Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Tandem C-N Coupling/Boulton-Katritzky Rearrangement Reactions of 3-Aminoisoxazoles or 1,2,4-Oxadiazol-3-amines with 2-Pyridyl Trifluoromethanesulfonate: A Rapid Access to [1,2,4]Triazolo[1,5-*a*]pyridines

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Supporting Information

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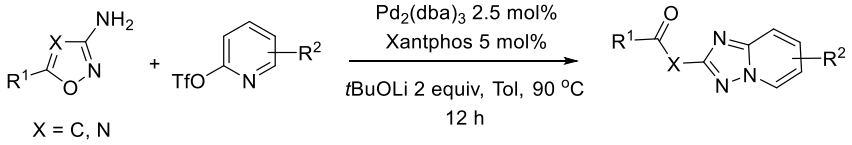
I. General Remarks

^{1}H NMR chemical shifts are reported in ppm with the $CDCl_3$ at 7.26 ppm or DMSO-d_6 at 2.50 ppm as standard. The ^{13}C NMR chemical shifts were given using $CDCl_3$ or DMSO-d_6 as the internal standard ($CDCl_3$: δ = 77.2 ppm, DMSO-d_6: δ = 39.5 ppm). Coupling constants, *J*, were reported in hertz unit (Hz). High resolution mass spectra (HRMS) were obtained on a Q-STAR Elite ESI-LC-MS/MS Spectrometer. Chemical names were generated using Cambridge Soft. ChemDraw Ultra 16.0. Commercially obtained reagents were used without further purification.

II. General procedure for the tandem C-N coupling/Boulton-Katritzky rearrangement reaction



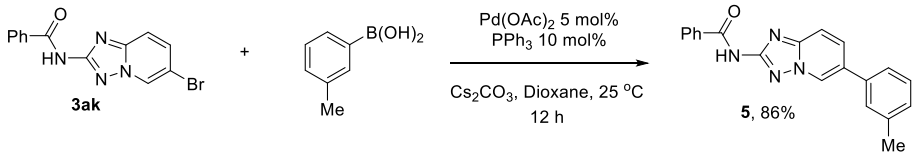
Under N_2, 1,2,4-oxadiazol-3-amines or 3-aminoisoxazoles (0.2 mmol), 2-pyridyl trifluoromethanesulfonate (0.22 mmol), $Pd_2(dba)_3$ (0.005 mmol), Xantphos (0.01 mmol), *t*BuOLi (0.4 mmol) and dry toluene (2.0 mL) were added to an oven-dried 15 mL Schlenk tube equipped with a stir bar were added. The tube was sealed and the reaction was stirred for 12 h at 90 °C with an oil bath. The reaction mixture was cooled to room temperature and diluted with CH_2Cl_2 (10 mL) and filtered through a short pad silica gel washing with CH_2Cl_2 (20 mL). The filtrate was concentrated and then purified by column chromatography on silica gel (PE/EA) to yield the desired products.

3-Amino-5-aryl-1,2,4-oxadiazoles[1-2] were synthesized according to the known procedures and their NMR data were in agreement with those described in the literature. Unless noted, all of the other substrates were commercially available.

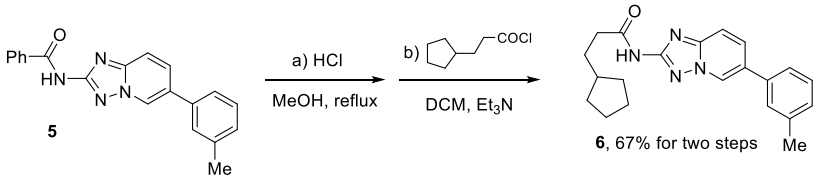
[1] K. Lu, L. Duan, B. Xu, W. Yin, D. Wu, Y. Zhao and P. Gong, Facile synthesis of 3-amino-5-aryl -1,2,4-oxadiazoles via PIDA-mediated intramolecular oxidative cyclization, *RSC Adv.*, **2016**, *6*, 54277.

[2] A. M. Polozov, G. Hategan, H. Cao, A. S. Kiselyov, W. Zeller, J. Singh, A general approach to indole-7-yl derivatives of isoxazole, oxadiazole, thiadiazole and pyrazole, *Tetrahedron Lett.*, **2010**, *51*, 575.

III. Synthesis of bioactive molecular 6



Under N_2, **3ak** (0.2 mmol), (3-methylphenyl)boronic acid (0.40 mmol), $Pd(OAc)_2$ (0.001 mmol), PPh_3 (0.002 mmol), Cs_2CO_3 (0.4 mmol) and dioxane (2.0 mL) were added to a 15 mL Schlenk tube equipped with a stir bar were added. The tube was sealed and the reaction was stirred for 12 h at room temperature. The reaction mixture was then diluted with CH_2Cl_2 (10 mL) and filtered through a short pad silica gel washing with CH_2Cl_2 (20 mL). The filtrate was concentrated and then purified by column chromatography on silica gel (PE/EA) to yield the desired product **5** in 86% yield.

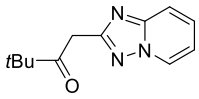


To a magnetically stirred solution of compound **5** (0.2 mmol) in MeOH (5.0mL) was added 1 M HCl solution (1 mL), and the resulting mixture was refluxed for 4h. After completion, the reaction mixture was neutralized by sat. $NaHCO_3$ (aq.) and the aqueous layer was extracted with CH_2Cl_2 (3 x 5 mL), the combined organic layers were washed by brine, dried over Na_2SO_4, filtered and concentrated under reduced pressure. The crude product was used directly for the next step.

To a solution of the above residue in dry CH_2Cl_2 (10 mL) was added Et_3N (0.3 mmol) and followed by the addition of cyclopentylpropionyl chloride (0.25 mmol) at 0 °C under argon atmosphere. The resulting mixture was stirred for 15 min, and then then quenched by sat. NH_4Cl (aq.) (5 mL). The aqueous layer was extracted with CH_2Cl_2 (3 x 5 mL), the combined organic layers were washed by brine, dried over Na_2SO_4 and concentrated under reduced pressure. The residue was purified by flash chromatography to furnish the product **6** as a white solid in 67% yield for two steps.

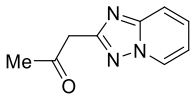
IV. NMR data for 3, 5, 6, 7

1-([1,2,4]triazolo[1,5-a]pyridin-2-yl)-3,3-dimethylbutan-2-one (3a)



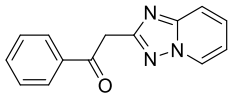
33.5 mg, 78%, white solid, m. p. 46-48 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.51 (d, *J* = 8.0 Hz, 1H), 7.66 (d, *J* = 8.0 Hz, 1H), 7.48-7.44 (m, 1H), 6.97-6.94 (m, 1H), 4.16 (s, 2H), 1.26 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 210.2, 161.4, 151.2, 129.3, 128.1, 116.2, 113.3, 44.6, 37.2, 26.3; HRMS (ESI) calcd for $C_{12}H_{16}N_3O$ $(M+H)^+$ 218.1288, found 218.1289.

1-([1,2,4]triazolo[1,5-a]pyridin-2-yl)propan-2-one (3b)



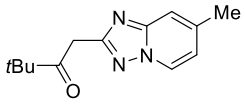
22.8 mg, 65%, colorless oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.55 (d, *J* = 8.0 Hz, 1H), 7.70 (d, *J* = 12.0 Hz, 1H), 7.54-7.50 (m, 1H), 7.04-7.00 (m, 1H), 4.06 (s, 2H), 2.31 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 203.3, 160.8, 151.4, 129.6, 128.2, 116.3, 113.6, 44.0, 29.8; HRMS (ESI) calcd for $C_9H_{10}N_3O$ $(M+H)^+$ 176.0819, found 176.0819.

2-([1,2,4]triazolo[1,5-a]pyridin-2-yl)-1-phenylethan-1-one (3c)



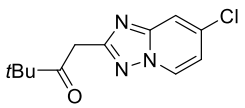
26.8 mg, 57%, colorless oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.54 (d, *J* = 8.0 Hz, 1H), 8.10 (d, *J* = 8.0 Hz, 2H), 7.70 (d, *J* = 8.0 Hz, 1H), 7.60-7.56 (m, 1H), 7.52-7.46 (m, 3H), 7.01-6.98 (m, 1H), 4.63 (s, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 194.8, 161.2, 151.4, 136.3, 133.4, 129.5, 128.7, 128.3, 116.4, 113.5, 42.7, 39.5; HRMS (ESI) calcd for $C_{14}H_{12}N_3O$ $(M+H)^+$ 238.0975, found 238.0974.

3,3-dimethyl-1-(7-methyl-[1,2,4]triazolo[1,5-a]pyridin-2-yl)butan-2-one (3d)



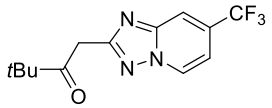
36.8 mg, 80%, white solid, m. p. 62-65 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.39 (d, *J* = 8.0 Hz, 1H), 7.44 (s, 1H), 6.80 (dd, *J* = 6.8, 1.2 Hz, 1H), 4.15 (s, 2H), 2.48 (s, 3H), 1.28 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 210.3, 161.4, 151.6, 140.9, 127.1, 115.8, 114.9, 44.6, 37.3, 26.4, 21.5; HRMS (ESI) calcd for $C_{13}H_{18}N_3O$ $(M+H)^+$ 232.1445, found 232.1444.

1-(7-chloro-[1,2,4]triazolo[1,5-a]pyridin-2-yl)-3,3-dimethylbutan-2-one (3e)



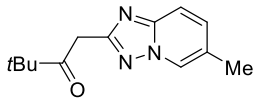
35.6 mg, 71%, yellow solid, m. p. 54-56 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.45 (d, *J* = 8.0 Hz, 1H), 7.69 (d, *J* = 2.0 Hz, 1H), 6.98 (dd, *J* = 7.2, 2.0 Hz, 1H), 4.16 (s, 2H), 1.28 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 210.1, 162.7, 151.5, 136.2, 128.3, 115.4, 115.0, 44.7, 37.2, 26.4; HRMS (ESI) calcd for $C_{12}H_{15}ClN_3O$ $(M+H)^+$ 252.0899, found 252.0899.

3,3-dimethyl-1-(7-(trifluoromethyl)-[1,2,4]triazolo[1,5-a]pyridin-2-yl)butan-2-one (3f)



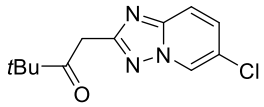
45.0 mg, 79%, white solid, m. p. 79-82 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.67 (d, *J* = 8.0 Hz, 1H), 8.01 (s, 1H), 7.20 (dd, *J* = 7.2, 1.2 Hz, 1H), 4.22 (s, 2H), 1.29 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 209.9, 163.4, 150.2, 131.6 (q, *J* = 34.0 Hz), 122.6 (q, *J* = 271.0 Hz), 114.2 (q, *J* = 15.0 Hz), 109.4 (q, *J* = 3.0 Hz), 44.7, 37.2, 26.3; HRMS (ESI) calcd for $C_{13}H_{15}F_3N_3O$ $(M+H)^+$ 286.1162, found 286.1160.

3,3-dimethyl-1-(6-methyl-[1,2,4]triazolo[1,5-a]pyridin-2-yl)butan-2-one (3g)



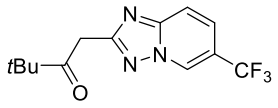
35.4 mg, 77%, yellow solid, m. p. 71-73 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.27 (s, 1H), 7.53 (d, *J* = 12.0 Hz, 1H), 7.29-7.27 (m, 1H), 4.12 (s, 2H), 2.34 (s, 3H), 1.23 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 210.2, 160.9, 149.8, 132.1, 126.02, 123.3, 115.3, 44.5, 37.1, 26.3, 17.8; HRMS (ESI) calcd for $C_{13}H_{18}N_3O$ $(M+H)^+$ 232.1445, found 232.1444.

1-(6-chloro-[1,2,4]triazolo[1,5-a]pyridin-2-yl)-3,3-dimethylbutan-2-one (3h)



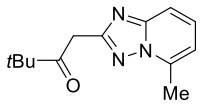
34.5 mg, 69%, yellow solid, m. p. 70-83 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.57 (s, 1H), 7.62 (d, *J* = 12.0 Hz, 1H), 7.45 (dd, *J* = 9.6, 1.6 Hz, 1H), 4.15 (s, 2H), 1.25 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 210.0, 162.2, 149.8, 130.8, 126.4, 121.4, 116.3, 44.6, 37.1, 26.3; HRMS (ESI) calcd for $C_{12}H_{15}ClN_3O$ $(M+H)^+$ 252.0899, found 252.0897.

3,3-dimethyl-1-(6-(trifluoromethyl)-[1,2,4]triazolo[1,5-a]pyridin-2-yl)butan-2-one (3i)



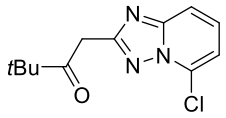
42.8 mg, 75%, yellow solid, m. p. 70-72 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.90 (s, 1H), 7.82 (d, *J* = 8.0 Hz, 1H), 7.67 (d, *J* = 9.2 Hz, 1H), 4.22 (s, 2H), 1.30 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 209.9, 163.7, 151.9, 127.1 (q, *J* = 9.2 Hz), 125.7 (q, *J* = 3.0 Hz), 123.0 (q, *J* = 271.0 Hz), 118.0 (q, *J* = 34.0 Hz), 117.0, 44.8, 37.2, 26.4; HRMS (ESI) calcd for $C_{13}H_{15}F_3N_3O$ $(M+H)^+$ 286.1162, found 286.1163.

3,3-dimethyl-1-(5-methyl-[1,2,4]triazolo[1,5-a]pyridin-2-yl)butan-2-one (3j)



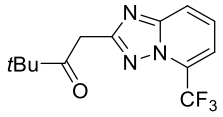
33.1 mg, 72%, yellow solid, m. p. 46-48 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.55 (d, *J* = 8.0 Hz, 1H), 7.40-7.36 (m, 1H), 6.78 (d, *J* = 7.2 Hz, 1H), 4.19 (s, 2H), 2.75 (s, 3H), 1.27 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 210.4, 160.8, 151.5, 138.5, 129.2, 113.4, 112.6, 44.54, 37.4, 26.4, 17.6; HRMS (ESI) calcd for $C_{13}H_{18}N_3O$ $(M+H)^+$ 232.1445, found 232.1445.

1-(5-chloro-[1,2,4]triazolo[1,5-a]pyridin-2-yl)-3,3-dimethylbutan-2-one (3k)



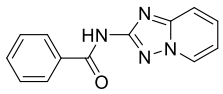
38.0 mg, 76%, yellow solid, m. p. 50-52 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.64 (d, *J* = 8.0 Hz, 1H), 7.47-7.43 (m, 1H), 7.08 (d, *J* = 8.0 Hz, 1H), 4.23 (s, 2H), 1.27 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 209.9, 161.6, 152.4, 129.6, 129.3, 114.5, 113.5, 44.6, 37.2, 26.4; HRMS (ESI) calcd for $C_{12}H_{15}ClN_3O$ $(M+H)^+$ 252.0899, found 252.0899.

3,3-dimethyl-1-(5-(trifluoromethyl)-[1,2,4]triazolo[1,5-a]pyridin-2-yl)butan-2-one (3l)



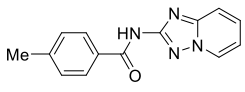
39.9 mg, 70%, yellow solid, m. p. 57-59 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.91 (d, *J* = 12.0 Hz, 1H), 7.60-7.56 (m, 1H), 7.42 (d, *J* = 8.0 Hz, 1H), 4.26 (s, 2H), 1.29 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 209.9, 162.5, 152.0, 128.4 (d, *J* = 37.0 Hz), 128, 120.1, 119.6 (d, *J* = 276 Hz), 112.9 (d, *J* = 5.0 Hz), 44.8, 37.2, 26.4; HRMS (ESI) calcd for $C_{13}H_{15}F_3N_3O$ $(M+H)^+$ 286.1162, found 286.1163.

***N*-([1,2,4]triazolo[1,5-a]pyridin-2-yl)benzamide (3aa)**



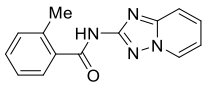
31.8 mg, 67%, white solid, m. p. 74-76 °C; ^{1}H NMR (400 MHz, DMSO-d_6) δ 11.20 (s, 1H), 8.90 (d, *J* = 6.8 Hz, 1H), 8.02 (d, *J* = 7.2 Hz, 2H), 7.77-7.73 (m, 1H), 7.68-7.60 (m, 2H), 7.55-7.51 (m, 2H), 7.19-7.15 (m, 1H); ^{13}C NMR (100 MHz, DMSO-d_6) δ 165.2, 158.6, 149.5, 133.8, 132.1, 130.5, 128.9, 128.5, 128.1, 114.9, 113.8; HRMS (ESI) calcd for $C_{13}H_{11}N_4O$ $(M+H)^+$ 239.0928, found 239.0927.

***N*-([1,2,4]triazolo[1,5-a]pyridin-2-yl)-4-methylbenzamide (3ba)**



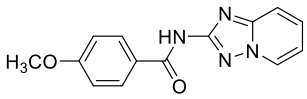
34.8 mg, 69%, white solid, m. p. 92-95 °C; ^{1}H NMR (400 MHz, DMSO-d_6) δ 11.10 (s, 1H), 8.90 (d, *J* = 6.8 Hz, 1H), 7.94 (d, *J* = 8.0 Hz, 2H), 7.74-7.63 (m, 2H), 7.32 (d, *J* = 7.6 Hz, 2H), 7.17-7.14 (m, 1H), 2.37 (s, 3H); ^{13}C NMR (100 MHz, DMSO-d_6) δ 164.9, 158.7, 149.4, 142.1, 130.9, 130.3, 128.9, 128.8, 128.1, 114.8, 113.7, 39.5, 21.0; HRMS (ESI) calcd for $C_{14}H_{13}N_4O$ $(M+H)^+$ 253.1084, found 253.1082.

***N*-([1,2,4]triazolo[1,5-a]pyridin-2-yl)-2-methylbenzamide (3ca)**



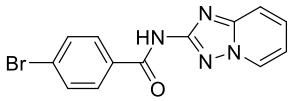
31.2 mg, 62%, white solid, m. p. 67-70 °C; ^{1}H NMR (400 MHz, DMSO-d_6) δ 11.22 (s, 1H), 8.98 (d, *J* = 8.0 Hz, 1H), 7.82-7.72 (m, 2H), 7.58 (d, *J* = 8.0 Hz, 1H), 7.50-7.47 (m, 1H), 7.40-7.36 (m, 2H), 7.27-7.23 (m, 1H), 2.49 (s, 3H); ^{13}C NMR (100 MHz, DMSO-d_6) δ 167.3, 158.4, 149.4, 136.1, 135.6, 130.6, 130.4, 130.0, 128.8, 127.5, 125.6, 114.8, 113.7, 19.4; HRMS (ESI) calcd for $C_{14}H_{13}N_4O$ $(M+H)^+$ 253.1084, found 253.1082.

***N*-([1,2,4]triazolo[1,5-a]pyridin-2-yl)-4-methoxybenzamide (3da)**



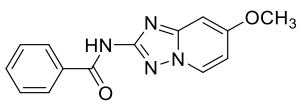
30.6 mg, 57%, white solid, m. p. 102-105 °C; ^{1}H NMR (400 MHz, DMSO-d_6) δ 10.52 (s, 1H), 8.39 (d, *J* = 6.8 Hz, 1H), 7.53 (d, *J* = 8.8 Hz, 2H), 7.23-7.13 (m, 2H), 6.67-7.64 (m, 1H), 6.55 (d, *J* = 8.0 Hz, 2H), 3.34 (s, 3H); ^{13}C NMR (100 MHz, DMSO-d_6) δ 164.4, 162.3, 158.8, 149.5, 130.3, 130.1, 128.8, 125.8, 114.8, 113.7, 55.5, 42.1; HRMS (ESI) calcd for $C_{14}H_{13}N_4O_2$ $(M+H)^+$ 269.1034, found 269.2034.

***N*-([1,2,4]triazolo[1,5-a]pyridin-2-yl)-4-bromobenzamide (3ea)**



37.2 mg, 59%, yellow solid, m. p. 87-89 °C; ^{1}H NMR (400 MHz, DMSO-d_6) δ 11.30 (s, 1H), 8.90 (d, *J* = 6.8 Hz, 1H), 7.95 (d, *J* = 8.4 Hz, 2H), 7.74 (d, *J* = 8.8 Hz, 3H), 7.69-7.65 (m, 1H), 7.19-7.16 (m, 1H); ^{13}C NMR (100 MHz, DMSO-d_6) δ 164.2, 158.5, 149.5, 132.9, 131.5, 130.5, 130.2, 128.9, 125.9, 114.9, 113.8; HRMS (ESI) calcd for $C_{13}H_{10}BrN_4O$ $(M+H)^+$ 317.0033, found 317.0033.

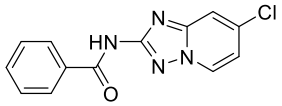
***N*-(7-methoxy-[1,2,4]triazolo[1,5-a]pyridin-2-yl)benzamide (3ab)**



37.5 mg, 70%, white solid, m. p. 92-95 °C; ^{1}H NMR (400 MHz, DMSO-d_6) δ 11.08 (s, 1H), 8.72 (d, *J* = 7.2 Hz, 1H), 8.01 (d, *J* = 7.6 Hz, 2H), 7.62-7.50 (m, 3H), 7.11 (d, *J* = 2.0 Hz, 1H), 6.80 (dd,

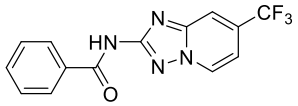
J = 7.2, 2.4 Hz, 1H), 3.90 (s, 3H); ^{13}C NMR (100z MHz, DMSO-d_6) δ 165.0, 160.9, 158.9, 151.1, 133.8, 132.0, 129.1, 128.4, 128.0, 106.9, 93.6, 56.2; HRMS (ESI) calcd for $C_{14}H_{13}N_4O_2$ $(M+H)^+$ 269.1034, found 269.2034.

***N*-(7-chloro-[1,2,4]triazolo[1,5-a]pyridin-2-yl)benzamide (3ac)**



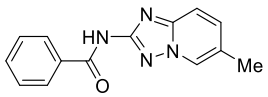
35.4 mg, 65%, yellow solid, m. p. 91-93 °C; ^{1}H NMR (400 MHz, DMSO-d_6) δ 11.29 (s, 1H), 8.95 (s, 1H), 8.02-7.96 (m, 3H), 7.63-7.51 (m, 3H), 7.26-7.24 (m, 1H); ^{13}C NMR (100 MHz, DMSO-d_6) δ 164.9, 159.5, 149.7, 135.4, 133.6, 132.1, 129.8, 128.4, 128.1, 114.6, 113.9; HRMS (ESI) calcd for $C_{13}H_{10}ClN_4O$ $(M+H)^+$ 273.0538, found 273.0539.

***N*-(7-(trifluoromethyl)-[1,2,4]triazolo[1,5-a]pyridin-2-yl)benzamide (3ad)**



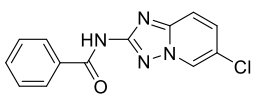
44.1 mg, 72%, yellow solid, m. p. 118-112 °C ; ^{1}H NMR (400 MHz, DMSO-d_6) δ 11.44 (s, 1H), 9.17 (d, *J* = 7.2 Hz, 1H), 8.30 (s, 1H), 8.03 (d, *J* = 7.2 Hz, 2H), 7.64-7.61 (m, 1H), 7.56-7.52 (m, 2H), 7.47 (dd, *J* = 7.2, 1.6 Hz, 1H); ^{13}C NMR (100 MHz, DMSO-d_6) δ 164.9, 160.1, 148.4, 133.6, 132.2, 130.4, 130.17 (q, *J* = 34.0 Hz), 128.4, 128.1, 123.0 (q, *J* = 272.0 Hz), 113.0 (q, *J* = 4.0 Hz), 109.2 (q, *J* = 3.0 Hz); HRMS (ESI) calcd for $C_{14}H_{10}F_3N_4O$ $(M+H)^+$ 307.0802, found 307.0803.

***N*-(6-methyl-[1,2,4]triazolo[1,5-a]pyridin-2-yl)benzamide (3ae)**



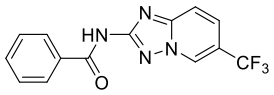
34.3 mg, 68%, white solid, m. p. 63-65 °C; ^{1}H NMR (400 MHz, DMSO-d_6) δ 11.12 (s, 1H), 8.73 (s, 1H), 8.02-8.00 (m, 2H), 7.64-7.58 (m, 2H), 7.54-7.50 (m, 3H), 2.36 (s, 3H); ^{13}C NMR (100 MHz, DMSO-d_6) δ 165.1, 158.3, 148.1, 133.8, 132.85, 132.0, 128.4, 128.0, 126.7, 123.5, 114.1, 17.3; HRMS (ESI) calcd for $C_{14}H_{13}N_4O$ $(M+H)^+$ 253.1084, found 253.1083.

***N*-(6-chloro-[1,2,4]triazolo[1,5-a]pyridin-2-yl)benzamide (3af)**



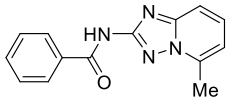
33.3 mg, 63%, yellow solid, m. p. 67-70 °C; ^{1}H NMR (400 MHz, DMSO-d_6) δ 11.45 (s, 1H), 9.63 (d, *J* = 1.2 Hz, 1H), 8.04 (d, *J* = 8.0 Hz, 2H), 7.93 (d, *J* = 1.2 Hz, 2H), 7.64-7.60 (m, 1H), 7.55-7.51 (m, 2H); ^{13}C NMR (100 MHz, DMSO-d_6) δ 165.0, 159.3, 148.3, 133.7, 132.1, 131.3, 128.4, 128.1, 127.4, 120.1, 115.4; HRMS (ESI) calcd for $C_{13}H_{10}ClN_4O$ $(M+H)^+$ 273.0538, found 273.0538.

***N*-(6-(trifluoromethyl)-[1,2,4]triazolo[1,5-a]pyridin-2-yl)benzamide (3ag)**



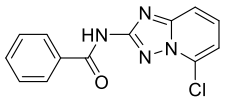
43.5 mg, 71%, yellow solid, m. p. 79-81 °C; ^{1}H NMR (400 MHz, DMSO-d_6) δ 11.29 (s, 1H), 9.30 (s, 1H), 8.01 (d, J = 7.2 Hz, 2H), 7.80-7.72 (m, 2H), 7.63-7.59 (m, 1H), 7.55-7.51 (m, 2H); ^{13}C NMR (100 MHz, DMSO-d_6) δ 165.0, 160.4, 150.4, 133.6, 132.20, 128.6 (q, J = 5.0 Hz), 128.4, 128.2, 126.3 (q, J = 8.0 Hz), 122.4 (q, J = 270.0 Hz), 116.0 (q, J = 34.0 Hz), 115.7; HRMS (ESI) calcd for $C_{14}H_{10}F_3N_4O$ $(M+H)^+$ 307.0802, found 307.0801.

N-(5-methyl-[1,2,4]triazolo[1,5-a]pyridin-2-yl)benzamide **(3ah)**



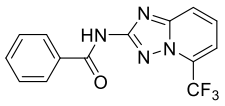
32.3 mg, 64%, white solid, m. p. 74-76 °C; ^{1}H NMR (400 MHz, DMSO-d_6) δ 11.19 (s, 1H), 8.04 (d, J = 8.0 Hz, 2H), 7.62-7.50 (m, 5H), 7.04 (d, J = 8.0 Hz, 1H), 2.71 (s, 3H); ^{13}C NMR (100 MHz, DMSO-d_6) δ 165.1, 158.3, 148.1, 133.8, 132.85, 132.0, 128.4, 128.0, 126.7, 123.5, 114.1, 17.3; HRMS (ESI) calcd for $C_{14}H_{13}N_4O$ $(M+H)^+$ 253.1084, found 253.1083.

***N*-(5-chloro-[1,2,4]triazolo[1,5-a]pyridin-2-yl)benzamide (3ai)**



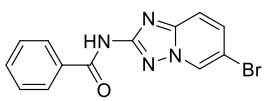
29.7 mg, 59%, yellow solid, m. p. 59-61 °C; ^{1}H NMR (400 MHz, DMSO-d_6) δ 11.38 (s, 1H), 8.05-8.03 (m, 2H), 7.76 (dd, J = 8.8, 0.8 Hz, 1H), 7.69-7.65 (m, 1H), 7.54-7.51 (m, 2H), 7.43-7.41 (m, 1H); ^{13}C NMR (100 MHz, DMSO-d_6) δ 165.1, 158.6, 150.8, 133.6, 132.2, 130.8, 128.4, 128.1, 114.0, 113.6; HRMS (ESI) calcd for $C_{13}H_{10}ClN_4O$ $(M+H)^+$ 273.0538, found 273.0538.

***N*-(5-(trifluoromethyl)-[1,2,4]triazolo[1,5-a]pyridin-2-yl)benzamide (3aj)**



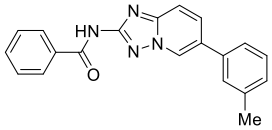
40.9 mg, 67%, yellow solid, m. p. 66-68 °C; ^{1}H NMR (400 MHz, DMSO-d_6) δ 11.45 (s, 1H), 8.11-8.04 (m, 3H), 7.83-7.74 (m, 2H), 7.62-7.59 (m, 1H), 7.54-7.50 (m, 2H); ^{13}C NMR (100 MHz, DMSO-d_6) δ 165.2, 159.4, 150.5, 133.5, 132.2, 129.6, 128.4, 128.2, 126.4 (q, J = 37.0 Hz), 119.8 (q, J = 275.0 Hz), 119.7, 114.0 (q, J = 4.0 Hz); HRMS (ESI) calcd for $C_{14}H_{10}F_3N_4O$ $(M+H)^+$ 307.0802, found 307.0801.

***N*-(6-bromo-[1,2,4]triazolo[1,5-a]pyridin-2-yl)benzamide (3ak)**



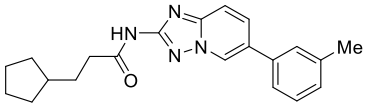
1.48 g, 47% (10 mmol scale), yellow solid, m. p. 79-81 °C; ^{1}H NMR (400 MHz, DMSO-d_6) δ 11.28 (s, 1H), 9.34 (d, J = 1.2 Hz, 1H), 8.01 (d, J = 7.2 Hz, 2H), 7.82-7.80 (m, 1H), 7.63-7.59 (m, 1H), 7.55-7.51 (m, 2H); ^{13}C NMR (100 MHz, DMSO-d_6) δ 164.9, 159.1, 148.4, 133.7, 133.5, 132.1, 129.3, 128.4, 128.1, 115.7, 106.8; HRMS (ESI) calcd for $C_{13}H_{10}BrN_4O$ $(M+H)^+$ 317.0033, found 317.0032.

_N_-(6-(m-tolyl)-[1,2,4]triazolo[1,5-a]pyridin-2-yl)benzamide (5)



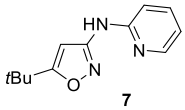
56.4 mg, 86%, yellow solid, m. p. 77-80 °C; ^{1}H NMR (400 MHz, DMSO-d_6) δ 11.24 (s, 1H), 9.24 (s, 1H), 8.04-8.00 (m, 3H), 7.80 (d, J = 12.0 Hz, 1H), 7.64-7.52 (m, 5H), 7.42-7.38 (m, 1H), 7.24 (d, J = 8.0 Hz, 1H); ^{13}C NMR (100 MHz, DMSO-d_6) δ 165.0, 159.0, 148.7, 138.4, 132.1, 130.0, 129.0, 128.7, 128.4, 128.1, 127.5, 125.8, 124.0, 114.7, 21.1; HRMS (ESI) calcd for $C_{20}H_{16}N_4O$ $(M+H)^+$ 329.1357, found 329.1355.

3-cyclopentyl-_N_-(6-(m-tolyl)-[1,2,4]triazolo[1,5-a]pyridin-2-yl)propanamide (6)



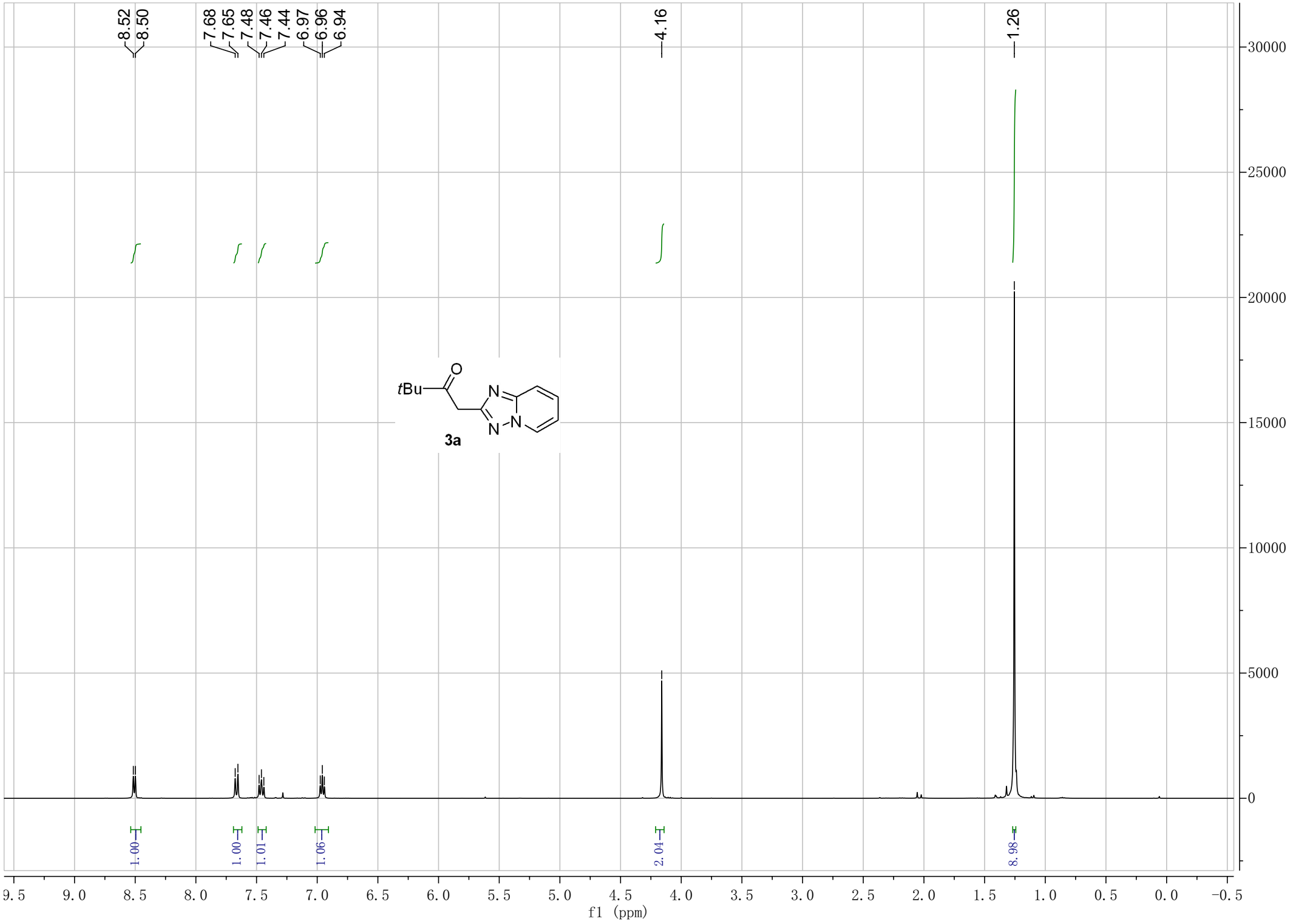
53.3 mg, 67% (two steps from **5**), white solid, m. p. 89-91 °C ; ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.84 (s, 1H), 8.81 (s, 1H), 7.76 (dd, J = 23.6, 9.2 Hz, 2H), 7.42-7.34 (m, 3H), 7.28-7.23 (m, 1H), 2.76-2.46 (m, 4H), 1.90-1.79 (m, 6H), 1.63-1.53 (m, 4H), 1.24-1.07 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 139.1, 136.1, 130.6, 129.1, 128.1, 127.6, 125.7, 124.0, 114.6, 39.7, 32.5, 31.3, 25.1, 21.5; HRMS (ESI) calcd for $C_{21}H_{25}N_4O$ $(M+H)^+$, 349.2023 found 349.2023.

