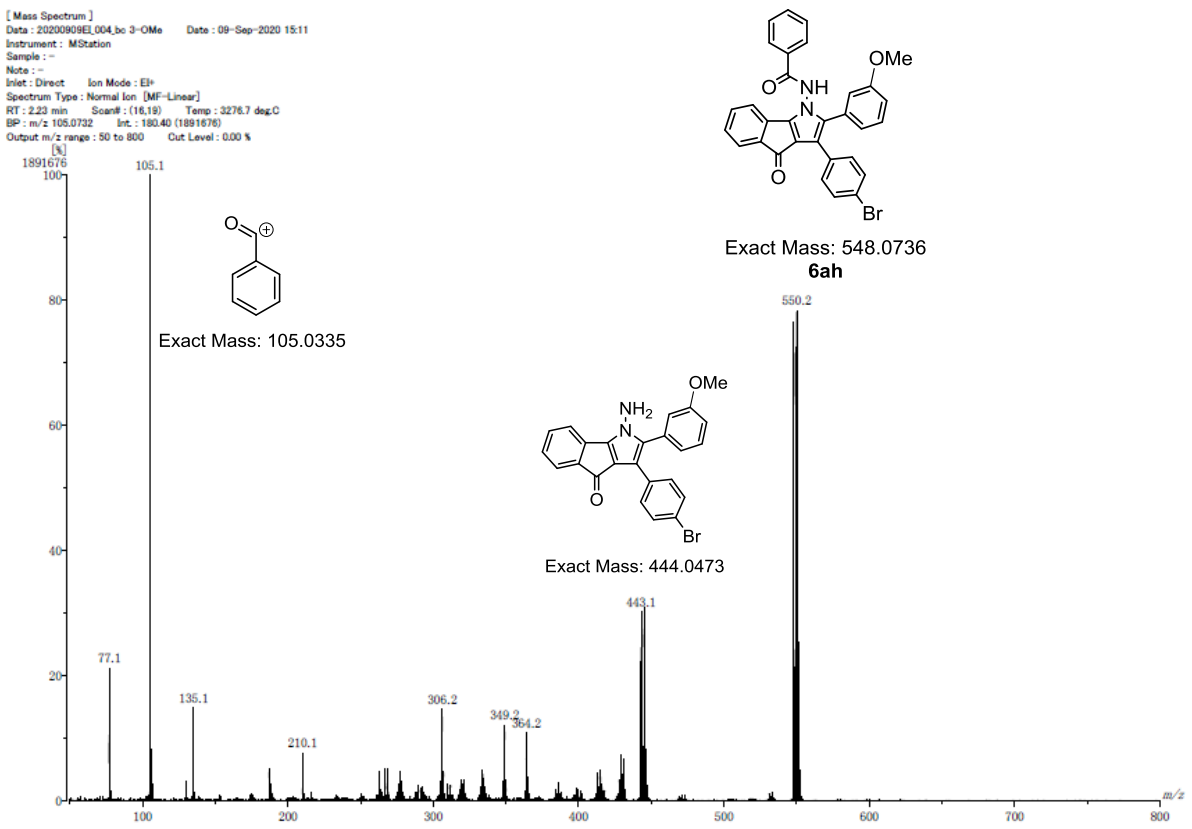


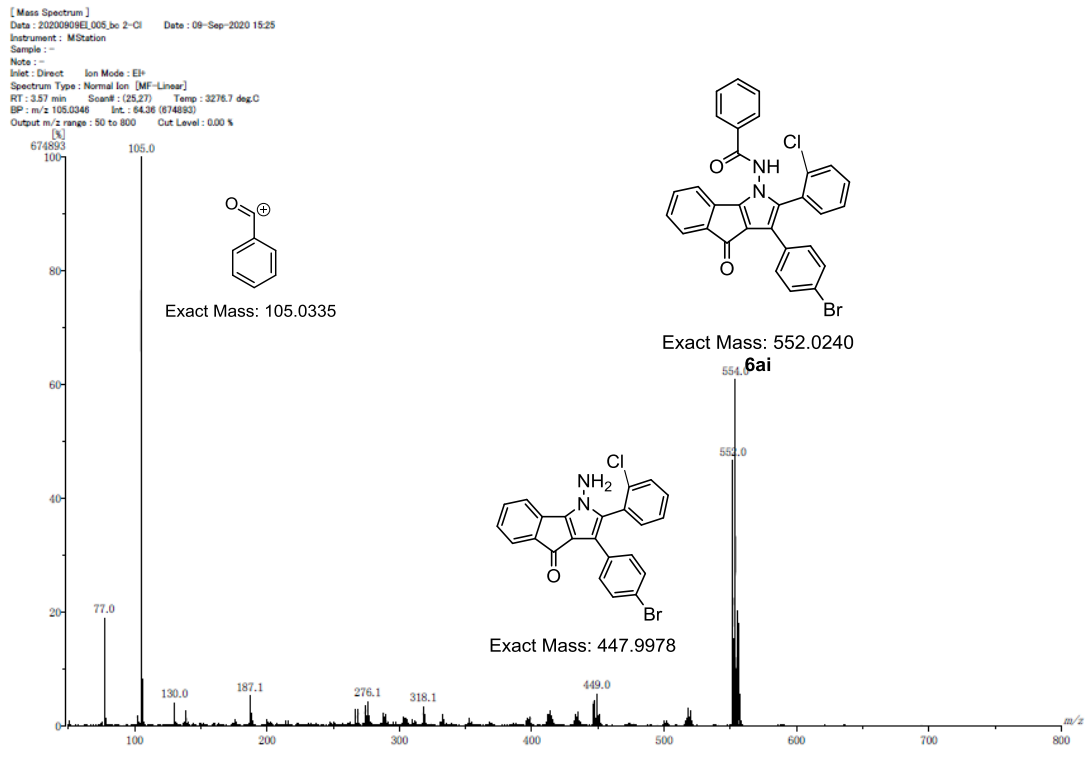

[Mass Spectrum]
Data : 20200923EI_004_bc 4-F Date : 23-Sep-2020 15:35
Instrument : MStation
Sample : -
Note : -
Inlet : Direct Ion Mode : EI+
Spectrum Type : Normal Ion [MF-Linear]
RT : 4.46 min Scan# : (31,35) Temp : 3276.7 deg.C
BP : m/z 105.0312 Int. : 318.49 (3339579)
Output m/z range : 50 to 800 Cut Level : 0.00 %
[%]
3339579
105.0
77.0
123.0
267.0
308.1
337.1
416.0
431.0
538.0
536.0
m/z
Exact Mass: 105.0335
Exact Mass: 536.0536
