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Supporting Information

para-Selective Copper-Catalyzed C(sp^2)–H Amidation/Dimerization of Anilides *via a* Radical Pathway

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1. General Information:

All reagents and solvents were used as received from commercial sources unless otherwise noted. All experiments were carried out in a Teflon screw cap glass tube. Precoated plates (silica gel 60 PF254, 0.25 mm or 0.5 mm) were utilized for thin-layer chromatography (TLC). Visualization of the developed TLC plate was performed by irradiation with UV light. Column chromatographic purifications were carried out on flash silica gel (240−400 mesh) using ethyl acetate and petroleum ether as eluents. The ^{1}H and ^{13}C NMR spectra were recorded on 400 and 100 MHz NMR spectrometers, respectively, in $CDCl_3$. Chemical shifts were reported as δ values from standard peaks. The ^{13}C NMR spectra of compounds **2a**, **2c**, **2m**, **2n and 2u** shows one carbon less and the compound **2o** shows two carbon less because of peak overlapping. The melting points were recorded on a Buchi instrument and are uncorrected. High-resolution mass spectrometry (HRMS) was performed on a TOF/Q-TOF mass spectrometer.

The NMR spectra of compounds **2a-g** show clean countable proton/carbon peaks. However, peak broadening was observed for aromatic peaks in the ^{1}H and ^{13}C NMR spectra of **2i-l**. Scanning the sample at various concentrations in $CDCl_3$ and other deuterated solvents at different concentrations and even for a longer time (24 h) on a 700 MHz Bruker NMR instrument also did not change this peculiar pattern. However, scanning the ^{1}H NMR of a representative compound **2j** at higher temperature provided clean spectra (see page nos. 37 and 38). These compounds with the presence of proton on the carbon adjacent to the carbonyl group may have a different kind of inter or intramolecular interaction leading to such a pattern. To clarify the doubt about the structure, we prepared the same compound **2j** by acylation of the corresponding commercially available diamine (page S4). The peculiar peak broadening was observed in the NMR, but the spectral and analytical data was in complete agreement with the data of the compound **2j** synthesized by our protocol. The matching data also confirms the regioselectivity of our protocol.

2. Experimental Procedures:

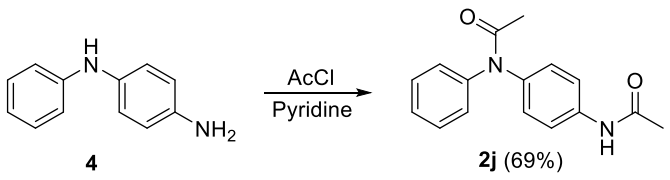
a] Synthesis of substrates 1a-z: The known substrates **1a-z** were prepared using the following procedure.[1-3] To a solution of amine (1 equiv) and NEt_3 (1.1 equiv) in dry CH_2Cl_2 was added the corresponding acid chloride (1.00 equiv) drop-wise over 30 min at 0 °C. The resulting reaction mixture was then allowed to warm to room temperature (rt) and stirred for 12-24 h. After completion of the reaction, the solution was transferred to a separatory funnel and washed three times with saturated aqueous $NaHCO_3$ and once with brine. The organic layer was dried over anhydrous Na_2SO_4, and concentrated in vacuo. The crude residue was purified by recrystallization from EtOH.

b] General procedure for *para*-selective dimerization of anilides to obtain 2a-x: An oven-dried screw cap glass tube equipped with a magnetic stirring bar was charged with anilide **1a-x** (0.2 mmol, 1 equiv), ammonium persulfate (APS, 46 mg, 0.2 mmol, 1 equiv) and copper acetate (3.6 mg, 0.02 mmol, 0.1 equiv) under argon atmosphere. To this mixture, DMSO (2.0 mL) was added and the glass tube was backfilled with argon and heated at 100 ^oC in a preheated oil bath. The progress of the reaction was monitored using TLC. After maximum conversion (18 h), the reaction mixture was diluted with ethyl acetate (40 mL) and washed with ice cold water (30 mL x 3). The organic layer was dried over Na_2SO_4, concentrated under vacuum, and the crude residue was purified by flash column chromatography using ethyl acetate and petroleum ether as eluents.

c] Typical experimental procedure for the preparation of representative product 2a:

An oven-dried screw cap glass tube, equipped with a magnetic stirring bar, was charged with *N*-phenylpivalamide (**1a**, 35.4 mg, 0.2 mmol, 1 equiv), APS (46 mg, 0.2 mmol, 1 equiv) and copper acetate (3.6 mg, 0.02 mmol, 0.1 equiv) under argon atmosphere. To this mixture, DMSO (2.0 mL) was added and the glass tube was backfilled with argon and heated at 100 ^{o}C in a preheated oil bath. The progress of the reaction was monitored using TLC. After 18 h, the reaction mixture was diluted with ethyl acetate (40 mL) and washed with ice cold water (30 mL x 3). The organic layer was dried over Na_2SO_4, concentrated under vacuum, and the crude residue was purified by flash column chromatography using ethyl acetate and petroleum ether (1:4) to afford pure dimer product **2a** in 62% yield (22 mg) and 6.5 mg of **1a** was recovered unchanged. Accordingly, the actual yield based on the recovered starting material (brsm) was 77%.

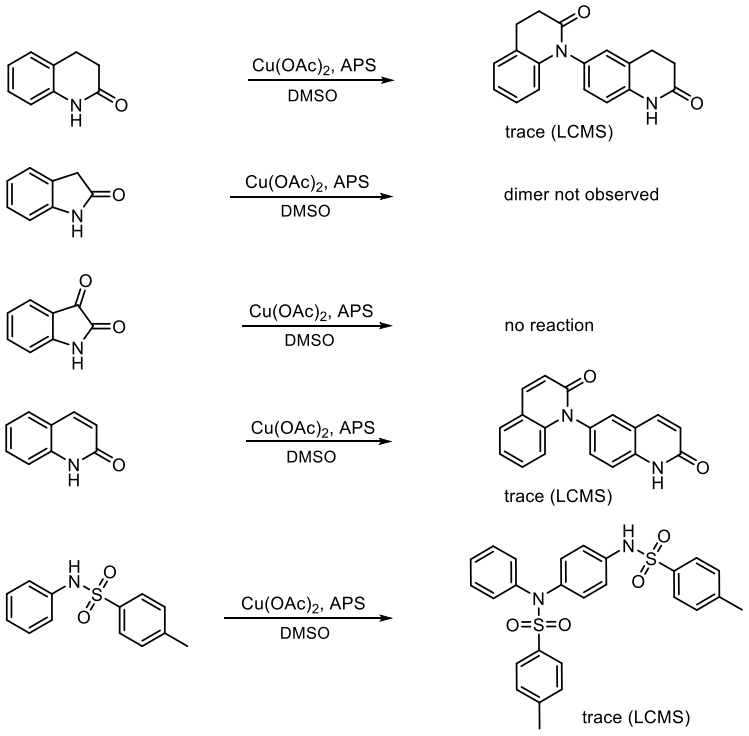
d] Alternate synthesis of product 2j: The procedure reported[4] for the acylation of amine was utilized. Acetyl chloride (86 µL, 1.2 mmol, 2.2 equiv) was added to a solution of commercially available amine **4** (100 mg, 0.55 mmol, 1 equiv) in dry pyridine (4 mL), and the reaction mixture was stirred for 1h at rt. After the removal of pyridine under vacuum, the residue was purified by silica gel column chromatography using ethyl acetate and petroleum ether (1:1) to afford **2j** in 69% yield (102 mg).



4 **2j** (69%)

e) General procedure for the attempted dimerization reaction of other amides:

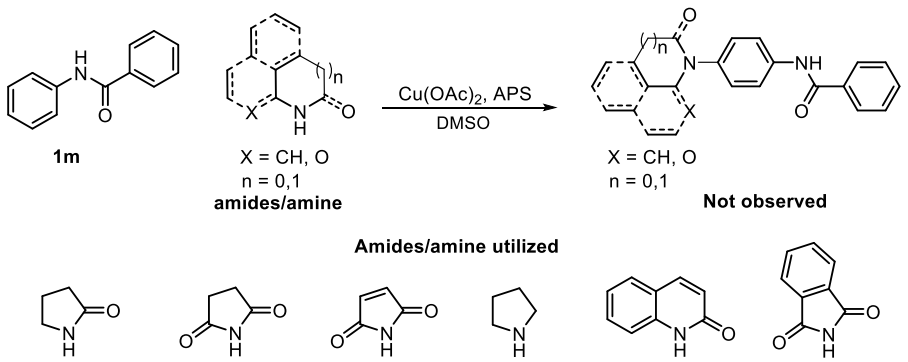
An oven-dried screw cap glass tube equipped with a magnetic stirring bar was charged with amides (0.2 mmol, 1 equiv), ammonium persulfate (APS, 46 mg, 0.2 mmol, 1 equiv) and copper acetate (3.6 mg, 0.02 mmol, 0.1 equiv) under argon atmosphere. To this mixture, DMSO (2.0 mL) was added and the glass tube was backfilled with argon and heated at 100 ^{o}C in a preheated oil bath. The progress of the reaction was monitored using TLC. All the reactions failed to give an isolable quantity of dimer product. A trace amount of dimer product formation was observed (LCMS) in the crude reaction mixture of 3,4-dihydroquinolin-2(1H)-one, quinolin-2(1H)-one and 4-methyl-N-phenylbenzenesulfonamide.



f) General procedure for attempted Cross-coupling reactions:

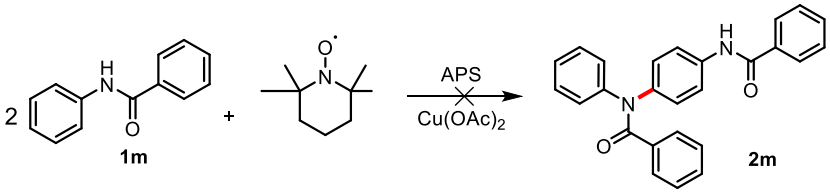
An oven-dried screw cap glass tube equipped with a magnetic stirring bar was charged with anilide **1m** (0.2 mmol, 1 equiv), other amide (0.4 mmol, 2 equiv), ammonium persulfate (APS,

46 mg, 0.2 mmol, 1 equiv), and copper acetate (3.6 mg, 0.02 mmol, 0.1 equiv) under argon atmosphere. To this mixture, DMSO (2.0 mL) was added and the glass tube was backfilled with argon and heated at 100 ^{o}C in a preheated oil bath. The reaction was monitored using TLC. All the reactions failed to give cross-coupled product as confirmed by LCMS of the crude reaction mixture.



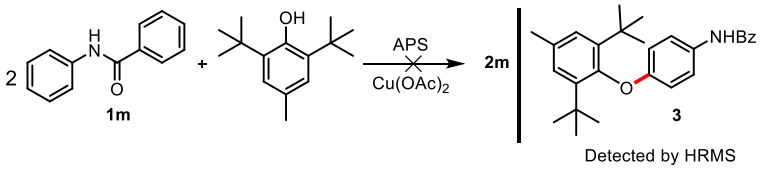
g) Radical trapping experiments:

An oven-dried screw cap glass tube, equipped with a magnetic stirring bar, was charged with anilide **1m** (20 mg, 0.1 mmol, 1 equiv), APS (23 mg, 0.1 mmol, 1 equiv), copper acetate (1.8 mg, 0.02 mmol, 0.1 equiv) and TEMPO (31 mg, 0.2 mmol, 2 equiv) under argon atmosphere. To this mixture, DMSO was added (1.0 mL) and the glass tube was backfilled with argon and heated at 100 ^{o}C in a preheated oil bath. The progress of the reaction was monitored using TLC, however the formation of the product **2m** was not observed and most of the starting material remained unreacted. LC-MS of the crude reaction mixture did not show any TEMPO adduct formation.



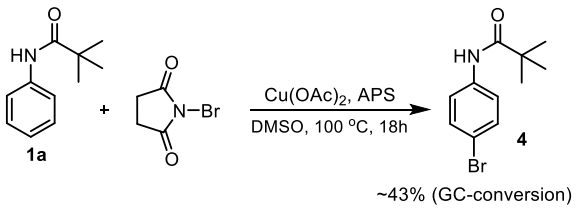
The same reaction was performed in the presence of BHT (44 mg, 0.2 mmol, 2 equiv) as a radical scavenger. In this case also, the formation of product **2m** was not observed. However, the peak corresponding to the molecular weight of BHT+**2m** was observed in LC-MS, which was reconfirmed by HRMS. HRMS of **3** (ESI−TOF) m/z $[M + H]^+$ calcd for $C_{28}H_{34}NO_2$, 416.2584 found, 416.2584.

Trapping of intermediate with BHT using the above mentioned procedure



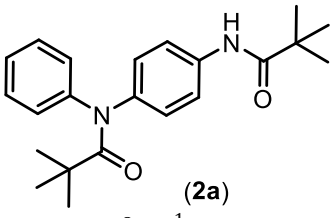
h) Bromination of anilide 1a with NBS under standard conditions:

An oven-dried screw cap glass tube, equipped with a magnetic stirring bar, was charged with *N*-phenylpivalamide (**1a**, 35.4mg, 0.2 mmol, 1 equiv), N-bromosuccinimide (71mg, 0.4 mmol, 2 equiv), APS (46 mg, 0.2 mmol, 1 equiv) and copper acetate (3.6 mg, 0.02 mmol, 0.1 equiv) under argon atmosphere. To this mixture, DMSO (2.0 mL) was added and the glass tube was backfilled with argon and heated at 100 ^oC in a preheated oil bath. The progress of the reaction was monitored by GC and GC-MS. After 18 h, the reaction mixture was diluted with ethyl acetate (40 mL) and washed with ice cold water (30 mL x 3). The organic layer was dried over Na_2SO_4, concentrated under vacuum, and the crude residue was passed through flash column chromatography using ethyl acetate and petroleum ether (1:3) to afford an inseparable mixture of **1a** and brominated product **4**. The ^1H NMR and GC/GC-MS analysis of inseparable mixture of **1a** and brominated product **4** shows 43% conversion.



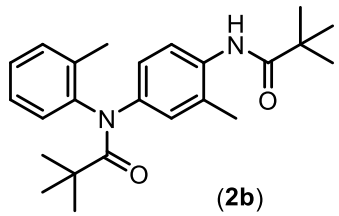
3. Characterization Data of Compounds.

N-Phenyl-N-(4-pivalamidophenyl)pivalamide (**2a**)


(**2a**)

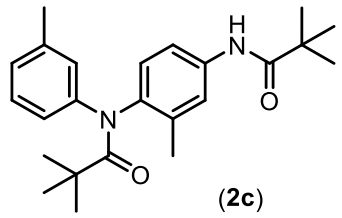
According to the general procedure, the title compound **2a** was obtained as a white solid (22 mg; 62% yield, [BRSM-77%]): Reaction time 18h, 100 ^{o}C; R_f 0.5 (ethyl acetate: pet. ether, 1:2); mp: 170-172 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 7.57-7.47 (m, 2H), 7.37-7.29 (m, 3H), 7.27-7.15 (m, 5H), 1.31 (s, 9H), 1.15 (m, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 179.5, 176.6, 144.5, 140.2, 136.8, 129.1, 128.2, 126.7, 120.6, 41.6, 39.6, 29.7, 27.7; HRMS (ESI−TOF) m/z $[M + H]^+$ calcd for $C_{22}H_{29}N_2O_2$, 353.2224; found, 353.2220.

N-(3-Methyl-4-pivalamidophenyl)-N-(o-tolyl)pivalamide (**2b**)


(**2b**)

According to the general procedure, the title compound **2b** was obtained as a white solid (23 mg; 60% yield, [BRSM-72%]): Reaction time 18h, 100 ^{o}C; R_f 0.5 (ethyl acetate:pet. ether, 1:2); mp: 140-142 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 7.85 (d, J = 8.54 Hz, 1H), 7.24-7.12 (m, 5H), 7.05-7.96 (m, 2H), 2.23 (s, 3H), 2.21 (s, 3H), 1.33 (s, 9H), 1.14 (s, 9H); ^{13}C NMR (100 MHz, CDCl3) δ (ppm) 179.5, 176.4, 142.7, 140.1, 135.7, 134.0, 131.4, 129.3, 129.2, 129.0, 127.6, 126.5, 125.9, 122.8, 41.7, 39.7, 29.5, 27.7, 18.6, 17.7; HRMS (ESI−TOF) m/z $[M + H]^+$ calcd for $C_{24}H_{33}N_2O_2$, 381.2542; found, 381.2547.

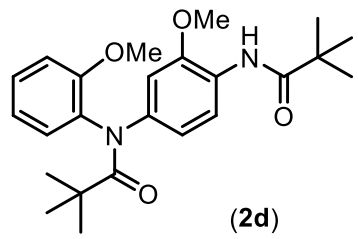
N-(2-Methyl-4-pivalamidophenyl)-N-(m-tolyl)pivalamide (**2c**)



(**2c**)

According to the general procedure, the title compound **2c** was obtained as a white solid (18 mg; 47% yield, [BRSM-80%]): Reaction time 18h, 100 ^{o}C; R_f 0.5 (ethyl acetate:pet. ether, 1:2); mp: 85-87 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 7.44 (d, *J* = 2.29 Hz, 1H), 7.41-7.34 (m, 2H), 7.19-7.14 (m, 1H), 7.13 (d, *J* = 8.70 Hz, 1H), 6.98 (d, *J* = 7.33 Hz, 1H), 6.95-6.90 (m, 2H), 2.29 (s, 3H), 2.2 (s, 3H), 1.31 (s, 9H), 1.14 (s, 9H); ^{13}C NMR (100 MHz, CDCl3) δ (ppm) 179.7, 176.6, 143.7, 138.6, 137.2, 136.7, 129.9, 128.5, 127.8, 127.0, 124.4, 122.5, 117.8, 41.8, 39.6, 29.5, 27.6, 21.4, 18.7; HRMS (ESI−TOF) m/z $[M + H]^+$ calcd for $C_{24}H_{33}N_2O_2$, 381.2542; found, 381.2540.

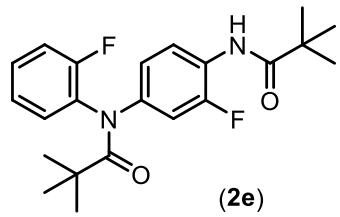
N-(3-Methoxy-4-pivalamidophenyl)-N-(2-methoxyphenyl*)pivalamide* (**2d**)



(**2d**)

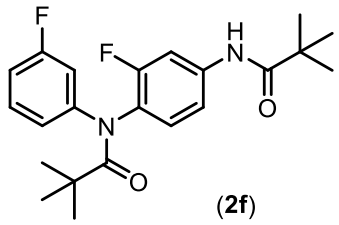
According to the general procedure, the title compound **2d** was obtained as a white solid (23 mg; 56% yield, [BRSM-68%]): Reaction time 18h, 100 ^{o}C; R_f 0.5 (ethyl acetate:pet. ether, 1:2); mp113-115 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.33 (d, *J* = 8.70 Hz, 1H), 8.05 (s, 1H), 7.26-7.18 (m, 2H), 6.93-6.88 (m, 4H), 3.86 (s, 3H), 3.86 (s, 3H), 1.30 (s, 9H), 1.15 (s, 9H); ^{13}C NMR (100 MHz, CDCl3) δ (ppm) 179.1, 176.4, 155.2, 147.9, 139.8, 133.5, 130.0, 128.7, 126.6, 120.83, 120.79, 119.3, 111.9, 110.3, 55.9, 55.4, 41.4, 40.0, 29.2, 27.6; HRMS (ESI−TOF) m/z $[M + H]^+$ calcd for $C_{24}H_{33}N_2O_4$, 413.2440; found, 413.2439.

N-(3-Fluoro-4-pivalamidophenyl)-N-(2-fluorophenyl)pivalamide (**2e**)


(**2e**)

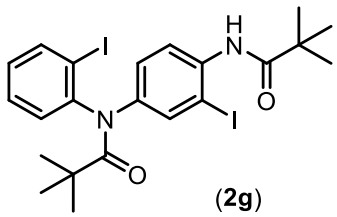
According to the general procedure, the title compound **2e** was obtained as a white solid (16 mg; 41% yield, [BRSM-62%]): Reaction time 18h, 100 ^{o}C; R_f 0.5 (ethyl acetate:pet. ether, 1:2); mp: 139-141 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.35 (t, *J* = 8.77 Hz, 1H), 7.60 (d, *J* = 2.29 Hz, 1H), 7.31-7.22 (m, 2H), 7.15-7.06 (m, 4H), 1.32 (s, 9H), 1.17 (s, 9H); ^{13}C NMR (100 MHz, CDCl3) δ (ppm) 178.6, 176.6, 158.0 (d, *J* = 249.2 Hz), 152.0 (d, *J* = 243.5), 139.3 (d, *J* = 9.59 Hz), 132.0 (d, *J* = 12.46), 130.4, 129.4 (d, *J* = 7.67 Hz), 125.8 (d, 10.54 Hz), 124.6 (d, *J* = 3.83), 124.5, 121.4, 116.7 (d, *J* = 21.09 Hz), 115.1 (d, *J* = 20.13 Hz), 41.5, 40.0, 29.1, 27.5; HRMS (ESI−TOF) m/z $[M + H]^+$ calcd for $C_{22}H_{27}N_2O_2F_2$, 389.2040; found, 389.2042.

N-(2-Fluoro-4-pivalamidophenyl)-N-(3-fluorophenyl)pivalamide (**2f**)


(**2f**)

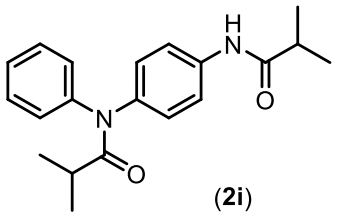
According to the general procedure, the title compound **2f** was obtained as a white solid (12 mg; 31% yield, [BRSM-74%]): Reaction time 18h, 100 ^{o}C; R_f 0.5 (ethyl acetate:pet. ether, 1:2); mp: 136-138 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 7.26 (m, 2H), 7.33-7.25 (m, 1H), 7.17 (d, *J* = 3.81 Hz, 2H), 7.06 (d, *J* = 7.63 Hz, 1H), 7.01-7.91 (m, 2H), 1.30 (s, 9H), 1.17 (s, 9H); ^{13}C NMR (100 MHz, CDCl3) δ (ppm) 179.1, 176.8, 162.7 (d, *J* = 248.28 Hz), 159.1 (d, *J* = 249.2 Hz), 145.3 (d, *J* = 8.63 Hz), 139.3 (d, *J* = 10.54), 130.6, 130.1 (d, *J* = 8.63 Hz), 127.0 (d, *J* = 13.42 Hz), 123.7, 115.5 (d, *J* = 5.75 HZ), 115.2, 114.1 (d, *J* = 21.09), 108.5 (d, *J* = 25.88), 41.5, 39.7, 29.1, 27.5; HRMS (ESI−TOF) m/z $[M + H]^+$ calcd for $C_{22}H_{27}N_2O_2F_2$, 389.2040; found, 389.2043.

N-(3-Iodo-4-pivalamidophenyl)-N-(2-iodophenyl)pivalamide (**2g**)


(**2g**)

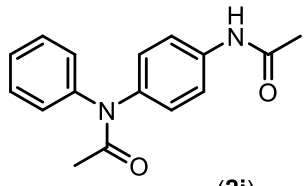
According to the general procedure, the title compound **2g** was obtained as a white solid (32 mg; 53% yield, [BRSM-72%]): Reaction time 18h, 100 ^{o}C; R_f 0.5 (ethyl acetate:pet. ether, 1:2); mp: 132-134 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.30 (d, J = 8.70 Hz, 1H), 7.90 (d, J = 7.79 Hz, 1H), 7.82 (s, 1H), 7.80 (d, J = 2.29 Hz, 1H), 7.40-7.30 (m, 2H), 7.24 (d, J = 7.78 Hz, 1H), 7.03-6.98 (t, J = 7.56, 1H), 1.36 (s, 9H), 1.20 (s, 9H); ^{13}C NMR (100 MHz, CDCl3) δ (ppm) 179.1, 176.7, 146.2, 140.5, 139.8, 138.0, 137.2, 130.2, 129.3, 129.1, 128.8, 120.8, 100.3, 88.9, 41.9, 40.2, 29.5, 27.6; HRMS (ESI−TOF) m/z $[M + H]^+$ calcd for $C_{22}H_{27}N_2O_2I_2$, 605.0162; found, 605.0164.

N-(4-Isobutyramidophenyl)-N-phenylisobutyramide (**2i**)


(**2i**)

According to the general procedure, the title compound **2i** was obtained as a sticky solid (18 mg; 56% yield, [BRSM-71%]): Reaction time 18h, 100 ^{o}C; R_f 0.5 (ethyl acetate:pet. ether, 1:2); mp: 140-142 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.71 (s, 1H), 7.59-7.29 (m, 5H), 7.26-7.05 (m, 4H), 2.79-2.67 (m, 1H), 2.55-2.44 (m, 1H), 1.22 (d, J = 6.71 Hz, 6H), 1.13 (d, J = 6.71 Hz, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 177.9, 175.5, 142.9, 138.6, 131-125 (5C's), 120.6, 36.4, 31.9, 19.6, 19.5; HRMS (ESI−TOF) m/z $[M + H]^+$ calcd for $C_{20}H_{25}N_2O_2$, 325.1916; found, 325.1919.

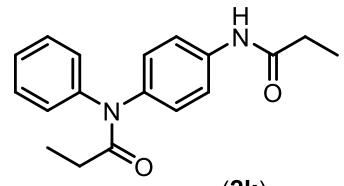
N-(4-Acetamidophenyl)-N-phenylacetamide (**2j**)



(**2j**)

According to the general procedure, the title compound **2j** was obtained as a sticky solid (14mg; 52% yield, [BRSM-68%]): Reaction time 18h, 100 ^{o}C; R_f 0.5 (ethyl acetate:pet. ether, 1:2); ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 7.77 (s, 1H), 7.55 (s, 1H), 7.45-7.32 (m, 4H), 7.28-7.23 (m, 2H), 7.22-7.14 (m, 2H); 2.14 (s, 3H), 2.07 (s, 3H); ^{13}C NMR (100 MHz, CDCl3) δ (ppm) 170.8, 168.5, 129.7-126.4 (7C's), 120.6, 24.4, 23.7; HRMS (ESI−TOF) m/z $[M + H]^+$ calcd for $C_{16}H_{17}N_2O_2$, 269.1290; found, 269.1295.

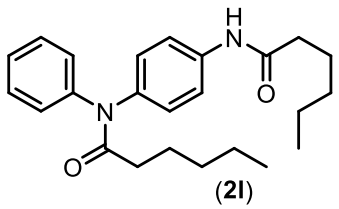
N-Phenyl-N-(4-propionamidophenyl)propionamide (**2k**)



(**2k**)

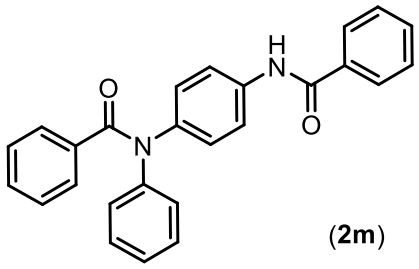
According to the general procedure, the title compound **2k** was obtained as a sticky solid (16mg; 54% yield, [BRSM-77%]): Reaction time 18h, 100 ^{o}C; R_f 0.5 (ethyl acetate:pet. ether, 1:2); ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 7.63 (s, 1H), 7.57 (m, 2H), 7.41-7.31 (m, 2H), 7.31-7.22 (m, 3H), 7.18 (d, J = 7.93 Hz, 2H), 2.35 (q, J = 7.52 Hz, 2H), 2.28 (q, J = 7.32 Hz, 2H), 1.22 (t, J = 7.32 Hz, 3H), 1.13 (t, J = 7.62 Hz, 3H); ^{13}C NMR (100 MHz, CDCl3) δ (ppm) 174.2, 172.2, 142.8, 138.5, 131-124 (5C's), 120.6, 30.6, 28.7, 9.7, 9.6; HRMS (ESI−TOF) m/z $[M + H]^+$ calcd for $C_{18}H_{21}N_2O_2$, 297.1603; found, 297.1605.

N-(4-Hexanamidophenyl)-N-phenylhexanamide (**2l**)


(**2l**)

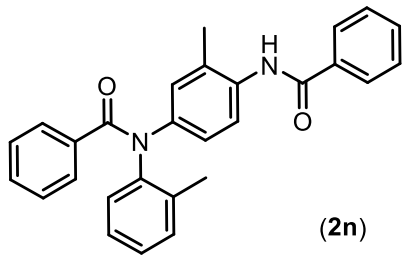
According to the general procedure, the title compound **2l** was obtained as a sticky solid (18 mg; 46% yield, [BRSM-65%]): Reaction time 18h, 100 ^{o}C; R_f 0.5 (ethyl acetate:pet. ether, 1:2); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.80 (s, 1H), 7.65-7.30 (m, 5H), 7.23 (d, J = 7.32 Hz, 2H), 7.20-7.10 (m, 2H); 2.39-2.22 (m, 4H), 1.78-1.59 (m, 4H), 1.40-1.30 (m, 4H), 1.29-1.21 (m, 4H), 0.95-0.8 (m, 6H); ^{13}C NMR (100 MHz, CDCl3) δ (ppm) 173.7, 171.7, 142.9, 138.5, 130-125 (5C's), 120.6, 37.5, 35.1, 33.7, 31.4, 29.7, 25.6, 22.4, 22.4, 13.9, 13.9; HRMS (ESI−TOF) m/z $[M + H]^+$ calcd for $C_{24}H_{33}N_2O_2$, 381.2542; found, 381.2538.

N-(4-Benzamidophenyl)-N-phenylbenzamide (**2m**)


(**2m**)

According to the general procedure, the title compound **2m** was obtained as a white solid (21 mg; 53% yield, [BRSM-72%]): Reaction time 18h, 100 ^{o}C; R_f 0.5 (ethyl acetate:pet. ether 1:2); mp: 188-190 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.16 (s, 1H), 7.85 (d, J = 7.32 Hz, 2H), 7.58 (d, J = 8.54 Hz, 2H), 7.53 (d, J = 7.32 Hz, 1H), 7.49-7.42 (m, 4H), 7.35-7.27 (m, 2H), 7.26-7.16 (m, 4H), 7.16-7.06 (m, 4H); ^{13}C NMR (100 MHz, CDCl3) δ (ppm) 170.8, 165.7, 143.8, 139.9, 136.3, 135.9, 134.8, 131.8, 130.3, 129.2, 129.1, 128.7, 127.9, 127.4, 127.1, 126.4, 120.8; HRMS (ESI−TOF) m/z $[M + H]^+$ calcd for $C_{26}H_{21}N_2O_2$, 393.1598; found, 393.1592.

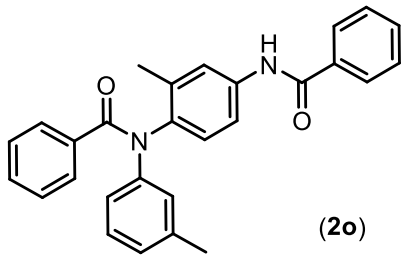
N-(4-Benzamido-3-methylphenyl)-N-(o-tolyl)benzamide (**2n**)



(**2n**)

According to the general procedure, the title compound **2n** was obtained as a white solid (21mg; 51% yield, [BRSM-71%]): Reaction time 18h, 100 ^{o}C; R_f 0.5 (ethyl acetate:pet. ether, 1:2); mp: 168-170 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) 7.91-7.82 (m, 3H), 7.68 (s, 1H), 7.62-7.52 (m, 2H), 7.52-7.44 (m, 4H), 7.30 (d, *J* = 7.32 Hz, 1H), 7.26-7.12 (m, 5H), 7.07 (d, *J* = 7.32 Hz, 1H), 6.97-6.92 (m, 1H), 2.29 (s, 3H), 2.25 (s, 3H); ^{13}C NMR (100 MHz, CDCl3) δ (ppm); 170.4, 165.5, 142.1, 136.0, 135.4, 134.8, 133.5, 131.9, 131.4, 130.3, 130.1, 129.6, 129.3, 128.9, 128.4, 128.1, 127.9, 127.6, 127.0, 124.7, 123.1, 18.4, 17.9; HRMS (ESI−TOF) m/z $[M + H]^+$ calcd for $C_{28}H_{25}N_2O_2$, 421.1916; found, 421.1921.

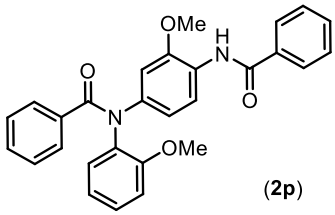
N-(4-Benzamido-2-methylphenyl)-N-(m-tolyl)benzamide (**2o**)



(**2o**)

According to the general procedure, the title compound **2o** was obtained as a white solid (18 mg; 42% yield, [BRSM-80%]): Reaction time 18h, 100 ^{o}C; R_f 0.5 (ethyl acetate:pet. ether, 1:2); mp: 138-140 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) 8.19 (s, 1H), 7.87 (d, *J* = 7.33 Hz, 2H), 7.57-7.41 (m, 8H), 7.32 (t, *J* = 7.33 Hz, 1H), 7.27-7.21 (m, 2H), 7.09 (t, *J* = 6.87 Hz, 1H), 7.0 (d, *J* = 8.7 Hz, 1H), 6.93 (d, *J* = 7.33 Hz, 1H), 6.86-6.79 (m, 1H), 2.26 (s, 3H), 2.24 (s, 3H); ^{13}C NMR (100 MHz, CDCl3) δ (ppm); 170.6, 165.8, 138.9, 138.3, 137.2, 136.1, 136.0, 134.9, 131.8, 130.3, 128.9, 128.7, 128.6, 127.9, 127.1, 126.8, 126.7, 123.6, 122.7, 118.8, 21.3, 18.5; HRMS (ESI−TOF) m/z $[M + H]^+$ calcd for $C_{28}H_{25}N_2O_2$, 421.1916; found, 421.1921.

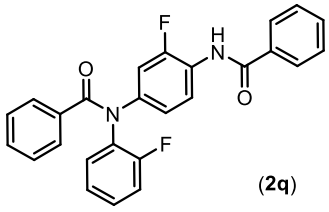
N-(4-Benzamido-3-methoxyphenyl)-N-(2-methoxyphenyl)benzamide (**2p**)



(**2p**)

According to the general procedure, the title compound **2p** was obtained as a white solid (23 mg; 50% yield, [BRSM-67%]): Reaction time 18h, 100 ^{o}C; R_f 0.5 (ethyl acetate:pet. ether, 1:2); mp: 152-154 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) 8.48 (s, 1H), 8.42 (d, *J* = 8.7 Hz, 1H), 7.88 (s, 1H), 7.86 (d, *J* = 1.34 Hz, 1H), 7.60-7.44 (m, 6H), 7.30-7.25 (m,1H), 7.24-7.17 (m, 4H), 6.91 (t, *J* = 7.56 Hz, 1H), 6.86 (s, 1H), 6.74 (dd, *J* = 8.70, 2.29 Hz, 1H), 3.82 (s, 3H), 3.71 (s, 3H); ^{13}C NMR (100 MHz, CDCl3) δ (ppm) 171.1, 165.1, 154.8, 148.1, 139.4, 136.4, 135.2, 132.6, 131.7, 129.9, 129.5, 128.8, 128.7, 128.5, 127.6, 127.0, 125.7, 121.1, 119.6, 118.8, 112.2, 109.3, 55.9, 55.5; HRMS (ESI−TOF) m/z $[M + H]^+$ calcd for $C_{28}H_{25}N_2O_4$, 453.1814; found, 453.1821.

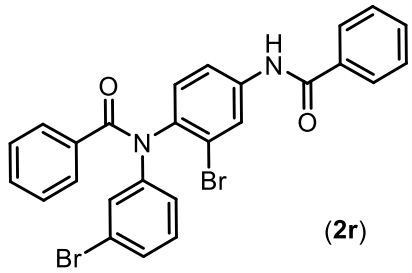
N-(4-Benzamido-3-fluorophenyl)-N-(2-fluorophenyl)benzamide (**2q**)



(**2q**)

According to the general procedure, the title compound **2q** was obtained as a white solid (17 mg; 40% yield, [BRSM-72%]): Reaction time 18h, 100 ^{o}C; R_f 0.5 (ethyl acetate:pet. ether, 1:2); mp: 162-164 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) *δ* (ppm) 8.41 (t, *J* = 8.77 Hz, 1H), 8.04 (s, 1H), 7.87 (d, *J* = 6.87 Hz, 2H), 7.61-7.5 (m, 1H), 7.54-7.47 (m, 4H), 7.37-7.31 (m, 1H), 7.31-7.22 (m, 3H), 7.22-7.16 (m, 1H), 7.16-7.03 (m, 3H), 7.98 (d, *J* = 8.39 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 170.5, 165.4, 157.6 (d, *J* = 251.12 Hz), 152.2 (d, *J* = 245.37 Hz), 139.0 (d, *J* = 10.54 Hz), 135.0, 134.2, 132.3, 131.0 (d, *J* = 12.46 Hz), 130.6, 129.8, 129.0 (d, *J* = 7.67 Hz), 128.9, 128.7, 128.0, 127.1, 124.9, 124.9 (d, *J* = 4.79 Hz), 122.8, 121.7, 116.8 (d, *J* = 20.13 Hz), 113.7 (d, *J* = 21.09 Hz); HRMS (ESI−TOF) m/z $[M + H]^+$ calcd for $C_{26}H_{19}N_2O_2F_2$, 429.1414; found, 429.1415.

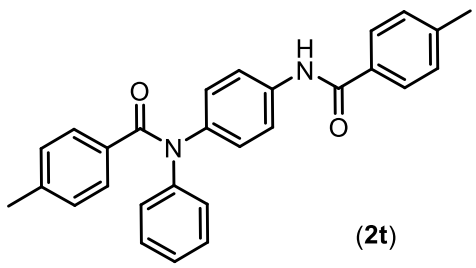
N-(4-Benzamido-2-bromophenyl)-N-(3-bromophenyl)benzamide (**2r**)



(**2r**)

According to the general procedure, the title compound **2r** was obtained as a white solid (20 mg; 36% yield, [BRSM-61%]): Reaction time 18h, 100 ^{o}C; R_f 0.5 (ethyl acetate:pet. ether, 1:2); mp: 202-204 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$); 8.37 (s, 1H), 7.96 (s, 1H), 7.88 (d, *J* = 7.32 Hz, 2H), 7.66 (d, *J* = 7.32 Hz, 1H), 7.60-7.52 (m, 3H), 7.50-7.43 (m, 2H), 7.41-7.36 (m, 1H), 7.33-7.26 (m, 3H), 7.22 (s, 1H), 7.10 (d, *J* = 7.93 Hz, 2H), 7.02 (s, 1H); ^{13}C NMR (100 MHz, CDCl3) δ (ppm) 170.7, 165.8, 138.8, 137.5, 135.0, 134.7, 134.4, 132.1, 130.9, 130.1, 129.3, 129.1, 128.9, 128.7, 128.1, 127.2, 127.1, 125.2, 124.9, 123.2, 122.4, 120.3; HRMS (ESI−TOF) m/z $[M + H]^+$ calcd for $C_{26}H_{19}N_2O_2{}^{79}Br_2$, 548.9813; found, 548.9824.

