Supporting Information

Perimidine Directed Rh(III)-Catalyzed [4+1] and [4+2] Annulations: Synthesis of Perimidine Linked Spiro-succinimides and Isoquinolines

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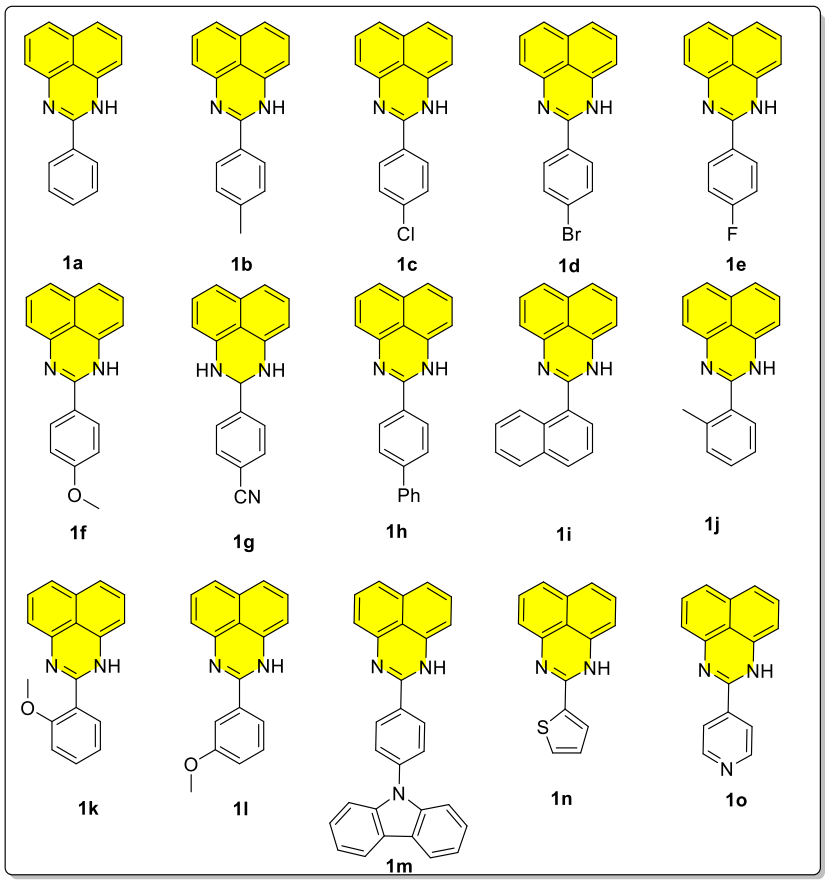
Table of Contents

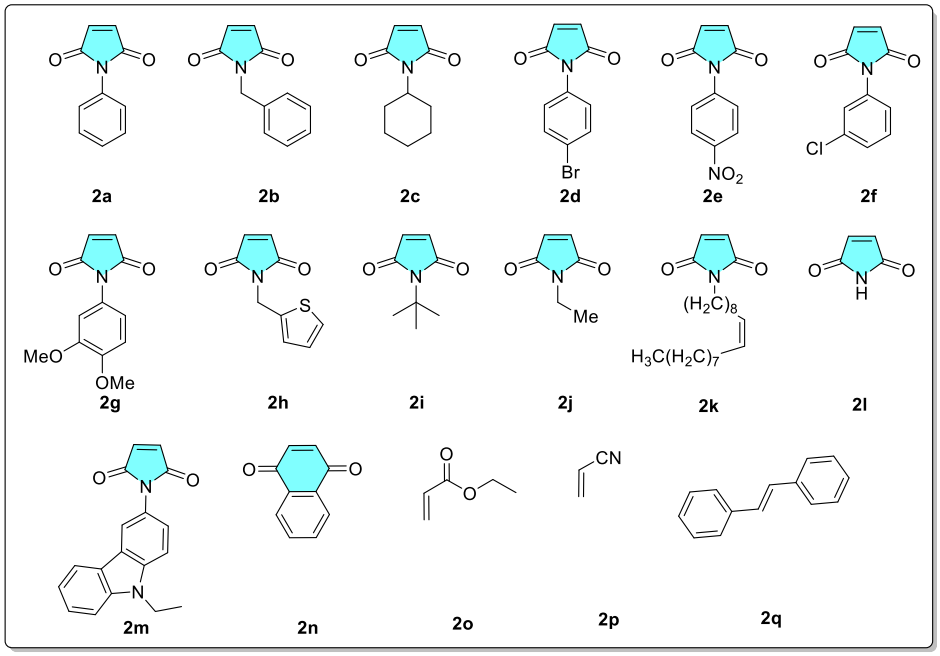
General Information

All the reagents were procured from commercial sources (Sigma-Aldrich, TCI, Alfa-Aesar, Chemscene) and used as such without any further purification. All the perimidine derivatives were prepared by reported method in the literature.[1] The maleimide derivatives **2a**, **2b**, **2c**, **2d**, **2e**, **2i**, **2j** and **2l** were procured from commercial sources such Sigma-Aldrich, TCI, Carbanio and Chemscene and were used as such without any further purification. The maleimide derivatives **2f**, **2g**, **2h**, **2k** and **2m** were synthesized by a reported method[2] using an amine and maleic anhydride in the presence of acetic acid. The alkenes **2n**, **2o**, **2p, 2q** and **5a** were procured from commercial sources such Sigma-Aldrich, TCI and Chemscene and were used as such without any further purification. Organic extracts were dried over anhydrous sodium sulphate. Solvents were removed using a Buchi rotavapor under reduced pressure. Reactions were performed in a sealed tube and no filter was used. For heating, silicone oil bath was used and heating was performed using a heating cum magnetic stirrer. Reactions were monitored by thin layer chromatography (TLC). Column chromatographic separations were performed using Avra silica gel (100−200 mesh). Melting points of products were recorded using an SRS EZ-Melt automated melting point apparatus by capillary methods and are uncorrected. A Bruker 400 MHz and Jeol 500 MHz spectrometer were used for recording NMR spectra. $CDCl_3$ and DMSO-D_6 were used as deuterated solvents for recording NMR spectra. Chemical shift (δ) values are reported in ppm. The abbreviations used for explaining the multiplicity are as follows: s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet, dd = doublet of doublet, tt = triplet of triplets, qt = quartet of triplets. HRMS analysis was carried out using a Bruker Impact HD mass spectrometer (Impact HD UHRTOF, ESI with positive mode), Agilent 6520 Q-TOF, or XEVO G2-XS QTOF mass spectrometer. Single-crystal XRD pattern was recorded in a Bruker D8 venture X-ray diffractometer.

List of 2-aryl-1H-perimidine Derivatives Used in the Study



List of Alkene Derivatives Used in the Study



General method for the synthesis of 3 and 4

To an oven dried pressure tube was added 0.1 mmol (1 equiv.) of perimidine **1**, 0.1 mmol (1 equiv.) alkene **2**, 5 mol% (3 mg) $[Cp^*RhCl_2]_2$, 0.1 mmol (8 mg, 1 equiv.) NaOAc was dissolved in 1 mL MeOH followed by the addition of 0.2 mmol (11 µL, 2 equiv.) AcOH. The resulting reaction mixture was then subjected to a pre-heated oil bath at 80 ℃ for 1 h. After cooling, reaction mixture was quenched with water and extracted with EtOAc (3 x 20 mL). The combined organic layers were washed with brine solution, dried over anhydrous Na_2SO_4, filtered and concentrated. The crude was then subjected to column chromatography using hexane:ethyl acetate as eluent to obtain the the pure product.

General method for the synthesis of 6

To an oven dried pressure tube was added 0.1 mmol (1 equiv.) of perimidine **1**, 5 mol% (3 mg) $[Cp^*RhCl_2]_2$, 0.1 mmol (18 mg, 1 equiv.) $Zn(OAc)_2$ was dissolved in 1 mL 1,2-DCE followed by the addition of 0.2 mmol (11 µL, 2 equiv.) AcOH. The resulting reaction mixture was then purged with N_2 gas for 5-10 mins followed by addition of 0.2 mmol (17 mg ≈ 13 µL, 0.2 equiv.) vinylene carbonate **5a**. The reaction mixture was then subjected to a pre-heated oil bath at 110 ℃ for 4 h. After cooling, reaction mixture was quenched with water and extracted with EtOAc (3 x 20 mL). The combined organic layers were washed with brine solution, dried over anhydrous Na_2SO_4, filtered and concentrated. The crude was then subjected to column chromatography using hexane:ethyl acetate as eluent to obtain the the pure product.

Procedure for 1 mmol Scale Synthesis of 3a

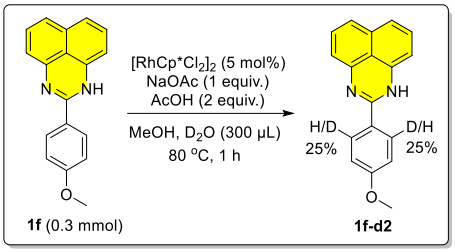
To an oven dried pressure tube was added 1 mmol (244 mg, 1 equiv.) of perimidine **1a**, 1 mmol (173 mg, 1 equiv.) maleimide **2a**, 5 mol% (31 mg) $[Cp^*RhCl_2]_2$, 1 mmol (82 mg, 1 equiv.) NaOAc was dissolved in 8 mL MeOH followed by the addition of 2 mmol (114 µL, 2 equiv.) AcOH. The resulting reaction mixture was then subjected to a pre-heated oil bath at 80

°C for 1 h. After cooling, reaction mixture was quenched with water and extracted with EtOAc (3 x 30 mL). The combined organic layers were washed with brine solution, dried over anhydrous Na_2SO_4, filtered and concentrated. The crude was then subjected to column chromatography using hexane:ethyl acetate (90:10) as eluent to obtain the the pure product in 68% yield.

General method for the synthesis of 7

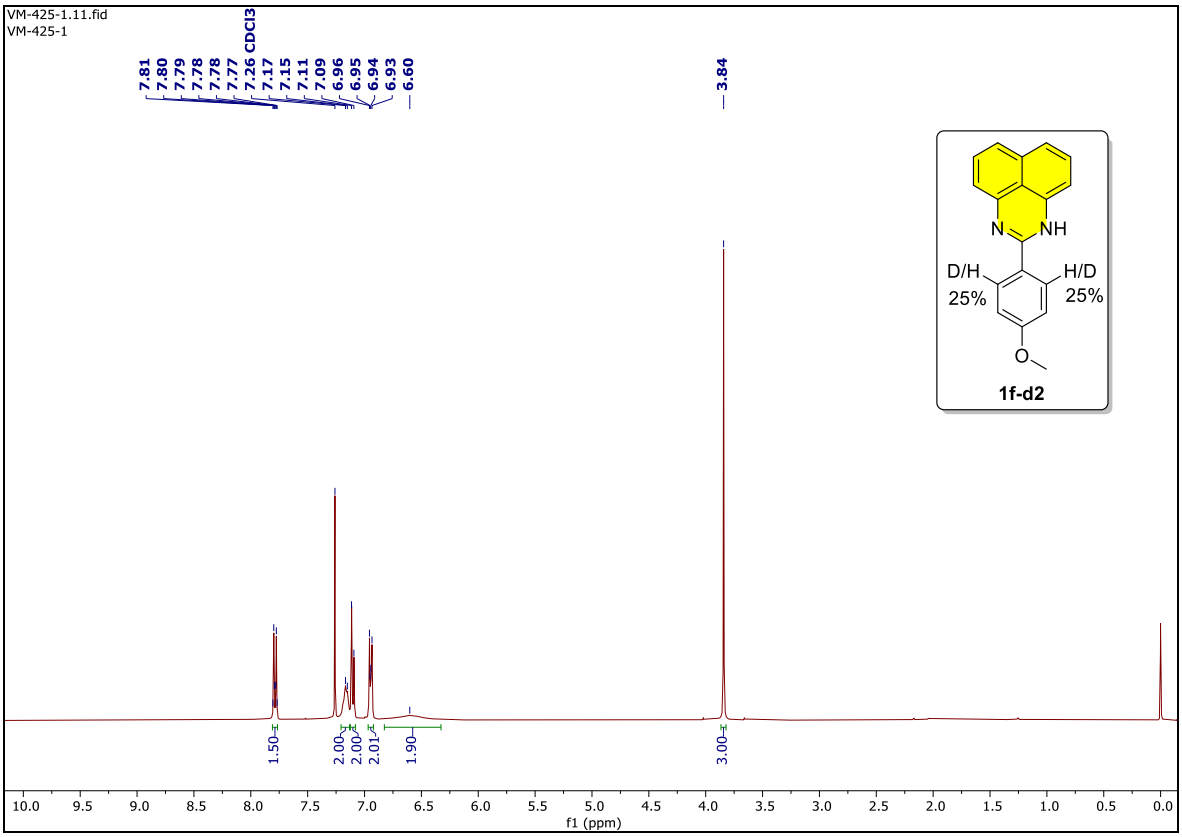
The spiro-succinimide **3a** 0.1 mmol (42 mg, 1 equiv.) was dissolved in 1 mL MeOH in an oven dried sealed tube followed by addition of 0.2 mmol (11 mg, 2 equiv.) NaOMe. The resulting reaction mixture was then heated at 80 °C for 3 h. The progress of the reaction was monitored using TLC. After completion of the reaction, the reaction mixture was acidified using 2N HCl solution. Then the reaction mixture was extracted using EtOAc (3 × 20 mL). Then combined organic layers were washed with brine solution, dried over anhydrous Na_2SO_4, filtered and concentrated. The crude was then subjected to column chromatography using hexane:ethyl acetate (60:40) as eluent to obtain the the pure product **7**.

Synthesis of 1f-d2

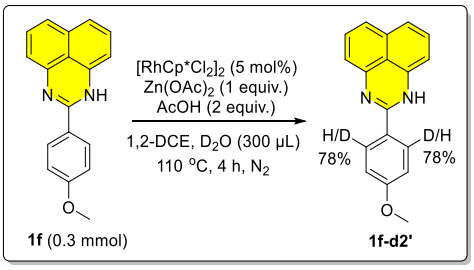


To an oven dried pressure tube was added 0.3 mmol (82 mg, 1 equiv.) 2-(4-methoxyphenyl)-1H-perimidine **1f**, 5 mol% (9 mg) $[Cp^*RhCl_2]_2$, 0.3 mmol (25 mg, 1 equiv.) NaOAc was dissolved in 3 mL MeOH followed by the addition of 0.6 mmol (34 µL, 2 equiv.) AcOH and 300 µL D_2O. The resulting reaction mixture was then subjected to a pre-heated oil bath at 80 °C for 1 h. After cooling, reaction mixture was quenched with water and extracted with EtOAc

(3 x 20 mL). The combined organic layers were washed with brine solution, dried over Na_2SO_4, filtered and concnetrated. The crude was then subjected to column chromatography using hexane:ethyl acetate (85:15) as eluent to obtain the **1f-d2** in 50% yield. The deuterium incorporation at both the ortho positions was determined by using a 400 MHz NMR spectrometer as 25%.

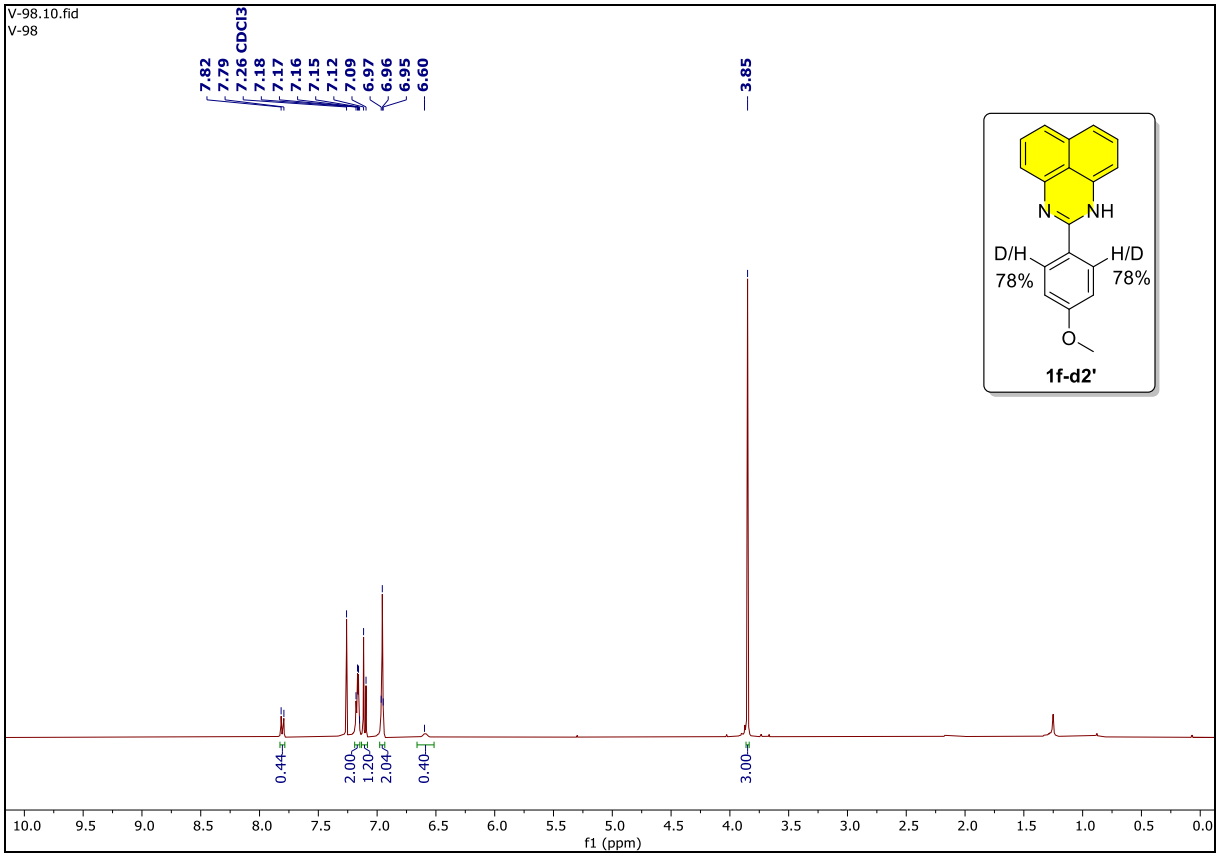


Synthesis of 1f-d2′

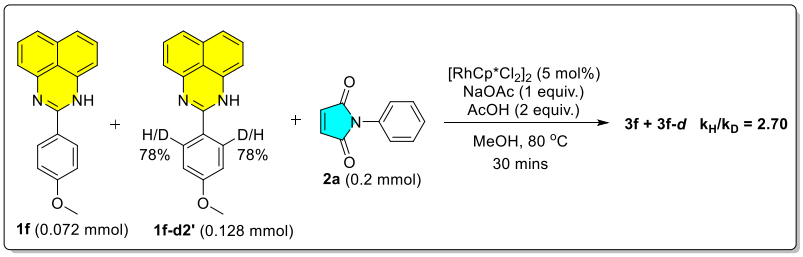


To an oven dried pressure tube was added 0.3 mmol (82 mg, 1 equiv.) 2-(4-methoxyphenyl)-1H-perimidine **1f**, 5 mol% (9 mg) $[Cp^*RhCl_2]_2$, 0.3 mmol (55 mg, 1 equiv.) $Zn(OAc)_2$ was dissolved in 3 mL 1,2-DCE followed by the addition of 0.6 mmol (34 µL, 2 equiv.) AcOH and

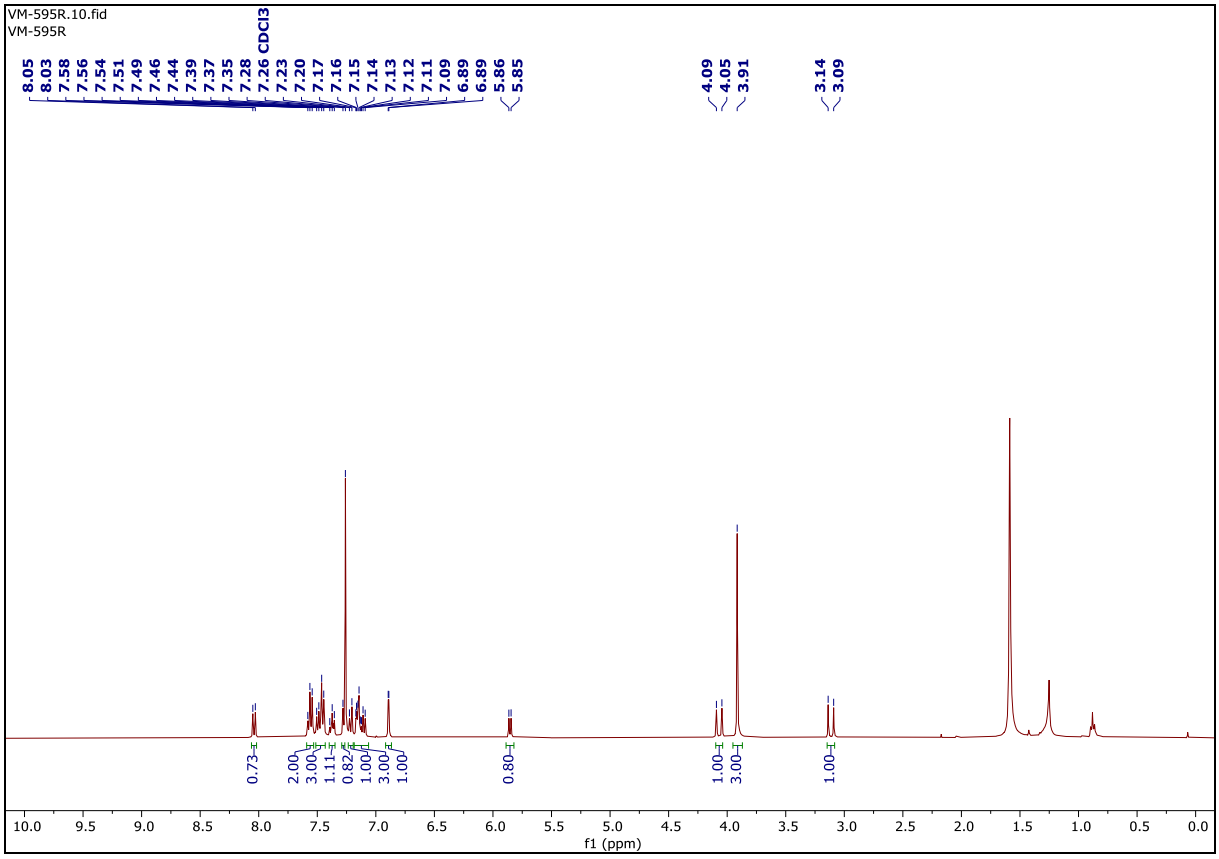
300 µL D_2O. The resulting reaction mixture was then purged with N_2 gas for 5-10 mins. The reaction mixture was then subjected to a pre-heated oil bath at 110 °C for 4 h. After cooling, reaction mixture was quenched with water and extracted with EtOAc (3 x 20 mL). The combined organic layers were washed with brine solution, dried over Na_2SO_4, filtered and concnetrated. The crude was then subjected to column chromatography using hexane:ethyl acetate (85:15) as eluent to obtain the **1f-d2'** in 87% yield. The deuterium incorporation at both the ortho positions was determined by using a 400 MHz NMR spectrometer as 78%.



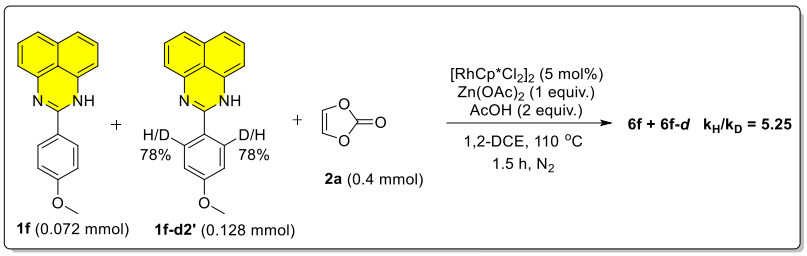
KIE Experiment for [4+1] cascade Annulation



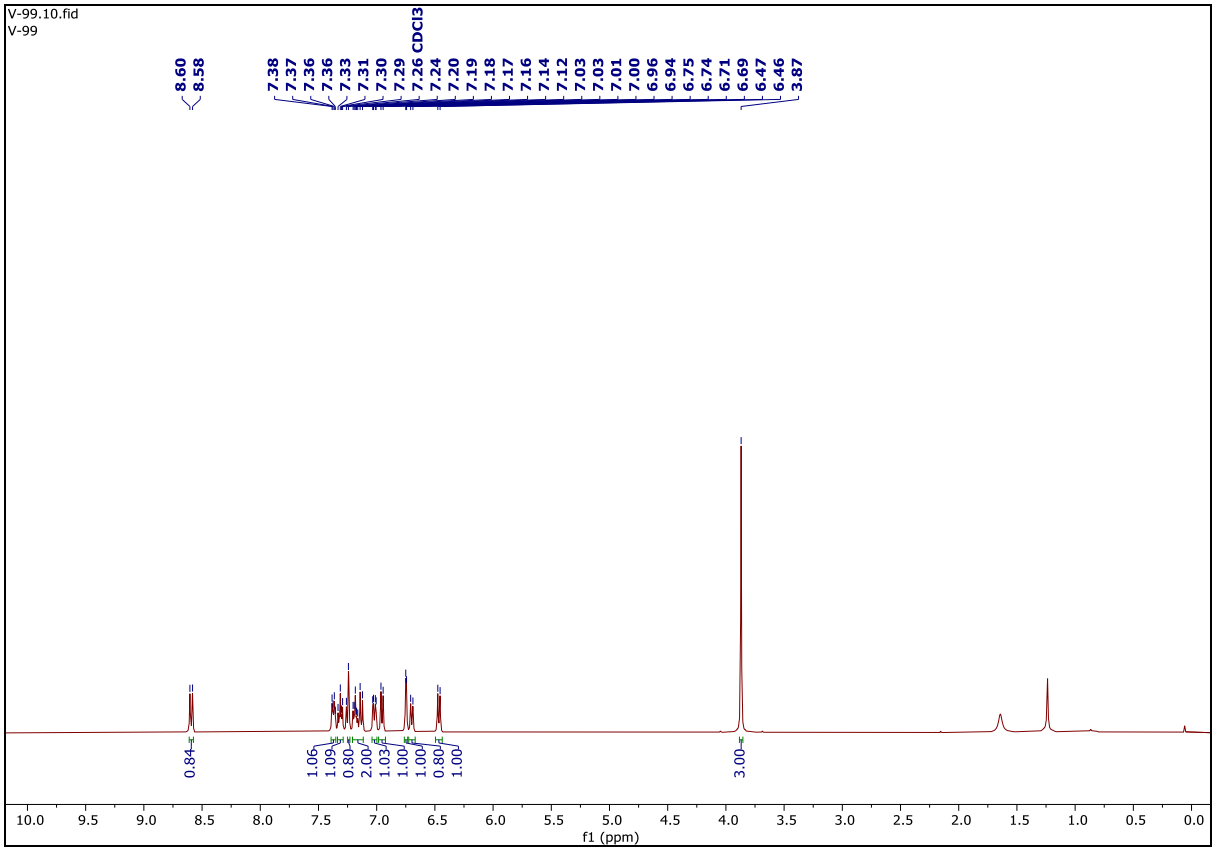
To an oven-dried pressure tube equipped with a magnetic stir bar was charged with 1:1 molar ratio of **1f:1f-d2'** [i.e., by weighing 0.128 mmol (35 mg) of **1f-d2'** which contains 0.1 mmol of **1f-d2'** (100% D) and 0.028 mmol of **1f** and by weighing 0.072 mmol (20 mg) of **1f**] followed by 0.2 mmol (35 mg) of **2a**, 5 mol% (6 mg) $[Cp^*RhCl_2]_2$, 0.2 mmol (16 mg, 1 equiv.) NaOAc was dissolved in 2 mL MeOH followed by the addition of 0.4 mmol (23 µL, 2 equiv.) AcOH. The resulting reaction mixture was then subjected to a pre-heated oil bath at 80 °C for 30 minutes. After cooling, reaction mixture was quenched with water and extracted with EtOAc (3 x 20 mL). The combined organic layers were washed with brine solution, dried over anhydrous Na_2SO_4, filtered and concnetrated. The crude was then subjected to column chromatography using hexane:ethyl acetate (80:20) as eluent to give k_H/k_D of 2.70.



KIE Experiment for [4+2] cascade Annulation



To an oven-dried pressure tube equipped with a magnetic stir bar was charged with 1:1 molar ratio of **1f:1f-d2'** [i.e., by weighing 0.128 mmol (35 mg) of **1f-d2'** which contains 0.1 mmol of **1f-d2'** (100% D) and 0.028 mmol of **1f** and by weighing 0.072 mmol (20 mg) of **1f**] followed by 5 mol% (6 mg) $[Cp^*RhCl_2]_2$, 0.2 mmol (37 mg, 1 equiv.) $Zn(OAc)_2$ was dissolved in 2 mL 1,2-DCE followed by the addition of 0.4 mmol (23 µL, 2 equiv.) AcOH. The resulting reaction mixture was then purged with N_2 gas for 5-10 mins followed by addition of 0.4 mmol (34 mg ≈ 25 µL, 0.2 equiv.) vinylene carbonate **5a**. The reaction mixture was then subjected to a pre-heated oil bath at 110 °C for 1.5 h. After cooling, reaction mixture was quenched with water and extracted with EtOAc (3 x 20 mL). The combined organic layers were washed with brine solution, dried over Na_2SO_4, filtered and concnetrated. The crude was then subjected to column chromatography using hexane:ethyl acetate (95:5) as eluent to give k_H/k_D of 5.25.


V-99.10.fid
V-99
8.60
8.58
7.38
7.37
7.36
7.36
7.33
7.31
7.30
7.29
7.26 CDCl3
7.24
7.20
7.19
7.18
7.17
7.16
7.14
7.12
7.03
7.03
7.01
7.00
6.96
6.94
6.75
6.74
6.71
6.69
6.47
6.46
3.87
0.84
1.06
1.09
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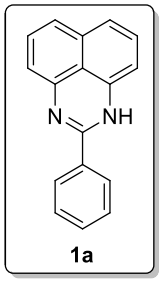
f1 (ppm)

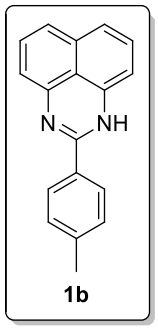
Characterization Data

***2-phenyl-1H-perimidine (1a)*[1,3,4,6,7,8]:** ^{1}H NMR (400 MHz, DMSO-D_6 + $CDCl_3$) δ 7.91 (d, J = 7.6 Hz, 2H), 7.48 – 7.40 (m, 3H), 7.06 (t, J = 7.8 Hz, 2H), 6.96 (d, J = 8.2 Hz, 2H), 6.58 (d, J = 7.3 Hz, 2H).



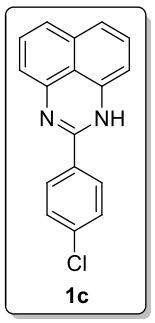
HRMS (ESI-TOF): m/z [M + H]$^+$ calcd for $C_{17}H_{13}N_2$ 245.1073; found 245.1067.

***2-(p-tolyl)-1H-perimidine (1b)*[1,3,4]:** ^{1}H NMR (500 MHz, DMSO-D_6) δ 10.57 (s, 1H), 7.92 (d, J = 8.3 Hz, 2H), 7.34 (d, J = 7.7 Hz, 2H), 7.19 – 7.16 (m, 1H), 7.13 – 7.10 (m, 1H), 7.04 (d, J = 8.3 Hz, 1H), 7.01 (d, J = 8.3 Hz, 1H), 6.66 (d, J = 7.3 Hz, 1H), 6.54 (d, J = 8.4 Hz, 1H), 2.39 (s, 3H).



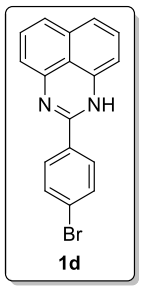
HRMS (ESI-TOF): m/z [M + H]$^+$ calcd for $C_{18}H_{15}N_2$ 259.1230; found 259.1232.

***2-(4-chlorophenyl)-1H-perimidine (1c)*[1,3,4]:** ^{1}H NMR (400 MHz, DMSO-D_6) δ 10.71 (s, 1H), 8.04 (d, J = 8.7 Hz, 2H), 7.61 (d, J = 8.7 Hz, 2H), 7.18 (t, J = 7.8 Hz, 1H), 7.12 (t, J = 7.9 Hz, 1H), 7.05 (dd, J = 17.7, 8.1 Hz, 2H), 6.68 (d, J = 7.1 Hz, 1H), 6.53 (d, J = 7.3 Hz, 1H).



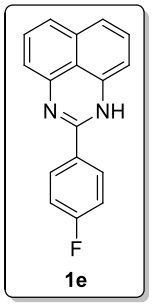
HRMS (ESI-TOF): m/z [M + H]$^+$ calcd for $C_{17}H_{12}ClN_2$ 279.0684; found 279.0675.

***2-(4-bromophenyl)-1H-perimidine (1d)*[3,4,8]:** ^{1}H NMR (500 MHz, DMSO-D_6) δ 10.70 (s, 1H), 7.97 (d, J = 8.7 Hz, 2H), 7.75 (d, J = 8.6 Hz, 2H), 7.15 (t, J = 7.9 Hz, 2H), 7.05 (d, J = 8.3 Hz, 2H), 6.62 (s, 2H).



HRMS (ESI-TOF): m/z [M + H]$^+$ calcd for $C_{17}H_{12}BrN_2$ 323.0178; found 323.0181.

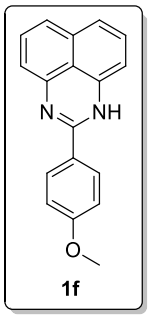
***2-(4-fluorophenyl)-1H-perimidine (1e)*[4]:** ^{1}H NMR (500 MHz, DMSO-D_6) δ 10.73 (s, 1H),



8.09 – 8.06 (m, 2H), 7.38 (t, J = 8.9 Hz, 2H), 7.15 (t, J = 7.9 Hz, 2H), 7.05 (d, J = 8.3 Hz, 2H), 6.61 (d, J = 7.5 Hz, 2H).

HRMS (ESI-TOF): m/z $[M + H]^+$ calcd for $C_{17}H_{12}FN_2$ 263.0979; found 263.0983.

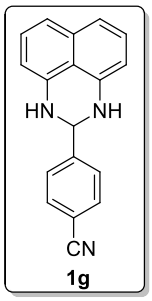
***2-(4-methoxyphenyl)-1H-perimidine (1f)*[1,8]:** ^{1}H NMR (500 MHz, DMSO-D_6) δ 10.62 (s, 1H),



8.00 (d, J = 8.9 Hz, 2H), 7.15 (t, J = 7.8 Hz, 2H), 7.08 (d, J = 9.0 Hz, 2H), 7.03 (d, J = 8.2 Hz, 2H), 6.60 (d, J = 7.4 Hz, 2H), 3.84 (s, 3H).

HRMS (ESI-TOF): m/z $[M + H]^+$ calcd for $C_{18}H_{15}N_2O$ 275.1179; found 275.1153.

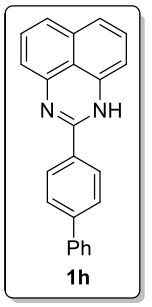
***4-(2,3-dihydro-1H-perimidin-2-yl)benzonitrile (1g)*[1]:** ^{1}H NMR (400 MHz, DMSO-D_6) δ 7.88



(d, J = 8.3 Hz, 2H), 7.75 (d, J = 8.3 Hz, 2H), 7.15 (t, J = 7.8 Hz, 2H), 6.98 (d, J = 8.2 Hz, 2H), 6.94 (s, 2H), 6.49 (d, J = 7.3 Hz, 2H), 5.47 (s, 1H).

HRMS (ESI-TOF): m/z $[M + H]^+$ calcd for $C_{18}H_{14}N_3$ 272.1182; found 272.1204.

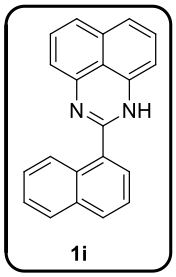
***2-([1,1'-biphenyl]-4-yl)-1H-perimidine (1h)*[4]:** ^{1}H NMR (500 MHz, DMSO-D_6)



δ 8.12 (d, J = 8.5 Hz, 2H), 7.87 (d, J = 8.5 Hz, 2H), 7.77 (d, J = 8.6 Hz, 2H), 7.52 (t, J = 7.6 Hz, 2H), 7.43 (t, J = 7.3 Hz, 1H), 7.18 (t, J = 7.8 Hz, 2H), 7.09 (d, J = 8.3 Hz, 2H), 6.66 (d, J = 7.3 Hz, 2H).

HRMS (ESI-TOF): m/z $[M + H]^+$ calcd for $C_{23}H_{17}N_2$ 321.1386; found 321.1385.

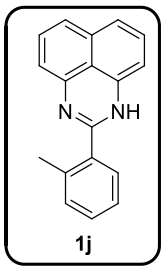
***2-(naphthalen-1-yl)-1H-perimidine (1i)*[6]:** ^{1}H NMR (500 MHz, DMSO-D_6) δ 10.94 (s, 1H), 8.34 – 8.31 (m, 1H), 8.09 (d, J = 8.3 Hz, 1H), 8.04 – 8.02 (m, 1H), 7.77 (d, J = 7.1 Hz, 1H), 7.65 – 7.59 (m, 3H), 7.22 – 7.19 (m, 1H), 7.13 – 7.10 (m, 2H), 7.05 (d, J = 7.3 Hz, 1H), 6.65 (d, J = 6.2 Hz, 1H), 6.39 (d, J = 7.3 Hz, 1H).



1i

HRMS (ESI-TOF): m/z [M + H]$^+$ calcd for $C_{21}H_{15}N_2$ 295.1230; found 295.1237.

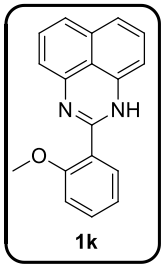
***2-(o-tolyl)-1H-perimidine (1j)*[4]:** ^{1}H NMR (400 MHz, DMSO-D_6) δ 10.75 (s, 1H), 7.47 (d, J = 7.6 Hz, 1H), 7.41 (t, J = 6.8 Hz, 1H), 7.35 – 7.30 (m, 2H), 7.13 (t, J = 7.9 Hz, 2H), 7.03 (d, J = 8.3 Hz, 2H), 6.47 (s, 2H), 2.44 (s, 3H).



1j

HRMS (ESI-TOF): m/z [M + H]$^+$ calcd for $C_{18}H_{15}N_2$ 259.1230; found 259.1234.

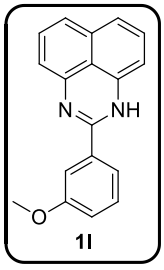
***2-(2-methoxyphenyl)-1H-perimidine (1k)*[7]:** ^{1}H NMR (500 MHz, DMSO-D_6) δ 10.51 (s, 1H), 7.59 (dd, J = 7.5, 1.8 Hz, 1H), 7.51 – 7.47 (m, 1H), 7.16 (t, J = 8.3 Hz, 2H), 7.09 – 7.02 (m, 3H), 6.98 (d, J = 7.3 Hz, 1H), 6.59 (d, J = 7.3 Hz, 1H), 6.35 (d, J = 7.3 Hz, 1H), 3.86 (s, 3H).



1k

HRMS (ESI-TOF): m/z [M + H]$^+$ calcd for $C_{18}H_{15}N_2O$ 275.1179; found 275.1204.

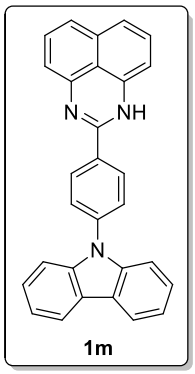
***2-(3-methoxyphenyl)-1H-perimidine (1l)*[4]:** ^{1}H NMR (500 MHz, DMSO-D_6) δ 10.69 (s, 1H), 7.59 (d, J = 7.9 Hz, 1H), 7.55 (s, 1H), 7.45 (t, J = 8.0 Hz, 1H), 7.16 (t, J = 7.8 Hz, 3H), 7.05 (d, J = 8.1 Hz, 2H), 6.62 (d, J = 7.3 Hz, 2H), 3.85 (s, 3H).



1l

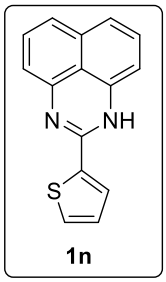
HRMS (ESI-TOF): m/z [M + H]$^+$ calcd for $C_{18}H_{15}N_2O$ 275.1179; found 275.1181.

2-(4-(9H-carbazol-9-yl)phenyl)-1H-perimidine *(1m)*: Yellow solid (360 mg, 88%), mp 187 - 190 °C. ^{1}H NMR (400 MHz, DMSO-*D*$_6$) δ 10.83 (s, 1H), 8.30 (dd, *J* = 15.0, 8.2 Hz, 4H), 7.84 (d, *J* = 8.6 Hz, 2H), 7.51 – 7.45 (m, 4H), 7.35 – 7.31 (m, 2H), 7.21 (t, *J* = 7.8 Hz, 1H), 7.15 (t, *J* = 7.8 Hz, 1H), 7.07 (dd, *J* = 17.2, 7.5 Hz, 2H), 6.73 (d, *J* = 7.3 Hz, 1H), 6.59 (d, *J* = 7.3 Hz, 1H). ^{13}C{^{1}H} NMR (101 MHz, DMSO-*D*$_6$) δ 139.8, 139.2, 132.2, 129.0, 128.7, 128.1, 126.4, 126.3, 123.0, 120.6, 120.4, 119.4, 114.1, 109.7, 102.9.



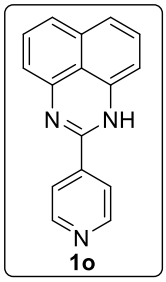
HRMS (ESI-TOF): m/z [M + H]$^{+}$ calcd for $C_{29}H_{20}N_3$ 410.1652; found 410.1657.

2-(thiophen-2-yl)-1H-perimidine *(1n)*[3]: ^{1}H NMR (400 MHz, DMSO-*D*$_6$) δ 10.69 (s, 1H), 7.92 (d, *J* = 3.8 Hz, 1H), 7.78 (d, *J* = 5.0 Hz, 1H), 7.23 – 7.21 (m, 1H), 7.19 – 7.11 (m, 2H), 7.07 – 7.01 (m, 2H), 6.62 (d, *J* = 7.2 Hz, 1H), 6.51 (d, *J* = 7.3 Hz, 1H).



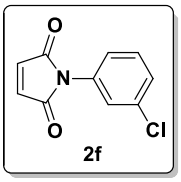
HRMS (ESI-TOF): m/z [M + H]$^{+}$ calcd for $C_{15}H_{11}N_2S$ 251.0637; found 251.0647.

2-(pyridin-4-yl)-1H-perimidine *(1o)*: ^{1}H NMR (500 MHz, DMSO-*D*$_6$) δ 10.96 (s, 1H), 8.75 – 8.73 (m, 1H), 8.30 (d, *J* = 7.9 Hz, 1H), 8.02 (td, *J* = 7.7, 1.8 Hz, 1H), 7.65 – 7.62 (m, 1H), 7.21 – 7.17 (m, 1H), 7.13 – 7.07 (m, 2H), 7.01 (d, *J* = 8.3 Hz, 1H), 6.77 (dd, *J* = 7.4, 1.1 Hz, 1H), 6.71 (dd, *J* = 7.3, 1.1 Hz, 1H). ^{13}C{^{1}H} NMR (126 MHz, DMSO-*D*$_6$) δ 150.8, 149.4, 148.4, 144.8, 138.0, 137.5, 135.2, 128.8, 128.1, 126.1, 122.3, 121.6, 119.8, 117.7, 114.1, 103.5.



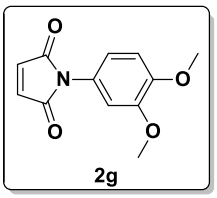
HRMS (ESI-TOF): m/z [M + H]$^{+}$ calcd for $C_{16}H_{12}N_3$ 246.1031; found 246.1025.

1-(3-chlorophenyl)-1H-pyrrole-2,5-dione (2f)[2a]***:*** Purified by silica gel column chromatography eluent: hexane/ethyl acetate (90:10). White solid (1.7 g, 82%), mp 95-98 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.42 – 7.33 (m, 3H), 7.28 (dt, *J* = 8.0, 1.7 Hz, 1H), 6.87 (s, 2H).



2f

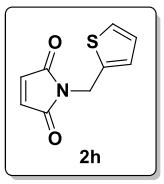
1-(3,4-dimethoxyphenyl)-1H-pyrrole-2,5-dione (2g): Purified by silica gel column chromatography eluent: hexane/ethyl acetate (90:10). Yellow solid (1.93 g, 83%), mp 165-168 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.94 (d, *J* = 8.6 Hz, 1H), 6.87 (dd, *J* = 8.5, 2.4 Hz, 1H), 6.84 (s, 2H), 6.81 (d, *J* = 2.3 Hz, 1H), 3.90 (s, 3H), 3.88 (s, 3H). ^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) δ 170.0, 149.4, 149.0, 134.3, 124.0, 119.0, 111.2, 110.0, 56.19, 56.15.



2g

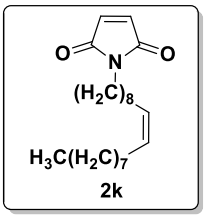
HRMS (ESI-TOF): m/z [M + H]$^+$ calcd for $C_{12}H_{12}NO_4$ 234.0761; found 234.0764.

1-(thiophen-2-ylmethyl)-1H-pyrrole-2,5-dione (2h)[2a]***:*** Purified by silica gel column chromatography eluent: hexane/ethyl acetate (90:10). White solid (1.54 g, 80%), mp 79-82 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.21 (d, *J* = 4.0 Hz, 1H), 7.07 (d, *J* = 4.0 Hz, 1H), 6.93 (dd, *J* = 4.0, 3.4 Hz, 1H), 6.71 (s, 2H), 4.85 (s, 2H).



2h

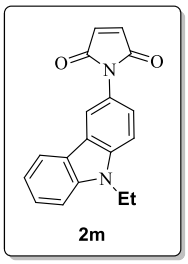
(Z)-1-(octadec-9-en-1-yl)-1H-pyrrole-2,5-dione(2k): Purified by silica gel column chromatography eluent: hexane/ethyl acetate (95:5). Yellow liquid (2.8 g, 81%), ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.68 (s, 2H), 5.38 – 5.32 (m, 2H), 3.50 (t, *J* = 7.3 Hz, 2H), 2.03 – 1.98 (m, 4H), 1.58 – 1.55 (m, 2H), 1.29 – 1.24 (m, 22H), 0.87 (t, *J* = 6.8 Hz, 3H). ^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) δ 171.1, 134.2, 130.1, 129.9, 38.1, 32.0, 29.9, 29.8, 29.7, 29.5, 29.3, 29.2, 28.7, 27.4, 26.9, 22.8, 14.3.



2k

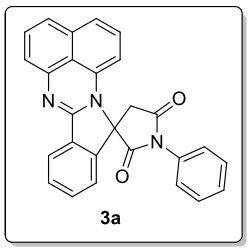
HRMS (ESI-TOF): m/z [M + H]$^+$ calcd for $C_{22}H_{38}NO_2$ 348.2897; found 348.2891.

1-(9-ethyl-9H-carbazol-3-yl)-1H-pyrrole-2,5-dione (2m)[2a]***:*** Purified by silica gel column chromatography eluent: hexane/ethyl acetate (85:15). Yellow solid (1.54 g, 53%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.07 (d, *J* = 7.8 Hz, 1H), 8.01 (d, *J* = 2.0 Hz, 1H), 7.52 – 7.46 (m, 2H), 7.43 (d, *J* = 8.3 Hz, 1H), 7.36 (dd, *J* = 8.6, 2.0 Hz, 1H), 7.24 (d, *J* = 6.8 Hz, 1H), 6.89 (s, 2H), 4.39 (q, *J* = 7.3 Hz, 2H), 1.44 (t, *J* = 7.3 Hz, 3H).



2m

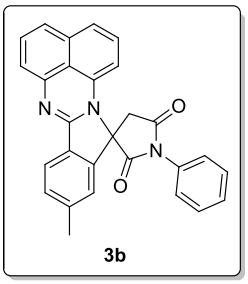
1'-phenylspiro[isoindolo[2,1-a]perimidine-12,3'-pyrrolidine]-2',5'-dione (3a)**:** Purified by silica gel column chromatography eluent: hexane/ethyl acetate (90:10). Yellow solid (35 mg, 84%), mp 254 - 256 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.12 (d, *J* = 7.0 Hz, 1H), 7.69 – 7.63 (m, 2H), 7.56 (t, *J* = 7.5 Hz, 2H), 7.50 – 7.45 (m, 4H), 7.38 (t, *J* = 7.8 Hz, 1H), 7.29 (d, *J* = 8.2 Hz, 1H), 7.22 (d, *J* = 8.2 Hz, 1H), 7.14 (dd, *J* = 14.1, 6.8 Hz, 2H), 5.88 (d, *J* = 7.3 Hz, 1H), 4.08 (d, *J* = 18.8 Hz, 1H), 3.12 (d, *J* = 18.8 Hz, 1H). ^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) δ 171.8, 171.2, 154.8, 143.0, 136.0, 134.6, 133.1, 131.4, 130.6, 129.7, 129.6, 129.4, 127.1, 126.2, 124.1, 121.9, 121.6, 120.8, 119.7, 117.2, 100.5, 69.8, 34.5.



3a

HRMS (ESI-TOF): m/z $[M + H]^+$ calcd for $C_{27}H_{18}N_3O_2$ 416.1394; found 416.1382.

10-methyl-1'-phenylspiro[isoindolo[2,1-a]perimidine-12,3'-pyrrolidine]-2',5'-dione (3b)**:** Purified by silica gel column chromatography eluent: hexane/ethyl acetate (88:12). Yellow solid (38 mg, 88%), mp 263 -265 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.96 (d, *J* = 7.9 Hz, 1H), 7.54 (t, *J* = 7.7 Hz, 2H), 7.48- 7.42 (m, 4H), 7.35 (t, *J* = 7.8 Hz, 1H), 7.24 (s, 1H), 7.19 (d, *J* = 8.5 Hz, 2H), 7.12 (t, *J* = 7.9 Hz, 1H), 7.09 (d, *J* = 7.3 Hz, 1H), 5.85 (d, *J* = 7.3 Hz, 1H), 4.04 (d, *J* = 18.8 Hz, 1H), 3.09 (d, *J* = 18.8 Hz, 1H), 2.49 (s, 3H). ^{13}C{^{1}H} (126 MHz, $CDCl_3$) δ 172.0, 171.4, 154.8, 144.2, 143.3, 143.1, 136.0, 134.7, 131.6, 131.4, 129.7,

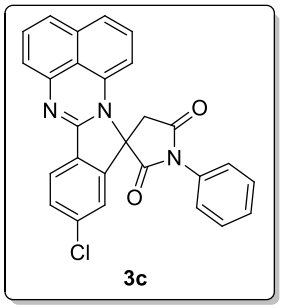


3b

129.5, 129.4, 128.9, 127.0, 126.2, 123.8, 121.7, 121.5, 120.6, 120.0, 117.2, 100.3, 69.6, 34.6, 22.3.

HRMS (ESI-TOF): m/z $[M + H]^+$ calcd for $C_{28}H_{20}N_3O_2$ 430.1556; found 430.1533.

10-chloro-1'-phenylspiro[isoindolo[2,1-a]perimidine-12,3'-pyrrolidine]-2',5'-dione (3c):

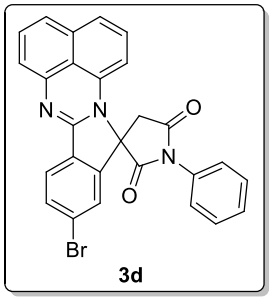


3c

Purified by silica gel column chromatography eluent: hexane/ethyl acetate (90:10). Orange solid (36 mg, 80%), mp 255 - 257 ºC. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.04 (d, *J* = 8.3 Hz, 1H), 7.63 (dd, *J* = 8.2, 1.8 Hz, 1H), 7.57 (t, *J* = 7.5, Hz, 2H), 7.50 (t, *J* = 7.4 Hz, 1H), 7.47 -7.45 (m, 2H), 7.42 (d, *J* = 1.5 Hz, 1H), 7.38 (t, *J* = 8.0 Hz, 1H), 7.29 (d, *J* = 7.7 Hz, 1H), 7.23 (d, *J* = 9.4 Hz, 1H), 7.16 – 7.13 (m, 1H), 7.10 (d, *J* = 6.3 Hz, 1H), 5.86 (d, *J* = 8.4 Hz, 1H), 4.07 (d, *J* = 18.9 Hz, 1H), 3.13 (d, *J* = 18.9 Hz, 1H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 171.4, 170.8, 153.7, 144.2, 142.8, 139.1, 136.0, 134.5, 131.2, 130.2, 129.74, 129.69, 129.4, 127.1, 126.2, 125.1, 122.2, 121.5, 120.9, 120.4, 117.5, 100.4, 69.5, 34.3.

HRMS (ESI-TOF): m/z $[M + H]^+$ calcd for $C_{27}H_{17}N_3O_2Cl$ 450.1004; found 445.1033.

10-bromo-1'-phenylspiro[isoindolo[2,1-a]perimidine-12,3'-pyrrolidine]-2',5'-dione (3d):

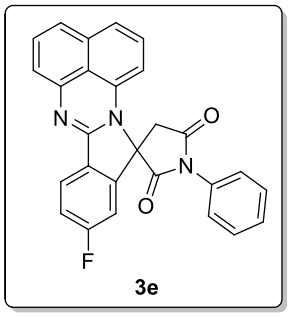


3d

Purified by silica gel column chromatography eluent: hexane/ethyl acetate (90:10). Orange solid (41 mg, 83%), mp 273 - 274 ºC. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.00 (d, *J* = 8.2 Hz, 1H), 7.79 (dd, *J* = 8.3, 1.7 Hz, 1H), 7.59 – 7.55 (m, 3H), 7.52 – 7.45 (m, 3H), 7.38 (t, *J* = 7.8 Hz, 1H), 7.30 (d, *J* = 7.1 Hz, 1H), 7.23 (d, *J* = 7.8 Hz, 1H), 7.17 – 7.11 (m, 2H), 5.86 (d, *J* = 7.3 Hz, 1H), 4.06 (d, *J* = 18.8 Hz, 1H), 3.13 (d, *J* = 19.0 Hz, 1H). ^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) δ 171.4, 170.7, 153.9, 144.4, 136.0, 134.4, 134.1, 131.2, 130.7, 129.73, 129.68, 129.4, 127.3, 127.1, 126.1, 125.4, 123.3, 122.2, 121.5, 121.0, 117.4, 100.5, 69.5, 34.3.

HRMS (ESI-TOF): m/z $[M + H]^+$ calcd for $C_{27}H_{17}N_3O_2Br$ 494.0499; found 494.0470.

10-fluoro-1'-phenylspiro[isoindolo[2,1-a]perimidine-12,3'-pyrrolidine]-2',5'-dione (3e):

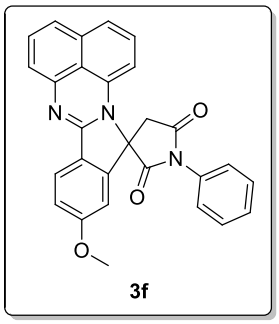


3e

Purified by silica gel column chromatography eluent: hexane/ethyl acetate (90:10). Yellow solid (27 mg, 62%), mp 305 - 308 ºC. ^{1}H NMR (400 MHz, DMSO-D_6 + $CDCl_3$) δ 8.04 – 8.01 (m, 2H), 7.58 – 7.47 (m, 6H), 7.34 (t, J = 7.8 Hz, 1H), 7.28 – 7.22 (m, 3H), 6.97 (d, J = 7.3 Hz, 1H), 6.09 (d, J = 8.3 Hz, 1H), 4.04 (d, J = 19.2 Hz, 1H), 3.45 (s, 1H). ^{13}C{^{1}H} NMR (126 MHz, DMSO-D_6 + $CDCl_3$) δ 171.6, 171.5, 165.2 (d, J = 252.0 Hz), 153.6, 145.2 (d, J = 10.08 Hz), 142.7, 135.4, 134.3, 131.6, 129.3, 129.2, 129.0, 127.8, 127.1, 127.0, 125.1 (d, J = 10.08 Hz), 121.3, 120.6, 120.0, 118.1 (d, J = 23.94 Hz), 116.3, 109.6 (d, J = 25.2 Hz), 100.9, 69.8, 34.2. ^{19}F NMR (471 MHz, DMSO-D_6 + $CDCl_3$) δ -104.5.

HRMS (ESI-TOF): m/z $[M + H]^+$ calcd for $C_{27}H_{17}N_3O_2F$ 434.1299; found 434.1305.

10-methoxy-1'-phenylspiro[isoindolo[2,1-a]perimidine-12,3'-pyrrolidine]-2',5'-dione (3f):

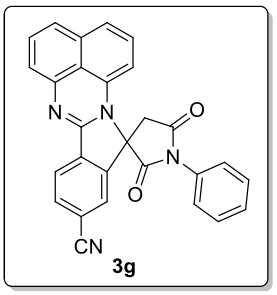


3f

Purified by silica gel column chromatography eluent: hexane/ethyl acetate (70:30). Yellow solid (39 mg, 88%), mp 272 - 274 ºC. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.04 (d, J = 8.6 Hz, 1H), 7.55 (t, J = 7.5 Hz, 2H), 7.50 – 7.44 (m, 3H), 7.37 (t, J = 7.8 Hz, 1H), 7.28 (s, 1H), 7.21 (d, J = 7.8 Hz, 1H), 7.16 – 7.09 (m, 3H), 6.89 (d, J = 2.2 Hz, 1H), 5.86 (d, J = 6.6 Hz, 1H), 4.06 (d, J = 18.8 Hz, 1H), 3.90 (s, 3H), 3.11 (d, J = 18.8 Hz, 1H). ^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) δ 171.8, 171.2, 163.8, 154.5, 144.9, 143.0, 136.0, 134.6, 131.4, 129.7, 129.5, 129.3, 127.0, 126.2, 125.5, 123.7, 121.6, 121.2, 120.6, 116.9, 116.2, 105.4, 100.2, 69.5, 56.1, 34.5.

HRMS (ESI-TOF): m/z $[M + H]^+$ calcd for $C_{28}H_{20}N_3O_3$ 446.1499; found 446.1519.

2',5'-dioxo-1'-phenylspiro[isoindolo[2,1-a]perimidine-12,3'-pyrrolidine]-10-carbonitrile

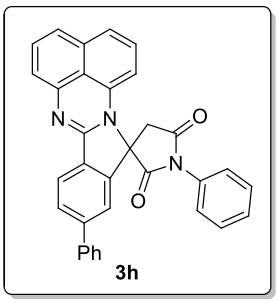


3g

(3g): Purified by silica gel column chromatography eluent: hexane/ethyl acetate (60:40). Red solid (18 mg, 41%), mp 313 - 316 ^{o}C. ^{1}H NMR (500 MHz, DMSO-D_6 + $CDCl_3$) δ 8.63 (s, 1H), 8.09 (d, J = 7.9 Hz, 1H), 7.99 – 7.97 (m, 1H), 7.52 (d, J = 4.3 Hz, 4H), 7.47 – 7.45 (m, 1H), 7.30 (t, J = 7.8 Hz, 1H), 7.25 (d, J = 8.2 Hz, 1H), 7.20 – 7.18 (m, 2H), 6.97 (d, J = 7.2 Hz, 1H), 6.02 (d, J = 5.9 Hz, 1H), 3.98 (d, J = 19.3 Hz, 1H), 3.41 (d, J = 19.2 Hz, 1H). ^{13}C{^{1}H} NMR (101 MHz, DMSO-D_6 + $CDCl_3$) δ 170.93, 170.89, 153.0, 143.1, 142.2, 135.3, 134.6, 134.0, 133.7, 131.3, 129.0, 128.83, 128.75, 127.3, 126.6, 126.1, 123.2, 121.6, 120.9, 120.1, 117.5, 116.7, 115.3, 100.6, 69.6, 34.0.

HRMS (ESI-TOF): m/z [M + H]$^{+}$ calcd for $C_{28}H_{17}N_4O_2$ 441.1346; found 441.1356.

1',10-diphenylspiro[isoindolo[2,1-a]perimidine-12,3'-pyrrolidine]-2',5'-dione (3h): Purified

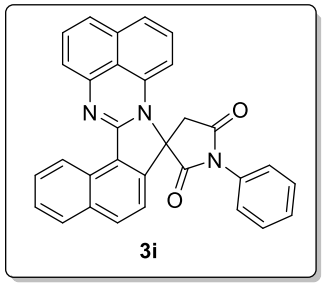


3h

by silica gel column chromatography eluent: hexane/ethyl acetate (80:20). Yellow solid (39 mg, 79%), mp 297 – 300 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.17 (d, J = 8.1 Hz, 1H), 7.85 (dd, J = 8.1, 1.5 Hz, 1H), 7.61 – 7.53 (m, 6H), , 7.51 – 7.45 (m,5H), 7.39 (t, J = 7.9 Hz, 1H), 7.29 (d, J = 8.3 Hz, 1H), 7.23 (d, J = 7.6 Hz, 1H), 7.15 (dd, J = 14.2, 6.7 Hz, 2H), 5.89 (d, J = 7.3 Hz, 1H), 4.11 (d, J = 18.8 Hz, 1H), 3.20 (d, J = 18.8 Hz, 1H).^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) δ 171.9, 171.3, 154.6, 146.7, 143.7, 143.1, 139.7, 136.0, 134.7, 131.4, 130.4, 129.9, 129.7, 129.6, 129.38, 129.34, 128.8, 127.6, 127.1, 126.2, 124.3, 121.9, 121.6, 120.7, 118.2, 117.3, 100.4, 69.8, 34.6.

HRMS (ESI-TOF): m/z [M + H]$^{+}$ calcd for $C_{33}H_{22}N_2O_2$ 492.1712; found 492.1708.

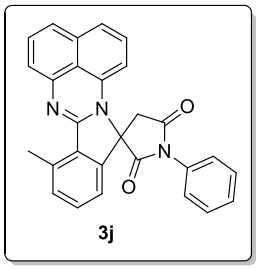
1'-phenylspiro[benzo[6,7]isoindolo[2,1-a]perimidine-14,3'-pyrrolidine]-2',5'-dione (3i):



Purified by silica gel column chromatography eluent: hexane/ethyl acetate (90:10). Orange solid (36 mg, 77%), mp 298-301 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.68 (d, *J* = 8.4 Hz, 1H), 8.13 (d, *J* = 8.6 Hz, 1H), 7.98 (d, *J* = 8.2 Hz, 1H), 7.81 (t, *J* = 7.7 Hz, 1H), 7.68 (t, *J* = 8.3 Hz, 1H), 7.57 (t, *J* = 8.0 Hz, 2H), 7.51 – 7.46 (m, 4H), 7.42 (t, *J* = 7.8 Hz, 1H), 7.31 (d, *J* = 8.3 Hz, 1H), 7.25 – 7.22 (m, 2H), 7.17 (t, *J* = 8.0 Hz, 1H), 5.91 (d, *J* = 6.6 Hz, 1H), 4.14 (d, *J* = 18.8 Hz, 1H), 3.18 (d, *J* = 18.8 Hz, 1H). ^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) δ 172.0, 171.4, 156.0, 143.4, 142.1, 136.0, 135.0, 134.4, 134.1, 131.5, 129.7, 129.5, 129.3, 129.2, 128.9, 128.6, 127.9, 127.1, 126.2, 125.5, 121.8, 121.0, 120.3, 117.9, 115.8, 100.0, 69.6, 34.0.

HRMS (ESI-TOF): m/z $[M + H]^+$ calcd for $C_{31}H_{20}N_3O_2$ 466.1550; found 466.1563.

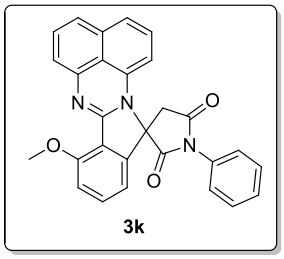
8-methyl-1'-phenylspiro[isoindolo[2,1-a]perimidine-12,3'-pyrrolidine]-2',5'-dione(3j):



Purified by silica gel column chromatography eluent: hexane/ethyl acetate (90:10). Yellow solid (23 mg, 54%), mp 236 - 239 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.59 – 7.54 (m, 2H), 7.52 – 7.46 (m, 4H), 7.41 – 7.37 (m, 2H), 7.30 – 7.28 (m, 2H), 7.22 (d, *J* = 7.6 Hz, 1H), 7.18 – 7.12 (m, 2H), 5.87 (d, *J* = 7.3 Hz, 1H), 4.08 (d, *J* = 18.7 Hz, 1H), 3.09 (d, *J* = 18.8 Hz, 1H), 2.93 (s, 3H).^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) δ 172.1, 171.6, 155.6, 143.4, 139.0, 135.9, 135.0, 132.6, 132.0, 131.5, 129.6, 129.5, 129.3, 128.8, 127.0, 126.2, 121.6, 121.1, 120.3, 117.7, 116.8, 100.1, 69.2, 34.7, 18.9.

HRMS (ESI-TOF): m/z $[M + H]^+$ calcd for $C_{28}H_{20}N_3O_2$ 430.1550; found 430.1565.

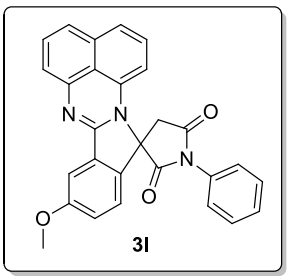
8-methoxy-1'-phenylspiro[isoindolo[2,1-a]perimidine-12,3'-pyrrolidine]-2',5'-dione (3k):



Purified by silica gel column chromatography eluent: hexane/ethyl acetate (70:30). Yellow solid (30 mg, 67%), mp 279 - 282 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.57 (t, *J* = 8.0 Hz, 1H), 7.53 (t, *J* = 7.7 Hz, 2H), 7.44 (dd, *J* = 18.8, 7.5 Hz, 3H), 7.35 (t, *J* = 7.8 Hz, 1H), 7.24 (s, 1H), 7.19 – 7.16 (m, 2H), 7.11 (t, *J* = 7.9 Hz, 1H), 7.06 (d, *J* = 8.3 Hz, 1H), 6.99 (d, *J* = 7.6 Hz, 1H), 5.83 (d, *J* = 7.3 Hz, 1H), 4.08 – 4.05 (m, 4H), 3.09 (d, *J* = 18.8 Hz, 1H).^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$) δ 172.0, 171.2, 157.5, 154.4, 145.2, 143.1, 135.8, 134.8, 134.6, 131.4, 129.6, 129.5, 129.2, 126.9, 126.2, 121.8, 120.9, 120.4, 118.8, 118.3, 112.6, 111.4, 100.1, 69.4, 56.7, 34.6.

HRMS (ESI-TOF): m/z $[M + H]^+$ calcd for $C_{28}H_{20}N_3O_3$ 446.1499; found 446.1477.

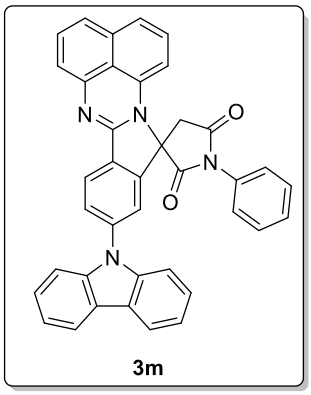
9-methoxy-1'-phenylspiro[isoindolo[2,1-a]perimidine-12,3'-pyrrolidine]-2',5'-dione (3l):



Purified by silica gel column chromatography eluent: hexane/ethyl acetate (75:25). Yellow solid (34 mg, 76%), mp 289 - 292 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.55 (t, *J* = 8.3 Hz, 3H), 7.46 (dd, *J* = 17.7, 7.4 Hz, 3H), 7.39 – 7.32 (m, 2H), 7.28 (d, *J* = 8.1 Hz, 1H), 7.23 – 7.19 (m, 2H), 7.13 (dd, *J* = 18.0, 7.3 Hz, 2H), 5.86 (d, *J* = 7.3 Hz, 1H), 4.06 (d, *J* = 18.7 Hz, 1H), 3.94 (s, 3H), 3.09 (d, *J* = 18.7 Hz, 1H). ^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) δ 171.9, 171.4, 161.7, 154.9, 143.0, 136.1, 135.1, 134.8, 133.1, 131.4, 129.6, 129.5, 129.3, 127.1, 126.2, 121.9, 121.7, 121.6, 120.65, 120.62, 117.2, 106.4, 100.3, 69.4, 56.2, 34.5.

HRMS (ESI-TOF): m/z $[M + H]^+$ calcd for $C_{28}H_{20}N_3O_3$ 446.1499; found 446.1499.

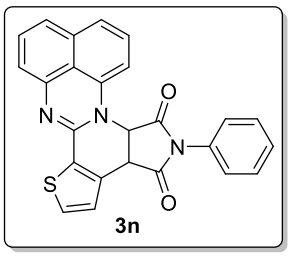
10-(9H-carbazol-9-yl)-1'-phenylspiro[isoindolo[2,1-a]perimidine-12,3'-pyrrolidine]-2',5'-



dione (3m): Purified by silica gel column chromatography eluent: hexane/ethyl acetate (75:25). Yellow solid (36 mg, 62%), mp 307 - 310 ºC. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.33 (d, *J* = 8.2 Hz, 1H), 8.15 (d, *J* = 7.7 Hz, 2H), 7.90 (dd, *J* = 8.2, 1.7 Hz, 1H), 7.69 (d, *J* = 1.8 Hz, 1H), 7.54 – 7.50 (m, 2H), 7.48 – 7.45 (m, 1H), 7.44 – 7.42 (m, 4H), 7.39 (t, *J* = 7.4 Hz, 3H), 7.36 – 7.31 (m, 3H), 7.25 – 7.24 (m, 1H), 7.19 – 7.15 (m, 2H), 5.91 (d, *J* = 6.8 Hz, 1H), 4.14 (d, *J* = 18.9 Hz, 1H), 3.21 (d, *J* = 19.0 Hz, 1H).^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$) δ 171.4, 171.2, 154.0, 144.7, 142.9, 142.3, 140.2, 136.1, 134.6, 131.2, 130.0, 129.7, 129.5, 129.0, 127.1, 126.6, 126.3, 125.6, 124.1, 122.2, 121.5, 121.2, 120.9, 120.8, 117.7, 117.6, 109.5, 100.5, 69.7, 34.4.

HRMS (ESI-TOF): m/z $[M + H]^+$ calcd for $C_{39}H_{25}N_4O_2$ 581.1972; found 581.1973.

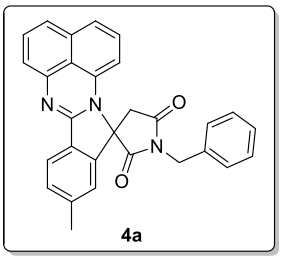
5-phenyl-3b,6a-dihydro-4H-pyrrolo[3',4':5,6]thieno[2',3':3,4]pyrido[1,2-a]perimidine-



4,6(5H)-dione (3n): Purified by silica gel column chromatography eluent: hexane/ethyl acetate (80:20). Red solid (16 mg, 38%), mp 254 - 257 ºC. ^{1}H NMR (500 MHz, DMSO-D_6) δ 7.92 (d, *J* = 3.8 Hz, 1H), 7.48 (t, *J* = 7.6 Hz, 2H), 7.42 (t, *J* = 7.3 Hz, 1H), 7.27 – 7.20 (m, 7H), 6.80 (d, *J* = 7.3 Hz, 2H), 6.25 (d, *J* = 9.0 Hz, 1H), 4.86 (d, *J* = 8.6 Hz, 1H), 3.45 (d, J = 30.0 Hz, 1H). ^{13}C{^{1}H} NMR (126 MHz, DMSO-D_6 + $CDCl_3$) δ 172.9, 172.2, 144.3, 141.9, 138.5, 134.8, 133.6, 133.5, 131.9, 131.3, 129.0, 128.6, 127.6, 126.5, 125.7, 121.4, 120.5, 119.2, 115.0, 102.7, 54.5, 42.0.

HRMS (ESI-TOF): m/z $[M + H]^+$ calcd for $C_{25}H_{16}N_3O_2S$ 422.0963; found 422.0957.

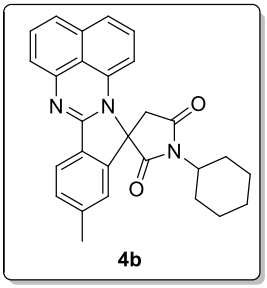
***1'-benzyl-10-methylspiro[isoindolo[2,1-a]perimidine-12,3'-pyrrolidine]-2',5'-dione (4a)*:**



Purified by silica gel column chromatography eluent: hexane/ethyl acetate (90:10). Yellow solid (38 mg, 86%), mp 264 - 266 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.92 (d, *J* = 7.8 Hz, 1H), 7.51 – 7.49 (m, 2H), 7.39 – 7.38 (m, 3H), 7.34 (dd, *J* = 15.4, 7.1 Hz, 2H), 7.23 (d, *J* = 8.2 Hz, 1H), 7.12 (d, *J* = 9.3 Hz, 1H), 7.06 (d, *J* = 7.4 Hz, 1H), 6.84 – 6.81 (m, 1H), 6.75 (s, 1H), 5.40 (d, *J* = 8.4 Hz, 1H), 4.94 (s, 2H), 3.81 (d, *J* = 18.7 Hz, 1H), 2.89 (d, *J* = 18.7 Hz, 1H), 2.35 (s, 3H). ^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$) δ 172.5, 172.2, 154.8, 143.9, 143.24, 143.16, 135.9, 135.2, 134.5, 131.4, 129.5, 129.2, 129.1, 128.80, 128.75, 126.9, 123.5, 121.6, 121.4, 120.4, 120.1, 117.0, 100.4, 69.4, 43.8, 34.6, 22.0.

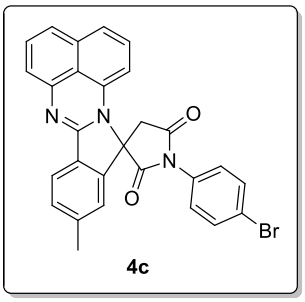
HRMS (ESI-TOF): m/z $[M + H]^+$ calcd for $C_{29}H_{22}N_3O_2$ 444.1707; found 444.1722 .

***1'-cyclohexyl-10-methylspiro[isoindolo[2,1-a]perimidine-12,3'-pyrrolidine]-2',5'-dione (4b)*:** Purified by silica gel column chromatography eluent: hexane/ethyl acetate (88:12). Yellow solid (39 mg, 90%), mp 297 - 299 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.01 (d, *J* = 7.9 Hz, 1H), 7.43 (d, *J* = 7.8 Hz, 1H), 7.37 (t, *J* = 7.8 Hz, 1H), 7.28 (s, 1H), 7.20 (d, *J* = 8.4 Hz, 1H), 7.13 – 7.05 (m, 3H), 5.70 (d, *J* = 7.3 Hz, 1H), 4.27 (t, *J* = 12.4 Hz, 1H), 3.84 (d, *J* = 18.6 Hz, 1H), 2.91 (d, *J* = 18.7 Hz, 1H), 2.50 (s, 3H), 2.36 – 2.23 (m, 2H), 1.93 (d, *J* = 13.6 Hz, 2H), 1.82 (t, *J* = 13.3 Hz, 2H), 1.73 (d, *J* = 12.8 Hz, 1H), 1.47 – 1.36 (m, 2H), 1.32 – 1.25 (m, 1H).^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) δ 172.9, 172.2, 155.0, 144.1, 143.6, 136.0, 134.6, 131.4, 129.3, 128.6, 126.9, 123.7, 121.6, 121.5, 120.5, 119.9, 116.8, 100.3, 69.3, 53.2, 34.4, 29.2, 28.8, 25.9, 25.8, 25.0, 22.3.



HRMS (ESI-TOF): m/z $[M + H]^+$ calcd for $C_{28}H_{26}N_3O_2$ 436.2020; found 436.2019.

1'-(4-bromophenyl)-10-methylspiro[isoindolo[2,1-a]perimidine-12,3'-pyrrolidine]-2',5'-

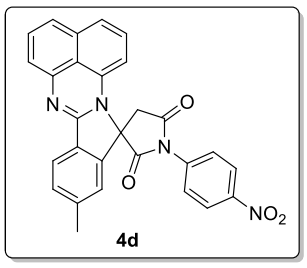


4c

***dione (4c)*:** Purified by silica gel column chromatography eluent: hexane/ethyl acetate (90:10). Yellow solid (35 mg, 69%), mp 232 - 234 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.99 (d, *J* = 7.8 Hz, 1H), 7.69 (d, *J* = 8.7 Hz, 2H), 7.46 (d, *J* = 7.9 Hz, 1H), 7.39 – 7.36 (m, 3H), 7.28 (d, *J* = 9.3 Hz, 1H), 7.22 – 7.18 (m, 2H), 7.14 – 7.10 (m, 2H), 5.80 (d, *J* = 6.7 Hz, 1H), 4.06 (d, *J* = 18.8 Hz, 1H), 3.11 (d, *J* = 18.9 Hz, 1H), 2.51 (s, 3H). ^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$) δ 171.6, 171.2, 154.7, 144.2, 143.13, 143.06, 136.0, 134.7, 132.8, 131.7, 130.4, 129.4, 129.0, 127.6, 127.0, 123.8, 123.4, 121.8, 121.5, 120.7, 120.0, 117.3, 100.1, 69.5, 34.5, 22.3.

HRMS (ESI-TOF): m/z $[M + H]^+$ calcd for $C_{28}H_{19}N_3O_2Br$ 508.0655; found 508.0682.

10-methyl-1'-(4-nitrophenyl)spiro[isoindolo[2,1-a]perimidine-12,3'-pyrrolidine]-2',5'-dione

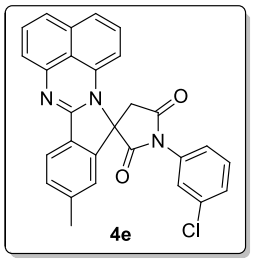


4d

***(4d)*:** Purified by silica gel column chromatography eluent: hexane/ethyl acetate (90:10). Yellow solid (37 mg, 78%), mp 291 - 293 °C. ^{1}H NMR (500 MHz, DMSO-D_6 + $CDCl_3$) δ 8.35 (d, *J* = 9.0 Hz, 2H), 7.87 (d, *J* = 7.8 Hz, 1H), 7.81 (d, *J* = 9.1 Hz, 2H), 7.47 (s, 1H), 7.43 (d, *J* = 7.9 Hz, 1H), 7.29 (t, *J* = 7.8 Hz, 1H), 7.20 (d, *J* = 8.1 Hz, 1H), 7.17 – 7.12 (m, 2H), 6.97 (d, *J* = 7.4 Hz, 1H), 5.99 (d, *J* = 6.4 Hz, 1H), 4.08 (d, *J* = 18.8 Hz, 1H), 3.22 (d, *J* = 18.9 Hz, 1H), 2.48 (s, 3H). ^{13}C{^{1}H} NMR (126 MHz, DMSO-D_6 + $CDCl_3$) δ 170.4, 170.2, 153.9, 146.9, 143.6, 142.5, 142.4, 136.5, 135.1, 134.0, 130.8, 128.4, 127.9, 126.8, 126.7, 123.8, 122.4, 120.7, 120.5, 120.2, 119.5, 116.2, 100.1, 69.1, 34.0, 21.2.

HRMS (ESI-TOF): m/z $[M + H]^+$ calcd for $C_{28}H_{19}N_4O_4$ 475.1401; found 475.1383.

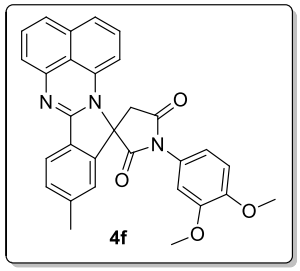
1'-(3-chlorophenyl)-10-methylspiro[isoindolo[2,1-a]perimidine-12,3'-pyrrolidine]-2',5'-



dione (4e)**:** Purified by silica gel column chromatography eluent: hexane/ethyl acetate (90:10). Yellow solid (33 mg, 71%), mp 279 - 282 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.99 (d, *J* = 7.8 Hz, 1H), 7.52 (s, 1H), 7.50 – 7.45 (m, 3H), 7.41 – 7.36 (m, 2H), 7.28 (d, *J* = 7.7 Hz, 1H), 7.23 – 7.19 (m, 2H), 7.17 – 7.10 (m, 2H), 5.81 (d, *J* = 7.2 Hz, 1H), 4.07 (d, *J* = 18.8 Hz, 1H), 3.11 (d, *J* = 18.8 Hz, 1H), 2.52 (s, 3H).^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) δ 171.5, 171.1, 154.7, 144.2, 143.11, 143.07, 136.0, 135.2, 134.7, 132.4, 131.8, 130.6, 129.7, 129.4, 128.9, 127.0, 126.4, 124.3, 123.8, 121.8, 121.5, 120.7, 120.0, 117.3, 100.2, 69.5, 34.5, 22.3.

HRMS (ESI-TOF): m/z [M + H]$^{+}$ calcd for $C_{28}H_{19}ClN_3O_2$ 464.1160; found 464.1183.

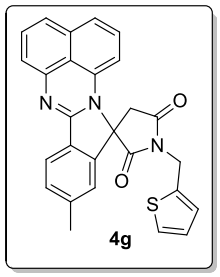
1'-(3,4-dimethoxyphenyl)-10-methylspiro[isoindolo[2,1-a]perimidine-12,3'-pyrrolidine]-



2',5'-dione (4f)**:** Purified by silica gel column chromatography eluent: hexane/ethyl acetate (80:20). Yellow solid (35 mg, 72%), mp 279 - 282 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.97 (d, *J* = 7.9 Hz, 1H), 7.43 (d, *J* = 7.9 Hz, 1H), 7.35 (t, *J* = 7.8 Hz, 1H), 7.24 (s, 1H), 7.19 (d, *J* = 6.0 Hz, 2H), 7.13 – 7.08 (m, 2H), 7.03 – 6.97 (m, 2H), 6.91 (d, *J* = 2.3 Hz, 1H), 5.83 (d, *J* = 7.2 Hz, 1H), 4.02 (d, *J* = 18.8 Hz, 1H), 3.91 (s, 3H), 3.90 (s, 3H), 3.08 (d, *J* = 18.8 Hz, 1H), 2.49 (s, 3H).^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) δ 172.2, 171.6, 154.8, 149.8, 149.6, 144.1, 143.3, 143.2, 136.0, 134.8, 131.6, 129.4, 129.0, 127.0, 124.2, 123.7, 121.7, 121.5, 120.6, 120.0, 118.7, 117.2, 111.4, 109.5, 100.2, 69.5, 56.4, 56.3, 34.6, 22.3.

HRMS (ESI-TOF): m/z [M + H]$^{+}$ calcd for $C_{30}H_{24}N_3O_4$ 490.1761; found 490.1749.

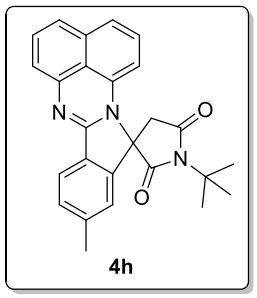
10-methyl-1'-(thiophen-2-ylmethyl)spiro[isoindolo[2,1-a]perimidine-12,3'-pyrrolidine]-



***2',5'-dione (4g)*:** Purified by silica gel column chromatography eluent: hexane/ethyl acetate (90:10). Yellow solid (36 mg, 80%), mp 231 - 234 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.84 (d, *J* = 7.8 Hz, 1H), 7.31 – 7.28 (m, 1H), 7.24 (d, *J* = 4.4 Hz, 1H), 7.18 – 7.13 (m, 3H), 7.05 (d, *J* = 8.3 Hz, 1H), 6.99 (d, *J* = 7.2 Hz, 1H), 6.93 (dd, *J* = 5.2, 3.5 Hz, 1H), 6.79 (t, *J* = 7.9 Hz, 1H), 6.70 (s, 1H), 5.33 (d, *J* = 7.5 Hz, 1H), 5.03 (s, 2H), 3.75 (d, *J* = 18.7 Hz, 1H), 2.83 (d, *J* = 18.7 Hz, 1H), 2.30 (s, 3H). ^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) δ 172.1, 171.7, 154.8, 143.9, 143.11, 143.09, 135.92, 135.87, 134.42, 131.35, 129.21, 129.19, 128.7, 127.3, 126.9, 126.6, 123.4, 121.5, 121.4, 120.3, 120.2, 117.0, 100.4, 69.4, 37.6, 34.6, 22.0.

HRMS (ESI-TOF): m/z $[M + H]^+$ calcd for $C_{27}H_{20}N_3O_2S$ 450.1271; found 450.1275.

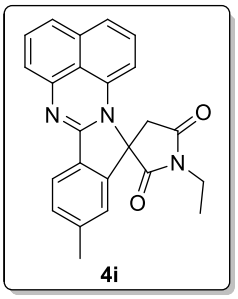
1'-(tert-butyl)-10-methylspiro[isoindolo[2,1-a]perimidine-12,3'-pyrrolidine]-2',5'-dione



***(4h)*:** Purified by silica gel column chromatography eluent: hexane/ethyl acetate (90:10). Yellow solid (31 mg, 76%), mp 234 - 236 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.95 (d, *J* = 7.9 Hz, 1H), 7.41 (d, *J* = 7.8 Hz, 1H), 7.36 – 7.33 (m, 1H), 7.24 (d, *J* = 8.3 Hz, 1H), 7.18 (d, *J* = 8.6 Hz, 1H), 7.11 – 7.06 (m, 3H), 5.67 (d, *J* = 7.4 Hz, 1H), 3.78 (d, *J* = 18.5 Hz, 1H), 2.83 (d, *J* = 18.6 Hz, 1H), 2.49 (s, 3H), 1.73 (s, 9H). ^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$) δ 174.0, 172.9, 155.0, 143.9, 143.8, 143.3, 136.0, 134.8, 131.4, 129.2, 128.9, 126.9, 123.6, 121.6, 121.4, 120.3, 119.7, 116.8, 100.2, 69.3, 60.5, 34.7, 28.5, 22.3.

HRMS (ESI-TOF): m/z $[M + H]^+$ calcd for $C_{26}H_{24}N_3O_2$ 410.1863; found 410.1872.

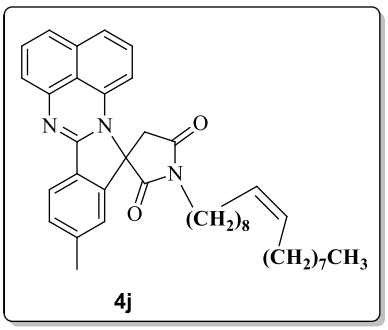
***1'-ethyl-10-methylspiro[isoindolo[2,1-a]perimidine-12,3'-pyrrolidine]-2',5'-dione (4i)*:**



Purified by silica gel column chromatography eluent: hexane/ethyl acetate (90:10). Yellow solid (32 mg, 84%), mp 281 - 283 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.00 (d, *J* = 4.0 Hz, 1H), 7.43 (d, *J* = 7.9 Hz, 1H), 7.37 (t, *J* = 7.8 Hz, 1H), 7.28 (s, 1H), 7.20 (d, *J* = 8.4 Hz, 1H), 7.13 – 7.08 (m, 2H), 7.05 (s, 1H), 5.67 (d, *J* = 7.3 Hz, 1H), 3.90 – 3.85 (m, 3H), 2.96 (d, *J* = 18.7 Hz, 1H), 2.49 (s, 3H), 1.38 (t, *J* = 7.2 Hz, 3H). ^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$) δ 172.7, 172.2, 154.9, 144.2, 143.4, 142.8, 135.9, 134.6, 131.5, 129.3, 128.6, 127.0, 123.8, 121.7, 121.4, 120.6, 120.0, 116.9, 100.3, 69.6, 35.2, 34.6, 22.2, 13.2.

HRMS (ESI-TOF): m/z [M + H]$^{+}$ calcd for $C_{24}H_{20}N_3O_2$ 382.1550; found 382.1571.

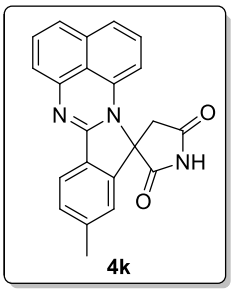
***(Z)-10-methyl-1'-(octadec-9-en-1-yl)spiro[isoindolo[2,1-a]perimidine-12,3'-pyrrolidine]-2',5'-dione (4j)*:**



Purified by silica gel column chromatography eluent: hexane/ethyl acetate (95:5). Yellow solid (46 mg, 76%), mp 96 – 99 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.94 (d, *J* = 7.9 Hz, 1H), 7.40 (d, *J* = 7.9 Hz, 1H), 7.35 (t, *J* = 7.8 Hz, 1H), 7.24 (d, *J* = 8.2 Hz, 1H), 7.17 (d, *J* = 8.4 Hz, 1H), 7.08 – 7.04 (m, 3H), 5.65 (d, *J* = 7.5 Hz, 1H), 5.43 – 5.31 (m, 2H), 3.86 (d, *J* = 18.7 Hz, 1H), 3.82 – 3.75 (m, 2H), 2.94 (d, *J* = 18.7 Hz, 1H), 2.46 (s, 3H), 2.06 – 1.95 (m, 4H), 1.79 – 1.71 (m, 2H), 1.38 – 1.26 (m, 22H), 0.88 (t, *J* = 6.8 Hz, 3H). ^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) δ 173.0, 172.5, 154.8, 143.9, 143.4, 143.2, 136.0, 134.8, 131.4, 130.2, 129.8, 129.2, 128.9, 126.9, 123.6, 121.53, 121.49, 120.4, 120.0, 117.0, 100.1, 69.5, 40.2, 34.5, 32.0, 29.9, 29.84, 29.77, 29.64, 29.58, 29.4, 29.34, 29.29, 27.9, 27.34, 27.29, 27.2, 22.8, 22.2, 14.2.

HRMS (ESI-TOF): m/z [M + H]$^{+}$ calcd for $C_{40}H_{50}N_3O_2$ 604.3898; found 604.3892.

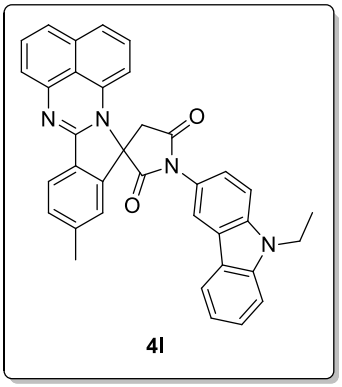
10-methylspiro[isoindolo[2,1-a]perimidine-12,3'-pyrrolidine]-2',5'-dione (4k): Purified by silica gel column chromatography eluent: hexane/ethyl acetate (80:20). Yellow solid (22 mg, 62%), mp 334 - 336 °C. ^{1}H NMR (500 MHz, DMSO-D_6) δ 12.50 (bs, 1H), 7.84 (d, J = 7.8 Hz, 1H), 7.52 (s, 1H), 7.49 (d, J = 7.9 Hz, 1H), 7.35 (t, J = 7.8 Hz, 1H), 7.27 (d, J = 8.1 Hz, 1H), 7.23 – 7.22 (m, 2H), 6.95 (d, J = 7.3 Hz, 1H), 5.97 (dd, J = 5.2, 3.1 Hz, 1H), 3.86 (d, J = 19.1 Hz, 1H), 3.07 (d, J = 19.1 Hz, 1H), 2.47 (s, 3H). ^{13}C{^{1}H} NMR (126 MHz, DMSO-D_6) δ 174.1, 173.9, 154.6, 143.9, 143.6, 143.1, 135.4, 134.5, 131.0, 129.0, 127.8, 127.7, 122.4, 121.1, 120.8, 120.7, 119.5, 115.9, 100.8, 70.9, 35.2, 21.4.



4k

HRMS (ESI-TOF): m/z [M + H]$^{+}$ calcd for $C_{22}H_{16}N_3O_2$ 354.1237; found 354.1231.

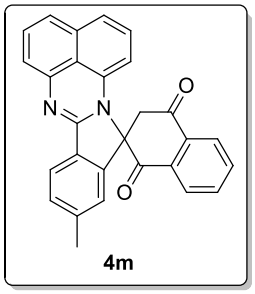
1'-(9-ethyl-9H-carbazol-3-yl)-10-methylspiro[isoindolo[2,1-a]perimidine-12,3'-pyrrolidine]-2',5'-dione (4l): Purified by silica gel column chromatography eluent: hexane/ethyl acetate (80:20). Yellow solid (42 mg, 77%), mp 338 -341 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.18 – 8.15 (m, 2H), 8.04 (d, J = 7.9 Hz, 1H), 7.59 – 7.48 (m, 5H), 7.41 (t, J = 7.8 Hz, 1H), 7.36 (s, 1H), 7.33 – 7.28 (m, 3H), 7.23 (d, J = 8.6 Hz, 1H), 7.15 (d, J = 7.3 Hz, 1H), 6.01 (d, J = 7.9 Hz, 1H), 4.45 (q, J = 7.2 Hz, 2H), 4.15 (d, J = 18.8 Hz, 1H), 3.20 (d, J = 18.8 Hz, 1H), 2.59 (s, 3H), 1.49 (t, J = 7.3 Hz, 3H). ^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) δ 172.8, 172.1, 154.9, 144.2, 143.6, 140.7, 139.9, 136.0, 134.8, 131.6, 129.3, 129.0, 127.1, 126.7, 123.8, 123.5, 123.4, 122.6, 122.4, 121.7, 121.0, 120.6, 120.2, 119.6, 118.7, 117.1, 109.2, 109.0, 100.4, 69.7, 37.9, 34.7, 22.3, 14.0.



4l

HRMS (ESI-TOF): m/z [M + H]$^{+}$ calcd for $C_{36}H_{27}N_4O_2$ 547.2129; found 547.2138.

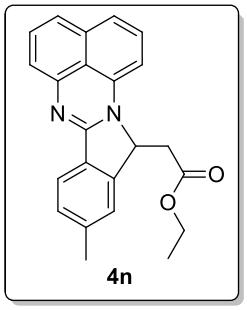
***10-methyl-1'H-spiro[isoindolo[2,1-a]perimidine-12,2'-naphthalene]-1',4'(3'H)-dione (4m)*:**



Purified by silica gel column chromatography eluent: hexane/ethyl acetate (90:10). Orange solid (34 mg, 82%), mp 236 - 237 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.35 – 8.32 (m, 2H), 8.01 – 7.98 (m, 1H), 7.97 (d, *J* = 7.9 Hz, 1H), 7.93 (t, *J* = 7.5 Hz, 1H), 7.37 – 7.33 (m, 2H), 7.24 (d, *J* = 7.2 Hz, 1H), 7.16 (d, *J* = 7.5 Hz, 1H), 7.07 (d, *J* = 7.4 Hz, 1H), 7.05 – 7.02 (m, 1H), 6.63 (s, 1H), 5.80 (d, *J* = 8.4 Hz, 1H), 4.51 (d, *J* = 16.7 Hz, 1H), 3.02 (d, *J* = 16.8 Hz, 1H), 2.28 (s, 3H). ^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$) δ 193.8, 186.5, 155.0, 143.7, 143.3, 143.0, 136.3, 136.1, 135.9, 135.3, 134.8, 134.4, 131.3, 129.5, 129.2, 128.9, 127.5, 126.8, 124.1, 122.0, 121.4, 121.3, 120.1, 116.6, 103.0, 74.0, 43.8, 22.2.

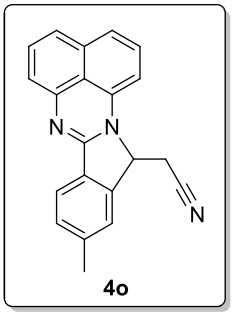
HRMS (ESI-TOF): m/z $[M + H]^+$ calcd for $C_{28}H_{19}N_2O_2$ 415.1441; found 415.1458.

