Electronic Supplementary Material (ESI) for ChemComm.

Supplementary Materials for

Coordination strategy induced selective C-H amination of 8-animoquinolines

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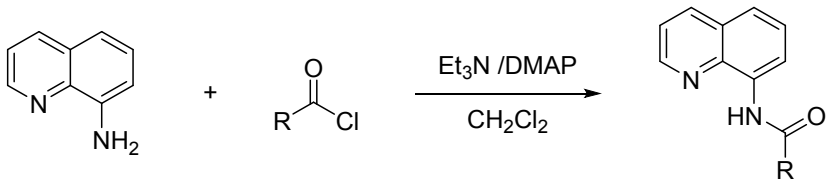
1. General Information

All manipulations were carried out by standard Schlenk techniques. Unless otherwise noted, analytical grade solvents and commercially available reagents were used to conduct the reactions. Thin layer chromatography (TLC) employed glass 0.25 mm silica gel plates. Flash chromatography columns were packed with 200-300 mesh silica gel in petroleum (boiling point is between 60-90°C). Gradient flash chromatography was conducted eluting with a continuous gradient using petroleum ether and ethyl acetate. The known compounds were characterized by ^{1}H NMR and ^{13}C NMR. GC-MS spectra were recorded on a Varian GC-MS 3900-2100T. The ^{1}H and ^{13}C NMR spectra were recorded on a Bruker 400 MHz NMR spectrometer with tetramethylsilane as an internal standard. The chemical shifts (δ) were given in part per million relative to internal tetramethyl silane (TMS, 0 ppm for ^{1}H), $CDCl_3$ (77.3 ppm for ^{13}C). High resolution mass spectra (HRMS) were measured with LTQ-Orbitrap Elite (Thermo-Fisher Scientific, Waltham, MA, USA) instrument and accurate masses were reported for the molecular ion + Hydrogen (M+H). The crystallography data collection were performed with APEX2 suite (BRUKER).

2. General Procedures for the Synthesis of 8-Aminoquinolines

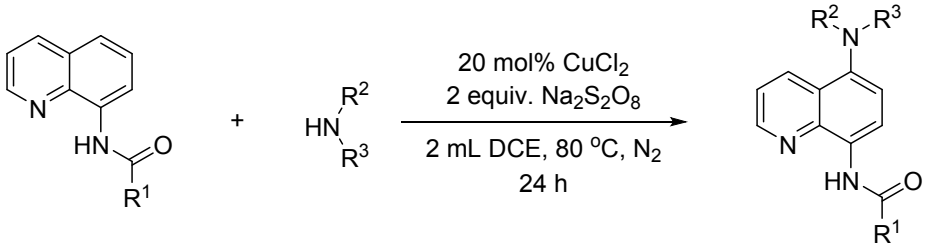


A mixture of 8-Aminoquinoline (10.0 mmol), Et_3N (2 mL) and DMAP (20.0 mg) were stirred in 20 mL CH_2Cl_2 under 0 ℃. Then acyl chloride (15.0 mmol) was added to the system dropwised. The solution was stirred at room temperature under air overnight. After completion of the reaction, the mixture was extracted three times using dilute hydrochloric acid (1.0 mol/L) and saturated sodium carbonate solution, the organic layer was dried over Na_2SO_4, the target product was obtained by flash column chromatography on silica gel using petroleum ether and ethyl acetate.

3. Condition Screening

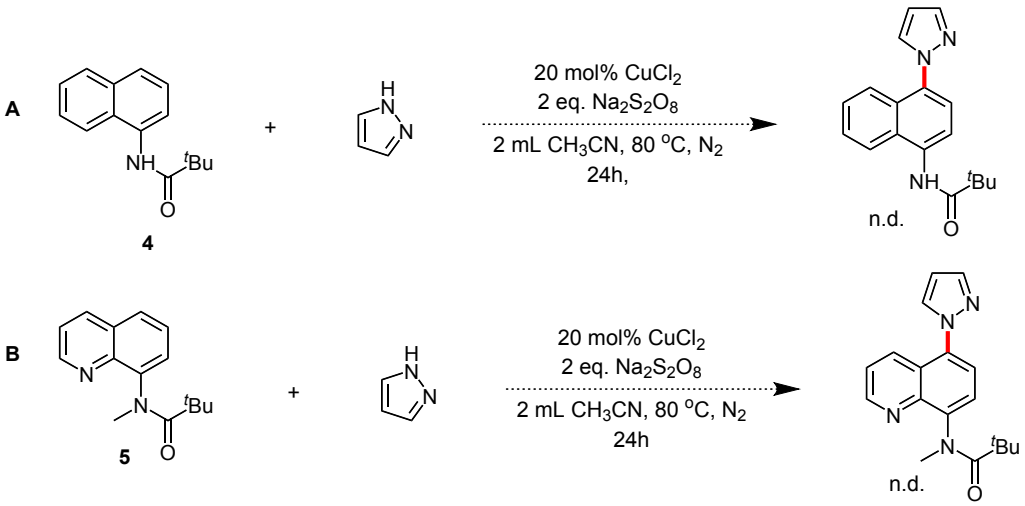
In a 25 mL schlenk tube, N-(5-(1H-pyrazol-1-yl)quinolin-8-yl)pivalamide (0.25 mmol), pyrazole (1.0 mmol), Cu catalyst (0.05 mmol) and oxidant (0.5 mmol) were stirred in 2 mL solvent at 80℃ under N_2 atmosphere for 24 hours, the mixture was diluted by ethyl acetate. The yield was determined by GC using biphenyl as internal standard.

4. General Procedures for the Amination of 8-Aminoquinolines

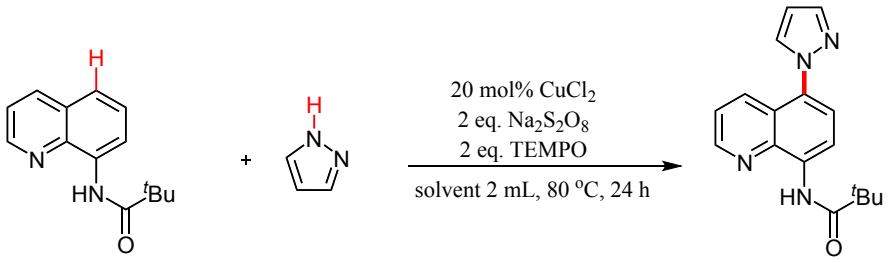


In a 25 mL schlenk tube, 8-Aminoquinolines (0.25 mmol), azoles (1.0 mmol), $CuCl_2$ or $Cu(OTf)_2$ (0.05 mmol) and $Na_2S_2O_8$ (0.5 mmol) were stirred in 2 mL DCE at 80℃ under N_2 atmosphere for 24 hours. After completion of the reaction, the mixture was diluted by ethyl acetate. As indicated by TLC, the pure product was obtained by flash column chromatography on silica gel using petroleum ether and ethyl acetate.

Scheme S1. (A) and (B) Control experiments.



5. Radical Inhibition Experiment



In a 25 mL schlenk tube, N-(5-(1H-pyrazol-1-yl)quinolin-8-yl)pivalamide (0.25 mmol), pyrazole (1.0 mmol), $CuCl_2$ (0.05 mmol), $Na_2S_2O_8$ (0.5 mmol) and TEMPO (0.5 mmol) were stirred in 2 mL DCE at 80℃ under N_2 atmosphere for 24 hours. Then the reaction mixture was monitored using TLC and GC-MS, no target product was detected.

6. Theoretical Calculation Details

6.1. Complete reference for Gaussian 09

Gaussian 09, Revision A.2, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, Jr., J. A.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, N. J.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, Ö.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. Gaussian, Inc., Wallingford CT, **2013**.

6.2. Computational methods.

All the density functional theory (DFT) calculations were carried out with the GAUSSIAN 09 series of programs. The B3LYP[1] method with a standard 6-31G(d,p) basis set was used for geometry optimizations in solvation. Acetonitrile is employed as the solvent. Harmonic frequency calculations were performed for all stationary points to confirm them as a local minima or and to derive the thermochemical corrections for the enthalpies and free energies. The solvent effects were considered by the geometry optimizations in solvent with a SMD continuum solvation model[2].

6.3. Table S1 Absolute calculation energies, enthalpies, and free energies.

Geometry	$E_{(elec\text{-}B3LYP)}$[1]	$G_{(corr\text{-}B3LYP)}$[2]	$H_{(corr\text{-}B3LYP)}$[3]	IF[5]
1a'	-727.742634	0.231729	0.291225	-

[1]The electronic energy calculated by B3LYP in acetonitrile. [2]The thermal correction to Gibbs free energy calculated by B3LYP in acetonitrile. [3]The thermal correction to enthalpy calculated by B3LYP in acetonitrile.

6.4. B3LYP geometries for the optimized compound 1a'.

C	-3.77451300	-1.88832100	0.01743700
C	-4.01298200	-0.52370800	0.01665500
C	-2.91163700	0.36299700	0.00155800
C	-1.61138700	-0.20592600	-0.01119000
C	-2.44430200	-2.34621300	0.00151700
H	-4.04984200	2.20922000	0.00796900
H	-4.59021600	-2.60325400	0.03009700
H	-5.02322000	-0.12568400	0.02823900
C	-3.05313600	1.77807800	0.00036500
C	-0.44424900	0.67925800	-0.01668100
H	-2.23029300	-3.41165500	0.00069800
C	-0.63826200	2.09091600	-0.01857900
C	-1.92303800	2.61156000	-0.01146200
H	0.22103400	2.74544100	-0.02722900
H	-2.05678600	3.68802900	-0.01542800
N	-1.38801900	-1.52974700	-0.01222900
N	0.75267400	0.06002000	-0.02011400
H	0.66623100	-0.95950000	-0.03809400
C	2.06826900	0.60551500	0.01662800
O	2.23742500	1.80987600	0.05886000
C	3.18587400	-0.44196400	-0.00053100
C	3.04995200	-1.35937300	1.24021700
H	2.11877700	-1.93522800	1.24035800
H	3.87925100	-2.07429400	1.23884100
H	3.09822000	-0.78032500	2.16861900
C	4.54033200	0.28239900	0.03642300
H	5.34173800	-0.46300700	0.02557300
H	4.66872700	0.93678900	-0.83126800
H	4.64723100	0.88866400	0.94106300

C	3.07833800	-1.28035800	-1.29778700
H	3.13227500	-0.64498500	-2.18818800
H	3.91557000	-1.98537000	-1.32878800
H	2.15375200	-1.86492500	-1.34437500

7. EXAFS Data Collection and Analysis

X-ray absorption measurements were acquired in transmission mode at beamline 17C11 at National Synchrotron Radiation Research Center (NSSRC) in Taiwan. A pure Cu foil spectrum (edge energy 8979 eV) was acquired simultaneously with each measurement for energy calibration. Multiple scans were taken to reduce the noise.

All solution samples were placed in a sample holder (the XAS solution cell) made of PEEK (polyether ether ketone) equipped with a screw top and O-ring fitting to prevent exposure to air and water[3]. For solution samples, the Cu concentration was adjusted to be 0.05 - 0.1 M with a path length of 3.5 mm. The sample holder was placed in a quartz tube (1–in. OD, 10–in. length) sealed with Kapton windows by two Ultra-Torr fittings and then used for transmission mode measurement.

The edge energy of the X-Ray absorption near edge structure (XANES) spectrum was determined from the inflection point of the edge. The data procedures were carried out using the Athena software package using standard methods[4]. Standard procedures based on Artemis software (Demeter 0.9.20) were used to extract the extended X-ray absorption fine structure (EXAFS) data.

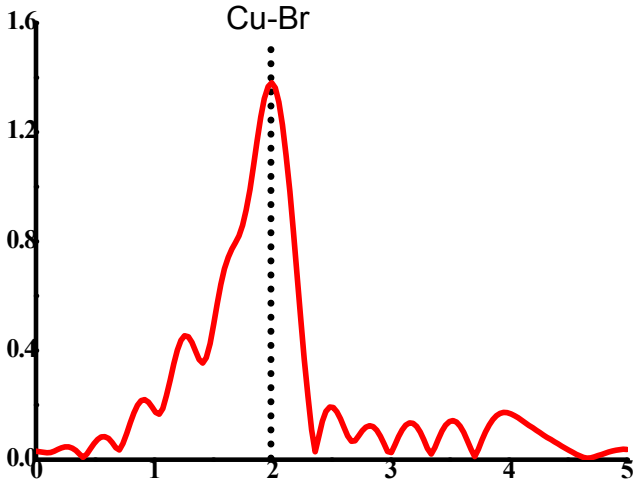


Figure S 1: The EXAFS spectrum of the reaction between CuBr2 and N-(5-(1H-pyrazol-1-yl)quinolin-8-yl)pivalamide in DMF at 80 ^{o}C.

8. Crystallography Data

Crystal structure determination of compound 3aa: A single crystal of the compound was selected, mounted onto a cryoloop, and transferred in a cold nitrogen gas stream. Intensity data were collected with a BRUKER Kappa-APEXII diffractometer with graphite-monochromated Mo-Kα radiation (λ = 0.71073 Å). Data collection were performed with APEX2 suite (BRUKER). Unit-cell parameters refinement, integration and data reduction were carried out with SAINT program (BRUKER). SADABS (BRUKER) was used for scaling and multi-scan absorption corrections. In the WinGX suite of programs, the structure were solved with Sir2014 program and refined by full-matrix least-squares methods using SHELXL-14.

CCDC 1486070 contain 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.

Empirical formula	C17H18N4O
Formula weight	294.35
Space group	P21/C
***a* (Å)**	7.4064
***b* (Å)**	21.4982
***c* (Å)**	10.1255
***α* (deg)**	90
***β* (deg)**	104.800
***γ* (deg)**	90
***V* (Å^3)**	1535
Z	4
***T* (K)**	296 K
ρ_{calcd} (g/cm^3)	1.274
μ (mm^{-1})	0.083
Significant reflections	3985
***R*[I > 2.5□ (*I*)]**	0.0501
R_w[I > 2.5□ (*I*)]	0.1536

Table S2. Crystallography Data

Number	Atom1	Atom2	Length
1	O1	C10	1.221(2)
2	H1	N1	0.89(2)
3	H1	C1	0.98(2)
4	C1	N3	1.314(2)
5	C1	C2	1.396(3)
6	N1	C8	1.399(2)
7	N1	C10	1.345(2)
8	H3	C3	1.02(2)
9	N3	C9	1.365(2)
10	C3	C2	1.361(3)
11	C3	C4	1.412(2)
12	N2	N4	1.360(2)
13	N2	C18	1.327(3)
14	H2	C2	0.99(2)
15	C4	C5	1.424(2)
16	C4	C9	1.411(2)
17	N4	C5	1.421(2)
18	N4	C16	1.356(2)
19	C5	C6	1.365(2)

20	C8	C7	1.366(2)
21	C8	C9	1.430(2)
22	C7	H7	0.98(2)
23	C7	C6	1.403(3)
24	C6	H6	0.99(2)
25	C10	C11	1.526(3)
26	C11	C13	1.515(3)
27	C11	C12	1.523(3)
28	C11	C14	1.507(3)

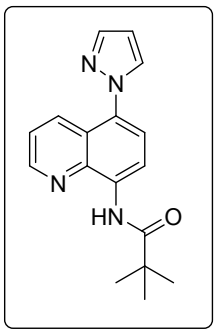
Table S3. Selected bond lengths

Atom1	**Atom2**	**Atom3**	**Angle**
N3	C1	C2	123.4(2)
C8	N1	C10	129.3(2)
C1	N3	C9	117.7(2)
C2	C3	C4	119.4(2)
N4	N2	C18	103.9(2)
C1	C2	C3	119.7(2)
C3	C4	C5	125.2(2)
C3	C4	C9	116.8(2)
C5	C4	C9	117.9(1)
N2	N4	C5	122.1(1)
N2	N4	C16	111.5(2)
C5	N4	C16	126.4(2)
C4	C5	N4	121.2(1)
C4	C5	C6	120.3(2)
N4	C5	C6	118.4(2)
N1	C8	C7	125.8(2)
N1	C8	C9	114.7(1)
C7	C8	C9	119.5(2)
C8	C7	H7	120(1)
C8	C7	C6	120.2(2)
H7	C7	C6	120(1)
C5	C6	C7	121.6(2)
C5	C6	H6	120(1)
C7	C6	H6	118(1)
O1	C10	N1	121.9(2)
O1	C10	C11	121.5(2)
N1	C10	C11	116.6(2)
N3	C9	C4	123.0(2)
N3	C9	C8	116.5(1)
C4	C9	C8	120.5(1)
C10	C11	C13	106.7(2)

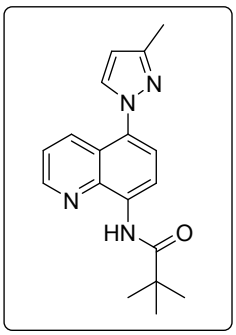
C10	C11	C12	113.8(2)
C10	C11	C14	108.4(2)
C13	C11	C12	108.1(2)
C13	C11	C14	110.5(2)
C12	C11	C14	109.3(2)
C18	C17	C16	105.1(2)
N2	C18	C17	112.6(2)
N4	C16	C17	106.9(2)

Table S4. Selected angles.

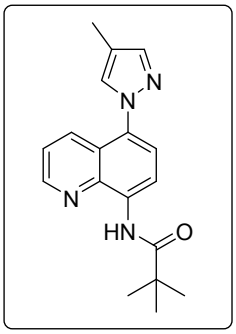
9. Characterization of Products



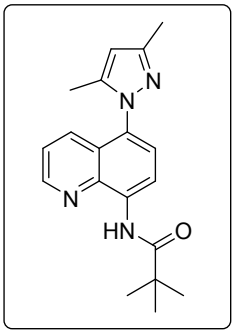
N-(5-(1H-pyrazol-1-yl)quinolin-8-yl)pivalamide (**3aa**): 53.1 mg (yield: 72%, 0.25 mmol scale), white solid. ^{1}H NMR (400 MHz, DMSO-d_6) δ = 10.24 (s, 1H), 9.02 (d, J = 4.0 Hz, 1H), 8.73 (d, J = 8.0 Hz, 1H), 8.36 (dd, J = 8.4, 1.6 Hz, 1H), 8.22 (d, J = 2.0 Hz, 1H), 7.86 (d, J = 1.6 Hz, 1H), 7.70-7.74 (m, 2H), 6.62 – 6.61 (m, 1H), 1.36 (s, 9H); ^{13}C NMR (101 MHz, DMSO-d_6) δ = 176.3, 149.7, 141.0, 137.9, 134.3, 132.9, 132.3, 130.7, 123.4, 123.3, 123.1, 114.6, 106.9, 39.9, 27.3. HRMS (ESI) calculated for $C_{17}H_{18}N_4O$ [M+H]$^+$: 295.1553; found: 295.1557.



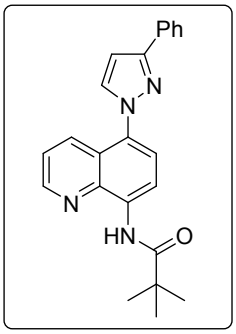
N-(5-(3-methyl-1H-pyrazol-1-yl)quinolin-8-yl)pivalamide (**3ab**): 43.6 mg (yield: 57%, 0.25 mmol scale),light yellow solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ = 10.33 (s, 1H), 8.87 – 8.80 (m, 1H), 8.38 (dd, J = 1.6, 7.2 Hz, 1H), 7.63 (d, J = 2.3 Hz, 1H), 7.52 (d, J = 8.3 Hz, 1H), 7.53-7.49 (m, 1H), 6.29 (d, J = 2.3 Hz, 1H), 2.41 (s, 3H), 1.44 (s, 9H); ^{13}C NMR (101 MHz, $CDCl_3$) δ = 177.5, 150.6, 148.8, 138.8, 135.0, 133.1, 132.3, 131.3, 124.3, 123.7, 122.4, 115.2, 106.8, 40.5, 27.8, 13.9. HRMS (ESI) calculated for $C_{18}H_{20}N_4O$ [M+H]$^+$: 309.1710; found: 309.1717.



N-(5-(4-methyl-1H-pyrazol-1-yl)quinolin-8-yl)pivalamide (**3ac**): 48.2 mg (yield: 62%, 0.25 mmol scale), white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ = 10.33 (s, 1H), 8.87 – 8.79 (m, 2H), 8.39 (dd, *J* = 8.6, 1.7 Hz, 1H), 7.62 (s, 1H), 7.55 – 7.50 (m, 2H), 7.49 –7.46 (m, 1H), 2.19 (s, 3H), 1.43 (s, 9H); ^{13}C NMR (101 MHz, $CDCl_3$) δ = 177.5, 148.8, 142.0, 138.8, 134.9, 133.2, 131.3, 130.2, 124.1, 123.5, 122.4, 117.4, 115.2, 40.5, 27.8, 9.0. HRMS (ESI) calculated for $C_{18}H_{20}N_4O$ $[M+H]^+$: 309.1710; found: 309.1712.

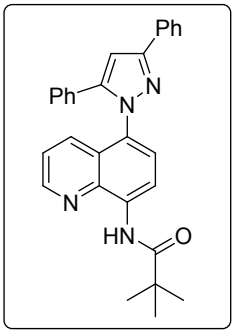


N-(5-(3,5-dimethyl-1H-pyrazol-1-yl)quinolin-8-yl)pivalamide (**3ad**): 50.9 mg (yield: 62%, 0.25 mmol scale), yellow solid. ^{1}H NMR (400 MHz, DMSO-d_6) δ = 10.24 (s, 1H), 9.01 (d, *J* = 5.8 Hz, 1H), 8.74 (d, *J* = 8.2 Hz, 1H), 7.78 – 7.76 (m, 1H), 7.71 – 7.68 (m, 1H), 7.64 (d, *J* = 8.4 Hz, 1H), 6.16 (s, 1H), 2.24 (s, 3H), 2.04 (s, 3H), 1.37 (s, 9H); ^{13}C NMR (101 MHz, DMSO-d_6) δ = 176.4, 149.6, 148.0, 141.2, 137.9, 134.7, 132.6, 129.5, 126.1, 125.2, 123.3, 114.4, 105.7, 39.5, 27.3, 13.4, 11.1. HRMS (ESI) calculated for $C_{19}H_{22}N_4O$ $[M+H]^+$: 323.1866; found: 323.1868.

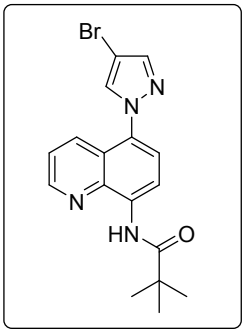


N-(5-(3-phenyl-1H-pyrazol-1-yl)quinolin-8-yl)pivalamide (**3ae**): 60.1 mg (yield: 65%, 0.25 mmol scale), white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ = 10.37 (s, 1H), 8.92 – 8.84 (m, 2H), 8.49 (dd, *J* = 1.6, 7.2 Hz, 1H), 7.99 – 7.88 (m, 2H), 7.78 (d, *J* = 2.4 Hz, 1H), 7.63 (d, *J* = 8.3 Hz, 1H), 7.52 (dd, *J* = 8.6, 4.2 Hz, 1H), 7.49 – 7.45 (m, 1H), 7.36 – 7.33 (m, 1H), 6.84 (d, *J* = 2.4 Hz, 1H), 1.46 (s, 9H); ^{13}C NMR (101 MHz, $CDCl_3$) δ = 177.5, 153.2, 148.9, 138.8, 135.2, 133.1, 133.1, 133.0,

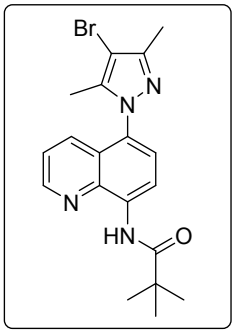
131.1, 128.8, 128.2, 125.9, 124.2, 123.7, 122.5, 115.1, 104.3, 40.5, 27.8. HRMS (ESI) calculated for $C_{23}H_{22}N_4O$ $[M+H]^+$: 371.1866; found: 371.1870.



N-(5-(3,5-diphenyl-1H-pyrazol-1-yl)quinolin-8-yl)pivalamide (**3af**): 79.8 mg (yield: 72%, 0.25 mmol scale), yellow solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ = 10.37 (s, 1H), 8.84 – 8.79 (m, 1H), 8.80 (d, *J* = 8.3 Hz, 1H), 8.12 – 8.04 (m, 1H), 8.00 – 7.91 (m, 2H), 7.51 – 7.41 (m, 4H), 7.40 – 7.33 (m, 1H), 7.23 – 7.12 (m, 5H), 6.97 (s, 1H), 1.45 (s, 9H); ^{13}C NMR (101 MHz, $CDCl_3$) δ = 177.5, 152.4, 148.8, 146.8, 138.8, 135.6, 133.0, 132.7, 130.2, 129.9, 128.8, 128.6, 128.4, 128.2, 128.1, 127.2, 125.9, 125.5, 122.6, 115.1, 103.9, 40.5, 27.8. HRMS (ESI) calculated for $C_{29}H_{26}N_4O$ $[M+H]^+$: 447.2179; found: 447.2184.