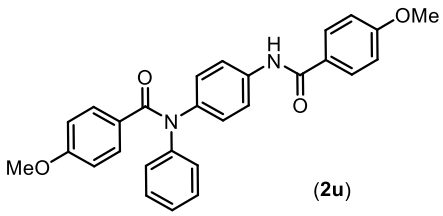
4-Methyl-N-(4-(4-methylbenzamido)phenyl)-N-phenylbenzamide (**2t**)



(**2t**)

According to the general procedure, the title compound **2t** was obtained as a white solid (22 mg; 52% yield, [BRSM-74%]): Reaction time 18h, 100 ^{o}C; R_f 0.5 (ethyl acetate:pet. ether, 1:2); mp: 162-164 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) *δ* (ppm) 8.02 (s, 1H), 7.78 (d, *J* = 5.95 HZ, 2H), 7.62-7.52 (m, 2H), 7.37 (d, *J* = 7.33 Hz, 2H), 7.32- 7.21 (m, 4H), 7.21-7.07 (m, 5H), 7.03 (d, *J* = 7.33 Hz, 2H), 2.42 (s, 3H), 2.30 (s, 3H); ^{13}C NMR (100 MHz, CDCl3) δ (ppm) 170.9, 165.8, 144.1, 142.5, 140.7, 140.1, 136.4, 133.0, 132.0, 129.51, 129.48, 129.2, 128.7, 128.1, 127.5, 127.2, 126.4, 120.9, 21.6, 21.5; HRMS (ESI−TOF) m/z $[M + H]^+$ calcd for $C_{28}H_{25}N_2O_2$, 421.1911; found, 421.1907.

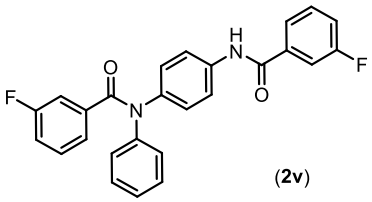
4-Methoxy-N-(4-(4-methoxybenzamido)phenyl)-N-phenylbenzamide (**2u**)



(**2u**)

According to the general procedure, the title compound **2u** was obtained as a white solid (25 mg; 56% yield, [BRSM-77%]): Reaction time 18h, 100 ^{o}C; R_f 0.5 (ethyl acetate:pet. ether, 1:2); mp: 190-192 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 7.99 (s, 1H), 8.83 (d, *J* = 8.55 Hz, 2H), 7.57 (d, *J* = 7.55 Hz, 2H), 7.45 (d, *J* = 9.16 Hz, 2H), 7.33-7.22 (m, 2H), 7.21-7.07 (m, 5H), 6.94 (d, *J* = 7.93 Hz, 2H), 6.73 (d, *J* = 8.55 Hz, 2H), 3.86 (s, 3H), 3.78 (s, 3H); ^{13}C NMR (100 MHz, CDCl3) δ (ppm) 170.4, 165.2, 162.5, 161.1, 144.2, 140.2, 136.2, 131.4, 129.1, 129.0, 127.9, 127.3, 126.9, 126.1, 120.8, 113.9, 113.2, 55.4, 55.2; HRMS (ESI−TOF) m/z $[M + H]^+$ calcd for $C_{28}H_{25}N_2O_4$, 453.1809; found, 453.1806.

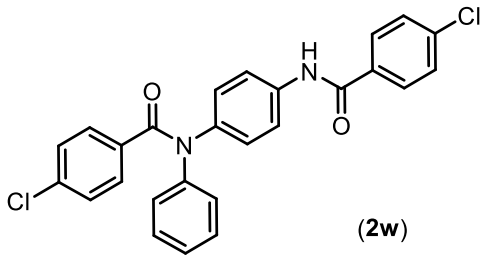
3-Fluoro-N-(4-(3-fluorobenzamido)phenyl)-N-phenylbenzamide (**2v**)



(**2v**)

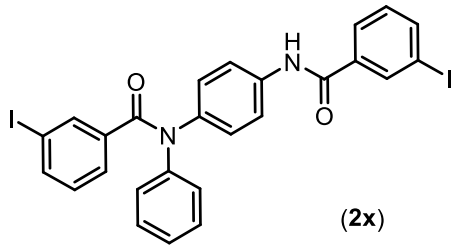
According to the general procedure, the title compound **2v** was obtained as a white solid (18 mg; 43% yield, [BRSM-63%]): Reaction time 18h, 100 ^{o}C; R_f 0.5 (ethyl acetate:pet. ether, 1:2); mp: 162-164 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.18 (s, 1H), 7.63 (d, *J* = 7.63 Hz, 1H), 7.58 (d, *J* = 8.39 Hz, 3H), 7.46-7.39 (m, 1H), 7.30 (d, *J* = 7.30 Hz, 1H), 7.26-7.16 (m, 6H), 7.15-7.07 (m, 4H), 7.04-7.98 (m, 1H); ^{13}C NMR (100 MHz, CDCl3) δ (ppm) 169.4, 164.4, 162.7 (d, *J* = 248.24 Hz), 162.1 (d, *J* = 247.3 Hz), 143.3, 139.6, 138.0 (d, *J* = 7.67 Hz), 137.0 (d, *J* = 6.71 Hz), 136.3, 130.4 (d, *J* = 7.67 Hz), 129.6 (d, *J* = 7.67 Hz), 129.3, 127.8, 127.3, 126.8, 124.8 (d, *J* = 2.88 Hz), 122.6 (d, *J* = 2.88 Hz), 121.0, 118.9 (d, *J* = 21.09 Hz), 117.4 (d, *J* = 21.09 Hz), 116.2 (d, *J* = 23 Hz), 114.6 (d, *J* = 23 Hz); HRMS (ESI−TOF) m/z $[M + H]^+$ calcd for $C_{26}H_{19}N_2O_2F_2$, 429.1409; found, 429.1404.

4-Chloro-N-(4-(4-chlorobenzamido)phenyl)-N-phenylbenzamide (**2w**)


(**2w**)

According to the general procedure, the title compound **2w** was obtained as a white solid (22 mg; 48% yield, [BRSM-75%]): Reaction time 18h, 100 ^{o}C; R_f 0.5 (ethyl acetate:pet. Ether; 1:2); mp: 161-163 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.12 (s, 1H), 7.80 (d, *J* = 8.24 Hz, 2H), 7.57 (d, *J* = 8.70 Hz, 2H), 7.41 (d, *J* = 7.41 Hz, 2H), 7.38 (d, *J* = 8.24 Hz, 2H), 7.33- 7.27 (m, 2H), 7.23-7.17 (m, 3H), 7.16-7.05 (m, 4H); ^{13}C NMR (100 MHz, CDCl3) δ (ppm) 169.7, 164.7, 143.4, 139.7, 138.2, 136.4, 136.3, 134.2, 133.0, 130.6, 129.3, 129.0, 128.6, 128.3, 127.8, 127.3, 126.7, 121.0; HRMS (ESI−TOF) m/z $[M + H]^+$ calcd for $C_{26}H_{19}N_2O_2Cl_2$, 461.0818; found, 461.0811.

3-Iodo-N-(4-(3-iodobenzamido)phenyl)-N-phenylbenzamide (**2x**)


(**2x**)

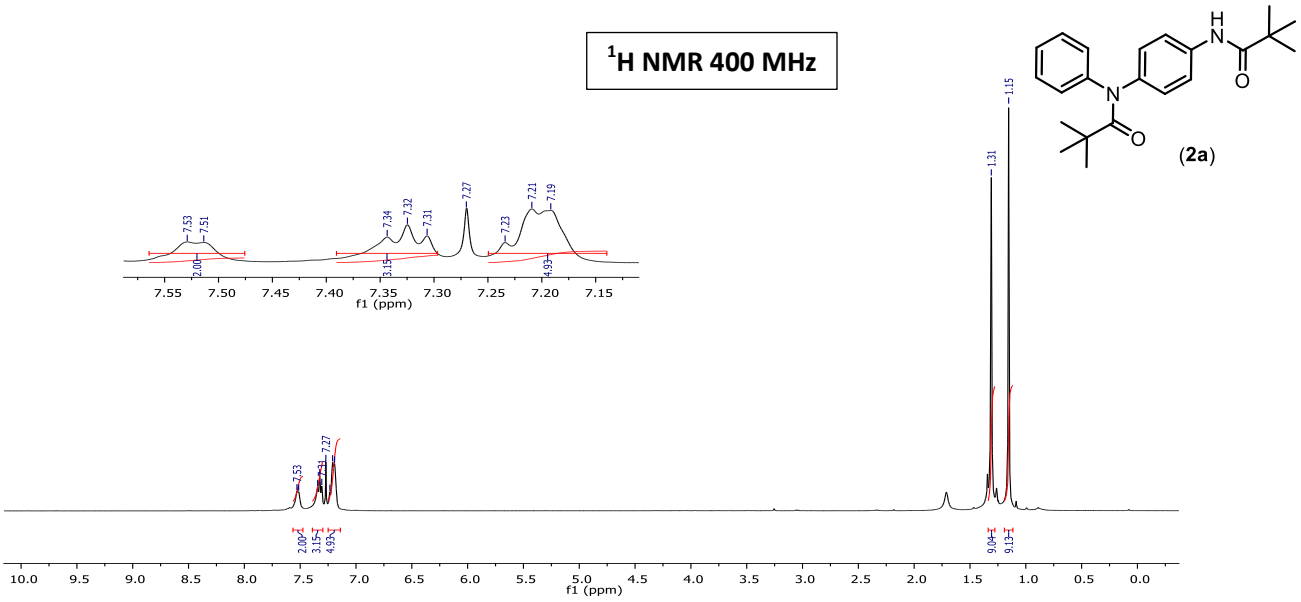
According to the general procedure, the title compound **2x** was obtained as a white solid (30 mg; 46% yield, [BRSM-68%]): Reaction time 18h, 100 ^{o}C; R_f 0.5 (ethyl acetate:pet. ether, 1:2); mp: 81-83 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.21-8.17 (m, 1H), 8.06 (s, 1H), 7.89-7.86 (m, 1H), 7.86-7.84 (m, 1H), 7.84-7.80 (m, 1H), 7.65-7.62 (m, 1H), 7.58 (d, *J* = 9.16 Hz, 2H), 7.37-7.34 (m, 1H), 7.32-7.28 (m, 2H), 7.23-7.18 (m, 2H), 7.16-7.09 (m, 4H) 6.97-6.91 (m, 1H); ^{13}C NMR (100 MHz, CDCl3) δ (ppm) 168.9, 164.1, 143.3, 140.8, 139.6, 139.2, 138.1, 137.8, 136.7, 136.2, 136.1, 130.4, 129.5, 129.3, 128.1, 127.9, 127.4, 126.8, 126.3, 121.0, 94.4, 93.5; HRMS (ESI−TOF) m/z $[M + H]^+$ calcd for $C_{26}H_{19}N_2O_2I_2$, 644.9530; found, 644.9526.

4. References:

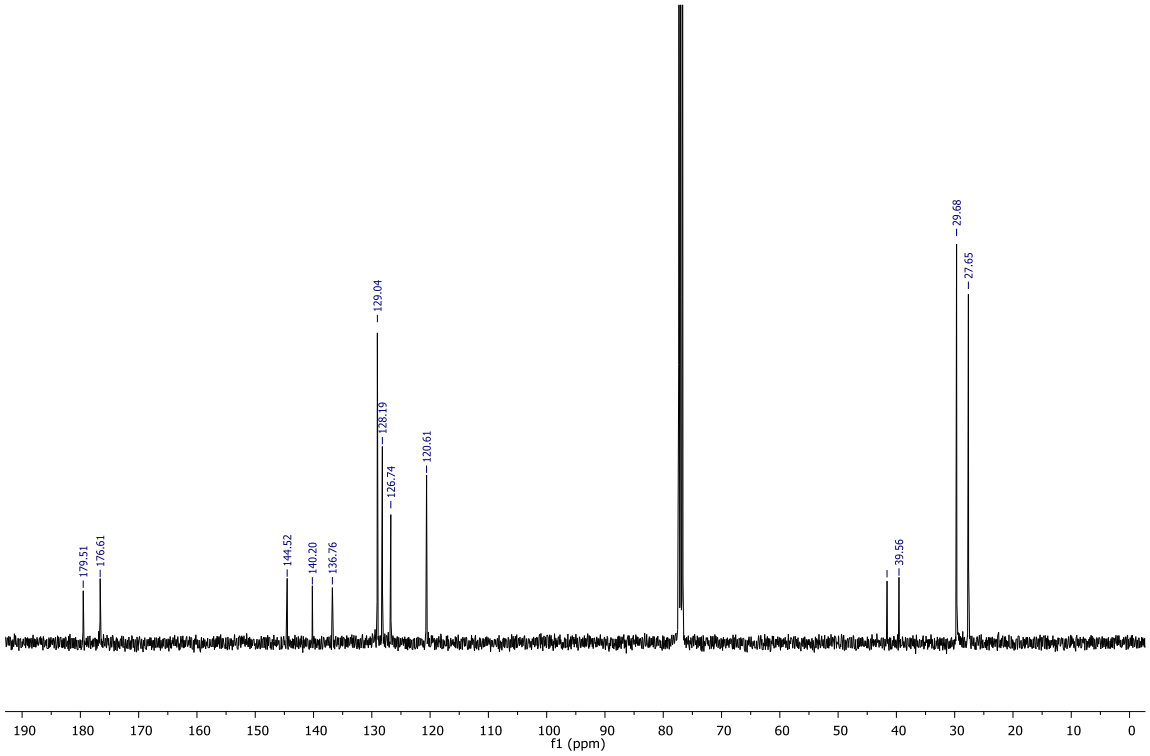
1. J. M. John, R. Loorthuraja, E. Antoniuk and S. H. Bergens, *Catal. Sci. Technol*., 2015, **5**, 1181.
2. J. Wanga, F. Li, W. Pei, M. Yang, Y. Wu, D. Ma, F. Zhang and J. Wang, *Tetrahedron Lett.*, 2018, **59**,1902.
3. F. Shi, J. Li, C. Li and X. Jia, *Tetrahedron Lett.*, 2010, **51**, 6049.
4. R. Yamasaki, A. Tanatani, I. Azumaya, S. Saito, K. Yamaguchi and H. Kagechika, *Org. Lett.*, 2003, **5**, 1265.

5. Copies of ^{1}H, ^{13}C and HRMS Spectra:

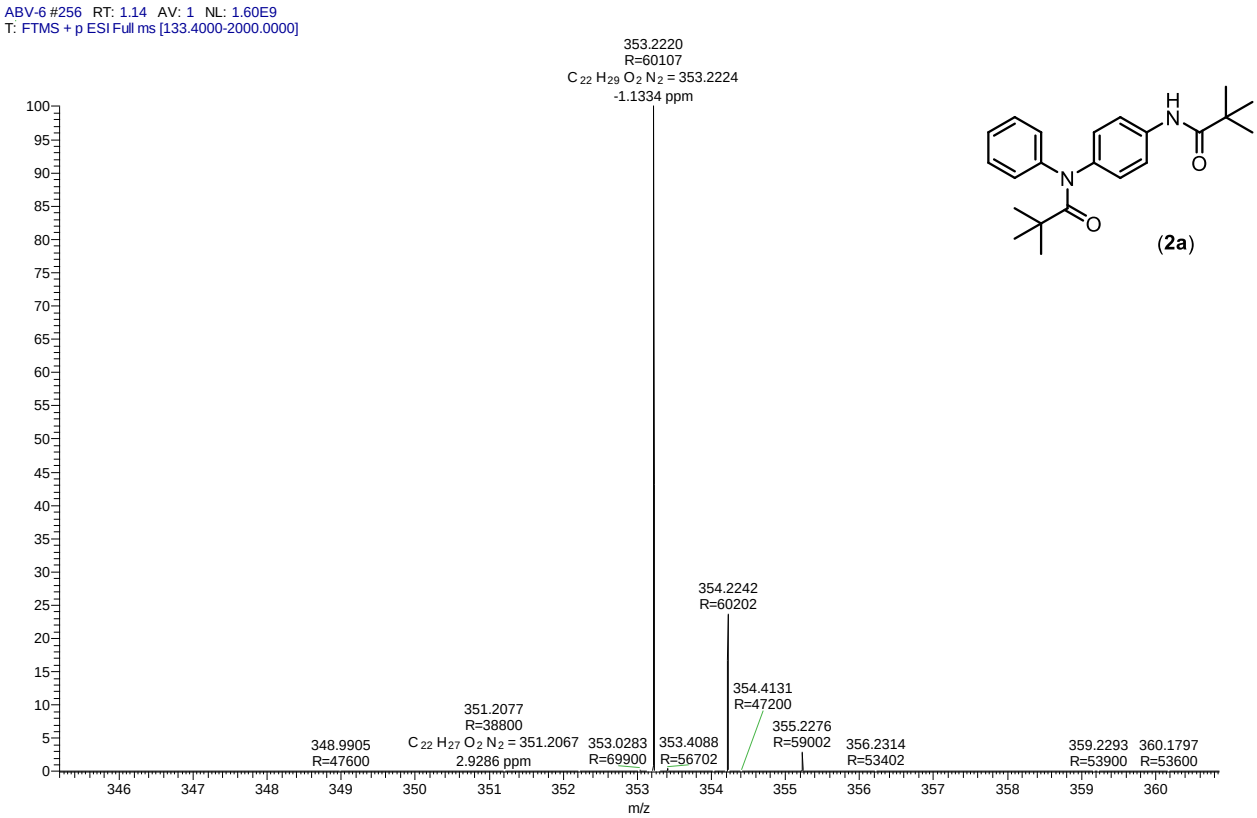
^{1}H NMR 400 MHz



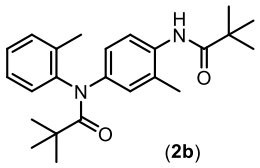
^{13}C NMR 100 MHz



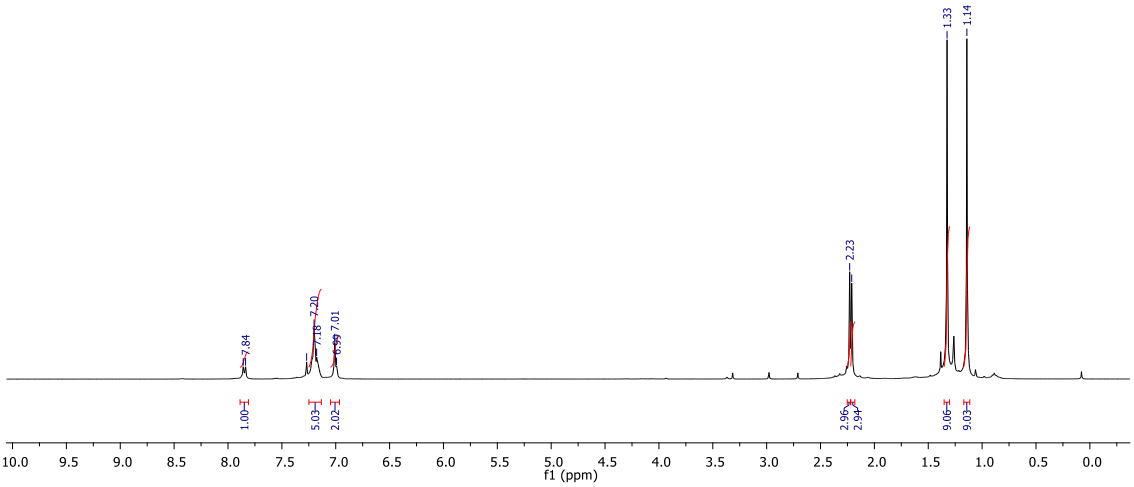
ESI-HRMS Chromatogram



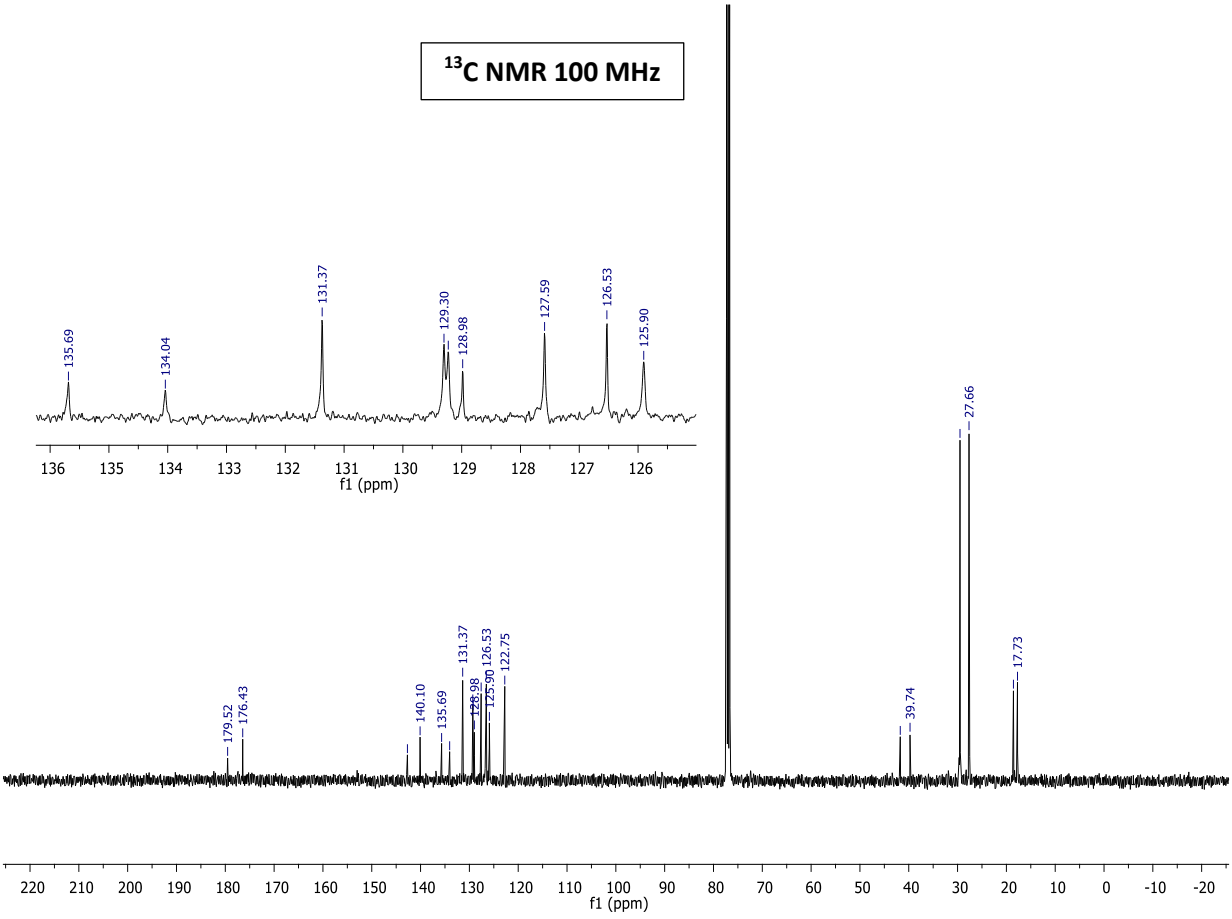
^{1}H NMR 400 MHz



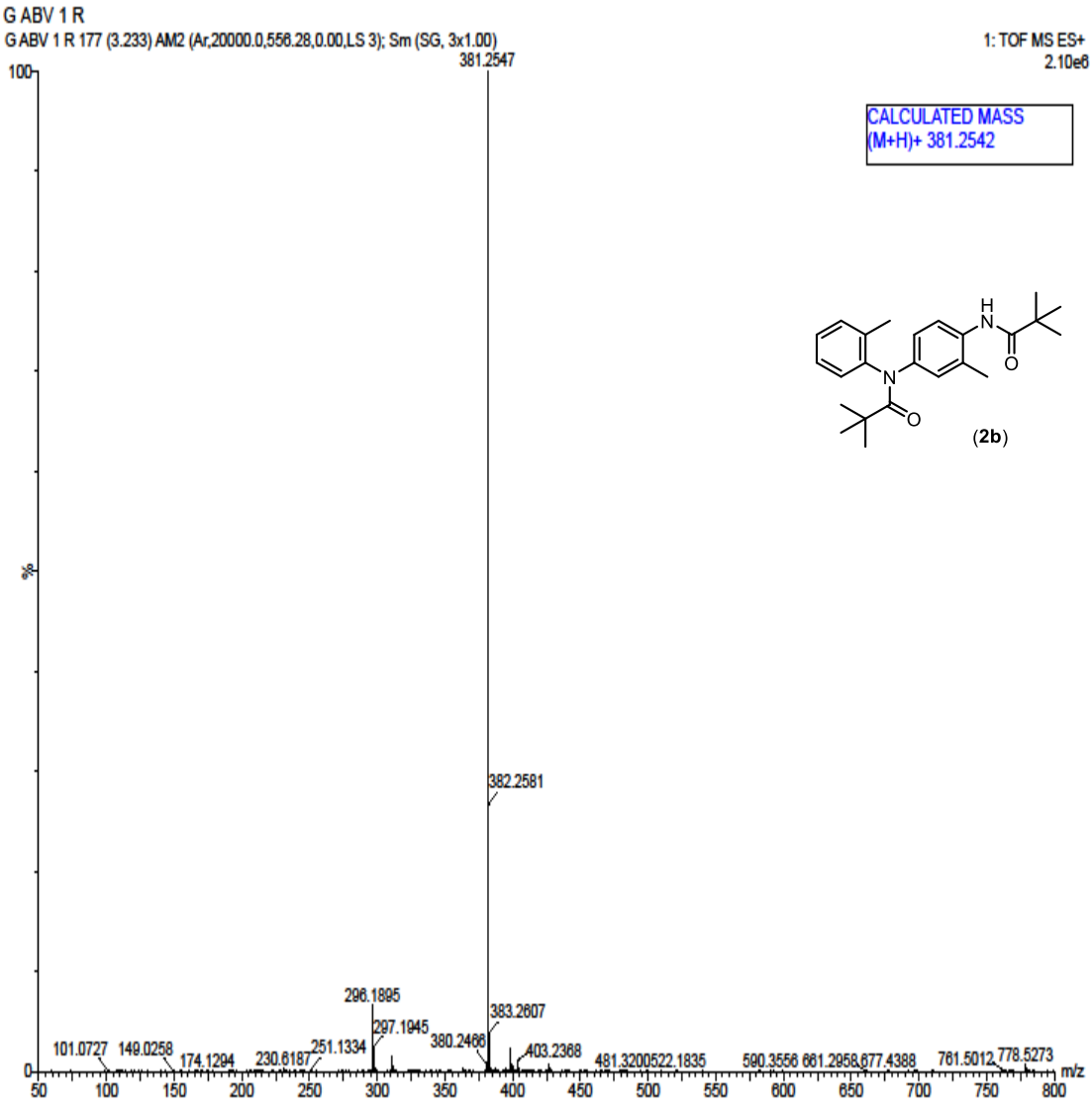
(**2b**)



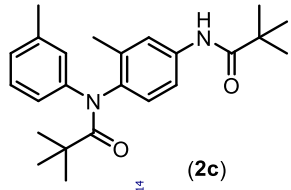
^{13}C NMR 100 MHz



ESI-HRMS Chromatogram



^{1}H NMR 400 MHz



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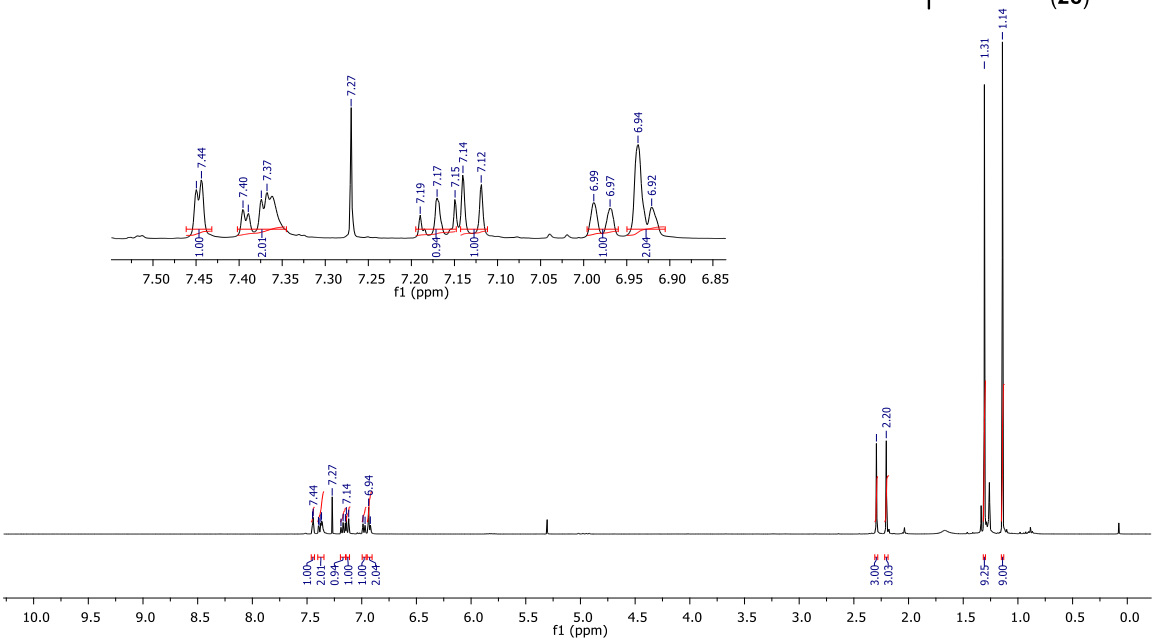

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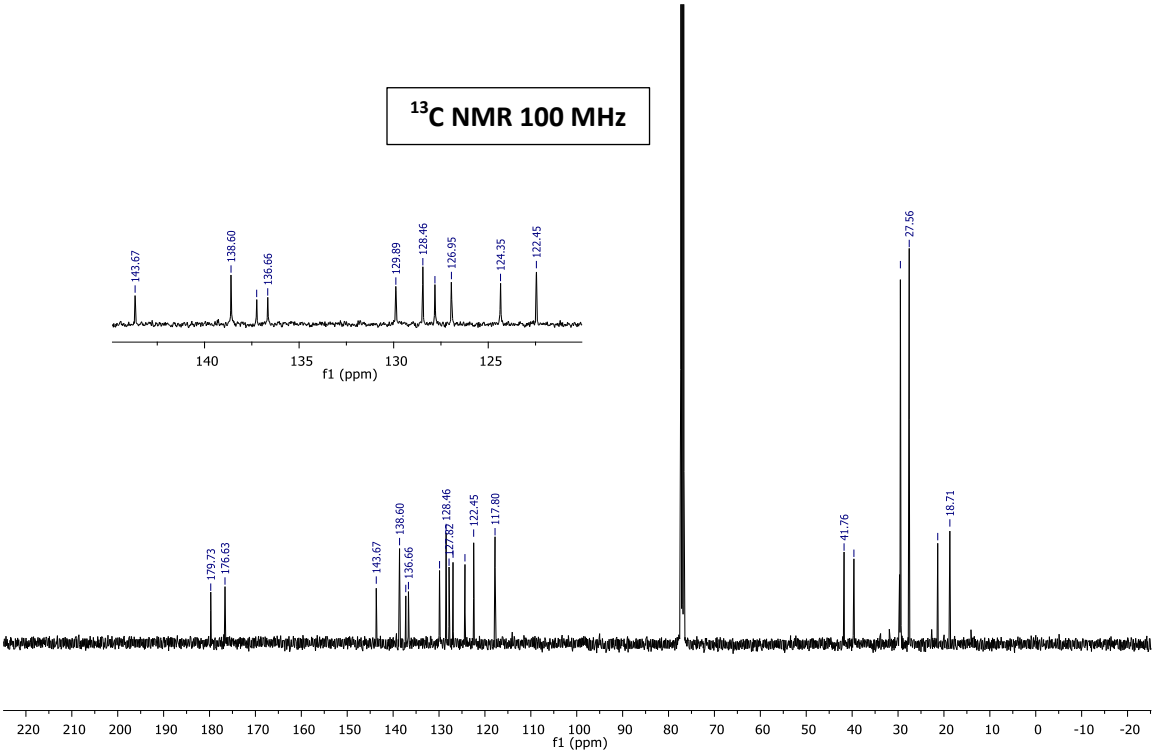
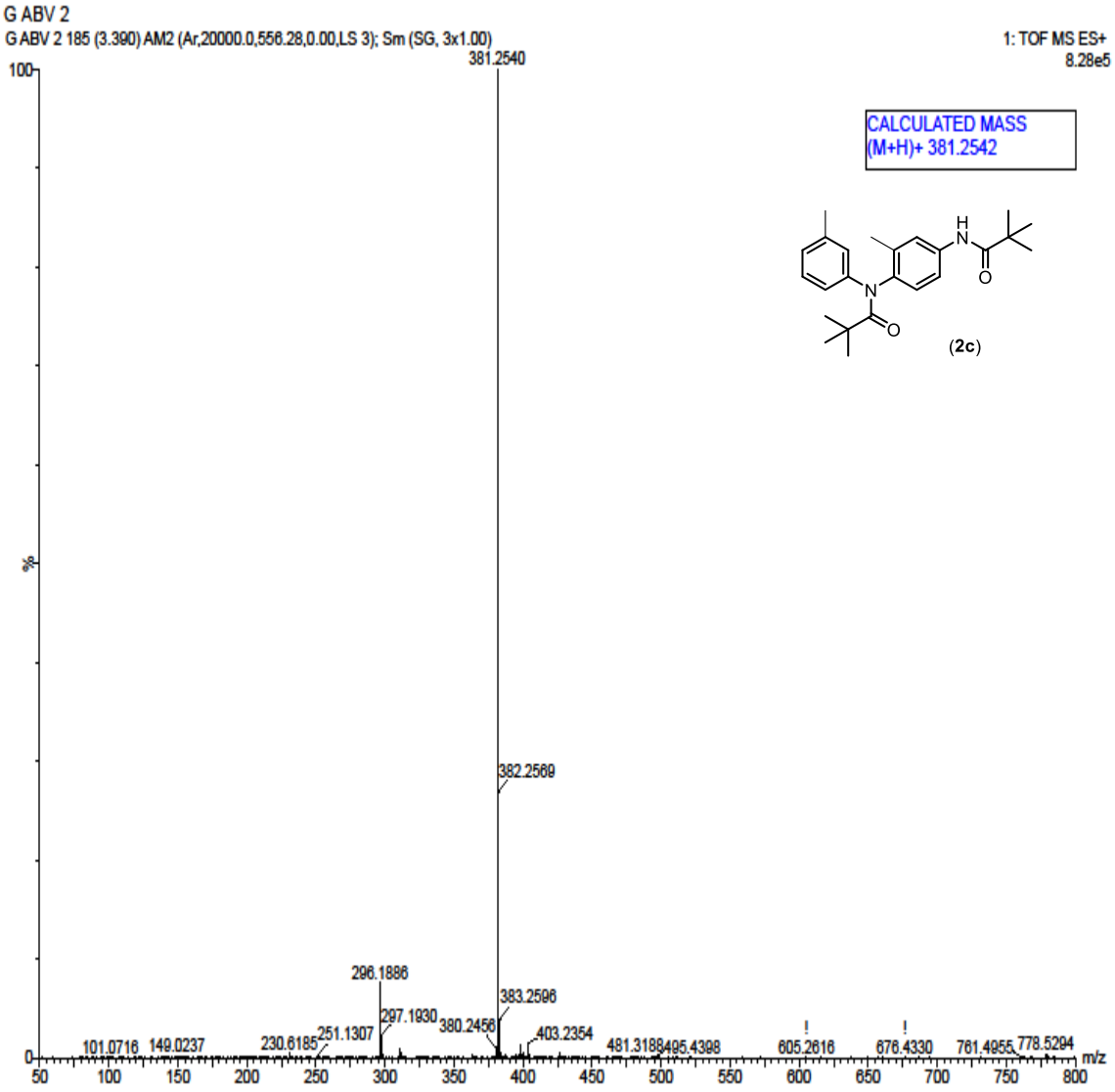
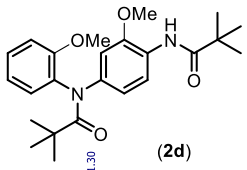