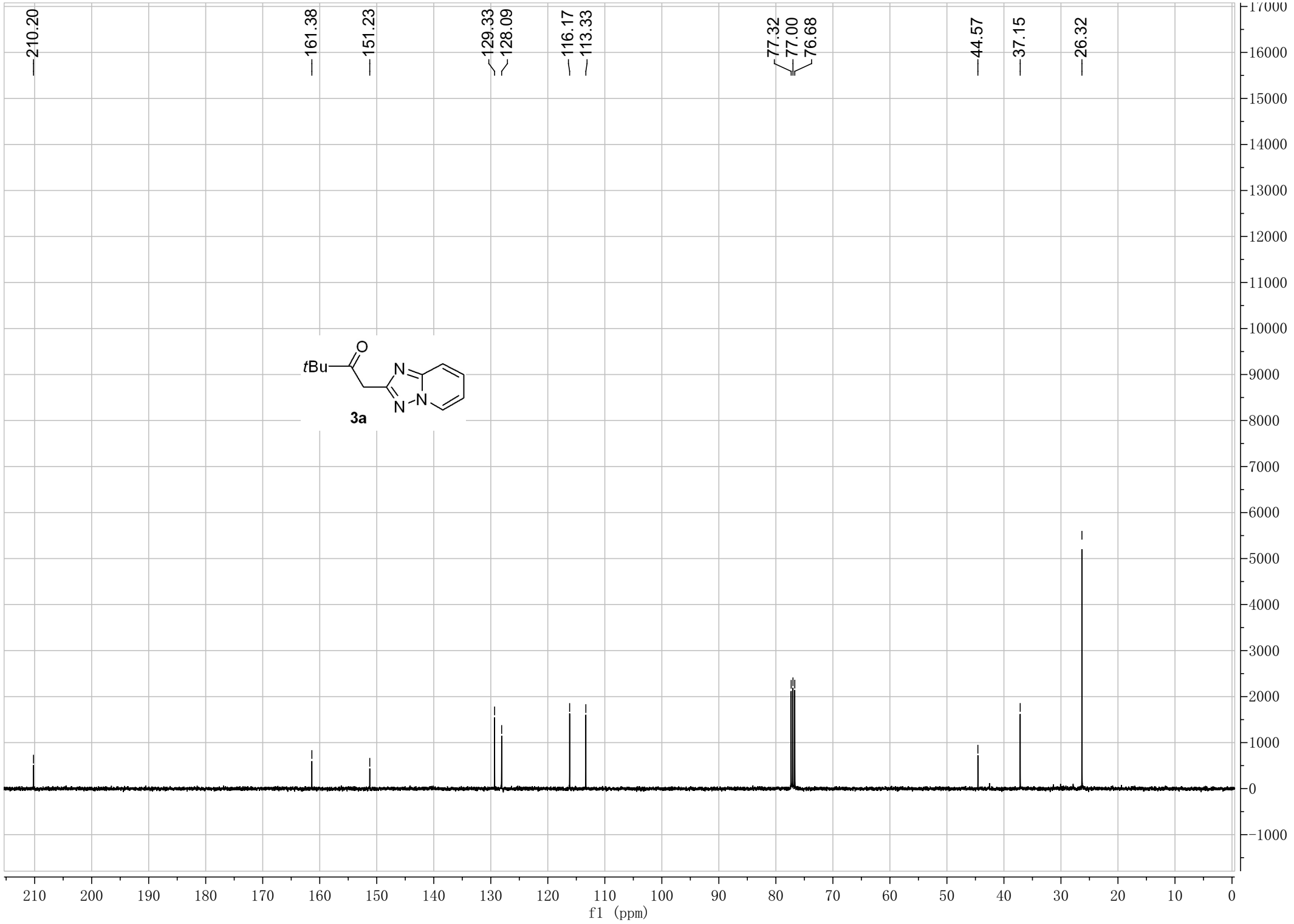
5-(tert-butyl)-_N_-(pyridin-2-yl)isoxazol-3-amine (7)

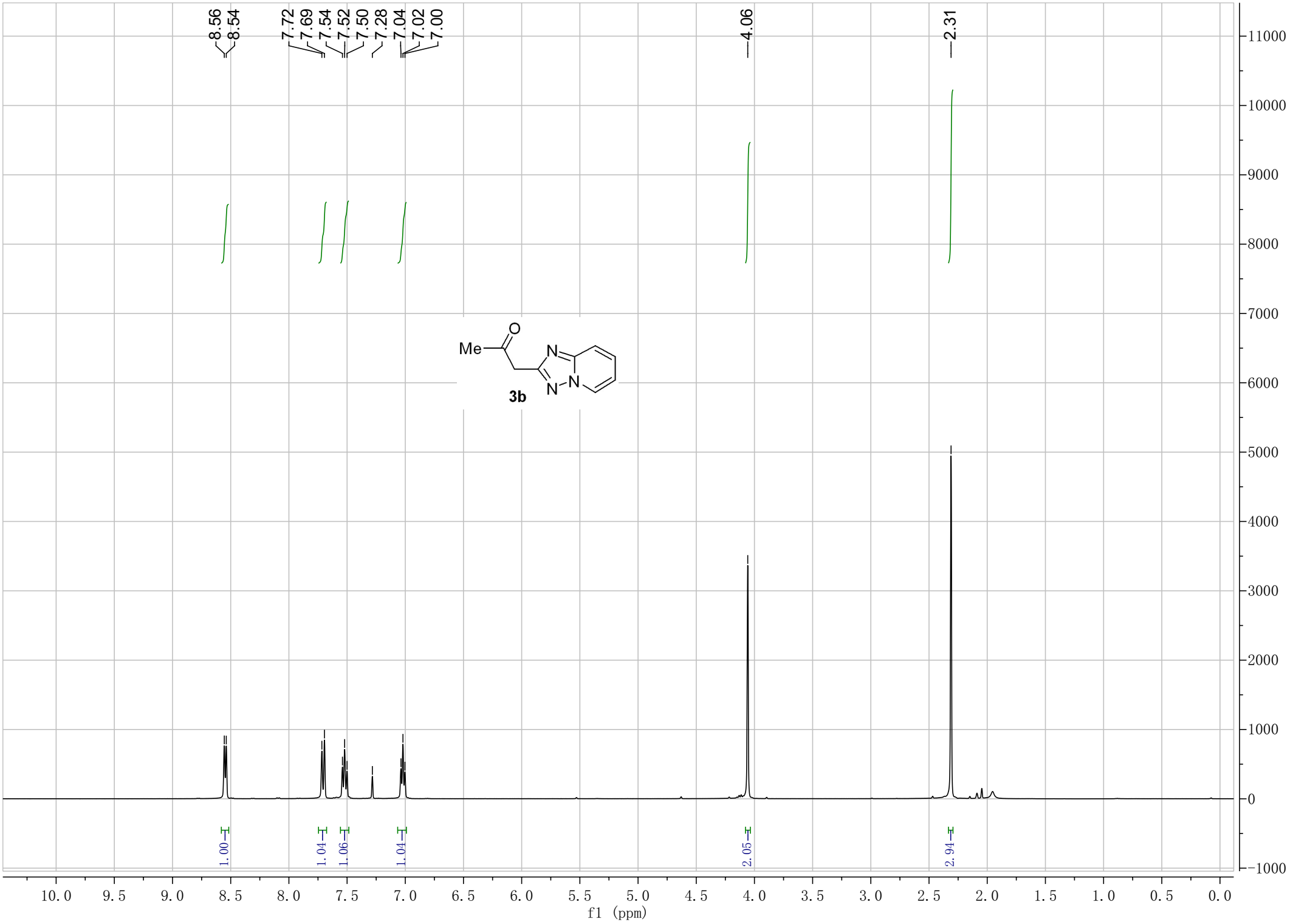


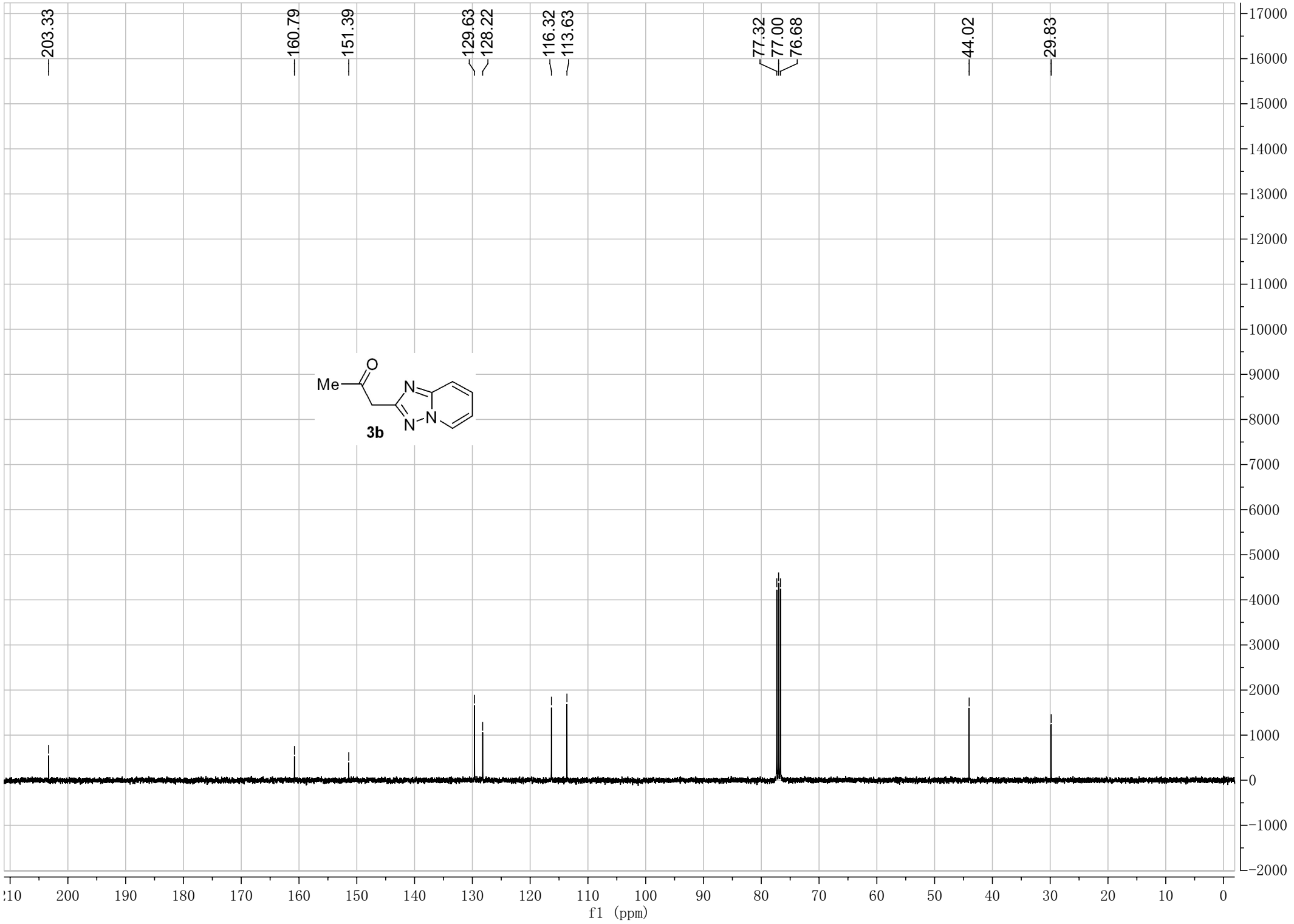
7

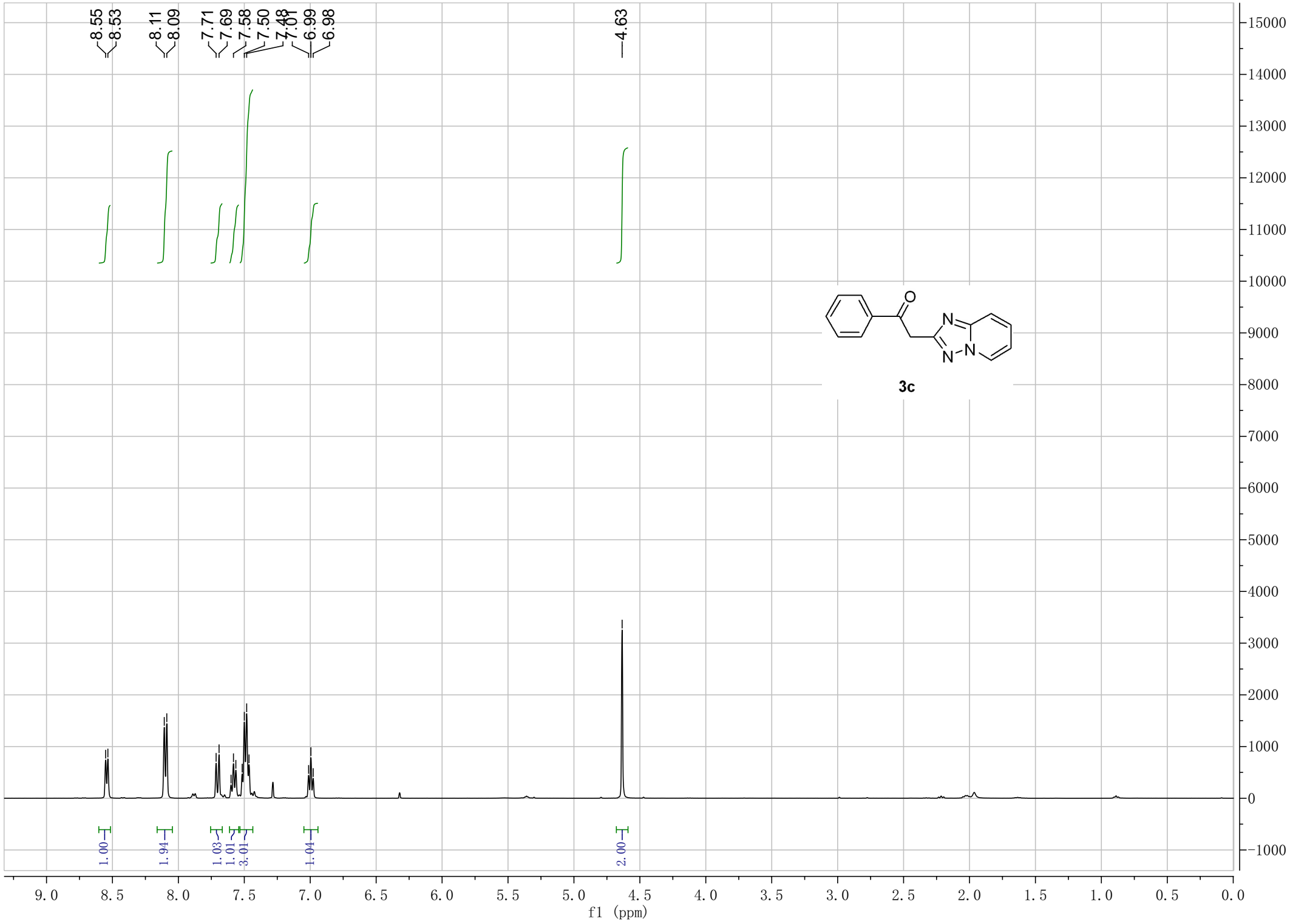
17.8 mg, 41%, yellow solid, m. p. 39-41 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.45 (s, 1H), 8.27-8.23 (m, 1H), 7.66-7.61 (m, 1H), 7.51 (d, J = 8.4 Hz, 1H), 6.88-6.85 (m, 1H), 6.11 (s, 1H), 1.35 (s, 9H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 180.4, 159.7, 153.7, 147.7, 138.3, 116.4, 111.1, 92.1, 32.8, 28.7. HRMS calcd for $C_{12}H_{16}N_3O$ $(M+H)^+$ 218.1288, found 218.1289.

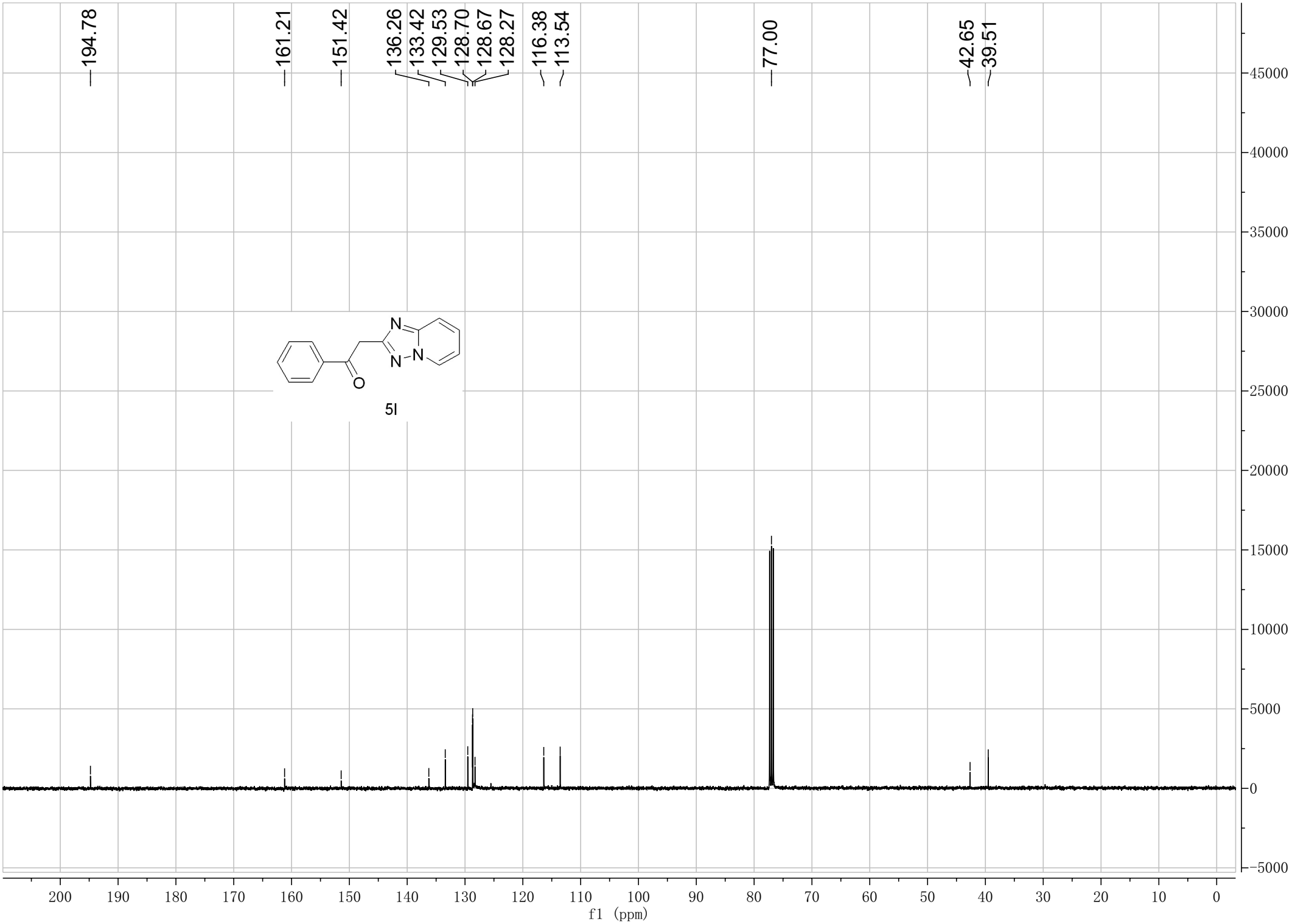

8.52
8.50
7.68
7.65
7.48
7.46
7.44
6.97
6.96
6.94
4.16
1.26
tBu
O
N
N
N
3a
1.00
1.00
1.01
1.06
2.04
8.98
30000
25000
20000
15000
10000
5000
0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

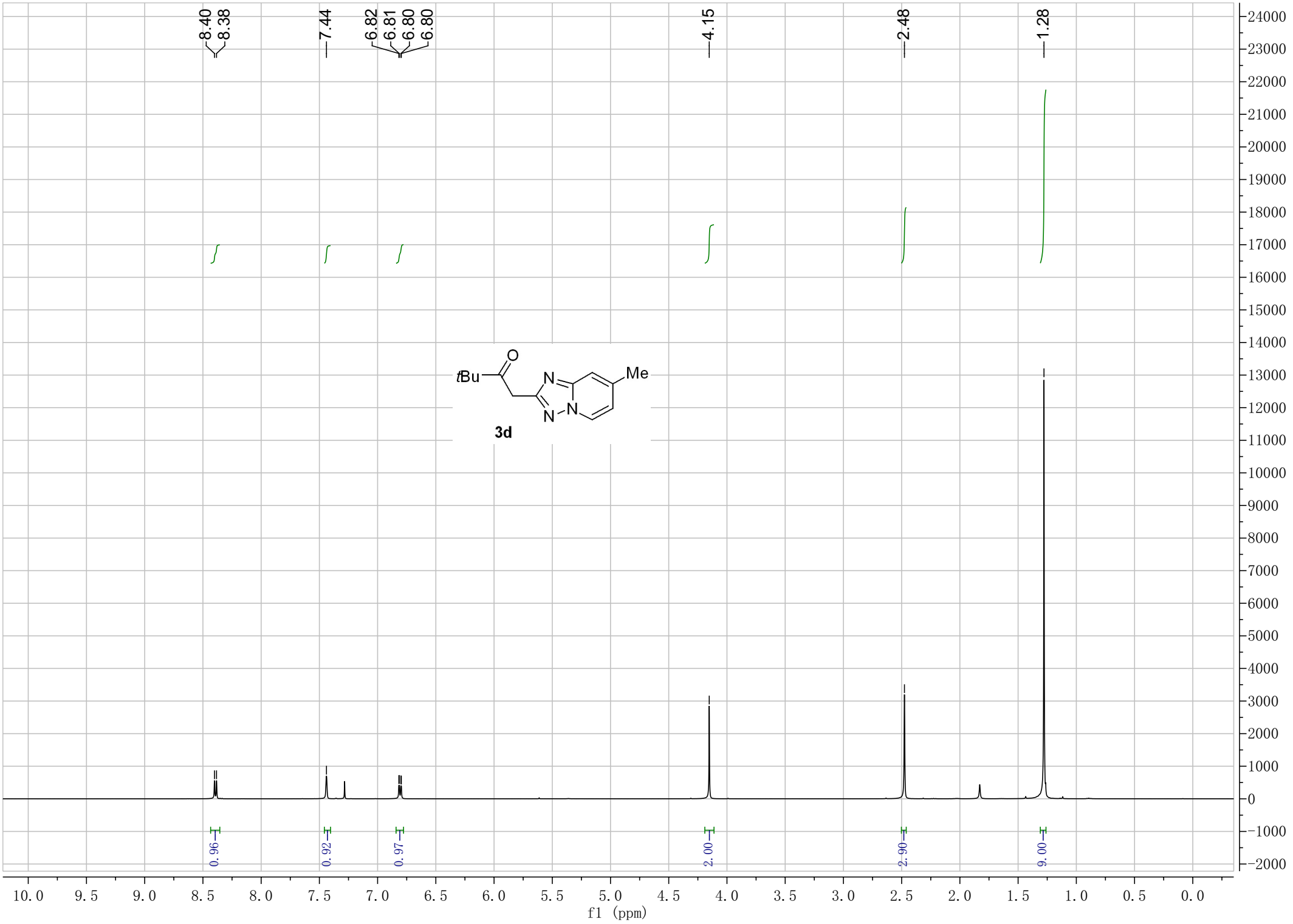

210.20
161.38
151.23
129.33
128.09
116.17
113.33
77.32
77.00
76.68
44.57
37.15
26.32
tBu
O
N
N
N
3a
f1 (ppm)

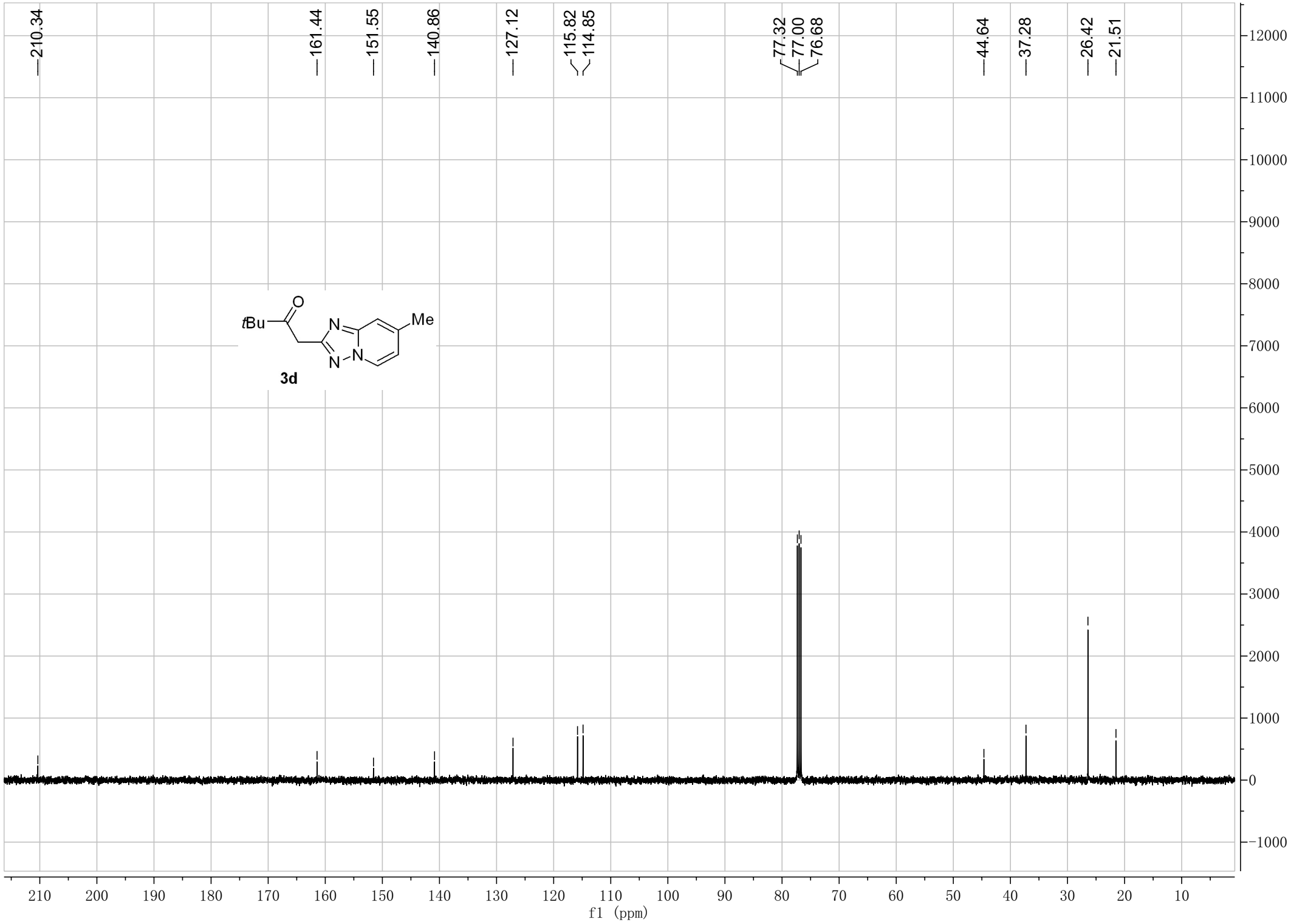

8.56
8.54
7.72
7.69
7.54
7.52
7.50
7.28
7.04
7.02
7.00
4.06
2.31
Me
O
N
N
N
3b
1.00
1.04
1.06
1.04
2.05
2.94
11000
10000
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
-1000
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


203.33
160.79
151.39
129.63
128.22
116.32
113.63
77.32
77.00
76.68
44.02
29.83
Me
O
N
N
N
3b
17000
16000
15000
14000
13000
12000
11000
10000
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
-1000
-2000
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


8.55
8.53
8.11
8.09
7.71
7.69
7.58
7.50
7.48
7.01
6.99
6.98
4.63
O
N
N
N
3c
1.00
1.94
1.03
1.01
3.01
1.04
2.00
f1 (ppm)


194.78
161.21
151.42
136.26
133.42
129.53
128.70
128.67
128.27
116.38
113.54
77.00
42.65
39.51
N
N
N
O
5l
45000
40000
35000
30000
25000
20000
15000
10000
5000
0
-5000
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


