Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Supporting Information for

2-Aminobenzaldehydes Synthesis by Rhodium(III)-Catalyzed C−H Amidation of Aldehydes with Dioxazolones

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and Lin Dong*

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1. General Methods

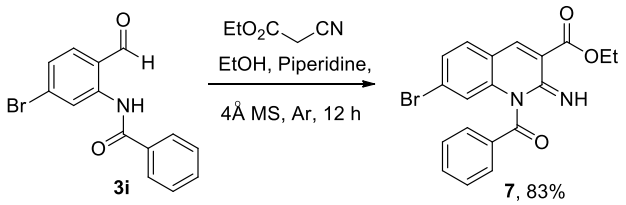
NMR data were obtained for ^{1}H at 400 MHz or 600 MHz, and for ^{13}C at 100 MHz or 151 MHz. Chemical shifts were reported in ppm from tetramethylsilane with the solvent resonance as the internal standard in $CDCl_3$ solution. ESI HRMS was recorded on a Waters SYNAPT G2 and Water XEVO G2 Q-ToF. UV detection was monitored at 220 nm. The UV-vis spectra were recorded on a Shimadzu UV-2450 spectrometer. TLC was performed on glass-backed silica plates. All benzaldehydes were commercially available. 1, 4, 2-Dioxazol-5-ones were prepared according to the literature procedures.[1,2]

2. General Procedure for Synthesis of 2-aminobenzaldehydes

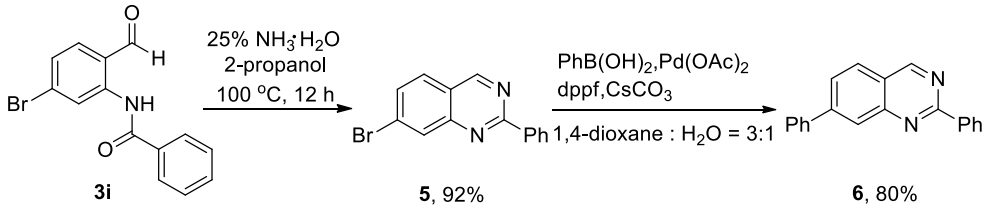
Benzaldehyde **1a** (5.3 mg, 0.05 mmol), 3-phenyl-1, 4, 2-dioxazol-5-one **2a** (24.5 mg, 3.0 equiv.), $[Cp^*RhCl_2]_2$ (1.6 mg, 5 mol %), $AgSbF_6$ (6.8 mg, 0.4 equiv.), $Zn(OAc)_2{\cdot}2H_2O$ (3.3 mg, 0.3 equiv.) and PhCOOH (6 mg, 1.0 equiv.) were stirred in DME (0.5 mL) at 120 °C for 24 h. After completion, the reaction mixture was purified by flash chromatography eluting with ethyl acetate and petroleum ether (1:50) to give the product **3a** as white solid (8.8 mg, 78%). The following products **3a**, **3b, 3e, 3g, 3h, 3i, 3j** and **8** have been reported by previous literatures, [3,4] therefore, only the ^{1}H NMR was attached accordingly. About the following products **3j, 3k, 3m** and **3p-3z** the single peak can be observed in the ^{1}H NMR illustrate that the amidation occured at the less hindered position.

Caution: With ethereal solvent, potentially explosive peroxides may be formed. Although the peroxides were not detected in the scale of 0.5 mmol, we'd like to remind the readers to pay attention to the possible peroxides when the reaction perform on a larger scale.

3. Synthetic Application of 2-aminobenzaldehydes



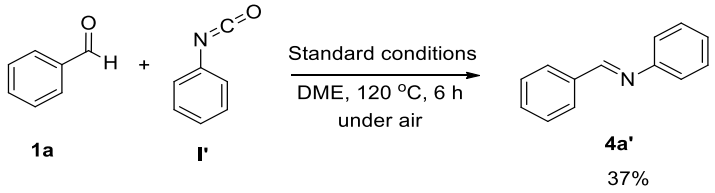
Ethyl-1-benzoyl-7-bromo-2-imino-1,2-dihydroquinoline-3-carboxylate **7**: A mixture of aldehyde **3i** (40 mg, 0.13 mmol, 1.0 equiv), molecular sieves 4 Å (40 mg), absolute ethanol (0.8 mL), ethylcyanoacetate (16.8 μL, 0.16 mmol, 1.2 equiv) and piperidine(0.2 μL, 2%, 2.6 μmol) in catalytic amount was stirred under argon at 60 °C for 24 h. The solution was diluted with CH_2Cl_2 and molecular sieves were filtered on a pad of Celite. The mixture was concentrated under vacuum and the compound **7** was obtained as a yellow solid (44 mg, yield 83%) after purification by flash column chromatography on silica gel.



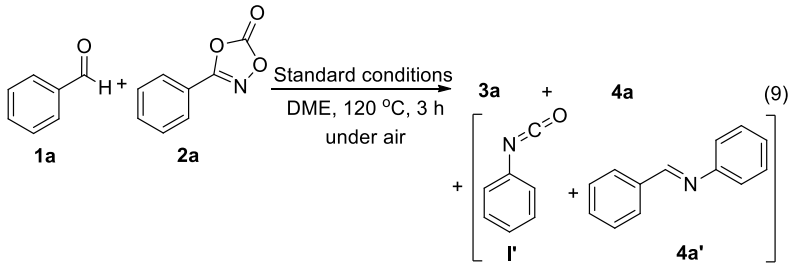
2,7-diphenylquinazoline **6**: To a dried tube equipped with stir bar was added Aldehyde **3i** (40 mg, 0.13 mmol, 1.0 equiv), 25% $NH_3 \cdot H_2O$ (1.2 mL) and 2-propanol (0.8 mL). The reaction mixture was stirred at 100 °C for 12 h. Then the reaction mixture was cooled to room temperature and concentrated under vacuum and the compound **5** was obtained (34 mg, yield 92%) after purification by flash column chromatography on silica gel. A mixture of compound **5** (40 mg, 0.14 mmol, 1.0 equiv), $PhB(OH)_2$ (22.4 mg, 0.18 mmol, 1.3 equiv), $Pd(OAc)_2$ (1.2 mg, 0.13% mmol, 0.036 equiv), dppf (2.8 mg, 0.13% mmol, 0.036 equiv), $CsCO_3$ (92 mg, 0.28 mmol, 2 equiv) and 1,4-dioxane : H_2O (1.2 mL: 0.4 mL) was stirred under argon at 60 °C for 24 h. The solution was concentrated under vacuum and **6** was obtained (32 mg, yield 80%) after purification by flash column chromatography on silica gel (PE/EA: 100/1).

4. Mechanistic Study

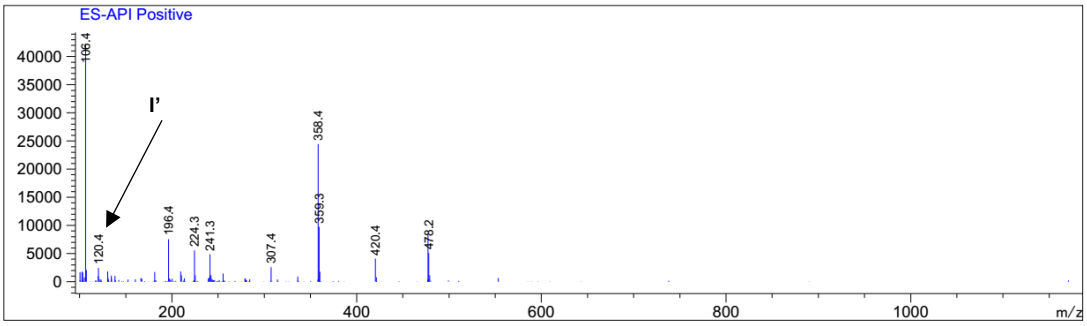
The benzaldehyde **1a** and phenyl isocyanate I' were performed under standard conditions in DME. The imine **4a'** was obtained in 37% yield.



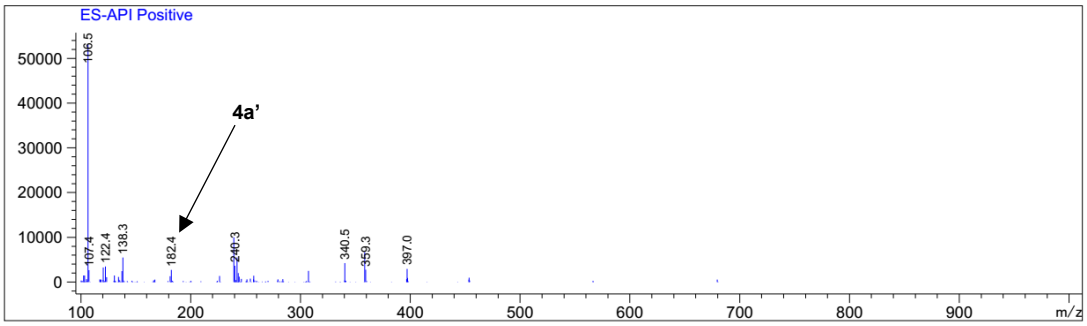
The reaction mixtures were tested respectively by LCMS when **1a** and **2a** reacted under standard conditions in DCE or DME for 3 h. **I'** and **4a'** were observed in DME (eq 9), while **4a'** was observed in DCE (eq 10).

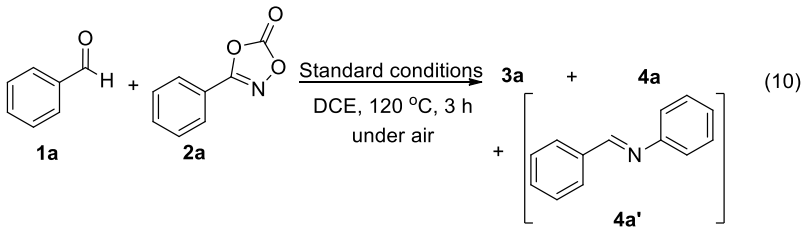


Ret. Time: 1.63

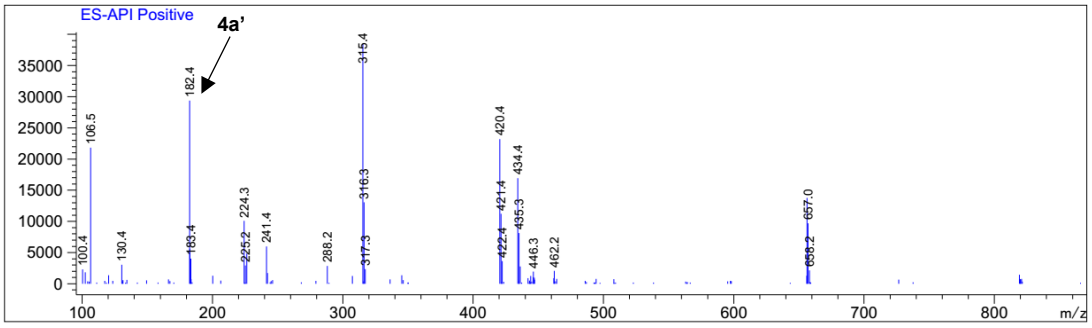


Ret. Time: 1.32

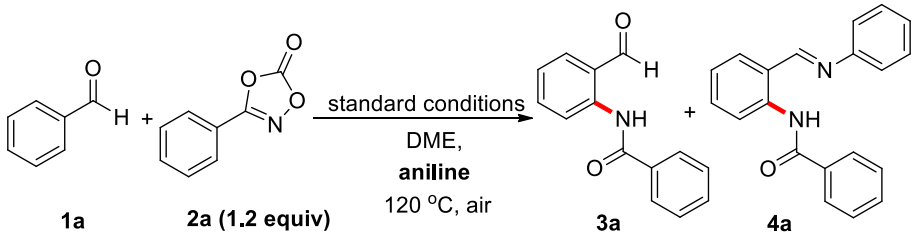




Ret. Time: 2.27

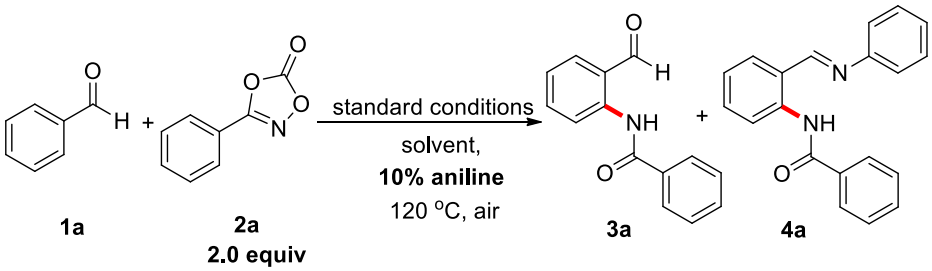


We tested the reaction in the presence of 5%, 10%, 20% aniline, respectively (shown in below scheme a and b). Only low yields of **3a** were obtained, while higher yields of **4a** were obtained in the presence of aniline. It implied that in the presence of catalytic amount of aniline, the yield of **4a** got a promotion, but the aniline catalyst may not work for the formation of **3a**. Therefore, low yield of **3a** indicated that ***imine-directed ortho-amidation pathway did not work smoothly in this reaction system***, and the results of that were same as eqs 5,6 in the Scheme 4.



Aniline	Yield/% 3a	4a
5%	32	11
10%	31	14
20%	31	21
without aniline	27	<5%

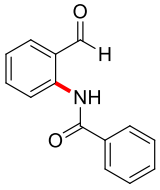
Scheme a



Solvent	Yield/% 3a	4a
DME	42	12
DCE	11	70
(without aniline, 2.0 equiv of 2a) entry 6 DCE	56	17
(without aniline, 2.0 equiv of 2a) entry 13 DME	58	<5

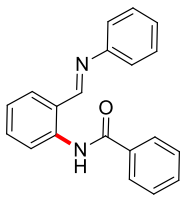
Scheme b

5. Characterization Data for Compounds



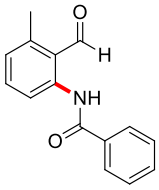
3a

N-(2-formylphenyl)benzamide (**3a**). White solid, m.p. 77.1-79.9 °C, 24 h, 8.8 mg, 78% yield; ^{1}H NMR (400 MHz, $CDCl_3$): δ = 12.10 (s, 1H), 10.01 (s, 1H), 8.97 (d, J = 8.4 Hz, 1H), 8.09-8.07 (m, 2H), 7.74 (dd, J_1 = 7.6 Hz, J_2 = 1.6 Hz, 1H), 7.71-7.67 (m, 1H), 7.59-7.52 (m, 3H), 7.29 (dd, J_1 = 7.6 Hz, J_2 = 0.8 Hz, 1H) ppm. The structure has been reported by previous literatures[3,4].



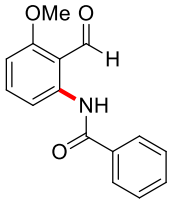
4a

N-(2-((phenylimino)methyl)phenyl)benzamide (**4a**). White solid, m.p. 102.2-104.9 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ = 13.58 (s, 1H), 9.02 (d, J = 8.8 Hz, 1H), 8.66 (s, 1H), 8.13 (d, J = 7.6 Hz, 2H), 7.56-7.44 (m, 7H), 7.34-7.19 (m, 4H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ = 166.4, 163.2, 149.9, 140.6, 135.3, 134.4, 132.7, 131.8, 129.5, 128.6, 127.7, 126.8, 122.8, 121.3, 120.8, 120.0 ppm. ESI HRMS: calcd. for $C_{20}H_{16}N_2O$+H 301.1341, found 301.1347.



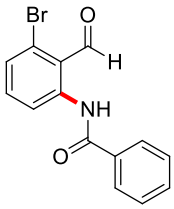
3b

N-(2-formyl-3-methylphenyl)benzamide (**3b**). White solid, m.p. 109.0-110.2 °C, 24 h, 8.1 mg, 68% yield; ^{1}H NMR (400 MHz, $CDCl_3$): δ = 12.56 (s, 1H), 10.52 (s, 1H), 8.83 (d, J = 8.4 Hz, 1H), 8.08 (d, J = 7.2 Hz, 2H), 7.57-7.43 (m, 4H), 6.97 (d, J = 7.2 Hz, 1H), 2.70 (s, 3H) ppm. The structure has been reported by previous literatures[4].



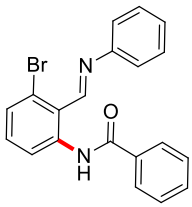
3c

N-(2-formyl-3-methoxyphenyl)benzamide (**3c**). White solid, m.p. 106.4-109.9 °C, 24 h, 11.4 mg, 72% yield; ^{1}H NMR (600 MHz, $CDCl_3$): δ = 12.64 (s, 1H), 10.58 (s, 1H), 8.52 (d, J = 9.0 Hz, 1H), 8.08-8.07 (m, 2H), 7.59-7.55 (m, 2H), 7.53-7.51 (m, 2H), 6.68 (d, J = 8.4 Hz, 1H), 3.93 (s, 3H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ = 193.7, 166.3, 163.3, 142.7, 138.1, 134.5, 132.1, 128.8, 127.6, 112.2, 111.2, 105.2, 55.9 ppm. ESI HRMS: calcd. for $C_{15}H_{13}NO_3$+H 256.0974, found 256.0977.



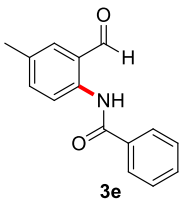
3d

N-(3-bromo-2-formylphenyl)benzamide (**3d**). White solid, m.p. 132.4-135.9 °C, 24 h, 6.4 mg, 42% yield; ^{1}H NMR (400 MHz, $CDCl_3$): δ = 12.42 (s, 1H), 10.46 (s, 1H), 8.87 (d, J = 8.4 Hz, 1H), 7.97 (d, J = 7.2 Hz, 2H), 7.51-7.43 (m, 3H), 7.37 (t, J = 8.0 Hz, 1H), 7.31 (d, J = 7.6 Hz, 1H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ = 197.2, 166.1, 143.5, 137.0, 134.2, 132.4, 129.9, 128.9, 128.2, 127.6, 119.9, 118.5 ppm. ESI HRMS: calcd. for $C_{14}H_{10}BrNO_2$+H 303.9973, found 303.9977, 305.9961.



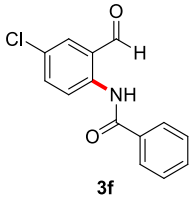
4d

N-(3-bromo-2-((phenylimino)methyl)phenyl)benzamide (**4d**). Light yellow solid, m.p. 145.1-146.0 °C, 24 h, 2.8 mg, 15% yield; ^{1}H NMR (400 MHz, $CDCl_3$): δ = 14.01 (s, 1H), 9.29 (s, 1H), 9.01 (d, J = 8.0 Hz, 1H), 8.10-8.08 (m, 2H), 7.57-7.53 (m, 1H), 7.50-7.45 (m, 4H), 7.42 (dd, J_1 = 8.0 Hz, J_2 = 1.2 Hz, 1H), 7.37-7.29 (m, 4H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ = 166.5, 165.3, 163.2, 159.4, 149.7, 148.5, 142.4, 140.0, 135.2, 134.9, 133.4, 132.7, 132.0, 130.5, 129.6, 129.4, 128.7, 128.6, 128.4, 128.2, 127.9, 127.7, 127.5, 127.3, 122.0, 121.1, 120.4, 119.8, 119.7, 118.9, 100.3, 58.4 ppm. ESI HRMS: calcd. for $C_{20}H_{15}BrN_2O$+H 379.0446, found 379.0443, 381.0427.



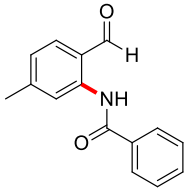
3e

N-(2-formyl-4-methylphenyl)benzamide (**3e**). White solid, m.p. 120.0-120.8 °C, 24 h, 9.3 mg, 78% yield; ^{1}H NMR (400 MHz, $CDCl_3$): δ = 11.99 (s, 1H), 9.96 (s, 1H), 8.85 (d, J = 8.4 Hz, 1H), 8.07 (d, J = 6.8 Hz, 2H), 7.57-7.48 (m, 5H), 2.42 (s, 3H) ppm.The structure has been reported by previous literatures[3,4].



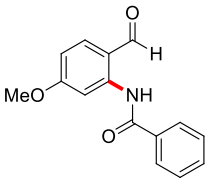
3f

N-(4-chloro-2-formylphenyl)benzamide (**3f**). White solid, m.p. 139.8-142.7 °C, 36 h, 6.2 mg, 48% yield; ^{1}H NMR (400 MHz, $CDCl_3$): δ = 11.97 (s, 1H), 9.94 (s, 1H), 8.96(d, J = 8.8 Hz, 1H), 8.05 (d, J = 7.2 Hz, 2H), 7.70-7.53 (m, 5H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ = 194.6, 166.1, 139.8, 136.1, 135.1, 134.0, 132.4, 128.9, 128.1, 127.5, 123.0, 121.7 ppm. ESI HRMS: calcd. for $C_{14}H_{10}ClNO_2$+H 282.0298, found 282.0296, 284.0270.



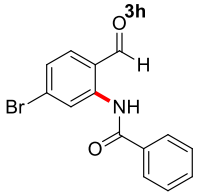
3g

N-(2-formyl-5-methylphenyl)benzamide (**3g**). White solid, m.p. 131.0 °C, 24 h, 8.0 mg, 67% yield; ^{1}H NMR (400 MHz, $CDCl_3$): δ = 12.11 (s, 1H), 9.93 (s, 1H), 8.81 (s, 1H), 8.09-8.06 (m, 2H), 7.61-7.51 (m, 4H), 7.07 (d, J = 7.6 Hz, 1H), 2.48 (s, 3H) ppm. The structure has been reported by previous literatures[3,4].



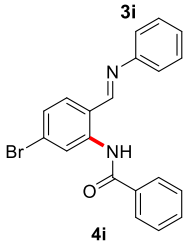
3h

N-(2-formyl-5-methoxyphenyl)benzamide (**3h**). White solid, m.p. 118.0-119.9 °C,24 h, 9.9 mg, 78% yield; ^{1}H NMR (400 MHz, $CDCl_3$): δ = 12.38 (s, 1H), 9.81 (s, 1H), 8.59 (s, 1H), 8.06 (d, J = 7.2 Hz, 2H), 7.60-7.50 (m, 4H), 6.74 (dd, J_1 = 8.4 Hz, J_2 = 1.6 Hz, 1H), 3.94 (s, 3H) ppm.The structure has been reported by previous literatures[3,4].



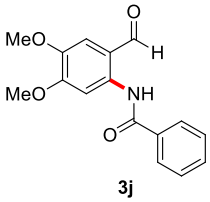
3i

N-(5-bromo-2-formylphenyl)benzamide (**3i**). White solid, m.p. 147.0-147.9 °C, 24 h, 6.5mg, 43% yield; ^{1}H NMR (400 MHz, $CDCl_3$): δ = 12.13 (s, 1H), 9.96 (s, 1H), 9.24 (s, 1H), 8.07 (d, J = 7.6 Hz, 2H), 7.63-7.54 (m, 4H), 7.42 (d, J = 8.0 Hz, 1H) ppm. The structure has been reported by previous literatures[4].



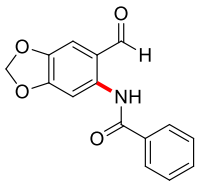
4i

N-(5-bromo-2-((phenylimino)methyl)phenyl)benzamide (**4i**). White solid, m.p. 140.5-144.2 °C, 24 h, 3 mg, 16% yield; ^{1}H NMR (400 MHz, $CDCl_3$): δ = 13.64 (s, 1H), 9.27 (d, J = 1.6 Hz, 1H), 8.60 (s, 1H), 8.11-8.09 (m, 2H), 7.56-7.27 (m, 10H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ = 166.4, 162.2, 149.6, 141.3, 135.2, 134.9, 132.0, 128.7, 127.7, 127.6, 127.1, 126.0, 123.0, 120.8, 120.1 ppm. ESI HRMS: calcd. for $C_{20}H_{15}BrN_2O$+H 379.0446, found 379.0441, 381.0423.



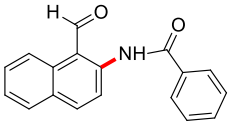
3j

N-(2-formyl-4,5-dimethoxyphenyl)benzamide (**3j**). White solid, m.p. 161.4-124.2 °C, 24 h, 12.5 mg, 82% yield; ^{1}H NMR (400 MHz, $CDCl_3$): δ = 12.33 (s, 1H), 9.83 (s, 1H), 8.72 (s, 1H), 8.07 (d, J = 7.2 Hz, 2H), 7.58-7.52 (m, 3H), 7.10 (s, 1H), 4.06 (s, 3H), 3.95 (s, 3H) ppm. The structure has been reported by previous literatures[4].



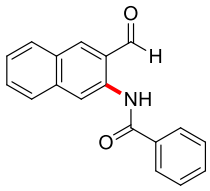
3k

N-(6-formylbenzo[*d*][1,3]dioxol-5-yl)benzamide (**3k**). Yellow solid, m.p. 182.1-183.5 °C, 24 h, 9.3 mg, 44% yield; ^{1}H NMR (400 MHz, $CDCl_3$): δ = 12.44 (s, 1H), 9.76 (s, 1H), 8.60 (s, 1H), 8.06 (d, J = 7.2 Hz, 2H), 7.58-7.51 (m, 3H), 7.07 (s, 1H), 6.10 (s, 2H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ = 193.1, 154.2, 139.7, 132.2, 128.8, 127.5, 116.0, 113.0, 102.4, 101.3 ppm. ESI HRMS: calcd. for $C_{15}H_{11}NO_4$+H 270.0766, found 270.0766.



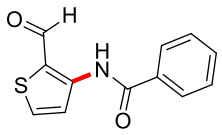
3l

N-(1-formylnaphthalen-2-yl)benzamide (**3l**). Yellow solid, m.p. 196.7-197.3 °C, 24 h, 9.9 mg, 72% yield; ^{1}H NMR (400 MHz, $CDCl_3$): δ = 13.14 (s, 1H), 11.10 (s, 1H), 9.17 (d, J = 9.2 Hz, 1H), 8.49 (d, J = 8.8 Hz, 1H), 8.15-8.12 (m, 3H), 7.88 (d, J = 8.0 Hz, 1H), 7.66-7.49 (m, 5H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ = 193.0, 193.0, 166.7, 143.0, 137.8, 134.4, 133.7, 132.4, 129.6, 129.4, 129.0, 128.9, 127.8, 125.2, 119.7, 112.9 ppm. ESI HRMS: calcd. for $C_{18}H_{13}NO_2$+H 276.1025, found 276.1025.



