Supporting Information

Green synthesis of *N*-sulfonyl amidine using CuI incorporated $CoFe_2O_4$ nano-catalyst in aqueous medium

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1. General information:

The reagents were obtained from commercial suppliers and used without further purification with the exception of *N*-sulfonyl azide, which were prepared by following the corresponding methods reported in the literature.[1] Commercially available terminal alkynes, ammonium chloride, were directly employed without any previous purification technique (distillation/use of molecular sieves). FT-IR spectra was recorded using Affinity-1 SHIMADZU. Powder X-ray diffraction (XRD) was recorded using a Rigaku X-ray diffractometer with Cu-Kα radiation at a wavelength of 1.5418 Å. FESEM and EDAX analyses was recorded using a ZEISS sigma 300 scanning along with energy dispersive X-ray spectrometer (EDX). TEM analysis was performed using a JEOL JEM-2100 electron microscope. Thermogravimetric analysis (TGA) was performed on a Mettler Toledo TGA/DSC 1, STAR system analyzer. Vibrating sample magnetometer (Lakeshore 7410) was used to determine the magnetic property of the prepared nanocatalyst. X-Ray Photoelectron Spectroscopy (XPS) data was determind using PHI 5000 VersaProbe III. ^{1}H and ^{13}C spectra were recorded on a Bruker Ultrashield 400/600 MHz spectrometer. Chemical shift are given in δ units relative to tetramethylsilane (TMS) signal as an internal reference in $CDCl_3$. ^{1}H NMR coupling constants were reported in Hz and multiplicity was indicated as follows: s (singlet); d (doublet); t (triplet); q (quartet); m (multiplet); br (broad); dd (doublet of doublets). Chromatographic purification was performed using column chromatography over a manually packed column containing silica gel (230-400 mesh). Melting points were measured in Relitech melting point apparatus. The NMR spectra for all the prepared compounds are included in the following sections of this supporting information.

2. Experimental procedures and characterization details:

2.1. General procedure for the synthesis of *N*-sulfonyl amidine compounds

To a stirred mixture of prepared catalyst (10 wt%), NH_4Cl (27 mg, 0.5 mmol), and phenylacetylene (51 mg, 0.5 mmol), in H_2O (2 ml), triethylamine (0.14 ml, 0.75 mmol) was

added slowly at room temperature. After 2-3 min, *p*-toluenesulfonyl azide (99 mg, 0.5 mmol) was added portionwise. The reaction was stirred at room temperature for 20 min. After the completion of the reaction (TLC), the catalyst was recovered with the help of an external magnet. The organic parts were separated out by adding ethyl acetate (15 ml). The combined organic layer was dried over Na_2SO_4 and concentrated in vacuo. The crude residue was then purified by column chromatography on silica gel (ethyl acetate: petroleum ether, 3:7) to afford the desired product.

3. Green Chemistry Metrics Calculations:

$$\text{E-factor (Environmental factor)} = \frac{\text{Mass of product}}{\text{Mass of waste}}$$

$$\text{Atom economy (\%) = (AE)} = \frac{\text{Molecular mass of desired product}}{\text{Molecular mass of all reactants}} \times 100$$

$$\text{Atom efficiency (\%)} = \frac{\text{Yield of the product (\%)}}{\text{Atom economy (\%)}} \times 100$$

$$\text{Carbon efficiency (\%)} = \frac{\text{Total no. of C in reactants}}{\text{Total no. of C in products}} \times 100$$

$$\text{Reaction mass efficiency (\%) = (RME)} = \frac{\text{Mass of desired product}}{\text{Mass of all reactants}} \times 100$$

Table S1. Evaluation of green chemistry metrics for the synthesis of **4i** from hex-1-yne.

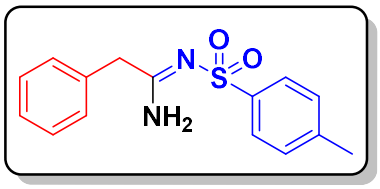
Reactant 1	**Hex-1-yne**	**0.029g**	**0.5 mmol**	**FW 82.14**
Reactant 2	**4-methyl benzenesulfonylazide**	**0.088g**	**0.5 mmol**	**FW 197.21**
Reactant 3	**Ammonium chloride**	**0.026g**	**0.5 mmol**	**FW 53.49**
Solvent	**Water**	**1.994g (2 mL)**	**------**	
Product	***N'*-tosyl hexanimidamide**	**0.122g**	**0.45 mmol**	**FW 268.37**
Product yield = 92%				
E-factor = (0.029+0.088+0.026+1.994-0.122)/0.122 = 16.51 Kg waste/1Kg product. **Atom economy = (268.37/332.84) x100 = 80.63%** **Atom efficiency = 92% x 80.63% /100 = 74.17%** **Carbon efficiency = 13/13 x100 = 100%** **Reaction mass efficiency = 0.122/(0.029+0.088+0.026)g x100 = 85.31%**				

Table S2. Evaluation of green chemistry metrics for the synthesis of **4i** by a known procedure.[25-26]

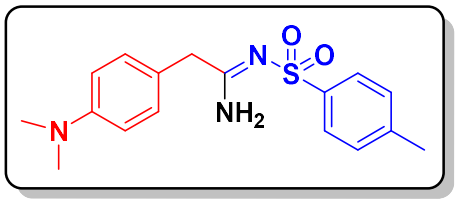
Reactant 1	**Hex-1-yne**	**0.029g**	**0.5 mmol**	**FW 82.14**
Reactant 2	**4-methyl benzenesulfonylazide**	**0.088g**	**0.5 mmol**	**FW 197.21**
Reactant 3	**Ammonium chloride**	**0.026g**	**0.5 mmol**	**FW 53.49**
Solvent	**Dichloromethane**	**1.33g (1 mL)**	**------**	
Product	***N'*-tosyl hexanimidamide**	**0.107g**	**0.39 mmol**	**FW 268.37**
Product yield = 81%				
E-factor = (0.029+0.088+0.026+1.994-0.107)/0.107 = 18.97 Kg waste/1Kg product. **Atom economy = (268.37/332.84) x100 = 80.63%** **Atom efficiency = 81% x 80.63% /100 = 65.31%** **Carbon efficiency = 13/13 x100 = 100%** **Reaction mass efficiency = 0.107/(0.029+0.088+0.026)g x100 = 74.82%**				

4. Spectroscopic data:

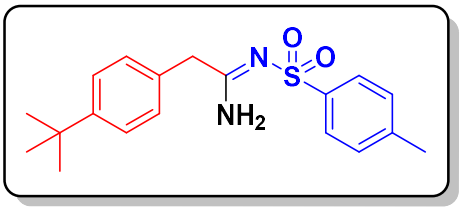
1. **2-phenyl-*N*'-tosylacetimidamide (4a)[1] :** White solid; m.p. 114-115 ˚C; **^{1}H NMR (500 MHz, $CDCl_3$) δ (ppm)** = 8.09 (br, 1H), 7.81 (d, *J* = 7.9 Hz, 2H), 7.37-7.32 (m, 3H), 7.28 (d, *J* = 8.2 Hz, 2H), 7.22 (d, *J* = 6.6 Hz, 2H), 5.69 (br, 1H), 3.65 (s, 2H), 2.43 (s, 3H); **^{13}C NMR (125 MHz, $CDCl_3$) δ (ppm)** = 167.21, 143.02, 139.12, 133.27, 129.62, 129.35, 129.27, 128.10, 126.41, 43.71, 21.49; **IR (KBr) υ** 3366, 3234, 3065, 3024, 2967, 2912, 2856, 1656, 1550, 1488, 1446, 1417, 1271, 1271, 1138, 1082, 1082, 957, 810, 705 cm^{-1}.



