Supporting Information

Ru(III)-catalyzed C4-H bond cyanoalkoxylation of 1-naphthylamine derivatives with azobisisobutyronitrile

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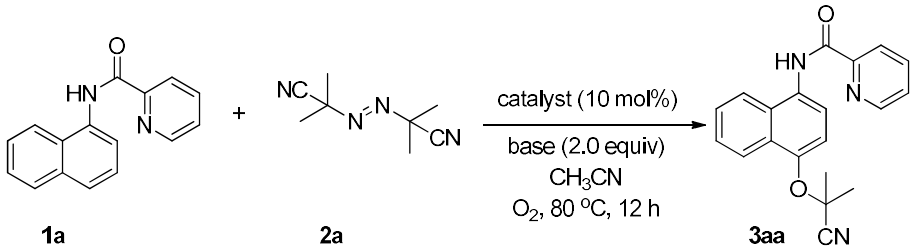
1. General Information

^{1}H NMR and ^{13}C NMR spectra were recorded on a Bruker DPX-400 spectrometer with $CDCl_3$ as the solvent and TMS as an internal standard. Melting points were measured using a WC-1 microscopic apparatus and are uncorrected. High resolution mass spectra were ensured on an Agilent Technologies 1290-6540 UHPLC/Accurate-Mass Quadrupole Time-of-Flight LC/MS. All solvents were used with further purification. Dichloromethane, ethyl acetate, and hexane were used for column chromatography. The commercials were obtained from commercial sources and used as-received without further purification unless otherwise noted.

2.Optimization of Reaction Conditions

Table S1. Optimization of Catalyst[a]

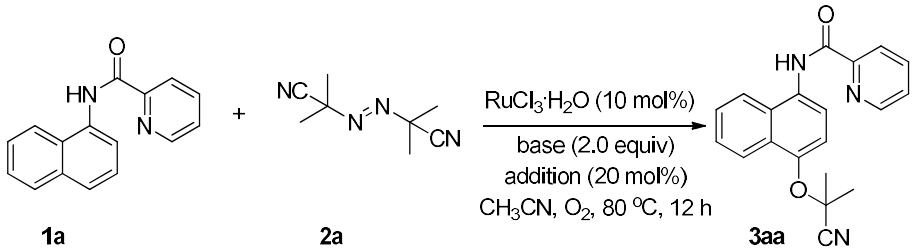


1a **2a** **3aa**

Entry	Catalyst	Base	Oxidant	Yield(%)[b]
1	$CuSO_4·H_2O$	PivONa	$K_2S_2O_8$	36
2	$Cu(OAc)_2·H_2O$	PivONa	$K_2S_2O_8$	26
3	$Cu(acac)_2$	PivONa	$K_2S_2O_8$	27
4	$Cu(OTf)_2$	PivONa	$K_2S_2O_8$	22
5	$CuBr_2$	PivONa	$K_2S_2O_8$	10
6	AgOAc	PivONa	$K_2S_2O_8$	24
7	$Fe(acac)_3$	PivONa	$K_2S_2O_8$	25
9	$FeCl_3·6H_2O$	PivONa	$K_2S_2O_8$	18
10	$FeCl_2·4H_2O$	PivONa	$K_2S_2O_8$	23
11	$Co(acac)_3$	PivONa	$K_2S_2O_8$	23
12	$Ni(OAc)_2·4H_2O$	PivONa	$K_2S_2O_8$	18
13	$NiCl_2·6H_2O$	PivONa	$K_2S_2O_8$	18
14	$PdCl_2$	PivONa	$K_2S_2O_8$	24
15	$Pd(OAc)_2$	PivONa	$K_2S_2O_8$	28
16	$Ru(pph_3)_3Cl_2$	PivONa	$K_2S_2O_8$	48
17	$Ru(bpy)_3PF_6$	PivONa	$K_2S_2O_8$	34
18	$Ru(bpy)_3Cl_3·6H_2O$	PivONa	$K_2S_2O_8$	32
19	$[RuCl_2(p\text{-cymene})_2]_2$	PivONa	$K_2S_2O_8$	51
20	$RuCl_3·H_2O$	PivONa	$K_2S_2O_8$	55
21	$RuCl_3·H_2O$	PivONa	-	68

[a] Reaction conditions: **1a** (0.2 mmol), **2a** (2.0 equiv), catalysts (10 mol%), base (0.4 mmol), oxidant (0.2 mmol), solvent (2 mL) at 80 °C under O_2 for 12 h. [b]Isolated yield.

Table S2. Optimization of Base and Additive [a]



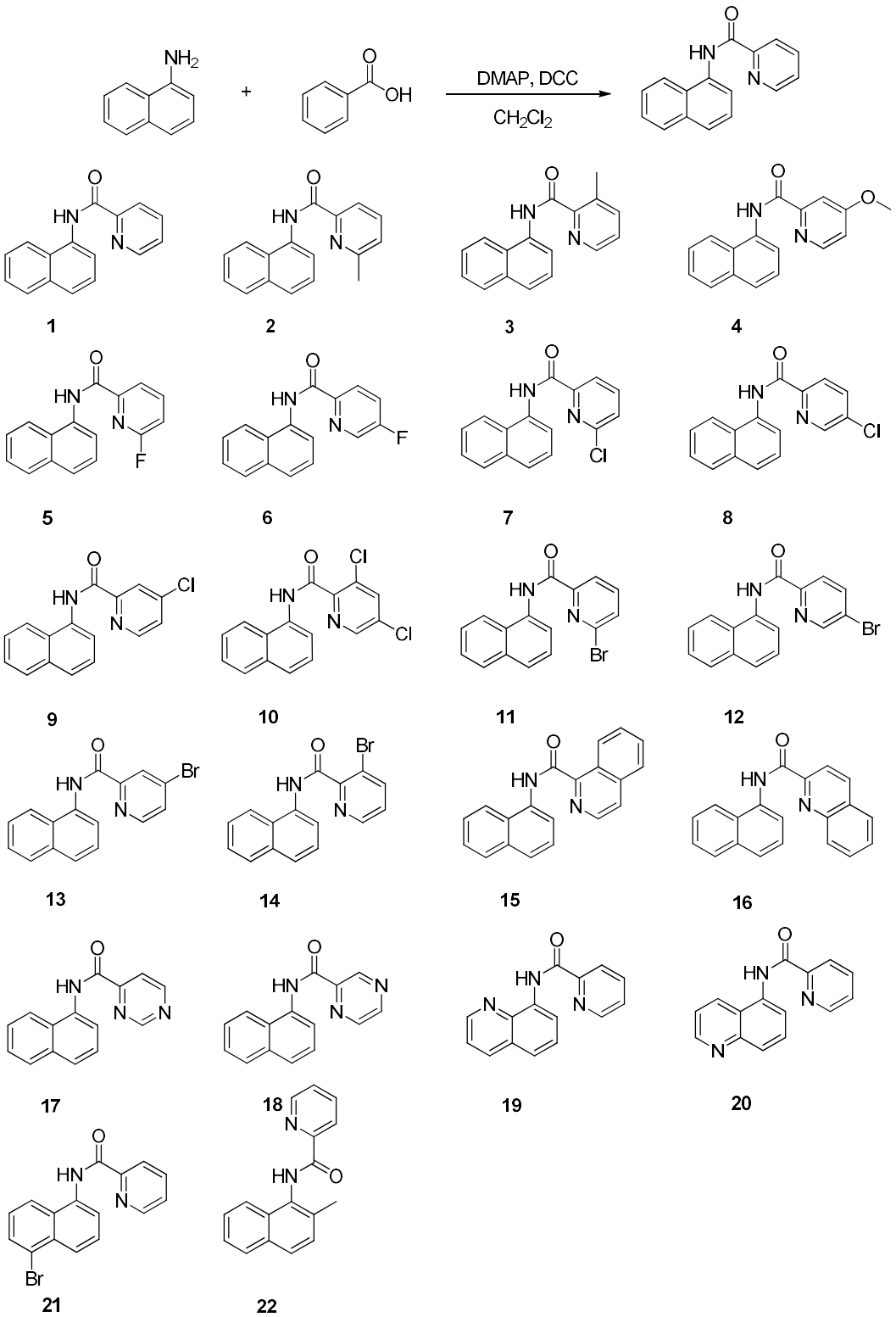
1a **2a** **3aa**

Entry	Catalyst	Base	Addition	Solvent	Yield(%)[b]
1	$RuCl_3·H_2O$	NaOAc	-	CH_3CN	61
2	$RuCl_3·H_2O$	KOAc	-	CH_3CN	63
3	$RuCl_3·H_2O$	$KHCO_3$	-	CH_3CN	54
4	$RuCl_3·H_2O$	KCO_3	-	CH_3CN	62
5	$RuCl_3·H_2O$	^tBuOK	-	CH_3CN	44
6	$RuCl_3·H_2O$	KI	-	CH_3CN	NR
7	$RuCl_3·H_2O$	NH_4OAc	-	CH_3CN	57
8	$RuCl_3·H_2O$	K_3PO_4	-	CH_3CN	55
9	$RuCl_3·H_2O$	PivOH	-	CH_3CN	42
10	$RuCl_3·H_2O$	NaCl	-	CH_3CN	49
11	$RuCl_3·H_2O$	PivONa	-	THF	<10
12	$RuCl_3·H_2O$	PivONa	-	1,4-Dioxane	NR
13	$RuCl_3·H_2O$	PivONa	-	DCE	NR
14	$RuCl_3·H_2O$	PivONa	-	Acetone	NR
15	$RuCl_3·H_2O$	PivONa	-	Dioxane	NR
16	$RuCl_3·H_2O$	PivONa	PPh_3	CH_3CN	61
17	$RuCl_3·H_2O$	PivONa	diMe-phen	CH_3CN	69
18	$RuCl_3·H_2O$	PivONa	TBAB	CH_3CN	58
19	$RuCl_3·H_2O$	PivONa	x-phos	CH_3CN	60
20	$RuCl_3·H_2O$	PivONa	1,10-phen	CH_3CN	67
21	$RuCl_3·H_2O$	PivONa	bpy	CH_3CN	72
22[c]	$RuCl_3·H_2O$	PivONa	bpy	CH_3CN	80

[a] Reaction conditions: **1a** (0.2 mmol), **2a** (2.0 equiv), catalysts (10 mol%), base (0.4 mmol), addition (20 mol%), solvent (2 mL) at 80 °C under O_2 for 12 h. [b]Isolated yield. [c]**2a** (0.8 mmol); 1,10-phen = 1,10-phenanthroline, bpy = 2, 2'-bipyridine, diMe-phen = 4,7-dimethyl-1,10-phenanthroline

3. Experimental Section

3.1. Typical procedure for the synthesis of substrate 1-22



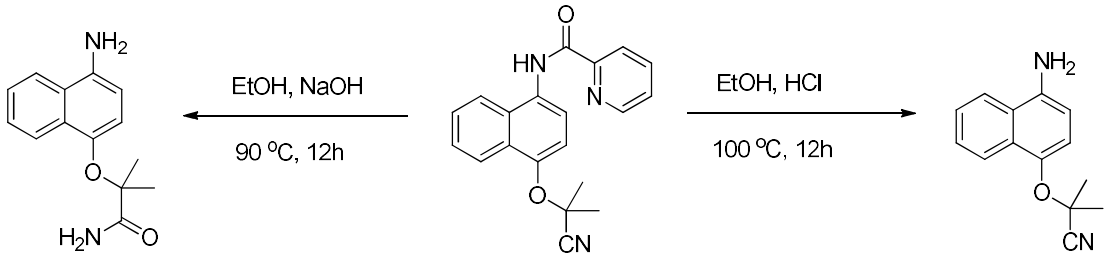
A 100 mL two-necked round-bottom flask was equipped with a magnetic stir bar and charged with 1-naphthylamine (20 mmol, 2.86 g), picolinic acid (1.1 equiv., 2.70 g), N,N-dimethyl-4-aminopyridine (DMAP, 0.1 equiv., 0.244 g) in 30 mL anhydrous CH_2Cl_2 at 0 °C. After DCC (4.54 g, 1.1 equiv.) in CH_2Cl_2 (20 mL) was added dropwise to the solution, the reaction was then warmed to room temperature, stirred for 12 h and quenched with water (30 mL). The reaction mixture was extracted with CH_2Cl_2 (3 × 20 mL), and the combined organic solvent was dried over Na_2SO_4, filtered and concentrated under reduced pressure. The resulting residue was purified by column chromatography (hexane/ethyl acetate = 3:1) (V/V) to afford the pure product **1** as a white solid (4.42 g, 89%).

All amides **2**-**22** were prepared from the corresponding 1-naphthylamine and 2-picolinic acid derivatives according to the reported procedure[1].

3.2. Typical procedure for the product 3aa

A Schlenk tube was equipped with a magnetic stir bar and charged with N-(naphthalen-1-yl)picolinamide **1a** (0.2 mmol, 49.6 mg), **2a** (0.8 mmol, 131 mg), $RuCl_3 \cdot H_2O$ (0.02 mmol, 5 mg), $PivONa \cdot H_2O$ (0.4 mmol, 56.8 mg), bpy (0.04 mmol, 6.2 mg), MeCN 2.0 mL. The resulting mixture was sealed under O_2, heated at 80 ℃ for 12 h, and cooled to room temperature. Upon completion, CH_2Cl_2 (30 mL) was added to the reaction system, and the resulting mixture was filtered through a pad of Celite. After the organic material was concentrated in vacuum, the product was purified by column chromatography on silica gel (100-200 mesh) using hexane/EtOAc as an eluent (5:1-3:1, V/V) to afford the pure product **3aa**.

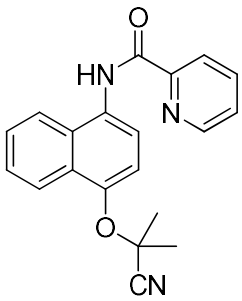
3.3. Typical procedure for the product 4a and 5a



A mixture of **3aa** (66.2 mg, 0.2 mmol) and HCl (1 mL) was heated in ethanol (2 mL) for 12 h at 100 °C. After the mixture was cooled to room temperature and diluted with water (3.0 mL). The saturated $NaHCO_3$ solution was then added until the pH value was about 7. The mixture was then extracted with CH_2Cl_2 and dried over anhydrous Na_2SO_4. After the organic material was concentrated in vacuum, the product was purified by column chromatography on silica gel (100-200 mesh) using hexane/EtOAc as an eluent (2:1, V/V) to afford the pure product **4a**.

A mixture of **3aa** (66.2 mg, 0.2 mmol) and NaOH (160 mg, 4 mmol, 20 equiv) was heated in ethanol (2 mL) for 12 h at 90 °C. After the mixture was cooled to room temperature and diluted with water (3.0 mL). The mixture was then extracted with CH_2Cl_2 and dried over anhydrous Na_2SO_4. After the organic material was concentrated in vacuum, the product was purified by column chromatography on silica gel (100-200 mesh) using hexane/EtOAc as an eluent (2:1, V/V) to afford the pure product **5a**.

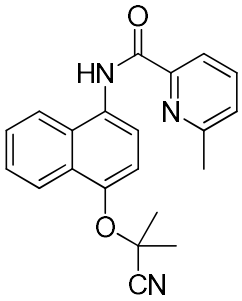
4. Characterization Data of the Products



3aa

N-(4-((2-cyanopropan-2-yl)oxy)naphthalen-1-yl)picolinamide

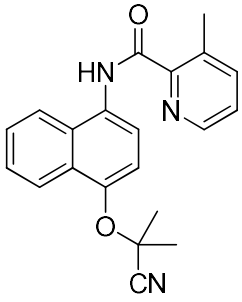
(3aa): pale yellow solid (52.7 mg, 80%), mp 124-126 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.60 (s, 1H), 8.71-8.70 (m, 1H), 8.35 (d, J = 7.80 Hz, 1H), 8.26 (d, J = 8.36 Hz, 1H), 8.19-8.17 (m, 1H), 8.06 (d, J = 8.22 Hz, 1H), 7.97-7.93 (m, 1H), 7.64-7.51 (m, 4H), 1.85 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$), δ 162.4, 149.9, 148.2, 147.7, 137.8, 128.8, 128.7, 128.0, 127.0, 126.6, 126.1, 122.9, 122.6, 121.1, 120.9, 119.0, 114.5, 72.4, 27.5; HRMS (ESI^+) m/z [$M+H^+$] calcd for $C_{20}H_{17}N_3O_2$: 332.1394, Found: 332.1394.



3ba

N-(4-((2-cyanopropan-2-yl)oxy)naphthalen-1-yl)-6-methylpicolinamide

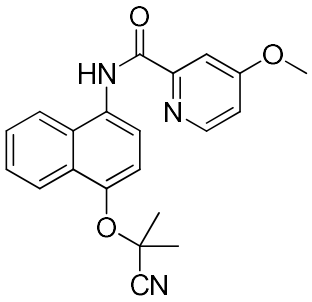
(3ba): yellow solid (45.5 mg, 66%), mp 123-125 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.66 (s, 1H), 8.24 (d, J=8.38 Hz, 1H), 8.19-8.15 (m, 2H), 8.04 (d, J = 8.36 Hz, 1H), 7.82 (t, J =7.72 Hz, 1H), 7.64-7.60 (m, 1H), 7.58-7.54 (m, 2H), 7.37 (d, J = 7.68 Hz, 1H), 2.70 (s, 3H);1.85 (s, 6H); ^{13}C NMR (100MHz, $CDCl_3$), δ 162.6, 157.3, 149.2, 147.6, 137.9, 128.9, 128.8, 128.1, 126.9, 126.3, 126.1, 122.9, 121.1, 121.0, 119.6, 119.1, 114.6, 72.3, 27.5, 24.5; HRMS (ESI^+) m/z [$M+H^+$] calcd for $C_{21}H_{19}N_3O_2$: 346.1550, Found: 346.1551.



3ca

N-(4-((2-cyanopropan-2-yl)oxy)naphthalen-1-yl)-3-methylpicolinamide

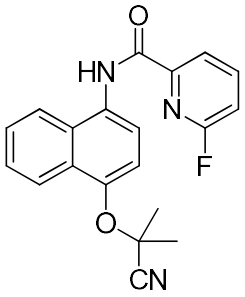
(3ca): white solid (48.2 mg, 69%), mp 97-99 °C; ^{1}H NMR (400MHz, CDCl3) δ 10.79 (s, 1H), 8.55-8.54 (m, 1H), 8.20-8.16 (m, 2H), 8.05 (d, J = 8.04 Hz, 1H), 7.69-7.67 (m, 1H) 7.62-7.53 (m, 3H), 7.41 (dd, J_1 = 7.72 Hz, J_2 = 4.60 Hz, 1H), 2.85 (s, 3H), 1.84 (s, 6H); ^{13}C NMR (100MHz, CDCl3), δ 164.0, 147.5, 146.8, 145.6, 141.4, 136.4, 129.2, 128.9, 128.3, 126.8, 126.2, 126.0, 122.8, 121.2, 121.1, 119.2, 114.6, 72.4, 27.5, 20.7; HRMS (ESI$^+$) m/z [M+H$^+$] calcd for $C_{21}H_{19}N_3O_2$: 346.1550, Found: 346.1550.



3da

N-(4-((2-cyanopropan-2-yl)oxy)naphthalen-1-yl)-4-methoxypicolinamide

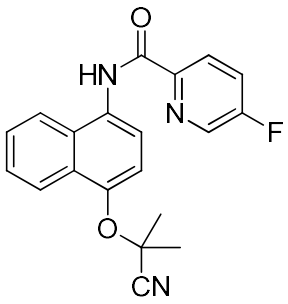
(3da): white solid (49.7 mg, 68%), mp 117-119 °C; ^{1}H NMR (400MHz, $CDCl_3$) δ 10.66 (s, 1H), 8.49 (d, J = 5.64 Hz, 1H), 8.26 (d, J = 8.36 Hz, 1H), 8.19-8.17 (m, 1H), 8.05 (d, J = 8.24 Hz, 1H), 7.88 (d, J = 2.52 Hz, 1H), 7.63-7.54 (m, 3H), 7.01 (dd, J_1 = 5.64 Hz, J_2 = 2.60 Hz, 1H), 3.96 (s, 3H), 1.85 (s, 6H); ^{13}C NMR (100MHz, $CDCl_3$), δ 167.3, 162.4, 152.0, 149.3, 147.6, 128.8, 127.9, 126.9, 126.1, 122.9, 121.1, 121.0, 118.9, 114.5, 113.4, 107.7, 72.3, 55.7, 27.5; HRMS (ESI$^+$) m/z [M+H$^+$] calcd for $C_{21}H_{19}N_3O_3$: 362.1499, Found: 362.1499.



3ea

N-(4-((2-cyanopropan-2-yl)oxy)naphthalen-1-yl)-6-fluoropicolinamide

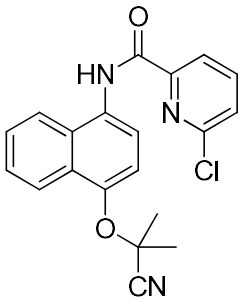
(3ea): white solid (45.5 mg, 65%); mp 123-125 °C ^{1}H NMR (400MHz, $CDCl_3$) δ 10.07 (s, 1H), 8.25 (dd, J_1 = 7.36 Hz, J_2 = 1.68 Hz, 1H), 8.19-8.16 (m, 2H), 8.09-8.00 (m, 2H), 7.65-7.54 (m, 3H), 7.19 (dd, J_1 = 8.16 Hz, J_2 = 2.00 Hz, 1H), 1.86 (s, 6H); ^{13}C NMR (100MHz, $CDCl_3$), δ 162.1 (d, $J_{C\text{-}F}$ = 243.32 Hz), 161.1, 148.5 (d, $J_{C\text{-}F}$ = 10.66 Hz), 148.1, 142.9 (d, $J_{C\text{-}F}$ = 7.56 Hz), 128.7, 128.2, 128.1, 127.1, 126.2, 122.9, 121.0, 120.9, 120.3 (d, $J_{C\text{-}F}$ = 3.69 Hz), 119.7, 114.2, 113.2 (d, $J_{C\text{-}F}$ = 35.57 Hz), 72.3, 27.5; ^{19}F NMR (376MHz, $CDCl_3$), δ -76.1 (s, 1F); HRMS (ESI$^+$) m/z [M+H$^+$] calcd for $C_{20}H_{16}FN_3O_2$: 350.1299, Found: 350.1299.



3fa

N-(4-((2-cyanopropan-2-yl)oxy)naphthalen-1-yl)-5-fluoropicolinamide

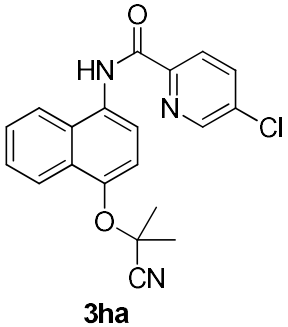
(3fa): white solid (55.1 mg, 79%), mp 128-130 °C; ^{1}H NMR (400MHz, $CDCl_3$) δ 10.33 (s, 1H), 8.54 (d, J = 2.72 Hz, 1H), 8.39 (dd, J_1 = 8.68 Hz, J_2 = 4.60 Hz, 1H), 8.22-8.17 (m, 2H), 8.01 (d, J = 8.12 Hz, 1H), 7.66-7.54 (m, 4H), 1.85 (s, 6H); ^{13}C NMR (100MHz, $CDCl_3$), δ 161.3 (d, $J_{C\text{-}F}$ = 259,79 Hz), 161.4, 147.8, 146.3 (d, $J_{C\text{-}F}$ = 3.74 Hz), 136.7 (d, $J_{C\text{-}F}$ = 25.39 Hz), 128.7, 128.5, 128.0, 127.0, 126.1, 124.4 (d, $J_{C\text{-}F}$ = 8.75 Hz), 124.3 (d, $J_{C\text{-}F}$ =21.40 Hz), 122.9, 121.0, 120.8, 119.3, 114.4, 72.3, 27.5; HRMS (ESI$^+$) m/z [M+H$^+$] calcd for $C_{20}H_{16}FN_3O_2$: 350.1299, Found: 350.1297.



3ga

6-chloro-N-(4-((2-cyanopropan-2-yl)oxy)naphthalen-1-yl)picolinamide

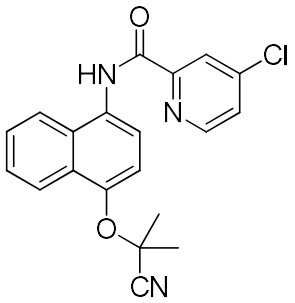
(3ga): white solid (50.9 mg, 70%), mp 94-96 °C; ^{1}H NMR (400MHz, $CDCl_3$) δ 10.19 (s, 1H), 8.29-8.27 (m, 1H), 8.19-8.17 (m, 1H), 8.15 (d, J = 8.32 Hz, 1H), 8.01 (d, J = 8.32 Hz, 1H), 7.91 (t, J = 7.80 Hz, 1H), 7.65-7.61 (m, 1H), 7.59-7.54 (m, 3H), 1.86 (s, 6H); ^{13}C NMR (100MHz, $CDCl_3$), δ 161.1, 150.4, 150.1, 148.1, 140.4, 128.7, 128.3, 128.2, 127.4, 127.1, 126.2, 122.9, 121.3, 121.0, 120.9, 119.8, 114.2, 72.3, 27.5; HRMS (ESI$^+$) m/z [M+H$^+$] calcd for $C_{20}H_{16}ClN_3O_2$: 366.1004, Found: 366.1003.



3ha

5-chloro-N-(4-((2-cyanopropan-2-yl)oxy)naphthalen-1-yl)picolinamide

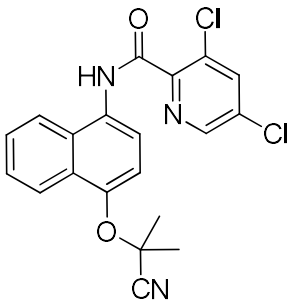
(3ha): pale yellow solid (50.4 mg, 69%), mp 117-119 °C; ^{1}H NMR (400MHz, $CDCl_3$) δ 10.36 (s, 1H), 8.65 (d, J = 2.28 Hz, 1H), 8.31 (d, J = 8.40 Hz, 1H), 8.23-8.18 (m, 2H), 8.01 (d, J = 8.36 Hz, 1H), 7.93-7,91 (m, 1H), 7.64-7.54 (m, 3H), 1.85 (s, 6H); ^{13}C NMR (100MHz, $CDCl_3$), δ 161.6, 148.1, 147.9, 147.3, 137.5, 135.5, 128.7, 128.3, 128.0, 127.1, 126.2, 123.6, 123.0, 121.0, 120.8, 119.3, 114.3, 72.3, 27.5; HRMS (ESI$^+$) m/z [M+H$^+$] calcd for $C_{20}H_{16}ClN_3O_2$: 366.1004, Found: 366.1001.



3ia

4-chloro-N-(4-((2-cyanopropan-2-yl)oxy)naphthalen-1-yl)picolinamide

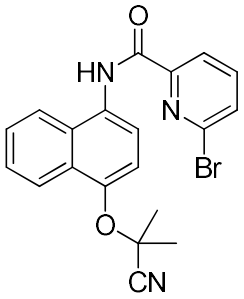
(3ia): yellow solid (48.8 mg, 67%), mp 120-122 °C; ^{1}H NMR (400MHz, $CDCl_3$) δ 10.46 (s, 1H), 8.59 (d, J = 5.24 Hz, 1H), 8.36 (d, J = 2.04 Hz, 1H), 8.23 (d, J = 8.36 Hz, 1H), 8.19-8.17 (m, 1H), 8.01 (d, J = 8.08 Hz, 1H), 7.64-7.52 (m, 4H), 1.85 (s, 6H); ^{13}C NMR (100MHz, $CDCl_3$), δ 161.2, 151.4, 149.1. 147.9, 146.4, 128.7, 128.3, 127.9, 126.8, 126.2, 123.2, 123.0, 121.0, 120.8, 119.3, 72.3, 27.5; HRMS (ESI$^+$) m/z [M+H$^+$] calcd for $C_{20}H_{16}ClN_3O_2$: 366.1004, Found: 366.1001.



3ja

3,5-dichloro-N-(4-((2-cyanopropan-2-yl)oxy)naphthalen-1-yl)picolinamide

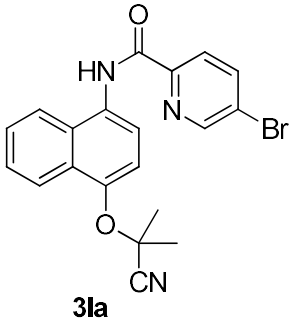
(3ja): white solid (50.2 mg, 63%), mp 127-129 °C; ^{1}H NMR (400MHz, $CDCl_3$) δ 10.22 (s, 1H), 8.56 (d, J = 2.04 Hz, 1H), 8.19-8.16 (m, 2H), 7.96-7.92 (m, 2H), 7.62-7.52 (m, 3H), 1.84 (s, 6H); ^{13}C NMR (100MHz, $CDCl_3$), δ 160.5, 148.0, 145.2, 143.8, 140.2, 134.7, 133.1, 128.7, 128.2, 128.1, 127.0, 126.2, 123.0, 121.0, 120.8, 119.6, 114.3, 72.3, 27.5; HRMS (ESI$^+$) m/z [M+H$^+$] calcd for $C_{20}H_{15}Cl_2N_3O_2$: 400.0614, Found: 400.0618.



3ka

6-bromo-N-(4-((2-cyanopropan-2-yl)oxy)naphthalen-1-yl)picolinamide

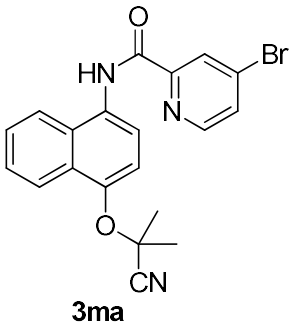
(3ka): white solid (61.5 mg, 75%), mp 103-105 °C; ^{1}H NMR (400MHz, $CDCl_3$) δ 10.17 (s, 1H), 8.32-8.30 (m, 1H), 8.18(d, J = 8.12 Hz, 1H), 8.14 (d, J = 8.32 Hz, 1H), 8.00 (d, J = 8.36 Hz, 1H), 7.81 (t, J = 7.68 Hz, 1H), 7.73-7.70 (m, 1H), 7.65-7.61 (m, 1H), 7.59-7.54 (m, 2H), 1.86 (s, 6H); ^{13}C NMR (100MHz, $CDCl_3$), δ 161.0, 151.0, 148.2, 140.6, 140.1, 131.2, 128.7, 128.3, 128.2, 127.2, 126.2, 122.9, 121.6, 121.1, 121.0, 119.9, 114.2, 72.3, 27.5; HRMS (ESI$^+$) m/z [M+H$^+$] calcd for $C_{20}H_{16}BrN_3O_2$: 410.0499, Found: 410.0501.



3la

5-bromo-N-(4-((2-cyanopropan-2-yl)oxy)naphthalen-1-yl)picolinamide

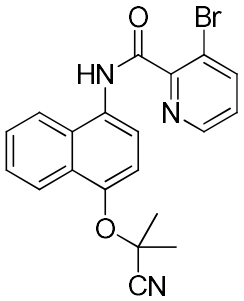
(3la): white solid (50.2 mg, 62%), mp 103-105 °C; ^{1}H NMR (400MHz, $CDCl_3$) δ 10.37 (s, 1H), 8.76(d, J = 1.88 Hz, 1H), 8.26-8.17 (m, 3H), 8.08 (dd, J_1 = 8.32 Hz, J_2 = 2.20 Hz, 1H), 8.00 (d, J = 8.20 Hz, 1H), 7.64-7.54 (m, 3H), 1.85 (s, 6H); ^{13}C NMR (100MHz, $CDCl_3$), δ 161.7, 149.4, 148.4, 147.9, 140.5, 128.7, 128.4, 128.0, 127.0, 126.2, 124.4, 124.0, 122.9, 121.0, 120.8, 119.3, 114.3, 72.3, 27.5; HRMS (ESI$^+$) m/z [M+H$^+$] calcd for $C_{20}H_{16}BrN_3O_2$: 410.0499, Found: 410.0499.



3ma

4-bromo-N-(4-((2-cyanopropan-2-yl)oxy)naphthalen-1-yl)picolinamide

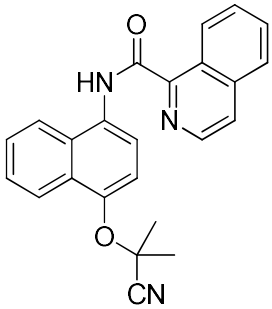
(3ma): white solid (56.9 mg, 70%), mp 124-126 °C; ^{1}H NMR (400MHz, $CDCl_3$) δ 10.45 (s, 1H), 8.53-8.51 (m, 2H), 8.23 (d, J = 8.36 Hz, 1H), 8.19-8.17 (m, 1H), 8.01 (d, J = 8.12 Hz, 1H), 7.70 (dd, J_1 = 5.16 Hz, J_2 = 1.96 Hz, 1H), 7.64-7.55 (m, 3H), 1.86 (s, 6H); ^{13}C NMR (100MHz, $CDCl_3$), δ 161.1, 151.1, 148.9, 147.9, 135.0, 129.9, 128.7, 128.3, 128.0, 127.0, 126.2, 126.1, 123.0, 121.0, 120.8, 119.3, 114.3, 72.3, 27.5; HRMS (ESI$^+$) m/z [M+H$^+$] calcd for $C_{20}H_{16}BrN_3O_2$: 410.0499, Found: 410.0498.



3na

3-bromo-N-(4-((2-cyanopropan-2-yl)oxy)naphthalen-1-yl)picolinamide

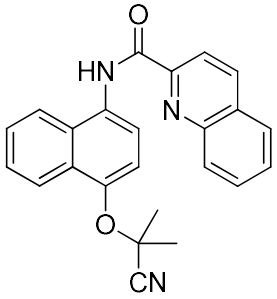
(3na): pale yellow solid (48.8 mg, 60%), mp 128-130 °C; ^{1}H NMR (400MHz, $CDCl_3$) δ 10.48 (s, 1H), 8.66-8.65 (m, 1H), 8.22 (d, J = 8.40 Hz, 1H), 8.19-8.13 (m, 2H), 8.00 (d, J = 8.08 Hz, 1H), 7.62-7.53 (m, 3H), 7.37 (dd, J_1 = 8.12 Hz, J_2 = 4.48 Hz, 1H), 1.85 (s, 6H); ^{13}C NMR (100MHz, $CDCl_3$), δ 161.5, 147.8, 146.7, 146.6, 144.5, 128.8, 128.6, 128.2, 127.0, 126.9, 126.1, 123.0, 121.0, 120.9, 120.0, 119.5, 114.5, 72.4, 27.5; HRMS (ESI$^+$) m/z [M+H$^+$] calcd for $C_{20}H_{16}BrN_3O_2$: 409.0499, Found: 410.0495.



3oa

N-(4-((2-cyanopropan-2-yl)oxy)naphthalen-1-yl)isoquinoline-1-carboxamide

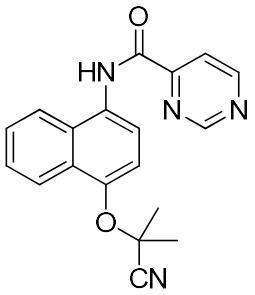
(3oa): Yellow liquid (51 mg, 67%); ^{1}H NMR (400MHz, $CDCl_3$) δ 10.90 (s, 1H), 9.80-9.77 (m, 1H), 8.62 (d, J = 5.48 Hz, 1H), 8.25 (d, J = 8.36 Hz, 1H), 8.20-8.18 (m, 1H), 8.11 (d, J = 8.16 Hz, 1H), 7.92-7.90 (m, 2H), 7.79-7.71 (m, 2H), 7.64-7.54 (m, 3H), 1.86 (s, 6H); ^{13}C NMR (100MHz, $CDCl_3$), δ 164.1, 147.8, 147.5, 140.2, 137.7, 130.7, 129.1, 129.0, 128.9, 128.5, 127.9, 127.4, 127.0, 126.9, 126.1, 125.1, 122.9, 121.3, 121.1, 119.5, 114.5, 72.4, 27.5; HRMS (ESI$^+$) m/z [M+H$^+$] calcd for $C_{24}H_{19}N_3O_2$: 382.1550, Found: 382.1550.



3pa

N-(4-((2-cyanopropan-2-yl)oxy)naphthalen-1-yl)quinoline-2-carboxamide

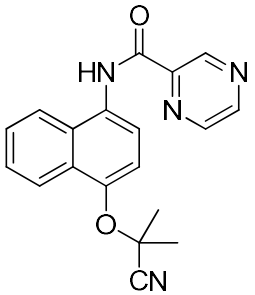
(3pa): pale yellow solid (39.8 mg, 55%), mp 175-176 ^{o}C; ^{1}H NMR (400MHz, $CDCl_3$) δ 10.81 (s, 1H), 8.48-8.41 (m, 2H), 8.30-8.26 (m, 2H), 8.20 (d, J = 7.84 Hz, 1H), 8.15 (d, J = 8.36 Hz, 1H), 7.95 (d, J = 8.16 Hz, 1H), 7.87-7.83 (m, 1H), 7.71-7.64 (m, 2H), 7.61-7.58 (m, 2H), 1.87 (s, 6H); ^{13}C NMR (100MHz, $CDCl_3$), δ 162.6, 149.7, 147.8, 146.4, 138.0, 130.4, 129.9, 129.6, 128.8, 128.7, 128.3, 128.2, 127.9, 127.0, 126.1, 123.0, 121.1, 121.0, 119.3, 119.0, 118.9, 114.5, 72.3, 27.5; HRMS (ESI$^+$) m/z [M+H$^+$] calcd for $C_{24}H_{19}N_3O_2$: 382.1550, Found: 382.1546.