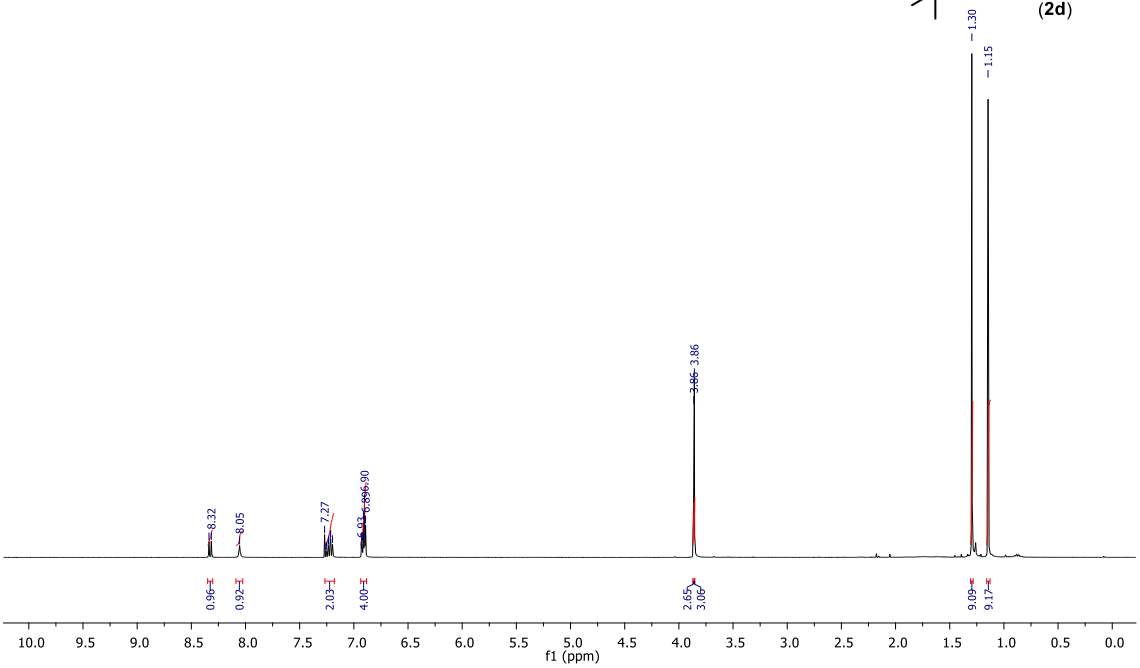
ESI-HRMS Chromatogram



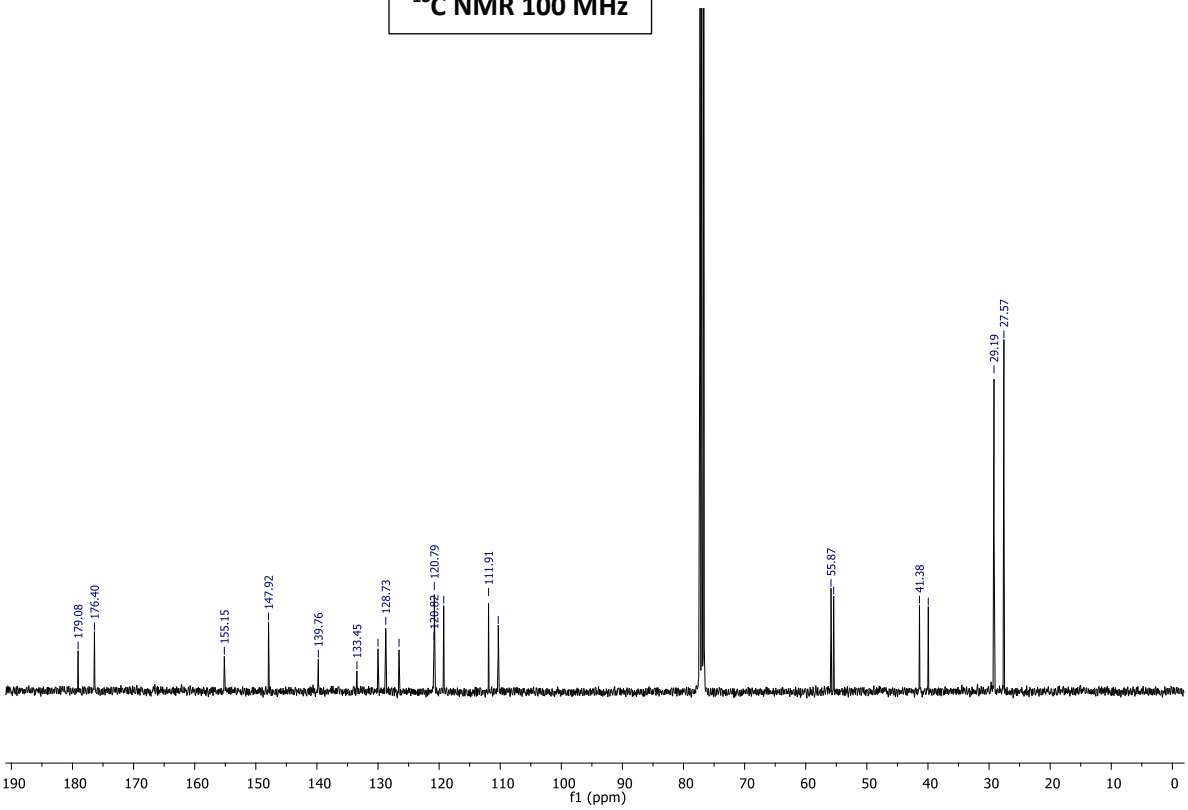
^{1}H NMR 400 MHz



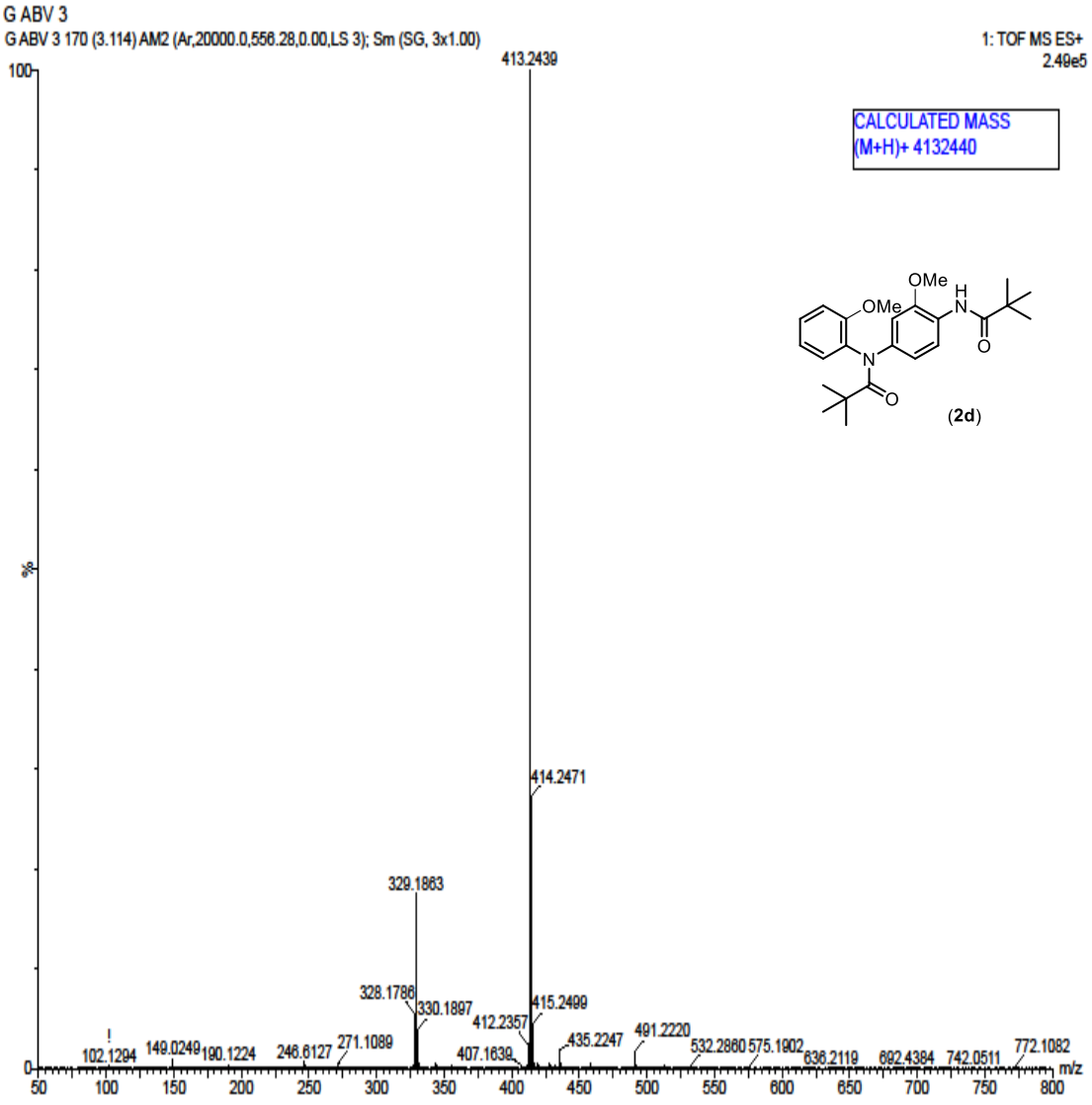
(**2d**)



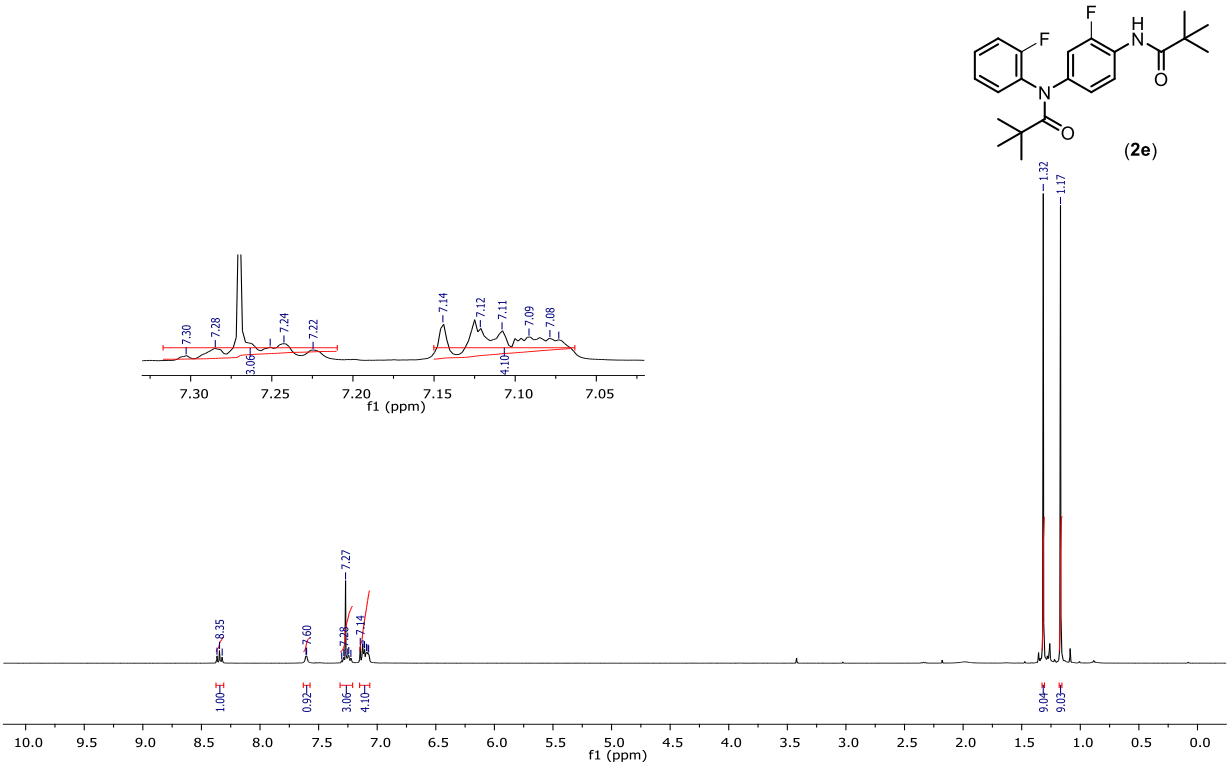
^{13}C NMR 100 MHz



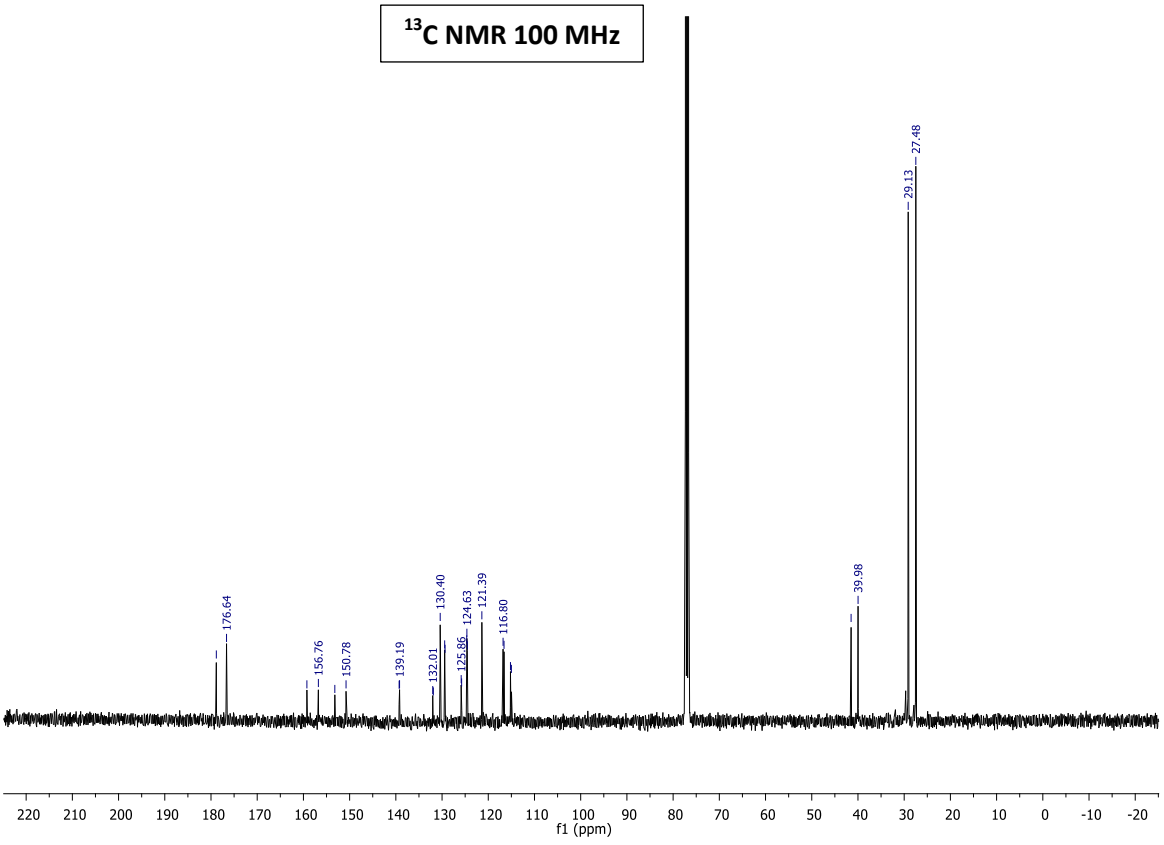
ESI-HRMS Chromatogram



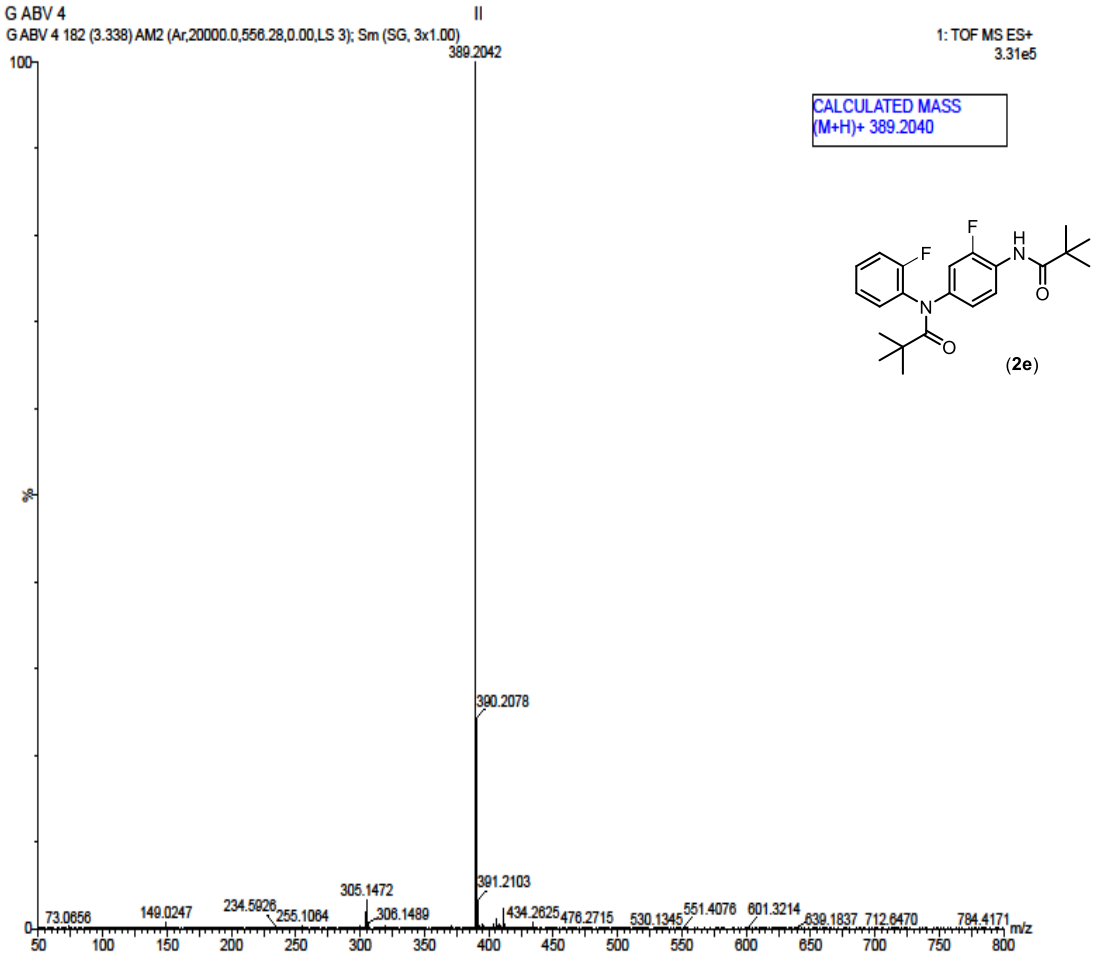
^{1}H NMR 400 MHz



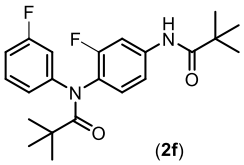
^{13}C NMR 100 MHz



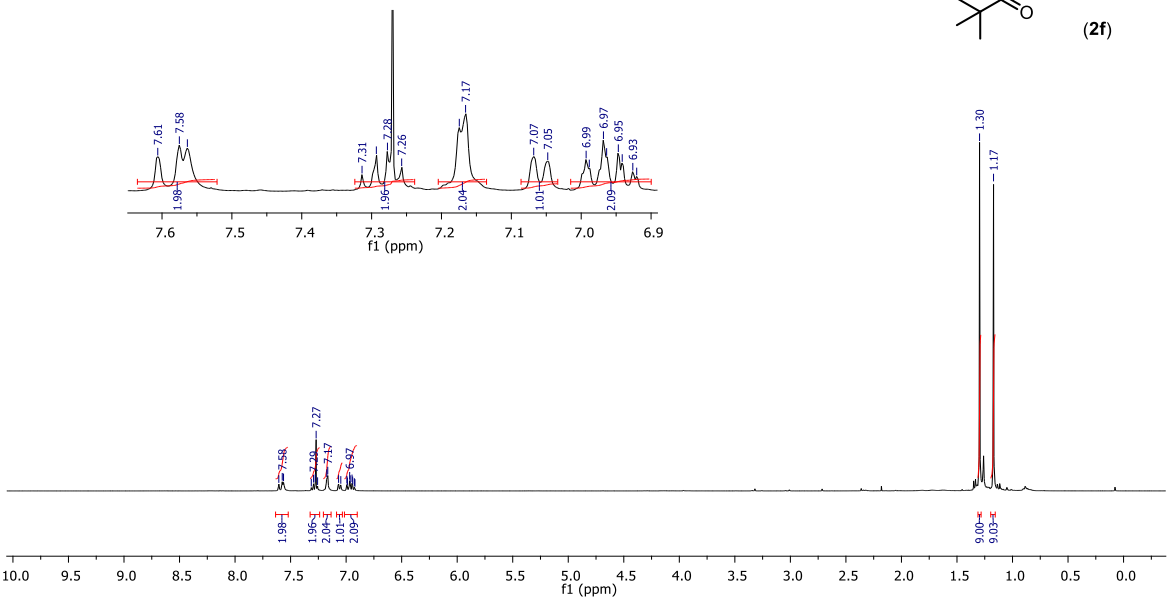
ESI-HRMS Chromatogram



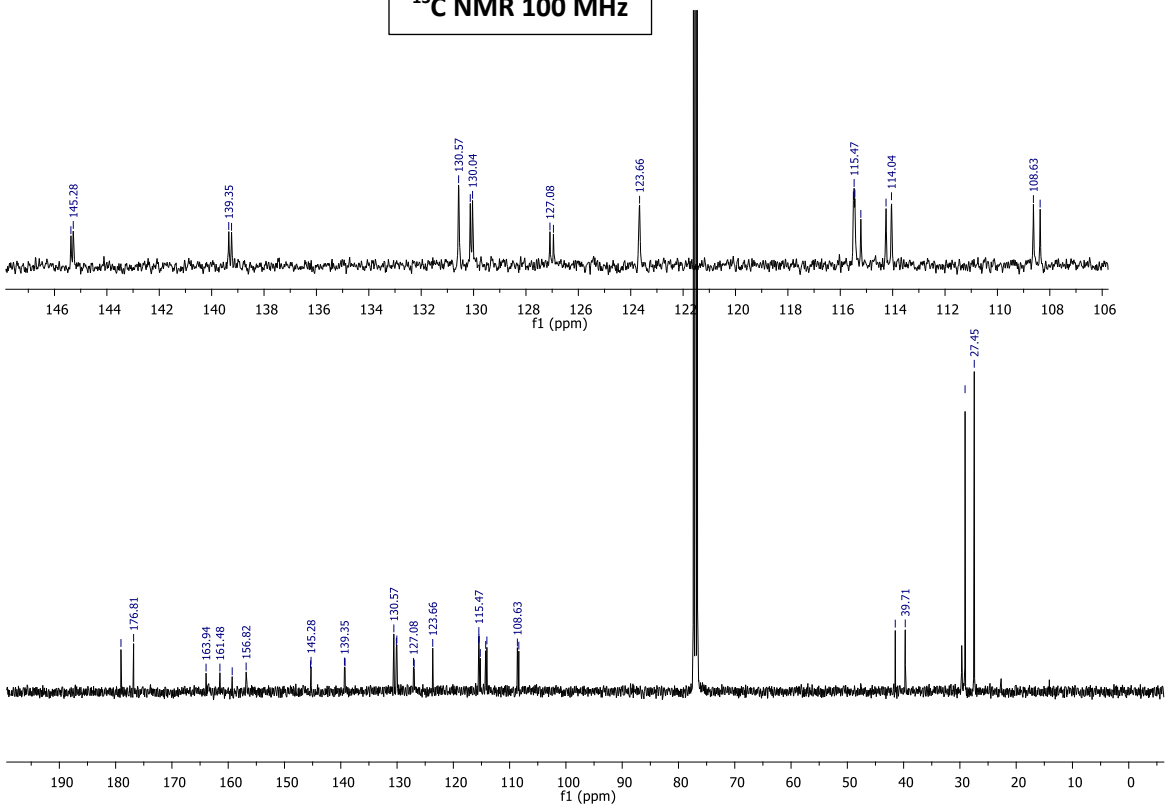
^{1}H NMR 400 MHz



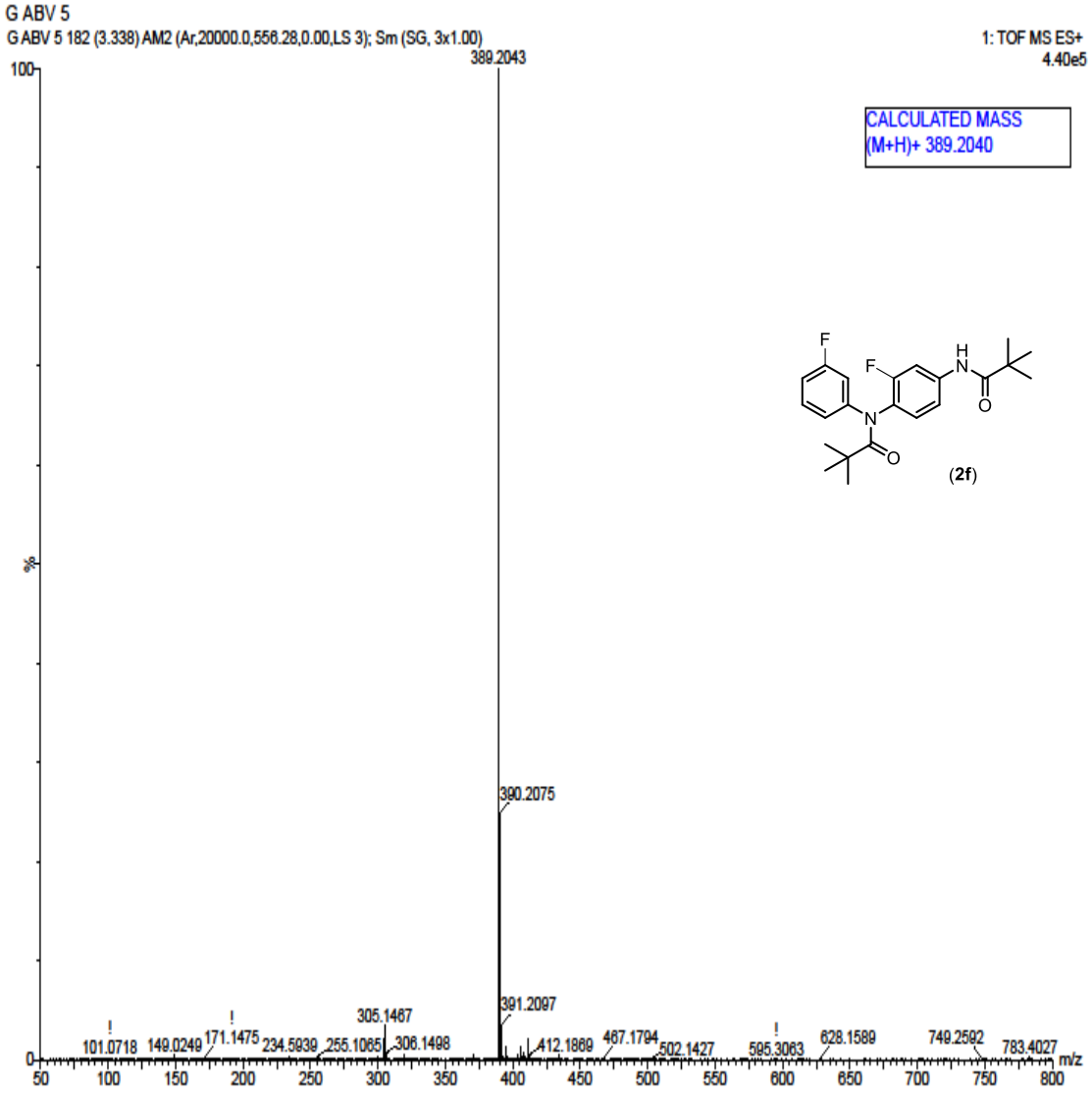
(**2f**)



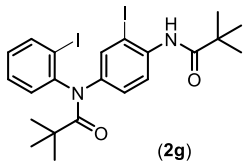
^{13}C NMR 100 MHz



ESI-HRMS Chromatogram



^{1}H NMR 400 MHz



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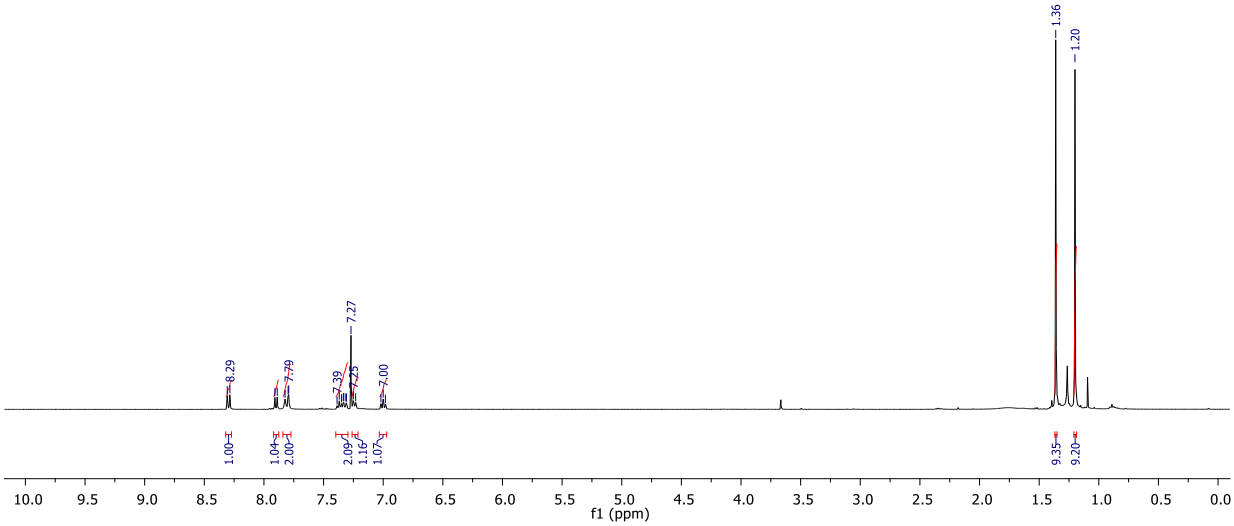
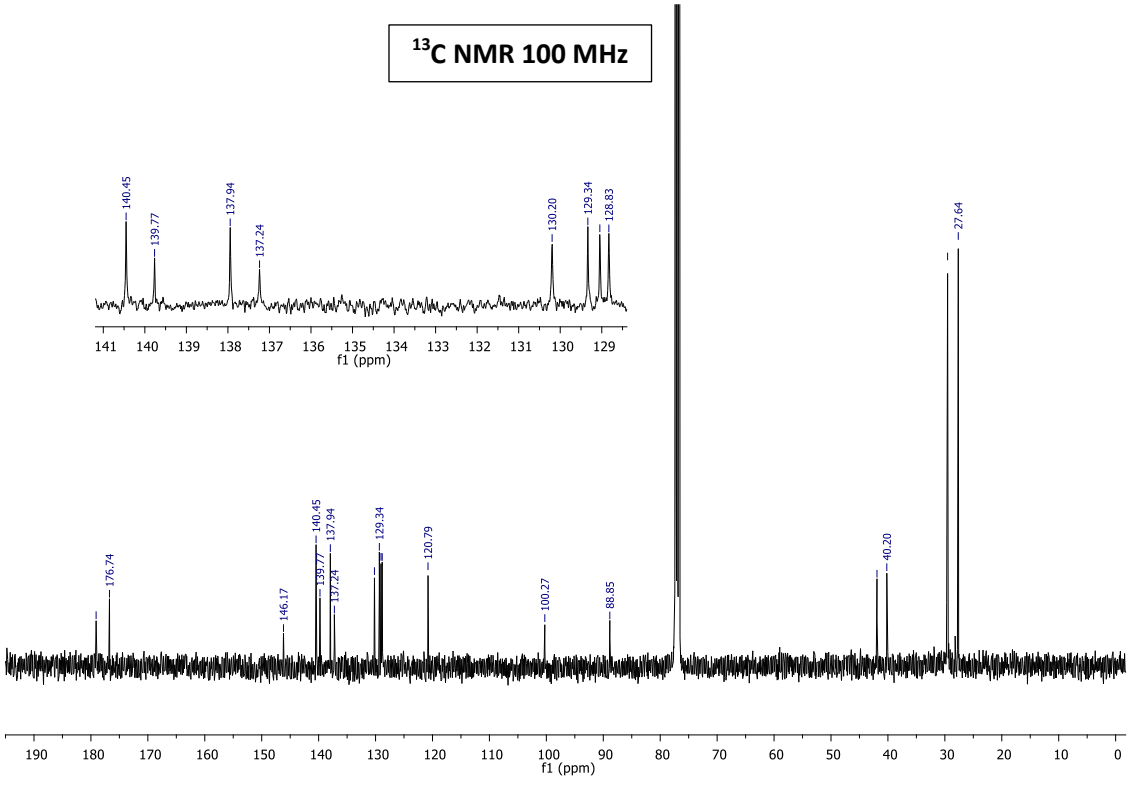
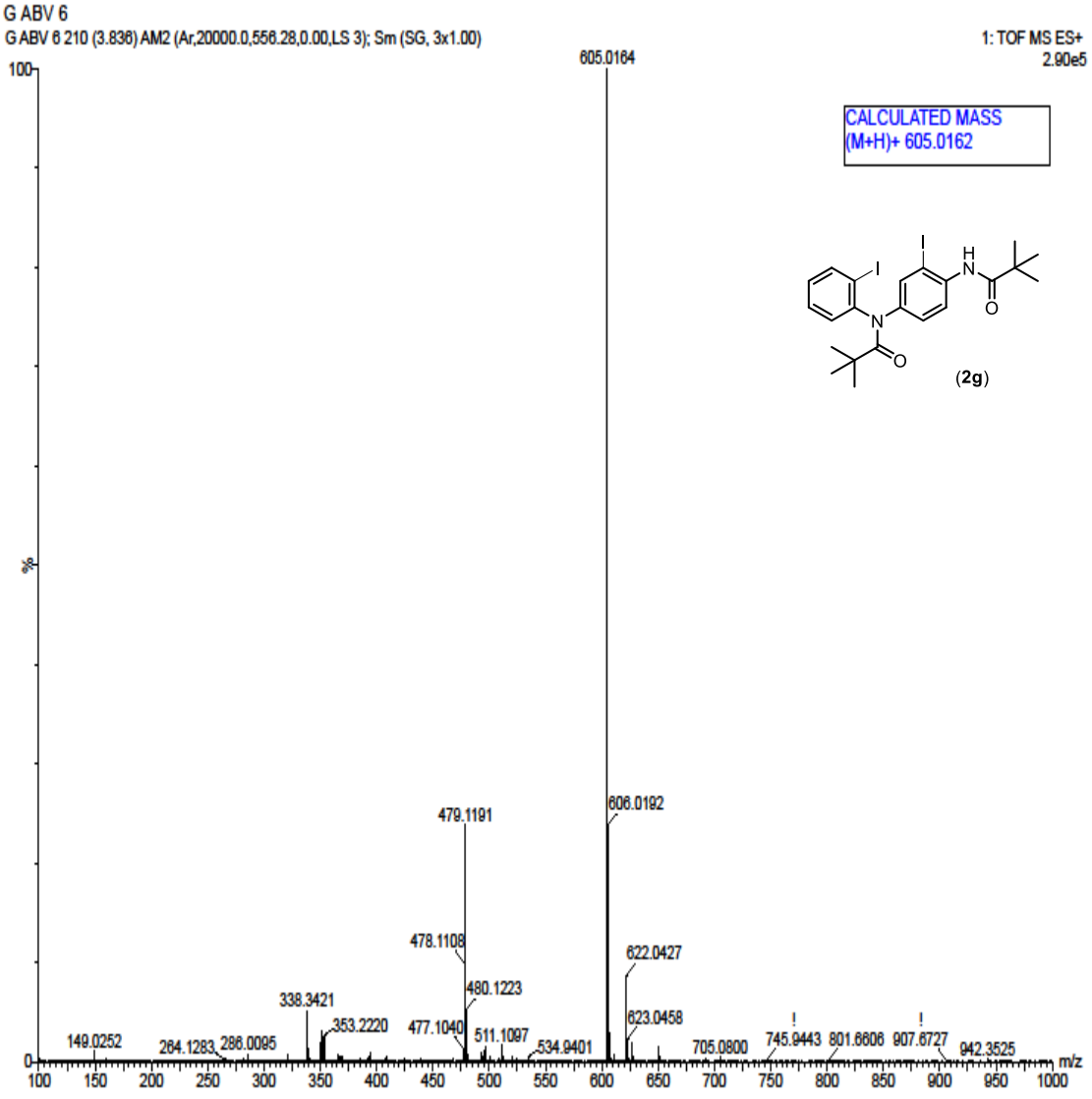