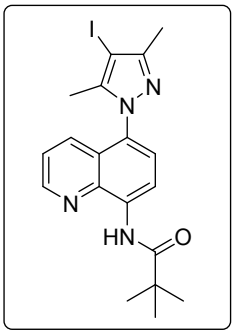


N-(5-(4-bromo-1H-pyrazol-1-yl)quinolin-8-yl)pivalamide (**3ag**): 54.9 mg (yield: 59%, 0.25 mmol scale), white solid. ^{1}H NMR (400 MHz, DMSO-d_6) δ = 10.23 (s, 1H), 9.00-8.99 (m, 1H), 8.70 (d, *J* = 8.3 Hz, 1H), 8.50 (s, 1H), 8.29 (d, *J* = 8.4 Hz, 1H), 7.97 (s, 1H), 7.77 – 7.67 (m, 2H), 1.34 (s, 9H); ^{13}C NMR (101 MHz, DMSO-d_6) δ = 176.3, 149.7, 141.3, 137.7, 134.7, 132.5, 132.5, 130.0, 123.8, 123.3, 123.1, 114.4, 94.0, 39.8, 27.2. HRMS (ESI) calculated for $C_{17}H_{17}BrN_4O$ $[M+H]^+$: 373.0659; found: 373.0666.

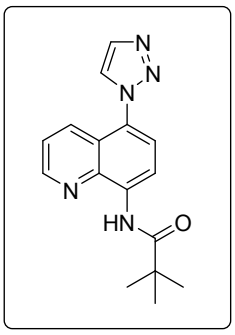


N-(5-(4-bromo-3,5-dimethyl-1H-pyrazol-1-yl)quinolin-8-yl)pivalamide (**3ah**): 78.3 mg (yield:

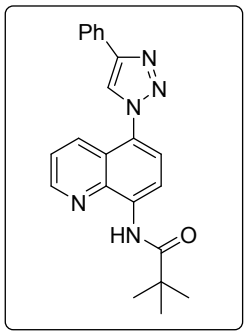
78%, 0.25 mmol scale), white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ = 10.33 (s, 1H), 8.92 – 8.76 (m, 2H), 7.77 (dd, *J* = 8.5, 1.7 Hz, 1H), 7.55 – 7.39 (m, 2H), 2.32 (s, 3H), 2.06 (s, 3H), 1.43 (s, 9H); ^{13}C NMR (101 MHz, $CDCl_3$) δ = 177.5, 148.9, 147.9, 139.8, 138.8, 135.9, 132.3, 129.3, 126.7, 125.6, 122.7, 115.0, 95.4, 40.5, 27.8, 12.6, 11.0. HRMS (ESI) calculated for $C_{19}H_{21}BrN_4O$ $[M+H]^+$: 401.0972; found: 401.0977.



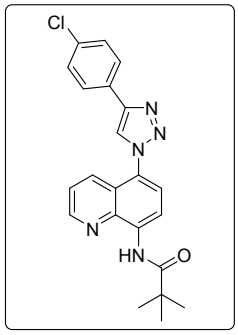
N-(5-(4-iodo-3,5-dimethyl-1H-pyrazol-1-yl)quinolin-8-yl)pivalamide (**3ai**): 91.7 mg (yield: 81%, 0.25 mmol scale), yellow solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ = 10.33 (s, 1H), 8.99 – 8.67 (m, 2H), 7.78 – 7.75 (m, 1H), 7.49-7.45 (m, 1H), 2.33 (s, 3H), 2.09 (s, 3H), 1.43 (s, 9H). ^{13}C NMR (101 MHz, $CDCl_3$) δ = 1776, 151.1, 148.9, 143.3, 138.8, 135.9, 132.3, 129.5, 126.7, 125.6, 122.8, 115.0, 64.0, 40.5, 27.8, 14.3, 12.7. HRMS (ESI) calculated for $C_{19}H_{21}IN_4O$ $[M+H]^+$: 449.0833; found: 449.0835



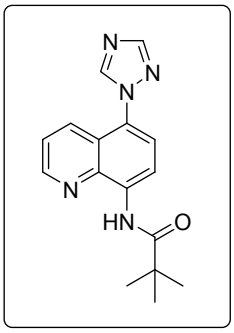
N-(5-(1H-1,2,3-triazol-1-yl)quinolin-8-yl)pivalamide (**3aj**): 48.7 mg (yield: 66%, 0.25 mmol scale), white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ = 10.36 (s, 1H), 8.88 (d, *J* = 8.5 Hz, 2H), 8.07 (d, *J* = 8.4 Hz, 1H), 7.93 (d, *J* = 3.7 Hz, 2H), 7.60 (d, *J* = 8.3 Hz, 1H), 7.52 (dd, *J* = 8.5, 4.1 Hz, 1H), 1.42 (s, 9H); ^{13}C NMR (101 MHz, $CDCl_3$) δ = 177.6, 149.2, 138.5, 136.5, 134.0, 132.0, 127.1, 126.2, 124.5, 123.8, 123.1, 114.8, 40.6, 27.7. HRMS (ESI) calculated for $C_{16}H_{17}N_5O$ $[M+H]^+$: 296.1506; found: 296.1509.



N-(5-(4-phenyl-1H-1,2,3-triazol-1-yl)quinolin-8-yl)pivalamide (**3ak**): 61.9 mg (yield: 67%, 0.25 mmol scale), white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ = 10.39 (s, 1H), 8.99 – 8.85 (m, 2H), 8.23 – 8.20 (m, 1H), 8.13 (s, 1H), 8.03 – 7.85 (m, 2H), 7.66 (d, *J* = 8.4 Hz, 1H), 7.55 (dd, *J* = 8.6, 4.2 Hz, 1H), 7.51 – 7.41 (m, 2H), 7.43 – 7.33 (m, 1H), 1.45 (s, 9H); ^{13}C NMR (101 MHz, $CDCl_3$) δ = 177.7, 149.3, 148.0, 138.6, 136.6, 132.2, 130.2, 129.1, 128.6, 127.2, 126.0, 124.4, 123.8, 123.1, 122.2, 114.9, 40.6, 27.8. HRMS (ESI) calculated for $C_{22}H_{21}N_5O$ $[M+H]^+$: 372.1819; found: 372.1825.

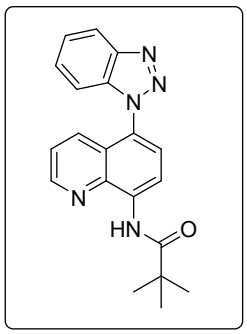


N-(5-(4-(4-chlorophenyl)-1H-1,2,3-triazol-1-yl)quinolin-8-yl)pivalamide (**3al**): 68.0 mg (yield: 67%, 0.25 mmol scale), white solid. ^{1}H NMR (400 MHz, DMSO-d_6) δ = 10.31 (s, 1H), 9.19 (s, 1H), 9.09 - 9.07 (m, 1H), 8.80 (d, *J* = 8.3 Hz, 1H), 8.22 (dd, *J* = 1.2, 7.6 Hz, 1H), 8.02 (d, *J* = 8.5 Hz, 2H), 7.93 (d, *J* = 8.3 Hz, 1H), 7.79 – 7.78 (m, 1H), 7.58 (d, *J* = 8.5 Hz, 2H), 1.38 (s, 9H); ^{13}C NMR (101 MHz, DMSO-d_6) δ = 176.6, 150.2, 145.7, 137.6, 135.8, 132.7, 132.2, 129.2, 129.1, 127.1, 126.9, 124.7, 124.5, 123.9, 123.1, 114.3, 40.0, 27.3. HRMS (ESI) calculated for $C_{22}H_{20}ClN_5O$ $[M+H]^+$: 406.1429; found: 406.1437.

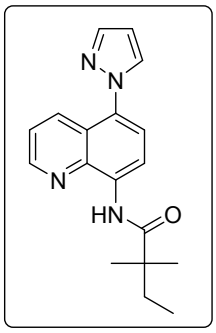


N-(5-(1H-1,2,4-triazol-1-yl)quinolin-8-yl)pivalamide (**3am**): 44.2 mg (yield: 60%, 0.25 mmol scale), yellow solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ = 10.36 (s, 1H), 8.90 – 8.86 (m, 2H), 8.42 (s, 1H), 8.22 (s, 1H), 8.19 (d, *J* = 8.6 Hz, 1H), 7.58 (d, *J* = 8.3 Hz, 1H), 7.54 (dd, *J* = 8.5, 4.1 Hz, 1H),

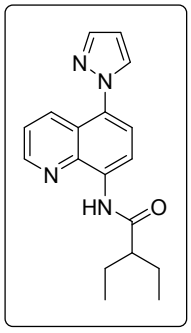
1.43 (s, 9H). ^{13}C NMR (101 MHz, $CDCl_3$) δ = 177.7, 152.9, 149.2, 144.8, 138.7, 136.5, 132.1, 126.8, 124.6, 123.9, 123.0, 114.8, 40.6, 27.8. HRMS (ESI) calculated for $C_{16}H_{17}N_5O$ $[M+H]^+$: 296.1506; found: 296.1511.



N-(5-(1H-benzo[d][1,2,3]triazol-1-yl)quinolin-8-yl)pivalamide (**3an**): 43.7 mg (yield: 51%, 0.25 mmol scale), white solid. ^{1}H NMR (400 MHz, DMSO-d_6) δ = 10.34 (s, 1H), 9. 07 (dd, J = 1.2, 4.0 Hz, 1H), 8.86 (d, J = 8.3 Hz, 1H), 8.25 (d, J = 8.2 Hz, 1H), 7.97 (d, J = 8.3 Hz, 1H), 7.85 (dd, J = 1.2, 8.8 Hz, 1H), 7.74-7.67 (m, 1H), 7.64 – 7.56 (m, 1H), 7.57 – 7.47 (m, 2H), 1.38 (s, 9H); ^{13}C NMR (101 MHz, DMSO-d_6) δ = 176.6, 150.1, 145.0, 138.0, 135.9, 134.3, 131.8, 128.8, 126.0, 125.5, 124.8, 124.0, 123.8, 119.7, 114.7, 110.5, 39.8, 27.3. HRMS (ESI) calculated for $C_{20}H_{19}N_5O$ $[M+H]^+$: 346.1662; found: 346.1666.

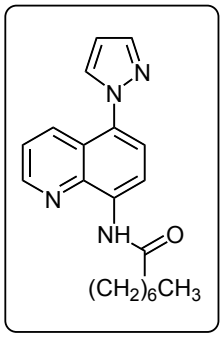


N-(5-(1H-pyrazol-1-yl)quinolin-8-yl)-2,2-dimethylbutanamide (**3ba**): 54.4 mg (yield: 71%, 0.25 mmol scale), white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ = 10.31 (s, 1H), 8.85 - 8.87 (m, 2H), 8.33（dd, J = 8.4, 1.6 Hz, 1H）,7.83 (d, J = 1.6 Hz, 1H), 7.76 (d, J = 2.4 Hz, 1H), 7.57 (d, J = 8.4Hz, 1 H), 7.50 (dd, J = 8.4, 4.2 Hz, 1H), 6.53 – 6.52 (m, 1H), 1.75-1.81 (m, 2H), 1.4 (s, 6H), 0.98 (t, J = 7.2 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ = 177.0, 148.9, 141.3, 138.8, 135.2, 133.0, 131.6, 131.1, 124.3, 123.9, 122.5, 115.1, 106.9, 44.3, 34.2, 25.2, 9.4. HRMS (ESI) calculated for $C_{18}H_{20}N_4O$ $[M+H]^+$: 309.1710; found: 309.1711.

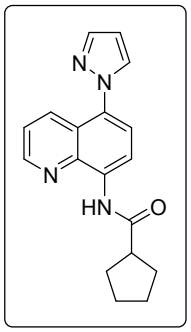


N-(5-(1H-pyrazol-1-yl)quinolin-8-yl)-2-ethylbutanamide (**3ca**): 52.7 mg (yield: 68%, 0.25 mmol scale), white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ = 9.94 (s, 1H), 8.91 (d, J = 8.4 Hz, 1H), 8.87

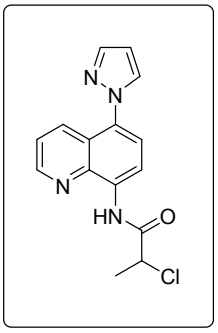
(dd, *J* = 4.4, 1.6 Hz, 1H), 8.34 (dd, *J* = 8.4, 1.6 Hz, 1H), 7.84 (d, *J* =1.2 Hz, 1H), 7.77 (d, *J* = 2.4 Hz, 1H), 7.58 (d, *J* = 8.0 Hz, 1H), 7.52 (dd, *J* =8.4, 4.0 Hz, 1H), 6.53 – 6.52 (m,1H), 2.39-2.32 (m, 1 H), 1.89-1.75 (m, 2H), 1.74-1.60 (m, 2H), 1.04 (t, *J* = 7.2 Hz, 6H); ^{13}C NMR (101 MHz, $CDCl_3$) δ = 175.1, 148.8, 141.3, 138.5, 135.1, 133.0, 131.6, 131.2, 124.3, 123.9, 122.5, 115.3, 106.9, 52.8, 26.0, 12.2. HRMS (ESI) calculated for $C_{18}H_{20}N_4O$ [M+H]$^+$: 309.1710; found: 309.1714.



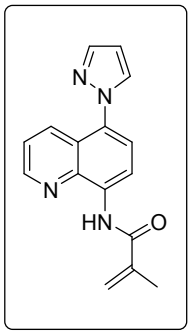
N-(5-(1H-pyrazol-1-yl)quinolin-8-yl)-2-methyl-2l5,7l3-heptanamide (**3da**): 56.9 mg (yield: 68%, 0.25 mmol scale), white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ = 9.88 (s, 1H), 8.92 – 8.75 (m, 2H), 8.31 (dd, *J* = 8.6, 1.6 Hz, 1H), 7.82 (d, *J* = 1.8 Hz, 1H), 7.76 (d, *J* = 2.3 Hz, 1H), 7.55 (d, *J* = 8.3 Hz, 1H), 7.48 (dd, *J* = 8.6, 4.2 Hz, 1H), 6.53 – 6.52 (m, 1H), 2.58 (t, *J* = 7.6 Hz, 2H), 1.86 – 1.75 (m, 2H), 1.50 – 1.26 (m, 8H), 0.96 – 0.80 (m, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ = 172.2, 148.8, 141.3, 138.3, 135.1, 133.0, 131.6, 131.1, 124.2, 123.9, 122.5, 115.3, 106.9, 38.3, 31.7, 29.4, 29.2, 25.7, 22.8, 14.2. HRMS (ESI) calculated for $C_{20}H_{24}N_4O$ [M+H]$^+$: 337.2023; found: 337.2024



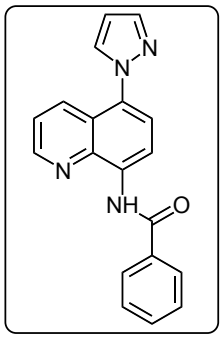
N-(5-(1H-pyrazol-1-yl)quinolin-8-yl)cyclopentanecarboxamide (**3ea**): 51.9 mg (yield: 68%, 0.25 mmol scale), buff solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ = 9.94 (s, 1H), 8.84-8.83 (m, 2H), 8.31 (d, *J* = 7.7 Hz, 1H), 7.80-7.79 (m, 2H), 7.65 – 7.39 (m, 2H), 6.53-6.52 (m, 1H), 2.97 (t, *J* = 7.2 Hz, 1H), 2.27 – 1.52 (m, 8H); ^{13}C NMR (101 MHz, $CDCl_3$) δ = 175.3, 148.7, 141.2, 138.4, 135.2, 133.0, 131.6, 131.0, 124.2, 123.9, 122.5, 115.2, 106.9, 47.5, 30.7, 26.1. HRMS (ESI) calculated for $C_{18}H_{18}N_4O$ [M+H]$^+$: 307.1553; found: 307.1556.



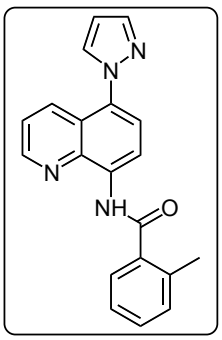
N-(5-(1H-pyrazol-1-yl)quinolin-8-yl)-2-chloropropanamide (**3fa**): 35.5 mg (yield: 47%, 0.25 mmol scale), yellow solid. ^{1}H NMR (400 MHz, DMSO-d_6) δ = 10.82 (s, 1H), 9.04 (dd, J = 8.4, 1.6 Hz, 1H), 8.72 (d, J = 8.3 Hz, 1H), 8.36 (dd, J = 8.4, 1.6 Hz, 1H), 8.24 (d, J = 2.3 Hz, 1H), 7.87 (d, J = 1.6 Hz, 1H), 7.77 – 7.71 (m, 2H), 6.63 – 6.62 (m, 1H), 5.29 (q, J = 6.8 Hz, 1H), 1.72 (d, J = 6.8 Hz, 3H); ^{13}C NMR (101 MHz, DMSO-d_6) δ = 168.1, 149.8, 141.1, 138.2, 134.0, 132.8, 132.4, 131.6, 123.4, 123.2, 123.1, 116.0, 107.0, 55.2, 21.5. HRMS (ESI) calculated for $C_{15}H_{13}ClN_4O$ $[M+H]^+$: 301.0851; found: 301.0858.



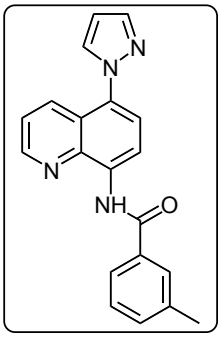
N-(5-(1H-pyrazol-1-yl)quinolin-8-yl)methacrylamide (**3ga**): 37.1 mg (yield: 53%, 0.25 mmol scale), yellow solid. ^{1}H NMR (400 MHz, DMSO-d_6) δ = 10.37 (s, 1H), 9.04 (dd, J = 4.4, 1.6 Hz, 1H), 8.76 (d, J = 8.0 Hz, 1H), 8.38 (dd, J = 8.8, 1.6 Hz, 1H), 8.25 (d, J = 2.4 Hz, 1H), 7.89 (d, J = 1.7 Hz, 1H), 7.76 (d, J = 1.6 Hz, 1H), 7.75 – 7.74 (m, 1H), 6.64 – 6.63 (m, 1H), 6.04 (s, 1H), 5.69 (s, 1H), 2.14 (s, 3H); ^{13}C NMR (101 MHz, DMSO-d_6) δ = 165.7, 149.8, 141.1, 140.0, 138.0, 134.1, 133.0, 132.4, 131.1, 123.4, 123.2, 121.5, 115.1, 107.0, 18.3. HRMS (ESI) calculated for $C_{16}H_{14}N_4O$ $[M+H]^+$: 279.1240; found: 279.1238.



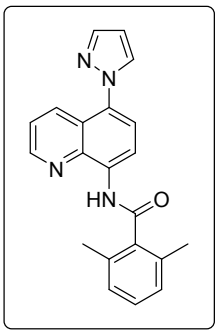
N-(5-(1H-pyrazol-1-yl)quinolin-8-yl)benzamide (**3ha**): 39.1 mg (yield: 50%, 0.25 mmol scale), buff solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ = 10.81 (s, 1H), 8.98 (d, J = 8.3 Hz, 1H), 8.87 (dd, J = 4.2, 1.5 Hz, 1H), 8.35 (dd, J = 8.6, 1.5 Hz, 1H), 8.10 – 8.08 (m, 2H), 7.84 (d, J = 1.7 Hz, 1H), 7.79 (d, J = 2.3 Hz, 1H), 7.57-7.52 (m, 4H), 7.50 (dd, J = 8.6, 4.2 Hz, 1H), 6.54-6.53 (m, 1H); ^{13}C NMR (101 MHz, $CDCl_3$) δ = 165.5, 148.9, 141.3, 138.7, 135.0, 134.9, 133.1, 132.1, 131.5, 131.4, 128.9, 127.4, 124.2, 123.8, 122.6, 115.4, 107.0. HRMS (ESI) calculated for $C_{19}H_{14}N_4O$ $[M+H]^+$: 315.1240; found: 315.1247.



N-(5-(1H-pyrazol-1-yl)quinolin-8-yl)-2-methylbenzamide (**3ia**): 44.9 mg (yield: 55%, 0.25 mmol scale), white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ = 10.31 (s, 1H), 9.00 (d, *J* = 8.3 Hz, 1H), 8.82 (dd, *J* = 4.2, 1.6 Hz, 1H), 8.36 (dd, *J* = 8.6, 1.6 Hz, 1H), 7.85 (d, *J* = 1.8 Hz, 1H), 7.80 (d, *J* = 2.4 Hz, 1H), 7.71 (d, *J* = 7.6 Hz , 1H), 7.62 (d, *J* = 8.3 Hz, 1H), 7.50 (dd, *J* = 8.6, 4.2 Hz, 1H), 7.46 – 7.39 (m, 1H), 7.36 -7.34 (t, *J* = 8.0 Hz, 2H), 6.55 – 6.54 (m, 1H), 2.62 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ = 168.3, 148.9, 141.3, 138.6, 136.9, 136.4, 135.2, 133.1, 131.6, 131.5, 130.7, 127.4, 126.2, 124.3, 123.8, 122.6, 115.4, 107.0, 20.4. HRMS (ESI) calculated for $C_{20}H_{16}N_4O$ $[M+H]^+$: 329.1397; found: 329.1403.

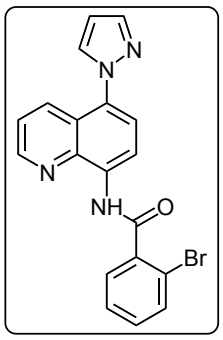


N-(5-(1H-pyrazol-1-yl)quinolin-8-yl)-3-methylbenzamide (**3ja**): 48.3 mg (yield: 59%, 0.25 mmol scale), white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ = 10.79 (s, 1H), 9.00 (d, *J* = 8.3 Hz, 1H), 8.90 (dd, *J* = 4.2, 1.7 Hz, 1H), 8.36 (dd, *J* = 8.5, 1.6 Hz, 1H), 7.94 – 7.82 (m, 3H), 7.80 (d, *J* = 2.3 Hz, 1H), 7.62 (d, *J* = 8.3 Hz, 1H), 7.52 (dd, *J* = 8.6, 4.2 Hz, 1H).), 7.48 – 7.37 (m, 2H), 6.55 -6.54 (m, 1H), 2.49 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ = 165.9, 149.0, 141.3, 138.9, 138.8, 135.2, 134.9, 133.1, 133.0, 131.6, 131.4, 128.8, 128.2, 124.4, 124.3, 123.9, 122.7, 115.5, 106.9, 21.5. HRMS (ESI) calculated for $C_{20}H_{16}N_4O$ $[M+H]^+$: 329.1397; found: 329.1401.

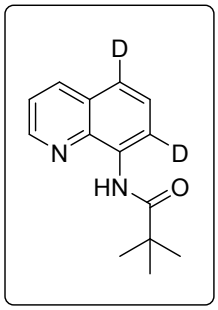


N-(5-(1H-pyrazol-1-yl)quinolin-8-yl)-2,6-dimethylbenzamide (**3ka**): 47.2 mg (yield: 55%, 0.25 mmol scale), white solid. ^{1}H NMR (400 MHz, DMSO-d_6) δ = 10.19 (s, 1H), 8.94 (d, *J* = 4.0 Hz,

1H), 8.80 (d, *J* = 8.3 Hz, 1H), 8.34 (dd, *J* = 8.4, 1.2 Hz, 1H), 8.23 (d, *J* = 2.2 Hz, 1H), 7.88 (d, *J* = 1.4 Hz, 1H), 7.78 (d, *J* = 8.3 Hz, 1H), 7.70 (dd, *J* = 8.6, 4.2 Hz, 1H), 7.32 – 7.26 (m, 1H), 7.16 (d, *J* = 7.6 Hz, 2H), 6.64 -6.63 (m, 1H), 2.34 (s, 6H); ^{13}C NMR (101 MHz, DMSO-d_6) δ = 168.3, 150.0, 141.3,138.5, 137.8, 134.2, 133.9, 132.9, 132.6, 131.8, 129.2, 127.7, 123.6, 123.5, 123.3, 116.5, 107.2, 19.1. HRMS (ESI) calculated for $C_{21}H_{18}N_4O$ $[M+H]^+$: 343.1553; found: 343.1559



N-(5-(1H-pyrazol-1-yl)quinolin-8-yl)-2-bromobenzamide (**3la**): 42.9 mg (yield: 44%, 0.25 mmol scale), white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ = 10.40 (s, 1H), 9.00 (d, *J* = 8.3 Hz, 1H), 8.83 (dd, *J* = 4.2, 1.5 Hz, 1H), 8.37 (dd, *J* = 8.6, 1.5 Hz, 1H), 7.85 (d, *J* = 1.5 Hz, 1H), 7.80 (d, *J* = 2.2 Hz, 1H), 7.74 (dd, *J* = 7.6, 1.6 Hz, 1H), 7.72 – 7.68 (m, 1H), 7.63 (d, *J* = 8.3 Hz, 1H), 7.53 – 7.43 (m, 2H), 7.39 – 7.35 (m, 1H), 6.55 – 6.54 (m, 1H); ^{13}C NMR (101 MHz, $CDCl_3$) δ = 166.1, 149.0, 141.4, 138.7, 138.1, 134.8, 133.9, 133.1, 131.9, 131.8, 131.6, 129.8, 127.8, 124.3, 123.7, 122.7, 119.8, 115.8, 107.1. HRMS (ESI) calculated for $C_{19}H_{13}BrN_4O$ $[M+H]^+$: 393.0346; found: 393.0345.



