Synthesis of two nitrogen-containing polyaromatic compounds through gold catalysis/DBU-promoted cyclizations

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Content:

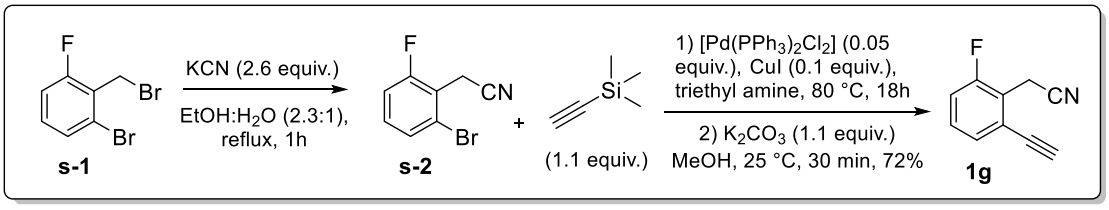
1. Representative synthetic procedures:

General procedure:

Unless otherwise noted, all the reactions for the preparation of the substrates were performed in oven-dried glassware under nitrogen atmosphere with freshly distilled solvents. The catalytic reactions were performed under nitrogen atmosphere. DCM and toluene were distilled from CaH_2 under nitrogen. THF was distilled from Na metal under nitrogen. Other solvents like 1, 2-dichloroethane, acetonitrile, benzene, trifluoromethyl benzene, MeOH, EtOH, ethyl acetate, $CHCl_3$ and DMF were used from commercial sources without further distillation. All other commercial reagents were used without further purification, unless otherwise indicated. ^{1}H NMR and ^{13}C NMR spectra were recorded on a Varian 700, 500 MHz, Bruker 400 and 500 MHz spectrometers using chloroform-*d* ($CDCl_3$) and *d*-THF as solvent and Me_4Si as an internal standard, with chemical shifts (δ) and spin−spin coupling constants (J). The following abbreviations were used to show the multiplicities: s, singlet; d, doublet; t, triplet; q, quadruplet; dd, doublet of doublet; m, multiplet. High-resolution mass spectral analysis (HRMS) data were measured on JMST100LP4G (JEOL) mass spectrometer or a TOF mass analyzer equipped with the ESI source, JEOL Model: JMS-T200GC AccuTOF GCx equipped with FD (field desorption) source. All heating reactions were carried out with an oil bath as the heat source. Reactions were magnetically stirred and monitored by thin layer chromatography carried out on 0.25 mm E. Merck silica gel plate (60f-254) using UV light as the visualizing agents. Single-crystal X-ray diffraction intensity data were collected on a Bruker X8 APEX diffractometer equipped with a CCD area detector and Mo Kα radiation (λ = 0.71073 Å) at 100 K; all data calculations were performed by using the PC version of the APEX2 program package.

2. General procedure for preparation of substrates:

(a) Preparation of 2-(2-ethynyl-6-fluorophenyl)acetonitrile (1g):



(a-1) Synthesis of 2-(2-bromo-6-fluorophenyl)acetonitrile[s1-a] (s-2).

To a refluxing solution of 3.16 gm (48.52 mmol) of potassium cyanide in 15 mL of 95% ethanol and 6.5 mL of water was added 5.0 gm (18.66 mmol) of 1-bromo-2-(bromomethyl)-3-fluorobenzene (**s-1**) over 0.5h. The mixture was refluxed in an oil bath as the heat source for an additional 0.5h, and 50 mL of ice water was added. The crystalline 2-(2-bromo-6-fluorophenyl)acetonitrile was collected and recrystallized from 70% aqueous ethanol to afford 3.30 gm (15.42 mmol, 83%) of 2-(2-bromo-6-fluorophenyl)acetonitrile (**s-2**).

(a-2) Synthesis of 2-(2-ethynyl-6-fluorophenyl)acetonitrile (1g).

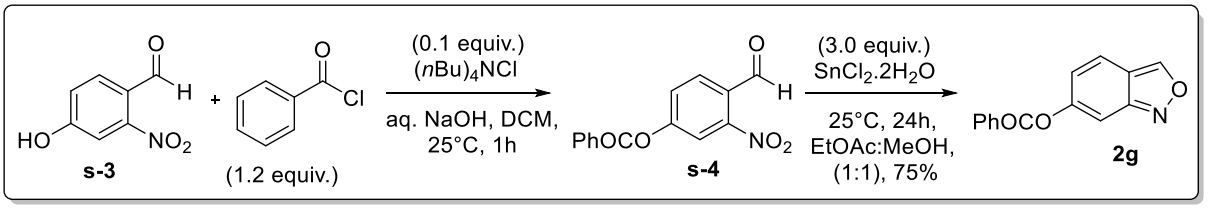
2-(2-bromo-6-fluorophenyl)acetonitrile (**s-2**). (2.0 gm, 9.34 mmol), $Pd(PPh_3)_2Cl_2$ (0.328 gm, 0.467 mmol, 5 mol %) and CuI (0.178 gm, 0.934 mmol, 10 mol %), were placed in an oven-dried and argon-filled Schlenk tube. After addition of triethylamine (20 mL), the mixture was stirred at 25 ºC for 5 min and (trimethylsilyl)acetylene (1.01 gm, 10.28 mmol) was added. After this mixture had been stirred at 80 ºC for 18h, the reaction mixture was quenched with saturated NH_4Cl solution (100 mL) and extracted with CH_2Cl_2 (3 x 75 mL). The combined organic layers were washed with water (50 mL), and saturated NaCl solution (50 mL) and dried with $MgSO_4$. After concentration under vacuum, the residue was purified by flash chromatography on silica column to afford 2-(2-fluoro-6-((trimethylsilyl)ethynyl)phenyl)acetonitrile 1.70 gm (7.35 mmol, 79%) as a light yellow oil.

To a methanol solution (20 mL) of 2-(2-fluoro-6-((trimethylsilyl)ethynyl)phenyl)acetonitrile (1.0 gm, 4.32 mmol) at 0 ºC was added K_2CO_3 (0.657 gm, 4.75 mmol); the resulting mixture was stirred at 25 °C for 0.5h. The solution was quenched with cold water, extracted with dichloromethane (3 X 20 mL), washed with saturated NaCl solution, dried over $MgSO_4$, and concentrated under reduced pressure. The residues were chromatographed on a silica column to afford pure 2-(2-ethynyl-6-fluorophenyl)acetonitrile (**1g**) 0.497 gm (3.12 mmol, 72%) as a brown oil.

The compound 2-(2-chloro-6-ethynylphenyl)acetonitrile **(1h)** was synthesized using the same synthetic procedure.

Synthesis of substrates **1a-1f** and **1i** were reported in literature.[s1-b] Synthesis of substrate **1j** was reported in literature.[s1-c] Synthesis of substrate **1k** was reported in literature.[s1-d]

(b) Preparation of benzo[*c*]isoxazol-6-yl benzoate (2g):



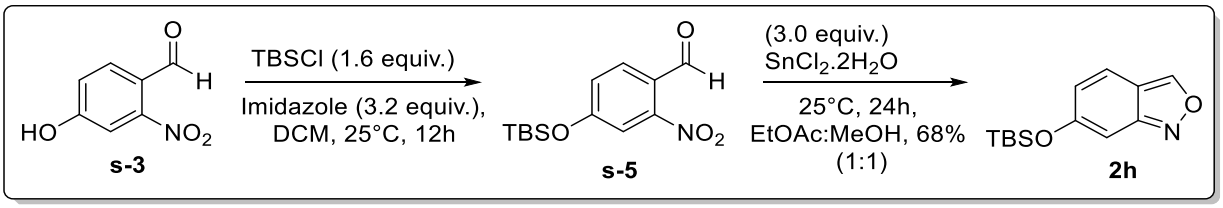
(b-1) Synthesis of 4-formyl-3-nitrophenyl benzoate (**s-4):**

To a solution of 4-hydroxy-2-nitrobenzaldehyde (**s-3**) (1 gm, 5.98 mmol) in 10 mL DCM at 0°C was added 10 ml aqueous sodium hydroxide (0.789 gm, 19.75 mmol) solution in a 100-ml flask. Solution of tetra-*n*-butylammonium chloride (0.166 gm, 0.598 mmol) in 5 mL of dichloromethane and benzoyl chloride (1.01 gm, 7.18 mmol) in 10 mL of dichloromethane were prepared and cooled to 0° C, further this solution was added dropwise to above reaction mixture at 0°C. The reaction mixture was stirred at 25° C for 1h and then poured over 50 mL of icy water. The organic layer was separated and the aqueous layer was extracted twice with 40 mL of diethyl ether. The combined organic extracts were washed with saturated NaCl solution and dried over $MgSO_4$. After concentration under vacuum, the residue was purified by flash chromatography on silica column to afford 1.30 gm (4.79 mmol, 80%) of 4-formyl-3-nitrophenyl benzoate (**s-4)** as off-white solid**.**

(b-2) Synthesis of benzo[*c*]isoxazol-6-yl benzoate (2g):

To a solution of 4-formyl-3-nitrophenyl benzoate (**s-4**) (1.0 g, 3.69 mmol) in ethyl acetate/methanol 1:1 (20 mL) was added $SnCl_2.2H_2O$ (2.50 g, 11.06 mmol). The reaction mixture was stirred at 25° C for 24h. The reaction was quenched by saturated $NaHCO_3$, filtered and washed with DCM. Organic layer was then washed with water and brine, dried over $MgSO_4$ and concentrated. Crude product was then purified by flash chromatography on silica gel using (EA/Hexane = 7:93) to give benzo[*c*]isoxazol-6-yl benzoate (**2g**) (0.660 gm, 2.76 mmol, 75%) as off-white solid.

(c) Preparation of 6-((tert-butyldimethylsilyl)oxy)benzo[*c*]isoxazole (2h):



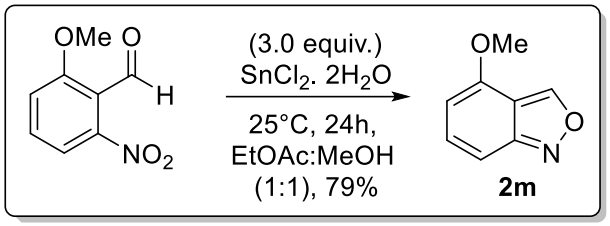
(c-1) Synthesis of 4-((*tert*-butyldimethylsilyl)oxy)-2-nitrobenzaldehyde (s-5):

In a typical procedure, 4-hydroxy-2-nitrobenzaldehyde (**s-3**) (1 gm, 5.98 mmol) was dissolved in 10 mL of dry dichloromethane in a 100-ml flask and cooled to 0°C. To this mixture at 0°C was added a dry dichloromethane (5.0 mL) solution of *tert*-butylchlorodimethylsilane (1.44 gm, 9.57 mmol). Further to above reaction mixture was added dropwise dry dichloromethane (5.0 mL) solution of 1*H*-imidazole (1.30 gm, 19.15 mmol) and stirred reaction mixture at 25°C for 12h. Reaction was monitered by TLC, after completion of the reaction, reaction mixture was quenched with cold water. The organic layer was separated and the aqueous layer was extracted twice with 40 mL of dichloromethane. The combined organic extracts were washed with saturated NaCl solution and dried over $MgSO_4$. After concentration under vacuum, the residue was purified by flash chromatography on silica column to afford 1.45 gm (5.15 mmol, 86%) of 4-((*tert*-butyldimethylsilyl)oxy)-2-nitrobenzaldehyde (**s-5)** as colorless oil**.**

(c-2) Preparation of 6-((*tert*-butyldimethylsilyl)oxy)benzo[*c*]isoxazole (2h):

To a solution of 4-((*tert*-butyldimethylsilyl)oxy)-2-nitrobenzaldehyde (**s-5**) (1.0 g, 3.55 mmol) in ethyl acetate/methanol 1:1 (20 mL) was added $SnCl_2.2H_2O$ (2.41 g, 10.66 mmol). The reaction mixture was stirred at 25°C for 24h. The reaction was quenched by saturated $NaHCO_3$, filtered and washed with DCM. Organic layer was then washed with water and brine, dried over $MgSO_4$ and concentrated. Crude product was then purified by flash chromatography on silica gel using (EA/Hexane = 6:94) to give 6-((*tert*-butyldimethylsilyl)oxy)benzo[*c*]isoxazole (**2h**) (0.605 gm, 2.43 mmol, 68%) as colorless oil.

(d) Preparation of 4-methoxybenzo[*c*]isoxazole (2m):

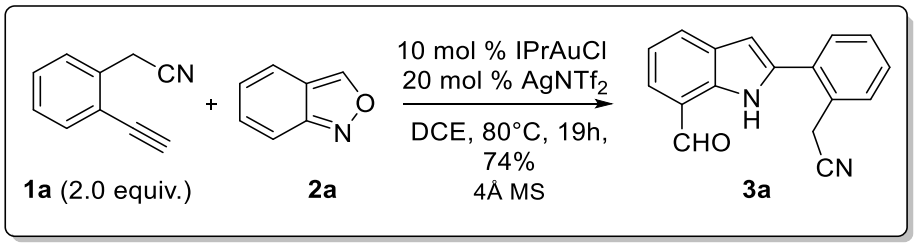


To a solution of 2-methoxy-6-nitrobenzaldehyde (1.0 g, 5.52 mmol) in ethyl acetate/methanol 1:1 (20 mL) was added $SnCl_2.2H_2O$ (3.74 g, 16.56 mmol). The reaction mixture was stirred at 25°C for 24h. The reaction was quenched by saturated $NaHCO_3$, filtered and washed with DCM. Organic layer was then washed with water and brine, dried over $MgSO_4$ and concentrated. Crude product was then purified by flash chromatography on silica gel using (EA/Hexane = 8:92) to give 4-methoxybenzo[*c*]isoxazole (**2m**) (0.650 gm, 4.36 mmol, 79%) as colorless solid.

Synthesis of substrates **2a-2f, 2i-2l** and **2n-2r** were reported in literature.[s2]

3. Standard procedure for catalytic operation:

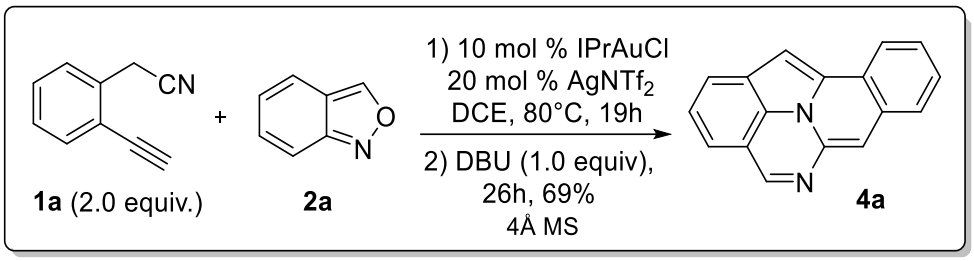
(a) Typical procedure for synthesis of 2-(2-(7-formyl-1*H*-indol-2-yl)phenyl)acetonitrile (3a):



A 15mL flask was charged with IPrAuCl (52.17 mg, 0.08 mmol) and $AgNTf_2$ (65.10 mg, 0.16 mmol), and to this mixture was added dry 1, 2-dichloroethane (0.5 mL). The resulting mixture was stirred at room temperature for 5 min. To this mixture was added dropwise a dry 1, 2-dichloroethane (2.5 mL) solution of 2-(2-ethynylphenyl)acetonitrile (**1a**) (237 mg, 1.68 mmol) and benzo[*c*]isoxazole (**2a**) (100 mg, 0.84 mmol) at room temperature. After addition the reaction mixture was stirred at 80 °C in oil bath for 19h. The reaction mixture was filtered over a short celite bed, concentrated under reduced pressure, and purified by silica column eluting with (EA/Hexane = 12/88) to afford 2-(2-(7-formyl-1*H*-indol-2-yl)phenyl)acetonitrile (**3a**) (162 mg, 0.62 mmol, 74%) as brown solid.

The compounds **3i, 3i', 3j** and **3k** were synthesized using the same catalytic procedure.

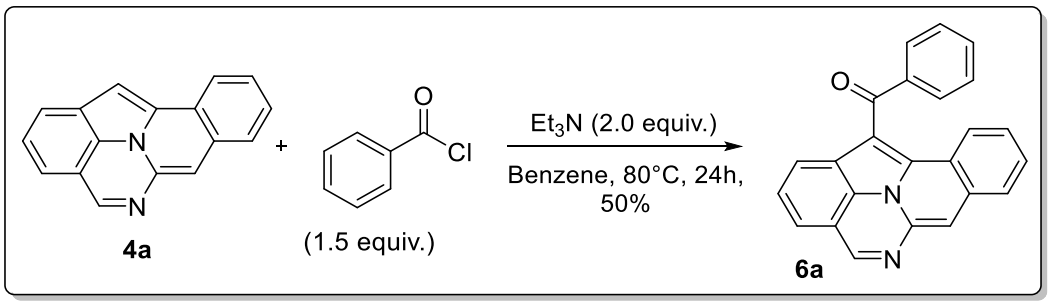
(b) Typical procedure for synthesis of benzo[7,8]indolizino[2,3,4,5-*ija*]quinazoline (4a):



A 15mL flask was charged with IPrAuCl (52.17 mg, 0.08 mmol) and $AgNTf_2$ (65.10 mg, 0.16 mmol), and to this mixture was added dry 1, 2-dichloroethane (0.5 mL). The resulting mixture was stirred at room temperature for 5 min. To this mixture was added dropwise a dry 1, 2-dichloroethane (2.5 mL) solution of 2-(2-ethynylphenyl)acetonitrile (**1a**) (237 mg, 1.68 mmol) and benzo[*c*]isoxazole (**2a**) (100 mg, 0.84 mmol) at room temperature. After addition the reaction mixture was stirred at 80 °C in oil bath for 19h, reaction was monitored by TLC. After completion of starting material **2a**, later at same temperature was added 1,8-diazabicyclo[5.4.0]undec-7-ene (DBU) (128 mg, 0.84 mmol) to the reaction mixture and further stirred for 26h. The reaction mixture was filtered over a short celite bed, concentrated under reduced pressure, and purified by silica column eluting with (EA/Hexane = 10/90) to afford benzo[7,8]indolizino[2,3,4,5-*ija*]quinazoline (**4a**) (140 mg, 0.57 mmol, 69%) as red solid.

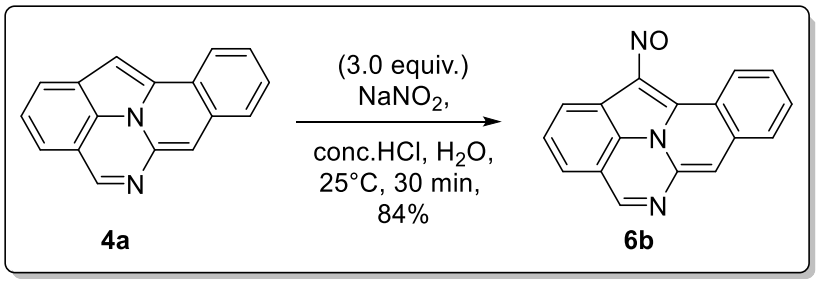
4. Synthetic procedure for chemical functionalization of 4a and 5o:

(a) Typical procedure for synthesis of benzo[7,8]indolizino[2,3,4,5-*ija*]quinazolin-11-yl(phenyl)methanone (6a):



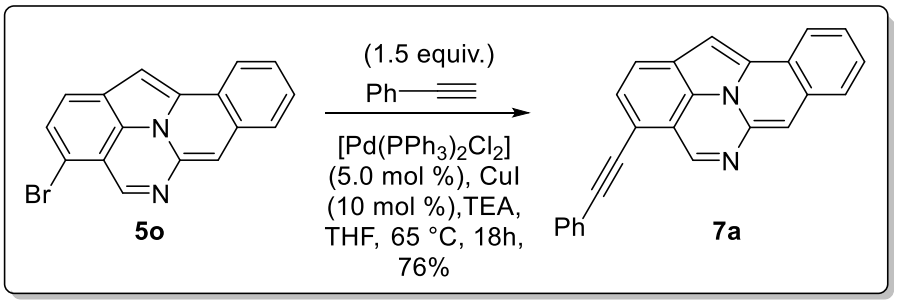
To a benzene (3.0 mL) solution of benzo[7,8]indolizino[2,3,4,5-*ija*]quinazoline **4a** (100 mg, 0.41 mmol) was added benzoyl chloride (87 mg, 0.61 mmol) at 25°C. To this mixture at 25°C was added triethyl amine (83.5 mg, 0.82 mmol). Further above reaction mixture was stirred at 80 °C in oil bath for 24h. Reaction was monitored by TLC, after completion of the reaction, reaction mixture was quenched with cold water. The organic layer was separated and the aqueous layer was extracted twice with 20 mL of dichloromethane. The combined organic extracts were dried over $MgSO_4$. After concentration under vacuum, the residue was purified by flash chromatography on silica column with (EA/Hexane = 14/86) to afford 72 mg (0.20 mmol, 50%) of benzo[7,8]indolizino[2,3,4,5-*ija*]quinazolin-11-yl(phenyl)methanone **(6a)** as orange solid**.**

(b) Typical procedure for the synthesis of 11-nitrosobenzo[7,8]indolizino[2,3,4,5-*ija*]quinazoline (6b):



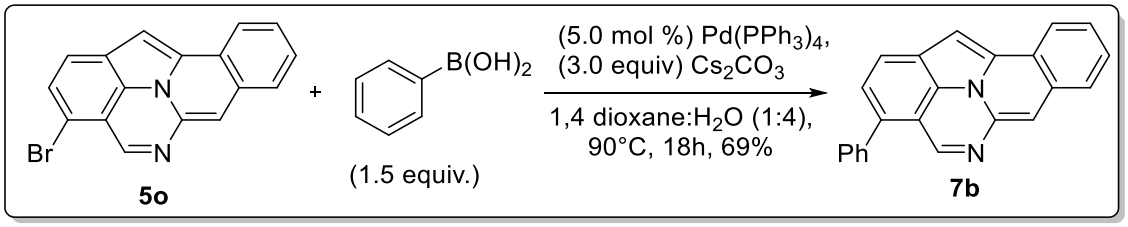
To a H_2O (1 mL) solution of benzo[7,8]indolizino[2,3,4,5-*ija*]quinazoline **4a** (100 mg, 0.41 mmol) was added 0.5 mL of conc. HCl at 0°C. With stirring and cooling, a solution of (85.4 mg, 1.24 mmol) of $NaNO_2$ in 2 mL of water was added to above reaction mixture and stirred at 25 °C for 30 min. Reaction was monitored by TLC, after completion of the reaction, reaction mixture was quenched by saturated NaOH solution. The organic layer was separated and the aqueous layer was extracted twice with 20 mL of dichloromethane. The combined organic extracts were dried over $MgSO_4$. After concentration under vacuum, the residue was purified by flash chromatography on silica column with (EA/Hexane = 50/50) to afford 94 mg (0.34 mmol, 84%) of 11-nitrosobenzo[7,8]indolizino[2,3,4,5-*ija*]quinazoline **(6b)** as brown solid**.**

(d) Typical procedure for the synthesis of 3-(phenylethynyl)benzo[7,8]indolizino[2,3,4,5-*ija*]quinazoline (7a):



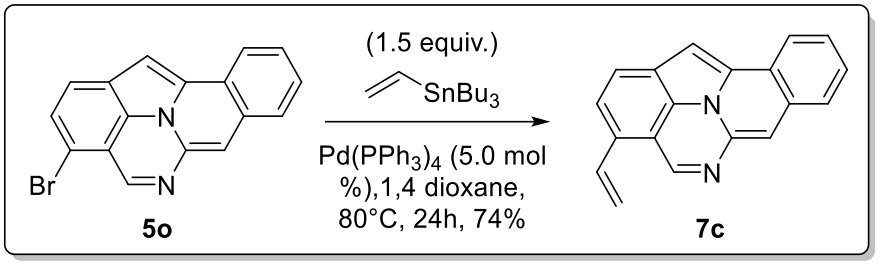
3-bromobenzo[7,8]indolizino[2,3,4,5-*ija*]quinazoline (**5o**) (100 mg, 0.31 mmol), $Pd(PPh_3)_2Cl_2$ (11 mg, 0.15 mmol, 5 mol %) and CuI (5.93 mg, 0.31 mmol, 10 mol %), were placed in an oven-dried argon-filled Schlenk tube and added 5 mL of THF. After addition of triethylamine (63 mg, 0.62 mmol), the mixture was stirred at 25 ºC for 5 min and phenyl acetylene (47.7 mg, 0.46 mmol) was added. After this reaction mixture had been stirred at 65 ºC in oil bath for 18h. After completion of reaction, reaction mixture was filtered over a short celite bed, concentrated under reduced pressure, and purified by silica column eluting with (EA/Hexane = 10/90) to afford 81 mg (0.23 mmol, 76%) 3-(phenylethynyl)benzo[7,8]indolizino[2,3,4,5-*ija*]quinazoline **(7a)** as red solid.

(e) Typical procedure for the synthesis of 3-phenylbenzo[7,8]indolizino[2,3,4,5-*ija*]quinazoline (7b):



3-bromobenzo[7,8]indolizino[2,3,4,5-*ija*]quinazoline (**5o**) (100 mg, 0.31 mmol), $Pd(PPh_3)_4$ (18 mg, 0.15 mmol, 5 mol %) and Cs_2CO_3 (304 mg, 0.93 mmol), were placed in an oven-dried argon-filled Schlenk tube and added 1,4 dioxane (4 mL): H_2O (1 mL). Later phenyl boronic acid (57 mg, 0.46 mmol) was added to the reaction mixture. After this reaction mixture was purged with argon gas for 10 min and had been stirred at 90 ºC in oil bath for 18h. After completion of reaction, reaction mixture was filtered over a short celite bed, concentrated under reduced pressure, and purified by silica column eluting with (EA/Hexane = 09/91) to afford 68 mg (0.21 mmol, 69%) 3-phenylbenzo[7,8]indolizino[2,3,4,5-*ija*]quinazoline **(7b)** as red solid.

(f) Typical procedure for the synthesis of 3-vinylbenzo[7,8]indolizino[2,3,4,5-*ija*]quinazoline (7c):



3-bromobenzo[7,8]indolizino[2,3,4,5-*ija*]quinazoline (**5o**) (100 mg, 0.31 mmol), $Pd(PPh_3)_4$ (18 mg, 0.15 mmol, 5 mol %) were placed in an oven-dried argon-filled Schlenk tube and added 1,4 dioxane (5 mL). Later tributyl(vinyl)stannane (148 mg, 0.46 mmol) was added to the reaction mixture. After this reaction mixture was purged with argon gas for 10 min and had been stirred at 80 ºC in oil bath for 24h. After completion of reaction, reaction mixture was filtered over a short celite bed, concentrated under reduced pressure, and purified by silica column eluting with (EA/Hexane = 10/90) to afford 62 mg (0.23 mmol, 74%) 3-vinylbenzo[7,8]indolizino[2,3,4,5-*ija*]quinazoline **(7c)** as red solid.

5. Optical and Photophysical Properties

All properties were examined in CH_2Cl_2 solution with a concentration of 10^{-5} and in quartz cuvettes with a layer thickness of 1 cm. UV-vis absorption spectra were recorded on a Hitachi U-3310 device. Fluorescence spectra were measured on a Hitachi F-7000 device. The excitation wavelength was at 394 nm.

Table s1. Photophysical data of representative N-containing polyaromatic compounds.

	λ_{abs} [nm] (log ε)	λ_{em}[a] [nm]	Stokes shift (nm)
4a	274 (4.80)	565	291
4b	274 (4.47)	568	294
4c	268 (4.72)	560	292
5a	274 (4.86)	573	299
5m	274 (4.91)	572	298

[a] Excited at λ_{abs}.

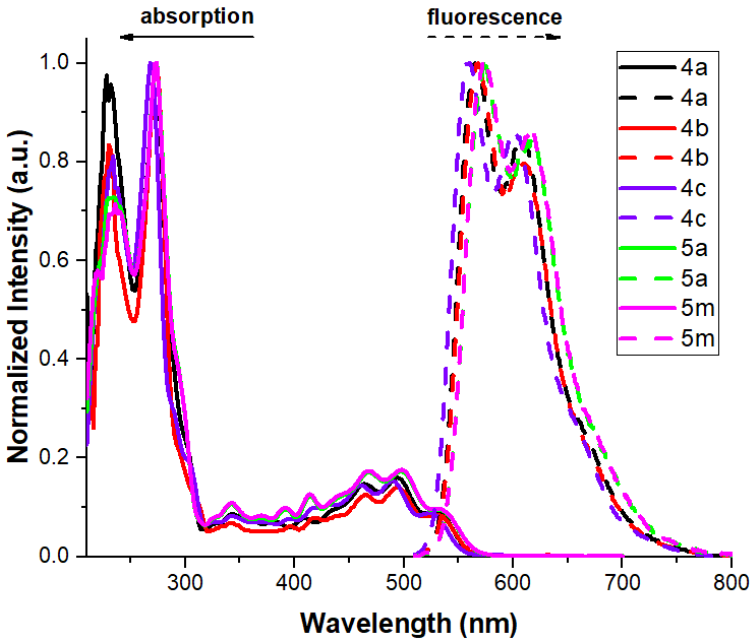


Figure s1. UV/Vis absorption (solid lines) and emission spectra (dotted ones) in dilute CH_2Cl_2.

6. Representative bioactive compounds

Figure s2 shows several small polyarenes containing two nitrogen atoms; species (**I-V**) are isolated from natural sources. Arnoamine A (**I**)[s3a] and B (**II**)[s3a] show cytotoxicity against human tumor cell lines. Pentralis (**III**, canthin-6-one)[s3b] is used to prevent infections caused by mycobacteria. Cordatanine (**IV**, 4-methoxycanthin-6-one)[s3c] is an anti-human immunodeficiency virus alkaloid. Drymaritin (**V**)[s3d] a novel indole alkaloid is reported to exhibit anti-HIV effects in H9 lymphocytes.

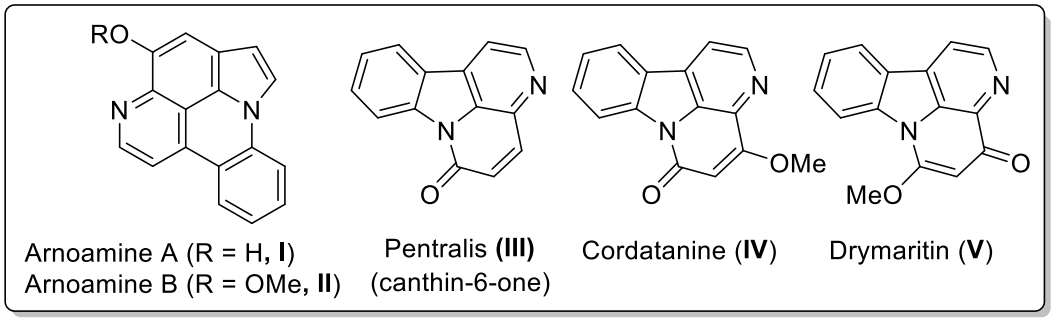


Figure s2. Bioactive compounds containing two nitrogen atoms

7. References:

[s1] (a) M. Adamczyk, D. S. Watt and D. A. Netzel, *J. Org. Chem*., 1984, **49**, 4226–4237; (b) S. N. Karad and R.-S. Liu, *Angew. Chem., Int. Ed.*, 2014, **53**, 5444−5448; (c) J. Sedelmeier, S. V. Ley, H. Lange and I. R. Baxendale, *Eur. J. Org. Chem*., 2009, 4412; (d) L. Song, G. Tian, Y. He and E. V. Van der Eycken, *Chem. Commun*., 2017, **53**, 12394.

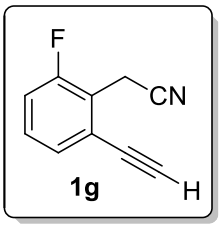
[s2] (a) J. Chauhan and S. Fletcher, *Tetrahedron Lett*., 2012, **53**, 4951- 4954; (b) H. Jin, B. Tian, X. Song, J. Xie, M. Rudolph, F. Rominger and A. S. K. Hashmi, *Angew. Chem., Int. Ed*., 2016, **55**, 12688−12692. (c) H. Jin, L. Huang, J. Xie, M. Rudolph, F. Rominger and A. S. K. Hashmi, *Angew. Chem., Int. Ed*., 2016, **55**, 794−797; (d) R. L. Sahani and R.-S. Liu, *Angew. Chem., Int. Ed.*, 2017, **56**, 12736−12740; (e) C. Wang, G. Xu, Y. Shao, S. Tang and J. Sun, *Org. Lett*., 2020, **22**, 5990−5994; (f) R. Shao, H. Zhao, S. Ding, L. Li, C. Chen, J. Wang and Y. Shang, *Chem. Commun*. 2022, **58**, 4771−4774.

[s3] (a) A. Plubrukarn and B. Davidson, *J. Org. Chem.*, 1998, **63**, 1657-1659. (b) Z. Zhang, A. Wang, Y. Wang, W. Sun, X. Zhou, Q. Xu, L. Mao and J. Zhang, *Molecules*, 2023, **28**, 3381; (c) S.

V. Shelar and N. P. Argade, *ACS Omega*, 2017, **2**, 3945; (d) I. Wetzel, L. Allmendinger and F. Bracher, *J. Nat. Prod*., 2009, **72**, 1908–1910.

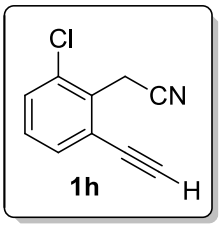
8. Spectral data of key compounds:

Spectral data for 2-(2-ethynyl-6-fluorophenyl)acetonitrile (1g):



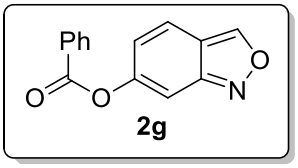
Compound **1g** was purified on silica gel column using ethyl acetate/hexane: (4:96) as the eluent; Colorless solid (497 mg, 3.12 mmol, 72%); ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.34-7.26 (m, 2H), 7.12 (d, *J* = 8.7 Hz, 1H), 3.87 (s, 2H), 3.44 (s, 1H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 161.3, 159.3, 129.9 (d), 128.8 (d), 124.0 (d), 120.0 (d), 116.7 (d), 116.0, 84.1, 79.2 (d), 15.5 (d); HRMS (FD) m/z: $[M]^+$ calcd for $C_{10}H_6NF$: 159.0489; found: 159.0495.

Spectral data for 2-(2-chloro-6-ethynylphenyl)acetonitrile (1h):



Compound **1h** was purified on silica gel column using ethyl acetate/hexane: (5:95) as the eluent; Colorless solid (531 mg, 3.02 mmol, 75%); ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.45-7.40 (m, 2H), 7.24 (t, *J* = 7.9 Hz, 1H), 4.02 (s, 2H), 3.45 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 134.6, 131.5, 130.6, 130.4, 129.4, 124.3, 115.8, 84.1, 79.8, 20.3; HRMS (ESI-TOF) m/z: [M-H] calcd for $C_{10}H_5NCl$: 174.0110; found: 174.0110.

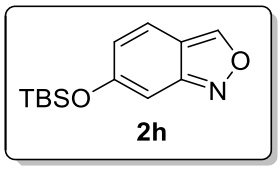
Spectral data for benzo[*c*]isoxazol-6-yl benzoate (2g):



2g

Compound **2g** was purified on silica gel column using ethyl acetate/hexane: (10:90) as the eluent; Off-white solid (660 mg, 2.76 mmol, 75%); ^{1}H NMR (500 MHz, $CDCl_3$): δ 9.11 (s, 1H), 8.18 (d, *J* = 7.6 Hz, 2H), 7.66 (q, *J* = 17.5 & 9.6 Hz, 2H), 7.50 (t, *J* = 7.7 Hz, 2H), 7.40 (s, 1H), 7.17 (d, 9.5 Hz, 1H; ^{13}C NMR (125 MHz, $CDCl_3$): δ 164.9, 154.8, 154.6, 147.1, 133.8, 130.1, 128.9, 128.6, 128.3, 117.6, 116.6, 109.4; HRMS (ESI-TOF) m/z: [M+H] calcd for $C_{14}H_{10}NO_3$: 240.0660; found: 240.0662.

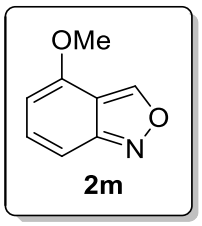
Spectral data for 6-((tert-butyldimethylsilyl)oxy)benzo[*c*]isoxazole (2h):



2h

Compound **2h** was purified on silica gel column using ethyl acetate/hexane: (9:91) as the eluent; Colorless oil (605 mg, 2.43 mmol, 68%); ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.90 (s, 1H), 7.50 (d, *J* = 9.4 Hz, 1H), 6.93 (d, *J* = 9.4 Hz, 1H), 6.72 (s, 1H), 0.96 (s, 9H), 0.20 (s, 6H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 154.1, 152.4, 151.5, 130.4, 118.5, 116.3, 102.5, 25.5, -4.5; HRMS (ESI-TOF) m/z: [M+H] calcd for $C_{13}H_{20}NO_2Si$: 250.1263; found: 250.1264.

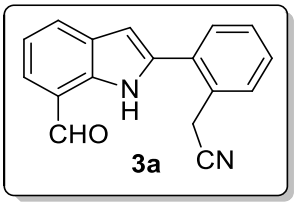
Spectral data for 4-methoxybenzo[*c*]isoxazole (2m):



2m

Compound **2m** was purified on silica gel column using ethyl acetate/hexane: (12:88) as the eluent; Colorless solid (650 mg, 4.36 mmol, 79%); ^{1}H NMR (500 MHz, $CDCl_3$): δ 9.09 (s, 1H), 7.18 (t, *J* = 8.9 Hz, 1H), 7.13 (d, *J* = 8.9 Hz, 1H), 6.12 (d, *J* = 7.0 Hz, 1H), 3.88 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 157.4, 153.4, 152.6, 132.2, 114.2, 106.8, 98.9, 55.4; HRMS (FD) m/z: $[M]^+$ calcd for $C_8H_7NO_2$: 149.0482; found: 149.0480.

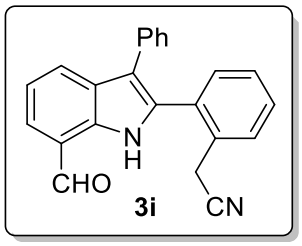
Spectral data for 2-(2-(7-formyl-1*H*-indol-2-yl)phenyl)acetonitrile (3a):



3a

Compound **3a** was purified on silica gel column using ethyl acetate/hexane: (12:88) as the eluent; Colorless solid (162 mg, 0.62 mmol, 74%); ^{1}H NMR (700 MHz, $CDCl_3$): δ 10.15 (s, 1H), 10.11 (s, 1H), 7.95 (d, *J* = 7.8 Hz, 1H), 7.69 (d, *J* = 7.3 Hz, 1H), 7.61-7.54 (m, 2H), 7.46 (t, *J* = 4.6 Hz, 2H), 7.31 (t, *J* = 7.6 Hz, 1H), 6.69 (s, 1H), 3.88 (s, 2H); ^{13}C NMR (175 MHz, $CDCl_3$): δ 193.4, 136.8, 134.1, 131.9, 130.0, 129.7, 129.6, 129.3, 129.1, 128.64, 128.63, 128.0, 120.1, 117.9, 103.2, 22.4; HRMS (ESI-TOF) m/z: $[M+Na]^+$ calcd for $C_{17}H_{12}N_2ONa$: 283.0847; found: 283.0846.

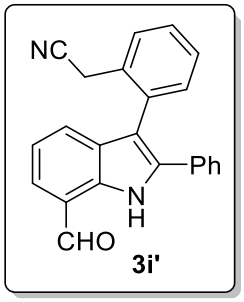
Spectral data for 2-(2-(7-formyl-3-phenyl-1*H*-indol-2-yl)phenyl)acetonitrile (3i):



3i

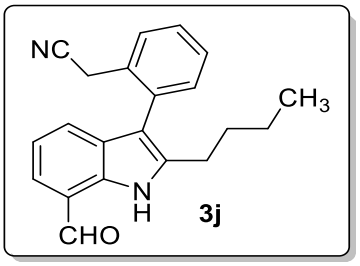
Compound **3i** was purified on silica gel column using ethyl acetate/hexane: (12:88) as the eluent; Colorless solid (73 mg, 0.21 mmol, 26%); ^{1}H NMR (700 MHz, $CDCl_3$): δ 10.16 (s, 1H, peak merged with CHO peak), 10.15 (s, 1H), 8.11 (d, *J* = 7.9 Hz, 1H), 7.75 (d, *J* = 7.3 Hz, 1H), 7.61-7.59 (m, 1H), 7.50-7.46 (m, 3H), 7.36-7.32 (m, 3H), 7.27-7.25 (m, 3H), 3.24 (s, 2H); ^{13}C NMR (175 MHz, $CDCl_3$): δ 193.4, 133.8, 133.7, 133.4, 131.4, 131.3, 129.7, 129.5, 129.4, 129.1, 129.0, 128.8, 128.5, 128.3, 127.0, 126.9, 120.49, 120.43, 117.5, 116.6, 21.6; HRMS (ESI-TOF) m/z: $[M+Na]^+$ calcd for $C_{23}H_{16}N_2ONa$: 359.1160; found: 359.1163.

Spectral data for 2-(2-(7-formyl-2-phenyl-1*H*-indol-3-yl)phenyl)acetonitrile (3i'):



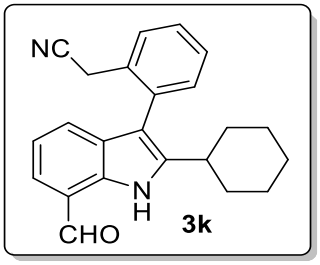
Compound **3i'** was purified on silica gel column using ethyl acetate/hexane: (12:88) as the eluent; Colorless solid (82 mg, 0.24 mmol, 29%); ^{1}H NMR (700 MHz, $CDCl_3$): δ 10.37 (s, 1H), 10.18 (s, 1H), 7.72 (d, *J* = 7.2 Hz, 1H), 7.59 (d, *J* = 7.8 Hz, 2H), 7.47-7.42 (m, 3H), 7.35-7.30 (m, 5H), 7.27 (t, *J* = 7.7 Hz, 1H), 3.44 (d, *J* = 18.8 Hz, 1H), 3.27 (d, *J* = 18.8 Hz, 1H); ^{13}C NMR (175 MHz, $CDCl_3$): δ 193.5, 136.2, 133.7, 133.4, 132.2, 131.2, 130.2, 129.7, 129.3, 129.1, 128.9, 128.6, 128.5, 128.4, 126.9, 126.5, 120.4, 120.3, 117.8, 111.9, 21.7; HRMS (ESI-TOF) m/z: $[M+Na]^+$ calcd for $C_{23}H_{16}N_2ONa$: 359.1160; found: 359.1159.

Spectral data for 2-(2-(2-butyl-7-formyl-1*H*-indol-3-yl)phenyl)acetonitrile (3j):



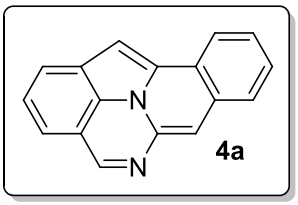
Compound **3j** was purified on silica gel column using ethyl acetate/hexane: (7:93) as the eluent; Colorless oil (80 mg, 0.25 mmol, 30%); ^{1}H NMR (500 MHz, $CDCl_3$): δ 10.13 (s, 1H), 10.05 (s, 1H), 7.62 (d, *J* = 7.2 Hz, 2H), 7. 46-7.38 (m, 3H), 7.29 (d, *J* = 7.2 Hz, 1H), 7.20 (t, *J* = 7.5 Hz, 1H), 3.51 (q, *J* = 31.7 & 18.5 Hz, 2H), 2.73-2.67 (m, 1H), 2.64-2.58 (m, 1H), 1.66-1.59 (m, 2H), 1.33-1.26 (m, 2H), 0.84 (t, *J* = 7.3 Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 193.6, 139.1, 133.4, 133.0, 132.3, 130.3, 129.2, 128.6, 128.3, 128.22, 128.21, 125.6, 120.0, 119.8, 118.0, 111.7, 31.5, 26.0, 22.3, 21.8, 13.6; HRMS (ESI-TOF) m/z: $[M+Na]^+$ calcd for $C_{21}H_{20}N_2ONa$: 339.1473; found: 339.1476.

Spectral data for 2-(2-(2-cyclohexyl-7-formyl-1*H*-indol-3-yl)phenyl)acetonitrile (3k):



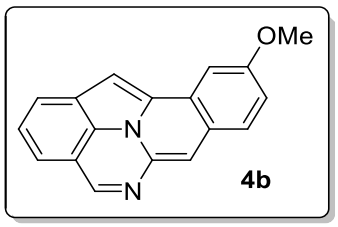
Compound **3k** was purified on silica gel column using ethyl acetate/hexane: (7:93) as the eluent; Colorless oil (89 mg, 0.26 mmol, 31%); ^{1}H NMR (500 MHz, $CDCl_3$): δ 10.13 (s, 1H), 10.00 (s, 1H), 7.62 (d, *J* = 7.1 Hz, 2H), 7.45 (t, *J* = 7.4 Hz, 1H), 7.40 (t, *J* = 7.9 Hz, 2H), 7.28 (d, *J* = 7.3 Hz, 1H), 7.19 (t, *J* = 7.5 Hz, 1H), 3.51 (q, *J* = 28.4 & 18.5 Hz, 2H), 2.67-2.61 (m, 1H), 1.91-1.79 (m, 4H), 1.71 (s, 1H), 1.58-1.49 (m, 2H), 1.32-1.24 (m, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 193.6, 143.6, 133.6, 132.9, 132.3, 130.3, 129.2, 128.6, 128.3, 128.24, 128.21, 125.6, 120.1, 119.7, 118.1, 110.3, 36.0, 33.3, 32.6, 26.25, 26.20, 25.6, 21.8; HRMS (ESI-TOF) m/z: $[M+Na]^+$ calcd for $C_{23}H_{22}N_2ONa$: 365.1629; found: 365.1631.

Spectral data for benzo[7,8]indolizino[2,3,4,5-*ija*]quinazoline (4a):



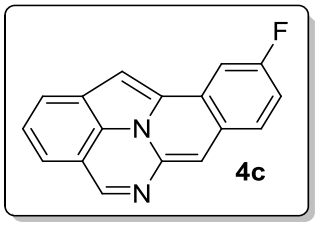
Compound **4a** was purified on silica gel column using ethyl acetate/hexane: (10:90) as the eluent; Red solid (140 mg, 0.57 mmol, 69%); ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.92 (s, 1H), 8.26 (t, *J* = 3.4 Hz, 1H), 7.88 (d, *J* = 7.9 Hz, 1H), 7.82 (t, *J* = 5.1 Hz, 1H), 7.56 (t, *J* = 3.9 Hz, 2H), 7.49 (t, *J* = 7.4 Hz, 1H), 7.37 (d, *J* = 7.1 Hz, 1H), 7.14 (s, 1H), 7.11 (s, 1H); ^{13}C NMR (175 MHz, $CDCl_3$): δ 156.2, 138.5, 134.9, 132.1, 130.6, 128.3, 127.7, 126.6, 126.4, 123.8, 123.7, 122.8, 122.2, 117.7, 113.8, 103.3, 90.4; HRMS (ESI-TOF) m/z: $[M+H]^+$ calcd for $C_{17}H_{11}N_2$: 243.0922; found: 243.0922.

Spectral data for 9-methoxybenzo[7,8]indolizino[2,3,4,5-*ija*]quinazoline (4b):



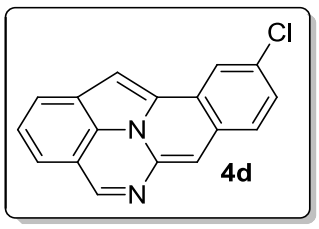
Compound **4b** was purified on silica gel column using ethyl acetate/hexane: (12:88) as the eluent; Red solid (149 mg, 0.54 mmol, 65%); ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.85 (s, 1H), 7.85 (d, *J* = 8.0 Hz, 1H), 7.75 (d, *J* = 8.7 Hz, 1H), 7.62 (s, 1H), 7.46 (t, *J* = 7.4 Hz, 1H), 7.32 (d, *J* = 7.1 Hz, 1H), 7.18 (d, *J* = 8.7 Hz, 1H), 7.09 (s, 2H), 3.97 (s, 3H); ^{13}C NMR (175 MHz, $CDCl_3$): δ 158.6, 154.9, 137.1, 134.4, 130.9, 129.8, 126.3, 125.9, 124.0, 123.8, 121.7, 117.9, 117.5, 113.2, 105.0, 103.3, 90.1, 55.5; HRMS (FD) m/z: $[M]^+$ calcd for $C_{18}H_{12}N_2O$: 272.0955; found: 272.0961.

Spectral data for 9-fluorobenzo[7,8]indolizino[2,3,4,5-*ija*]quinazoline (4c):



Compound **4c** was purified on silica gel column using ethyl acetate/hexane: (9:91) as the eluent; Red solid (146 mg, 0.56 mmol, 67%); ^{1}H NMR (700 MHz, $CDCl_3$): δ 8.83 (s, 1H), 7.83 (d, *J* = 7.9 Hz, 1H), 7.79 (d, *J* = 9.0 Hz, 1H), 7.72 (t, *J* = 7.9 Hz, 1H), 7.44 (t, *J* = 7.4 Hz, 1H), 7.31 (d, *J* = 7.0 Hz, 1H), 7.22 (d, *J* = 10.6 Hz, 1H), 7.01 (s, 1H), 6.99 (s,1H); ^{13}C NMR (175 MHz, $CDCl_3$): δ 161.9, 160.5, 155.8, 137.9, 133.9 (d), 130.5, 130.2 (d), 128.4 (d), 126.2, 124.0 (d), 122.3, 117.7, 116.4 (d), 114.1, 108.9 (d), 102.6, 91.1; ^{19}F NMR (500 MHz, $CDCl_3$): δ -112.39; HRMS (FD) m/z: $[M]^+$ calcd for $C_{17}H_9N_2F$: 260.0755; found: 260.0757.

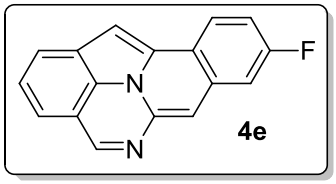
Spectral data for 9-chlorobenzo[7,8]indolizino[2,3,4,5-*ija*]quinazoline (4d):



Compound **4d** was purified on silica gel column using ethyl acetate/hexane: (8:92) as the eluent; Red solid (144 mg, 0.52 mmol, 62%); ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.91 (s, 1H), 8.17 (s, 1H), 7.91 (d, *J* = 7.8 Hz, 1H), 7.72 (d, *J* = 8.1 Hz, 1H), 7.52-7.39 (m, 3H), 7.11 (s, 1H), 7.03 (s, 1H); ^{13}C NMR (175 MHz, $CDCl_3$): δ 156.3, 138.5, 133.6, 132.2, 130.6, 130.4, 129.5, 128.1, 126.3,

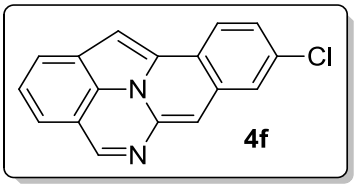
124.1, 123.7, 123.1, 122.7, 117.6, 114.4, 102.5, 91.3; HRMS (FD) m/z: $[M]^+$ calcd for $C_{17}H_9N_2Cl$: 276.0459; found: 276.0467.

Spectral data for 8-fluorobenzo[7,8]indolizino[2,3,4,5-*ija*]quinazoline (4e):



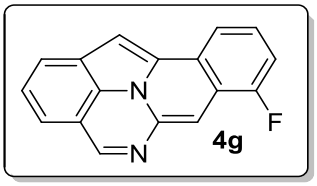
Compound **4e** was purified on silica gel column using ethyl acetate/hexane: (9:91) as the eluent; Red solid (123 mg, 0.47 mmol, 56%); ^{1}H NMR (700 MHz, *d*-THF): δ 9.18 (s, 1H), 8.52 (dd, *J* = 8.6 & 5.6 Hz, 1H), 8.06 (d, *J* = 7.8 Hz, 1H), 7.76 (d, *J* = 10.0 Hz, 1H), 7.67 (t, *J* = 7.3 Hz, 1H), 7.63 (d, *J* = 7.1 Hz, 1H), 7.51 (t, *J* = 8.5 Hz, 1H), 7.36 (s, 1H), 7.27 (s,1H); ^{13}C NMR (175 MHz, *d*-THF): δ 164.0, 162.6, 158.1, 140.8, 135.7 (t), 131.6, 127.9, 127.1 (d), 125.1, 123.2, 120.6 (d), 119.0, 115.9 (d), 115.2, 113.8 (d), 103.4 (d), 91.4 (d); ^{19}F NMR (500 MHz, *d*-THF): δ -113.61; HRMS (FD) m/z: $[M]^+$ calcd for $C_{17}H_9N_2F$: 260.0755; found: 260.0754.

Spectral data for 8-chlorobenzo[7,8]indolizino[2,3,4,5-*ija*]quinazoline (4f):



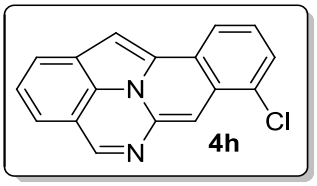
Compound **4f** was purified on silica gel column using ethyl acetate/hexane: (9:91) as the eluent; Red solid (128 mg, 0.46 mmol, 55%); ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.94 (s, 1H), 8.15 (d, *J* = 8.3 Hz, 1H), 7.91 (d, *J* = 7.7 Hz, 1H), 7.75 (s, 1H), 7.52-7.40 (m, 3H), 7.12 (s, 1H), 6.97 (s, 1H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 156.8, 139.2, 134.2, 133.5, 133.4, 130.5, 127.2, 126.9, 126.5, 125.0, 124.1, 122.6, 121.0, 117.6, 114.4, 102.1, 90.9; HRMS (FD) m/z: $[M]^+$ calcd for $C_{17}H_9N_2Cl$: 276.0459; found: 276.0468.

Spectral data for 7-fluorobenzo[7,8]indolizino[2,3,4,5-ija]quinazoline (4g):



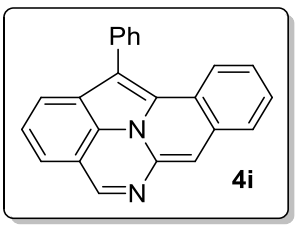
Compound **4g** was purified on silica gel column using ethyl acetate/hexane: (9:91) as the eluent; Red solid (134 mg, 0.51 mmol, 61%); ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.92 (s, 1H), 8.00 (d, *J* = 7.9 Hz, 1H), 7.90 (d, *J* = 7.9 Hz, 1H), 7.52-7.44 (m, 2H), 7.38 (d, *J* = 7.0 Hz, 1H), 7.28 (s, 1H), 7.24 (t, *J* = 5.6 Hz, 1H), 7.13 (s, 1H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 160.0, 158.0, 156.5, 138.6, 133.9, 130.5, 126.8 (d), 126.3, 124.2 (t), 122.6, 121.6 (d), 119.3 (d), 117.6, 114.4, 112.7 (d), 95.4, 91.3; ^{19}F NMR (500 MHz, $CDCl_3$): δ -118.44; HRMS (FD) m/z: $[M]^+$ calcd for $C_{17}H_9N_2F$: 260.0755; found: 260.0756.

Spectral data for 7-chlorobenzo[7,8]indolizino[2,3,4,5-*ija*]quinazoline (4h):



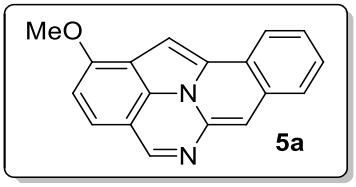
Compound **4h** was purified on silica gel column using ethyl acetate/hexane: (9:91) as the eluent; Red solid (133 mg, 0.48 mmol, 57%); ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.92 (s, 1H), 8.09 (d, *J* = 7.9 Hz, 1H), 7.88 (d, *J* = 8.0 Hz, 1H), 7.57 (d, *J* = 7.6 Hz, 1H), 7.49 (t, *J* = 7.4 Hz, 2H), 7.39 (q, *J* = 14.7 & 7.8 Hz, 2H), 7.10 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 156.8, 139.1, 134.1, 132.2, 130.2, 130.0, 128.1, 126.4, 124.2, 124.0, 122.7, 122.3, 117.6, 114.4, 99.4, 91.4, one carbon merged with other peaks; HRMS (FD) m/z: $[M]^+$ calcd for $C_{17}H_9N_2Cl$: 276.0459; found: 276.0462.

Spectral data for 11-phenylbenzo[7,8]indolizino[2,3,4,5-*ija*]quinazoline (4i):



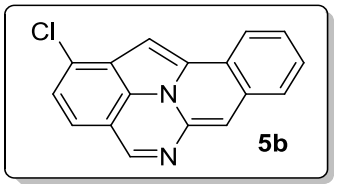
Compound **4i** was purified on silica gel column using ethyl acetate/hexane: (9:91) as the eluent; Red solid (56 mg, 0.17 mmol, 21%); ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.97 (s, 1H), 8.27 (d, *J* = 8.1 Hz, 1H), 7.83 (t, *J* = 7.8 Hz, 2H), 7.73 (d, *J* = 7.1 Hz, 2H), 7.58-7.49 (m, 4H), 7.48-7.42 (m, 2H), 7.34 (t, *J* = 7.4 Hz, 1H), 7.18 (s, 1H); ^{13}C NMR (175 MHz, $CDCl_3$): δ 156.0, 138.3, 135.2, 132.6, 130.3, 129.9, 129.7, 128.9, 128.4, 127.7, 127.1, 127.0, 126.3, 124.1, 123.8, 123.5, 121.2, 117.6, 114.6, 109.4, 103.9; HRMS (FD) m/z: $[M]^+$ calcd for $C_{23}H_{14}N_2$: 318.1162; found: 318.1168.

Spectral data for 1-methoxybenzo[7,8]indolizino[2,3,4,5-*ija*]quinazoline (5a):



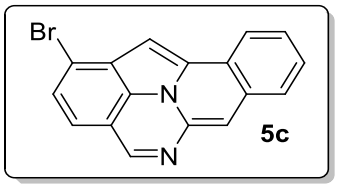
Compound **5a** was purified on silica gel column using ethyl acetate/hexane: (12:88) as the eluent; Red solid (124 mg, 0.45 mmol, 68%); ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.69 (s, 1H), 8.11 (t, *J* = 5.3 Hz, 1H), 7.70 (t, *J* = 3.4 Hz, 1H), 7.48 (q, *J* = 5.7 & 3.0 Hz, 2H), 7.31 (d, *J* = 7.9 Hz, 1H), 7.08 (s, 1H), 6.91 (s, 1H), 6.84 (d, *J* = 7.9 Hz, 1H), 4.10 (s, 3H); ^{13}C NMR (175 MHz, $CDCl_3$): δ 155.6, 138.4, 133.8, 132.3, 132.2, 128.1, 127.8, 126.5, 123.4, 122.9, 117.1, 116.4, 112.3, 104.8, 102.0, 88.8, 56.1 (one carbon merged with other peaks); HRMS (FD) m/z: $[M]^+$ calcd for $C_{18}H_{12}N_2O$: 272.0955; found: 272.0963.

Spectral data for 1-chlorobenzo[7,8]indolizino[2,3,4,5-*ija*]quinazoline (5b):



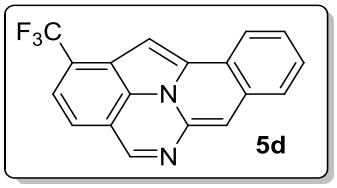
Compound **5b** was purified on silica gel column using ethyl acetate/hexane: (10:90) as the eluent; Red solid (119 mg, 0.43 mmol, 66%); ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.89 (s, 1H), 8.26 (t, *J* = 3.8 Hz, 1H), 7.83 (t, *J* = 5.1 Hz, 1H), 7.60-7.58 (m, 2H), 7.45 (d, *J* = 7.6 Hz, 1H), 7.28 (d, *J* = 7.6 Hz, 1H), 7.15 (d, *J* = 8.5 Hz, 2H); ^{13}C NMR (125 MHz, $CDCl_3$): δ; 155.2, 138.0, 135.1, 132.1, 130.8, 128.4, 128.2, 127.2, 127.0, 125.3, 123.8, 123.7, 122.5, 116.1, 114.5, 104.3, 89.3; HRMS (FD) m/z: $[M]^+$ calcd for $C_{17}H_9N_2Cl$: 276.0459; found: 276.0463.

Spectral data for 1-bromobenzo[7,8]indolizino[2,3,4,5-*ija*]quinazoline (5c):



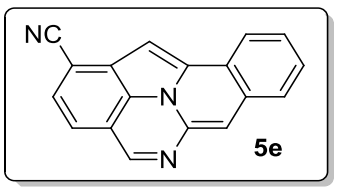
Compound **5c** was purified on silica gel column using ethyl acetate/hexane: (9:91) as the eluent; Red solid (101 mg, 0.31 mmol, 62%); ^{1}H NMR (500 MHz, *d*-THF): δ 9.14 (s, 1H), 8.59 (d, *J* = 8.4 Hz, 1H), 8.09 (d, *J* = 8.4 Hz, 1H), 7.84-7.78 (m, 3H), 7.49 (d, *J* = 7.6 Hz, 1H), 7.42 (d, *J* = 7.4 Hz, 2H); ^{13}C NMR (175 MHz, *d*-THF): δ 156.6, 139.7, 136.5, 133.7, 131.5, 129.5, 129.3, 128.6, 128.1, 127.8, 125.1, 123.8, 118.2, 116.0, 115.8, 105.6, 91.6; HRMS (FD) m/z: $[M]^+$ calcd for $C_{17}H_9N_2Br$: 319.9954; found: 319.9945.

Spectral data for 1-(trifluoromethyl)benzo[7,8]indolizino[2,3,4,5-*ija*]quinazoline (5d):



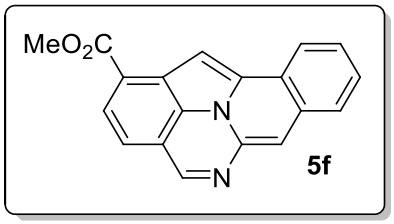
Compound **5d** was purified on silica gel column using ethyl acetate/hexane: (8:92) as the eluent; Red solid (125 mg, 0.40 mmol, 75%); ^{1}H NMR (500 MHz, $CDCl_3$): δ 9.00 (s, 1H), 8.36 (d, *J* = 8.6 Hz, 1H), 7.91 (d, *J* = 8.6 Hz, 1H), 7.76 (d, *J* = 7.5 Hz, 1H), 7.67-7.62 (m, 2H), 7.39 (d, *J* = 7.5 Hz, 1H), 7.33 (s, 2H); ^{13}C NMR (175 MHz, $CDCl_3$): δ 154.7, 137.5, 135.8, 132.0, 131.1, 128.6, 128.4, 127.4, 125.4, 124.0 (d), 122.8 (d), 122.5, 121.8, 121.5 (q), 119.6, 112.5, 105.7, 90.2; ^{19}F NMR (500 MHz, $CDCl_3$): δ -61.83; HRMS (FD) m/z: $[M]^+$ calcd for $C_{18}H_9N_2F_3$: 310.0723; found: 310.0729.

Spectral data for benzo[7,8]indolizino[2,3,4,5-*ija*]quinazoline-1-carbonitrile (5e):



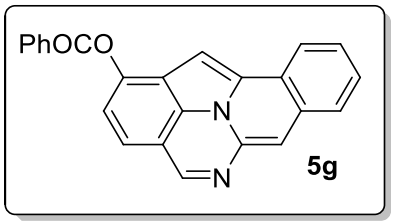
Compound **5e** was purified on silica gel column using ethyl acetate/hexane: (10:90) as the eluent; Red solid (104 mg, 0.38 mmol, 56%); ^{1}H NMR (500 MHz, $CDCl_3$): δ 9.00 (s, 1H), 8.35 (d, *J* = 7.1 Hz, 1H), 7.94 (d, *J* = 7.0 Hz, 1H), 7.77 (d, *J* = 7.4 Hz, 1H), 7.72-7.67 (m, 2H), 7.40 (s, 1H), 7.34 (d, *J* = 7.4 Hz, 1H), 7.29 (s, 1H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 154.1, 137.1, 136.2, 132.0, 130.3, 129.5, 128.8, 128.7, 127.9, 127.0, 124.1, 122.2, 119.9, 118.6, 112.4, 106.8, 101.6, 90.0; HRMS (FD) m/z: $[M]^+$ calcd for $C_{18}H_9N_3$: 267.0802; found: 267.0805.

Spectral data for methyl benzo[7,8]indolizino[2,3,4,5-*ija*]quinazoline-1-carboxylate (5f):



Compound **5f** was purified on silica gel column using ethyl acetate/hexane: (10:90) as the eluent; Red solid (107 mg, 0.35 mmol, 63%); ^{1}H NMR (700 MHz, $CDCl_3$): δ 8.89 (s, 1H), 8.27 (d, *J* = 8.8 Hz, 1H), 8.16 (d, *J* = 7.5 Hz, 1H), 7.83 (d, *J* = 8.8 Hz, 1H), 7.59-7.56 (m, 2H), 7.45 (s, 1H), 7.24 (d, *J* = 7.5 Hz, 2H), 4.01 (s, 3H); ^{13}C NMR (175 MHz, $CDCl_3$): δ 167.2, 154.7, 137.5, 135.8, 132.0, 131.4, 128.4, 128.2, 127.4, 127.3, 125.6, 124.0, 122.6, 120.9, 120.2, 112.4, 105.8, 92.7, 52.0; HRMS (FD) m/z: $[M]^+$ calcd for $C_{19}H_{12}N_2O_2$: 300.0904; found: 300.0901.

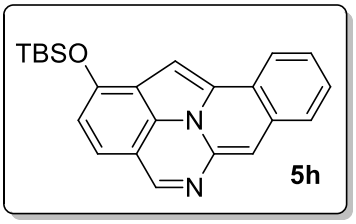
Spectral data for benzo[7,8]indolizino[2,3,4,5-*ija*]quinazolin-1-yl benzoate (5g):



Compound **5g** was purified on silica gel column using ethyl acetate/hexane: (11:91) as the eluent; Red solid (102 mg, 0.28 mmol, 67%); ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.90 (s, 1H), 8.26 (d, *J* = 7.6 Hz, 3H), 7.85 (s, 1H), 7.66 (q, *J* = 16.0 & 8.4 Hz, 2H), 7.59-7.51 (m, 4H), 7.35 (s, 1H), 7.17 (d, *J* = 13.2 Hz, 2H); ^{13}C NMR (175 MHz, $CDCl_3$): δ 165.9, 155.0, 147.8, 138.0, 135.6, 133.6, 132.0, 129.5, 128.7, 128.6, 128.4, 127.9, 126.9, 126.5, 123.8, 122.6, 117.4, 115.0, 108.0, 104.2,

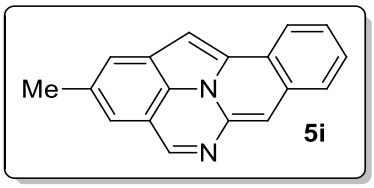
90.8, one carbon merged with other peaks; HRMS (FD) m/z: $[M]^+$ calcd for $C_{24}H_{14}N_2O_2$: 362.1060; found: 362.1061.