8.40
8.38
7.44
6.82
6.81
6.80
6.80
4.15
2.48
1.28
tBu
O
N
N
N
Me
3d
0.96
0.92
0.97
2.00
2.90
9.00
f1 (ppm)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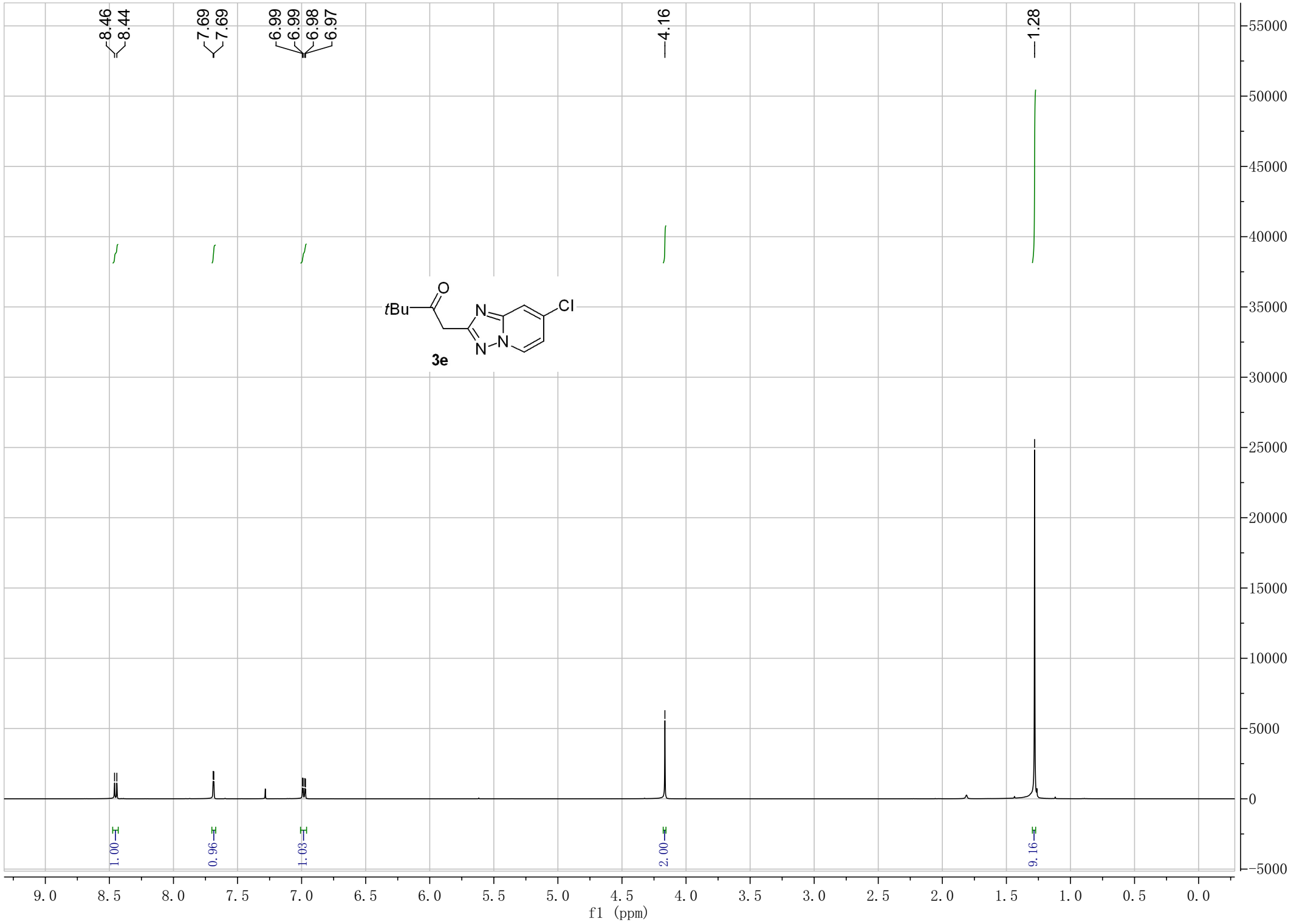
161.44
151.55
140.86
127.12
115.82
114.85
77.32
77.00
76.68
44.64
37.28
26.42
21.51
tBu
O
N
N
N
Me
3d
12000
11000
10000
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
-1000
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)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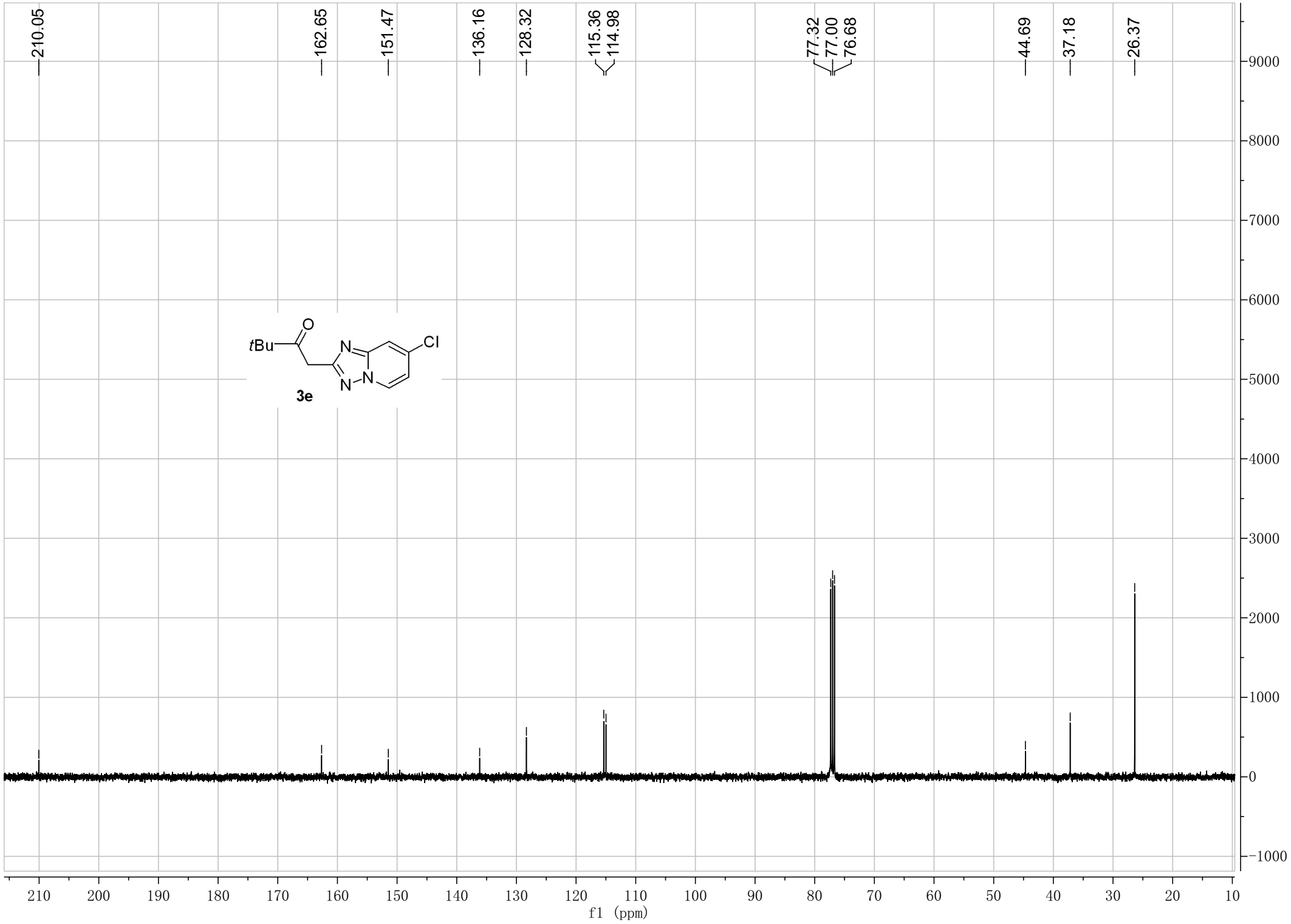
8.44
7.69
7.69
6.99
6.99
6.98
6.97
4.16
1.28
tBu
O
N
N
N
Cl
3e
1.00
0.96
1.03
2.00
9.16
55000
50000
45000
40000
35000
30000
25000
20000
15000
10000
5000
0
-5000
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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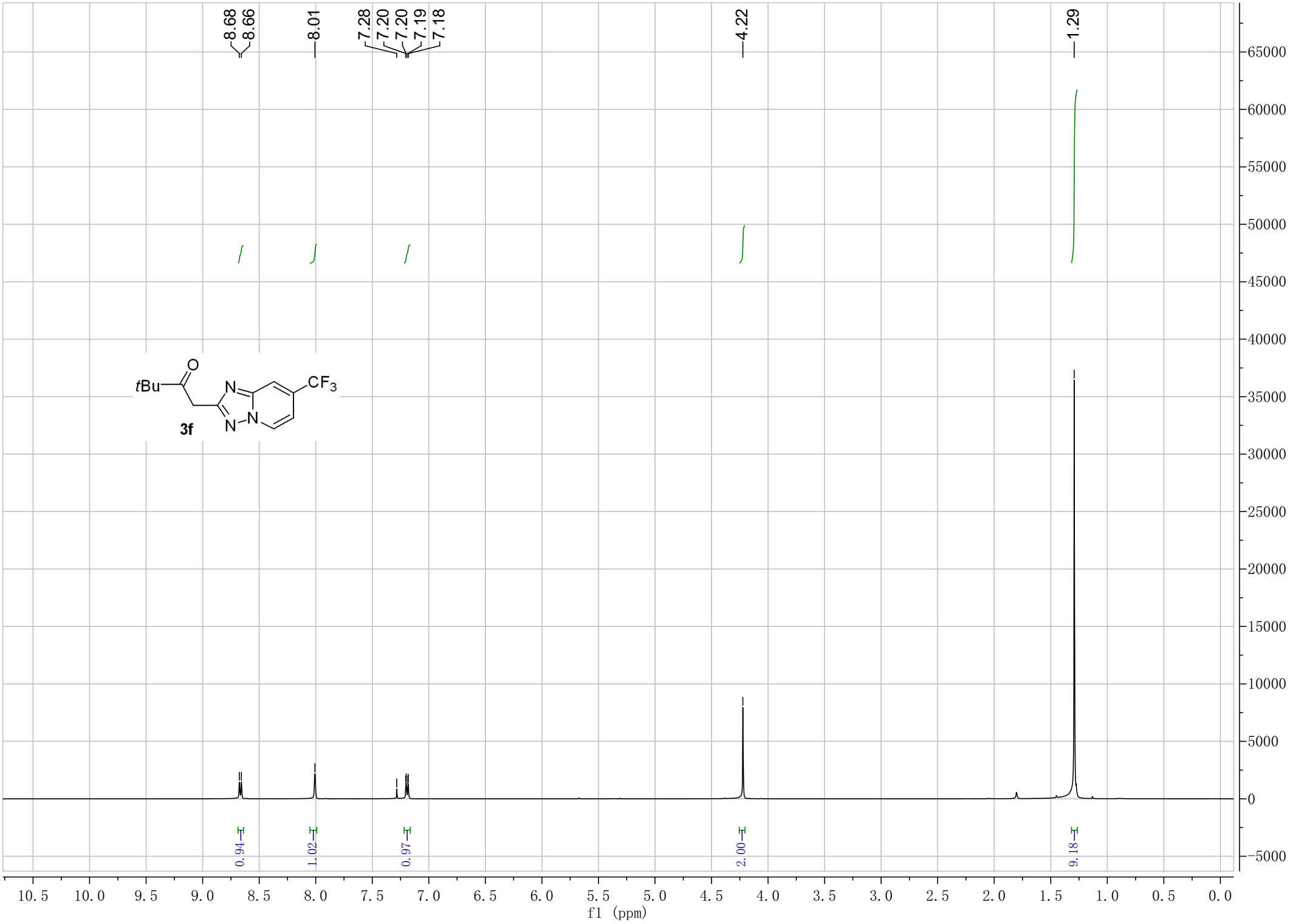
162.65
151.47
136.16
128.32
115.36
114.98
77.32
77.00
76.68
44.69
37.18
26.37
tBu
O
N
N
N
Cl
3e
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
−1000
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)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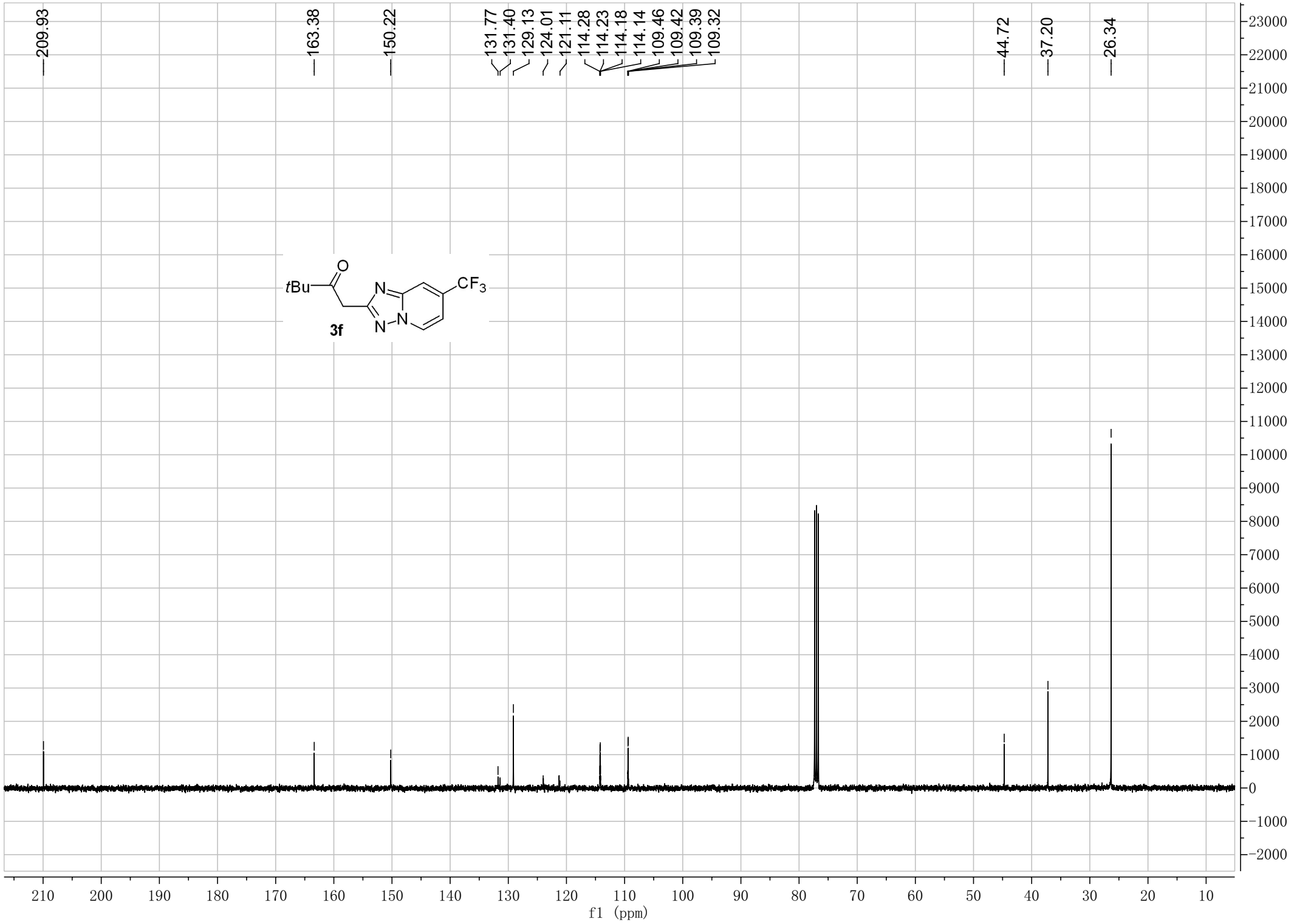
8.66
8.01
7.28
7.20
7.20
7.19
7.18
4.22
1.29
tBu
O
N
N
N
CF3
3f
0.94
1.02
0.97
2.00
9.18
65000
60000
55000
50000
45000
40000
35000
30000
25000
20000
15000
10000
5000
0
-5000
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


209.93
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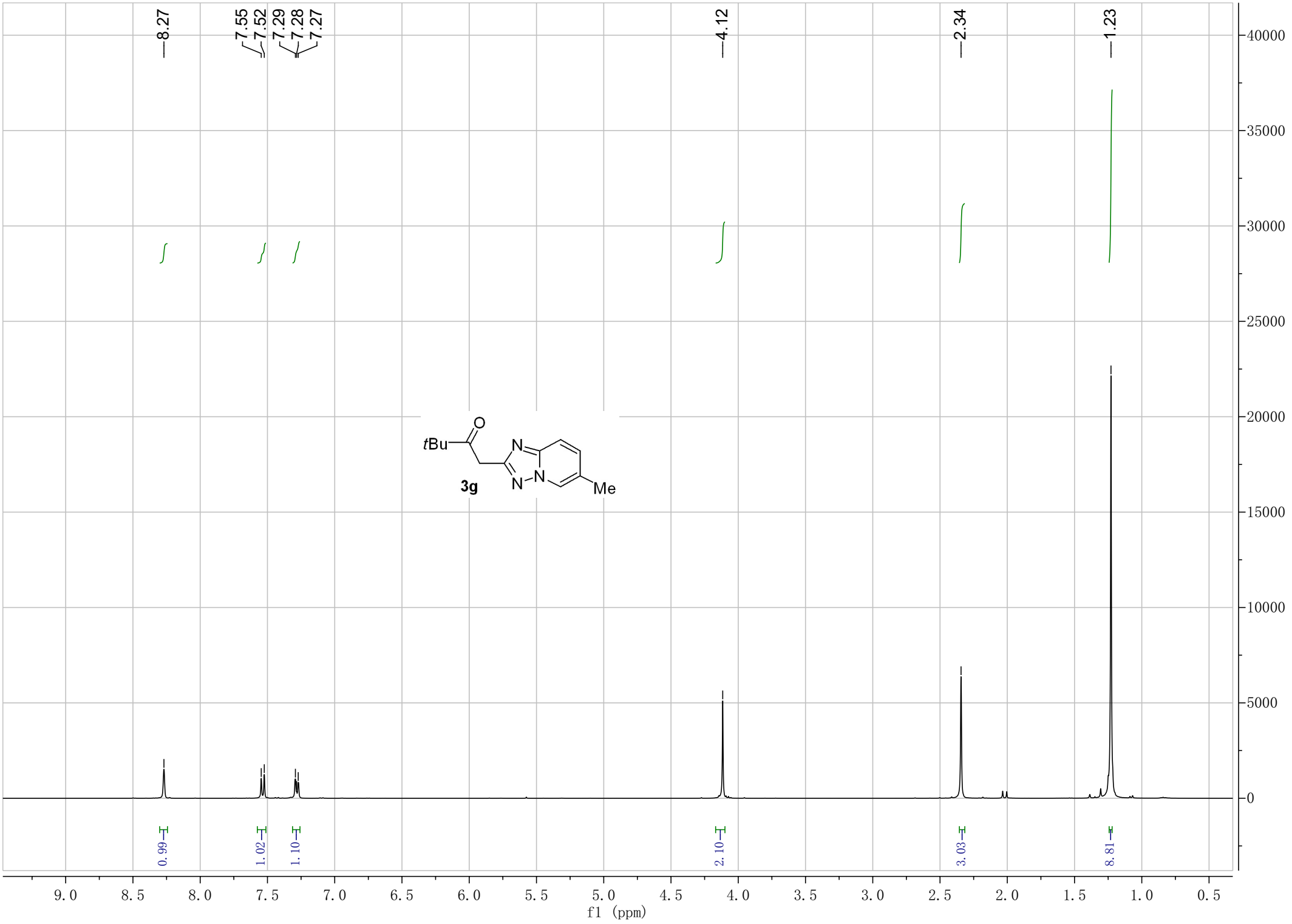
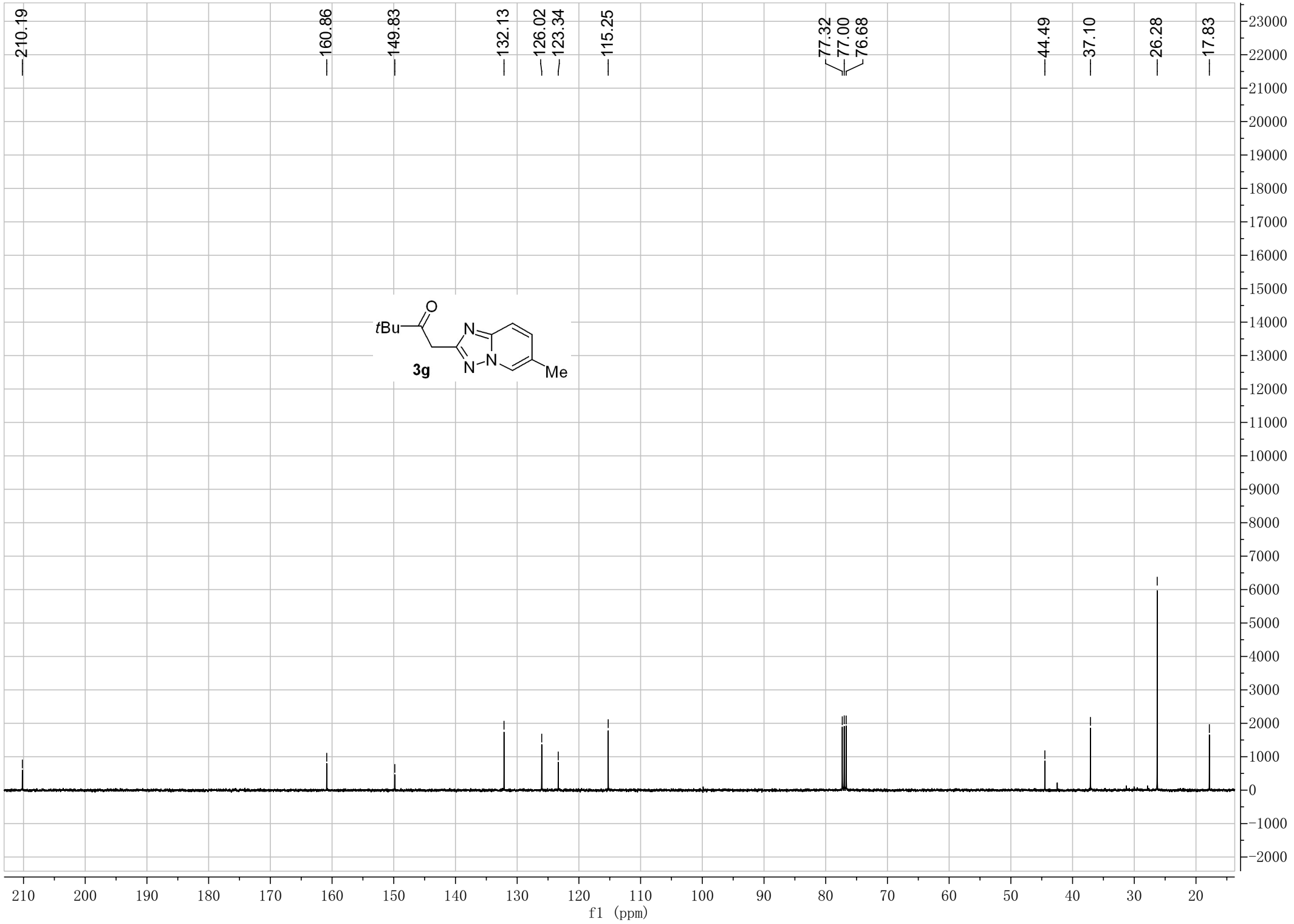
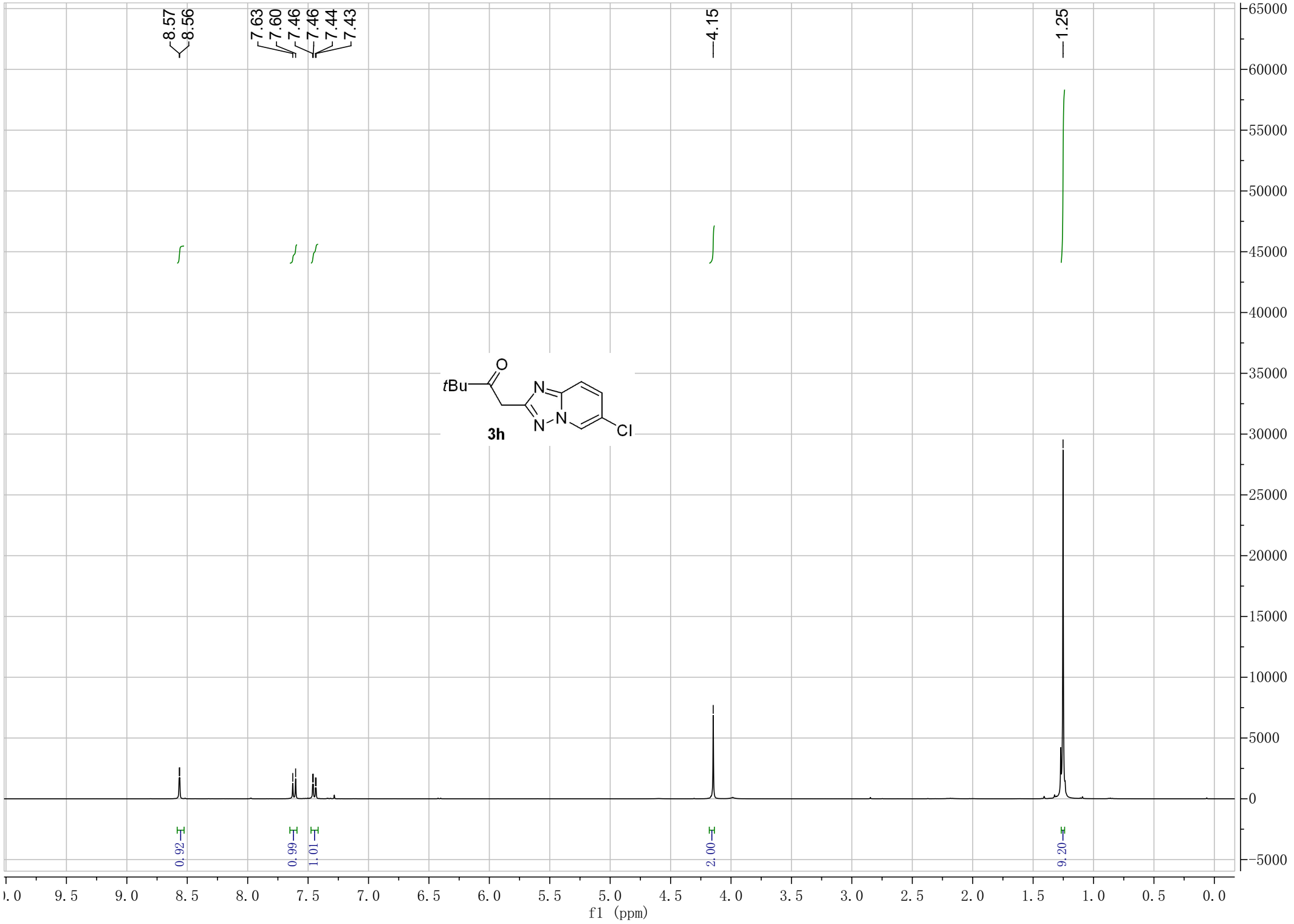
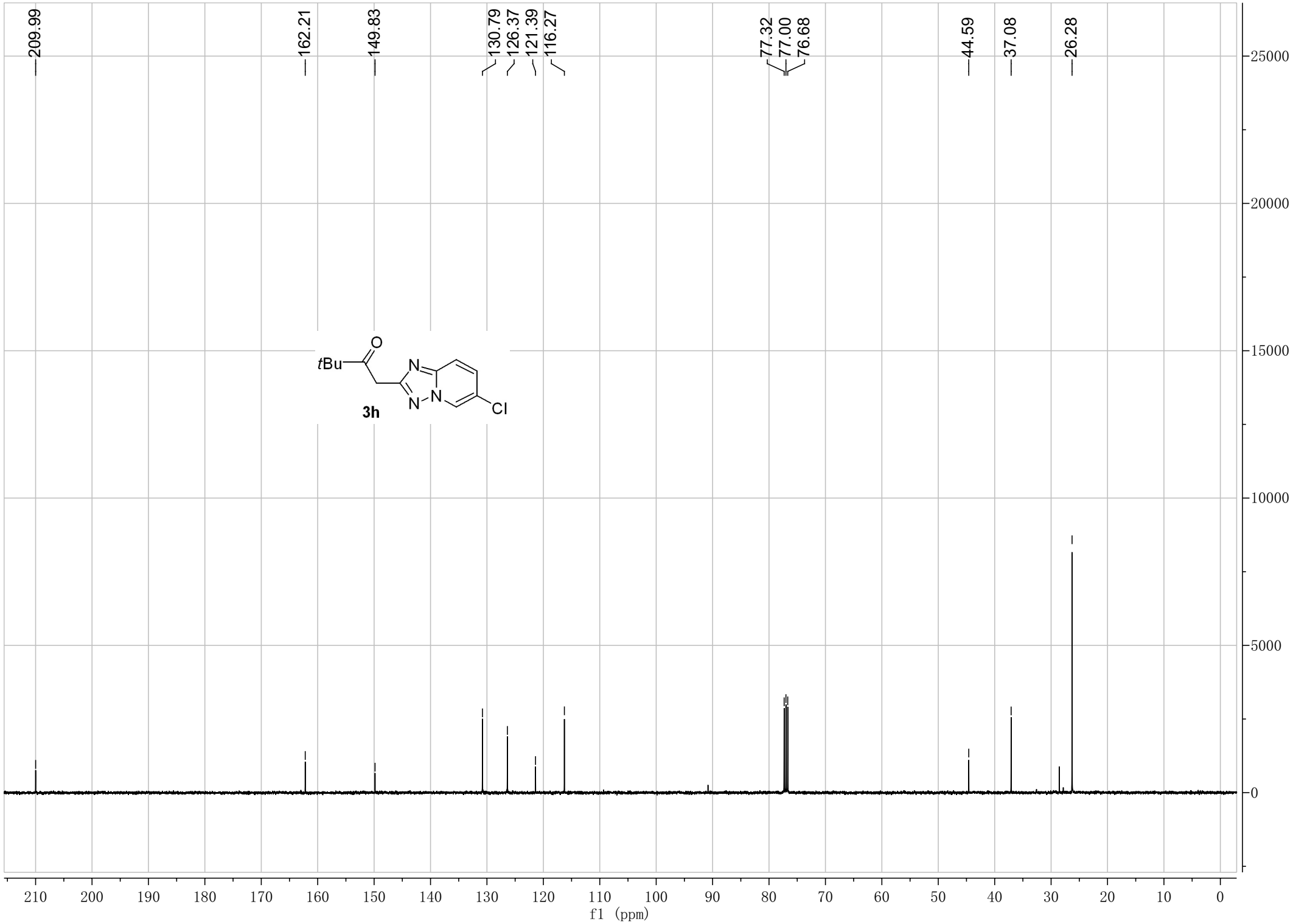
150.22
131.77
131.40
129.13
124.01
121.11
114.28
114.23
114.18
114.14
109.46
109.42
109.39
109.32
44.72
37.20
26.34
tBu
O
N
N
N
CF3
3f
f1 (ppm)


8.27
7.55
7.52
7.29
7.28
7.27
4.12
2.34
1.23
tBu
O
N
N
N
Me
3g
0.99
1.02
1.10
2.10
3.03
8.81
40000
35000
30000
25000
20000
15000
10000
5000
0
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
f1 (ppm)


210.19
160.86
149.83
132.13
126.02
123.34
115.25
77.32
77.00
76.68
44.49
37.10
26.28
17.83
tBu
O
N
N
N
Me
3g
f1 (ppm)


8.57
8.56
7.63
7.60
7.46
7.46
7.44
7.43
4.15
1.25
tBu
O
N
N
N
Cl
3h
0.92
0.99
1.01
2.00
9.20
f1 (ppm)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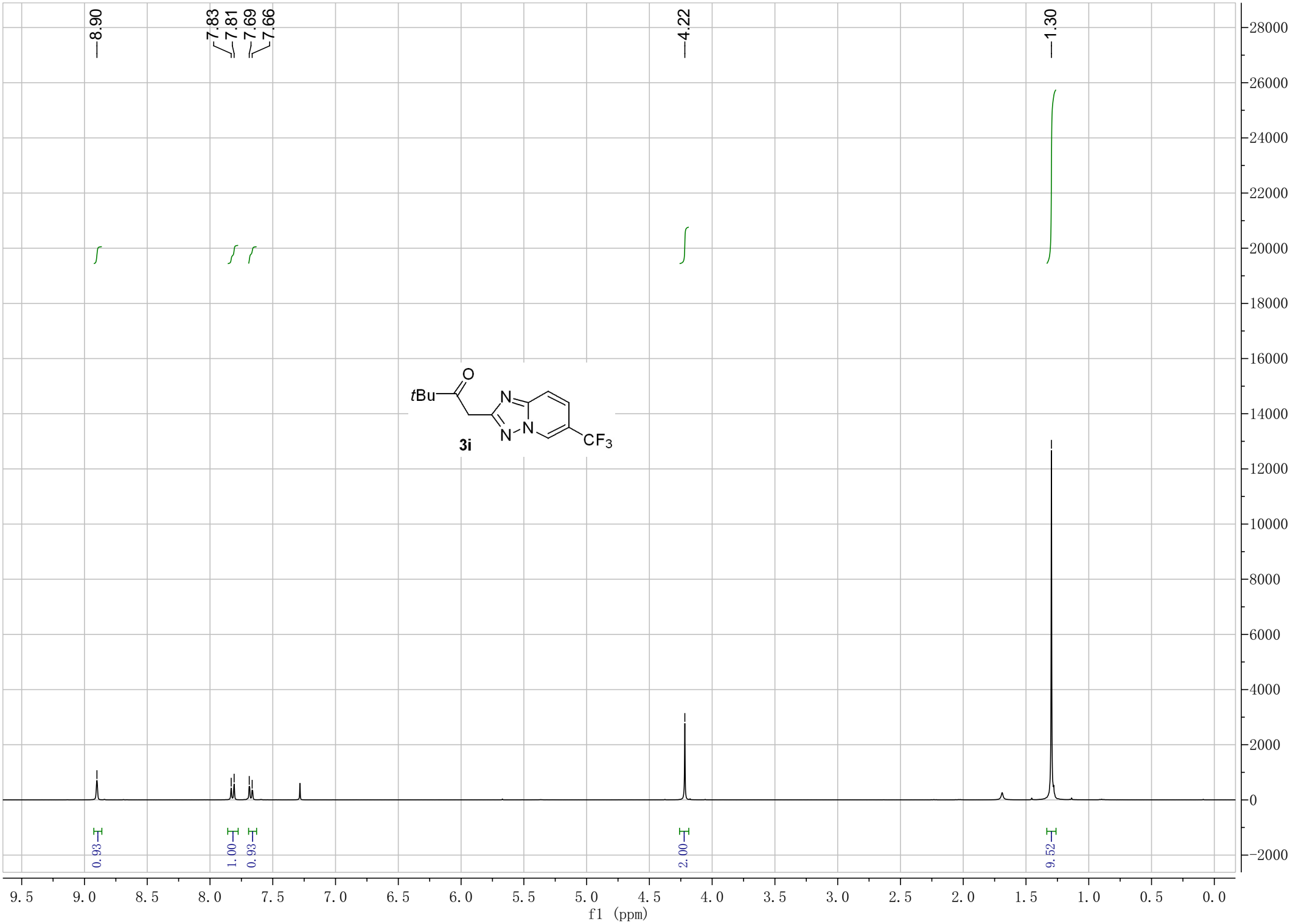
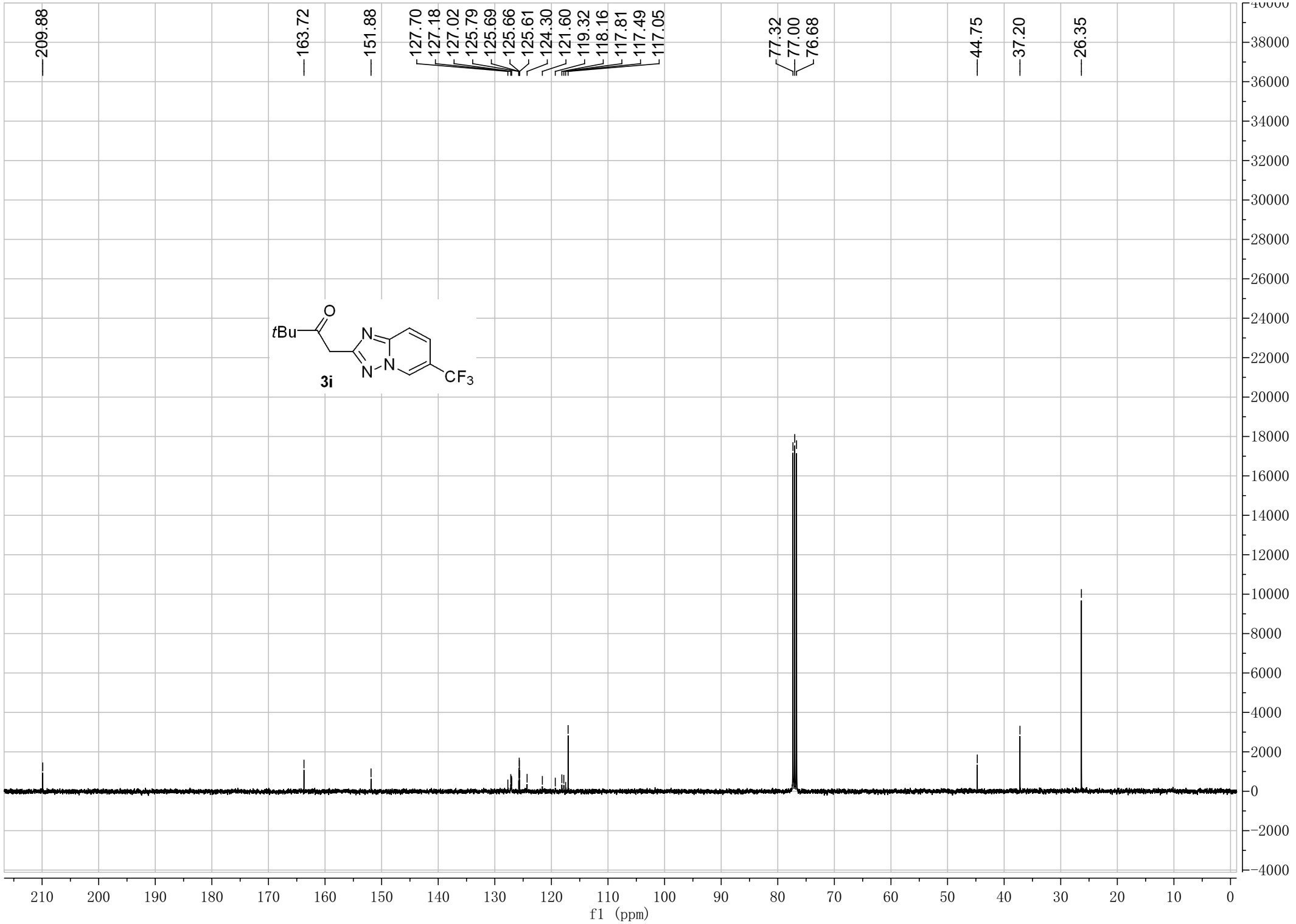
162.21
149.83
130.79
126.37
121.39
116.27
77.32
77.00
76.68
44.59
37.08
26.28
tBu
O
N
N
N
Cl
3h
25000
20000
15000
10000
5000
0
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