N-(quinolin-8-yl-5,7-d2)pivalamide: yellow liquid. ^{1}H NMR (400 MHz, $CDCl_3$) δ = 10.22 (s, 1H), 8.70 (d, *J* = 4.2 Hz, 1H), 7.98 (d, *J* = 8.2 Hz, 1H), 7.42 (s, 1H), 7.29 (dd, *J* = 8.2, 4.2 Hz, 1H), 1.38 (s, 9H); ^{13}C NMR (101 MHz, $CDCl_3$) δ = 177.0, 148.0, 138.5, 136.1, 136.0, 134.4, 127.6, 127.0, 126.9, 121.4, 40.2, 27.6.

10. Reference

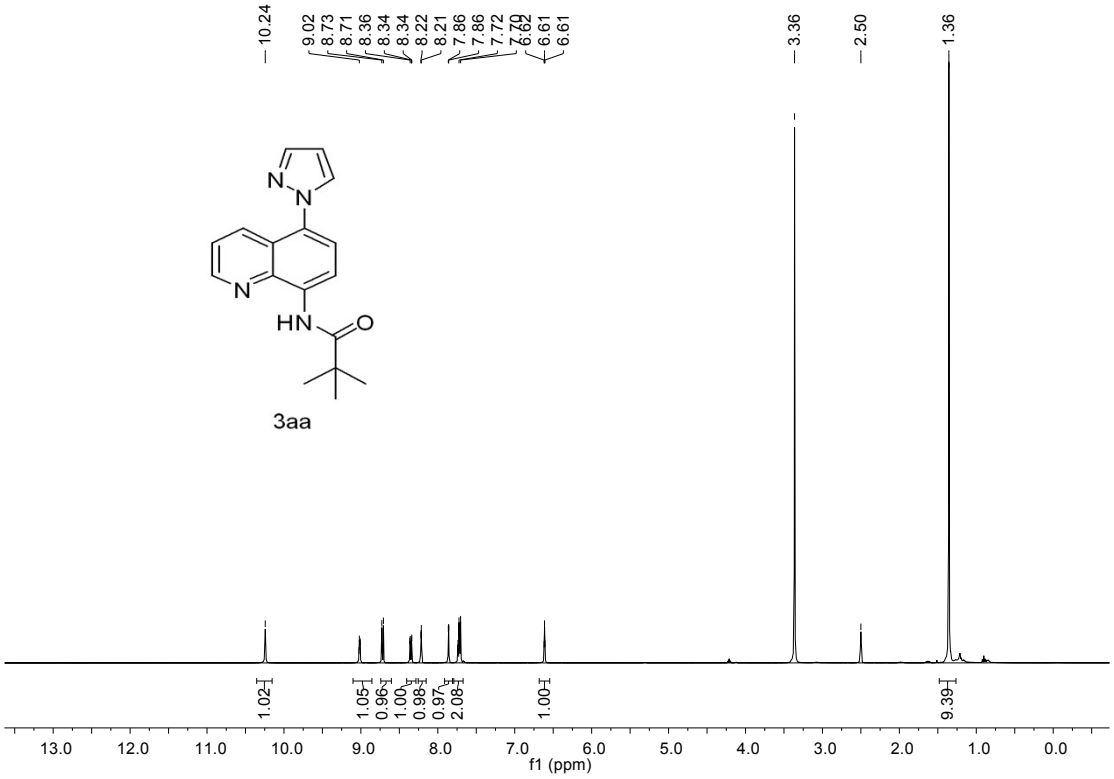
1) (a) Lee, C.; Yang, W.; R. G. Parr. R. G. *Phys. Rev. B* **1988**, *37*, 785; (b) Becke. A. D. *J. Chem. Phys.* **1993**, *98*, 5648.

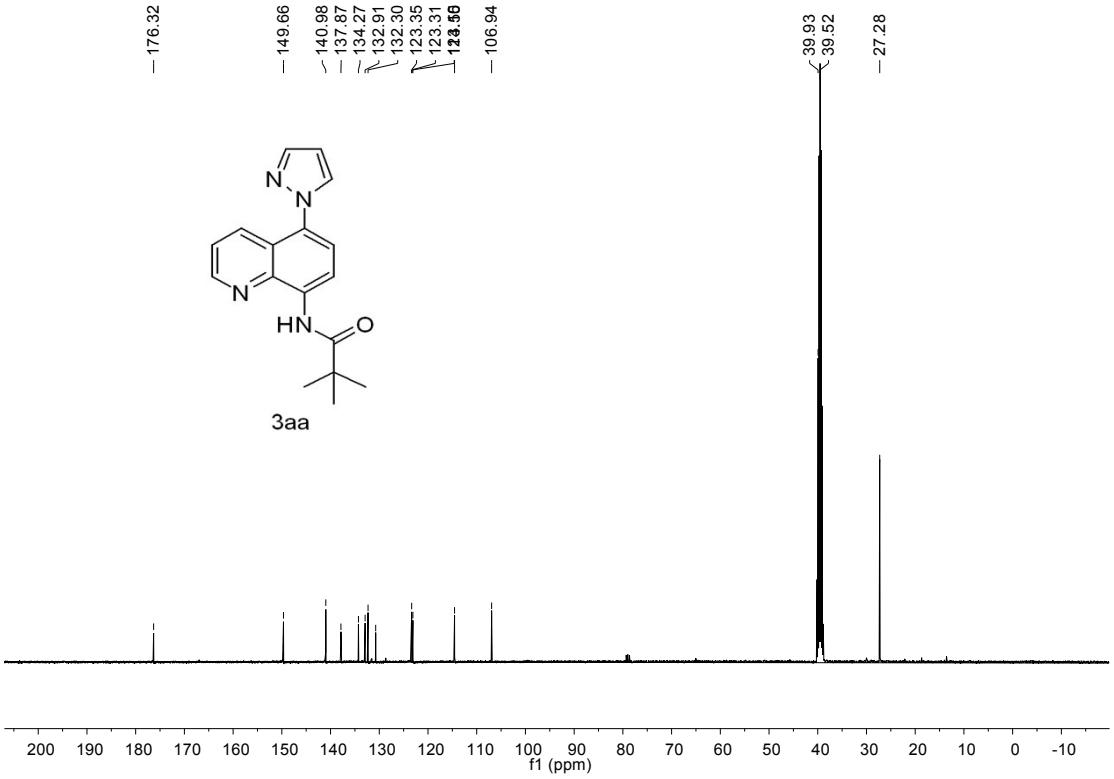
2) Marenich, A. V.; Cramer, C. J.; Truhlar. D. G. *J. Phys. Chem. B* **2009**, *113*, 6378.

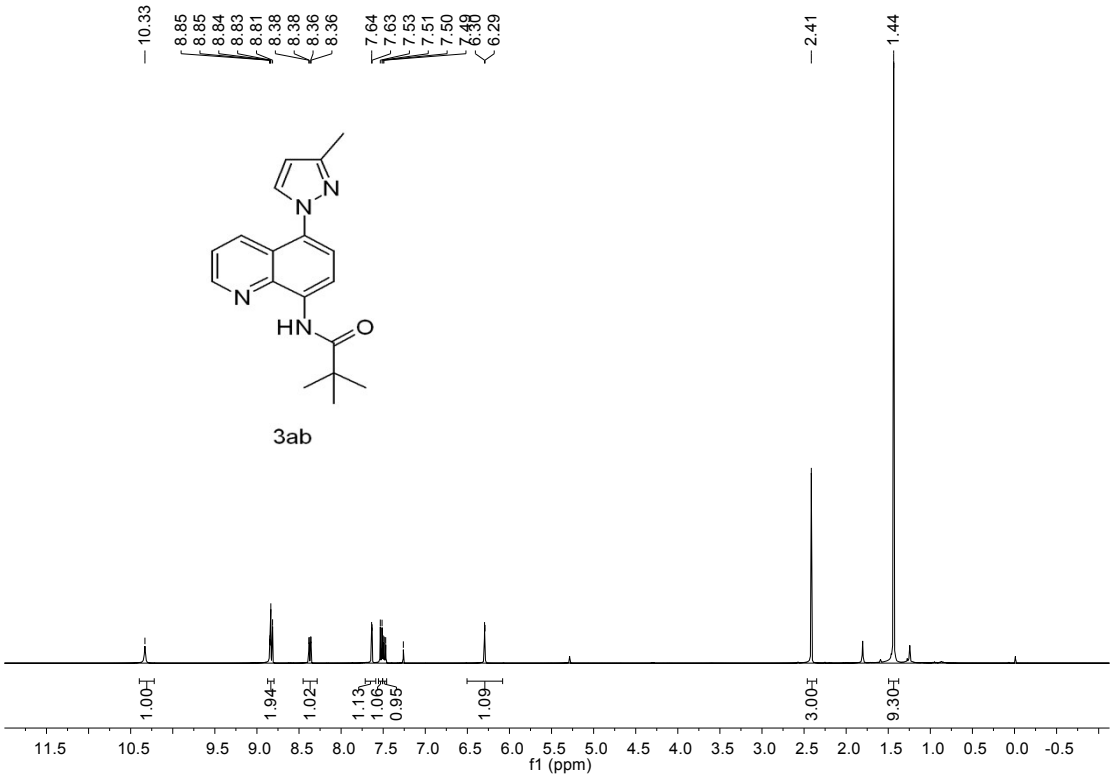
3) Nelson, R. C.; Miller. J. T. *Catal. Sci. Technol.* **2012**, *2*, 461-470.

4) Ravel, B.; Newville. M. *J. Synchrotron. Radiat.* **2005**, *12*, 537-541.

