Supporting Information

Visible-light Promoted α-Alkylation of Glycine Derivatives with Alkyl Boronic Acids

Jiayuan Wang, Yingpeng Su*, Zhengjun Quan*, Jun Li, Jie Yang, Yong Yuan, Congde Huo*

Gansu International Scientific and Technological Cooperation Base of Water-Retention Chemical Functional Materials; College of Chemistry and Chemical Engineering, Northwest Normal University, Lanzhou, Gansu 730070, China.

E-mail: huocongde1978@hotmail.com

Table of Contents Graphic

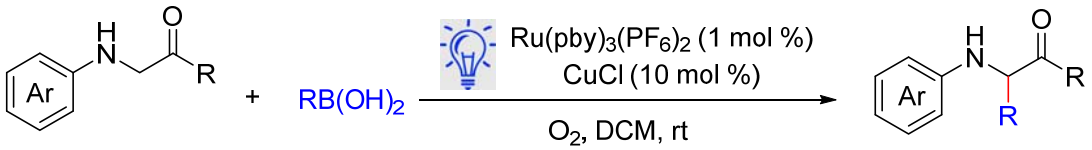
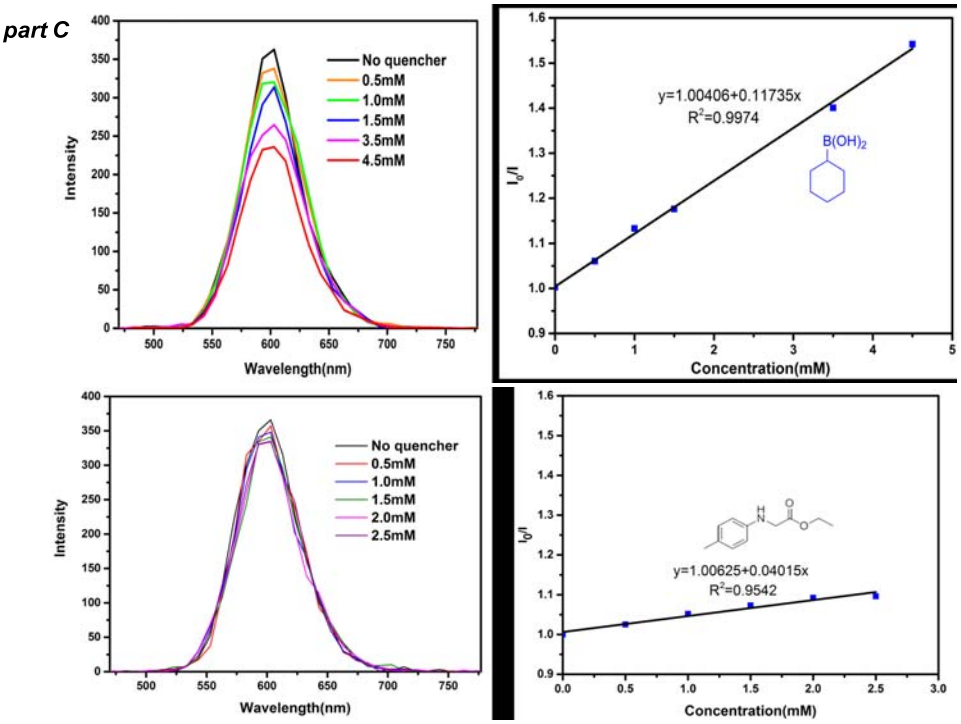


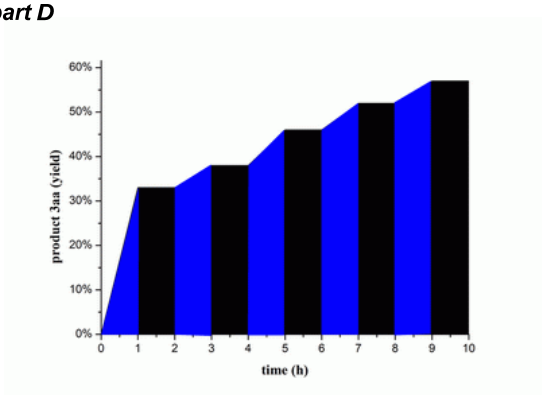
Table of Contents

Part C and Part D of **Scheme 5.** Control Experiments

part C



part D



General Information

The starting materials, reagents and solvents, purchased from commercial suppliers, were used without further purification. Literature procedures were used for the preparation of glycine derivatives (*PNAS*, 2009, **106**, 4106). Analytical TLC was performed with silica gel GF254 plates, and the products were visualized by UV detection. Flash chromatography was carried out using silica gel 200−300. ^{1}HNMR (400 MHz or 600 Hz) and ^{13}CNMR (150 MHz) spectra were measured with $CDCl_3$ as solvent. All chemical shifts (δ) are reported in ppm and coupling constants (*J*) in Hz. High resolution mass spectra (HR-MS) were recorded under electrospray ionization (ESI) conditions.

General procedure for the visible-light promoted C-H alkylation of glycine derivatives with alkyl boronic acids

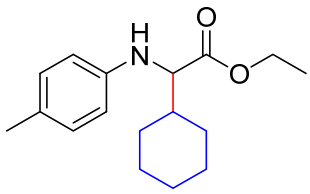
To a dried reaction tube (10 mL) with a magnetic stirring bar were added glycine esters (**1,** 0.2 mmol), alkyl boronic acids (**2**, 0.4 mmol), $Ru(bpy)_3(PF_6)_2$ (1 mol %), CuCl (10 mol %) and DCM (2 mL) successively under oxygen atmosphere (O_2 balloon). The resulting reaction mixture was performed at room temperature under blue LEDs irradiation (6 W) for 8-14 hours. After the reaction was completed, the reaction mixture was concentrated under reduced pressure, and the residue was purified by column chromatography to afford the desired compounds **3** (ethyl acetate/petroleum ether = 1:40 to 1:15).

Scale-up experiment

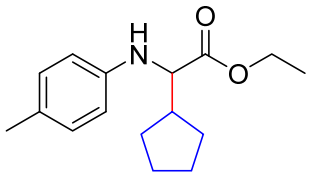
To a dried reaction tube (50 mL) with a magnetic stirring bar were added glycine esters (**1n,** 10 mmol), alkyl boronic acids (**2a**, 20 mmol), $Ru(bpy)_3(PF_6)_2$ (1 mol %), CuCl (10 mol %) and DCM (30 mL) successively under oxygen atmosphere (O_2 balloon). The resulting reaction mixture was performed at room temperature under blue LEDs irradiation (24 W) for 10 hours. After the reaction was completed, the reaction mixture was concentrated under reduced pressure, and the residue was purified by column chromatography to afford the desired compounds **3na** (1.8 g, 62% yield, ethyl acetate/petroleum ether = 1:40).

Photos of reaction set-up

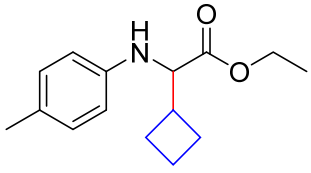
Characterization of theproducts



Ethyl 2-cyclohexyl-2-(p-tolylamino)acetate (3aa). The desired pure product was obtained in 71% yield (39.5 mg) as a yellow oil. ^{1}H NMR (600 MHz, $CDCl_3$) δ 6.96 (d, *J* = 8.0 Hz, 2H), 6.54 (d, *J* = 8.4 Hz, 2H), 4.15 (q, *J* = 7.1 Hz, 2H), 3.81 (d, *J* = 6.2 Hz, 1H), 2.21 (s, 3H), 1.88 – 1.63 (m, 7H), 1.30 – 1.26 (m, 1H), 1.23 (t, *J* = 7.1 Hz, 3H), 1.21 – 1.11 (m, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 173.8, 145.2, 129.7, 127.3, 113.7, 62.4, 60.7, 41.3, 29.6, 29.2, 26.2, 26.1, 26.0, 20.3,14.3. HRMS (ESI) exact mass calcd for $C_{17}H_{26}NO_2$ [M+H] m/z 276.1958, found 276.1951.

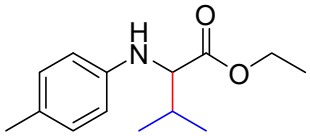


Ethyl 2-cyclopentyl-2-(p-tolylamino)acetate (3ab). The desired pure product was obtained in 58% yield (30.5 mg) as a yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.97 (d, *J* = 8.1 Hz, 2H), 6.56 (d, *J* = 8.4 Hz, 2H), 4.15 (q, *J* = 7.1 Hz, 2H), 3.82 (d, *J* = 7.9 Hz, 1H), 2.22 (s, 3H), 1.96 – 1.39 (m, 9H), 1.23 (t, *J* = 7.1 Hz, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 174.3, 145.1, 129.7, 127.4, 113.7, 61.3, 60.7, 43.2, 29.4, 29.0, 25.3, 25.1, 20.4, 14.3. HRMS (ESI) exact mass calcd for $C_{16}H_{24}NO_2$ [M+H] m/z 262.1802, found 262.1800.

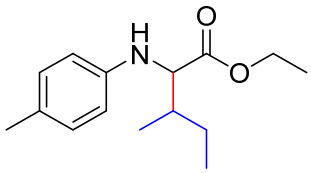


Ethyl 2-cyclobutyl-2-(p-tolylamino)acetate (3ac). The desired pure product was obtained in 42% yield (23.5 mg) as a yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.98 (d, *J* = 8.1 Hz, 2H), 6.55 (d, *J* = 8.4 Hz, 2H), 4.15 (q, *J* = 7.1 Hz, 2H), 3.92 (s, 1H), 2.67 – 2.57 (m, 1H), 2.23 (s, 3H), 2.11 – 1.74 (m, 6H), 1.23 (t, *J* = 7.1 Hz, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 173.5, 145.1, 129.7, 127.5, 113.7, 61.5, 60.7, 38.4,

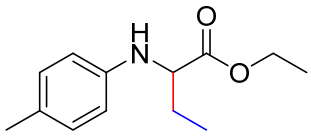
25.4, 24.8, 20.4, 18.1, 14.3. HRMS (ESI) exact mass calcd for $C_{15}H_{22}NO_2$ [M+H] m/z 248.1645, found 248.1642.



Ethyl p-tolylvalinate (3ad). The desired pure product was obtained in 62% yield (29.3 mg) as a yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.98 (d, *J* = 8.0 Hz, 2H), 6.57 (d, *J* = 8.3 Hz, 2H), 4.17 (q, *J* = 7.1 Hz, 2H), 3.82 (d, *J* = 5.8Hz, 1H), 2.23 (s, 3H), 2.12 – 2.02 (m, 1H), 1.25 (t, *J* = 7.2 Hz, 3H), 1.05 (d, *J* = 6.9 Hz, 3H), 1.02 (d, *J* = 6.8 Hz, 3H).^{13}C NMR (150 MHz, $CDCl_3$) δ 173.8, 145.1, 129.7, 127.4, 113.8, 62.9, 60.7, 31.5, 20.4, 19.1, 18.7, 14.3. HRMS (ESI) exact mass calcd for $C_{14}H_{22}NO_2$ [M+H] m/z 236.1645, found 236.1647.

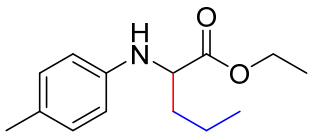


Ethyl 3-methyl-2-(p-tolylamino)pentanoate (3ae). The desired pure product was obtained in 61% yield (28.9 mg) as a yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.98 (d, *J* = 8.5 Hz, 2H), 6.57 (d, *J* = 8.3 Hz, 2H), 4.17 (q, *J* = 7.1 Hz, 2H), 3.93 (dd, *J* = 20.6, 5.5 Hz, 1H), 1.96 – 1.82 (m, 1H), 1.71 – 1.50 (m, 1H), 1.36 – 1.29 (m, 1H), 1.25 (t, *J* = 7.1 Hz, 3H), 1.01 (d, *J* = 6.9 Hz, 3H), 0.96 (t, *J* = 8.5 Hz, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 174.0, 145.2, 129.7, 127.4, 113.8, 61.6, 60.7, 38.0, 26.2, 20.4, 15.5, 14.3, 11.7. HRMS (ESI) exact mass calcd for $C_{15}H_{24}NO_2$ [M+H] m/z 250.1802, found 250.1801.

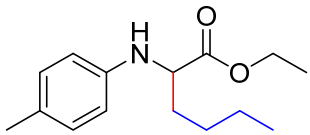


Ethyl 2-(p-tolylamino)butanoate (3af). The desired pure product was obtained in 52% yield (23.2 mg) as a yellow oil ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.98 (d, *J* = 8.3 Hz, 2H), 6.55 (d, *J* = 8.4 Hz, 2H), 4.18 (q, *J* = 7.1 Hz, 2H), 3.98 (t, *J* = 6.3 Hz, 1H), 2.23 (s, 3H), 1.95 – 1.71 (m, 2H), 1.25 (t, *J* = 7.1 Hz, 3H), 1.00 (t, *J* = 7.4 Hz, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 174.1, 144.6, 129.8, 127.4, 113.7, 60.9, 58.2,

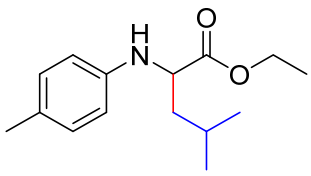
26.1, 20.4, 14.2, 9.9. HRMS (ESI) exact mass calcd for $C_{13}H_{20}NO_2$ [M+H] m/z 222.1489, found 222.1493.



Ethyl 2-(p-tolylamino)pentanoate (3ag). The desired pure product was obtained in 64% yield (30.2 mg) as a yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.97 (d, *J* = 7.8 Hz, 2H), 6.54 (d, *J* = 6.8 Hz, 2H), 4.16 (q, *J* = 7.2 Hz, 2H), 4.01 (t, *J* = 6.1 Hz, 1H), 2.22 (s, 3H), 1.88 – 1.63 (m, 2H), 1.55 – 1.35 (m, 2H), 1.24 (t, *J* = 7.1 Hz, 3H), 0.94 (t, *J* = 7.4Hz, 3H).^{13}C NMR (150 MHz, $CDCl_3$) δ 174.4, 144.6, 129.8, 127.5, 113.7, 60.9, 56.9, 35.2, 20.4, 18.9, 14.2, 13.8. HRMS (ESI) exact mass calcd for $C_{14}H_{22}NO_2$ [M+H] m/z 236.1645, found 236.1650.

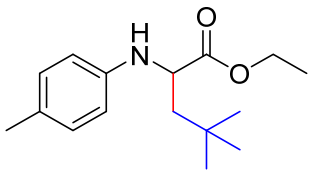


Ethyl 2-(phenylamino)hexanoate (3ah). The desired pure product was obtained in 65% yield (32.3 mg) as a yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.97 (d, *J* = 8.1 Hz, 2H), 6.55 (d, *J* = 6.8 Hz, 2H), 4.17 (q, *J* = 7.1 Hz, 2H), 4.00 (t, *J* = 6.5 Hz, 1H), 2.23 (s, 3H), 1.92 – 1.56 (m, 2H), 1.45 – 1.30 (m, 4H), 1.24 (t, *J* = 7.1 Hz, 3H), 0.90 (t, *J* = 7.1 Hz, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 174.4, 144.7, 129.8, 127.4, 113.7, 60.8, 57.0, 32.9, 27.7, 22.4, 20.4, 14.2, 13.9. HRMS (ESI) exact mass calcd for $C_{15}H_{24}NO_2$ [M+H] m/z 250.1802, found 250.1806.

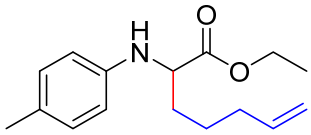


Ethyl p-tolylleucinate (3ai). The desired pure product was obtained in 65% yield (32.4 mg) as a yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.97 (d, *J* = 8.0 Hz, 2H), 6.55 (d, *J* = 8.4 Hz, 2H), 4.15 (q, *J* = 7.1 Hz, 2H), 4.04 (s, 1H), 3.85 (s, 1H), 2.23 (s, 3H), 1.91 – 1.72 (m, 1H), 1.65 – 1.60 (m, 2H), 1.23 (t, *J* = 7.1 Hz, 3H), 0.99 (d, *J* = 6.6 Hz, 3H), 0.94 (d, *J* = 6.6 Hz, 3H).^{13}C NMR (150 MHz, $CDCl_3$) δ 174.9,

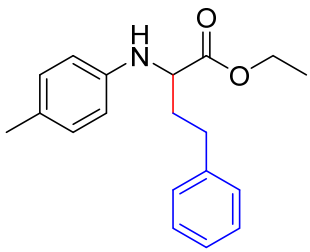
144.7, 129.8, 127.5, 113.7, 60.8, 55.6, 42.4, 24.9, 22.7, 22.2, 20.4, 14.2. HRMS (ESI) exact mass calcd for $C_{15}H_{24}NO_2$ [M+H] m/z 250.1802, found 250.1800.



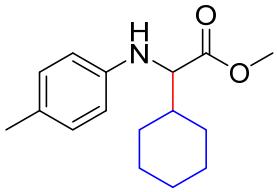
Ethyl 4,4-dimethyl-2-(p-tolylamino)pentanoate (3aj). The desired pure product was obtained in 62% yield (32.5 mg) as a yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.98 (d, *J* = 8.5 Hz, 2H), 6.55 (d, *J* = 8.4 Hz, 2H), 4.21 – 4.08 (m, 2H), 4.05 (s, 1H), 3.77 (s, 1H), 2.23 (s, 3H), 1.76 (dd, *J* = 14.2, 5.0 Hz, 1H), 1.58 (dd, *J* = 14.2, 7.4 Hz, 1H), 1.22 (t, *J* = 7.1 Hz, 3H), 1.00 (s, 9H).^{13}C NMR (150 MHz, $CDCl_3$) δ 175.1, 144.5, 129.7, 127.5, 113.7, 60.8, 54.9, 47.0, 30.7, 29.8, 20.4, 14.1. HRMS (ESI) exact mass calcd for $C_{16}H_{26}NO_2$ [M+H] m/z 264.1958, found 264.1963.



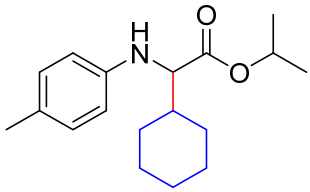
Ethyl 2-(p-tolylamino)hept-6-enoate (3ak). The desired pure product was obtained in 53% yield (27.3 mg) as a yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.98 (d, *J* = 0.6 Hz, 2H), 6.55 (d, *J* = 8.4 Hz, 2H), 5.89 – 5.64 (m, 1H), 5.13 – 4.91 (m, 2H), 4.18 (q, *J* = 7.1 Hz, 2H), 4.04 (s, 1H), 4.02 (d, *J* = 6.8 Hz, 1H), 2.24 (s, 3H), 2.15 – 2.04 (m, 2H), 1.90 – 1.71 (m, 2H), 1.61 – 1.51 (m, 2H), 1.25 (t, *J* = 7.1 Hz, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 174.3, 144.6, 138.1, 129.8, 127.5, 115.0, 113.7, 60.9, 56.9, 33.3, 32.5, 24.8, 20.4, 14.2. HRMS (ESI) exact mass calcd for $C_{16}H_{24}NO_2$ [M+H] m/z 262.1802, found 262.1804.



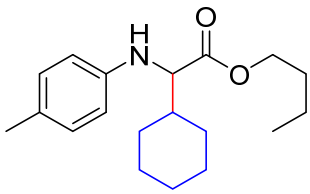
Ethyl 4-phenyl-2-(p-tolylamino)butanoate (3al). The desired pure product was obtained in 70% yield (41.4 mg) as a yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.32 – 7.27 (m, 2H), 7.23 – 7.18 (m, 3H), 6.98 (d, *J* = 8.0 Hz, 2H), 6.52 (d, *J* = 8.5 Hz, 2H), 4.16 (q, *J* = 7.1 Hz, 2H), 4.03 (d, *J* = 5.8 Hz, 2H), 2.77 (t, *J* = 7.9 Hz, 2H), 2.23 (s, 3H), 2.21 – 2.11 (m, 1H), 2.09 – 1.99 (m, 1H), 1.25 (t, *J* = 7.1 Hz, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 174.1, 144.5, 141.0, 129.8, 128.5, 128.4, 127.6, 126.1, 113.8, 61.0, 56.5, 34.7, 31.8, 20.4, 14.2. HRMS (ESI) exact mass calcd for $C_{19}H_{24}NO_2$ [M+H] m/z 298.1802, found 298.1798.



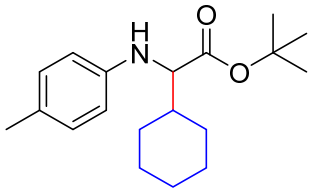
Methyl 2-cyclohexyl-2-(p-tolylamino)acetate (3ba). The desired pure product was obtained in 62% yield (32.3 mg) as a yellow oil. ^{1}H NMR (600 MHz, $CDCl_3$) δ 6.97 (d, *J* = 8.0 Hz, 2H), 6.54 (d, *J* = 8.4 Hz, 2H), 3.98 (s, 1H), 3.84 (d, *J* = 6.2 Hz, 1H), 3.69 (s, 3H), 2.22 (s, 3H), 1.89 – 1.58 (m, 6H), 1.30 – 1.08 (m, 5H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 174.4, 145.1, 129.8, 127.4, 113.7, 62.4, 51.7, 41.3, 29.7, 29.2, 26.2, 26.1, 26.0, 20.4. HRMS (ESI) exact mass calcd for $C_{16}H_{24}NO_2$ [M+H] m/z 262.1802, found 262.1805.



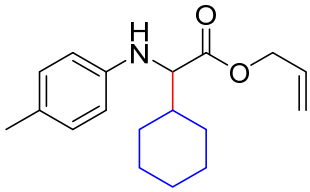
Isopropyl 2-cyclohexyl-2-(p-tolylamino)acetate (3ca). The desired pure product was obtained in 59% yield (32.4 mg) as a yellow oily liquid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.97 (d, *J* = 7.8Hz, 2H), 6.56 (d, *J* = 8.3 Hz, 2H), 5.17 – 4.72 (m, 1H), 4.03 (s, 1H), 3.80 (d, *J* = 5.9 Hz, 1H), 2.23 (s, 3H), 1.92 – 1.61 (m, 6H), 1.28 (d, *J* = 6.2 Hz, 2H), 1.22 (t, *J* = 7.2 Hz, 7H), 1.19 – 1.11 (m, 2H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 173.3, 145.2, 129.7, 127.2, 113.8, 68.3, 62.5, 41.3, 29.6, 29.2, 26.2, 26.1, 26.0, 21.9, 21.9, 20.4. HRMS (ESI) exact mass calcd for $C_{18}H_{28}NO_2$ [M+H] m/z 290.2115, found 290.2116.



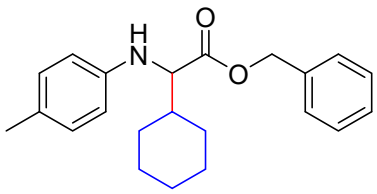
Butyl 2-cyclohexyl-2-(p-tolylamino)acetate (3da). The desired pure product was obtained in 59% yield (34.4 mg) as a red oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.97 (d, *J* = 8.5 Hz, 2H), 6.55 (d, *J* = 8.4 Hz, 2H), 4.10 (t, *J* = 6.7 Hz, 2H), 4.00 (s, 1H), 3.83 (d, *J* = 6.1 Hz, 1H), 2.23 (s, 3H), 1.90 – 1.63 (m, 7H), 1.64 – 1.54 (m, 2H), 1.39 – 1.29 (m, 2H), 1.29 – 1.12 (m, 4H), 0.91 (t, *J* = 7.4 Hz, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 174.0, 145.2, 129.7, 127.3, 113.7, 64.6, 62.5, 41.3, 30.6, 29.6, 29.2, 26.2, 26.1, 26.0, 20.3, 19.1, 13.6. HRMS (ESI) exact mass calcd for $C_{19}H_{30}NO_2$ [M+H] m/z 304.2271, found 304.2274.



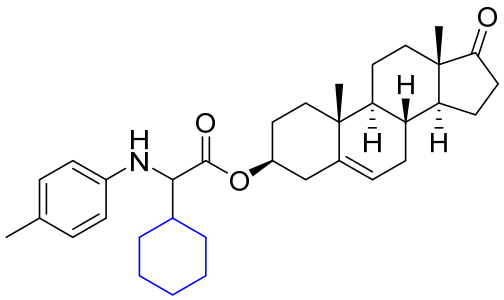
Tert-butyl 2-cyclohexyl-2-(p-tolylamino)acetate (3ea). The desired pure product was obtained in 50% yield (29.4 mg) as a red oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.97 (d, *J* = 8.0 Hz, 2H), 6.55 (d, *J* = 8.4 Hz, 2H), 4.00 (s, 1H), 3.72 (d, *J* = 5.7 Hz, 1H), 2.23 (s, 3H), 1.86 – 1.62 (m, 6H), 1.42 (s, 9H), 1.27 – 1.12 (m, 5H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 173.0, 145.4, 129.6, 127.0, 113.7, 81.3, 62.8, 41.3, 29.5, 29.1, 28.1, 26.3, 26.2, 26.1, 20.4. HRMS (ESI) exact mass calcd for $C_{19}H_{30}NO_2$ [M+H] m/z 304.2271, found 304.2277.



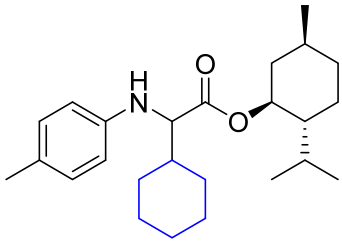
Allyl 2-cyclohexyl-2-(p-tolylamino)acetate (3fa). The desired pure product was obtained in 40% yield (19.8 mg) as a yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.97 (d, *J* = 8.4 Hz, 2H), 6.55 (d, *J* = 8.4 Hz, 2H), 6.00 – 5.76 (m, 1H), 5.28 (dd, *J* = 12.7, 7.1, 1.3 Hz, 2H), 4.60 (d, *J* = 5.8 Hz, 2H), 3.99 (s, 1H), 3.87 (s, 1H), 2.22 (s, 3H), 1.90 – 1.62 (m, 6H), 1.29 – 1.11 (m, 5H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 173.5, 145.1, 131.9, 129.7, 127.4, 118.6, 113.7, 65.3, 62.5, 41.3, 29.7, 29.1, 26.2, 26.1, 26.0, 20.4. HRMS (ESI) exact mass calcd for $C_{18}H_{26}NO_2$ [M+H] m/z 288.1958, found 288.1961.



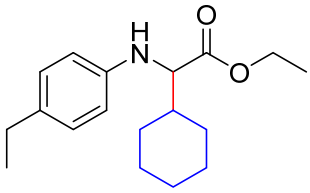
Benzyl 2-cyclohexyl-2-(p-tolylamino)acetate (3ga). The desired pure product was obtained in 54% yield (36.1 mg) as a red oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.47 – 7.28 (m, 5H), 6.99 (d, *J* = 8.0 Hz, 2H), 6.58 (d, *J* = 8.4 Hz, 2H), 5.16 (s, 2H), 4.04 (d, *J* = 9.1 Hz, 1H), 3.97 – 3.90 (m, 1H), 2.26 (s, 3H), 1.91 – 1.64 (m, 6H), 1.28 – 1.14 (m, 5H).^{13}C NMR (100 MHz, $CDCl_3$) δ 174.1, 145.4, 135.9, 130.1, 128.8, 128.6, 128.5, 127.7, 114.1, 66.8, 62.8, 41.6, 29.9, 29.4, 26.4, 26.32, 26.3, 20.7. HRMS (ESI) exact mass calcd for $C_{22}H_{28}NO_2$ [M+H] m/z 338.2115, found 338.2119.



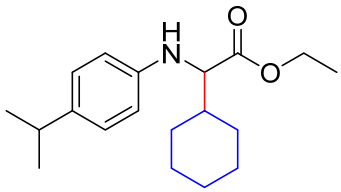
(3S,8R,9S,10R,13S,14S)-10,13-dimethyl-17-oxo-2,3,4,7,8,9,10,11,12,13,14,15,16,17-tetradecahydro-1H-cyclopenta[a]phenanthren-3-yl 2-cyclohexyl-2-(p-tolylamino)acetate (3ha). The desired pure product was obtained in 51% yield (54.7 mg) as a red oil. ^{1}H NMR (600 MHz, $CDCl_3$) δ 6.96 (dd, *J* = 8.2, 1.6 Hz, 2H), 6.54 (d, *J* = 8.4 Hz, 2H), 5.39 (t, *J* = 5.0 Hz, 1H), 4.67 – 4.62 (m, 1H), 4.00 (s, 1H), 3.82 (d, *J* = 36.9 Hz, 1H), 2.45 (dd, *J* = 19.3, 8.7 Hz, 1H), 2.38 – 2.27 (m, 2H), 2.22 (s, 3H), 2.14 – 2.04 (m, 2H), 1.98 – 1.91 (m, 1H), 1.87 – 1.45 (m, 14H), 1.33 – 1.11 (m, 9H), 1.05 (s, 3H), 0.88 (s, 3H).^{13}C NMR (150 MHz, $CDCl_3$) δ 220.9, 173.2, 145.2, 139.7, 129.7, 127.2, 122.0, 113.7, 74.2, 62.5, 51.7, 50.1, 47.5, 41.3, 38.1, 36.8, 36.7, 35.8, 31.4, 31.4, 30.7, 29.6, 29.2, 27.8, 26.2, 26.1, 26.06, 21.9, 20.4, 20.3, 19.3, 13.5. HRMS (ESI) exact mass calcd for $C_{34}H_{48}NO_3$ [M+H] m/z 518.3629, found 518.3625.



(1S,2R,5S)-2-isopropyl-5-methylcyclohexyl 2-cyclohexyl-2-(p-tolylamino)acetate (3ia). The desired pure product was obtained in 61% yield (48.6 mg) as a red oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.95 (d, *J* = 8.4 Hz, 2H), 6.55 (d, *J* = 8.4 Hz, 2H), 4.72 – 4.60 (m, 1H), 3.95 (d, *J* = 9.0 Hz, 1H), 3.83 – 3.74 (m, 1H), 2.22 (s, 3H), 1.99 – 1.60 (m, 11H), 1.50 – 1.10 (m, 8H), 0.88 (d, *J* = 6.5 Hz, 3H), 0.85 (d, *J* = 7.0 Hz, 3H), 0.62 (d, *J* = 6.9 Hz, 3H).^{13}C NMR (150 MHz, $CDCl_3$) δ 173.5, 145.2, 129.6, 127.4, 114.1, 74.9, 62.8, 46.9, 41.3, 40.8, 34.2, 31.4, 29.6, 29.4, 26.3, 26.1, 26.0, 25.9, 23.1, 22.0, 20.8, 20.4, 15.9. HRMS (ESI) exact mass calcd for $C_{25}H_{40}NO_2$ [M+H] m/z 386.3054, found 386.3053.

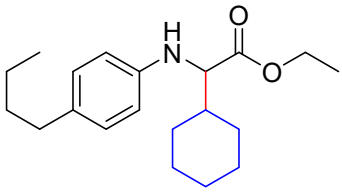


Ethyl 2-cyclohexyl-2-((4-ethylphenyl)amino)acetate (3ja). The desired pure product was obtained in 63% yield (36.5 mg) as a red oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.00 (d, *J* = 8.5 Hz, 2H), 6.57 (d, *J* = 8.5 Hz, 2H), 4.16 (q, *J* = 7.1 Hz, 2H), 4.03 (s, 1H), 3.83 (d, *J* = 6.1 Hz, 1H), 2.53 (q, *J* = 7.6 Hz, 2H), 1.96 – 1.56 (m, 7H), 1.40 – 1.27 (m, 1H), 1.25 (t, *J* = 7.1 Hz, 3H), 1.18 (t, *J* = 7.6 Hz, 3H), 1.15 – 1.08 (m, 1H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 173.7, 145.4, 133.9, 128.5, 113.8, 62.5, 60.6, 41.4, 29.6, 29.2, 27.8, 26.2, 26.1, 26.06, 15.7, 14.2. HRMS (ESI) exact mass calcd for $C_{18}H_{28}NO_2$ [M+H] m/z 290.2115, found 290.2115.