***ethyl 2-(10-methyl-12H-isoindolo[2,1-a]perimidin-12-yl)acetate (4n)*:** Purified by silica gel column chromatography eluent: hexane/ethyl acetate (90:10). Yellow solid (33 mg, 93%), mp 122 - 125 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.92 (d, *J* = 7.9 Hz, 1H), 7.33 (t, J = 8.2 Hz, 3H), 7.22 – 7.14 (m, 3H), 7.02 (d, *J* = 8.6 Hz, 1H), 6.25 (d, *J* = 7.0 Hz, 1H), 5.38 (dd, *J* = 9.4, 2.8 Hz, 1H), 4.29 – 4.20 (m, 2H), 3.48 (dd, *J* = 16.4, 2.8 Hz, 1H), 2.47 (s, 3H), 2.45 – 2.41 (m, 1H), 1.28 (t, *J* = 7.2 Hz, 3H). ^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) δ 170.8, 155.3, 144.4, 144.3, 142.8, 136.1, 135.9, 130.2, 129.3, 129.2, 127.3, 123.2, 123.0, 121.7, 120.5, 119.5, 115.9, 100.4, 61.4, 58.0, 34.5, 22.2, 14.3.



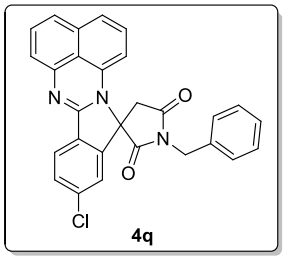
HRMS (ESI-TOF): m/z $[M + H]^+$ calcd for $C_{23}H_{21}N_2O_2$ 357.1598; found 357.1619.

***2-(10-methyl-12H-isoindolo[2,1-a]perimidin-12-yl)acetonitrile (4o)*:** Purified by silica gel column chromatography eluent: hexane/ethyl acetate (80:20). Yellow solid (26 mg, 84%), mp 225 - 226 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.94 (d, *J* = 7.9 Hz, 1H), 7.55 (s, 1H), 7.39 (d, *J* = 7.9 Hz, 1H), 7.35 (t, J = 7.6 Hz, 1H), 7.24 (d, *J* = 8.2 Hz, 1H), 7.19 – 7.17 (m, 2H), 7.05 (d, *J* = 7.5 Hz, 1H), 6.18 (dd, *J* = 5.5, 2.8 Hz, 1H), 5.14 (dd, *J* = 8.3, 3.1 Hz, 1H), 3.43 (dd, *J* = 16.9, 3.1 Hz, 1H), 2.77 (dd, *J* = 16.9, 8.3 Hz, 1H), 2.52 (s, 3H). ^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) δ 154.6, 143.5, 141.6, 135.8, 135.5, 131.1, 129.4, 129.2, 127.2, 123.5, 123.1, 121.2, 120.2, 116.6, 115.8, 100.2, 57.0, 22.3, 19.5.



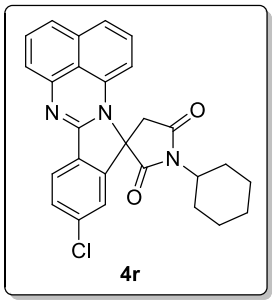
HRMS (ESI-TOF): m/z $[M + H]^+$ calcd for $C_{21}H_{16}N_3$ 310.1339; found 310.1364.

1'-benzyl-10-chlorospiro[isoindolo[2,1-a]perimidine-12,3'-pyrrolidine]-2',5'-dione (4q): Purified by silica gel column chromatography eluent: hexane/ethyl acetate (90:10). Yellow solid (37 mg, 80%), mp 279 - 281 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.97 (d, *J* = 8.3 Hz, 1H), 7.55 (dd, *J* = 8.2, 1.8 Hz, 1H), 7.50 – 7.48 (m, 2H), 7.40 – 7.39 (m, 3H), 7.33 (t, *J* = 7.6 Hz, 1H), 7.24 (d, *J* = 7.2 Hz, 1H), 7.13 (d, *J* = 8.1 Hz, 1H), 7.06 (d, *J* = 7.4 Hz, 1H), 7.00 (d, *J* = 1.7 Hz, 1H), 6.79 (t, *J* = 8.1 Hz, 1H), 5.35 (d, *J* = 6.9 Hz, 1H), 4.93 (s, 2H), 3.81 (d, *J* = 18.9 Hz, 1H), 2.91 (d, *J* = 18.8 Hz, 1H). ^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$) δ 172.0, 171.6, 153.7, 144.2, 142.8, 138.9, 135.9, 134.9, 134.2, 131.0, 130.0, 129.4, 129.3, 129.2, 129.0, 126.9, 124.9, 122.0, 121.5, 120.7, 120.5, 117.3, 100.6, 69.4, 44.0, 34.4.



HRMS (ESI-TOF): m/z $[M + H]^+$ calcd for $C_{28}H_{19}N_3O_2Cl$ 464.1160; found 464.1181.

10-chloro-1'-cyclohexylspiro[isoindolo[2,1-a]perimidine-12,3'-pyrrolidine]-2',5'-dione (4r):

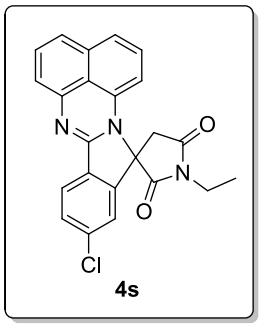


4r

Purified by silica gel column chromatography eluent: hexane/ethyl acetate (90:10). Yellow solid (39 mg, 85%), mp 302 - 303 ºC. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.00 (d, *J* = 8.2 Hz, 1H), 7.58 (dd, *J* = 8.2, 1.8 Hz, 1H), 7.36 (t, *J* = 8.2 Hz, 1H), 7.27 (s, 1H), 7.22 (d, *J* = 1.5 Hz, 1H), 7.19 (d, *J* = 7.6 Hz, 1H), 7.09 – 7.06 (m, 2H), 5.66 (d, *J* = 8.4 Hz, 1H), 4.24 (tt, *J* = 12.4, 3.9 Hz, 1H), 3.83 (d, *J* = 18.7 Hz, 1H), 2.90 (d, *J* = 18.8 Hz, 1H), 2.33 – 2.20 (m, 2H), 1.91 (d, *J* = 13.3 Hz, 2H), 1.79 (t, J = 15.0 Hz, 2H), 1.71 (d, *J* = 12.8 Hz, 1H), 1.45 – 1.34 (m, 2H), 1.26 (qt, *J* = 13.0, 3.4 Hz, 1H). ^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$) δ 172.4, 171.7, 153.9, 144.5, 142.9, 138.9, 136.0, 134.5, 131.0, 130.1, 129.3, 127.0, 125.0, 122.0, 121.5, 120.7, 120.2, 117.3, 100.3, 69.1, 53.4, 34.2, 29.1, 28.8, 25.84, 25.79, 25.0.

HRMS (ESI-TOF): m/z $[M + H]^+$ calcd for $C_{27}H_{23}N_3O_2Cl$ 456.1473; found 456.1497.

10-chloro-1'-ethylspiro[isoindolo[2,1-a]perimidine-12,3'-pyrrolidine]-2',5'-dione (4s):

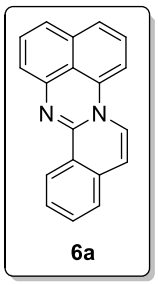


4s

Purified by silica gel column chromatography eluent: hexane/ethyl acetate (90:10). Yellow solid (33 mg, 82%), mp 292 - 295 ºC. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.00 (d, *J* = 8.3 Hz, 1H), 7.59 (dd, *J* = 8.2, 1.8 Hz, 1H),7.36 (t, *J* = 7.8 Hz, 1H), 7.28 (d, *J* = 1.1 Hz, 1H), 7.24 (d, *J* = 1.6 Hz, 1H), 7.20 (d, *J* = 8.5 Hz, 1H), 7.09– 7.06 (m, 2H) 5.64 (d, *J* = 6.5 Hz, 1H), 3.89 – 3.85 (m, 3H), 2.95 (d, *J* = 18.8 Hz, 1H), 1.37 (t, *J* = 7.2 Hz, 3H). ^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$) δ 172.2, 171.6, 153.8, 144.3, 142.9, 139.0, 136.0, 134.5, 131.0, 130.1, 129.4, 127.0, 125.0, 122.1, 121.5, 120.8, 120.3, 117.4, 100.3, 69.5, 35.4, 34.4, 13.2.

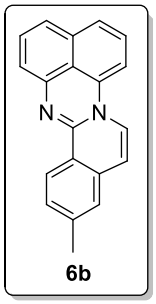
HRMS (ESI-TOF): m/z $[M + H]^+$ calcd for $C_{23}H_{17}N_3O_2Cl$ 402.1004; found 402.1027.

isoquinolino[2,1-a]perimidine (6a): Purified by silica gel column chromatography eluent: hexane/ethyl acetate (98:2). Orange solid (16 mg, 60%), mp 161 - 163 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.69 (d, *J* = 8.1 Hz, 1H), 7.56 (t, *J* = 7.5 Hz, 1H), 7.47 (t, *J* = 6.9 Hz, 1H), 7.39 – 7.32 (m, 3H), 7.28 (s, 1H), 7.19 (dd, *J* = 17.7, 7.8 Hz, 2H), 7.00 (d, *J* = 7.5 Hz, 1H), 6.72 (d, *J* = 7.7 Hz, 1H), 6.54 (d, *J* = 7.7 Hz, 1H). ^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) δ 147.6, 142.6, 136.9, 135.9, 133.6, 131.8, 129.3, 128.1, 127.8, 127.19, 127.15, 125.8, 123.2, 122.2, 121.7, 119.3, 115.5, 110.0, 101.8.



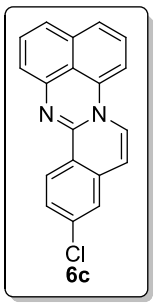
HRMS (ESI-TOF): m/z [M + H]$^+$ calcd for $C_{19}H_{13}N_2$ 269.1079; found 269.1057.

10-methylisoquinolino[2,1-a]perimidine (6b): Purified by silica gel column chromatography eluent: hexane/ethyl acetate (98:2). Orange solid (19 mg, 67%), mp 165 - 168 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.58 (d, *J* = 8.3 Hz, 1H), 7.40 (d, *J* = 7.8 Hz, 1H), 7.36 – 7.27 (m, 3H), 7.24 – 7.16 (m, 3H), 6.99 (d, *J* = 7.5 Hz, 1H), 6.74 (d, *J* = 7.5 Hz, 1H), 6.52 (d, *J* = 7.7 Hz, 1H), 2.45 (s, 3H). ^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) δ 147.6, 142.8, 142.3, 136.9, 135.9, 133.7, 129.5, 129.3, 127.2, 125.8, 125.4, 123.2, 122.1, 121.6, 119.1, 115.3, 110.0, 101.7, 21.7.



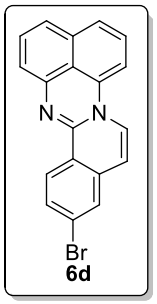
HRMS (ESI-TOF): m/z [M + H]$^+$ calcd for $C_{20}H_{15}N_2$ 283.1235; found 283.1212.

10-chloroisoquinolino[2,1-a]perimidine (6c): Purified by silica gel column chromatography eluent: hexane/ethyl acetate (98:2). Orange solid (16 mg, 53%), mp 194 - 197 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.50 (d, *J* = 8.7 Hz, 1H), 7.32 – 7.29 (m, 2H), 7.25 (d, *J* = 6.7 Hz, 1H), 7.22 – 7.17 (m, 2H), 7.14 – 7.08 (m, 2H), 6.88 (dd, *J* = 7.4, 1.2 Hz, 1H), 6.63 (d, *J* = 7.6 Hz, 1H), 6.35 (d, *J* = 7.8 Hz, 1H). ^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) δ 147.0, 142.3, 138.1, 136.6, 135.9, 135.0, 129.3, 128.9, 128.4, 127.2, 126.3, 125.2, 124.6, 122.1, 122.0, 119.7, 115.8, 108.7, 102.0.



HRMS (ESI-TOF): m/z [M + H]$^+$ calcd for $C_{19}H_{12}N_2Cl$ 303.0689; found 303.0672.

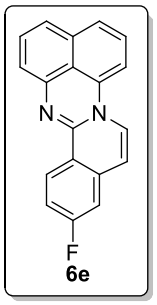
10-bromoisoquinolino[2,1-a]perimidine (6d): Purified by silica gel column chromatography



eluent: hexane/ethyl acetate (98:2). Orange solid (19 mg, 55%), mp 204 - 207 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.51 (d, *J* = 8.5 Hz, 1H), 7.55 – 7.52 (m, 2H), 7.40 (d, *J* = 8.3 Hz, 1H), 7.35 – 7.32 (m, 1H), 7.28 (d, *J* = 8.4 Hz, 1H), 7.23 – 7.18 (m, 2H), 6.97 (dd, *J* = 7.4, 1.1 Hz, 1H), 6.73 (d, *J* = 7.5 Hz, 1H), 6.44 (d, *J* = 7.7 Hz, 1H). ^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$) δ 147.1, 142.3, 136.6, 135.9, 135.2, 131.2, 129.3, 129.0, 128.3, 127.2, 126.70, 126.66, 124.6, 122.1, 122.0, 119.8, 115.8, 108.6, 102.0.

HRMS (ESI-TOF): m/z $[M + H]^+$ calcd for $C_{19}H_{12}N_2Br$ 347.0184; found 347.0171.

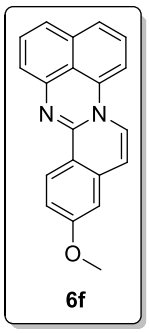
10-fluoroisoquinolino[2,1-a]perimidine (6e): Purified by silica gel column chromatography



eluent: hexane/ethyl acetate (95:5). Orange solid (12 mg, 42%), mp 169 - 172 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.65 (dd, *J* = 8.9, 5.7 Hz, 1H), 7.39 (d, *J* = 7.8 Hz, 1H), 7.30 (t, *J* = 7.8 Hz, 1H), 7.21 (dd, *J* = 16.1, 7.8 Hz, 2H), 7.16 – 7.09 (m, 2H), 6.99 (dd, *J* = 8.8, 2.7 Hz, 1H), 6.94 (d, *J* = 7.5 Hz, 1H), 6.70 (d, *J* = 7.6 Hz, 1H), 6.44 (d, *J* = 7.8 Hz, 1H). ^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) δ 165.0, (d, *J* = 253.5 Hz), 147.0, 142.4, 136.6, 135.85, 135.76, 130.3 (d, *J* = 9.1 Hz), 129.3, 127.2, 124.6, 124.2, 122.01, 121.97, 119.5, 116.2 (d, *J* = 23.2 Hz), 115.6, 111.0 (d, *J* = 22.2 Hz), 109.1, (d, *J* = 3.0 Hz), 102.0. ^{19}F NMR (471 MHz, $CDCl_3$) δ -107.8.

HRMS (ESI-TOF): m/z $[M + H]^+$ calcd for $C_{19}H_{12}N_2F$ 287.0985; found 287.0960.

10-methoxyisoquinolino[2,1-a]perimidine (6f): Purified by silica gel column chromatography

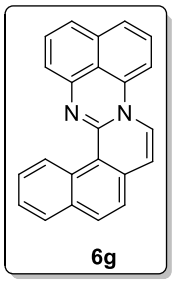


6f

eluent: hexane/ethyl acetate (95:5). Orange solid (20 mg, 67%), mp 178 - 181 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.60 (d, *J* = 9.0 Hz, 1H), 7.38 (d, *J* = 7.8 Hz, 1H), 7.31 (t, *J* = 7.8 Hz, 1H), 7.24 (s, 1H), 7.19 (t, *J* = 7.9 Hz, 1H), 7.13 (d, *J* = 8.2 Hz, 1H), 7.02 (dd, *J* = 9.0, 2.6 Hz, 1H), 6.95 (d, *J* = 7.5 Hz, 1H), 6.76 (d, *J* = 2.7 Hz, 1H), 6.71 (d, *J* = 7.6 Hz, 1H), 6.47 (d, *J* = 7.7 Hz, 1H), 3.87 (s, 3H). ^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) δ 162.5, 147.4, 142.8, 136.8, 135.9, 135.5, 129.3, 129.2, 127.1, 123.8, 121.8, 121.7, 121.2, 118.8, 116.8, 115.1, 109.8, 107.5, 101.7, 55.6.

HRMS (ESI-TOF): m/z [M + H]$^{+}$ calcd for $C_{20}H_{15}N_2O$ 299.1184; found 299.1158.

benzo[7,8]isoquinolino[2,1-a]perimidine (6g): Purified by silica gel column chromatography

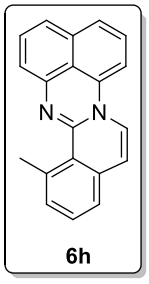


6g

eluent: hexane/ethyl acetate (98:2). Orange solid (16 mg, 50%), mp 165 - 168 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.58 (d, *J* = 8.9 Hz, 1H), 7.96 (d, *J* = 8.4 Hz, 1H), 7.88 (d, *J* = 7.9 Hz, 1H), 7.75 – 7.71 (m, 1H), 7.58 (dd, *J* = 16.6, 7.9 Hz, 2H), 7.43 – 7.39 (m, 2H), 7.36 – 7.34 (m, 1H), 7.29 (d, *J* = 7.7 Hz, 1H), 7.24 (d, *J* = 7.2 Hz, 1H), 7.17 (d, *J* = 7.5 Hz, 1H), 6.80 (d, *J* = 7.5 Hz, 1H), 6.68 (d, *J* = 7.5 Hz, 1H). ^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) δ 148.6, 142.2, 137.5, 135.7, 135.6, 133.8, 133.5, 131.4, 129.3, 128.8, 128.2, 127.3, 126.5, 125.3, 124.2, 121.9, 121.6, 119.2, 115.8, 110.8, 103.0.

HRMS (ESI-TOF): m/z [M + H]$^{+}$ calcd for $C_{23}H_{15}N_2$ 319.1235; found 319.1216.

8-methylisoquinolino[2,1-a]perimidine (6h): Purified by silica gel column chromatography



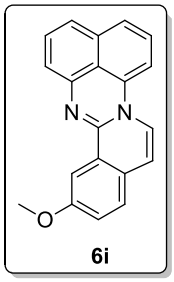
6h

eluent: hexane/ethyl acetate (98:2). Orange solid (14 mg, 50%), mp 170 - 173 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.39 (t, *J* = 7.6 Hz, 1H), 7.35 – 7.30 (m, 2H), 7.29 – 7.26 (m, 2H), 7.25 – 7.19 (m, 3H), 7.00 (dd, *J* = 7.4, 1.1 Hz, 1H), 6.71 (d, *J* = 7.4 Hz, 1H), 6.49 (d, *J* = 7.6 Hz, 1H), 3.03 (s, 3H). ^{13}C{^{1}H} NMR (126 MHz,

$CDCl_3$) δ 148.3, 142.2, 141.3, 137.6, 135.7, 135.6, 132.2, 130.7, 129.2, 127.4, 126.5, 124.2, 123.9, 121.8, 121.2, 119.4, 115.8, 110.7, 102.3, 26.5.

HRMS (ESI-TOF): m/z $[M + H]^+$ calcd for $C_{20}H_{15}N_2$ 283.1235; found 283.1211.

9-methoxyisoquinolino[2,1-a]perimidine (6i): Purified by silica gel column chromatography

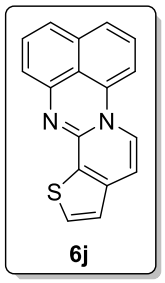


6i

eluent: hexane/ethyl acetate (98:2). Orange solid (16 mg, 54%), mp 156 - 158 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.15 (d, *J* = 2.7 Hz, 1H), 7.36 – 7.27 (m, 4H), 7.22 (d, *J* = 7.7 Hz, 1H), 7.19 – 7.15 (m, 2H), 7.01 (d, *J* = 8.2 Hz, 1H), 6.72 (d, *J* = 7.6 Hz, 1H), 6.52 (d, *J* = 7.7 Hz, 1H), 3.99 (s, 3H). $^{13}C\{^1H\}$ NMR (101 MHz, $CDCl_3$) δ 159.6, 147.3, 142.8, 137.0, 135.9, 129.2, 129.1, 127.6, 127.4, 127.2, 122.2, 121.8, 121.6, 121.0, 119.1, 115.2, 109.8, 107.8, 101.9, 55.8.

HRMS (ESI-TOF): m/z $[M + H]^+$ calcd for $C_{20}H_{15}N_2O$ 299.1184; found 299.1161.

Thieno[2',3':3,4]pyrido[1,2-a]perimidine (6j): Purified by silica gel column chromatography

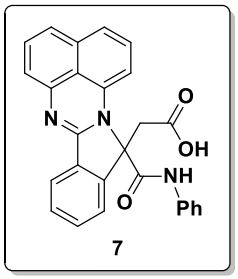


6j

eluent: hexane/ethyl acetate (80:20). Red solid (11 mg, 40%), mp 202 - 205 °C. ^{1}H NMR (500 MHz, $CDCl_3$) 7.61 (d, *J* = 5.1 Hz, 1H), 7.53 (d, *J* = 8.0 Hz, 1H), 7.32 – 7.27 (m, 2H), 7.19 (t, *J* = 8.0 Hz, 1H), 7.14 – 7.12 (m, 2H), 6.98 (d, *J* = 7.4 Hz, 1H), 6.79 (d, *J* = 7.6 Hz, 1H), 6.72 (d, *J* = 7.4 Hz, 1H). $^{13}C\{^1H\}$ NMR (126 MHz, $CDCl_3$) δ 145.7, 142.4, 141.2, 136.1, 136.0, 132.9, 129.3, 127.0, 124.2, 124.0, 122.6, 121.7, 118.8, 114.7, 106.7, 102.6.

HRMS (ESI-TOF): m/z $[M + H]^+$ calcd for $C_{17}H_{11}N_2S$ 275.0643; found 275.0632.

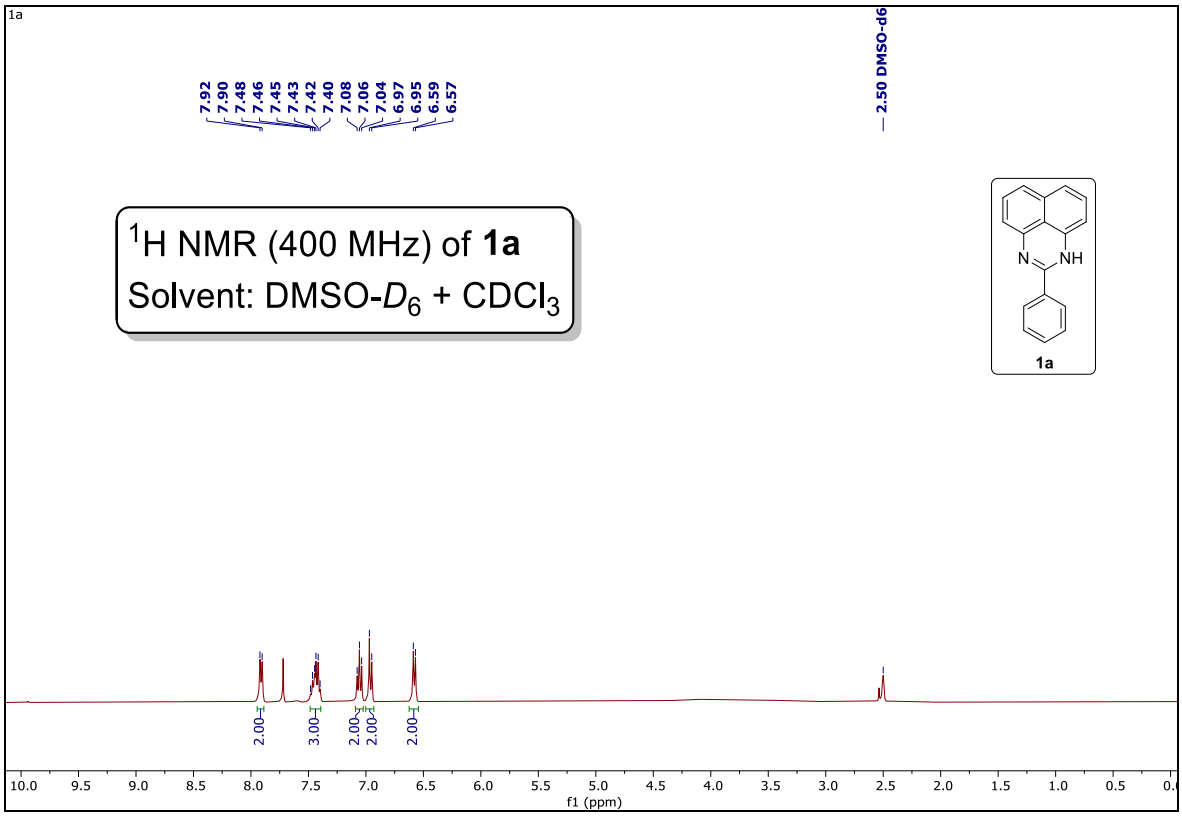
2-(12-(phenylcarbamoyl)-12H-isoindolo[2,1-a]perimidin-12-yl)acetic acid (7): Purified by silica gel column chromatography eluent: hexane/ethyl acetate (60:40). Yellow solid (37 mg, 85%), mp 187 - 190 ºC. ^{1}H NMR (500 MHz, DMSO-D_6 + $CDCl_3$) δ 10.01 (s, 1H), 8.11 (s, 1H), 7.91 (d, J = 7.4 Hz, 1H), 7.61 – 7.58 (m, 2H), 7.57 – 7.54 (m, 1H), 7.39 (d, J = 7.4 Hz, 2H), 7.29 – 7.26 (m, 1H), 7.18 (t, J = 8.0 Hz, 3H), 7.13 – 7.09 (m, 2H), 7.00 (t, J = 7.4 Hz, 1H), 6.90 (d, J = 6.2 Hz, 1H), 6.16 (d, J = 5.5 Hz, 1H), 3.78 (d, J = 15.9 Hz, 1H), 3.57 (d, J = 16.0 Hz, 1H). ^{13}C{^{1}H} NMR (126 MHz, DMSO-D_6 + $CDCl_3$) δ 169.2, 165.4, 156.1, 143.9, 142.7, 137.6, 135.41, 135.37, 132.2, 131.8, 129.2, 128.4, 128.2, 127.2, 124.3, 122.3, 121.7, 121.5, 121.3, 120.2, 118.8, 115.2, 101.6, 71.5, 33.2.



7

HRMS (ESI-TOF): m/z $[M + H]^+$ calcd for $C_{27}H_{20}N_3O_3$ 434.1505; found 434.1506.

^{1}H NMR and ^{13}C NMR and HRMS Spectra



Display Report

Analysis Info

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Method	DEFAULT.m	Operator	Gudipati SrinivasaRao
Sample Name	VM-100	Instrument	impact HD 1819696.00197
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
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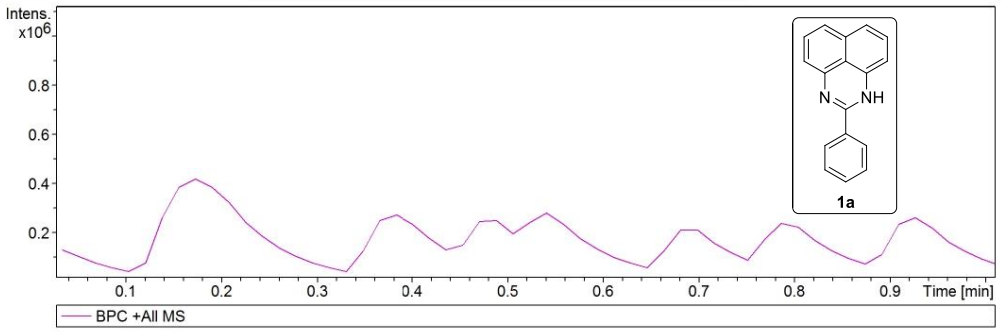
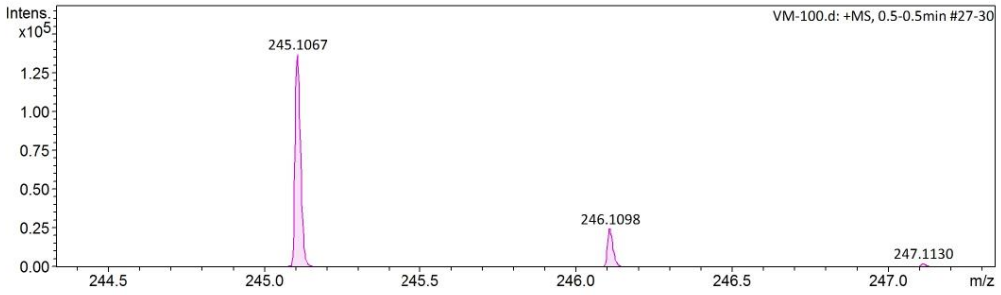
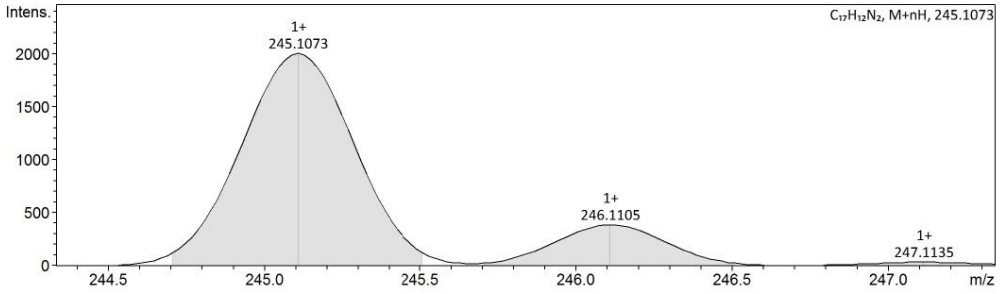
Scan Begin	150 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 °C

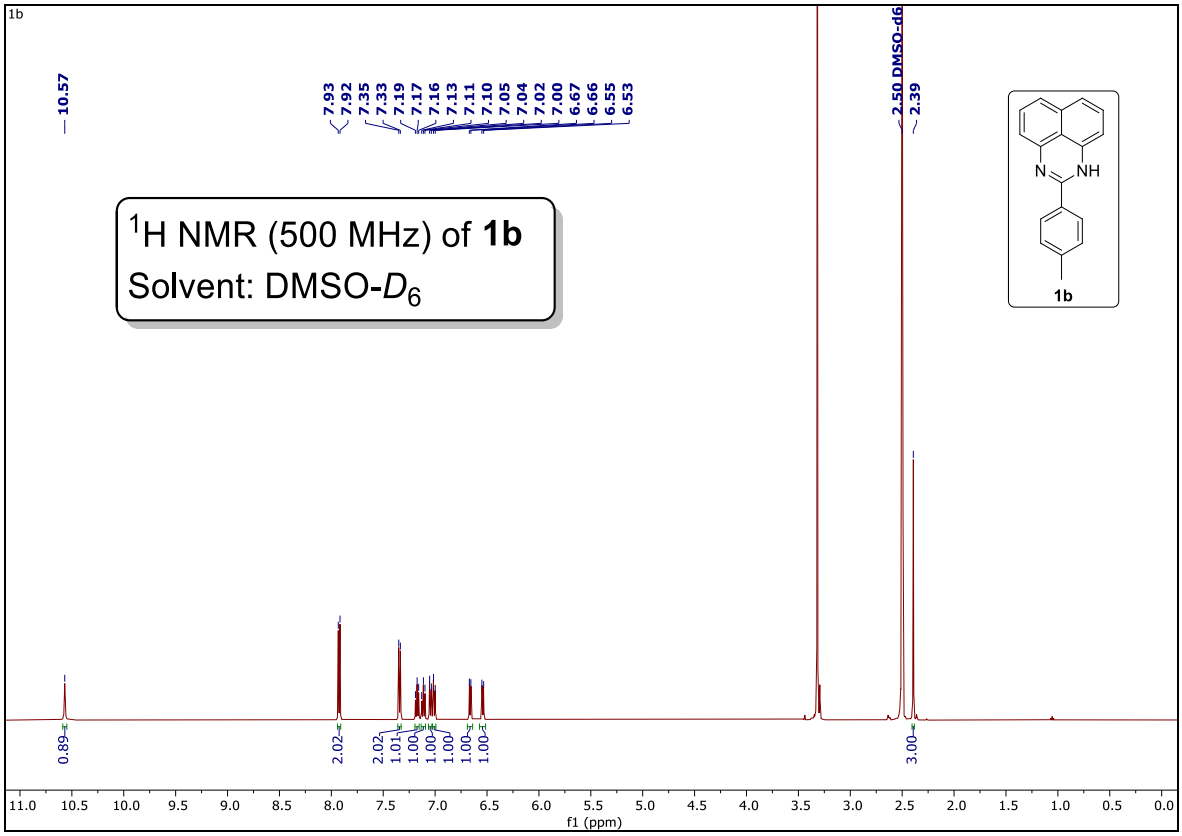






VM-100.d

Gudipati


1b
10.57
7.93
7.92
7.35
7.33
7.19
7.17
7.16
7.13
7.11
7.10
7.05
7.04
7.02
7.00
6.67
6.66
6.55
6.53
2.50 DMSO-d6
2.39
^{1}H NMR (500 MHz) of **1b**
Solvent: DMSO-D_6
N
NH
1b
0.89
2.02
2.02
1.01
1.00
1.00
1.00
1.00
1.00
3.00
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

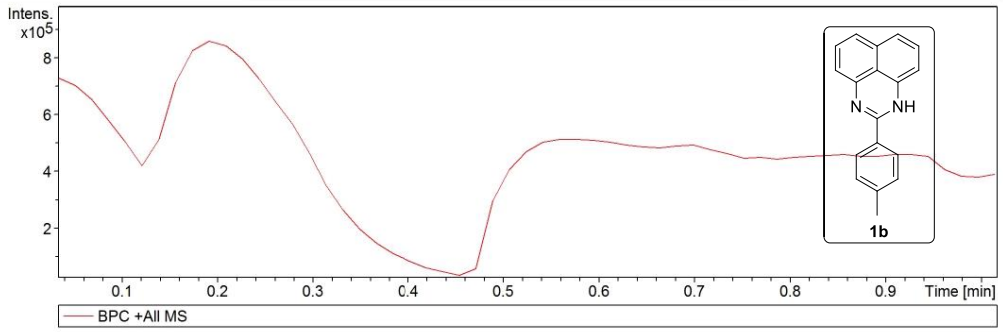
Display Report

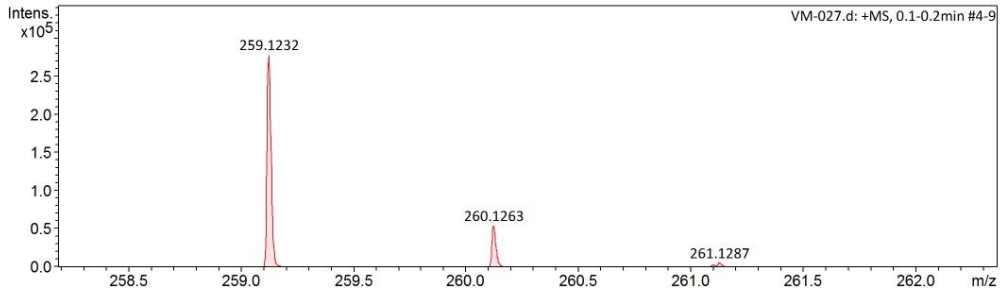
Analysis Info

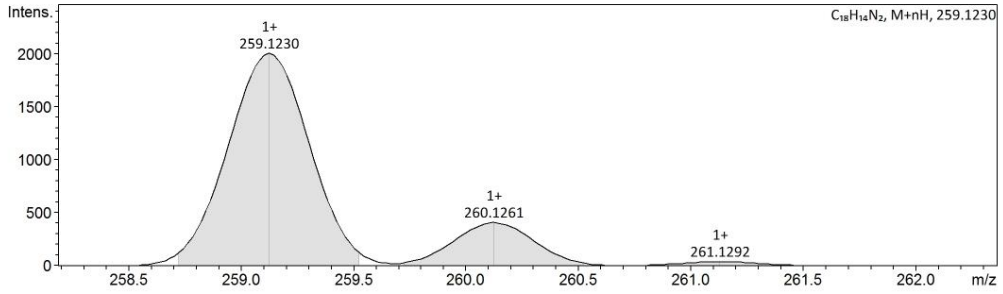
Analysis Name	D:\Data\user data\Dr. Lokman\27-09-24\VM-027.d	Acquisition Date	9/29/2024 1:01:25 AM
Method	DEFAULT.m	Operator	Gudipati SrinivasaRao
Sample Name	VM-027	Instrument	impact HD 1819696.00197
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active	Set Capillary	3500 V	Set Dry Heater	200 °C
Scan Begin	150 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 °C

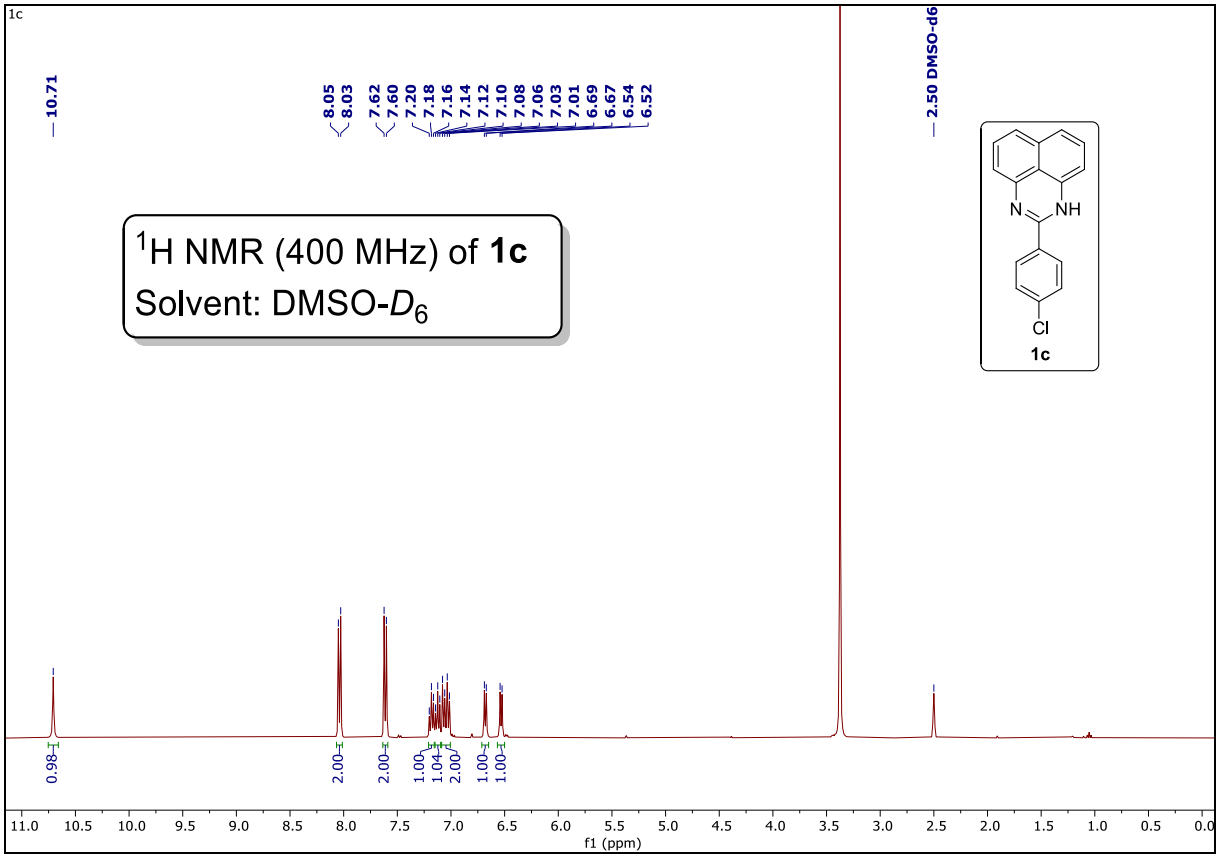






VM-027.d

Gudipati


1c
10.71
8.05
8.03
7.62
7.60
7.20
7.18
7.16
7.14
7.12
7.10
7.08
7.06
7.03
7.01
6.69
6.67
6.54
6.52
2.50 DMSO-d6
^{1}H NMR (400 MHz) of **1c**
Solvent: DMSO-D_6
N
NH
Cl
1c
0.98
2.00
2.00
1.00
1.04
2.00
1.00
1.00
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

Display Report

Analysis Info

Analysis Name	D:\Data\user data\Dr. Lokman\27-09-24\VM-020.d	Acquisition Date	9/27/2024 11:33:58 AM
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Sample Name	VM-020	Instrument	impact HD 1819696.00197
Comment			

Acquisition Parameter

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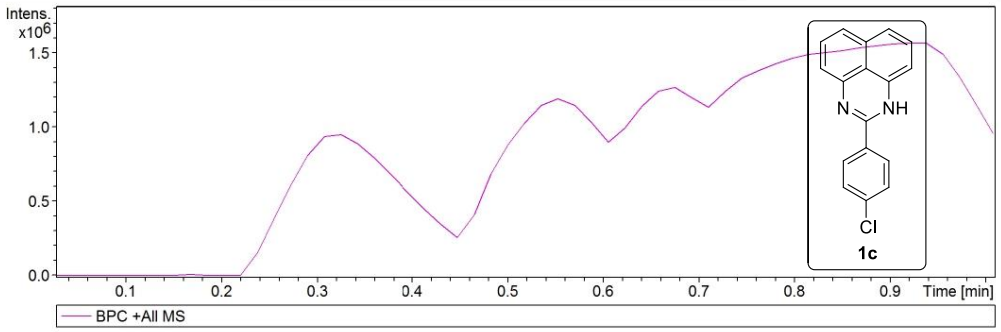
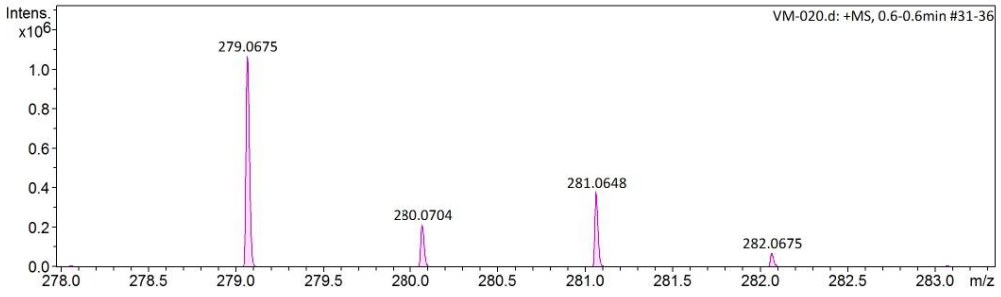
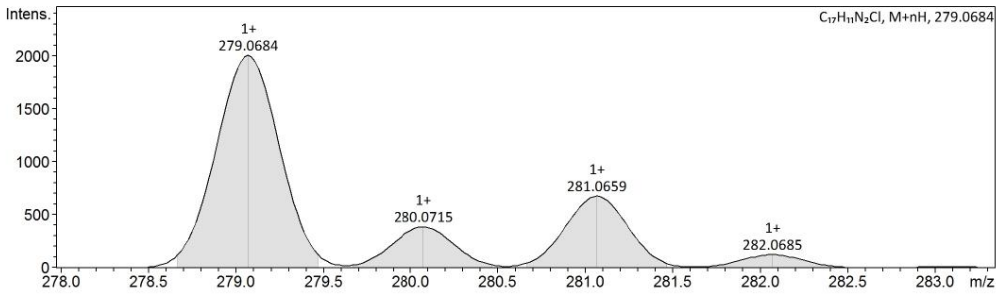
Scan Begin	150 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 °C

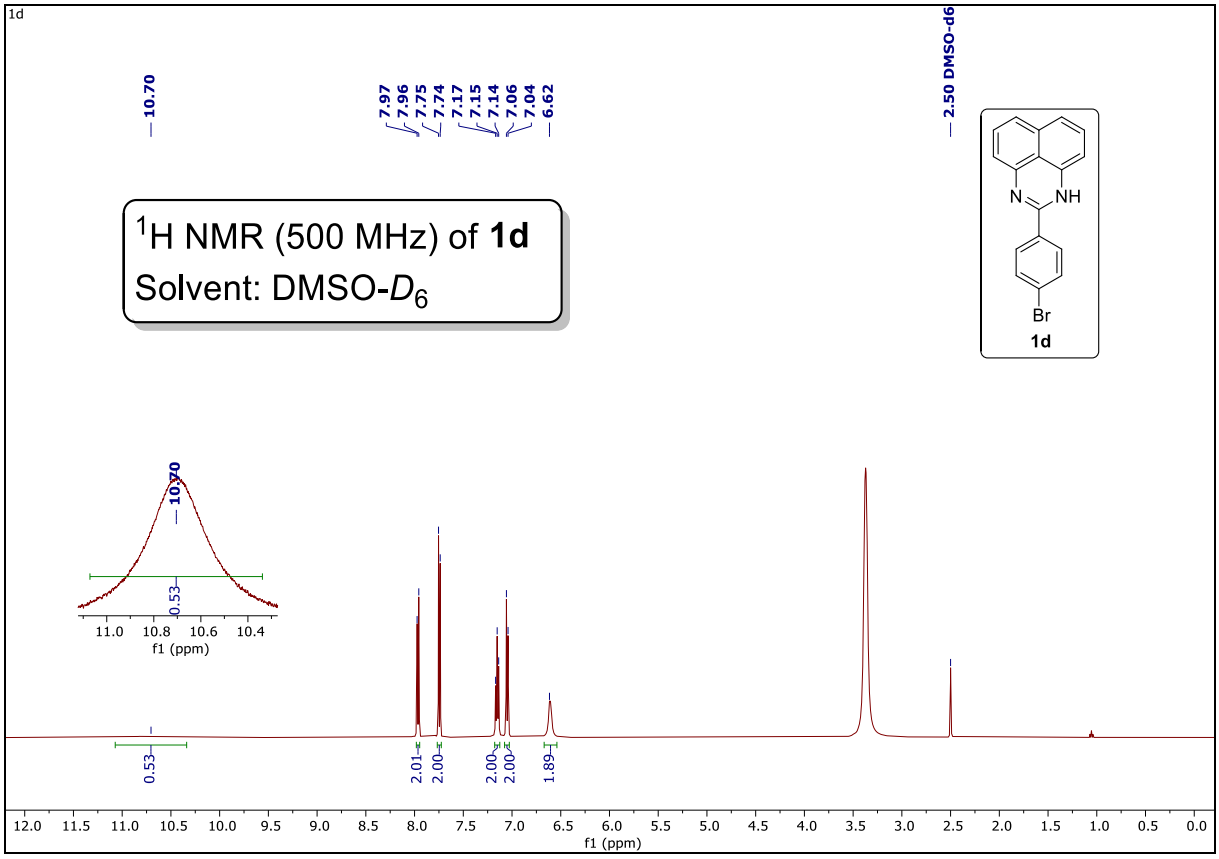






VM-020.d

Gudipati


1d
10.70
7.97
7.96
7.75
7.74
7.17
7.15
7.14
7.06
7.04
6.62
2.50 DMSO-d6
^{1}H NMR (500 MHz) of **1d**
Solvent: DMSO-D_6
N
NH
Br
1d
10.70
0.53
11.0 10.8 10.6 10.4
f1 (ppm)
0.53
2.01
2.00
2.00
2.00
1.89
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

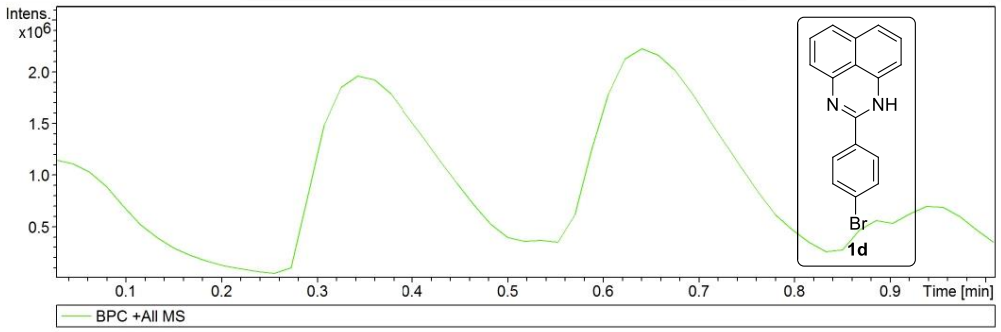
Display Report

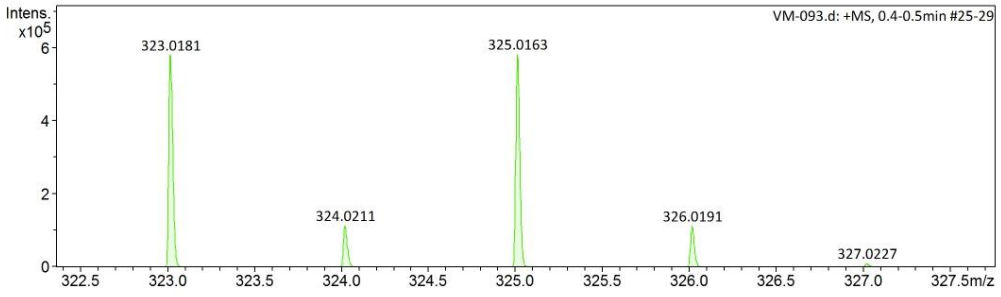
Analysis Info

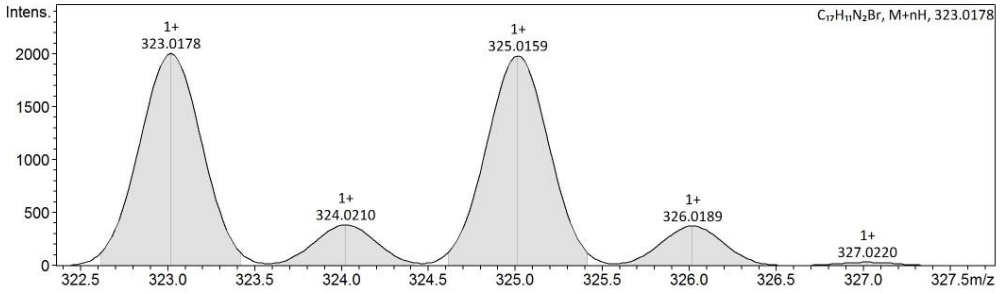
Analysis Name	D:\Data\user data\Dr. Lokman\27-09-24\VM-093.d	Acquisition Date	9/27/2024 12:07:22 PM
Method	DEFAULT.m	Operator	Gudipati SrinivasaRao
Sample Name	VM-093	Instrument	impact HD 1819696.00197
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active	Set Capillary	3500 V	Set Dry Heater	200 °C
Scan Begin	150 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 °C

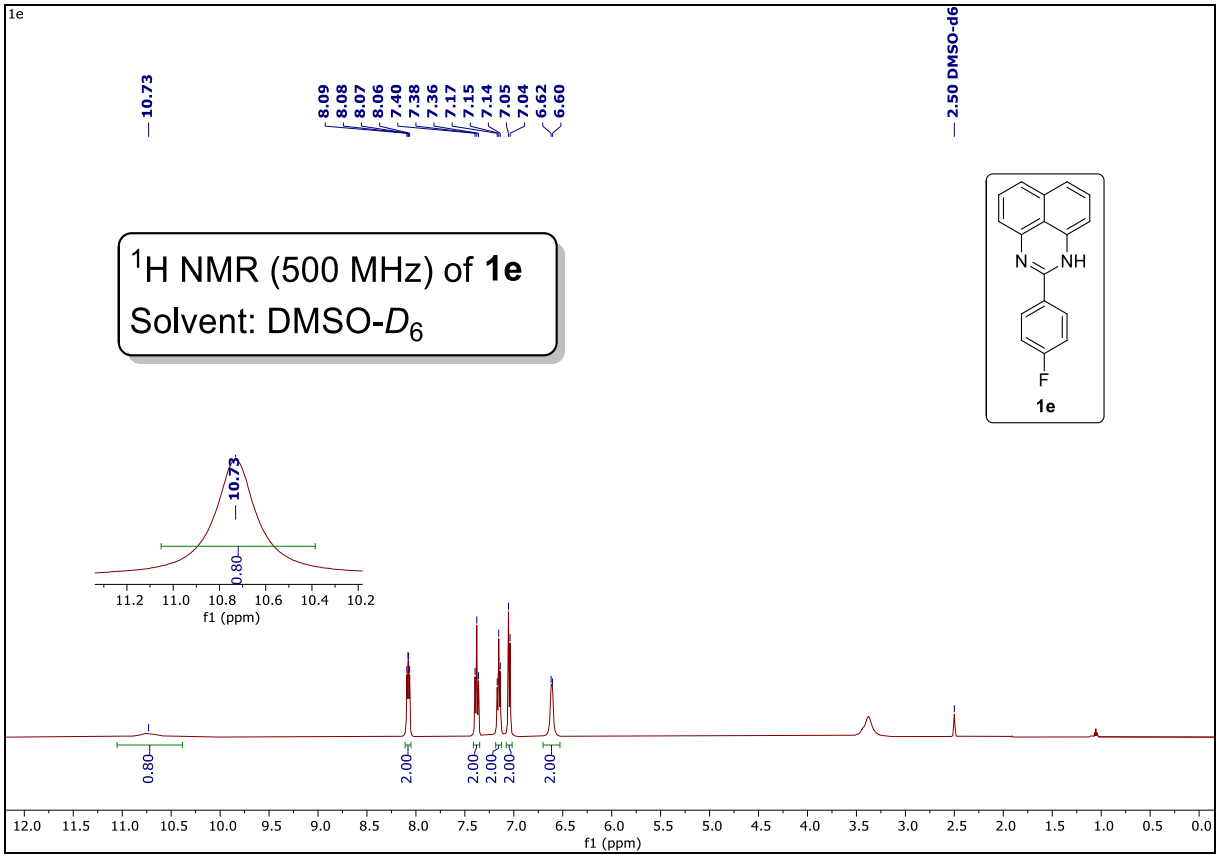






VM-093.d

Gudipati


1e
10.73
8.09
8.08
8.07
8.06
7.40
7.38
7.36
7.17
7.15
7.14
7.05
7.04
6.62
6.60
2.50 DMSO-d6
1H NMR (500 MHz) of 1e
Solvent: DMSO-D6
N
NH
F
1e
0.80
2.00
2.00
2.00
2.00
f1 (ppm)

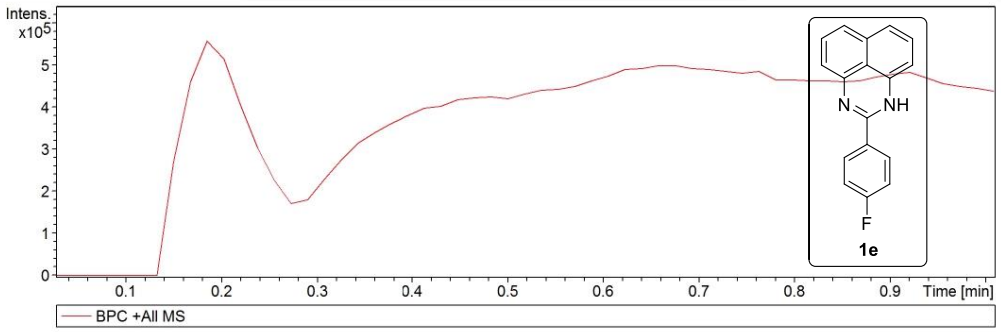
Display Report

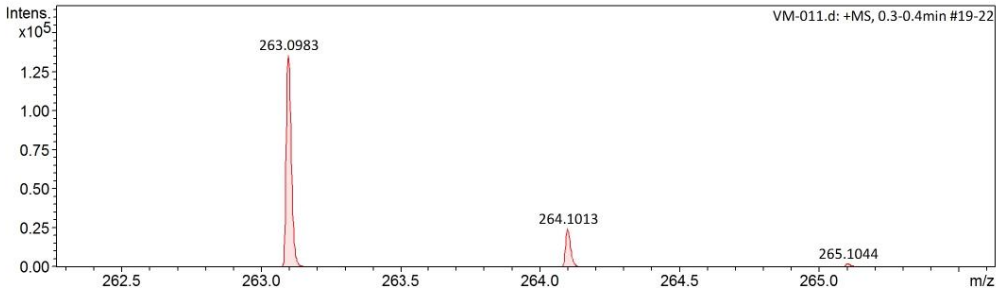
Analysis Info

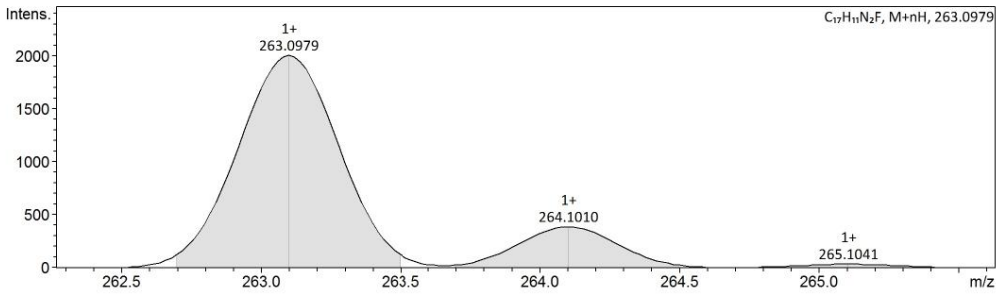
Analysis Name	D:\Data\user data\Dr. Lokman\27-09-24\VM-011.d	Acquisition Date	9/29/2024 2:00:09 AM
Method	DEFAULT.m	Operator	Gudipati SrinivasaRao
Sample Name	VM-011	Instrument	impact HD 1819696.00197
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.5 Bar
Focus	Not active	Set Capillary	3500 V	Set Dry Heater	200 °C
Scan Begin	150 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 °C

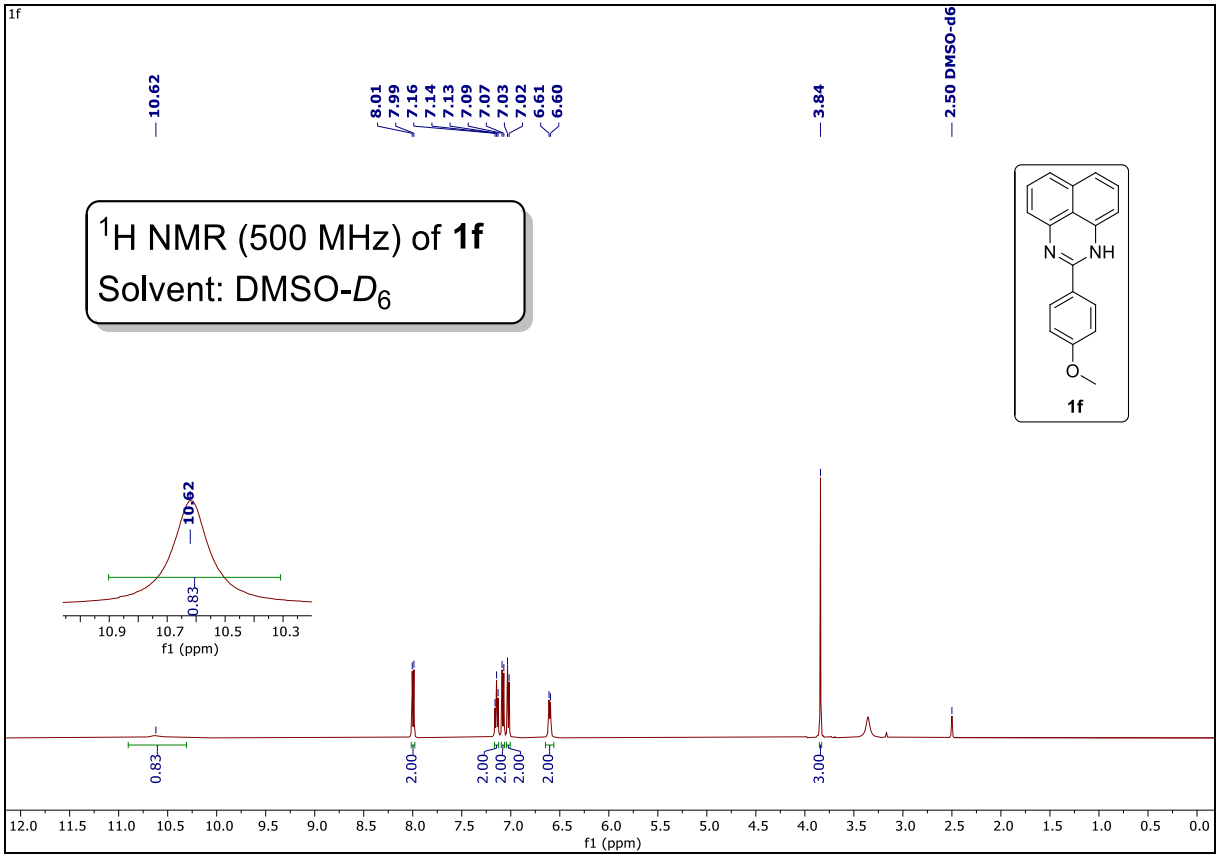






VM-011.d

Gudipati


1f
10.62
8.01
7.99
7.16
7.14
7.13
7.09
7.07
7.03
7.02
6.61
6.60
3.84
2.50 DMSO-d6
^{1}H NMR (500 MHz) of **1f**
Solvent: DMSO-D_6
N
NH
O
1f
10.62
0.83
10.9
10.7
10.5
10.3
f1 (ppm)
0.83
2.00
2.00
2.00
2.00
3.00
12.0
11.5
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

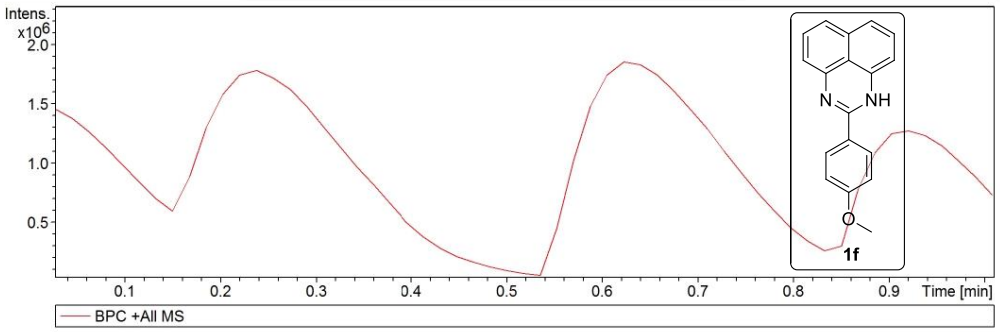
Display Report

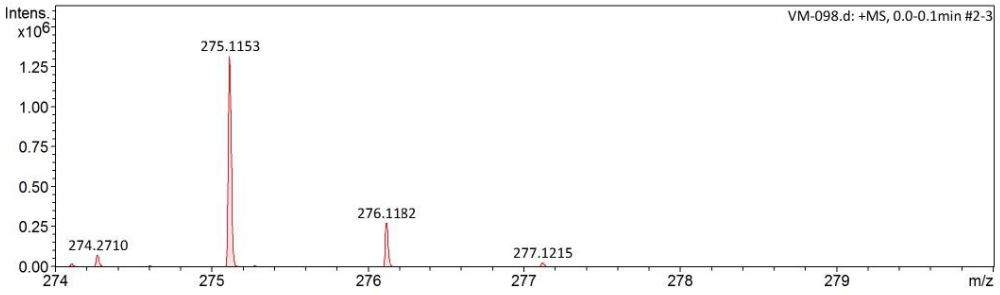
Analysis Info

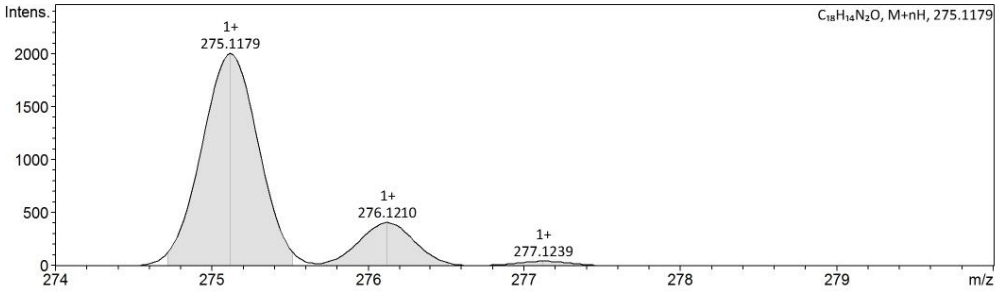
Analysis Name	D:\Data\user data\Dr. Lokman\27-09-24\VM-098.d	Acquisition Date	9/27/2024 12:03:45 PM
Method	DEFAULT.m	Operator	Gudipati SrinivasaRao
Sample Name	VM-098	Instrument	impact HD 1819696.00197
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active	Set Capillary	3500 V	Set Dry Heater	200 °C
Scan Begin	150 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 °C

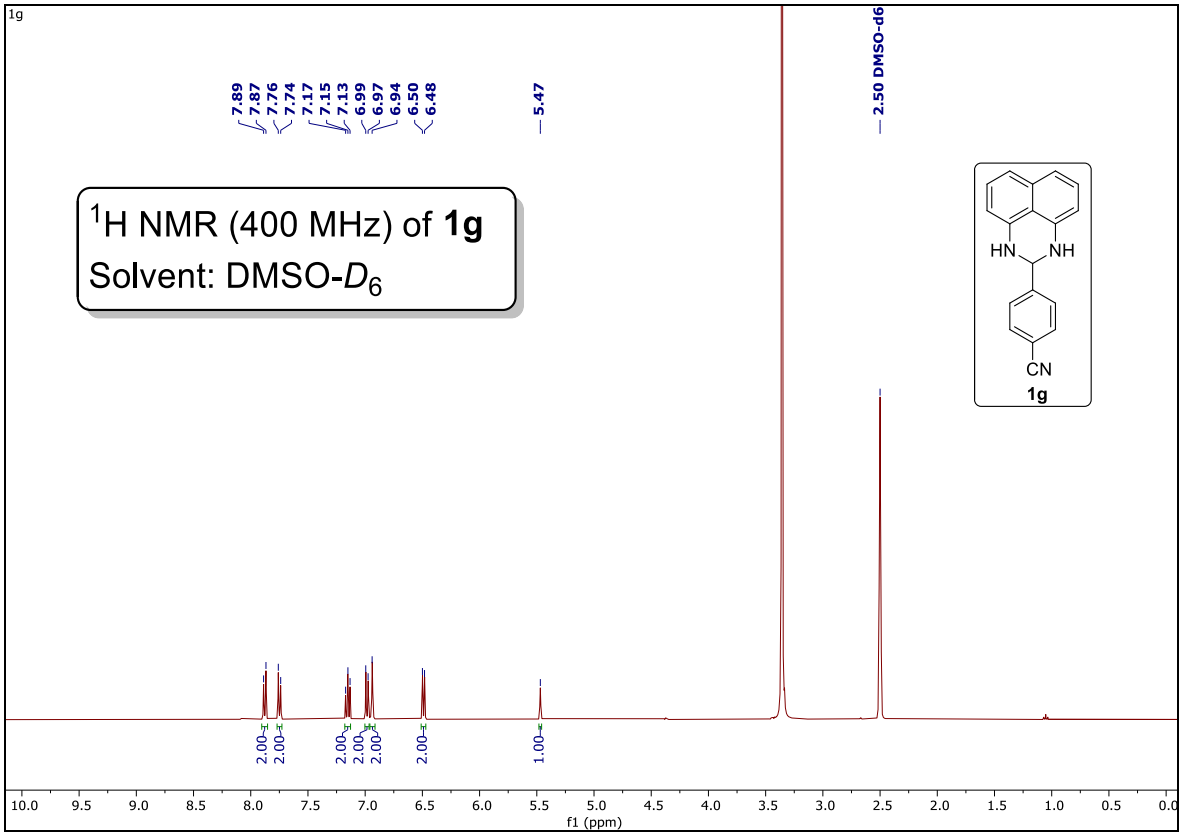






VM-098.d

Gudipati


1g
7.89
7.87
7.76
7.74
7.17
7.15
7.13
6.99
6.97
6.94
6.50
6.48
5.47
2.50 DMSO-d6
^{1}H NMR (400 MHz) of **1g**
Solvent: DMSO-D_6
HN
NH
CN
1g
2.00
2.00
2.00
2.00
2.00
2.00
1.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

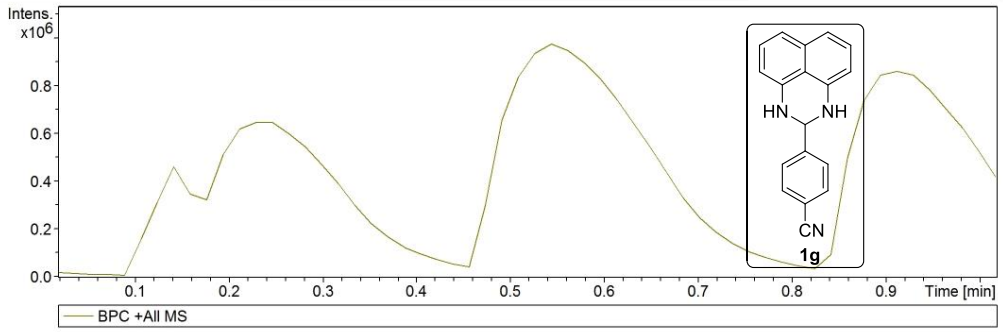
Display Report

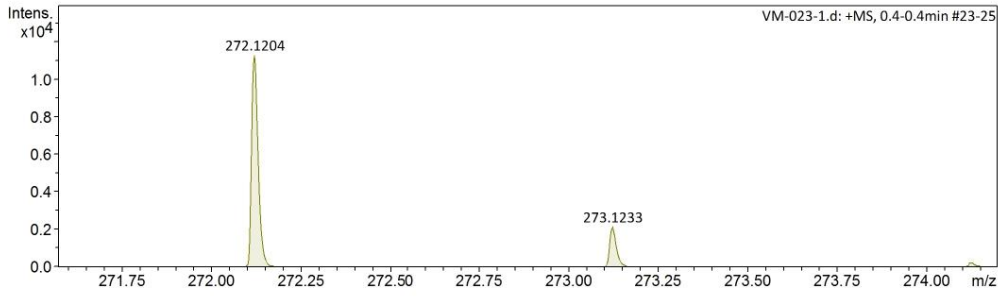
Analysis Info

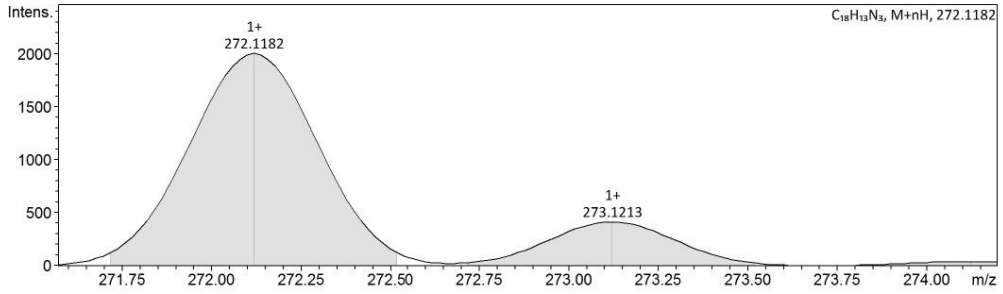
Analysis Name	D:\Data\user data\Dr. Lokman\27-09-24\VM-023-1.d	Acquisition Date	9/27/2024 12:22:52 PM
Method	DEFAULT.m	Operator	Gudipati SrinivasaRao
Sample Name	VM-023-1	Instrument	impact HD 1819696.00197
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.5 Bar
Focus	Not active	Set Capillary	3500 V	Set Dry Heater	200 °C
Scan Begin	150 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 °C

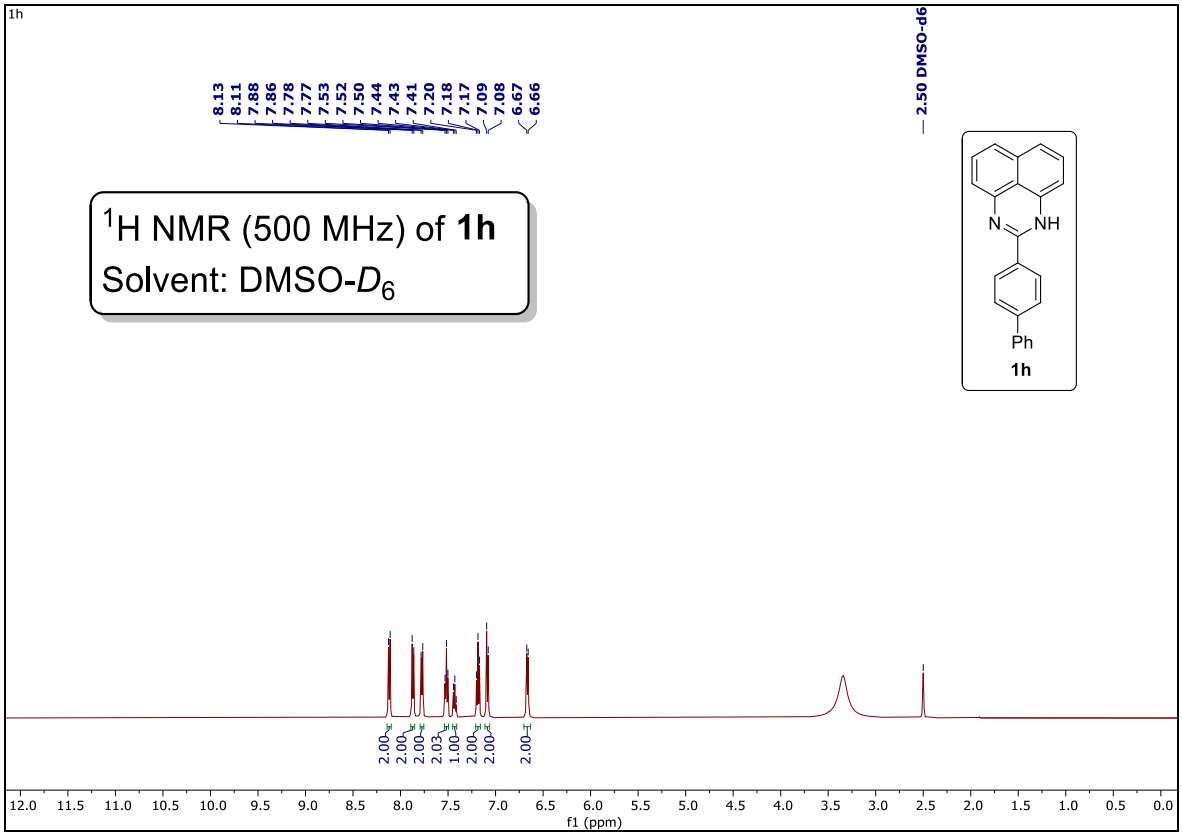






VM-023-1.d

Gudipati


1h
8.13
8.11
7.88
7.86
7.78
7.77
7.53
7.52
7.50
7.44
7.43
7.41
7.20
7.18
7.17
7.09
7.08
6.67
6.66
2.50 DMSO-d6
^{1}H NMR (500 MHz) of **1h**
Solvent: DMSO-D_6
N
NH
Ph
1h
2.00
2.00
2.00
2.03
1.00
2.00
2.00
2.00
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

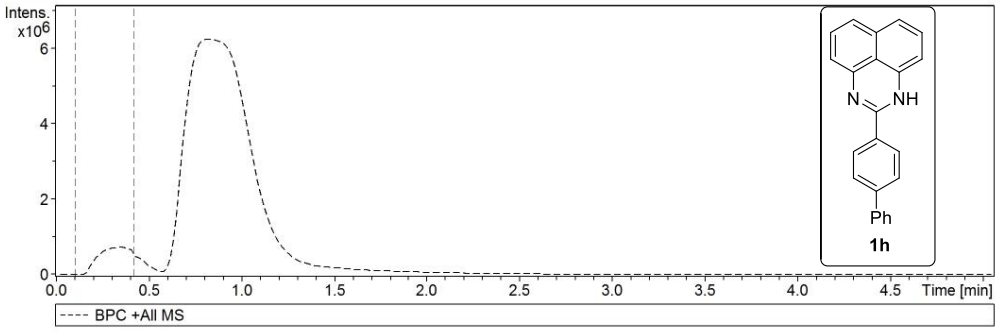
Display Report

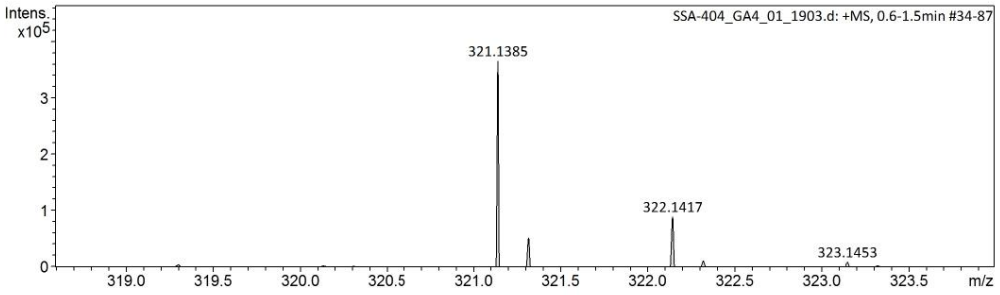
Analysis Info

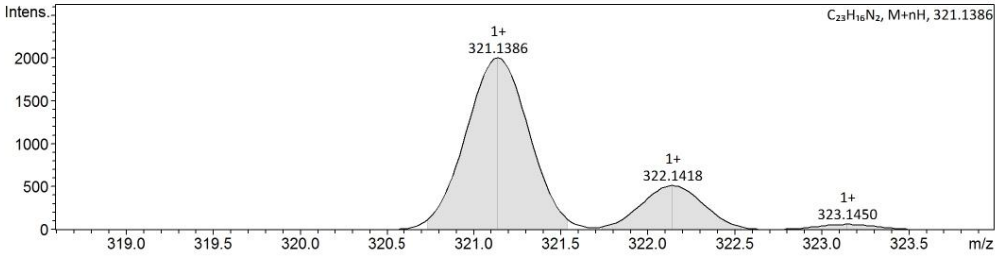
Analysis Name	D:\Data\user data\HPLC\DR LOKMAN\SWADHIN\SSA-404_GA4_01_1903.d	Acquisition Date	5/16/2022 2:50:28 PM
Method	low mass bruker.m	Operator	vidhi
Sample Name	SSA-404	Instrument	impact HD 1819696.00197
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.8 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	1500 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C

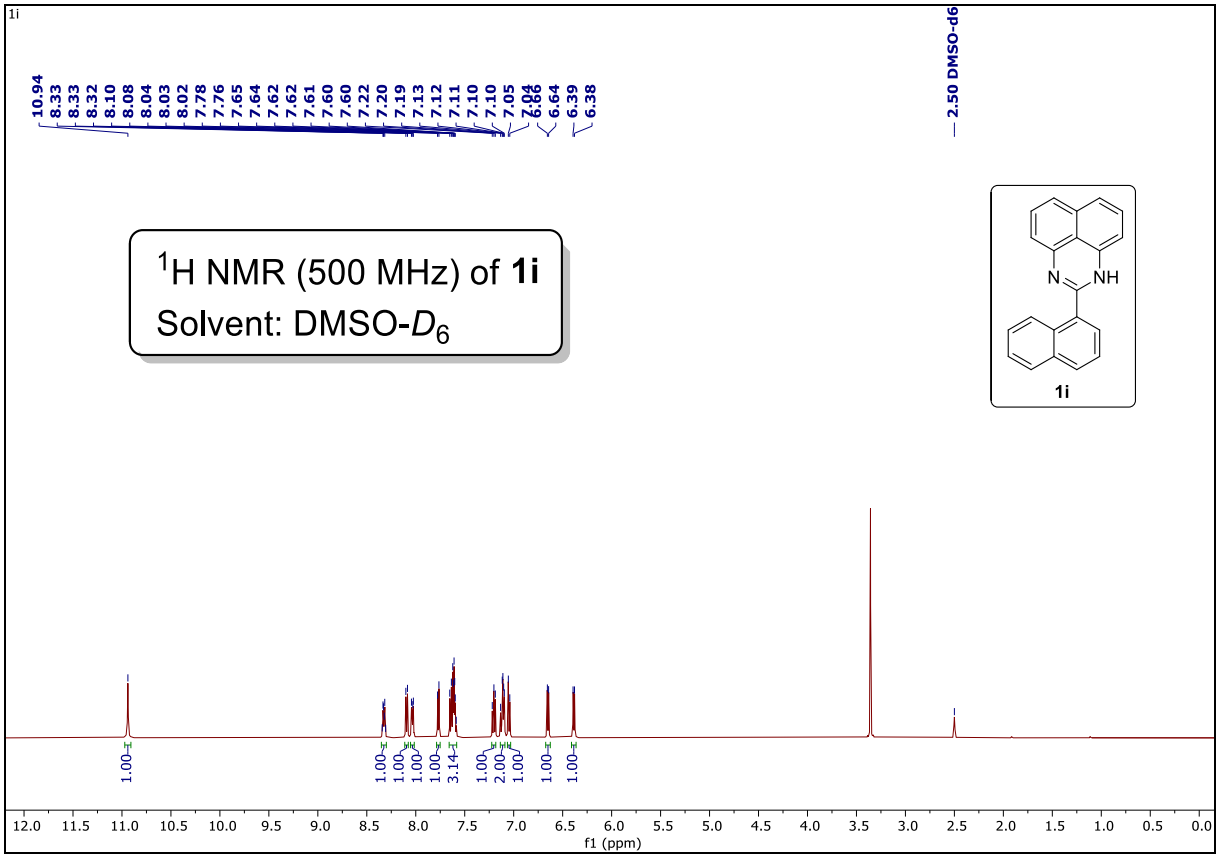






SSA-404_GA4_01_1903.d

Bruker Compass DataAnalysis 4.2 printed: 5/16/2022 2:59:08 PM by: vidhi Page 1 of 1


1i
10.94
8.33
8.33
8.32
8.10
8.08
8.04
8.03
8.02
7.78
7.76
7.65
7.64
7.62
7.61
7.60
7.60
7.22
7.20
7.19
7.13
7.12
7.11
7.10
7.05
6.64
6.39
6.38
2.50 DMSO-d6
^{1}H NMR (500 MHz) of **1i**
Solvent: DMSO-D_6
N
NH
1i
1.00
1.00
1.00
1.00
3.14
1.00
2.00
1.00
1.00
1.00
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

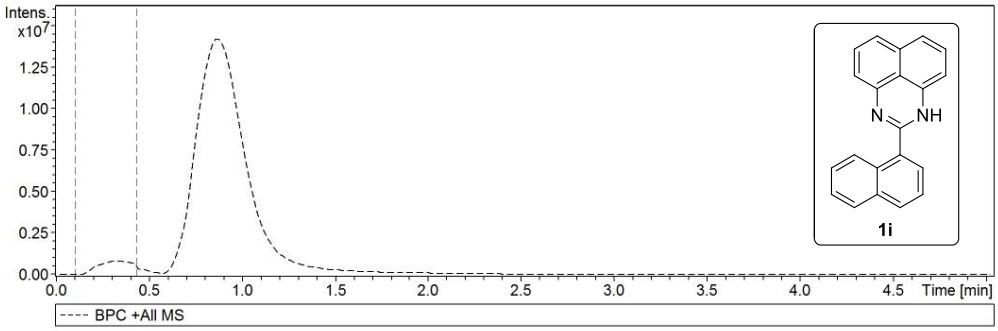
Display Report

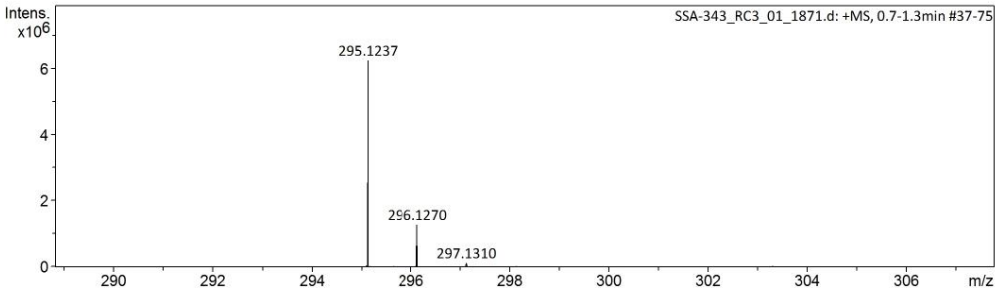
Analysis Info

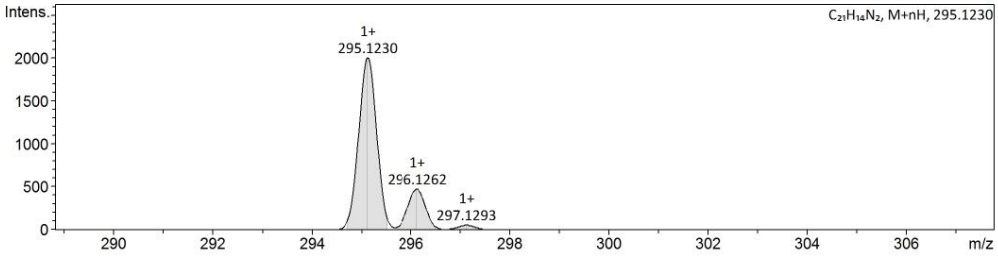
Analysis Name	D:\Data\user data\HPLC\DR LOKMAN\SWADHIN\SSA-343_RC3_01_1871.d	Acquisition Date	5/10/2022 12:50:36 PM
Method	low mass bruker.m	Operator	vidhi
Sample Name	SSA-343	Instrument	impact HD 1819696.00197
Comment			

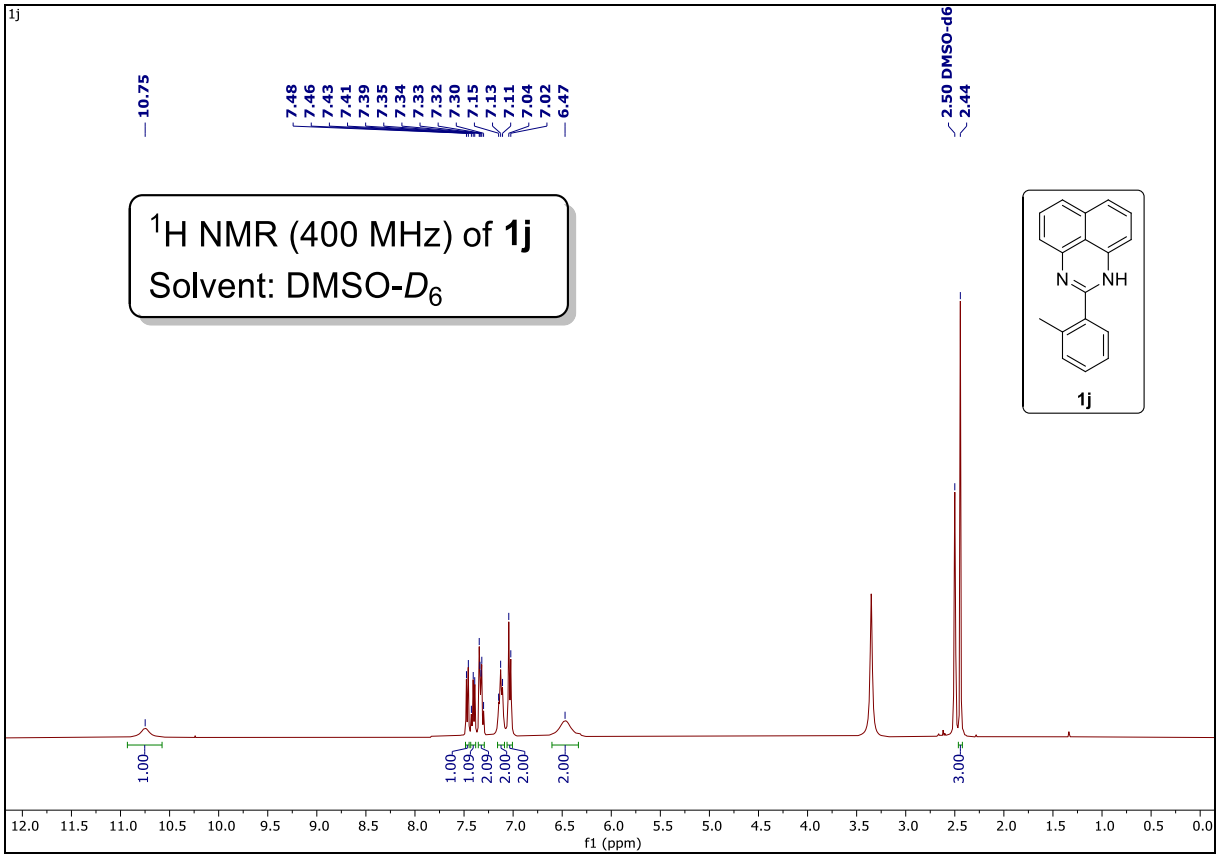
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.8 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	1500 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C








1j
10.75
7.48
7.46
7.43
7.41
7.39
7.35
7.34
7.33
7.32
7.30
7.15
7.13
7.11
7.04
7.02
6.47
2.50 DMSO-d6
2.44
1H NMR (400 MHz) of 1j
Solvent: DMSO-D6
N
NH
1j
1.00
1.00
1.09
2.09
2.00
2.00
2.00
3.00
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

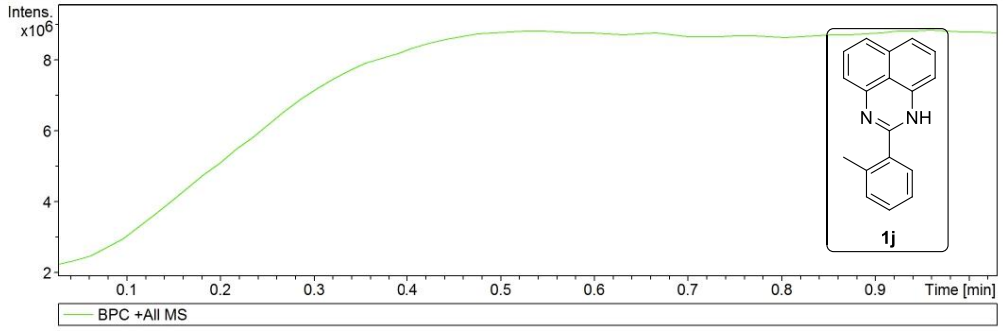
Display Report

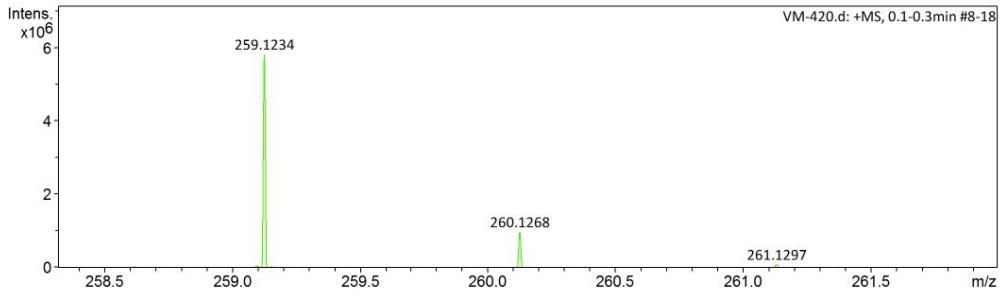
Analysis Info

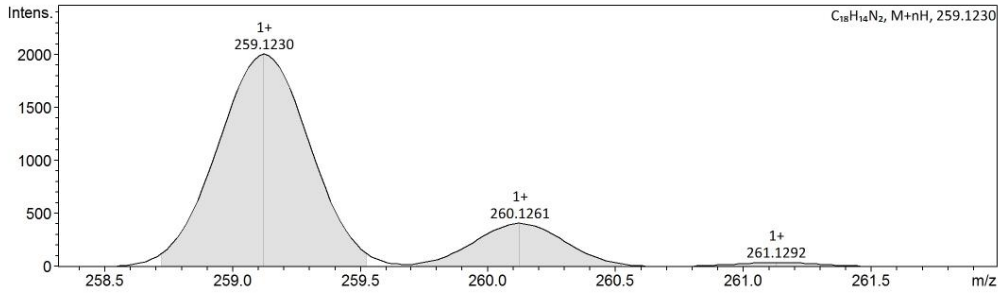
Analysis Name	D:\Data\user data\Dr. Lokman\25-02-25\VM-420.d	Acquisition Date	2/25/2025 12:39:01 PM
Method	low_mass.m	Operator	Gudipati SrinivasaRao
Sample Name	VM-420	Instrument	impact HD 1819696.00197
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.6 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	5.0 l/min
Scan End	1500 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C

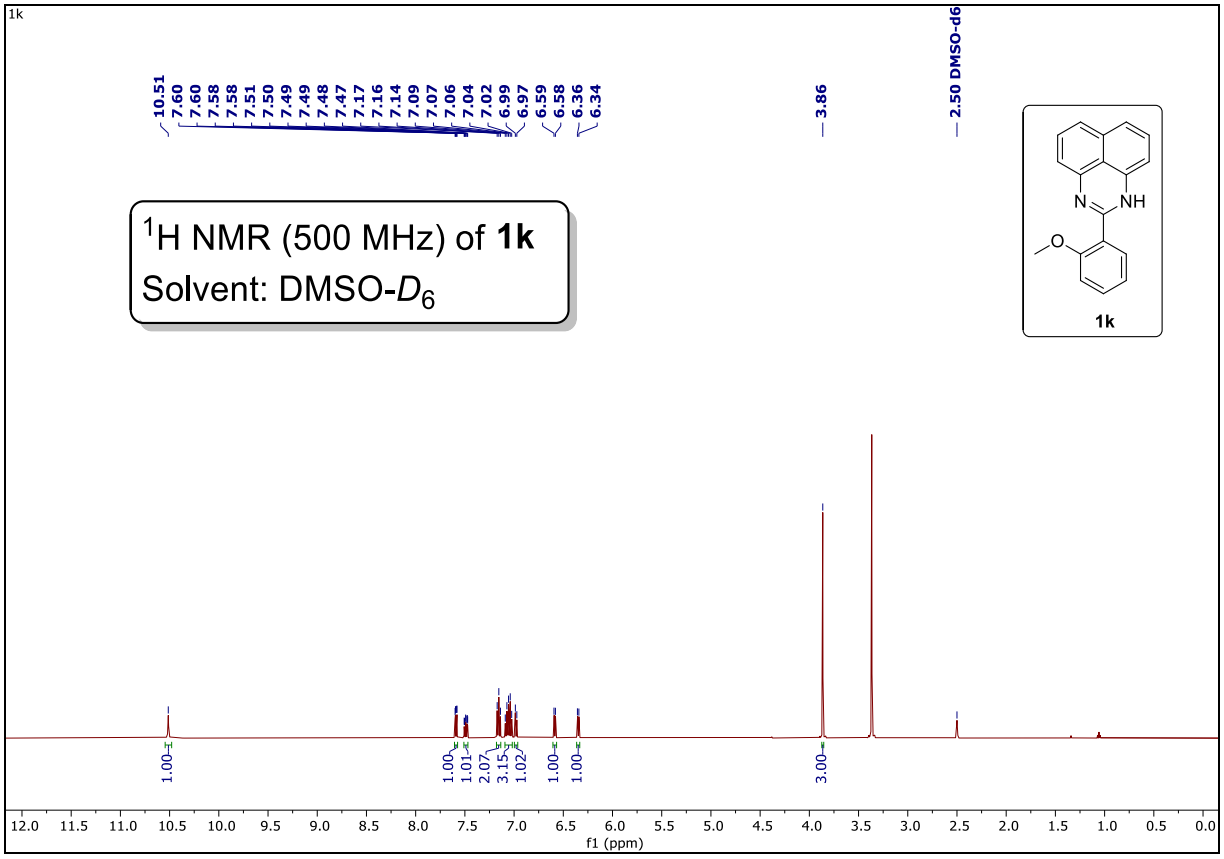






VM-420.d

Gudipati


1k
10.51
7.60
7.60
7.58
7.58
7.51
7.50
7.49
7.49
7.48
7.47
7.17
7.16
7.14
7.09
7.07
7.06
7.04
7.02
6.99
6.97
6.59
6.58
6.36
6.34
3.86
2.50 DMSO-d6
1H NMR (500 MHz) of 1k
Solvent: DMSO-D6
N
NH
O
1k
1.00
1.00
1.01
2.07
3.15
1.02
1.00
1.00
3.00
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

