Supporting Information

Copper-Catalyzed N-Arylation of Amines with Part-per-Million Catalyst Loadings under Air at Room Temperature

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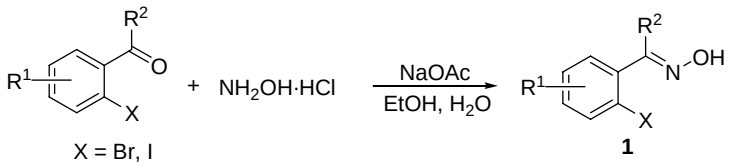
General experimental procedures

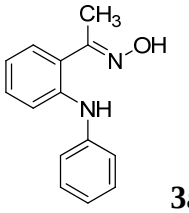
All reagents were weighed and handled in air at room temperature. Column chromatography was performed on silica gel (200 ~ 300 mesh). Proton magnetic resonance spectra (^{1}H NMR) were recorded using tetramethylsilane (TMS) (at 0.00 ppm) in the solvent, remaining $CHCl_3$ in $CDCl_3$ (at 7.26 ppm) or remaining DMSO in DMSO-d_6 (at 2.50 ppm) as the internal standard. Carbon magnetic resonance spectra (^{13}C NMR) were recorded using $CDCl_3$ (at 77.2 ppm) or DMSO-d_6 (at 39.5 ppm) as the internal standard.



General procedures for synthesis of oximes 1a-f: Oximes were prepared according to the previous procedure.[1] Ketone (10 mmol), hydroxylamine hydrochloride (15 mmol) and AcONa (15 mmol) were added a round bottom flask with 8 mL of H_2O/EtOH (v/v = 1:1) and a magnetic stirrer at room temperature. The solution was refluxed till consumption of the ketone (TLC determination). After cooling to room temperature, ethanol in the resulting solution was removed in vacuo, and 25 mL of water was added to the residue. The crude product was extracted with EtOAc (3 × 50 mL), and the organic phase was dried over anhydrous Na_2SO_4 and concentrated. The residue was purified by crystallization or flash chromatography to get oxime (**1a-f**).

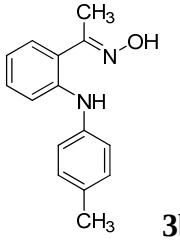
General procedure for synthesis of compounds 3a-b': 12.1 mg of $CuCl_2$ was dissolved in 4 mL of methanol at room temperature to get 22.5 mM $CuCl_2$ solution. 0.89 uL of the $CuCl_2$ solution (2.0×10^{-5} mmol, 2.69×10^{-3} mg of $CuCl_2$) was added to a round bottom flask, then methanol was removed with the aid of a rotary evaporator, and $CuCl_2$ was remained in the flask. Substituted (*E*)-1-(2-halophenyl)alkanone oxime (**1**) (0.25 mmol), amine (**2**) (0.50 mmol), *N,N'*-dimethylenediamine (0.025 mmol, 2.2 mg), 99.997% K_2CO_3 (0.50 mmol, 69 mg for free amine; 1.0 mmol, 138 mg for amine hydrochloride), cyclohexane (1.8 mL) and ethanol (0.2 mL) were added to the round bottom flask equipped with $CuCl_2$ (2.0×10^{-5} mmol, 2.69×10^{-3} mg) and a magnetic

stirrer. The mixture was allowed to stir under air (without extrusion of air) at room temperature (ca. 25 ^{o}C) for 24 h. The resulting solution was concentrated with the aid of a rotary evaporator. The residue was purified by column chromatography on silica gel using hexane/ ethyl acetate as eluent to provide the desired product (**3**).



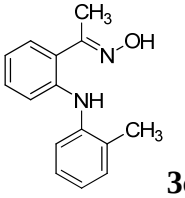
3a

(*E*)-1-(2-(Phenylamino)phenyl)ethanone oxime (3a).[2] Eluent: hexane/ethyl acetate (15:1). For substrate **1a**, yield 90% (51 mg); for substrate **1e**, yield 88% (50 mg). Light yellow oil. ^{1}H NMR ($CDCl_3$, 300 MHz) δ 8.94 (br s, 1H), 7.44-7.14 (m, 8H), 6.98 (t, J = 7.2 Hz, 1H), 6.84 (t, J = 7.4 Hz, 1H), 2.34 (s, 3H). ^{13}C NMR ($CDCl_3$, 75 MHz) δ 158.5, 142.7, 142.2, 129.6, 129.4, 122.3, 121.5, 120.8, 118.8, 116.0, 13.4. ESI-MS $[M+H]^+$ m/z 227.2, $[M+Na]^+$ m/z 249.2.



3b

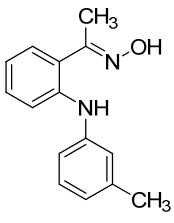
(*E*)-1-(2-(*p*-Tolylamino)phenyl)ethanone oxime (3b).[2] Eluent: hexane/ethyl acetate (15:1). Yield 88% (53 mg). Light yellow oil. ^{1}H NMR ($CDCl_3$, 300 MHz) δ 8.88 (br s, 1H), 7.50 (br s, 1H), 7.41 (dd, J = 7.9 Hz, J = 1.4 Hz 1H), 7.24-7.04 (m, 6H), 6.82-6.77 (m, 1H), 2.38 (s, 3H), 2.34 (s, 3H). ^{13}C NMR ($CDCl_3$, 75 MHz) δ 158.6, 143.6, 139.5, 132.3, 130.0, 129.6, 129.4, 121.8, 120.7, 118.1, 115.3, 20.9, 13.3. ESI-MS $[M+H]^+$ m/z 241.2, $[M+Na]^+$ m/z 263.2.



3c

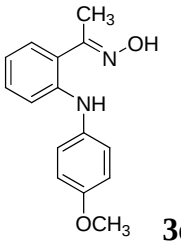
(*E*)-1-(2-(*o*-Tolylamino)phenyl)ethanone oxime (3c). Eluent: hexane/ethyl acetate (12:1). For substrate **1a**, yield 63% (38 mg); for substrate **1e**, yield 65% (39 mg).

Light yellow oil. ^{1}H NMR ($CDCl_3$, 300 MHz) δ 8.82 (br s, 1H), 7.44 (dd, *J* = 7.9 Hz, *J* = 1.4 Hz 1H), 7.30-7.11 (m, 5H), 7.05-6.96 (m, 2H), 6.83-6.78 (m, 1H), 2.36 (s, 3H), 2.24 (s, 3H). ^{13}C NMR ($CDCl_3$, 75 MHz) δ 158.7, 143.6, 140.5, 131.0, 129.6, 129.3, 126.7, 123.2, 121.7, 120.5, 117.9, 115.4, 18.3, 13.2. HR-MS $[M+H]^+$ m/z Calcd for $C_{15}H_{17}N_2O$: 241.1341. Found: 241.1343.



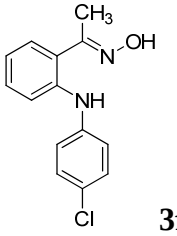
3d

(*E*)-1-(2-(*m*-Tolylamino)phenyl)ethanone oxime (3d). Eluent: hexane/ethyl acetate (12:1). Yield 85% (51 mg). Light yellow oil. ^{1}H NMR ($CDCl_3$, 300 MHz) δ 8.88 (br s, 1H), 7.44-7.40 (m, 2H), 7.32 (d, *J* = 8.3 Hz, 1H), 7.20-7.14 (m, 2H), 6.98-6.96 (m, 2H), 6.86-6.79 (m, 2H), 2.34 (s, 3H), 2.30 (s, 3H). ^{13}C NMR ($CDCl_3$, 75 MHz) δ158.4, 142.8, 142.2, 139.3, 129.5, 129.4, 129.2, 123.1, 121.4, 118.6, 117.7, 116.1, 21.6, 13.4. HR-MS $[M+H]^+$ m/z Calcd for $C_{15}H_{17}N_2O$: 241.1341. Found: 241.1344.



3e

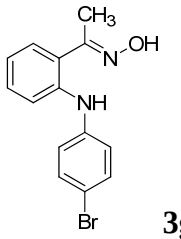
(*E*)-1-(2-(4-Methoxyphenylamino)phenyl)ethanone oxime (3e).[2] Eluent: hexane/ethyl acetate (10:1). Yield 90% (58 mg). Light yellow oil. ^{1}H NMR ($CDCl_3$, 300 MHz) δ 8.92 (br s, 1H), 7.47 (br s, 1H), 7.42 (d, *J* = 7.9 Hz, 1H), 7.14-7.02 (m, 4H), 6.88 (s, 1H), 6.85 (s, 1H), 6.78 (t, *J* = 7.4 Hz, 1H), 3.80 (s, 3H), 2.36 (s, 3H). ^{13}C NMR ($CDCl_3$, 75 MHz) δ 158.7, 156.0, 144.8, 134.9, 129.6, 129.3, 124.8, 119.5, 117.3, 114.7, 114.2, 55.7, 13.0. ESI-MS $[M+H]^+$ m/z 257.2, $[M+Na]^+$ m/z 279.2.



3f

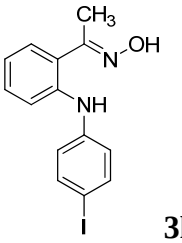
(*E*)-1-(2-(4-Chlorophenylamino)phenyl)ethanone oxime (3f).[2] Eluent: hexane/ethyl

acetate (12:1). Yield 86% (56 mg). Light yellow oil. ^{1}H NMR ($CDCl_3$, 300 MHz) δ 8.92 (br s, 1H), 7.50 (br s, 1H), 7.43 (dd, *J* = 7.9 Hz, *J* = 1.4 Hz, 1H), 7.27-7.04 (m, 6H), 6.87 (t, *J* = 7.6 Hz, 1H), 2.34 (s, 3H). ^{13}C NMR ($CDCl_3$, 75 MHz) δ 158.5, 142.3, 140.9, 129.6, 129.5, 129.4, 126.9, 121.8, 119.2, 116.0, 13.4. ESI-MS $[M+H]^+$ m/z 261.2, $[M+Na]^+$ m/z 283.1.



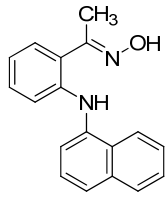
3g

(*E*)-1-(2-(4-Bromophenylamino)phenyl)ethanone oxime (3g). Eluent: hexane/ethyl acetate (12:1). Yield 84% (64 mg). Light yellow oil. ^{1}H NMR ($CDCl_3$, 300 MHz) δ 8.97 (br s, 1H), 7.44 (dd, *J* = 7.9 Hz, *J* = 1.4 Hz, 1H), 7.38-7.26 (m, 4H), 7.21-7.16 (m, 1H), 7.04-6.99 (m, 2H), 6.90-6.85 (m, 1H), 2.35 (s, 3H). ^{13}C NMR ($CDCl_3$, 75 MHz) δ 158.4, 142.1, 141.4, 132.3, 129.6, 129.5, 122.0, 121.8, 119.3, 116.1, 114.2, 13.4. HR-MS $[M+H]^+$ m/z Calcd for $C_{14}H_{14}BrN_2O$: 305.0290. Found: 305.0293.



3h

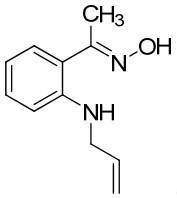
(*E*)-1-(2-(4-Iodophenylamino)phenyl)ethanone oxime (3h). Eluent: hexane/ethyl acetate (12:1). Yield 90% (79 mg). Light yellow oil. ^{1}H NMR ($CDCl_3$, 300 MHz) δ 8.93 (br s, 1H), 7.54 (s, 1H), 7.51 (s, 1H), 7.45-7.42 (m, 2H), 7.30 (d, *J* = 7.2 Hz, 1H), 7.19 (t, *J* = 6.9 Hz, 1H), 6.92-6.86 (m, 3H), 2.34 (s, 3H). ^{13}C NMR ($CDCl_3$, 75 MHz) δ 158.4, 142.2, 141.8, 138.2, 129.6, 129.5, 122.1, 119.5, 116.3, 83.9, 13.4. HR-MS $[M+H]^+$ m/z Calcd for $C_{14}H_{14}IN_2O$: 353.0151. Found: 353.0149.



3i

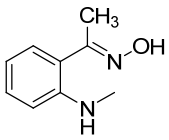
(*E*)-1-(2-(Naphthalen-1-ylamino)phenyl)ethanone oxime (3i). Eluent: hexane/ethyl

acetate (10:1). Yield 75% (52 mg). Light yellow oil. ^{1}H NMR ($CDCl_3$, 300 MHz) δ 9.56 (br s, 1H), 8.08-8.05 (m, 1H), 7.87-7.84 (m, 1H), 7.61 (d, *J* = 7.9 Hz, 1H), 7.52-7.39 (m, 5H), 7.23 (s, 1H), 7.15-7.06 (m, 2H), 6.85-6.79 (m, 1H), 2.42 (s, 3H). ^{13}C NMR ($CDCl_3$, 75 MHz) δ 159.0, 144.5, 138.1, 134.9, 129.7, 129.3, 129.2, 128.5, 126.2, 126.1, 126.0, 123.8, 122.6, 120.2, 118.7, 118.0, 115.5, 13.0. HR-MS $[M+H]^+$ m/z Calcd for $C_{18}H_{17}N_2O$: 277.1341. Found: 277.1345.



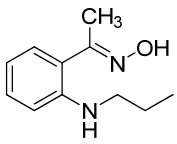
3j

(*E*)-1-(2-(Allylamino)phenyl)ethanone oxime (3j).[3] Eluent: hexane/ethyl acetate (10:1). Yield 80% (38 mg). Light yellow oil. ^{1}H NMR ($CDCl_3$, 300 MHz) δ 7.46 (br s, 1H), 7.41-7.38 (m, 1H), 7.25-7.17 (m, 2H), 6.70-6.66 (m, 2H), 6.02-5.90 (m, 1H), 5.31-5.13 (m, 2H), 3.86-3.84 (m, 2H), 2.34 (s, 3H). ^{13}C NMR ($CDCl_3$, 75 MHz) δ 159.2, 146.9, 135.3, 130.0, 129.2, 118.1, 116.0, 115.5, 111.4, 46.0, 12.7. ESI-MS $[M+H]^+$ m/z 191.2.



3k

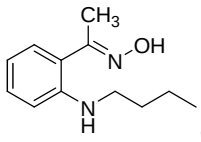
(*E*)-1-(2-(Methylamino)phenyl)ethanone oxime (3k).[3] Eluent: hexane/ethyl acetate (15:1). Yield 76% (31 mg). Light yellow solid. mp 71-72 °C. ^{1}H NMR ($CDCl_3$, 300 MHz) δ 7.39 (dd, *J* = 8.1 Hz, *J* = 1.4 Hz, 1H), 7.30-7.22 (m, 3H), 6.71-6.66 (m, 2H), 2.88 (s, 3H), 2.33 (s, 3H),. ^{13}C NMR ($CDCl_3$, 75 MHz) δ 159.2, 148.0, 130.2, 129.1, 118.0, 115.2, 110.6, 30.2, 12.6. ESI-MS $[M+H]^+$ m/z 165.2.



3l

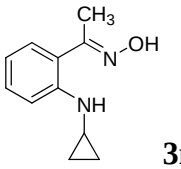
(*E*)-1-(2-(Propylamino)phenyl)ethanone oxime (3l). Eluent: hexane/ethyl acetate (15:1). Yield 77% (37 mg). Light yellow oil. ^{1}H NMR ($CDCl_3$, 300 MHz) δ 7.39 (dd, *J* = 7.9 Hz, *J* = 1.4 Hz, 1H), 7.24-7.18 (m, 3H), 6.70-6.63 (m, 2H), 3.14 (t, *J* = 6.9 Hz, 2H), 2.33 (s, 3H), 1.74-1.62 (m, 2H), 1.00 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR ($CDCl_3$, 75

MHz) δ 159.2, 147.2, 130.1, 129.2, 117.8, 115.0, 111.0, 45.4, 22.5, 12.6, 12.0. HR-MS $[M+H]^+$ m/z Calcd for $C_{11}H_{17}N_2O$: 193.1341. Found: 193.1339.



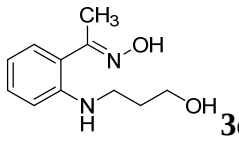
3m

(*E*)-1-(2-(Butylamino)phenyl)ethanone oxime (3m). Eluent: hexane/ethyl acetate (15:1). Yield 80% (41 mg). Light yellow solid. mp 56-57 °C. ^{1}H NMR ($CDCl_3$, 300 MHz) δ 7.44 (br s, 1H), 7.37 (dd, *J* = 7.9 Hz, *J* = 1.7 Hz, 1H), 7.23-7.18 (m, 2H), 6.70-6.63 (m, 2H), 3.16 (t, *J* = 7.2 Hz, 2H), 2.32 (s, 3H), 1.69-1.59 (m, 2H), 1.49-1.37 (m, 2H), 0.95 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR ($CDCl_3$, 75 MHz) δ 159.2, 147.2, 130.1, 129.2, 117.9, 115.1, 111.1, 43.3, 31.5, 20.6, 14.0, 12.8. HR-MS $[M+H]^+$ m/z Calcd for $C_{12}H_{19}N_2O$: 207.1497. Found: 207.1495.



3n

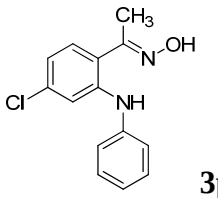
(*E*)-1-(2-(Cyclopropylamino)phenyl)ethanone oxime (3n). Eluent: hexane/ethyl acetate (15:1). Yield 86% (41 mg). Light yellow oil. ^{1}H NMR ($CDCl_3$, 300 MHz) δ 7.43 (br s, 1H), 7.36 (dd, *J* = 7.9 Hz, *J* = 1.4 Hz, 1H), 7.32 (br s, 1H), 7.27-7.15 (m, 2H), 6.74-6.69 (m, 1H), 2.47-2.40 (m, 1H), 2.31 (s, 3H), 0.79-0.73 (m, 2H), 0.56-0.51 (m, 2H). ^{13}C NMR ($CDCl_3$, 75 MHz) δ 159.0, 147.6, 130.0, 129.0, 118.0, 115.9, 112.6, 24.9, 12.7, 7.6. HR-MS $[M+H]^+$ m/z Calcd for $C_{11}H_{15}N_2O$: 191.1184. Found: 191.1181.



3o

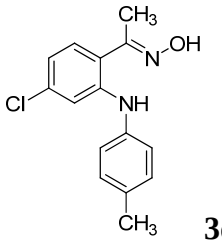
(*E*)-1-(2-(3-Hydroxypropylamino)phenyl)ethanone oxime (3o). Eluent: hexane/ethyl acetate (1:1). Yield 56% (29 mg). Light yellow solid. mp 96-97 °C. ^{1}H NMR (DMSO-d_6, 600 MHz) δ 11.02 (br s, 1H), 7.68 (t, *J* = 4.5 Hz, 1H), 7.12 (d, *J* = 7.6 Hz, 1H), 7.10 (t, *J* = 7.6 Hz, 1H), 6.62 (d, *J* = 8.2 Hz, 1H), 6.54 (t, *J* = 7.6 Hz, 1H), 4.47 (t, *J* = 5.5 Hz, 1H), 3.49 (q, *J* = 6.2 Hz, 2H), 3.14 (q, *J* = 6.2 Hz, 2H), 2.16 (s,

3H), 1.72-1.68 (m, 2H). ^{13}C NMR ($CDCl_3$, 75 MHz) δ 158.6, 147.0, 130.0, 129.1, 118.7, 115.7, 111.2, 61.9, 41.3, 31.5, 12.7. HR-MS $[M+H]^+$ m/z Calcd for $C_{11}H_{17}N_2O_2$: 209.1290. Found: 209.1293.



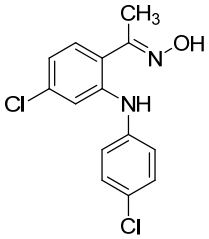
3p

(*E*)-1-(4-Chloro-2-(phenylamino)phenyl)ethanone oxime (3p). Eluent: hexane/ethyl acetate (10:1). Yield 69% (45 mg). Light yellow oil. ^{1}H NMR (DMSO-d_6, 300 MHz) δ 11.43 (br s, 1H), 9.67 (br s, 1H), 7.49 (d, J = 8.6 Hz, 1H), 7.38-7.33 (m, 2H), 7.17-7.13 (m, 3H), 7.05 (t, J = 7.3 Hz, 1H), 6.89-6.85 (m, 1H), 2.22 (s, 3H). ^{13}C NMR (DMSO-d_6, 75 MHz) δ 155.7, 144.2, 141.6, 134.0, 131.6, 130.1, 123.2, 121.2, 121.1, 118.6, 114.4, 13.3. HR-MS $[M+H]^+$ m/z Calcd for $C_{14}H_{14}ClN_2O$: 261.0795. Found: 261.0792.



3q

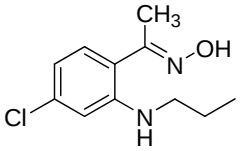
(*E*)-1-(4-Chloro-2-(*p*-tolylamino)phenyl)ethanone oxime (3q). Eluent: hexane/ethyl acetate (10:1). Yield 74% (51 mg). Light yellow oil. ^{1}H NMR ($CDCl_3$, 300 MHz) δ 9.18 (br s, 1H), 7.33 (d, J = 8.2 Hz, 2H), 7.15-7.05 (m, 5H), 6.74-6.70 (m, 1H), 2.33 (s, 6H). ^{13}C NMR ($CDCl_3$, 75 MHz) δ 158.2, 145.3, 138.2, 135.6, 133.5, 130.4, 130.2, 122.9, 118.0, 117.5, 113.9, 21.0, 13.0. HR-MS $[M+H]^+$ m/z Calcd for $C_{15}H_{16}ClN_2O$: 275.0951. Found: 275.0955.



3r

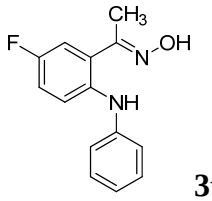
(*E*)-1-(4-Chloro-2-(4-chlorophenylamino)phenyl)ethanone oxime (3r). Eluent: hexane/ethyl acetate (10:1). Yield 62% (46 mg). White solid, mp 120-122 ^{o}C. ^{1}H

NMR (DMSO-d_6, 300 MHz) δ 11.36 (br s, 1H), 9.49 (br s, 1H), 7.43 (d, J = 8.6 Hz, 1H), 7.32 (d, J = 8.6 Hz, 2H), 7.10-7.07 (m, 3H), 6.88 (dd, J = 8.6 Hz, J = 2.1 Hz, 1H), 2.13 (s, 3H). ^{13}C NMR (DMSO-d_6, 75 MHz) δ 155.4, 143.5, 141.0, 134.1, 131.7, 129.9, 126.2, 122.5, 121.8, 119.6, 115.5, 13.5. HR-MS $[M+H]^+$ m/z Calcd for $C_{14}H_{13}Cl_2N_2O$: 295.0405. Found: 295.0402.



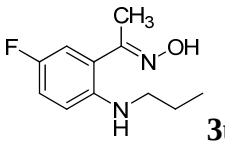
3s

(*E*)-1-(4-Chloro-2-(propylamino)phenyl)ethanone oxime (3s). Eluent: hexane/ethyl acetate (10:1). Yield 60% (34 mg). White solid, Light yellow oil. ^{1}H NMR (DMSO-d_6, 300 MHz) δ 11.24 (br s, 1H), 8.11 (t, J = 5.2 Hz, 1H), 7.41 (d, J = 8.3 Hz, 1H), 6.66-6.61 (m, 2H), 3.16-3.10 (q, 2H), 2.24 (s, 3H), 1.71-1.59 (m, 2H), 1.07 (t, J = 7.6 Hz, 3H). ^{13}C NMR (DMSO-d_6, 75 MHz) δ 156.2, 148.3, 134.5, 130.7, 116.9, 114.3, 109.8, 44.5, 22.1, 12.4, 12.1. HR-MS $[M+H]^+$ m/z Calcd for $C_{11}H_{16}ClN_2O$: 227. 0951. Found: 227. 0949.



3t

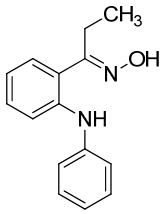
(*E*)-1-(5-Fluoro-2-(phenylamino)phenyl)ethanone oxime (3t). Eluent: hexane/ethyl acetate (12:1). Yield 85% (52 mg). Light yellow solid, mp 106-107 ^{o}C. ^{1}H NMR (DMSO-d_6, 600 MHz) δ 11.38 (br s, 1H), 8.87 (br s, 1H), 7.24-7.18 (m, 4H), 7.06 (td, J = 8.2 Hz, J = 2.8 Hz, 1H), 6.95 (d, J = 8.2 Hz, 2H), 6.83 (t, J = 7.6 Hz, 1H), 2.11 (s, 3H). ^{13}C NMR (DMSO-d_6, 150 MHz) δ 156.6 (d, J = 235.5 Hz), 155.1, 143.8, 138.3, 129.8, 127.0 (d, J = 5.8 Hz), 121.0, 120.3 (d, J = 7.2 Hz), 118.1, 116.2 (d, J = 21.7 Hz), 116.0 (d, J = 23.1 Hz), 13.8. HR-MS $[M+H]^+$ m/z Calcd for $C_{14}H_{14}FN_2O$: 245.1090. Found: 245.1091.



3u

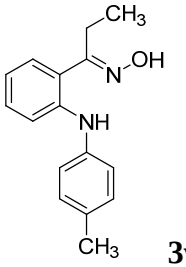
(*E*)-1-(5-Fluoro-2-(propylamino)phenyl)ethanone oxime (3u). Eluent: hexane/ethyl

acetate (15:1). Yield 76% (40 mg). Light yellow oil. ^{1}H NMR (DMSO-d_6, 600 MHz) δ 11.21 (br s, 1H), 7.55 (t, J = 4.8 Hz, 1H), 7.16 (dd, J = 11.0 Hz, J = 2.8 Hz, 1H), 6.96 (td, J = 8.2 Hz, J = 2.8 Hz, 1H), 6.58-6.56 (m, 1H), 3.02 (q, J = 6.2 Hz, 2H), 2.16 (s, 3H), 1.58-1.52 (m, 2H), 0.92 (t, J = 7.6 Hz, 3H). ^{13}C NMR (DMSO-d_6, 150 MHz) δ 156.2, 153.6 (d, J = 228.3 Hz), 144.1, 118.8 (d, J = 7.2 Hz), 116.3 (d, J = 21.7 Hz), 115.3 (d, J = 23.1 Hz), 111.7 (d, J = 7.2 Hz), 45.3, 22.4, 12.6, 12.2. HR-MS $[M+H]^+$ m/z Calcd for $C_{11}H_{16}FN_2O$: 211.1247. Found: 211.1244.



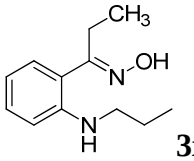
3v

(*E*)-1-(2-(Phenylamino)phenyl)propan-1-one oxime (3v). Eluent: hexane/ethyl acetate (10:1). Yield 45% (27 mg). Light yellow oil. ^{1}H NMR ($CDCl_3$, 300 MHz) δ 8.82 (br s, 1H), 7.43 (dd, J = 7.9 Hz, J = 1.4 Hz, 1H), 7.35-7.14 (m, 7H), 7.00-6.96 (m, 1H), 6.88-6.83 (m, 1H), 2.86 (q, J = 7.6 Hz, 2H), 1.21 (t, J = 7.6 Hz, 3H). ^{13}C NMR ($CDCl_3$, 75 MHz) δ 163.2, 143.1, 142.3, 129.5, 129.4, 129.1, 122.2, 120.7, 120.5, 118.8, 116.1, 20.6, 11.4. HR-MS $[M+H]^+$ m/z Calcd for $C_{15}H_{17}N_2O$: 241.1341. Found: 241.1345.



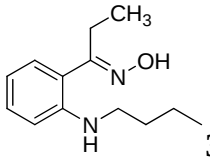
3w

(*E*)-1-(2-(*p*-Tolylamino)phenyl)propan-1-one oxime (3w). Eluent: hexane/ethyl acetate (10:1). Yield 52% (33 mg). Light yellow oil. ^{1}H NMR ($CDCl_3$, 300 MHz) δ 8.73 (br s, 1H), 7.43 (br s, 1H), 7.42 (d, J = 8.3 Hz, 1H), 7.24-7.03 (m, 6H), 6.80 (t, J = 7.2 Hz, 1H), 2.86 (q, J = 7.6 Hz, 2H), 2.31 (s, 3H), 1.21 (t, J = 7.6 Hz, 3H). ^{13}C NMR ($CDCl_3$, 75 MHz) δ 163.3, 143.9, 139.5, 132.2, 130.0, 129.6, 129.1, 121.7, 119.8, 118.2, 115.4, 20.9, 20.6, 11.4. HR-MS $[M+H]^+$ m/z Calcd for $C_{16}H_{19}N_2O$: 255.1497. Found: 255.1496.



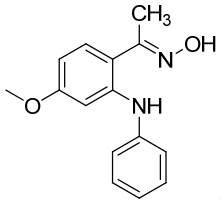
3x

(*E*)-1-(2-(Propylamino)phenyl)propan-1-one oxime (3x). Eluent: hexane/ethyl acetate (15:1). Yield 60% (31 mg). Light yellow oil. ^{1}H NMR ($CDCl_3$, 300 MHz) δ 7.39-7.36 (m, 2H), 7.24-7.16 (m, 2H), 6.71-6.64 (m, 2H), 2.85 (t, *J* = 6.9 Hz, 2H), 2.85 (q, *J* = 7.6 Hz, 2H), 1.74-1.62 (m, 2H), 1.20 (t, *J* = 7.6 Hz, 3H), 1.00 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR ($CDCl_3$, 75 MHz) δ 164.0, 147.6, 130.1, 128.9, 116.7, 115.1, 111.2, 45.4, 22.5, 20.0, 12.0, 11.6. HR-MS $[M+H]^+$ m/z Calcd for $C_{12}H_{19}N_2O$: 207.1497. Found: 207.1493.



3y

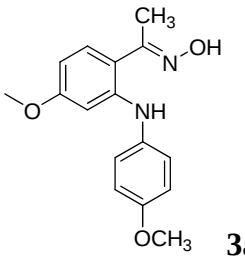
(*E*)-1-(2-(Butylamino)phenyl)propan-1-one oxime (3y). Eluent: hexane/ethyl acetate (15:1). Yield 62% (34 mg). Light yellow oil. ^{1}H NMR ($CDCl_3$, 300 MHz) δ 7.38 (dd, *J* = 7.9 Hz, *J* = 1.4 Hz, 1H), 7.24-7.16 (m, 3H), 6.70-6.63 (m, 2H), 3.16 (t, *J* = 6.9 Hz, 2H), 2.86 (q, *J* = 7.6 Hz, 2H), 1.69-1.60 (m, 2H), 1.50-1.37 (m, 2H), 1.20 (t, *J* = 7.6 Hz, 3H), 0.95 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR ($CDCl_3$, 75 MHz) δ 164.0, 147.7, 130.1, 128.9, 116.6, 115.0, 111.1, 43.3, 31.5, 20.6, 20.0, 14.0, 11.6. HR-MS $[M+H]^+$ m/z Calcd for $C_{13}H_{21}N_2O$: 221.1654. Found: 221.1652.



3z

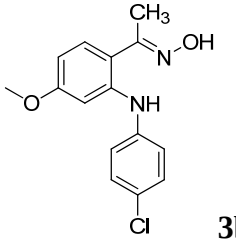
(*E*)-1-(4-Methoxy-2-(phenylamino)phenyl)ethanone oxime (3z). Eluent: hexane/ethyl acetate (10:1). Yield 84% (54 mg). White solid, mp 108-109 °C. ^{1}H NMR (DMSO-d_6, 300 MHz) δ 11.15 (br s, 1H), 9.72 (br s, 1H), 7.46 (d, *J* = 8.9 Hz, 1H), 7.35 (t, *J* = 8.3 Hz, 2H), 7.18 (d, *J* = 7.6 Hz, 2H), 7.01 (t, *J* = 7.6 Hz, 1H), 6.79 (d, *J* = 2.8 Hz, 1H), 6.50 (dd, *J* = 8.8 Hz, *J* = 2.4 Hz, 1H), 3.74 (s, 3H), 2.23 (s, 3H). ^{13}C NMR (DMSO-d_6, 75 MHz) δ 160.3, 156.0, 143.9, 142.4, 131.2, 130.0, 127.2, 120.1, 115.8, 105.2, 100.8, 55.5, 13.3. HR-MS $[M+H]^+$ m/z Calcd for $C_{15}H_{17}N_2O_2$:

257.1290. Found: 257.1293.



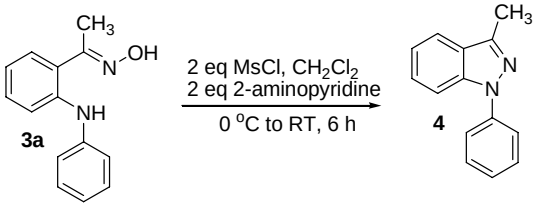
3a'

(*E*)-1-(4-Methoxy-2-(4-methoxyphenylamino)phenyl)ethanone oxime (3a'). Eluent: hexane/ethyl acetate (10:1). Yield 92% (66 mg). White solid, mp 154-156 ^{o}C. ^{1}H NMR (DMSO-d_6, 300 MHz) δ 11.09 (br s, 1H), 9.66 (br s, 1H), 7.44 (d, J = 8.9 Hz, 1H), 7.17-6.96 (m, 4H), 6.50 (d, J = 2.8 Hz, 1H), 6.40 (dd, J = 8.8 Hz, J = 2.8 Hz, 1H), 3.79 (s, 3H), 3.69 (s, 3H), 2.26 (s, 3H). ^{13}C NMR (DMSO-d_6, 75 MHz) δ 160.4, 156.4, 155.9, 146.1, 134.6, 131.1, 124.4, 115.2, 113.7, 103.5, 98.7, 55.7, 55.3, 12.9. HR-MS $[M+H]^+$ m/z Calcd for $C_{16}H_{19}N_2O_3$: 287.1396. Found: 287.1397.



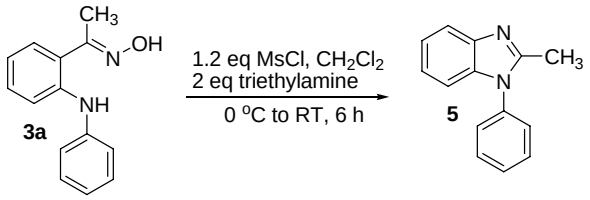
3b'

(*E*)-1-(2-(4-Chlorophenylamino)-4-methoxyphenyl)ethanone oxime (3b'). Eluent: hexane/ethyl acetate (10:1). Yield 80% (58 mg). White solid, mp 127-128 ^{o}C. ^{1}H NMR (DMSO-d_6, 300 MHz) δ 11.16 (br s, 1H), 9.63 (br s, 1H), 7.46 (d, J = 8.6 Hz, 1H), 7.38-7.15 (m, 4H), 6.78 (d, J = 2.8 Hz, 1H), 6.56 (dd, J = 8.6 Hz, J = 2.4 Hz, 1H), 3.77 (s, 3H), 2.21 (s, 3H). ^{13}C NMR (DMSO-d_6, 75 MHz) δ 160.3, 155.8, 143.1, 141.8, 131.3, 129.7, 125.1, 120.9, 117.0, 106.1, 101.8, 55.5, 13.5. HR-MS $[M+H]^+$ m/z Calcd for $C_{15}H_{16}ClN_2O_2$: 291.0900. Found: 291.0906.