2. **2-(4-(dimethylamino)phenyl)-*N*'-tosylacetimidamide (4b) :** Brown solid; m.p. 100-101 ˚C; **^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm)** = 8.79 (d, *J* = 7.3 Hz, 1H), 8.41 (d, *J* = 9 Hz, 1H), 8.20 (br, 1H), 7.92 (d, *J* = 8.2 Hz, 1H), 7.82 (d, *J* = 8.2 Hz, 1H), 7.53-7.50 (m, 1H), 7.46 (br, 1H), 7.33-7.30 (m, 2H), 7.17 (t, *J* = 6.9 Hz, 1H), 2.42 (s, 2H), 1.60 (br, 6H), 1.26 (s, 3H); **^{13}C NMR (125 MHz, $CDCl_3$) δ (ppm)** = 155.74, 143.02, 139.54, 129.72, 129.43, 126.41, 125.74, 120.69, 116.81, 31.91, 29.68, 21.51; **IR (KBr) υ** 3315, 3022, 2983, 2845, 1625, 1589, 1448, 1340, 815, 765 cm^{-1}; **HRMS (ESI) m/z** calcd. for $[M+H]^+$: 332.1427, found: 332.1421.

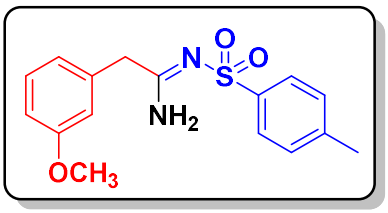


3. **2-(4-(*tert*-butyl)phenyl)-*N*'-tosylacetimidamide (4c) :** White solid; m.p. 89-90 ˚C; **^{1}H NMR (500 MHz, $CDCl_3$) δ (ppm)** = 8.10 (br, 1H), 7.84 (d, *J* = 7.9 Hz, 2H), 7.38 (d, *J* = 8.2 Hz, 2H), 7.30 (d, *J* = 7.9 Hz, 2H), 7.15 (d, *J* = 7.9 Hz, 2H), 5.59 (br, 1H), 3.64 (s, 2H), 2.43 (s, 3H), 1.32 (s, 9H); **^{13}C NMR (125 MHz, $CDCl_3$) δ (ppm)** =

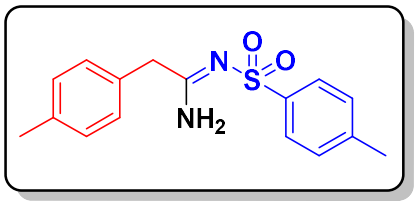


167.43, 151.34, 142.98, 139.24, 129.97, 129.46, 129.35, 126.47, 126.29, 43.23, 34.59, 31.25, 21.52; **IR (KBr)** υ 3366, 3226, 3073, 3017, 2961, 2905, 2864, 1669, 1564, 1508, 1467, 1397, 1355, 1250, 1194, 1079, 1013, 957, 845, 810, 768 cm^{-1}; **HRMS (ESI) m/z** calcd. for $[M+H]^+$: 345.1631, found: 345.1638.

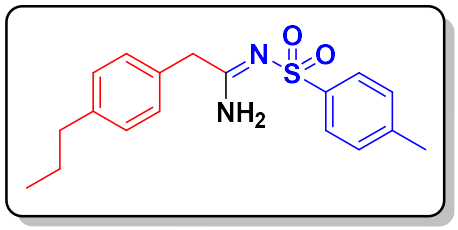
4. **2-(3-methoxyphenyl)-*N*'-tosylacetimidamide (4d) :** White solid; m.p. 100-101 ˚C; **^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm)** = 8.13 (br, 1H), 7.84 (d, *J* = 8.2 Hz, 2H), 7.32-7.28 (m, 3H), 6.88 (dd, *J* = 2.2 Hz, 8.2 Hz, 1H), 6.81 (d, *J* = 7.7 Hz, 1H), 6.76 (s, 1H), 5.69 (br, 1H), 3.79 (s, 3H), 3.64 (s, 2H), 2.44 (s, 3H); **^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm)** = 167.02, 160.20, 143.06, 139.08, 134.58, 130.38, 129.36, 126.44, 121.82, 115.12, 113.72, 55.23, 43.74, 21.51; **IR (KBr)** υ 3436, 3324, 3051, 3010, 2968, 2919, 2842, 1613, 1586, 1536, 1494, 1257, 1187, 1076, 943, 908, 873, 810, 754 cm^{-1}; **HRMS (ESI) m/z** calcd. for $[M+H]^+$: 319.1111, found: 319.1095.



5. **2-(*p*-tolyl)-*N*'-tosylacetimidamide (4e)[1] :** White solid; m.p. 123-124 ˚C; **^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm)** = 8.10 (br, 1H), 7.83 (d, *J* = 8.2 Hz, 2H), 7.30 (d, *J* = 8.2 Hz, 2H), 7.18-7.09 (m, 4H), 5.76 (br, 1H), 3.59 (s, 2H), 2.41 (s, 3H), 2.33 (s, 3H); **^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm)** = 167.68, 142.88, 139.10, 137.72, 130.22, 129.78, 129.39, 129.25, 126.29, 43.15, 21.42, 20.98; **IR (KBr)** υ 3436, 3366, 3234, 3065, 3024, 2912, 2856, 1732, 1655, 1550, 1488, 1411, 1180, 1082, 894, 859, 796 cm^{-1}.

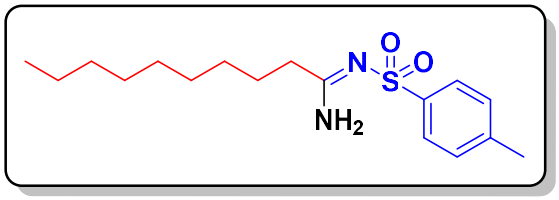


6. **2-(4-propylphenyl)-*N*'-tosylacetimidamide (4f) :** White solid; m.p. 79-80 ˚C; **^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm)** = 8.00 (br, 1H), 7.73 (d, *J* = 8.2 Hz, 2H), 7.23-7.19 (m, 2H), 7.08-7.02 (m, 4H), 5.65 (br, 1H), 3.54 (s, 2H), 2.49 (t, *J* = 7.5 Hz, 2H), 2.34 (s, 3H), 1.59-1.50 (m, 9H), 0.86 (t, *J* = 7.3 Hz, 3H); **^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm)** = 167.62, 142.97, 142.71, 139.10, 130.26, 129.53, 129.32, 128.39, 126.38, 43.26,

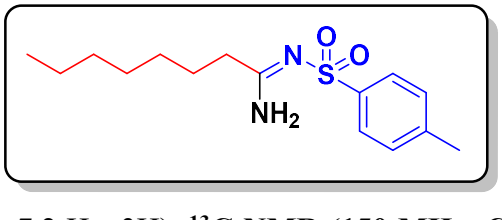


37.57, 24.41, 24.38, 21.49, 13.79, 13.75; **IR (KBr) υ** 3359, 3234, 2968, 2927, 2870, 1648, 1544, 1502, 1417, 1271, 1146, 1082, 943, 810, 761 cm^{-1}; **HRMS (ESI) m/z** calcd. for $[M+H]^+$: 331.1475, found: 331.1468.