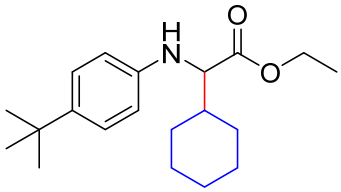


Ethyl 2-cyclohexyl-2-((4-isopropylphenyl)amino)acetate (3ka) The desired pure product was obtained in 61% yield (36.6 mg) as a red oil.^{1}H NMR (400 MHz, $CDCl_3$) δ 7.03 (d, *J* = 8.5 Hz, 2H), 6.58 (d, *J* = 8.5 Hz, 2H), 4.16 (q, *J* = 7.1 Hz, 2H), 4.05 (s, 1H), 3.83 (d, *J* = 6.0 Hz, 1H), 1.90 – 1.62 (m, 7H), 1.43

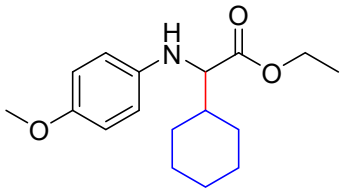
– 1.27 (m, 2H), 1.25 (t, *J* = 7.1 Hz, 3H), 1.19 (d, *J* = 6.9 Hz, 6H), 1.17 – 1.10 (m, 2H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 173.9, 145.5, 138.5, 127.1, 113.5, 62.3, 60.7, 41.4, 33.1, 29.6, 29.2, 26.2, 26.1, 26.0, 24.2, 24.1, 14.3. HRMS (ESI) exact mass calcd for $C_{19}H_{30}NO_2$ [M+H] m/z 304.2271, found 304.2276.



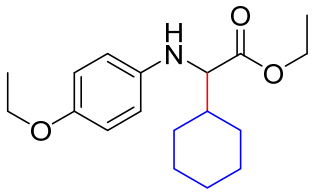
Ethyl 2-((4-butylphenyl)amino)-2-cyclohexylacetate (3la). The desired pure product was obtained in 62% yield (38.8 mg) as a red oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.97 (d, *J* = 8.3 Hz, 2H), 6.56 (d, *J* = 8.4 Hz, 2H), 4.16 (q, *J* = 7.1 Hz, 2H), 4.02 (s, 1H), 3.82 (d, *J* = 6.0 Hz, 1H), 2.48 (t, J=7.1Hz,2H), 1.90 – 1.59 (m, 7H), 1.57 – 1.47 (m, 2H), 1.38 – 1.28 (m, 3H), 1.24 (t, *J* = 7.1 Hz, 3H), 1.20 – 1.09 (m, 3H), 0.90 (t, *J* = 7.3 Hz, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 173.9, 145.3, 132.5, 129.1, 113.6, 62.4, 60.7, 41.3, 34.7, 33.9, 29.6, 29.2, 26.2, 26.1, 26.0, 22.3, 14.3, 14.0. HRMS (ESI) exact mass calcd for $C_{20}H_{32}NO_2$ [M+H] m/z 318.2428, found 318.2432.



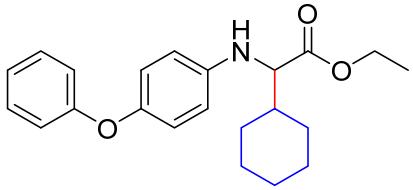
Ethyl 2-((4-(tert-butyl)phenyl)amino)-2-cyclohexylacetate (3ma). The desired pure product was obtained in 58% yield (36.5 mg) as a red oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.19 (d, *J* = 7.9 Hz, 2H), 6.58 (d, *J* = 7.9 Hz, 2H), 4.17 (q, *J* = 7.1 Hz, 2H), 4.07 (s, 1H), 3.84 (d, *J* = 5.9 Hz, 1H), 1.89 – 1.64 (m, 3H), 1.36 – 1.28 (m, 1H), 1.27 (s, 9H), 1.25 (t, 3H), 1.23 – 1.09 (m, 4H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 173.7, 145.1, 140.8, 125.9, 113.3, 62.4, 60.6, 41.4, 33.8, 31.5, 29.6, 29.2, 26.2, 26.1, 26.0, 14.2. HRMS (ESI) exact mass calcd for $C_{20}H_{32}NO_2$ [M+H] m/z 318.2428, found 318.2429.



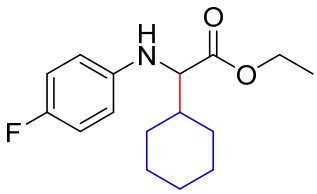
Ethyl 2-cyclohexyl-2-((4-methoxyphenyl)amino)acetate (3na). The desired pure product was obtained in 64% yield (37.3 mg) as a red oil.^{1}H NMR (400 MHz, $CDCl_3$) δ 6.75 (d, *J* = 8.7 Hz, 2H), 6.60 (d, *J* = 8.7 Hz, 2H), 4.14 (q, *J* = 7.1 Hz, 2H), 3.87 (s, 1H), 3.76 (d, *J* = 5.9 Hz, 1H), 3.72 (s, 3H), 2.02 – 1.56 (m, 7H), 1.34 – 1.25 (m, 1H), 1.22 (t, *J* = 7.1 Hz, 3H), 1.19 – 1.11 (m, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 174.0, 152.6, 141.6, 115.2, 114.8, 63.4, 60.7, 55.7, 41.3, 29.7, 29.2, 26.2, 26.1, 26.0, 14.3. HRMS (ESI) exact mass calcd for $C_{17}H_{26}NO_3$ [M+H] m/z 292.1907, found 292.1910.



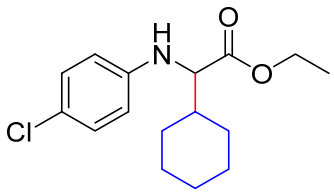
Ethyl 2-cyclohexyl-2-((4-ethoxyphenyl)amino)acetate (3oa). The desired pure product was obtained in 62% yield (32.7 mg) as a red oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.74 (d, *J* = 9.0 Hz, 2H), 6.58 (d, *J* = 9.0 Hz, 2H), 4.14 (q, *J* = 6.8 Hz, 2H), 3.94 (q, *J* = 7.0 Hz, 2H), 3.85 (s, 1H), 3.75 (d, *J* = 5.8 Hz, 1H), 1.90 – 1.63 (m, 7H), 1.36 (t, *J* = 7.0 Hz, 3H), 1.32 – 1.24 (m, 2H), 1.22 (t, *J* = 7.1 Hz, 3H), 1.18 – 1.09 (m, 2H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 174.0, 151.9, 141.6, 115.7, 115.2, 64.0, 63.4, 60.7, 41.3, 29.7, 29.2, 26.2, 26.1, 26.0, 15.0, 14.3. HRMS (ESI) exact mass calcd for $C_{18}H_{28}NO_3$ [M+H] m/z 306.2064, found 306.2063.



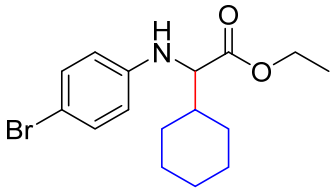
Ethyl 2-cyclohexyl-2-((4-phenoxyphenyl)amino)acetate (3pa). The desired pure product was obtained in 50% yield (35.5 mg) as a red oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.28 (dd, *J* = 7.0, 1.6 Hz, 1H), 7.25 (d, *J* = 2.6 Hz, 1H), 7.00 (dd, *J* = 14.7, 0.8 Hz, 1H), 6.92 (d, *J* = 8.5 Hz, 2H), 6.89 (d, *J* = 8.8 Hz, 2H), 6.62 (d, *J* = 8.8 Hz, 2H), 4.18 (q, *J* = 7.1 Hz, 2H), 4.06 (s, 1H), 3.81 (d, *J* = 6.1 Hz, 1H), 1.92 – 1.65 (m, 6H), 1.42 – 1.28 (m, 2H), 1.25 (t, *J* = 7.1 Hz, 3H), 1.23 – 1.10 (m, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 173.7, 158.9, 148.3, 144.0, 129.5, 122.0, 121.1, 117.2, 114.7, 62.8, 60.8, 41.3, 29.6, 29.2, 26.2, 26.1, 26.0, 14.3. HRMS (ESI) exact mass calcd for $C_{22}H_{28}NO_3$ [M+H] m/z 354.2064, found 354.2066.



Ethyl 2-cyclohexyl-2-((4-fluorophenyl)amino)acetate (3qa). The desired pure product was obtained in 45% yield (22.7 mg) as a yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.99 – 6.73 (m, 2H), 6.60 – 6.39 (m, 2H), 4.15 (q, *J* = 7.1 Hz, 2H), 3.99 (s, 1H), 3.76 (d, *J* = 6.1 Hz, 1H), 2.07 – 1.50 (m, 7H), 1.30 – 1.26 (m, 1H), 1.23 (t, *J* = 7.1 Hz, 3H), 1.19 – 1.07 (m, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 173.5, 156.3 (d, *J* = 235.8 Hz), 143.9, 115.6 (d, *J* = 22.4 Hz), 114.7 (d, *J* = 7.5 Hz), 63.1, 60.7, 41.3, 29.6, 29.2, 26.2, 26.1, 26.0, 14.2. HRMS (ESI) exact mass calcd for $C_{16}H_{23}FNO_2$ [M+H] m/z 280.1707, found 280.1711.

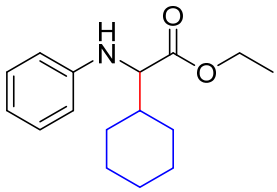


Ethyl 2-((4-chlorophenyl)amino)-2-cyclohexylacetate (3ra). The desired pure product was obtained in 43% yield (25.1 mg) as a yellow oil. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.09 (d, *J* = 8.9 Hz, 2H), 6.53 (d, *J* = 8.9 Hz, 2H), 4.16 (q, *J* = 7.1 Hz, 2H), 4.11 (s, 1H), 3.79 (d, 1H), 1.85 – 1.65 (m, 6H), 1.31 – 1.26 (m, 1H), 1.24 (t, *J* = 7.1 Hz, 3H), 1.22 – 1.09 (m, 4H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 173.3, 146.0, 129.1, 122.7, 114.6, 62.2, 60.9, 41.2, 29.6, 29.1, 26.1, 26.0, 25.9, 14.3. HRMS (ESI) exact mass calcd for $C_{16}H_{23}ClNO_2$ [M+H] m/z 296.1412, found 296.1411.

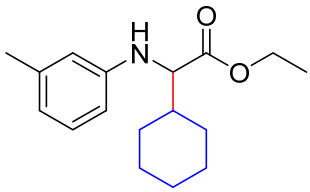


Ethyl 2-((4-bromophenyl)amino)-2-cyclohexylacetate (3sa). The desired pure product was obtained in 42% yield (28.2 mg) as a yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.23 (d, *J* = 8.9 Hz, 1H), 7.09 (d, *J* = 8.9 Hz, 1H), 6.52 (dd, *J* = 17.8, 8.9 Hz, 2H), 4.16 (q, *J* = 7.1 Hz, 2H), 3.79 (d, *J* = 6.1 Hz, 1H), 1.87 – 1.62 (m, 6H), 1.34 – 1.27 (m, 1H), 1.24 (t, *J* = 7.1 Hz, 3H), 1.21 – 1.09 (m, 4H). ^{13}C NMR (150 MHz,

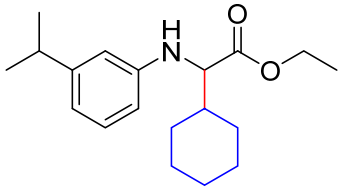
$CDCl_3$) δ 173.3, 146.5, 131.9, 115.1, 109.7, 62.0, 60.9, 41.2, 29.6, 29.1, 26.1, 26.0, 25.9, 14.3. HRMS (ESI) exact mass calcd for $C_{16}H_{23}BrNO_2$ [M+H] m/z 340.0907, found 340.0909.



Ethyl 2-cyclohexyl-2-(phenylamino)acetate (3ta). The desired pure product was obtained in 34% yield (17.8 mg) as a yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.16 (dd, *J* = 8.5, 7.4 Hz, 2H), 6.75 – 6.69 (m, 1H), 6.63 (dd, *J* = 8.6, 0.9 Hz, 2H), 4.17 (q, *J* = 7.1 Hz, 2H), 4.12 (s, 1H), 3.87 (d, *J* = 6.3 Hz, 1H), 1.89 – 1.60 (m, 7H), 1.34 – 1.27 (m, 1H), 1.25 (t, *J* = 7.1 Hz, 3H), 1.22 – 1.09 (m, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 173.7, 147.4, 129.2, 118.0, 113.5, 62.0, 60.8, 41.3, 29.6, 29.2, 26.2, 26.1, 26.0, 14.3. HRMS (ESI) exact mass calcd for $C_{16}H_{24}NO_2$ [M+H] m/z 262.1802, found 262.1801.

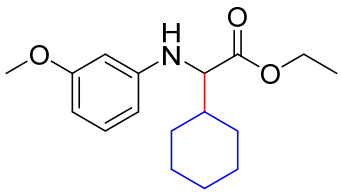


Ethyl 2-cyclohexyl-2-(m-tolylamino)acetate (3ua). The desired pure product was obtained in 34% yield (23.5 mg) as a red oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.05 (t, *J* = 7.7 Hz, 1H), 6.54 (d, *J* = 7.3 Hz, 1H), 6.44 (d, *J* = 13.3 Hz, 2H), 4.23 – 4.13 (m, 2H), 4.08 (s, 1H), 3.85 (s, 1H), 2.26 (s, 3H), 1.89 – 1.61 (m, 7H), 1.25 (t, *J* = 7.1 Hz, 3H), 1.22 – 1.07 (m, 4H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 173.7, 147.5, 139.0, 129.1, 119.0, 114.4, 110.5, 62.0, 60.7, 41.3, 29.6, 29.2, 26.2, 26.1, 26.0, 21.6, 14.3. HRMS (ESI) exact mass calcd for $C_{17}H_{26}NO_2$ [M+H] m/z 276.1958, found 276.1960.

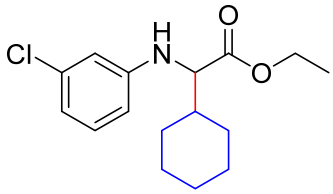


Ethyl 2-cyclohexyl-2-((3-isopropylphenyl)amino)acetate (3va). The desired pure product was obtained in 34% yield (31.3 mg) as a red oily liquid.^{1}H NMR (400 MHz, $CDCl_3$) δ 7.09 (t, *J* = 7.8 Hz, 1H), 6.61 (d, *J* = 8.1 Hz, 1H), 6.51 (s, 1H), 6.45 (dd, *J* = 8.0, 2.4 Hz, 1H), 4.17 (q, *J* = 7.1 Hz, 2H), 4.12 (d, *J* =

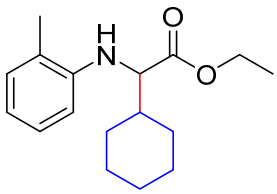
8.7 Hz, 1H), 3.88 (d, *J* = 6.3 Hz, 1H), 2.87 – 2.73 (m, 1H), 1.93 – 1.65 (m, 7H), 1.36 – 1.27 (m, 2H), 1.25 (t, *J* = 7.2 Hz, 3H), 1.22 (d, *J* = 6.9 Hz, 6H), 1.16 (dd, *J* = 19.9, 7.7 Hz, 2H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 173.8, 150.1, 147.5, 129.1, 116.4, 111.9, 110.8, 62.1, 60.7, 41.4, 34.2, 29.6, 29.2, 26.2, 26.1, 26.0, 23.9, 23,8, 14.3. HRMS (ESI) exact mass calcd for $C_{19}H_{30}NO_2$ [M+H] m/z 304.2271, found 304.2275.



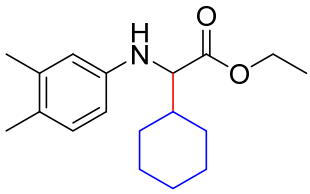
Ethyl 2-cyclohexyl-2-((3-methoxyphenyl)amino)acetate (3wa). The desired pure product was obtained in 59% yield (34.5 mg) as a yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.06 (t, *J* = 8.1 Hz, 1H), 6.30 – 6.21 (m, 2H), 6.17 (t, *J* = 2.3 Hz, 1H), 4.18 (q, *J* = 9.0, 5.3 Hz, 2H), 4.14 (s, 1H), 3.87 – 3.81 (m, 1H), 3.75 (s, 3H), 1.86 – 1.63 (m, 6H), 1.38 – 1.28 (m, 1H), 1.25 (t, *J* = 7.1 Hz, 3H), 1.23 – 1.09 (m, 4H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 173.6, 160.8, 148.8, 130.0, 106.4, 103.3, 99.4, 61.9, 60.8, 55.0, 41.3, 29.6, 29.2, 26.2, 26.1, 26.0, 14.3. HRMS (ESI) exact mass calcd for $C_{17}H_{26}NO_3$ [M+H] m/z 292.1907, found 292.1906.



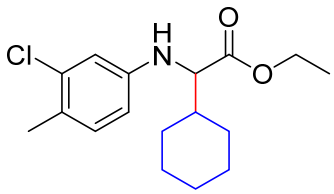
Ethyl 2-((3-chlorophenyl)amino)-2-cyclohexylacetate (3xa). The desired pure product was obtained in 47% yield (27.7 mg) as a yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.09 – 7.00 (m, 1H), 6.70 – 6.65 (m, 1H), 6.60 (d, *J* = 1.8 Hz, 1H), 6.48 (dd, *J* = 8.1, 2.0 Hz, 1H), 4.25 – 4.14 (m, 2H), 4.17 (s, 1H), 3.82 (dd, *J* = 9.2, 6.0 Hz, 1H), 1.85 – 1.58 (m, 7H), 1.26 (t, *J* = 7.1 Hz, 3H), 1.22 – 1.09 (m, 4H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 173.2, 148.6, 135.0, 130.2, 117.9, 113.2, 111.7, 61.7, 61.0, 41.2, 29.6, 29.1, 26.1, 26.0, 25.9, 14.3. HRMS (ESI) exact mass calcd for $C_{16}H_{23}ClNO_2$ [M+H] m/z 296.1412, found 296.1414.



Ethyl 2-cyclohexyl-2-(o-tolylamino)acetate (3ya). The desired pure product was obtained in 68% yield (37.3 mg) as a yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.07 (dd, *J* = 12.7, 7.0 Hz, 2H), 6.66 (t, *J* = 7.4 Hz, 1H), 6.56 (d, *J* = 8.0 Hz, 1H), 4.17 (q, *J* = 7.2 Hz, 2H), 4.05 (d, *J* = 9.0 Hz, 1H), 3.92 (d, *J* = 6.1 Hz, 1H), 2.21 (s, 3H), 1.94 – 1.65 (m, 6H), 1.37 – 1.28 (m, 2H), 1.26 (t, *J* = 7.1 Hz, 3H), 1.21 – 1.10 (m, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 173.8, 145.4, 130.3, 127.0, 122.7, 117.6, 110.4, 61.9, 60.8, 41.4, 29.6, 29.3, 26.2, 26.1, 26.0, 17.5, 14.3. HRMS (ESI) exact mass calcd for $C_{17}H_{26}NO_2$ [M+H] m/z 276.1958, found 276.1954.

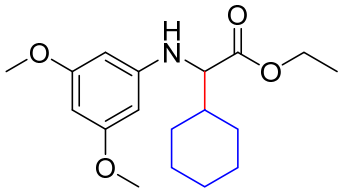


Ethyl 2-cyclohexyl-2-((3,4-dimethylphenyl)amino)acetate (3za). The desired pure product was obtained in 34% yield (18.9 mg) as a red oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.92 (d, *J* = 8.1 Hz, 1H), 6.47 (d, *J* = 2.4 Hz, 1H), 6.39 (dd, *J* = 8.1, 2.5 Hz, 1H), 4.20 – 4.13 (m, 2H), 3.82 (d, *J* = 6.1 Hz, 1H), 2.18 (s, 3H), 2.14 (s, 3H), 1.91 – 1.63 (m, 6H), 1.32 – 1.27 (m, 1H), 1.25 (t, *J* = 7.1 Hz, 3H), 1.22 – 1.09 (m, 4H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 173.9, 145.6, 137.3, 130.3, 126.1, 115.5, 110.9, 62.3, 60.7, 41.3, 29.6, 29.2, 26.2, 26.1, 26.0, 20.0, 18.7, 14.3. HRMS (ESI) exact mass calcd for $C_{18}H_{28}NO_2$ [M+H] m/z 290.2115, found 290.2111.

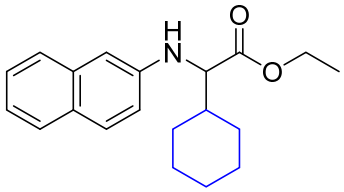


Ethyl 2-((3-chloro-4-methylphenyl)amino)-2-cyclohexylacetate (3aaa). The desired pure product was obtained in 48% yield (30.2 mg) as a red oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.97 (d, *J* = 8.2 Hz, 1H), 6.63 (d, *J* = 2.4 Hz, 1H), 6.44 (dd, *J* = 8.2, 2.4 Hz, 1H), 4.21 – 4.13 (m, 2H), 4.07 (d, *J* = 9.5 Hz, 1H), 3.79 (dd, *J* = 9.5, 6.1 Hz, 1H), 2.23 (s, 3H), 1.87 – 1.62 (m, 7H), 1.25 (t, *J* = 7.1 Hz, 3H), 1.22 – 1.07

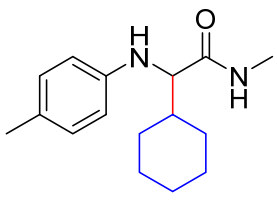
(m, 4H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 173.4, 146.6, 134.8, 131.3, 125.0, 113.9, 112.3, 62.1, 60.9, 41.2, 29.6, 29.1, 26.1, 26.0, 25.9, 18.8, 14.3. HRMS (ESI) exact mass calcd for $C_{17}H_{25}ClNO_2$ [M+H] m/z 310.1568, found 310.1575.



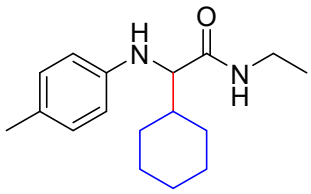
Ethyl 2-cyclohexyl-2-((3,5-dimethoxyphenyl)amino)acetate (3aba). The desired pure product was obtained in 23% yield (14.5 mg) as a red oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 5.88 (d, *J* = 1.9 Hz, 1H), 5.81 (d, *J* = 1.8 Hz, 2H), 4.20 – 4.16 (m, 2H), 4.15 (s, 1H), 3.85 – 3.79 (m, 1H), 3.74 (s, 3H), 3.73 (s, 3H), 1.86 – 1.62 (m, 6H), 1.34 – 1.29 (m, 1H), 1.26 (t, *J* = 5.4 Hz, 3H), 1.20 – 1.09 (m, 4H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 173.5, 161.7, 149.3, 92.2, 90.5, 61.8, 60.8, 55.1, 41.3, 29.6, 29.1, 26.2, 26.1, 26.0, 14.3. HRMS (ESI) exact mass calcd for $C_{18}H_{28}NO_4$ [M+H] m/z 322.2013, found 322.2011.



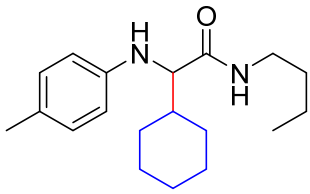
Ethyl 2-cyclohexyl-2-(naphthalen-2-ylamino)acetate (3aca). The desired pure product was obtained in 33% yield (20.5 mg) as a colourless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.69 – 7.58 (m, 1H), 7.38 – 7.32 (m, 1H), 7.23 – 7.18 (m, 1H), 6.93 (dd, *J* = 8.8, 2.4 Hz, 1H), 6.82 (d, *J* = 2.3 Hz, 1H), 4.33 (s, 1H), 4.24 – 4.14 (m, 2H), 4.02 (d, *J* = 6.0 Hz, 1H), 1.96 – 1.65 (m, 6H), 1.38 – 1.28 (m, 2H), 1.26 (t, *J* = 7.1 Hz, 3H), 1.23 – 1.14 (m, 3H).^{13}C NMR (150 MHz, $CDCl_3$) δ 173.6, 145.1, 135.0, 129.0, 127.8, 127.6, 126.3, 126.0, 122.2, 118.2, 105.4, 62.0, 60.9, 41.3, 29.7, 29.3, 26.2, 26.1, 26,0, 14.3. HRMS (ESI) exact mass calcd for $C_{20}H_{26}NO_4$ [M+H] m/z 312.1958, found 312.1963.



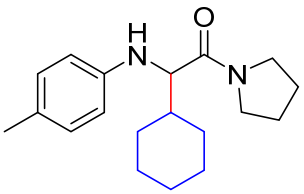
2-cyclohexyl-N-methyl-2-(p-tolylamino)acetamide (3ada). The desired pure product was obtained in 83% yield (42.7 mg) as a red oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.00 (d, *J* = 8.3 Hz, 2H), 6.87 (s, 1H), 6.52 (d, *J* = 8.0 Hz, 2H), 3.86 (s, 1H), 3.53 (d, *J* = 4.0 Hz, 1H), 2.78 (d, *J* = 4.8 Hz, 3H), 2.24 (s, 3H), 2.08 – 1.98 (m, 1H), 1.77 (d, *J* = 11.5 Hz, 2H), 1.68 (d, *J* = 11.9 Hz, 3H), 1.35 – 1.05 (m, 5H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 173.6, 145.1, 129.8, 128.2, 113.6, 65.1, 41.1, 30.3, 28.1, 26.3, 26.2, 26.1, 25.9, 20.3. HRMS (ESI) exact mass calcd for $C_{16}H_{25}N_2O$ [M+H] m/z 261.1961, found 261.1966.



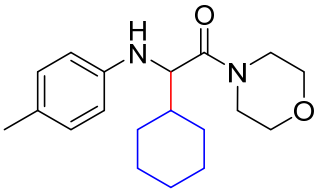
2-cyclohexyl-N-ethyl-2-(p-tolylamino)acetamide (3aea). The desired pure product was obtained in 91% yield (49.9 mg) as a red oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.00 (d, *J* = 8.4 Hz, 2H), 6.83 (s, 1H), 6.52 (d, *J* = 8.3 Hz, 2H), 3.77 (s, 1H), 3.49 (d, *J* = 3.0 Hz, 1H), 3.39 – 3.13 (m, 2H), 2.24 (s, 3H), 2.08 – 1.97 (m, 1H), 1.88 – 1.61 (m, 6H), 1.33 – 1.14 (m, 4H), 1.07 (t, *J* = 7.3 Hz, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 172.6, 145.2, 129.8, 128.2, 113.7, 65.2, 41.0, 33.9, 30.3, 28.0, 26.3, 26.2, 26.1, 20.3, 14.9. HRMS (ESI) exact mass calcd for $C_{17}H_{27}N_2O$ [M+H] m/z 275.2118, found 275.2122.



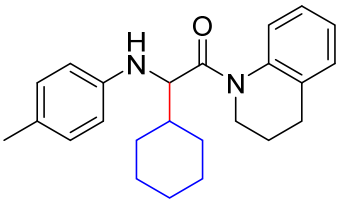
N-butyl-2-cyclohexyl-2-(p-tolylamino)acetamide (3afa). The desired pure product was obtained in 74% yield (44.8 mg) as a red oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.00 (d, *J* = 8.4 Hz, 2H), 6.83 (s, 1H), 6.52 (d, *J* = 8.4 Hz, 2H), 3.77 (s, 1H), 3.50 (d, *J* = 3.9 Hz, 1H), 3.34 – 3.13 (m, 2H), 2.24 (s, 3H), 2.10 – 1.93 (m, 1H), 1.82 – 1.64 (m, 6H), 1.46 – 1.34 (m, 2H), 1.33 – 1.20 (m, 4H), 1.20 – 1.10 (m, 2H), 0.86 (t, *J* = 7.3 Hz, 3H).^{13}C NMR (150 MHz, $CDCl_3$) δ 172.6, 145.2, 129.8, 128.2, 113.7, 65.3, 41.0, 38.8, 31.7, 30.4, 28.0, 26.3, 26.2, 26.1, 20.3, 20.0, 13.6. HRMS (ESI) exact mass calcd for $C_{19}H_{31}N_2O$ [M+H] m/z 303.2431, found 303.2438.



2-cyclohexyl-1-(pyrrolidin-1-yl)-2-(p-tolylamino)ethan-1-one (3aga). The desired pure product was obtained in 75% yield (44.7 mg) as a red oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.94 (d, *J* = 8.0 Hz, 2H), 6.55 (d, *J* = 8.4 Hz, 2H), 4.32 (s, 1H), 3.90 (d, *J* = 5.8 Hz, 1H), 3.55 – 3.38 (m, 4H), 2.21 (s, 3H), 2.00 – 1.78 (m, 5H), 1.80 – 1.61 (m, 6H), 1.32 – 1.03 (m, 4H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 171.9, 146.1, 129.7, 126.8, 113.9, 61.2, 46.6, 45.7, 42.0, 30.2, 29.0, 26.3, 26.28, 26.2, 26.1, 24.1, 20.3. HRMS (ESI) exact mass calcd for $C_{19}H_{29}N_2O$ [M+H] m/z 301.2274, found 301.2278.

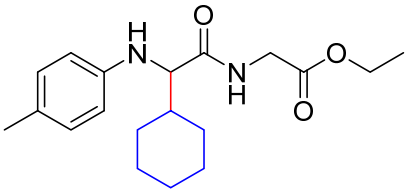


2-cyclohexyl-1-morpholino-2-(p-tolylamino)ethan-1-one (3aha). The desired pure product was obtained in 78% yield (50.7 mg) as a red oil.^{1}H NMR (400 MHz, $CDCl_3$) δ 6.95 (d, *J* = 8.2 Hz, 2H), 6.54 (d, *J* = 7.9 Hz, 2H), 4.31 (s, 1H), 4.04 (d, *J* = 5.8 Hz, 1H), 3.66 – 3.53 (m, 8H), 2.21 (s, 3H), 1.88 (d, *J* = 11.6 Hz, 1H), 1.82 – 1.54 (m, 6H), 1.27 – 1.12 (m, 4H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 172.0, 145.8, 129.8, 127.4, 114.3, 67.0, 66.6, 59.0, 46.3, 42.4, 41.9, 30.3, 28.8, 26.2, 26.18, 26.1, 20.4. HRMS (ESI) exact mass calcd for $C_{19}H_{29}N_2O_2$ [M+H] m/z 317.2224, found 317.2220.

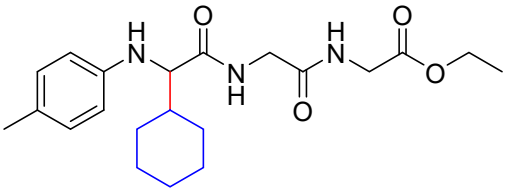


2-cyclohexyl-1-(3,4-dihydroquinolin-1(2H)-yl)-2-(p-tolylamino)ethan-1-one (3aia). The desired pure product was obtained in 76% yield (53.9 mg) as a red oil. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.18 (s, 3H), 7.03 (s, 1H), 6.93 (dd, *J* = 35.5, 6.7Hz, 2H), 6.37 (s, 2H), 4.44 (s, 1H), 4.19 (s, 1H), 3.96 (d, *J* = 4.5 Hz, 1H), 3.58 (s, 1H), 2.54 (s, 2H), 2.22 (s, 3H), 2.01 (d, *J* = 5.8 Hz, 1H), 1.87 – 1.50 (m, 5H), 1.31 – 0.85 (m, 6H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 173.8, 145.2, 138.9, 134.7, 129.6, 128.4, 126.4, 125.9, 124.7,

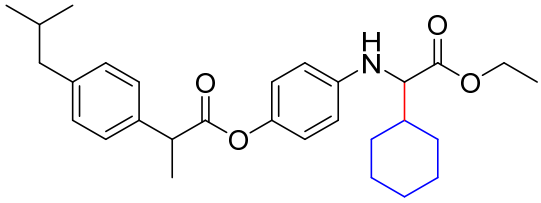
115.2, 114.0, 59.1, 42.6, 29.9, 29.1, 26.5, 26.3, 26.2, 24.1, 20.4. HRMS (ESI) exact mass calcd for $C_{24}H_{31}N_2O$ [M+H] m/z 363.2431, found 363.2437.