11. NMR Spectra of Products



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7.50
6.30
6.29
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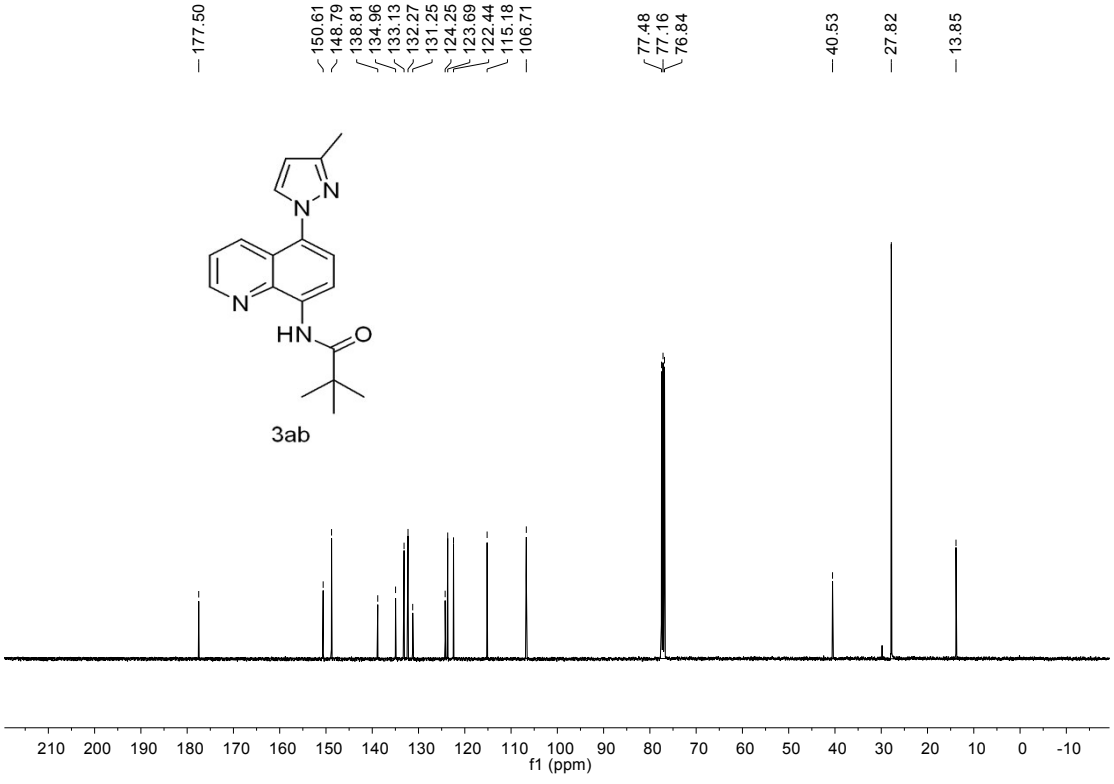
f1 (ppm)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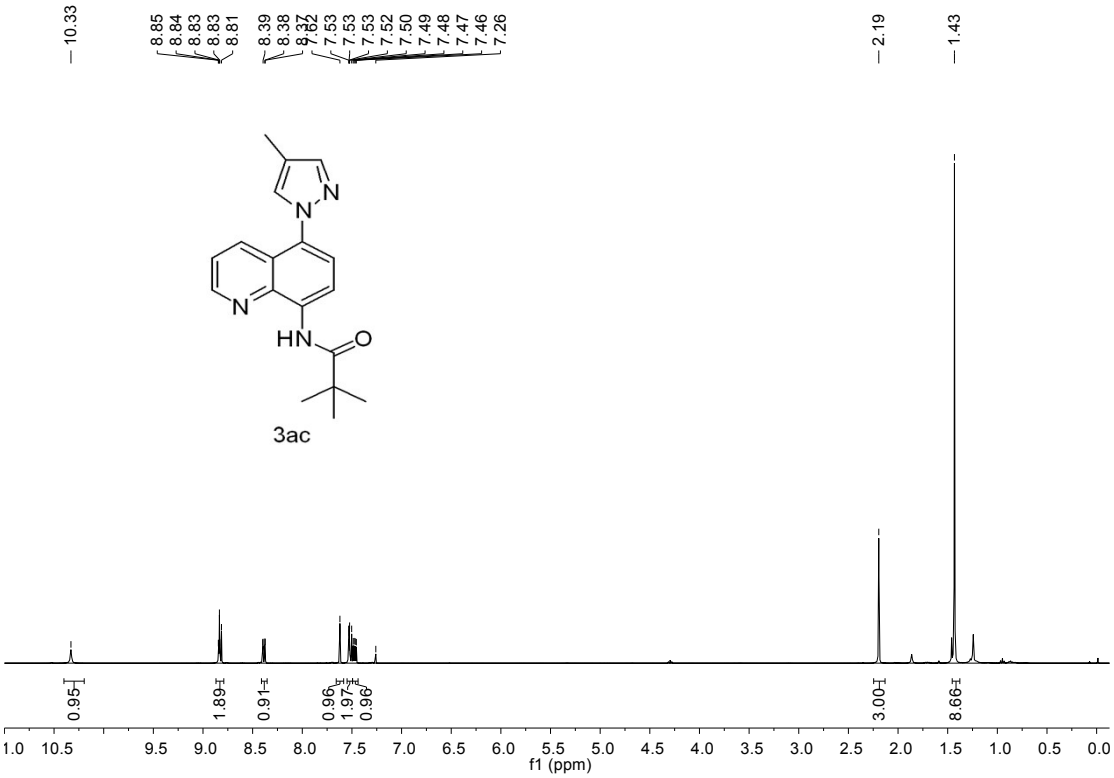
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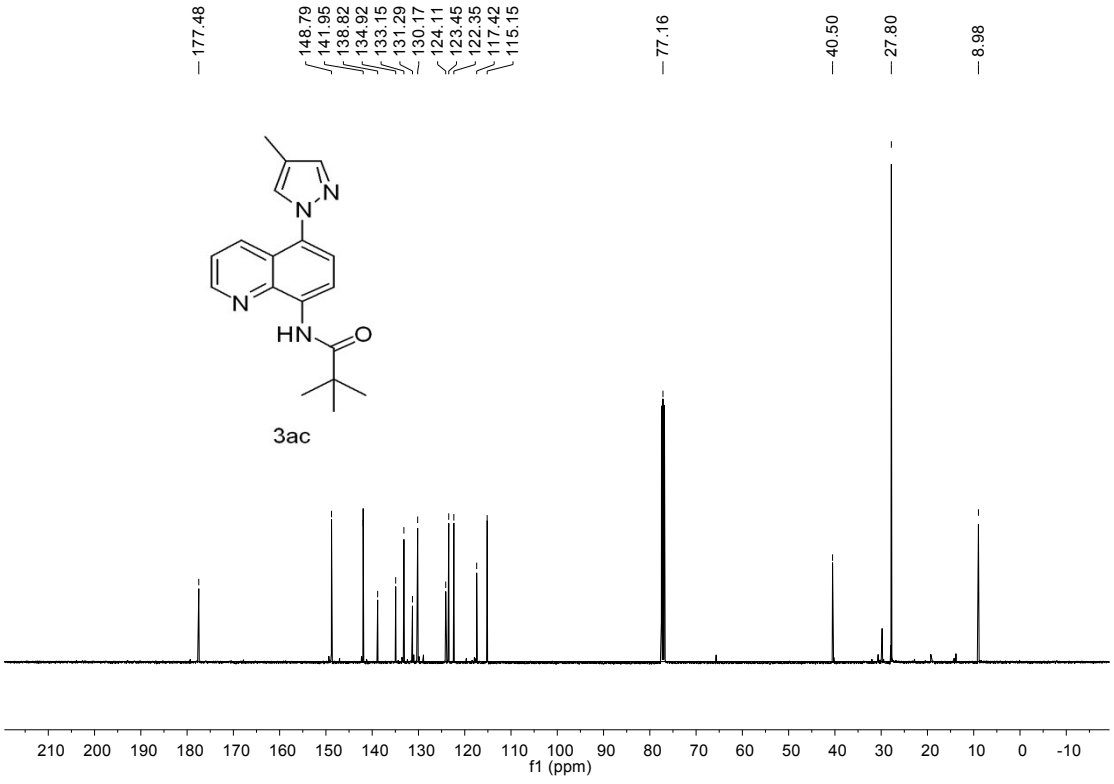
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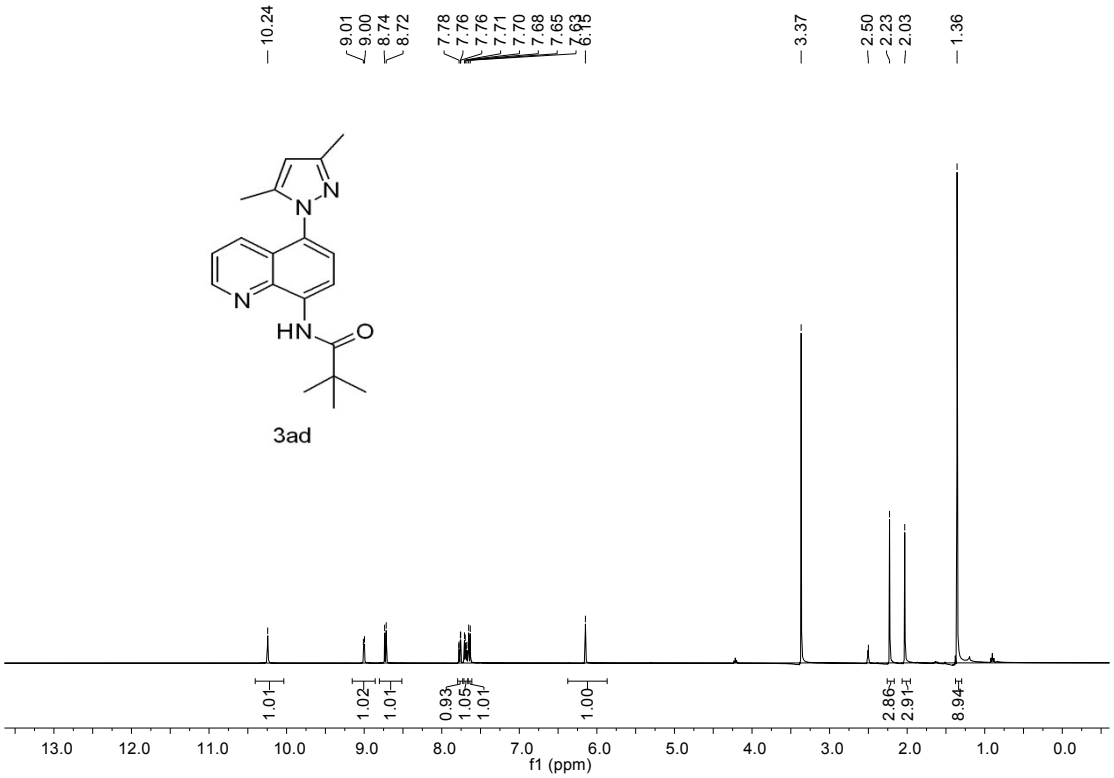
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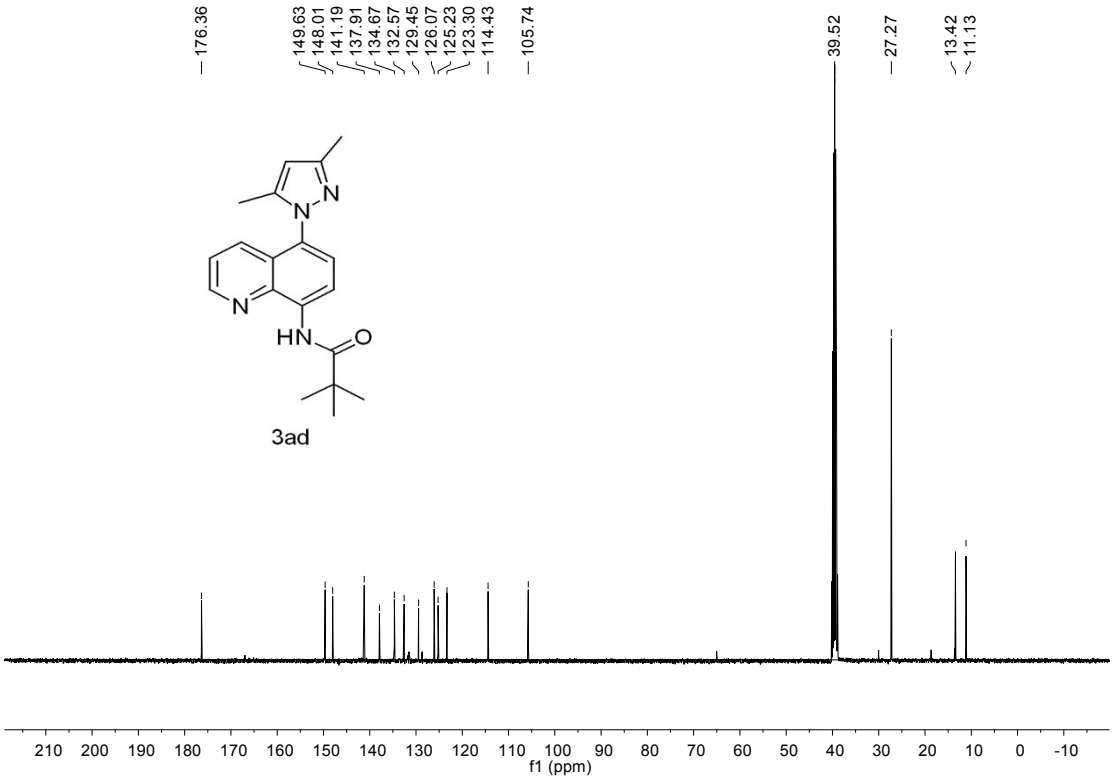
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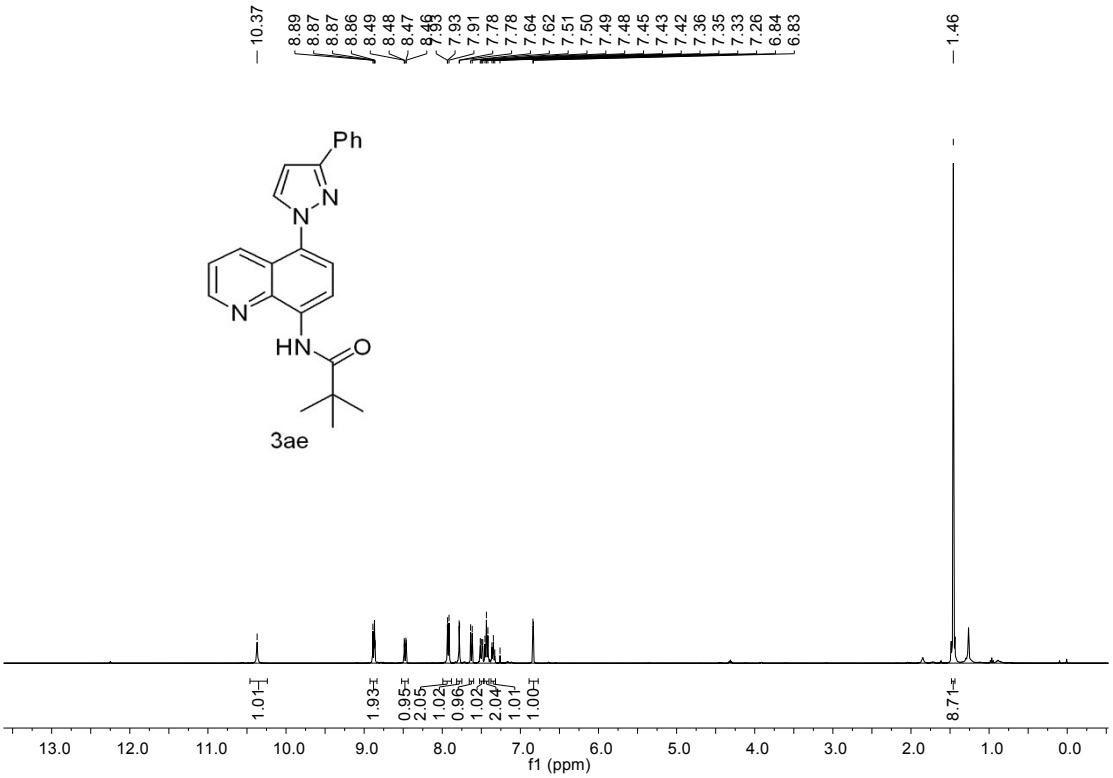
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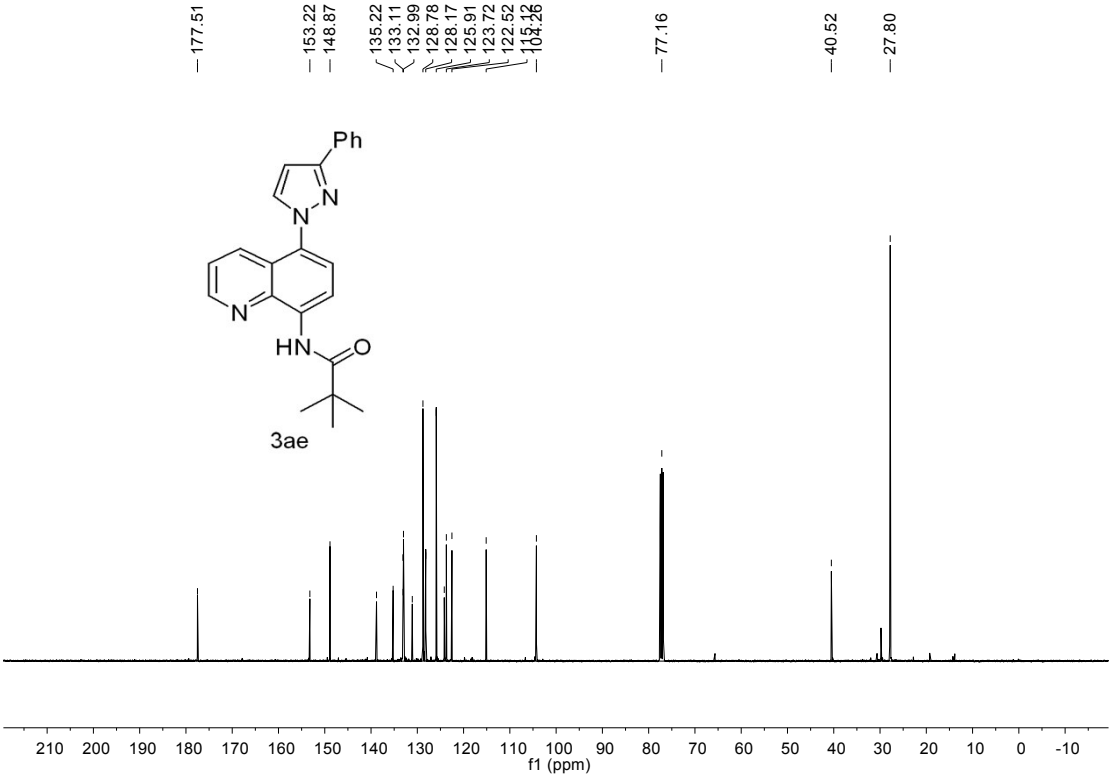
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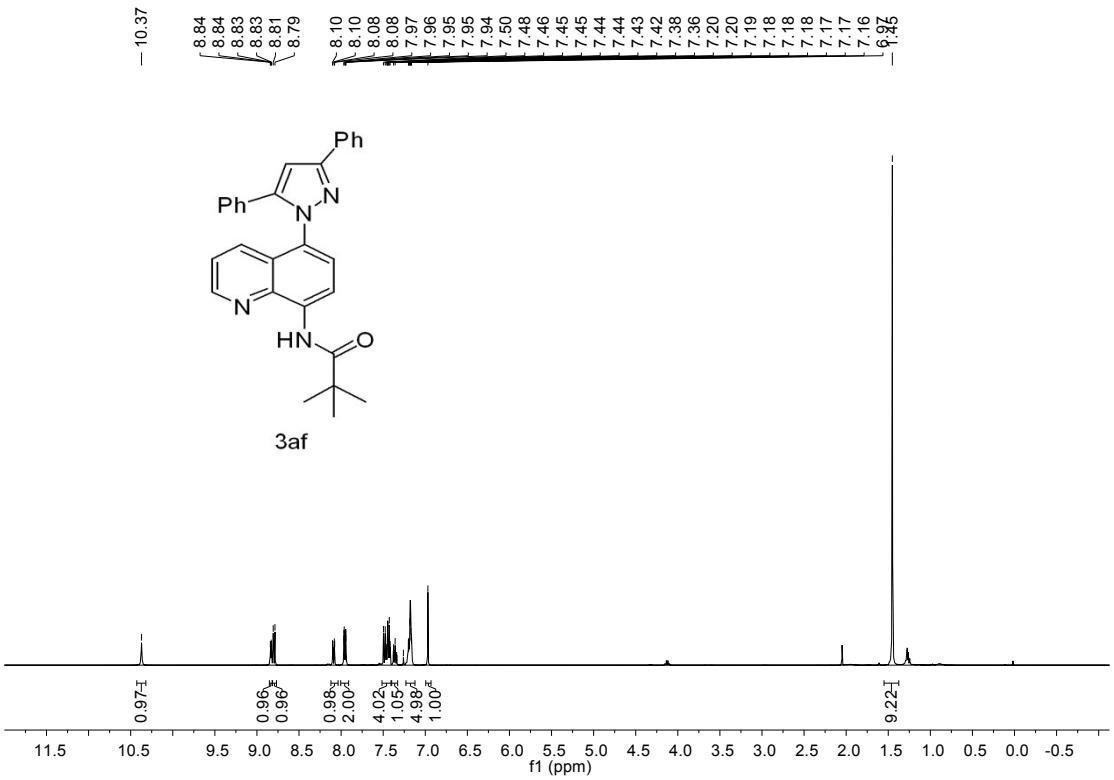
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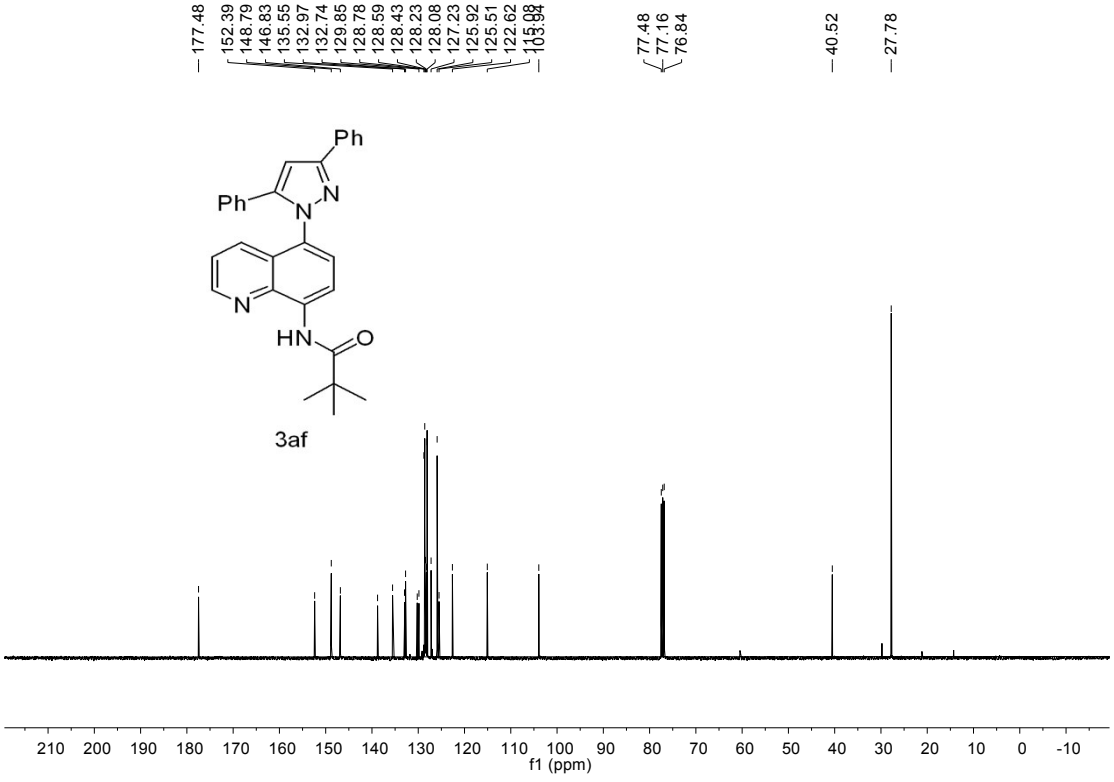
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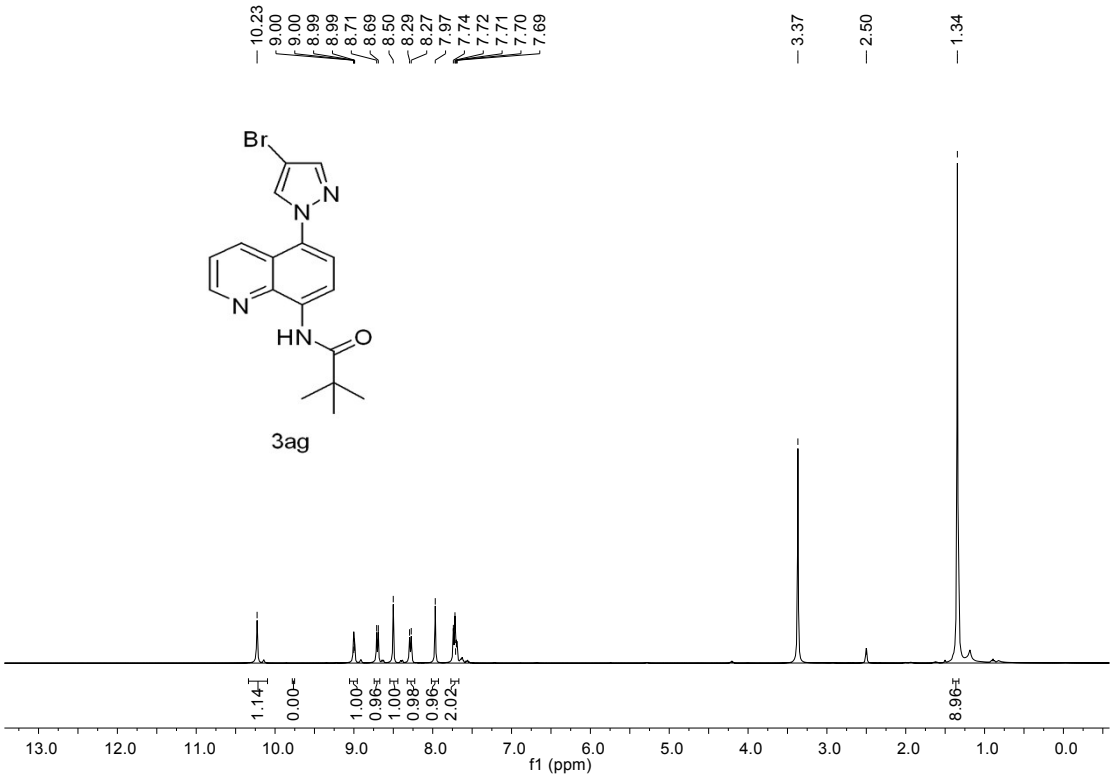
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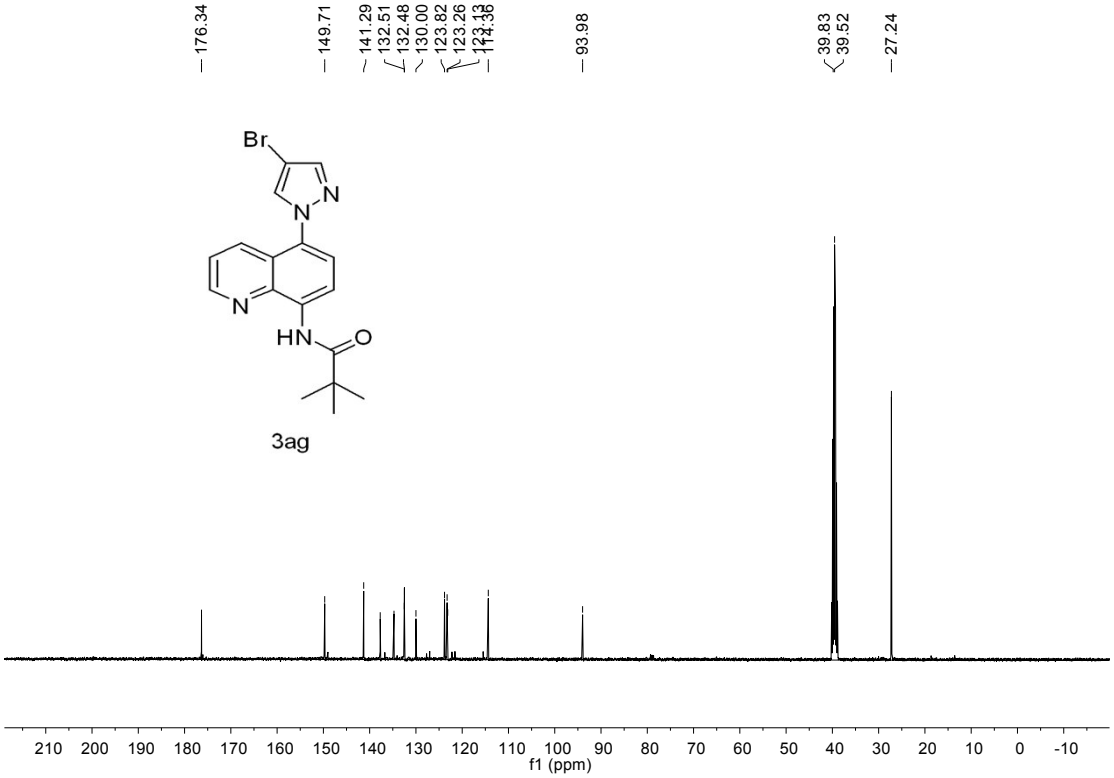
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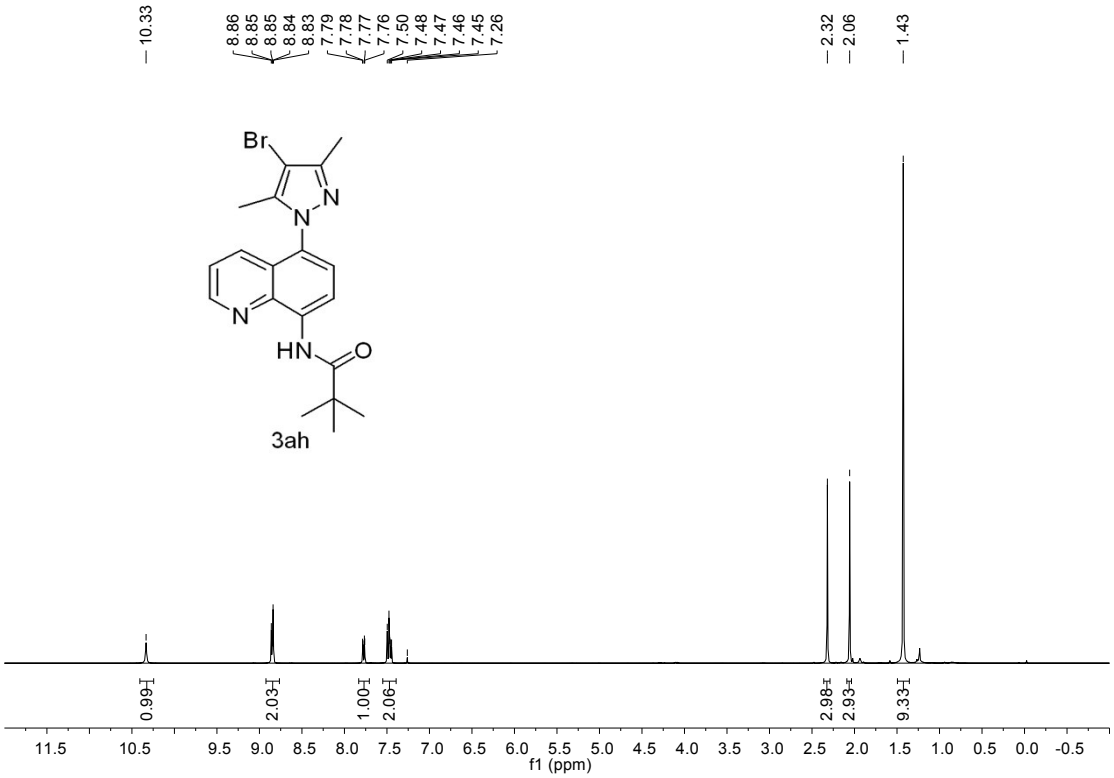
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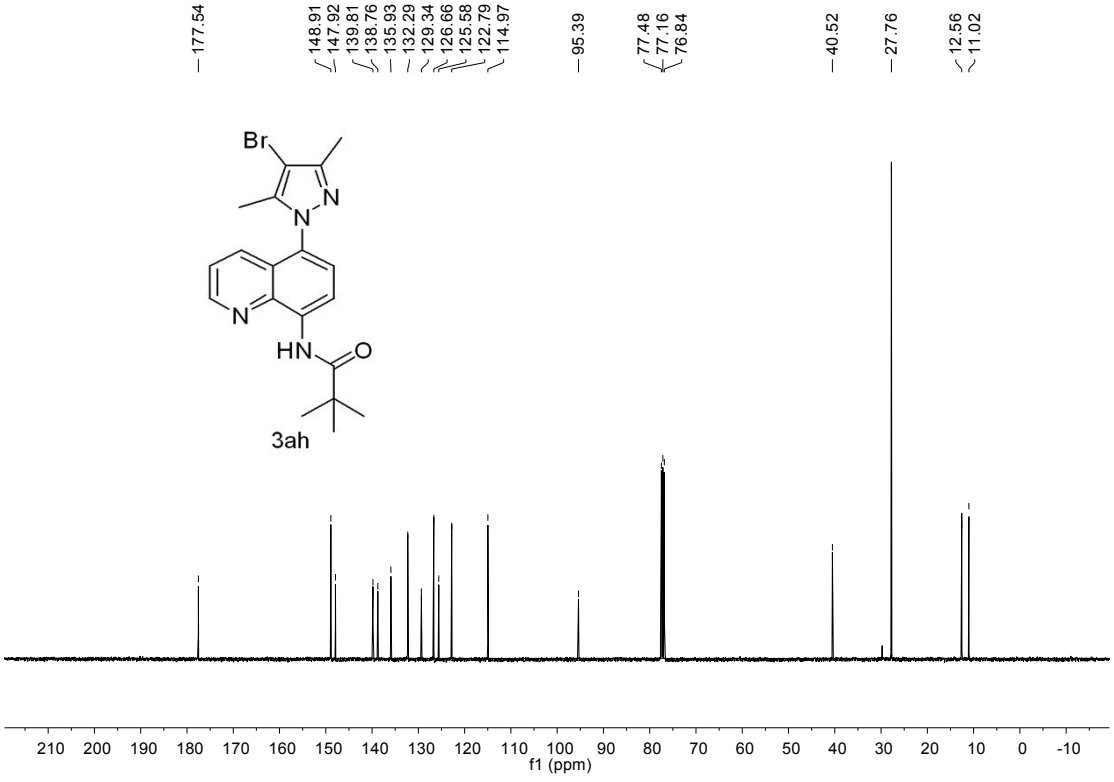
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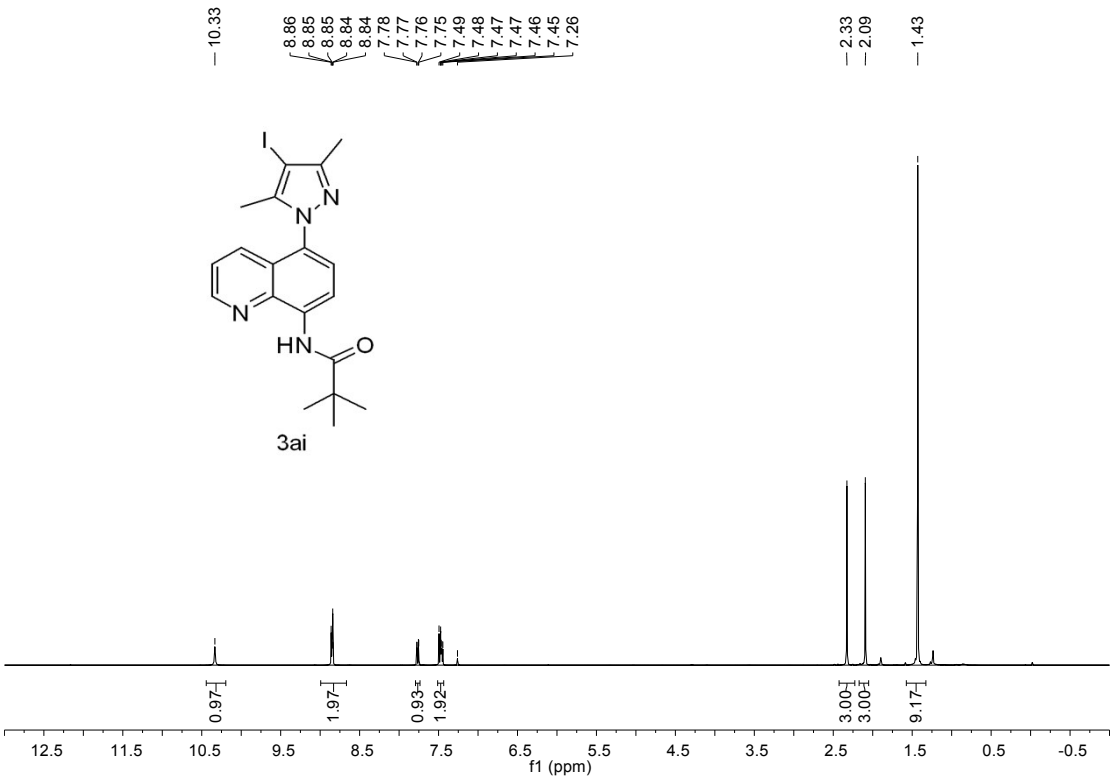
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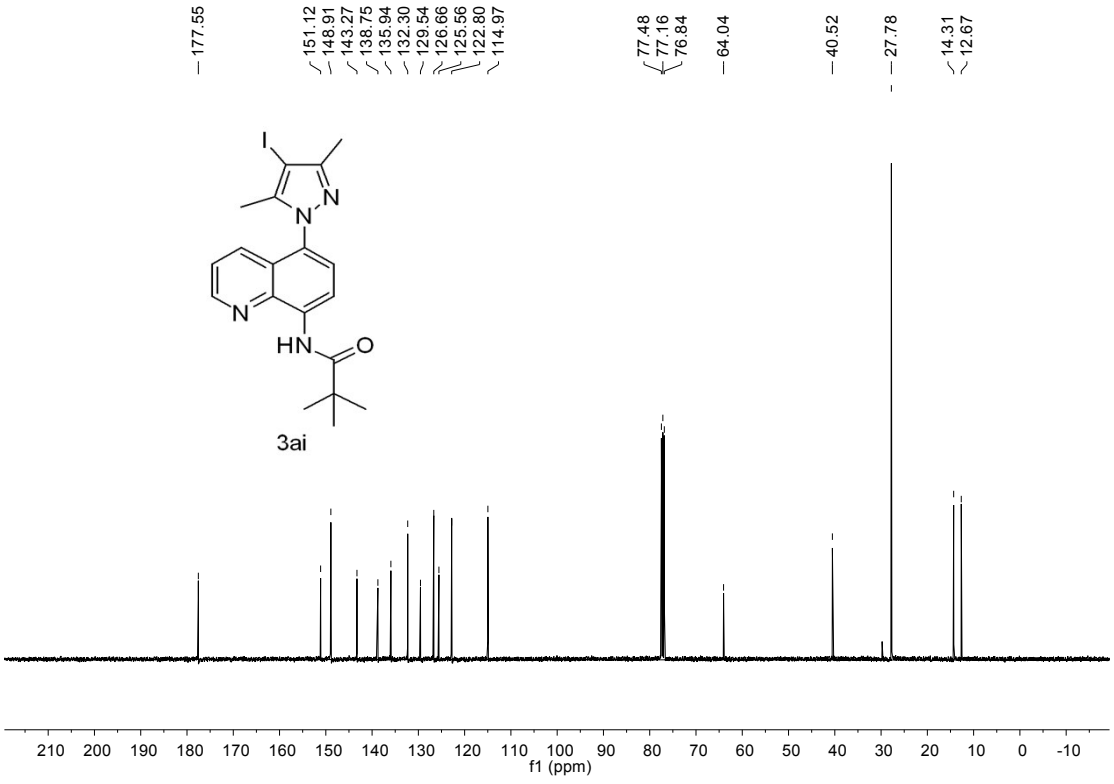
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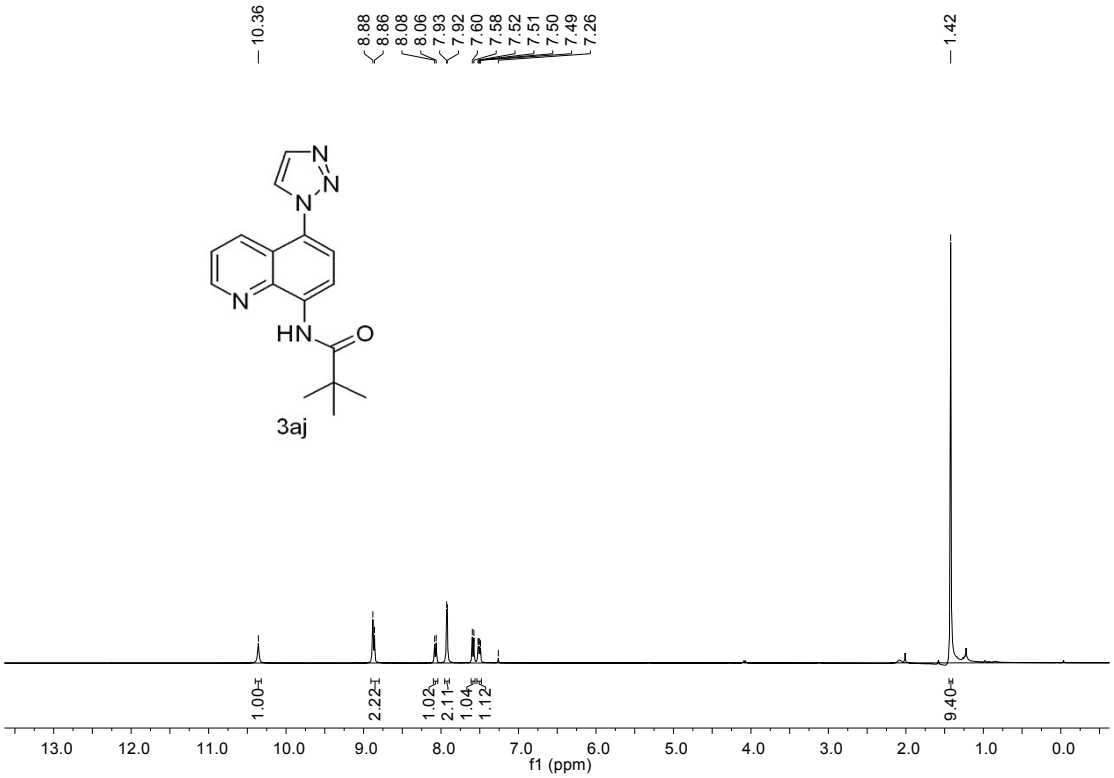
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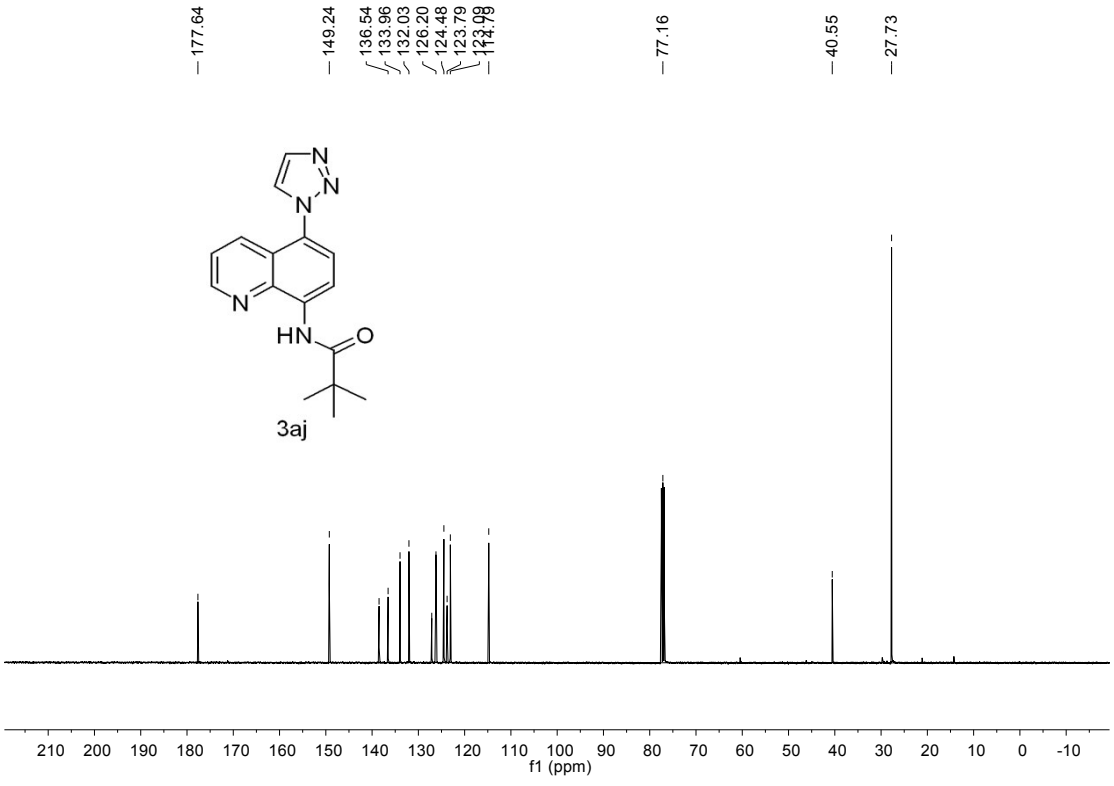
f1 (ppm)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124.48
123.79
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40.55
27.73
3aj
210
200
190
180
170
160
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120
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100
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80
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60
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30
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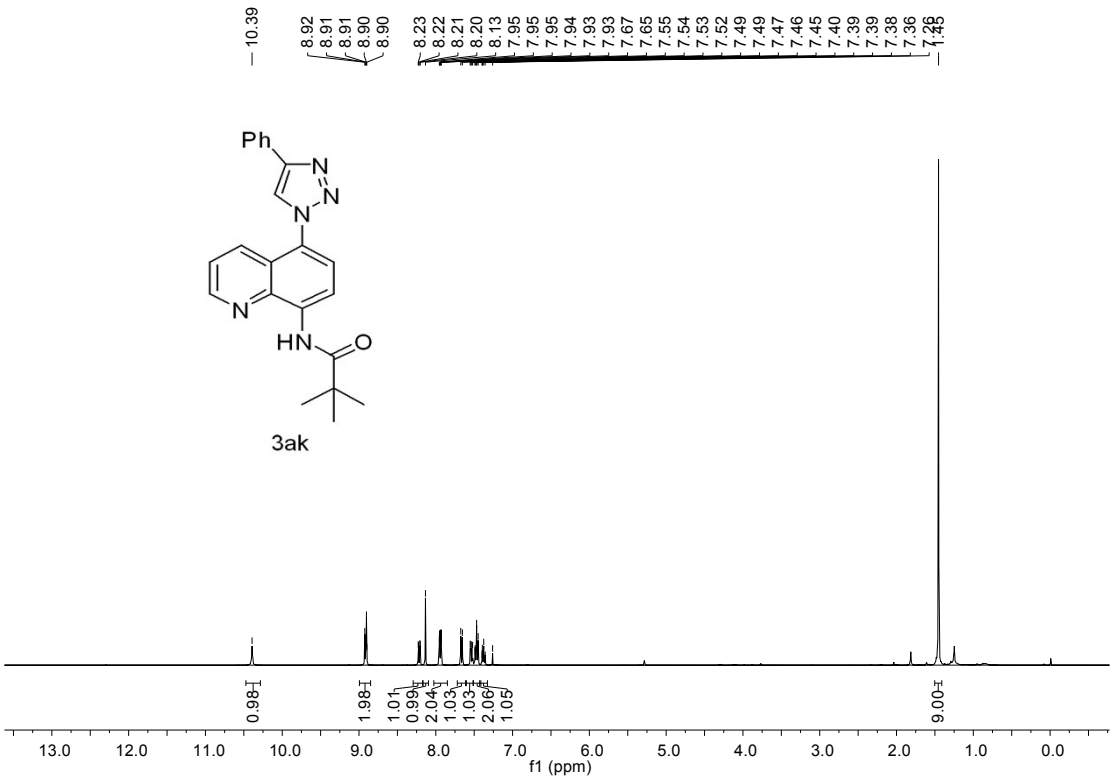
-10
f1 (ppm)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8.13
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7.95
7.94
7.93
7.93
7.67
7.65
7.55
7.54
7.53
7.52
7.49
7.49
7.47
7.46
7.45
7.40
7.39
7.39
7.38
7.36
1.45
Ph
N
N
N
N
HN
O
3ak
0.98
1.98
1.01
0.99
2.04
1.03
1.03
2.06
1.05
9.00
13.0
12.0
11.0
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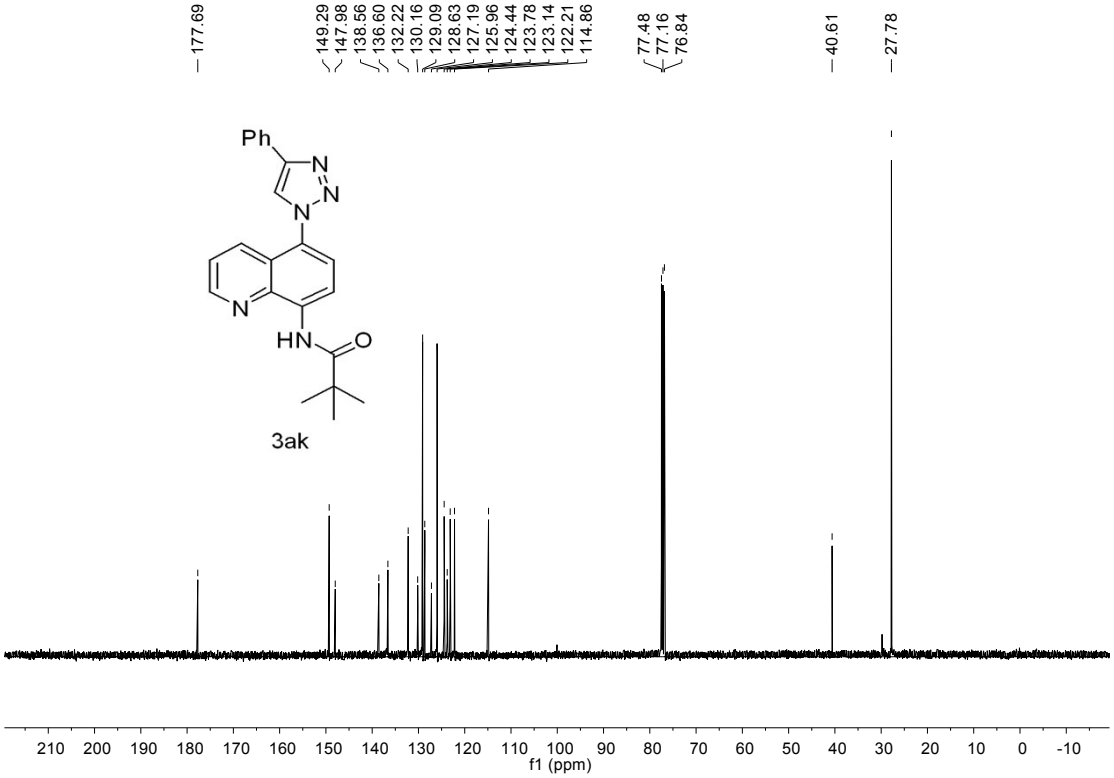
f1 (ppm)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124.44
123.78
123.14
122.21
114.86
77.48