Spectral data for 1-((tert-butyldimethylsilyl)oxy)benzo[7,8]indolizino[2,3,4,5-*ija*]quinazoline (5h):



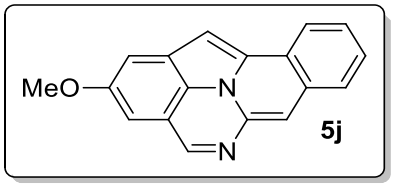
Compound **5h** was purified on silica gel column using ethyl acetate/hexane: (9:91) as the eluent; Red solid (67 mg, 0.17 mmol, 45%); ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.90 (s, 1H), 8.27 (d, *J* = 8.5 Hz, 1H), 7.84 (d, *J* = 8.3 Hz, 1H), 7.56 (t, *J* = 3.7 Hz, 2H), 7.37 (s, 1H), 7.15 (s, 1H), 7.08 (s, 1H), 6.96 (s, 1H), 1.03 (s, 9H), 0.24 (s, 6H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 155.4, 153.1, 138.3, 135.4, 132.1, 128.3, 127.6, 127.09, 127.00, 126.5, 123.6, 122.6, 117.6, 112.9, 107.4, 103.1, 89.9, 25.7, -4.3 ; HRMS (FD) m/z: $[M]^+$ calcd for $C_{23}H_{24}N_2OSi$: 372.1663; found: 372.1668.

Spectral data for 2-methylbenzo[7,8]indolizino[2,3,4,5-*ija*]quinazoline (5i):



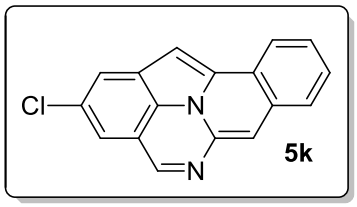
Compound **5i** was purified on silica gel column using ethyl acetate/hexane: (11:89) as the eluent; Red solid (137 mg, 0.53 mmol, 71%); ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.84 (s, 1H), 8.22 (d, *J* = 5.0 Hz, 1H), 7.79 (t, *J* = 4.6 Hz, 1H), 7.66 (s, 1H), 7.53 (t, *J* = 3.7 Hz, 2H), 7.16 (s, 1H), 7.04 (d, *J* = 14.0 Hz, 2H), 2.60 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): δ155.9, 138.5, 134.9, 133.7, 132.1, 129.2, 128.2, 127.6, 126.5, 126.4, 123.6, 122.8, 122.2, 117.2, 115.0, 102.8, 89.8, 22.5; HRMS (FD) m/z: $[M]^+$ calcd for $C_{18}H_{12}N_2$: 256.1006; found: 256.1006.

Spectral data for 2-methoxybenzo[7,8]indolizino[2,3,4,5-*ija*]quinazoline (5j):



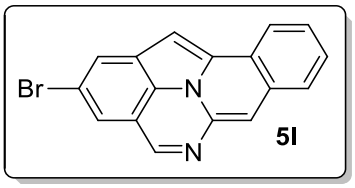
Compound **5j** was purified on silica gel column using ethyl acetate/hexane: (13:87) as the eluent; Red solid (128 mg, 0.47 mmol, 70%); ^{1}H NMR (700 MHz, $CDCl_3$): δ 8.88 (s, 1H), 8.25 (d, *J* = 5.5 Hz, 1H), 7.83 (d, *J* = 4.7 Hz, 1H), 7.55 (t, *J* = 3.5 Hz, 2H), 7.37 (s, 1H), 7.13 (s, 1H), 7.06 (s, 1H), 6.99 (s, 1H), 3.92 (s, 3H); ^{13}C NMR (175 MHz, $CDCl_3$): δ 157.8, 155.4, 138.1, 135.2, 132.0, 128.3, 127.6, 126.8, 126.6, 124.2, 123.6, 122.6, 117.6, 105.7, 103.4, 102.5, 90.0, 56.3; HRMS (FD) m/z: $[M]^+$ calcd for $C_{18}H_{12}N_2O$: 272.0955; found: 272.0959.

Spectral data for 2-chlorobenzo[7,8]indolizino[2,3,4,5-*ija*]quinazoline (5k):



Compound **5k** was purified on silica gel column using ethyl acetate/hexane: (9:91) as the eluent; Red solid (99 mg, 0.35 mmol, 55%); ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.83 (s, 1H), 8.23 (t, *J* = 3.3 Hz, 1H), 7.84 (t, *J* = 5.6 Hz, 1H), 7.78 (s, 1H), 7.58 (q, *J* = 5.8 & 3.2 Hz, 2H), 7.28 (s, 1H), 7.17 (s, 1H), 7.03 (s, 1H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 154.5, 137.8, 135.6, 132.0, 129.7, 129.0, 128.5, 128.1, 127.1, 127.0, 123.8, 122.6, 121.4, 117.8, 113.6, 104.6, 90.0 ; HRMS (FD) m/z: $[M]^+$ calcd for $C_{17}H_9N_2Cl$: 276.0459; found: 276.0464.

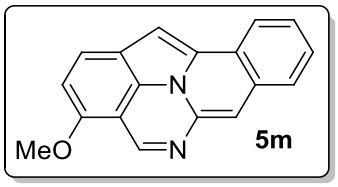
Spectral data for 2-bromobenzo[7,8]indolizino[2,3,4,5-*ija*]quinazoline (5l):



Compound **5l** was purified on silica gel column using ethyl acetate/hexane: (10:90) as the eluent; Red solid (79 mg, 0.24 mmol, 49%); ^{1}H NMR (500 MHz, *d*-THF): δ 9.14 (s, 1H), 8.57 (t, *J* = 3.7 Hz, 1H), 8.21 (s, 1H), 8.12 (t, *J* = 5.4, 1H), 7.80 (t, *J* = 4.6 Hz, 2H), 7.75 (s, 1H), 7.47 (s, 1H), 7.43

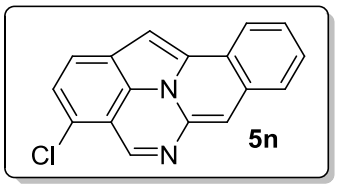
(s, 1H); ^{13}C NMR (125 MHz, *d*-THF): δ 155.1, 138.7, 136.2, 132.9, 129.7, 129.0, 128.6, 128.4, 127.5, 124.4, 124.3, 123.3, 119.3, 117.6, 116.6, 105.1, 90.4; HRMS (FD) m/z: $[M]^+$ calcd for $C_{17}H_9N_2Br$: 319.9954; found: 319.9952.

Spectral data for 3-methoxybenzo[7,8]indolizino[2,3,4,5-*ija*]quinazoline (5m):



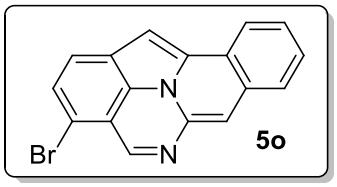
Compound **5m** was purified on silica gel column using ethyl acetate/hexane: (12:88) as the eluent; Red solid (97 mg, 0.35 mmol, 53%); ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.94 (s, 1H), 8.10 (d, *J* = 9.0 Hz, 1H), 7.75 (d, *J* = 8.6 Hz, 1H), 7.68 (d, *J* = 9.0 Hz, 1H), 7.47-7.44 (m, 2H), 7.03 (d, *J* = 8.6 Hz, 1H), 6.94 (s, 1H), 6.81 (s, 1H), 3.98 (s, 3H); ^{13}C NMR (175 MHz, $CDCl_3$): δ 152.6, 148.8, 139.2, 134.7, 132.3, 131.3, 127.9, 127.5, 126.2, 123.5, 123.29, 123.26, 120.9, 108.2, 106.5, 101.5, 90.0, 56.5; HRMS (FD) m/z: $[M]^+$ calcd for $C_{18}H_{12}N_2O$: 272.0955; found: 272.0953.

Spectral data for 3-chlorobenzo[7,8]indolizino[2,3,4,5-*ija*]quinazoline (5n):



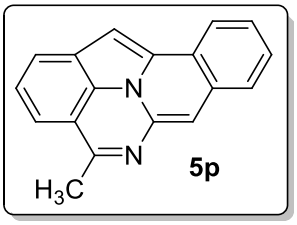
Compound **5n** was purified on silica gel column using ethyl acetate/hexane: (9:91) as the eluent; Red solid (130 mg, 0.46 mmol, 72%); ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.97 (s, 1H), 8.20 (d, *J* = 8.5 Hz, 1H), 7.78 (d, *J* = 8.5 Hz, 1H), 7.72 (d, *J* = 8.4 Hz, 1H), 7.58-7.54 (m, 2H), 7.38 (d, *J* = 8.4 Hz, 1H), 7.09 (s, 1H), 7.05 (s, 1H); ^{13}C NMR (125 MHz, $CDCl_3$): δ; 152.5, 137.9, 135.0, 131.8, 131.1, 128.4, 128.0, 127.0, 125.0, 124.6, 123.6, 122.9, 122.6, 119.1, 115.2, 104.4, 90.6; HRMS (FD) m/z: $[M]^+$ calcd for $C_{17}H_9N_2Cl$: 276.0459; found: 276.0460.

Spectral data for 3-bromobenzo[7,8]indolizino[2,3,4,5-*ija*]quinazoline (5o):



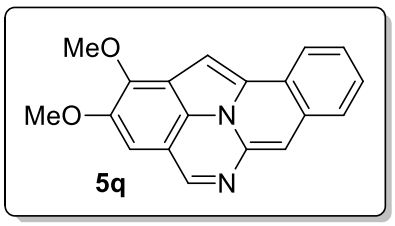
Compound **5o** was purified on silica gel column using ethyl acetate/hexane: (9:91) as the eluent; Red solid (115 mg, 0.35 mmol, 71%); ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.90 (s, 1H), 8.22 (d, *J* = 5.8 Hz, 1H), 7.79 (s, 1H), 7.67 (d, *J* = 8.3 Hz, 1H), 7.58 (d, *J* = 3.1 Hz, 2H), 7.53 (d, *J* = 8.4 Hz, 1H), 7.12 (s, 1H), 7.07 (s, 1H); ^{13}C NMR (125 MHz, $CDCl_3$): δ; 154.3, 138.0, 134.9, 131.9, 131.5, 128.4, 128.0, 127.3, 127.1, 125.5, 123.7, 122.9, 122.8, 117.0, 107.3, 104.5, 90.6; HRMS (FD) m/z: $[M]^+$ calcd for $C_{17}H_9N_2Br$: 319.9954; found: 319.9953.

Spectral data for 4-methylbenzo[7,8]indolizino[2,3,4,5-*ija*]quinazoline (5p):



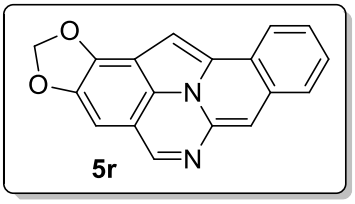
Compound **5p** was purified on silica gel column using ethyl acetate/hexane: (8:92) as the eluent; Red solid (131 mg, 0.51 mmol, 68%); ^{1}H NMR (700 MHz, $CDCl_3$): δ 8.24 (t, *J* = 4.7 Hz, 1H), 7.88 (d, *J* = 7.9 Hz, 1H), 7.82 (t, *J* = 3.8 Hz, 1H), 7.56-7.53 (m, 2H), 7.47 (t, *J* = 7.4 Hz, 1H), 7.38 (d, *J* = 7.1 Hz, 1H), 7.12 (s, 1H), 7.07 (s, 1H), 2.80 (s, 3H); ^{13}C NMR (175 MHz, $CDCl_3$): δ 164.1, 134.5, 132.1, 130.0, 128.1, 127.6, 126.5, 126.2, 123.6, 123.5, 122.3, 122.2, 117.4, 112.7, 101.8, 90.4, 21.7, one carbon merged with other peaks; HRMS (ESI-TOF) m/z: $[M+H]^+$ calcd for $C_{18}H_{13}N_2$: 257.1078; found: 257.1078.

Spectral data for benzo 1,2-dimethoxybenzo[7,8]indolizino[2,3,4,5-*ija*]quinazoline (5q):



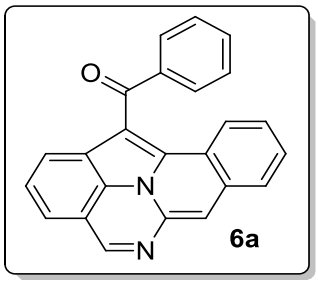
Compound **5q** was purified on silica gel column using ethyl acetate/hexane: (12:88) as the eluent; Red solid (118 mg, 0.39 mmol, 70%); ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.66 (s, 1H), 8.07 (d, *J* = 7.6 Hz, 1H), 7.69 (d, *J* = 7.6 Hz, 1H), 7.49-7.43 (m, 2H), 7.10 (s, 1H), 7.02 (s, 1H), 6.83 (s, 1H), 4.44 (s, 3H), 3.95 (s, 3H); ^{13}C NMR (175 MHz, $CDCl_3$): δ 155.1, 146.3, 145.1, 139.1, 134.8, 132.7, 129.6, 127.9, 127.8, 125.9, 123.3, 121.8, 116.5, 111.1, 102.3, 101.1, 89.1, 59.3, 57.8; HRMS (FD) m/z: $[M]^+$ calcd for $C_{19}H_{14}N_2O_2$: 302.1060; found: 302.1066.

Spectral data for benzo[7,8]indolizino[2,3,4,5-*ija*][1,3]dioxolo[4,5-*g*]quinazoline (5r):



Compound **5r** was purified on silica gel column using ethyl acetate/hexane: (10:90) as the eluent; Red solid (67 mg, 0.23 mmol, 38%); ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.66 (s, 1H), 8.09 (d, *J* = 7.5 Hz, 1H), 7.71 (d, *J* = 7.5 Hz, 1H), 7.51-7.45 (m, 2H), 6.91 (d, *J* = 15.9 Hz, 2H), 6.83 (s, 1H), 6.12 (s, 2H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 155.0, 143.8, 140.8, 138.6, 136.3, 132.6, 131.0, 128.1, 127.9, 126.1, 123.6, 121.7, 111.5, 111.3, 101.6, 101.1, 97.1, 86.1; HRMS (FD) m/z: $[M]^+$ calcd for $C_{18}H_{10}N_2O_2$: 286.0747; found: 286.0746.

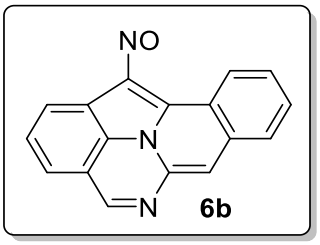
Spectral data for benzo[7,8]indolizino[2,3,4,5-*ija*]quinazolin-11-yl(phenyl)methanone (6a):



Compound **6a** was purified on silica gel column using ethyl acetate/hexane: (20:80) as the eluent; Red solid (72 mg, 0.20 mmol, 50%); ^{1}H NMR (500 MHz, $CDCl_3$): δ 9.38 (d, *J* = 8.4 Hz, 1H), 9.01 (s, 1H), 7.97 (d, *J* = 7.9 Hz, 1H), 7.91 (d, *J* = 7.6 Hz, 2H), 7.71 (t, *J* = 7.3 Hz, 1H), 7.61 (q, *J* = 15.0 & 7.8 Hz, 2H), 7.56 (s, 1H), 7.51-7.45 (m, 3H), 7.40 (t, *J* = 7.7 Hz, 1H), 7.18 (d, *J* = 7.9 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 192.1, 155.6, 141.1, 137.6, 137.3, 133.7, 132.1, 130.1, 129.7,

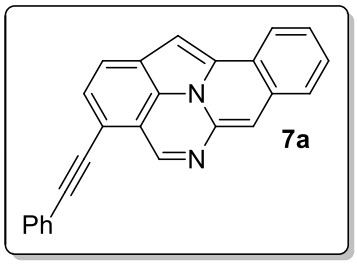
129.4, 128.6, 128.4, 127.7, 127.4, 127.3, 125.4, 123.7, 122.6, 117.4, 115.7, 108.8, 108.4; HRMS (FD) m/z: $[M]^+$ calcd for $C_{24}H_{14}N_2O$: 346.1111; found: 346.1115.

Spectral data for 11-nitrosobenzo[7,8]indolizino[2,3,4,5-*ija*]quinazoline (6b):



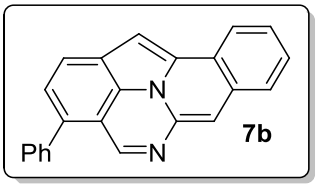
Compound **6b** was purified on silica gel column using ethyl acetate/hexane: (40:60) as the eluent; Brownish solid (94 mg, 0.34 mmol, 84%); ^{1}H NMR (500 MHz, $CDCl_3$): δ 9.83 (d, *J* = 8.1 Hz, 1H), 9.17 (s, 1H), 8.61 (d, *J* = 7.6 Hz, 1H), 8.15 (d, *J* = 8.0 Hz, 1H), 7.96-7.83 (m, 4H), 7.75 (d, *J* = 7.5 Hz, 1H); ^{13}C NMR (175 MHz, $CDCl_3$): δ 155.6, 153.0, 140.6, 136.6, 135.8, 131.8, 131.0, 130.9, 130.1, 129.1, 128.7, 125.1, 122.4, 120.2, 116.2, 113.5, 111.9; HRMS (FD) m/z: $[M]^+$ calcd for $C_{17}H_9N_3O$: 271.0751; found: 271.0750.

Spectral data for 3-(phenylethynyl)benzo[7,8]indolizino[2,3,4,5-*ija*]quinazoline (7a):



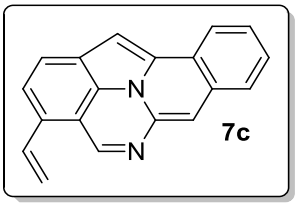
Compound **7a** was purified on silica gel column using ethyl a cetate/hexane: (8:92) as the eluent; Red solid (81 mg, 0.23 mmol, 76%); ^{1}H NMR (500 MHz, $CDCl_3$): δ 9.20 (s, 1H), 8.27 (d, *J* = 8.9 Hz, 1H), 7.86-7.81 (m, 2H), 7.61-7.58 (m, 5H), 7.40-7.34 (m, 4H), 7.16 (s, 1H); ^{13}C NMR (175 MHz, $CDCl_3$): δ 154.5, 138.2, 135.6, 132.2, 131.5 130.5, 128.49, 128.41, 128.1, 127.5, 127.1, 126.0, 123.7, 123.2, 122.8, 121.8, 118.3, 108.0, 104.6, 94.0, 91.3, 86.3, one carbon merged with other peaks; HRMS (FD) m/z: $[M]^+$ calcd for $C_{25}H_{14}N_2$: 342.1162; found: 342.1160.

Spectral data for 3-phenylbenzo[7,8]indolizino[2,3,4,5-*ija*]quinazoline (7b):



Compound **7b** was purified on silica gel column using ethyl acetate/hexane: (8:92) as the eluent; Orange solid (68 mg, 0.21 mmol, 69%); ^{1}H NMR (700 MHz, $CDCl_3$): δ 9.07 (s, 1H), 8.27 (d, *J* = 8.4 Hz, 1H), 7.93 (d, *J* = 8.1 Hz, 1H), 7.83 (d, *J* = 7.9 Hz, 1H), 7.61 (d, *J* = 7.2 Hz, 2H), 7.58-7.52 (m, 5H), 7.43 (t, *J* = 7.3 Hz, 1H), 7.18 (s, 1H), 7.12 (s, 1H); ^{13}C NMR (175 MHz, $CDCl_3$): δ 155.2, 138.4, 138.2, 135.2, 132.1, 131.0, 129.5, 129.2, 128.9, 128.3, 127.9, 127.5, 126.7, 125.7, 125.5, 123.6, 122.9, 122.4, 114.7, 103.1, 90.6; HRMS (FD) m/z: $[M]^+$ calcd for $C_{23}H_{14}N_2$: 318.1162; found: 318.1163.

Spectral data for 3-vinylbenzo[7,8]indolizino[2,3,4,5-*ija*]quinazoline (7c):



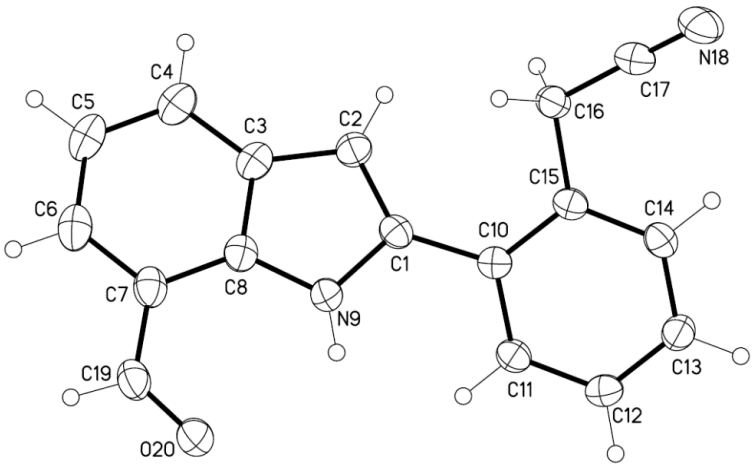
Compound **7c** was purified on silica gel column using ethyl acetate/hexane: (10:90) as the eluent; Red solid (62 mg, 0.23 mmol, 74%); ^{1}H NMR (500 MHz, $CDCl_3$): δ 9.13 (s, 1H), 8.19 (s, 1H), 7.78 (d, *J* = 6.9 Hz, 2H), 7.64 (d, *J* = 7.9 Hz, 1H), 7.52 (s, 2H), 7.30 (q, *J* = 16.8 & 11.2 Hz, 1H), 7.07 (s, 2H), 5.88 (d, *J* = 17.4 Hz, 1H), 5.43 (d, *J* = 10.6 Hz, 1H) ; ^{13}C NMR (175 MHz, $CDCl_3$): δ 153.5, 138.3, 134.9, 132.0, 130.7, 130.5, 128.2, 127.7, 126.7, 125.7, 123.9, 123.5, 122.9, 122.2, 120.9, 115.5, 114.7, 103.6, 90.9 ; HRMS (FD) m/z: $[M]^+$ calcd for $C_{19}H_{12}N_2$: 268.1006; found: 268.1009.

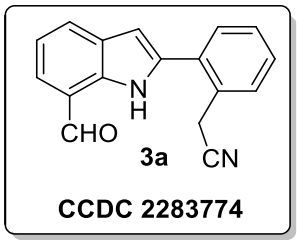
9. X-ray crystallographic structure and data for compound 3a, 3i, 3i', 4a, 6a, 6b, 7a, 7c:

(a) X-ray crystallographic data of compound (3a)

Ellipsoid contour % probability level = 50%

Sample Preparation for Crystal Growth: The compound **3a** was dissolved in Ethyl acetate/Pentane (1:5) and kept for slow evaporation (4 days). A needle-shaped crystal was formed whose X-ray analysis was performed.





230521lt_auto

Table S1 Crystal data and structure refinement for 230521lt_auto.

Identification code	230521lt_auto
Empirical formula	$C_{17}H_{12}N_2O$
Formula weight	260.29
Temperature/K	100.00(10)
Crystal system	monoclinic
Space group	C2/c
a/Å	16.3278(3)
b/Å	7.4345(2)

c/Å	21.1425(4)
α/°	90
β/°	99.071(2)
γ/°	90
Volume/Å^3	2534.37(10)
Z	8
ρ_{calc}g/cm^3	1.364
μ/mm^{-1}	0.690
F(000)	1088.0
Crystal size/mm^3	0.18 × 0.15 × 0.03
Radiation	Cu Kα (λ = 1.54184)
2Θ range for data collection/°	8.47 to 134.15
Index ranges	-19 ≤ h ≤ 19, -8 ≤ k ≤ 6, -25 ≤ l ≤ 25
Reflections collected	8719
Independent reflections	2263 [R_{int} = 0.0239, R_{sigma} = 0.0263]
Data/restraints/parameters	2263/0/182
Goodness-of-fit on F^2	1.039
Final R indexes [I>=2σ (I)]	R_1 = 0.0390, wR_2 = 0.1036
Final R indexes [all data]	R_1 = 0.0448, wR_2 = 0.1077
Largest diff. peak/hole / e Å^{-3}	0.24/-0.20

Table S2 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for 230521lt_auto. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
C1	2880.4(8)	1993.3(18)	2679.6(7)	22.8(3)
C2	2550.2(9)	1529.5(19)	3212.8(7)	25.9(3)

Table S2 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for 230521lt_auto. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
C3	3163.2(9)	1889(2)	3761.5(7)	27.1(3)
C4	3193.8(10)	1657(2)	4420.5(7)	33.1(4)
C5	3903.6(11)	2139(2)	4837.3(7)	36.2(4)
C6	4582.5(10)	2865(2)	4600.1(7)	33.8(4)
C7	4580.1(9)	3121(2)	3948.4(7)	28.7(3)
C8	3861.7(9)	2601.8(19)	3527.2(7)	25.2(3)
C10	2562.4(8)	1824.1(18)	1990.2(7)	21.7(3)
C11	3118.9(8)	1336.4(19)	1579.2(7)	23.8(3)
C12	2871.1(9)	1189.9(19)	925.4(7)	26.1(3)
C13	2054.5(9)	1549(2)	664.2(7)	27.4(3)
C14	1495.4(9)	2021.2(19)	1065.6(7)	25.8(3)
C15	1731.2(8)	2153.8(18)	1723.3(7)	22.6(3)
C16	1103.0(8)	2660(2)	2151.7(7)	25.2(3)
C17	337.1(9)	3392(2)	1790.0(7)	29.2(4)
C19	5296.1(9)	3906(2)	3725.7(7)	31.7(4)
N9	3683.5(7)	2644.3(16)	2875.8(5)	24.0(3)
N18	−266.4(8)	3911(2)	1495.6(7)	40.3(4)
O20	5355.5(6)	4181.8(15)	3164.5(5)	33.9(3)

Table S3 Anisotropic Displacement Parameters (Å^2×10^3) for 230521lt_auto. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C1	20.9(6)	20.3(7)	26.9(7)	−0.9(6)	2.6(5)	2.4(5)
C2	27.3(7)	24.8(7)	26.1(8)	−0.8(6)	5.5(6)	0.5(6)

Table S3 Anisotropic Displacement Parameters ($Å^2×10^3$) for 230521lt_auto. The Anisotropic displacement factor exponent takes the form: $-2π^2[h^2a^{*2}U_{11}+2hka*b*U_{12}+…]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C3	33.9(8)	22.6(7)	25.0(8)	-0.6(6)	5.1(6)	2.8(6)
C4	43.3(9)	29.7(8)	26.8(8)	1.2(6)	6.7(6)	-1.0(7)
C5	51.2(10)	34.3(9)	22.1(8)	1.1(7)	2.4(7)	2.4(7)
C6	39.0(8)	31.0(8)	28.3(8)	-2.7(7)	-4.0(6)	6.2(7)
C7	30.2(8)	26.9(8)	27.2(8)	-2.2(6)	-1.5(6)	6.7(6)
C8	27.3(7)	22.4(7)	25.0(7)	-0.8(6)	1.8(6)	5.8(6)
C10	22.9(7)	18.3(7)	24.6(7)	-0.7(5)	5.2(5)	-0.7(5)
C11	21.6(7)	22.0(7)	27.7(7)	0.3(6)	3.8(5)	1.2(5)
C12	26.6(7)	25.9(7)	27.5(8)	-1.8(6)	9.0(6)	-0.1(6)
C13	29.4(7)	30.1(8)	22.6(7)	-0.8(6)	3.8(6)	-2.9(6)
C14	21.7(7)	26.5(8)	28.4(8)	0.0(6)	1.6(5)	-2.7(6)
C15	21.7(7)	19.6(7)	26.9(7)	0.1(6)	5.2(5)	-1.1(5)
C16	21.6(7)	27.4(8)	27.0(8)	-1.6(6)	4.6(5)	-0.6(6)
C17	24.6(8)	30.0(8)	34.8(8)	-1.3(6)	10.0(6)	0.6(6)
C19	25.8(7)	36.0(9)	30.9(8)	-6.3(7)	-2.7(6)	6.9(6)
N9	21.9(6)	27.0(6)	22.8(6)	-0.4(5)	2.3(4)	1.3(5)
N18	27.9(7)	49.3(9)	44.8(8)	4.0(7)	9.5(6)	10.6(6)
O20	27.3(6)	42.1(7)	31.7(6)	-3.0(5)	2.6(4)	3.7(5)

Table S4 Bond Lengths for 230521lt_auto.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
C1	C2	1.3683(19)	C8	N9	1.3624(18)
C1	C10	1.4735(19)	C10	C11	1.4004(18)

Table S4 Bond Lengths for 230521lt_auto.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
C1	N9	1.3979(17)	C10	C15	1.4068(19)
C2	C3	1.433(2)	C11	C12	1.382(2)
C3	C4	1.397(2)	C12	C13	1.386(2)
C3	C8	1.416(2)	C13	C14	1.386(2)
C4	C5	1.388(2)	C14	C15	1.387(2)
C5	C6	1.395(2)	C15	C16	1.5189(18)
C6	C7	1.390(2)	C16	C17	1.464(2)
C7	C8	1.410(2)	C17	N18	1.1462(19)
C7	C19	1.450(2)	C19	O20	1.2230(18)

Table S5 Bond Angles for 230521lt_auto.

Atom	Atom	Atom	Angle/˚	Atom	Atom	Atom	Angle/˚
C2	C1	C10	132.09(13)	N9	C8	C7	130.98(13)
C2	C1	N9	108.41(12)	C11	C10	C1	118.29(12)
N9	C1	C10	119.40(12)	C11	C10	C15	118.40(13)
C1	C2	C3	107.72(13)	C15	C10	C1	123.30(12)
C4	C3	C2	134.04(14)	C12	C11	C10	121.65(13)
C4	C3	C8	119.39(14)	C11	C12	C13	119.65(13)
C8	C3	C2	106.56(12)	C14	C13	C12	119.33(13)
C5	C4	C3	119.77(15)	C13	C14	C15	121.77(13)
C4	C5	C6	120.19(15)	C10	C15	C16	120.23(12)
C7	C6	C5	122.08(15)	C14	C15	C10	119.19(12)
C6	C7	C8	117.40(14)	C14	C15	C16	120.59(12)
C6	C7	C19	120.04(14)	C17	C16	C15	112.46(12)

Table S5 Bond Angles for 230521lt_auto.

Atom	Atom	Atom	Angle/˚	Atom	Atom	Atom	Angle/˚
C8	C7	C19	122.56(13)	N18	C17	C16	177.67(17)
C7	C8	C3	121.15(13)	O20	C19	C7	125.02(14)
N9	C8	C3	107.87(12)	C8	N9	C1	109.44(11)

Table S6 Torsion Angles for 230521lt_auto.

A	B	C	D	Angle/˚	A	B	C	D	Angle/˚
C1	C2	C3	C4	−178.29(16)	C7	C8	N9	C1	−179.52(14)
C1	C2	C3	C8	0.67(16)	C8	C3	C4	C5	0.5(2)
C1	C10	C11	C12	−178.54(12)	C8	C7	C19	O20	-0.6(2)
C1	C10	C15	C14	177.75(12)	C10	C1	C2	C3	175.85(14)
C1	C10	C15	C16	-1.9(2)	C10	C1	N9	C8	−176.93(12)
C2	C1	C10	C11	−140.85(16)	C10	C11	C12	C13	0.6(2)
C2	C1	C10	C15	40.1(2)	C10	C15	C16	C17	165.35(13)
C2	C1	N9	C8	-0.22(15)	C11	C10	C15	C14	-1.3(2)
C2	C3	C4	C5	179.32(16)	C11	C10	C15	C16	179.10(12)
C2	C3	C8	C7	179.34(13)	C11	C12	C13	C14	-1.0(2)
C2	C3	C8	N9	-0.81(16)	C12	C13	C14	C15	0.3(2)
C3	C4	C5	C6	0.5(2)	C13	C14	C15	C10	0.9(2)
C3	C8	N9	C1	0.65(15)	C13	C14	C15	C16	−179.49(13)
C4	C3	C8	C7	-1.5(2)	C14	C15	C16	C17	-14.27(19)
C4	C3	C8	N9	178.34(13)	C15	C10	C11	C12	0.5(2)

Table S6 Torsion Angles for 230521lt_auto.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
C4	C5	C6	C7	-0.4(2)	C19	C7	C8	C3	-178.09(13)
C5	C6	C7	C8	-0.6(2)	C19	C7	C8	N9	2.1(2)
C5	C6	C7	C19	179.06(14)	N9	C1	C2	C3	-0.29(16)
C6	C7	C8	C3	1.6(2)	N9	C1	C10	C11	34.94(18)
C6	C7	C8	N9	-178.26(14)	N9	C1	C10	C15	-144.08(13)
C6	C7	C19	O20	179.80(14)					

Table S7 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for 230521lt_auto.

Atom	*x*	*y*	*z*	U(eq)
H2	2011.22	1054.39	3218.27	31
H4	2730.33	1171.98	4582.83	40
H5	3927.36	1974.16	5285.38	43
H6	5061.47	3193.62	4893.05	41
H11	3680.88	1100.23	1754.23	29
H12	3258.43	845.26	656.33	31
H13	1879.83	1471.18	214.67	33
H14	935.63	2260.69	885.3	31
H16A	968.52	1580.42	2389.81	30
H16B	1352.34	3563.37	2468.64	30
H19	5754.29	4230.65	4039.89	38
H9	4021.46	3022.86	2618.49	29

Experimental

Single crystals of $C_{17}H_{12}N_2O$ **[230521lt_auto]** were **[]**. A suitable crystal was selected and **[]** on a **XtaLAB Synergy R, DW system, HyPix-Arc 150** diffractometer. The crystal was kept at 100.00(10) K during data collection. Using Olex2 [1], the structure was solved with the SHELXT [2] structure solution program using Intrinsic Phasing and refined with the SHELXL [3] refinement package using Least Squares minimisation.

1. Dolomanov, O.V., Bourhis, L.J., Gildea, R.J, Howard, J.A.K. & Puschmann, H. (2009), J. Appl. Cryst. 42, 339-341.
2. Sheldrick, G.M. (2015). Acta Cryst. A71, 3-8.
3. Sheldrick, G.M. (2015). Acta Cryst. C71, 3-8.

Crystal structure determination of [230521lt_auto]

Crystal Data for $C_{17}H_{12}N_2O$ (M =260.29 g/mol): monoclinic, space group C2/c (no. 15), a = 16.3278(3) Å, b = 7.4345(2) Å, c = 21.1425(4) Å, β = 99.071(2)°, V = 2534.37(10) Å^3, Z = 8, T = 100.00(10) K, μ(Cu Kα) = 0.690 mm^{-1}, *Dcalc* = 1.364 g/cm^3, 8719 reflections measured (8.47° ≤ 2Θ ≤ 134.15°), 2263 unique (R_{int} = 0.0239, R_{sigma} = 0.0263) which were used in all calculations. The final R_1 was 0.0390 (I > 2σ(I)) and wR_2 was 0.1077 (all data).

Refinement model description

Number of restraints - 0, number of constraints - unknown.

Details:

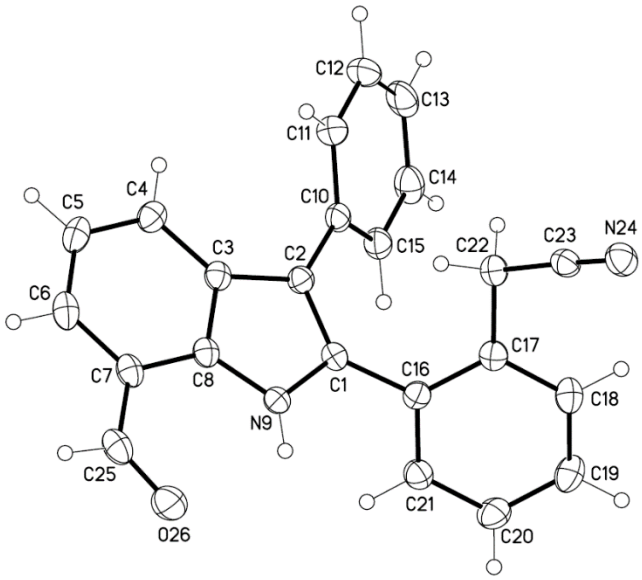
```
1. Fixed Uiso
 At 1.2 times of:
  All C(H) groups, All C(H,H) groups, All N(H) groups
2.a Secondary CH2 refined with riding coordinates:
 C16(H16A,H16B)
2.b Aromatic/amide H refined with riding coordinates:
 C2(H2), C4(H4), C5(H5), C6(H6), C11(H11), C12(H12), C13(H13), C14(H14),
 C19(H19), N9(H9)
```

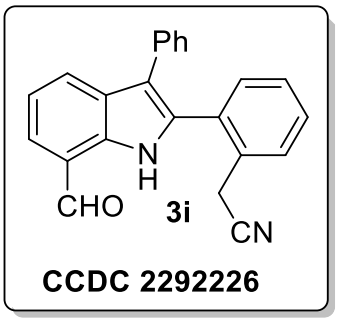
This report has been created with Olex2, compiled on 2023.03.06 svn.rbb2c1857 for OlexSys. Please let us know if there are any errors or if you would like to have additional features.

(b) X-ray crystallographic data of compound (3i)

Ellipsoid contour % probability level = 50%

Sample Preparation for Crystal Growth: The compound **3i** was dissolved in Ethyl acetate/Hexane (1:5) and kept for slow evaporation (7 days). A needle-shaped crystal was formed whose X-ray analysis was performed.





230884lt_auto

Table S8 Crystal data and structure refinement for 230884lt_auto.

Identification code	230884lt_auto
Empirical formula	$C_{23}H_{16}N_2O$
Formula weight	336.38
Temperature/K	109(6)
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	12.43235(13)
b/Å	12.20419(15)
c/Å	11.52302(14)
α/°	90
β/°	102.4803(11)
γ/°	90
Volume/Å^3	1707.04(4)

Z	4
ρ_{calc}g/cm^3	1.309
μ/mm^{-1}	0.639
F(000)	704.0
Crystal size/mm^3	0.24 × 0.07 × 0.06
Radiation	Cu Kα (λ = 1.54184)
2Θ range for data collection/°	7.282 to 149.472
Index ranges	-15 ≤ h ≤ 10, -15 ≤ k ≤ 14, -13 ≤ l ≤ 13
Reflections collected	11901
Independent reflections	3318 [R_{int} = 0.0265, R_{sigma} = 0.0224]
Data/restraints/parameters	3318/0/236
Goodness-of-fit on F^2	1.050
Final R indexes [I>=2σ (I)]	R_1 = 0.0337, wR_2 = 0.0869
Final R indexes [all data]	R_1 = 0.0368, wR_2 = 0.0890
Largest diff. peak/hole / e Å^{-3}	0.24/-0.25

Table S9 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for 230884lt_auto. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
C1	2677.2(9)	258.7(9)	3058.5(9)	19.0(2)
C2	1805.4(8)	735.3(9)	3429.8(9)	19.3(2)
C3	1878.0(9)	371.6(9)	4637.1(9)	19.8(2)
C4	1223.0(9)	532.9(9)	5474.3(10)	23.2(2)
C5	1495.2(10)	4.6(10)	6561.0(10)	26.7(3)
C6	2415.7(10)	-677.5(10)	6832.8(10)	26.2(3)

Table S9 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for 230884lt_auto. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
C7	3097.1(9)	-851.0(9)	6038.7(10)	22.3(2)
C8	2806.6(9)	-323.0(9)	4926.9(9)	19.4(2)
C10	911.8(9)	1394.3(9)	2708.7(10)	20.9(2)
C11	499.9(10)	2319.8(10)	3181.3(11)	26.9(3)
C12	-377.9(10)	2905.7(11)	2510.0(12)	33.6(3)
C13	-855.6(10)	2585.9(11)	1364.3(12)	33.8(3)
C14	-448.4(10)	1679.4(11)	880.5(11)	29.8(3)
C15	428.1(9)	1090.9(10)	1540.6(10)	23.9(2)
C16	3007.4(8)	321.9(9)	1902.7(9)	19.8(2)
C17	3243.5(9)	1324.1(9)	1417.3(9)	21.1(2)
C18	3561.4(10)	1330.4(10)	327.7(10)	26.5(3)
C19	3647.7(10)	364.0(11)	-275.4(10)	30.2(3)
C20	3420.9(10)	-629.3(10)	205.5(10)	28.6(3)
C21	3106.5(9)	-647.9(10)	1285.9(10)	23.9(2)
C22	3172.8(9)	2390.0(9)	2077.5(10)	23.5(2)
C23	4006.9(9)	3179.2(9)	1892.8(10)	22.6(2)
C25	4082.1(10)	-1519.5(10)	6386.4(10)	27.8(3)
N9	3277.4(7)	-381.2(7)	3962.8(8)	19.4(2)
N24	4675.9(8)	3771.4(8)	1741.4(9)	28.5(2)
O26	4728.6(7)	-1724.8(8)	5758.3(8)	34.2(2)

Table S10 Anisotropic Displacement Parameters ($Å^2×10^3$) for 230884lt_auto. The Anisotropic displacement factor exponent takes the form: $-2π^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+…]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C1	19.9(5)	17.4(5)	19.0(5)	1.4(4)	2.9(4)	-1.0(4)
C2	19.4(5)	18.4(5)	20.4(5)	-0.1(4)	5.0(4)	-1.6(4)
C3	20.5(5)	18.4(5)	20.4(5)	-1.0(4)	4.3(4)	-4.2(4)
C4	22.0(5)	24.2(6)	24.3(6)	-3.2(4)	6.9(4)	-4.8(5)
C5	28.4(6)	31.1(6)	22.7(6)	-2.7(5)	10.6(4)	-9.1(5)
C6	31.9(6)	27.1(6)	18.7(5)	2.1(4)	3.2(4)	-9.5(5)
C7	25.4(5)	19.6(5)	20.1(5)	0.9(4)	1.1(4)	-6.2(4)
C8	20.7(5)	17.7(5)	19.3(5)	-0.8(4)	3.0(4)	-4.8(4)
C10	18.2(5)	21.2(5)	24.7(6)	4.3(4)	7.5(4)	-0.3(4)
C11	27.3(6)	24.9(6)	30.3(6)	1.2(5)	9.7(5)	2.5(5)
C12	32.0(6)	26.1(6)	46.1(8)	7.3(5)	15.8(6)	9.6(5)
C13	24.4(6)	34.6(7)	42.1(7)	16.7(6)	6.7(5)	7.8(5)
C14	24.1(6)	35.8(7)	28.0(6)	9.4(5)	2.6(5)	-0.4(5)
C15	22.1(5)	24.7(6)	25.2(6)	4.1(4)	6.1(4)	0.0(5)
C16	16.7(5)	23.3(6)	19.0(5)	1.4(4)	2.7(4)	1.6(4)
C17	18.3(5)	24.0(6)	19.7(5)	1.4(4)	1.6(4)	0.1(4)
C18	29.8(6)	28.9(6)	20.6(6)	3.0(4)	5.2(4)	-4.1(5)
C19	34.7(7)	37.5(7)	19.9(6)	-1.6(5)	9.3(5)	-3.2(5)
C20	33.8(6)	28.7(6)	23.7(6)	-5.2(5)	7.1(5)	1.3(5)
C21	26.2(6)	22.6(6)	22.7(6)	1.5(4)	4.8(4)	1.2(5)
C22	24.2(5)	22.1(6)	25.1(6)	1.8(4)	7.6(4)	-2.1(4)
C23	23.5(5)	20.4(5)	23.3(5)	1.7(4)	3.6(4)	3.1(5)
C25	34.0(6)	23.8(6)	22.6(6)	4.4(5)	-0.3(5)	-1.8(5)
N9	19.9(4)	19.0(5)	19.0(4)	2.2(3)	3.5(3)	2.0(4)

Table S10 Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for 230884lt_auto. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
N24	27.5(5)	25.2(5)	32.9(6)	1.5(4)	6.7(4)	−2.0(4)
O26	35.4(5)	34.5(5)	31.4(5)	5.6(4)	4.6(4)	8.6(4)

Table S11 Bond Lengths for 230884lt_auto.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
C1	C2	1.3772(15)	C11	C12	1.3914(17)
C1	C16	1.4780(14)	C12	C13	1.3816(19)
C1	N9	1.3844(13)	C13	C14	1.3832(19)
C2	C3	1.4444(15)	C14	C15	1.3869(16)
C2	C10	1.4739(15)	C16	C17	1.4021(15)
C3	C4	1.4043(15)	C16	C21	1.3997(16)
C3	C8	1.4128(15)	C17	C18	1.3954(15)
C4	C5	1.3838(16)	C17	C22	1.5190(15)
C5	C6	1.3949(18)	C18	C19	1.3847(17)
C6	C7	1.3910(16)	C19	C20	1.3870(18)
C7	C8	1.4095(15)	C20	C21	1.3833(16)
C7	C25	1.4539(16)	C22	C23	1.4641(15)
C8	N9	1.3649(13)	C23	N24	1.1434(15)
C10	C11	1.3983(16)	C25	O26	1.2182(15)
C10	C15	1.4003(16)			

Table S12 Bond Angles for 230884lt_auto.

Atom	Atom	Atom	Angle/˚	Atom	Atom	Atom	Angle/˚
C2	C1	C16	130.42(10)	C15	C10	C2	120.82(10)
C2	C1	N9	109.68(9)	C12	C11	C10	120.52(12)
N9	C1	C16	119.88(9)	C13	C12	C11	120.64(12)
C1	C2	C3	106.25(9)	C12	C13	C14	119.46(11)
C1	C2	C10	127.10(10)	C13	C14	C15	120.39(12)
C3	C2	C10	126.39(9)	C14	C15	C10	120.90(11)
C4	C3	C2	133.93(10)	C17	C16	C1	121.86(10)
C4	C3	C8	119.16(10)	C21	C16	C1	119.04(10)
C8	C3	C2	106.85(9)	C21	C16	C17	119.09(10)
C5	C4	C3	119.45(11)	C16	C17	C22	120.49(10)
C4	C5	C6	120.63(10)	C18	C17	C16	119.22(10)
C7	C6	C5	122.00(10)	C18	C17	C22	120.28(10)
C6	C7	C8	117.09(10)	C19	C18	C17	120.97(11)
C6	C7	C25	120.04(10)	C18	C19	C20	119.96(11)
C8	C7	C25	122.84(10)	C21	C20	C19	119.69(11)
C7	C8	C3	121.66(10)	C20	C21	C16	121.07(11)
N9	C8	C3	108.12(9)	C23	C22	C17	111.78(9)
N9	C8	C7	130.18(10)	N24	C23	C22	178.07(12)
C11	C10	C2	121.07(10)	O26	C25	C7	125.18(11)
C11	C10	C15	118.08(10)	C8	N9	C1	109.09(9)

Table S13 Torsion Angles for 230884lt_auto.

A	B	C	D	Angle/˚	A	B	C	D	Angle/˚
C1	C2	C3	C4	−177.23(12)	C8	C7	C25	O26	−2.68(18)
C1	C2	C3	C8	−0.31(12)	C10	C2	C3	C4	−2.72(19)
C1	C2	C10	C11	−140.87(12)	C10	C2	C3	C8	174.19(10)
C1	C2	C10	C15	41.10(16)	C10	C11	C12	C13	−0.21(18)
C1	C16	C17	C18	179.39(10)	C11	C10	C15	C14	−1.25(16)
C1	C16	C17	C22	0.37(16)	C11	C12	C13	C14	−0.54(19)
C1	C16	C21	C20	−179.53(10)	C12	C13	C14	C15	0.38(18)
C2	C1	C16	C17	58.27(16)	C13	C14	C15	C10	0.53(18)
C2	C1	C16	C21	−122.91(13)	C15	C10	C11	C12	1.09(16)
C2	C1	N9	C8	−0.26(12)	C16	C1	C2	C3	178.92(11)
C2	C3	C4	C5	176.23(11)	C16	C1	C2	C10	4.47(19)
C2	C3	C8	C7	−177.98(10)	C16	C1	N9	C8	−179.01(9)
C2	C3	C8	N9	0.16(12)	C16	C17	C18	C19	−0.11(17)
C2	C10	C11	C12	−177.00(10)	C16	C17	C22	C23	145.50(10)
C2	C10	C15	C14	176.84(10)	C17	C16	C21	C20	−0.68(17)
C3	C2	C10	C11	45.75(16)	C17	C18	C19	C20	−0.26(19)
C3	C2	C10	C15	−132.28(12)	C18	C17	C22	C23	−33.50(14)
C3	C4	C5	C6	0.47(17)	C18	C19	C20	C21	0.16(19)
C3	C8	N9	C1	0.05(12)	C19	C20	C21	C16	0.31(18)
C4	C3	C8	C7	−0.52(16)	C21	C16	C17	C18	0.57(16)

Table S13 Torsion Angles for 230884lt_auto.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
C4	C3	C8	N9	177.62(9)	C21	C16	C17	C22	−178.44(10)
C4	C5	C6	C7	0.39(18)	C22	C17	C18	C19	178.91(11)
C5	C6	C7	C8	−1.25(16)	C25	C7	C8	C3	−176.39(10)
C5	C6	C7	C25	176.53(11)	C25	C7	C8	N9	5.92(18)
C6	C7	C8	C3	1.32(16)	N9	C1	C2	C3	0.35(12)
C6	C7	C8	N9	−176.37(11)	N9	C1	C2	C10	−174.10(10)
C6	C7	C25	O26	179.68(12)	N9	C1	C16	C17	−123.28(11)
C7	C8	N9	C1	177.98(11)	N9	C1	C16	C21	55.54(14)
C8	C3	C4	C5	−0.39(16)					

Table S14 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for 230884lt_auto.

Atom	*x*	*y*	*z*	U(eq)
H4	598.29	1000.72	5296.18	28
H5	1050.89	107.41	7127.27	32
H6	2582.32	−1034.33	7583	31
H11	822.06	2550.46	3966.98	32
H12	−651.53	3531.67	2842.57	40
H13	−1458.9	2985.46	912.51	41
H14	−770.88	1458.59	91.5	36
H15	704.03	473.48	1195.46	29
H18	3720.91	2007.56	−5.34	32

Table S14 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for 230884lt_auto.

Atom	*x*	*y*	*z*	U(eq)
H19	3862.13	381.41	-1018.09	36
H20	3481.18	-1293.74	-205.17	34
H21	2955.35	-1330.07	1614.53	29
H22A	2431.48	2713.28	1799.54	28
H22B	3274.13	2235.59	2937.79	28
H25	4233.62	-1820.17	7165.29	33
H9	3867.95	-764.24	3922.54	23

Experimental

Single crystals of $C_{23}H_{16}N_2O$ **[230884lt_auto]** were **[]**. A suitable crystal was selected and **[]** on a **XtaLAB Synergy R, DW system, HyPix-Arc 150** diffractometer. The crystal was kept at 109(6) K during data collection. Using Olex2 [1], the structure was solved with the SHELXT [2] structure solution program using Intrinsic Phasing and refined with the SHELXL [3] refinement package using Least Squares minimisation.

1. Dolomanov, O.V., Bourhis, L.J., Gildea, R.J, Howard, J.A.K. & Puschmann, H. (2009), J. Appl. Cryst. 42, 339-341.
2. Sheldrick, G.M. (2015). Acta Cryst. A71, 3-8.
3. Sheldrick, G.M. (2015). Acta Cryst. C71, 3-8.

Crystal structure determination of [230884lt_auto]

Crystal Data for $C_{23}H_{16}N_2O$ (M =336.38 g/mol): monoclinic, space group $P2_1/c$ (no. 14), a = 12.43235(13) Å, b = 12.20419(15) Å, c = 11.52302(14) Å, β = 102.4803(11)°, V = 1707.04(4) Å^3, Z = 4, T = 109(6) K, μ(Cu Kα) = 0.639 mm^{-1}, *Dcalc* = 1.309 g/cm^3, 11901 reflections measured (7.282° ≤ 2Θ ≤ 149.472°), 3318 unique (R_{int} = 0.0265, R_{sigma} = 0.0224) which were used in all calculations. The final R_1 was 0.0337 (I > 2σ(I)) and wR_2 was 0.0890 (all data).

Refinement model description

Number of restraints - 0, number of constraints - unknown.

Details:

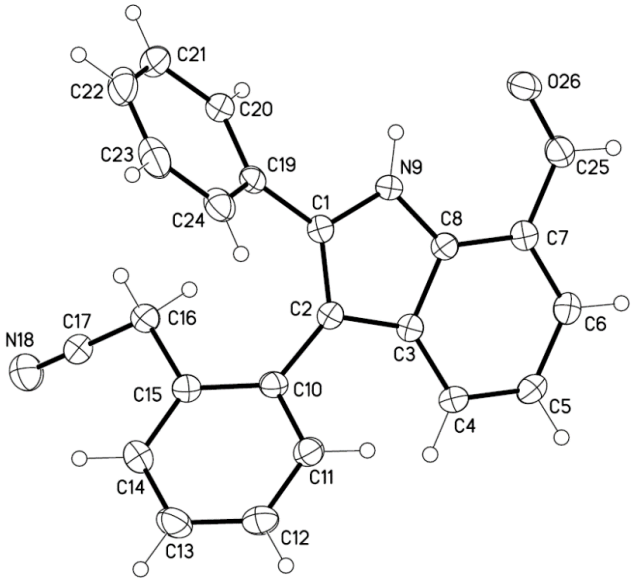
```
1. Fixed Uiso
 At 1.2 times of:
  All C(H) groups, All C(H,H) groups, All N(H) groups
2.a Secondary CH2 refined with riding coordinates:
 C22(H22A,H22B)
2.b Aromatic/amide H refined with riding coordinates:
 C4(H4), C5(H5), C6(H6), C11(H11), C12(H12), C13(H13), C14(H14), C15(H15),
 C18(H18), C19(H19), C20(H20), C21(H21), C25(H25), N9(H9)
```

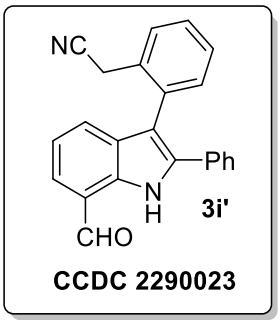
This report has been created with Olex2, compiled on 2023.08.24 svn.re1ec1418 for OlexSys. Please let us know if there are any errors or if you would like to have additional features.

(c) X-ray crystallographic data of compound (3i')

Ellipsoid contour % probability level = 50%

Sample Preparation for Crystal Growth: The compound **3i'** was dissolved in Ethyl acetate/Hexane (1:5) and kept for slow evaporation (7 days). A needle-shaped crystal was formed whose X-ray analysis was performed.





230861LT_auto

Table S15 Crystal data and structure refinement for 230861LT_auto.

Identification code	230861LT_auto
Empirical formula	$C_{23}H_{16}N_2O$
Formula weight	336.38
Temperature/K	99.99(10)
Crystal system	triclinic
Space group	P-1
a/Å	8.22512(19)
b/Å	10.0169(4)
c/Å	12.1195(4)
α/°	104.088(3)
β/°	101.613(2)

γ/°	109.165(3)
Volume/Å^3	870.66(5)
Z	2
ρ_{calc}g/cm^3	1.283
μ/mm^{-1}	0.627
F(000)	352.0
Crystal size/mm^3	0.22 × 0.21 × 0.19
Radiation	Cu Kα (λ = 1.54184)
2Θ range for data collection/°	7.902 to 147.672
Index ranges	-10 ≤ h ≤ 7, -12 ≤ k ≤ 12, -14 ≤ l ≤ 15
Reflections collected	9944
Independent reflections	3312 [R_{int} = 0.0123, R_{sigma} = 0.0128]
Data/restraints/parameters	3312/0/236
Goodness-of-fit on F^2	1.053
Final R indexes [I>=2σ (I)]	R_1 = 0.0327, wR_2 = 0.0845
Final R indexes [all data]	R_1 = 0.0343, wR_2 = 0.0858
Largest diff. peak/hole / e Å^{-3}	0.24/-0.16

Table S16 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for 230861LT_auto. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
C1	4151.0(14)	2472.9(11)	-1719.9(9)	20.9(2)
C2	3078.0(14)	3278.9(11)	-1716.2(9)	20.8(2)
C3	2144.3(14)	3000.2(11)	-854.4(9)	21.1(2)
C4	845.3(14)	3444.9(12)	-473.5(9)	23.5(2)
C5	218.0(15)	2971.6(12)	404.7(10)	25.9(2)

Table S16 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for 230861LT_auto. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
C6	856.7(15)	2058.2(12)	909.9(10)	25.0(2)
C7	2107.2(14)	1552.2(12)	525.8(9)	22.8(2)
C8	2724.0(14)	2021.6(11)	-373.5(9)	21.0(2)
C10	2879.1(13)	4263.1(12)	-2420.9(9)	21.1(2)
C11	3041.6(14)	5706.5(12)	-1814.8(10)	24.0(2)
C12	2814.7(15)	6678.6(12)	-2413.8(11)	28.1(3)
C13	2437.9(16)	6230.5(13)	-3646.1(11)	31.2(3)
C14	2272.5(16)	4807.7(13)	-4264.3(10)	29.0(3)
C15	2468.5(14)	3812.3(12)	-3672.8(9)	23.0(2)
C16	2235.2(15)	2248.8(13)	-4382.1(9)	26.2(2)
C17	856.0(15)	1617.6(13)	-5558.8(10)	26.5(2)
C19	5422.5(14)	2355.4(12)	-2399.9(9)	22.6(2)
C20	5428.3(16)	955.8(13)	-2940.8(10)	27.4(2)
C21	6613.5(18)	843.0(16)	-3591.9(11)	36.3(3)
C22	7793.7(18)	2108.8(18)	-3710.0(11)	40.0(3)
C23	7798.0(16)	3500.2(16)	-3178.8(11)	36.3(3)
C24	6613.4(15)	3631.7(14)	-2525.5(10)	28.3(3)
C25	2703.2(15)	544.5(12)	1018.1(10)	25.8(2)
N9	3912.4(12)	1699.3(10)	-921.8(7)	21.0(2)
N18	-231.0(15)	1102.8(12)	-6470.9(9)	36.4(3)
O26	3772.9(10)	54.2(9)	701.9(7)	29.3(2)

Table S17 Anisotropic Displacement Parameters ($Å^2×10^3$) for 230861LT_auto. The Anisotropic displacement factor exponent takes the form: $-2π^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+…]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C1	23.1(5)	22.7(5)	18.3(5)	6.9(4)	6.0(4)	10.8(4)
C2	23.3(5)	22.4(5)	18.6(5)	6.2(4)	7.1(4)	11.3(4)
C3	23.6(5)	22.3(5)	18.9(5)	6.5(4)	6.6(4)	11.0(4)
C4	27.7(5)	24.1(5)	23.1(5)	7.8(4)	8.6(4)	15.2(4)
C5	28.4(6)	28.1(6)	26.6(5)	8.3(4)	13.1(4)	15.6(5)
C6	28.2(6)	27.7(5)	21.9(5)	9.3(4)	10.9(4)	12.2(4)
C7	24.4(5)	24.6(5)	20.4(5)	8.1(4)	7.1(4)	10.5(4)
C8	22.1(5)	22.6(5)	19.2(5)	6.2(4)	5.9(4)	10.9(4)
C10	20.7(5)	23.7(5)	22.8(5)	9.5(4)	8.0(4)	11.6(4)
C11	24.2(5)	24.7(5)	24.6(5)	7.4(4)	8.5(4)	11.6(4)
C12	29.6(6)	21.9(5)	35.5(6)	10.0(5)	11.2(5)	12.6(4)
C13	37.0(6)	29.6(6)	35.7(6)	18.9(5)	11.9(5)	17.5(5)
C14	35.6(6)	33.0(6)	24.6(5)	14.1(5)	10.4(5)	17.2(5)
C15	24.1(5)	26.2(5)	23.0(5)	9.7(4)	8.4(4)	13.3(4)
C16	31.8(6)	29.6(6)	20.9(5)	7.7(4)	6.5(4)	18.0(5)
C17	32.8(6)	29.2(6)	23.7(6)	9.7(4)	11.8(5)	17.5(5)
C19	22.2(5)	32.5(6)	18.4(5)	10.9(4)	6.1(4)	15.9(4)
C20	33.1(6)	35.7(6)	22.6(5)	12.0(5)	10.4(4)	21.8(5)
C21	43.4(7)	54.9(8)	26.2(6)	14.2(5)	14.9(5)	35.5(6)
C22	34.3(7)	73.5(10)	29.1(6)	23.2(6)	17.8(5)	32.7(7)
C23	25.0(6)	59.3(8)	30.9(6)	25.7(6)	10.1(5)	15.8(6)
C24	24.5(6)	37.0(6)	25.7(5)	14.6(5)	6.1(4)	13.0(5)
C25	27.3(6)	29.7(6)	24.6(5)	12.5(4)	9.3(4)	12.9(5)
N9	24.4(4)	24.2(4)	20.6(4)	9.9(3)	8.5(3)	14.6(4)

Table S17 Anisotropic Displacement Parameters ($Å^2×10^3$) for 230861LT_auto. The Anisotropic displacement factor exponent takes the form: $-2π^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+…]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
N18	42.0(6)	38.7(6)	26.7(5)	8.5(4)	5.6(5)	18.4(5)
O26	29.9(4)	34.8(4)	33.4(4)	17.8(4)	12.2(3)	19.3(4)

Table S18 Bond Lengths for 230861LT_auto.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
C1	C2	1.3779(14)	C11	C12	1.3853(15)
C1	C19	1.4722(14)	C12	C13	1.3870(17)
C1	N9	1.3843(13)	C13	C14	1.3867(17)
C2	C3	1.4431(14)	C14	C15	1.3931(15)
C2	C10	1.4791(14)	C15	C16	1.5197(14)
C3	C4	1.4014(14)	C16	C17	1.4693(15)
C3	C8	1.4147(14)	C17	N18	1.1442(15)
C4	C5	1.3892(15)	C19	C20	1.3976(15)
C5	C6	1.3953(16)	C19	C24	1.3964(16)
C6	C7	1.3970(15)	C20	C21	1.3872(16)
C7	C8	1.4078(15)	C21	C22	1.381(2)
C7	C25	1.4545(15)	C22	C23	1.384(2)
C8	N9	1.3658(13)	C23	C24	1.3920(16)
C10	C11	1.4016(14)	C25	O26	1.2207(13)
C10	C15	1.4071(15)			

Table S19 Bond Angles for 230861LT_auto.

Atom	Atom	Atom	Angle/˚	Atom	Atom	Atom	Angle/˚
C2	C1	C19	130.53(9)	C15	C10	C2	123.65(9)
C2	C1	N9	109.54(9)	C12	C11	C10	121.83(10)
N9	C1	C19	119.93(9)	C11	C12	C13	119.63(10)
C1	C2	C3	106.39(9)	C14	C13	C12	119.53(10)
C1	C2	C10	128.93(9)	C13	C14	C15	121.30(10)
C3	C2	C10	124.67(9)	C10	C15	C16	120.46(9)
C4	C3	C2	134.08(10)	C14	C15	C10	119.66(10)
C4	C3	C8	119.04(9)	C14	C15	C16	119.88(9)
C8	C3	C2	106.84(9)	C17	C16	C15	113.30(9)
C5	C4	C3	119.39(10)	N18	C17	C16	178.77(13)
C4	C5	C6	121.06(10)	C20	C19	C1	120.06(10)
C5	C6	C7	121.20(10)	C24	C19	C1	120.55(10)
C6	C7	C8	117.52(10)	C24	C19	C20	119.39(10)
C6	C7	C25	120.86(10)	C21	C20	C19	120.07(11)
C8	C7	C25	121.61(10)	C22	C21	C20	120.36(12)
C7	C8	C3	121.69(9)	C21	C22	C23	120.05(11)
N9	C8	C3	107.99(9)	C22	C23	C24	120.29(12)
N9	C8	C7	130.32(9)	C23	C24	C19	119.85(11)
C11	C10	C2	118.27(9)	O26	C25	C7	123.44(10)
C11	C10	C15	118.04(9)	C8	N9	C1	109.22(8)

Table S20 Torsion Angles for 230861LT_auto.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
C1	C2	C3	C4	−177.57(11)	C8	C7	C25	O26	0.72(17)
C1	C2	C3	C8	0.15(11)	C10	C2	C3	C4	3.01(18)
C1	C2	C10	C11	−129.74(11)	C10	C2	C3	C8	−179.27(9)
C1	C2	C10	C15	52.73(16)	C10	C11	C12	C13	−0.81(17)
C1	C19	C20	C21	179.34(10)	C10	C15	C16	C17	145.30(10)
C1	C19	C24	C23	−179.52(10)	C11	C10	C15	C14	1.23(15)
C2	C1	C19	C20	−135.65(12)	C11	C10	C15	C16	−178.67(9)
C2	C1	C19	C24	43.46(16)	C11	C12	C13	C14	0.74(17)
C2	C1	N9	C8	−1.47(12)	C12	C13	C14	C15	0.33(18)
C2	C3	C4	C5	−179.60(11)	C13	C14	C15	C10	−1.32(17)
C2	C3	C8	C7	178.20(9)	C13	C14	C15	C16	178.58(10)
C2	C3	C8	N9	−1.03(11)	C14	C15	C16	C17	−34.60(14)
C2	C10	C11	C12	−177.85(10)	C15	C10	C11	C12	−0.18(15)
C2	C10	C15	C14	178.77(10)	C19	C1	C2	C3	−178.57(10)
C2	C10	C15	C16	−1.14(16)	C19	C1	C2	C10	0.81(19)
C3	C2	C10	C11	49.54(14)	C19	C1	N9	C8	177.97(9)
C3	C2	C10	C15	−127.99(11)	C19	C20	C21	C22	0.03(17)
C3	C4	C5	C6	−0.19(16)	C20	C19	C24	C23	−0.41(15)
C3	C8	N9	C1	1.53(11)	C20	C21	C22	C23	−0.08(18)
C4	C3	C8	C7	−3.67(15)	C21	C22	C23	C24	−0.11(18)

Table S20 Torsion Angles for 230861LT_auto.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
C4	C3	C8	N9	177.10(9)	C22	C23	C24	C19	0.36(17)
C4	C5	C6	C7	-1.92(17)	C24	C19	C20	C21	0.22(16)
C5	C6	C7	C8	1.18(16)	C25	C7	C8	C3	179.92(10)
C5	C6	C7	C25	−177.14(10)	C25	C7	C8	N9	-1.04(18)
C6	C7	C8	C3	1.62(15)	N9	C1	C2	C3	0.79(11)
C6	C7	C8	N9	−179.34(10)	N9	C1	C2	C10	−179.83(10)
C6	C7	C25	O26	178.97(10)	N9	C1	C19	C20	45.05(14)
C7	C8	N9	C1	−177.61(11)	N9	C1	C19	C24	−135.84(10)
C8	C3	C4	C5	2.90(15)					

Table S21 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for 230861LT_auto.