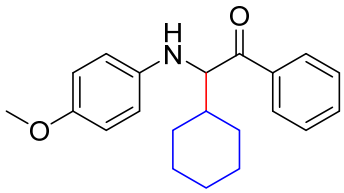
Ethyl (2-cyclohexyl-2-(p-tolylamino)acetyl)glycinate (3aja). The desired pure product was obtained in 82% yield (54.7 mg) as a red oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.29 (t, *J* = 5.5 Hz, 1H), 7.00 (d, *J* = 8.5 Hz, 2H), 6.54 (d, *J* = 8.4 Hz, 2H), 4.21 – 4.12 (m, 3H), 3.86 (dd, *J* = 18.2, 4.9 Hz, 1H), 3.57 (d, *J* = 4.2 Hz, 1H), 2.23 (s, 3H), 2.09 – 1.98 (m, 1H), 1.84 – 1.65 (m, 6H), 1.37 – 1.26 (m, 2H), 1.24 (t, *J* = 7.1 Hz, 3H), 1.20 – 1.09 (m, 2H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 173.4, 169.6, 145.1, 129.8, 128.3, 113.8, 65.1, 61.3, 41.2, 41.0, 30.2, 28.0, 26.3, 26.2, 26.1, 20.3, 14.1. HRMS (ESI) exact mass calcd for $C_{19}H_{29}N_2O_3$ [M+H] m/z 333.2173, found 333.2179.



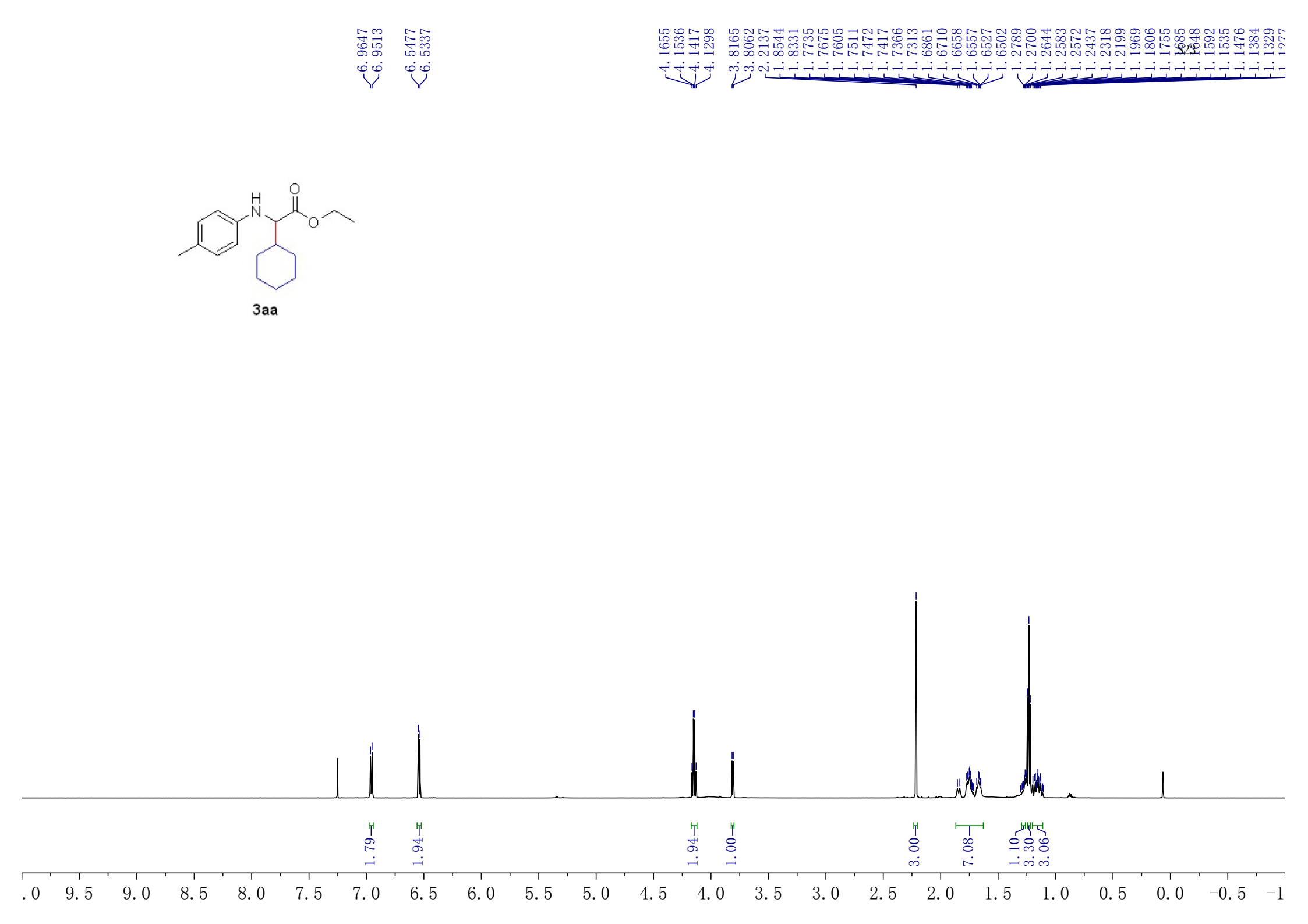
2-cyclohexyl-N-(2-((3-methoxy-2-oxopropyl)amino)-2-oxoethyl)-2-(p-tolylamino)acetamide (3aka) The desired pure product was obtained in 62% yield (48.8 mg) as a yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.48 (s, 1H), 6.98 (d, *J* = 8.2 Hz, 2H), 6.60 (s, 1H), 6.54 (d, *J* = 8.2 Hz, 2H), 4.17 (q, *J* = 7.1 Hz, 2H), 3.96 (d, *J* = 5.3 Hz, 2H), 3.93 – 3.87 (m, 2H), 3.62 (d, *J* = 4.5 Hz, 1H), 2.22 (s, 3H), 2.07 – 1.88 (m, 1H), 1.83 – 1.58 (m, 5H), 1.43 – 1.30 (m, 1H), 1.26 (t, *J* = 7.1 Hz, 3H), 1.24 – 1.11 (m, 4H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 173.9, 169.4, 169.0, 144.9, 129.9, 128.3, 113.6, 64.8, 61.5, 42.8, 41.2, 41.1, 30.2, 28.4, 26.2, 26.1, 26.0, 20.3, 14.1. HRMS (ESI) exact mass calcd for $C_{21}H_{32}N_3O_4$ [M+H] m/z 390.2387, found 390.2395.

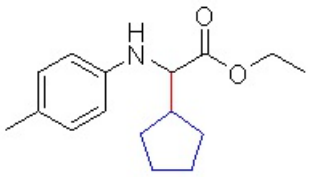


4-((1-cyclohexyl-2-ethoxy-2-oxoethyl)amino)phenyl 2-(4-isobutylphenyl)propanoate ***(3ala)*** The desired pure product was obtained in 63% yield (58.9 mg) as a yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.28 (d, *J* = 8.0 Hz, 2H), 7.13 (d, *J* = 8.0 Hz, 2H), 6.79 (d, *J* = 8.8 Hz, 2H), 6.55 (d, *J* = 8.8 Hz, 2H), 4.15 (q, *J* = 14.2, 7.1 Hz, 2H), 3.89 (q, *J* = 14.2, 7.1 Hz, 1H), 3.78 (s, 1H), 2.46 (d, *J* = 7.1 Hz, 2H), 1.89 – 1.62 (m, 7H), 1.57 (d, *J* = 7.1 Hz, 3H), 1.47 – 1.28 (m, 1H), 1.23 (t, *J* = 7.1 Hz, 3H), 1.20 – 1.02 (m, 3H), 0.91 (d, *J* = 6.6 Hz, 6H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 173.7, 173.5, 145.2, 142.7, 140.6, 137.5, 129.4, 127.2, 121.9, 113.9, 62.4, 60.8, 45.2, 45.0, 41.2, 30.2, 29.6, 29.2, 26.2, 26.1, 26.0, 22.4, 18.6, 14.3. HRMS (ESI) exact mass calcd for $C_{29}H_{40}NO_4$ [M+H] m/z 466.2952, found 466.2956.

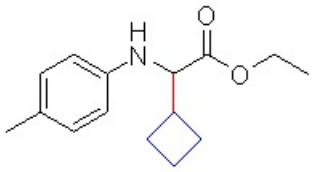


2-cyclohexyl-2-((4-methoxyphenyl)amino)-1-phenylethan-1-one (3ama) The desired pure product was obtained in 60% yield (38.6 mg) as a yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.95 (d, *J* = 7.4 Hz, 2H), 7.59 (t, *J* = 7.4 Hz, 1H), 7.49 (t, *J* = 7.7 Hz, 2H), 6.74 (d, *J* = 9.0 Hz, 2H), 6.68 (d, *J* = 8.9 Hz, 2H), 4.77 (d, *J* = 4.2 Hz, 1H), 4.39 (s, 1H), 3.71 (s, 3H), 1.88 – 1.67 (m, 4H), 1.60 (s, 2H), 1.46 – 1.34 (m, 1H), 1.30 – 1.19 (m, 1H), 1.17 – 1.04 (m, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 201.8, 152.5, 142.5, 136.2, 133.4, 128.8, 128.3, 115.7, 114.9, 64.7, 55.7, 41.8, 30.9, 27.7, 26.4, 26.2, 26.0. HRMS (ESI) exact mass calcd for $C_{21}H_{26}NO_2$ [M+H] m/z 324.1958, found 324.1962.


6.9647
6.9513
6.5477
6.5337
4.1655
4.1536
4.1417
4.1298
3.8165
3.8062
2.2137
1.8544
1.8331
1.7735
1.7675
1.7605
1.7511
1.7472
1.7417
1.7366
1.7313
1.6861
1.6710
1.6658
1.6557
1.6527
1.6502
1.2789
1.2700
1.2644
1.2583
1.2572
1.2437
1.2318
1.2199
1.1969
1.1806
1.1755
1.1685
1.1648
1.1592
1.1535
1.1476
1.1384
1.1329
1.1977
H
N
O
O
3aa
1.79
1.94
1.94
1.00
3.00
7.08
1.10
3.30
3.06
.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
-1

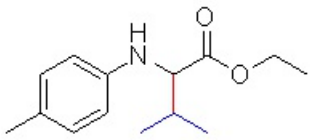


3ab

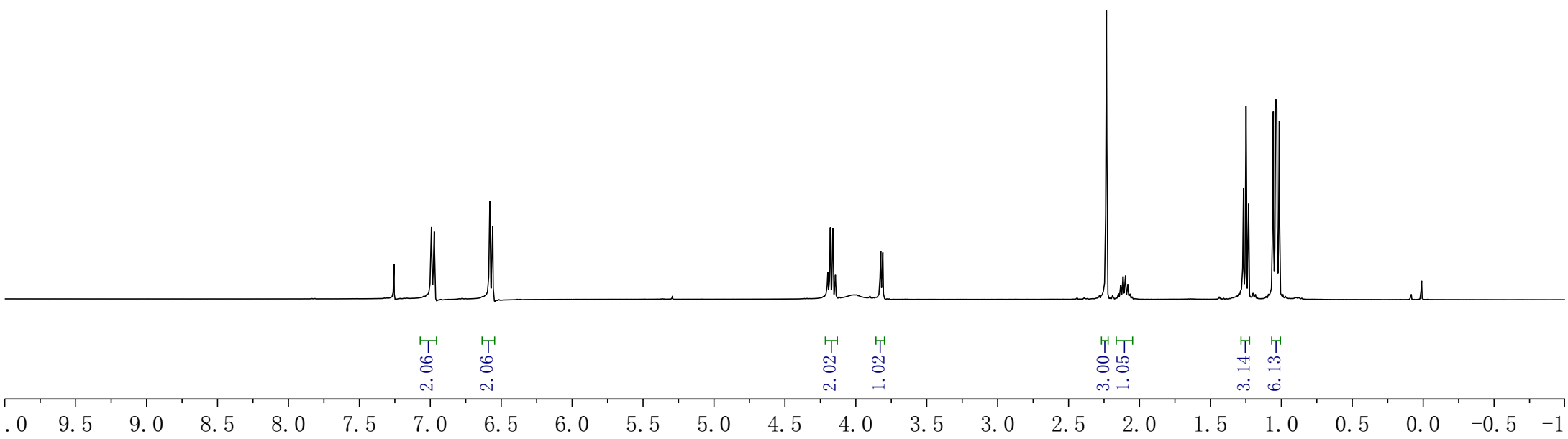


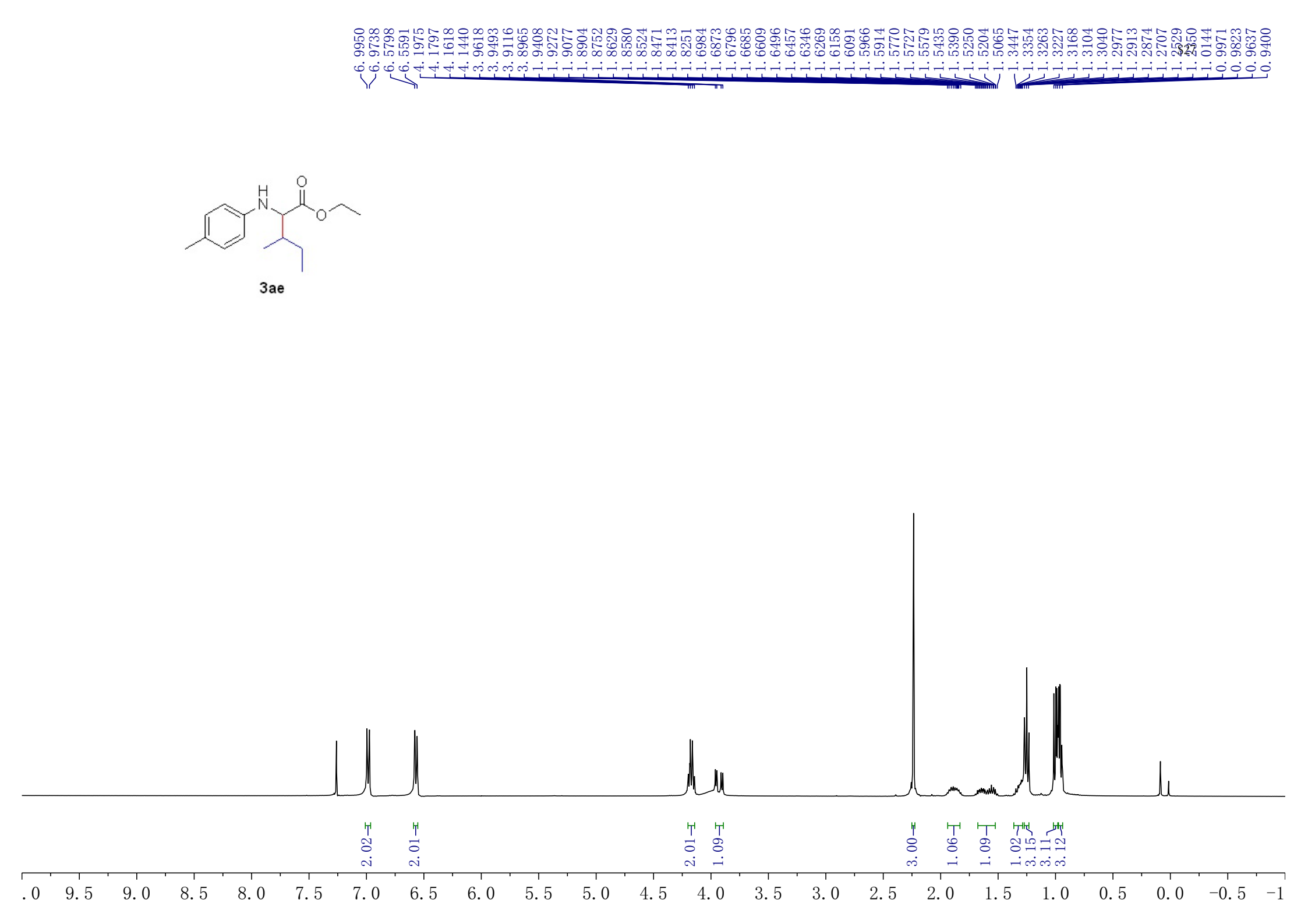
3ac

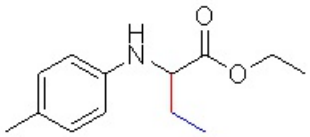
6.9893
6.9691
6.5641
6.5431
4.1792
4.1614
4.1436
4.1259
3.9237
2.7011
2.6821
2.6628
2.6432
2.6236
2.2318
2.0900
2.0824
2.0776
2.0705
2.0626
2.0542
2.0412
2.0295
2.0203
2.0002
1.9978
1.9917
1.9518
1.9313
1.9173
1.8984
1.8796
1.8710
1.8548
1.8440
1.8386
1.8259
1.2503
1.2325
1.91
2.01
2.00
1.03
0.97
3.00
6.07
3.02
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5



3ad

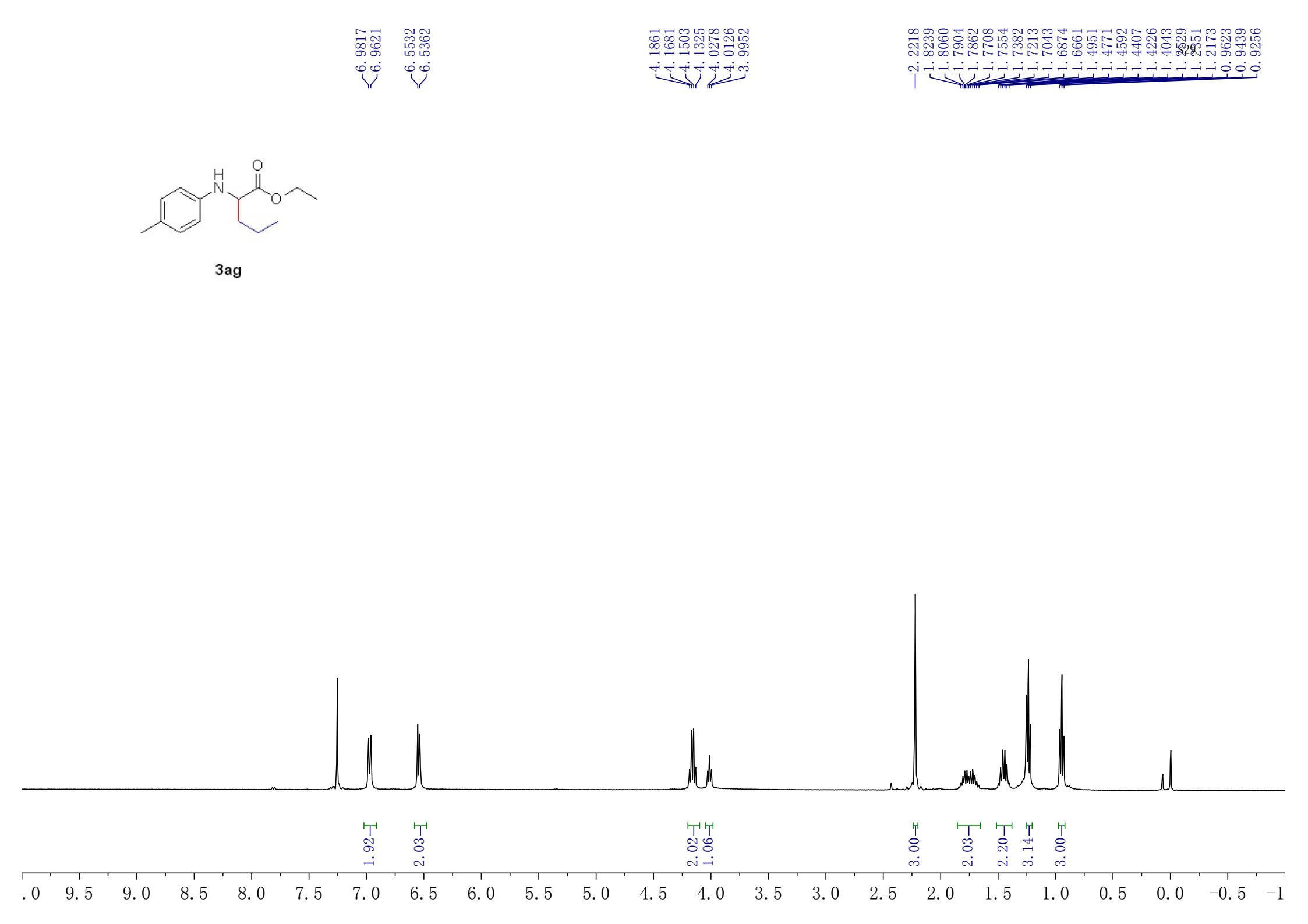

6.9923
6.9723
6.5802
6.5594
4.1976
4.1798
4.1618
4.1440
3.8242
3.8096
2.2328
2.1481
2.1316
2.1155
2.0989
2.0821
1.2666
1.2487
1.2309
1.0565
1.0393
1.0315
1.0144
2.06
2.06
2.02
1.02
3.00
1.05
3.14
6.13
.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 −0.5 −1

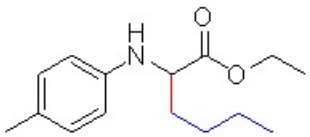

6.9950
6.9738
6.5798
6.5591
4.1975
4.1797
4.1618
4.1440
3.9618
3.9493
3.9116
3.8965
3.9408
1.9272
1.9077
1.8904
1.8752
1.8629
1.8580
1.8524
1.8471
1.8413
1.8251
1.6984
1.6873
1.6796
1.6685
1.6609
1.6496
1.6457
1.6346
1.6269
1.6158
1.6091
1.5966
1.5914
1.5770
1.5727
1.5579
1.5435
1.5390
1.5250
1.5204
1.5065
1.3447
1.3354
1.3263
1.3227
1.3168
1.3104
1.3040
1.2977
1.2913
1.2874
1.2707
1.2529
1.2350
1.0144
0.9971
0.9823
0.9637
0.9400
3ae
2.02
2.01
2.01
1.09
3.00
1.06
1.09
1.02
3.15
3.11
3.12
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1



3af

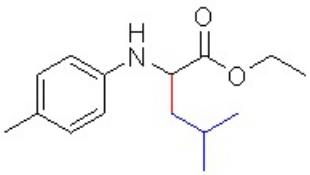
6.9952
6.9741
6.5674
6.5468
4.2109
4.1932
4.1753
4.1575
4.0043
3.9889
3.9730
2.2341
1.9346
1.9172
1.9001
1.8830
1.8654
1.8473
1.8278
1.8094
1.7924
1.7747
1.7569
1.7395
1.2731
1.2552
1.2374
1.0224
1.0041
0.9852
1.91
1.93
2.00
1.05
3.00
2.00
3.03
3.01
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
−0.5
−1


6.9817
6.9621
6.5532
6.5362
4.1861
4.1681
4.1503
4.1325
4.0278
4.0126
3.9952
2.2218
1.8239
1.8060
1.7904
1.7862
1.7708
1.7554
1.7382
1.7213
1.7043
1.6874
1.6661
1.4951
1.4771
1.4592
1.4407
1.4226
1.4043
1.2529
1.2351
1.2173
0.9623
0.9439
0.9256
3ag
1.92
2.03
2.02
1.06
3.00
2.03
2.20
3.14
3.00
.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
-1



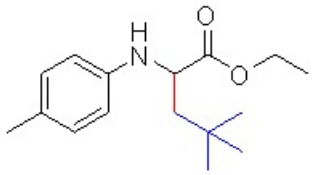
3ah

6.9969
6.9756
6.5665
6.5454
4.2042
4.1863
4.1685
4.1507
4.0328
4.0169
4.0005
2.2370
1.8439
1.8244
1.8091
1.7893
1.7704
1.7524
1.4385
1.4297
1.4184
1.4093
1.3990
1.3909
1.3831
1.3740
1.3683
1.3552
1.3510
1.3342
1.2688
1.2509
1.2331
0.9340
0.9162
2.00
2.01
2.00
1.09
3.00
2.03
4.09
3.01
3.03
f1 (ppm)

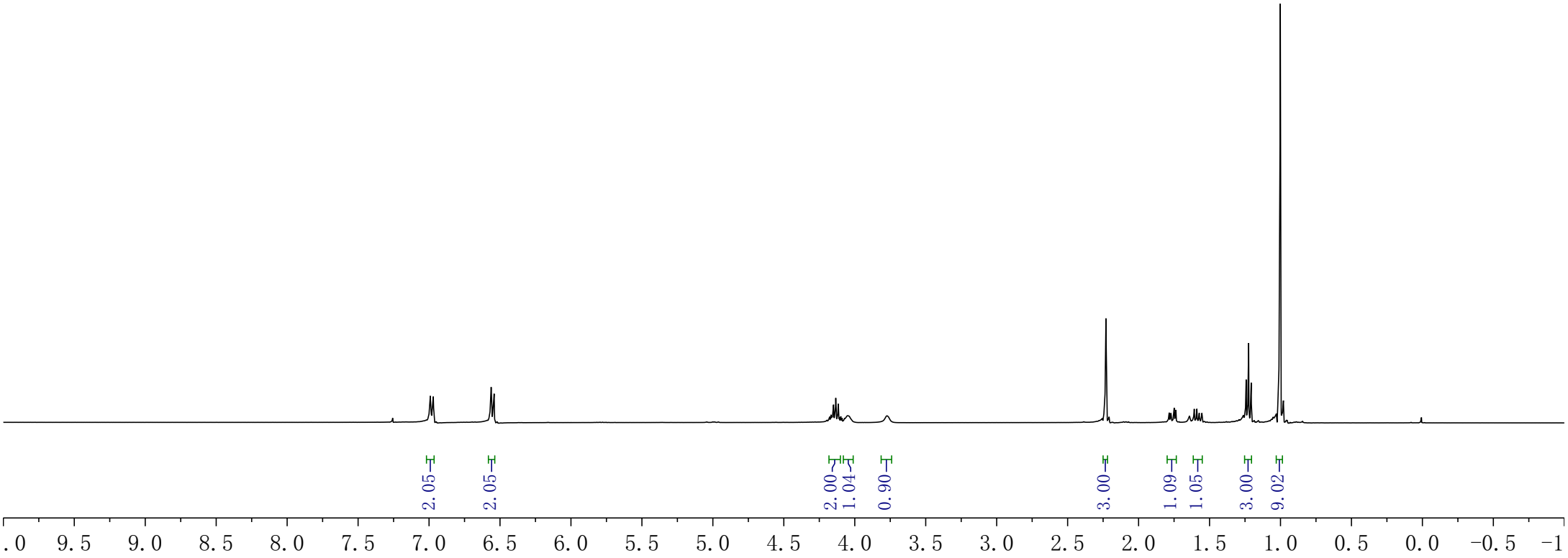


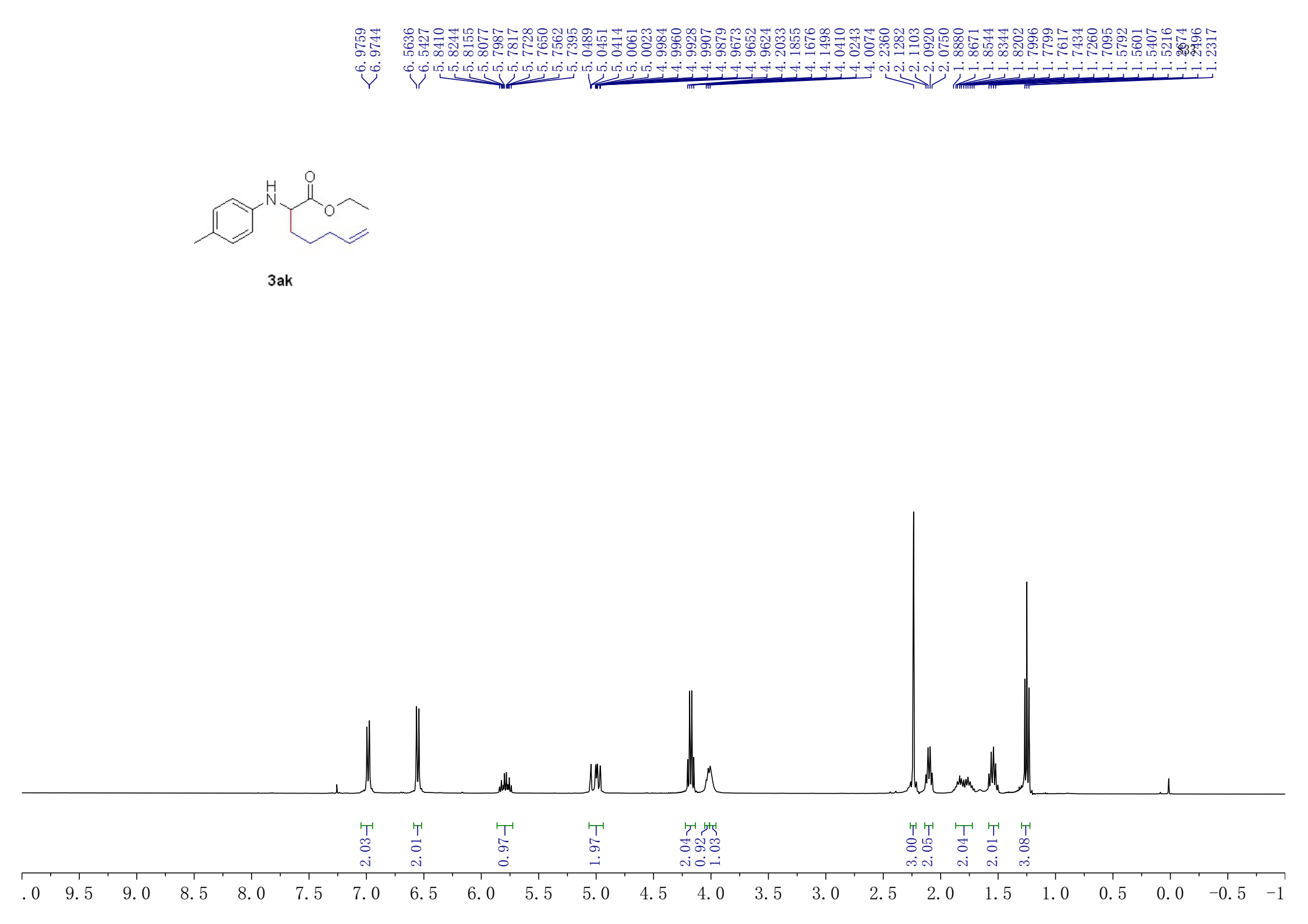
3ai

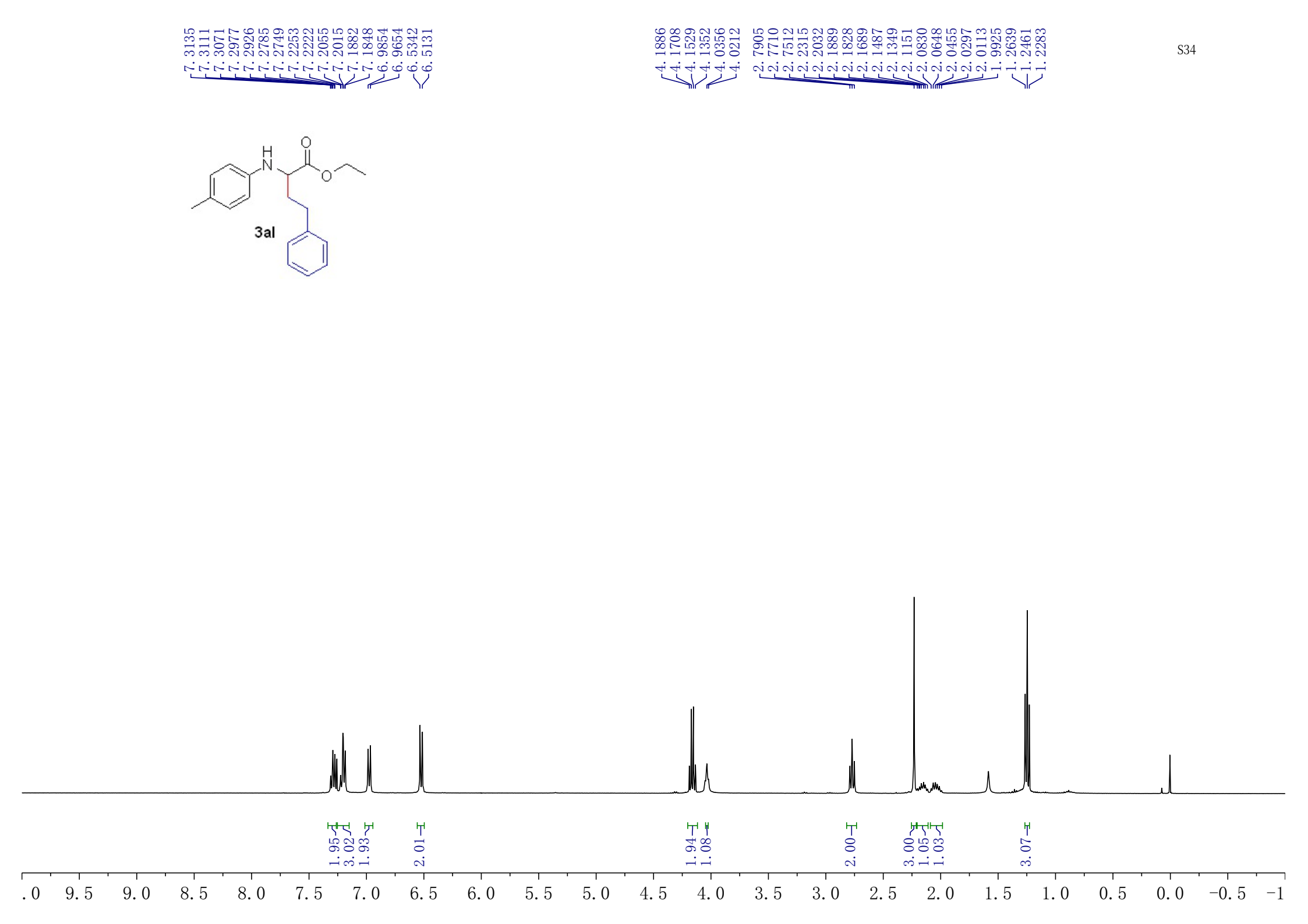
6.9849
6.9650
6.5602
6.5391
4.1750
4.1572
4.1395
4.1217
4.0395
3.8529
2.2254
1.8607
1.8438
1.8269
1.8101
1.7933
1.7763
1.7596
1.6458
1.6290
1.6254
1.6117
1.6070
1.2469
1.2291
1.2113
0.9969
0.9804
0.9513
0.9349
1.95
2.00
2.01
0.96
0.89
3.00
0.90
2.08
3.00
3.00
3.00
.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
−0.5
−1