3qa

N-(4-((2-cyanopropan-2-yl)oxy)naphthalen-1-yl)pyrimidine-4-carboxamide

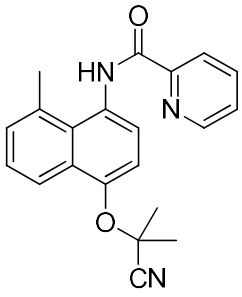
(3qa): yellow solid (35.1 mg, 53%); mp 118-120 ^{o}C; ^{1}H NMR (400MHz, $CDCl_3$) δ 10.43 (s, 1H), 9.40 (d, J = 1.32 Hz, 1H), 9.09 (d, J = 5.00 Hz, 1H), 8.29-8.19 (m, 3H), 8.02 (d, J = 8.36 Hz, 1H), 7.67-7.55 (m, 3H), 1.86 (s, 6H); ^{13}C NMR (100MHz, $CDCl_3$), δ 160.6, 159.7, 157.8, 156.4, 148.2, 128.7, 127.9, 127.7, 127.2, 126.3, 123.0, 120.9, 120.6, 119.5, 118.8, 114.1, 72.3, 27.5; HRMS (ESI$^+$) m/z [M+H$^+$] calcd for $C_{19}H_{14}N_4O_2$: 333.1346, Found: 333.1346.



3ra

N-(4-((2-cyanopropan-2-yl)oxy)naphthalen-1-yl)pyrazine-2-carboxamide

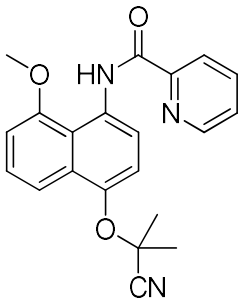
(3ra): pale yellow solid (35 mg, 52%), mp 164-166 °C; ^{1}H NMR (400MHz, $CDCl_3$) δ 10.19 (s, 1H), 9.57 (d, J = 1.28 Hz, 1H), 8.86 (d, J = 2.44 Hz, 1H), 8.68-8.67 (m, 1H), 8.22-8.18 (m, 2H), 8.00 (d, J = 8.12 Hz, 1H), 7.64-7.55 (m, 3H), 1.86 (s, 6H); ^{13}C NMR (100MHz, $CDCl_3$), δ 161.1, 148.1, 147.7, 144.8, 144.5, 142.6, 128.7, 128.0, 127.9, 127.1, 126.3, 123.0, 121.0, 120.7, 119.7, 114.2, 72.3, 27.5; HRMS (ESI$^+$) m/z [M+H$^+$] calcd for $C_{19}H_{14}N_4O_2$: 333.1346, Found: 333.1343.



3ab

N-(4-((2-cyanopropan-2-yl)oxy)-8-methylnaphthalen-1-yl)picolinamide

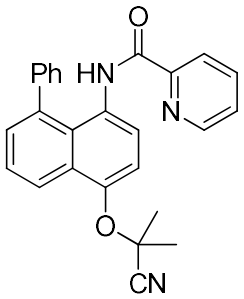
(3ab): white solid (23.2 mg, 33%), mp 125-127 °C; ^{1}H NMR (400MHz, $CDCl_3$) δ 10.45 (s, 1H), 8.67-8.65 (m, 1H), 8.36 (d, J = 7.80 Hz, 1H), 8.06 (d, J = 8.16 Hz, 1H), 7.96-7.12 (m, 2H), 7.54-7.50 (m, 2H), 7.39-7.30 (m, 2H), 2.95 (s, 3H), 1.84 (s, 6H), ^{13}C NMR (100MHz, $CDCl_3$), δ 161.5, 149.0, 147.9, 147.2, 136.6, 131.9, 129.8, 129.2, 128.6. 128.3, 125.4, 124.6, 122.7, 121.7, 120.2, 120.1, 112.9, 72.2, 26.4, 23.9; HRMS (ESI$^+$) m/z [M+H$^+$] calcd for $C_{21}H_{19}N_3O_2$: 346.1550, Found: 346.1548.



3ac

N-(4-((2-cyanopropan-2-yl)oxy)-8-methoxynaphthalen-1-yl)picolinamide

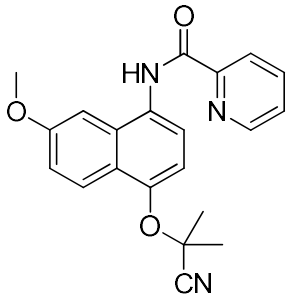
(3ac): yellow solid (36.8 mg, 52%), mp 132-134 °C; ^{1}H NMR (400MHz, $CDCl_3$) δ 13.14 (s, 1H), 8.94 (d, J = 8.68 Hz, 1H), 8.69 (d, J = 4.24 Hz, 1H), 8.34 (d, J = 7.80 Hz, 1H), 7.92 (m, 1H), 7.76 (d, J = 8.48 Hz, 1H), 7.55 (d, J = 8.64 Hz, 1H), 7.49-7.46 (m, 1H), 7.43-7.39 (m, 1H), 6.96 (d, J = 7.68 Hz, 1H), 4.20 (s, 3H), 1.82 (s, 6H); ^{13}C NMR (100MHz, $CDCl_3$), δ 162.3, 156.3, 151.1, 148.1, 156.0, 137.6, 131.8, 131.1, 126.1, 125.9, 122.6, 121.2, 117.8, 116.2, 116.1, 115.6, 106.5, 72.6, 56.3, 27.5; HRMS (ESI$^+$) m/z [M+H$^+$] calcd for $C_{21}H_{19}N_3O_3$: 362.1499, Found: 362.1497.



3ad

N-(4-((2-cyanopropan-2-yl)oxy)-8-phenylnaphthalen-1-yl)picolinamide

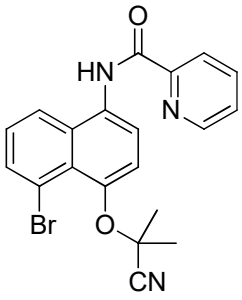
(3ad): yellow solid (54.4 mg, 66%), mp 141-143 °C; ^{1}H NMR (400MHz, $CDCl_3$) δ 9.44 (s, 1H), 8.24-8.22 (m, 1H), 8.19-8.17 (m, 1H), 8.10 (d, J = 8.44 Hz, 1H), 8.06 (d, J = 7.80 Hz, 1H), 7.78-7.74 (m, 1H), 7.61 (d, J = 8.44 Hz, 1H), 7.54-7.50 (m, 1H), 7.38-7.30 (m, 4H), 7.17-7.14 (m, 2H), 6.99-6.95 (m, 1H), 1.89 (s, 6H); ^{13}C NMR (100MHz, $CDCl_3$), δ 162.0, 149.7, 148.3, 147.4, 142.6, 137.9, 137.0, 131.2, 130.0, 129.1, 129.0, 128.1, 126.7, 126.5, 125.8, 125.0, 122.7, 122.4, 121.8, 121.1, 114.5, 72.4, 27.6; HRMS (ESI$^+$) m/z [M+H$^+$] calcd for $C_{26}H_{21}N_3O_2$: 408.1701, Found: 408.1707.



3ae

N-(4-((2-cyanopropan-2-yl)oxy)-7-methoxynaphthalen-1-yl)picolinamide

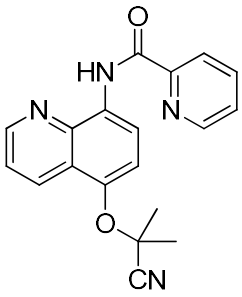
(3ae): pale yellow solid (21.2 mg, 29%), mp 120-122 °C; ^{1}H NMR (400MHz, $CDCl_3$) δ 10.36 (s, 1H), 8.68 (d, J = 4.20 Hz, 1H), 8.35 (d, J = 7.80 Hz, 1H), 8.11-8.07 (m, 2H), 7.97-7.53 (m, 1H), 7.54-7.51 (m, 1H), 7.40 (d, J = 8.32 Hz, 1H), 7.28 (d, J = 2.32 Hz, 1H), 7.20 (dd, J_1 = 9.20 Hz, J_2 = 2.40 Hz, 1H), 3.95 (s, 3H), 1.84 (s, 6H); ^{13}C NMR (100MHz, $CDCl_3$), δ 162.5, 158.6, 150.0, 148.2, 148.1, 137.8. 129.9, 127.5, 126.6, 124.7, 124.0, 122.6, 121.1, 120.8, 118.1, 112.1, 100.5, 72.2, 55.4. 27.5; HRMS (ESI$^+$) m/z [M+H$^+$] calcd for $C_{21}H_{19}N_3O_3$: 362.1499, Found: 362.1502.



3af

N-(5-bromo-4-((2-cyanopropan-2-yl)oxy)naphthalen-1-yl)picolinamide

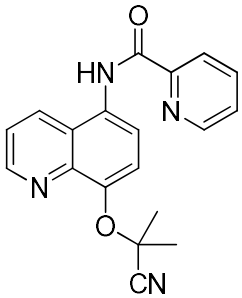
(3af): white solid (21.2 mg, 29%), mp 141-143 °C; ^{1}H NMR (400MHz, $CDCl_3$) δ 10.47 (s, 1H), 8.70-8.69 (m, 1H), 8.34 (d, J = 7.80 Hz, 1H), 8.19 (d, J = 8.44 Hz, 1H), 8.06-8.04 (m, 1H), 7.98-7.94 (m, 1H), 7.98-7.94 (m, 1H), 7.89-7.87 (m, 1H), 7.74 (d, J = 8.44 Hz, 1H), 7.56-7.53 (m, 1H), 1.86 (s, 6H); ^{13}C NMR (100MHz, $CDCl_3$), δ 162.6, 149.7, 148.2, 147.6, 137.9, 134.3, 130.8, 129.3, 126.8, 126.7, 122.7, 121.4, 121.3, 121.0, 118.2, 117.0, 73.8, 27.0; HRMS (ESI$^+$) m/z [M+H$^+$] calcd for $C_{20}H_{16}BrN_3O_2$: 410.0499, Found: 410.0501.



3ag

N-(5-((2-cyanopropan-2-yl)oxy)quinolin-8-yl)picolinamide

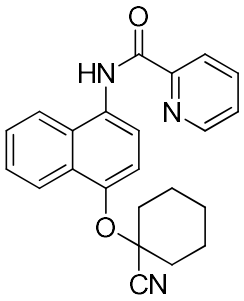
(3ag): white solid (49.4 mg, 74%), mp 147-149 °C; ^{1}H NMR (400MHz, $CDCl_3$) δ 12.15 (s, 1H), 8.99-8.97 (m, 2H), 8.79-8.77 (m, 1H), 8.48-8.46 (m, 1H), 8.35 (d, J = 7.80 Hz, 1H), 7.95-7.91 (m, 1H), 7.56 (d, J = 8.56 Hz, 1H), 7.53-7.49 (m, 2H), 1.85 (s, 6H); ^{13}C NMR (100MHz, $CDCl_3$), δ 162.6, 150.4, 149.2, 148.6, 144.9, 139.9, 137.5, 131.2, 131.1, 126.3, 123.5, 122.5, 121.5, 121.0, 116.3, 115.9, 72.6, 27.5; HRMS (ESI$^+$) m/z [M+H$^+$] calcd for $C_{19}H_{16}N_4O_2$: 333.1346, Found: 333.1348.



3ah

N-(8-((2-cyanopropan-2-yl)oxy)quinolin-5-yl)picolinamide

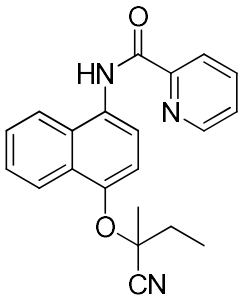
(3ah): pale yellow solid (21.9 mg, 33%), mp 135-137 °C; ^{1}H NMR (400MHz, $CDCl_3$) δ 10.55 (s, 1H), 9.02-9.00 (m, 1H), 8.71-8.70 (m, 1H), 8.43-8.40 (m, 1H), 8.35 (d, J = 7.80 Hz, 1H), 8.26 (d, J = 8.40 Hz, 1H), 7.99-7.95 (m, 1H), 7.79 (d, J = 8.40 Hz, 1H), 7.58-7.52 (m, 2H), 1.89 (s, 6H); ^{13}C NMR (100MHz, $CDCl_3$), δ 162.6, 150.2, 149.5, 148.2, 148.1, 143.2, 137.9, 130.0, 129.1, 126.9, 123.6, 122.7, 121.5, 121.1, 120.5, 120.0, 73.9, 27.6; HRMS (ESI$^+$) m/z [M+H$^+$] calcd for $C_{19}H_{16}N_4O_2$: 333.1346, Found: 333.1349.



3ak

N-(4-((1-cyanocyclohexyl)oxy)naphthalen-1-yl)picolinamide

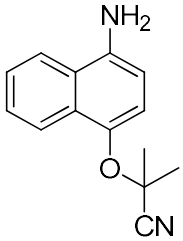
(3ak): pale yellow solid (25.8 mg, 35%), mp 121-123 °C; ^{1}H NMR (400MHz, $CDCl_3$) δ 10.57 (s, 1H), 8.71-8.70 (m, 1H), 8.36 (d, J = 7.80 Hz, 1H), 8.26-8.22 (m, 2H), 8.05 (d, J = 8.12 Hz, 1H), 7.97-7.93 (m, 1H), 7.63-7.52 (m, 4H), 2.37-2.33 (m, 2H), 2.06-2.00 (m, 2H), 1.86-1.83 (m, 2H), 1.70-1.62 (m, 3H), 1.43-1.36 (m, 1H); ^{13}C NMR (100MHz, $CDCl_3$), δ 162.4, 150.0, 148.2, 147.3, 137.8, 128.5, 128.3, 128.1, 126.9, 126.6, 126.0, 122.9, 122.6, 121.0, 120.3, 119.2, 113.9, 35.8, 24.6, 22.4; HRMS (ESI$^+$) m/z [M+H$^+$] calcd for $C_{23}H_{21}N_3O_2$: 372.1707, Found: 372.1710.



3al

N-(4-((2-cyanobutan-2-yl)oxy)naphthalen-1-yl)picolinamide

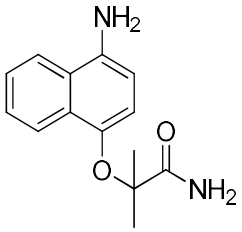
(3al): pale yellow solid (17.3 mg, 28%), mp 125-127 °C; ^{1}H NMR (400MHz, $CDCl_3$) δ 10.59 (s, 1H), 8.71-8.70 (m, 1H), 8.36 (d, J = 7.40 Hz, 1H), 8.25 (d, J = 8.36 Hz, 1H), 8.20-8.18 (m, 1H), 8.06 (d, J = 8.28 Hz, 1H), 7.97-7.93 (m, 1H), 7.63-7.59 (m, 1H), 7.57-7.52 (m, 3H), 2.31-2.21 (m, 1H), 2.17-2.11 (m, 1H), 1.72 (s, 3H), 1.27 (t, J = 7.55Hz, 3H); ^{13}C NMR (100MHz, $CDCl_3$), δ 162.4, 150.0, 148.2, 147.6, 137.8, 128.7, 128.5, 128.0, 126.9, 126.6, 126.1, 122.9, 122.6, 121.0, 120.4, 119.1, 114.1, 76.4, 34.2, 24.2, 8.7; HRMS (ESI$^+$) m/z [M+H$^+$] calcd for $C_{21}H_{19}N_3O_2$: 346.1550, Found: 346.1554.



4a

2-((4-aminonaphthalen-1-yl)oxy)-2-methylpropanenitrile

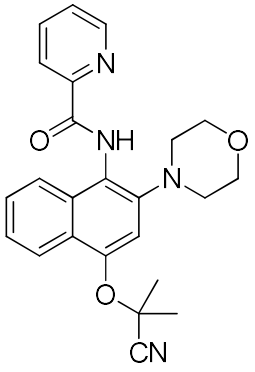
(4a): brown liquid (34.4 mg, 76%), ^{1}H NMR (400MHz, $CDCl_3$) δ 8.07-8.05 (m, 1H), 7.82-7.80 (m, 1H), 7.51-7.48 (m, 2H), 7.37 (d, J = 8.12 Hz, 1H), 6.72 (d, J = 8.12 Hz, 1H), 1.76 (s, 6H); ^{13}C NMR (100MHz, $CDCl_3$), δ 143.2, 139.0, 129.5, 126.0, 125.5, 124.6, 122.8, 121.6, 121.2, 116.9, 109.1, 73.1, 27.4; HRMS (ESI$^+$) m/z [M+H$^+$] calcd for $C_{14}H_{14}N_2O$: 227.1173, Found: 227.1180.



5a

2-((4-aminonaphthalen-1-yl)oxy)-2-methylpropanamide

(5a): brown solid (40.1 mg, 82%), mp 94-96 ^{o}C; ^{1}H NMR (400MHz, $CDCl_3$) δ 8.17-8.15 (m, 1H), 7.83-7.80 (m, 1H), 7.51-7.49 (m, 2H), 6.88 (d, J = 8.08 Hz, 1H), 6.66 (d, J = 8.04 Hz, 1H), 1.57 (s, 6H); ^{13}C NMR (100MHz, $CDCl_3$), δ 178.3, 143.1, 137.9, 129.4, 125.8, 125.5, 124.8, 123.0, 121.2, 115.9, 109.0, 82.1, 25.0; HRMS (ESI$^+$) m/z [M+H$^+$] calcd for $C_{14}H_{16}N_2O_2$: 245.1285, Found: 245.1283.

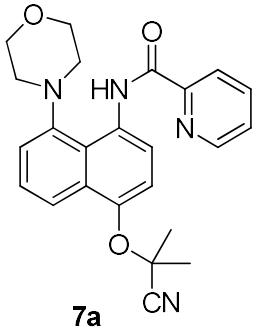


6a

N-(4-((2-cyanopropan-2-yl)oxy)-2-morpholinonaphthalen-1-yl)picolinamide

(6a): brown solid (50.7 mg, 61%), mp 187-189 ^{o}C; ^{1}H NMR (400MHz, $CDCl_3$) δ 10.17 (s, 1H), 8.73 (d, J = 4.68 Hz, 1H), 8.35 (d, J = 7.76 Hz, 1H), 8.04 (d, J = 8.36 Hz, 1H), 7.98-7.94 (m, 1H), 7.87 (d, J = 8.36 Hz, 1H), 7.57-7.49 (m, 3H), 7.45-7.41 (m, 1H), 3.82-3.80 (m, 4H), 3.04-3.02 (m,

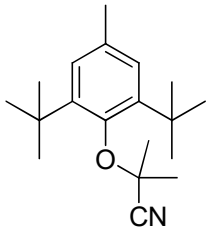
4H), 1.84 (s, 6H); ^{13}C NMR (100MHz, $CDCl_3$), δ 163.6, 150.2, 149.9, 148.3, 144.2, 137.7, 130.7, 127.0, 126.6, 125.9, 124.9, 124.5, 122.8, 122.3, 122.1, 121.3, 108.3, 72.7, 67.4, 51.9, 27.5; HRMS (ESI^+) m/z [$M+H^+$] calcd for $C_{24}H_{24}N_4O_3$: 417.1921, Found: 417.1921.



7a

N-(4-((2-cyanopropan-2-yl)oxy)-8-morpholinonaphthalen-1-yl)picolinamide

(7a): white solid (40.1 mg, 48%), mp 144-146 °C; ^{1}H NMR (400MHz, $CDCl_3$) δ 13.79 (s, 1H), 9.10 (d, J = 8.72 Hz, 1H), 8.74-8.73 (m, 1H), 8.38 (d, J = 7.84 Hz, 1H), 8.02-7.92 (m, 2H), 7.56-7.42 (m, 4H), 4.28-4.22 (m, 2H), 3.86-3.84 (m, 2H), 3.20-3.18 (m, 2H), 3.06-3.00 (m, 2H), 1.83 (s, 6H), ^{13}C NMR (100MHz, $CDCl_3$), δ 163.1, 151.2, 149.3, 147.9, 146.5, 137.6, 132.0, 130.9, 126.4, 125.7, 123.4, 121.1, 121.0, 119.8, 117.9, 116.6, 115.3, 72.5, 65.6, 54.5, 27.5; HRMS (ESI^+) m/z [$M+H^+$] calcd for $C_{24}H_{24}N_4O_3$: 417.1921, Found: 417.1925.



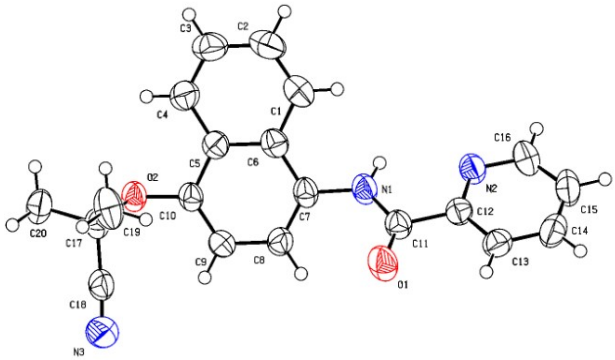
14a

2-(2,6-di-tert-butyl-4-methylphenoxy)-2-methylpropanenitrile

(**14a**): white solid, mp 106-108 ℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.54 (s, 2H), 1.41 (s, 3H), 1.29 (s, 6H), 1.25 (s, 18H); ^{13}C NMR (100 MHz, $CDCl_3$), δ 185.6, 149.3, 140.7, 123.5, 42.7, 39.8, 35.1, 29.4, 22.9, 22.6; HRMS (ESI^+) m/z [$M+H^+$] calcd for $C_{19}H_{29}NO$: 288.2322, Found: 288.2317.

5. The Single Crystal X-ray Diffraction Study

The Single Crystal X-ray Diffraction Study of **3aa**



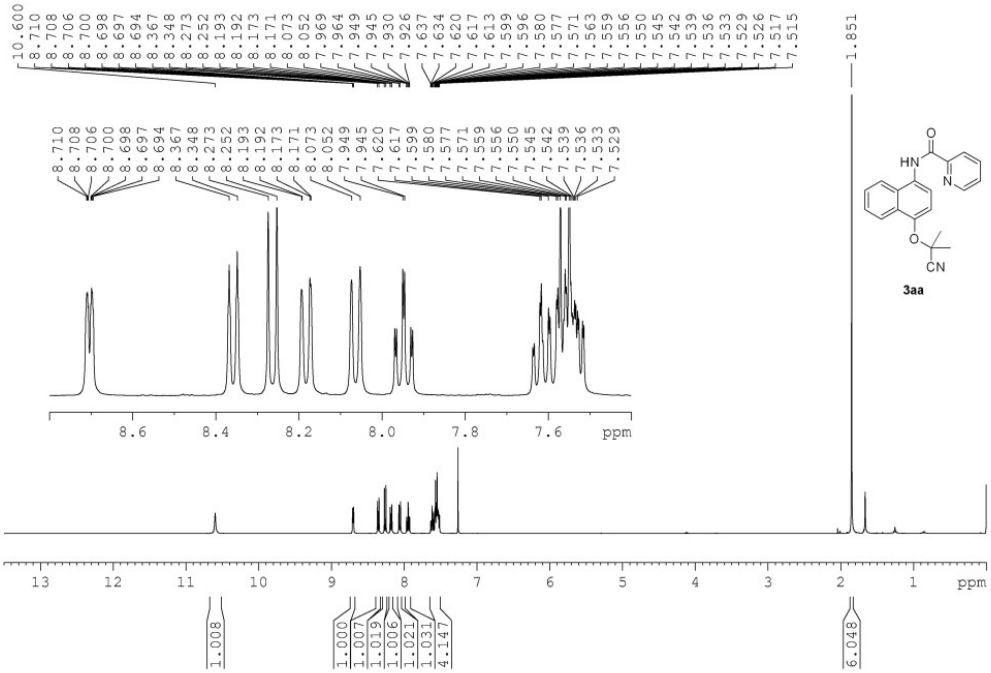
CCDC 2156275 (**3aa**) contains the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre *via* www.ccdc.cam.ac.uk/data_request/cif.

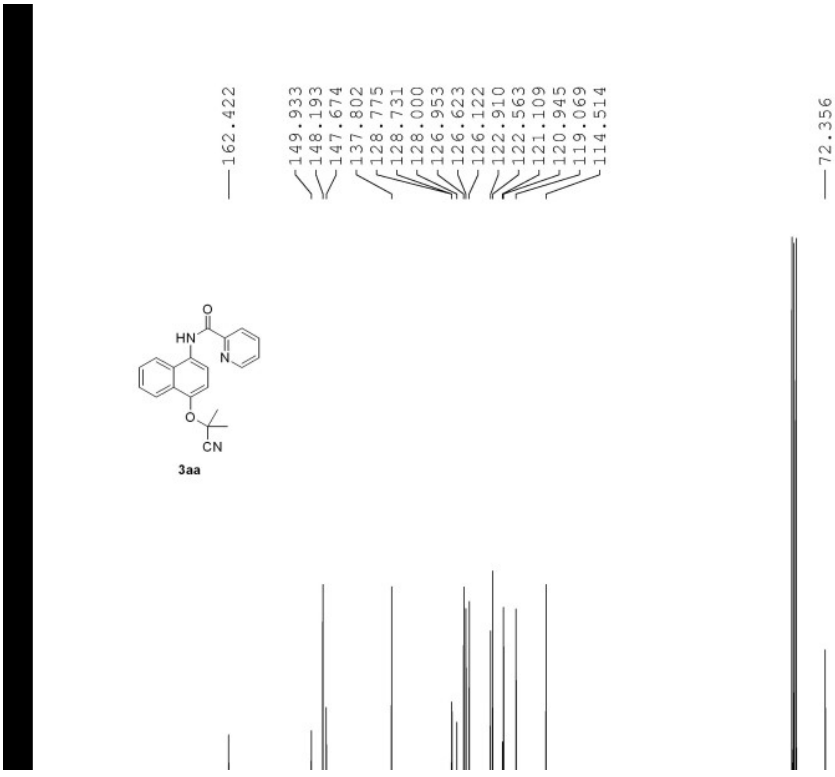
Table S3 Crystal data and structure refinement for CCDC 2156275.

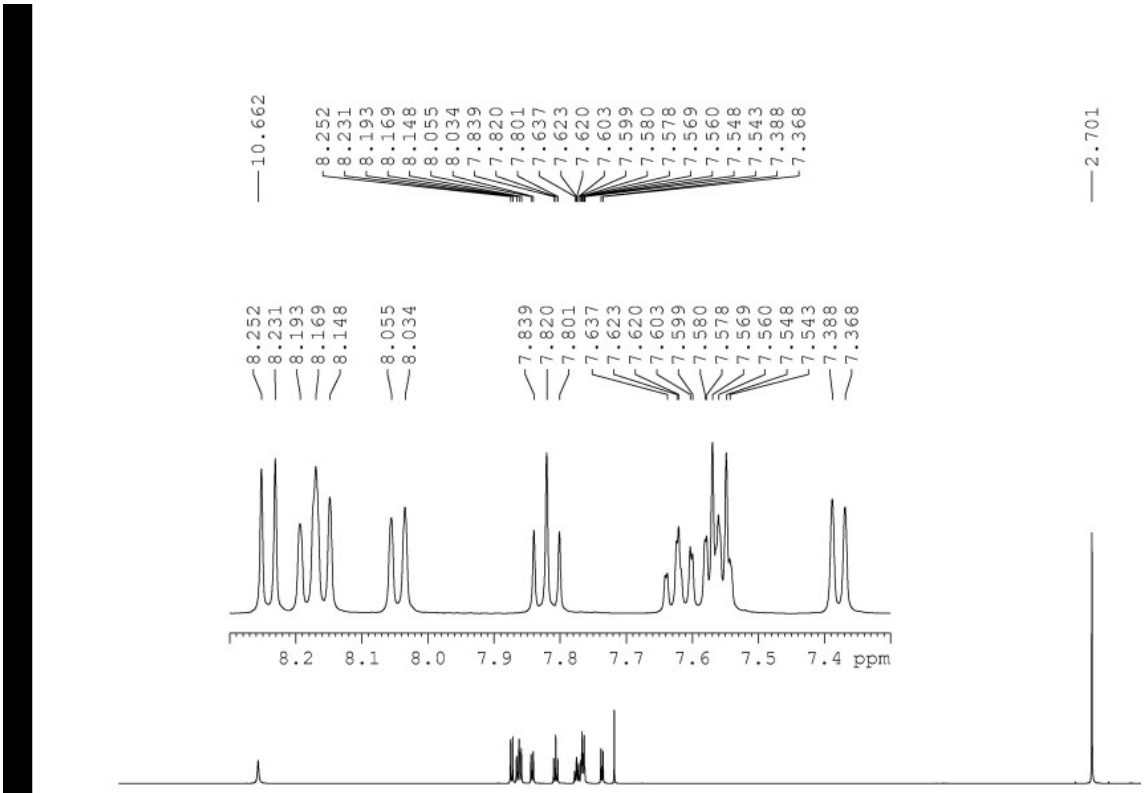
Empirical formula	$C_{20}H_{17}N_3O_2$
Formula weight	331.36
Temperature/K	293 (2)
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	9.5434 (4)
b/Å	10.6963 (7)
c/Å	16.8676 (6)
α/°	90
β/°	101.643 (4)
γ/°	90
Volume/Å^3	1686.40 (13)
Z	4
ρ_{calc}g/cm^3	1.305
μ/mm^{-1}	0.696
F(000)	696.0
Crystal size/mm^3	0.22 × 0.15 × 0.1
Radiation	CuKα (λ = 1.54184)
2Θ range for data collection/°	9.462 to 134.158
Index ranges	$-11 \le h \le 11$, $-6 \le k \le 12$, $-17 \le l \le 20$
Reflections collected	6134
Independent reflections	3002 [R_{int} = 0.0277, R_{sigma} = 0.0364]
Data/restraints/parameters	3002/0/232
Goodness-of-fit on F^2	1.031

Final R indexes [I>=2σ (I)]	R_1 = 0.0444, wR_2 = 0.1194
Final R indexes [all data]	R_1 = 0.0600, wR_2 = 0.1358
Largest diff. peak/hole / e Å^{-3}	0.16/-0.21