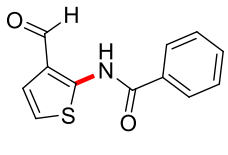
3m

N-(1-acetylnaphthalen-2-yl)benzamide (**3m**). Yellow solid, m.p. 142.9-145.3 °C, 24 h, 24 h, 8.0 mg, 58% yield; ^{1}H NMR (400 MHz, $CDCl_3$): δ = 11.90 (s, 1H), 10.14 (s, 1H), 9.35 (s, 1H), 8.25 (s, 1H), 8.11 (dd, J_1 = 7.6 Hz, J_2 = 1.6 Hz, 2H), 7.91 (d, J = 8.8 Hz, 2H), 7.66-7.46 (m, 5H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ = 195.8, 166.0, 140.4, 137.2, 135.8, 134.5, 132.0, 130.5, 129.0, 128.9, 128.7, 128.1, 127.4, 125.9, 123.1, 117.4 ppm. ESI HRMS: calcd. for $C_{18}H_{13}NO_2$+H 276.1025, found 276.1030.



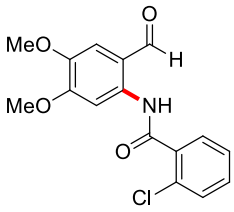
3n

N-(2-formylthiophen-3-yl)benzamide (**3n**). White solid, m.p. 97.9-103.7 °C, 24 h, 3.1 mg, 27% yield; ^{1}H NMR (400 MHz, $CDCl_3$): δ = 11.63 (s, 1H), 9.79 (s, 1H), 8.37 (d, J = 5.2 Hz, 1H), 8.03 (d, J = 7.6 Hz, 2H), 7.77 (d, J = 5.2 Hz, 1H), 7.62-7.52 (m, 3H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ = 184.5, 164.8, 145.2, 136.5, 133.1, 132.5, 128.9, 127.6, 123.1, 121.4 ppm. ESI HRMS: calcd. for $C_{12}H_9NO_2S$+H 232.0432, found 232.0430.



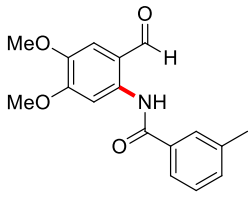
3o

N-(3-acetylthiophen-2-yl)benzamide (**3o**). White solid, m.p. 110.3-114.9 °C, 24 h, 3.4 mg, 21% yield; ^{1}H NMR (400 MHz, $CDCl_3$): δ = 12.43 (s, 1H), 9.93 (s, 1H), 8.06-8.04 (m, 2H), 7.65-7.61 (m, 1H), 7.58-7.54 (m, 2H), 7.24 (d, J = 5.6 Hz, 1H), 6.83 (d, J = 5.6 Hz, 1H) ppm; ^{13}C NMR (151 MHz, $CDCl_3$): δ = 187.2, 164.1, 150.3, 132.9, 131.3, 128.9, 128.9, 128.9, 127.5, 127.5, 127.5, 127.5, 127.5, 125.0, 122.3, 117.1 ppm. ESI HRMS: calcd. for $C_{12}H_9NO_2S$+Na 254.0252, found 254.0253.



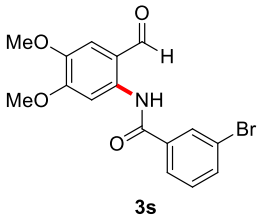
3p

2-chloro-*N*-(2-formyl-4,5-dimethoxyphenyl)benzamide (**3p**). Yellow solid, m.p. 152.9-155.5 °C, 24 h, 9.6 mg, 60% yield; ^{1}H NMR (400 MHz, $CDCl_3$): δ = 11.80 (s, 1H), 9.77 (s, 1H), 8.66 (s, 1H), 7.65 (dd, J_1 = 7.2 Hz, J_2 = 1.6 Hz, 1H), 7.49 (dd, J_1 = 8.0 Hz, J_2 = 1.2 Hz, 1H), 7.44 (dd, J_1 = 7.6 Hz, J_2 = 1.6 Hz, 1H), 7.41-7.36 (m, 1H), 7.10 (s, 1H), 4.06 (s, 3H), 3.95 (s, 3H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ = 193.2, 166.0, 155.5, 144.9, 137.1, 135.7, 131.4，130.7, 129.3, 127.1, 116.5, 115.0, 103.4, 56.5，56.3 ppm. ESI HRMS: calcd. for $C_{16}H_{14}ClNO_4$+H 320.0690, found 320.0698.



3r

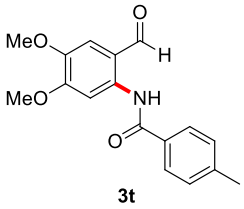
N-(2-formyl-4,5-dimethoxyphenyl)-3-methylbenzamide (**3r**). Yellow solid, m.p. 139.0-139.8 °C, 24 h, 12.7 mg, 80% yield; ^{1}H NMR (400 MHz, $CDCl_3$): δ = 12.31 (s, 1H), 9.83 (s, 1H), 8.70 (s, 1H), 7.65-7.61 (m, 2H), 7.40 (t, J = 8.0 Hz, 1H), 7.13-7.10 (m, 2H), 4.05 (s, 3H), 3.94 (s, 3H), 3.90 (s, 3H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ = 193.5, 166.0, 160.0, 155.7, 144.6, 137.8, 135.7, 129.9, 119.3, 118.9, 116.5, 115.0, 112.2, 103.1, 56.4, 56.2, 55.4 ppm. ESI HRMS: calcd. for $C_{17}H_{17}NO_4$+H 300.1236, found 300.1238.



3s

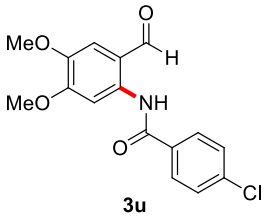
3-bromo-*N*-(2-formyl-4,5-dimethoxyphenyl)benzamide (**3s**). Yellow solid, m.p. 162.8-163.8 °C, 24 h, 9.5 mg, 52% yield; ^{1}H NMR (400 MHz, $CDCl_3$): δ = 11.71 (s, 1H), 9.77 (s, 1H), 8.64 (s, 1H), 7.67 (dd, J_1 = 8.0 Hz, J_2 = 1.2 Hz, 1H), 7.60 (dd, J_1 = 7.6 Hz, J_2 = 1.6 Hz, 1H), 7.43 (td, J_1 = 7.6 Hz, J_2 = 1.2 Hz, 1H), 7.34 (td, J_1 = 7.6 Hz, J_2 = 1.6 Hz, 1H), 7.09 (s, 1H),

4.05 (s, 3H), 3.94 (s, 3H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ = 193.2, 191.6, 166.8, 163.0, 155.5, 149.3, 144.9, 144.0, 137.9, 137.1, 134.4, 133.9, 131.7, 129.1, 127.7, 119.8, 116.5, 115.0, 103.3, 56.6, 56.3 ppm. ESI HRMS: calcd. for $C_{16}H_{14}BrNO_4$+Na 386.0004, found 386.0005, 387.9954.



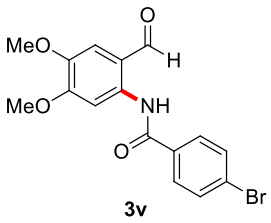
3t

N-(2-formyl-4,5-dimethoxyphenyl)-4-methylbenzamide (**3t**). Light yellow solid, m.p. 146.7-149.5 °C, 24 h, 13.0 mg, 81% yield; ^{1}H NMR (400 MHz, $CDCl_3$): δ = 12.27 (s, 1H), 9.83 (s, 1H), 8.72 (s, 1H), 7.96 (d, J = 8.4 Hz, 2H), 7.33 (d, J = 8.0 Hz, 2H), 7.09 (s, 1H), 4.05 (s, 3H), 3.94 (s, 3H), 2.43 (s, 3H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ = 193.5, 166.2, 155.7, 144.5, 142.8, 138.1, 131.5, 129.5, 127.4, 116.5, 114.9, 103.1, 56.4, 56.2, 21.5 ppm. ESI HRMS: calcd. for $C_{17}H_{17}NO_4$+H 300.1236, found 300.1241.



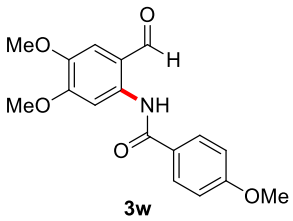
3u

4-chloro-*N*-(2-formyl-4,5-dimethoxyphenyl)benzamide (**3u**). Light brown, solid, m.p. 165.3-168.7 °C, 24 h, 9.6 mg, 60% yield; ^{1}H NMR (400 MHz, $CDCl_3$): δ = 12.32 (s, 1H), 9.83 (s, 1H), 8.67 (s, 1H), 8.00 (d, J = 8.4 Hz, 2H), 7.50 (d, J = 8.4 Hz, 2H), 7.11 (s, 1H), 4.05 (s, 3H), 3.95 (s, 3H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ = 193.6, 165.0, 155.7, 144.8, 138.6, 137.7, 132.7, 129.2, 128.8, 116.5, 114.9, 103.1, 56.5, 56.3 ppm. ESI HRMS: calcd. for $C_{16}H_{14}ClNO_4$+H 320.0690, found 320.0683, 322.0670.



3v

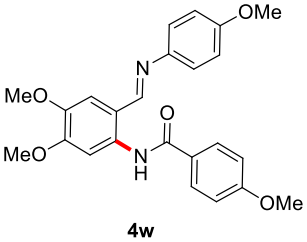
4-bromo-*N*-(2-formyl-4,5-dimethoxyphenyl)benzamide (**3v**). Light yellow solid, m.p. 168.3-171.2 °C, 24 h, 9.3 mg, 51% yield; ^{1}H NMR (600 MHz, $CDCl_3$): δ = 12.33 (s, 1H), 9.83 (s, 1H), 8.67 (s, 1H), 7.93 (d, J = 8.4 Hz, 2H), 7.67 (d, J = 8.4 Hz, 2H), 7.11 (s, 1H), 4.05 (s, 3H), 3.95 (s, 3H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ = 193.6, 165.1, 155.7, 144.8, 137.7, 133.1, 132.1, 129.0, 127.1, 116.5, 114.9, 103.1, 56.5, 56.3 ppm. ESI HRMS: calcd. for C16H14BrNO4+H 364.0184, found 364.0186, 366.0169.



3w

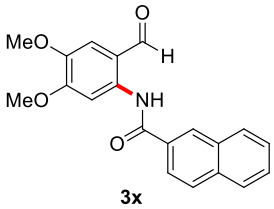
N-(2-formyl-4,5-dimethoxyphenyl)-4-methoxybenzamide (**3w**). Yellow solid, m.p. 151.8-152.1 °C, 24 h, 8.7 mg, 55% yield; ^{1}H NMR (400 MHz, $CDCl_3$): δ = 12.25 (s, 1H), 9.83 (s, 1H), 8.71 (s, 1H), 8.04 (d, J = 8.4 Hz, 2H), 7.09 (s, 1H), 7.02 (d, J = 8.8 Hz, 2H), 4.05 (s, 3H), 3.95 (s, 3H), 3.89 (s, 3H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ = 193.5, 165.8, 162.8, 155.7, 144.4, 138.3, 129.4, 126.6, 116.5, 114.8, 114.1, 103.0, 56.4, 56.2, 55.4 ppm. ESI HRMS: calcd. for $C_{17}H_{17}NO_5$+H 316.1185, found 316.1183.

N-(4,5-dimethoxy-2-(((4-methoxyphenyl)imino)methyl)phenyl)-4-methoxybenzamide (**4w**).



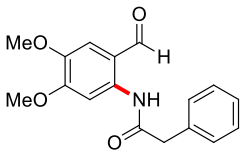
4w

Yellow solid, m.p. 185.8-187.3 °C, 24 h, 3.6 mg, 17% yield; ^{1}H NMR (600 MHz, $CDCl_3$): δ = 13.64 (s, 1H), 8.79 (s, 1H), 8.54 (s, 1H), 8.08 (d, J = 8.4 Hz, 2H), 7.27-7.25 (m, 2H), 6.97 (t, J = 7.8 Hz, 5H), 4.02 (s, 3H), 3.93 (s, 3H), 3.88 (s, 3H), 3.86 (s, 3H) ppm; ^{13}C NMR (151 MHz, $CDCl_3$): δ = 165.9, 162.3, 160.2, 158.4, 151.9, 144.1, 143.3, 136.2, 129.4, 127.7, 121.7, 115.6, 114.6, 113.9, 113.7, 103.5, 56.2, 56.1, 55.5, 55.4 ppm. ESI HRMS: calcd. for $C_{24}H_{24}N_2O_5$+H 421.1763, found 421.1769.



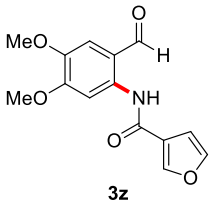
3x

N-(2-formyl-4,5-dimethoxyphenyl)-2-naphthamide (**3x**). Yellow solid, m.p. 173.9-174.4 °C, 24 h, 7.7 mg, 46% yield; ^{1}H NMR (400 MHz, $CDCl_3$): δ = 12.49 (s, 1H), 9.87 (s, 1H), 8.77 (s, 1H), 8.60 (s, 1H), 8.11 (d, J = 8.4 Hz, 1H), 8.04-7.97 (m, 2H), 7.90 (d, J = 7.6 Hz, 1H), 7.62-7.55 (m, 2H), 7.12 (s, 1H), 4.07 (s, 3H), 3.95 (s, 3H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ = 193.5, 166.2, 155.7, 144.6, 138.0, 135.1, 132.7, 131.5, 129.4, 128.8, 128.6, 128.1, 127.7, 126.8, 123.5, 116.5, 115.0, 103.2, 56.5, 56.3 ppm. ESI HRMS: calcd. for $C_{20}H_{17}NO_4$+H 336.1236, found 336.1240.



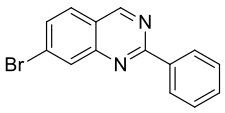
3y

N-(2-formyl-4,5-dimethoxyphenyl)-2-phenylacetamide (**3y**). White solid, m.p. 117.8-119.6 °C, 24 h, 8.7 mg, 58% yield; ^{1}H NMR (600 MHz, $CDCl_3$): δ = 11.33 (s, 1H), 9.67 (s, 1H), 8.49 (s, 1H), 7.41-7.32 (m, 5H), 7.00 (s, 1H), 3.97 (s, 3H), 3.90 (s, 3H), 3.77 (s, 2H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ = 193.0, 170.7, 155.4, 144.5, 137.4, 134.0, 129.6, 128.9, 127.4, 116.3, 114.7, 103.0, 56.4, 56.2, 45.6 ppm. ESI HRMS: calcd. for $C_{17}H_{18}NO_4$+Na 322.1055, found 322.1056.



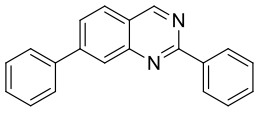
3z

N-(2-formyl-4,5-dimethoxyphenyl)furan-2-carboxamide (**3z**). White solid, m.p. 154.0-154.5 °C, 24 h, 3.0 mg, 22% yield; ^{1}H NMR (400 MHz, $CDCl_3$): δ = 11.99 (s, 1H), 9.81 (s, 1H), 8.60 (s, 1H), 8.15 (s, 1H), 7.51 (s, 1H), 7.08 (s, 1H), 6.91 (s, 1H), 4.03 (s, 3H), 3.94 (s, 3H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ = 193.5, 161.6, 155.7, 145.8, 144.6, 144.2, 137.8, 123.4, 116.4, 114.5, 108.4, 102.9, 56.4, 56.2 ppm. ESI HRMS: calcd. for $C_{14}H_{13}NO_5$+H 276.0872, found 276.0819.



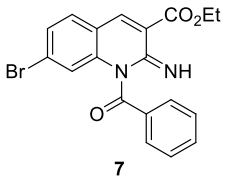
5

2-(4-bromophenyl)quinazoline (**5**). White solid, m.p. 172.9-175.3 °C, 24 h, 34 mg, 92% yield; ^{1}H NMR (600 MHz, $CDCl_3$): δ = 9.43 (s, 1H), 8.59 (d, J = 6.0 Hz, 2H), 8.28 (s, 1H), 7.79 (d, J = 9.0 Hz, 1H), 7.69 (d, J = 8.4 Hz, 1H), 7.54-7.52 (m, 3H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ = 161.8, 160.3, 151.4, 137.6, 131.1, 130.9, 130.9, 128.9, 128.7, 128.6, 128.3, 122.1 ppm. ESI HRMS: calcd. for $C_{14}H_9BrN_2$+H 285.0027, found 285.0021.



6

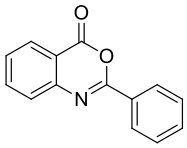
2,7-diphenylquinazoline (**6**).White solid, m.p. 211.3-212.8 °C, 24 h, 32 mg, 80% yield; ^{1}H NMR (400 MHz, $CDCl_3$): δ = 9.49 (s, 1H), 8.63 (d, J = 6.8 Hz, 2H), 8.31 (s, 1H), 8.01 (d, J = 8.0 Hz, 1H), 7.89 (d, J = 8.0 Hz, 1H), 7.79 (d, J = 7.6 Hz, 2H), 7.56-7.47 (m, 6H) ppm; ^{13}C NMR (151 MHz, $CDCl_3$) δ 161.4, 160.1, 151.1, 146.8, 139.6, 138.0, 130.6, 129.1, 128.6, 128.5, 128.5, 127.6, 127.5, 127.0, 126.1, 122.5 ppm. ESI HRMS: calcd. for $C_{20}H_{14}N_2$+H 283.1235, found 283.1251.



7

ethyl 1-benzoyl-7-bromo-2-imino-1,2-dihydroquinoline-3-carboxylate (**7**). White solid, m.p. 161.3-162.8 °C, 24 h, 43 mg, 83% yield; ^{1}H NMR (400 MHz, $CDCl_3$): δ = 11.90 (s, 1H), 8.87 (s, 1H), 8.32 (d, J = 1.2 Hz, 1H), 8.11-8.09 (m, 2H), 7.67 (d, J = 8.8 Hz, 1H), 7.60-7.51 (m, 4H), 4.49 (q, J = 7.2 Hz,

2H), 1.48 (t, J = 7.2 Hz, 3H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ = 166.9, 164.4, 149.5, 142.2 , 134.7, 132.2, 131.1, 129.6, 129.6, 128.8, 127.6, 127.5, 122.7, 112.7, 77.3, 77.0, 76.7, 62.5, 14.2 ppm. ESI HRMS: calcd. for $C_{19}H_{15}BrN_2O_3$+H 399.0344, found 399.0343, 401.0330.



8

2-phenyl-4H-benzo[*d*][1,3]oxazin-4-one (**8**). White solid, m.p. 121.9-124.7 °C, 24 h, 22 mg, 76% yield; ^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.32 (d, J = 7.6 Hz, 2H), 8.25 (d, J = 7.6 Hz, 1H), 7.83 (d, J = 7.2 Hz, 1H), 7.70 (d, J = 8.0 Hz, 1H), 7.60-7.58 (m, 4H) ppm. T+he structure has been reported by previous literatures[4].

References

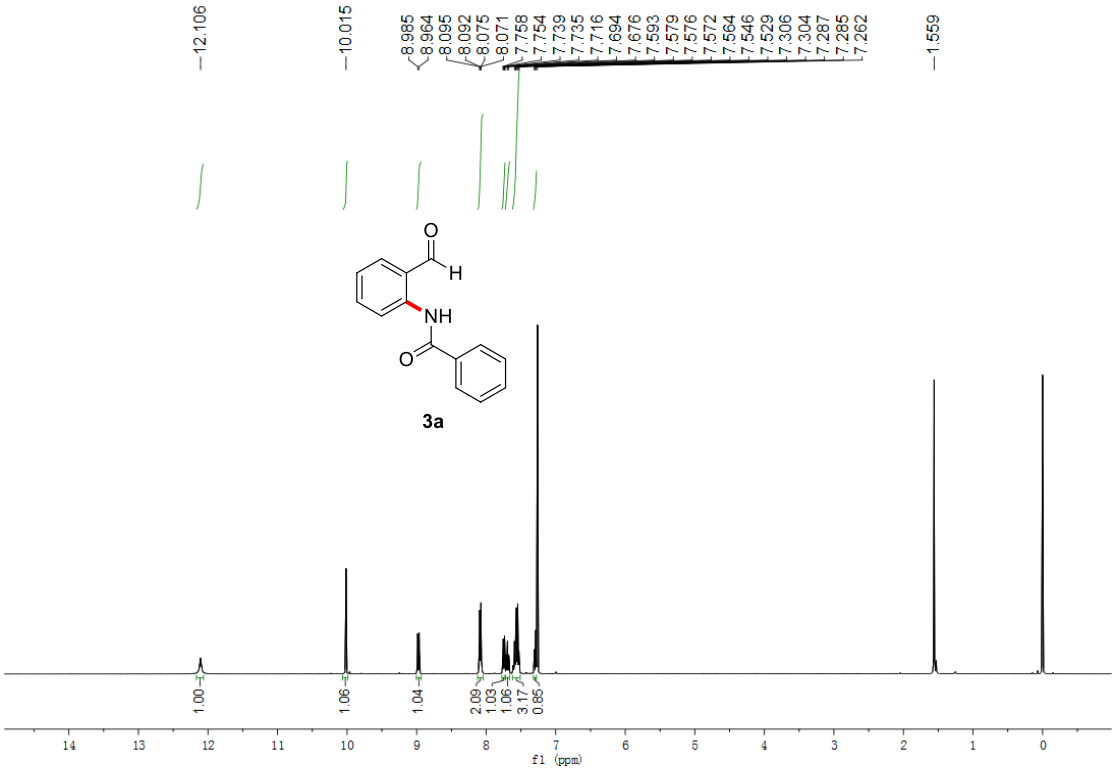
[1]. Bizet, V.; Buglioni, L.; Bolm, C. *Angew. Chem. Int. Ed.* **2014**, *53*, 5639.

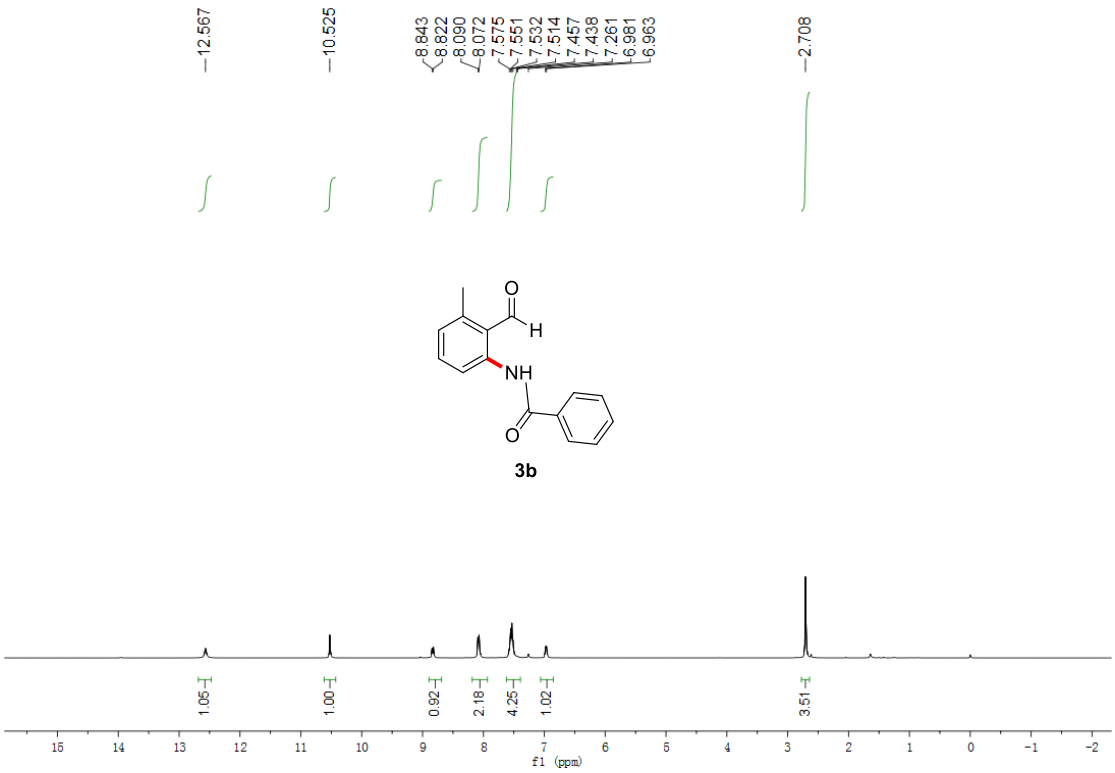
[2]. Wang, Q.; Wang, F.; Yang, X. F.; Zhou, X. K.; Li, X. W. *Org. Lett.* **2016**, *18*, 6144.

[3]. Deng, H.; Li, H. J.; Zhang, W. G.; Wang, L. *Chem. Commun.* **2017**, *53*, 10322.

[4]. Yu, J. C.; Zhang-Negrerie, D.; Du, Y. F. *Eur. J. Org. Chem.* **2016**, 562.