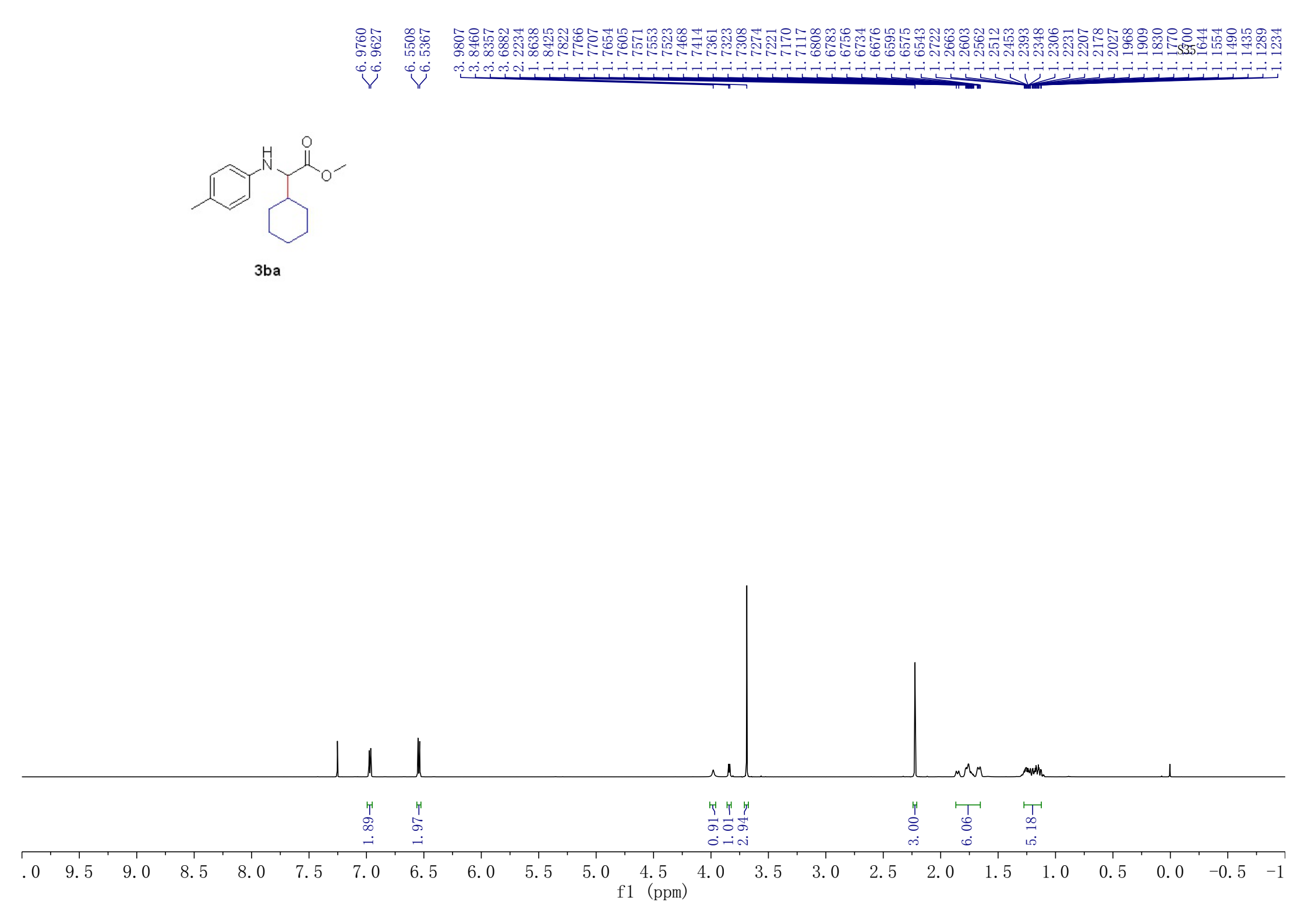


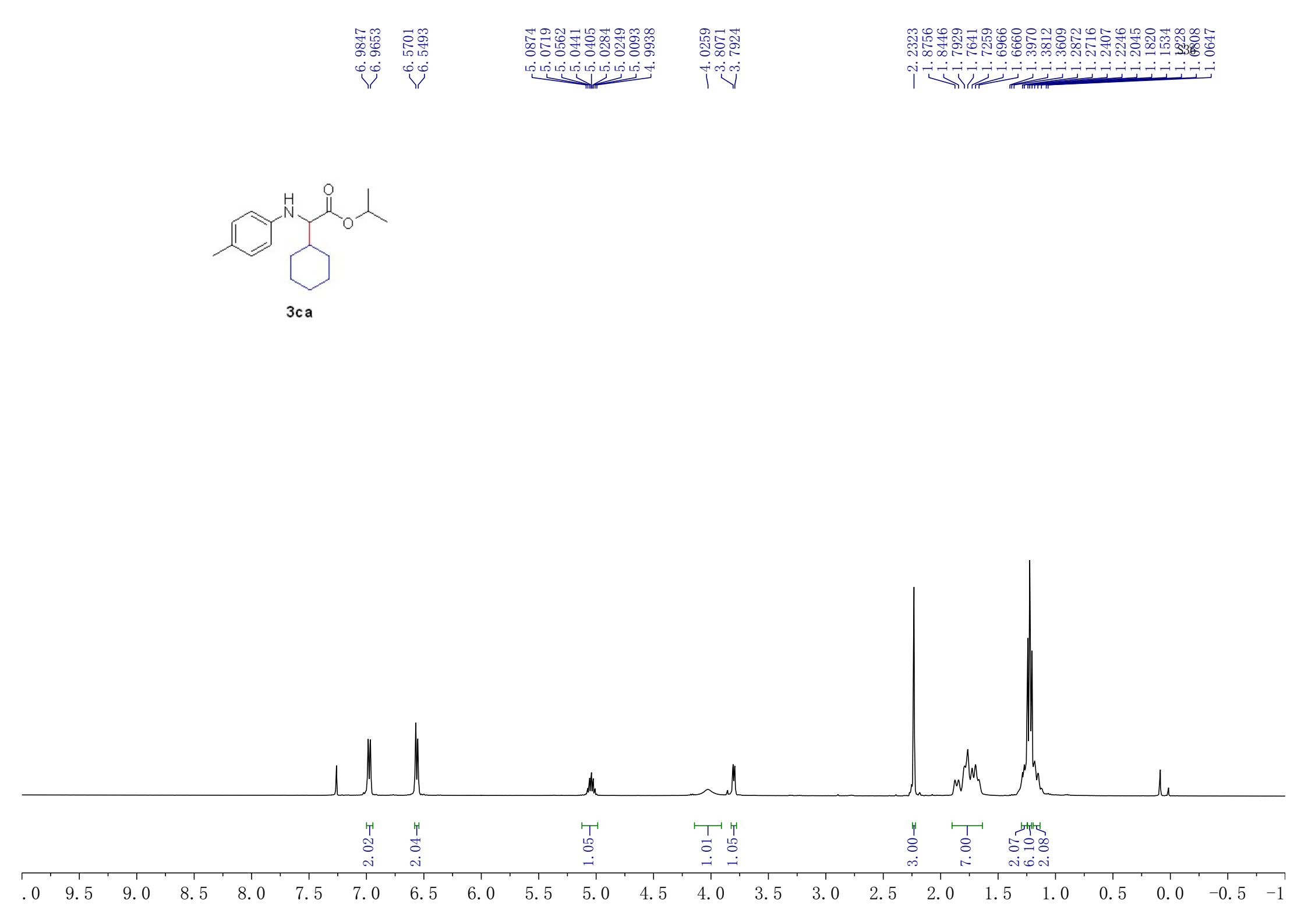
3aj

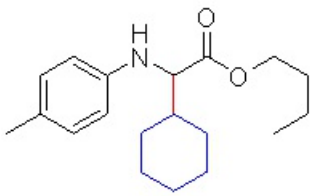

6.9914
6.9703
6.5623
6.5413
4.1978
4.1945
4.1800
4.1766
4.1674
4.1621
4.1586
4.1496
4.1337
4.1319
4.1160
4.1068
4.0982
4.0932
4.0889
4.0487
3.7733
2.2297
1.7845
1.7721
1.7492
1.7367
1.6078
1.5893
1.5724
1.5539
1.2421
1.2242
1.2064
1.0016
2.05
2.05
2.00
1.04
0.90
3.00
1.09
1.05
3.00
9.02
.0
9.5
9.0
8.5
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
-1


6.9759
6.9744
6.5636
6.5427
5.8410
5.8244
5.8155
5.8077
5.7987
5.7817
5.7728
5.7650
5.7562
5.7395
5.0489
5.0451
5.0414
5.0061
5.0023
4.9984
4.9960
4.9928
4.9907
4.9879
4.9673
4.9652
4.9624
4.2033
4.1855
4.1676
4.1498
4.0410
4.0243
4.0074
2.2360
2.1282
2.1103
2.0920
2.0750
1.8880
1.8671
1.8544
1.8344
1.8202
1.7996
1.7799
1.7617
1.7434
1.7260
1.7095
1.5792
1.5601
1.5407
1.5216
1.2674
1.2496
1.2317
3ak
2.03
2.01
0.97
1.97
2.04
0.92
1.03
3.00
2.05
2.04
2.01
3.08
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1


7.3135
7.3111
7.3071
7.2977
7.2926
7.2785
7.2749
7.2253
7.2222
7.2055
7.2015
7.1882
7.1848
6.9854
6.9654
6.5342
6.5131
4.1886
4.1708
4.1529
4.1352
4.0356
4.0212
2.7905
2.7710
2.7512
2.2315
2.2032
2.1889
2.1828
2.1689
2.1487
2.1349
2.1151
2.0830
2.0648
2.0455
2.0297
2.0113
1.9925
1.2639
1.2461
1.2283
3al
1.95
3.02
1.93
2.01
1.94
1.08
2.00
3.00
1.05
1.03
3.07
.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
-1

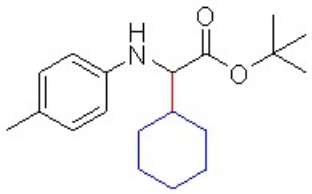

6.9760
6.9627
6.5508
6.5367
3.9807
3.8460
3.8357
3.6882
2.2234
1.8638
1.8425
1.7822
1.7766
1.7707
1.7654
1.7605
1.7571
1.7553
1.7523
1.7468
1.7414
1.7361
1.7323
1.7308
1.7274
1.7221
1.7170
1.7117
1.6808
1.6783
1.6756
1.6734
1.6676
1.6595
1.6575
1.6543
1.2722
1.2663
1.2603
1.2562
1.2512
1.2453
1.2393
1.2348
1.2306
1.2231
1.2207
1.2178
1.2027
1.1968
1.1909
1.1830
1.1770
1.1644
1.1554
1.1490
1.1435
1.1289
1.1234
O
N
H
O
3ba
1.89
1.97
0.91
1.01
2.94
3.00
6.06
5.18
f1 (ppm)


6.9847
6.9653
6.5701
6.5493
5.0874
5.0719
5.0562
5.0441
5.0405
5.0284
5.0249
5.0093
4.9938
4.0259
3.8071
3.7924
2.2323
1.8756
1.8446
1.7929
1.7641
1.7259
1.6966
1.6660
1.3970
1.3812
1.3609
1.2872
1.2716
1.2407
1.2246
1.2045
1.1820
1.1534
1.0808
1.0647
3ca
2.02
2.04
1.05
1.01
1.05
3.00
7.00
2.07
6.10
2.08
.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
-1

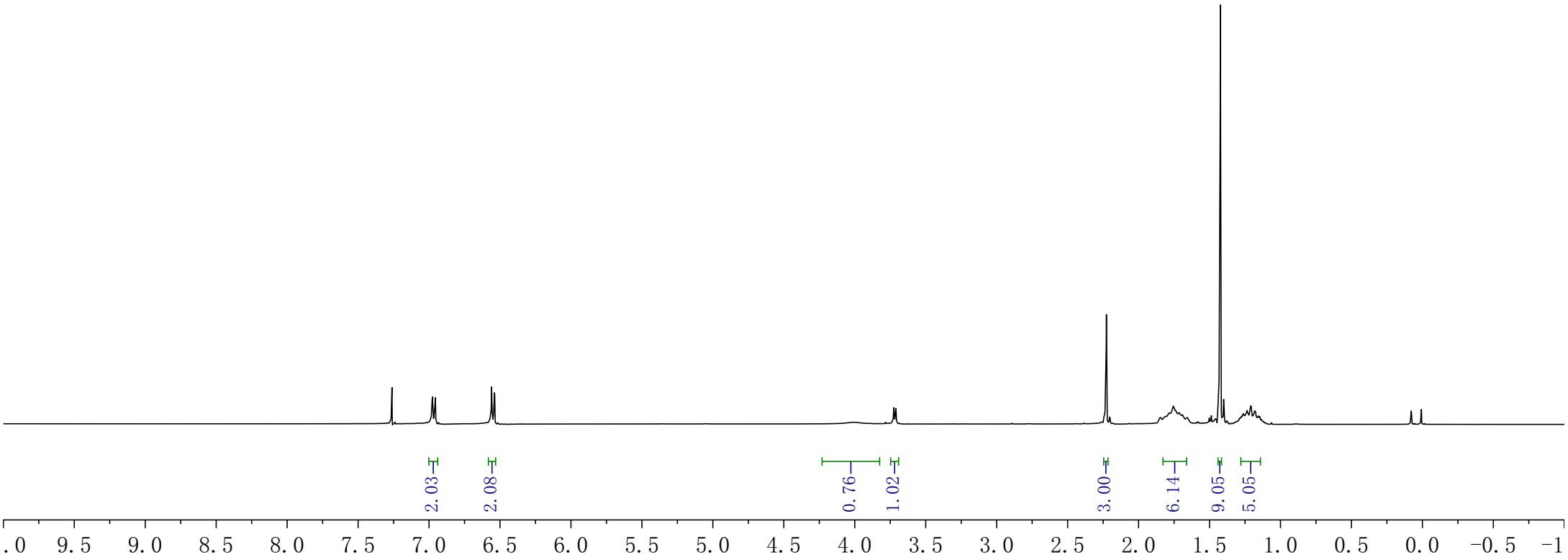

H
N
O
O

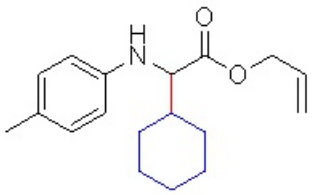
3da

6.9805
6.9593
6.5629
6.5418
4.1126
4.0960
4.0793
4.0026
3.8383
3.8231
2.2255
1.8728
1.8411
1.7892
1.7824
1.7586
1.6963
1.6802
1.6684
1.6255
1.6225
1.6085
1.6002
1.5913
1.5870
1.5746
1.5697
1.5530
1.3862
1.3677
1.3492
1.3304
1.3114
1.2924
1.2841
1.2760
1.2622
1.2542
1.2442
1.2377
1.2263
1.2102
1.1972
1.1915
1.1852
1.1798
1.1681
1.1396
1.1322
0.9256
0.9071
0.8887
2.01
2.04
2.05
0.95
1.00
3.00
7.07
2.02
2.03
4.10
3.03
.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
-1



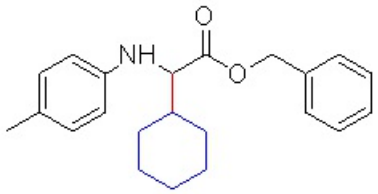
3ea


6.9767
6.9566
6.5592
6.5383
4.0028
3.7240
3.7098
2.2265
1.8475
1.8054
1.7858
1.7557
1.7400
1.7195
1.7144
1.6996
1.6912
1.6576
1.4238
1.2622
1.2519
1.2430
1.2360
1.2081
1.1825
2.03
2.08
0.76
1.02
3.00
6.14
9.05
5.05
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1



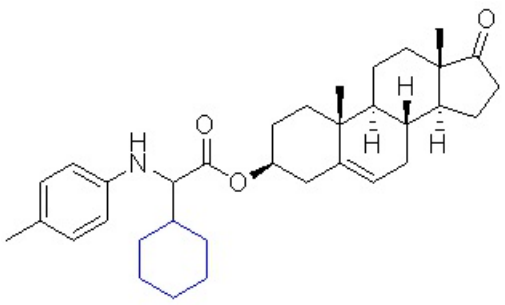
3fa

6.9803
6.9592
6.5632
6.5422
5.9266
5.9121
5.9005
5.8976
5.8860
5.8717
5.8691
5.8576
5.8547
5.8431
5.8285
5.3153
5.3118
5.3082
5.2723
5.2688
5.2652
5.2399
5.2370
5.2338
5.2139
5.2110
5.2078
4.6027
4.5882
3.9881
3.8667
2.2230
1.8699
1.8388
1.7802
1.7556
1.6934
1.6678
1.2574
1.2424
1.2396
1.2217
1.2039
1.1951
1.1661
1.1363
2.00
2.03
0.69
0.81
0.82
1.76
1.01
1.08
3.06
6.08
5.06
.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
-1

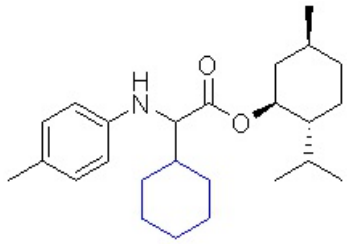

O
NH
O

3ga

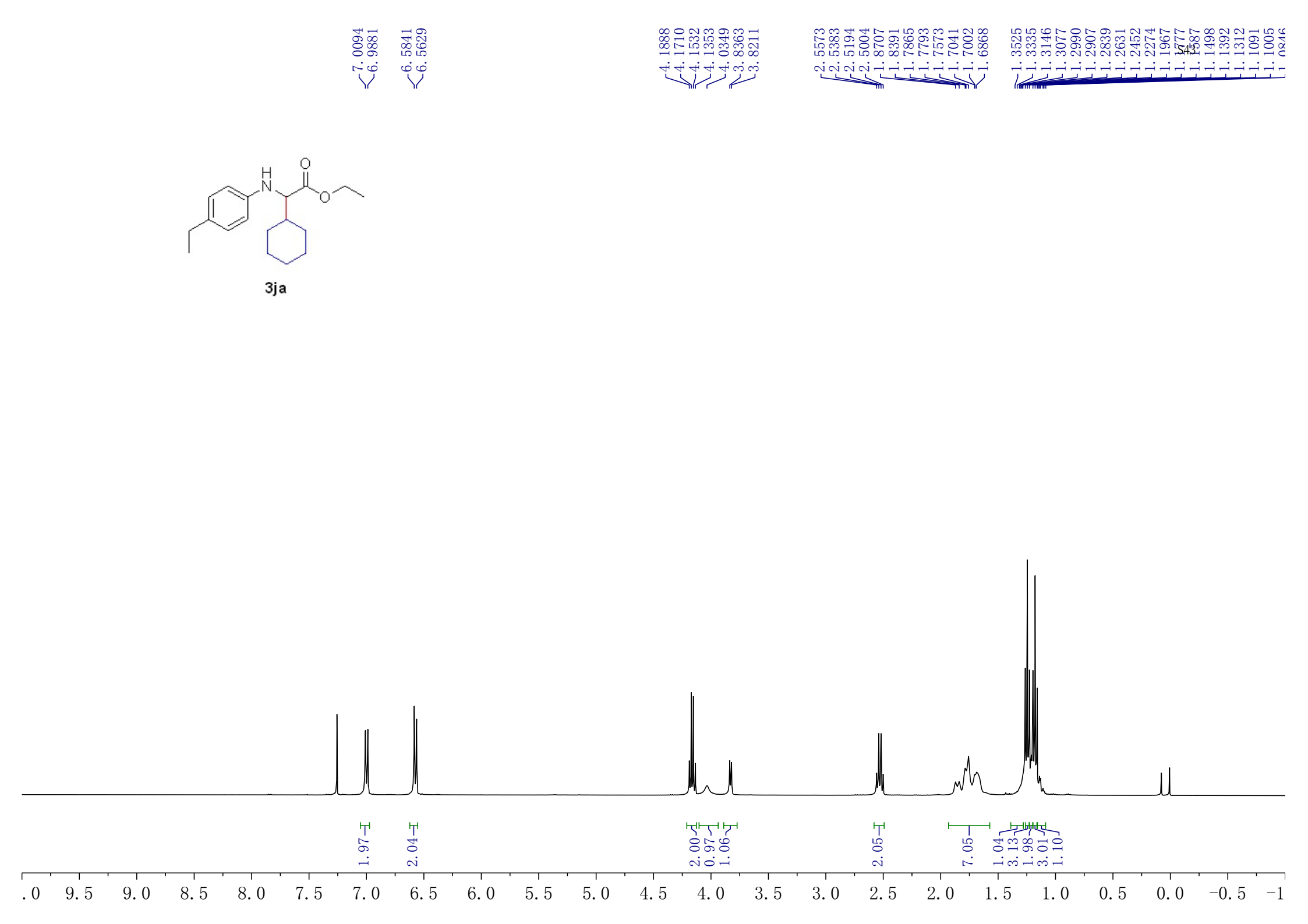
7.3691
7.3665
7.3649
7.3614
7.3547
7.3514
7.3389
7.3154
7.3095
7.2966
7.2921
7.0049
6.9849
6.5938
6.5729
5.1571
4.0510
4.0283
3.9457
3.9309
3.9074
2.2644
1.8735
1.8393
1.7895
1.7627
1.6998
1.6697
1.6647
1.2906
1.2728
1.2549
1.2408
1.2275
1.2043
1.1742
1.1436
4.86
2.02
2.05
1.89
1.03
0.97
3.00
6.02
5.06
.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
−1

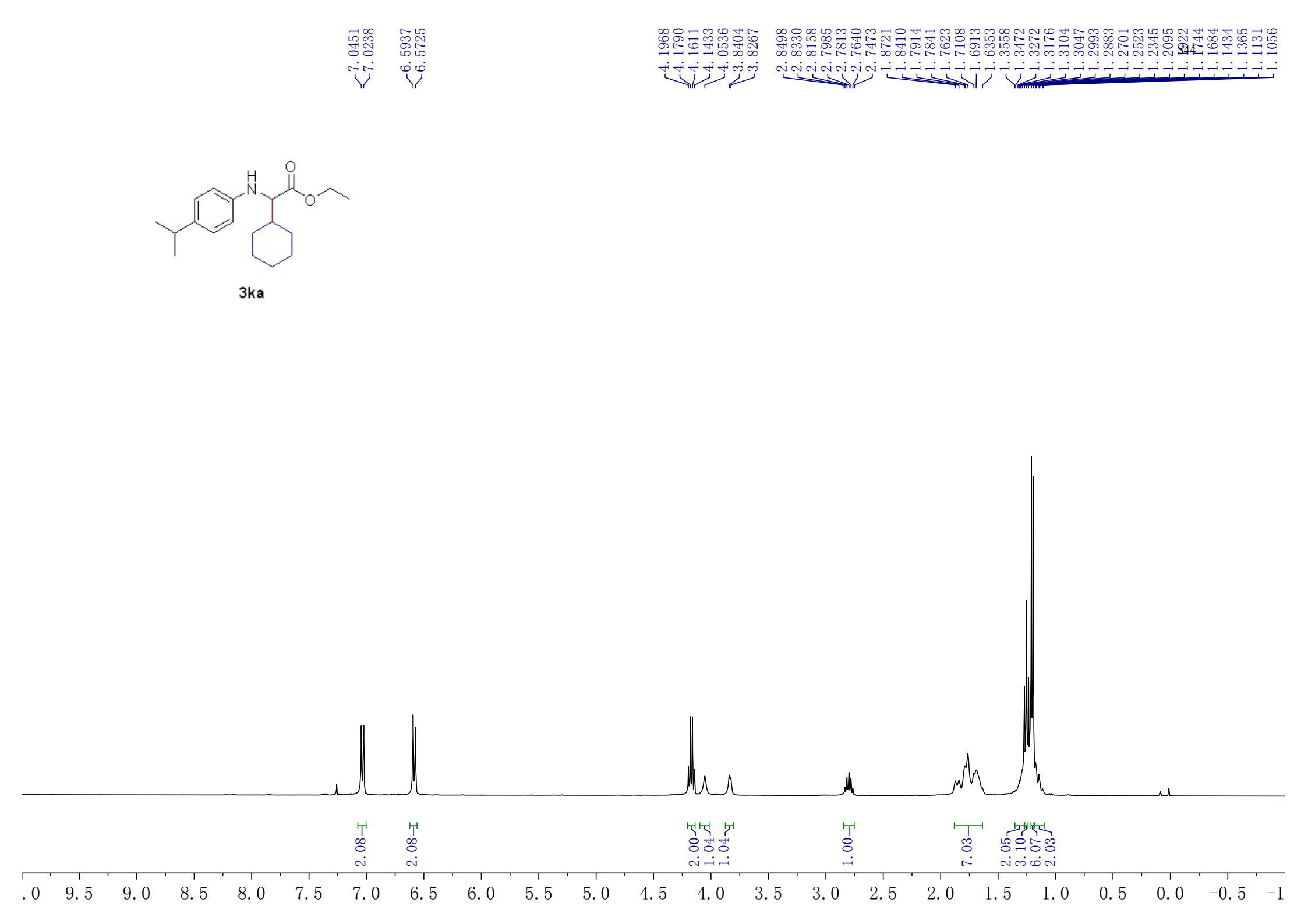


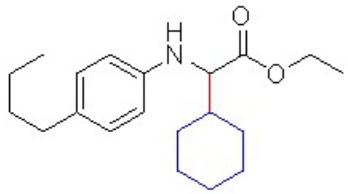
3ha



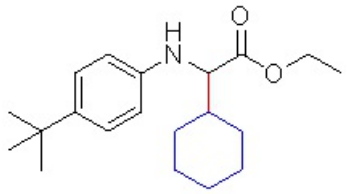
3ia


7.0094
6.9881
6.5841
6.5629
4.1888
4.1710
4.1532
4.1353
4.0349
3.8363
3.8211
2.5573
2.5383
2.5194
2.5004
1.8707
1.8391
1.7865
1.7793
1.7573
1.7041
1.7002
1.6868
1.3525
1.3335
1.3146
1.3077
1.2990
1.2907
1.2839
1.2631
1.2452
1.2274
1.1967
1.1777
1.1587
1.1498
1.1392
1.1312
1.1091
1.1005
NH
O
O
3ja
1.97
2.04
2.00
0.97
1.06
2.05
7.05
1.04
3.13
1.98
3.01
1.10
.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
-0.5
-1

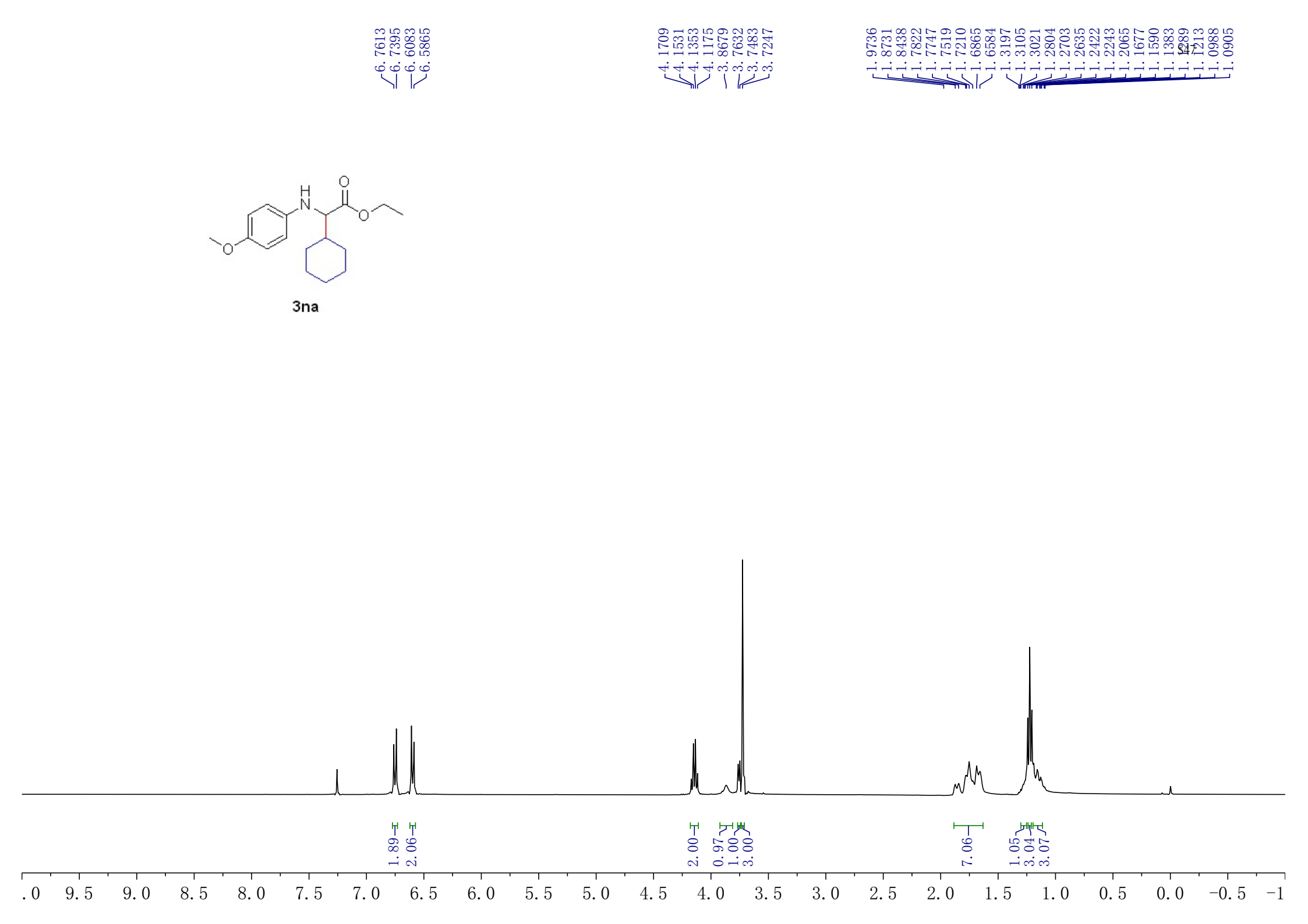

7.0451
7.0238
6.5937
6.5725
4.1968
4.1790
4.1611
4.1433
4.0536
3.8404
3.8267
2.8498
2.8330
2.8158
2.7985
2.7813
2.7640
2.7473
1.8721
1.8410
1.7914
1.7841
1.7623
1.7108
1.6913
1.6353
1.3558
1.3472
1.3272
1.3176
1.3104
1.3047
1.2993
1.2883
1.2701
1.2523
1.2345
1.2095
1.1922
1.1744
1.1684
1.1434
1.1365
1.1131
1.1056
3ka
2.08
2.08
2.00
1.04
1.04
1.00
7.03
2.05
3.10
6.07
2.03
.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
-1