Synthesis of 3-methyl-1-phenyl-1*H*-indazole (4).[2] Compound **4** was synthesized according to the previous procedure.[2] (*E*)-1-(2-(Phenylamino)phenyl)ethanone oxime

(**3a**) (0.25 mmol, 57 mg) and 2-aminopyridine (0.50 mmol) were added to a round bottom flask equipped with 5 mL of CH_2Cl_2 and a magnetic stirrer. The solution was stirred at ambient temperature for 15 min, and then cooled to 0 ^oC. A solution of methanesulfonyl chloride (MsCl) (0.5 mmol) in CH_2Cl_2 (2 mL) was slowly added to the flask, and the solution was allowed to warm to ambient temperature over 6 h. The resulting solution was concentrated in vacuo, and the residue was purified by column chromatography on silica gel using hexane/ ethyl acetate (9:1) as eluent to provide the desired product (**4**). Yield 75% (39 mg). Yellow oil. ^1H NMR ($CDCl_3$, 600 MHz) δ 7.72-7.70 (m, 4H), 7.50 (t, *J* = 8.2 Hz, 2H), 7.40 (t, *J* = 7.6 Hz, 1H), 7.31 (t, *J* = 7.6 Hz, 1H), 7.20 (t, *J* = 8.2 Hz, 1H), 2.65 (s, 3H). ^{13}C NMR ($CDCl_3$, 150 MHz) δ 144.1, 140.4, 139.5, 129.5, 127.2, 126.2, 125.0, 122.5, 120.9, 120.7, 110.4, 12.0. ESI-MS $[M+H]^+$ m/z 209.2.



Synthesis of 2-methyl-1-phenyl-1*H*-benzo[*d*]imidazole (5).[2] Compound **5** was synthesized according to the previous procedure.[2] (*E*)-1-(2-(Phenylamino)phenyl)ethanone oxime (**3a**) (0.25 mmol, 57mg) and Et_3N (0.50 mmol) were added to a round bottom flask equipped with 5 mL of CH_2Cl_2 and a magnetic stirrer. The solution was stirred at ambient temperature for 15 min, and then cooled to 0 ^oC. A solution of MsCl (0.30 mmol) in CH_2Cl_2 (2 mL) was slowly added to the flask, and the solution was allowed to warm to ambient temperature over 6 h. The resulting solution was concentrated, and the residue was dissolved in EtOAc. The solution was washed twice with water, and the organic phase was dried over Na_2SO_4 and concentrated. The residue was purified by column chromatography on silica gel using hexane/ ethyl acetate (1:1) as eluent to provide the desired product (**5**). Yield 52% (27 mg). Yellow oil. ^1H NMR ($CDCl_3$, 600 MHz) δ 7.75 (d, *J* = 8.2 Hz, 1H), 7.59-7.52 (m, 3H), 7.37 (d, *J* = 8.2 Hz, 2H), 7.26 (t, *J* = 7.6 Hz, 1H), 7.19 (t, *J* = 7.6 Hz, 1H), 7.12 (t, *J* = 7.6 Hz, 1H), 2.51 (s, 3H). ^{13}C NMR ($CDCl_3$, 150 MHz) δ 151.6,

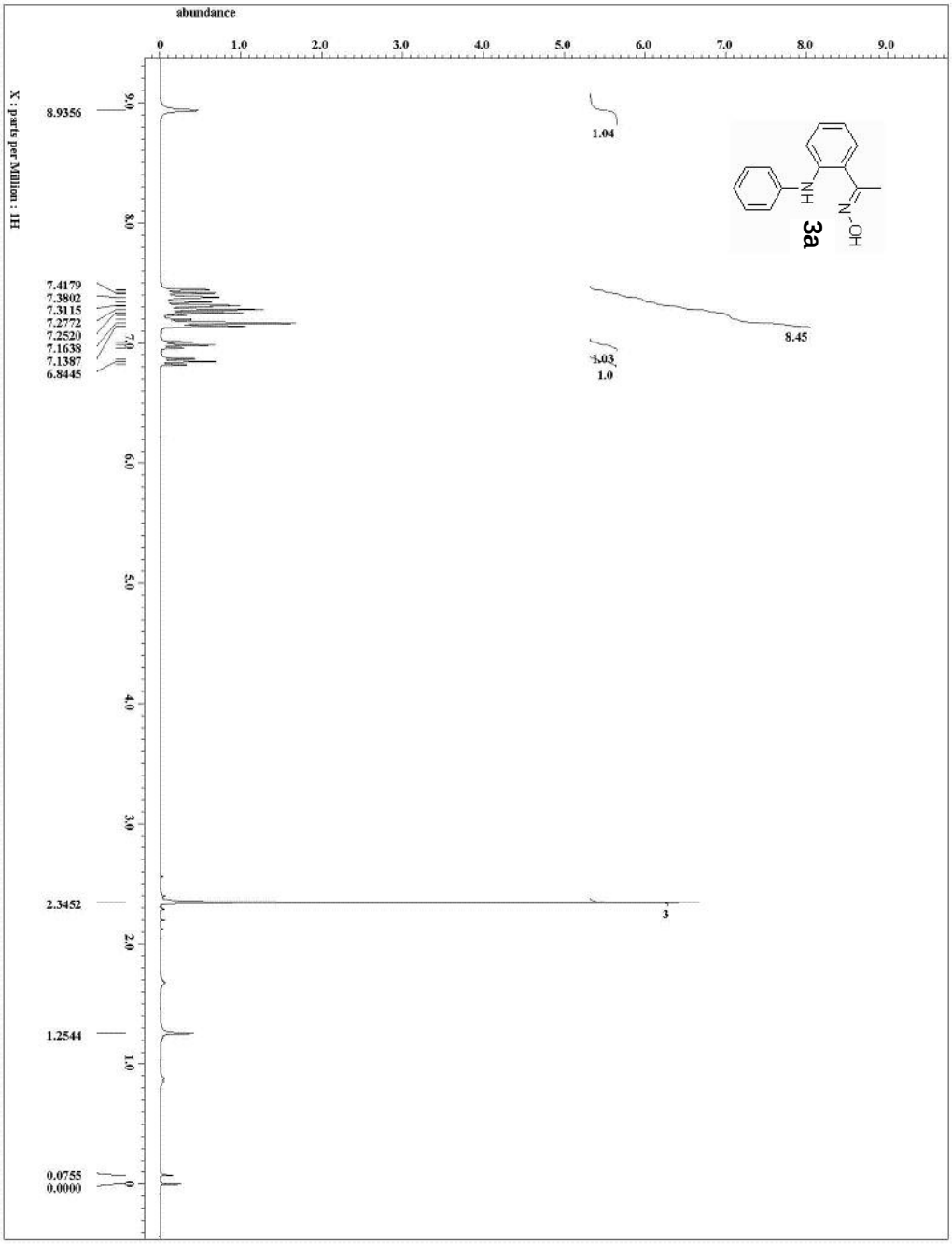
142.7, 136.5, 136.2, 130.0, 128.9, 127.2, 122.6, 122.5, 119.0, 110.0, 14.5. ESI-MS $[M+H]^+$ m/z 209.2.

References

1 Y.-J. Chen and C. Chen, *Tetrahedron: Asymmetry,* **2008**, *19*, 2201.

2 B. C. Wray and J. P. Stambuli, *Org. Lett.,* **2010**, *12*, 4576.

3 C. M. Counceller, C. C. Eichman, B. C. Wray and J. P. Stambuli, *Org. Lett.,* **2008**, *10*, 1021.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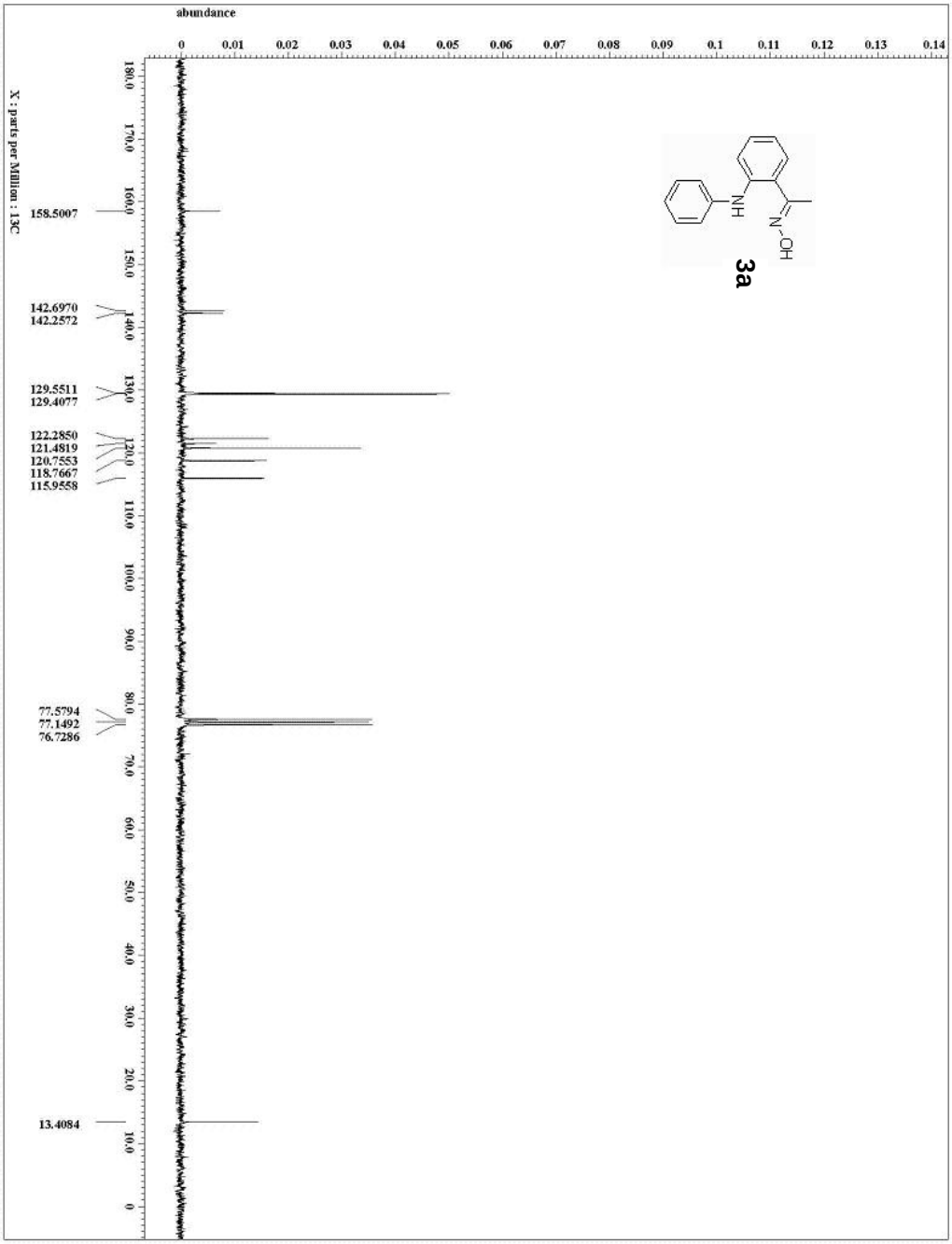
N
OH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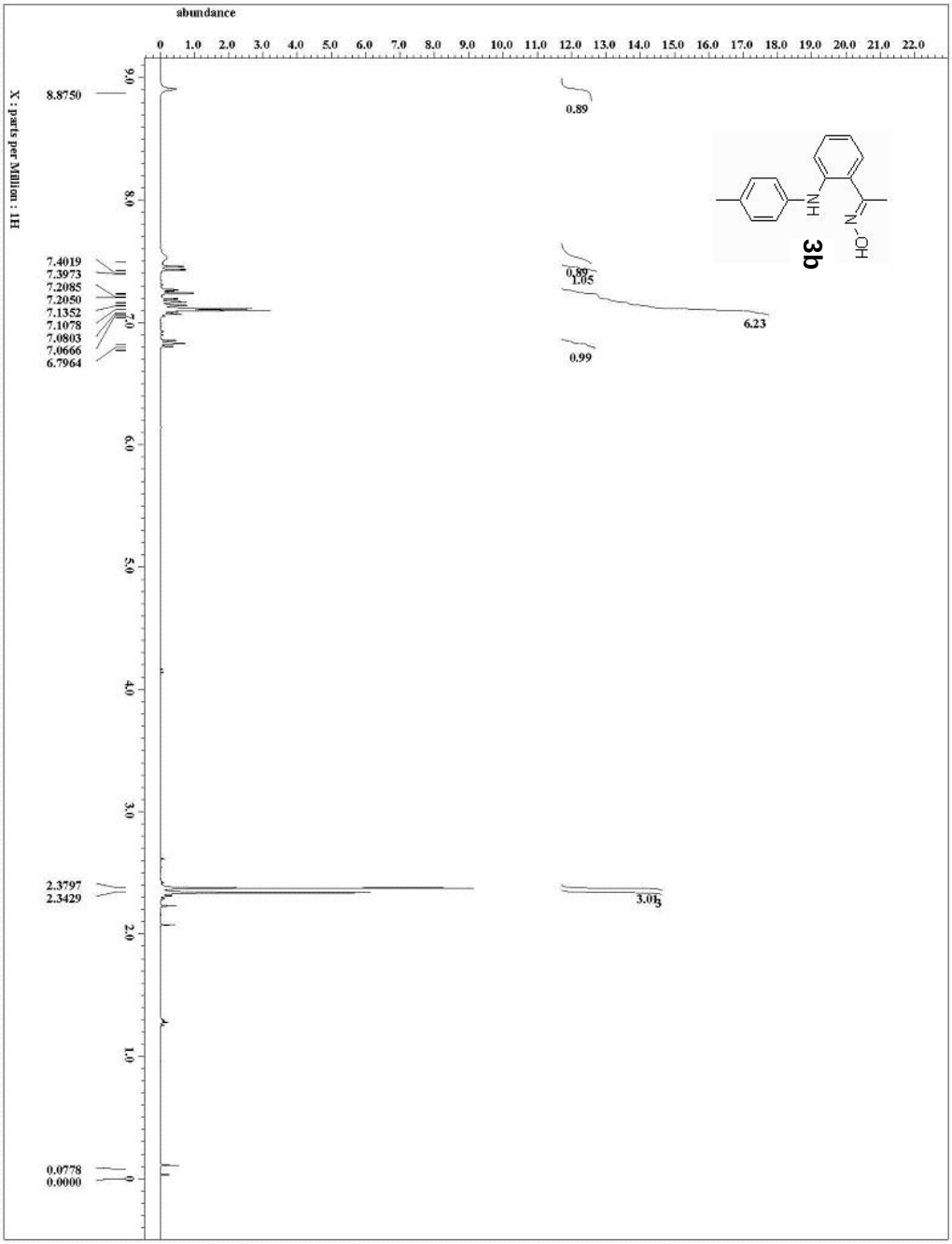
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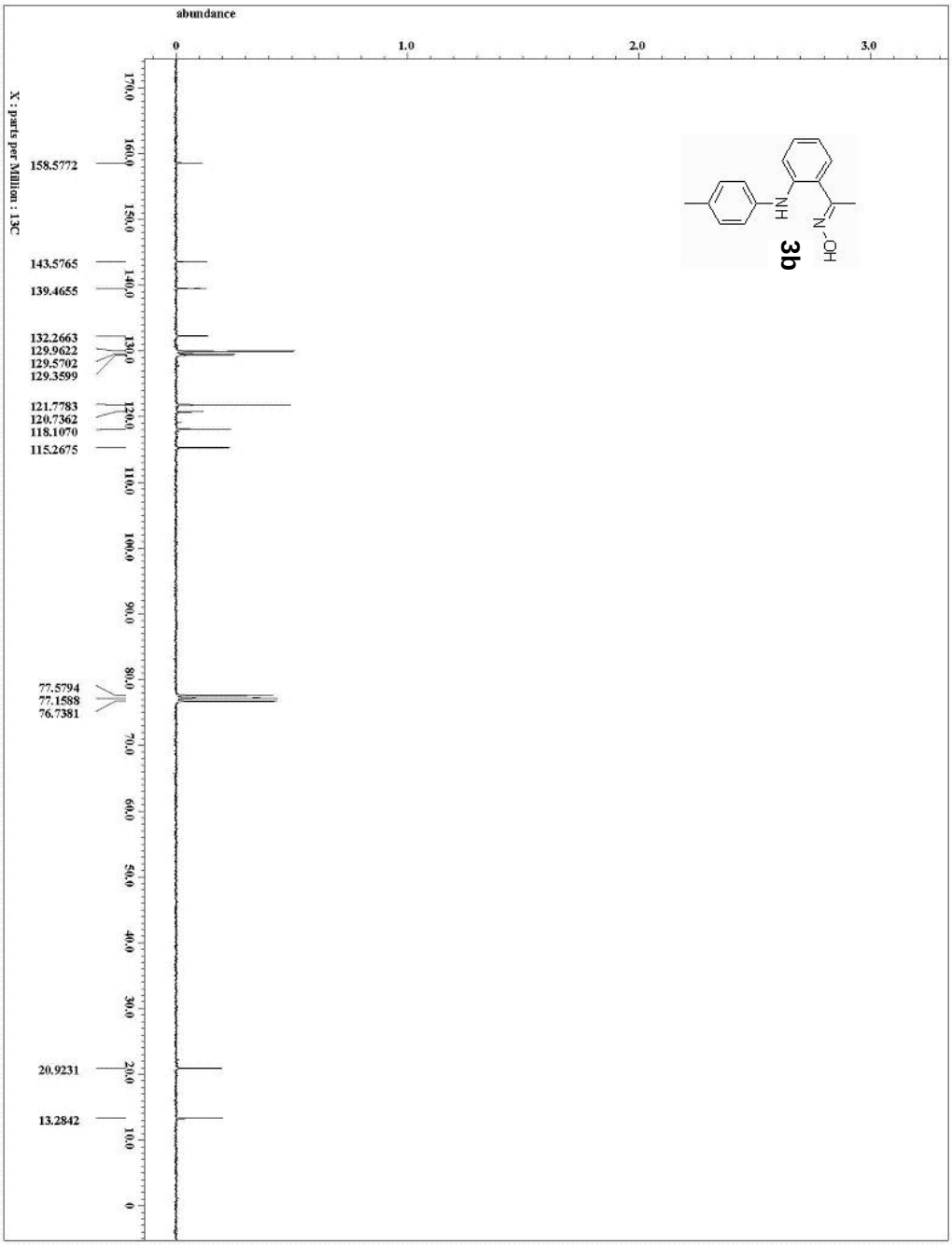
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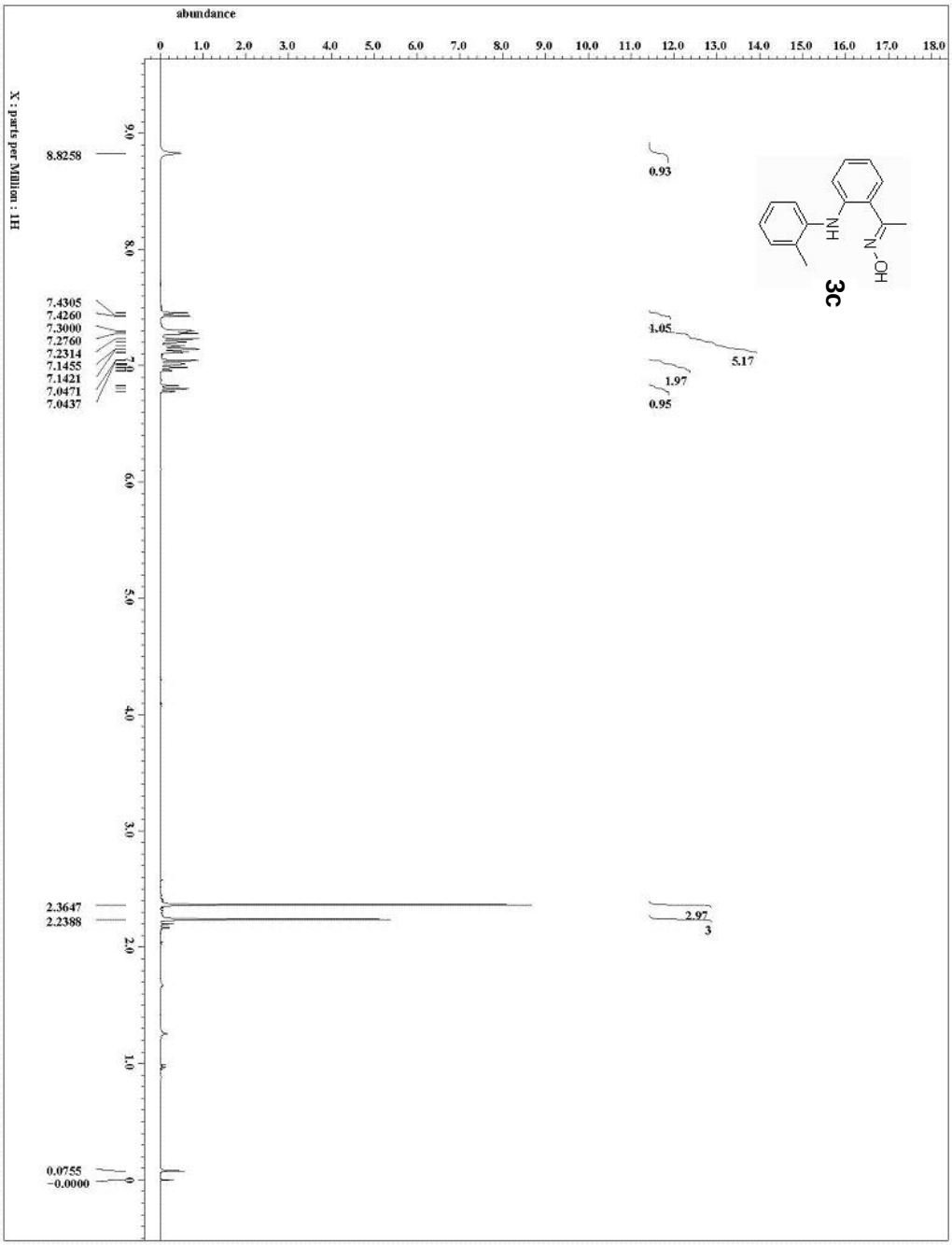
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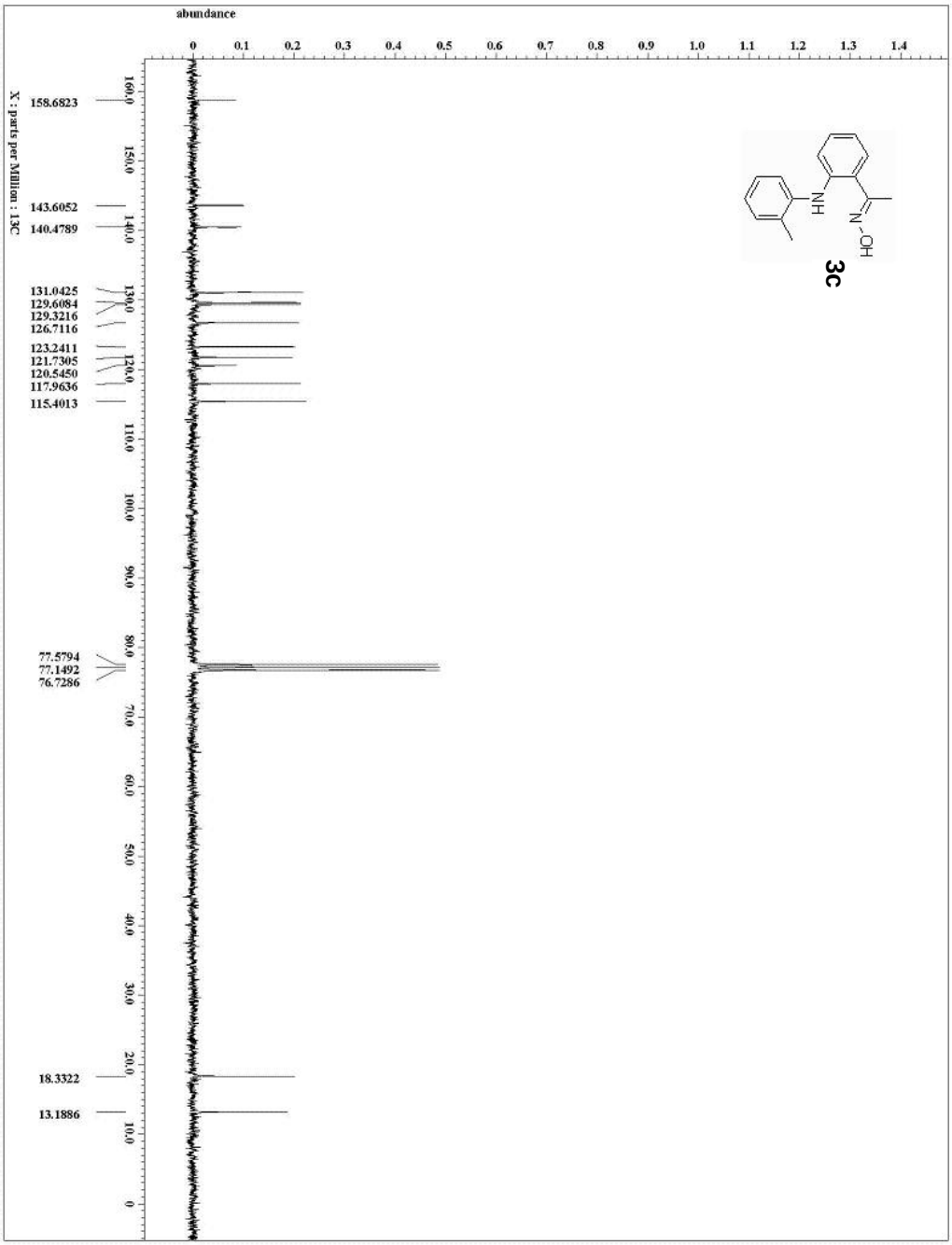
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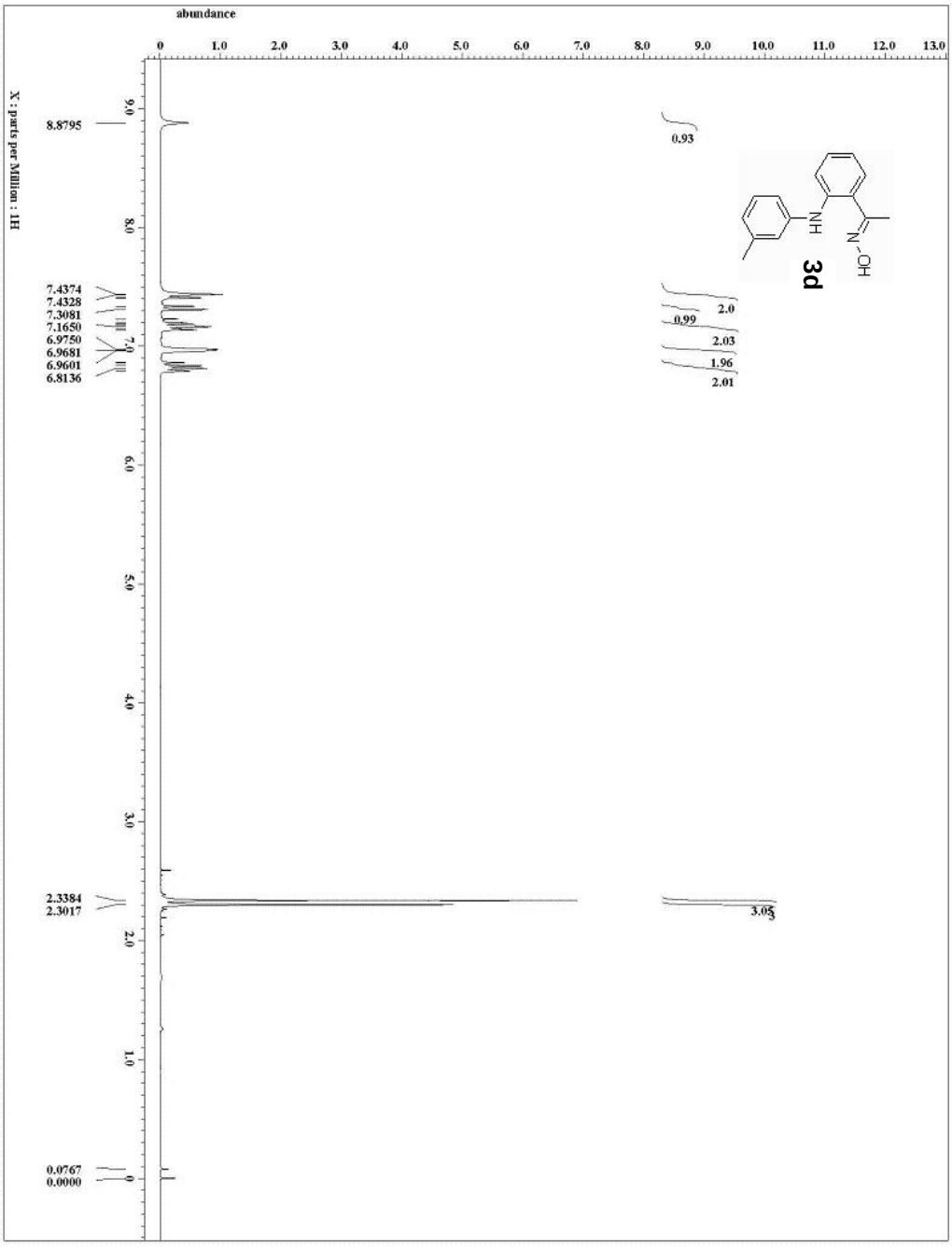
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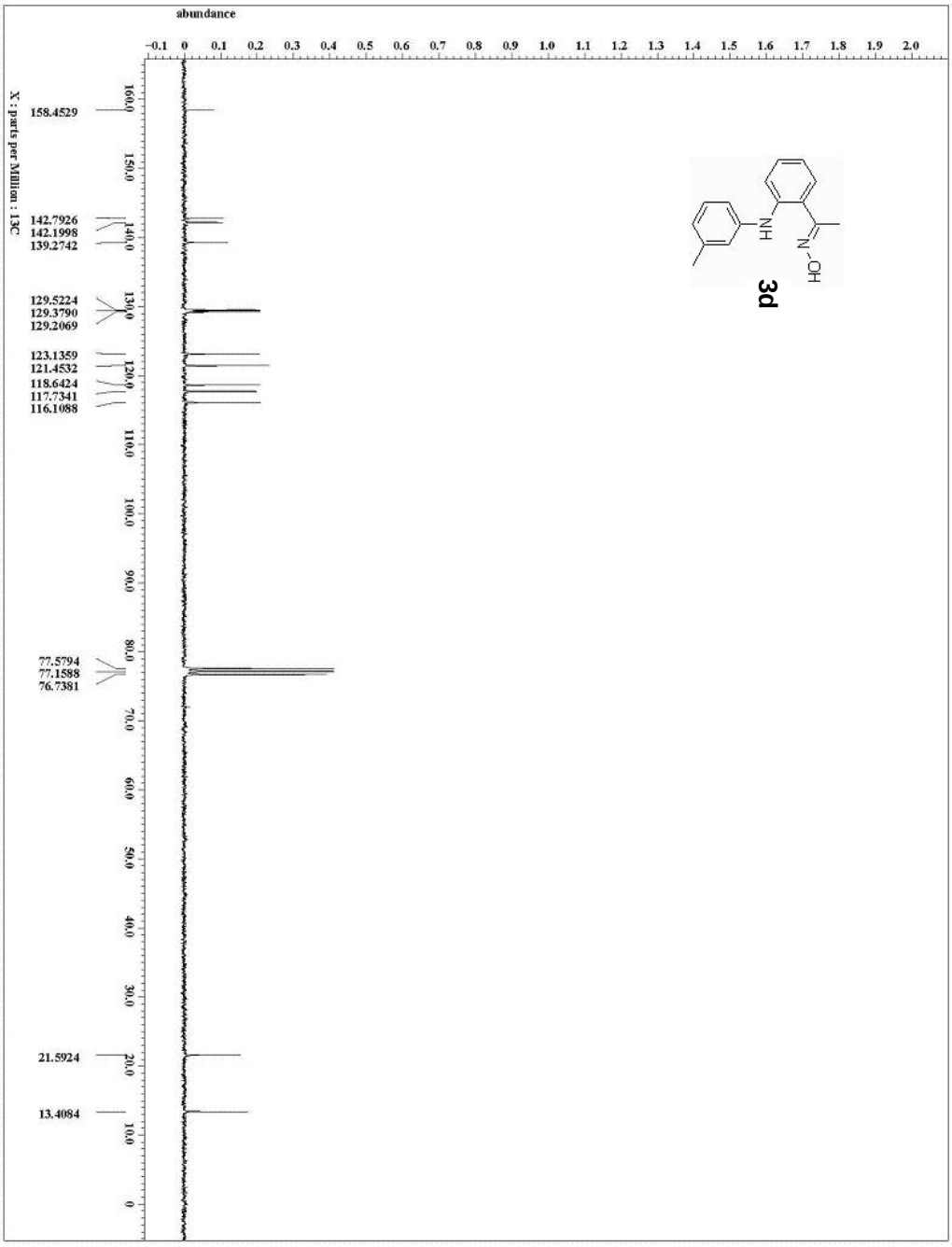
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NH
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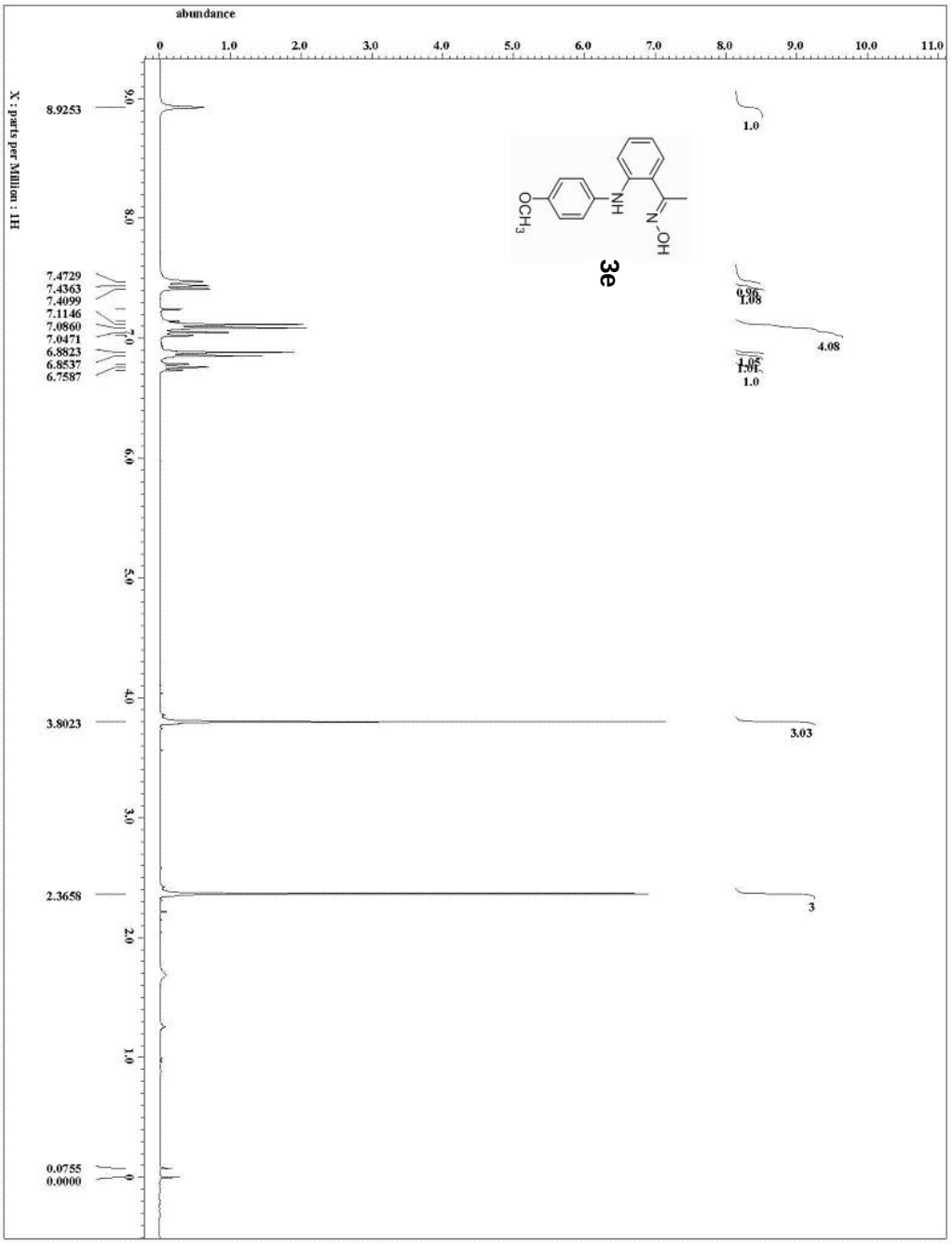
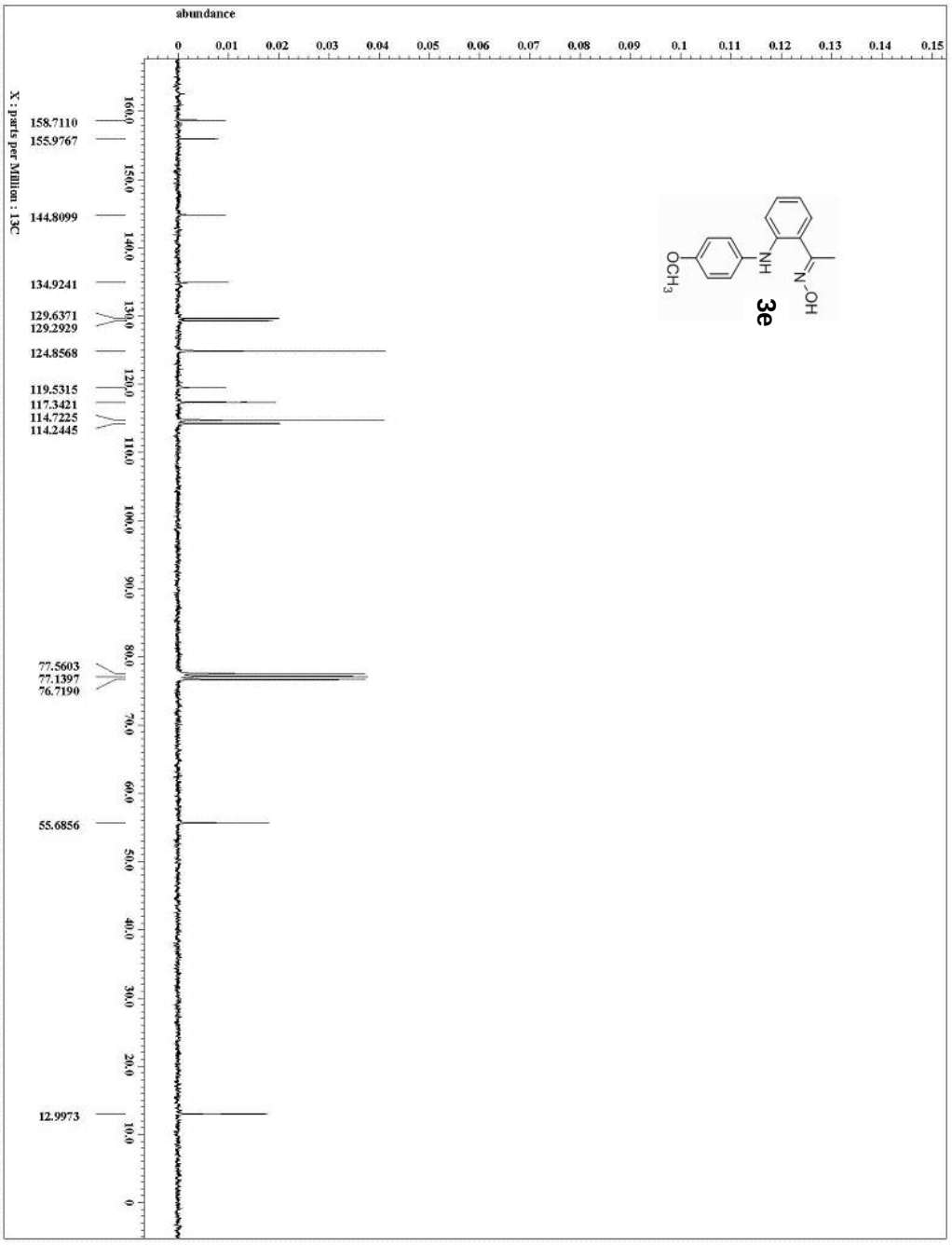
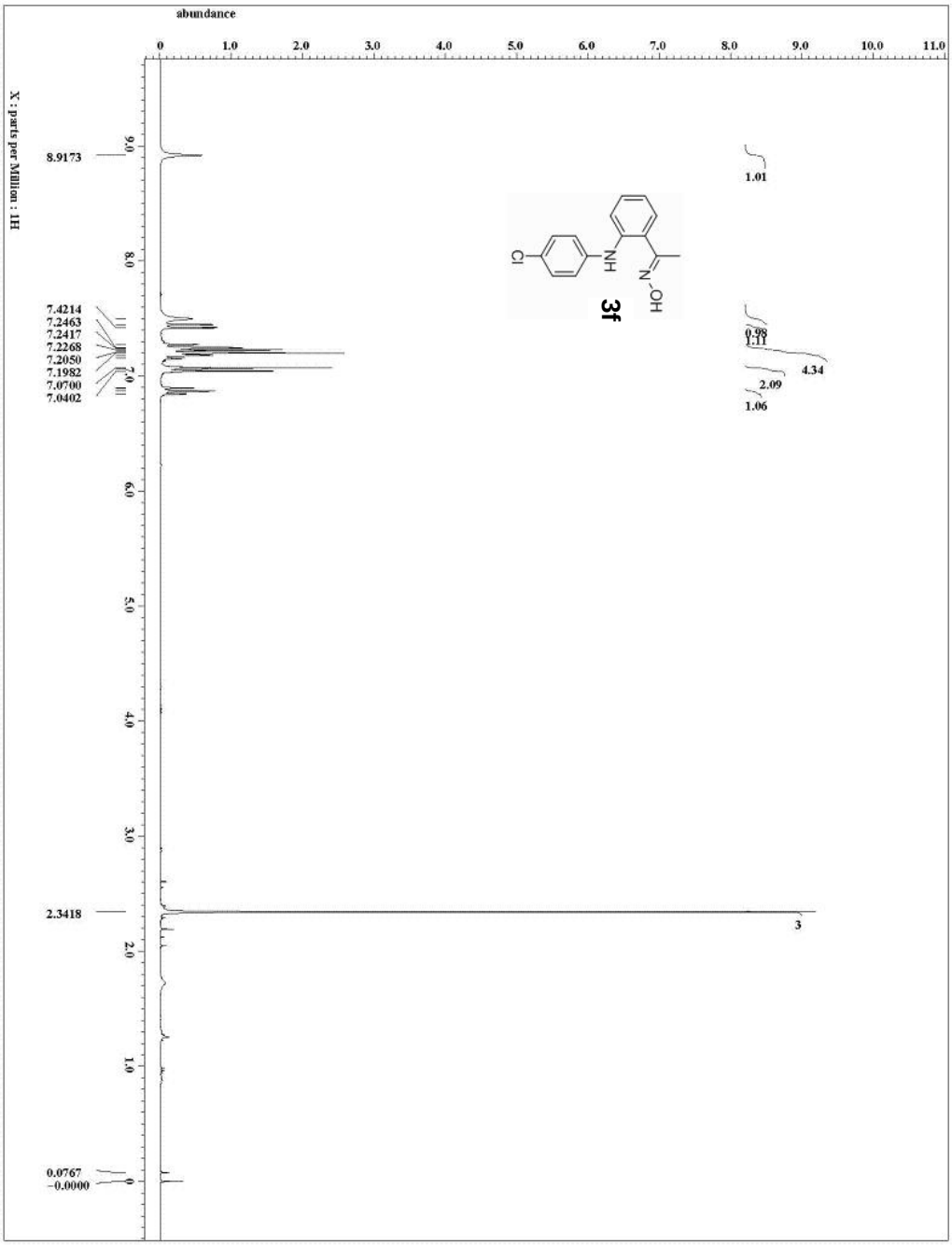
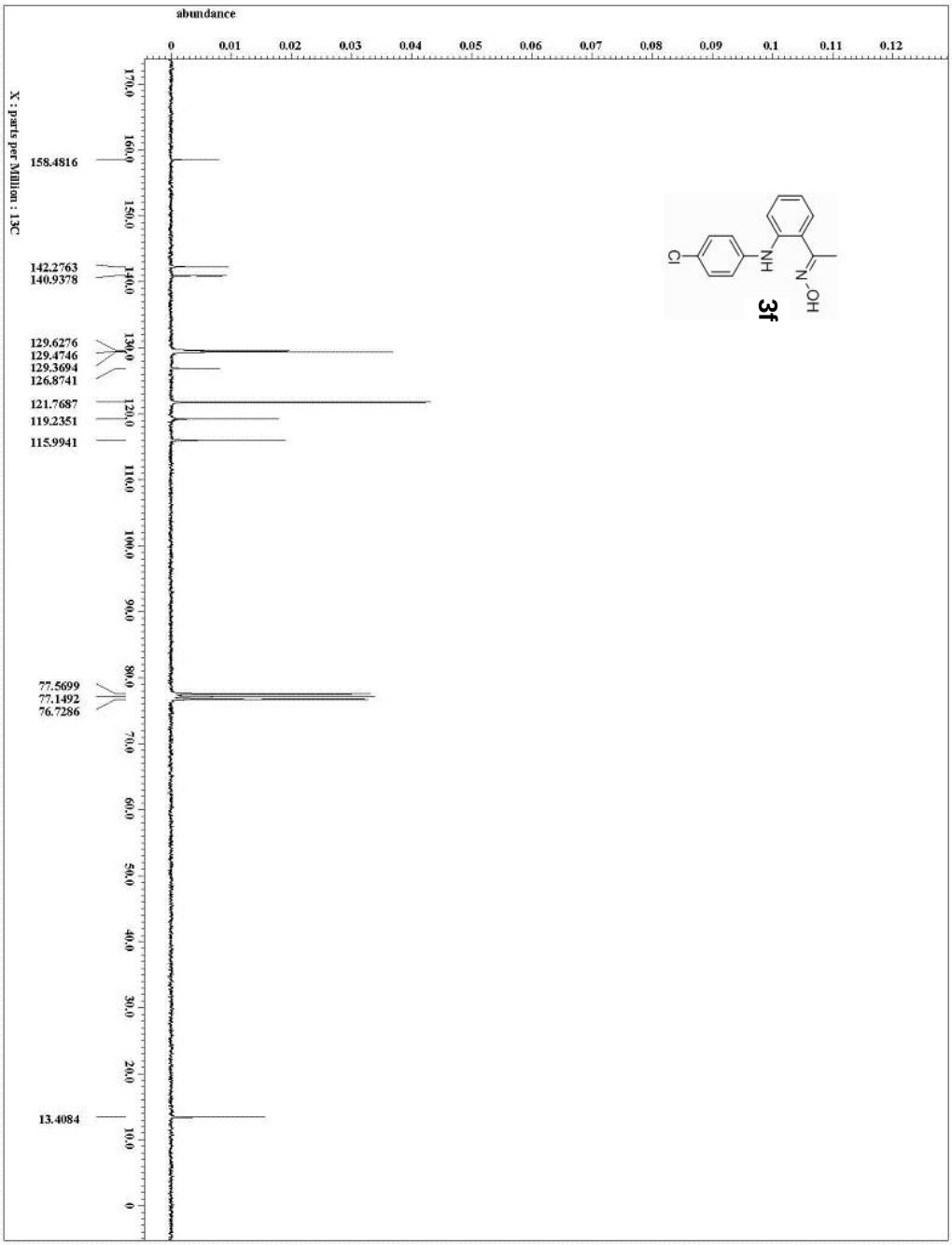
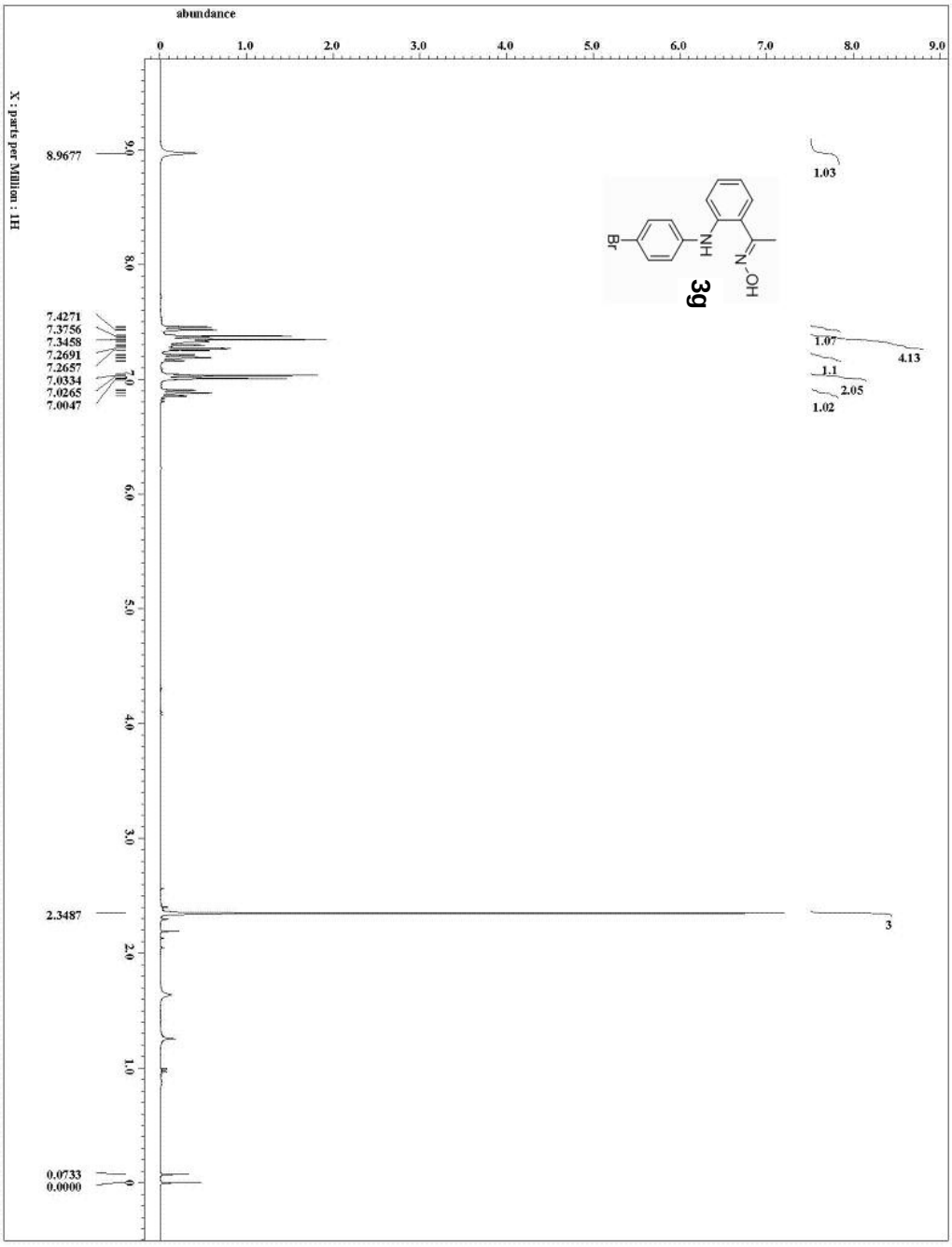
HO
3d