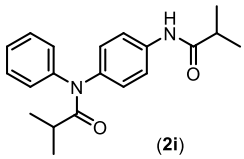
^{13}C NMR 100 MHz



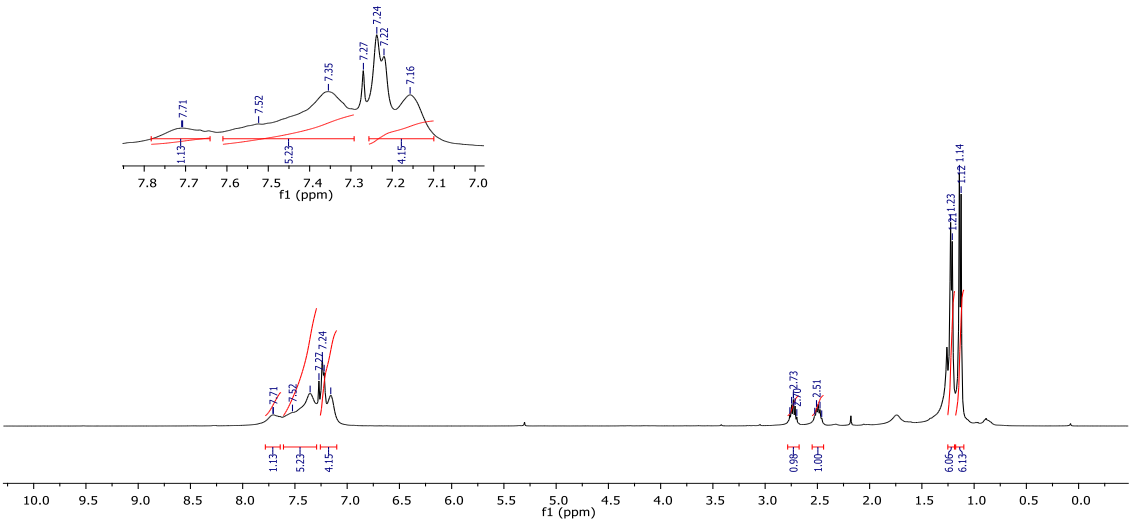
ESI-HRMS Chromatogram



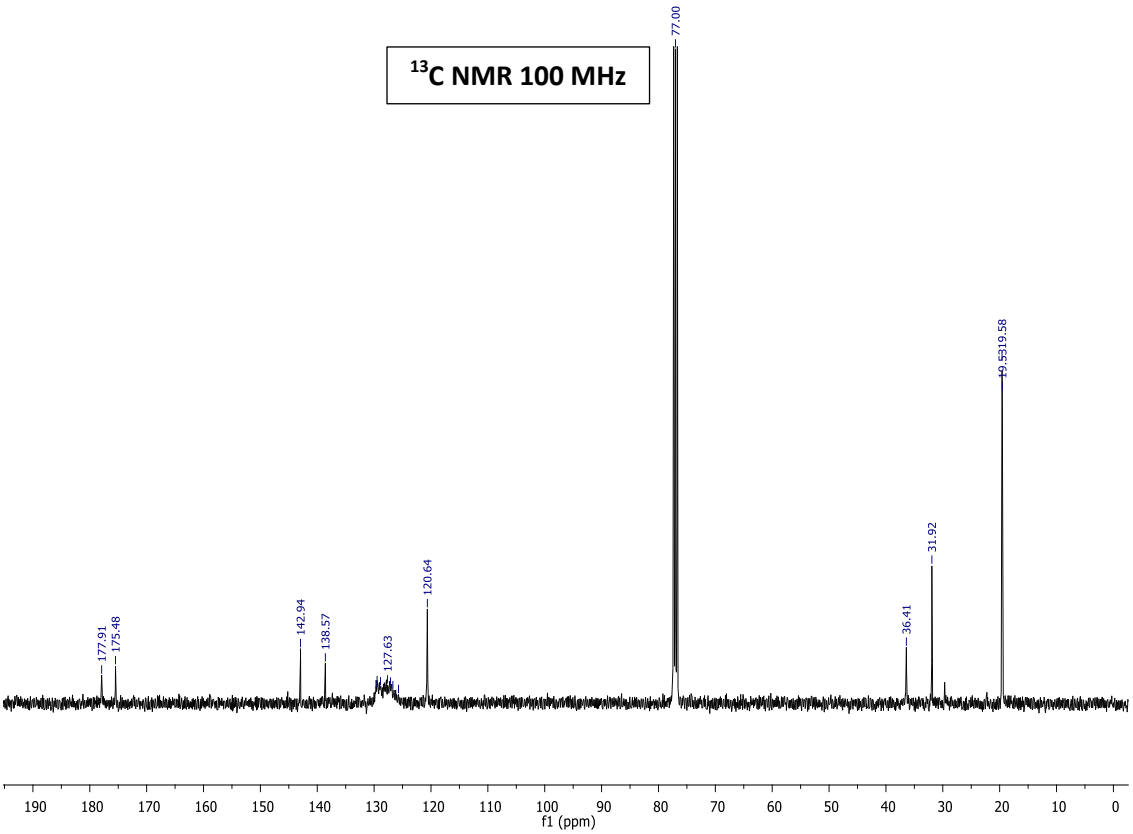
^{1}H NMR 400 MHz



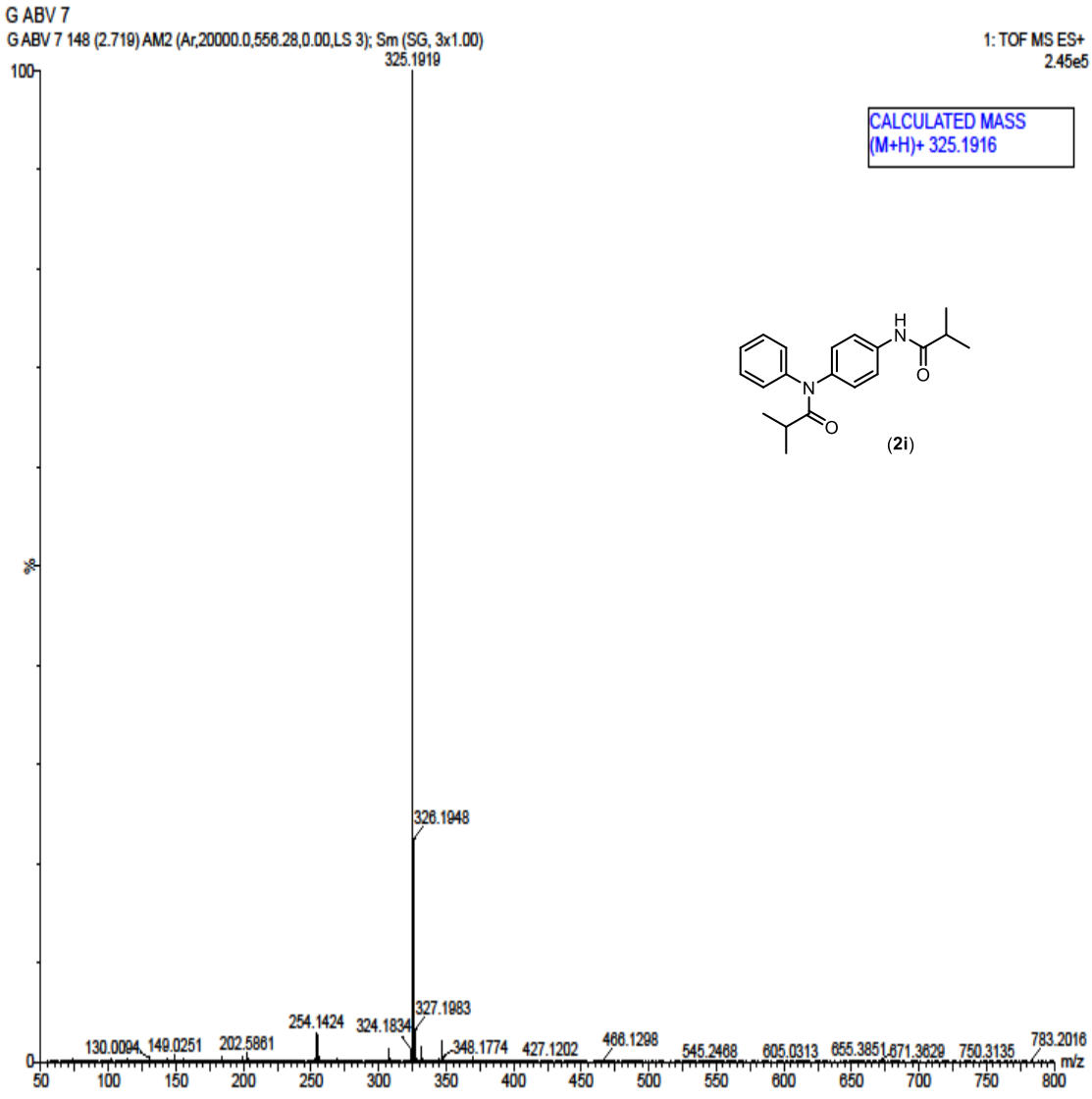
(**2i**)



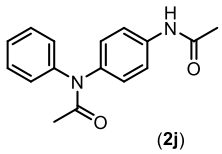
^{13}C NMR 100 MHz



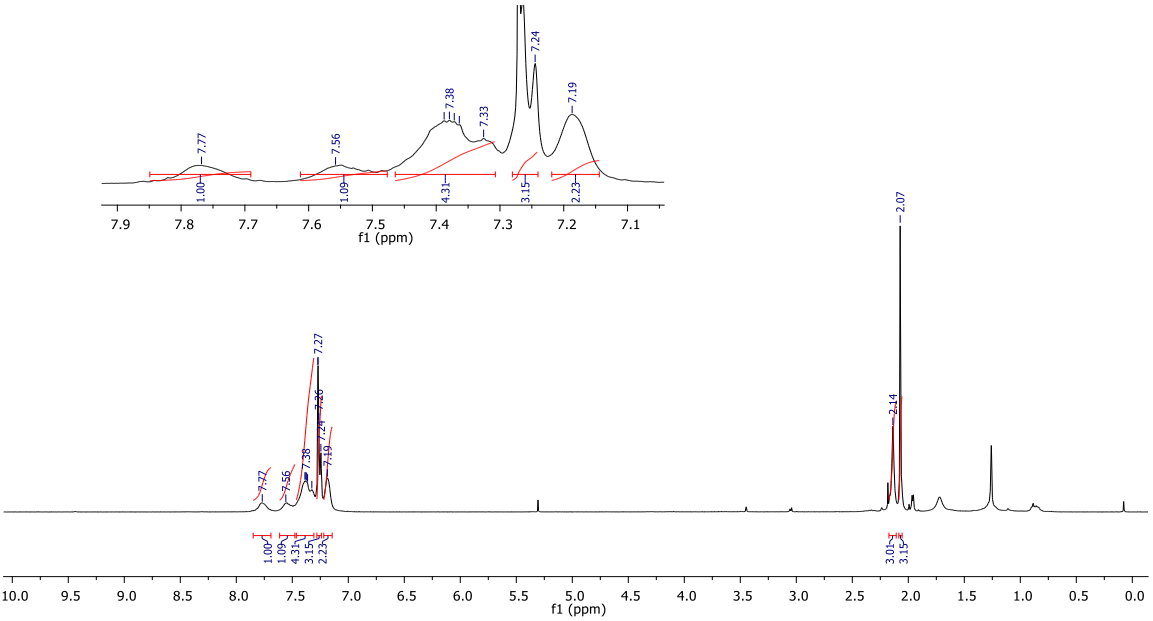
ESI-HRMS Chromatogram



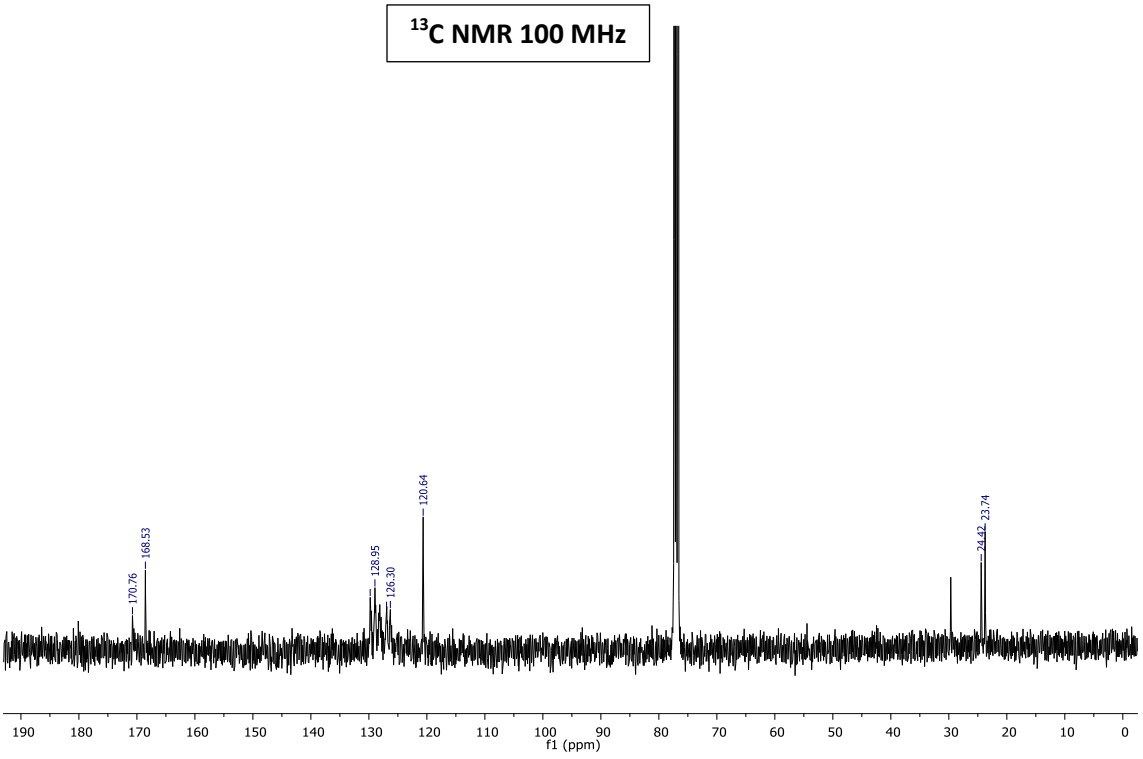
^{1}H NMR 400 MHz



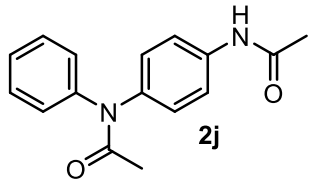
(**2j**)



^{13}C NMR 100 MHz

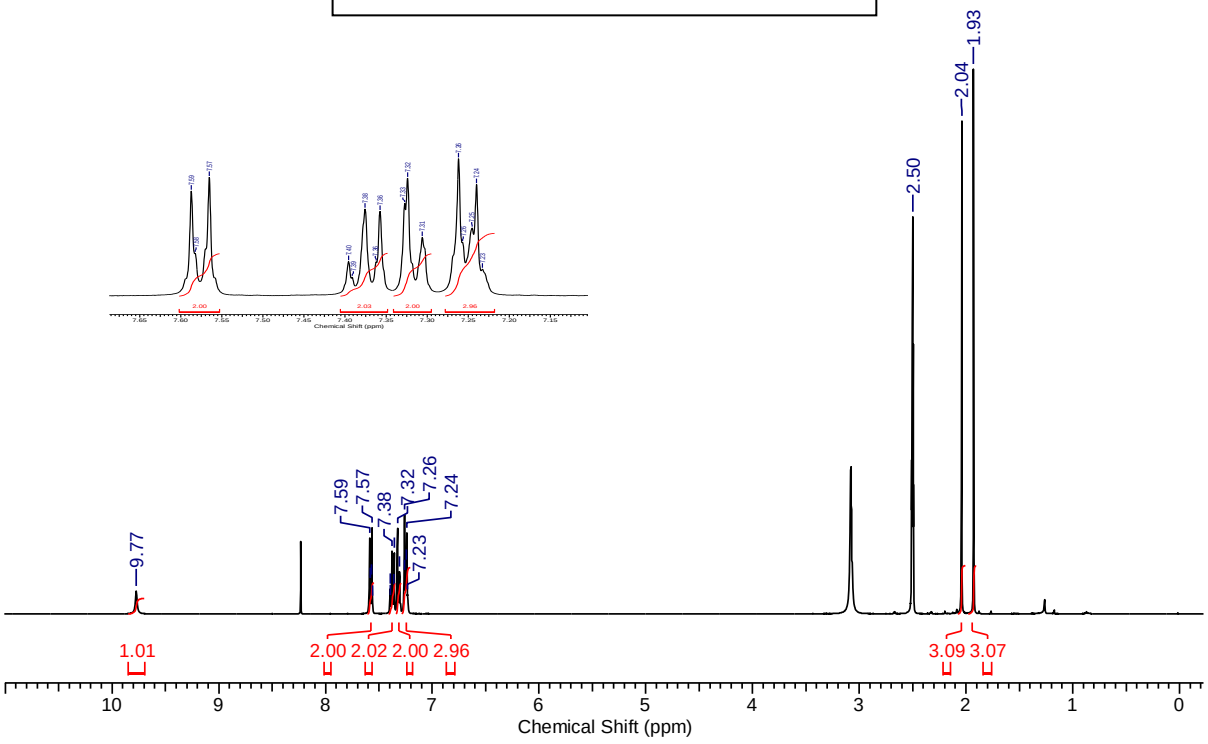


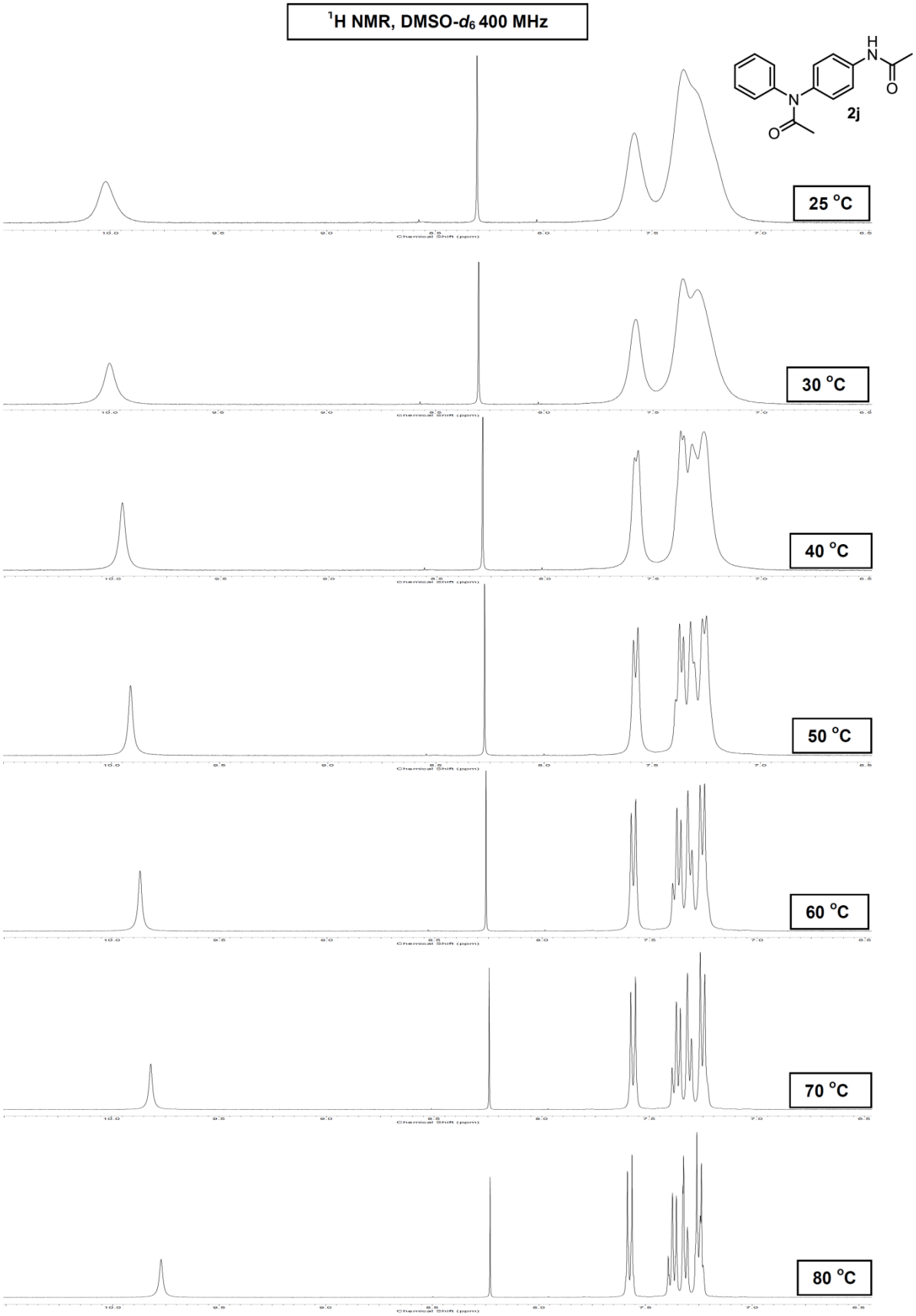
^{1}H NMR, $CDCl_3$ 400 MHz at 30 ^{o}C



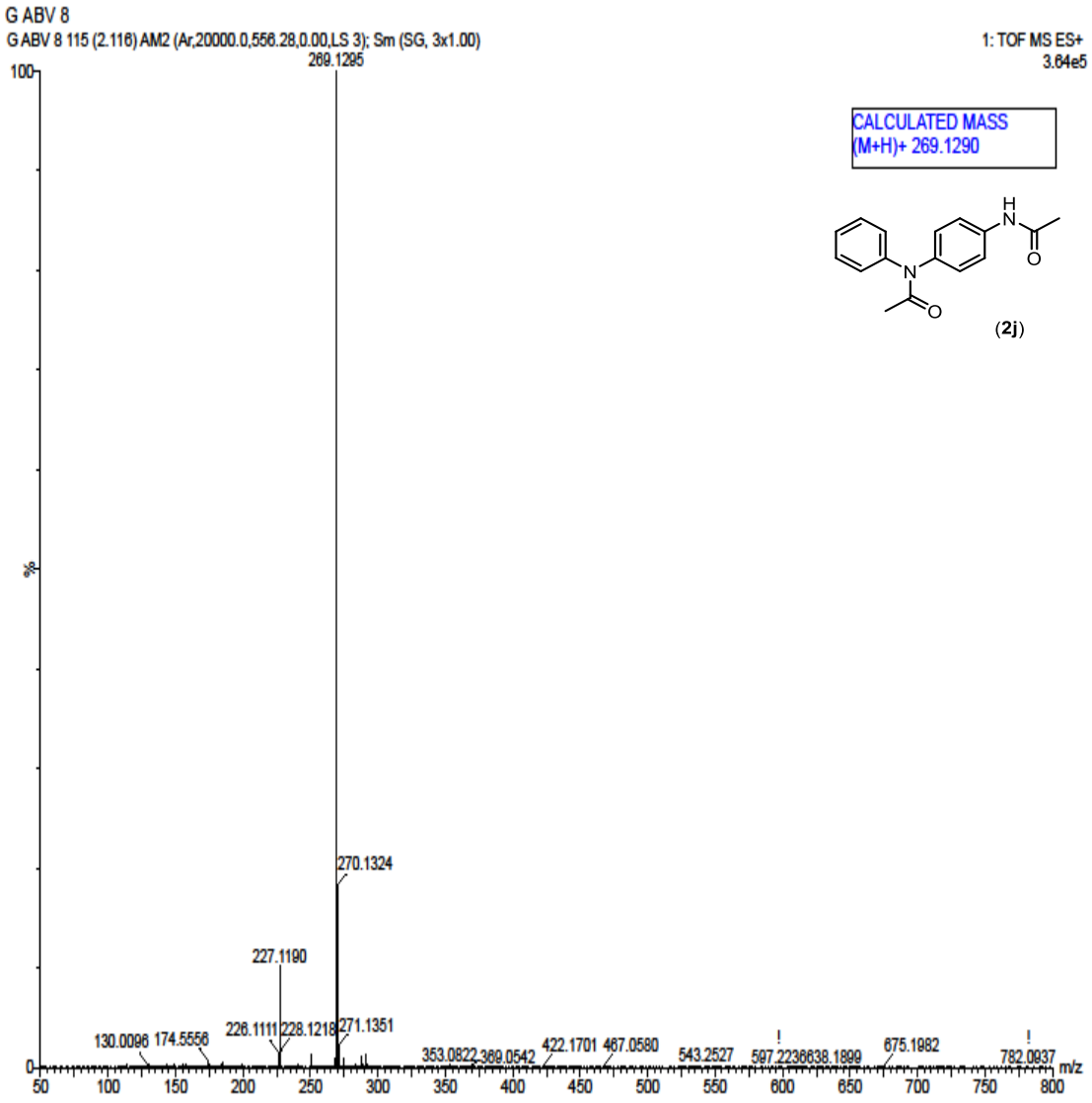
2j

^{1}H NMR, DMSO-d_6 400 MHz at 80 ^{o}C

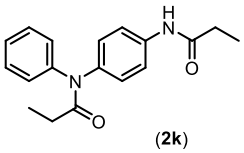



^{1}H NMR, DMSO-d_6 400 MHz
2j
25 °C
30 °C
40 °C
50 °C
60 °C
70 °C
80 °C

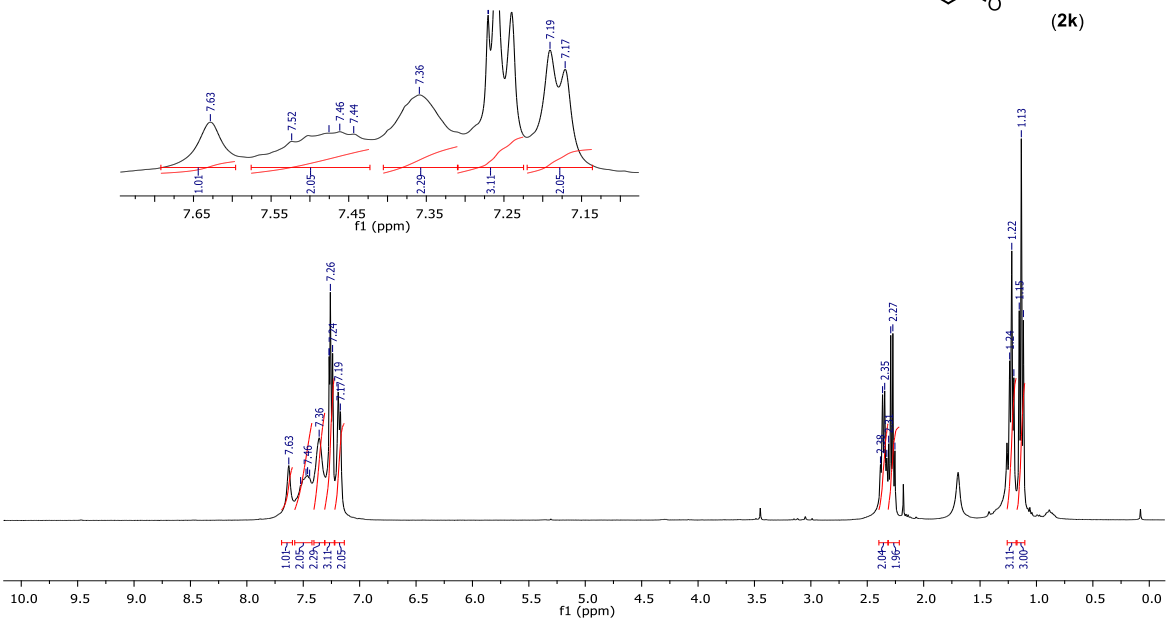
ESI-HRMS Chromatogram



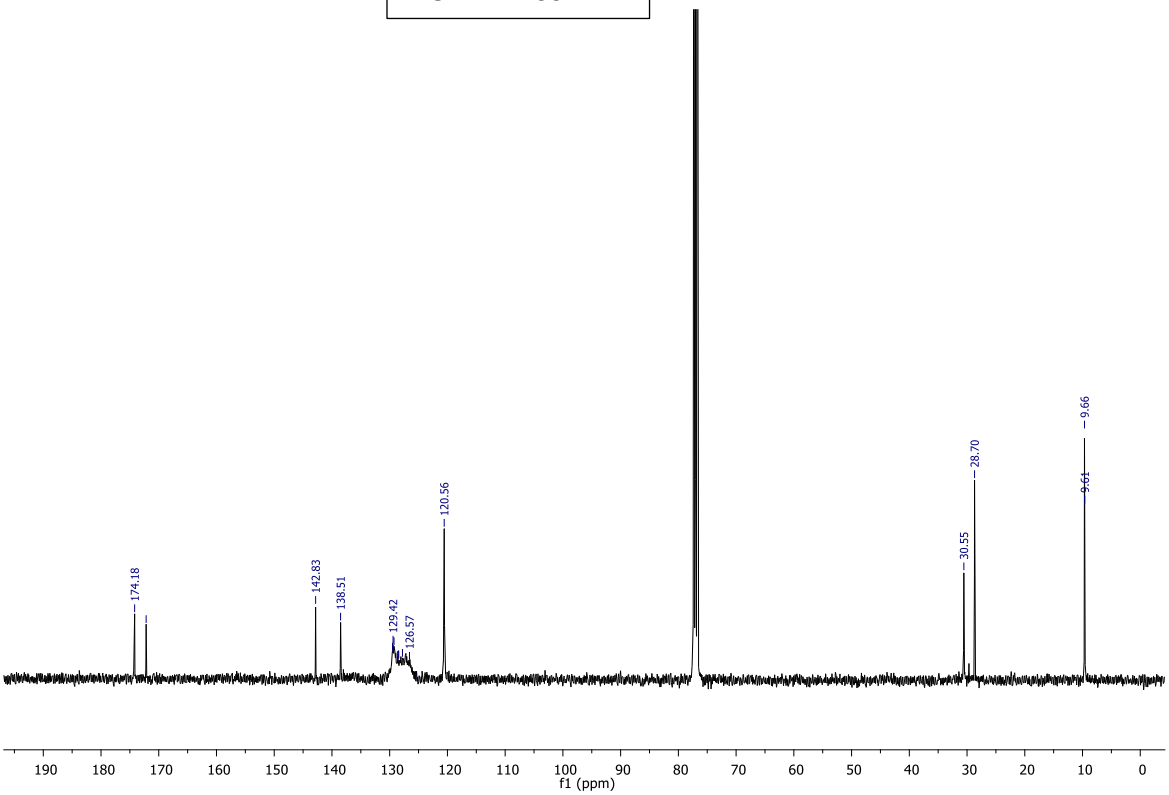
^{1}H NMR 400 MHz



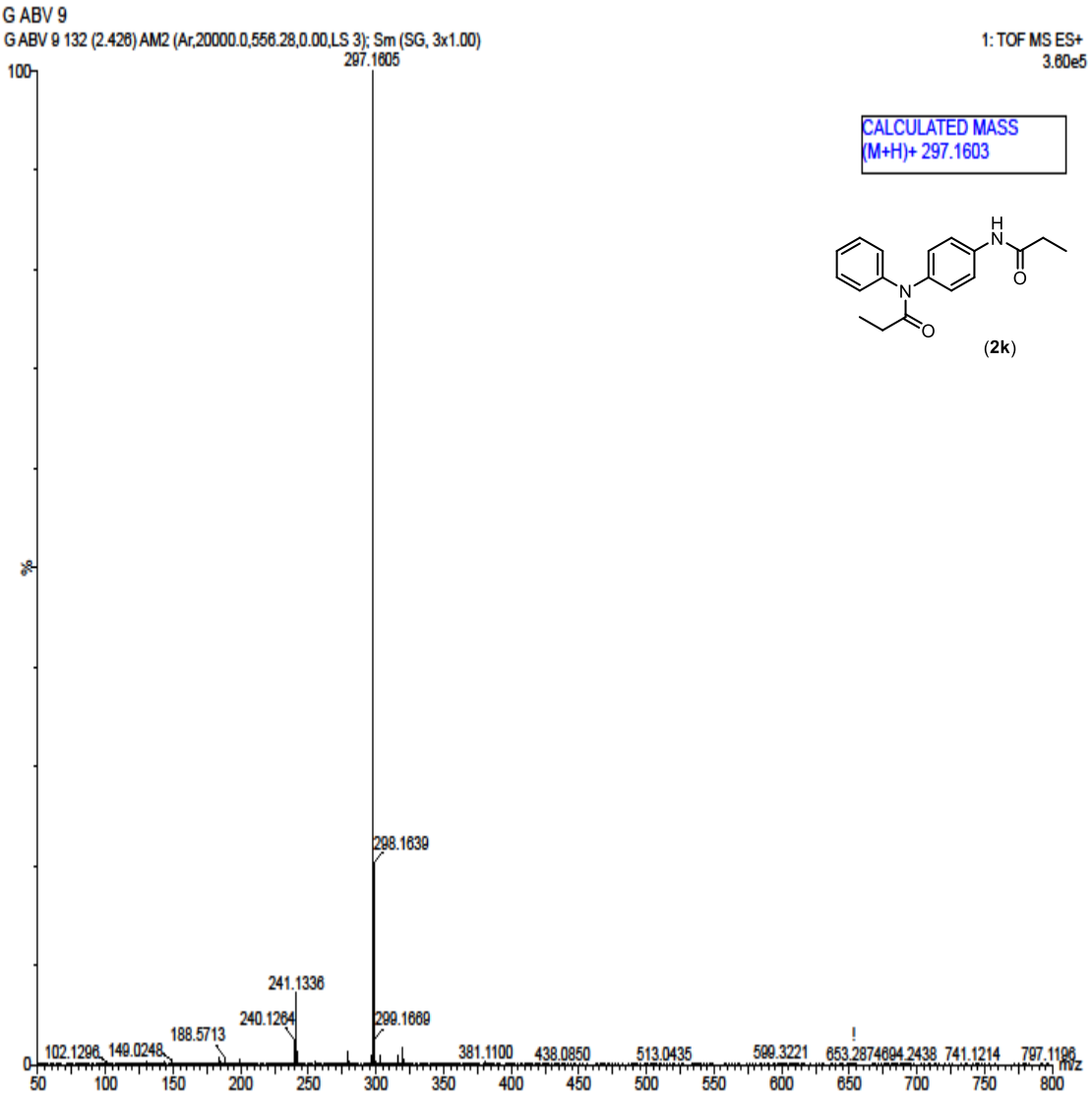
(**2k**)



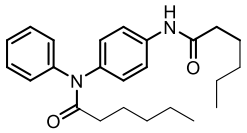
^{13}C NMR 100 MHz



ESI-HRMS Chromatogram



^{1}H NMR 400 MHz



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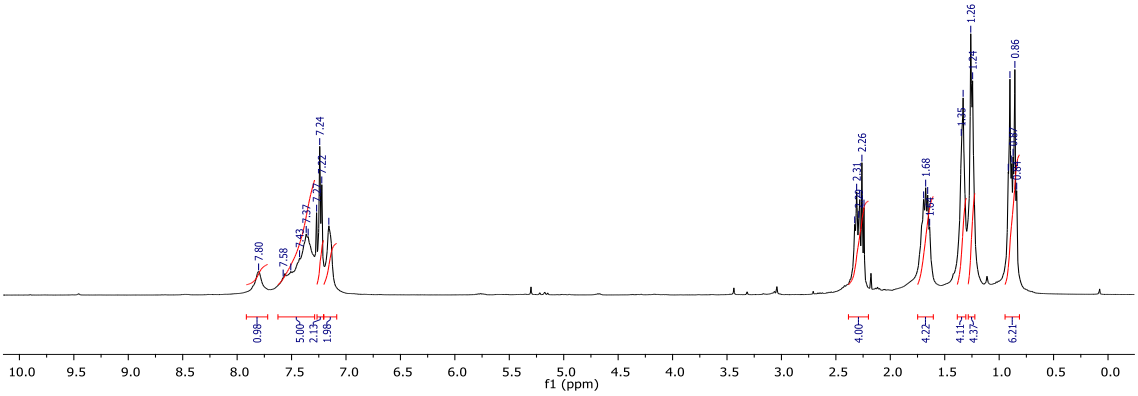
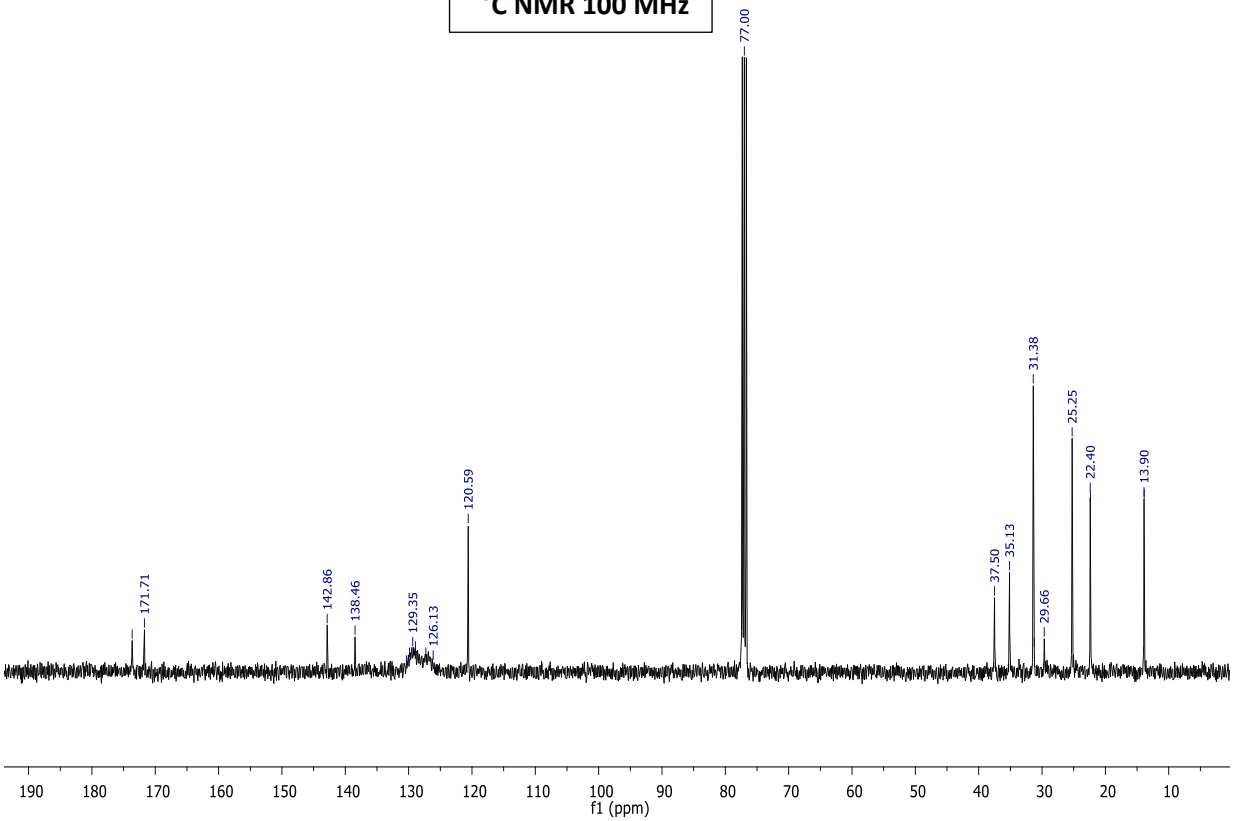
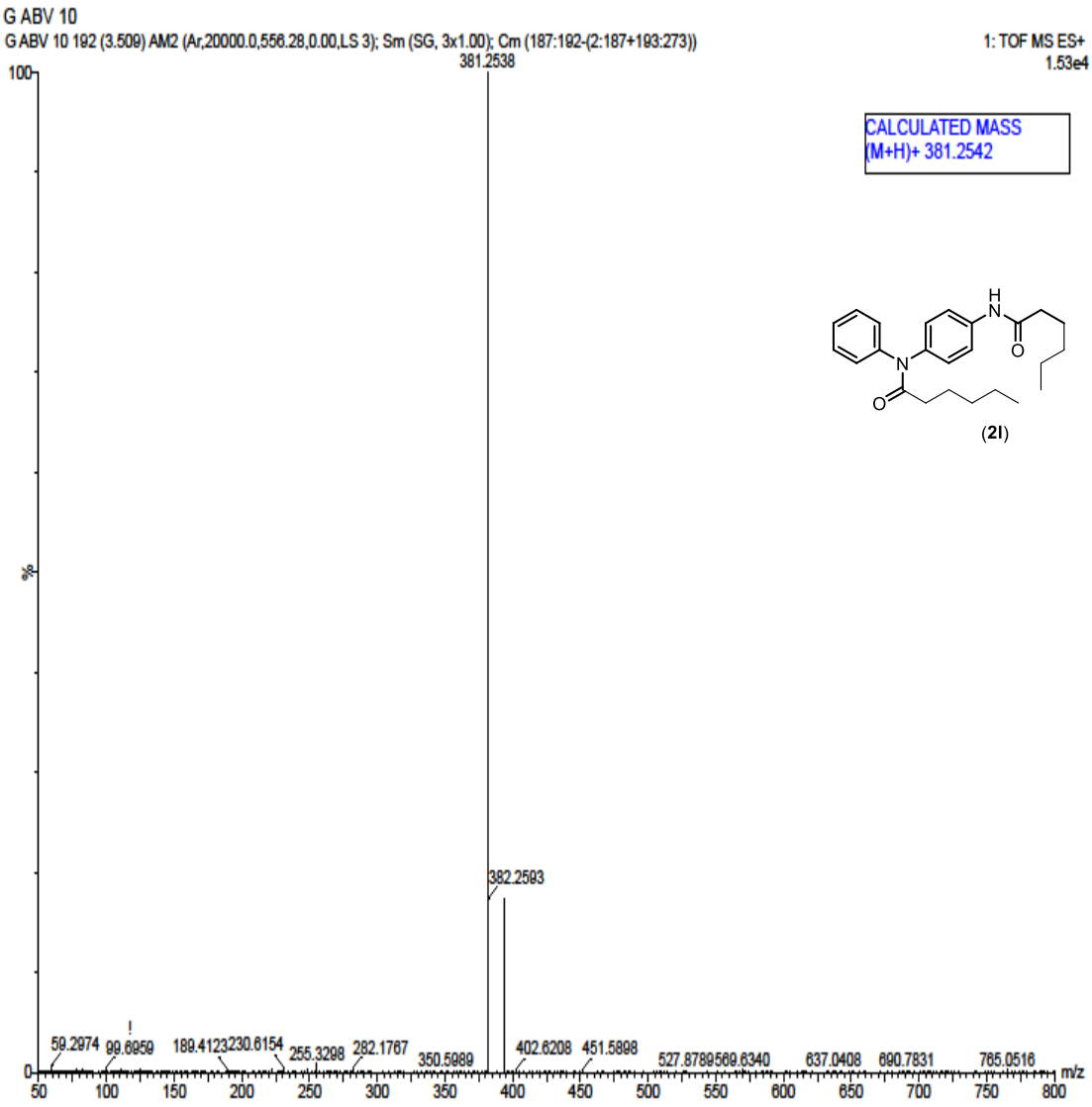