6. NMR Spectra of Amidation Compounds and Structure Determination

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8.090
8.072
7.575
7.551
7.532
7.514
7.457
7.438
7.261
6.981
6.963
2.708
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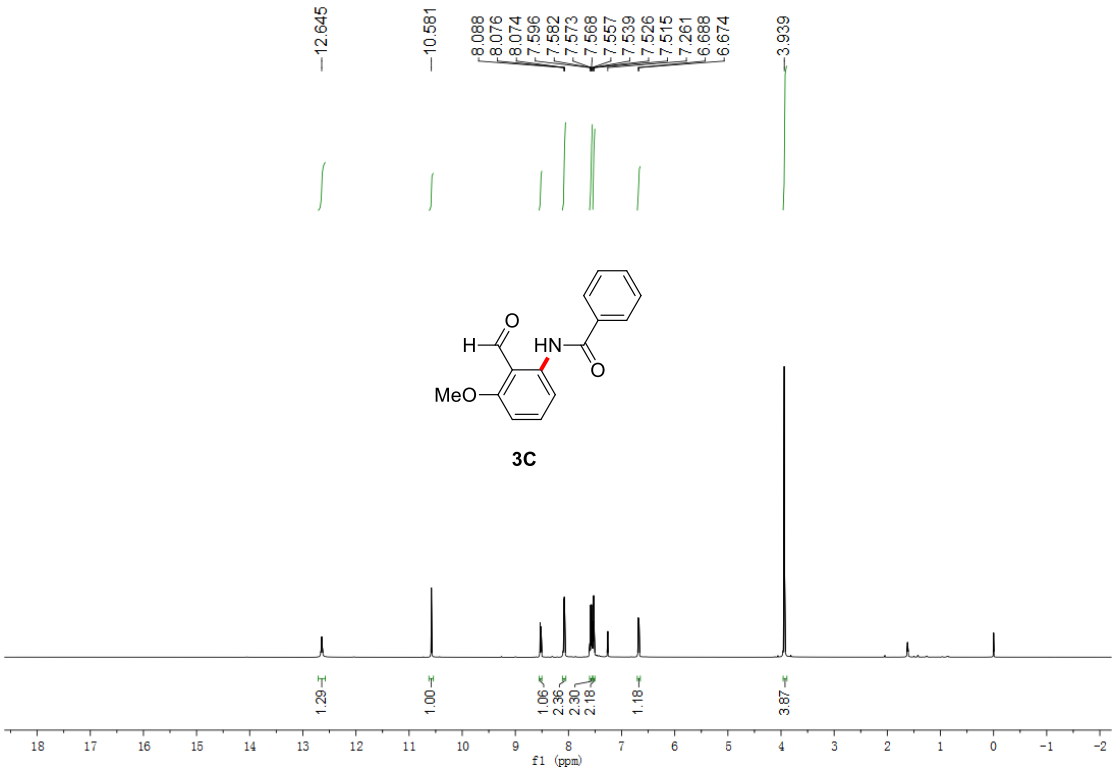
H
NH
O
1.05
1.00
0.92
2.18
4.25
1.02
3.51
f1 (ppm)

3b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7.515
7.261
6.688
6.674
3.939
O
H
HN
O
MeO
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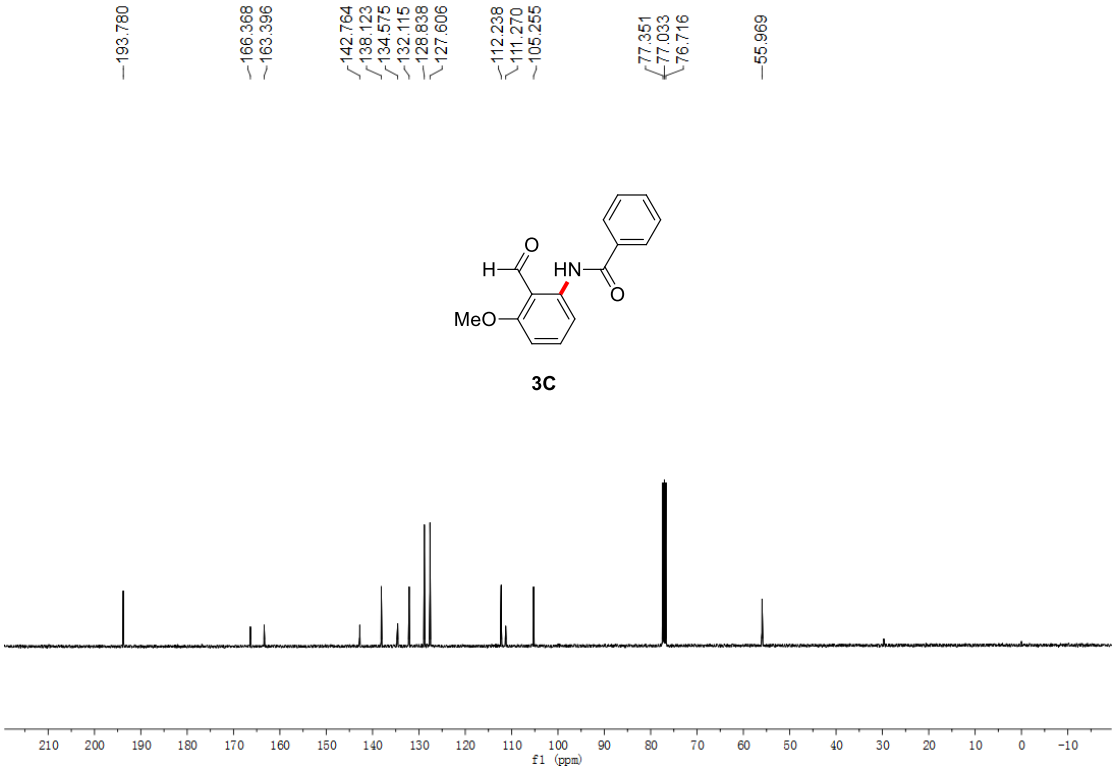
1.00
1.06
2.36
2.30
2.18
1.18
3.87
f1 (ppm)

3C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77.351
77.033
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HN
O
MeO
3C
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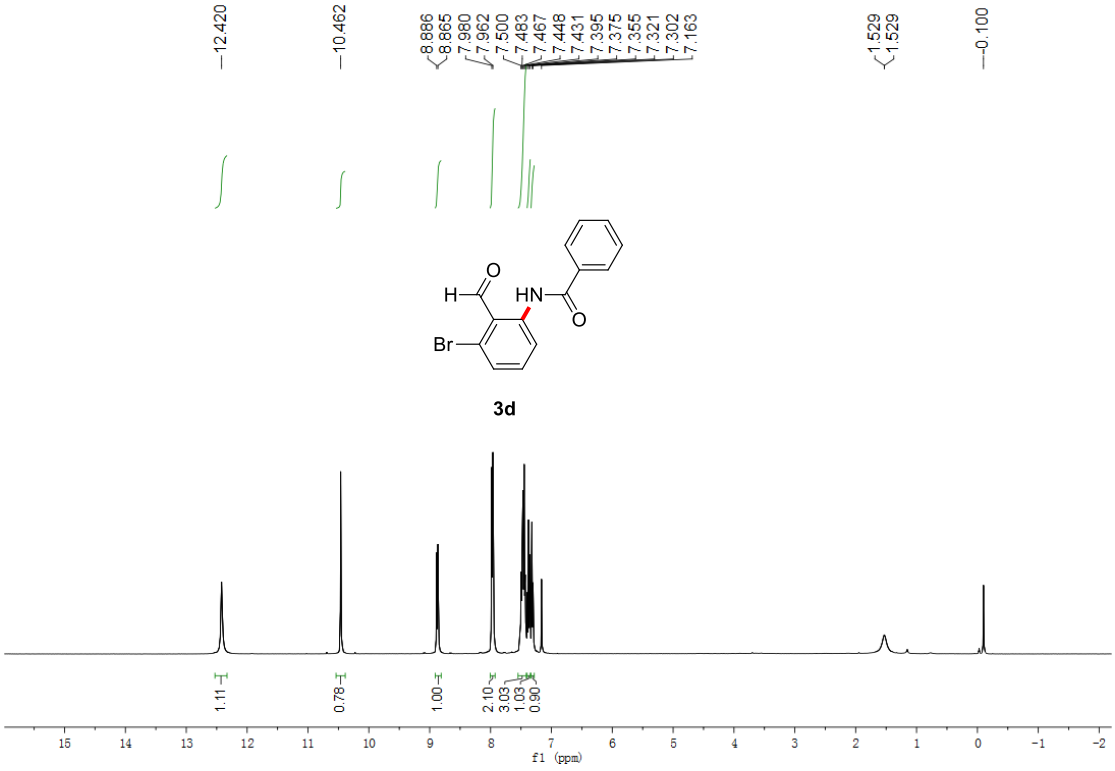
f1 (ppm)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7.375
7.355
7.321
7.302
7.163
1.529
1.529
0.100
O
H
HN
O
Br
3d
1.11
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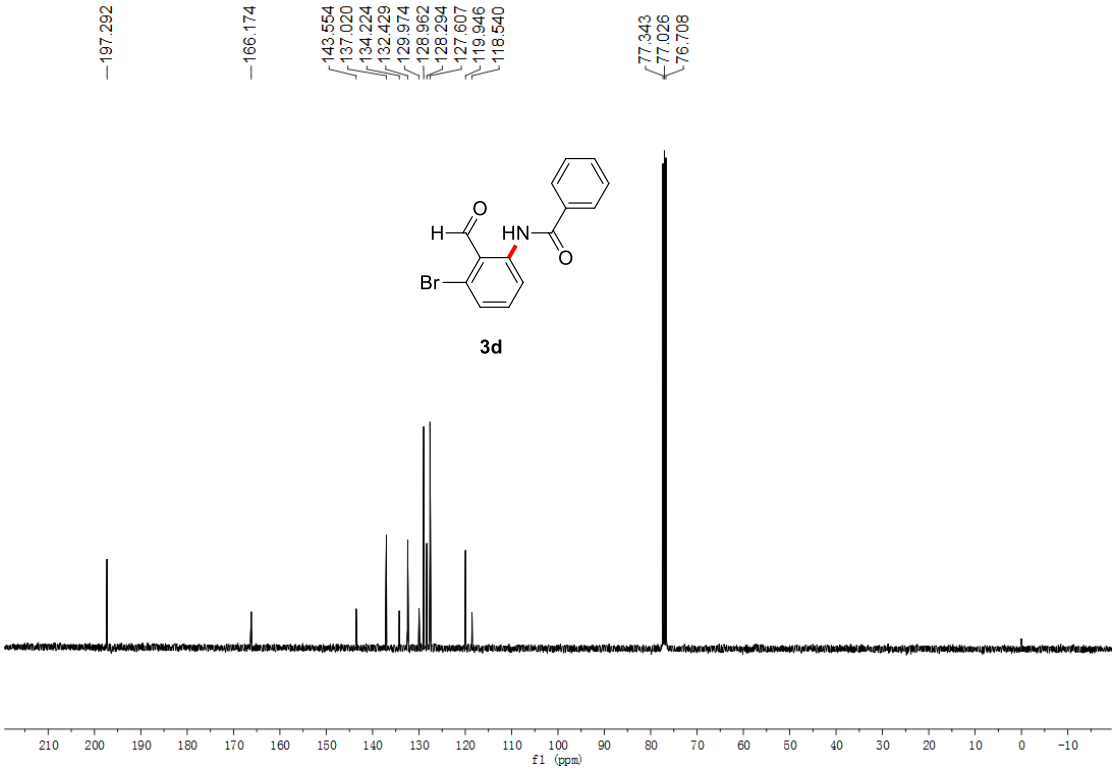
2.10
3.03
1.03
0.90
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2
f1 (ppm)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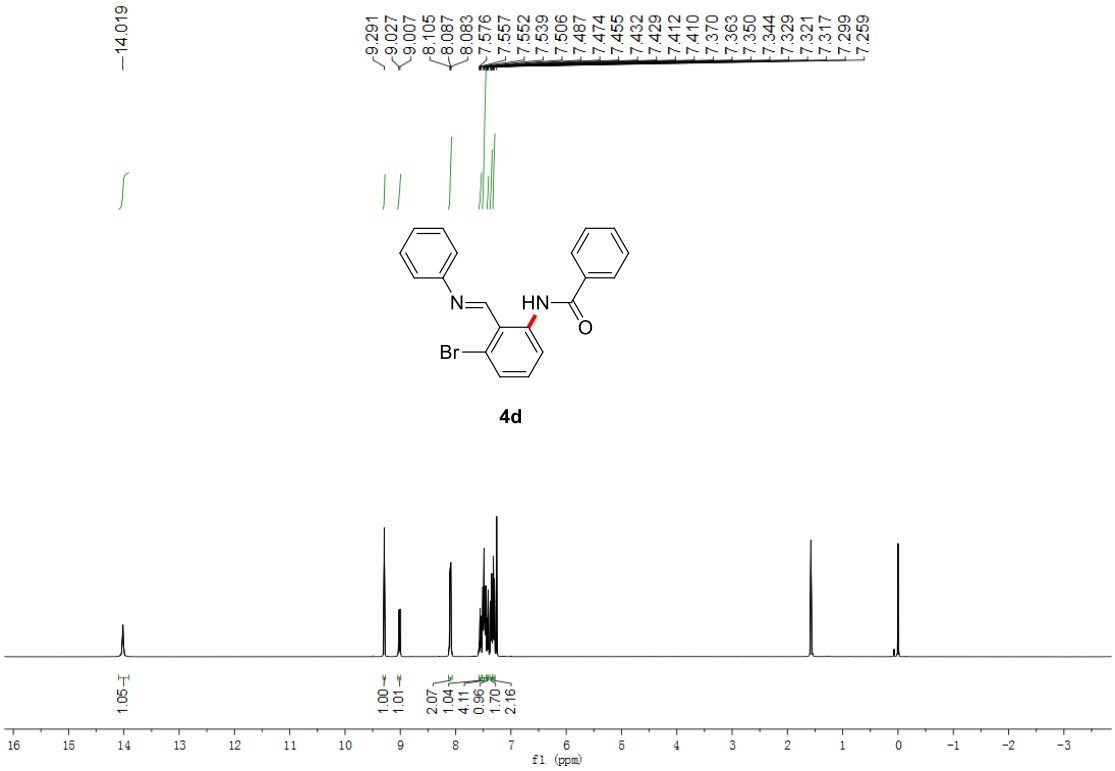
H
HN
O
Br
3d
f1 (ppm)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7.487
7.474
7.455
7.432
7.429
7.412
7.410
7.370
7.363
7.350
7.344
7.329
7.321
7.317
7.299
7.259
N
HN
O
Br
4d
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1.00
1.01
2.07
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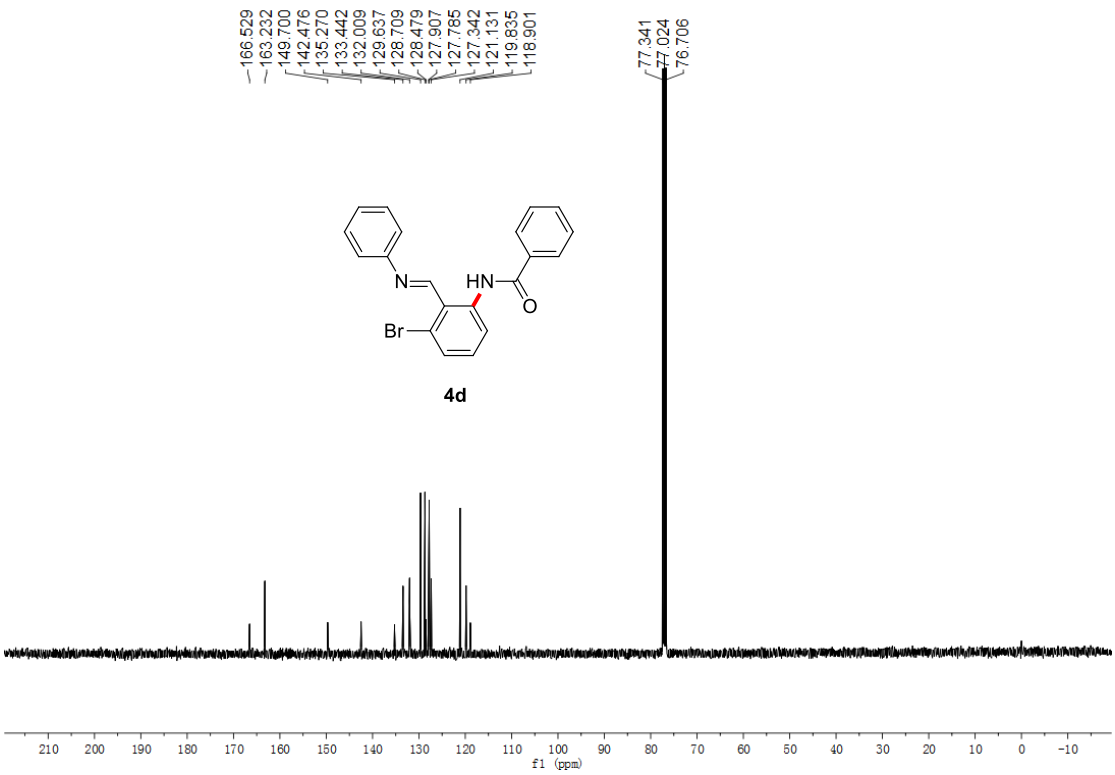
2.16
f1 (ppm)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127.907
127.785
127.342
121.131
119.835
118.901
77.341
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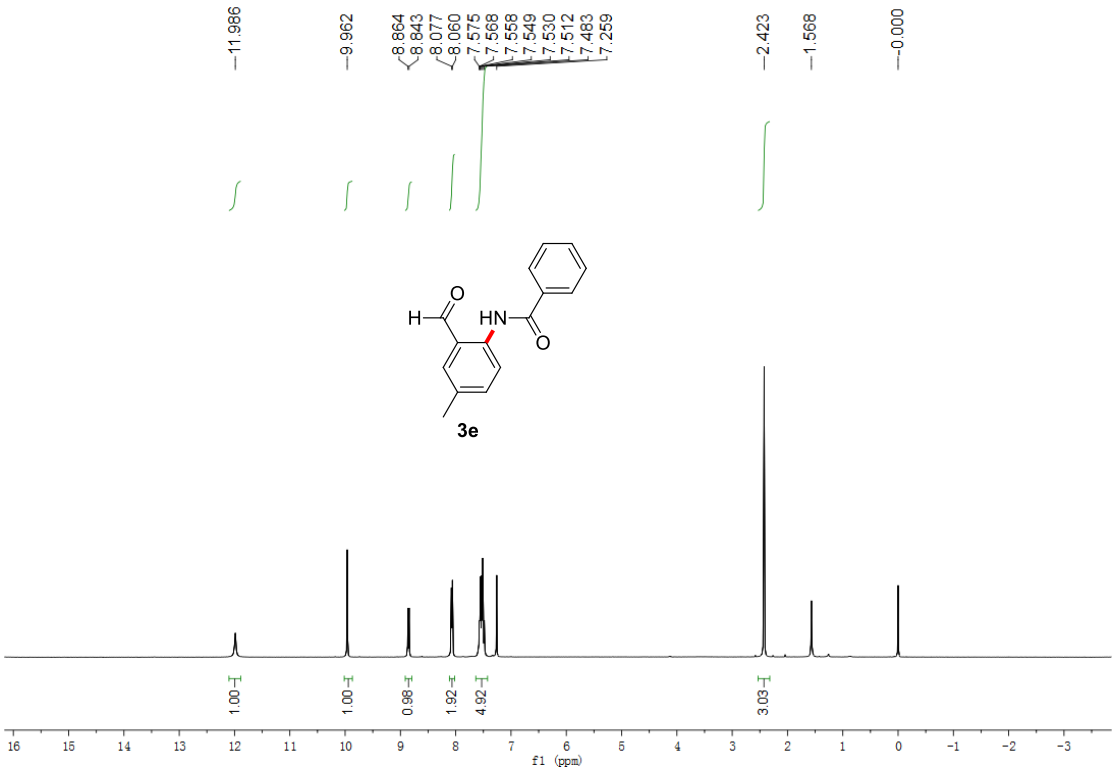
O
Br
4d
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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7.568
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7.549
7.530
7.512
7.483
7.259
2.423
1.568
0.000
O
H
HN
O
3e
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3.03
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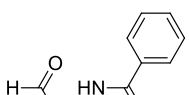
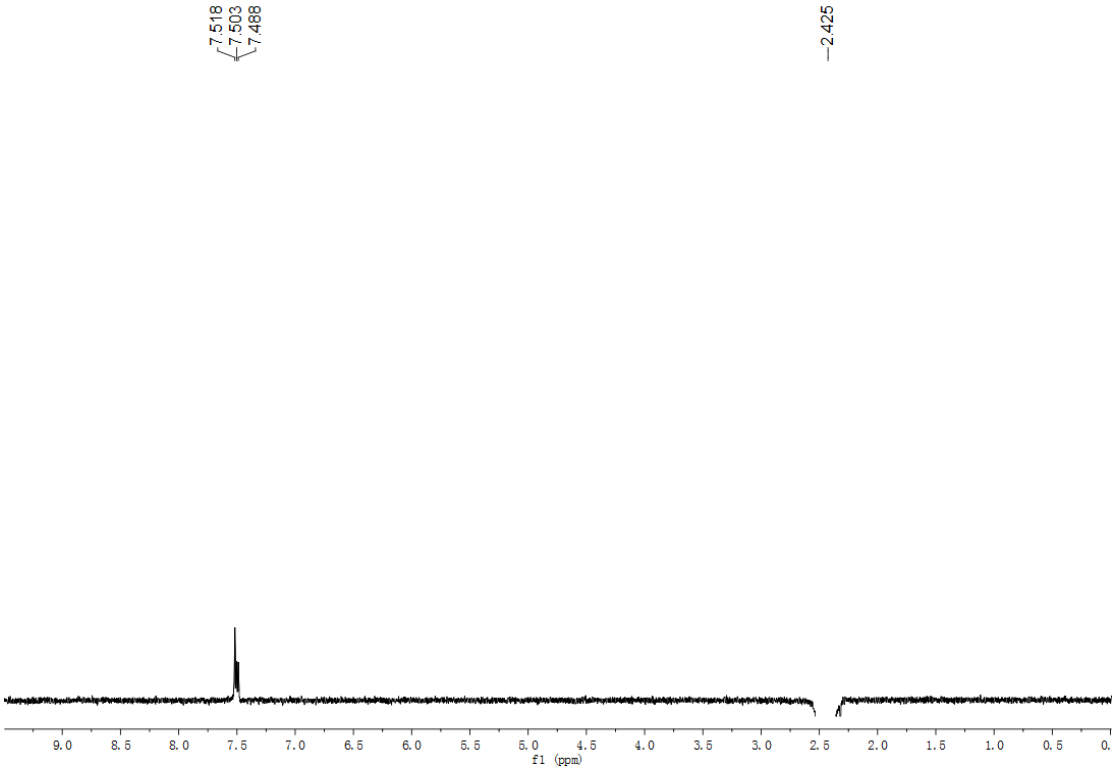
f1 (ppm)


O
H
HN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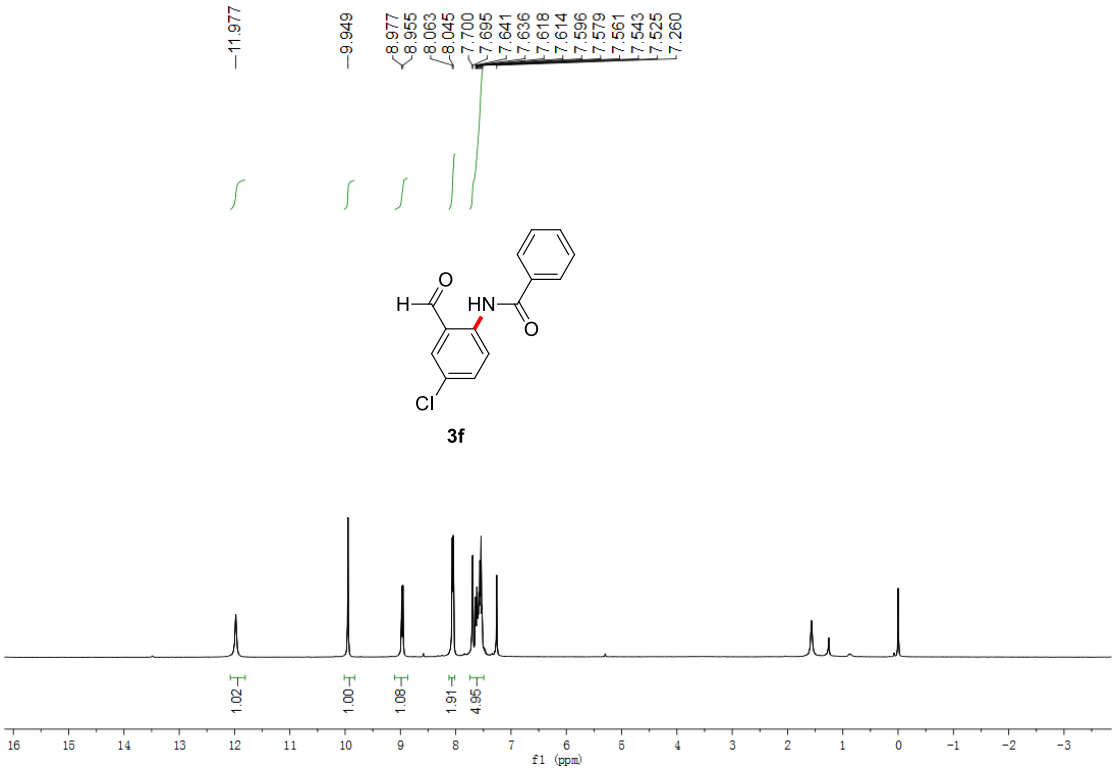
7.503
7.488
2.425
f1 (ppm)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7.700
7.695
7.641
7.636
7.618
7.614
7.596
7.579
7.561
7.543
7.525
7.260
O
H
HN
O
Cl
1.02
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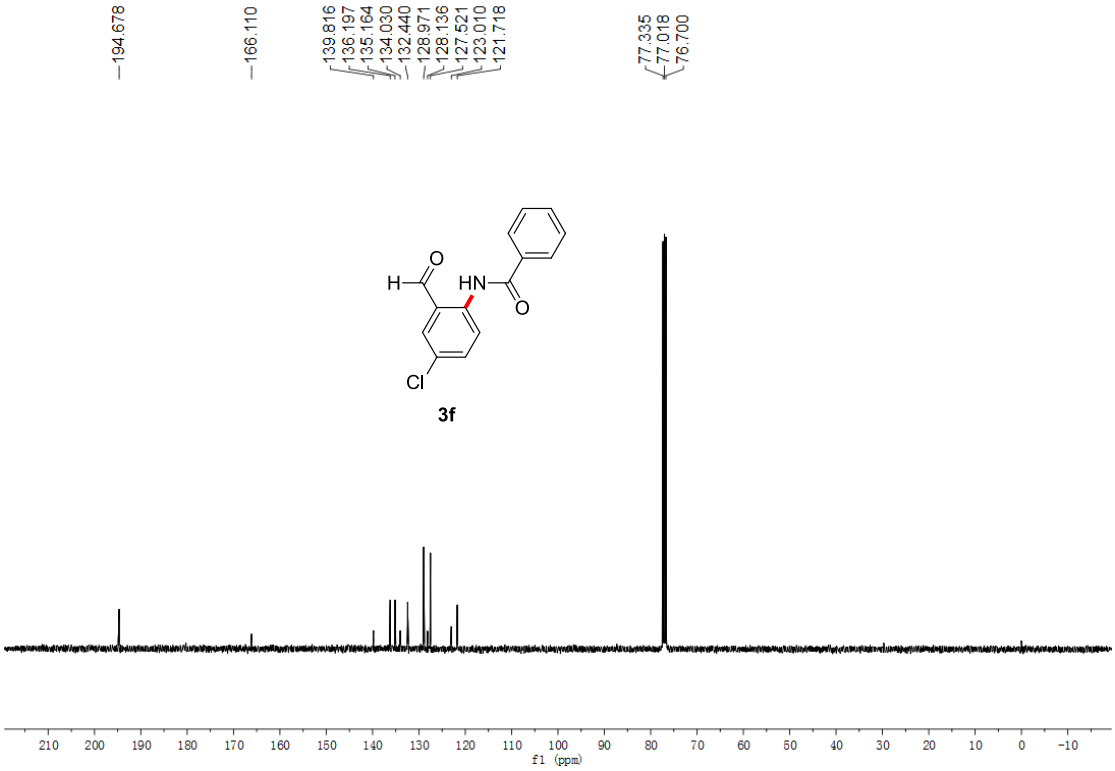
1.08
1.91
4.95
f1 (ppm)

