Supporting Information

Ni-catalyzed Radical Cyclization of Vinyl Azides with Cyclobutanone Oxime Esters to Access Cyanoalkyl Containing Quinoxalin-2(1*H*)-ones

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General Information:

All reactions were carried out under Ar atmosphere unless otherwise noted. All catalysts and solvents were obtained from commercial suppliers. Reactions were monitored by TLC on silica gel plates (GF254), and the analytical thin-layer chromatography (TLC) was performed on precoated, glass-backed silica gel plates. ^{1}H NMR, ^{13}C NMR and ^{19}F NMR spectra were recorded on 400 MHz spectrometer at room temperature. Chemical shifts (δ) are reported in ppm downfield fromtetramethylsilane. High resolution mass spectra were obtained on a high–resolution mass spectrometer in the ESI mode. All of vinyl azides **1** were synthesized according to the literature.[1] And all of cycloketone oxime esters **2** were synthesized from the corresponding cycloketones and carboxylic acids according to the literature.[2a] The substituted cycloketones were prepared according to the reported procedure.[2b]

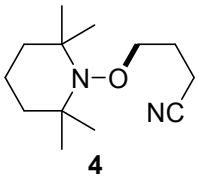
General procedure for the synthesis of 3

An oven-dried Schlenk tube (10 mL) was equipped with a magnetic stir bar, **1** (0.1 mmol), cycloketone *O*-acyl oximes **2** (2 equiv, 0.2 mmol), $NiCl_2$•glyme (5 mol%). The flask was evacuated and backfilled with Ar for 3 times. 1 mL DMF was added with syringe under Ar. The tube was then sealed and the mixture was stirred at 70 °C for 24 h. After the reaction was finished, 10 ml water was added and the resulting mixture was extracted with EtOAc (3 × 10 mL). The combined organic phase was washed with brine (10 mL), dried over Na_2SO_4, and concentrated under reduced pressure. The residue was purified by column chromatography on silica gel (petroleum ether/ethyl acetate, 3:1, v/v) to obtain the desired product **3**.

Trapping experiment with TEMPO

An oven-dried Schlenk tube (10 mL) was equipped with a magnetic stir bar, **1** (0.1 mmol), cyclobutanone *O*-acyl oximes **2** (2 equiv, 0.2 mmol), $NiCl_2$•glyme (5 mol%). The flask was evacuated and backfilled with Ar for 3 times. 1 mL DMF was added with syringe under Ar. The tube was then sealed and the mixture was stirred at 70 °C for 24 h. However, product **3aa** could not be detected, the intermediate **4** was formed, suggesting that this transformation proceeds through a radical pathway.

The HRMS (ESI) for the intermediate 4



4

HRMS [**4**+H]$^{+}$： Calcd：225.1691；Found: 225.1694.

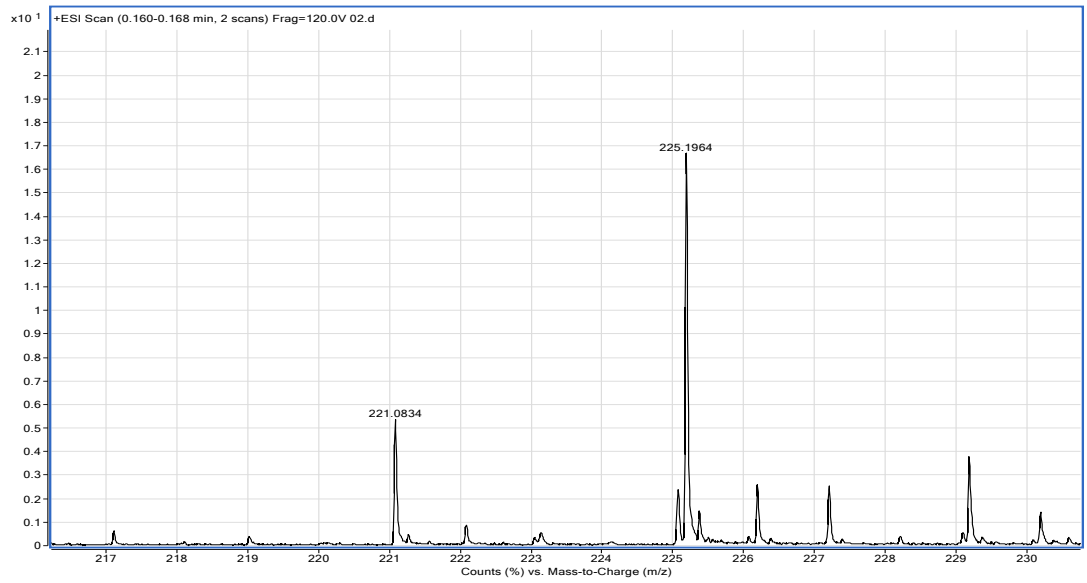
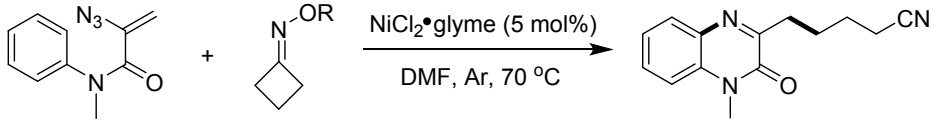


Table 1. Optimization of Reaction Conditions[a]



1a **2a**, R = *p*-$CF_3C_6H_4CO$ **2a-2**, R = C_6F_5CO **3aa**
2a-1, R = *p*-$NO_2C_6H_4CO$ **2a-3**, R = C_6H_5CO

Entry	Variation from the standard conditions	Yield(%)[b]
1	none	75
2	**2a-1** instead of **2a**	61
3	**2a-2** instead of **2a**	56
4	**2a-3** instead of **2a**	24
5	without $NiCl_2$•glyme	0
6	5 mol % $FeCl_2$ as the catalyst	23
7	5 mol % $Fe(OAc)_2$ as the catalyst	38
8	5 mol % $CuCl_2$ as the catalyst	17
9	5 mol % CuCl as the catalyst	6
10	5 mol % $CuBr_2$ as the catalyst	16
11	5 mol % CuO as the catalyst	23
12	5 mol % $Cu(OAc)_2$ as the catalyst	15
13	5 mol % $NiCl_2$ as the catalyst	35
14	5 mol % $NiBr_2$ as the catalyst	31
15	5 mol % $Ni(OAc)_2$ as the catalyst	58
16	5 mol % $Ni(acac)_2$ as the catalyst	43
17[c]	2 mol % *fac*-$Ir(ppy)_3$ as the catalyst	48
18[c]	2 mol % $Ru(bpy)_3(PF_6)_2$ as the catalyst	32
19[c]	2 mol % 4CzIPN as the catalyst	38
20[c]	2 mol % Eosin Y as the catalyst	0
21	10 mol % $NiCl_2$•glyme was used	73
22	1,4-dioxane as the solvent	26

23	CH_3CN as the solvent	70
24	toluene as the solvent	41
25	DMSO as the solvent	51
26	DMA as the solvent	45
27	1.5 equiv **2a**	67
28	at 60 °C	61
29	at 80 °C	53

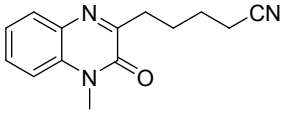
Reaction conditions: **1a** (0.1 mmol, 0.1 M), **2a** (0.2 mmol, 2 equiv), 5 mol % $NiCl_2$•glyme, and DMF (1 mL) at 70 °C (oil bath) in an argon atmosphere for 24 h. [b] Yield of isolated product. [c] Under 12 W blue LED irradiation for 24 h.

Reference

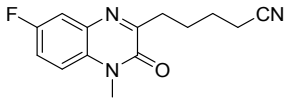
1, (a) T. Yang, H. Zhu, W. Yu, *Org. Biomol. Chem.,* 2016, **14**, 3376; (b) E. G. Mackay, A. Studer, *Chem. Eur. J.* 2016, **22**, 13455.

2, (a) T. Nishimura, Y. Nishiguchi, Y. Maeda, S. Uemura, *J. Org. Chem.* 2004, **69**, 5342. (b) Y.-R. Gu, X.-H. Duan, L. Yang, L.-N. Guo, *Org. Lett.* 2017, **19**, 5908.

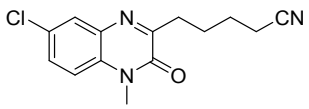
B. Zhao, H. Tan, C. Chen, N. Jiao, N. and Z. Shi, *Chin. J. Chem.* 2018, **36**, 995.



*5-(4-methyl-3-oxo-3,4-dihydroquinoxalin-2-yl)pentanenitrile (**3aa**)*. Yellow solid; (18 mg, 75%); mp: 103-107 °C; R_f = 0.20 (petroleum ether/ethyl acetate 3:1); ^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.85-7.82 (m, 1H), 7.57-7.53 (m, 1H), 7.38-7.30 (m, 2H), 3.71 (s, 3H), 2.99 (t, *J* = 7.2 Hz, 2H), 2.44 (t, *J* = 7.2 Hz, 2H), 2.03-1.95 (m, 2H), 1.86-1.79 (m, 2H) ppm; ^{13}C NMR (101 MHz, $CDCl_3$): δ 159.6, 154.8, 133.0, 132.6, 129.8, 129.7, 123.6, 119.6, 113.6, 32.8, 29.0, 25.4, 25.1, 17.0 ppm. ESI-HRMS: m/z Calcd for $C_{14}H_{15}N_3O$ [M+H$^+$]: 241.1215, found 241.1217.

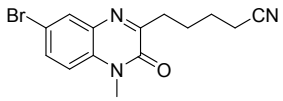


*5-(7-fluoro-4-methyl-3-oxo-3,4-dihydroquinoxalin-2-yl)pentanenitrile (**3ba**)*. Yellow solid; (14.8 mg, 57%); mp: 115-117 °C; R_f = 0.20 (petroleum ether/ethyl acetate 3:1); ^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.55-7.52 (m, 1H), 7.32-7.25 (m, 1H), 3.70 (s, 3H), 2.99 (t, *J* = 7.2 Hz, 2H), 2.44 (t, *J* = 7.2 Hz, 2H), 2.02-1.94 (m, 2H), 1.86-1.78 (m, 2H) ppm; ^{13}C NMR (101 MHz, $CDCl_3$): δ 161.3, 158.7 (d, *J* = 305 Hz), 154.4, 133.1 (d, *J* = 14 Hz), 129.7 (d, *J* = 3 Hz), 119.6, 117.5 (d, *J* = 30 Hz), 115.2 (d, *J* = 28 Hz), 114.7 (d, *J* = 11 Hz), 32.9, 29.3, 25.2, 25.0, 17.0 ppm; ^{19}F NMR (376 MHz, $CDCl_3$): *δ* -118.9 ppm. ESI-HRMS: m/z Calcd for $C_{14}H_{14}FN_3O$ [M+H$^+$]: 259.1121, found 259.1123.

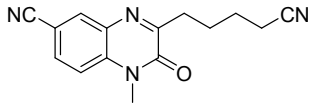


*5-(7-chloro-4-methyl-3-oxo-3,4-dihydroquinoxalin-2-yl)pentanenitrile (**3ca**)*. Yellow solid; (19.6 mg, 72%); mp: 121-124 °C; R_f = 0.20 (petroleum ether/ethyl acetate 3:1); ^{1}H NMR (400 MHz,

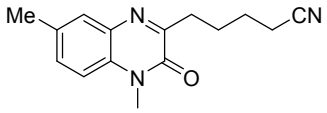
$CDCl_3$): δ = 7.82 (s, 1H), 7.51-7.48 (m, 1H), 7.25-7.23 (m, 1H), 3.69 (s, 3H), 2.98 (t, *J* = 7.2 Hz, 2H), 2.44 (t, *J* = 7.2 Hz, 2H), 2.01-1.94 (m, 2H), 1.85-1.78 (m, 2H) ppm; ^{13}C NMR (101 MHz, $CDCl_3$): δ 161.1, 154.4, 133.1, 131.7, 129.7, 129.0, 128.9, 119.5, 114.7, 32.8, 29.2, 25.1, 25.0, 17.0 ppm. ESI-HRMS: m/z Calcd for $C_{14}H_{15}ClN_3O$ [M+H$^+$]: 276.0898, found 276.0895.



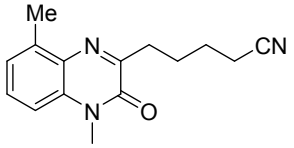
*5-(7-bromo-4-methyl-3-oxo-3,4-dihydroquinoxalin-2-yl)pentanenitrile (**3da**)*. Yellow solid; (20.2 mg, 63%); mp: 131-134 °C; R_f = 0.20 (petroleum ether/ethyl acetate 3:1); ^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.982-7.978 (m, 1H), 7.64-7.61 (m, 1H), 7.19-7.13 (m, 1H), 3.68 (s, 3H), 2.98 (t, *J* = 7.2 Hz, 2H), 2.44 (t, *J* = 7.2 Hz, 2H), 2.01-1.94 (m, 2H), 1.85-1.78 (m, 2H) ppm; ^{13}C NMR (101 MHz, $CDCl_3$): δ 161.1, 154.4, 133.4, 132.5, 132.2, 132.1, 119.5, 116.2, 115.0, 32.8, 29.2, 25.1, 25.0, 17.0 ppm. ESI-HRMS: m/z Calcd for $C_{14}H_{15}BrN_3O$ [M+H$^+$]: 320.0393, found 320.0396.



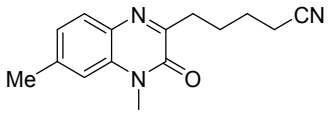
*3-(4-cyanobutyl)-1-methyl-2-oxo-1,2-dihydroquinoxaline-6-carbonitrile (**3ea**)*. Yellow solid; (20.3 mg, 76%); mp: 124-127 °C; R_f = 0.20 (petroleum ether/ethyl acetate 3:1); ^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.15-8.14 (m, 1H), 7.79-7.76 (m, 1H), 7.40-7.38 (m, 1H), 3.72 (s, 3H), 3.00 (t, *J* = 7.2 Hz, 2H), 2.45 (t, *J* = 7.2 Hz, 2H), 2.03-1.95 (m, 2H), 1.86-1.78 (m, 2H) ppm; ^{13}C NMR (101 MHz, $CDCl_3$): δ 162.0, 154.4, 136.3, 134.0, 132.4, 132.1, 119.4, 117.9, 114.7, 107.1, 32.8, 29.3, 25.0, 24.9, 17.0 ppm. ESI-HRMS: m/z Calcd for $C_{15}H_{15}N_4O$ [M+H$^+$]: 267.1240, found 267.1237.



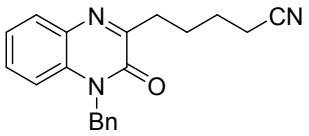
*5-(4,7-dimethyl-3-oxo-3,4-dihydroquinoxalin-2-yl)pentanenitrile (**3fa**)*. Yellow solid; (13.6 mg, 53%); mp: 108-110°C; R_f = 0.20 (petroleum ether/ethyl acetate 3:1); ^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.66-7.65 (m, 1H), 7.39-7.36 (m, 1H), 7.23-7.21 (m, 1H), 3.71 (s, 3H), 3.00 (t, *J* = 7.2 Hz, 2H), 2.48 (s, 3H), 2.45 (t, *J* = 7.2 Hz, 2H), 2.03-1.96 (m, 2H), 1.88-1.80 (m, 2H) ppm; ^{13}C NMR (101 MHz, $CDCl_3$): δ 159.6, 154.8, 133.5, 132.5, 131.0, 130.9, 129.6, 119.6, 113.4, 32.9, 29.0, 25.4, 25.1, 20.6, 17.0 ppm. ESI-HRMS: m/z Calcd for $C_{15}H_{18}N_3O$ [M+H$^+$]: 256.1444, found 256.1441.



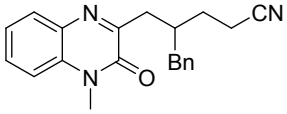
*5-(4,8-dimethyl-3-oxo-3,4-dihydroquinoxalin-2-yl)pentanenitrile (**3ga**)*. Yellow solid; (14.8 mg, 58%); mp: 114-116 °C; R_f = 0.25 (petroleum ether/ethyl acetate 3:1); ^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.42 (t, *J* = 8.0 Hz, 1H), 7.21 (d, *J* = 7.6 Hz, 1H), 7.15 (d, *J* = 7.6 Hz, 1H), 3.70 (s, 3H), 3.00 (t, *J* = 7.2 Hz, 2H), 2.68 (s, 3H), 2.45 (t, *J* = 7.2 Hz, 2H), 2.06-1.98 (m, 2H), 1.87-1.80 (m, 2H) ppm; ^{13}C NMR (101 MHz, $CDCl_3$): δ 157.5, 154.8, 138.5, 133.1, 131.1, 129.5, 124.9, 119.7, 111.4, 32.6, 29.2, 25.0, 24.9, 17.5, 17.0 ppm. ESI-HRMS: m/z Calcd for $C_{15}H_{18}N_3O$ [M+H$^+$]: 256.1444, found 256.1441.



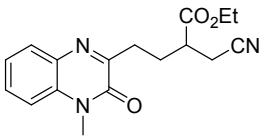
*5-(4,6-dimethyl-3-oxo-3,4-dihydroquinoxalin-2-yl)pentanenitrile (**3ga'**).* Yellow solid; (8.2 mg, 32%); mp: 115-117 °C; R_f = 0.20 (petroleum ether/ethyl acetate 3:1); ^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.70 (d, *J* = 7.2 Hz, 1H), 7.18-7.16 (m, 1H), 7.10 (s, 1H), 3.69 (s, 3H), 2.97 (t, *J* = 7.2 Hz, 2H), 2.52 (s, 3H), 2.43 (t, *J* = 7.2 Hz, 2H), 2.01-1.93 (m, 2H), 1.85-1.78 (m, 2H) ppm; ^{13}C NMR (101 MHz, $CDCl_3$): δ 158.4, 155.0, 140.5, 132.9, 130.8, 129.4, 124.9, 119.7, 113.7, 32.8, 29.0, 25.5, 25.1, 22.0, 17.0 ppm. ESI-HRMS: m/z Calcd for $C_{15}H_{18}N_3O$ [M+H$^+$]: 256.1444, found 256.1441.



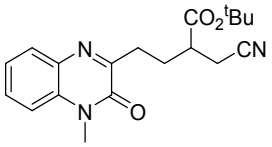
*5-(4-benzyl-3-oxo-3,4-dihydroquinoxalin-2-yl)pentanenitrile (**3ha**).* Yellow solid; (15.2 mg, 48%); mp: 135-137 °C; R_f = 0.25 (petroleum ether/ethyl acetate 3:1); ^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.85-7.83 (m, 1H), 7.44-7.39 (m, 1H), 7.34-7.28 (m, 3H), 7.24-7.22 (m, 5H), 5.50 (s, 3H), 3.05 (t, *J* = 7.2 Hz, 2H), 2.07-1.99 (m, 2H), 1.89-1.82 (m, 2H) ppm; ^{13}C NMR (101 MHz, $CDCl_3$): δ 159.8, 154.9, 135.2, 132.9, 132.4, 129.9, 129.8, 128.9, 127.7, 126.8, 123.7, 119.6, 114.4, 45.9, 32.9, 25.4, 25.2, 17.1 ppm. ESI-HRMS: m/z Calcd for $C_{20}H_{19}N_3O$ [M+H$^+$]: 317.1528, found 317.1530.



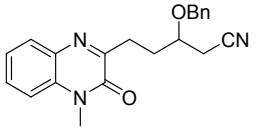
*4-benzyl-5-(4-methyl-3-oxo-3,4-dihydroquinoxalin-2-yl)pentanenitrile (**3ab**).* Yellow oil; (15.9 mg, 48%); R_f = 0.50 (petroleum ether/ethyl acetate 3:1); ^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.86-7.84 (m, 1H), 7.57-7.52 (m, 1H), 7.38-7.33 (m, 1H), 7.30-7.19 (m, 5H), 7.17-7.13 (m, 1H), 3.67 (s, 3H), 2.94 (d, *J* = 6.0 Hz, 2H), 2.84-2.77 (m, 1H), 2.71-2.63 (m, 2H), 2.42 (t, *J* = 8.0 Hz, 2H), 1.80-1.75 (m, 2H) ppm; ^{13}C NMR (101 MHz, $CDCl_3$): δ 158.9, 154.9, 139.5, 133.0, 129.9, 129.8, 129.2, 128.3, 126.2, 123.6, 119.8, 113.6, 40.3, 37.6, 36.7, 29.5, 29.1, 14.8 ppm. ESI-HRMS: m/z Calcd for $C_{21}H_{22}N_3O$ [M+H$^+$]: 332.1757, found 332.1759.



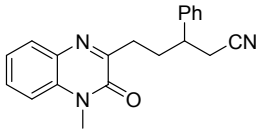
*ethyl 2-(cyanomethyl)-4-(4-methyl-3-oxo-3,4-dihydroquinoxalin-2-yl)butanoate (**3ac**).*Yellow oil; (14.4 mg, 46%); R_f = 0.20 (petroleum ether/ethyl acetate 3:1); ^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.85-7.83 (m, 1H), 7.57-7.53 (m, 1H), 7.38-7.33 (m, 1H), 7.32-7.30 (m, 1H), 4.19 (q, *J* = 14.0 Hz, *J* = 7.2 Hz, 2H), 3.71 (s, 3H), 3.09-2.98 (m, 2H), 2.96-2.89 (m, 1H), 2.81-2.67 (m, 2H), 2.35-2.20 (m, 2H), 1.28 (t, *J* = 7.2 Hz, 3H) ppm; ^{13}C NMR (101 MHz, $CDCl_3$): δ 172.4, 158.8, 154.7, 133.0, 132.5, 129.9, 129.8, 123.7, 117.8, 113.6, 61.4, 41.0, 30.5, 29.0, 27.5, 19.5, 14.1 ppm. ESI-HRMS: m/z Calcd for $C_{17}H_{20}N_3O_3$ [M+H$^+$]: 314.1499, found 314.1495.