^{13}C NMR 100 MHz

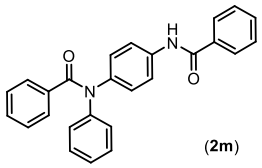


ESI-HRMS Chromatogram



(**2l**)

^{1}H NMR 400 MHz



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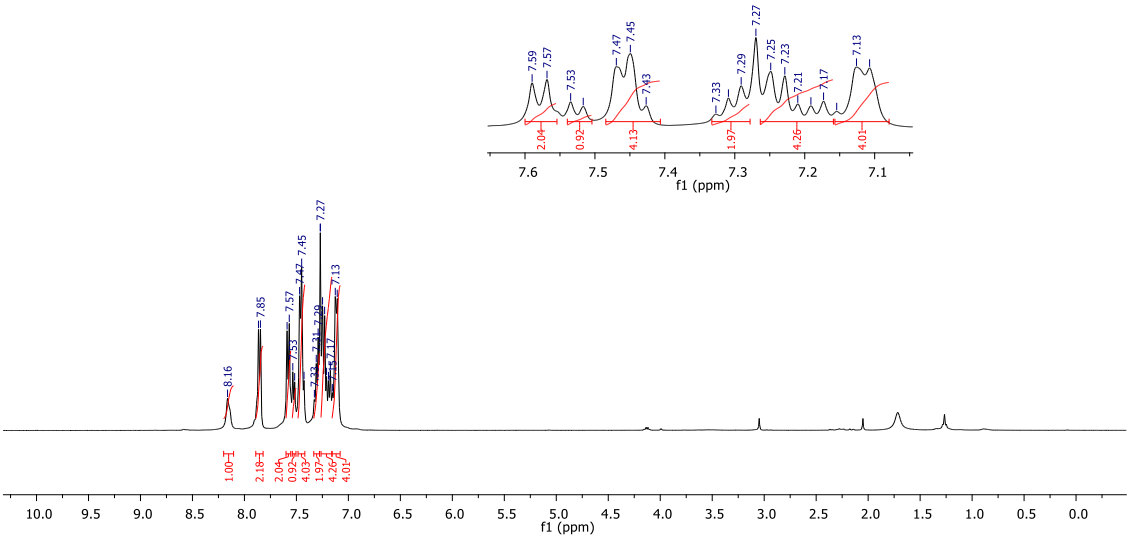
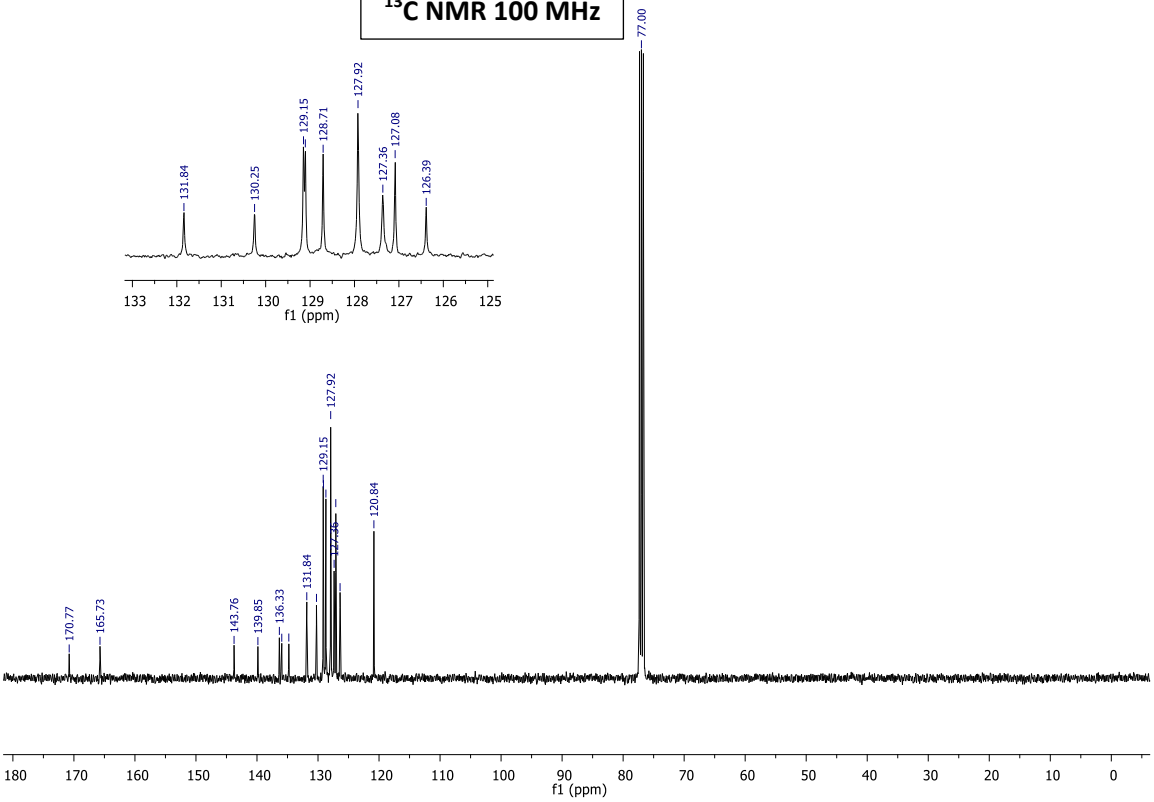
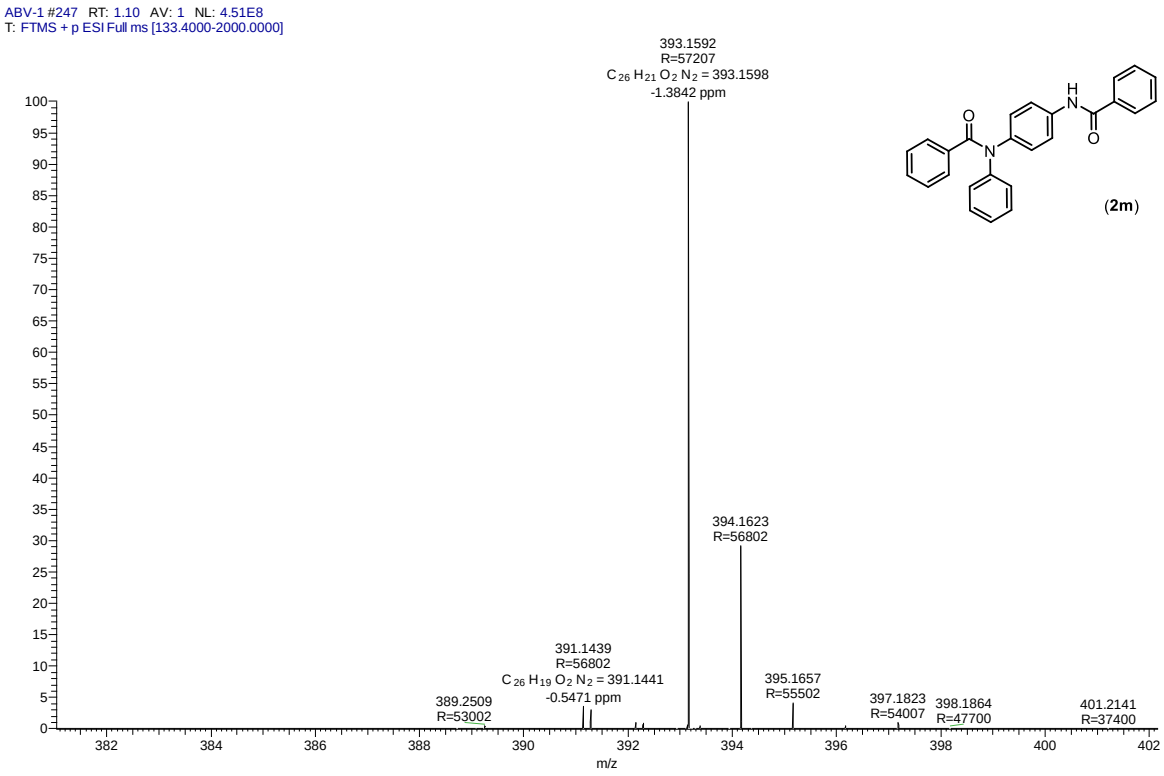


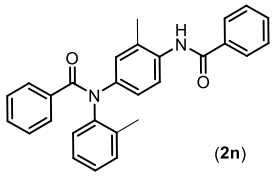
^{13}C NMR 100 MHz



ESI-HRMS Chromatogram



^{1}H NMR 400 MHz



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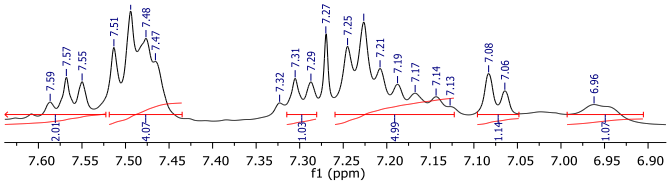
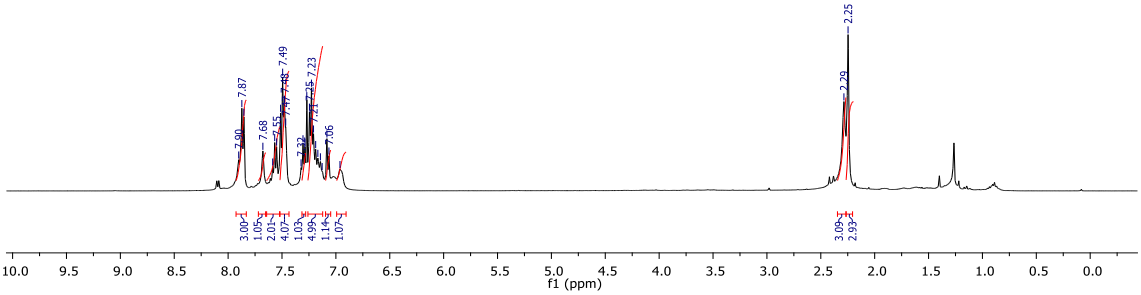
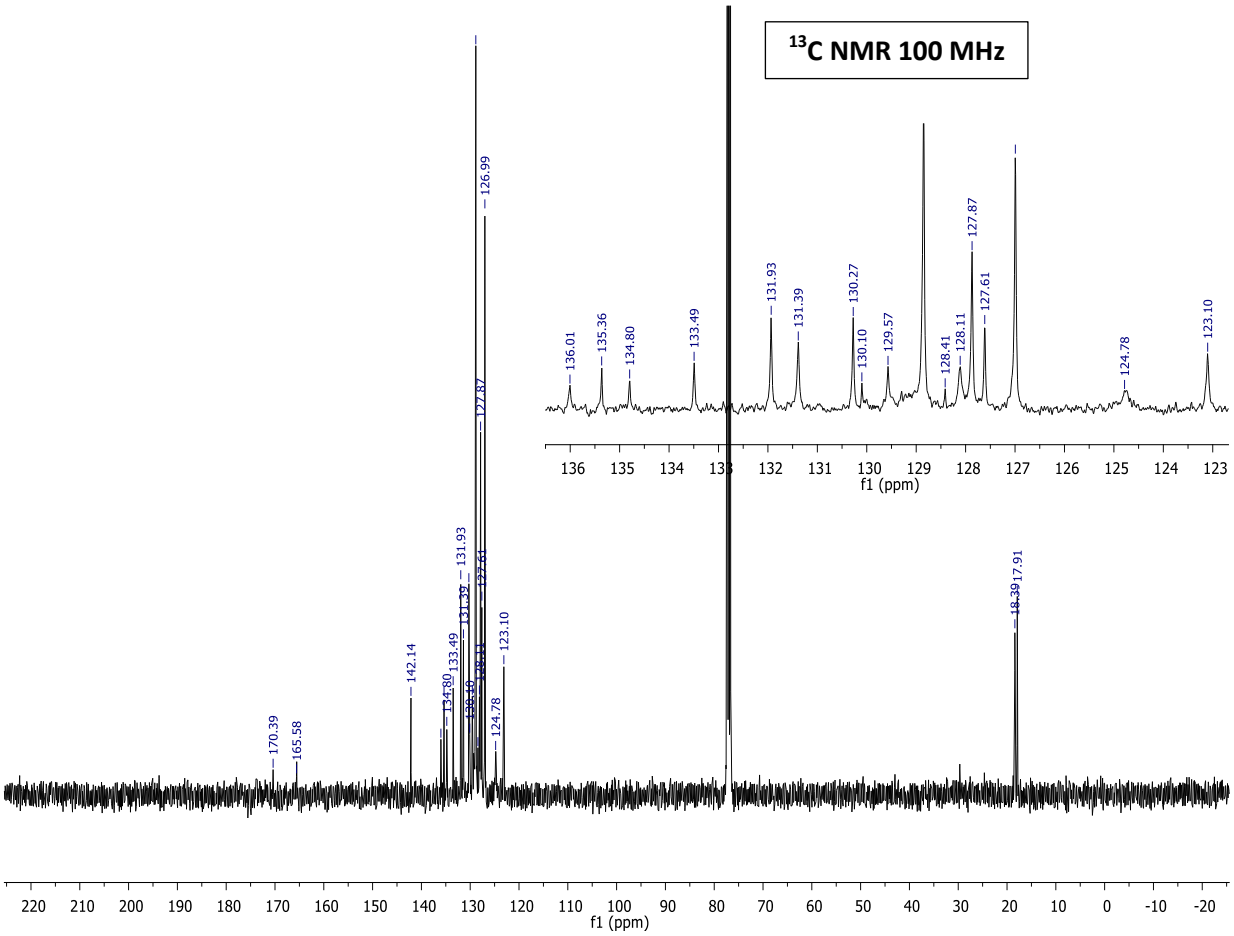
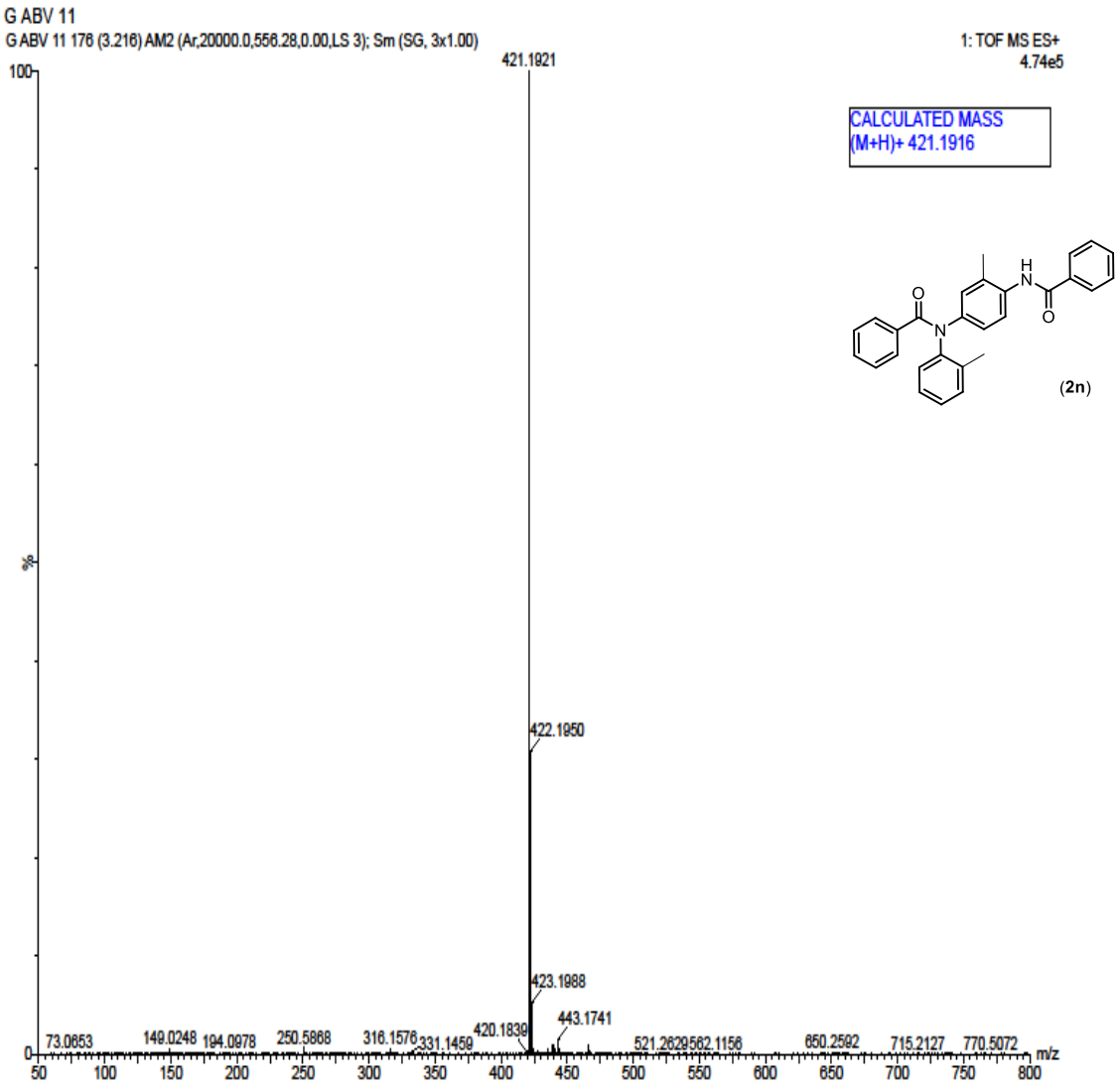




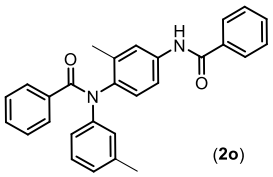
^{13}C NMR 100 MHz



ESI-HRMS Chromatogram



^{1}H NMR 400 MHz



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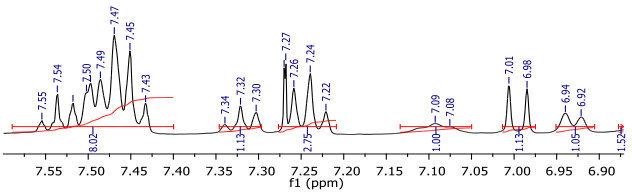
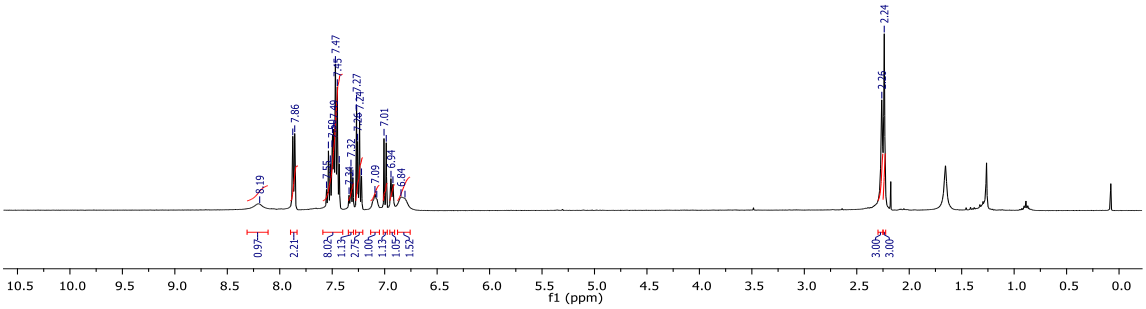
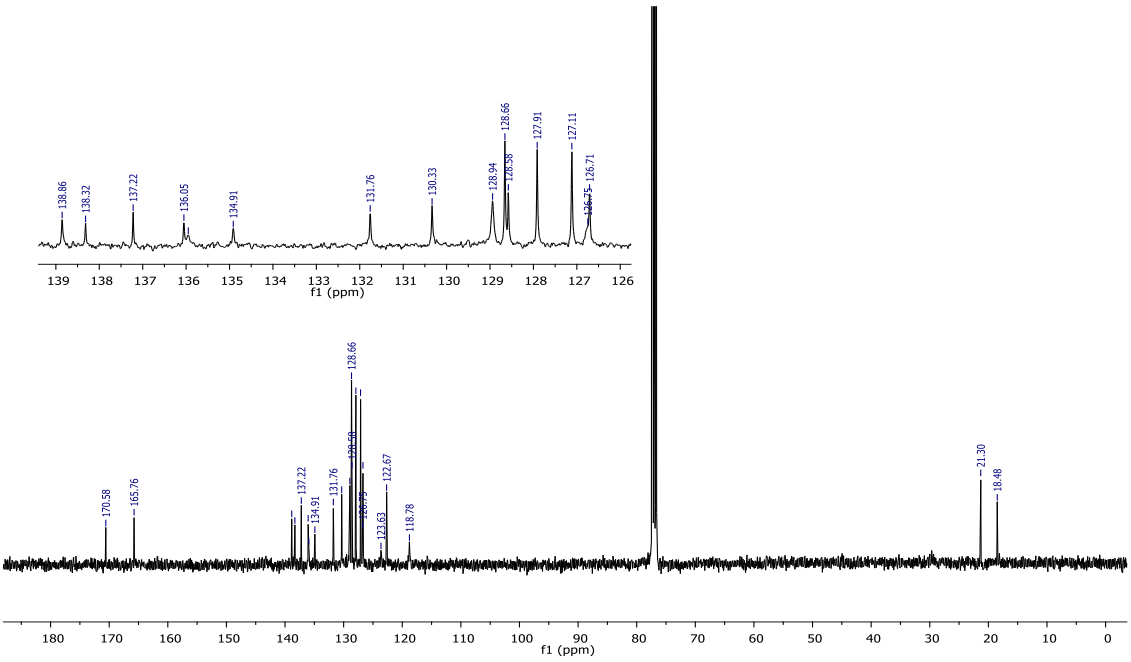
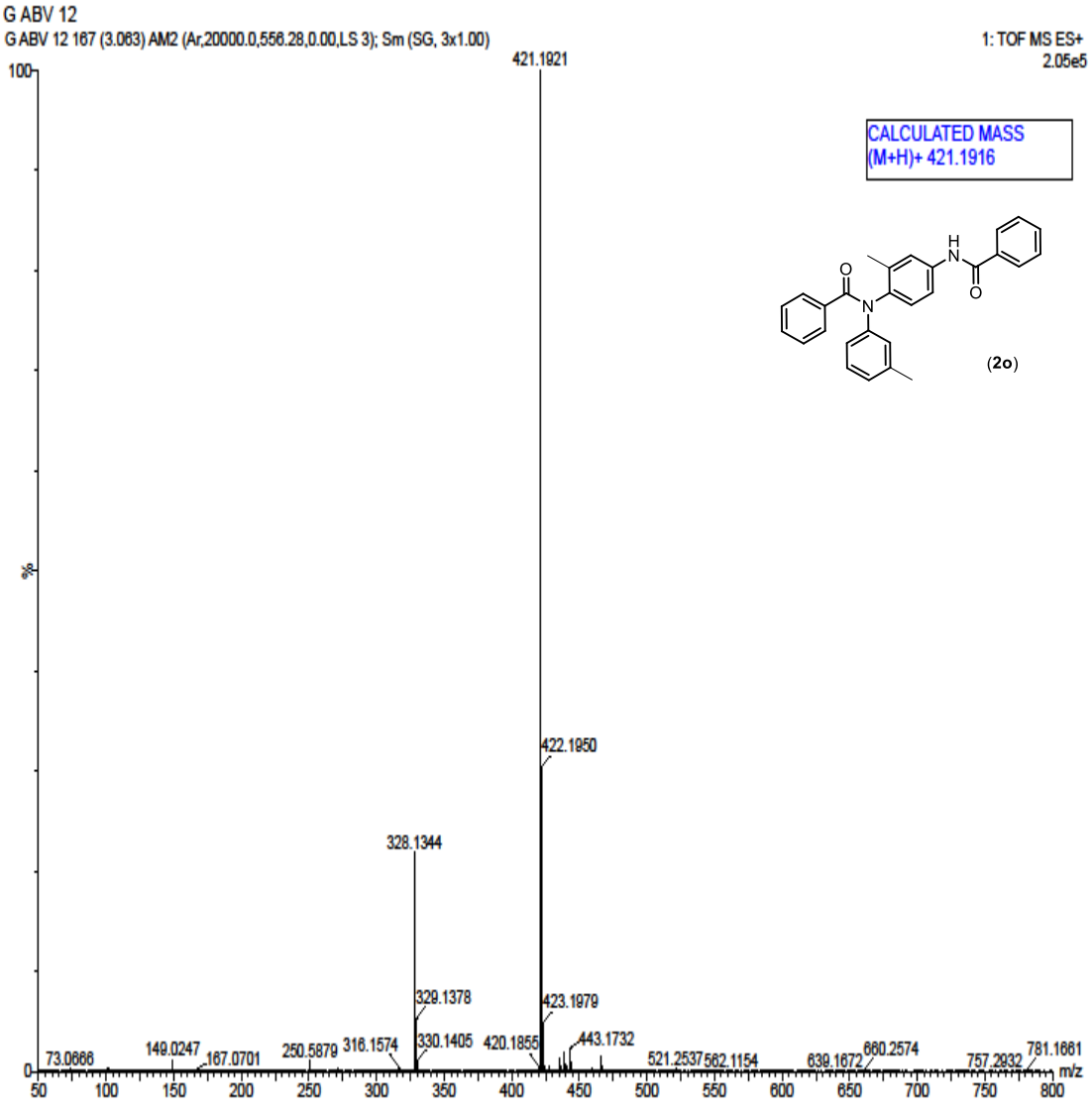




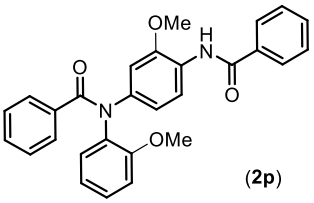
^{13}C NMR 100 MHz



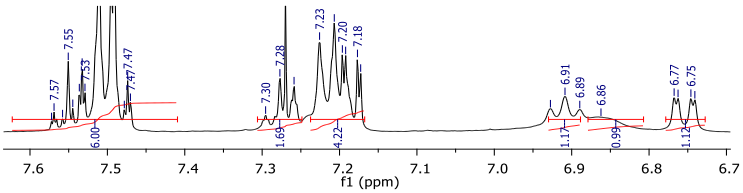
ESI-HRMS Chromatogram

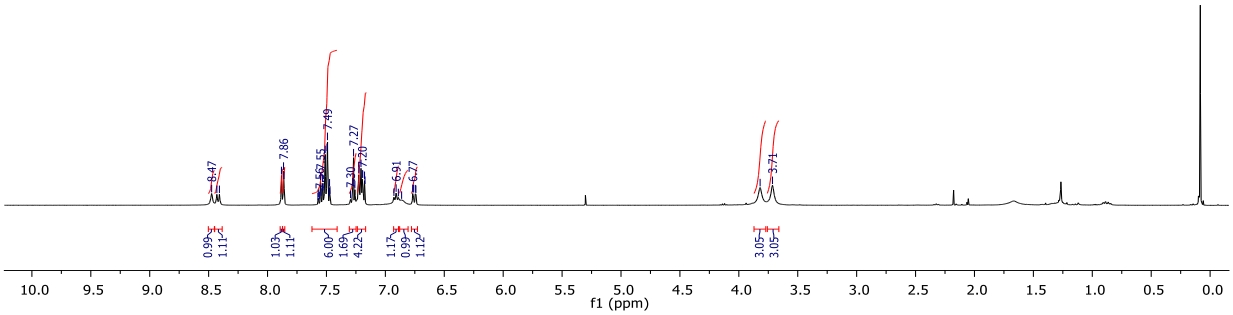


^{1}H NMR 400 MHz

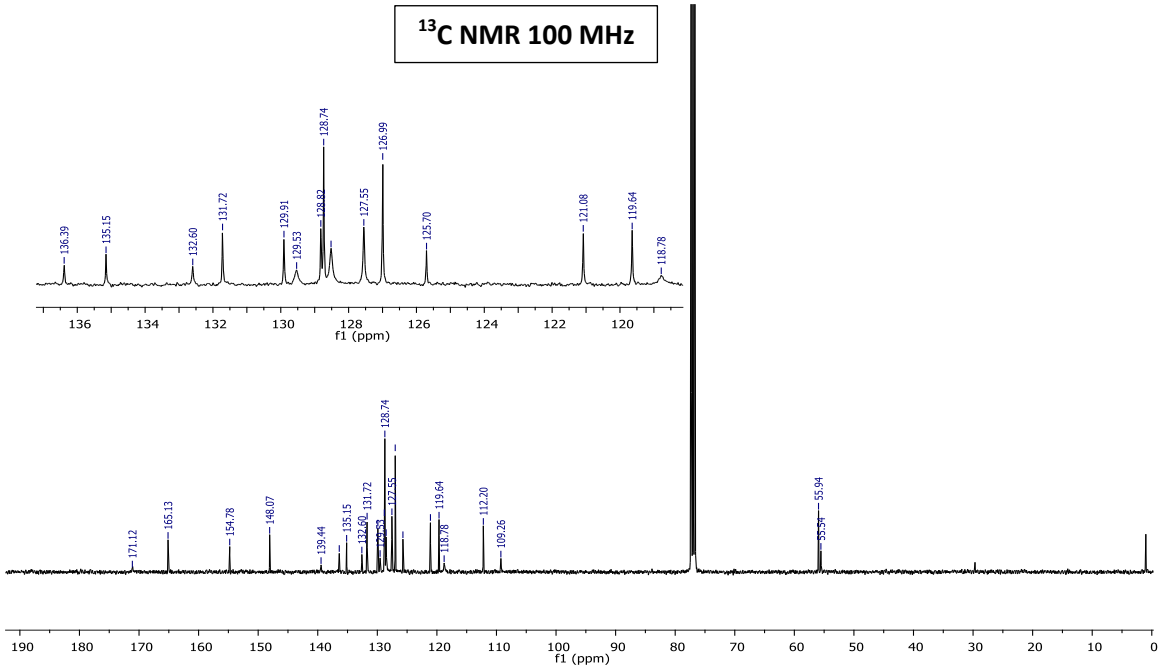


(**2p**)

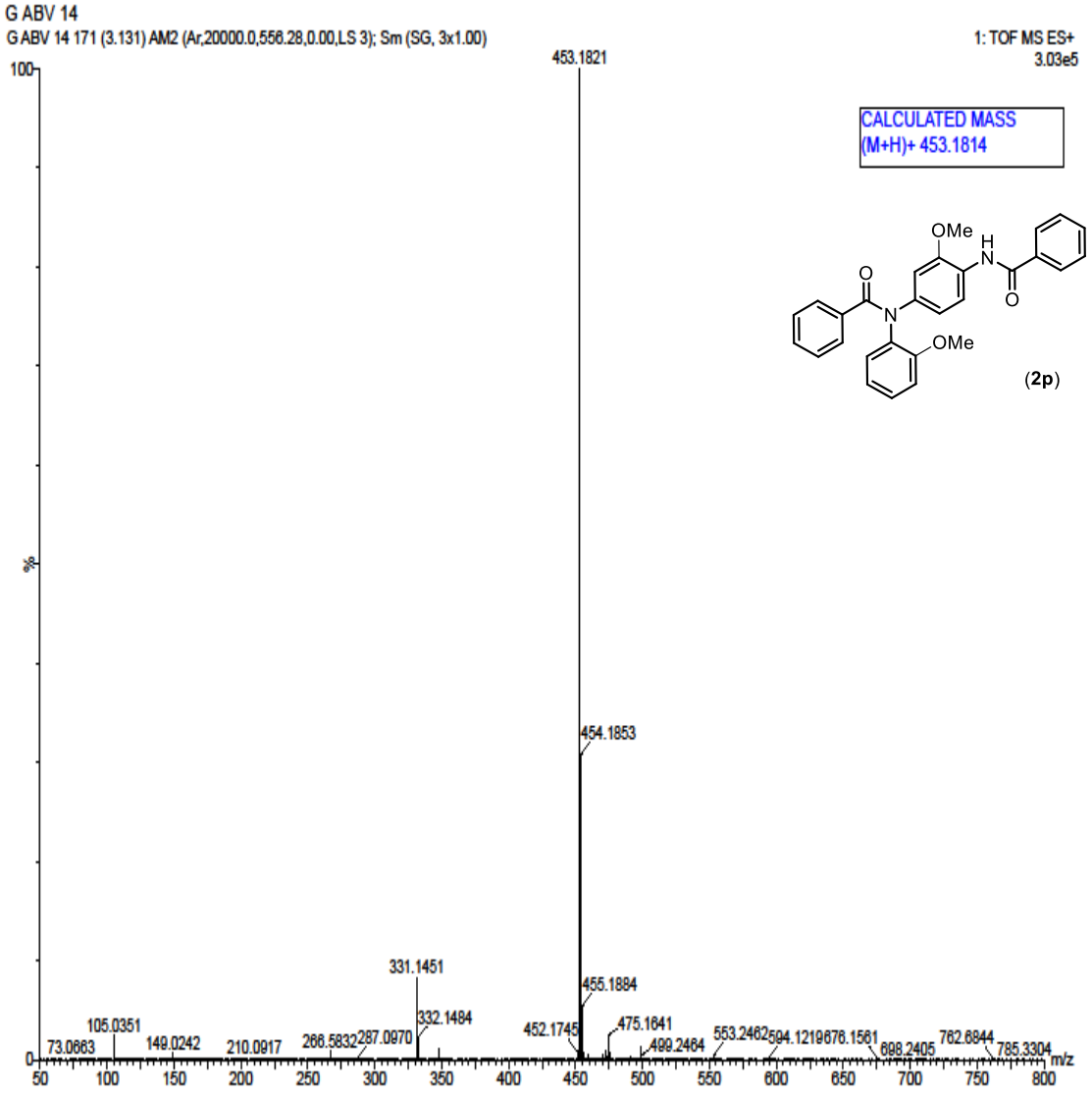




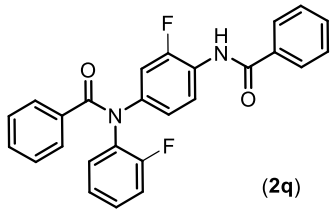
^{13}C NMR 100 MHz



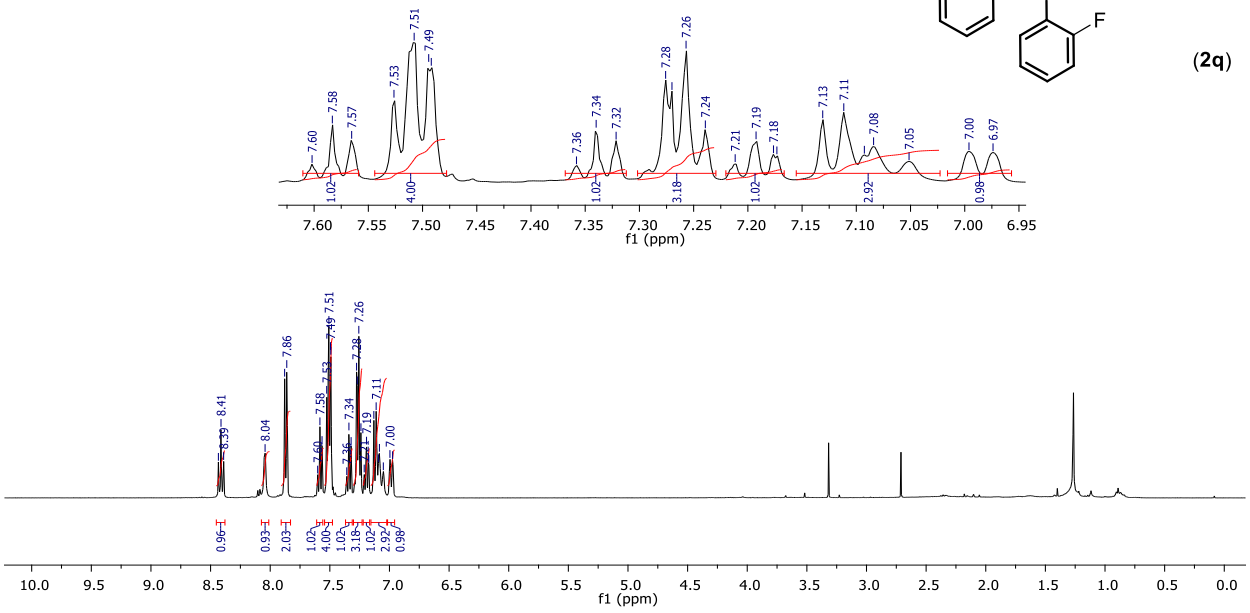
ESI-HRMS Chromatogram



^{1}H NMR 400 MHz



(**2q**)