6ad
Exact Mass: 432.0274

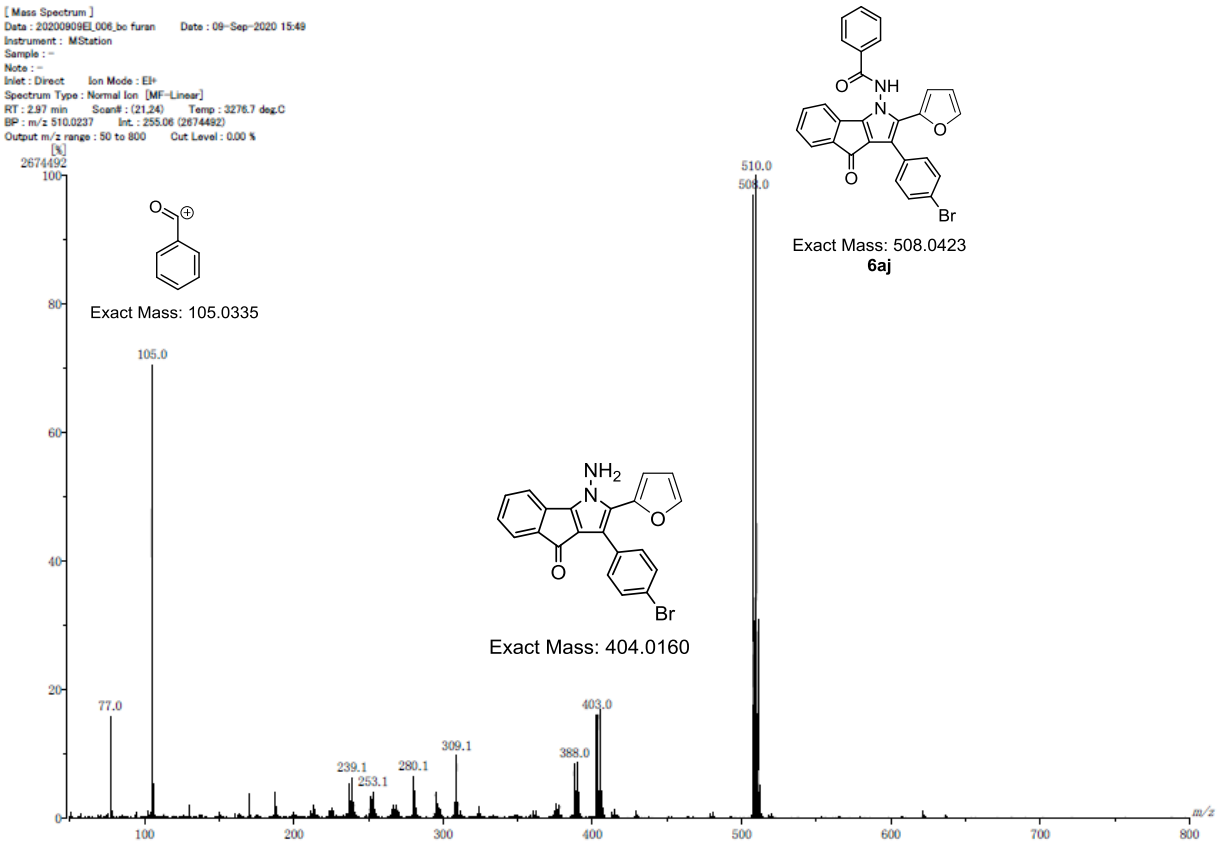

[Mass Spectrum]
Data : 20200908EI_003_bc 4-Me Date : 08-Sep-2020 16:27
Instrument : MStation
Sample : -
Note : -
Inlet : Direct Ion Mode : EI+
Spectrum Type : Normal Ion [MF-Linear]
RT : 3.12 min Scan# : (22,24) Temp : 3276.7 deg.C
BP : m/z 534.0476 Int. : 178.95 (1876445)
Output m/z range : 50 to 800 Cut Level : 0.00 %
[%]
1876445
105.0
77.0
119.1
194.1
333.1
348.1
412.0
429.0
534.0
m/z
Exact Mass: 105.0335
Exact Mass: 532.0786
6ae
Exact Mass: 428.0524