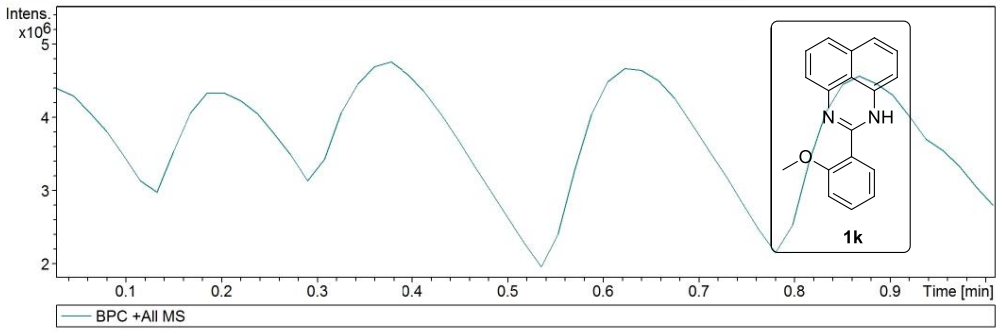
Display Report

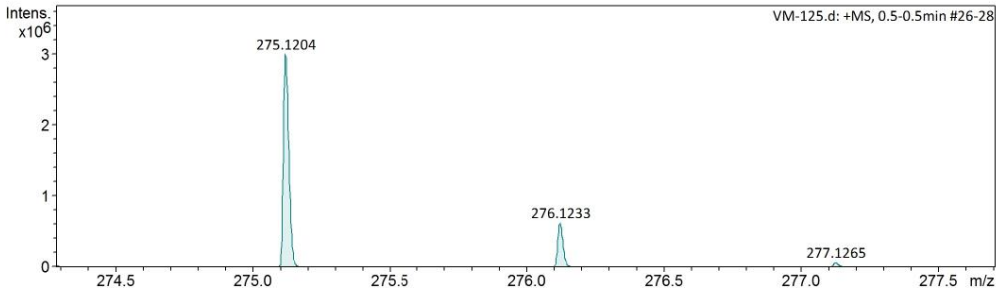
Analysis Info

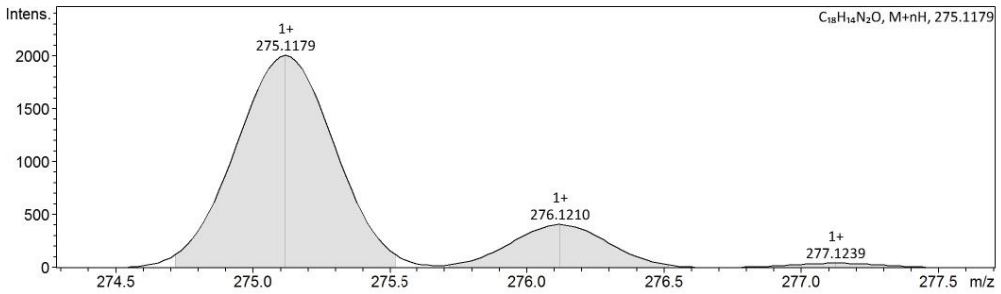
Analysis Name	D:\Data\user data\Dr. Lokman\27-09-24\VM-125.d	Acquisition Date	9/27/2024 11:43:14 AM
Method	DEFAULT.m	Operator	Gudipati SrinivasaRao
Sample Name	VM-125	Instrument	impact HD 1819696.00197
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active	Set Capillary	3500 V	Set Dry Heater	200 °C
Scan Begin	150 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 °C

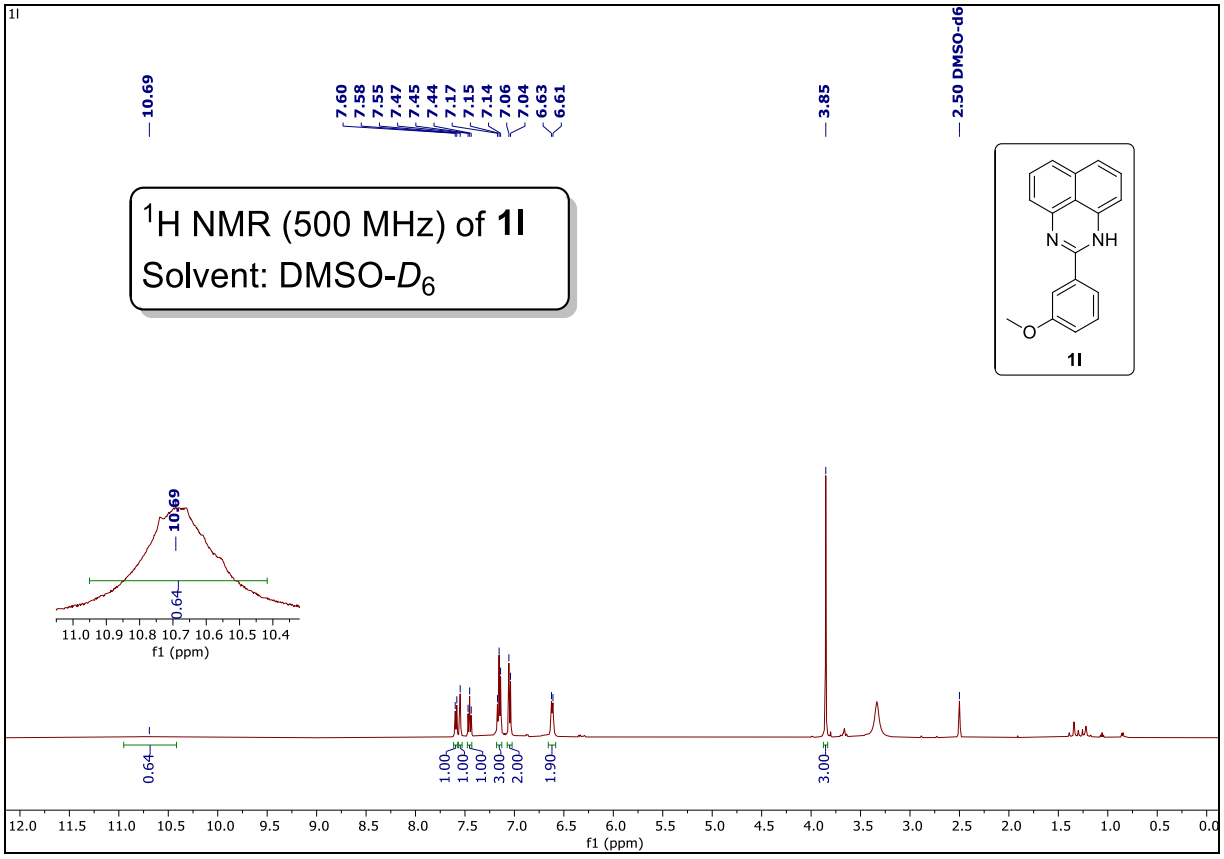






VM-125.d

Gudipati


1l
10.69
7.60
7.58
7.55
7.47
7.45
7.44
7.17
7.15
7.14
7.06
7.04
6.63
6.61
3.85
2.50 DMSO-d6
1H NMR (500 MHz) of 1l
Solvent: DMSO-D6
N
NH
O
1l
11.0 10.9 10.8 10.7 10.6 10.5 10.4
f1 (ppm)
0.64
1.00
1.00
1.00
3.00
2.00
1.90
3.00
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

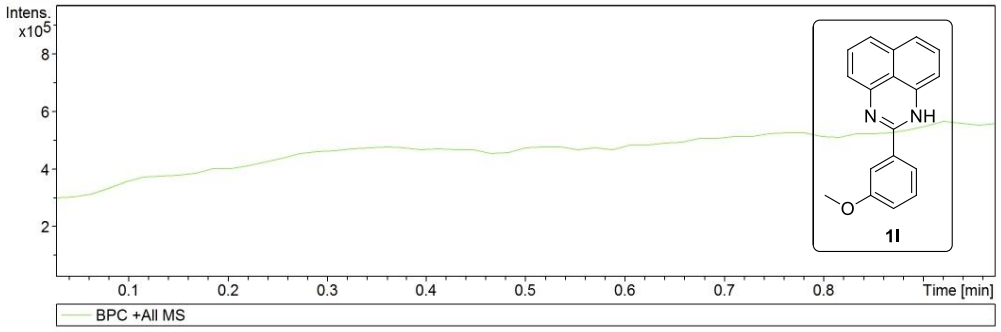
Display Report

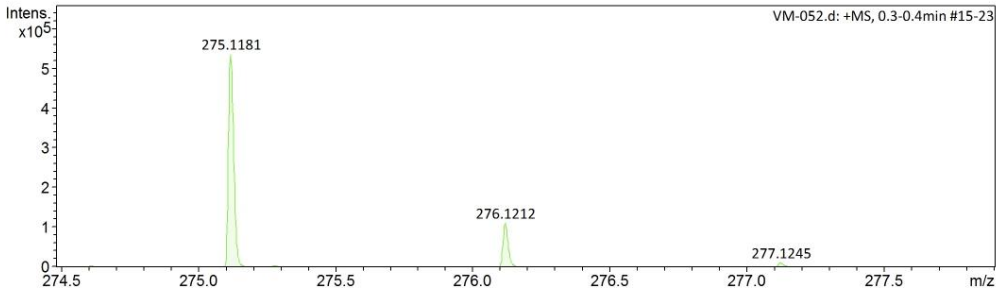
Analysis Info

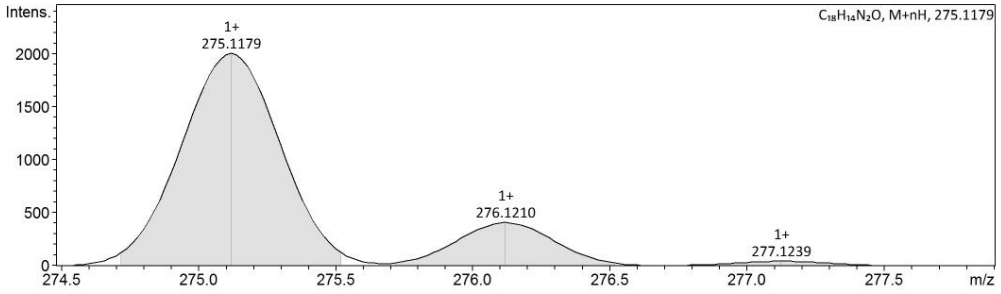
Analysis Name	D:\Data\user data\Dr. Lokman\27-09-24\VM-052.d	Acquisition Date	9/29/2024 1:05:08 AM
Method	DEFAULT.m	Operator	Gudipati SrinivasaRao
Sample Name	VM-052	Instrument	impact HD 1819696.00197
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active	Set Capillary	3500 V	Set Dry Heater	200 °C
Scan Begin	150 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 °C

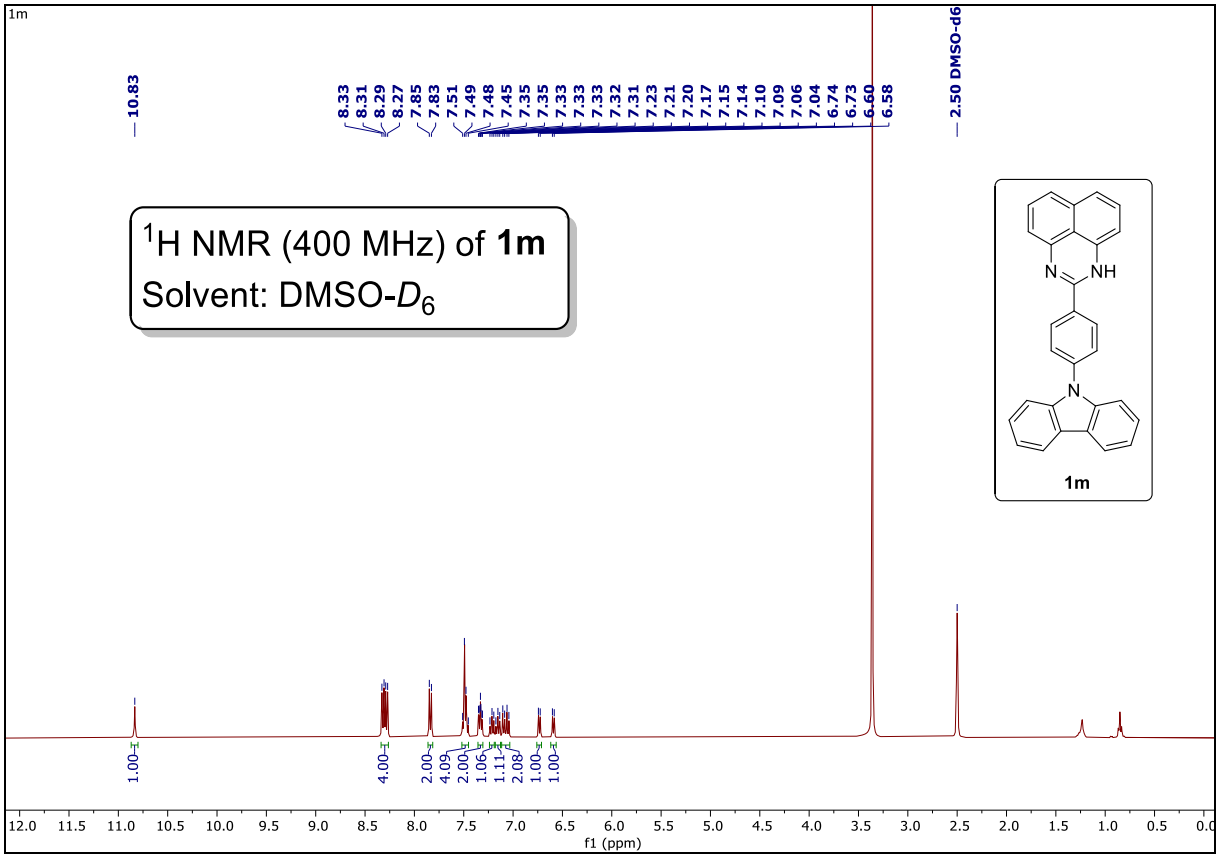


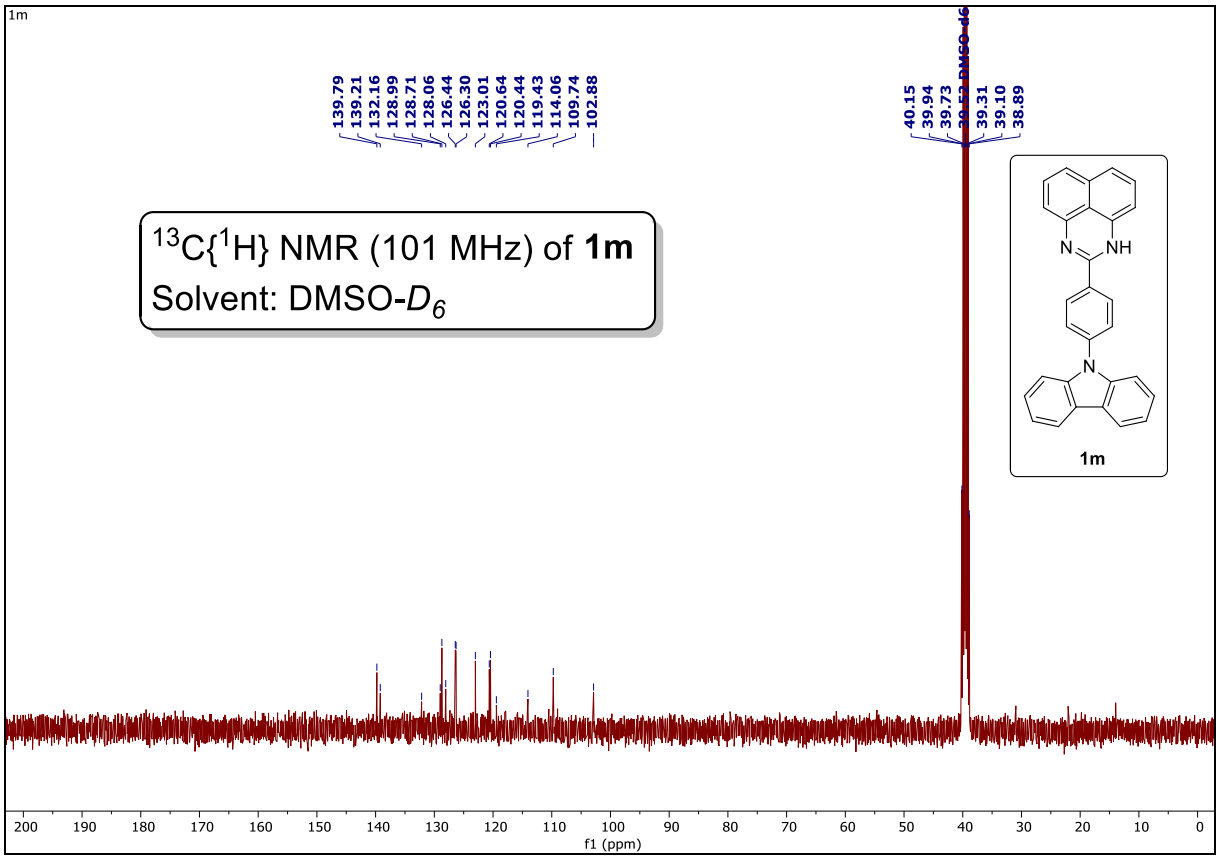




VM-052.d

Gudipati


1m
10.83
8.33
8.31
8.29
8.27
7.85
7.83
7.51
7.49
7.48
7.45
7.35
7.35
7.33
7.33
7.32
7.31
7.23
7.21
7.20
7.17
7.15
7.14
7.10
7.09
7.06
7.04
6.74
6.73
6.60
6.58
2.50 DMSO-d6
1H NMR (400 MHz) of 1m
Solvent: DMSO-D6
N
NH
N
1m
1.00
4.00
2.00
4.09
2.00
1.06
1.11
2.08
1.00
1.00
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


1m
139.79
139.21
132.16
128.99
128.71
128.06
126.44
126.30
123.01
120.64
120.44
119.43
114.06
109.74
102.88
40.15
39.94
39.73
39.52 DMSO-d6
39.31
39.10
38.89
13C{1H} NMR (101 MHz) of 1m
Solvent: DMSO-D6
N
NH
N
1m
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

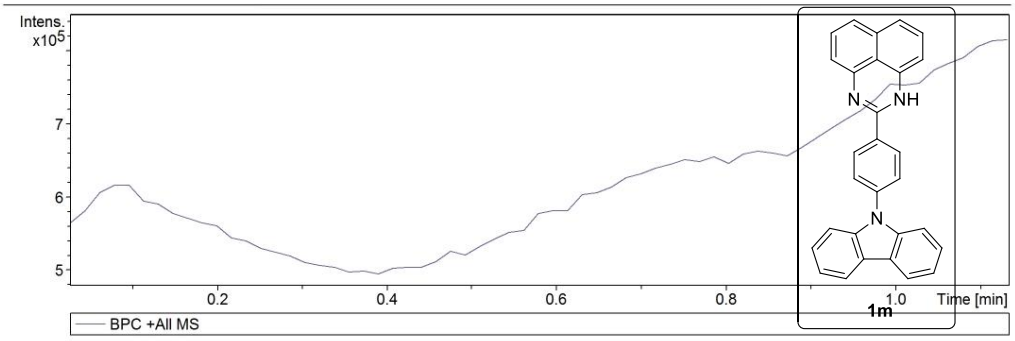
Display Report

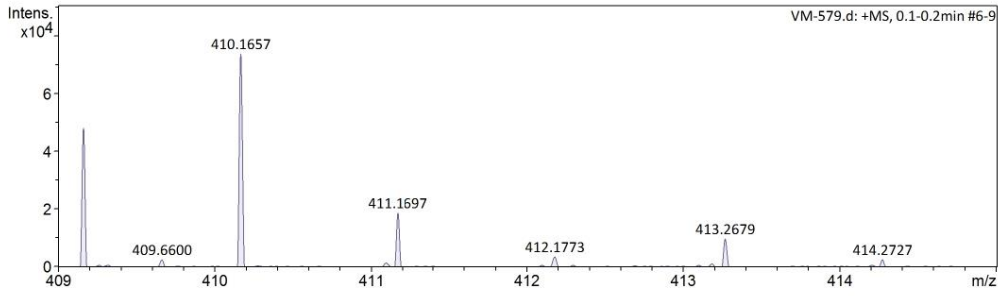
Analysis Info

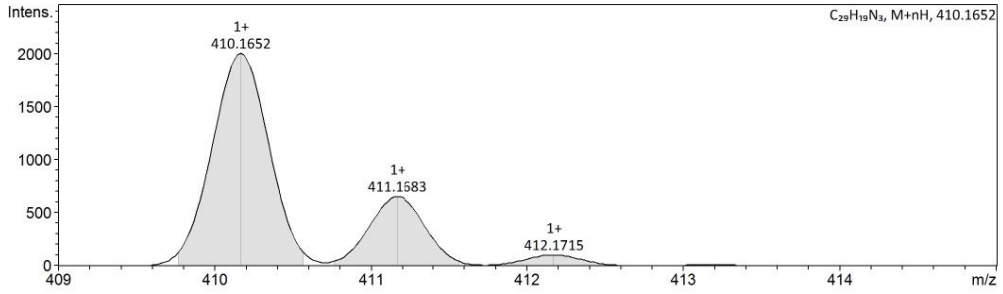
Analysis Name	D:\Data\user data\Dr. Lokman\24-02-2025\VM-579.d	Acquisition Date	2/24/2025 1:21:16 PM
Method	low_mass.m	Operator	Gudipati SrinivasaRao
Sample Name	VM-579	Instrument	impact HD 1819696.00197
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.6 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	5.0 l/min
Scan End	1500 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C

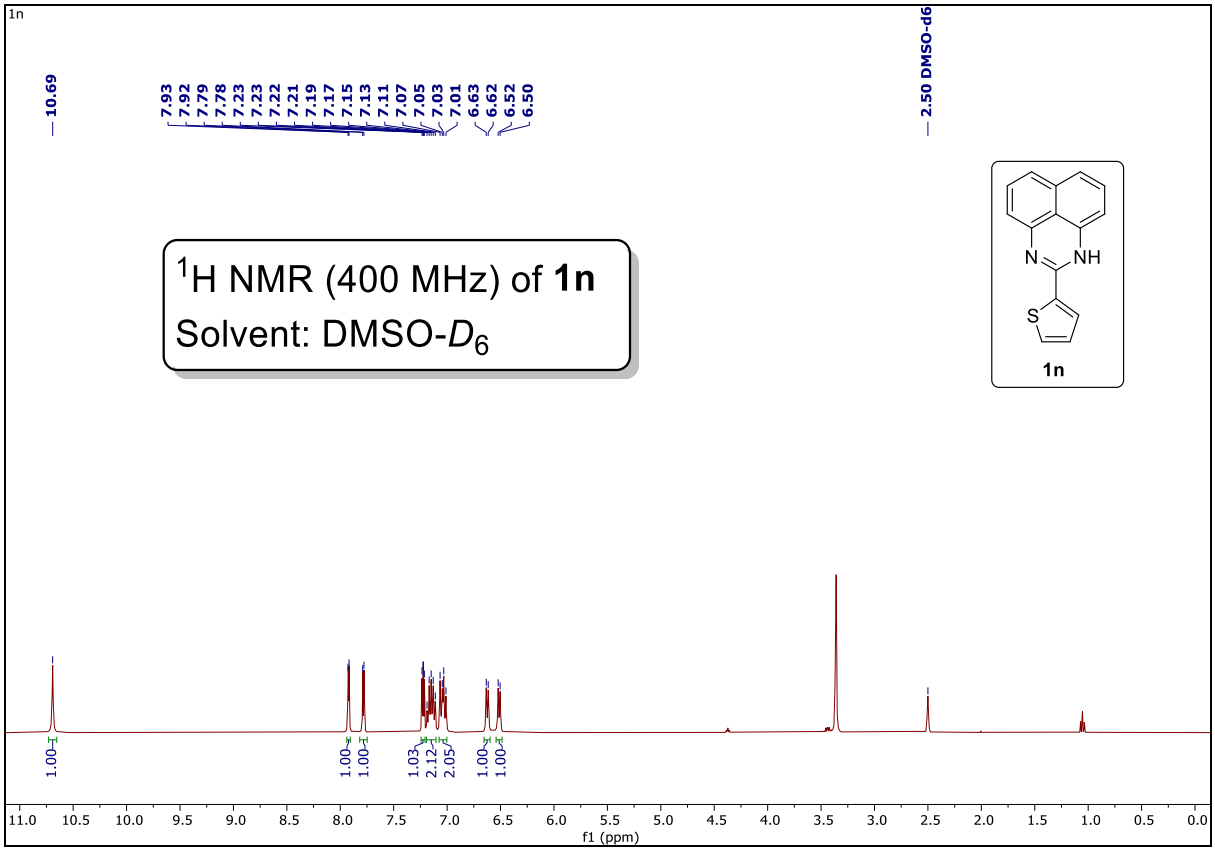






VM-579.d

Gudipati


1n
10.69
7.93
7.92
7.79
7.78
7.23
7.23
7.22
7.21
7.19
7.17
7.15
7.13
7.11
7.07
7.05
7.03
7.01
6.63
6.62
6.52
6.50
2.50 DMSO-d6
1H NMR (400 MHz) of 1n
Solvent: DMSO-D6
N
NH
S
1n
1.00
1.00
1.00
1.03
2.12
2.05
1.00
1.00
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

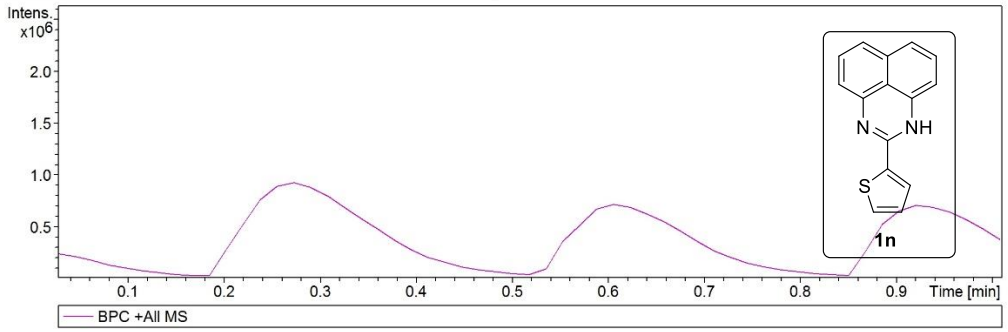
Display Report

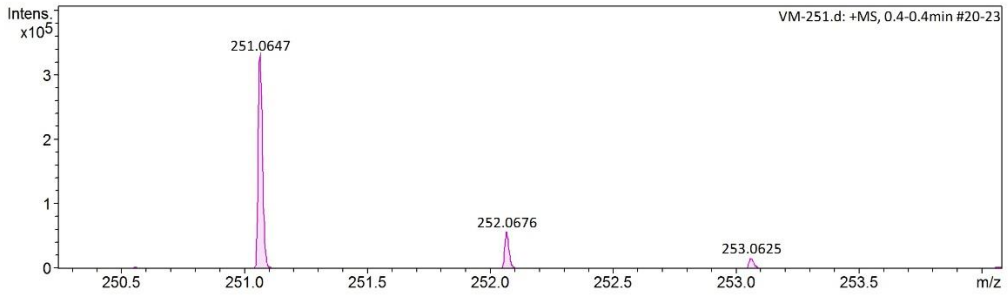
Analysis Info

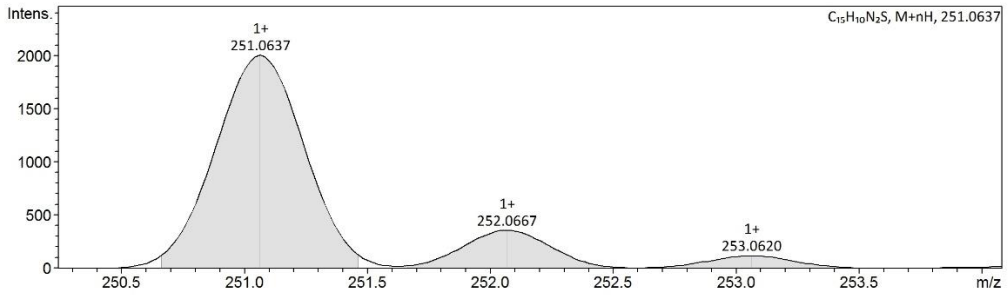
Analysis Name	D:\Data\user data\Dr. Lokman\27-09-24\VM-251.d	Acquisition Date	9/27/2024 12:10:59 PM
Method	DEFAULT.m	Operator	Gudipati SrinivasaRao
Sample Name	VM-251	Instrument	impact HD 1819696.00197
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active	Set Capillary	3500 V	Set Dry Heater	200 °C
Scan Begin	150 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 °C

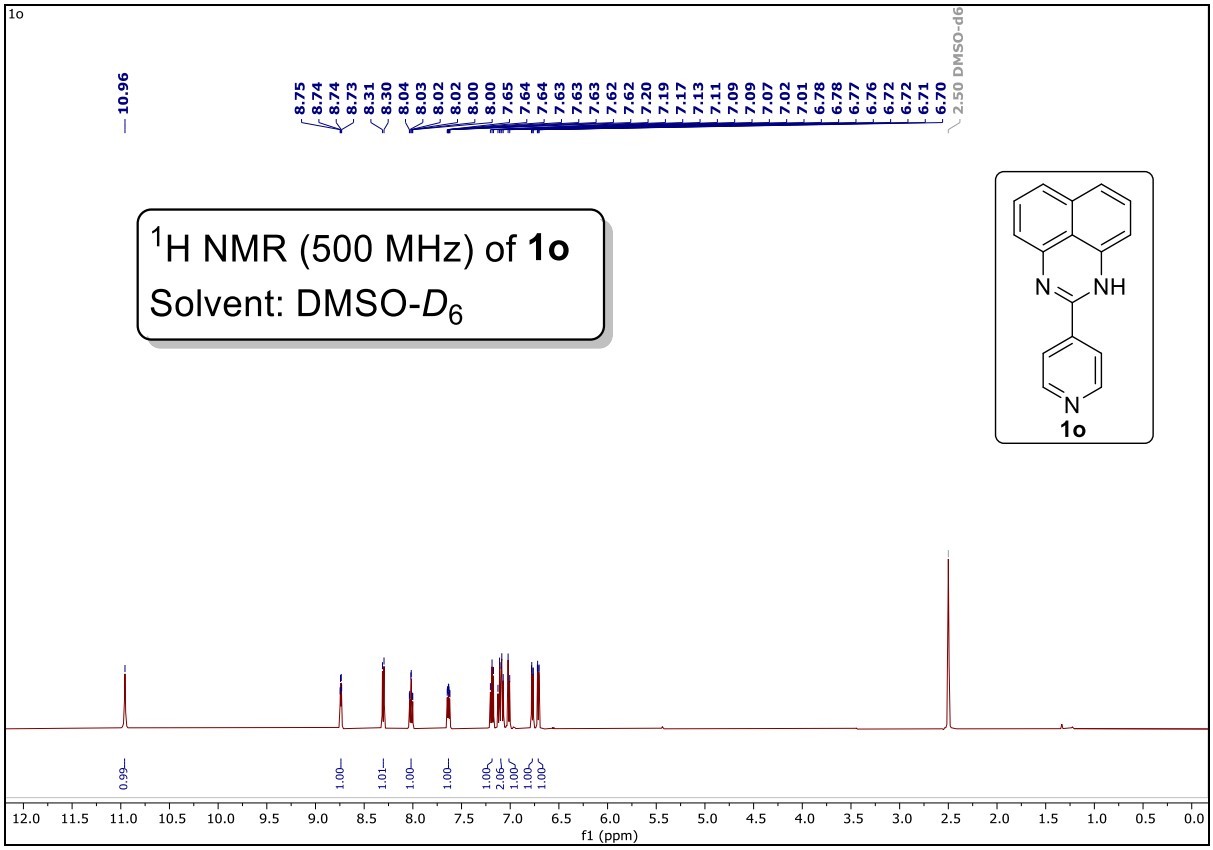


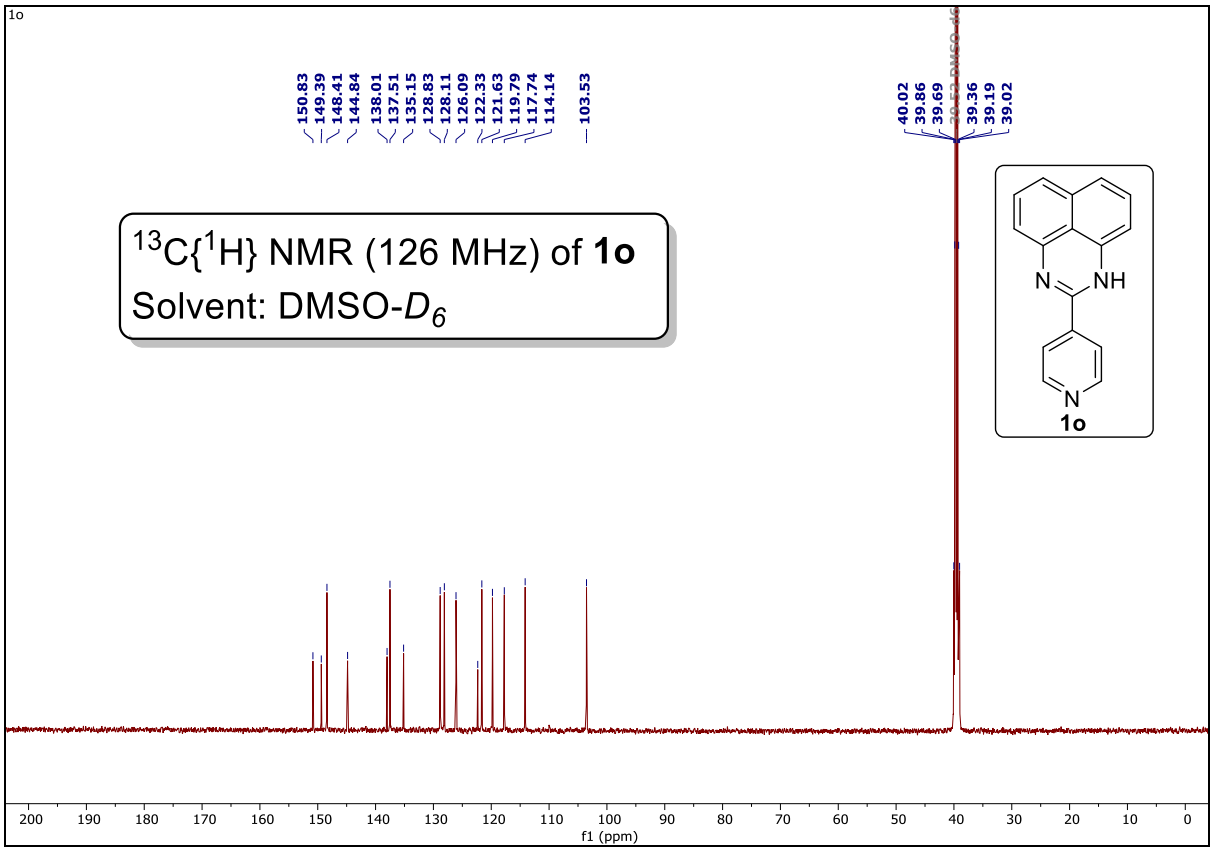


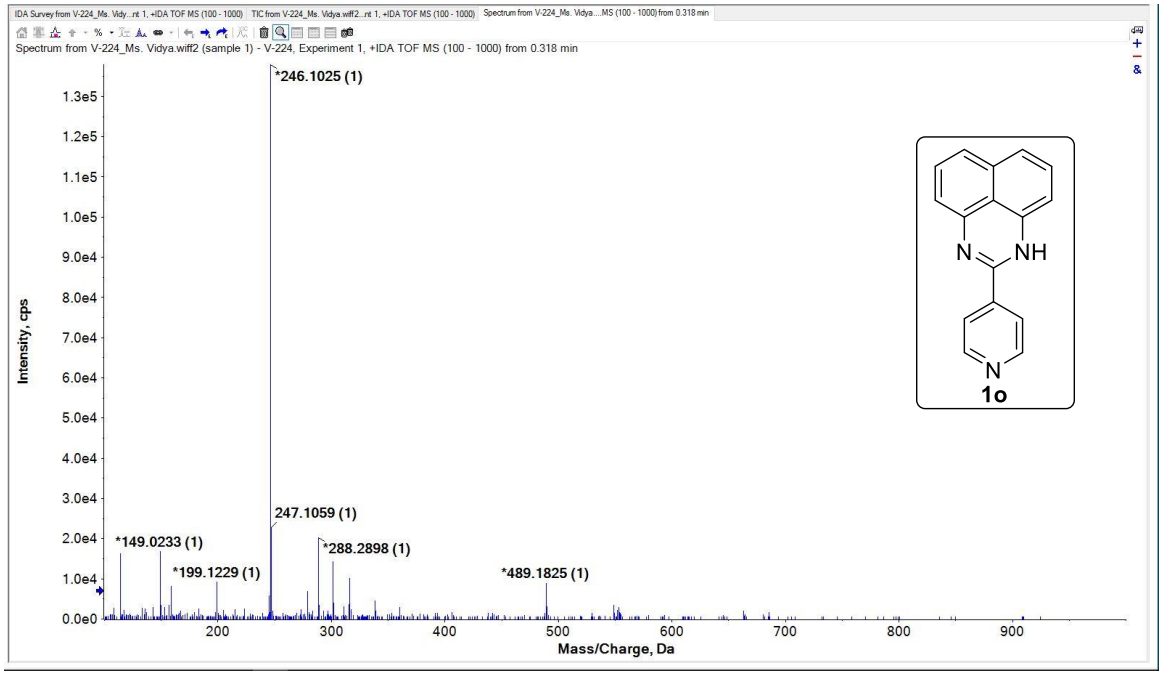


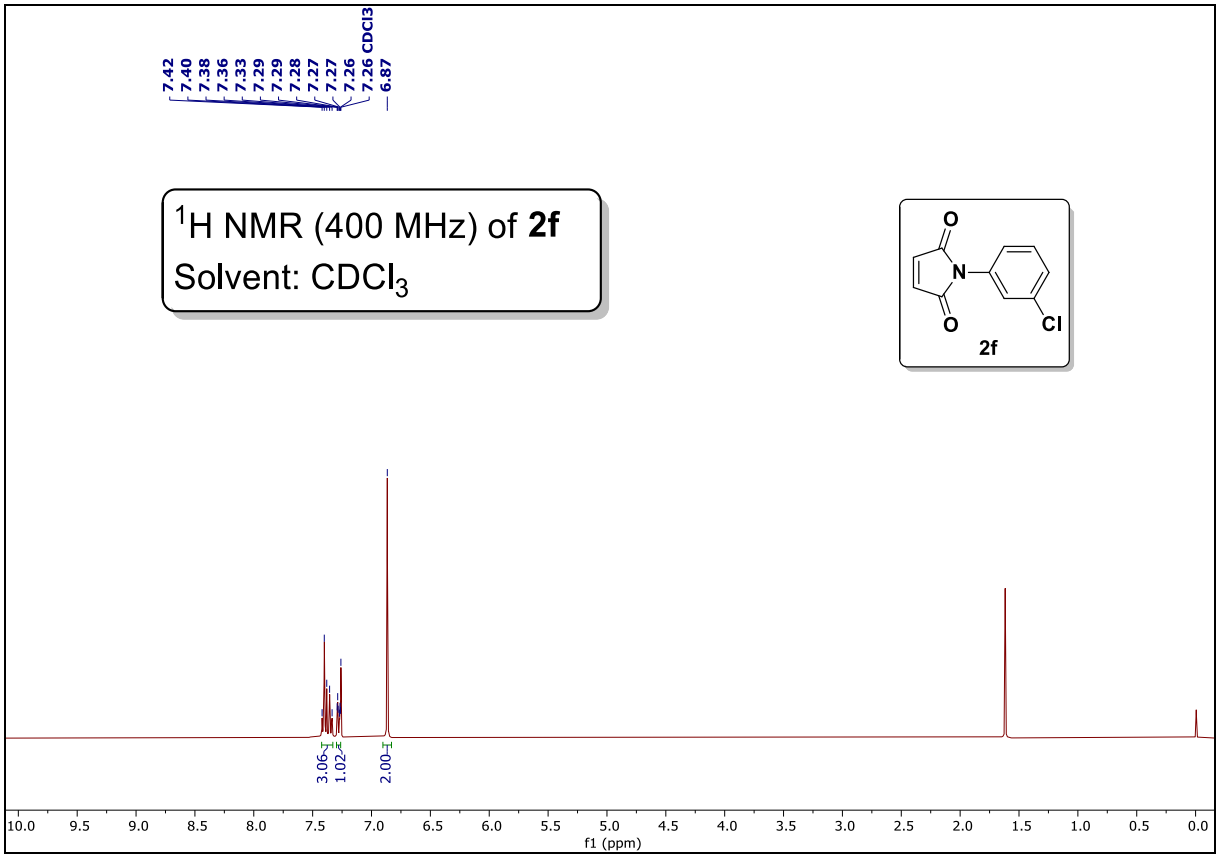
VM-251.d

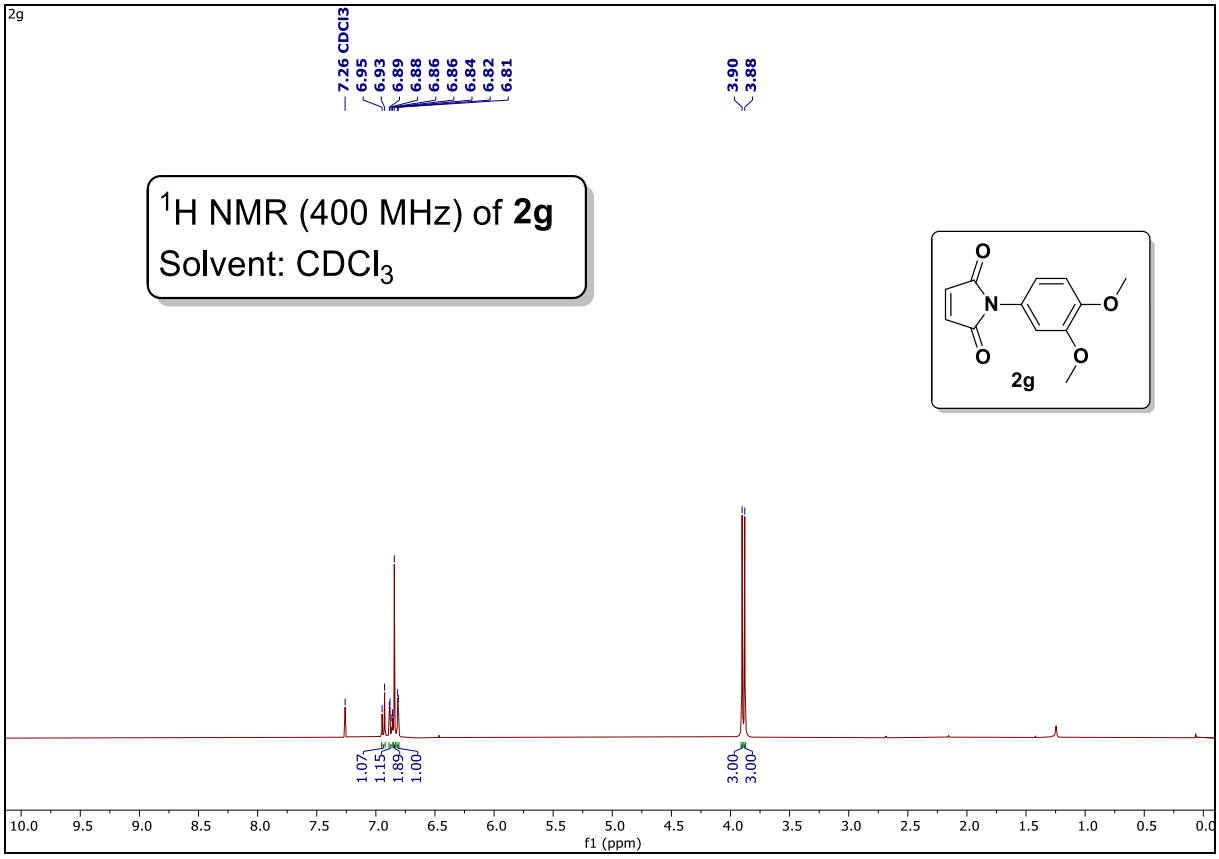
Gudipati

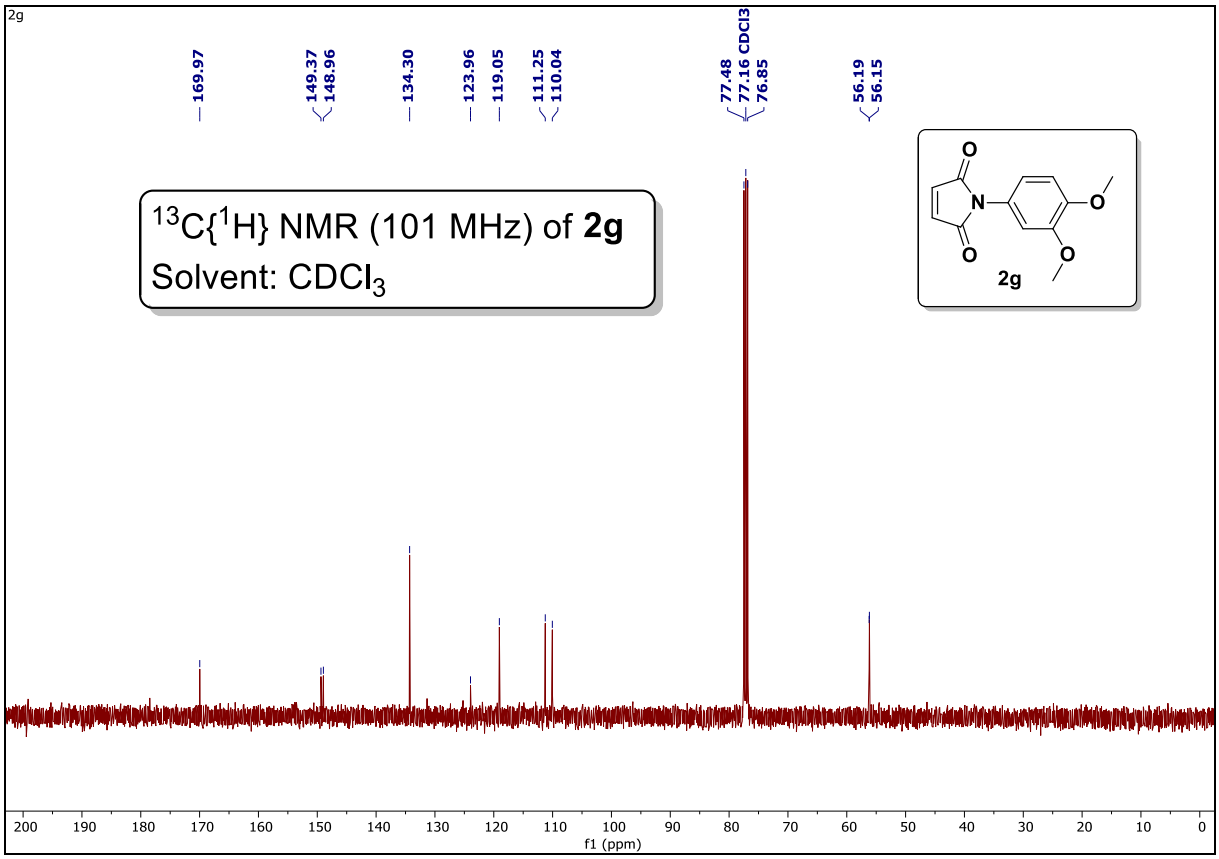

1o
10.96
8.75
8.74
8.74
8.73
8.31
8.30
8.04
8.03
8.02
8.02
8.00
8.00
7.65
7.64
7.64
7.63
7.63
7.62
7.62
7.20
7.19
7.17
7.13
7.11
7.09
7.09
7.07
7.02
7.01
6.78
6.78
6.77
6.76
6.72
6.72
6.71
6.70
2.50 DMSO-d6
^{1}H NMR (500 MHz) of **1o**
Solvent: DMSO-D_6
N
NH
N
1o
0.99
1.00
1.01
1.00
1.00
1.00
2.06
1.00
1.00
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


1o
150.83
149.39
148.41
144.84
138.01
137.51
135.15
128.83
128.11
126.09
122.33
121.63
119.79
117.74
114.14
103.53
40.02
39.86
39.69
39.52 DMSO-d6
39.36
39.19
39.02
^{13}C{^{1}H} NMR (126 MHz) of **1o**
Solvent: DMSO-D_6
N
NH
N
1o
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


Spectrum from V-224_Ms. Vidya.wiff2 (sample 1) - V-224, Experiment 1, +IDA TOF MS (100 - 1000) from 0.318 min
Intensity, cps
Mass/Charge, Da
*246.1025 (1)
247.1059 (1)
*149.0233 (1)
*199.1229 (1)
*288.2898 (1)
*489.1825 (1)
1.3e5
1.2e5
1.1e5
1.0e5
9.0e4
8.0e4
7.0e4
6.0e4
5.0e4
4.0e4
3.0e4
2.0e4
1.0e4
0.0e0
200
300
400
500
600
700
800
900
N
NH
N
1o


7.42
7.40
7.38
7.36
7.33
7.29
7.29
7.28
7.27
7.27
7.26
7.26 CDCl3
6.87
1H NMR (400 MHz) of 2f
Solvent: CDCl3
O
N
O
Cl
2f
3.06
1.02
2.00
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


2g
7.26 CDCl3
6.95
6.93
6.89
6.88
6.86
6.86
6.84
6.82
6.81
3.90
3.88
1H NMR (400 MHz) of 2g
Solvent: CDCl3
2g
1.07
1.15
1.89
1.00
3.00
3.00
f1 (ppm)


2g
169.97
149.37
148.96
134.30
123.96
119.05
111.25
110.04
77.48
77.16 CDCl3
76.85
56.19
56.15
13C{1H} NMR (101 MHz) of 2g
Solvent: CDCl3
2g
f1 (ppm)

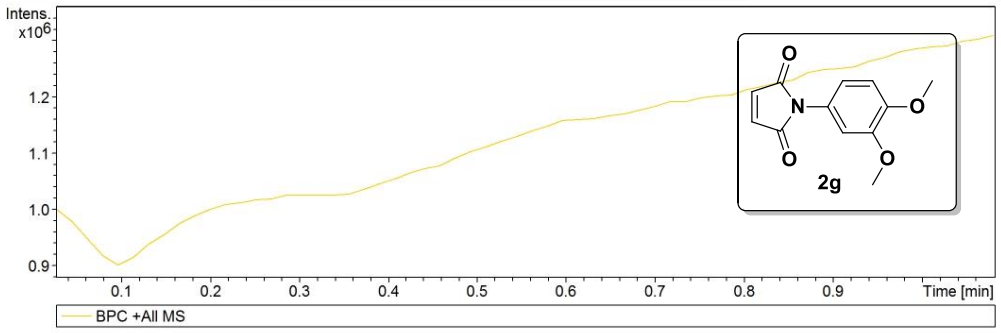
Display Report

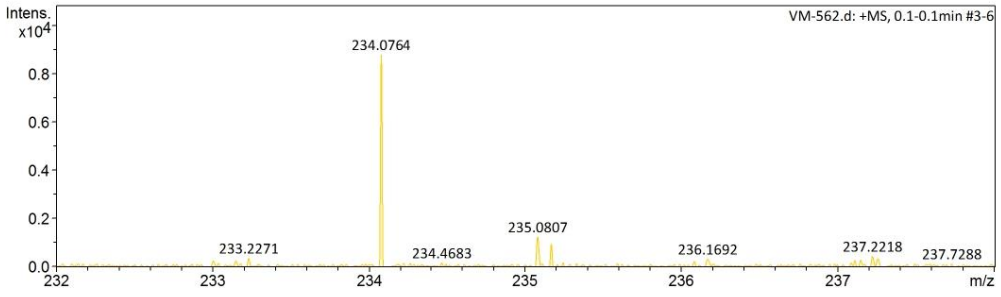
Analysis Info

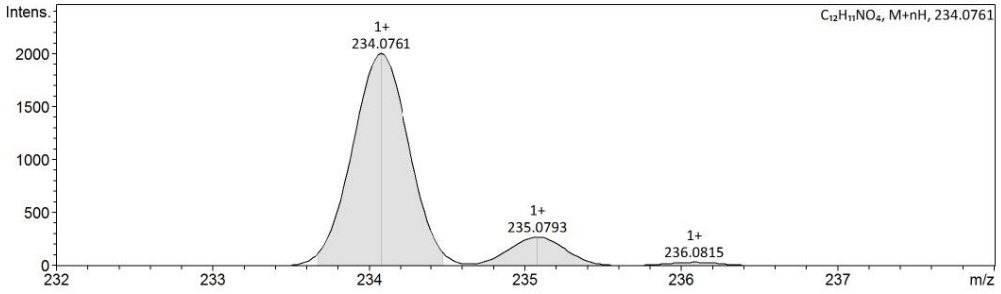
Analysis Name	D:\Data\user data\Dr. Lokman\24-02-2025\VM-562.d	Acquisition Date	2/24/2025 1:07:26 PM
Method	low_mass.m	Operator	Gudipati SrinivasaRao
Sample Name	VM-562	Instrument	impact HD 1819696.00197
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.6 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	5.0 l/min
Scan End	1500 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C

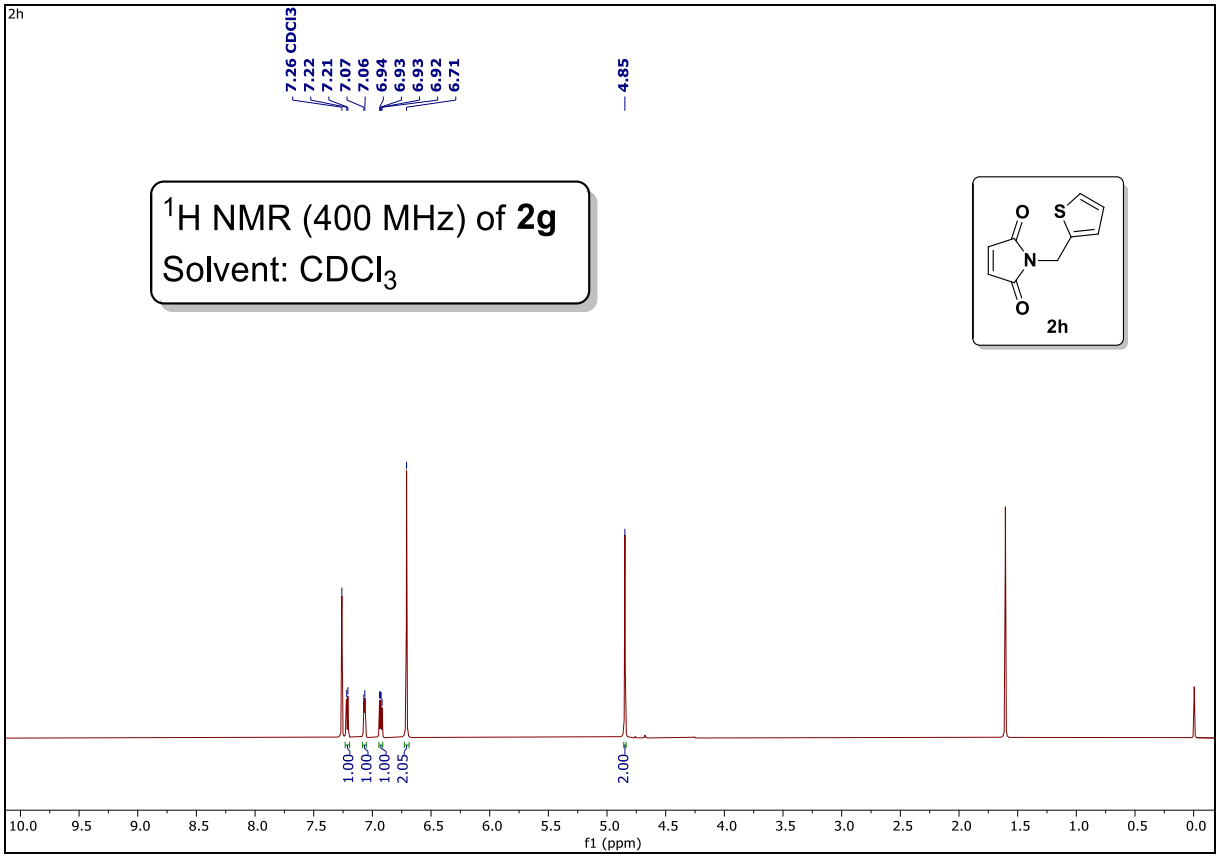


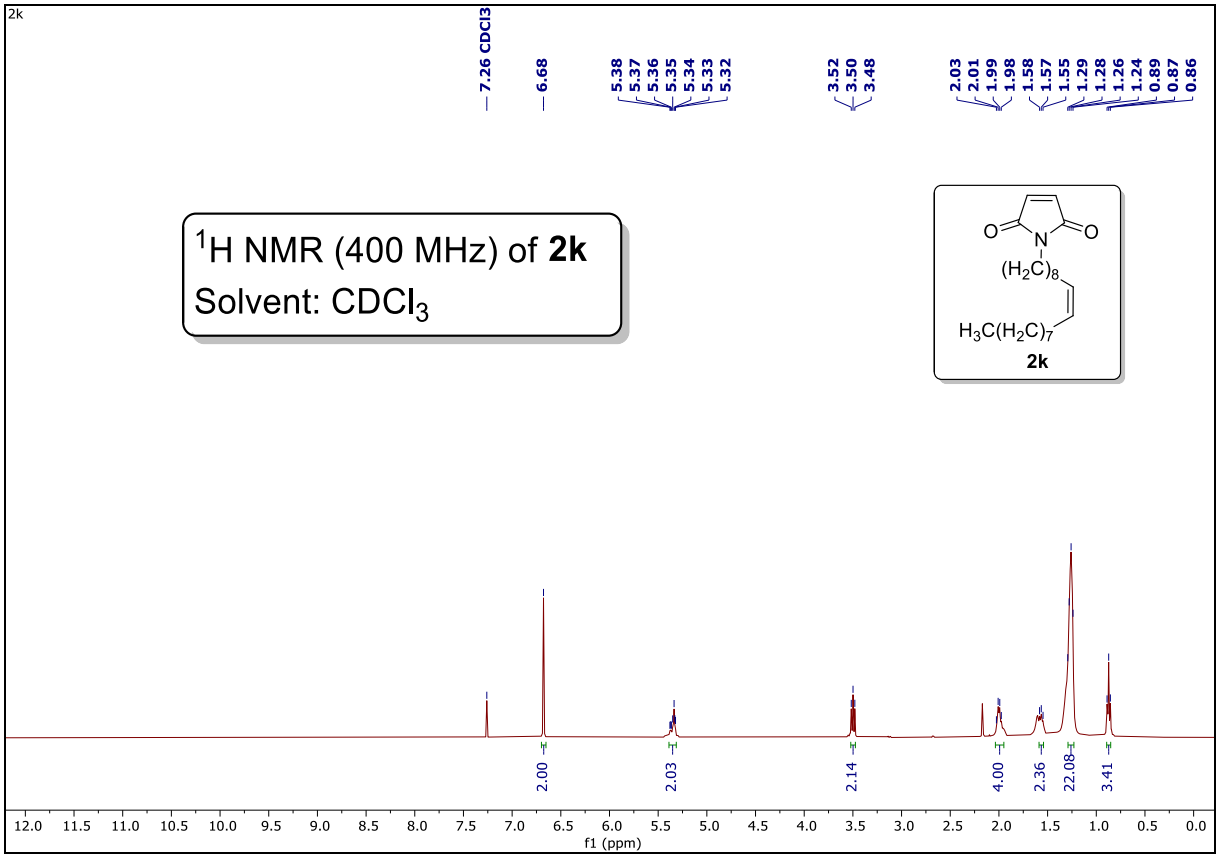


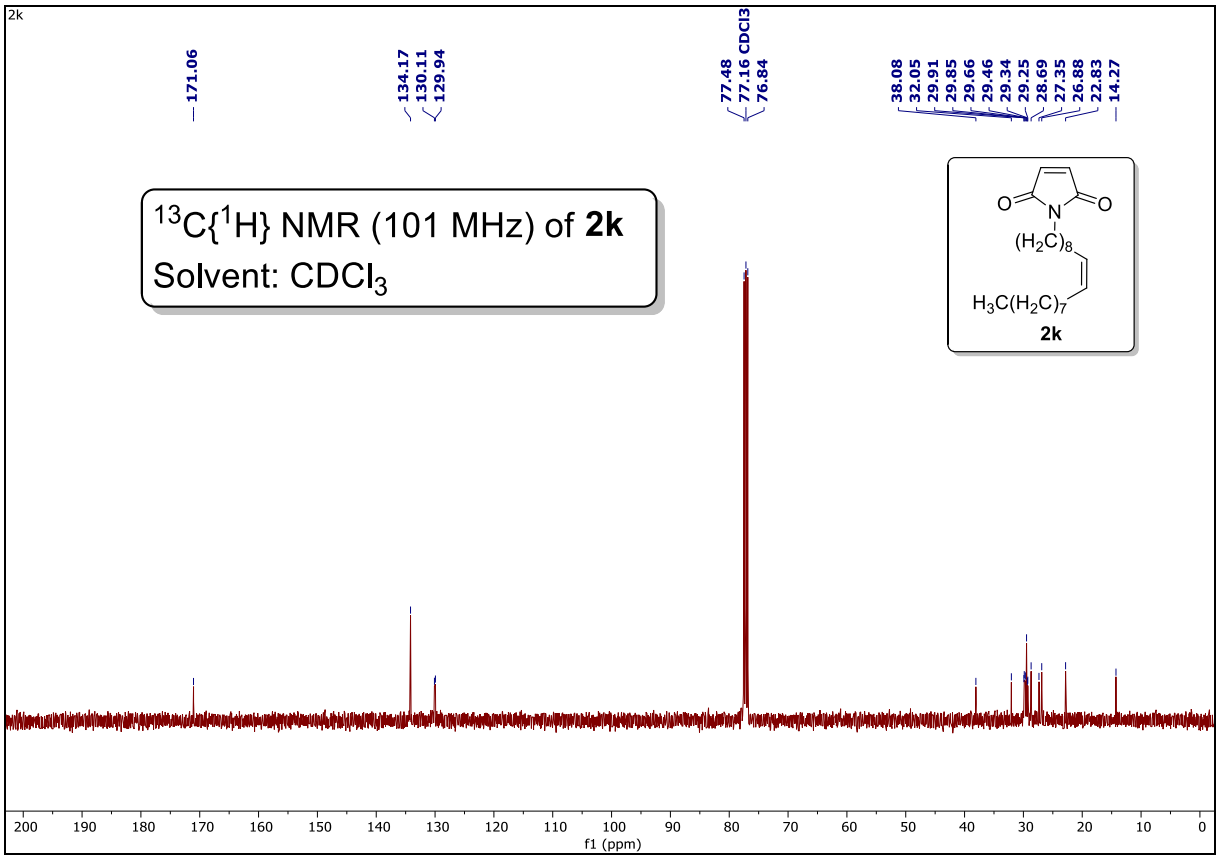


VM-562.d

Gudipati


2h
7.26 CDCl3
7.22
7.21
7.07
7.06
6.94
6.93
6.93
6.92
6.71
4.85
1H NMR (400 MHz) of 2g
Solvent: CDCl3
O
S
N
O
2h
1.00
1.00
1.00
2.05
2.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


2k
7.26 CDCl3
6.68
5.38
5.37
5.36
5.35
5.34
5.33
5.32
3.52
3.50
3.48
2.03
2.01
1.99
1.98
1.58
1.57
1.55
1.29
1.28
1.26
1.24
0.89
0.87
0.86
1H NMR (400 MHz) of 2k
Solvent: CDCl3
2k
2.00
2.03
2.14
4.00
2.36
22.08
3.41
f1 (ppm)


2k
171.06
134.17
130.11
129.94
77.48
77.16 CDCl3
76.84
38.08
32.05
29.91
29.85
29.66
29.46
29.34
29.25
28.69
27.35
26.88
22.83
14.27
13C{1H} NMR (101 MHz) of 2k
Solvent: CDCl3
2k
f1 (ppm)

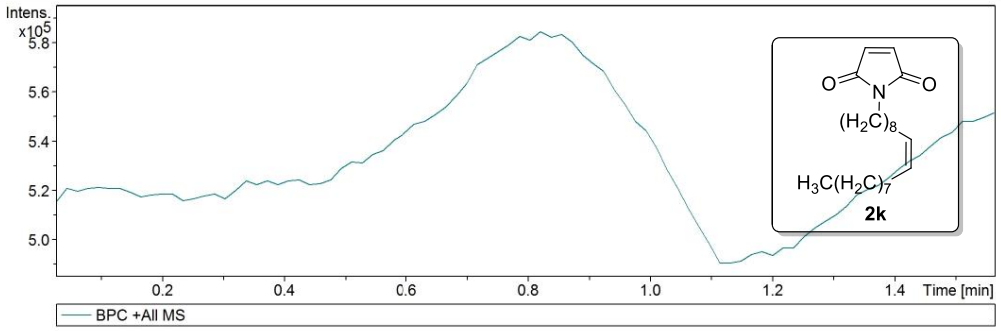
Display Report

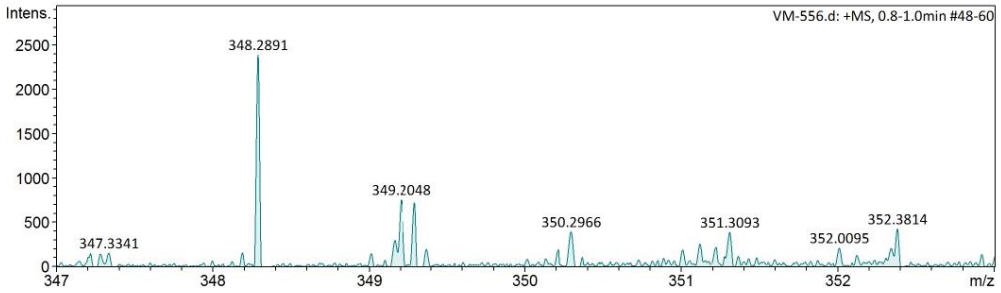
Analysis Info

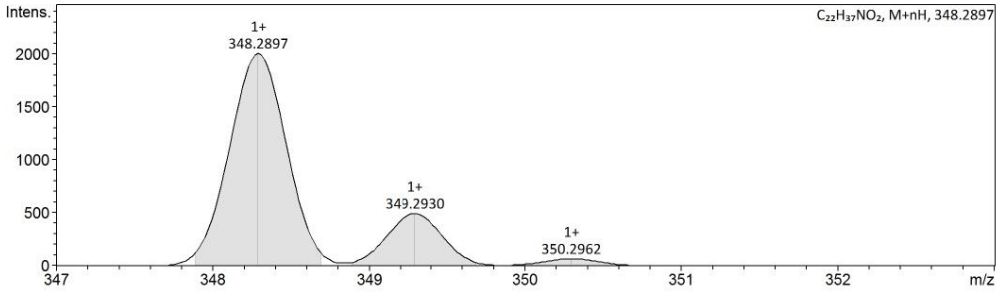
Analysis Name	D:\Data\user data\Dr. Lokman\24-02-2025\VM-556.d	Acquisition Date	2/24/2025 12:13:10 PM
Method	low_mass.m	Operator	Gudipati SrinivasaRao
Sample Name	VM-556	Instrument	impact HD 1819696.00197
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.6 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	5.0 l/min
Scan End	1500 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C

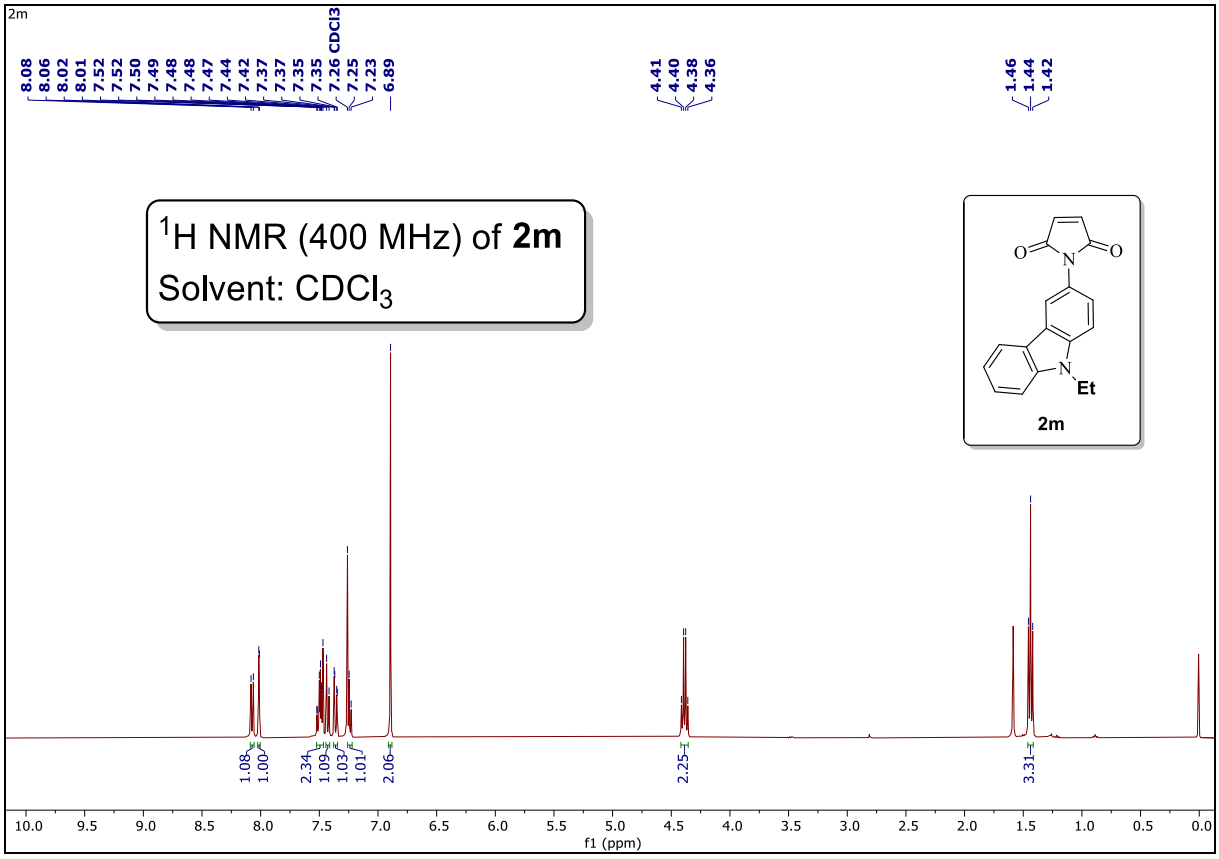


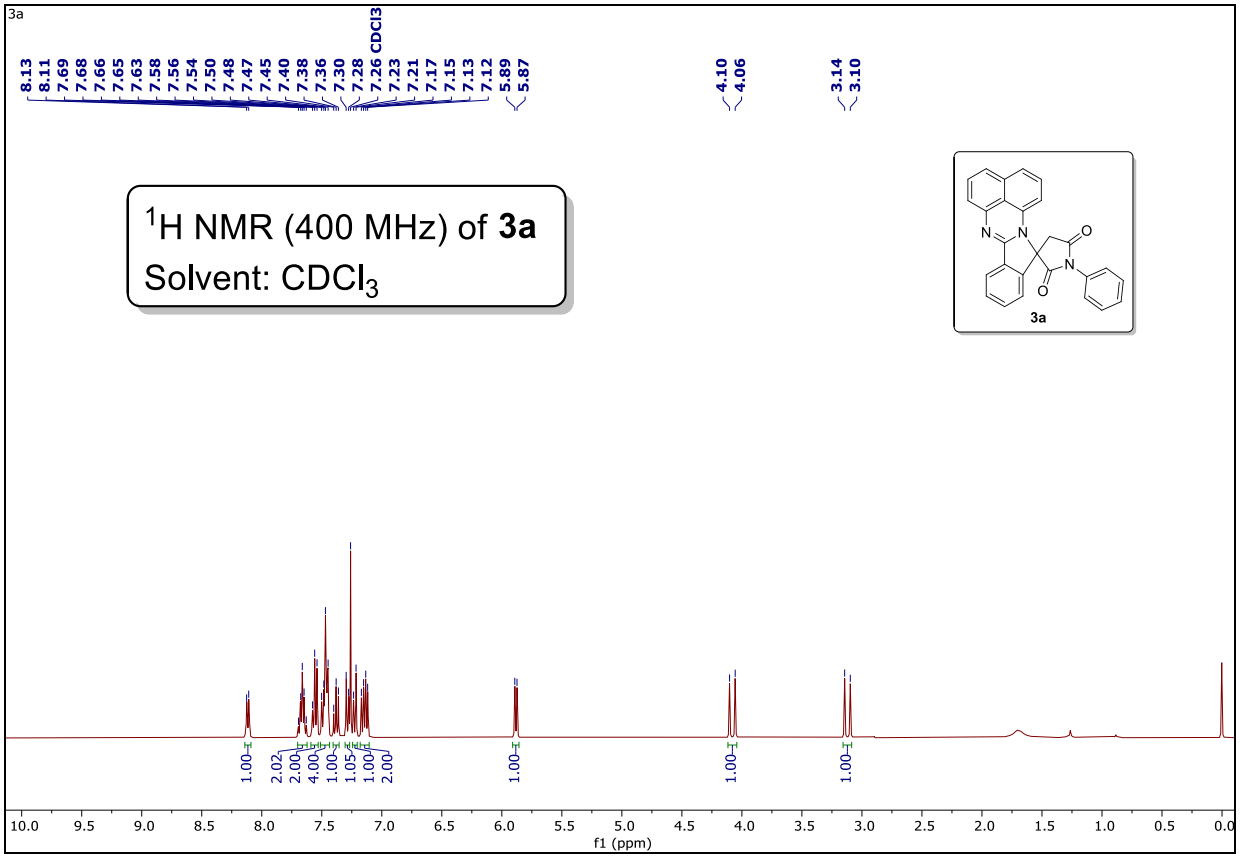


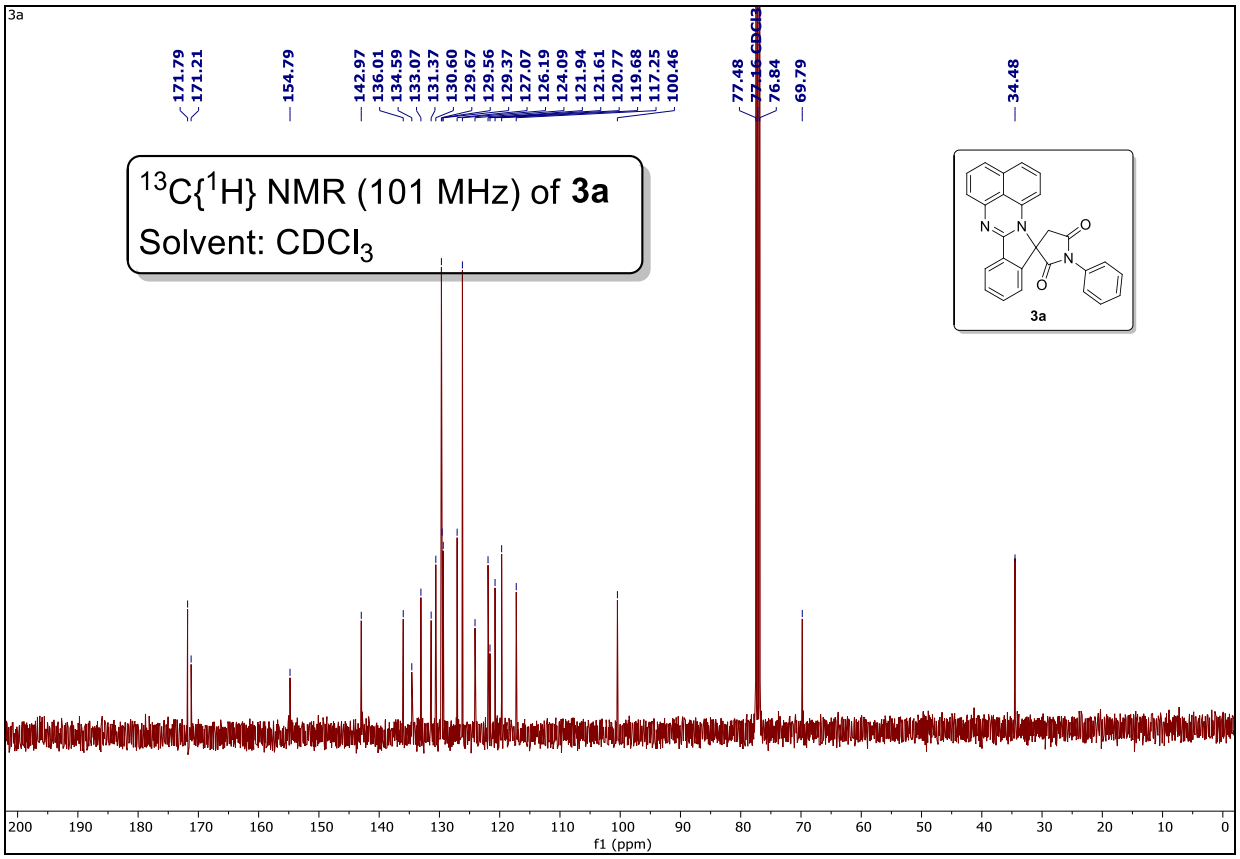


VM-556.d

Gudipati


2m
8.08
8.06
8.02
8.01
7.52
7.52
7.50
7.49
7.48
7.48
7.47
7.44
7.42
7.37
7.37
7.35
7.35
7.26 CDCl3
7.25
7.23
6.89
4.41
4.40
4.38
4.36
1.46
1.44
1.42
1H NMR (400 MHz) of 2m
Solvent: CDCl3
Et
2m
1.08
1.00
2.34
1.09
1.03
1.01
2.06
2.25
3.31
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


3a
8.13
8.11
7.69
7.68
7.66
7.65
7.63
7.58
7.56
7.54
7.50
7.48
7.47
7.45
7.40
7.38
7.36
7.30
7.28
7.26 CDCl3
7.23
7.21
7.17
7.15
7.13
7.12
5.89
5.87
4.10
4.06
3.14
3.10
1H NMR (400 MHz) of 3a
Solvent: CDCl3
3a
1.00
2.02
2.00
4.00
1.00
1.05
1.00
2.00
1.00
1.00
1.00
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


3a
171.79
171.21
154.79
142.97
136.01
134.59
133.07
131.37
130.60
129.67
129.56
129.37
127.07
126.19
124.09
121.94
121.61
120.77
119.68
117.25
100.46
77.48
77.16 CDCl3
76.84
69.79
34.48
13C{1H} NMR (101 MHz) of 3a
Solvent: CDCl3
3a
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

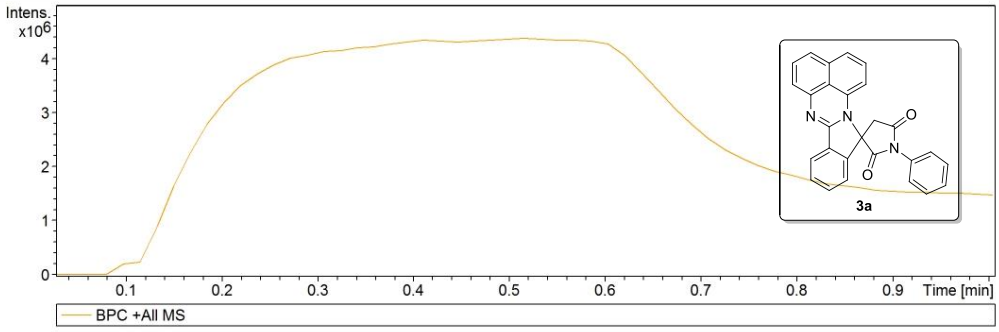
Display Report

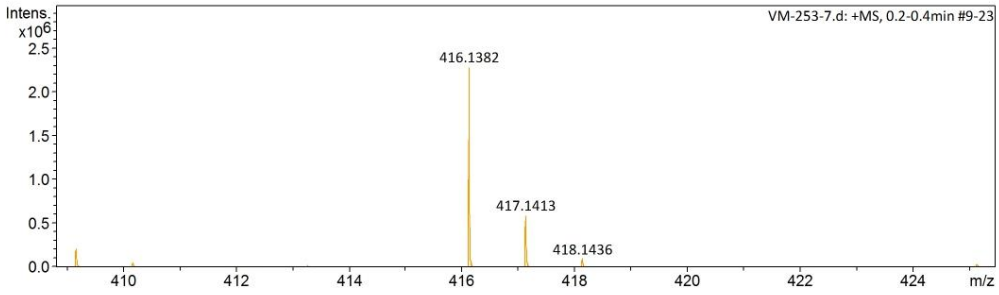
Analysis Info

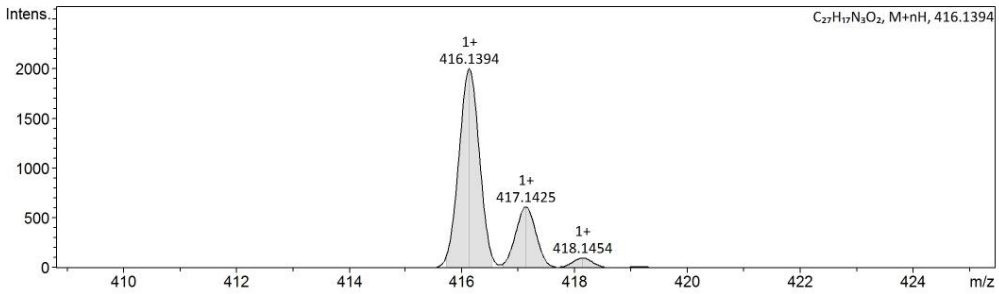
Analysis Name	D:\Data\user data\Dr. Lokman\16-04-2024\VM-253-7.d	Acquisition Date	4/16/2024 11:30:31 AM
Method	Tune_pos_Mid.m	Operator	vidhi
Sample Name	VM-253-7	Instrument	impact HD 1819696.00197
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	219 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 °C

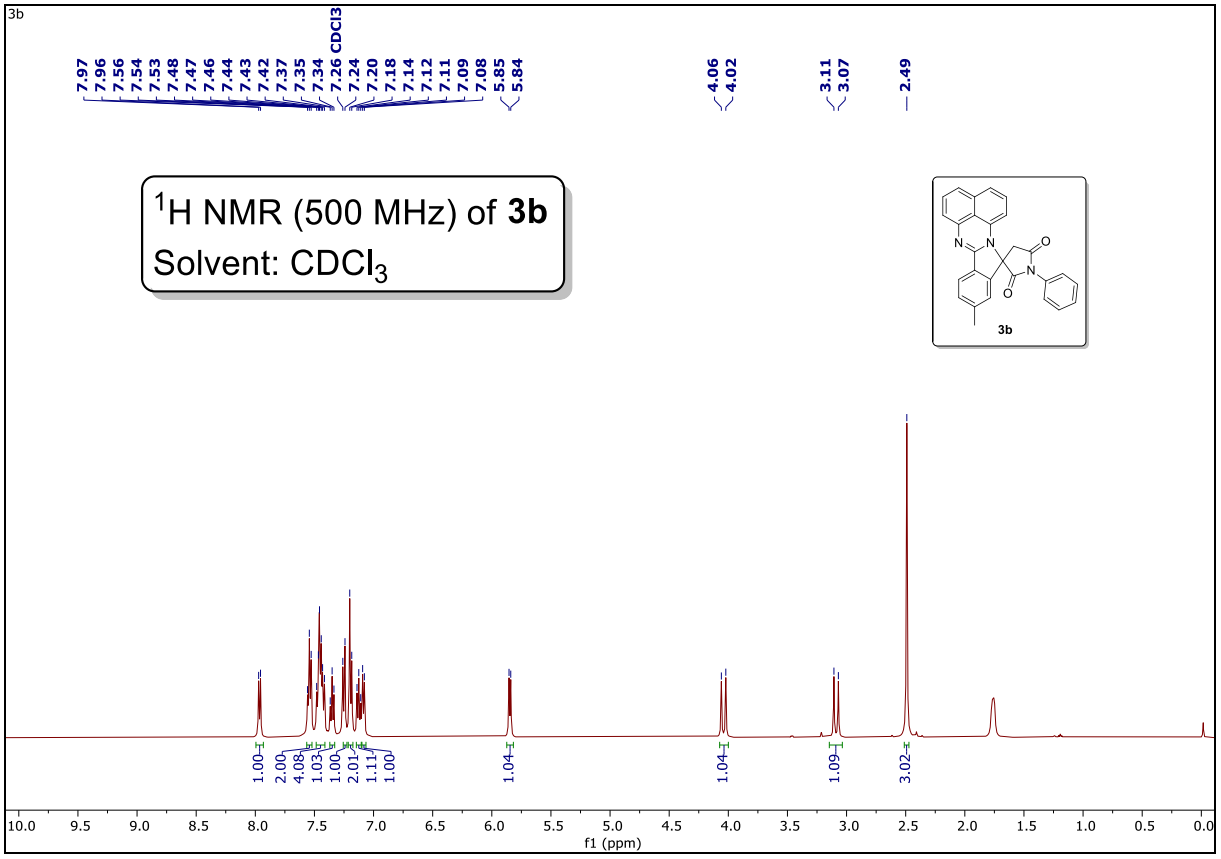


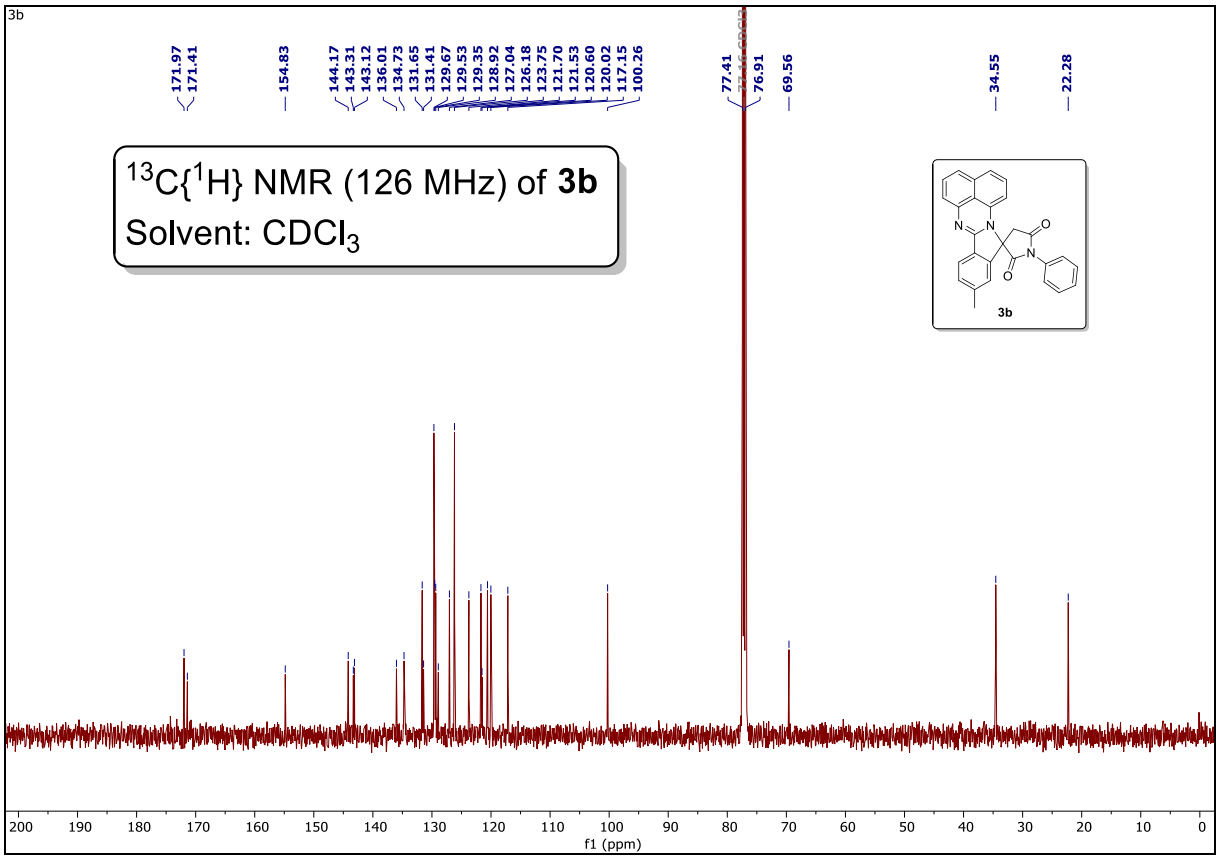


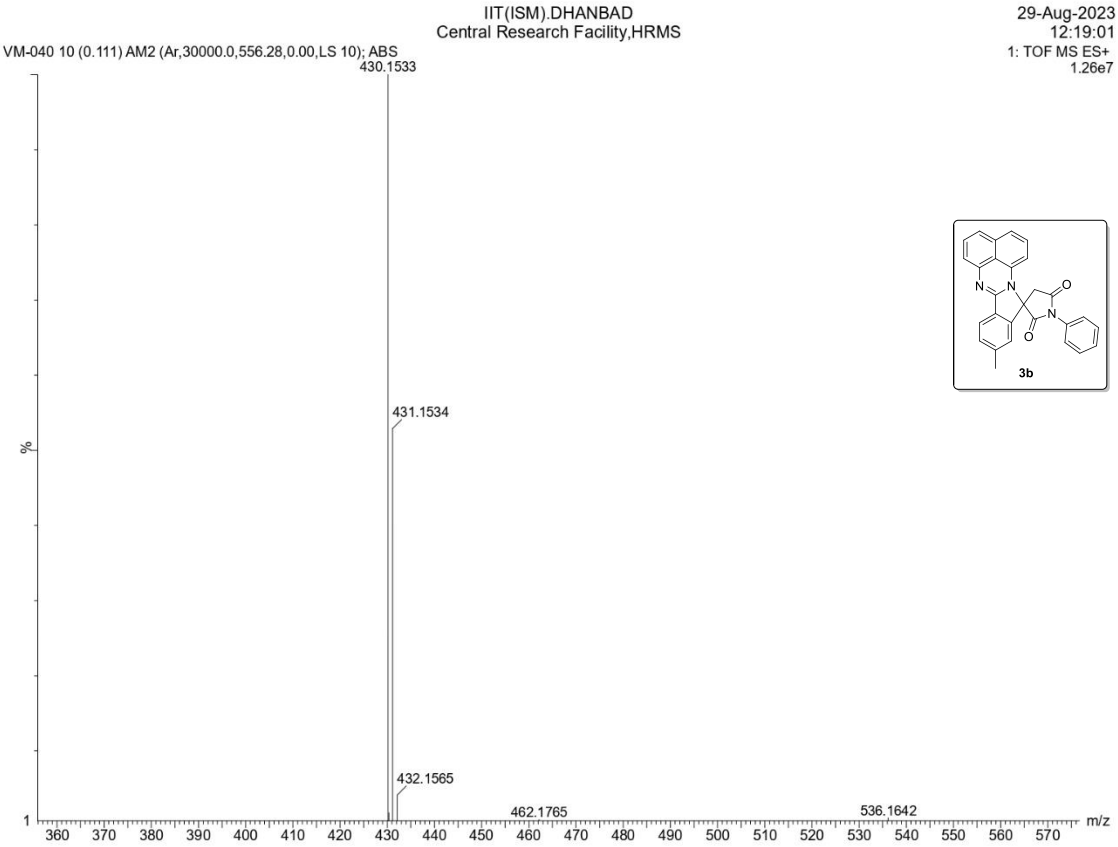


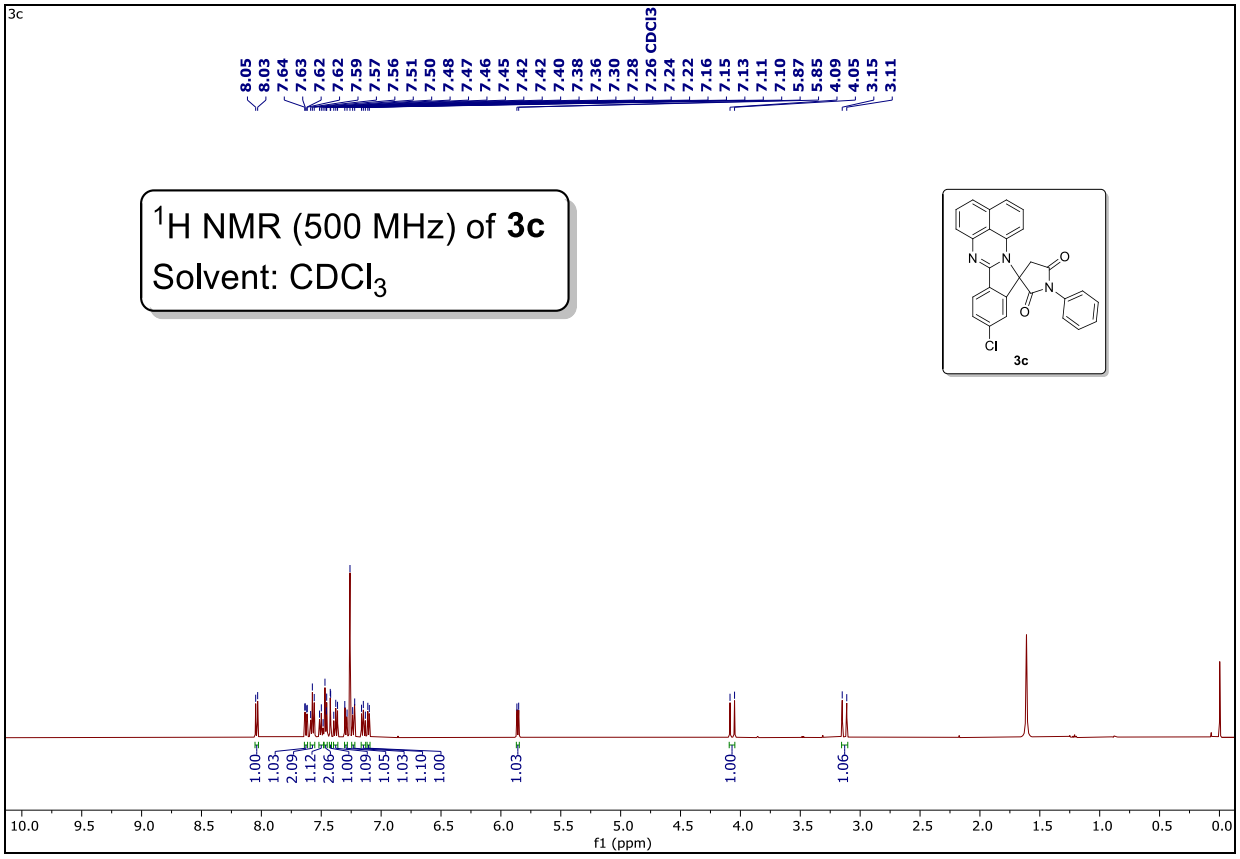
VM-253-7.d

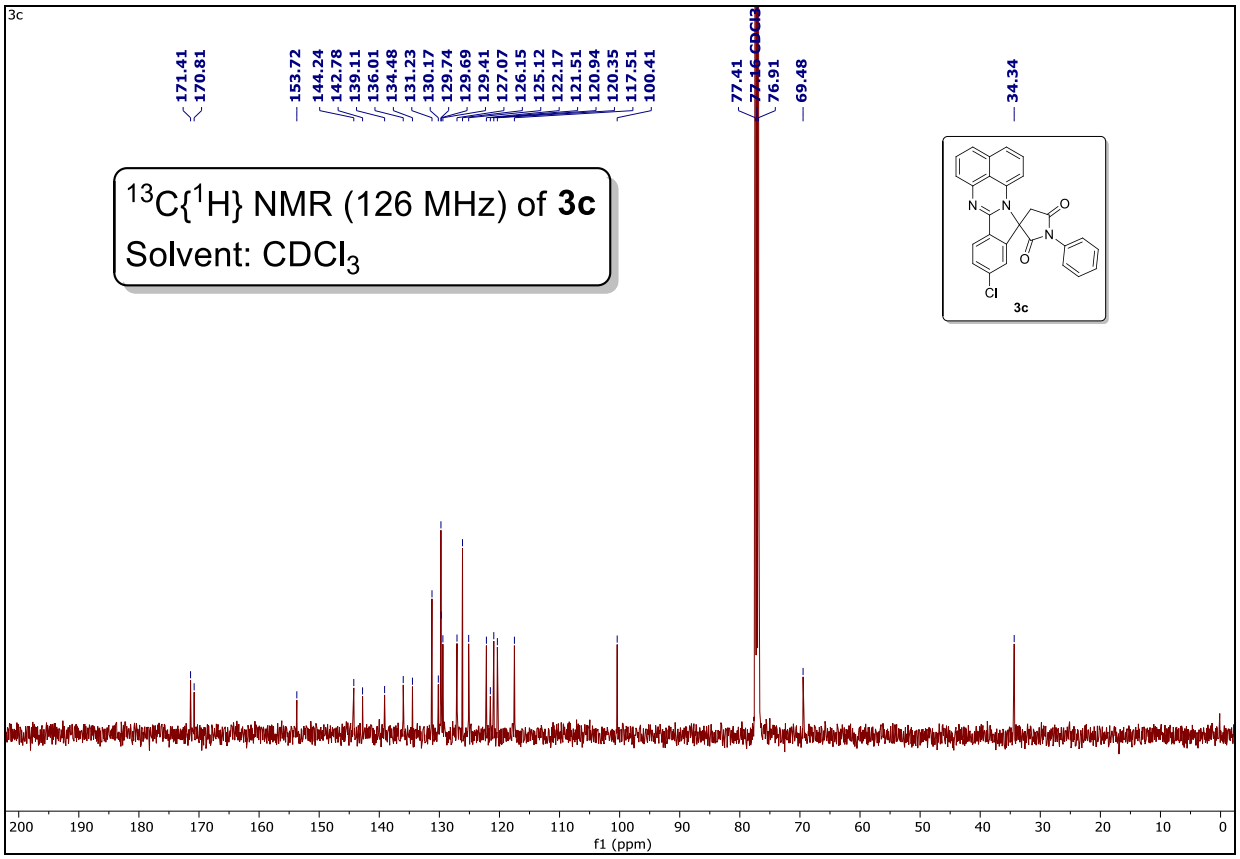
Bruker Compass DataAnalysis 4.2 printed: 4/16/2024 11:34:05 AM by: vidhi Page 1 of 1