Atom	*x*	*y*	*z*	U(eq)
H4	397.81	4064.22	-812.64	28
H5	-659.79	3274.76	665.51	31
H6	433.51	1775.23	1526.29	30
H11	3314.86	6027.06	-969.65	29
H12	2916.69	7646.73	-1983.04	34
H13	2294.09	6893.68	-4063.62	37
H14	2020.65	4505.74	-5107.76	35
H16A	3407.08	2286.95	-4494.2	31
H16B	1896.84	1574.24	-3915.3	31
H20	4619.87	80.97	-2862.4	33

Table S21 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for 230861LT_auto.

Atom	*x*	*y*	*z*	U(eq)
H21	6613.09	-110.34	-3958.52	44
H22	8603.35	2024.67	-4156.11	48
H23	8612.99	4369.27	-3260.53	44
H24	6615.19	4587.67	-2165.96	34
H25	2235.43	252.54	1617.15	31
H9	4442.53	1095.42	-788.66	25

Experimental

Single crystals of $C_{23}H_{16}N_2O$ **[230861LT_auto]** were **[]**. A suitable crystal was selected and **[]** on a **XtaLAB Synergy R, DW system, HyPix-Arc 150** diffractometer. The crystal was kept at 99.99(10) K during data collection. Using Olex2 [1], the structure was solved with the SHELXT [2] structure solution program using Intrinsic Phasing and refined with the SHELXL [3] refinement package using Least Squares minimisation.

1. Dolomanov, O.V., Bourhis, L.J., Gildea, R.J, Howard, J.A.K. & Puschmann, H. (2009), J. Appl. Cryst. 42, 339-341.
2. Sheldrick, G.M. (2015). Acta Cryst. A71, 3-8.
3. Sheldrick, G.M. (2015). Acta Cryst. C71, 3-8.

Crystal structure determination of [230861LT_auto]

Crystal Data for $C_{23}H_{16}N_2O$ (M =336.38 g/mol): triclinic, space group P-1 (no. 2), a = 8.22512(19) Å, b = 10.0169(4) Å, c = 12.1195(4) Å, α = 104.088(3)°, β = 101.613(2)°, γ = 109.165(3)°, V = 870.66(5) Å^3, Z = 2, T = 99.99(10) K, μ(Cu Kα) = 0.627 mm^{-1}, *Dcalc* = 1.283 g/cm^3, 9944 reflections measured (7.902° ≤ 2Θ ≤ 147.672°), 3312 unique (R_{int} = 0.0123, R_{sigma} = 0.0128) which were used in all calculations. The final R_1 was 0.0327 (I > 2σ(I)) and wR_2 was 0.0858 (all data).

Refinement model description

Number of restraints - 0, number of constraints - unknown.

Details:

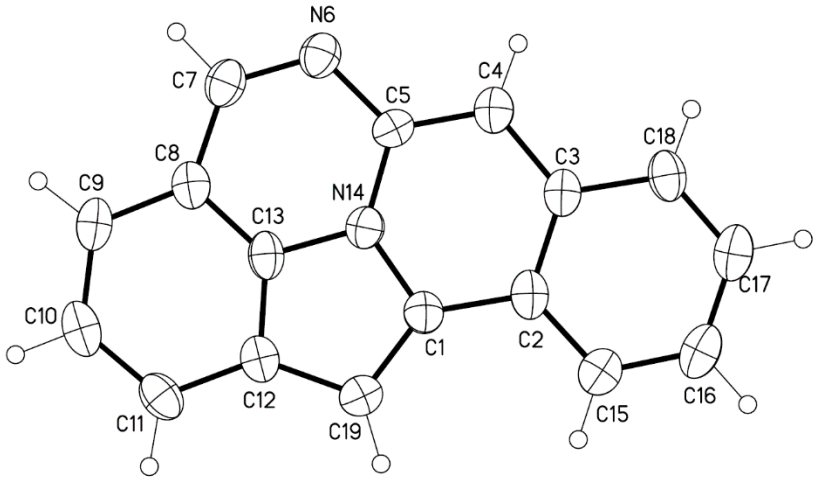
```
1. Fixed Uiso
 At 1.2 times of:
  All C(H) groups, All C(H,H) groups, All N(H) groups
2.a Secondary CH2 refined with riding coordinates:
 C16(H16A,H16B)
2.b Aromatic/amide H refined with riding coordinates:
 C4(H4), C5(H5), C6(H6), C11(H11), C12(H12), C13(H13), C14(H14), C20(H20),
 C21(H21), C22(H22), C23(H23), C24(H24), C25(H25), N9(H9)
```

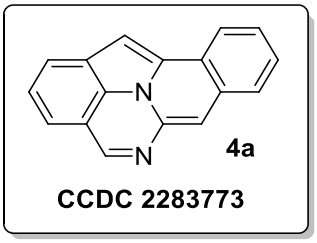
This report has been created with Olex2, compiled on 2023.08.17 svn.r577a77a9 for OlexSys. Please let us know if there are any errors or if you would like to have additional features.

(d) X-ray crystallographic data of compound (4a)

Ellipsoid contour % probability level = 50%

Sample Preparation for Crystal Growth: The compound **4a** was dissolved in Tetrahydrofuran and kept for slow evaporation (3 days). A needle-shaped crystal was formed whose X-ray analysis was performed.





230522LT2_auto

Table S22 Crystal data and structure refinement for 230522LT2_auto.

Identification code	230522LT2_auto
Empirical formula	$C_{17}H_{10}N_2$
Formula weight	242.27
Temperature/K	99.98(10)
Crystal system	orthorhombic
Space group	$P2_12_12_1$
a/Å	4.50440(10)
b/Å	12.6636(5)
c/Å	19.6473(8)
α/°	90
β/°	90

γ/°	90
Volume/Å^3	1120.72(7)
Z	4
ρ_{calc}g/cm^3	1.436
μ/mm^{-1}	0.671
F(000)	504.0
Crystal size/mm^3	0.17 × 0.03 × 0.02
Radiation	Cu Kα (λ = 1.54184)
2Θ range for data collection/°	8.306 to 134.11
Index ranges	-4 ≤ h ≤ 5, -15 ≤ k ≤ 15, -23 ≤ l ≤ 23
Reflections collected	12127
Independent reflections	2008 [R_{int} = 0.0669, R_{sigma} = 0.0348]
Data/restraints/parameters	2008/0/174
Goodness-of-fit on F^2	1.120
Final R indexes [I>=2σ (I)]	R_1 = 0.0554, wR_2 = 0.1506
Final R indexes [all data]	R_1 = 0.0594, wR_2 = 0.1530
Largest diff. peak/hole / e Å^{-3}	0.20/-0.24
Flack parameter	-0.3(13)

Table S23 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for 230522LT2_auto. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
C1	5149(8)	5503(3)	6919.4(18)	29.7(8)
C2	7189(8)	5199(3)	7448.4(19)	30.4(9)
C3	8483(8)	4167(3)	7405.9(17)	30.2(9)

Table S23 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for 230522LT2_auto. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
C4	7738(8)	3439(3)	6871.5(18)	32.7(8)
C5	5752(8)	3735(3)	6377.9(17)	27.9(8)
C7	2923(9)	3486(3)	5399.4(18)	34.7(9)
C8	1638(8)	4527(3)	5429.4(17)	30.8(9)
C9	-411(8)	5020(3)	5000.6(19)	34.7(9)
C10	-1301(9)	6060(3)	5148(2)	38.1(10)
C11	-248(8)	6632(3)	5708.7(18)	35.4(9)
C12	1842(7)	6154(3)	6146.6(18)	30.0(8)
C13	2599(8)	5129(3)	5969.1(18)	30.5(8)
C15	7937(8)	5860(3)	7993.1(18)	34.4(9)
C16	9934(9)	5542(3)	8480.0(19)	38.5(9)
C17	11223(9)	4548(3)	8440.7(19)	39.5(10)
C18	10533(8)	3881(3)	7922.0(18)	34.2(9)
C19	3484(8)	6396(3)	6756.5(18)	31.0(8)
N6	4848(7)	3104(3)	5842.6(15)	34.6(8)
N14	4611(7)	4741(2)	6432.9(15)	28.9(7)

Table S24 Anisotropic Displacement Parameters (Å^2×10^3) for 230522LT2_auto. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C1	25.5(16)	35.3(18)	28.1(18)	0.3(15)	2.7(15)	1.3(16)
C2	20.6(16)	44(2)	27.1(17)	5.7(15)	2.3(14)	-4.3(16)
C3	24.0(17)	42(2)	24.8(18)	3.5(15)	1.3(15)	-2.7(16)
C4	29.2(18)	40(2)	29.2(18)	2.2(16)	0.2(15)	-1.5(16)

Table S24 Anisotropic Displacement Parameters ($Å^2×10^3$) for 230522LT2_auto. The Anisotropic displacement factor exponent takes the form: $-2π^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+…]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C5	26.5(17)	28.2(18)	28.9(18)	-3.3(14)	3.9(14)	-3.5(15)
C7	34(2)	43(2)	27.4(18)	-0.3(17)	0.7(16)	-5.0(17)
C8	25.1(18)	42(2)	25.4(18)	5.0(16)	3.1(15)	-0.4(17)
C9	28.0(19)	51(2)	25.2(18)	4.0(16)	-2.7(15)	-5.2(17)
C10	26.7(19)	52(2)	36(2)	15.0(18)	-0.7(16)	0.8(19)
C11	28.6(18)	39(2)	39(2)	9.2(17)	4.5(16)	5.1(17)
C12	24.0(16)	38(2)	28.4(18)	6.8(16)	2.6(15)	-1.9(15)
C13	22.4(17)	43(2)	26.3(18)	5.9(15)	-0.4(14)	-2.0(16)
C15	29.5(17)	41(2)	32(2)	-1.5(16)	4.1(16)	-5.3(16)
C16	35(2)	54(2)	26.8(18)	-0.9(18)	1.5(17)	-14(2)
C17	33(2)	55(3)	30(2)	5.6(19)	-2.9(16)	-11(2)
C18	24.3(17)	46(2)	32.1(19)	7.9(17)	-0.8(15)	-1.7(17)
C19	29.2(18)	31.5(19)	32.4(19)	-2.3(15)	3.9(15)	-3.3(15)
N6	34.6(16)	40.3(18)	28.9(16)	-1.7(14)	0.8(14)	-1.0(15)
N14	28.7(15)	32.6(16)	25.4(15)	1.8(12)	1.3(13)	-2.0(13)

Table S25 Bond Lengths for 230522LT2_auto.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
C1	C2	1.440(5)	C8	C9	1.397(5)
C1	C19	1.393(5)	C8	C13	1.376(5)
C1	N14	1.380(5)	C9	C10	1.407(5)
C2	C3	1.433(5)	C10	C11	1.401(6)
C2	C15	1.400(5)	C11	C12	1.412(5)

Table S25 Bond Lengths for 230522LT2_auto.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
C3	C4	1.437(5)	C12	C13	1.387(5)
C3	C18	1.419(5)	C12	C19	1.441(5)
C4	C5	1.371(5)	C13	N14	1.376(4)
C5	N6	1.382(4)	C15	C16	1.374(5)
C5	N14	1.379(5)	C16	C17	1.388(6)
C7	C8	1.440(6)	C17	C18	1.360(5)
C7	N6	1.321(5)			

Table S26 Bond Angles for 230522LT2_auto.

Atom	Atom	Atom	Angle/˚	Atom	Atom	Atom	Angle/˚
C19	C1	C2	136.6(3)	C11	C10	C9	123.3(4)
N14	C1	C2	115.1(3)	C10	C11	C12	118.9(4)
N14	C1	C19	108.3(3)	C11	C12	C19	139.3(4)
C3	C2	C1	117.5(3)	C13	C12	C11	114.3(3)
C15	C2	C1	123.1(4)	C13	C12	C19	106.4(3)
C15	C2	C3	119.5(3)	C8	C13	C12	129.4(3)
C2	C3	C4	122.2(3)	C8	C13	N14	121.4(3)
C18	C3	C2	117.2(3)	N14	C13	C12	109.2(3)
C18	C3	C4	120.7(3)	C16	C15	C2	121.0(4)
C5	C4	C3	119.6(3)	C15	C16	C17	120.1(4)
C4	C5	N6	125.0(3)	C18	C17	C16	120.6(4)
C4	C5	N14	116.1(3)	C17	C18	C3	121.7(4)
N14	C5	N6	119.0(3)	C1	C19	C12	107.2(3)
N6	C7	C8	124.9(3)	C7	N6	C5	118.9(3)

Table S26 Bond Angles for 230522LT2_auto.

Atom	Atom	Atom	Angle/˚	Atom	Atom	Atom	Angle/˚
C9	C8	C7	130.5(4)	C5	N14	C1	129.5(3)
C13	C8	C7	114.3(3)	C13	N14	C1	109.0(3)
C13	C8	C9	115.2(4)	C13	N14	C5	121.6(3)
C8	C9	C10	118.9(4)				

Table S27 Torsion Angles for 230522LT2_auto.

A	B	C	D	Angle/˚	A	B	C	D	Angle/˚
C1	C2	C3	C4	-1.8(5)	C10	C11	C12	C19	-179.5(4)
C1	C2	C3	C18	178.9(3)	C11	C12	C13	C8	0.9(5)
C1	C2	C15	C16	-178.9(3)	C11	C12	C13	N14	-179.3(3)
C2	C1	C19	C12	-179.2(4)	C11	C12	C19	C1	178.4(4)
C2	C1	N14	C5	-0.3(5)	C12	C13	N14	C1	0.8(4)
C2	C1	N14	C13	179.0(3)	C12	C13	N14	C5	-179.8(3)
C2	C3	C4	C5	0.8(5)	C13	C8	C9	C10	0.1(5)
C2	C3	C18	C17	0.8(5)	C13	C12	C19	C1	-0.2(4)
C2	C15	C16	C17	-0.6(6)	C15	C2	C3	C4	178.0(3)
C3	C2	C15	C16	1.2(5)	C15	C2	C3	C18	-1.3(5)
C3	C4	C5	N6	-179.6(3)	C15	C16	C17	C18	0.1(6)
C3	C4	C5	N14	0.5(5)	C16	C17	C18	C3	-0.2(6)
C4	C3	C18	C17	-178.5(3)	C18	C3	C4	C5	-180.0(3)
C4	C5	N6	C7	-179.8(4)	C19	C1	C2	C3	-178.6(4)
C4	C5	N14	C1	-0.7(5)	C19	C1	C2	C15	1.5(7)
C4	C5	N14	C13	-180.0(3)	C19	C1	N14	C5	179.8(3)
C7	C8	C9	C10	-179.8(4)	C19	C1	N14	C13	-0.9(4)

Table S27 Torsion Angles for 230522LT2_auto.

A	B	C	D	Angle/˚	A	B	C	D	Angle/˚
C7	C8	C13	C12	179.5(3)	C19	C12	C13	C8	179.8(4)
C7	C8	C13	N14	-0.3(5)	C19	C12	C13	N14	-0.4(4)
C8	C7	N6	C5	-0.4(5)	N6	C5	N14	C1	179.4(3)
C8	C9	C10	C11	-0.4(6)	N6	C5	N14	C13	0.1(5)
C8	C13	N14	C1	-179.4(3)	N6	C7	C8	C9	-179.6(4)
C8	C13	N14	C5	0.0(5)	N6	C7	C8	C13	0.5(5)
C9	C8	C13	C12	-0.4(6)	N14	C1	C2	C3	1.6(5)
C9	C8	C13	N14	179.8(3)	N14	C1	C2	C15	-178.3(3)
C9	C10	C11	C12	0.9(6)	N14	C1	C19	C12	0.6(4)
C10	C11	C12	C13	-1.0(5)	N14	C5	N6	C7	0.1(5)

Table S28 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for 230522LT2_auto.

Atom	*x*	*y*	*z*	U(eq)
H4	8615.62	2757.47	6860.18	39
H7	2342.35	3041.71	5033.39	42
H9	-1189.75	4659.25	4616.14	42
H10	-2685.65	6391.92	4852.09	46
H11	-929.53	7329.48	5792.97	42
H15	7050.08	6538.78	8026.48	41
H16	10433.8	6002.05	8844.12	46
H17	12599.3	4331.46	8779.51	47
H18	11447.49	3205.09	7904.7	41
H19	3440.43	7042.08	7001.46	37

Experimental

Single crystals of $C_{17}H_{10}N_2$ **[230522LT2_auto]** were **[]**. A suitable crystal was selected and **[]** on a **XtaLAB Synergy R, DW system, HyPix-Arc 150** diffractometer. The crystal was kept at 99.98(10) K during data collection. Using Olex2 [1], the structure was solved with the SHELXT [2] structure solution program using Intrinsic Phasing and refined with the SHELXL [3] refinement package using Least Squares minimisation.

1. Dolomanov, O.V., Bourhis, L.J., Gildea, R.J, Howard, J.A.K. & Puschmann, H. (2009), J. Appl. Cryst. 42, 339-341.
2. Sheldrick, G.M. (2015). Acta Cryst. A71, 3-8.
3. Sheldrick, G.M. (2015). Acta Cryst. C71, 3-8.

Crystal structure determination of [230522LT2_auto]

Crystal Data for $C_{17}H_{10}N_2$ (M =242.27 g/mol): orthorhombic, space group $P2_12_12_1$ (no. 19), a = 4.50440(10) Å, b = 12.6636(5) Å, c = 19.6473(8) Å, V = 1120.72(7) Å^3, Z = 4, T = 99.98(10) K, μ(Cu Kα) = 0.671 mm^{-1}, *Dcalc* = 1.436 g/cm^3, 12127 reflections measured (8.306° ≤ 2Θ ≤ 134.11°), 2008 unique (R_{int} = 0.0669, R_{sigma} = 0.0348) which were used in all calculations. The final R_1 was 0.0554 (I > 2σ(I)) and wR_2 was 0.1530 (all data).

Refinement model description

Number of restraints - 0, number of constraints - unknown.

Details:

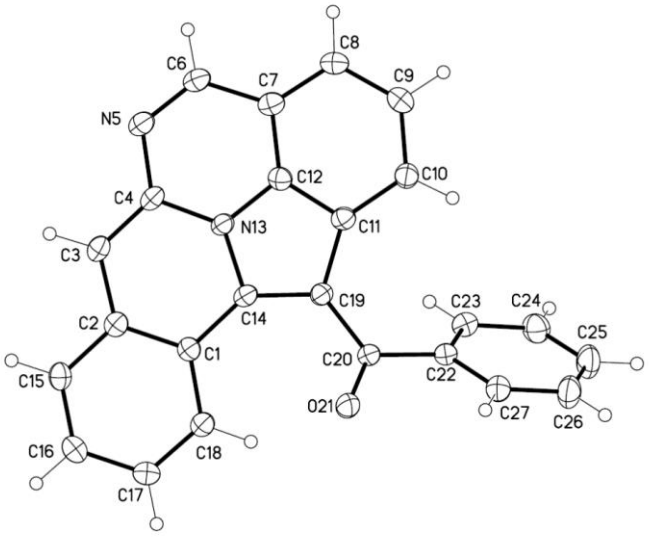
```
1. Twinned data refinement
 Scales: 1.3(13)
 -0.3(13)
2. Fixed Uiso
 At 1.2 times of:
  All C(H) groups
3.a Aromatic/amide H refined with riding coordinates:
 C4(H4), C7(H7), C9(H9), C10(H10), C11(H11), C15(H15), C16(H16), C17(H17),
 C18(H18), C19(H19)
```

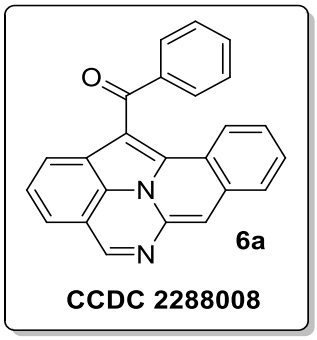
This report has been created with Olex2, compiled on 2023.03.06 svn.rbb2c1857 for OlexSys. Please let us know if there are any errors or if you would like to have additional features.

(e) X-ray crystallographic data of compound (6a)

Ellipsoid contour % probability level = 50%

Sample Preparation for Crystal Growth: The compound **6a** was dissolved in Methanol/Tetrahydrofuran (1:1) and kept for slow evaporation (6 days). A needle-shaped crystal was formed whose X-ray analysis was performed.





230766lt_auto

Table S29 Crystal data and structure refinement for 230766lt_auto.

Identification code	230766lt_auto
Empirical formula	$C_{24}H_{14}N_2O$
Formula weight	346.37
Temperature/K	100.00(10)
Crystal system	triclinic
Space group	P-1
a/Å	7.67160(10)
b/Å	9.16801(15)
c/Å	12.73071(19)
α/°	106.1712(14)
β/°	91.1629(11)
γ/°	109.9674(13)
Volume/Å^3	801.64(2)
Z	2

ρ_{calc}g/cm^3	1.435
μ/mm^{-1}	0.703
F(000)	360.0
Crystal size/mm^3	0.22 × 0.15 × 0.06
Radiation	Cu Kα (λ = 1.54184)
2Θ range for data collection/°	10.776 to 149.508
Index ranges	-7 ≤ h ≤ 9, -11 ≤ k ≤ 11, -15 ≤ l ≤ 15
Reflections collected	8120
Independent reflections	3101 [R_{int} = 0.0125, R_{sigma} = 0.0152]
Data/restraints/parameters	3101/0/245
Goodness-of-fit on F^2	1.053
Final R indexes [I>=2σ (I)]	R_1 = 0.0358, wR_2 = 0.0959
Final R indexes [all data]	R_1 = 0.0378, wR_2 = 0.0973
Largest diff. peak/hole / e Å^{-3}	0.44/-0.18

Table S30 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for 230766lt_auto. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
C1	3927.0(15)	11481.3(14)	4806.6(9)	18.4(2)
C2	3544.2(15)	10083.8(14)	3862.4(9)	19.3(2)
C3	2277.2(16)	8508.3(14)	3843.1(10)	20.6(3)
C4	1361.3(15)	8321.1(14)	4729.2(10)	19.3(2)
C6	-635.3(16)	6799.3(14)	5706.0(10)	22.3(3)
C7	-284.4(16)	8198.6(14)	6671.4(10)	20.6(3)
C8	-990.7(16)	8300.2(14)	7676.8(10)	22.4(3)
C9	-369.5(17)	9817.6(15)	8499.3(10)	23.9(3)

Table S30 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for 230766lt_auto. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
C10	934.5(16)	11237.4(14)	8372.5(10)	21.8(3)
C11	1659.5(15)	11176.2(14)	7353.9(10)	19.5(2)
C12	968.9(15)	9644.3(14)	6571.3(9)	19.0(2)
C14	3041.6(15)	11264.7(13)	5769.5(9)	18.2(2)
C15	4453.2(16)	10276.3(15)	2928.2(10)	21.7(3)
C16	5648.9(17)	11767.7(15)	2905.2(10)	23.4(3)
C17	5981.7(16)	13145.6(15)	3823.6(10)	22.7(3)
C18	5139.4(16)	13004.3(14)	4754.2(10)	20.8(3)
C19	3021.2(15)	12223.4(14)	6851.2(9)	19.1(2)
C20	4340.0(16)	13876.7(13)	7439.5(9)	18.8(2)
C22	3674.2(16)	14967.4(14)	8304.1(9)	20.8(3)
C23	1832.7(17)	14901.0(14)	8206.0(10)	24.3(3)
C24	1275.0(18)	15993.4(16)	8986.7(11)	29.3(3)
C25	2550(2)	17150.2(17)	9867.2(11)	33.5(3)
C26	4389.8(19)	17236.0(17)	9964.0(11)	31.5(3)
C27	4955.5(17)	16155.1(15)	9182.9(10)	24.3(3)
N5	113.6(14)	6854.5(12)	4800.0(8)	22.4(2)
N13	1769.5(13)	9706.8(11)	5631.8(8)	18.1(2)
O21	5982.5(11)	14379.8(10)	7258.6(7)	25.4(2)

Table S31 Anisotropic Displacement Parameters (Å^2×10^3) for 230766lt_auto. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C1	16.5(5)	19.6(6)	20.4(6)	6.0(4)	2.6(4)	8.2(4)

Table S31 Anisotropic Displacement Parameters ($Å^2×10^3$) for 230766lt_auto. The Anisotropic displacement factor exponent takes the form: $-2π^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+…]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C2	17.0(5)	19.9(6)	22.0(6)	5.4(5)	1.4(4)	8.6(4)
C3	20.1(6)	17.6(6)	22.1(6)	2.1(4)	0.7(4)	7.6(5)
C4	17.2(5)	14.8(5)	23.3(6)	2.5(4)	-0.7(4)	5.6(4)
C6	18.2(6)	17.5(6)	29.8(6)	7.1(5)	1.9(5)	5.0(4)
C7	16.5(5)	19.5(6)	26.5(6)	7.9(5)	1.7(4)	6.6(4)
C8	18.7(6)	21.4(6)	28.2(6)	11.4(5)	3.8(5)	5.6(5)
C9	22.7(6)	28.5(6)	23.4(6)	11.0(5)	6.3(5)	9.9(5)
C10	21.9(6)	21.3(6)	20.9(6)	4.7(4)	2.9(4)	7.6(5)
C11	16.6(5)	18.8(6)	22.8(6)	6.2(4)	2.4(4)	6.3(4)
C12	16.8(5)	20.2(6)	21.3(6)	7.0(4)	3.3(4)	7.8(4)
C14	15.9(5)	14.8(5)	22.6(6)	4.7(4)	1.3(4)	5.0(4)
C15	22.0(6)	24.2(6)	19.7(6)	3.9(5)	2.5(4)	11.4(5)
C16	22.5(6)	29.2(6)	21.2(6)	9.4(5)	5.5(5)	11.3(5)
C17	20.3(6)	22.2(6)	25.4(6)	9.6(5)	3.5(5)	5.7(5)
C18	20.4(6)	19.0(6)	21.9(6)	4.8(4)	1.8(4)	6.7(5)
C19	18.5(5)	16.9(5)	21.0(5)	5.0(4)	4.0(4)	6.0(4)
C20	19.6(5)	16.2(5)	18.5(5)	5.0(4)	2.5(4)	4.2(4)
C22	24.6(6)	16.7(5)	20.2(5)	6.2(4)	5.5(4)	5.8(5)
C23	24.9(6)	20.3(6)	25.6(6)	6.5(5)	4.3(5)	6.0(5)
C24	27.7(7)	30.7(7)	32.8(7)	9.6(5)	9.4(5)	14.3(5)
C25	40.6(8)	31.5(7)	28.8(7)	2.1(5)	9.8(6)	18.9(6)
C26	35.0(7)	30.3(7)	22.8(6)	-0.9(5)	2.5(5)	11.4(6)
C27	24.8(6)	23.7(6)	22.3(6)	5.1(5)	3.9(5)	7.7(5)
N5	19.9(5)	16.9(5)	27.6(5)	4.5(4)	1.7(4)	5.4(4)

Table S31 Anisotropic Displacement Parameters ($Å^2×10^3$) for 230766lt_auto. The Anisotropic displacement factor exponent takes the form: $-2π^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+…]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
N13	16.5(5)	14.9(5)	21.1(5)	4.1(4)	2.0(4)	4.5(4)
O21	22.4(4)	21.3(4)	26.2(4)	2.3(3)	6.6(3)	3.8(3)

Table S32 Bond Lengths for 230766lt_auto.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
C1	C2	1.4295(16)	C11	C19	1.4516(16)
C1	C14	1.4426(15)	C12	N13	1.3620(14)
C1	C18	1.4095(16)	C14	C19	1.4161(15)
C2	C3	1.4325(16)	C14	N13	1.3873(14)
C2	C15	1.4136(16)	C15	C16	1.3707(17)
C3	C4	1.3614(17)	C16	C17	1.4046(17)
C4	N5	1.3871(15)	C17	C18	1.3774(16)
C4	N13	1.3903(14)	C19	C20	1.4736(15)
C6	C7	1.4496(17)	C20	C22	1.4936(15)
C6	N5	1.3049(16)	C20	O21	1.2359(14)
C7	C8	1.3916(16)	C22	C23	1.3946(17)
C7	C12	1.3879(16)	C22	C27	1.3962(17)
C8	C9	1.4051(17)	C23	C24	1.3890(17)
C9	C10	1.3984(17)	C24	C25	1.387(2)
C10	C11	1.4156(16)	C25	C26	1.388(2)
C11	C12	1.3917(16)	C26	C27	1.3862(17)

Table S33 Bond Angles for 230766lt_auto.

Atom	Atom	Atom	Angle/˚	Atom	Atom	Atom	Angle/˚
C2	C1	C14	118.22(10)	N13	C14	C1	114.62(10)
C18	C1	C2	118.75(10)	N13	C14	C19	107.12(10)
C18	C1	C14	123.03(10)	C16	C15	C2	121.48(11)
C1	C2	C3	121.81(11)	C15	C16	C17	119.77(11)
C15	C2	C1	118.56(11)	C18	C17	C16	120.47(11)
C15	C2	C3	119.63(10)	C17	C18	C1	120.93(11)
C4	C3	C2	119.97(11)	C11	C19	C20	125.02(10)
C3	C4	N5	124.74(11)	C14	C19	C11	107.06(10)
C3	C4	N13	116.56(10)	C14	C19	C20	127.13(10)
N5	C4	N13	118.67(10)	C19	C20	C22	118.61(10)
N5	C6	C7	124.37(11)	O21	C20	C19	122.42(10)
C8	C7	C6	129.86(11)	O21	C20	C22	118.95(10)
C12	C7	C6	114.30(11)	C23	C22	C20	121.19(11)
C12	C7	C8	115.83(11)	C23	C22	C27	119.46(11)
C7	C8	C9	118.40(11)	C27	C22	C20	119.18(11)
C10	C9	C8	123.86(11)	C24	C23	C22	120.14(12)
C9	C10	C11	119.02(11)	C25	C24	C23	119.98(12)
C10	C11	C19	139.65(11)	C24	C25	C26	120.23(12)
C12	C11	C10	114.19(10)	C27	C26	C25	119.98(12)
C12	C11	C19	106.07(10)	C26	C27	C22	120.19(12)
C7	C12	C11	128.67(11)	C6	N5	C4	119.75(10)
N13	C12	C7	121.61(11)	C12	N13	C4	121.29(10)
N13	C12	C11	109.68(10)	C12	N13	C14	110.04(9)
C19	C14	C1	138.19(11)	C14	N13	C4	128.57(10)

Table S34 Torsion Angles for 230766lt_auto.

A	B	C	D	Angle/˚	A	B	C	D	Angle/˚
C1	C2	C3	C4	1.80(17)	C12	C11	C19	C14	1.52(12)
C1	C2	C15	C16	-1.38(17)	C12	C11	C19	C20	−168.90(11)
C1	C14	C19	C11	175.99(13)	C14	C1	C2	C3	1.84(16)
C1	C14	C19	C20	-13.8(2)	C14	C1	C2	C15	−177.99(10)
C1	C14	N13	C4	5.71(17)	C14	C1	C18	C17	178.70(10)
C1	C14	N13	C12	-177.96(9)	C14	C19	C20	C22	152.37(11)
C2	C1	C14	C19	178.33(13)	C14	C19	C20	O21	-29.08(18)
C2	C1	C14	N13	-5.11(15)	C15	C2	C3	C4	−178.37(10)
C2	C1	C18	C17	-1.63(17)	C15	C16	C17	C18	1.09(18)
C2	C3	C4	N5	−179.73(10)	C16	C17	C18	C1	-0.08(18)
C2	C3	C4	N13	-1.74(16)	C18	C1	C2	C3	−177.84(10)
C2	C15	C16	C17	-0.33(18)	C18	C1	C2	C15	2.33(16)
C3	C2	C15	C16	178.78(10)	C18	C1	C14	C19	-2.0(2)
C3	C4	N5	C6	177.40(11)	C18	C1	C14	N13	174.56(10)
C3	C4	N13	C12	−178.21(10)	C19	C11	C12	C7	175.92(11)
C3	C4	N13	C14	-2.25(17)	C19	C11	C12	N13	-1.77(13)
C6	C7	C8	C9	177.96(11)	C19	C14	N13	C4	−176.69(10)
C6	C7	C12	C11	−177.03(11)	C19	C14	N13	C12	-0.36(12)
C6	C7	C12	N13	0.42(16)	C19	C20	C22	C23	-33.75(16)

Table S34 Torsion Angles for 230766lt_auto.

A	B	C	D	Angle/˚	A	B	C	D	Angle/˚
C7	C6	N5	C4	1.20(17)	C19	C20	C22	C27	151.07(11)
C7	C8	C9	C10	−0.58(18)	C20	C22	C23	C24	−176.13(11)
C7	C12	N13	C4	0.12(17)	C20	C22	C27	C26	176.65(11)
C7	C12	N13	C14	−176.52(10)	C22	C23	C24	C25	−0.16(19)
C8	C7	C12	C11	2.13(18)	C23	C22	C27	C26	1.39(18)
C8	C7	C12	N13	179.58(10)	C23	C24	C25	C26	0.9(2)
C8	C9	C10	C11	1.37(18)	C24	C25	C26	C27	−0.5(2)
C9	C10	C11	C12	−0.45(16)	C25	C26	C27	C22	−0.7(2)
C9	C10	C11	C19	−176.40(13)	C27	C22	C23	C24	−0.96(18)
C10	C11	C12	C7	−1.35(18)	N5	C4	N13	C12	−0.10(16)
C10	C11	C12	N13	−179.04(9)	N5	C4	N13	C14	175.87(10)
C10	C11	C19	C14	177.68(14)	N5	C6	C7	C8	179.87(11)
C10	C11	C19	C20	7.3(2)	N5	C6	C7	C12	−1.12(17)
C11	C12	N13	C4	178.01(10)	N13	C4	N5	C6	−0.55(16)
C11	C12	N13	C14	1.37(13)	N13	C14	C19	C11	−0.73(12)
C11	C19	C20	C22	−39.14(16)	N13	C14	C19	C20	169.43(10)
C11	C19	C20	O21	139.41(12)	O21	C20	C22	C23	147.65(11)
C12	C7	C8	C9	−1.05(16)	O21	C20	C22	C27	−27.53(16)

Table S35 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for 230766lt_auto.

Atom	*x*	*y*	*z*	U(eq)
H3	2076.22	7594.53	3212.27	25

Table S35 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for 230766lt_auto.

Atom	*x*	*y*	*z*	U(eq)
H6	-1465.84	5773.65	5734.84	27
H8	-1871.51	7366.25	7804.01	27
H9	-864.59	9882.79	9181.7	29
H10	1327.99	12228.43	8961.21	26
H15	4230.32	9351.19	2302.3	26
H16	6250.45	11869.16	2270.36	28
H17	6793.52	14182.46	3802.81	27
H18	5378.91	13946.74	5369.43	25
H23	957.79	14106.86	7604.03	29
H24	20.71	15947.95	8917.42	35
H25	2161.79	17886.71	10406.14	40
H26	5261.62	18035.31	10565.48	38
H27	6218.75	16222.69	9245.73	29

Experimental

Single crystals of $C_{24}H_{14}N_2O$ **[230766lt_auto]** were **[]**. A suitable crystal was selected and **[]** on a **XtaLAB Synergy R, DW system, HyPix-Arc 150** diffractometer. The crystal was kept at 100.00(10) K during data collection. Using Olex2 [1], the structure was solved with the SHELXT [2] structure solution program using Intrinsic Phasing and refined with the SHELXL [3] refinement package using Least Squares minimisation.

1. Dolomanov, O.V., Bourhis, L.J., Gildea, R.J, Howard, J.A.K. & Puschmann, H. (2009), J. Appl. Cryst. 42, 339-341.
2. Sheldrick, G.M. (2015). Acta Cryst. A71, 3-8.
3. Sheldrick, G.M. (2015). Acta Cryst. C71, 3-8.

Crystal structure determination of [230766lt_auto]

Crystal Data for $C_{24}H_{14}N_2O$ (M =346.37 g/mol): triclinic, space group P-1 (no. 2), a = 7.67160(10) Å, b = 9.16801(15) Å, c = 12.73071(19) Å, α = 106.1712(14)°, β = 91.1629(11)°, γ = 109.9674(13)°, V = 801.64(2) Å^3, Z = 2, T = 100.00(10) K, μ(Cu Kα) = 0.703 mm^{-1}, *Dcalc* = 1.435 g/cm^3, 8120 reflections measured (10.776° ≤ 2Θ ≤ 149.508°), 3101 unique (R_{int} = 0.0125, R_{sigma} = 0.0152) which were used in all calculations. The final R_1 was 0.0358 (I > 2σ(I)) and wR_2 was 0.0973 (all data).

Refinement model description

Number of restraints - 0, number of constraints - unknown.
Details:

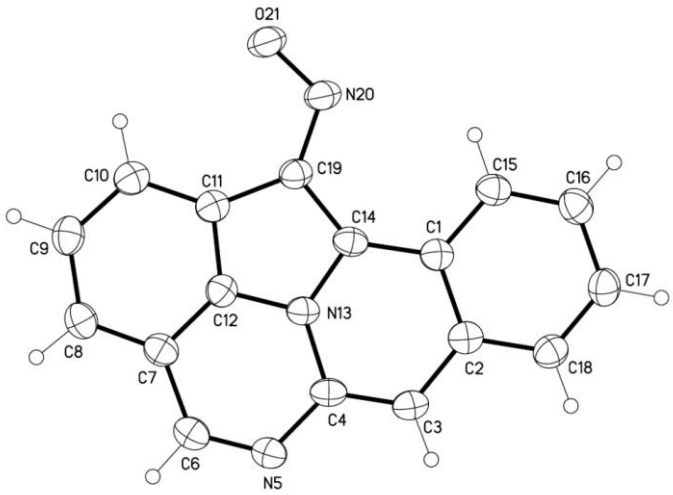
```
1. Fixed Uiso
 At 1.2 times of:
  All C(H) groups
2.a Aromatic/amide H refined with riding coordinates:
 C3(H3), C6(H6), C8(H8), C9(H9), C10(H10), C15(H15), C16(H16), C17(H17),
 C18(H18), C23(H23), C24(H24), C25(H25), C26(H26), C27(H27)
```

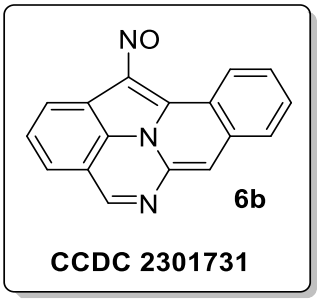
This report has been created with Olex2, compiled on 2023.03.06 svn.rbb2c1857 for OlexSys. Please let us know if there are any errors or if you would like to have additional features.

(f) X-ray crystallographic data of compound (6b)

Ellipsoid contour % probability level = 50%

Sample Preparation for Crystal Growth: The compound **6b** was dissolved in Acetonitrile and kept for slow evaporation (8 days). A needle-shaped crystal was formed whose X-ray analysis was performed.





231041lt_auto

Table S36 Crystal data and structure refinement for 231041lt_auto.

Identification code	231041lt_auto
Empirical formula	$C_{17}H_9N_3O$
Formula weight	271.27
Temperature/K	100.01(10)
Crystal system	monoclinic

Space group	$P2_1/c$
a/Å	3.77916(13)
b/Å	16.2226(5)
c/Å	19.1757(6)
α/°	90
β/°	93.565(3)
γ/°	90
Volume/Å^3	1173.34(7)
Z	4
ρ_{calc}g/cm^3	1.536
μ/mm^{-1}	0.804
F(000)	560.0
Crystal size/mm^3	0.09 × 0.07 × 0.04
Radiation	Cu Kα (λ = 1.54184)
2Θ range for data collection/°	7.144 to 149.604
Index ranges	-4 ≤ h ≤ 4, -20 ≤ k ≤ 18, -23 ≤ l ≤ 21
Reflections collected	6065
Independent reflections	2257 [R_{int} = 0.0282, R_{sigma} = 0.0338]
Data/restraints/parameters	2257/0/190
Goodness-of-fit on F^2	1.039
Final R indexes [I>=2σ (I)]	R_1 = 0.0404, wR_2 = 0.1013
Final R indexes [all data]	R_1 = 0.0548, wR_2 = 0.1090
Largest diff. peak/hole / e Å^{-3}	0.15/-0.19

Table S37 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for 231041lt_auto. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
O21	-6212(3)	-2559.4(7)	1975.1(6)	39.2(3)
N5	2442(4)	318.8(8)	3940.5(7)	31.7(3)
N13	-479(3)	-891.9(8)	3493.4(6)	27.0(3)
N20	-4870(4)	-2541.5(8)	2596.6(7)	32.7(3)
C1	-1206(4)	-2143.0(9)	4112.1(8)	27.8(4)
C2	588(4)	-1740.7(10)	4698.8(8)	29.1(4)
C3	1878(4)	-917.2(10)	4651.1(8)	29.9(4)
C4	1345(4)	-485.1(10)	4046.6(8)	28.5(4)
C6	1680(4)	683.7(10)	3341.9(8)	32.3(4)
C7	-239(4)	297.4(10)	2748.2(8)	30.5(4)
C8	-1175(4)	605.5(10)	2085.1(8)	33.2(4)
C9	-2942(5)	85.1(11)	1593.0(8)	34.8(4)
C10	-3868(4)	-729.5(10)	1733.7(8)	32.1(4)
C11	-2997(4)	-1049.6(10)	2400.8(8)	28.8(4)
C12	-1206(4)	-511.8(10)	2863.1(8)	28.1(3)
C14	-1745(4)	-1685.3(9)	3477.1(8)	27.7(3)
C15	-2420(4)	-2959.3(10)	4180.3(8)	30.8(4)
C16	-1907(4)	-3359.5(10)	4811.4(8)	34.8(4)
C17	-214(4)	-2961.8(11)	5389.8(9)	34.2(4)
C18	1024(4)	-2174.5(10)	5334.6(8)	32.0(4)
C19	-3367(4)	-1812.0(10)	2794.4(7)	27.9(3)

Table S38 Anisotropic Displacement Parameters ($Å^2×10^3$) for 231041lt_auto. The Anisotropic displacement factor exponent takes the form: $-2π^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+…]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
O21	46.1(7)	35.1(7)	34.7(7)	-7.6(5)	-10.8(5)	0.8(6)
N5	33.3(8)	27.7(7)	34.1(7)	-3.5(6)	2.2(6)	-2.8(6)
N13	27.8(7)	24.9(7)	28.2(7)	-4.1(5)	0.3(5)	-0.9(5)
N20	34.4(8)	30.1(8)	32.7(8)	-6.9(6)	-5.9(6)	1.5(6)
C1	25.7(8)	26.9(8)	30.9(8)	-2.4(6)	1.5(6)	2.9(6)
C2	24.2(7)	30.8(9)	32.4(8)	-3.0(7)	1.7(6)	2.4(7)
C3	28.5(8)	30.3(9)	30.6(8)	-6.7(6)	-0.8(6)	0.4(7)
C4	26.6(8)	27.4(8)	31.6(8)	-8.5(6)	2.1(6)	-0.6(7)
C6	31.8(9)	27.3(9)	38.3(9)	-2.7(7)	5.8(7)	-1.1(7)
C7	29.7(8)	26.8(8)	35.2(9)	-2.5(6)	4.4(7)	1.3(7)
C8	33.0(9)	29.0(9)	37.7(9)	3.6(7)	3.8(7)	2.6(7)
C9	36.0(9)	35.0(9)	33.4(9)	4.7(7)	2.7(7)	7.4(7)
C10	31.0(8)	32.3(9)	32.7(9)	-3.5(7)	0.5(6)	3.4(7)
C11	27.3(8)	28.8(8)	30.2(8)	-3.2(6)	1.1(6)	4.0(6)
C12	27.5(8)	28.0(8)	28.6(8)	0.2(6)	1.5(6)	3.0(7)
C14	24.7(8)	25.1(8)	33.3(8)	-4.9(6)	1.6(6)	0.8(6)
C15	29.4(8)	28.1(8)	34.7(9)	-3.6(7)	0.4(6)	0.9(7)
C16	33.1(9)	30.6(9)	40.5(10)	3.0(7)	1.2(7)	1.4(7)
C17	32.5(9)	35.3(9)	34.5(9)	6.2(7)	0.0(7)	3.1(7)
C18	29.7(8)	34.4(9)	31.5(8)	-1.8(7)	-0.9(6)	2.2(7)
C19	27.8(8)	27.0(8)	28.6(8)	-3.7(6)	-1.2(6)	2.1(7)

Table S39 Bond Lengths for 231041lt_auto.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
O21	N20	1.2662(17)	C6	C7	1.454(2)
N5	C4	1.387(2)	C7	C8	1.391(2)
N5	C6	1.308(2)	C7	C12	1.384(2)
N13	C4	1.3946(19)	C8	C9	1.404(2)
N13	C12	1.3695(19)	C9	C10	1.398(2)
N13	C14	1.373(2)	C10	C11	1.401(2)
N20	C19	1.357(2)	C11	C12	1.389(2)
C1	C2	1.434(2)	C11	C19	1.460(2)
C1	C14	1.430(2)	C14	C19	1.425(2)
C1	C15	1.410(2)	C15	C16	1.376(2)
C2	C3	1.427(2)	C16	C17	1.403(2)
C2	C18	1.408(2)	C17	C18	1.367(2)
C3	C4	1.359(2)			

Table S40 Bond Angles for 231041lt_auto.

Atom	Atom	Atom	Angle/˚	Atom	Atom	Atom	Angle/˚
C6	N5	C4	120.18(13)	C7	C8	C9	118.79(15)
C12	N13	C4	121.38(14)	C10	C9	C8	123.59(15)
C12	N13	C14	110.59(12)	C9	C10	C11	118.64(15)
C14	N13	C4	128.03(13)	C10	C11	C19	139.60(15)
O21	N20	C19	114.80(13)	C12	C11	C10	115.30(15)
C14	C1	C2	117.86(14)	C12	C11	C19	105.11(13)
C15	C1	C2	119.69(14)	N13	C12	C7	121.82(14)
C15	C1	C14	122.45(14)	N13	C12	C11	110.07(14)

Table S40 Bond Angles for 231041lt_auto.

Atom	Atom	Atom	Angle/˚	Atom	Atom	Atom	Angle/˚
C3	C2	C1	121.50(14)	C7	C12	C11	128.10(15)
C18	C2	C1	118.41(15)	N13	C14	C1	115.87(13)
C18	C2	C3	120.08(14)	N13	C14	C19	106.58(13)
C4	C3	C2	120.30(14)	C19	C14	C1	137.53(15)
N5	C4	N13	118.13(14)	C16	C15	C1	119.71(15)
C3	C4	N5	125.46(14)	C15	C16	C17	120.70(16)
C3	C4	N13	116.41(14)	C18	C17	C16	120.68(15)
N5	C6	C7	124.36(15)	C17	C18	C2	120.79(15)
C8	C7	C6	130.33(16)	N20	C19	C11	130.26(14)
C12	C7	C6	114.08(14)	N20	C19	C14	122.09(14)
C12	C7	C8	115.57(15)	C14	C19	C11	107.65(13)

Table S41 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for 231041lt_auto.

Atom	*x*	*y*	*z*	U(eq)
H3	3114.53	-669.88	5043.74	36
H6	2431.77	1238.21	3291.78	39
H8	-627.43	1157.85	1967.42	40
H9	-3540.95	298.32	1139.54	42
H10	-5064.01	-1059.35	1383.99	38
H15	-3587.93	-3231.75	3792.44	37
H16	-2707.53	-3911.07	4855.68	42
H17	75.08	-3242.61	5824.31	41
H18	2192.24	-1916.72	5729.78	38

Experimental

Single crystals of $C_{17}H_9N_3O$ **[231041lt_auto]** were **[]**. A suitable crystal was selected and **[]** on a **XtaLAB Synergy R, DW system, HyPix-Arc 150** diffractometer. The crystal was kept at 100.01(10) K during data collection. Using Olex2 [1], the structure was solved with the SHELXT [2] structure solution program using Intrinsic Phasing and refined with the SHELXL [3] refinement package using Least Squares minimisation.

1. Dolomanov, O.V., Bourhis, L.J., Gildea, R.J, Howard, J.A.K. & Puschmann, H. (2009), J. Appl. Cryst. 42, 339-341.
2. Sheldrick, G.M. (2015). Acta Cryst. A71, 3-8.
3. Sheldrick, G.M. (2015). Acta Cryst. C71, 3-8.

Crystal structure determination of [231041lt_auto]

Crystal Data for $C_{17}H_9N_3O$ (M =271.27 g/mol): monoclinic, space group $P2_1/c$ (no. 14), a = 3.77916(13) Å, b = 16.2226(5) Å, c = 19.1757(6) Å, β = 93.565(3)°, V = 1173.34(7) Å^3, Z = 4, T = 100.01(10) K, μ(Cu Kα) = 0.804 mm^{-1}, *Dcalc* = 1.536 g/cm^3, 6065 reflections measured (7.144° ≤ 2Θ ≤ 149.604°), 2257 unique (R_{int} = 0.0282, R_{sigma} = 0.0338) which were used in all calculations. The final R_1 was 0.0404 (I > 2σ(I)) and wR_2 was 0.1090 (all data).

Refinement model description

Number of restraints - 0, number of constraints - unknown.

Details:

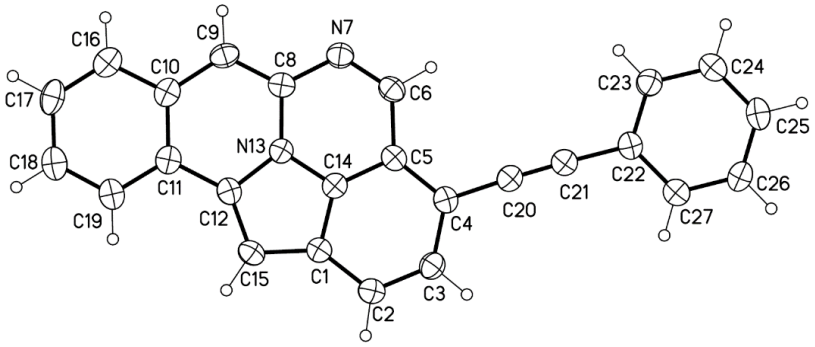
```
1. Fixed Uiso
 At 1.2 times of:
  All C(H) groups
2.a Aromatic/amide H refined with riding coordinates:
 C3(H3), C6(H6), C8(H8), C9(H9), C10(H10), C15(H15), C16(H16), C17(H17),
 C18(H18)
```

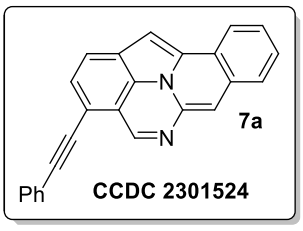
This report has been created with Olex2, compiled on 2022.04.12 svn.rca3783a0 for Rigaku Oxford Diffraction. Please let us know if there are any errors or if you would like to have additional features.

(g) X-ray crystallographic data of compound (7a)

Ellipsoid contour % probability level = 50%

Sample Preparation for Crystal Growth: The compound **7a** was dissolved in Tetrahydrofuran and kept for slow evaporation (4 days). A needle-shaped crystal was formed whose X-ray analysis was performed.





231020lt_auto

Table S42 Crystal data and structure refinement for 231020lt_auto.

Identification code	231020lt_auto
Empirical formula	$C_{25}H_{14}N_2$
Formula weight	342.38
Temperature/K	99.98(10)
Crystal system	orthorhombic
Space group	$P2_12_12_1$
a/Å	5.78180(10)
b/Å	12.8402(3)
c/Å	21.6872(5)
α/°	90
β/°	90
γ/°	90
Volume/Å^3	1610.05(6)
Z	4
ρ_{calc}g/cm^3	1.412
μ/mm^{-1}	0.647
F(000)	712.0
Crystal size/mm^3	0.17 × 0.03 × 0.02
Radiation	Cu Kα (λ = 1.54184)
2Θ range for data collection/°	8.002 to 149.586
Index ranges	-6 ≤ h ≤ 3, -15 ≤ k ≤ 15, -25 ≤ l ≤ 27
Reflections collected	9467
Independent reflections	2997 [R_{int} = 0.0356, R_{sigma} = 0.0403]
Data/restraints/parameters	2997/0/245

Goodness-of-fit on F^2	1.045
Final R indexes [I>=2σ (I)]	R_1 = 0.0404, wR_2 = 0.1029
Final R indexes [all data]	R_1 = 0.0463, wR_2 = 0.1062
Largest diff. peak/hole / e $Å^{-3}$	0.23/-0.22
Flack parameter	0.8(8)

Table S43 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters ($Å^2$×10^3) for 231020lt_auto. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
C1	6845(4)	7104(2)	3751.6(11)	26.9(5)
C2	5118(4)	7611(2)	4097.6(11)	31.2(6)
C3	3442(5)	7021(2)	4393.3(11)	31.1(6)
C4	3343(4)	5912(2)	4377.7(11)	28.0(5)
C5	5083(4)	5390.1(19)	4046.1(11)	27.4(5)
C6	5515(4)	4285(2)	3963.0(12)	29.8(6)
C8	8754(4)	4547(2)	3341.0(12)	28.3(5)
C9	10580(4)	4243(2)	2989.3(12)	31.6(6)
C10	12061(4)	5010(2)	2710.0(11)	30.1(6)
C11	11687(4)	6097(2)	2795.1(11)	28.9(5)
C12	9759(4)	6422(2)	3172.8(11)	28.0(5)
C14	6688(4)	6016.7(19)	3753.3(10)	26.2(5)
C15	8824(4)	7353(2)	3380.6(11)	29.5(5)
C16	13977(4)	4702(2)	2347.6(13)	35.2(6)
C17	15420(5)	5431(2)	2084.2(12)	37.1(6)
C18	15020(5)	6497(2)	2170.6(12)	35.9(6)

Table S43 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for 231020lt_auto. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
C19	13178(4)	6822(2)	2520.7(11)	32.7(6)
C20	1545(4)	5373(2)	4698.4(11)	29.3(5)
C21	27(4)	4951(2)	4984.4(11)	29.6(5)
C22	-1792(4)	4482(2)	5341.9(11)	28.5(5)
C23	-1853(4)	3406(2)	5441.8(12)	33.0(6)
C24	-3652(4)	2968(2)	5773.2(13)	35.9(6)
C25	-5388(4)	3584(2)	6014.6(12)	34.8(6)
C26	-5327(4)	4651(2)	5926.7(12)	33.4(6)
C27	-3555(4)	5100(2)	5588.6(11)	30.6(5)
N7	7209(4)	3894.1(17)	3638.7(10)	31.1(5)
N13	8424(3)	5614.9(16)	3411.8(9)	26.3(5)

Table S44 Anisotropic Displacement Parameters (Å^2×10^3) for 231020lt_auto. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C1	26.4(12)	28.1(12)	26.1(11)	1.0(10)	-3.3(10)	0.2(10)
C2	34.2(13)	28.5(13)	30.8(12)	0.0(10)	-1.3(11)	-0.4(11)
C3	32.1(13)	34.9(14)	26.3(12)	-1.6(11)	0.4(11)	1.8(11)
C4	27.8(12)	32.0(13)	24.1(11)	2.1(10)	-2.3(10)	-1.6(10)
C5	28.4(12)	29.1(12)	24.6(12)	2.3(10)	-4.1(11)	-2.0(11)
C6	31.0(13)	28.6(13)	29.9(13)	4.2(11)	-4.1(11)	-2.1(10)
C8	30.1(12)	27.9(12)	26.9(12)	0.0(10)	-5.2(11)	0.1(10)
C9	33.6(13)	29.9(13)	31.1(13)	-2.3(11)	-5.6(11)	6.0(11)
C10	26.7(13)	39.2(14)	24.6(12)	-1.0(11)	-4.5(10)	2.8(11)

Table S44 Anisotropic Displacement Parameters ($Å^2×10^3$) for 231020lt_auto. The Anisotropic displacement factor exponent takes the form: $-2π^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+…]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C11	27.5(13)	37.1(13)	22.1(11)	0.3(10)	-5.0(10)	0.4(11)
C12	27.9(12)	32.3(13)	23.7(11)	3.1(10)	-2.8(10)	-1.6(11)
C14	25.9(12)	29.9(12)	22.9(11)	-1.0(10)	-4.1(10)	0.6(10)
C15	32.8(13)	26.7(12)	28.9(12)	1.1(10)	-3.2(10)	-4.2(10)
C16	32.8(14)	43.3(16)	29.4(13)	-4.7(12)	-3.8(11)	4.6(12)
C17	27.3(13)	60.1(18)	23.9(12)	-0.5(12)	0.0(11)	3.5(13)
C18	28.9(13)	50.0(16)	28.8(13)	3.9(12)	-3.3(11)	-5.6(13)
C19	29.7(13)	41.8(15)	26.7(12)	3.0(11)	-3.4(10)	-4.3(12)
C20	30.1(13)	32.5(13)	25.4(12)	-0.9(10)	-1.8(11)	1.8(11)
C21	30.7(14)	31.5(12)	26.6(11)	-1.0(10)	-3.1(11)	-1.0(11)
C22	28.1(12)	33.9(13)	23.5(12)	0.5(10)	-2.3(10)	-3.3(10)
C23	31.7(13)	34.3(13)	33.1(13)	0.3(11)	0.8(11)	1.0(12)
C24	37.8(14)	32.5(13)	37.4(14)	4.3(11)	-1.6(12)	-4.0(12)
C25	29.4(13)	45.8(16)	29.2(13)	5.6(12)	0.3(11)	-5.3(12)
C26	27.7(13)	42.9(15)	29.6(13)	-4.3(11)	0.9(11)	1.9(11)
C27	30.8(13)	32.3(13)	28.8(12)	0.8(11)	-4.5(11)	-1.8(11)
N7	32.2(11)	29.9(11)	31.2(11)	2.0(9)	-2.4(9)	1.8(9)
N13	26.3(10)	28.2(10)	24.6(10)	0.5(8)	-0.8(9)	0.9(9)

Table S45 Bond Lengths for 231020lt_auto.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
C1	C2	1.408(3)	C11	C12	1.445(3)
C1	C14	1.400(3)	C11	C19	1.402(4)

Table S45 Bond Lengths for 231020lt_auto.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
C1	C15	1.435(3)	C12	C15	1.387(4)
C2	C3	1.387(4)	C12	N13	1.392(3)
C3	C4	1.425(3)	C14	N13	1.350(3)
C4	C5	1.407(3)	C16	C17	1.378(4)
C4	C20	1.430(4)	C17	C18	1.401(4)
C5	C6	1.452(4)	C18	C19	1.373(4)
C5	C14	1.383(3)	C20	C21	1.203(4)
C6	N7	1.306(3)	C21	C22	1.439(3)
C8	C9	1.360(4)	C22	C23	1.399(4)
C8	N7	1.385(3)	C22	C27	1.398(3)
C8	N13	1.393(3)	C23	C24	1.384(4)
C9	C10	1.438(4)	C24	C25	1.381(4)
C10	C11	1.425(4)	C25	C26	1.383(4)
C10	C16	1.415(4)	C26	C27	1.386(4)

Table S46 Bond Angles for 231020lt_auto.

Atom	Atom	Atom	Angle/˚	Atom	Atom	Atom	Angle/˚
C2	C1	C15	139.6(2)	N13	C12	C11	115.1(2)
C14	C1	C2	114.4(2)	C5	C14	C1	128.7(2)
C14	C1	C15	106.0(2)	N13	C14	C1	109.4(2)
C3	C2	C1	119.3(2)	N13	C14	C5	121.9(2)
C2	C3	C4	124.2(2)	C12	C15	C1	107.5(2)
C3	C4	C20	120.1(2)	C17	C16	C10	121.0(3)
C5	C4	C3	117.3(2)	C16	C17	C18	120.5(3)

Table S46 Bond Angles for 231020lt_auto.

Atom	Atom	Atom	Angle/˚	Atom	Atom	Atom	Angle/˚
C5	C4	C20	122.5(2)	C19	C18	C17	120.0(3)
C4	C5	C6	130.7(2)	C18	C19	C11	120.6(3)
C14	C5	C4	116.0(2)	C21	C20	C4	177.4(3)
C14	C5	C6	113.3(2)	C20	C21	C22	177.8(3)
N7	C6	C5	124.8(2)	C23	C22	C21	121.0(2)
C9	C8	N7	126.1(2)	C27	C22	C21	120.1(2)
C9	C8	N13	116.8(2)	C27	C22	C23	118.9(2)
N7	C8	N13	117.1(2)	C24	C23	C22	120.0(2)
C8	C9	C10	120.1(2)	C25	C24	C23	120.7(3)
C11	C10	C9	121.7(2)	C24	C25	C26	119.8(3)
C16	C10	C9	120.6(2)	C25	C26	C27	120.2(3)
C16	C10	C11	117.7(2)	C26	C27	C22	120.3(2)
C10	C11	C12	118.3(2)	C6	N7	C8	120.2(2)
C19	C11	C10	120.2(2)	C12	N13	C8	128.0(2)
C19	C11	C12	121.5(2)	C14	N13	C8	122.6(2)
C15	C12	C11	137.2(2)	C14	N13	C12	109.4(2)
C15	C12	N13	107.7(2)				

Table S47 Torsion Angles for 231020lt_auto.

A	B	C	D	Angle/˚	A	B	C	D	Angle/˚
C1	C2	C3	C4	0.6(4)	C11	C12	N13	C14	−179.92(19)
C1	C14	N13	C8	178.3(2)	C12	C11	C19	C18	179.1(2)
C1	C14	N13	C12	−0.4(3)	C14	C1	C2	C3	−1.0(3)

Table S47 Torsion Angles for 231020lt_auto.

A	B	C	D	Angle/˚	A	B	C	D	Angle/˚
C2	C1	C14	C5	0.0(4)	C14	C1	C15	C12	0.4(3)
C2	C1	C14	N13	-179.7(2)	C14	C5	C6	N7	-1.1(3)
C2	C1	C15	C12	180.0(3)	C15	C1	C2	C3	179.4(3)
C2	C3	C4	C5	0.9(4)	C15	C1	C14	C5	179.7(2)
C2	C3	C4	C20	180.0(2)	C15	C1	C14	N13	0.0(3)
C3	C4	C5	C6	177.3(2)	C15	C12	N13	C8	-177.9(2)
C3	C4	C5	C14	-1.7(3)	C15	C12	N13	C14	0.7(3)
C4	C5	C6	N7	179.8(2)	C16	C10	C11	C12	-179.0(2)
C4	C5	C14	C1	1.4(4)	C16	C10	C11	C19	0.5(3)
C4	C5	C14	N13	-178.9(2)	C16	C17	C18	C19	0.1(4)
C5	C6	N7	C8	-0.2(4)	C17	C18	C19	C11	0.1(4)
C5	C14	N13	C8	-1.4(3)	C19	C11	C12	C15	-1.1(4)
C5	C14	N13	C12	179.8(2)	C19	C11	C12	N13	179.7(2)
C6	C5	C14	C1	-177.8(2)	C20	C4	C5	C6	-1.8(4)
C6	C5	C14	N13	1.9(3)	C20	C4	C5	C14	179.2(2)
C8	C9	C10	C11	0.6(4)	C21	C22	C23	C24	-178.3(2)
C8	C9	C10	C16	179.5(2)	C21	C22	C27	C26	179.2(2)
C9	C8	N7	C6	-179.8(2)	C22	C23	C24	C25	-0.8(4)
C9	C8	N13	C12	-1.0(4)	C23	C22	C27	C26	0.1(4)
C9	C8	N13	C14	-179.4(2)	C23	C24	C25	C26	-0.2(4)
C9	C10	C11	C12	-0.1(3)	C24	C25	C26	C27	1.1(4)
C9	C10	C11	C19	179.4(2)	C25	C26	C27	C22	-1.1(4)
C9	C10	C16	C17	-179.2(2)	C27	C22	C23	C24	0.8(4)
C10	C11	C12	C15	178.3(3)	N7	C8	C9	C10	-179.5(2)
C10	C11	C12	N13	-0.8(3)	N7	C8	N13	C12	178.5(2)

Table S47 Torsion Angles for 231020lt_auto.

A	B	C	D	Angle/˚	A	B	C	D	Angle/˚
C10	C11	C19	C18	-0.4(3)	N7	C8	N13	C14	0.0(3)
C10	C16	C17	C18	0.1(4)	N13	C8	C9	C10	-0.1(3)
C11	C10	C16	C17	-0.3(4)	N13	C8	N7	C6	0.8(3)
C11	C12	C15	C1	-179.9(3)	N13	C12	C15	C1	-0.7(3)
C11	C12	N13	C8	1.5(3)					

Table S48 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for 231020lt_auto.

Atom	*x*	*y*	*z*	U(eq)
H2	5101.68	8348.94	4128.29	37
H3	2285.91	7379.15	4621.04	37
H6	4489.08	3810.73	4158.88	36
H9	10879.33	3523.18	2927.85	38
H15	9390.85	8031.49	3293.19	35
H16	14272.18	3981.9	2284.92	42
H17	16697.39	5208.19	1842.01	45
H18	16022.88	6994.04	1987.02	43
H19	12912.09	7546.17	2577.56	39
H23	-658.75	2975.34	5282.02	40
H24	-3693.99	2236.04	5835.35	43
H25	-6618.88	3276.4	6240.35	42
H26	-6505.01	5076.76	6098.77	40
H27	-3537.5	5831.44	5524.04	37

Experimental

Single crystals of $C_{25}H_{14}N_2$ **[231020lt_auto]** were **[]**. A suitable crystal was selected and **[]** on a **XtaLAB Synergy R, DW system, HyPix-Arc 150** diffractometer. The crystal was kept at 99.98(10) K during data collection. Using Olex2 [1], the structure was solved with the SHELXT [2] structure solution program using Intrinsic Phasing and refined with the SHELXL [3] refinement package using Least Squares minimisation.

1. Dolomanov, O.V., Bourhis, L.J., Gildea, R.J, Howard, J.A.K. & Puschmann, H. (2009), J. Appl. Cryst. 42, 339-341.
2. Sheldrick, G.M. (2015). Acta Cryst. A71, 3-8.
3. Sheldrick, G.M. (2015). Acta Cryst. C71, 3-8.

Crystal structure determination of [231020lt_auto]

Crystal Data for $C_{25}H_{14}N_2$ (M =342.38 g/mol): orthorhombic, space group $P2_12_12_1$ (no. 19), a = 5.78180(10) Å, b = 12.8402(3) Å, c = 21.6872(5) Å, V = 1610.05(6) Å^3, Z = 4, T = 99.98(10) K, μ(Cu Kα) = 0.647 mm^{-1}, *Dcalc* = 1.412 g/cm^3, 9467 reflections measured (8.002° ≤ 2Θ ≤ 149.586°), 2997 unique (R_{int} = 0.0356, R_{sigma} = 0.0403) which were used in all calculations. The final R_1 was 0.0404 (I > 2σ(I)) and wR_2 was 0.1062 (all data).

Refinement model description

Number of restraints - 0, number of constraints - unknown.