77.16
76.84
40.61
27.78
Ph
N
N
N
N
HN
O
3ak
210
200
190
180
170
160
150
140
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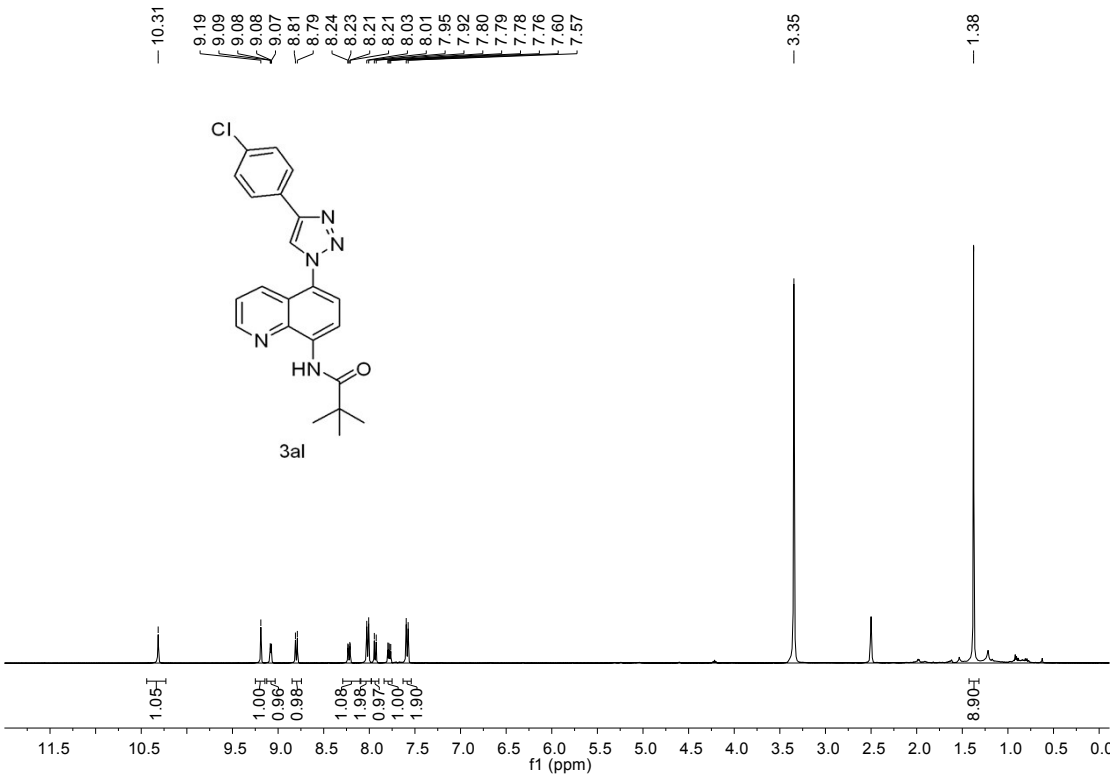
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)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9.07
8.81
8.79
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8.23
8.21
8.21
8.03
8.01
7.95
7.92
7.80
7.79
7.78
7.76
7.60
7.57
3.35
1.38
Cl
N
N
N
N
HN
O
3al
1.05
1.00
0.96
0.98
1.08
1.98
0.97
1.00
1.90
8.90
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
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4.0
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3.0
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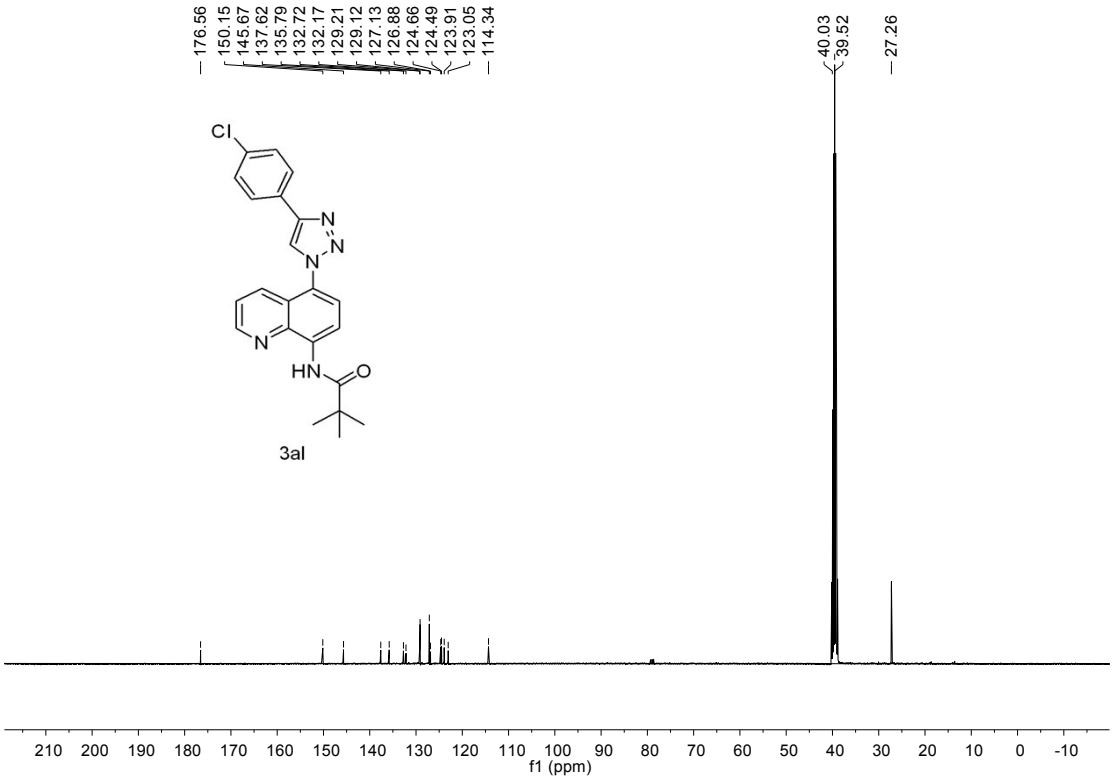
f1 (ppm)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126.88
124.66
124.49
123.91
123.05
114.34
40.03
39.52
27.26
Cl
N
N
N
N
HN
O
3al
210
200
190
180
170
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140
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120
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100
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80
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60
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40
30
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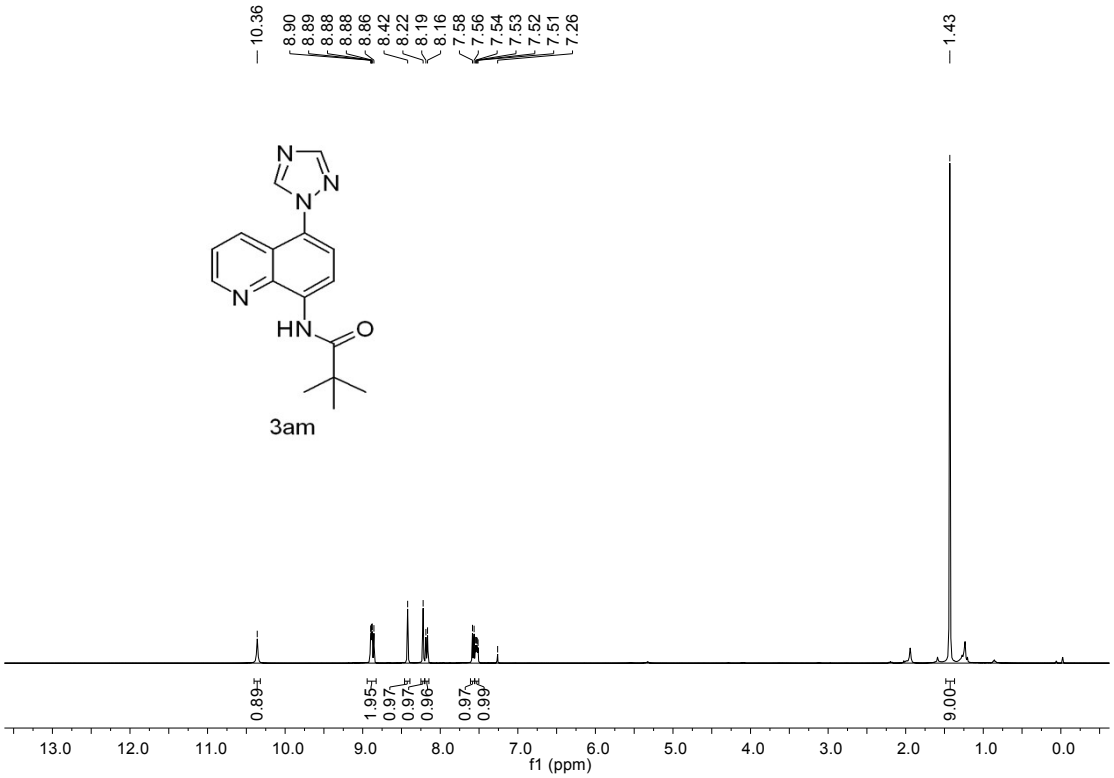
0
-10
f1 (ppm)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8.22
8.19
8.16
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7.56
7.54
7.53
7.52
7.51
7.26
1.43
3am
0.89
1.95
0.97
0.97
0.96
0.97
0.99
9.00
13.0
12.0
11.0
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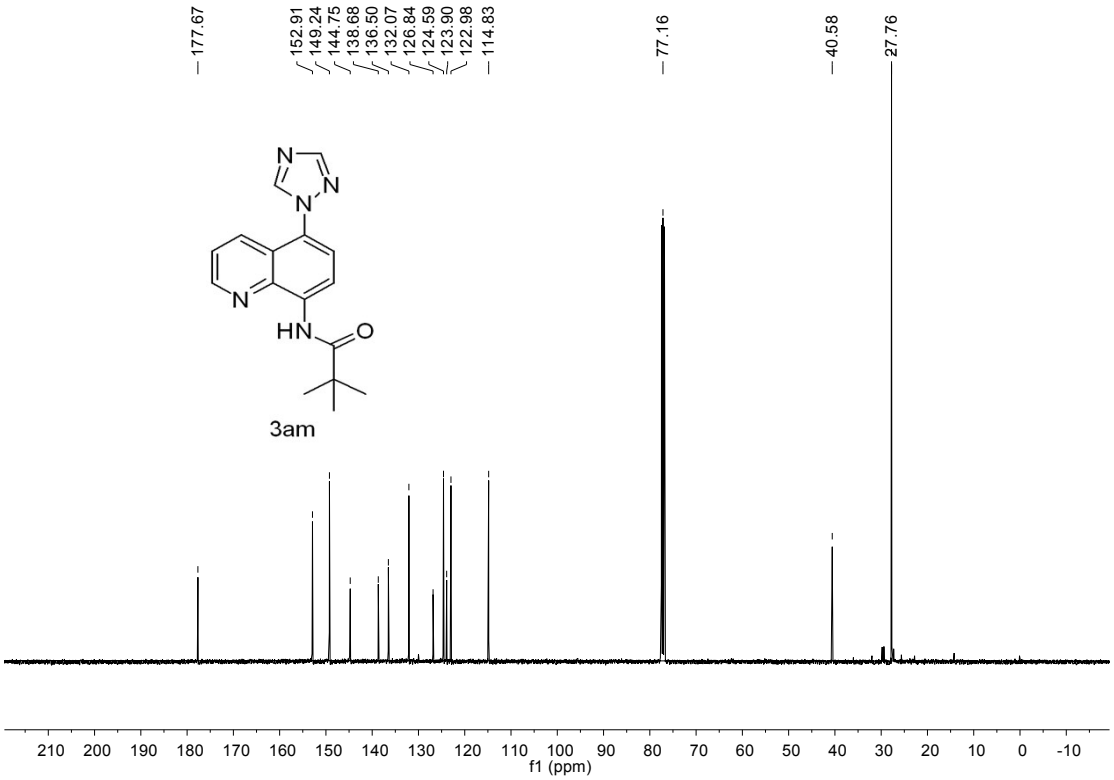
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)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136.50
132.07
126.84
124.59
123.90
122.98
114.83
77.16
40.58
27.76
3am
210
200
190
180
170
160
150
140
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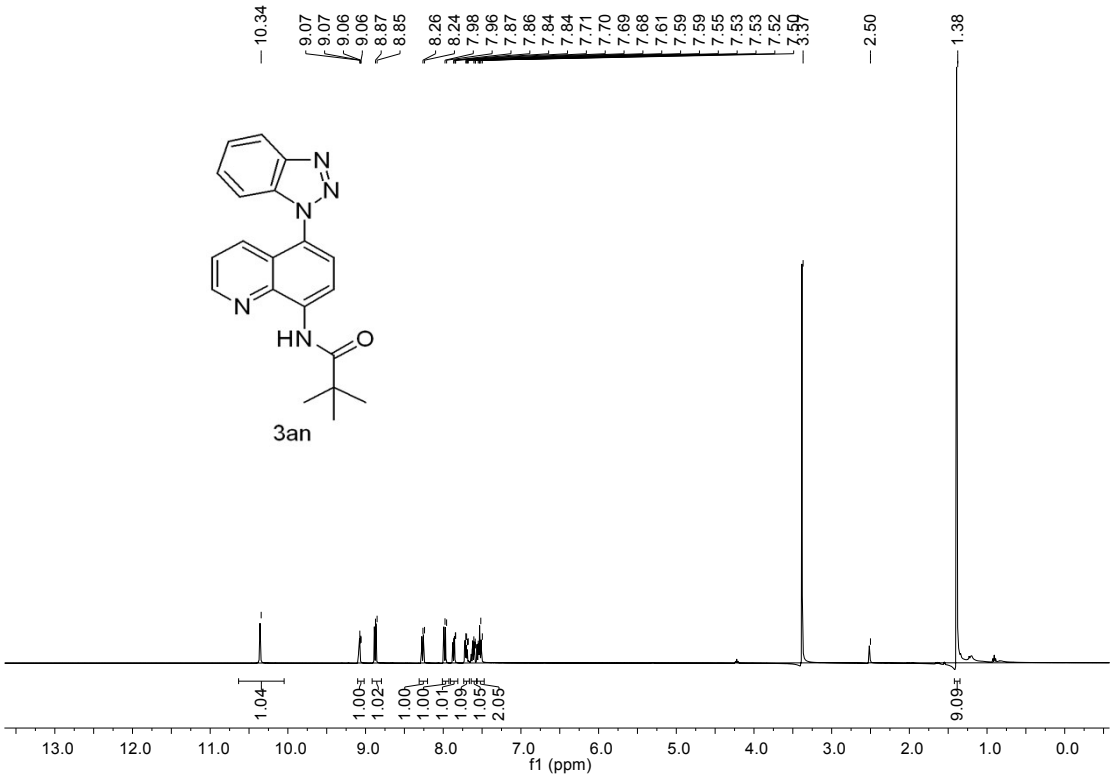
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)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9.07
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8.85
8.26
8.24
7.98
7.96
7.87
7.86
7.84
7.84
7.71
7.70
7.69
7.68
7.61
7.59
7.59
7.55
7.53
7.53
7.52
7.50
3.37
2.50
1.38
N
N
N
N
HN
O
3an
1.04
1.00
1.02
1.00
1.00
1.01
1.09
1.05
2.05
9.09
13.0
12.0
11.0
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6.0
5.0
4.0
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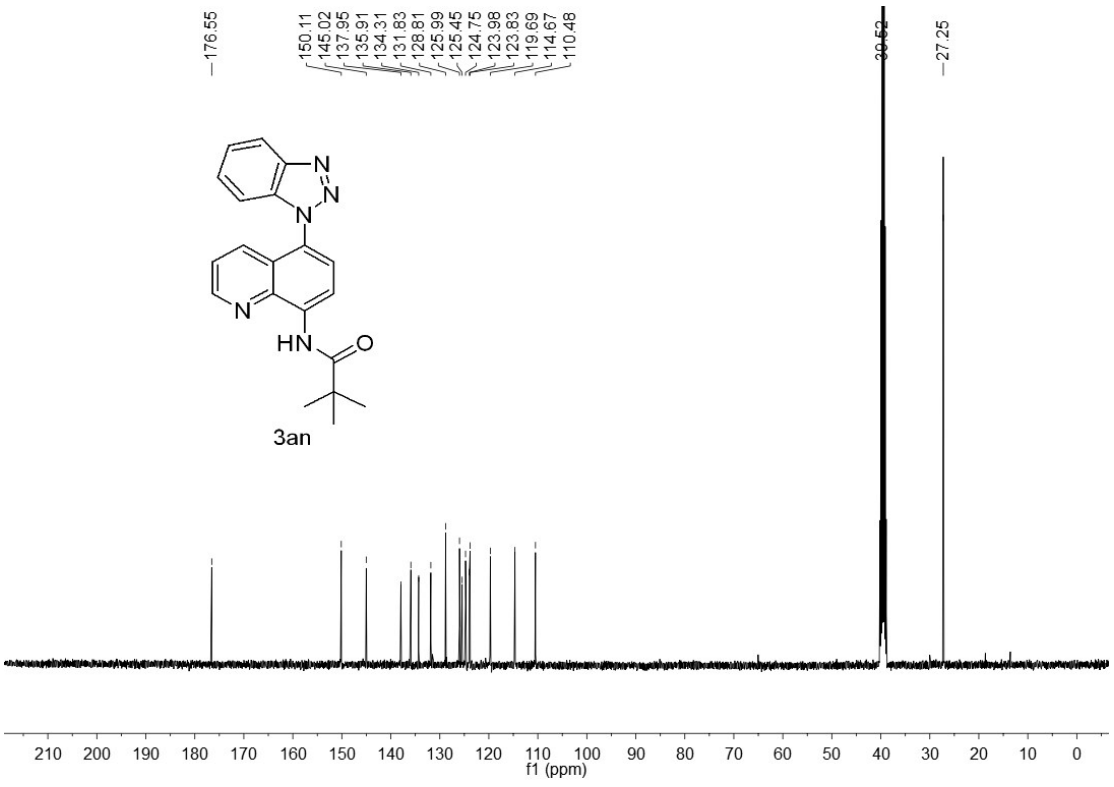
2.0
1.0
0.0
f1 (ppm)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145.02
137.95
135.91
134.31
131.83
128.81
125.99
125.45
124.75
123.98
123.83
119.69
114.67
110.48
39.52
27.25
N
N
N
N
HN
O
3an
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