3b
7.97
7.96
7.56
7.54
7.53
7.48
7.47
7.46
7.44
7.43
7.42
7.37
7.35
7.34
7.26 CDCl3
7.24
7.20
7.18
7.14
7.12
7.11
7.09
7.08
5.85
5.84
4.06
4.02
3.11
3.07
2.49
1H NMR (500 MHz) of 3b
Solvent: CDCl3
3b
1.00
2.00
4.08
1.03
1.00
2.01
1.11
1.00
1.04
1.04
1.09
3.02
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


3b
171.97
171.41
154.83
144.17
143.31
143.12
136.01
134.73
131.65
131.41
129.67
129.53
129.35
128.92
127.04
126.18
123.75
121.70
121.53
120.60
120.02
117.15
100.26
77.41
76.91
69.56
34.55
22.28
13C{1H} NMR (126 MHz) of 3b
Solvent: CDCl3
3b
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


IIT(ISM).DHANBAD
Central Research Facility,HRMS
29-Aug-2023
12:19:01
1: TOF MS ES+
1.26e7
VM-040 10 (0.111) AM2 (Ar,30000.0,556.28,0.00,LS 10); ABS
430.1533
431.1534
432.1565
462.1765
536.1642
%
1
m/z
360 370 380 390 400 410 420 430 440 450 460 470 480 490 500 510 520 530 540 550 560 570
3b


3c
8.05
8.03
7.64
7.63
7.62
7.62
7.59
7.57
7.56
7.51
7.50
7.48
7.47
7.46
7.45
7.42
7.42
7.40
7.38
7.36
7.30
7.28
7.26 CDCl3
7.24
7.22
7.16
7.15
7.13
7.11
7.10
5.87
5.85
4.09
4.05
3.15
3.11
1H NMR (500 MHz) of 3c
Solvent: CDCl3
Cl
3c
1.00
1.03
2.09
1.12
2.06
1.00
1.09
1.05
1.03
1.10
1.00
1.03
1.00
1.06
f1 (ppm)


3c
171.41
170.81
153.72
144.24
142.78
139.11
136.01
134.48
131.23
130.17
129.74
129.69
129.41
127.07
126.15
125.12
122.17
121.51
120.94
120.35
117.51
100.41
77.41
77.16 CDCl3
76.91
69.48
34.34
13C{1H} NMR (126 MHz) of 3c
Solvent: CDCl3
Cl
3c
f1 (ppm)

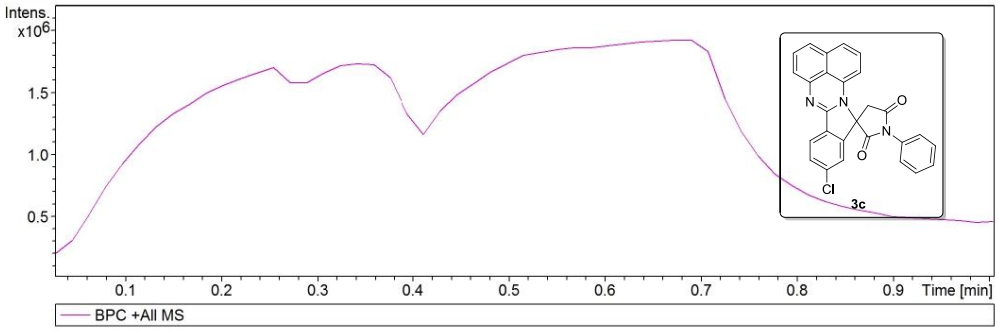
Display Report

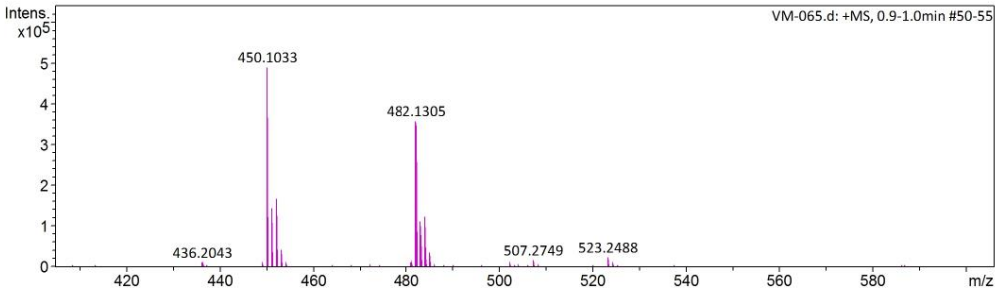
Analysis Info

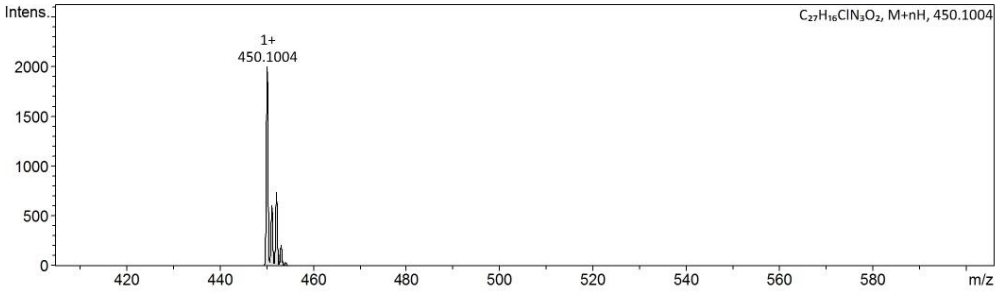
Analysis Name	D:\Data\user data\Dr. Lokman\09-04-2024\VM-065.d	Acquisition Date	4/9/2024 4:03:06 PM
Method	Tune_pos_Mid.m	Operator	vidhi
Sample Name	VM-065	Instrument	impact HD 1819696.00197
Comment			

Acquisition Parameter

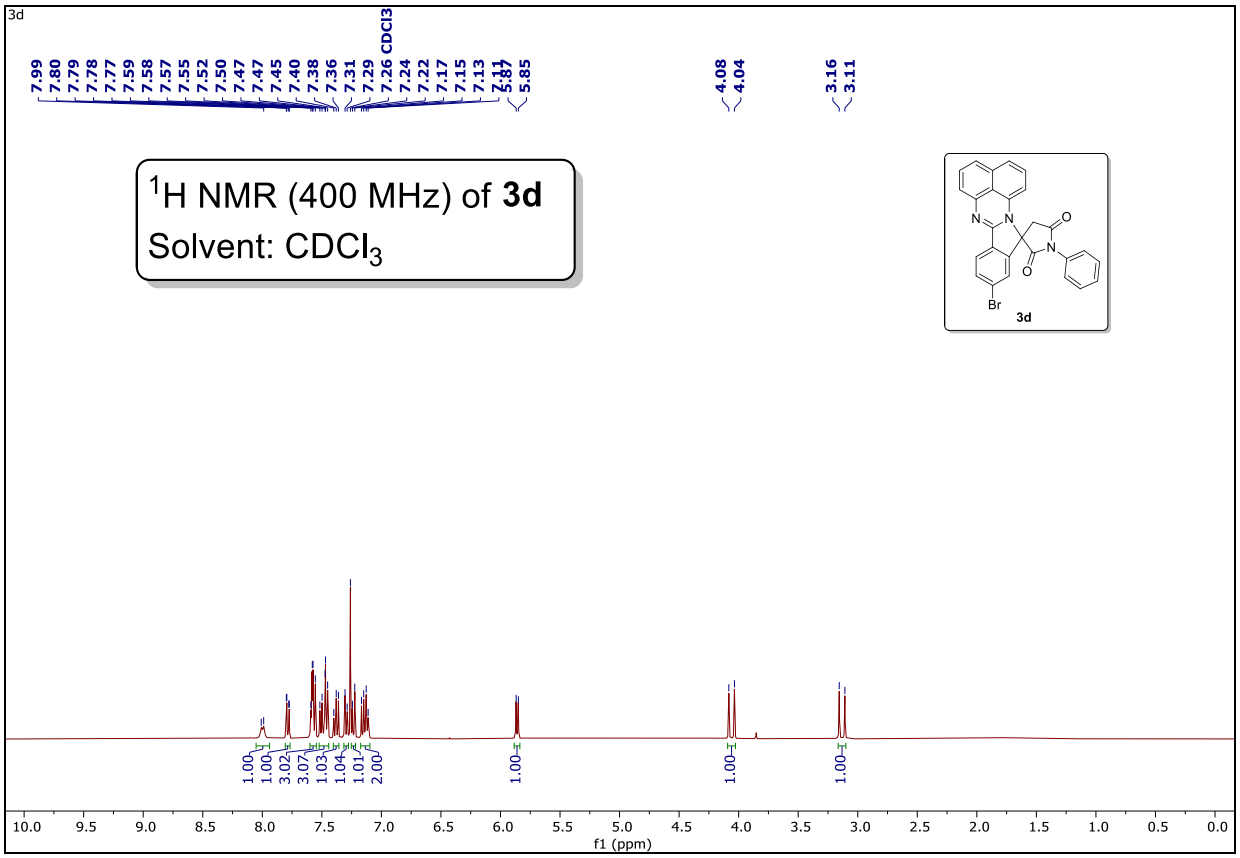
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	219 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 °C

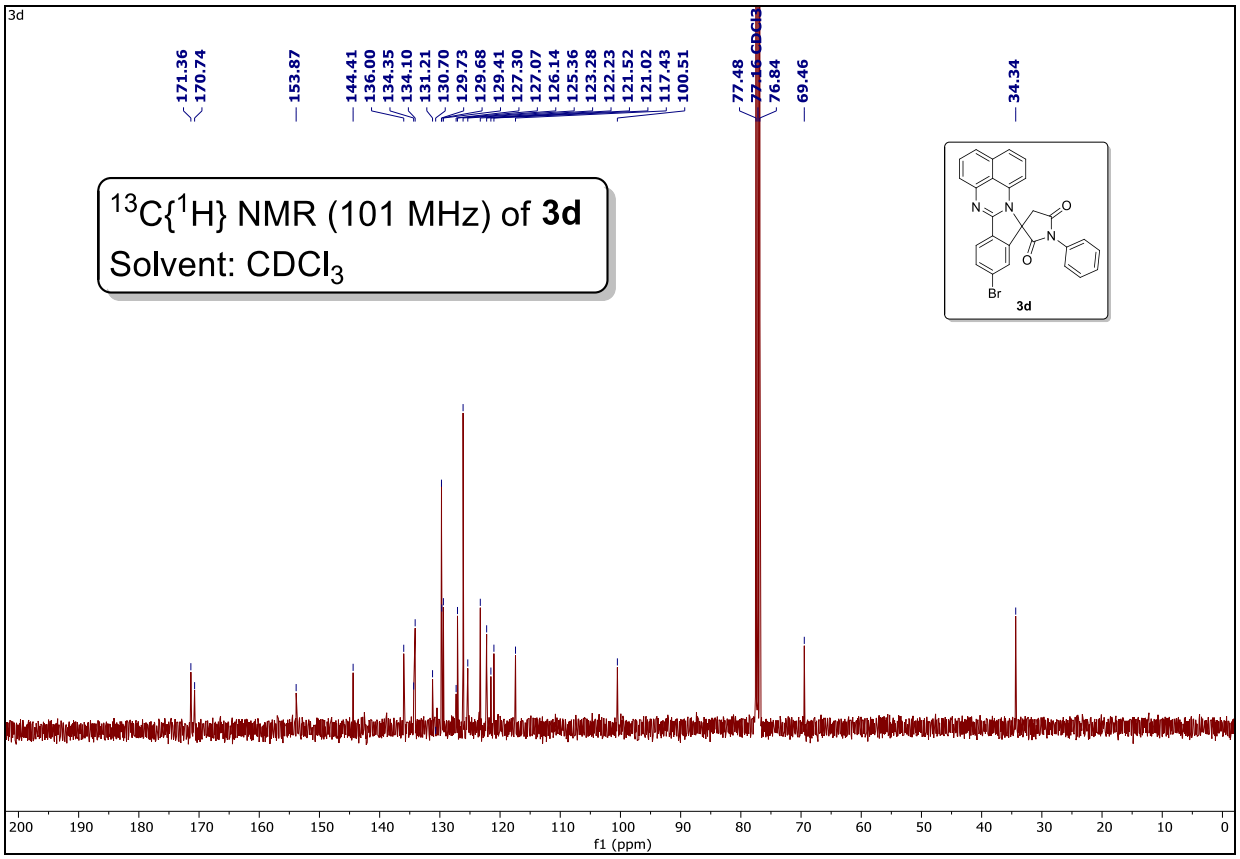






VM-065.d


3d
7.99
7.80
7.79
7.78
7.77
7.59
7.58
7.57
7.55
7.52
7.50
7.47
7.47
7.45
7.40
7.38
7.36
7.31
7.29
7.26 CDCl3
7.24
7.22
7.17
7.15
7.13
5.87
5.85
4.08
4.04
3.16
3.11
1H NMR (400 MHz) of 3d
Solvent: CDCl3
Br
3d
1.00
1.00
3.02
3.07
1.03
1.04
1.01
2.00
1.00
1.00
1.00
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


3d
171.36
170.74
153.87
144.41
136.00
134.35
134.10
131.21
130.70
129.73
129.68
129.41
127.30
127.07
126.14
125.36
123.28
122.23
121.52
121.02
117.43
100.51
77.48
77.16 CDCl3
76.84
69.46
34.34
13C{1H} NMR (101 MHz) of 3d
Solvent: CDCl3
Br
3d
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

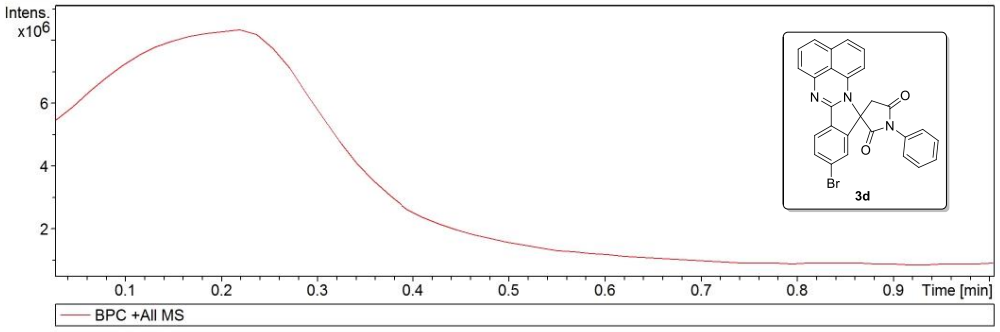
Display Report

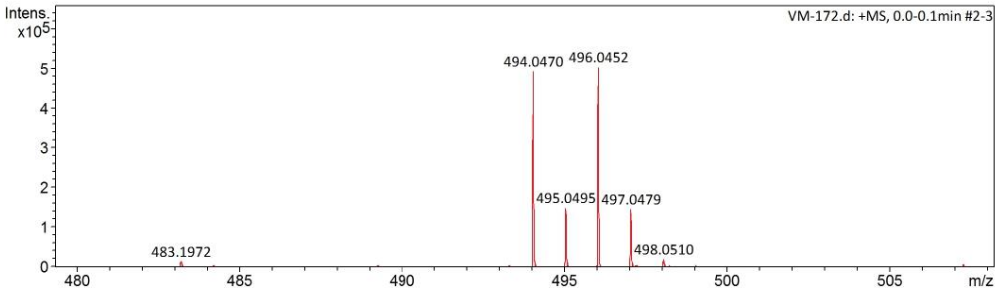
Analysis Info

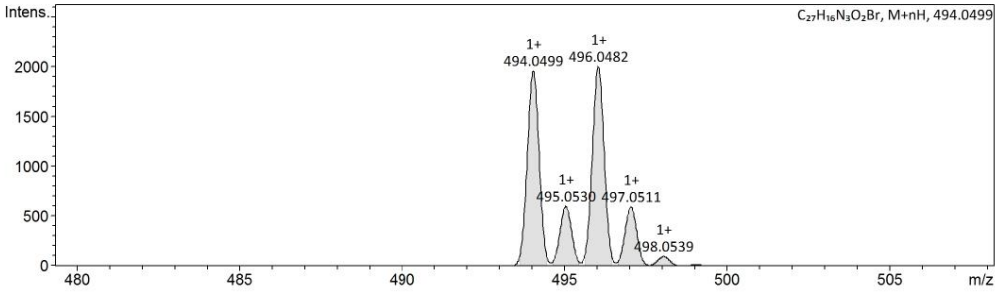
Analysis Name	D:\Data\user data\Dr. Lokman\16-04-2024\VM-172.d	Acquisition Date	4/16/2024 11:03:16 AM
Method	Tune_pos_Mid.m	Operator	vidhi
Sample Name	VM-172	Instrument	impact HD 1819696.00197
Comment			

Acquisition Parameter

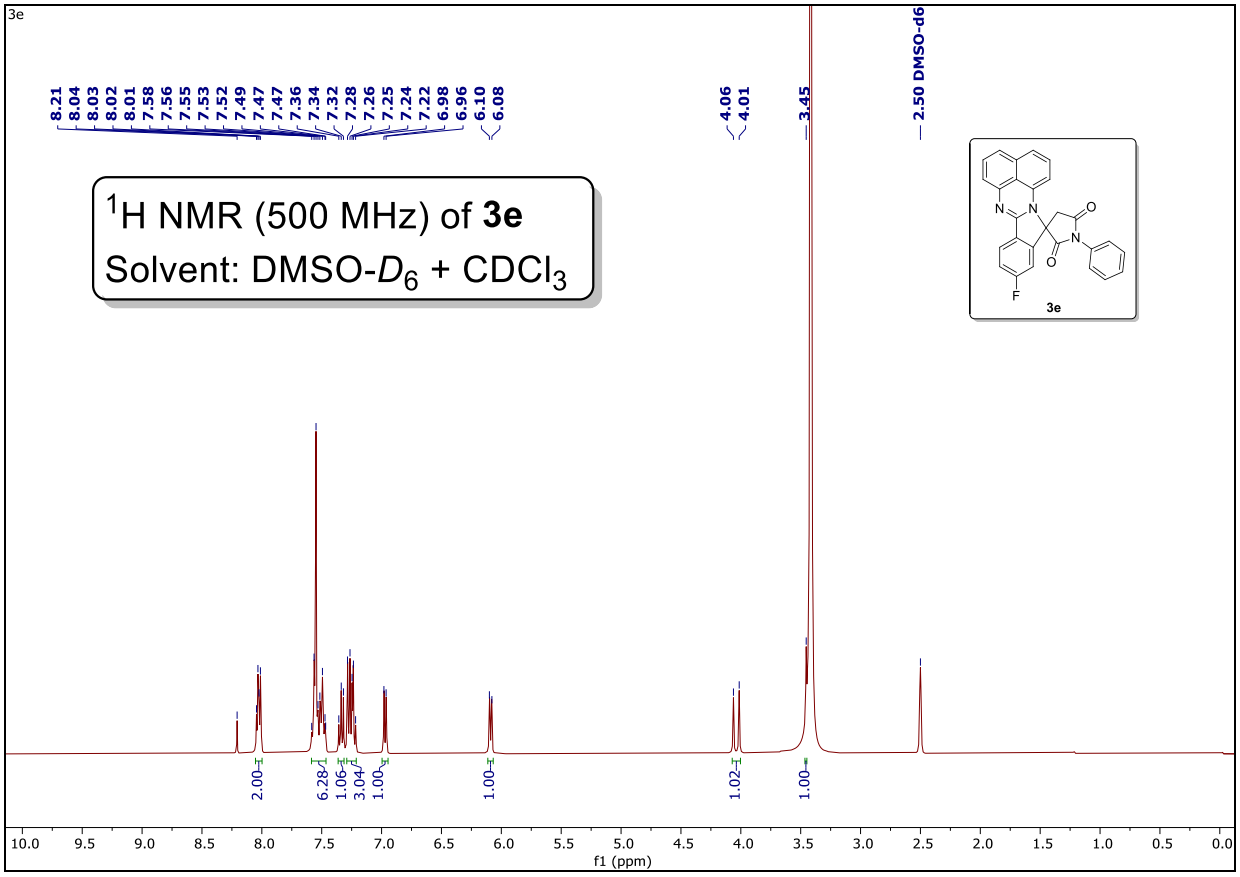
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	219 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 °C

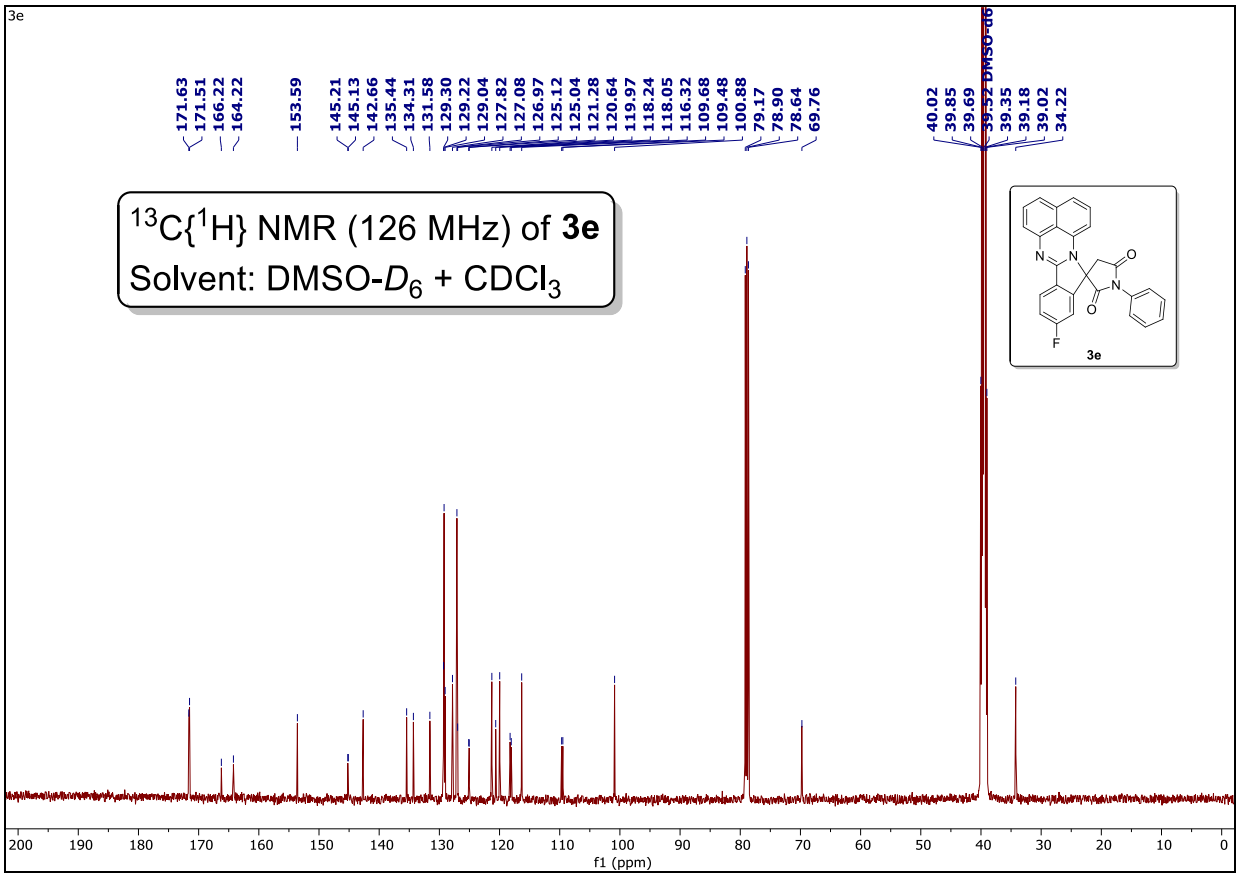


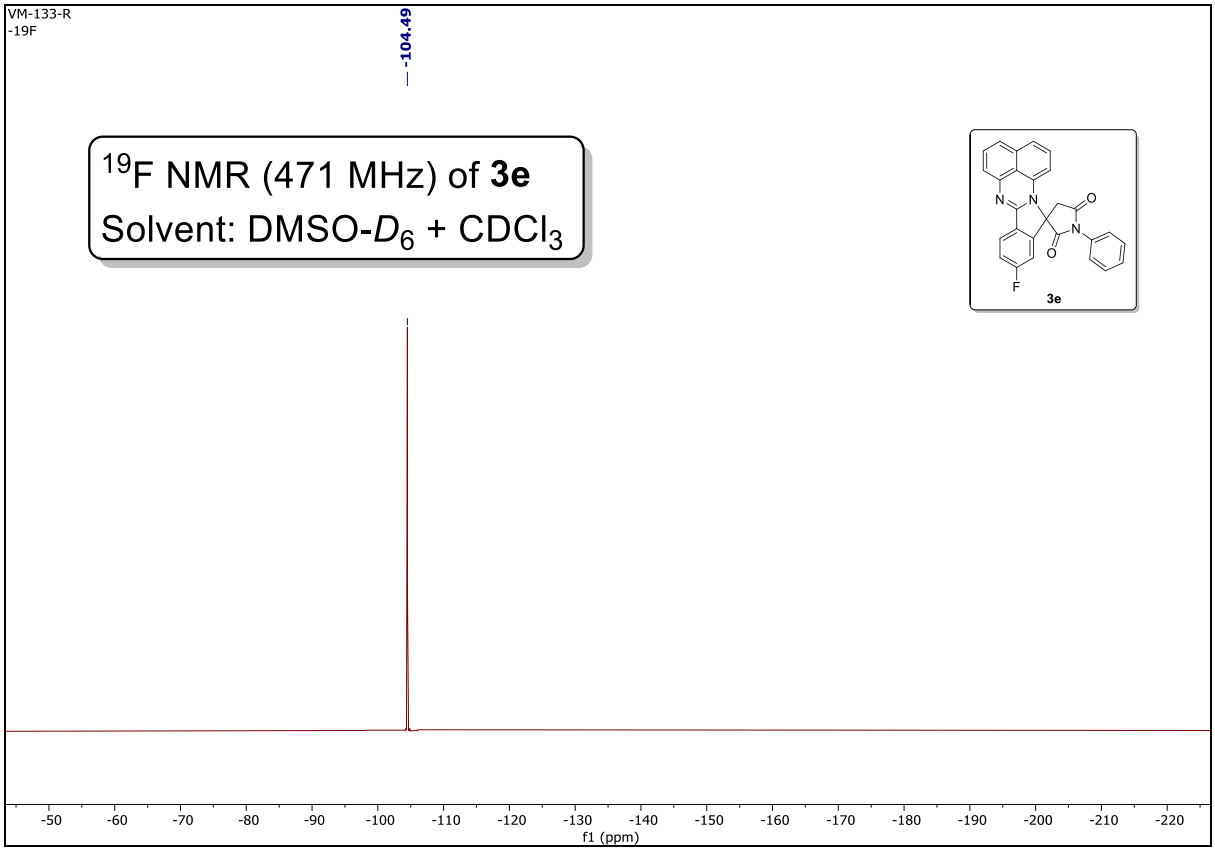




VM-172.d


3e
8.21
8.04
8.03
8.02
8.01
7.58
7.56
7.55
7.53
7.52
7.49
7.47
7.47
7.36
7.34
7.32
7.28
7.26
7.25
7.24
7.22
6.98
6.96
6.10
6.08
4.06
4.01
3.45
2.50 DMSO-d6
^{1}H NMR (500 MHz) of **3e**
Solvent: DMSO-D_6 + $CDCl_3$
3e
2.00
6.28
1.06
3.04
1.00
1.00
1.02
1.00
f1 (ppm)


3e
171.63
171.51
166.22
164.22
153.59
145.21
145.13
142.66
135.44
134.31
131.58
129.30
129.22
129.04
127.82
127.08
126.97
125.12
125.04
121.28
120.64
119.97
118.24
118.05
116.32
109.68
109.48
100.88
79.17
78.90
78.64
69.76
40.02
39.85
39.69
39.52 DMSO-d6
39.35
39.18
39.02
34.22
^{13}C{^{1}H} NMR (126 MHz) of **3e**
Solvent: DMSO-D_6 + $CDCl_3$
3e
f1 (ppm)


VM-133-R
-19F
-104.49
^{19}F NMR (471 MHz) of **3e**
Solvent: DMSO-D_6 + $CDCl_3$
N
N
O
N
O
F
3e
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
-220
f1 (ppm)

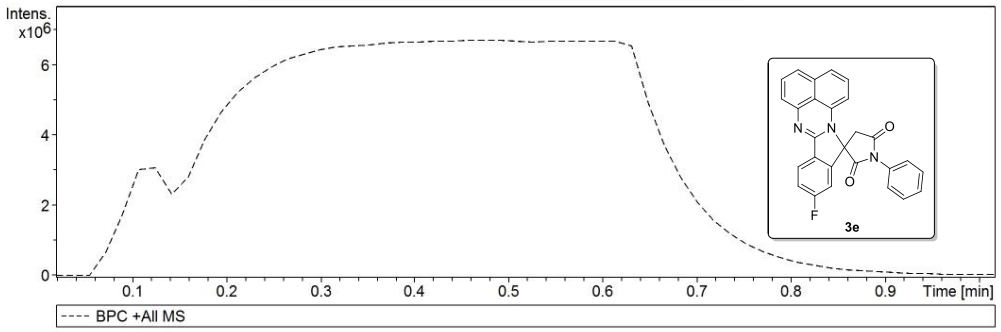
Display Report

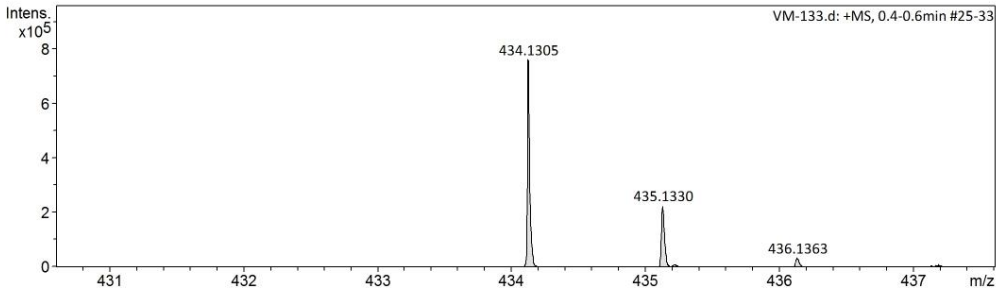
Analysis Info

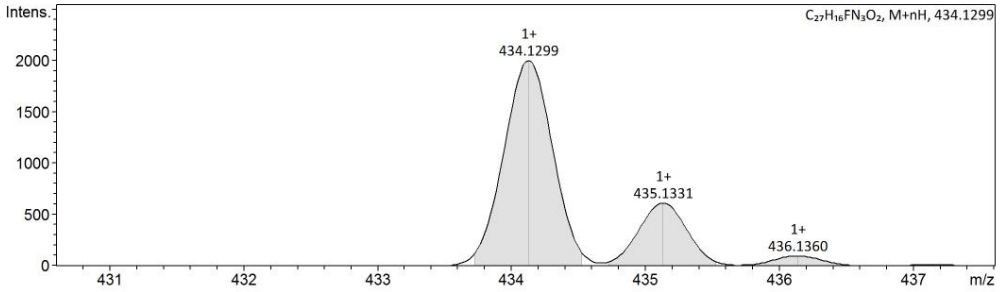
Analysis Name	D:\Data\user data\Dr. Lokman\17-04-2024\VM-133.d	Acquisition Date	4/17/2024 5:41:35 PM
Method	Tune_pos_Mid.m	Operator	vidhi
Sample Name	VM-133	Instrument	impact HD 1819696.00197
Comment			

Acquisition Parameter

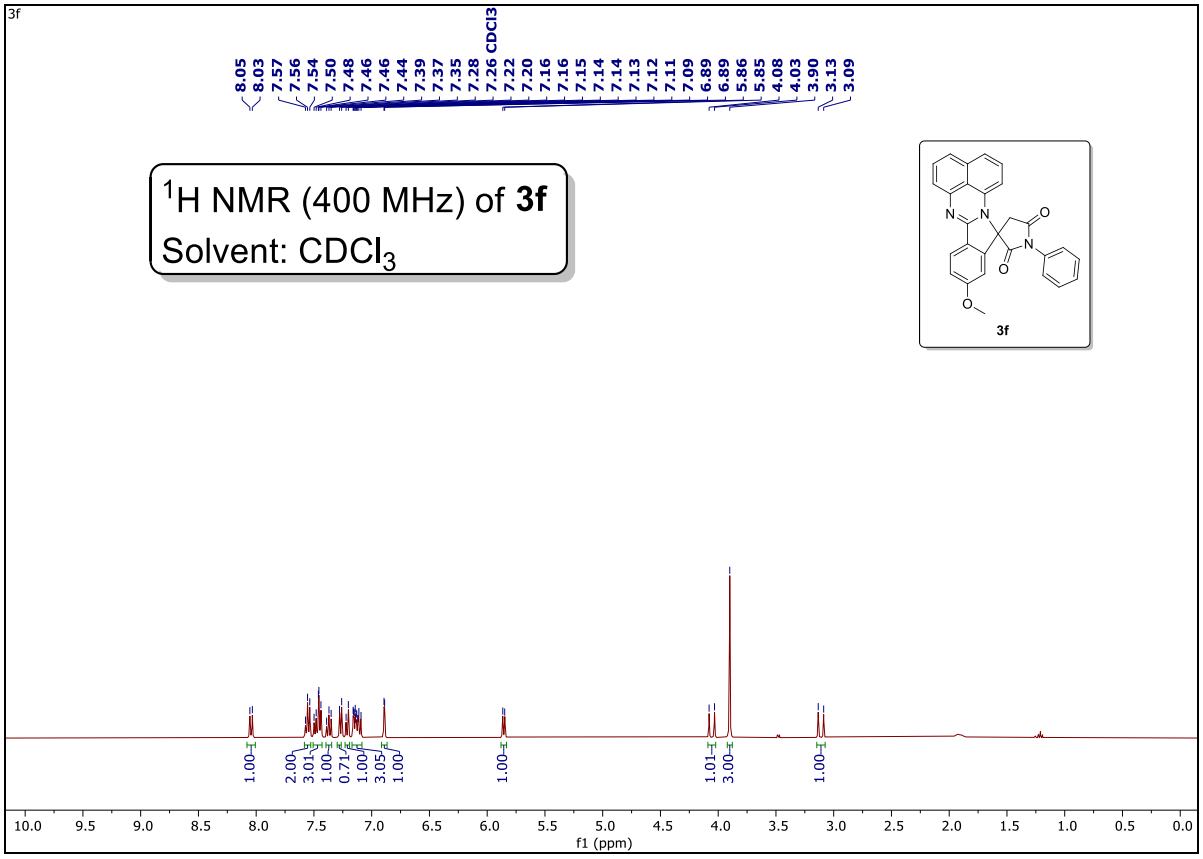
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	200 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 °C

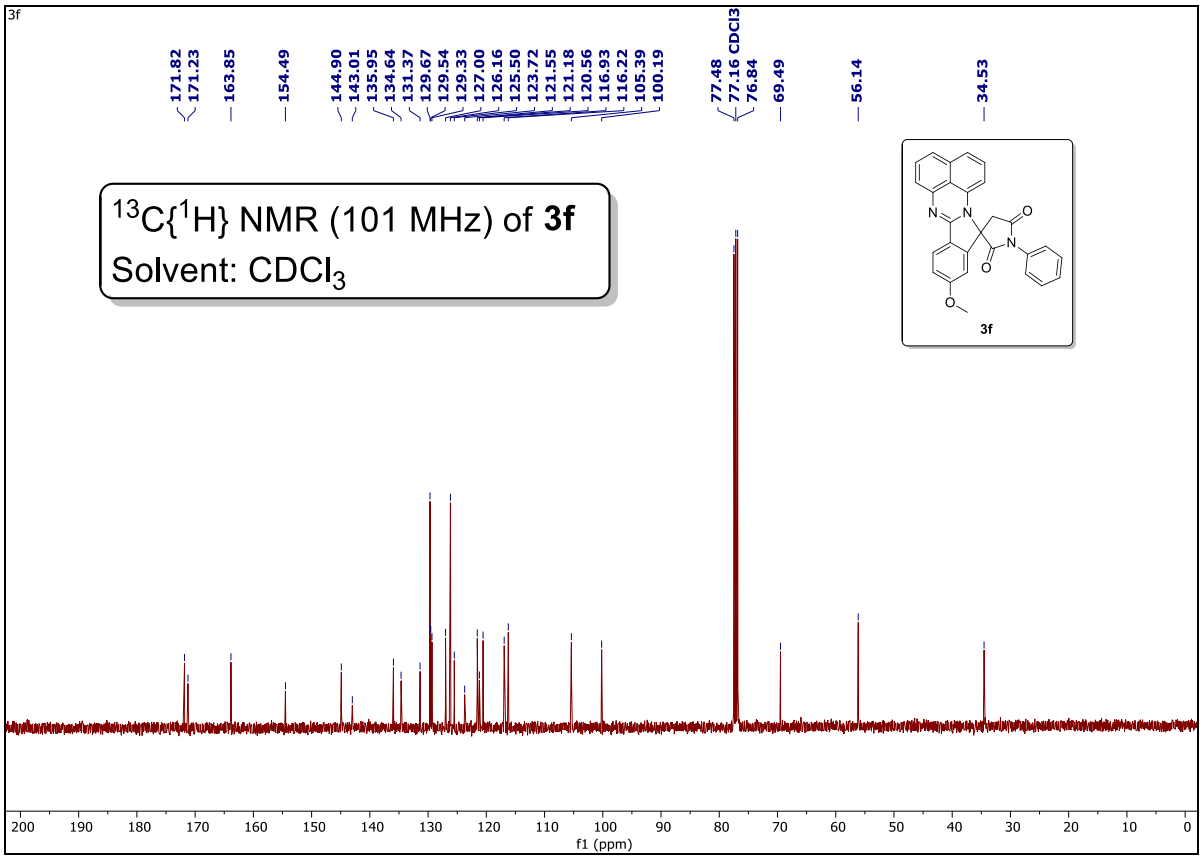






VM-133.d


3f
8.05
8.03
7.57
7.56
7.54
7.50
7.48
7.46
7.46
7.44
7.39
7.37
7.35
7.28
7.26 CDCl3
7.22
7.20
7.16
7.15
7.14
7.14
7.13
7.12
7.11
7.09
6.89
6.89
5.86
5.85
4.08
4.03
3.90
3.13
3.09
1H NMR (400 MHz) of 3f
Solvent: CDCl3
3f
1.00
2.00
3.01
1.00
0.71
1.00
3.05
1.00
1.00
1.01
3.00
1.00
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


3f
171.82
171.23
163.85
154.49
144.90
143.01
135.95
134.64
131.37
129.67
129.54
129.33
127.00
126.16
125.50
123.72
121.55
121.18
120.56
116.93
116.22
105.39
100.19
77.48
77.16 CDCl3
76.84
69.49
56.14
34.53
13C{1H} NMR (101 MHz) of 3f
Solvent: CDCl3
3f
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

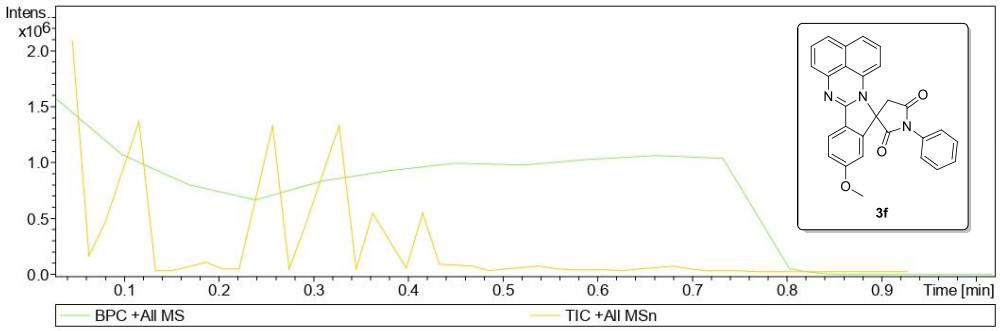
Display Report

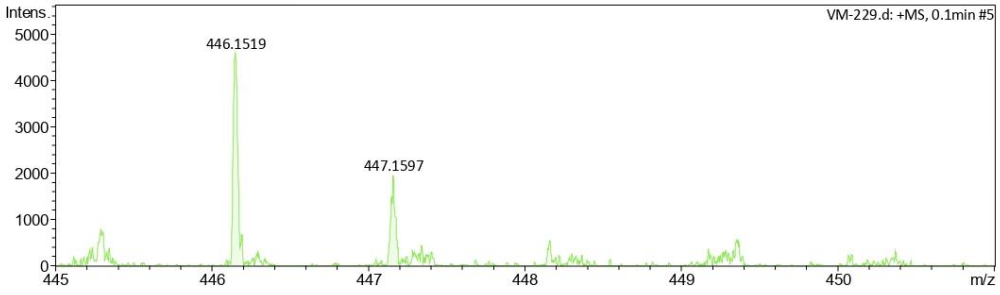
Analysis Info

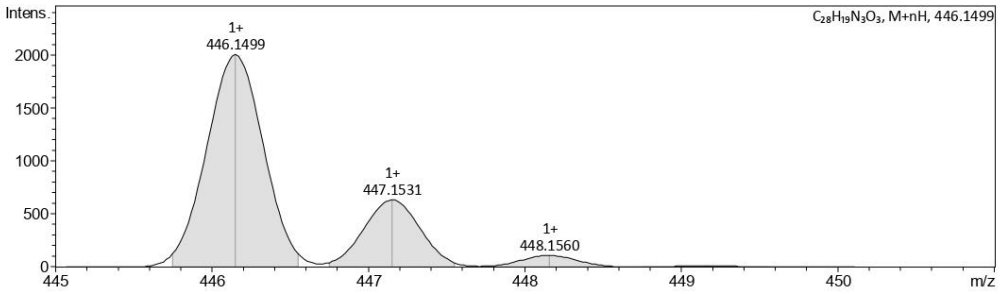
Analysis Name	D:\Data\user data\Dr. Lokman\14.03.2024\VM-229.d	Acquisition Date	3/14/2024 5:01:39 PM
Method	Tune_pos_Standard.m	Operator	vidhi
Sample Name	VM-229	Instrument	impact HD 1819696.00197
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 °C

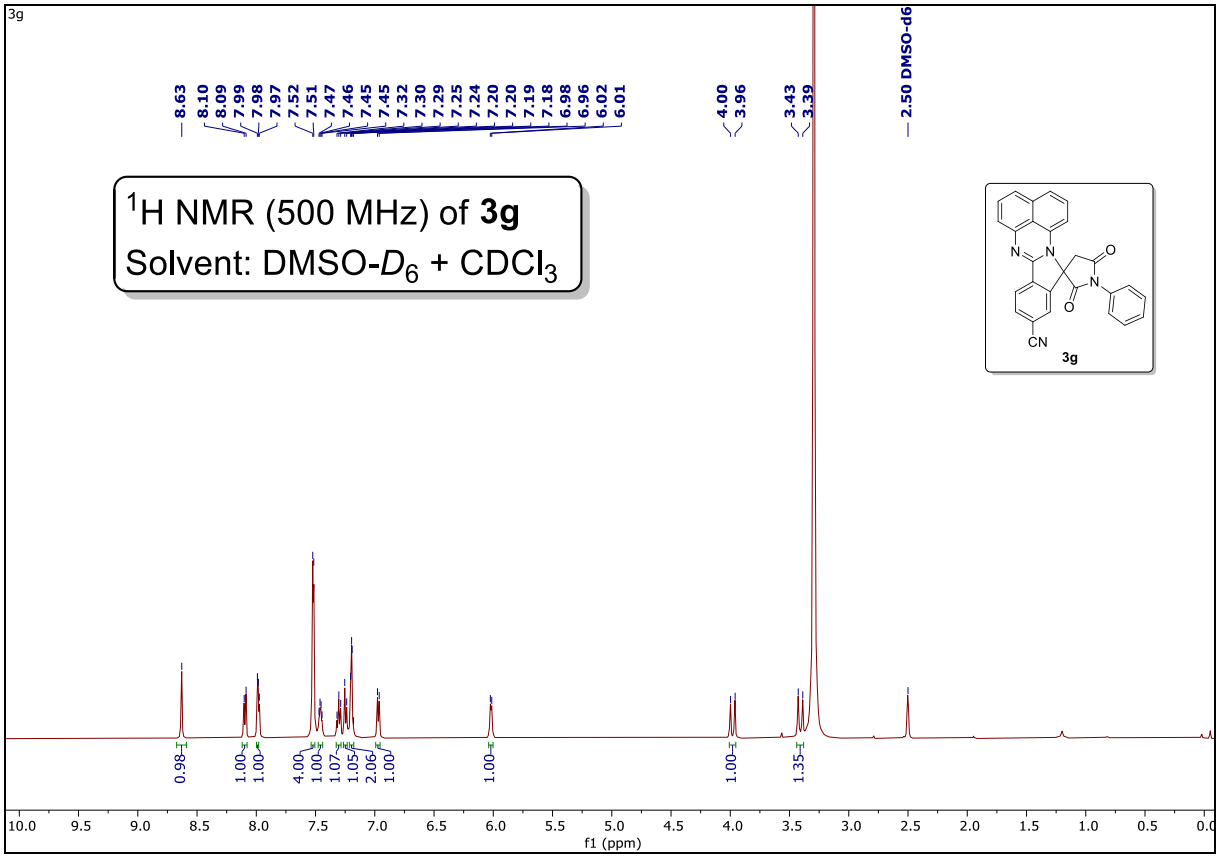


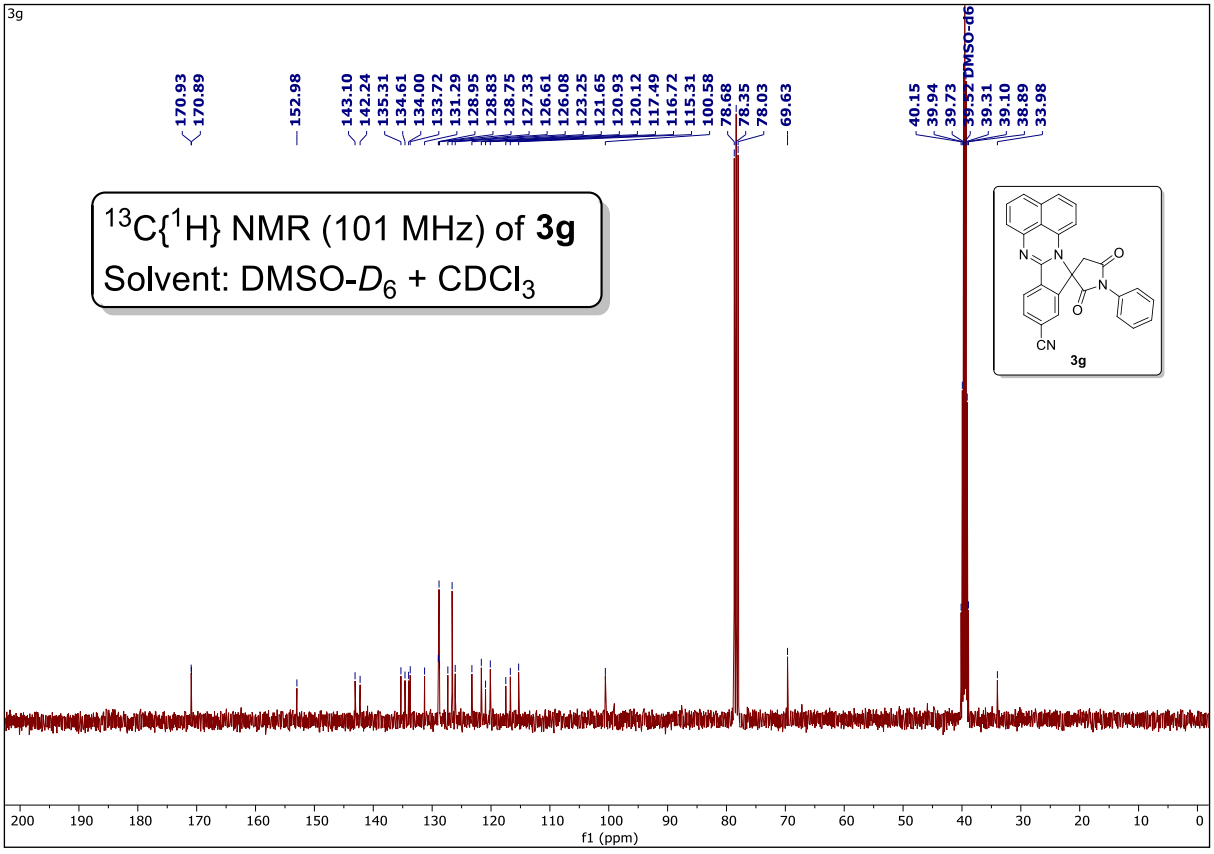




VM-229.d

Bruker Compass DataAnalysis 4.2 printed: 3/14/2024 5:14:22 PM by: vidhi Page 1 of 1


3g
8.63
8.10
8.09
7.99
7.98
7.97
7.52
7.51
7.47
7.46
7.45
7.45
7.32
7.30
7.29
7.25
7.24
7.20
7.20
7.19
7.18
6.98
6.96
6.02
6.01
4.00
3.96
3.43
3.39
2.50 DMSO-d6
^{1}H NMR (500 MHz) of **3g**
Solvent: DMSO-D_6 + $CDCl_3$
CN
3g
0.98
1.00
1.00
4.00
1.00
1.07
1.05
2.06
1.00
1.00
1.00
1.35
f1 (ppm)


3g
170.93
170.89
152.98
143.10
142.24
135.31
134.61
134.00
133.72
131.29
128.95
128.83
128.75
127.33
126.61
126.08
123.25
121.65
120.93
120.12
117.49
116.72
115.31
100.58
78.68
78.35
78.03
69.63
40.15
39.94
39.73
39.52 DMSO-d6
39.31
39.10
38.89
33.98
^{13}C{^{1}H} NMR (101 MHz) of **3g**
Solvent: DMSO-D_6 + $CDCl_3$
CN
3g
f1 (ppm)

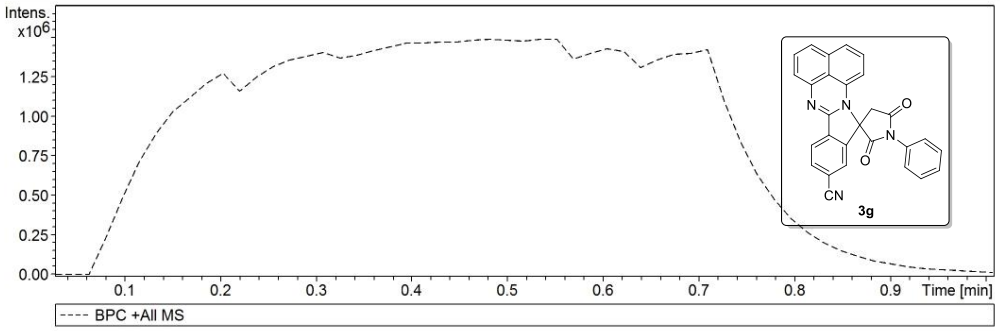
Display Report

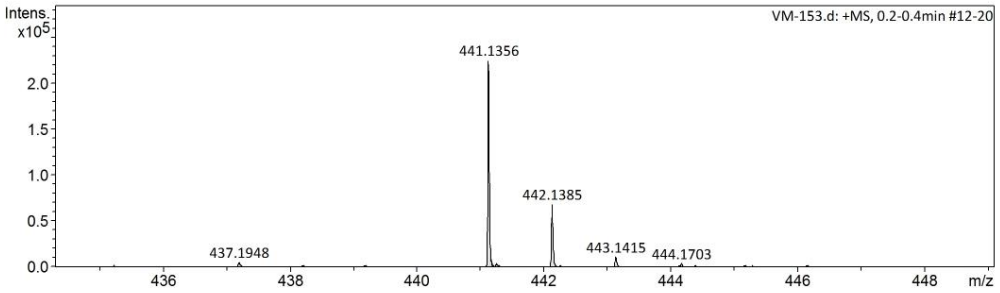
Analysis Info

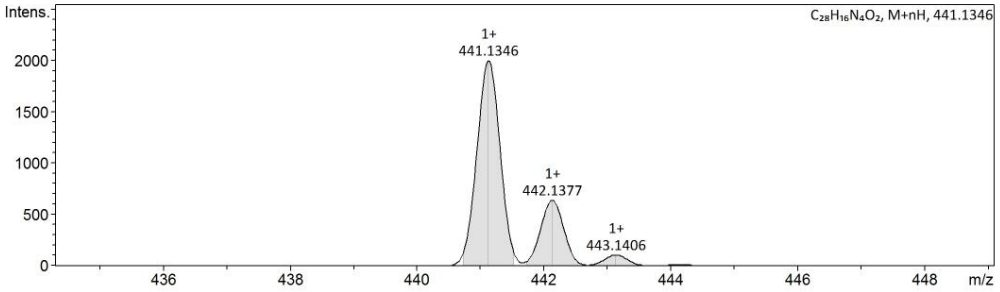
Analysis Name	D:\Data\user data\Dr. Lokman\17-04-2024\VM-153.d	Acquisition Date	4/17/2024 5:59:43 PM
Method	Tune_pos_Mid.m	Operator	vidhi
Sample Name	VM-153	Instrument	impact HD 1819696.00197
Comment			

Acquisition Parameter

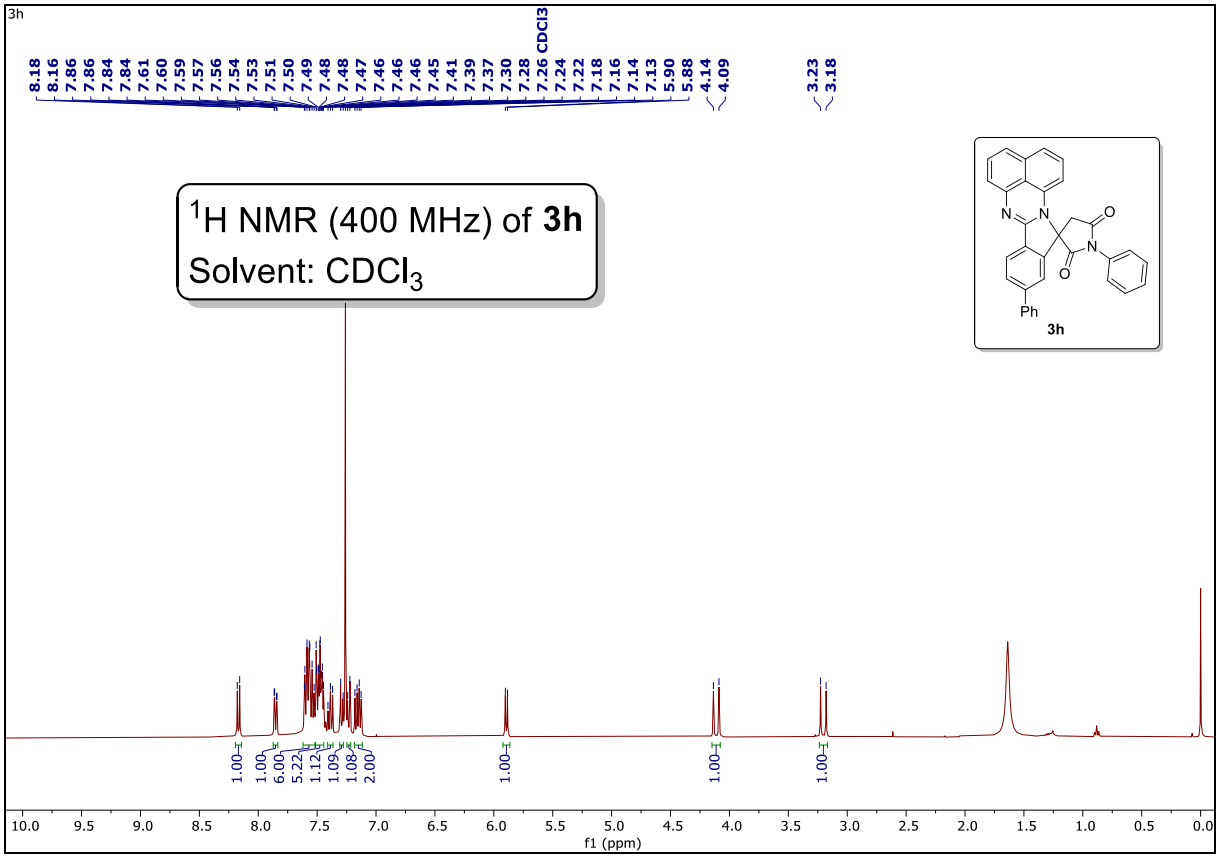
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	200 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 °C

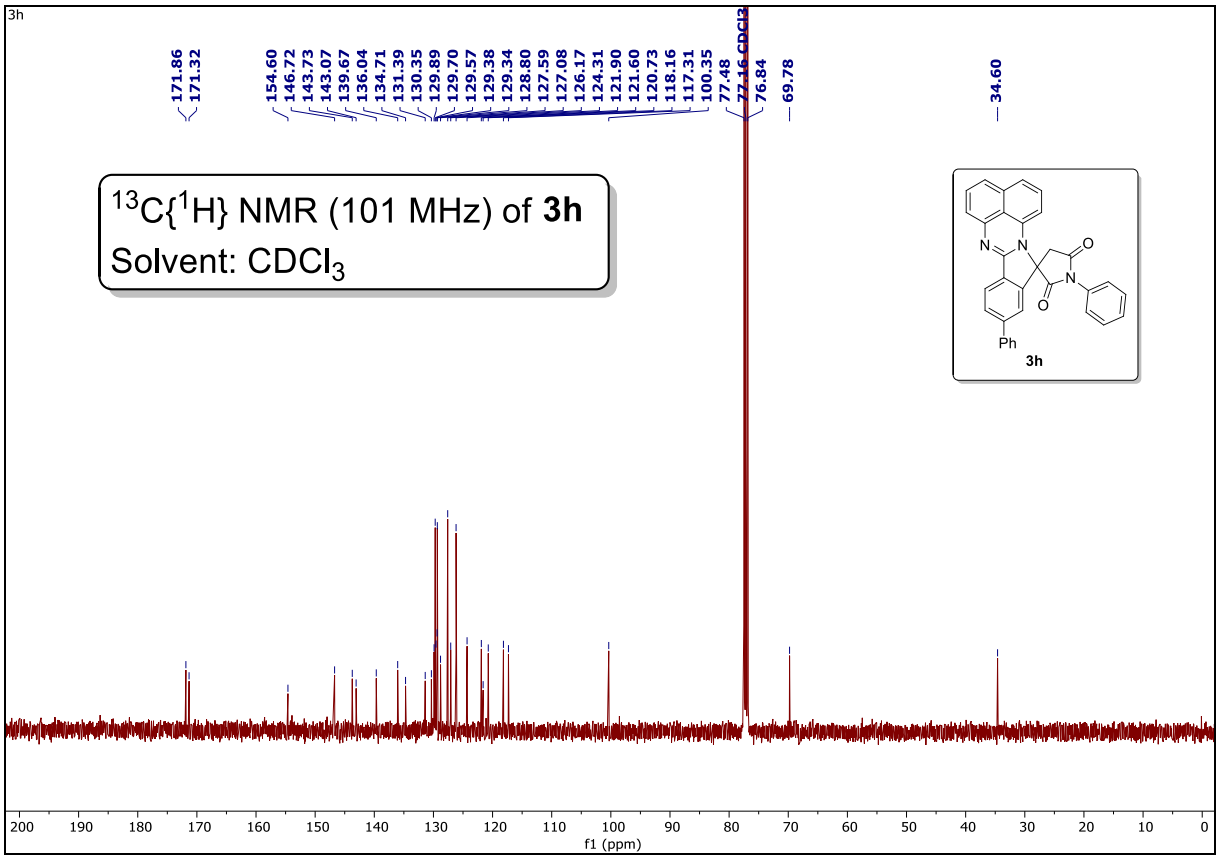


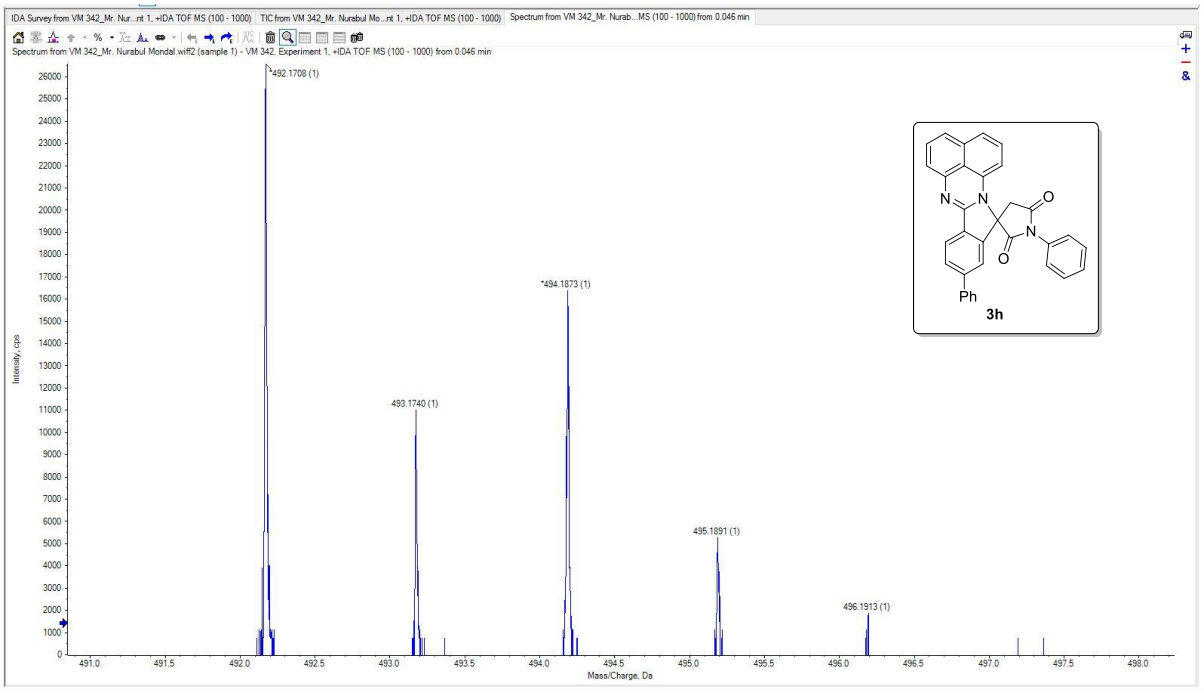


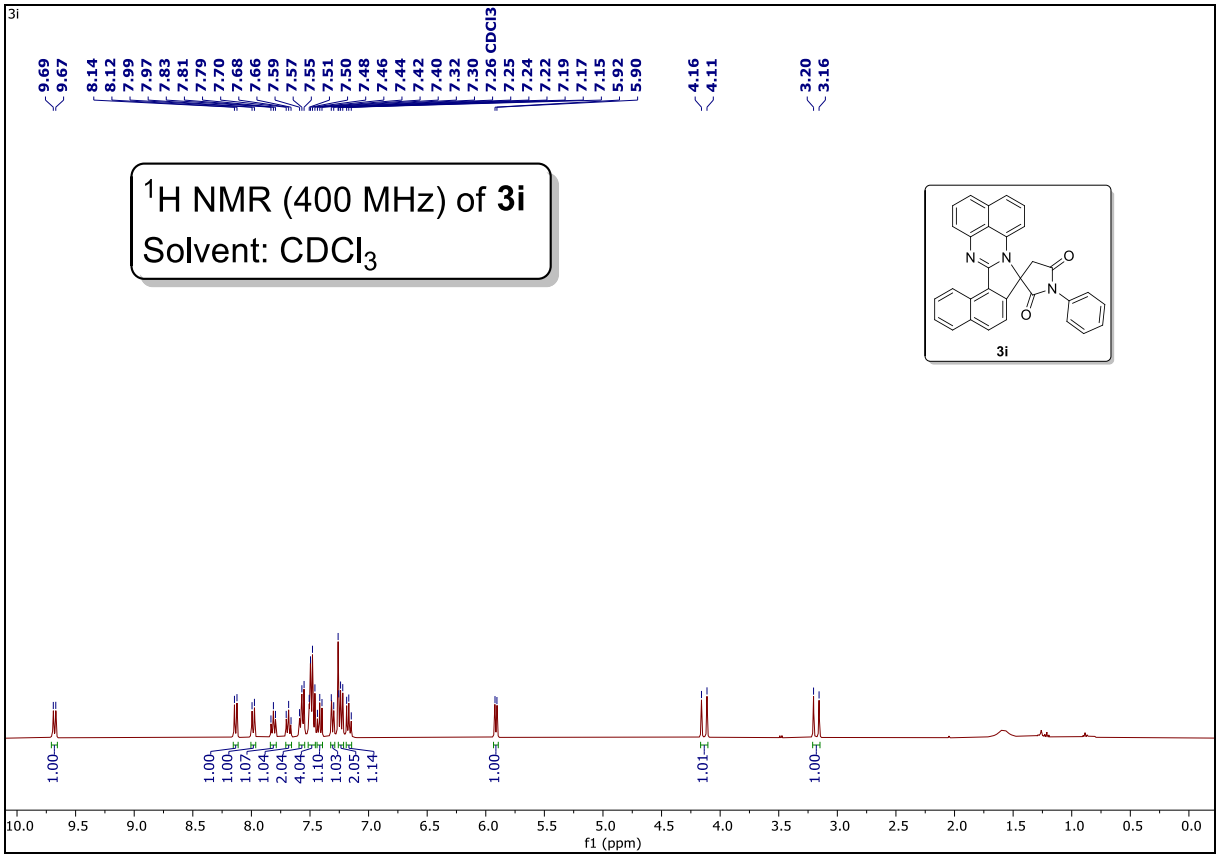


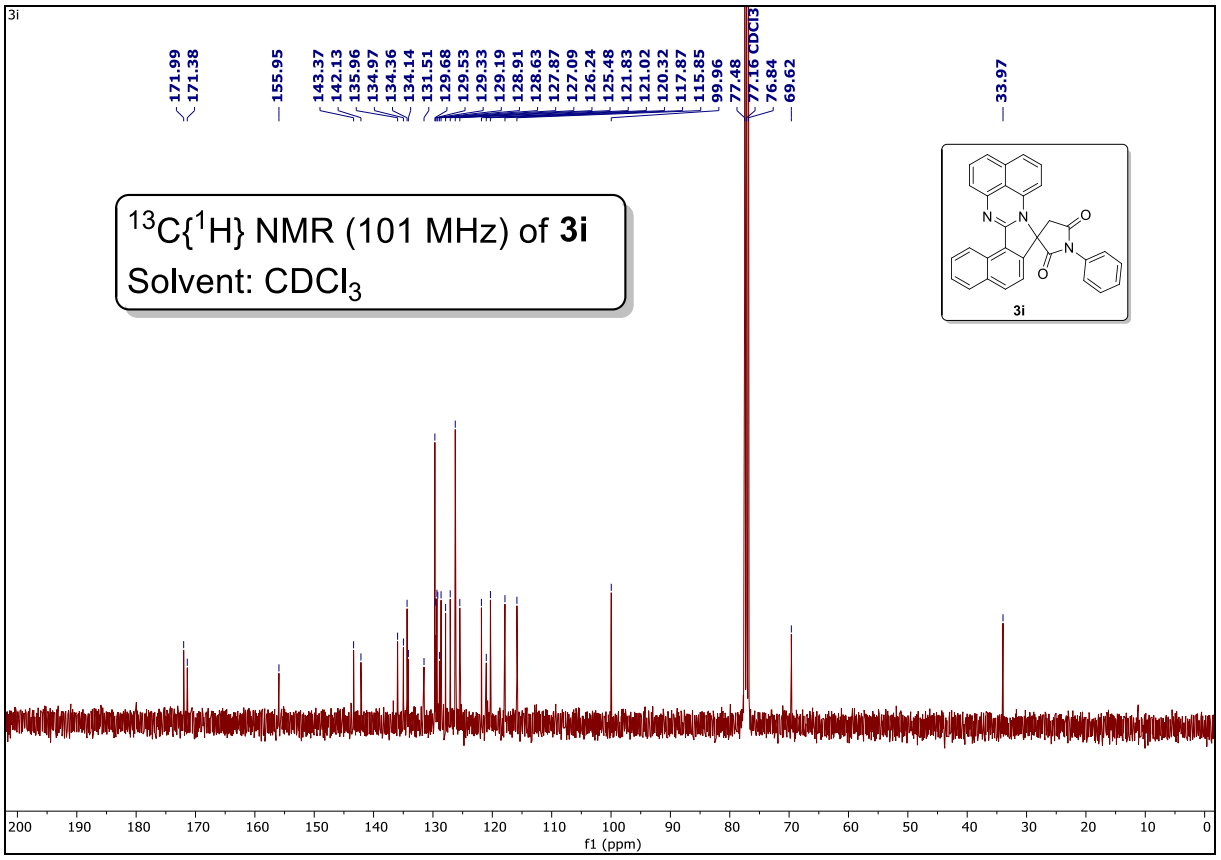
VM-153.d


3h
CDCl3
^{1}H NMR (400 MHz) of **3h**
Solvent: $CDCl_3$
Ph
3h
f1 (ppm)


3h
$^{13}C\{^{1}H\}$ NMR (101 MHz) of **3h**
Solvent: $CDCl_3$
Ph
3h
f1 (ppm)


IDA Survey from VM 342_Mr. Nur...nt 1, +IDA TOF MS (100 - 1000)
TIC from VM 342_Mr. Nurabul Mo...nt 1, +IDA TOF MS (100 - 1000)
Spectrum from VM 342_Mr. Nurab...MS (100 - 1000) from 0.046 min
Spectrum from VM 342_Mr. Nurabul Mondal.wiff2 (sample 1) - VM 342, Experiment 1, +IDA TOF MS (100 - 1000) from 0.046 min
492.1708 (1)
494.1873 (1)
493.1740 (1)
495.1891 (1)
496.1913 (1)
Intensity, cps
Mass/Charge, Da
N
N
O
N
O
Ph
3h


3i
9.69
9.67
8.14
8.12
7.99
7.97
7.83
7.81
7.79
7.70
7.68
7.66
7.59
7.57
7.55
7.51
7.50
7.48
7.46
7.44
7.42
7.40
7.32
7.30
7.26 CDCl3
7.25
7.24
7.22
7.19
7.17
7.15
5.92
5.90
4.16
4.11
3.20
3.16
1H NMR (400 MHz) of 3i
Solvent: CDCl3
3i
1.00
1.00
1.00
1.07
1.04
2.04
4.04
1.10
1.03
2.05
1.14
1.00
1.01
1.00
f1 (ppm)


3i
171.99
171.38
155.95
143.37
142.13
135.96
134.97
134.36
134.14
131.51
129.68
129.53
129.33
129.19
128.91
128.63
127.87
127.09
126.24
125.48
121.83
121.02
120.32
117.87
115.85
99.96
77.48
77.16 CDCl3
76.84
69.62
33.97
13C{1H} NMR (101 MHz) of 3i
Solvent: CDCl3
3i
f1 (ppm)

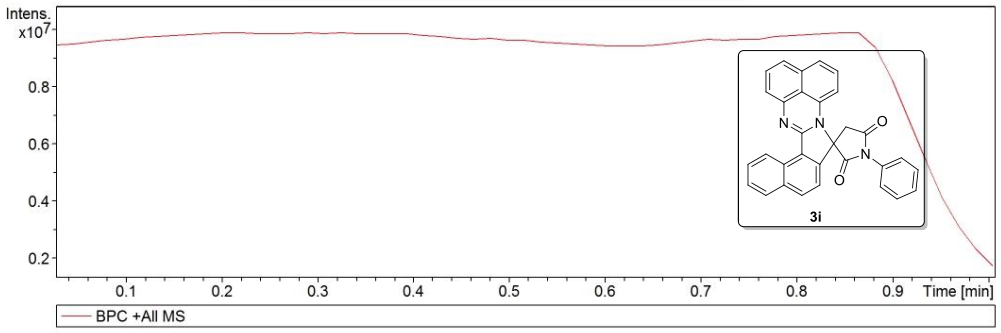
Display Report

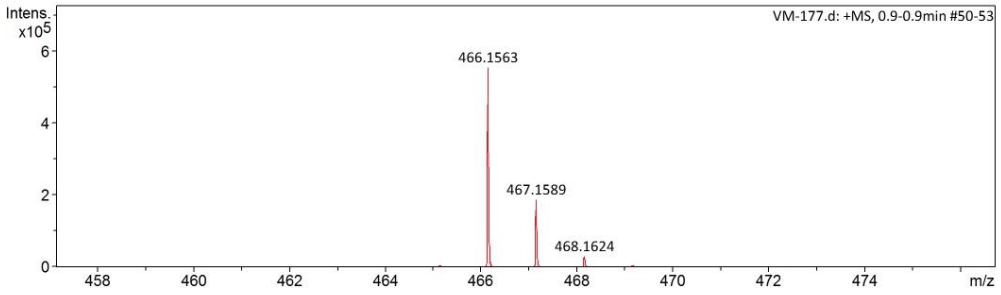
Analysis Info

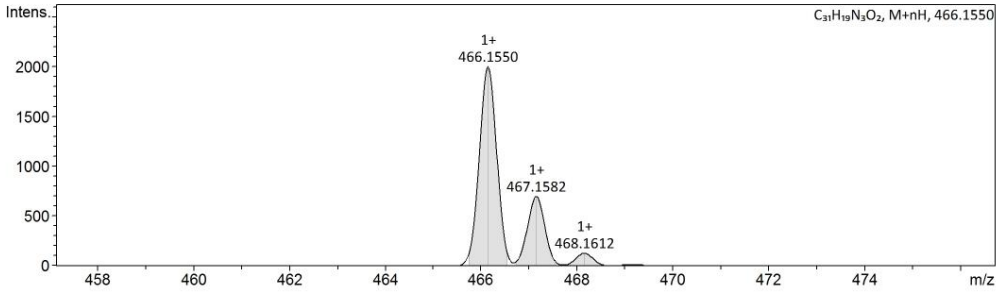
Analysis Name	D:\Data\user data\Dr. Lokman\16-04-2024\VM-177.d	Acquisition Date	4/16/2024 11:15:30 AM
Method	Tune_pos_Mid.m	Operator	vidhi
Sample Name	VM-177	Instrument	impact HD 1819696.00197
Comment			

Acquisition Parameter

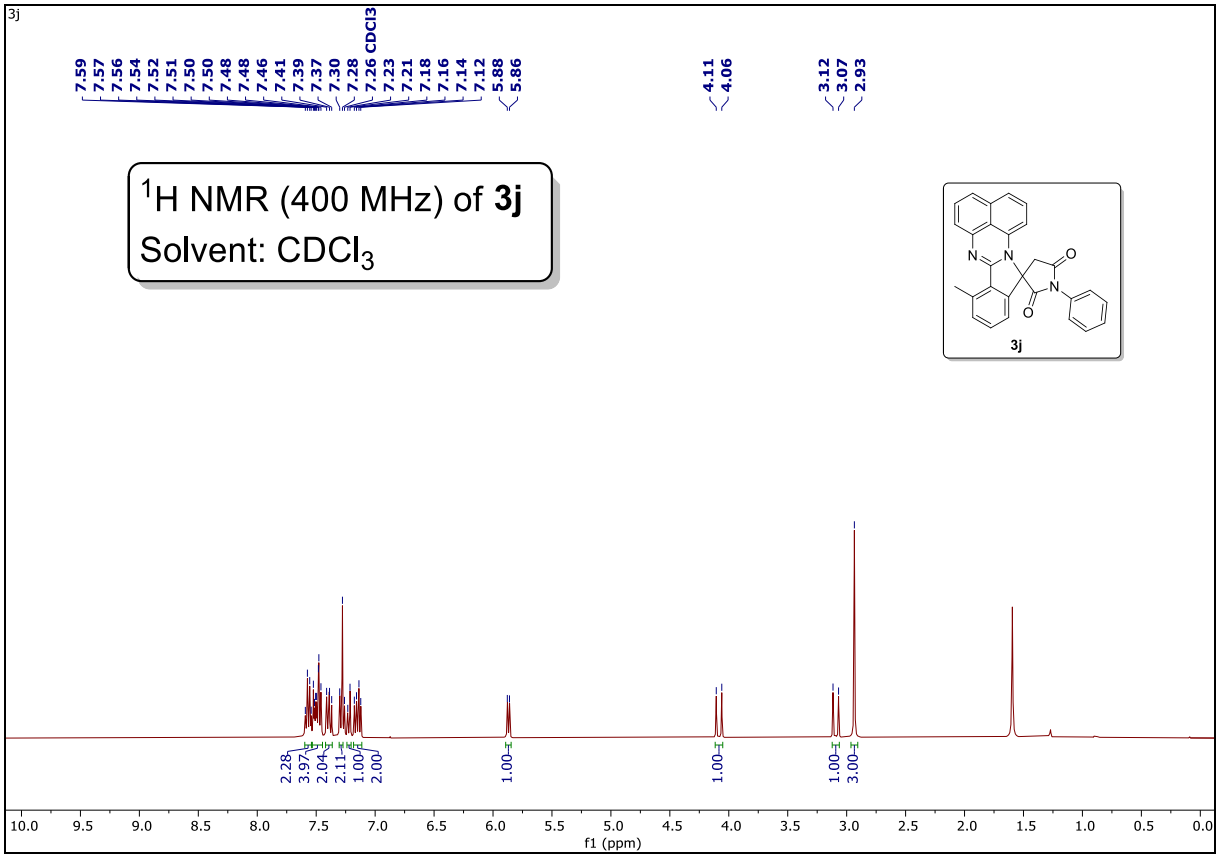
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	219 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 °C

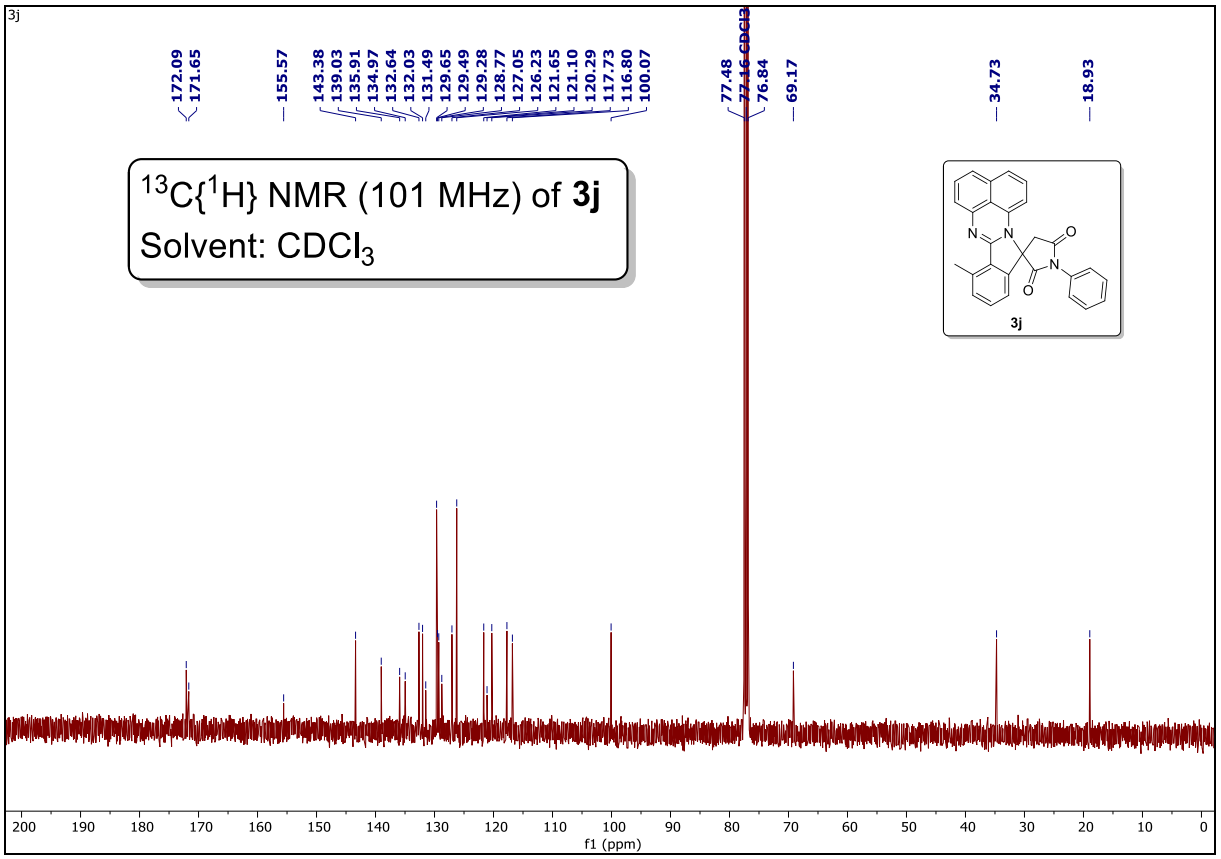






VM-177.d


3j
7.59
7.57
7.56
7.54
7.52
7.51
7.50
7.50
7.48
7.48
7.46
7.41
7.39
7.37
7.30
7.28
7.26 CDCl3
7.23
7.21
7.18
7.16
7.14
7.12
5.88
5.86
4.11
4.06
3.12
3.07
2.93
1H NMR (400 MHz) of 3j
Solvent: CDCl3
3j
2.28
3.97
2.04
2.11
1.00
2.00
1.00
1.00
1.00
3.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


3j
172.09
171.65
155.57
143.38
139.03
135.91
134.97
132.64
132.03
131.49
129.65
129.49
129.28
128.77
127.05
126.23
121.65
121.10
120.29
117.73
116.80
100.07
77.48
77.16 CDCl3
76.84
69.17
34.73
18.93
13C{1H} NMR (101 MHz) of 3j
Solvent: CDCl3
3j
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

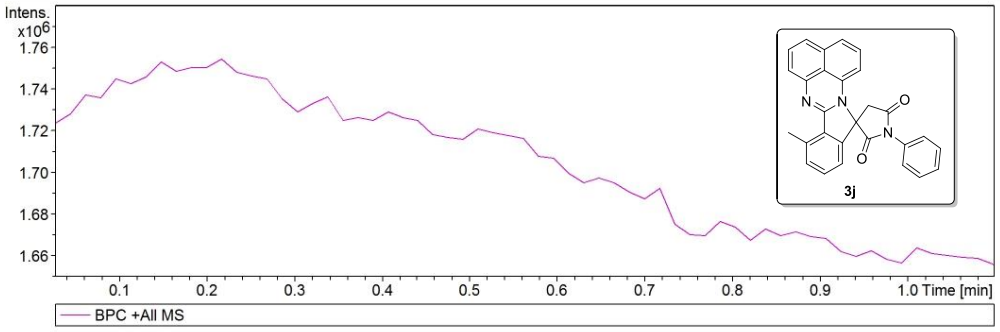
Display Report

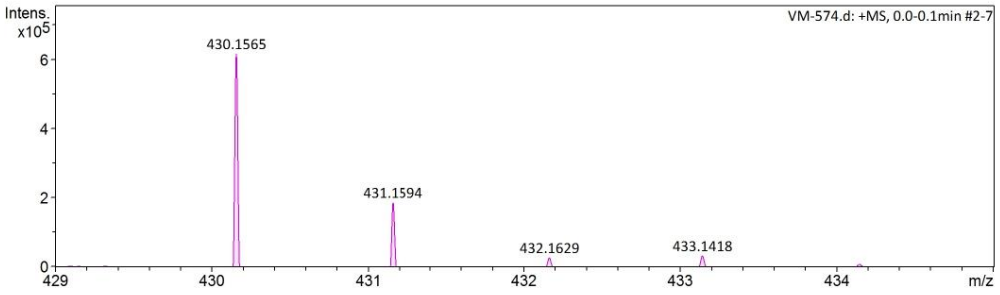
Analysis Info

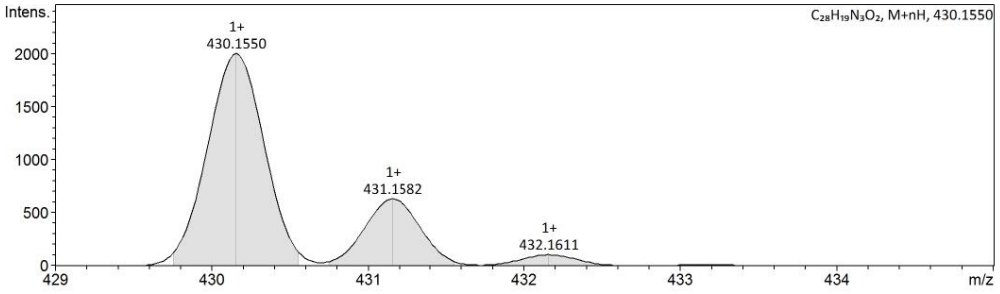
Analysis Name	D:\Data\user data\Dr. Lokman\18-02-2025\VM-574.d	Acquisition Date	2/18/2025 1:03:50 PM
Method	low_mass.m	Operator	Gudipati SrinivasaRao
Sample Name	VM-574	Instrument	impact HD 1819696.00197
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.6 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	5.0 l/min
Scan End	1500 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C

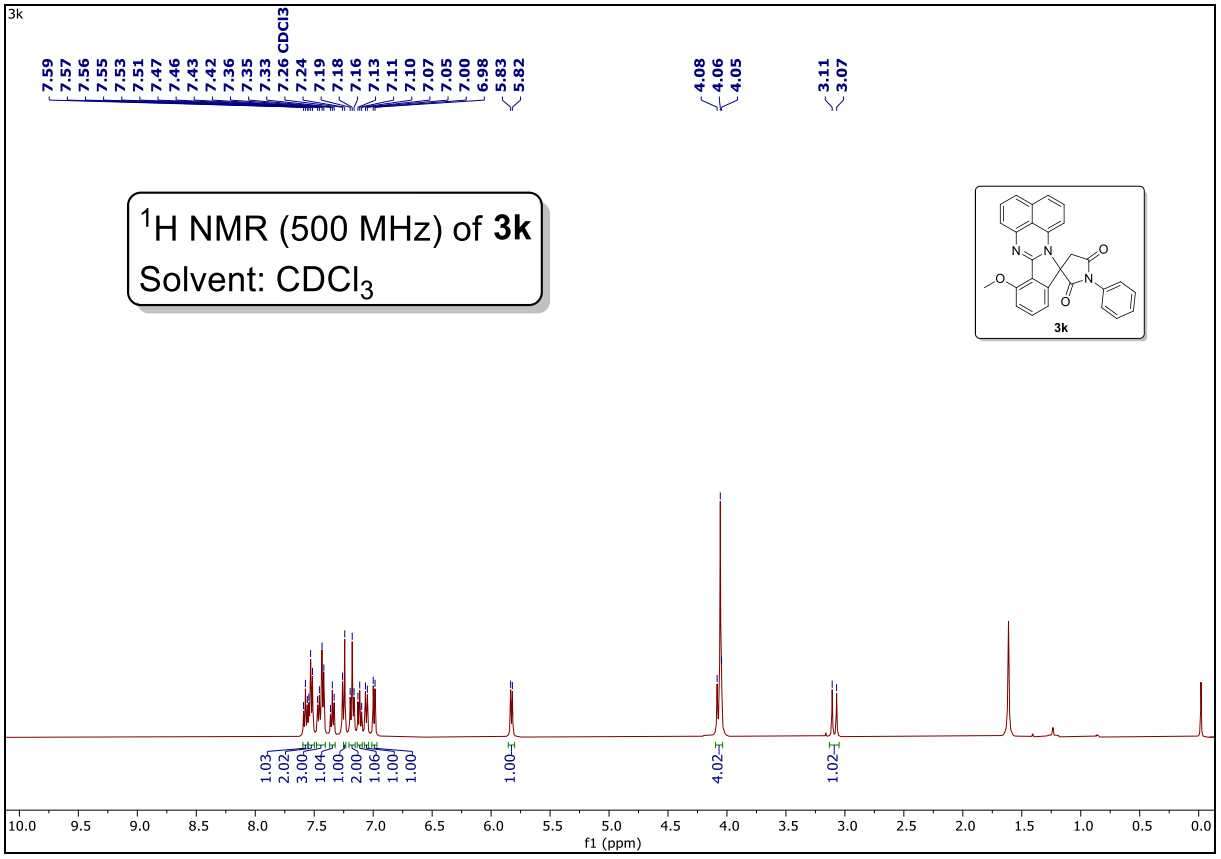


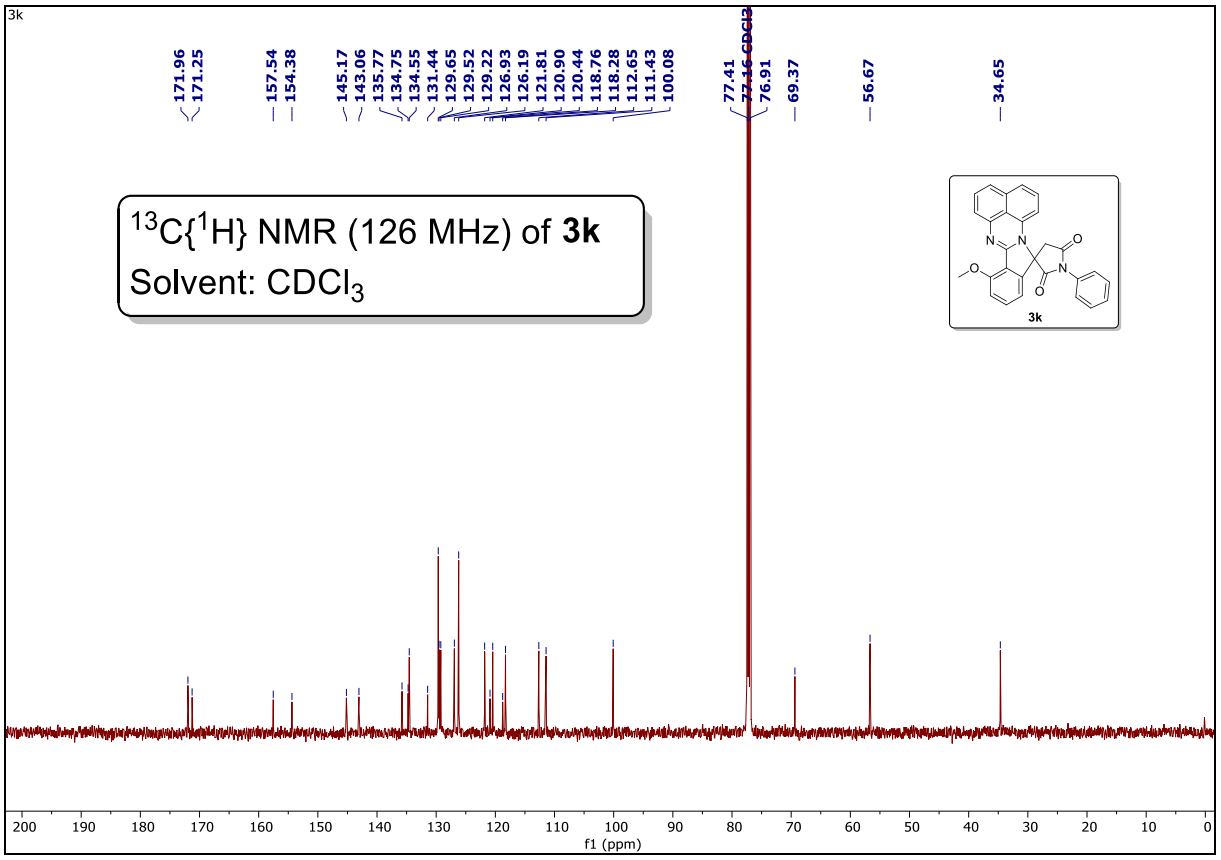




VM-574.d

Gudipati


3k
7.59
7.57
7.56
7.55
7.53
7.51
7.47
7.46
7.43
7.42
7.36
7.35
7.33
7.26 CDCl3
7.24
7.19
7.18
7.16
7.13
7.11
7.10
7.07
7.05
7.00
6.98
5.83
5.82
4.08
4.06
4.05
3.11
3.07
1H NMR (500 MHz) of 3k
Solvent: CDCl3
3k
1.03
2.02
3.00
1.04
1.00
2.00
1.06
1.00
1.00
1.00
4.02
1.02
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


3k
171.96
171.25
157.54
154.38
145.17
143.06
135.77
134.75
134.55
131.44
129.65
129.52
129.22
126.93
126.19
121.81
120.90
120.44
118.76
118.28
112.65
111.43
100.08
77.41
77.16 CDCl3
76.91
69.37
56.67
34.65
13C{1H} NMR (126 MHz) of 3k
Solvent: CDCl3
3k
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