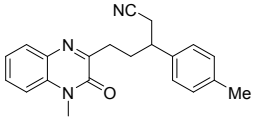
tert-butyl 2-(cyanomethyl)-4-(4-methyl-3-oxo-3,4-dihydroquinoxalin-2-yl)butanoate ***(3ad)***. Yellow solid; (16.0 mg, 47%); mp: 123-125 °C; R_f = 0.20 (petroleum ether/ethyl acetate 3:1); ^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.85-7.83 (m, 1H), 7.57-7.53 (m, 1H), 7.37-7.33 (m, 1H), 7.32-7.30 (m, 1H), 3.71 (s, 3H), 3.04-3.00 (m, 2H), 2.85-2.78 (m, 1H), 2.75-2.61 (m, 2H), 2.30-2.15 (m, 2H), 1.49 (s, 9H) ppm; ^{13}C NMR (101 MHz, $CDCl_3$): δ 171.7, 158.9, 154.7, 133.0, 132.5, 129.9, 129.8, 123.7, 117.9, 113.6, 82.1, 41.8, 30.6, 29.0, 28.0, 27.8, 19.6 ppm. ESI-HRMS: m/z Calcd for $C_{19}H_{24}N_3O_3$ [M+H$^+$]: 342.1812, found 342.1815.



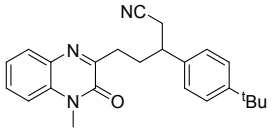
3-(benzyloxy)-5-(4-methyl-3-oxo-3,4-dihydroquinoxalin-2-yl)pentanenitrile ***(3ae)***. Yellow oil; (15.6 mg, 45%); R_f = 0.20 (petroleum ether/ethyl acetate 3:1); ^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.82-7.79 (m, 1H), 7.55-7.50 (m, 1H), 7.36-7.32 (m, 1H), 7.28-7.21 (m, 6H), 4.59 (q, J = 30.8 Hz, J = 7.2 Hz, 2H), 3.94-3.88 (m, 1H), 3.62 (s, 3H), 3.06 (t, J = 7.2 Hz, 2H), 2.67 (d, J = 6.0 Hz, 2H), 2.23 (q, J = 13.6 Hz, J = 7.2 Hz, 2H) ppm; ^{13}C NMR (101 MHz, $CDCl_3$): δ 159.6, 154.7, 137.4, 133.0, 132.5, 129.7, 129.6, 128.3, 127.7, 123.6, 117.6, 113.6, 74.0, 71.6, 30.6, 29.4, 28.9, 22.9 ppm. ESI-HRMS: m/z Calcd for $C_{21}H_{23}N_3O_2$ [M+H$^+$]: 347.1634, found 347.1631.



5-(4-methyl-3-oxo-3,4-dihydroquinoxalin-2-yl)-3-phenylpentanenitrile ***(3af)***. Yellow solid; (16.7 mg, 53%); mp: 151-153 °C; R_f = 0.30 (petroleum ether/ethyl acetate 3:1); ^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.84-7.82 (m, 1H), 7.55-7.51 (m, 1H), 7.37-7.32 (m, 2H), 7.31-7.22 (m, 5H), 3.66 (s, 3H), 3.19-3.11 (m, 1H), 3.89-2.84 (m, 2H), 2.71-2.69 (m, 2H), 2.37-2.30 (m, 2H) ppm; ^{13}C NMR (101 MHz, $CDCl_3$): δ 159.6, 154.7, 141.1, 133.0, 132.6, 129.8, 129.7, 128.9, 127.5, 127.4, 123.6, 118.5, 113.5, 41.9, 31.7, 31.3, 29.0, 25.3 ppm. ESI-HRMS: m/z Calcd for $C_{20}H_{19}N_3O$ [M+H$^+$]: 317.1528, found 317.1531.

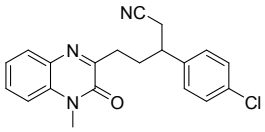


5-(4-methyl-3-oxo-3,4-dihydroquinoxalin-2-yl)-3-(p-tolyl)pentanenitrile ***(3ag)***. Yellow oil; (13.2 mg, 41%); R_f = 0.20 (petroleum ether/ethyl acetate 3:1); ^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.83-7.81 (m, 1H), 7.54-7.50 (m, 1H), 7.36-7.32 (m, 1H), 7.28-7.26 (m, 1H), 7.16-7.10 (m, 4H), 3.65 (s, 3H), 3.14-3.07 (m, 1H), 2.87-2.84 (m, 2H), 2.68-2.66 (m, 2H), 2.35-2.31 (m, 2H), 2.29 (s, 3H) ppm; ^{13}C NMR (101 MHz, $CDCl_3$): δ 159.7, 154.6, 138.0, 137.0, 133.0, 132.8, 129.708, 129.687, 129.5, 127.2, 123.6, 118.6, 113.5, 41.6, 31.8, 31.3, 28.9, 25.4, 21.0 ppm. ESI-HRMS: m/z Calcd for $C_{21}H_{21}N_3O$ [M+H$^+$]: 331.1685, found 331.1687.

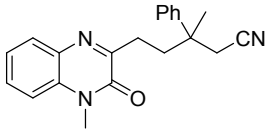


3-(4-(tert-butyl)phenyl)-5-(4-methyl-3-oxo-3,4-dihydroquinoxalin-2-yl)pentanenitrile ***(3ah)***.

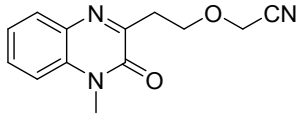
Yellow solid; (20.1 mg, 54%); mp: 155-157 °C; R_f = 0.20 (petroleum ether/ethyl acetate 3:1); ^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.84-7.81 (m, 1H), 7.54-7.50 (m, 1H), 7.36-7.28 (m, 4H), 7.20-7.18 (m, 2H), 3.66 (s, 3H), 3.16-3.09 (m, 1H), 2.88 (t, *J* = 8.0 Hz, 2H), 2.69-2.67 (m, 2H), 2.37-2.31 (m, 2H), 1.28 (s, 9H) ppm; ^{13}C NMR (101 MHz, $CDCl_3$): δ 159.7, 154.7, 150.2, 138.0, 133.0, 132.6, 129.7, 127.0, 125.7, 123.6, 118.7, 113.5, 41.4, 34.4, 31.8, 31.3, 31.1, 29.7, 28.9, 25.3 ppm. ESI-HRMS: m/z Calcd for $C_{24}H_{28}N_3O$ [M+H$^+$]: 374.2227, found 374.2229.



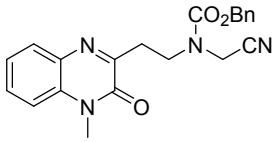
3-(4-chlorophenyl)-5-(4-methyl-3-oxo-3,4-dihydroquinoxalin-2-yl)pentanenitrile ***(3ai)***. Yellow solid; (13.6 mg, 39%); mp: 141-143 °C; R_f = 0.20 (petroleum ether/ethyl acetate 3:1); ^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.83-7.81 (m, 1H), 7.56-7.52 (m, 1H), 7.37-7.33 (m, 1H), 7.30-7.26 (m, 3H), 7.21-7.19 (m, 2H), 3.65 (s, 3H), 3.17-3.10 (m, 1H), 2.86 (t, *J* = 8.0 Hz, 2H), 2.69-2.66 (m, 2H), 2.35-2.28 (m, 2H) ppm; ^{13}C NMR (101 MHz, $CDCl_3$): δ 159.3, 154.6, 139.5, 133.2, 133.0, 132.5, 129.9, 129.7, 129.0, 128.8, 123.7, 118.1, 113.6, 41.4, 31.7, 31.2, 29.0, 25.2 ppm. ESI-HRMS: m/z Calcd for $C_{20}H_{18}ClN_3O$ [M+H$^+$]: 351.1138, found 351.1135.



3-methyl-5-(4-methyl-3-oxo-3,4-dihydroquinoxalin-2-yl)-3-phenylpentanenitrile ***(3aj)***. Yellow solid; (16.2 mg, 49%); mp: 129-131 °C; R_f = 0.35 (petroleum ether/ethyl acetate 3:1); ^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.81 (d, *J* = 8.0 Hz, 1H), 7.52 (t, *J* = 8.0 Hz, 1H), 7.39-7.24 (m, 6H), 7.20-7.17 (m, 1H), 3.63 (s, 3H), 2.86-2.65 (m, 4H), 2.53-2.45 (m, 1H), 2.28-2.21 (m, 1H), 1.66 (s, 3H) ppm; ^{13}C NMR (101 MHz, $CDCl_3$): δ 159.8, 154.6, 143.3, 133.0, 132.6, 129.7, 129.6, 128.6, 126.8, 125.9, 123.6, 118.1, 113.5, 40.1, 37.7, 31.9, 29.5, 28.9, 24.8 ppm. ESI-HRMS: m/z Calcd for $C_{21}H_{22}N_3O$ [M+H$^+$]: 332.1757, found 332.1755.

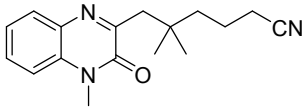


2-(2-(4-methyl-3-oxo-3,4-dihydroquinoxalin-2-yl)ethoxy)acetonitrile ***(3ak)***. Yellow solid; (10.9 mg, 45%); mp: 119-121 °C; R_f = 0.25 (petroleum ether/ethyl acetate 3:1); ^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.87-7.85 (m, 1H), 7.58-7.54 (m, 1H), 7.38-7.31 (m, 2H), 4.32 (s, 3H), 4.15 (t, *J* = 6.4 Hz, 2H), 3.71 (s, 3H), 2.82 (t, *J* = 5.6 Hz, 2H) ppm; ^{13}C NMR (101 MHz, $CDCl_3$): δ 157.1, 154.8, 133.2, 132.6, 130.1, 130.0, 123.7, 116.0, 113.7, 68.4, 56.2, 33.8, 29.1 ppm. ESI-HRMS: m/z Calcd for $C_{13}H_{14}N_3O_2$ [M+H$^+$]: 244.1081, found 244.1078.

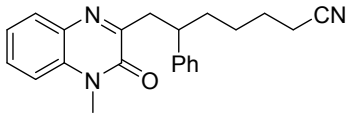


benzyl (cyanomethyl)(2-(4-methyl-3-oxo-3,4-dihydroquinoxalin-2-yl)ethyl)carbamate ***(3al)***. Yellow oil; (23.6 mg, 63%); R_f = 0.20 (petroleum ether/ethyl acetate 3:1); ^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.79 (d, *J* = 8.0 Hz, 1H), 7.55 (t, *J* = 8.0 Hz, 1H), 7.37-7.23 (m, 7H), 5.09-5.03 (m, 2H),

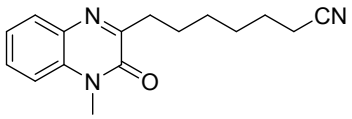
4.45-4.38 (m, 2H), 3.94 (t, J = 6.4 Hz, 1H), 3.68-3.58 (m, 3H), 3.29-3.23 (m, 2H) ppm; ^{13}C NMR (101 MHz, $CDCl_3$): δ 157.4, 155.6, 154.7, 135.6, 133.1, 132.3, 130.1, 129.6, 129.3, 128.5, 128.2, 128.0, 127.7, 123.7, 115.9, 113.7, 68.1, 45.2, 44.4, 36.2, 32.8, 32.5, 28.9 ppm. ESI-HRMS: m/z Calcd for $C_{21}H_{20}N_4O_3$ [M+H$^+$]: 376.1535, found 376.1539.



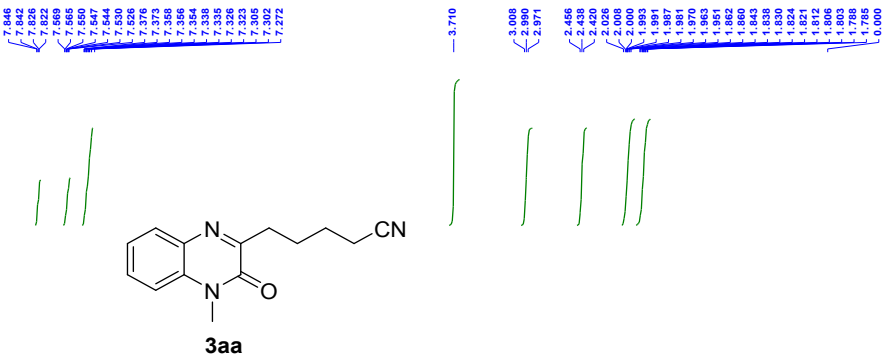
*5,5-dimethyl-6-(4-methyl-3-oxo-3,4-dihydroquinoxalin-2-yl)hexanenitrile (**3am**)*. Yellow oil; (16.2 mg, 57%); R_f = 0.25 (petroleum ether/ethyl acetate 3:1); ^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.85-7.83 (m, 1H), 7.56-7.52 (m, 1H), 7.37-7.32 (m, 1H), 7.31-7.29 (m, 1H), 3.70 (s, 3H), 2.92 (s, 2H), 2.36 (t, J = 7.2 Hz, 2H), 1.85-1.79 (m, 2H), 1.53-1.48 (m, 2H), 1.04 (s, 6H) ppm; ^{13}C NMR (101 MHz, $CDCl_3$): δ 159.5, 155.5, 133.1, 132.5, 129.915, 129.872, 123.6, 119.9, 113.6, 42.4, 41.0, 29.3, 27.5, 20.6, 17.9 ppm. ESI-HRMS: m/z Calcd for $C_{17}H_{22}N_3O$ [M+H$^+$]: 284.1757, found 284.1756.



*7-(4-methyl-3-oxo-3,4-dihydroquinoxalin-2-yl)-6-phenylheptanenitrile (**3an**)*.Yellow oil; (14.5 mg, 42%); R_f = 0.45 (petroleum ether/ethyl acetate 3:1); ^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.80 (t, J = 8.0 Hz, 1H), 7.51 (t, J = 8.0 Hz, 1H), 7.33 (t, J = 8.0 Hz, 1H), 7.28-7.24 (m, 5H), 7.18-7.13 (m, 1H), 3.67 (s, 3H), 3.49-3.41 (m, 1H), 3.32-3.19 (m, 2H), 2.31-2.18 (m, 2H), 1.81-1.70 (m, 2H), 1.68-1.55 (m, 2H), 1.39-1.25 (m, 3H) ppm; ^{13}C NMR (101 MHz, $CDCl_3$): δ 159.2, 155.0, 144.4, 133.0, 132.6, 129.749, 129.695, 128.4, 127.8, 126.3, 123.6, 119.8, 113.6, 42.5, 41.0, 35.1, 29.1, 26.6, 25.4, 17.0 ppm. ESI-HRMS: m/z Calcd for $C_{22}H_{24}N_3O$ [M+H$^+$]: 346.1914, found 346.1911.



*7-(4-methyl-3-oxo-3,4-dihydroquinoxalin-2-yl)heptanenitrile (**3ao**)*. Yellow oil; (6.8 mg, 23%); R_f = 0.26 (petroleum ether/ethyl acetate 3:1); ^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.76 (s, 1H), 7.34-7.27 (m, 1H), 7.14 (d, J = 7.6 Hz, 1H), 3.50 (s, 3H), 1.71-1.53 (m, 8H), 1.48-1.43 (m, 2H), 1.27-1.24 (m, 2H) ppm; ^{13}C NMR (101 MHz, $CDCl_3$): δ 163.6, 159.8, 153.1, 142.6, 129.3, 128.0, 127.2, 108.4, 37.1, 32.9, 25.2, 23.7 ppm. ESI-HRMS: m/z Calcd for $C_{17}H_{22}N_3O$ [M+H$^+$]: 270.1601, found 270.1605.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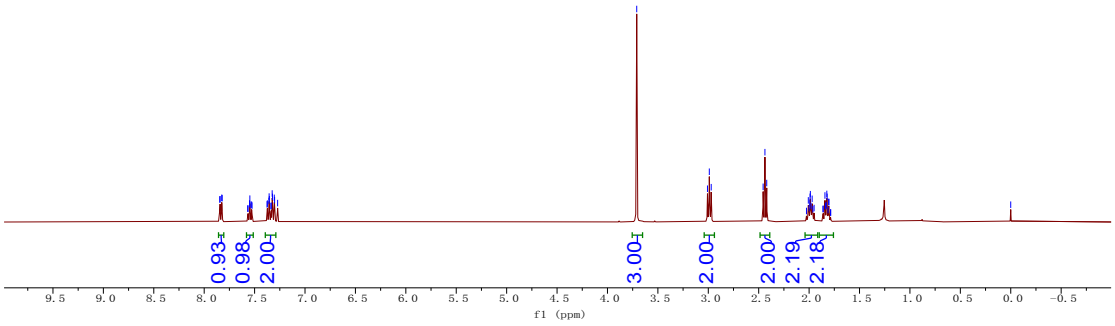
3aa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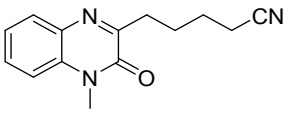
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CN
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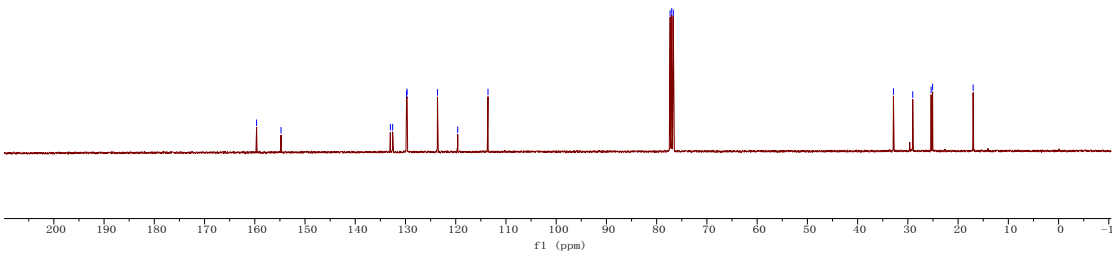
3aa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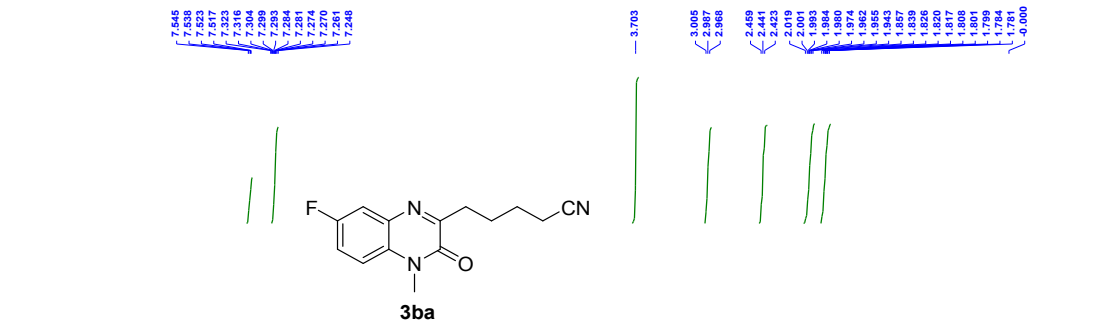
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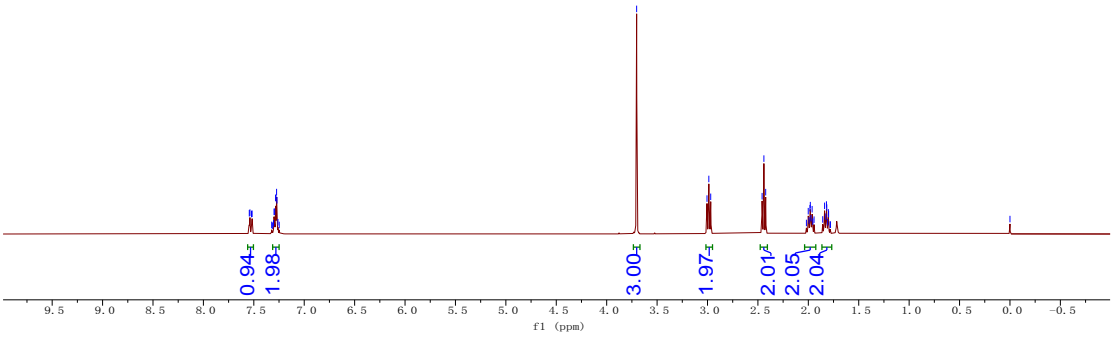
3ba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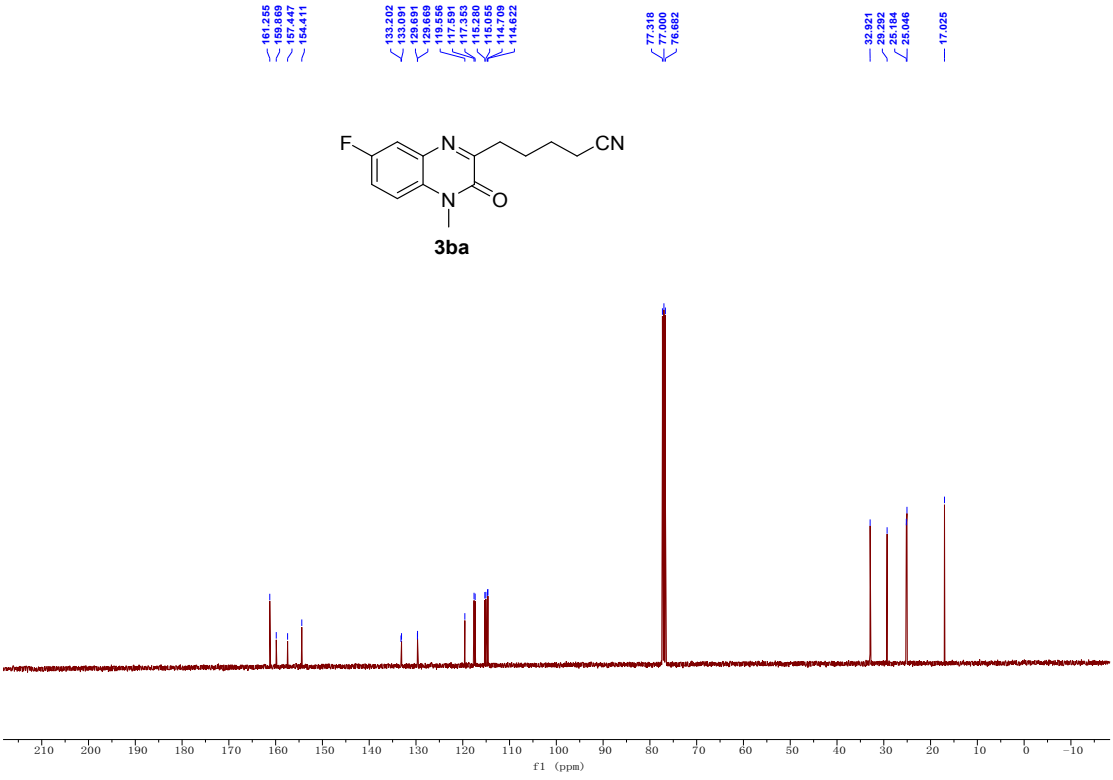
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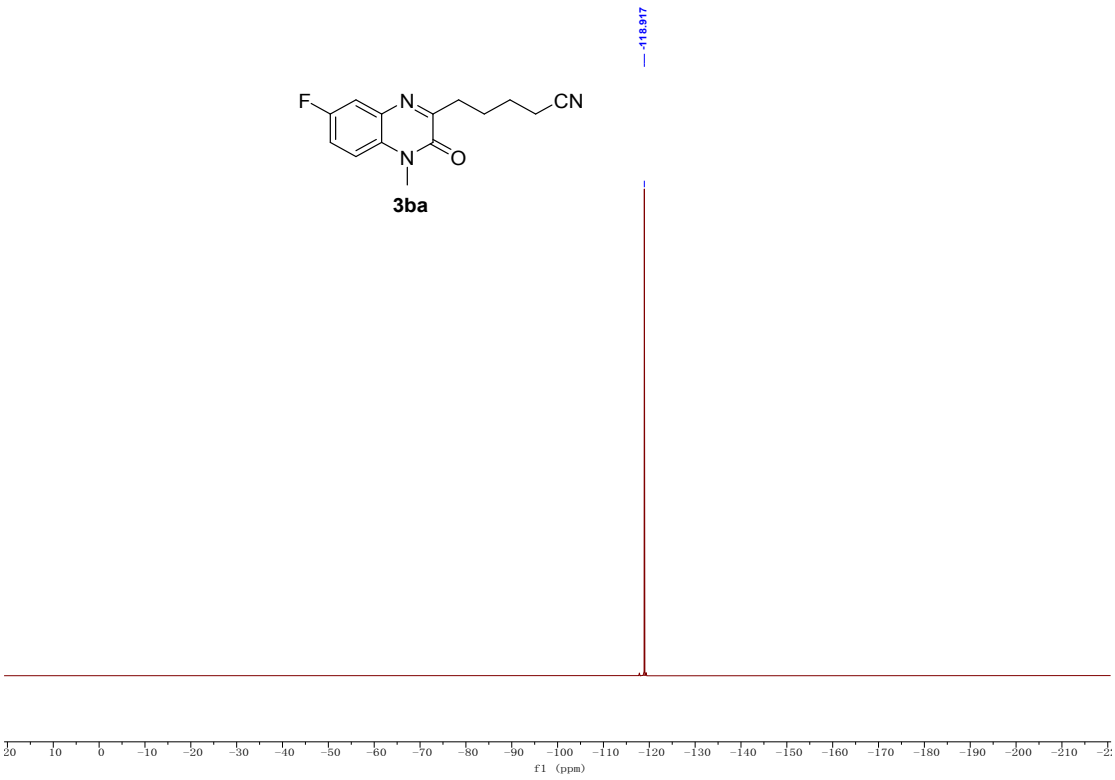
O
f1 (ppm)