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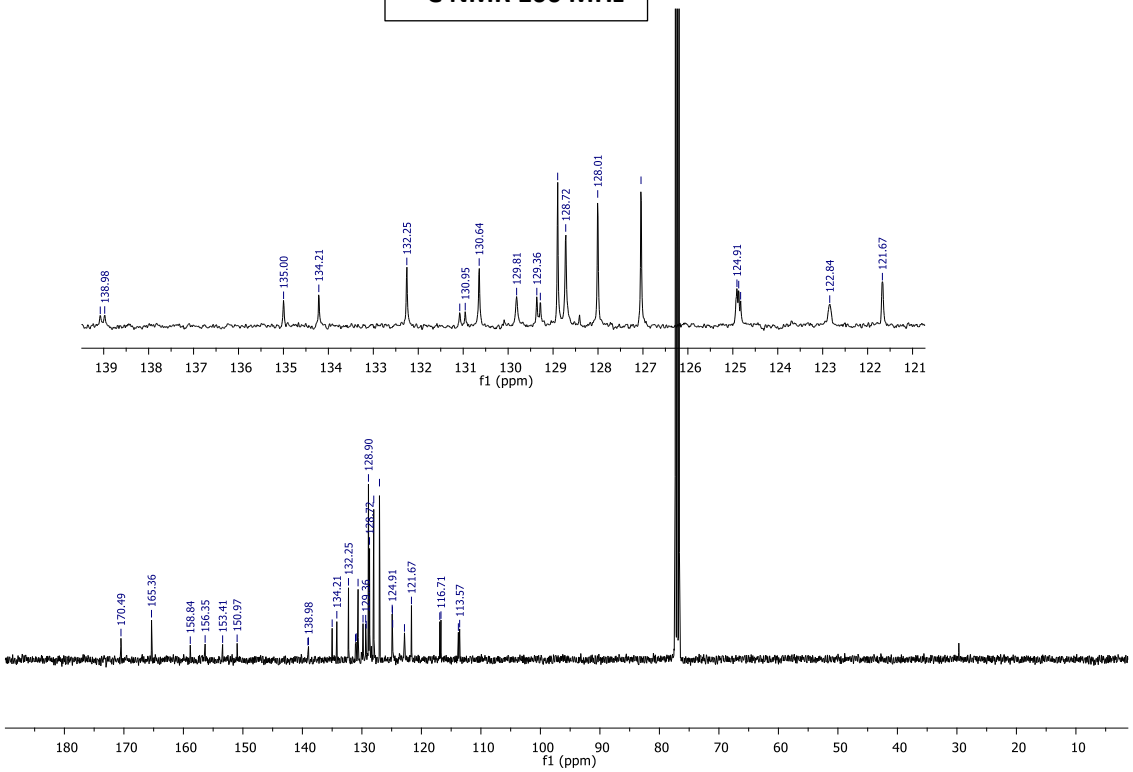
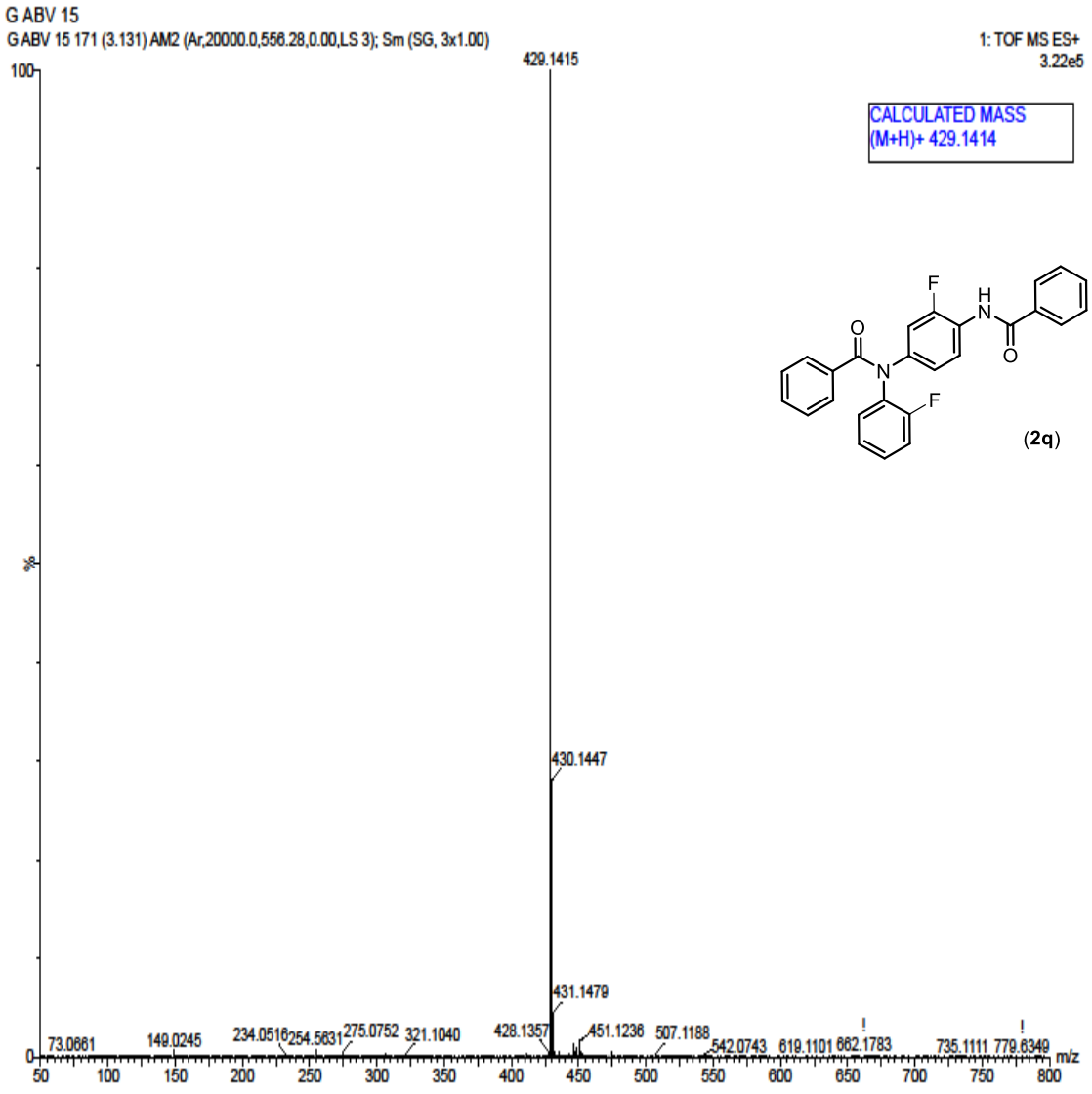
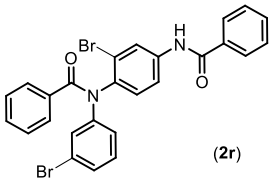


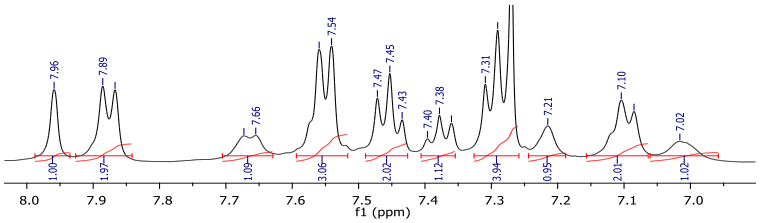
ESI-HRMS Chromatogram

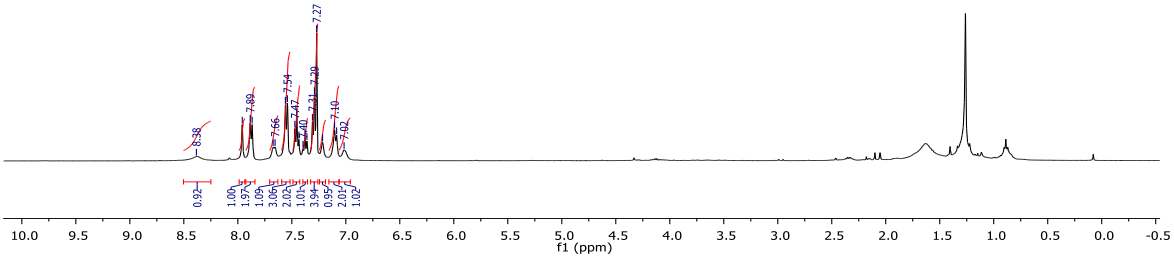


^{1}H NMR 400 MHz

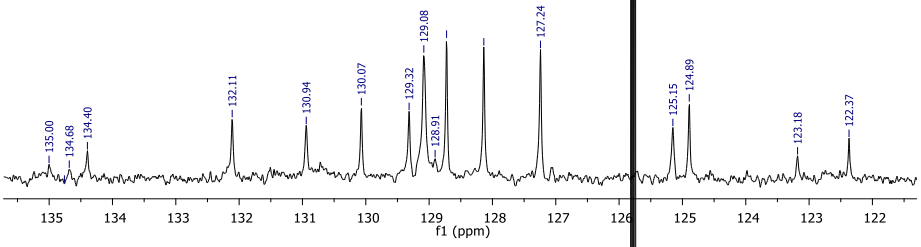


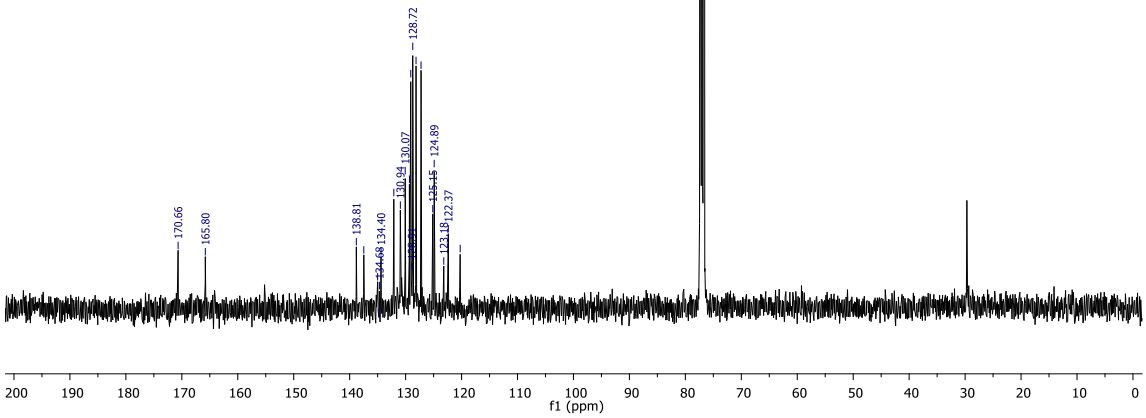
(**2r**)