8.90
7.83
7.81
7.69
7.66
4.22
1.30
tBu
O
N
N
N
CF3
3i
0.93
1.00
0.93
2.00
9.52
f1 (ppm)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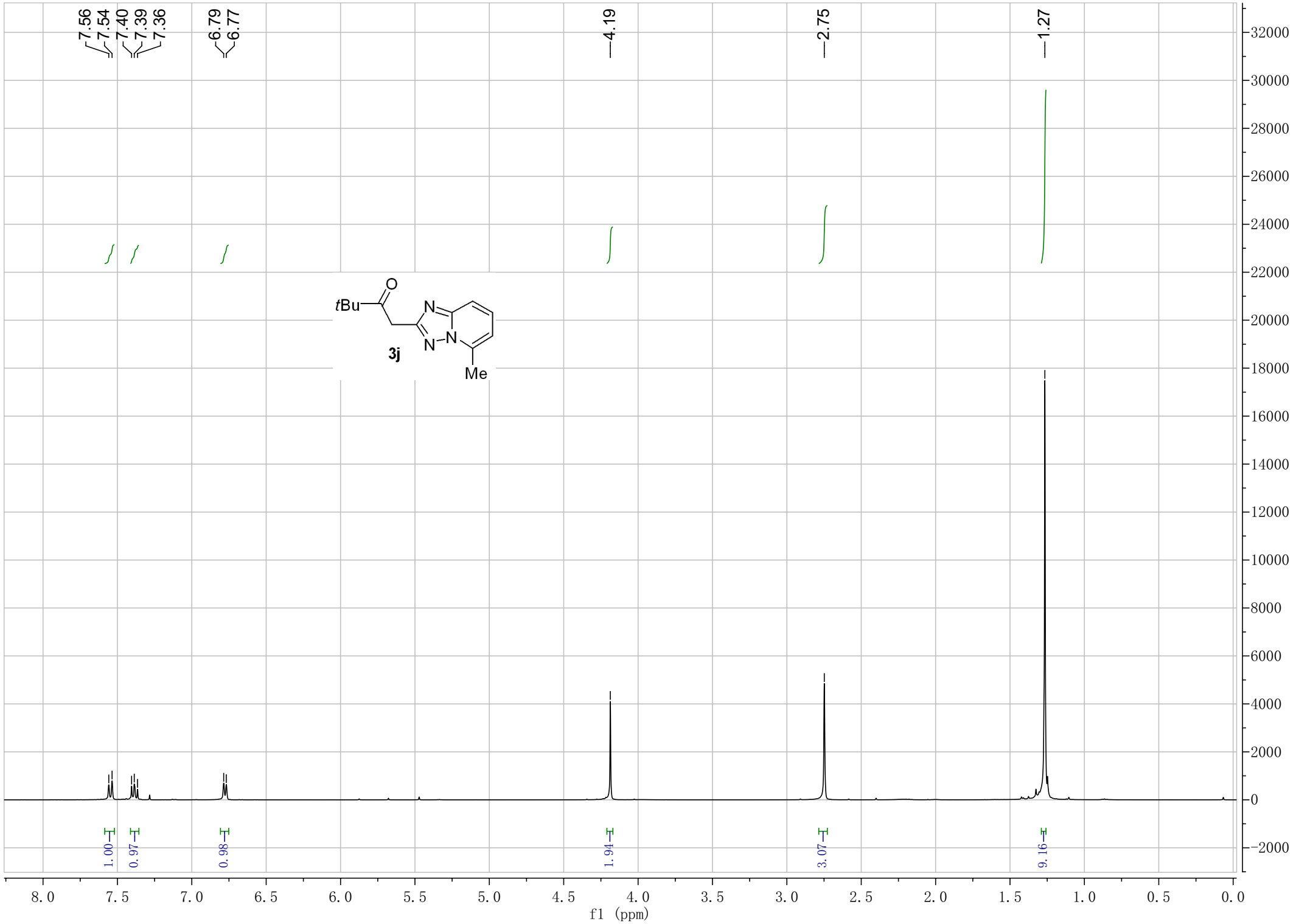
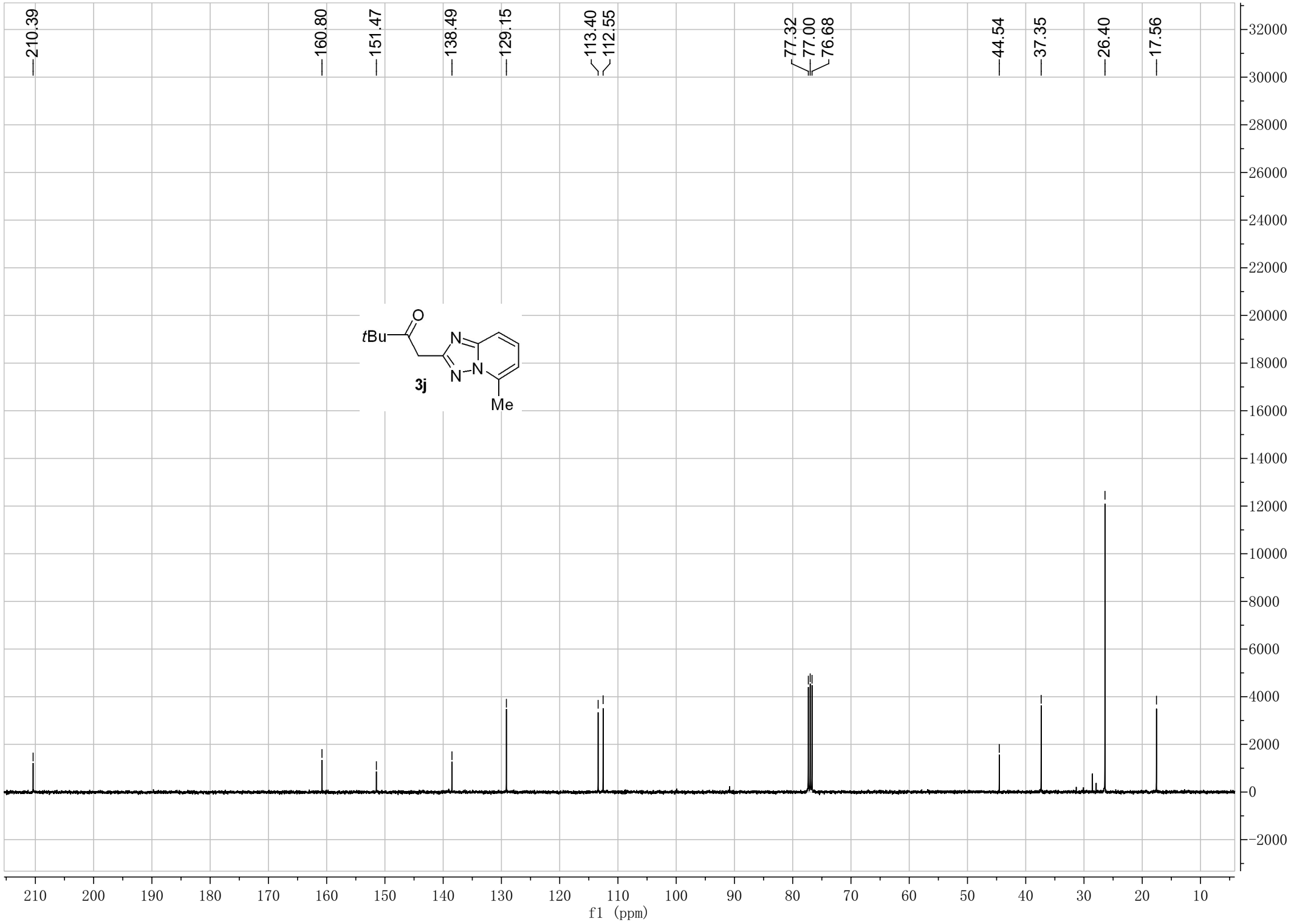
163.72
151.88
127.70
127.18
127.02
125.79
125.69
125.66
125.61
124.30
121.60
119.32
118.16
117.81
117.49
117.05
77.32
77.00
76.68
44.75
37.20
26.35
tBu
O
N
N
N
CF3
3i
f1 (ppm)


7.56
7.54
7.40
7.39
7.36
6.79
6.77
4.19
2.75
1.27
tBu
O
N
N
N
Me
3j
1.00
0.97
0.98
1.94
3.07
9.16
f1 (ppm)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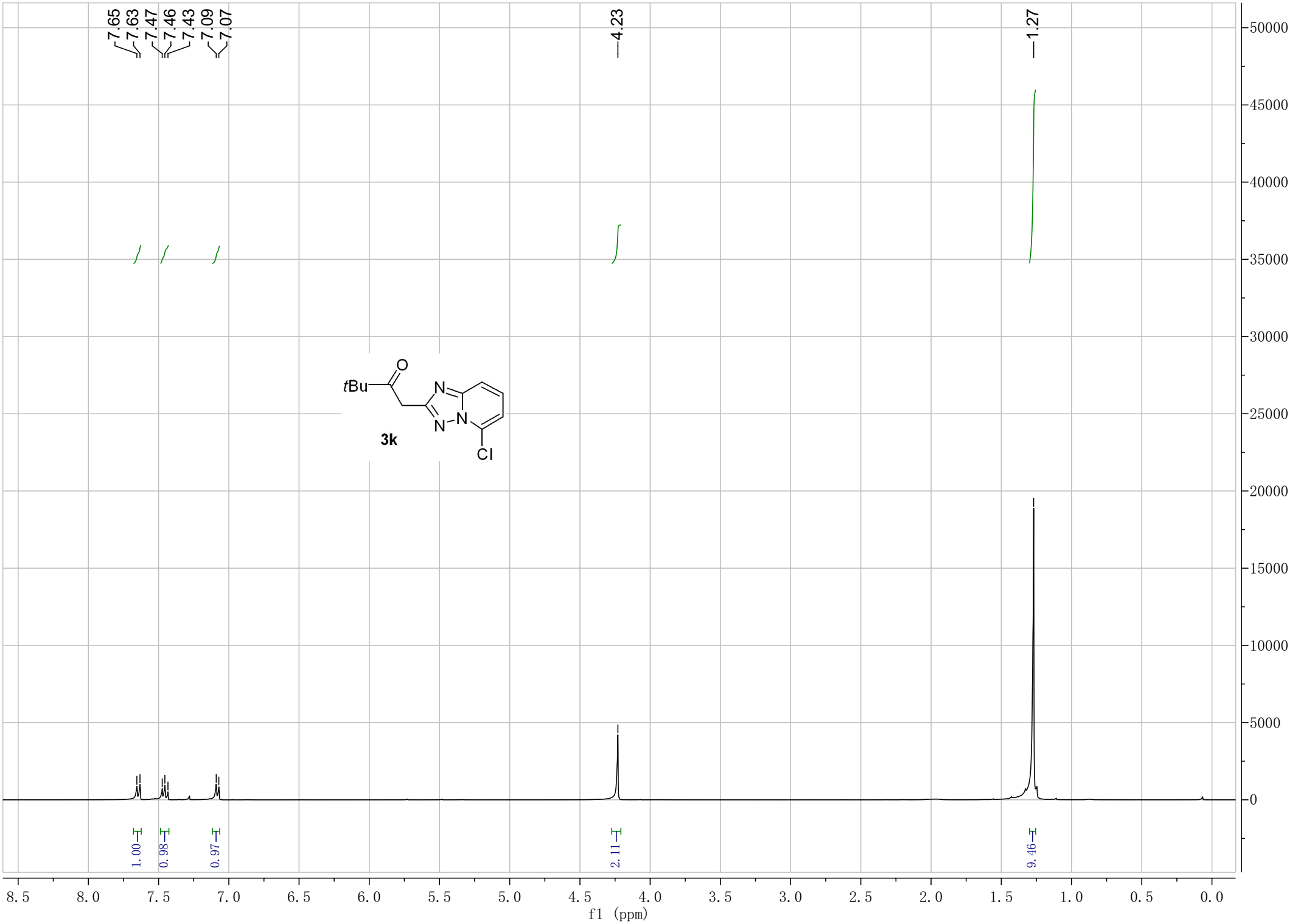
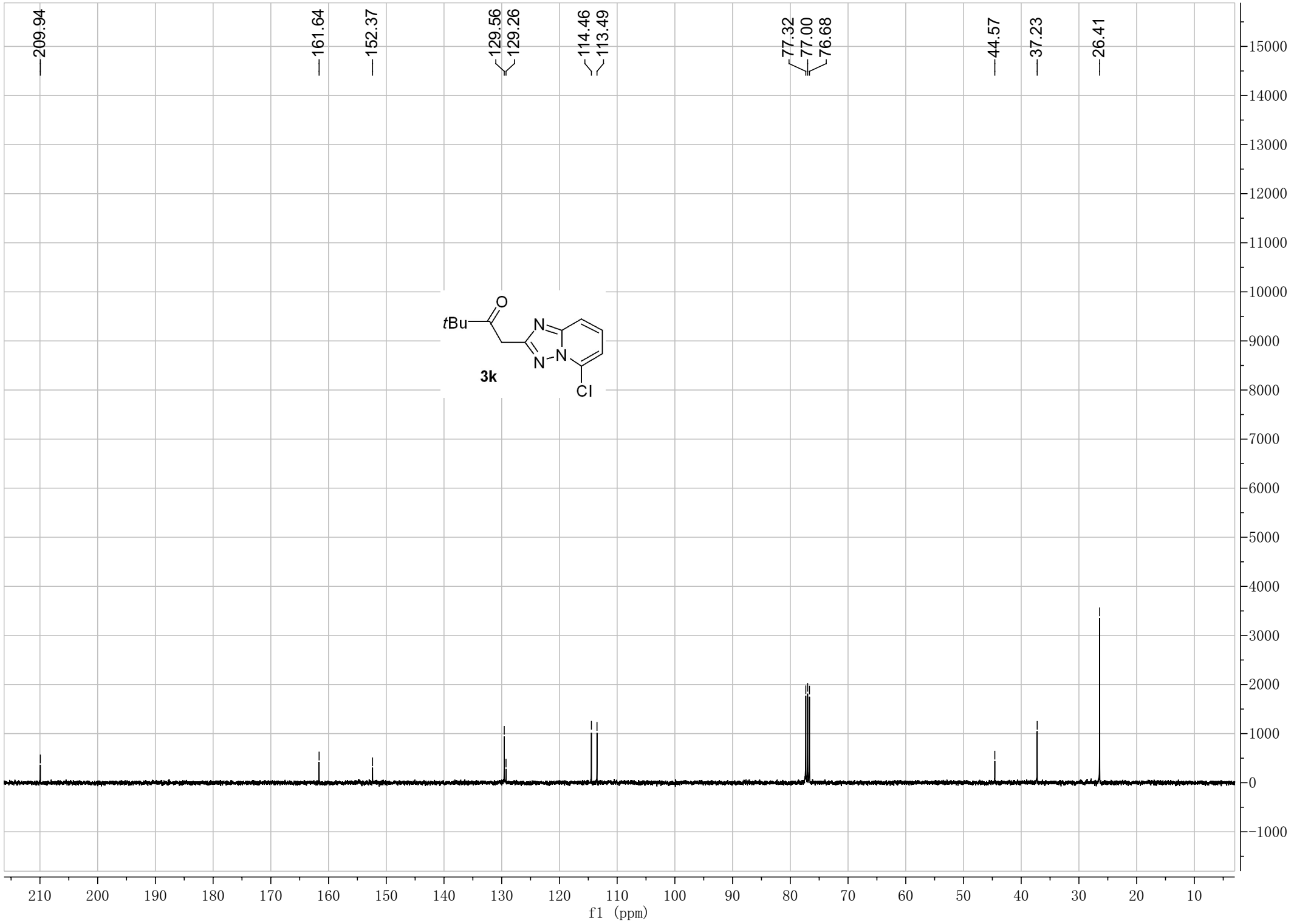
160.80
151.47
138.49
129.15
113.40
112.55
77.32
77.00
76.68
44.54
37.35
26.40
17.56
tBu
O
N
N
N
Me
3j
32000
30000
28000
26000
24000
22000
20000
18000
16000
14000
12000
10000
8000
6000
4000
2000
0
-2000
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)


7.65
7.63
7.47
7.46
7.43
7.09
7.07
4.23
1.27
tBu
O
N
N
N
Cl
3k
1.00
0.98
0.97
2.11
9.46
50000
45000
40000
35000
30000
25000
20000
15000
10000
5000
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)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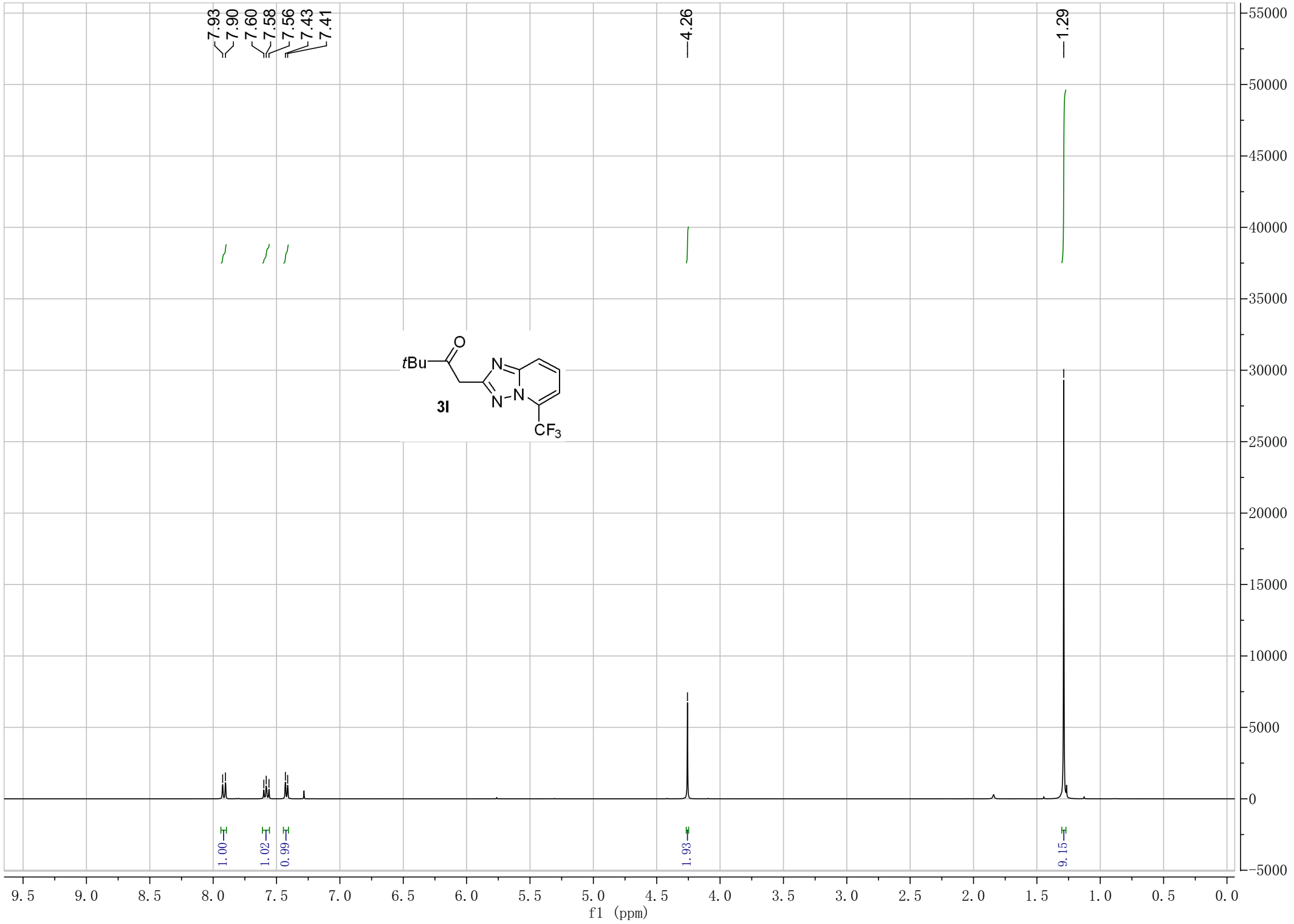
152.37
129.56
129.26
114.46
113.49
77.32
77.00
76.68
44.57
37.23
26.41
tBu
O
N
N
N
Cl
3k
15000
14000
13000
12000
11000
10000
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
-1000
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)