6. Copies of ^{1}H, ^{13}C NMR Spectra for the Products



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7.623
7.620
7.603
7.599
7.580
7.578
7.569
7.560
7.548
7.543
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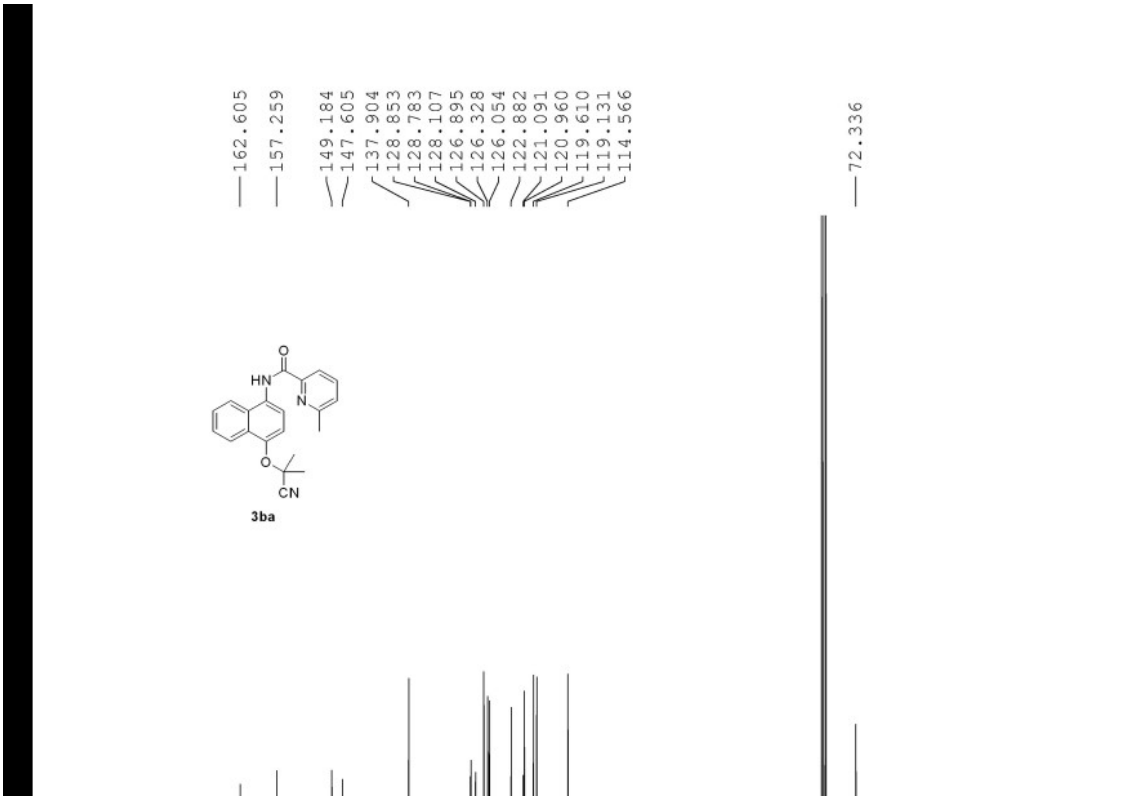
7.5
7.4 ppm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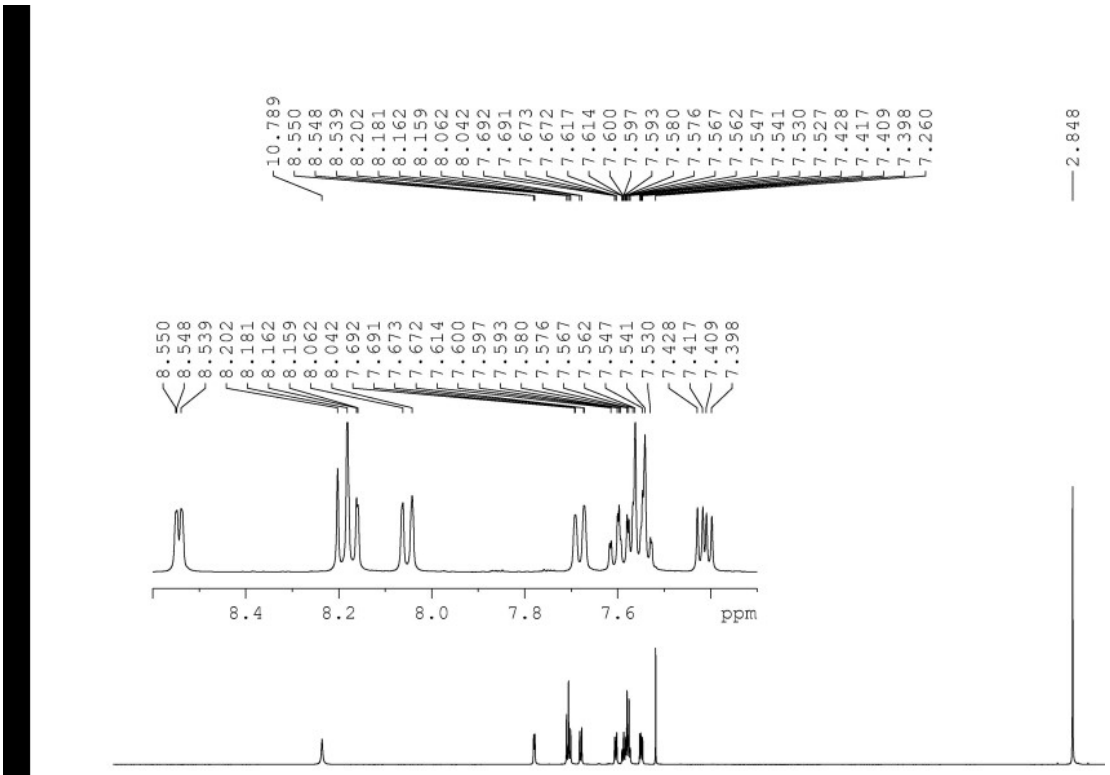
O
CN
3ba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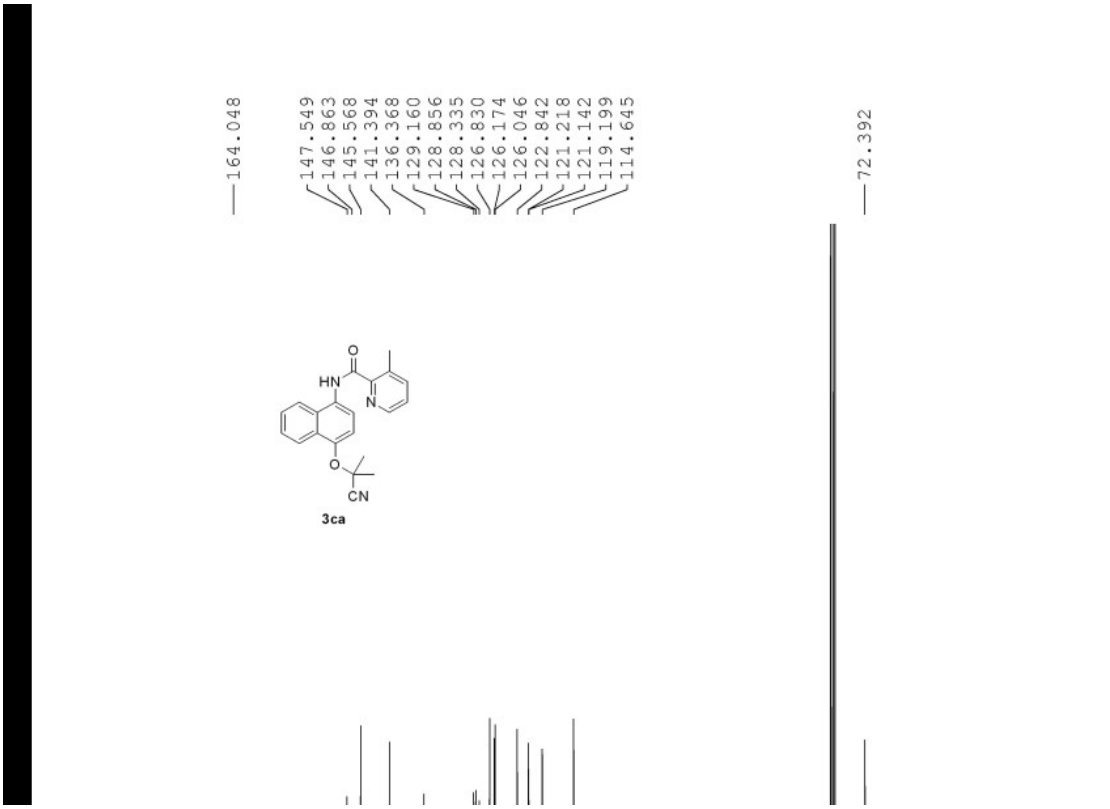
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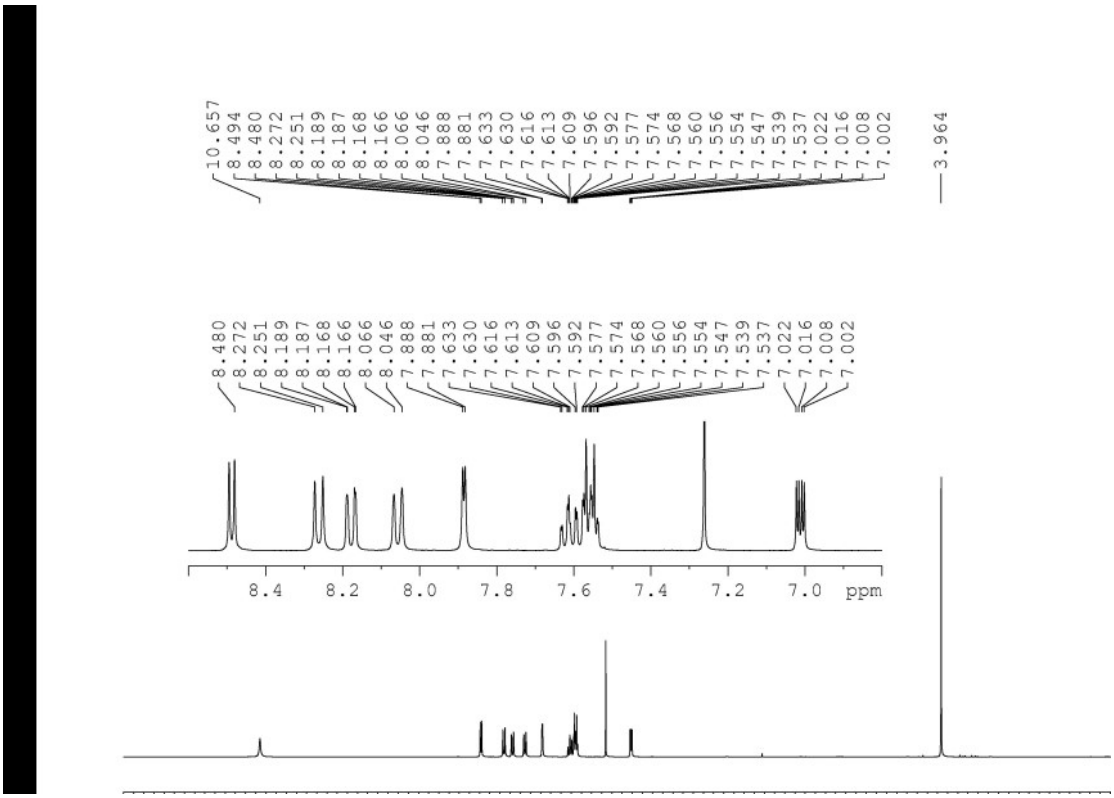
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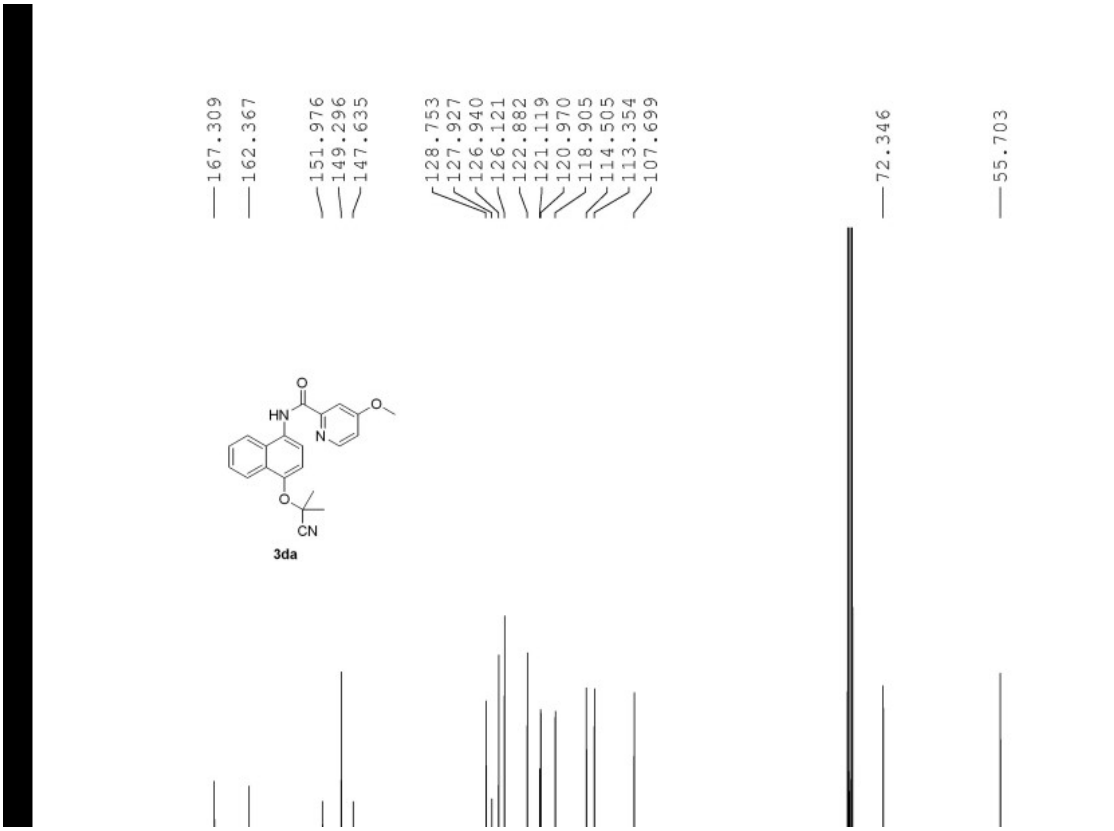
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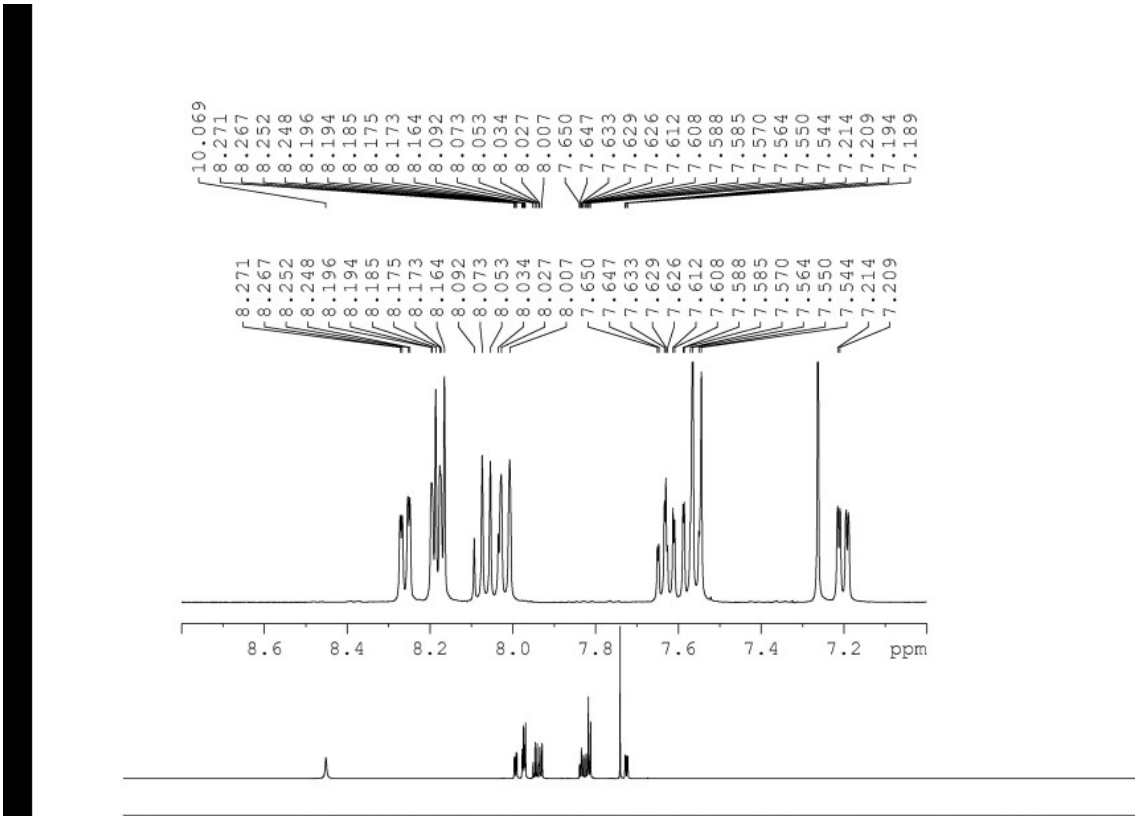
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8.053
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8.027
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7.585
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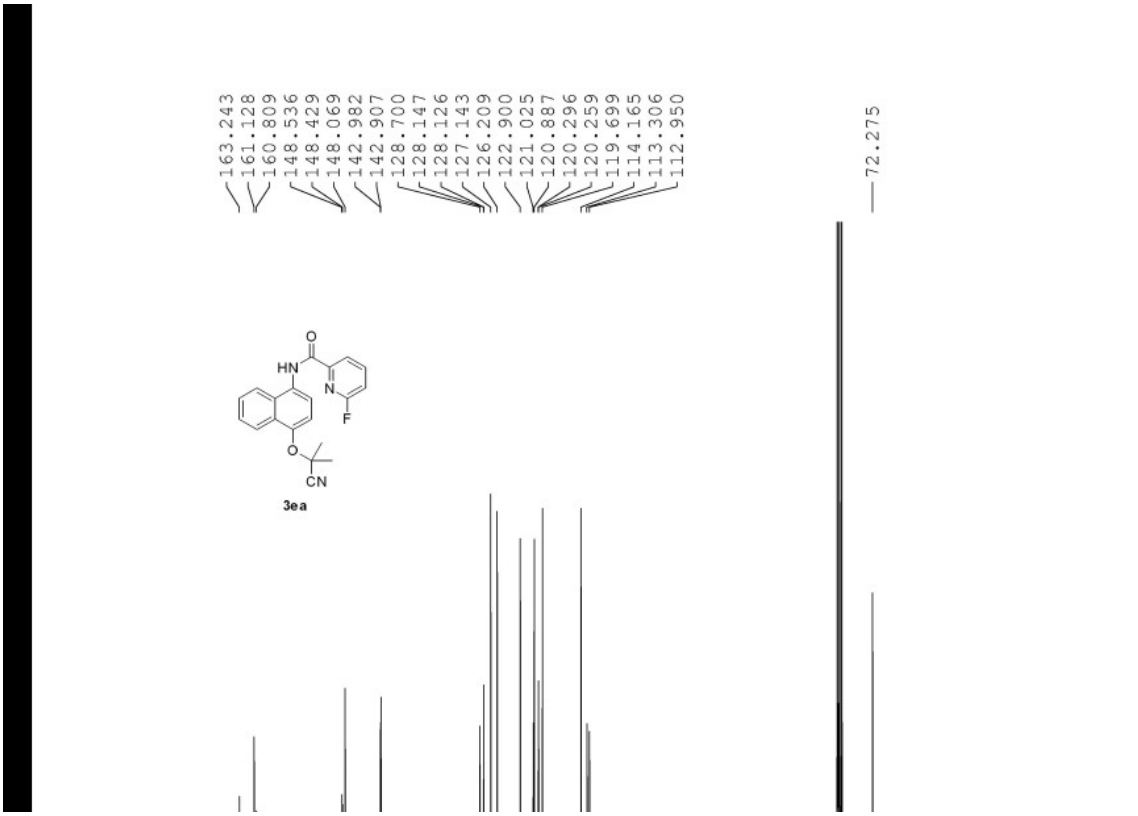
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F
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CN
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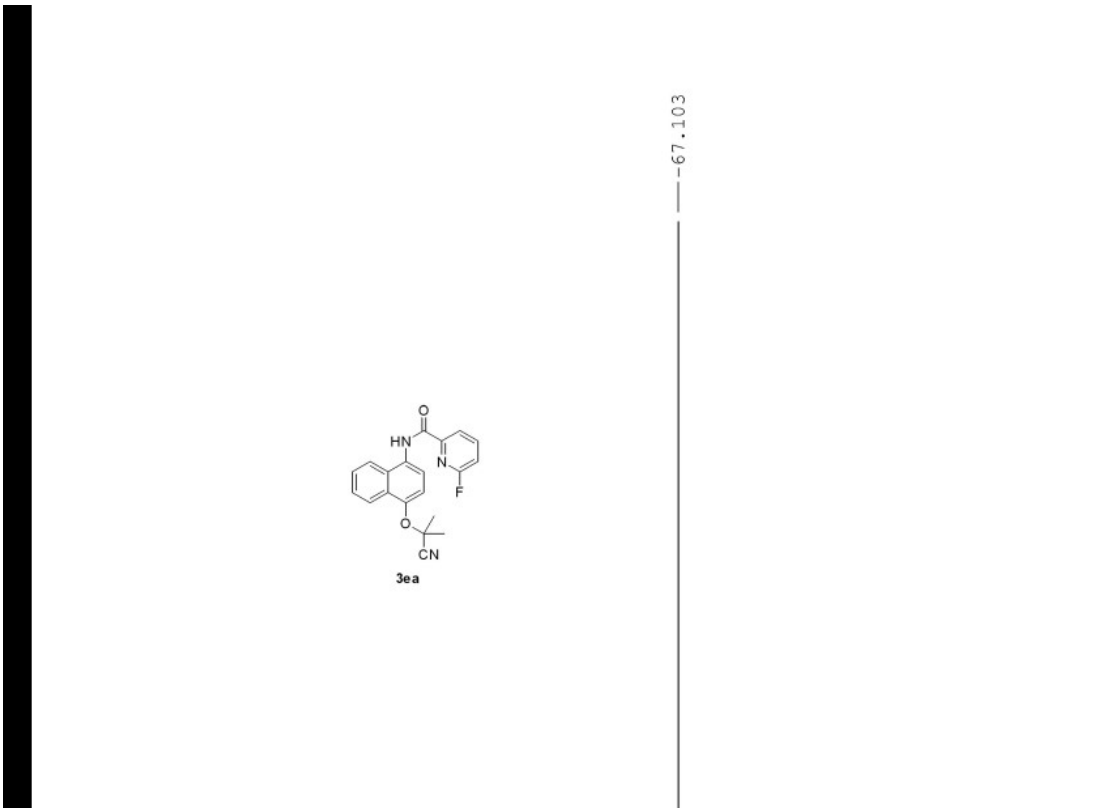
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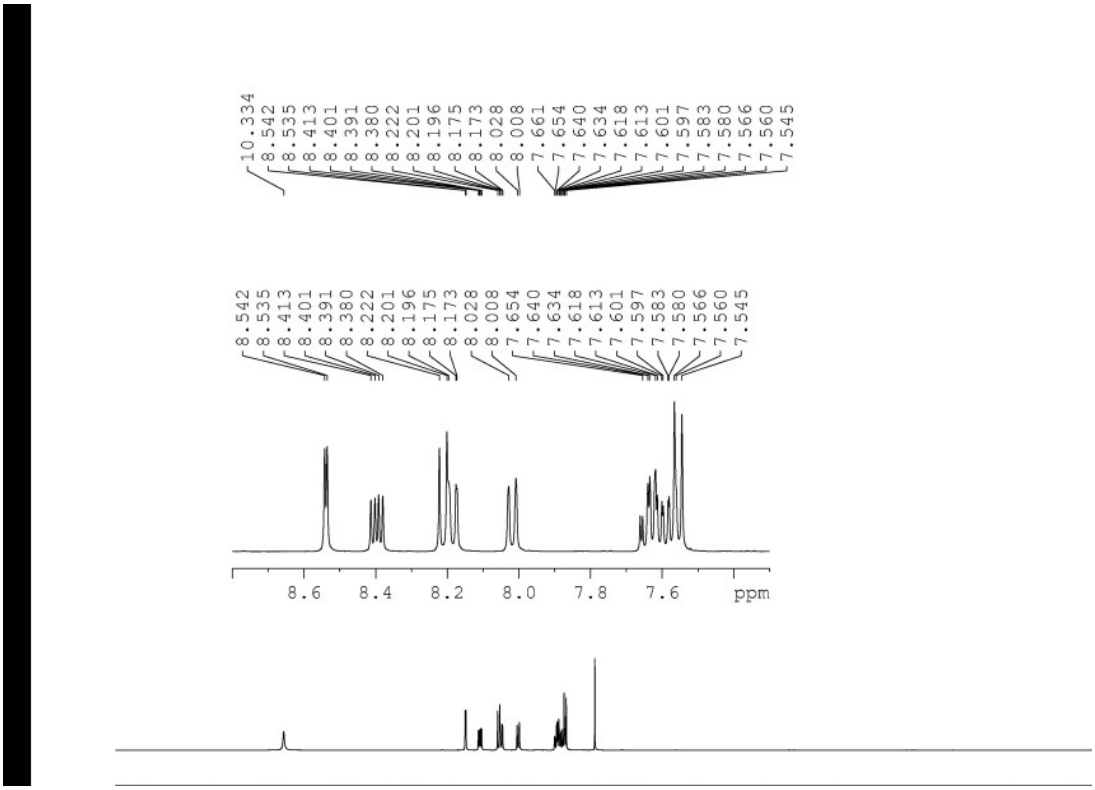
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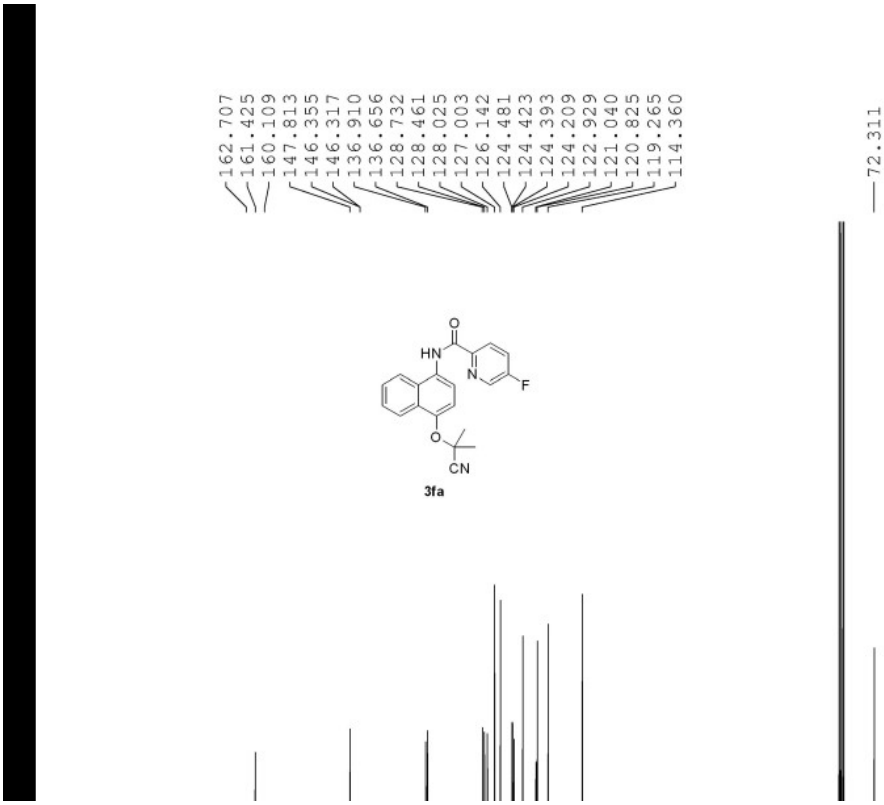
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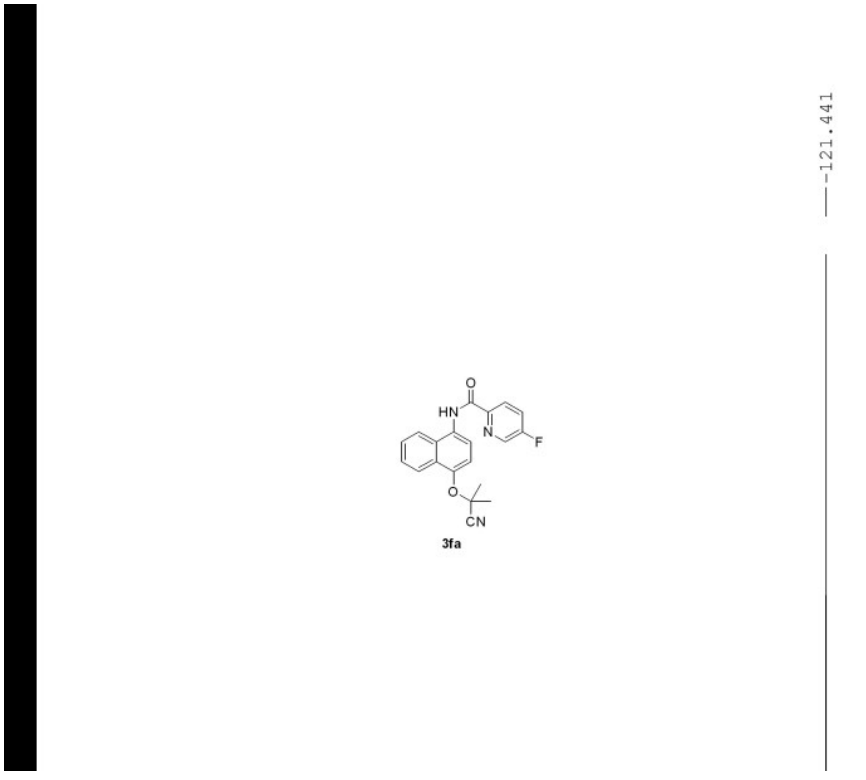
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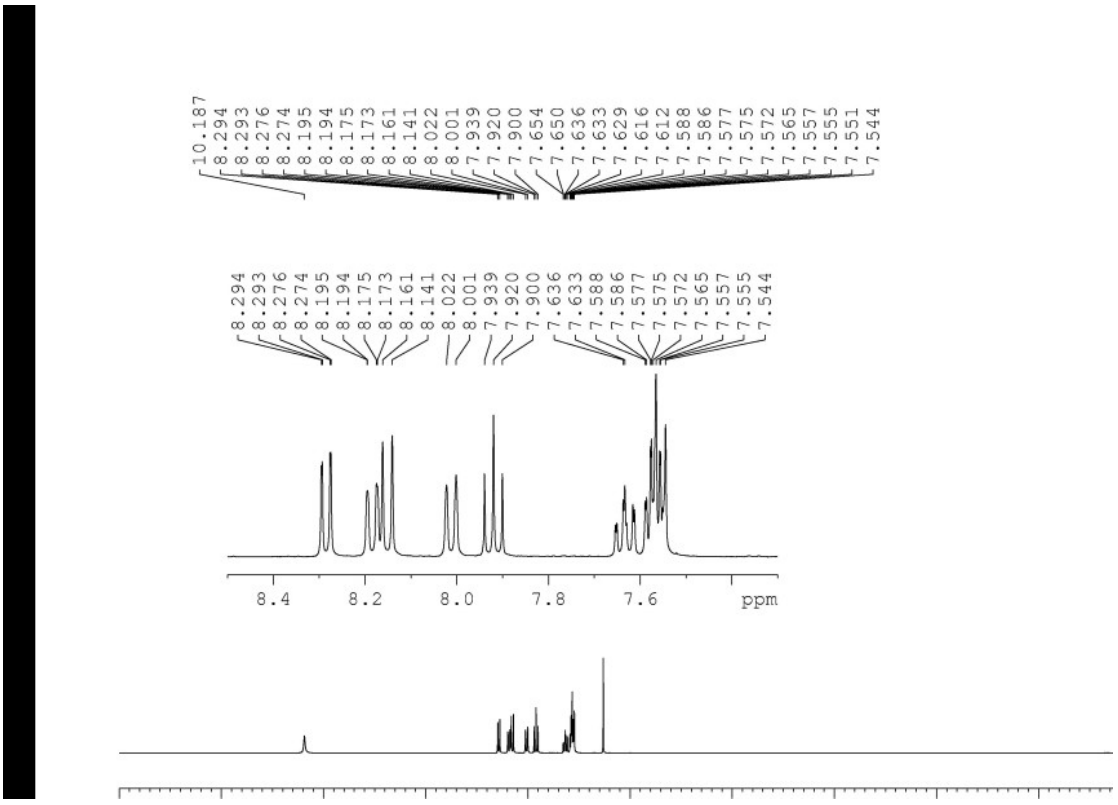
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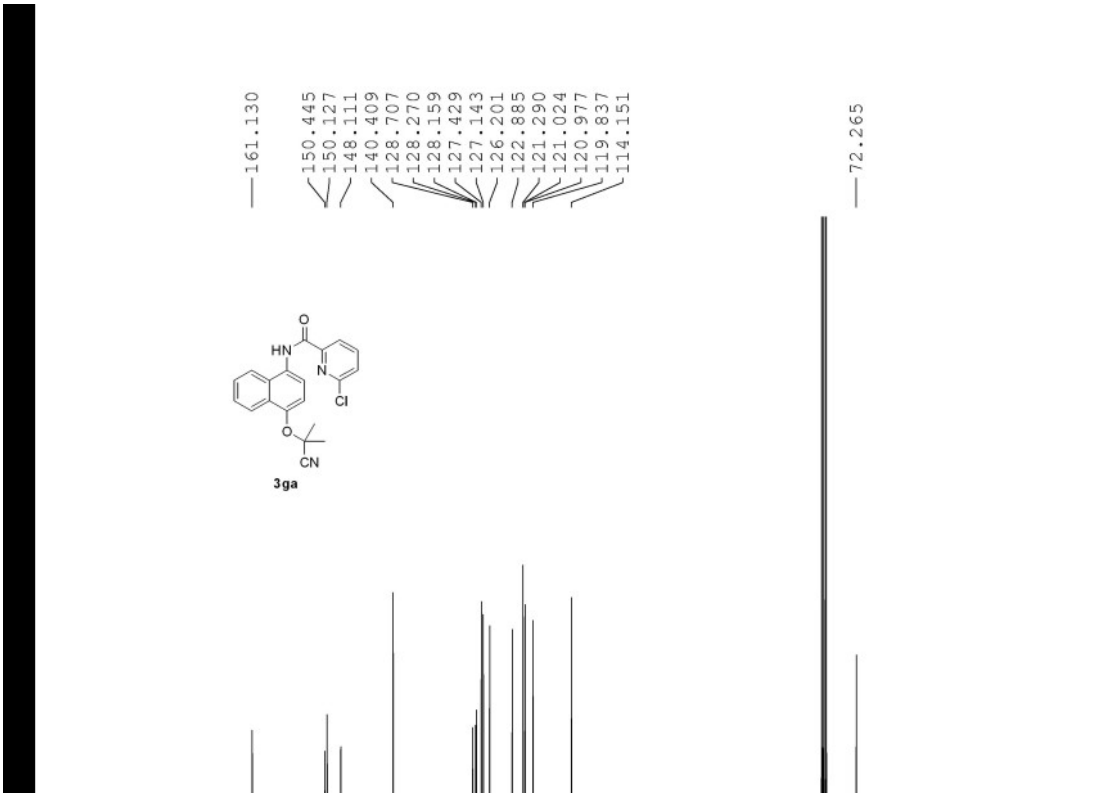
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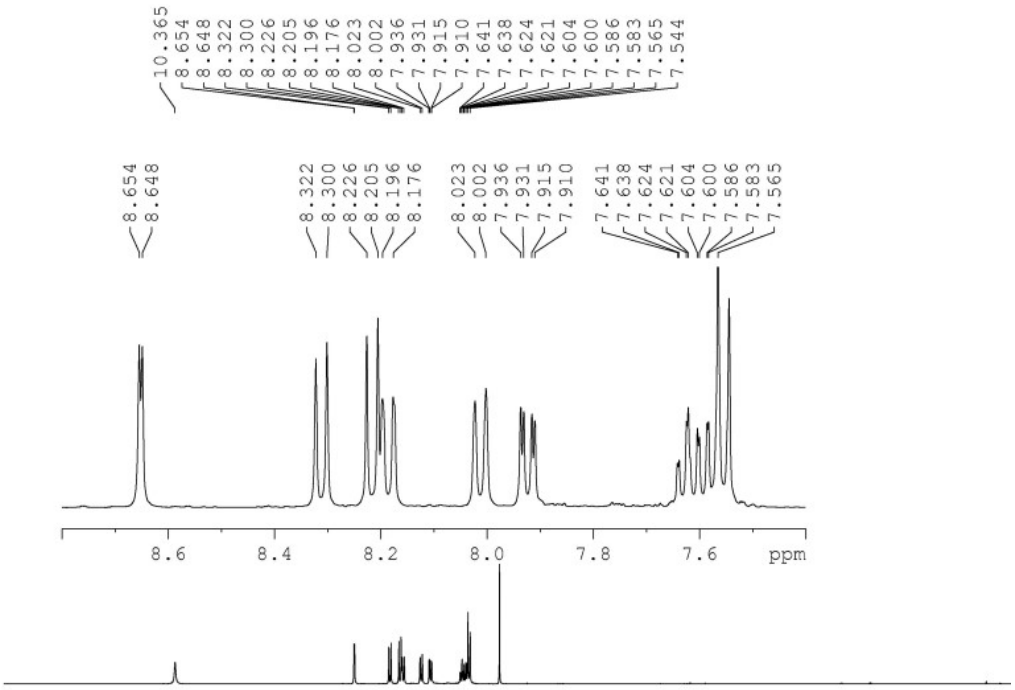
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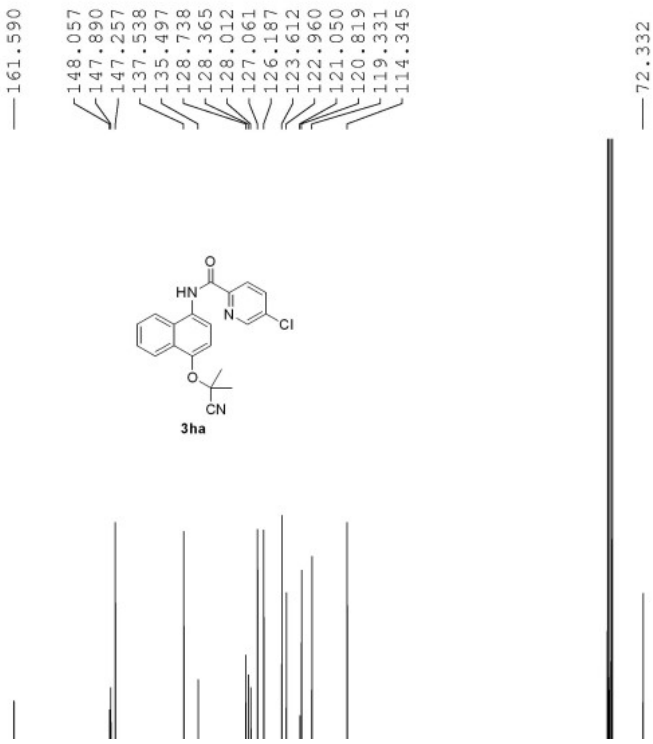
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Cl
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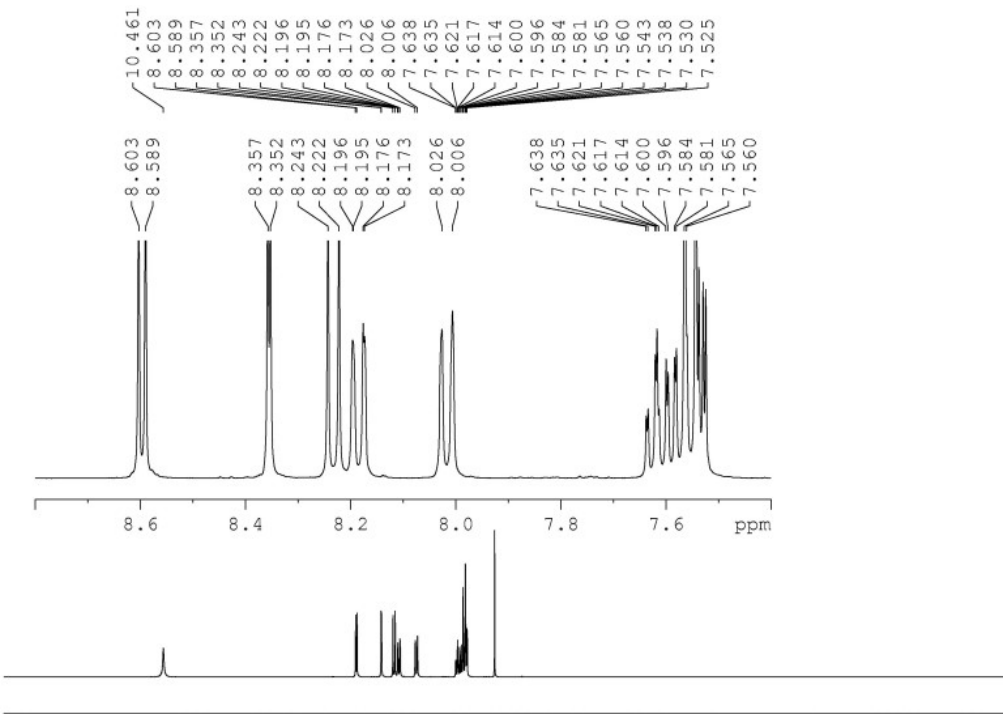
3ha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7.8
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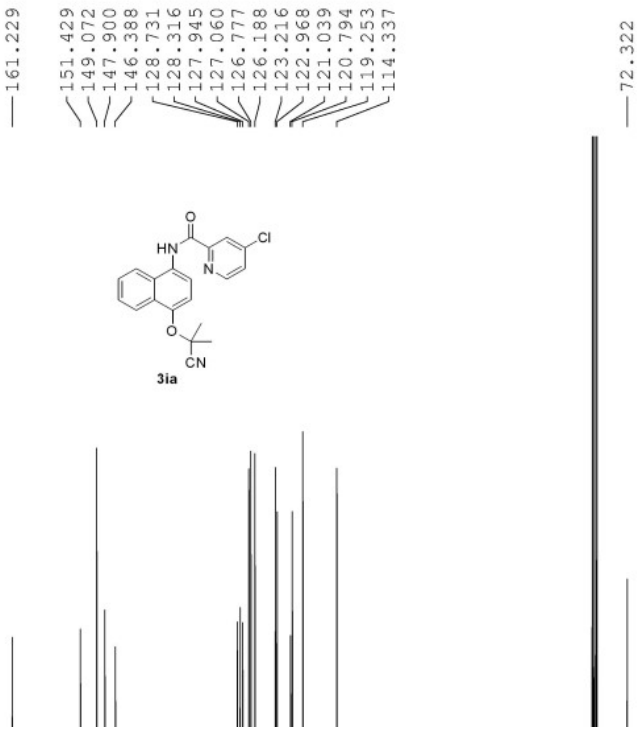
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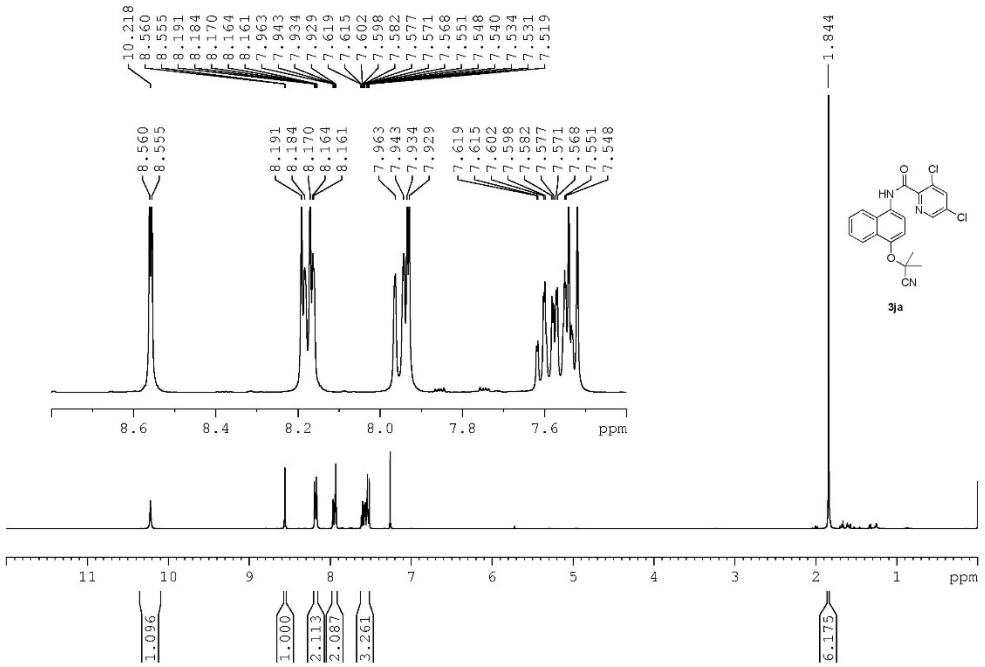
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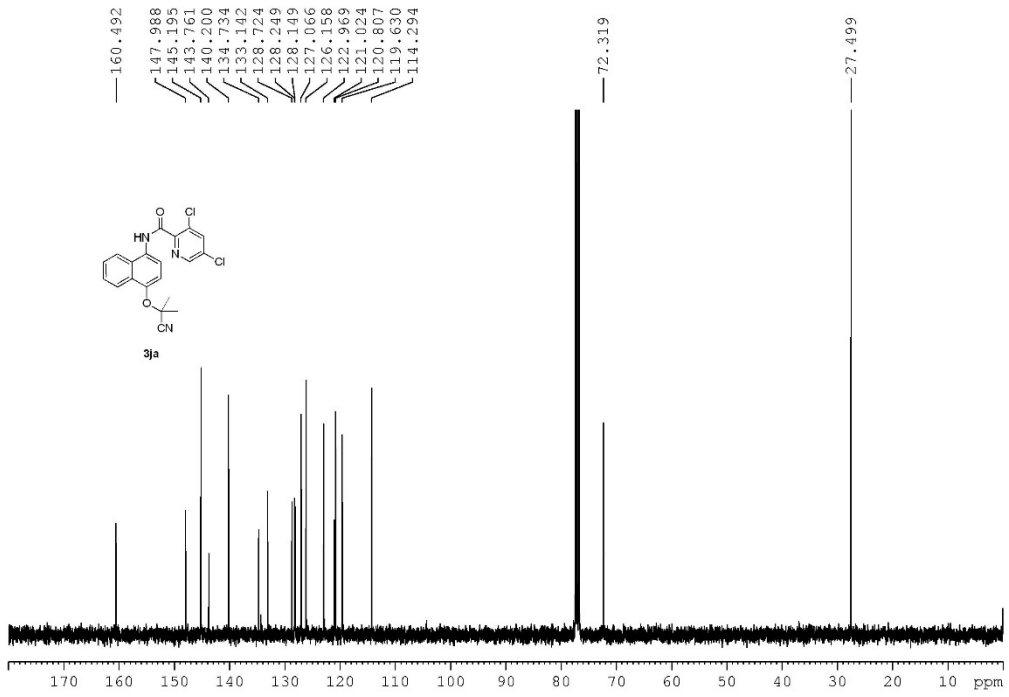