3f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134.030
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76.700
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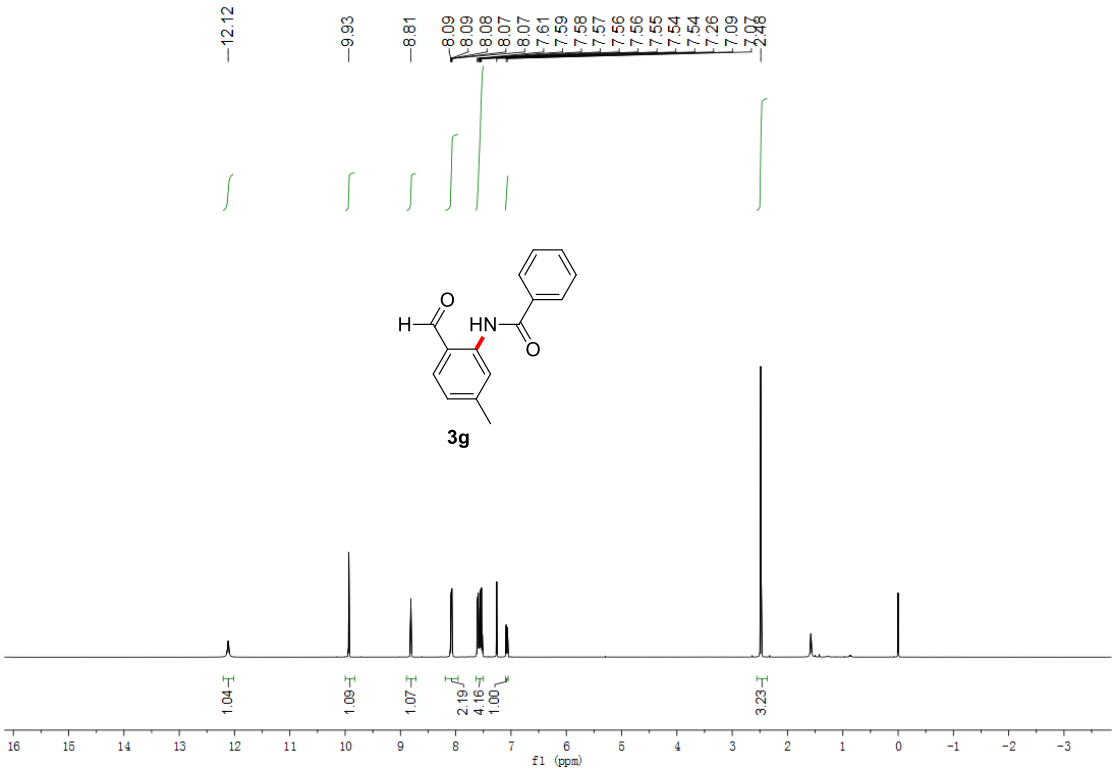
H
HN
O
Cl
3f
f1 (ppm)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8.09
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8.07
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7.58
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7.56
7.56
7.55
7.54
7.54
7.26
7.09
7.07
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O
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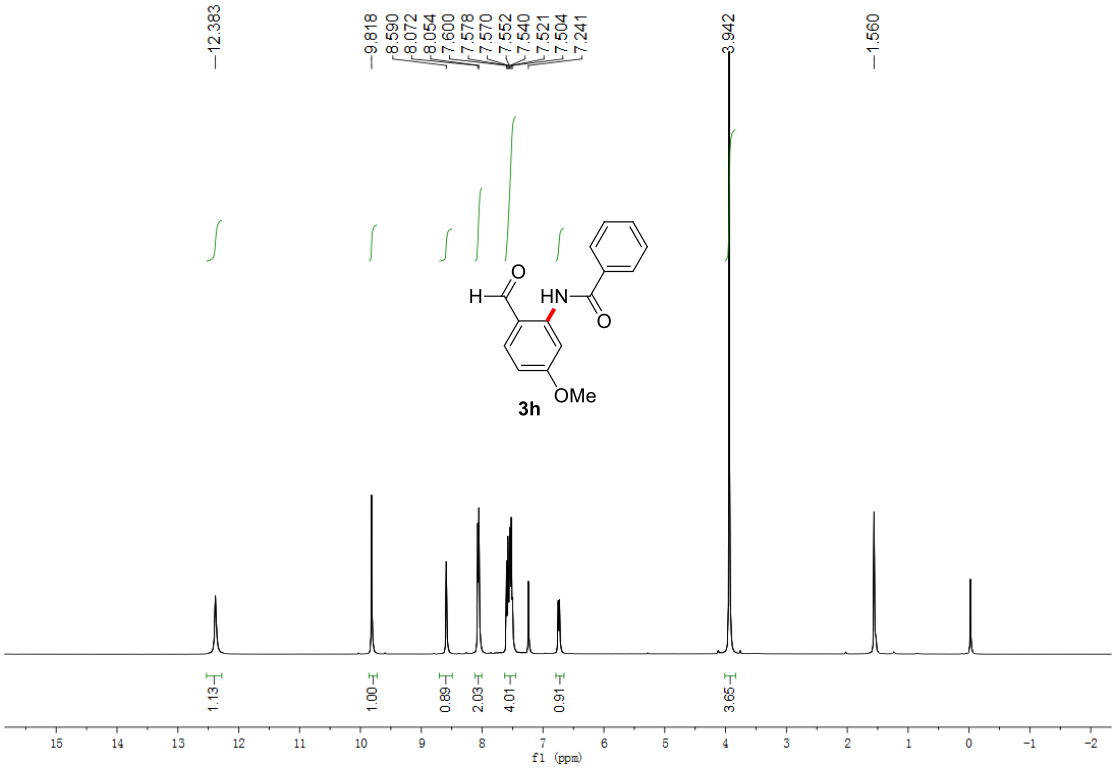
1.09
1.07
2.19
4.16
1.00
3.23
f1 (ppm)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7.540
7.521
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7.241
3.942
1.560
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OMe
3h
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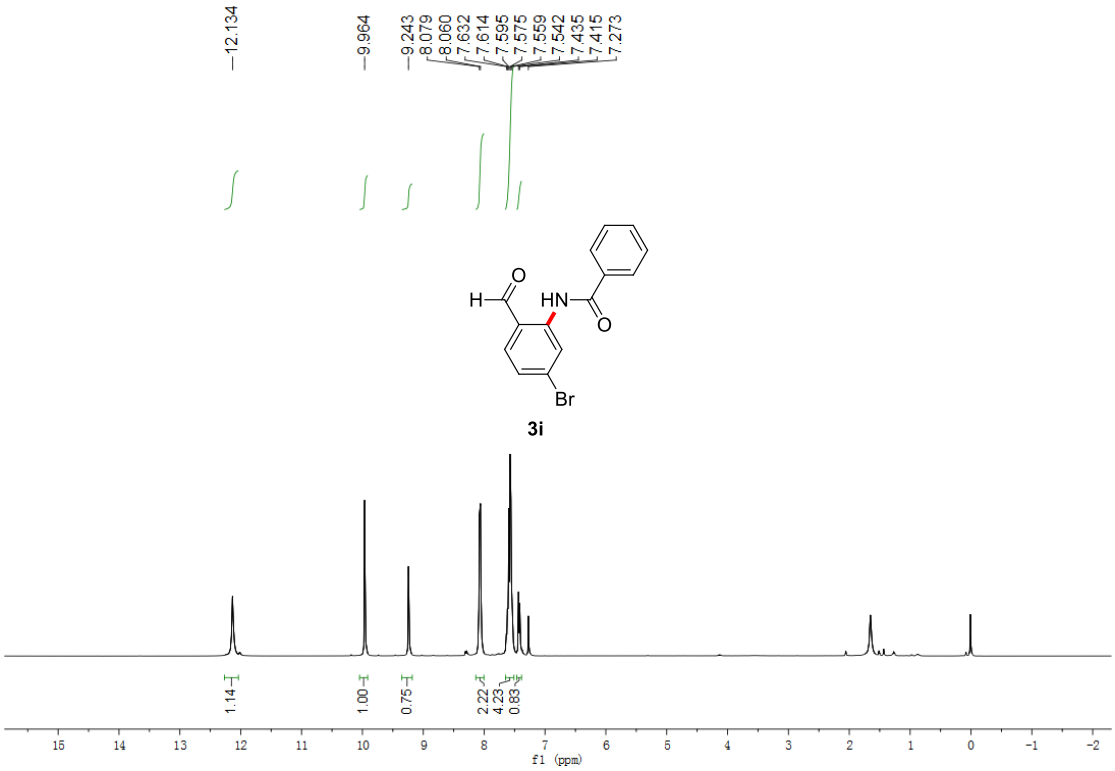
4.01
0.91
3.65
f1 (ppm)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8.060
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7.614
7.595
7.575
7.559
7.542
7.435
7.415
7.273
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H
HN
O
Br
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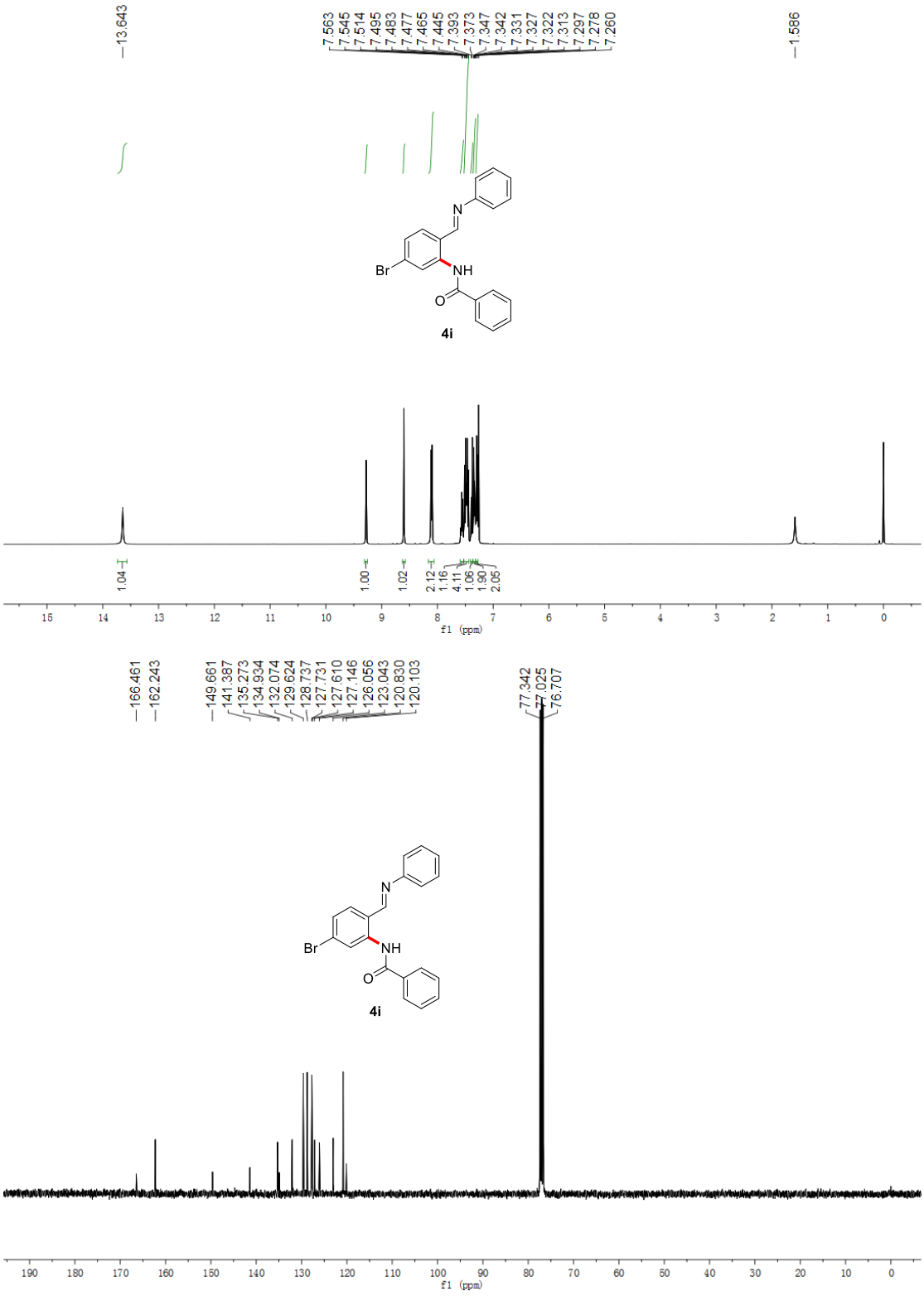
4.23
0.83
f1 (ppm)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7.393
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7.342
7.331
7.327
7.322
7.313
7.297
7.278
7.260
1.586
N
Br
NH
O
4i
1.04
1.00
1.02
2.12
1.16
4.11
1.06
1.90
2.05
f1 (ppm)
166.461
162.243
149.661
141.387
135.273
134.934
132.074
129.624
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127.146
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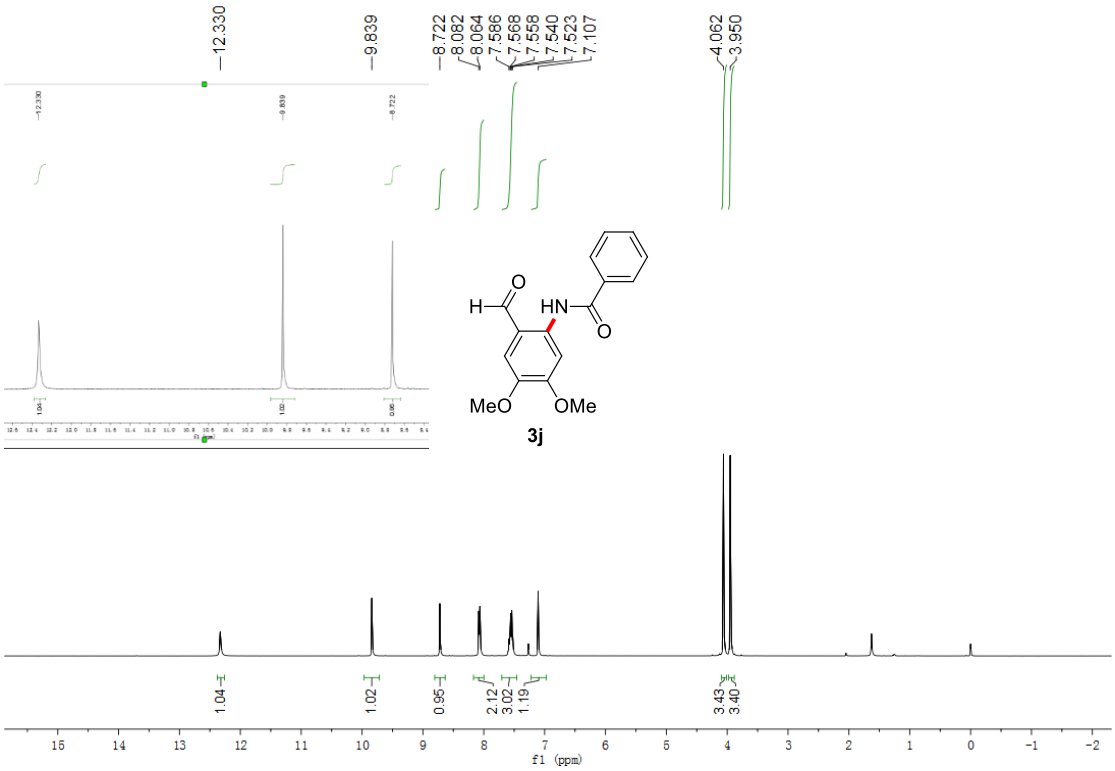
f1 (ppm)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7.523
7.107
4.062
3.950
H
O
HN
O
MeO
OMe
3j
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1.02
0.96
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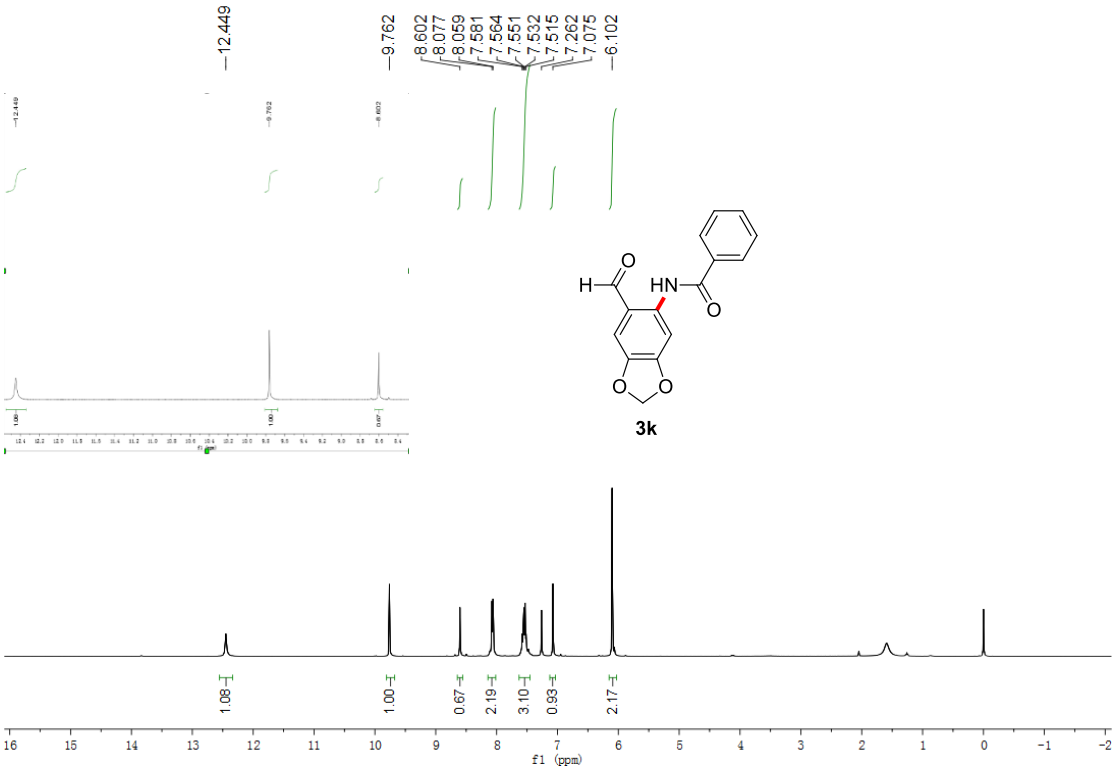
f1 (ppm)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7.515
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7.075
6.102
H
O
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O
O
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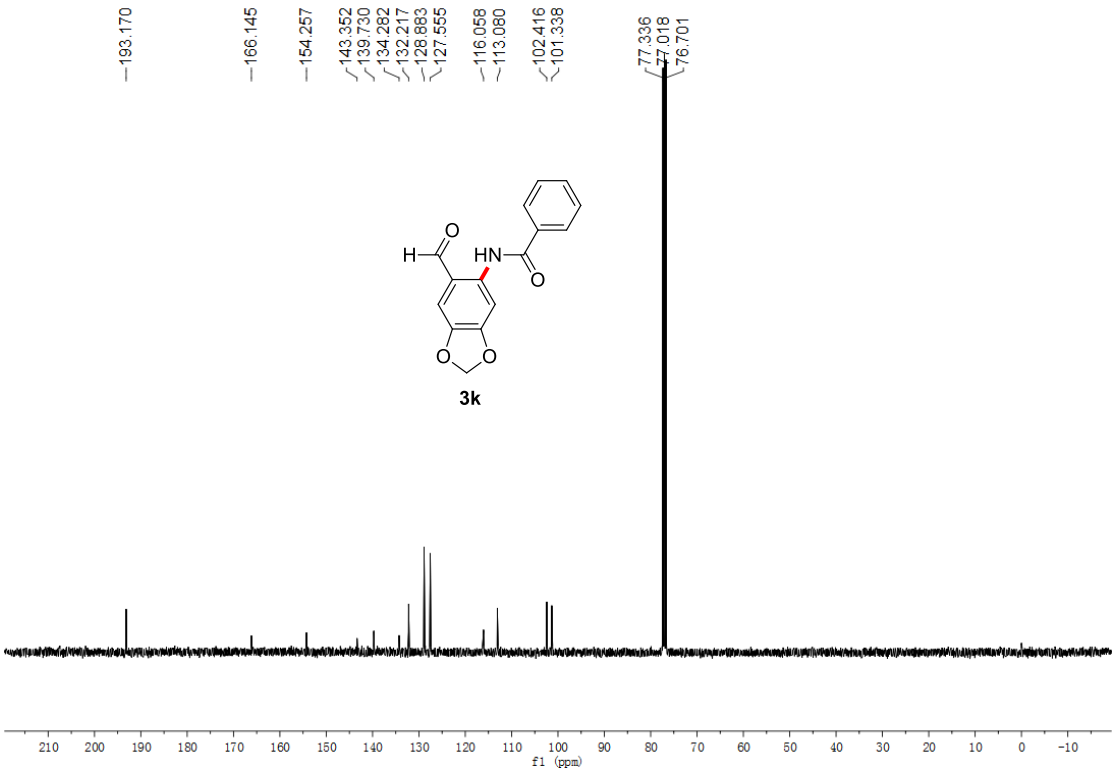
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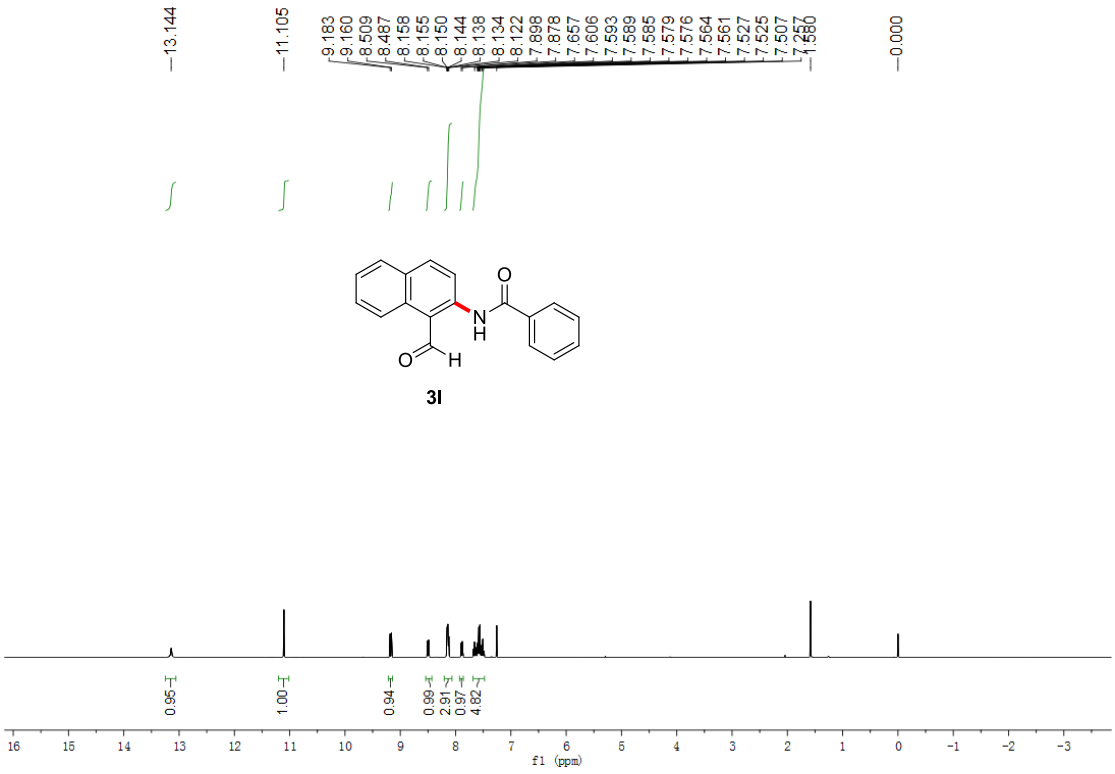
O
3k
f1 (ppm)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7.878
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7.606
7.593
7.589
7.585
7.579
7.576
7.564
7.561
7.527
7.525
7.507
7.257
1.580
0.000
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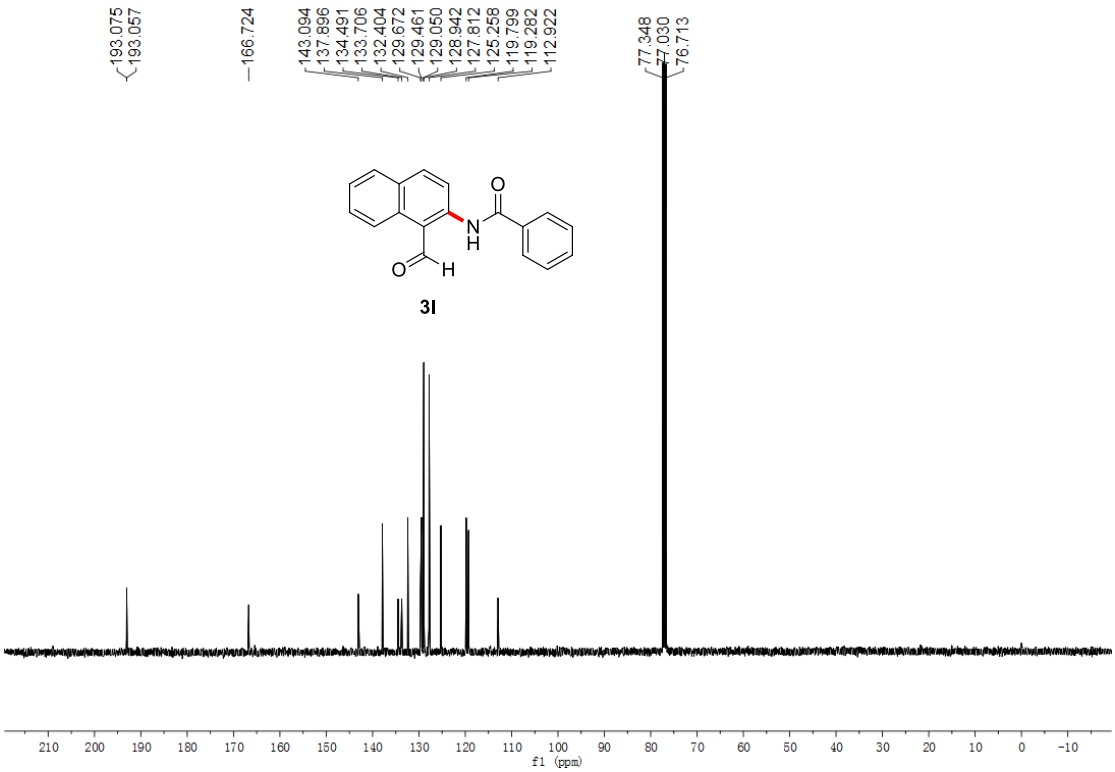
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132.404
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128.942
127.812
125.258
119.799
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112.922
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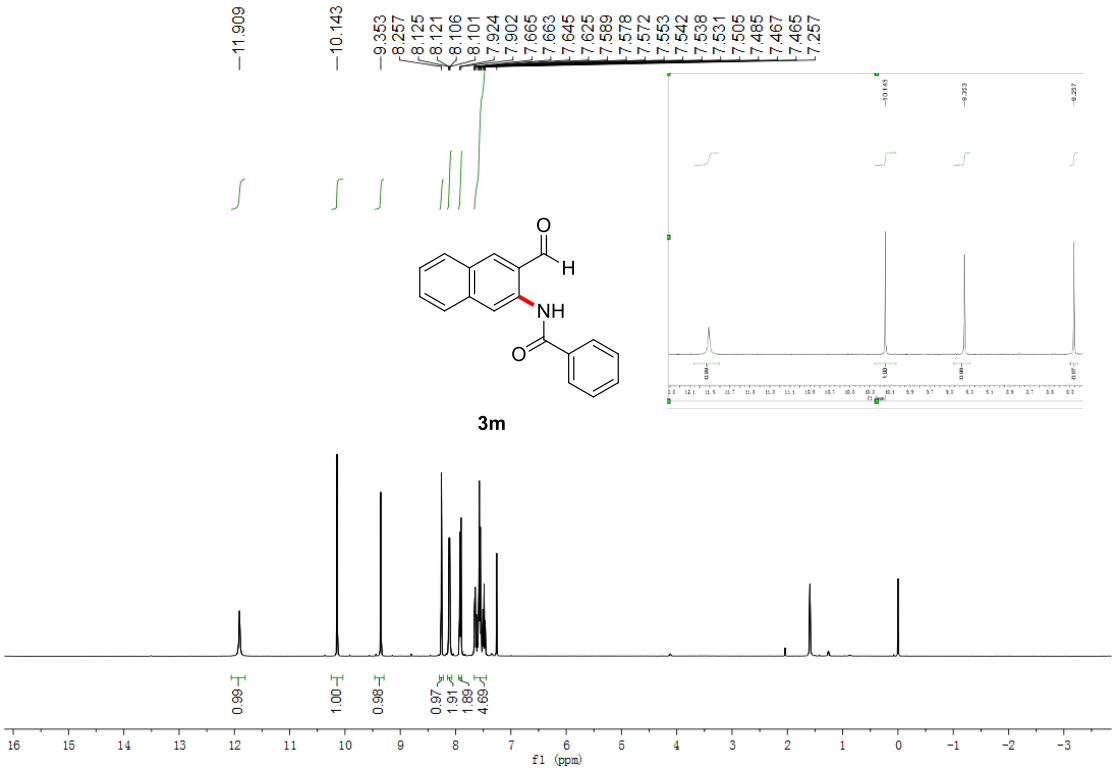
77.030
76.713
O
N
H
O
H
3l
f1 (ppm)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7.902
7.665
7.663
7.645
7.625
7.589
7.578
7.572
7.553
7.542
7.538
7.531
7.505
7.485
7.467
7.465
7.257
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O
3m
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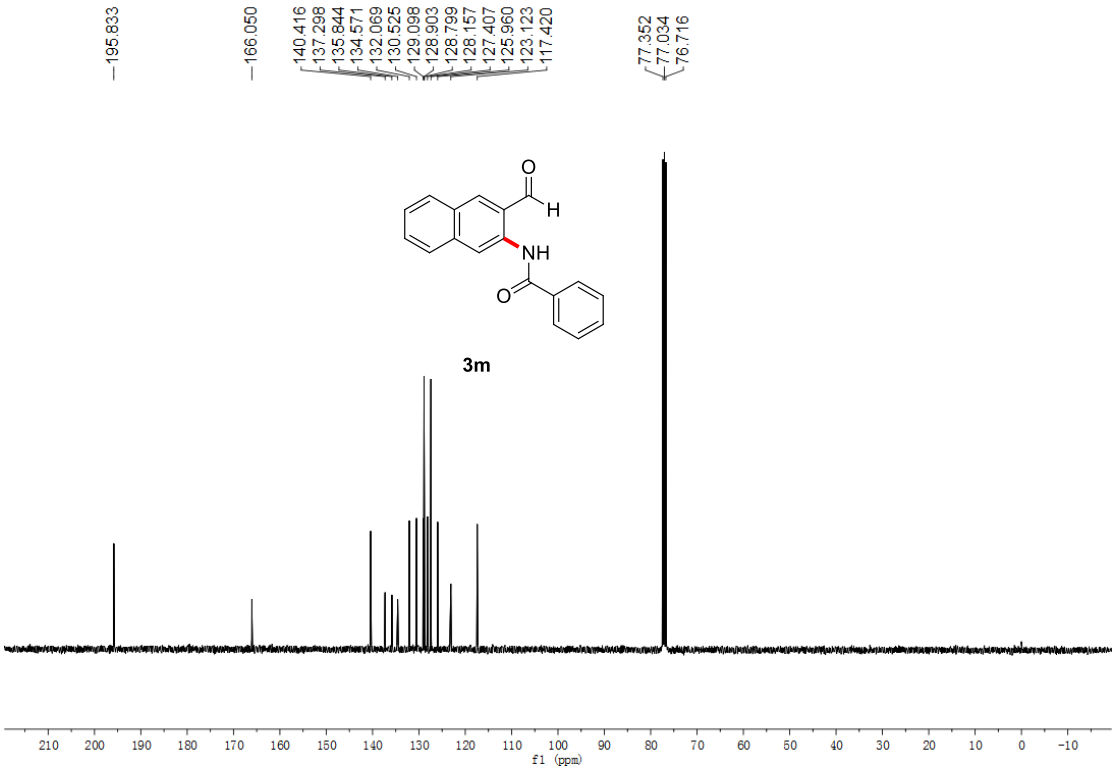
1.89
4.69
f1 (ppm)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134.571
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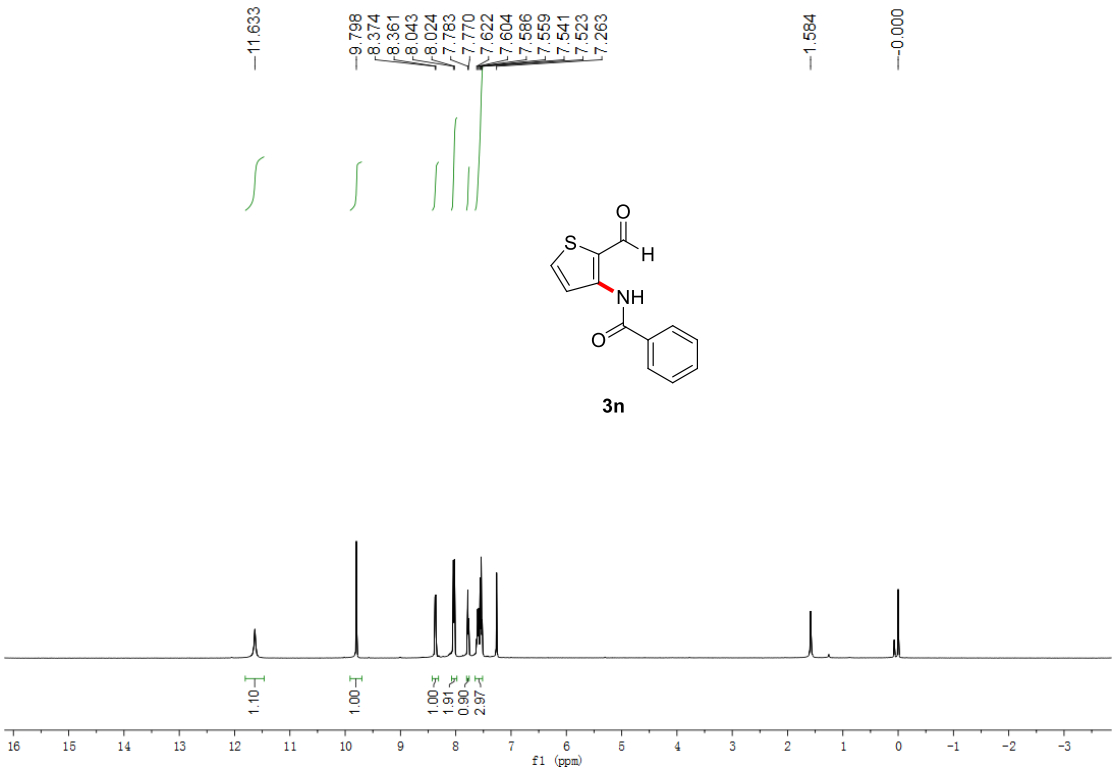
128.903
128.799
128.157
127.407
125.960
123.123
117.420
77.352
77.034
76.716
O
H
NH
O
3m
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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8.024
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7.770
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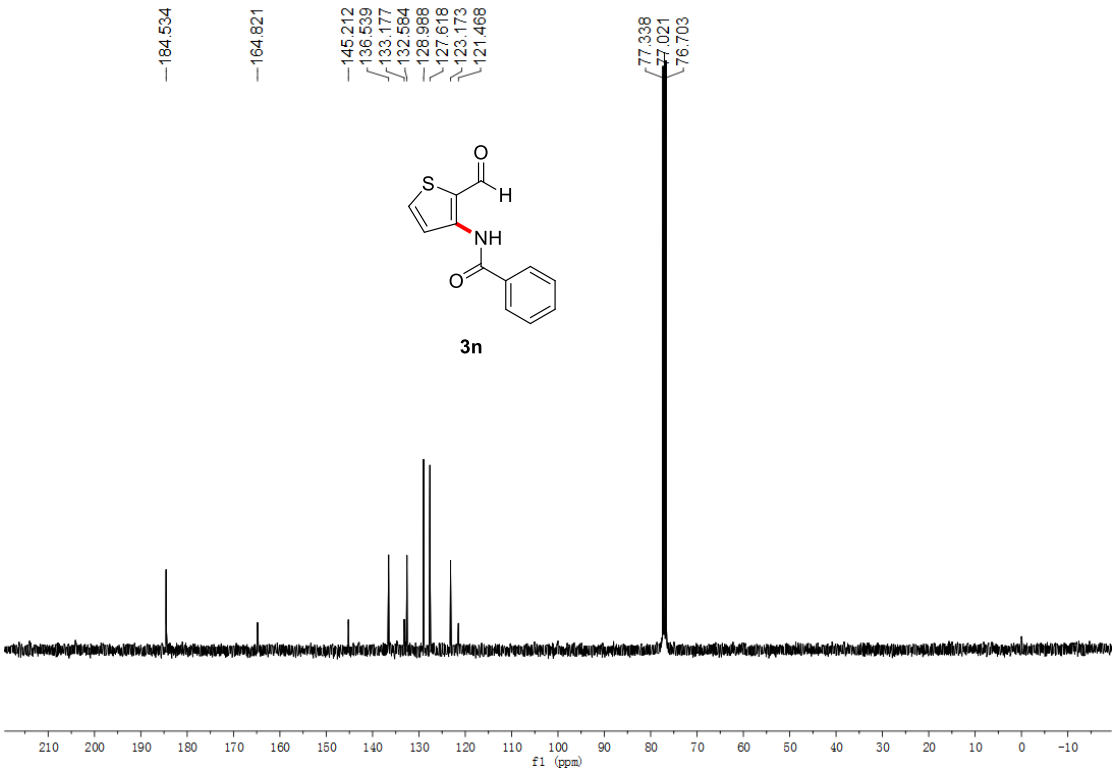
7.604
7.586
7.559
7.541
7.523
7.263
1.584
0.000
O
S
H
NH
O
3n
1.10
1.00
1.00
1.91
0.90
2.97
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3
f1 (ppm)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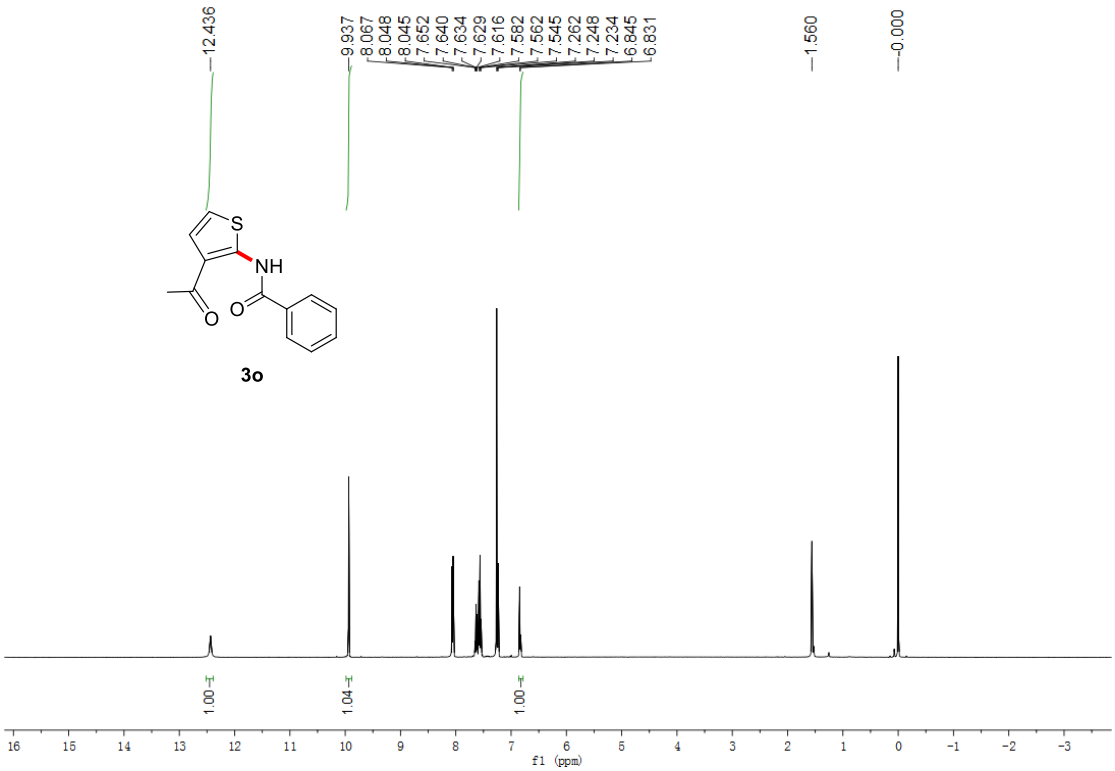
76.703
O
S
H
NH
O
3n
f1 (ppm)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7.616
7.582
7.562
7.545
7.262
7.248
7.234
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1.560
0.000
S
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O
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3o
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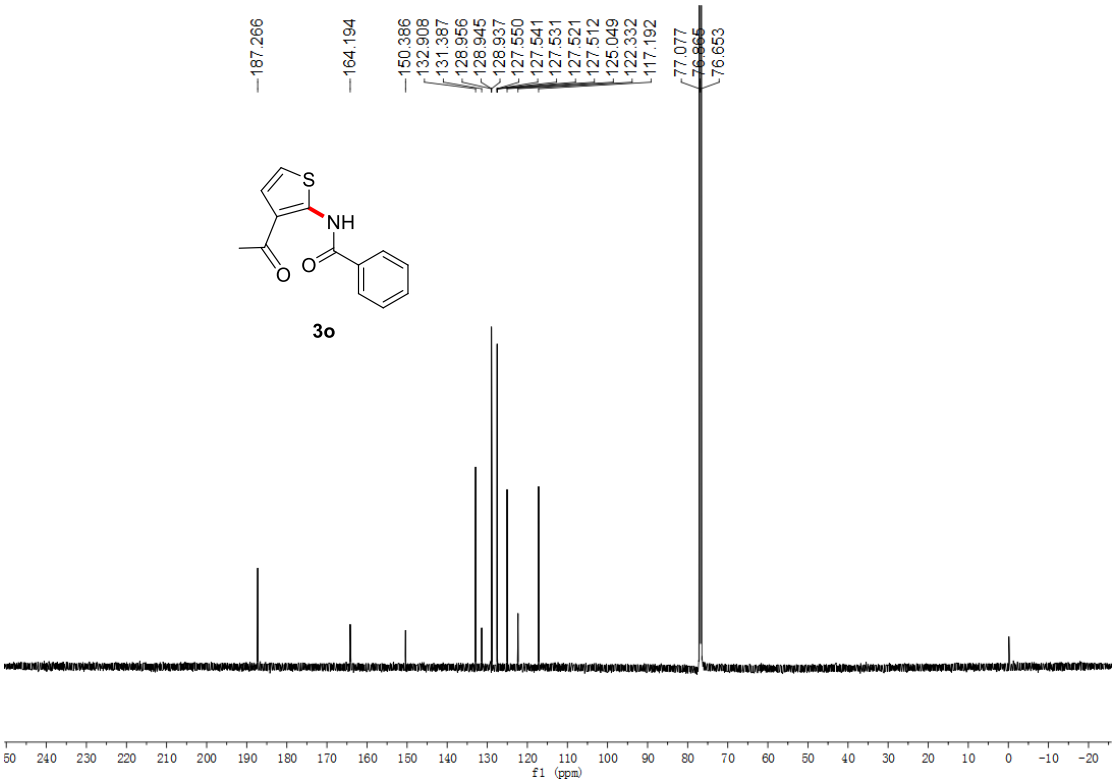
1.04
1.00
f1 (ppm)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128.937
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127.521
127.512
125.049
122.332
117.192
77.077
76.865
76.653
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O
O
3o
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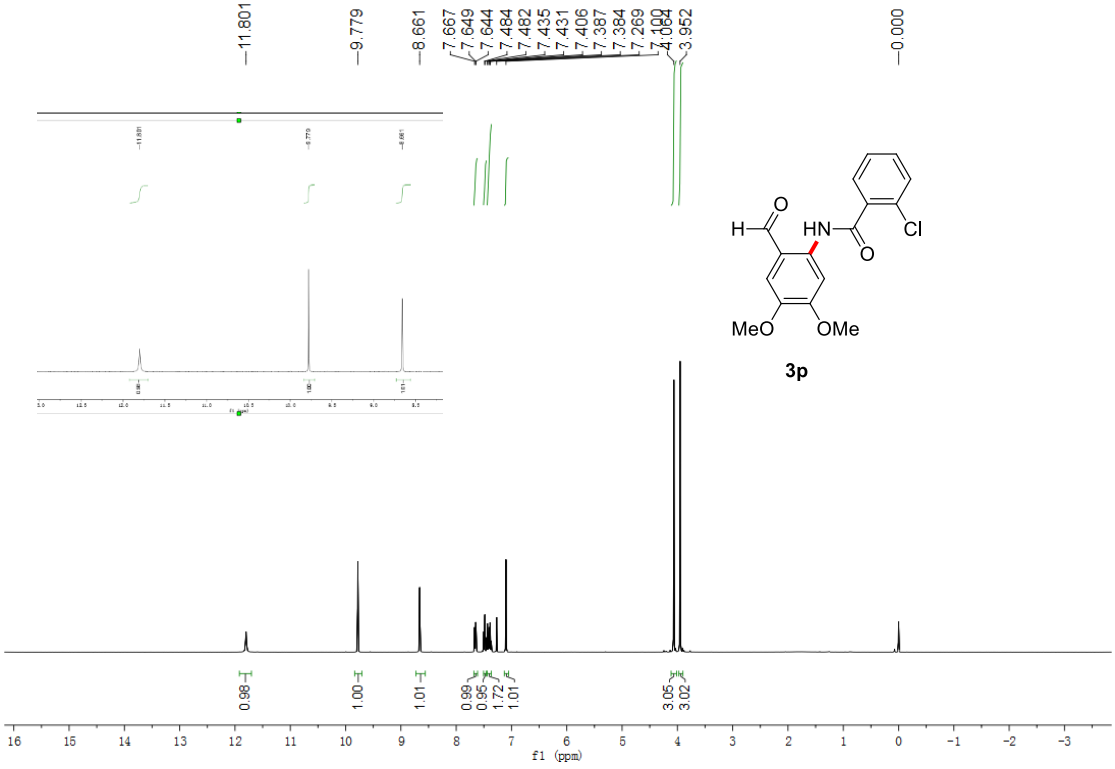
f1 (ppm)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7.482
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7.431
7.406
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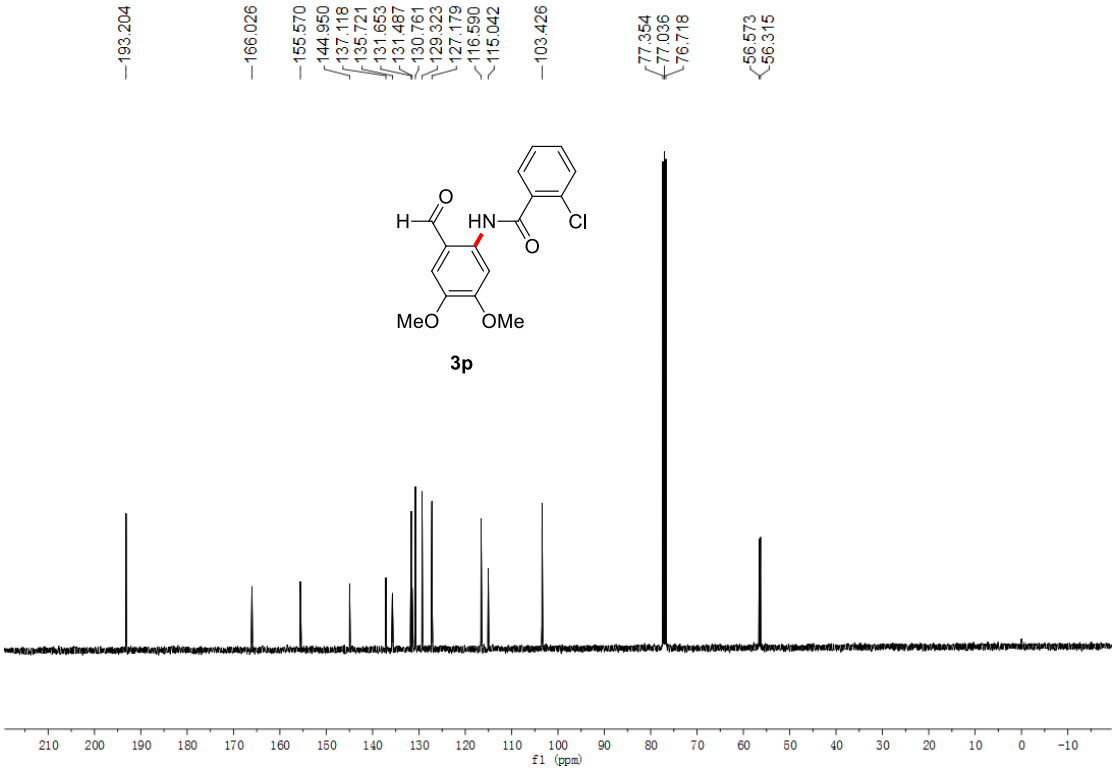
7.269
7.100
4.064
3.952
0.000
H
O
HN
O
Cl
MeO
OMe
3p
0.98
1.00
1.01
0.99
0.95
1.72
1.01
3.05
3.02
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3
f1 (ppm)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129.323
127.179
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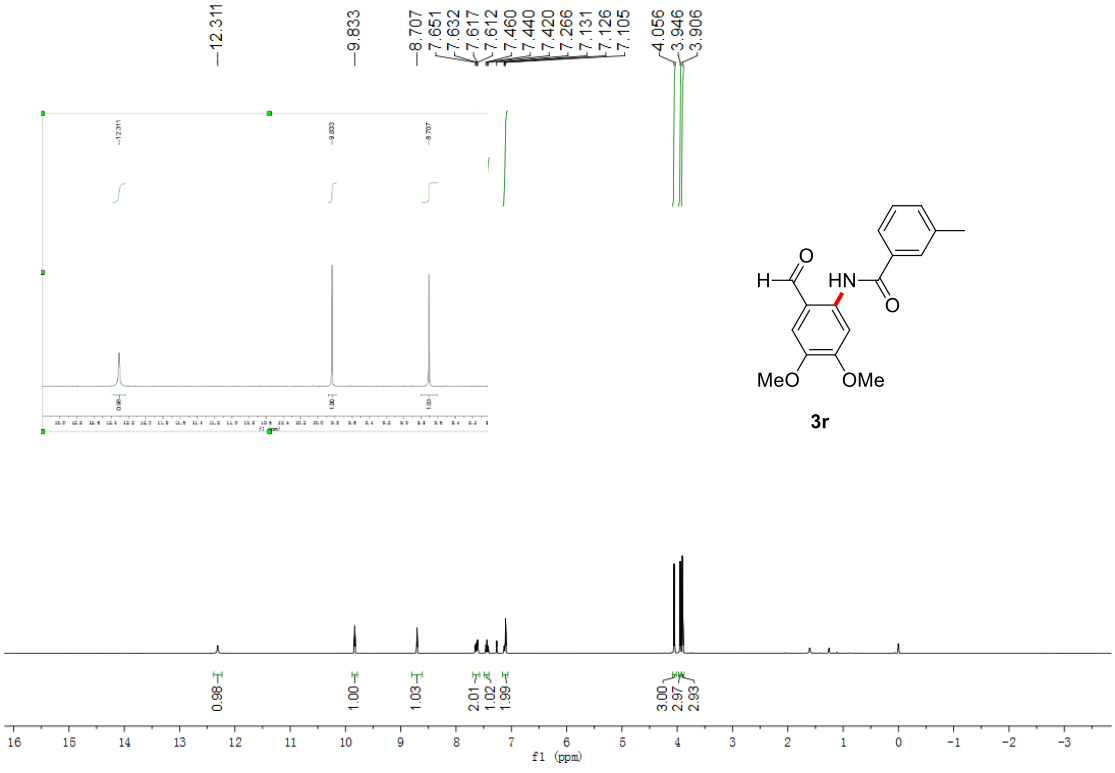
115.042
103.426
77.354
77.036
76.718
56.573
56.315
O
H
HN
O
Cl
MeO
OMe
3p
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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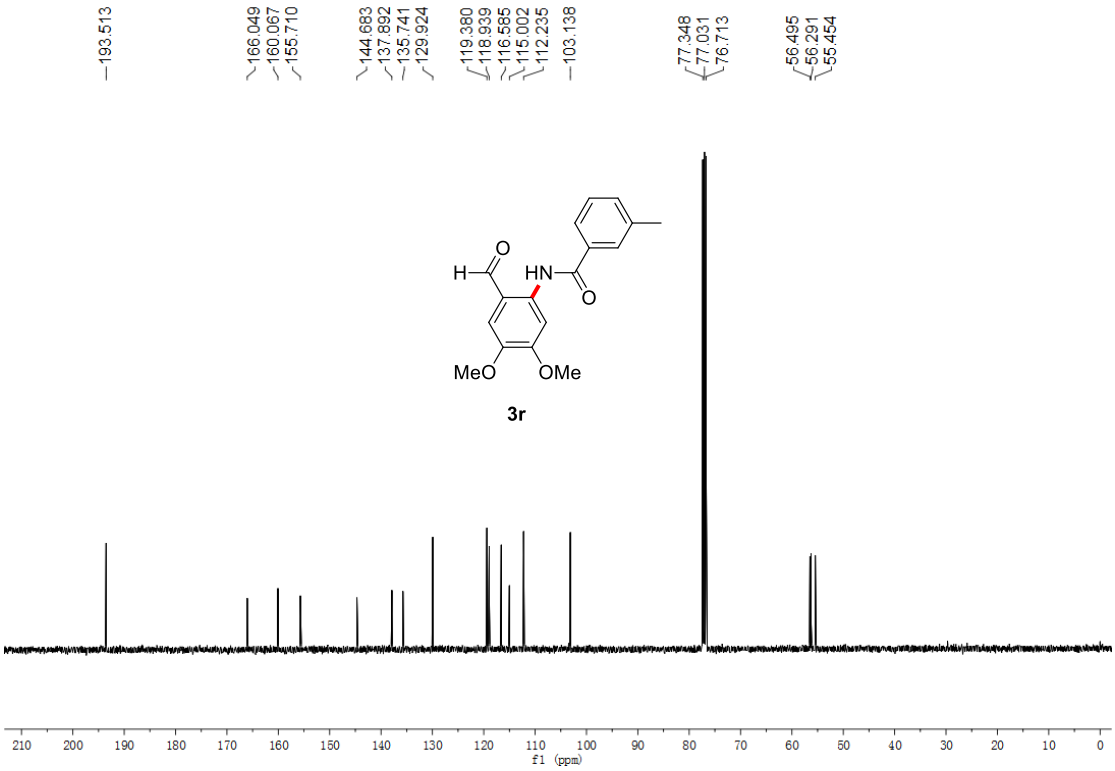
9.833
8.707
7.651
7.632
7.617
7.612
7.460
7.440
7.420
7.266
7.131
7.126
7.105
4.056
3.946
3.906
O
H
HN
O
MeO
OMe
3r
0.98
1.00
1.03
2.01
1.02
1.99
3.00
2.97
2.93
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3
f1 (ppm)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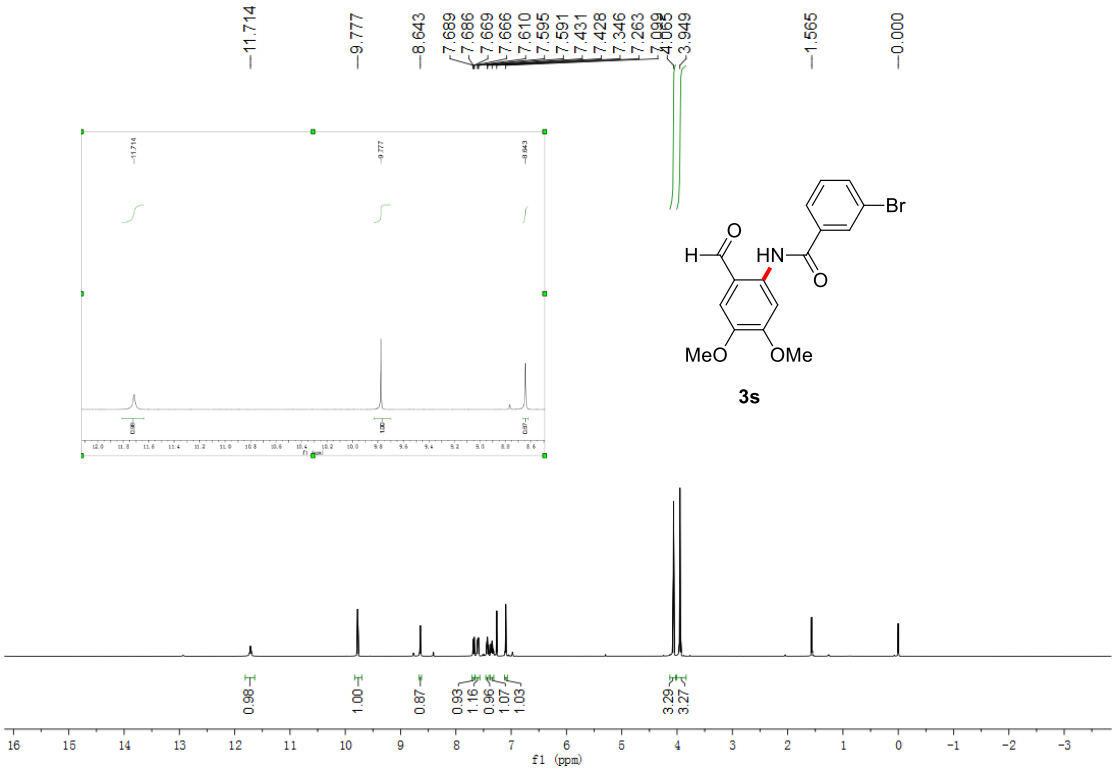
160.067
155.710
144.683
137.892
135.741
129.924
119.380
118.939
116.585
115.002
112.235
103.138
77.348
77.031
76.713
56.495
56.291
55.454
O
H
HN
O
MeO
OMe
3r
f1 (ppm)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8.643
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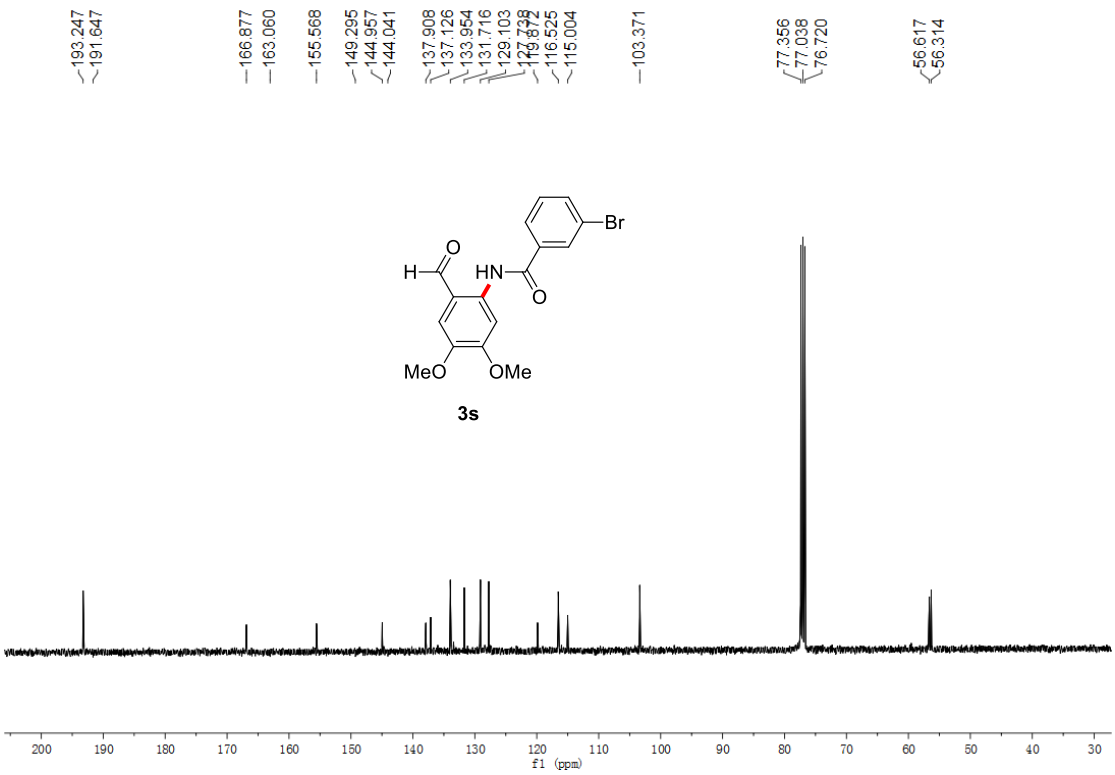
7.686
7.669
7.666
7.610
7.595
7.591
7.431
7.428
7.346
7.263
7.099
4.065
3.949
1.565
0.000
Br
O
H
HN
O
MeO
OMe
3s
0.98
1.00
0.87
0.93
1.16
0.96
1.07
1.03
3.29
3.27
f1 (ppm)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144.957
144.041
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131.716
129.103
116.525
115.004
103.371
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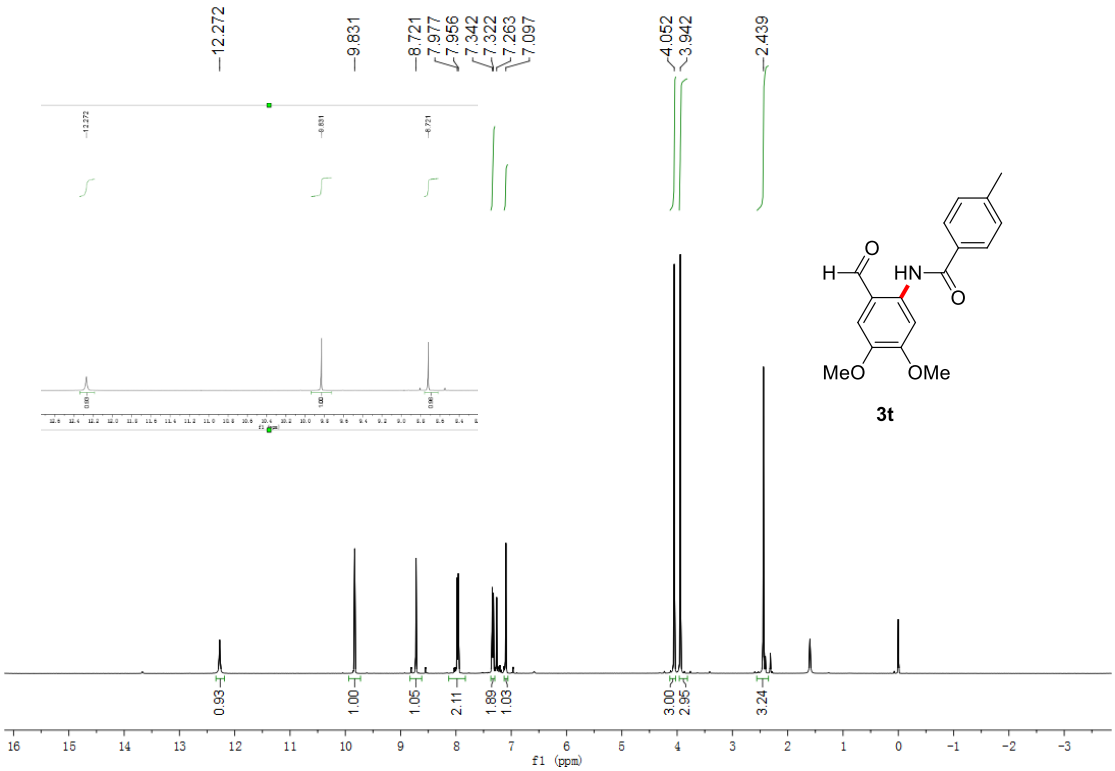
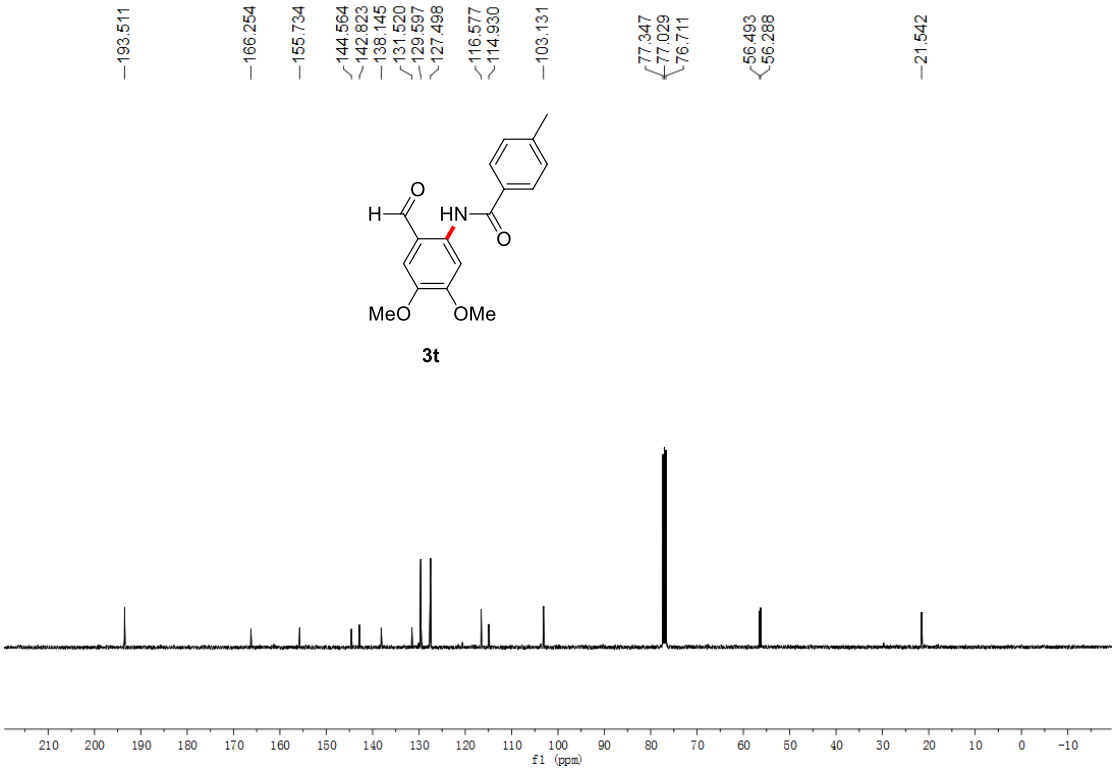
76.720
56.617
56.314
Br
O
H
HN
O
MeO
OMe
3s
f1 (ppm)