7.93
7.90
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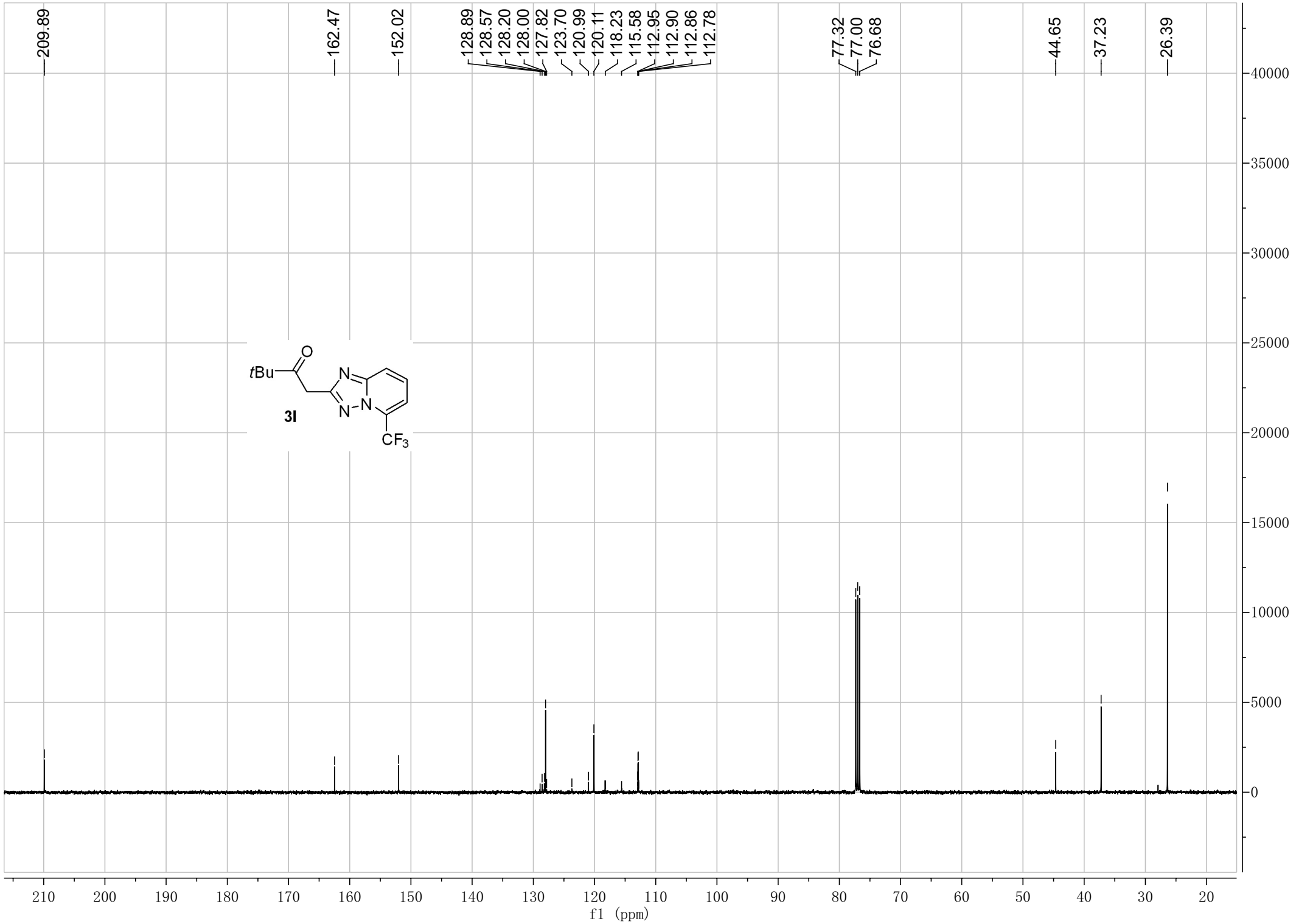
7.58
7.56
7.43
7.41
4.26
1.29
tBu
O
N
N
N
CF3
3l
1.00
1.02
0.99
1.93
9.15
55000
50000
45000
40000
35000
30000
25000
20000
15000
10000
5000
0
-5000
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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128.89
128.57
128.20
128.00
127.82
123.70
120.99
120.11
118.23
115.58
112.95
112.90
112.86
112.78
77.32
77.00
76.68
44.65
37.23
26.39
tBu
O
N
N
N
CF3
3l
40000
35000
30000
25000
20000
15000
10000
5000
0
210
200
190
180
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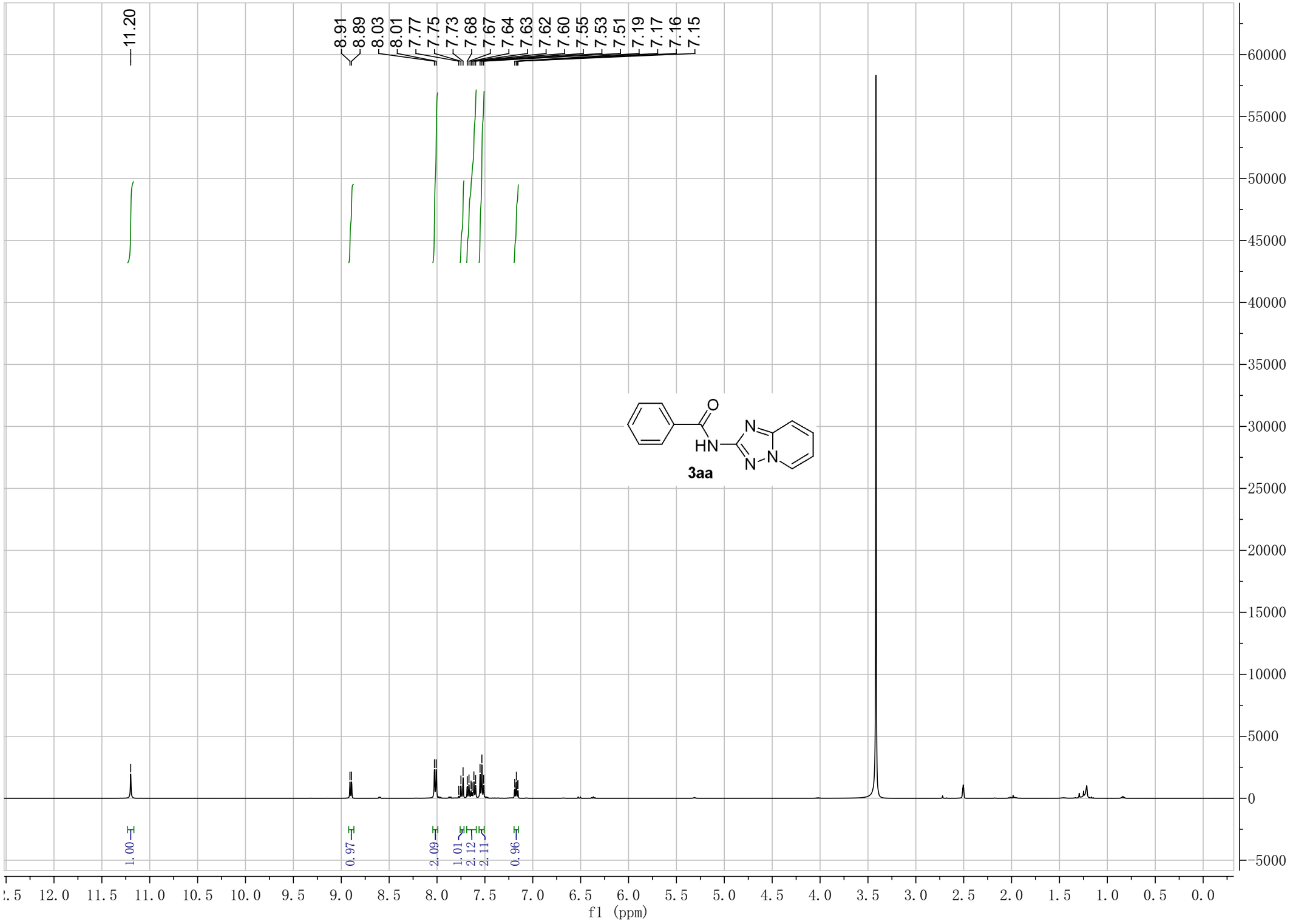
150
140
130
120
110
100
90
80
70
60
50
40
30
20
f1 (ppm)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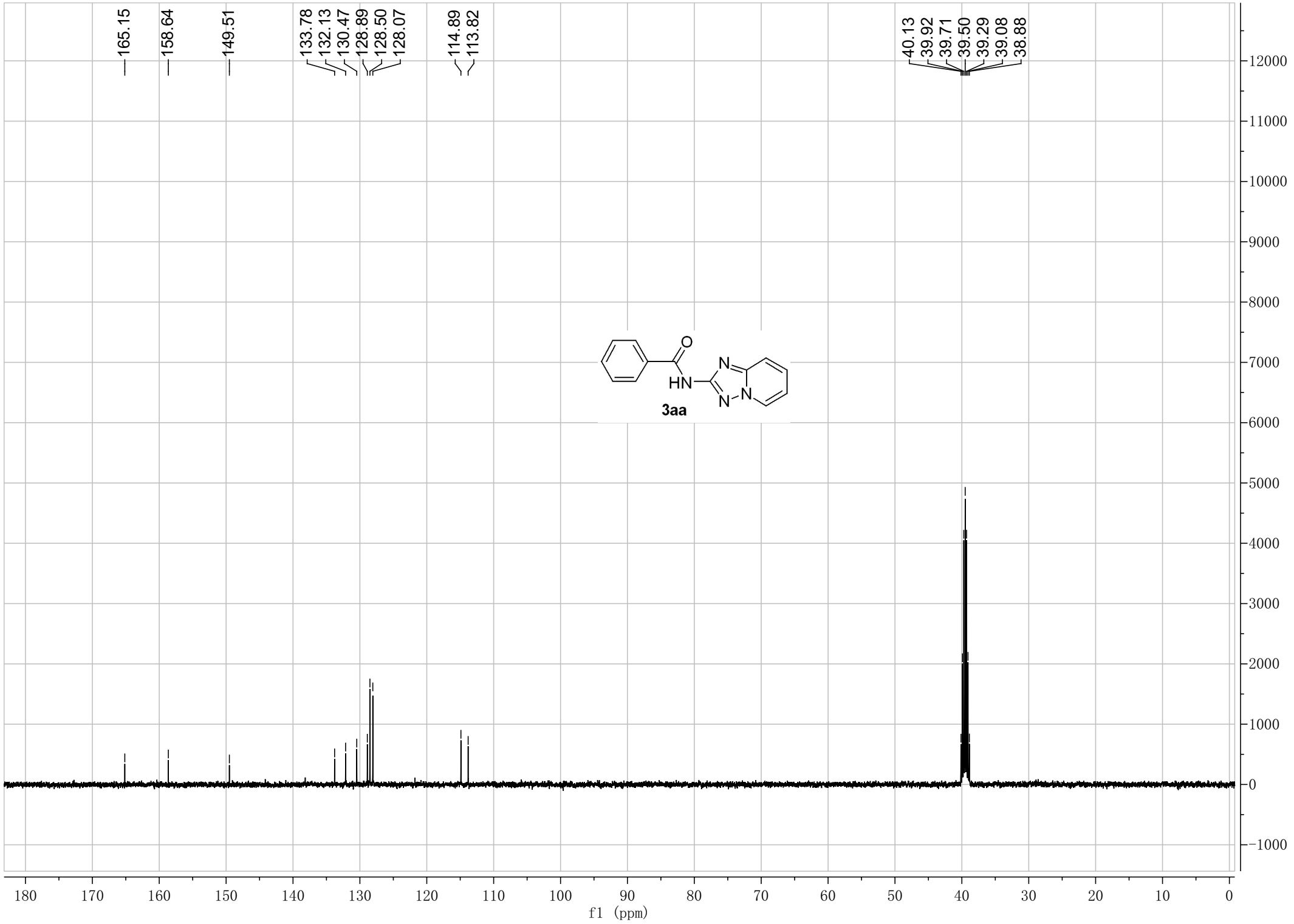
8.89
8.03
8.01
7.77
7.75
7.73
7.68
7.67
7.64
7.63
7.62
7.60
7.55
7.53
7.51
7.19
7.17
7.16
7.15
O
HN
N
N
N
3aa
1.00
0.97
2.09
1.01
2.12
2.11
0.96
60000
55000
50000
45000
40000
35000
30000
25000
20000
15000
10000
5000
0
-5000
12.0
11.5
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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158.64
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133.78
132.13
130.47
128.89
128.50
128.07
114.89
113.82
40.13
39.92
39.71
39.50
39.29
39.08
38.88
O
HN
N
N
N
3aa
12000
11000
10000
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
-1000
180
170
160
150
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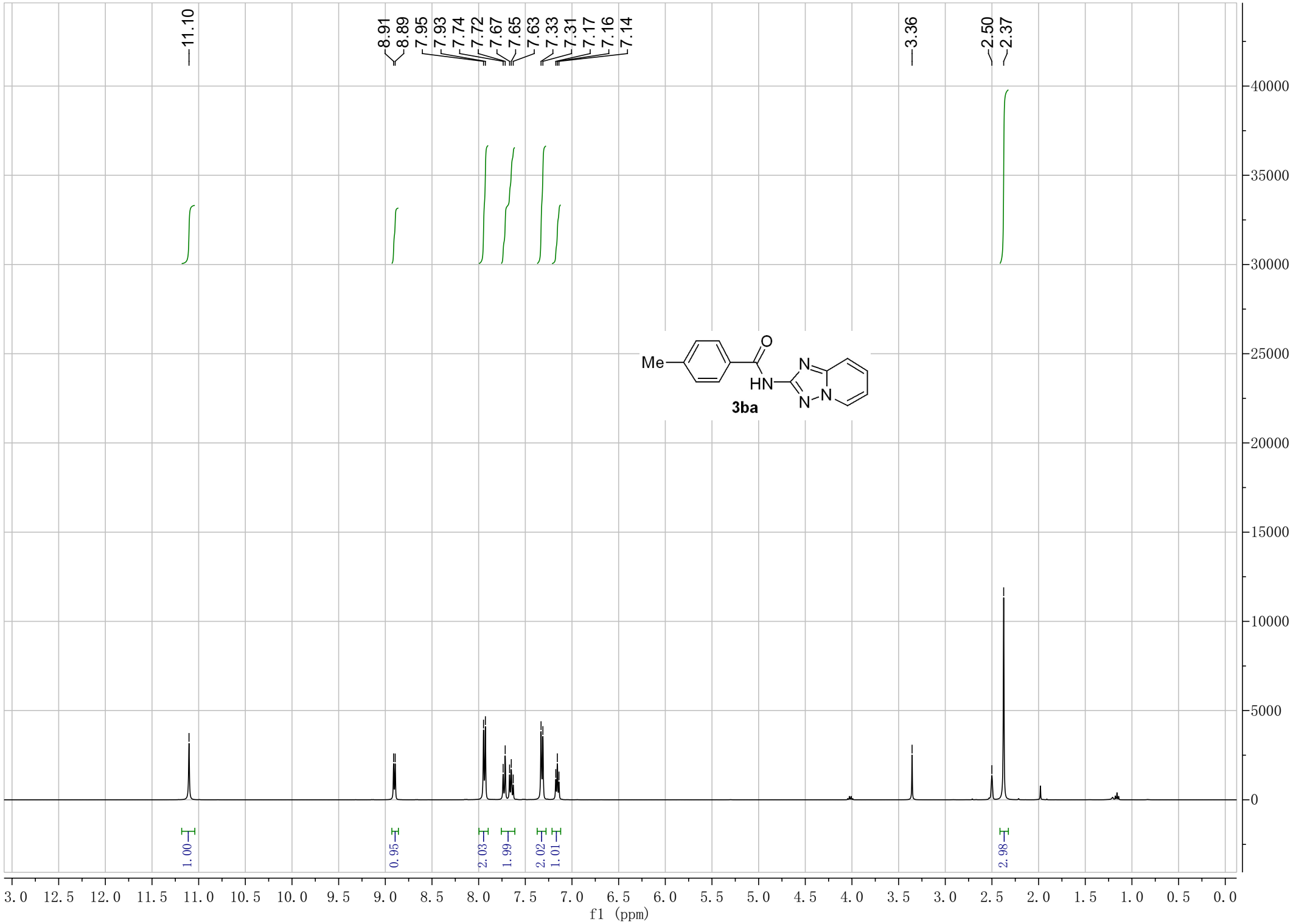
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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8.91
8.89
7.95
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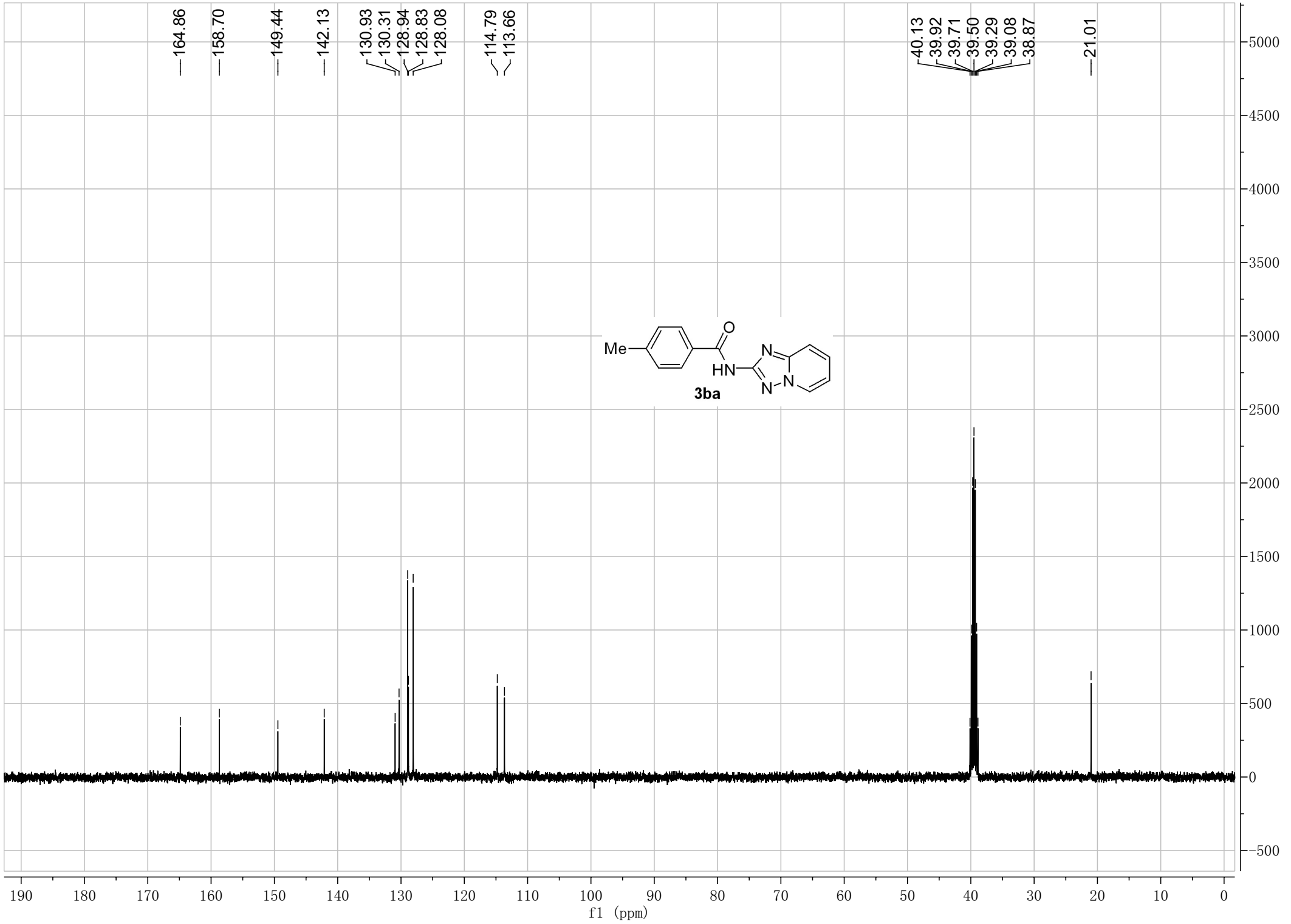
7.74
7.72
7.67
7.65
7.63
7.33
7.31
7.17
7.16
7.14
3.36
2.50
2.37
Me
O
HN
N
N
N
3ba
1.00
0.95
2.03
1.99
2.02
1.01
2.98
40000
35000
30000
25000
20000
15000
10000
5000
0
3.0 12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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142.13
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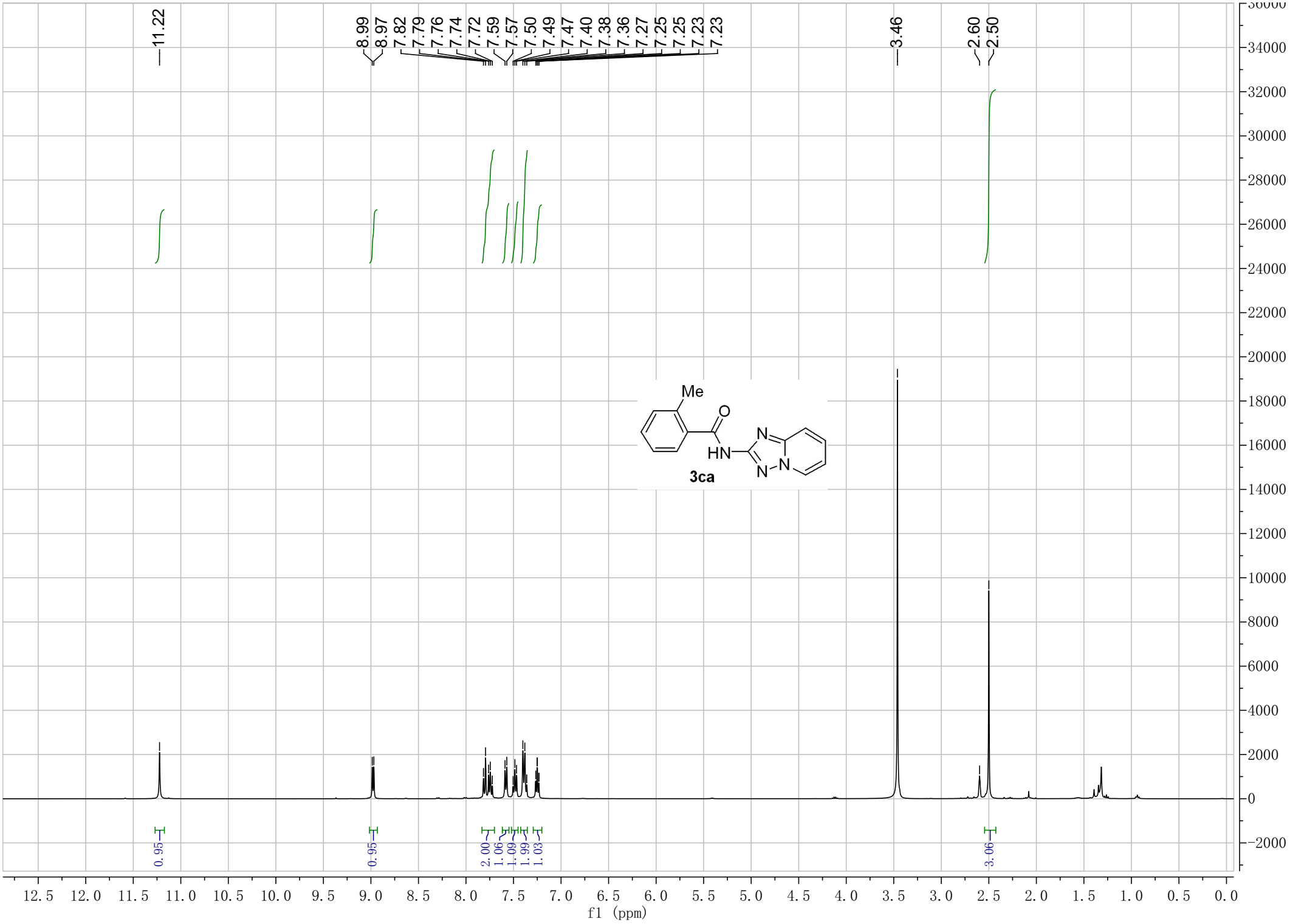
130.31
128.94
128.83
128.08
114.79
113.66
40.13
39.92
39.71
39.50
39.29
39.08
38.87
21.01
Me
O
HN
N
N
N
3ba
5000
4500
4000
3500
3000
2500
2000
1500
1000
500
0
−500
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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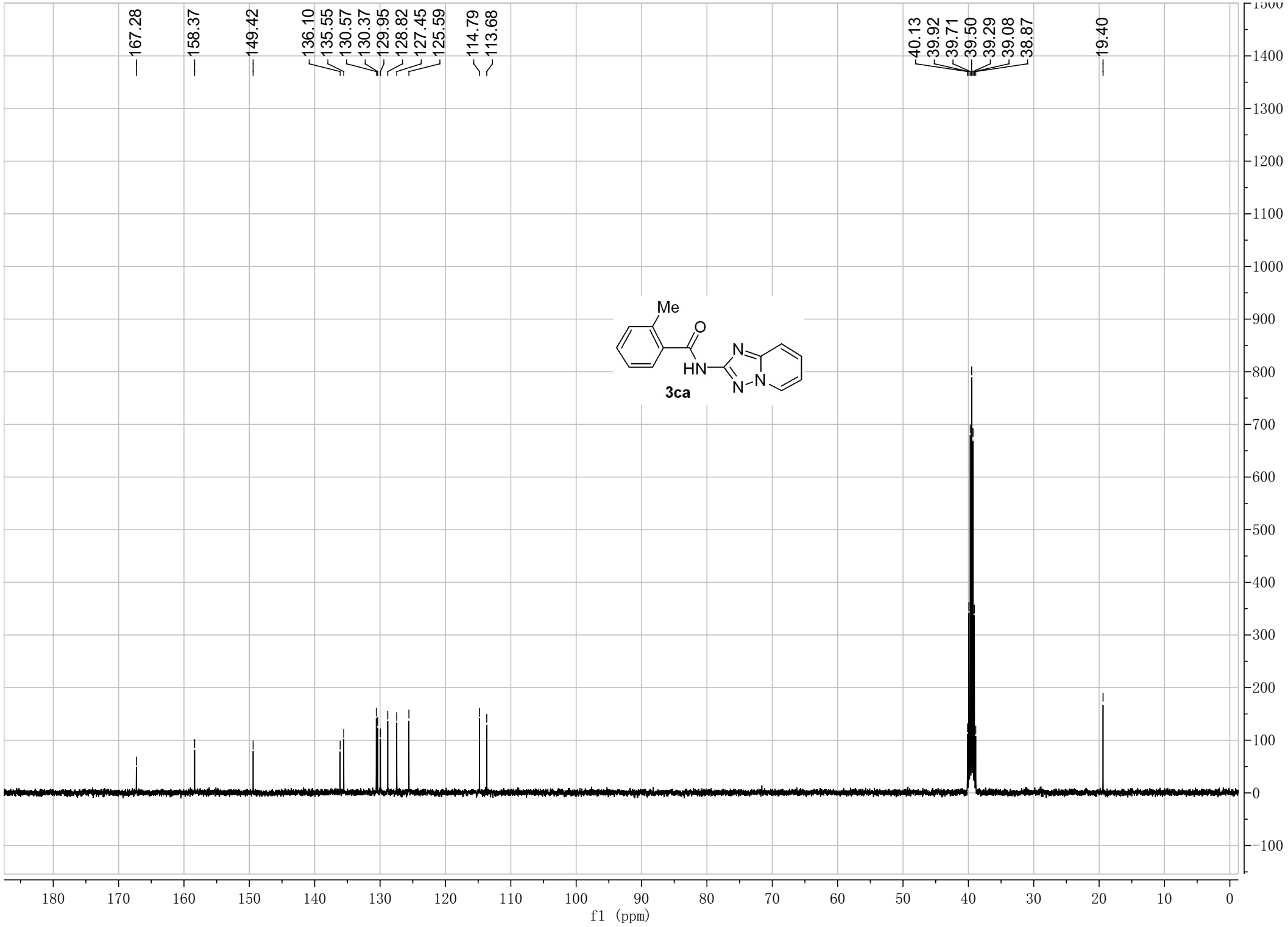
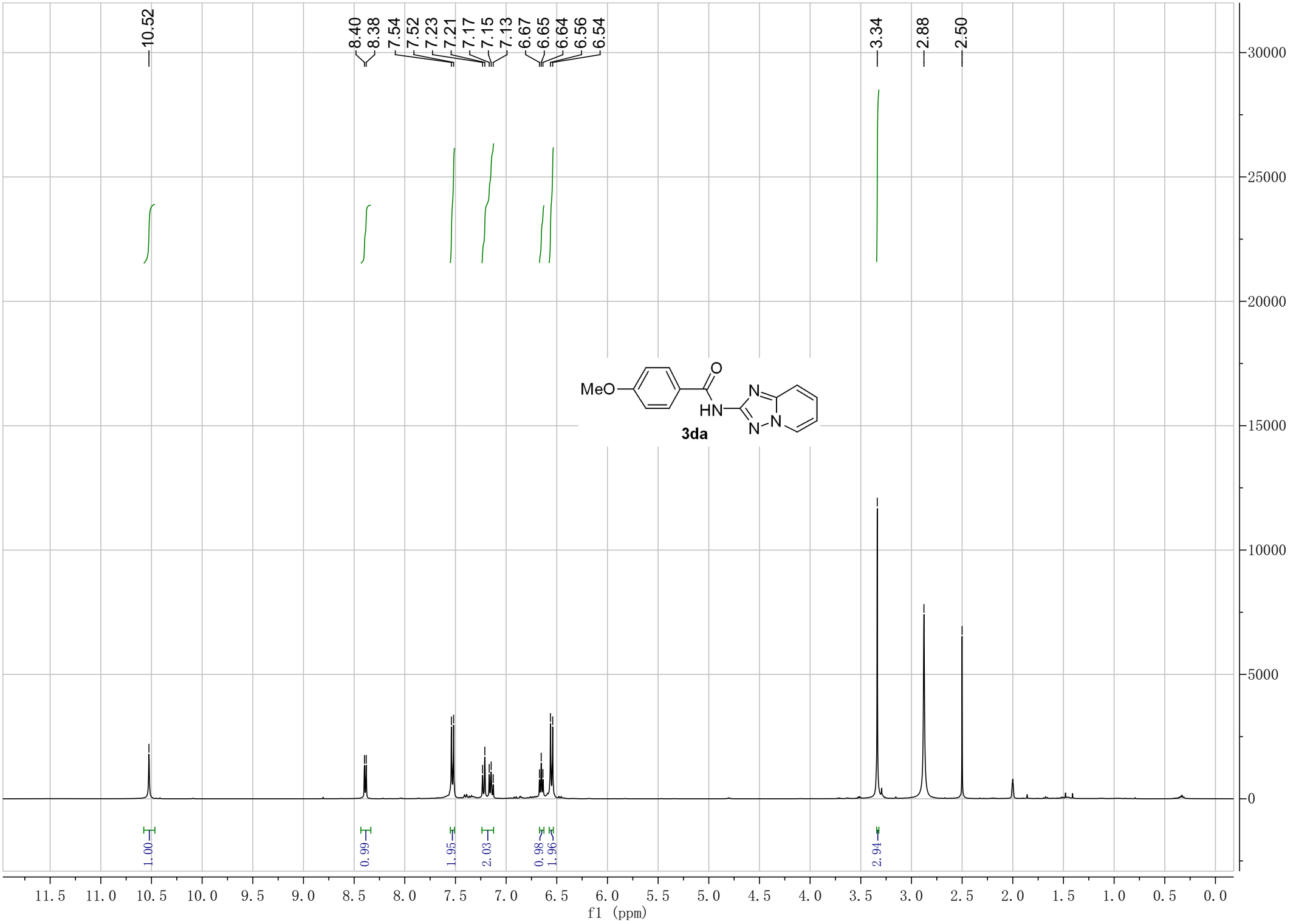
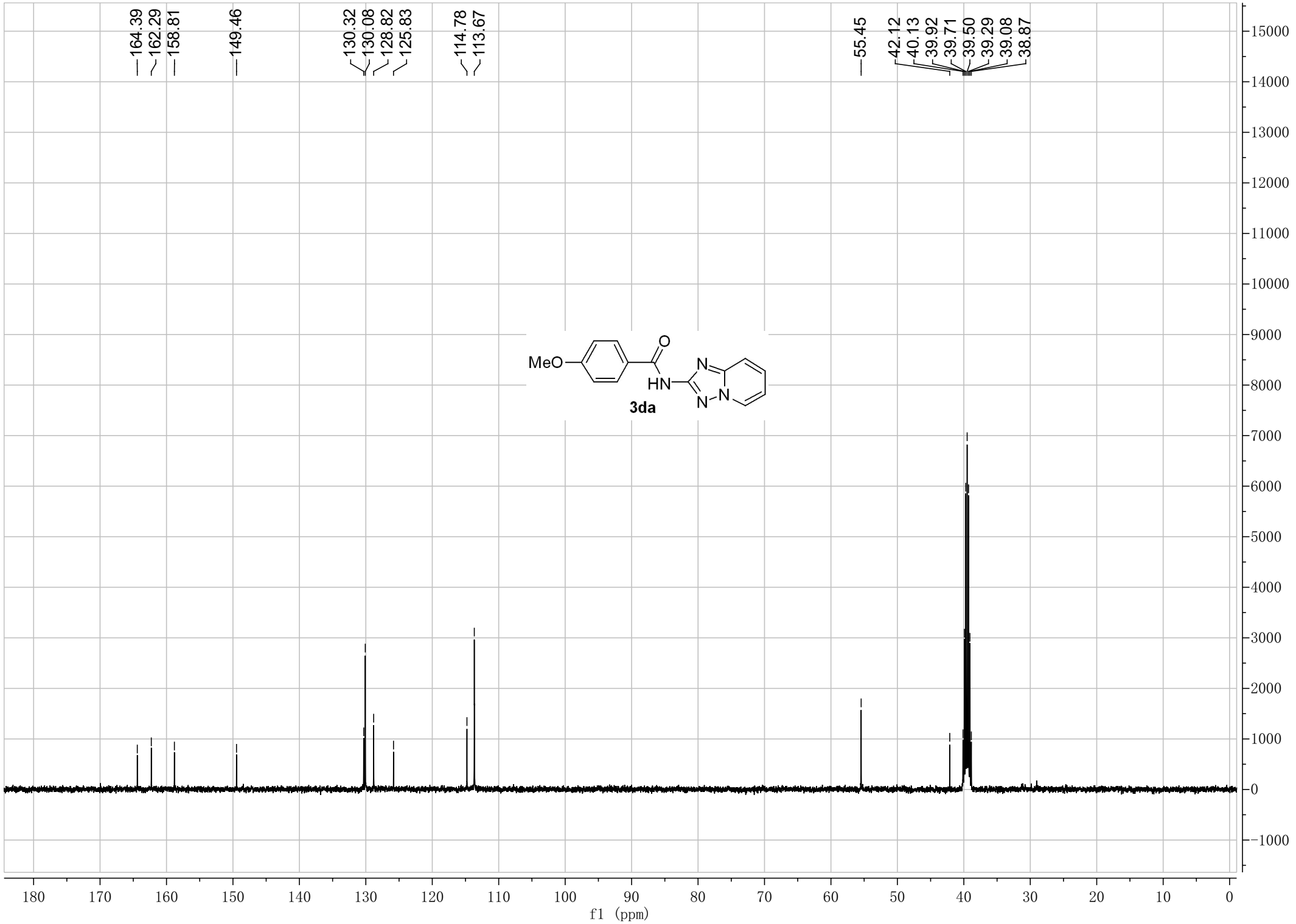
7.82
7.79
7.76
7.74
7.72
7.59
7.57
7.50
7.49
7.47
7.40
7.38
7.36
7.27
7.25
7.25
7.23
7.23
3.46
2.60
2.50
Me
O
HN
N
N
N
3ca
0.95
0.95
2.00
1.06
1.09
1.99
1.03
3.06
f1 (ppm)


167.28
158.37
149.42
136.10
135.55
130.57
130.37
129.95
128.82
127.45
125.59
114.79
113.68
40.13
39.92
39.71
39.50
39.29
39.08
38.87
19.40
Me
O
HN
N
N
N
3ca
f1 (ppm)


10.52
8.40
8.38
7.54
7.52
7.23
7.21
7.17
7.15
7.13
6.67
6.65
6.64
6.56
6.54
3.34
2.88
2.50
MeO
O
HN
N
N
N
3da
30000
25000
20000
15000
10000
5000
0
1.00
0.99
1.95
2.03
0.98
1.96
2.94
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 1.5 1.0 0.5 0.0
f1 (ppm)