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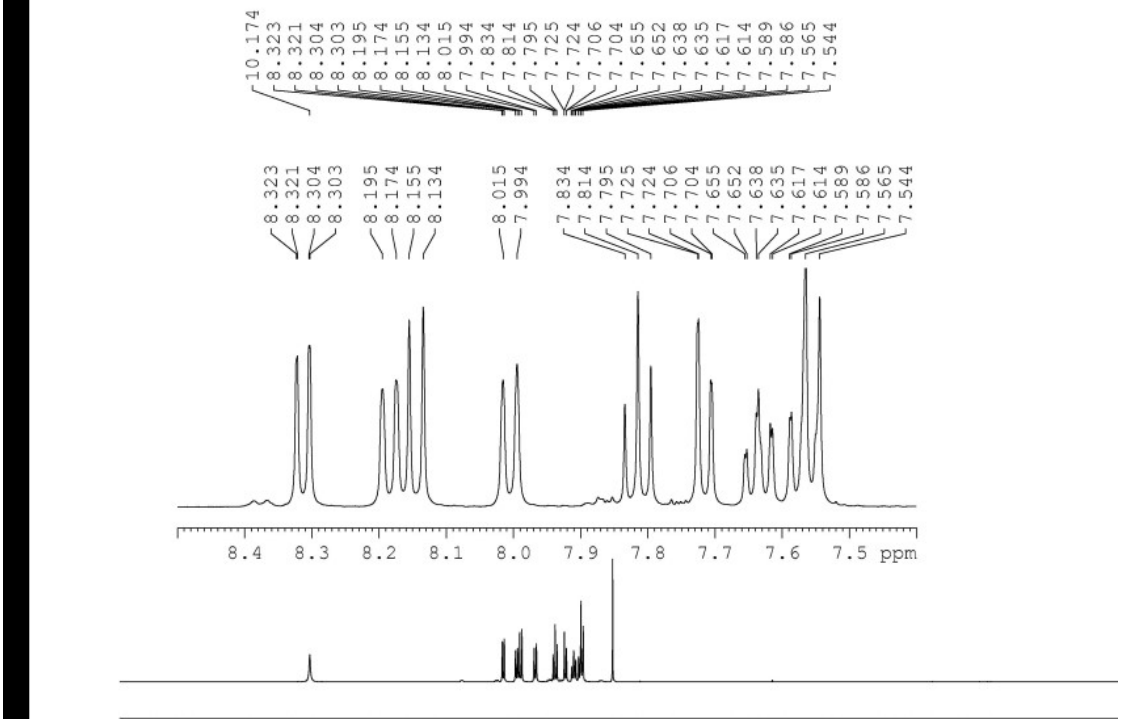
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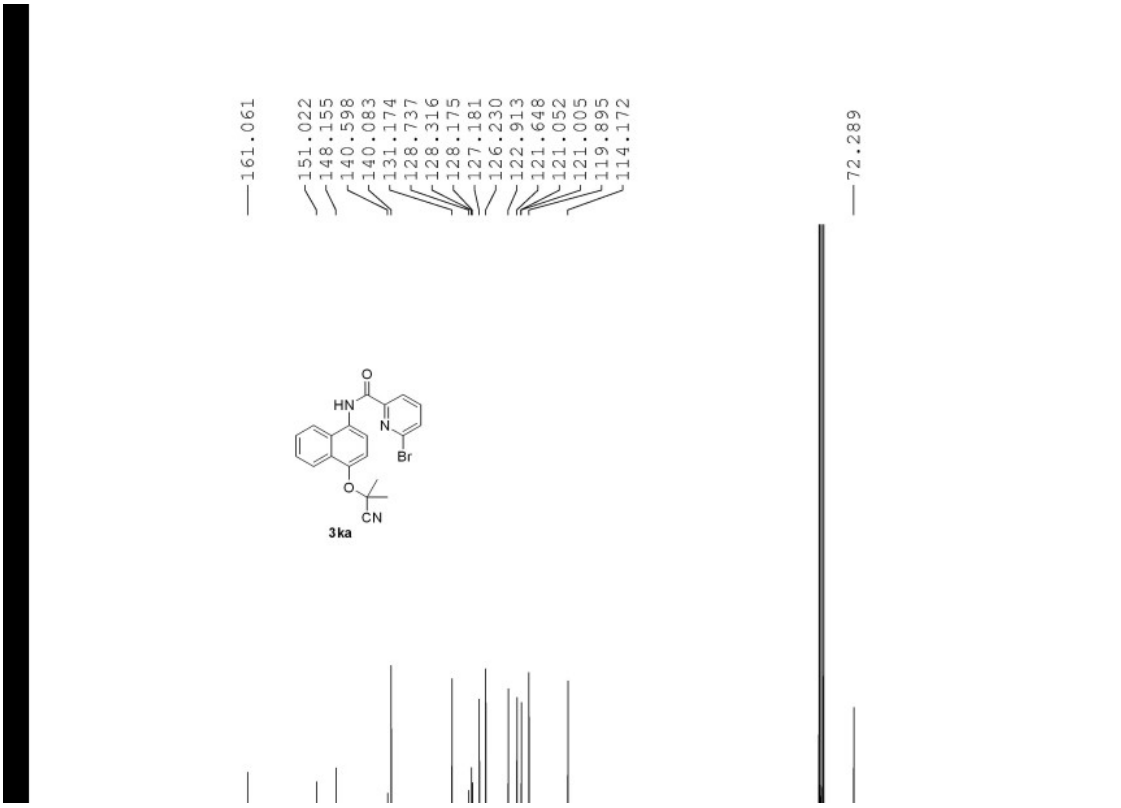
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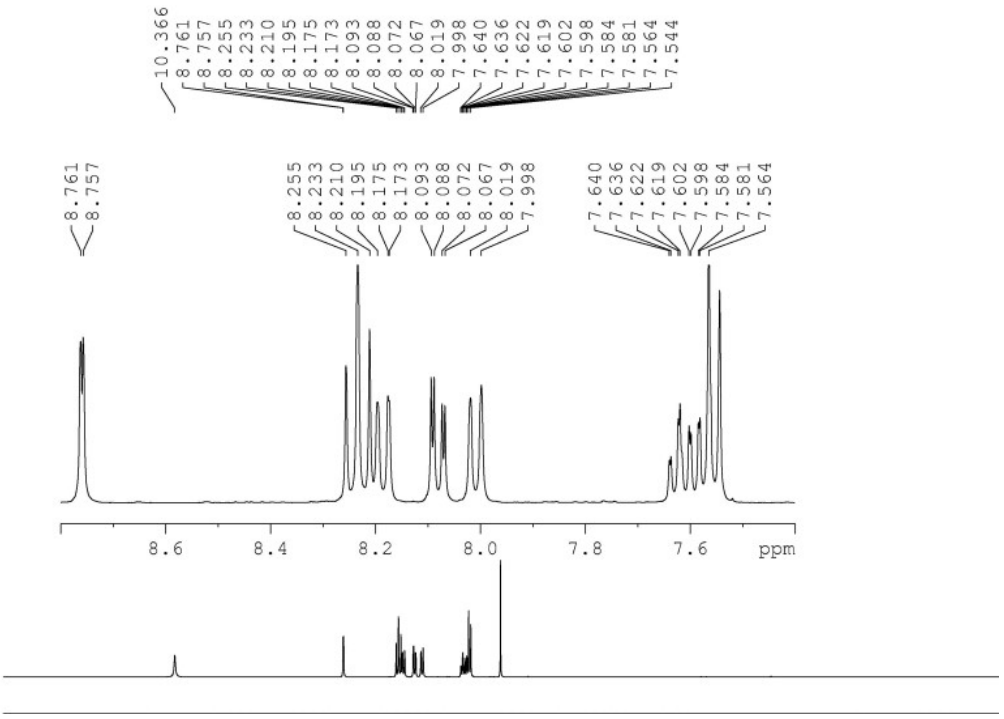
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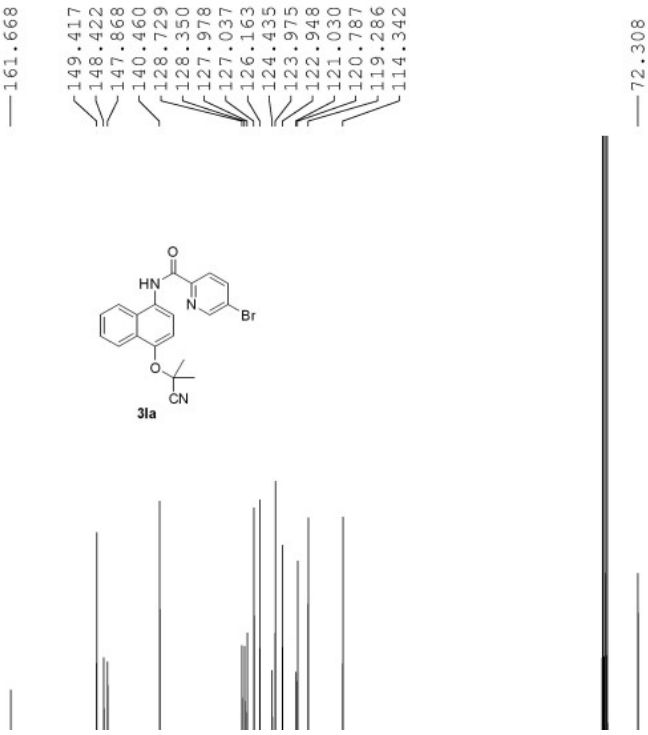
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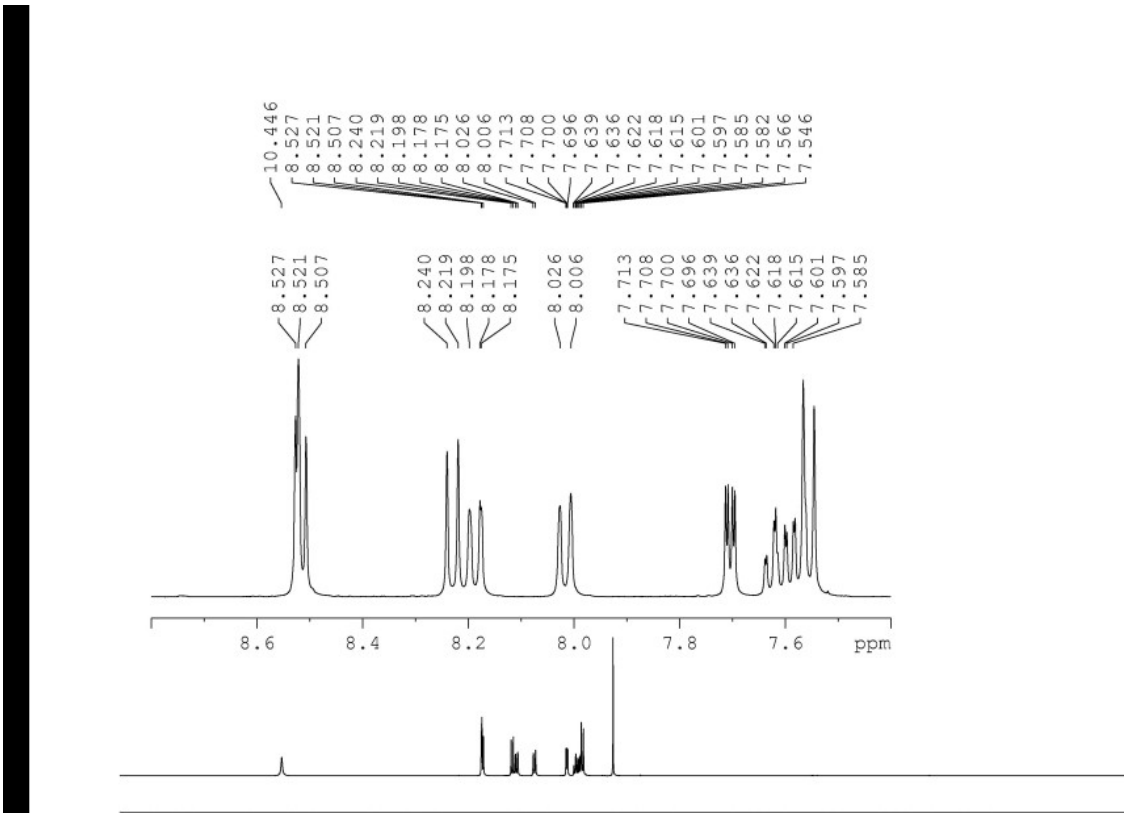
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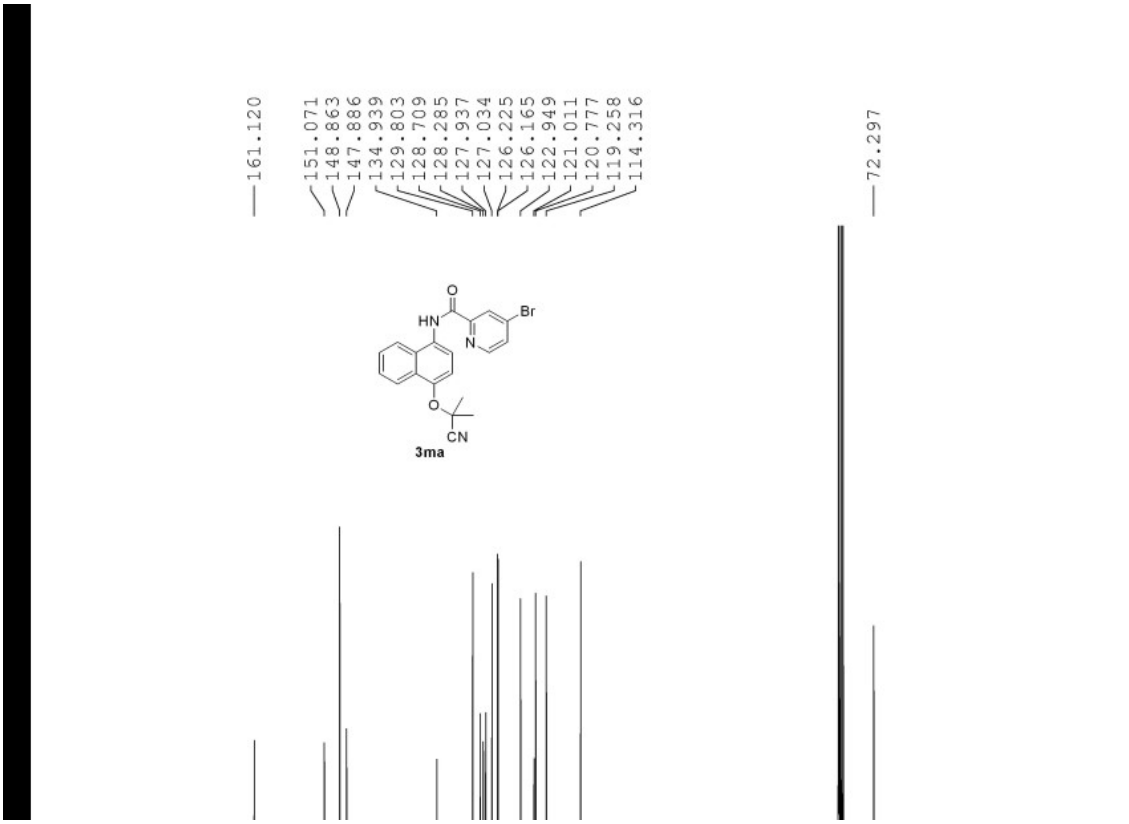
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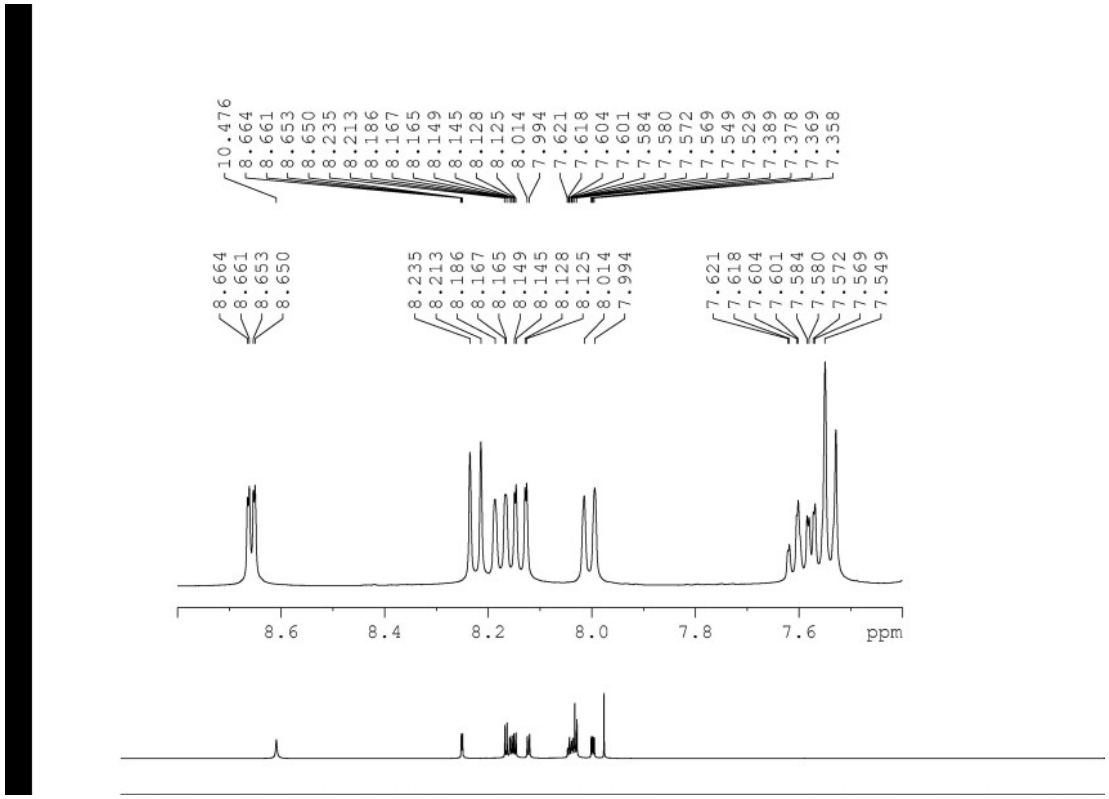
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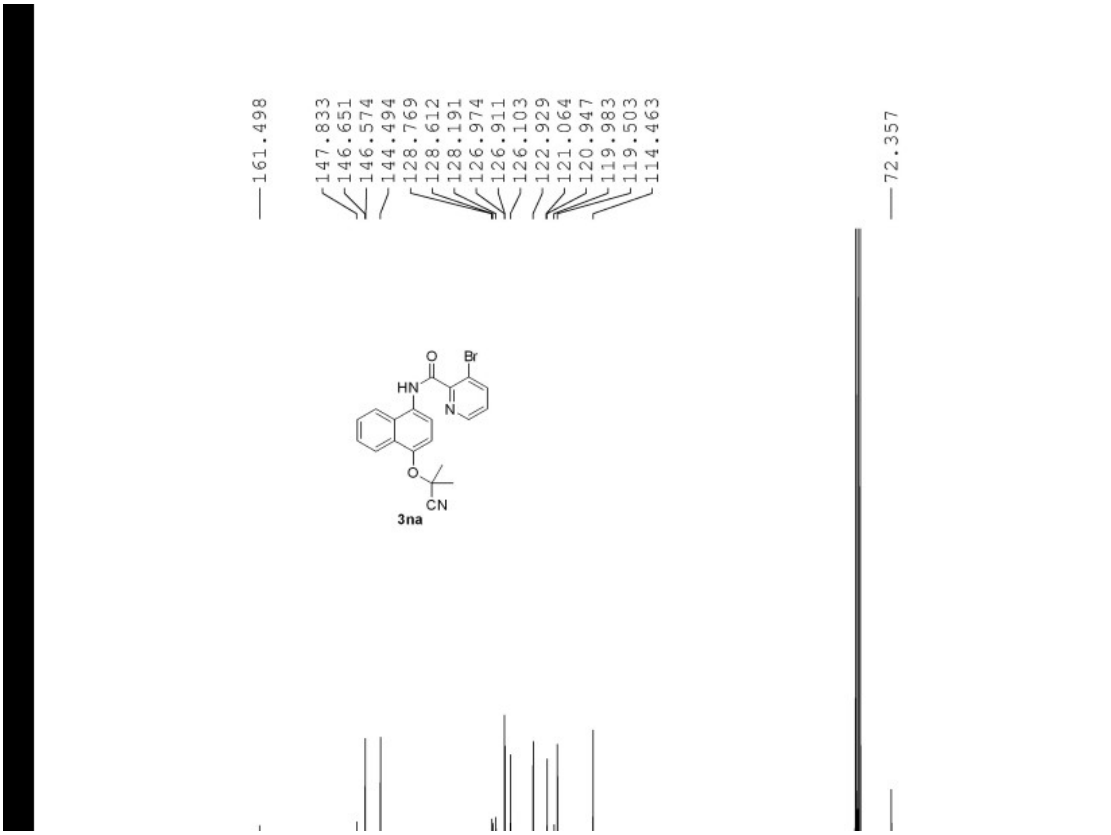
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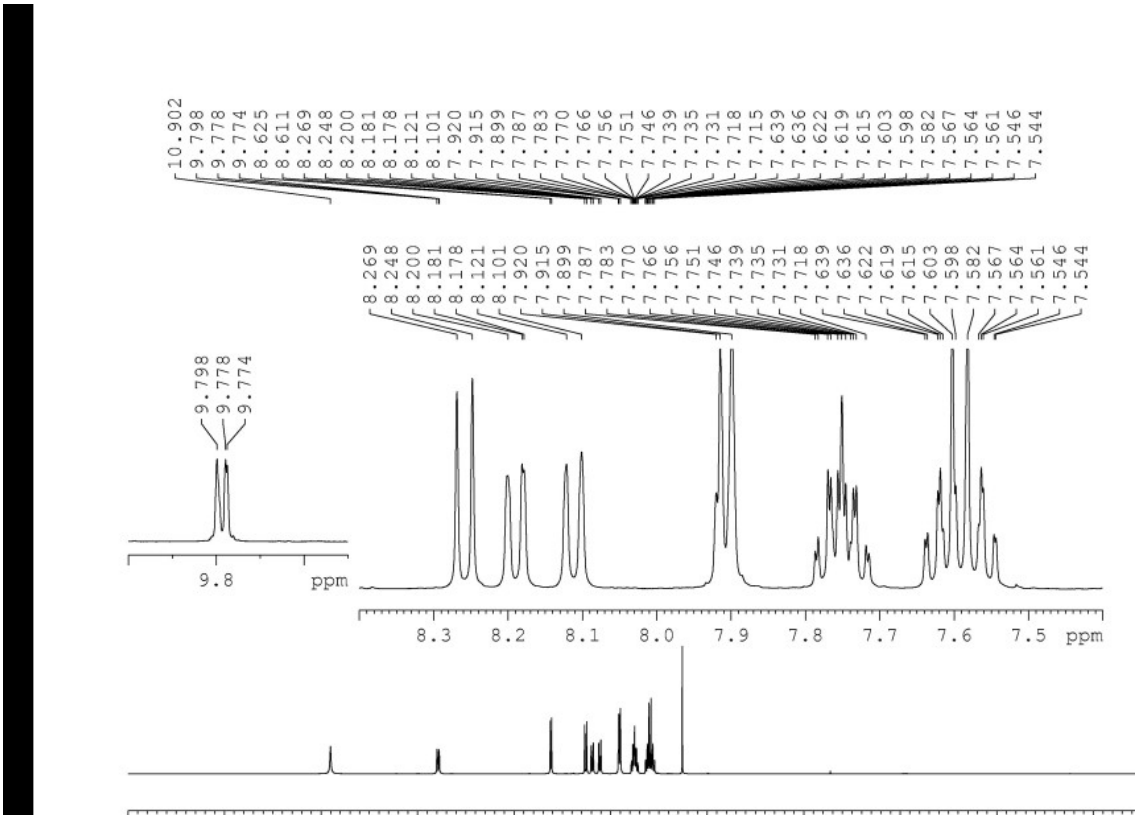
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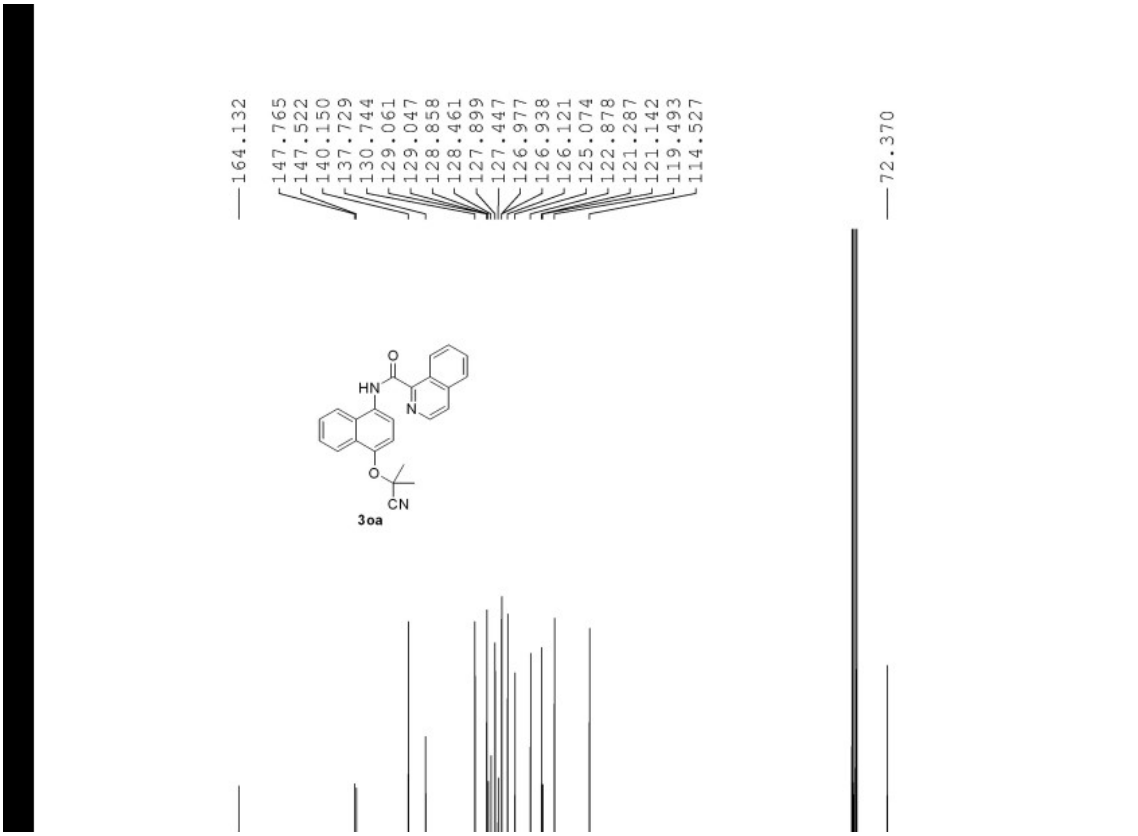
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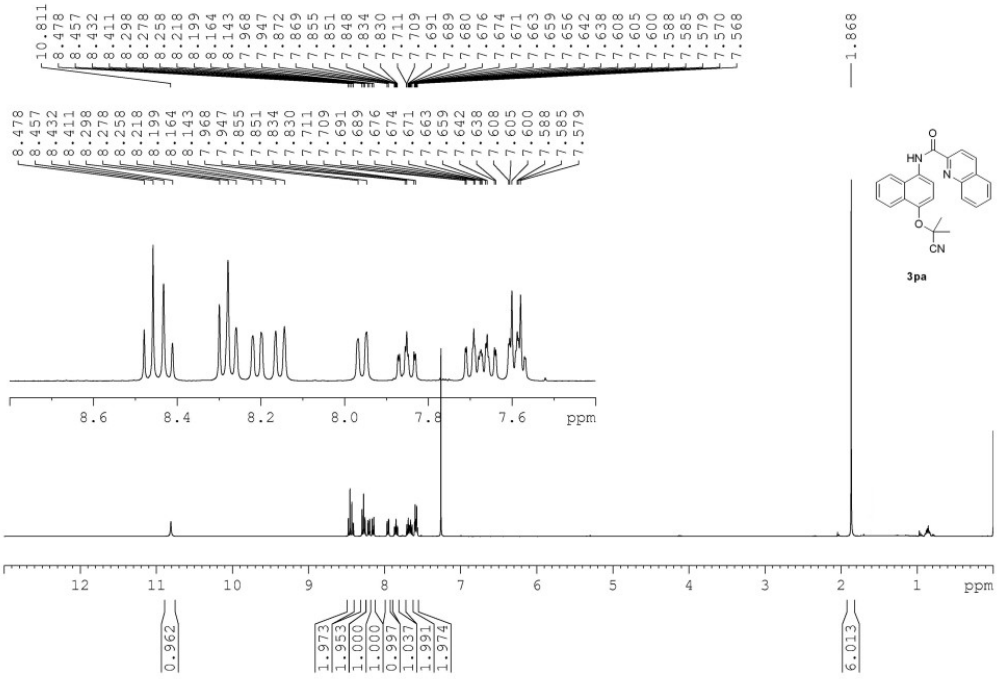
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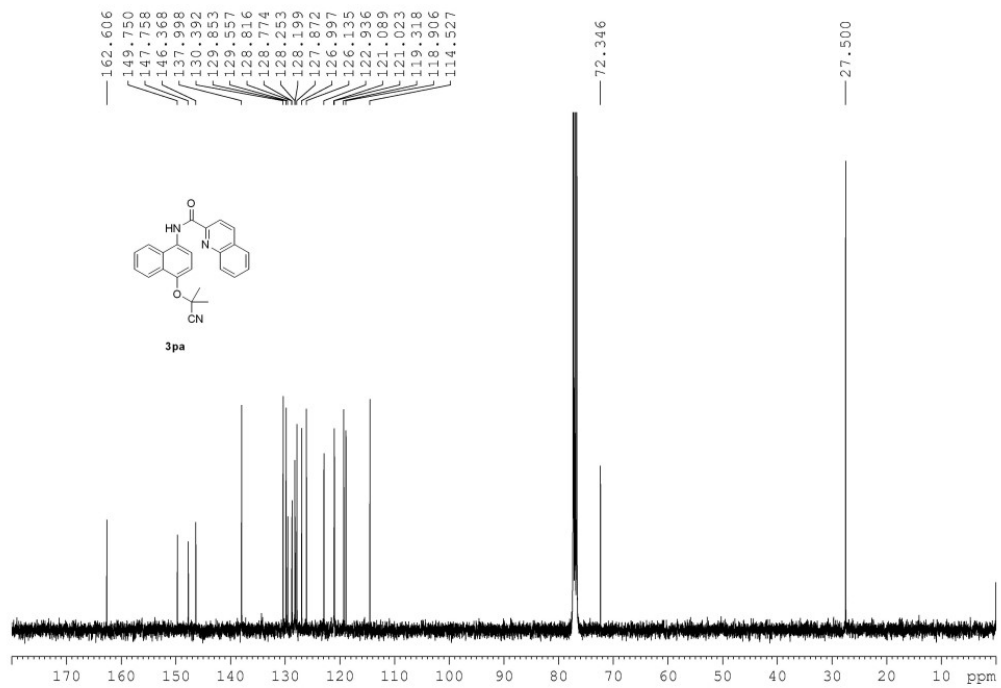
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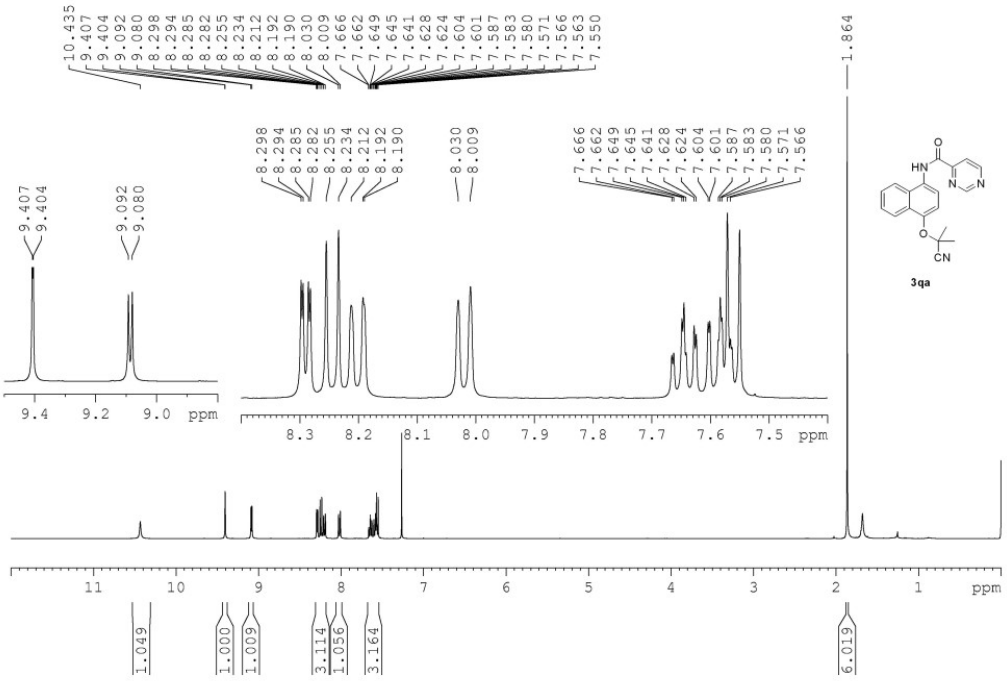
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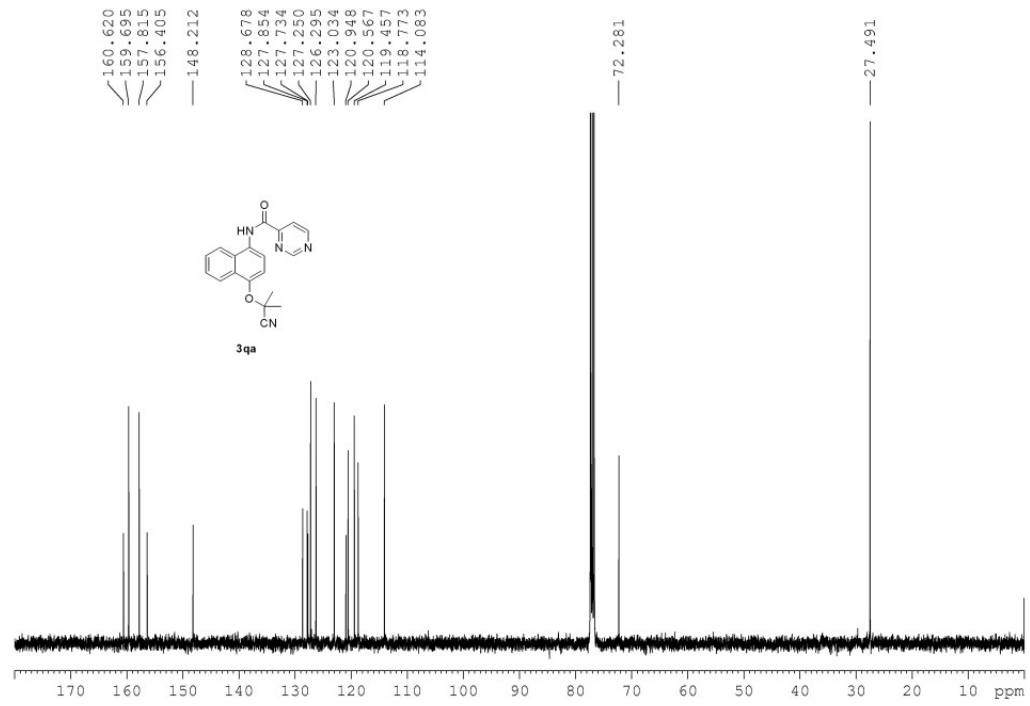
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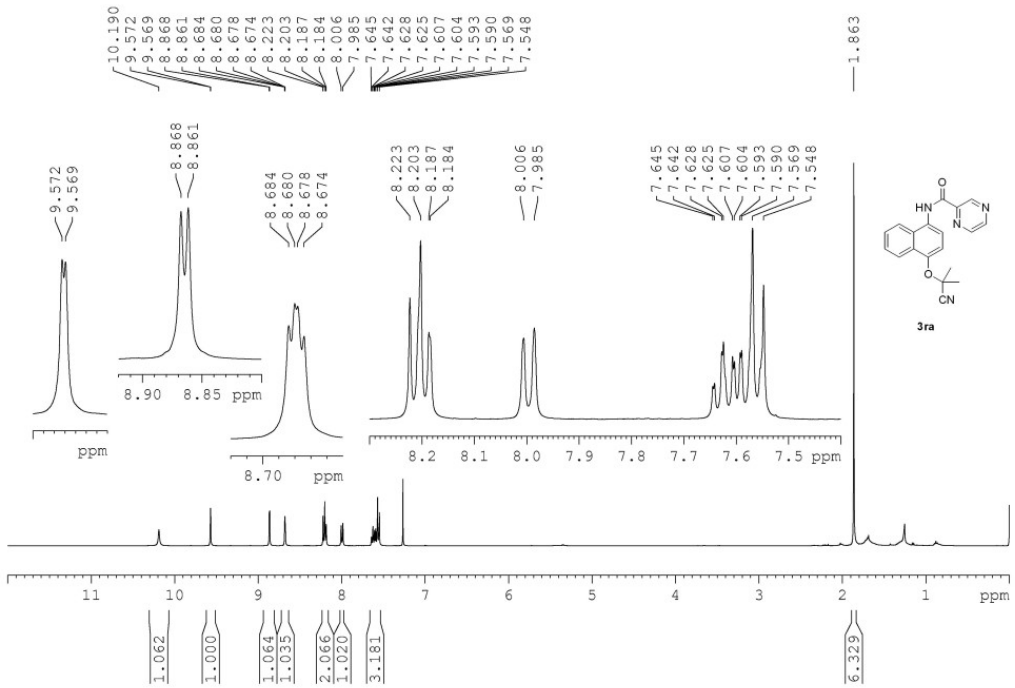
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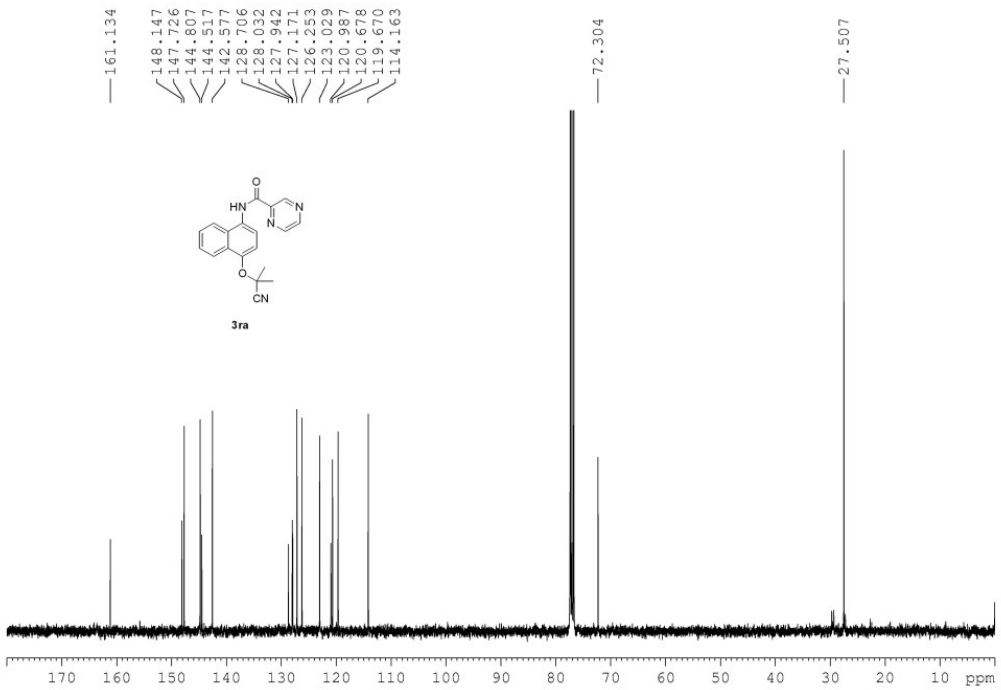
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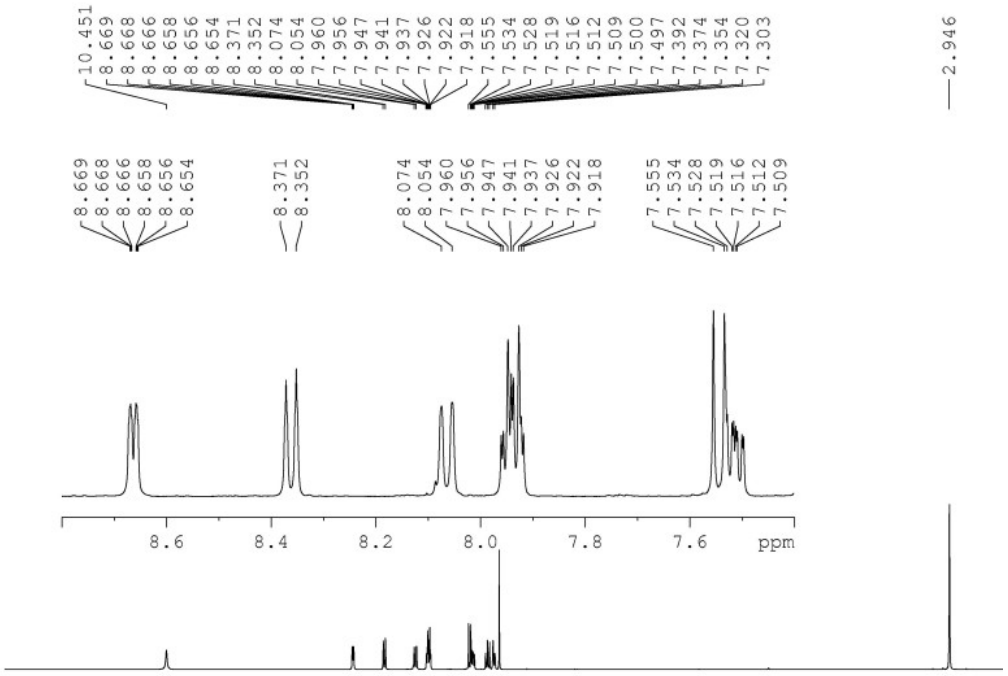
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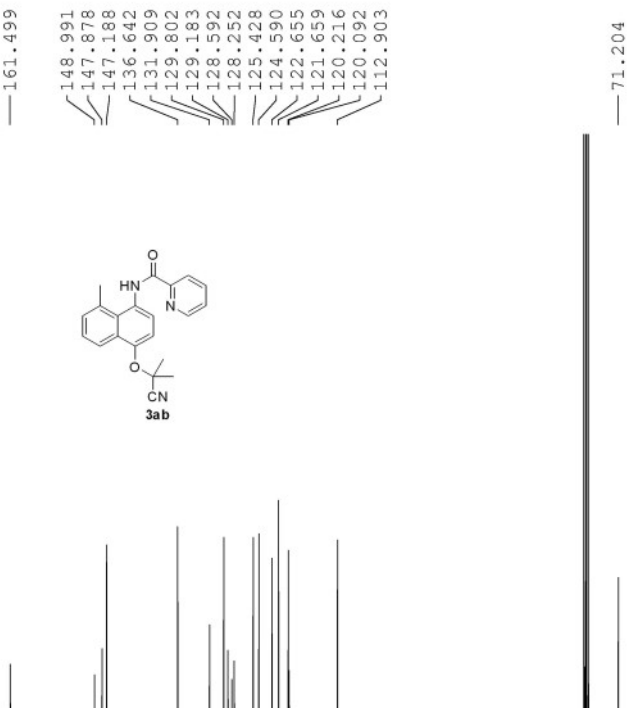
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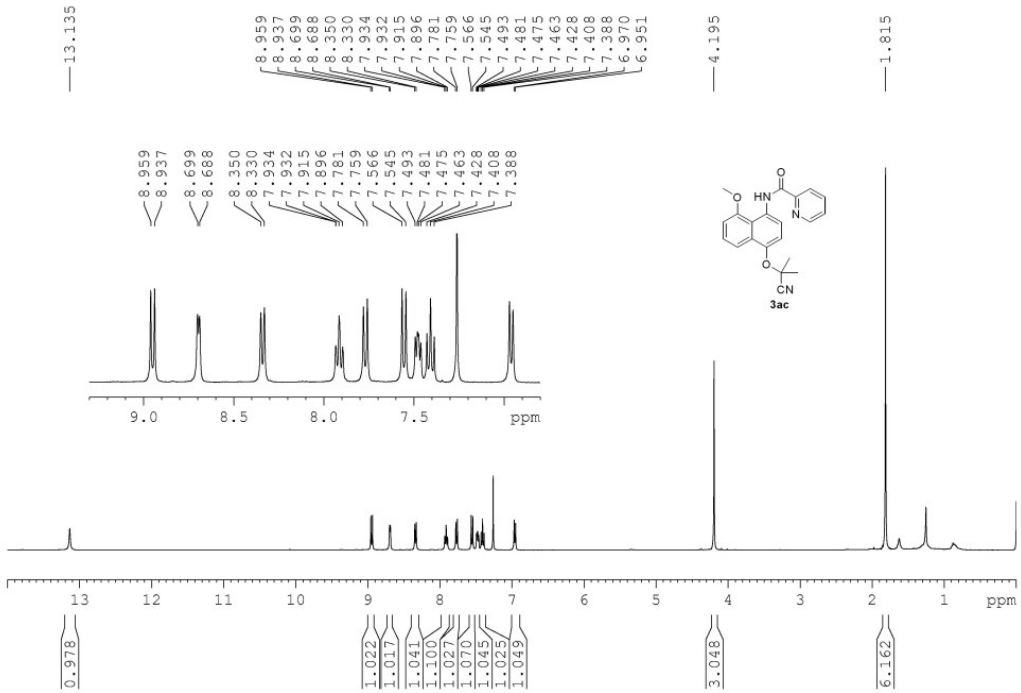
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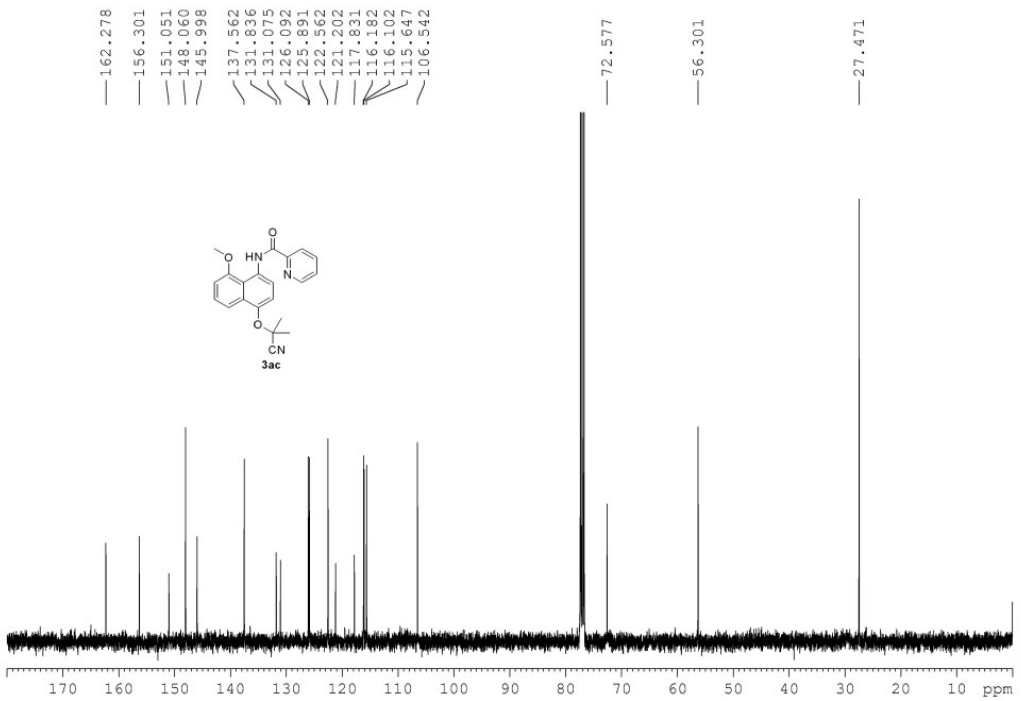
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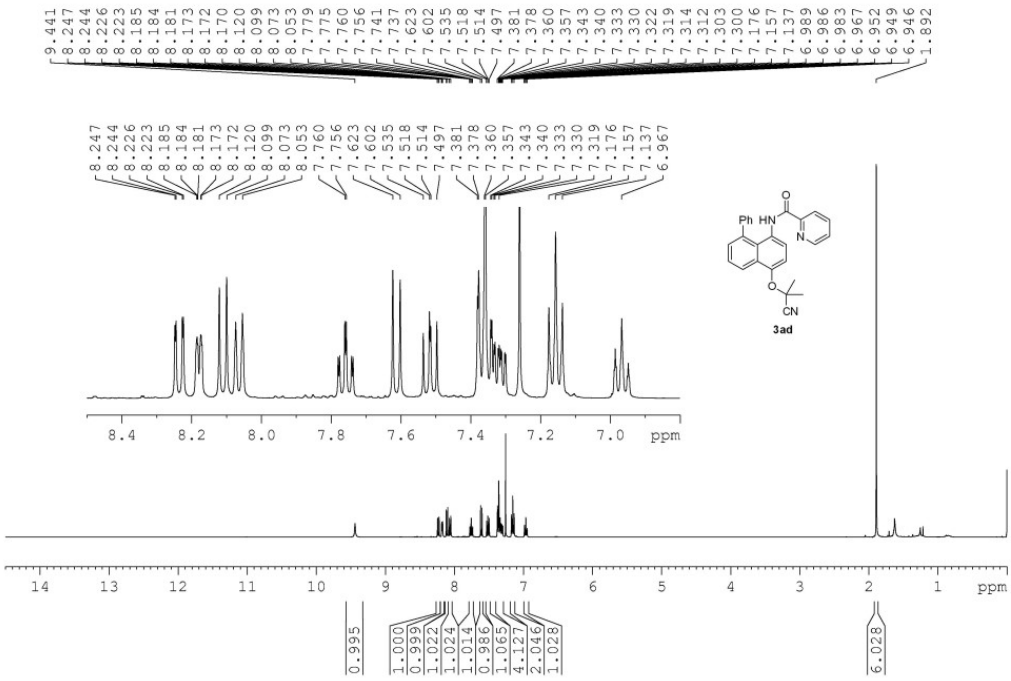
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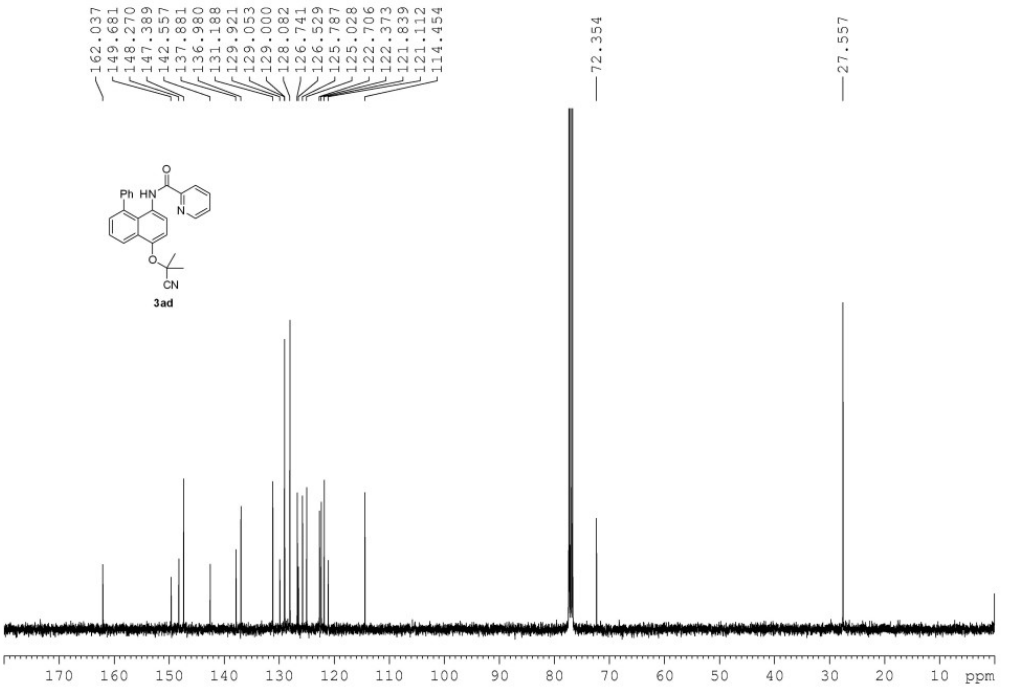
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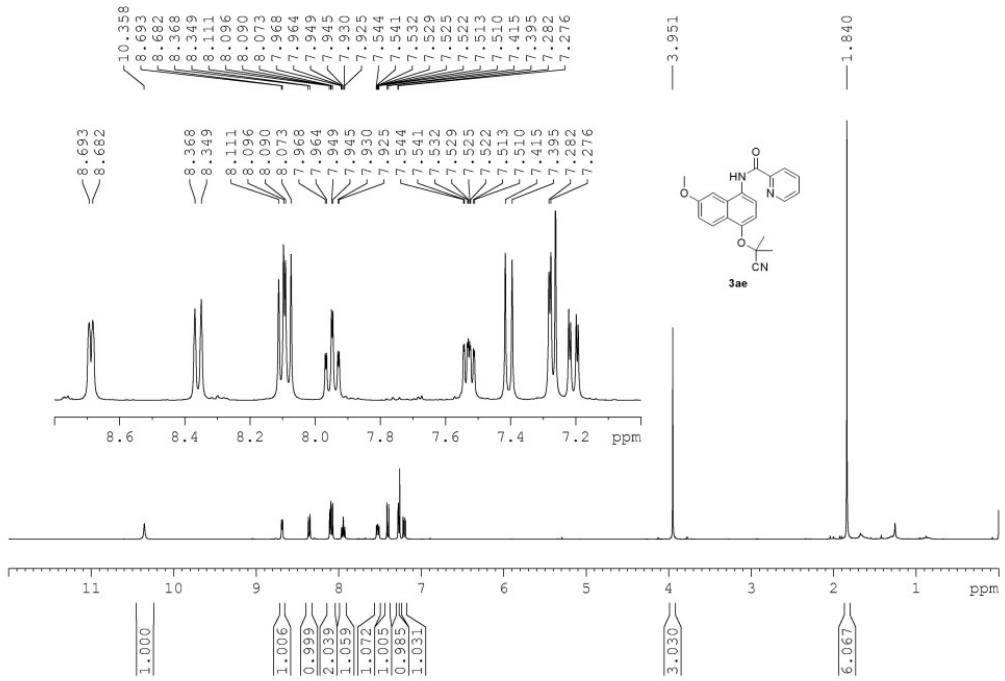
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1.840
3ae
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0.999
2.039
1.059
1.072
1.005