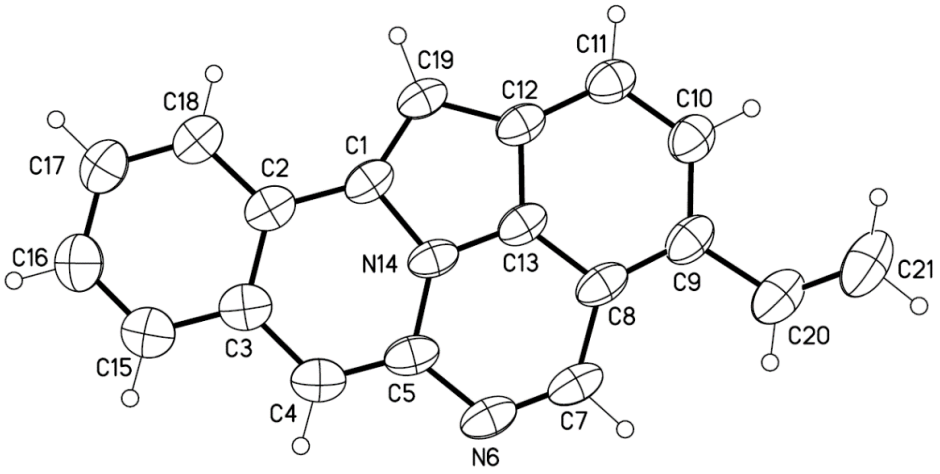
Details:

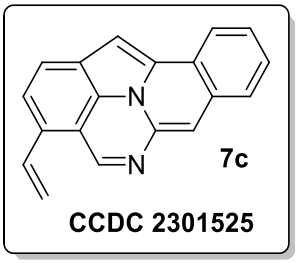
```
1. Twinned data refinement
 Scales: 0.2(8)
 0.8(8)
2. Fixed Uiso
 At 1.2 times of:
  All C(H) groups
3.a Aromatic/amide H refined with riding coordinates:
 C2(H2), C3(H3), C6(H6), C9(H9), C15(H15), C16(H16), C17(H17), C18(H18),
 C19(H19), C23(H23), C24(H24), C25(H25), C26(H26), C27(H27)
```


(h) X-ray crystallographic data of compound (7c)

Ellipsoid contour % probability level = 50%

Sample Preparation for Crystal Growth: The compound **7c** was dissolved in Tetrahydrofuran and kept for slow evaporation (5 days). A needle-shaped crystal was formed whose X-ray analysis was performed.





231019lt

Table S49 Crystal data and structure refinement for 231019lt.

Identification code	231019lt
Empirical formula	$C_{19}H_{12}N_2$
Formula weight	268.31
Temperature/K	99.9(3)
Crystal system	monoclinic
Space group	$P2_1/n$
a/Å	17.6032(6)
b/Å	3.85280(10)
c/Å	18.9019(6)
α/°	90
β/°	99.580(3)
γ/°	90
Volume/Å^3	1264.08(7)
Z	4
ρ_{calc}g/cm^3	1.410

μ/mm^{-1}	0.652
F(000)	560.0
Crystal size/mm^3	0.16 × 0.03 × 0.03
Radiation	Cu Kα (λ = 1.54184)
2Θ range for data collection/°	6.354 to 149.728
Index ranges	-21 ≤ h ≤ 21, -3 ≤ k ≤ 4, -22 ≤ l ≤ 23
Reflections collected	17727
Independent reflections	2556 [R_{int} = 0.0423, R_{sigma} = 0.0281]
Data/restraints/parameters	2556/0/190
Goodness-of-fit on F^2	1.058
Final R indexes [I>=2σ (I)]	R_1 = 0.0605, wR_2 = 0.1762
Final R indexes [all data]	R_1 = 0.0657, wR_2 = 0.1814
Largest diff. peak/hole / e Å^{-3}	0.27/-0.25

Table S50 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for 231019lt. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
C1	3712.3(11)	6775(4)	7088.0(9)	38.3(4)
C2	4231.0(11)	6605(5)	7762.7(10)	40.6(4)
C3	4971.6(11)	5066(5)	7785.6(11)	43.7(5)
C4	5201.4(11)	3634(5)	7144.9(11)	45.1(5)
C5	4712.3(11)	3730(5)	6512.1(11)	41.8(5)
C7	4327.4(12)	2638(5)	5286.2(11)	44.7(5)
C8	3580.6(11)	4294(4)	5246.5(10)	42.2(5)
C9	2979.8(12)	4776(5)	4678.5(10)	45.4(5)
C10	2305.2(12)	6458(5)	4820.8(10)	45.6(5)

Table S50 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for 231019lt. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
C11	2209.6(12)	7681(5)	5495.4(10)	44.0(5)
C12	2810.3(11)	7258(4)	6079.6(10)	39.1(4)
C13	3461.7(11)	5568(4)	5913.3(9)	38.3(4)
C15	5472.9(12)	4909(5)	8450.6(11)	50.6(5)
C16	5246.3(13)	6208(6)	9064.1(12)	53.5(5)
C17	4521.8(12)	7715(5)	9033.4(11)	49.5(5)
C18	4021.2(12)	7918(5)	8396.1(10)	44.1(5)
C19	2982.8(10)	8004(4)	6831.0(9)	38.8(4)
C20	3047.3(15)	3527(5)	3949.2(11)	55.8(6)
C21	2571.3(17)	4240(6)	3360.9(12)	69.8(7)
N6	4850.3(10)	2368(4)	5863.4(9)	46.5(4)
N14	3999.4(8)	5287(4)	6505.3(8)	37.5(4)

Table S51 Anisotropic Displacement Parameters (Å^2×10^3) for 231019lt. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C1	50.2(10)	29.2(8)	40.7(9)	-0.1(7)	22.5(8)	-4.4(7)
C2	47.8(10)	30.7(8)	47.2(10)	0.9(7)	19.4(8)	-5.6(7)
C3	45.5(10)	33.1(9)	55.1(11)	4.0(8)	16.2(8)	-5.3(7)
C4	43.3(10)	37.1(9)	58.2(12)	6.3(8)	17.8(8)	1.0(8)
C5	45.3(10)	31.2(9)	54.7(11)	2.7(7)	24.9(8)	0.6(7)
C7	58.0(11)	32.1(9)	52.1(11)	0.0(8)	32.7(9)	0.7(8)
C8	57.0(11)	30.6(9)	45.9(10)	0.7(7)	28.6(9)	-1.5(8)
C9	65.4(12)	34.6(9)	41.3(10)	0.7(7)	24.1(9)	-2.5(8)

Table S51 Anisotropic Displacement Parameters ($Å^2×10^3$) for 231019lt. The Anisotropic displacement factor exponent takes the form: $-2π^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+…]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C10	59.2(11)	38.7(9)	41.3(10)	3.5(7)	15.2(8)	1.8(8)
C11	53.0(11)	36.6(9)	46.2(10)	2.8(8)	19.5(8)	3.4(8)
C12	49.4(10)	30.5(8)	42.3(9)	2.3(7)	22.3(8)	-0.2(7)
C13	49.8(10)	28.6(8)	41.6(9)	0.6(7)	22.8(8)	-2.4(7)
C15	50.5(11)	41.6(10)	60.7(13)	3.5(9)	12.0(9)	-4.4(8)
C16	60.5(12)	47.8(11)	50.9(11)	1.4(9)	5.3(9)	-10.0(9)
C17	60.2(12)	43.4(11)	46.8(11)	-3.4(8)	14.0(9)	-9.7(9)
C18	53.5(11)	36.2(9)	46.0(10)	-1.8(7)	18.4(8)	-6.3(8)
C19	48.5(10)	30.6(8)	42.6(9)	0.4(7)	22.8(8)	1.3(7)
C20	82.8(15)	40.4(10)	50.1(12)	-0.9(8)	28.5(11)	-0.4(10)
C21	114(2)	53.9(13)	47.2(12)	-7.5(10)	28.8(13)	-6.7(13)
N6	55.9(10)	37.2(8)	54.0(10)	1.5(7)	31.6(8)	0.8(7)
N14	42.2(8)	30.0(7)	45.4(8)	1.7(6)	22.6(7)	0.6(6)

Table S52 Bond Lengths for 231019lt.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
C1	C2	1.441(3)	C8	C13	1.401(2)
C1	C19	1.379(3)	C9	C10	1.417(3)
C1	N14	1.408(2)	C9	C20	1.483(3)
C2	C3	1.426(3)	C10	C11	1.396(3)
C2	C18	1.405(3)	C11	C12	1.405(3)
C3	C4	1.448(3)	C12	C13	1.399(2)
C3	C15	1.412(3)	C12	C19	1.431(3)

Table S52 Bond Lengths for 231019lt.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
C4	C5	1.353(3)	C13	N14	1.344(2)
C5	N6	1.392(2)	C15	C16	1.381(3)
C5	N14	1.389(2)	C16	C17	1.394(3)
C7	C8	1.452(3)	C17	C18	1.371(3)
C7	N6	1.309(3)	C20	C21	1.305(3)
C8	C9	1.389(3)			

Table S53 Bond Angles for 231019lt.

Atom	Atom	Atom	Angle/˚	Atom	Atom	Atom	Angle/˚
C19	C1	C2	137.98(16)	C10	C9	C20	121.59(19)
C19	C1	N14	107.39(16)	C11	C10	C9	124.05(19)
N14	C1	C2	114.63(16)	C10	C11	C12	119.29(18)
C3	C2	C1	119.14(17)	C11	C12	C19	139.81(17)
C18	C2	C1	121.35(17)	C13	C12	C11	114.53(16)
C18	C2	C3	119.51(19)	C13	C12	C19	105.66(17)
C2	C3	C4	120.94(18)	C12	C13	C8	128.03(19)
C15	C3	C2	118.52(18)	N14	C13	C8	122.07(17)
C15	C3	C4	120.53(18)	N14	C13	C12	109.90(15)
C5	C4	C3	120.24(17)	C16	C15	C3	120.5(2)
C4	C5	N6	126.15(17)	C15	C16	C17	120.4(2)
C4	C5	N14	117.44(17)	C18	C17	C16	120.67(19)
N14	C5	N6	116.40(17)	C17	C18	C2	120.43(19)
N6	C7	C8	125.66(17)	C1	C19	C12	108.17(16)
C9	C8	C7	131.71(17)	C21	C20	C9	125.7(2)

Table S53 Bond Angles for 231019lt.

Atom	Atom	Atom	Angle/˚	Atom	Atom	Atom	Angle/˚
C9	C8	C13	116.12(17)	C7	N6	C5	120.17(16)
C13	C8	C7	112.16(18)	C5	N14	C1	127.59(17)
C8	C9	C10	117.96(17)	C13	N14	C1	108.88(14)
C8	C9	C20	120.45(19)	C13	N14	C5	123.53(15)

Table S54 Torsion Angles for 231019lt.

A	B	C	D	Angle/˚	A	B	C	D	Angle/˚
C1	C2	C3	C4	-1.0(3)	C10	C11	C12	C19	-179.8(2)
C1	C2	C3	C15	179.82(15)	C11	C12	C13	C8	0.3(3)
C1	C2	C18	C17	179.66(16)	C11	C12	C13	N14	-179.86(14)
C2	C1	C19	C12	-179.32(19)	C11	C12	C19	C1	179.3(2)
C2	C1	N14	C5	-0.3(2)	C12	C13	N14	C1	0.51(19)
C2	C1	N14	C13	179.22(13)	C12	C13	N14	C5	-179.92(15)
C2	C3	C4	C5	-0.2(3)	C13	C8	C9	C10	-0.6(3)
C2	C3	C15	C16	0.3(3)	C13	C8	C9	C20	179.91(16)
C3	C2	C18	C17	-0.2(3)	C13	C12	C19	C1	-0.02(19)
C3	C4	C5	N6	-178.05(17)	C15	C3	C4	C5	178.65(16)
C3	C4	C5	N14	1.0(3)	C15	C16	C17	C18	0.3(3)
C3	C15	C16	C17	-0.5(3)	C16	C17	C18	C2	0.1(3)
C4	C3	C15	C16	-178.59(18)	C18	C2	C3	C4	178.94(16)

Table S54 Torsion Angles for 231019lt.

A	B	C	D	Angle/˚	A	B	C	D	Angle/˚
C4	C5	N6	C7	−179.87(17)	C18	C2	C3	C15	0.1(3)
C4	C5	N14	C1	−0.8(3)	C19	C1	C2	C3	−179.2(2)
C4	C5	N14	C13	179.73(15)	C19	C1	C2	C18	0.9(3)
C7	C8	C9	C10	178.54(18)	C19	C1	N14	C5	179.94(16)
C7	C8	C9	C20	−0.9(3)	C19	C1	N14	C13	−0.51(19)
C7	C8	C13	C12	−179.03(16)	C19	C12	C13	C8	179.80(17)
C7	C8	C13	N14	1.1(2)	C19	C12	C13	N14	−0.30(19)
C8	C7	N6	C5	0.1(3)	C20	C9	C10	C11	179.93(18)
C8	C9	C10	C11	0.5(3)	N6	C5	N14	C1	178.37(15)
C8	C9	C20	C21	−170.1(2)	N6	C5	N14	C13	−1.1(2)
C8	C13	N14	C1	−179.59(15)	N6	C7	C8	C9	179.67(18)
C8	C13	N14	C5	0.0(3)	N6	C7	C8	C13	−1.2(3)
C9	C8	C13	C12	0.3(3)	N14	C1	C2	C3	1.2(2)
C9	C8	C13	N14	−179.59(15)	N14	C1	C2	C18	−178.74(15)
C9	C10	C11	C12	0.1(3)	N14	C1	C19	C12	0.32(19)
C10	C9	C20	C21	10.5(3)	N14	C5	N6	C7	1.1(2)
C10	C11	C12	C13	−0.4(3)					

Table S55 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for 231019lt.

Atom	*x*	*y*	*z*	U(eq)
H4	5697.34	2623.87	7169.06	54

Table S55 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for 231019lt.

Atom	*x*	*y*	*z*	U(eq)
H7	4447	1667.24	4856.01	54
H10	1892.58	6772.77	4432.91	55
H11	1743.45	8787.77	5559.12	53
H15	5969.38	3902.11	8476.4	61
H16	5586.5	6074.34	9509.61	64
H17	4373.15	8610.46	9458.32	59
H18	3529.27	8953.71	8382.89	53
H19	2652	9148.44	7105.25	47
H20	3474.5	2081.92	3906.5	67
H21A	2136.07	5675.77	3378.31	84
H21B	2660.16	3322.82	2915.33	84

Experimental

Single crystals of $C_{19}H_{12}N_2$ **[231019lt]** were **[]**. A suitable crystal was selected and **[]** on a **XtaLAB Synergy R, DW system, HyPix-Arc 150** diffractometer. The crystal was kept at 99.9(3) K during data collection. Using Olex2 [1], the structure was solved with the SHELXT [2] structure solution program using Intrinsic Phasing and refined with the SHELXL [3] refinement package using Least Squares minimisation.

1. Dolomanov, O.V., Bourhis, L.J., Gildea, R.J, Howard, J.A.K. & Puschmann, H. (2009), J. Appl. Cryst. 42, 339-341.
2. Sheldrick, G.M. (2015). Acta Cryst. A71, 3-8.
3. Sheldrick, G.M. (2015). Acta Cryst. C71, 3-8.

Crystal structure determination of [231019lt]

Crystal Data for $C_{19}H_{12}N_2$ (M =268.31 g/mol): monoclinic, space group $P2_1/n$ (no. 14), a = 17.6032(6) Å, b = 3.85280(10) Å, c = 18.9019(6) Å, β = 99.580(3)°, V = 1264.08(7) Å^3, Z = 4, T = 99.9(3) K, μ(Cu Kα) = 0.652 mm^{-1}, *Dcalc* = 1.410 g/cm^3, 17727 reflections measured (6.354° ≤ 2Θ ≤ 149.728°), 2556 unique (R_{int} = 0.0423, R_{sigma} = 0.0281) which were used in all calculations. The final R_1 was 0.0605 (I > 2σ(I)) and wR_2 was 0.1814 (all data).

Refinement model description

Number of restraints - 0, number of constraints - unknown.

Details:

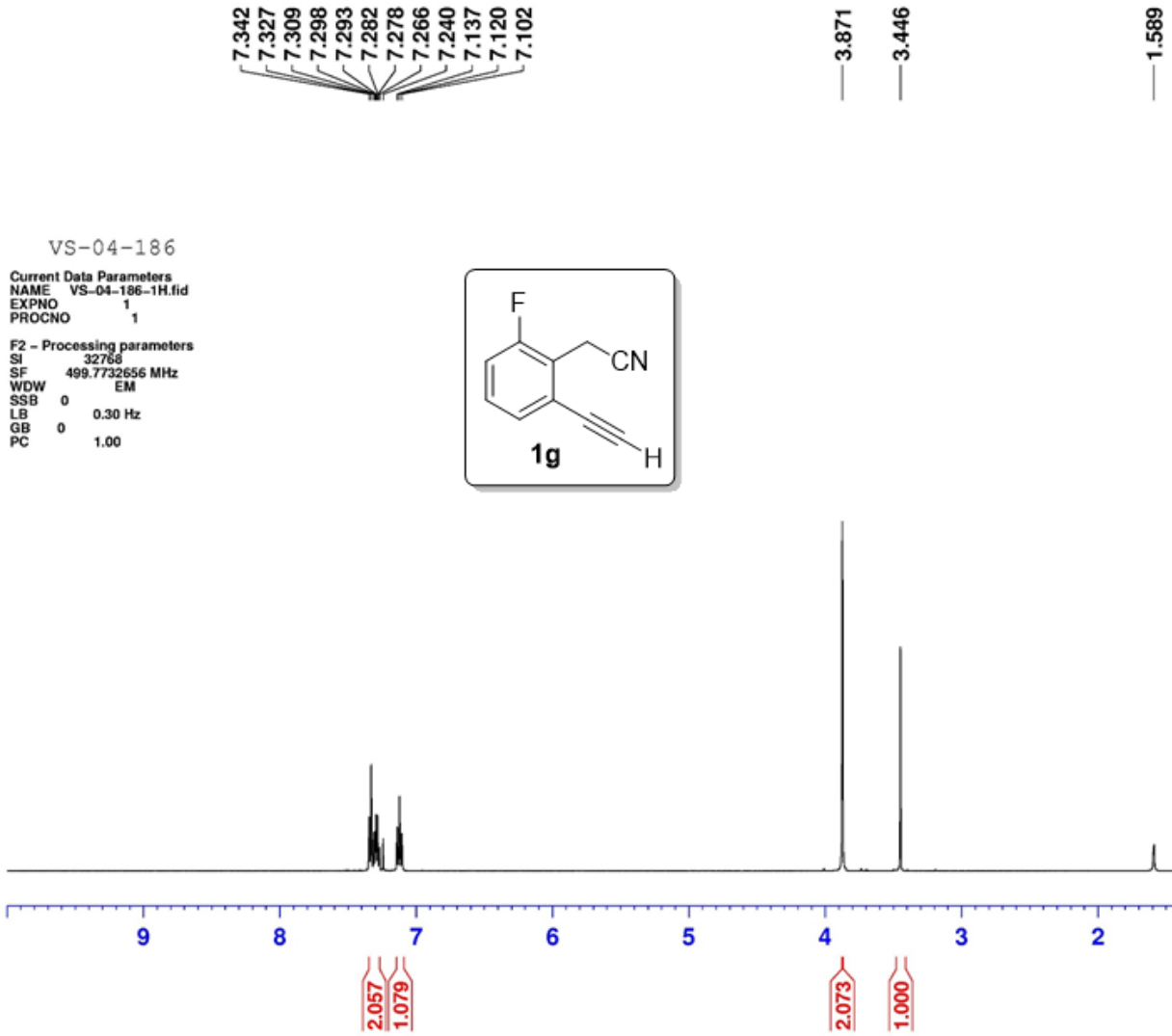
```
1. Fixed Uiso
 At 1.2 times of:
  All C(H) groups, All C(H,H) groups
2.a Aromatic/amide H refined with riding coordinates:
 C4(H4), C7(H7), C10(H10), C11(H11), C15(H15), C16(H16), C17(H17), C18(H18),
 C19(H19), C20(H20)
```

```
2.b X=CH2 refined with riding coordinates:
 C21(H21A,H21B)
```

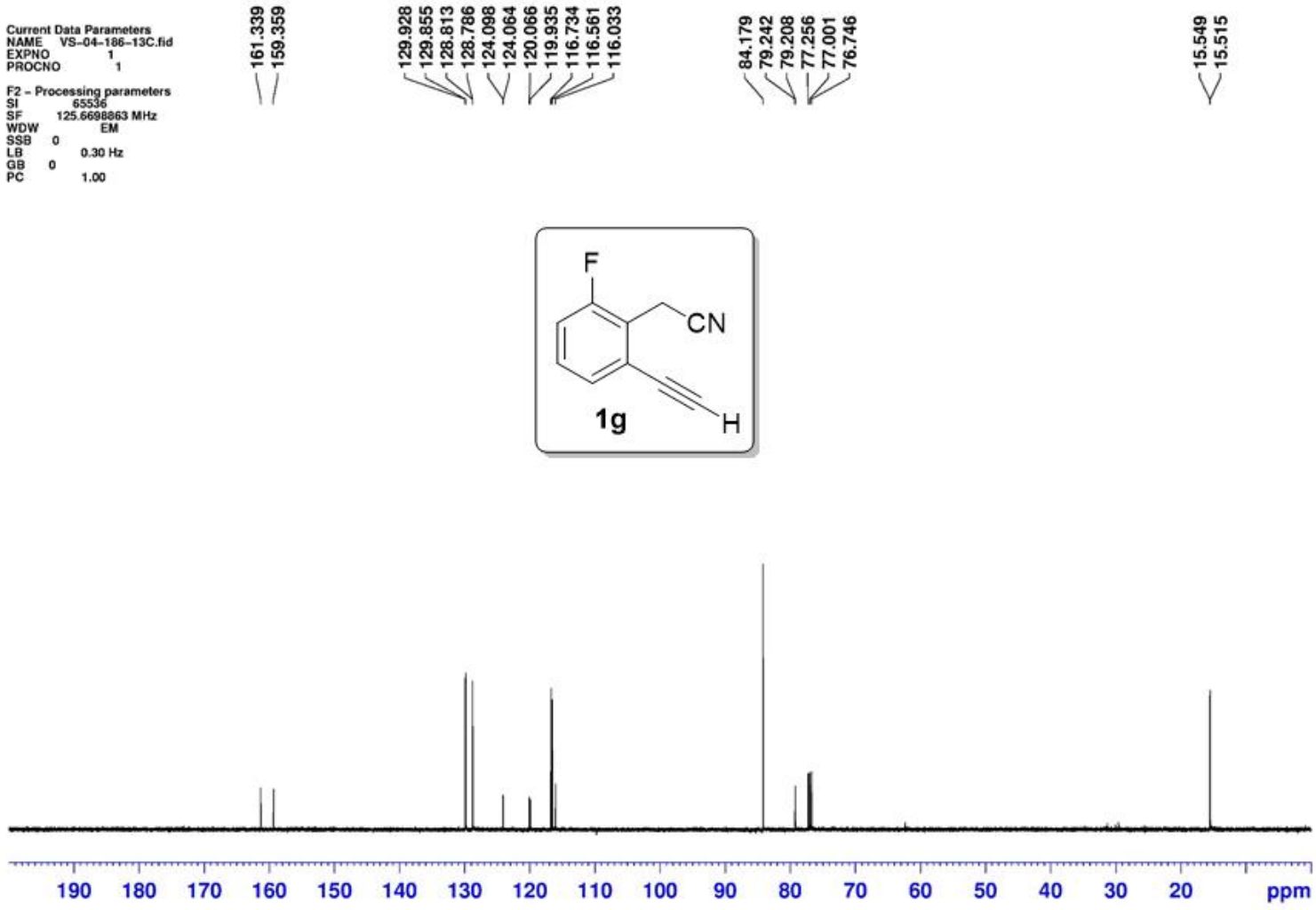
This report has been created with Olex2, compiled on 2023.08.24 svn.re1ec1418 for OlexSys. Please let us know if there are any errors or if you would like to have additional features.

10. ^{1}H,^{13}C spectra of key compounds

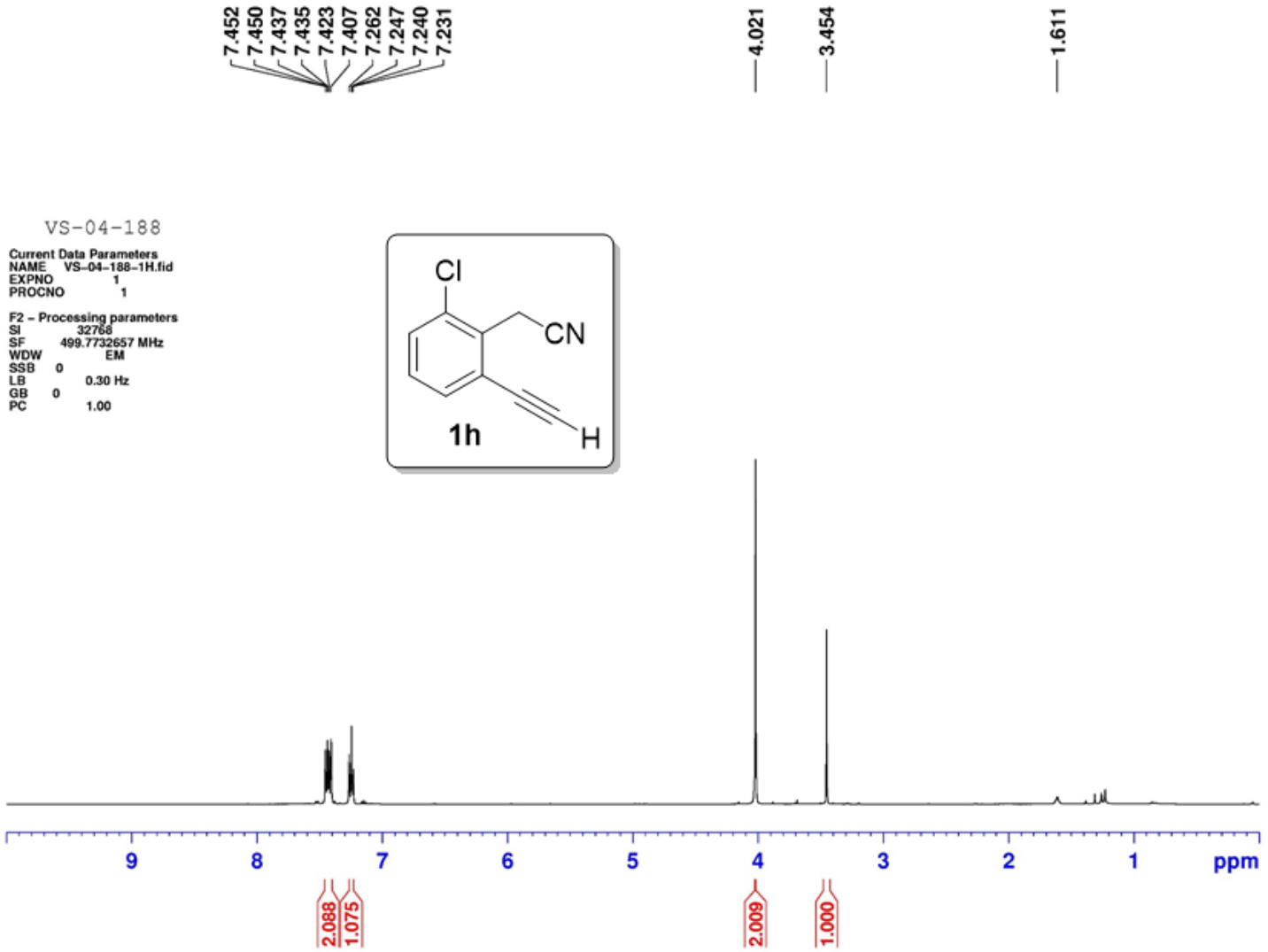
^{1}H-NMR (500 MHz, $CDCl_3$)



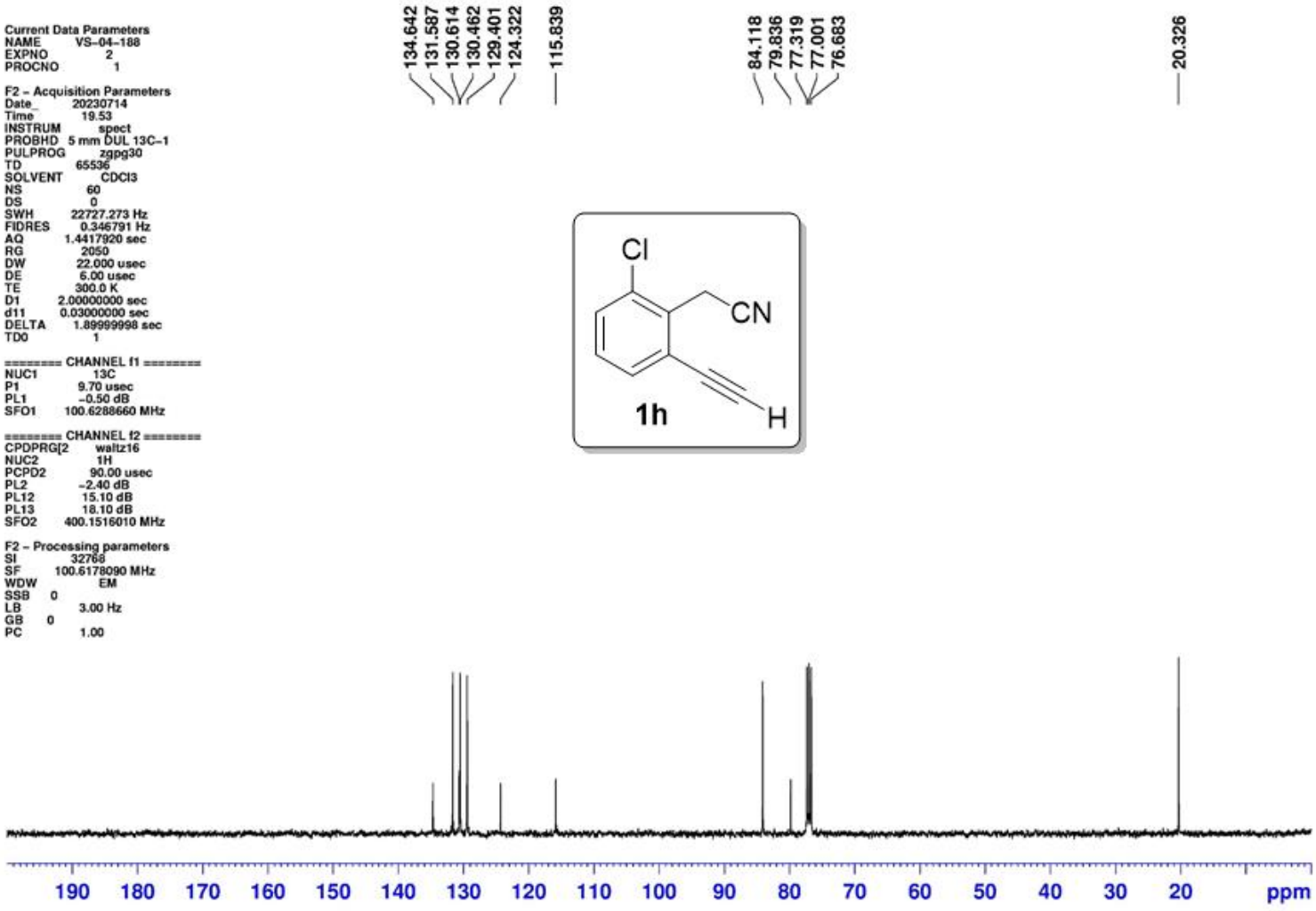
$^{13}C\{^{1}H\}$ NMR (125 MHz, $CDCl_3$)



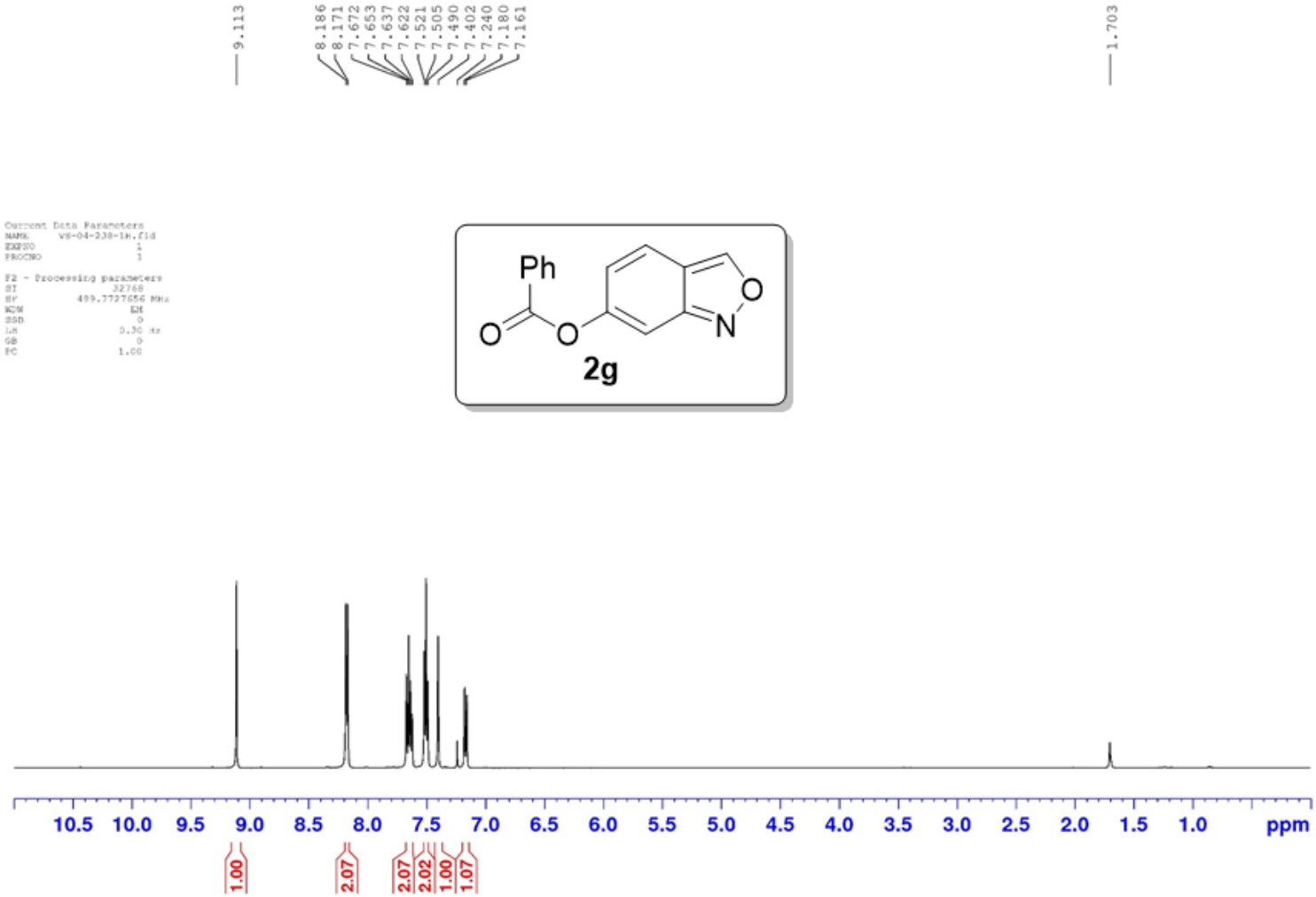
^{1}H-NMR (500 MHz, $CDCl_3$)



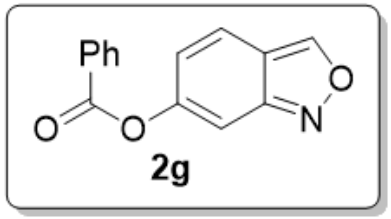
$^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$)



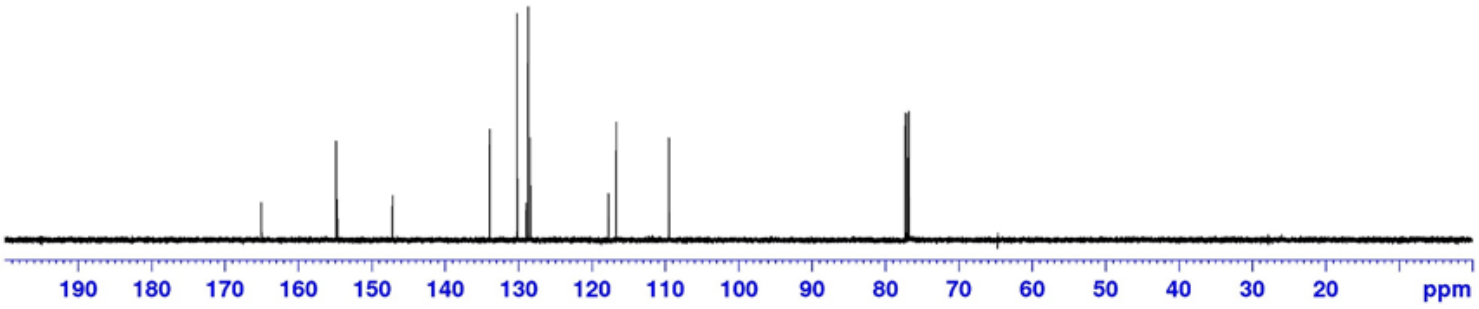
^{1}H-NMR (500 MHz, $CDCl_3$)



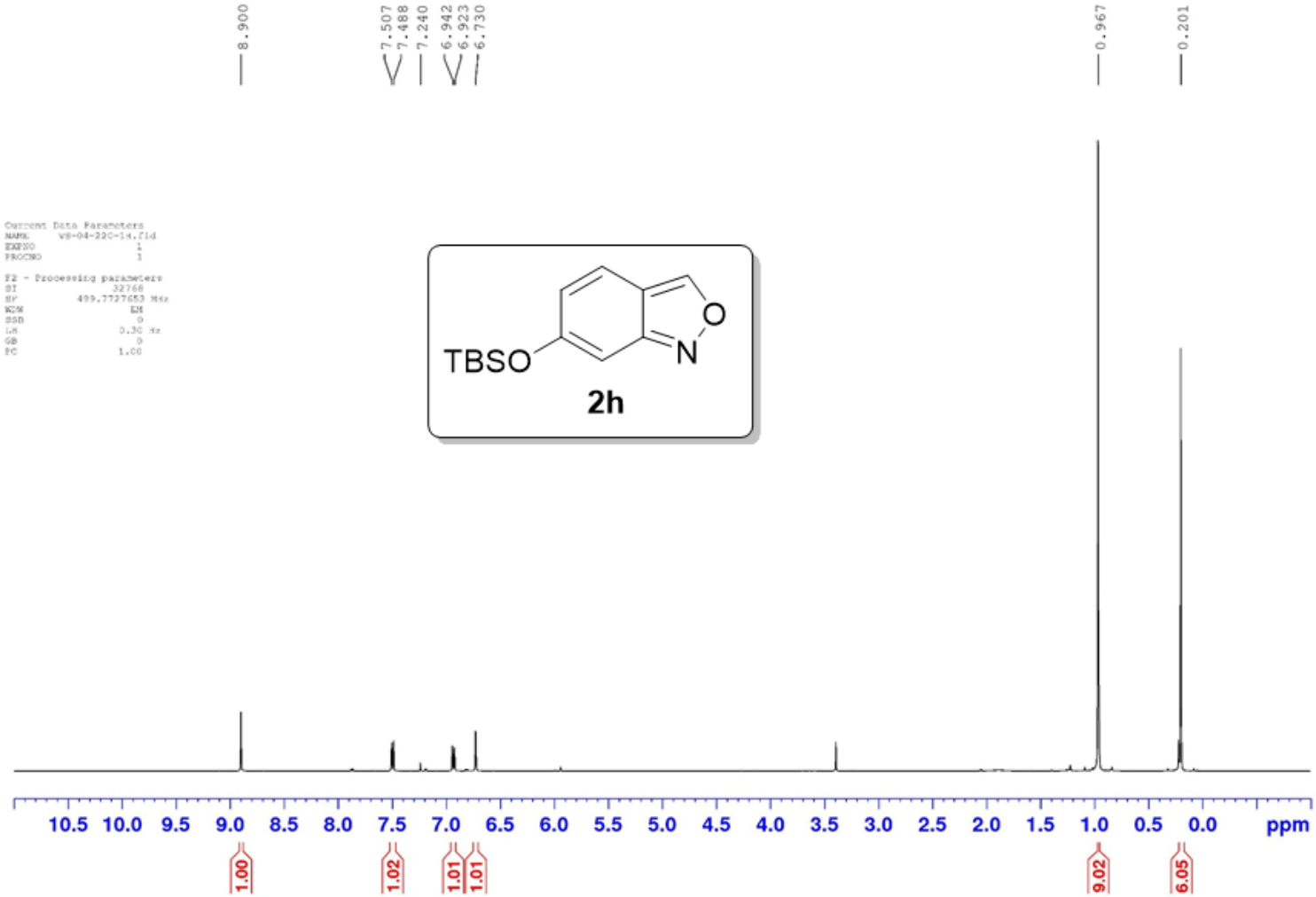
$^{13}C\{^{1}H\}$ NMR (125 MHz, $CDCl_3$)



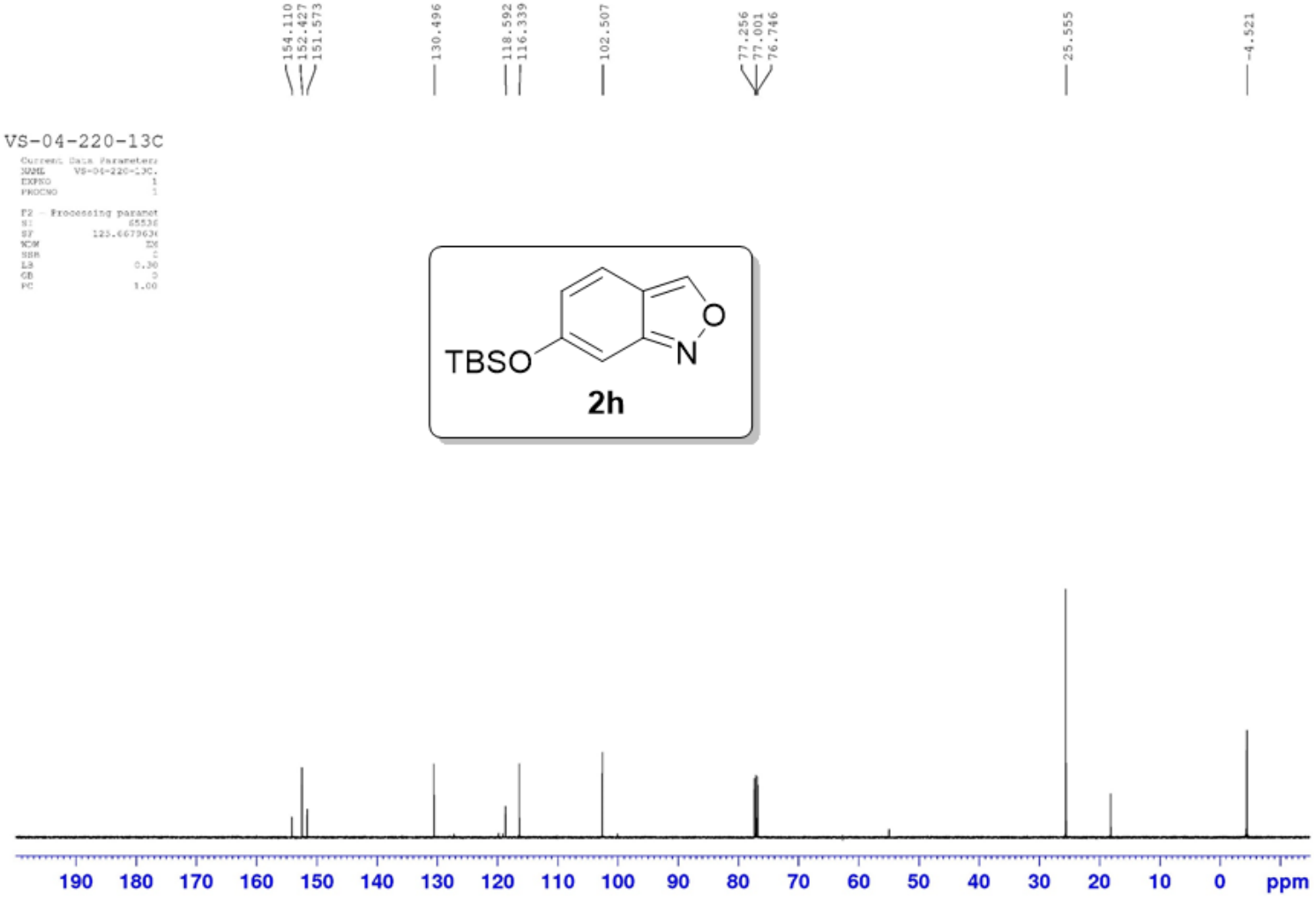
2g



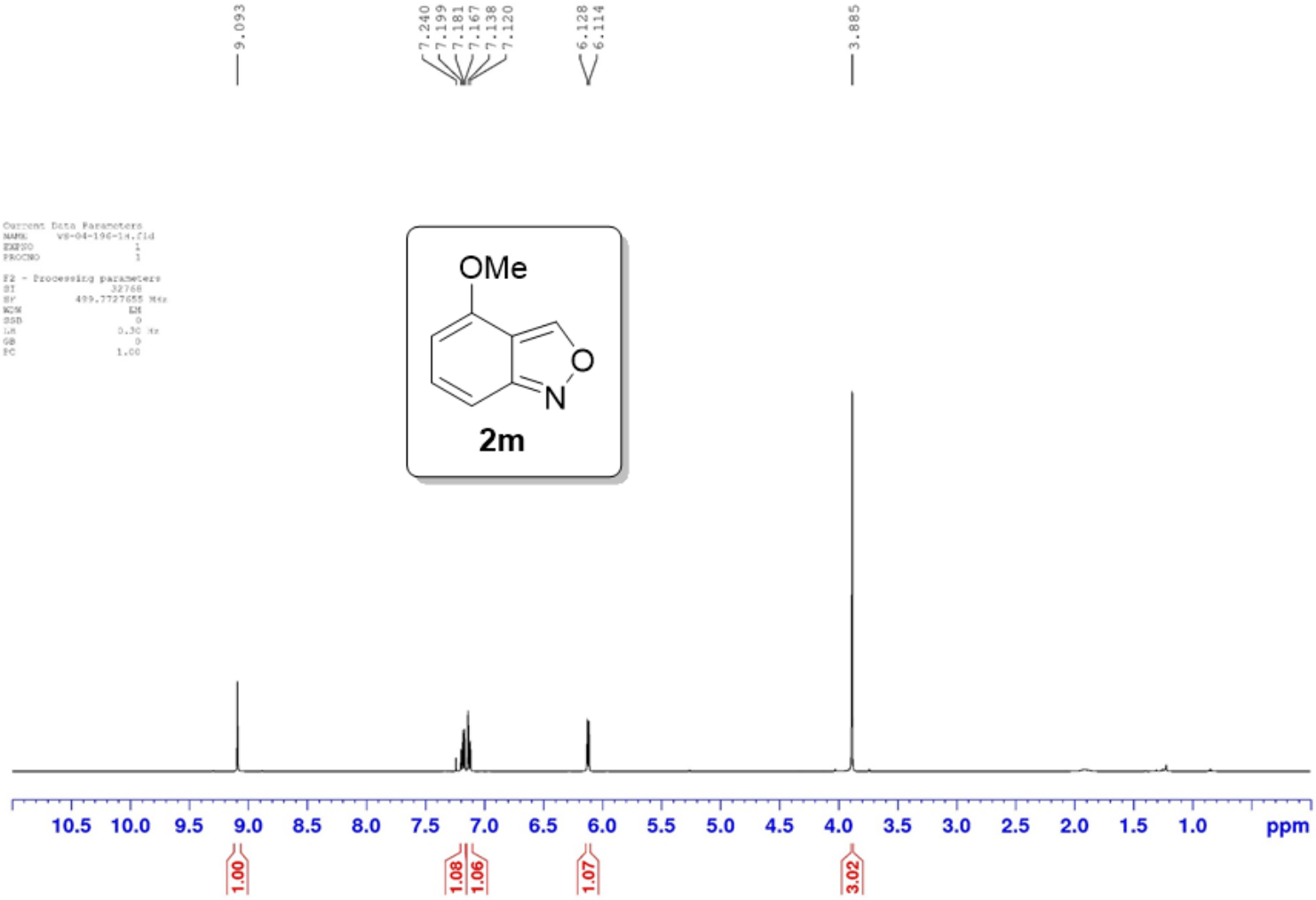
^{1}H-NMR (500 MHz, $CDCl_3$)



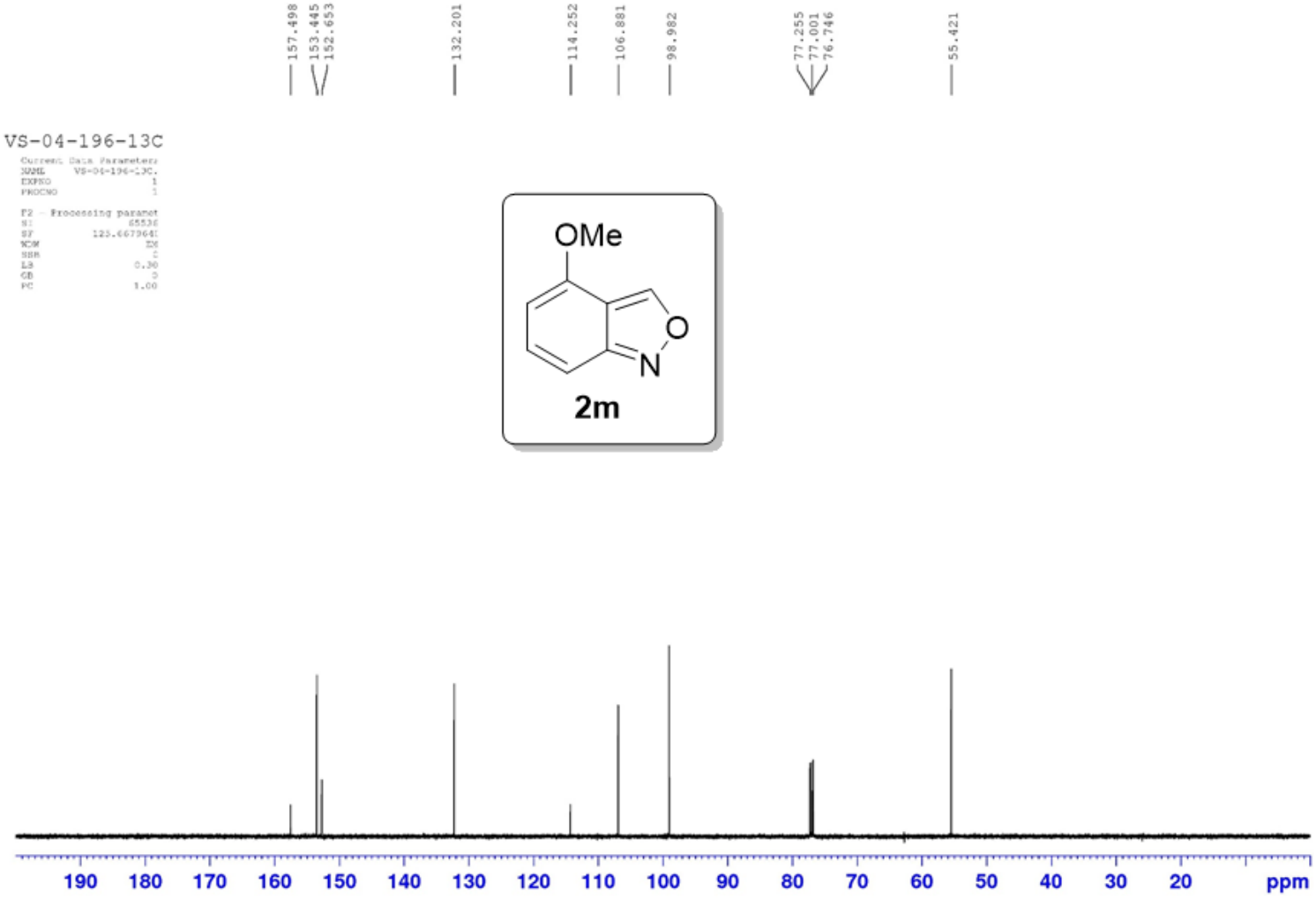
$^{13}C\{^{1}H\}$ NMR (125 MHz, $CDCl_3$)



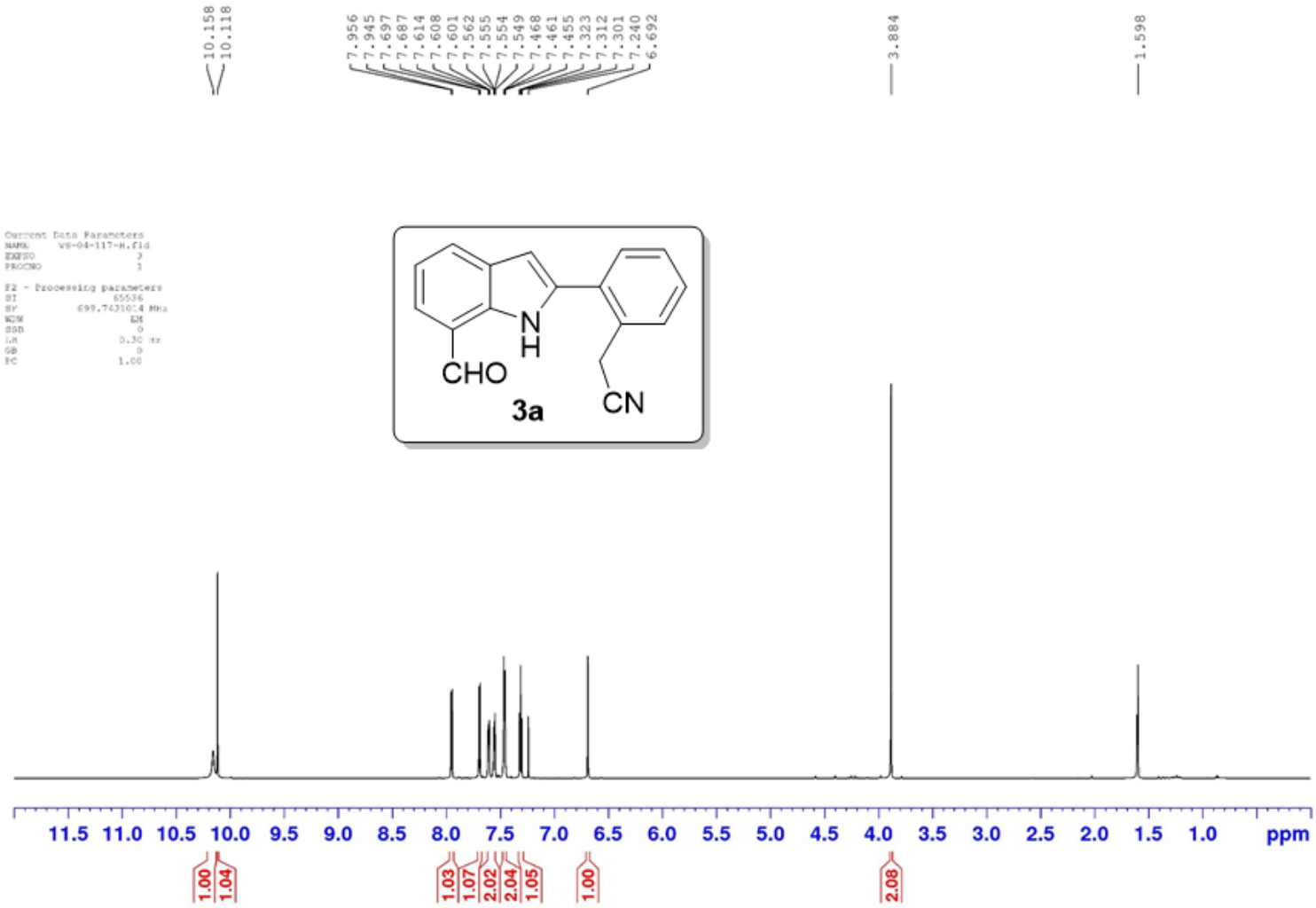
^{1}H-NMR (500 MHz, $CDCl_3$)



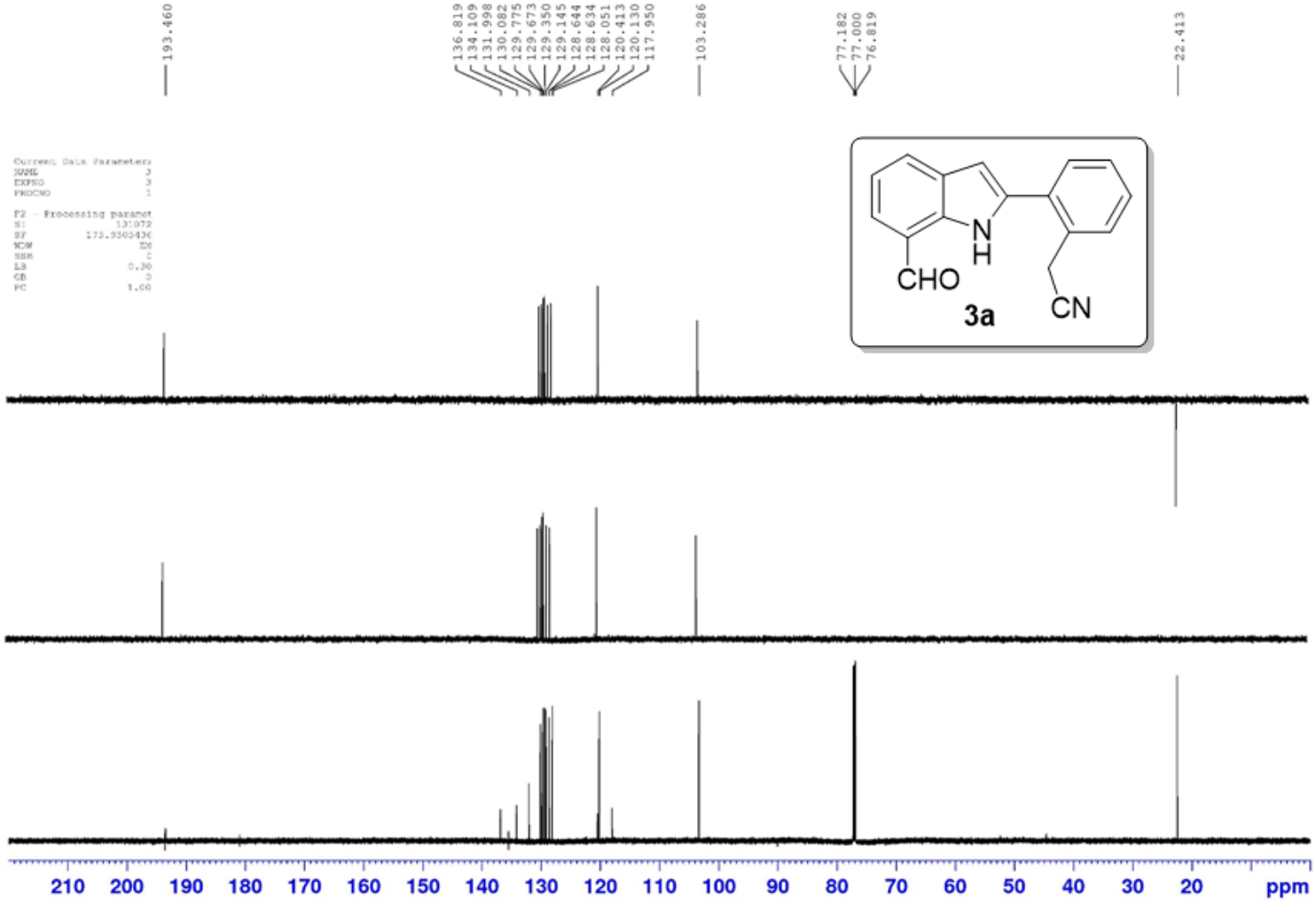
$^{13}C\{^{1}H\}$ NMR (125 MHz, $CDCl_3$)



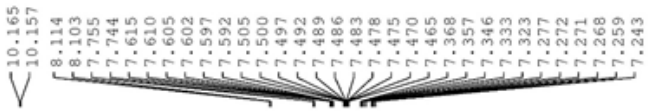
^{1}H-NMR (700 MHz, $CDCl_3$)

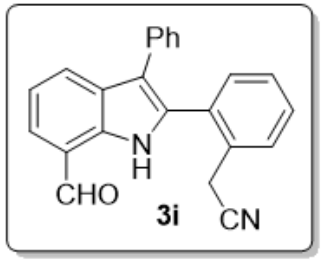


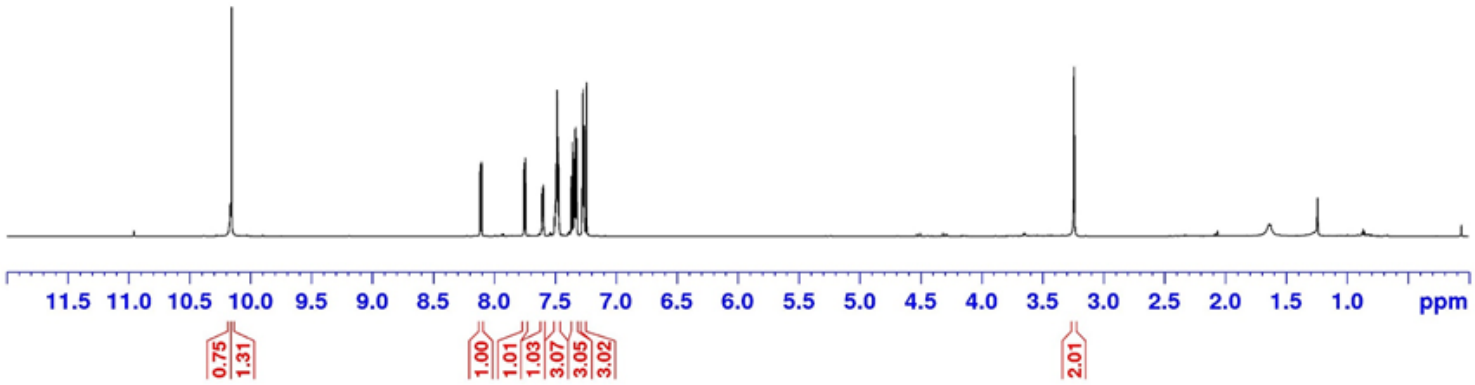
$^{13}C\{^{1}H\}$ and DEPT NMR (175 MHz, $CDCl_3$)



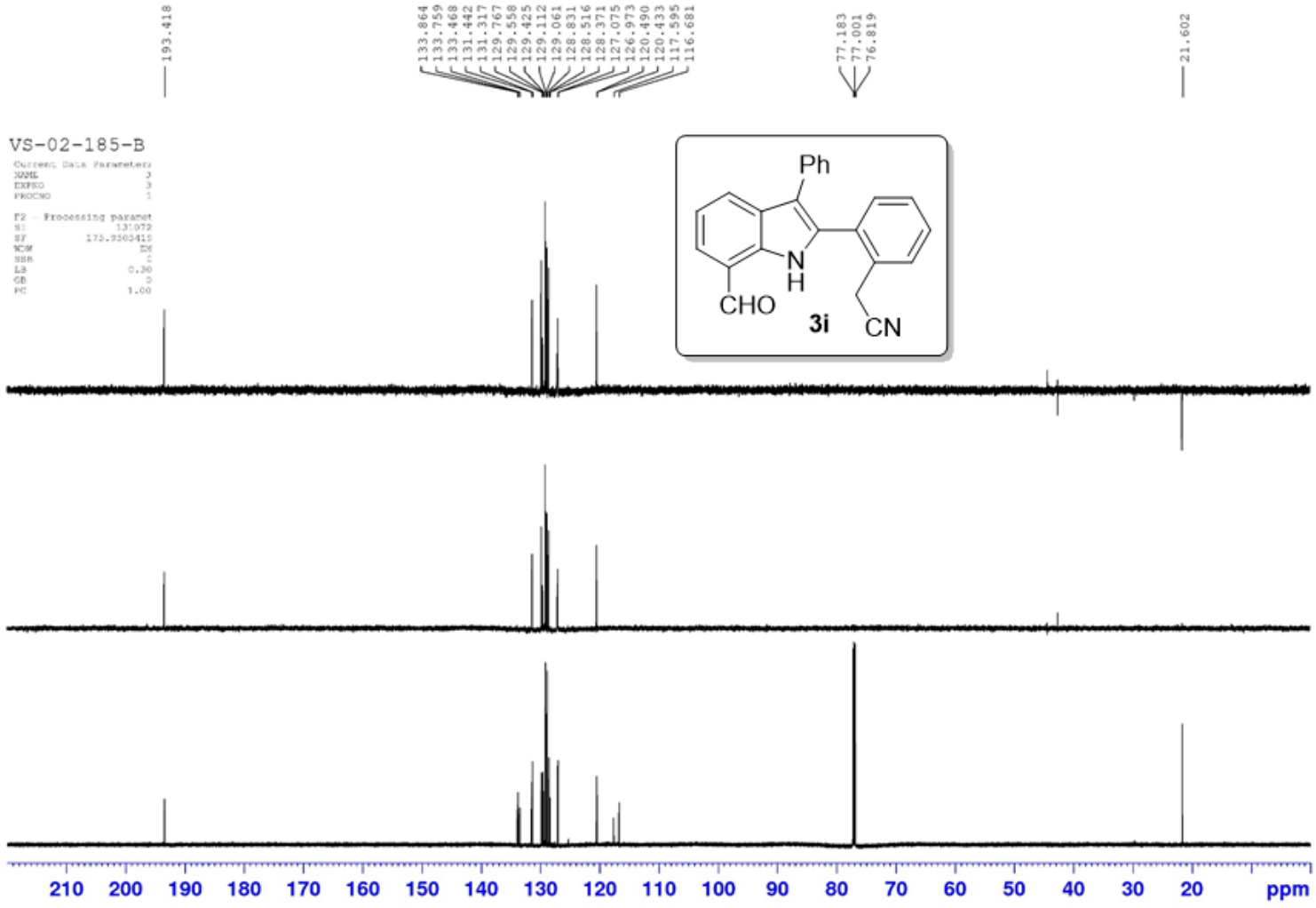
^{1}H-NMR (700 MHz, $CDCl_3$)