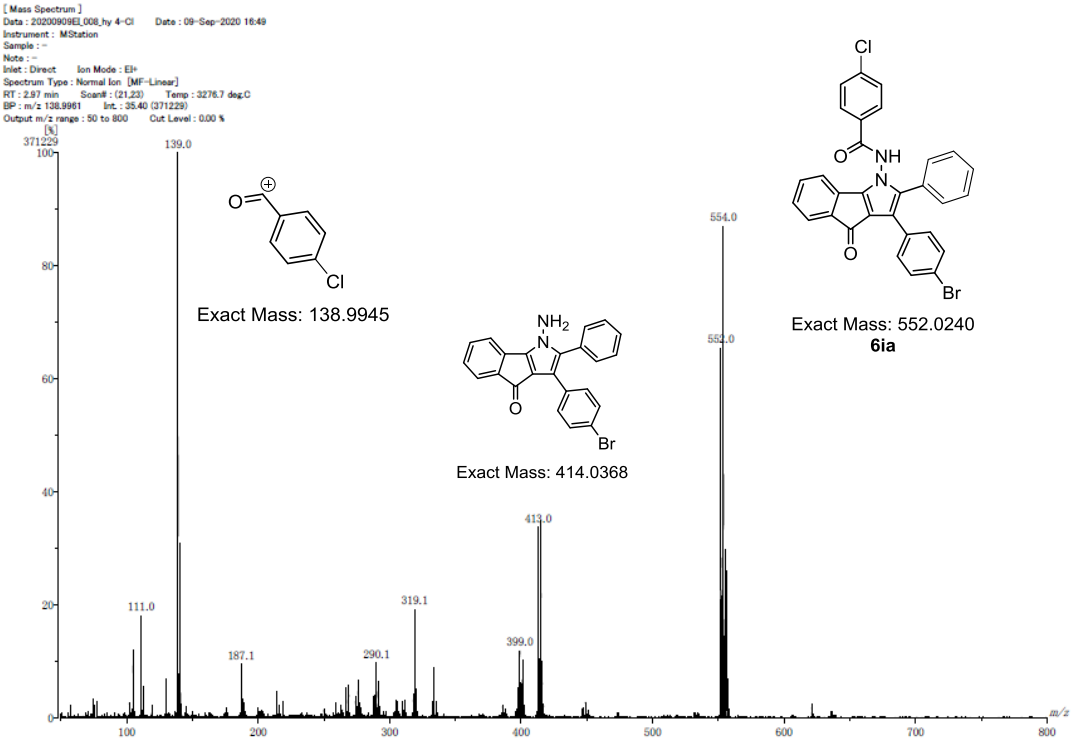

[Mass Spectrum]
Data : 20200922EI_009_bc 3-Cl Date : 22-Sep-2020 19:37
Instrument : MStation
Sample : -
Note : -
Inlet : Direct Ion Mode : EI+
Spectrum Type : Normal Ion [MF-Linear]
RT : 1.79 min Scan# : (13,14) Temp : 3276.7 deg.C
BP : m/z 554.0237 Int. : 129.35 (1356302)
Output m/z range : 50 to 800 Cut Level : 0.00 %
[%]
1356302
Exact Mass: 105.0335
Exact Mass: 552.0240
6af
Exact Mass: 447.9978
554.0
552.0
105.0
449.0
77.0
187.1
269.0
353.0
412.0
m/z