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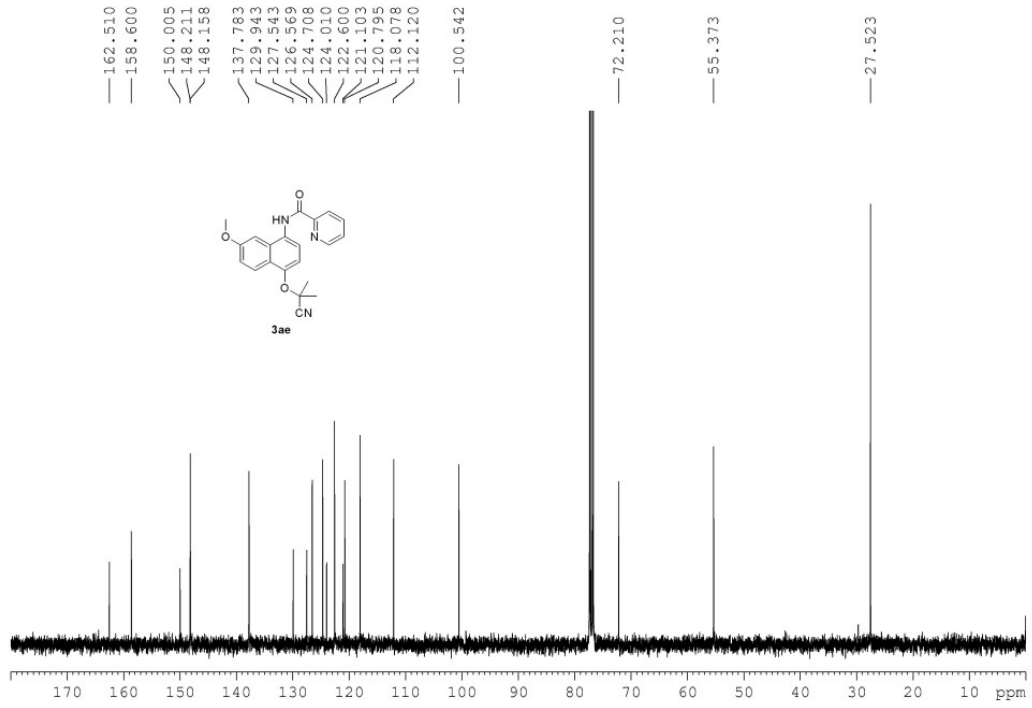
1.031
3.030
6.067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158.600
150.005
148.211
148.158
137.783
129.943
127.543
126.569
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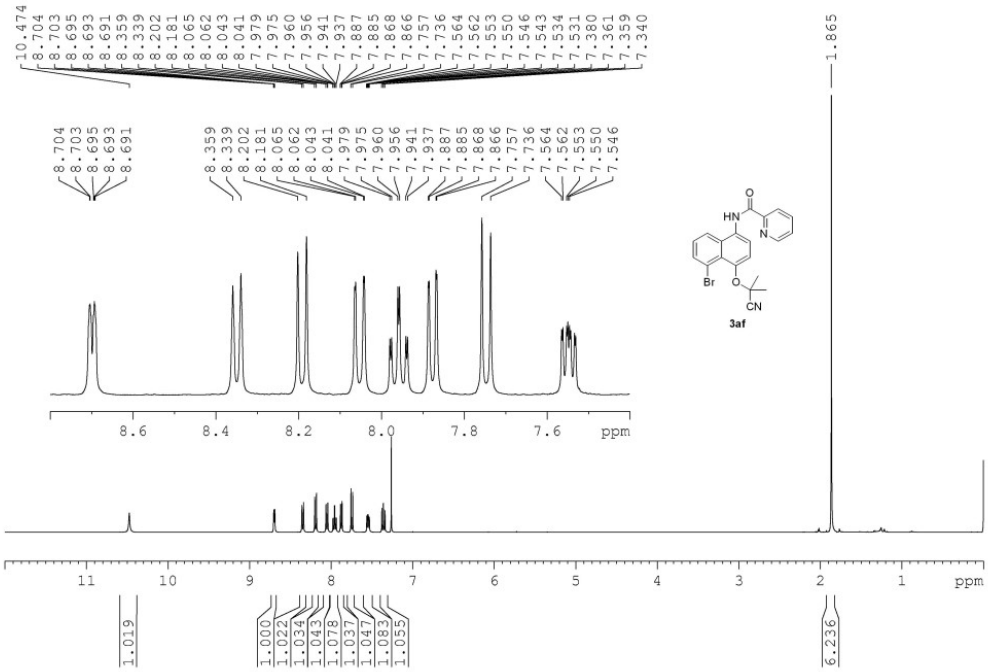
121.103
120.795
118.078
112.120
100.542
72.210
55.373
27.523
3ae
ppm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8.704
8.703
8.695
8.693
8.691
8.359
8.339
8.202
8.181
8.065
8.062
8.043
8.041
7.979
7.975
7.960
7.956
7.941
7.937
7.887
7.885
7.868
7.866
7.757
7.736
7.564
7.562
7.553
7.550
7.546
7.543
7.534
7.531
7.380
7.361
7.359
7.340
1.865
HN
O
N
Br
O
CN
3af
ppm
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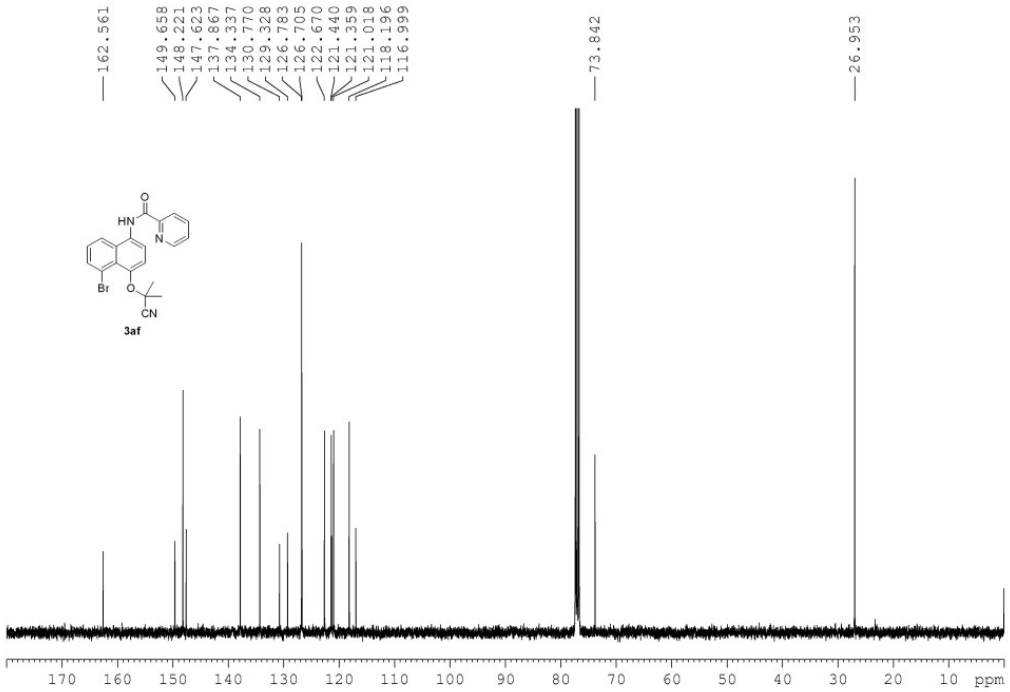
1.000
1.022
1.034
1.043
1.078
1.037
1.047
1.083
1.055
6.236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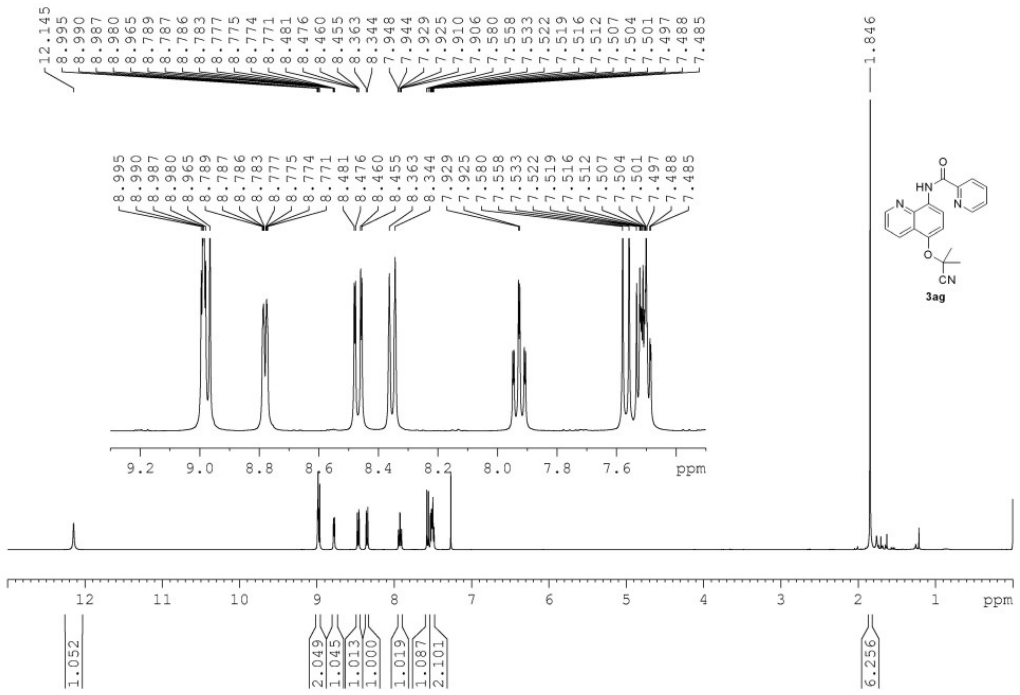
149.658
148.221
147.623
137.867
134.337
130.770
129.328
126.783
126.705
122.670
121.440
121.359
121.018
118.196
116.999
73.842
26.953
HN
O
N
Br
O
CN
3af
ppm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8.995
8.990
8.987
8.980
8.965
8.789
8.787
8.786
8.783
8.777
8.775
8.774
8.771
8.481
8.476
8.460
8.455
8.363
8.344
7.948
7.944
7.929
7.925
7.910
7.906
7.580
7.558
7.533
7.522
7.519
7.516
7.512
7.507
7.504
7.501
7.497
7.488
7.485
1.846
3ag
9.2
9.0
8.8
8.6
8.4
8.2
8.0
7.8
7.6
ppm
12
11
10
9
8
7
6
5
4
3
2
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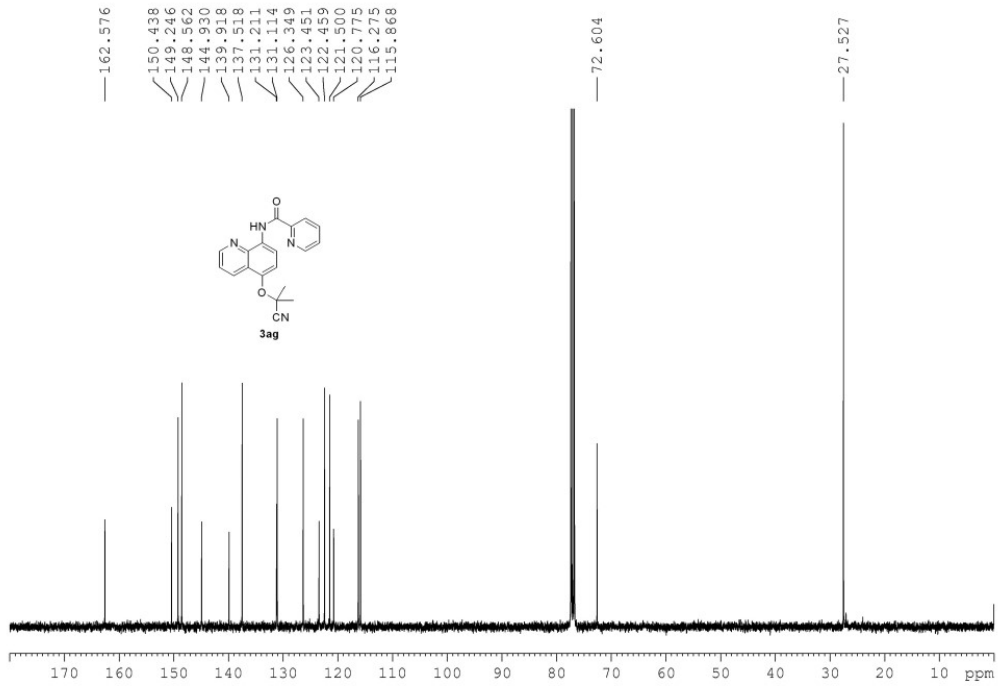
ppm
1.052
2.049
1.045
1.013
1.000
1.019
1.087
2.101
6.256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149.246
148.562
144.930
139.918
137.518
131.211
131.114
126.349
123.451
122.459
121.500
120.775
116.275
115.868
72.604
27.527
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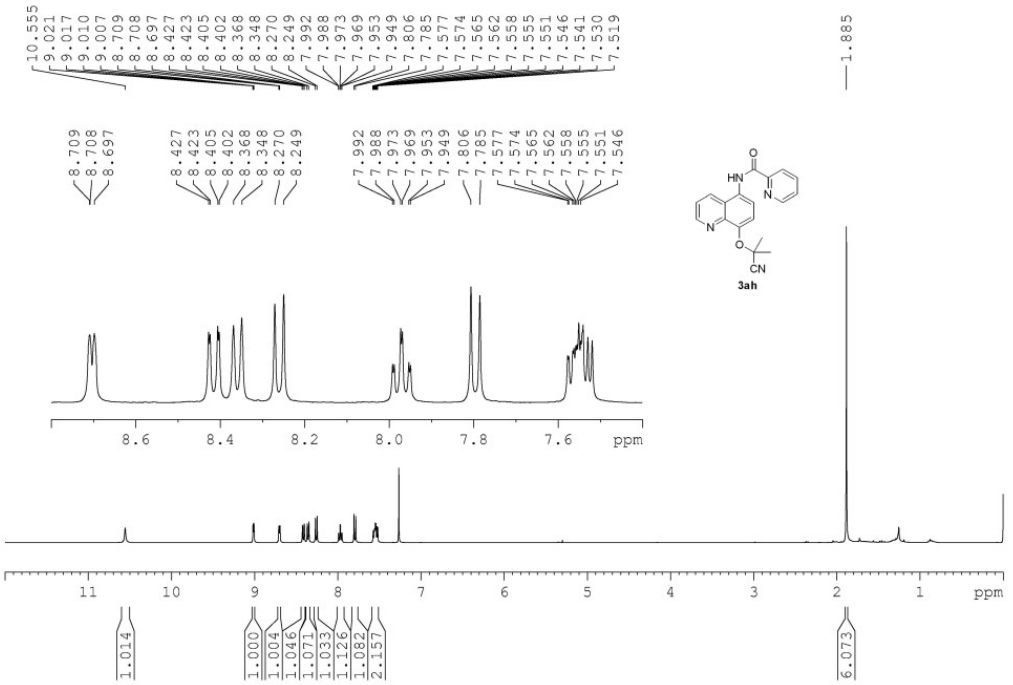
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm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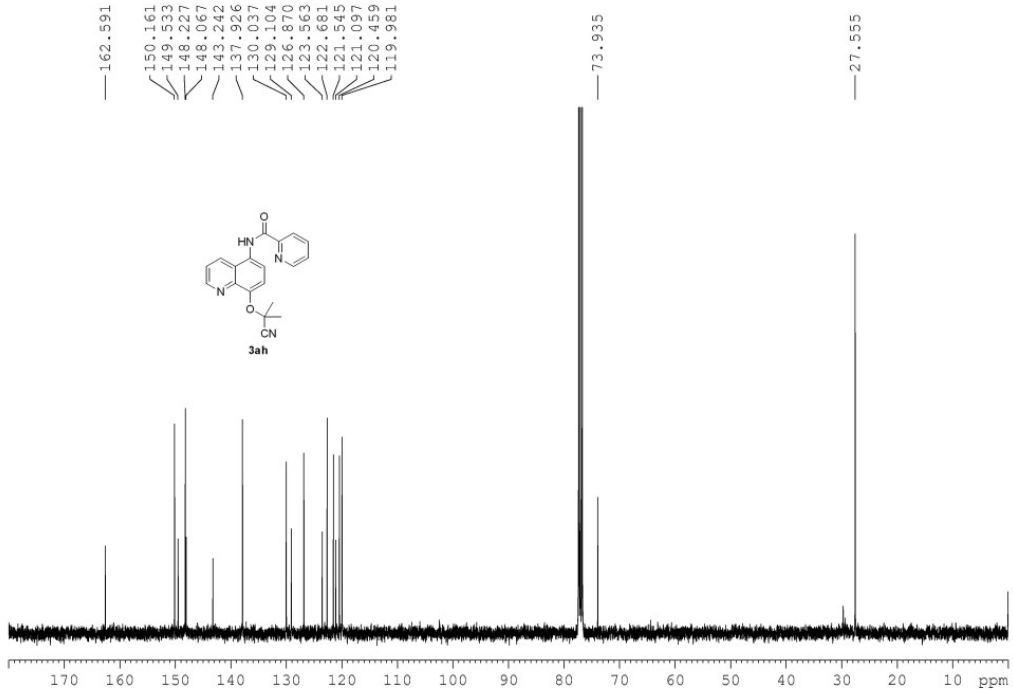
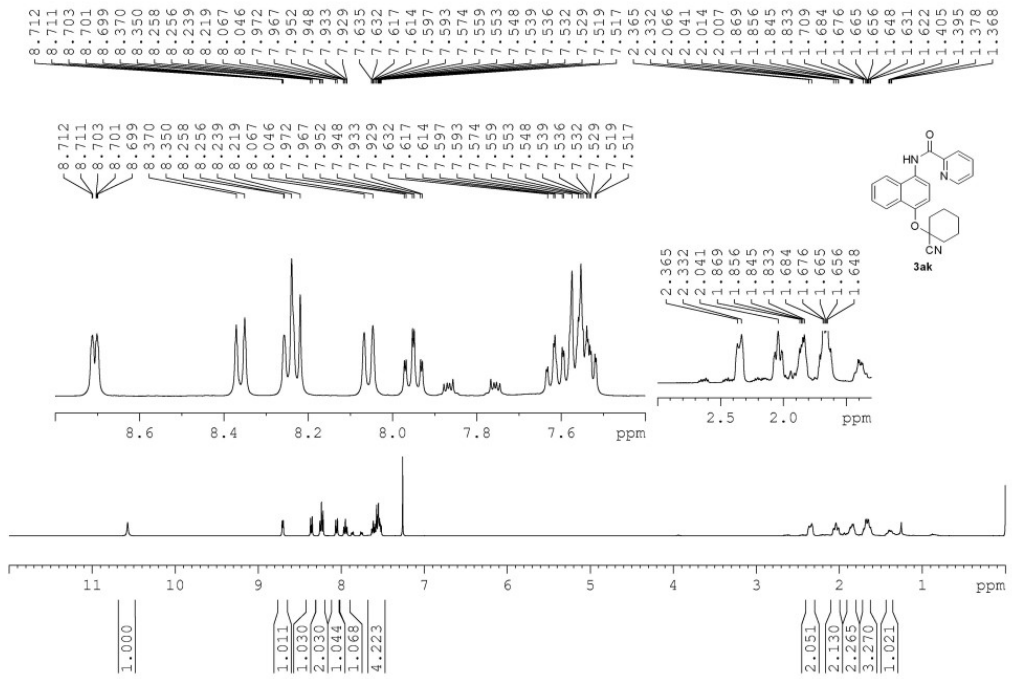
9.021
9.017
9.010
9.007
8.709
8.708
8.697
8.427
8.423
8.405
8.402
8.368
8.348
8.270
8.249
7.992
7.988
7.973
7.969
7.953
7.949
7.806
7.785
7.577
7.574
7.565
7.562
7.558
7.555
7.551
7.546
7.541
7.530
7.519
1.885
HN
N
O
CN
3ah
8.6
8.4
8.2
8.0
7.8
7.6
ppm
11
10
9
8
7
6
5
4
3
2
1
ppm
1.014
1.000
1.004
1.046
1.071
1.033
1.126
1.082
2.157
6.073