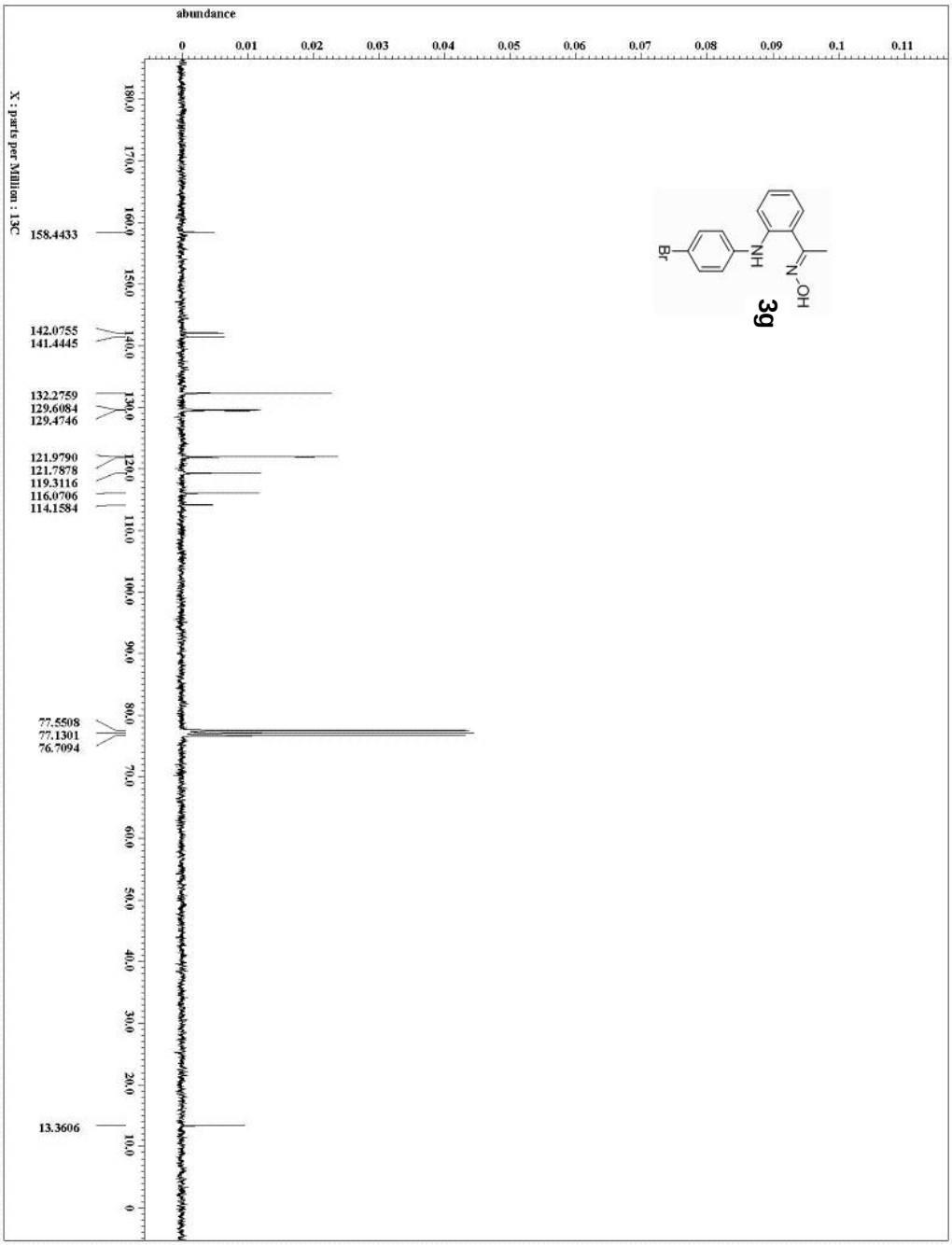

abundance
X : parts per Million : 1H
8.9253
7.4729
7.4363
7.4099
7.1146
7.0860
7.0471
6.8823
6.8537
6.7587
3.8023
2.3658
0.0755
0.0000
1.0
4.08
3.03
3
3e

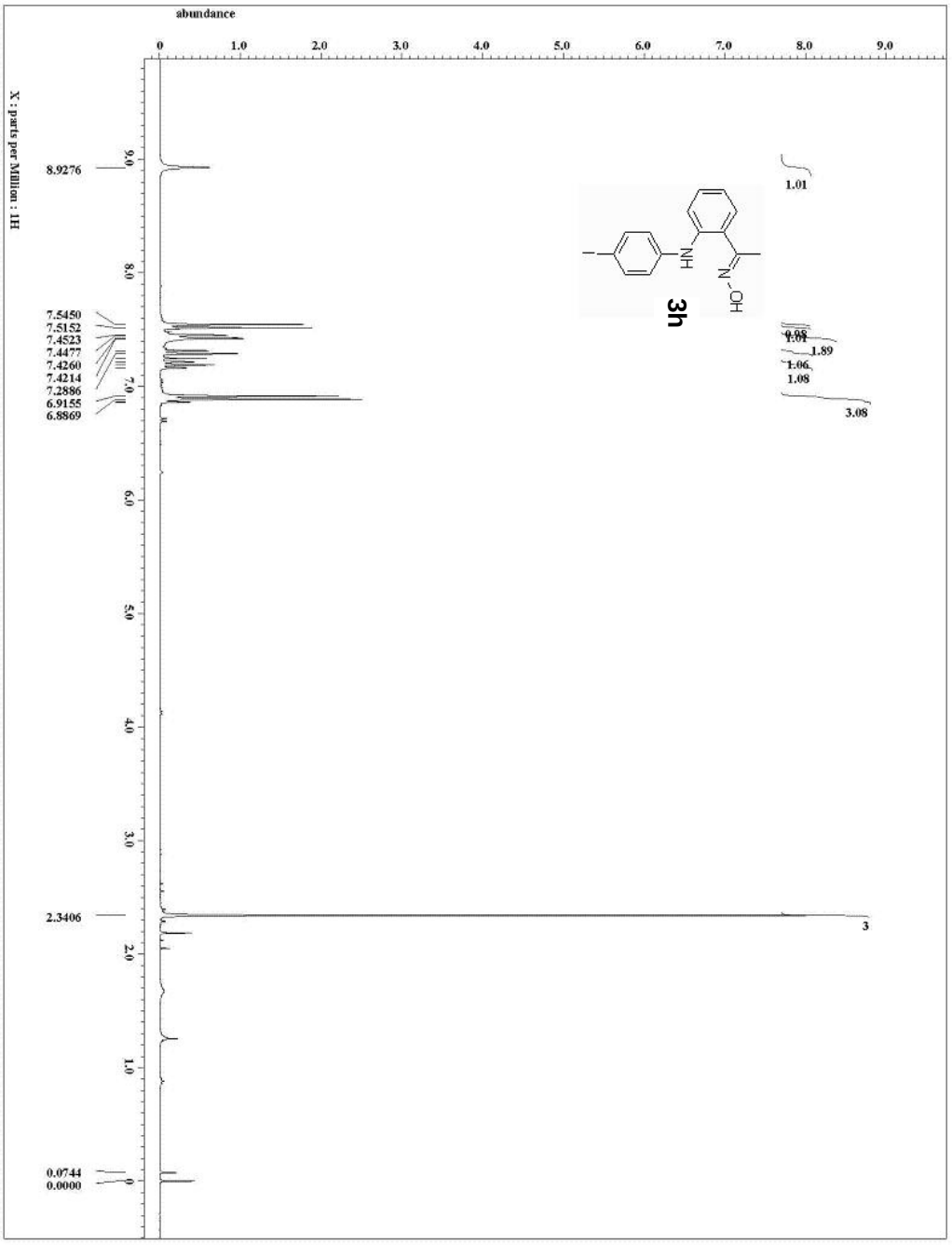

abundance
0
0.01
0.02
0.03
0.04
0.05
0.06
0.07
0.08
0.09
0.1
0.11
0.12
0.13
0.14
0.15
X : parts per Million : 13C
158.7110
155.9767
144.8099
134.9241
129.6371
129.2929
124.8568
119.5315
117.3421
114.7225
114.2445
77.5603
77.1397
76.7190
55.6856
12.9973
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
NH
N
OH
OCH3
3e

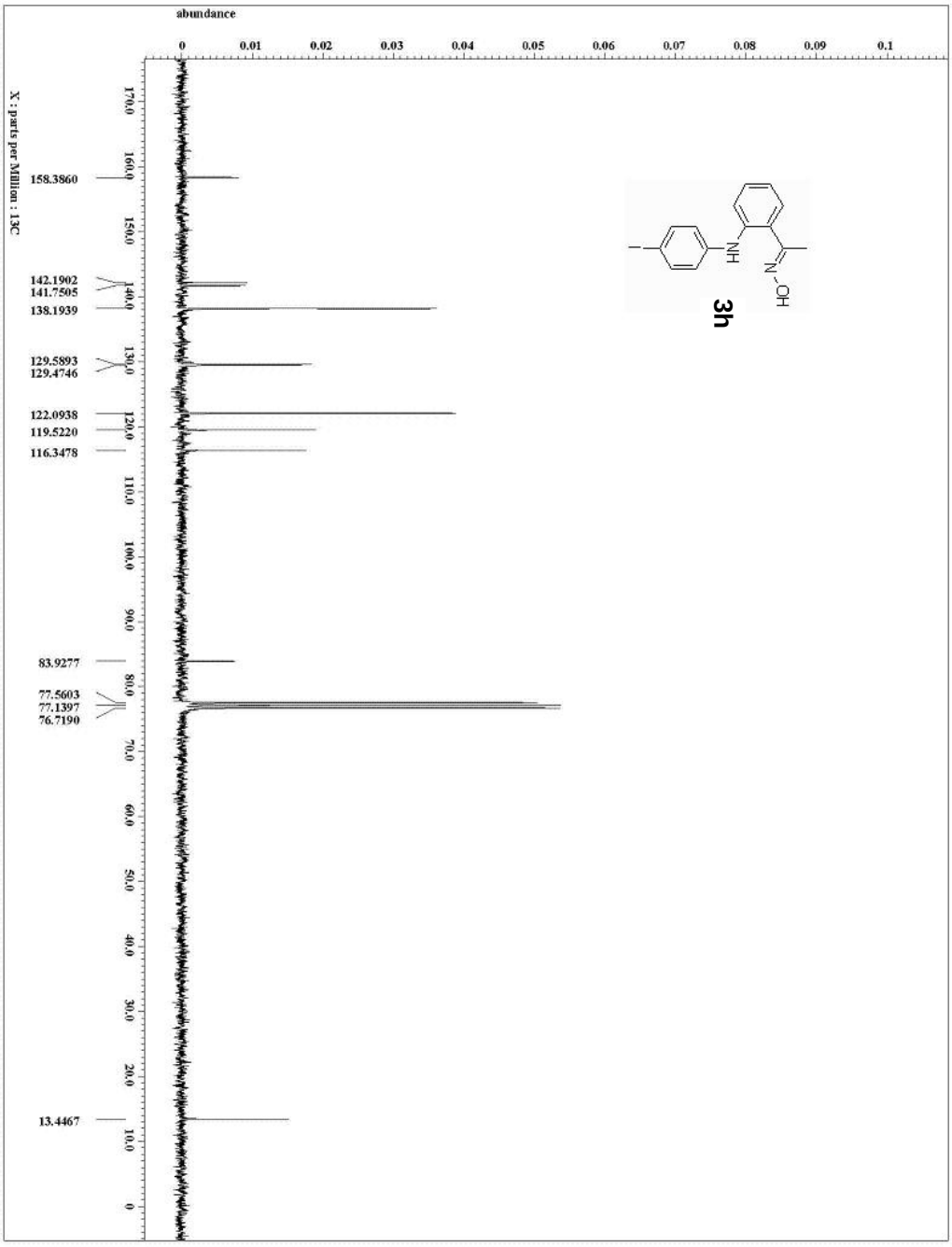

abundance
X : parts per Million : 1H
8.9173
7.4214
7.2463
7.2417
7.2268
7.2050
7.1982
7.0700
7.0402
2.3418
0.0767
-0.0000
1.01
0.99
1.11
4.34
2.09
1.06
3
Cl
NH
N
OH
3f

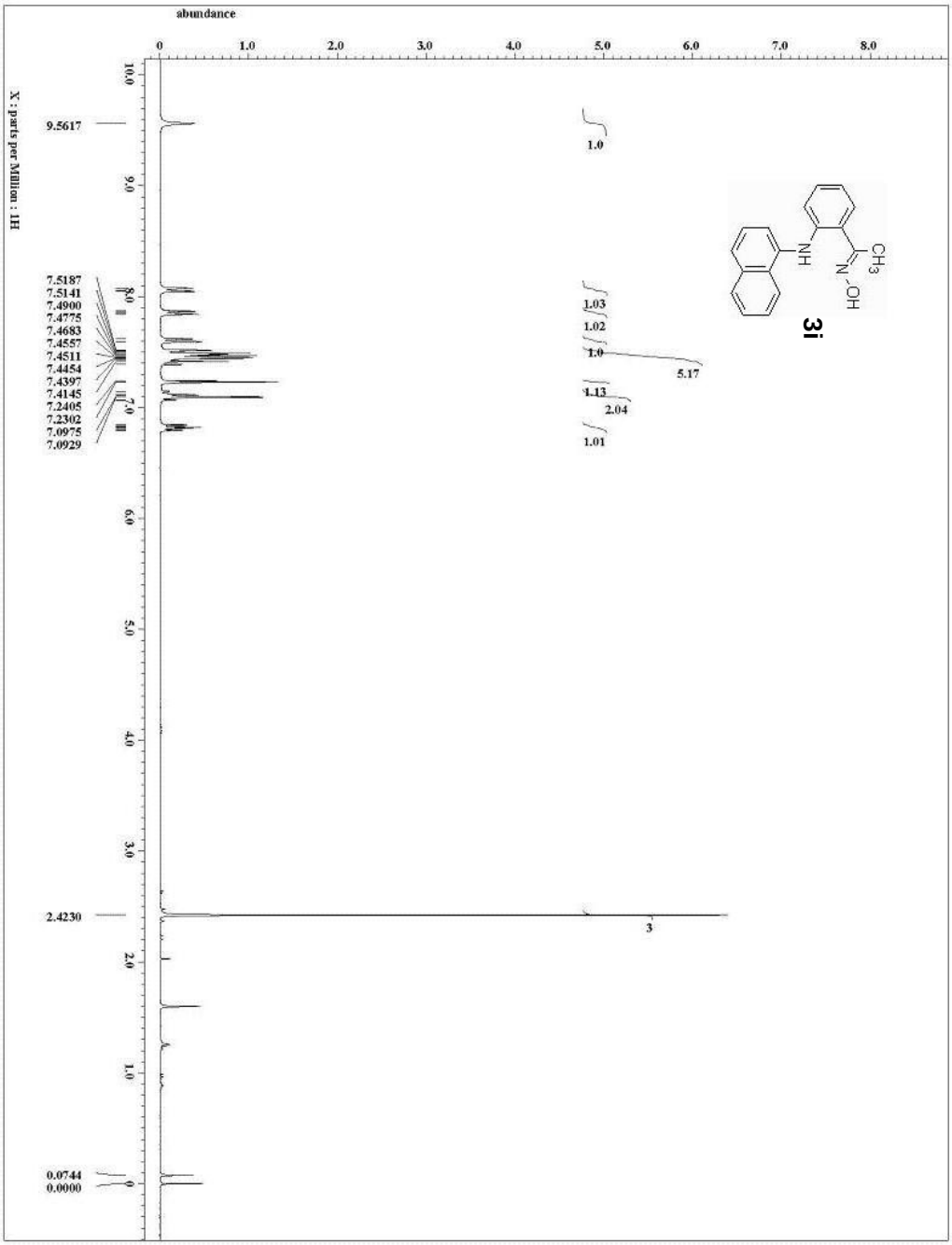

abundance
0
0.01
0.02
0.03
0.04
0.05
0.06
0.07
0.08
0.09
0.1
0.11
0.12
X : parts per Million : 13C
158.4816
142.2763
140.9378
129.6276
129.4746
129.3694
126.8741
121.7687
119.2351
115.9941
77.5699
77.1492
76.7286
13.4084
Cl
NH
N
OH
3f