12.272
9.831
8.721
7.977
7.956
7.342
7.322
7.263
7.097
4.052
3.942
2.439
O
H
HN
O
MeO
OMe
3t
0.93
1.00
1.05
2.11
1.89
1.03
3.00
2.95
3.24
f1 (ppm)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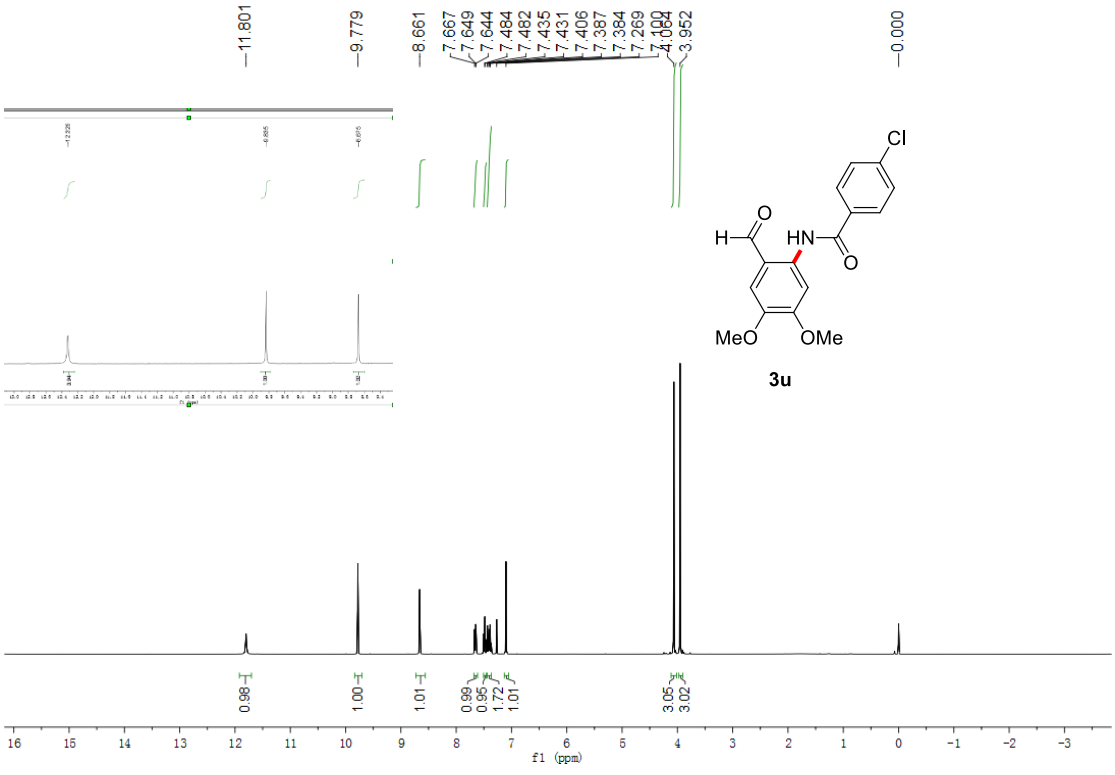
131.520
129.597
127.498
116.577
114.930
103.131
77.347
77.029
76.711
56.493
56.288
21.542
O
H
HN
O
MeO
OMe
3t
f1 (ppm)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7.482
7.435
7.431
7.406
7.387
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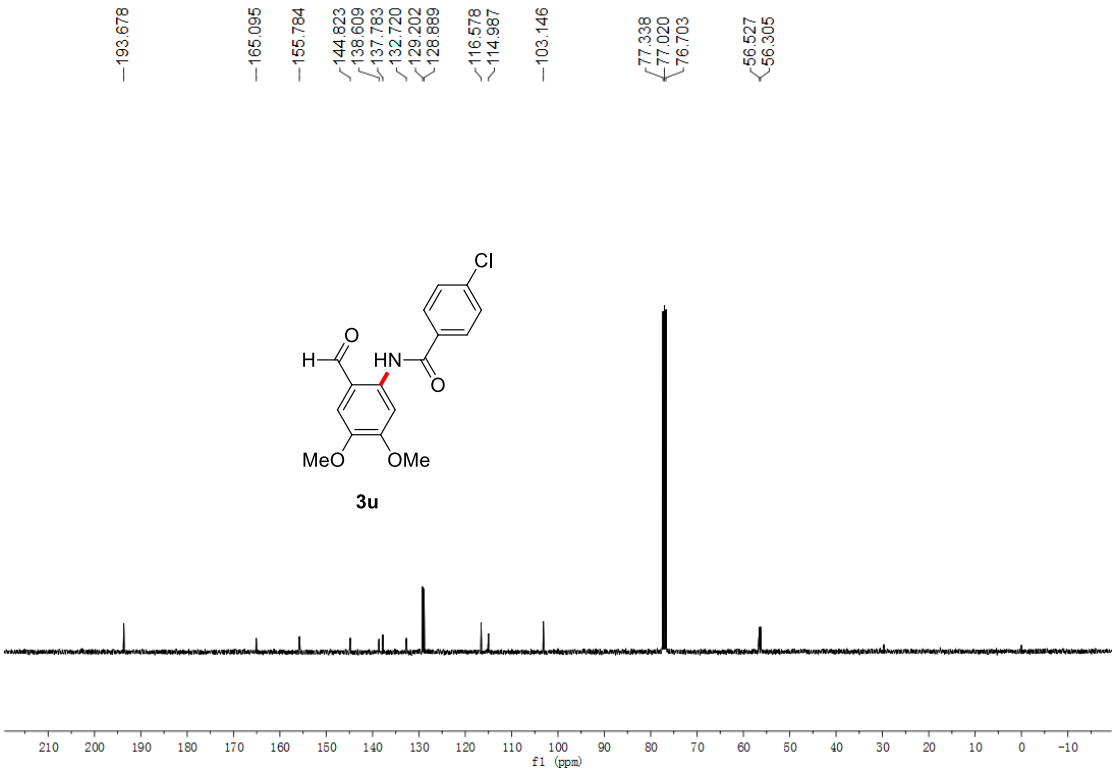
7.269
7.100
7.064
3.952
0.000
Cl
O
H
HN
O
MeO
OMe
3u
0.98
1.00
1.01
0.99
0.95
1.72
1.01
3.05
3.02
f1 (ppm)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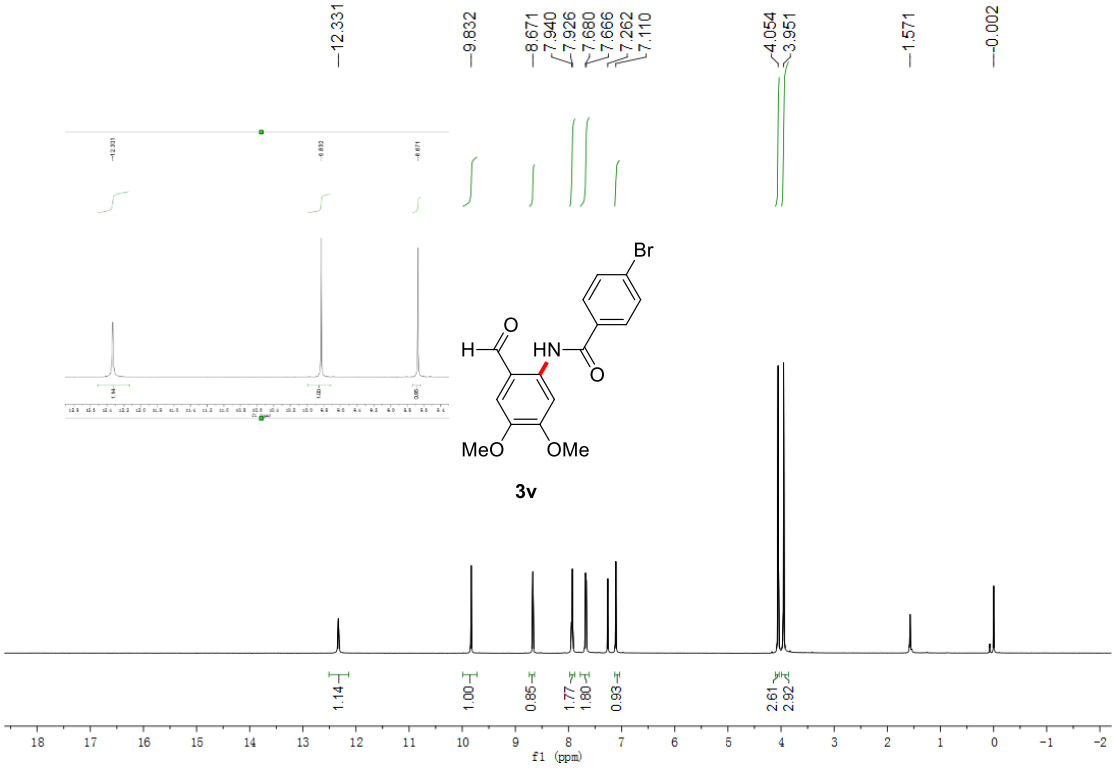
155.784
144.823
138.609
137.783
132.720
129.202
128.889
116.578
114.987
103.146
77.338
77.020
76.703
56.527
56.305
Cl
O
H
HN
O
MeO
OMe
3u
f1 (ppm)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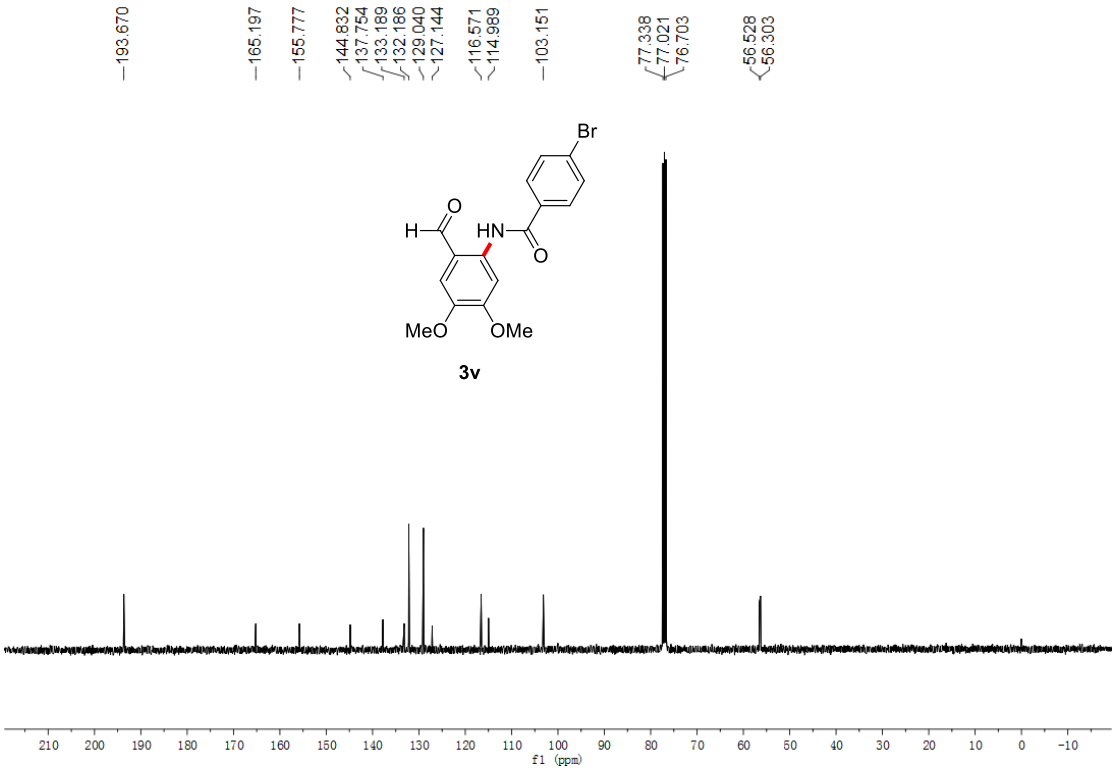
9.832
8.671
7.940
7.926
7.680
7.666
7.262
7.110
4.054
3.951
1.571
0.002
Br
O
H
HN
O
MeO
OMe
3v
1.14
1.00
0.85
1.77
1.80
0.93
2.61
2.92
f1 (ppm)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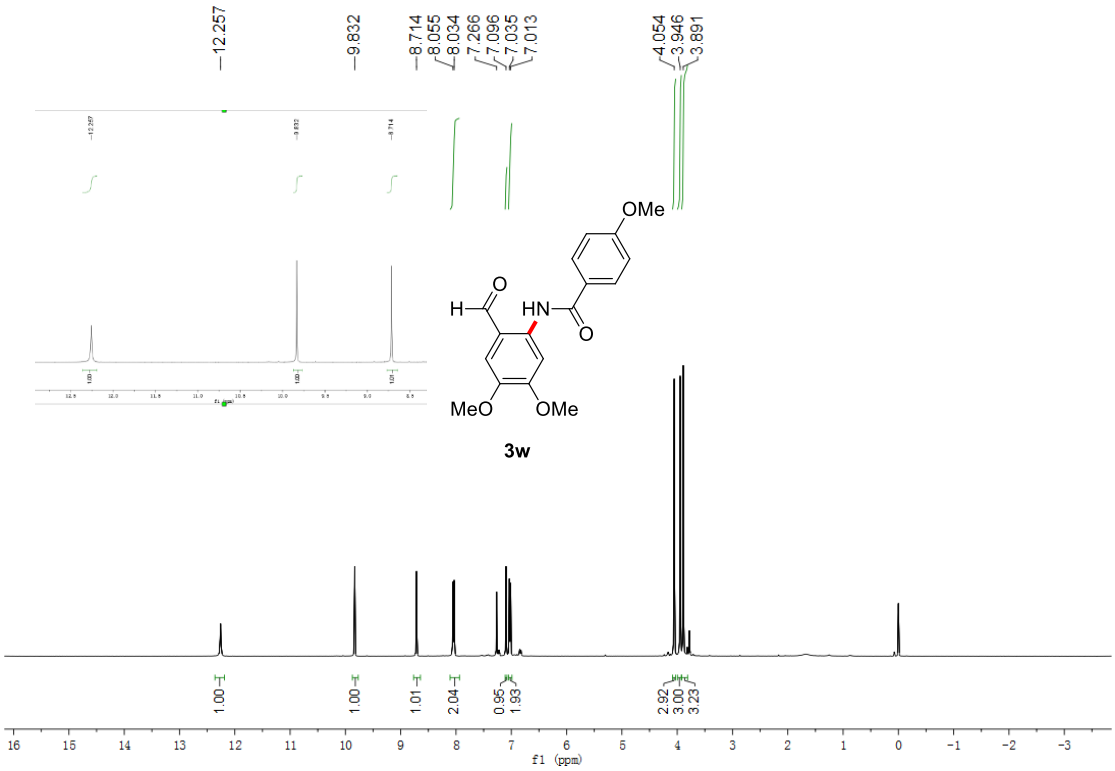
144.832
137.754
133.189
132.186
129.040
127.144
116.571
114.989
103.151
77.338
77.021
76.703
56.528
56.303
Br
O
H
HN
O
MeO
OMe
3v
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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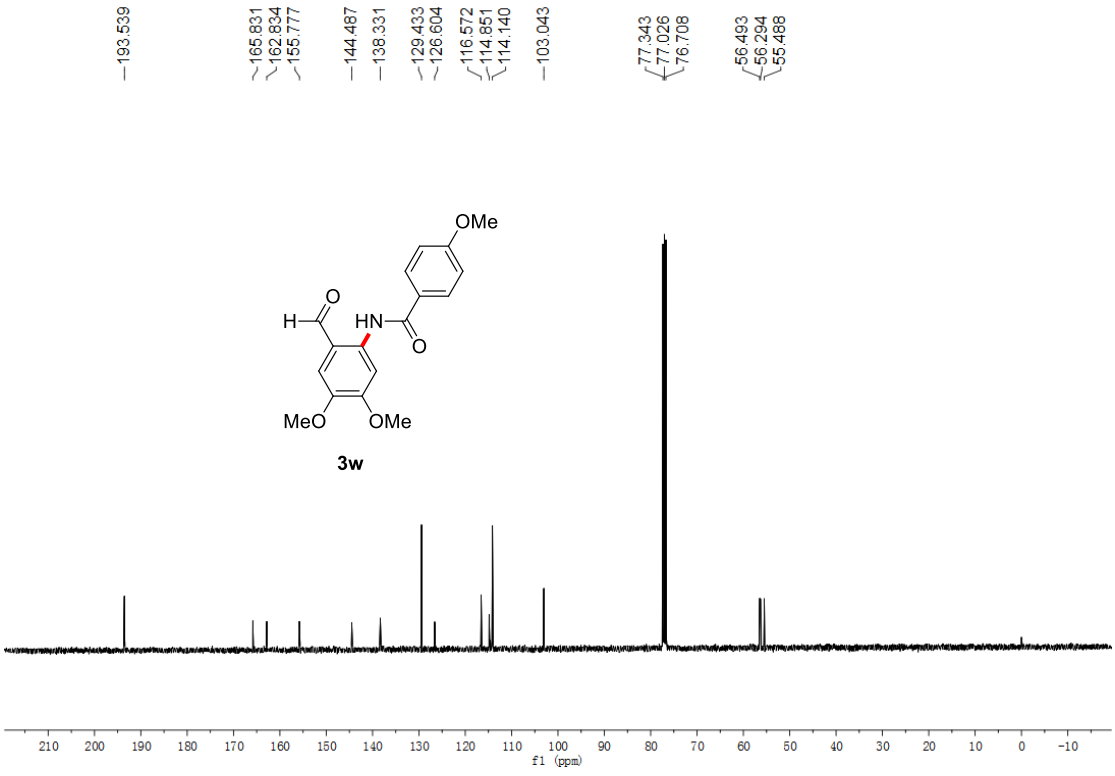
8.714
8.055
8.034
7.266
7.096
7.035
7.013
4.054
3.946
3.891
OMe
O
H
HN
O
MeO
OMe
3w
1.00
1.00
1.01
2.04
0.95
1.93
2.92
3.00
3.23
f1 (ppm)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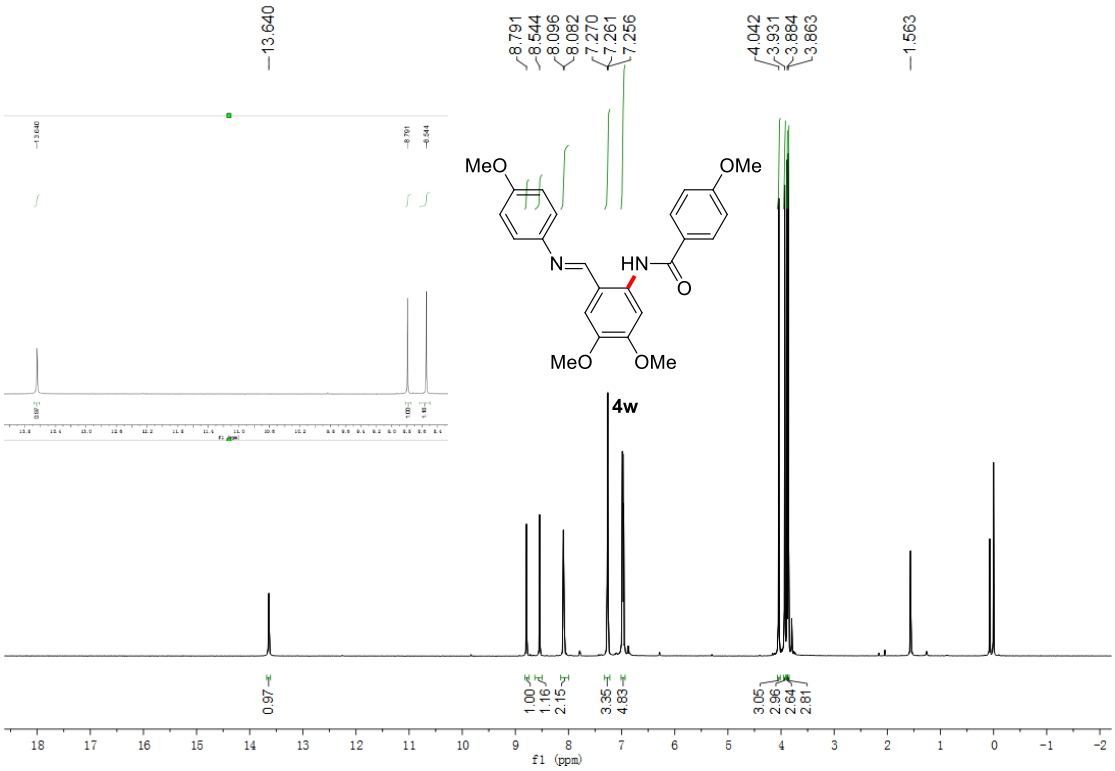
165.831
162.834
155.777
144.487
138.331
129.433
126.604
116.572
114.851
114.140
103.043
77.343
77.026
76.708
56.493
56.294
55.488
OMe
O
H
HN
O
MeO
OMe
3w
f1 (ppm)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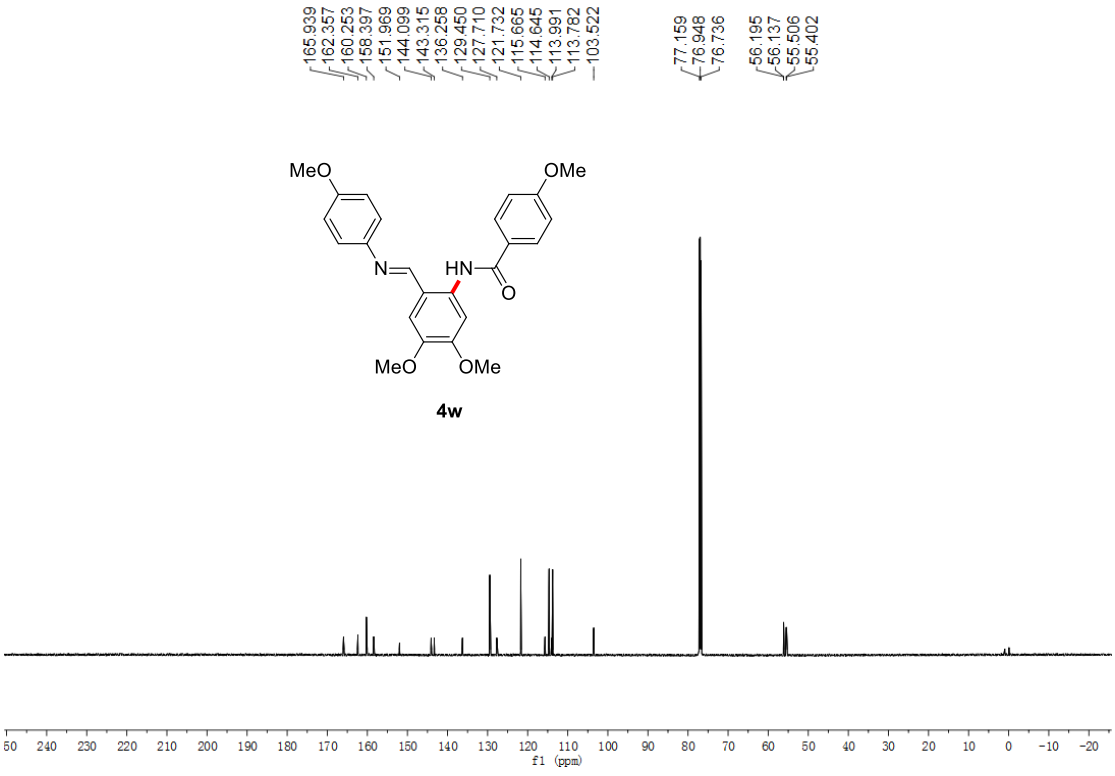
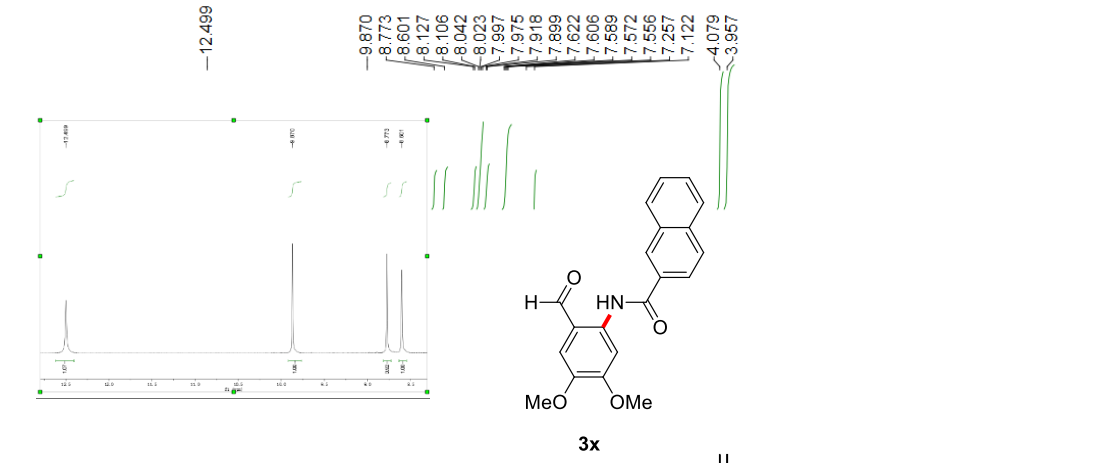
8.791
8.544
8.096
8.082
7.270
7.261
7.256
4.042
3.931
3.884
3.863
1.563
MeO
OMe
N
HN
O
MeO
OMe
4w
0.97
1.00
1.16
2.15
3.35
4.83
3.05
2.96
2.64
2.81
f1 (ppm)