164.39
162.29
158.81
149.46
130.32
130.08
128.82
125.83
114.78
113.67
55.45
42.12
40.13
39.92
39.71
39.50
39.29
39.08
38.87
MeO
O
HN
N
N
N
3da
15000
14000
13000
12000
11000
10000
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
-1000
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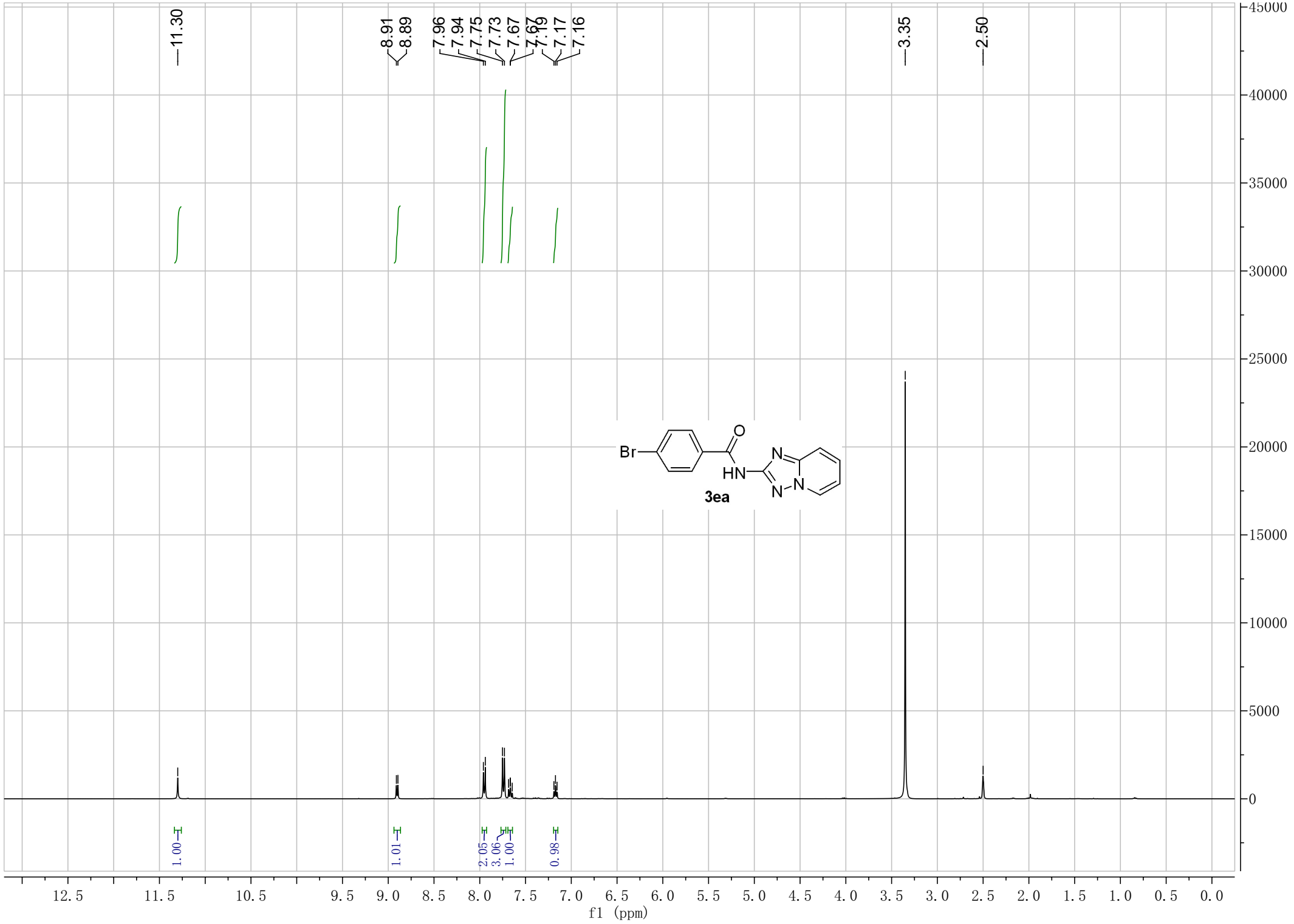
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7.17
7.16
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2.50
Br
O
HN
N
N
N
3ea
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1.01
2.05
3.06
1.00
0.98
45000
40000
35000
30000
25000
20000
15000
10000
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11.5
10.5
9.5
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5.5
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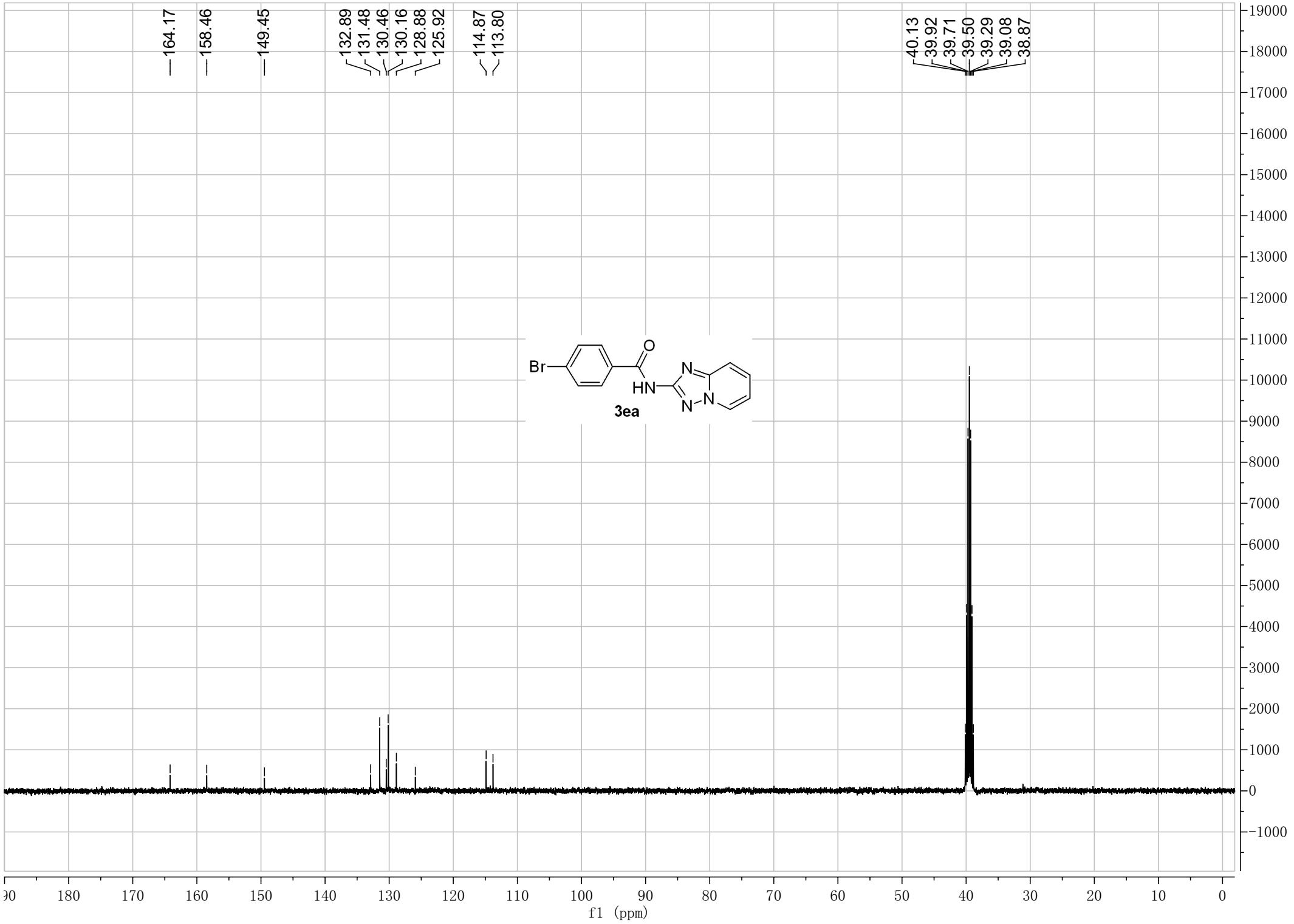
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39.71
39.50
39.29
39.08
38.87
Br
O
HN
N
N
N
3ea
19000
18000
17000
16000
15000
14000
13000
12000
11000
10000
9000
8000
7000
6000
5000
4000
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2000
1000
0
-1000
180
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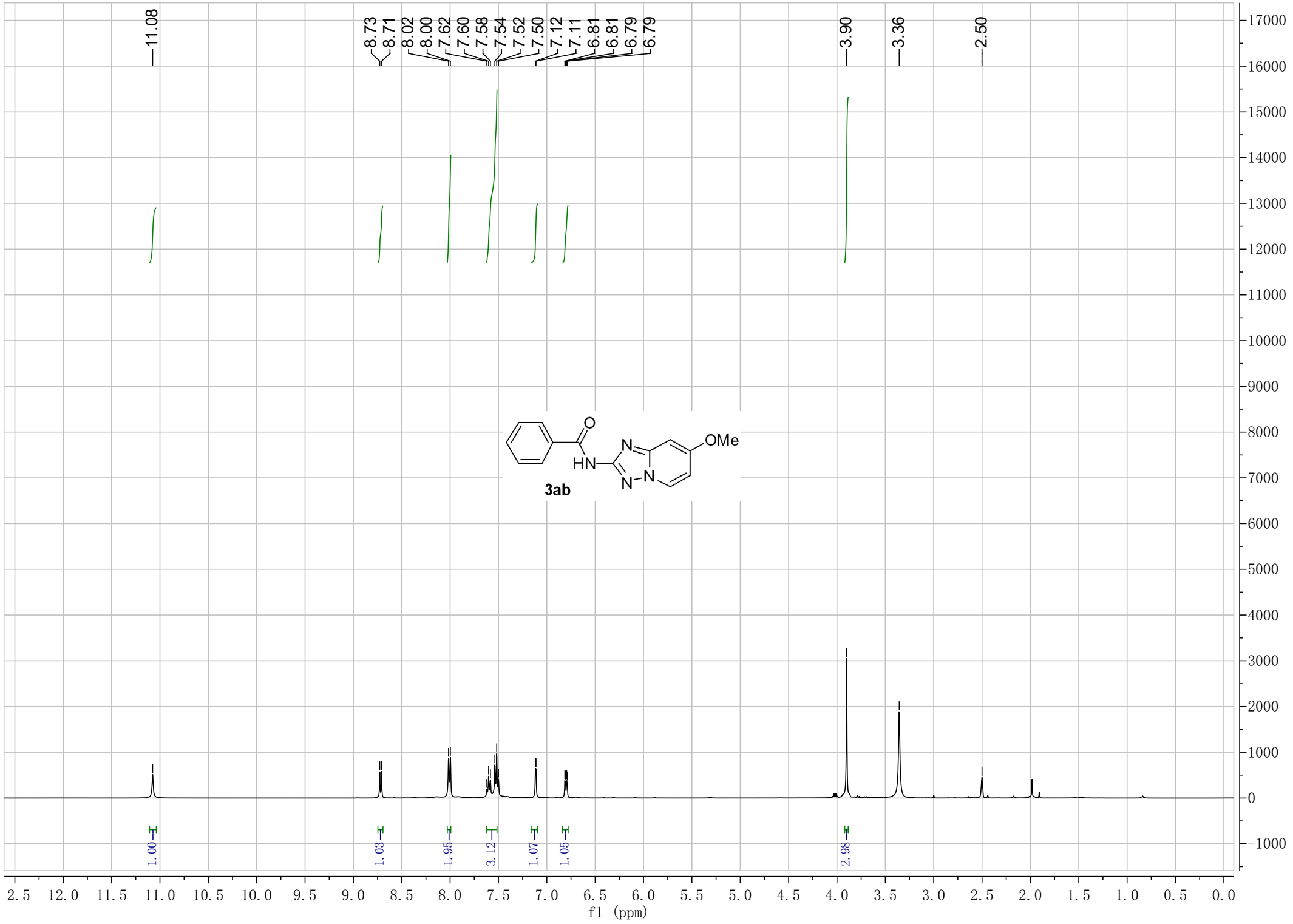
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7.11
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6.81
6.79
6.79
3.90
3.36
2.50
O
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1.03
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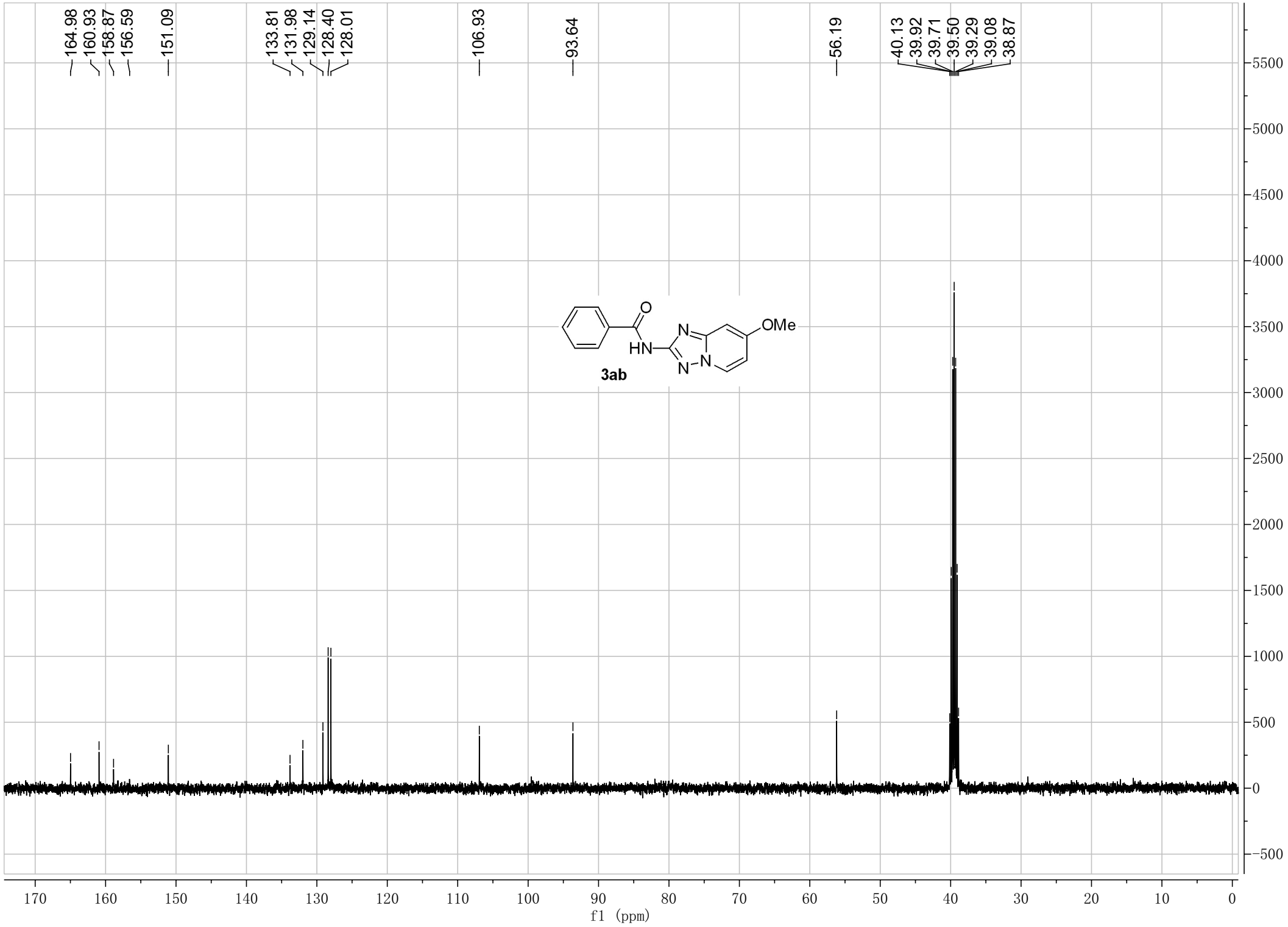
1.07
1.05
2.98
f1 (ppm)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39.92
39.71
39.50
39.29
39.08
38.87
O
HN
N
N
N
OMe
3ab
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5000
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3500
3000
2500
2000
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1000
500
0
−500
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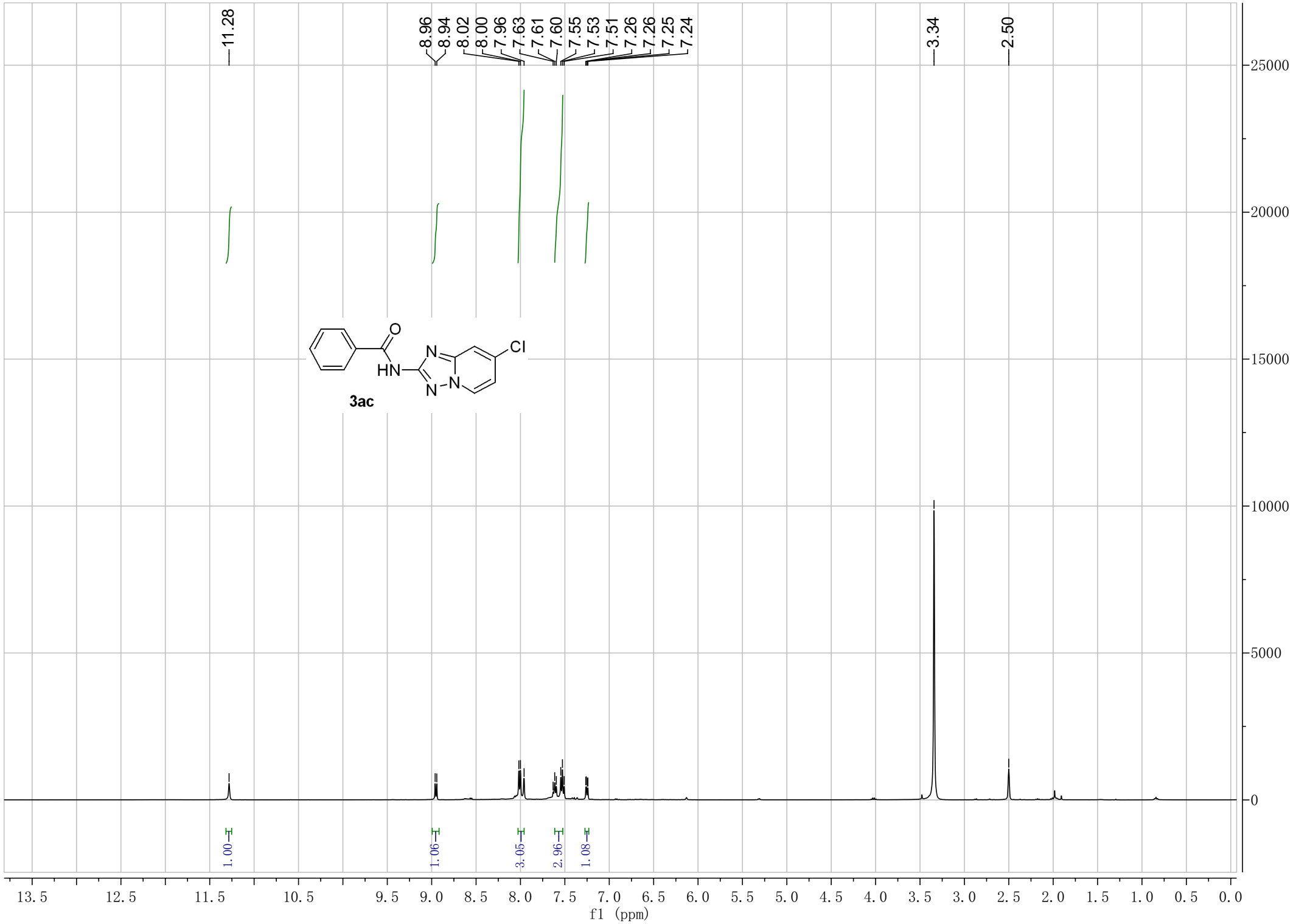
f1 (ppm)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7.26
7.25
7.24
3.34
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O
HN
N
N
N
Cl
3ac
1.00
1.06
3.05
2.96
1.08
25000
20000
15000
10000
5000
0
13.5
12.5
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
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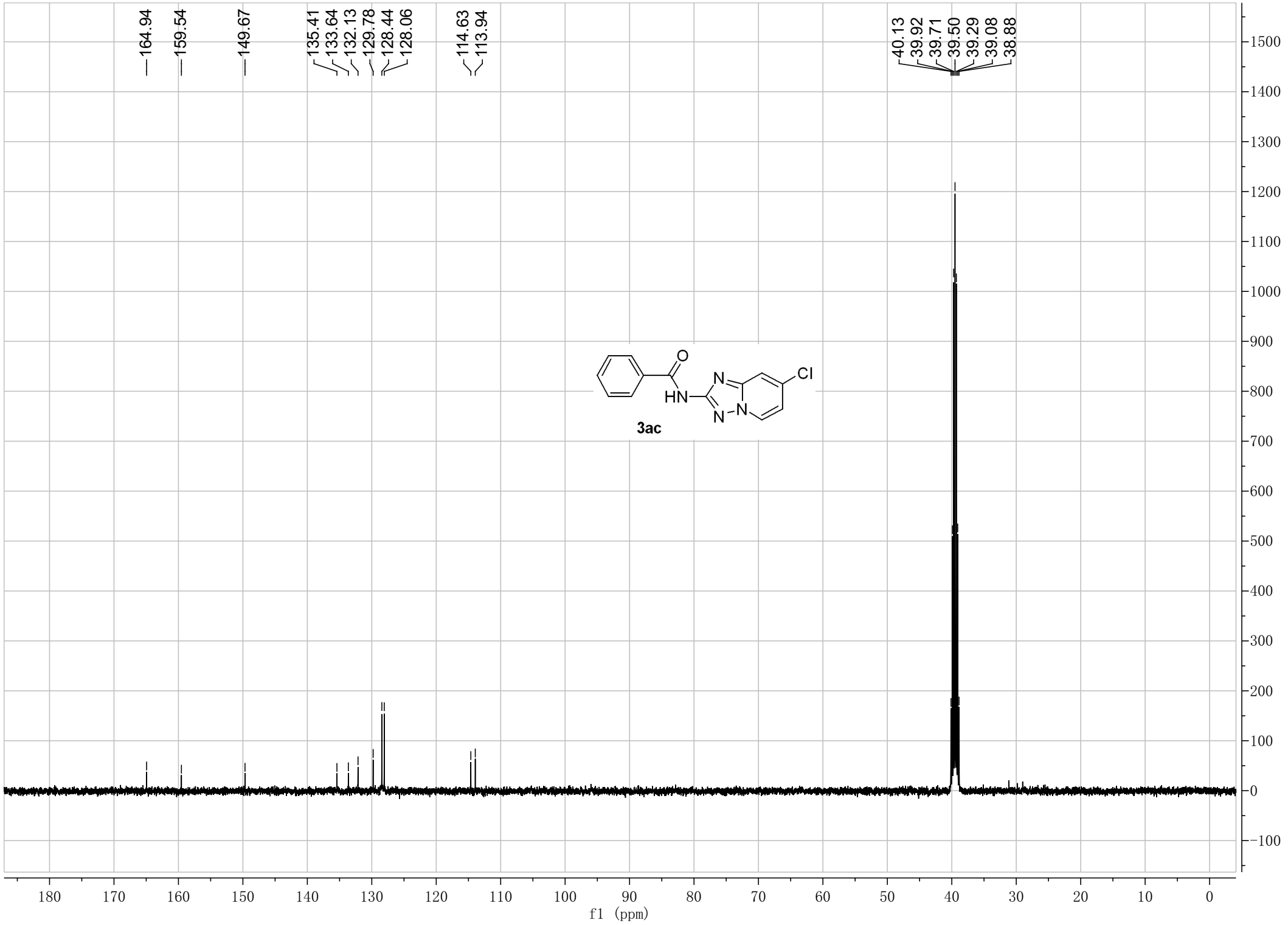
0.0
f1 (ppm)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39.71
39.50
39.29
39.08
38.88
O
HN
N
N
N
Cl
3ac
1500
1400
1300
1200
1100
1000
900
800
700
600
500
400
300
200
100
0
−100
180
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50
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30
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10
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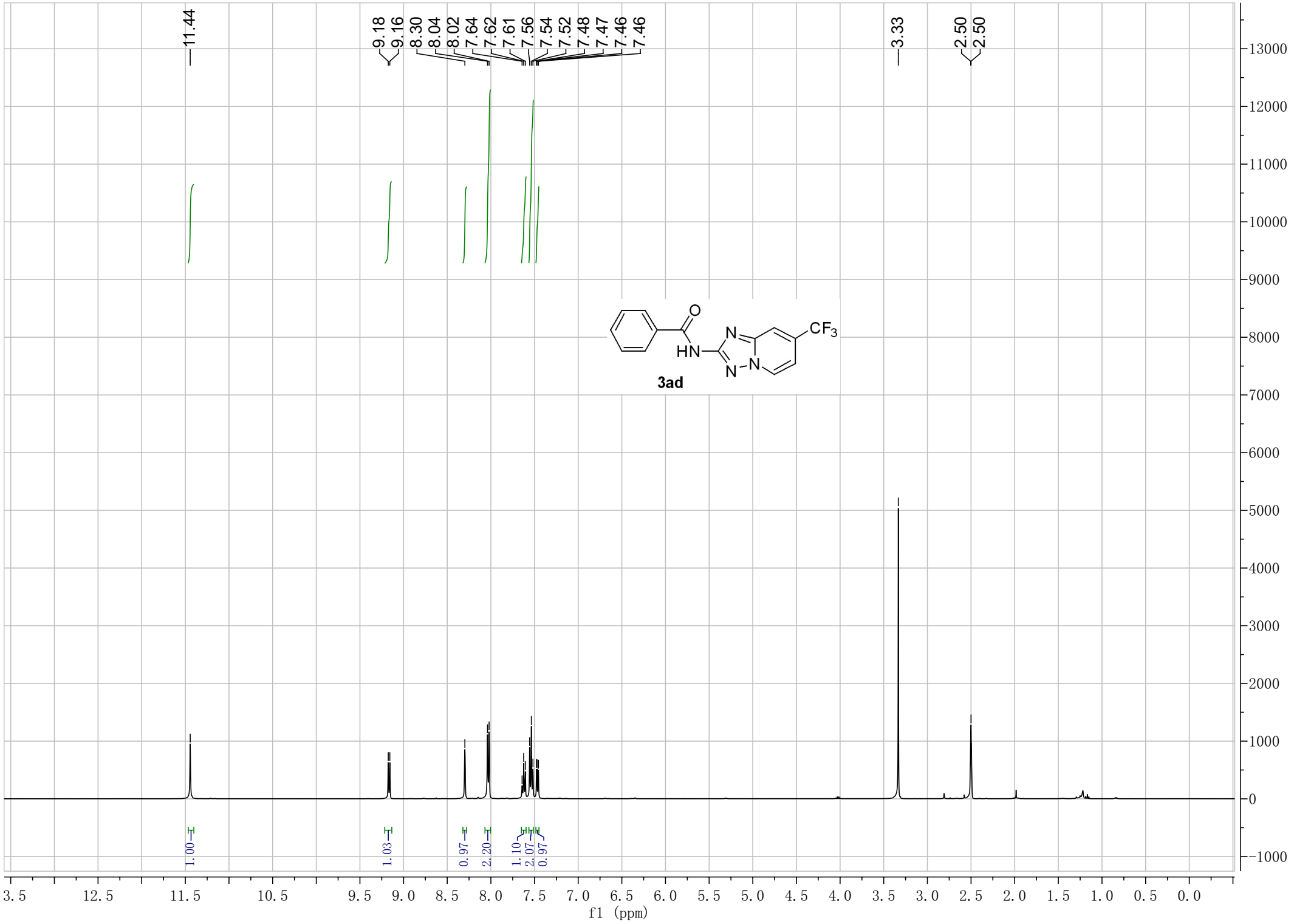
f1 (ppm)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7.61
7.56
7.54
7.52
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7.47
7.46
7.46
3.33
2.50
2.50
O
HN
N
N
N
CF3
3ad
1.00
1.03
0.97
2.20
1.10
2.07
0.97
13000
12000
11000
10000
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
-1000
3.5
12.5
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
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3.0
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1.0
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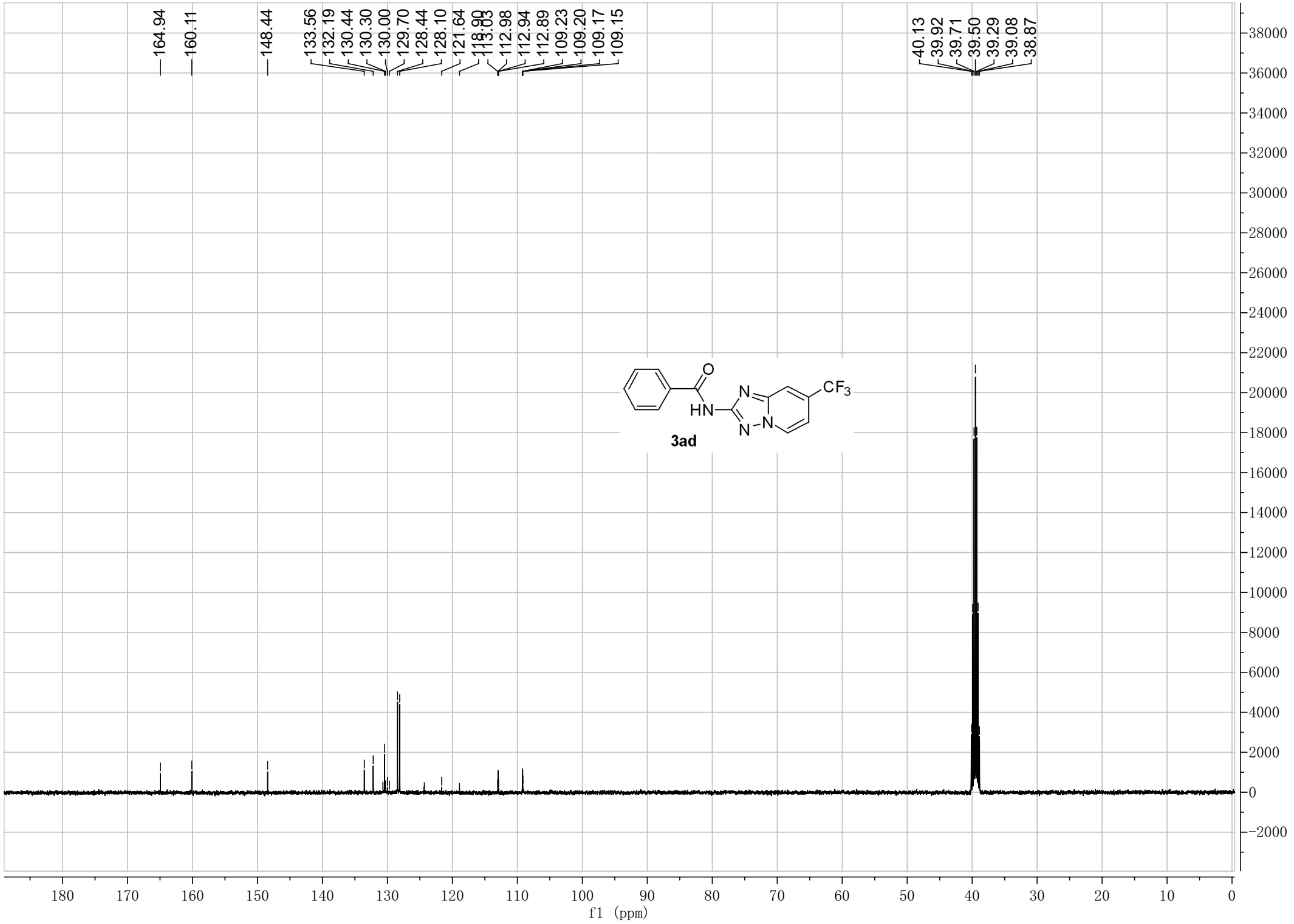
0.0
f1 (ppm)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128.44
128.10
121.64
118.90
113.03
112.98
112.94
112.89
109.23
109.20
109.17
109.15
40.13
39.92
39.71
39.50
39.29
39.08
38.87
O
HN
N
N
N
CF3
3ad
38000
36000
34000
32000
30000
28000
26000
24000
22000
20000
18000
16000
14000
12000
10000
8000
6000
4000