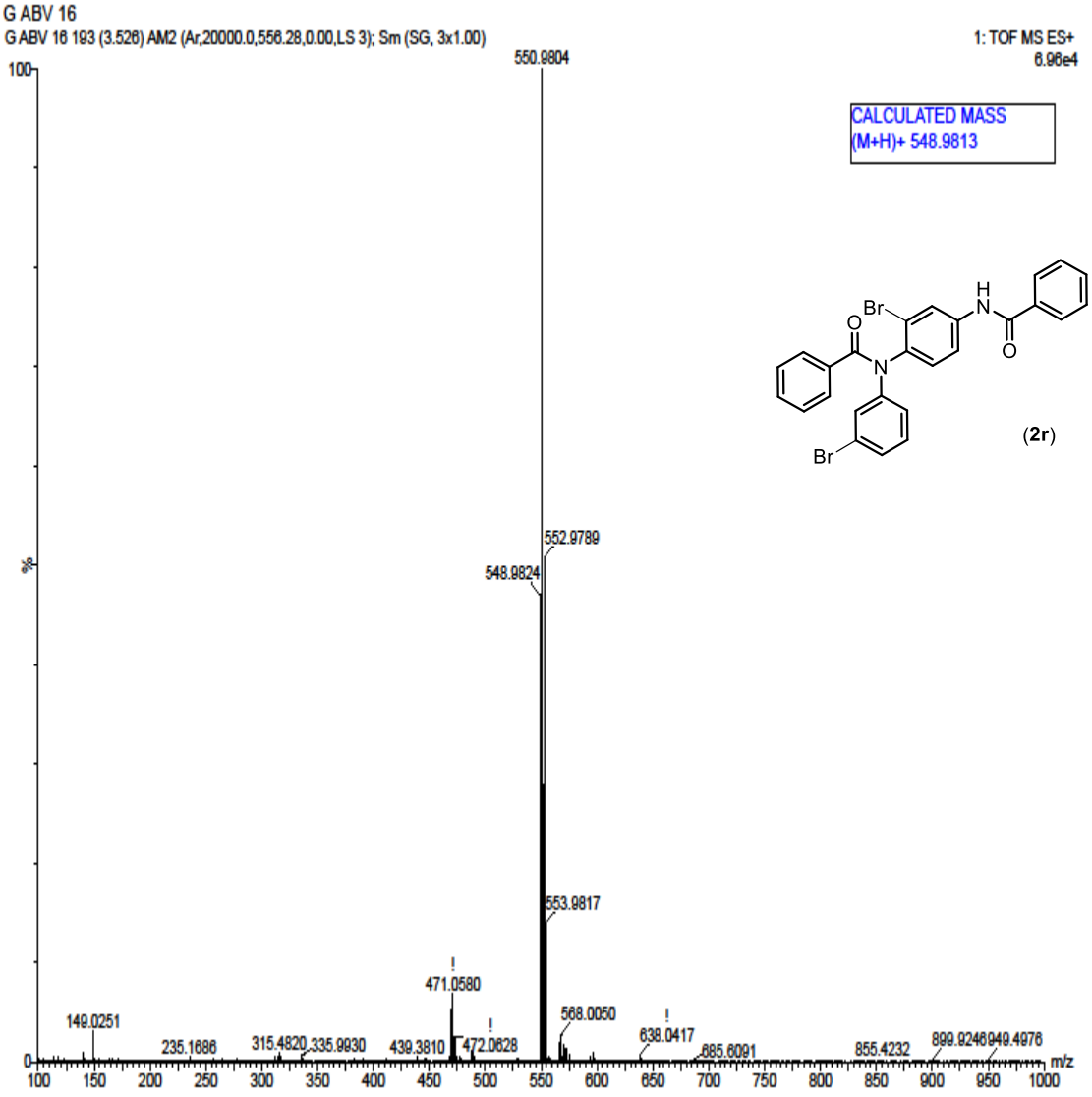


^{13}C NMR 100 MHz

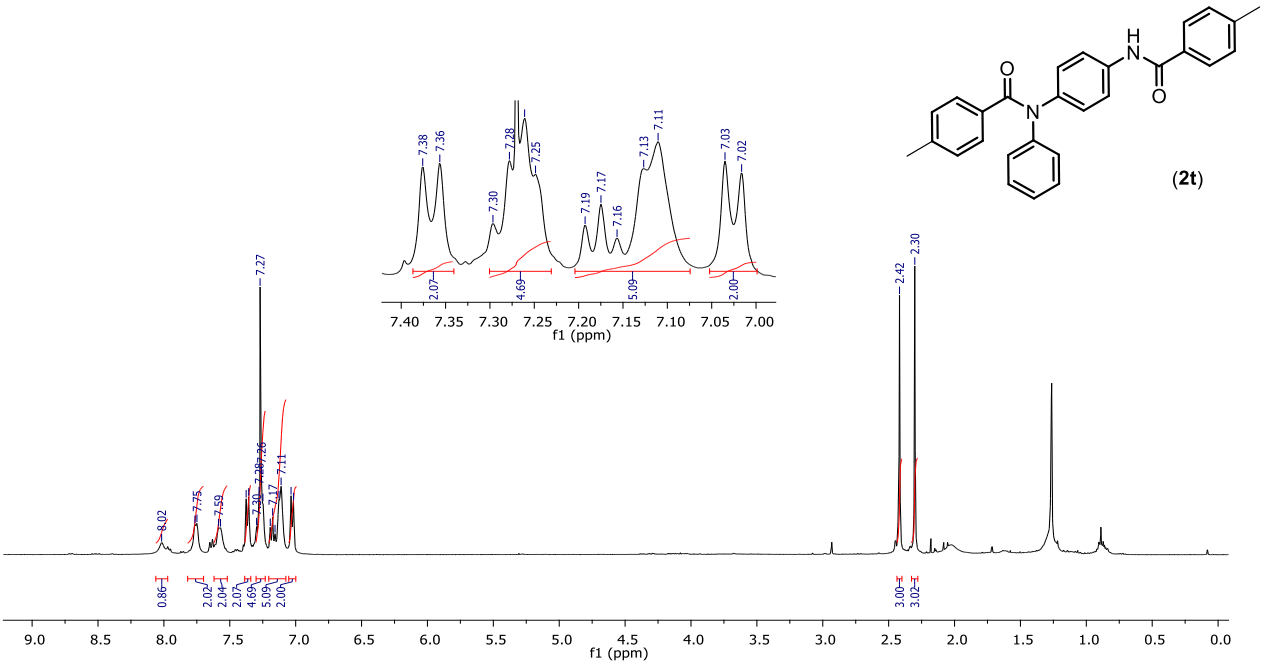




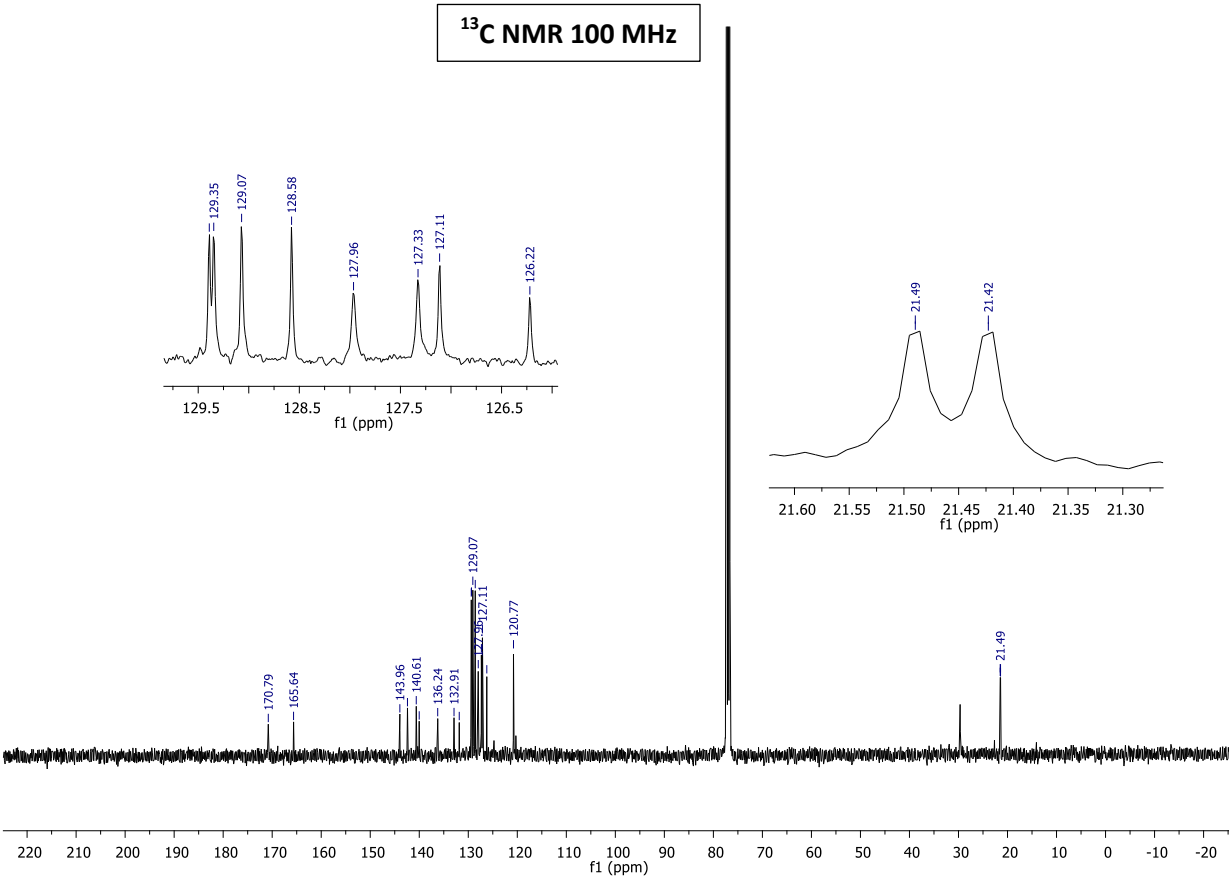
ESI-HRMS Chromatogram



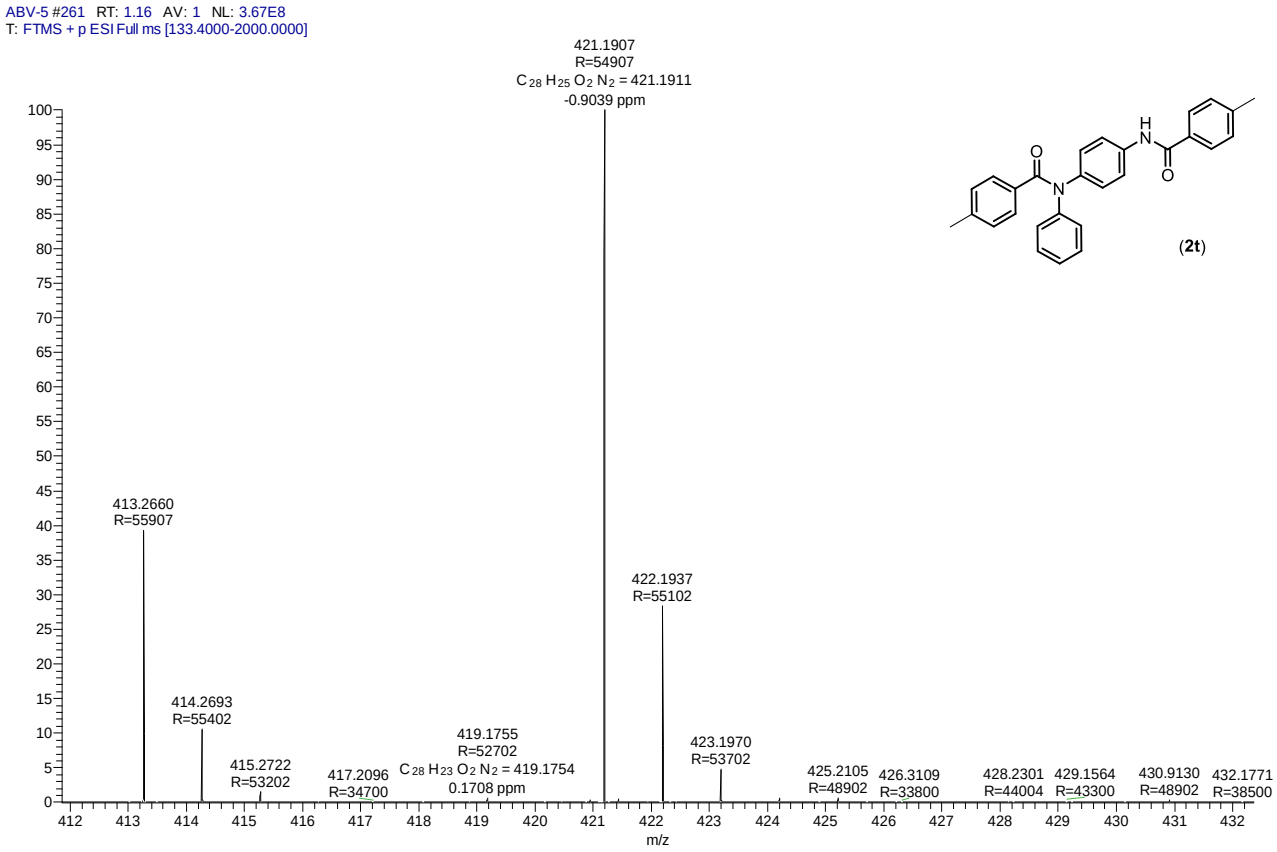
^{1}H NMR 400 MHz



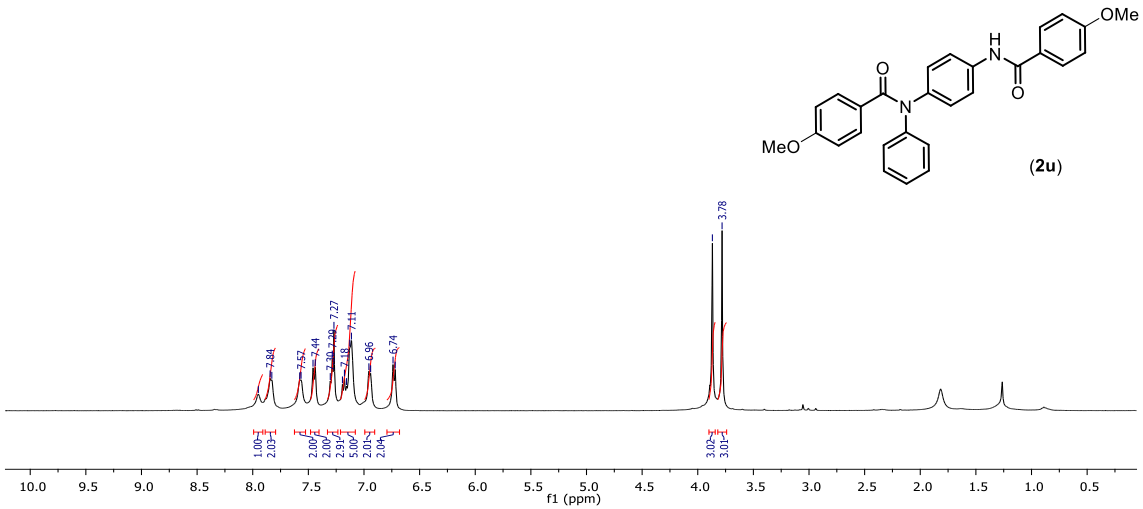
^{13}C NMR 100 MHz



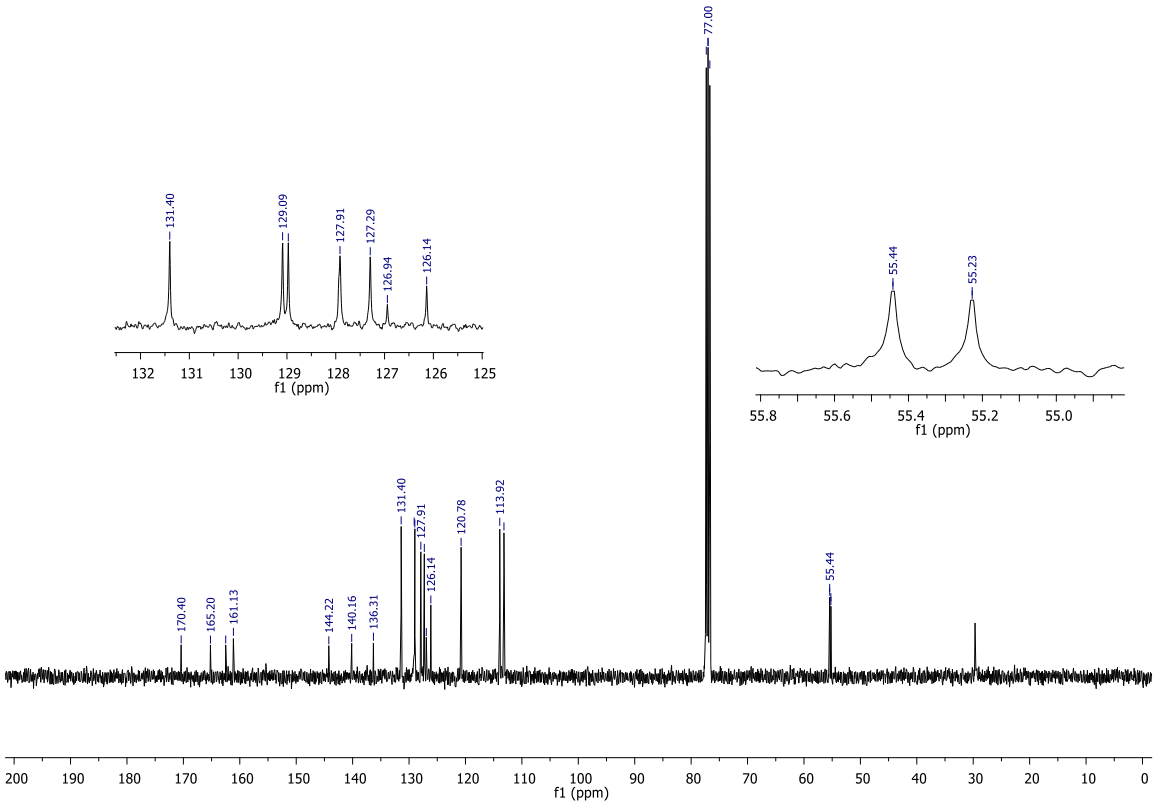
ESI-HRMS Chromatogram



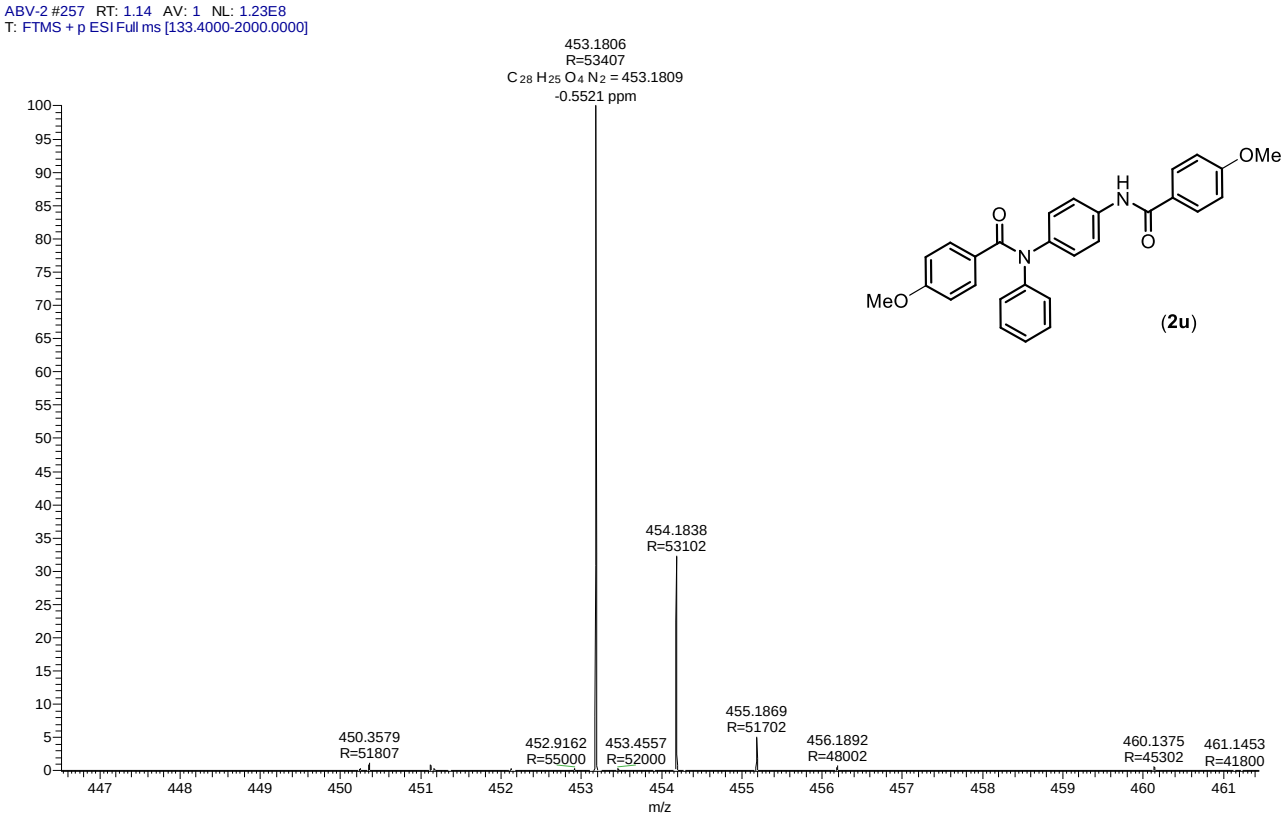
^{1}H NMR 400 MHz



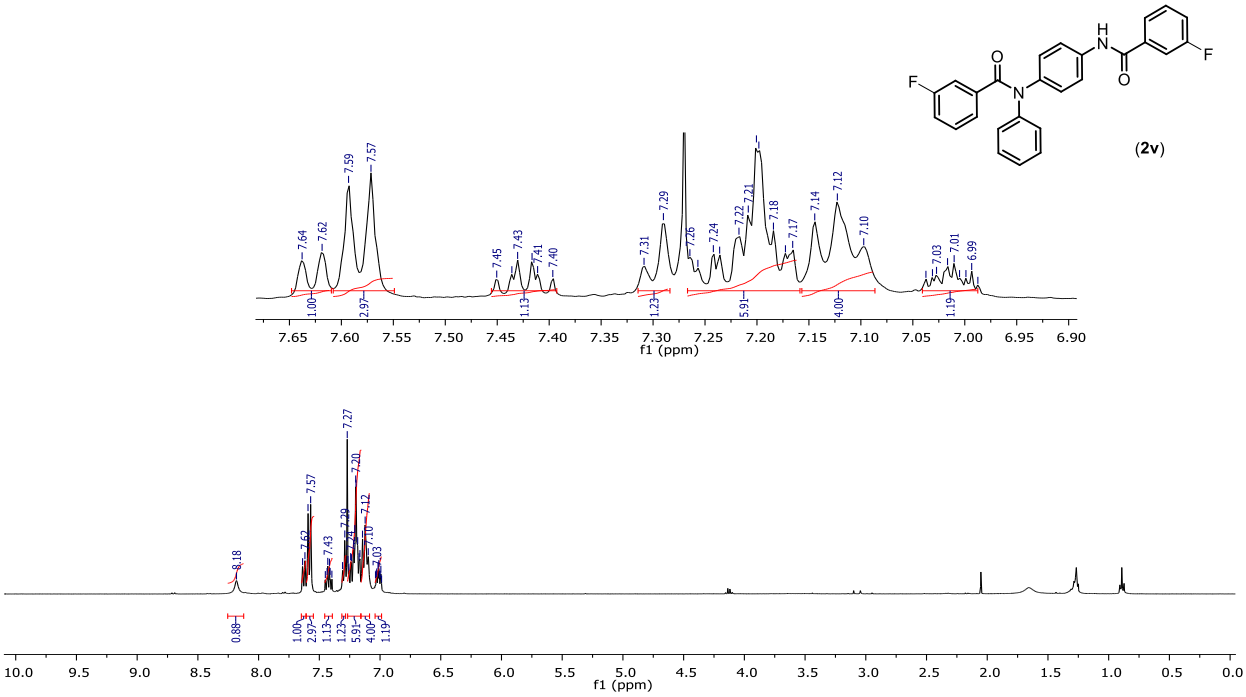
^{13}C NMR 100 MHz



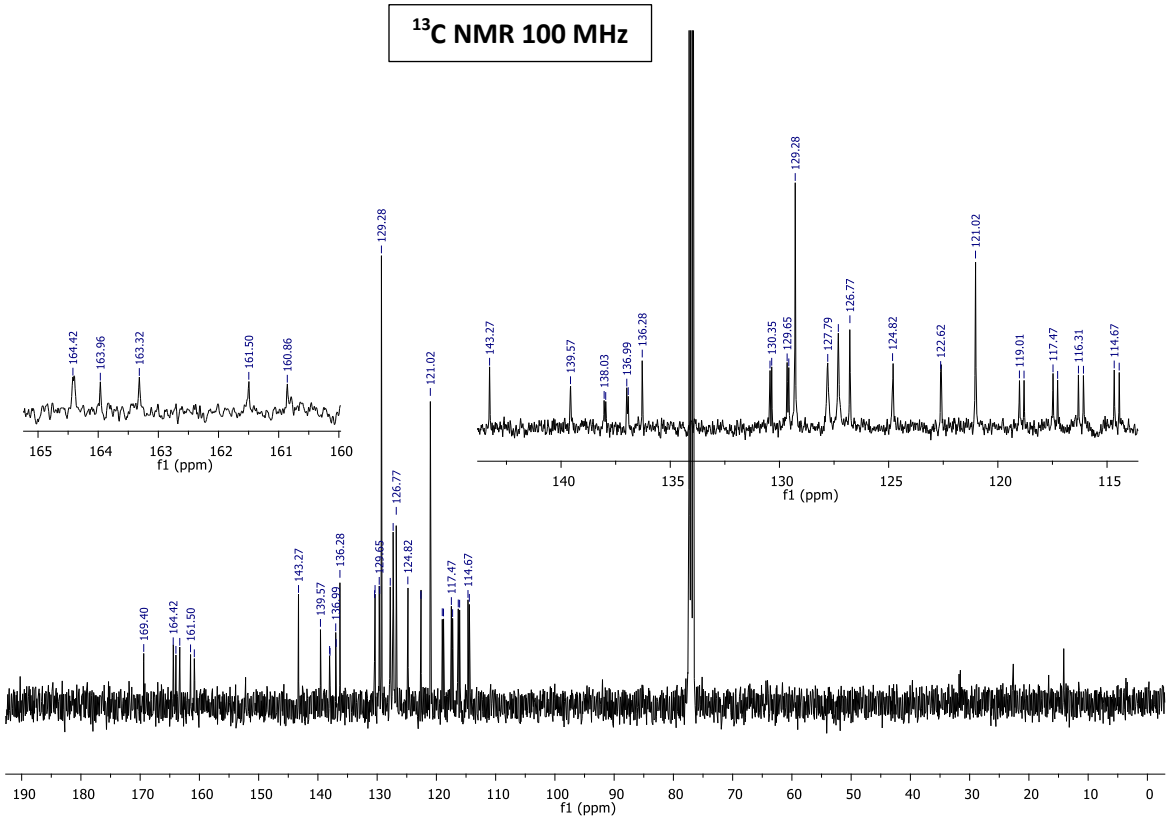
ESI-HRMS Chromatogram



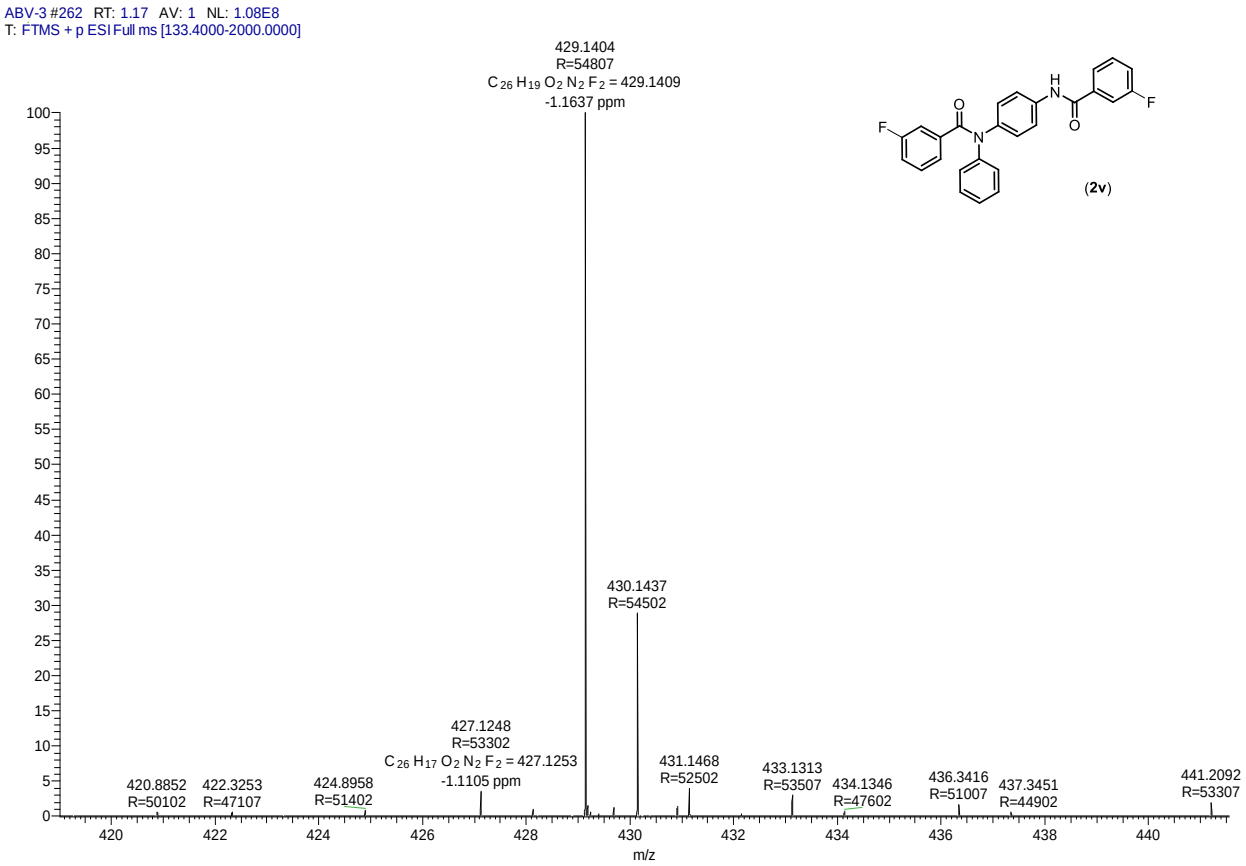
^{1}H NMR 400 MHz



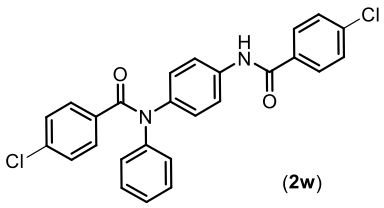
^{13}C NMR 100 MHz



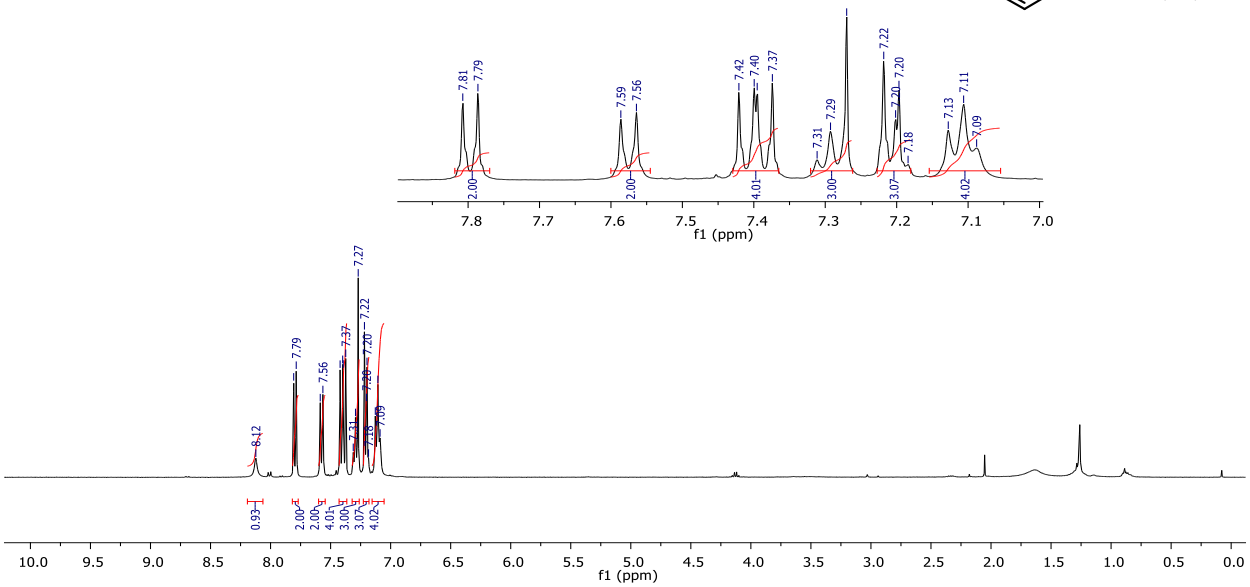
ESI-HRMS Chromatogram



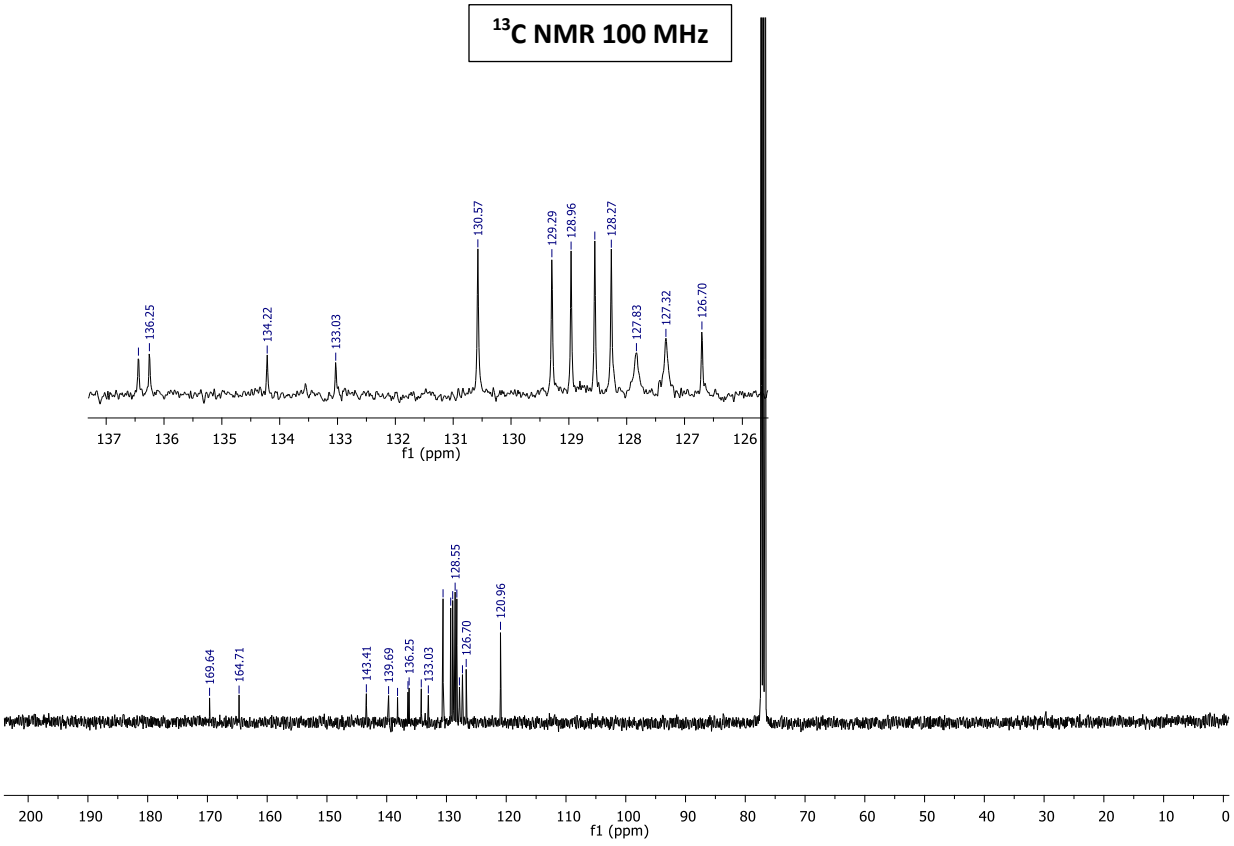
^{1}H NMR 400 MHz



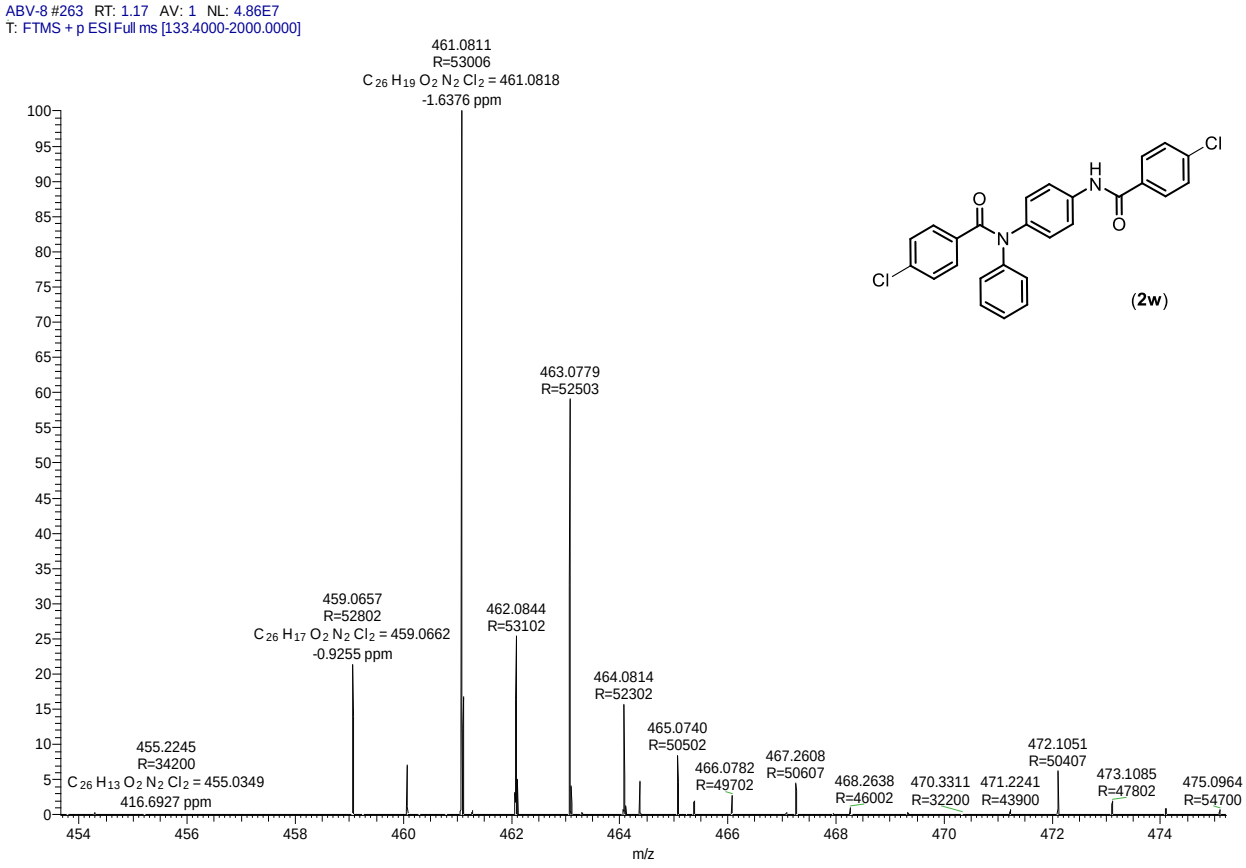
(**2w**)



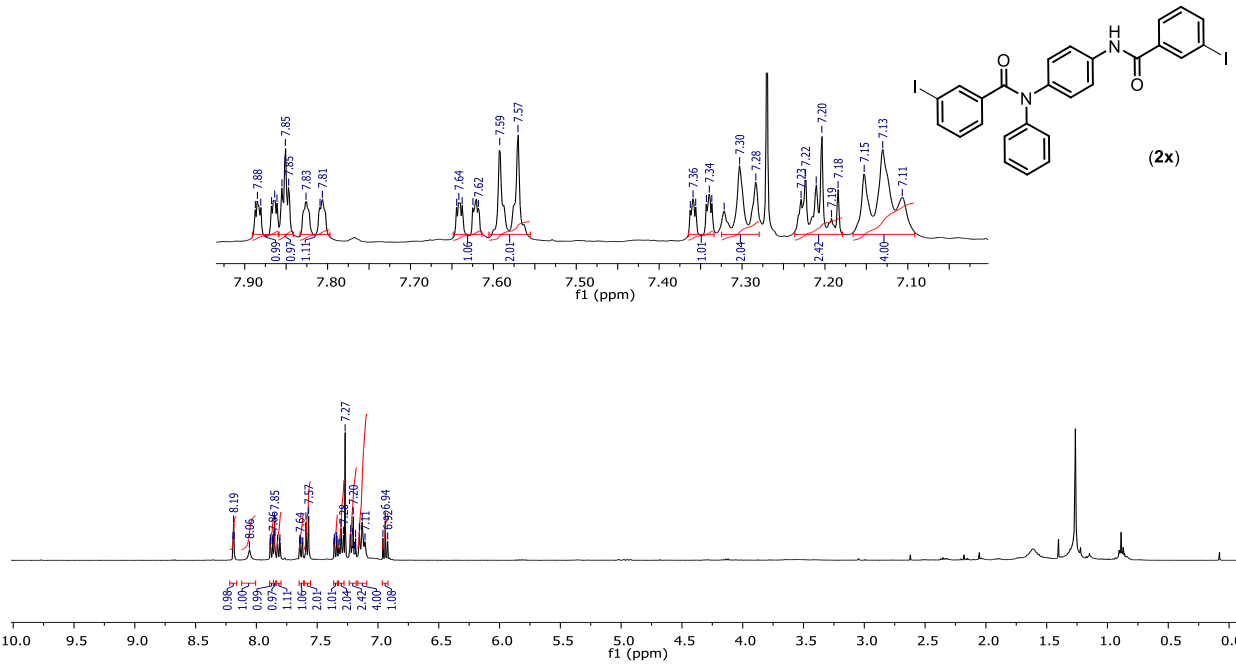
^{13}C NMR 100 MHz



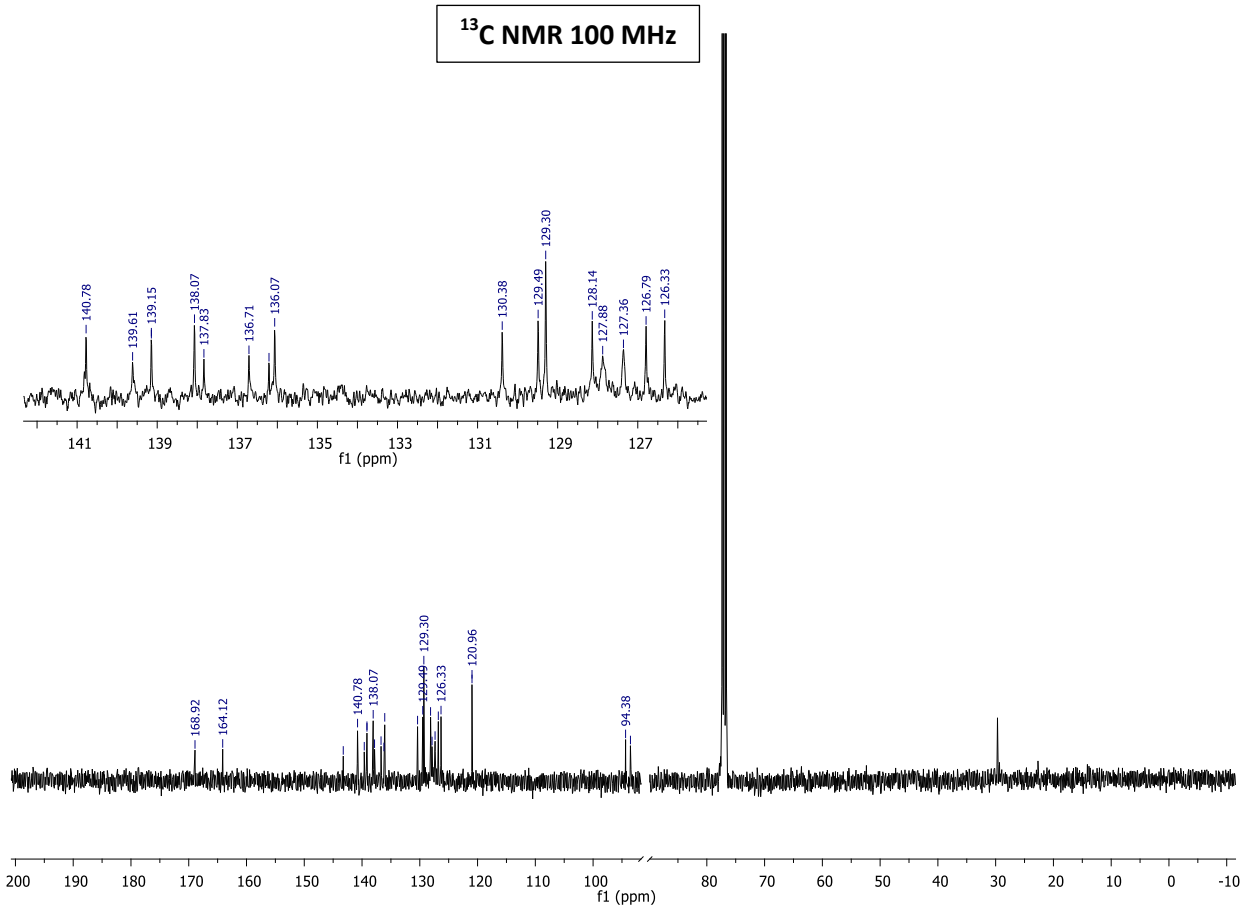
ESI-HRMS Chromatogram



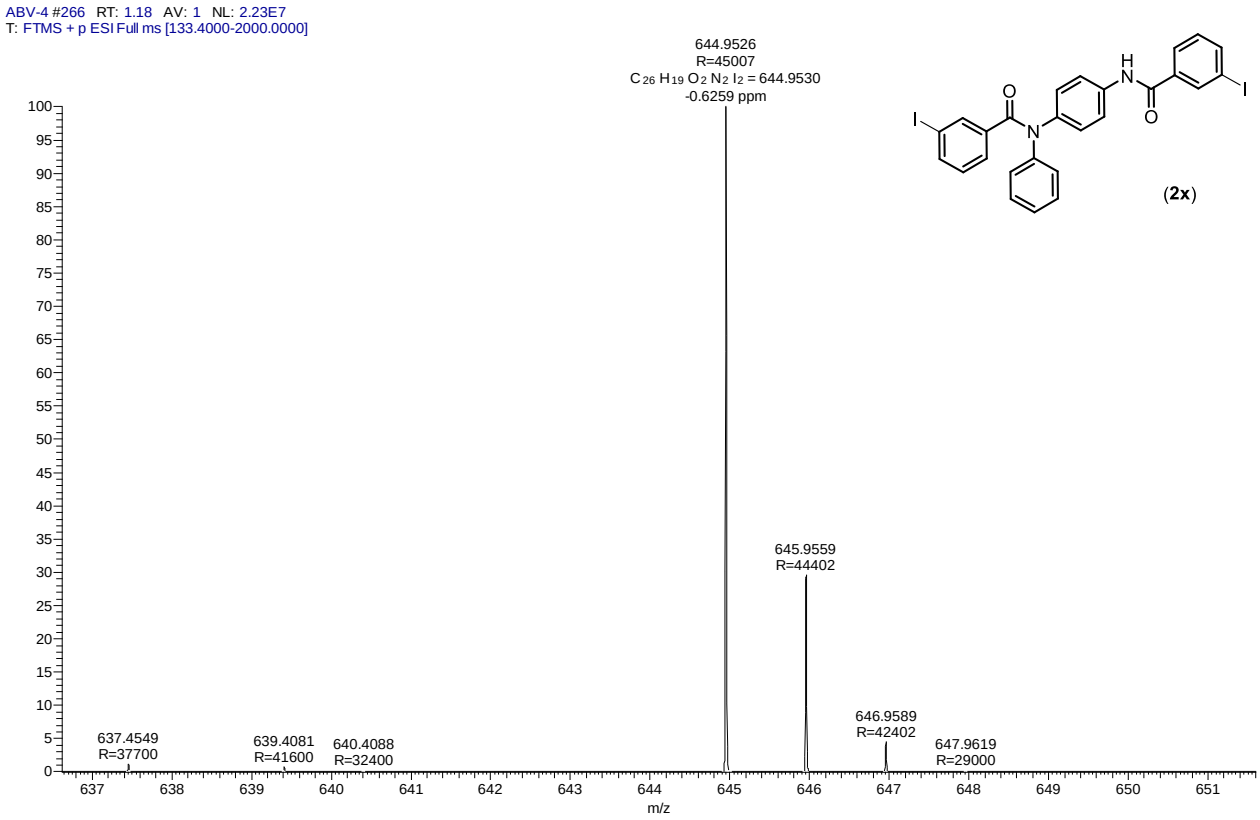
^{1}H NMR 400 MHz



^{13}C NMR 100 MHz



ESI-HRMS Chromatogram



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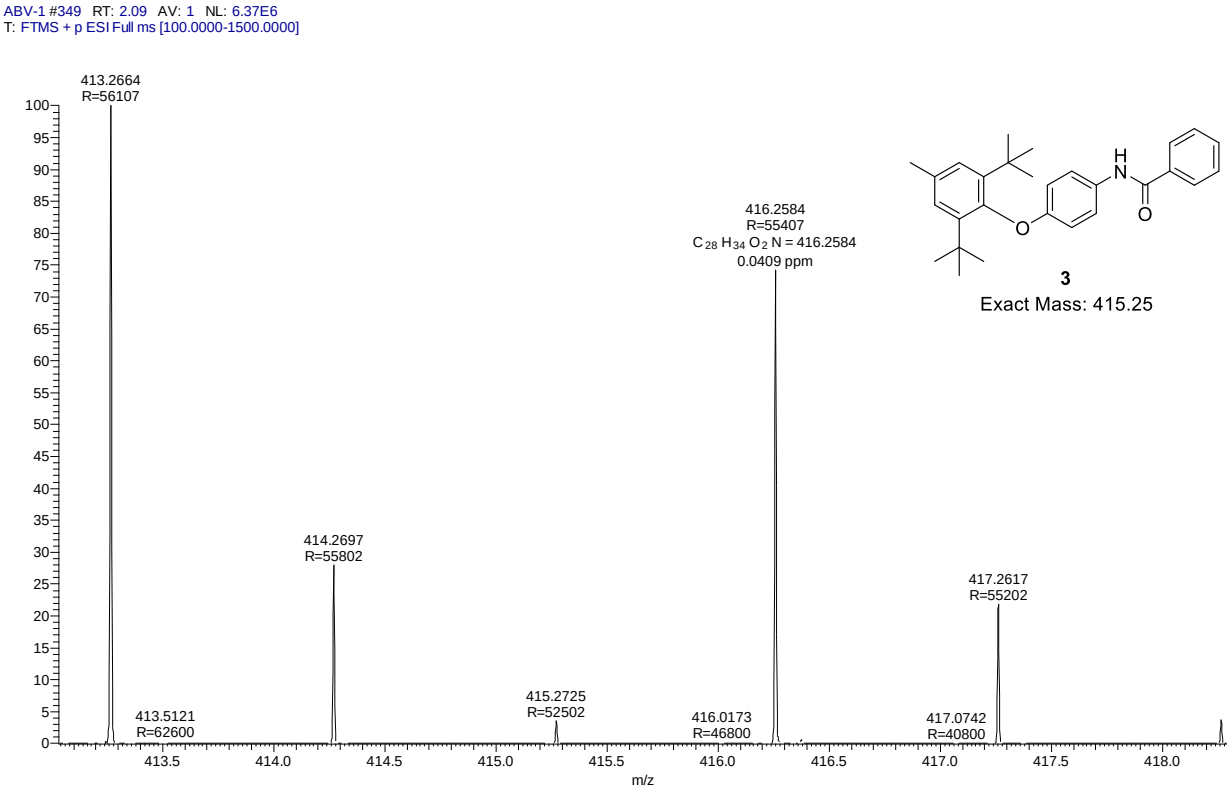
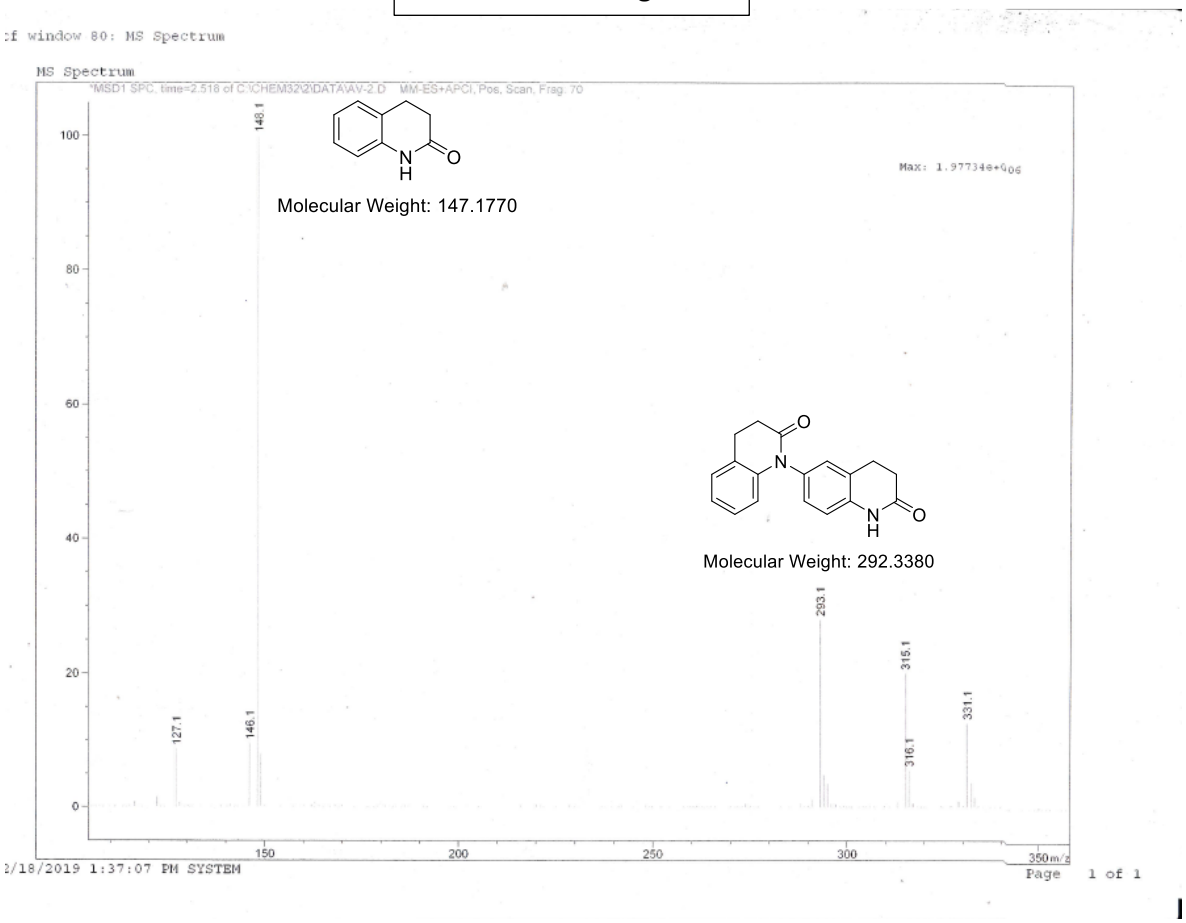
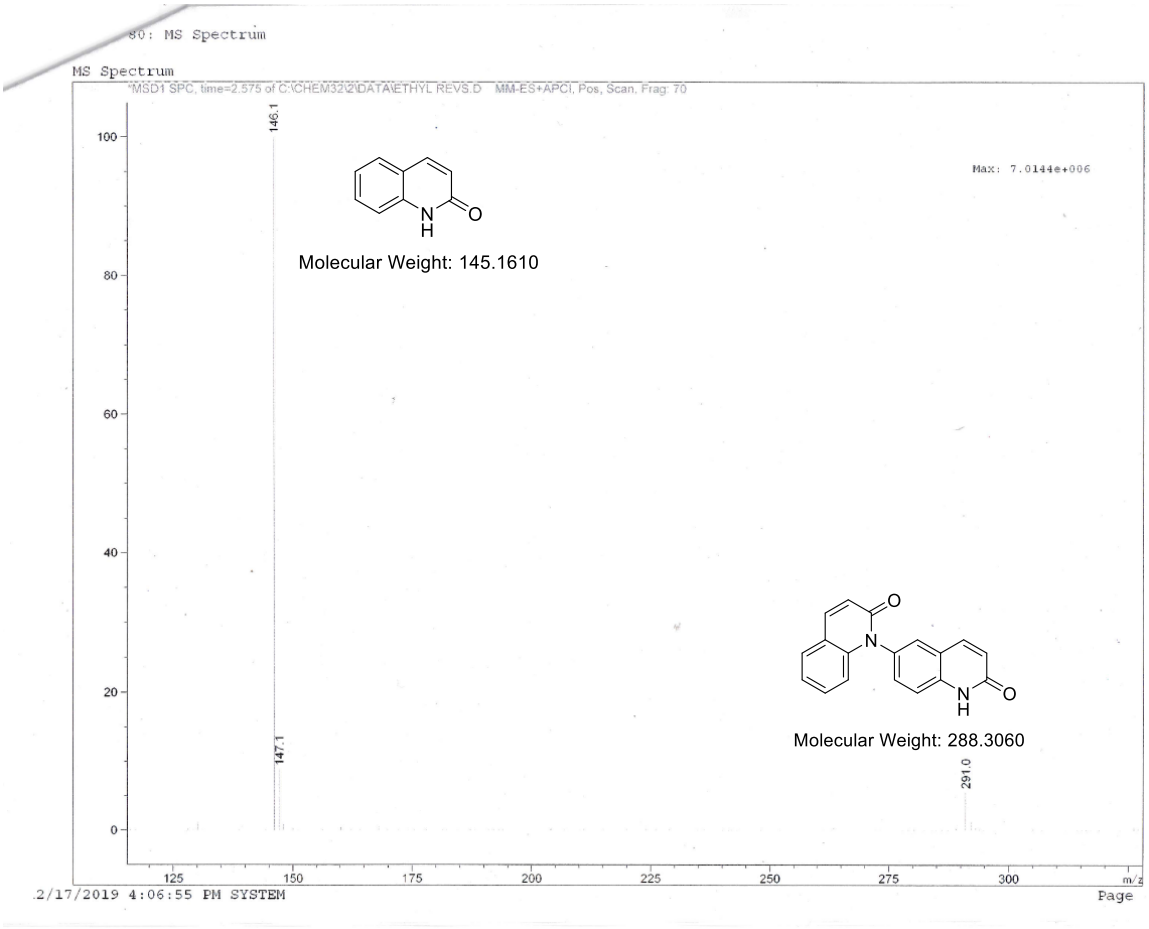


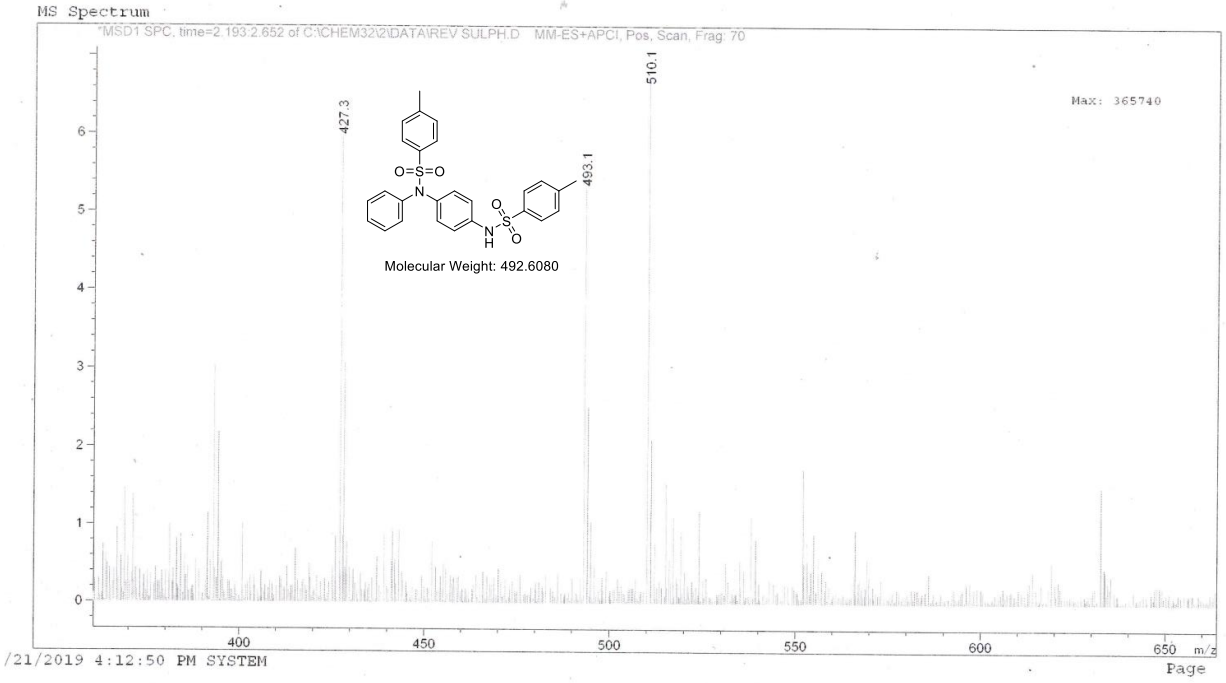
LCMS Chromatogram



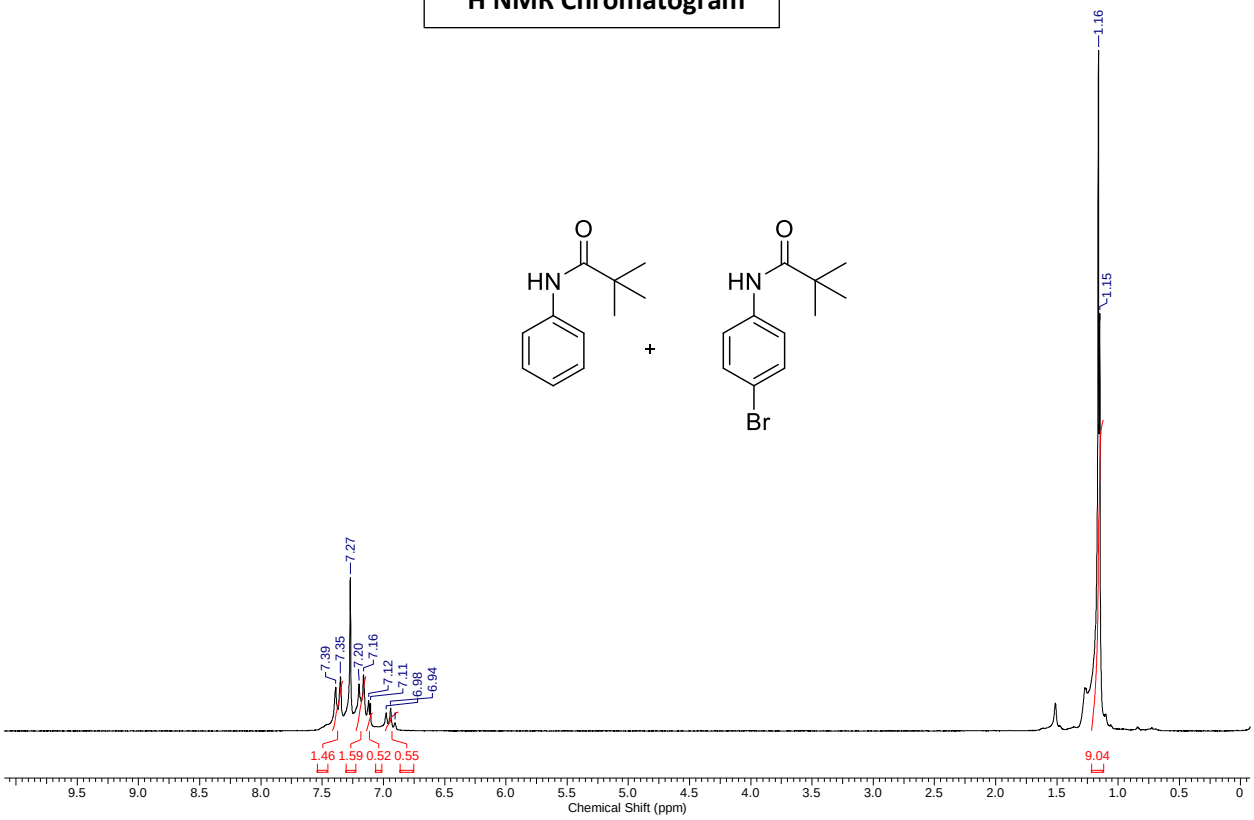
LCMS Chromatogram



LCMS Chromatogram



^{1}H NMR Chromatogram



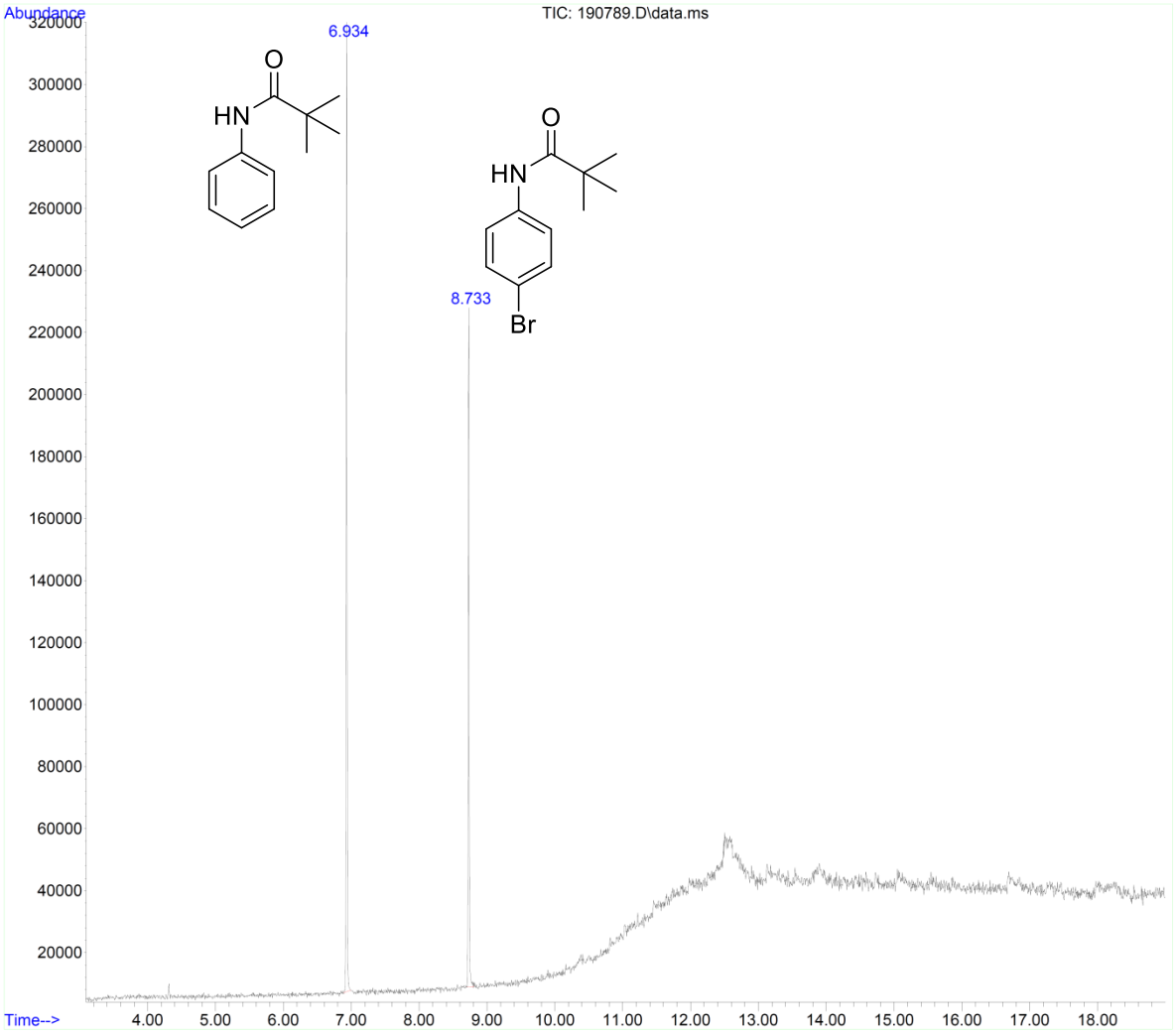
GC Chromatogram

```
  Acq On    : 25 Nov 2019  12:30
  Operator  :
  Sample    : ABV-1
  Misc      :
  ALS Vial  : 2   Sample Multiplier: 1

  Integration Parameters: autoint1.e
  Integrator: ChemStation

  Method    : D:\NCL\DATA\OCD\Year_2019\1PPM.D\SDP_Jan2019.M
  Title     :

  Signal     : TIC: 190789.D\data.ms
```