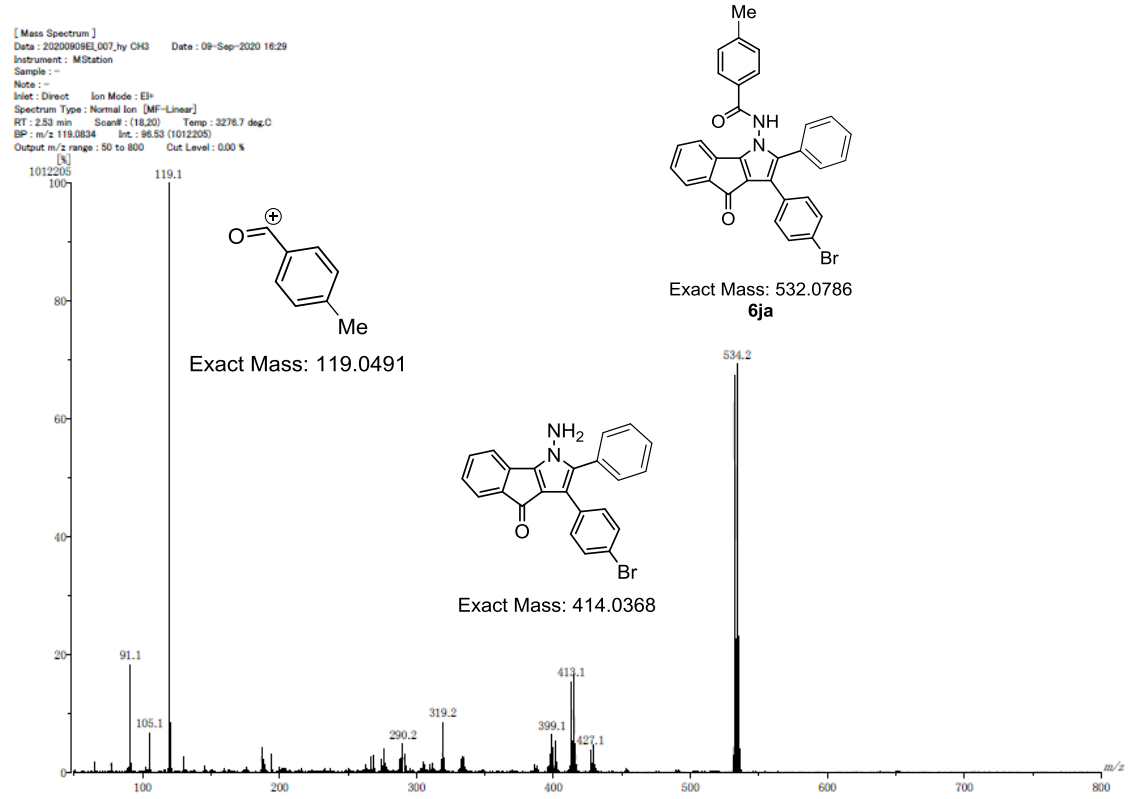

[Mass Spectrum]
Data : 20200923EI_003_bc 3-Me Date : 23-Sep-2020 15:19
Instrument : MStation
Sample : -
Note : -
Inlet : Direct Ion Mode : EI+
Spectrum Type : Normal Ion [MF-Linear]
RT : 1.64 min Scan# : 12 Temp : 3276.7 deg.C
BP : m/z 534.0629 Int. : 66.10 (693071)
Output m/z range : 50 to 800 Cut Level : 0.00 %
[%]
693071
Exact Mass: 105.0335
Exact Mass: 532.0786
6ag
Exact Mass: 428.0524
534.1
532.1
105.0
427.0
119.1
347.1
77.0
333.1
414.0
289.1
m/z

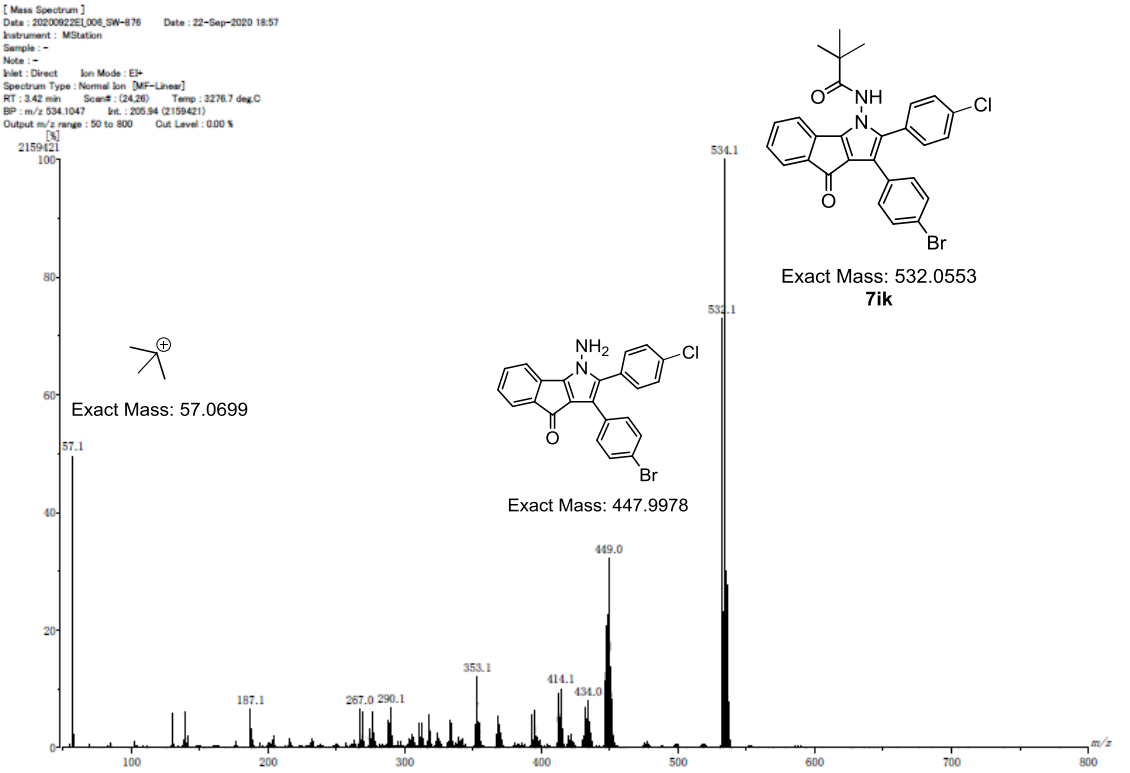

[Mass Spectrum]
Data : 20200909EI_004_bc 3-OMe Date : 09-Sep-2020 15:11
Instrument : MStation
Sample : -
Note : -
Inlet : Direct Ion Mode : EI+
Spectrum Type : Normal Ion [MF-Linear]
RT : 2.23 min Scan# : (16,19) Temp : 3276.7 deg.C
BP : m/z 105.0732 Int. : 180.40 (1891676)
Output m/z range : 50 to 800 Cut Level : 0.00 %
[%]
1891676
105.1
77.1
135.1
210.1
306.2
349.2
364.2
443.1
550.2
m/z
Exact Mass: 105.0335
Exact Mass: 444.0473
Exact Mass: 548.0736
6ah