2000
0
-2000
180
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150
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130
120
110
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90
80
70
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50
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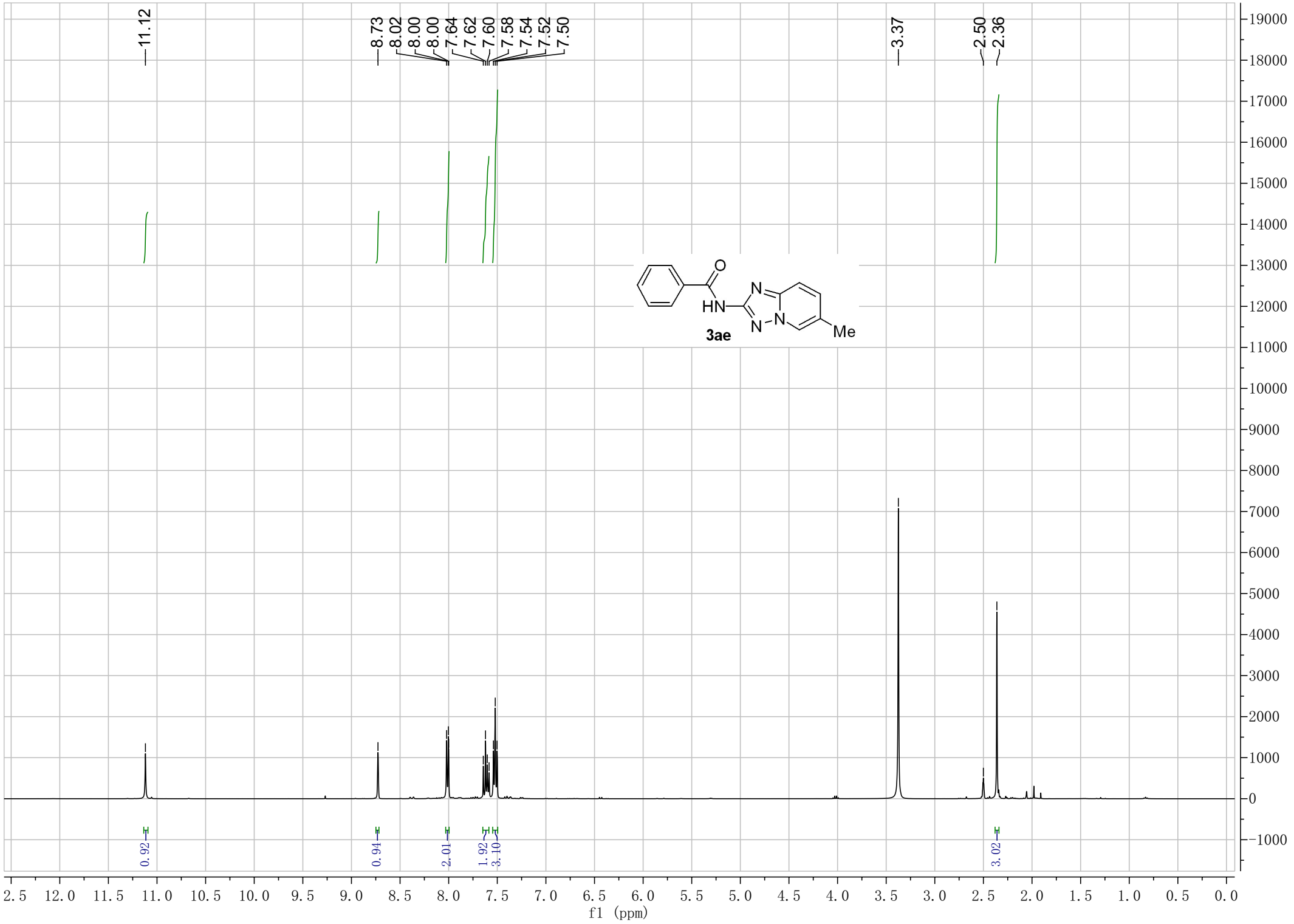
10
0
f1 (ppm)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2.50
2.36
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N
N
Me
3ae
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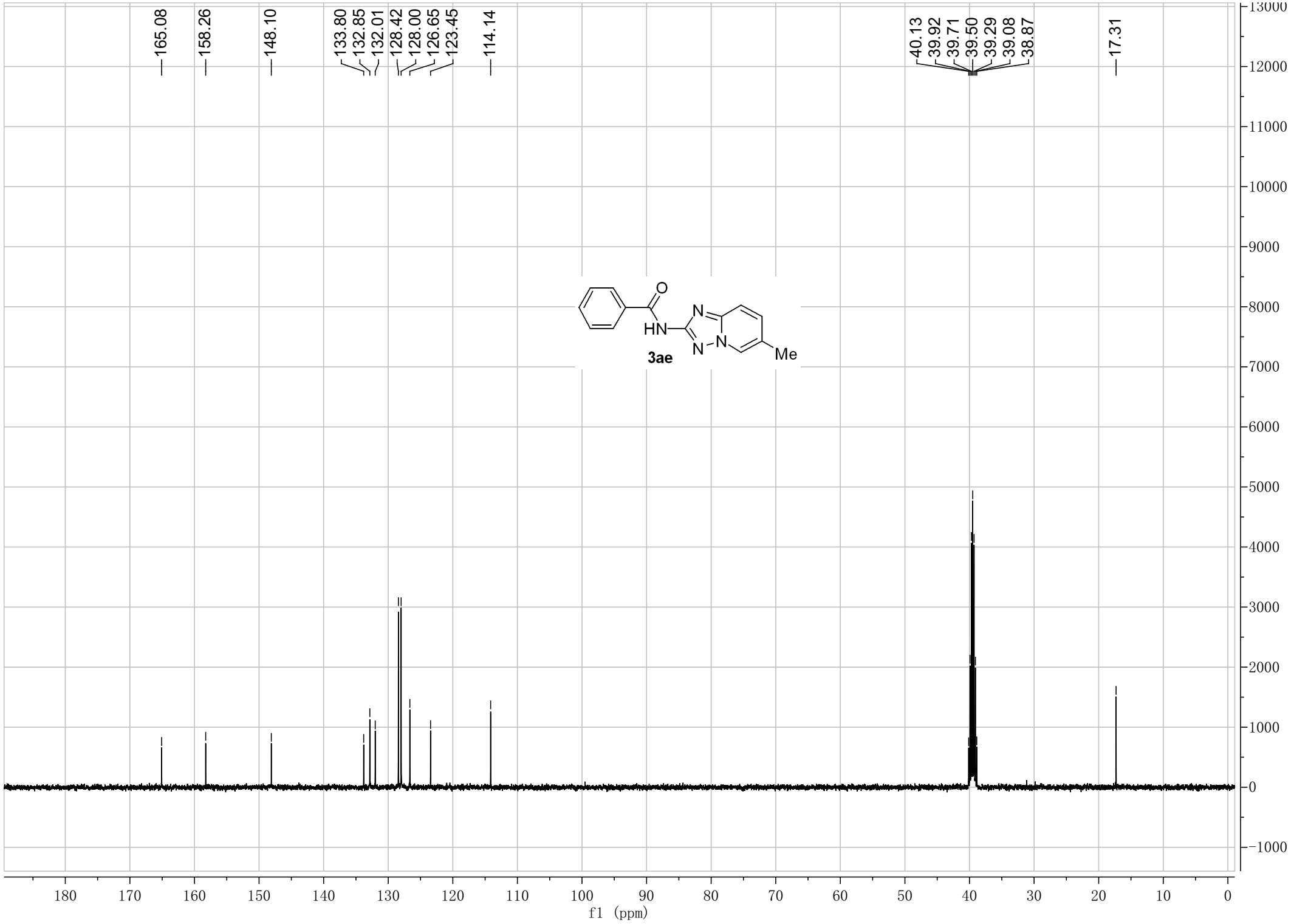
0.94
2.01
1.92
3.10
3.02
f1 (ppm)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126.65
123.45
114.14
40.13
39.92
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39.29
39.08
38.87
17.31
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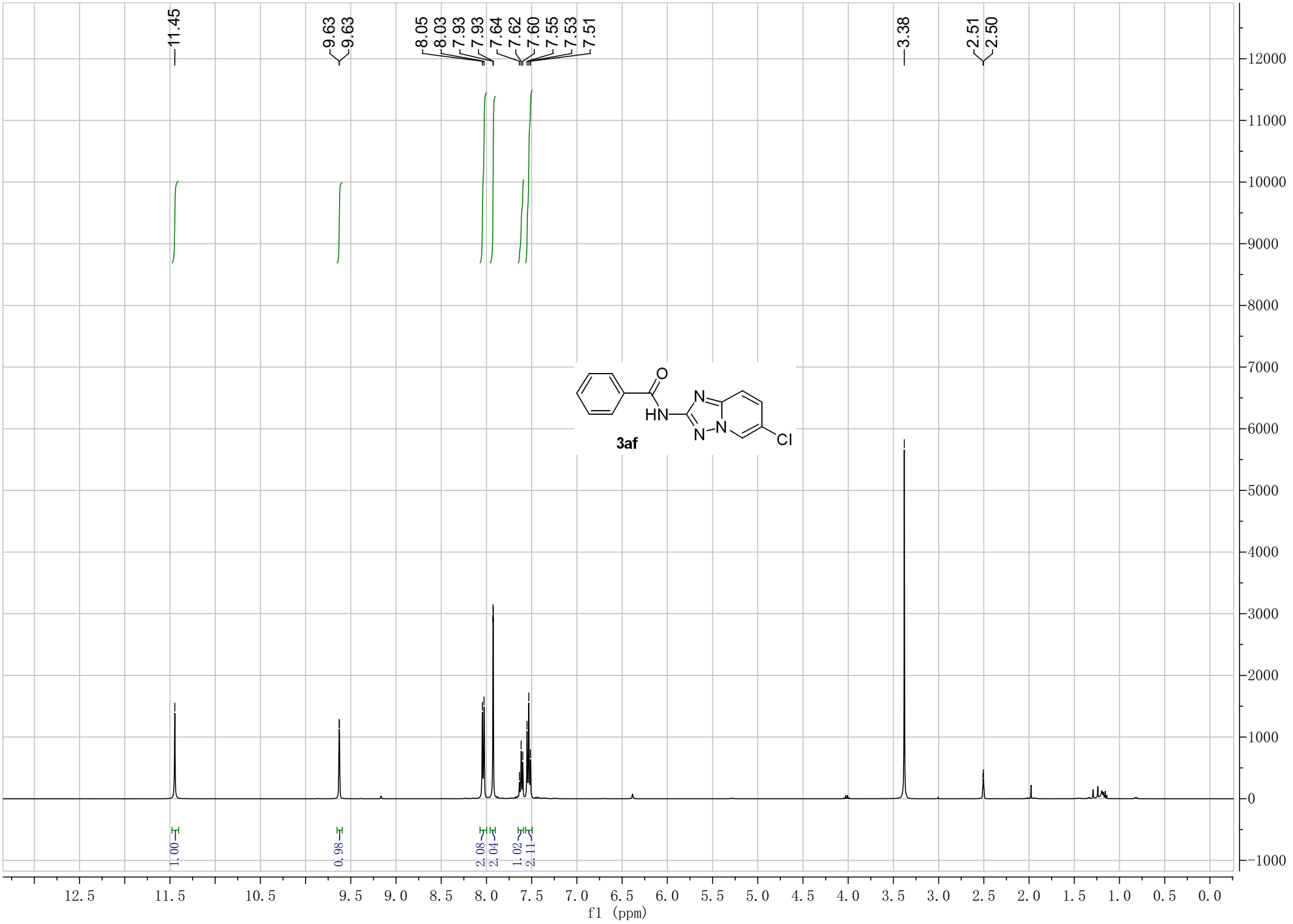
N
N
N
Me
3ae
f1 (ppm)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7.60
7.55
7.53
7.51
3.38
2.51
2.50
O
HN
N
N
N
Cl
3af
1.00
0.98
2.08
2.04
1.02
2.11
12000
11000
10000
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
-1000
12.5
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
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3.5
3.0
2.5
2.0
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1.0
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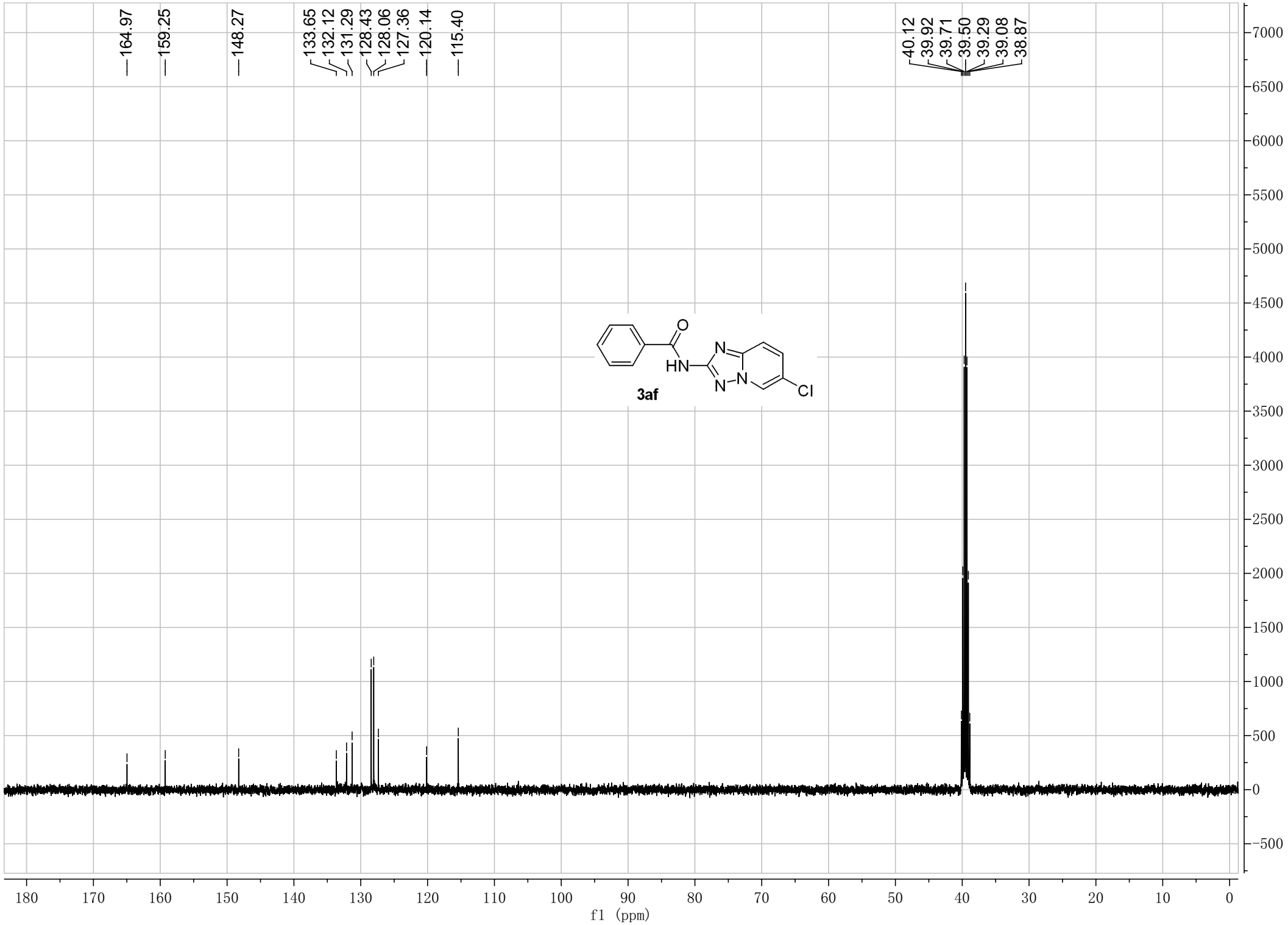
0.0
f1 (ppm)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120.14
115.40
40.12
39.92
39.71
39.50
39.29
39.08
38.87
O
HN
N
N
N
Cl
3af
7000
6500
6000
5500
5000
4500
4000
3500
3000
2500
2000
1500
1000
500
0
-500
180
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90
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50
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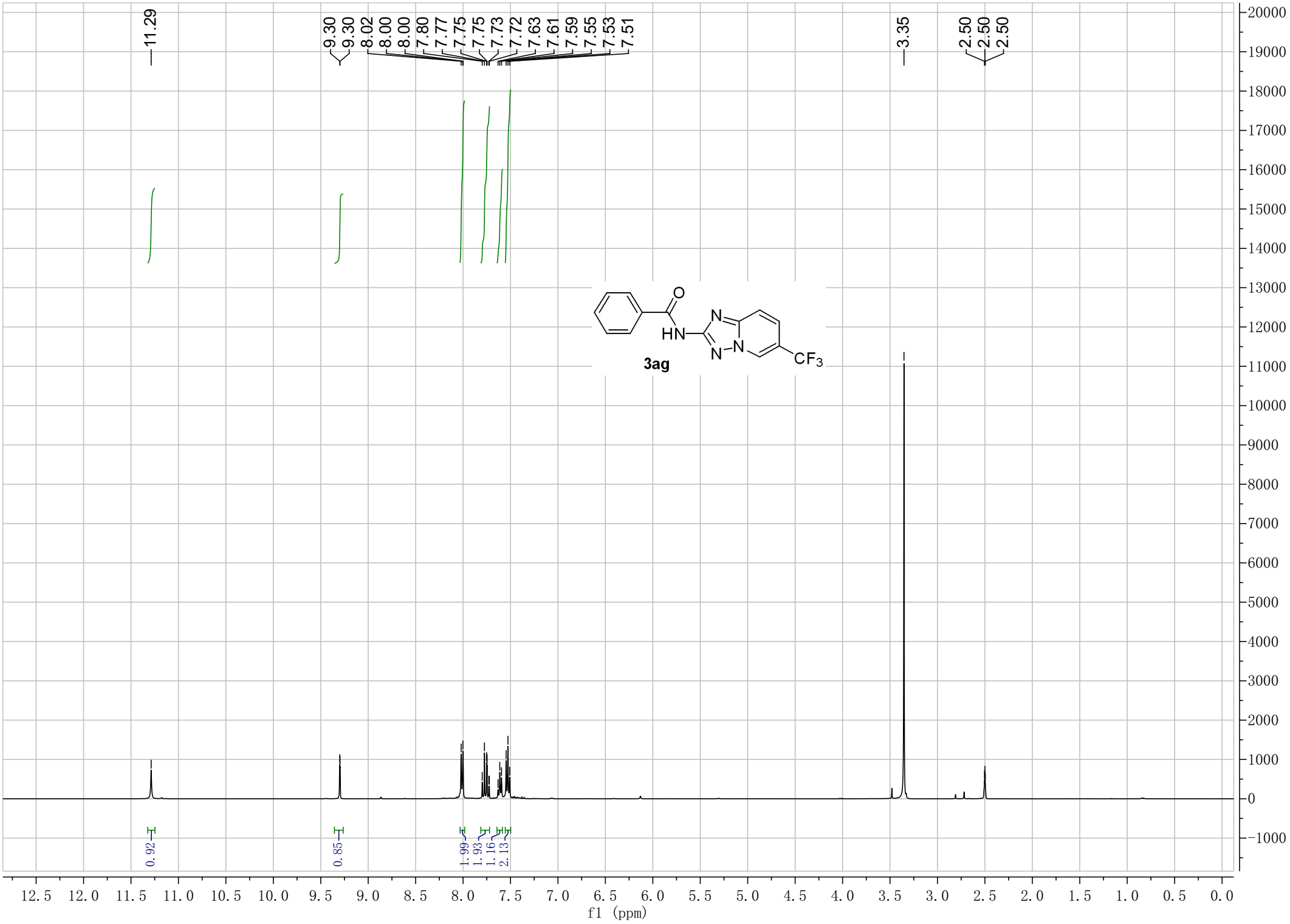
10
0
f1 (ppm)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7.72
7.63
7.61
7.59
7.55
7.53
7.51
3.35
2.50
2.50
2.50
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N
CF3
3ag
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0.85
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1.93
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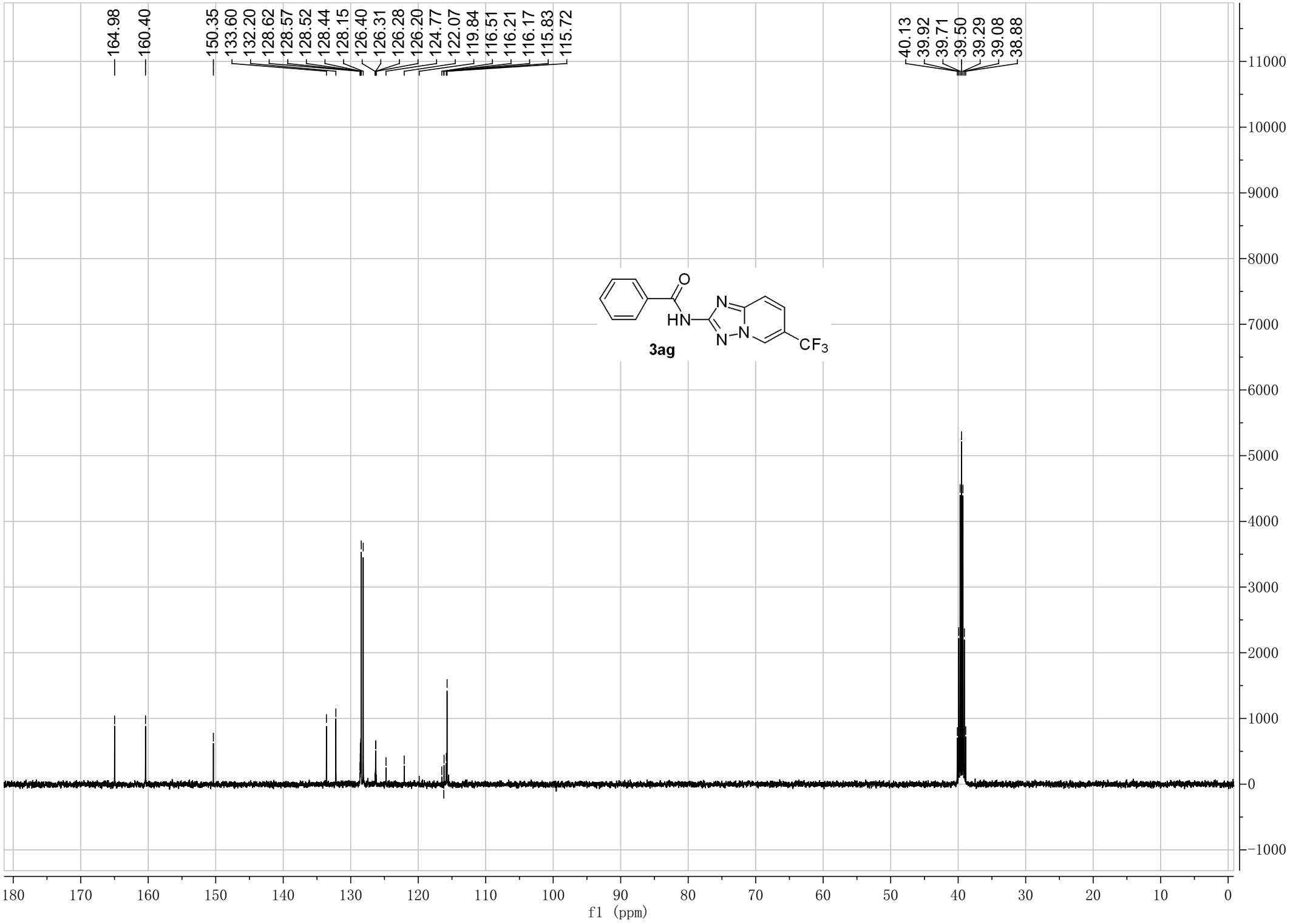
2.13
f1 (ppm)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126.31
126.28
126.20
124.77
122.07
119.84
116.51
116.21
116.17
115.83
115.72
40.13
39.92
39.71
39.50
39.29
39.08
38.88
O
HN
N
N
N
CF3
3ag
11000
10000
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
-1000
180
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120
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50
40
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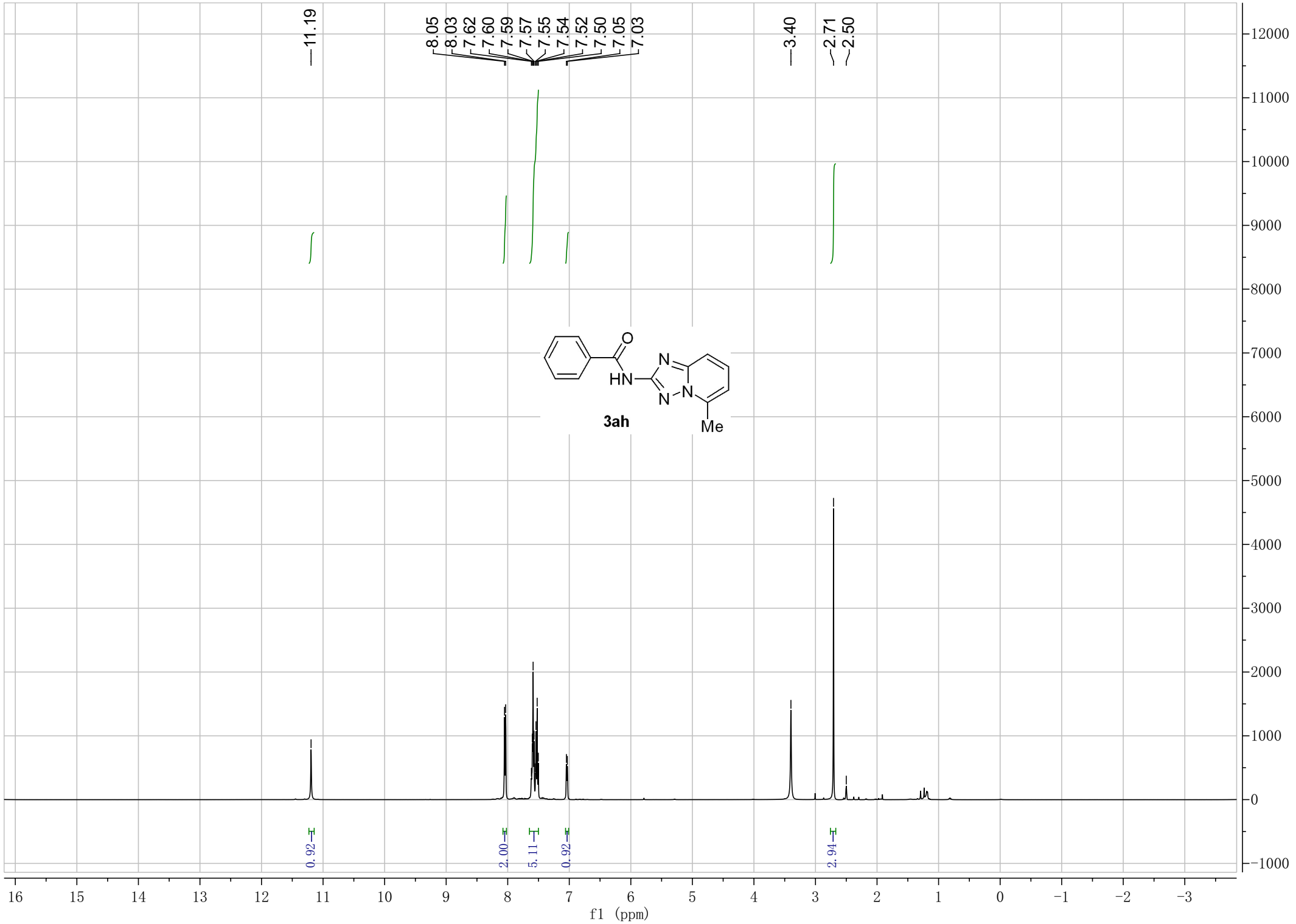
10
0
f1 (ppm)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7.05
7.03
3.40
2.71
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N
Me
3ah
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5.11
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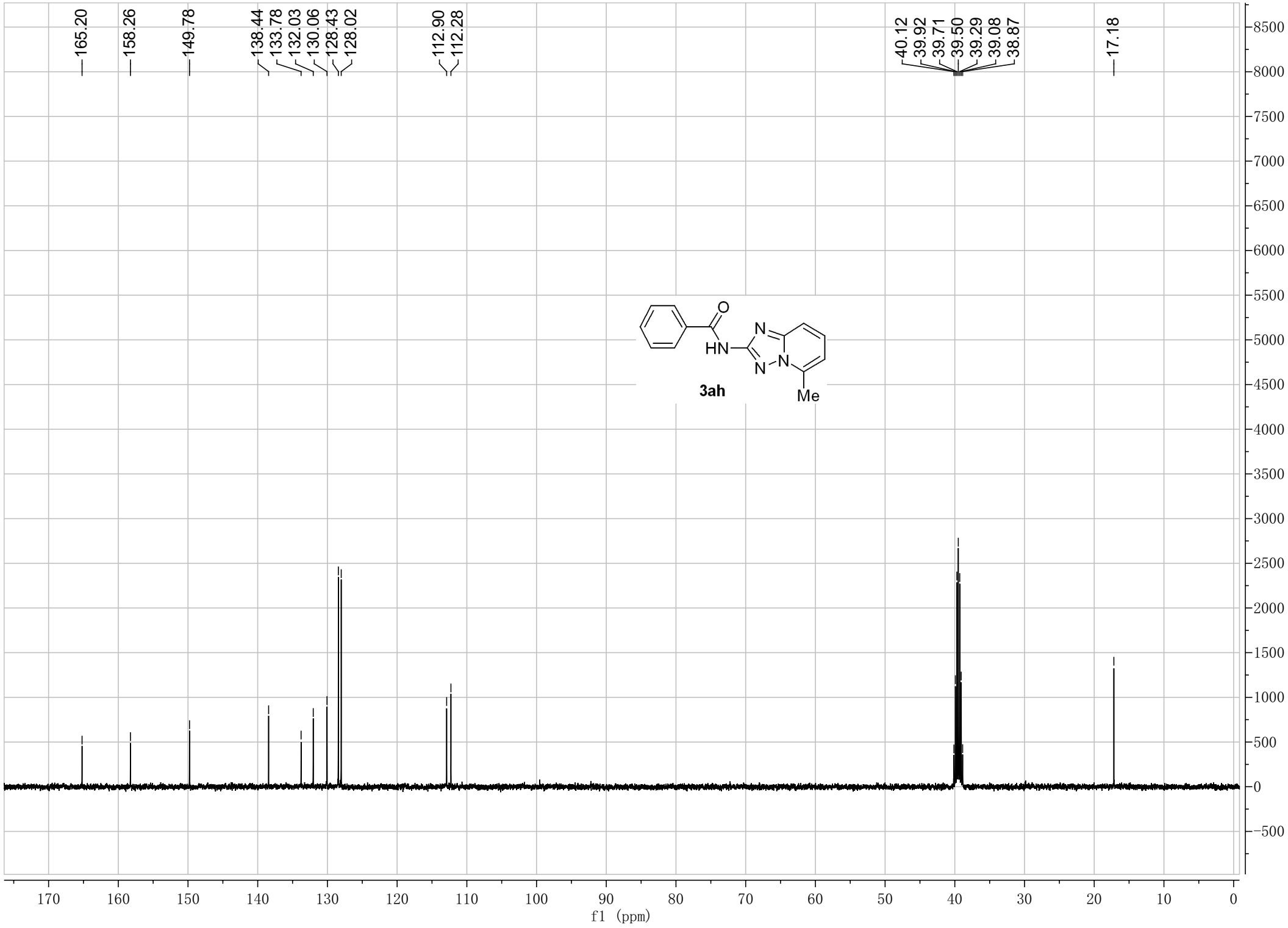
2.94
f1 (ppm)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39.92
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39.08
38.87
17.18
O
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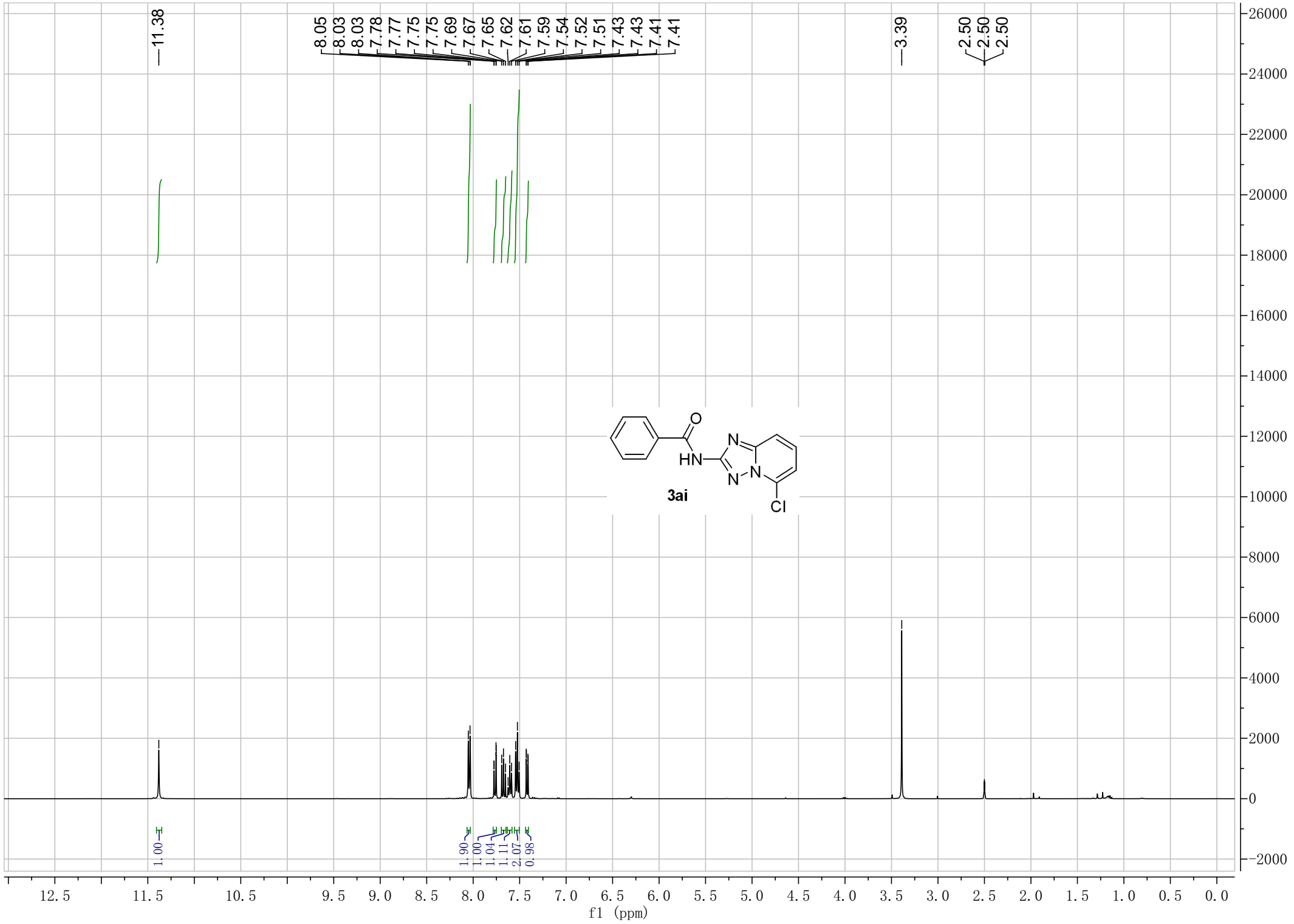
N
N
N
Me
3ah
f1 (ppm)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7.59
7.54
7.52
7.51
7.43
7.43
7.41
7.41
3.39
2.50
2.50
2.50
O
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1.00
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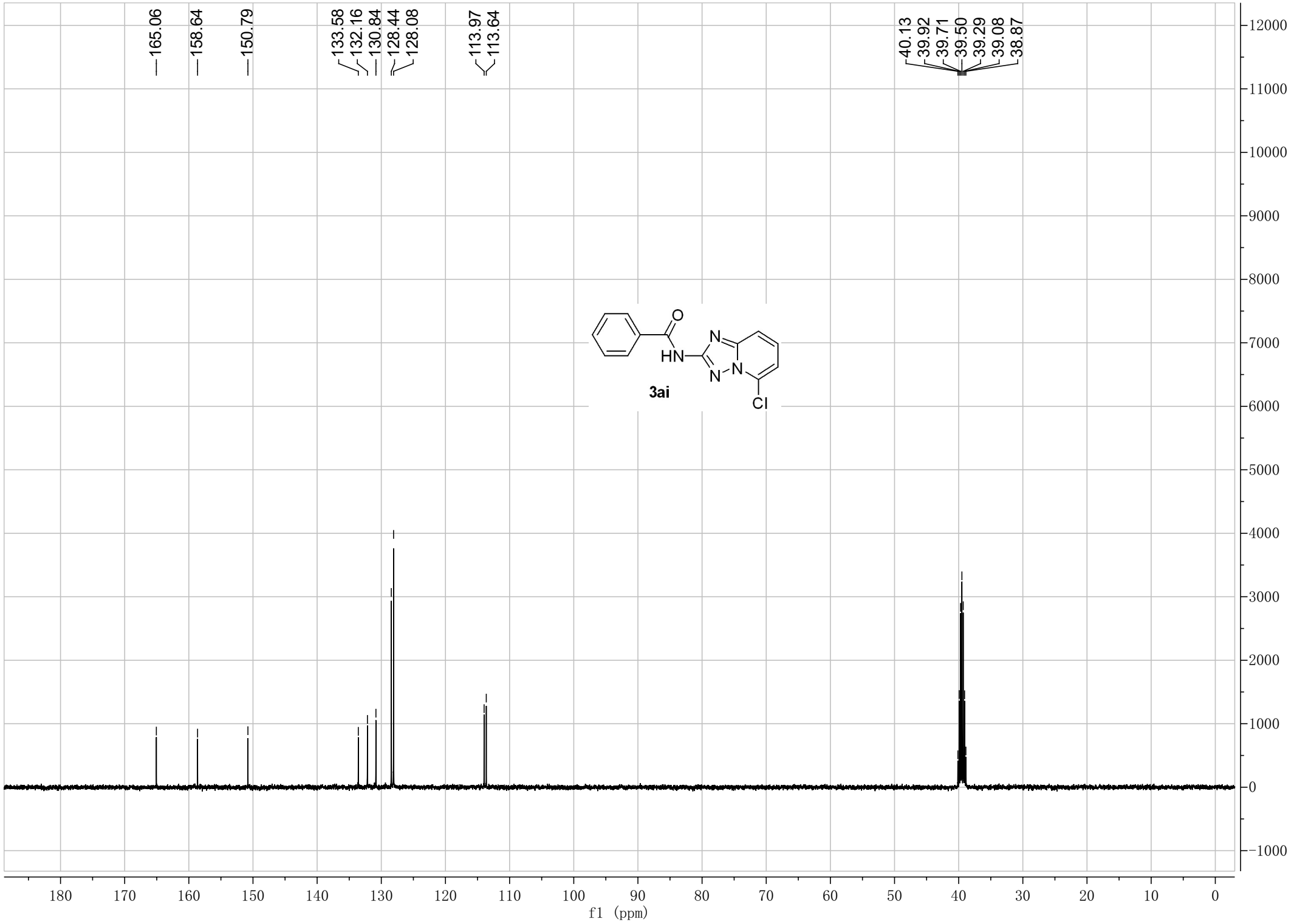
1.11
2.07
0.98
f1 (ppm)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39.92