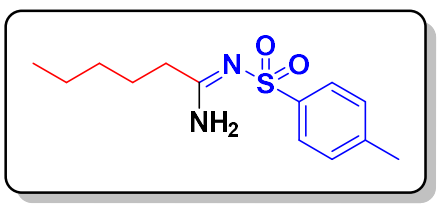
7. ***N*'-tosyldecanimidamide (4g) :** White solid; m.p. 60-61 ˚C; **^{1}H NMR (600 MHz, $CDCl_3$) δ (ppm)** = 8.05 (br, 1H), 7.82 (d, *J* = 7.7 Hz, 2H), 7.28-7.27 (m, 3H), 5.78 (br, 1H), 2.41 (s, 3H), 2.25 (t, *J* = 7.5 Hz, 2H), 1.29-1.22 (m, 14H), 0.88 (t, *J* = 7.0 Hz, 3H); **^{13}C NMR (150 MHz, $CDCl_3$) δ (ppm)** = 169.02, 142.87, 139.23, 129.28, 126.36, 37.97, 31.81, 29.34, 29.17, 28.80, 26.52, 22.63, 21.49, 14.08; **IR (KBr) υ** 3394, 3317, 3248, 2961, 2919, 2842, 1641, 1544, 1453, 1271, 1132, 1082, 915, 796, 712 cm^{-1}; **HRMS (ESI) m/z** calcd. for $[M+H]^+$: 325.1944, found: 325.1945.



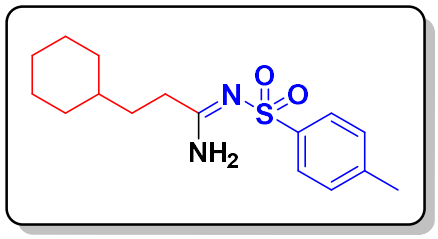
8. ***N*'-tosyloctanimidamide (4h) :** White solid; m.p. 70-71 ˚C; **^{1}H NMR (600 MHz, $CDCl_3$) δ (ppm)** = 8.05 (br, 1H), 7.83 (d, *J* = 8.1 Hz, 2H), 7.3 (d, *J* = 7 Hz, 2H), 5.96 (br, 1H), 2.43 (s, 3H), 2.27 (t, *J* = 7.5 Hz, 2H), 1.69 (s, 2H), 1.62-1.60 (m, 2H), 1.28-1.20 (m, 6H), 0.88 (t, *J* = 7.2 Hz, 3H); **^{13}C NMR (150 MHz, $CDCl_3$) δ (ppm)** = 169.19, 142.87, 139.22, 129.28, 126.33, 37.91, 31.56, 28.82, 28.73, 26.53, 22.50, 21.48, 14.01; **IR (KBr) υ** 3388, 3322, 3243, 2913, 2848, 1642, 1541, 1455, 1416, 1271, 1145, 1079, 928, 875, 810 cm^{-1}; **HRMS (ESI) m/z** calcd. for $[M+H]^+$: 297.1631, found: 297.1628.



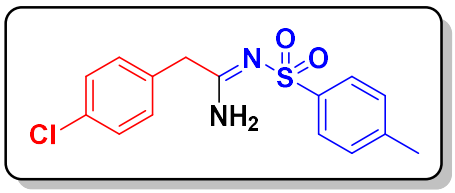
9. ***N*'-tosylhexanimidamide (4i)[1] :** Yellow solid; m.p. 70-71 ˚C; **^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm)** = 8.05 (br, 1H), 7.82 (d, *J* = 8.2 Hz, 2H), 7.29 (d, *J* = 6.9 Hz, 2H), 6.02 (br, 1H), 2.43 (s, 3H), 2.26 (t, *J* = 7.7 Hz, 2H), 1.65-1.57 (m, 2H), 1.30-1.20 (m, 4H), 0.84 (t, *J* = 6.9 Hz, 3H); **^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm)** = 169.28, 142.90, 139.16, 129.27, 126.33, 37.81, 30.91, 26.22, 22.21, 21.48, 13.79; **IR (KBr) υ** 3372, 3310, 3225, 2910, 2908, 2867, 1640, 1535, 1442, 1138, 1089, 805.



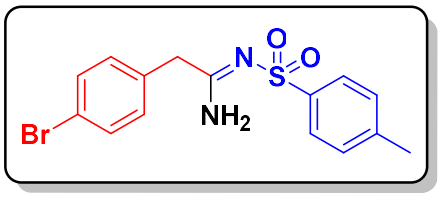
10. 3-cyclohexyl-*N*'-tosylpropanimidamide (4j) : White solid; m.p. 98-99 ˚C; **^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm)** = 8.02 (br, 1H), 7.81 (d, *J* = 8.6 Hz, 2H), 7.28 (d, *J* = 5.6, 2H), 6.14 (br, 1H), 2.42 (s, 3H), 2.29-2.25 (m, 2H), 1.80 (br, 1H), 1.65-1.60 (m, 4H), 1.50-1.45 (m, 2H), 1.16-1.06 (m, 4H), 0.86-0.80 (m, 2H); **^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm)** = 169.75, 142.88, 139.17, 129.28, 126.30, 36.97, 35.39, 33.89, 32.85, 26.35, 26.07, 21.47; **IR (KBr) υ** 3443, 3338, 3248, 2912, 2842, 1627, 1530, 1453, 1403, 1264, 1138, 935, 817, 782, 706 cm^{-1}; **HRMS (ESI) m/z** calcd. for $[M+H]^+$: 309.1631, found: 309.1637.



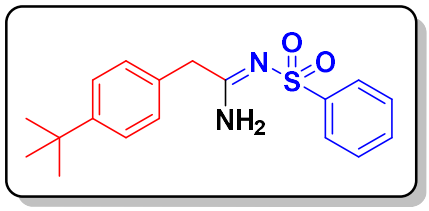
11. 2-(4-chlorophenyl)-*N*'-tosylacetimidamide (4k) : White solid; m.p. 123-124 ˚C; **^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm)** = 8.07 (br, 1H), 7.78 (d, *J* = 8.2 Hz, 2H), 7.31-7.26 (m, 4H), 7.15 (d, *J* = 8.2 Hz, 2H), 5.75 (br, 1H), 3.59 (s, 2H), 2.42 (s, 3H); **^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm)** = 166.56, 143.17, 138.88, 134.06, 131.89, 130.80, 129.37, 129.31, 126.37, 43.09, 21.51; **IR (KBr) υ** 3365, 3235, 1648, 1559, 1445, 1370, 1269, 1145, 1137, 860, 769, 550, 525 cm^{-1}; **HRMS (ESI) m/z** calcd. for $[M+H]^+$: 323.0616, found: 323.0612.



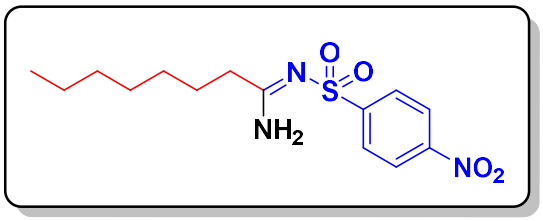
12. 2-(4-chlorophenyl)-*N*'-tosylacetimidamide (4l)[1] : White solid; m.p. 176-177 ˚C; **^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) =** 8.09 (br, 1H), 7.8 (d, *J* = 8.2 Hz, 2H), 7.48 (d, *J* = 8.2 Hz, 2H), 7.29 (d, *J* = 8.2 Hz, 2H), 7.1 (d, *J* = 8.2 Hz, 2H), 5.63 (br, 1H), 3.59 (s, 2H), 2.43 (s, 3H); **^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm)** = 166.28, 143.18, 138.90, 132.36, 132.33, 131.17, 129.38, 126.43, 122.24, 43.23, 21.53; **IR (KBr) υ** 3370, 3215, 1654, 1578, 1425, 1350, 1289, 1151, 1127, 854, 780, 550, 514 cm^{-1}.