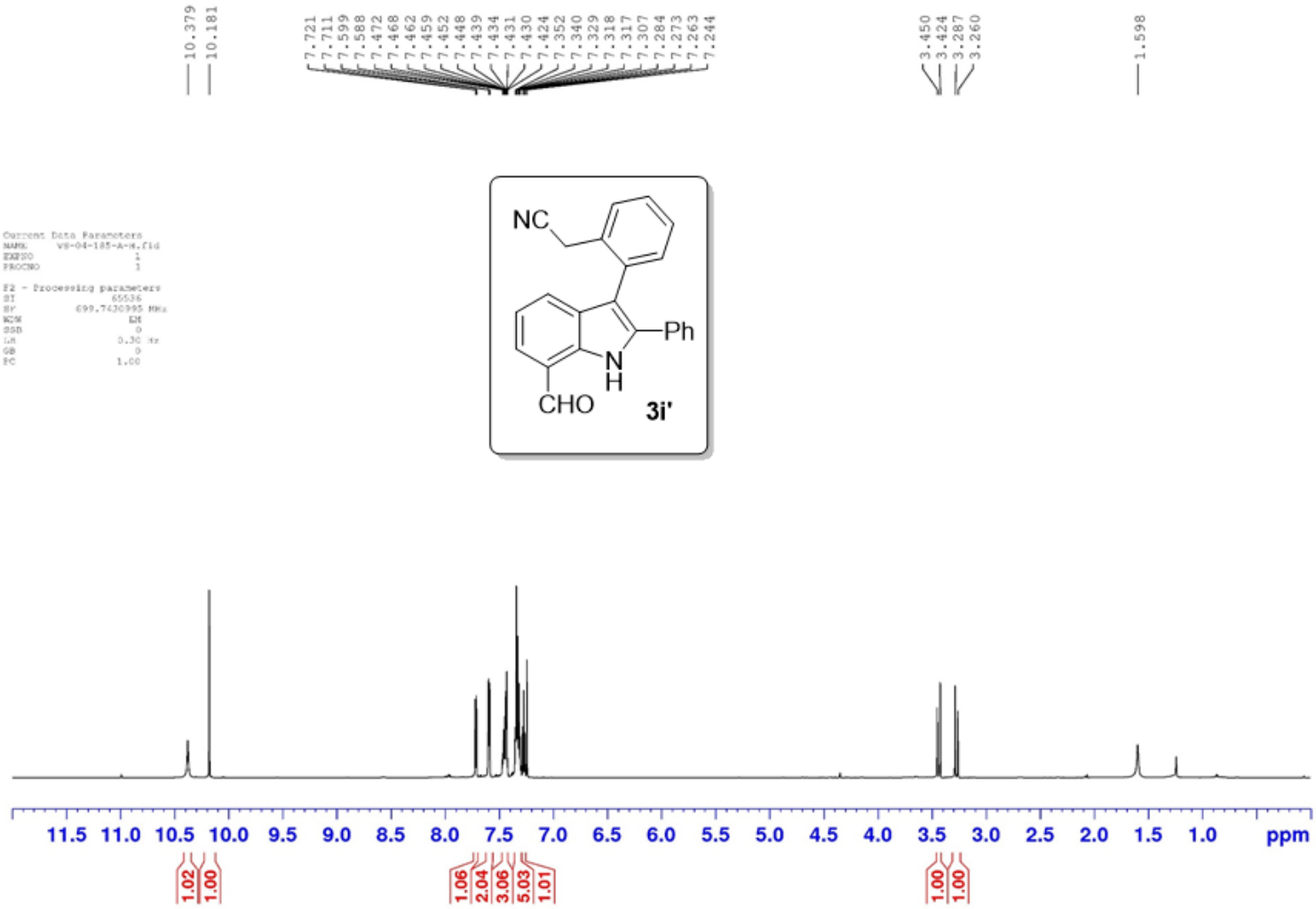




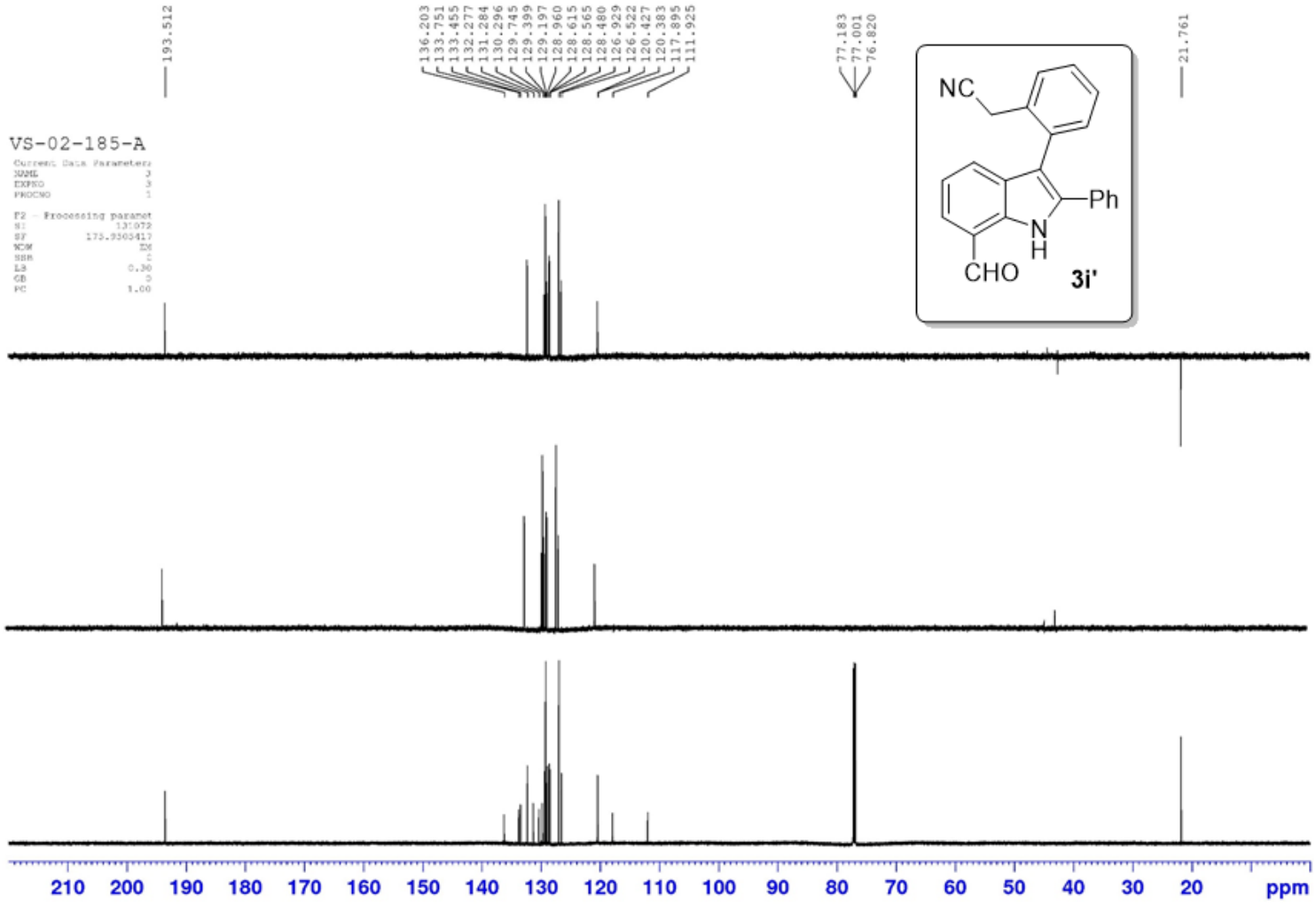
$^{13}C\{^{1}H\}$ and DEPT NMR (175 MHz, $CDCl_3$)



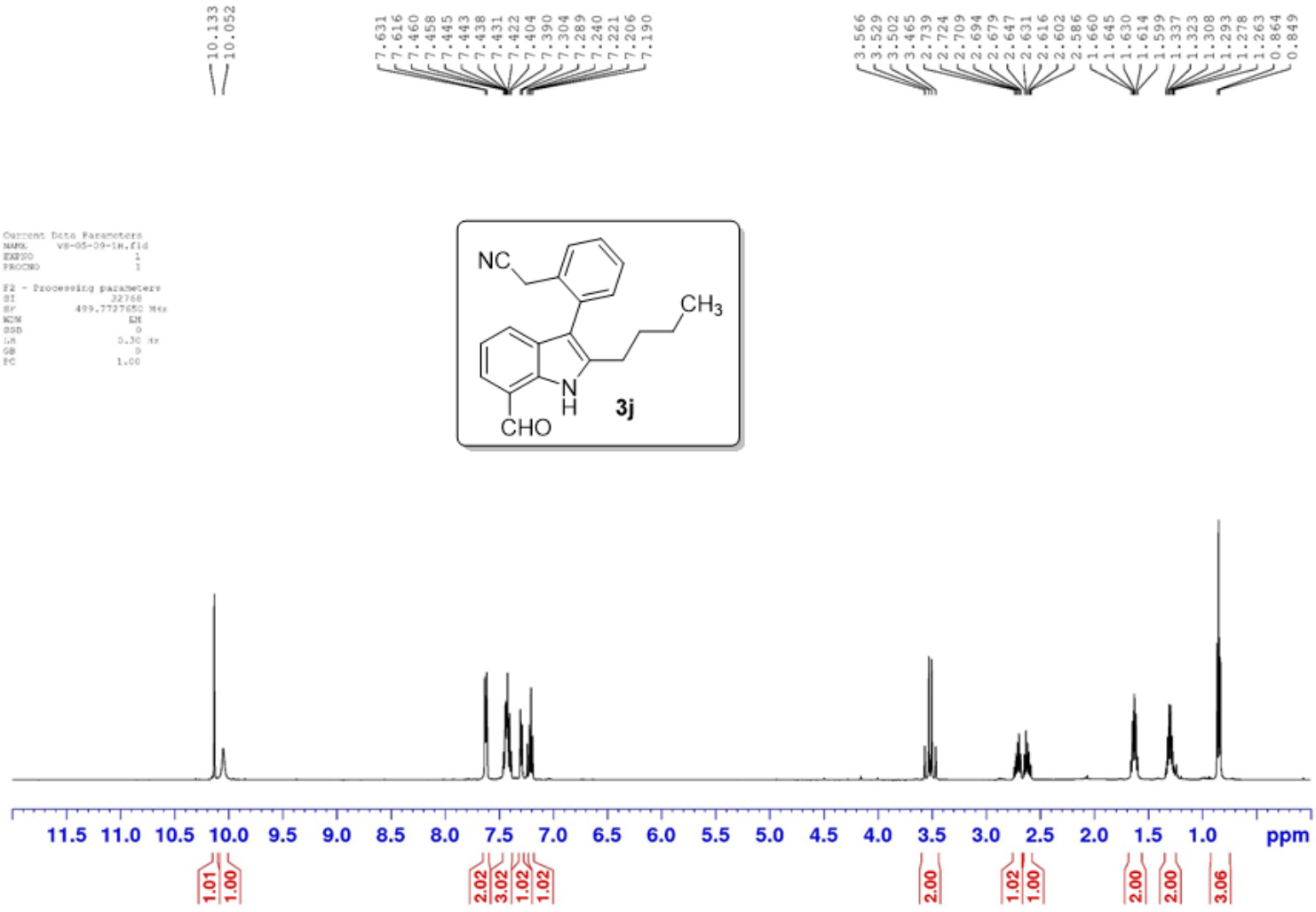
^{1}H-NMR (700 MHz, $CDCl_3$)



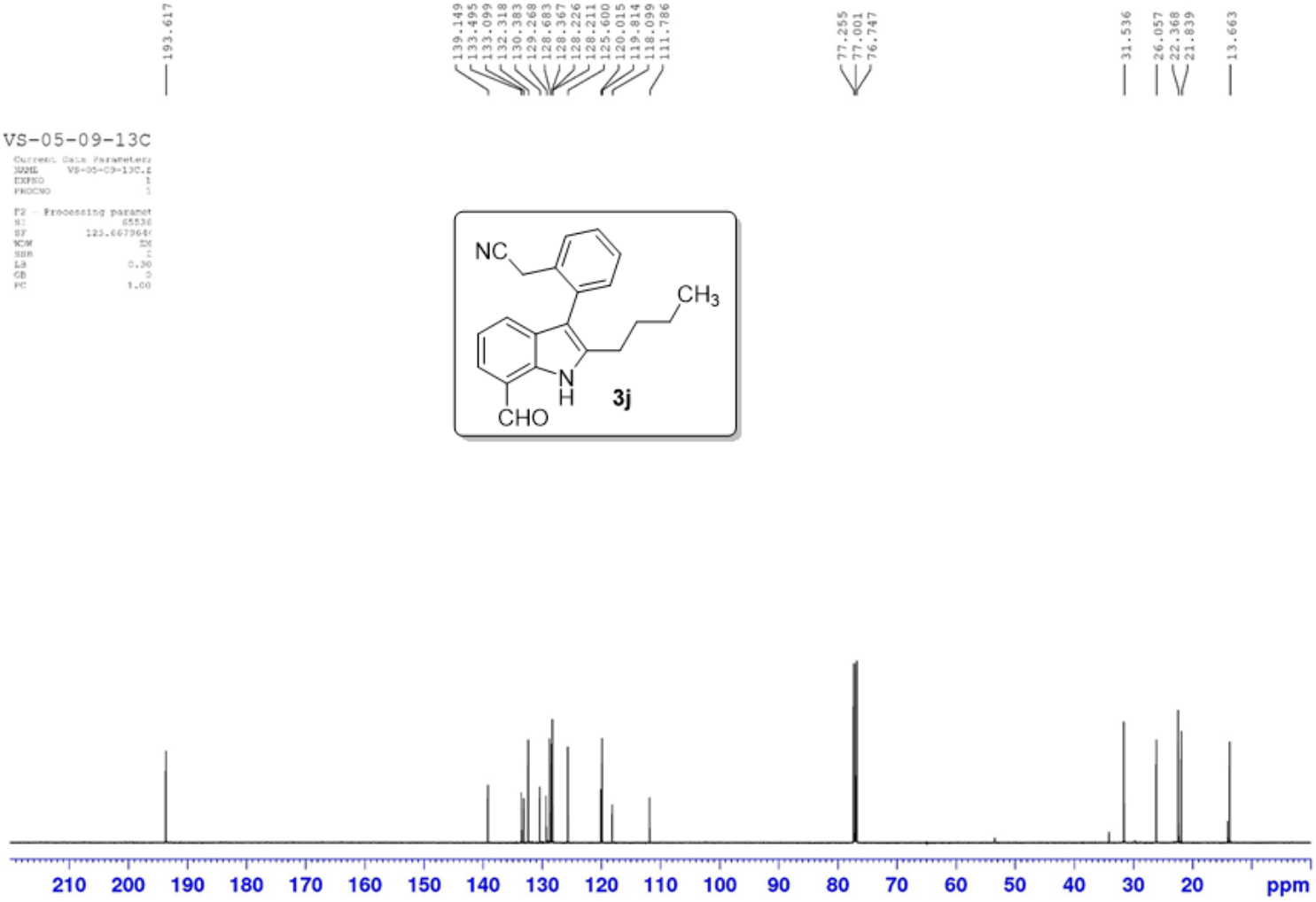
$^{13}C\{^{1}H\}$ and DEPT NMR (175 MHz, $CDCl_3$)



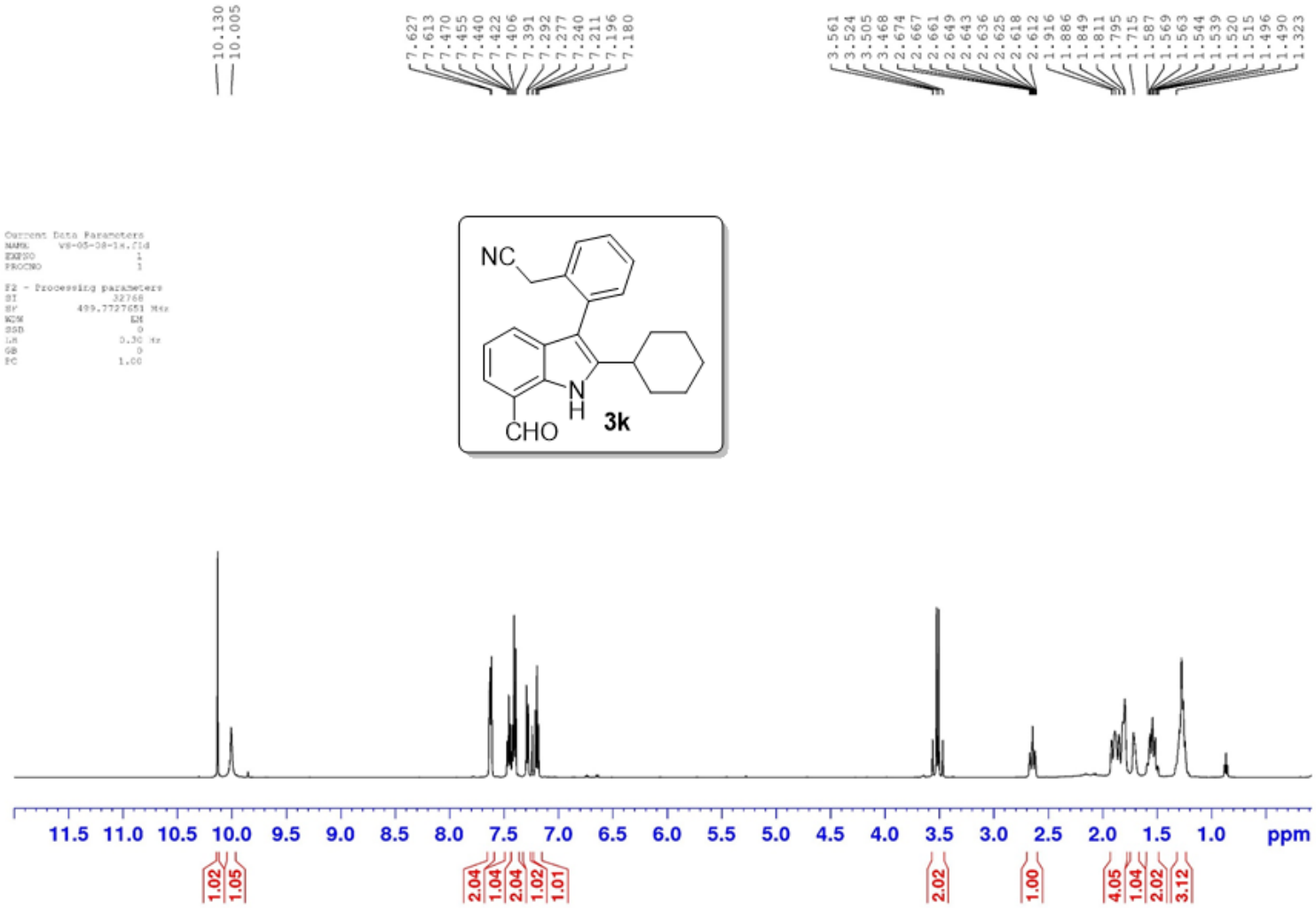
^{1}H-NMR (500 MHz, $CDCl_3$)



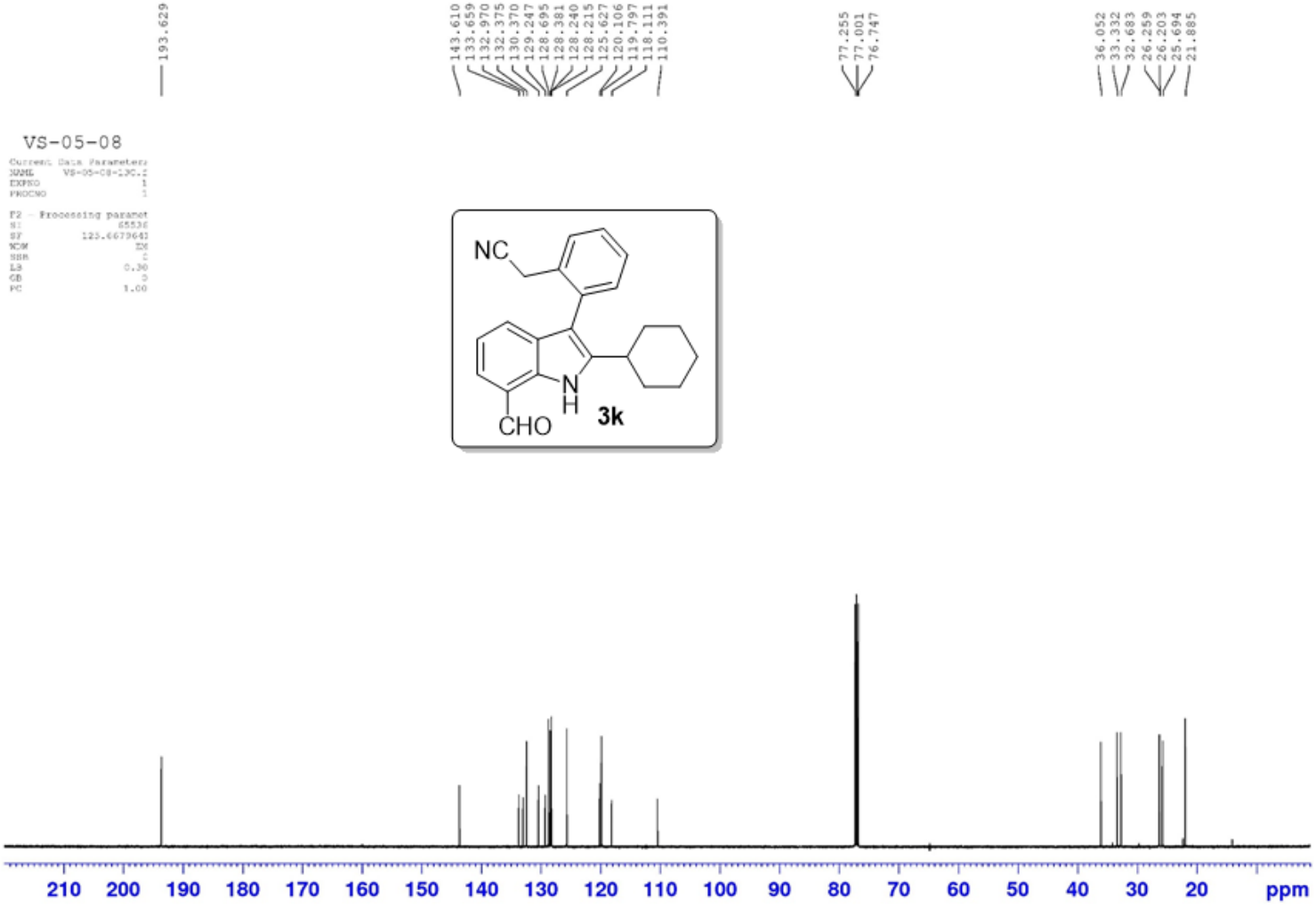
$^{13}C\{^{1}H\}$ NMR (125 MHz, $CDCl_3$)



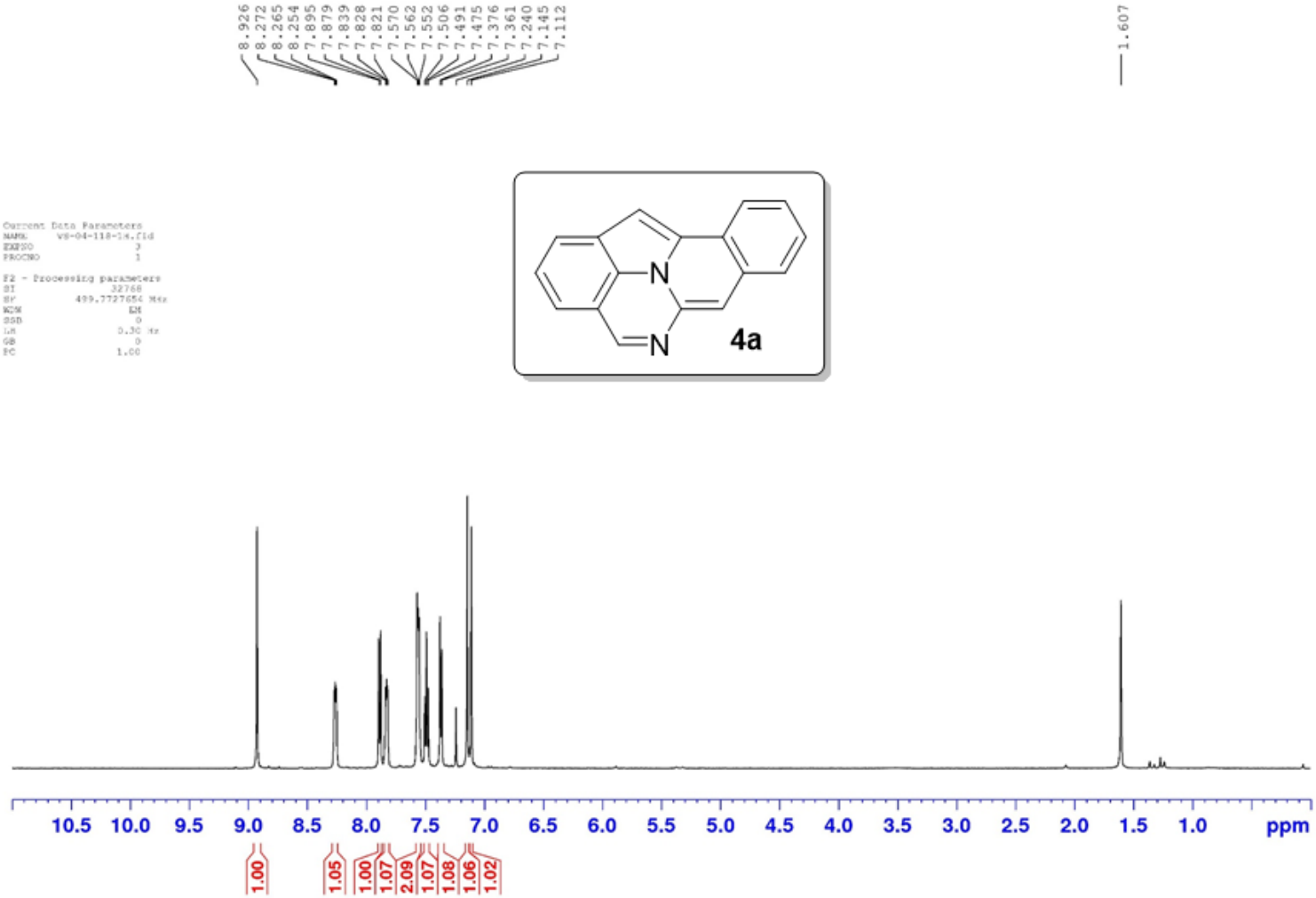
^{1}H-NMR (500 MHz, $CDCl_3$)



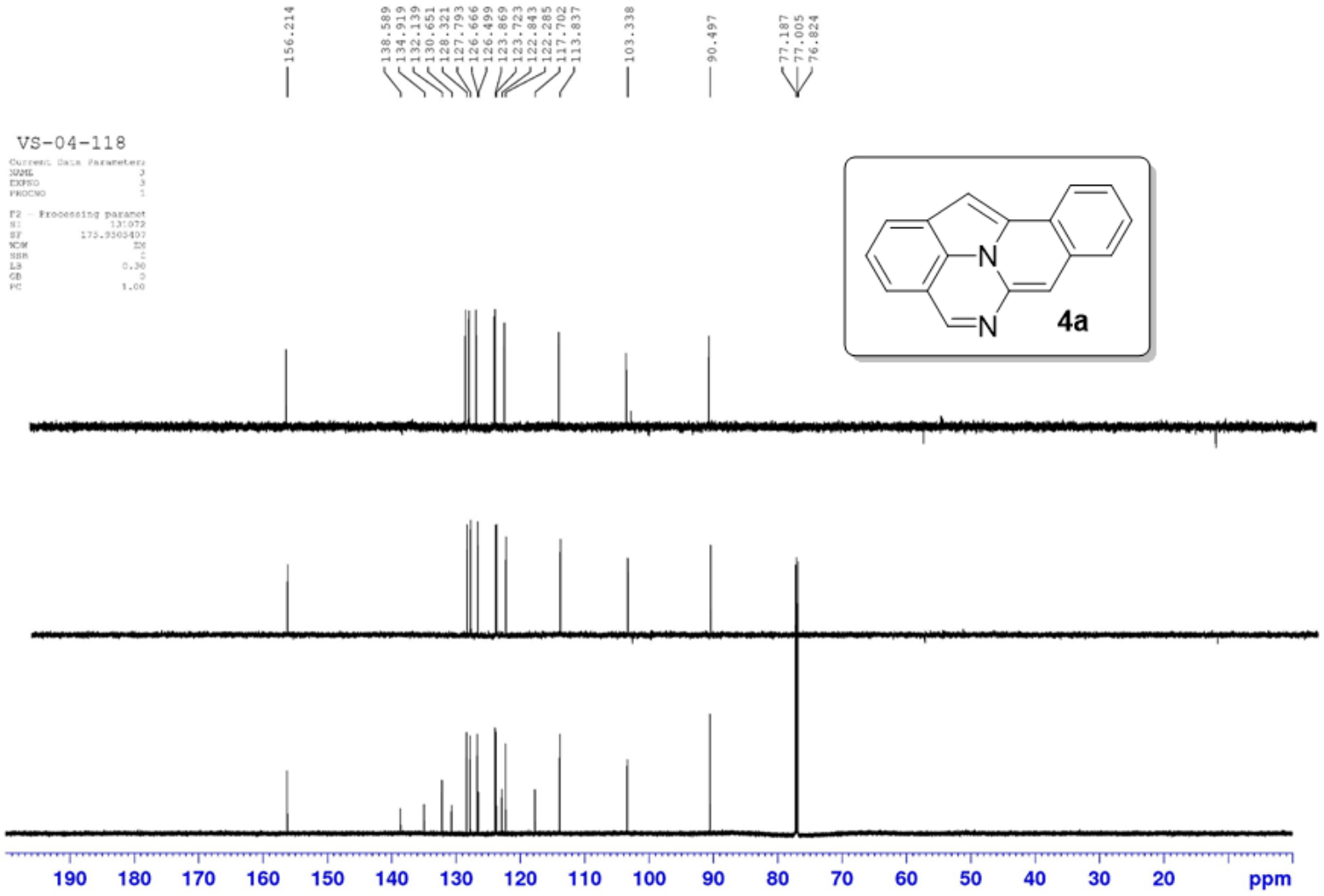
$^{13}C\{^{1}H\}$ NMR (125 MHz, $CDCl_3$)



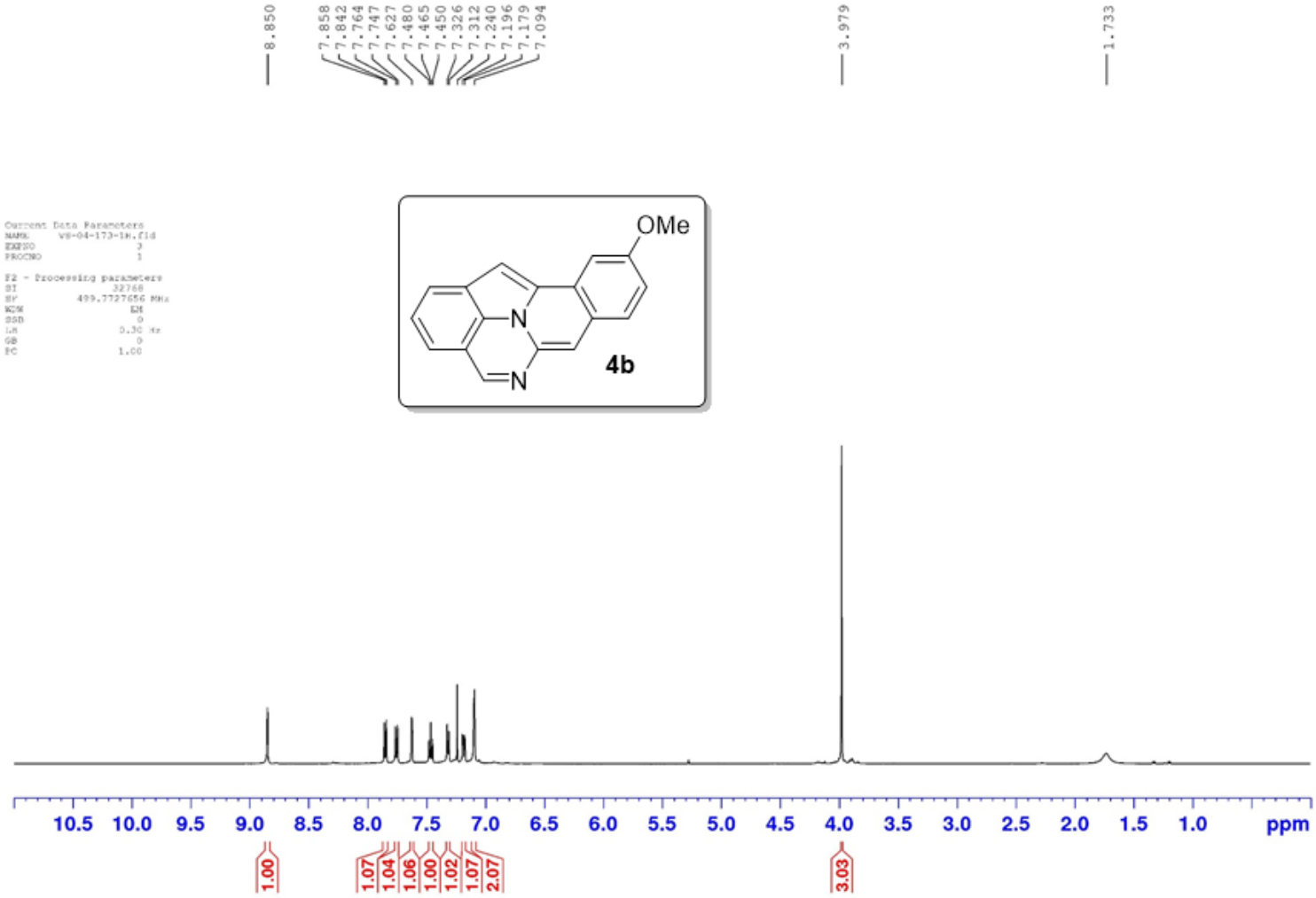
^{1}H-NMR (500 MHz, $CDCl_3$)



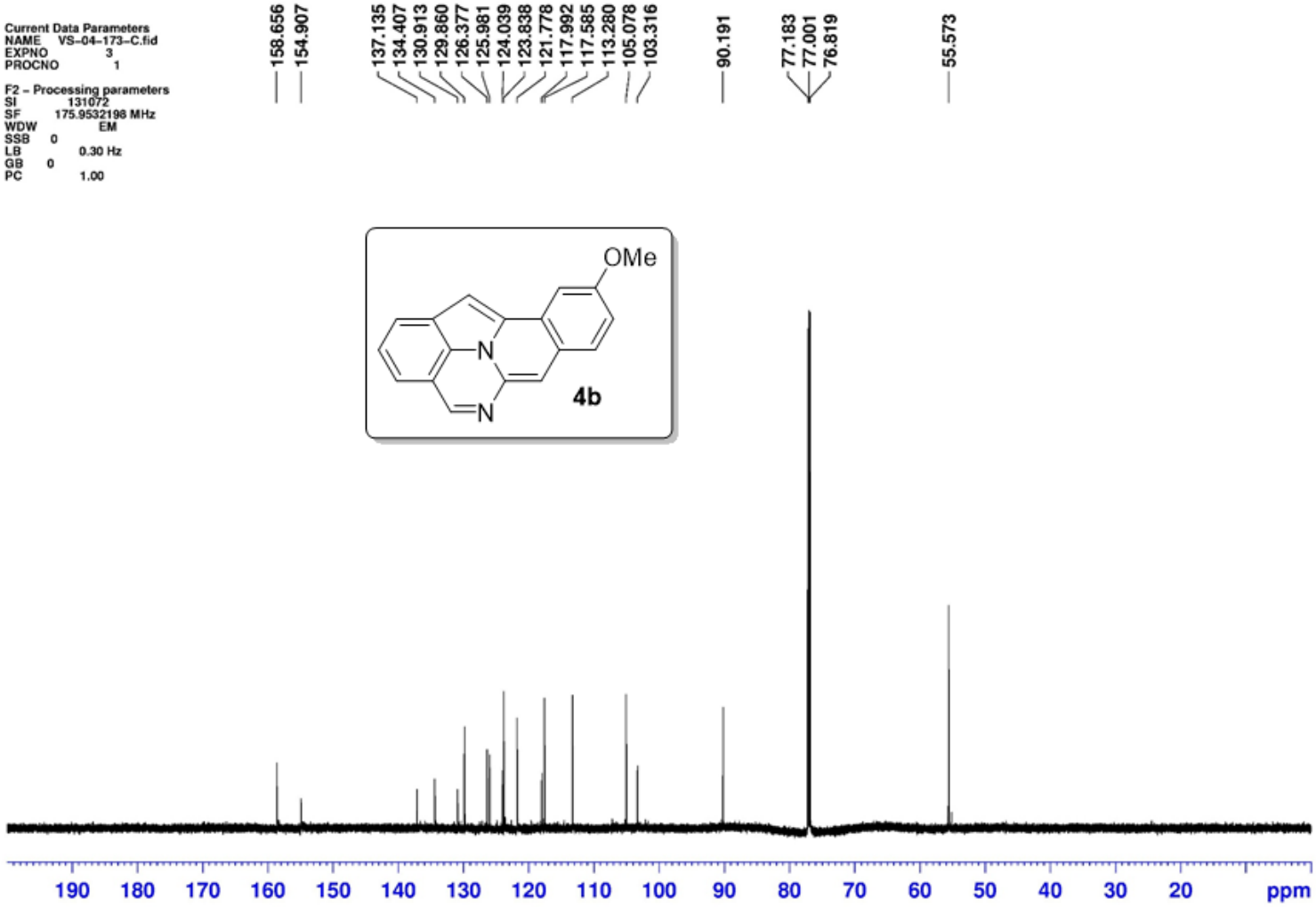
$^{13}C\{^{1}H\}$ and DEPT NMR (175 MHz, $CDCl_3$)



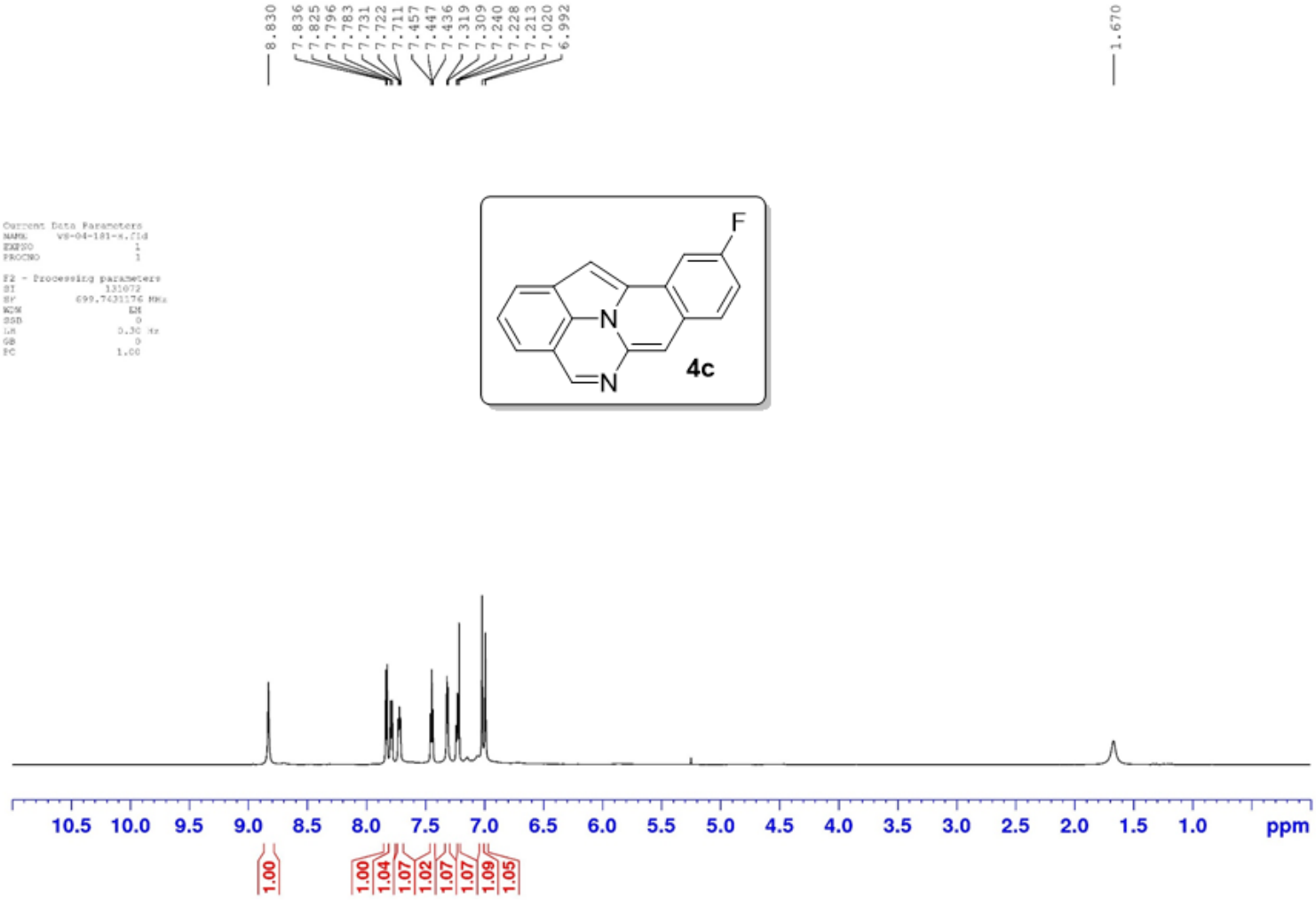
^{1}H-NMR (500 MHz, $CDCl_3$)



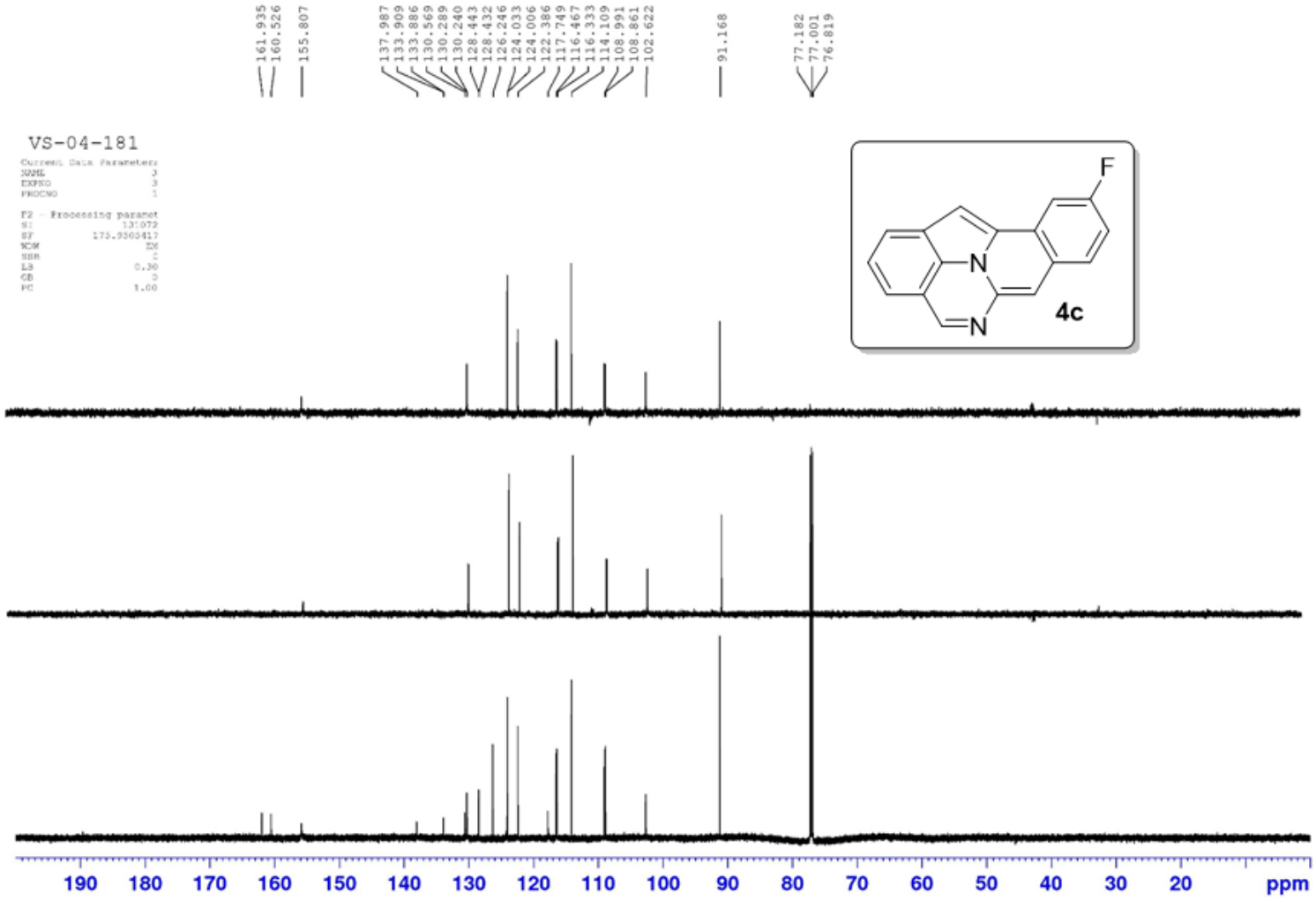
$^{13}C\{^{1}H\}$ NMR (175 MHz, $CDCl_3$)



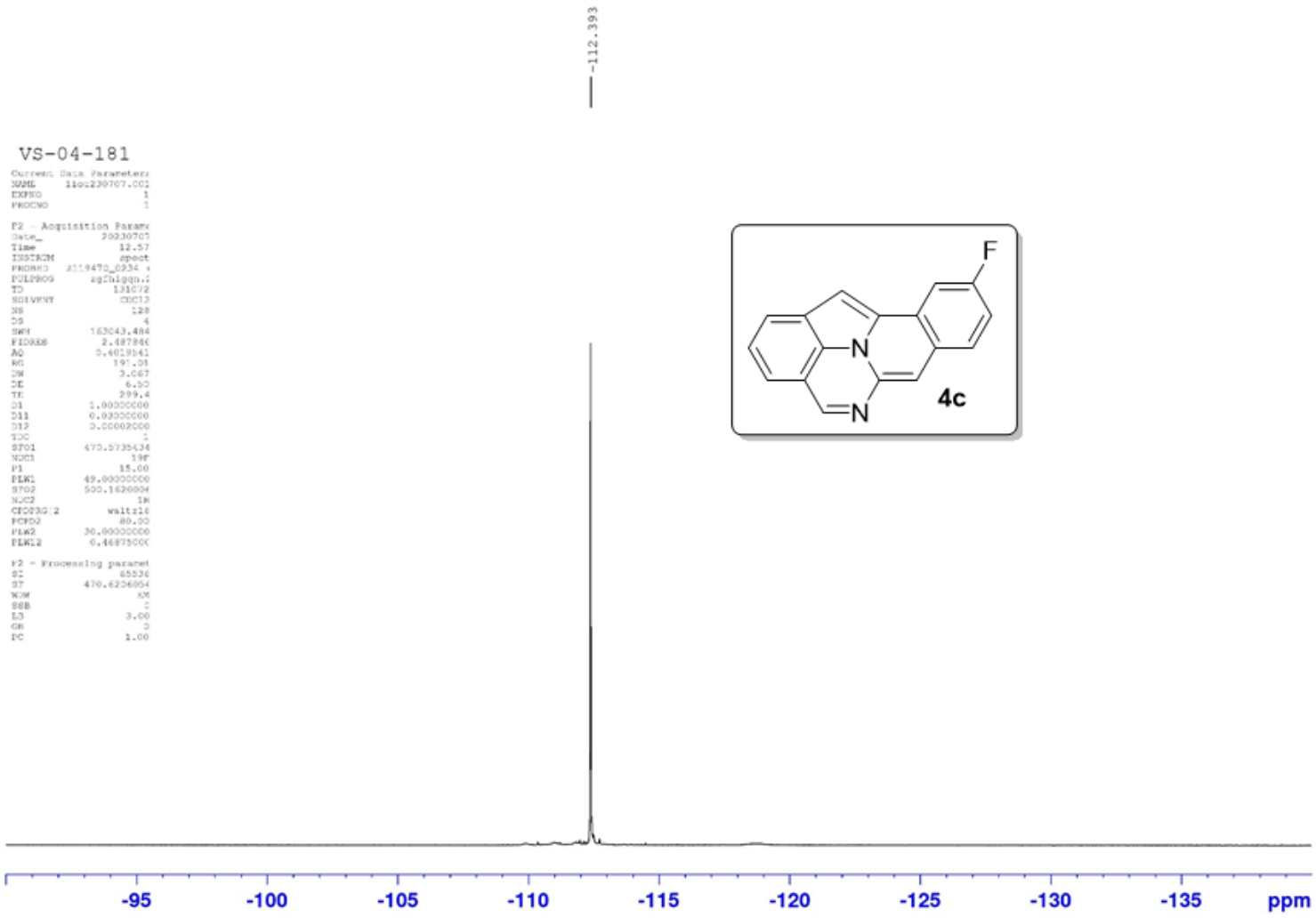
^{1}H-NMR (700 MHz, $CDCl_3$)



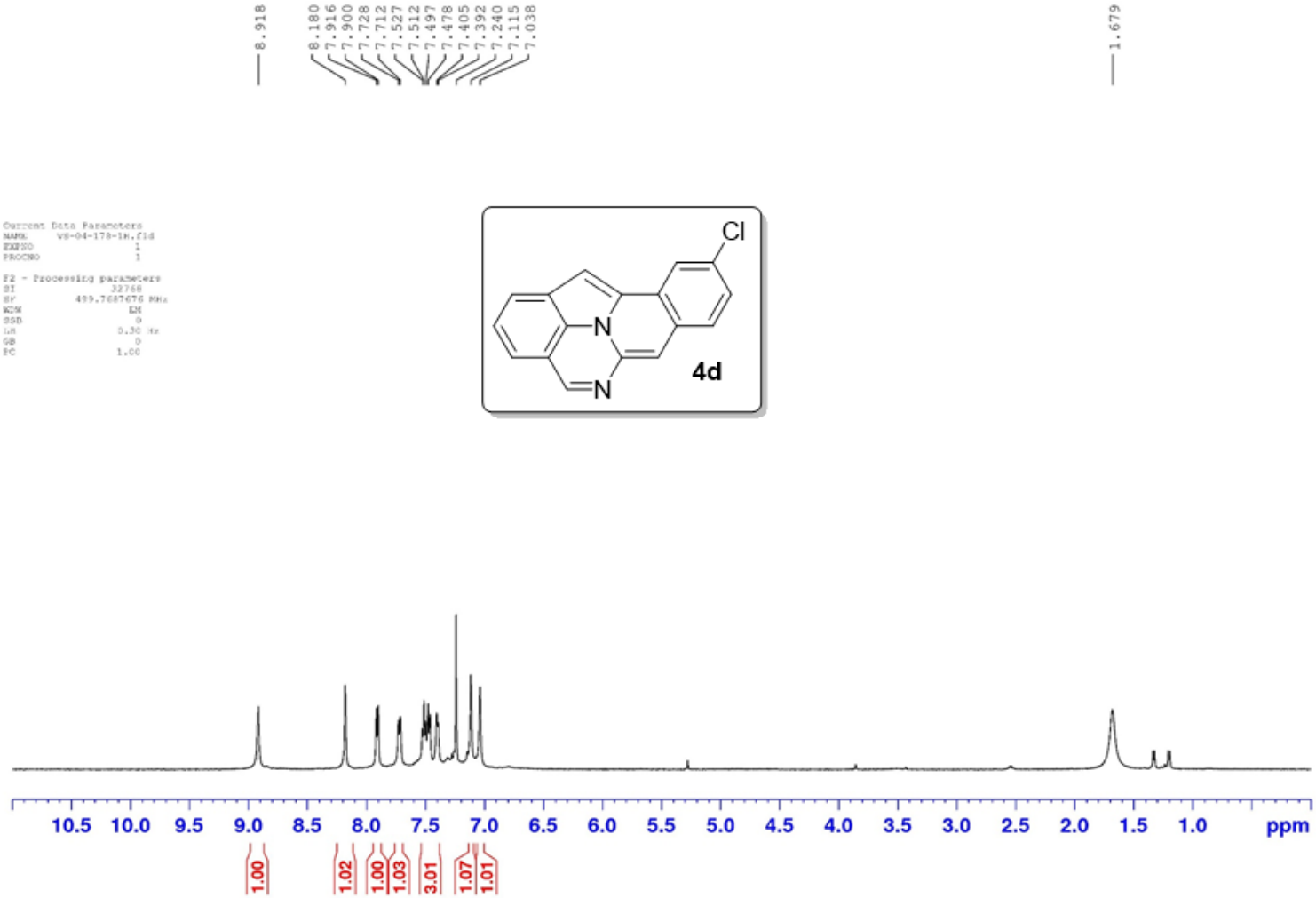
$^{13}C\{^{1}H\}$ and DEPT NMR (175 MHz, $CDCl_3$)



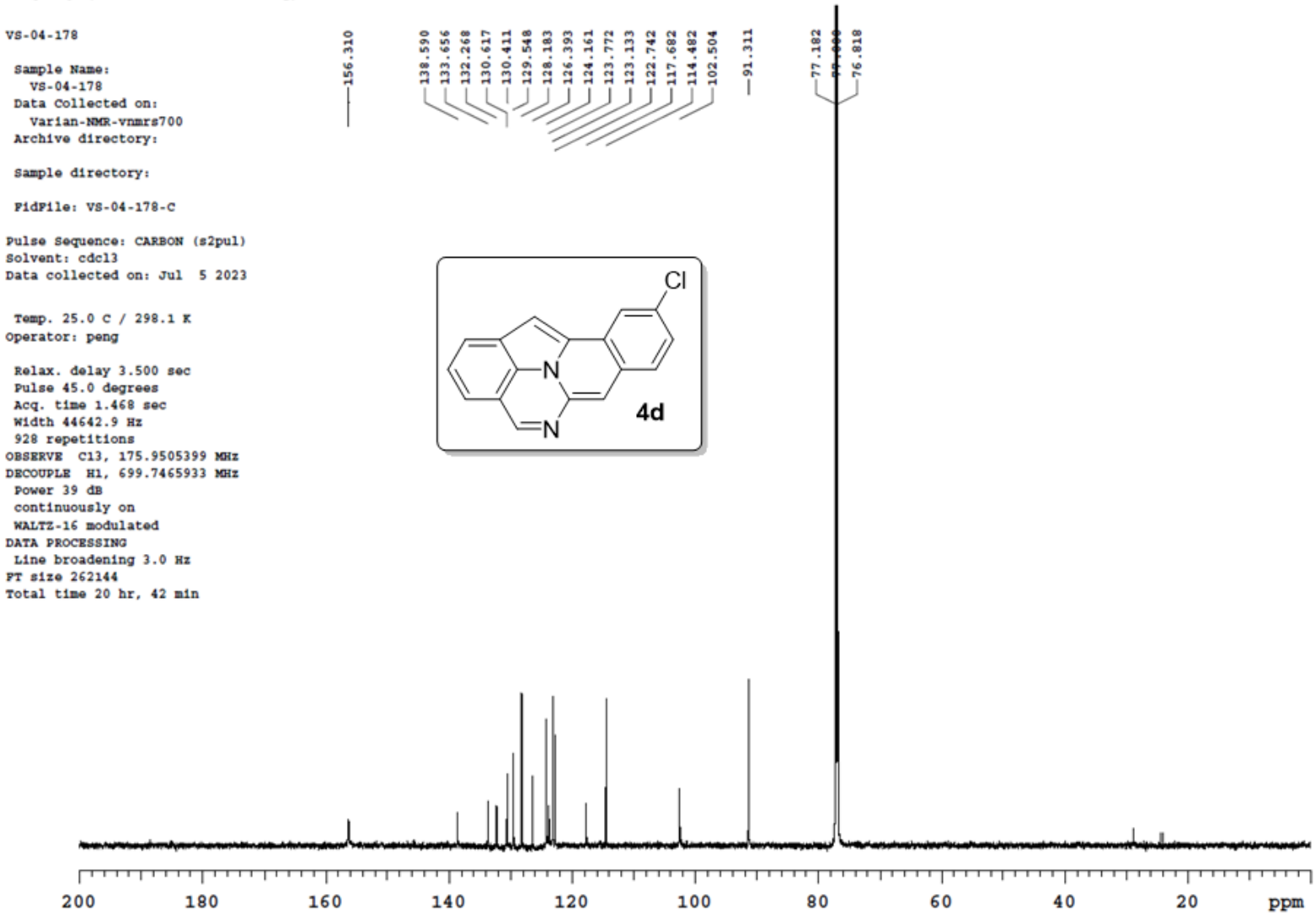
^{19}F {^{1}H} NMR (500 MHz, $CDCl_3$)



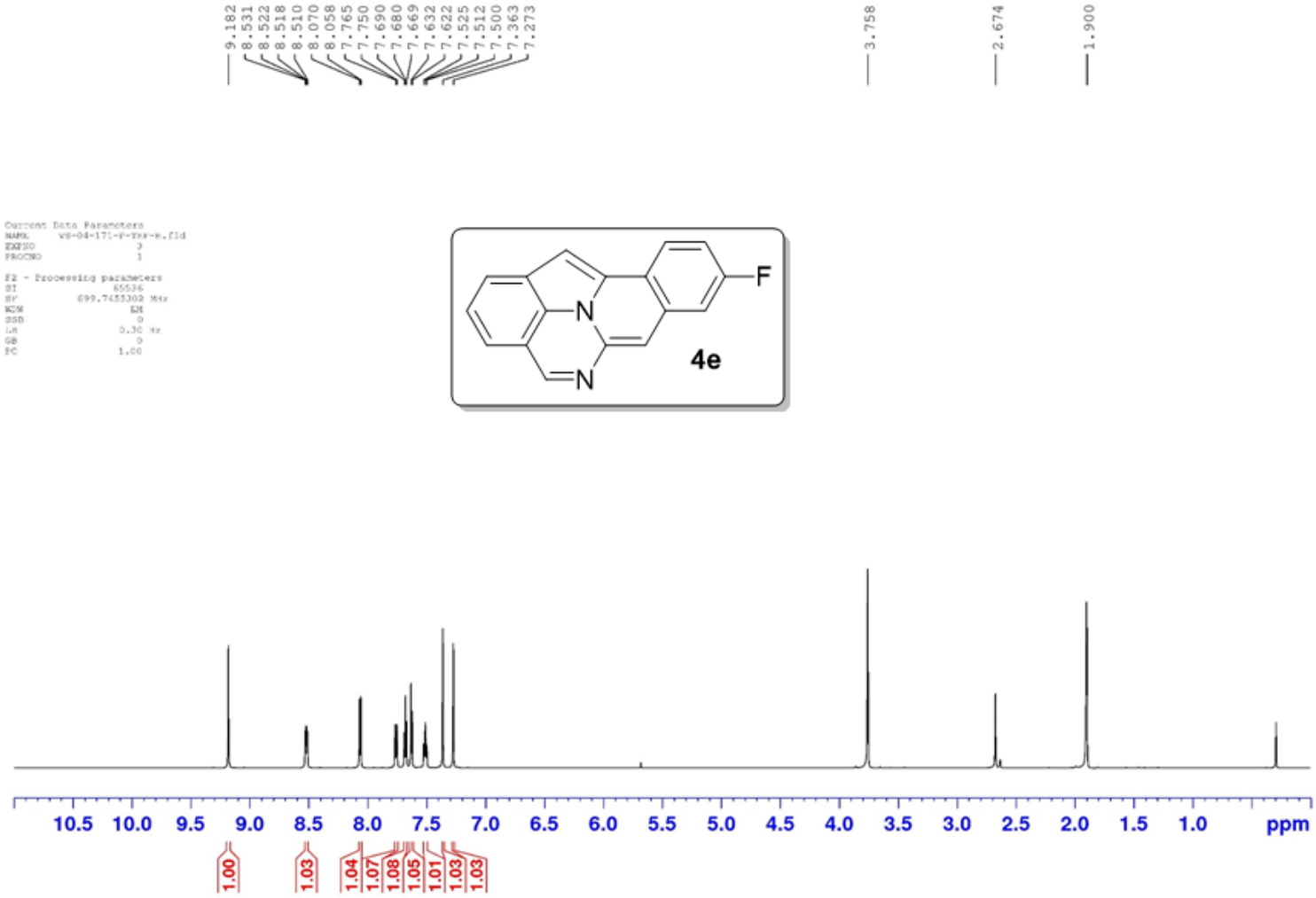
^{1}H-NMR (500 MHz, $CDCl_3$)



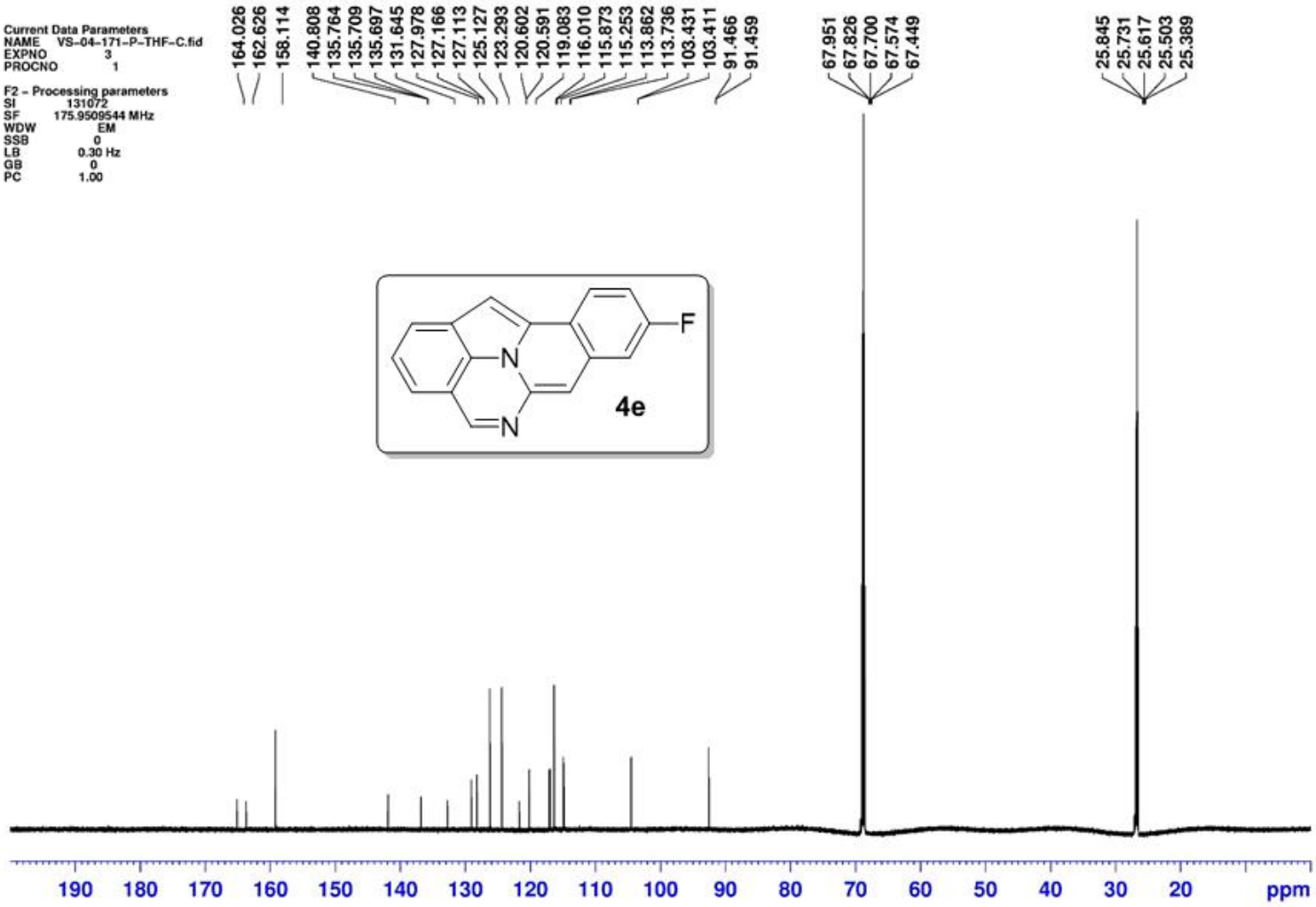
$^{13}C\{^{1}H\}$ (175 MHz, $CDCl_3$)



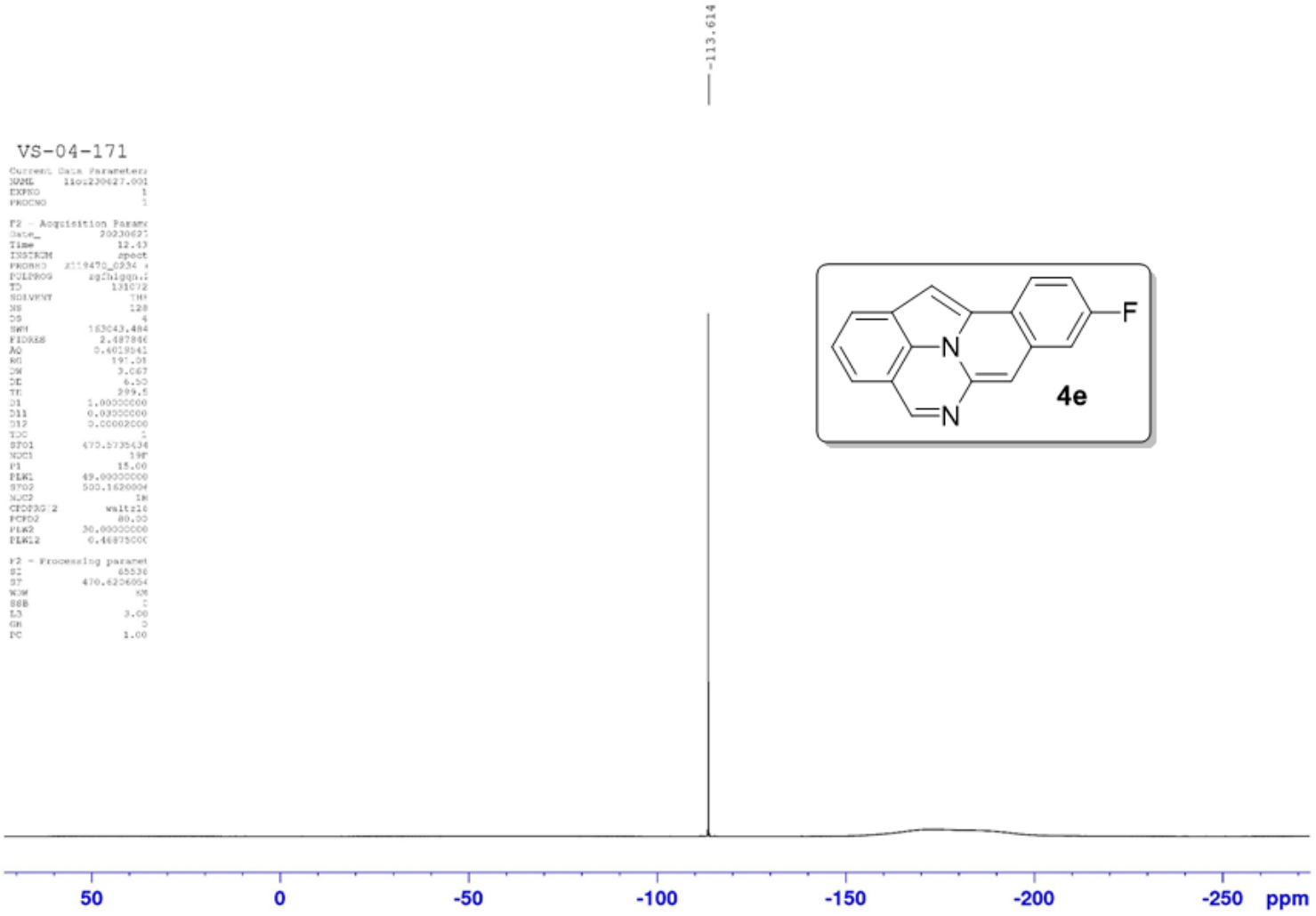
^{1}H-NMR (700 MHz, *d*-THF)