3ba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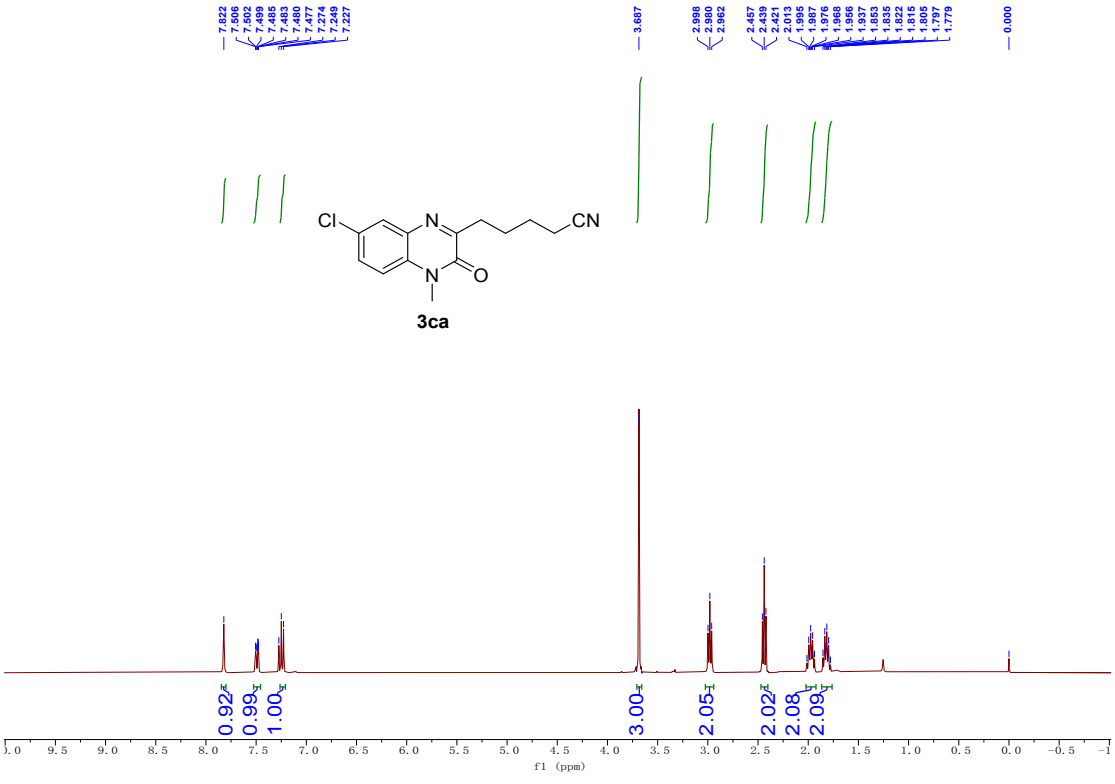
f1 (ppm)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CN
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3.00
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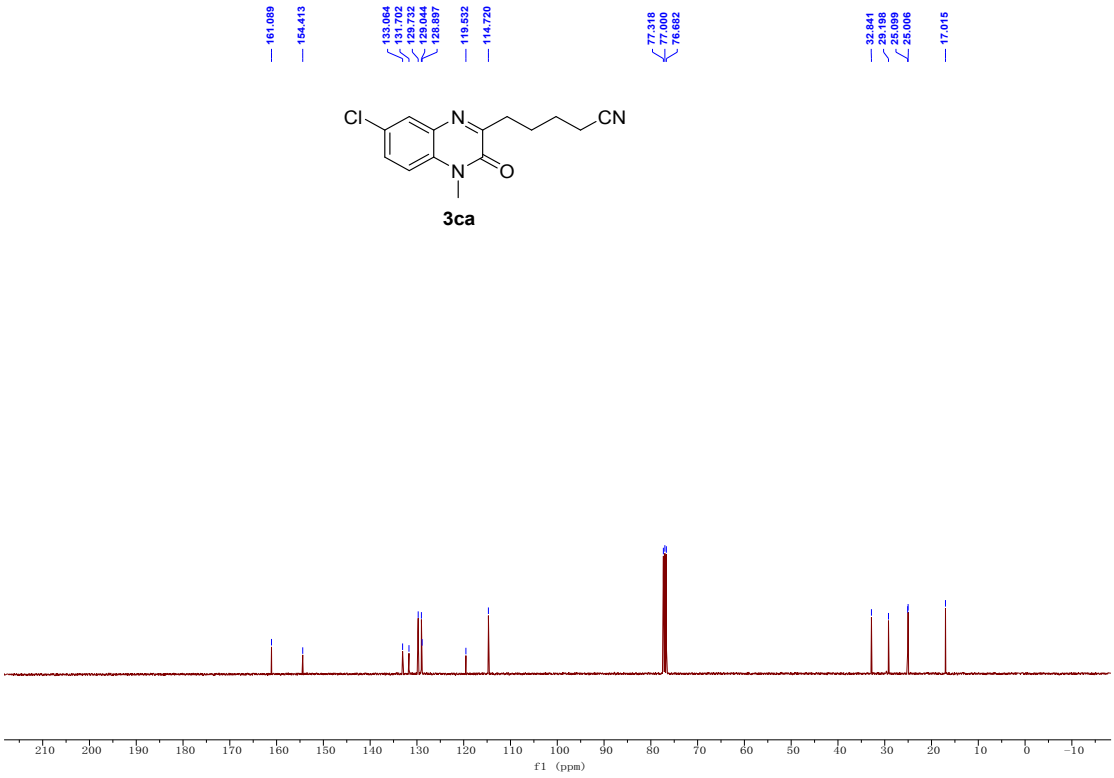
2.08
2.09
f1 (ppm)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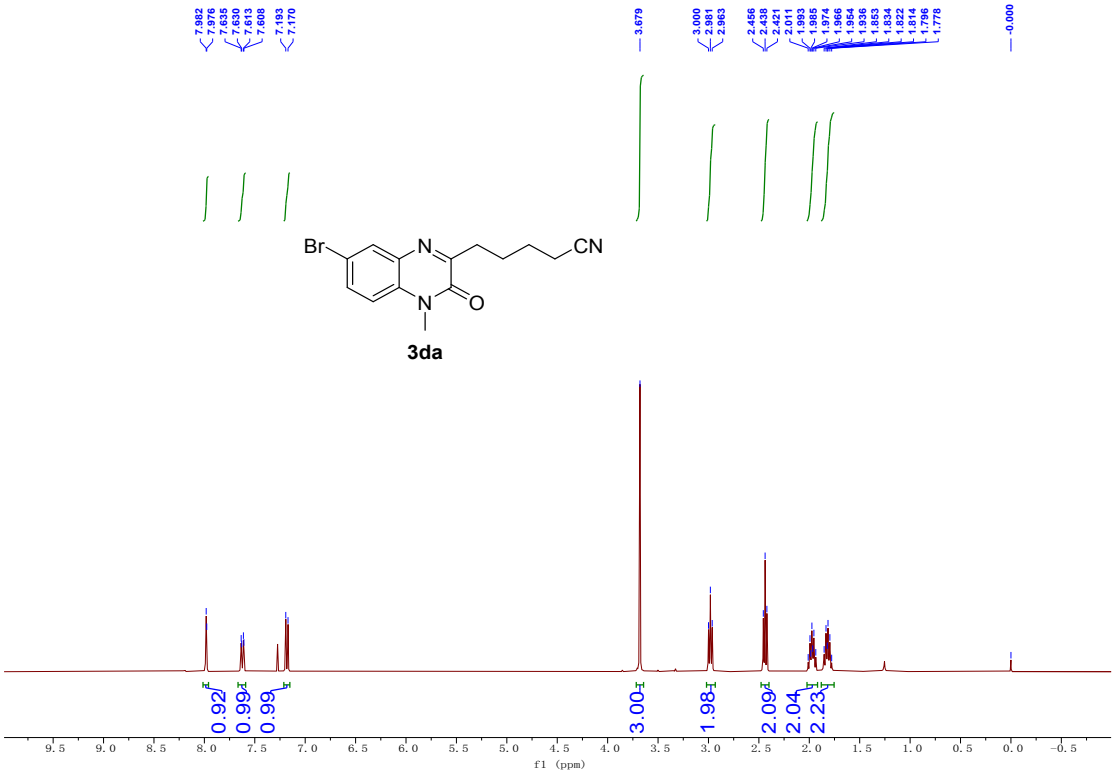
154.413
133.064
131.702
129.732
129.044
128.897
119.532
114.720
77.318
77.000
76.682
32.841
29.195
25.099
25.006
17.015
Cl
N
CN
N
O
3ca
f1 (ppm)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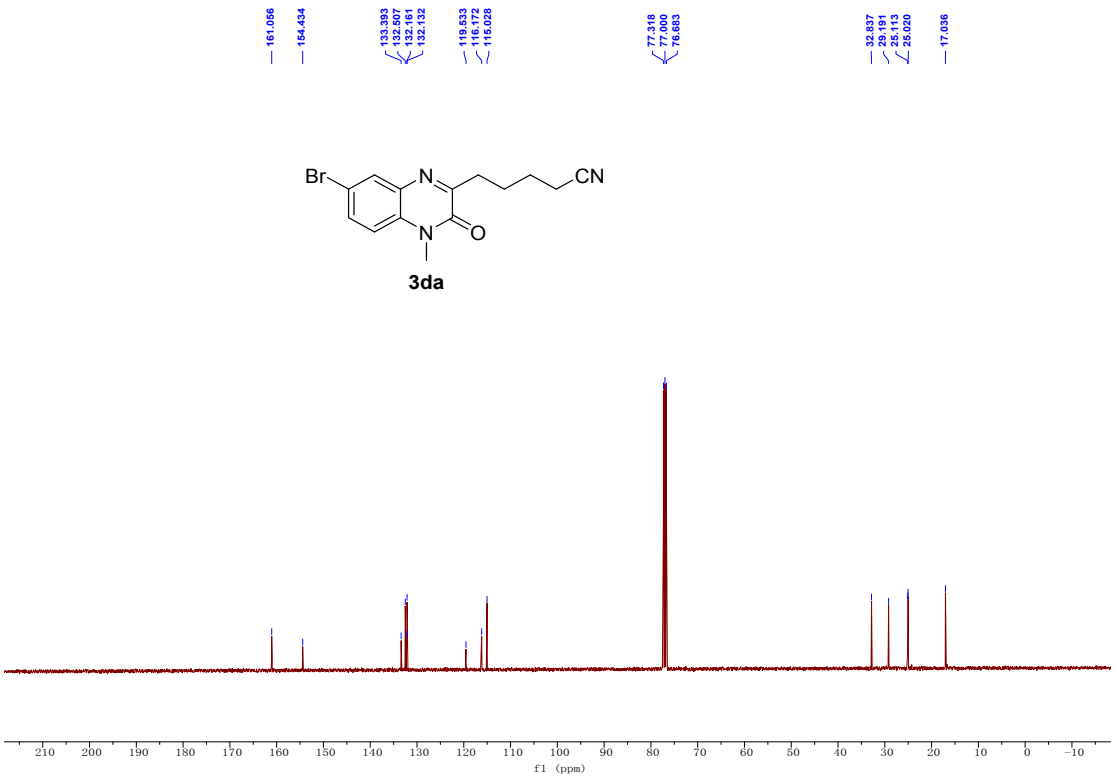
7.976
7.635
7.630
7.613
7.608
7.193
7.170
3.679
3.000
2.981
2.963
2.466
2.438
2.421
2.011
1.993
1.985
1.974
1.966
1.954
1.936
1.853
1.834
1.822
1.814
1.796
1.778
-0.000
Br
N
CN
N
O
3da
0.92
0.99
0.99
3.00
1.98
2.09
2.04
2.23
f1 (ppm)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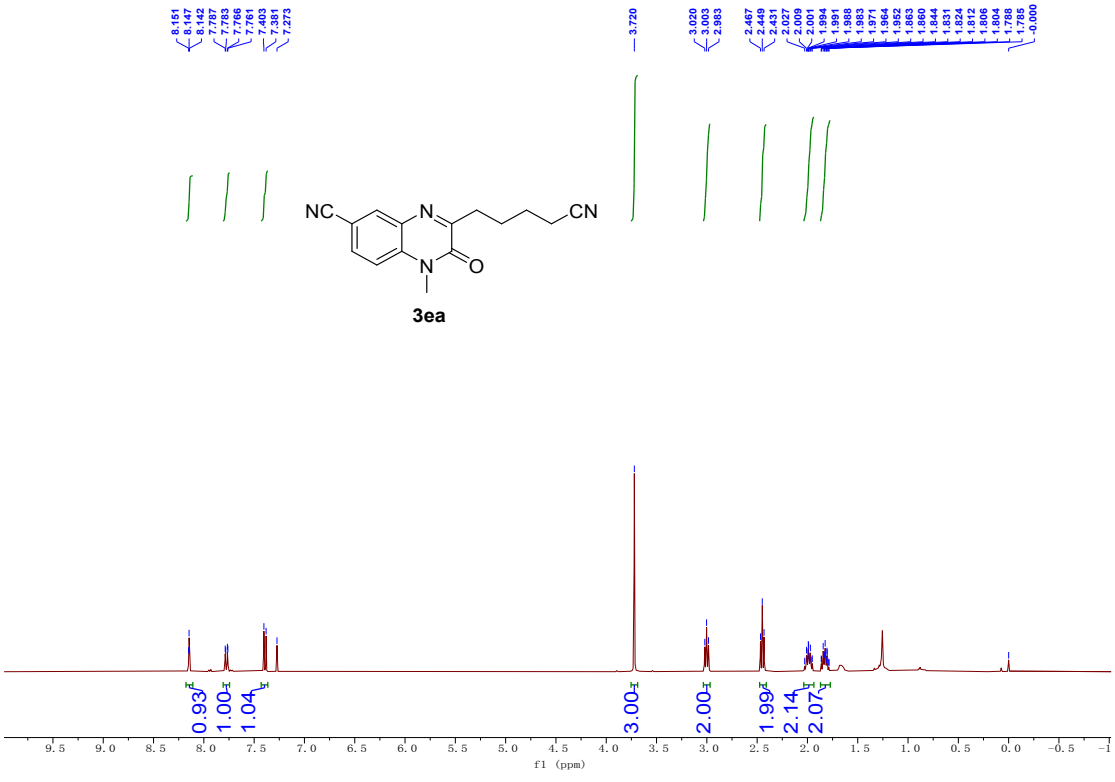
154.434
133.393
132.507
132.161
132.152
119.533
116.172
115.028
77.318
77.000
76.683
32.637
29.191
25.113
25.020
17.036
Br
N
CN
N
O
3da
f1 (ppm)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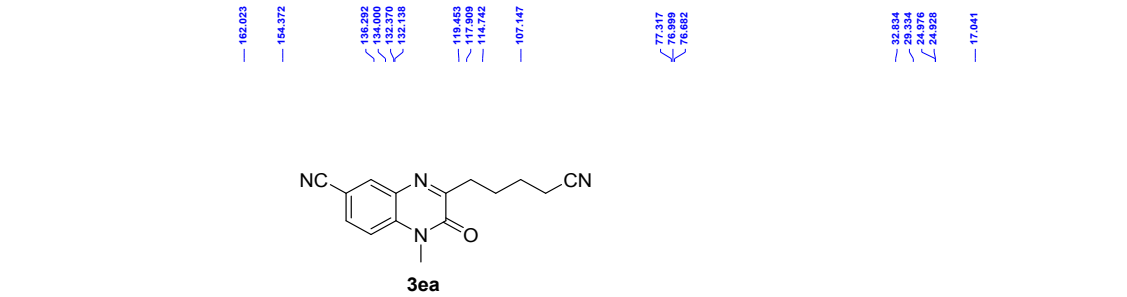
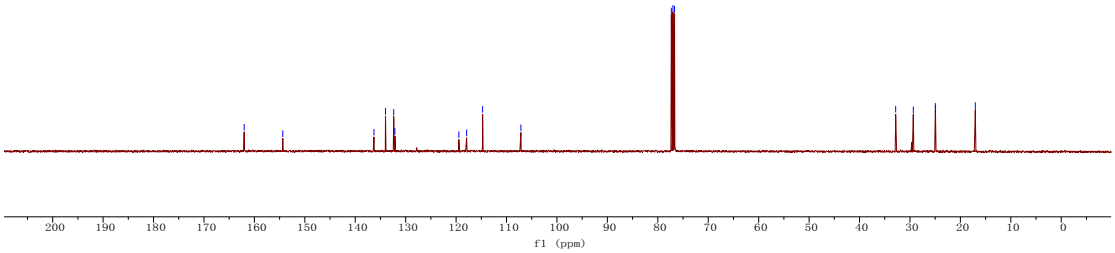
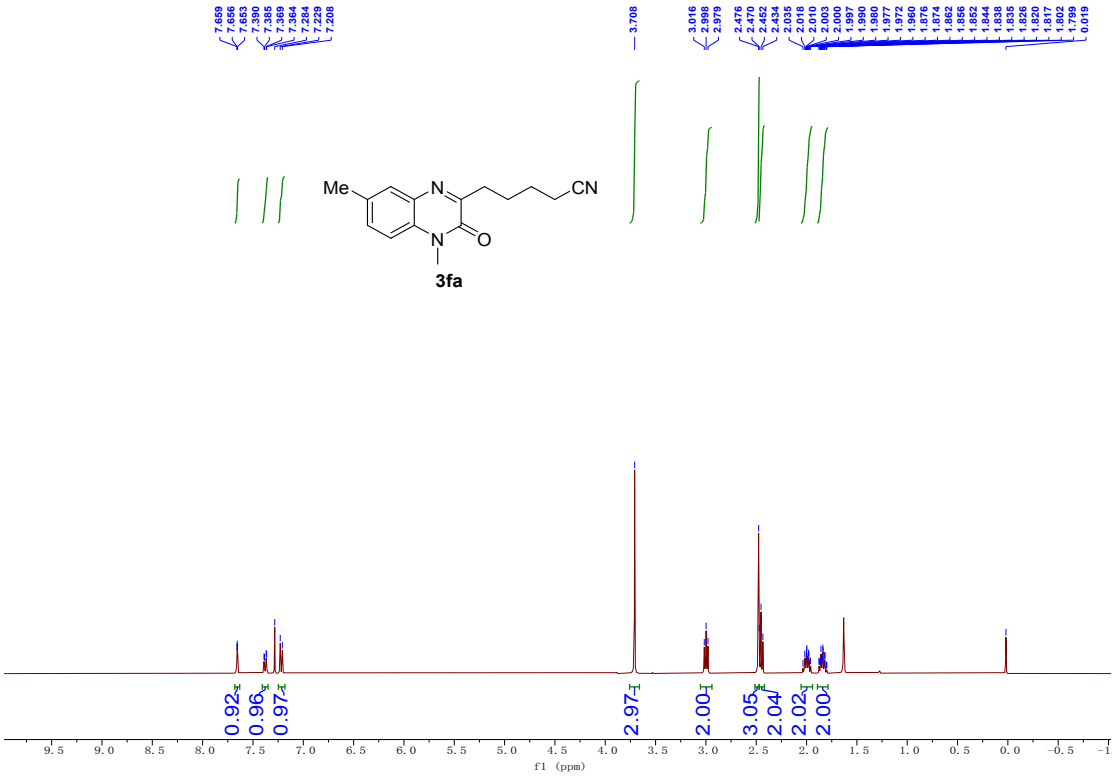
8.147
8.142
7.787
7.783
7.766
7.761
7.403
7.381
7.273
3.720
3.020
3.003
2.983
2.467
2.449
2.431
2.077
2.009
2.001
1.994
1.991
1.988
1.983
1.971
1.964
1.952
1.863
1.860
1.844
1.831
1.824
1.812
1.806
1.804
1.798
1.785
-0.000
NC
N
CN
N
O
3ea
0.93
1.00
1.04
3.00
2.00
1.99
2.14
2.07
f1 (ppm)