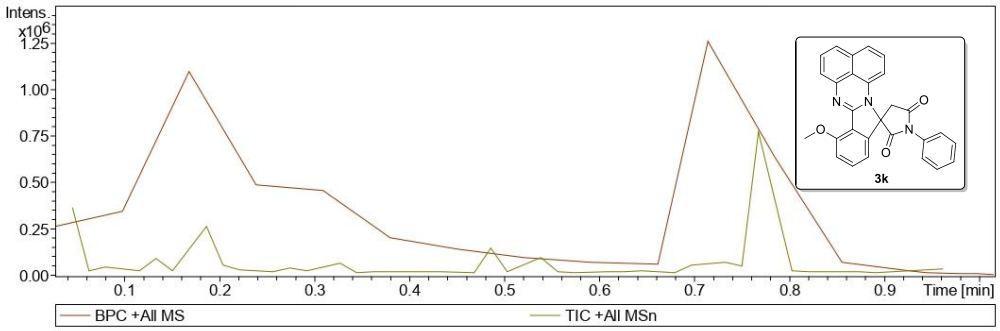
Display Report

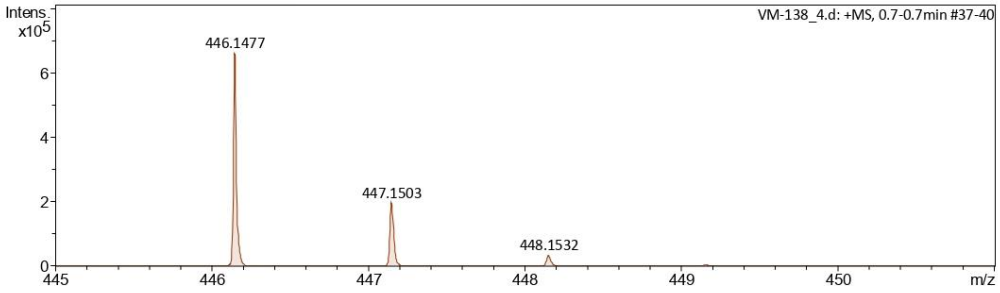
Analysis Info

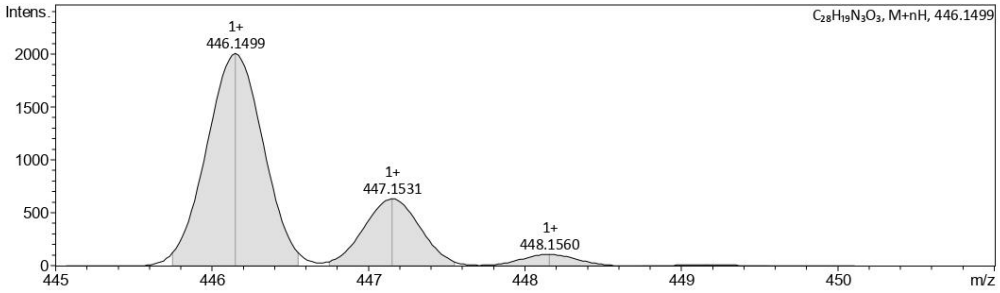
Analysis Name	D:\Data\user data\Dr. Lokman\14.03.2024\VM-138_4.d	Acquisition Date	3/14/2024 4:20:02 PM
Method	Tune_pos_Standard.m	Operator	vidhi
Sample Name	VM-138_4	Instrument	impact HD 1819696.00197
Comment			

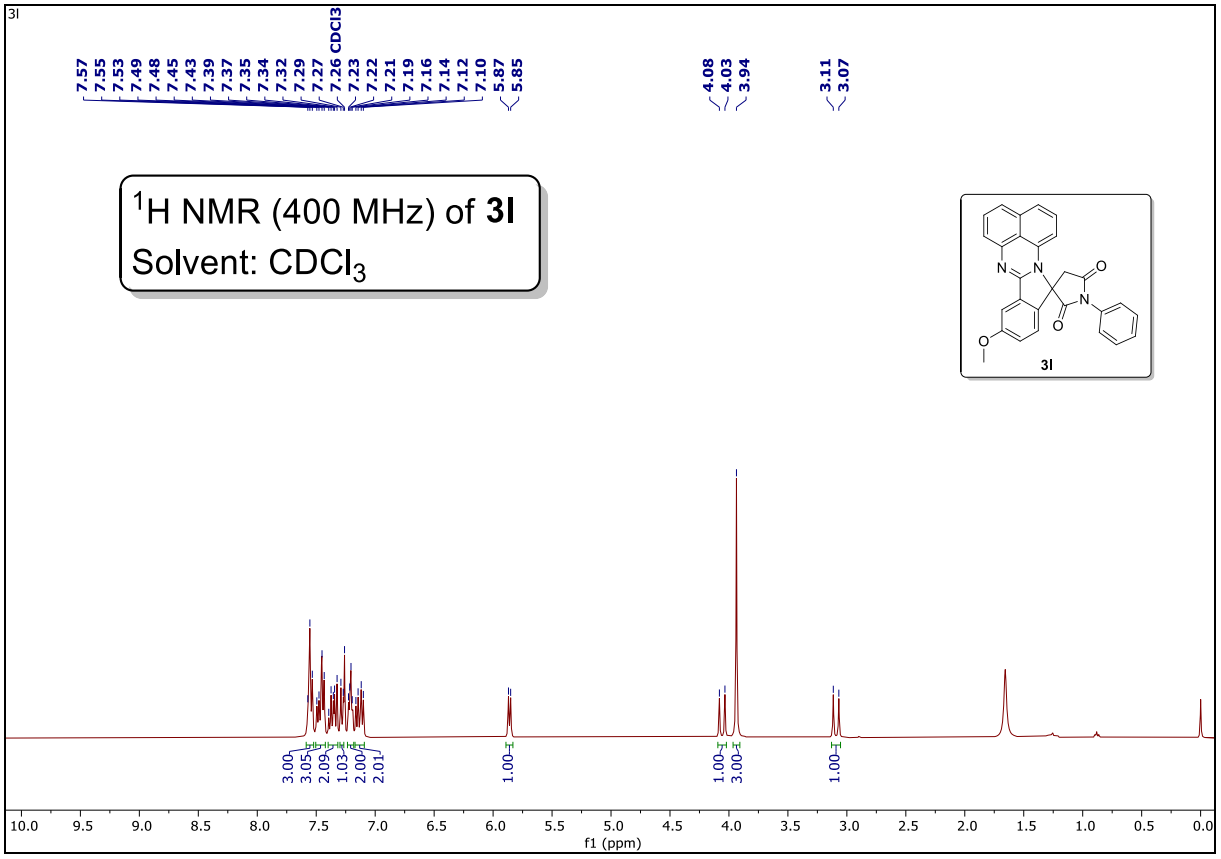
Acquisition Parameter

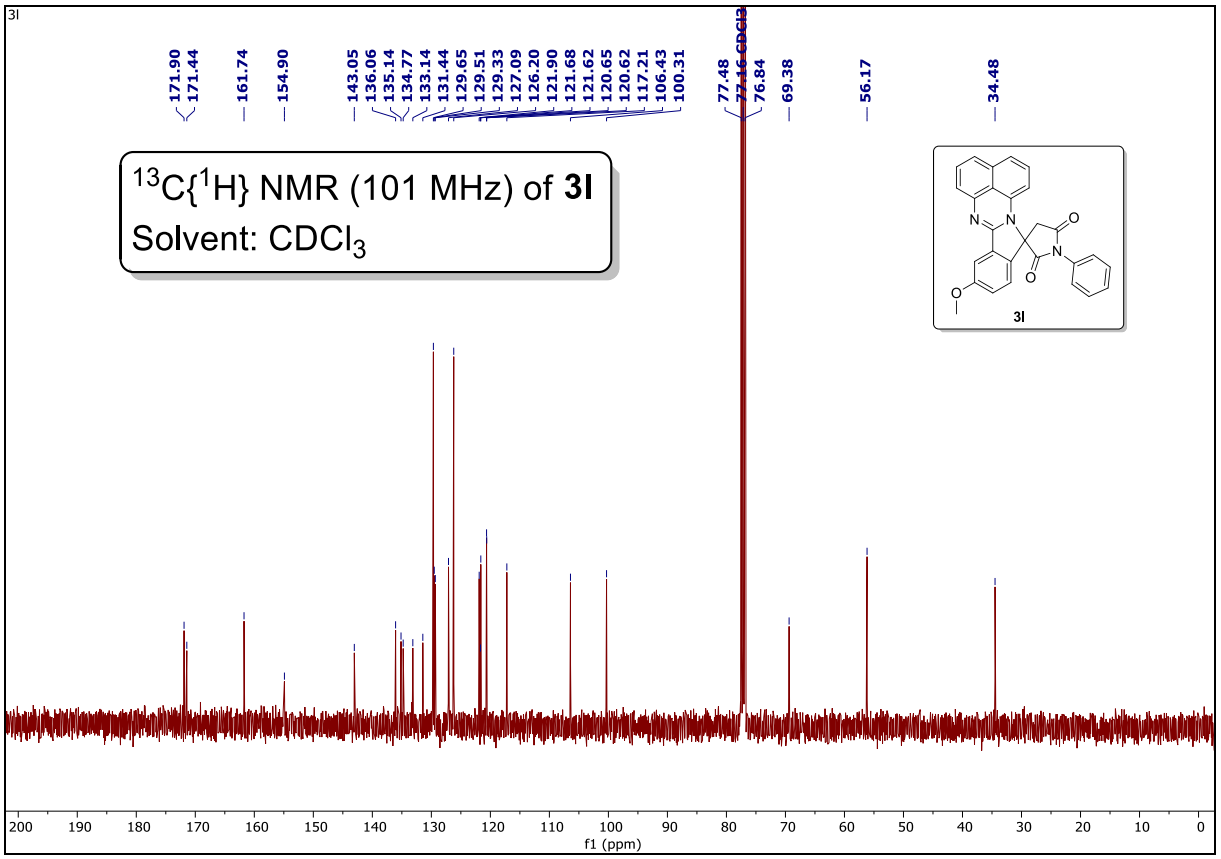
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.7 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 °C








3l
7.57
7.55
7.53
7.49
7.48
7.45
7.43
7.39
7.37
7.35
7.34
7.32
7.29
7.27
7.26 CDCl3
7.23
7.22
7.21
7.19
7.16
7.14
7.12
7.10
5.87
5.85
4.08
4.03
3.94
3.11
3.07
^{1}H NMR (400 MHz) of **3l**
Solvent: $CDCl_3$
3l
3.00
3.05
2.09
1.03
2.00
2.01
1.00
1.00
3.00
1.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


3l
171.90
171.44
161.74
154.90
143.05
136.06
135.14
134.77
133.14
131.44
129.65
129.51
129.33
127.09
126.20
121.90
121.68
121.62
120.65
120.62
117.21
106.43
100.31
77.48
77.16 CDCl3
76.84
69.38
56.17
34.48
^{13}C{^{1}H} NMR (101 MHz) of **3l**
Solvent: $CDCl_3$
3l
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

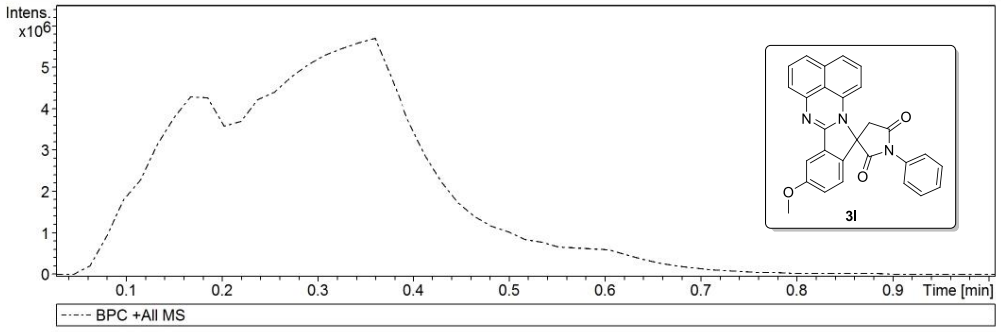
Display Report

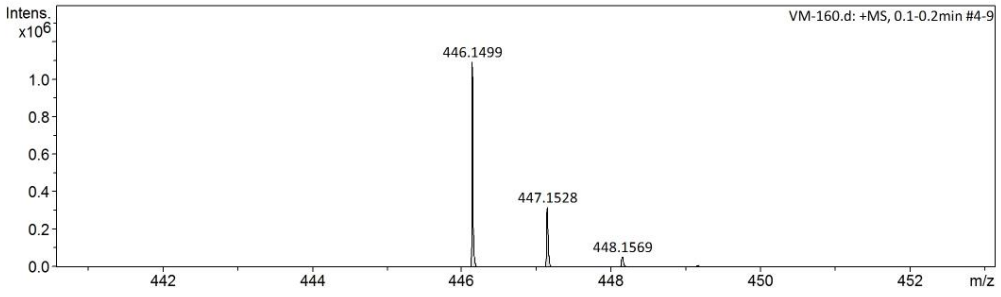
Analysis Info

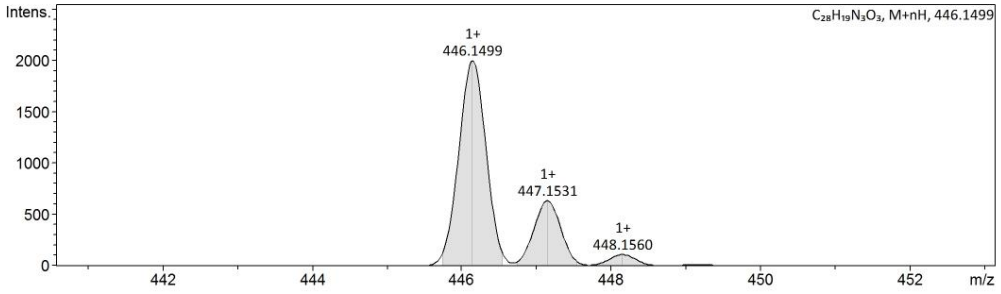
Analysis Name	D:\Data\user data\Dr. Lokman\17-04-2024\VM-160.d	Acquisition Date	4/17/2024 5:54:40 PM
Method	Tune_pos_Mid.m	Operator	vidhi
Sample Name	VM-160	Instrument	impact HD 1819696.00197
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	200 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 °C

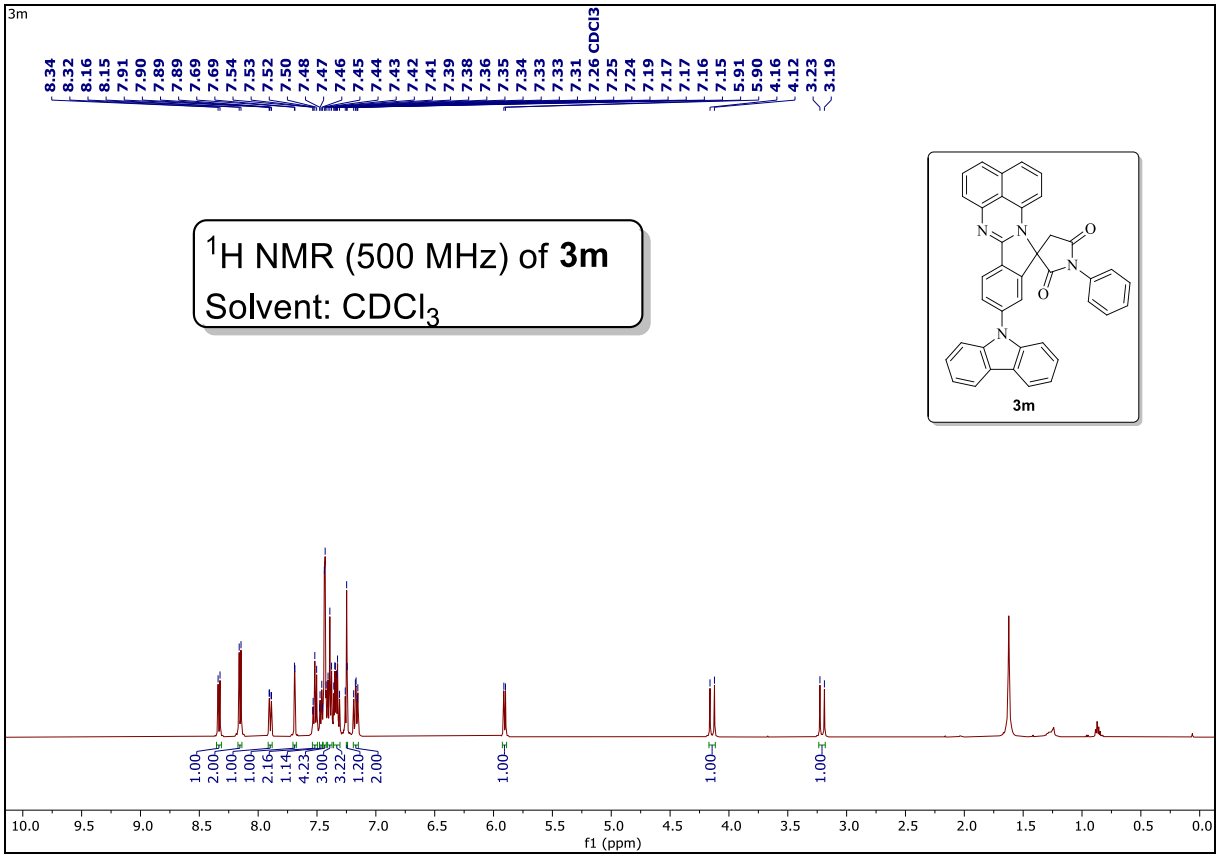


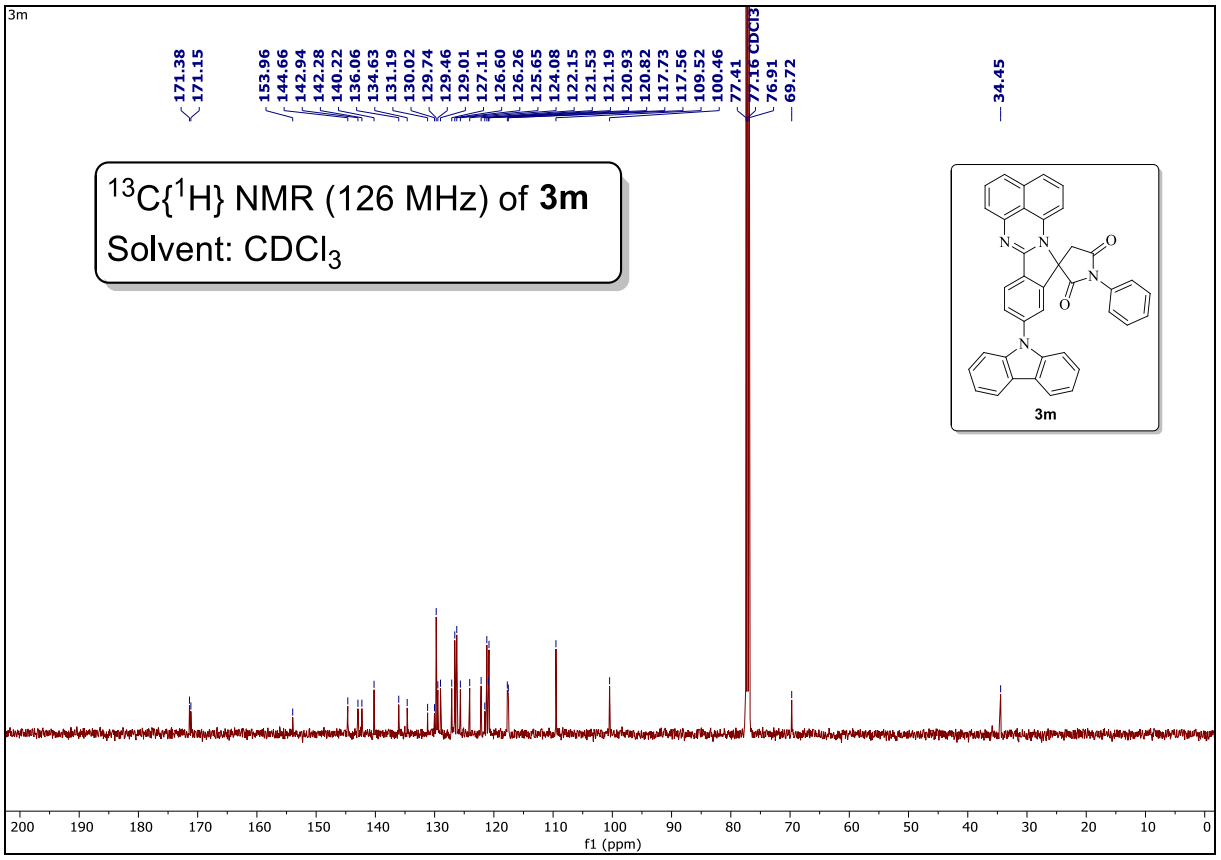




VM-160.d

Bruker Compass DataAnalysis 4.2 printed: 4/17/2024 5:56:56 PM by: vidhi Page 1 of 1


3m
8.34 8.32 8.16 8.15 7.91 7.90 7.89 7.89 7.69 7.69 7.54 7.53 7.52 7.50 7.48 7.47 7.46 7.45 7.44 7.43 7.42 7.41 7.39 7.38 7.36 7.35 7.34 7.33 7.33 7.31 7.26 CDCl3 7.25 7.24 7.19 7.17 7.17 7.16 7.15 5.91 5.90 4.16 4.12 3.23 3.19
1H NMR (500 MHz) of 3m
Solvent: CDCl3
3m
1.00 2.00 1.00 1.00 2.16 1.14 4.23 3.00 3.22 1.20 2.00 1.00 1.00 1.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


3m
171.38 171.15 153.96 144.66 142.94 142.28 140.22 136.06 134.63 131.19 130.02 129.74 129.46 129.01 127.11 126.60 126.26 125.65 124.08 122.15 121.53 121.19 120.93 120.82 117.73 117.56 109.52 100.46 77.41 77.16 CDCl3 76.91 69.72 34.45
13C{1H} NMR (126 MHz) of 3m
Solvent: CDCl3
3m
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

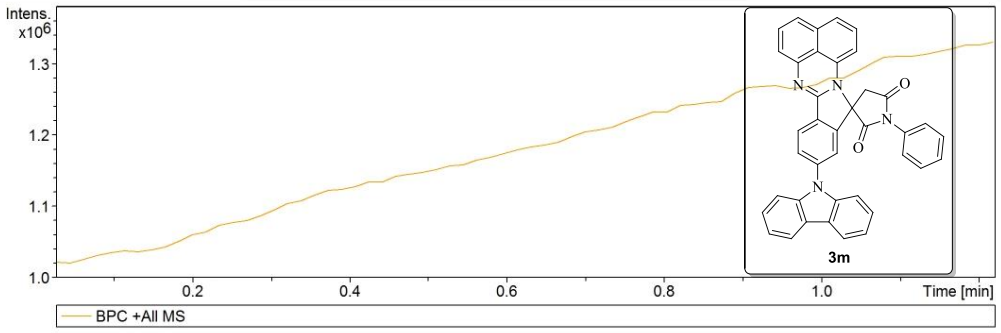
Display Report

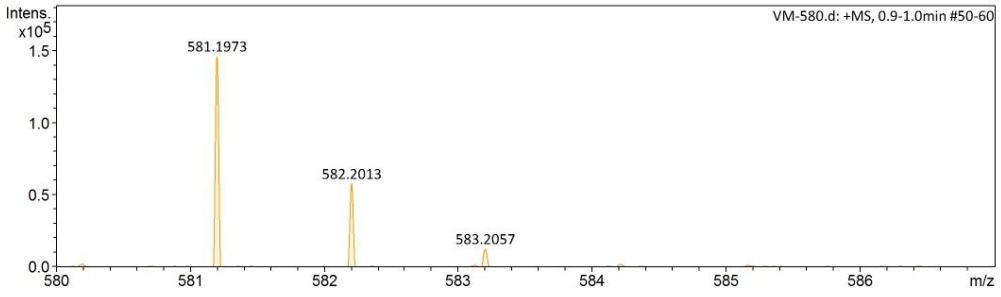
Analysis Info

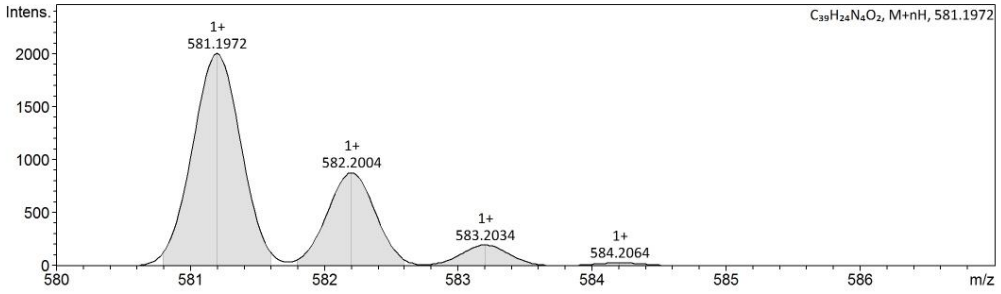
Analysis Name	D:\Data\user data\Dr. Lokman\24-02-2025\VM-580.d	Acquisition Date	2/24/2025 11:53:27 AM
Method	low_mass.m	Operator	Gudipati SrinivasaRao
Sample Name	VM-580	Instrument	impact HD 1819696.00197
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.6 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	5.0 l/min
Scan End	1500 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C

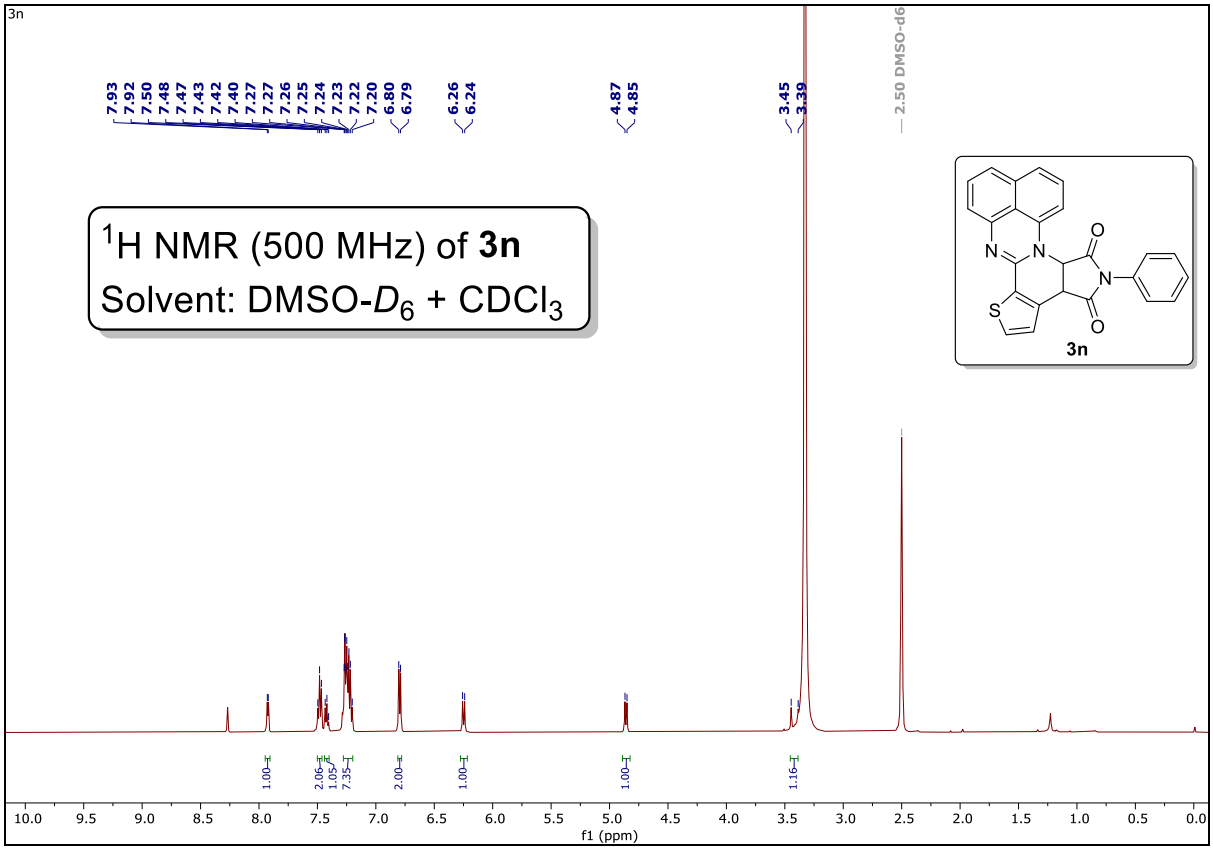


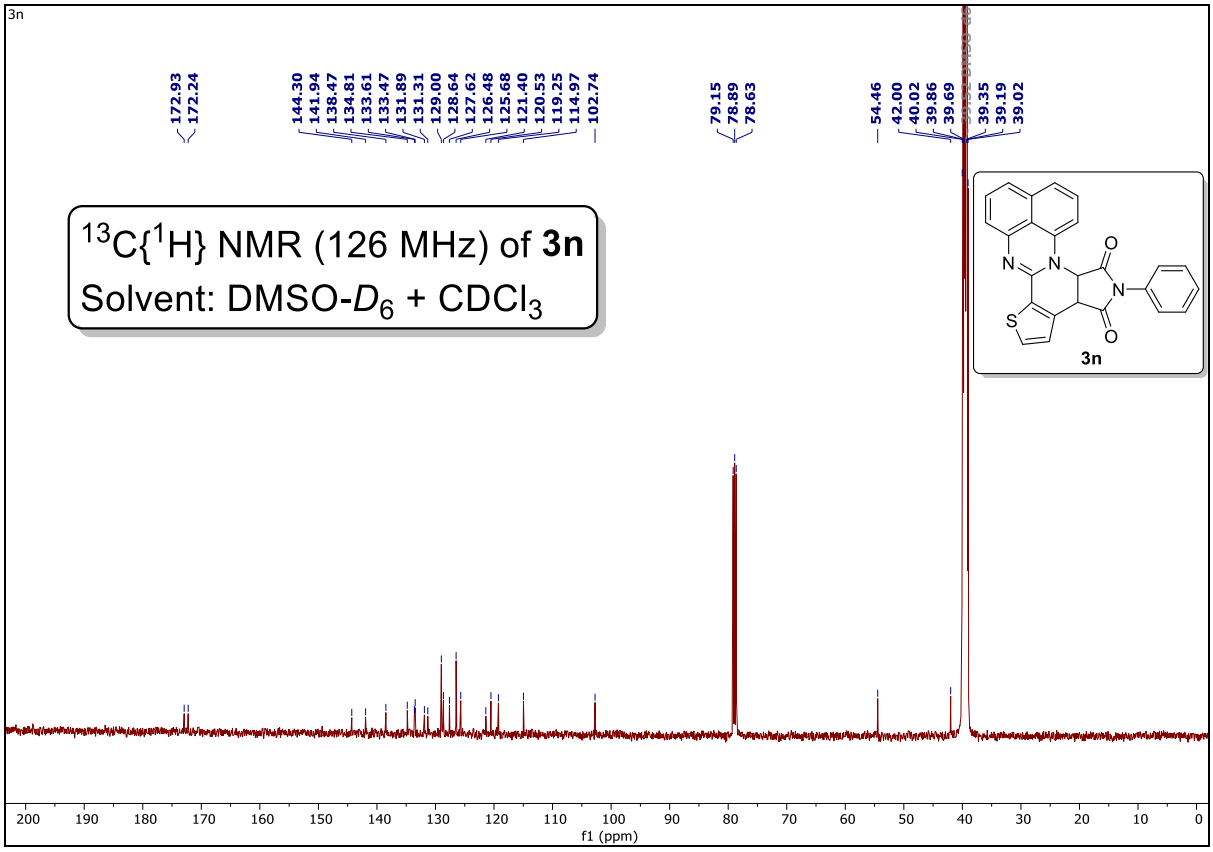


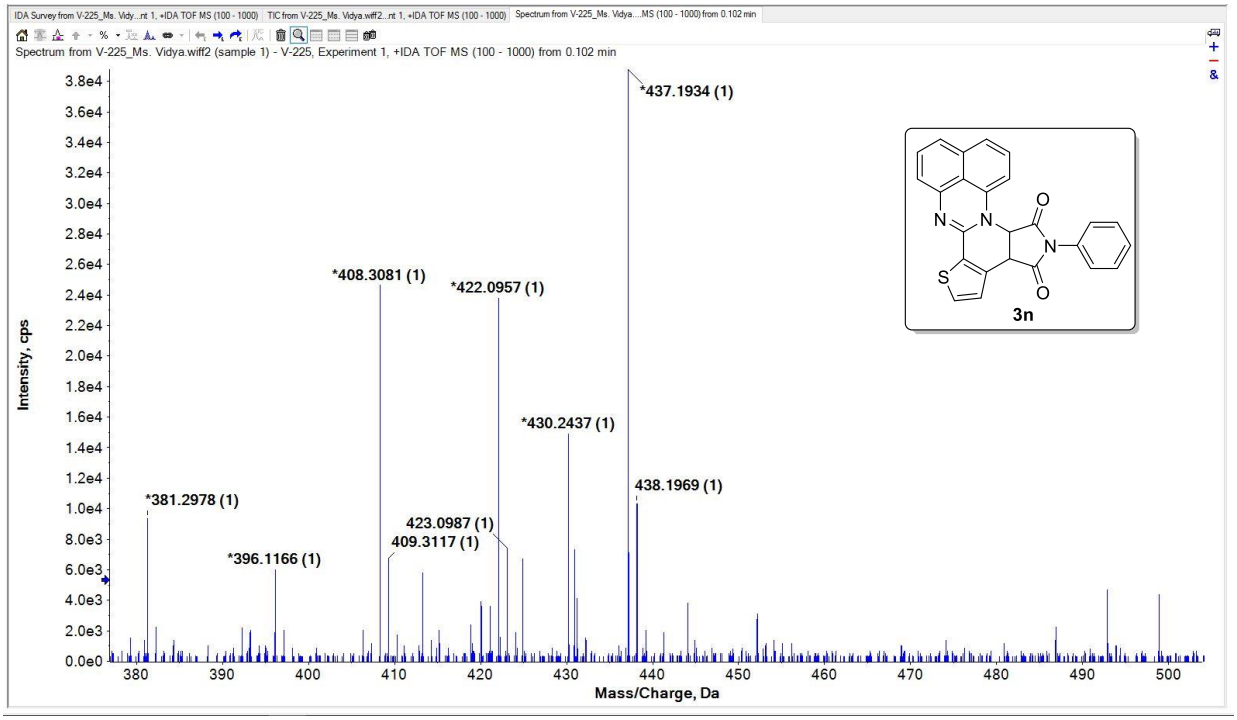


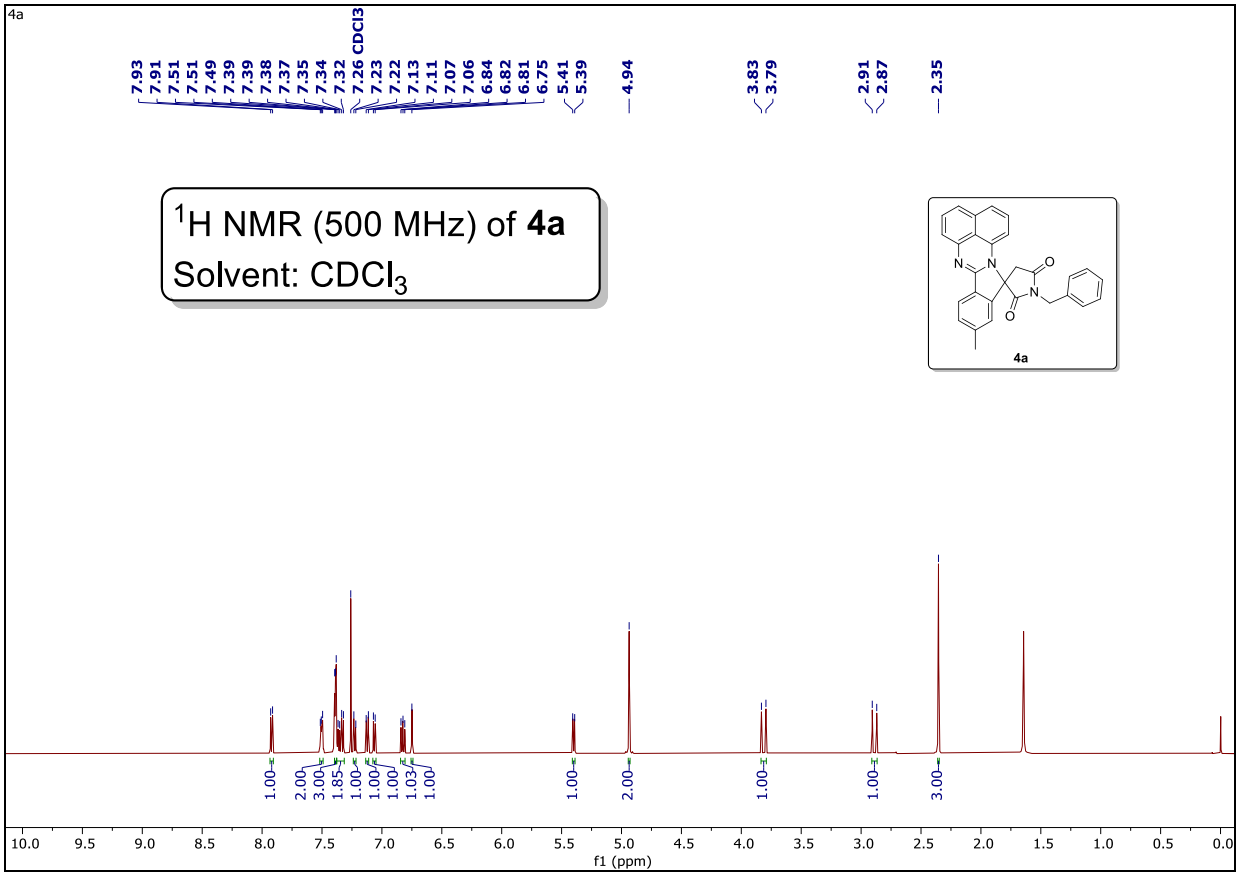
VM-580.d

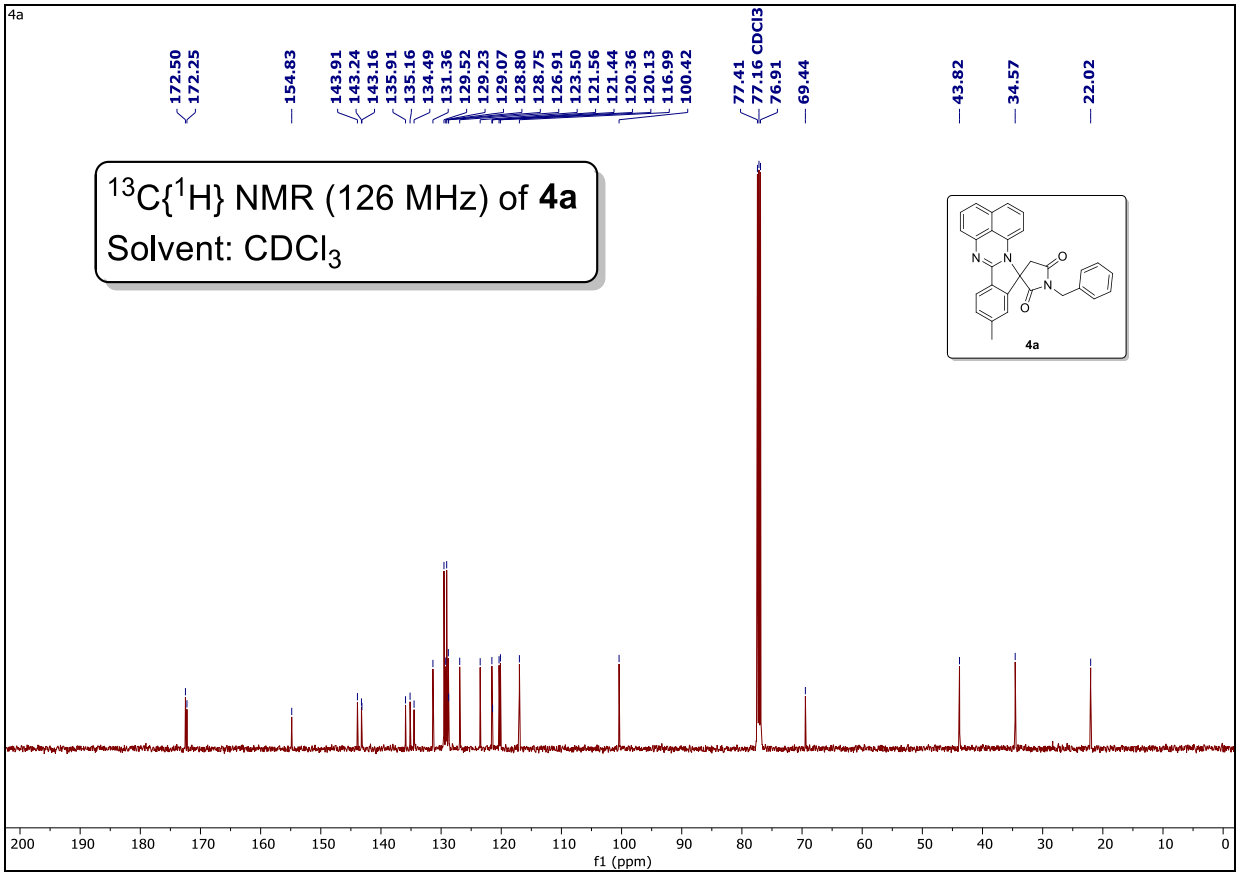
Gudipati


3n
7.93
7.92
7.50
7.48
7.47
7.43
7.42
7.40
7.27
7.27
7.26
7.25
7.24
7.23
7.22
7.20
6.80
6.79
6.26
6.24
4.87
4.85
3.45
3.39
2.50 DMSO-d6
1H NMR (500 MHz) of 3n
Solvent: DMSO-D6 + CDCl3
3n
1.00
2.06
1.05
7.35
2.00
1.00
1.00
1.16
f1 (ppm)


3n
172.93
172.24
144.30
141.94
138.47
134.81
133.61
133.47
131.89
131.31
129.00
128.64
127.62
126.48
125.68
121.40
120.53
119.25
114.97
102.74
79.15
78.89
78.63
54.46
42.00
40.02
39.86
39.69
39.35
39.19
39.02
13C{1H} NMR (126 MHz) of 3n
Solvent: DMSO-D6 + CDCl3
3n
f1 (ppm)


IDA Survey from V-225_Ms. Vidy...nt 1, +IDA TOF MS (100 - 1000)
TIC from V-225_Ms. Vidya.wiff2...nt 1, +IDA TOF MS (100 - 1000)
Spectrum from V-225_Ms. Vidya....MS (100 - 1000) from 0.102 min
Spectrum from V-225_Ms. Vidya.wiff2 (sample 1) - V-225, Experiment 1, +IDA TOF MS (100 - 1000) from 0.102 min
*437.1934 (1)
*408.3081 (1)
*422.0957 (1)
*430.2437 (1)
438.1969 (1)
*381.2978 (1)
423.0987 (1)
409.3117 (1)
*396.1166 (1)
Intensity, cps
Mass/Charge, Da
3n


4a
7.93
7.91
7.51
7.51
7.49
7.39
7.39
7.38
7.37
7.35
7.34
7.32
7.26 CDCl3
7.23
7.22
7.13
7.11
7.07
7.06
6.84
6.82
6.81
6.75
5.41
5.39
4.94
3.83
3.79
2.91
2.87
2.35
1H NMR (500 MHz) of 4a
Solvent: CDCl3
4a
1.00
2.00
3.00
1.85
1.00
1.00
1.00
1.03
1.00
1.00
2.00
1.00
1.00
3.00
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


4a
172.50
172.25
154.83
143.91
143.24
143.16
135.91
135.16
134.49
131.36
129.52
129.23
129.07
128.80
128.75
126.91
123.50
121.56
121.44
120.36
120.13
116.99
100.42
77.41
77.16 CDCl3
76.91
69.44
43.82
34.57
22.02
13C{1H} NMR (126 MHz) of 4a
Solvent: CDCl3
4a
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

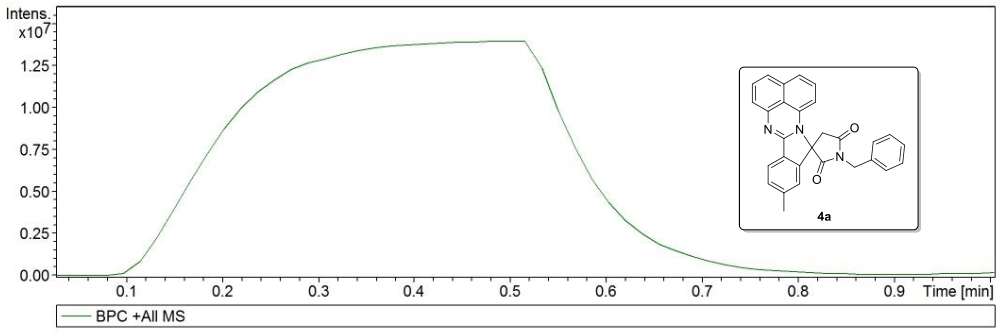
Display Report

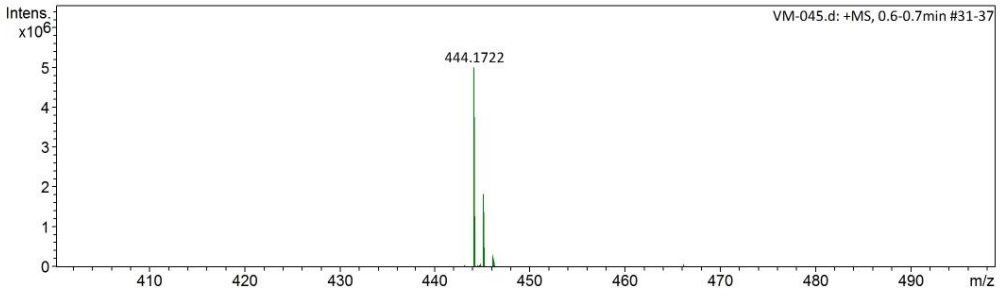
Analysis Info

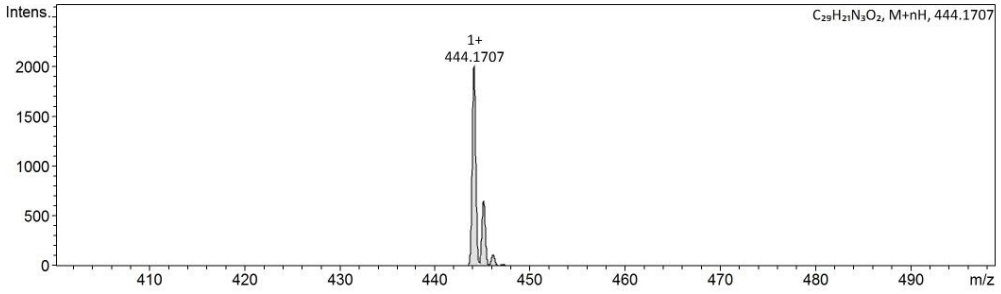
Analysis Name	D:\Data\user data\Dr. Lokman\09-04-2024\VM-045.d	Acquisition Date	4/9/2024 4:41:20 PM
Method	Tune_pos_Mid.m	Operator	vidhi
Sample Name	VM-045	Instrument	impact HD 1819696.00197
Comment			

Acquisition Parameter

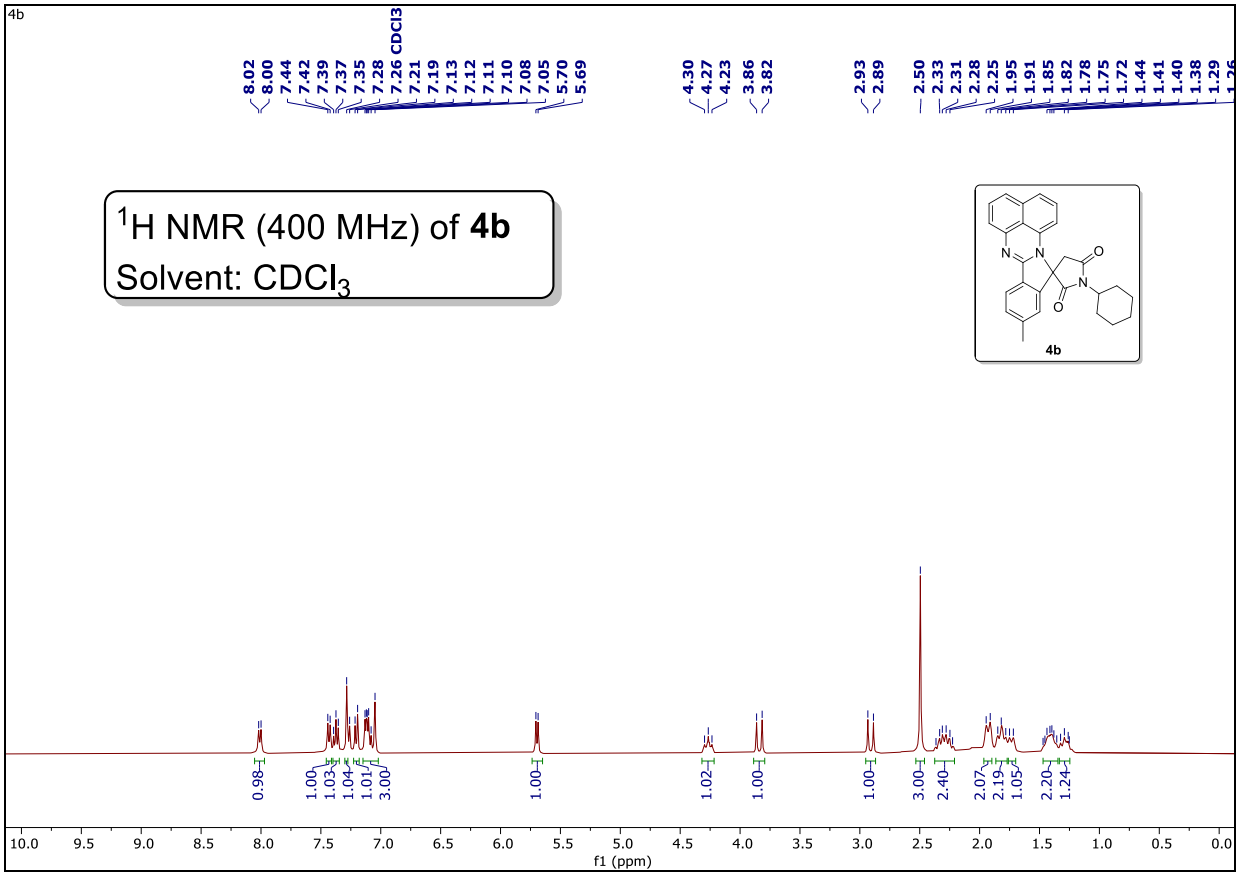
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	219 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 °C

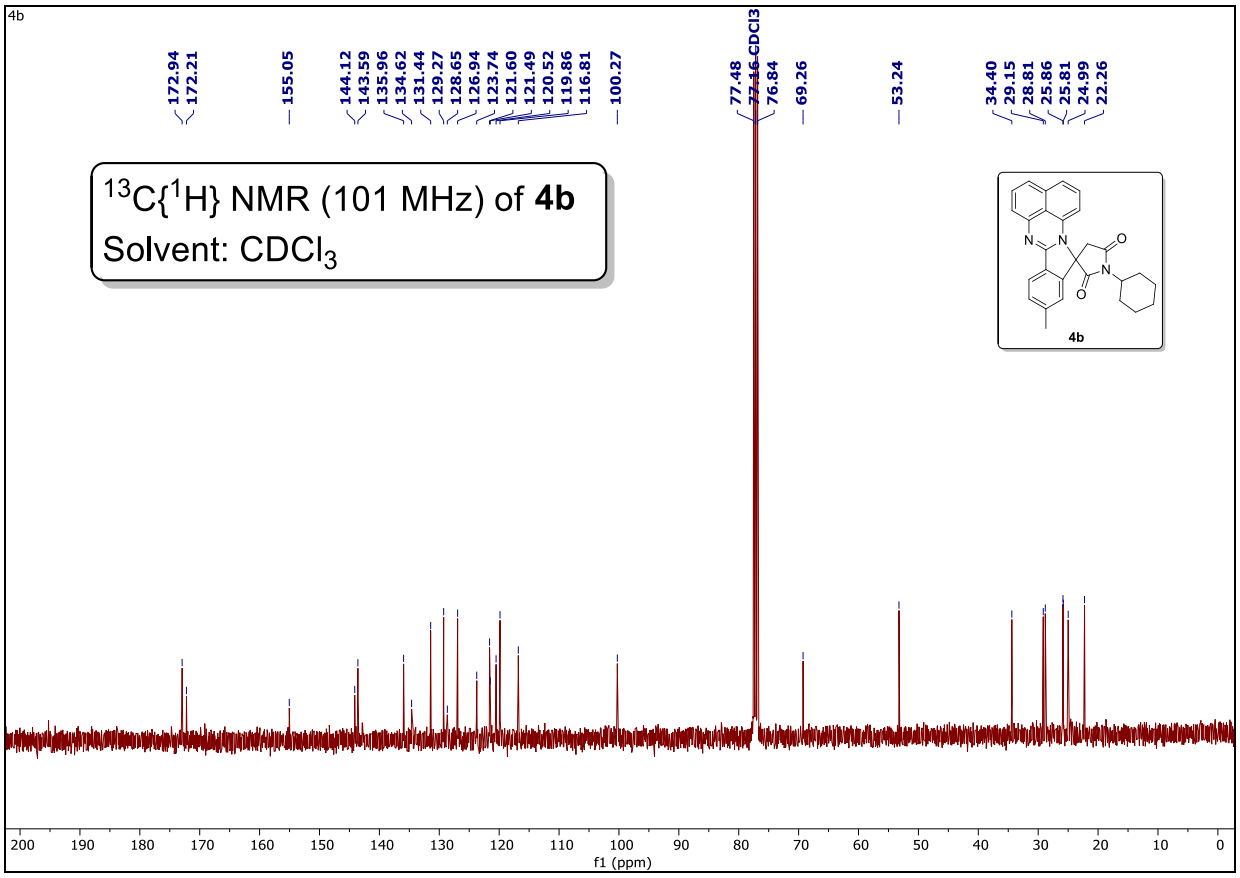






VM-045.d


4b
8.02
8.00
7.44
7.42
7.39
7.37
7.35
7.28
7.26 CDCl3
7.21
7.19
7.13
7.12
7.11
7.10
7.08
7.05
5.70
5.69
4.30
4.27
4.23
3.86
3.82
2.93
2.89
2.50
2.33
2.31
2.28
2.25
1.95
1.91
1.85
1.82
1.78
1.75
1.72
1.44
1.41
1.40
1.38
1.29
1H NMR (400 MHz) of 4b
Solvent: CDCl3
4b
0.98
1.00
1.03
1.04
1.01
3.00
1.00
1.02
1.00
1.00
3.00
2.40
2.07
2.19
1.05
2.20
1.24
f1 (ppm)


4b
172.94
172.21
155.05
144.12
143.59
135.96
134.62
131.44
129.27
128.65
126.94
123.74
121.60
121.49
120.52
119.86
116.81
100.27
77.48
77.16 CDCl3
76.84
69.26
53.24
34.40
29.15
28.81
25.86
25.81
24.99
22.26
13C{1H} NMR (101 MHz) of 4b
Solvent: CDCl3
4b
f1 (ppm)

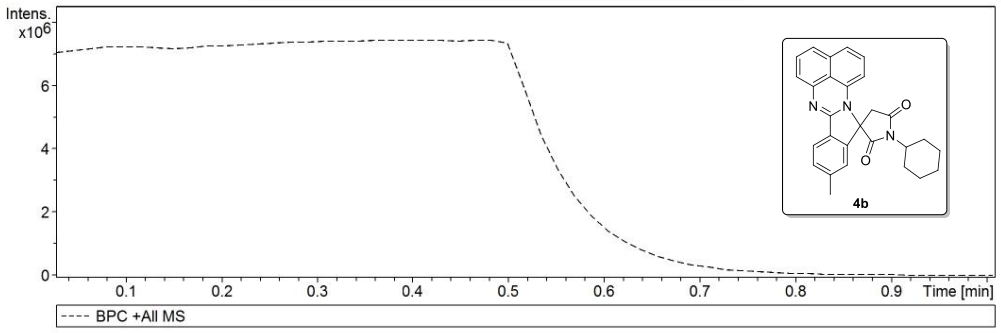
Display Report

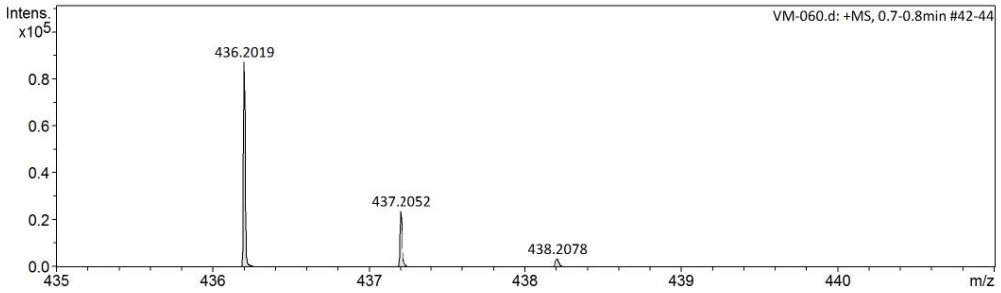
Analysis Info

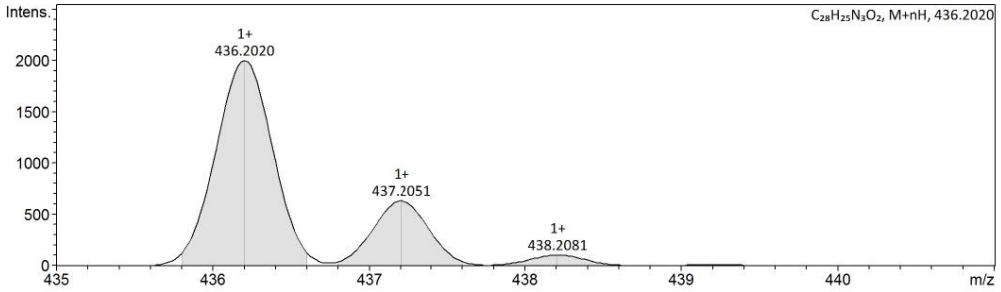
Analysis Name	D:\Data\user data\Dr. Lokman\17-04-2024\VM-060.d	Acquisition Date	4/17/2024 4:15:07 PM
Method	Tune_pos_Mid.m	Operator	vidhi
Sample Name	VM-060	Instrument	impact HD 1819696.00197
Comment			

Acquisition Parameter

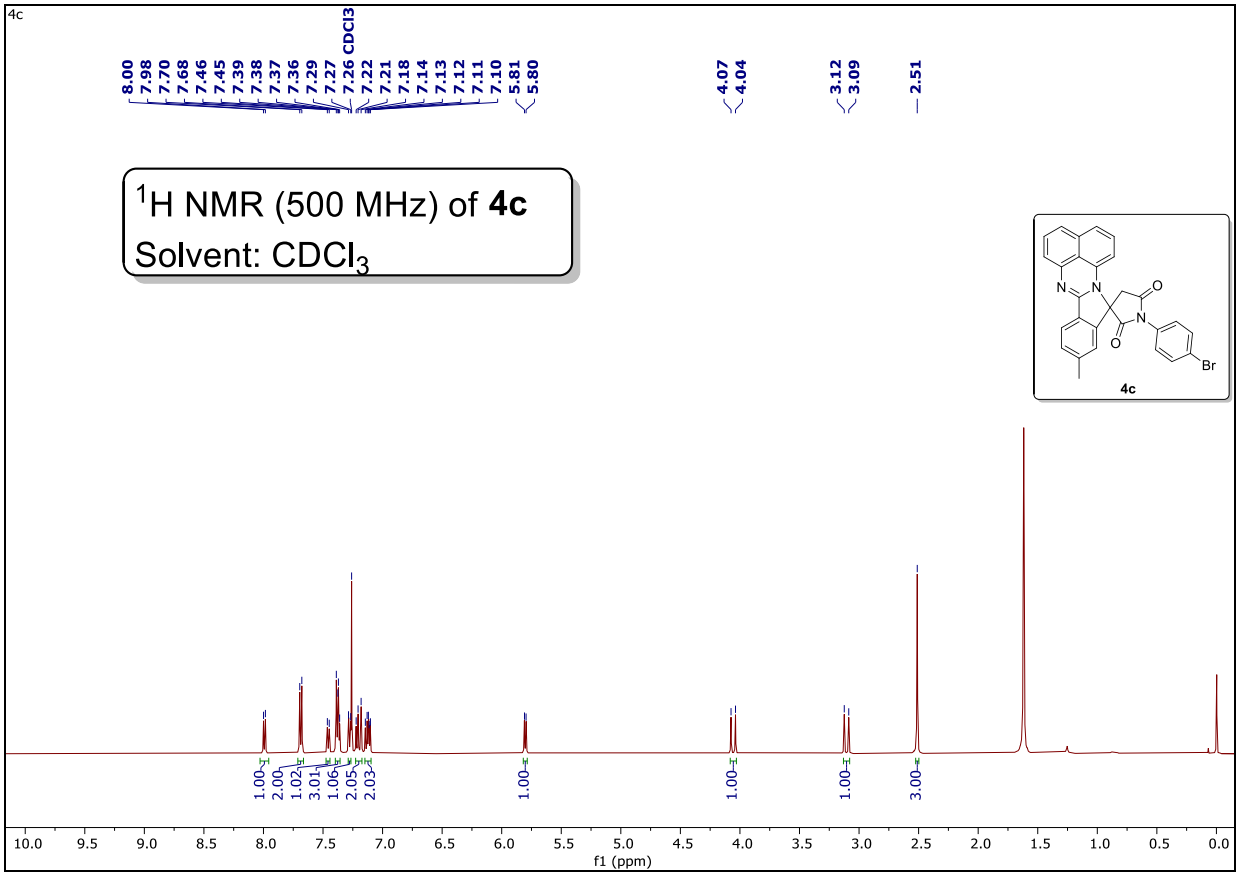
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	200 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 °C

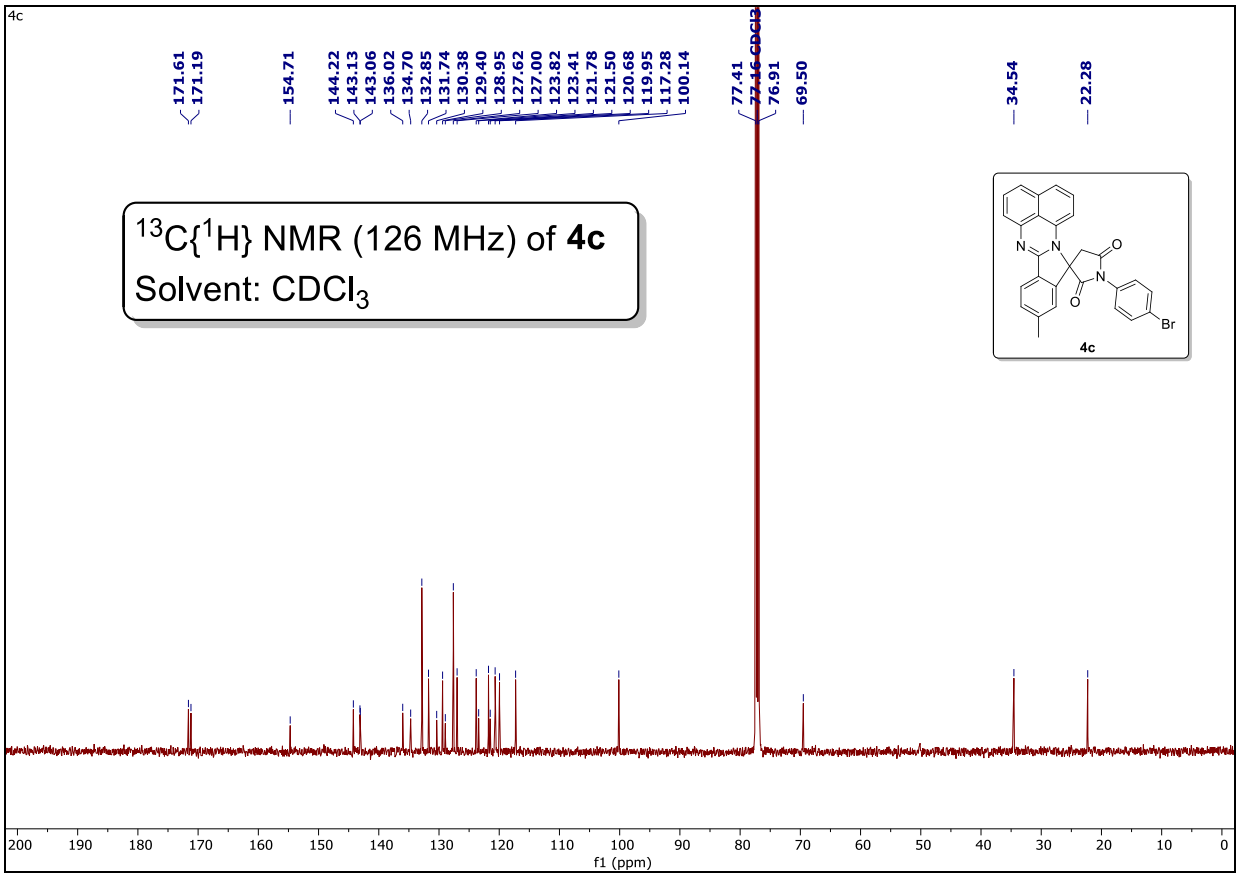






VM-060.d


4c
8.00
7.98
7.70
7.68
7.46
7.45
7.39
7.38
7.37
7.36
7.29
7.27
7.26 CDCl3
7.22
7.21
7.18
7.14
7.13
7.12
7.11
7.10
5.81
5.80
4.07
4.04
3.12
3.09
2.51
1H NMR (500 MHz) of 4c
Solvent: CDCl3
Br
4c
1.00
2.00
1.02
3.01
1.06
2.05
2.03
1.00
1.00
1.00
3.00
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


4c
171.61
171.19
154.71
144.22
143.13
143.06
136.02
134.70
132.85
131.74
130.38
129.40
128.95
127.62
127.00
123.82
123.41
121.78
121.50
120.68
119.95
117.28
100.14
77.41
77.16 CDCl3
76.91
69.50
34.54
22.28
13C{1H} NMR (126 MHz) of 4c
Solvent: CDCl3
Br
4c
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

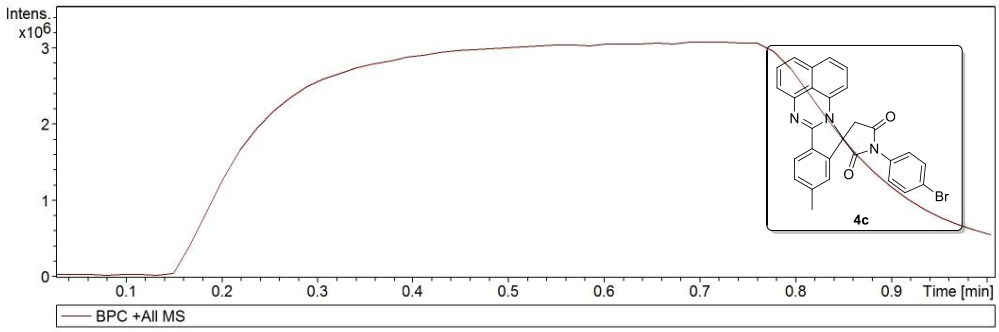
Display Report

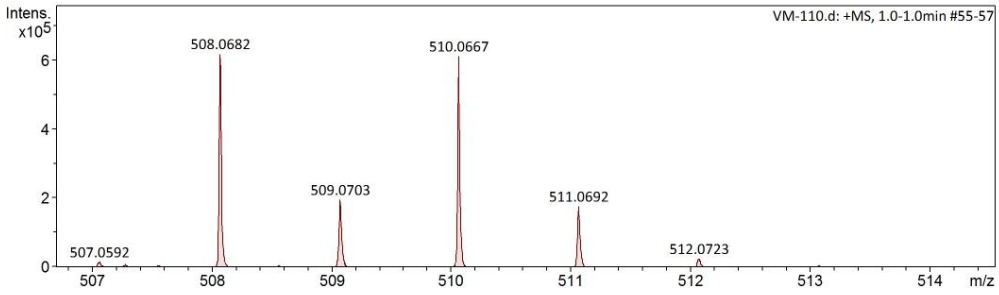
Analysis Info

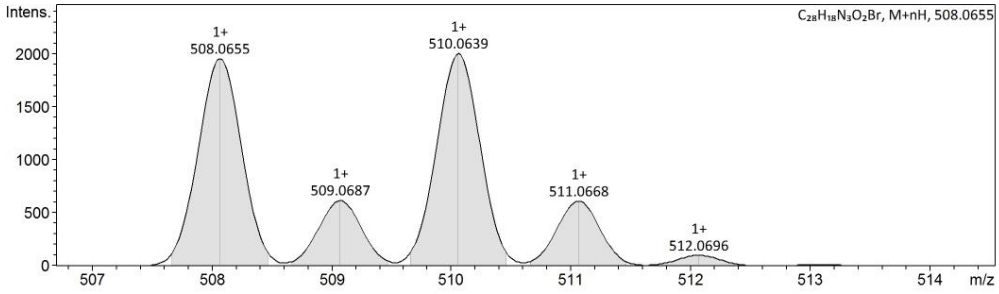
Analysis Name	D:\Data\user data\Dr. Lokman\09-04-2024\VM-110.d	Acquisition Date	4/9/2024 4:49:15 PM
Method	Tune_pos_Mid.m	Operator	vidhi
Sample Name	VM-110	Instrument	impact HD 1819696.00197
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	219 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 °C

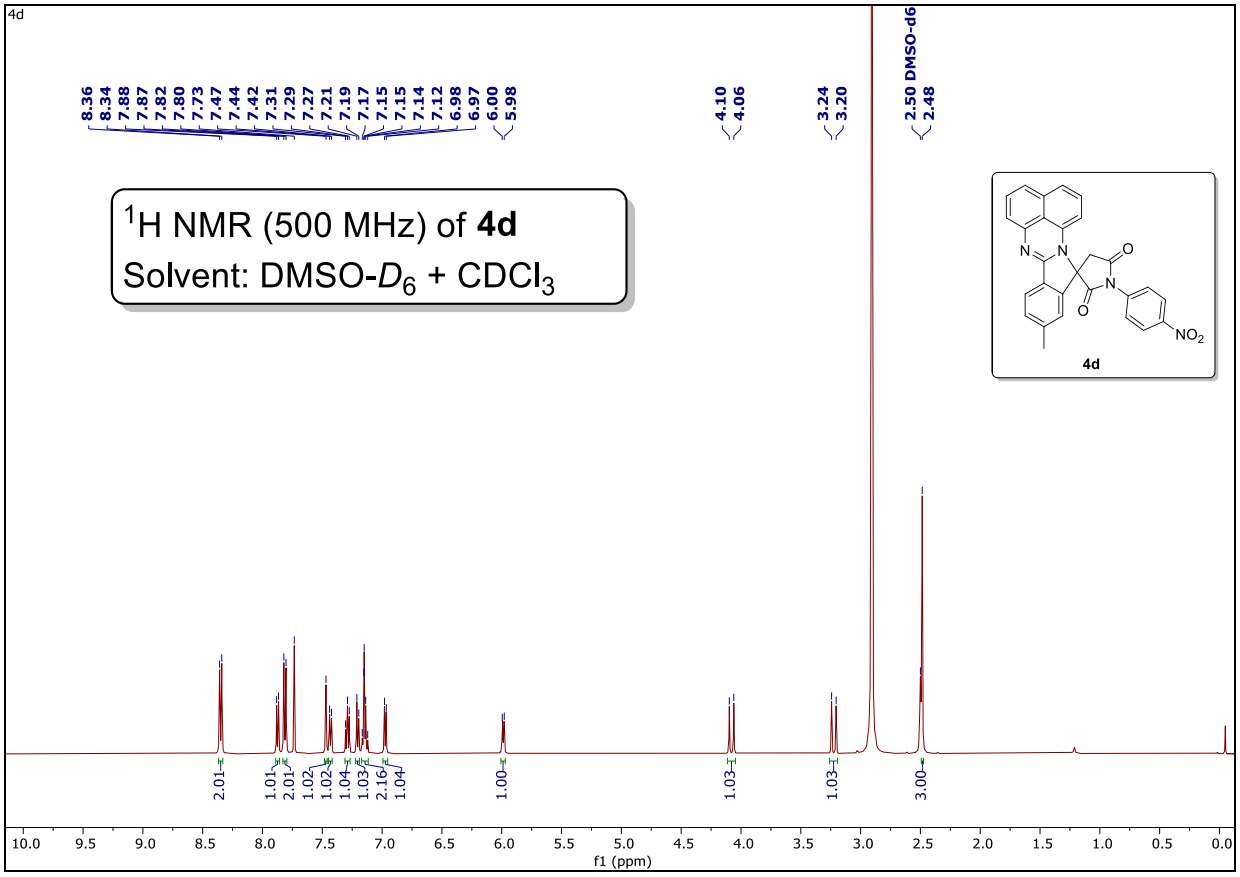


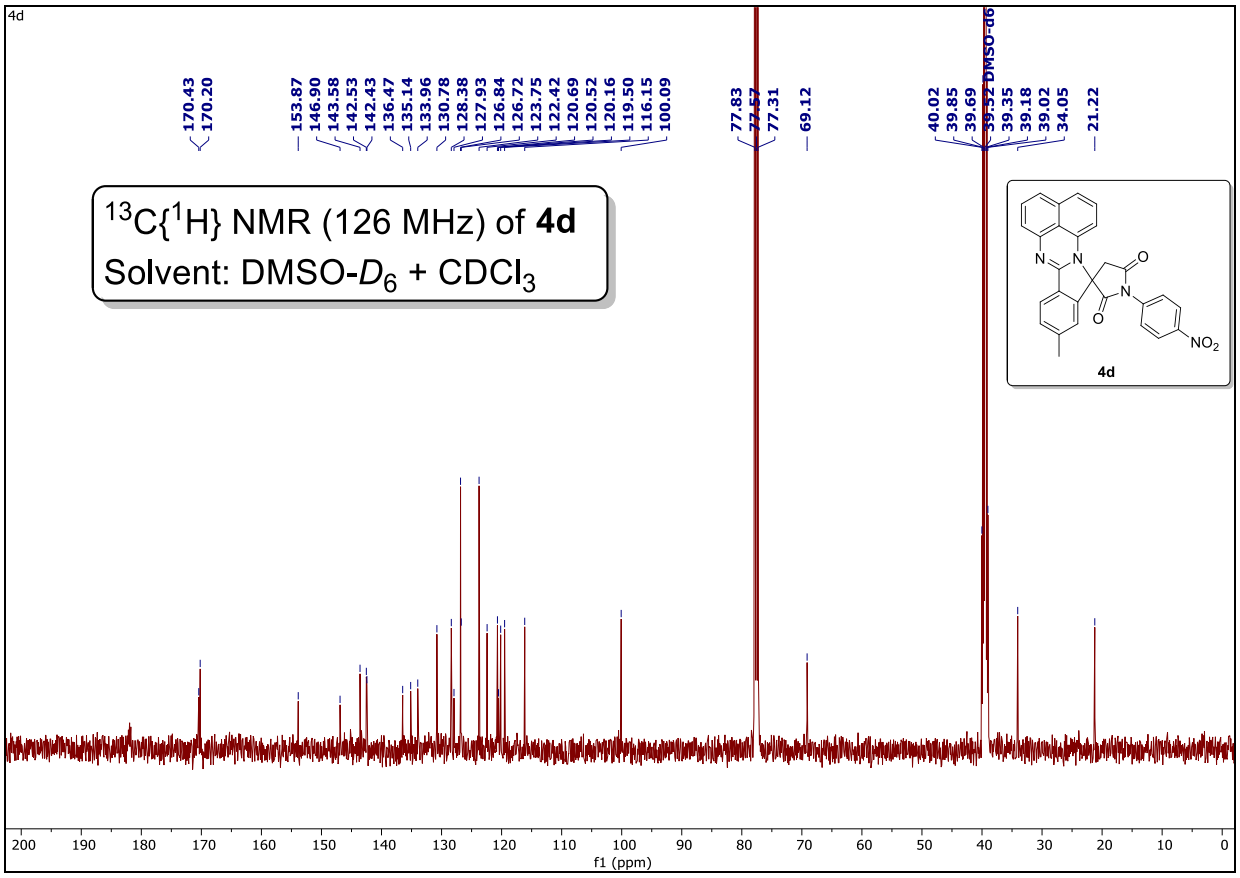




VM-110.d

Gudipati


4d
8.36
8.34
7.88
7.87
7.82
7.80
7.73
7.47
7.44
7.42
7.31
7.29
7.27
7.21
7.19
7.17
7.15
7.15
7.14
7.12
6.98
6.97
6.00
5.98
4.10
4.06
3.24
3.20
2.50 DMSO-d6
2.48
^{1}H NMR (500 MHz) of **4d**
Solvent: DMSO-D_6 + $CDCl_3$
4d
2.01
1.01
2.01
1.02
1.02
1.04
1.03
2.16
1.04
1.00
1.03
1.03
3.00
f1 (ppm)


4d
170.43
170.20
153.87
146.90
143.58
142.53
142.43
136.47
135.14
133.96
130.78
128.38
127.93
126.84
126.72
123.75
122.42
120.69
120.52
120.16
119.50
116.15
100.09
77.83
77.57
77.31
69.12
40.02
39.85
39.69
39.52 DMSO-d6
39.35
39.18
39.02
34.05
21.22
^{13}C{^{1}H} NMR (126 MHz) of **4d**
Solvent: DMSO-D_6 + $CDCl_3$
4d
f1 (ppm)

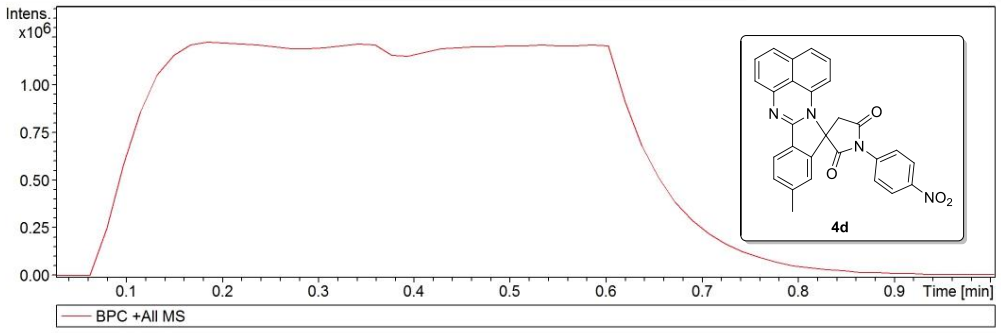
Display Report

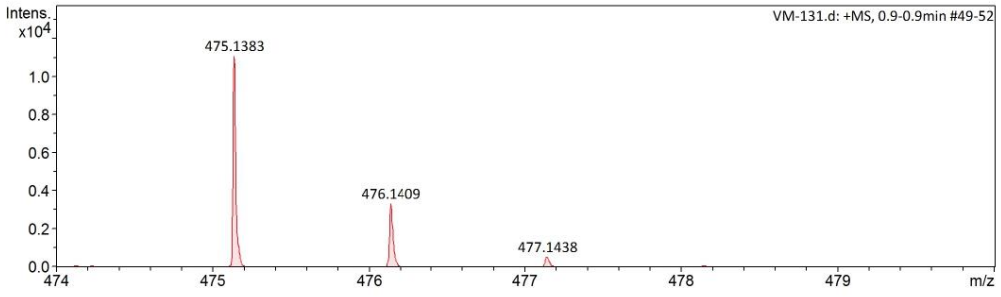
Analysis Info

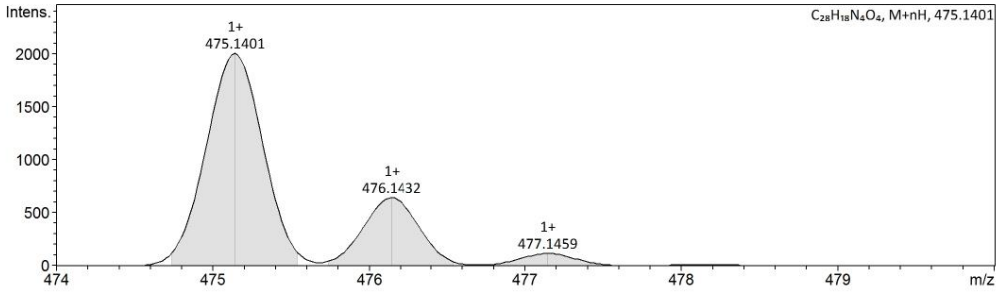
Analysis Name	D:\Data\user data\Dr. Lokman\09-04-2024\VM-131.d	Acquisition Date	4/9/2024 4:57:36 PM
Method	Tune_pos_Mid.m	Operator	vidhi
Sample Name	VM-131	Instrument	impact HD 1819696.00197
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	219 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 °C

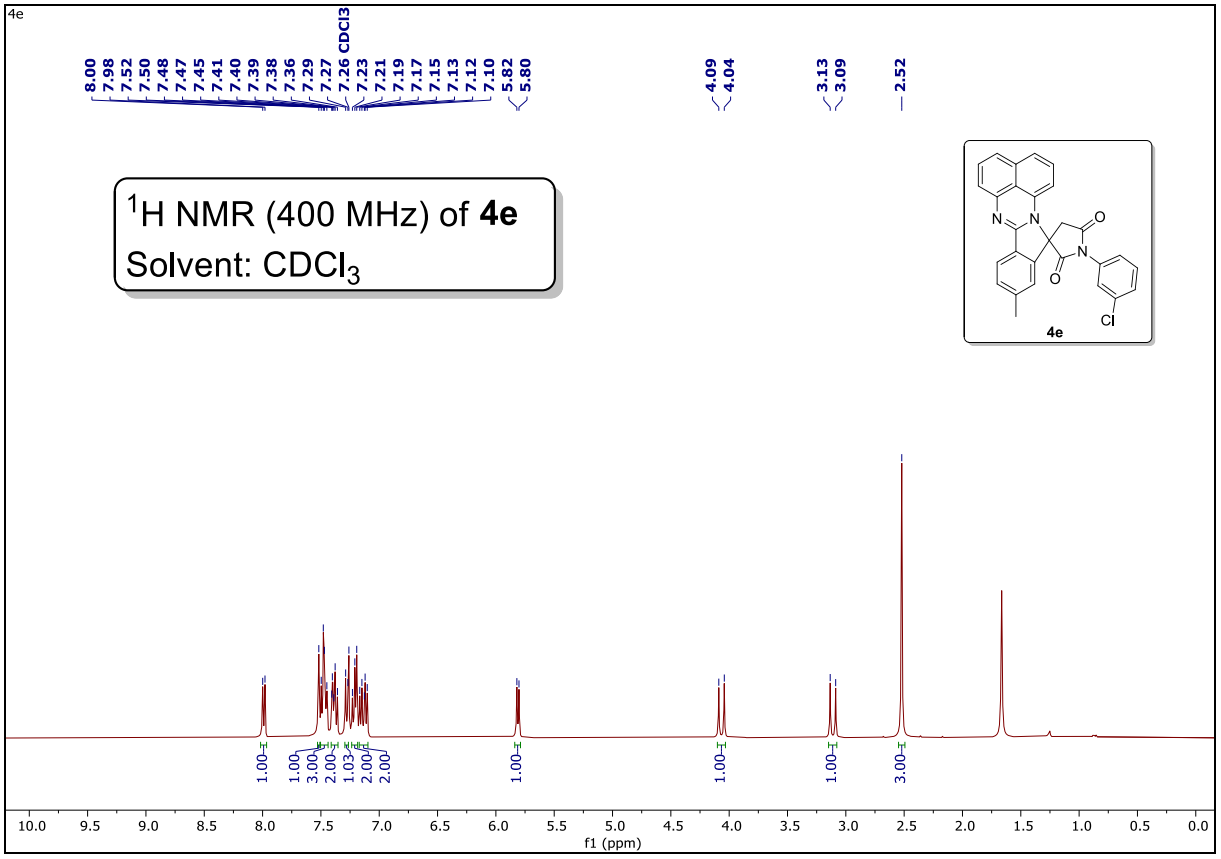


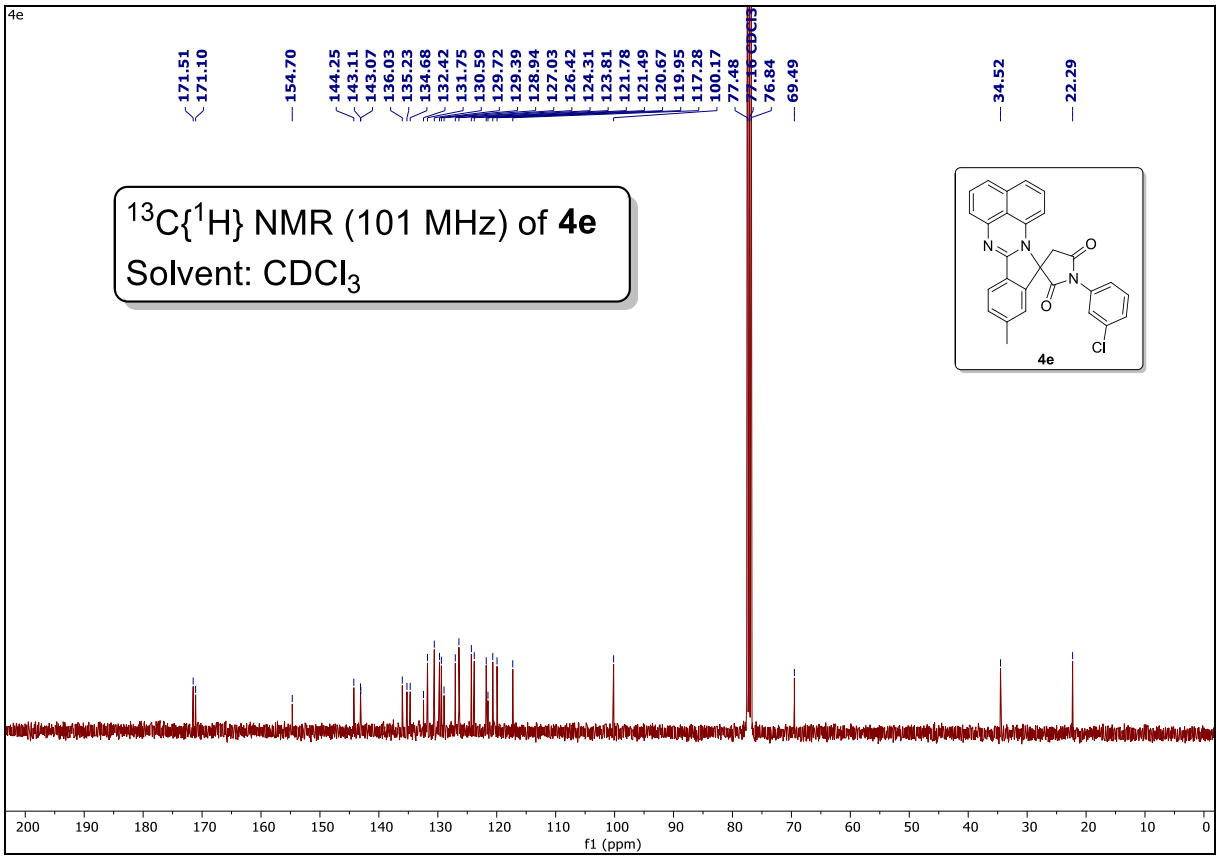




VM-131.d

Gudipati


4e
8.00
7.98
7.52
7.50
7.48
7.47
7.45
7.41
7.40
7.39
7.38
7.36
7.29
7.27
7.26 CDCl3
7.23
7.21
7.19
7.17
7.15
7.13
7.12
7.10
5.82
5.80
4.09
4.04
3.13
3.09
2.52
1H NMR (400 MHz) of 4e
Solvent: CDCl3
4e
1.00
1.00
3.00
2.00
1.03
2.00
2.00
1.00
1.00
1.00
3.00
f1 (ppm)


4e
171.51
171.10
154.70
144.25
143.11
143.07
136.03
135.23
134.68
132.42
131.75
130.59
129.72
129.39
128.94
127.03
126.42
124.31
123.81
121.78
121.49
120.67
119.95
117.28
100.17
77.48
77.16 CDCl3
76.84
69.49
34.52
22.29
13C{1H} NMR (101 MHz) of 4e
Solvent: CDCl3
4e
f1 (ppm)

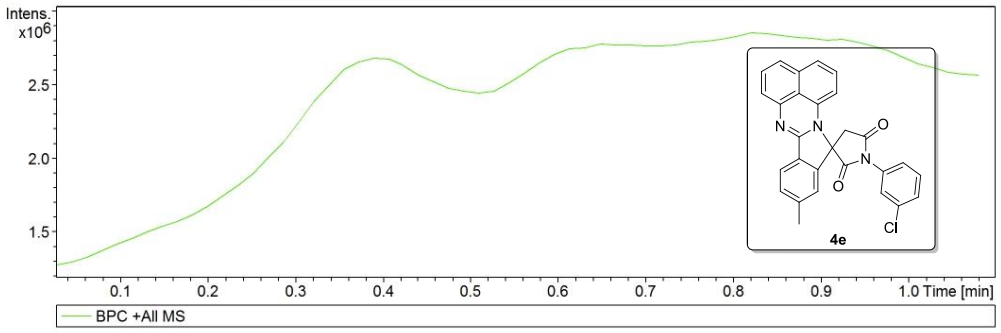
Display Report

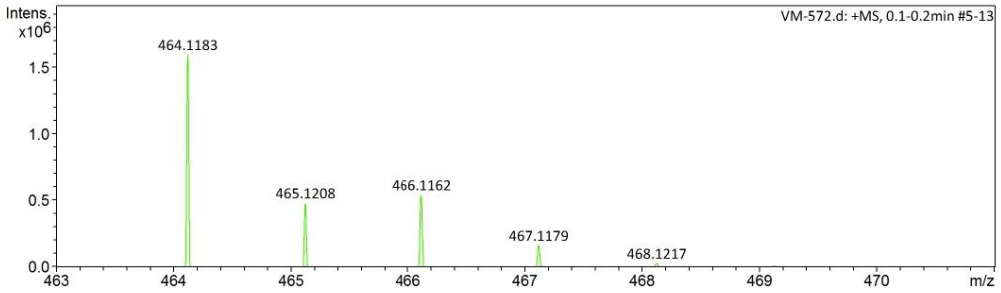
Analysis Info

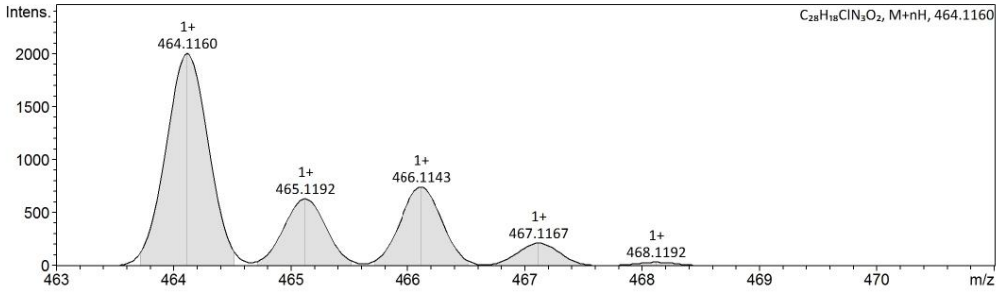
Analysis Name	D:\Data\user data\Dr. Lokman\18-02-2025\VM-572.d	Acquisition Date	2/18/2025 12:37:22 PM
Method	low_mass.m	Operator	Gudipati SrinivasaRao
Sample Name	VM-572	Instrument	impact HD 1819696.00197
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.6 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	5.0 l/min
Scan End	1500 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C

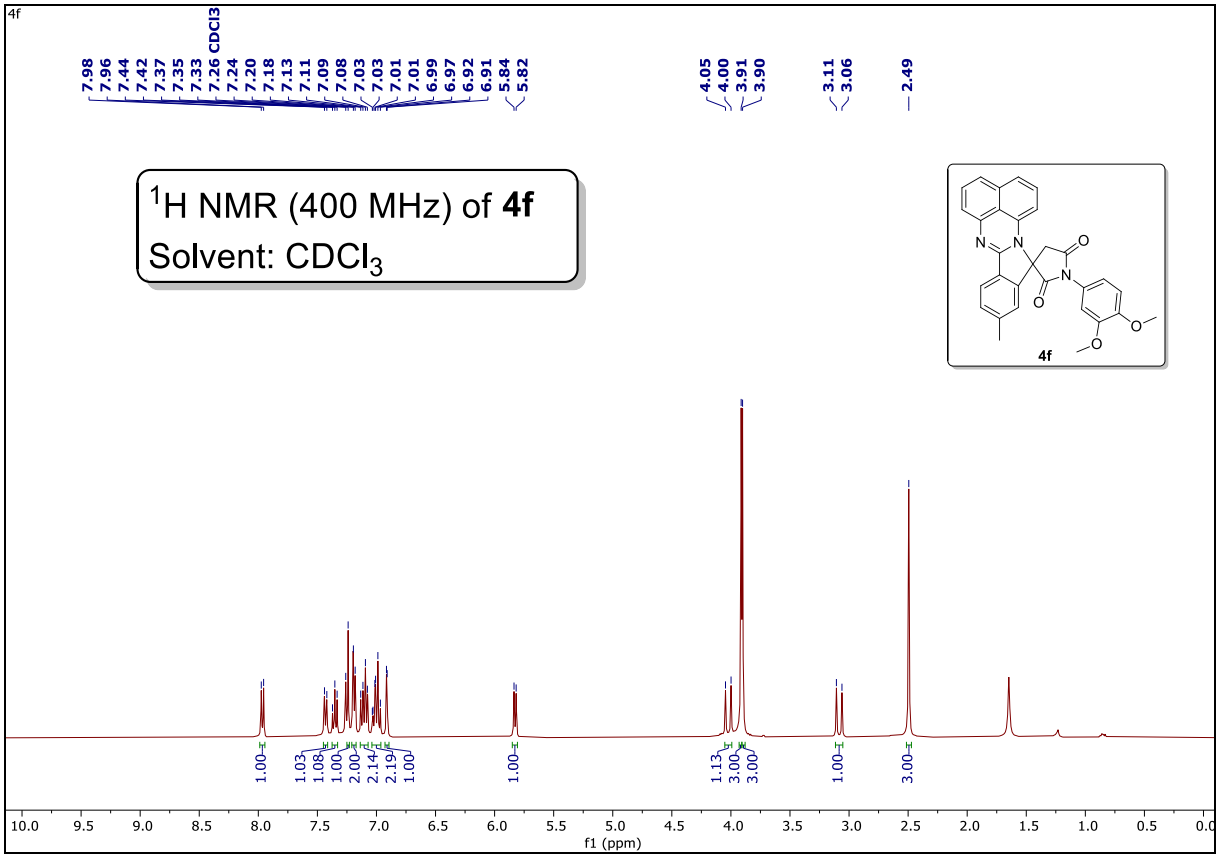


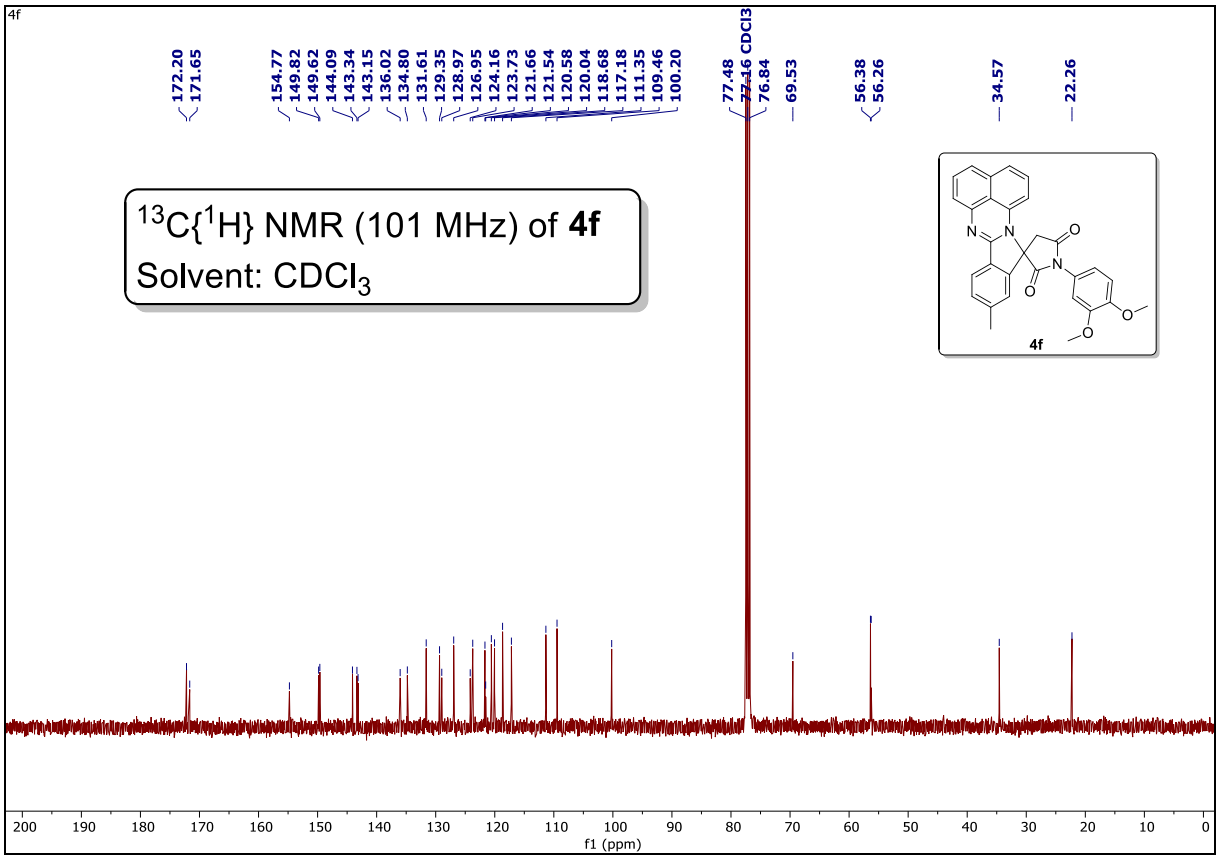




VM-572.d

Gudipati


4f
7.98
7.96
7.44
7.42
7.37
7.35
7.33
7.26 CDCl3
7.24
7.20
7.18
7.13
7.11
7.09
7.08
7.03
7.03
7.01
7.01
6.99
6.97
6.92
6.91
5.84
5.82
4.05
4.00
3.91
3.90
3.11
3.06
2.49
1H NMR (400 MHz) of 4f
Solvent: CDCl3
4f
1.00
1.03
1.08
1.00
2.00
2.14
2.19
1.00
1.00
1.13
3.00
3.00
1.00
3.00
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