39.71
39.50
39.29
39.08
38.87
O
HN
N
N
N
Cl
3ai
12000
11000
10000
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
-1000
180
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90
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70
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10
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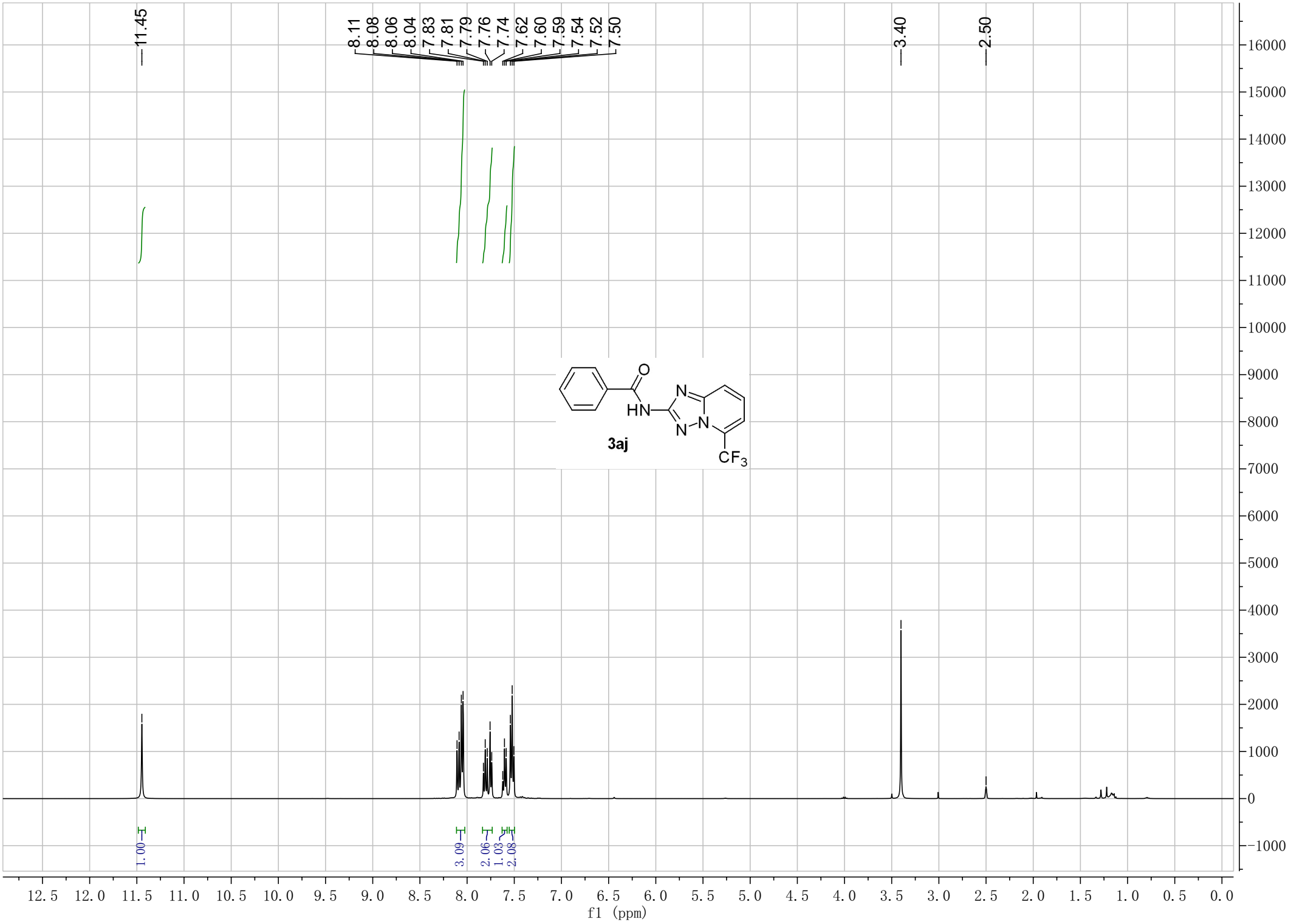
f1 (ppm)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7.59
7.54
7.52
7.50
3.40
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N
N
CF3
3aj
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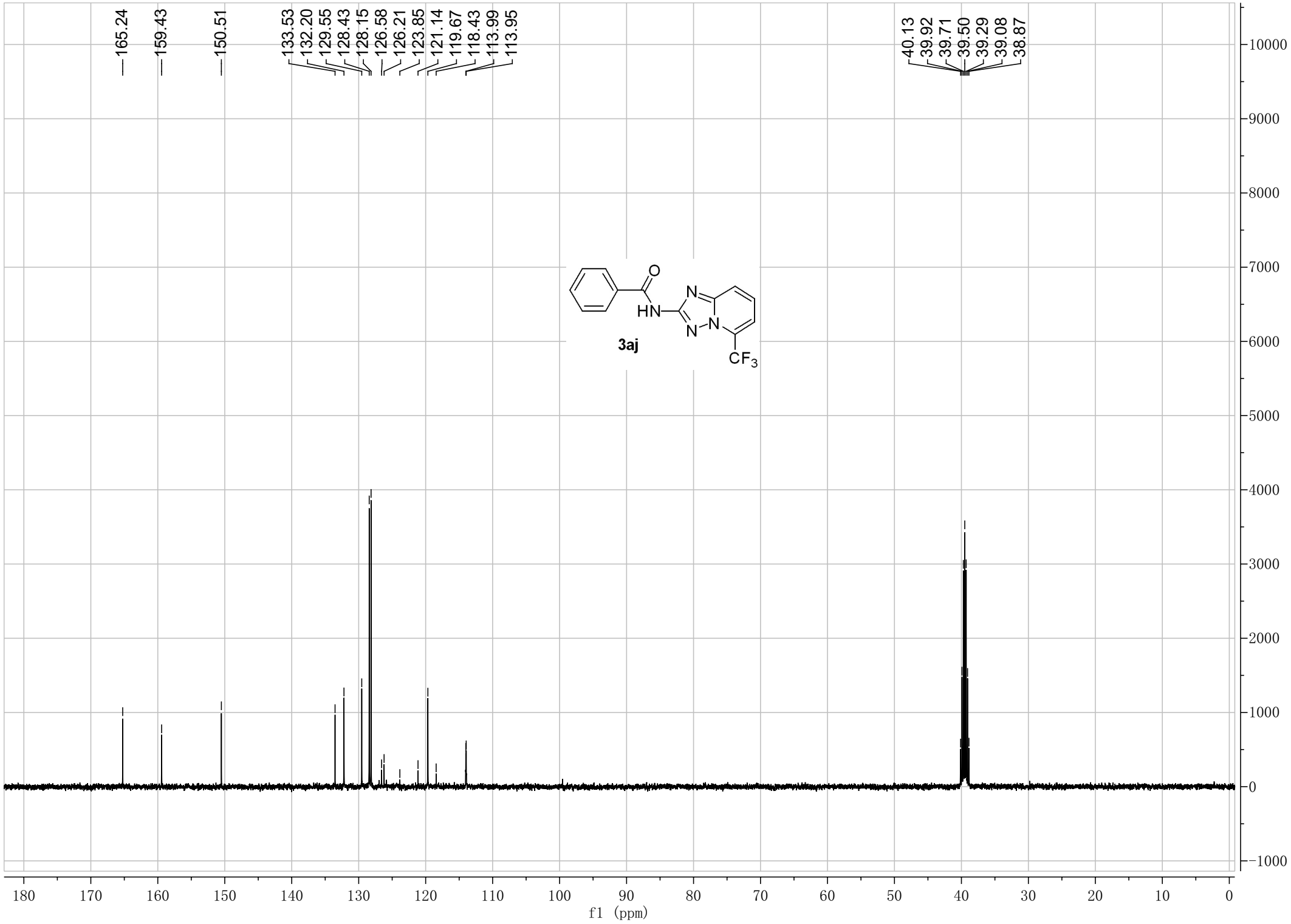
3.09
2.06
1.03
2.08
f1 (ppm)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121.14
119.67
118.43
113.99
113.95
40.13
39.92
39.71
39.50
39.29
39.08
38.87
O
HN
N
N
N
CF3
3aj
10000
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
−1000
180
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70
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50
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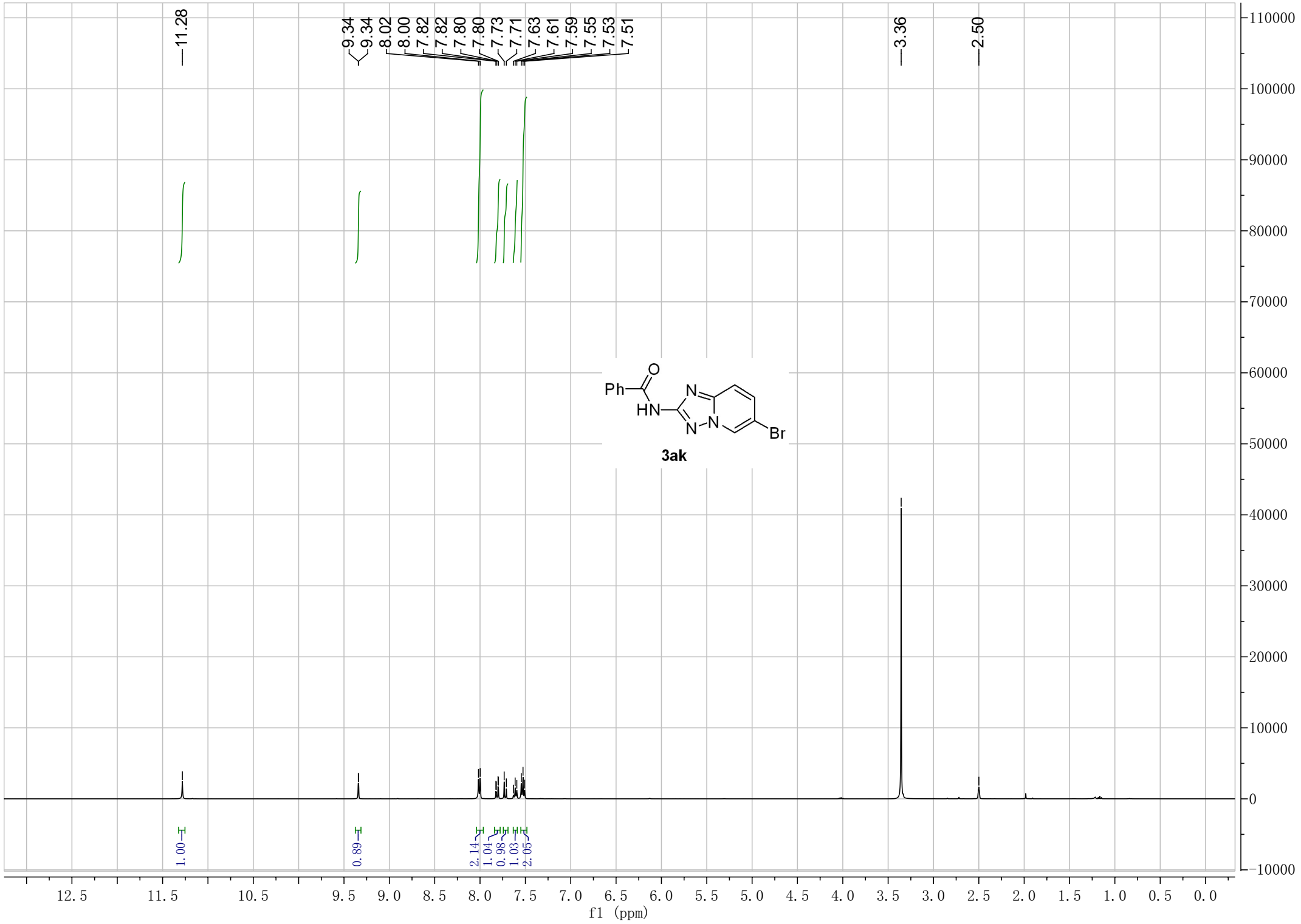
0
f1 (ppm)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7.71
7.63
7.61
7.59
7.55
7.53
7.51
3.36
2.50
Ph
O
HN
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N
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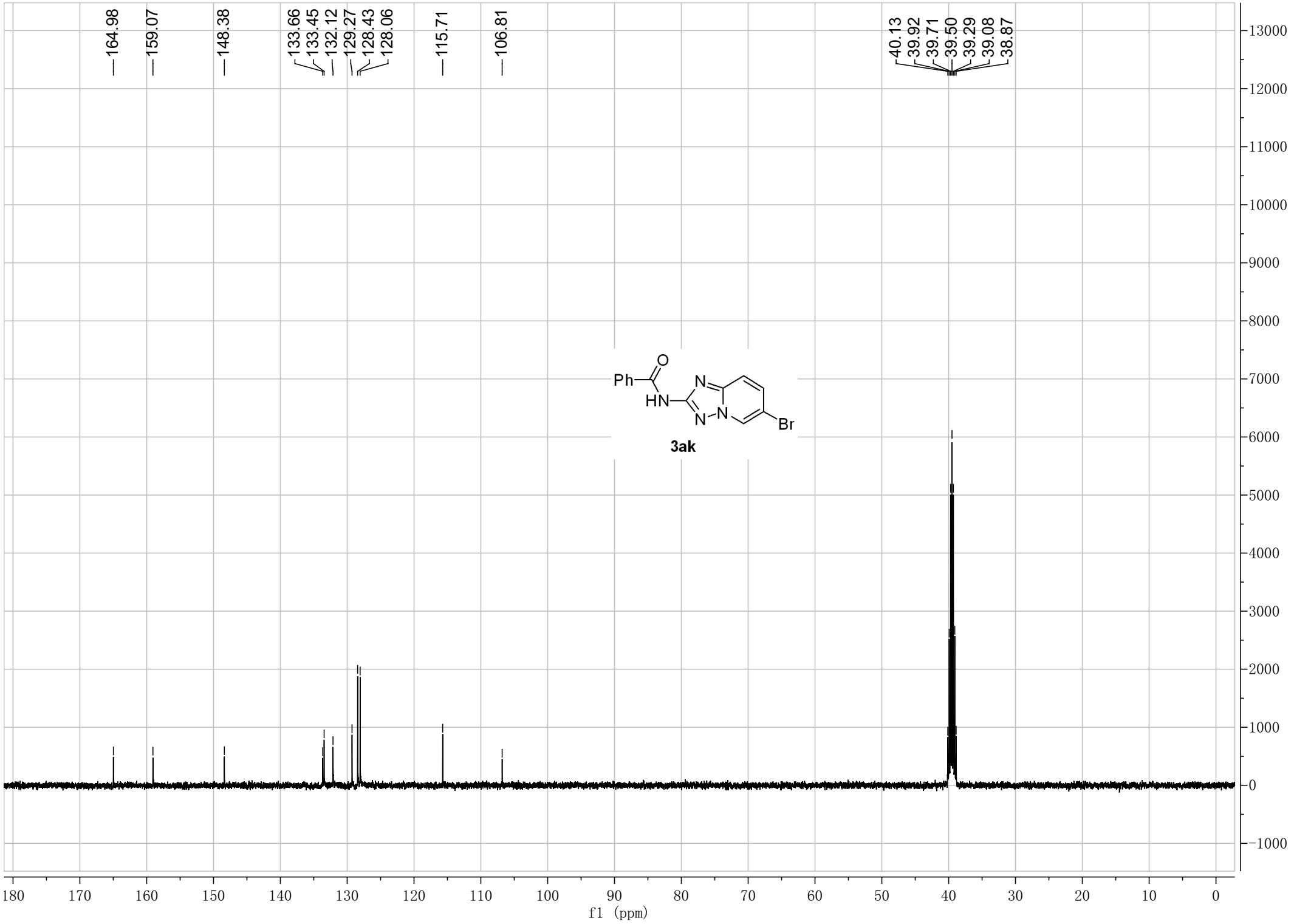
Br
3ak
1.00
0.89
2.14
1.04
0.98
1.03
2.05
f1 (ppm)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129.27
128.43
128.06
115.71
106.81
40.13
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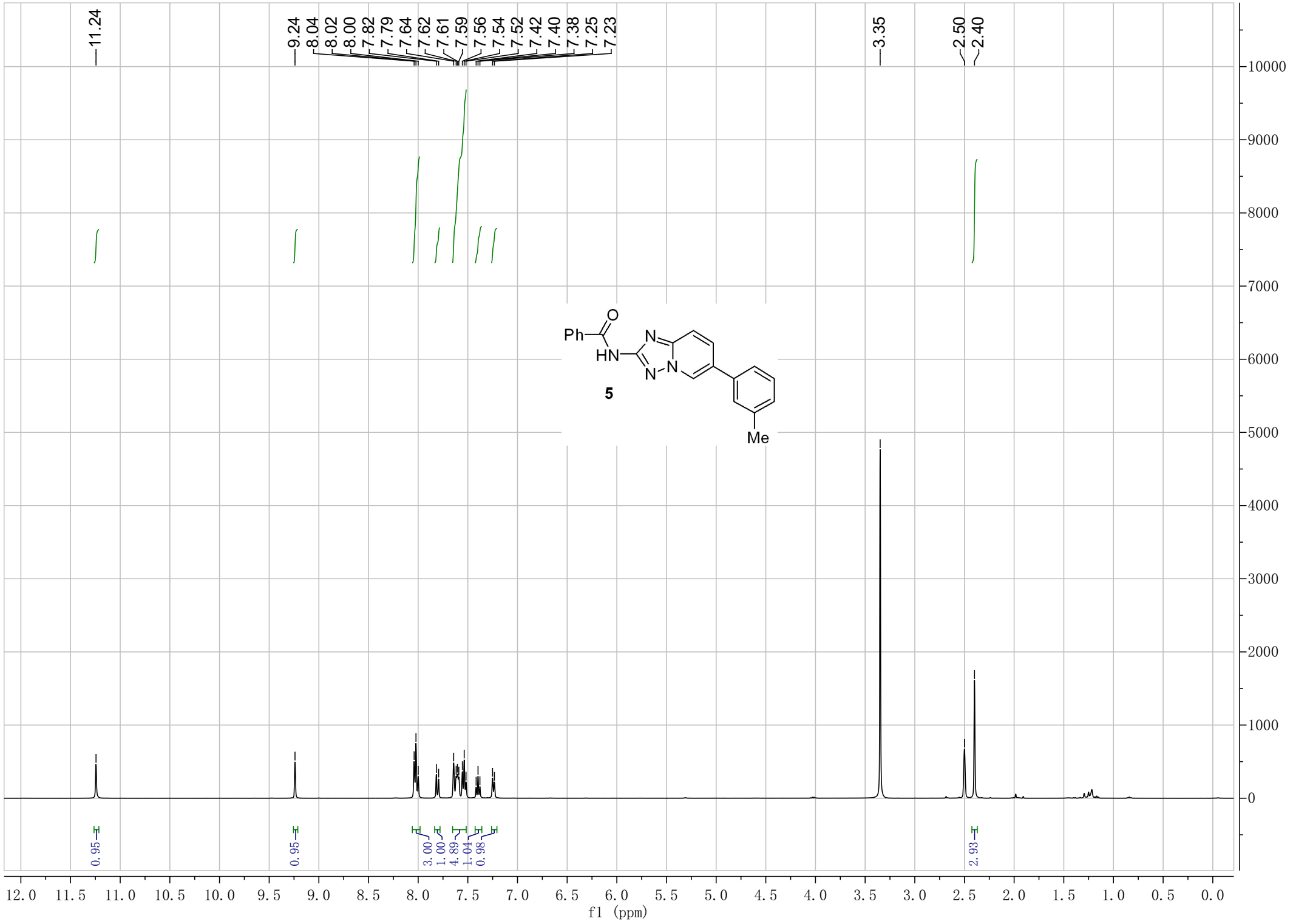
39.29
39.08
38.87
Ph
O
HN
N
N
N
Br
3ak
f1 (ppm)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7.61
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7.54
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7.38
7.25
7.23
3.35
2.50
2.40
Ph
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N
N
Me
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0.95
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1.00
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8000
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5000
4000
3000
2000
1000
0
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11.0
10.5
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3.5
3.0
2.5
2.0
1.5
1.0
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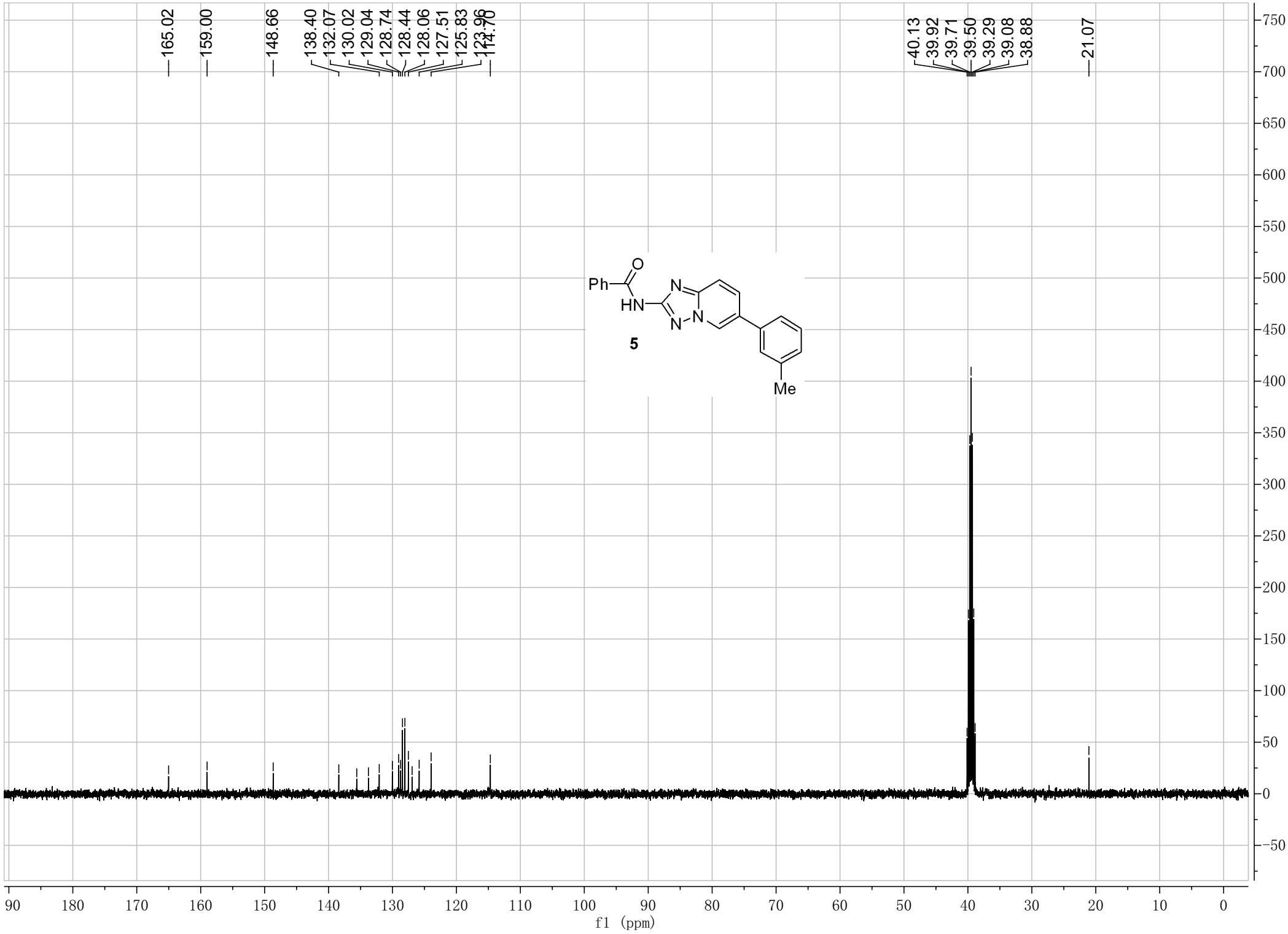
0.0
f1 (ppm)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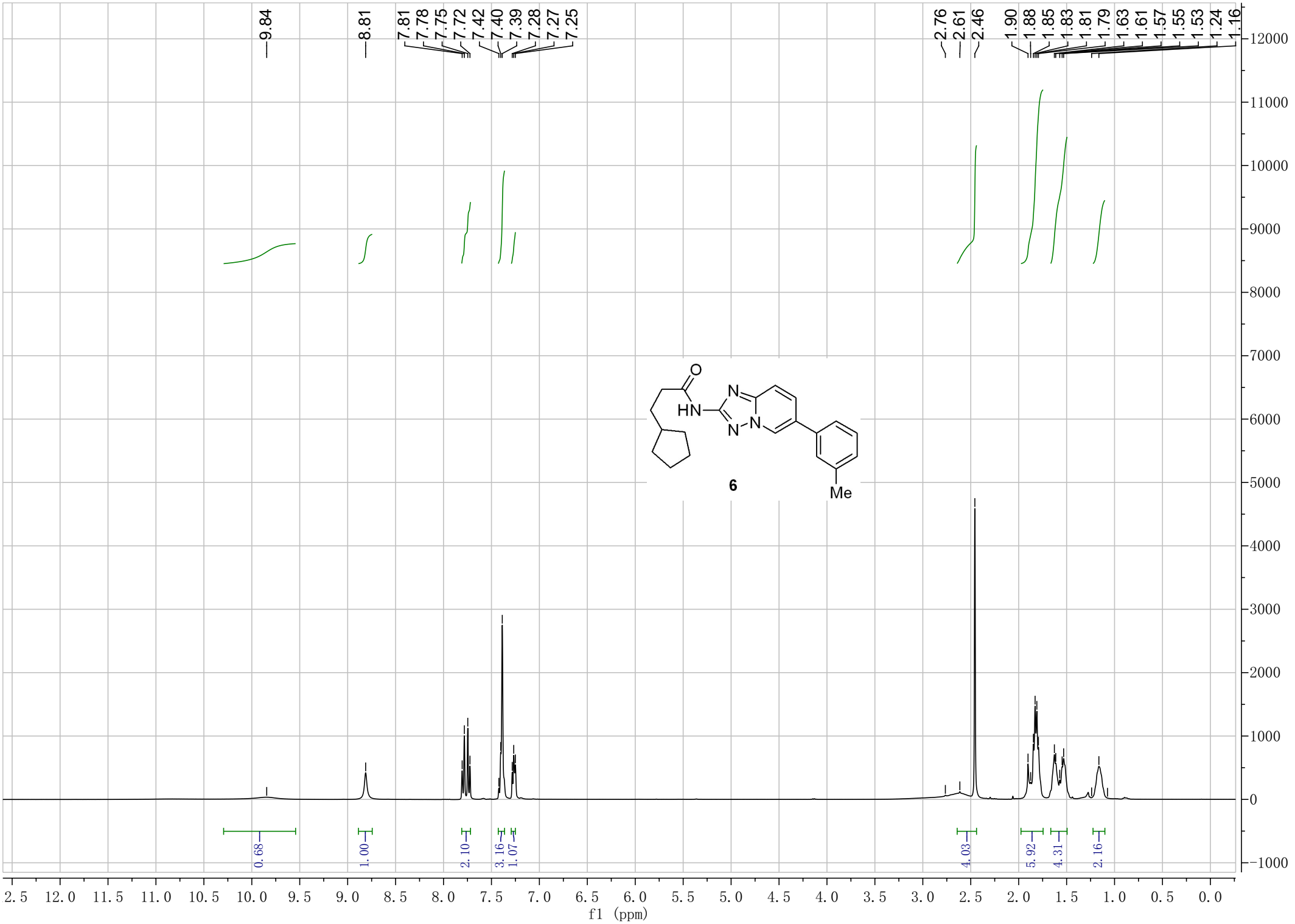
159.00
148.66
138.40
132.07
130.02
129.04
128.74
128.44
128.06
127.51
125.83
123.96
114.70
40.13
39.92
39.71
39.50
39.29
39.08
38.88
21.07
Ph
O
HN
N
N
N
Me
5
f1 (ppm)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7.81
7.78
7.75
7.72
7.42
7.40
7.39
7.28
7.27
7.25
2.76
2.61
2.46
1.90
1.88
1.85
1.83
1.81
1.79
1.63
1.61
1.57
1.55
1.53
1.24
1.16
O
HN
N
N
N
6
Me
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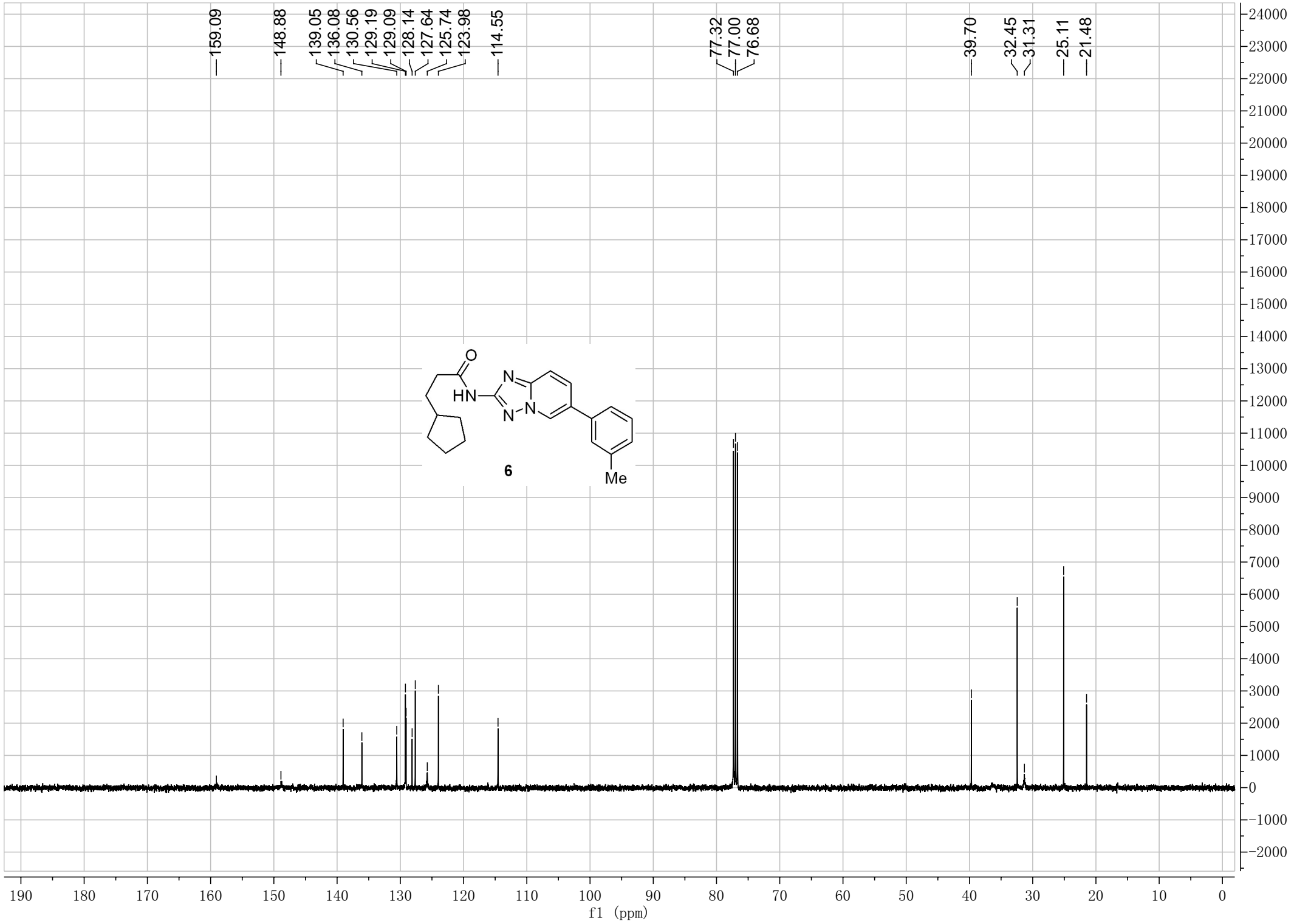
1.00
2.10
3.16
1.07
4.03
5.92
4.31
2.16
f1 (ppm)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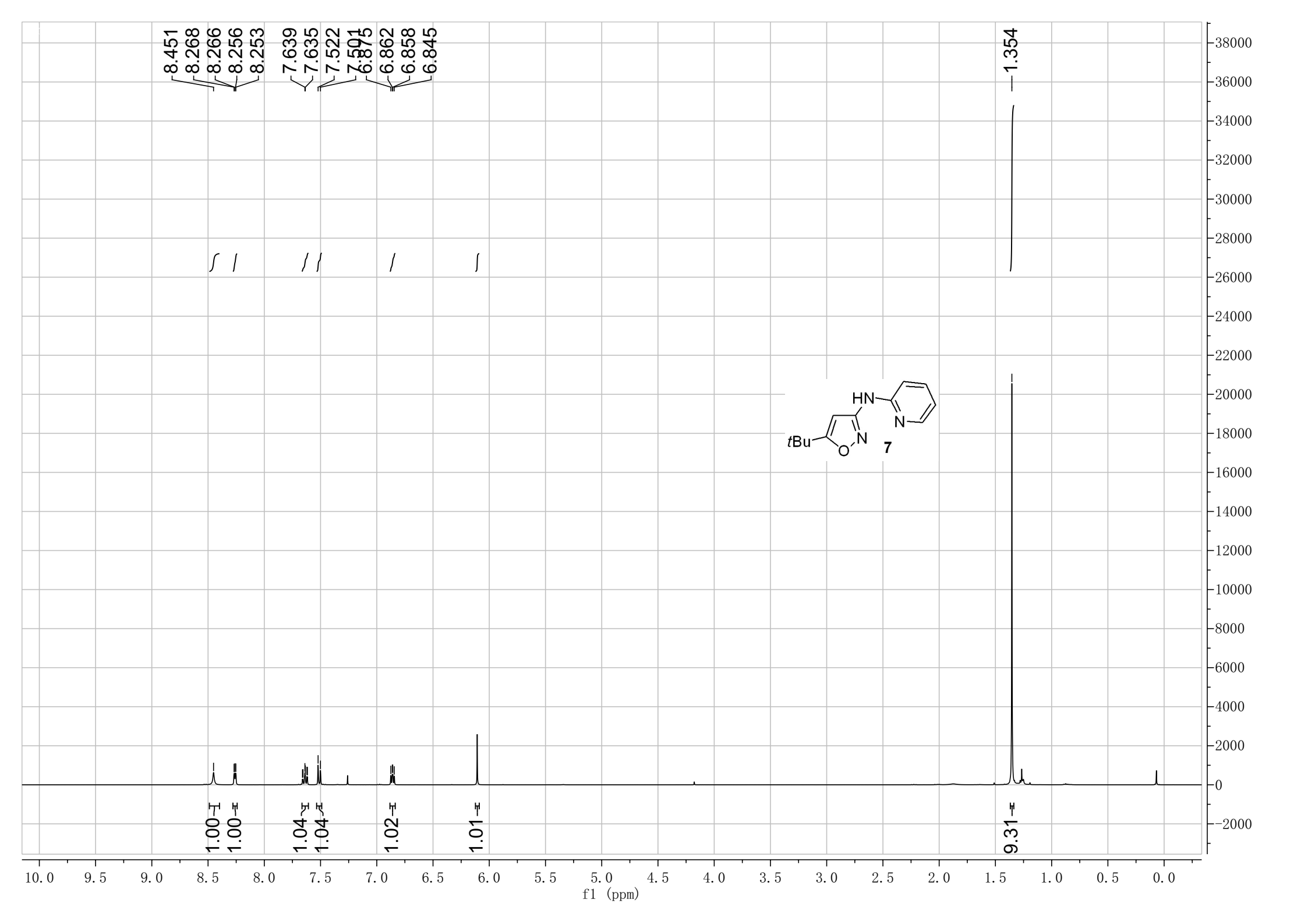
148.88
139.05
136.08
130.56
129.19
129.09
128.14
127.64
125.74
123.98
114.55
77.32
77.00
76.68
39.70
32.45
31.31
25.11
21.48
O
HN
N
N
N
6
Me
f1 (ppm)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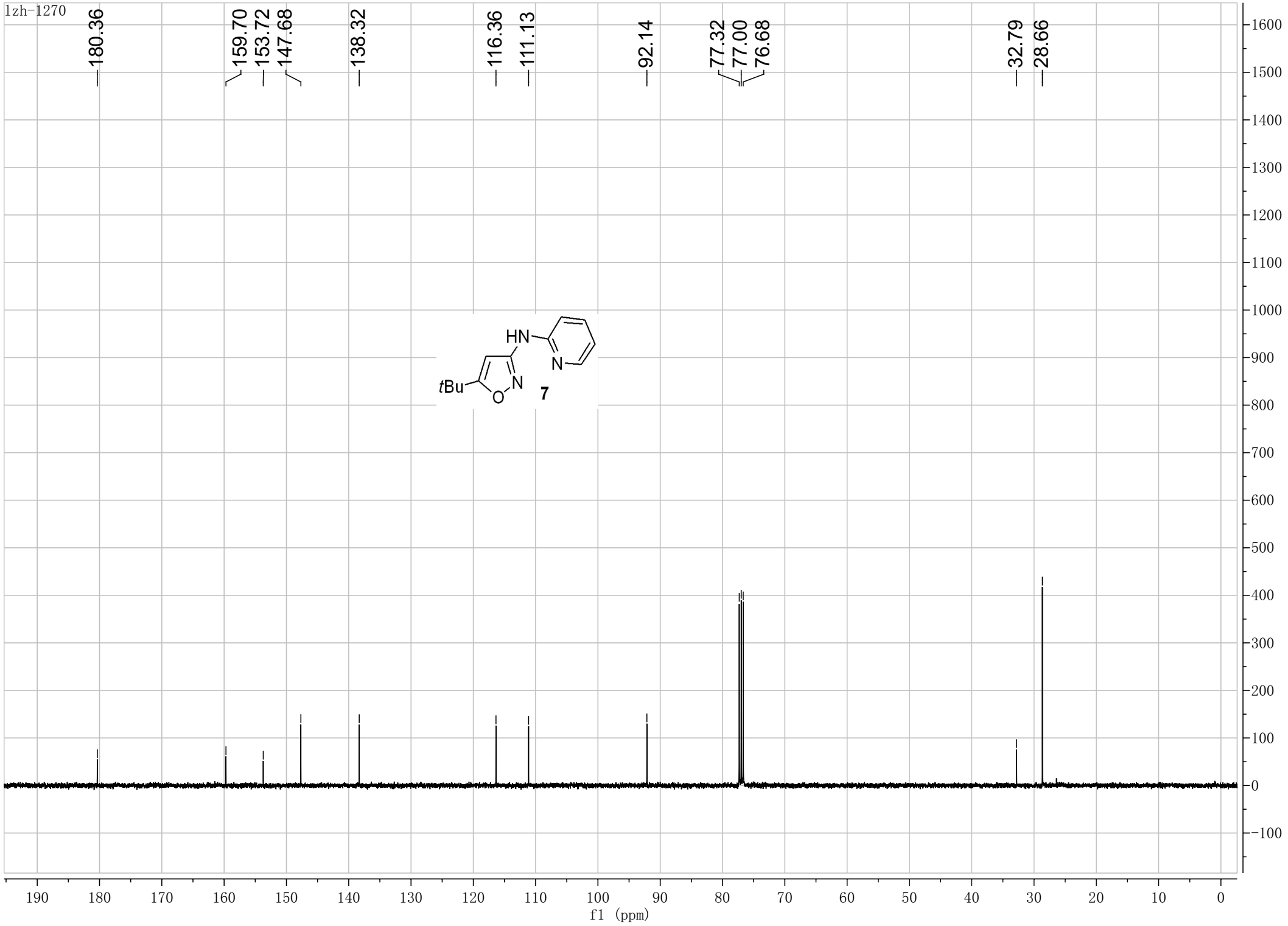
8.268
8.266
8.256
8.253
7.639
7.635
7.522
7.501
6.875
6.862
6.858
6.845
1.354
HN
N
tBu
O
N
7
1.00
1.00
1.04
1.04
1.02
1.01
9.31
f1 (ppm)


1zh-1270
180.36
159.70
153.72
147.68
138.32
116.36
111.13
92.14
77.32
77.00
76.68
32.79
28.66
HN
N
tBu
O
N
7
f1 (ppm)