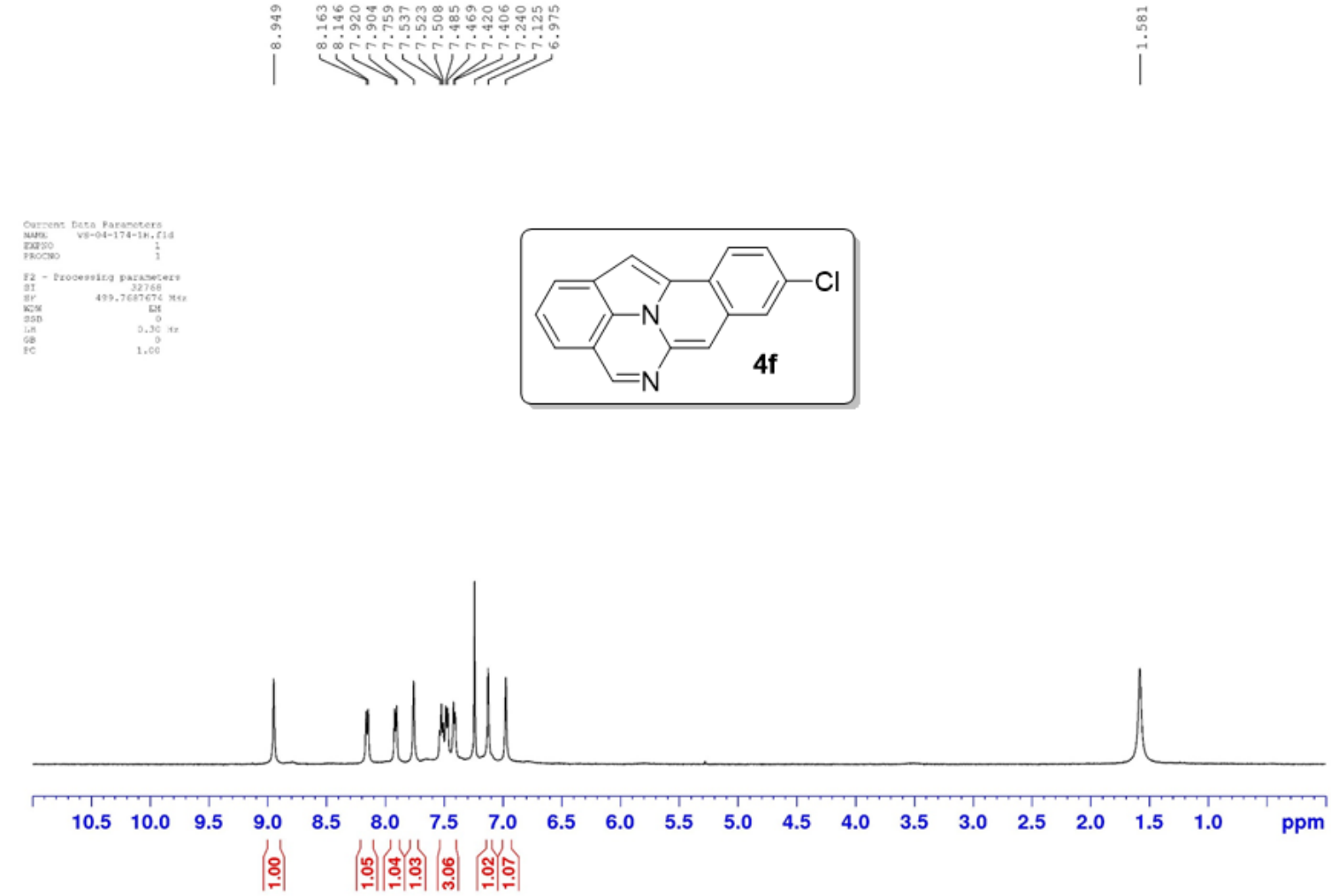
$^{13}C\{^{1}H\}$ NMR (175 MHz, *d*-THF)



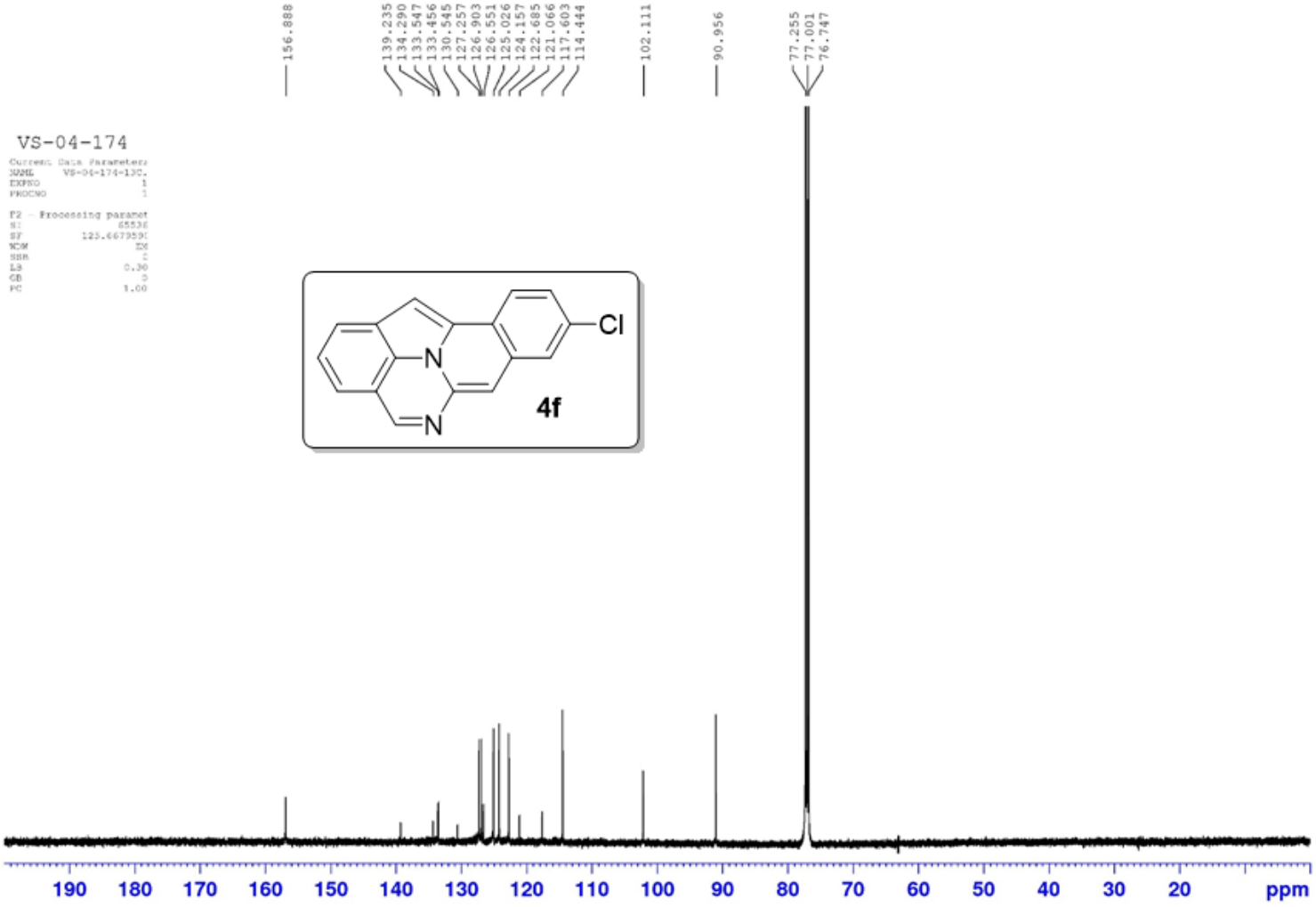
^{19}F {^{1}H} NMR (500 MHz, *d*-THF)



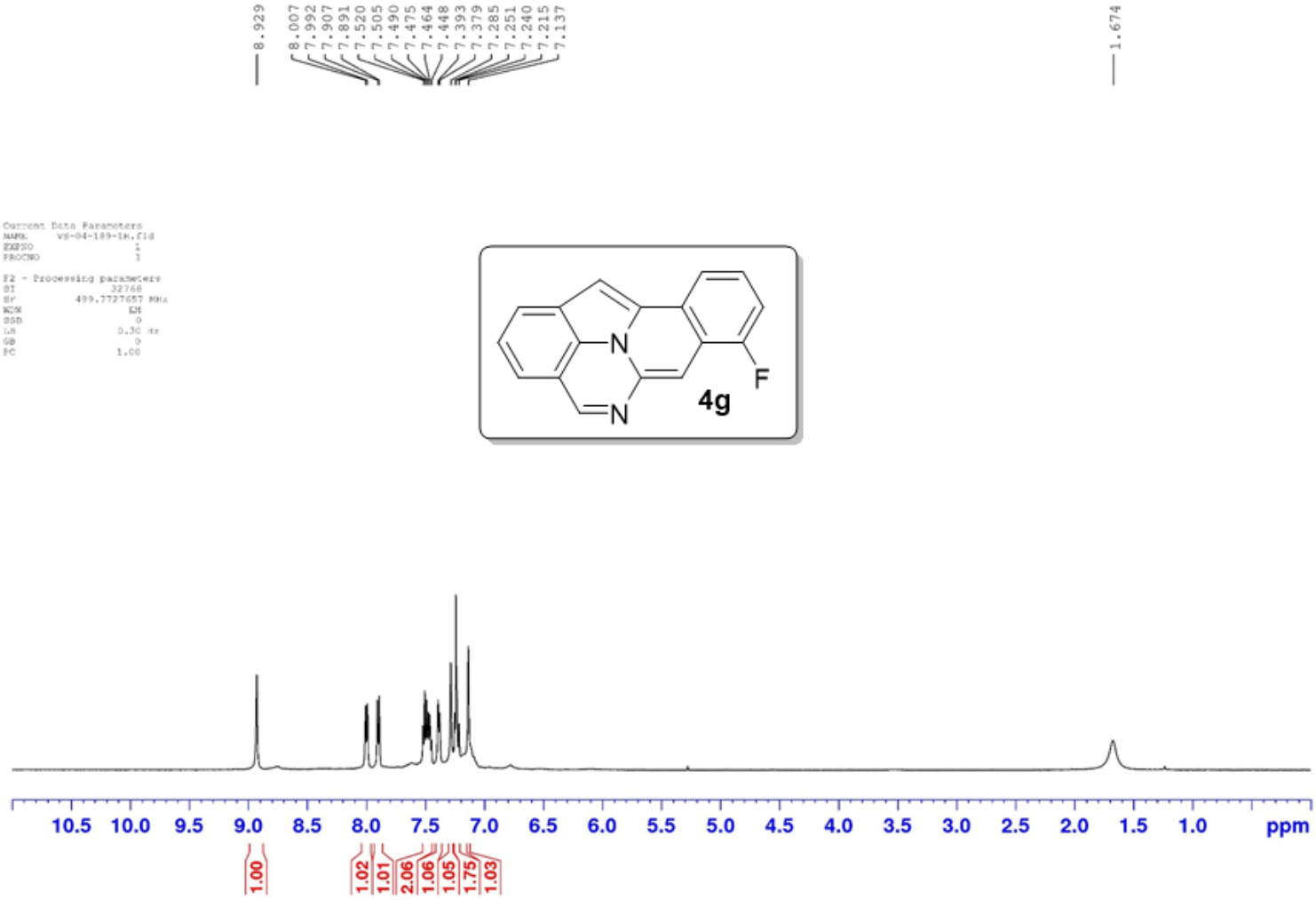
^{1}H-NMR (500 MHz, $CDCl_3$)



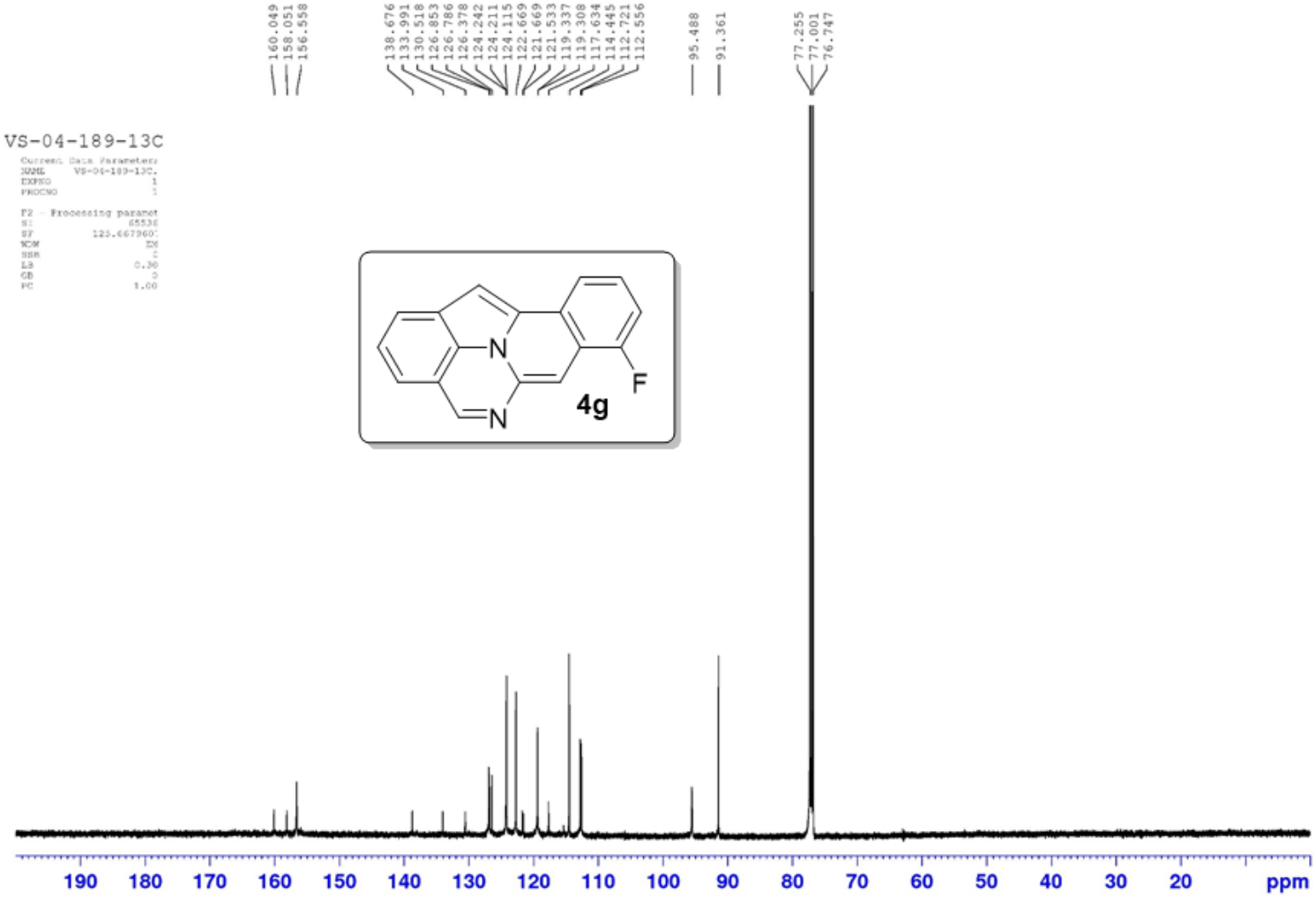
$^{13}C\{^{1}H\}$ NMR (125 MHz, $CDCl_3$)



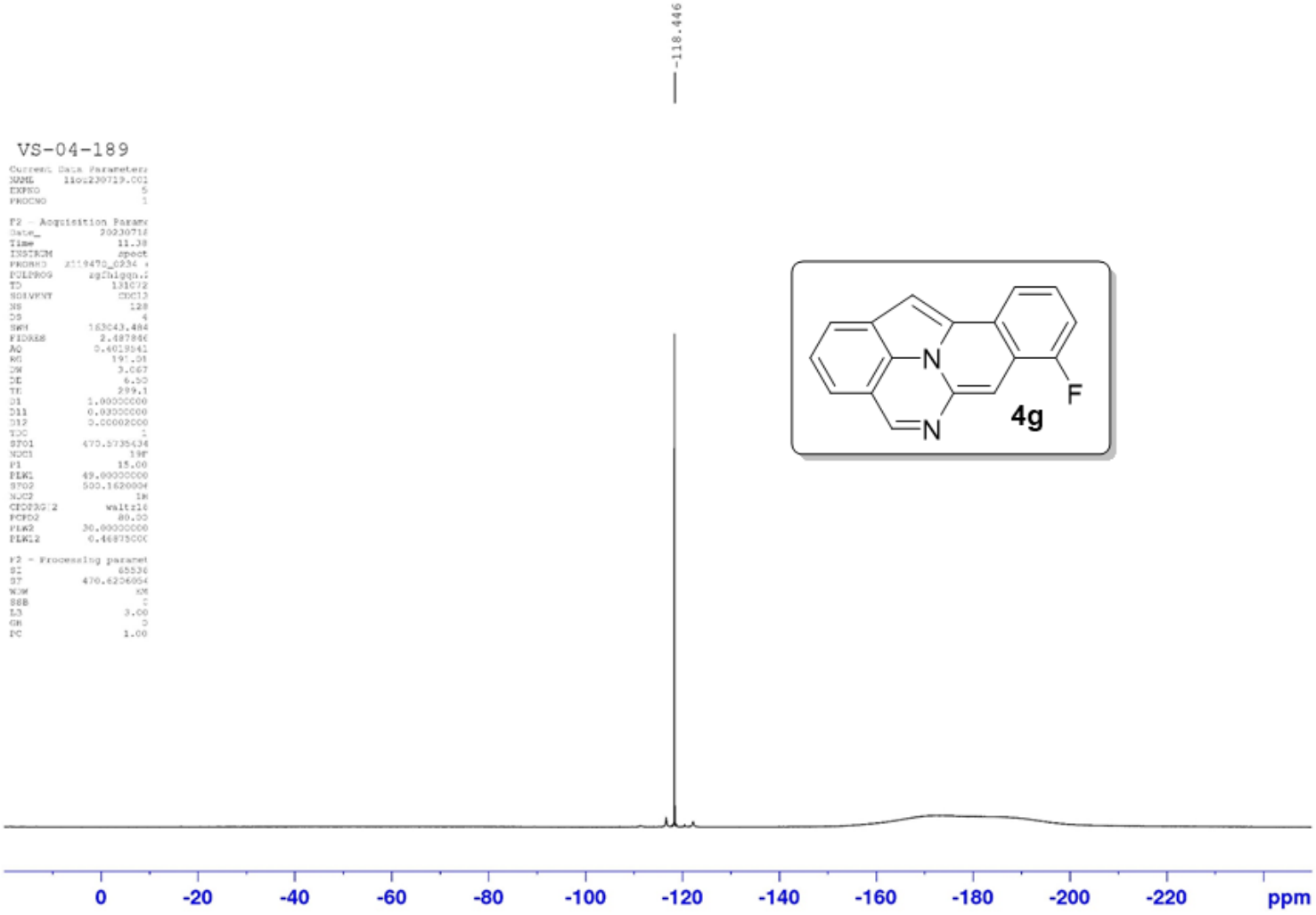
^{1}H-NMR (500 MHz, $CDCl_3$)



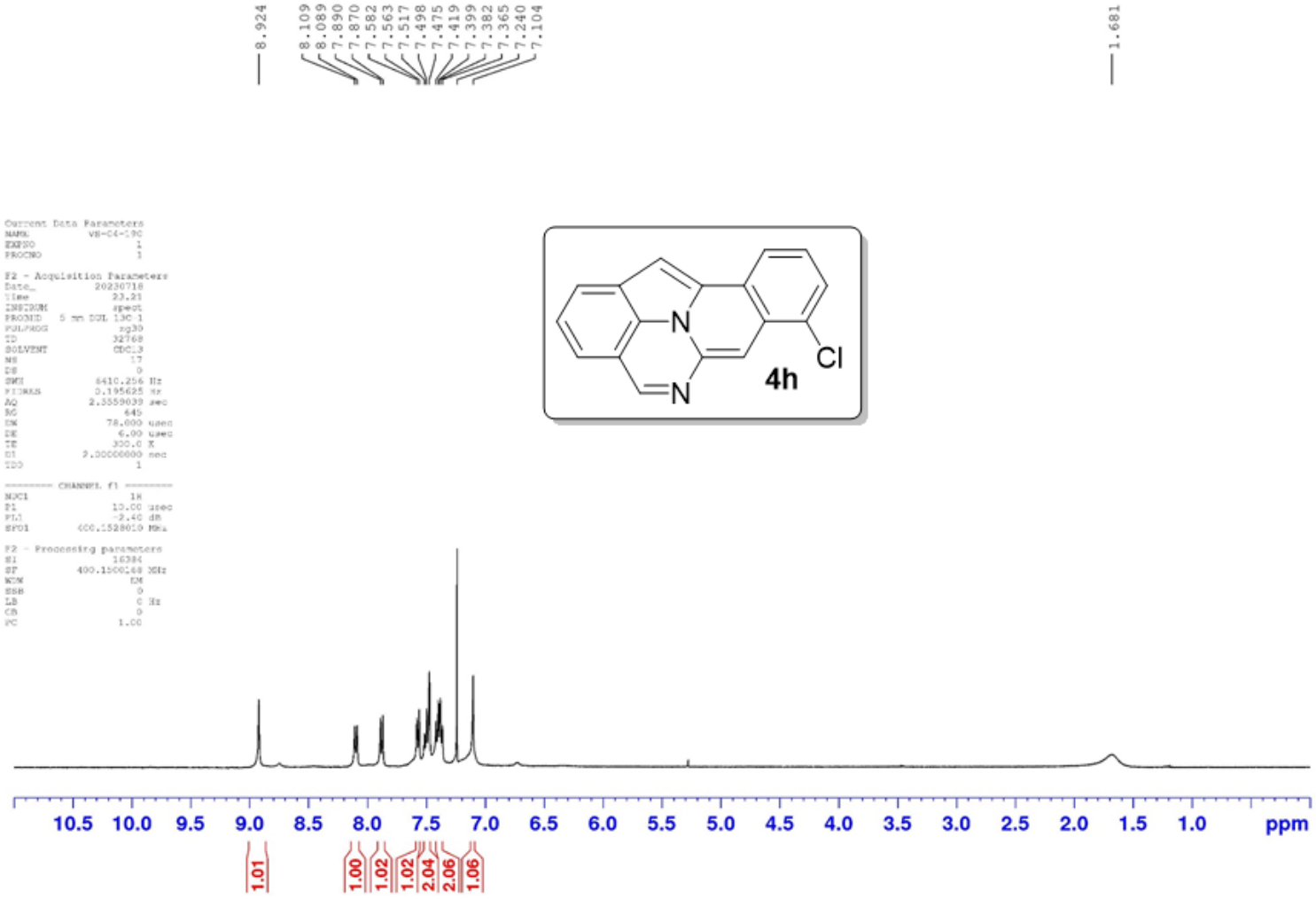
$^{13}C\{^{1}H\}$ NMR (125 MHz, $CDCl_3$)



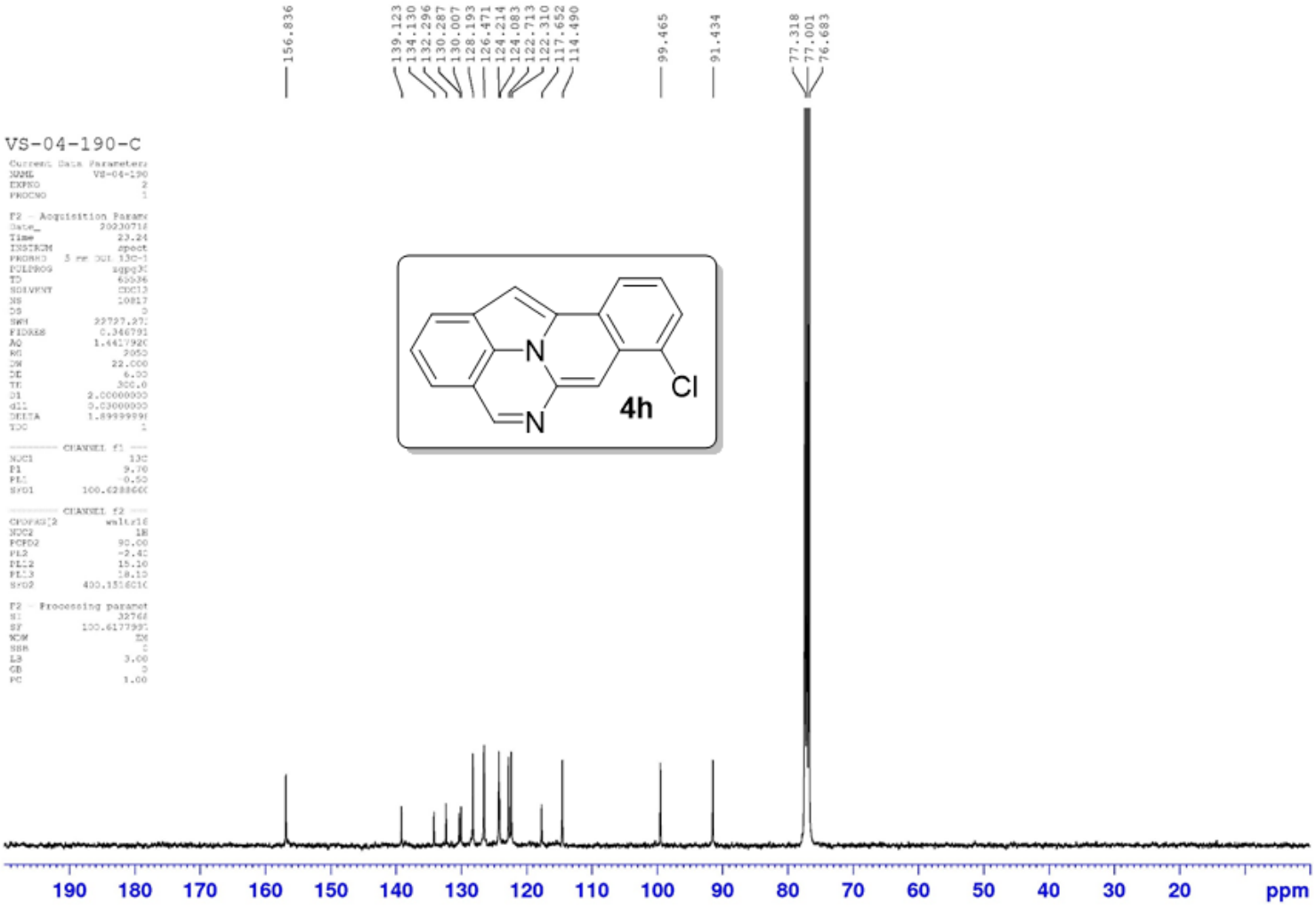
^{19}F {^{1}H} NMR (500 MHz, $CDCl_3$)



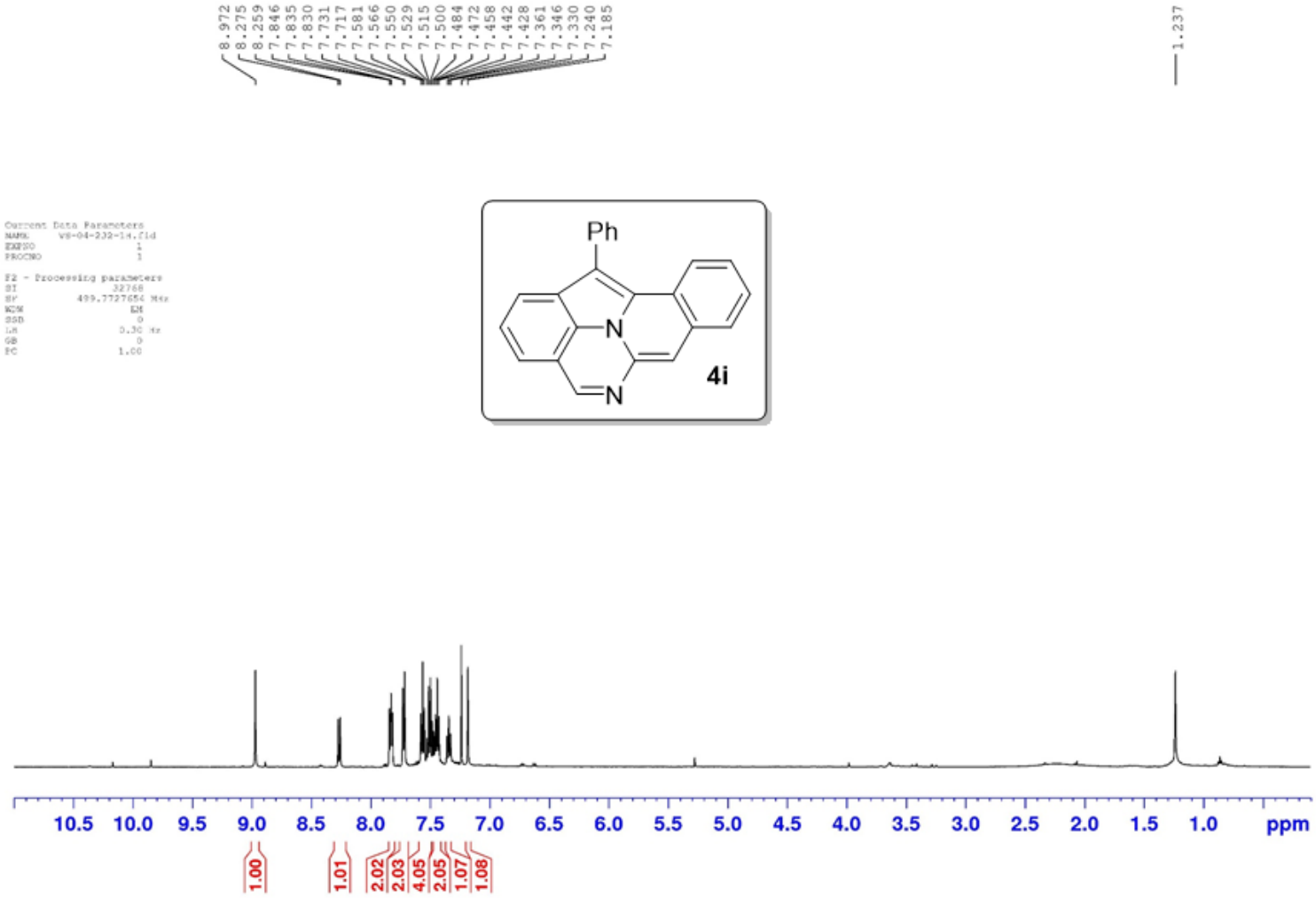
^{1}H-NMR (400 MHz, $CDCl_3$)



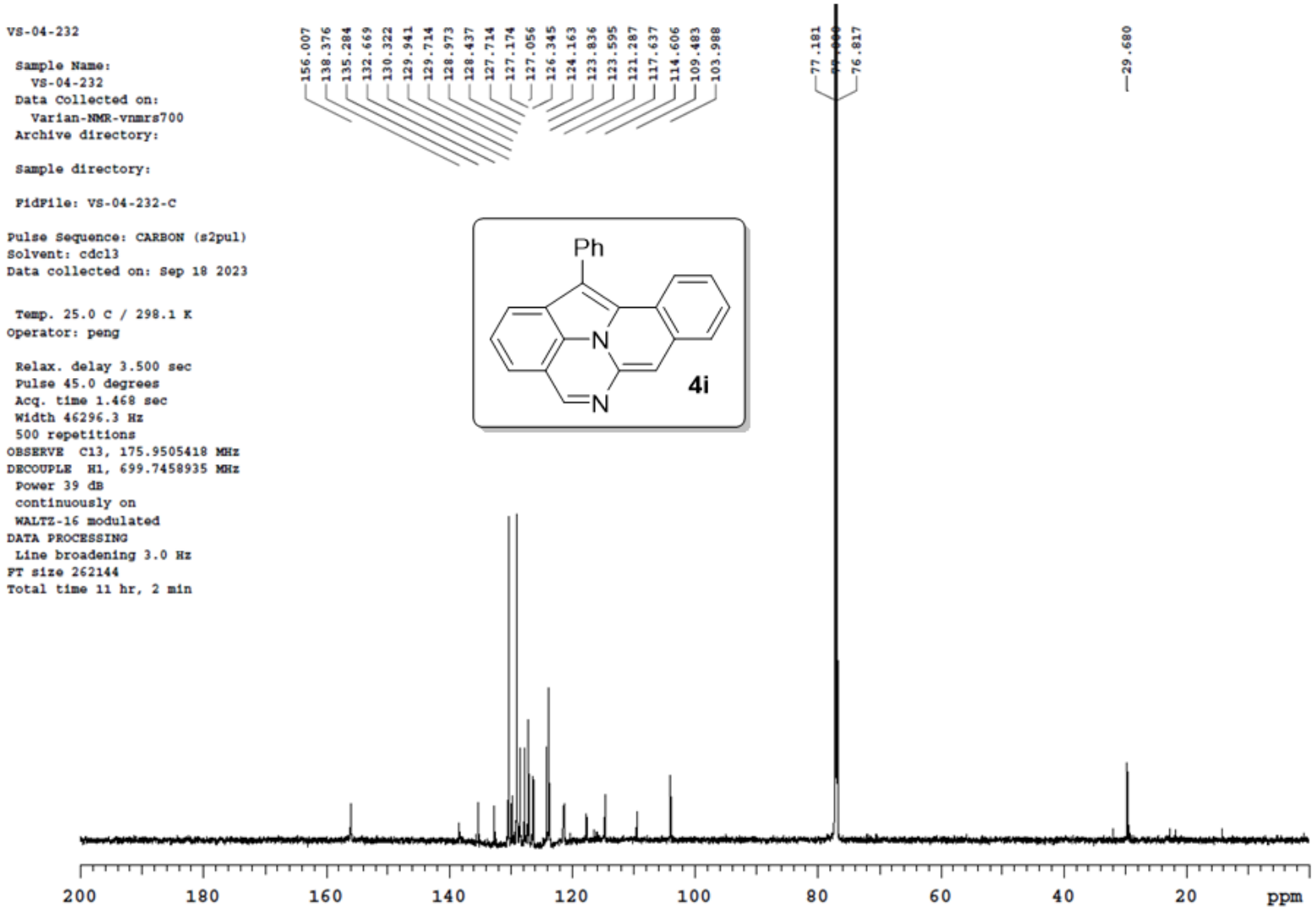
$^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$)



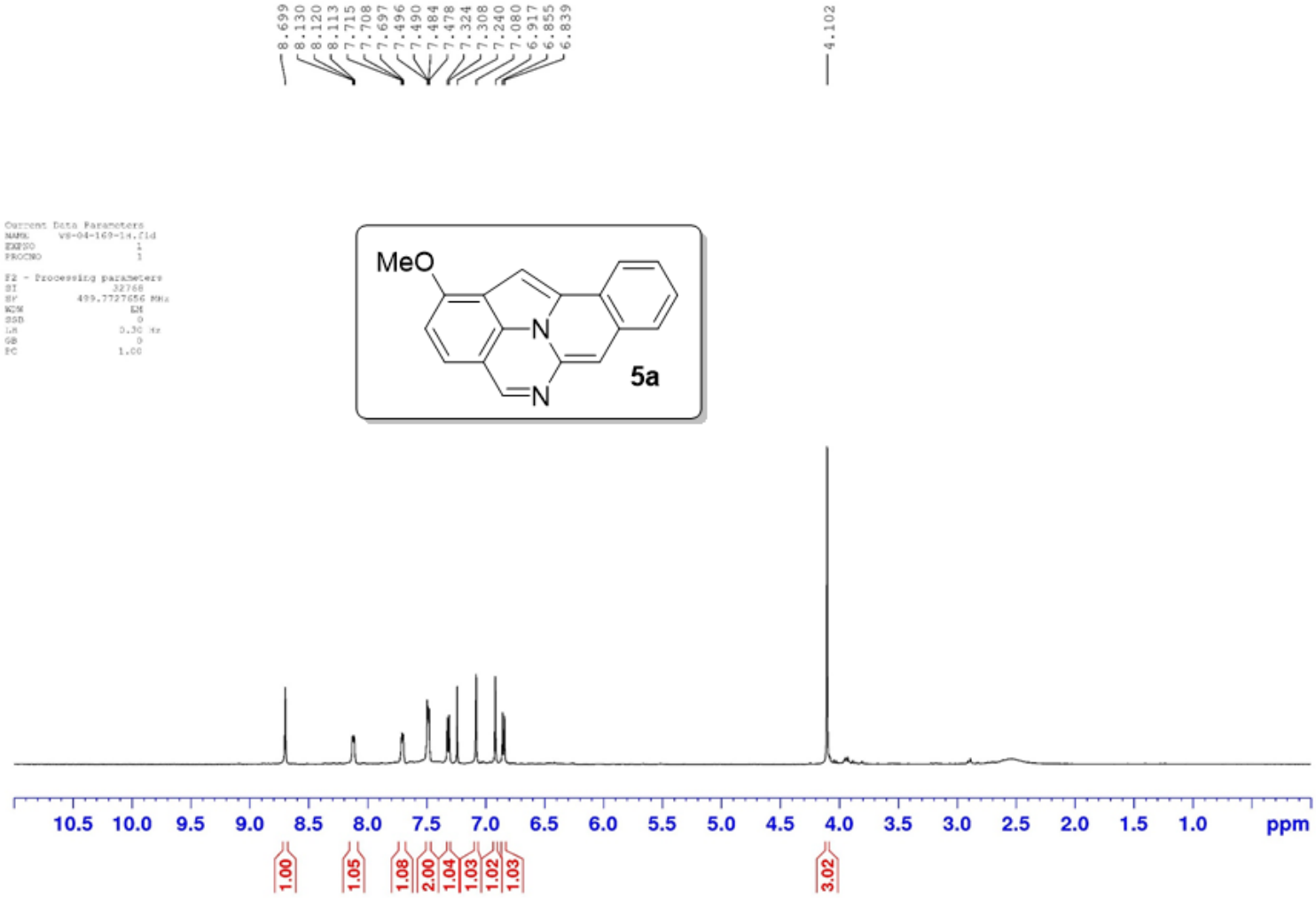
^{1}H-NMR (500 MHz, $CDCl_3$)



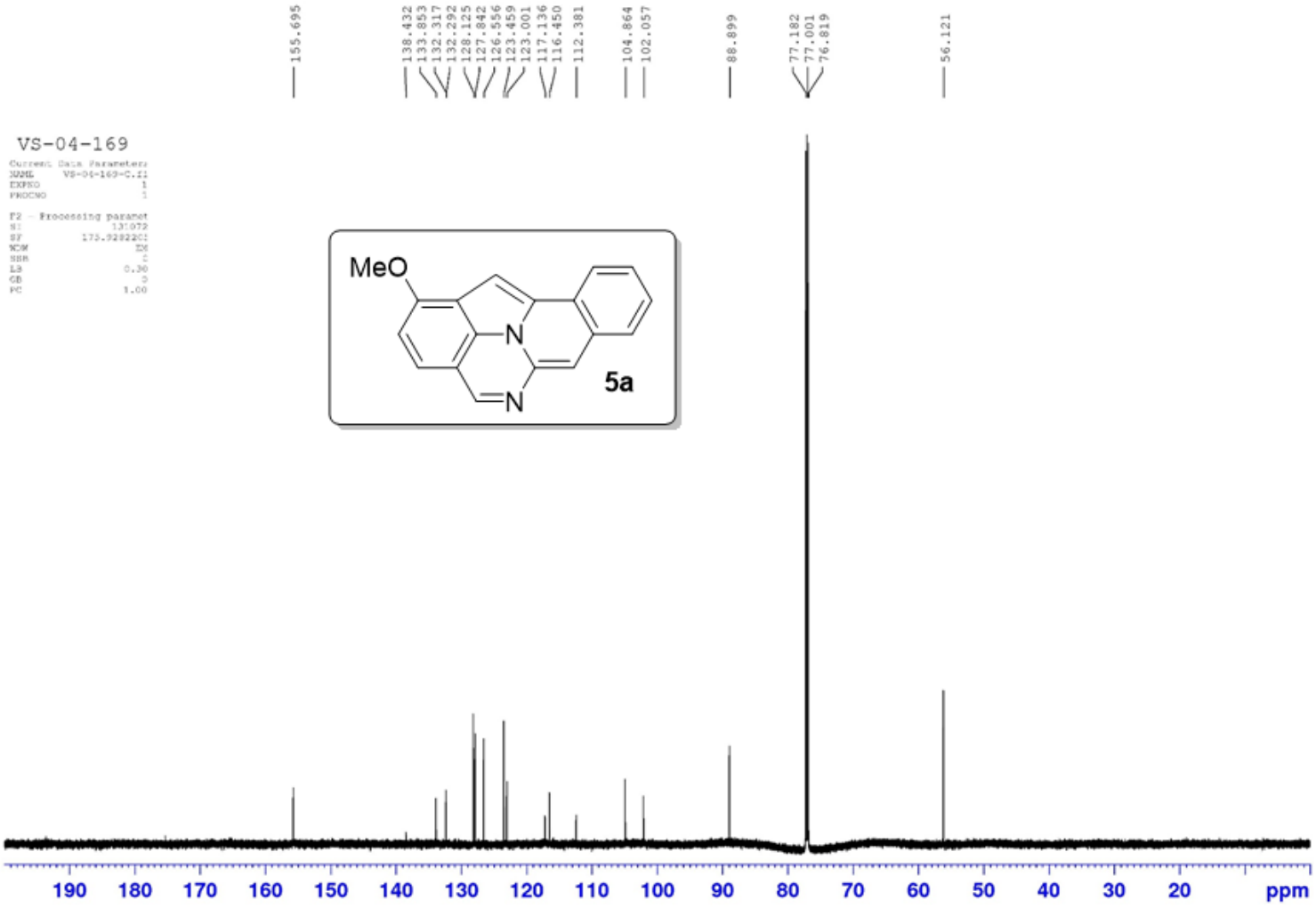
$^{13}C\{^{1}H\}$ NMR (175 MHz, $CDCl_3$)



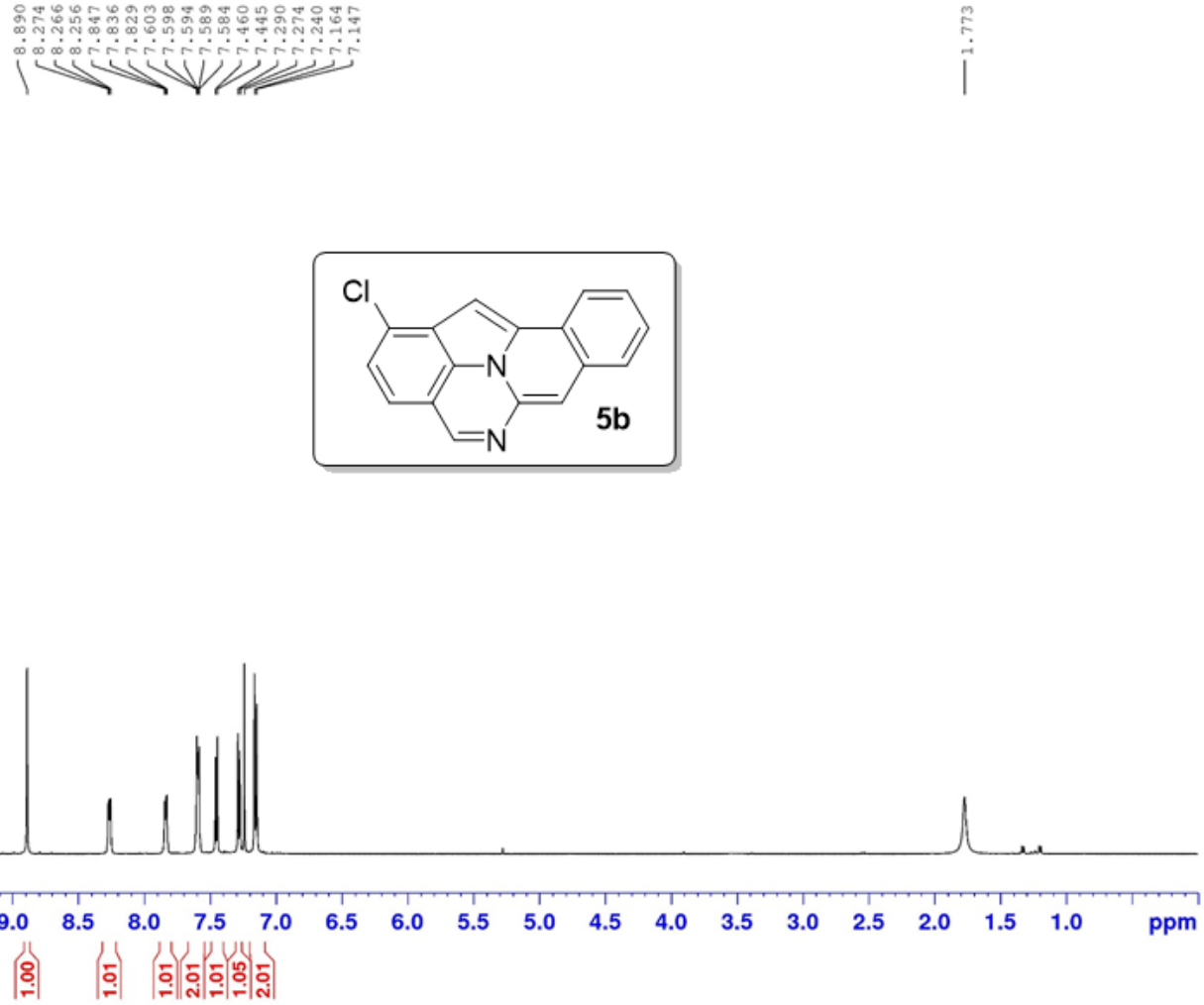
^{1}H-NMR (500 MHz, $CDCl_3$)



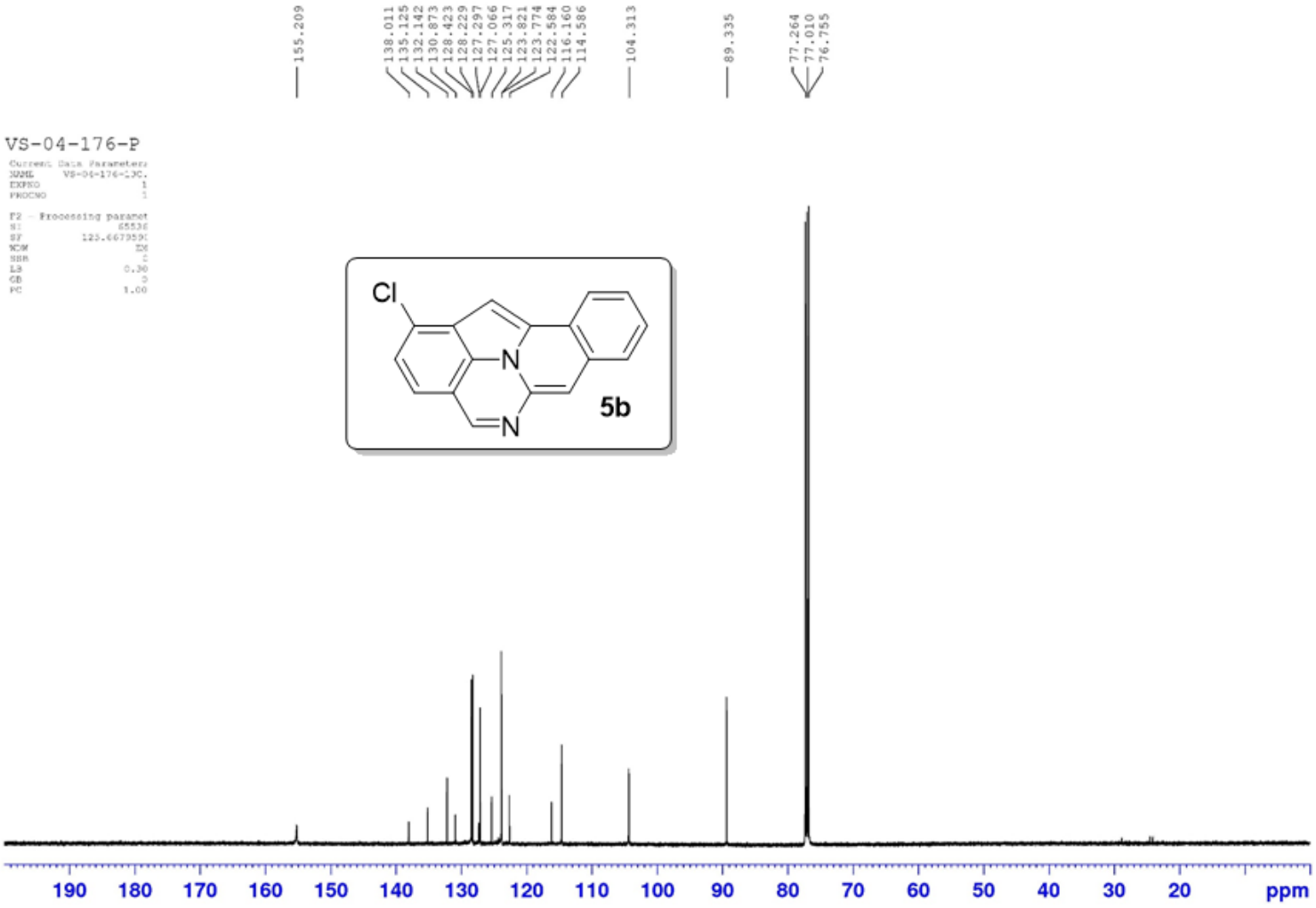
$^{13}C\{^{1}H\}$ NMR (175 MHz, $CDCl_3$)



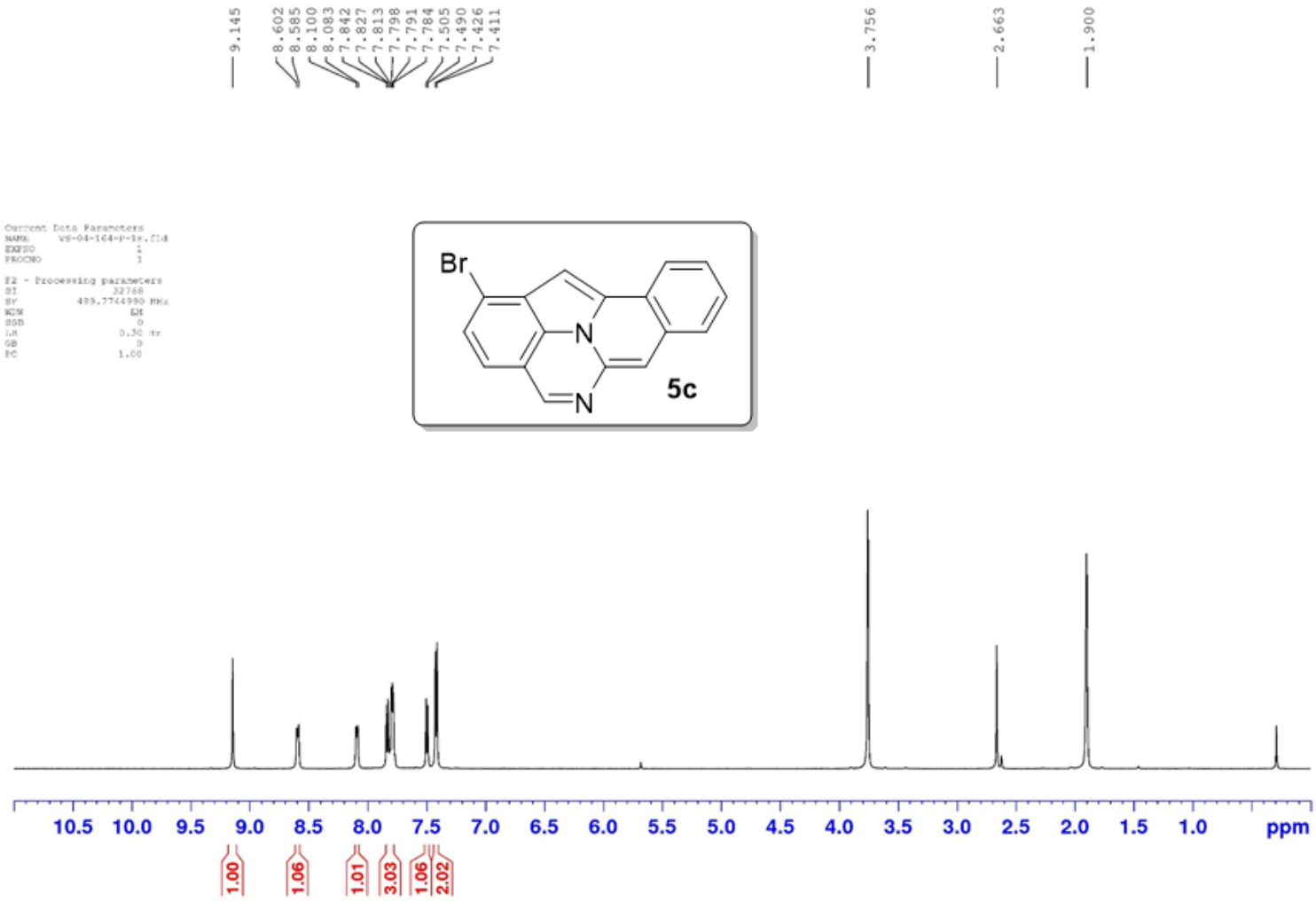
^{1}H-NMR (500 MHz, $CDCl_3$)



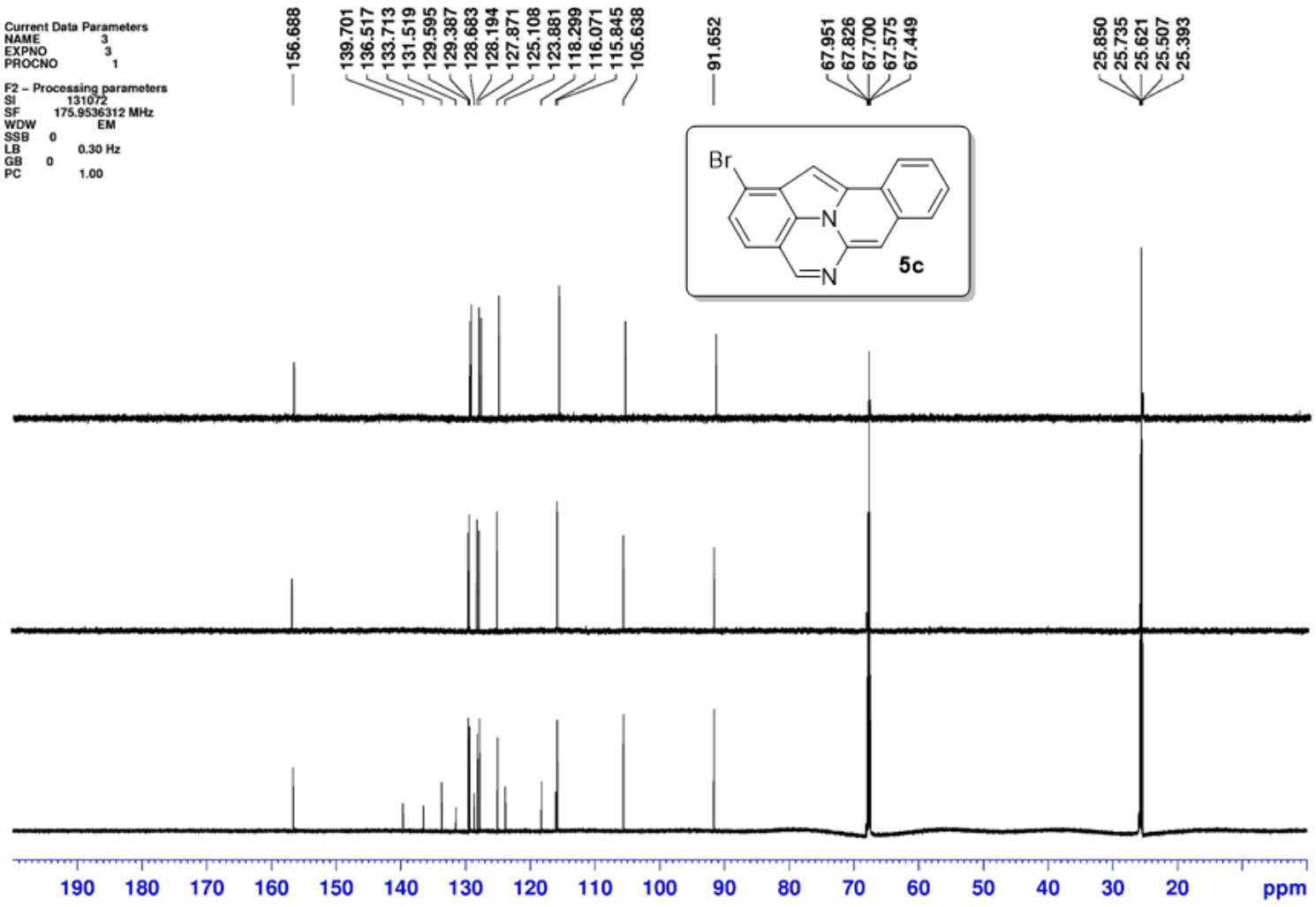
$^{13}C\{^{1}H\}$ NMR (125 MHz, $CDCl_3$)



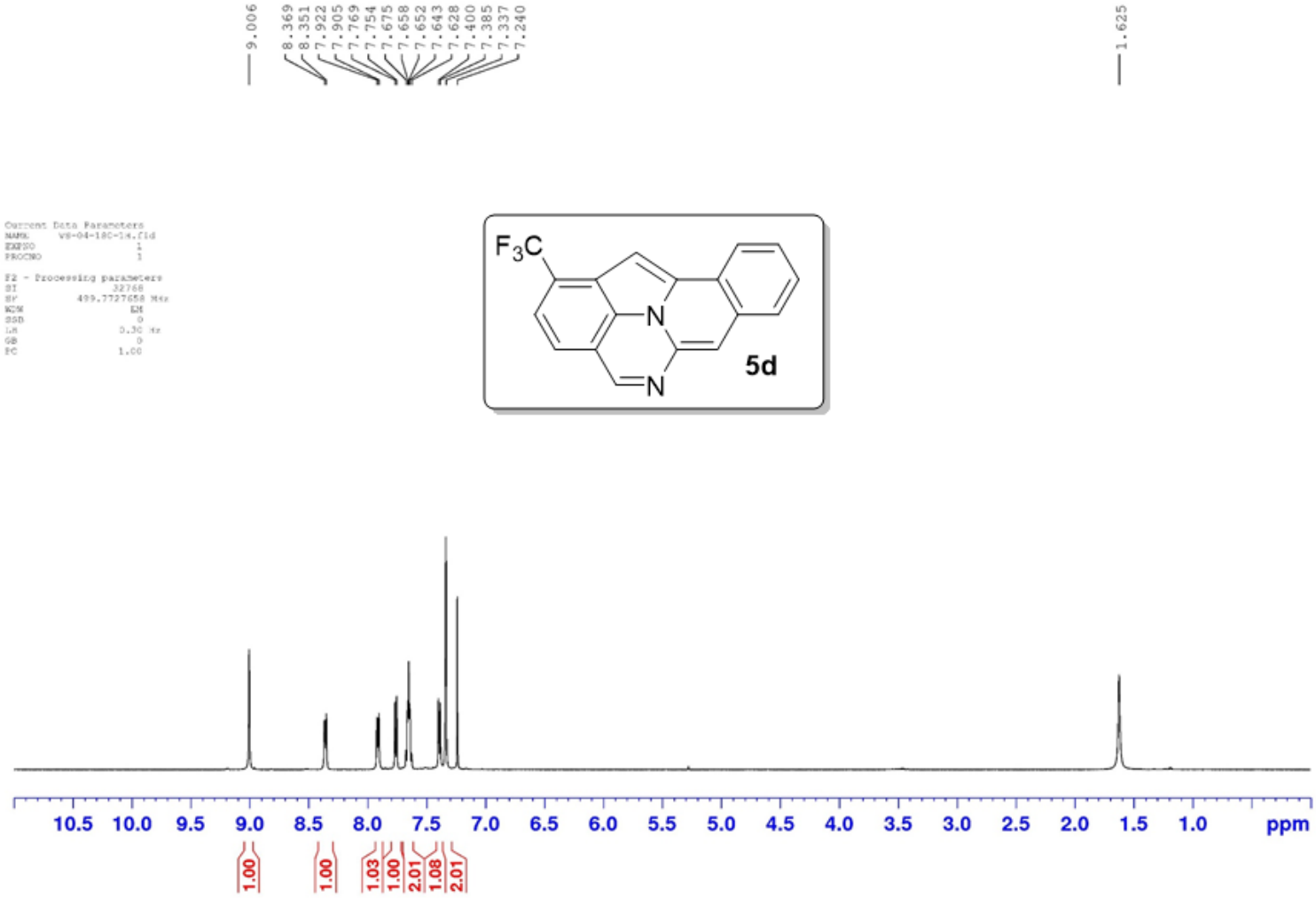
^{1}H-NMR (500 MHz, *d*-THF)



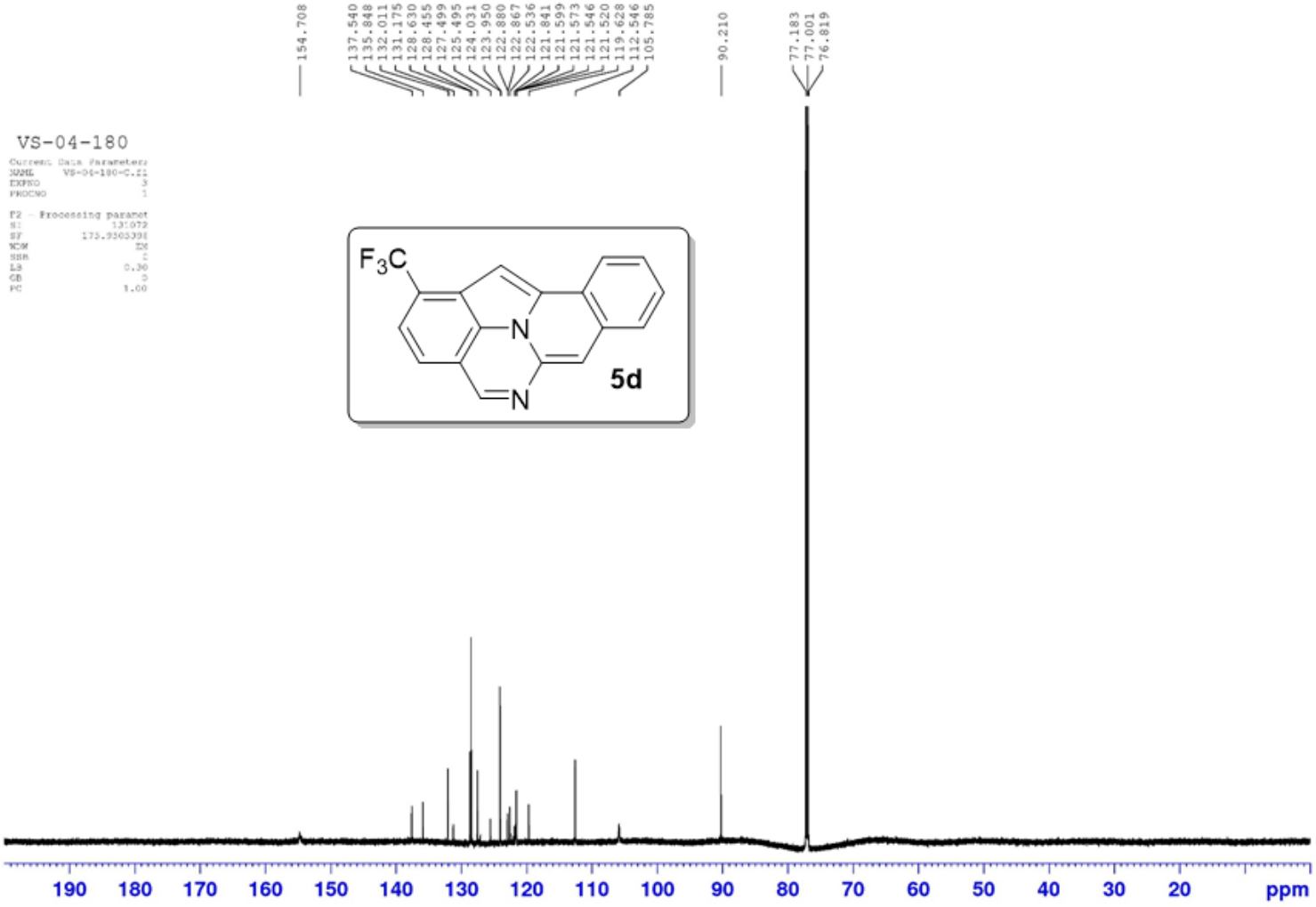
$^{13}C\{^{1}H\}$ and DEPT NMR (175 MHz, *d*-THF)