4f
172.20
171.65
154.77
149.82
149.62
144.09
143.34
143.15
136.02
134.80
131.61
129.35
128.97
126.95
124.16
123.73
121.66
121.54
120.58
120.04
118.68
117.18
111.35
109.46
100.20
77.48
77.16 CDCl3
76.84
69.53
56.38
56.26
34.57
22.26
13C{1H} NMR (101 MHz) of 4f
Solvent: CDCl3
4f
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

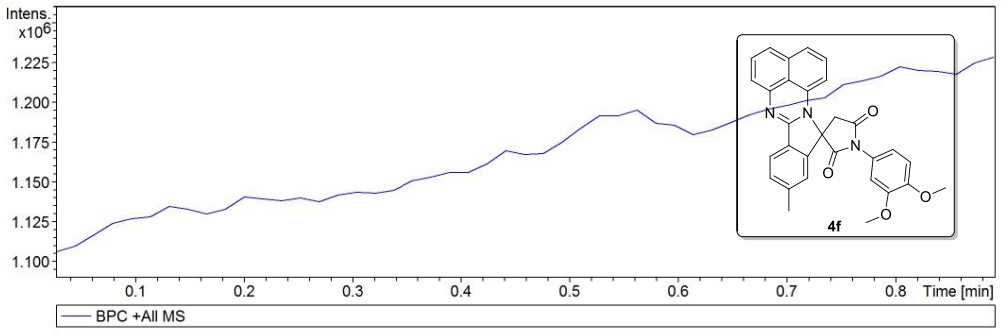
Display Report

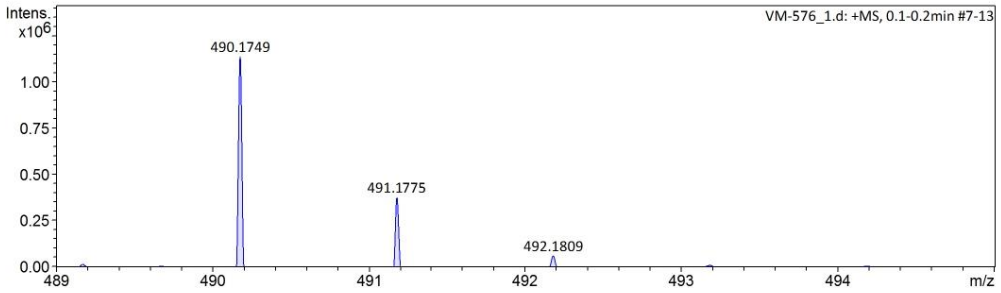
Analysis Info

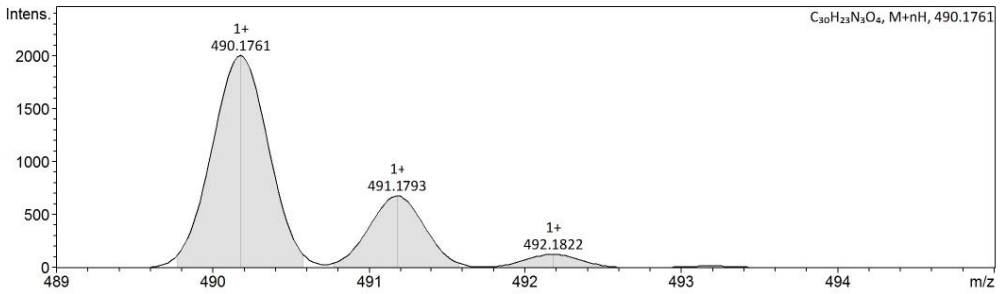
Analysis Name	D:\Data\user data\Dr. Lokman\24-02-2025\VM-576_1.d	Acquisition Date	2/24/2025 11:35:14 AM
Method	low_mass.m	Operator	Gudipati SrinivasaRao
Sample Name	VM-576_1	Instrument	impact HD 1819696.00197
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.7 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	5.0 l/min
Scan End	1500 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C

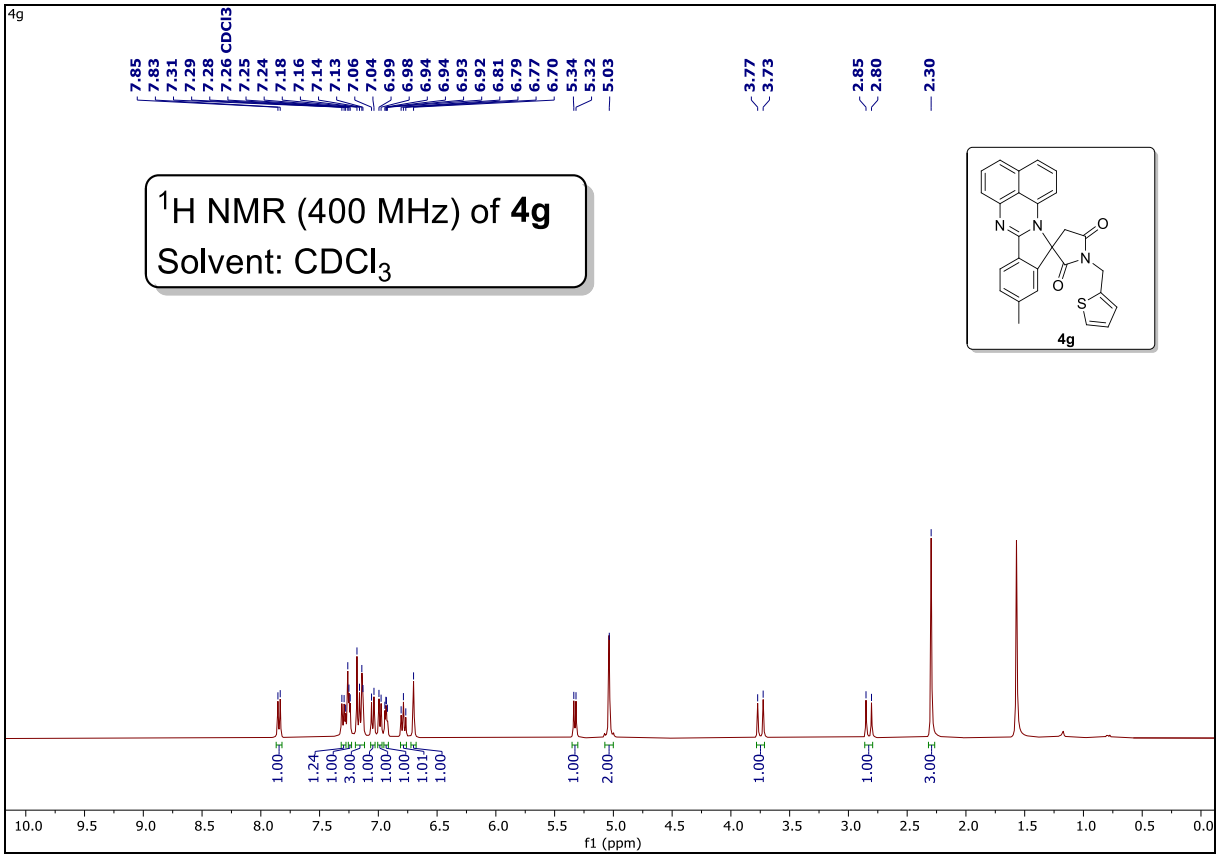


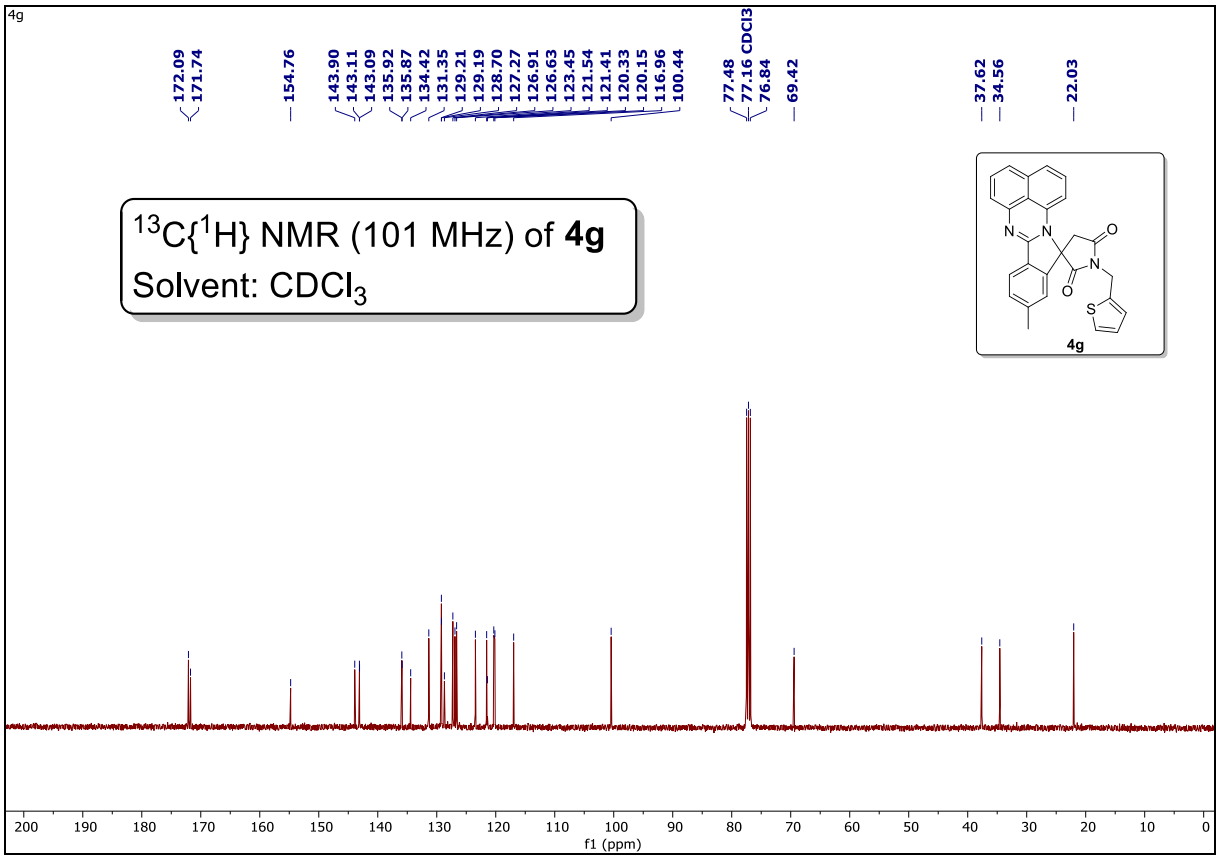




VM-576_1.d

Gudipati


4g
7.85
7.83
7.31
7.29
7.28
7.26 CDCl3
7.25
7.24
7.18
7.16
7.14
7.13
7.06
7.04
6.99
6.98
6.94
6.94
6.93
6.92
6.81
6.79
6.77
6.70
5.34
5.32
5.03
3.77
3.73
2.85
2.80
2.30
1H NMR (400 MHz) of 4g
Solvent: CDCl3
4g
1.00
1.24
1.00
3.00
1.00
1.00
1.01
1.00
1.00
2.00
1.00
1.00
3.00
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


4g
172.09
171.74
154.76
143.90
143.11
143.09
135.92
135.87
134.42
131.35
129.21
129.19
128.70
127.27
126.91
126.63
123.45
121.54
121.41
120.33
120.15
116.96
100.44
77.48
77.16 CDCl3
76.84
69.42
37.62
34.56
22.03
13C{1H} NMR (101 MHz) of 4g
Solvent: CDCl3
4g
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

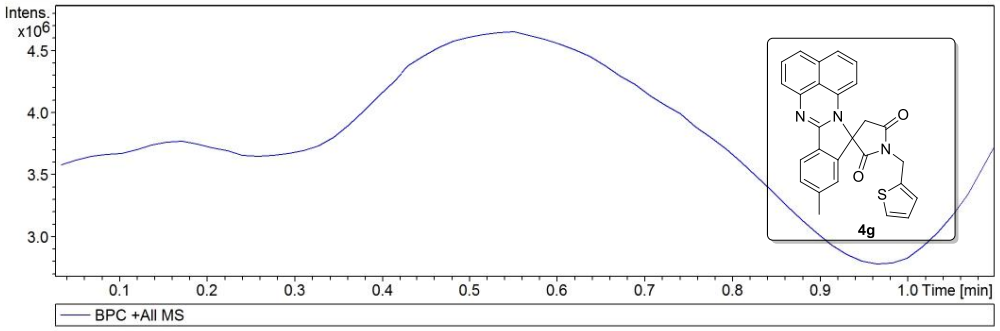
Display Report

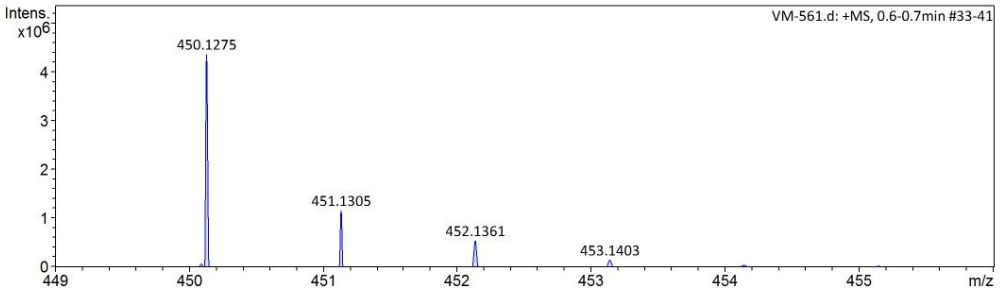
Analysis Info

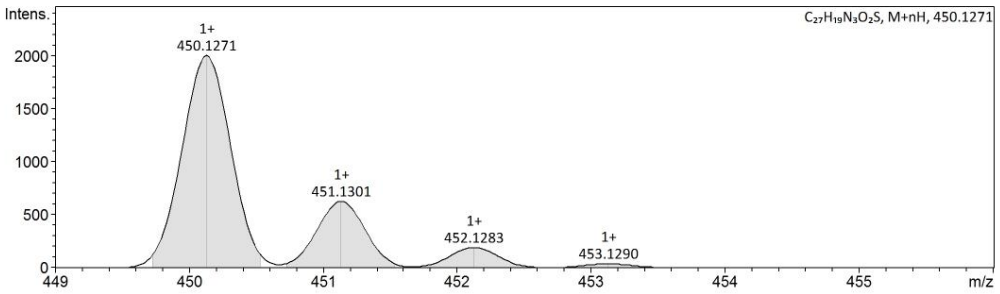
Analysis Name	D:\Data\user data\Dr. Lokman\18-02-2025\VM-561.d	Acquisition Date	2/18/2025 1:21:32 PM
Method	low_mass.m	Operator	Gudipati SrinivasaRao
Sample Name	VM-561	Instrument	impact HD 1819696.00197
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.6 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	5.0 l/min
Scan End	1500 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C

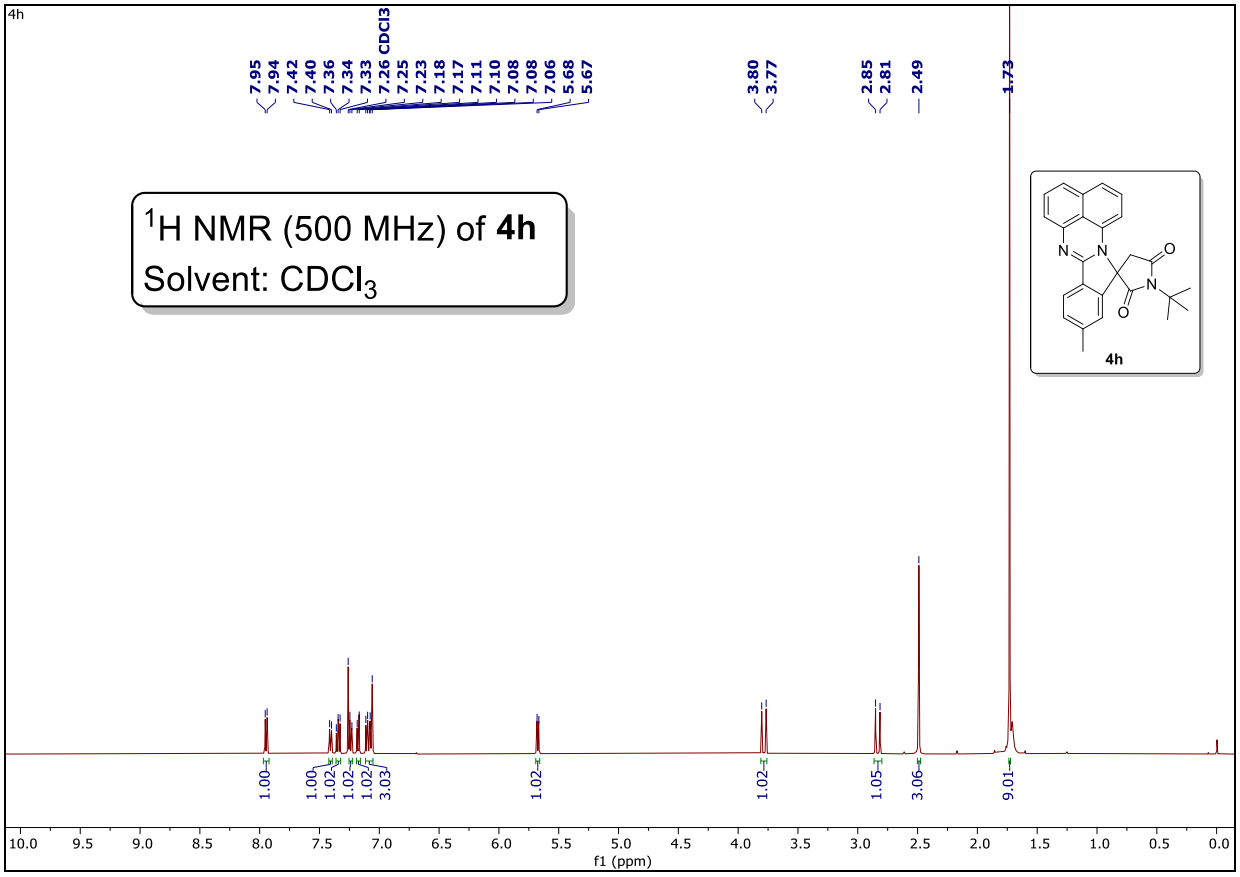


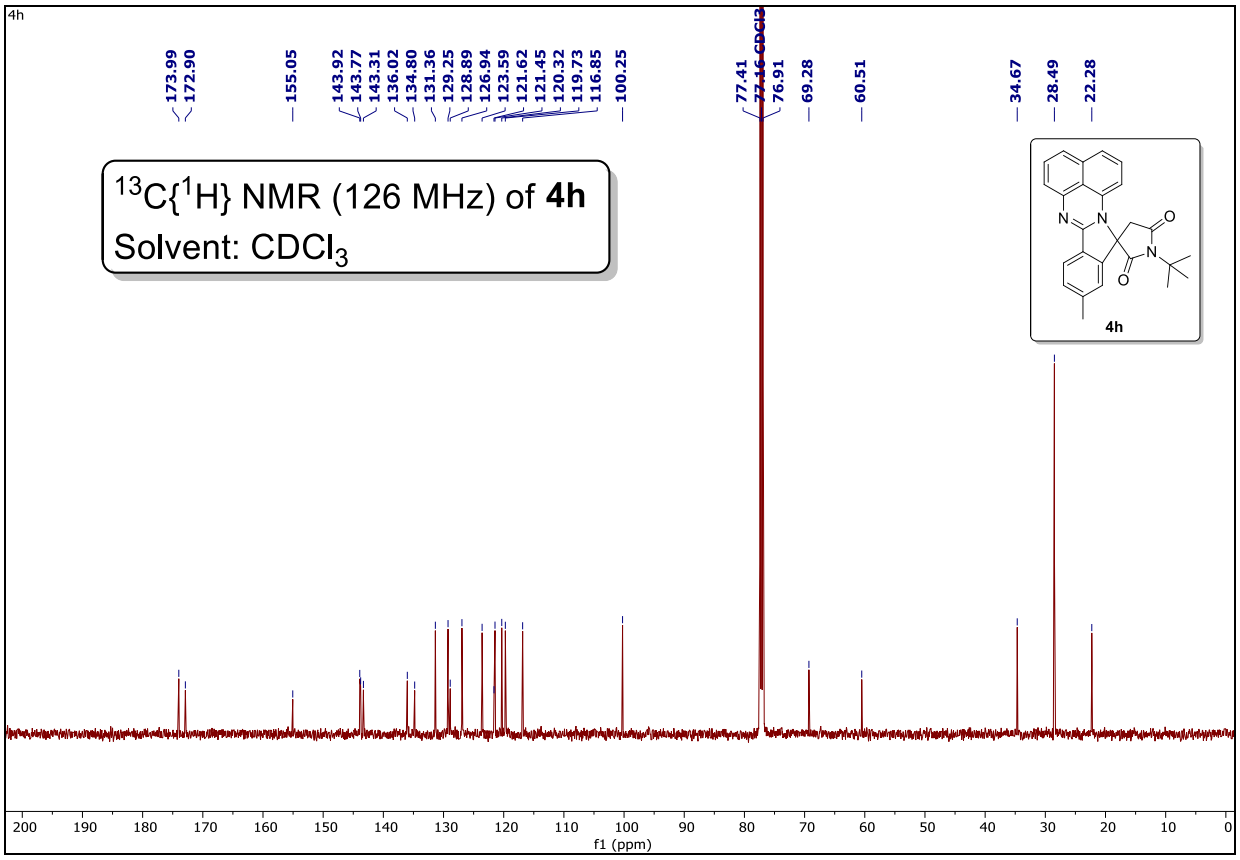




VM-561.d

Gudipati


4h
7.95
7.94
7.42
7.40
7.36
7.34
7.33
7.26 CDCl3
7.25
7.23
7.18
7.17
7.11
7.10
7.08
7.08
7.06
5.68
5.67
3.80
3.77
2.85
2.81
2.49
1.73
1H NMR (500 MHz) of 4h
Solvent: CDCl3
4h
1.00
1.00
1.02
1.02
1.02
3.03
1.02
1.02
1.05
3.06
9.01
f1 (ppm)


4h
173.99
172.90
155.05
143.92
143.77
143.31
136.02
134.80
131.36
129.25
128.89
126.94
123.59
121.62
121.45
120.32
119.73
116.85
100.25
77.41
77.16 CDCl3
76.91
69.28
60.51
34.67
28.49
22.28
13C{1H} NMR (126 MHz) of 4h
Solvent: CDCl3
4h
f1 (ppm)

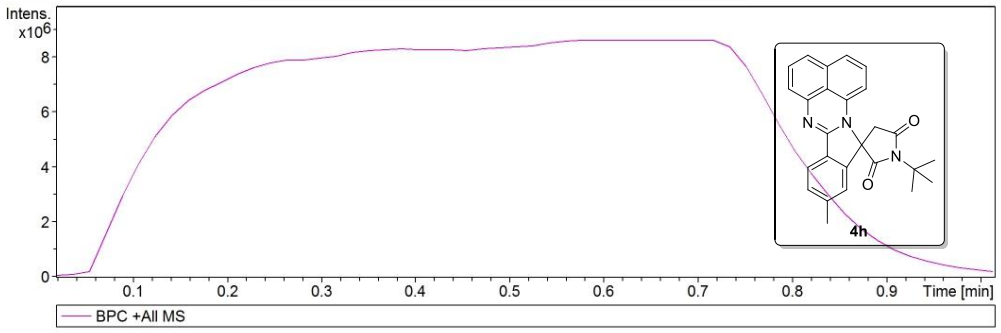
Display Report

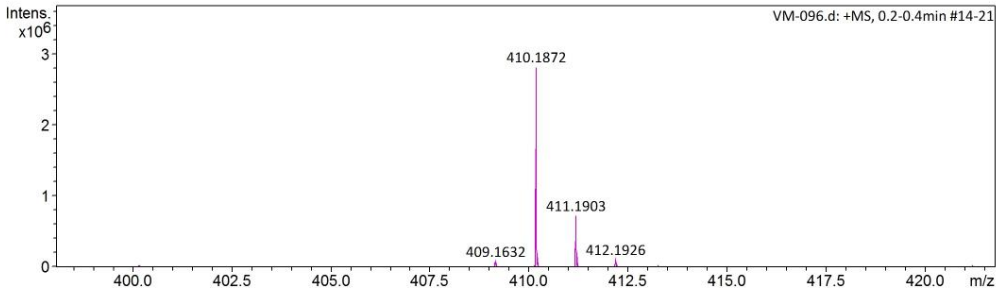
Analysis Info

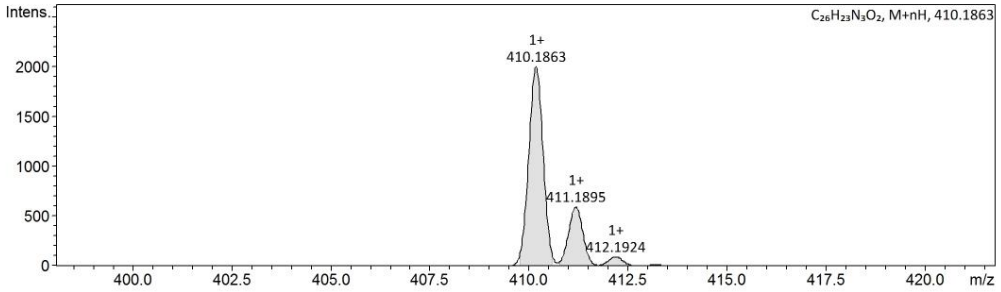
Analysis Name	D:\Data\user data\Dr. Lokman\16-04-2024\VM-096.d	Acquisition Date	4/16/2024 11:23:36 AM
Method	Tune_pos_Mid.m	Operator	vidhi
Sample Name	VM-096	Instrument	impact HD 1819696.00197
Comment			

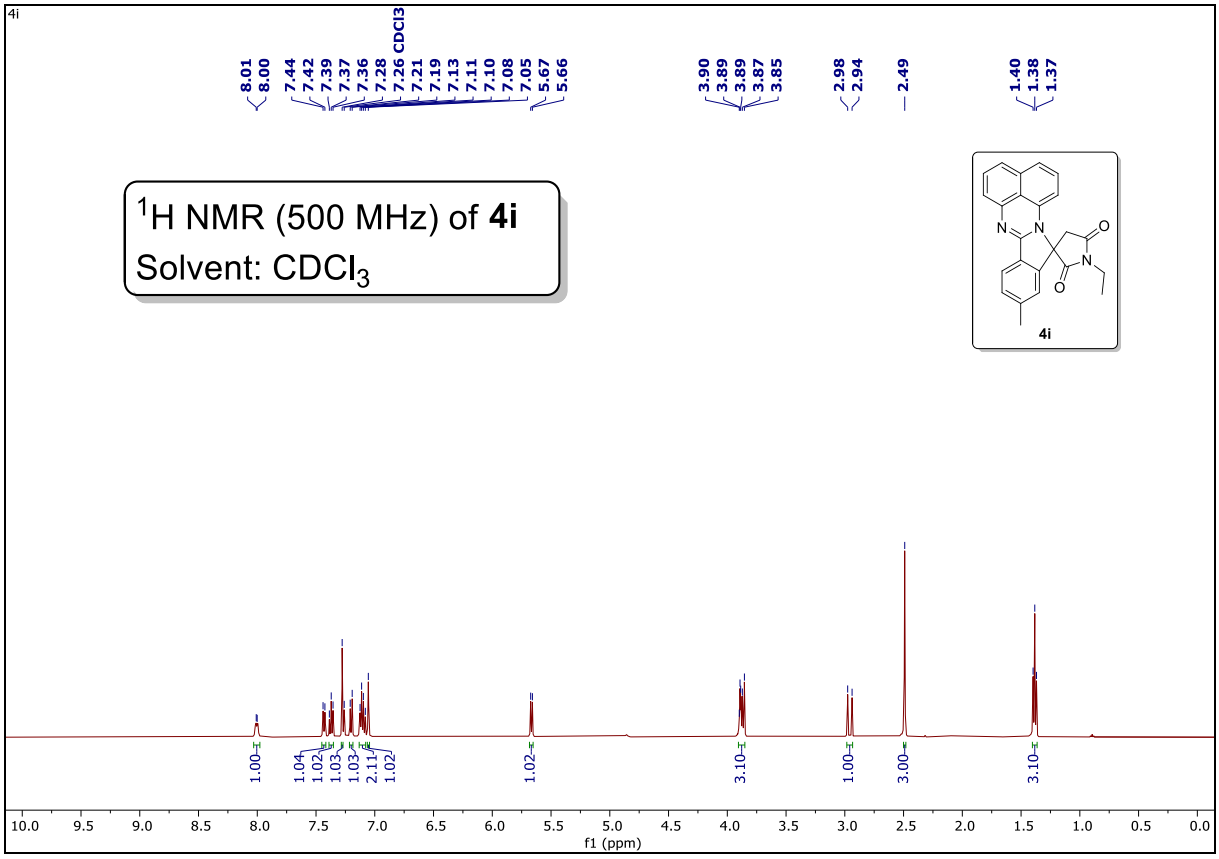
Acquisition Parameter

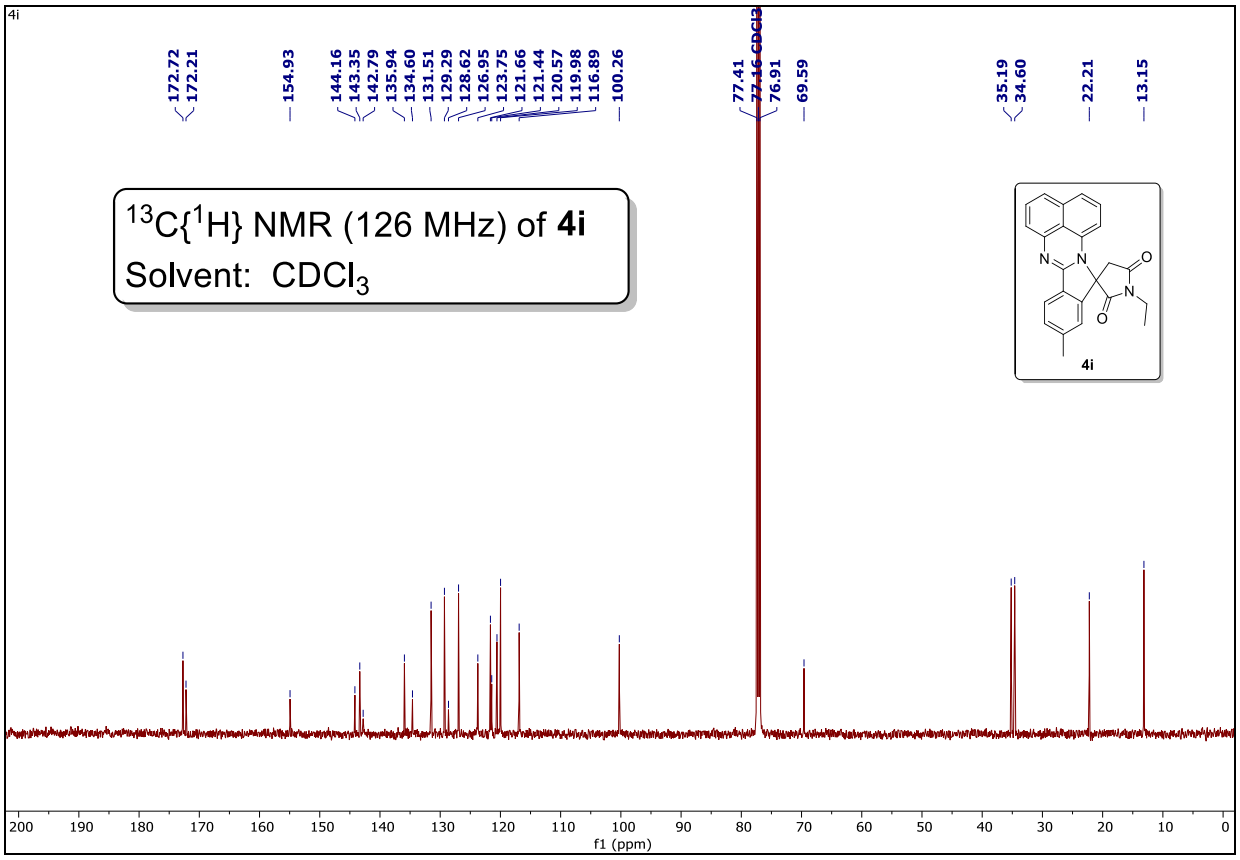
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	219 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 °C








4i
8.01
8.00
7.44
7.42
7.39
7.37
7.36
7.28
7.26 CDCl3
7.21
7.19
7.13
7.11
7.10
7.08
7.05
5.67
5.66
3.90
3.89
3.89
3.87
3.85
2.98
2.94
2.49
1.40
1.38
1.37
1H NMR (500 MHz) of 4i
Solvent: CDCl3
4i
1.00
1.04
1.02
1.03
1.03
2.11
1.02
1.02
3.10
1.00
3.00
3.10
f1 (ppm)


4i
172.72
172.21
154.93
144.16
143.35
142.79
135.94
134.60
131.51
129.29
128.62
126.95
123.75
121.66
121.44
120.57
119.98
116.89
100.26
77.41
77.16 CDCl3
76.91
69.59
35.19
34.60
22.21
13.15
13C{1H} NMR (126 MHz) of 4i
Solvent: CDCl3
4i
f1 (ppm)

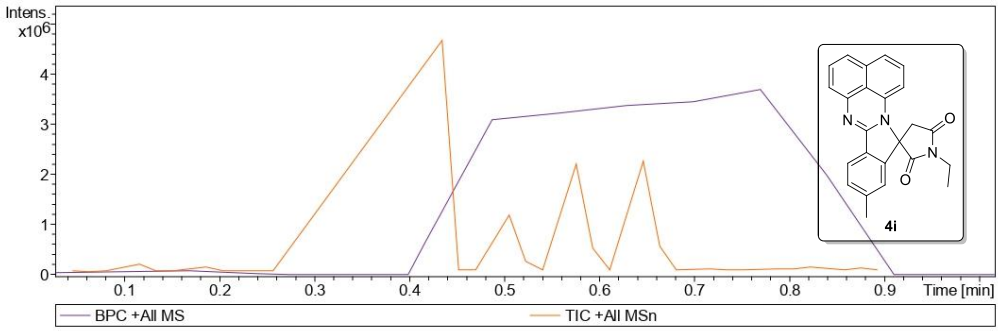
Display Report

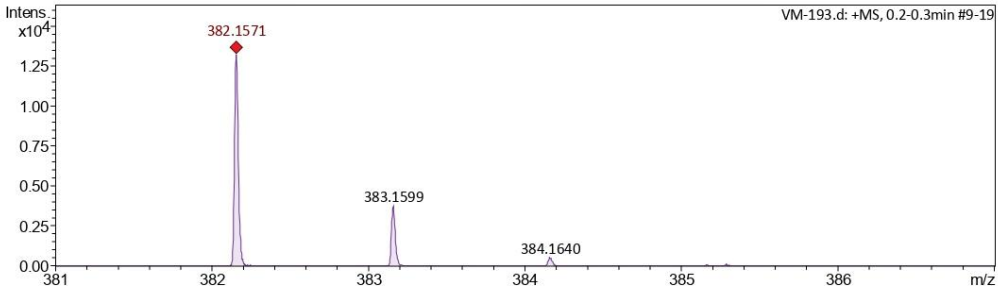
Analysis Info

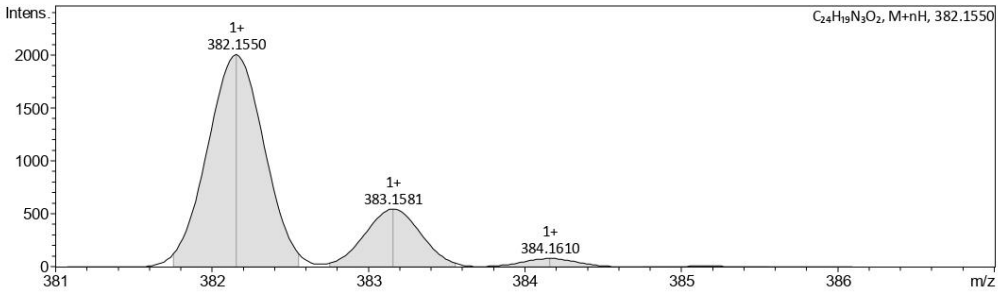
Analysis Name	D:\Data\user data\Dr. Lokman\14.03.2024\VM-193.d	Acquisition Date	3/14/2024 4:53:54 PM
Method	Tune_pos_Standard.m	Operator	vidhi
Sample Name	VM-193	Instrument	impact HD 1819696.00197
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 °C

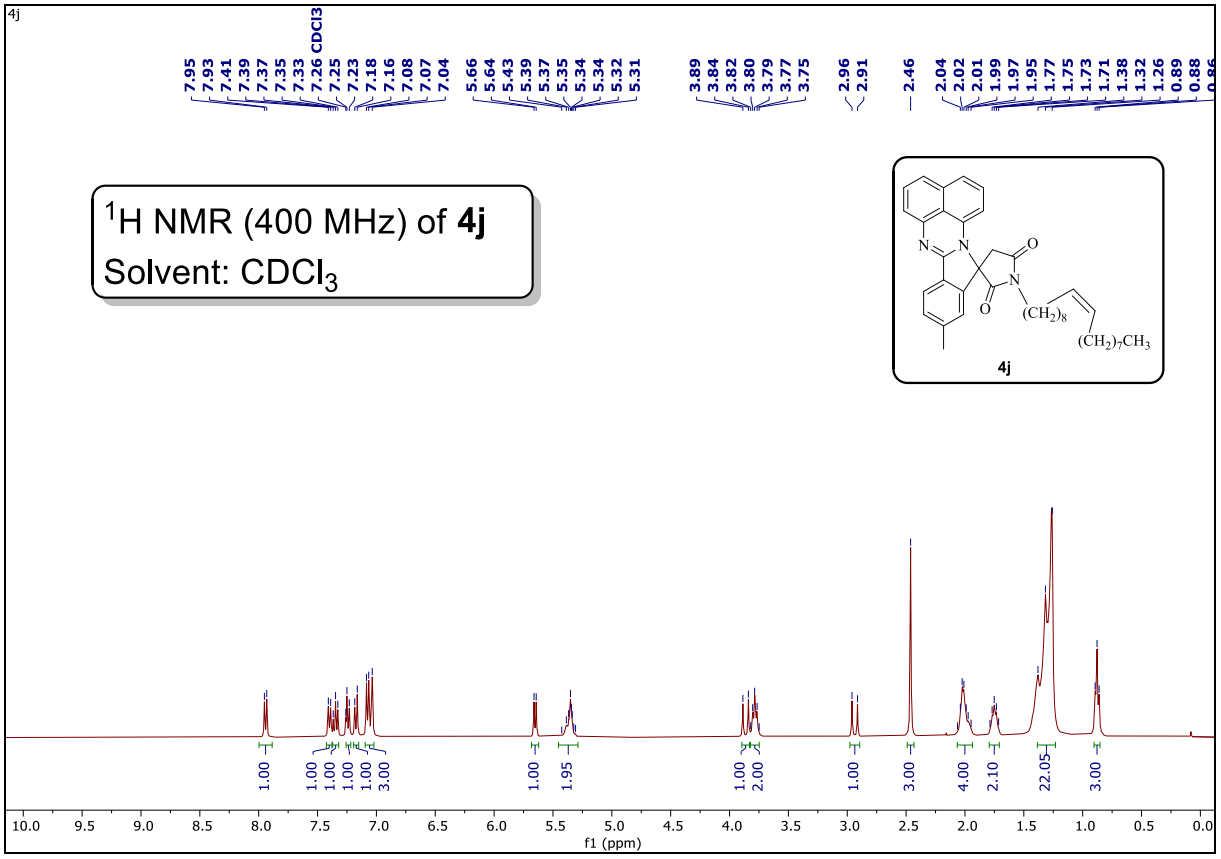


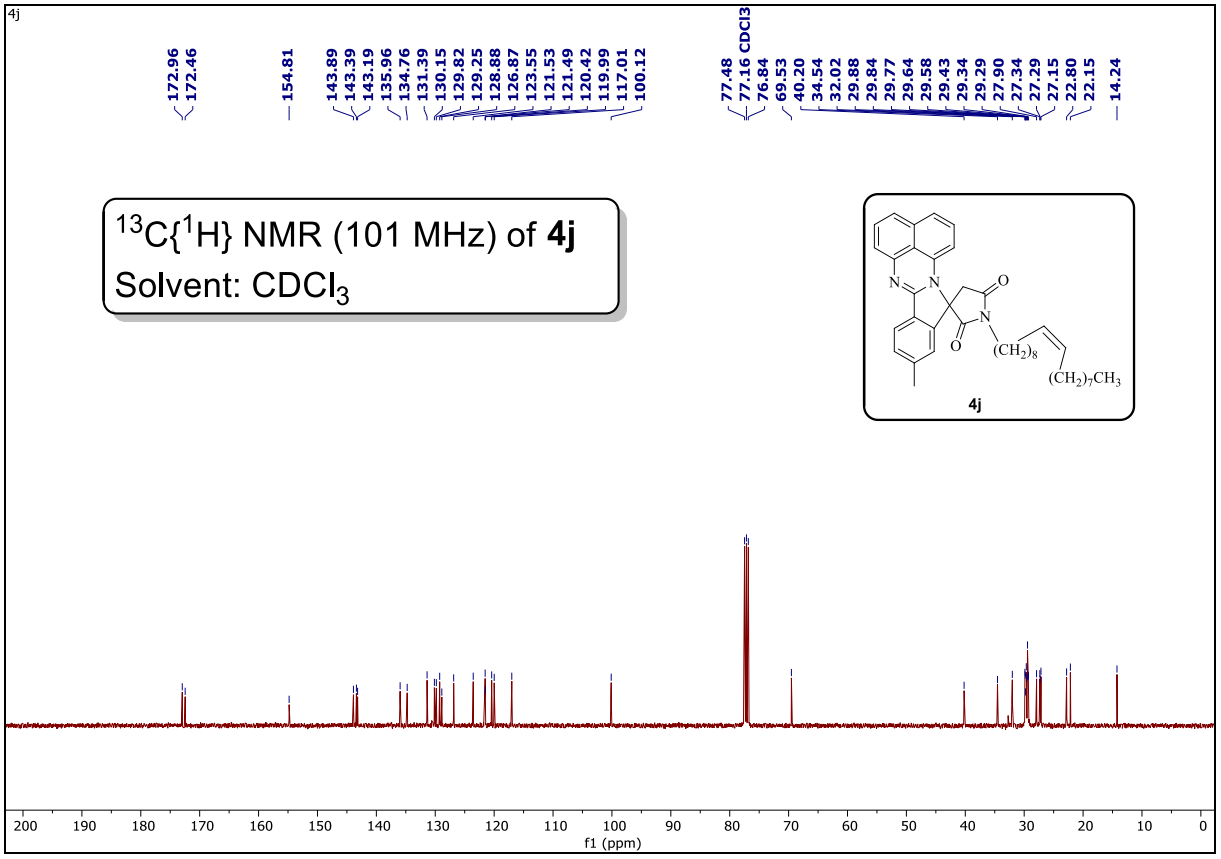




VM-193.d

Bruker Compass DataAnalysis 4.2 printed: 3/14/2024 5:21:29 PM by: vidhi Page 1 of 1


4j
7.95 7.93 7.41 7.39 7.37 7.35 7.33 CDCl3 7.26 7.25 7.23 7.18 7.16 7.08 7.07 7.04
5.66 5.64 5.43 5.39 5.37 5.35 5.34 5.34 5.32 5.31
3.89 3.84 3.82 3.80 3.79 3.77 3.75
2.96 2.91
2.46
2.04 2.02 2.01 1.99 1.97 1.95 1.77 1.75 1.73 1.71 1.38 1.32 1.26 0.89 0.88
1H NMR (400 MHz) of 4j
Solvent: CDCl3
4j
1.00 1.00 1.00 1.00 3.00 1.00 1.95 1.00 2.00 1.00 3.00 4.00 2.10 22.05 3.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


4j
172.96 172.46
154.81
143.89 143.39 143.19 135.96 134.76 131.39 130.15 129.82 129.25 128.88 126.87 123.55 121.53 121.49 120.42 119.99 117.01 100.12
77.48 77.16 CDCl3 76.84 69.53 40.20 34.54 32.02 29.88 29.84 29.77 29.64 29.58 29.43 29.34 29.29 27.90 27.34 27.29 27.15 22.80 22.15
14.24
13C{1H} NMR (101 MHz) of 4j
Solvent: CDCl3
4j
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

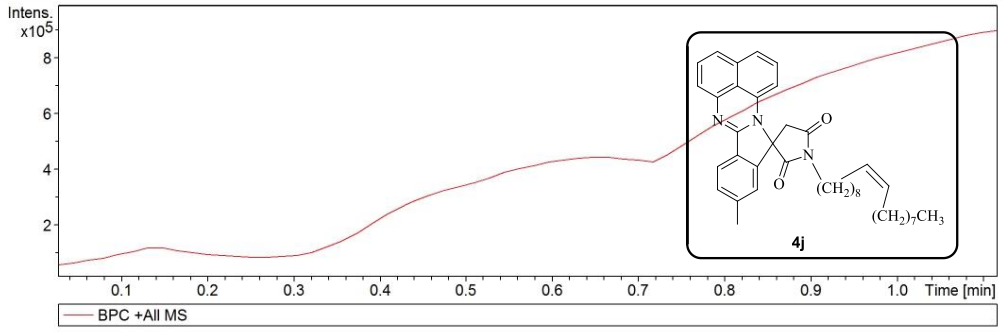
Display Report

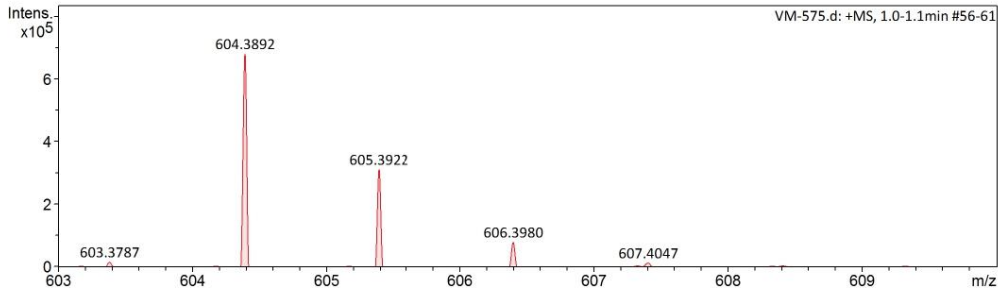
Analysis Info

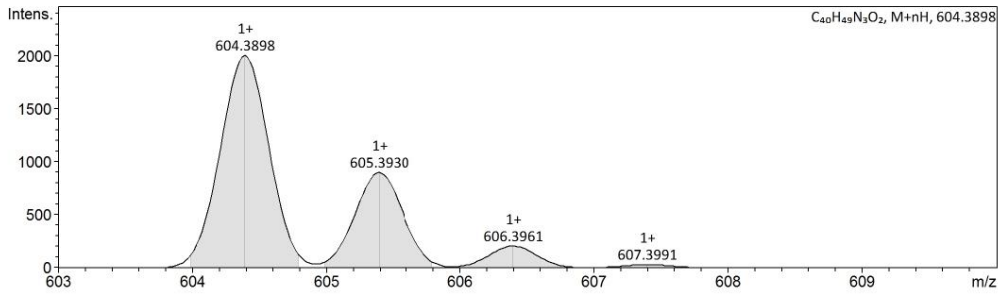
Analysis Name	D:\Data\user data\Dr. Lokman\24-02-2025\VM-575.d	Acquisition Date	2/24/2025 10:55:20 AM
Method	low_mass.m	Operator	Gudipati SrinivasaRao
Sample Name	VM-575	Instrument	impact HD 1819696.00197
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.6 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	5.0 l/min
Scan End	1500 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C

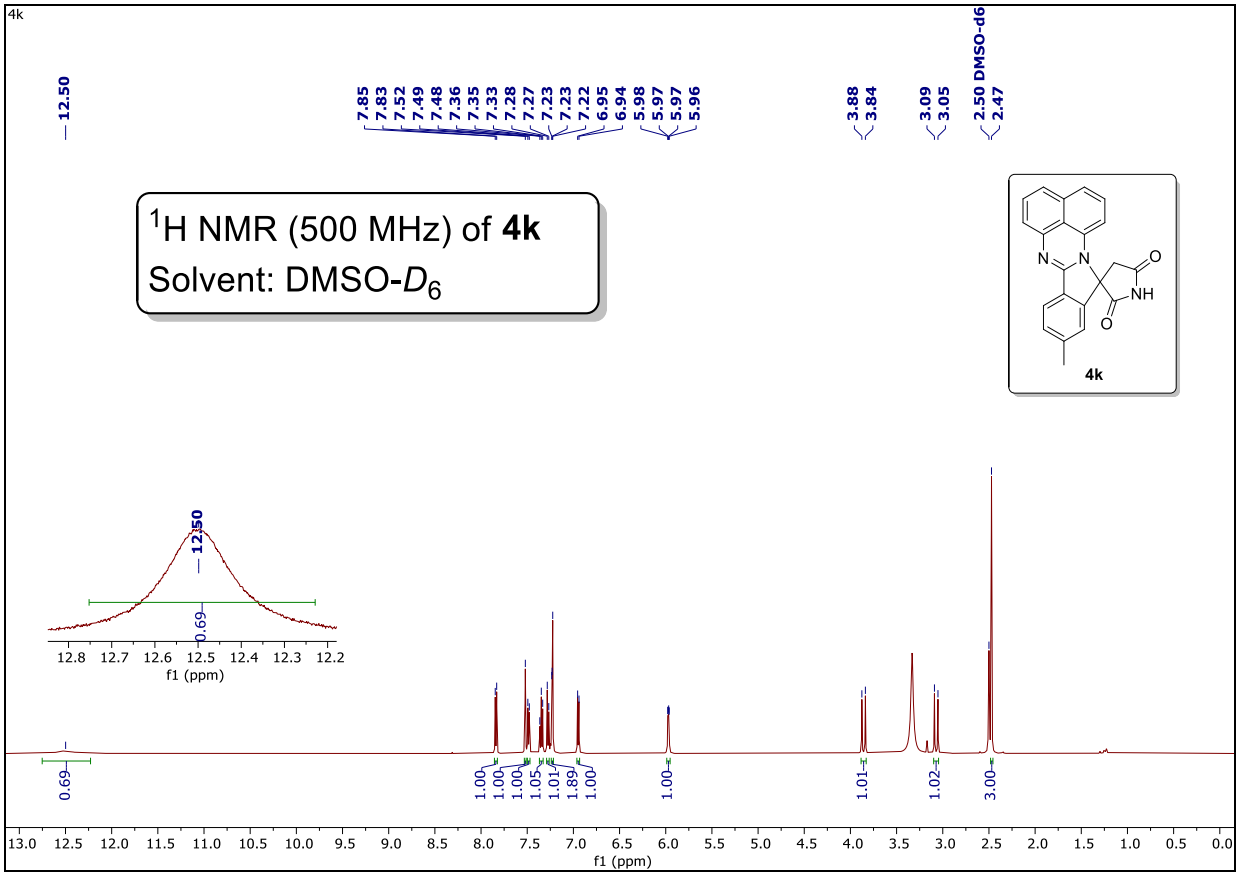


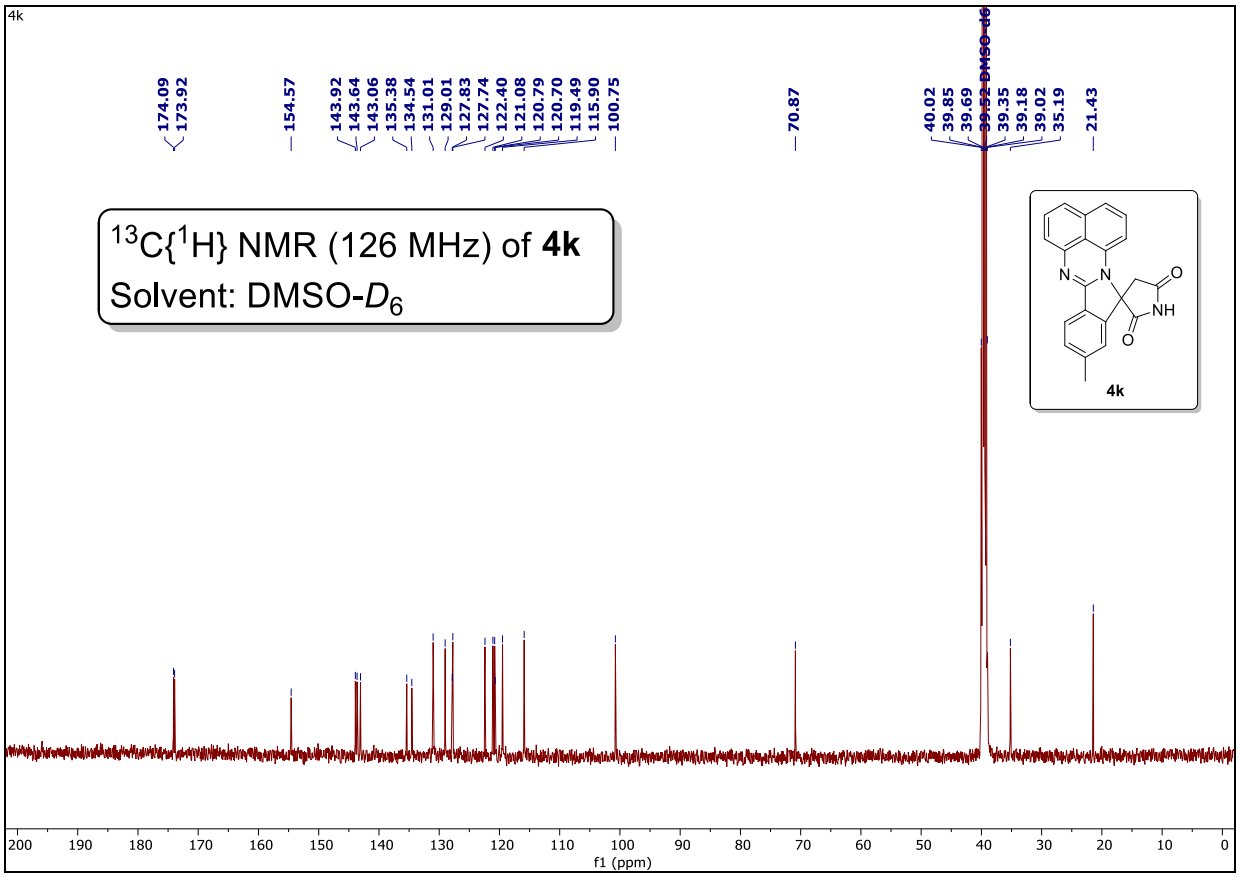




VM-575.d

Gudipati


4k
12.50
7.85
7.83
7.52
7.49
7.48
7.36
7.35
7.33
7.28
7.27
7.23
7.23
7.22
6.95
6.94
5.98
5.97
5.97
5.96
3.88
3.84
3.09
3.05
2.50 DMSO-d6
2.47
1H NMR (500 MHz) of 4k
Solvent: DMSO-D6
4k
f1 (ppm)


4k
174.09
173.92
154.57
143.92
143.64
143.06
135.38
134.54
131.01
129.01
127.83
127.74
122.40
121.08
120.79
120.70
119.49
115.90
100.75
70.87
40.02
39.85
39.69
39.52 DMSO-d6
39.35
39.18
39.02
35.19
21.43
13C{1H} NMR (126 MHz) of 4k
Solvent: DMSO-D6
4k
f1 (ppm)

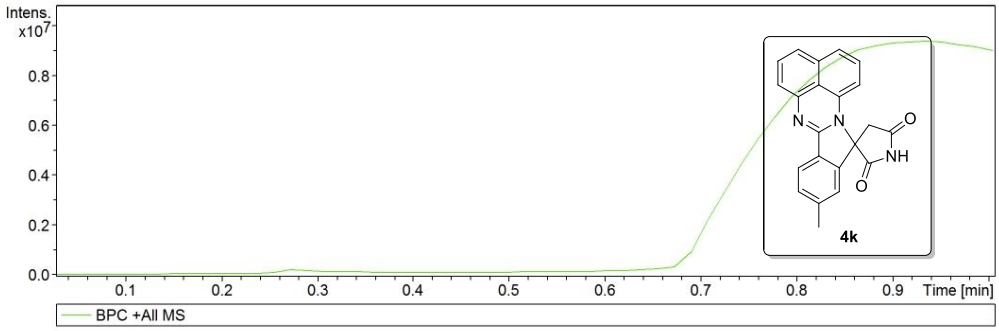
Display Report

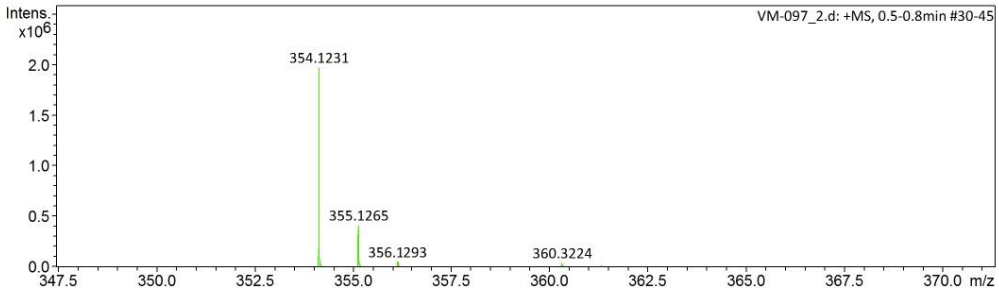
Analysis Info

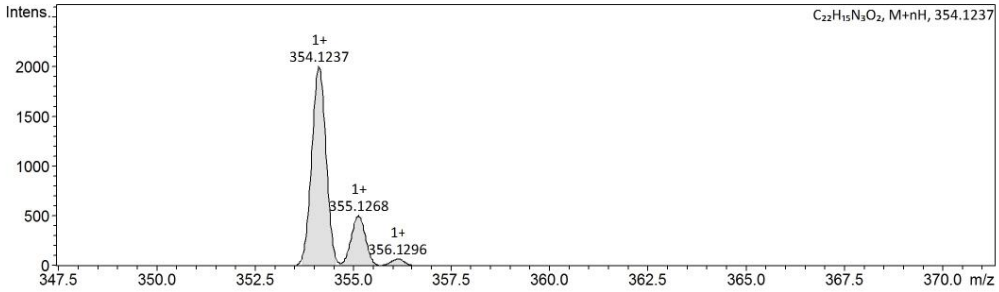
Analysis Name	D:\Data\user data\Dr. Lokman\09-04-2024\VM-097_2.d	Acquisition Date	4/9/2024 3:41:15 PM
Method	Tune_pos_Mid.m	Operator	vidhi
Sample Name	VM-097_2	Instrument	impact HD 1819696.00197
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	219 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 °C

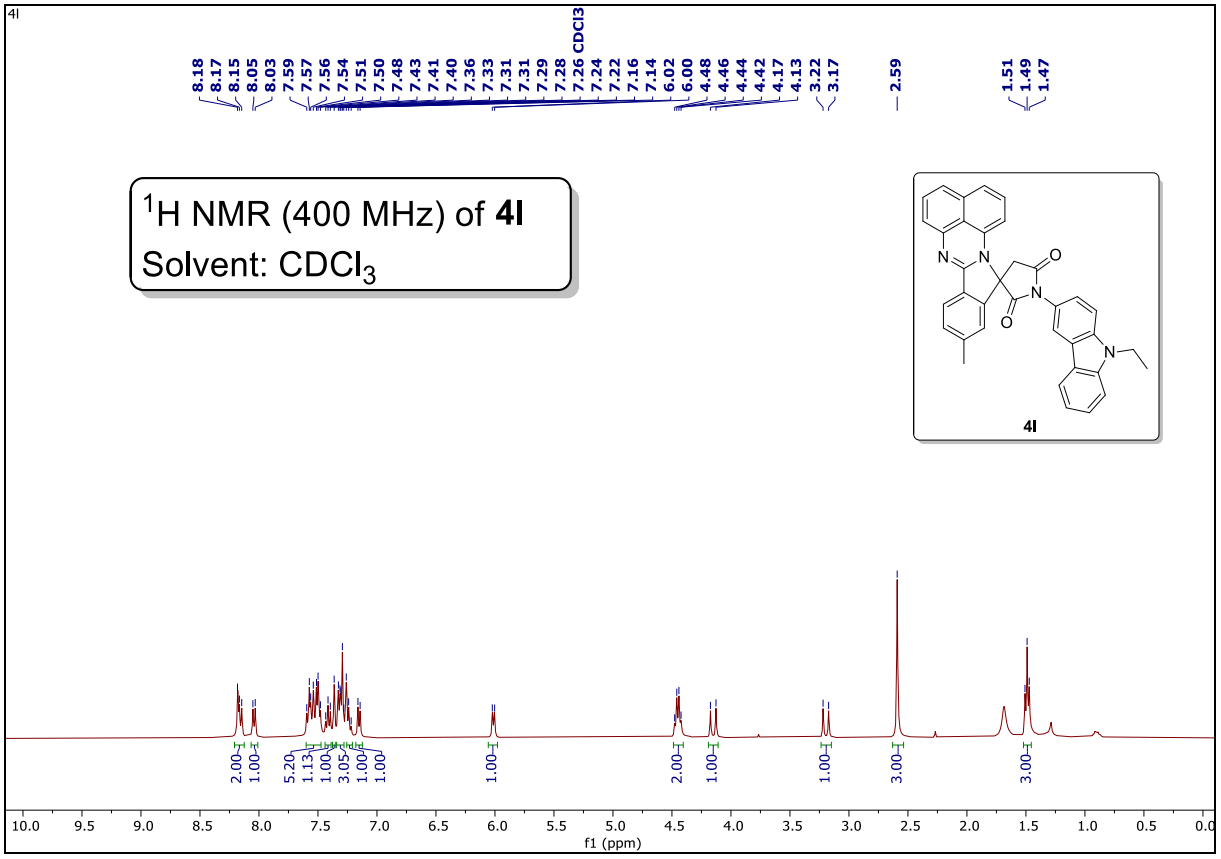


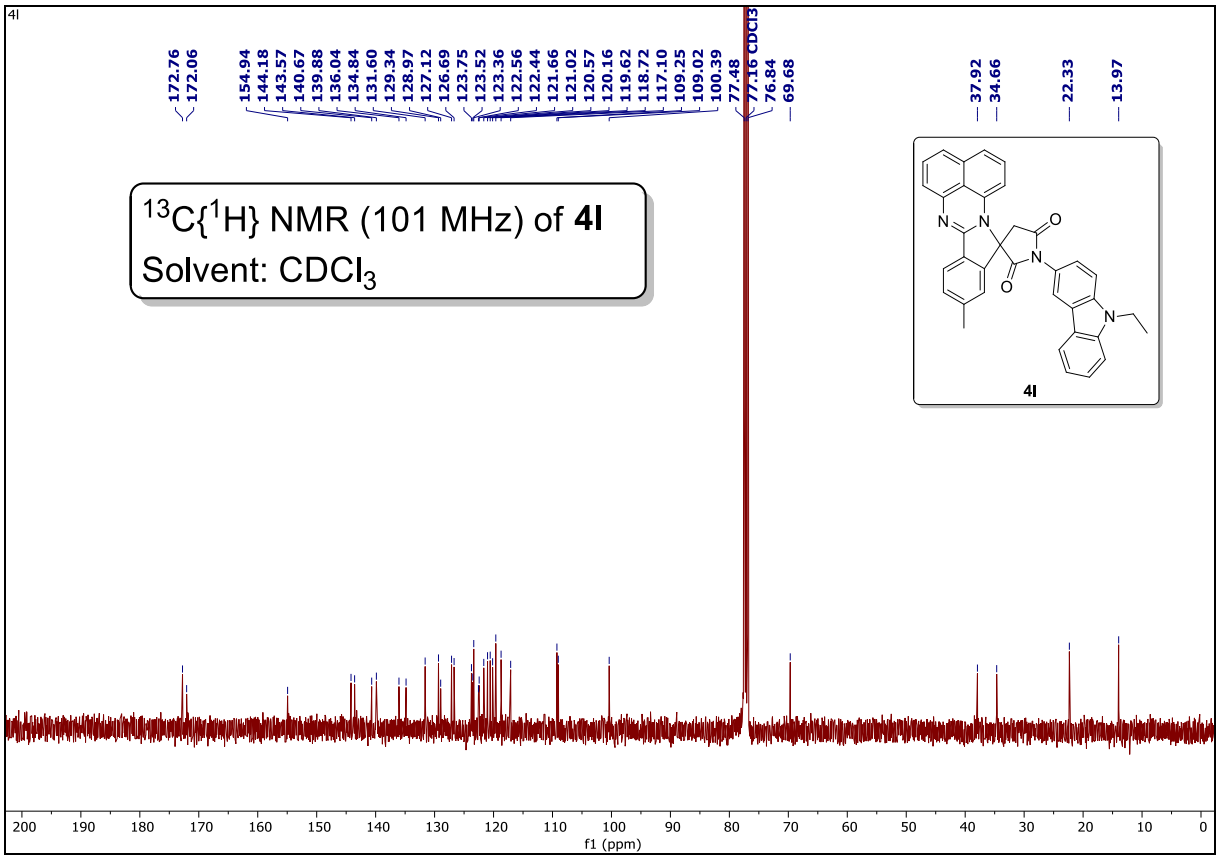




VM-097_2.d

Bruker Compass DataAnalysis 4.2 printed: 4/9/2024 3:43:41 PM by: vidhi Page 1 of 1


4l
8.18
8.17
8.15
8.05
8.03
7.59
7.57
7.56
7.54
7.51
7.50
7.48
7.43
7.41
7.40
7.36
7.33
7.31
7.31
7.29
7.28
7.26 CDCl3
7.24
7.22
7.16
7.14
6.02
6.00
4.48
4.46
4.44
4.42
4.17
4.13
3.22
3.17
2.59
1.51
1.49
1.47
^{1}H NMR (400 MHz) of **4l**
Solvent: $CDCl_3$
4l
2.00
1.00
5.20
1.13
1.00
3.05
1.00
1.00
1.00
1.00
2.00
1.00
1.00
3.00
3.00
f1 (ppm)


4l
172.76
172.06
154.94
144.18
143.57
140.67
139.88
136.04
134.84
131.60
129.34
128.97
127.12
126.69
123.75
123.52
123.36
122.56
122.44
121.66
121.02
120.57
120.16
119.62
118.72
117.10
109.25
109.02
100.39
77.48
77.16 CDCl3
76.84
69.68
37.92
34.66
22.33
13.97
^{13}C{^{1}H} NMR (101 MHz) of **4l**
Solvent: $CDCl_3$
4l
f1 (ppm)

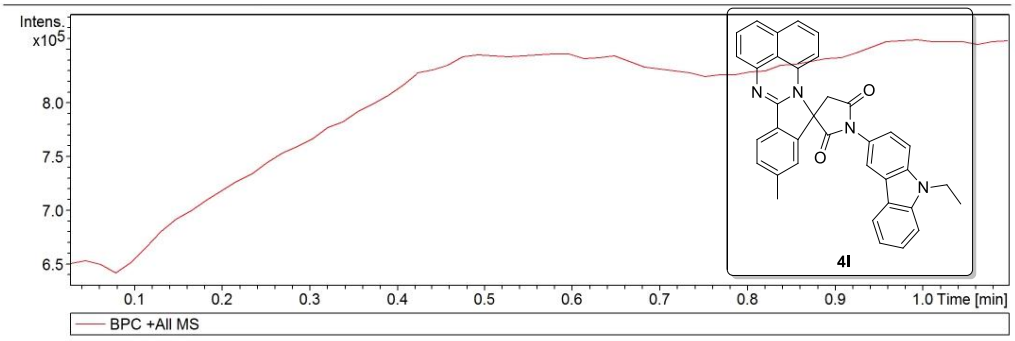
Display Report

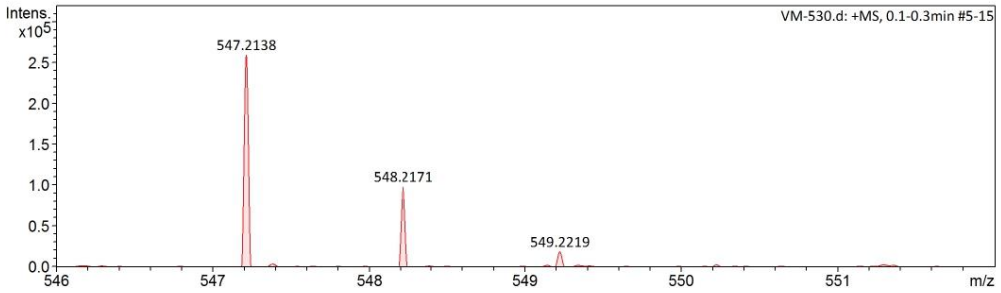
Analysis Info

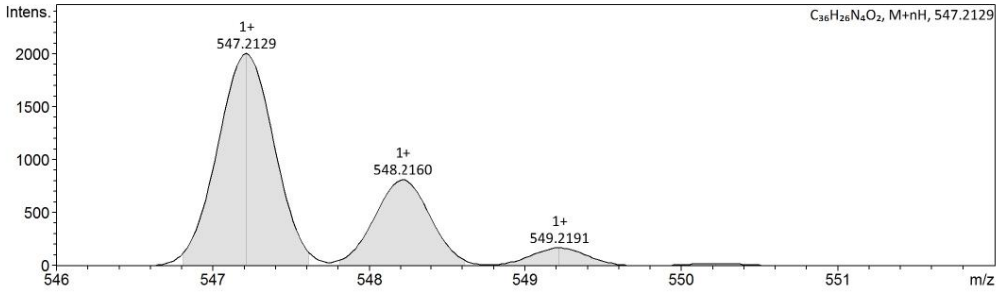
Analysis Name	D:\Data\user data\Dr. Lokman\18-02-2025\VM-530.d	Acquisition Date	2/18/2025 12:18:03 PM
Method	low_mass.m	Operator	Gudipati SrinivasaRao
Sample Name	VM-530	Instrument	impact HD 1819696.00197
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.6 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	5.0 l/min
Scan End	1500 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C

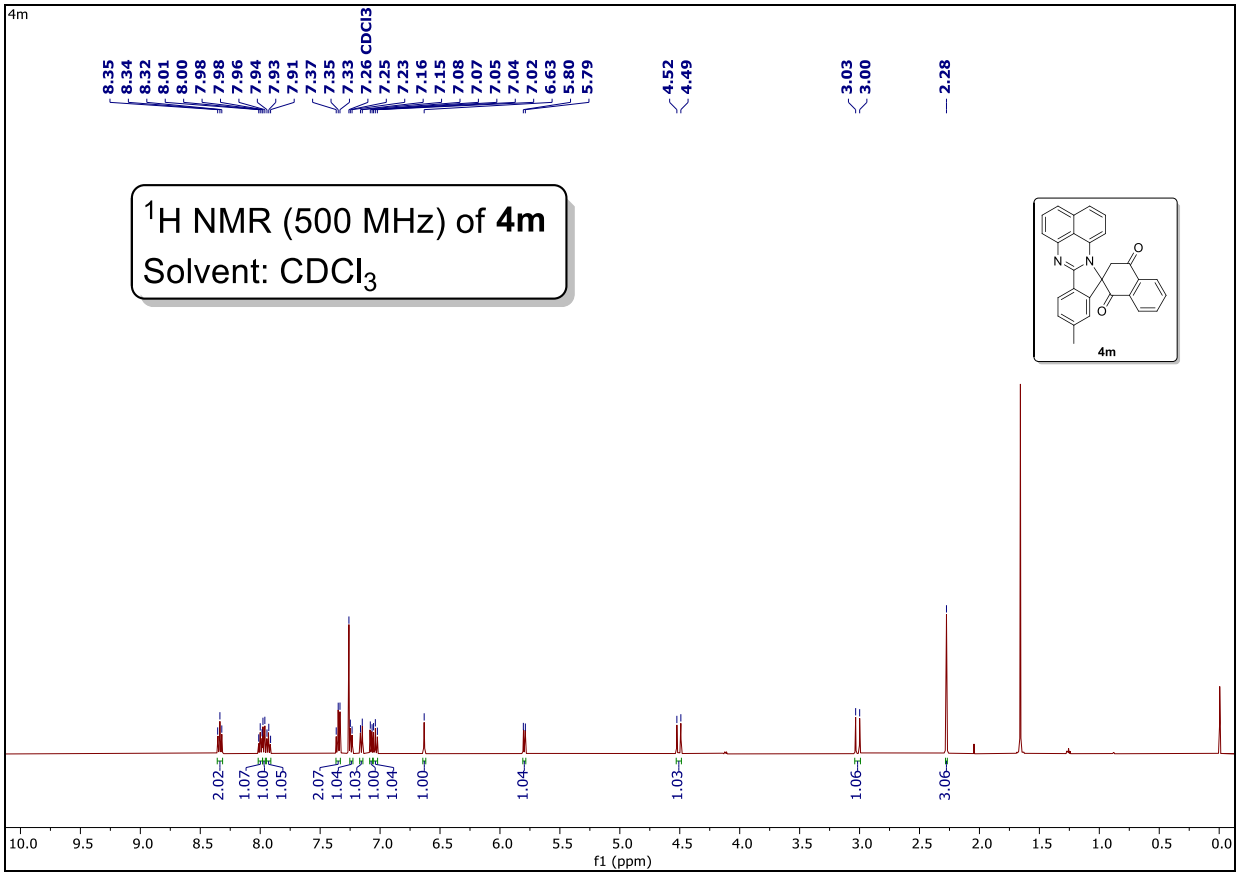


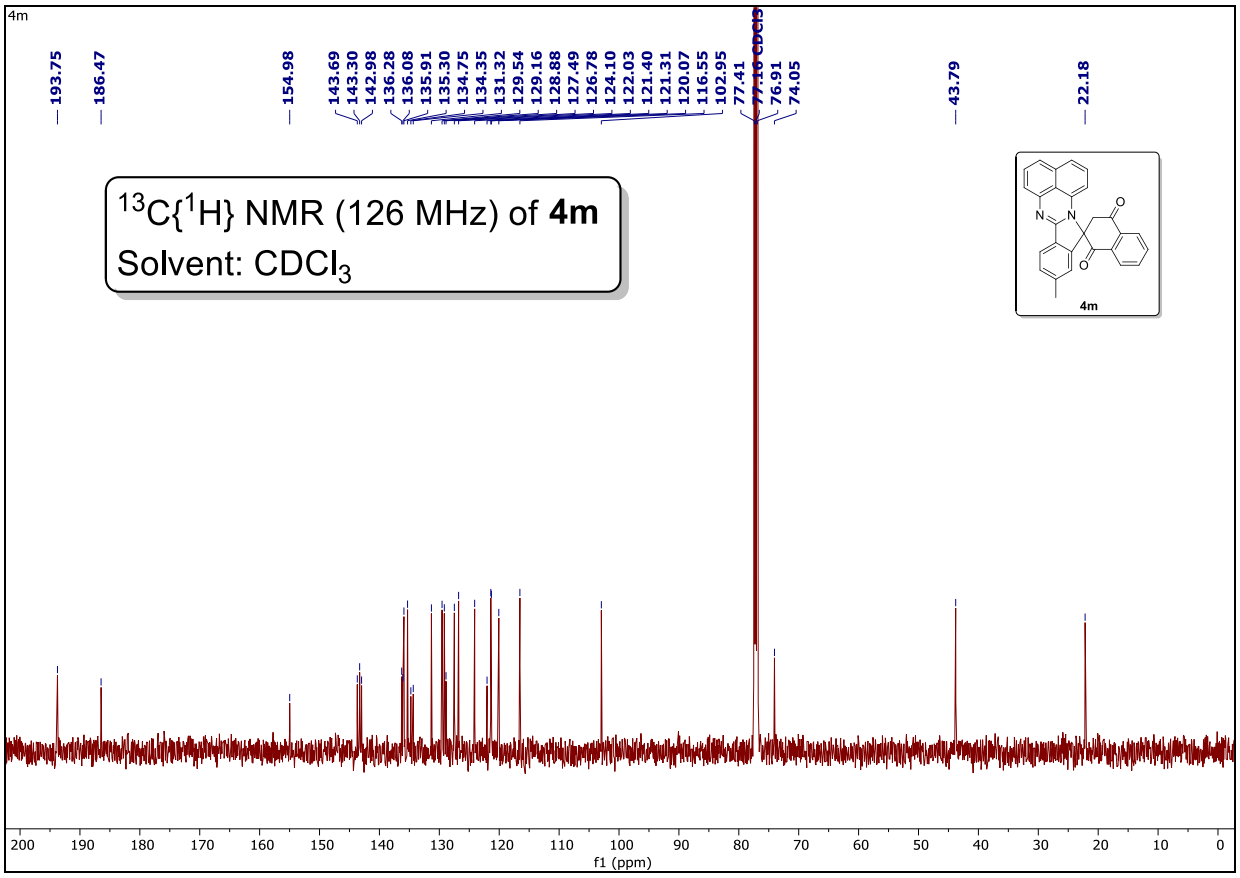




VM-530.d

Gudipati


4m
8.35
8.34
8.32
8.01
8.00
7.98
7.98
7.96
7.94
7.93
7.91
7.37
7.35
7.33
7.26 CDCl3
7.25
7.23
7.16
7.15
7.08
7.07
7.05
7.04
7.02
6.63
5.80
5.79
4.52
4.49
3.03
3.00
2.28
1H NMR (500 MHz) of 4m
Solvent: CDCl3
4m
2.02
1.07
1.00
1.05
2.07
1.04
1.03
1.00
1.04
1.00
1.04
1.03
1.06
3.06
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


4m
193.75
186.47
154.98
143.69
143.30
142.98
136.28
136.08
135.91
135.30
134.75
134.35
131.32
129.54
129.16
128.88
127.49
126.78
124.10
122.03
121.40
121.31
120.07
116.55
102.95
77.41
77.10 CDCl3
76.91
74.05
43.79
22.18
13C{1H} NMR (126 MHz) of 4m
Solvent: CDCl3
4m
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

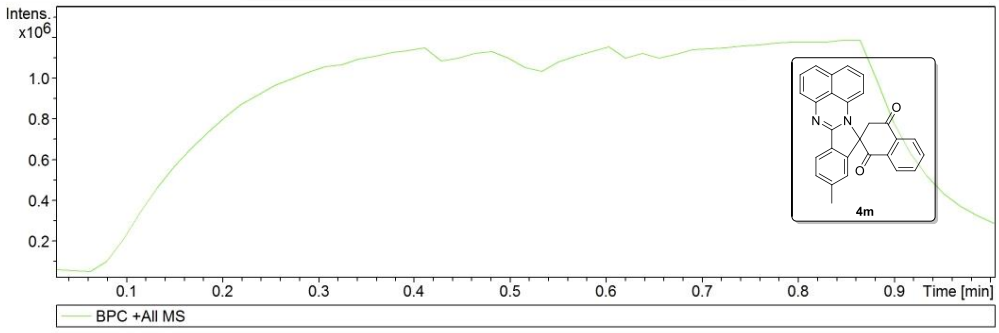
Display Report

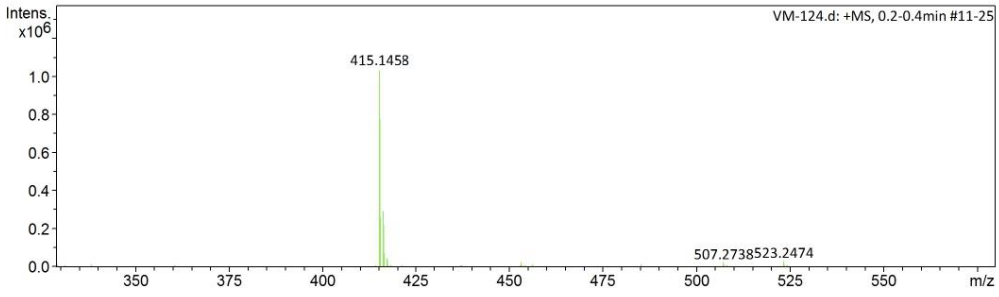
Analysis Info

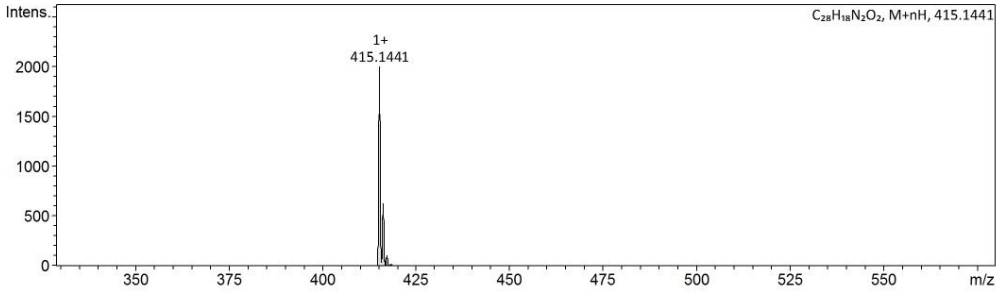
Analysis Name	D:\Data\user data\Dr. Lokman\09-04-2024\VM-124.d	Acquisition Date	4/9/2024 4:11:14 PM
Method	Tune_pos_Mid.m	Operator	vidhi
Sample Name	VM-124	Instrument	impact HD 1819696.00197
Comment			

Acquisition Parameter

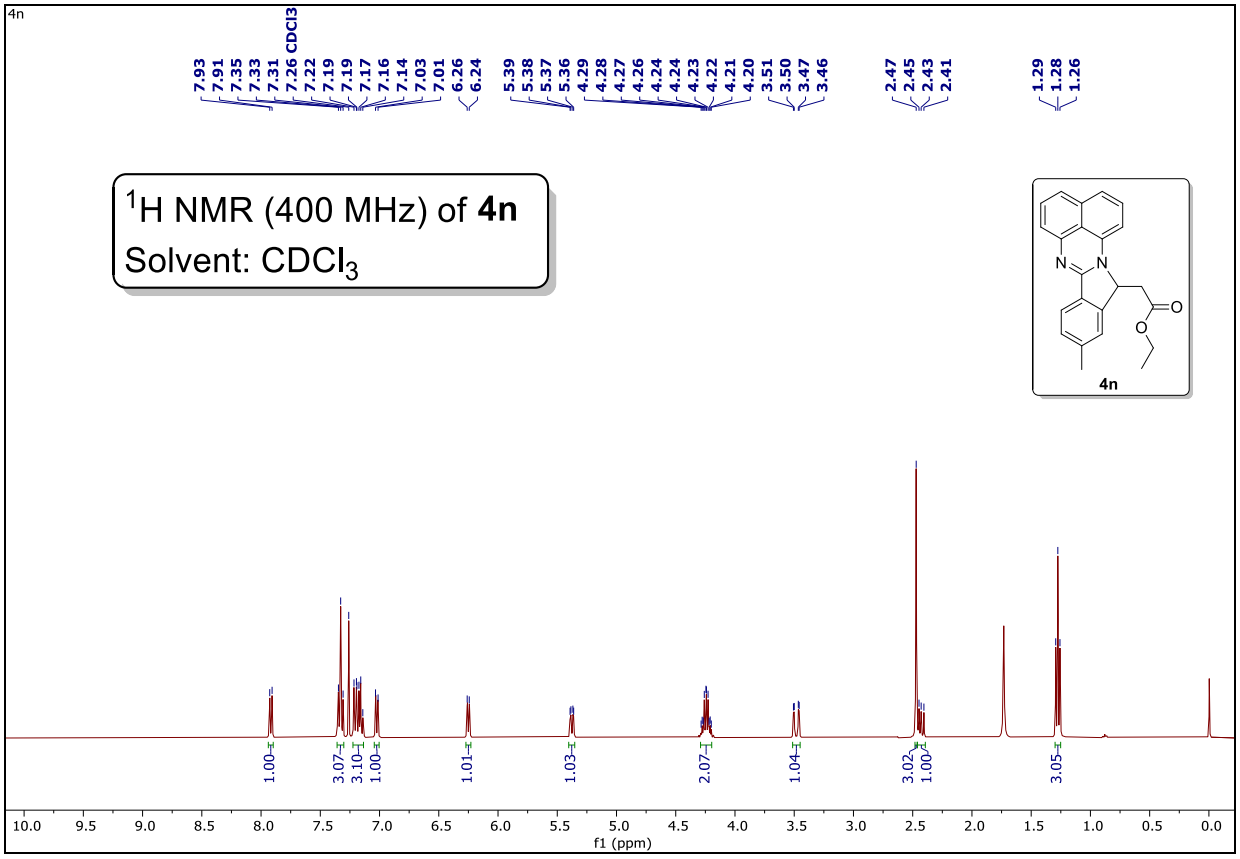
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	219 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 °C

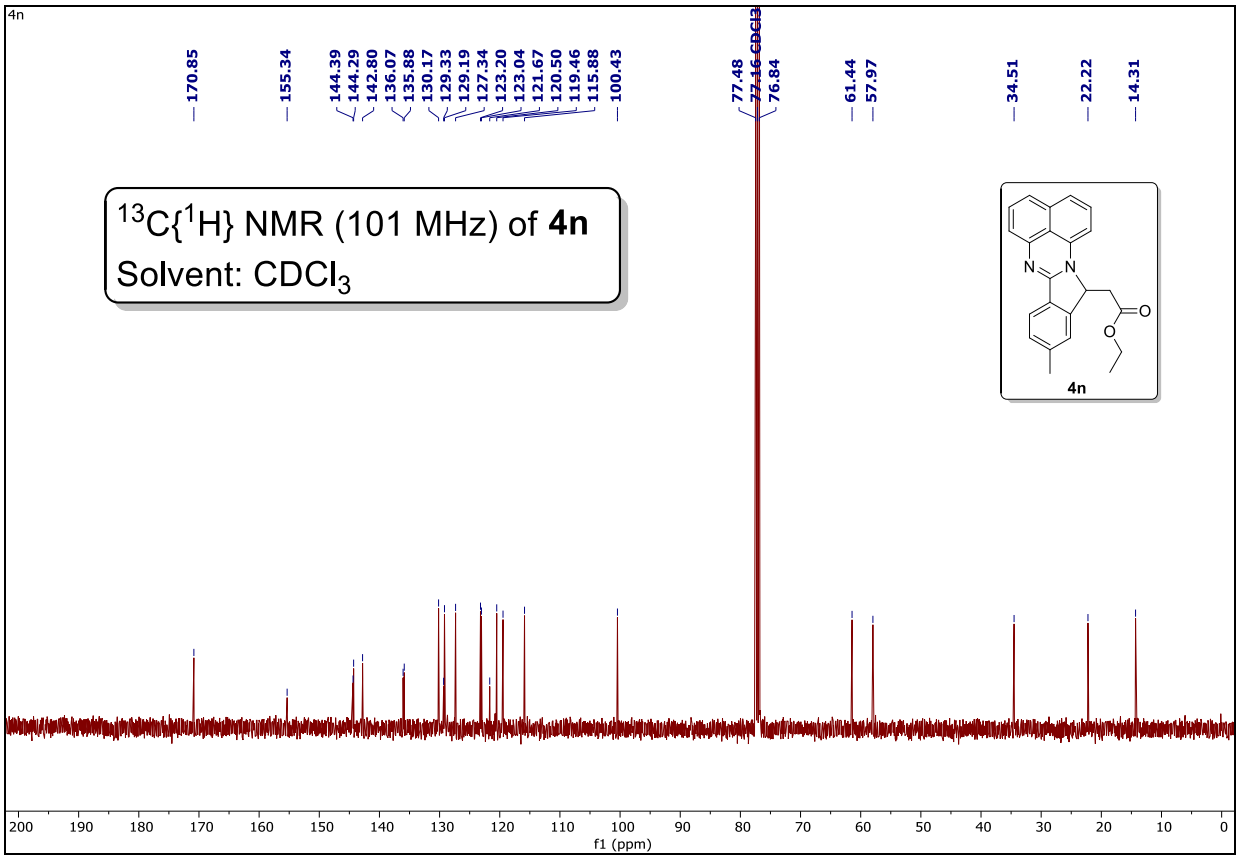






VM-124.d


4n
7.93 7.91 7.35 7.33 7.31 7.26 CDCl3 7.22 7.19 7.19 7.17 7.16 7.14 7.03 7.01 6.26 6.24
5.39 5.38 5.37 5.36 4.29 4.28 4.27 4.26 4.24 4.24 4.23 4.22 4.21 4.20 3.51 3.50 3.47 3.46
2.47 2.45 2.43 2.41
1.29 1.28 1.26
^{1}H NMR (400 MHz) of **4n**
Solvent: $CDCl_3$
4n
1.00 3.07 3.10 1.00 1.01 1.03 2.07 1.04 3.02 1.00 3.05
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


4n
170.85 155.34 144.39 144.29 142.80 136.07 135.88 130.17 129.33 129.19 127.34 123.20 123.04 121.67 120.50 119.46 115.88 100.43
77.48 77.16 CDCl3 76.84
61.44 57.97
34.51 22.22 14.31
^{13}C{^{1}H} NMR (101 MHz) of **4n**
Solvent: $CDCl_3$
4n
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

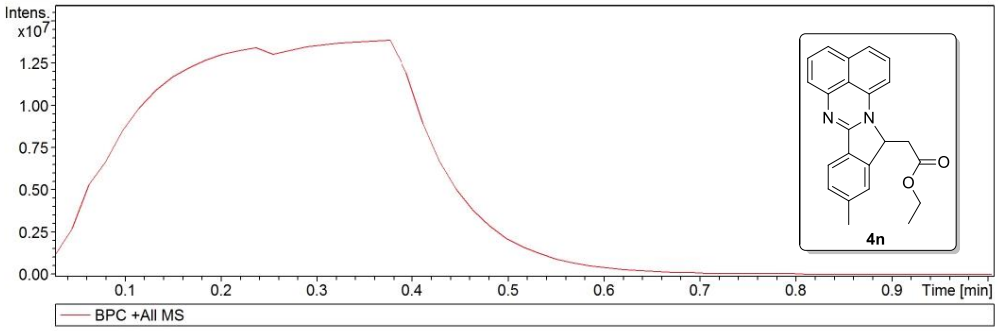
Display Report

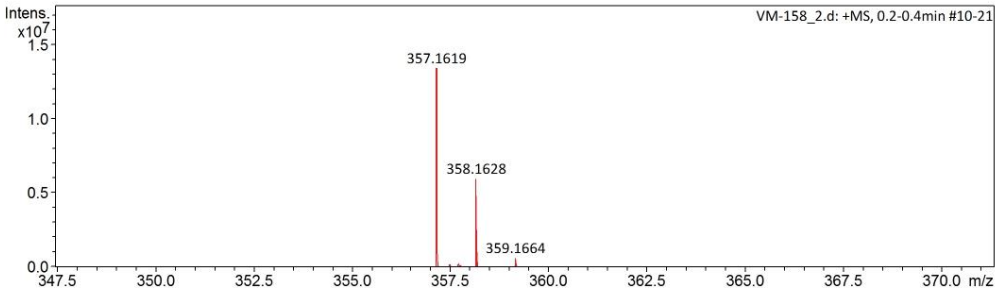
Analysis Info

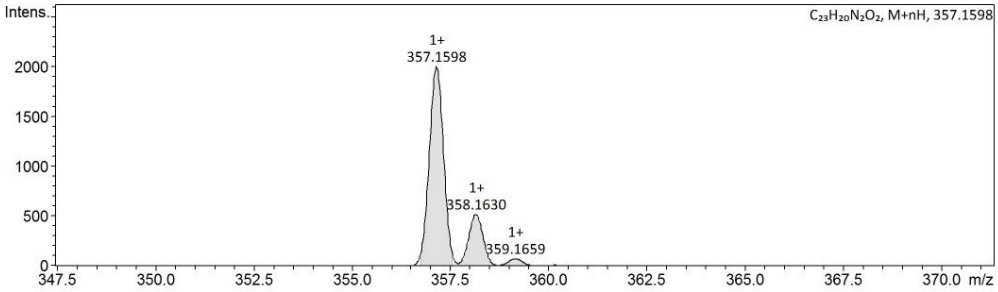
Analysis Name	D:\Data\user data\Dr. Lokman\09-04-2024\VM-158_2.d	Acquisition Date	4/9/2024 3:47:37 PM
Method	Tune_pos_Mid.m	Operator	vidhi
Sample Name	VM-158_2	Instrument	impact HD 1819696.00197
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	219 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 °C