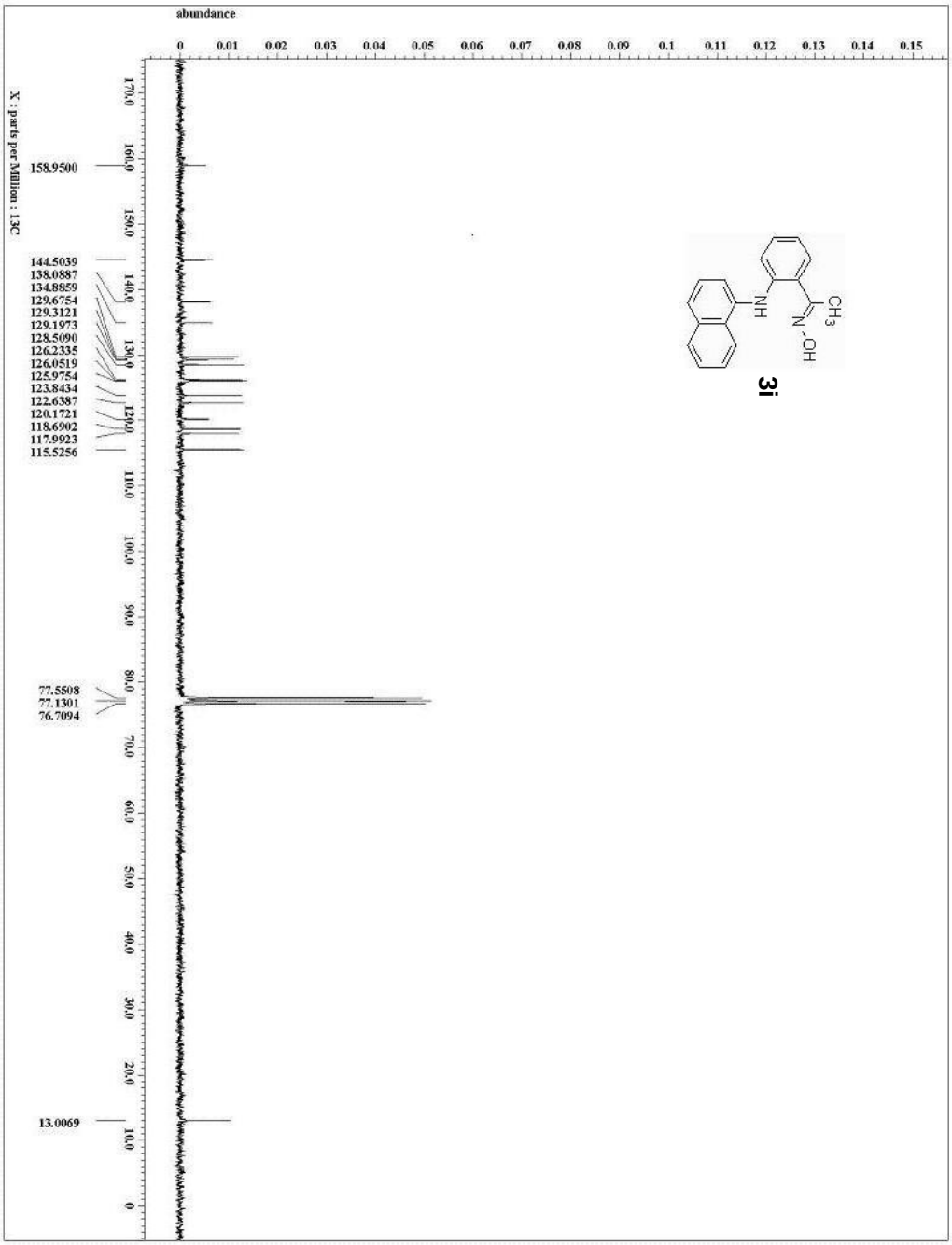

abundance
X : parts per Million : 1H
8.9677
7.4271
7.3756
7.3458
7.2691
7.2657
7.0334
7.0265
7.0047
2.3487
0.0733
0.0000
1.03
1.07
4.13
1.1
2.05
1.02
3
Br
NH
N
OH
3g


abundance
0
0.01
0.02
0.03
0.04
0.05
0.06
0.07
0.08
0.09
0.1
0.11
X : parts per Million : 13C
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
158.4433
142.0755
141.4445
132.2759
129.6084
129.4746
121.9790
121.7878
119.3116
116.0706
114.1584
77.5508
77.1301
76.7094
13.3606
Br
NH
N
OH
3g

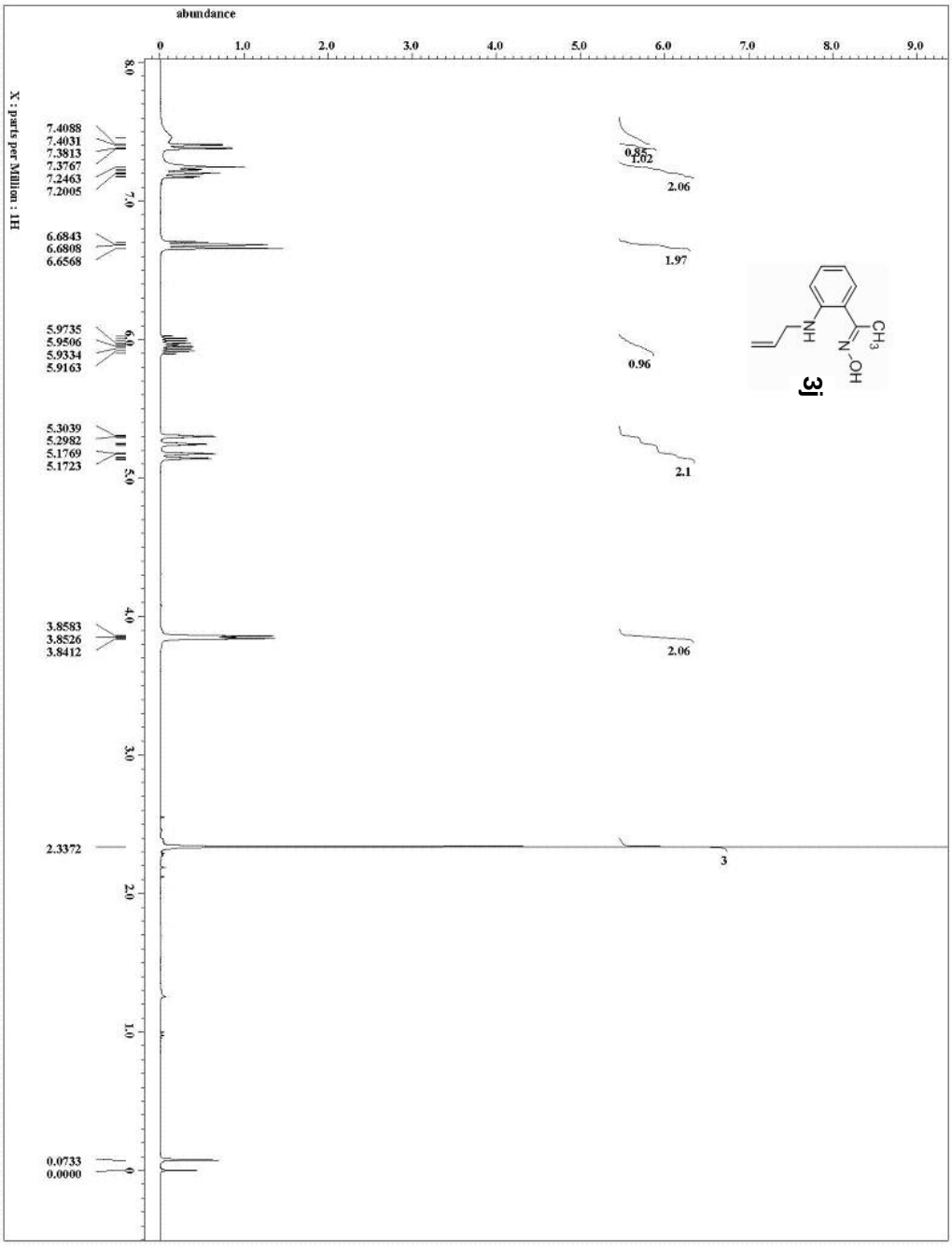

abundance
X : parts per Million : 1H
8.9276
7.5450
7.5152
7.4523
7.4477
7.4260
7.4214
7.2886
6.9155
6.8869
2.3406
0.0744
0.0000
1.01
1.89
1.06
1.08
3.08
3
3h


abundance
0
0.01
0.02
0.03
0.04
0.05
0.06
0.07
0.08
0.09
0.1
X : parts per Million : 13C
158.3860
142.1902
141.7505
138.1939
129.5893
129.4746
122.0938
119.5220
116.3478
83.9277
77.5603
77.1397
76.7190
13.4467
NH
N
OH
3h

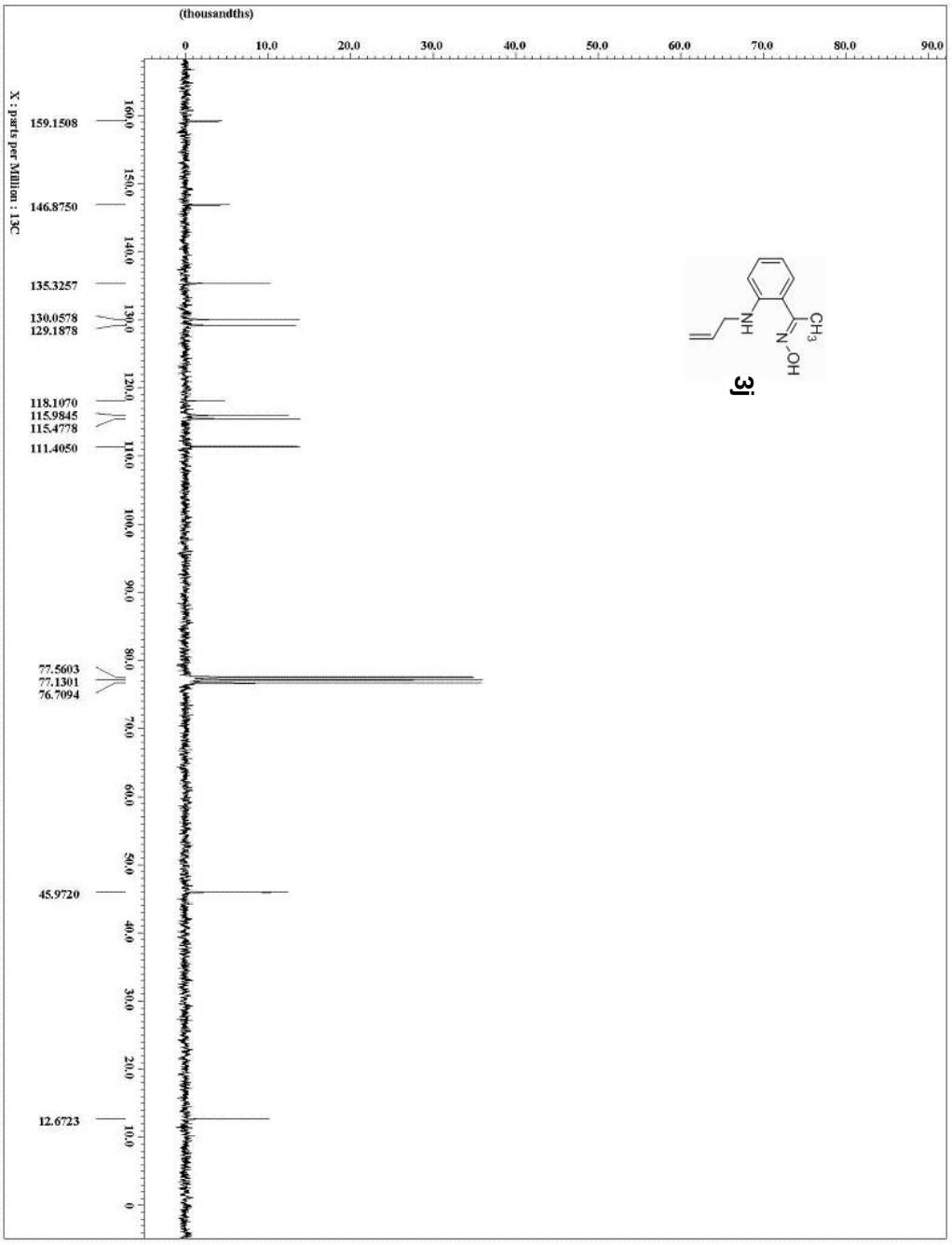

abundance
X : parts per Million : 1H
9.5617
7.5187
7.5141
7.4900
7.4775
7.4683
7.4557
7.4511
7.4454
7.4397
7.4145
7.2405
7.2302
7.0975
7.0929
2.4230
0.0744
0.0000
1.0
1.03
1.02
1.0
5.17
1.13
2.04
1.01
3
HN
N
OH
CH3
3i


abundance
0 0.01 0.02 0.03 0.04 0.05 0.06 0.07 0.08 0.09 0.1 0.11 0.12 0.13 0.14 0.15
X : parts per Million : 13C
170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0
158.9500
144.5039
138.0887
134.8859
129.6754
129.3121
129.1973
128.5090
126.2335
126.0519
125.9754
123.8434
122.6387
120.1721
118.6902
117.9923
115.5256
77.5508
77.1301
76.7094
13.0069
NH
N
OH
CH3

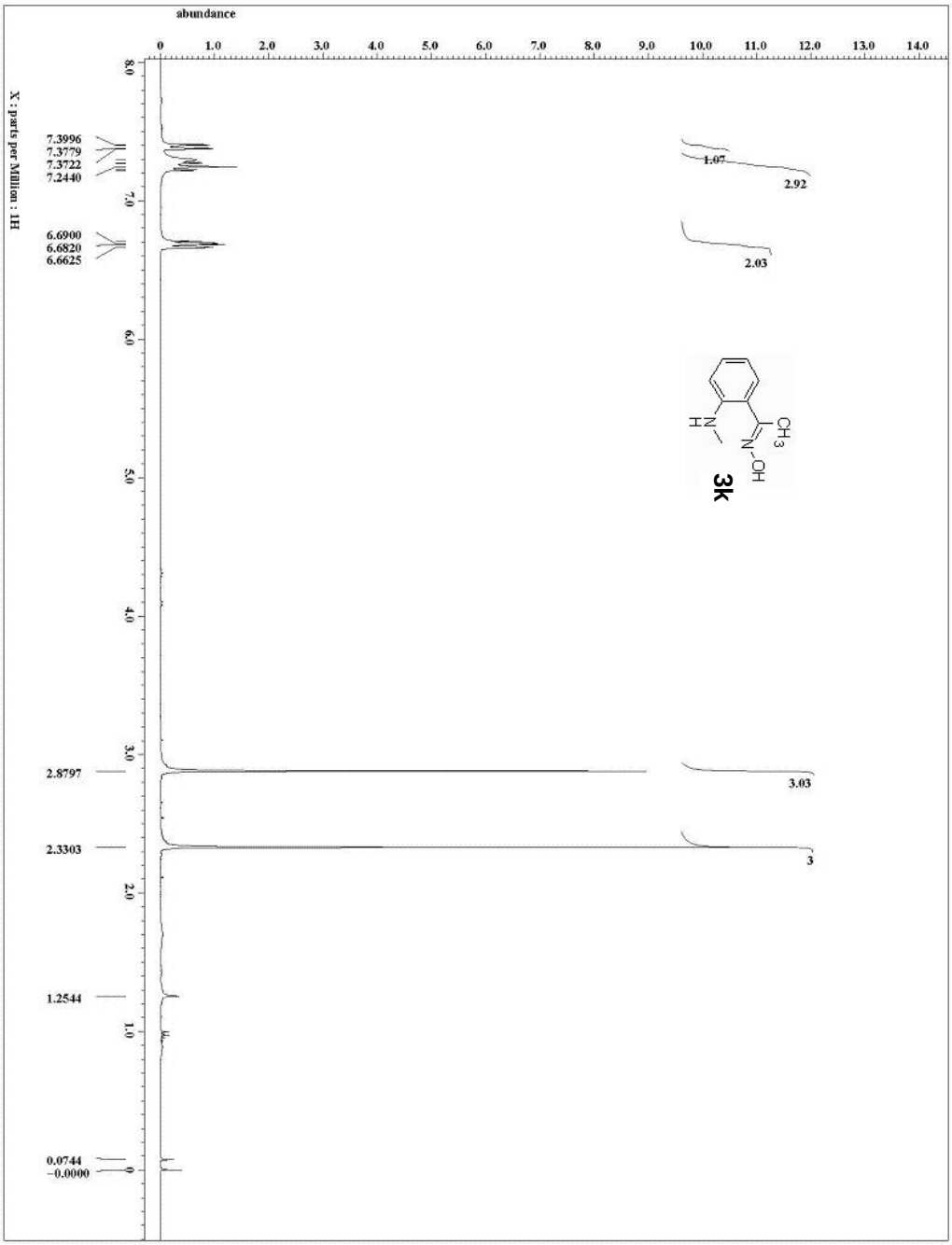
3i

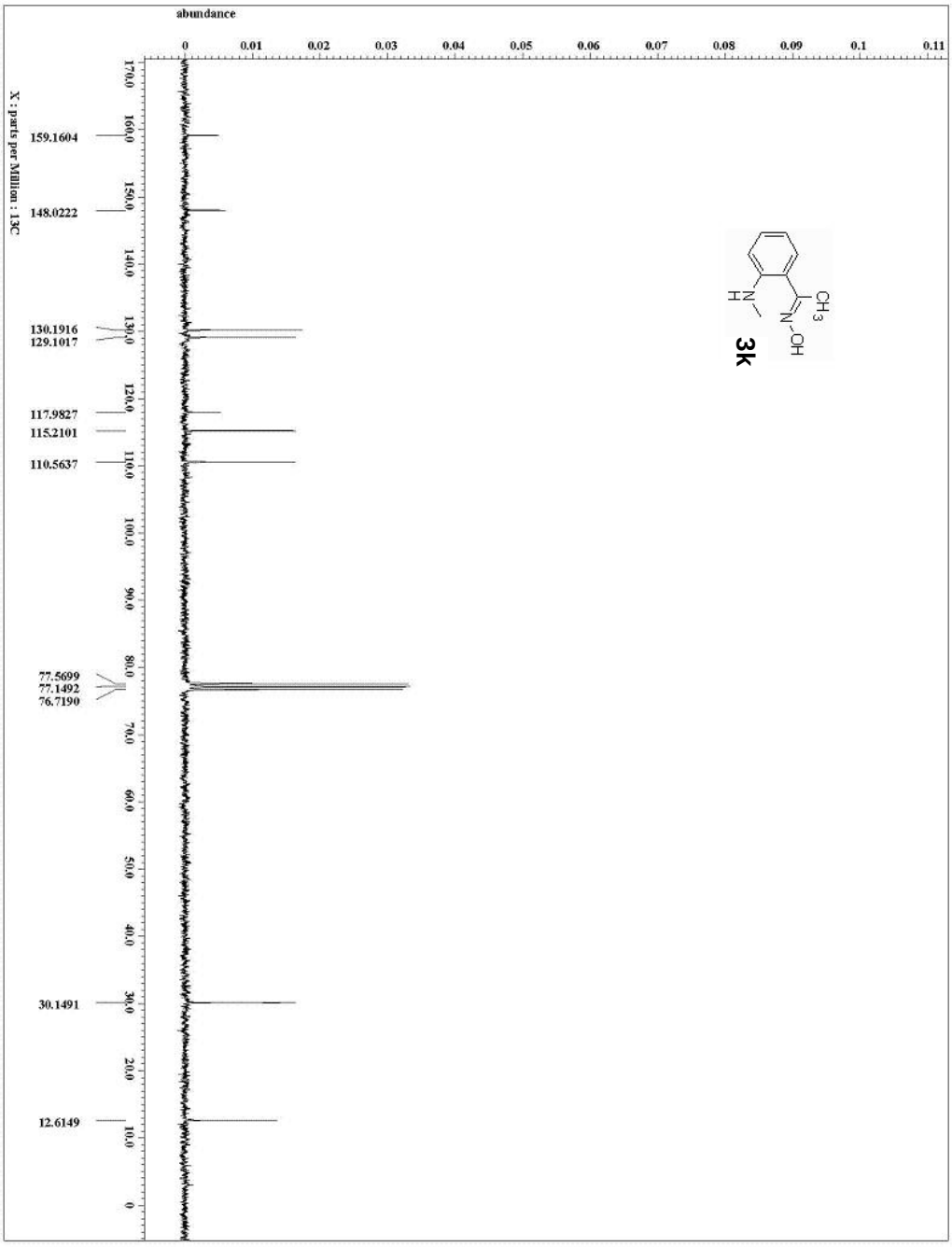

abundance
X : parts per Million : 1H
7.4088
7.4031
7.3813
7.3767
7.2463
7.2005
6.6843
6.6808
6.6568
5.9735
5.9506
5.9334
5.9163
5.3039
5.2982
5.1769
5.1723
3.8583
3.8526
3.8412
2.3372
0.0733
0.0000
0.85
1.02
2.06
1.97
0.96
2.1
2.06
3
NH
N
OH
CH3

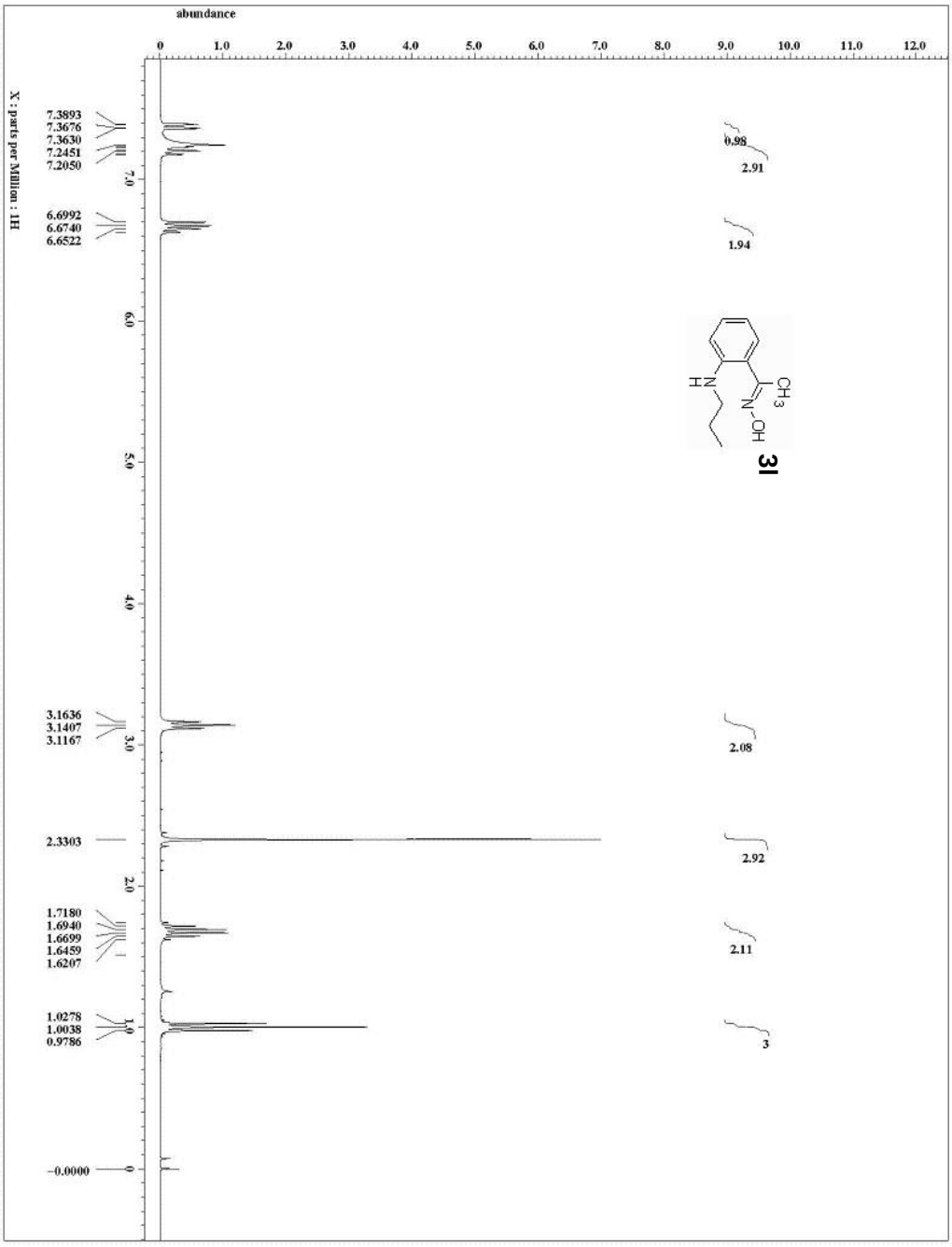
3

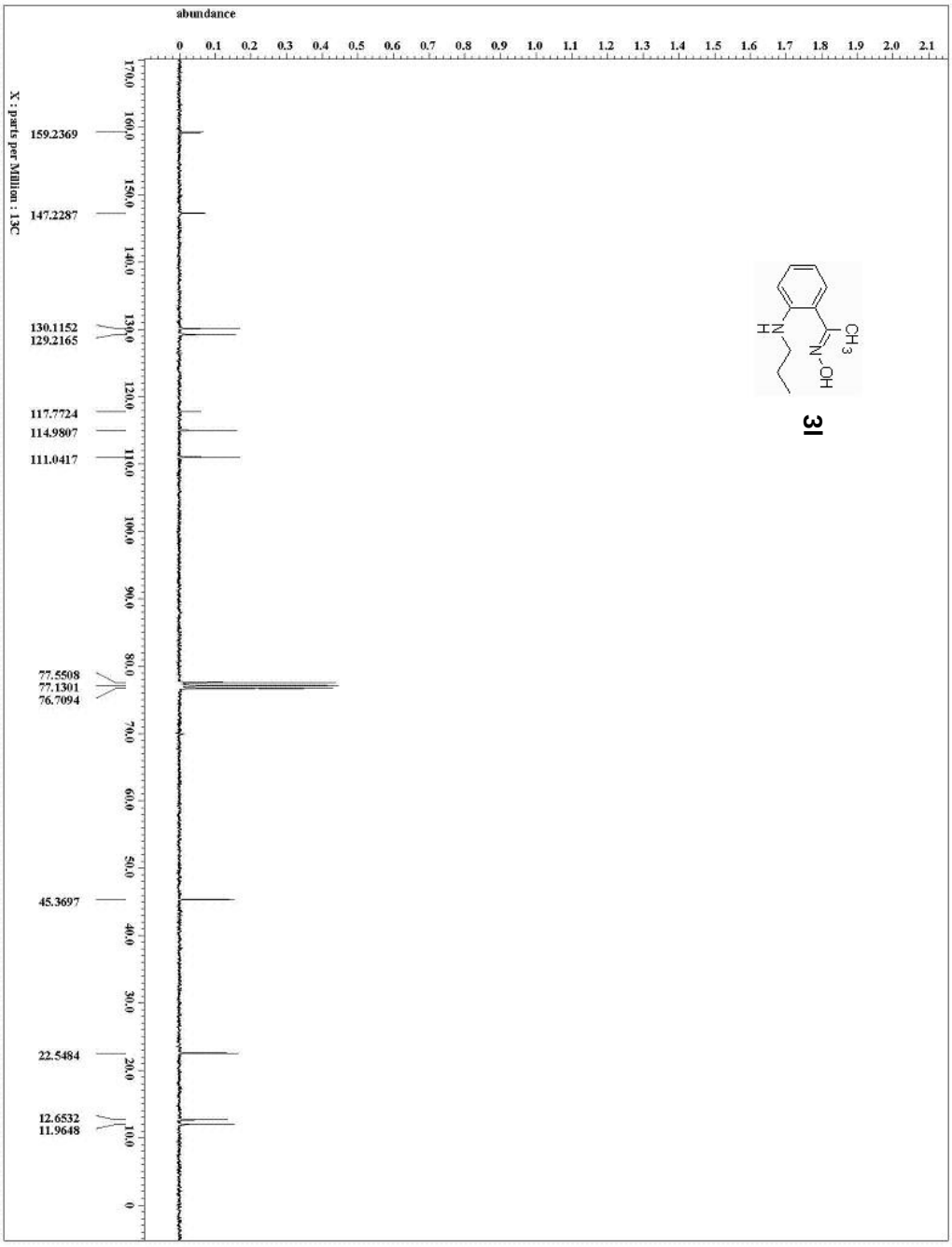

(thousandths)
0
10.0
20.0
30.0
40.0
50.0
60.0
70.0
80.0
90.0
X : parts per Million : 13C
159.1508
146.8750
135.3257
130.0578
129.1878
118.1070
115.9845
115.4778
111.4050
77.5603
77.1301
76.7094
45.9720
12.6723
NH
N
OH
CH3

3

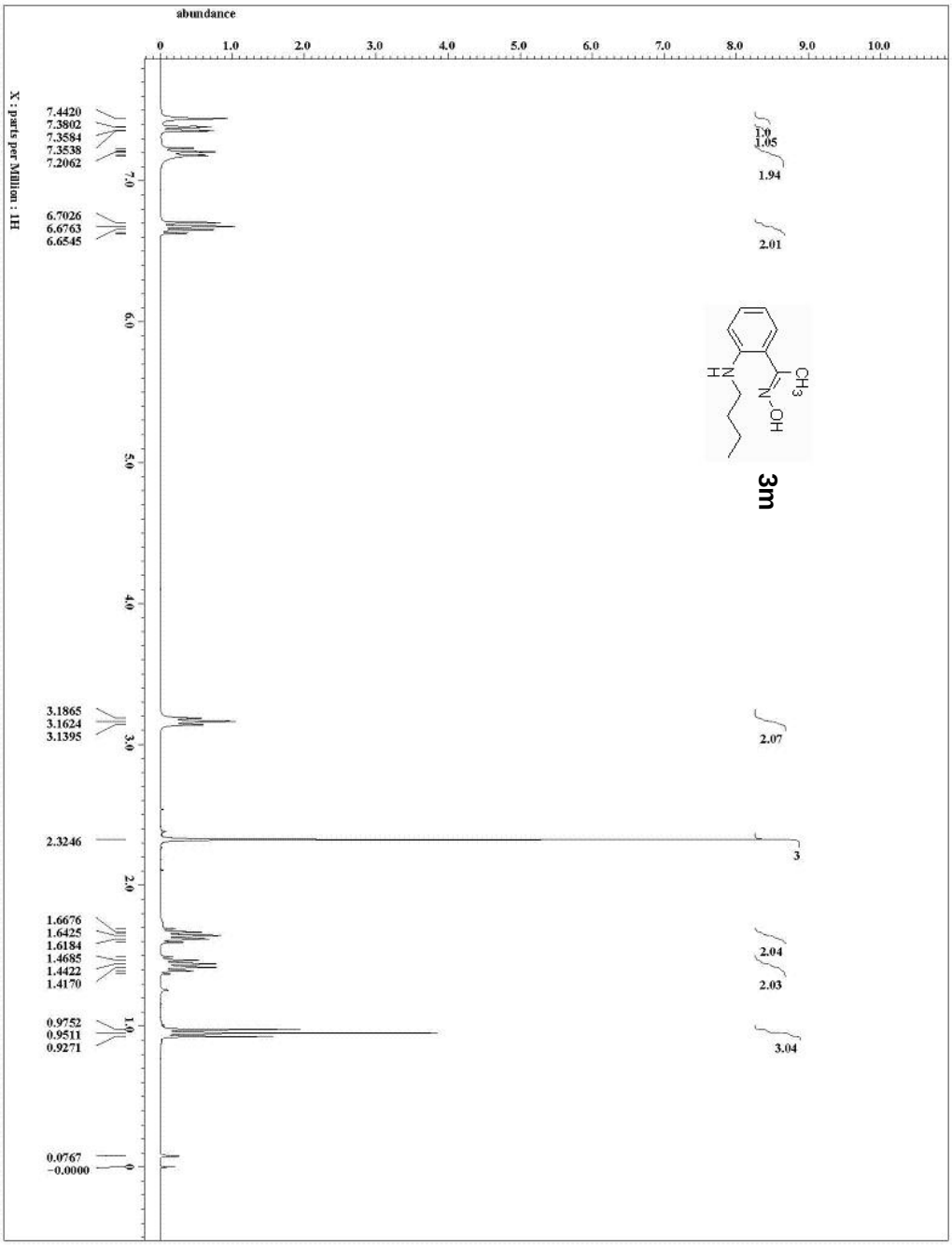

abundance
X : parts per Million : 1H
7.3996
7.3779
7.3722
7.2440
6.6900
6.6820
6.6625
2.8797
2.3303
1.2544
0.0744
−0.0000
1.07
2.92
2.03
3.03
3
3k

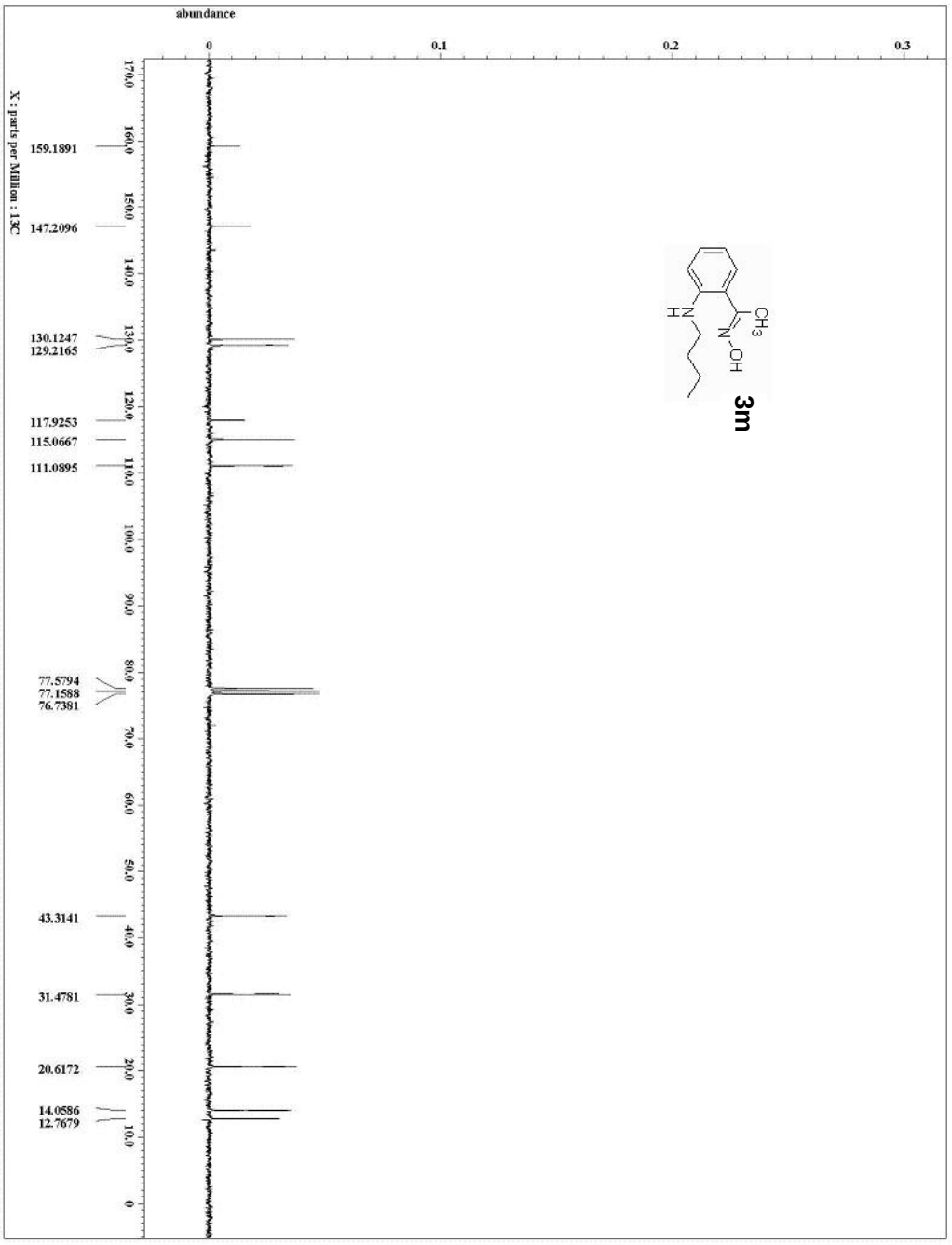

abundance
0
0.01
0.02
0.03
0.04
0.05
0.06
0.07
0.08
0.09
0.1
0.11
X : parts per Million : 13C
159.1604
148.0222
130.1916
129.1017
117.9827
115.2101
110.5637
77.5699
77.1492
76.7190
30.1491
12.6149
CH3
N
H
N
OH
3k