162.591
150.161
149.533
148.227
148.067
143.242
137.926
130.037
129.104
126.870
123.563
122.681
121.545
121.097
120.459
119.981
73.935
27.555
HN
N
O
CN
3ah
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm


8.712
8.711
8.703
8.701
8.699
8.370
8.350
8.258
8.256
8.239
8.219
8.067
8.046
7.972
7.967
7.952
7.948
7.933
7.929
7.635
7.632
7.617
7.614
7.597
7.593
7.574
7.559
7.553
7.548
7.539
7.536
7.532
7.529
7.519
7.517
2.365
2.332
2.066
2.041
2.014
2.007
1.869
1.856
1.845
1.833
1.709
1.684
1.676
1.665
1.656
1.648
1.631
1.622
1.405
1.395
1.378
1.368
HN
O
N
O
CN
3ak
8.6
8.4
8.2
8.0
7.8
7.6
ppm
2.5
2.0
ppm
11
10
9
8
7
6
5
4
3
2
1
ppm
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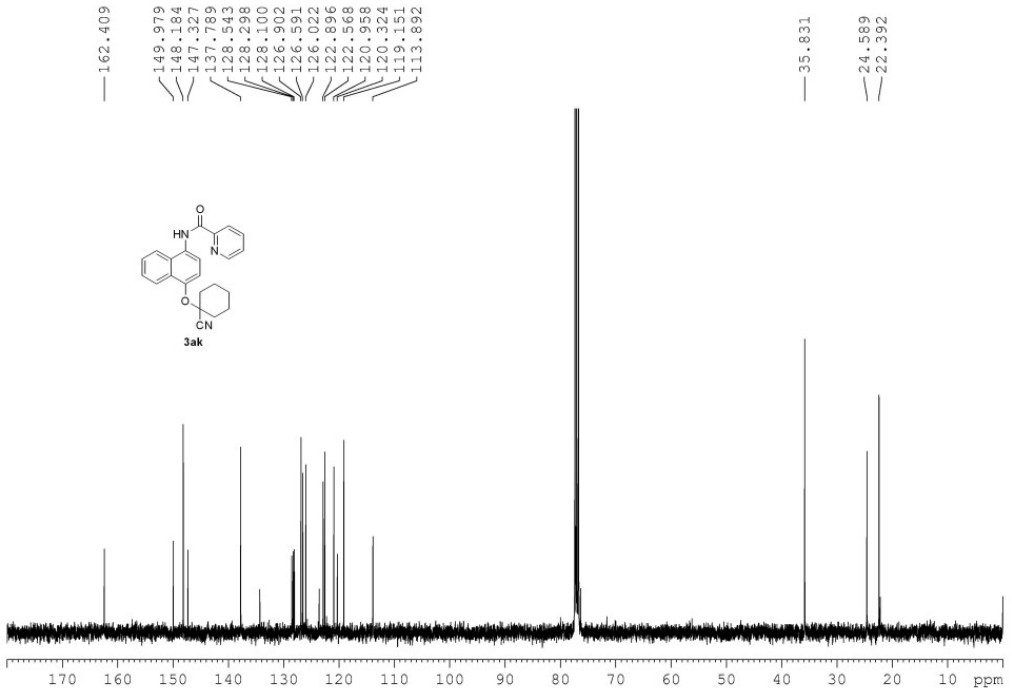
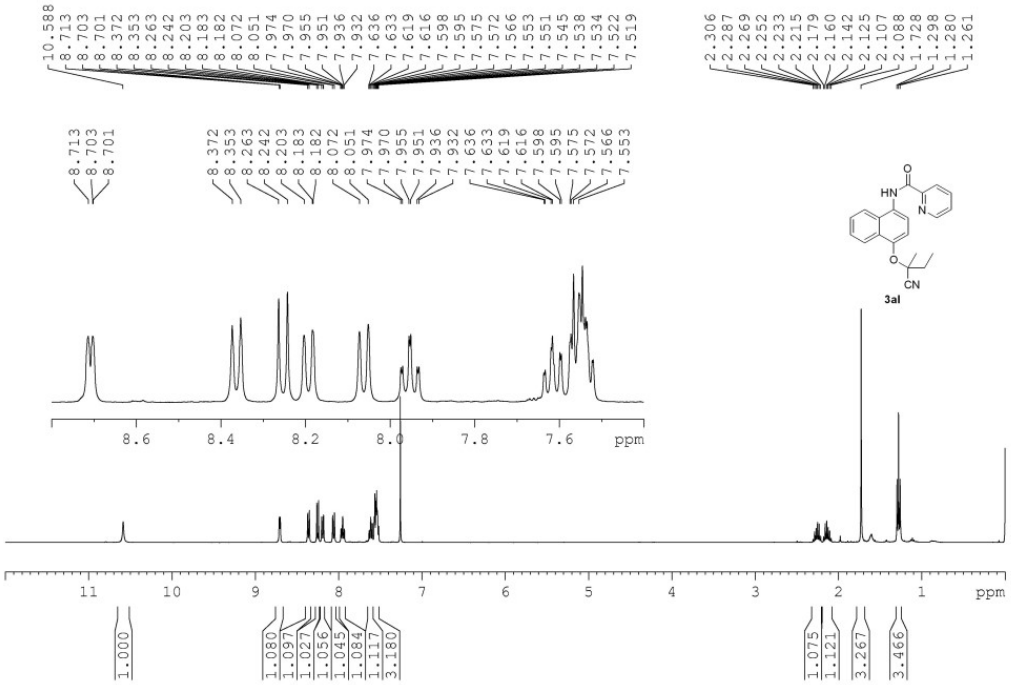
1.030
2.030
1.044
1.068
4.223
2.051
2.130
2.265
3.270
1.021


162.409
149.979
148.184
147.327
137.789
128.543
128.298
128.100
126.902
126.591
126.022
122.896
122.568
120.958
120.324
119.151
113.892
35.831
24.589
22.392
HN
O
N
O
CN
3ak
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm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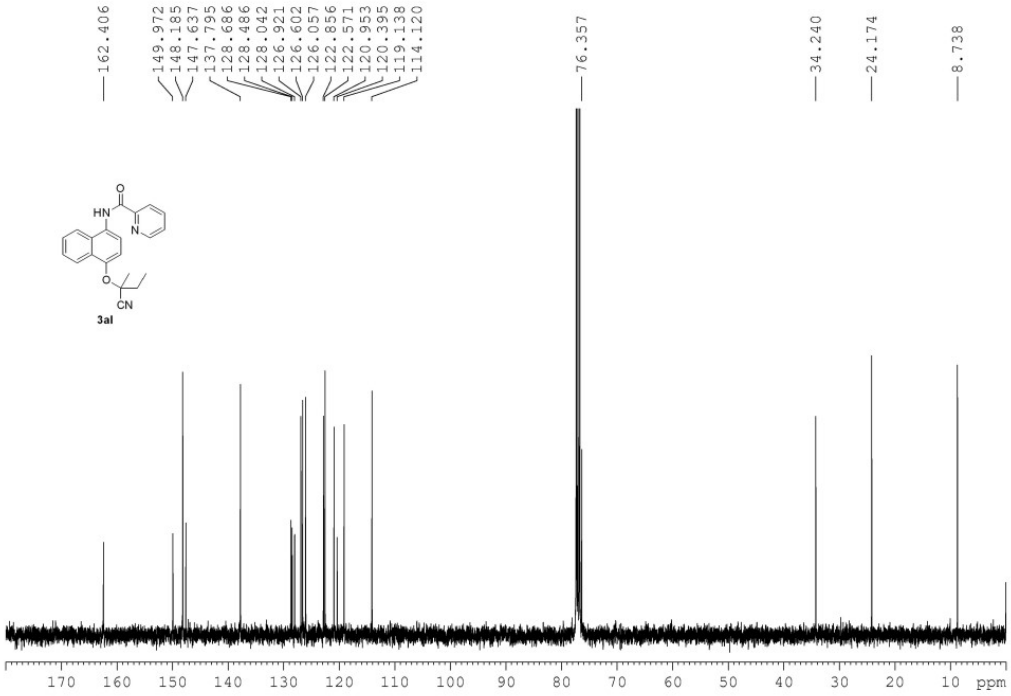
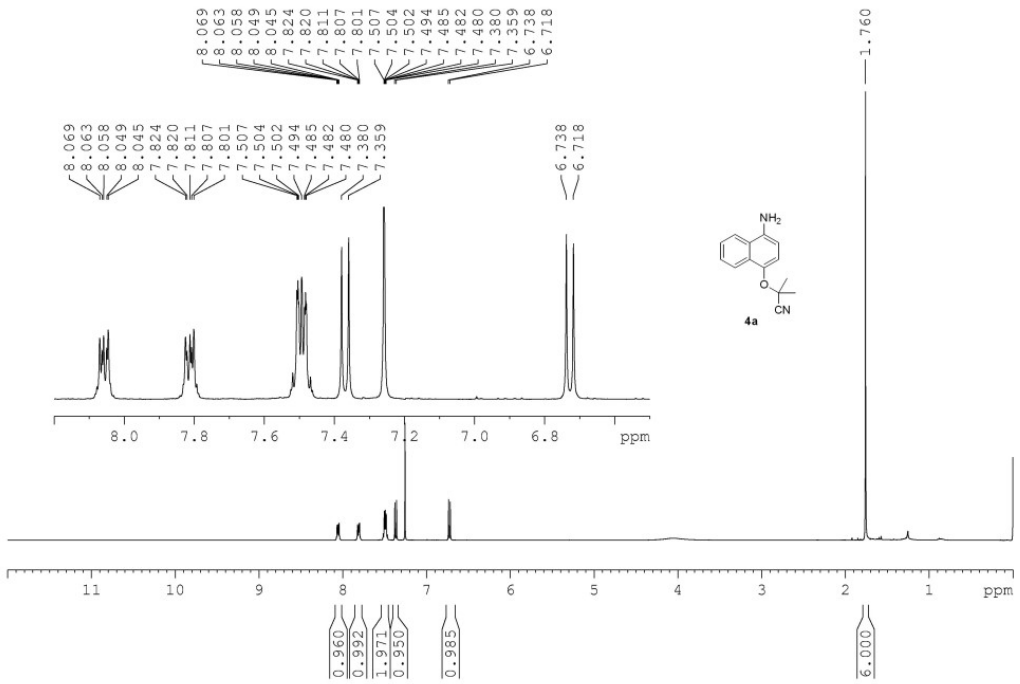
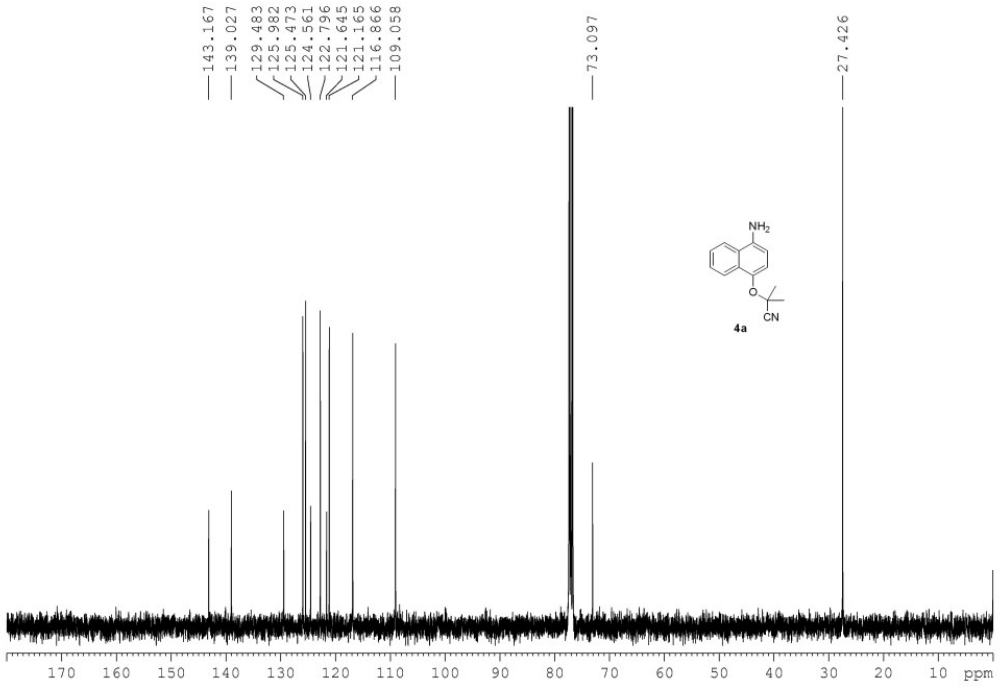
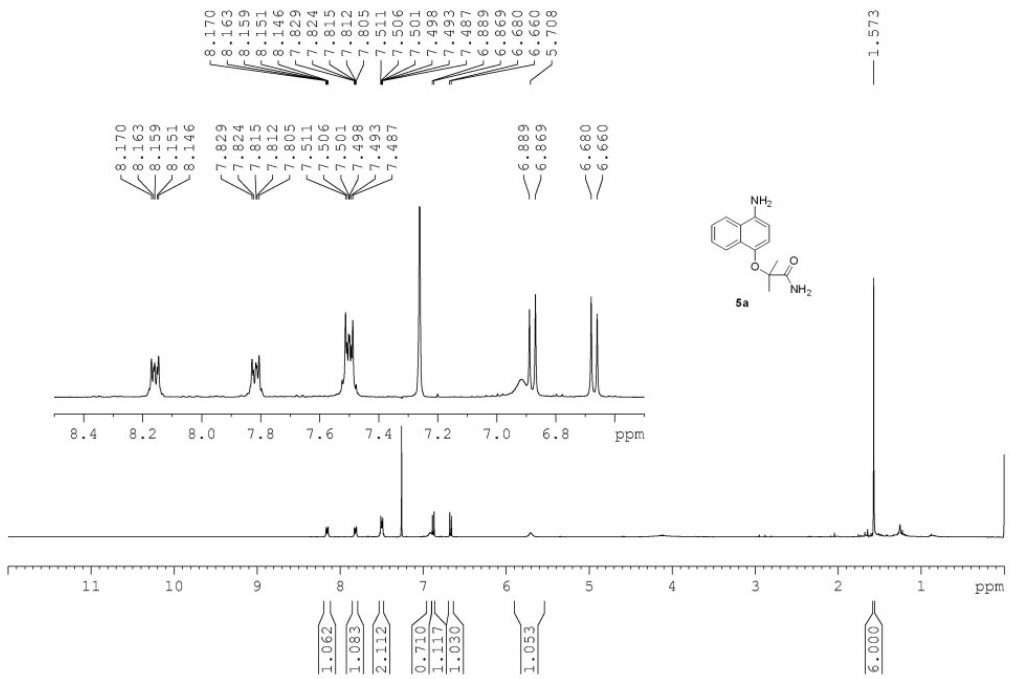
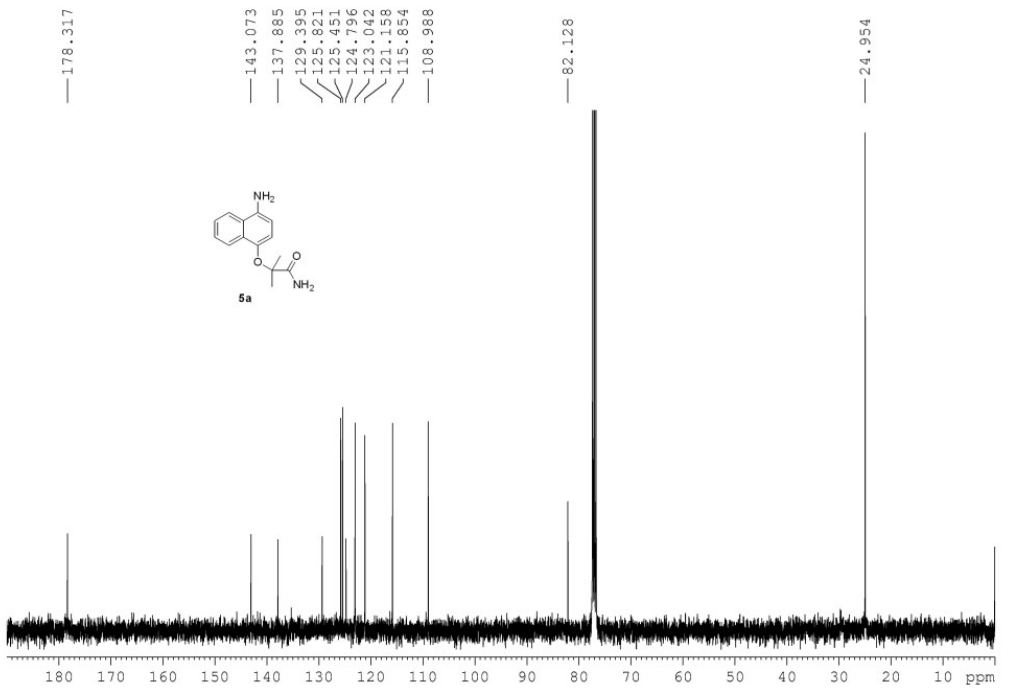
8.713
8.703
8.701
8.372
8.353
8.263
8.242
8.203
8.183
8.182
8.072
8.051
7.974
7.970
7.955
7.951
7.936
7.932
7.636
7.633
7.619
7.616
7.598
7.595
7.575
7.572
7.566
7.553
7.545
7.538
7.534
7.522
7.519
2.306
2.287
2.269
2.252
2.233
2.215
2.179
2.160
2.142
2.125
2.107
2.088
1.728
1.298
1.280
1.261
HN
N
O
CN
3al
8.6
8.4
8.2
8.0
7.8
7.6
ppm
11
10
9
8
7
6
5
4
3
2
1
ppm
1.000
1.080
1.097
1.027
1.056
1.045
1.084
1.117
3.180
1.075
1.121
3.267
3.466

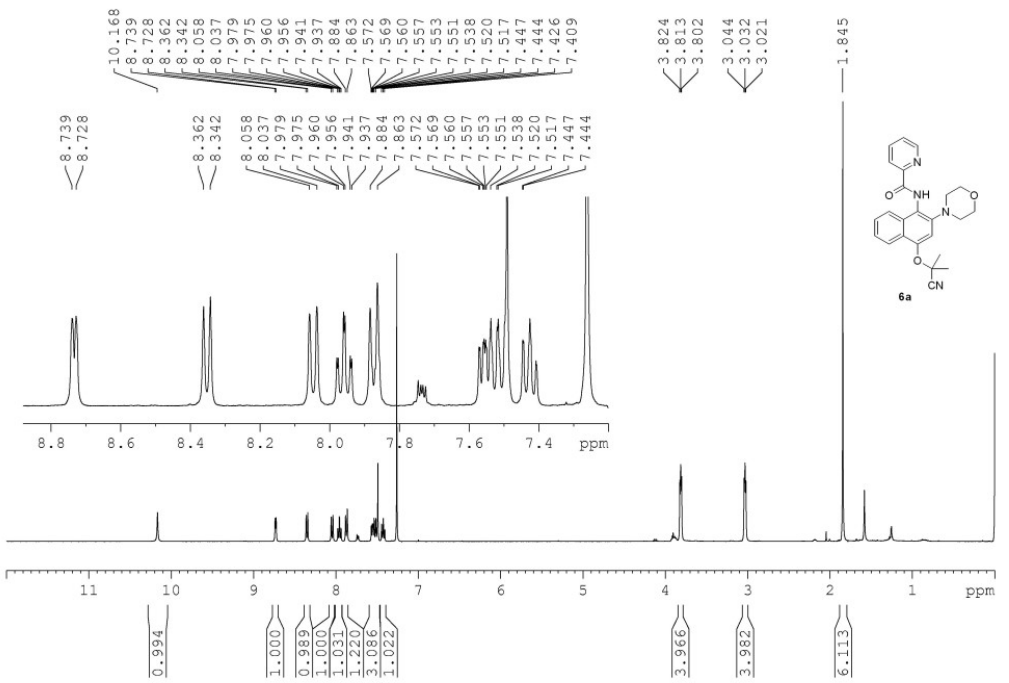

162.406
149.972
148.185
147.637
137.795
128.686
128.486
128.042
126.921
126.602
126.057
122.856
122.571
120.953
120.395
119.138
114.120
76.357
34.240
24.174
8.738
HN
N
O
CN
3al
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

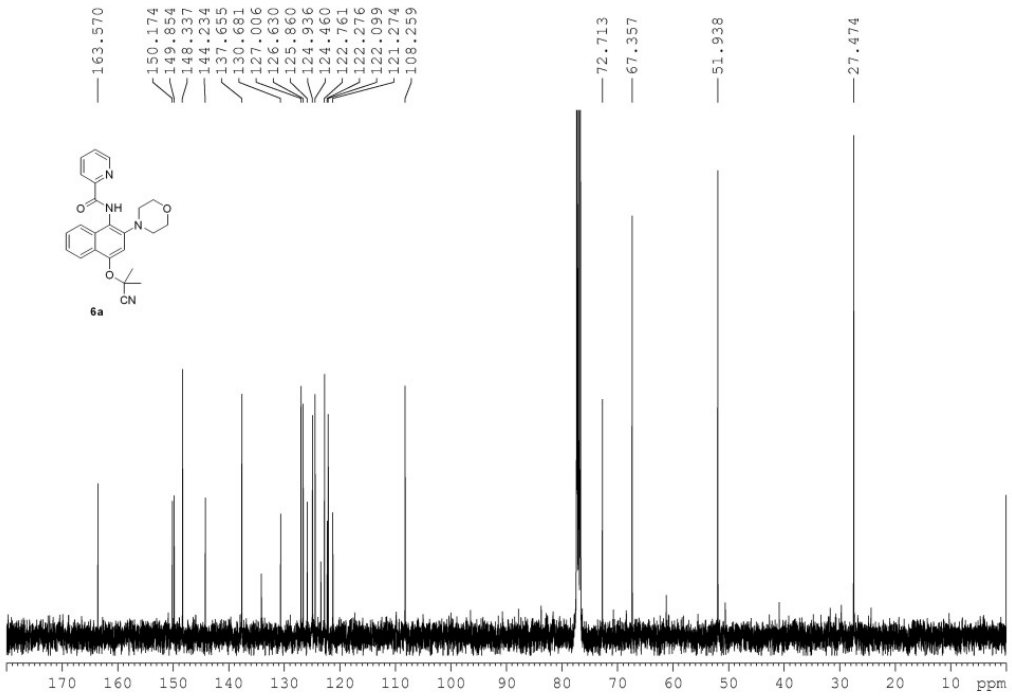

8.069
8.063
8.058
8.049
8.045
7.824
7.820
7.811
7.807
7.801
7.507
7.504
7.502
7.494
7.485
7.482
7.480
7.380
7.359
6.738
6.718
1.760
NH2
O
CN
4a
8.0
7.8
7.6
7.4
7.2
7.0
6.8
ppm
11
10
9
8
7
6
5
4
3
2
1
ppm
0.960
0.992
1.971
0.950
0.985
6.000

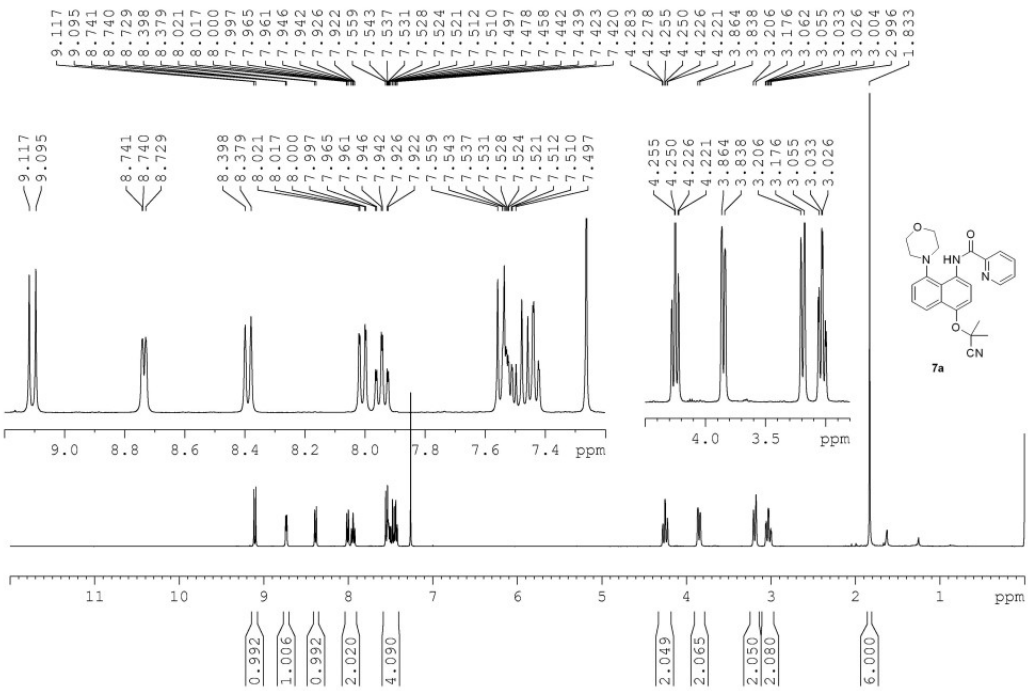

143.167
139.027
129.483
125.982
125.473
124.561
122.796
121.645
121.165
116.866
109.058
73.097
27.426
NH2
O
CN
4a
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

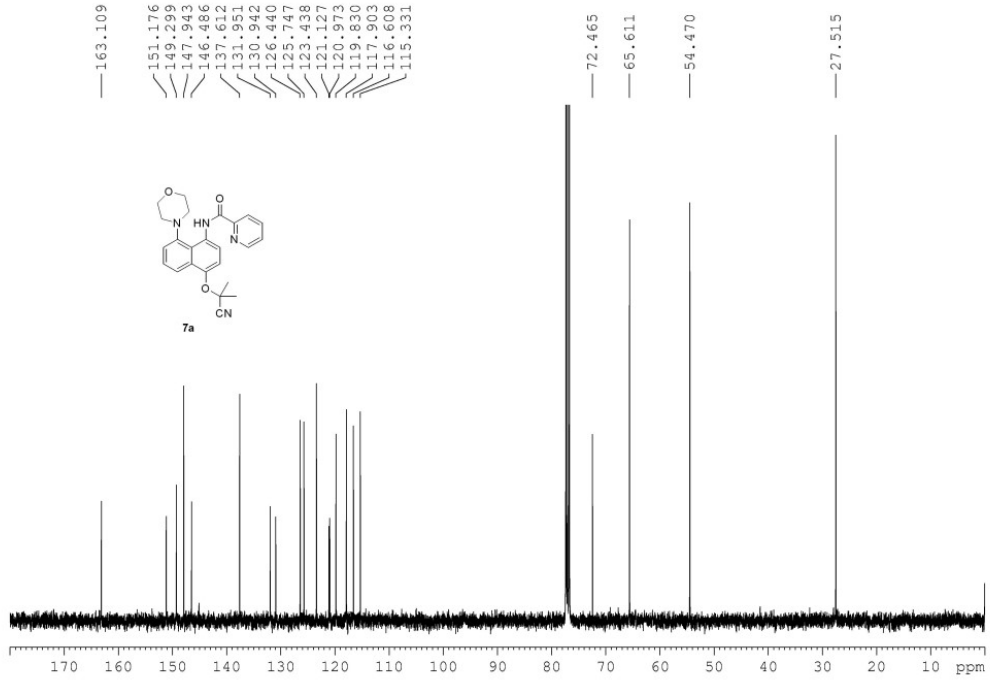

8.170
8.163
8.159
8.151
8.146
7.829
7.824
7.815
7.812
7.805
7.511
7.506
7.501
7.498
7.493
7.487
6.889
6.869
6.680
6.660
5.708
1.573
NH2
O
NH2
5a
8.4
8.2
8.0
7.8
7.6
7.4
7.2
7.0
6.8
ppm
11
10
9
8
7
6
5
4
3
2
1
ppm
1.062
1.083
2.112
0.710
1.117
1.030
1.053
6.000

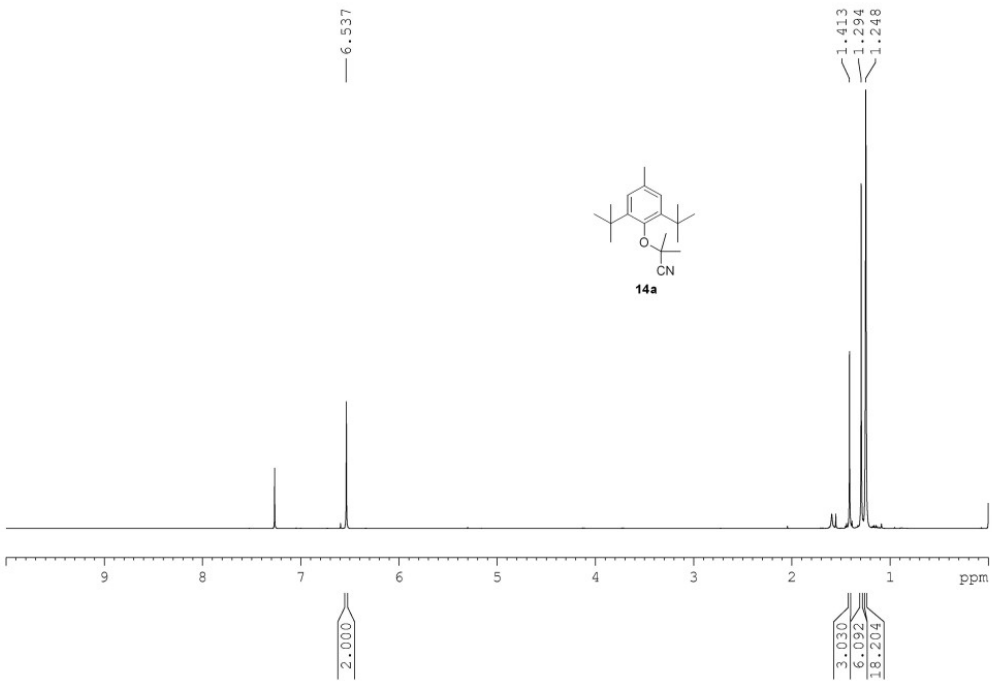

178.317
143.073
137.885
129.395
125.821
125.451
124.796
123.042
121.158
115.854
108.988
82.128
24.954
NH2
O
NH2
5a
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

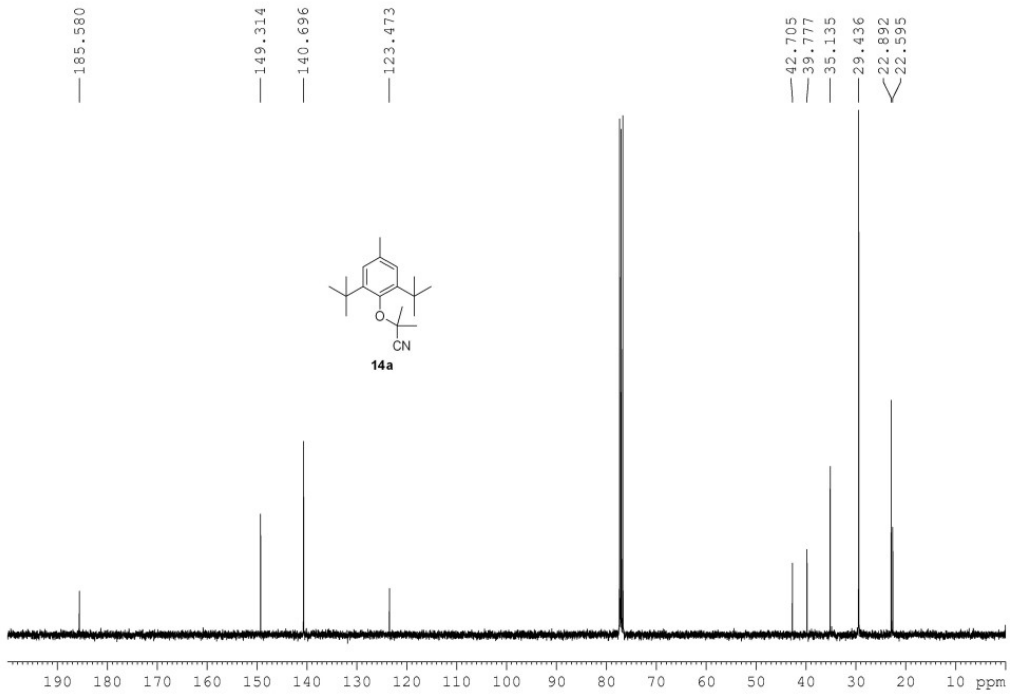

10.168
8.739
8.728
8.362
8.342
8.058
8.037
7.979
7.975
7.960
7.956
7.941
7.937
7.884
7.863
7.572
7.569
7.560
7.557
7.553
7.551
7.538
7.520
7.517
7.447
7.444
7.426
7.409
3.824
3.813
3.802
3.044
3.032
3.021
1.845
6a
ppm
0.994
1.000
0.989
1.000
1.031
1.220
3.086
1.022
3.966
3.982
6.113


163.570
150.174
149.854
148.337
144.234
137.655
130.681
127.006
126.630
125.860
124.936
124.460
122.761
122.276
122.099
121.274
108.259
72.713
67.357
51.938
27.474
6a
ppm