162.023
154.372
136.292
134.000
132.370
132.138
119.453
117.909
114.742
107.147
77.317
76.999
76.682
32.834
29.334
24.976
24.928
17.041
NC
N
CN
N
O

3ea


200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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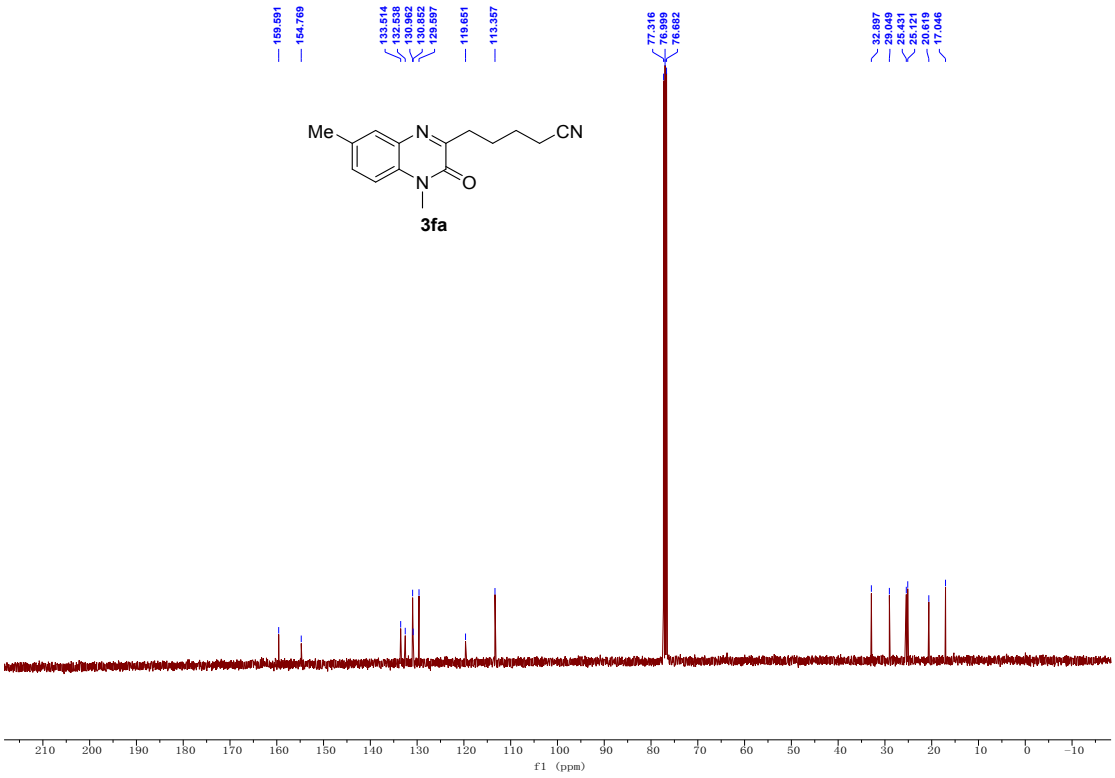
7.656
7.653
7.390
7.385
7.369
7.364
7.284
7.229
7.208
3.708
3.016
2.998
2.979
2.476
2.470
2.462
2.434
2.035
2.018
2.010
2.003
2.000
1.997
1.990
1.980
1.977
1.972
1.960
1.876
1.874
1.862
1.856
1.852
1.844
1.838
1.835
1.826
1.820
1.817
1.802
1.799
0.019
Me
N
CN
N
O
0.92
0.96
0.97
2.97
2.00
3.05
2.04
2.02
2.00
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1
f1 (ppm)

3fa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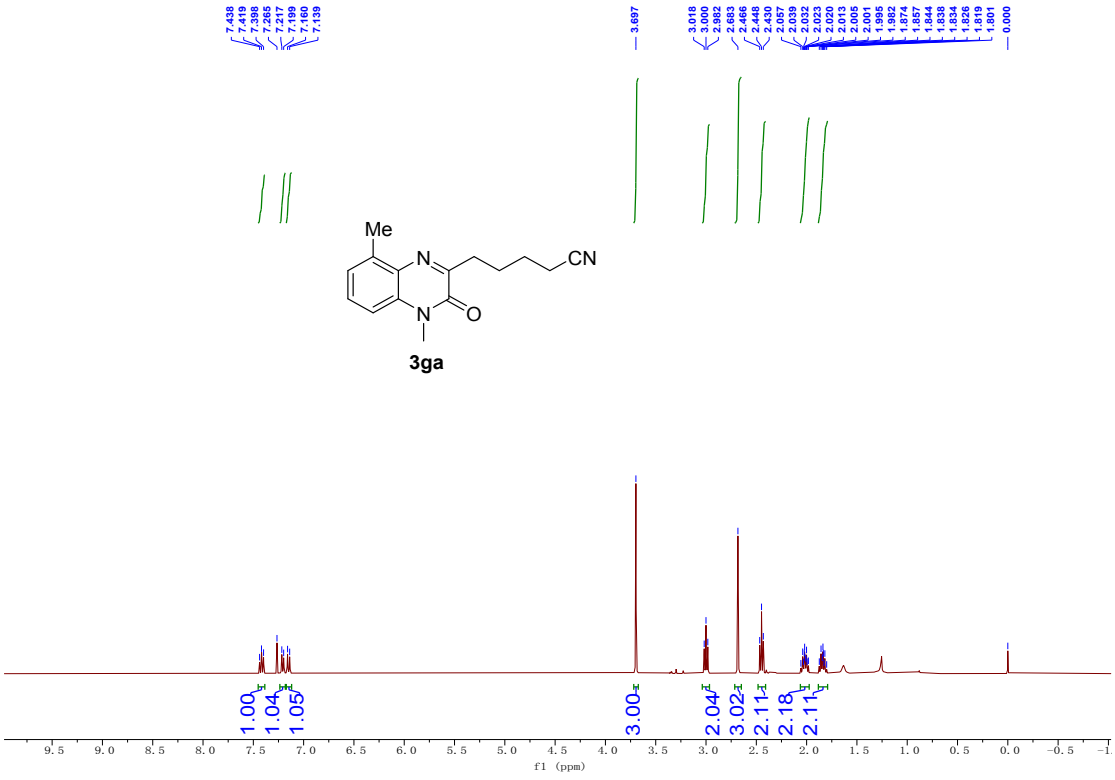
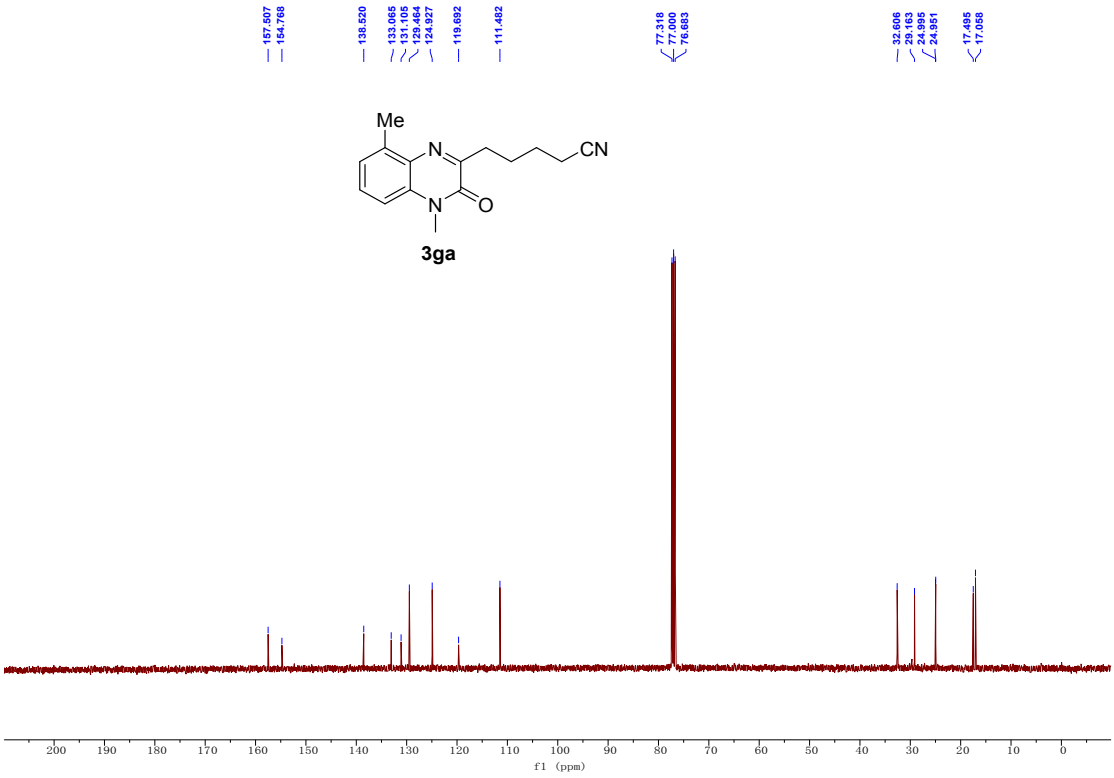
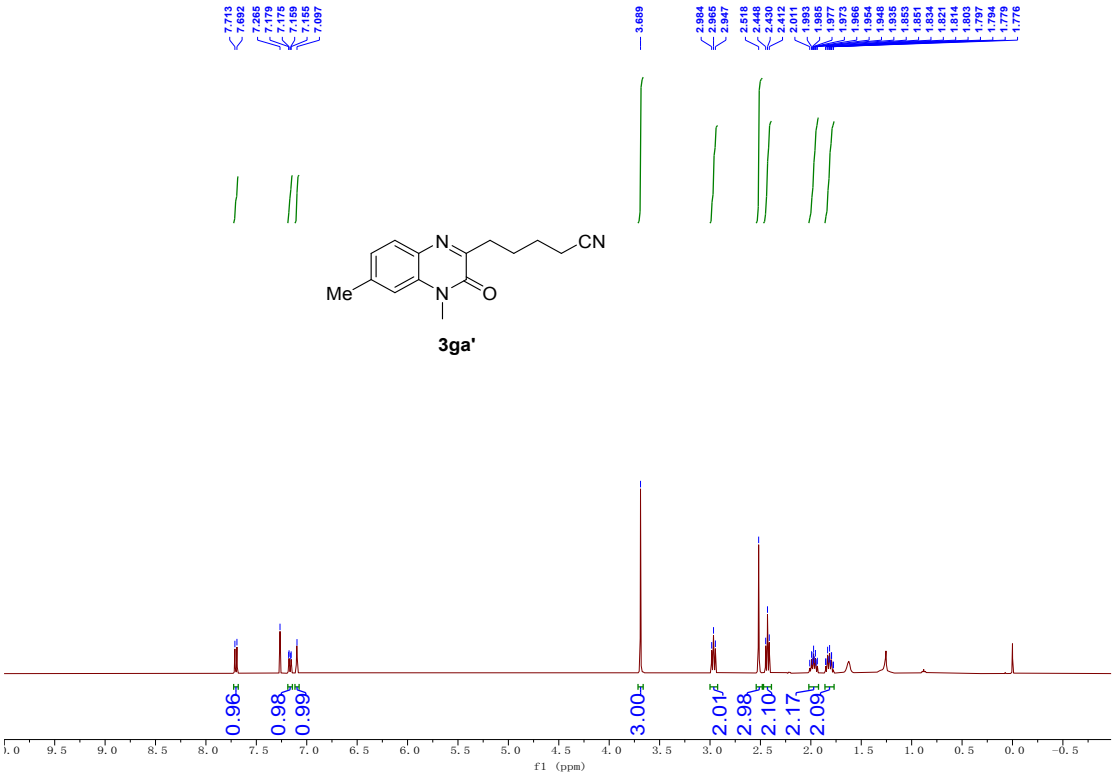
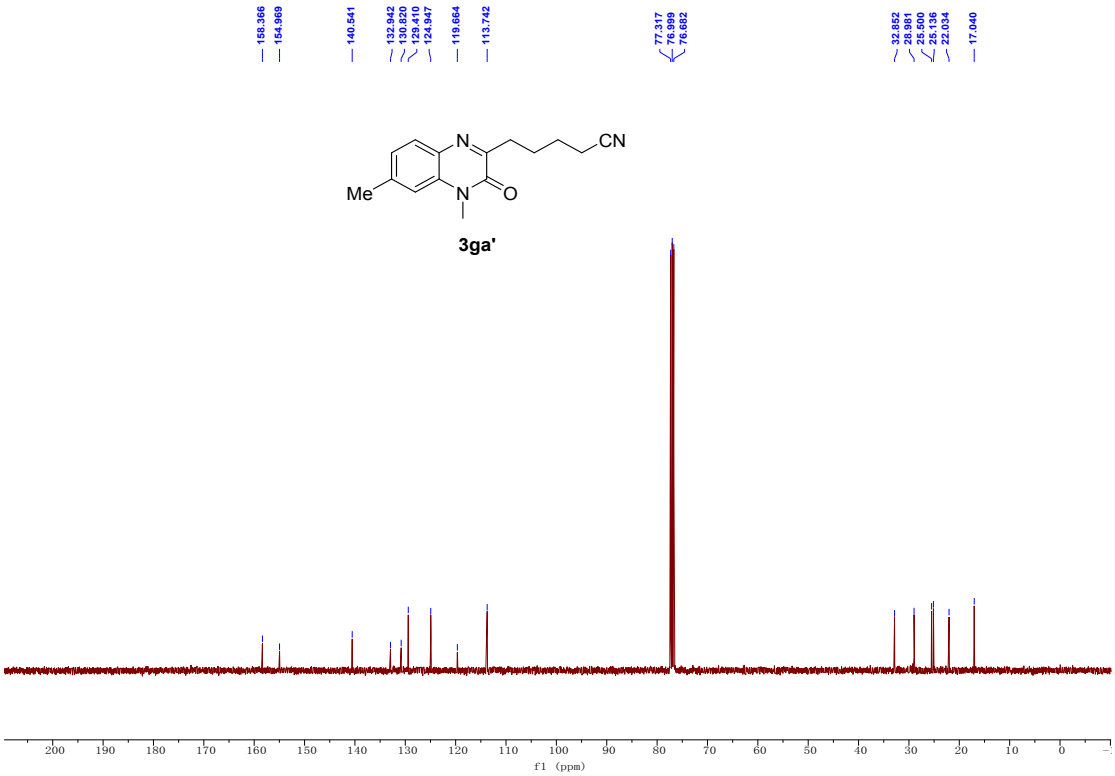
154.769
133.514
132.538
130.862
130.552
129.597
119.651
113.357
77.316
76.999
76.682
32.897
29.049
25.431
25.121
20.159
17.046
Me
N
CN
N
O
3fa
f1 (ppm)


7.438
7.419
7.398
7.255
7.217
7.199
7.160
7.139
3.697
3.018
3.000
2.982
2.683
2.466
2.448
2.430
2.057
2.039
2.032
2.023
2.020
2.015
2.005
2.001
1.995
1.982
1.874
1.857
1.844
1.838
1.834
1.826
1.819
1.801
0.000
Me
N
CN
N
O
3ga
1.00
1.04
1.05
3.00
2.04
3.02
2.11
2.18
2.11
f1 (ppm)


157.507
154.768
138.520
133.065
131.105
129.464
124.927
119.692
111.482
77.318
77.000
76.683
32.606
29.163
24.995
24.951
17.495
17.058
Me
N
CN
N
O
3ga
f1 (ppm)


7.713
7.692
7.266
7.179
7.175
7.159
7.155
7.097
3.689
2.984
2.965
2.947
2.518
2.448
2.430
2.412
2.011
1.993
1.986
1.977
1.973
1.966
1.954
1.948
1.935
1.853
1.851
1.834
1.821
1.814
1.803
1.797
1.794
1.779
1.776
N
CN
Me
N
O
3ga'
0.96
0.98
0.99
3.00
2.01
2.98
2.10
2.17
2.09
f1 (ppm)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130.820
129.410
124.947
119.664
113.742
77.317
76.999
76.682
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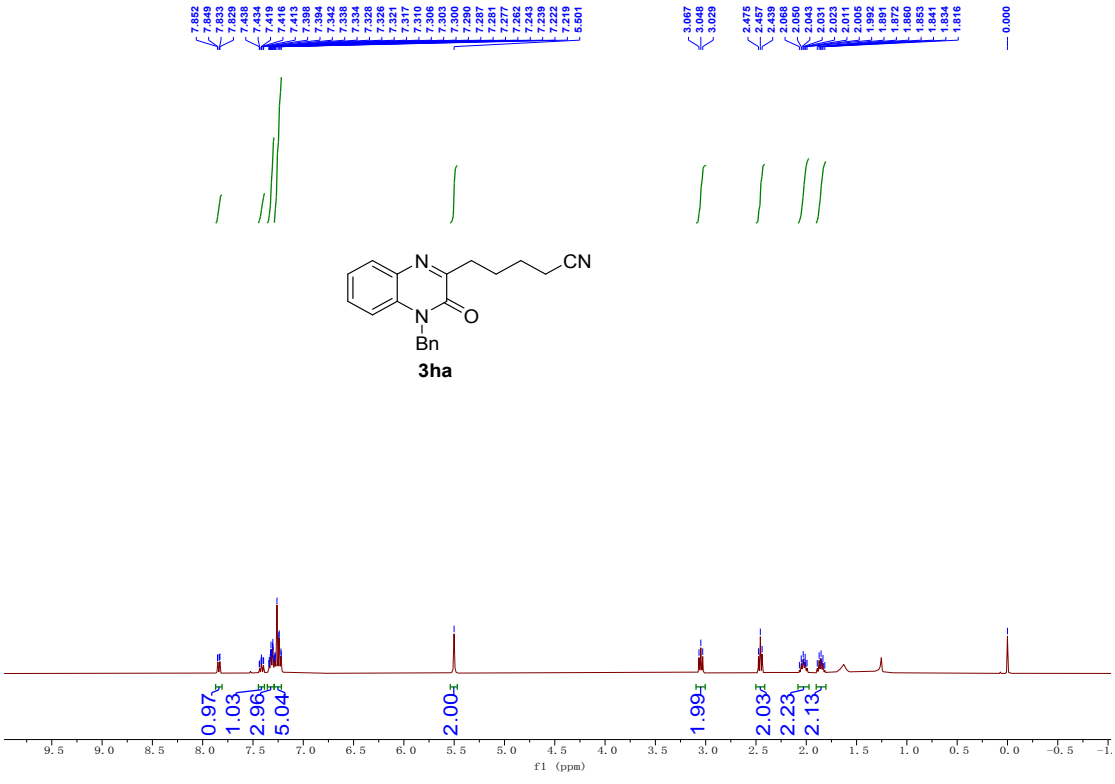
25.500
25.136
22.034
17.040
N
CN
Me
N
O
f1 (ppm)