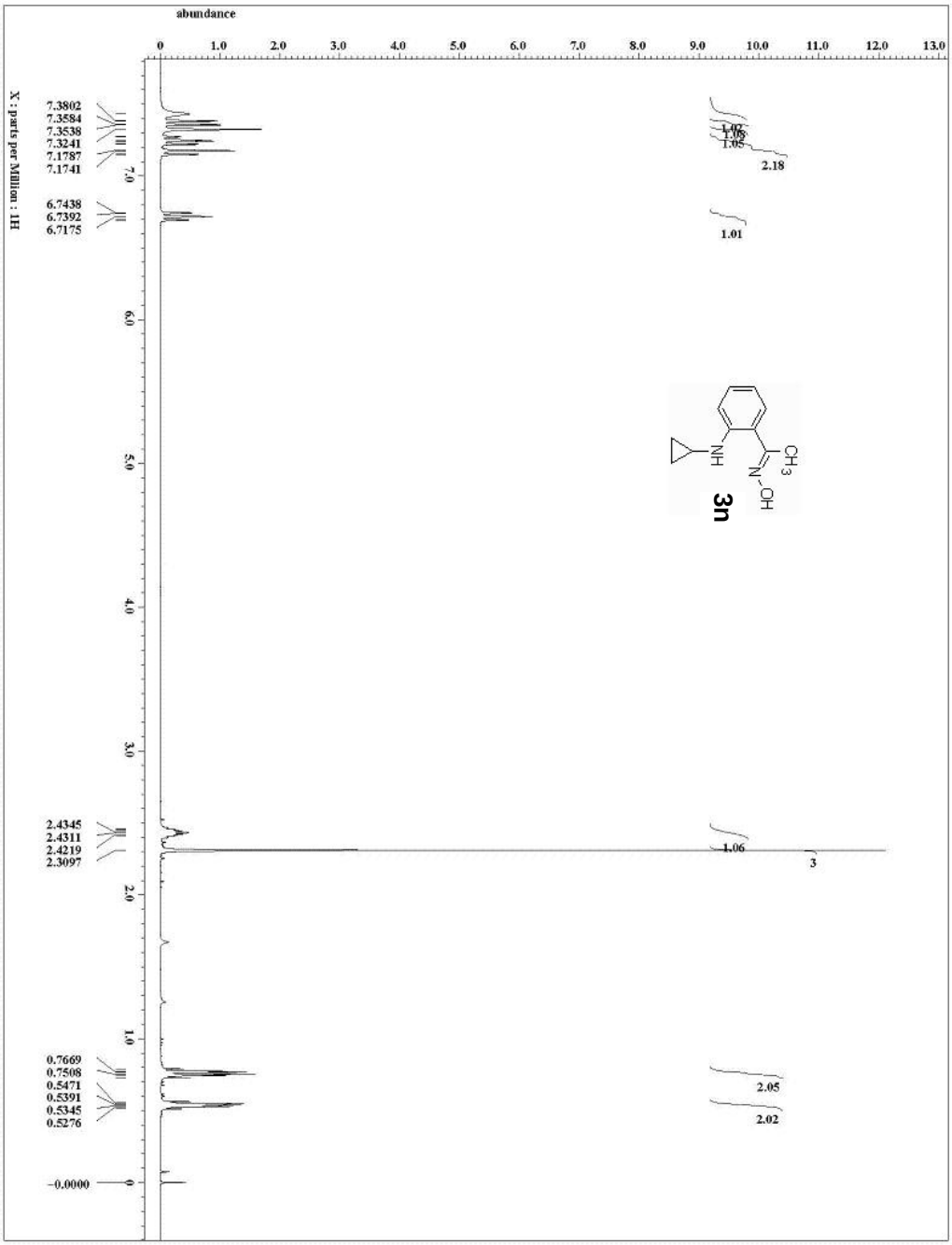

abundance
0
1.0
2.0
3.0
4.0
5.0
6.0
7.0
8.0
9.0
10.0
11.0
12.0
X : parts per Million : 1H
7.3893
7.3676
7.3630
7.2451
7.2050
6.6992
6.6740
6.6522
3.1636
3.1407
3.1167
2.3303
1.7180
1.6940
1.6699
1.6459
1.6207
1.0278
1.0038
0.9786
-0.0000
0.98
2.91
1.94
2.08
2.92
2.11
3
CH3
N
H
N
OH
3l

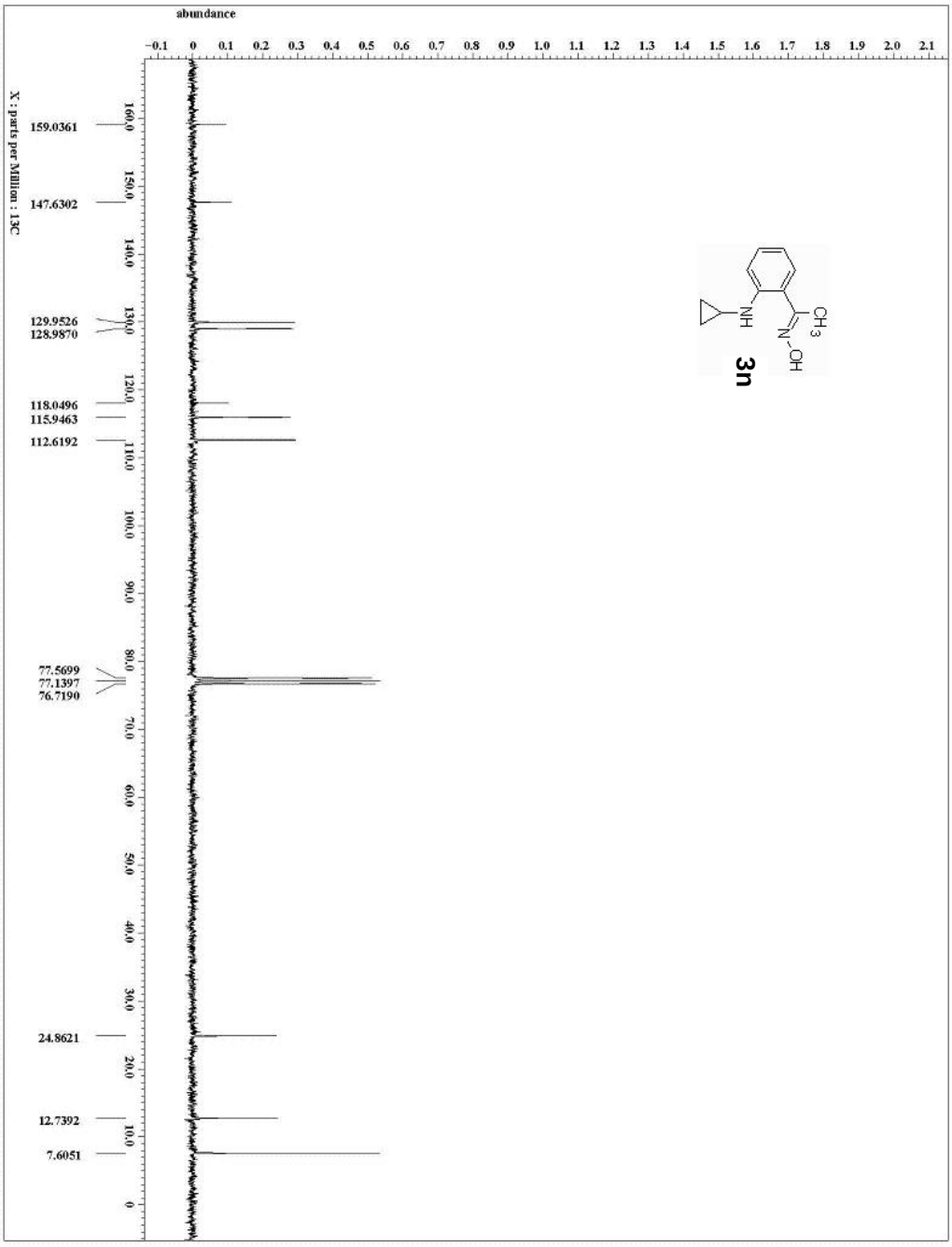

abundance
X : parts per Million : 13C
159.2369
147.2287
130.1152
129.2165
117.7724
114.9807
111.0417
77.5508
77.1301
76.7094
45.3697
22.5484
12.6532
11.9648
CH3
N
H
N
OH

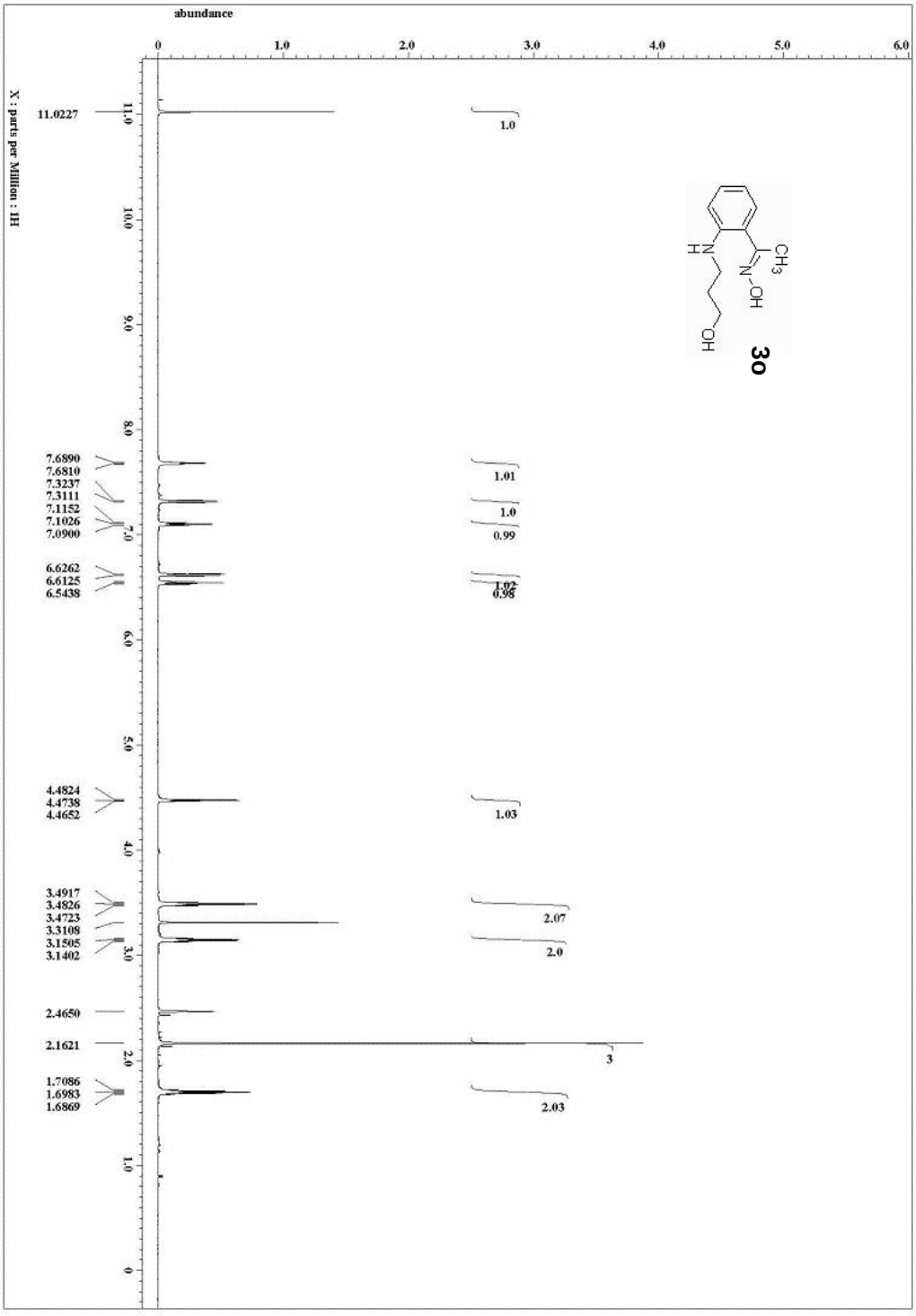
3l

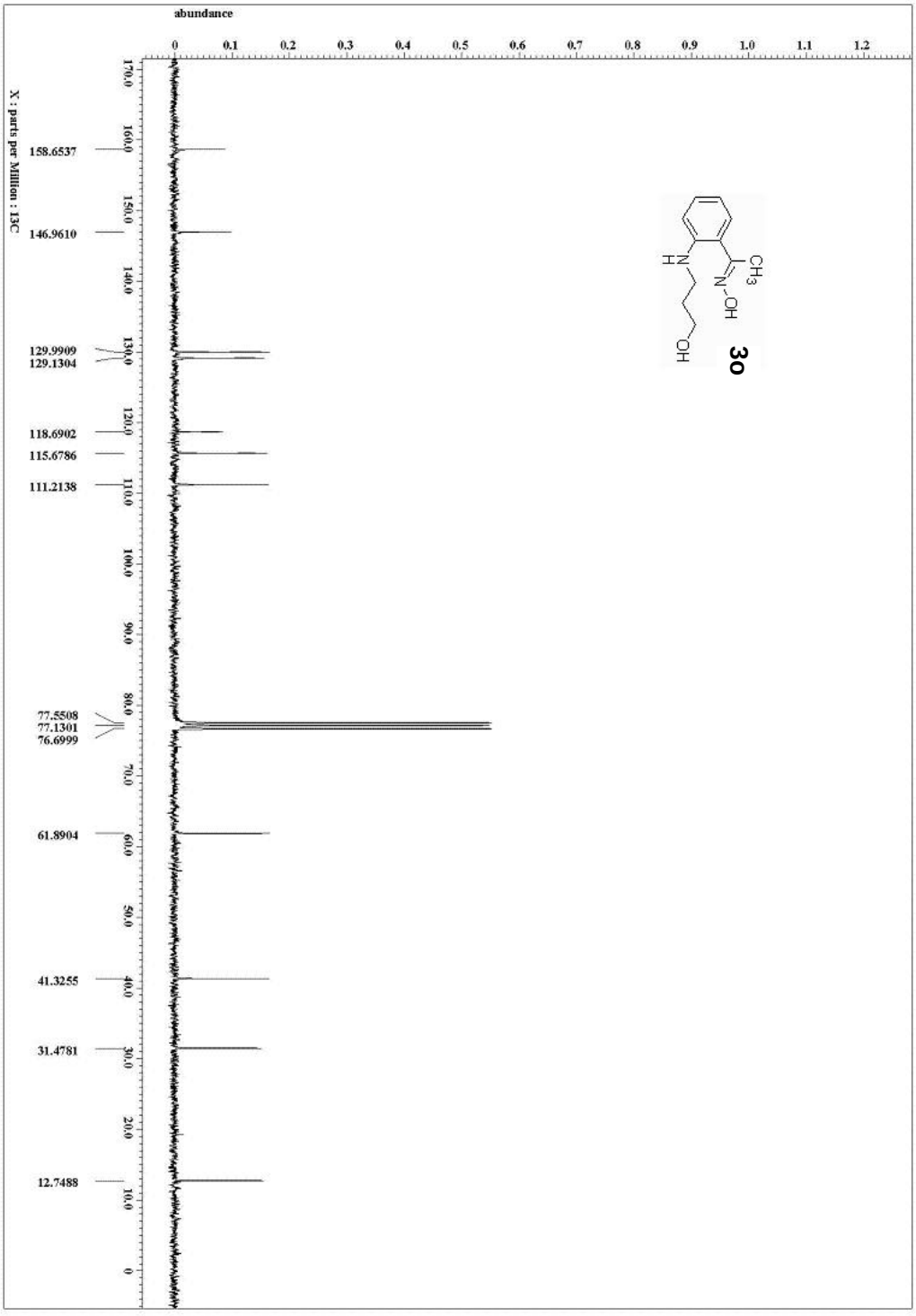

abundance
X : parts per Million : 1H
7.4420
7.3802
7.3584
7.3538
7.2062
6.7026
6.6763
6.6545
3.1865
3.1624
3.1395
2.3246
1.6676
1.6425
1.6184
1.4685
1.4422
1.4170
0.9752
0.9511
0.9271
0.0767
-0.0000
1.94
2.01
2.07
3
2.04
2.03
3.04
3m

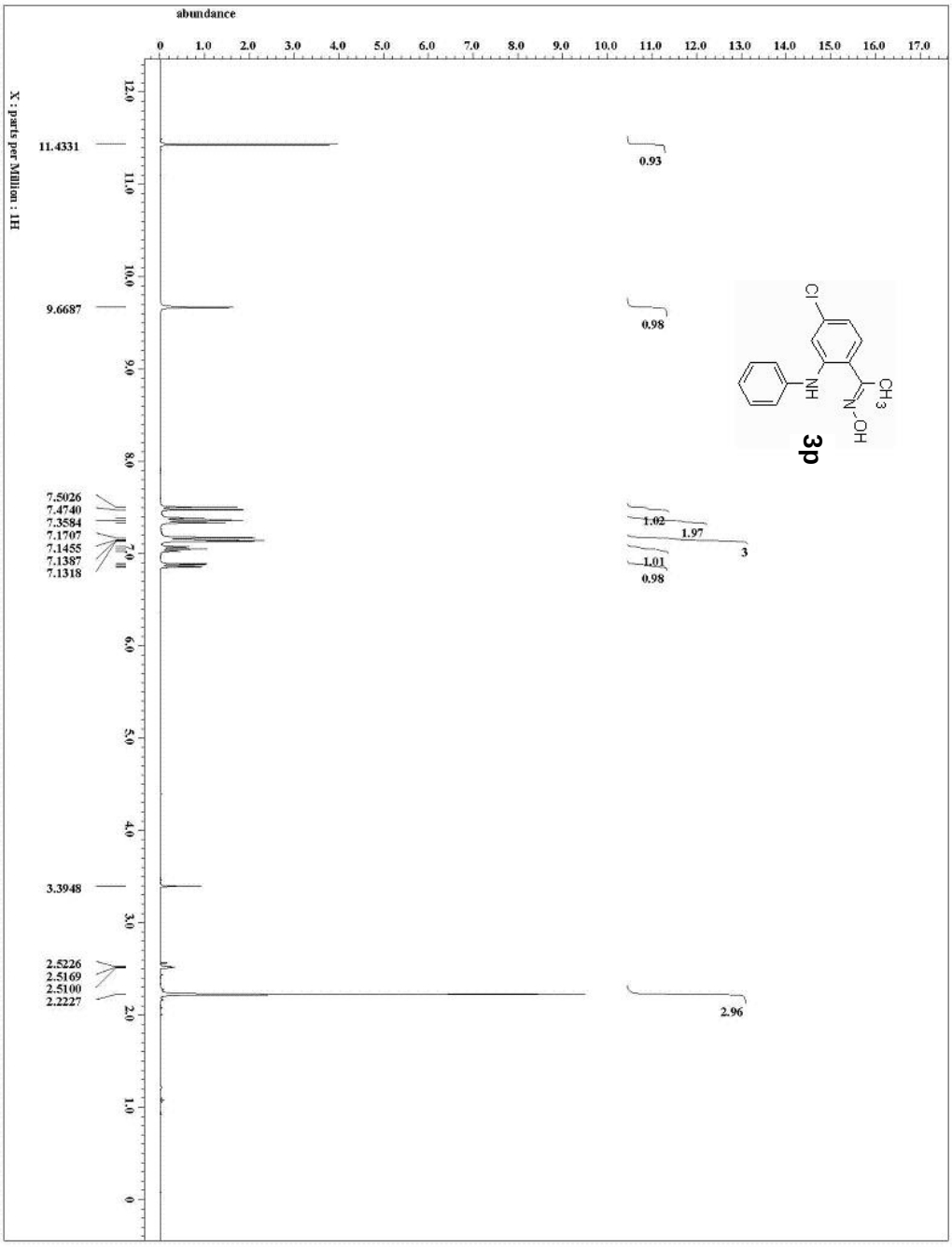

abundance
0
0.1
0.2
0.3
X : parts per Million : 13C
159.1891
147.2096
130.1247
129.2165
117.9253
115.0667
111.0895
77.5794
77.1588
76.7381
43.3141
31.4781
20.6172
14.0586
12.7679
3m

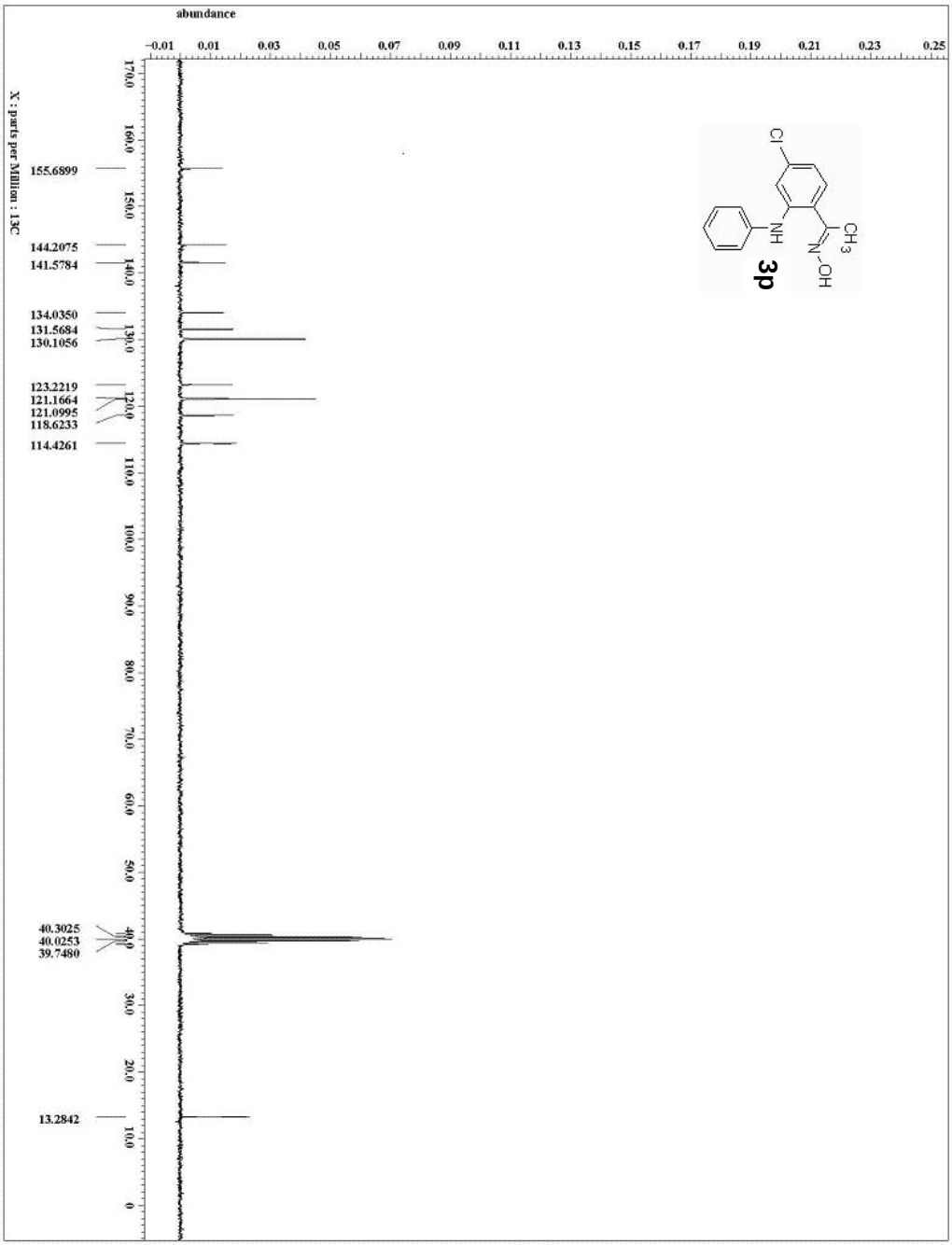

abundance
X : parts per Million : 1H
7.3802
7.3584
7.3538
7.3241
7.1787
7.1741
6.7438
6.7392
6.7175
2.4345
2.4311
2.4219
2.3097
0.7669
0.7508
0.5471
0.5391
0.5345
0.5276
-0.0000
2.18
1.01
1.06
3
2.05
2.02
NH
CH3
N
OH
3n

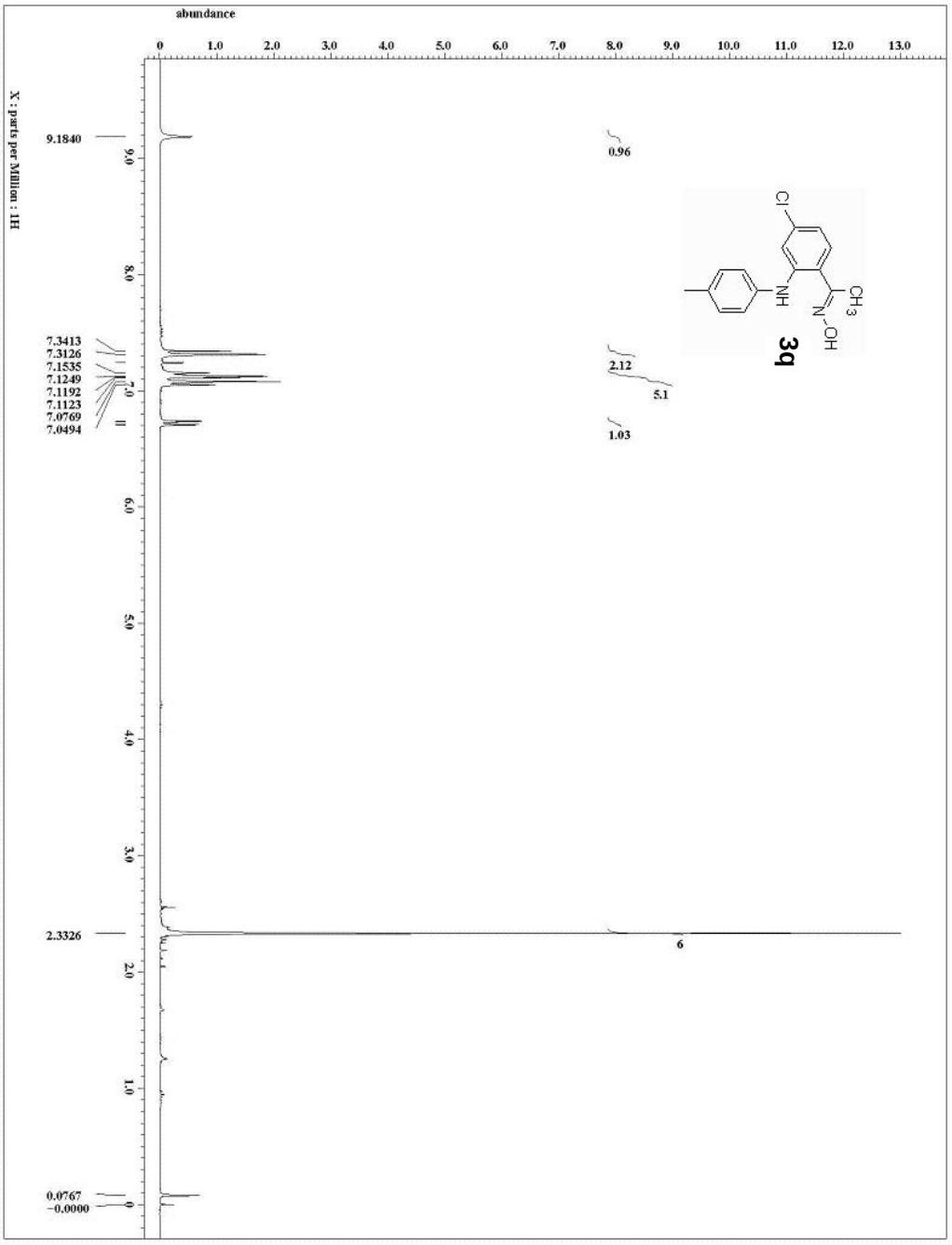

abundance
X : parts per Million : 13C
159.0361
147.6302
129.9526
128.9870
118.0496
115.9463
112.6192
77.5699
77.1397
76.7190
24.8621
12.7392
7.6051
NH
CH3
N
OH
3n

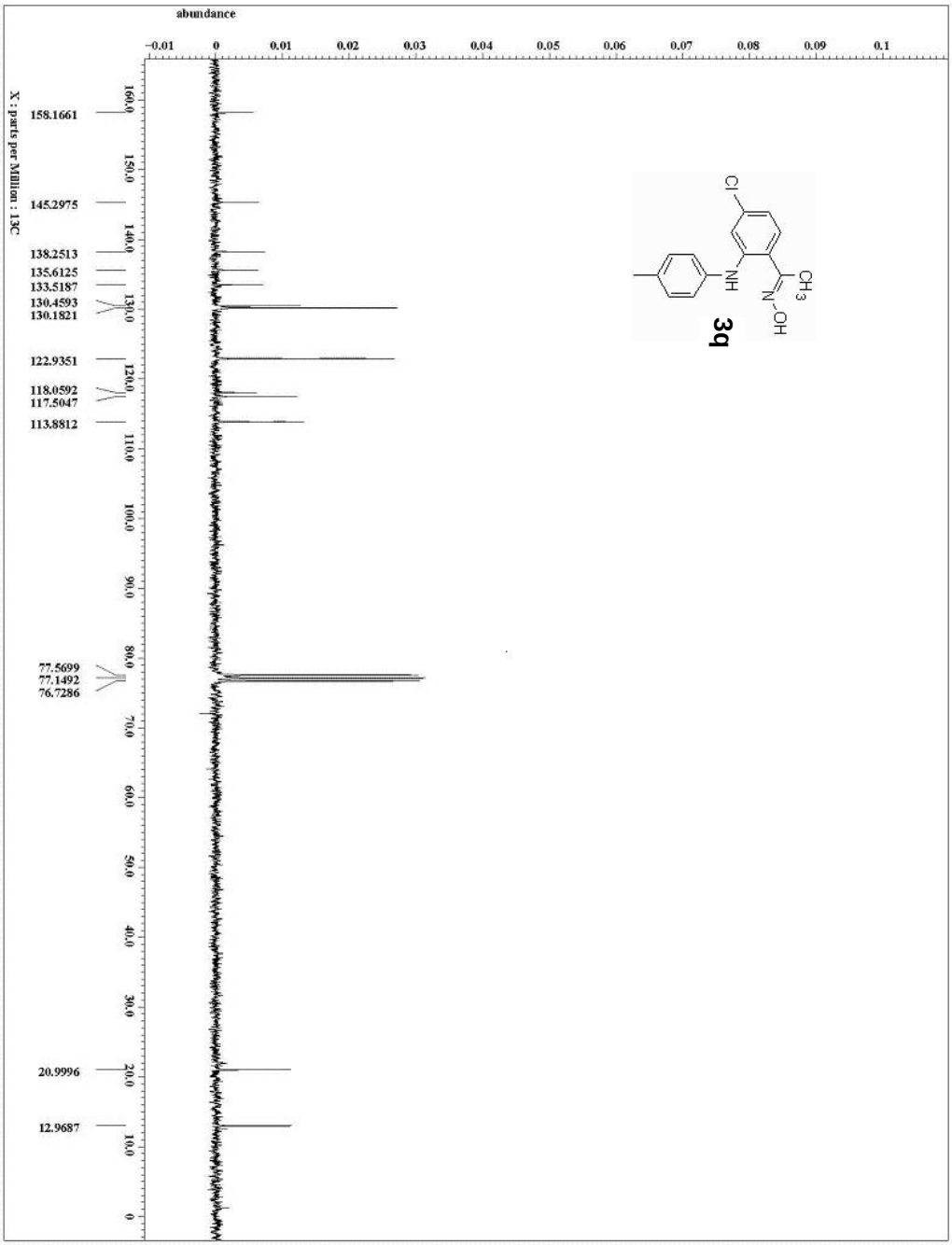

abundance
X : parts per Million : 1H
11.0227
7.6890
7.6810
7.3237
7.3111
7.1152
7.1026
7.0900
6.6262
6.6125
6.5438
4.4824
4.4738
4.4652
3.4917
3.4826
3.4723
3.3108
3.1505
3.1402
2.4650
2.1621
1.7086
1.6983
1.6869
1.0
1.01
1.0
0.99
1.03
2.07
2.0
3
2.03
30

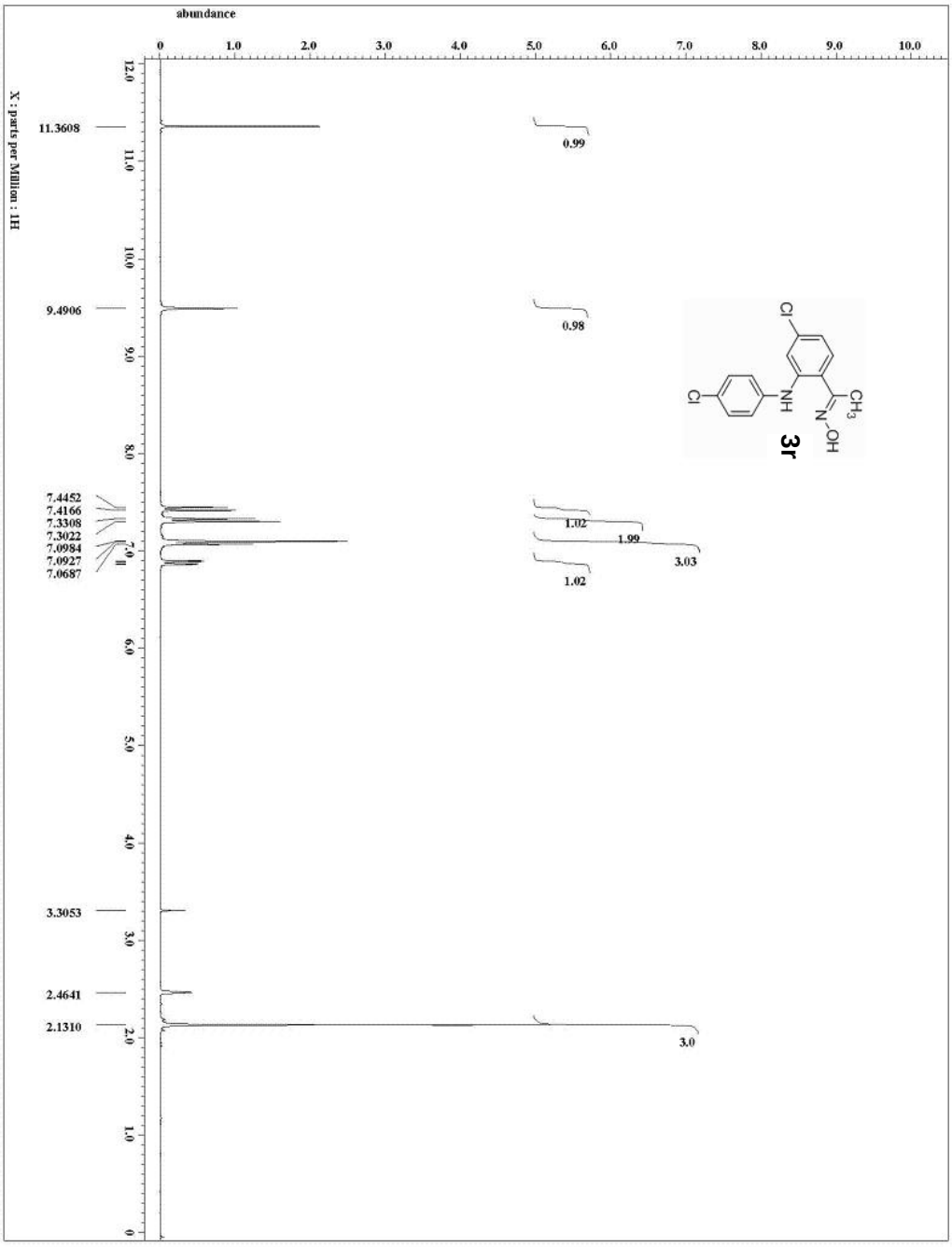

abundance
X : parts per Million : 13C
158.6537
146.9610
129.9909
129.1304
118.6902
115.6786
111.2138
77.5508
77.1301
76.6999
61.8904
41.3255
31.4781
12.7488
30