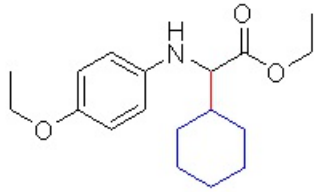


3la

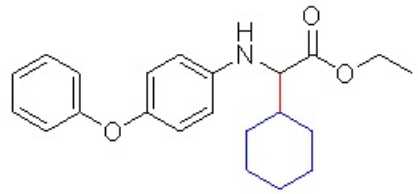


3ma

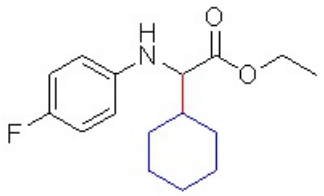

6.7613
6.7395
6.6083
6.5865
4.1709
4.1531
4.1353
4.1175
3.8679
3.7632
3.7483
3.7247
1.9736
1.8731
1.8438
1.7822
1.7747
1.7519
1.7210
1.6865
1.6584
1.3197
1.3105
1.3021
1.2804
1.2703
1.2635
1.2422
1.2243
1.2065
1.1677
1.1590
1.1383
1.1289
1.1213
1.0988
1.0905
3na
1.89
2.06
2.00
0.97
1.00
3.00
7.06
1.05
3.04
3.07
.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
-1



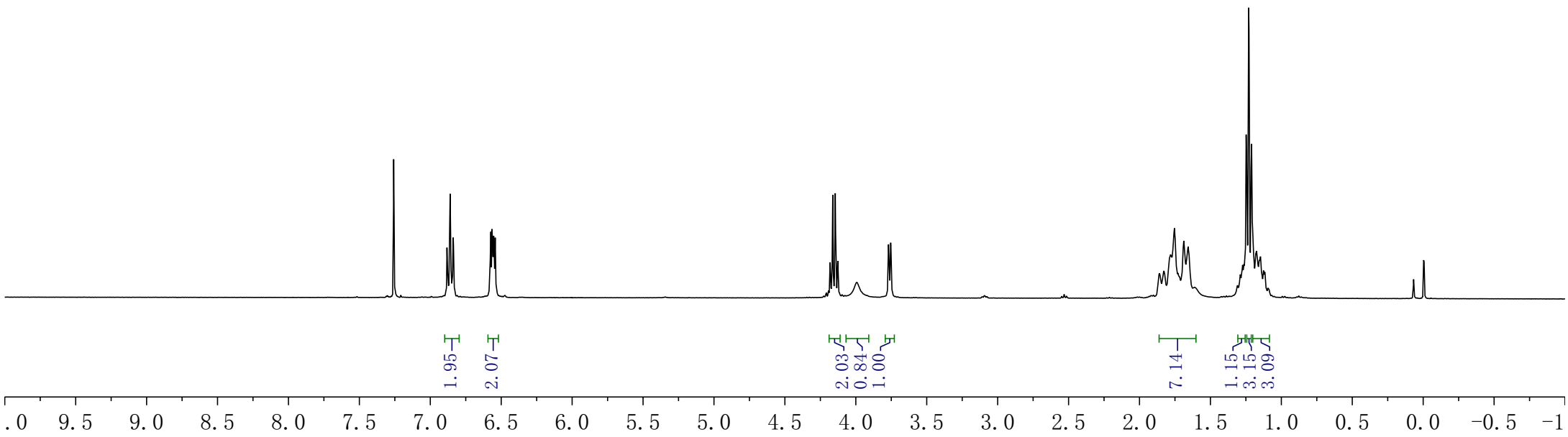
3oa

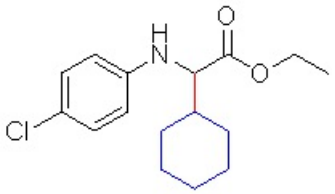


3pa



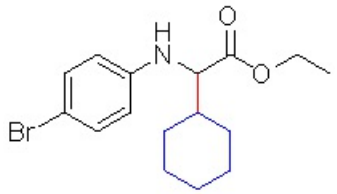
3qa


6.8822
6.8799
6.8597
6.8386
6.5733
6.5645
6.5508
6.5419
4.1806
4.1628
4.1450
4.1273
3.9926
3.7691
3.7539
1.8588
1.8274
1.7805
1.7537
1.7287
1.6878
1.6570
1.3102
1.2896
1.2728
1.2635
1.2480
1.2302
1.2123
1.1751
1.1470
1.1253
1.1167
1.0949
1.95
2.07
2.03
0.84
1.00
7.14
1.15
3.15
3.09
.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
-1


H
N
O
O
Cl

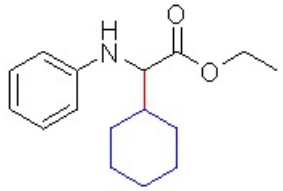
3ra

7.1090
7.0868
6.5520
6.5298
4.1935
4.1756
4.1577
4.1400
4.1189
3.8164
3.8011
3.7932
3.7779
1.8432
1.8042
1.7837
1.7560
1.7282
1.7200
1.7128
1.6895
1.6600
1.2621
1.2443
1.2264
1.2120
1.1878
1.1829
1.1544
1.1333
1.1245
1.1174
1.1020
1.0948
2.02
2.00
3.05
1.00
7.09
3.05
4.04
.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
-1


H
N
O
O
Br

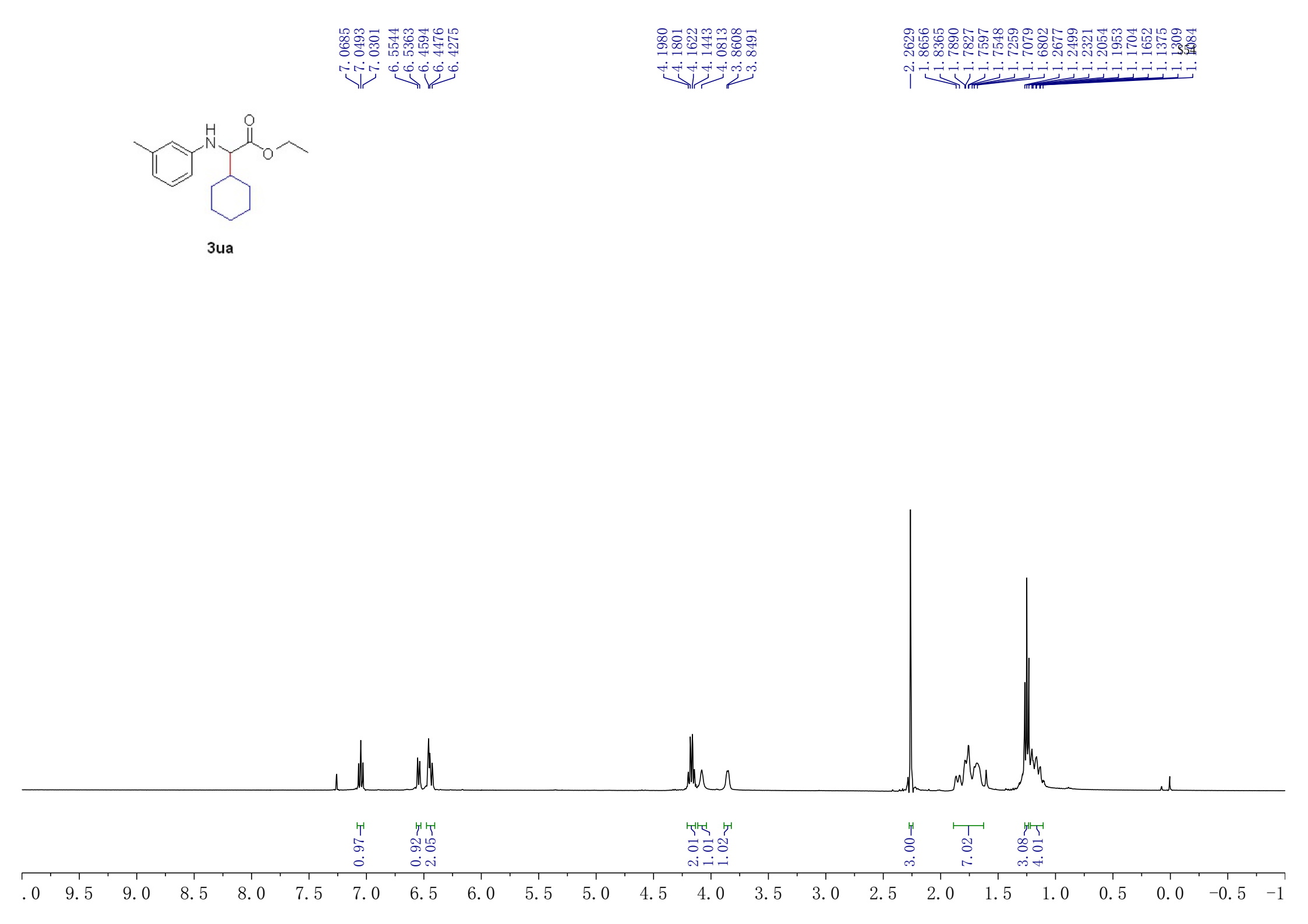
3sa

7.2393
7.2194
6.5060
6.4856
4.1947
4.1926
4.1767
4.1746
4.1589
4.1568
4.1410
3.8131
3.7968
1.8378
1.7918
1.7829
1.7546
1.6887
1.6579
1.2645
1.2467
1.2288
1.2107
1.1933
1.1822
1.1525
1.1454
1.1306
1.1216
1.1149
1.0914
1.91
2.00
3.06
1.01
7.04
3.01
4.06
.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
-1



3ta

7.1801
7.1616
7.1588
7.1403
6.7375
6.7352
6.7328
6.7169
6.7010
6.6985
6.6960
6.6378
6.6354
6.6163
6.6140
4.1943
4.1764
4.1586
4.1408
4.1240
3.8805
3.8648
1.8716
1.8405
1.7926
1.7844
1.7808
1.7713
1.7637
1.7360
1.7284
1.7114
1.6899
1.6823
1.6622
1.6076
1.3233
1.3153
1.3038
1.2913
1.2835
1.2629
1.2450
1.2272
1.2100
1.2051
1.1738
1.1407
1.1150
1.1098
2.00
0.98
2.01
2.00
0.94
1.00
7.08
1.08
3.09
3.03
.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
-1

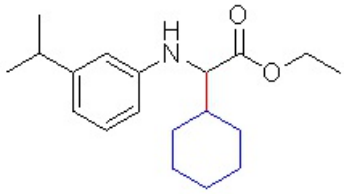

7.0685
7.0493
7.0301
6.5544
6.5363
6.4594
6.4476
6.4275
4.1980
4.1801
4.1622
4.1443
4.0813
3.8608
3.8491
2.2629
1.8656
1.8365
1.7890
1.7827
1.7597
1.7548
1.7259
1.7079
1.6802
1.2677
1.2499
1.2321
1.2054
1.1953
1.1704
1.1652
1.1375
1.1309
1.1084
NH
O
O
3ua
0.97
0.92
2.05
2.01
1.01
1.02
3.00
7.02
3.08
4.01
.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
-1

7.1090
7.0894
7.0700
6.6173
6.5971
6.5133
6.4583
6.4524
6.4383
6.4323

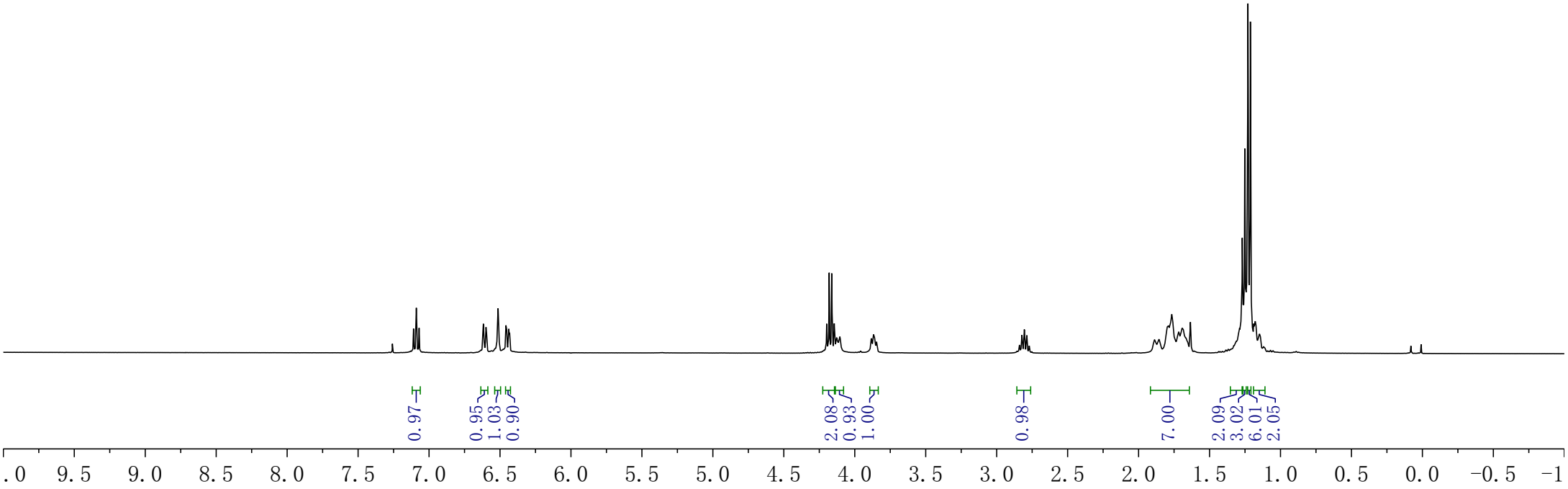
4.1979
4.1801
4.1622
4.1444
4.1273
4.1055
3.8830
3.8672

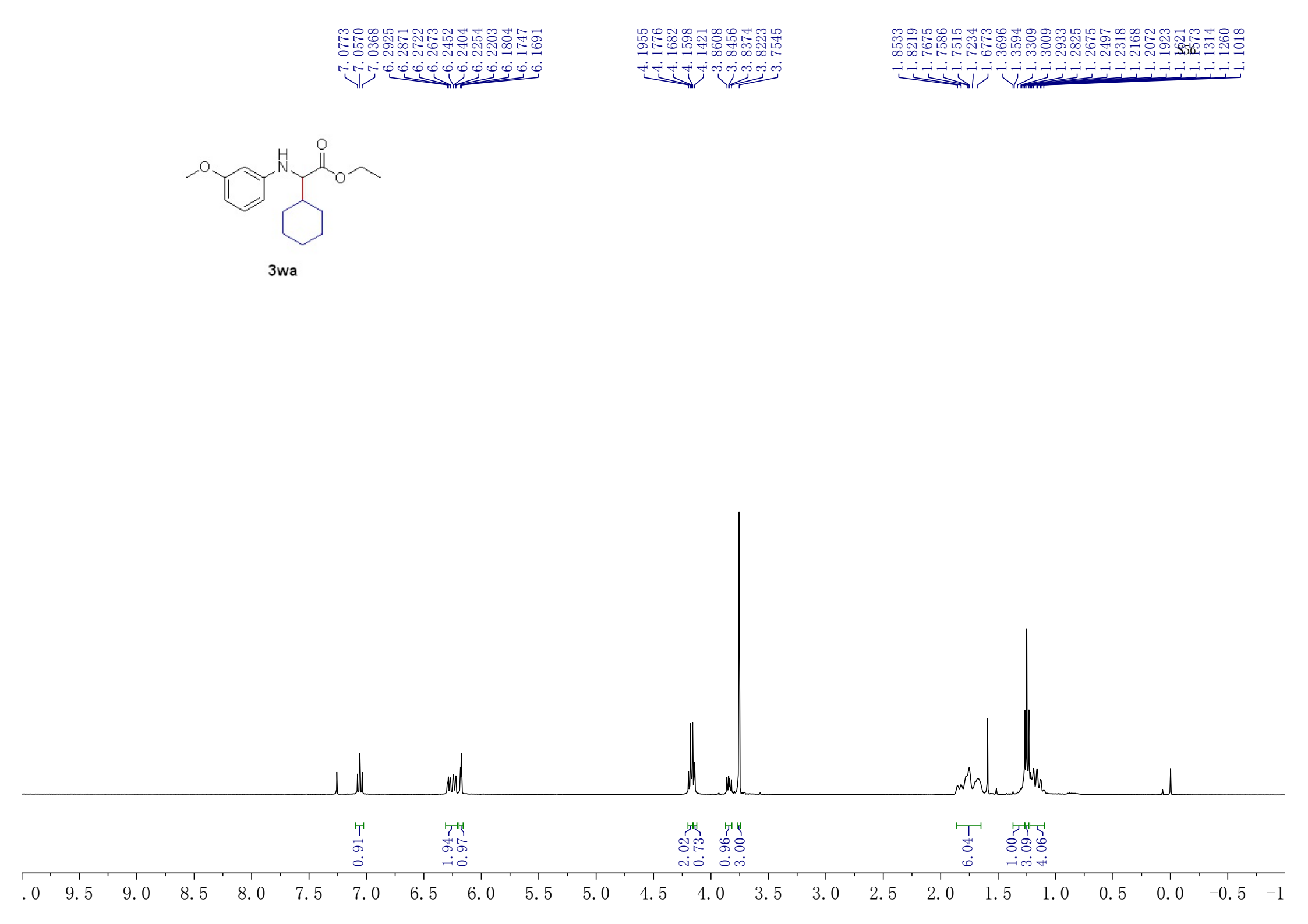
2.8393
2.8220
2.8047
2.7874
2.7701

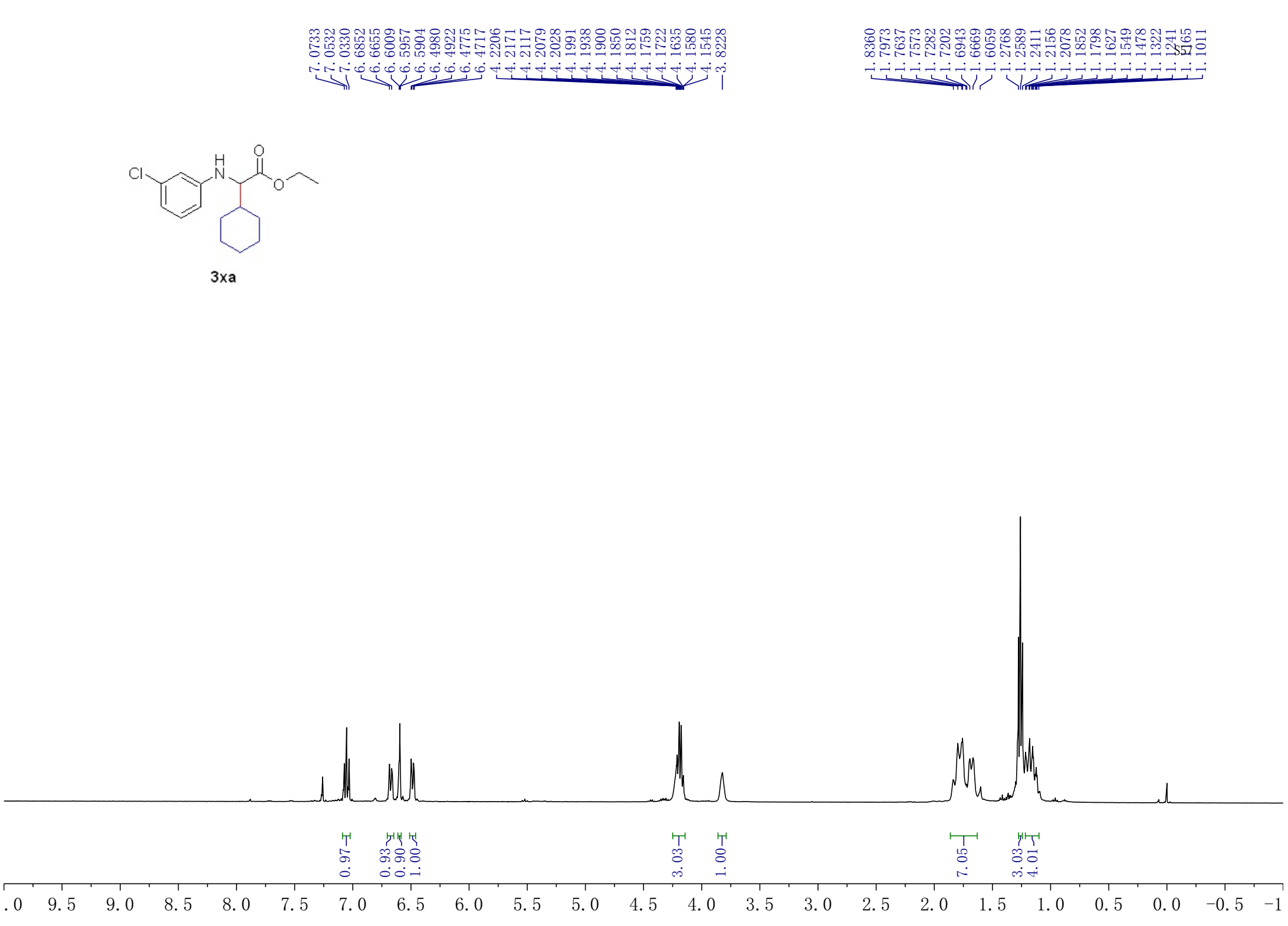
1.8879
1.8567
1.7958
1.7891
1.7665
1.7167
1.6933
1.3679
1.3290
1.3115
1.2880
1.2695
1.2517
1.2336
1.2294
1.2121
1.1884
1.1780
1.1475
1.1196

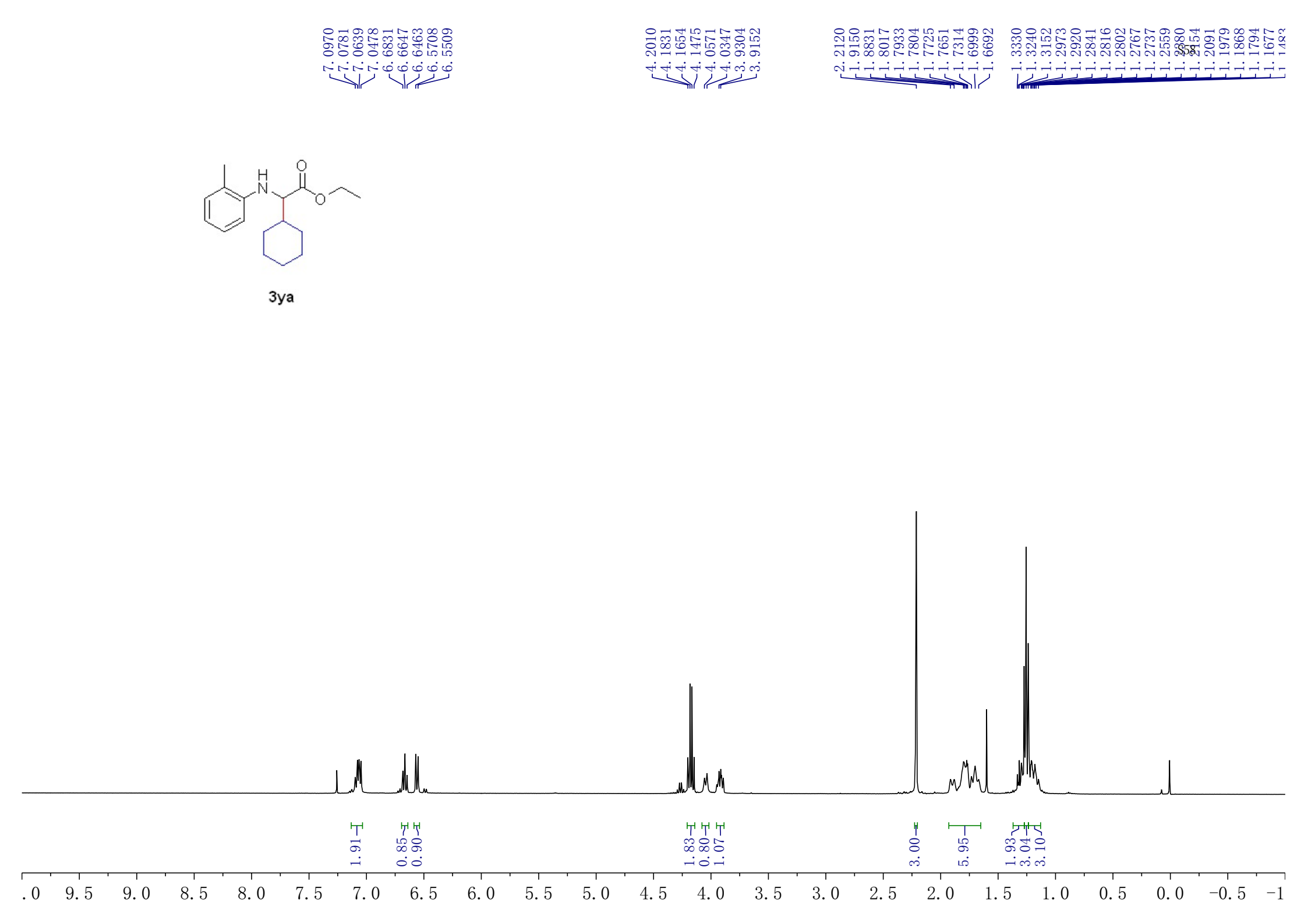


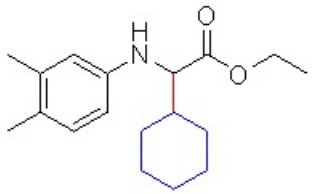
3va




7.0773
7.0570
7.0368
6.2925
6.2871
6.2722
6.2673
6.2452
6.2404
6.2254
6.2203
6.1804
6.1747
6.1691
4.1955
4.1776
4.1682
4.1598
4.1421
3.8608
3.8456
3.8374
3.8223
3.7545
1.8533
1.8219
1.7675
1.7586
1.7515
1.7234
1.6773
1.3696
1.3594
1.3309
1.3009
1.2933
1.2825
1.2675
1.2497
1.2318
1.2168
1.2072
1.1923
1.1621
1.1573
1.1314
1.1260
1.1018
3wa
0.91
1.94
0.97
2.02
0.73
0.96
3.00
6.04
1.00
3.09
4.06
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1

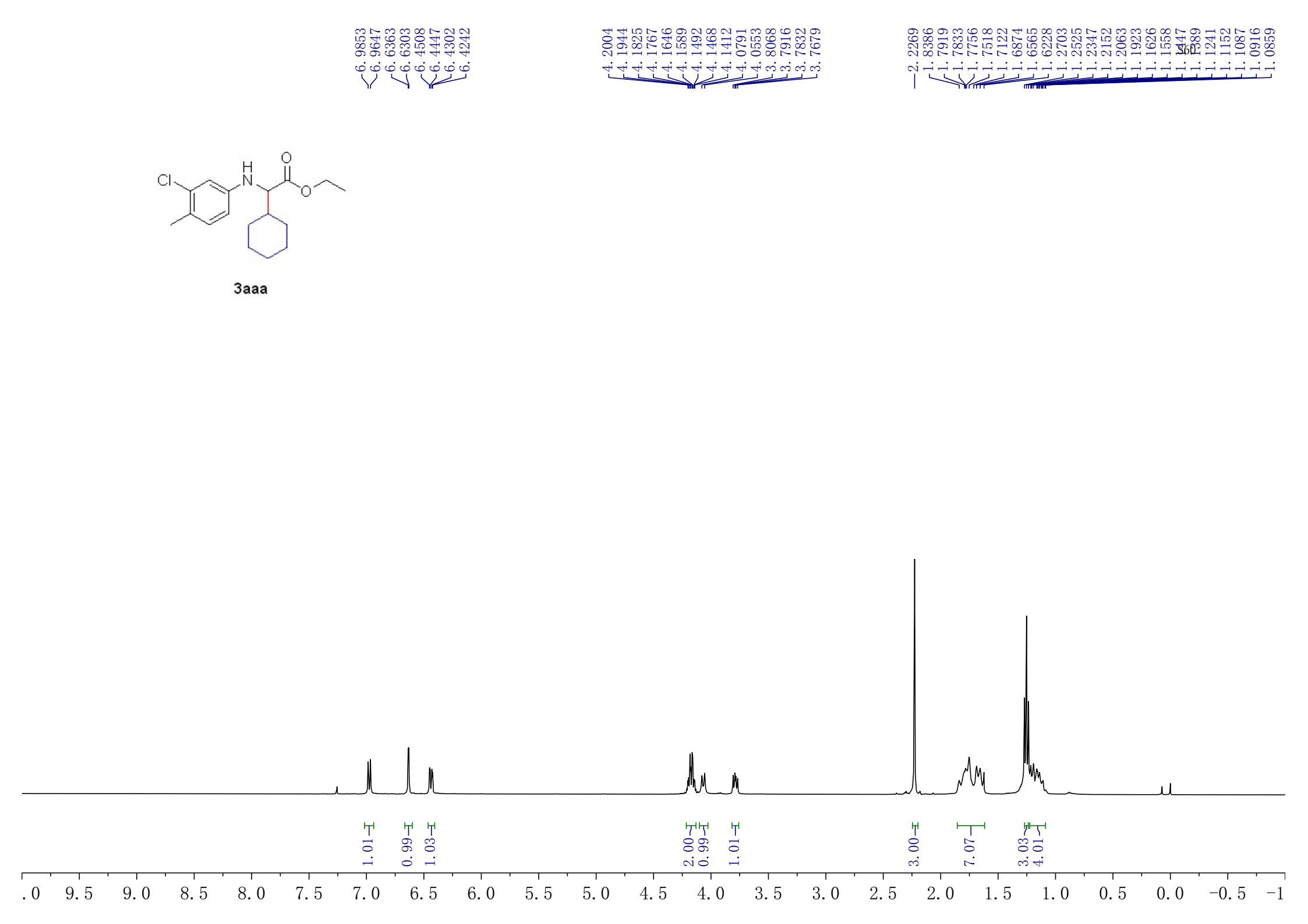

7.0733
7.0532
7.0330
6.6852
6.6655
6.6009
6.5957
6.5904
6.4980
6.4922
6.4775
6.4717
4.2206
4.2171
4.2117
4.2079
4.2028
4.1991
4.1938
4.1900
4.1850
4.1812
4.1759
4.1722
4.1635
4.1580
4.1545
3.8228
1.8360
1.7973
1.7637
1.7573
1.7282
1.7202
1.6943
1.6669
1.6059
1.2768
1.2589
1.2411
1.2156
1.2078
1.1852
1.1798
1.1627
1.1549
1.1478
1.1322
1.1241
1.1165
1.1011
Cl
N
H
O
O
3xa
0.97
0.93
0.90
1.00
3.03
1.00
7.05
3.03
4.01
.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
-1