10.31
8.87
8.86
8.86
8.85
8.85
8.30
7.83
7.82
7.76
7.75
7.57
6.53
6.52
6.52
1.81
1.80
1.78
1.77
1.75
1.40
0.98
0.96
0.94
HN
O
3ba
1.00
2.02
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1.01
0.53
0.49
1.04
1.00
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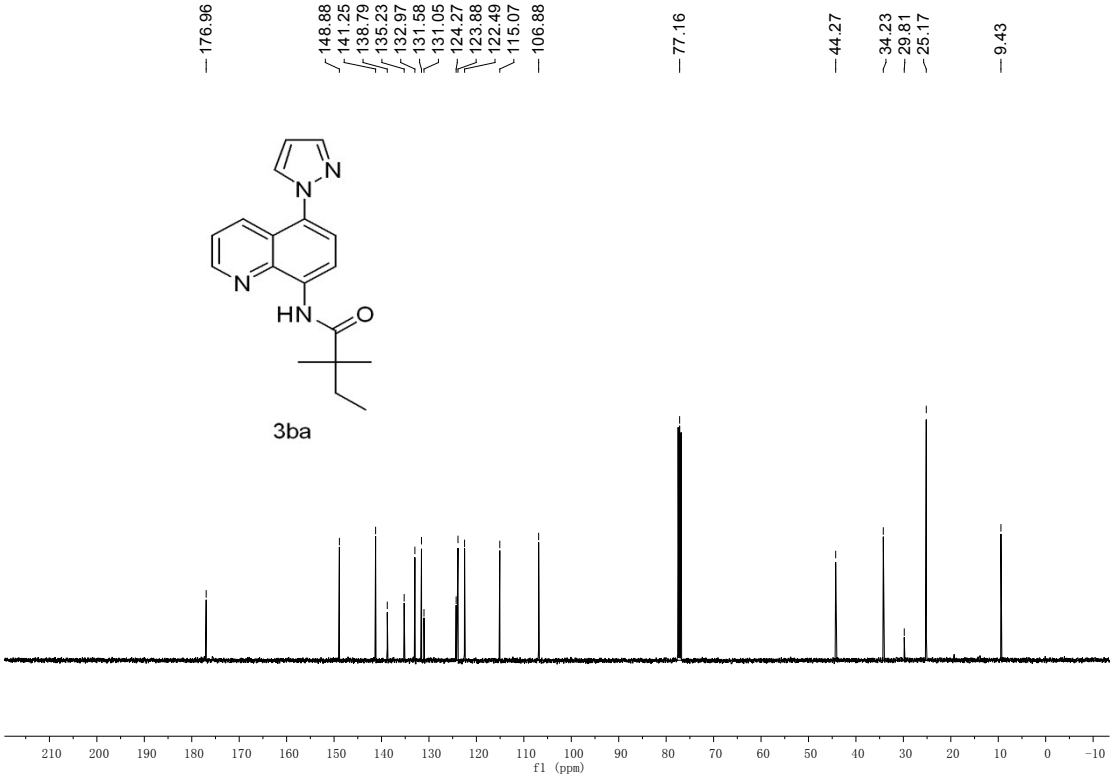
3.30
f1 (ppm)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123.88
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77.16
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34.23
29.81
25.17
9.43
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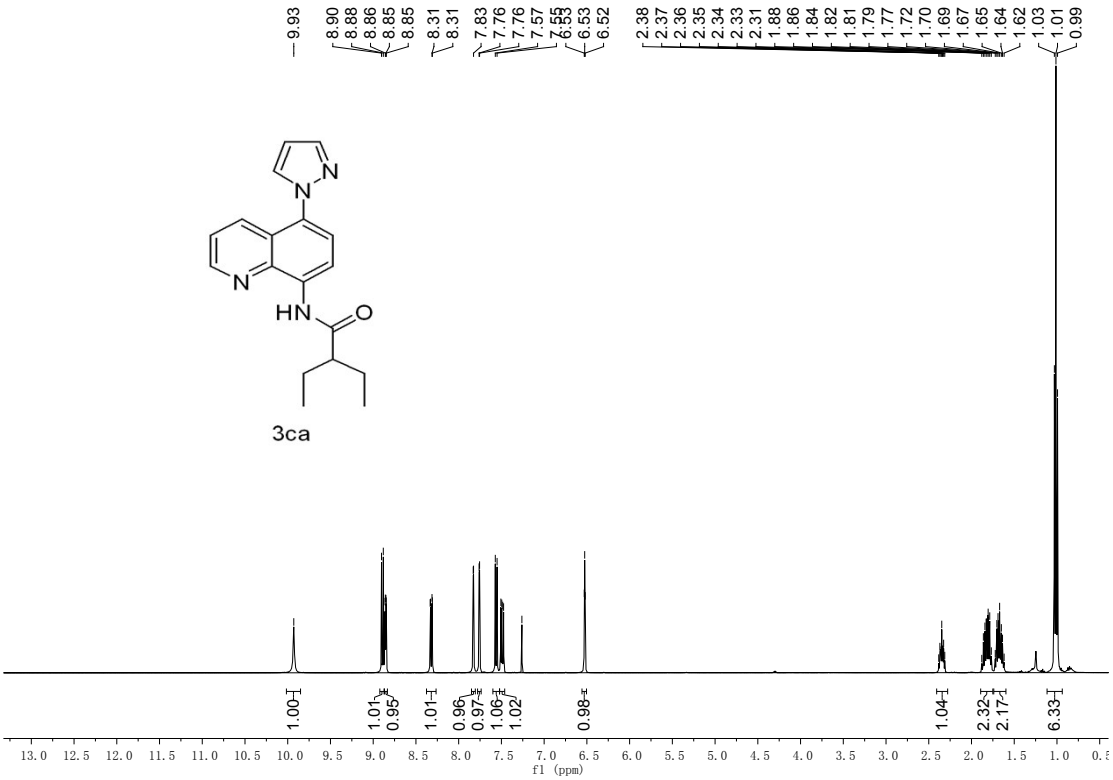
O
3ba
f1 (ppm)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8.31
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7.76
7.76
7.57
7.55
6.53
6.52
2.38
2.37
2.36
2.35
2.34
2.33
2.31
1.88
1.86
1.84
1.82
1.81
1.79
1.77
1.72
1.70
1.69
1.67
1.65
1.64
1.62
1.03
1.01
0.99
N
N
N
HN
O
3ca
1.00
1.01
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1.01
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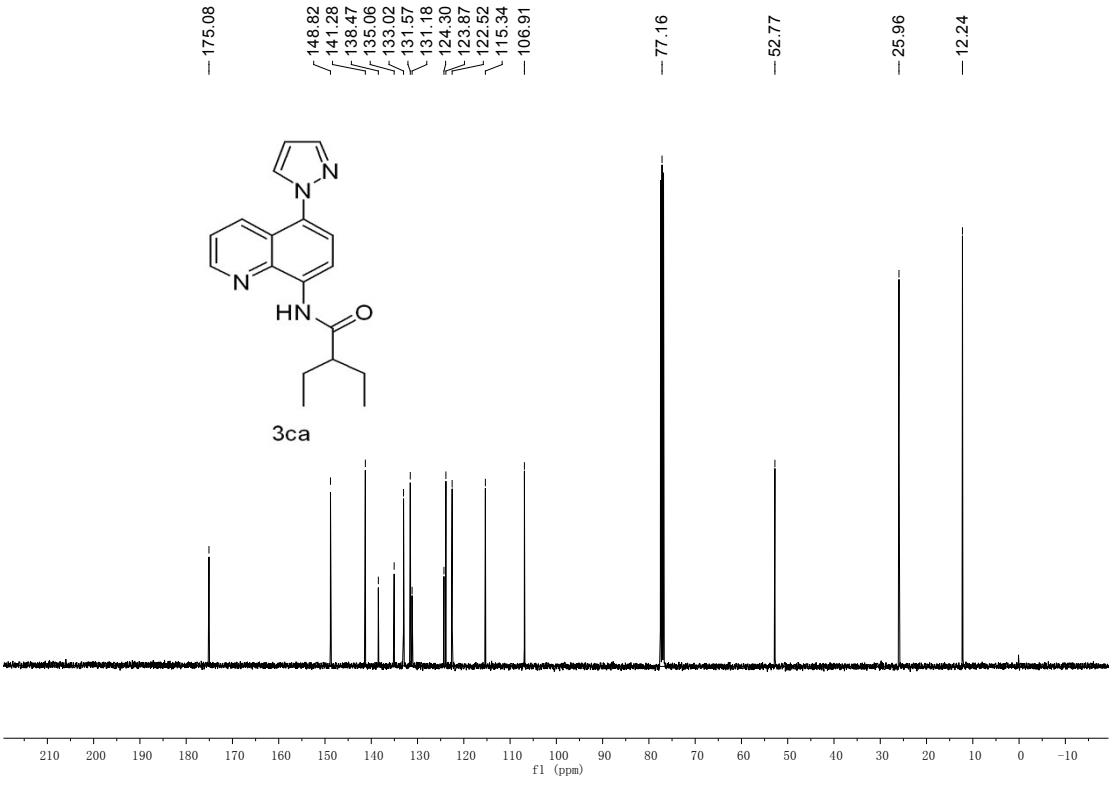
0.97
1.06
1.02
0.98
1.04
2.32
2.17
6.33
f1 (ppm)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133.02
131.57
131.18
124.30
123.87
122.52
115.34
106.91
77.16
52.77
25.96
12.24
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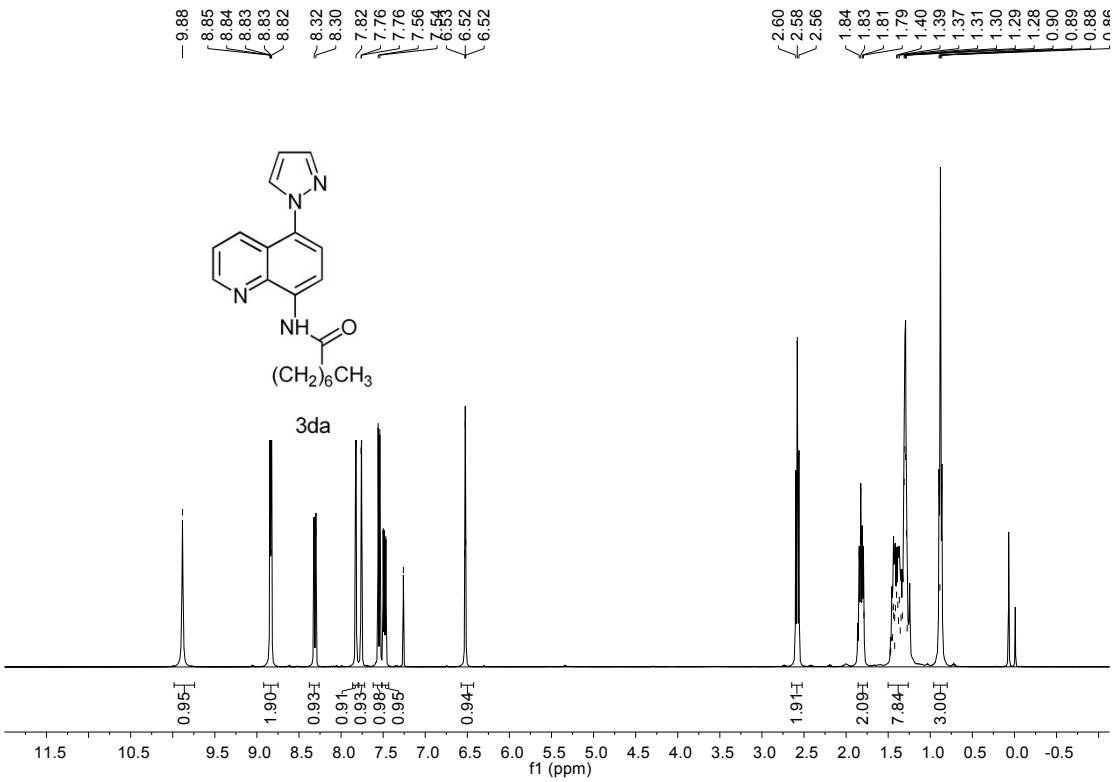
N
N
HN
O
3ca
f1 (ppm)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8.32
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7.76
7.76
7.56
7.54
6.53
6.52
6.52
2.60
2.58
2.56
1.84
1.83
1.81
1.79
1.40
1.39
1.37
1.31
1.30
1.29
1.28
0.90
0.89
0.88
N
N
NH
O
(CH2)6CH3
3da
0.95
1.90
0.93
0.91
0.93
0.98
0.95
0.94
1.91
2.09
7.84
3.00
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
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4.0
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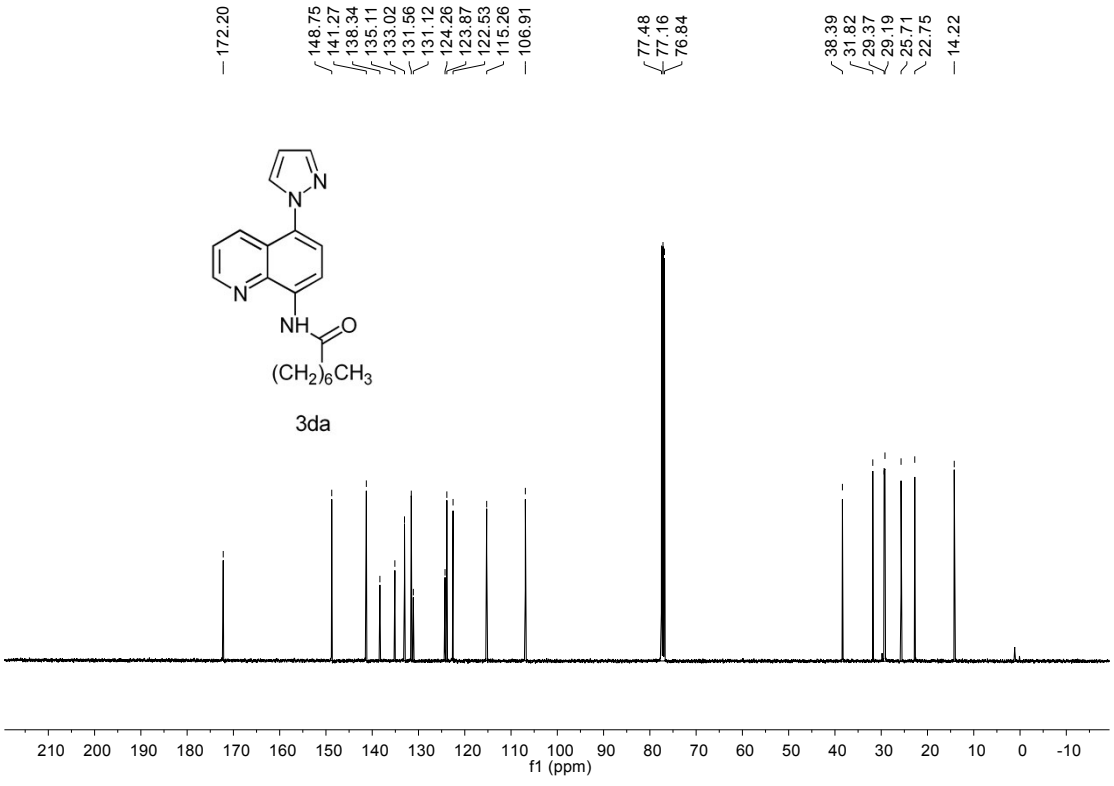
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)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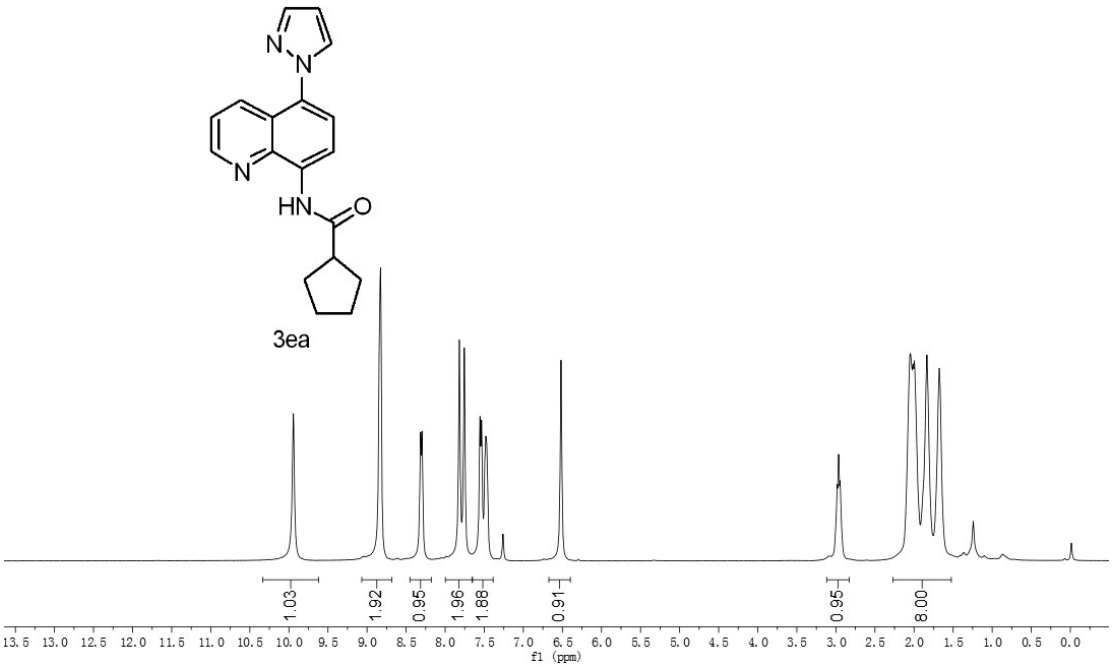
123.87
122.53
115.26
106.91
77.48
77.16
76.84
38.39
31.82
29.37
29.19
25.71
22.75
14.22
N
N
NH
O
(CH2)6CH3
3da
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)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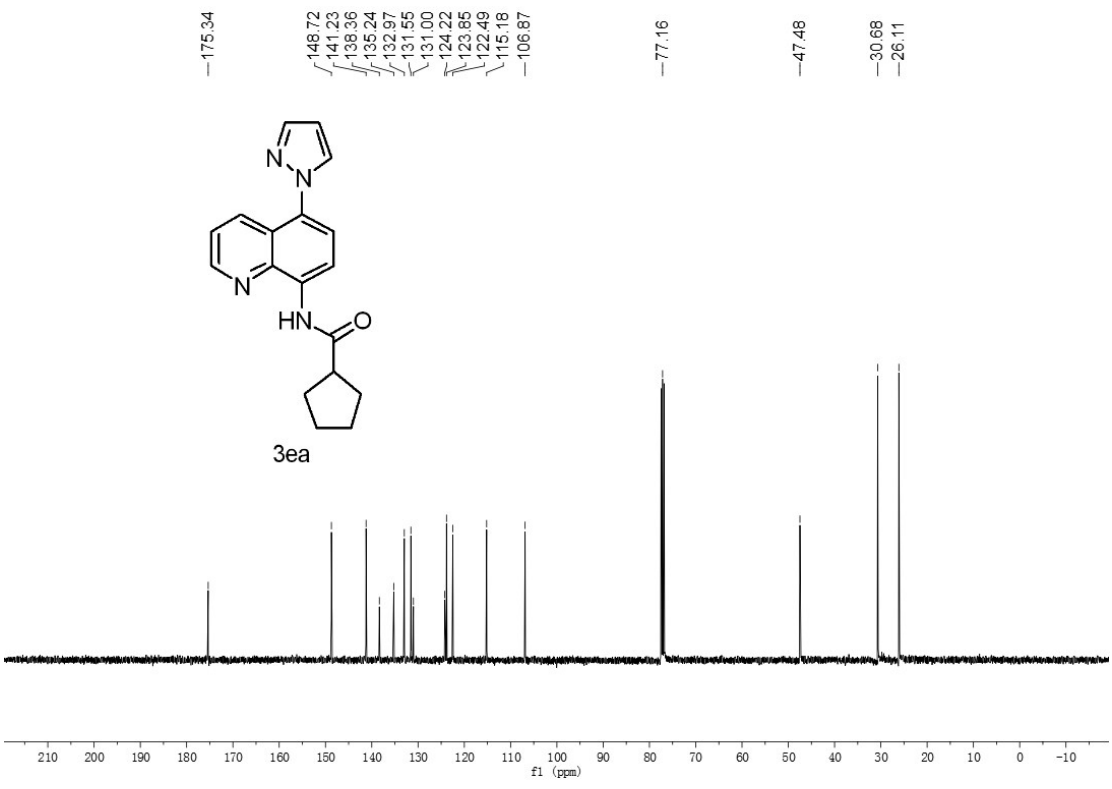
8.00
f1 (ppm)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124.22
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122.49
115.18
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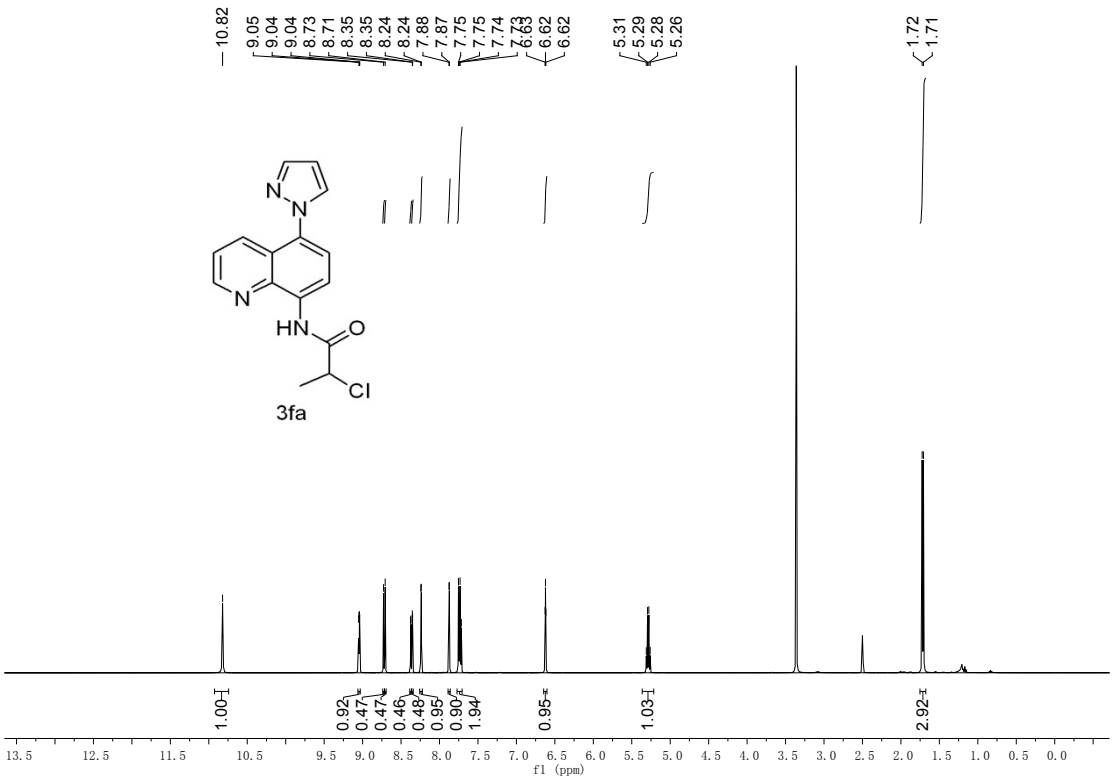
47.48
30.68
26.11
3ea
f1 (ppm)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9.04
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5.29
5.28
5.26
1.72
1.71
3fa
1.00
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0.48
0.95
0.90