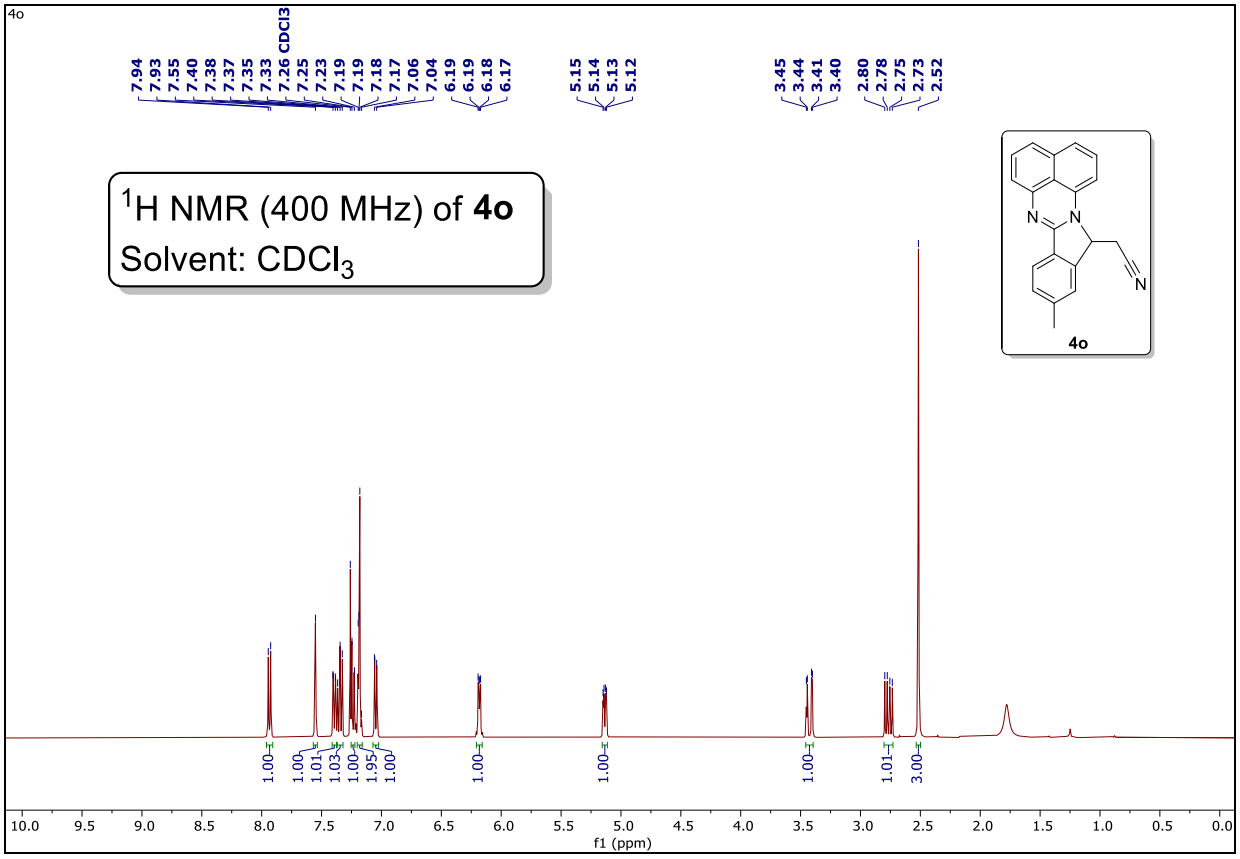


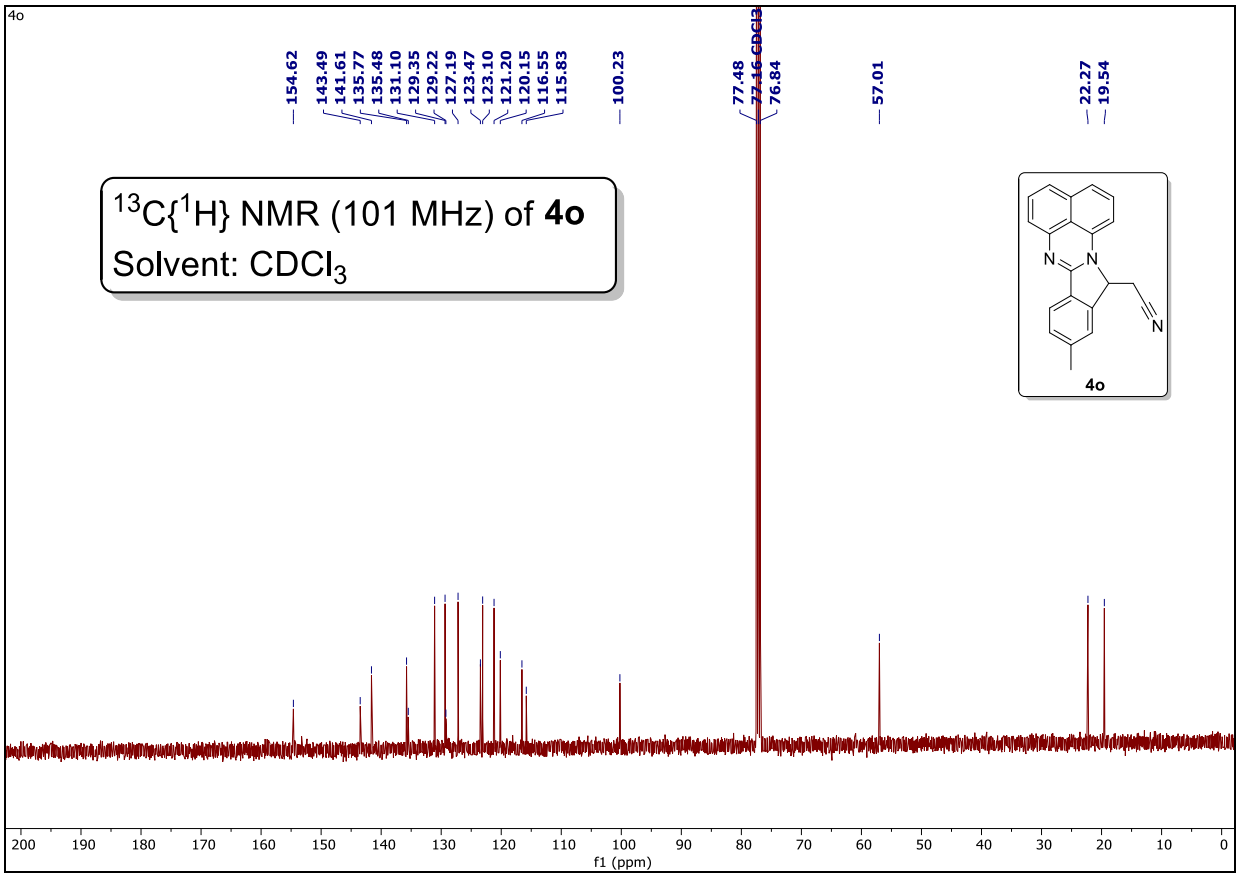




VM-158_2.d

Bruker Compass DataAnalysis 4.2 printed: 4/9/2024 3:49:49 PM by: vidhi Page 1 of 1


4o
7.94
7.93
7.55
7.40
7.38
7.37
7.35
7.33
7.26 CDCl3
7.25
7.23
7.19
7.19
7.18
7.17
7.06
7.04
6.19
6.19
6.18
6.17
5.15
5.14
5.13
5.12
3.45
3.44
3.41
3.40
2.80
2.78
2.75
2.73
2.52
1H NMR (400 MHz) of 4o
Solvent: CDCl3
4o
1.00
1.00
1.01
1.03
1.00
1.95
1.00
1.00
1.00
1.00
1.01
3.00
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


4o
154.62
143.49
141.61
135.77
135.48
131.10
129.35
129.22
127.19
123.47
123.10
121.20
120.15
116.55
115.83
100.23
77.48
77.16 CDCl3
76.84
57.01
22.27
19.54
13C{1H} NMR (101 MHz) of 4o
Solvent: CDCl3
4o
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

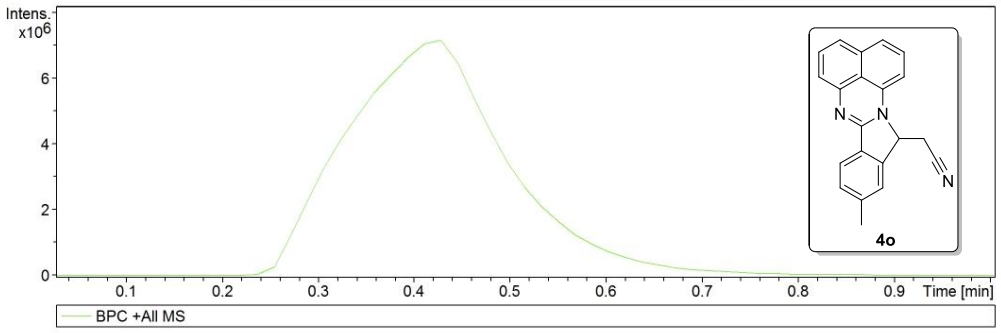
Display Report

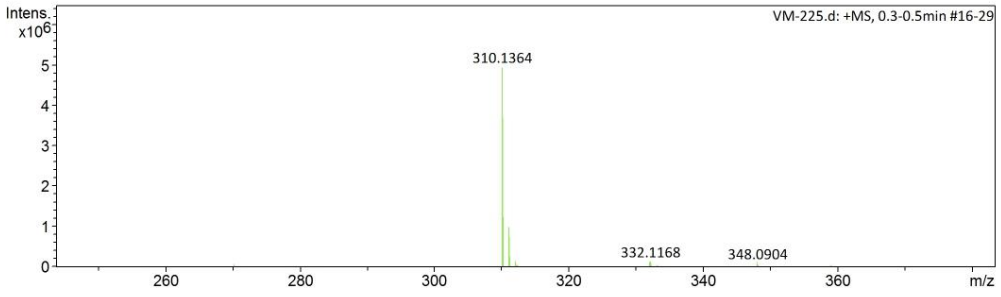
Analysis Info

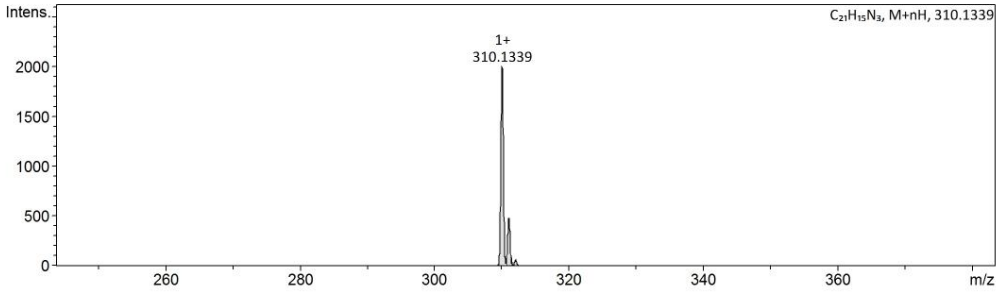
Analysis Name	D:\Data\user data\Dr. Lokman\09-04-2024\VM-225.d	Acquisition Date	4/9/2024 12:31:15 PM
Method	Tune_pos_Mid.m	Operator	vidhi
Sample Name	VM-225	Instrument	impact HD 1819696.00197
Comment			

Acquisition Parameter

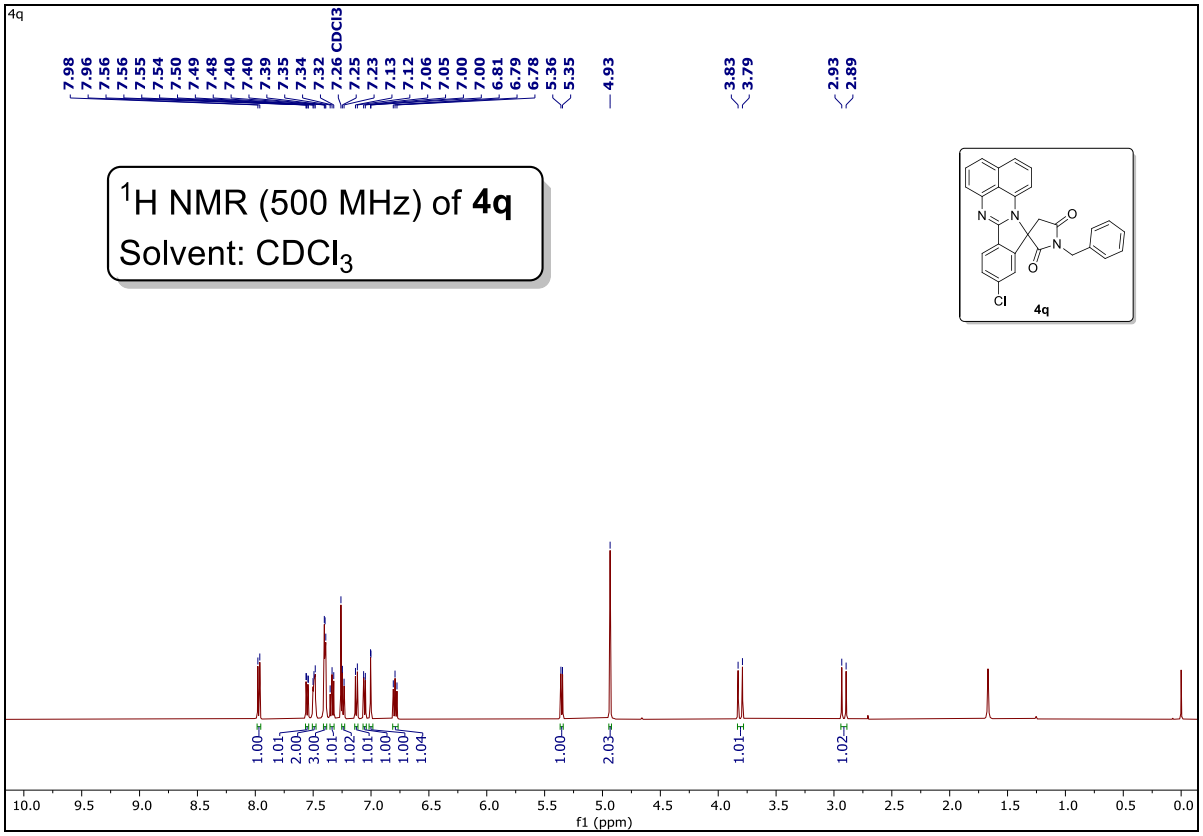
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	219 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 °C

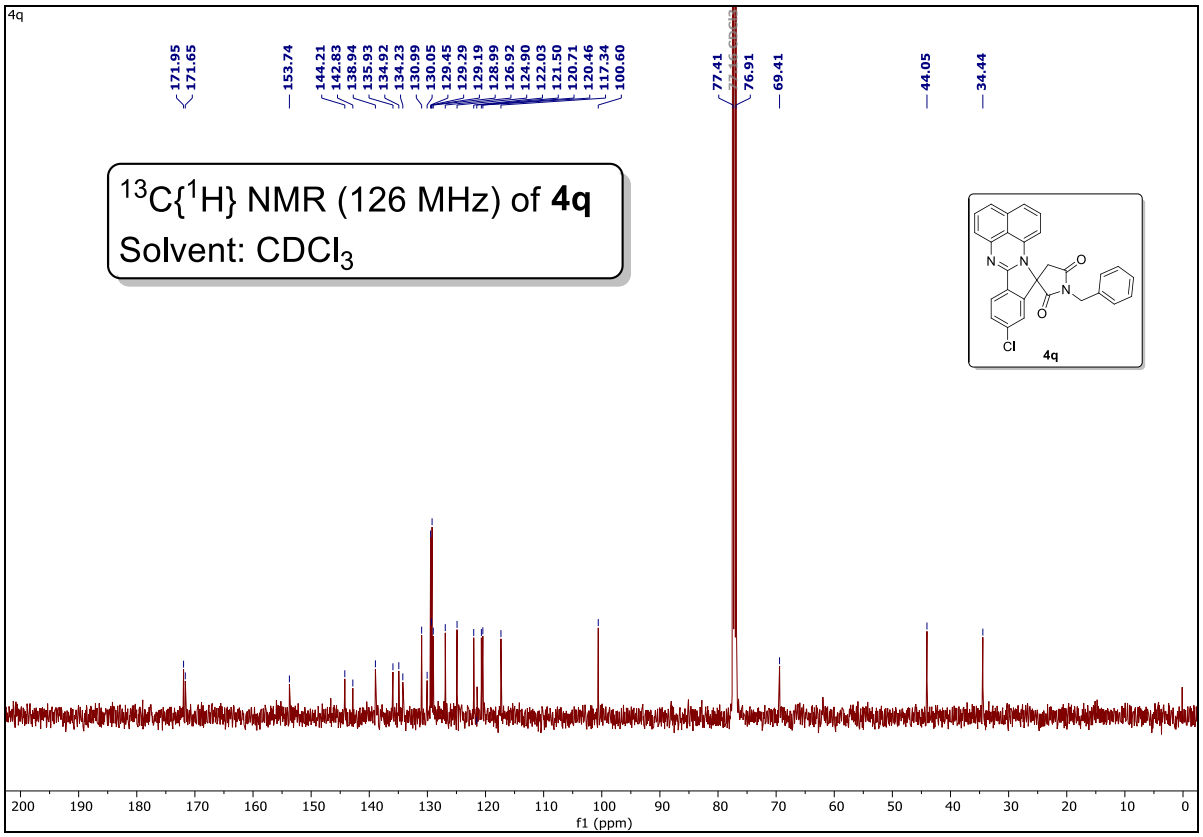






VM-225.d


4q
7.98 7.96 7.56 7.56 7.55 7.54 7.50 7.49 7.48 7.40 7.40 7.39 7.35 7.34 7.32 7.26 CDCl3 7.25 7.23 7.13 7.12 7.06 7.05 7.00 7.00 6.81 6.79 6.78 5.36 5.35 4.93 3.83 3.79 2.93 2.89
1H NMR (500 MHz) of 4q
Solvent: CDCl3
4q
1.00 1.01 2.00 3.00 1.01 1.02 1.01 1.00 1.00 1.04 1.00 2.03 1.01 1.02
f1 (ppm)


4q
171.95 171.65 153.74 144.21 142.83 138.94 135.93 134.92 134.23 130.99 130.05 129.45 129.29 129.19 128.99 126.92 124.90 122.03 121.50 120.71 120.46 117.34 100.60 77.41 76.91 69.41 44.05 34.44
13C{1H} NMR (126 MHz) of 4q
Solvent: CDCl3
4q
f1 (ppm)

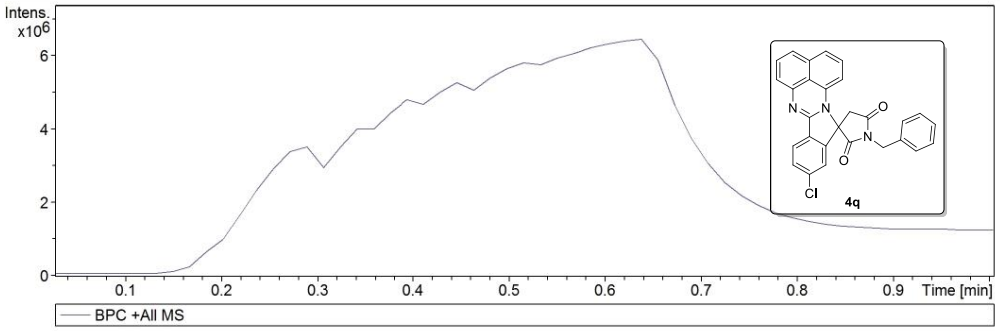
Display Report

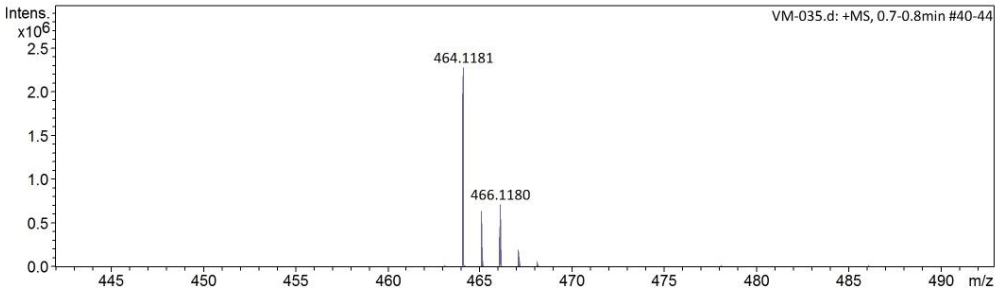
Analysis Info

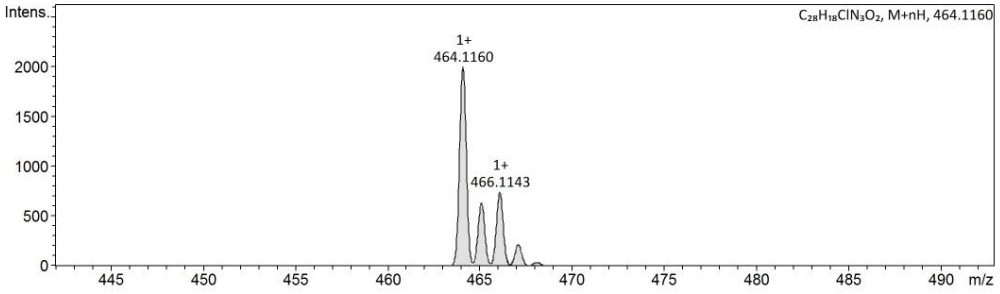
Analysis Name	D:\Data\user data\Dr. Lokman\09-04-2024\VM-035.d	Acquisition Date	4/9/2024 4:15:37 PM
Method	Tune_pos_Mid.m	Operator	vidhi
Sample Name	VM-035	Instrument	impact HD 1819696.00197
Comment			

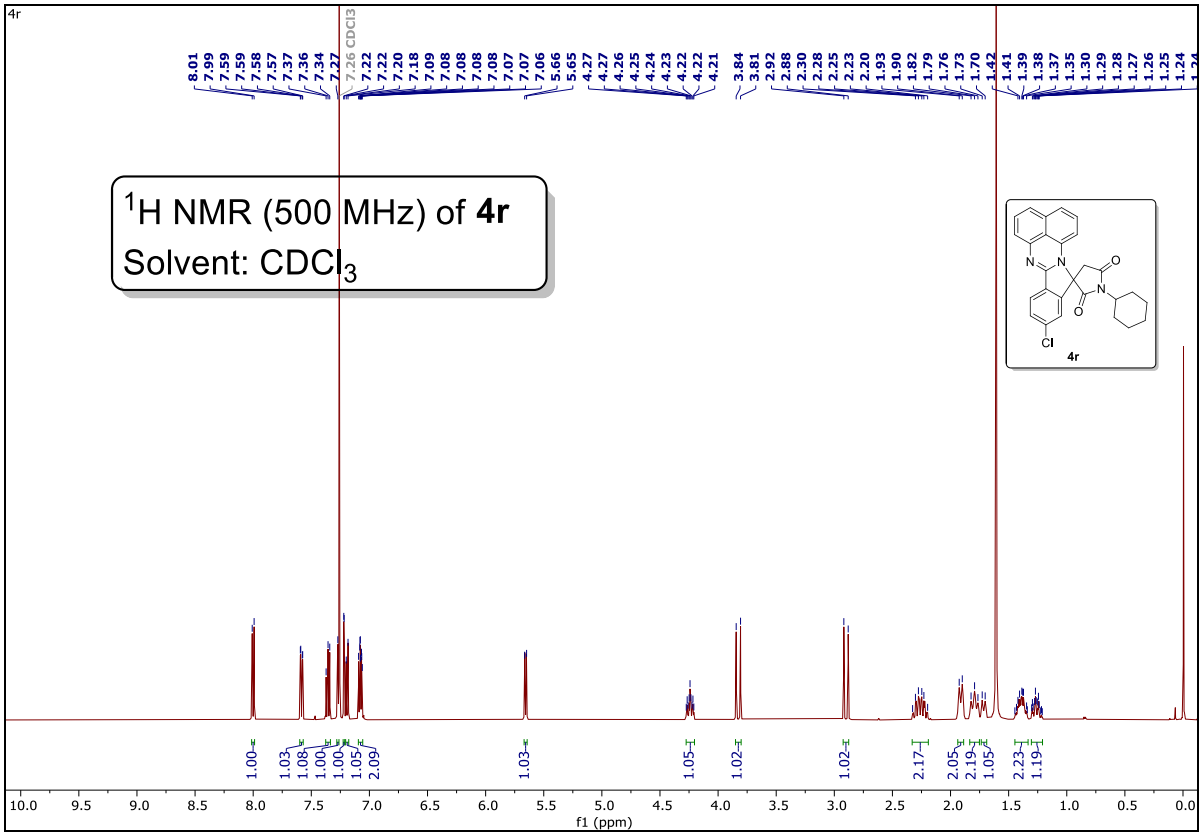
Acquisition Parameter

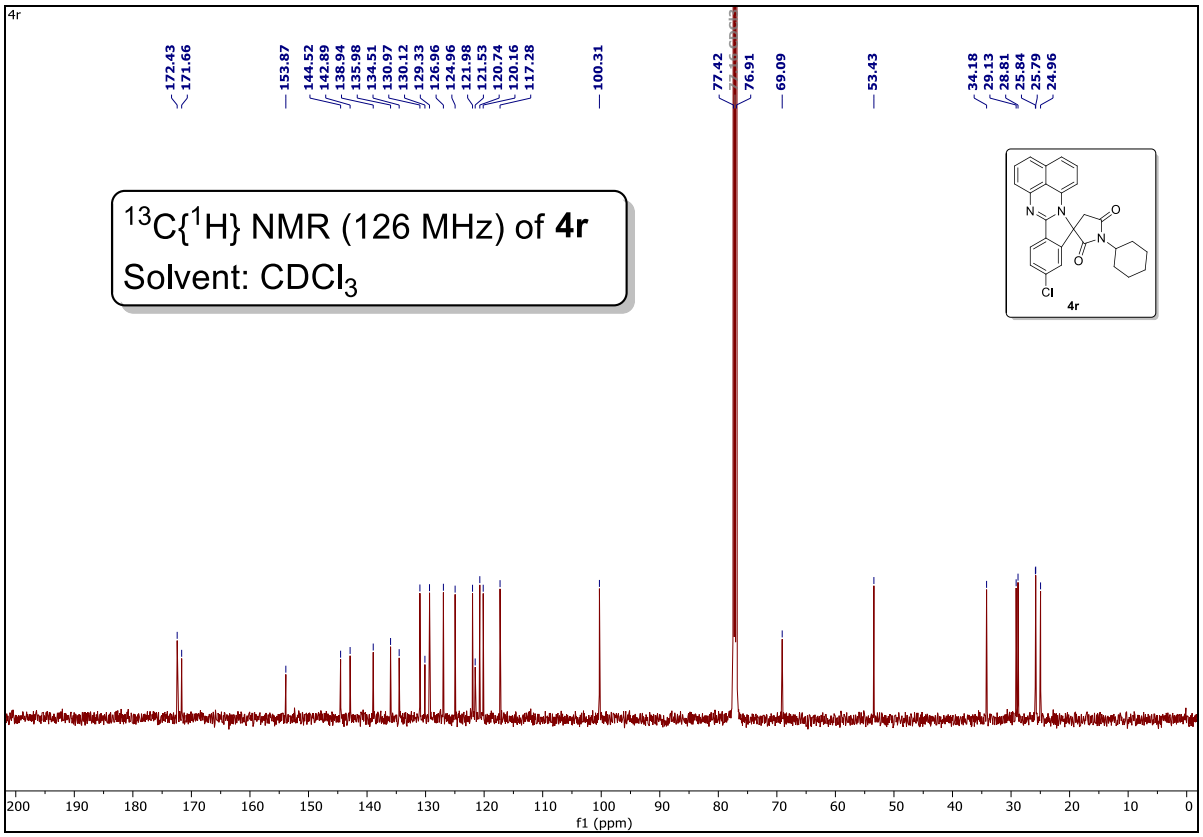
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	219 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 °C








4r
^{1}H NMR (500 MHz) of **4r**
Solvent: $CDCl_3$
f1 (ppm)


4r
$^{13}C\{^{1}H\}$ NMR (126 MHz) of **4r**
Solvent: $CDCl_3$
f1 (ppm)

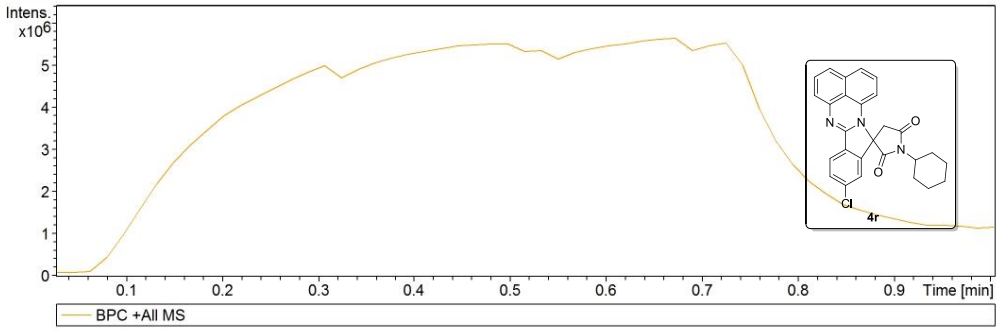
Display Report

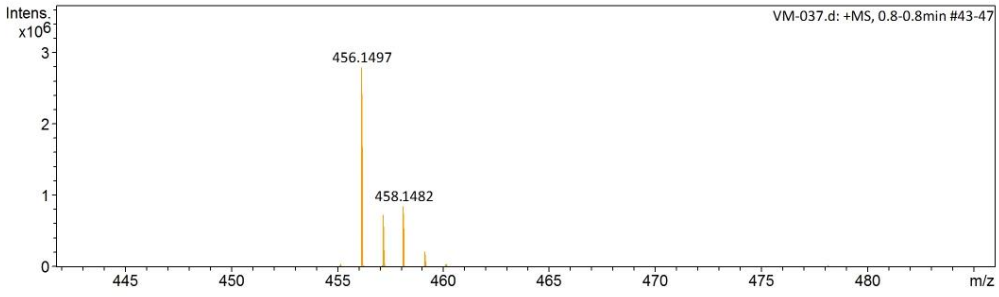
Analysis Info

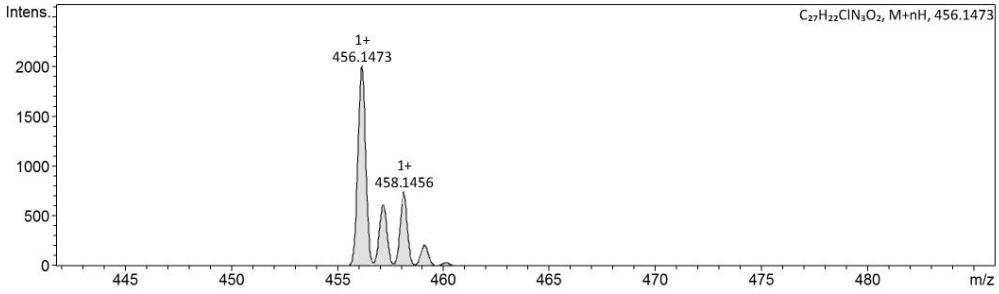
Analysis Name	D:\Data\user data\Dr. Lokman\09-04-2024\VM-037.d	Acquisition Date	4/9/2024 4:07:23 PM
Method	Tune_pos_Mid.m	Operator	vidhi
Sample Name	VM-037	Instrument	impact HD 1819696.00197
Comment			

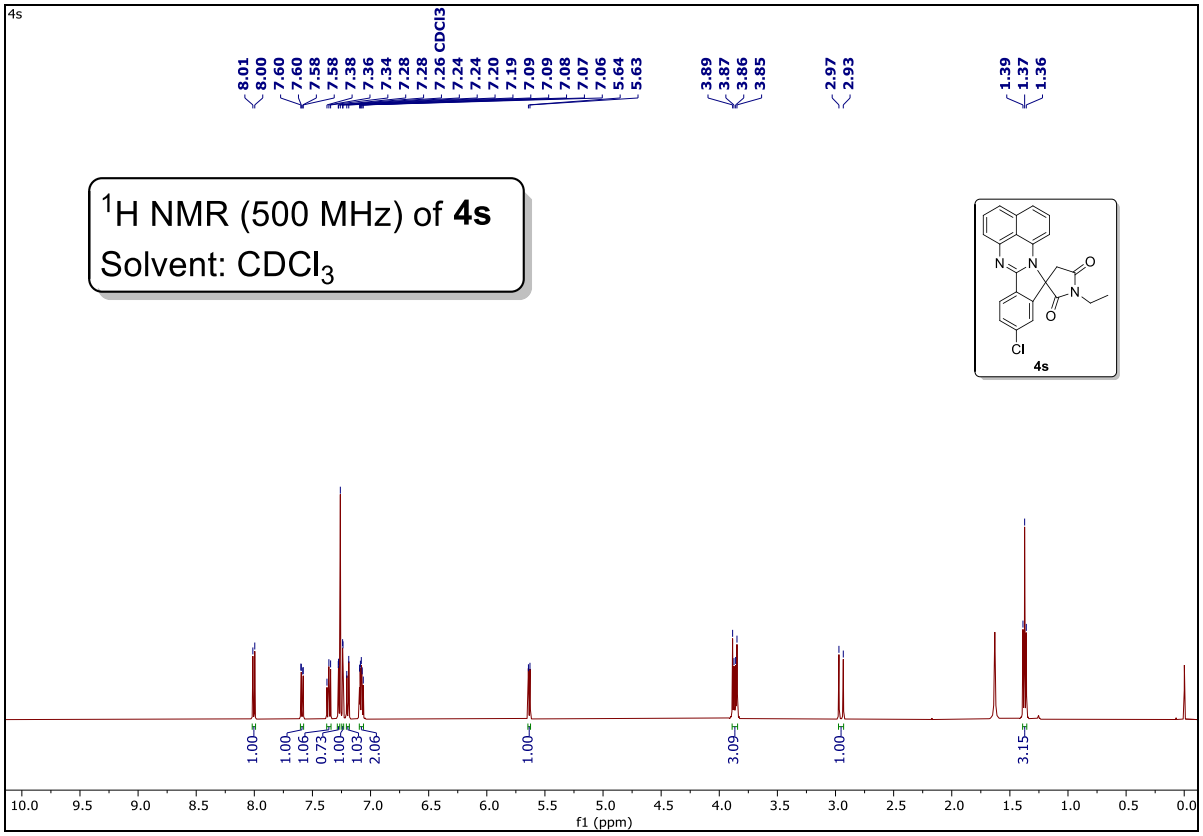
Acquisition Parameter

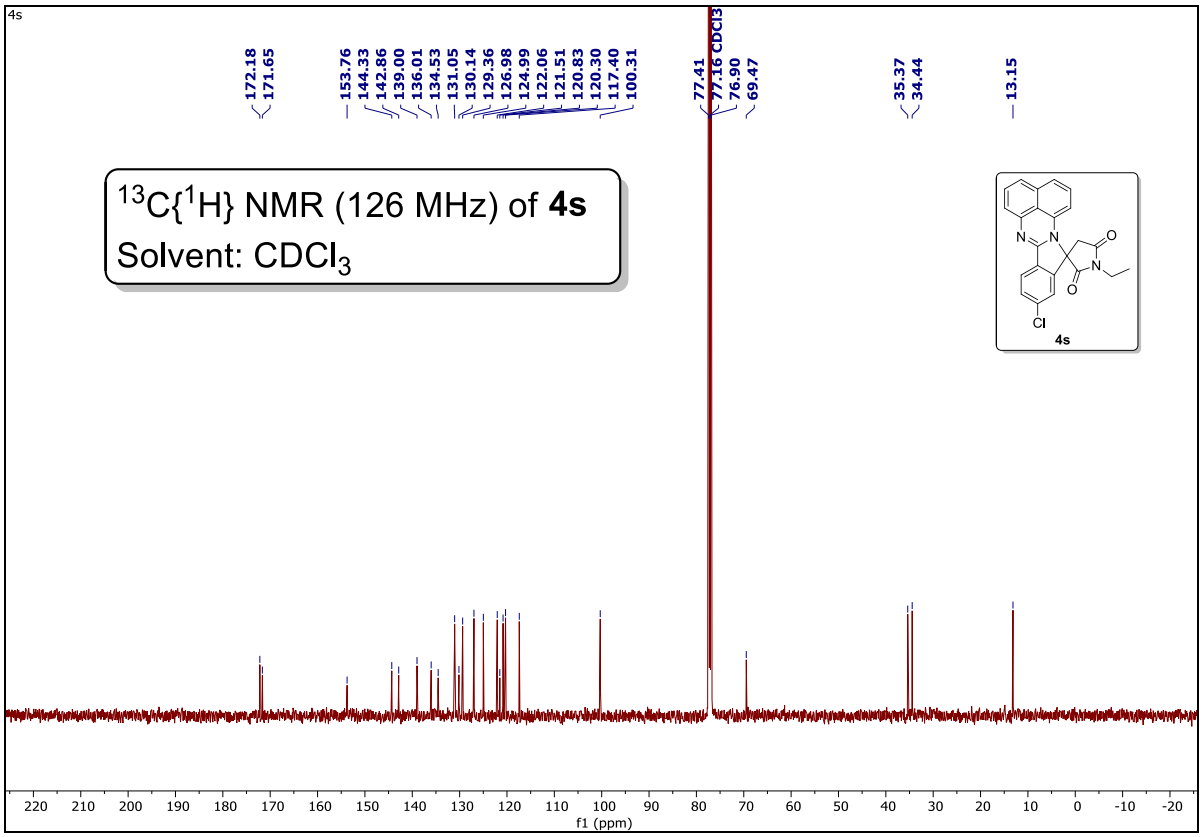
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	219 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 °C








4s
8.01
8.00
7.60
7.60
7.58
7.58
7.38
7.36
7.34
7.28
7.28
7.26 CDCl3
7.24
7.24
7.20
7.19
7.09
7.09
7.08
7.07
7.06
5.64
5.63
3.89
3.87
3.86
3.85
2.97
2.93
1.39
1.37
1.36
1H NMR (500 MHz) of 4s
Solvent: CDCl3
4s
1.00
1.00
1.06
0.73
1.00
1.03
2.06
1.00
3.09
1.00
3.15
f1 (ppm)


4s
172.18
171.65
153.76
144.33
142.86
139.00
136.01
134.53
131.05
130.14
129.36
126.98
124.99
122.06
121.51
120.83
120.30
117.40
100.31
77.41
77.16 CDCl3
76.90
69.47
35.37
34.44
13.15
13C{1H} NMR (126 MHz) of 4s
Solvent: CDCl3
4s
f1 (ppm)

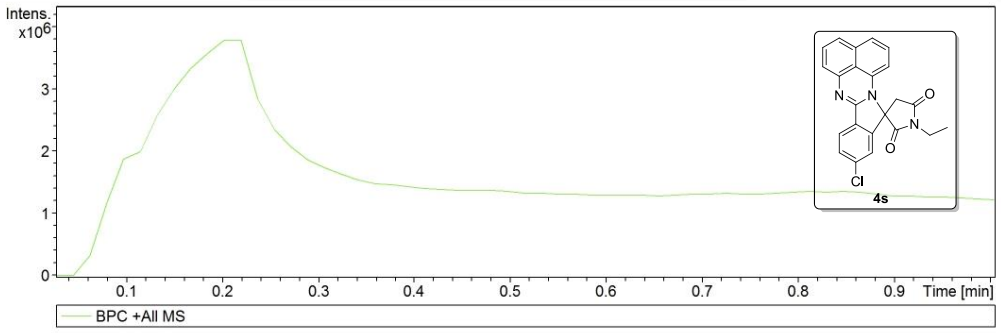
Display Report

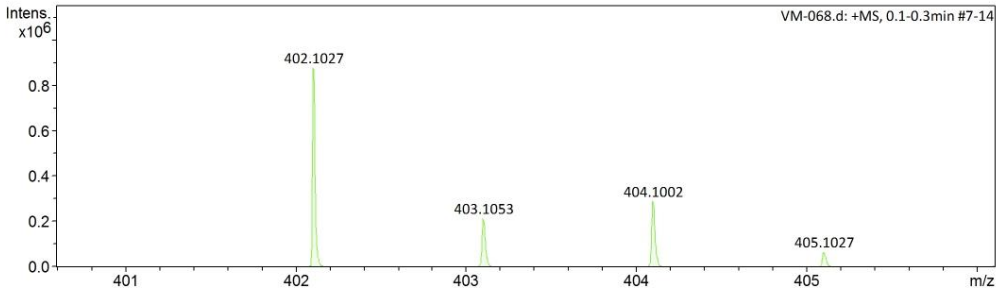
Analysis Info

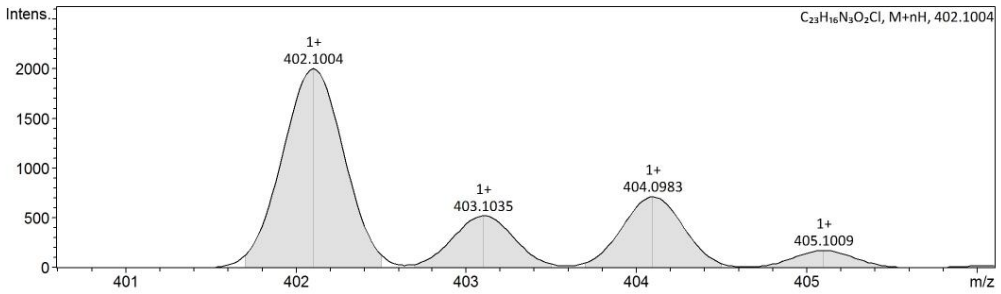
Analysis Name	D:\Data\user data\Dr. Lokman\16-04-2024\VM-068.d	Acquisition Date	4/16/2024 11:37:01 AM
Method	Tune_pos_Mid.m	Operator	vidhi
Sample Name	VM-068	Instrument	impact HD 1819696.00197
Comment			

Acquisition Parameter

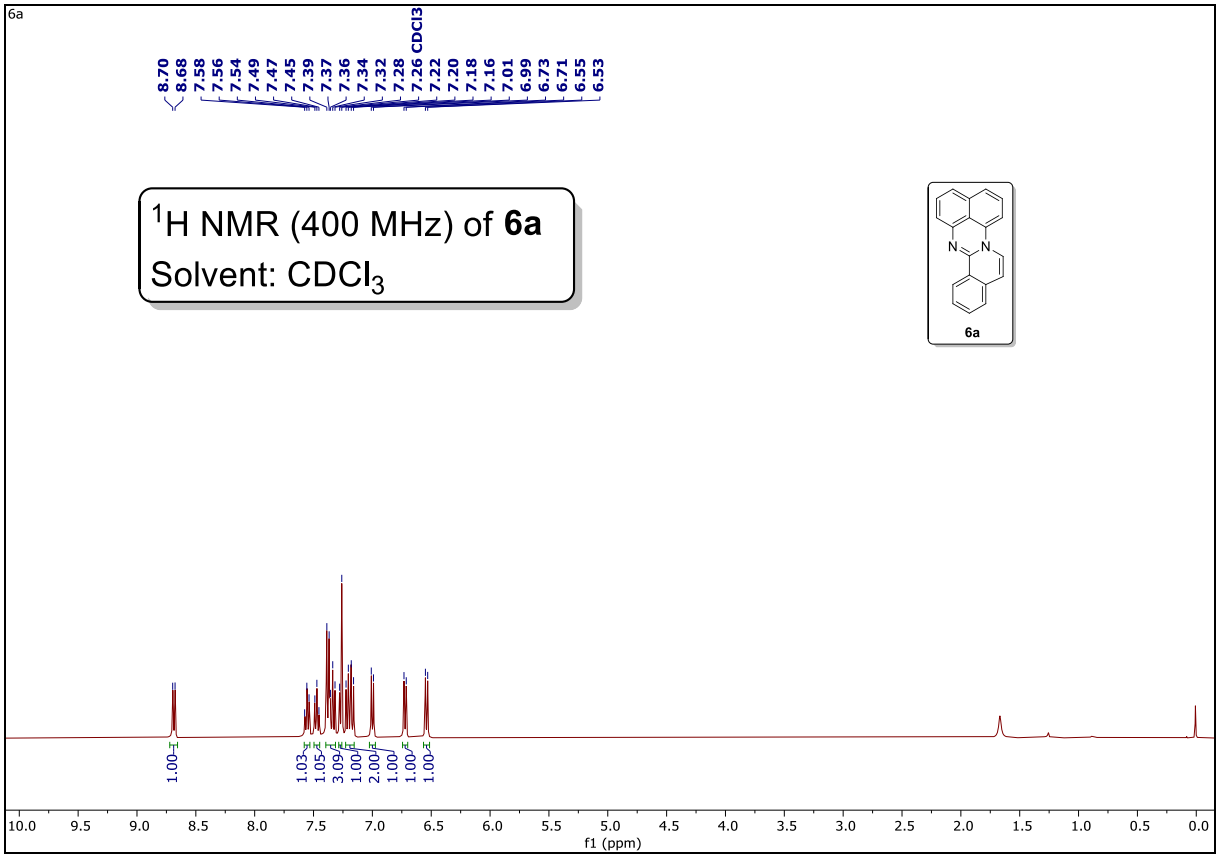
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	219 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 °C

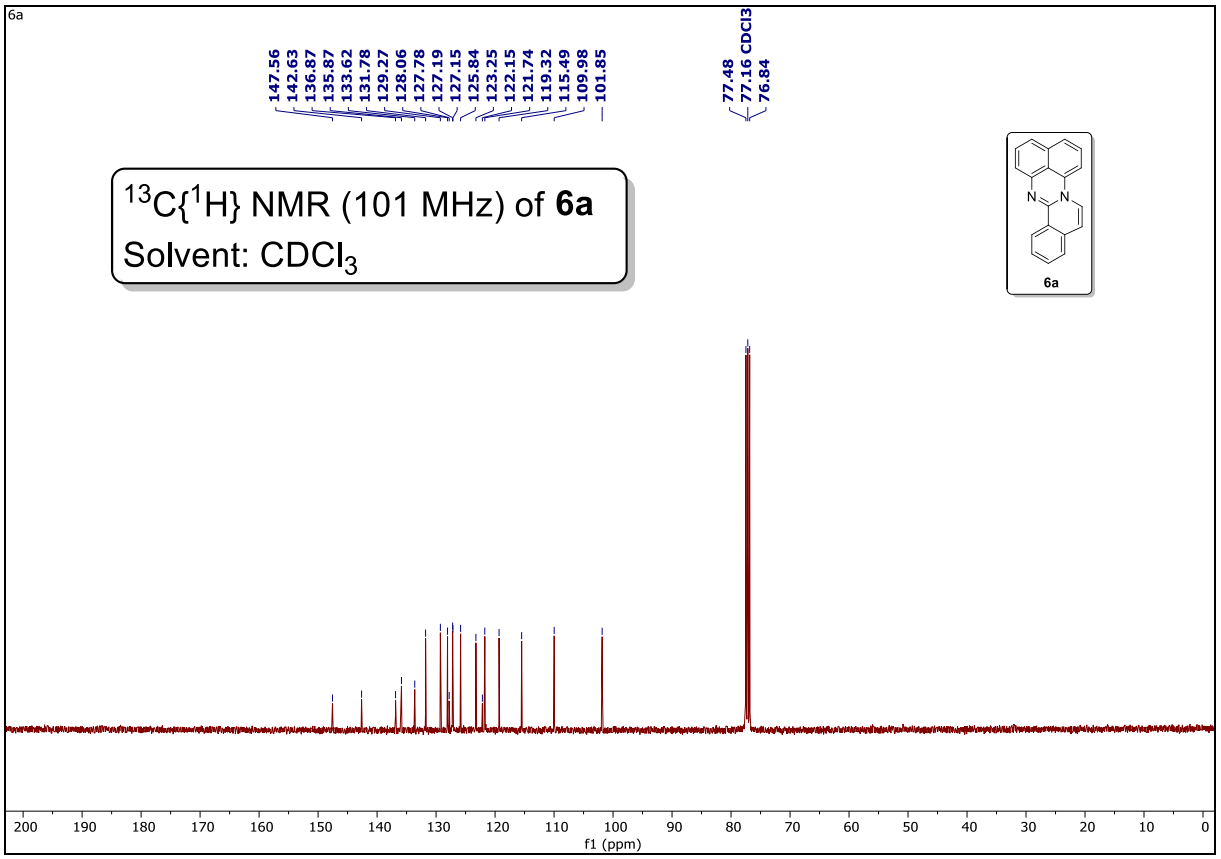


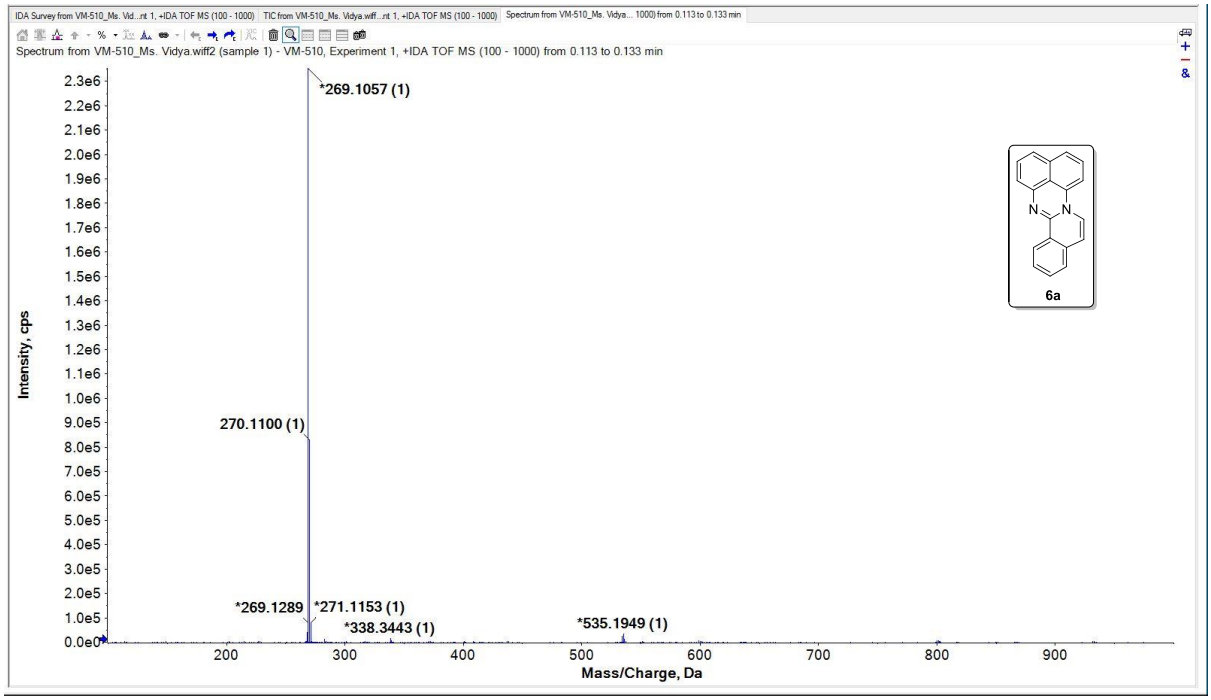


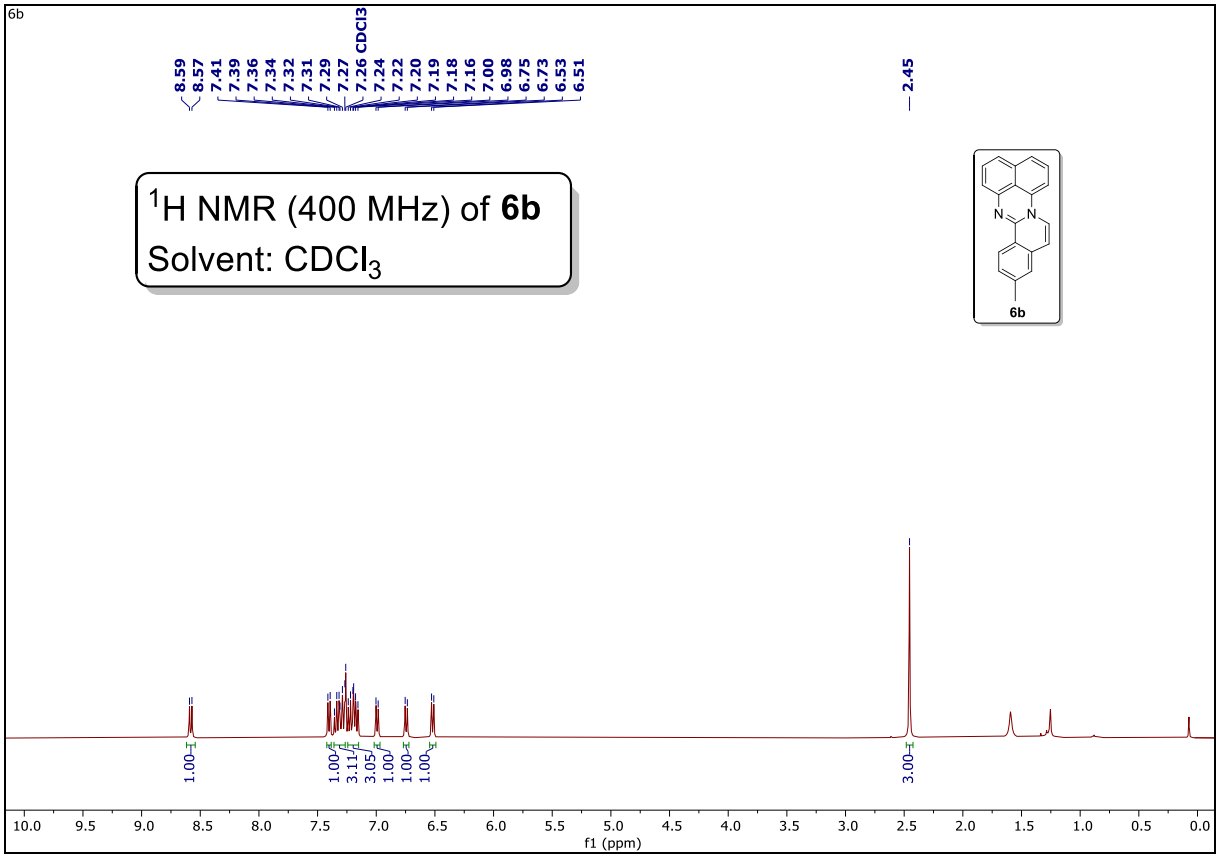


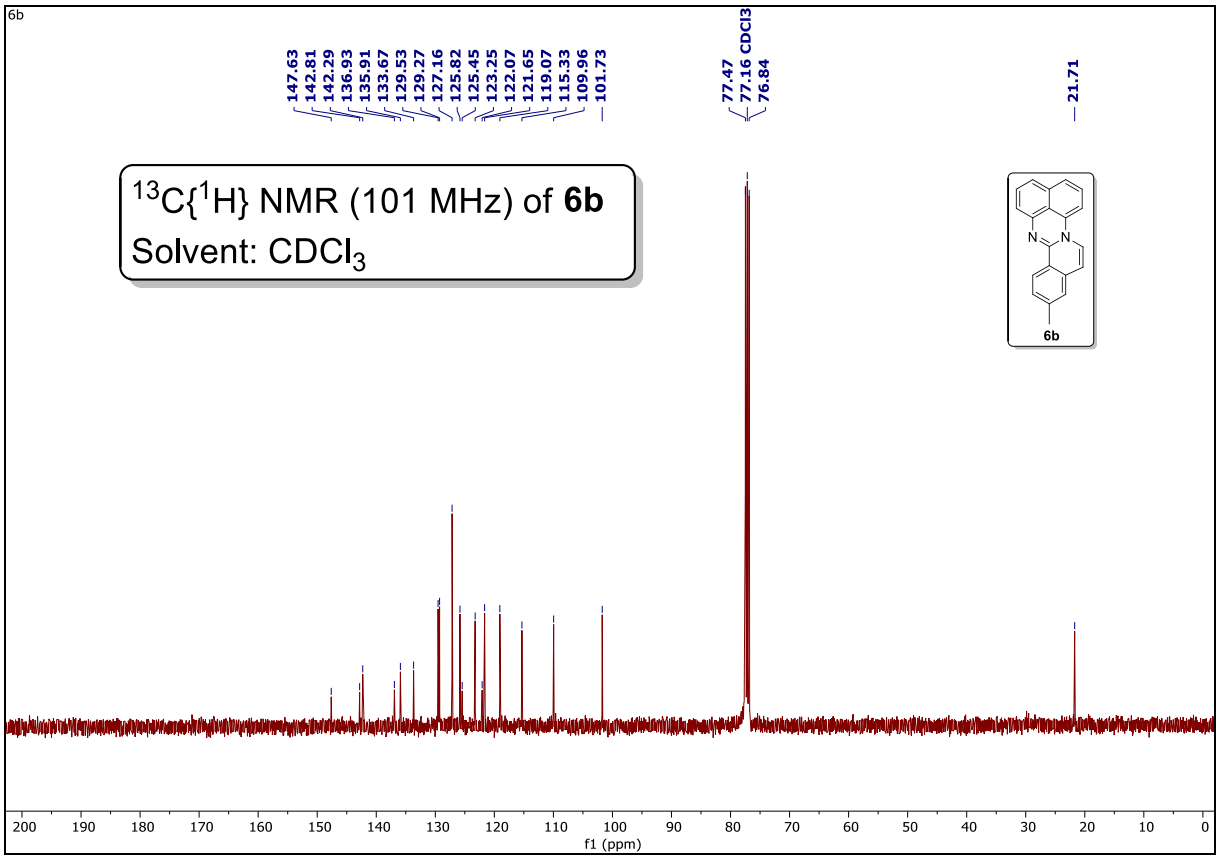
VM-068.d

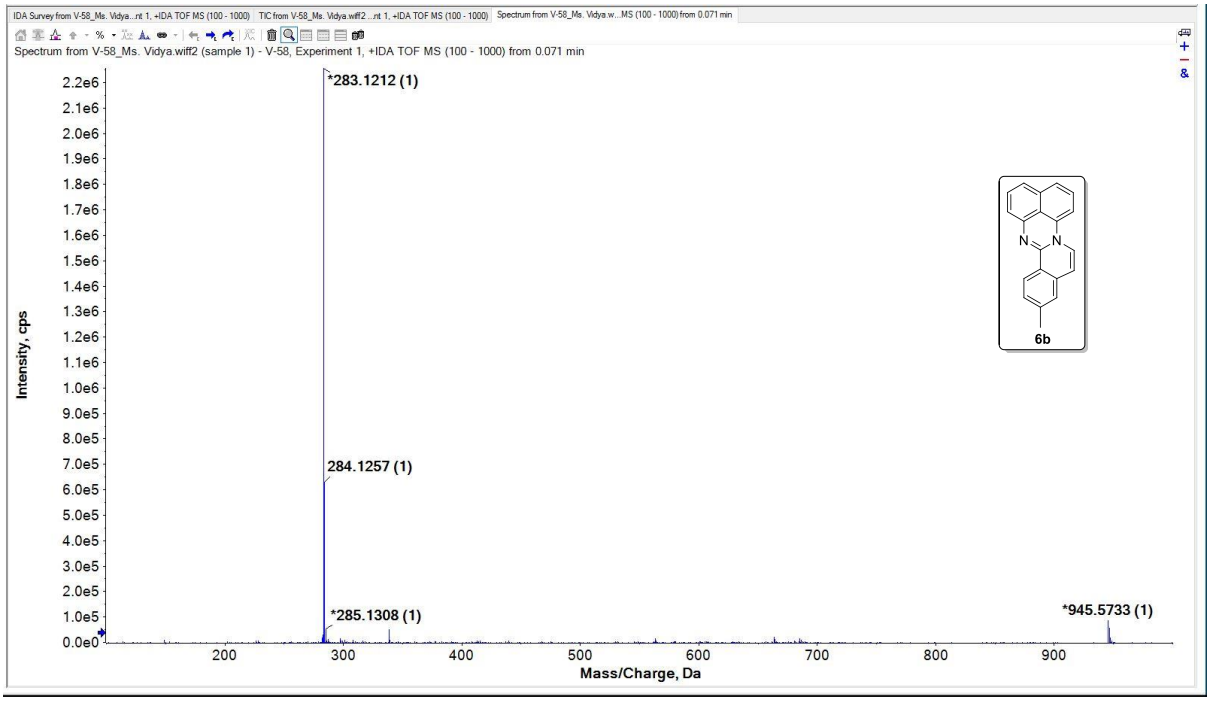

6a
8.70
8.68
7.58
7.56
7.54
7.49
7.47
7.45
7.39
7.37
7.36
7.34
7.32
7.28
7.26 CDCl3
7.22
7.20
7.18
7.16
7.01
6.99
6.73
6.71
6.55
6.53
1H NMR (400 MHz) of 6a
Solvent: CDCl3
6a
1.00
1.03
1.05
3.09
1.00
2.00
1.00
1.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

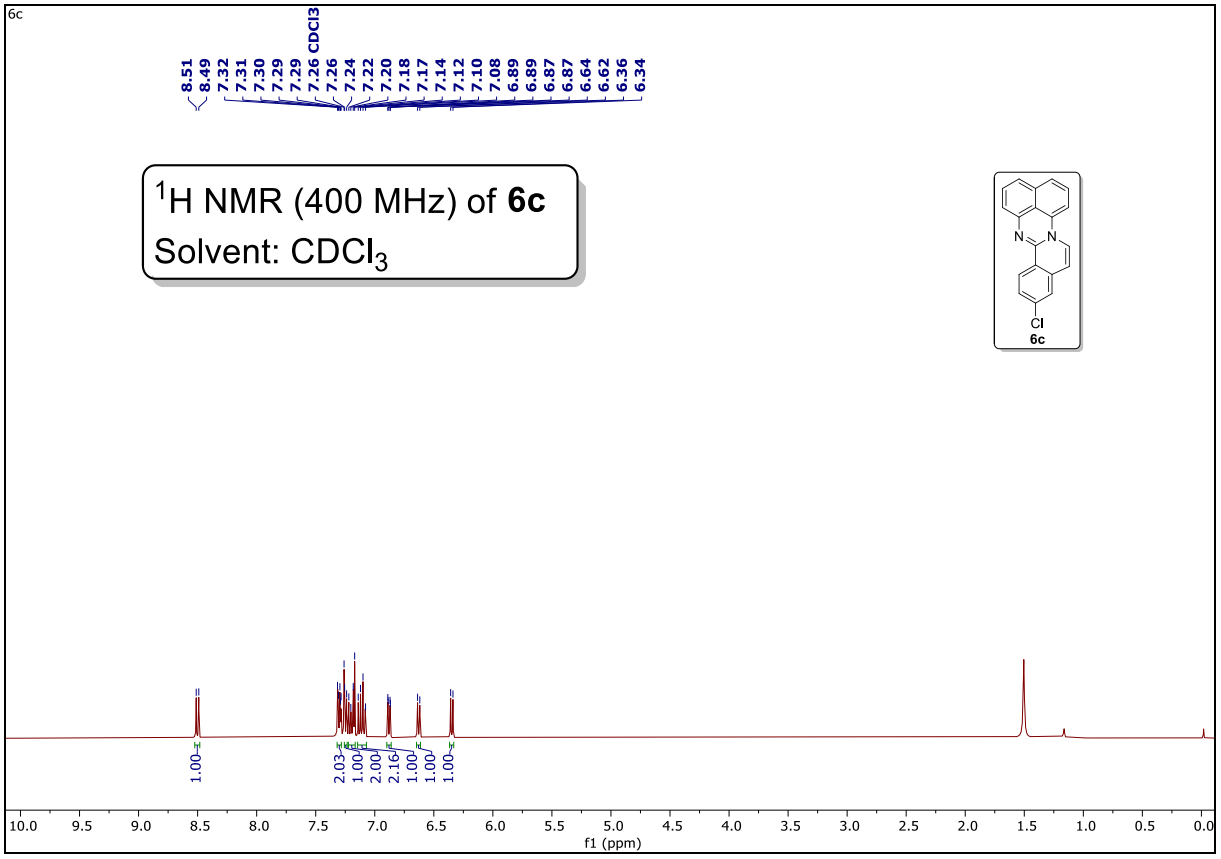

6a
147.56
142.63
136.87
135.87
133.62
131.78
129.27
128.06
127.78
127.19
127.15
125.84
123.25
122.15
121.74
119.32
115.49
109.98
101.85
77.48
77.16 CDCl3
76.84
13C{1H} NMR (101 MHz) of 6a
Solvent: CDCl3
6a
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

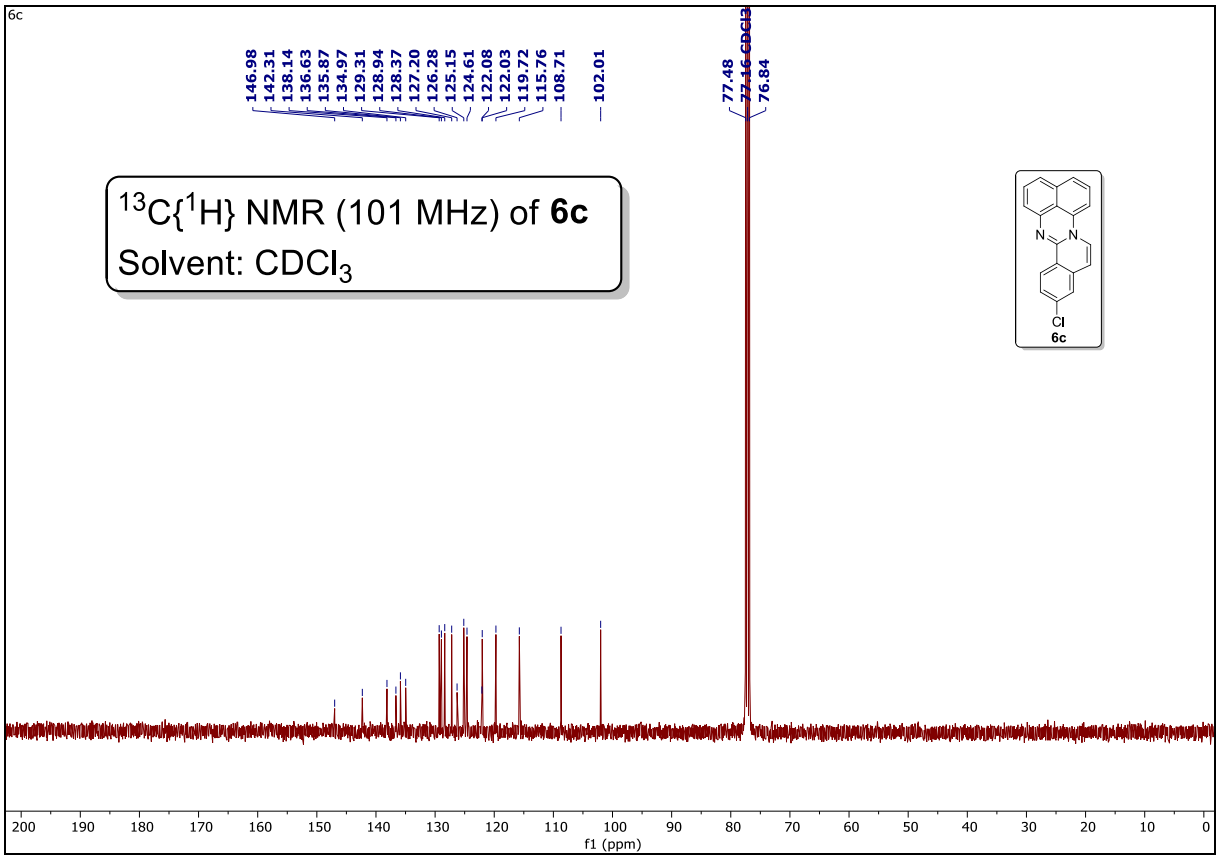

Spectrum from VM-510_Ms. Vidya.wiff2 (sample 1) - VM-510, Experiment 1, +IDA TOF MS (100 - 1000) from 0.113 to 0.133 min
*269.1057 (1)
270.1100 (1)
*269.1289
*271.1153 (1)
*338.3443 (1)
*535.1949 (1)
Intensity, cps
Mass/Charge, Da
6a

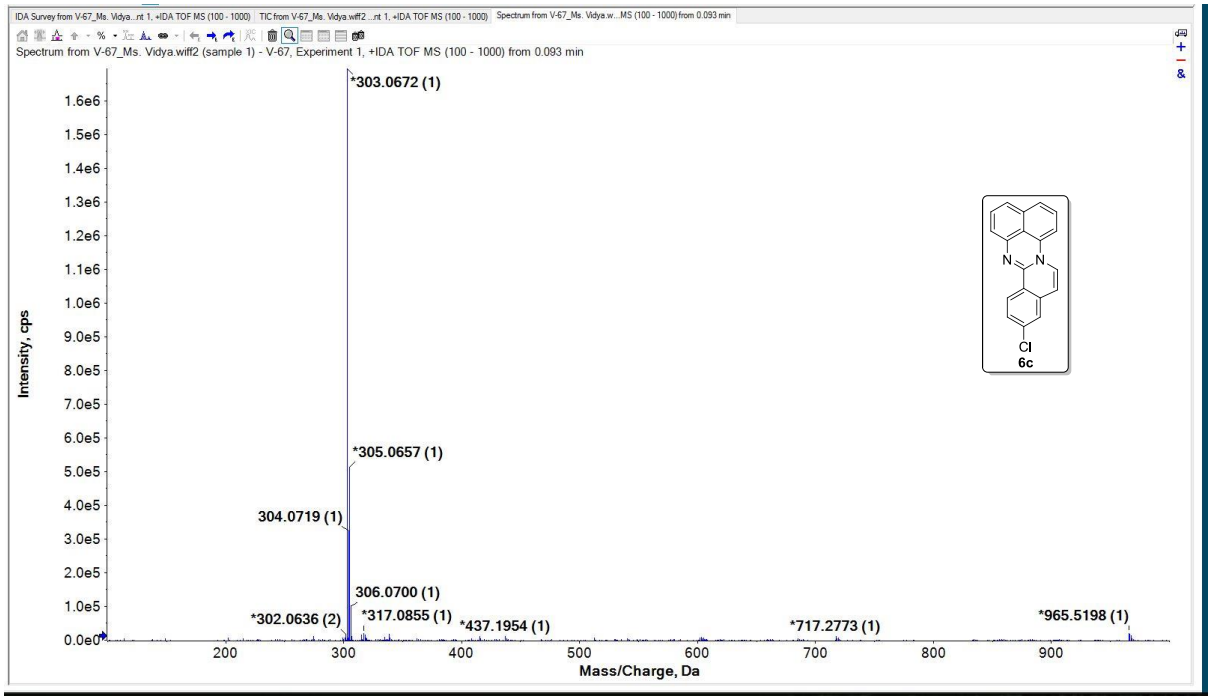

6b
8.59
8.57
7.41
7.39
7.36
7.34
7.32
7.31
7.29
7.27
7.26 CDCl3
7.24
7.22
7.20
7.19
7.18
7.16
7.00
6.98
6.75
6.73
6.53
6.51
2.45
1H NMR (400 MHz) of 6b
Solvent: CDCl3
6b
1.00
1.00
3.11
3.05
1.00
1.00
1.00
3.00
f1 (ppm)

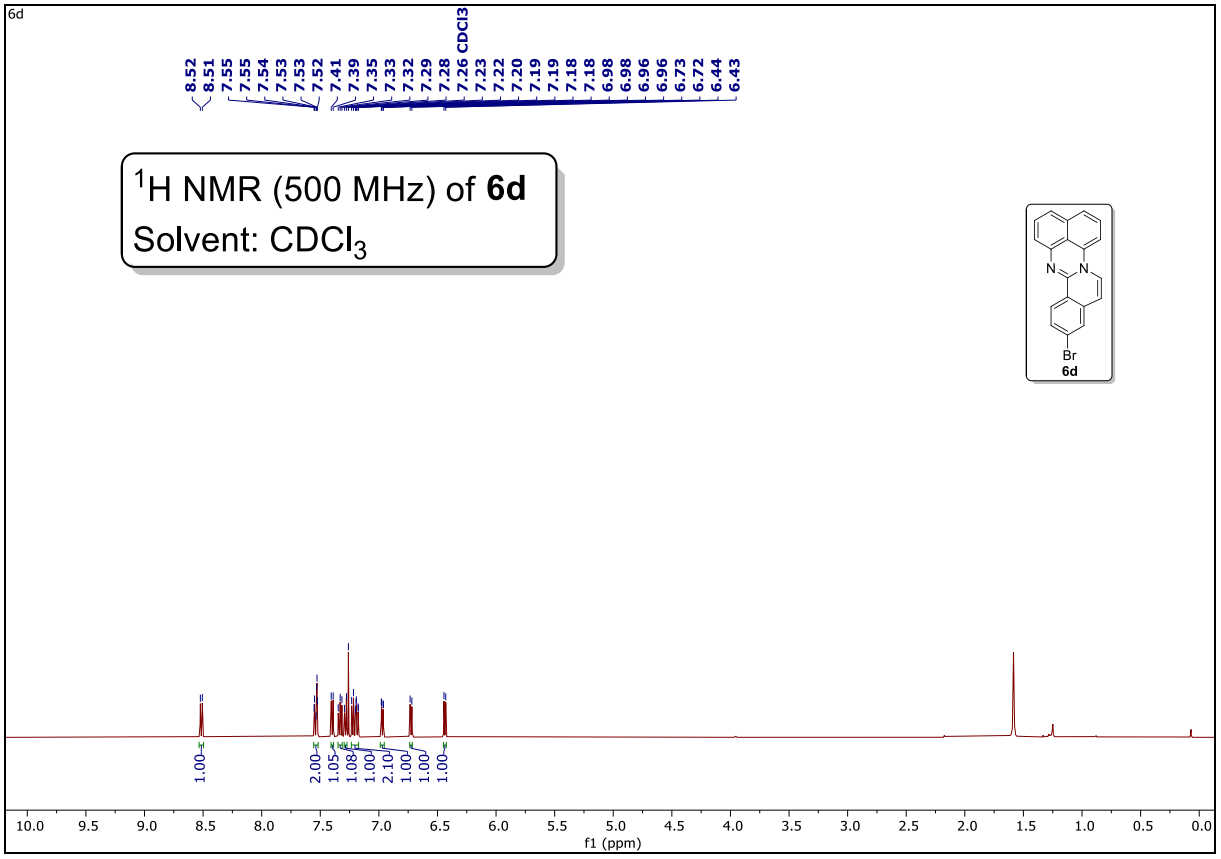

6b
147.63
142.81
142.29
136.93
135.91
133.67
129.53
129.27
127.16
125.82
125.45
123.25
122.07
121.65
119.07
115.33
109.96
101.73
77.47
77.16 CDCl3
76.84
21.71
13C{1H} NMR (101 MHz) of 6b
Solvent: CDCl3
6b
f1 (ppm)

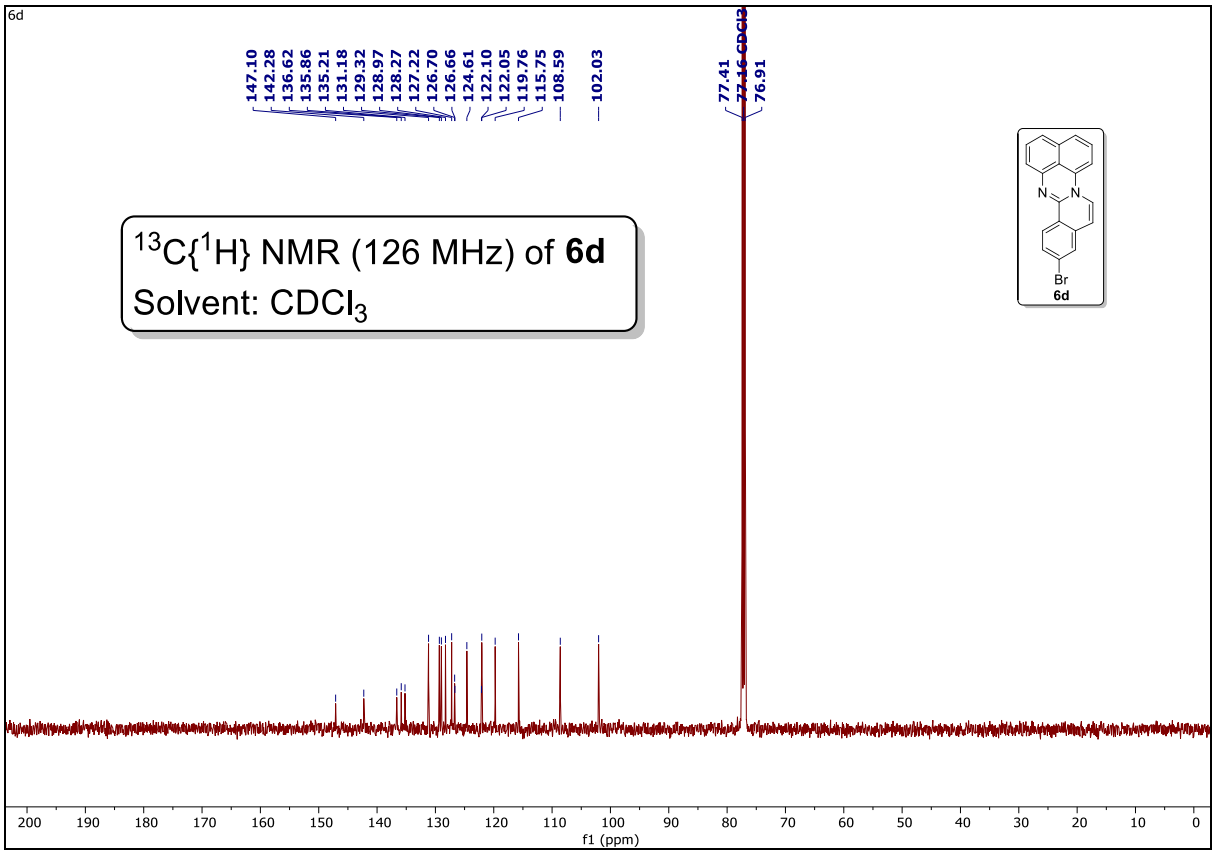

IDA Survey from V-58_Ms. Vidya...nt 1, +IDA TOF MS (100 - 1000)
TIC from V-58_Ms. Vidya.wiff2...nt 1, +IDA TOF MS (100 - 1000)
Spectrum from V-58_Ms. Vidya.w...MS (100 - 1000) from 0.071 min
Spectrum from V-58_Ms. Vidya.wiff2 (sample 1) - V-58, Experiment 1, +IDA TOF MS (100 - 1000) from 0.071 min
*283.1212 (1)
284.1257 (1)
*285.1308 (1)
*945.5733 (1)
Intensity, cps
Mass/Charge, Da
6b

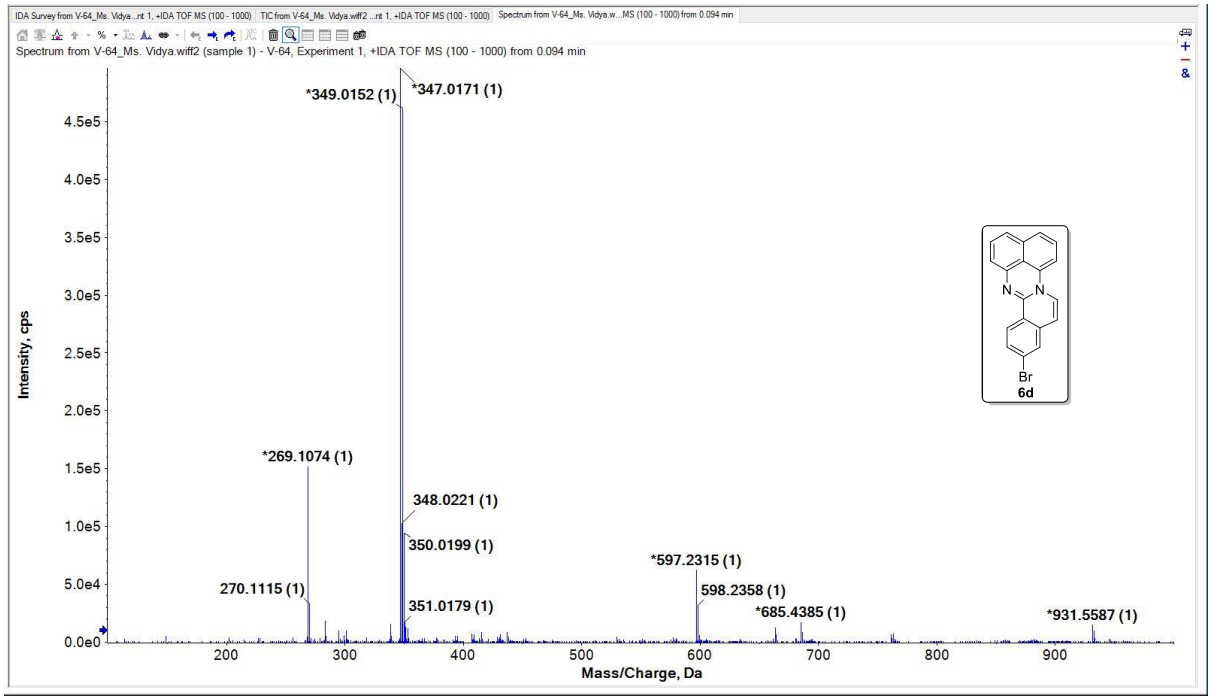

6c
8.51
8.49
7.32
7.31
7.30
7.29
7.29
7.26 CDCl3
7.26
7.24
7.22
7.20
7.18
7.17
7.14
7.12
7.10
7.08
6.89
6.89
6.87
6.87
6.64
6.62
6.36
6.34
1H NMR (400 MHz) of 6c
Solvent: CDCl3
N
N
Cl
6c
1.00
2.03
1.00
2.00
2.16
1.00
1.00
1.00
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

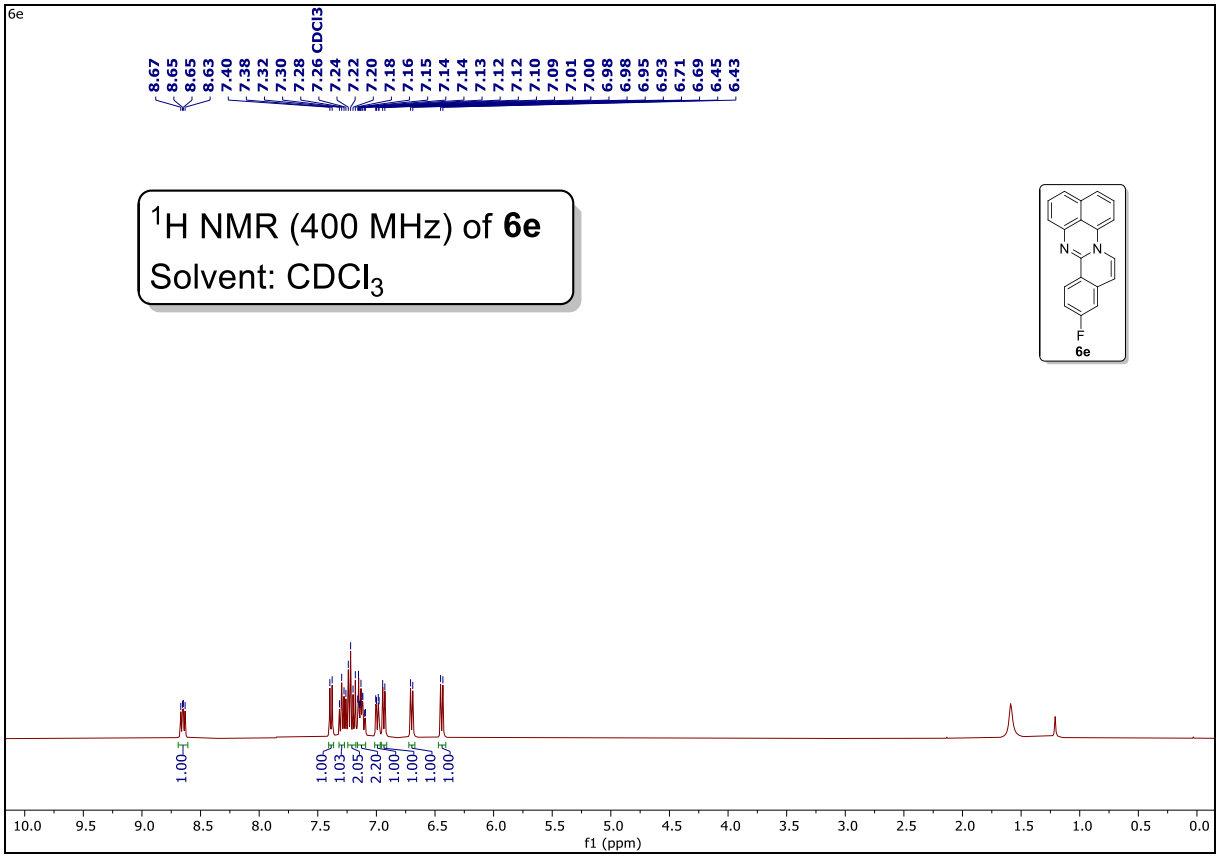

6c
146.98
142.31
138.14
136.63
135.87
134.97
129.31
128.94
128.37
127.20
126.28
125.15
124.61
122.08
122.03
119.72
115.76
108.71
102.01
77.48
77.16 CDCl3
76.84
13C{1H} NMR (101 MHz) of 6c
Solvent: CDCl3
N
N
Cl
6c
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

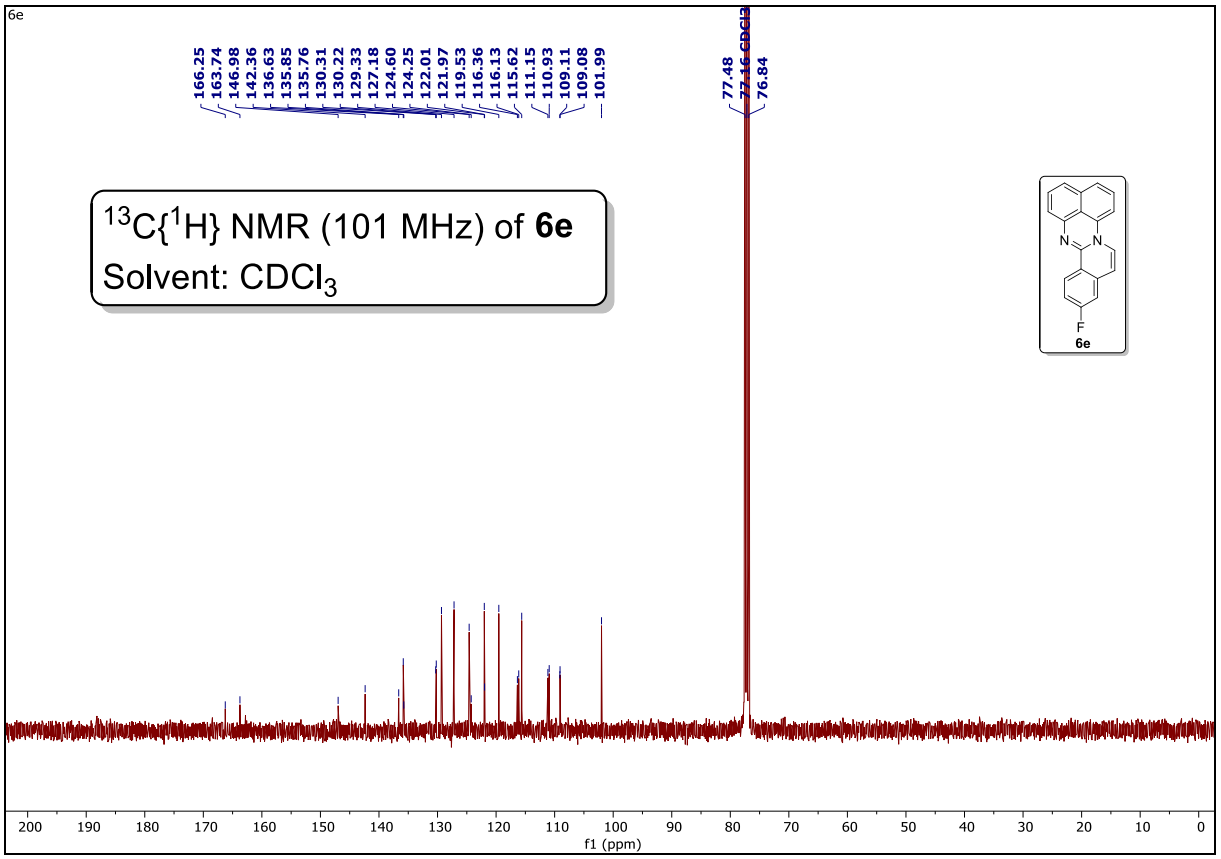

Spectrum from V-67_Ms. Vidya.wiff2 (sample 1) - V-67, Experiment 1, +IDA TOF MS (100 - 1000) from 0.093 min
Intensity, cps
Mass/Charge, Da
*303.0672 (1)
*305.0657 (1)
304.0719 (1)
306.0700 (1)
*302.0636 (2)
*317.0855 (1)
*437.1954 (1)
*717.2773 (1)
*965.5198 (1)
Cl
6c

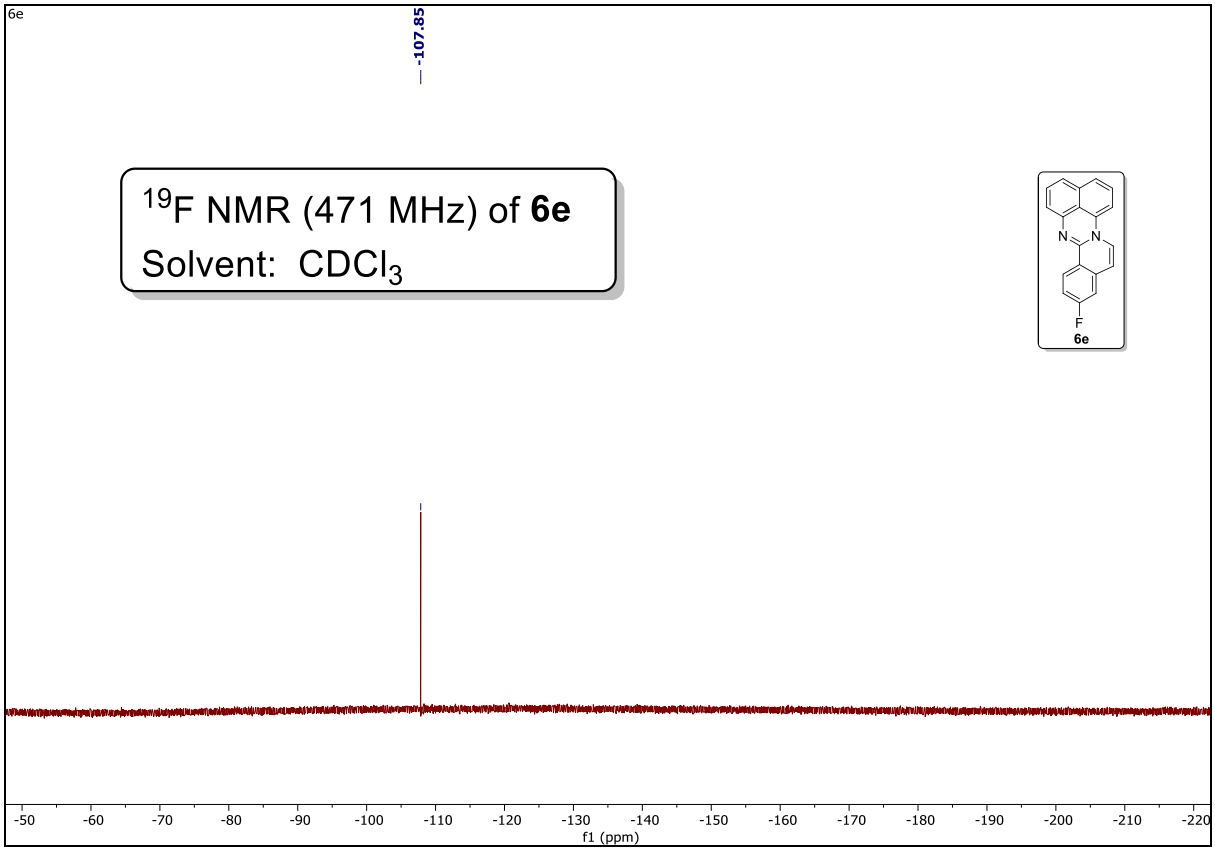

6d
8.52
8.51
7.55
7.55
7.54
7.53
7.53
7.52
7.41
7.39
7.35
7.33
7.32
7.29
7.28
7.26 CDCl3
7.23
7.22
7.20
7.19
7.19
7.18
7.18
6.98
6.98
6.96
6.96
6.73
6.72
6.44
6.43
1H NMR (500 MHz) of 6d
Solvent: CDCl3
N
N
Br
6d
1.00
2.00
1.05
1.08
1.00
2.10
1.00
1.00
1.00
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

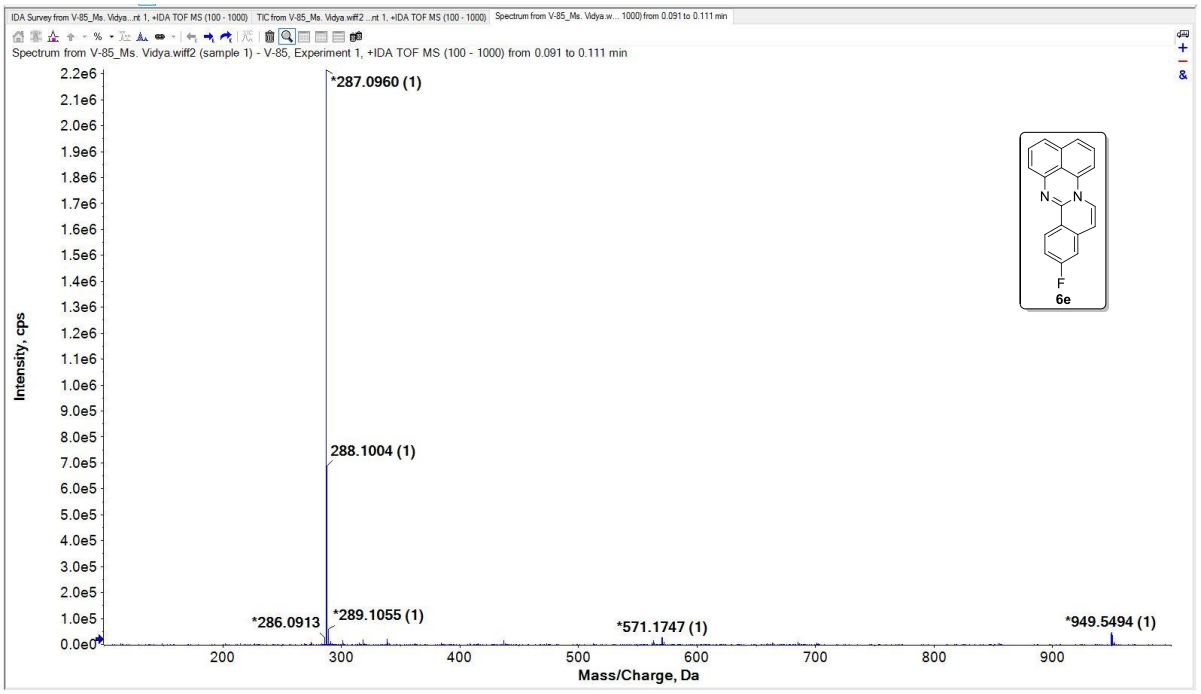

6d
147.10
142.28
136.62
135.86
135.21
131.18
129.32
128.97
128.27
127.22
126.70
126.66
124.61
122.10
122.05
119.76
115.75
108.59
102.03
77.41
77.16 CDCl3
76.91
13C{1H} NMR (126 MHz) of 6d
Solvent: CDCl3
N
N
Br
6d
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