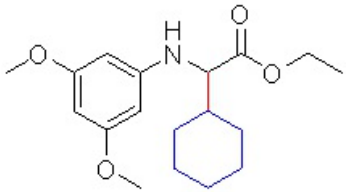

7.0970
7.0781
7.0639
7.0478
6.6831
6.6647
6.6463
6.5708
6.5509
4.2010
4.1831
4.1654
4.1475
4.0571
4.0347
3.9304
3.9152
2.2120
1.9150
1.8831
1.8017
1.7933
1.7804
1.7725
1.7651
1.7314
1.6999
1.6692
1.3330
1.3240
1.3152
1.2973
1.2920
1.2841
1.2816
1.2802
1.2767
1.2737
1.2559
1.2380
1.2354
1.2091
1.1979
1.1868
1.1794
1.1677
1.1483
3ya
1.91
0.85
0.90
1.83
0.80
1.07
3.00
5.95
1.93
3.04
3.10
.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
-0.5
-1



3za

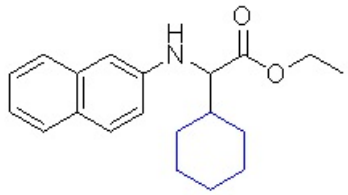
6.9263
6.9061
6.4713
6.4653
6.4049
6.3986
6.3848
6.3785
4.1896
4.1847
4.1810
4.1718
4.1670
4.1539
4.1492
4.1399
4.1360
4.1314
3.8298
3.8145
2.1777
2.1366
1.8673
1.8357
1.7849
1.7770
1.7539
1.7334
1.6977
1.6890
1.6847
1.6761
1.6663
1.3213
1.3126
1.3051
1.2973
1.2901
1.2825
1.2723
1.2659
1.2480
1.2302
1.2114
1.1893
1.1819
1.1684
1.1602
1.1522
1.1380
1.1298
0.90
0.96
0.96
1.88
0.96
3.00
3.03
6.08
1.03
3.00
4.01
.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
-1


6.9853
6.9647
6.6363
6.6303
6.4508
6.4447
6.4302
6.4242
4.2004
4.1944
4.1825
4.1767
4.1646
4.1589
4.1492
4.1468
4.1412
4.0791
4.0553
3.8068
3.7916
3.7832
3.7679
2.2269
1.8386
1.7919
1.7833
1.7756
1.7518
1.7122
1.6874
1.6565
1.6228
1.2703
1.2525
1.2347
1.2152
1.2063
1.1923
1.1626
1.1558
1.1447
1.1389
1.1241
1.1152
1.1087
1.0916
1.0859
Cl
H
N
O
O
3aaa
1.01
0.99
1.03
2.00
0.99
1.01
3.00
7.07
3.03
4.01
.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
−1

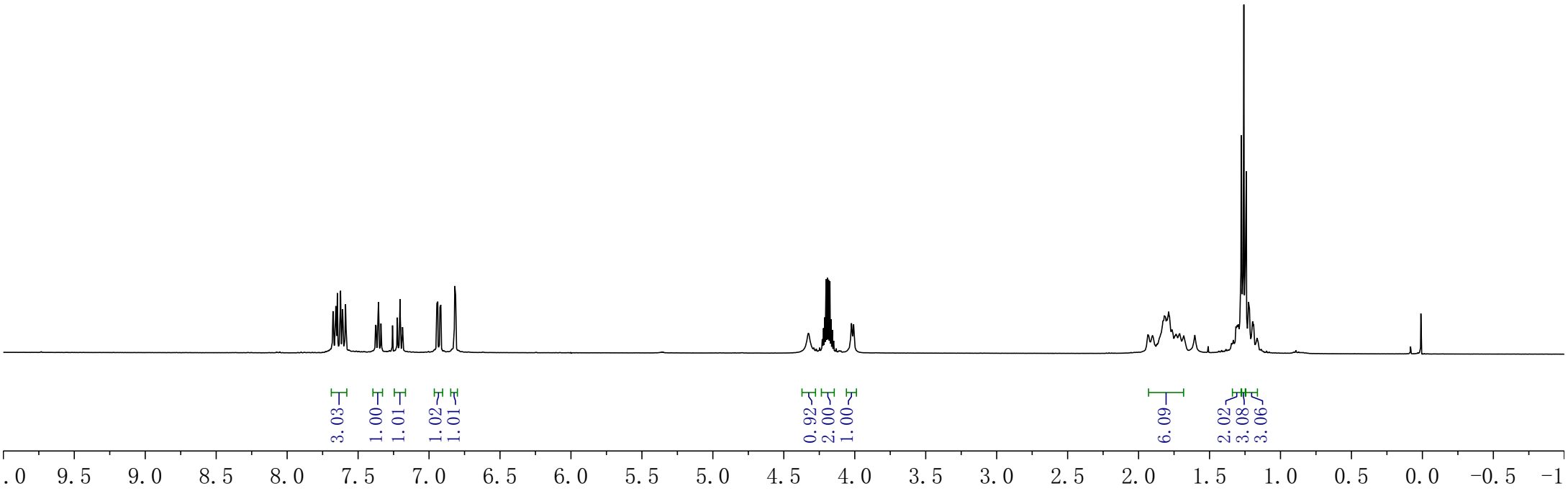


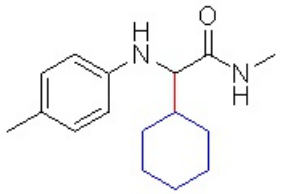
3aba

5.8806
5.8759
5.8090
5.8045
4.2012
4.1974
4.1834
4.1795
4.1656
4.1616
4.1479
3.8398
3.8255
3.8194
3.8041
3.7357
3.7318
1.8408
1.8094
1.7736
1.7471
1.6581
1.3270
1.2979
1.2909
1.2711
1.2575
1.2396
1.2087
1.1845
1.1554
1.1244
1.0955
0.82
1.86
1.88
0.72
1.04
6.00
6.07
1.09
3.04
4.03
.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
−1



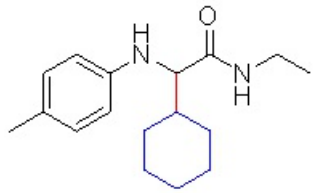
3aca



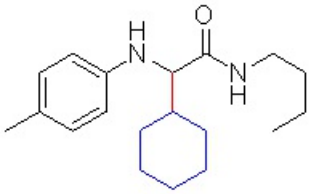


3ada

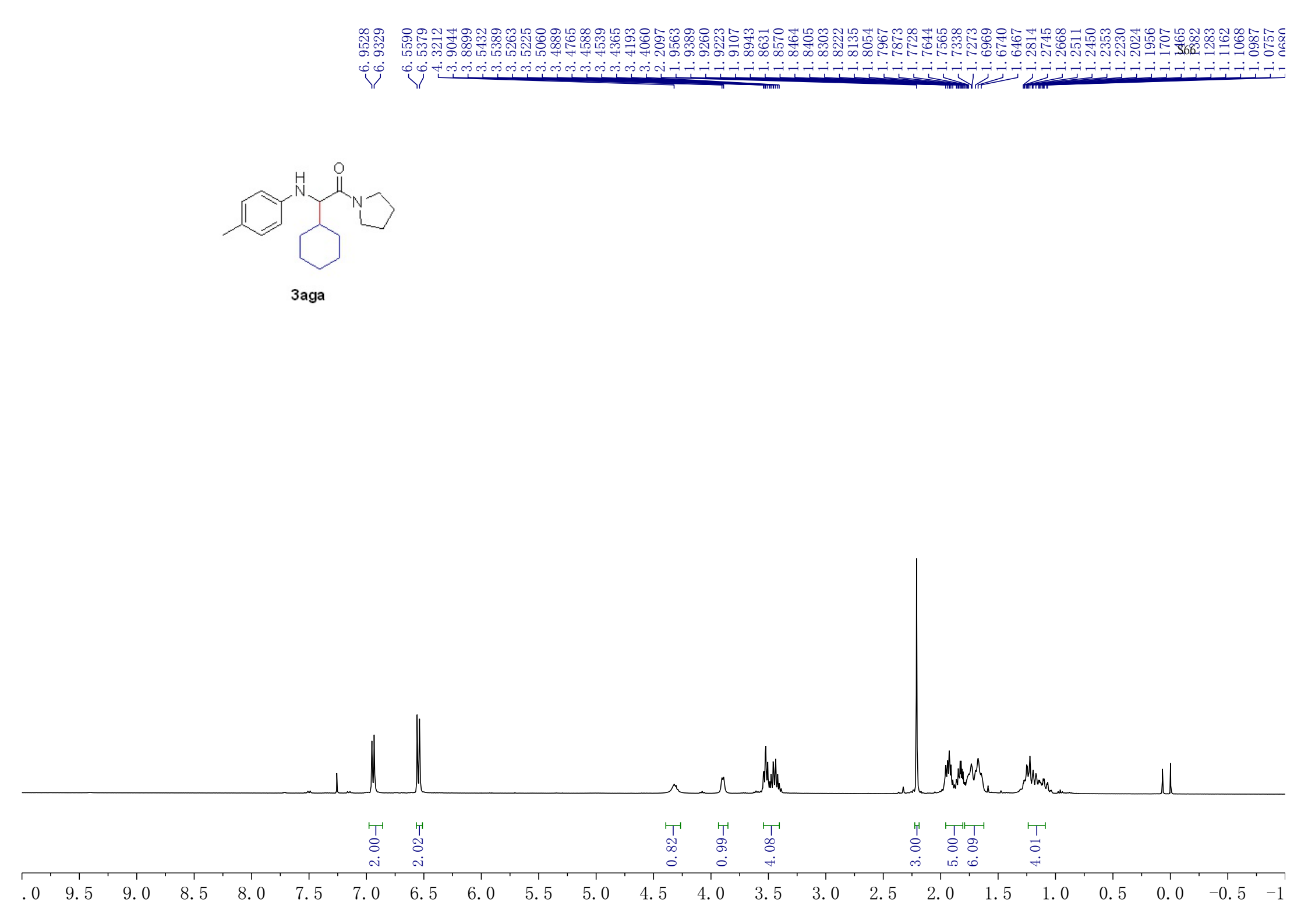
7.0080
6.9873
6.8710
6.5274
6.5075
3.8582
3.5309
3.5208
2.7878
2.7756
2.2378
2.0422
2.0338
2.0125
2.0042
1.9824
1.9746
1.7878
1.7591
1.6968
1.6671
1.3556
1.3237
1.3158
1.2850
1.2598
1.2522
1.2180
1.1865
1.1560
1.1252
1.0946
1.93
1.03
2.02
1.05
1.05
3.03
3.00
1.02
2.05
3.09
5.04
.0
9.5
9.0
8.5
8.0
7.5
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
-1



3aea

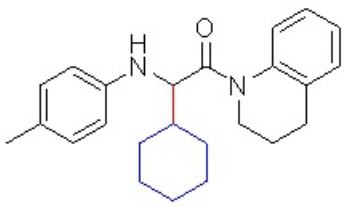


3afa (74 %)

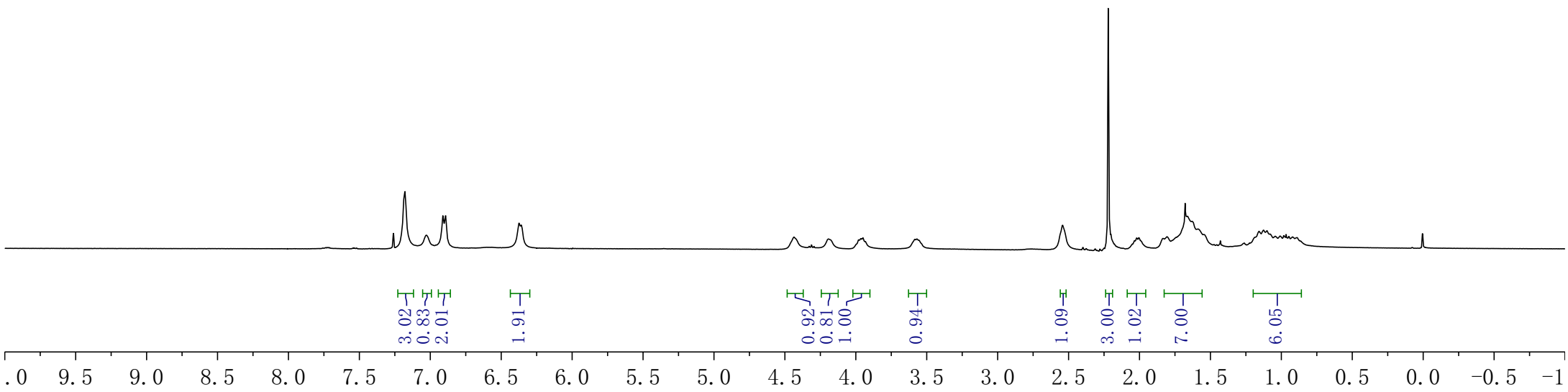

6.9528
6.9329
6.5590
6.5379
4.3212
3.9044
3.8899
3.5432
3.5389
3.5263
3.5225
3.5060
3.4889
3.4765
3.4588
3.4539
3.4365
3.4193
3.4060
2.2097
1.9563
1.9389
1.9260
1.9223
1.9107
1.8943
1.8631
1.8570
1.8464
1.8405
1.8303
1.8222
1.8135
1.8054
1.7967
1.7873
1.7728
1.7644
1.7565
1.7338
1.7273
1.6969
1.6740
1.6467
1.2814
1.2745
1.2668
1.2511
1.2450
1.2353
1.2230
1.2024
1.1956
1.1707
1.1465
1.1382
1.1283
1.1162
1.1068
1.0987
1.0757
1.0680
H
N
O
N
3aga
2.00
2.02
0.82
0.99
4.08
3.00
5.00
6.09
4.01
.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
-1

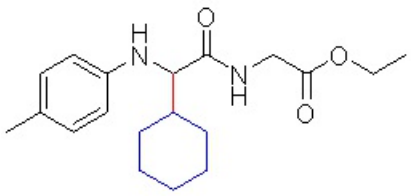
3aha

6.9626
6.9422
6.5523
6.5326
4.3126
4.0442
4.0298
3.6261
3.6147
3.5863
3.5647
3.5533
2.2145
1.8986
1.8695
1.7496
1.6995
1.6762
1.6520
1.5610
1.2646
1.2417
1.2151
1.1764
1.1463
1.1157
1.0864
1.90
1.93
0.72
0.95
8.05
3.00
1.06
6.02
4.04
.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
−1



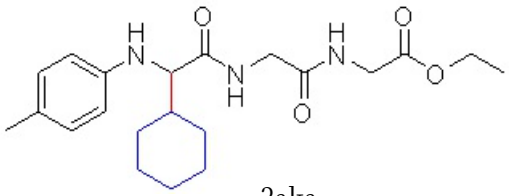
3aia


7.1793
7.0284
6.9108
6.8920
6.3742
6.3580
4.4368
4.1931
3.9803
3.9643
3.9502
3.5845
3.5694
2.5419
2.2205
2.0352
2.0201
2.0044
1.8348
1.8060
1.6784
1.1581
1.1263
1.1017
1.0428
1.0080
0.9835
0.9664
0.9471
0.9210
0.8867
3.02
0.83
2.01
1.91
0.92
0.81
1.00
0.94
1.09
3.00
1.02
7.00
6.05
.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
-1



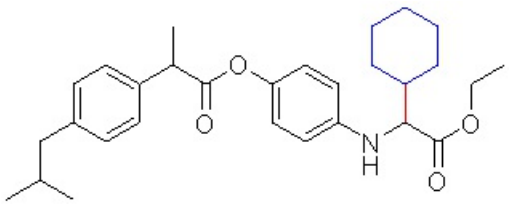
3aja

7.3028
7.2894
7.2754
7.0099
6.9887
6.5552
6.5342
4.1946
4.1871
4.1783
4.1692
4.1510
4.1332
3.8856
3.8734
3.8402
3.8280
3.5760
3.5656
2.2346
2.0708
2.0623
2.0531
2.0408
2.0327
2.0235
2.0149
2.0030
1.9939
1.7933
1.7701
1.7123
1.6995
1.6923
1.6802
1.3605
1.3368
1.3290
1.3062
1.2971
1.2867
1.2688
1.2638
1.2554
1.2376
1.2196
1.2018
1.1926
1.1714
1.1596
1.1501
1.1398
1.1282
1.01
1.94
2.01
0.84
2.02
1.01
1.00
2.99
1.08
6.04
2.02
3.00
2.07
.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
-1

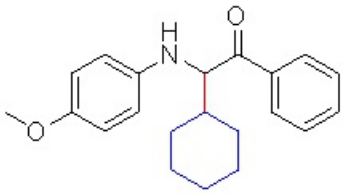


3aka

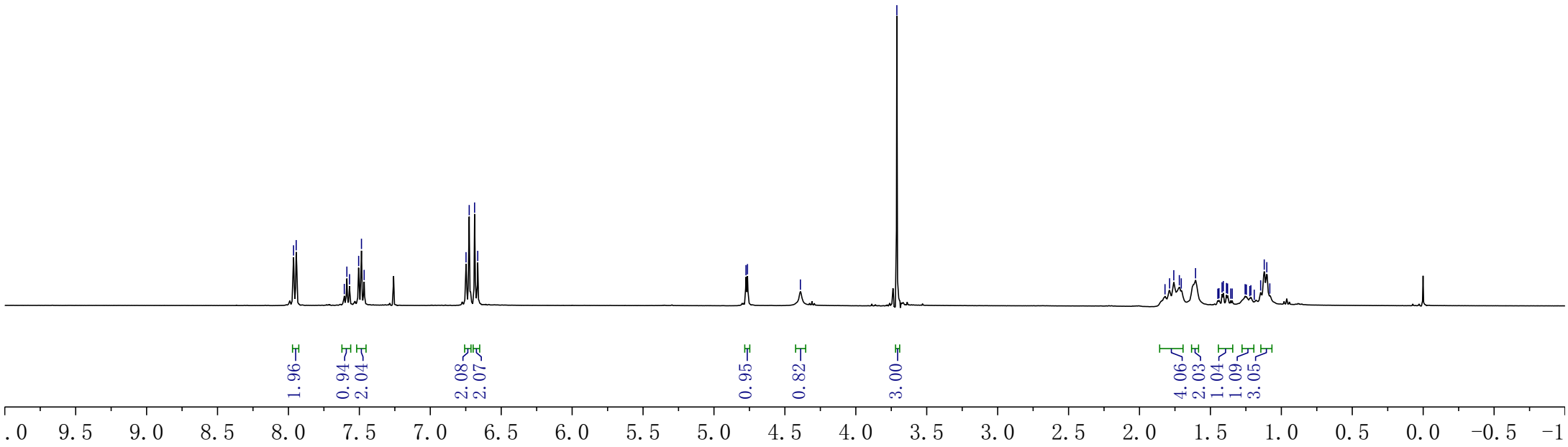
7.48
6.99
6.97
6.60
6.55
6.53
4.19
4.18
4.16
4.14
3.97
3.96
3.93
3.91
3.89
3.88
3.63
3.61
2.22
2.06
1.99
1.98
1.97
1.96
1.95
1.94
1.77
1.73
1.71
1.69
1.67
1.42
1.40
1.39
1.31
1.28
1.26
1.24
1.23
1.22
1.21
1.20
1.19
1.18
1.16
1.15
1.13
0.91
1.97
0.97
2.01
1.95
1.95
1.89
0.91
3.00
1.07
5.02
0.95
3.08
4.07
.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
−1

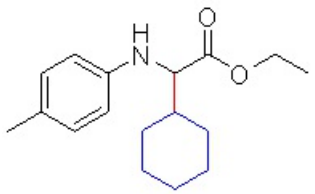


3ala



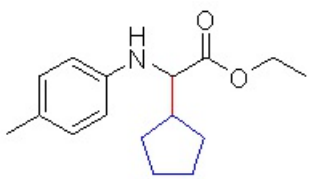
3ama


7.96
7.95
7.61
7.59
7.57
7.51
7.49
7.47
6.75
6.73
6.69
6.67
4.77
4.76
4.39
3.71
1.82
1.79
1.76
1.72
1.71
1.60
1.45
1.44
1.42
1.41
1.39
1.38
1.36
1.35
1.26
1.25
1.22
1.21
1.19
1.15
1.12
1.10
1.08
1.96
0.94
2.04
2.08
2.07
0.95
0.82
3.00
4.06
2.03
1.04
1.09
3.05
.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
−1



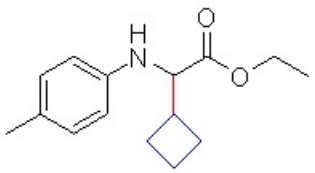
3aa

173.80
145.17
129.71
127.29
113.71
62.44
60.68
41.31
29.61
29.18
26.19
26.09
26.05
20.33
14.28
10
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-1



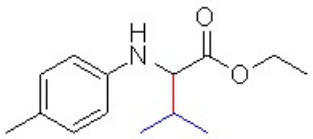
3ab

174.29
145.05
129.71
127.41
113.66
61.25
60.69
43.19
29.36
29.03
25.33
25.10
20.35
14.26
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0



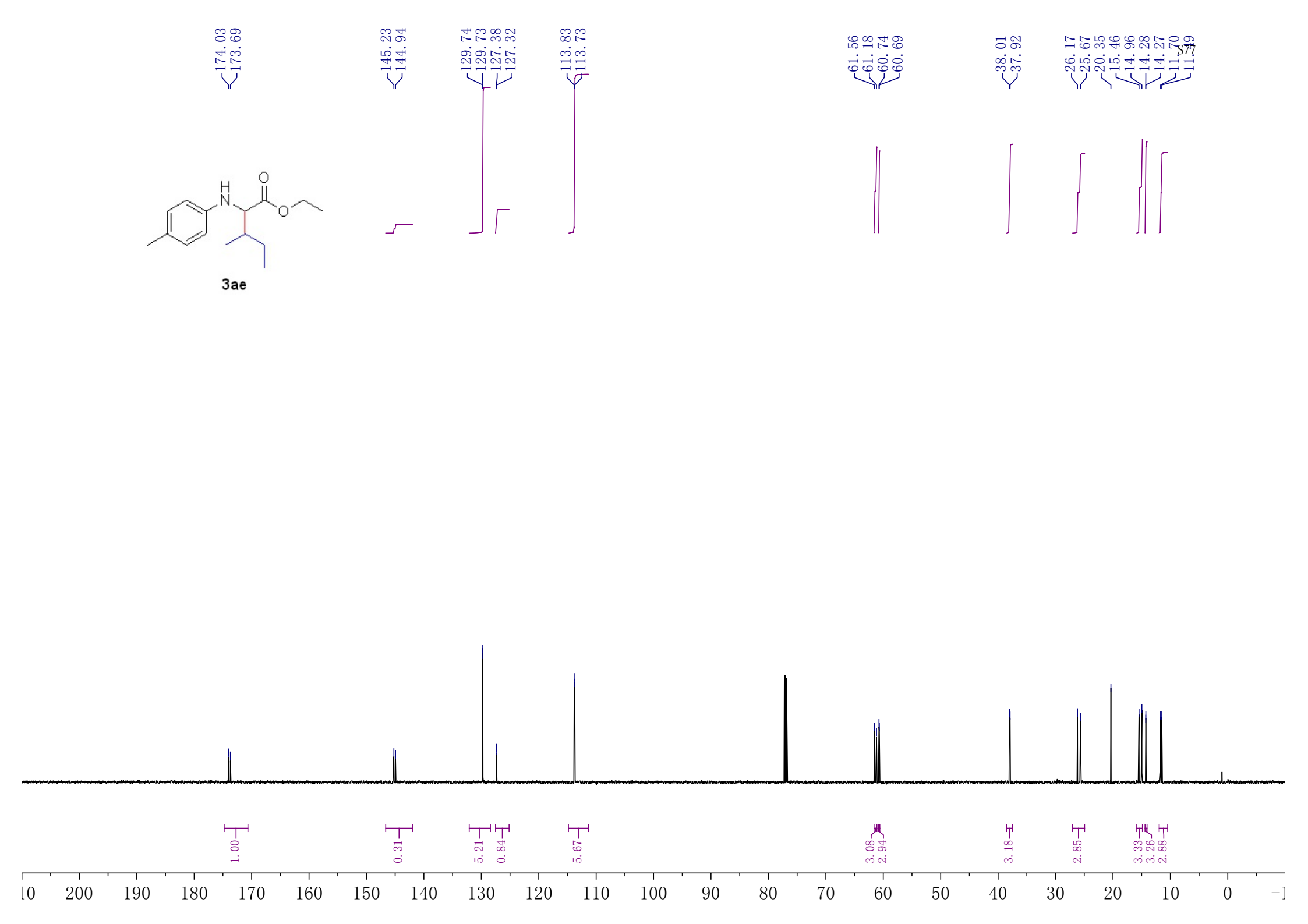
3ac

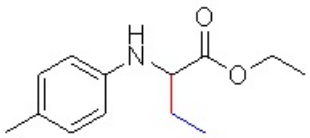
173.52
145.05
129.71
127.46
113.68
61.48
60.74
38.37
25.41
24.75
20.36
18.06
14.31
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0



3ad

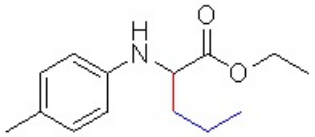
173.78
145.11
129.74
127.38
113.81
62.89
60.73
31.53
20.35
19.07
18.68
14.29
10
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-1


174.03
173.69
145.23
144.94
129.74
129.73
127.38
127.32
113.83
113.73
61.56
61.18
60.74
60.69
38.01
37.92
26.17
25.67
20.35
15.46
14.96
14.28
14.27
11.70
11.59
3ae
1.00
0.31
5.21
0.84
5.67
3.08
2.94
3.18
2.85
3.33
3.26
2.88
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10



3af

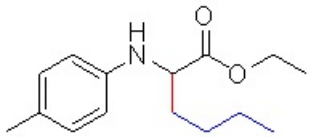
174.14
144.61
129.75
127.38
113.66
60.87
58.16
26.11
20.36
14.24
9.89
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0



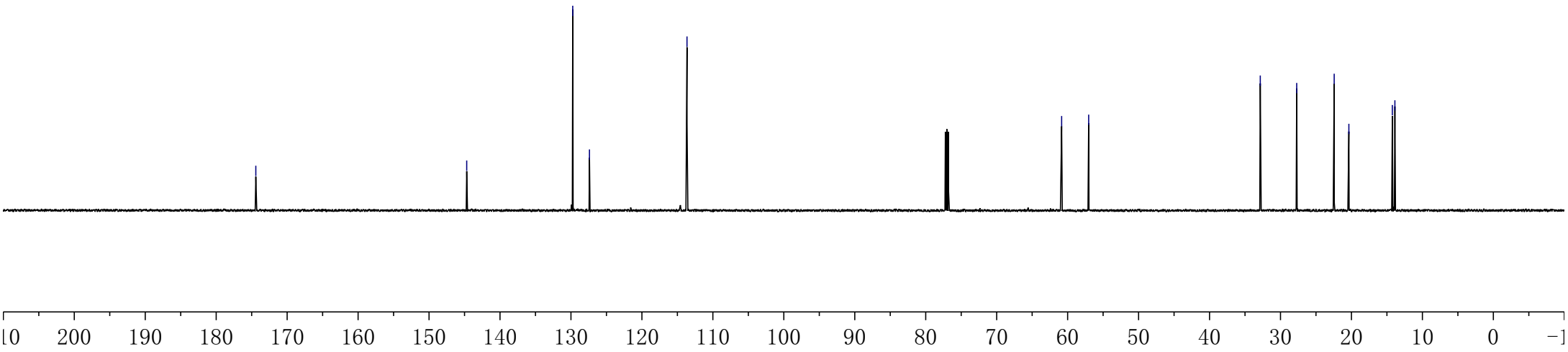
3ag

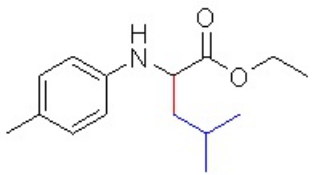
174.40
144.62
129.75
127.46
113.67
60.86
56.86
35.22
20.36
18.87
14.23
13.80
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10

^{13}C NMR (151 MHz, cdcl$_3$) δ 174.41, 144.69, 129.75, 127.39, 113.65, 60.84, 57.03, 32.85, 27.71, 22.43, 20.36, 14.24, 13.88.