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0.95
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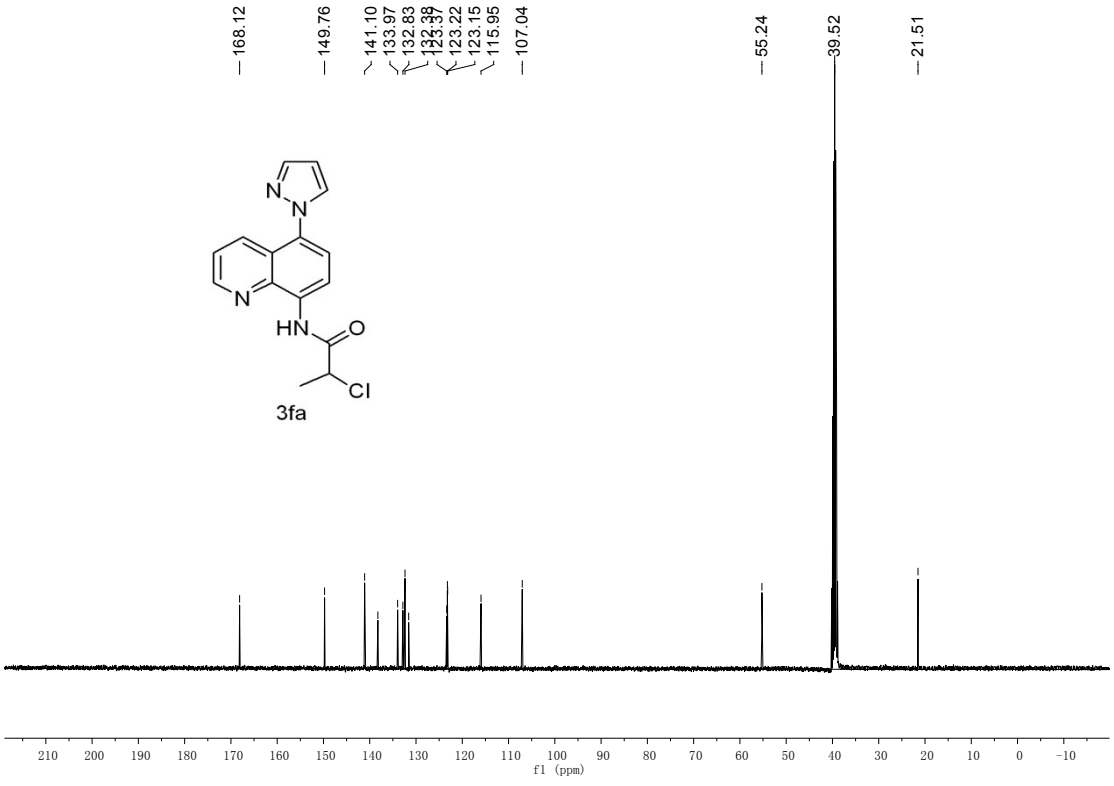
2.92
f1 (ppm)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123.15
115.95
107.04
55.24
39.52
21.51
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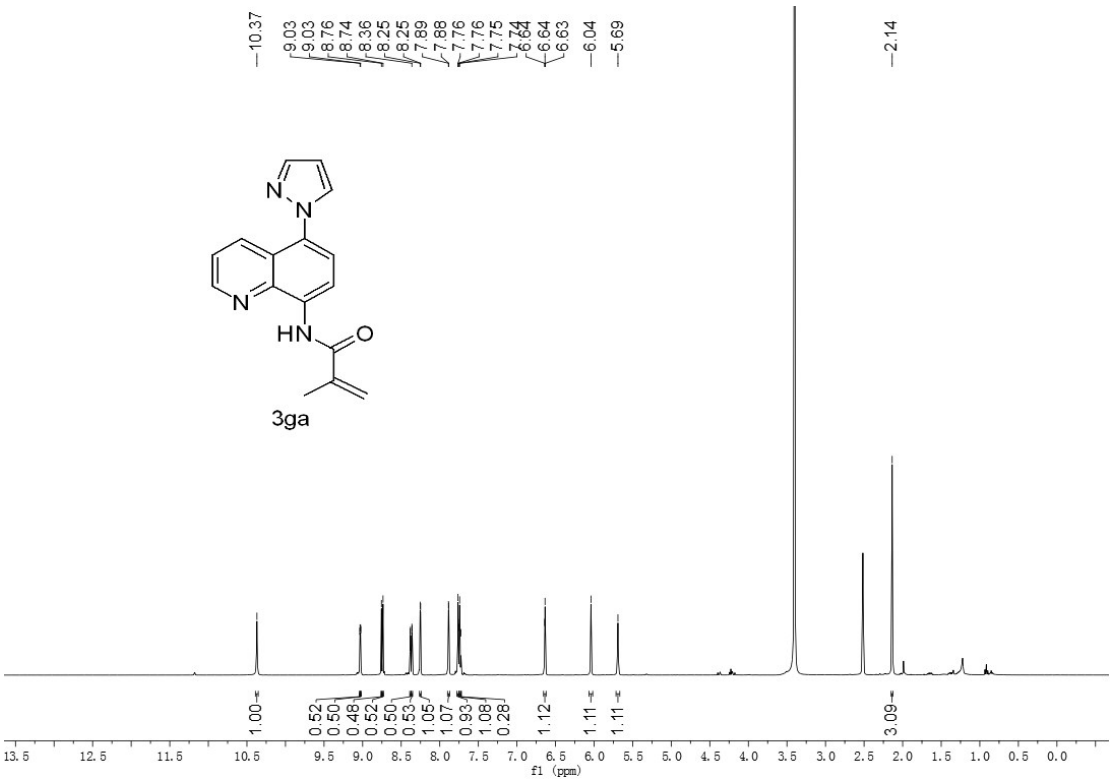
f1 (ppm)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7.76
7.76
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6.63
6.04
5.69
2.14
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N
N
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O
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0.50
0.48
0.52
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1.08
0.28
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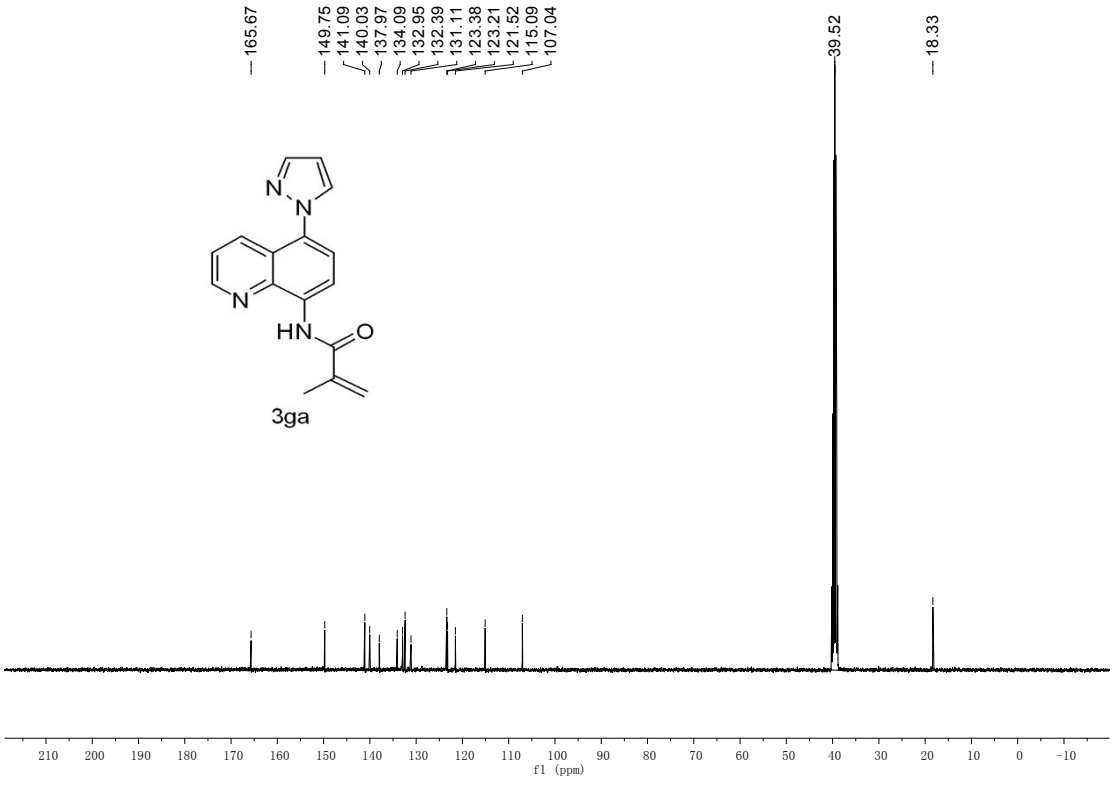
1.11
1.11
3.09
f1 (ppm)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132.39
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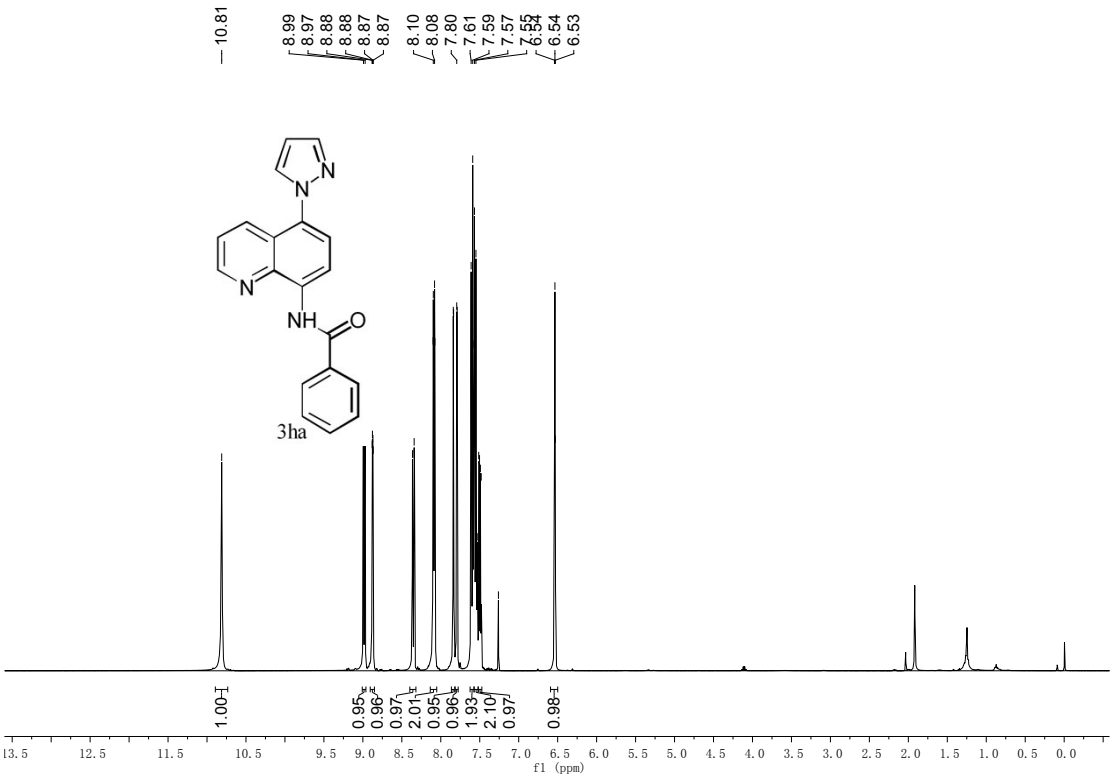
115.09
107.04
39.52
18.33
N
N
N
HN
O
3ga
f1 (ppm)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7.80
7.61
7.59
7.57
7.55
6.54
6.53
3ha
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0.97
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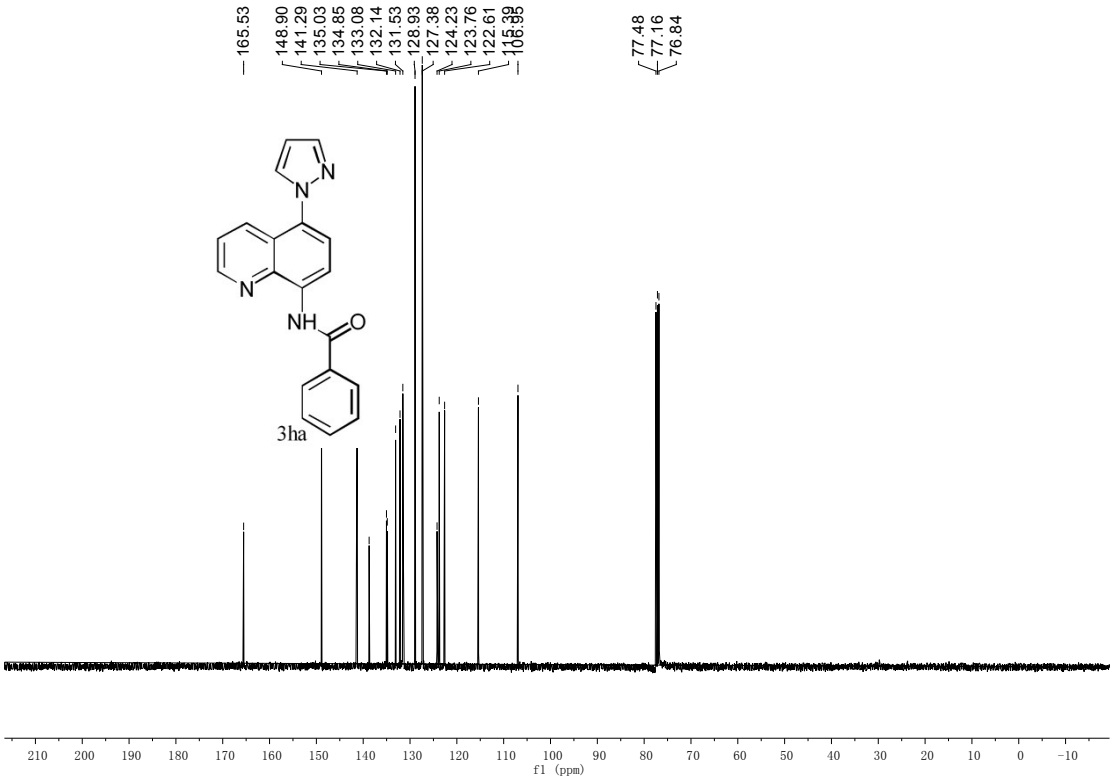
0.95
0.96
1.93
2.10
0.97
0.98
f1 (ppm)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133.08
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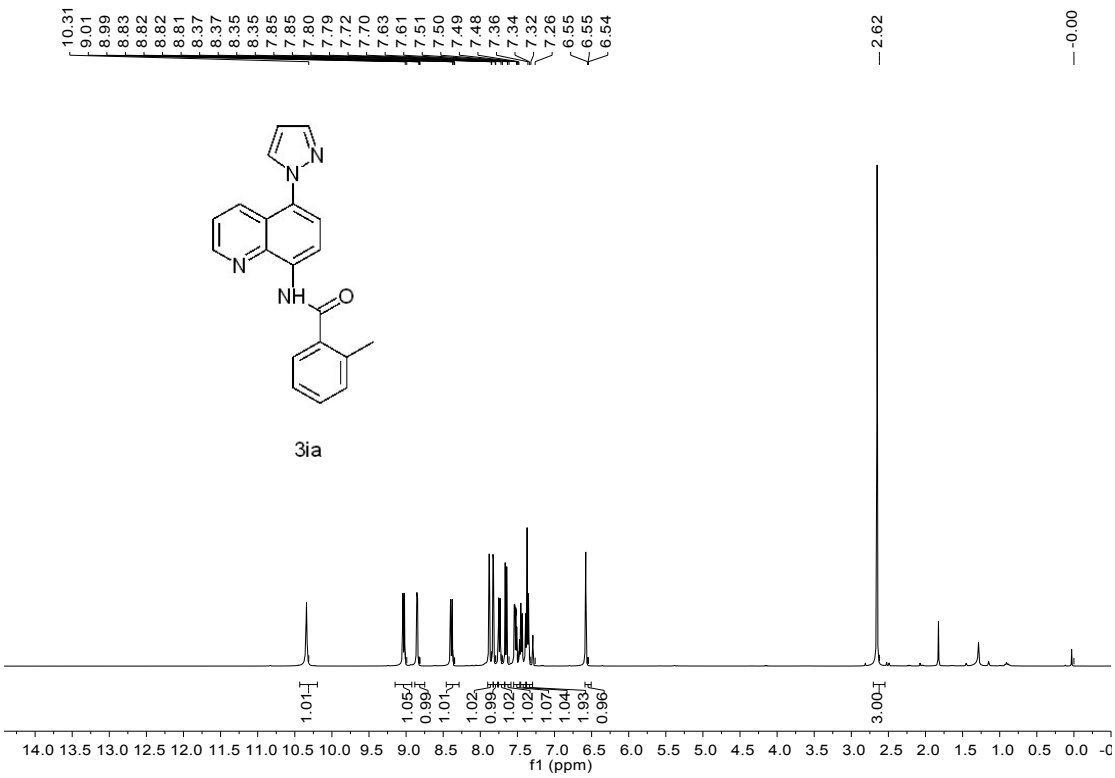
123.76
122.61
77.48
77.16
76.84
3ha
f1 (ppm)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8.81
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8.35
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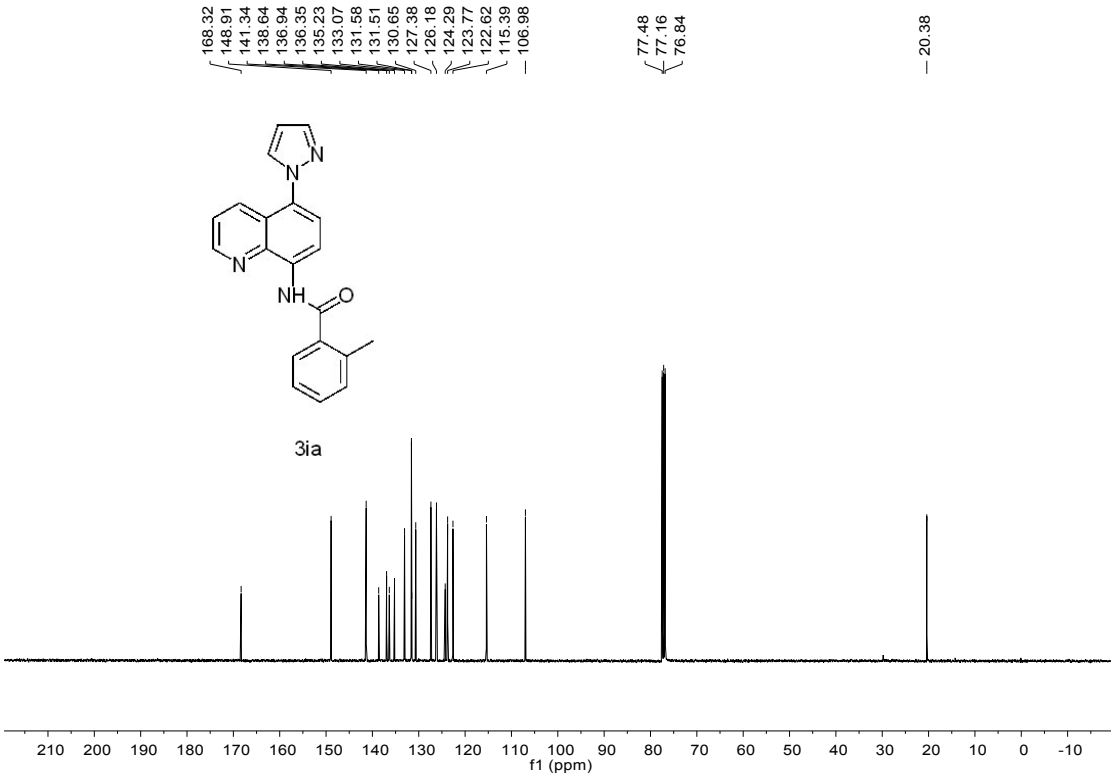
7.85
7.80
7.79
7.72
7.70
7.63
7.61
7.51
7.50
7.49
7.48
7.36
7.34
7.32
7.26
6.55
6.55
6.54
2.62
-0.00
3ia
1.01
1.05
0.99
1.01
1.02
0.99
1.02
1.02
1.07
1.04
1.93
0.96
3.00
f1 (ppm)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141.34
138.64
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131.51
130.65
127.38
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124.29
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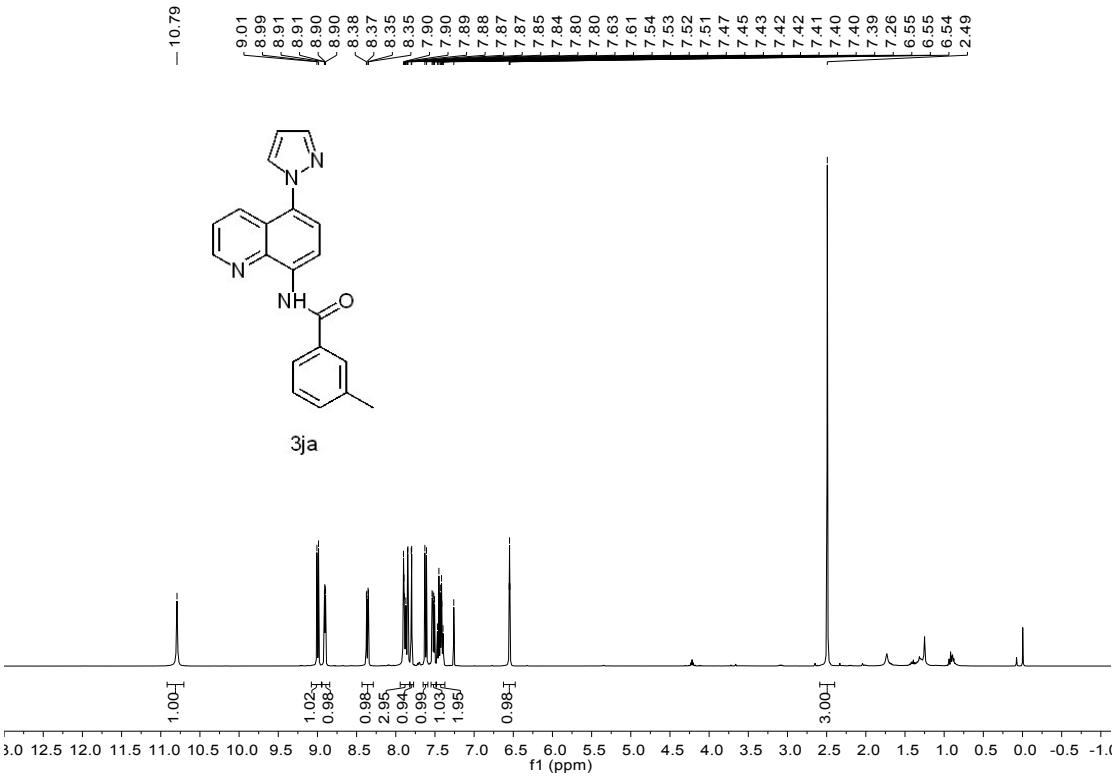
77.48
77.16
76.84
20.38
3ia
f1 (ppm)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7.90
7.89
7.88
7.87
7.87
7.85
7.84
7.80
7.80
7.63
7.61
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7.51
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7.43
7.42
7.42
7.41
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6.55
6.55
6.54
2.49
N
N
NH
O
3ja
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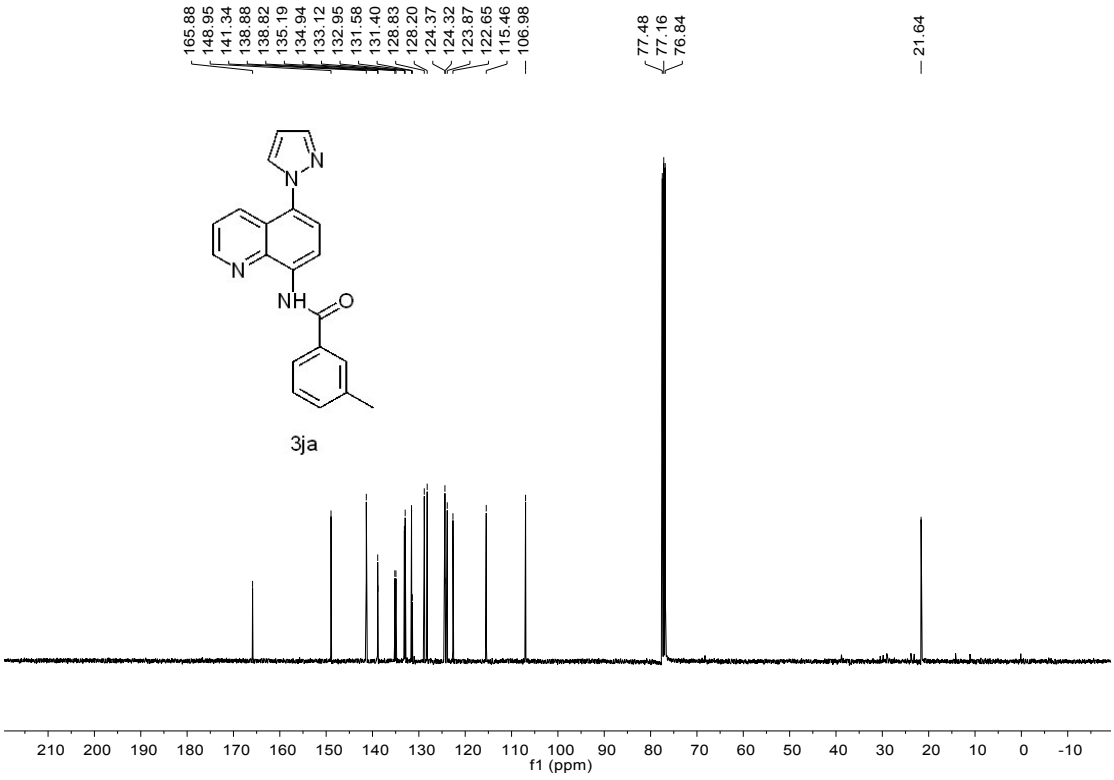
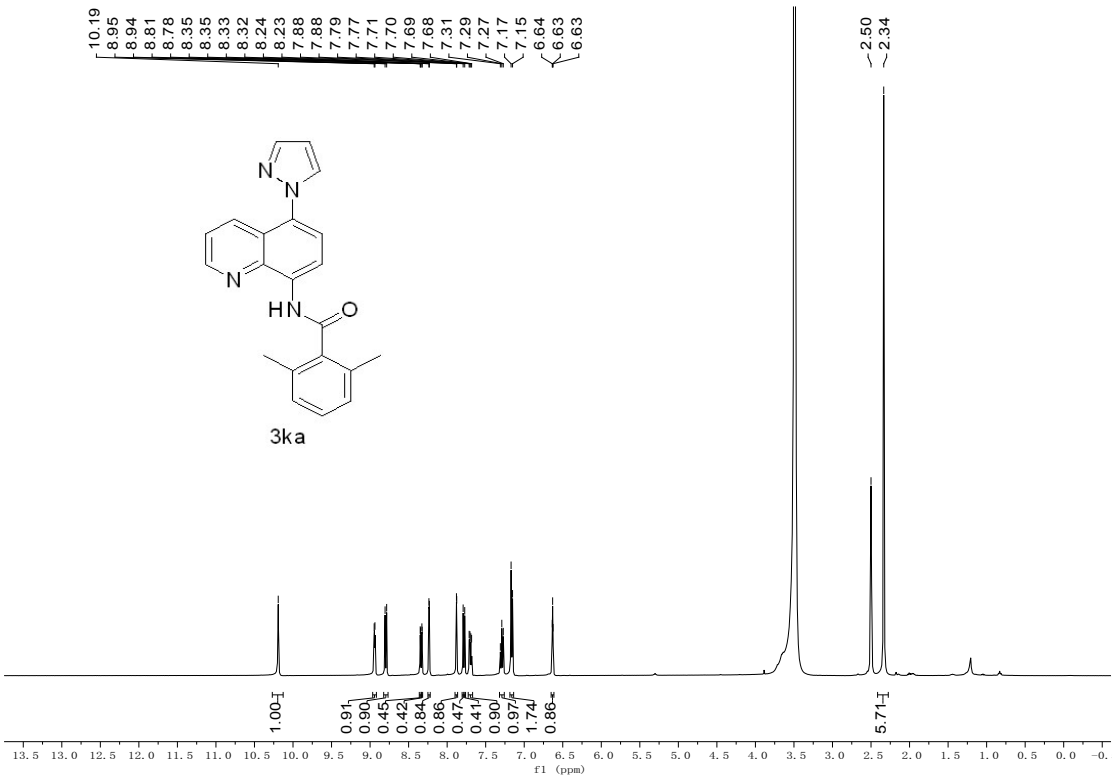
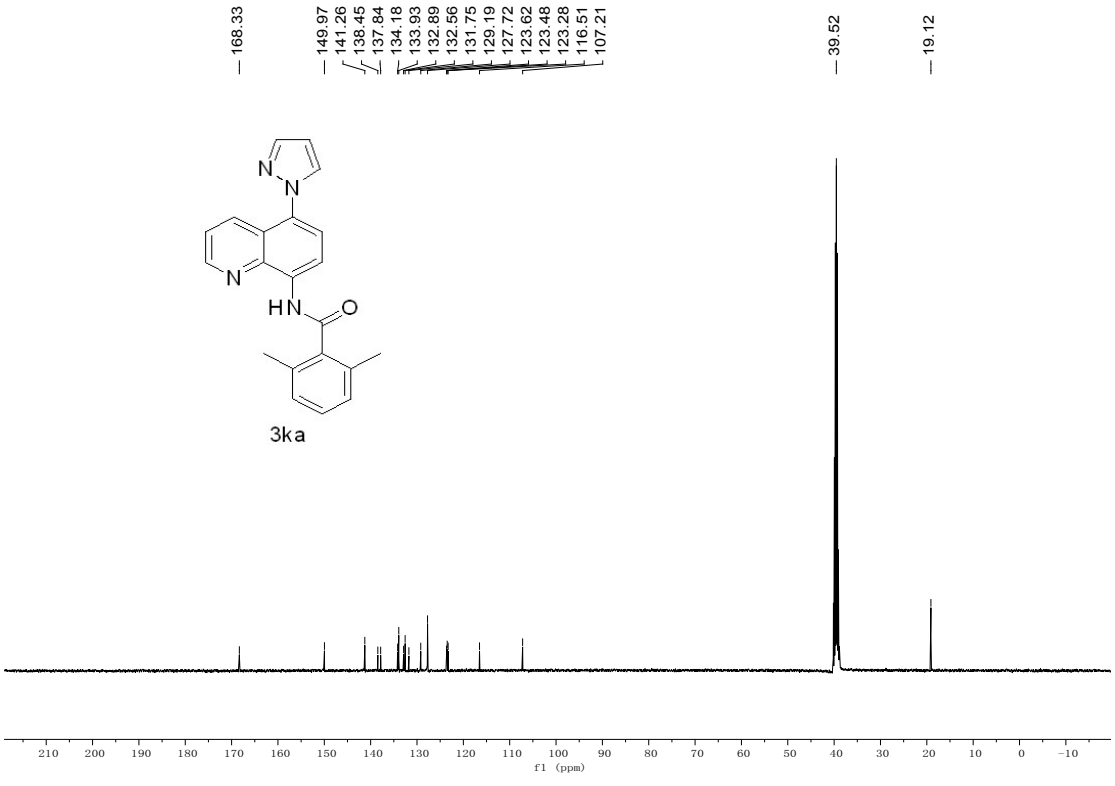
0.98
2.95
0.94
0.99
1.03
1.95
0.98
3.00
f1 (ppm)