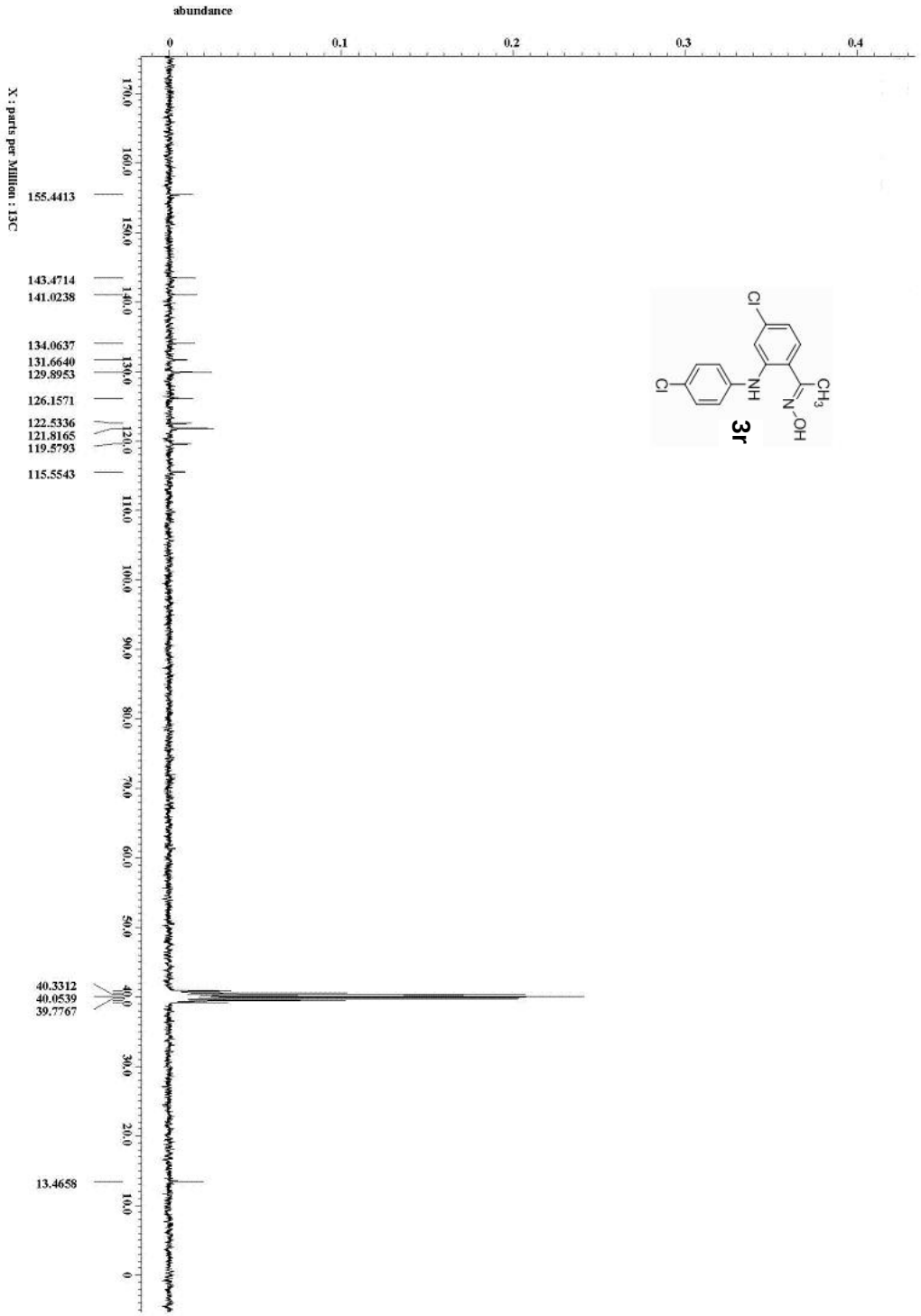

abundance
X : parts per Million : 1H
11.4331
9.6687
7.5026
7.4740
7.3584
7.1707
7.1455
7.1387
7.1318
3.3948
2.5226
2.5169
2.5100
2.2227
0.93
0.98
1.02
1.97
3
1.01
0.98
2.96
Cl
NH
N
OH
CH3
3p

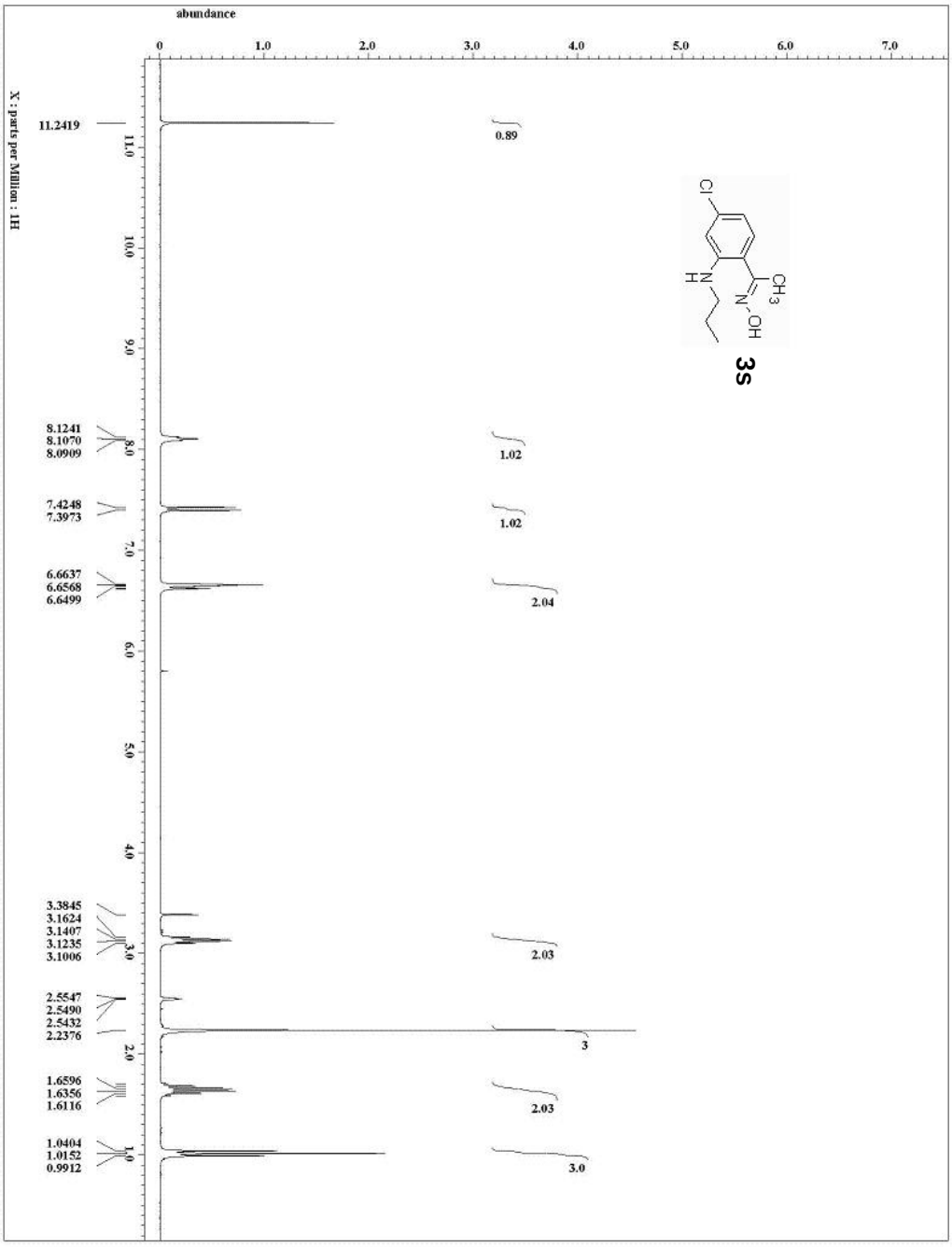

abundance
X : parts per Million : 13C
155.6899
144.2075
141.5784
134.0350
131.5684
130.1056
123.2219
121.1664
121.0995
118.6233
114.4261
40.3025
40.0253
39.7480
13.2842
Cl
HN
N
OH
CH3
3p

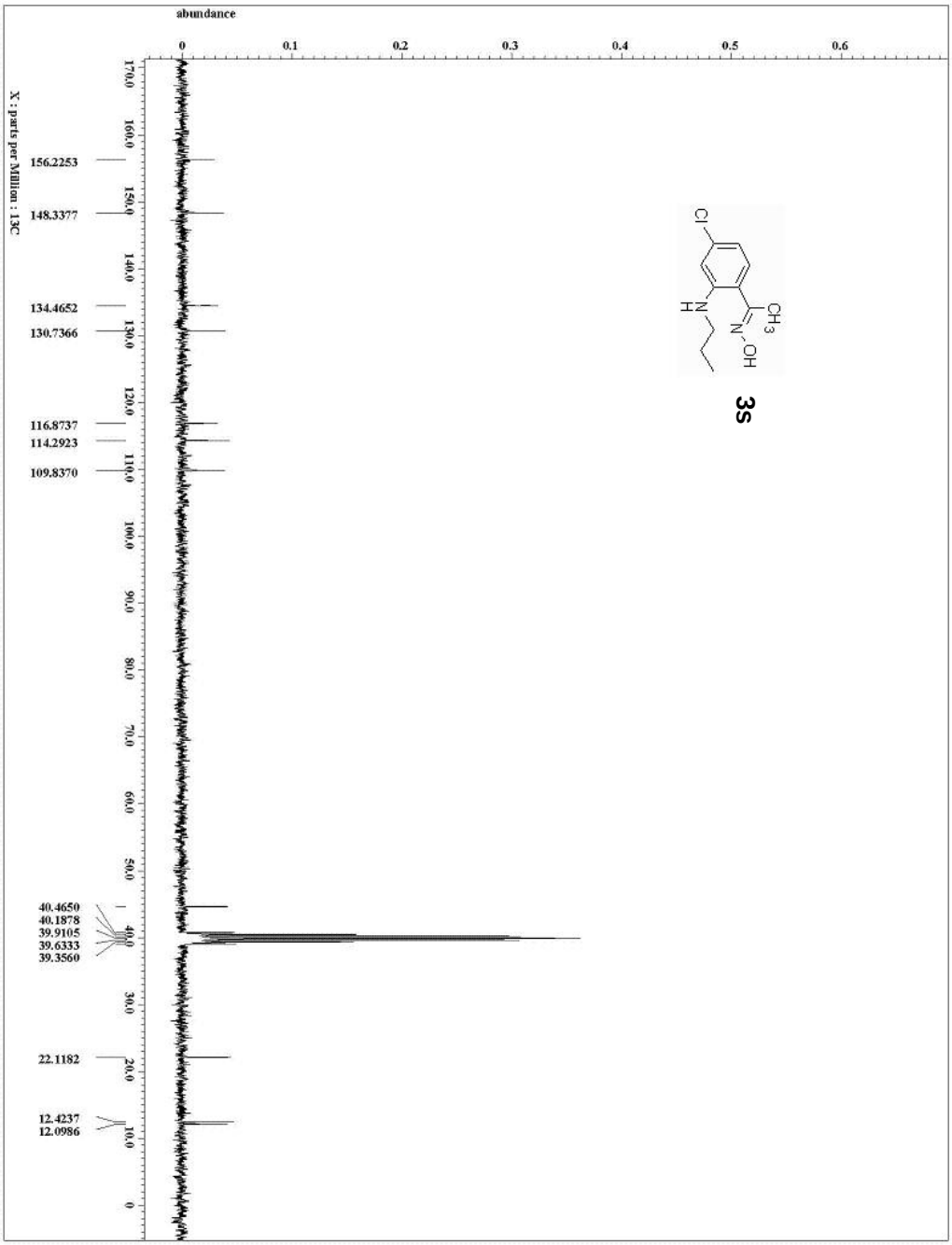

abundance
X : parts per Million : 1H
9.1840
7.3413
7.3126
7.1535
7.1249
7.1192
7.1123
7.0769
7.0494
2.3326
0.0767
−0.0000
0.96
2.12
5.1
1.03
6
Cl
NH
N
OH
CH3
3q

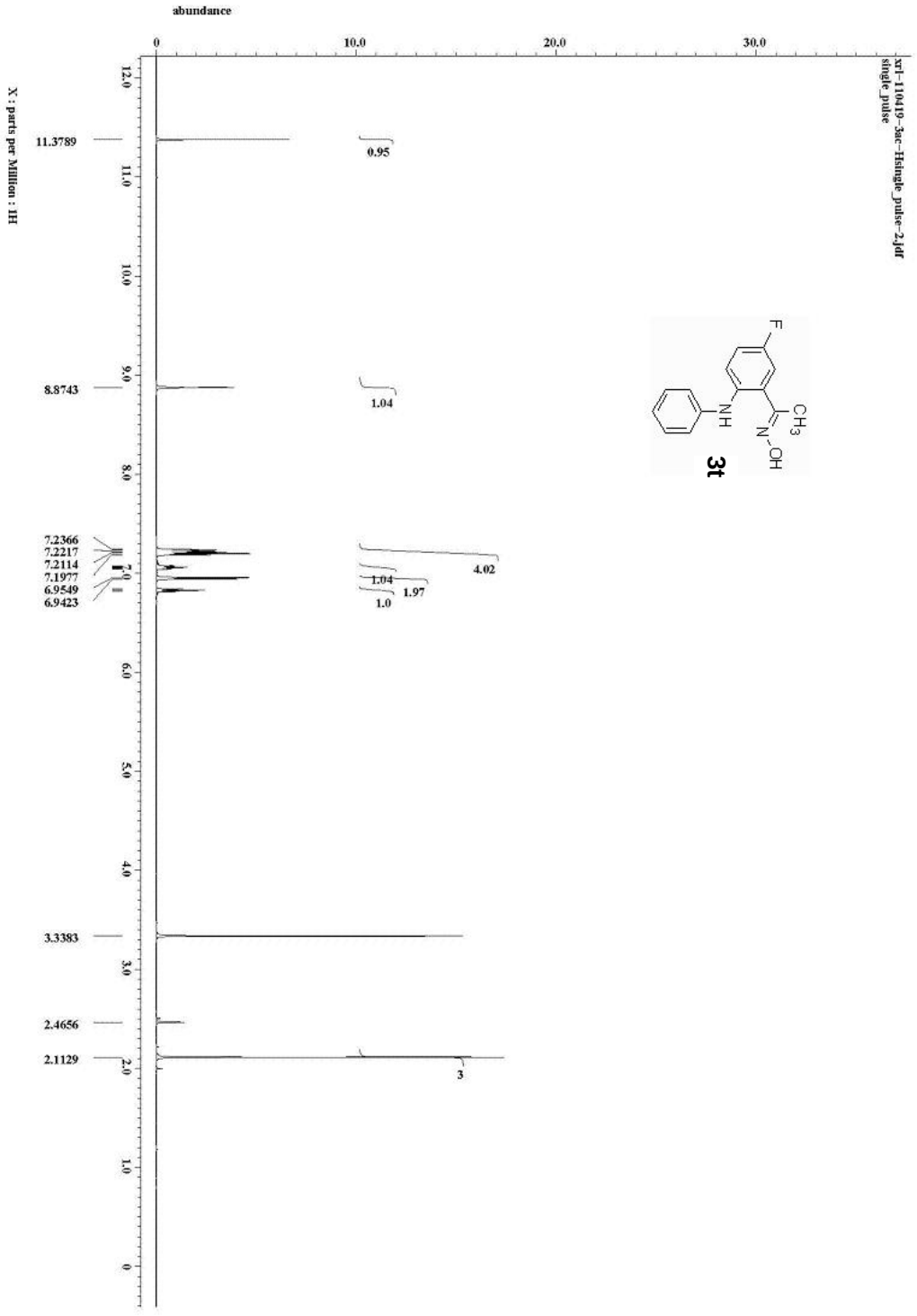

abundance
X : parts per Million : 13C
158.1661
145.2975
138.2513
135.6125
133.5187
130.4593
130.1821
122.9351
118.0592
117.5047
113.8812
77.5699
77.1492
76.7286
20.9996
12.9687
Cl
NH
CH3
N
OH
3q

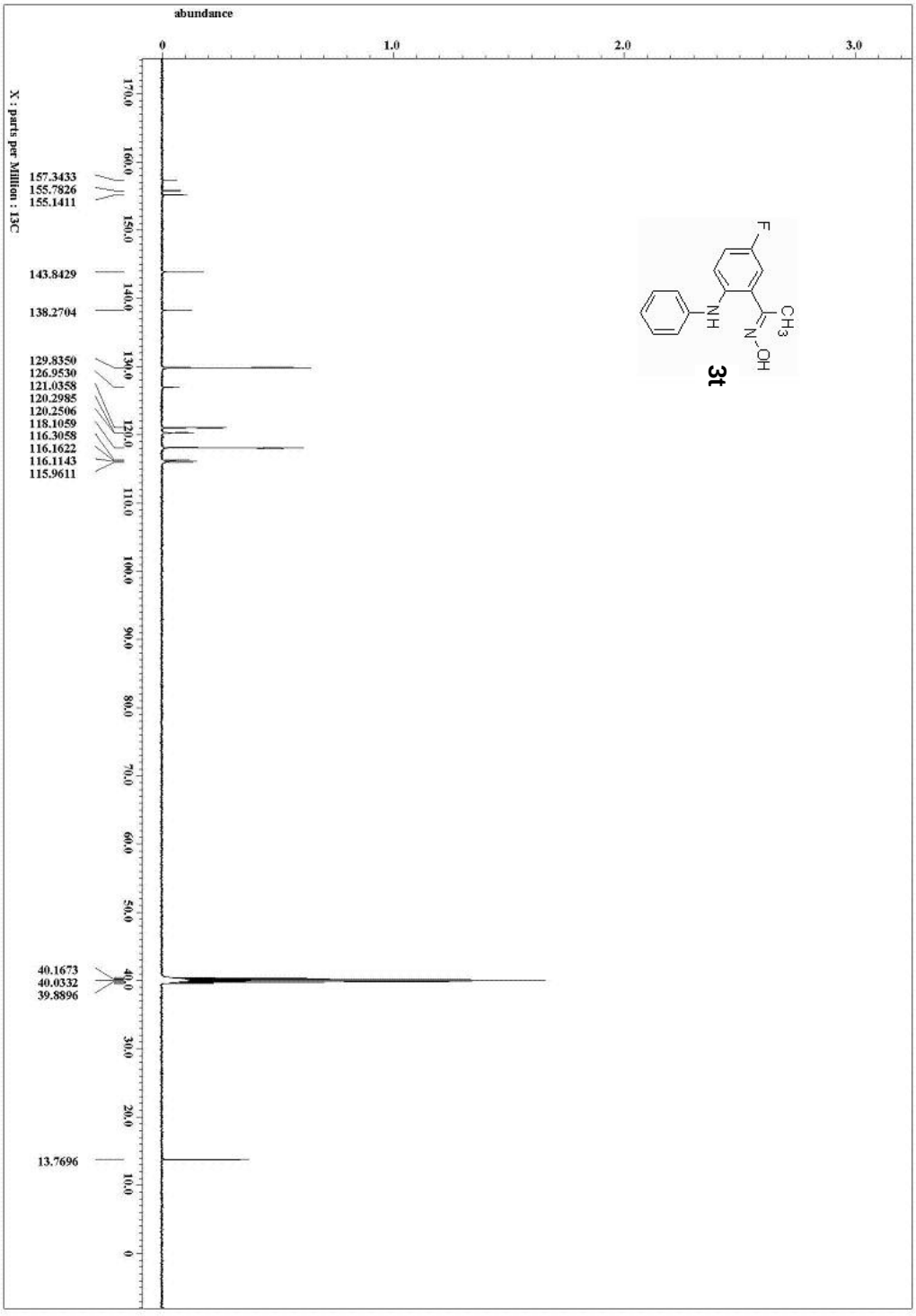

abundance
X : parts per Million : 1H
11.3608
9.4906
7.4452
7.4166
7.3308
7.3022
7.0984
7.0927
7.0687
3.3053
2.4641
2.1310
0.99
0.98
1.02
1.99
3.03
1.02
3.0
Cl
NH
Cl
N
OH
CH3
3r

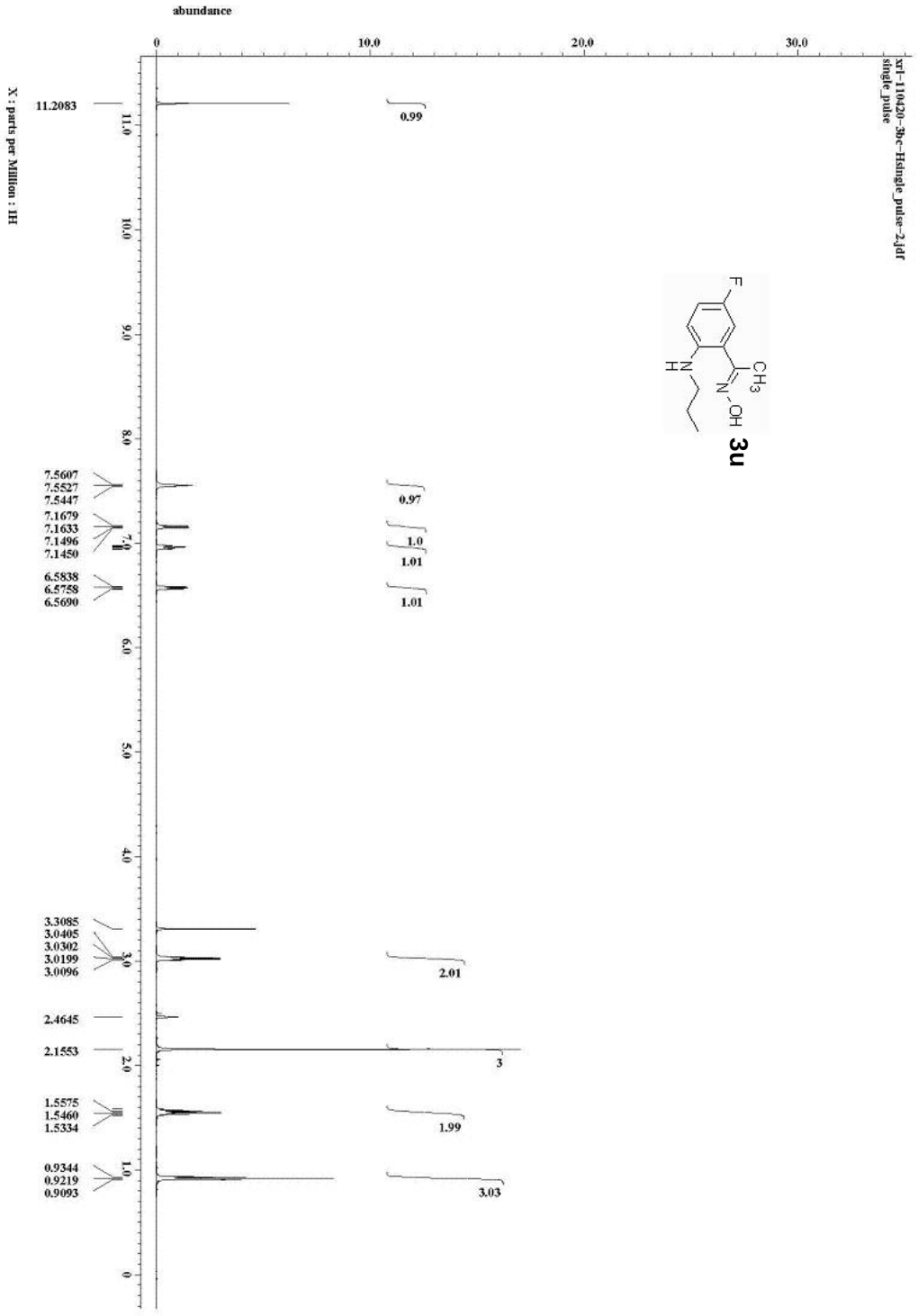

abundance
0
0.1
0.2
0.3
0.4
X : parts per Million : 13C
155.4413
143.4714
141.0238
134.0637
131.6640
129.8953
126.1571
122.5336
121.8165
119.5793
115.5543
40.3312
40.0539
39.7767
13.4658
Cl
NH
Cl
CH3
N
OH
3r

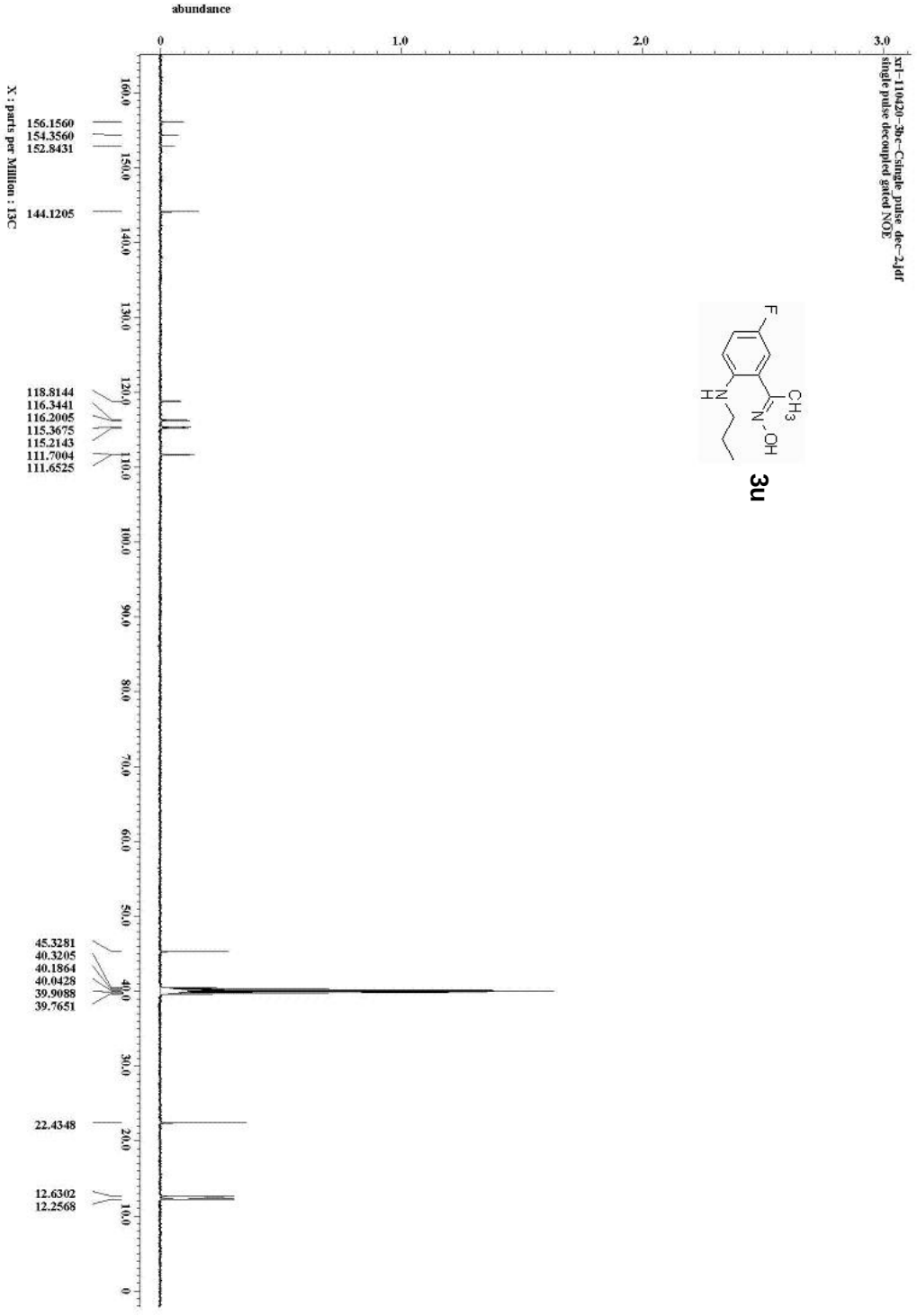

abundance
X : parts per Million : 1H
11.2419
8.1241
8.1070
8.0909
7.4248
7.3973
6.6637
6.6568
6.6499
3.3845
3.1624
3.1407
3.1235
3.1006
2.5547
2.5490
2.5432
2.2376
1.6596
1.6356
1.6116
1.0404
1.0152
0.9912
0.89
1.02
1.02
2.04
2.03
3
2.03
3.0
Cl
H
N
N
OH
CH3
3s

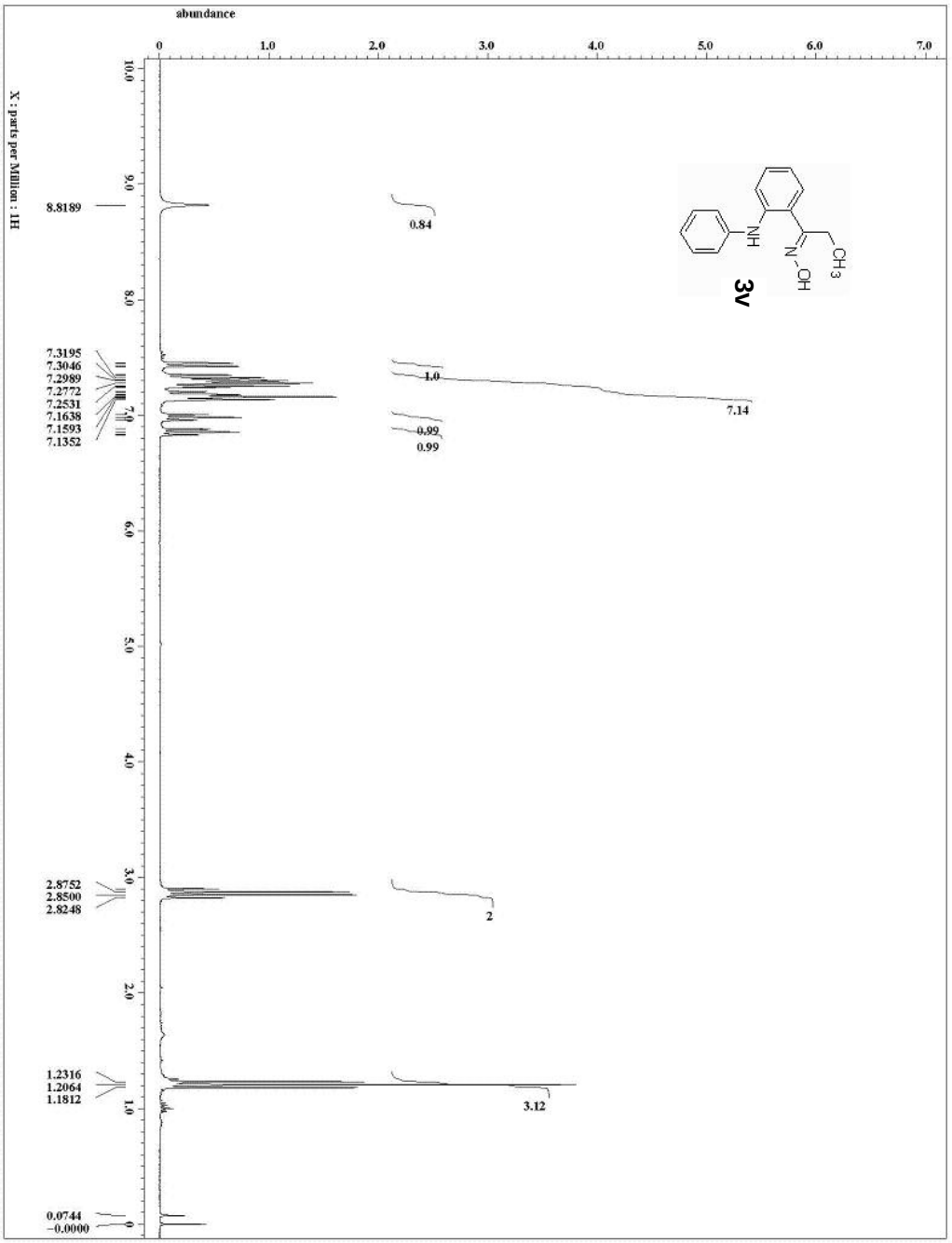

abundance
0
0.1
0.2
0.3
0.4
0.5
0.6
X : parts per Million : 13C
156.2253
148.3377
134.4652
130.7366
116.8737
114.2923
109.8370
40.4650
40.1878
39.9105
39.6333
39.3560
22.1182
12.4237
12.0986
Cl
H
N
CH3
N
OH
3s