165.939
162.357
160.253
158.397
151.969
144.099
143.315
136.258
129.450
127.710
121.732
115.665
114.645
113.991
113.782
103.522
77.159
76.948
76.736
56.195
56.137
55.506
55.402
MeO
OMe
N
HN
O
MeO
OMe
4w
f1 (ppm)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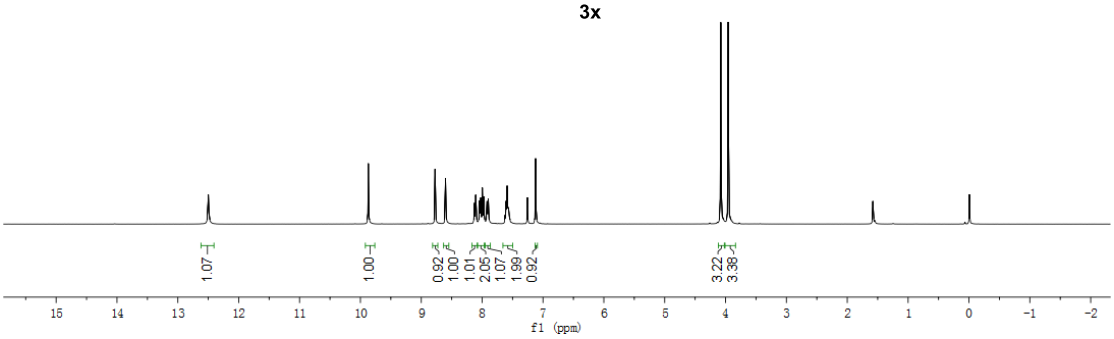
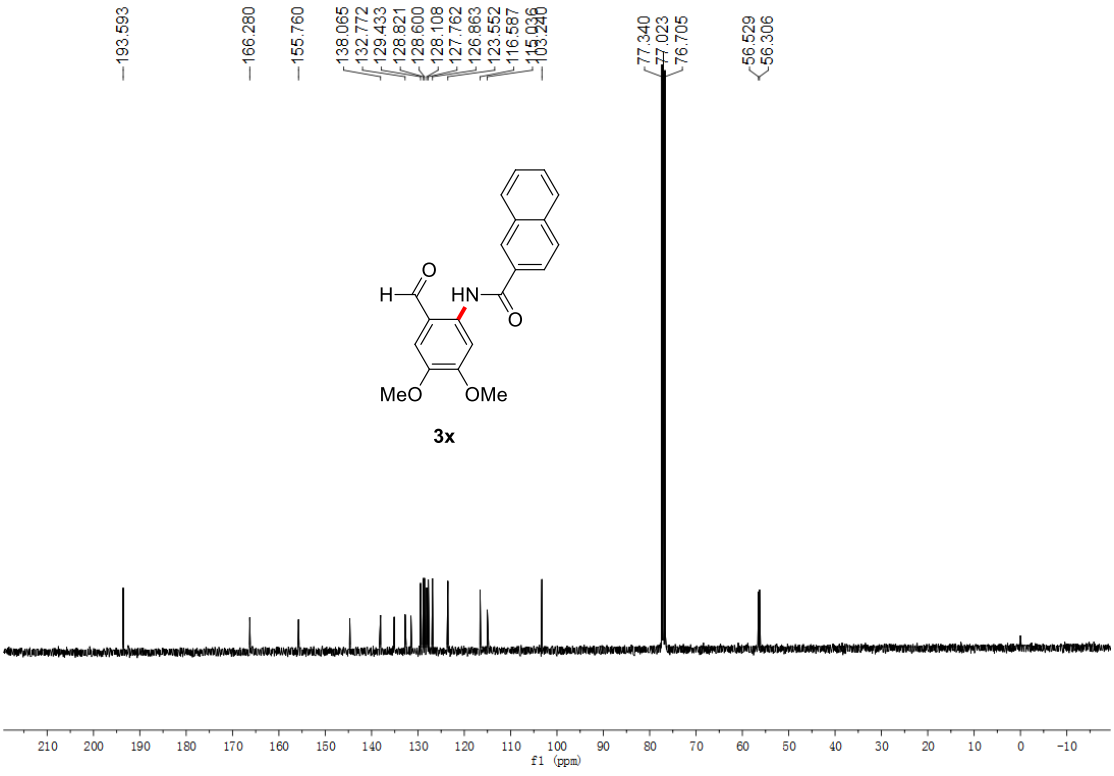
8.773
8.601
8.127
8.106
8.042
8.023
7.997
7.975
7.918
7.899
7.622
7.606
7.589
7.572
7.556
7.257
7.122
4.079
3.957
H
O
HN
O
MeO
OMe