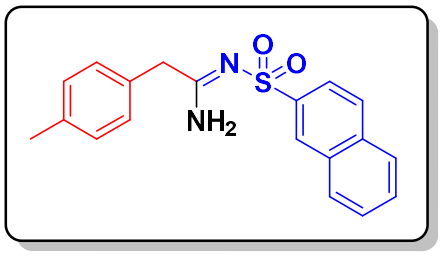
13. 2-(4-(*tert*-butyl)phenyl)-*N*'-(phenylsulfonyl)acetimidamide (4m) : White solid; m.p. 82-83 ˚C; **^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm)** = 8.14 (br, 1H), 7.96 (d, *J* = 7.3 Hz, 2H), 7.60-7.56 (m, 1H), 7.53-7.50 (m, 2H), 7.39 (d, *J* = 8.2 Hz, 2H), 7.17 (d, *J* = 8.2 Hz, 2H), 5.75 (br, 1H), 3.66 (s, 2H), 1.33 (s, 9H); **^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm)** = 167.81, 151.27, 142.00, 132.28, 129.90, 129.40, 128.73, 126.37, 126.25, 43.18, 34.56, 31.23; **IR (KBr) υ** 3352, 3206, 2954, 2326, 2172, 1655, 1550, 1278, 1138, 1090, 943, 810 cm^{-1}; **HRMS (ESI) m/z** calcd. for $[M+H]^+$: 331.1475, found: 331.1477.



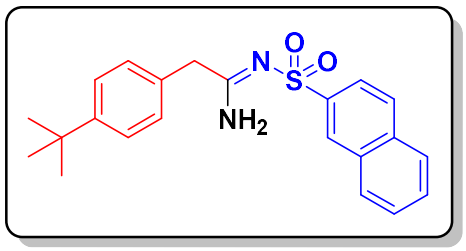
14. *N*'-((4-nitrophenyl)sulfonyl)octanimidamide (4n) : White solid; m.p. 60-61 ˚C; **^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm)** = 8.34 (d, *J* = 8.6 Hz, 2H), 8.12 (d, *J* = 9 Hz, 2H), 6.31 (br, 1H), 2.31 (t, *J* = 7.5 Hz, 2H), 1.85 (br, 1H), 1.62-1.59 (m, 2H), 1.25-1.20 (m, 8H), 0.85 (t, *J* = 6.9 Hz, 3H); **^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm)** = 170.55, 149.73, 147.73, 127.60, 123.98, 37.83, 31.51, 28.74, 28.71, 26.43, 22.45, 13.94; **IR (KBr) υ** 3352, 3206, 2954, 2326, 2172, 1655, 1550, 1278, 1138, 1090, 943, 810 cm^{-1}; **HRMS (ESI) m/z** calcd. for $[M+H]^+$: 328.1326, found: 328.1322.



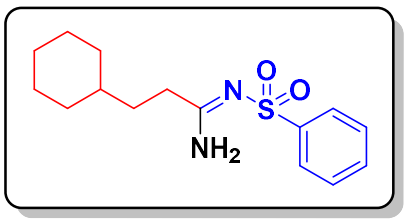
15. *N*'-(naphthalen-2-ylsulfonyl)-2-(*p*-tolyl)acetimidamide (4o) : Light Brown solid; m.p. 110-111 ˚C; **^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm)** = 8.48 (s, 1H), 8.18 (br, 1H), 7.96-7.92 (m, 4H), 7.65-7.60 (m, 2H), 7.15-7.09 (m, 4H), 5.76 (br, 1H), 3.64 (s, 2H), 2.33 (s, 3H); **^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm)** = 167.89, 138.87, 138.00, 129.97, 129.56, 129.25, 129.04, 128.45, 127.81, 127.81, 127.23, 127.12, 122.30, 43.23, 21.05; **IR (KBr) υ** 3369, 3324, 3247, 2965, 2984, 2845, 1658, 1524, 1306, 1287, 1108, 813 cm^{-1}; **HRMS (ESI) m/z** calcd. for $[M+H]^+$: 339.1162, found: 339.1160.



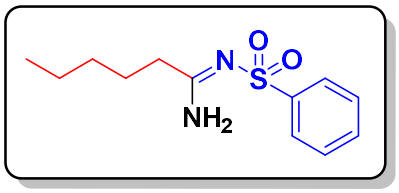
16. 2-(4-(*tert*-butyl)phenyl)-*N*'-(naphthalen-2-ylsulfonyl)acetimidamide (4p) : Light Brown solid; m.p. 115-116 ˚C; **^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm)** = 8.49 (s, 1H), 8.19 (br, 1H), 7.96-7.90 (m, 4H), 7.65-7.58 (m, 2H), 7.36 (d, *J* = 7.7 Hz, 2H), 7.15 (d, *J* = 7.7 Hz, 2H), 5.73 (br, 1H), 3.66 (s, 2H), 1.31 (s, 9H); **^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm)** = 167.83, 151.29, 138.90, 134.74, 132.08, 129.89, 129.43, 129.40, 129.27, 129.05, 128.46, 127.83, 127.24, 127.15, 126.26, 122.33, 43.20, 34.56, 31.23; **IR (KBr) υ** 3408, 3303, 3254, 2954, 2926, 2870, 1641, 1544, 1502, 1389, 1250, 1166, 1118, 1068, 1013, 935, 817 cm^{-1}; **HRMS (ESI) m/z** calcd. for $[M+H]^+$: 381.1631, found: 381.1624.



17. 3-cyclohexyl-*N*'-(phenylsulfonyl)propanimidamide (4q) : White solid; m.p. 80-81 ˚C; **^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm)** = 8.07 (br, 1H), 7.93 (d, *J* = 6.9 Hz, 2H), 7.57-7.47 (m, 3H), 6.04 (br, 1H), 2.34-2.27 (m, 2H), 1.77 (br, 1H), 1.65-1.60 (m, 4H), 1.52-1.46 (m, 2H), 1.14-1.09 (m, 4H), 0.89-0.79 (m, 2H); **^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm)** = 169.89, 142.05, 132.22, 128.69, 126.29, 36.98, 35.47, 33.86, 32.67, 26.35, 26.07; **IR (KBr) υ** 3436, 3324, 2912, 2836, 1613, 1522, 1439, 1411, 1271, 1138, 1082, 929, 789 cm^{-1}; **HRMS (ESI) m/z** calcd. for $[M+H]^+$: 295.1475, found: 295.1471.



18. *N*'-(phenylsulfonyl)hexanimidamide (4r) : Yellow solid; m.p. 52-53 ˚C; **^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm)** = 8.03 (br, 1H), 7.92 (d, *J* = 7.3 Hz, 2H), 7.56-7.46 (m, 3H), 6.28 (br, 1H), 2.25 (t, *J* = 7.7 Hz, 2H), 1.62-1.55 (m, 2H), 1.27-1.17 (m, 4H), 0.81 (t, *J* = 6.9 Hz, 3H); **^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm)** = 169.82, 142.02, 132.20, 128.67, 126.20, 37.72, 30.86, 26.21, 22.16, 13.78; **IR (KBr) υ** 3443, 3324, 3234, 3059, 2954, 2918, 2864, 1613, 1530, 1417, 1264, 1146, 1090, 929, 789, 754 cm^{-1}; **HRMS (ESI) m/z** calcd. for $[M+H]^+$: 255.1162, found: 255.1158.