3ga'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7.833
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7.438
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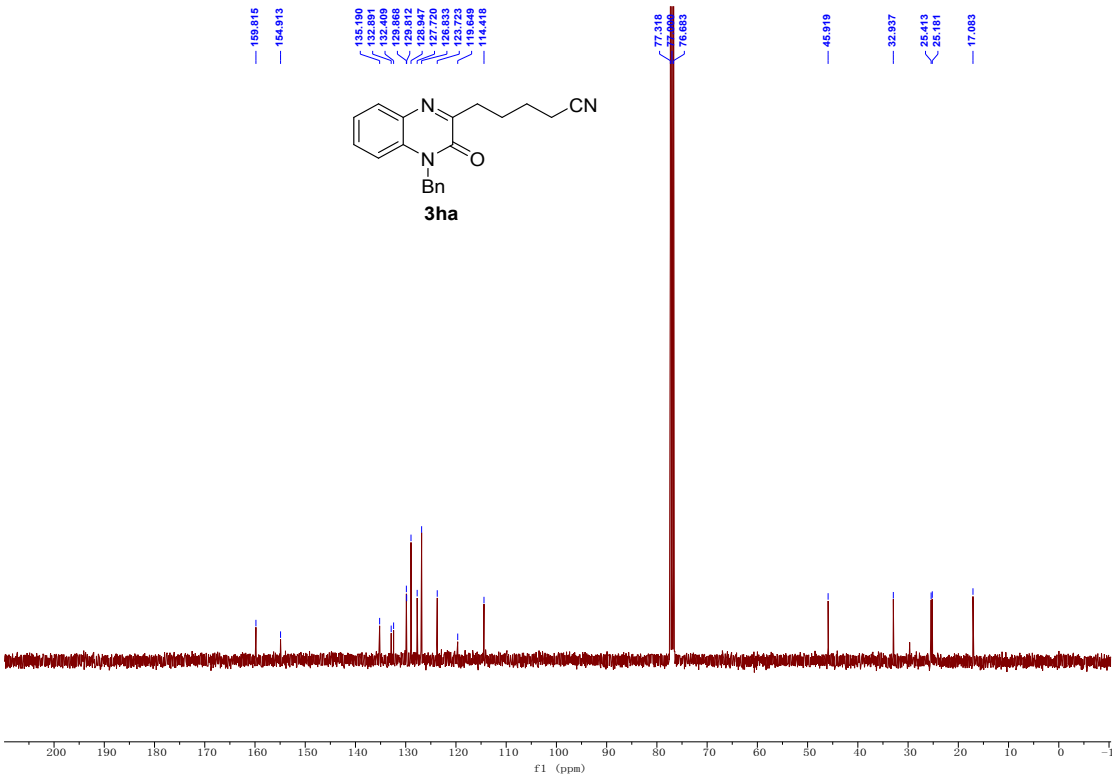
7.419
7.416
7.413
7.398
7.394
7.342
7.338
7.334
7.328
7.326
7.321
7.317
7.310
7.306
7.303
7.300
7.290
7.287
7.281
7.277
7.262
7.243
7.239
7.222
7.219
6.501
3.067
3.048
3.029
2.475
2.457
2.439
2.068
2.050
2.043
2.031
2.023
2.011
2.005
1.892
1.891
1.872
1.860
1.853
1.841
1.834
1.816
0.000
N
CN
N
O
Bn
0.97
1.03
2.96
5.04
2.00
1.99
2.03
2.23
2.13
f1 (ppm)

3ha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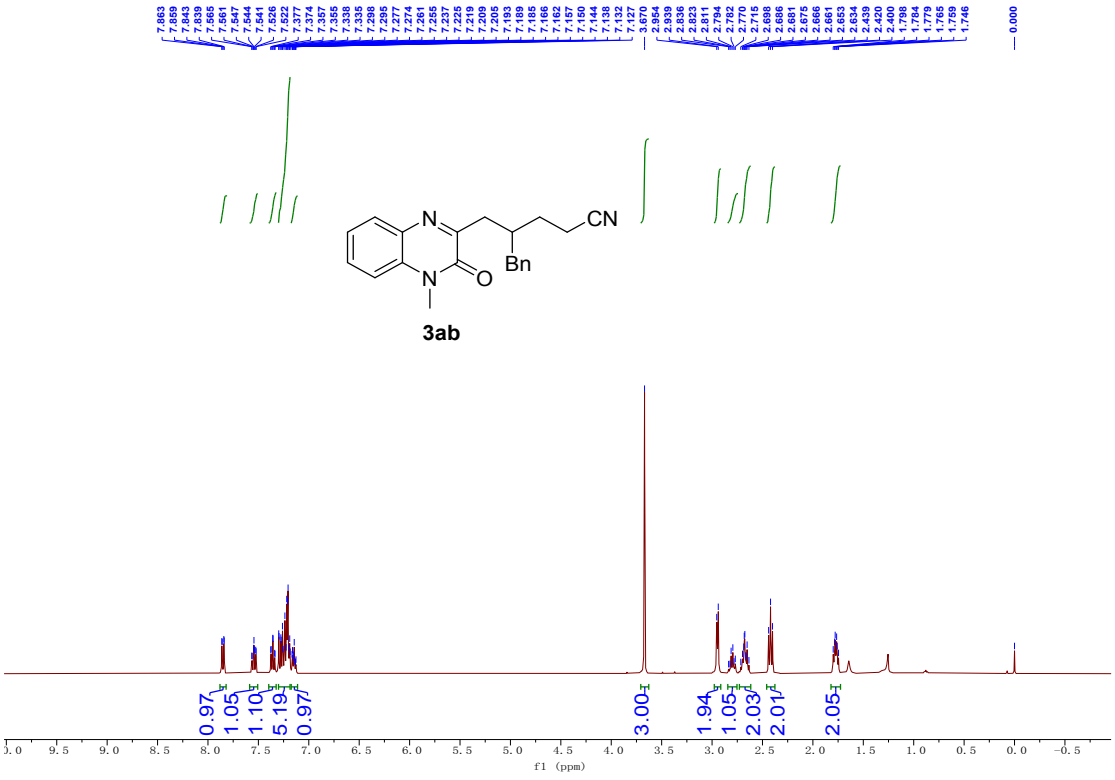
154.913
135.190
132.891
132.409
129.868
129.512
128.947
127.720
126.833
123.723
119.649
114.418
77.318
77.000
76.683
45.919
32.937
25.413
25.181
17.083
N
CN
N
O
Bn
f1 (ppm)

3ha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7.544
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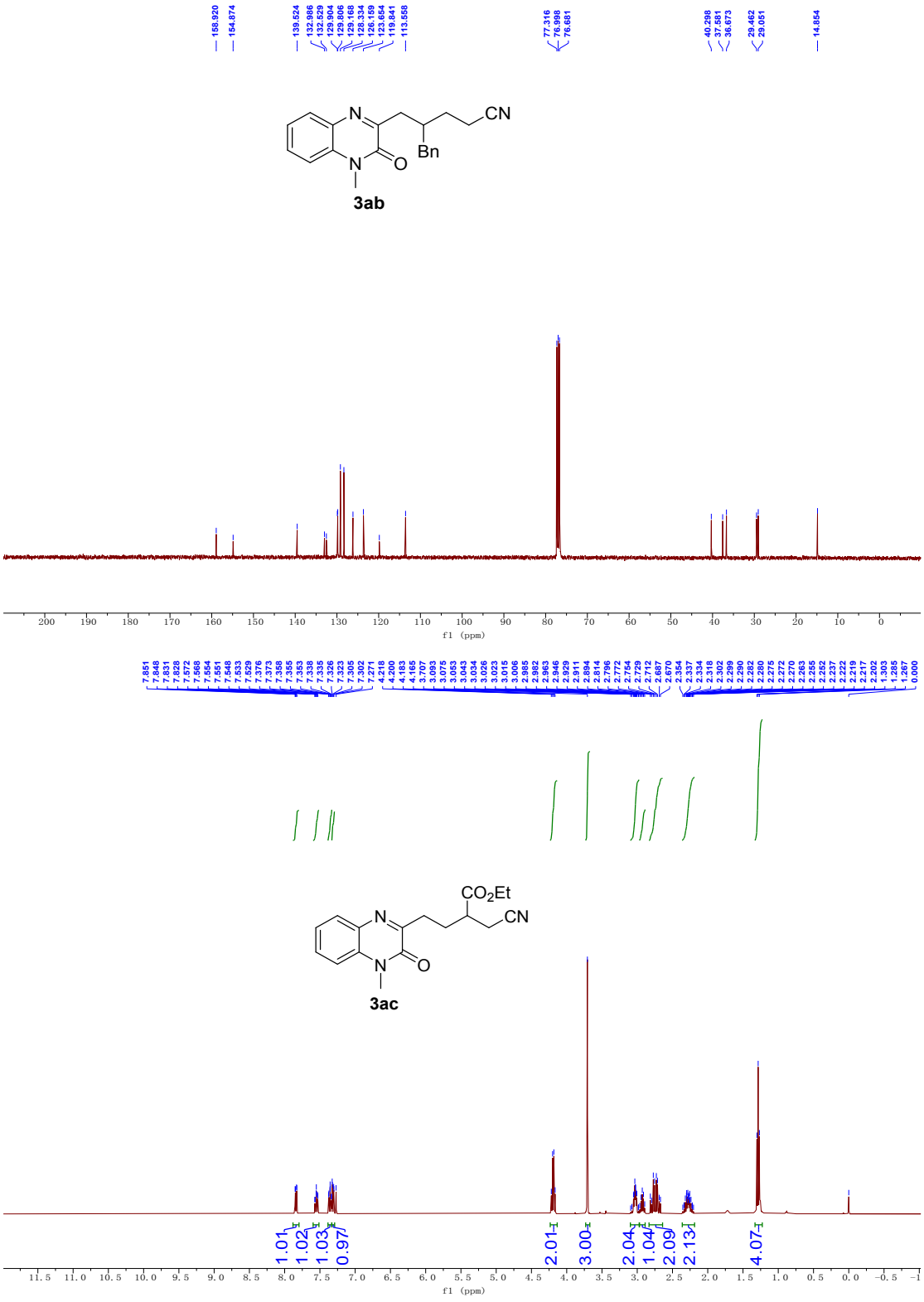
7.526
7.522
7.377
7.374
7.357
7.355
7.338
7.335
7.298
7.296
7.277
7.274
7.261
7.255
7.237
7.225
7.219
7.209
7.205
7.193
7.189
7.185
7.166
7.162
7.157
7.160
7.144
7.138
7.132
7.127
3.670
2.954
2.939
2.836
2.823
2.811
2.794
2.782
2.770
2.715
2.698
2.686
2.681
2.675
2.666
2.661
2.653
2.634
2.439
2.420
2.400
1.798
1.784
1.779
1.765
1.759
1.746
0.000
N
CN
Bn
N
O
0.97
1.05
1.10
5.19
0.97
3.00
1.94
1.05
2.03
2.01
2.05
f1 (ppm)