3x


1.07
1.00
0.92
1.00
1.01
2.05
1.07
1.99
0.92
3.22
3.38
f1 (ppm)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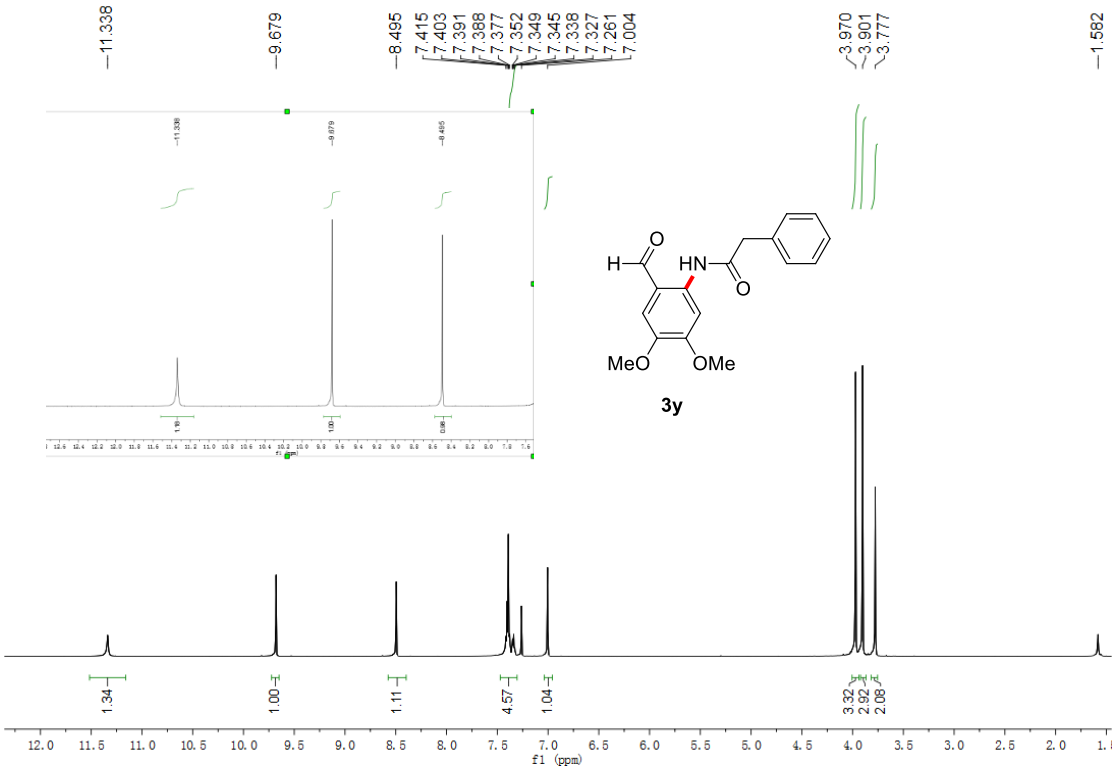
132.772
129.433
128.821
128.600
128.108
127.762
126.863
123.552
116.587
115.036
77.340
77.023
76.705
56.529
56.306
H
O
HN
O
MeO
OMe
f1 (ppm)