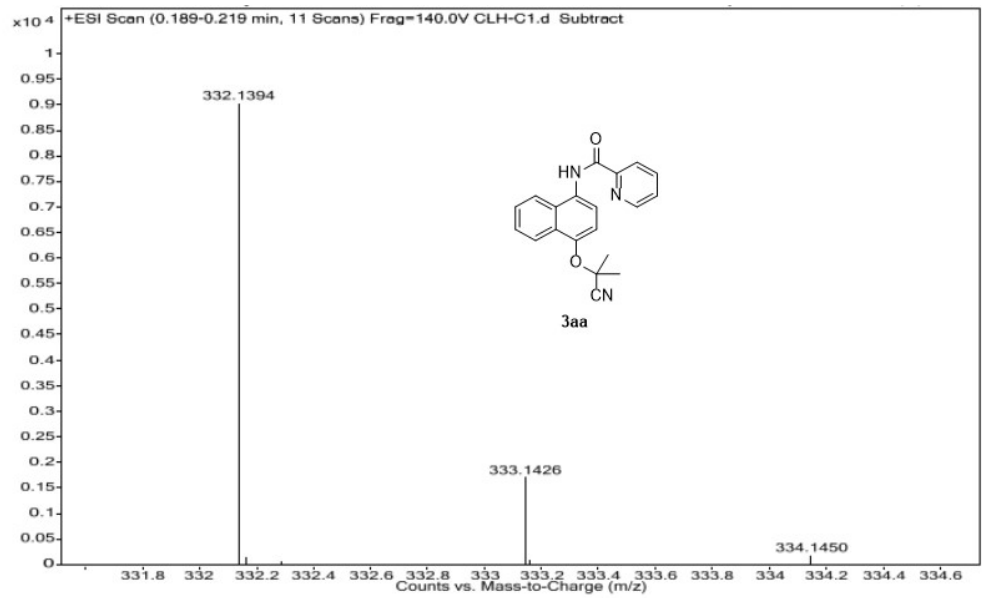

9.117
9.095
8.741
8.740
8.729
8.398
8.379
8.021
8.017
8.000
7.997
7.965
7.961
7.946
7.942
7.926
7.922
7.559
7.543
7.537
7.531
7.528
7.524
7.521
7.512
7.510
7.497
7.478
7.458
7.442
7.439
7.423
7.420
4.283
4.278
4.255
4.250
4.226
4.221
3.864
3.838
3.206
3.176
3.062
3.055
3.033
3.026
3.004
2.996
1.833
9.0 8.8 8.6 8.4 8.2 8.0 7.8 7.6 7.4 ppm
4.0 3.5 ppm
11 10 9 8 7 6 5 4 3 2 1 ppm
0.992
1.006
0.992
2.020
4.090
2.049
2.065
2.050
2.080
6.000
HN
O
N
CN
7a

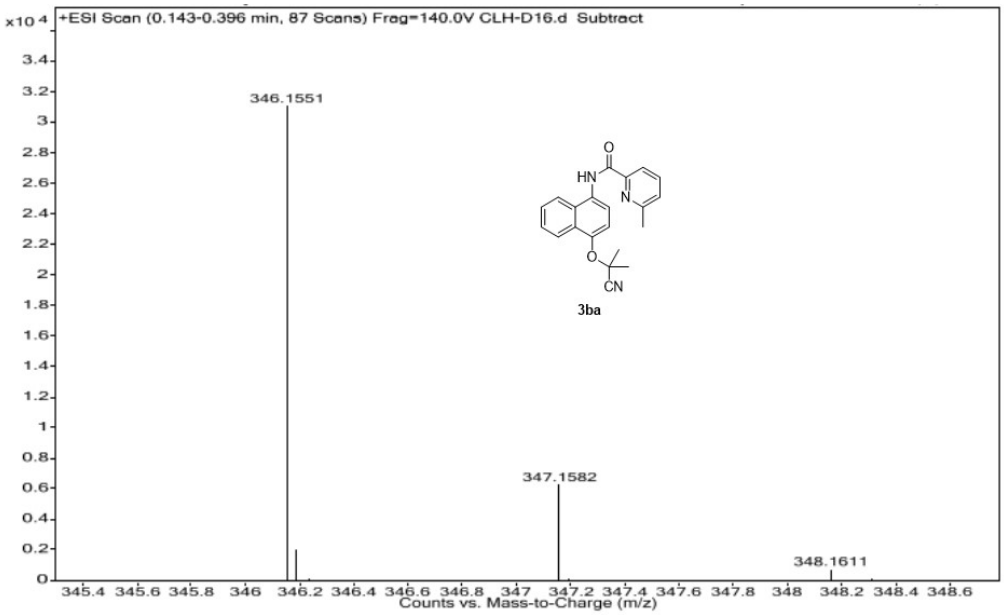

163.109
151.176
149.299
147.943
146.486
137.612
131.951
130.942
126.440
125.747
123.438
121.127
120.973
119.830
117.903
116.608
115.331
72.465
65.611
54.470
27.515
HN
O
N
CN
7a
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

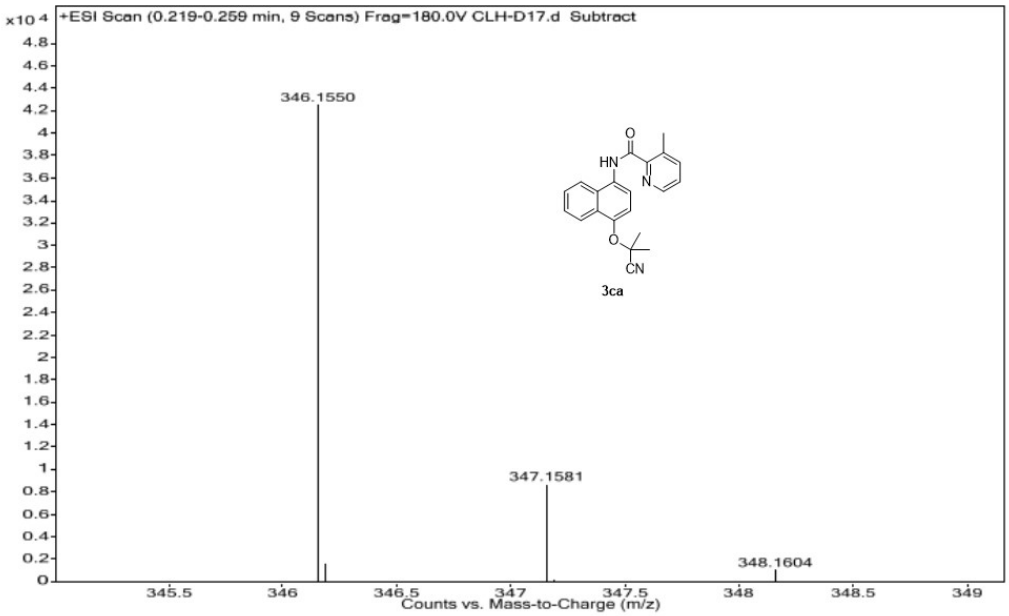


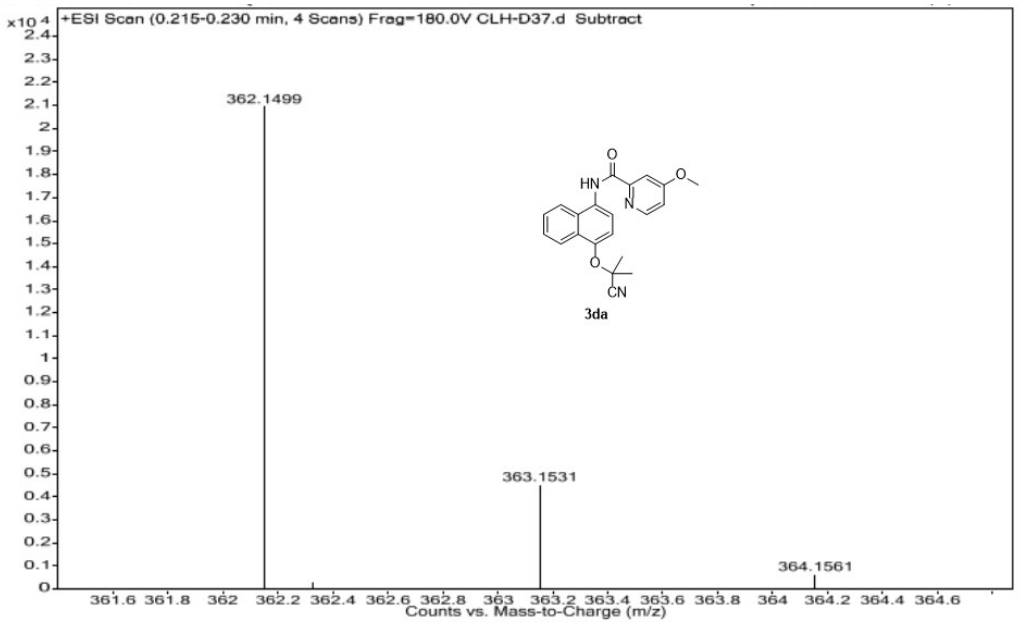


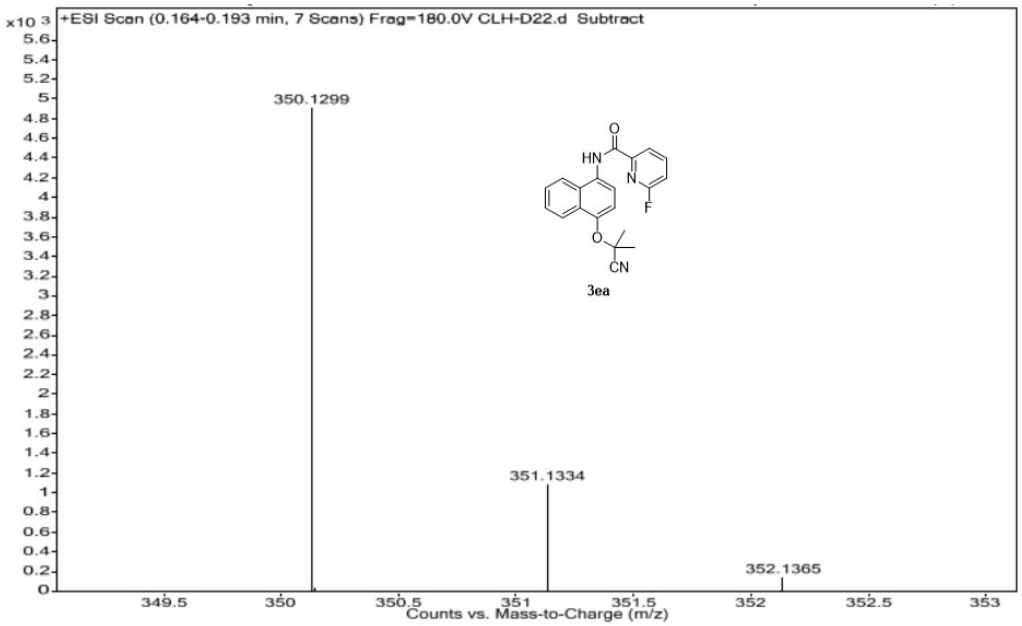
7. HRMS (ESI$^+$) m/z [M+H$^+$] calcd for the Products

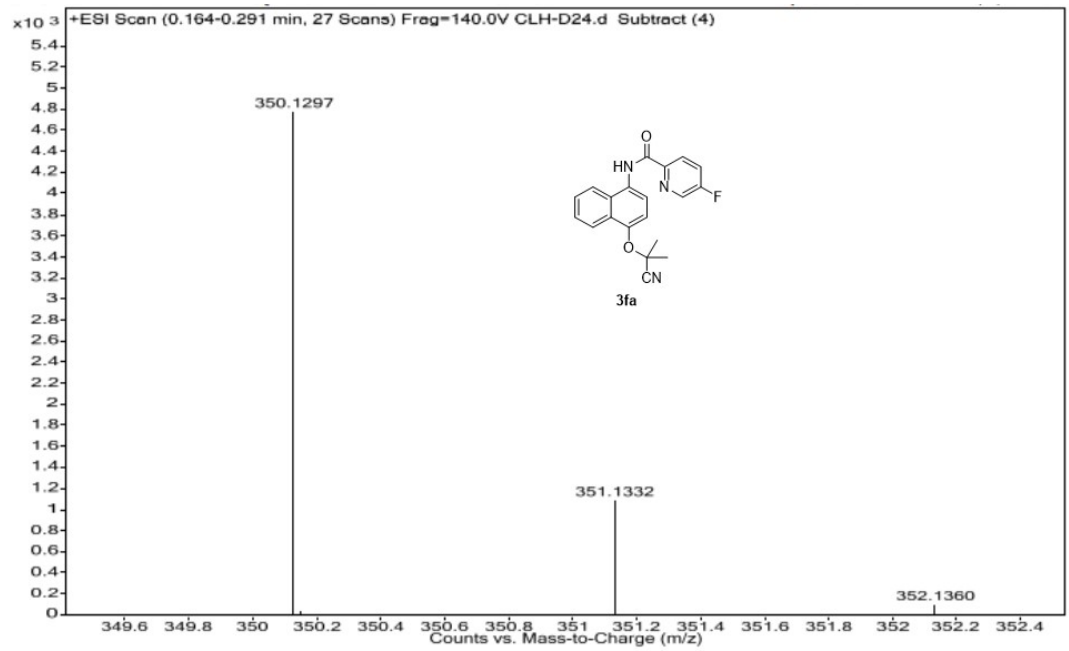

+ESI Scan (0.189-0.219 min, 11 Scans) Frag=140.0V CLH-C1.d Subtract
x10 4
332.1394
333.1426
334.1450
HN
O
N
O
CN
3aa
Counts vs. Mass-to-Charge (m/z)

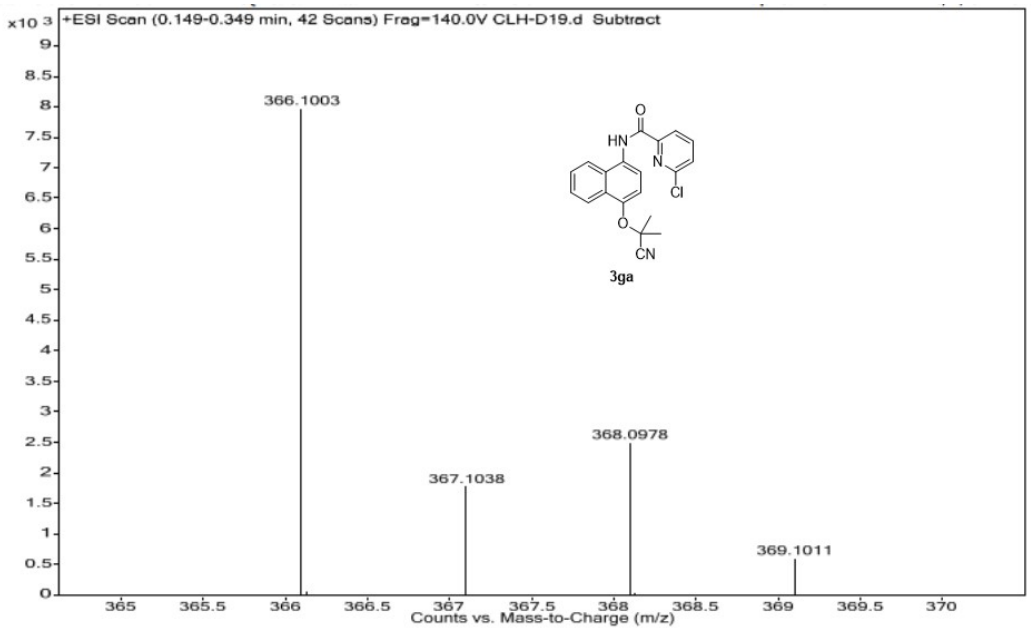

+ESI Scan (0.143-0.396 min, 87 Scans) Frag=140.0V CLH-D16.d Subtract
x10 4
346.1551
347.1582
348.1611
HN
O
N
O
CN
3ba
Counts vs. Mass-to-Charge (m/z)

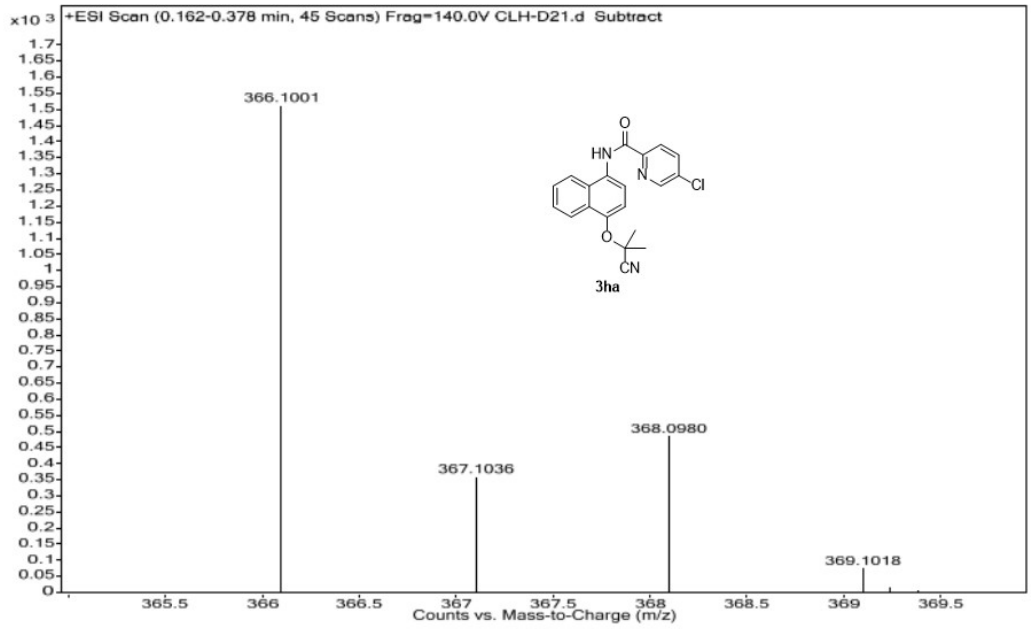

x10 4
+ESI Scan (0.219-0.259 min, 9 Scans) Frag=180.0V CLH-D17.d Subtract
346.1550
347.1581
348.1604
HN
O
N
O
CN
3ca
Counts vs. Mass-to-Charge (m/z)

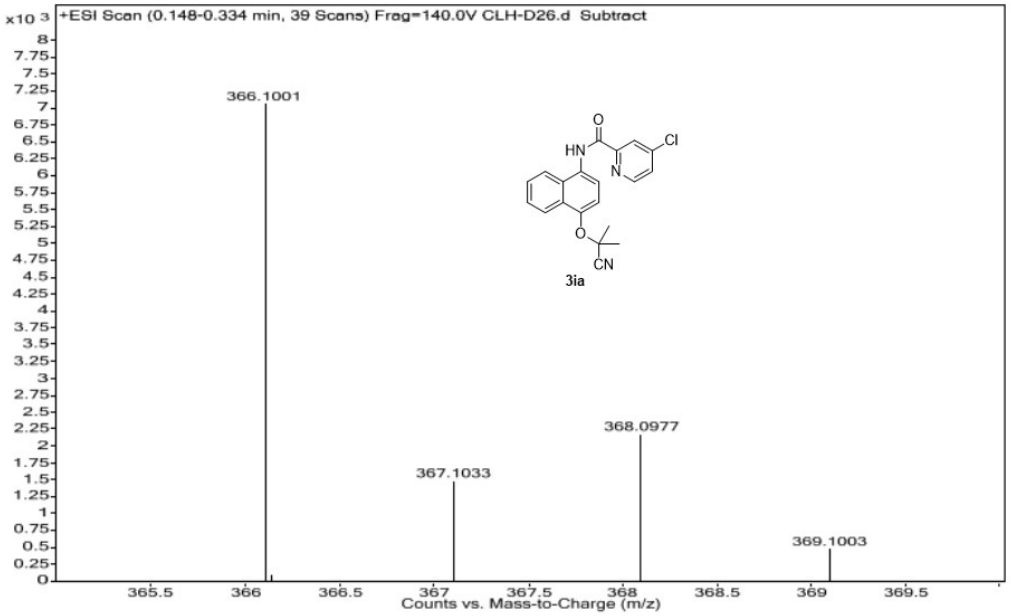

x10 4
+ESI Scan (0.215-0.230 min, 4 Scans) Frag=180.0V CLH-D37.d Subtract
362.1499
363.1531
364.1561
HN
O
N
O
O
CN
3da
Counts vs. Mass-to-Charge (m/z)

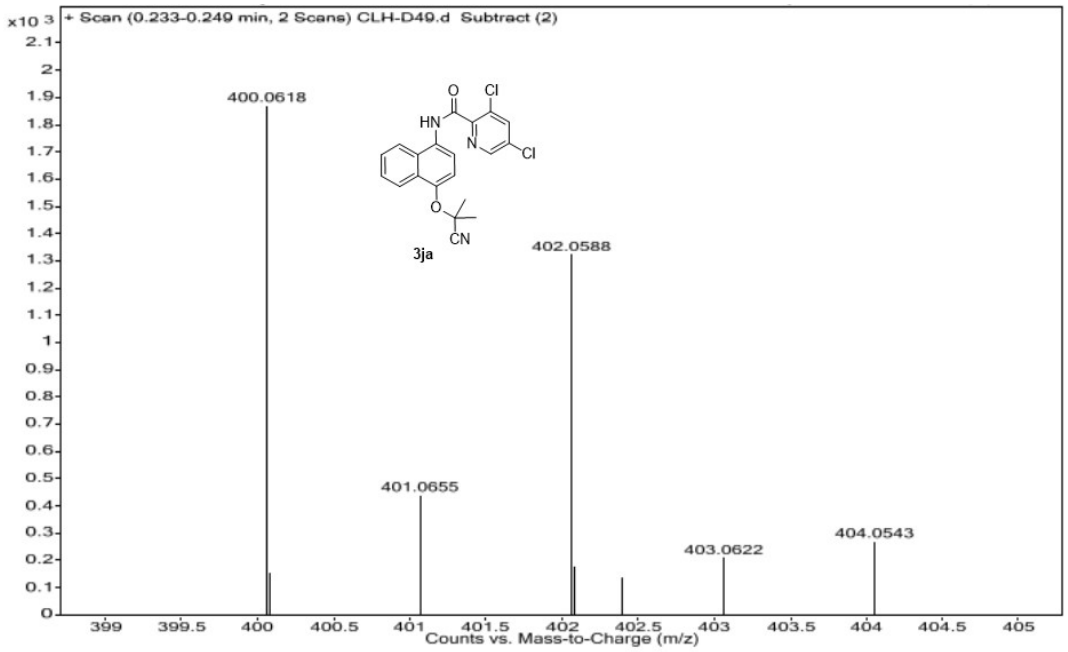

+ESI Scan (0.164-0.193 min, 7 Scans) Frag=180.0V CLH-D22.d Subtract
x10 3
350.1299
351.1334
352.1365
HN
O
N
F
O
CN
3ea
Counts vs. Mass-to-Charge (m/z)

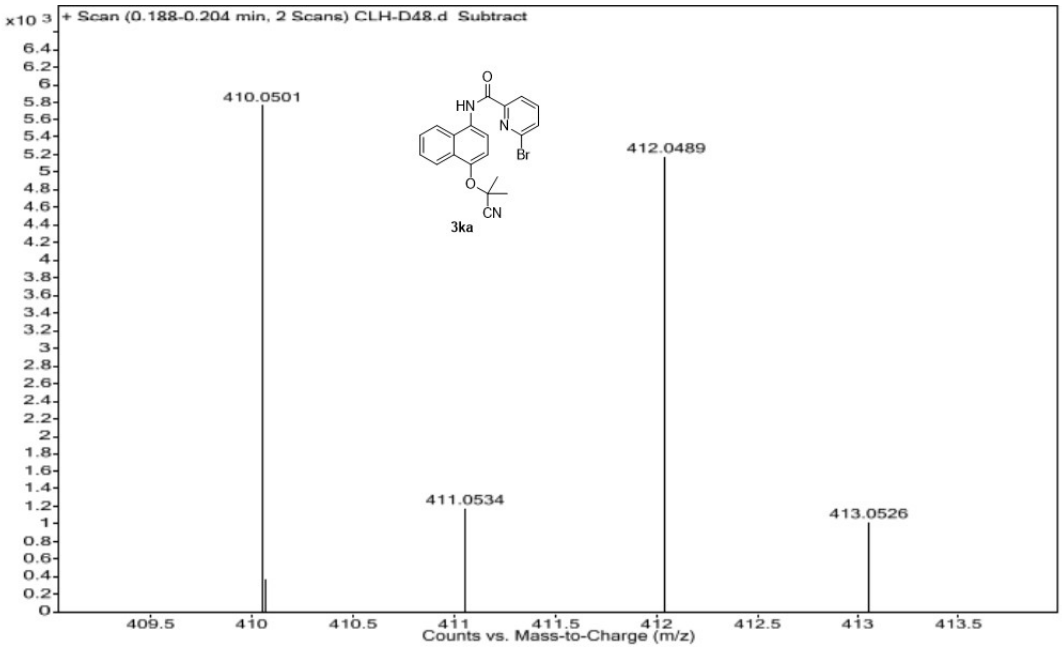

+ESI Scan (0.164-0.291 min, 27 Scans) Frag=140.0V CLH-D24.d Subtract (4)
x10 3
350.1297
351.1332
352.1360
HN
O
N
F
O
CN
3fa
Counts vs. Mass-to-Charge (m/z)

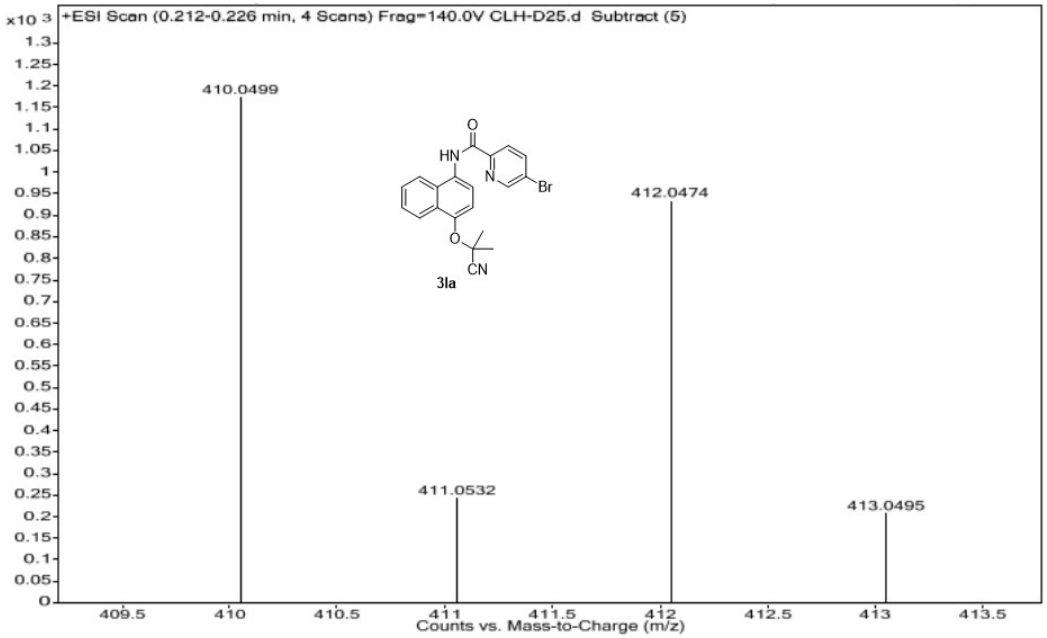

+ESI Scan (0.149-0.349 min, 42 Scans) Frag=140.0V CLH-D19.d Subtract
x10 3
366.1003
368.0978
367.1038
369.1011
3ga
Counts vs. Mass-to-Charge (m/z)

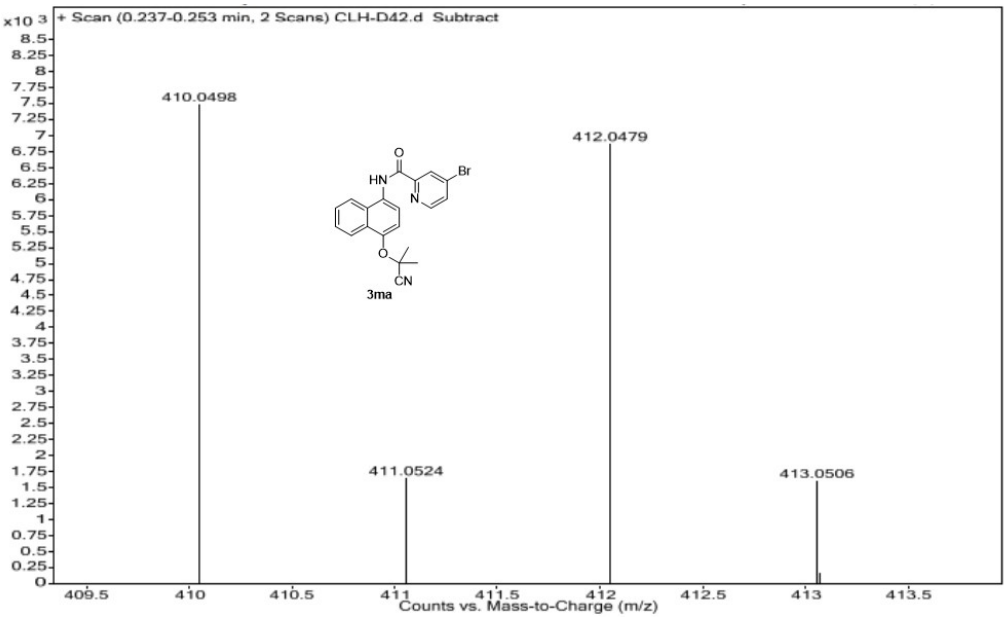

+ESI Scan (0.162-0.378 min, 45 Scans) Frag=140.0V CLH-D21.d Subtract
x10 3
366.1001
368.0980
367.1036
369.1018
3ha
Counts vs. Mass-to-Charge (m/z)

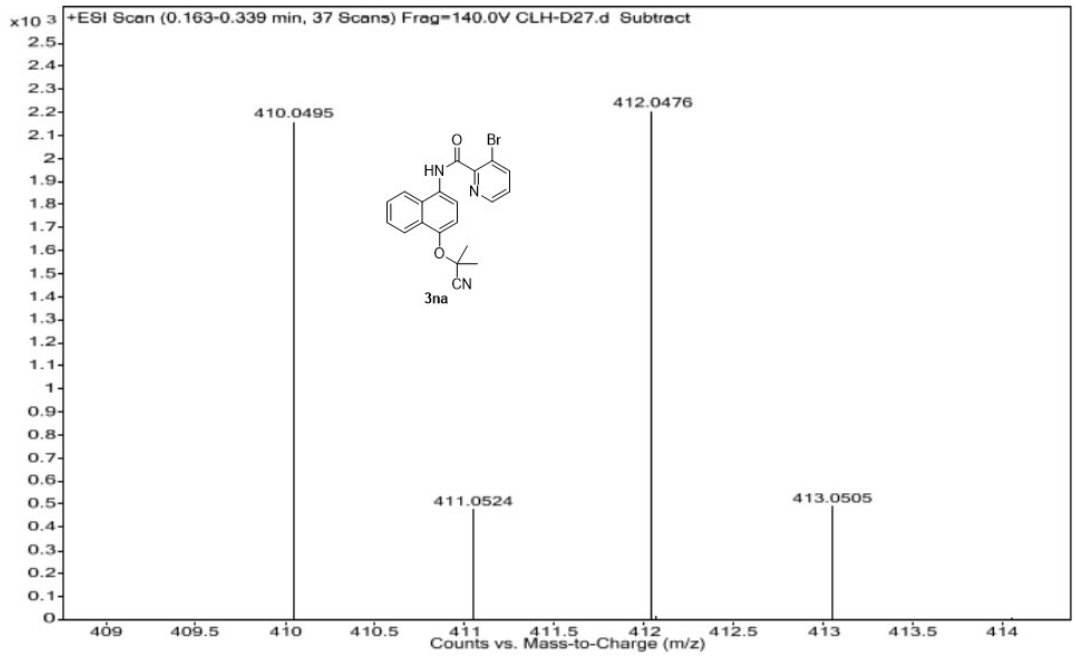

x10 3
+ESI Scan (0.148-0.334 min, 39 Scans) Frag=140.0V CLH-D26.d Subtract
366.1001
367.1033
368.0977
369.1003
HN
O
Cl
N
O
CN
3ia
Counts vs. Mass-to-Charge (m/z)

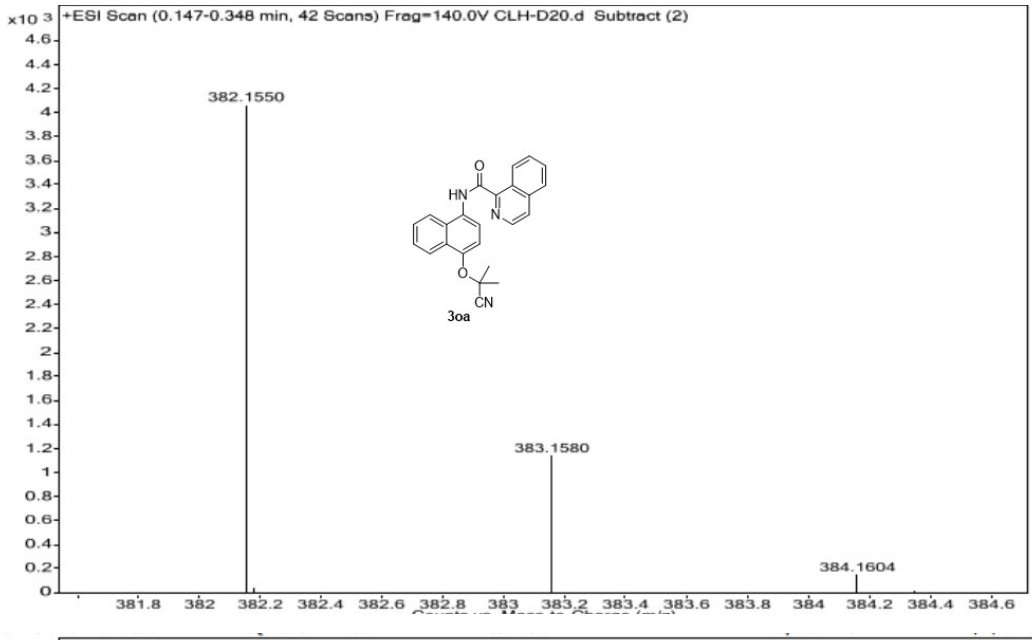

x10 3
+ Scan (0.233-0.249 min, 2 Scans) CLH-D49.d Subtract (2)
400.0618
401.0655
402.0588
403.0622
404.0543
HN
O
Cl
N
Cl
O
CN
3ja
Counts vs. Mass-to-Charge (m/z)

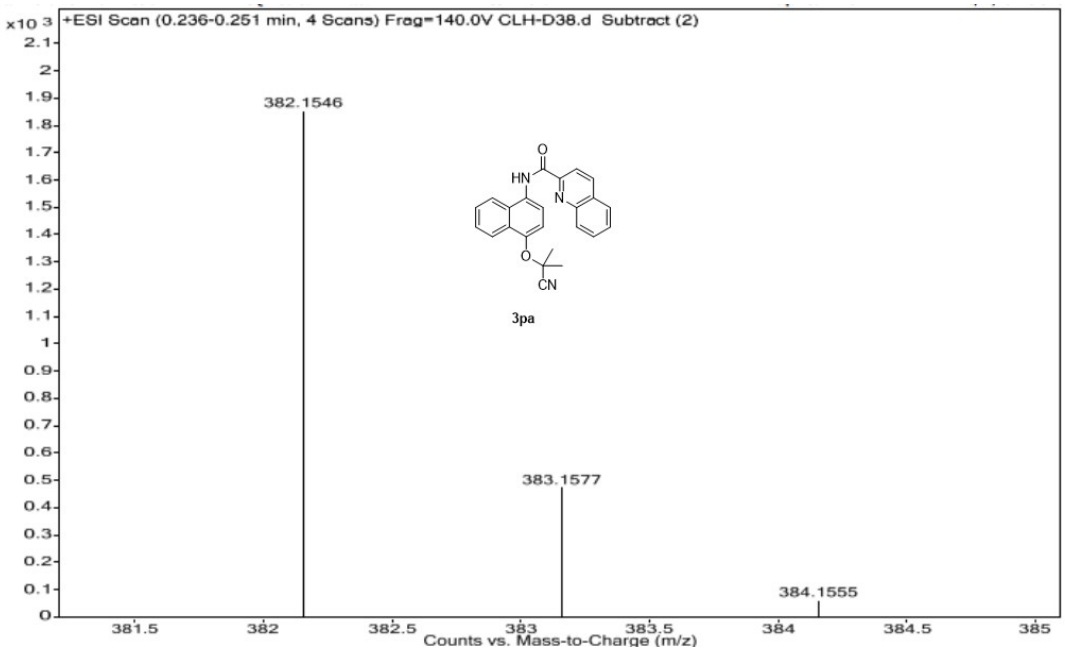

+ Scan (0.188-0.204 min, 2 Scans) CLH-D48.d Subtract
x10 3
410.0501
412.0489
411.0534
413.0526
3ka
Counts vs. Mass-to-Charge (m/z)

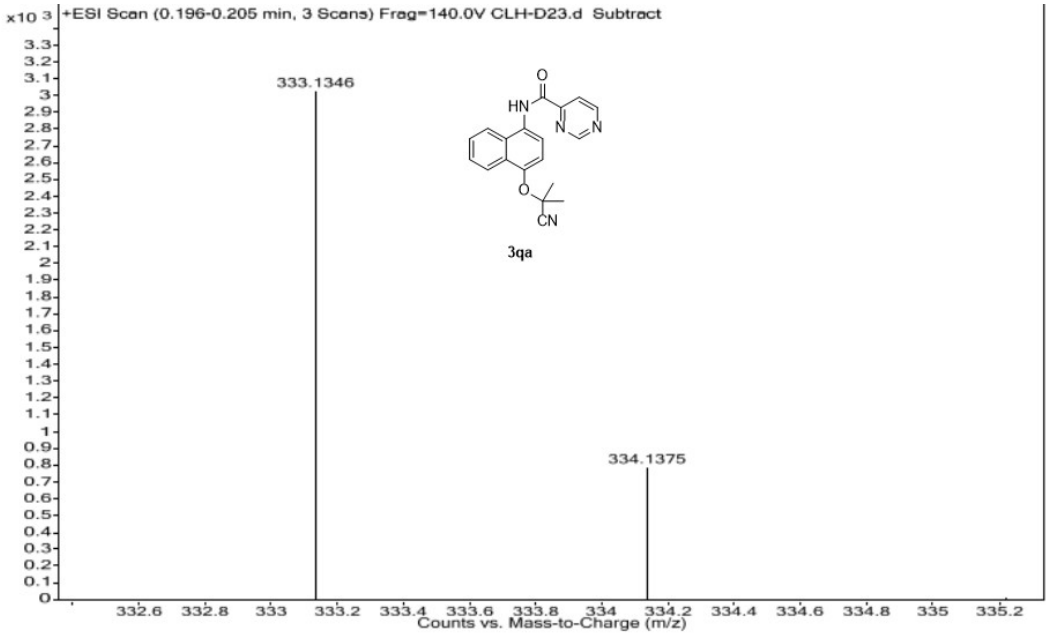

+ESI Scan (0.212-0.226 min, 4 Scans) Frag=140.0V CLH-D25.d Subtract (5)
x10 3
410.0499
412.0474
411.0532
413.0495
3la
Counts vs. Mass-to-Charge (m/z)