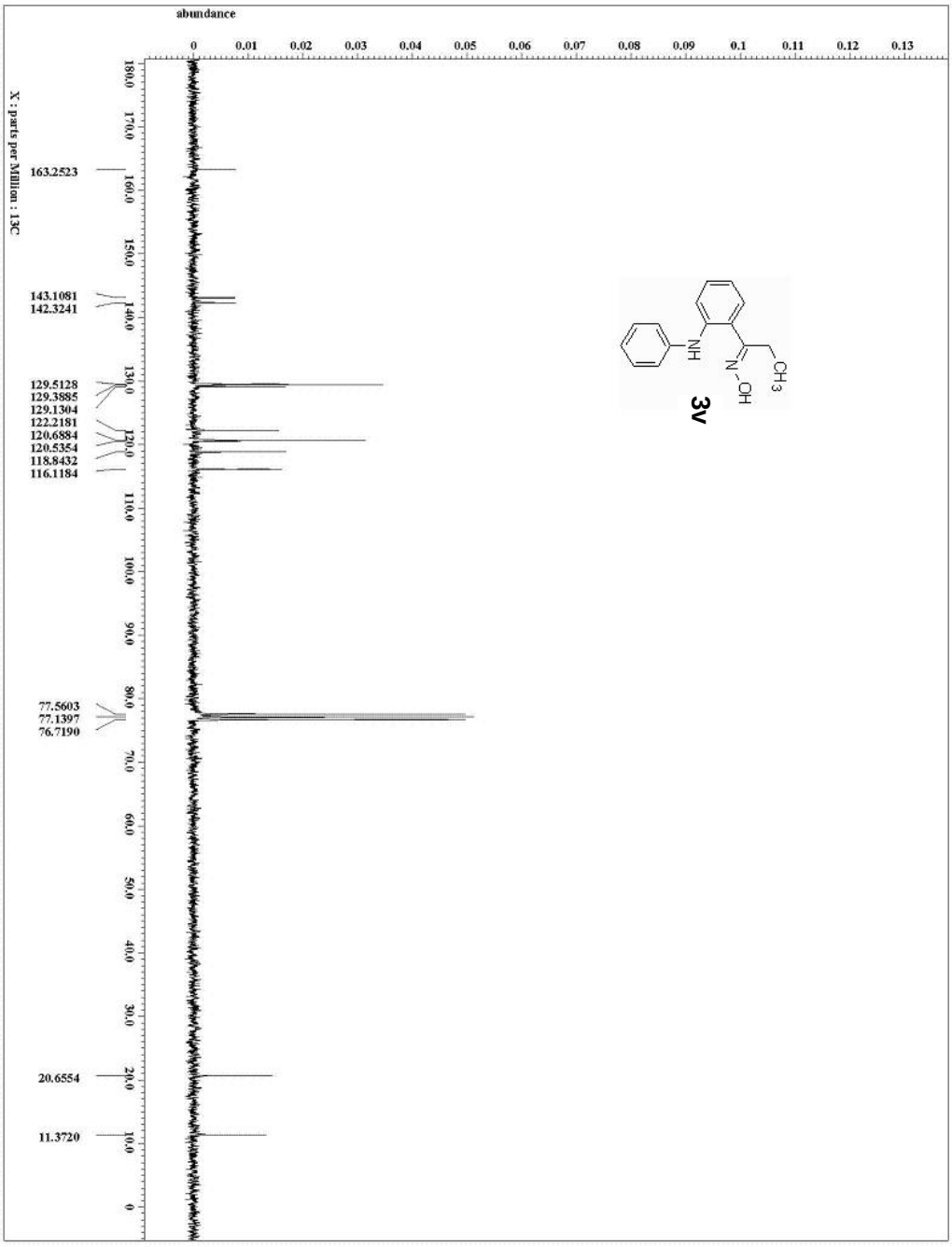

abundance
0
10.0
20.0
30.0
xrl-110419-3ac-Hsingle_pulse-2.jdf
single_pulse
X : parts per Million : 1H
11.3789
8.8743
7.2366
7.2217
7.2114
7.1977
6.9549
6.9423
3.3383
2.4656
2.1129
0.95
1.04
4.02
1.04
1.97
1.0
3
F
NH
N
OH
CH3
3t

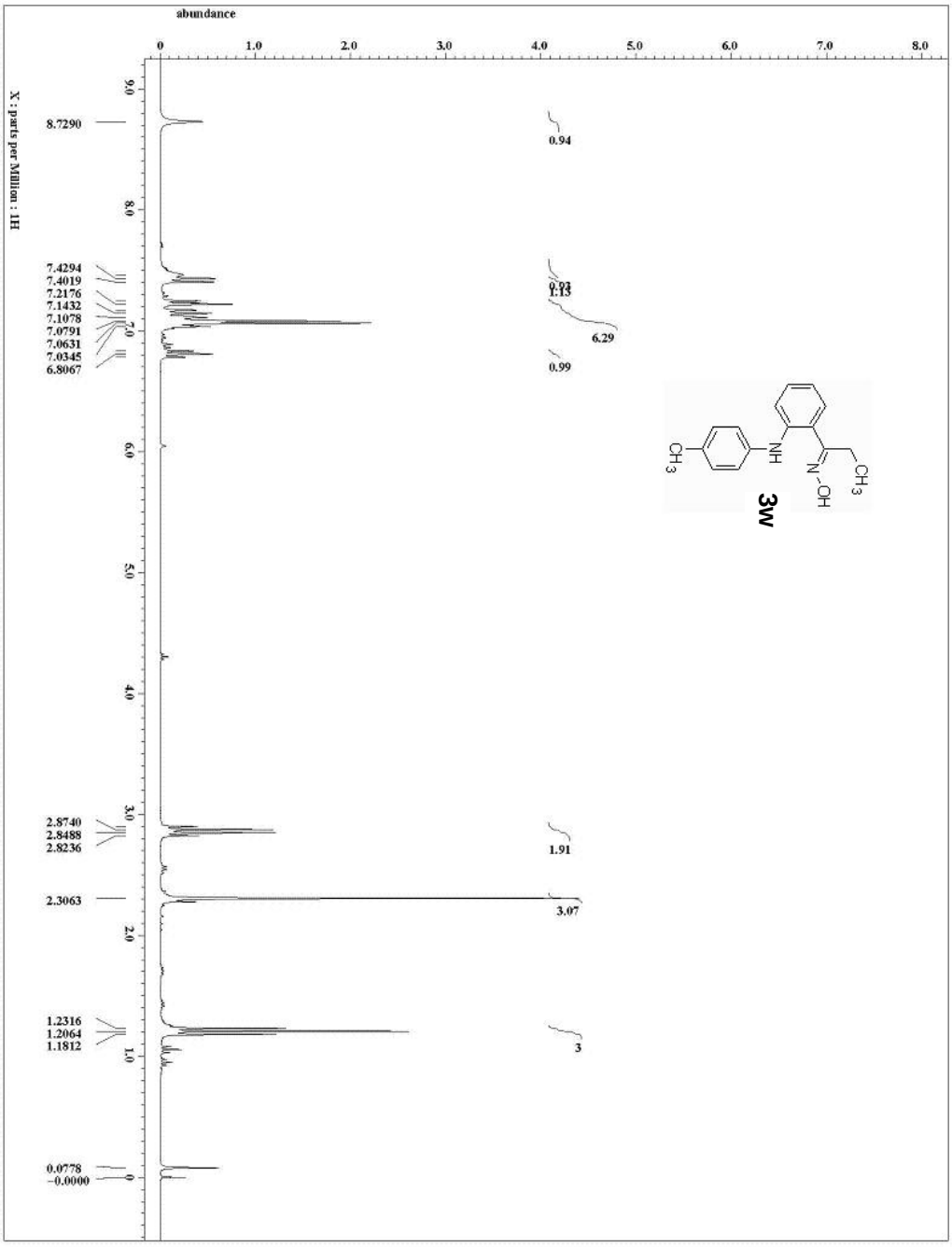

abundance
0
1.0
2.0
3.0
X : parts per Million : 13C
157.3433
155.7826
155.1411
143.8429
138.2704
129.8350
126.9530
121.0358
120.2985
120.2506
118.1059
116.3058
116.1622
116.1143
115.9611
40.1673
40.0332
39.8896
13.7696
F
NH
CH3
N
OH
3t

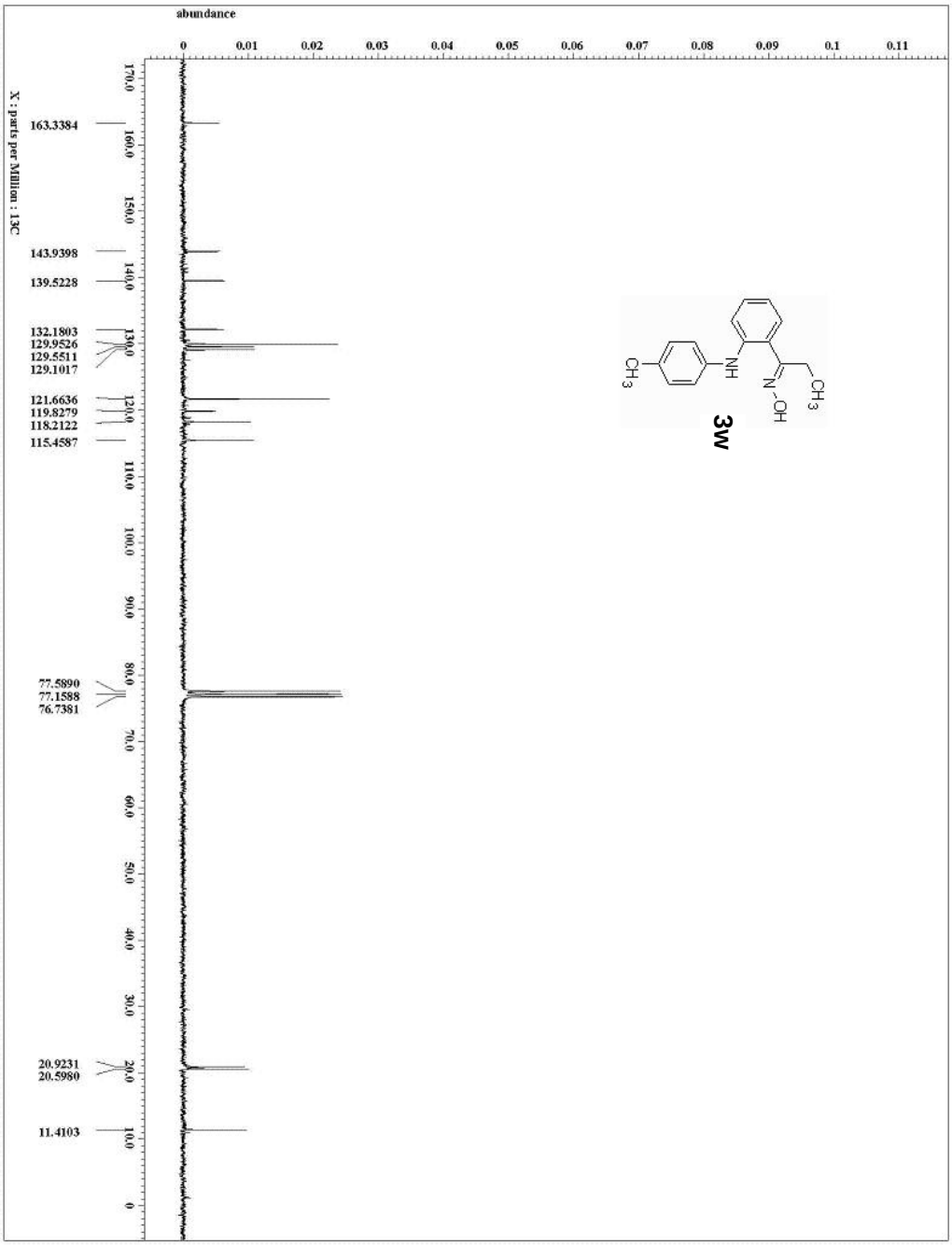

abundance
X : parts per Million : 1H
xr1-110420-3bc-Hsingle_pulse-2.jdf
single_pulse
11.2083
7.5607
7.5527
7.5447
7.1679
7.1633
7.1496
7.1450
6.5838
6.5758
6.5690
3.3085
3.0405
3.0302
3.0199
3.0096
2.4645
2.1553
1.5575
1.5460
1.5334
0.9344
0.9219
0.9093
0.99
0.97
1.0
1.01
1.01
2.01
3
1.99
3.03
3u

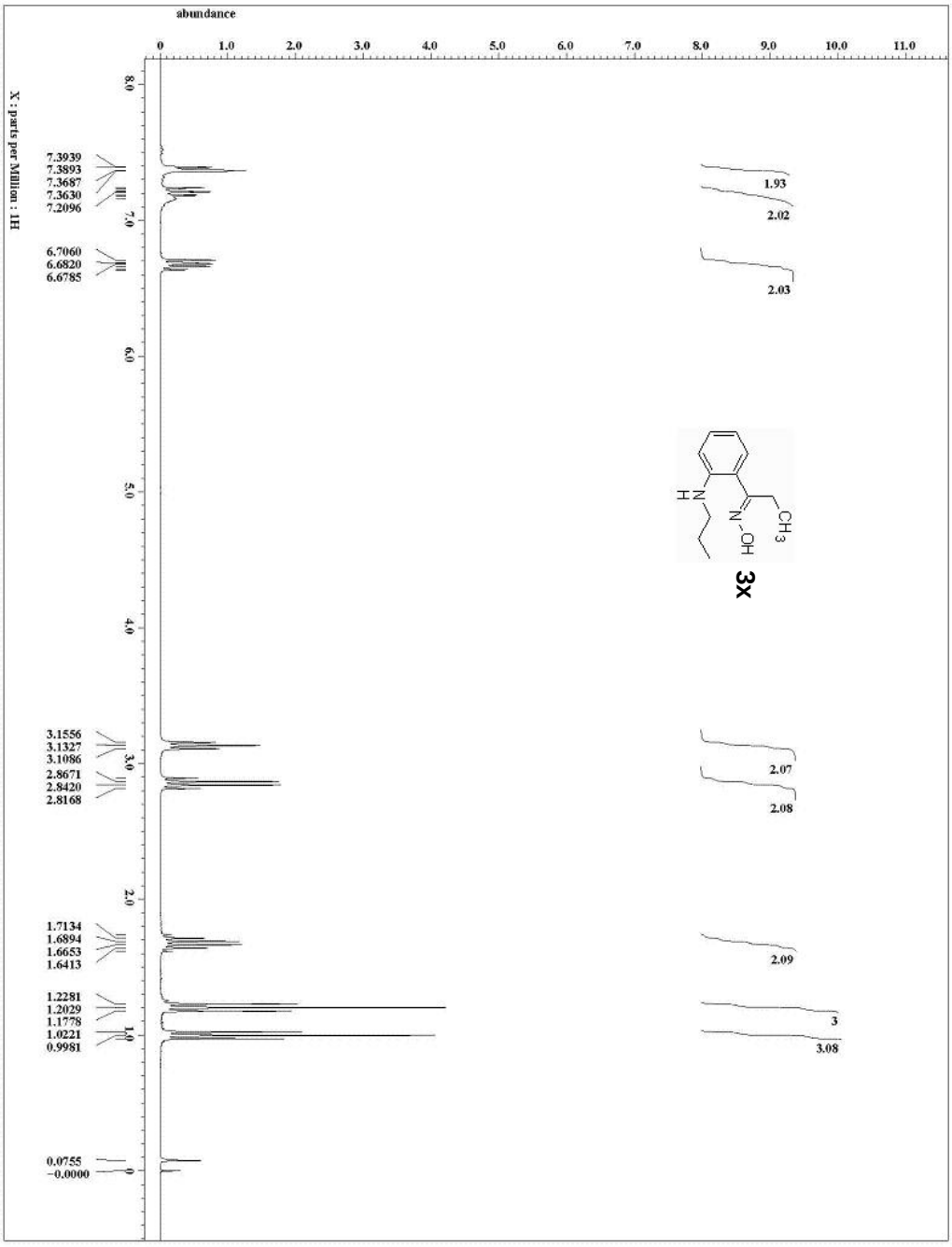

abundance
0
1.0
2.0
3.0
xr1-110420-3bc-Csingle_pulse_dec-2.jdf
single pulse decoupled gated NOE
X : parts per Million : 13C
156.1560
154.3560
152.8431
144.1205
118.8144
116.3441
116.2005
115.3675
115.2143
111.7004
111.6525
45.3281
40.3205
40.1864
40.0428
39.9088
39.7651
22.4348
12.6302
12.2568
F
CH3
N
OH
H
3u

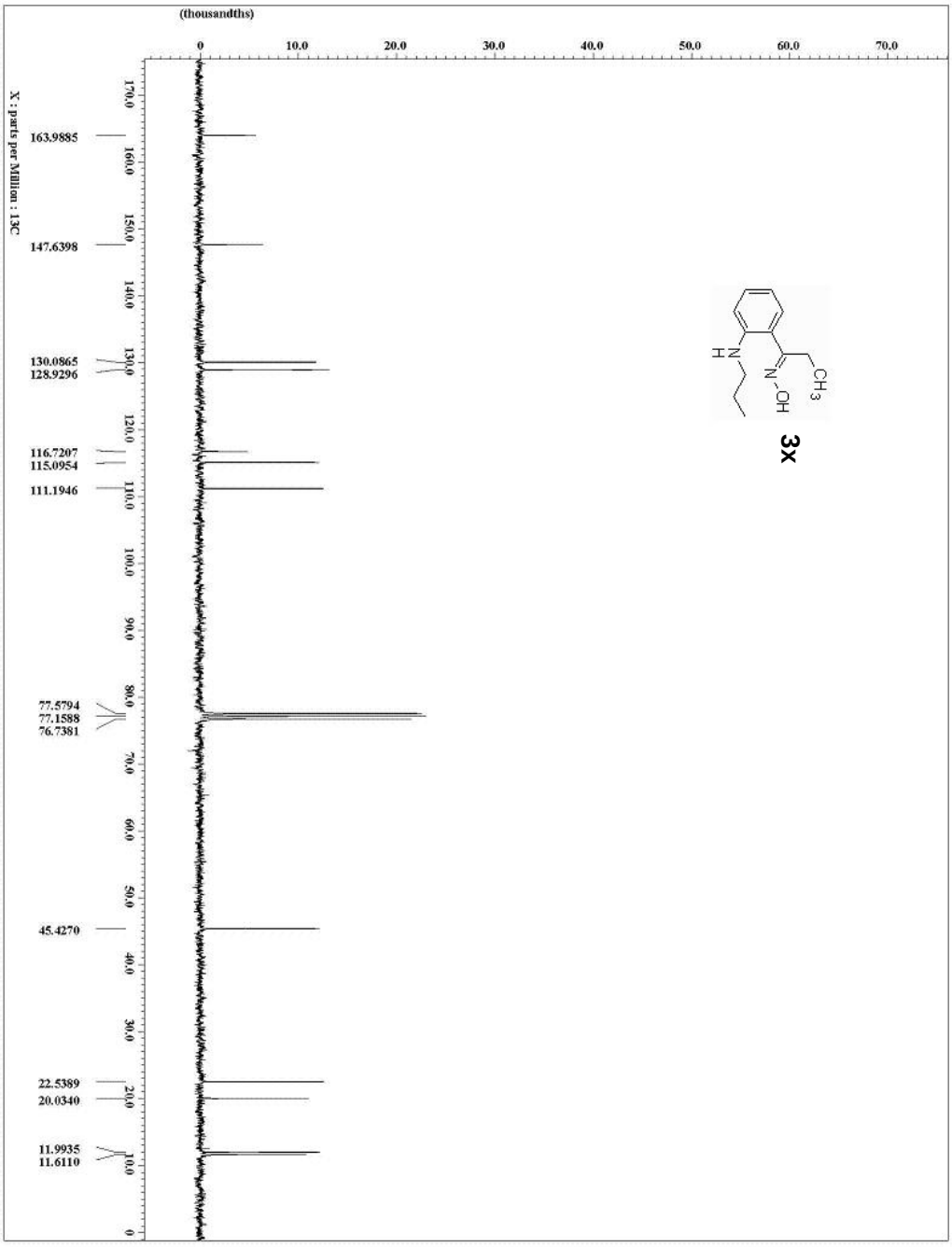

abundance
X : parts per Million : 1H
8.8189
7.3195
7.3046
7.2989
7.2772
7.2531
7.1638
7.1593
7.1352
2.8752
2.8500
2.8248
1.2316
1.2064
1.1812
0.0744
−0.0000
0.84
1.0
7.14
0.99
0.99
2
3.12
NH
N
OH
CH3
3v

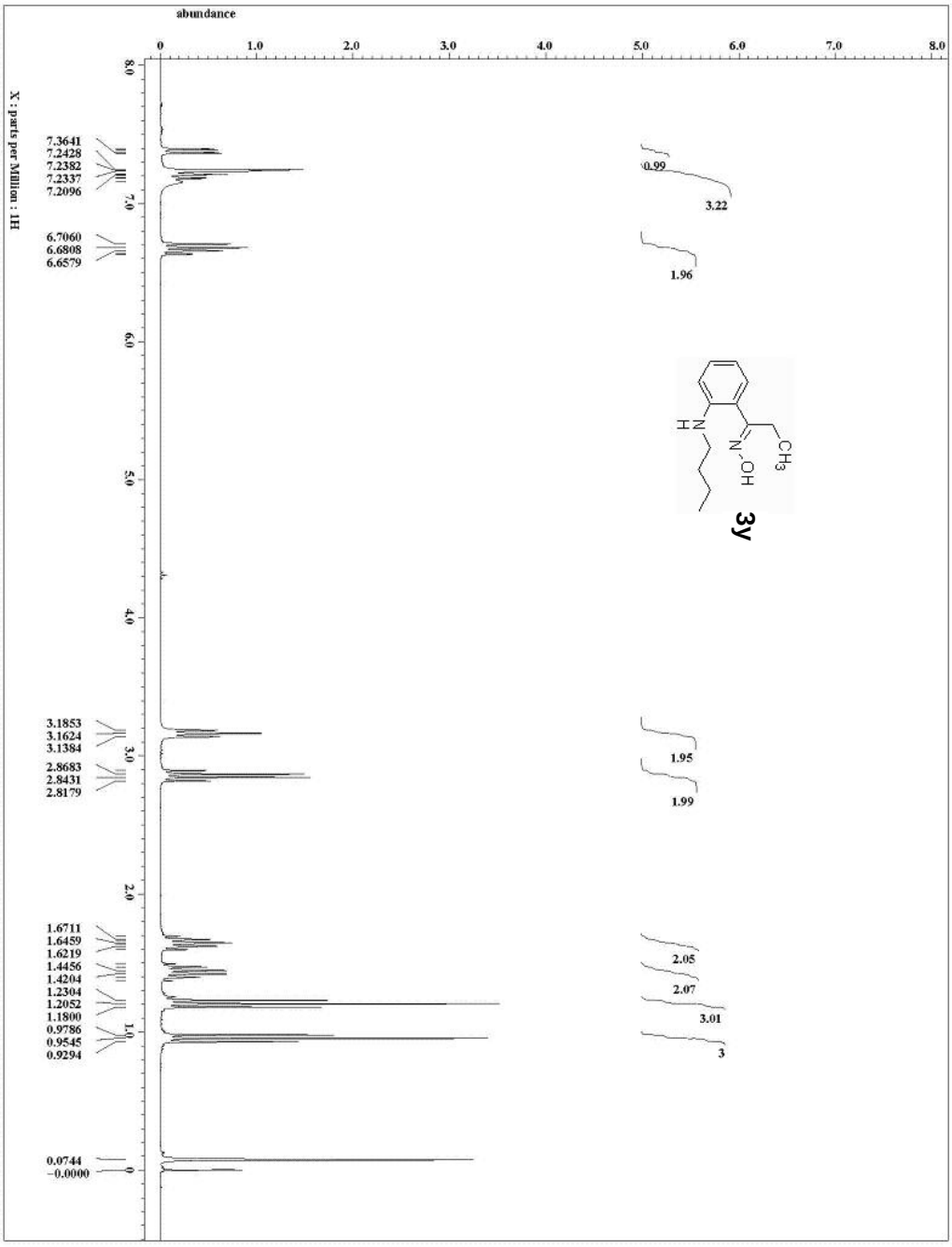

abundance
X : parts per Million : 13C
163.2523
143.1081
142.3241
129.5128
129.3885
129.1304
122.2181
120.6884
120.5354
118.8432
116.1184
77.5603
77.1397
76.7190
20.6554
11.3720
NH
N
OH
CH3
3v

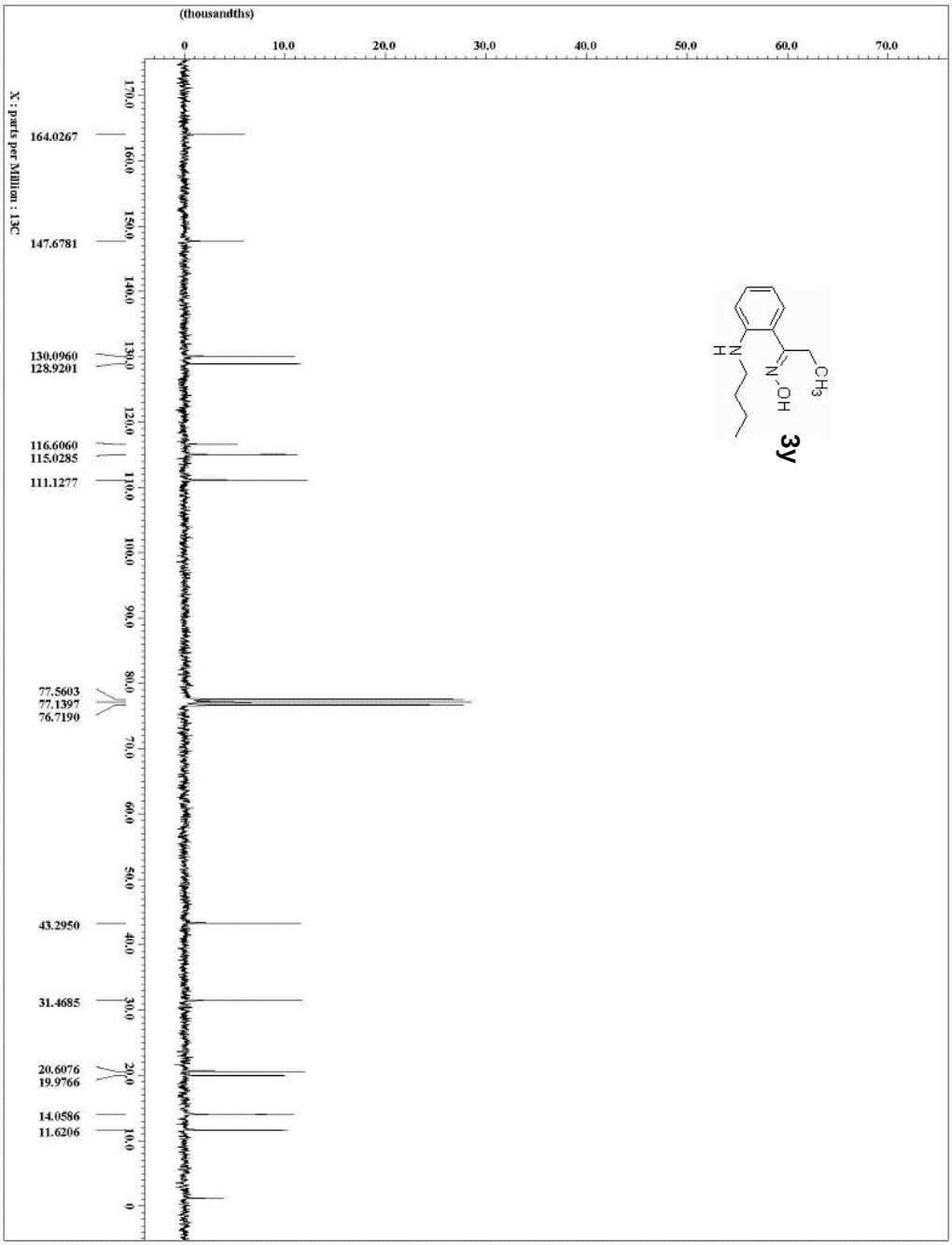

abundance
X : parts per Million : 1H
8.7290
7.4294
7.4019
7.2176
7.1432
7.1078
7.0791
7.0631
7.0345
6.8067
2.8740
2.8488
2.8236
2.3063
1.2316
1.2064
1.1812
0.0778
−0.0000
0.94
1.13
6.29
0.99
1.91
3.07
3
CH3
NH
N
OH
CH3
3w

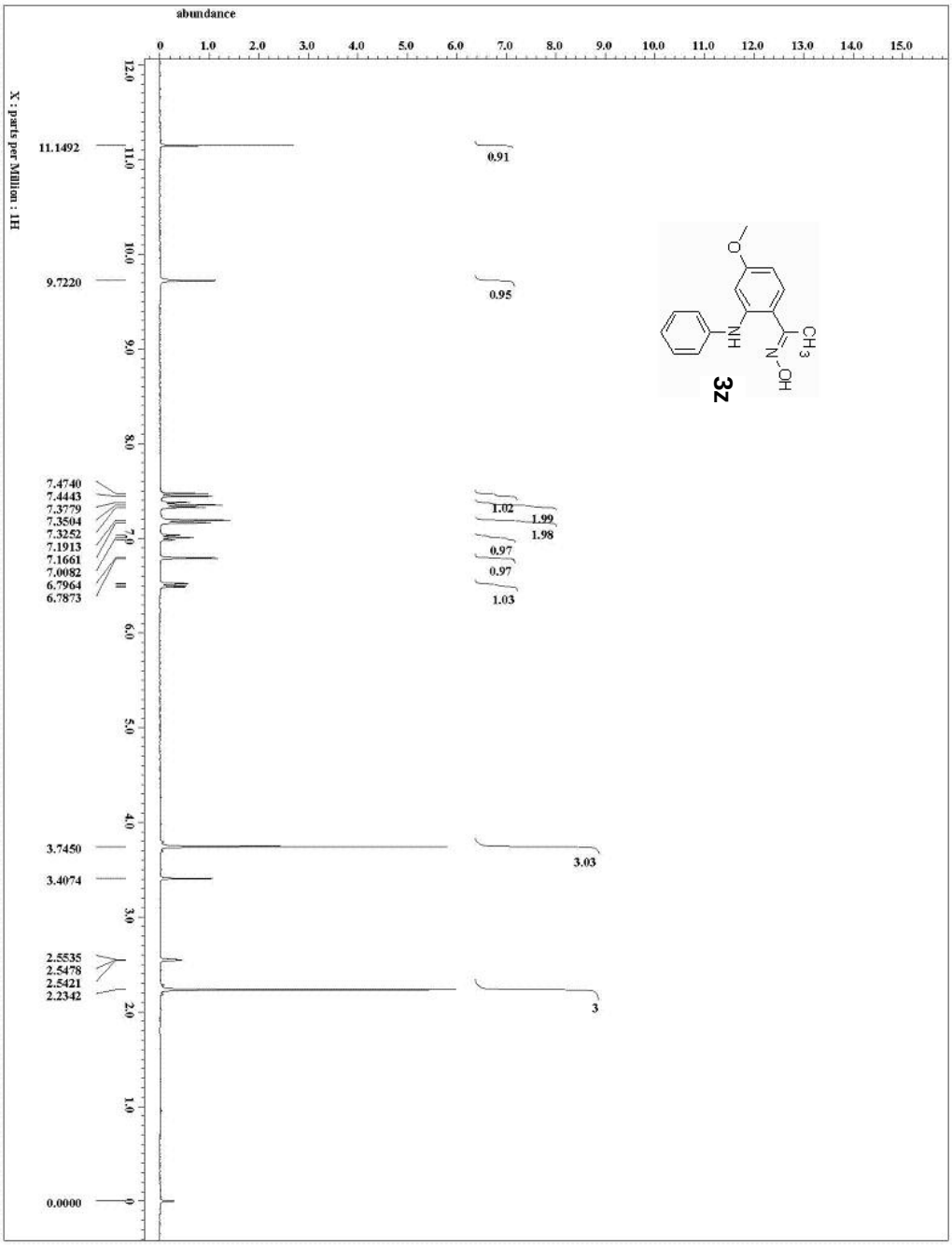

abundance
0
0.01
0.02
0.03
0.04
0.05
0.06
0.07
0.08
0.09
0.1
0.11
X : parts per Million : 13C
163.3384
143.9398
139.5228
132.1803
129.9526
129.5511
129.1017
121.6636
119.8279
118.2122
115.4587
77.5890
77.1588
76.7381
20.9231
20.5980
11.4103
CH3
NH
N
OH
CH3
3w

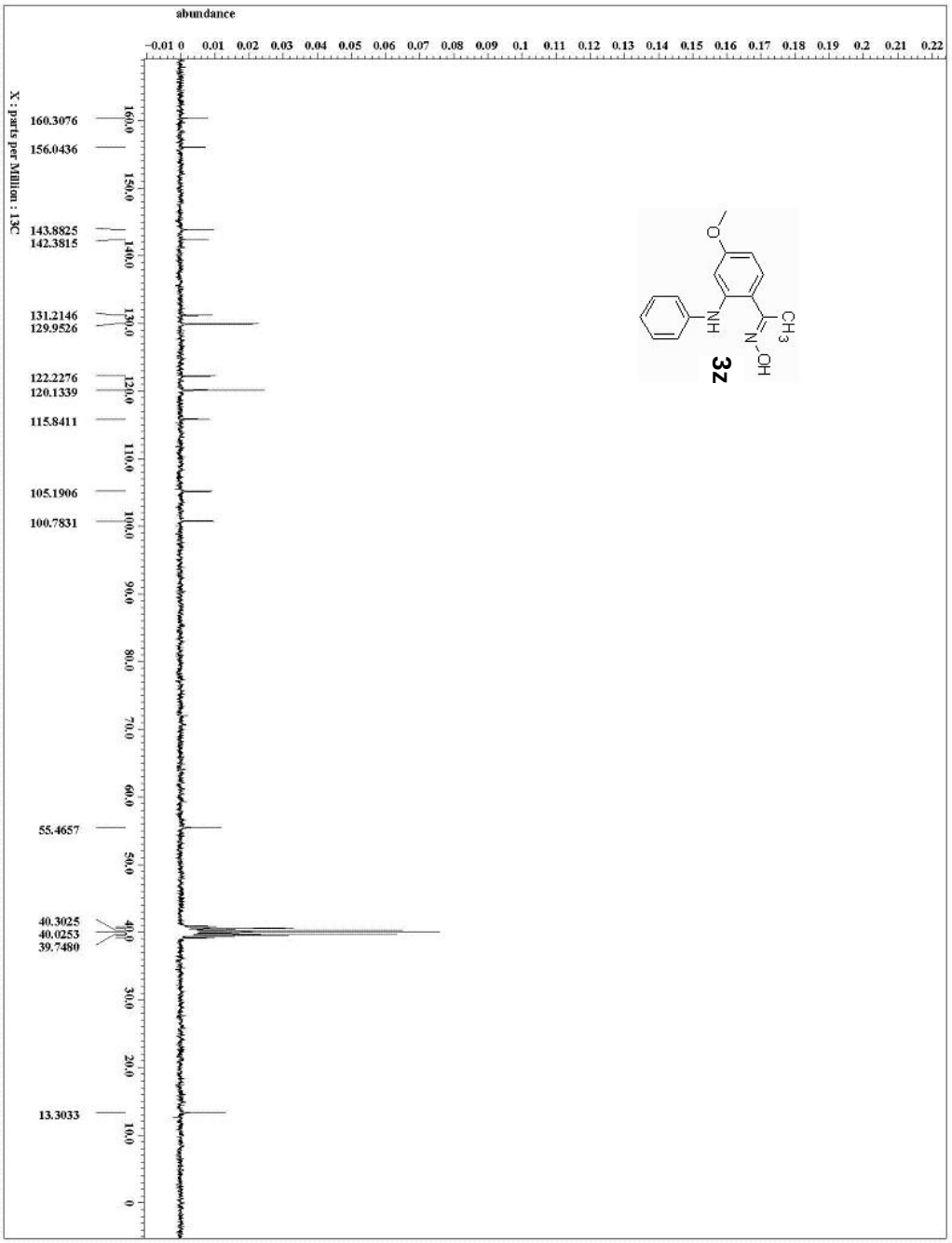

abundance
X : parts per Million : 1H
7.3939
7.3893
7.3687
7.3630
7.2096
6.7060
6.6820
6.6785
3.1556
3.1327
3.1086
2.8671
2.8420
2.8168
1.7134
1.6894
1.6653
1.6413
1.2281
1.2029
1.1778
1.0221
0.9981
0.0755
-0.0000
1.93
2.02
2.03
2.07
2.08
2.09
3
3.08
3x