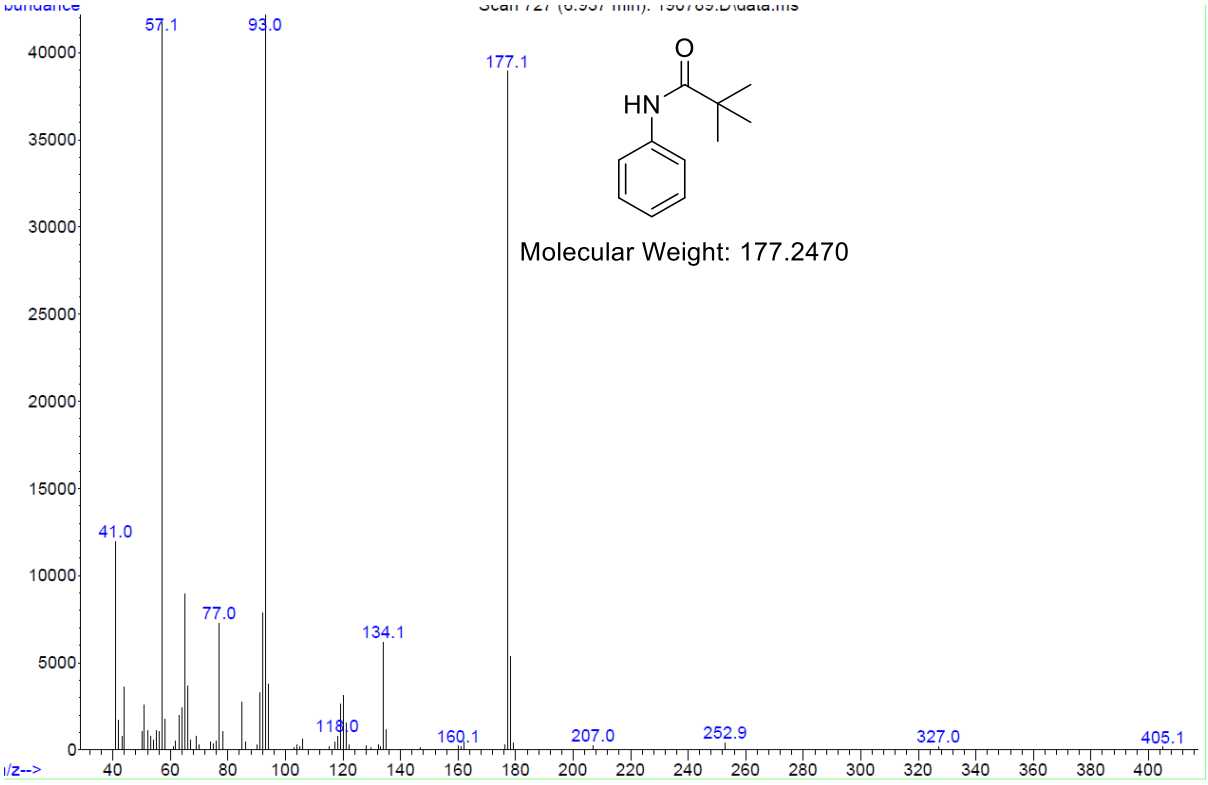
peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	6.934	718	726	737	BB	294213	2923095	100.00%	57.627%
2	8.733	1061	1066	1079	BV	210770	2149386	73.53%	42.373%

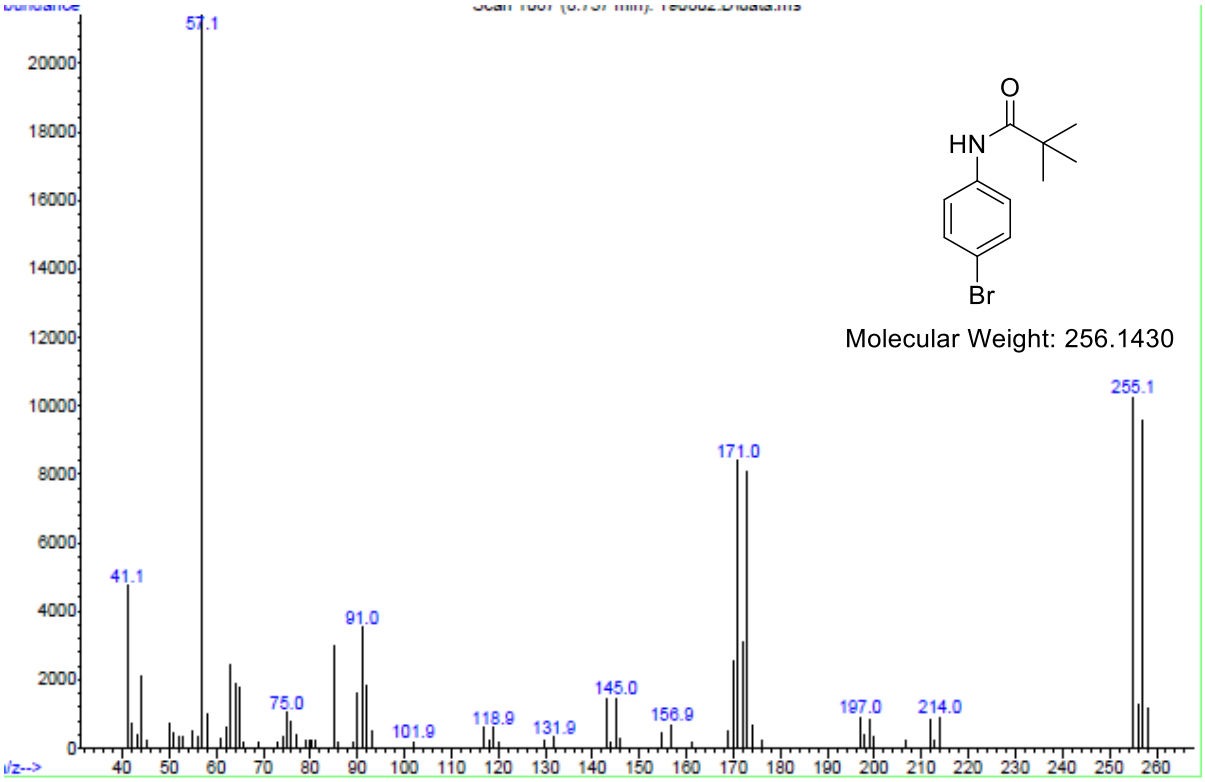
Sum of corrected areas: 5072480

SDP_Jan2019.M Tue Nov 26 19:01:42 2019



GCMS Chromatogram





6. X-ray data:

X-ray intensity data measurements of compounds **Amol_Vivek** (**2a**) and **Amol_2R** (**2m**) were carried out on a Bruker D8 VENTURE Kappa Duo PHOTON II CPAD diffractometer equipped with Incoatech multilayer mirrors optics. The intensity measurements were carried out with Mo micro-focus sealed tube diffraction source (Mo-Kα = 0.71073 Å) at 100(2) K temperature. The X-ray generator was operated at 50 kV and 1.4 mA. A preliminary set of cell constants and an orientation matrix were calculated from three sets of 12 frames for Mo radiations. Data were collected with φ and ω scan width of 0.5º at different settings of φ, ω and θ with a frame time of 10-20 sec keeping the sample-to-detector distance fixed at 5.00 cm. The X-ray data collection was monitored by APEX3 program (Bruker, 2016). All the data were corrected for Lorentzian, polarization and absorption effects using SAINT and SADABS programs (Bruker, 2016). Using APEX3 (Bruker) program suite, the structure was solved with the ShelXS-97 (Sheldrick, 2008)[2] structure solution program, using direct methods. The model was refined with the version of ShelXL-2013 (Sheldrick, 2015)[3] using Least Squares minimization. All the hydrogen atoms were placed in a geometrically idealized position and constrained to ride on their parent atoms except N-H (N2-H2) proton in Amol_2R which has been located in the difference Fourier map and refined isotropically. An *ORTEP* III[4] view of compound was drawn at the 50% probability displacement ellipsoids, and H atoms are shown as small spheres of arbitrary radii.

Crystal data of Amol_Vivek (2a): $C_{22}H_{28}N_2O_2$, M = 352.46, colorless plate, 0.32 x 0.21 x 0.10 mm^3, monoclinic, space group $P2_1/c$, a = 18.3781(7) Å, b = 9.6218(4) Å, c = 11.0075(4) Å, V = 101.862(2) $Å^3$, Z = 4, T = 100(2) K, λ = 0.71073 Å, $2\theta_{max}$ = 52.00°, D_{calc} (g cm^{-3}) = 1.229, $F(000)$ = 760, μ(mm^{-1}) = 0.079, 31398 reflections collected, 3721 unique reflections (R_{int} = 0.0661, $Rsig$ = 0.0451), 2813 observed ($I > 2\sigma(I)$) reflections, multi-scan absorption correction, T_{min} = 0.975, T_{max} = 0.992, 241 refined parameters, Good of Fit = S = 1.018, $R1$ = 0.0473, $wR2$ = 0.0965 (all data R = 0.0715, $wR2$ = 0.1065), maximum and minimum residual electron densities; $\Delta\rho_{max}$ = 0.270, $\Delta\rho_{min}$ = -0.209 ($eÅ^{-3}$).

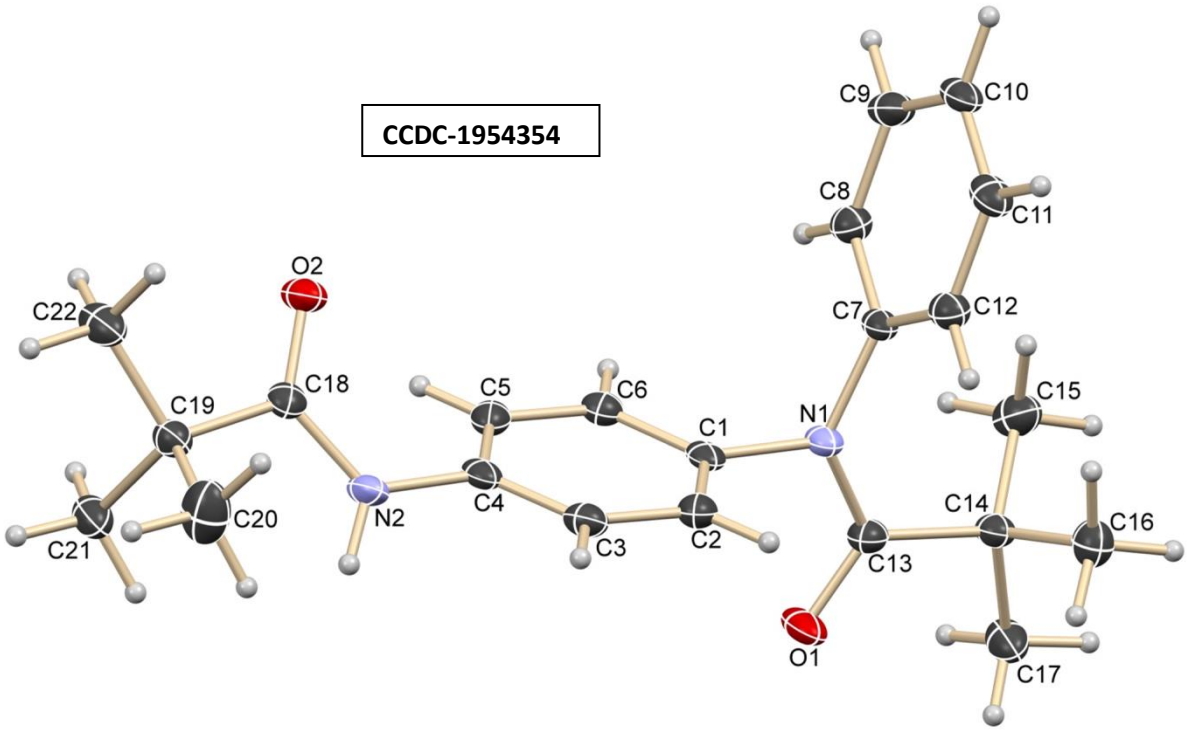


Table 1. Crystal data and structure refinement for AMOL (**2a**).

Identification code	AMOL
Empirical formula	C22 H28 N2 O2
Formula weight	352.46
Temperature	100(2) K
Wavelength	0.71073 Å

Crystal system	Monoclinic	
Space group	$P2_1/c$	
Unit cell dimensions	a = 18.3781(7) Å	α= 90°.
	b = 9.6218(4) Å	β= 101.862(2)°.
	c = 11.0075(4) Å	γ = 90°.
Volume	1904.89(13) $Å^3$	
Z	4	
Density (calculated)	1.229 Mg/m^3	
Absorption coefficient	0.079 mm^{-1}	
F(000)	760	
Crystal size	0.320 x 0.210 x 0.100 mm^3	
Theta range for data collection	2.265 to 26.000°.	
Index ranges	-22<=h<=22, -11<=k<=11, -13<=l<=13	
Reflections collected	31398	
Independent reflections	3721 [R(int) = 0.0661]	
Completeness to theta = 25.242°	99.4 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.992 and 0.975	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3721 / 0 / 241	
Goodness-of-fit on F^2	1.018	
Final R indices [I>2sigma(I)]	R1 = 0.0473, wR2 = 0.0965	
R indices (all data)	R1 = 0.0715, wR2 = 0.1065	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.270 and -0.209 $e.Å^{-3}$	

Table 2. Bond lengths [Å] and angles [°] for AMOL.

O(1)-C(13)	1.2231(19)
O(2)-C(18)	1.2304(19)
N(1)-C(13)	1.379(2)
N(1)-C(7)	1.449(2)
N(1)-C(1)	1.458(2)
N(2)-C(18)	1.356(2)
N(2)-C(4)	1.427(2)
N(2)-H(2N)	0.8800
C(1)-C(2)	1.384(2)
C(1)-C(6)	1.385(2)
C(2)-C(3)	1.385(2)
C(2)-H(2)	0.9500
C(3)-C(4)	1.388(2)
C(3)-H(3)	0.9500
C(4)-C(5)	1.384(2)
C(5)-C(6)	1.384(2)
C(5)-H(5)	0.9500
C(6)-H(6)	0.9500
C(7)-C(12)	1.386(2)
C(7)-C(8)	1.386(2)
C(8)-C(9)	1.391(2)
C(8)-H(8)	0.9500
C(9)-C(10)	1.384(2)
C(9)-H(9)	0.9500
C(10)-C(11)	1.382(2)
C(10)-H(10)	0.9500
C(11)-C(12)	1.391(2)
C(11)-H(11)	0.9500
C(12)-H(12)	0.9500
C(13)-C(14)	1.546(2)
C(14)-C(17)	1.530(2)
C(14)-C(16)	1.533(2)
C(14)-C(15)	1.535(2)
C(15)-H(15A)	0.9800

C(15)-H(15B)	0.9800
C(15)-H(15C)	0.9800
C(16)-H(16A)	0.9800
C(16)-H(16B)	0.9800
C(16)-H(16C)	0.9800
C(17)-H(17A)	0.9800
C(17)-H(17B)	0.9800
C(17)-H(17C)	0.9800
C(18)-C(19)	1.536(2)
C(19)-C(22)	1.528(2)
C(19)-C(20)	1.532(2)
C(19)-C(21)	1.533(2)
C(20)-H(20A)	0.9800
C(20)-H(20B)	0.9800
C(20)-H(20C)	0.9800
C(21)-H(21A)	0.9800
C(21)-H(21B)	0.9800
C(21)-H(21C)	0.9800
C(22)-H(22A)	0.9800
C(22)-H(22B)	0.9800
C(22)-H(22C)	0.9800

C(13)-N(1)-C(7)	129.36(13)
C(13)-N(1)-C(1)	117.84(13)
C(7)-N(1)-C(1)	112.80(12)
C(18)-N(2)-C(4)	124.97(14)
C(18)-N(2)-H(2N)	117.5
C(4)-N(2)-H(2N)	117.5
C(2)-C(1)-C(6)	119.95(15)
C(2)-C(1)-N(1)	119.89(14)
C(6)-C(1)-N(1)	120.04(15)
C(1)-C(2)-C(3)	119.90(15)
C(1)-C(2)-H(2)	120.0
C(3)-C(2)-H(2)	120.0
C(2)-C(3)-C(4)	120.23(16)
C(2)-C(3)-H(3)	119.9

C(4)-C(3)-H(3)	119.9
C(5)-C(4)-C(3)	119.65(15)
C(5)-C(4)-N(2)	122.04(14)
C(3)-C(4)-N(2)	118.27(15)
C(4)-C(5)-C(6)	120.16(15)
C(4)-C(5)-H(5)	119.9
C(6)-C(5)-H(5)	119.9
C(5)-C(6)-C(1)	120.10(15)
C(5)-C(6)-H(6)	120.0
C(1)-C(6)-H(6)	120.0
C(12)-C(7)-C(8)	119.88(15)
C(12)-C(7)-N(1)	119.98(14)
C(8)-C(7)-N(1)	119.67(14)
C(7)-C(8)-C(9)	120.05(16)
C(7)-C(8)-H(8)	120.0
C(9)-C(8)-H(8)	120.0
C(10)-C(9)-C(8)	120.07(16)
C(10)-C(9)-H(9)	120.0
C(8)-C(9)-H(9)	120.0
C(11)-C(10)-C(9)	119.80(16)
C(11)-C(10)-H(10)	120.1
C(9)-C(10)-H(10)	120.1
C(10)-C(11)-C(12)	120.34(16)
C(10)-C(11)-H(11)	119.8
C(12)-C(11)-H(11)	119.8
C(7)-C(12)-C(11)	119.85(16)
C(7)-C(12)-H(12)	120.1
C(11)-C(12)-H(12)	120.1
O(1)-C(13)-N(1)	118.52(15)
O(1)-C(13)-C(14)	120.22(14)
N(1)-C(13)-C(14)	121.24(14)
C(17)-C(14)-C(16)	107.32(14)
C(17)-C(14)-C(15)	108.04(14)
C(16)-C(14)-C(15)	110.66(14)
C(17)-C(14)-C(13)	107.48(13)
C(16)-C(14)-C(13)	109.31(14)

C(15)-C(14)-C(13)	113.77(13)
C(14)-C(15)-H(15A)	109.5
C(14)-C(15)-H(15B)	109.5
H(15A)-C(15)-H(15B)	109.5
C(14)-C(15)-H(15C)	109.5
H(15A)-C(15)-H(15C)	109.5
H(15B)-C(15)-H(15C)	109.5
C(14)-C(16)-H(16A)	109.5
C(14)-C(16)-H(16B)	109.5
H(16A)-C(16)-H(16B)	109.5
C(14)-C(16)-H(16C)	109.5
H(16A)-C(16)-H(16C)	109.5
H(16B)-C(16)-H(16C)	109.5
C(14)-C(17)-H(17A)	109.5
C(14)-C(17)-H(17B)	109.5
H(17A)-C(17)-H(17B)	109.5
C(14)-C(17)-H(17C)	109.5
H(17A)-C(17)-H(17C)	109.5
H(17B)-C(17)-H(17C)	109.5
O(2)-C(18)-N(2)	121.62(15)
O(2)-C(18)-C(19)	122.64(14)
N(2)-C(18)-C(19)	115.74(14)
C(22)-C(19)-C(20)	109.00(15)
C(22)-C(19)-C(21)	109.72(14)
C(20)-C(19)-C(21)	109.13(15)
C(22)-C(19)-C(18)	109.12(13)
C(20)-C(19)-C(18)	111.42(14)
C(21)-C(19)-C(18)	108.44(13)
C(19)-C(20)-H(20A)	109.5
C(19)-C(20)-H(20B)	109.5
H(20A)-C(20)-H(20B)	109.5
C(19)-C(20)-H(20C)	109.5
H(20A)-C(20)-H(20C)	109.5
H(20B)-C(20)-H(20C)	109.5
C(19)-C(21)-H(21A)	109.5
C(19)-C(21)-H(21B)	109.5

H(21A)-C(21)-H(21B)	109.5
C(19)-C(21)-H(21C)	109.5
H(21A)-C(21)-H(21C)	109.5
H(21B)-C(21)-H(21C)	109.5
C(19)-C(22)-H(22A)	109.5
C(19)-C(22)-H(22B)	109.5
H(22A)-C(22)-H(22B)	109.5
C(19)-C(22)-H(22C)	109.5
H(22A)-C(22)-H(22C)	109.5
H(22B)-C(22)-H(22C)	109.5

Symmetry transformations used to generate equivalent atoms:

Table 3. Torsion angles [°] for AMOL.

C(13)-N(1)-C(1)-C(2)	86.57(19)
C(7)-N(1)-C(1)-C(2)	-92.74(17)
C(13)-N(1)-C(1)-C(6)	-97.34(18)
C(7)-N(1)-C(1)-C(6)	83.36(18)
C(6)-C(1)-C(2)-C(3)	1.0(2)
N(1)-C(1)-C(2)-C(3)	177.10(14)
C(1)-C(2)-C(3)-C(4)	-0.3(2)
C(2)-C(3)-C(4)-C(5)	-0.4(2)
C(2)-C(3)-C(4)-N(2)	177.33(15)
C(18)-N(2)-C(4)-C(5)	-53.3(2)
C(18)-N(2)-C(4)-C(3)	129.04(17)
C(3)-C(4)-C(5)-C(6)	0.2(2)
N(2)-C(4)-C(5)-C(6)	-177.37(15)
C(4)-C(5)-C(6)-C(1)	0.5(2)
C(2)-C(1)-C(6)-C(5)	-1.1(2)
N(1)-C(1)-C(6)-C(5)	-177.23(14)
C(13)-N(1)-C(7)-C(12)	-92.7(2)
C(1)-N(1)-C(7)-C(12)	86.45(17)
C(13)-N(1)-C(7)-C(8)	95.1(2)
C(1)-N(1)-C(7)-C(8)	-85.74(18)
C(12)-C(7)-C(8)-C(9)	-0.6(2)
N(1)-C(7)-C(8)-C(9)	171.61(15)
C(7)-C(8)-C(9)-C(10)	0.7(3)
C(8)-C(9)-C(10)-C(11)	0.1(2)
C(9)-C(10)-C(11)-C(12)	-1.1(2)
C(8)-C(7)-C(12)-C(11)	-0.4(2)
N(1)-C(7)-C(12)-C(11)	-172.55(15)
C(10)-C(11)-C(12)-C(7)	1.2(3)
C(7)-N(1)-C(13)-O(1)	-179.11(16)
C(1)-N(1)-C(13)-O(1)	1.7(2)
C(7)-N(1)-C(13)-C(14)	2.5(3)
C(1)-N(1)-C(13)-C(14)	-176.71(14)
O(1)-C(13)-C(14)-C(17)	9.6(2)
N(1)-C(13)-C(14)-C(17)	-172.04(15)

O(1)-C(13)-C(14)-C(16)	-106.61(18)
N(1)-C(13)-C(14)-C(16)	71.79(19)
O(1)-C(13)-C(14)-C(15)	129.13(17)
N(1)-C(13)-C(14)-C(15)	-52.5(2)
C(4)-N(2)-C(18)-O(2)	2.8(2)
C(4)-N(2)-C(18)-C(19)	-177.33(14)
O(2)-C(18)-C(19)-C(22)	-10.2(2)
N(2)-C(18)-C(19)-C(22)	169.89(14)
O(2)-C(18)-C(19)-C(20)	-130.60(17)
N(2)-C(18)-C(19)-C(20)	49.5(2)
O(2)-C(18)-C(19)-C(21)	109.27(17)
N(2)-C(18)-C(19)-C(21)	-70.63(18)

Symmetry transformations used to generate equivalent atoms:

Table 4. Hydrogen bonds for AMOL [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)

Crystal data of Amol_2R (2m): $C_{26}H_{20}N_2O_2$, M = 392.44, colorless plate, 0.21 x 0.15 x 0.09 mm^3, monoclinic, space group $P2_1/c$, a = 12.6898(9) Å, b = 8.3673(6) Å, c = 19.2488(12) Å, β = 106.184(2)°, V = 1962.8(2) $Å^3$, Z = 4, T = 100(2) K, λ = 0.71073 Å, $2\theta_{max}$ = 52.0°, D_{calc} (g cm^{-3}) = 1.328, $F(000)$ = 824, μ (mm^{-1}) = 0.085, 16767 reflections collected, 3847 unique reflections (R_{int} = 0.0566, *Rsig* = 0.0541), 3067 observed ($I > 2\sigma(I)$) reflections, multi-scan absorption correction, T_{min} = 0.982, T_{max} = 0.992, 275 refined parameters, Good of Fit = S = 1.169, $R1$ = 0.0801, $wR2$ = 0.1470 (all data R = 0.1024, $wR2$ = 0.1551), maximum and minimum residual electron densities; $\Delta\rho_{max}$ = 0.318, $\Delta\rho_{min}$ = -0.303 ($eÅ^{-3}$).

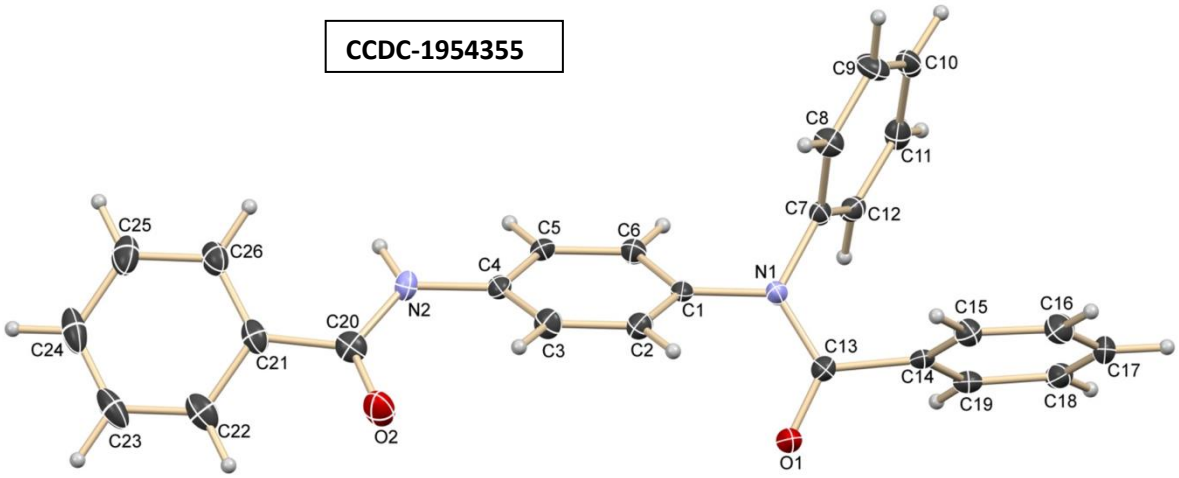


Table 1. Crystal data and structure refinement for mo_amol_2_r_0m_a. (**2m**)

Identification code	mo_amol_2_r_0m_a	
Empirical formula	C26 H20 N2 O2	
Formula weight	392.44	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1/c$	
Unit cell dimensions	a = 12.6898(9) Å	α= 90°.
	b = 8.3673(6) Å	β= 106.184(2)°.

	c = 19.2488(12) Å γ = 90°.
Volume	1962.8(2) $Å^3$
Z	4
Density (calculated)	1.328 Mg/m^3
Absorption coefficient	0.085 mm^{-1}
F(000)	824
Crystal size	0.210 x 0.150 x 0.090 mm^3
Theta range for data collection	2.672 to 25.997°.
Index ranges	-15<=h<=15, -10<=k<=10, -23<=l<=19
Reflections collected	16767
Independent reflections	3847 [R(int) = 0.0566]
Completeness to theta = 25.242°	99.7 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.992 and 0.982
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3847 / 0 / 275
Goodness-of-fit on F^2	1.169
Final R indices [I>2sigma(I)]	R1 = 0.0801, wR2 = 0.1470
R indices (all data)	R1 = 0.1024, wR2 = 0.1551
Extinction coefficient	n/a
Largest diff. peak and hole	0.318 and -0.303 $e.Å^{-3}$

Table 2. Bond lengths [Å] and angles [°] for mo_amol_2_r_0m_a.

O(1)-C(13)	1.236(4)
O(2)-C(20)	1.223(4)
N(1)-C(13)	1.356(4)
N(1)-C(1)	1.441(4)
N(1)-C(7)	1.456(4)
N(2)-C(20)	1.365(4)
N(2)-C(4)	1.419(4)
N(2)-H(2N)	0.90(3)
C(1)-C(2)	1.377(4)
C(1)-C(6)	1.388(4)
C(2)-C(3)	1.390(4)
C(2)-H(2)	0.9500
C(3)-C(4)	1.390(4)
C(3)-H(3)	0.9500
C(4)-C(5)	1.382(4)
C(5)-C(6)	1.379(4)
C(5)-H(5)	0.9500
C(6)-H(6)	0.9500
C(7)-C(12)	1.375(4)
C(7)-C(8)	1.382(4)
C(8)-C(9)	1.386(4)
C(8)-H(8)	0.9500
C(9)-C(10)	1.377(4)
C(9)-H(9)	0.9500
C(10)-C(11)	1.379(4)
C(10)-H(10)	0.9500
C(11)-C(12)	1.393(4)
C(11)-H(11)	0.9500
C(12)-H(12)	0.9500
C(13)-C(14)	1.505(4)
C(14)-C(15)	1.387(4)
C(14)-C(19)	1.391(4)
C(15)-C(16)	1.389(4)
C(15)-H(15)	0.9500

C(16)-C(17)	1.375(5)
C(16)-H(16)	0.9500
C(17)-C(18)	1.384(5)
C(17)-H(17)	0.9500
C(18)-C(19)	1.387(4)
C(18)-H(18)	0.9500
C(19)-H(19)	0.9500
C(20)-C(21)	1.497(4)
C(21)-C(26)	1.392(5)
C(21)-C(22)	1.400(4)
C(22)-C(23)	1.383(5)
C(22)-H(22)	0.9500
C(23)-C(24)	1.385(5)
C(23)-H(23)	0.9500
C(24)-C(25)	1.388(5)
C(24)-H(24)	0.9500
C(25)-C(26)	1.377(5)
C(25)-H(25)	0.9500
C(26)-H(26)	0.9500

C(13)-N(1)-C(1)	121.7(2)
C(13)-N(1)-C(7)	120.6(2)
C(1)-N(1)-C(7)	117.5(2)
C(20)-N(2)-C(4)	125.8(3)
C(20)-N(2)-H(2N)	116(2)
C(4)-N(2)-H(2N)	117(2)
C(2)-C(1)-C(6)	119.9(3)
C(2)-C(1)-N(1)	121.7(3)
C(6)-C(1)-N(1)	118.4(3)
C(1)-C(2)-C(3)	120.2(3)
C(1)-C(2)-H(2)	119.9
C(3)-C(2)-H(2)	119.9
C(4)-C(3)-C(2)	119.8(3)
C(4)-C(3)-H(3)	120.1
C(2)-C(3)-H(3)	120.1
C(5)-C(4)-C(3)	119.4(3)

C(5)-C(4)-N(2)	117.0(3)
C(3)-C(4)-N(2)	123.6(3)
C(6)-C(5)-C(4)	120.7(3)
C(6)-C(5)-H(5)	119.7
C(4)-C(5)-H(5)	119.7
C(5)-C(6)-C(1)	119.8(3)
C(5)-C(6)-H(6)	120.1
C(1)-C(6)-H(6)	120.1
C(12)-C(7)-C(8)	121.0(3)
C(12)-C(7)-N(1)	120.3(3)
C(8)-C(7)-N(1)	118.7(3)
C(7)-C(8)-C(9)	119.0(3)
C(7)-C(8)-H(8)	120.5
C(9)-C(8)-H(8)	120.5
C(10)-C(9)-C(8)	120.4(3)
C(10)-C(9)-H(9)	119.8
C(8)-C(9)-H(9)	119.8
C(9)-C(10)-C(11)	120.2(3)
C(9)-C(10)-H(10)	119.9
C(11)-C(10)-H(10)	119.9
C(10)-C(11)-C(12)	119.7(3)
C(10)-C(11)-H(11)	120.1
C(12)-C(11)-H(11)	120.1
C(7)-C(12)-C(11)	119.5(3)
C(7)-C(12)-H(12)	120.2
C(11)-C(12)-H(12)	120.2
O(1)-C(13)-N(1)	123.2(3)
O(1)-C(13)-C(14)	120.9(3)
N(1)-C(13)-C(14)	115.9(2)
C(15)-C(14)-C(19)	120.2(3)
C(15)-C(14)-C(13)	119.3(3)
C(19)-C(14)-C(13)	120.4(3)
C(14)-C(15)-C(16)	119.6(3)
C(14)-C(15)-H(15)	120.2
C(16)-C(15)-H(15)	120.2
C(17)-C(16)-C(15)	120.2(3)

C(17)-C(16)-H(16)	119.9
C(15)-C(16)-H(16)	119.9
C(16)-C(17)-C(18)	120.4(3)
C(16)-C(17)-H(17)	119.8
C(18)-C(17)-H(17)	119.8
C(17)-C(18)-C(19)	120.0(3)
C(17)-C(18)-H(18)	120.0
C(19)-C(18)-H(18)	120.0
C(18)-C(19)-C(14)	119.6(3)
C(18)-C(19)-H(19)	120.2
C(14)-C(19)-H(19)	120.2
O(2)-C(20)-N(2)	122.4(3)
O(2)-C(20)-C(21)	121.3(3)
N(2)-C(20)-C(21)	116.2(3)
C(26)-C(21)-C(22)	118.7(3)
C(26)-C(21)-C(20)	124.9(3)
C(22)-C(21)-C(20)	116.4(3)
C(23)-C(22)-C(21)	120.4(3)
C(23)-C(22)-H(22)	119.8
C(21)-C(22)-H(22)	119.8
C(22)-C(23)-C(24)	120.1(3)
C(22)-C(23)-H(23)	119.9
C(24)-C(23)-H(23)	119.9
C(23)-C(24)-C(25)	119.9(3)
C(23)-C(24)-H(24)	120.0
C(25)-C(24)-H(24)	120.0
C(26)-C(25)-C(24)	120.0(4)
C(26)-C(25)-H(25)	120.0
C(24)-C(25)-H(25)	120.0
C(25)-C(26)-C(21)	120.9(3)
C(25)-C(26)-H(26)	119.5
C(21)-C(26)-H(26)	119.5

Symmetry transformations used to generate equivalent atoms:

Table 3. Torsion angles [°] for mo_amol_2_r_0m_a.

C(13)-N(1)-C(1)-C(2)	49.5(4)
C(7)-N(1)-C(1)-C(2)	-136.2(3)
C(13)-N(1)-C(1)-C(6)	-131.6(3)
C(7)-N(1)-C(1)-C(6)	42.7(4)
C(6)-C(1)-C(2)-C(3)	1.9(4)
N(1)-C(1)-C(2)-C(3)	-179.2(3)
C(1)-C(2)-C(3)-C(4)	0.7(5)
C(2)-C(3)-C(4)-C(5)	-2.8(4)
C(2)-C(3)-C(4)-N(2)	177.3(3)
C(20)-N(2)-C(4)-C(5)	149.6(3)
C(20)-N(2)-C(4)-C(3)	-30.5(4)
C(3)-C(4)-C(5)-C(6)	2.4(4)
N(2)-C(4)-C(5)-C(6)	-177.8(3)
C(4)-C(5)-C(6)-C(1)	0.2(5)
C(2)-C(1)-C(6)-C(5)	-2.4(4)
N(1)-C(1)-C(6)-C(5)	178.7(3)
C(13)-N(1)-C(7)-C(12)	69.1(4)
C(1)-N(1)-C(7)-C(12)	-105.3(3)
C(13)-N(1)-C(7)-C(8)	-110.4(3)
C(1)-N(1)-C(7)-C(8)	75.2(3)
C(12)-C(7)-C(8)-C(9)	-1.6(5)
N(1)-C(7)-C(8)-C(9)	177.8(3)
C(7)-C(8)-C(9)-C(10)	-1.1(5)
C(8)-C(9)-C(10)-C(11)	2.8(5)
C(9)-C(10)-C(11)-C(12)	-1.9(5)
C(8)-C(7)-C(12)-C(11)	2.5(5)
N(1)-C(7)-C(12)-C(11)	-176.9(3)
C(10)-C(11)-C(12)-C(7)	-0.7(5)
C(1)-N(1)-C(13)-O(1)	2.5(5)
C(7)-N(1)-C(13)-O(1)	-171.7(3)
C(1)-N(1)-C(13)-C(14)	-175.5(3)
C(7)-N(1)-C(13)-C(14)	10.3(4)
O(1)-C(13)-C(14)-C(15)	-94.0(4)
N(1)-C(13)-C(14)-C(15)	84.1(4)

O(1)-C(13)-C(14)-C(19)	83.0(4)
N(1)-C(13)-C(14)-C(19)	-98.9(3)
C(19)-C(14)-C(15)-C(16)	-0.8(5)
C(13)-C(14)-C(15)-C(16)	176.3(3)
C(14)-C(15)-C(16)-C(17)	1.5(5)
C(15)-C(16)-C(17)-C(18)	-0.5(5)
C(16)-C(17)-C(18)-C(19)	-1.2(5)
C(17)-C(18)-C(19)-C(14)	1.9(5)
C(15)-C(14)-C(19)-C(18)	-0.9(4)
C(13)-C(14)-C(19)-C(18)	-177.9(3)
C(4)-N(2)-C(20)-O(2)	4.2(5)
C(4)-N(2)-C(20)-C(21)	-173.6(3)
O(2)-C(20)-C(21)-C(26)	161.5(3)
N(2)-C(20)-C(21)-C(26)	-20.7(4)
O(2)-C(20)-C(21)-C(22)	-17.7(4)
N(2)-C(20)-C(21)-C(22)	160.1(3)
C(26)-C(21)-C(22)-C(23)	1.2(5)
C(20)-C(21)-C(22)-C(23)	-179.5(3)
C(21)-C(22)-C(23)-C(24)	-0.2(5)
C(22)-C(23)-C(24)-C(25)	-0.8(5)
C(23)-C(24)-C(25)-C(26)	0.8(5)
C(24)-C(25)-C(26)-C(21)	0.2(5)
C(22)-C(21)-C(26)-C(25)	-1.2(5)
C(20)-C(21)-C(26)-C(25)	179.6(3)

Symmetry transformations used to generate equivalent atoms:

Table 4. Hydrogen bonds for mo_amol_2_r_0m_a [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(2)-H(2N)...O(1)#1	0.90(3)	2.24(3)	3.111(4)	162(3)
C(3)-H(3)...O(2)	0.95	2.39	2.870(4)	111.0

Symmetry transformations used to generate equivalent atoms:

#1 x,y-1,z

References for X-ray data:

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