3x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7.388
7.377
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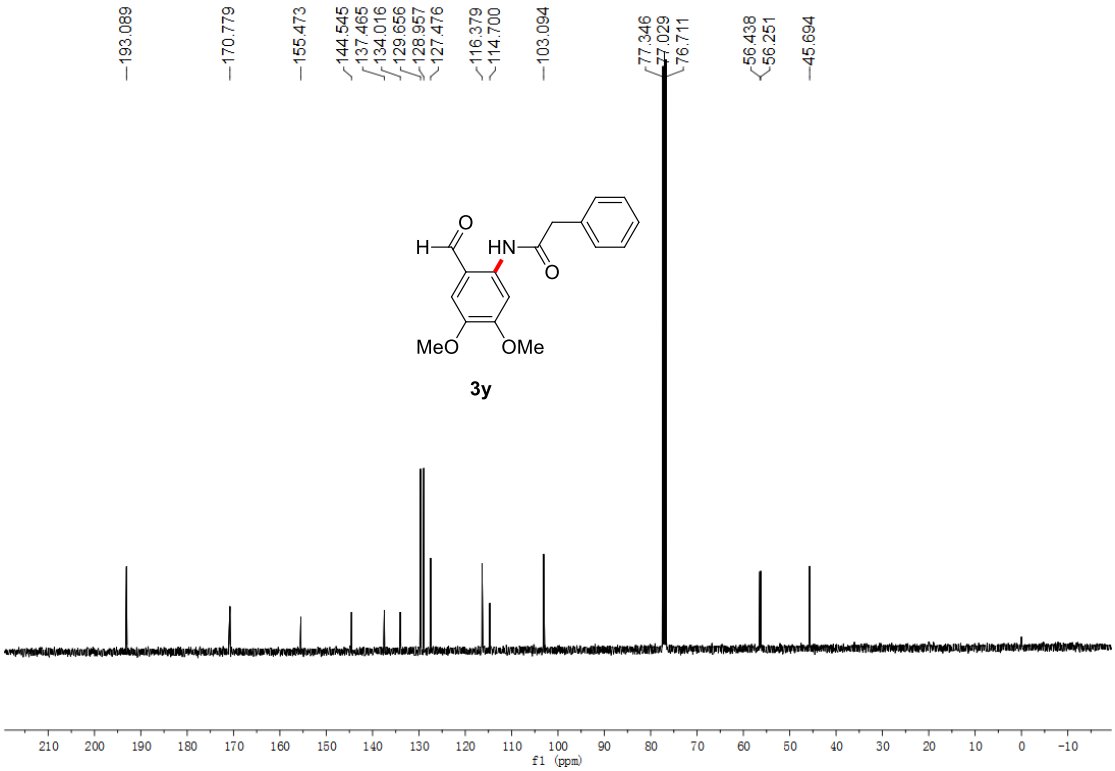
7.349
7.345
7.338
7.327
7.261
7.004
3.970
3.901
3.777
1.582
H
O
HN
O
MeO
OMe
3y
1.34
1.00
1.11
4.57
1.04
3.32
2.92
2.08
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0
f1 (ppm)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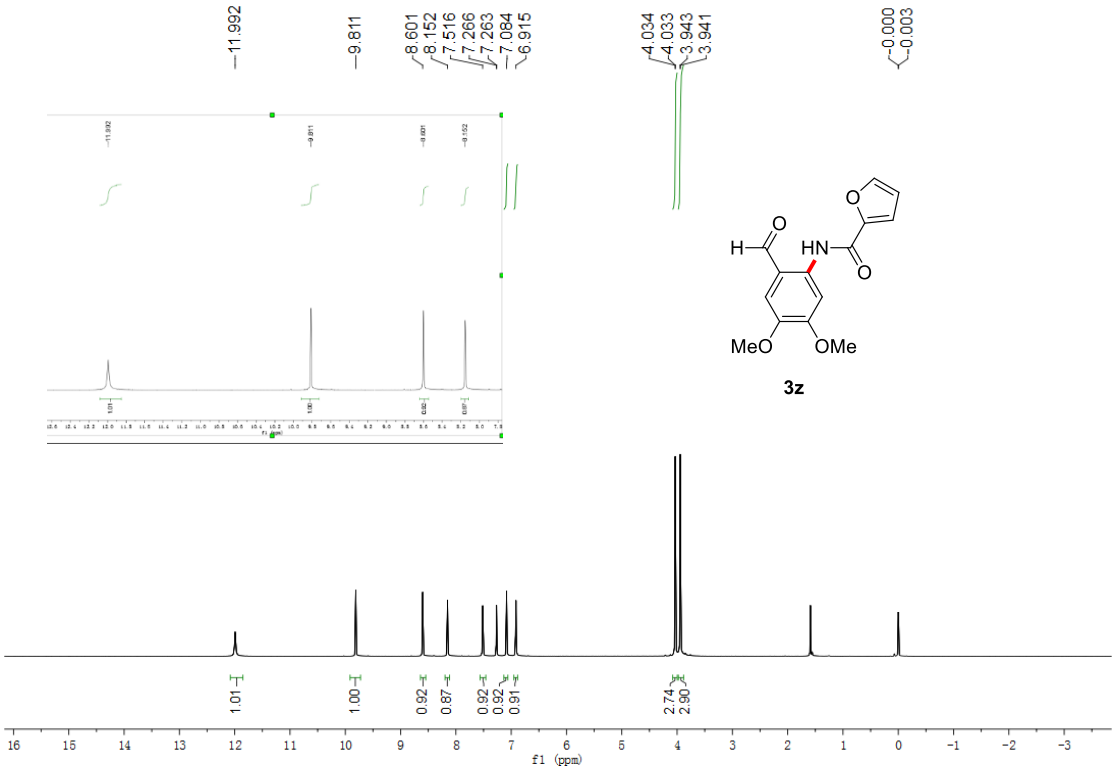
137.465
134.016
129.656
128.957
127.476
116.379
114.700
103.094
77.346
77.029
76.711
56.438
56.251
45.694
H
O
HN
O
MeO
OMe
3y
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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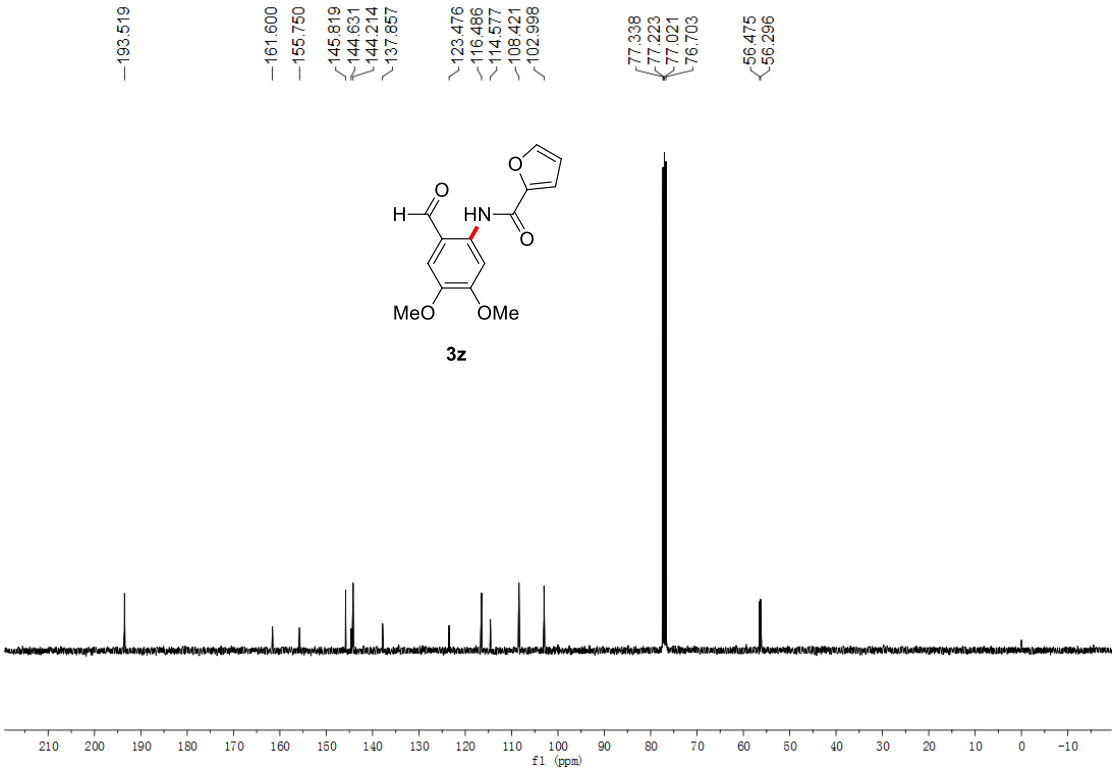
7.266
7.263
7.084
6.915
4.034
4.033
3.943
3.941
0.000
0.003
O
H
HN
O
O
MeO
OMe
3z
1.01
1.00
0.92
0.87
0.92
0.92
0.91
2.74
2.90
f1 (ppm)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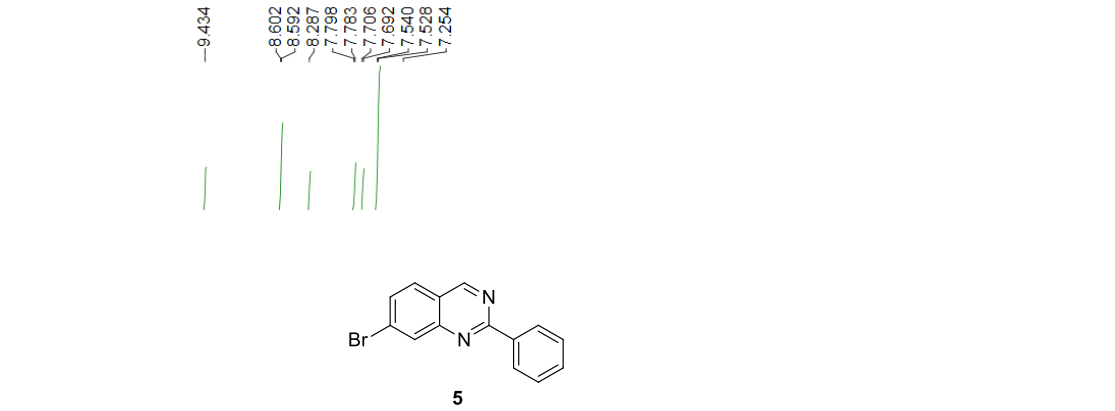
144.631
144.214
137.857
123.476
116.486
114.577
108.421
102.998
77.338
77.223
77.021
76.703
56.475
56.296
O
H
HN
O
O
MeO
OMe
3z
f1 (ppm)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7.783
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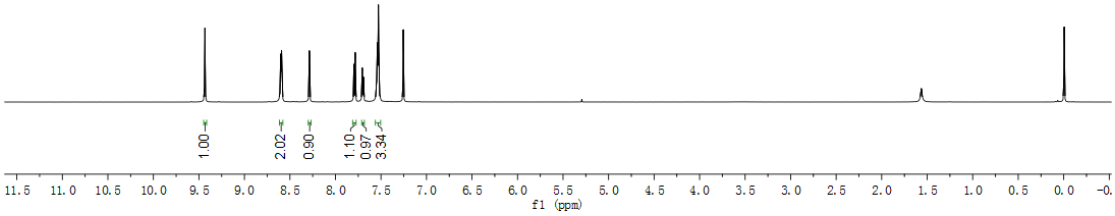
7.692
7.540
7.528
7.254
Br
N
N
5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2.02
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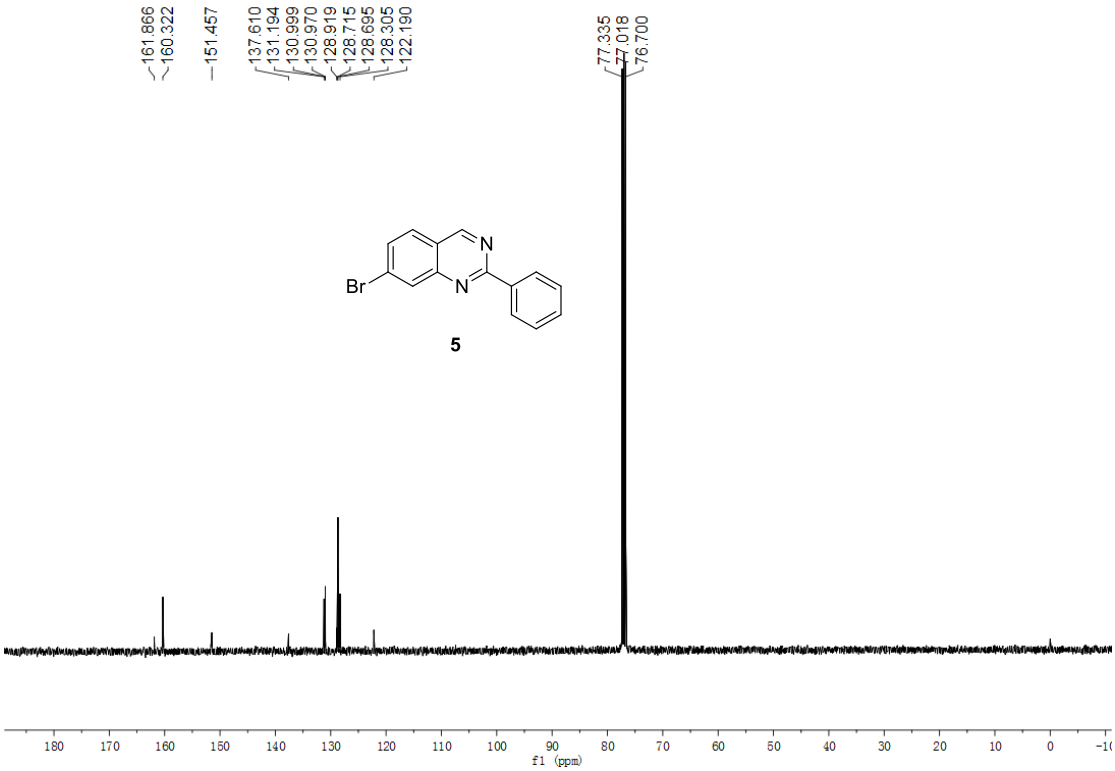
1.10
0.97
3.34
f1 (ppm)


161.866
160.322
151.457
137.610
131.194
130.999
130.970
128.919
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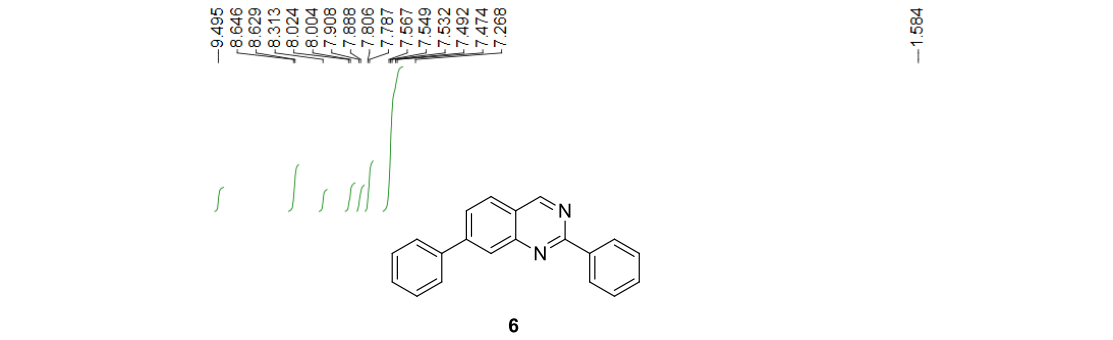
128.695
128.305
122.190
77.335
77.018
76.700
Br
N
N
5
f1 (ppm)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8.646
8.629
8.313
8.024
8.004
7.908
7.888
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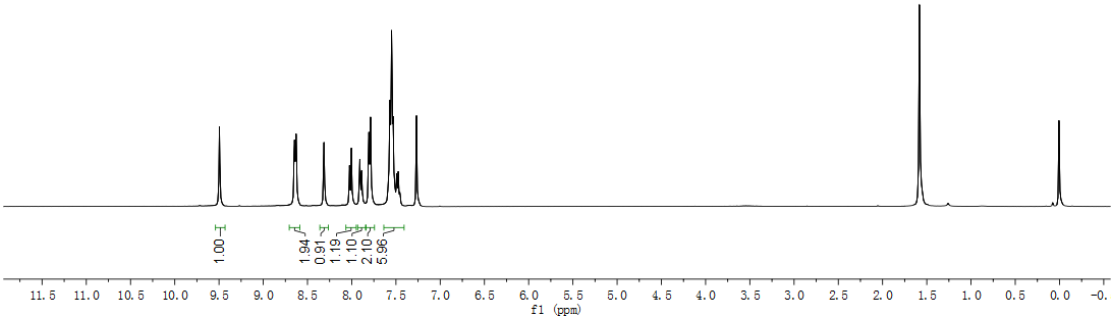
7.567
7.549
7.532
7.492
7.474
7.268
1.584
N
N

6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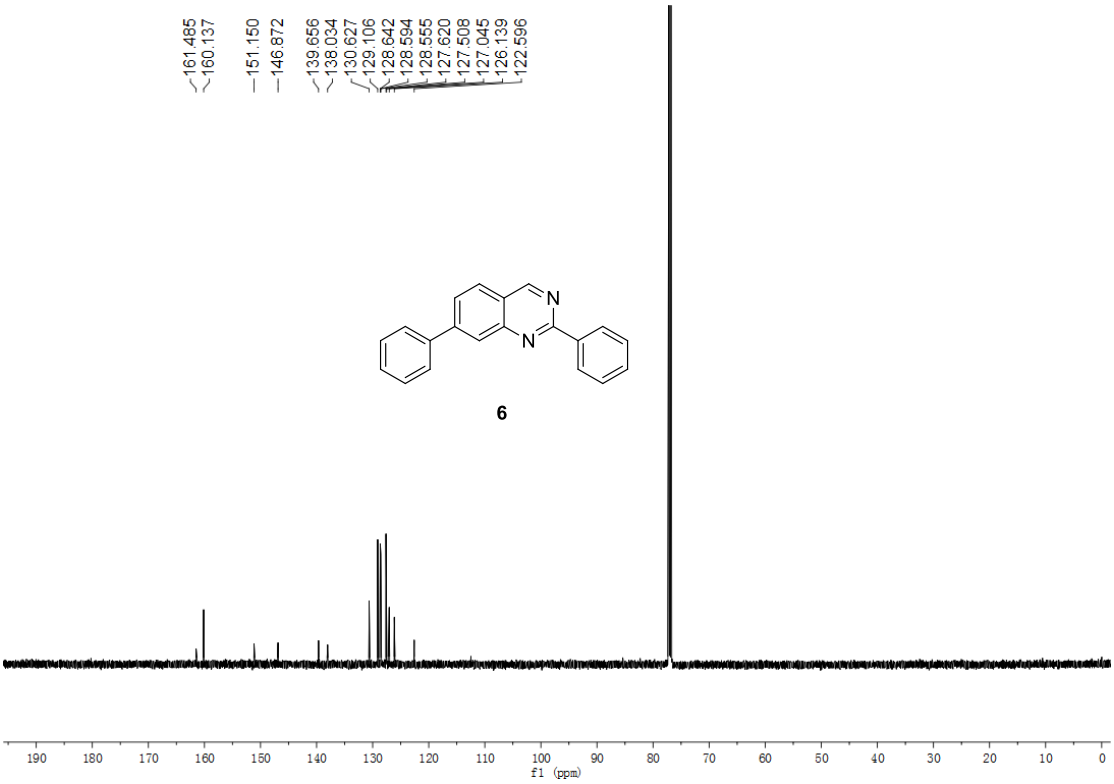
0.91
1.19
1.10
2.10
5.96
f1 (ppm)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151.150
146.872
139.656
138.034
130.627
129.106
128.642
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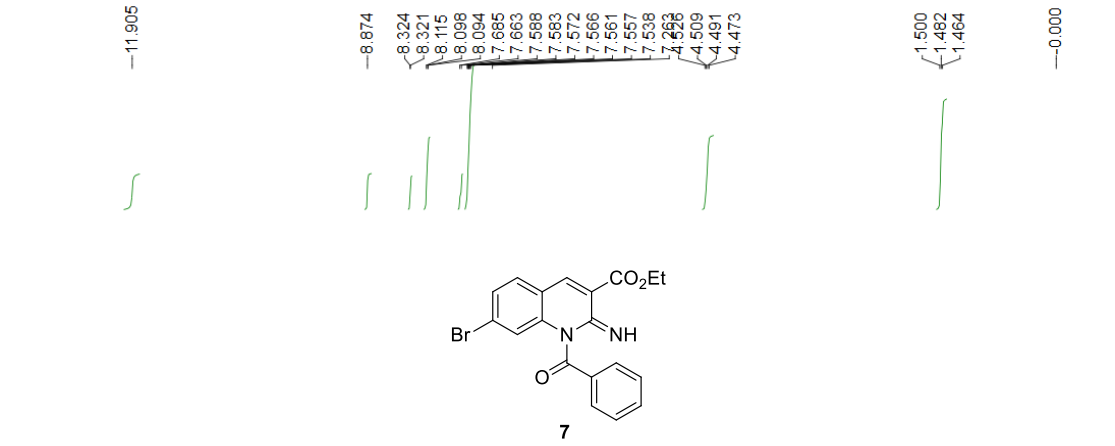
128.555
127.620
127.508
127.045
126.139
122.596
N
N
f1 (ppm)

6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8.324
8.321
8.115
8.098
8.094
7.685
7.663
7.588
7.583
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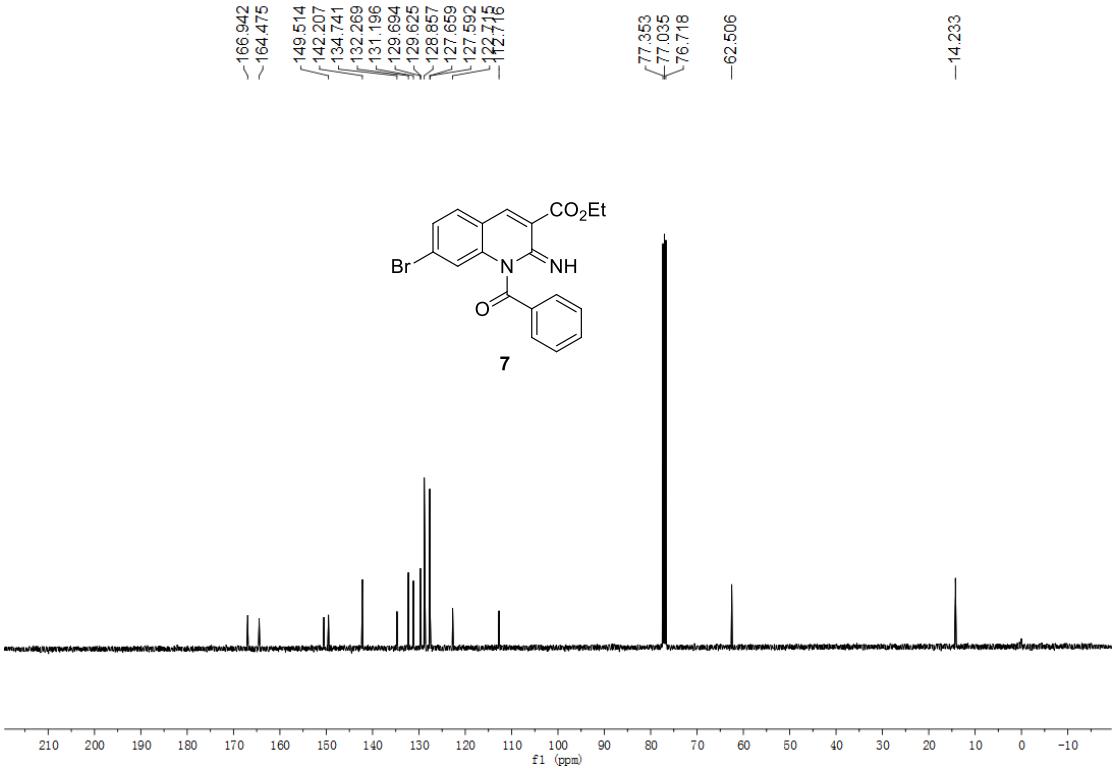
7.566
7.561
7.557
7.538
4.509
4.491
4.473
1.500
1.482
1.464
0.000
CO2Et
Br
N
NH
O
7
0.98
1.00
0.94
2.01
1.00
4.01
2.05
3.07
f1 (ppm)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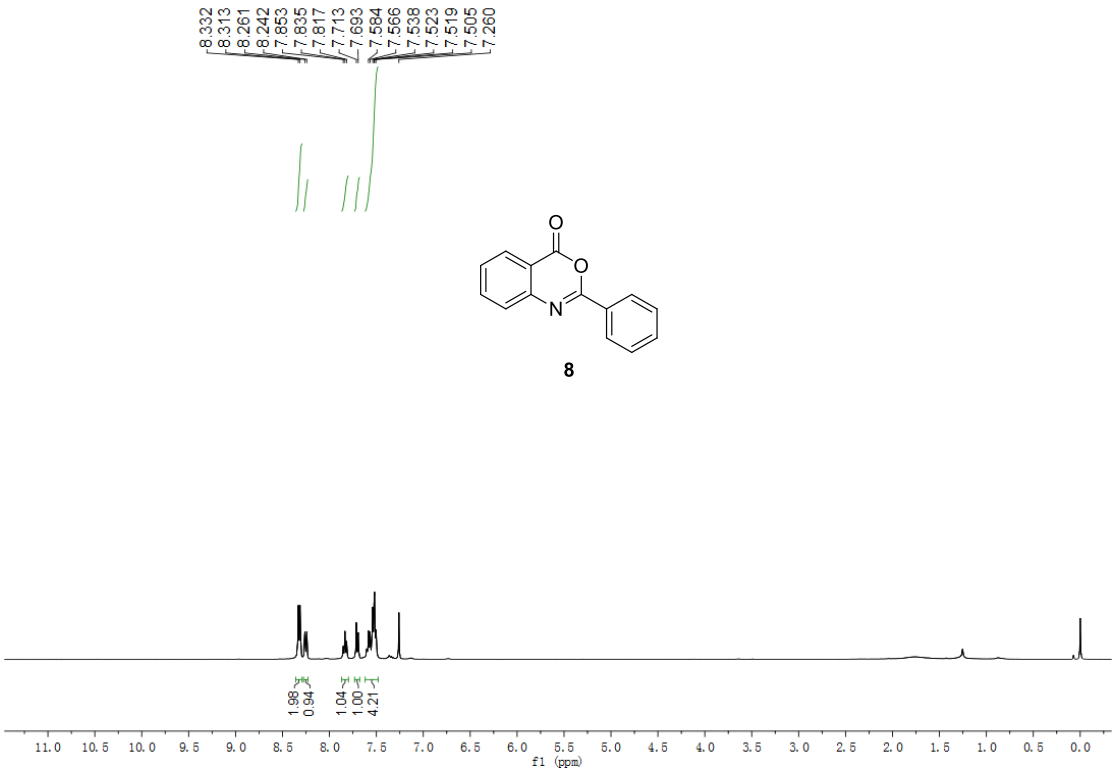
149.514
142.207
134.741
132.269
131.196
129.694
129.625
128.857
127.659
127.592
122.715
122.716
77.353
77.035
76.718
62.506
14.233
CO2Et
Br
N
NH
O
7
f1 (ppm)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7.835
7.817
7.713
7.693
7.584
7.566
7.538
7.523
7.519
7.505
7.260
O
O
N
1.98
0.94
1.04
1.00
4.21
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

8