165.88
148.95
141.34
138.88
138.82
135.19
134.94
133.12
132.95
131.58
131.40
128.83
128.20
124.37
124.32
123.87
122.65
115.46
106.98
77.48
77.16
76.84
21.64
N
N
NH
O
3ja
f1 (ppm)


10.19
8.95
8.94
8.81
8.78
8.35
8.35
8.33
8.32
8.24
8.23
7.88
7.88
7.79
7.77
7.71
7.70
7.69
7.68
7.31
7.29
7.27
7.17
7.15
6.64
6.63
6.63
2.50
2.34
N
N
N
HN
O
3ka
1.00
0.91
0.90
0.45
0.42
0.84
0.86
0.47
0.41
0.90
0.97
1.74
0.86
5.71
f1 (ppm)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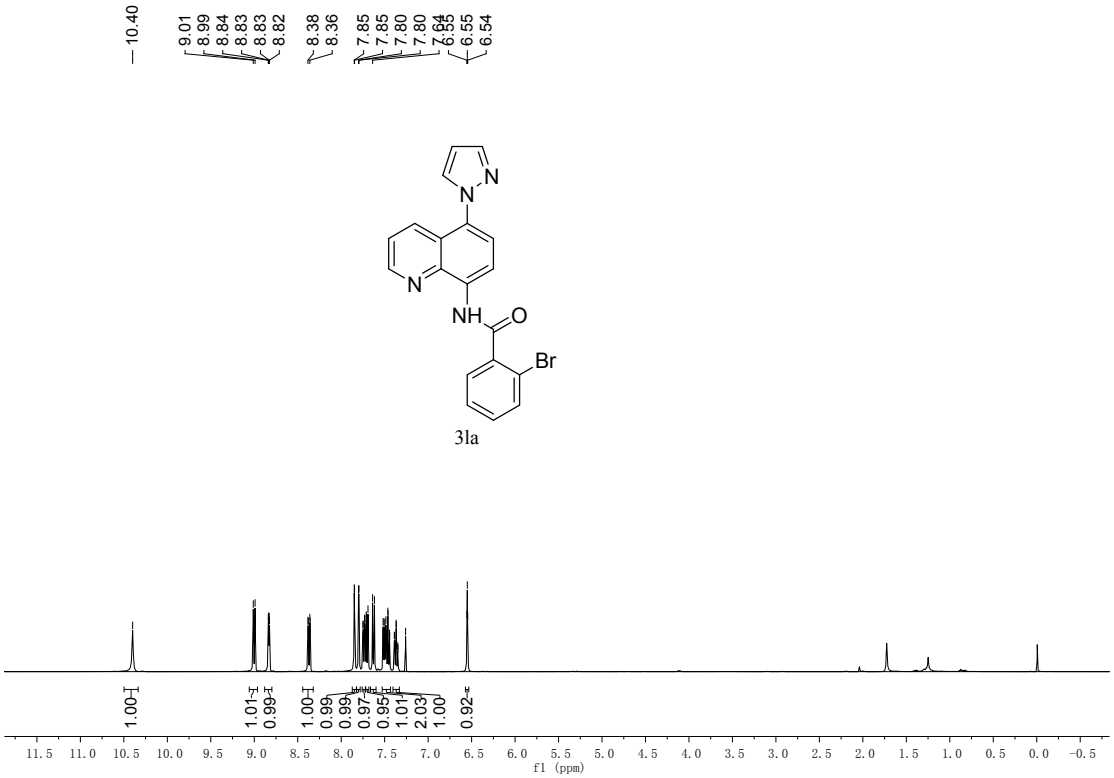
141.26
138.45
137.84
134.18
133.93
132.89
132.56
131.75
129.19
127.72
123.62
123.48
123.28
116.51
107.21
39.52
19.12
N
N
N
HN
O
3ka
f1 (ppm)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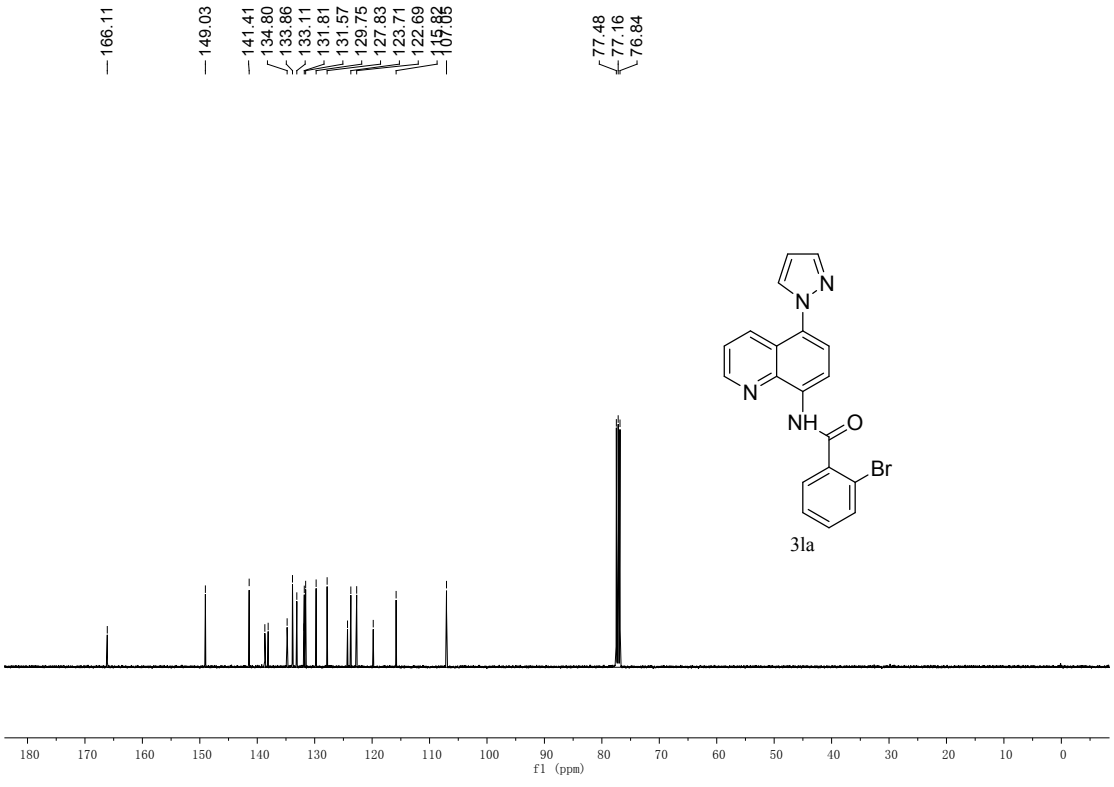
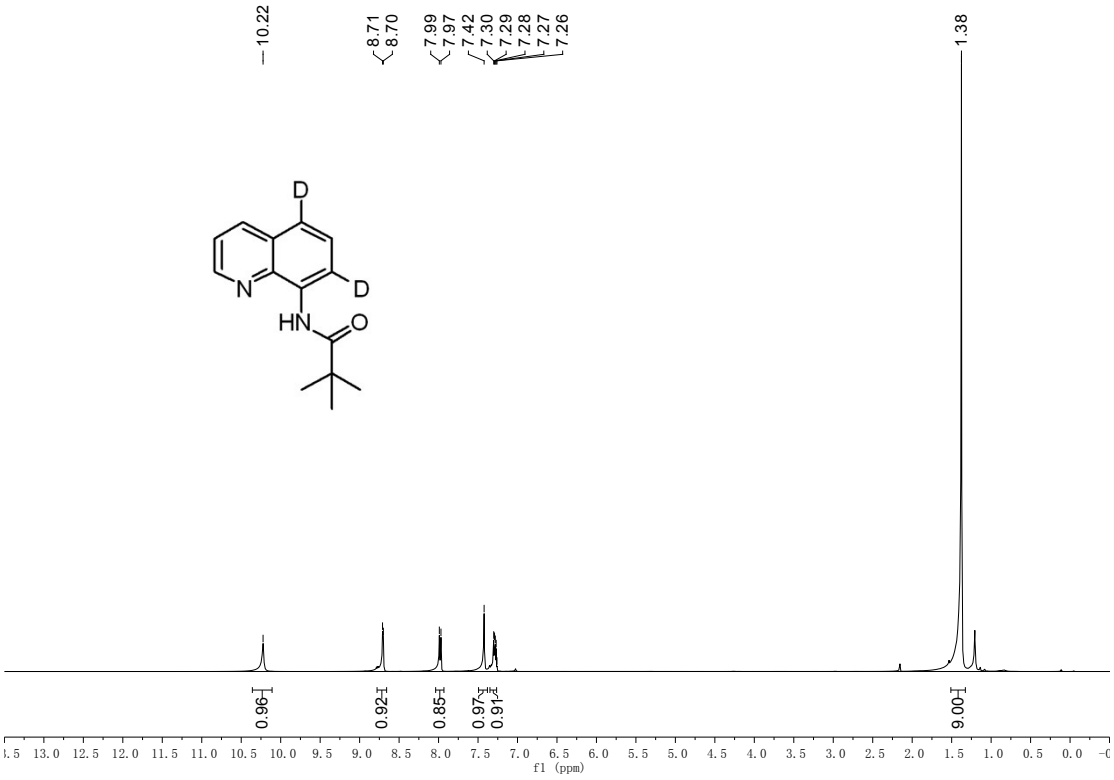
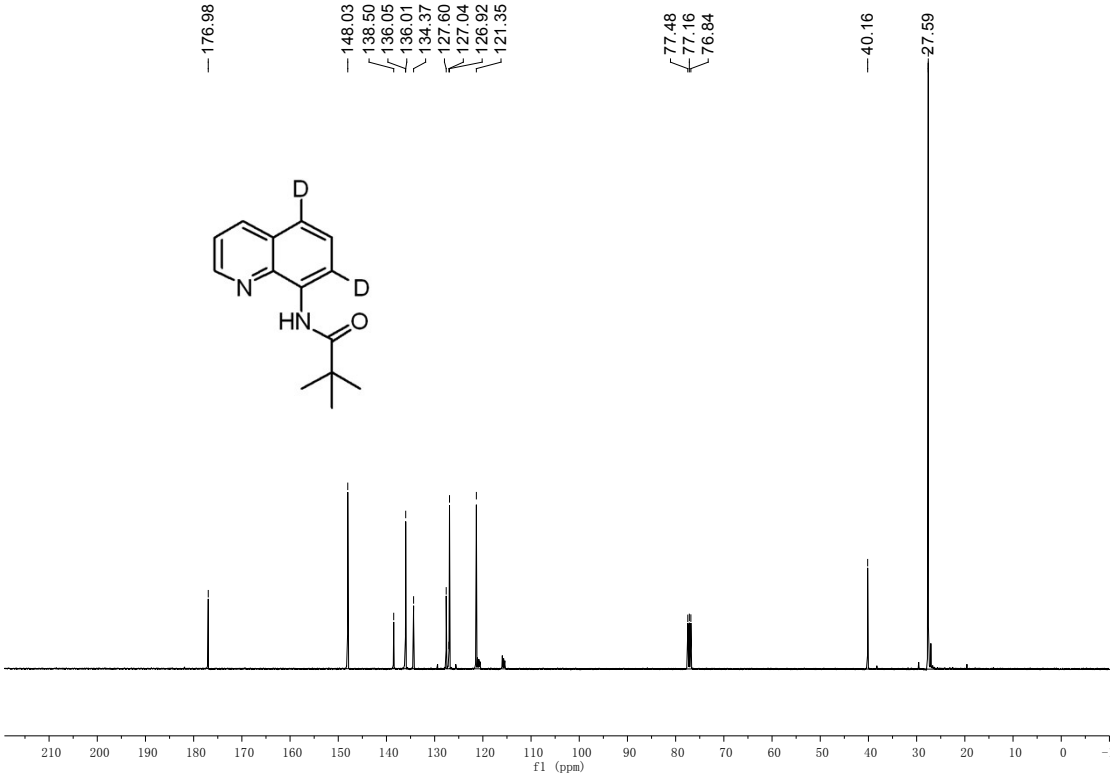
9.01
8.99
8.84
8.83
8.83
8.82
8.38
8.36
7.85
7.85
7.80
7.80
6.55
6.54
N
N
N
NH
O
Br
3la
1.00
1.01
0.99
1.00
0.99
0.97
0.95
1.01
2.03
1.00
0.92
f1 (ppm)


166.11
149.03
141.41
134.80
133.86
133.11
131.81
131.57
129.75
127.83
123.71
122.69
77.48
77.16
76.84
N
N
N
NH
O
Br
3la
f1 (ppm)


10.22
8.71
8.70
7.99
7.97
7.42
7.30
7.29
7.28
7.27
7.26
1.38
D
D
N
HN
O
0.96
0.92
0.85
0.97
0.91
9.00
f1 (ppm)


176.98
148.03
138.50
136.05
136.01
134.37
127.60
127.04
126.92
121.35
77.48
77.16
76.84
40.16
27.59
D
D
N
HN
O
f1 (ppm)