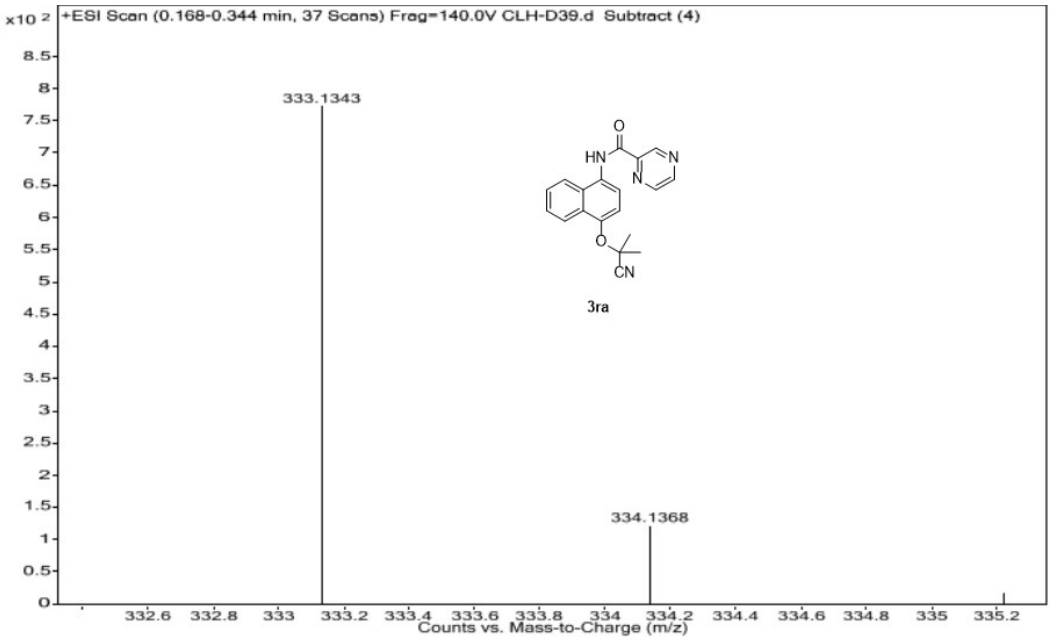

+ Scan (0.237-0.253 min, 2 Scans) CLH-D42.d Subtract
x10 3
410.0498
412.0479
411.0524
413.0506
HN
O
Br
N
O
CN
3ma
Counts vs. Mass-to-Charge (m/z)

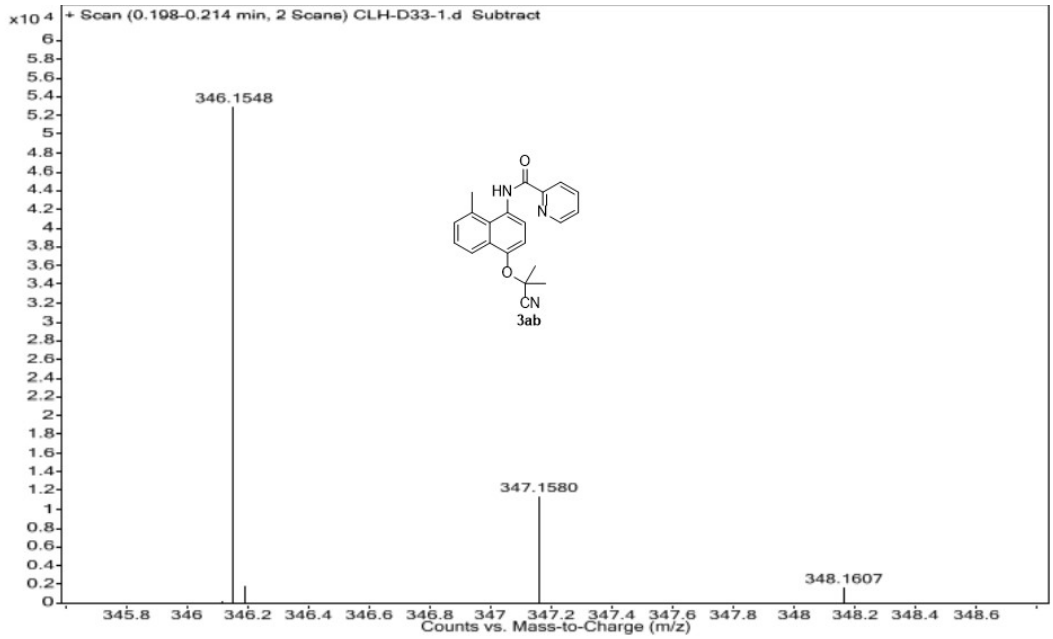

+ESI Scan (0.163-0.339 min, 37 Scans) Frag=140.0V CLH-D27.d Subtract
x10 3
410.0495
412.0476
411.0524
413.0505
HN
O
Br
N
O
CN
3na
Counts vs. Mass-to-Charge (m/z)

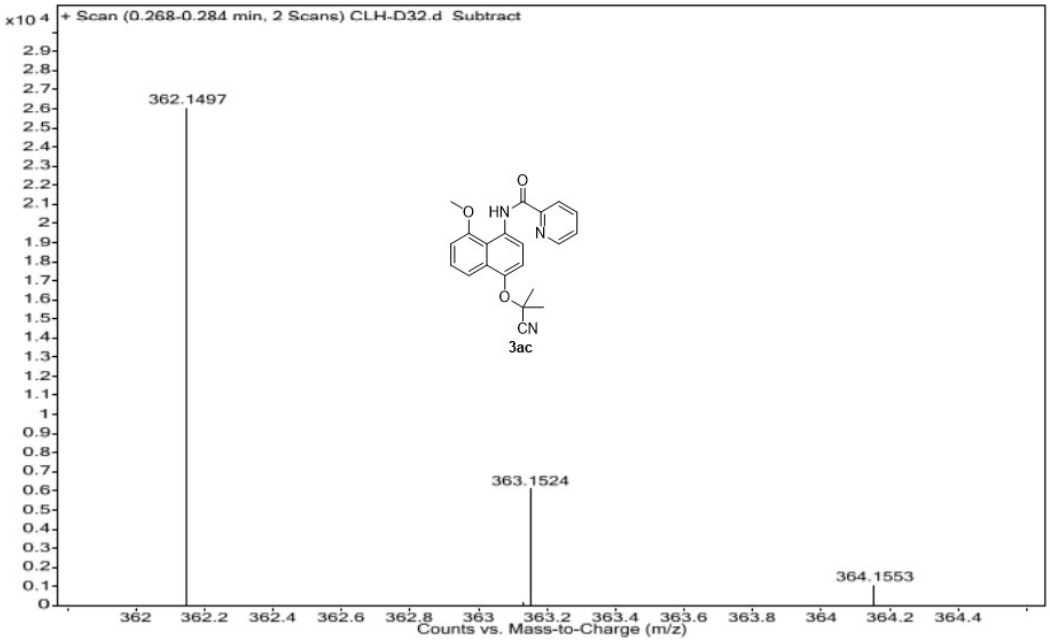

+ESI Scan (0.147-0.348 min, 42 Scans) Frag=140.0V CLH-D20.d Subtract (2)
x10 3
382.1550
383.1580
384.1604
3oa

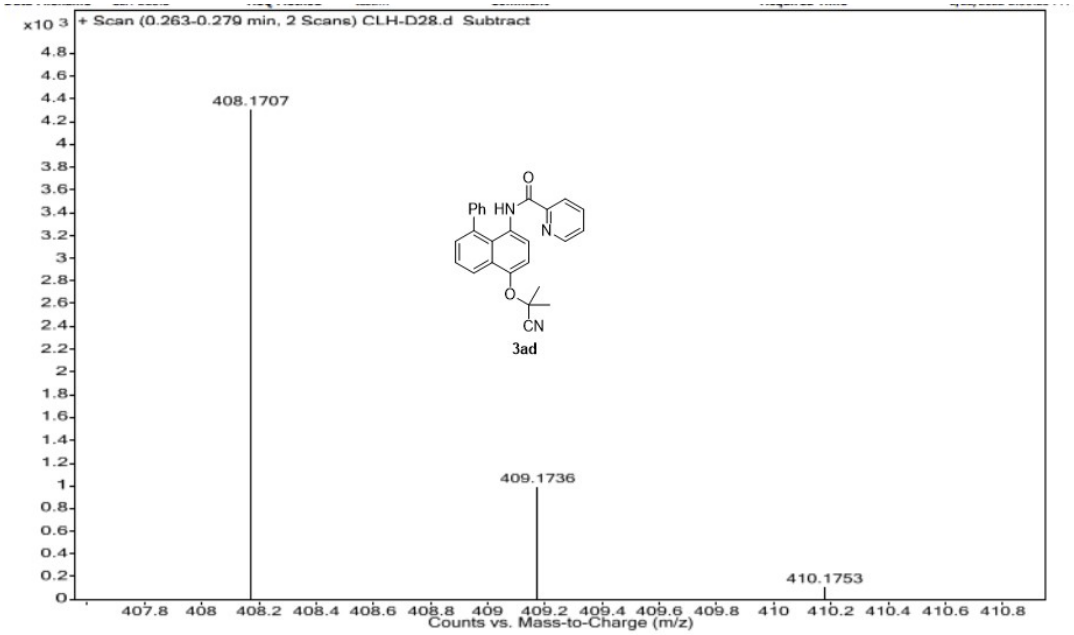

+ESI Scan (0.236-0.251 min, 4 Scans) Frag=140.0V CLH-D38.d Subtract (2)
x10 3
382.1546
383.1577
384.1555
3pa
Counts vs. Mass-to-Charge (m/z)

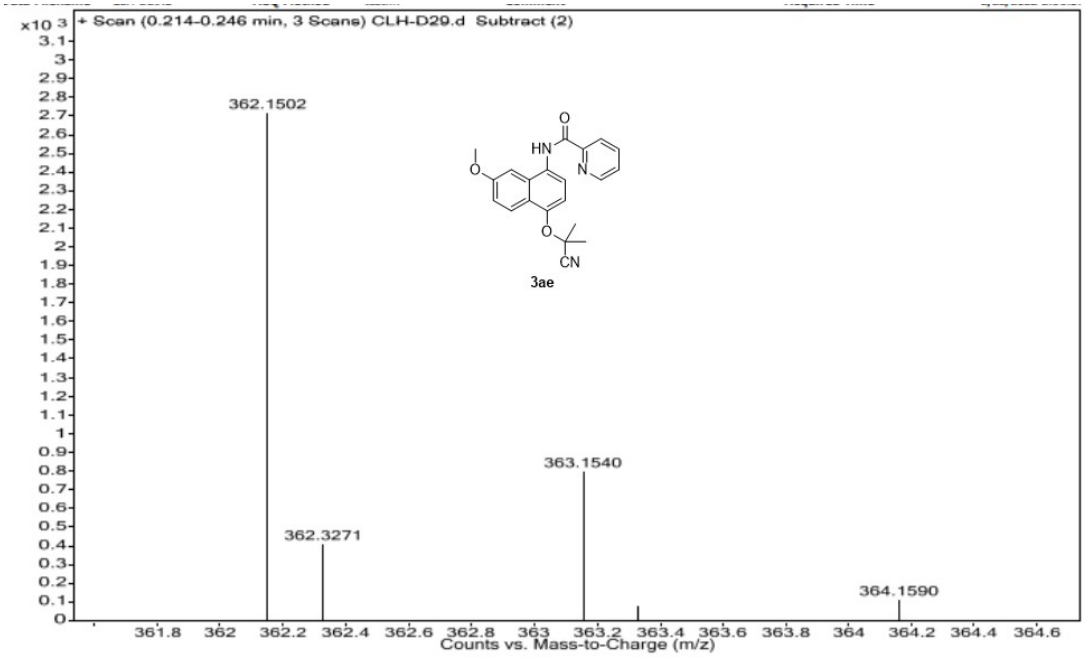

+ESI Scan (0.196-0.205 min, 3 Scans) Frag=140.0V CLH-D23.d Subtract
x10 3
333.1346
334.1375
3qa
Counts vs. Mass-to-Charge (m/z)

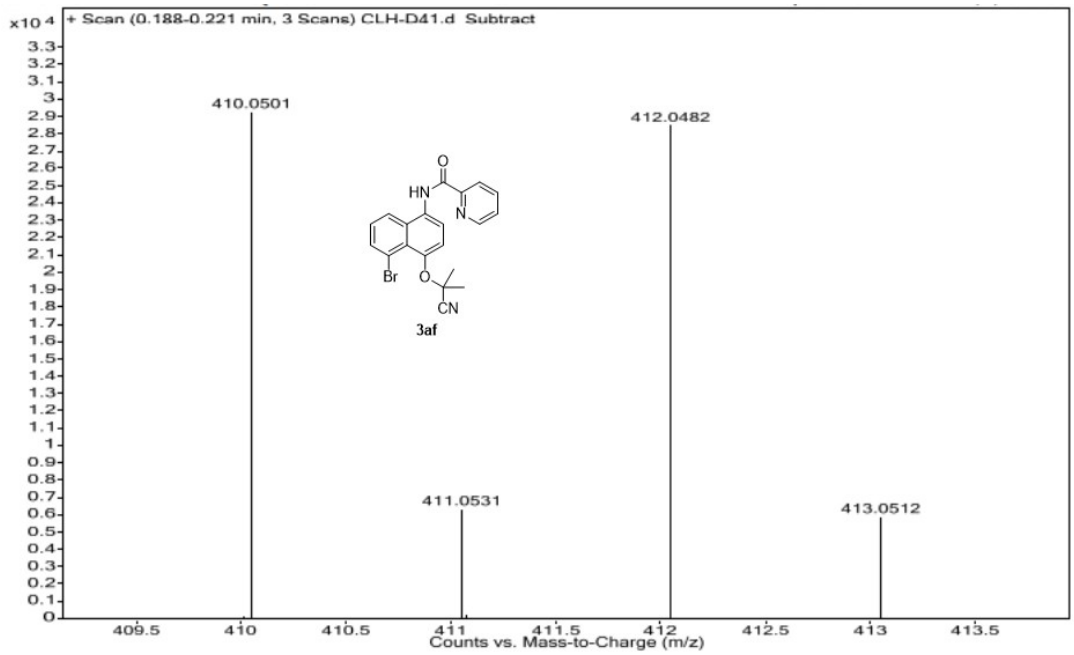

+ESI Scan (0.168-0.344 min, 37 Scans) Frag=140.0V CLH-D39.d Subtract (4)
x10 2
333.1343
334.1368
3ra
Counts vs. Mass-to-Charge (m/z)

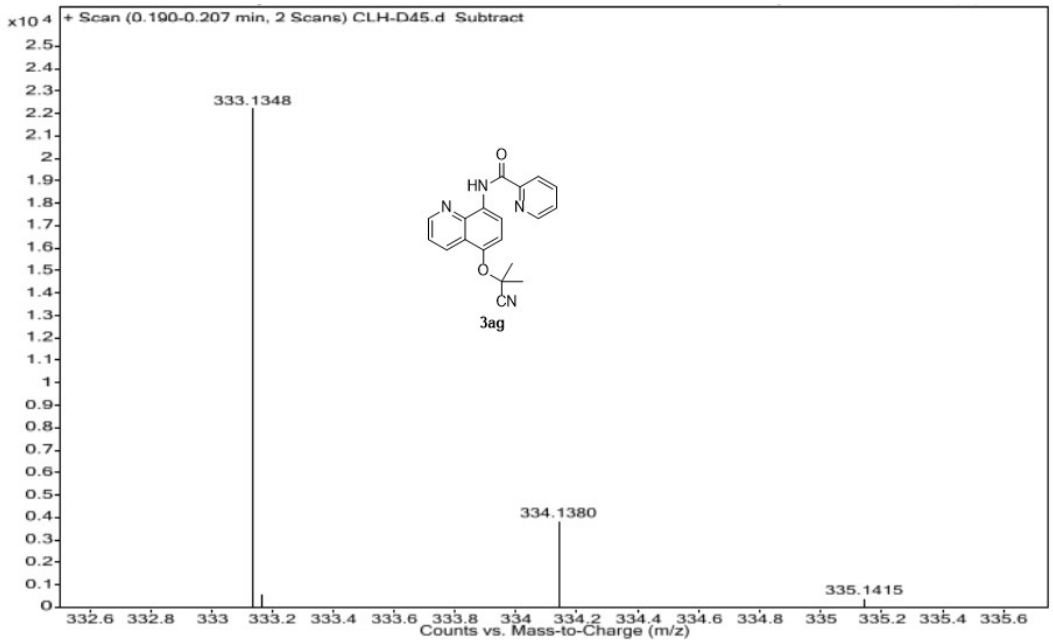

+ Scan (0.198-0.214 min, 2 Scans) CLH-D33-1.d Subtract
x10 4
346.1548
347.1580
348.1607
HN
O
N
O
CN
3ab
Counts vs. Mass-to-Charge (m/z)

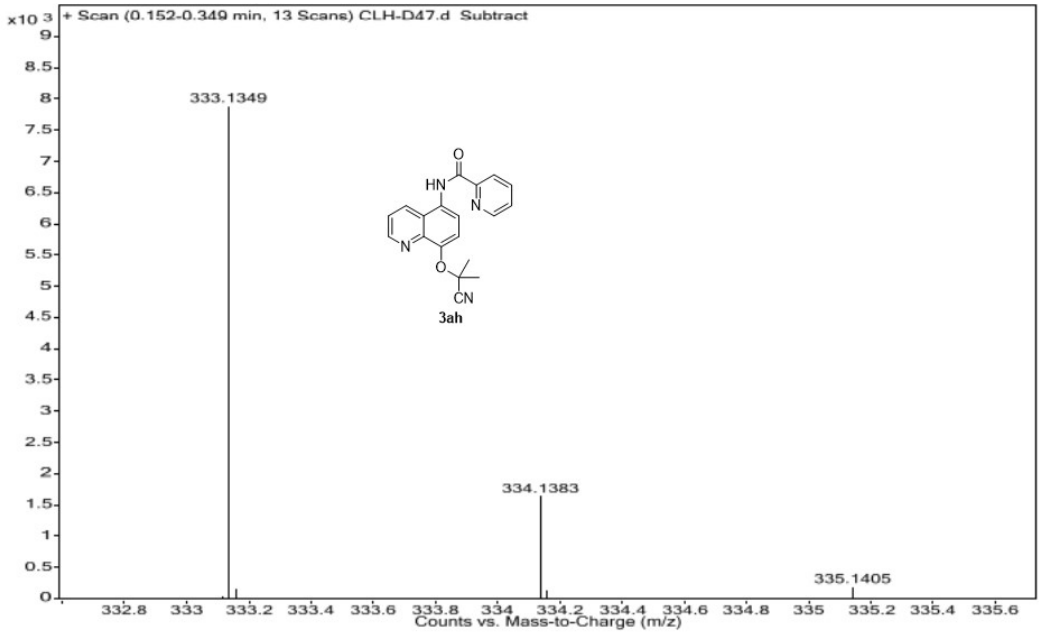

+ Scan (0.268-0.284 min, 2 Scans) CLH-D32.d Subtract
x10 4
362.1497
363.1524
364.1553
O
HN
N
O
CN
3ac
Counts vs. Mass-to-Charge (m/z)

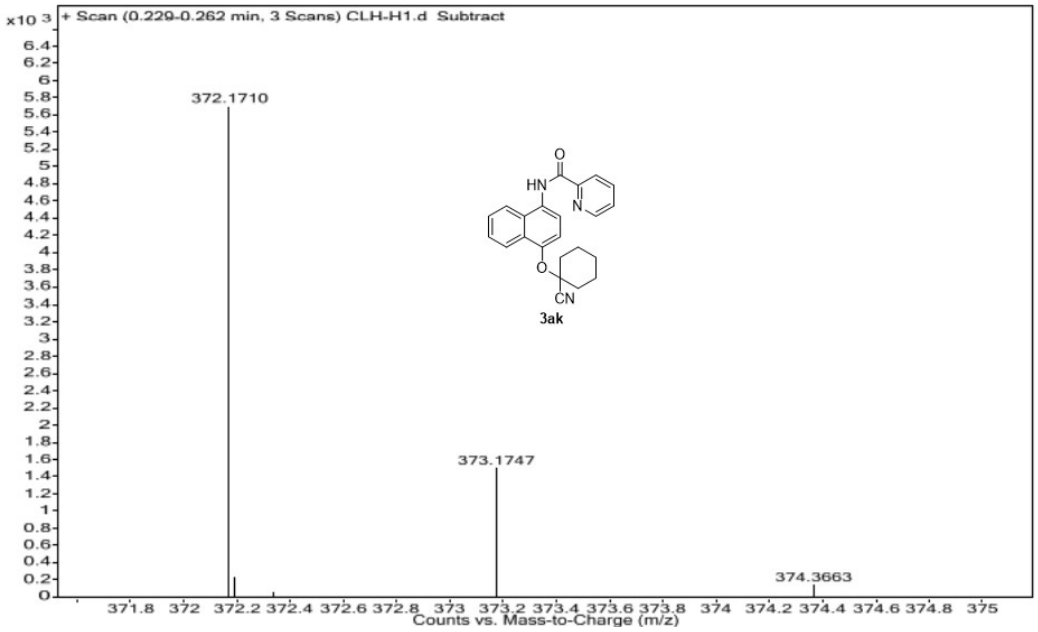

+ Scan (0.263-0.279 min, 2 Scans) CLH-D28.d Subtract
x10 3
408.1707
409.1736
410.1753
Ph HN
O
N
O
CN
3ad
Counts vs. Mass-to-Charge (m/z)

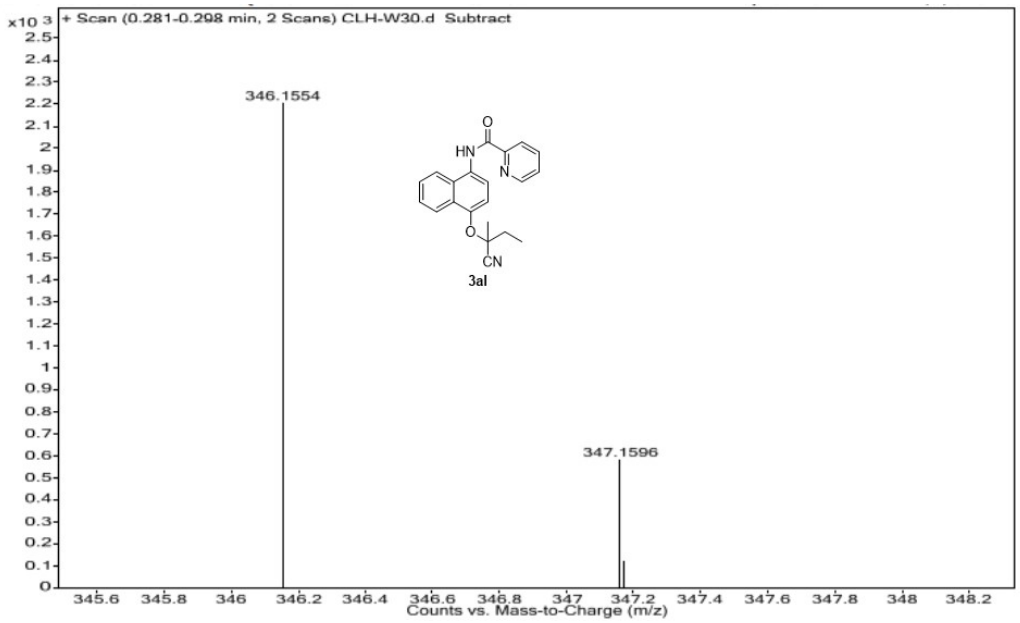

+ Scan (0.214-0.246 min, 3 Scans) CLH-D29.d Subtract (2)
x10 3
362.1502
362.3271
363.1540
364.1590
HN
O
N
O
O
CN
3ae
Counts vs. Mass-to-Charge (m/z)

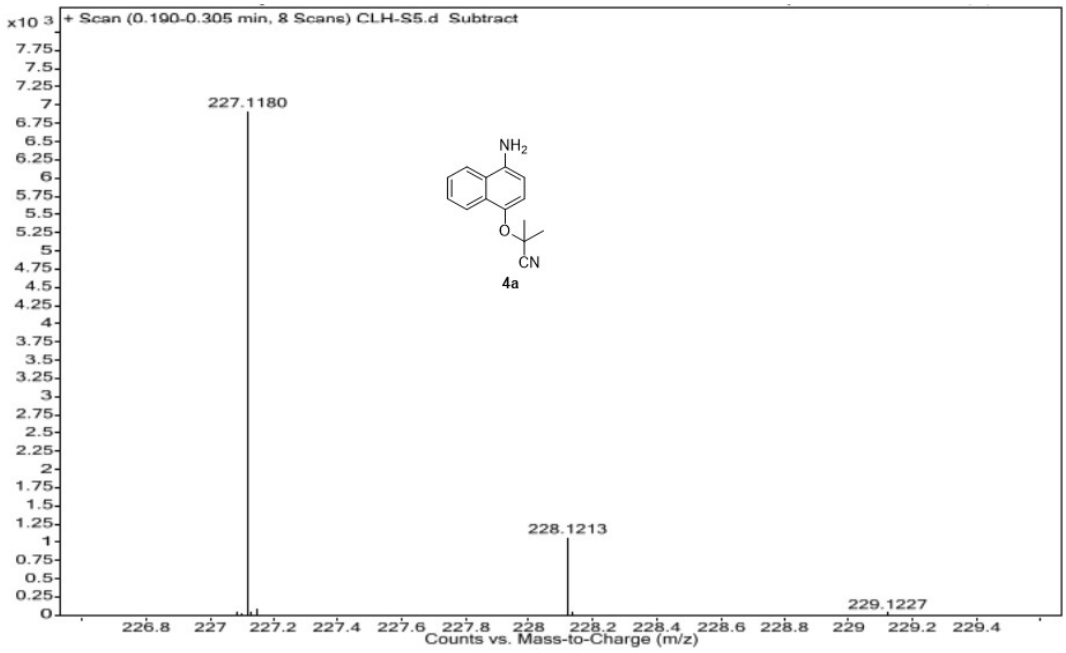

+ Scan (0.188-0.221 min, 3 Scans) CLH-D41.d Subtract
x10 4
410.0501
412.0482
411.0531
413.0512
Br
O
HN
N
O
CN
3af
409.5
410
410.5
411
411.5
412
412.5
413
413.5
Counts vs. Mass-to-Charge (m/z)

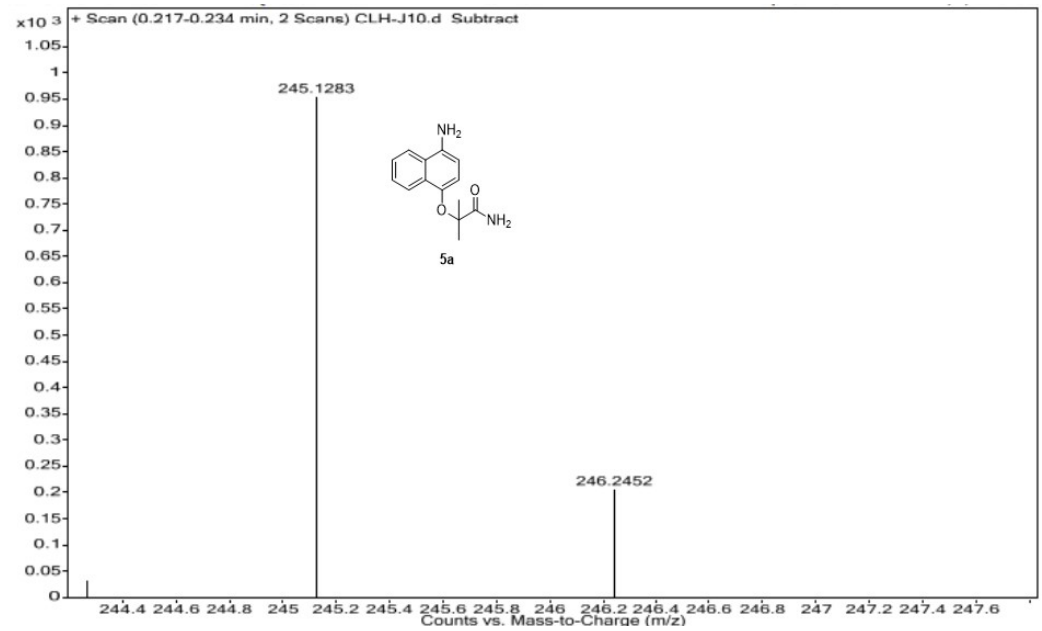

+ Scan (0.190-0.207 min, 2 Scans) CLH-D45.d Subtract
x10 4
333.1348
334.1380
335.1415
N
HN
O
N
O
CN
3ag
332.6
332.8
333
333.2
333.4
333.6
333.8
334
334.2
334.4
334.6
334.8
335
335.2
335.4
335.6
Counts vs. Mass-to-Charge (m/z)

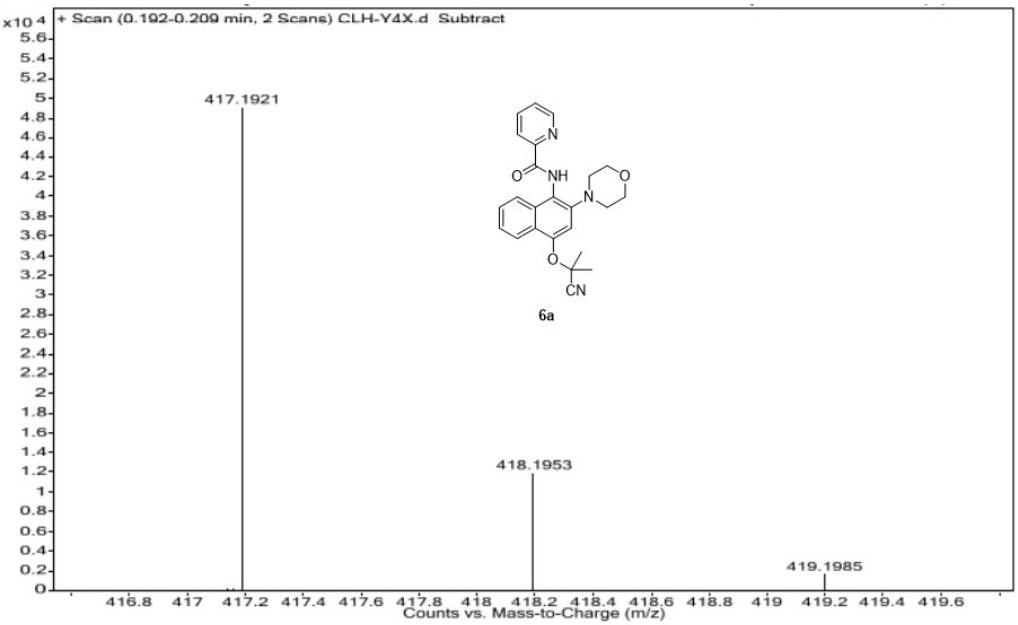

+ Scan (0.152-0.349 min, 13 Scans) CLH-D47.d Subtract
x10 3
333.1349
334.1383
335.1405
3ah
Counts vs. Mass-to-Charge (m/z)

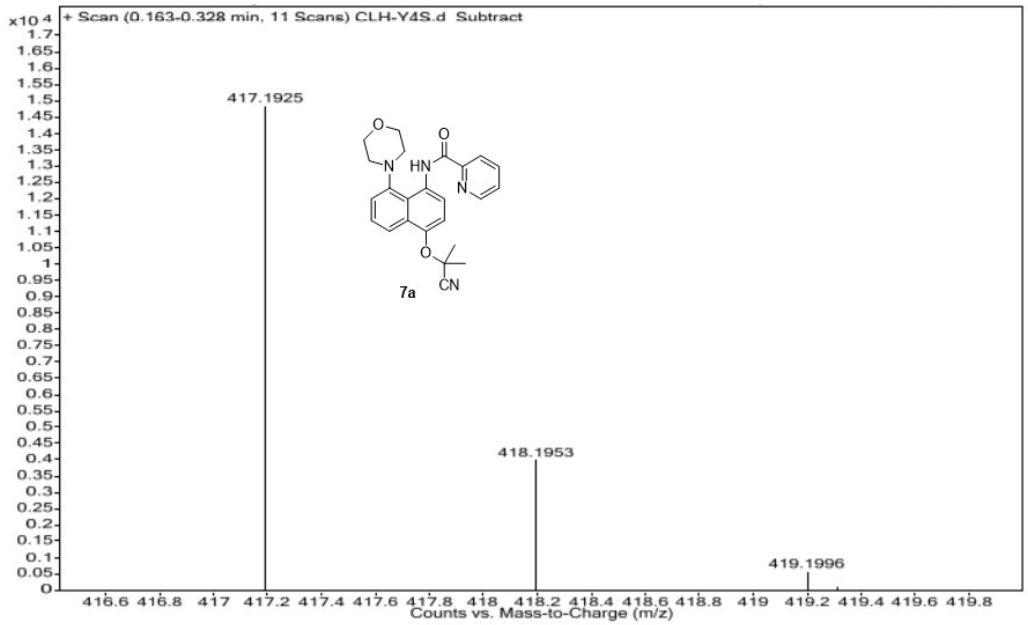

+ Scan (0.229-0.262 min, 3 Scans) CLH-H1.d Subtract
x10 3
372.1710
373.1747
374.3663
3ak
Counts vs. Mass-to-Charge (m/z)

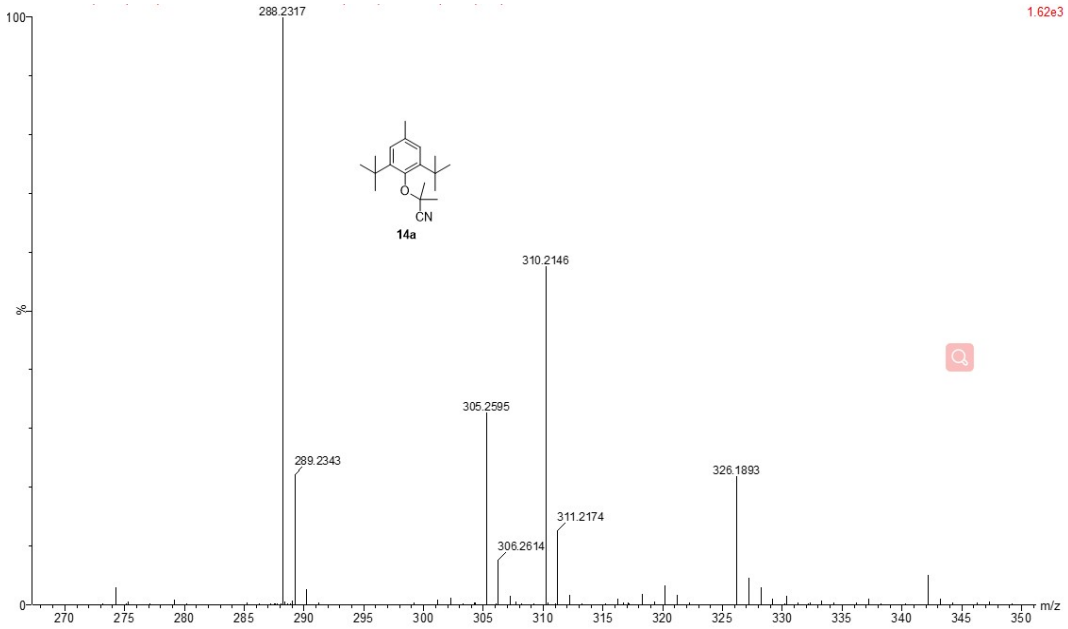

+ Scan (0.281-0.298 min, 2 Scans) CLH-W30.d Subtract
x10 3
346.1554
347.1596
HN
O
N
O
CN
3al
Counts vs. Mass-to-Charge (m/z)


+ Scan (0.190-0.305 min, 8 Scans) CLH-S5.d Subtract
x10 3
227.1180
228.1213
229.1227
NH2
O
CN
4a
Counts vs. Mass-to-Charge (m/z)


+ Scan (0.217-0.234 min, 2 Scans) CLH-J10.d Subtract
x10 3
245.1283
246.2452
NH2
O
NH2
5a
Counts vs. Mass-to-Charge (m/z)


+ Scan (0.192-0.209 min, 2 Scans) CLH-Y4X.d Subtract
x10 4
417.1921
418.1953
419.1985
N
NH
O
N
O
CN
6a
Counts vs. Mass-to-Charge (m/z)





8. Reference

[1]. R. Shang, L. Ilies, E. Nakamura, J. Am. Chem. Soc. 2015, 137, 7660.