19. *N*'-(phenylsulfonyl)-2-(*p*-tolyl)acetimidamide (4s) : White solid; m.p. 76-77 ˚C; **^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm)** = 8.11 (br, 1H), 7.94 (d, *J* = 7.3 Hz, 2H), 7.59-7.48 (m, 3H), 7.17-7.09 (m, 4H), 5.71 (br, 1H), 3.63 (s, 2H), 2.35 (s, 3H); **^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm)** = 167.81, 141.99, 138.01, 132.29, 129.98, 129.92, 129.56, 128.73, 126.37, 43.27, 21.06; **IR (KBr) υ** 3443, 3324, 2912, 2856, 1606, 1522, 1439, 1375, 1264, 1146, 1068, 908, 852, 789, 754, 712 cm^{-1}; **HRMS (ESI) m/z** calcd. for $[M+H]^+$: 289.1005, found: 289.1001.

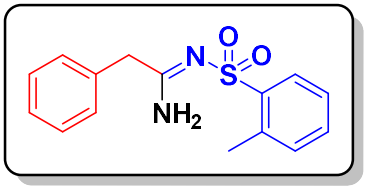
20. *N*'-((4-nitrophenyl)sulfonyl)hexanimidamide (4t) : Yellow solid; m.p. 55-56 ˚C; **^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm)** = 8.33 (d, *J* = 8.6 Hz, 2H), 8.11 (d, *J* = 8.6 Hz, 2H), 6.27 (br, 1H), 2.3 (t, *J* = 7.7 Hz, 2H), 1.85 (br, 1H), 1.65-1.57 (m, 2H), 1.27-1.22 (m, 4H), 0.83 (t, *J* = 6.9 Hz, 3H); **^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm)** = 170.49, 149.75, 147.72, 127.62, 123.98, 37.83, 30.88, 26.09, 22.14, 13.78; **IR (KBr) υ** 3388, 3322, 3243, 3104, 2933, 2854, 1641, 1528, 1436, 1344, 1271, 1140, 1079, 961, 855, 803, 684; **HRMS (ESI) m/z** calcd. for $[M+H]^+$: 300.1013, found: 300.1009.

21. 2-(4-(*tert*-butyl)phenyl)-*N*'-(*o*-tolylsulfonyl)acetimidamide (4u) : White solid; m.p. 82-83 ˚C; **^{1}H NMR (500 MHz, $CDCl_3$) δ (ppm)** = 8.07 (br, 1H), 8.03 (d, *J* = 7.3 Hz, 1H), 7.46-7.43 (m, 1H), 7.38 (d, *J* = 8.2 Hz, 2H), 7.30 (d, *J* = 7.5 Hz, 2H), 7.15 (d, *J* = 8.2 Hz, 2H), 5.73 (br, 1H), 3.65 (s, 2H), 2.67 (s, 3H), 1.32 (s, 9H); **^{13}C NMR (125 MHz, $CDCl_3$) δ (ppm)** = 167.73, 151.29, 139.75, 137.64, 132.78, 132.24, 129.42, 127.79, 126.25, 125.79, 42.95, 34.56, 31.23, 20.29; **IR (KBr) υ** 3394, 3317, 3248, 2961, 2891, 2864, 1655, 1558, 1453, 1411, 1250, 1110, 1054, 971, 817, 740 cm^{-1}; **HRMS (ESI) m/z** calcd. for $[M+H]^+$: 345.1631, found: 345.1628.

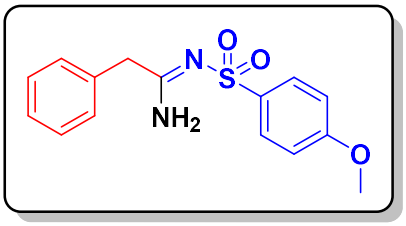
22. 2-phenyl-*N*'-(phenylsulfonyl)acetimidamide (4v) : White solid; m.p. 86-87 ˚C; **^{1}H NMR (600 MHz, $CDCl_3$) δ (ppm)** = 8.11 (br, 1H), 7.93

(d, *J* = 7.7 Hz, 2H), 7.57-7.55 (m, 1H), 7.50-7.48 (m, 2H), 7.36-7.32 (m, 3H), 7.22 (d, *J* = 7 Hz, 2H), 5.79 (br, 1H), 3.66 (s, 2H); **^{13}C NMR (150 MHz, CDCl$_3$) δ(ppm)** = 167.56, 141.90, 133.18, 132.32, 129.59, 129.26, 128.74, 128.10, 126.34; **IR (KBr) υ** 3436, 3324, 1627, 1530, 1389, 1264, 1138, 1082, 929, 775, 740 cm^{-1}; **HRMS (ESI) m/z** calcd. for [M+H] $^+$: 275.0849, found: 275.0843.

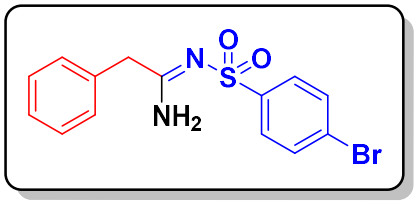
23. 2-phenyl-*N*'-(*o*-tolylsulfonyl)acetimidamide (4w) : White solid; m.p. 70-71 ˚C; **^{1}H NMR (400 MHz, CDCl$_3$) δ (ppm)** = 7.92 (d, *J* = 7.7 Hz, 1H), 7.37-7.33 (m, 1H), 7.28-7.19 (m, 5H), 7.14-7.12 (m, 2H), 5.77 (br, 1H), 3.57 (s, 2H), 2.56 (s, 3H), 1.65 (br, 1H); **^{13}C NMR (100 MHz, CDCl$_3$) δ (ppm)** = 167.38, 139.86, 137.50, 133.36, 133.33, 132.32, 132.16, 129.53, 129.14, 129.12, 127.96, 127.94, 127.59, 125.69, 43.69, 20.21; **IR (KBr) υ** 3450, 3380, 3338, 2933, 1620, 1550, 1446, 1257, 1187, 1124, 817 cm^{-1}; **HRMS (ESI) m/z** calcd. for [M+H] $^+$: 289.1005, found: 289.1002.



24. *N*'-((4-methoxyphenyl)sulfonyl)-2-phenylacetimidamide (4x) : White solid; m.p. 100-101 ˚C; **^{1}H NMR (400 MHz, CDCl$_3$) δ (ppm)** = 8.06 (br, 1H), 7.85 (d, *J* = 9 Hz, 2H), 7.36-7.31 (m, 3H), 7.21 (dd, *J* = 1.5 Hz, 7.5 Hz, 2H), 6.95 (d, *J* = 9 Hz, 2H), 5.79 (br, 1H), 3.86 (s, 3H), 3.63 (s, 2H); **^{13}C NMR (100 MHz, CDCl$_3$) δ (ppm)** = 167.09, 162.61, 133.81, 129.50, 129.14, 128.39, 127.94, 113.87, 55.52, 43.61; **IR (KBr) υ** 3401, 3324, 3248, 2933, 1634, 1592, 1488, 1124, 1076, 817 cm^{-1}; **HRMS (ESI) m/z** calcd. for [M+H] $^+$: 305.0954, found: 305.0948.