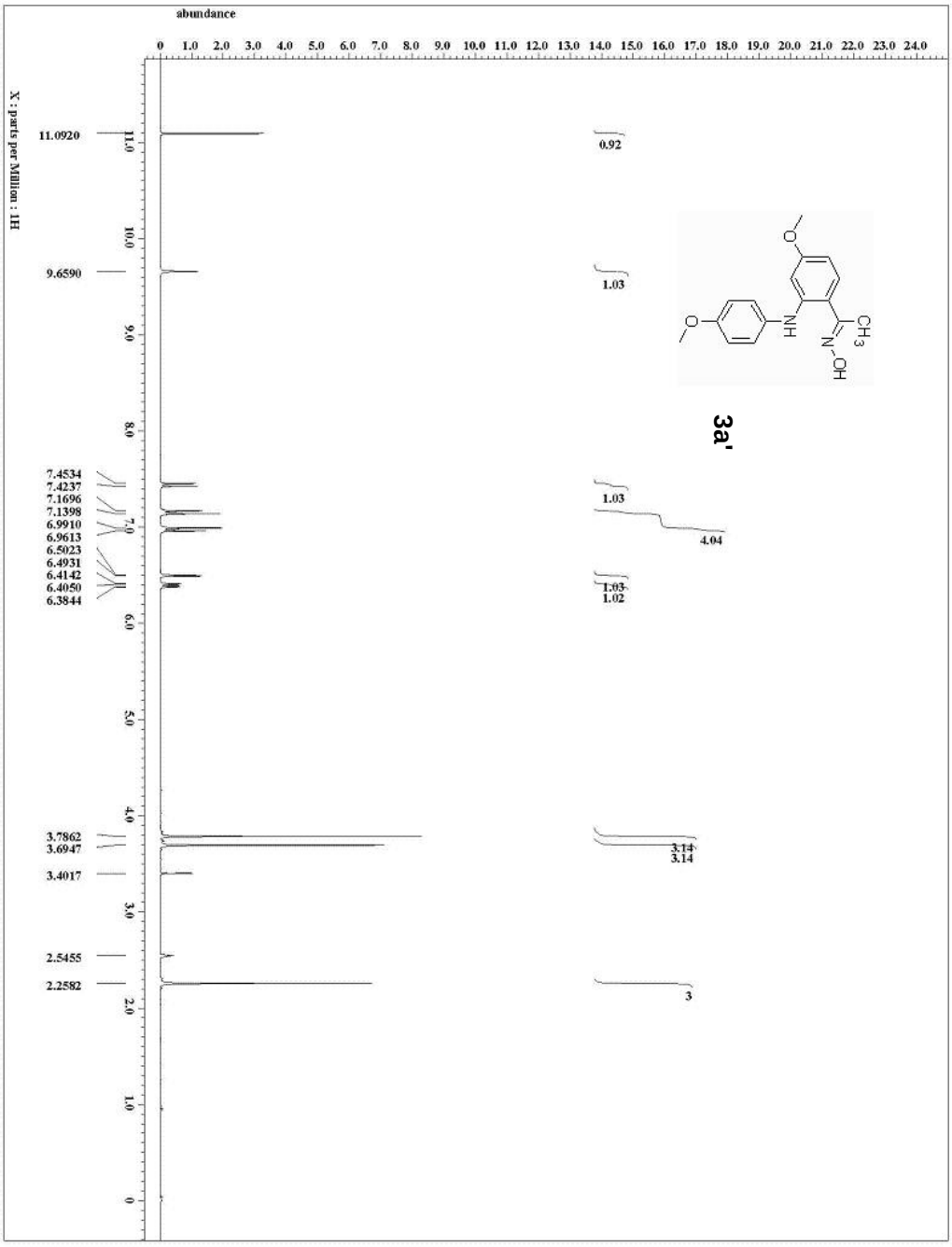

(thousandths)
X : parts per Million : 13C
163.9885
147.6398
130.0865
128.9296
116.7207
115.0954
111.1946
77.5794
77.1588
76.7381
45.4270
22.5389
20.0340
11.9935
11.6110
3x

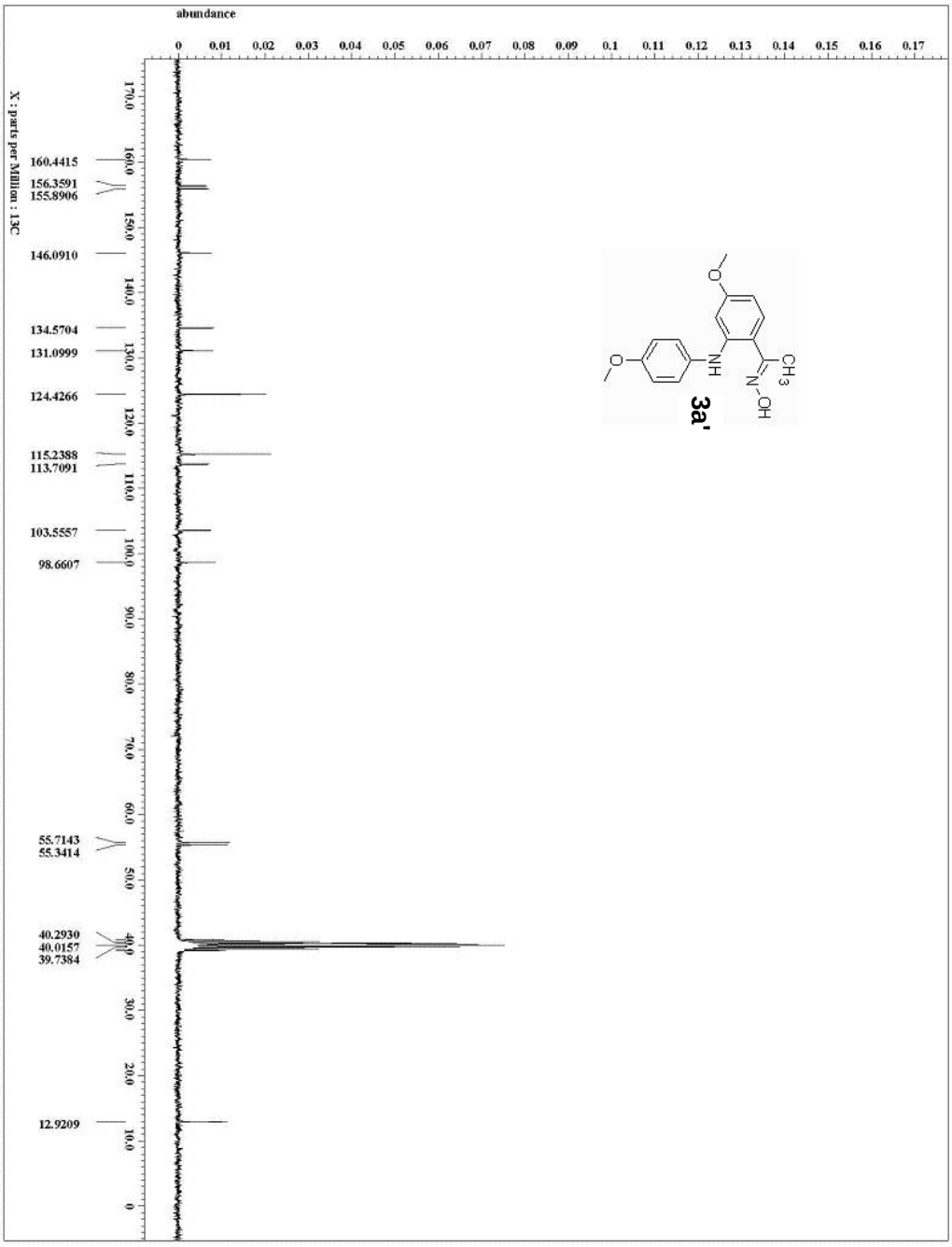

abundance
X : parts per Million : 1H
7.3641
7.2428
7.2382
7.2337
7.2096
6.7060
6.6808
6.6579
3.1853
3.1624
3.1384
2.8683
2.8431
2.8179
1.6711
1.6459
1.6219
1.4456
1.4204
1.2304
1.2052
1.1800
0.9786
0.9545
0.9294
0.0744
-0.0000
0.99
3.22
1.96
1.95
1.99
2.05
2.07
3.01
3
3y

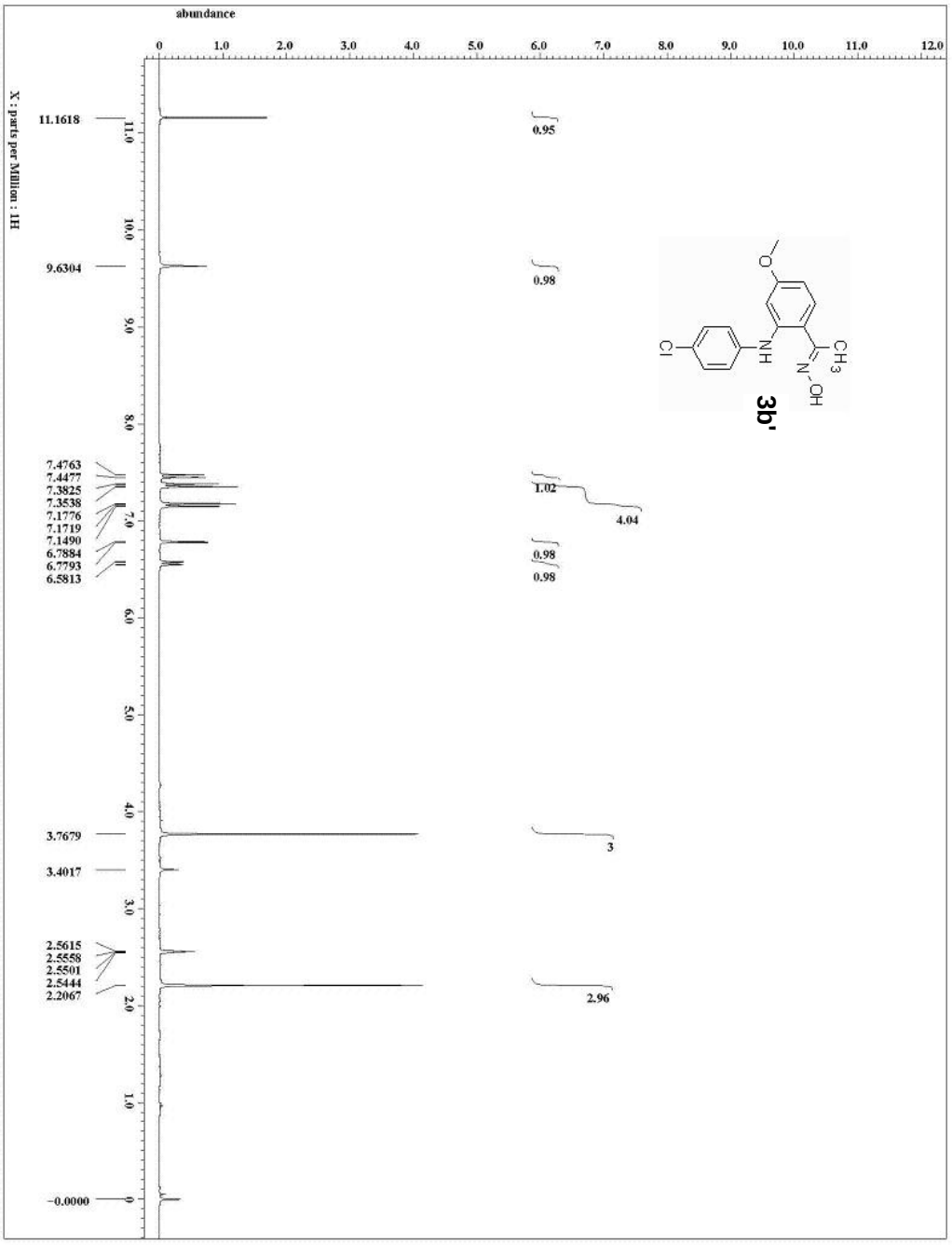

(thousandths)
0
10.0
20.0
30.0
40.0
50.0
60.0
70.0
X : parts per Million : 13C
164.0267
147.6781
130.0960
128.9201
116.6060
115.0285
111.1277
77.5603
77.1397
76.7190
43.2950
31.4685
20.6076
19.9766
14.0586
11.6206
H
N
N
OH
CH3
3y

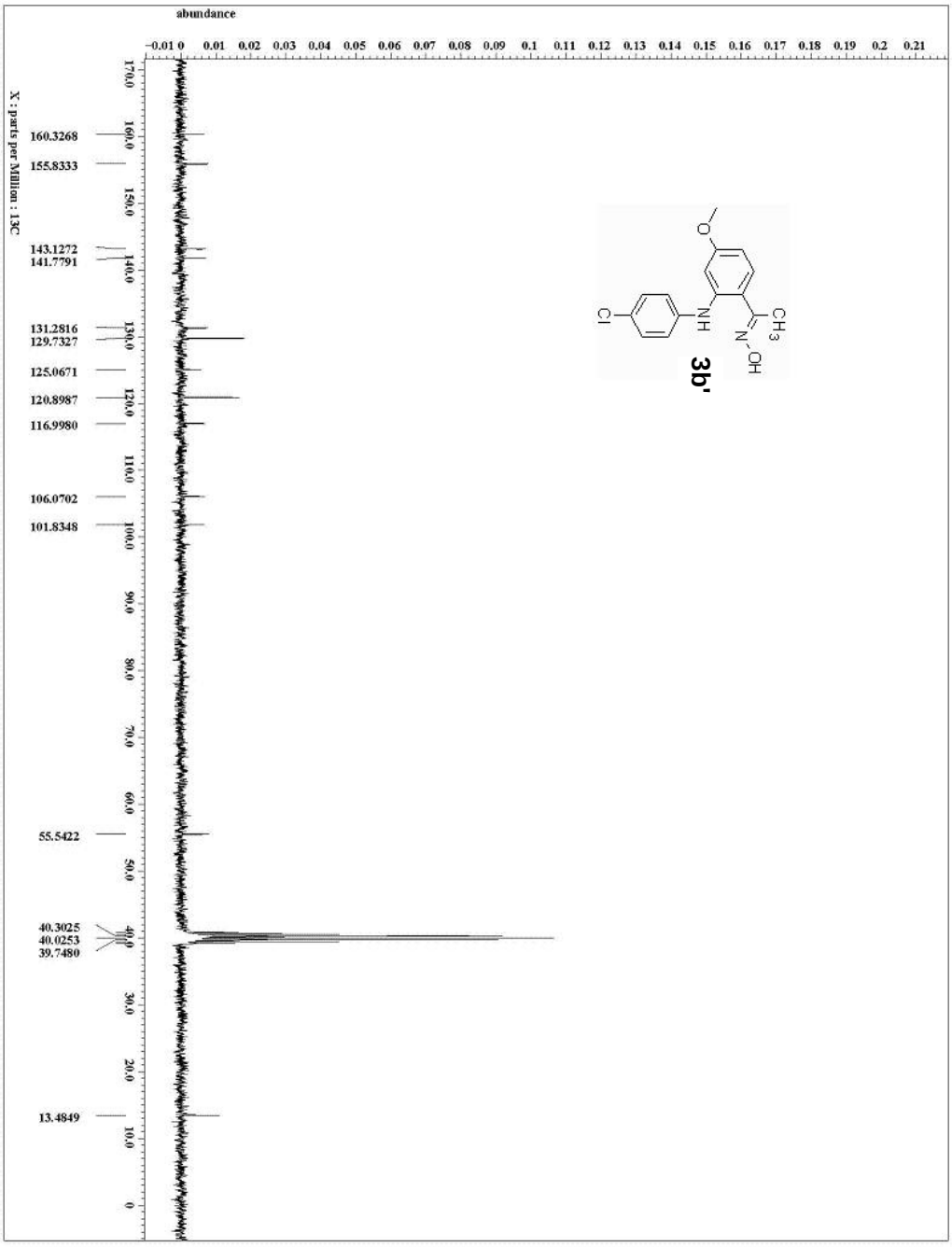

abundance
X : parts per Million : 1H
11.1492
9.7220
7.4740
7.4443
7.3779
7.3504
7.3252
7.1913
7.1661
7.0082
6.7964
6.7873
3.7450
3.4074
2.5535
2.5478
2.5421
2.2342
0.0000
0.91
0.95
1.02
1.99
1.98
0.97
0.97
1.03
3.03
3
NH
N
OH
CH3
O
3z

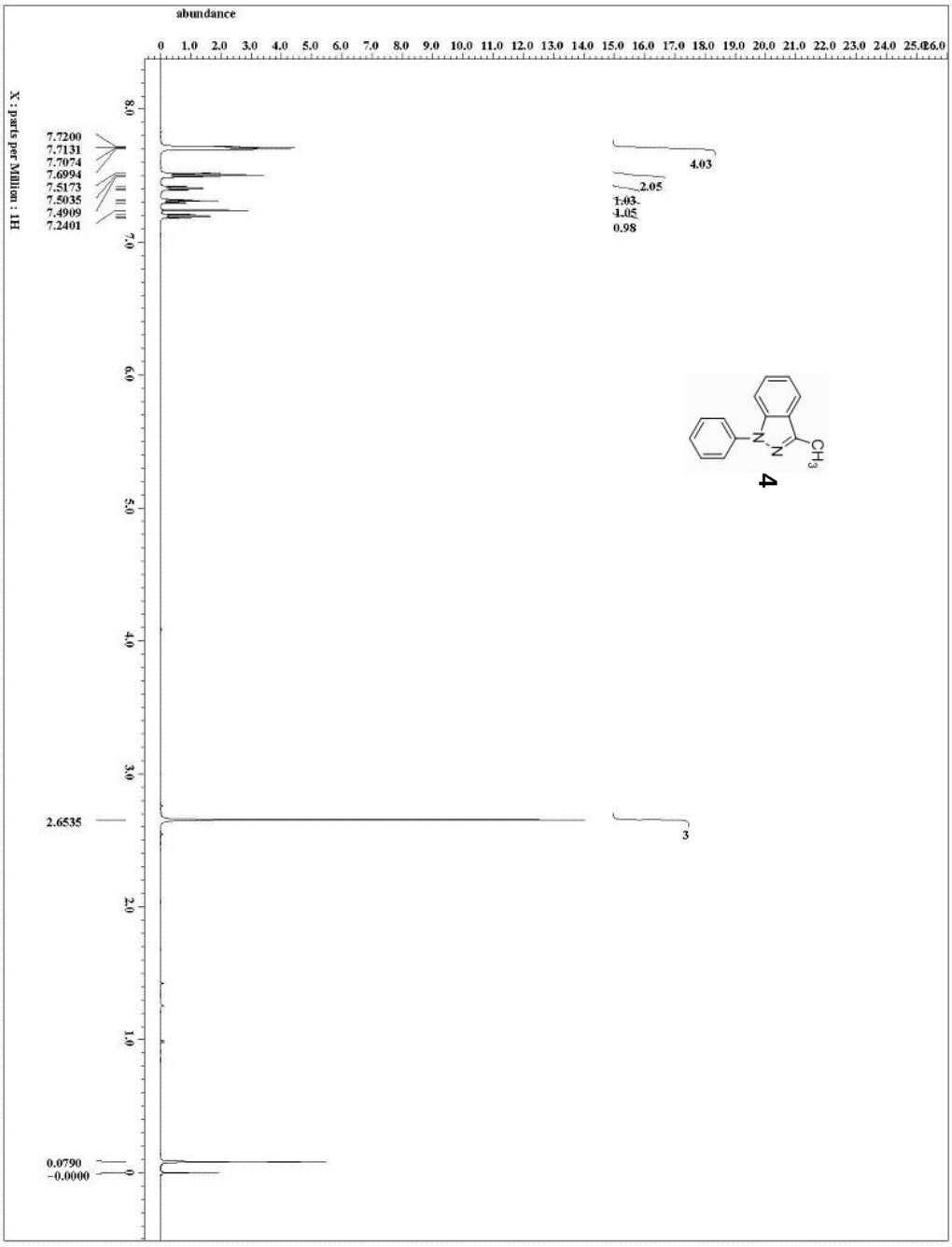

abundance
X : parts per Million : 13C
160.3076
156.0436
143.8825
142.3815
131.2146
129.9526
122.2276
120.1339
115.8411
105.1906
100.7831
55.4657
40.3025
40.0253
39.7480
13.3033
NH
N
OH
CH3
3z

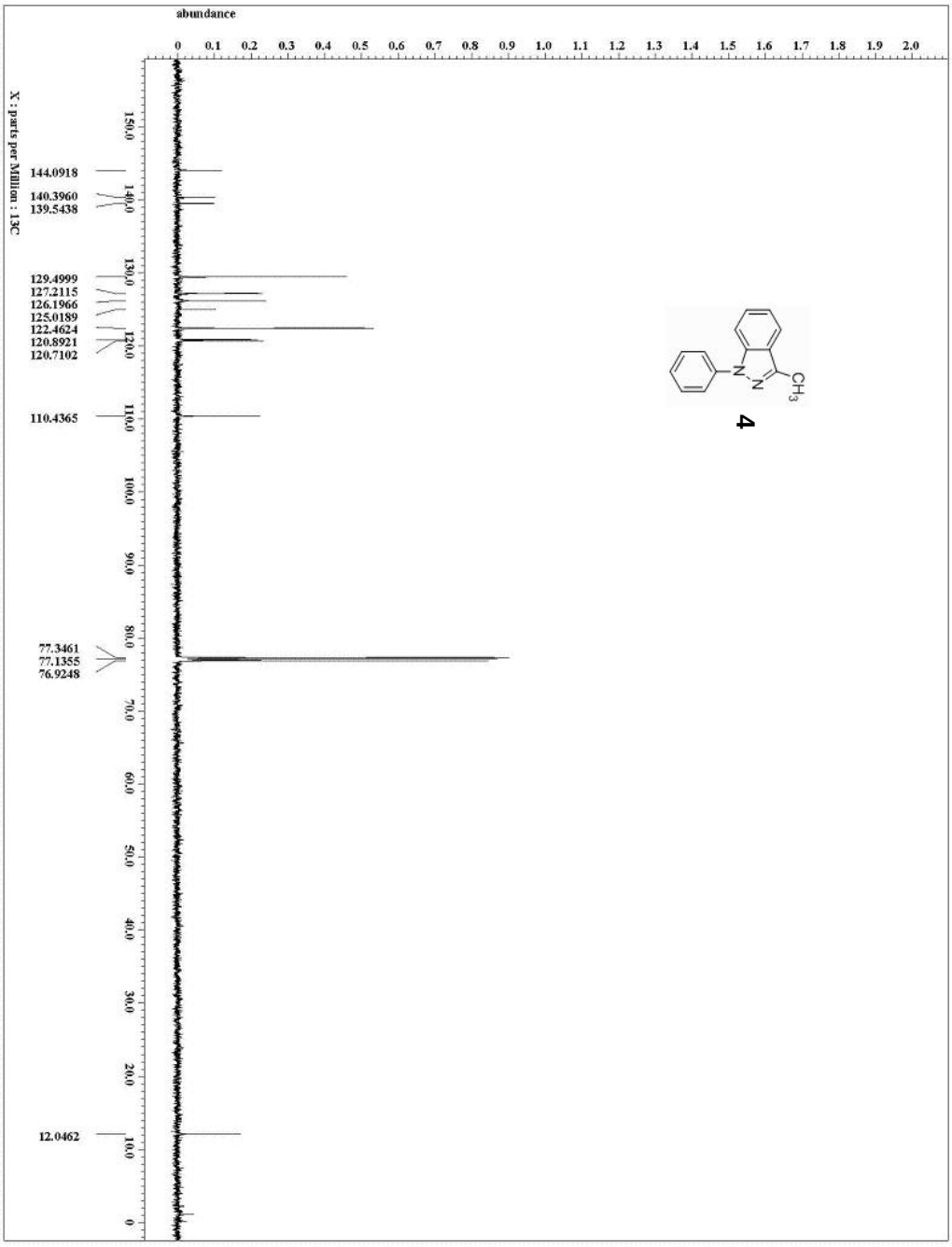

abundance
X : parts per Million : 1H
11.0920
9.6590
7.4534
7.4237
7.1696
7.1398
6.9910
6.9613
6.5023
6.4931
6.4142
6.4050
6.3844
3.7862
3.6947
3.4017
2.5455
2.2582
0.92
1.03
1.03
4.04
1.03
1.02
3.14
3.14
3
3a'

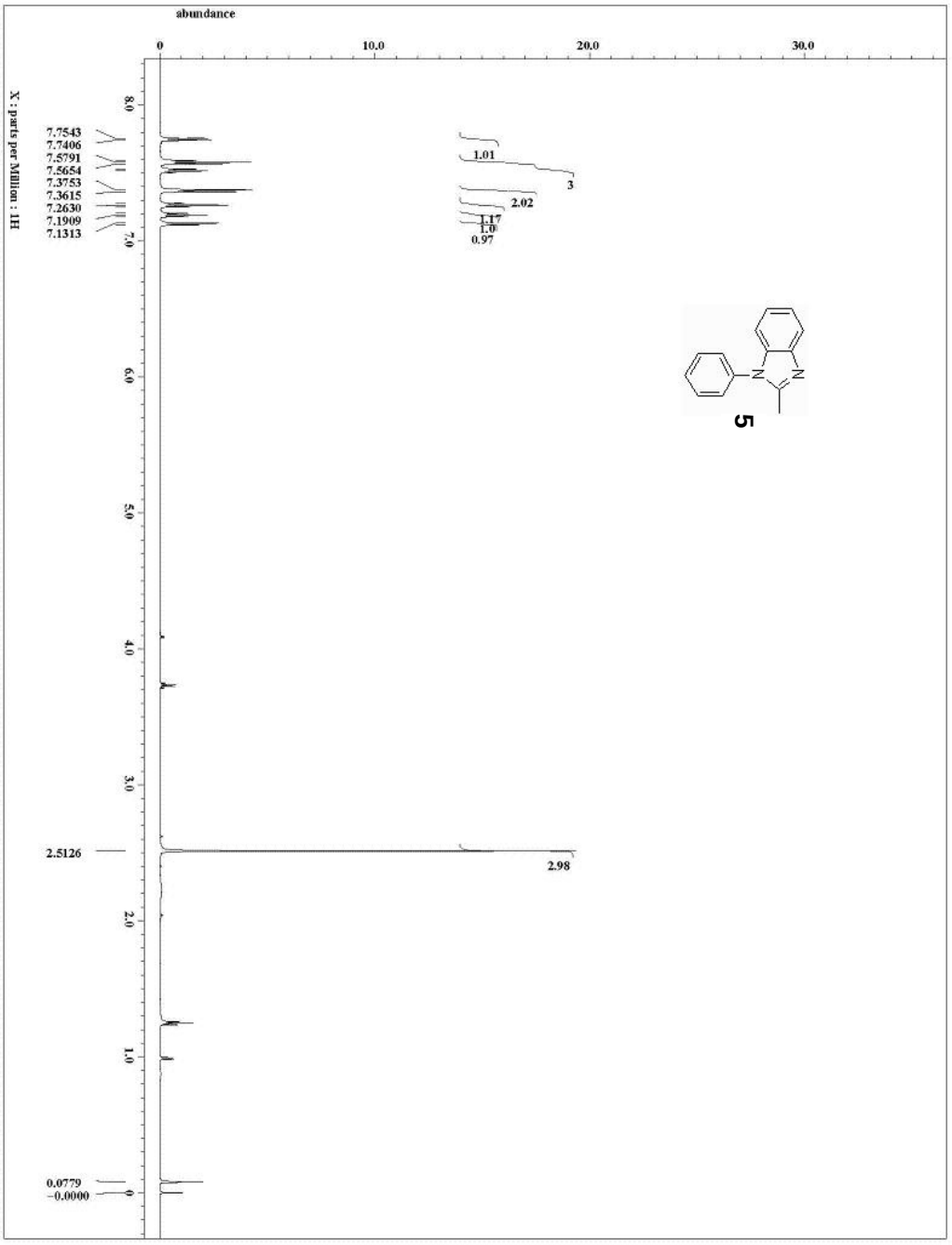

abundance
0 0.01 0.02 0.03 0.04 0.05 0.06 0.07 0.08 0.09 0.1 0.11 0.12 0.13 0.14 0.15 0.16 0.17
X : parts per Million : 13C
160.4415
156.3591
155.8906
146.0910
134.5704
131.0999
124.4266
115.2388
113.7091
103.5557
98.6607
55.7143
55.3414
40.2930
40.0157
39.7384
12.9209
170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0
O
NH
CH3
N
OH
3a'

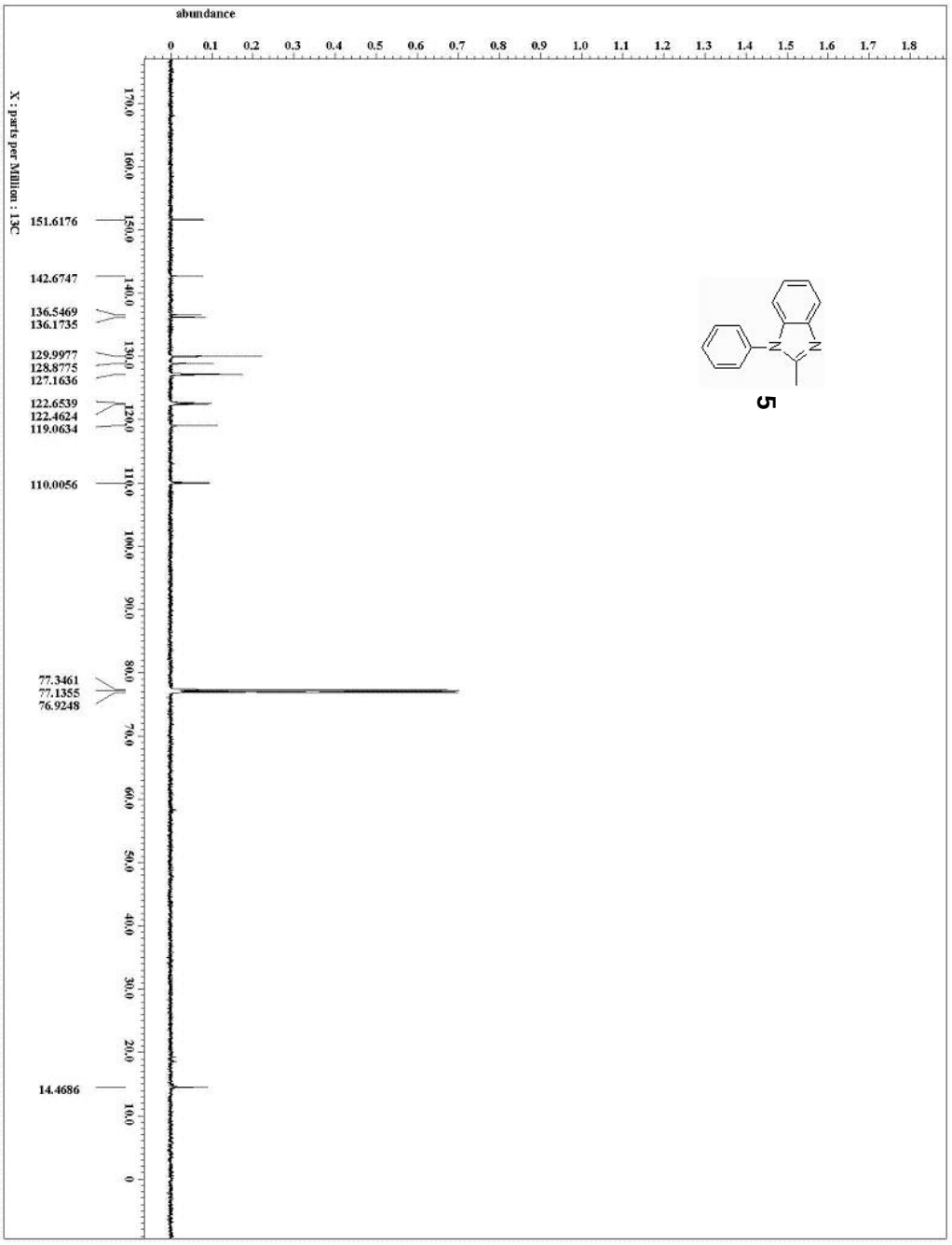

abundance
X : parts per Million : 1H
11.1618
9.6304
7.4763
7.4477
7.3825
7.3538
7.1776
7.1719
7.1490
6.7884
6.7793
6.5813
3.7679
3.4017
2.5615
2.5558
2.5501
2.5444
2.2067
-0.0000
0.95
0.98
1.02
4.04
0.98
0.98
3
2.96
Cl
NH
N
OH
CH3
O
3b'


abundance
X : parts per Million : 13C
160.3268
155.8333
143.1272
141.7791
131.2816
129.7327
125.0671
120.8987
116.9980
106.0702
101.8348
55.5422
40.3025
40.0253
39.7480
13.4849
3b'


abundance
X : parts per Million : 1H
7.7200
7.7131
7.7074
7.6994
7.5173
7.5035
7.4909
7.2401
4.03
2.05
1.03
1.05
0.98
2.6535
3
0.0790
-0.0000
CH3
4


abundance
X : parts per Million : 13C
144.0918
140.3960
139.5438
129.4999
127.2115
126.1966
125.0189
122.4624
120.8921
120.7102
110.4365
77.3461
77.1355
76.9248
12.0462
CH3
4


abundance
0
10.0
20.0
30.0
X : parts per Million : 1H
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
7.7543
7.7406
7.5791
7.5654
7.3753
7.3615
7.2630
7.1909
7.1313
1.01
3
2.02
1.17
1.0
0.97
2.5126
2.98
0.0779
-0.0000
5


abundance
X : parts per Million : 13C
151.6176
142.6747
136.5469
136.1735
129.9977
128.8775
127.1636
122.6539
122.4624
119.0634
110.0056
77.3461
77.1355
76.9248
14.4686
5