3ab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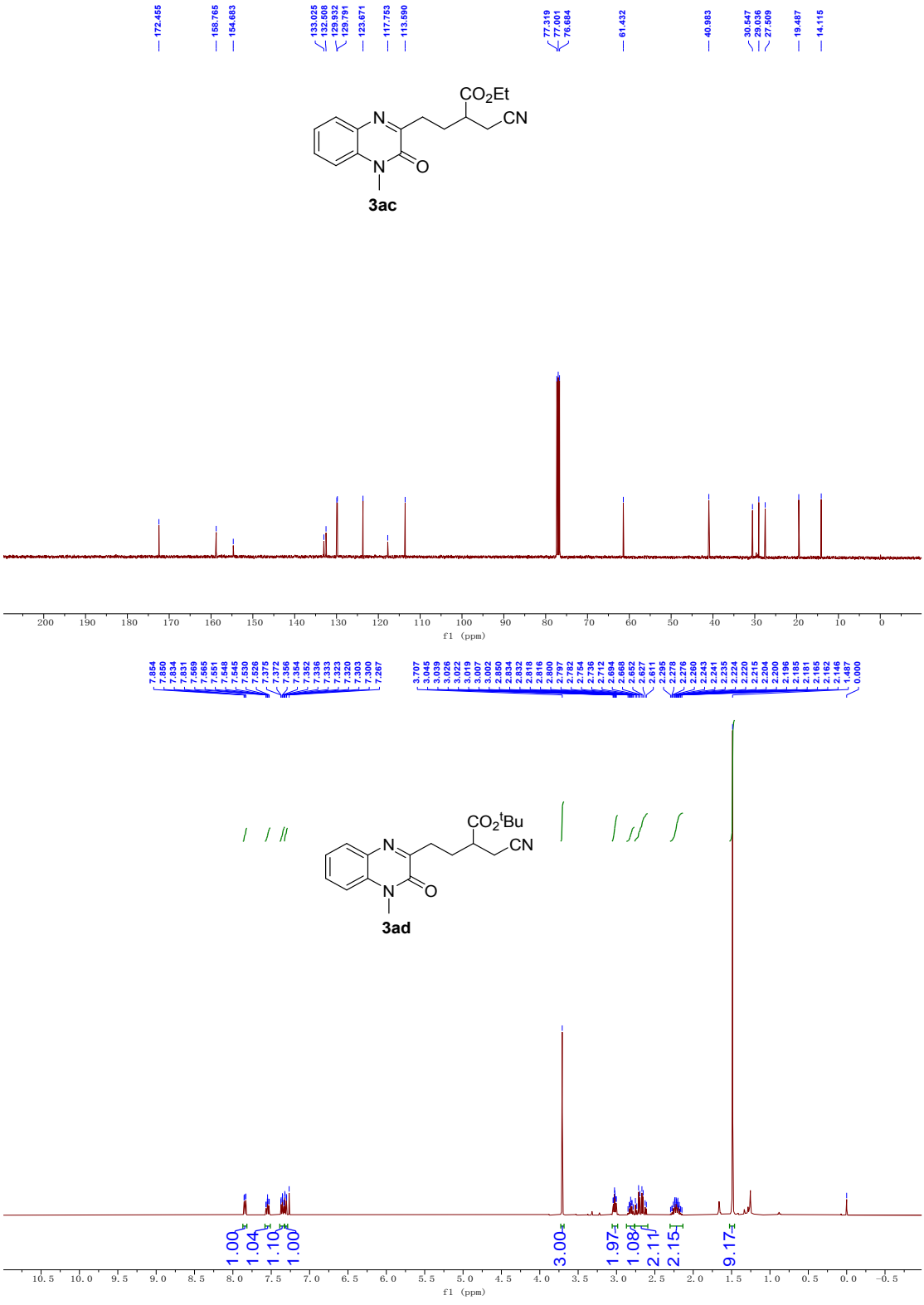
113.558
77.316
76.998
76.681
40.236
37.681
36.673
29.462
29.051
14.854
N
CN
Bn
N
O
3ab
f1 (ppm)
7.851
7.848
7.831
7.828
7.572
7.568
7.554
7.551
7.548
7.533
7.529
7.376
7.373
7.368
7.355
7.353
7.338
7.335
7.326
7.323
7.305
7.302
7.271
4.218
4.200
4.183
4.165
3.707
3.093
3.075
3.055
3.043
3.034
3.026
3.023
3.015
3.006
2.985
2.982
2.963
2.946
2.929
2.911
2.894
2.814
2.796
2.772
2.754
2.729
2.712
2.687
2.670
2.354
2.337
2.334
2.316
2.302
2.299
2.290
2.282
2.280
2.275
2.272
2.270
2.265
2.255
2.252
2.237
2.222
2.219
2.217
2.202
1.303
1.285
1.267
0.000
CO2Et
CN
N
O
3ac
1.01
1.02
1.03
0.97
2.01
3.00
2.04
1.04
2.09
2.13
4.07
f1 (ppm)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113.590
77.319
77.001
76.684
61.432
40.983
30.547
29.038
27.509
19.487
14.115
CO2Et
CN
N
N
O
3ac
f1 (ppm)
CO2tBu
CN
N
N
O
3ad
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1.04
1.10
1.00
3.00
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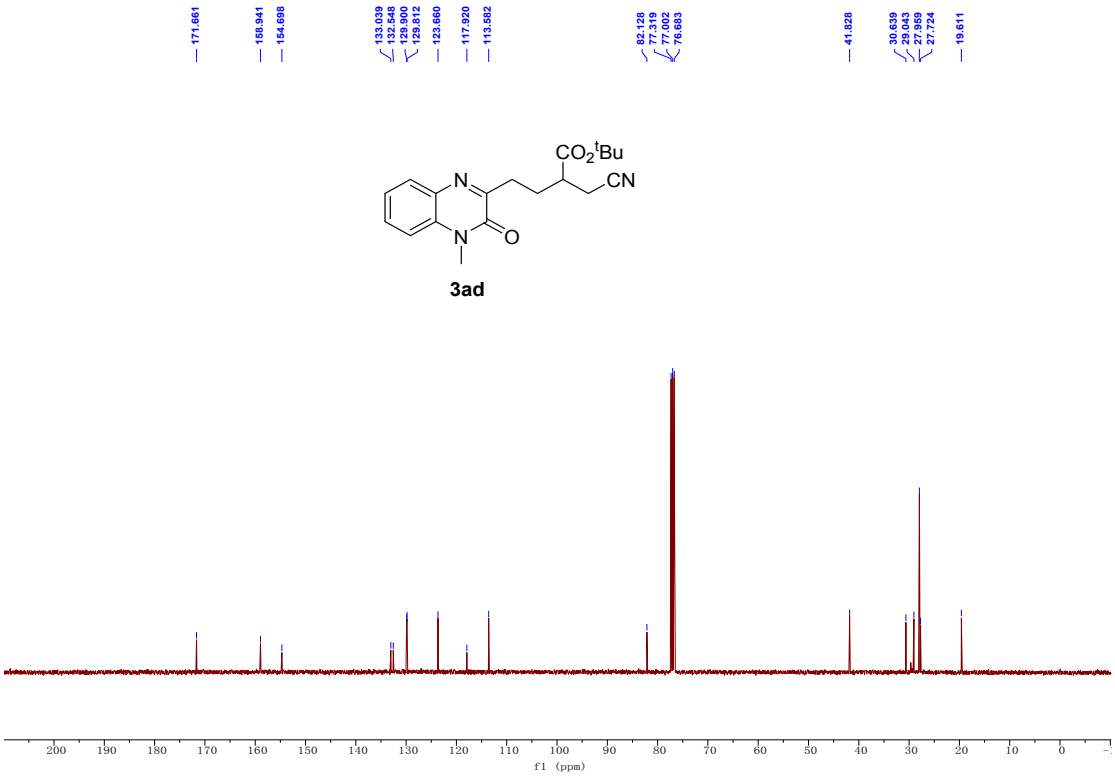
1.08
2.11
2.15
9.17
f1 (ppm)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129.812
123.660
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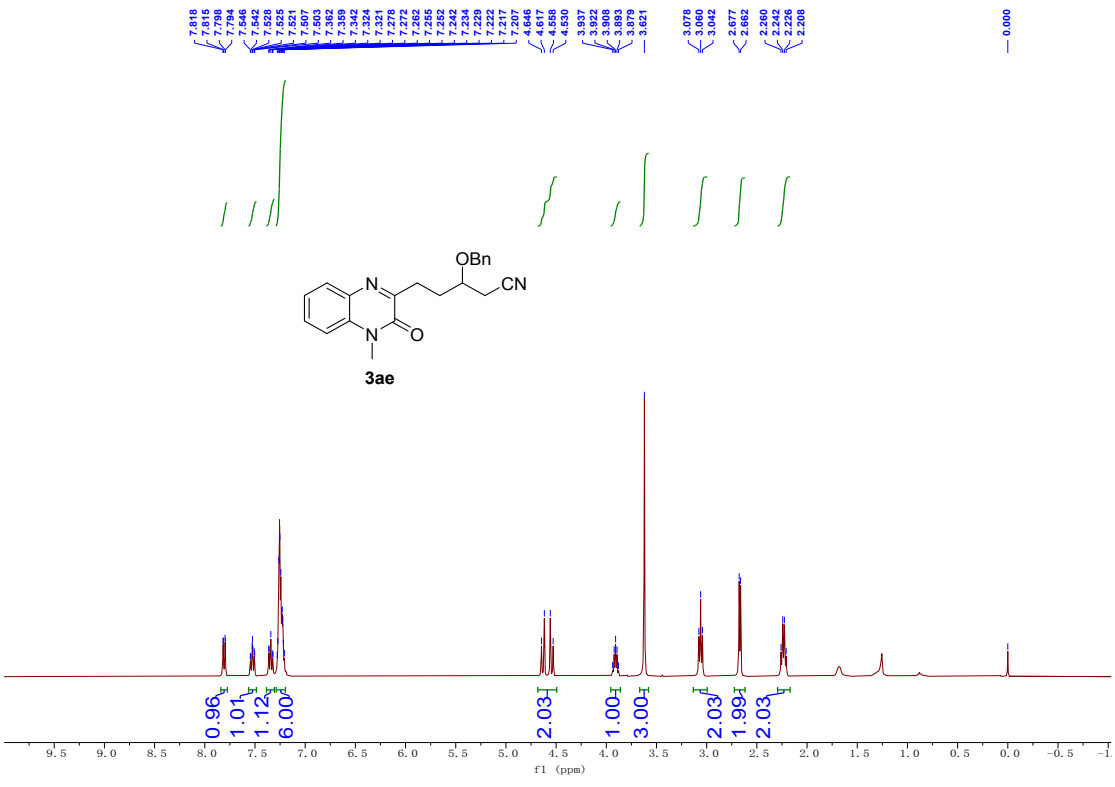
113.582
82.128
77.319
77.002
76.683
41.828
30.639
29.043
27.959
27.724
19.611
CO2tBu
CN
N
N
O
3ad
f1 (ppm)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7.535
7.521
7.507
7.503
7.362
7.359
7.342
7.334
7.321
7.278
7.272
7.262
7.255
7.252
7.242
7.234
7.229
7.222
7.217
7.207
4.646
4.617
4.558
4.530
3.937
3.922
3.908
3.893
3.879
3.621
3.078
3.060
3.042
2.677
2.662
2.260
2.242
2.226
2.208
0.000
OBn
CN
N
N
O
3ae
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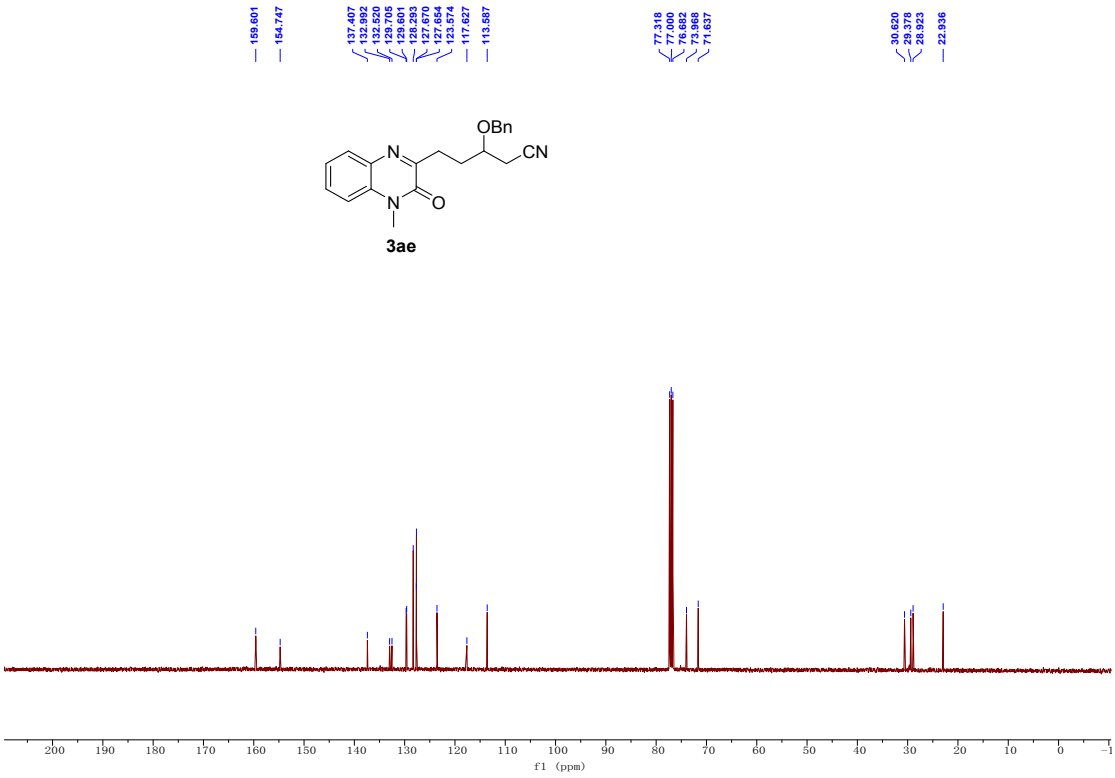
1.12
6.00
2.03
1.00
3.00
2.03
1.99
2.03
f1 (ppm)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154.747
137.407
132.992
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129.705
129.601
128.293
127.670
127.654
123.574
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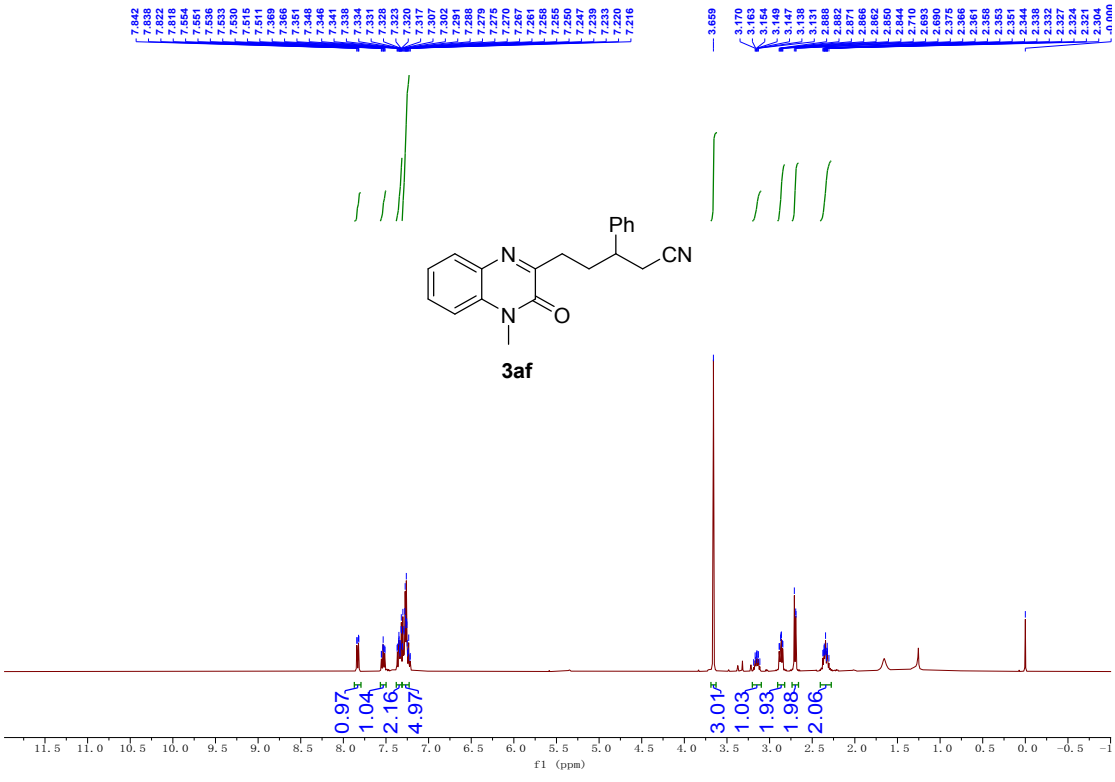
113.587
77.318
77.000
76.682
73.968
71.637
30.620
29.378
28.923
22.936
OBn
CN
N
N
O
3ae
f1 (ppm)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7.536
7.533
7.530
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7.369
7.366
7.351
7.348
7.346
7.341
7.338
7.334
7.331
7.328
7.323
7.320
7.317
7.307
7.302
7.291
7.288
7.279
7.275
7.270
7.267
7.261
7.258
7.255
7.250
7.247
7.239
7.233
7.230
7.216
3.659
3.170
3.163
3.154
3.149
3.147
3.138
3.131
2.888
2.882
2.871
2.866
2.862
2.850
2.844
2.710
2.693
2.690
2.375
2.366
2.361
2.358
2.353
2.351
2.344
2.338
2.332
2.327
2.324
2.321
2.304
Ph
CN
N
N
O
3af
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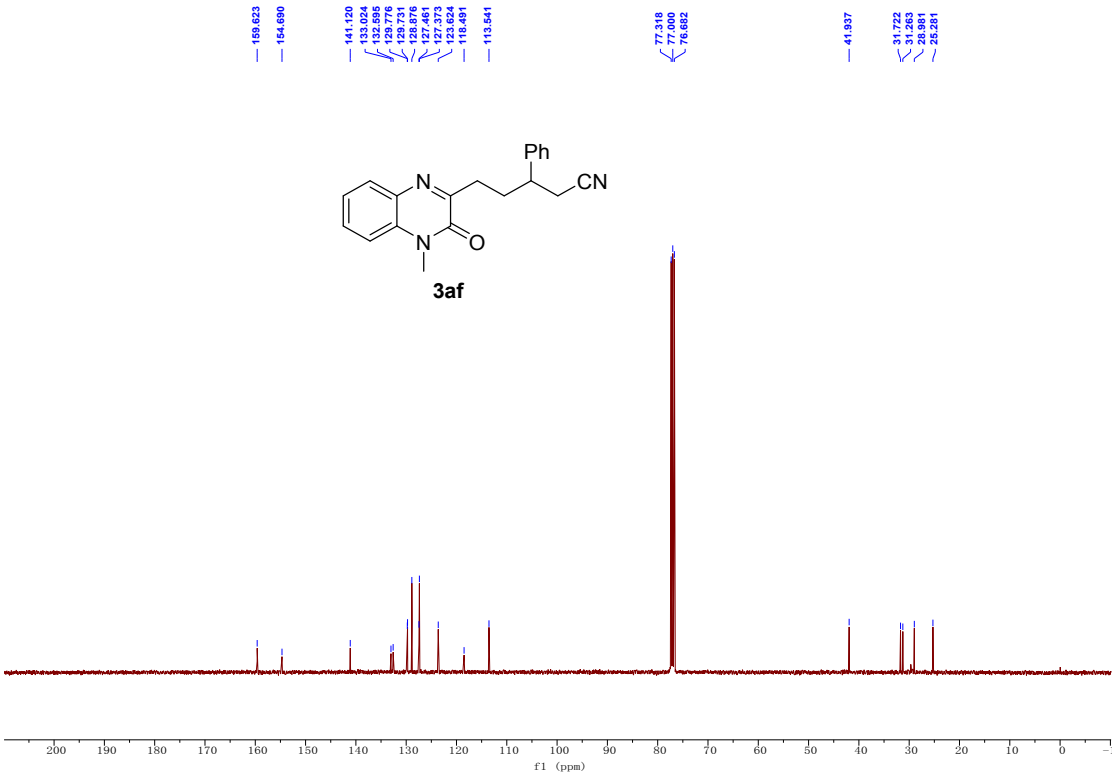
1.04
2.16
4.97
3.01
1.03
1.93
1.98
2.06
f1 (ppm)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128.876
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127.373
123.654
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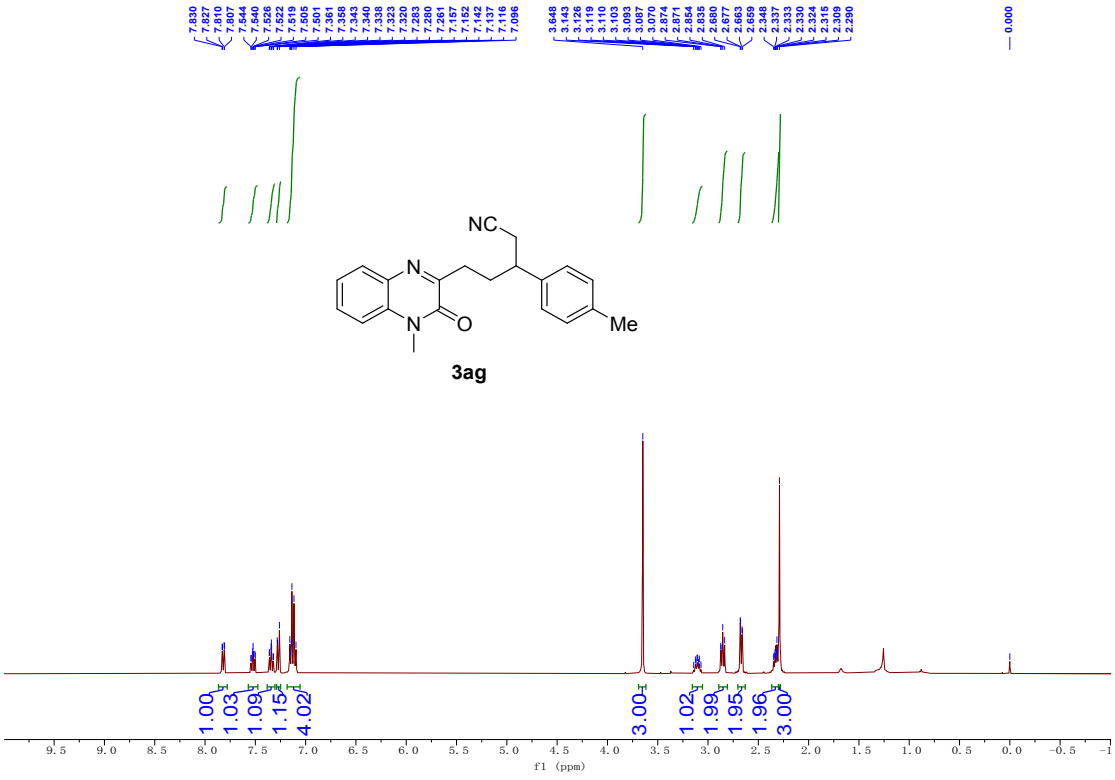
113.541
77.318
77.000
76.682
41.937
31.722
31.263
28.881
25.281
Ph
CN
N
N
O
3af
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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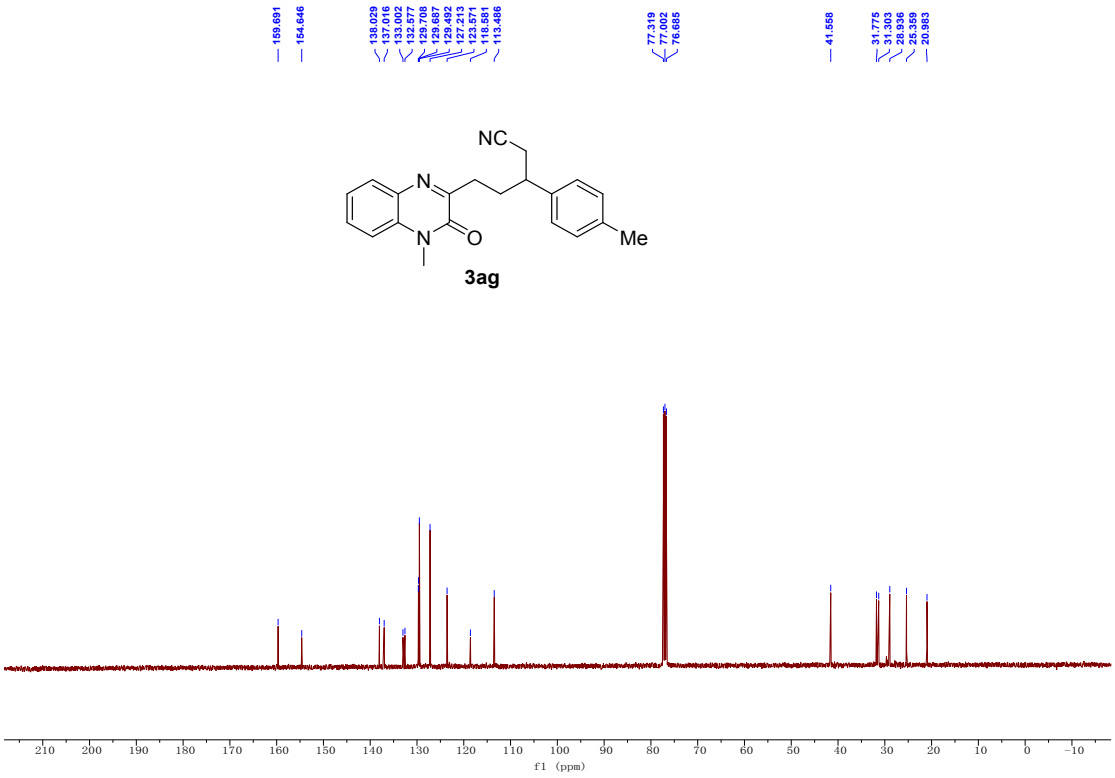
7.505
7.501
7.361
7.358
7.343
7.340
7.338
7.323
7.320
7.283
7.280
7.261
7.157
7.152
7.142
7.137
7.116
7.096
3.648
3.143
3.126
3.119
3.110
3.103
3.093
3.087
3.070
2.874
2.871
2.854
2.835
2.680
2.677
2.663
2.659
2.348
2.337
2.333
2.330
2.324
2.315
2.309
2.290
0.000
NC
N
N
O
Me
3ag
1.00
1.03
1.09
1.15
4.02
3.00
1.02
1.99
1.95
1.96
3.00
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1
f1 (ppm)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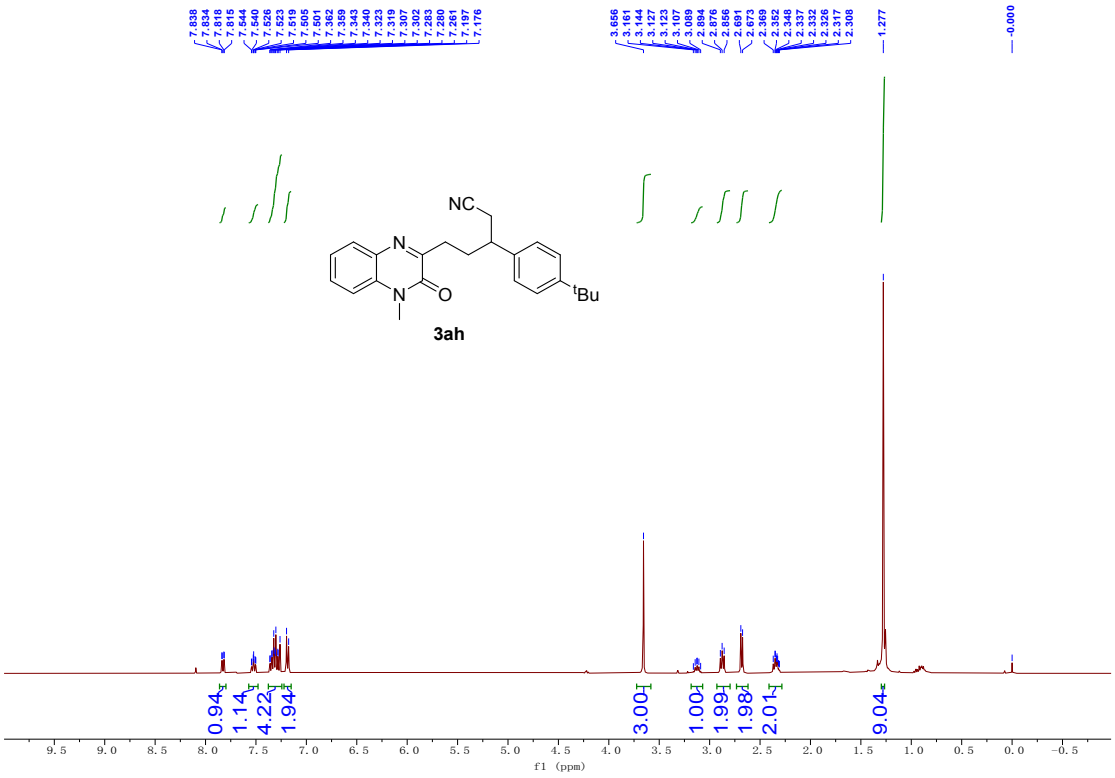
138.029
137.016
133.002
132.577
129.708
129.657
129.492
127.213
123.571
118.581
113.486
77.319
77.002
76.685
41.558
31.775
31.303
28.936
25.389
20.983
NC
N
N
O
Me
3ag
f1 (ppm)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7.818
7.815
7.644
7.640
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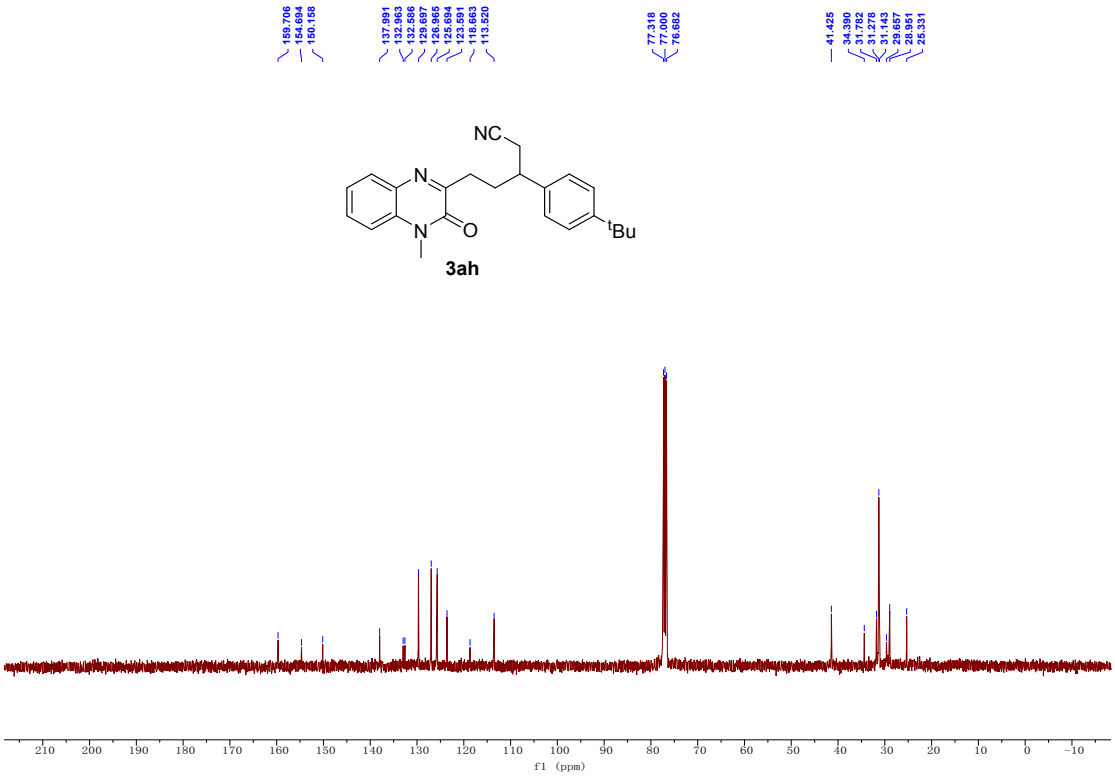
7.523
7.519
7.505
7.501
7.362
7.359
7.343
7.340
7.323
7.319
7.307
7.302
7.283