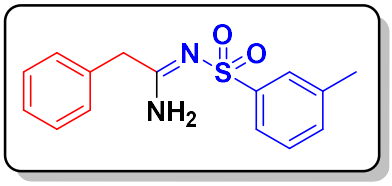


25. *N*'-((4-bromophenyl)sulfonyl)-2-phenylacetimidamide (4y) : White solid; m.p. 76-77 ˚C; **^{1}H NMR (400 MHz, CDCl$_3$) δ (ppm)** = 8.12 (br, 1H), 7.8 (d, *J* = 8.6 Hz, 2H), 7.63 (d, *J* = 8.6 Hz, 2H), 7.38-7.35 (m, 3H), 7.24-7.22 (m, 2H), 5.65 (br, 1H), 3.67 (s, 2H); **^{13}C NMR (100 MHz, CDCl$_3$) δ (ppm)** = 167.62, 141.04, 132.90, 131.99, 129.67, 129.40, 128.30, 128.05, 127.21, 43.75; **IR (KBr)**



υ 3401, 3303, 3240, 2905, 2850, 1648, 1550, 1425, 1348, 1257, 1160, 1068, 957, 796, 601 cm^{-1}; **HRMS (ESI) m/z** calcd. for $[M+H]^+$: 352.9954, found: 352.9948.

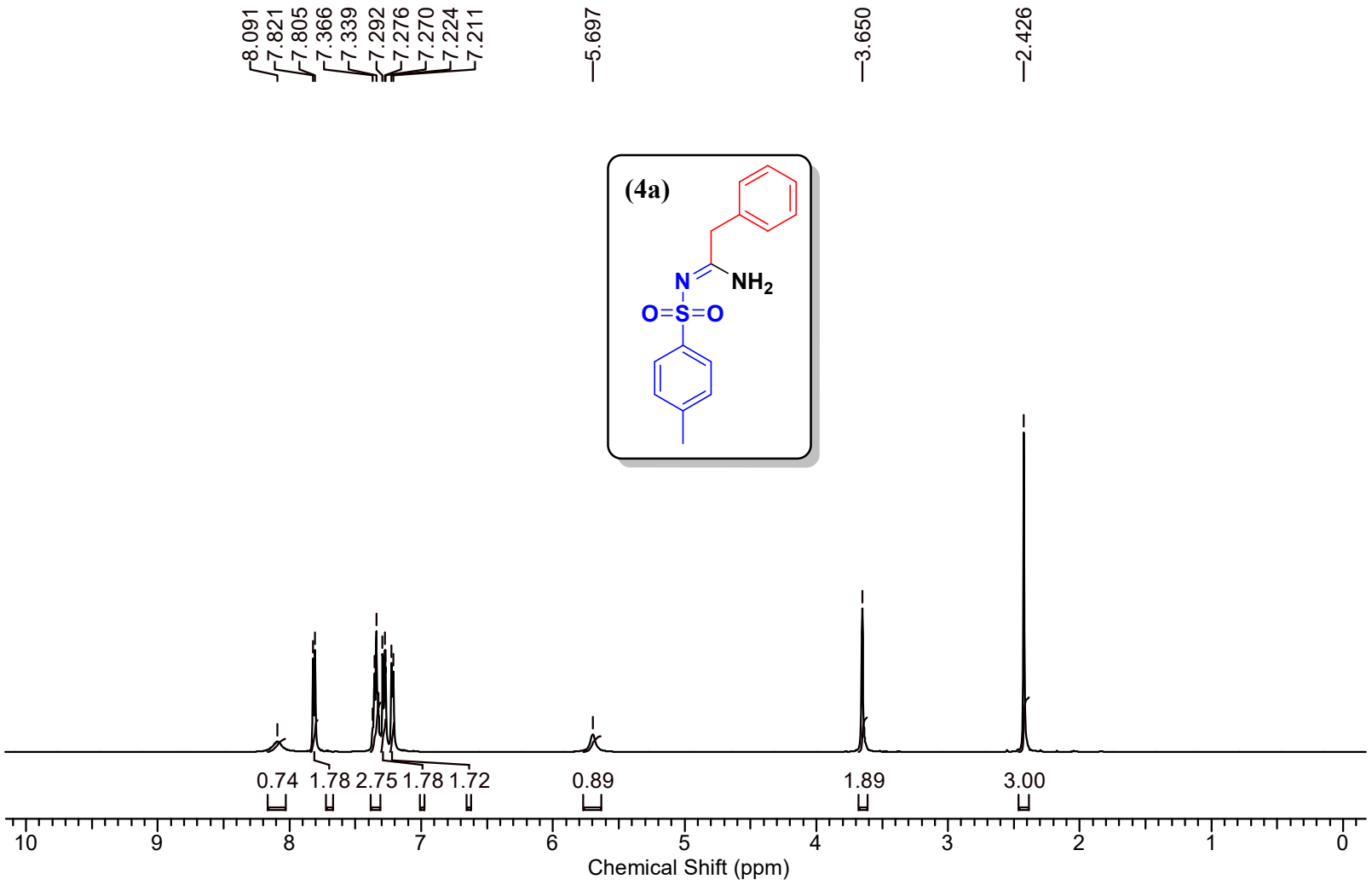
26. 2-phenyl-*N*'-(*m*-tolylsulfonyl)acetimidamide (4z) : White solid; m.p. 85-86 ˚C; **^{1}H NMR (500 MHz, $CDCl_3$) δ (ppm)** = 8.15 (br, 1H), 7.74-7.3 (m, 2H), 7.38-7.22 (m, 5H), 7.23 (dd, *J* = 1.5 Hz, 7.8 Hz, 2H), 5.74 (br, 1H), 3.68 (s, 2H), 2.42 (s, 3H); **^{13}C NMR (125 MHz, $CDCl_3$) δ (ppm)** = 167.41, 141.62, 138.94, 133.19, 133.10, 129.67, 129.30, 128.64, 128.17, 126.82, 123.48, 43.63, 21.33; **IR (KBr) υ** 3366, 3240, 3065, 3017, 2912, 2850, 1648, 1550, 1417, 1271, 1138, 1090, 963, 859, 803 cm^{-1}; **HRMS (ESI) m/z** calcd. for $[M+H]^+$: 289.1005, found: 289.1009.