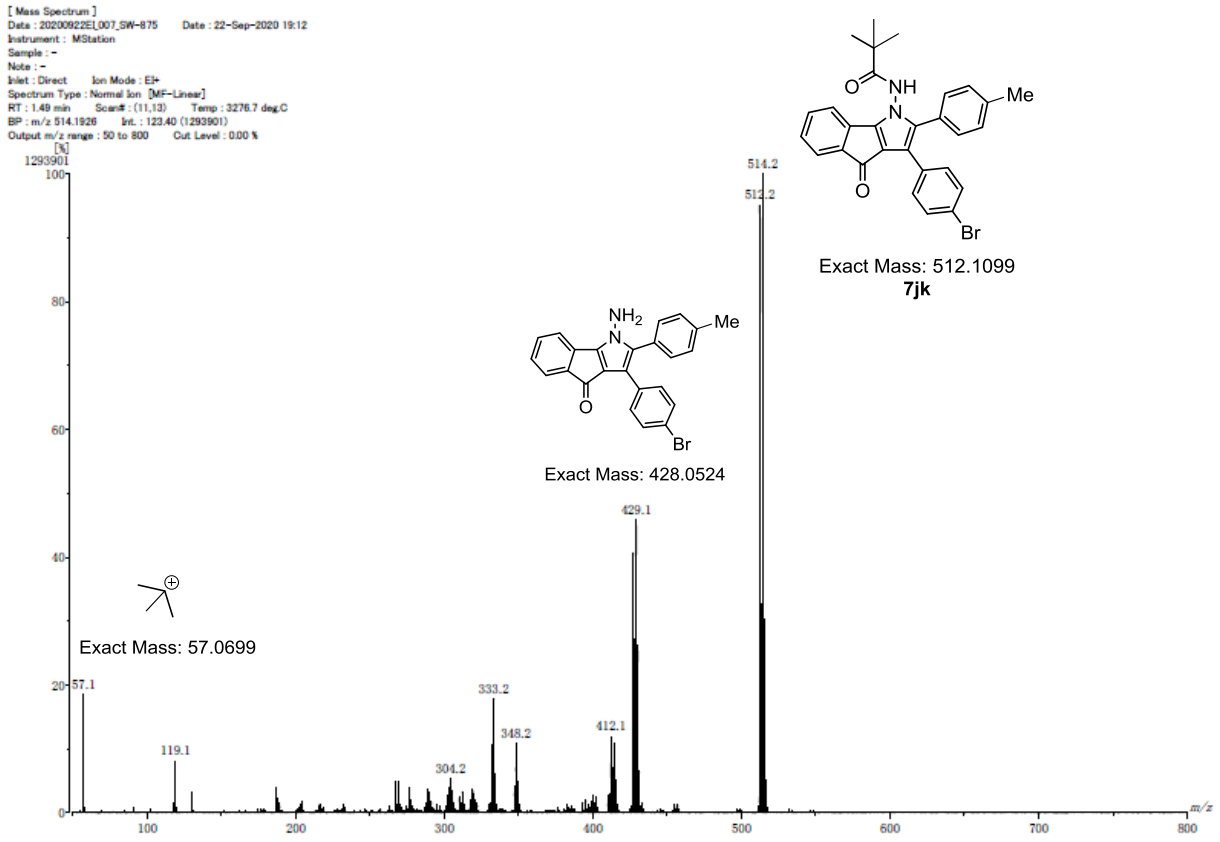

[Mass Spectrum]
Data : 20200909EI_005_bc 2-Cl Date : 09-Sep-2020 15:25
Instrument : MStation
Sample : -
Note : -
Inlet : Direct Ion Mode : EI+
Spectrum Type : Normal Ion [MF-Linear]
RT : 3.57 min Scan# : (25,27) Temp : 3276.7 deg.C
BP : m/z 105.0346 Int. : 64.36 (674893)
Output m/z range : 50 to 800 Cut Level : 0.00 %
[%]
674893
105.0
77.0
130.0
187.1
276.1
318.1
449.0
552.0
554.0
m/z
Exact Mass: 105.0335
Exact Mass: 447.9978
Exact Mass: 552.0240
6ai

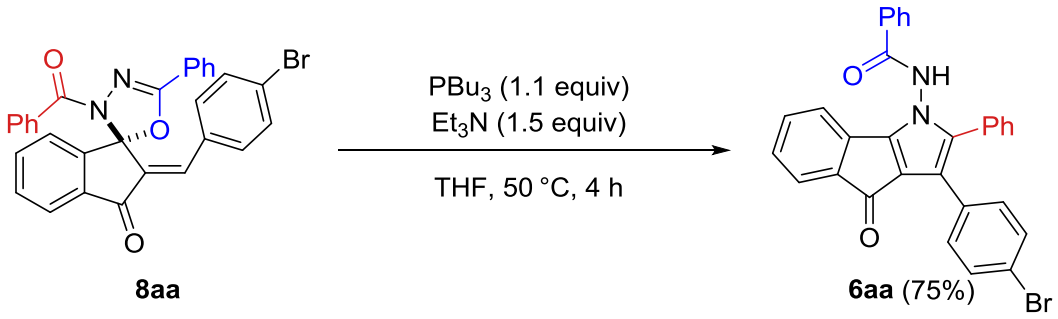

[Mass Spectrum]
Data : 20200909EI_006_bc furan Date : 09-Sep-2020 15:49
Instrument : MStation
Sample : –
Note : –
Inlet : Direct Ion Mode : EI+
Spectrum Type : Normal Ion [MF-Linear]
RT : 2.97 min Scan# : (21,24) Temp : 3276.7 deg.C
BP : m/z 510.0237 Int. : 255.06 (2674492)
Output m/z range : 50 to 800 Cut Level : 0.00 %
[%]
2674492
Exact Mass: 105.0335
Exact Mass: 508.0423
6aj
Exact Mass: 404.0160
m/z


[Mass Spectrum]
Data : 20200909EI_008_hy 4-Cl Date : 09-Sep-2020 16:49
Instrument : MStation
Sample : –
Note : –
Inlet : Direct Ion Mode : EI+
Spectrum Type : Normal Ion [MF-Linear]
RT : 2.97 min Scan# : (21,23) Temp : 3276.7 deg.C
BP : m/z 138.9961 Int. : 35.40 (371229)
Output m/z range : 50 to 800 Cut Level : 0.00 %
[%]
371229
Exact Mass: 138.9945
Exact Mass: 552.0240
6ia
Exact Mass: 414.0368
m/z