7.280
7.261
7.197
7.176
3.656
3.161
3.144
3.127
3.123
3.107
3.089
3.084
2.876
2.866
2.691
2.673
2.369
2.352
2.348
2.337
2.332
2.326
2.317
2.308
1.277
-0.000
NC
N
N
O
tBu
3ah
0.94
1.14
4.22
1.94
3.00
1.00
1.99
1.98
2.01
9.04
f1 (ppm)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150.158
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132.586
129.697
128.965
125.694
123.591
118.663
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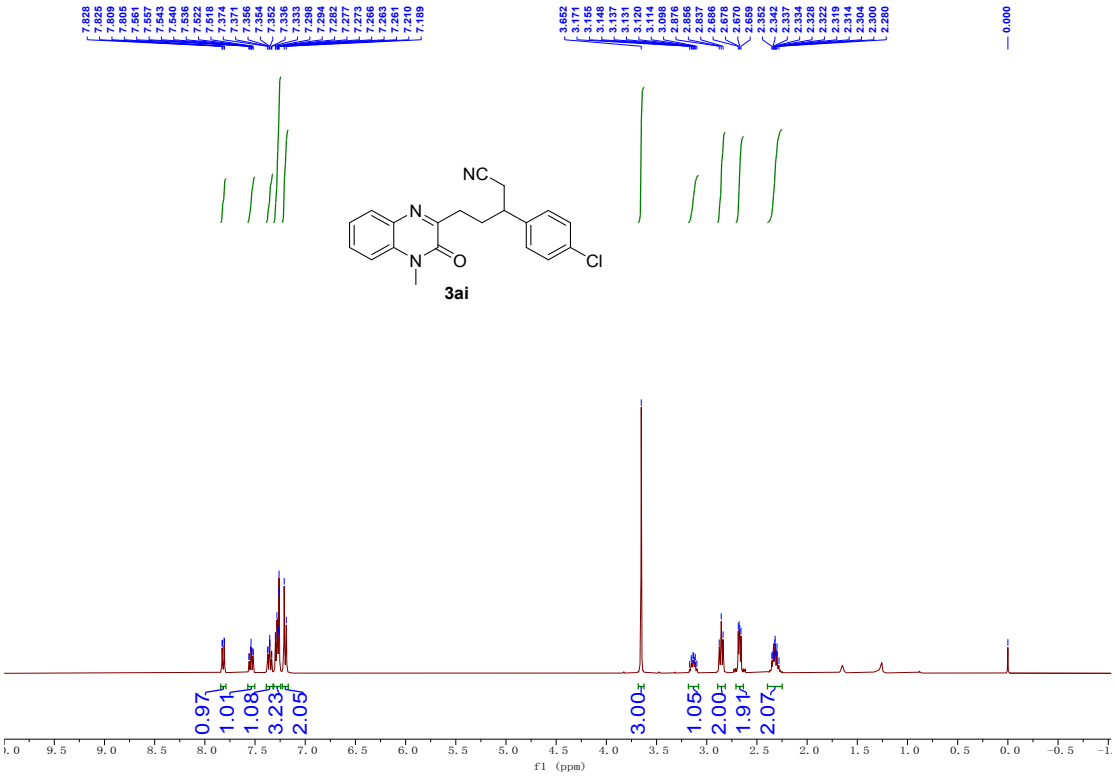
77.318
77.000
76.682
41.425
34.390
31.782
31.278
31.143
29.657
28.951
25.331
NC
N
N
O
tBu
3ah
f1 (ppm)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7.609
7.805
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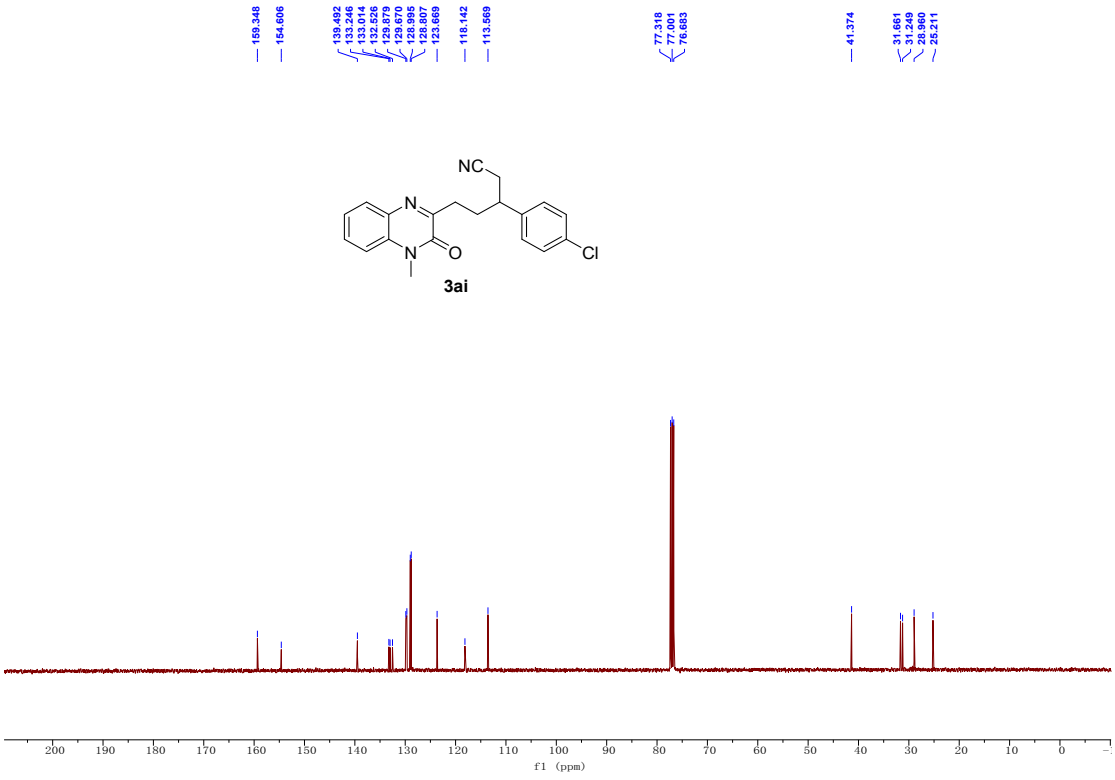
7.557
7.543
7.540
7.536
7.532
7.518
7.374
7.371
7.356
7.354
7.352
7.336
7.333
7.298
7.294
7.282
7.277
7.273
7.266
7.263
7.261
7.210
7.189
3.652
3.171
3.155
3.148
3.137
3.131
3.120
3.114
3.098
2.876
2.866
2.637
2.686
2.678
2.670
2.659
2.352
2.342
2.337
2.334
2.328
2.322
2.319
2.314
2.304
2.300
2.280
0.000
NC
N
N
O
Cl
3ai
0.97
1.01
1.08
3.23
2.05
3.00
1.05
2.00
1.91
2.07
f1 (ppm)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154.606
139.492
133.246
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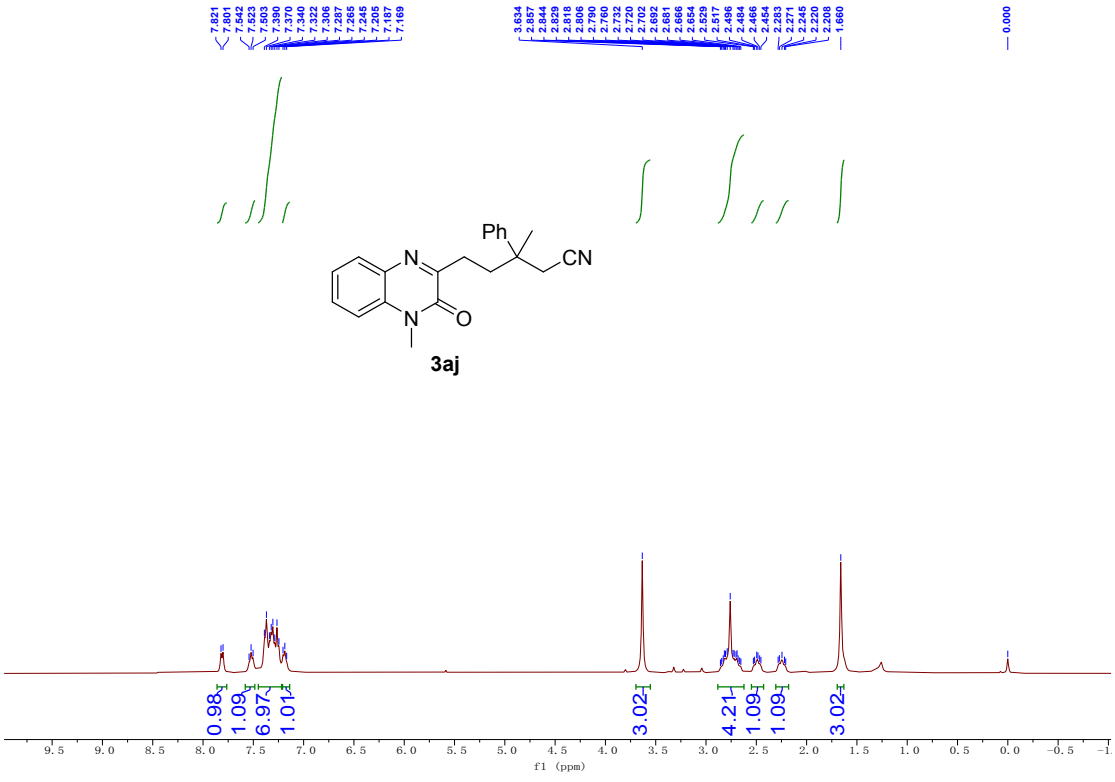
132.526
129.879
129.670
128.995
128.807
123.669
118.142
113.569
77.316
77.001
76.683
41.374
31.661
31.249
28.980
25.211
NC
N
N
O
Cl
3ai
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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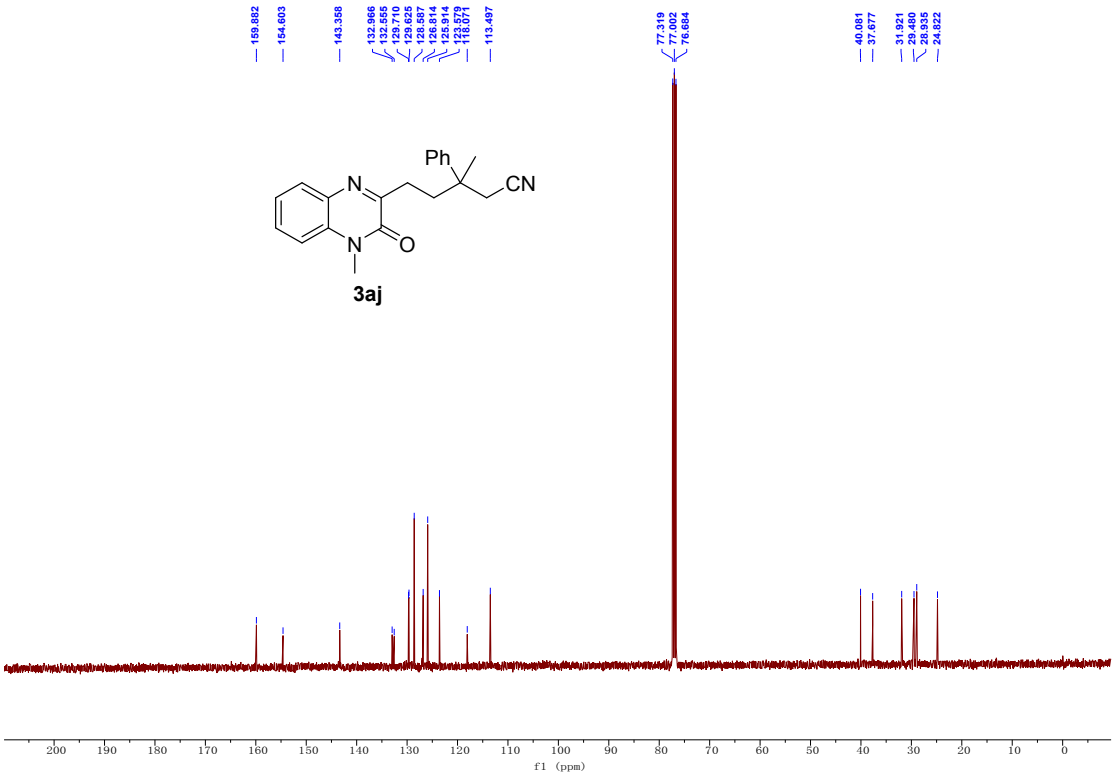
7.542
7.523
7.503
7.390
7.370
7.340
7.322
7.306
7.287
7.265
7.245
7.205
7.187
7.169
3.634
2.857
2.844
2.829
2.818
2.806
2.790
2.780
2.732
2.720
2.702
2.692
2.681
2.666
2.654
2.529
2.517
2.496
2.484
2.466
2.454
2.283
2.271
2.245
2.220
2.200
1.660
0.000
Ph
CN
N
N
O
3aj
0.98
1.09
6.97
1.01
3.02
4.21
1.09
1.09
3.02
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.
f1 (ppm)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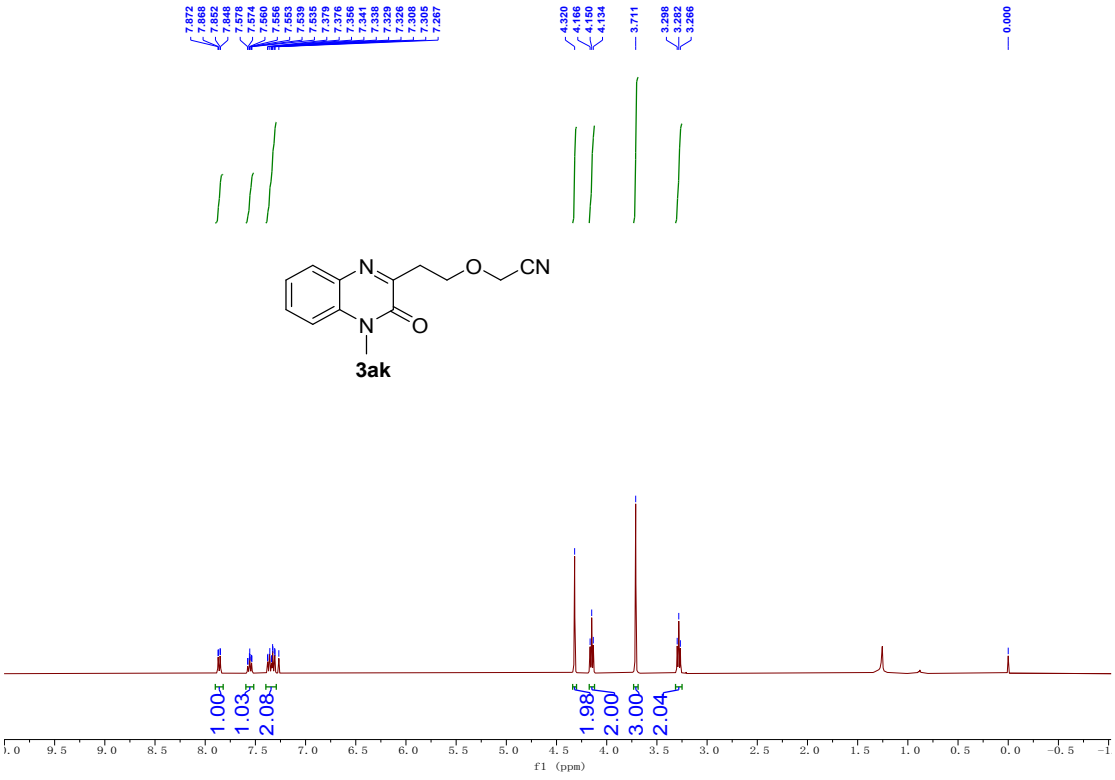
154.603
143.358
132.966
132.555
129.710
129.055
128.567
126.814
125.914
123.579
118.071
113.497
77.319
77.002
76.684
40.081
37.677
31.921
24.600
23.935
24.822
Ph
CN
N
O
3aj
f1 (ppm)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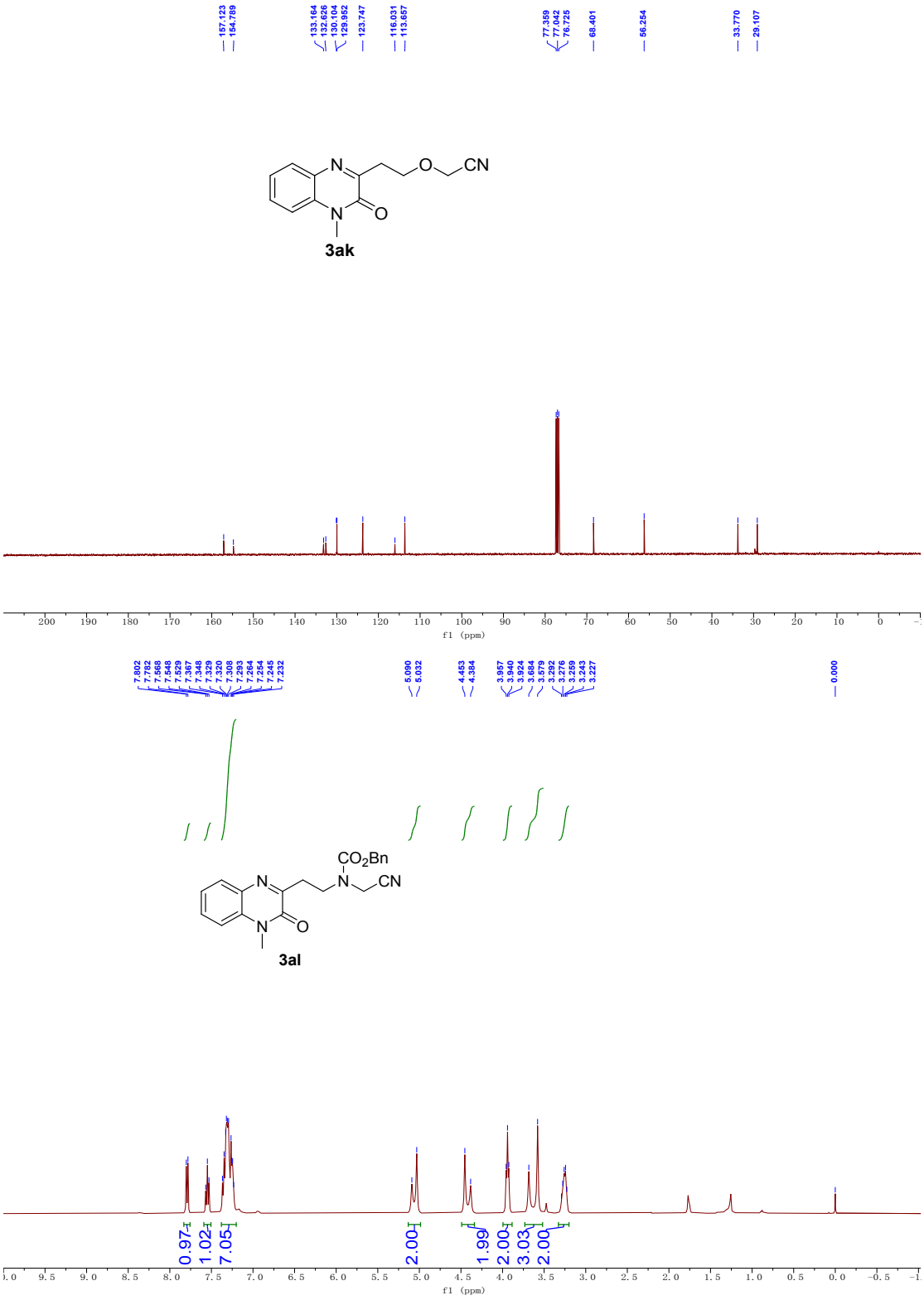
7.852
7.848
7.575
7.574
7.560
7.556
7.553
7.539
7.535
7.379
7.376
7.356
7.341
7.338
7.329
7.326
7.308
7.305
7.287
4.320
4.166
4.150
4.134
3.711
3.298
3.282
3.266
0.000
N
O
CN
O
3ak
1.00
1.03
2.08
1.98
2.00
3.00
2.04
f1 (ppm)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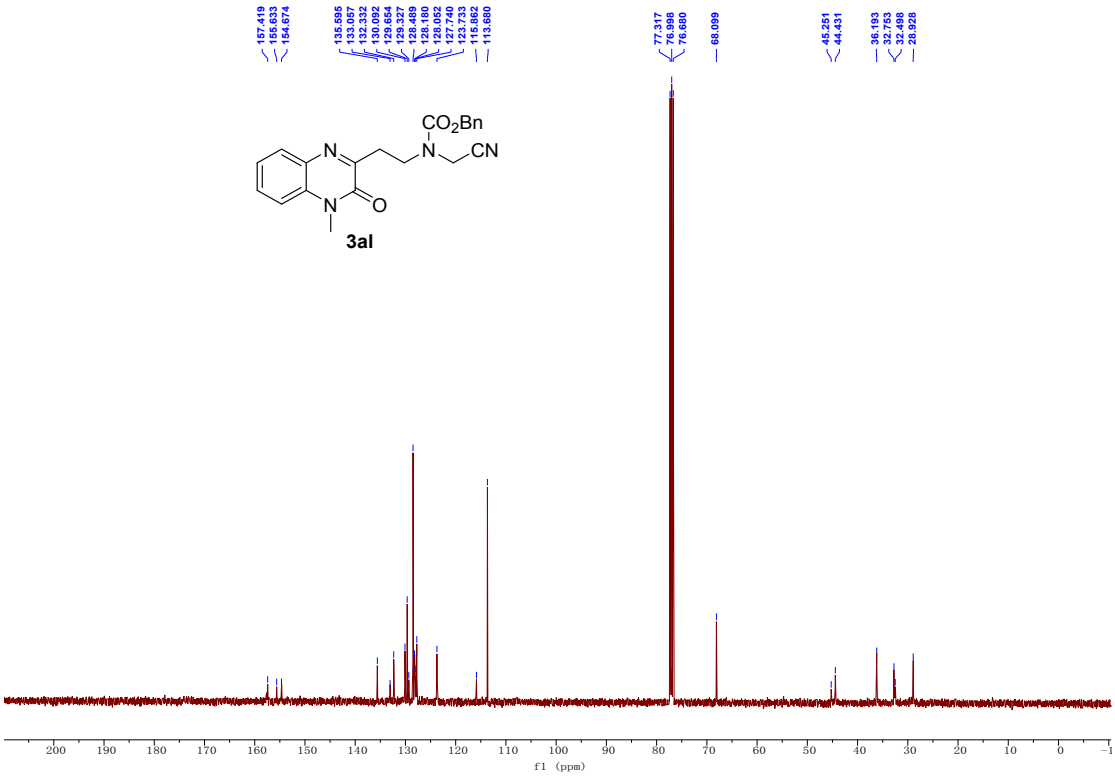
154.769
133.164
132.626
130.104
129.952
123.747
116.031
113.657
77.359
77.042
76.725
68.401
56.254
33.770
29.107
N
O
CN
N
O
3ak
f1 (ppm)
7.802
7.782
7.568
7.548
7.529
7.367
7.348
7.329
7.320
7.308
7.293
7.264
7.254
7.245
7.232
5.090
5.032
4.453
4.384
3.957
3.940
3.924
3.684
3.579
3.292
3.276
3.259
3.243
3.227
0.000
CO2Bn
N
N
CN
N
O
3al
0.97
1.02
7.05
2.00
1.99
2.00
3.03
2.00
f1 (ppm)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154.674
135.595
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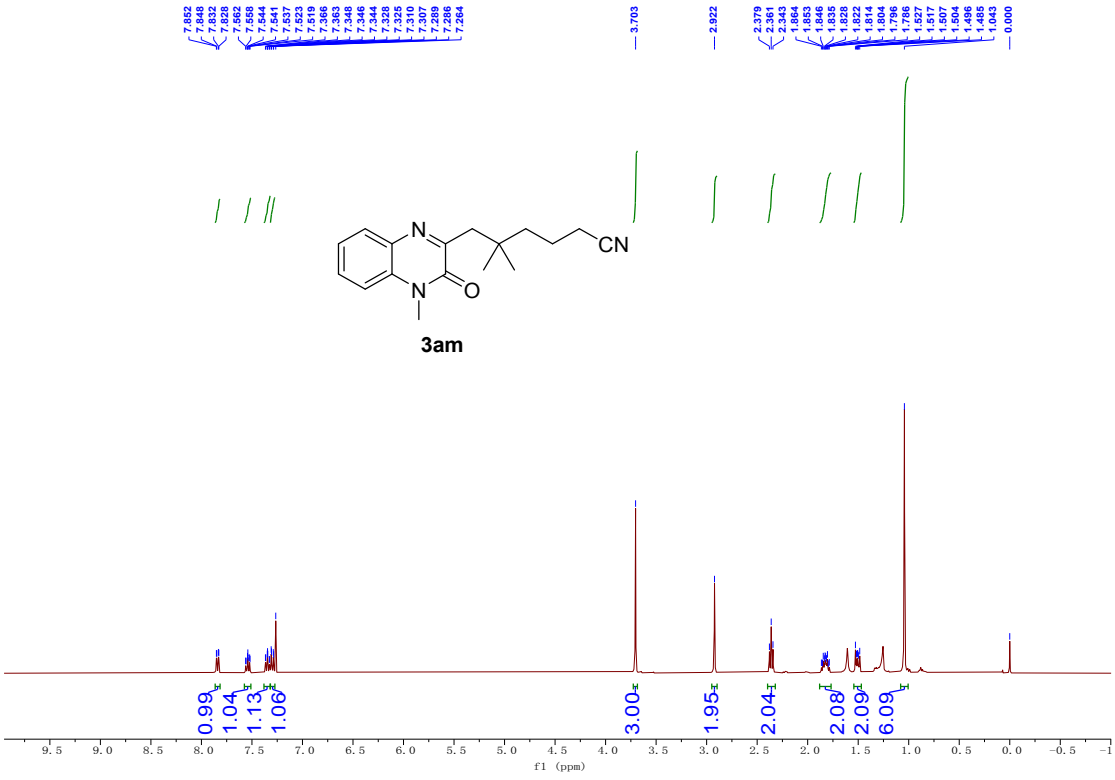
132.332
130.092
129.654
129.327
128.489
128.180
128.052
127.740
123.733
115.862
113.680
77.317
76.998
76.680
68.099
45.251
44.431
36.193
32.753
32.498
28.928
CO2Bn
N
N
CN
N
O
3al
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 −1
f1 (ppm)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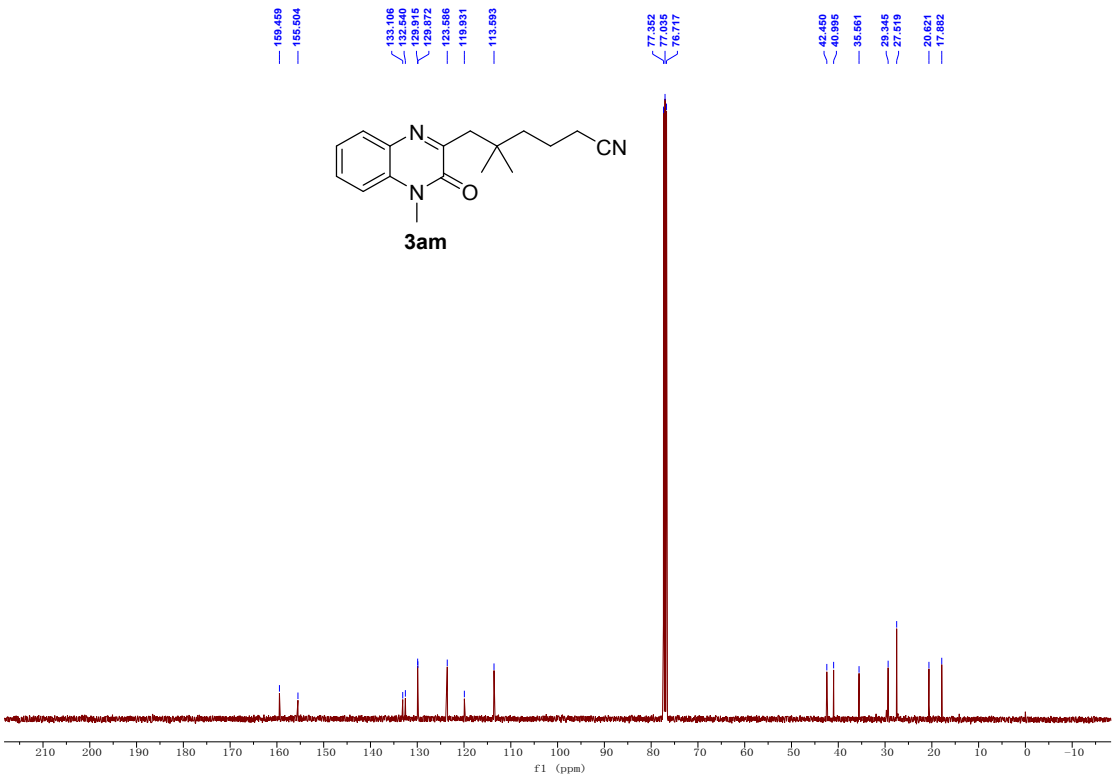
7.562
7.558
7.544
7.541
7.537
7.523
7.519
7.366
7.363
7.348
7.346
7.344
7.328
7.325
7.310
7.307
7.289
7.286
7.264
3.703
2.922
2.379
2.361
2.343
1.864
1.853
1.846
1.835
1.828
1.822
1.814
1.804
1.796
1.786
1.527
1.517
1.507
1.504
1.486
1.485
1.043
0.000
N
N
CN
O
3am
0.99
1.04
1.13
1.06
3.00
1.95
2.04
2.08
2.09
6.09
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 −0.5 −1
f1 (ppm)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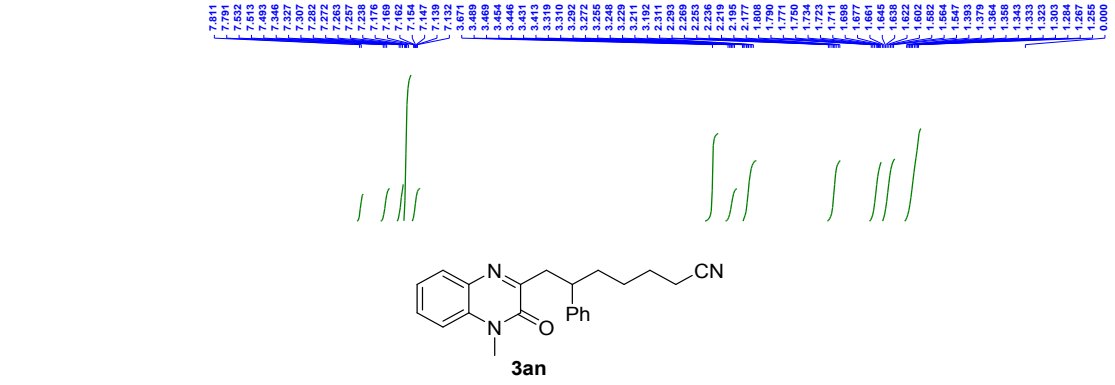
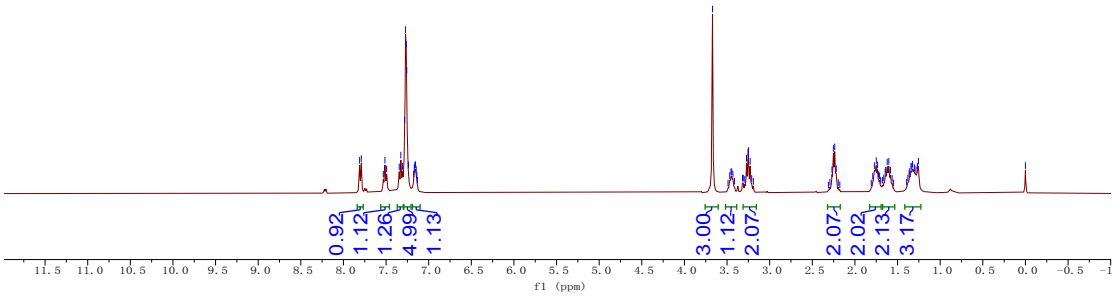
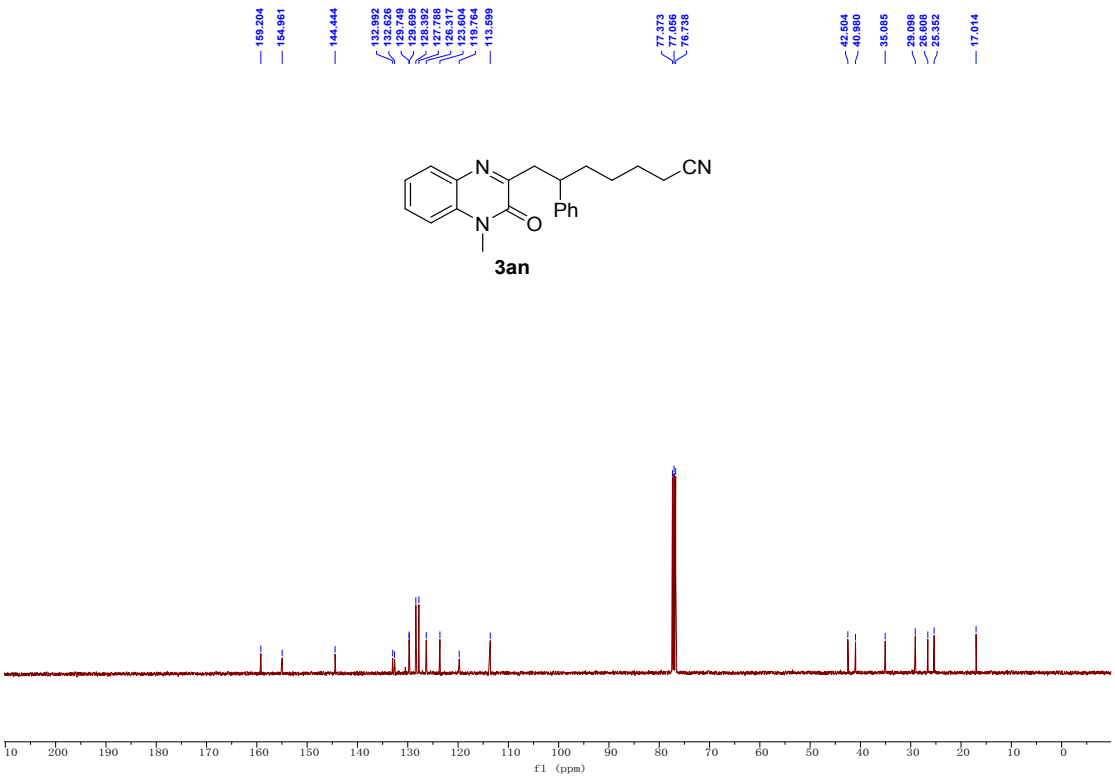
119.931
113.593
77.352
77.035
76.717
42.450
40.995
35.561
29.345
27.519
20.621
17.882
N
CN
N
O
3am
f1 (ppm)