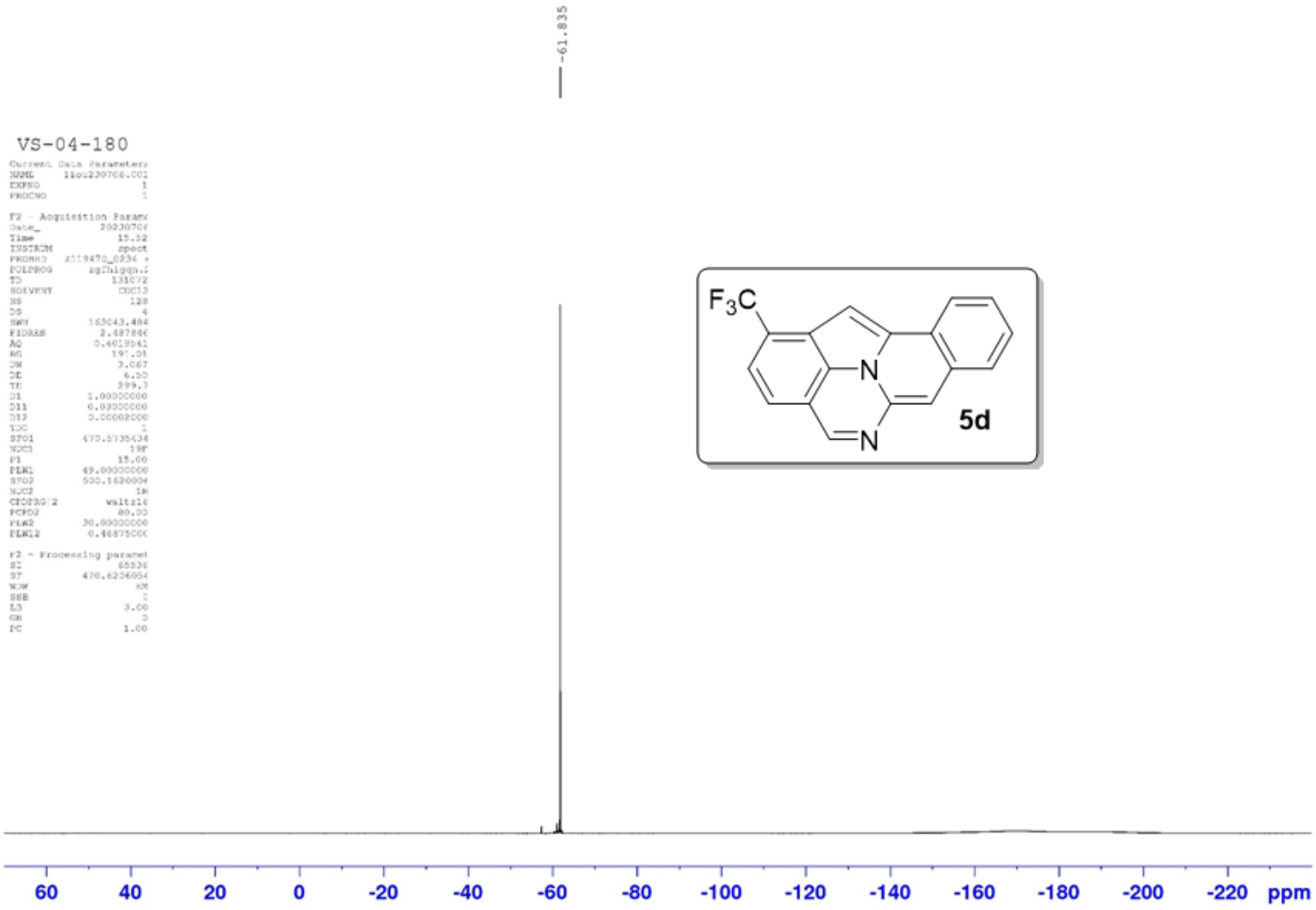
^{1}H-NMR (500 MHz, $CDCl_3$)



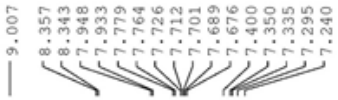
$^{13}C\{^{1}H\}$ NMR (175 MHz, $CDCl_3$)

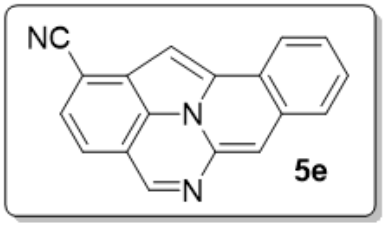


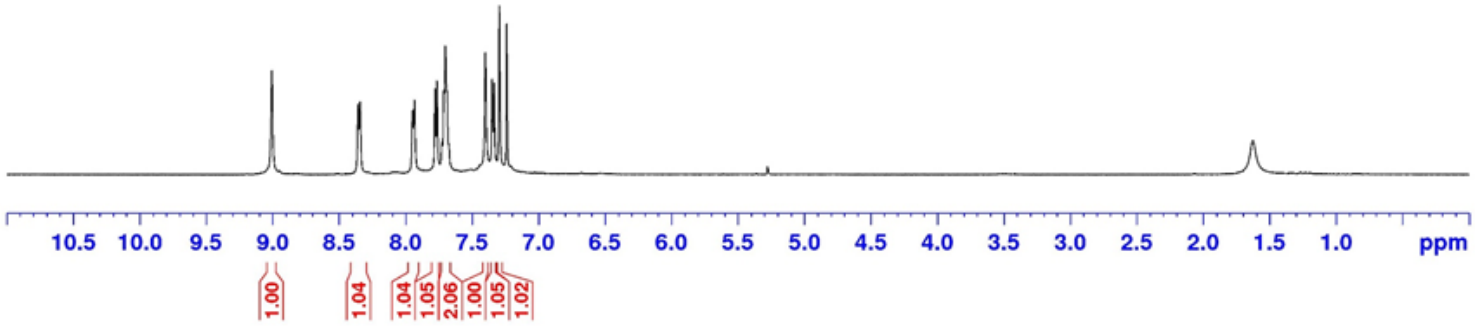
^{19}F {^{1}H} NMR (500 MHz, $CDCl_3$)



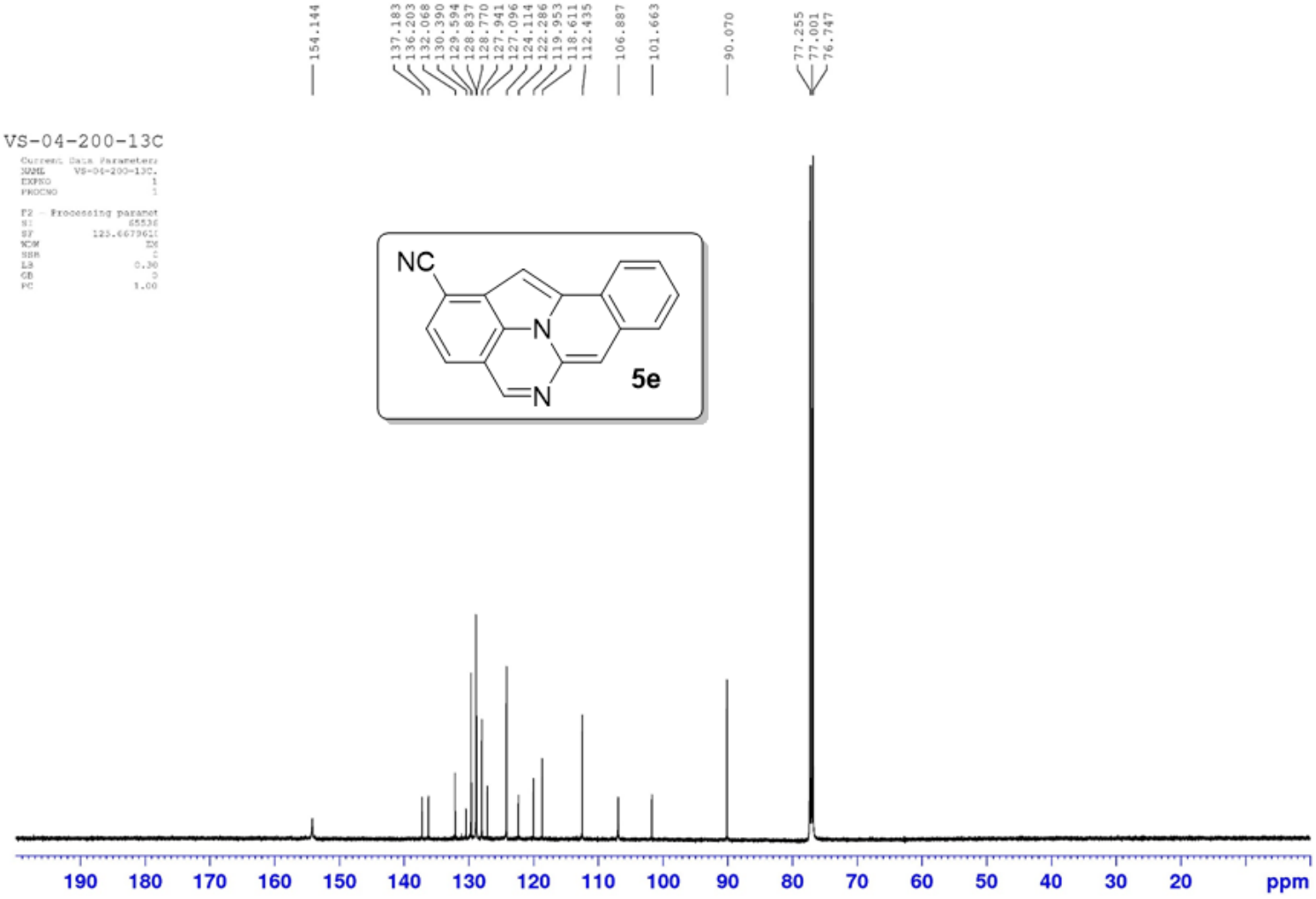
^{1}H-NMR (500 MHz, $CDCl_3$)



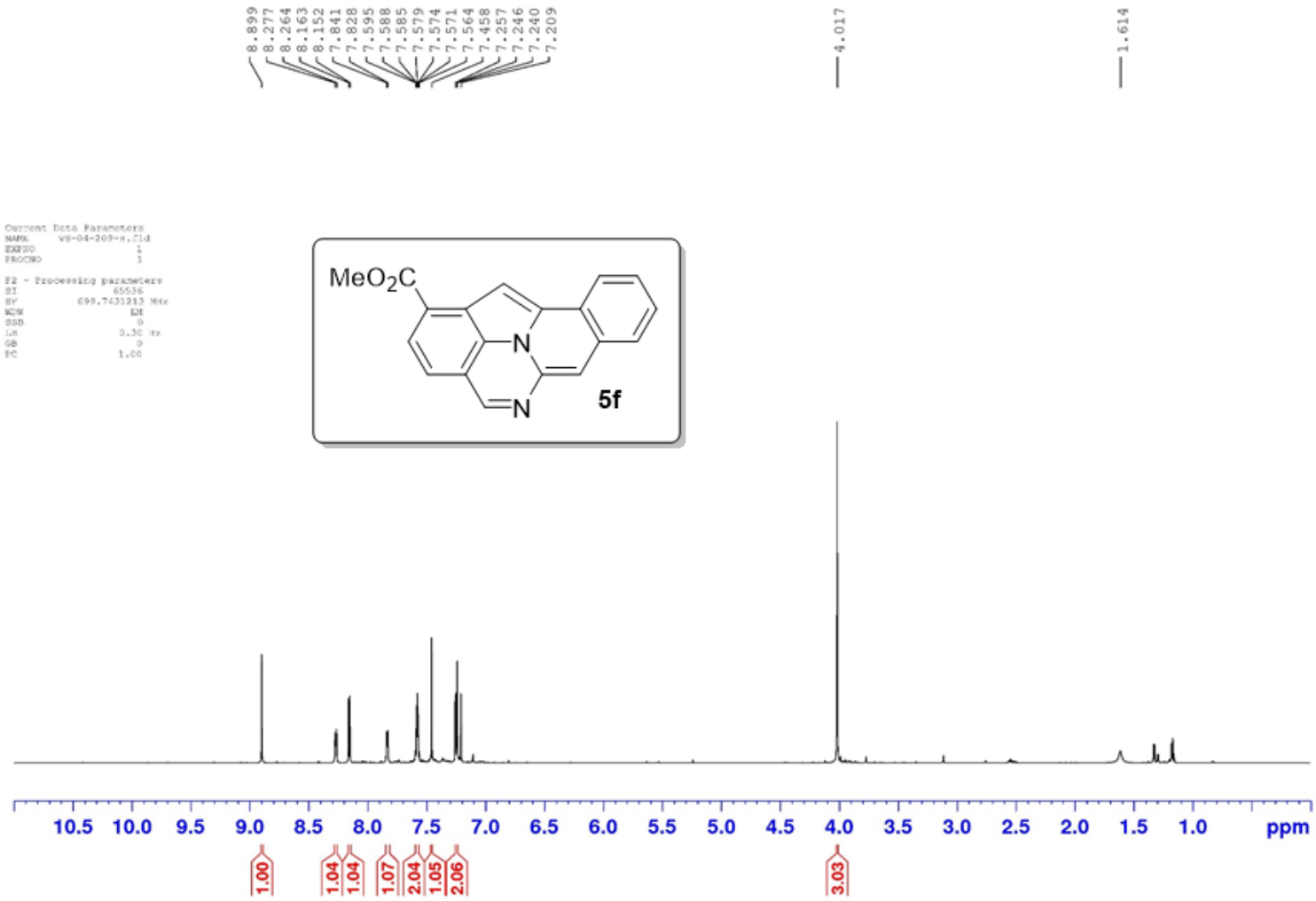




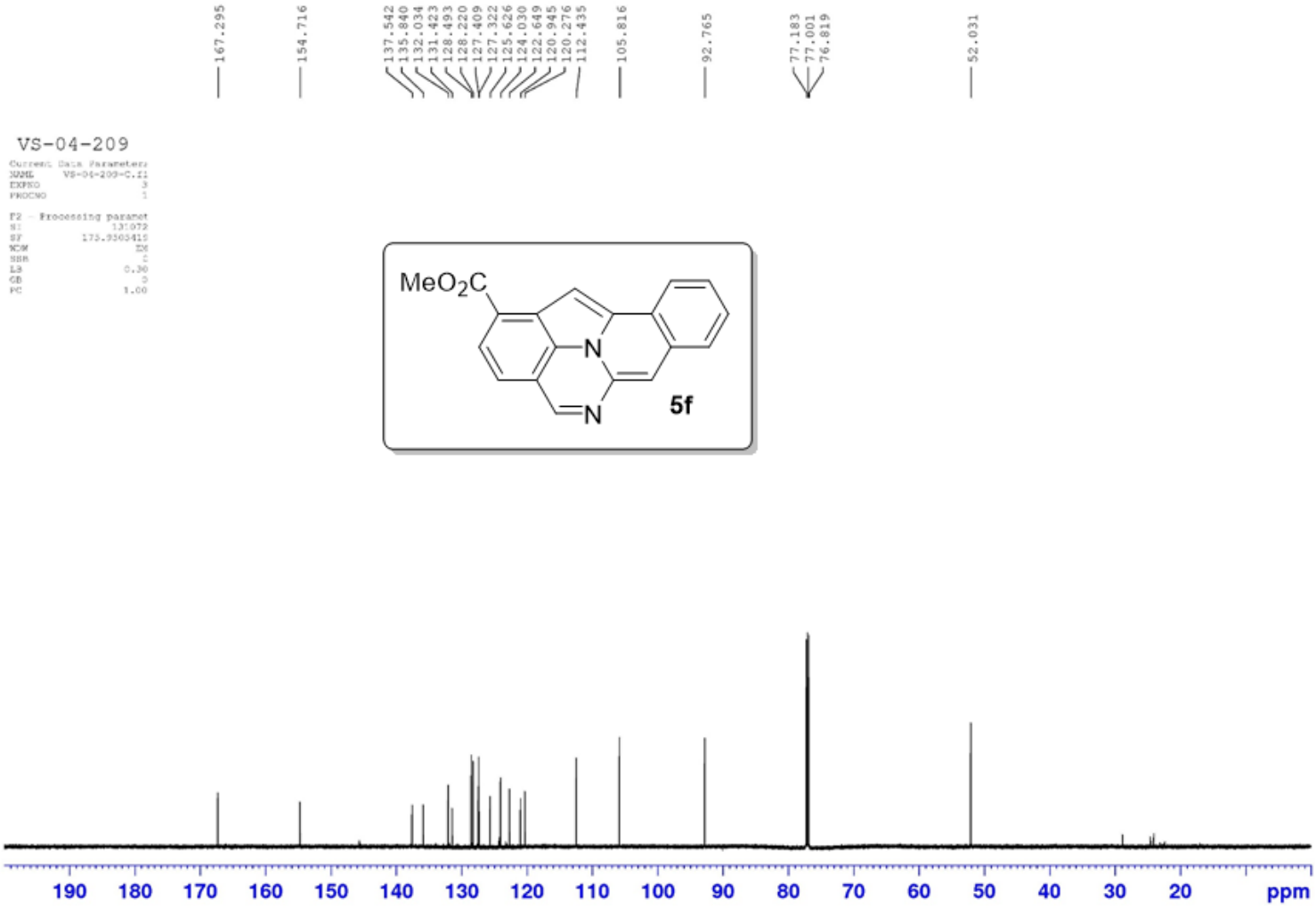
$^{13}C\{^{1}H\}$ NMR (125 MHz, $CDCl_3$)



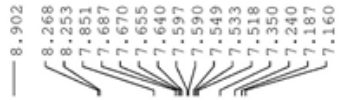
^{1}H-NMR (700 MHz, $CDCl_3$)

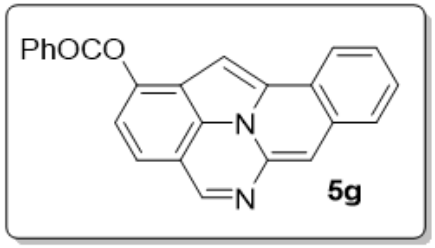


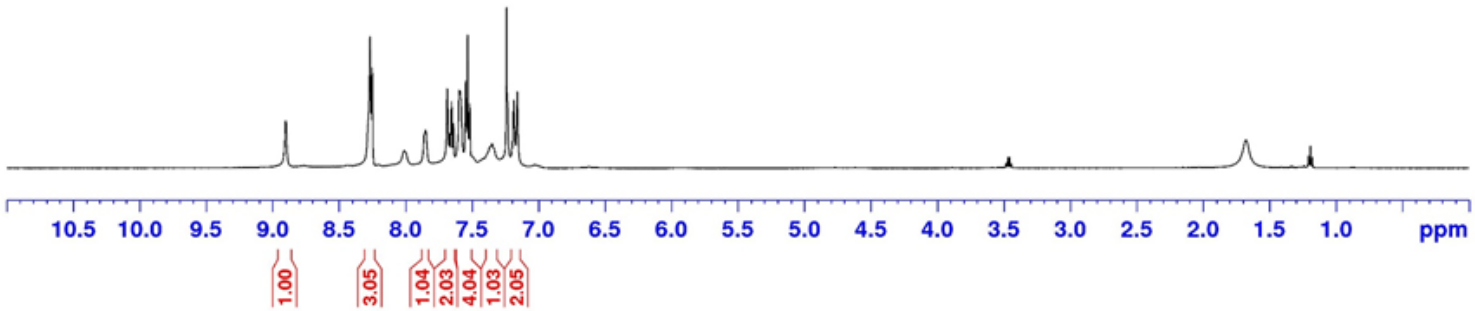
$^{13}C\{^{1}H\}$ NMR (175 MHz, $CDCl_3$)



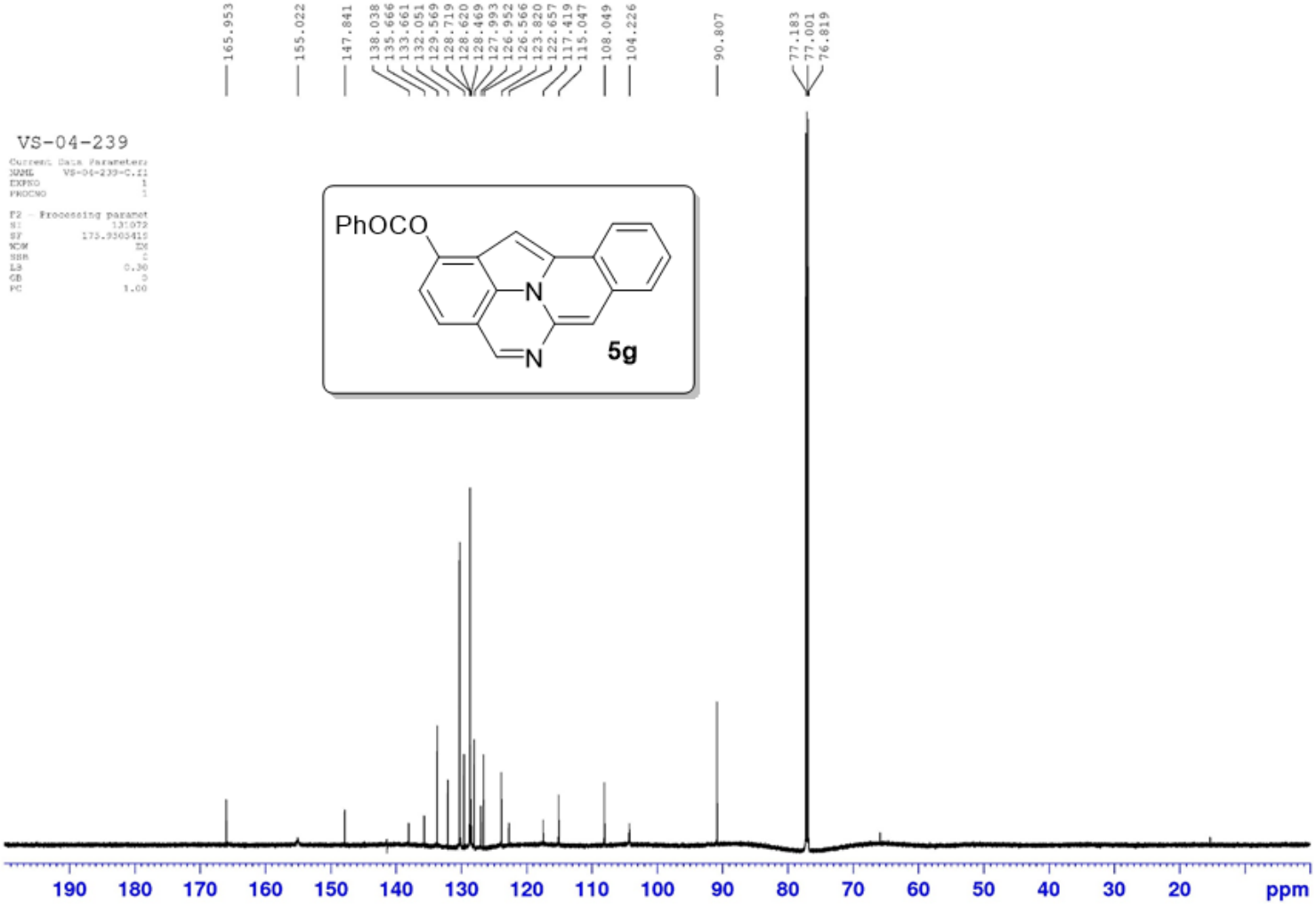
^{1}H-NMR (500 MHz, $CDCl_3$)



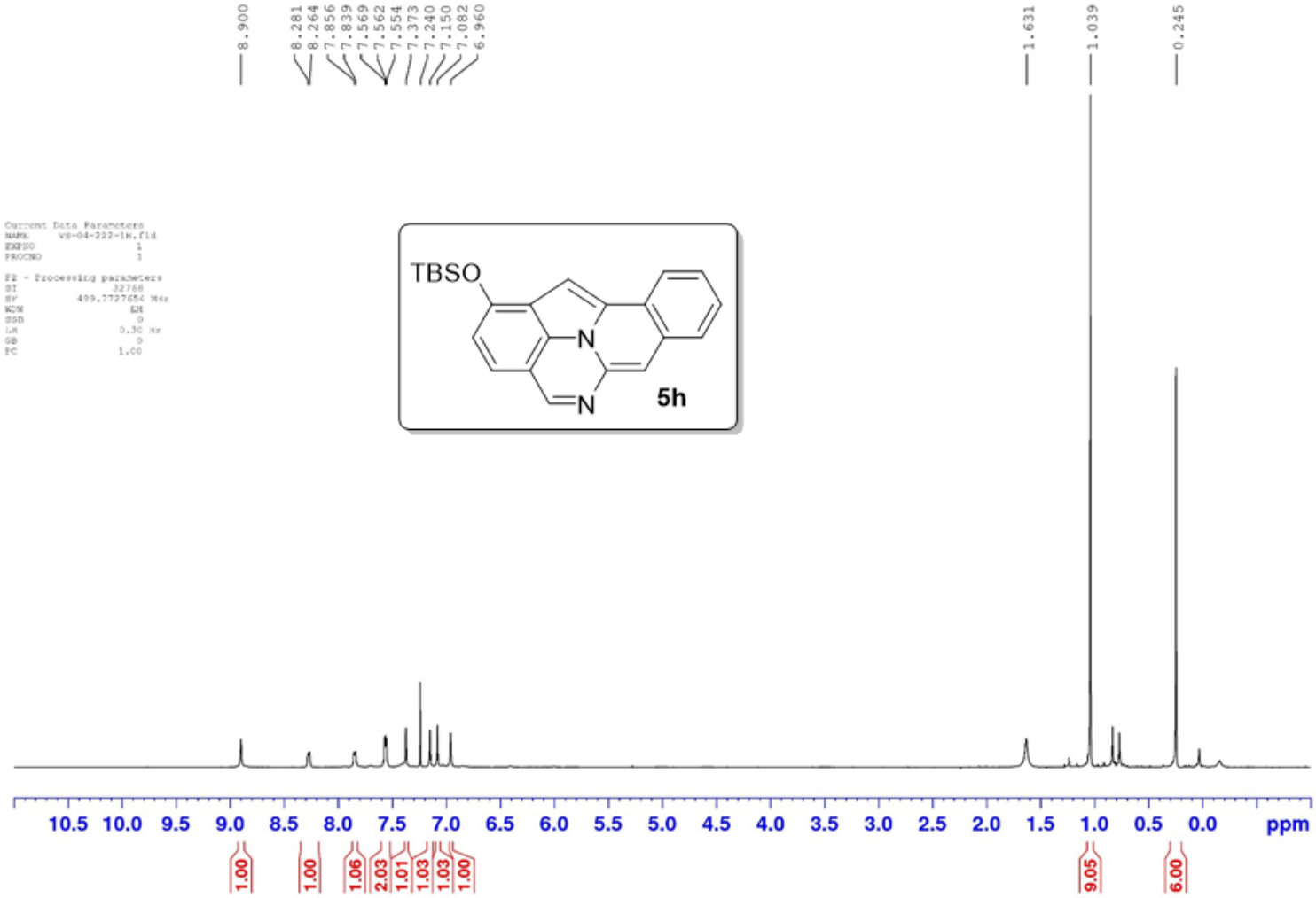




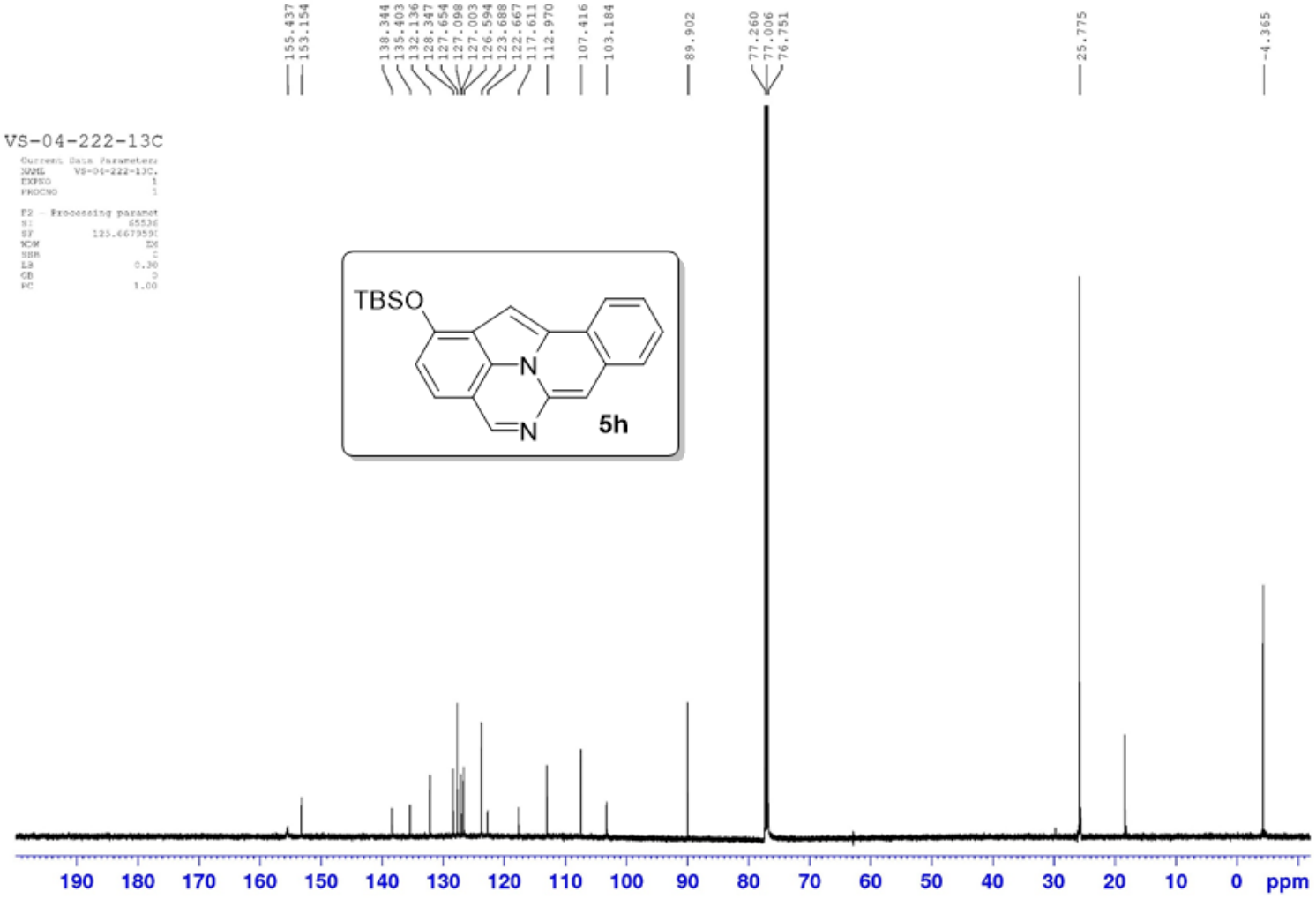
$^{13}C\{^{1}H\}$ NMR (175 MHz, $CDCl_3$)



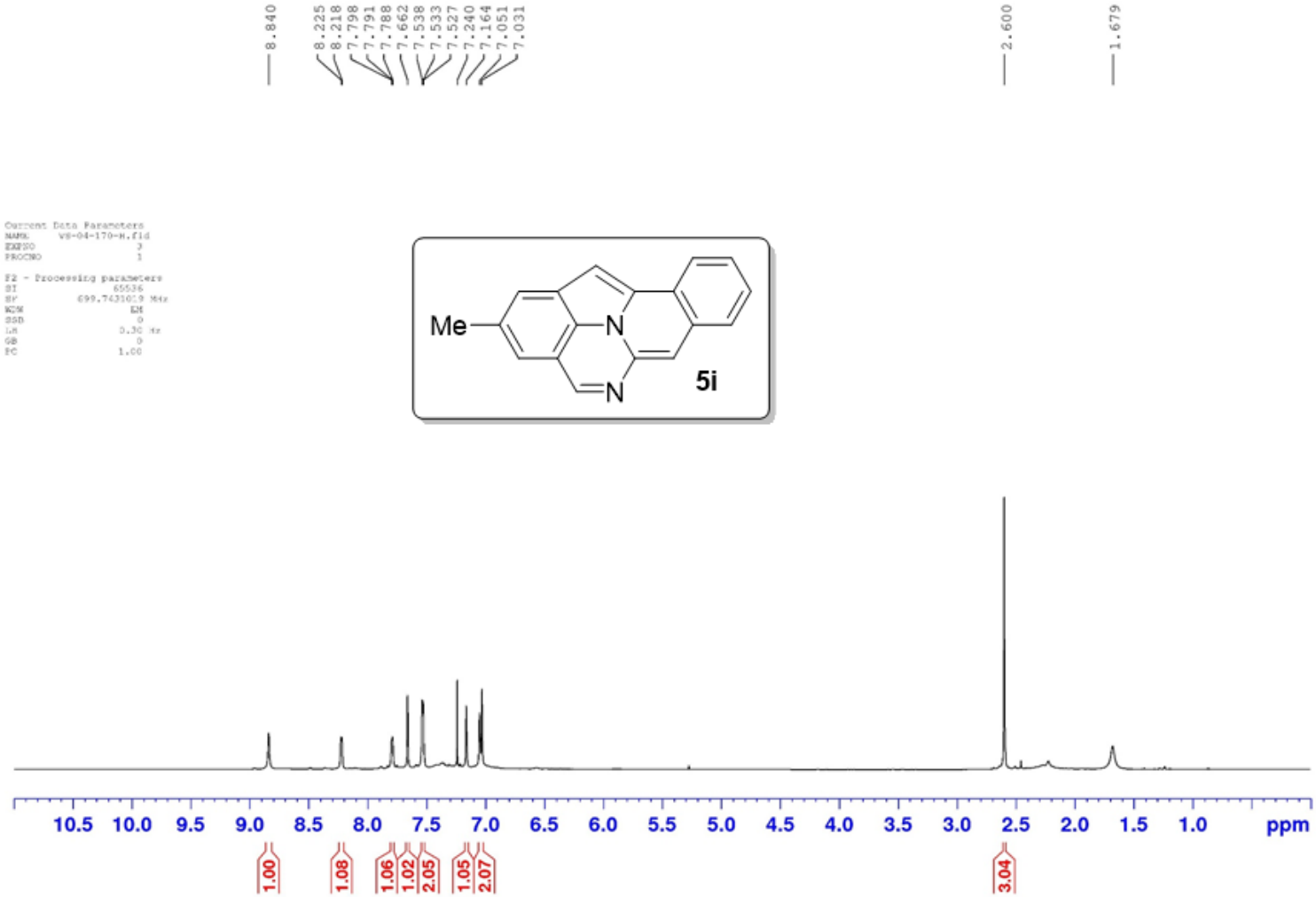
^{1}H-NMR (500 MHz, $CDCl_3$)



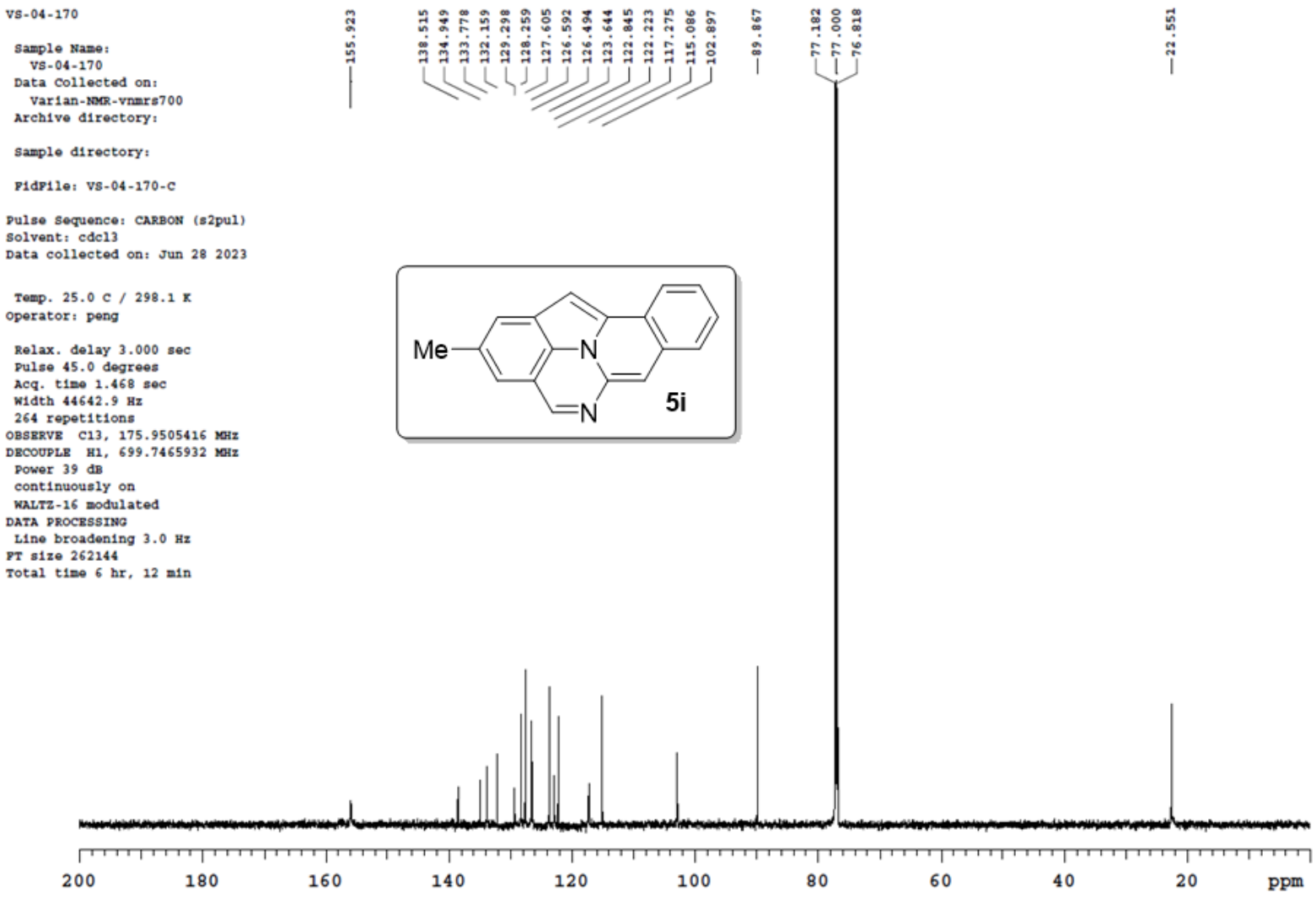
$^{13}C\{^{1}H\}$ NMR (125 MHz, $CDCl_3$)



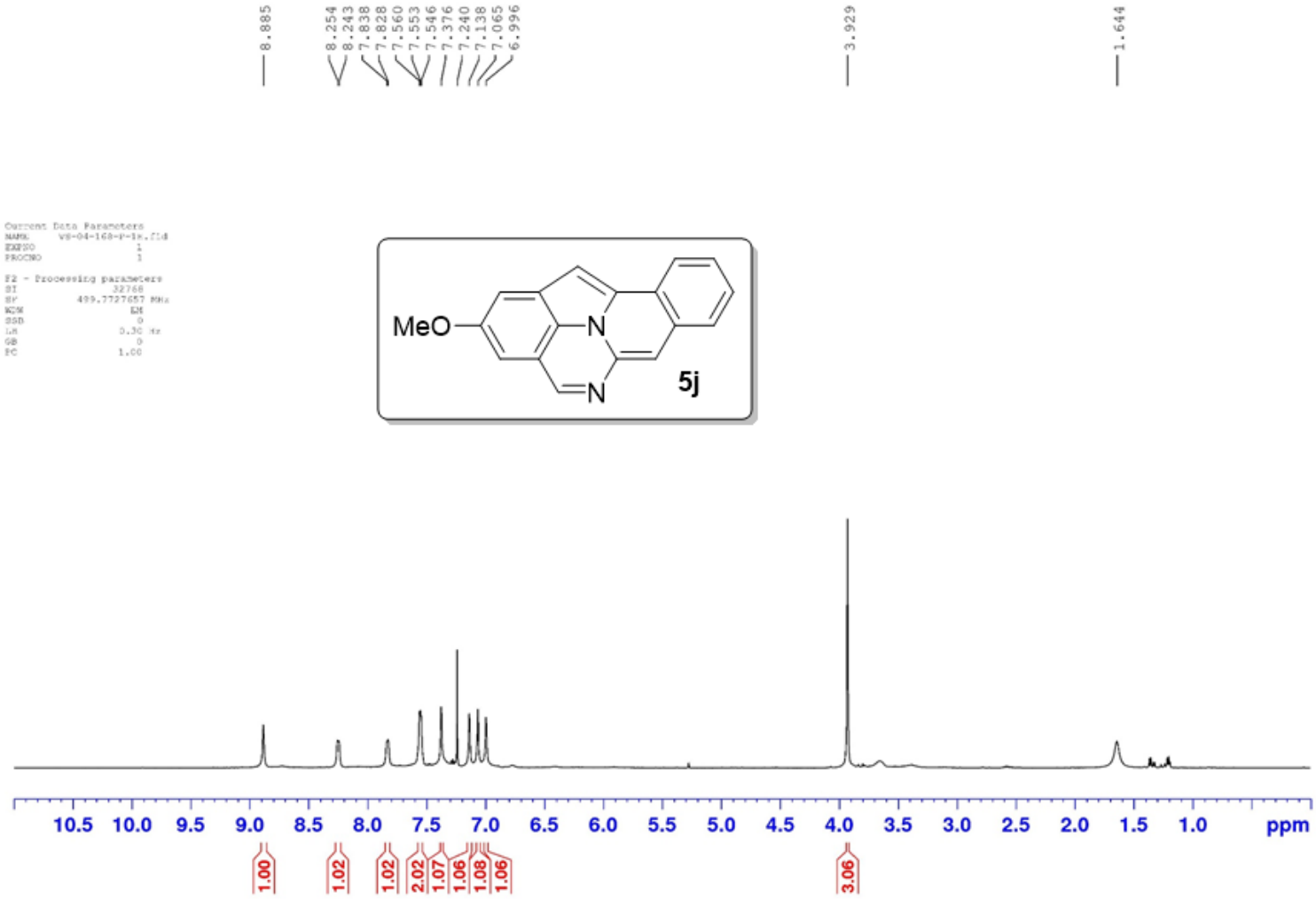
^{1}H-NMR (700 MHz, $CDCl_3$)



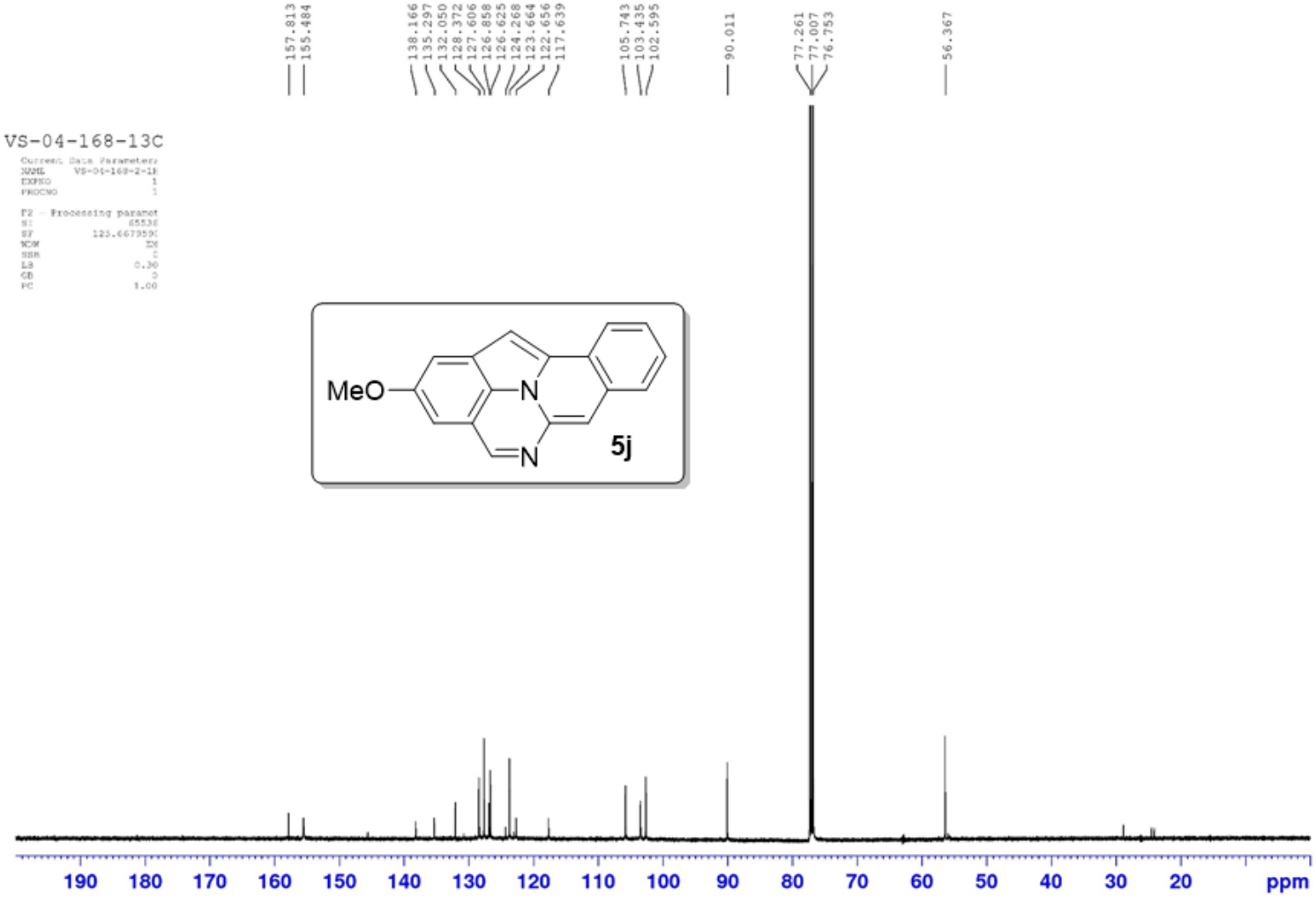
$^{13}C\{^{1}H\}$ NMR (175 MHz, $CDCl_3$)



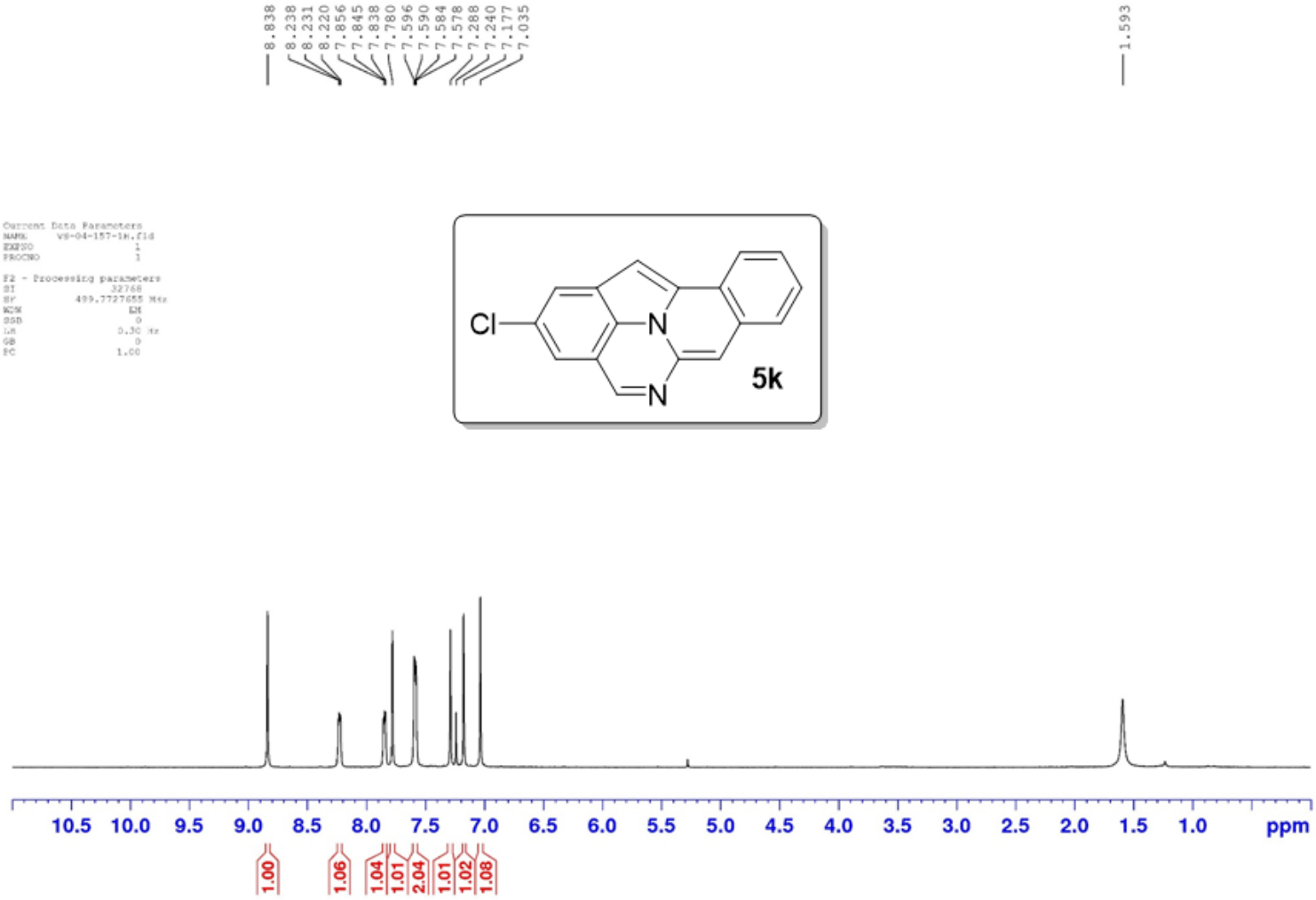
^{1}H-NMR (500 MHz, $CDCl_3$)



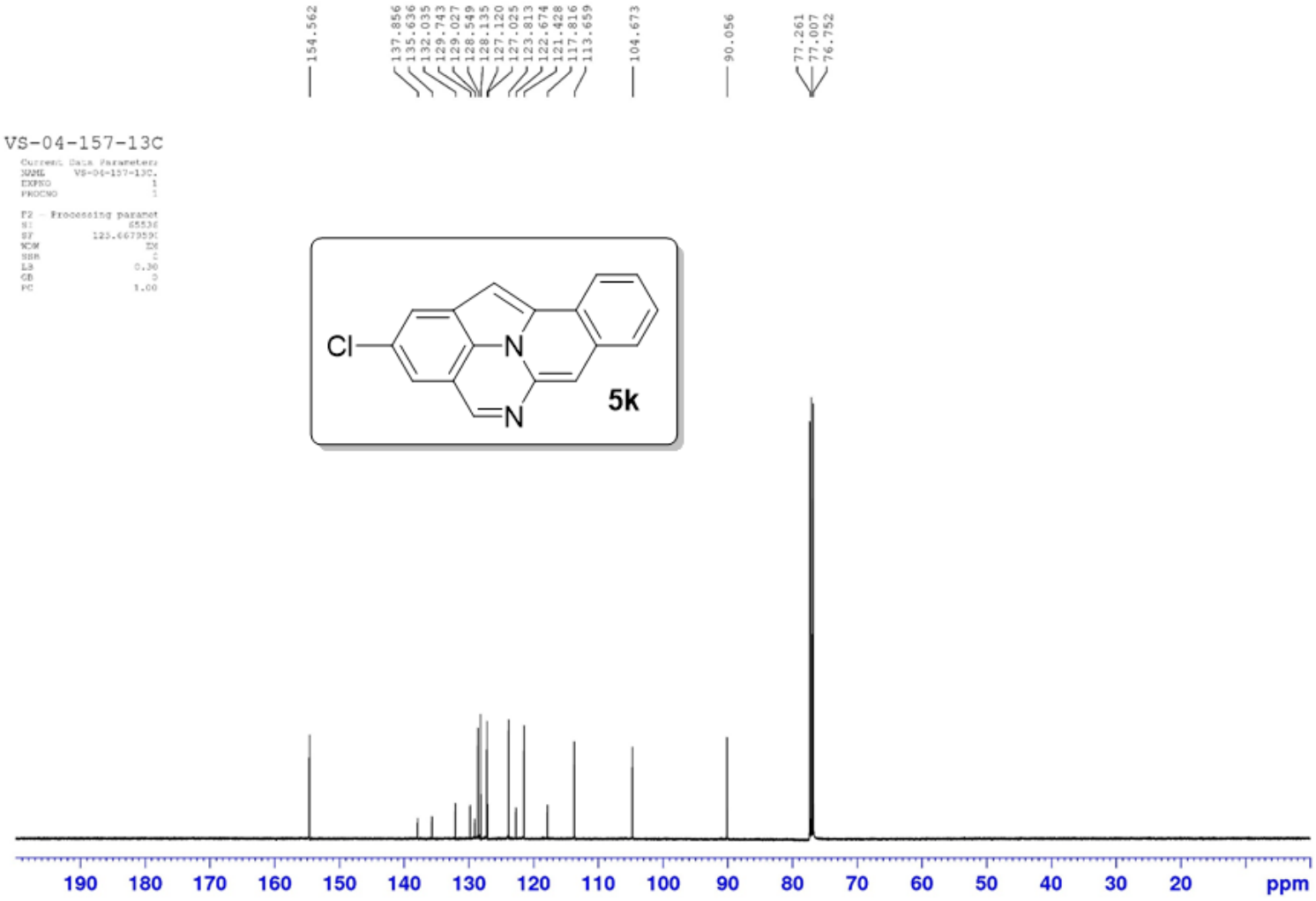
$^{13}C\{^{1}H\}$ NMR (125 MHz, $CDCl_3$)



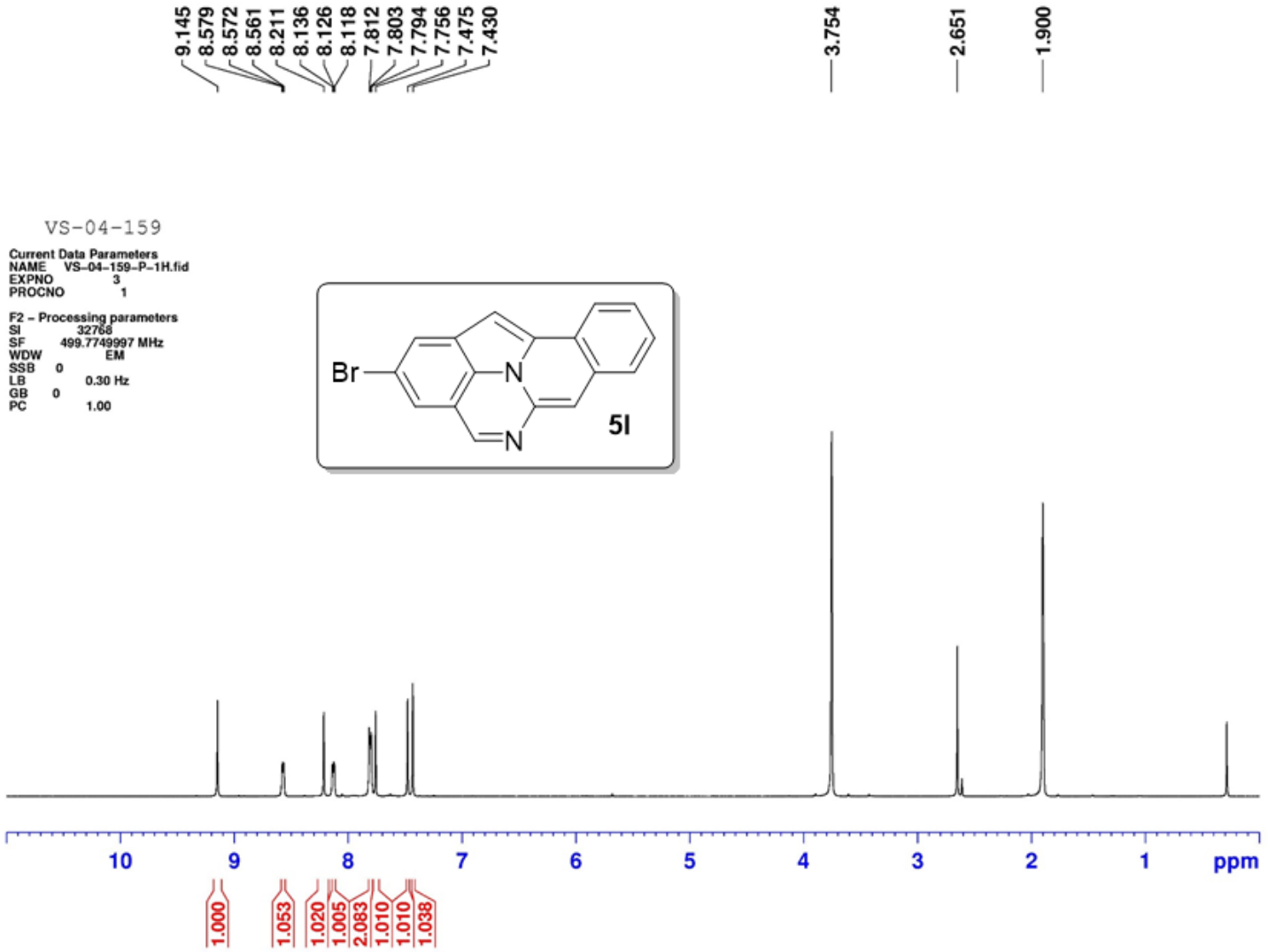
^{1}H-NMR (500 MHz, $CDCl_3$)



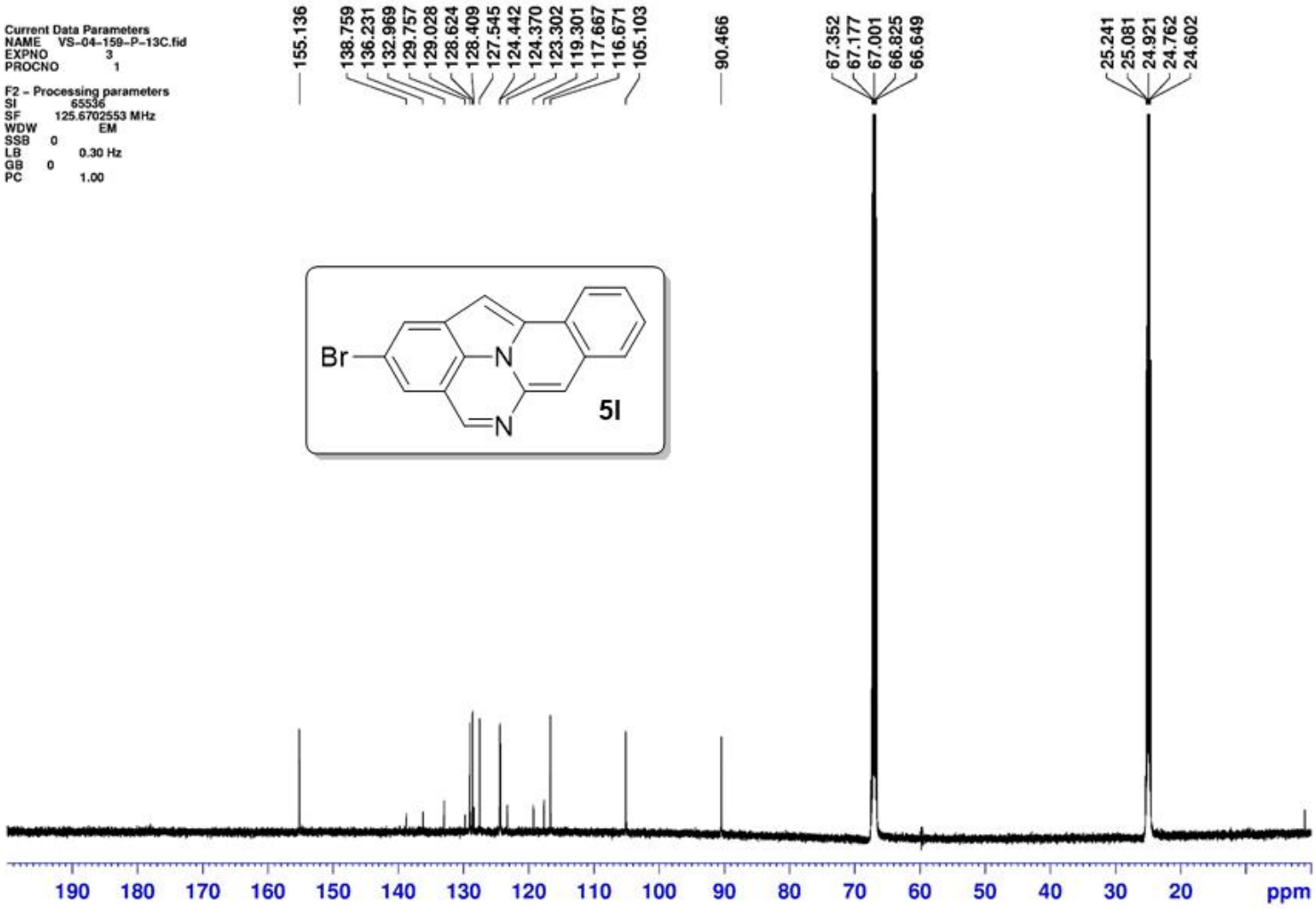
$^{13}C\{^{1}H\}$ NMR (125 MHz, $CDCl_3$)



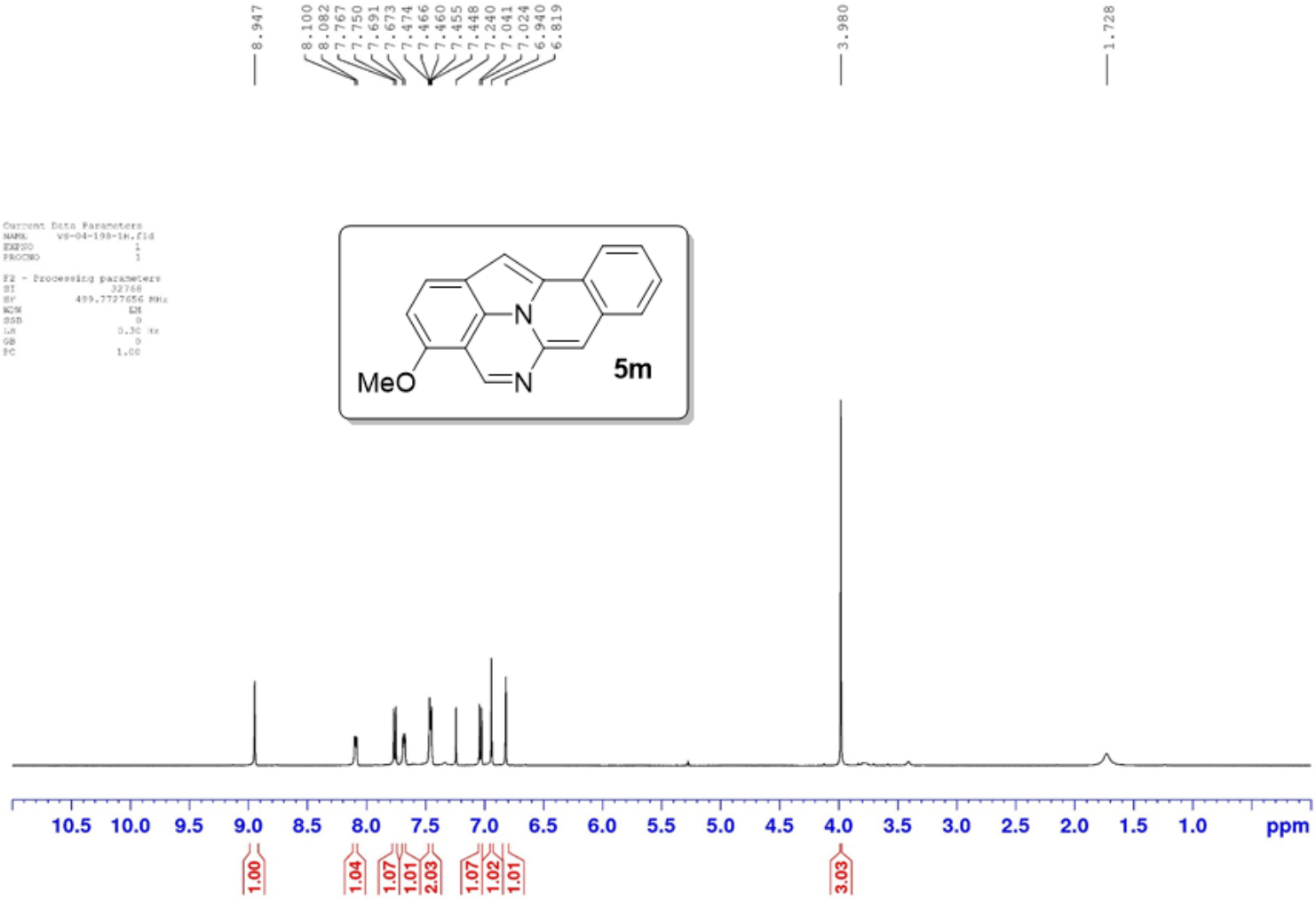
^{1}H-NMR (500 MHz, *d*-THF)



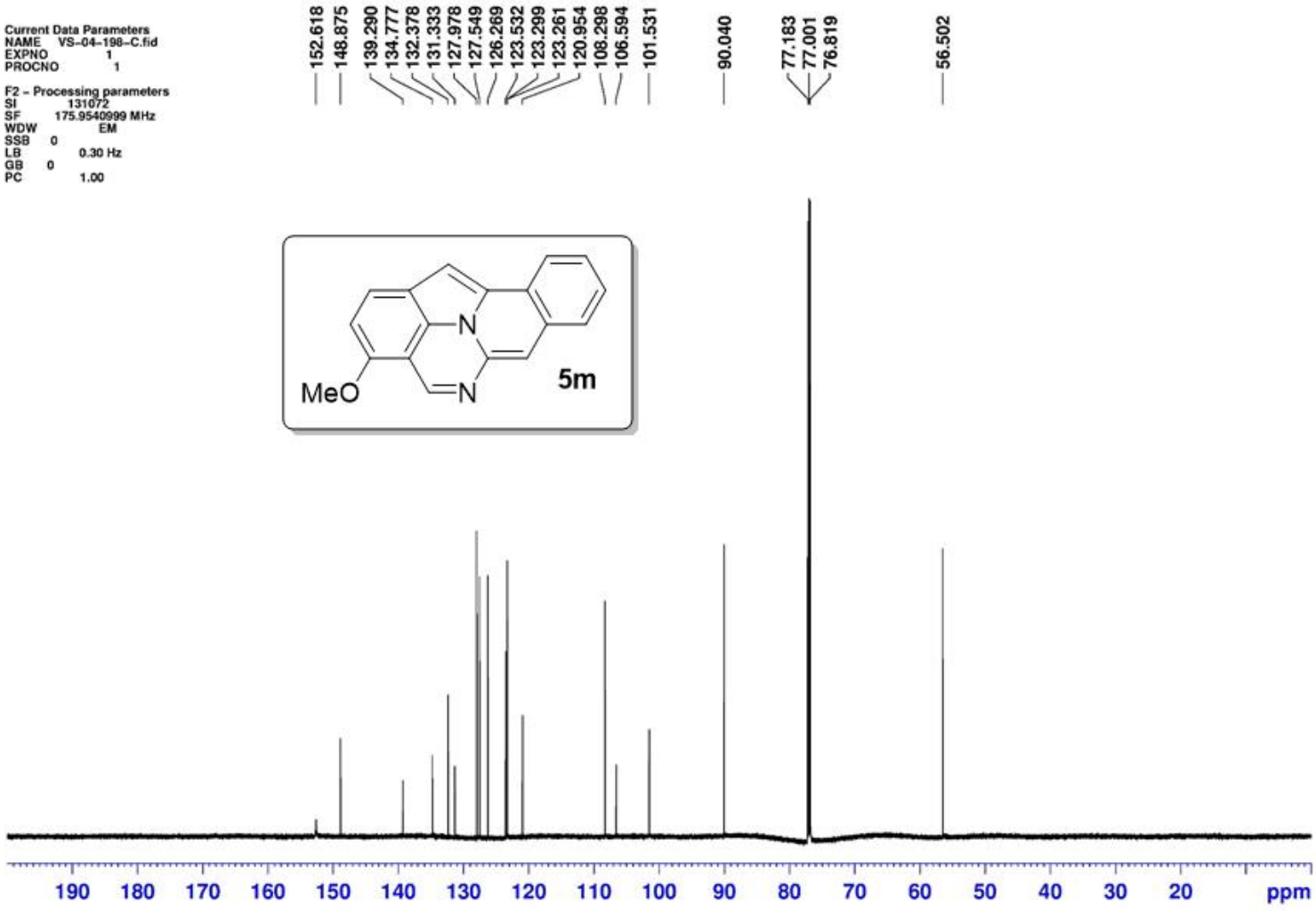
$^{13}C\{^{1}H\}$ NMR (125 MHz, *d*-THF)