3ah

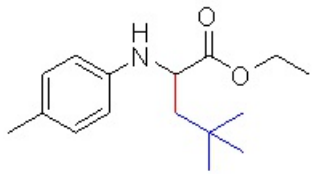




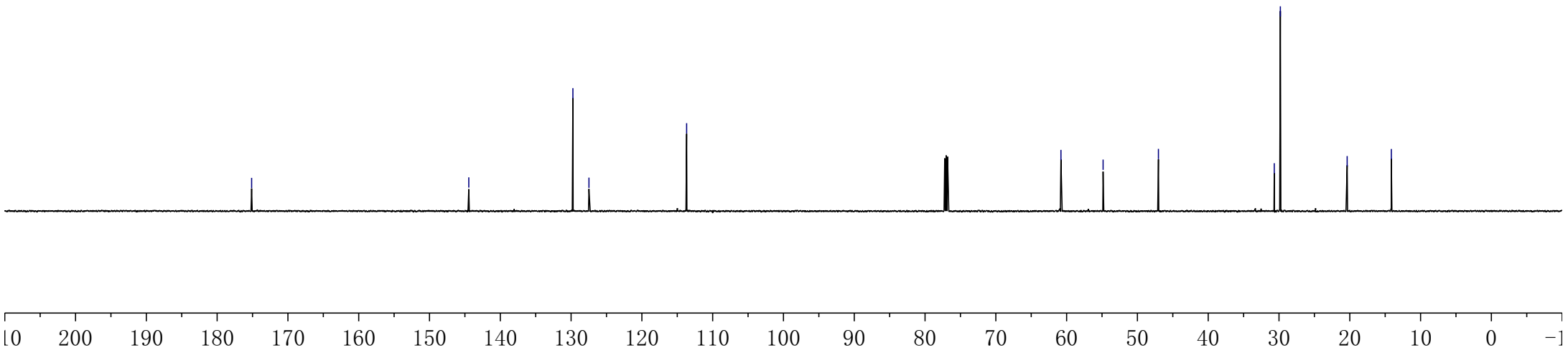
3ai

174.86
144.73
129.75
127.51
113.66
60.80
55.58
42.40
24.87
22.73
22.23
20.37
14.21
10
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-1

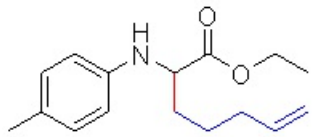
175.13
144.45
129.74
127.48
113.68
60.80
54.85
47.03
30.67
29.81
20.37
14.13



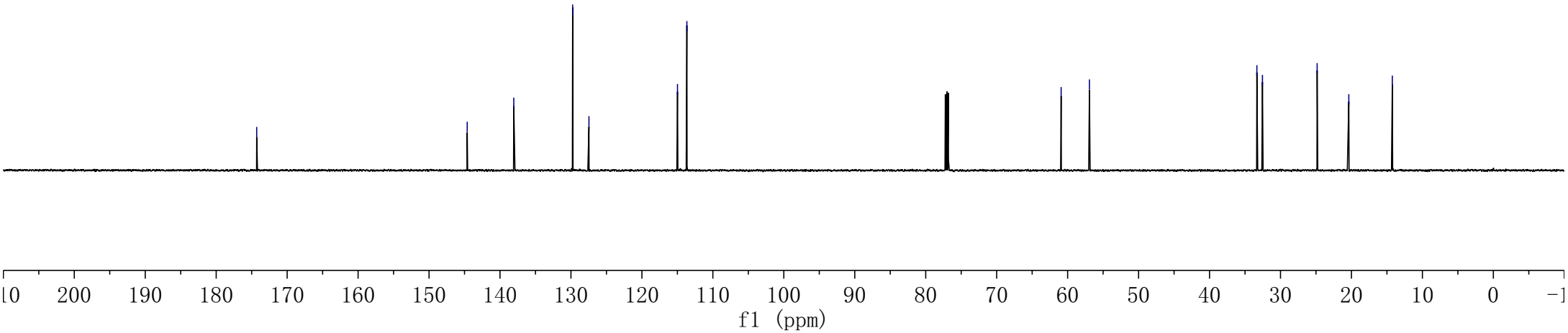
3aj

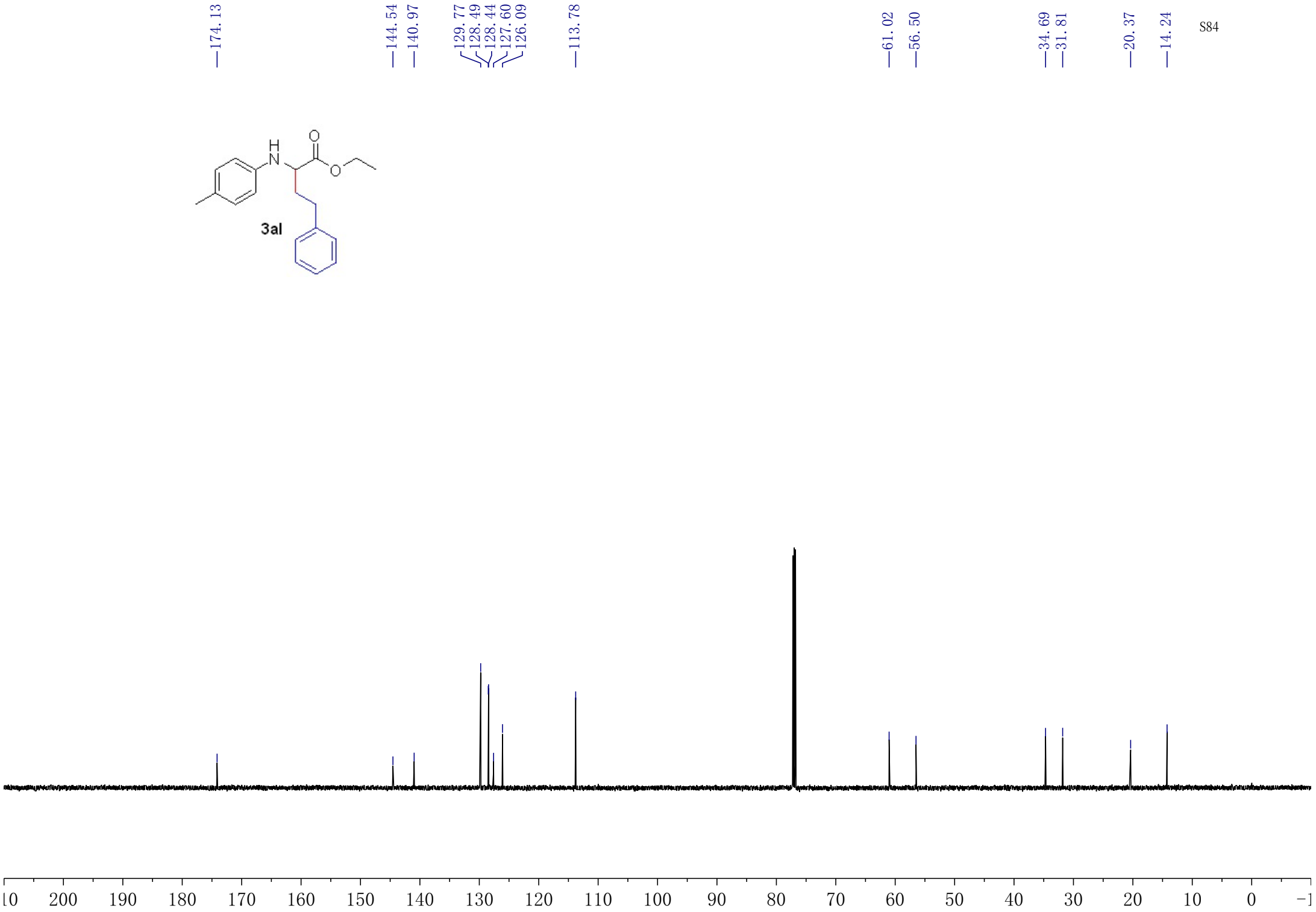


174.29
144.62
138.06
129.76
127.46
114.99
113.66
60.92
56.93
33.33
32.54
24.83
20.37
14.24

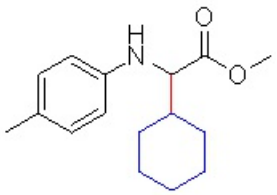


3ak

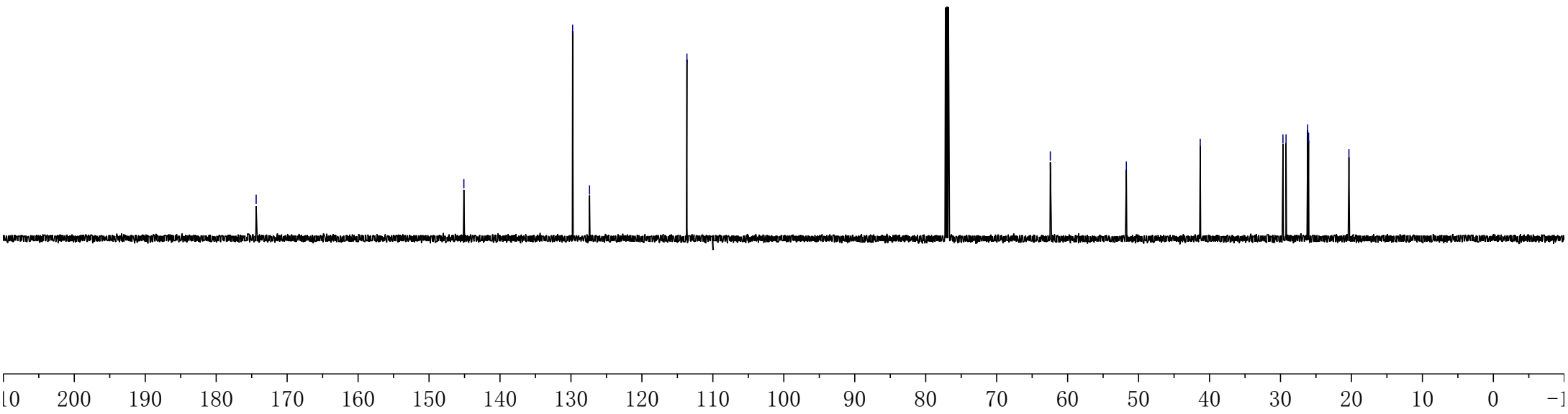


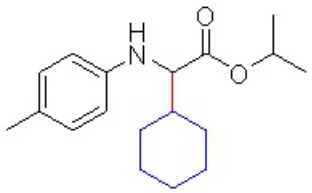

174.13
144.54
140.97
129.77
128.49
128.44
127.60
126.09
113.78
61.02
56.50
34.69
31.81
20.37
14.24
3al
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0

174.37
145.09
129.77
127.38
113.65
62.44
51.73
41.31
29.65
29.22
26.17
26.07
26.04
20.35



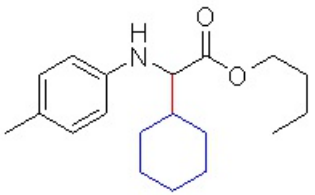
3ba




H
N
O
O

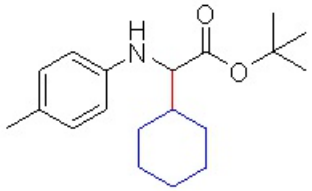
3ca

173.29
145.24
129.67
127.20
113.75
68.27
62.46
41.29
29.56
29.18
26.24
26.13
26.08
21.90
21.85
20.35
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10



3da

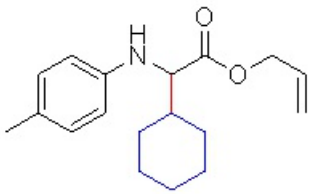
173.95
145.19
129.71
127.29
113.72
64.58
62.51
41.31
30.63
29.64
29.20
26.20
26.09
26.06
20.34
19.08
13.60
10
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-1



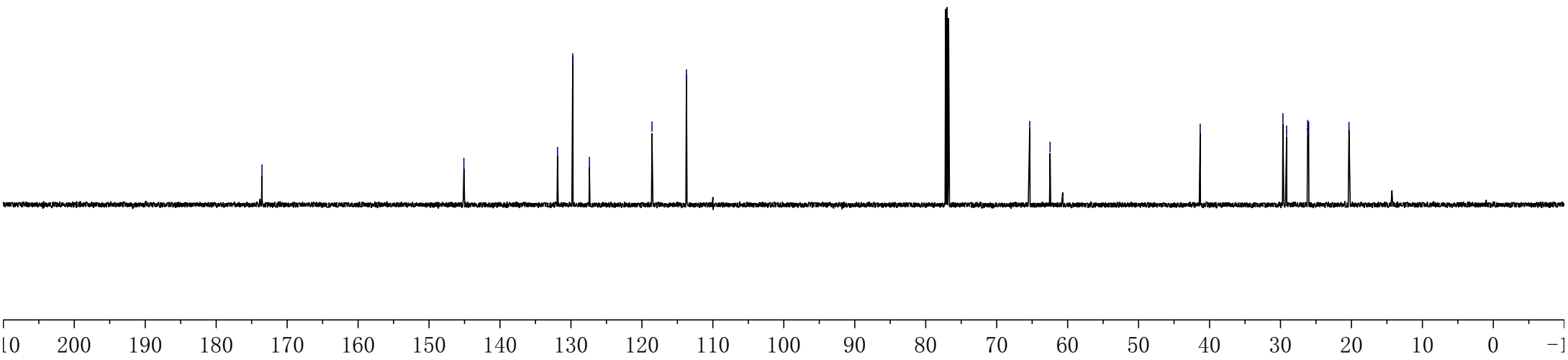
3ea

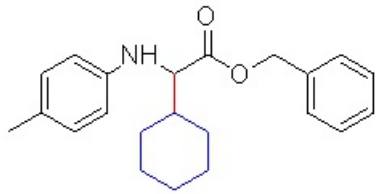
172.97
145.37
129.63
127.01
113.72
81.28
62.82
41.32
29.53
29.14
28.10
26.28
26.18
26.11
20.35
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0

173.54
145.09
131.89
129.74
127.40
118.58
113.72
65.34
62.47
41.32
29.66
29.14
26.17
26.06
26.03
20.35



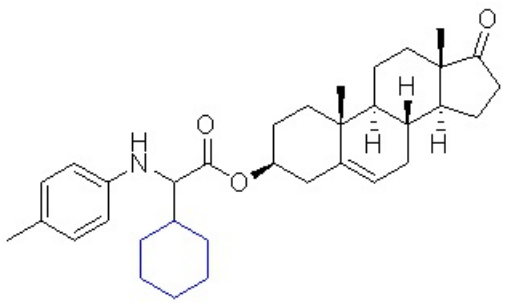
3fa




NH
O
O

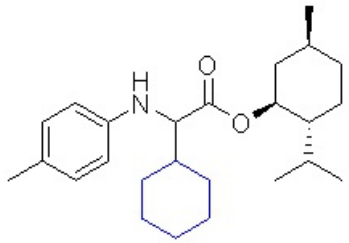
3ga

174.05
145.38
135.89
130.05
128.77
128.55
128.52
127.70
114.07
66.82
62.78
41.57
29.91
29.42
26.43
26.32
26.30
20.67
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10



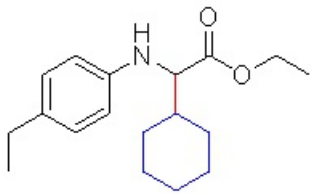
3ha

173.15
145.20
139.71
139.69
129.69
129.68
127.24
127.22
122.00
113.74
113.71
74.17
62.48
62.44
51.66
50.09
47.48
41.29
38.07
38.06
36.84
36.69
35.81
31.43
31.38
30.74
29.58
29.22
27.78
27.77
26.82
26.11
26.06
21.85
20.36
20.30
19.33
10
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-1



3ia

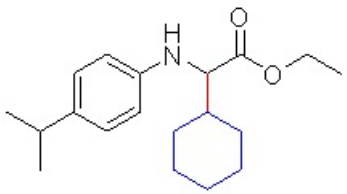
173.46
145.18
129.60
127.37
114.11
74.90
62.80
46.92
41.27
40.75
34.20
31.37
29.62
29.36
26.28
26.09
26.03
25.93
23.06
21.99
20.80
20.36
15.66



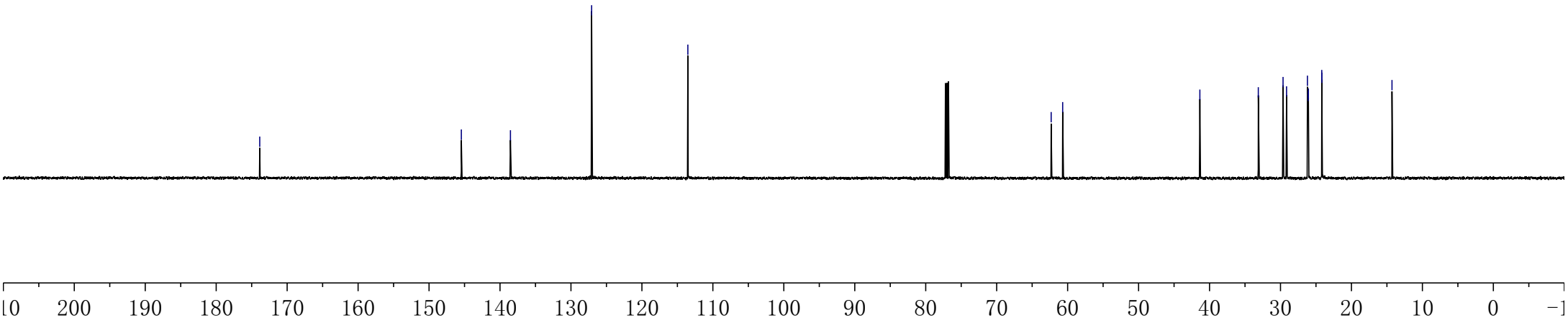
3ja

173.68
145.44
133.93
128.47
113.77
62.49
60.57
41.40
29.62
29.18
27.84
26.21
26.09
26.06
15.66
14.21
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0

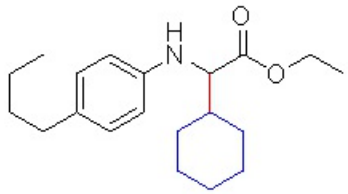
^{13}C NMR (151 MHz, cdcl$_3$) δ 173.86, 145.45, 138.53, 127.09, 113.52, 62.32, 60.70, 41.36, 33.13, 29.64, 29.15, 26.20, 26.10, 26.07, 24.18, 24.17, 14.29.



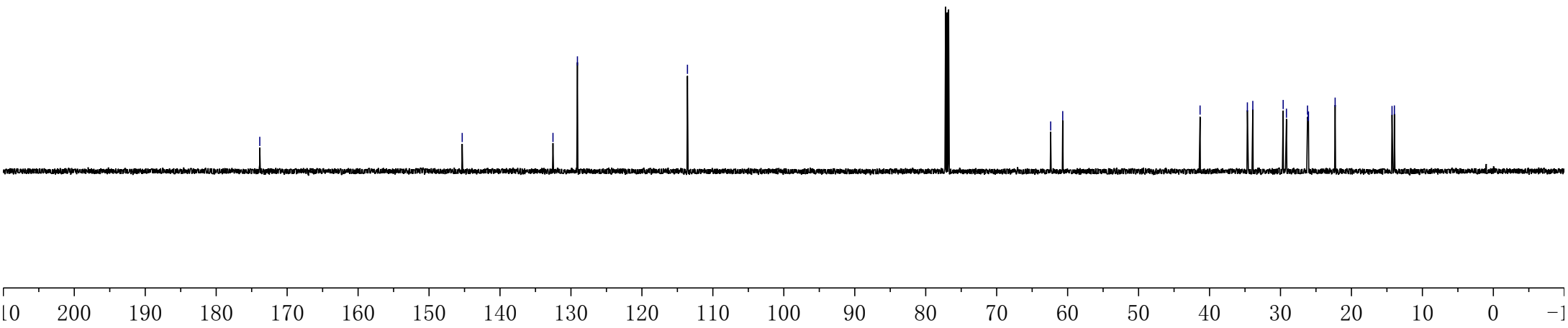
3ka

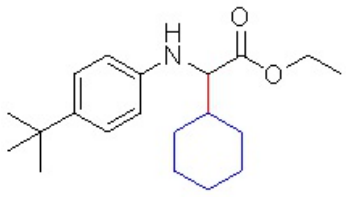


173.86
145.33
132.53
129.09
113.58
62.39
60.69
41.33
34.67
33.90
29.62
29.16
26.19
26.09
26.06
22.30
14.28
13.95



3la

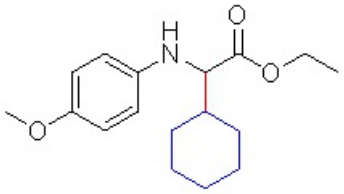




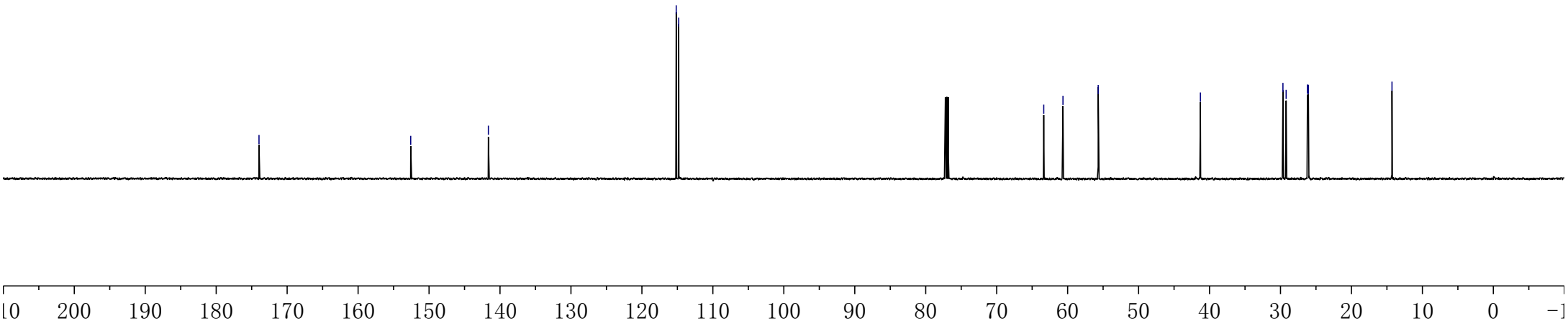
3ma

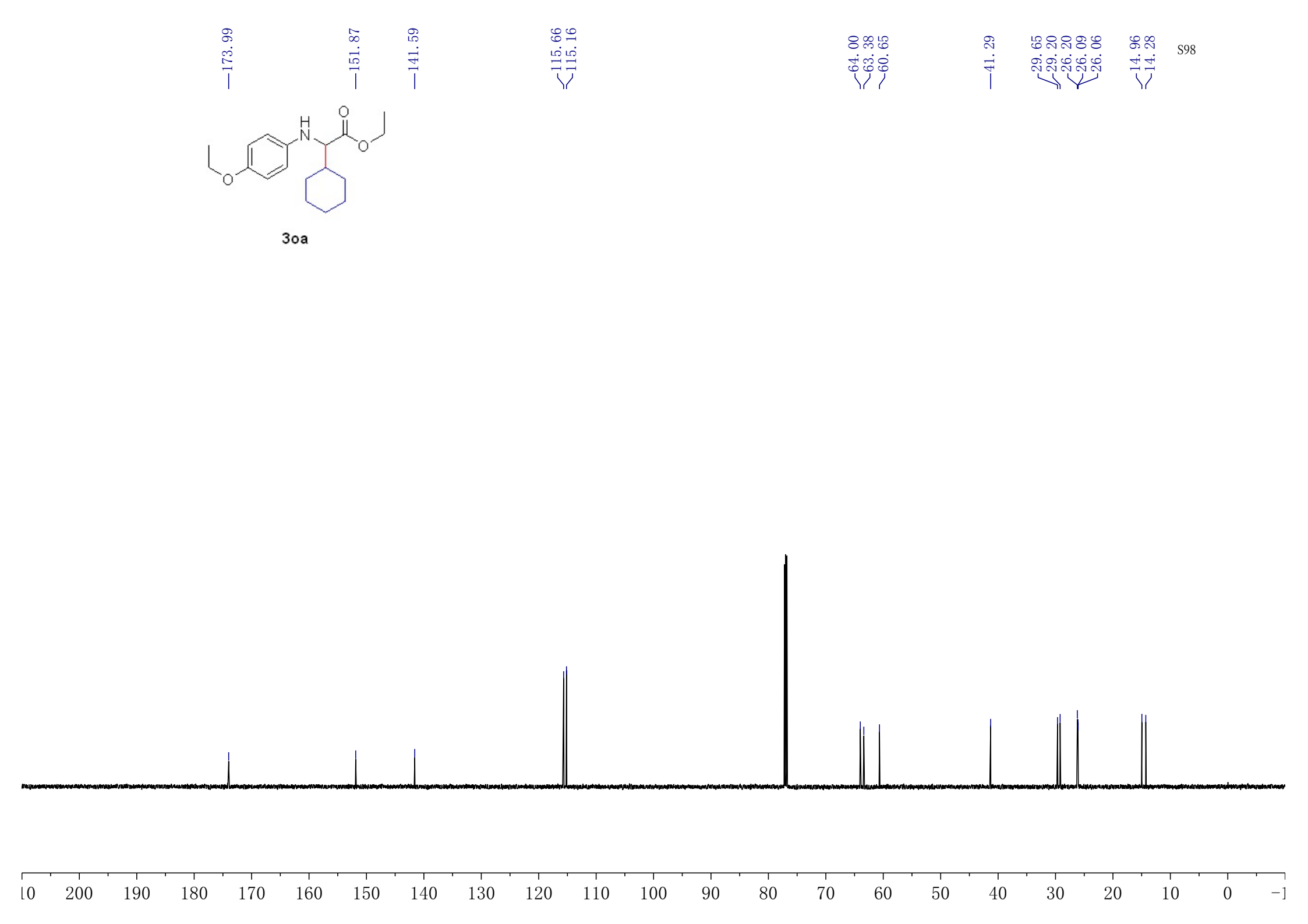
173.70
145.10
140.84
125.94
113.30
62.35
60.59
41.44
33.79
31.45
29.64
29.15
26.21
26.10
26.06
14.21
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0

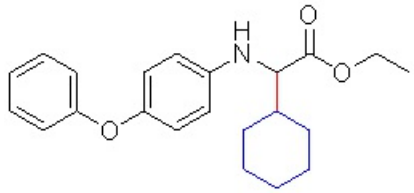
173.97
152.58
141.64
115.16
114.81
63.37
60.66
55.69
41.29
29.66
29.20
26.20
26.09
26.06
14.29



3na

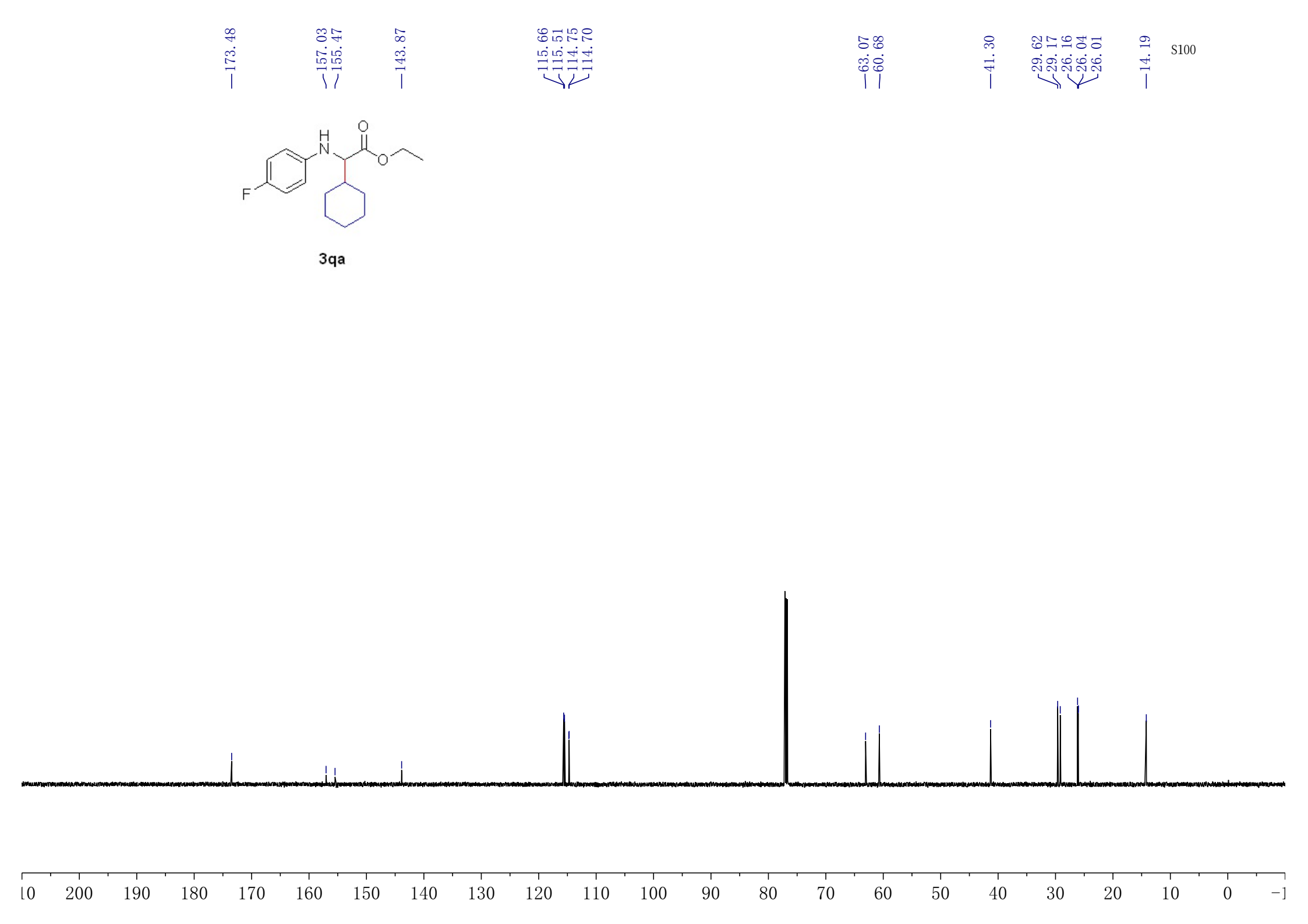


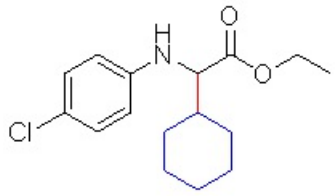

173.99
151.87
141.59
115.66
115.16
64.00
63.38
60.65
41.29
29.65
29.20
26.20
26.09
26.06
14.96
14.28
3oa



3pa

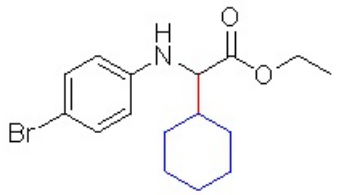
173.73
158.88
148.26
144.04
129.45
121.99
121.07
117.21
114.71
62.78
60.80
41.30
29.65
29.18
26.18
26.08
26.05
14.31
10
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-1


173.48
157.03
155.47
143.87
115.66
115.51
114.75
114.70
63.07
60.68
41.30
29.62
29.17
26.16
26.04
26.01
14.19
H
N
O
O
F
3qa
10
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-1


NH
O
O
Cl

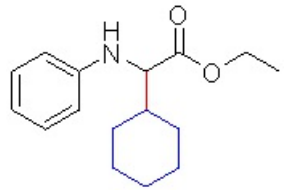
3ra

173.32
146.04
129.06
122.65
114.61
62.16
60.89
41.21
29.57
29.14
26.13
26.03
26.00
14.28
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10


Br
H
N
O
O

3sa

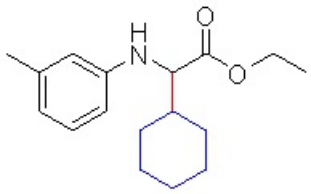
173.27
146.45
131.94
115.06
109.67
62.01
60.92
41.19
29.55
29.13
26.12
26.03
25.99
14.28
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0



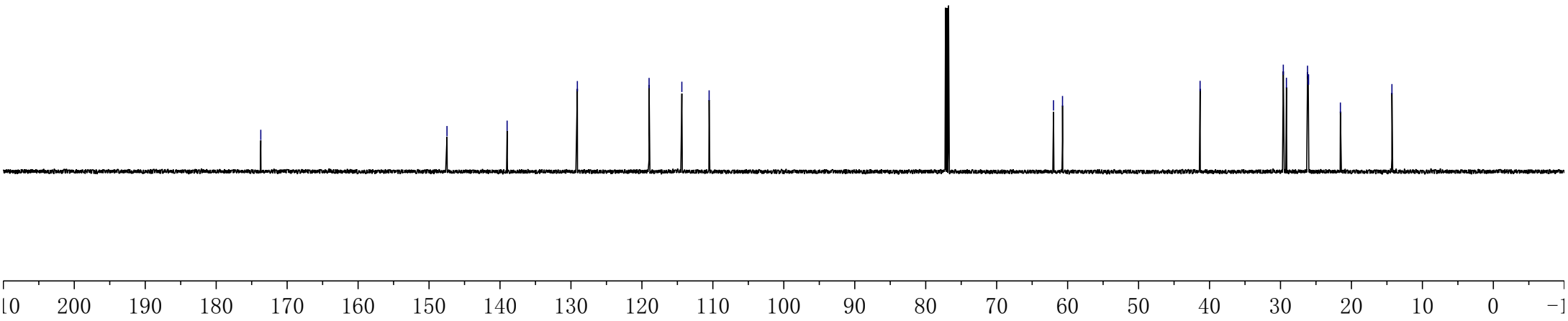
3ta

173.65
147.44
129.23
118.04
113.49
62.01
60.77
41.30
29.59
29.18
26.18
26.09
26.04
14.28
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10

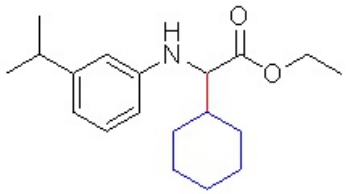
173.71
147.47
139.00
129.10
118.99
114.37
110.53
61.99
60.72
41.33
29.61
29.17
26.19
26.09
26.04
21.56
14.29



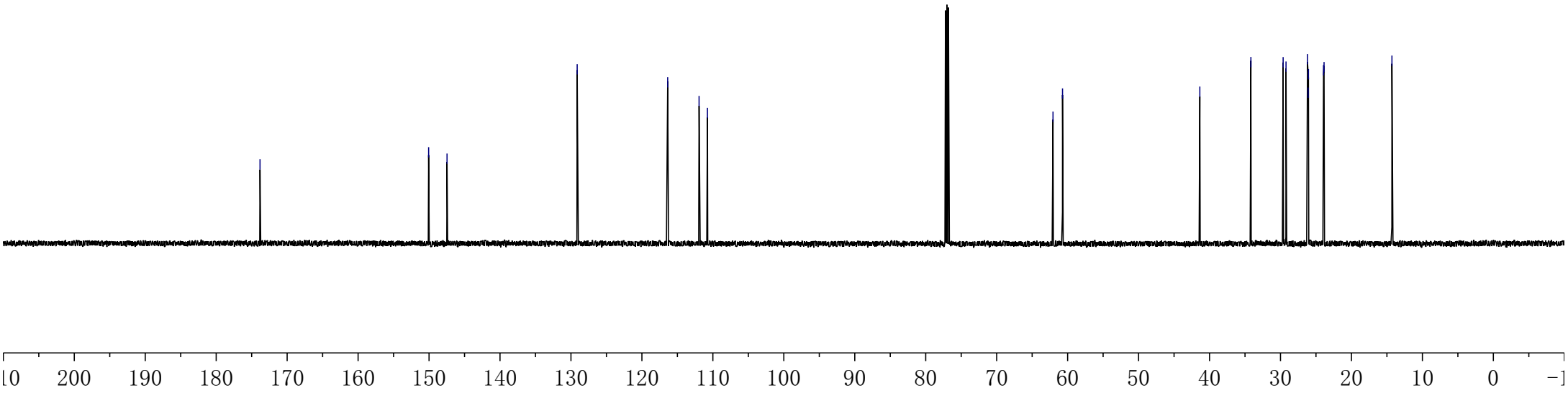
3ua



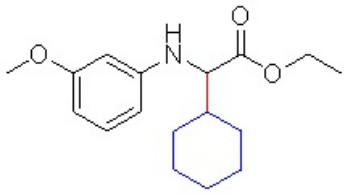
173.82
150.06
147.46
129.12
116.37
111.94
110.77
62.06
60.72
41.37
34.17
29.63
29.22
26.19
26.10
26.06
23.94
23.86
14.29