N
CN
Ph
N
O
3an


0.92
1.12
1.26
4.99
1.13
3.00
1.12
2.07
2.07
2.02
2.13
3.17
f1 (ppm)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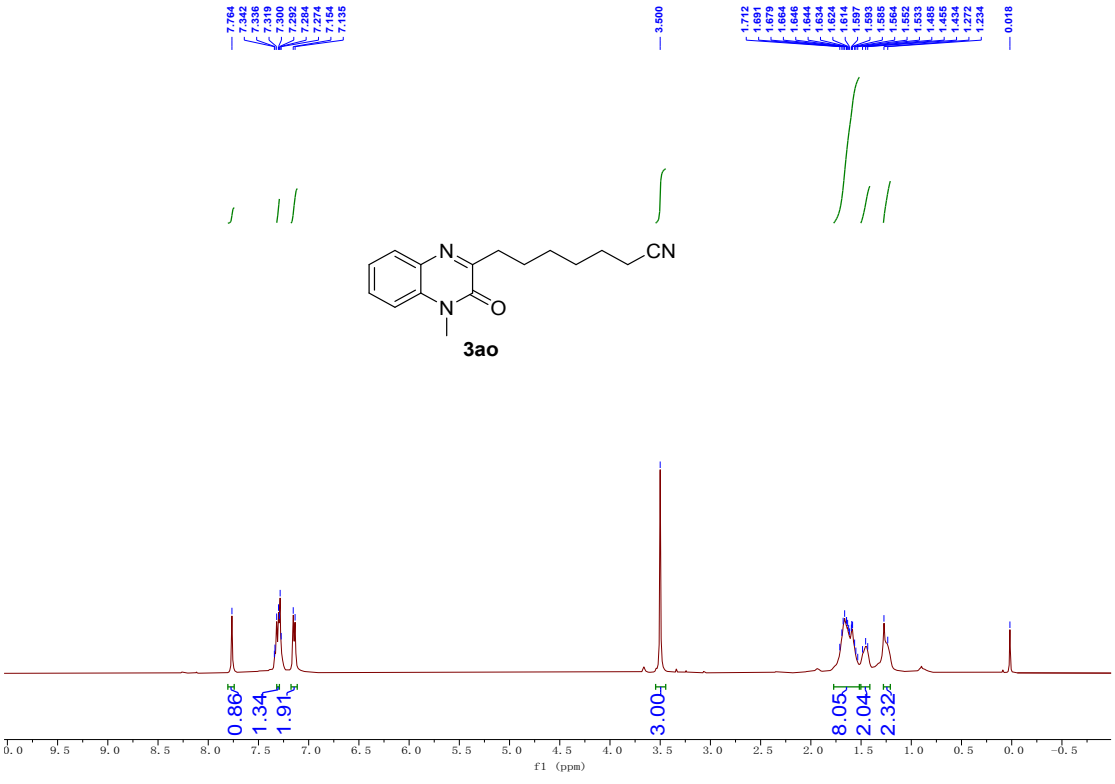
154.961
144.444
132.992
132.626
129.749
129.695
128.392
127.708
126.177
123.604
119.764
113.599
77.373
77.056
76.738
42.604
40.980
35.085
29.098
26.608
25.352
17.014
N
CN
Ph
N
O
3an
f1 (ppm)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7.284
7.274
7.154
7.135
3.500
1.712
1.691
1.679
1.664
1.646
1.644
1.634
1.624
1.614
1.597
1.593
1.585
1.564
1.552
1.533
1.485
1.455
1.434
1.272
1.234
0.018
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CN
N
O
3ao
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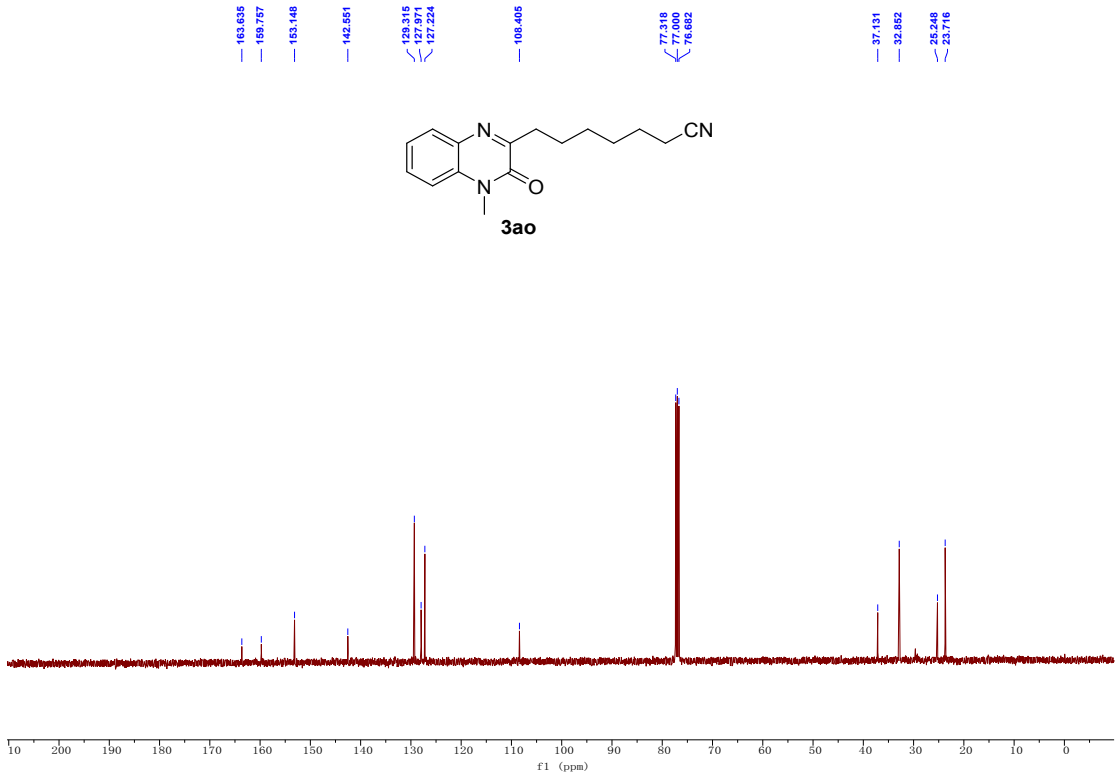
3.00
8.05
2.04
2.32
f1 (ppm)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127.224
108.405
77.318
77.000
76.682
37.131
32.852
25.248
23.716
N
N
O
CN
3ao
10
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)