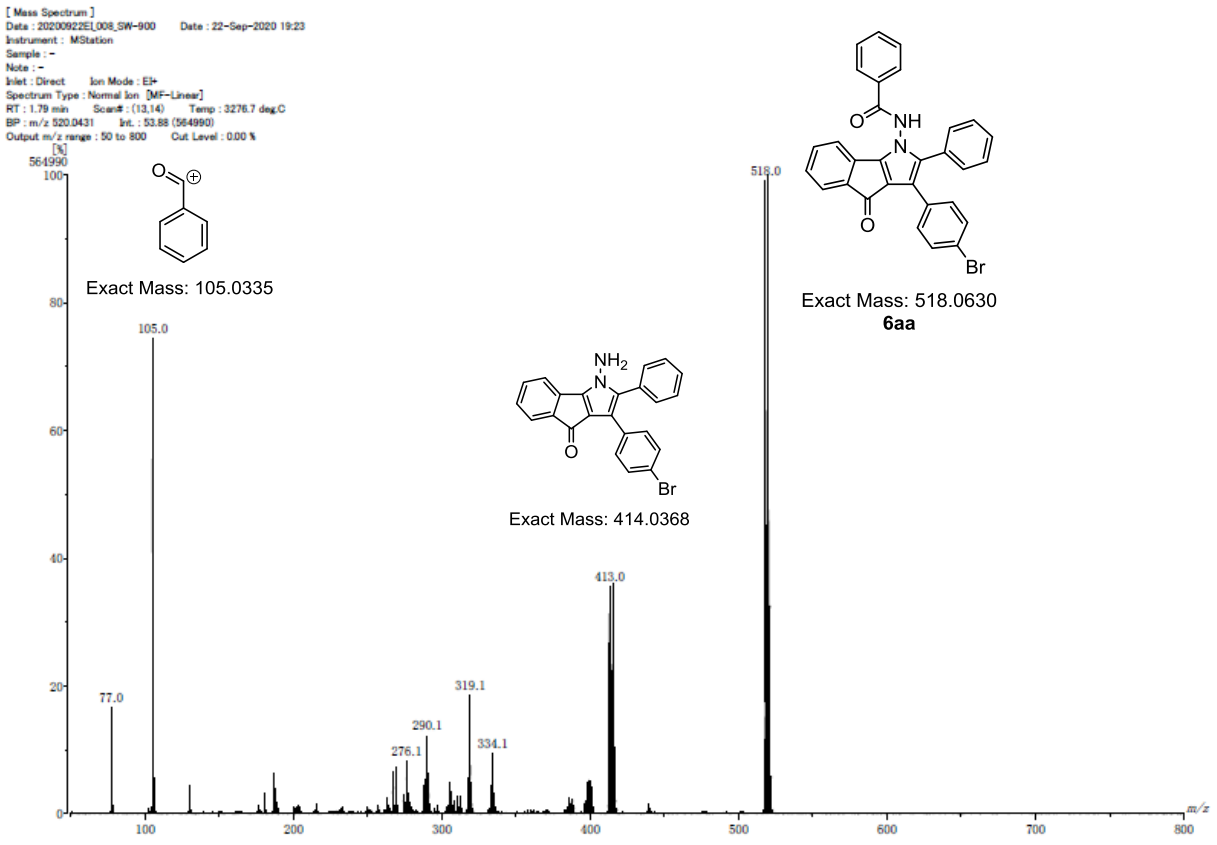

[Mass Spectrum]
Data : 20200909EI_007_hy CH3 Date : 09-Sep-2020 16:29
Instrument : MStation
Sample : -
Note : -
Inlet : Direct Ion Mode : EI+
Spectrum Type : Normal Ion [MF-Linear]
RT : 2.53 min Scan# : (18,20) Temp : 3276.7 deg.C
BP : m/z 119.0834 Int. : 96.53 (1012205)
Output m/z range : 50 to 800 Cut Level : 0.00 %
[%]
1012205
119.1
91.1
105.1
290.2
319.2
399.1
413.1
427.1
534.2
m/z
Exact Mass: 119.0491
Exact Mass: 414.0368
Exact Mass: 532.0786
6ja

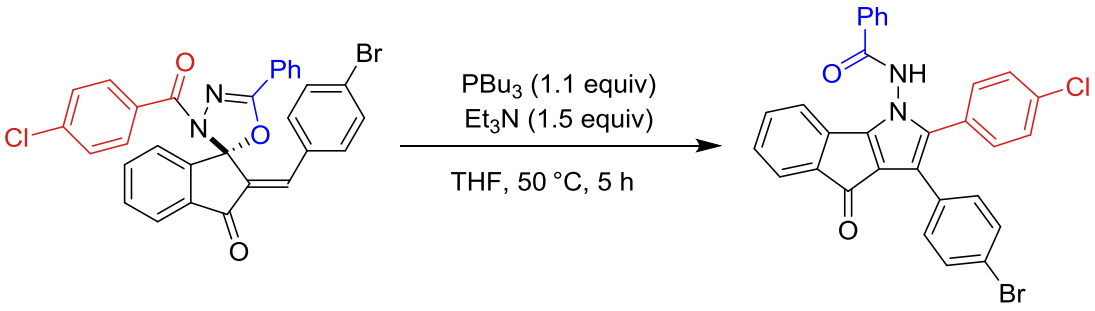

[Mass Spectrum]
Data : 20200922EI_006_SW-876 Date : 22-Sep-2020 18:57
Instrument : MStation
Sample : -
Note : -
Inlet : Direct Ion Mode : EI+
Spectrum Type : Normal Ion [MF-Linear]
RT : 3.42 min Scan# : (24,26) Temp : 3276.7 deg.C
BP : m/z 534.1047 Int. : 205.94 (2159421)
Output m/z range : 50 to 800 Cut Level : 0.00 %
[%]
2159421
57.1
187.1
267.0
290.1
353.1
414.1
434.0
449.0
532.1
534.1
m/z
Exact Mass: 57.0699
Exact Mass: 447.9978
Exact Mass: 532.0553
7ik