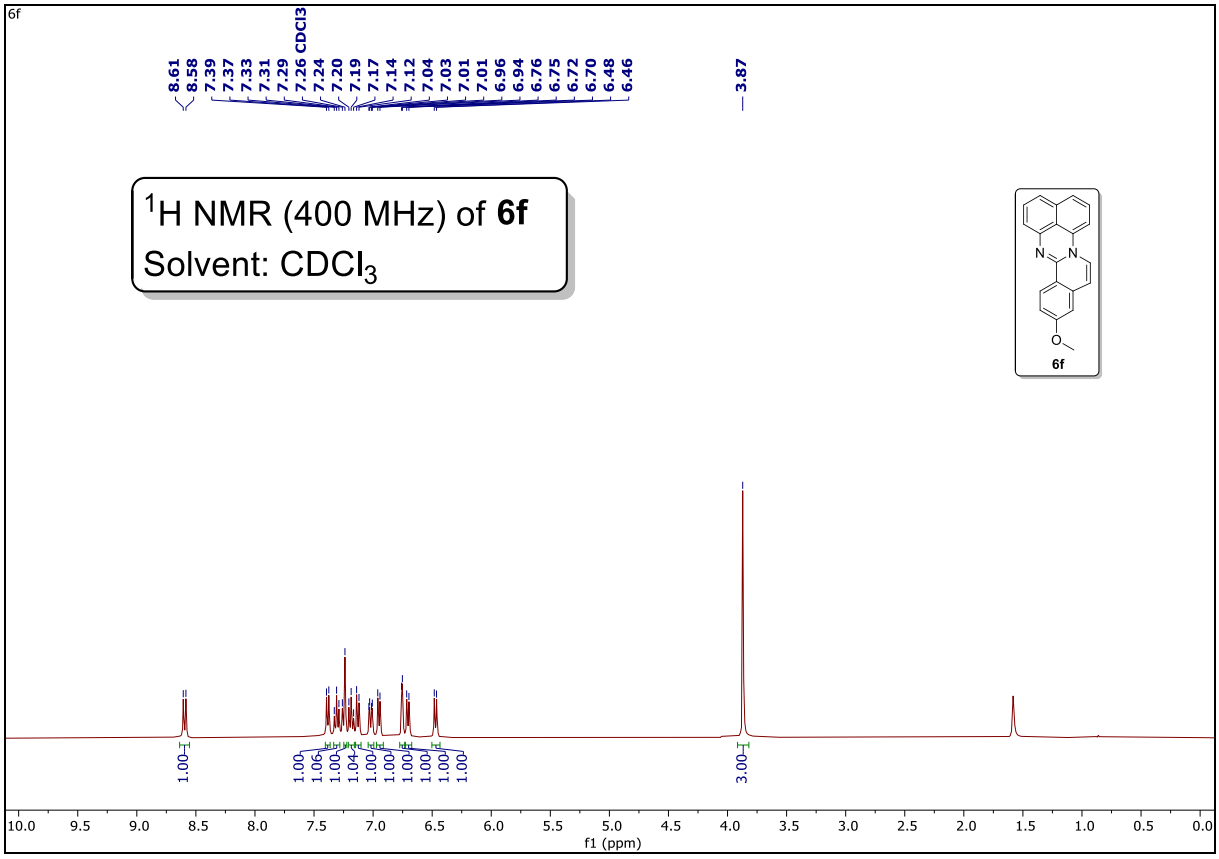

Spectrum from V-64_Ms. Vidya.wiff2 (sample 1) - V-64, Experiment 1, +IDA TOF MS (100 - 1000) from 0.094 min
*349.0152 (1)
*347.0171 (1)
*269.1074 (1)
348.0221 (1)
350.0199 (1)
*597.2315 (1)
598.2358 (1)
270.1115 (1)
351.0179 (1)
*685.4385 (1)
*931.5587 (1)
Intensity, cps
Mass/Charge, Da
Br
6d

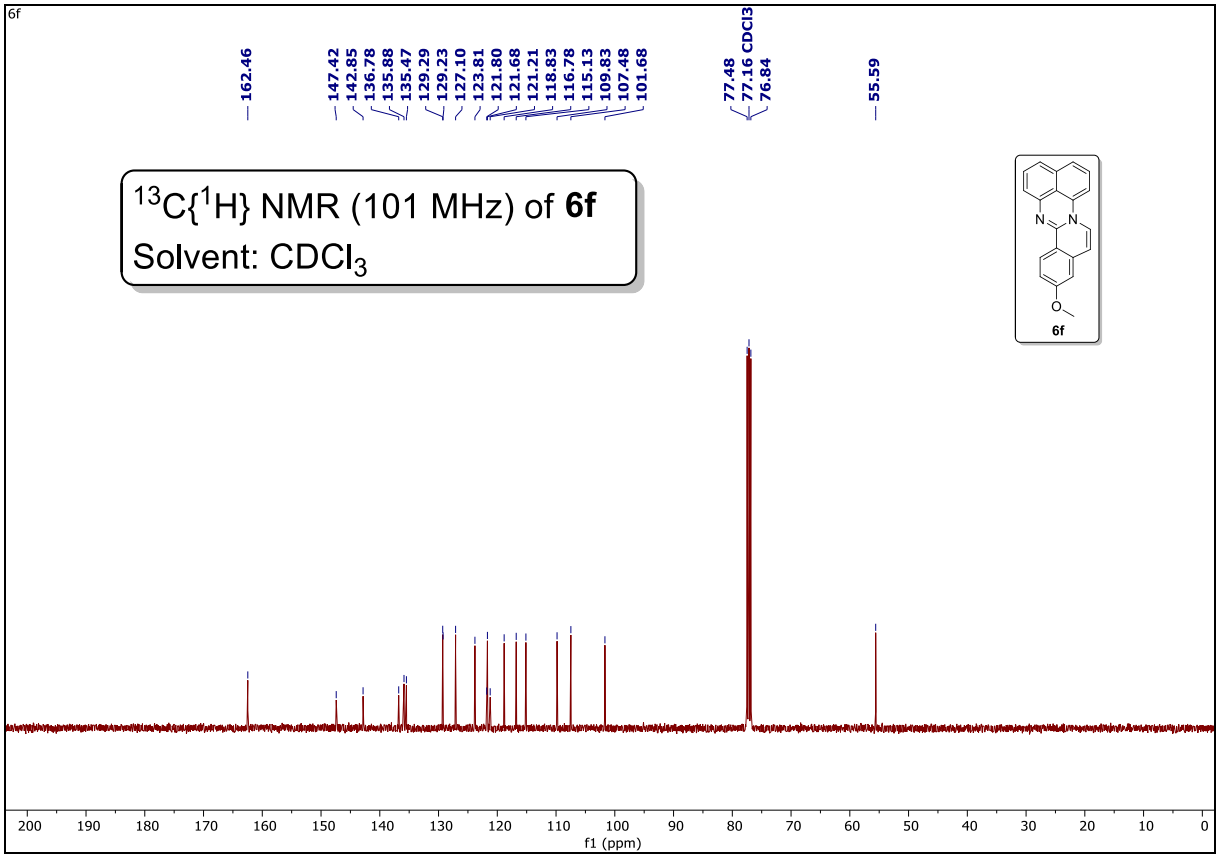

6e
8.67
8.65
8.65
8.63
7.40
7.38
7.32
7.30
7.28
CDCl3
7.26
7.24
7.22
7.20
7.18
7.16
7.15
7.14
7.14
7.13
7.12
7.12
7.10
7.09
7.01
7.00
6.98
6.98
6.95
6.93
6.71
6.69
6.45
6.43
1H NMR (400 MHz) of 6e
Solvent: CDCl3
N
N
F
6e
1.00
1.00
1.03
2.05
2.20
1.00
1.00
1.00
1.00
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

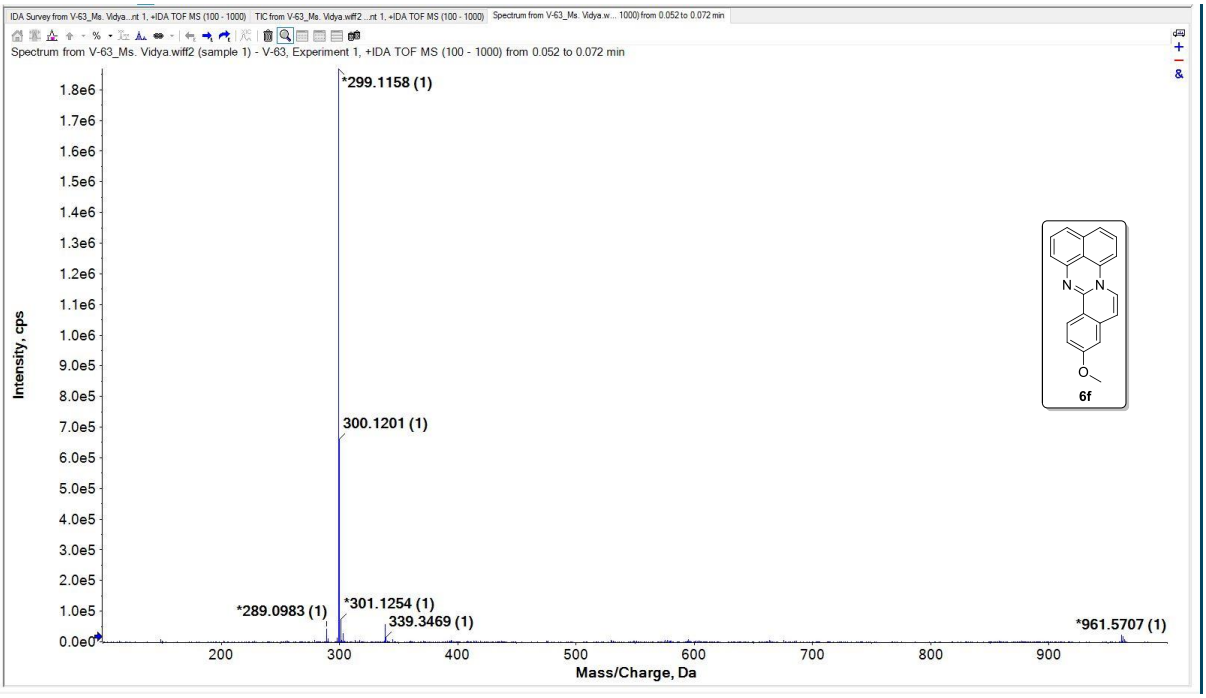

6e
166.25
163.74
146.98
142.36
136.63
135.85
135.76
130.31
130.22
129.33
127.18
124.60
124.25
122.01
121.97
119.53
116.36
116.13
115.62
111.15
110.93
109.11
109.08
101.99
77.48
77.16 CDCl3
76.84
13C{1H} NMR (101 MHz) of 6e
Solvent: CDCl3
N
N
F
6e
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

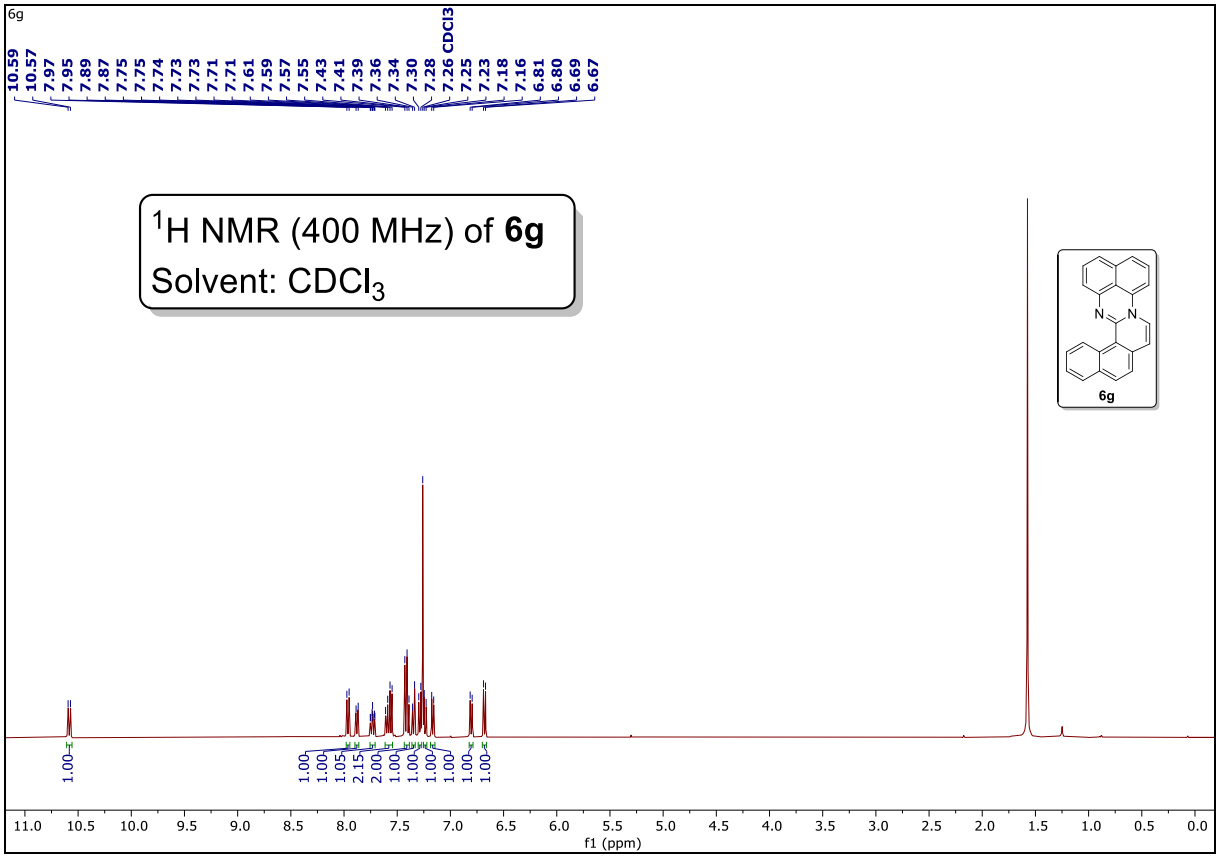

6e
-107.85
^{19}F NMR (471 MHz) of **6e**
Solvent: $CDCl_3$
N
N
F
6e
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
-220
f1 (ppm)

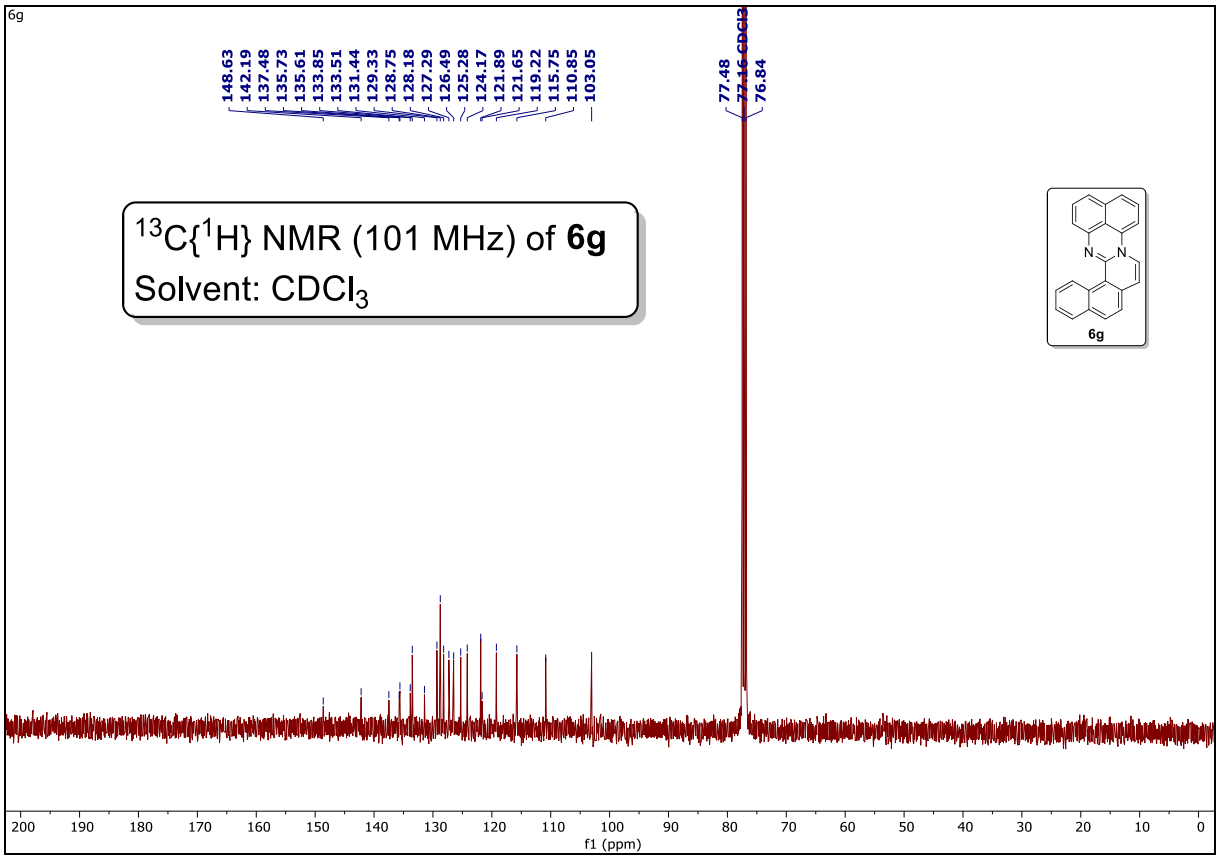

Spectrum from V-85_Ms. Vidya.wiff2 (sample 1) - V-85, Experiment 1, +IDA TOF MS (100 - 1000) from 0.091 to 0.111 min
Intensity, cps
Mass/Charge, Da
*287.0960 (1)
288.1004 (1)
*286.0913
*289.1055 (1)
*571.1747 (1)
*949.5494 (1)
N
N
F
6e

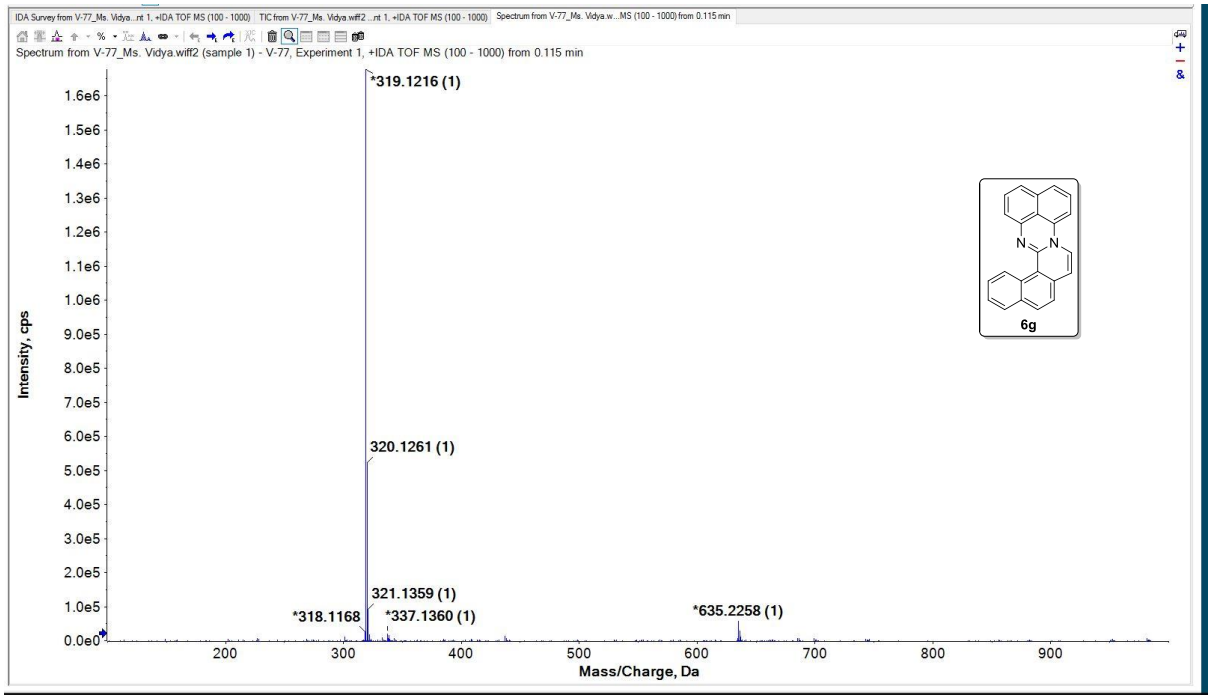

6f
8.61
8.58
7.39
7.37
7.33
7.31
7.29
7.26 CDCl3
7.24
7.20
7.19
7.17
7.14
7.12
7.04
7.03
7.01
7.01
6.96
6.94
6.76
6.75
6.72
6.70
6.48
6.46
3.87
1H NMR (400 MHz) of 6f
Solvent: CDCl3
6f
1.00
1.06
1.00
1.04
1.00
1.00
1.00
1.00
1.00
1.00
3.00
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

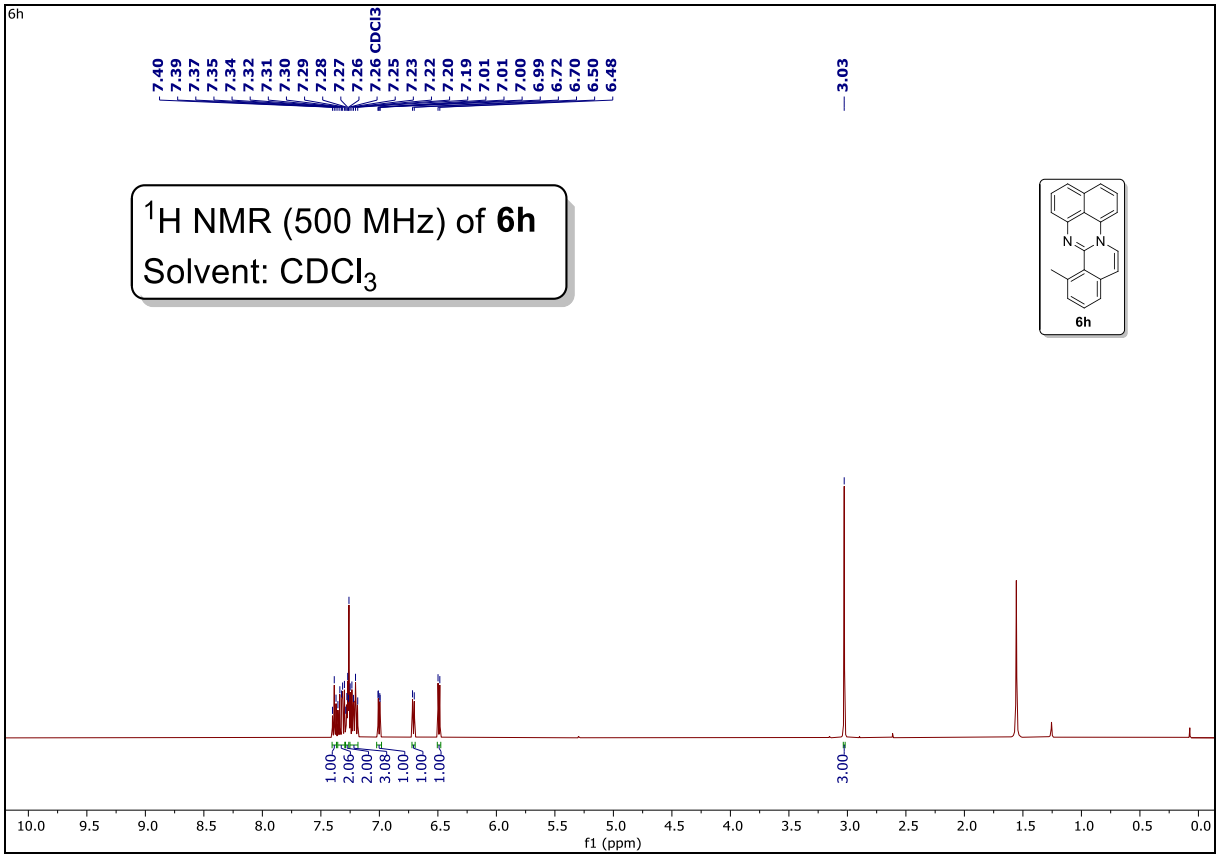

6f
162.46
147.42
142.85
136.78
135.88
135.47
129.29
129.23
127.10
123.81
121.80
121.68
121.21
118.83
116.78
115.13
109.83
107.48
101.68
77.48
77.16 CDCl3
76.84
55.59
13C{1H} NMR (101 MHz) of 6f
Solvent: CDCl3
6f
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

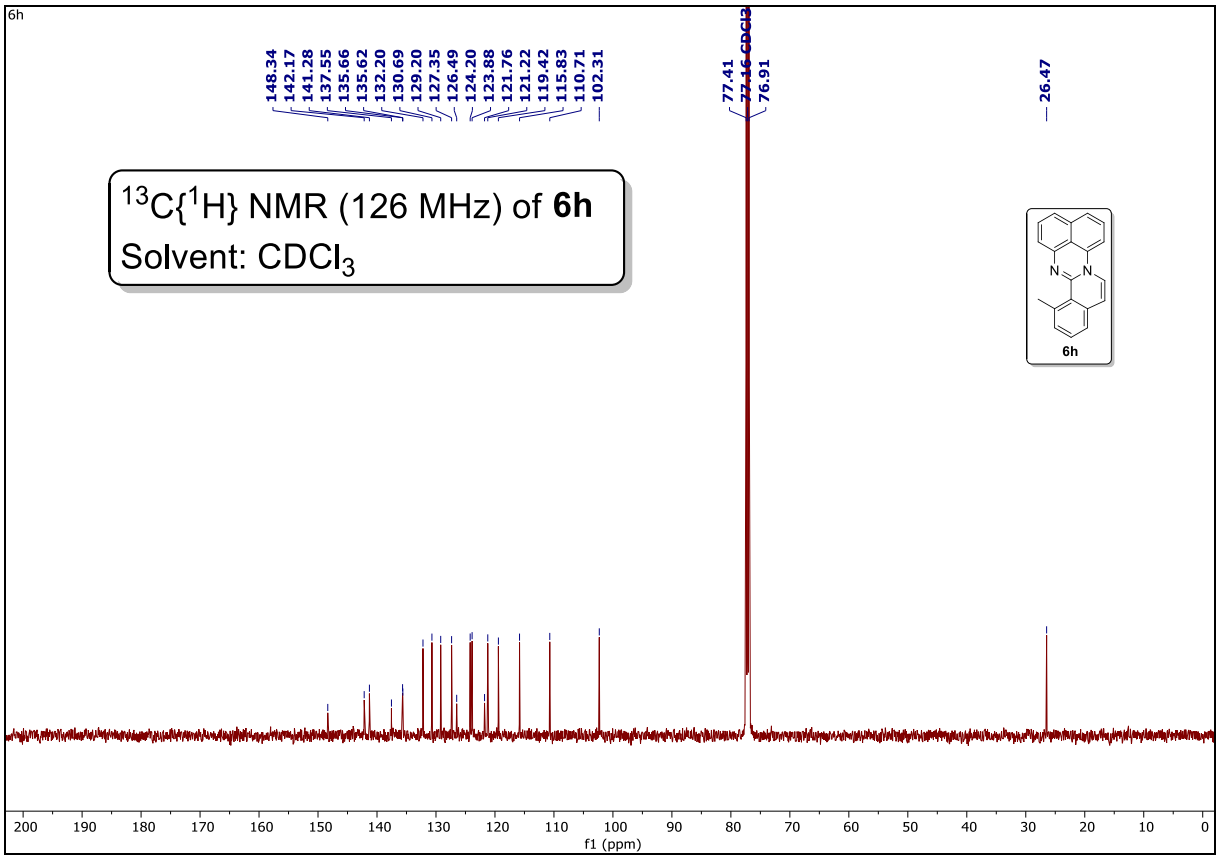

Spectrum from V-63_Ms. Vidya.wiff2 (sample 1) - V-63, Experiment 1, +IDA TOF MS (100 - 1000) from 0.052 to 0.072 min
Intensity, cps
Mass/Charge, Da
*299.1158 (1)
300.1201 (1)
*289.0983 (1)
*301.1254 (1)
339.3469 (1)
*961.5707 (1)
6f

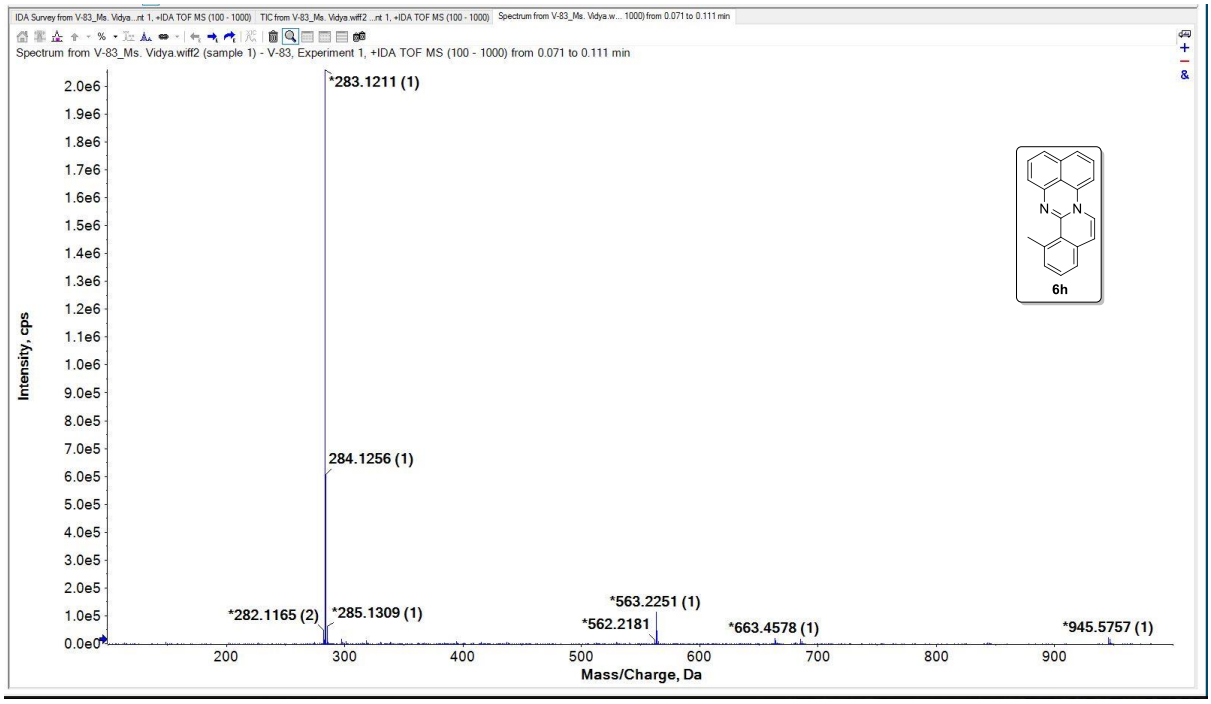

6g
10.59
10.57
7.97
7.95
7.89
7.87
7.75
7.75
7.74
7.73
7.73
7.71
7.71
7.61
7.59
7.57
7.55
7.43
7.41
7.39
7.36
7.34
7.30
7.28
7.26 CDCl3
7.25
7.23
7.18
7.16
6.81
6.80
6.69
6.67
1H NMR (400 MHz) of 6g
Solvent: CDCl3
6g
1.00
1.00
1.00
1.05
2.15
2.00
1.00
1.00
1.00
1.00
1.00
1.00
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

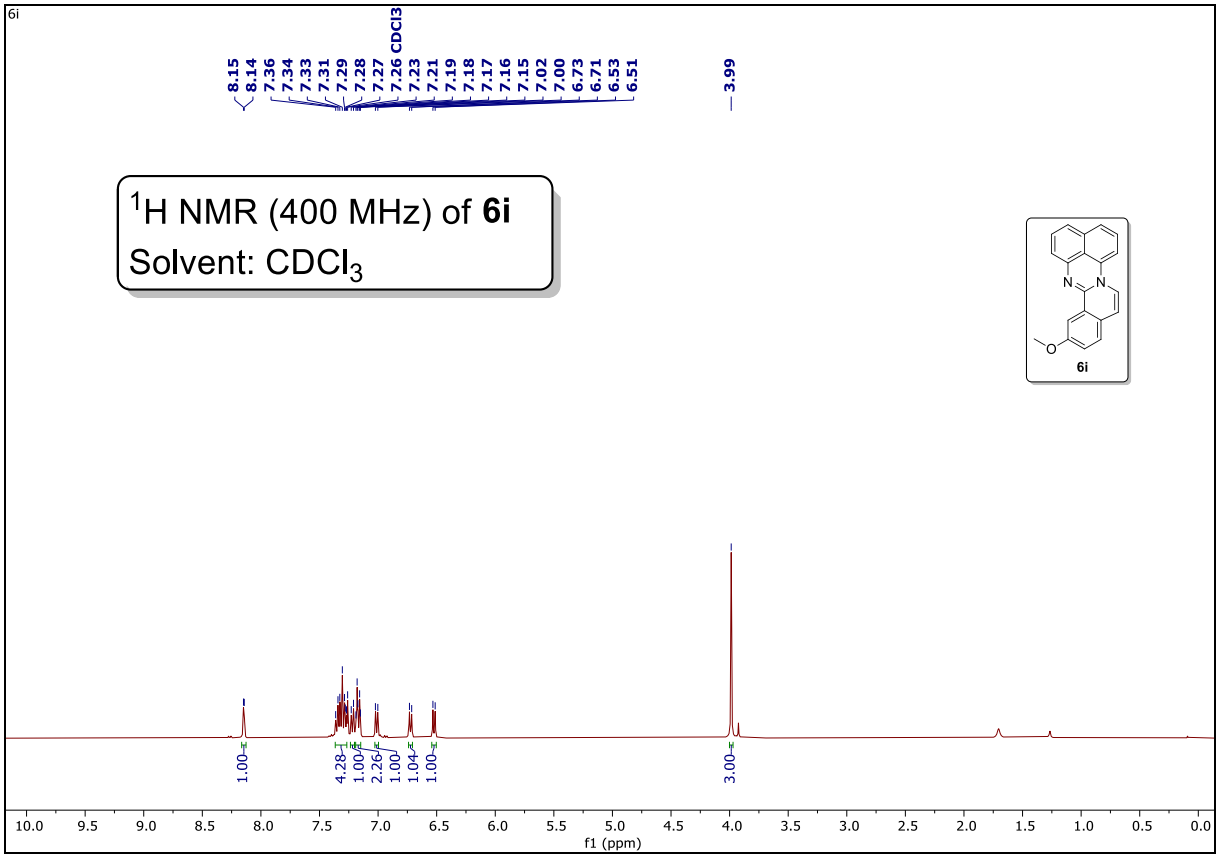

6g
148.63
142.19
137.48
135.73
135.61
133.85
133.51
131.44
129.33
128.75
128.18
127.29
126.49
125.28
124.17
121.89
121.65
119.22
115.75
110.85
103.05
77.48
77.16 CDCl3
76.84
13C{1H} NMR (101 MHz) of 6g
Solvent: CDCl3
6g
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

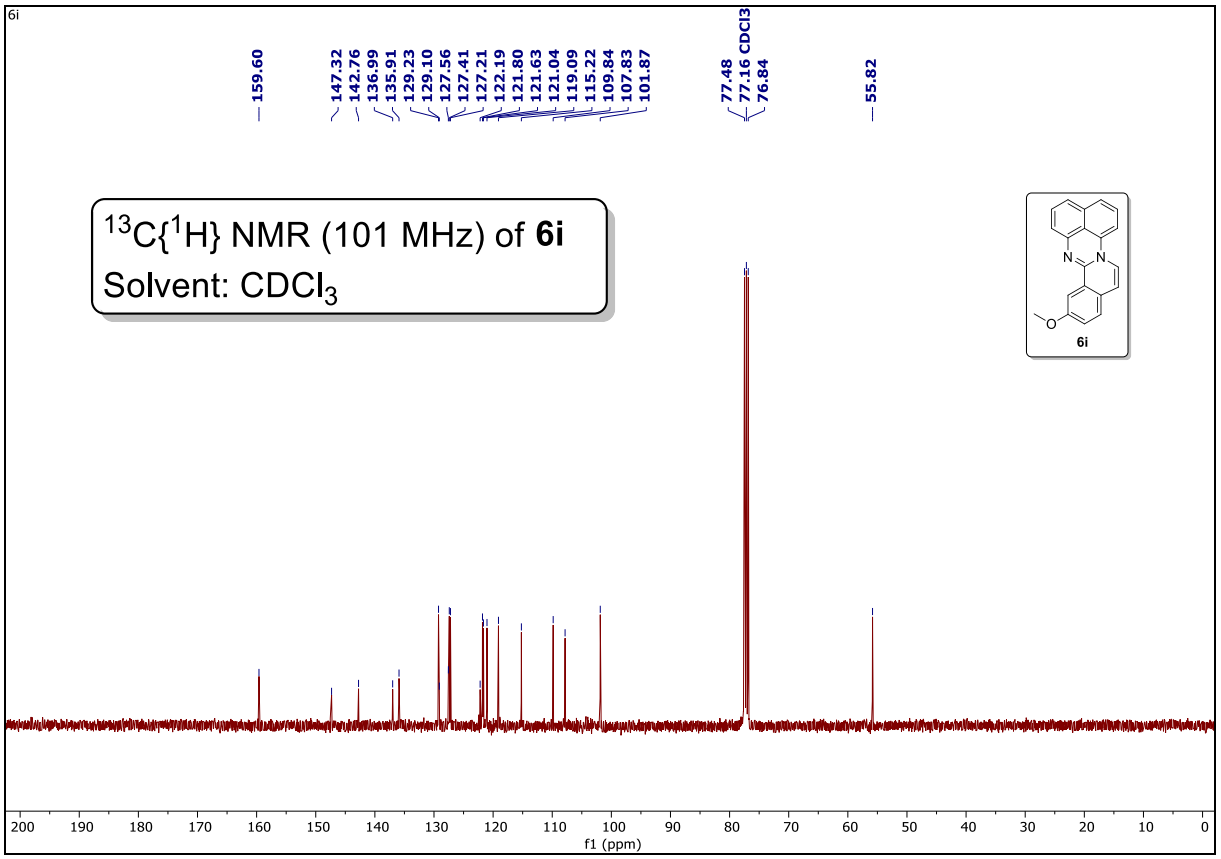

Spectrum from V-77_Ms. Vidya.wiff2 (sample 1) - V-77, Experiment 1, +IDA TOF MS (100 - 1000) from 0.115 min
*319.1216 (1)
320.1261 (1)
321.1359 (1)
*318.1168
*337.1360 (1)
*635.2258 (1)
Intensity, cps
Mass/Charge, Da
6g

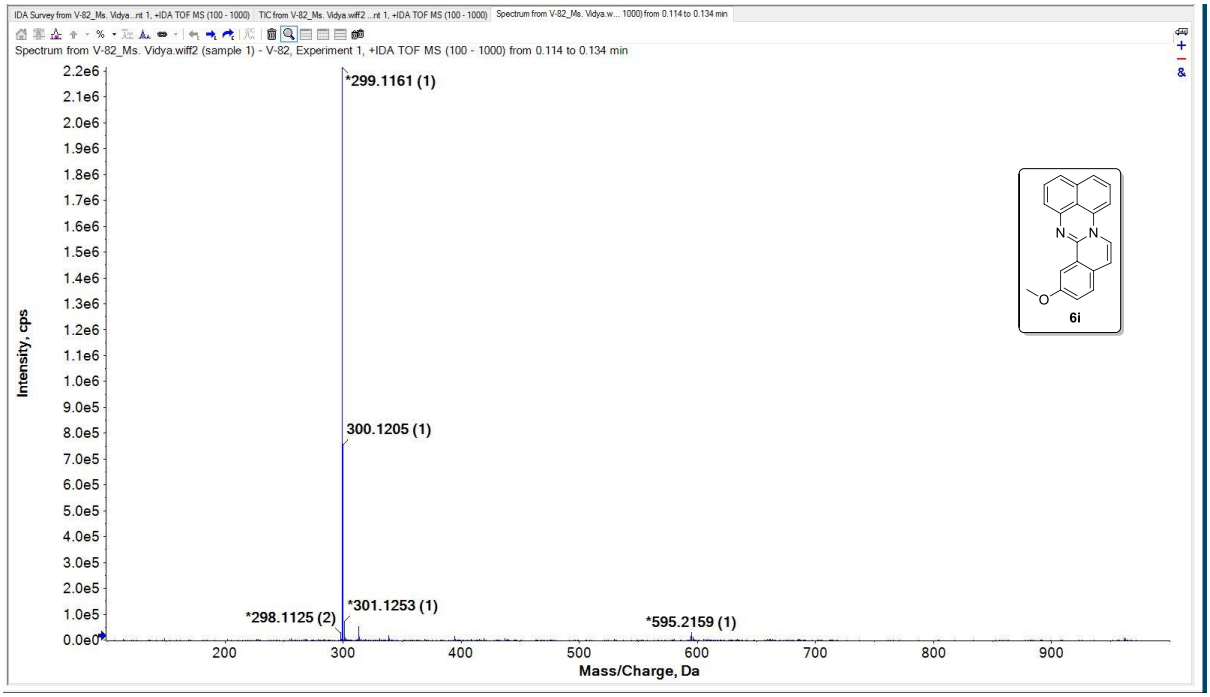

6h
7.40
7.39
7.37
7.35
7.34
7.32
7.31
7.30
7.29
7.28
7.27
7.26 CDCl3
7.25
7.23
7.22
7.20
7.19
7.01
7.01
7.00
6.99
6.72
6.70
6.50
6.48
3.03
1H NMR (500 MHz) of 6h
Solvent: CDCl3
6h
1.00
2.06
2.00
3.08
1.00
1.00
1.00
3.00
f1 (ppm)

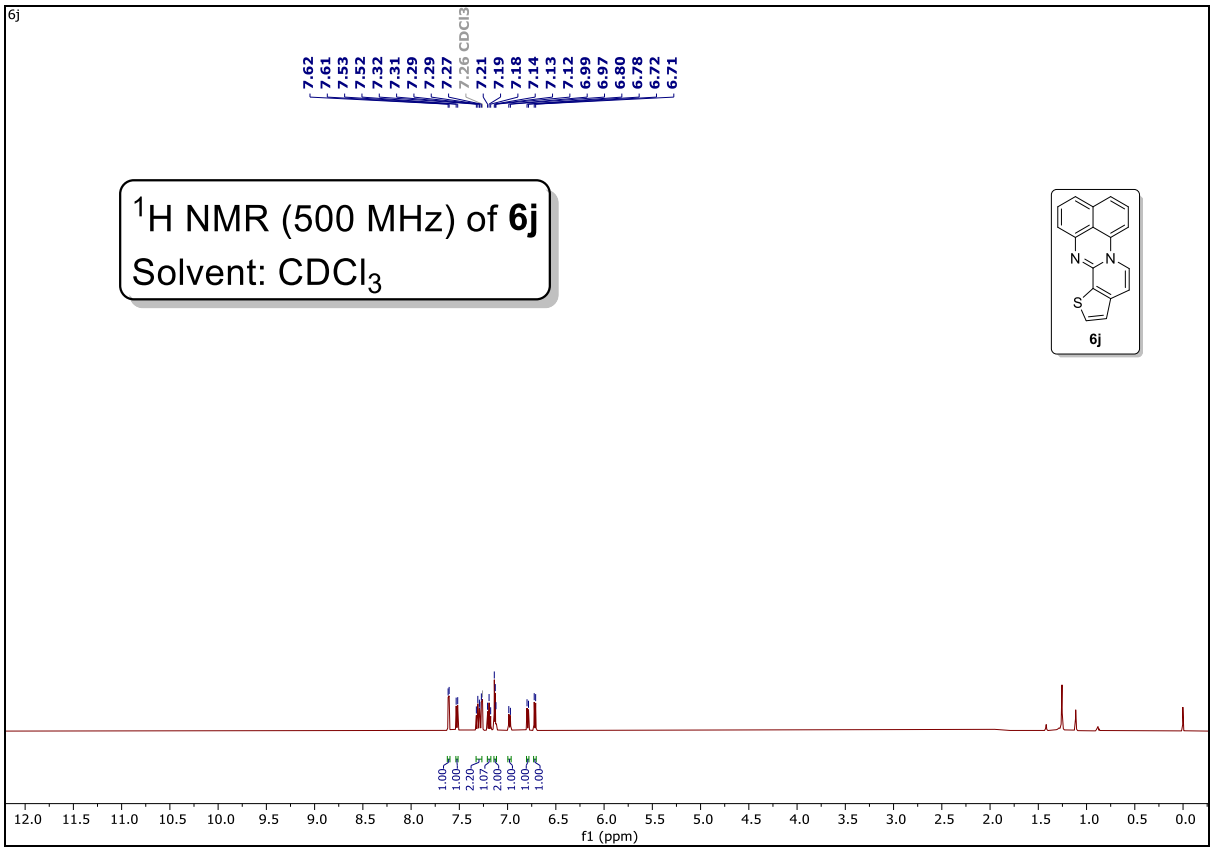

6h
148.34
142.17
141.28
137.55
135.66
135.62
132.20
130.69
129.20
127.35
126.49
124.20
123.88
121.76
121.22
119.42
115.83
110.71
102.31
77.41
77.16 CDCl3
76.91
26.47
13C{1H} NMR (126 MHz) of 6h
Solvent: CDCl3
6h
f1 (ppm)

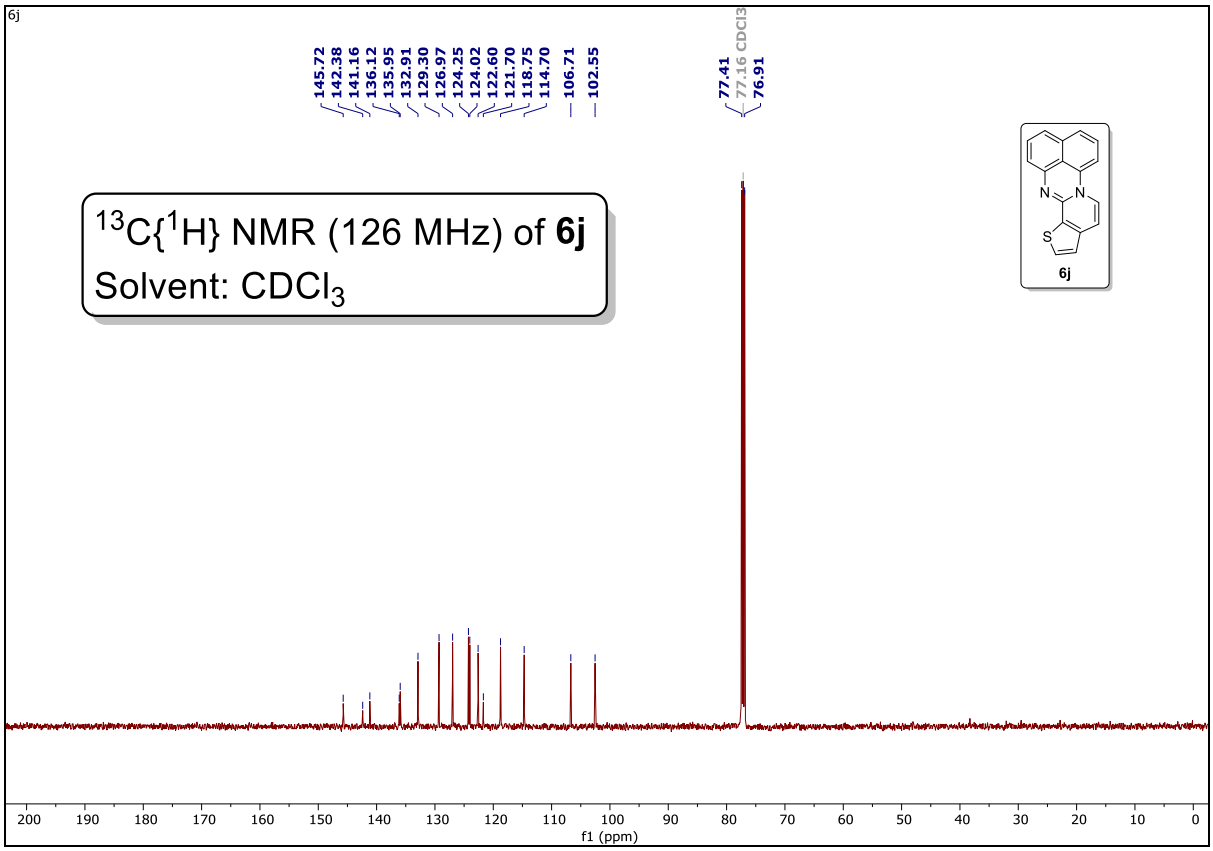

Spectrum from V-83_Ms. Vidya.wiff2 (sample 1) - V-83, Experiment 1, +IDA TOF MS (100 - 1000) from 0.071 to 0.111 min
Intensity, cps
Mass/Charge, Da
*283.1211 (1)
284.1256 (1)
*282.1165 (2)
*285.1309 (1)
*563.2251 (1)
*562.2181
*663.4578 (1)
*945.5757 (1)
6h

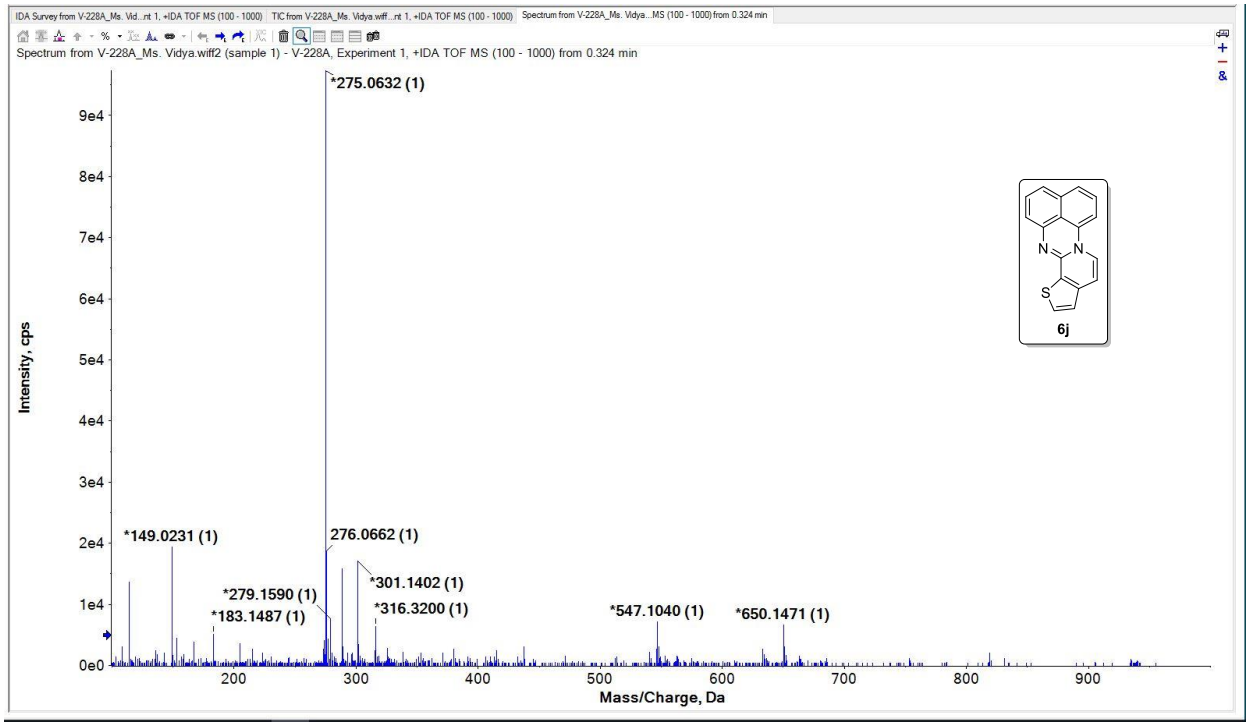

6i
8.15
8.14
7.36
7.34
7.33
7.31
7.29
7.28
7.27
7.26 CDCl3
7.23
7.21
7.19
7.18
7.17
7.16
7.15
7.02
7.00
6.73
6.71
6.53
6.51
3.99
1H NMR (400 MHz) of 6i
Solvent: CDCl3
6i
1.00
4.28
1.00
2.26
1.00
1.04
1.00
3.00
f1 (ppm)

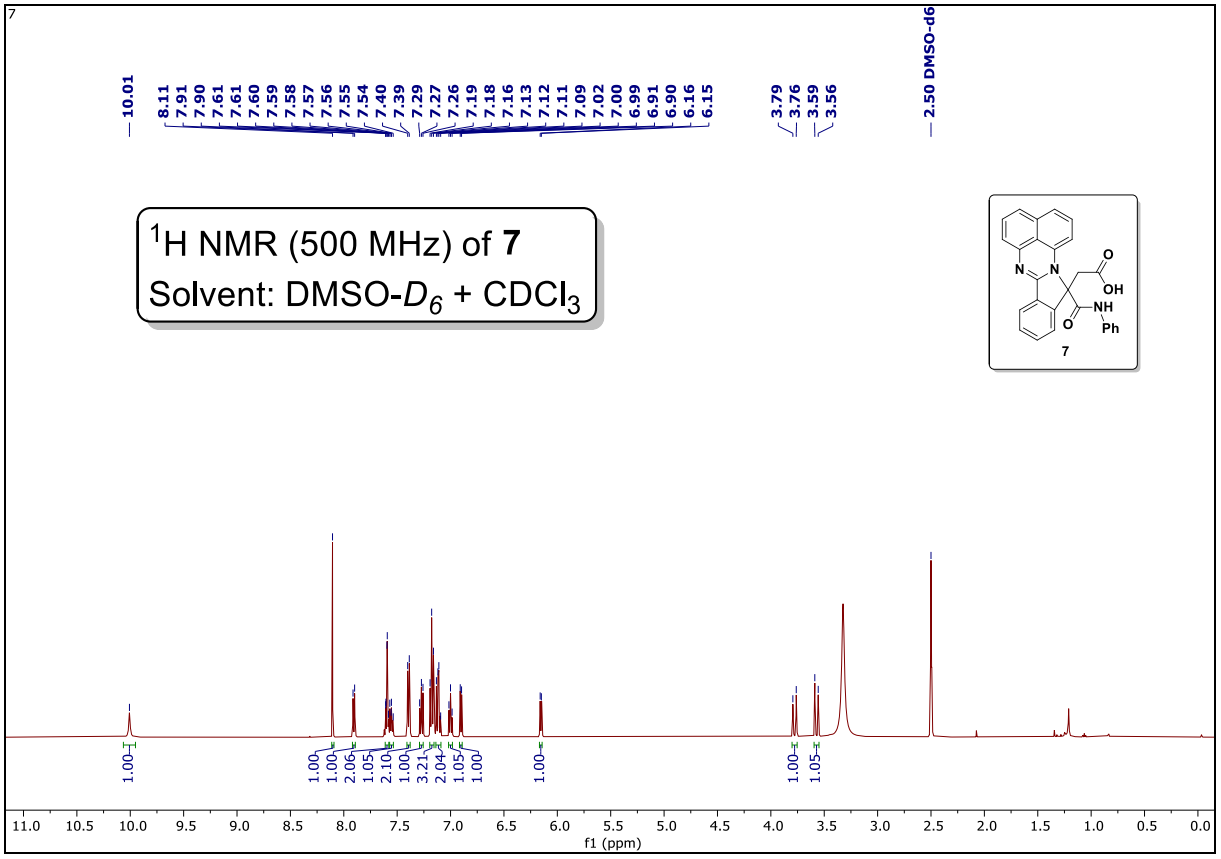

6i
159.60
147.32
142.76
136.99
135.91
129.23
129.10
127.56
127.41
127.21
122.19
121.80
121.63
121.04
119.09
115.22
109.84
107.83
101.87
77.48
77.16 CDCl3
76.84
55.82
13C{1H} NMR (101 MHz) of 6i
Solvent: CDCl3
6i
f1 (ppm)

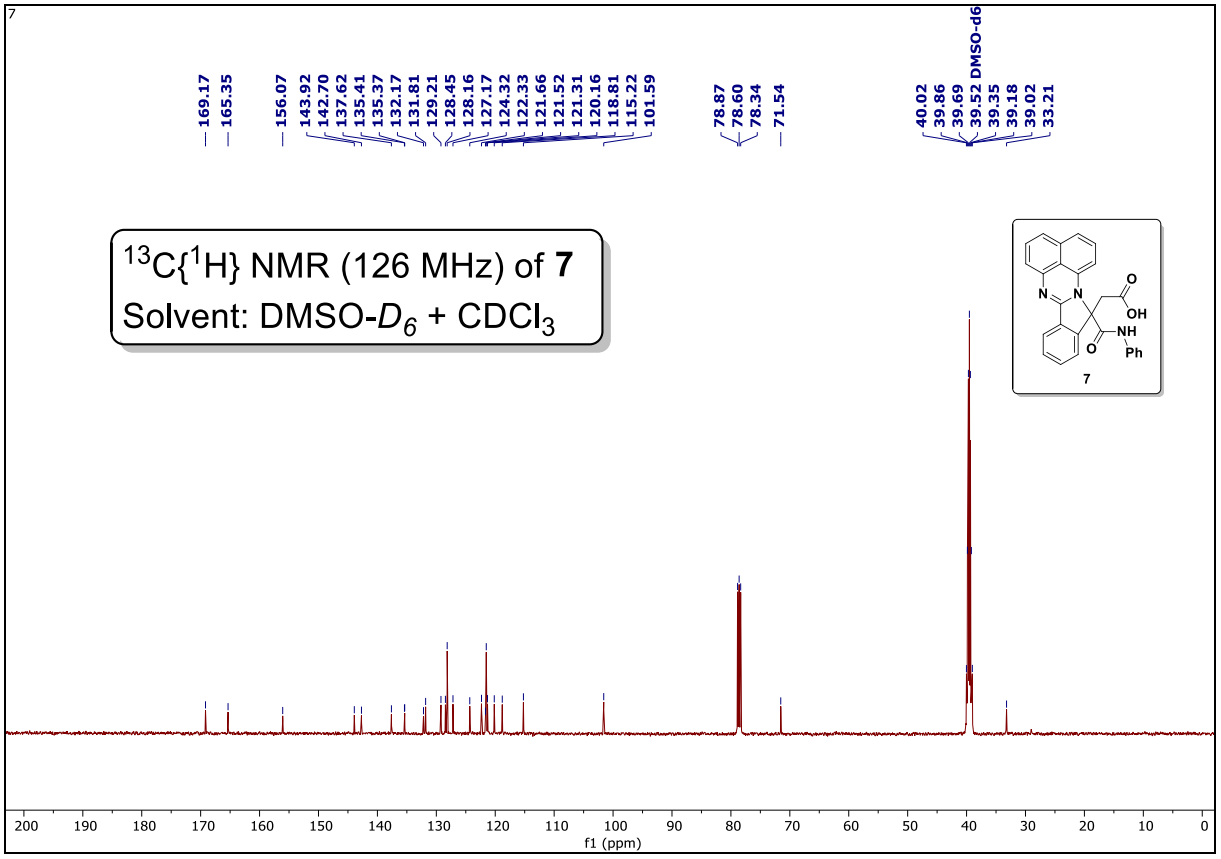

Spectrum from V-82_Ms. Vidya.wiff2 (sample 1) - V-82, Experiment 1, +IDA TOF MS (100 - 1000) from 0.114 to 0.134 min
Intensity, cps
Mass/Charge, Da
*299.1161 (1)
300.1205 (1)
*301.1253 (1)
*298.1125 (2)
*595.2159 (1)
6i

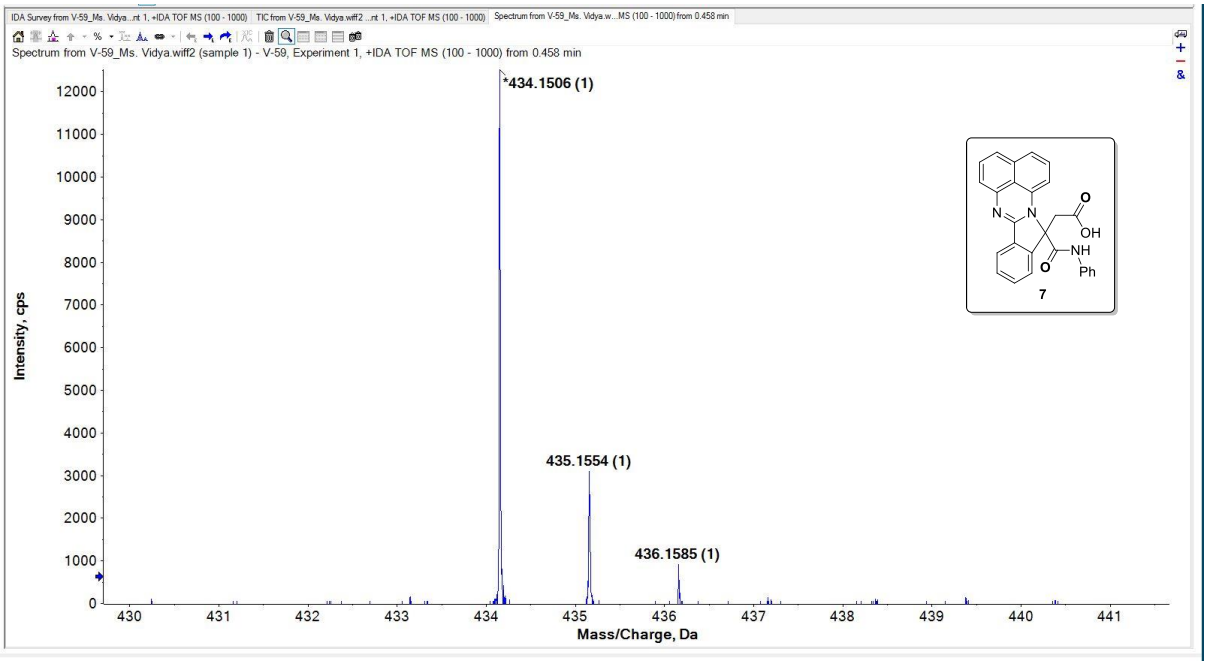

6j
7.62
7.61
7.53
7.52
7.32
7.31
7.29
7.29
7.27
7.26 CDCl3
7.21
7.19
7.18
7.14
7.13
7.12
6.99
6.97
6.80
6.78
6.72
6.71
^{1}H NMR (500 MHz) of **6j**
Solvent: $CDCl_3$
6j
f1 (ppm)


6j
145.72
142.38
141.16
136.12
135.95
132.91
129.30
126.97
124.25
124.02
122.60
121.70
118.75
114.70
106.71
102.55
77.41
77.16 CDCl3
76.91
^{13}C{^{1}H} NMR (126 MHz) of **6j**
Solvent: $CDCl_3$
6j
f1 (ppm)


Spectrum from V-228A_Ms. Vidya.wiff2 (sample 1) - V-228A, Experiment 1, +IDA TOF MS (100 - 1000) from 0.324 min
*275.0632 (1)
*149.0231 (1)
276.0662 (1)
*301.1402 (1)
*279.1590 (1)
*316.3200 (1)
*183.1487 (1)
*547.1040 (1)
*650.1471 (1)
Intensity, cps
Mass/Charge, Da
6j


7
10.01
8.11
7.91
7.90
7.61
7.61
7.60
7.59
7.58
7.57
7.56
7.55
7.54
7.40
7.39
7.29
7.27
7.26
7.19
7.18
7.16
7.13
7.12
7.11
7.09
7.02
7.00
6.99
6.91
6.90
6.16
6.15
3.79
3.76
3.59
3.56
2.50 DMSO-d6
1H NMR (500 MHz) of 7
Solvent: DMSO-D6 + CDCl3
O
OH
NH
Ph
O
N
N
7
1.00
1.00
1.00
2.06
1.05
2.10
1.00
3.21
2.04
1.05
1.00
1.00
1.00
1.05
f1 (ppm)


7
169.17
165.35
156.07
143.92
142.70
137.62
135.41
135.37
132.17
131.81
129.21
128.45
128.16
127.17
124.32
122.33
121.66
121.52
121.31
120.16
118.81
115.22
101.59
78.87
78.60
78.34
71.54
40.02
39.86
39.69
39.52 DMSO-d6
39.35
39.18
39.02
33.21
13C{1H} NMR (126 MHz) of 7
Solvent: DMSO-D6 + CDCl3
O
OH
NH
Ph
O
N
N
7
f1 (ppm)


IDA Survey from V-59_Ms. Vidya...nt 1, +IDA TOF MS (100 - 1000)
TIC from V-59_Ms. Vidya.wiff2 ...nt 1, +IDA TOF MS (100 - 1000)
Spectrum from V-59_Ms. Vidya.w...MS (100 - 1000) from 0.458 min
Spectrum from V-59_Ms. Vidya.wiff2 (sample 1) - V-59, Experiment 1, +IDA TOF MS (100 - 1000) from 0.458 min
*434.1506 (1)
435.1554 (1)
436.1585 (1)
Intensity, cps
Mass/Charge, Da
12000
11000
10000
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
430
431
432
433
434
435
436
437
438
439
440
441
N
N
O
OH
NH
O
Ph
7

HRMS of Intermediates

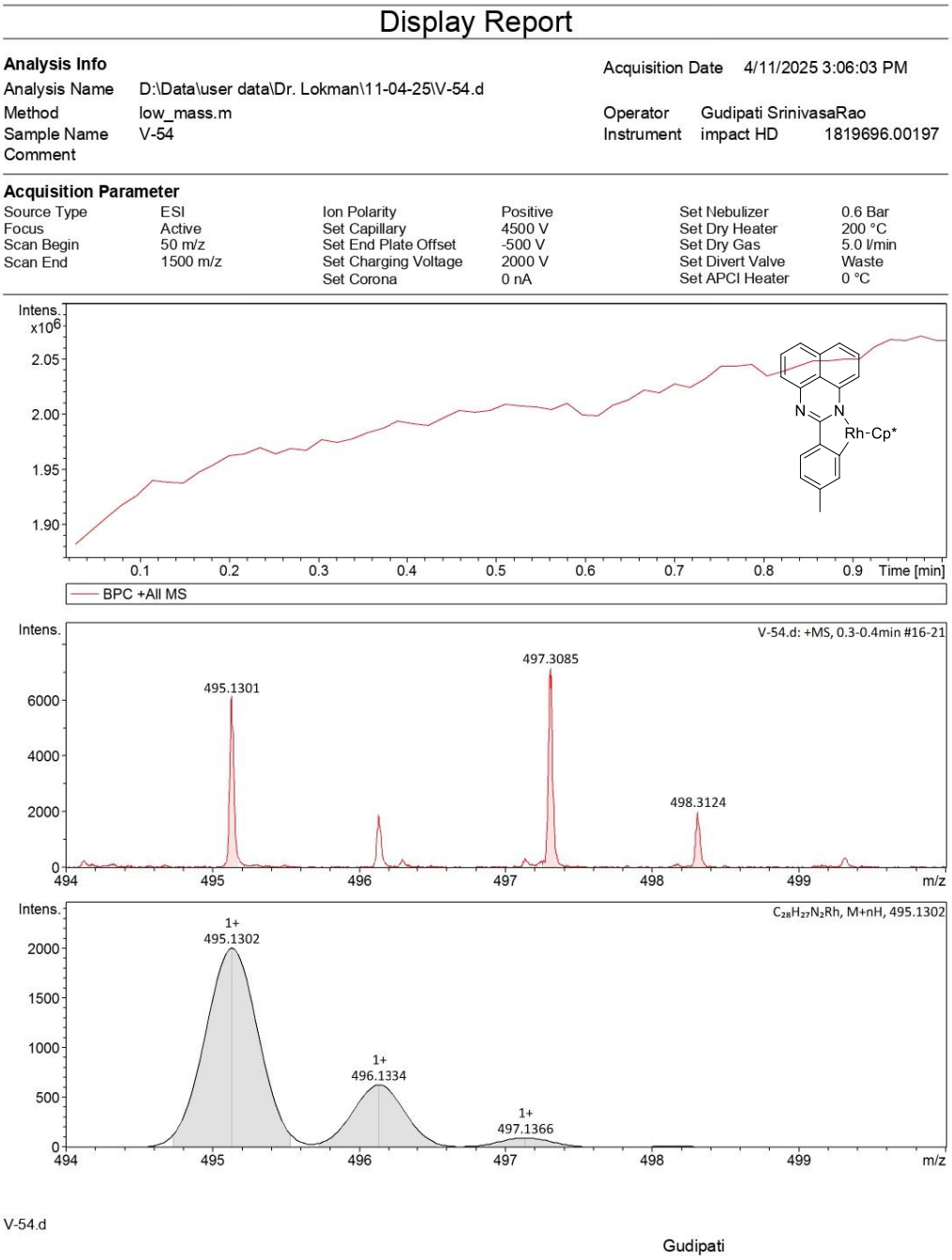


Figure S1: HRMS of Intermediate B (detected for **1b**)

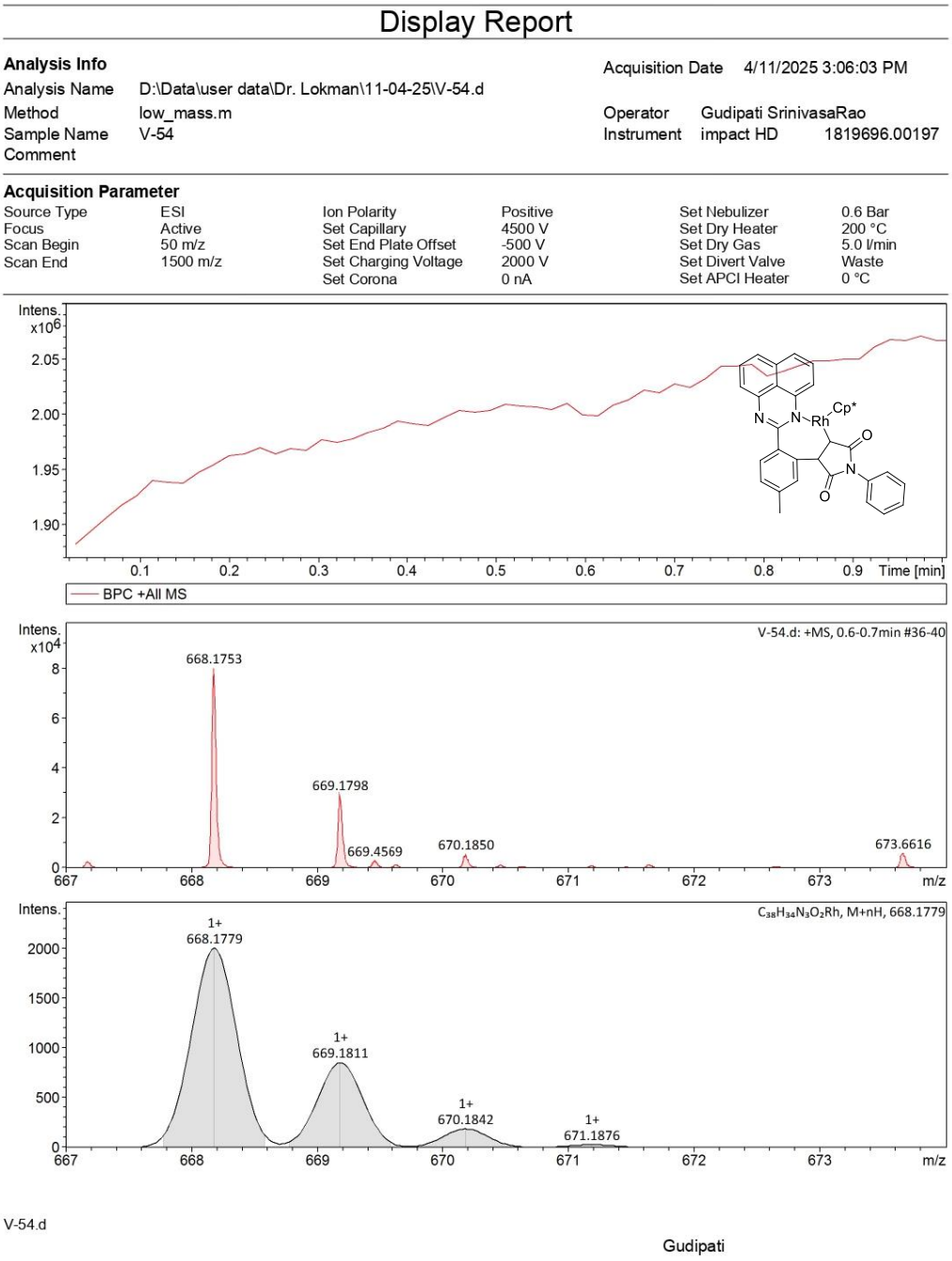


Figure S2: HRMS of Intermediate D (detected for **1b**)

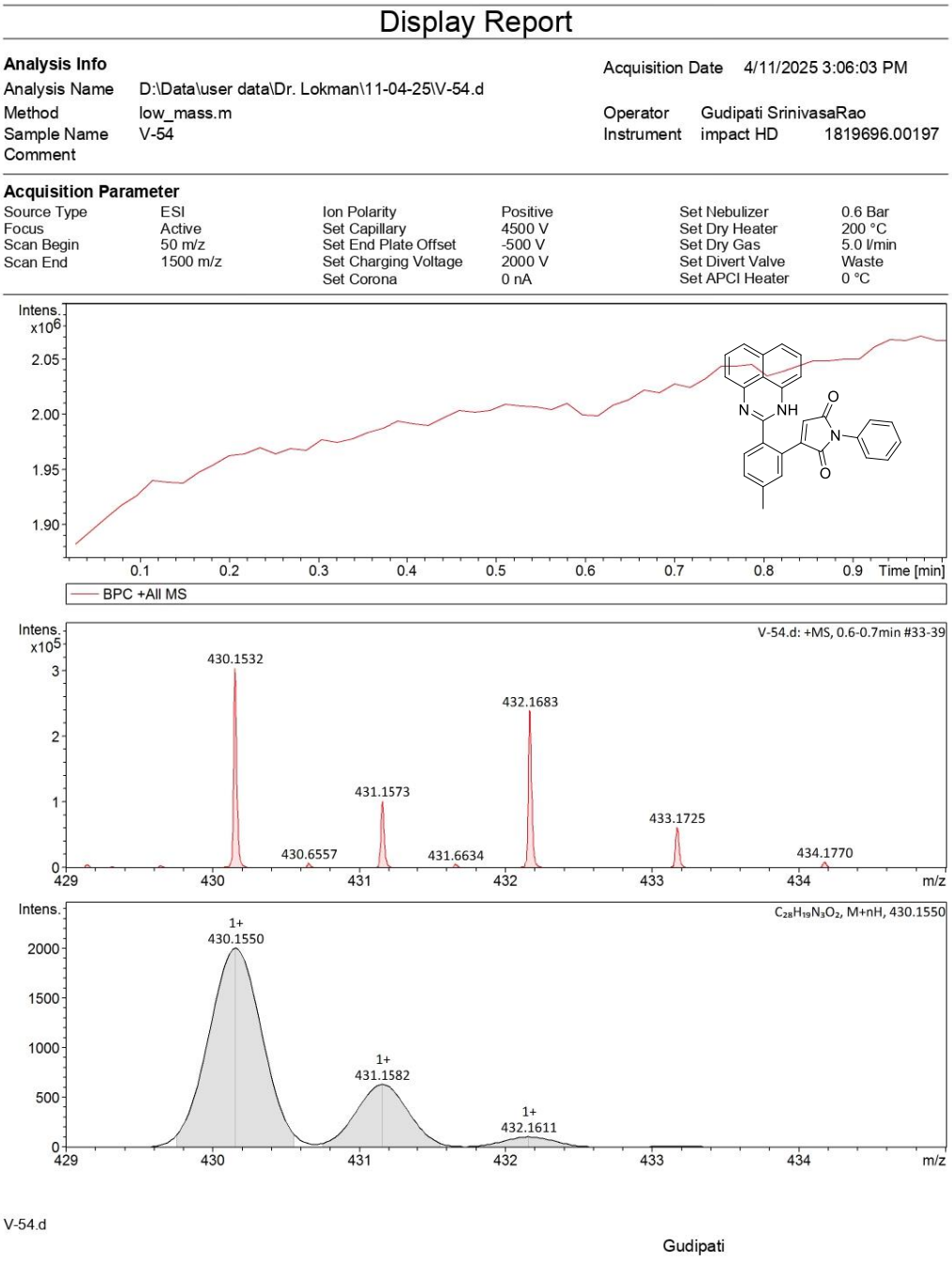


Figure S3: HRMS of Intermediate F (detected for **1b**)

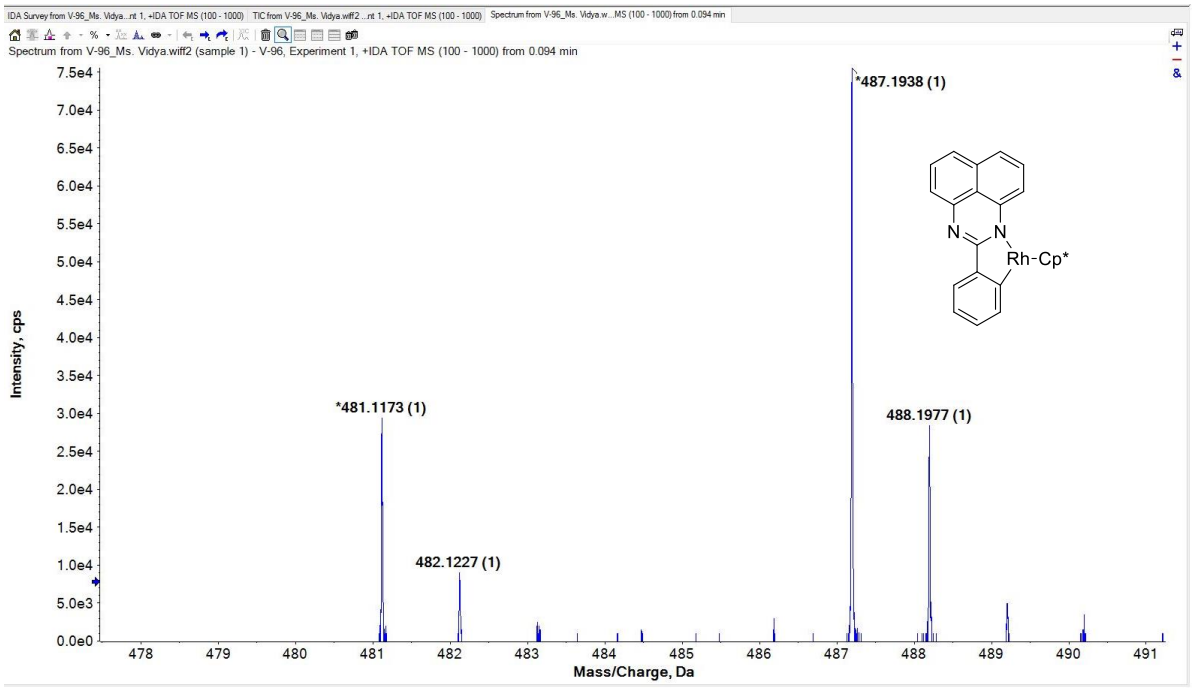


Figure S4: HRMS of Intermediate B' (detected for **1a**)

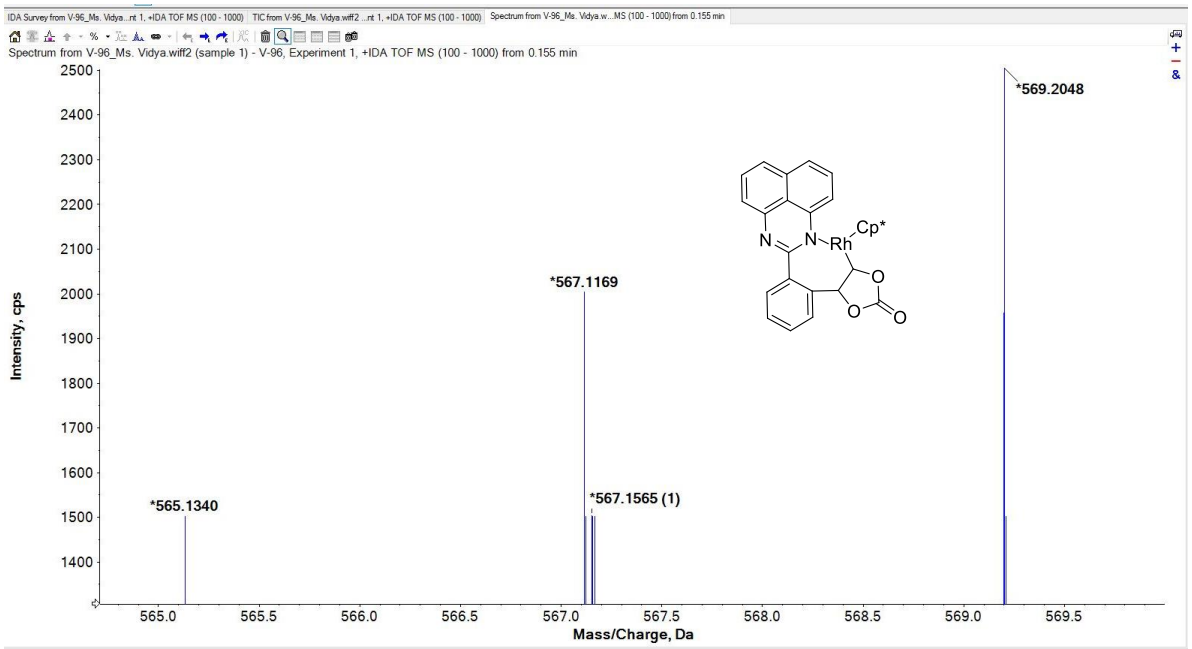


Figure S5: HRMS of Intermediate D' (detected for **1a**)

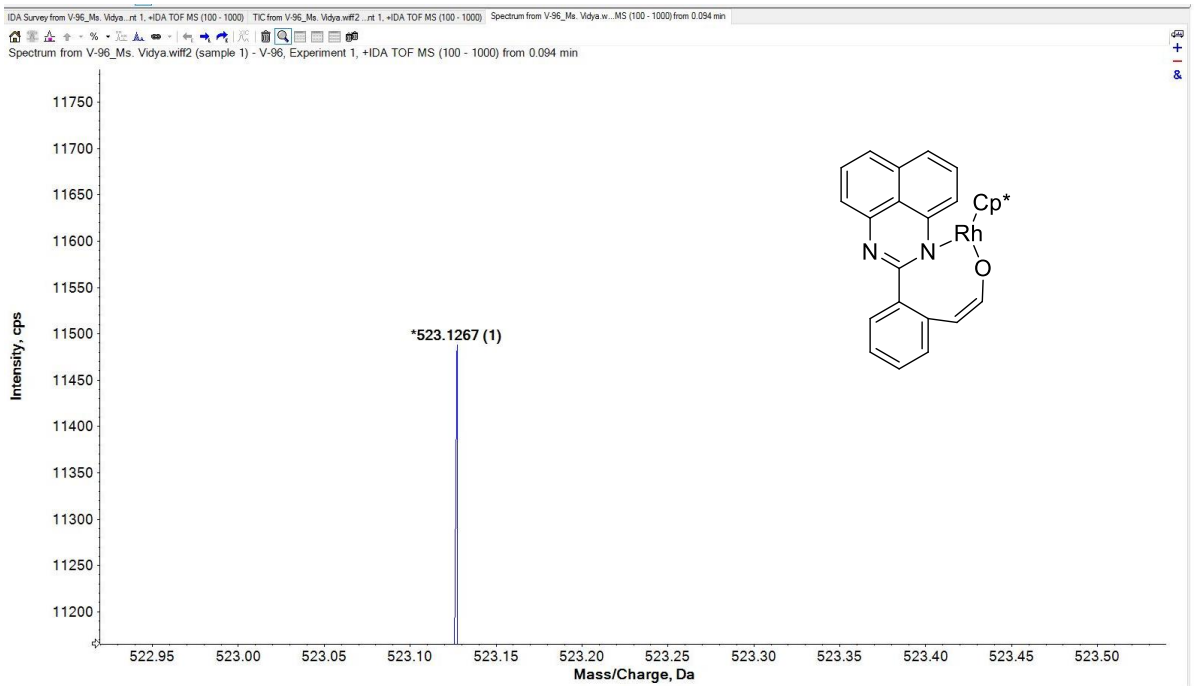


Figure S6: HRMS of Intermediate E' (detected for **1a**)

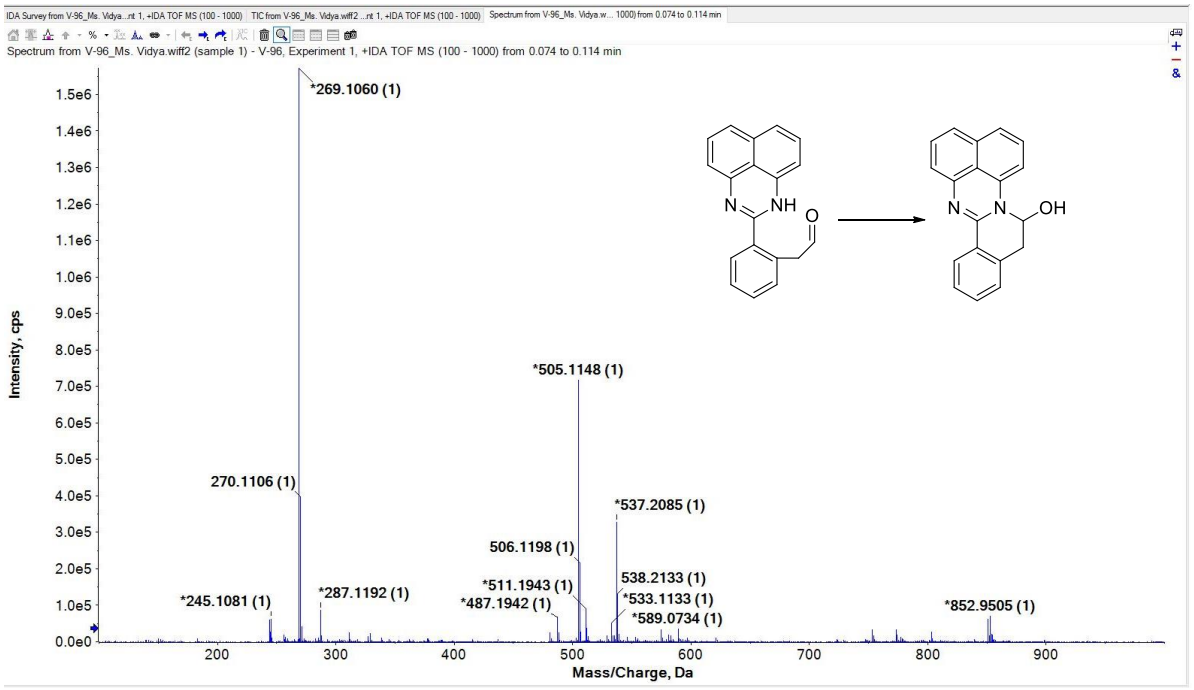


Figure S7: HRMS of Intermediate G'/H' (detected for **1a**)

SC-XRD of 3b

Method for crystal growth 3b:

In a 5 mL vial, 30 mg of the pure **3b** was dissolved in 2 mL volume of EtOAc and gently warmed in water bath and shaken well. After getting a clear homogeneous solution, the vial

was covered with a porous cap and kept undisturbed for 24-36 hrs at room temperature. The slow evaporation of the solvent mixture afforded the crystals of **3b**. The details of SC-XRD analysis is given below.

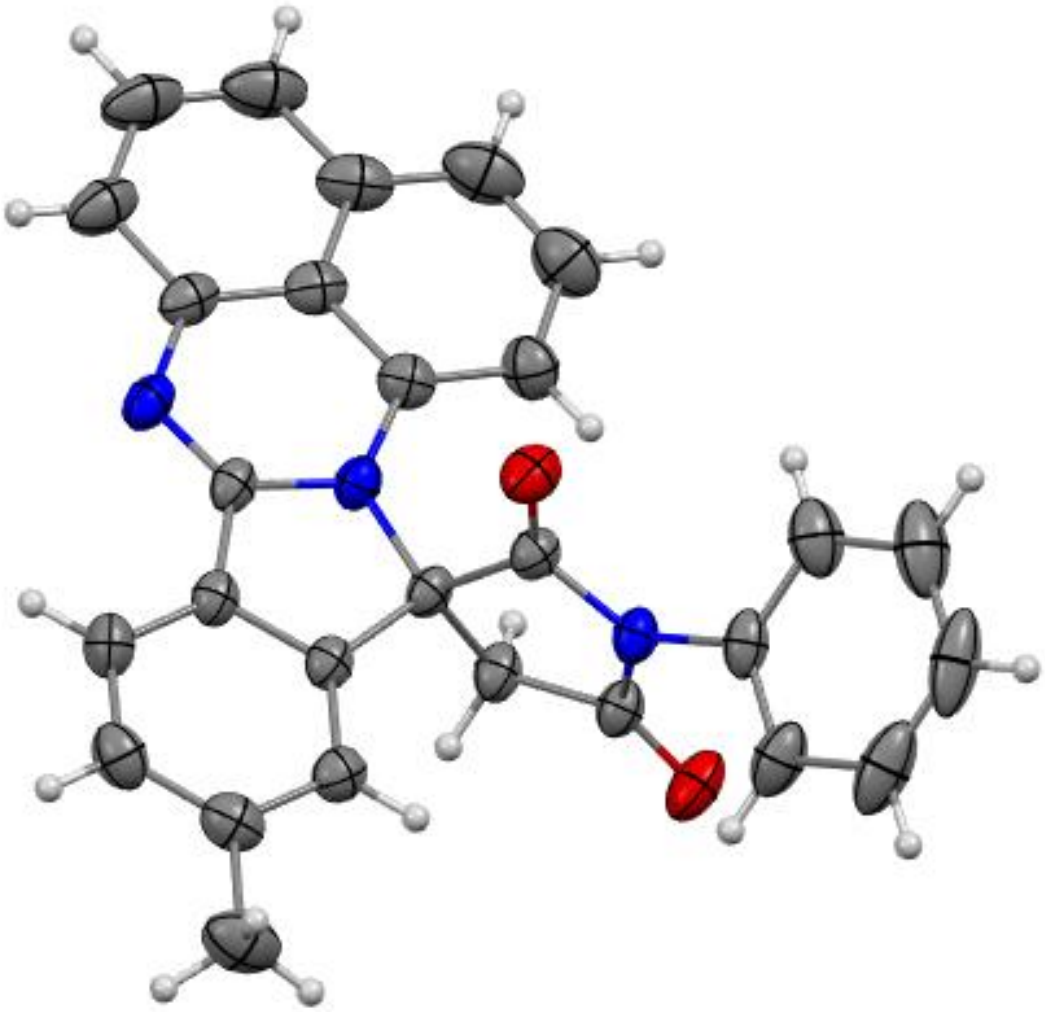


Figure S8: SC-XRD of **3b** (ellipsoid contour % probability - 30)

A specimen of $C_{28}H_{19}N_3O_2$, approximate dimensions 0.31 mm x 0.303 mm x 0.16 mm, was used for the X-ray crystallographic analysis. The X-ray intensity data were measured.

Table 1 Crystal data and structure refinement for 2279344.	
Identification code	2279344
Empirical formula	$C_{28}H_{19}N_3O_2$
Formula weight	429.46
Temperature/K	298
Crystal system	monoclinic
Space group	$P2_1/c$

a/Å	12.219(3)
b/Å	9.929(3)
c/Å	20.262(5)
α/°	90
β/°	97.500(9)
γ/°	90
Volume/Å^3	2437.1(11)
Z	4
ρ_{calc}g/cm^3	1.170
μ/mm^{-1}	0.075
F(000)	896.0
Crystal size/mm^3	0.31 × 0.303 × 0.16
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	5.52 to 53.09
Index ranges	-15 ≤ h ≤ 15, -12 ≤ k ≤ 12, -25 ≤ l ≤ 24
Reflections collected	36401
Independent reflections	5047 [R_{int} = 0.0660, R_{sigma} = 0.0386]
Data/restraints/parameters	5047/0/301
Goodness-of-fit on F^2	1.026
Final R indexes [I>=2σ (I)]	R_1 = 0.0590, wR_2 = 0.1512
Final R indexes [all data]	R_1 = 0.0671, wR_2 = 0.1566
Largest diff. peak/hole / e Å^{-3}	0.21/-0.16

SC-XRD of 3l

Method for crystal growth 3l:

In a 5 mL vial, 25 mg of the pure **3l** was dissolved in 2 mL volume of EtOAc and gently warmed in water bath and shaken well. After getting a clear homogeneous solution, the vial was covered with a porous cap and kept undisturbed for 24-36 hrs at room temperature. The slow evaporation of the solvent mixture afforded the crystals of **3l**. The details of SC-XRD analysis is given below.

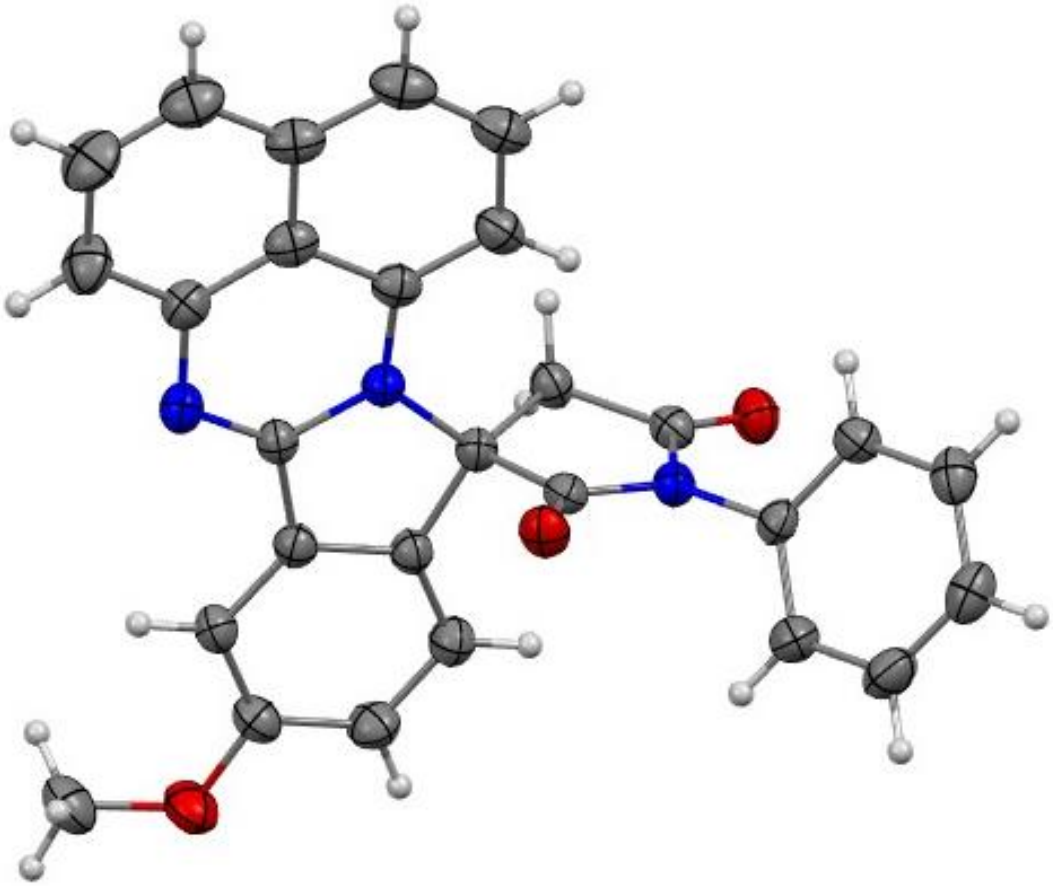


Figure S9: SC-XRD of **3l** (ellipsoid contour % probability - 30)

A specimen of $C_{28}H_{19}N_3O_2$, approximate dimensions 0.2154 mm x 0.156 mm x 0.123 mm, was used for the X-ray crystallographic analysis. The X-ray intensity data were measured.

Table 1 Crystal data and structure refinement for MONO.	
Identification code	2495811
Empirical formula	$C_{30}H_{23}N_3O_4$
Formula weight	489.51
Temperature/K	298
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	11.832(3)
b/Å	21.918(5)
c/Å	11.449(3)
α/°	90
β/°	117.514(10)
γ/°	90
Volume/Å^3	2633.2(11)
Z	4

ρ_{calc}g/cm^3	1.235
μ/mm^{-1}	0.083
F(000)	1024.0
Crystal size/mm^3	0.2154 × 0.156 × 0.123
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	6.796 to 52.934
Index ranges	-14 ≤ h ≤ 14, -27 ≤ k ≤ 27, -14 ≤ l ≤ 14
Reflections collected	39000
Independent reflections	5356 [R_{int} = 0.0709, R_{sigma} = 0.0421]
Data/restraints/parameters	5356/0/308
Goodness-of-fit on F^2	1.056
Final R indexes [I>=2σ (I)]	R_1 = 0.0811, wR_2 = 0.2164
Final R indexes [all data]	R_1 = 0.1183, wR_2 = 0.2474
Largest diff. peak/hole / e Å^{-3}	0.23/-0.26

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