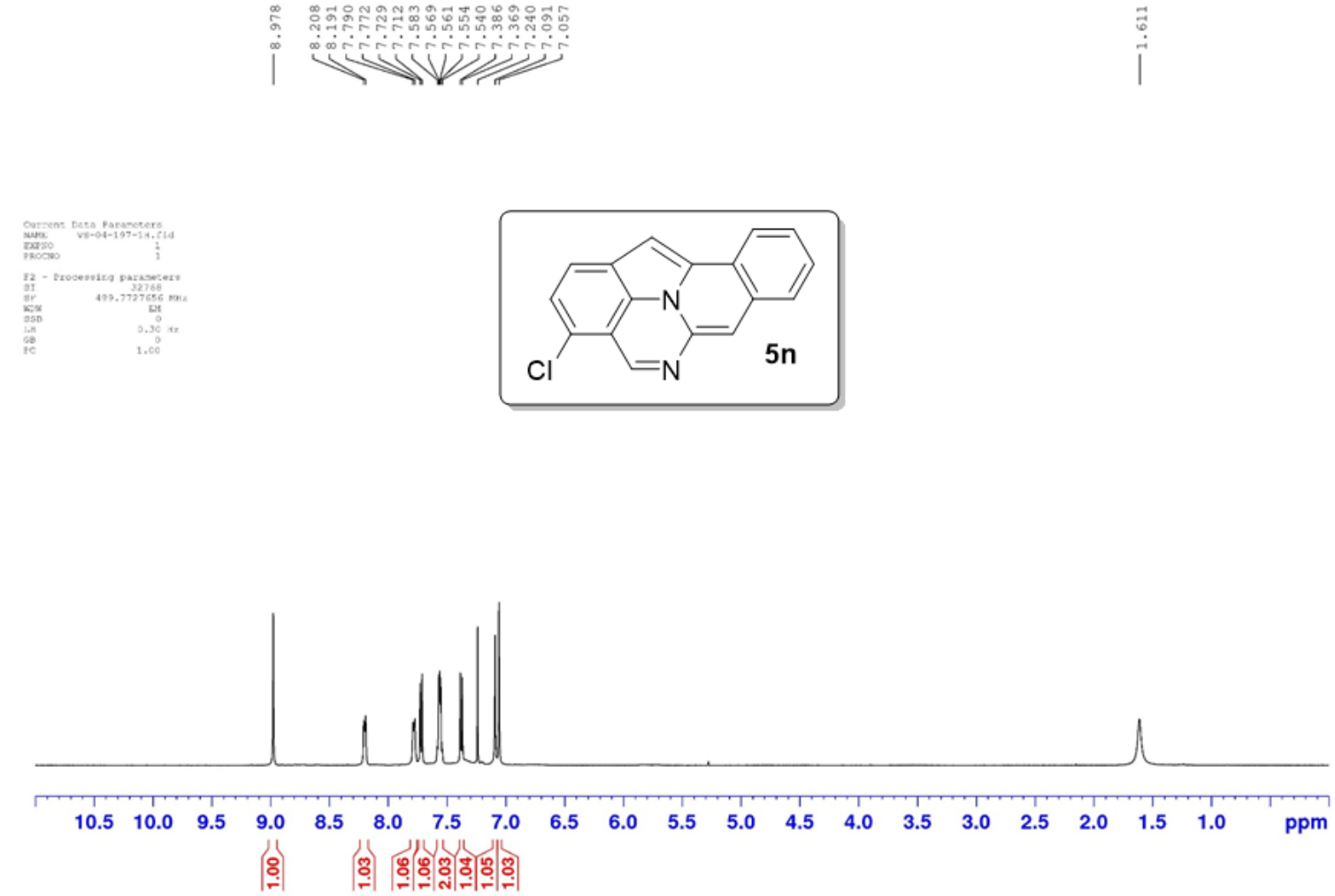
^{1}H-NMR (500 MHz, $CDCl_3$)



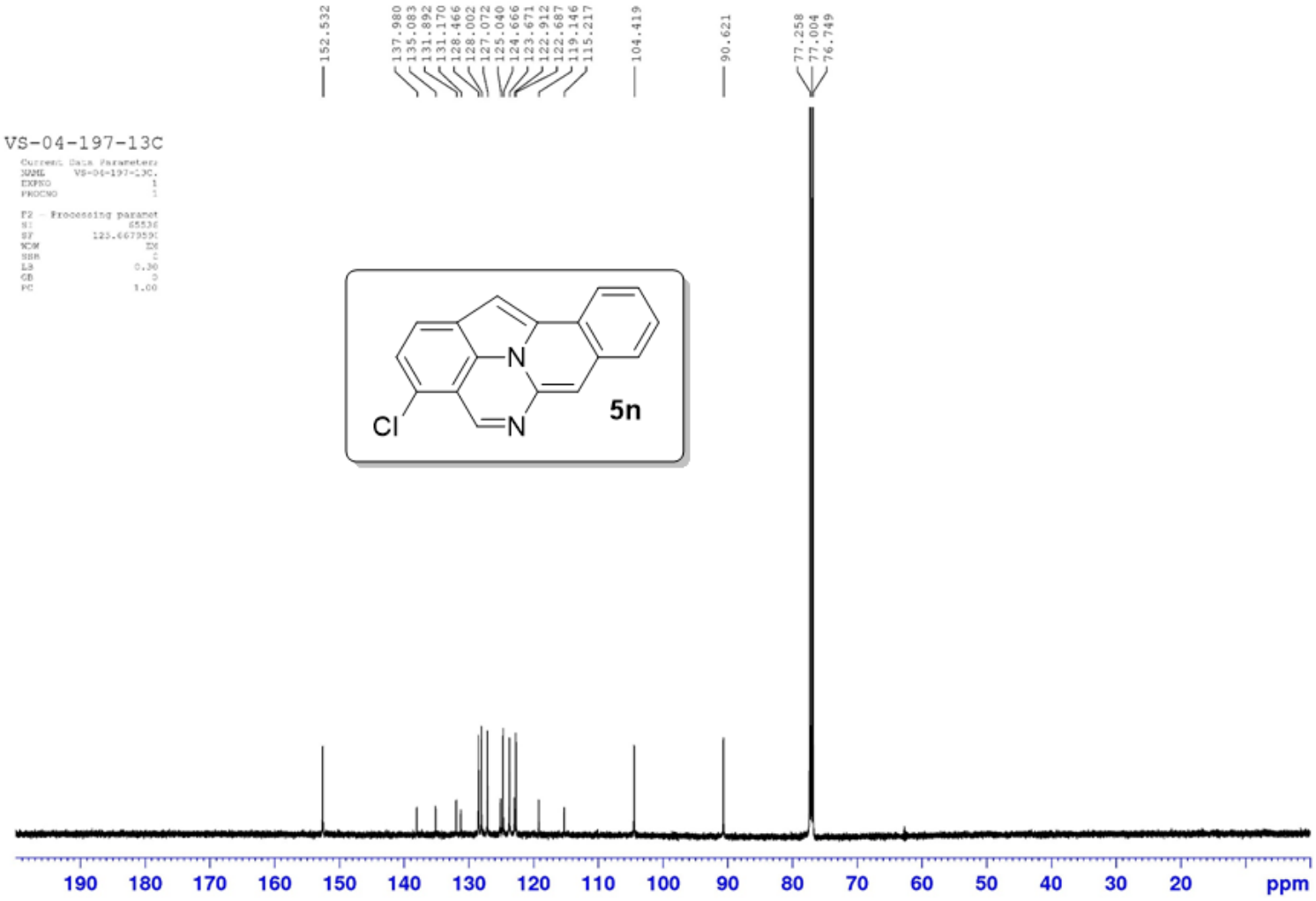
$^{13}C\{^{1}H\}$ NMR (175 MHz, $CDCl_3$)



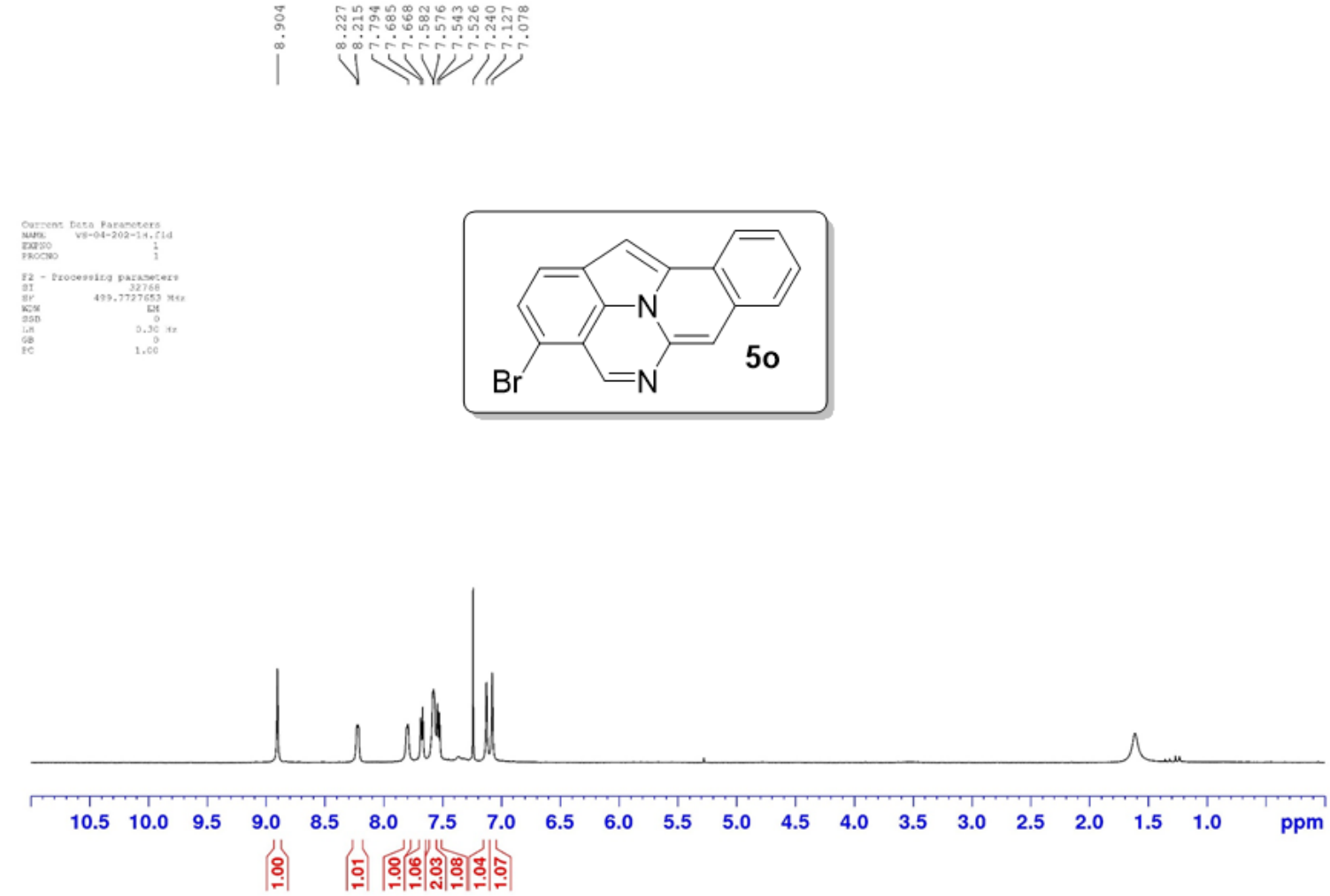
^{1}H-NMR (500 MHz, $CDCl_3$)



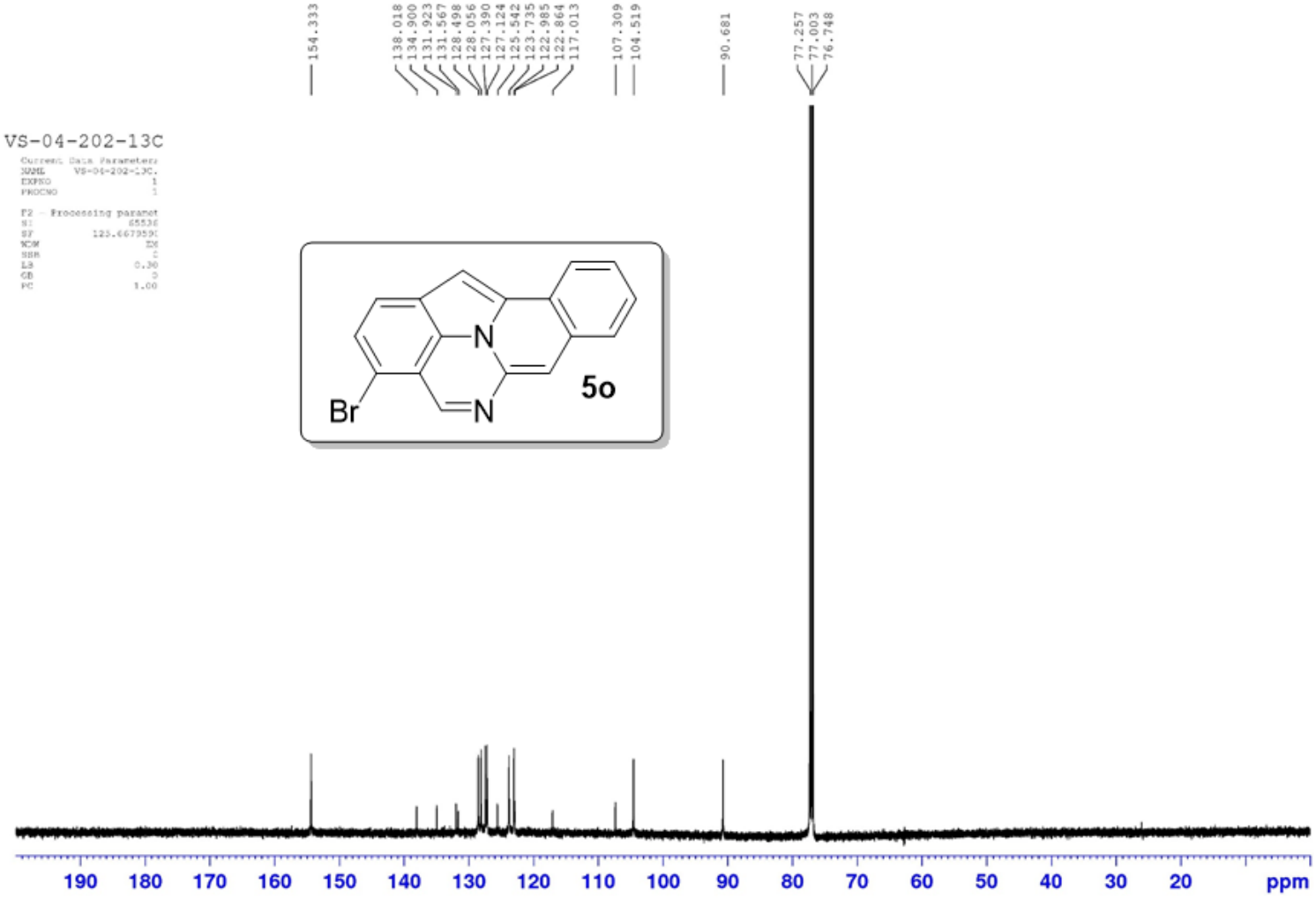
$^{13}C\{^{1}H\}$ NMR (125 MHz, $CDCl_3$)



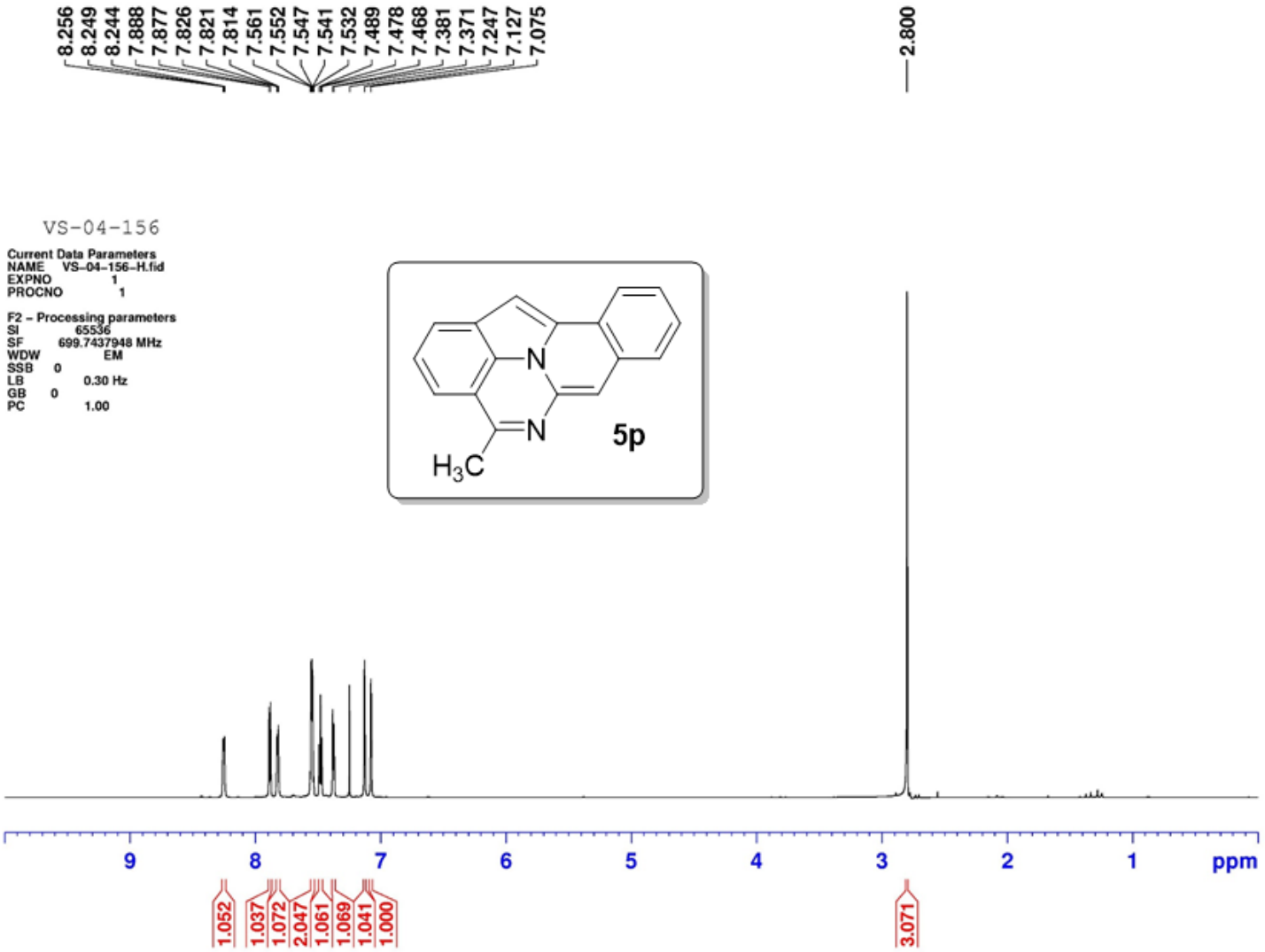
^{1}H-NMR (500 MHz, $CDCl_3$)



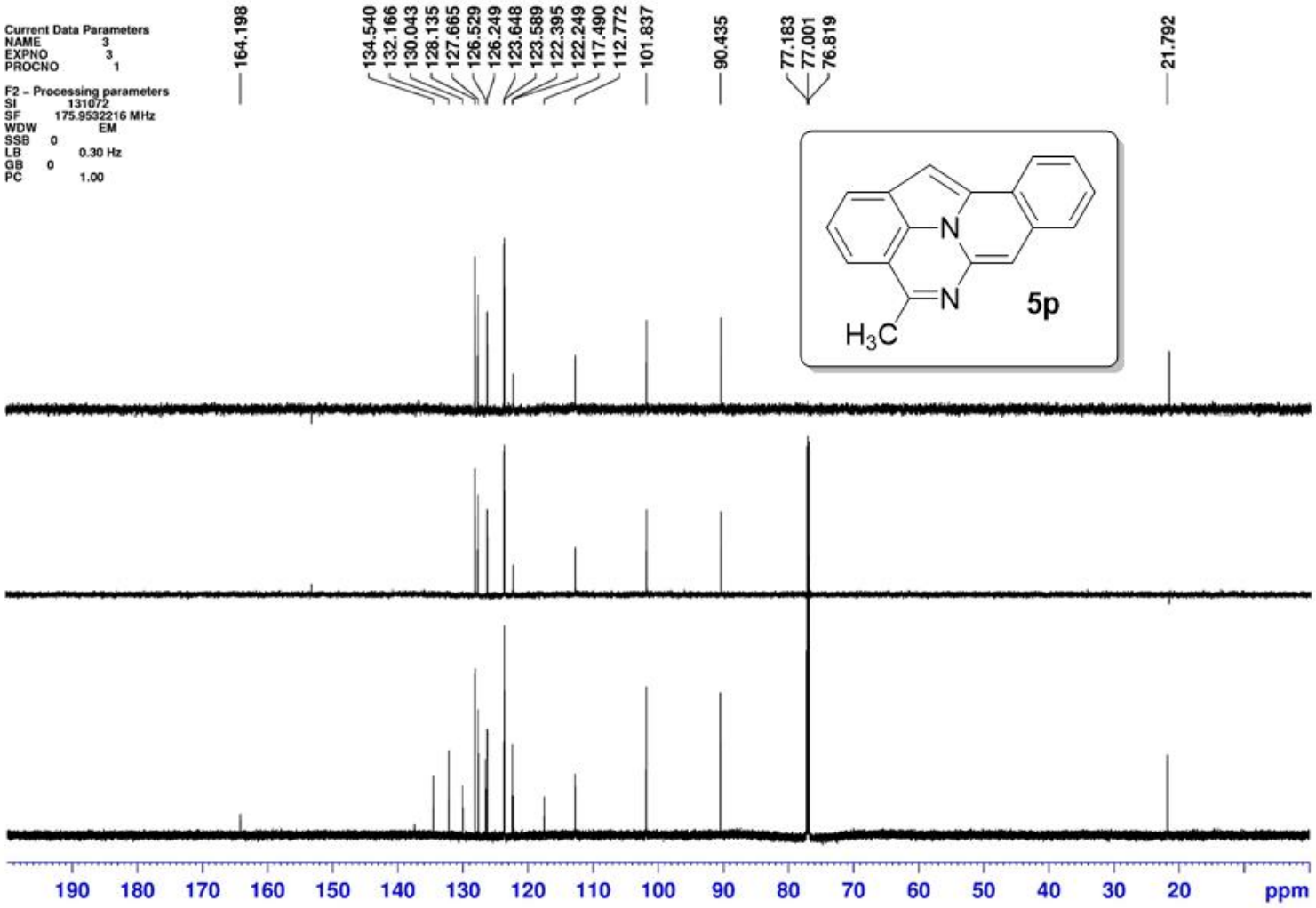
$^{13}C\{^{1}H\}$ NMR (125 MHz, $CDCl_3$)



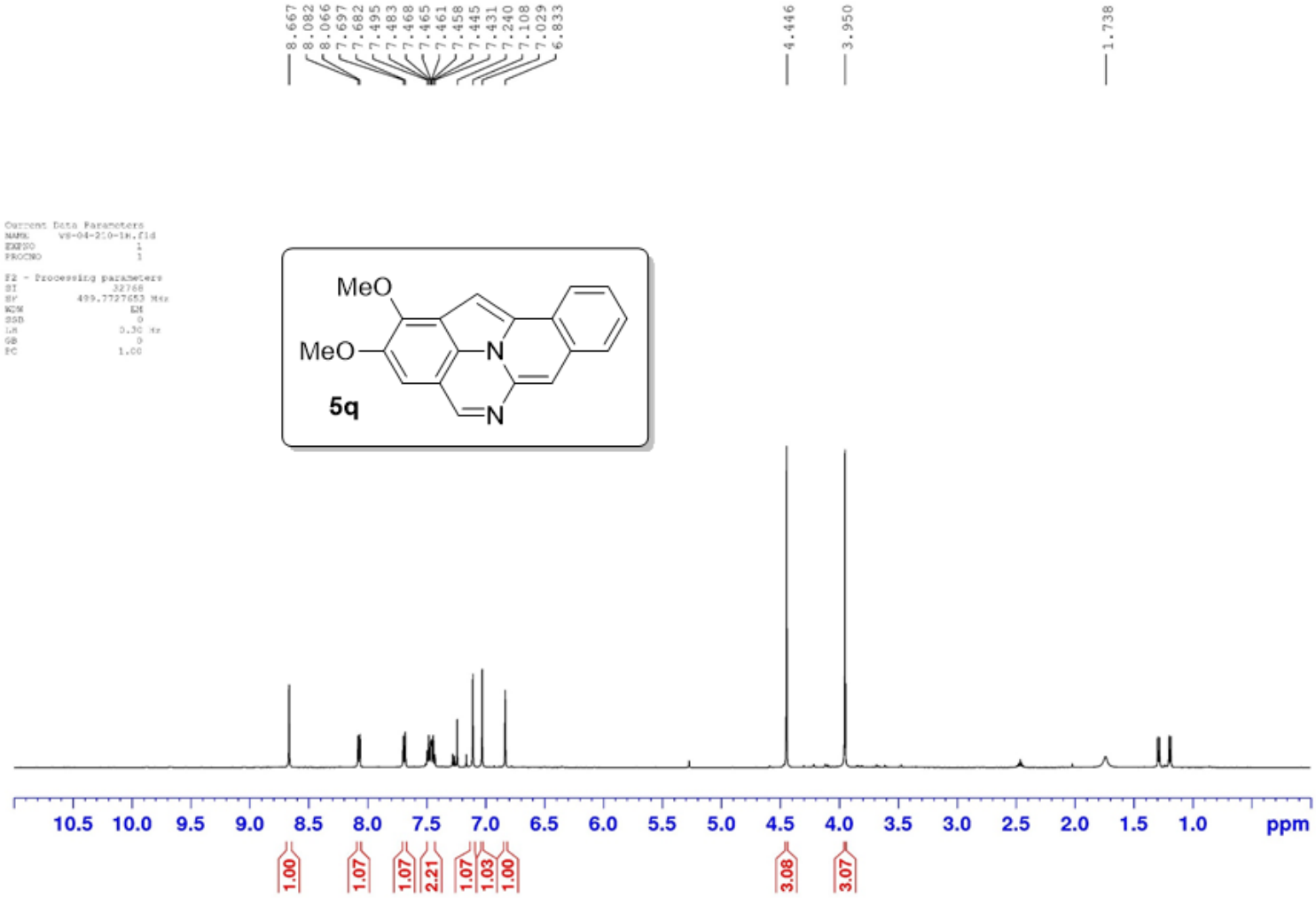
^{1}H-NMR (700 MHz, $CDCl_3$)



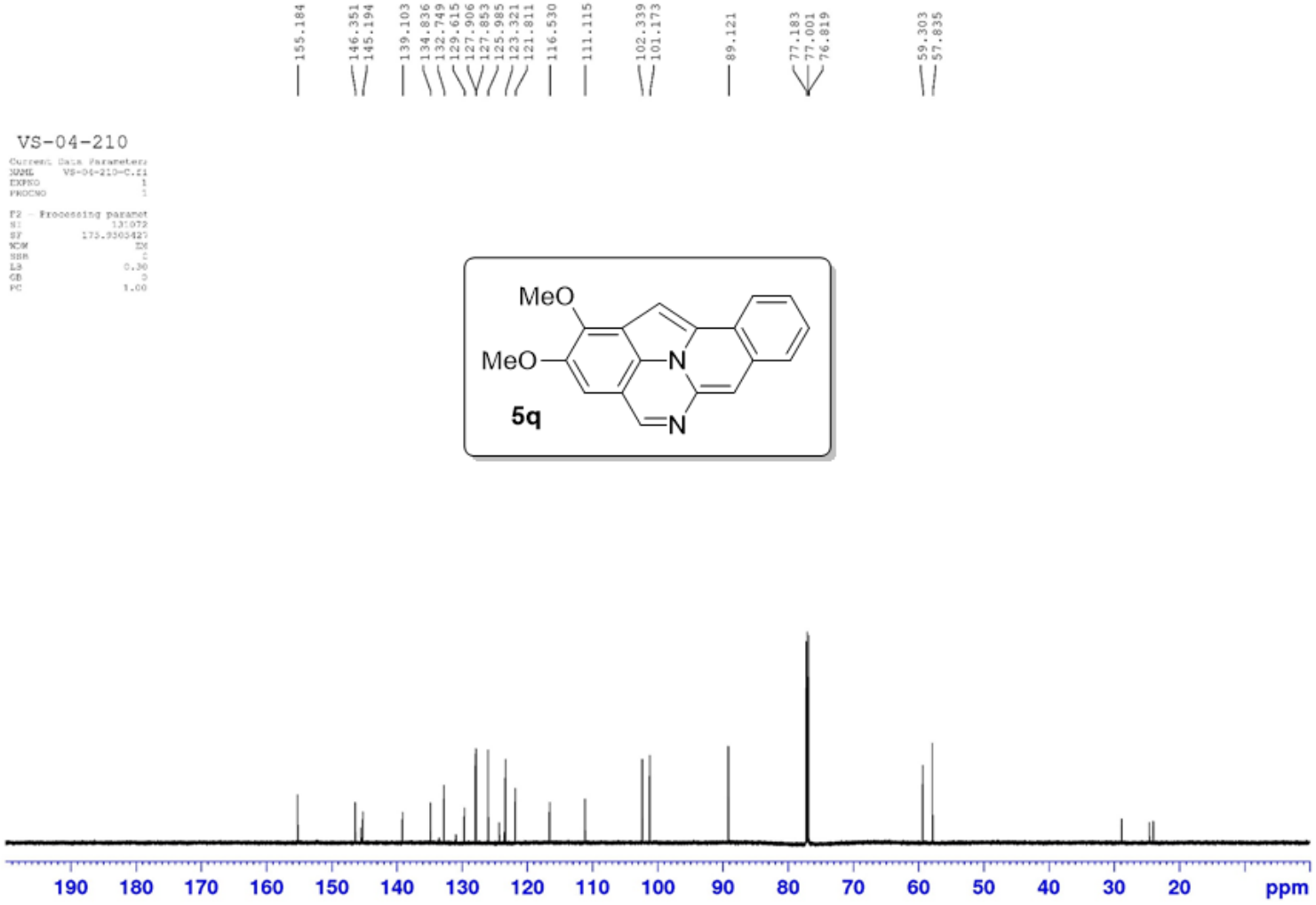
$^{13}C\{^{1}H\}$ and DEPT NMR (175 MHz, $CDCl_3$)



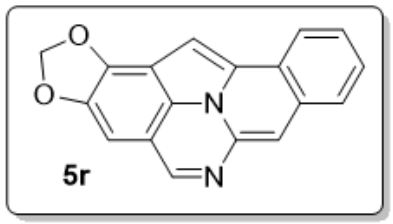
^{1}H-NMR (500 MHz, $CDCl_3$)

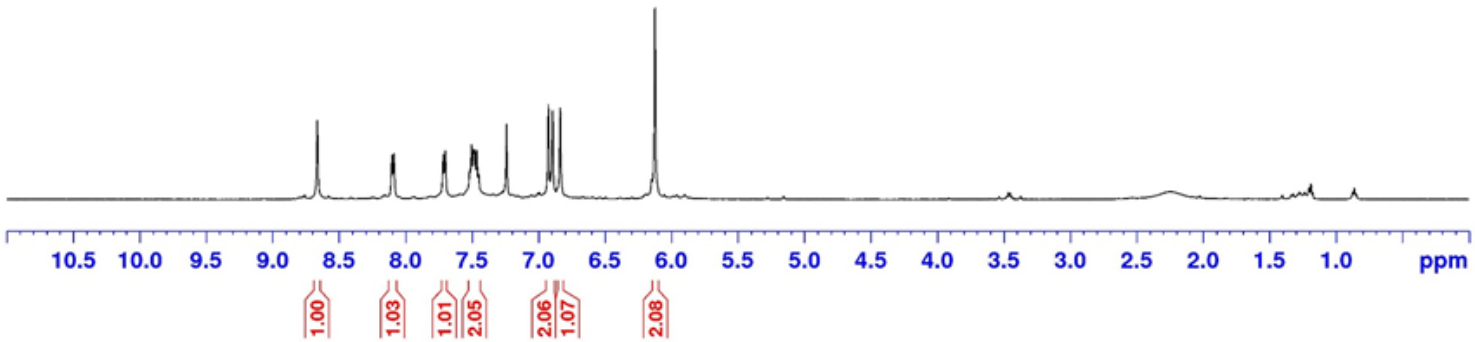


$^{13}C\{^{1}H\}$ NMR (175 MHz, $CDCl_3$)

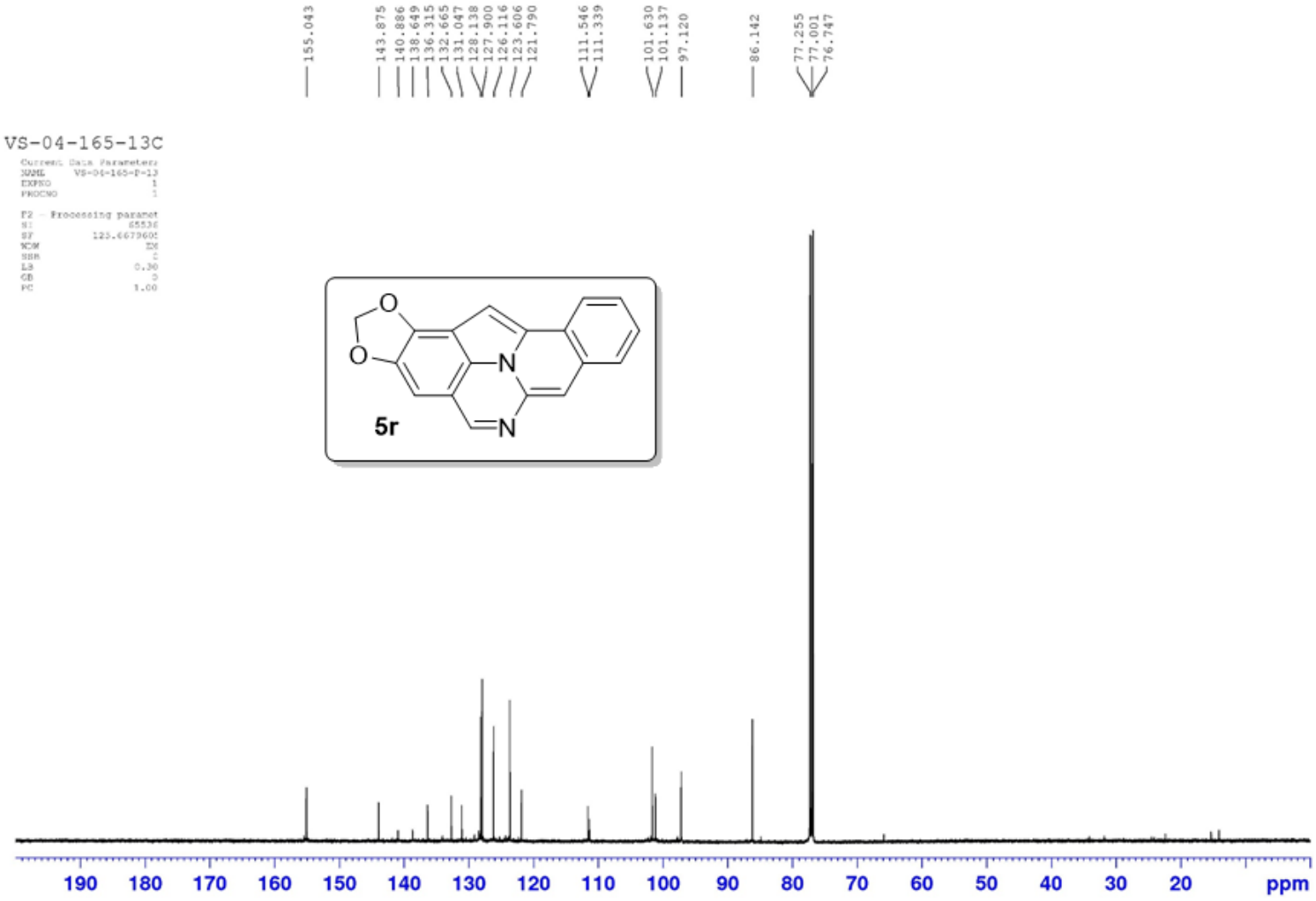


^{1}H-NMR (500 MHz, $CDCl_3$)

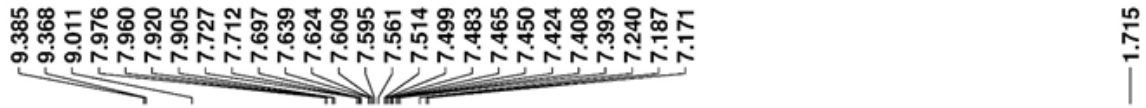




$^{13}C\{^{1}H\}$ NMR (125 MHz, $CDCl_3$)



^{1}H-NMR (500 MHz, $CDCl_3$)



VS-04-193-P

Current Data Parameters
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EXPNO 1
PROCNO 1

F2 – Processing parameters
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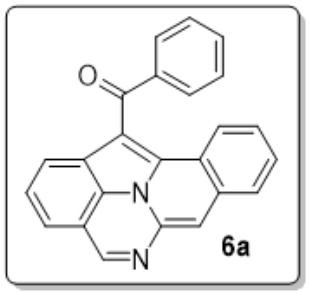
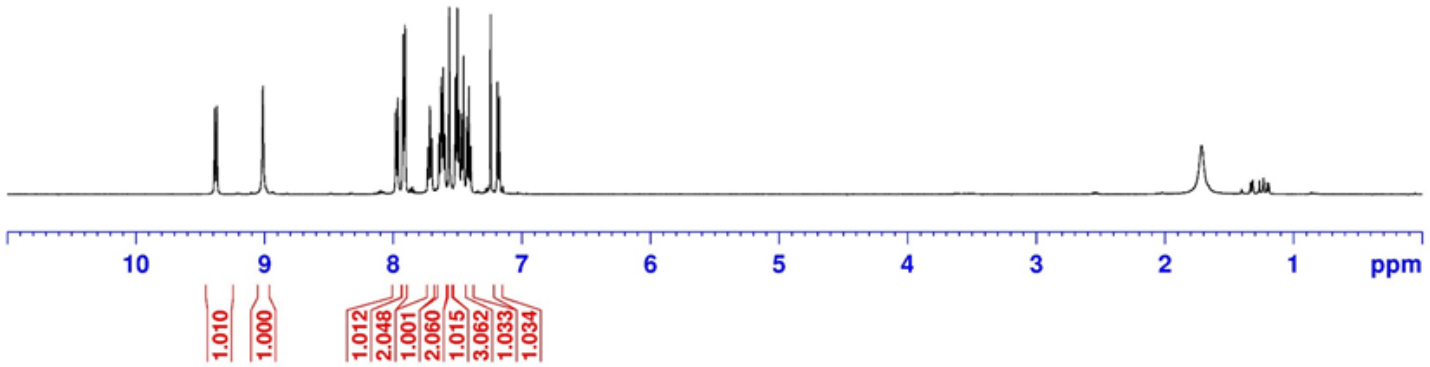
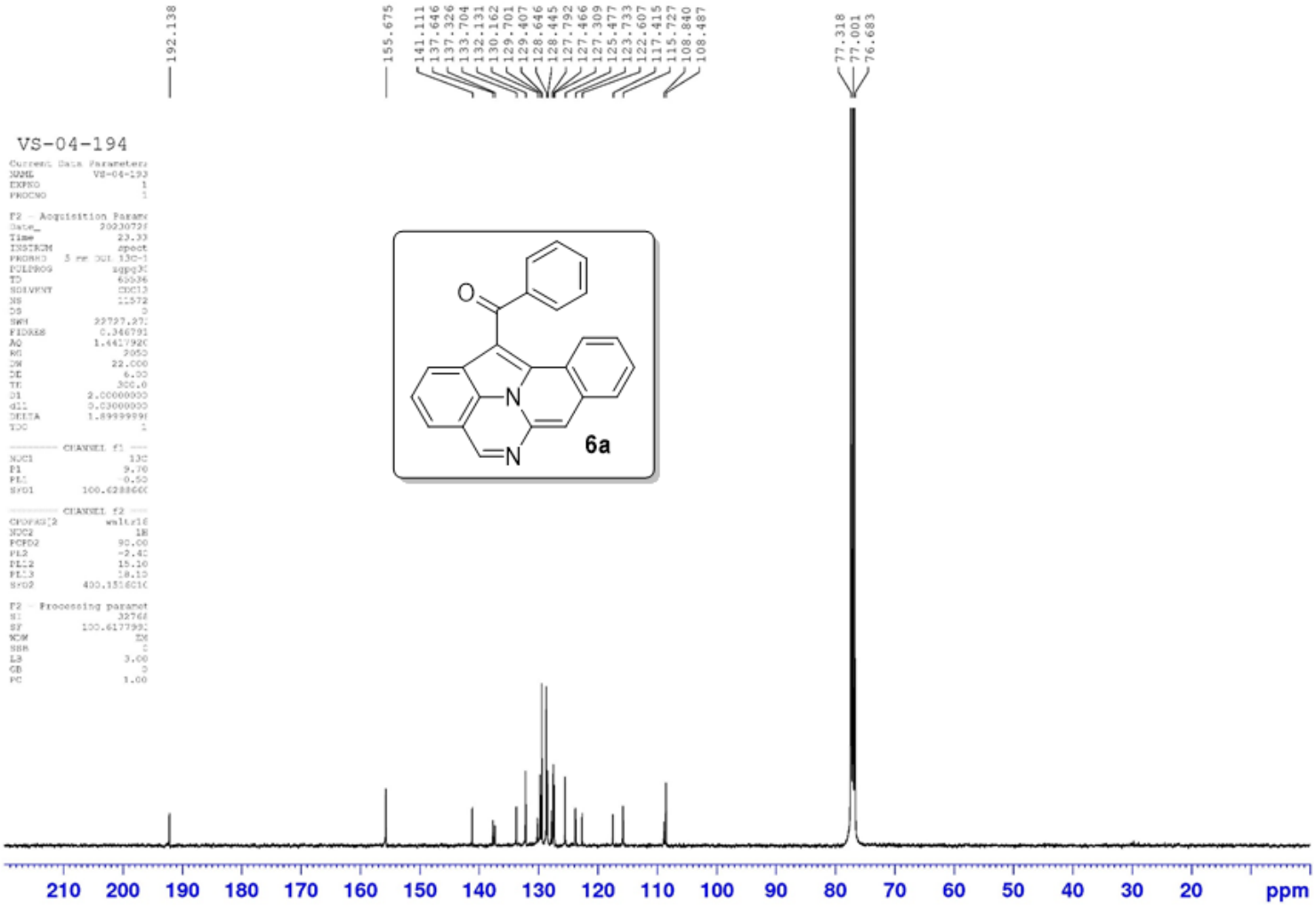
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

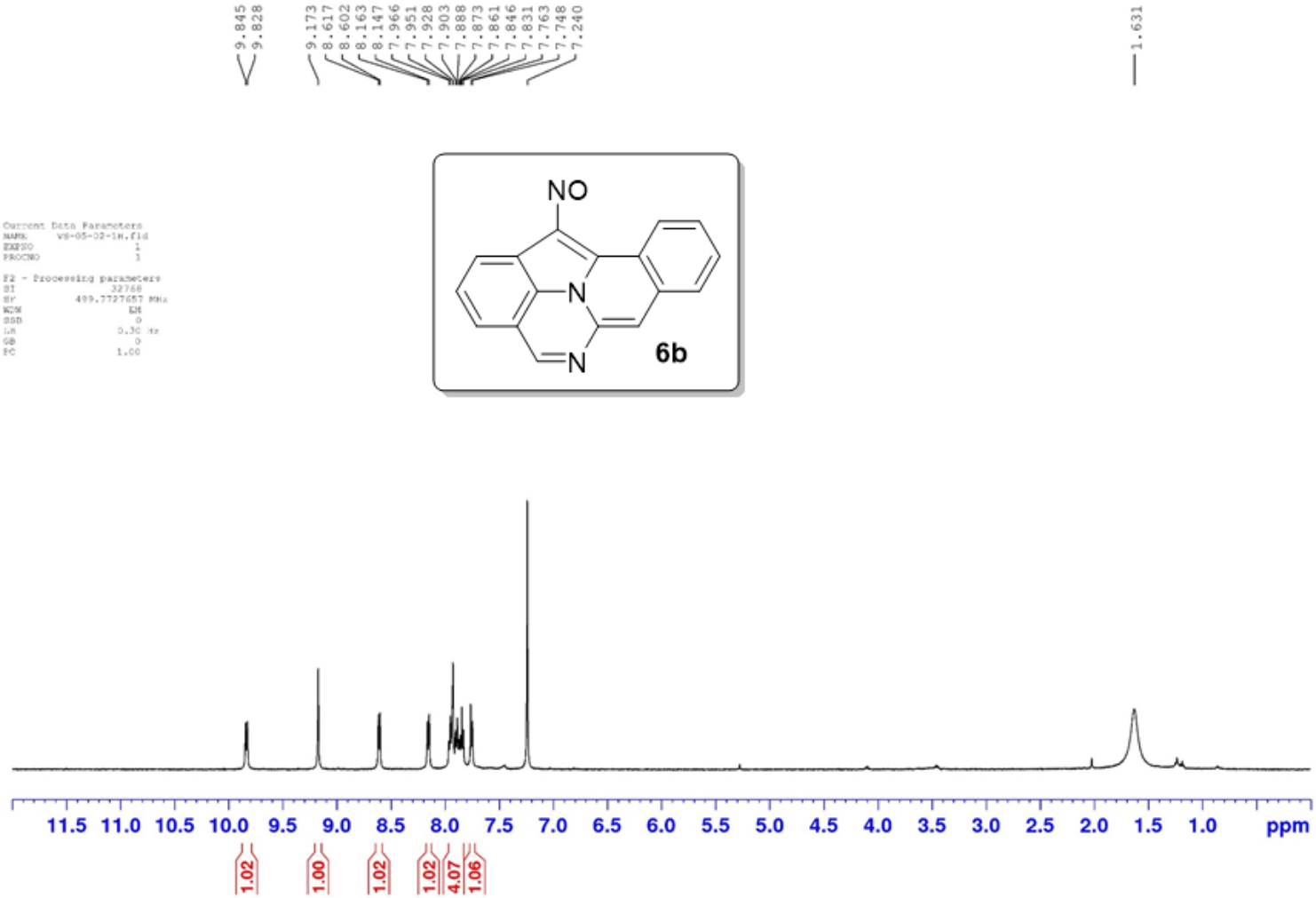




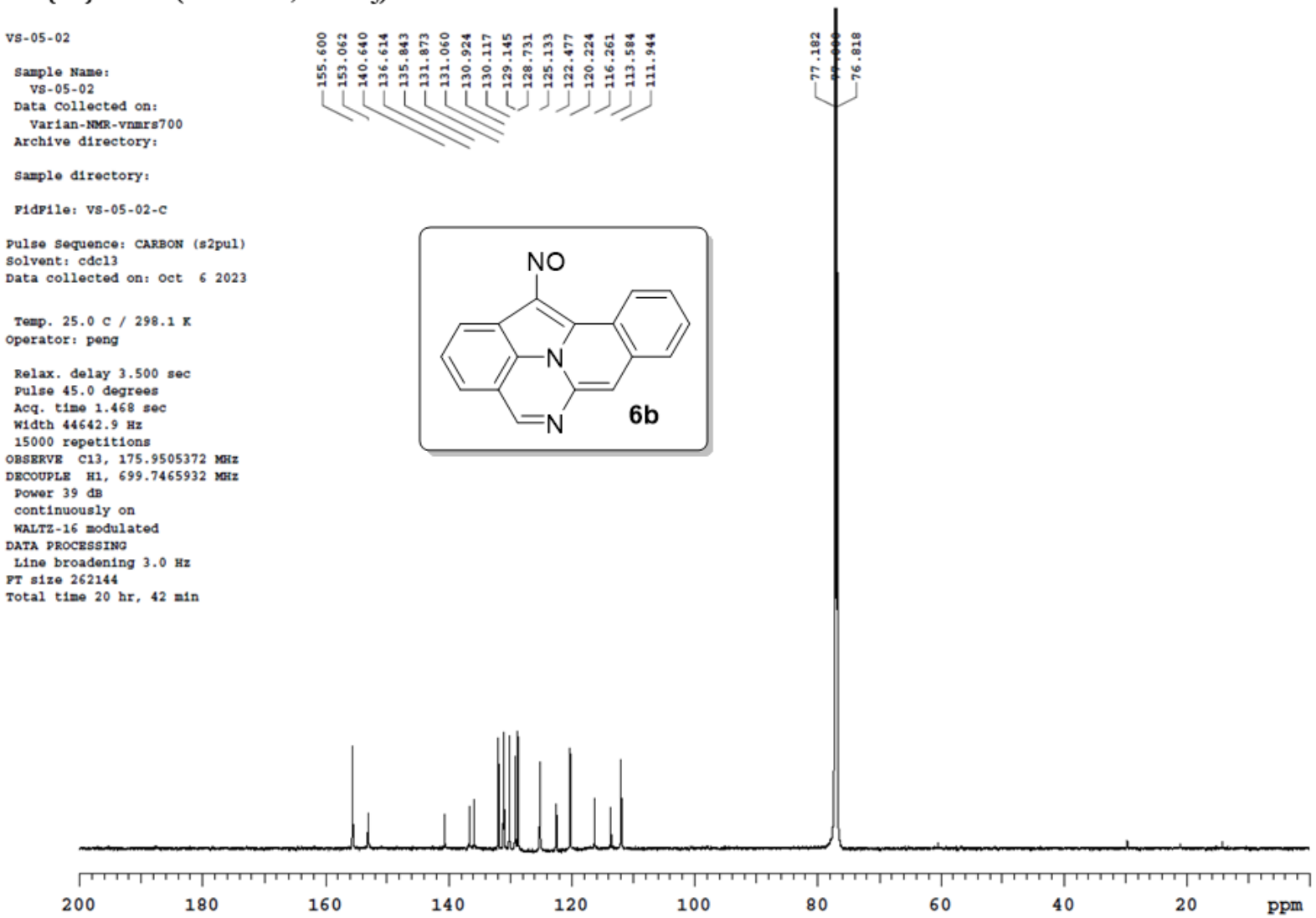
$^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$)



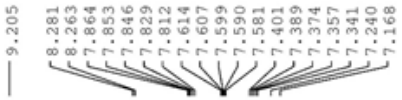
^{1}H-NMR (500 MHz, $CDCl_3$)

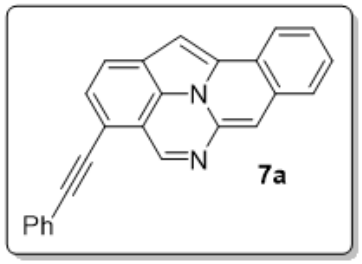


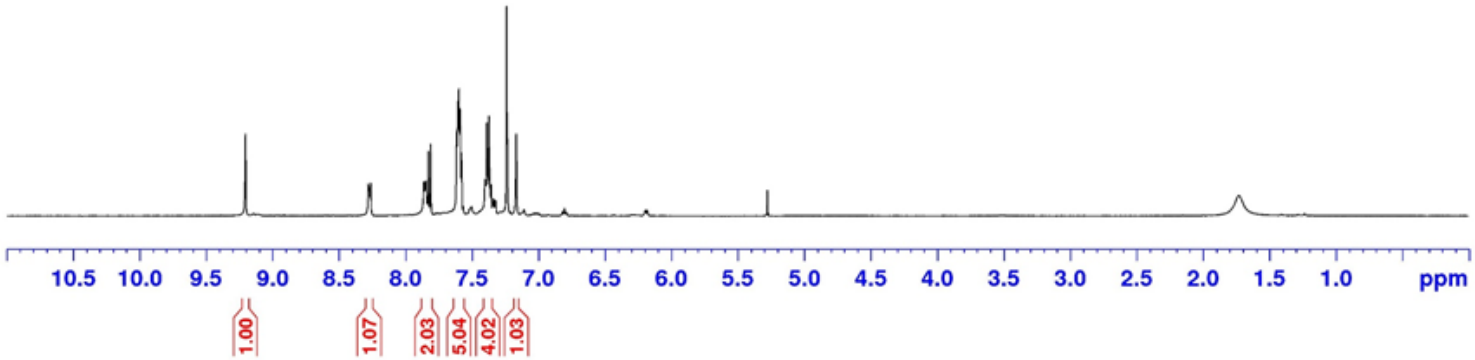
$^{13}C\{^{1}H\}$ NMR (175 MHz, $CDCl_3$)



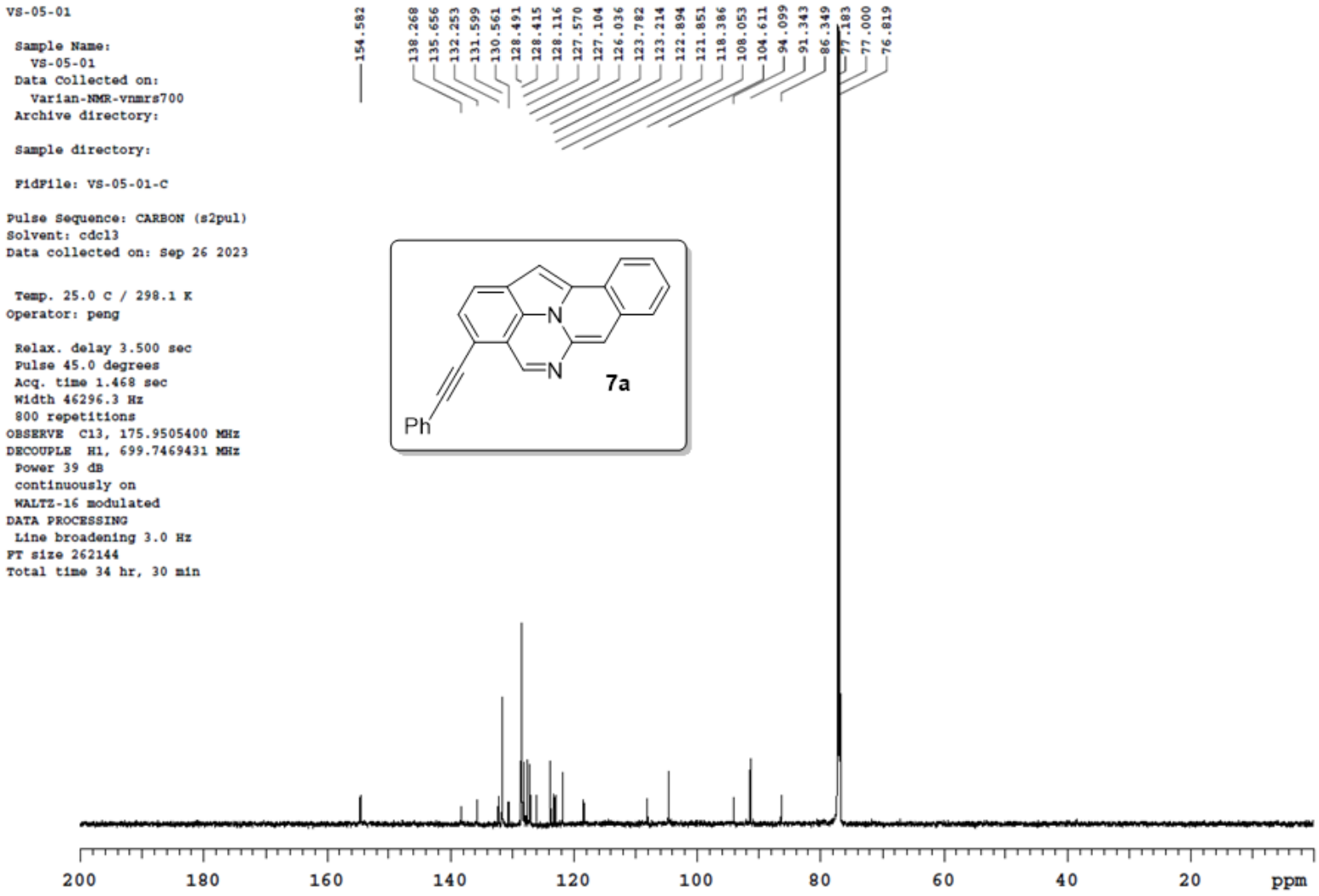
^{1}H-NMR (500 MHz, $CDCl_3$)



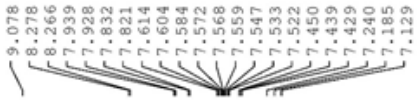


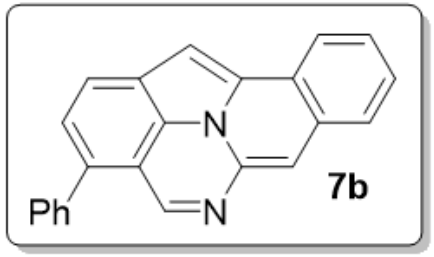


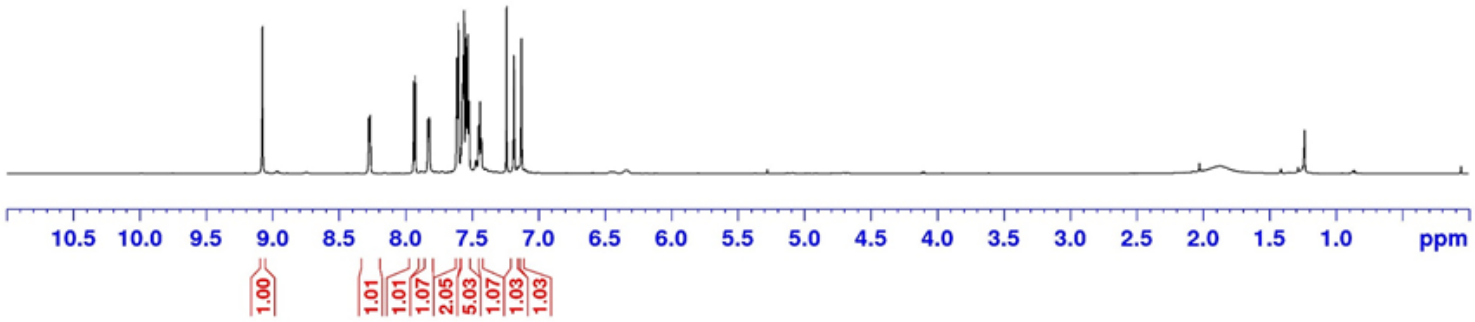
$^{13}C\{^{1}H\}$ NMR (175 MHz, $CDCl_3$)



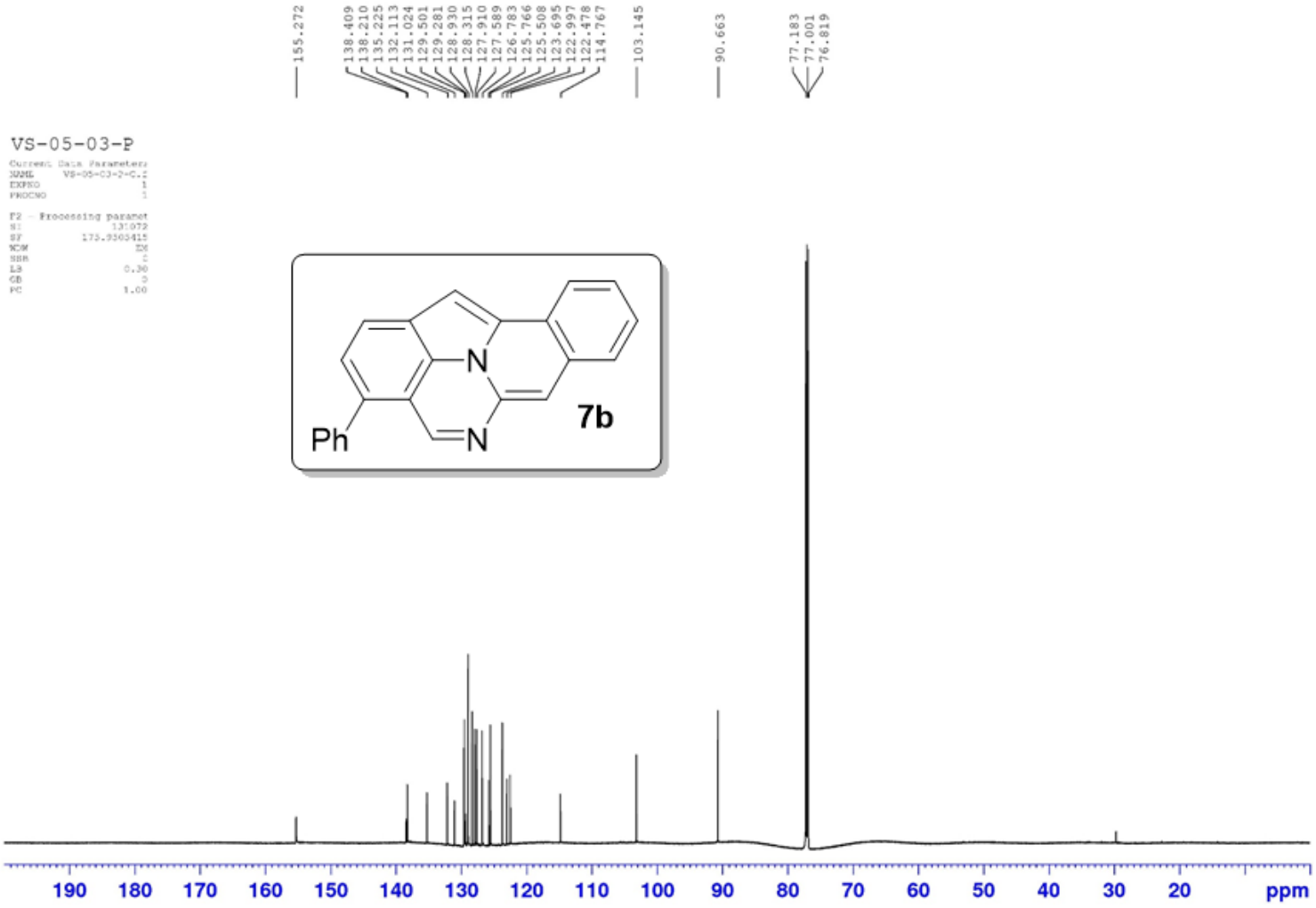
^{1}H-NMR (700 MHz, $CDCl_3$)



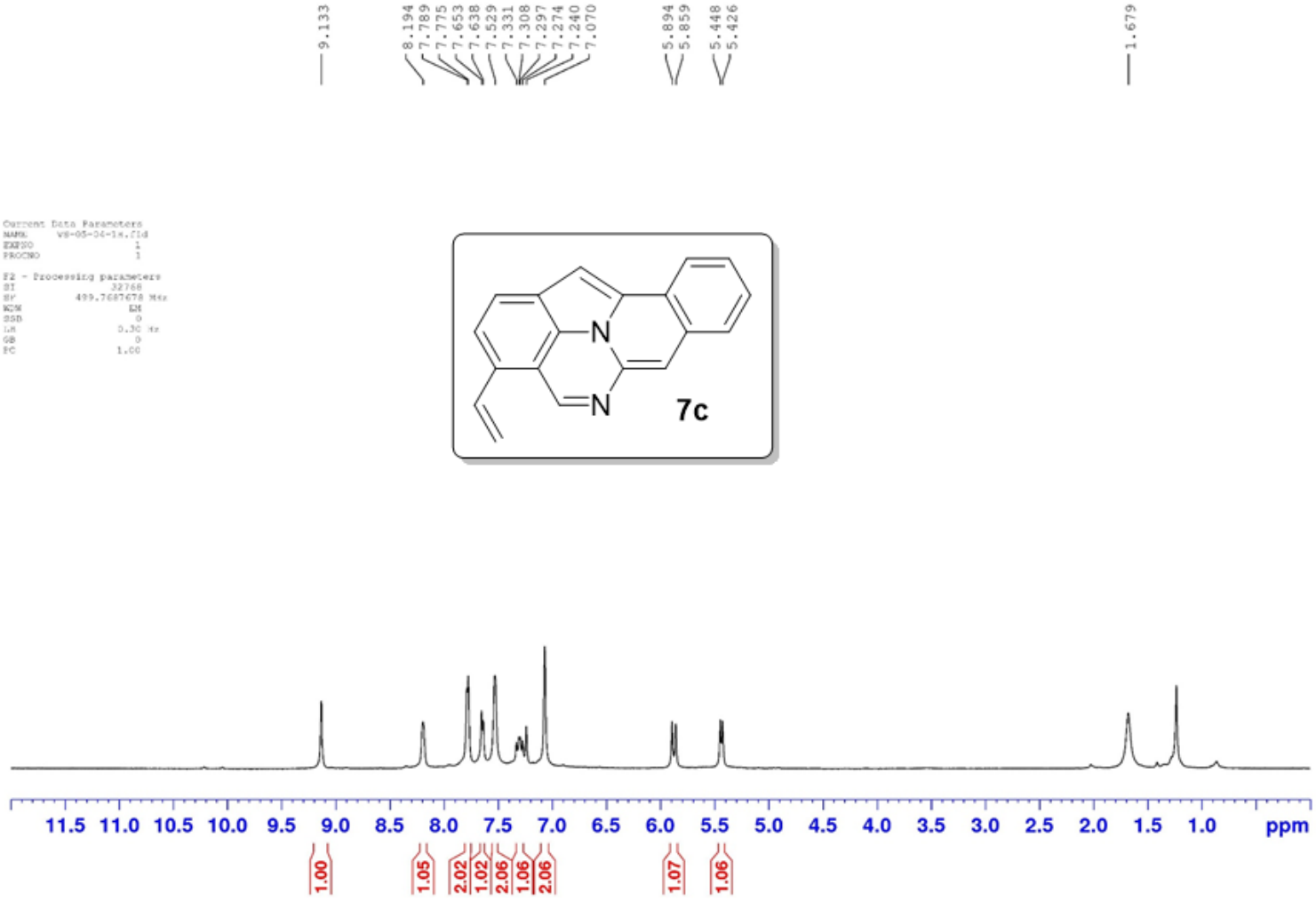




$^{13}C\{^{1}H\}$ NMR (175 MHz, $CDCl_3$)



^{1}H-NMR (500 MHz, $CDCl_3$)



$^{13}C\{^{1}H\}$ NMR (175 MHz, $CDCl_3$)