[Mass Spectrum]
Data : 20200922EI_007_SW-875 Date : 22-Sep-2020 19:12
Instrument : MStation
Sample : -
Note : -
Inlet : Direct Ion Mode : EI+
Spectrum Type : Normal Ion [MF-Linear]
RT : 1.49 min Scan# : (11,13) Temp : 3276.7 deg.C
BP : m/z 514.1926 Int. : 123.40 (1293901)
Output m/z range : 50 to 800 Cut Level : 0.00 %
[%]
1293901
514.2
512.2
429.1
333.2
348.2
412.1
304.2
119.1
57.1
Exact Mass: 57.0699
Exact Mass: 428.0524
Exact Mass: 512.1099
7jk
m/z



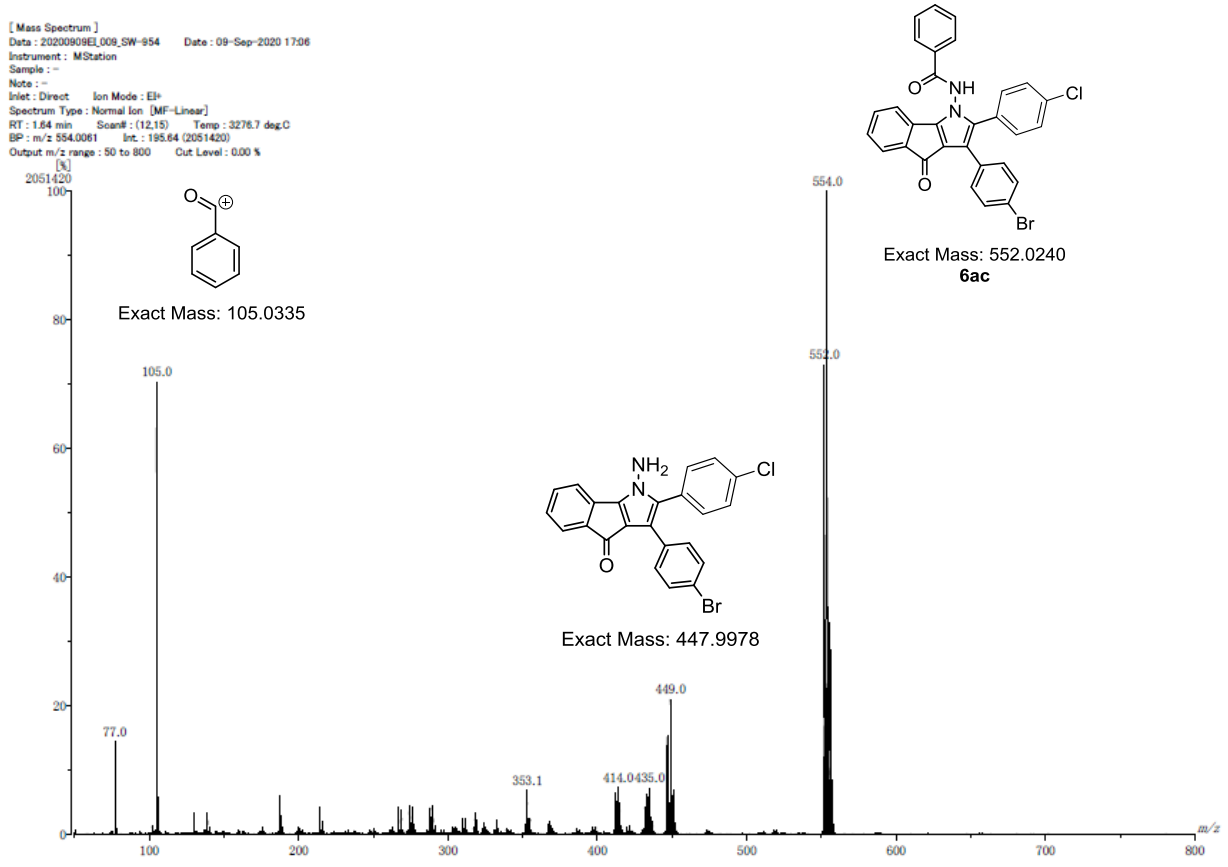
We have examined the reaction between phenyl substituted **8aa**, PBu_3 (1.1 equiv) and Et_3N (1.5 equiv) in the presence of THF at 50 °C. The desired indeno[1,2-*b*]pyrrole **6aa** was observed in 75% yield after 4 h, and further confirmed by using ^1H NMR as well as EIMS analysis.

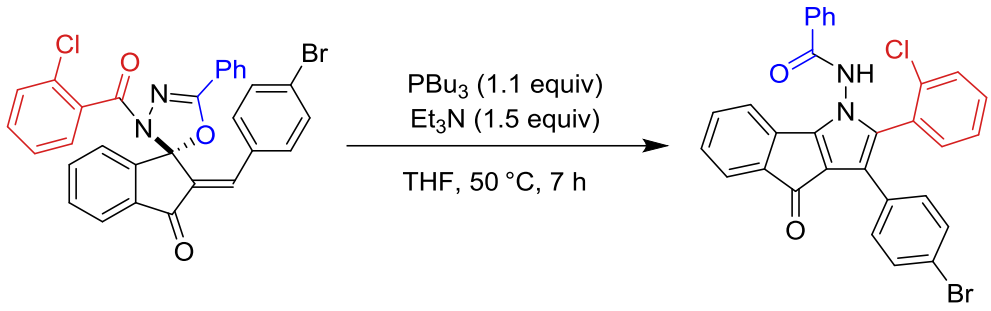




8ac **6ac** (69%)