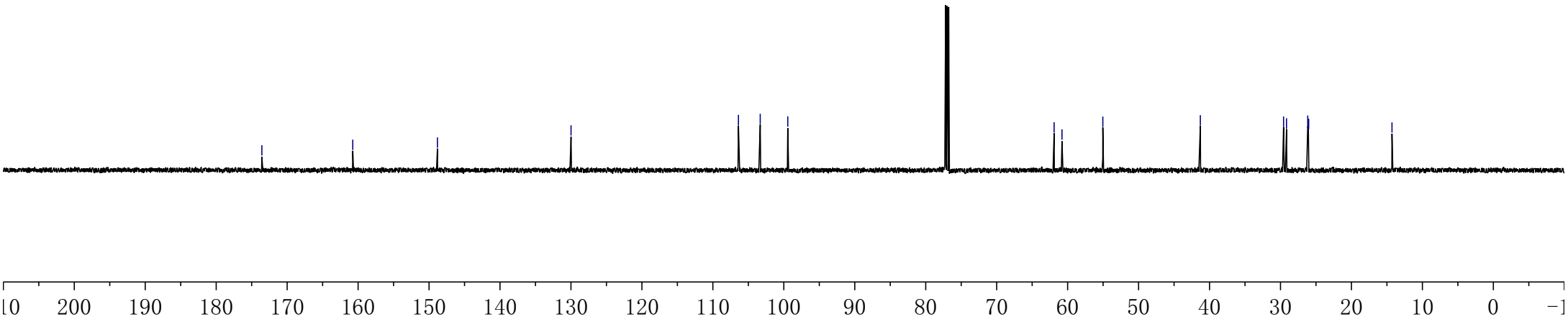
3va



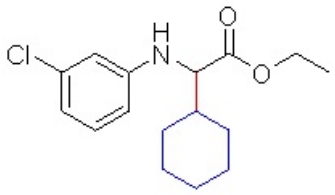
173.56
160.75
148.82
129.99
106.39
103.33
99.44
61.91
60.80
55.04
41.30
29.57
29.15
26.16
26.07
26.03
14.29



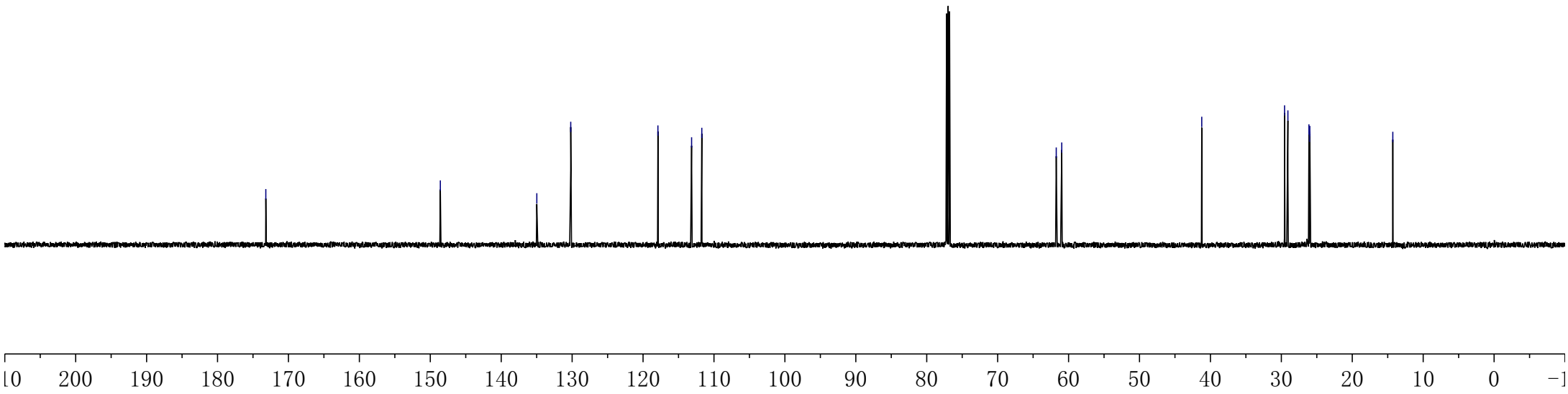
3wa



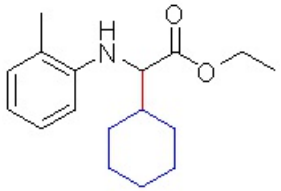
173.19
148.58
134.98
130.20
117.90
113.16
111.72
61.74
60.96
41.22
29.55
29.08
26.11
26.02
25.98
14.28



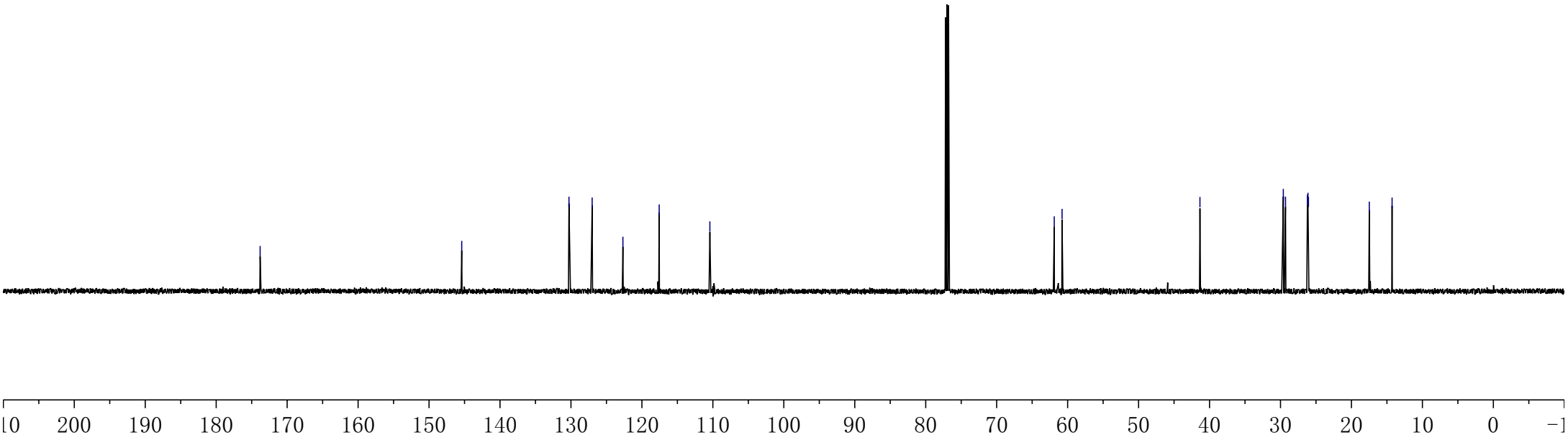
3xa

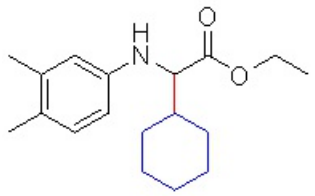


173.81
145.40
130.28
127.01
122.68
117.57
110.42
61.89
60.78
41.35
29.60
29.29
26.21
26.13
26.06
17.49
14.27



3ya

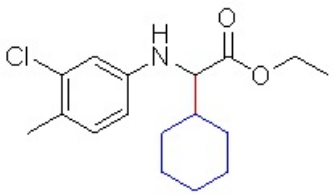




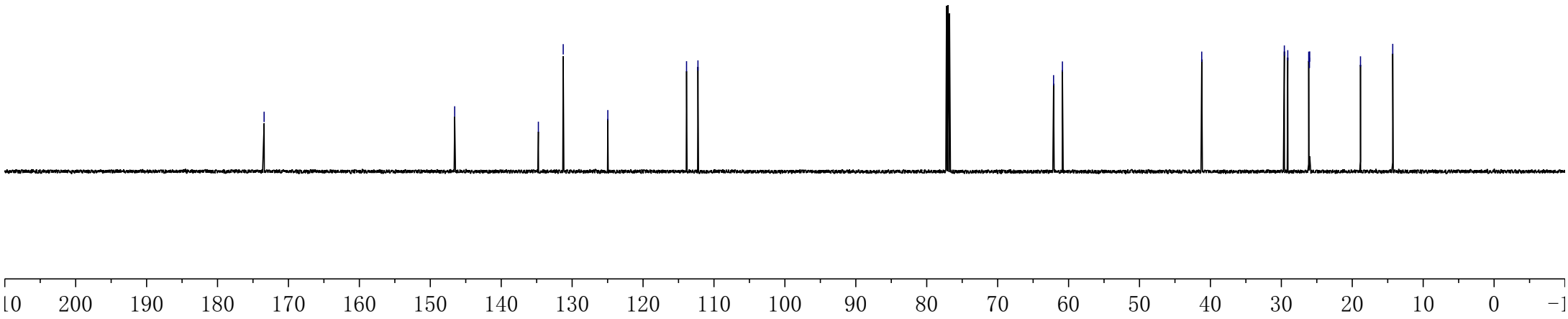
3za

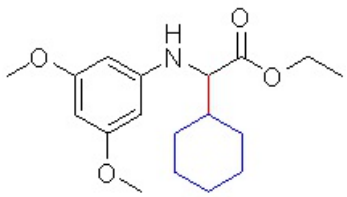
173.91
145.58
137.28
130.25
126.07
115.49
110.85
62.33
60.66
41.33
29.63
29.16
26.21
26.09
26.06
19.98
18.65
14.31
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10

173.43
146.56
134.76
131.26
124.97
113.87
112.26
62.12
60.87
41.23
29.58
29.09
26.14
26.04
26.00
18.84
14.29



3aaa

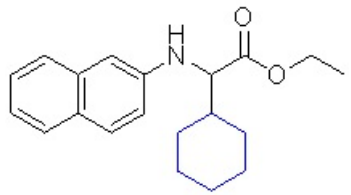




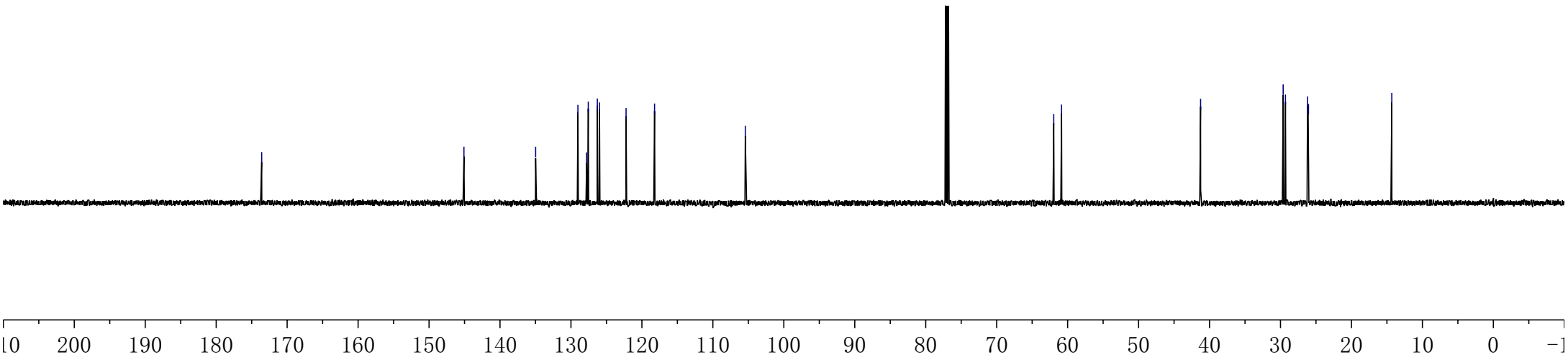
3aba

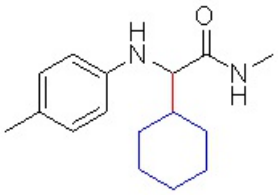
173.52
161.66
149.34
92.21
90.47
61.81
60.82
55.11
41.29
29.55
29.14
26.15
26.06
26.02
14.30
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0

173.59
145.08
134.98
129.02
127.80
127.56
126.28
125.98
122.23
118.22
105.43
61.96
60.85
41.26
29.62
29.30
26.19
26.10
26.05
14.31



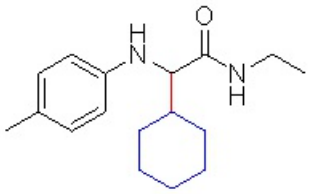
3aca





3ada

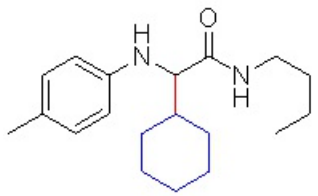
173.45
145.14
129.85
128.23
113.60
65.12
41.06
30.32
28.05
26.25
26.22
26.10
25.86
20.32
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10



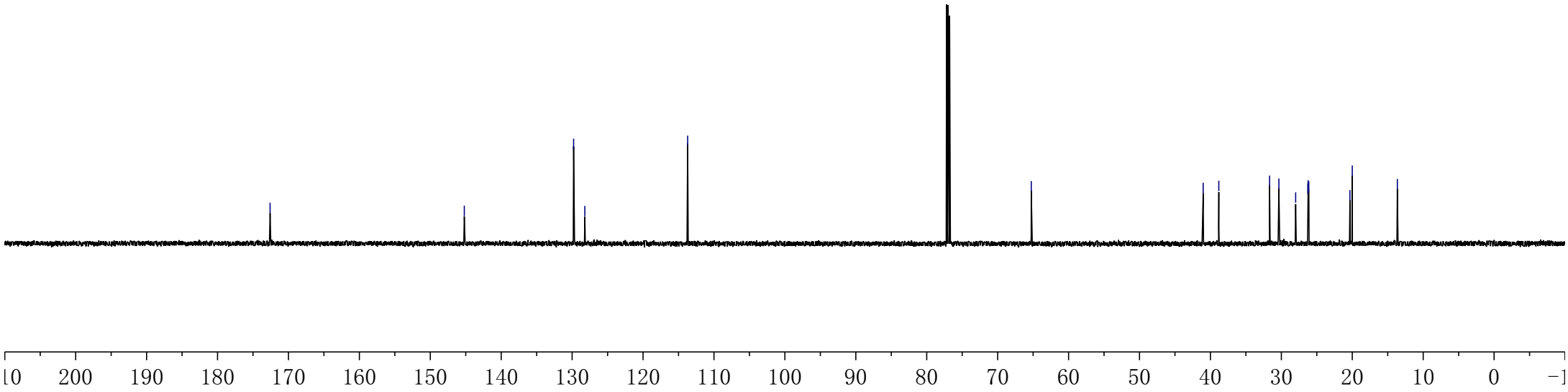
3aea

172.52
145.23
129.80
128.19
113.68
65.20
41.04
33.91
30.34
27.97
26.27
26.22
26.12
20.32
14.91
10
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-1

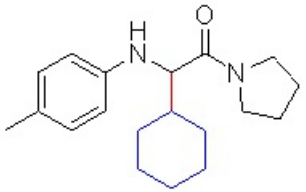
172.59
145.21
129.79
128.21
113.71
65.26
41.02
38.82
31.66
30.35
27.98
26.27
26.23
26.13
20.33
20.00
13.64



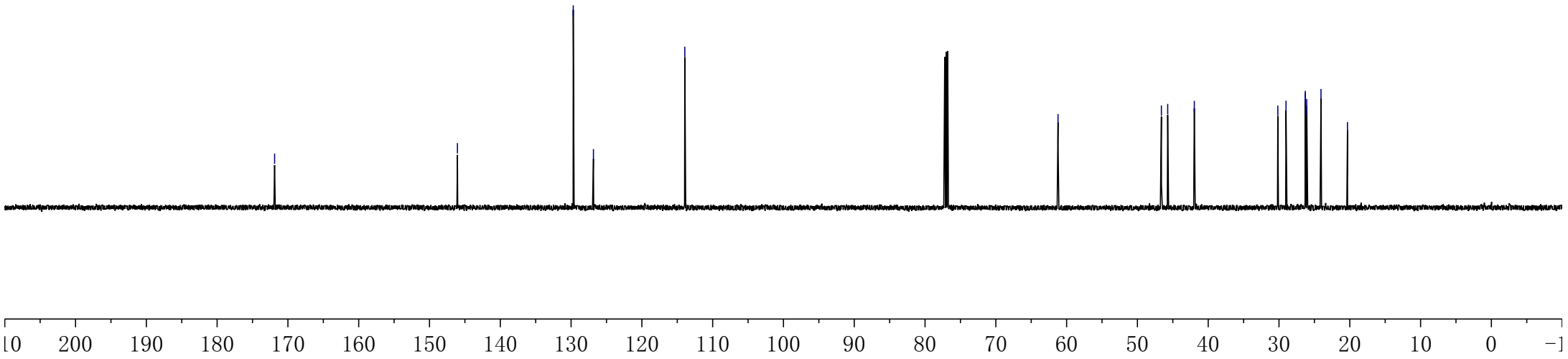
3afa



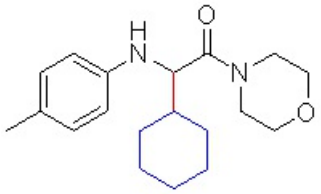
171.88
146.06
129.69
126.84
113.94
61.21
46.61
45.72
41.96
30.17
29.01
26.29
26.28
26.17
26.08
24.07
20.33



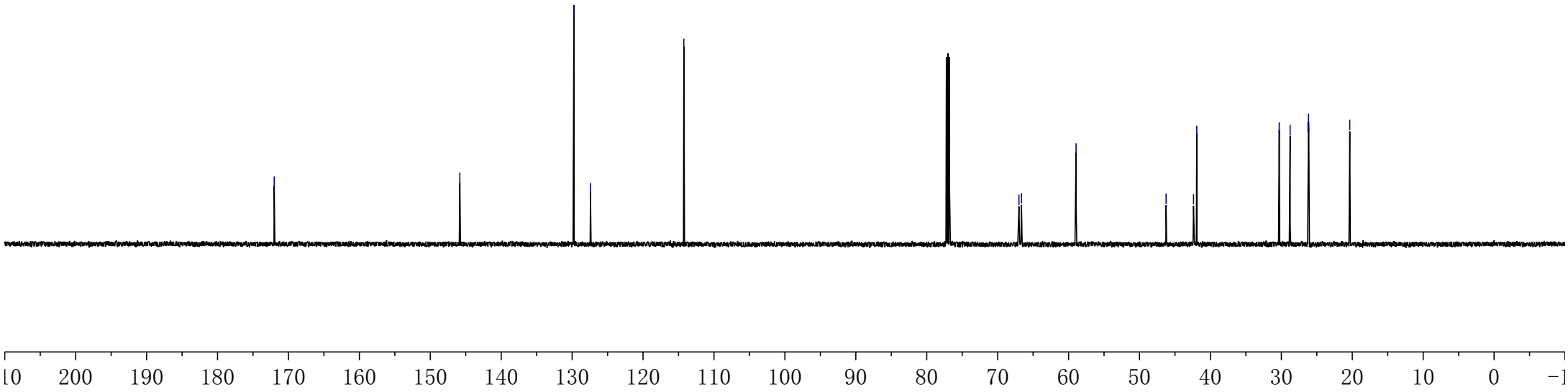
3aga

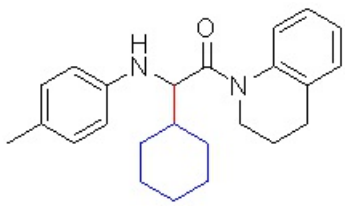


172.01
145.83
129.75
127.41
114.25
67.00
66.64
58.95
46.25
42.38
41.93
30.30
28.76
26.24
26.18
26.13
20.35



3aha

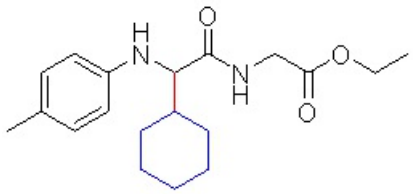




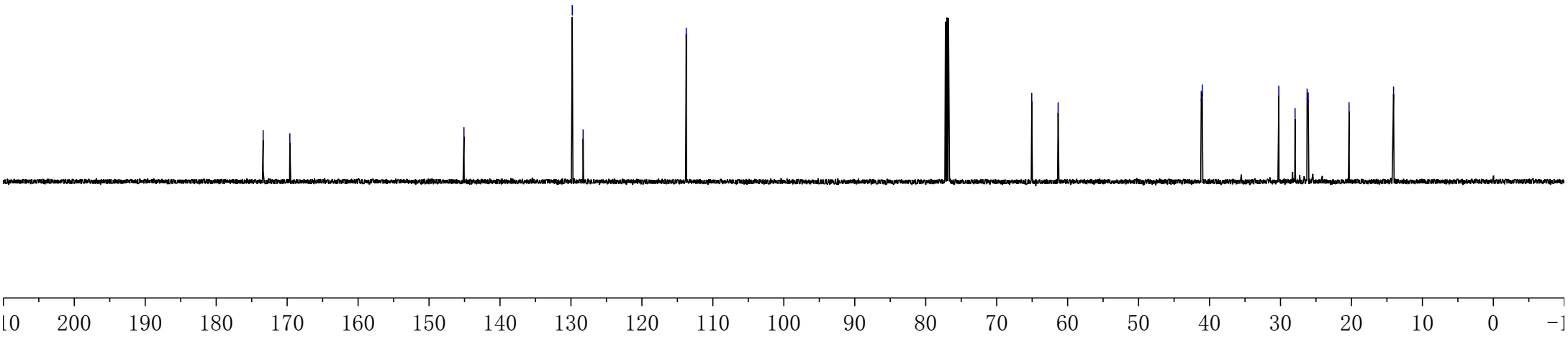
3aia

173.77
145.20
138.88
134.67
130.87
129.61
128.81
128.35
126.81
126.39
125.89
124.74
114.00
59.08
42.62
29.90
29.12
26.52
26.27
26.19
24.07
20.36
19.17
13.71
10
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-1

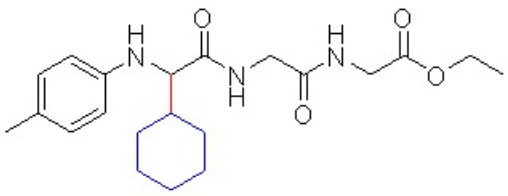
173.38
169.62
145.08
129.82
128.29
113.75
65.06
61.34
41.17
41.02
30.23
27.95
26.25
26.21
26.10
20.34
14.06



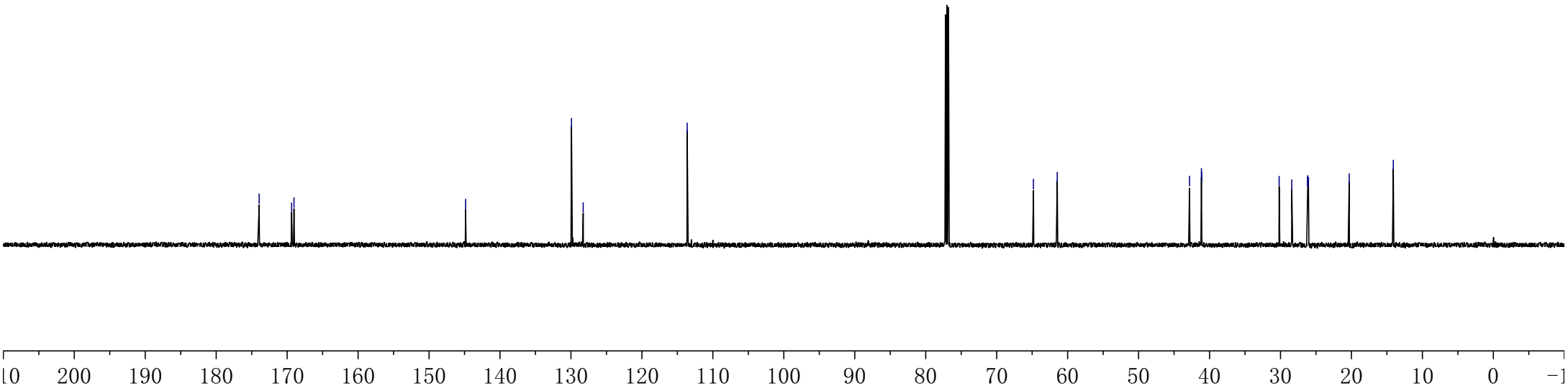
3aja

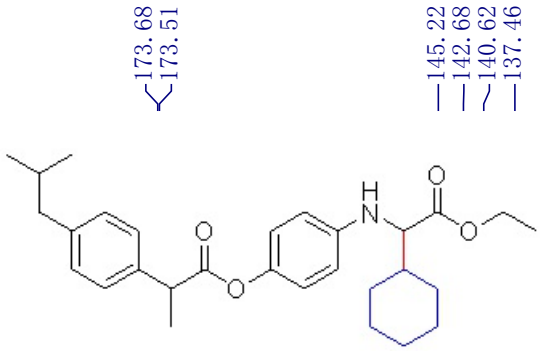


173.94
169.37
169.03
144.85
129.92
128.27
113.62
64.82
61.47
42.82
41.15
41.10
30.19
28.41
26.18
26.16
26.06
20.31
14.10

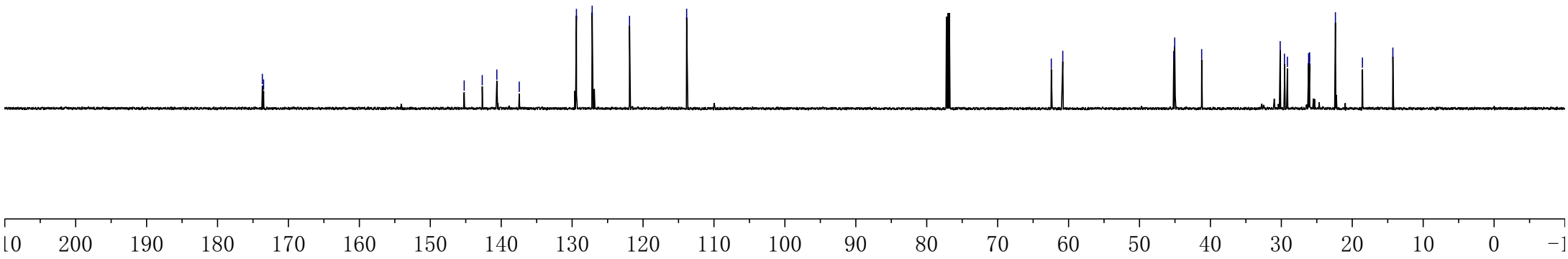


3aka

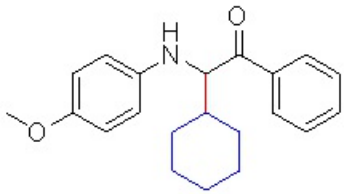



173.68
173.51
145.22
142.68
140.62
137.46
129.39
127.18
121.91
113.85
62.44
60.82
45.18
45.03
41.23
30.16
29.56
29.15
26.16
26.05
26.01
22.38
18.56
14.28
O
O
O
O
H
N

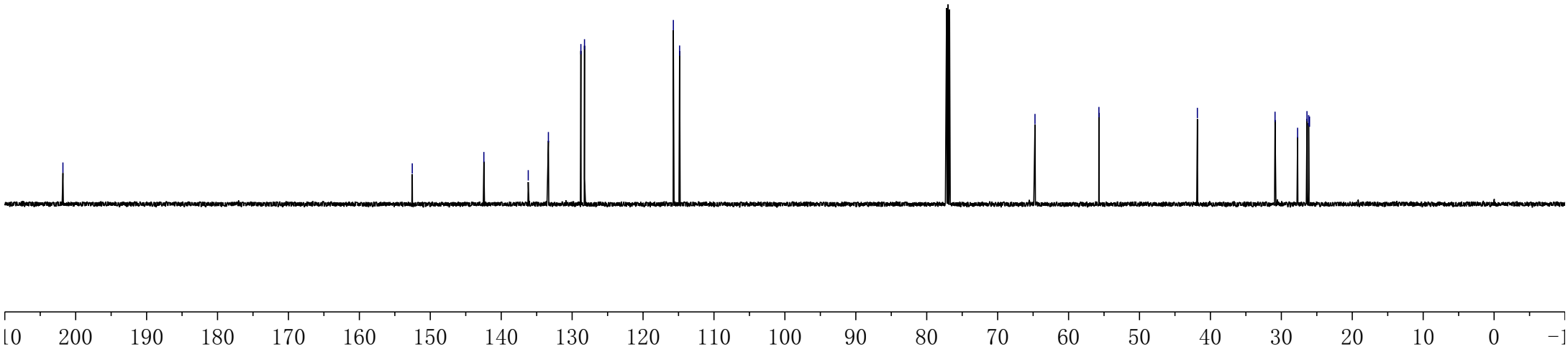
3ala

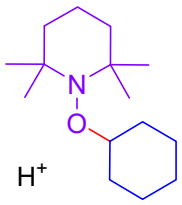

210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10

201.80
152.54
142.45
136.19
133.35
128.77
128.26
115.73
114.85
64.74
55.72
41.84
30.89
27.71
26.39
26.15
26.03

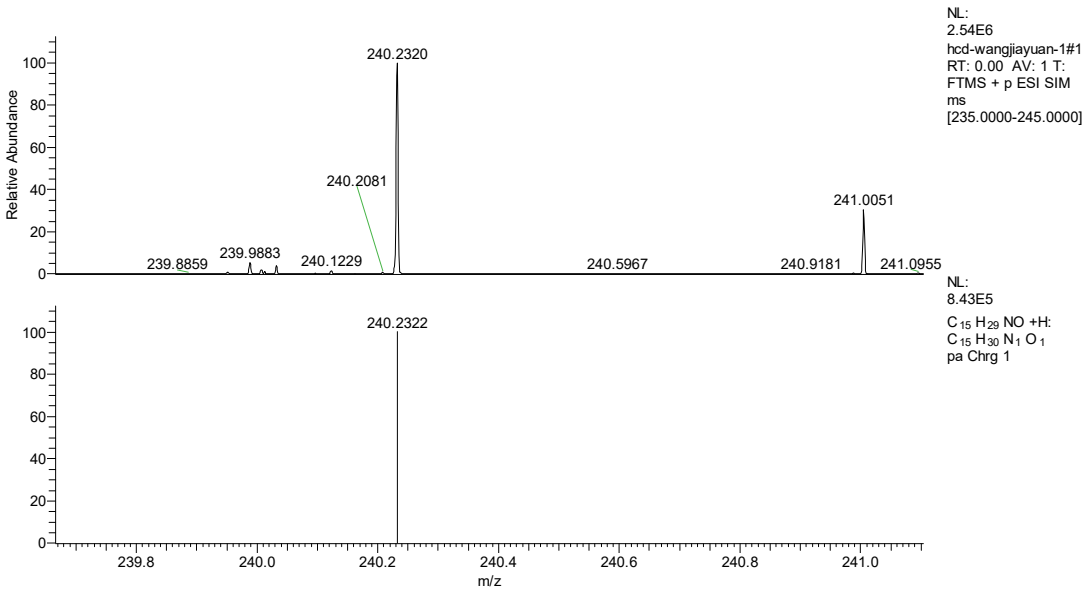


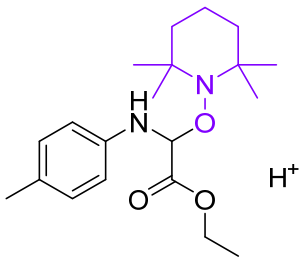
3ama





G:\7.16\hcd-wangjiayuan-1 2020/6/9 17:07:22
Error = 0.8 ppm





G:\7.16\hcd-wangjiayuan-1 2020/6/9 17:07:22
Error = 1.4 ppm