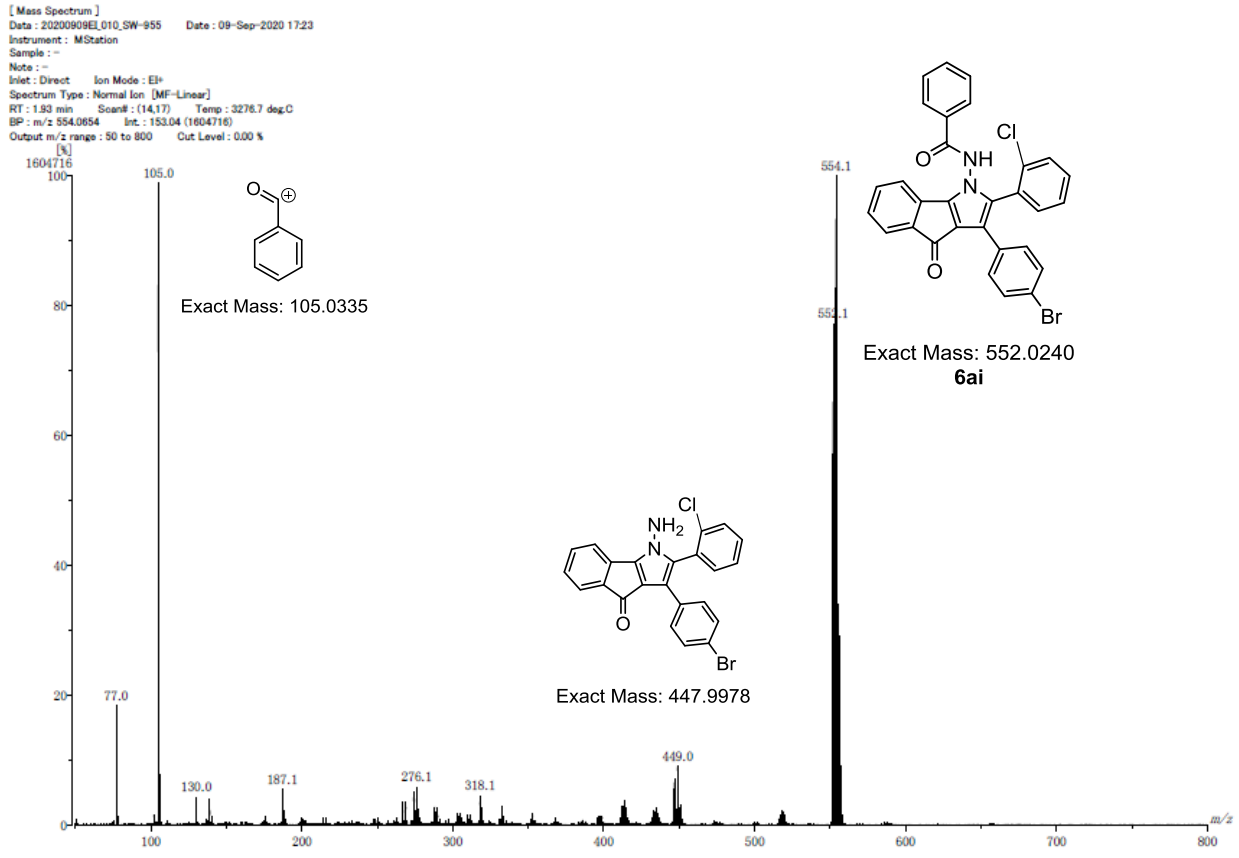
We have examined the reaction between *para*-chloro substituted **8ac**, PBu_3 (1.1 equiv) and Et_3N (1.5 equiv) in the presence of THF at 50 °C. The desired indeno[1,2-*b*]pyrrole **6ac** was observed in 69% yield after 5 h, and further confirmed by using ^1H NMR as well as EIMS analysis.

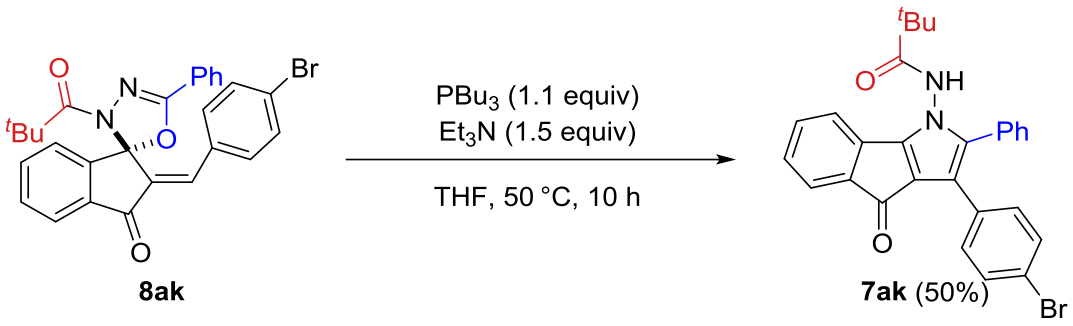




8ai **6ai** (63%)

We have also carried out the reaction between *ortho*-chloro substituted **8ai**, PBu_3 (1.1 equiv) and Et_3N (1.5 equiv) in presence of THF at 50 °C. The desired indeno[1,2-*b*]pyrrole **6ai** was observed in 63% yield after 7 h, and further confirmed by using ^1H NMR as well as EIMS analysis.





Similarly, we performed the reaction between pivaloyl substituted **8ak**, PBu_3 (1.1 equiv) and Et_3N (1.5 equiv) in presence of THF at 50 °C. The desired indeno[1,2-*b*]pyrrole **7ak** was observed in 50% yield after longer reaction time (10 h), and further confirmed by using ^1H NMR as well as EIMS analysis.