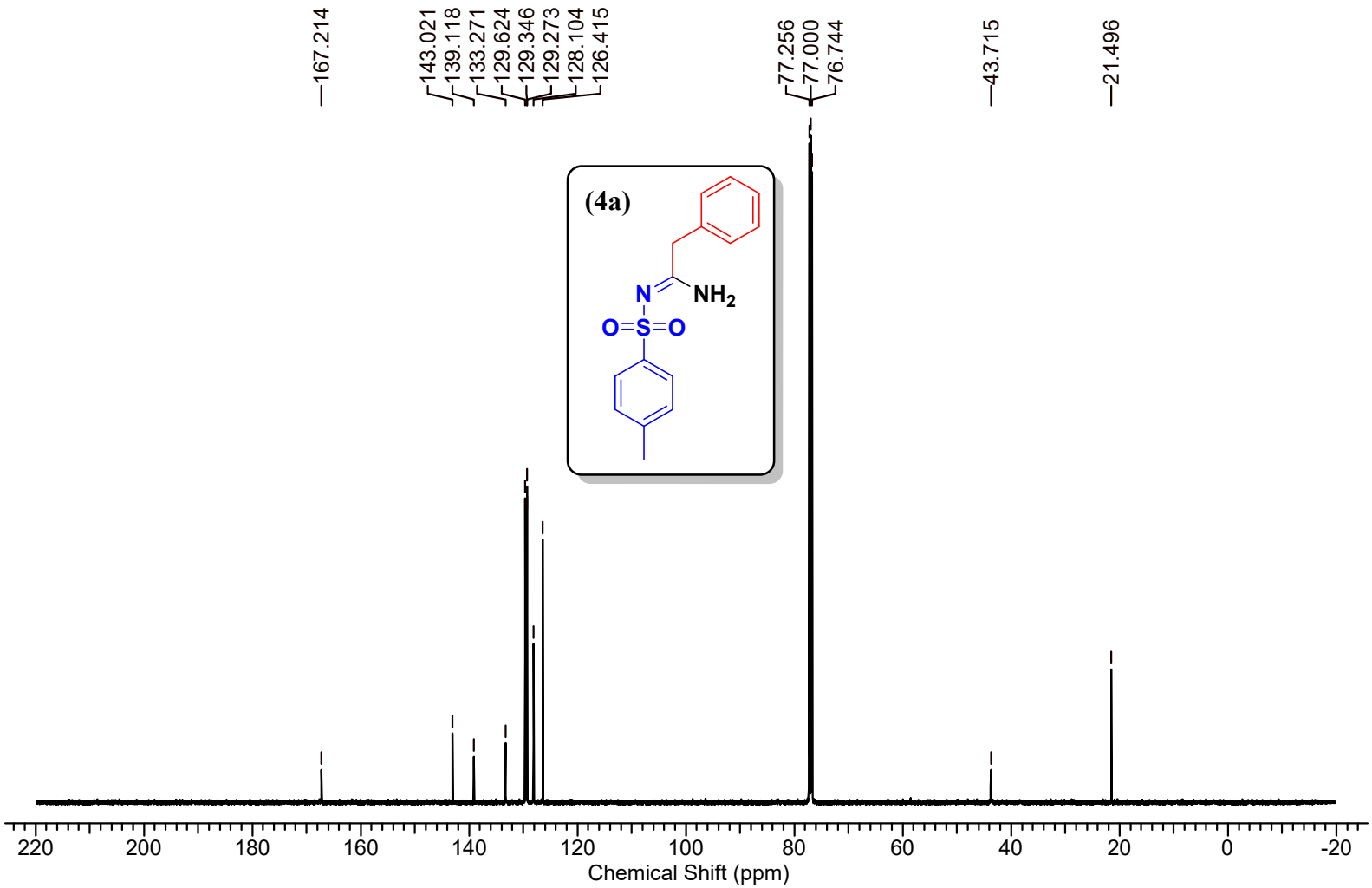


References:

1. J. Kim, S. Y. Lee, J. Lee, Y. Do and S. Chang, *J. Org. Chem.*, 2008, **73**, 9454–9457.

3. ^{1}H and ^{13}C NMR spectra:

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133.271
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129.273
128.104
126.415
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77.000
76.744
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21.496
(4a)
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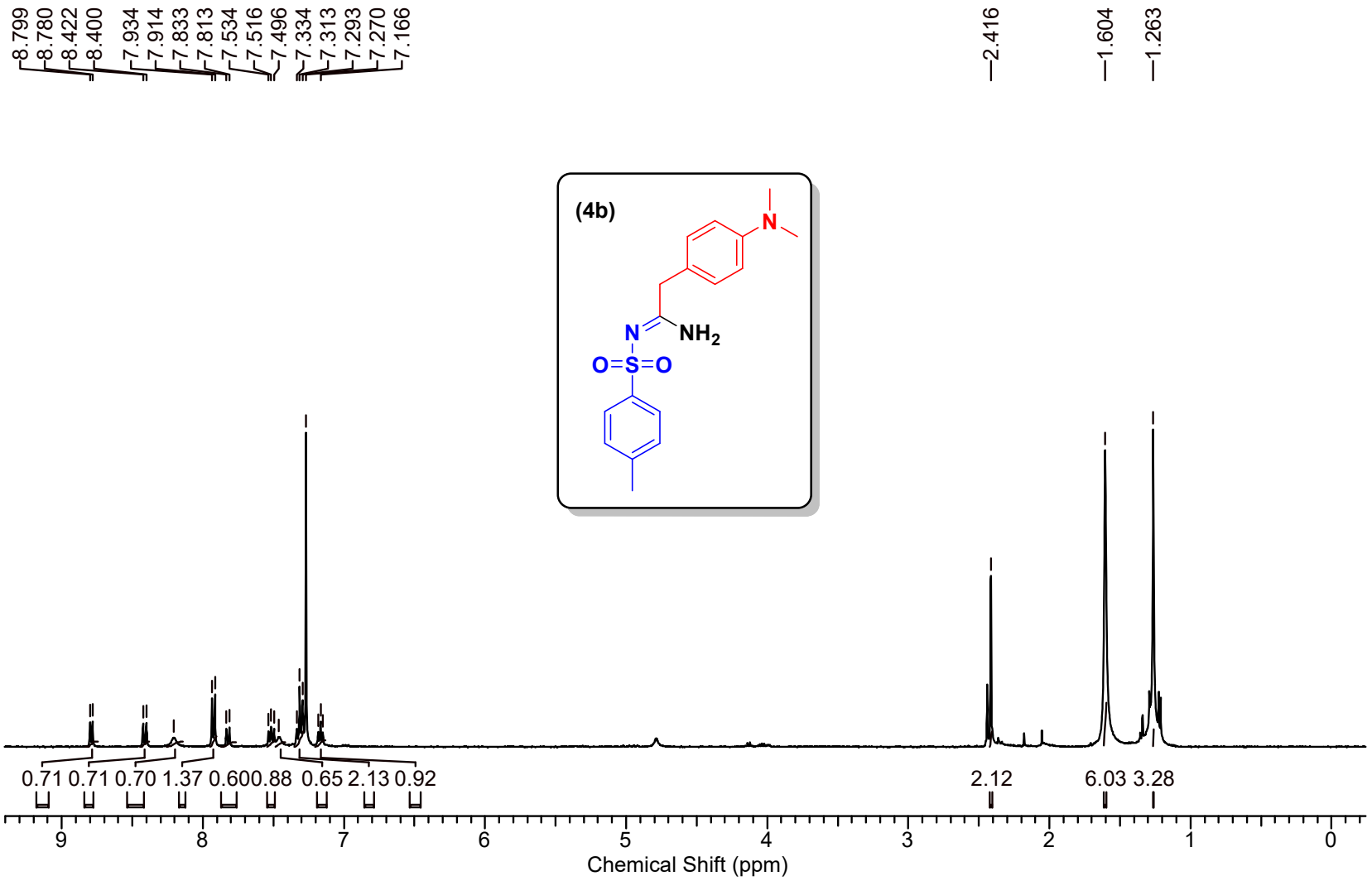
200
180
160
140
120
100
80
60
40
20
0
-20
Chemical Shift (ppm)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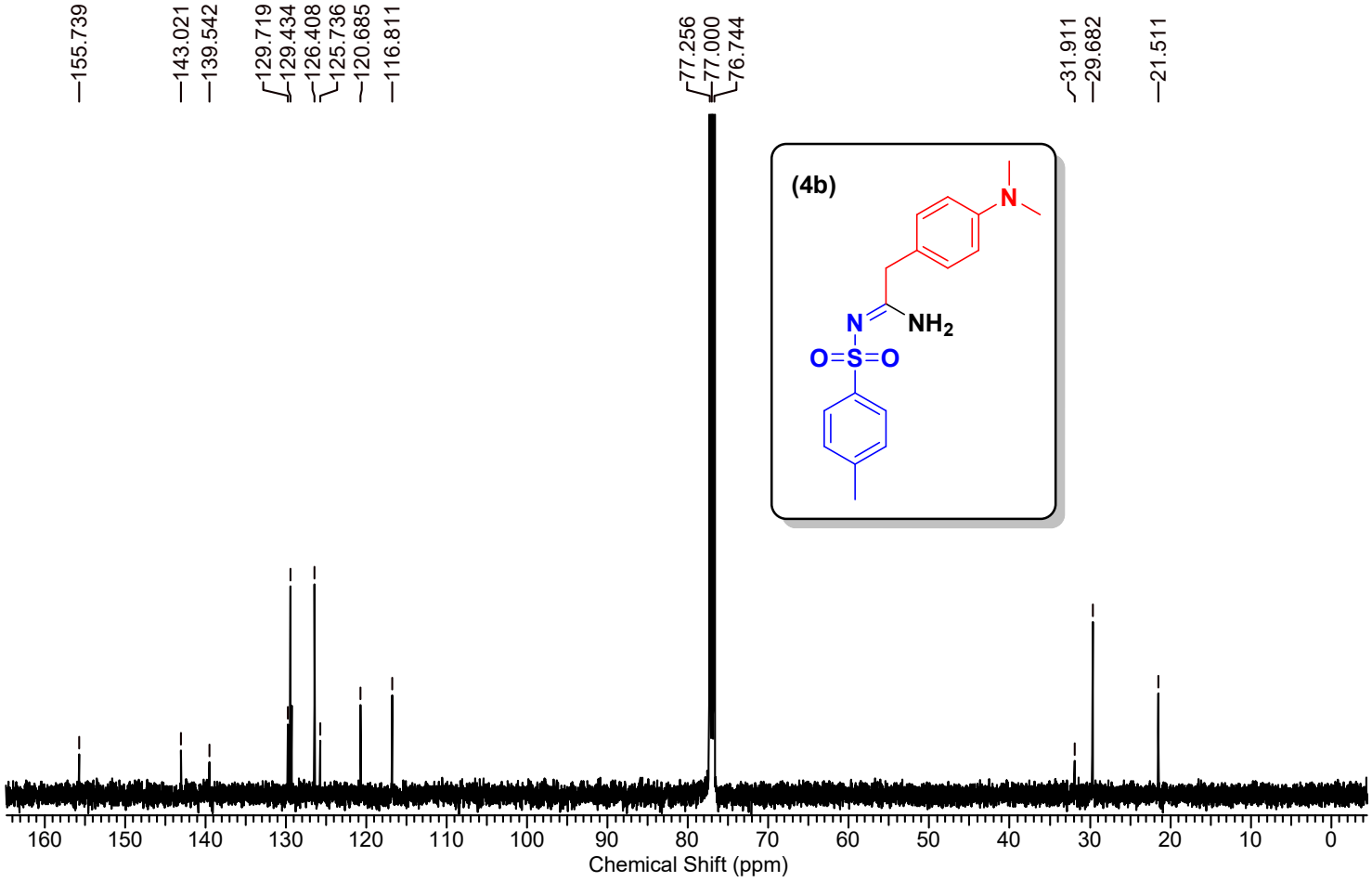
7.914
7.833
7.813
7.534
7.516
7.496
7.334
7.313
7.293
7.270
7.166
2.416
1.604
1.263
(4b)
N
NH2
O=S=O
0.71 0.71 0.70 1.37 0.60 0.88 0.65 2.13 0.92
2.12
6.03 3.28
9
8
7
6
5
4
3
2
1
0
Chemical Shift (ppm)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129.434
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120.685
116.811
77.256
77.000
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31.911
29.682
21.511
(4b)
N
N
NH2
O=S=O
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150
140
130
120
110
100
90
80
70
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50
40
30
20
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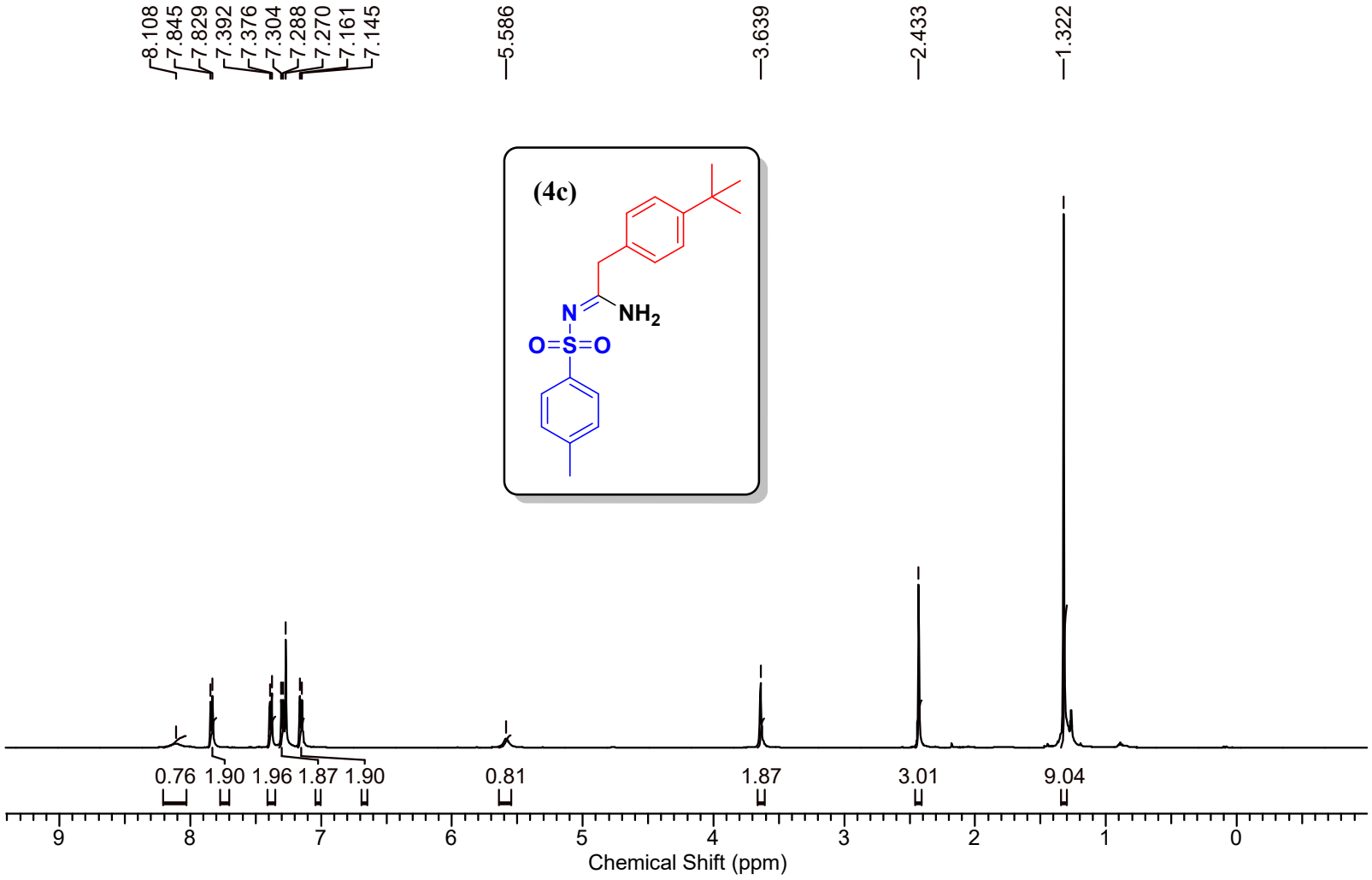
Chemical Shift (ppm)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7.376
7.304
7.288
7.270
7.161
7.145
5.586
3.639
2.433
1.322
(4c)
N
NH2
O=S=O
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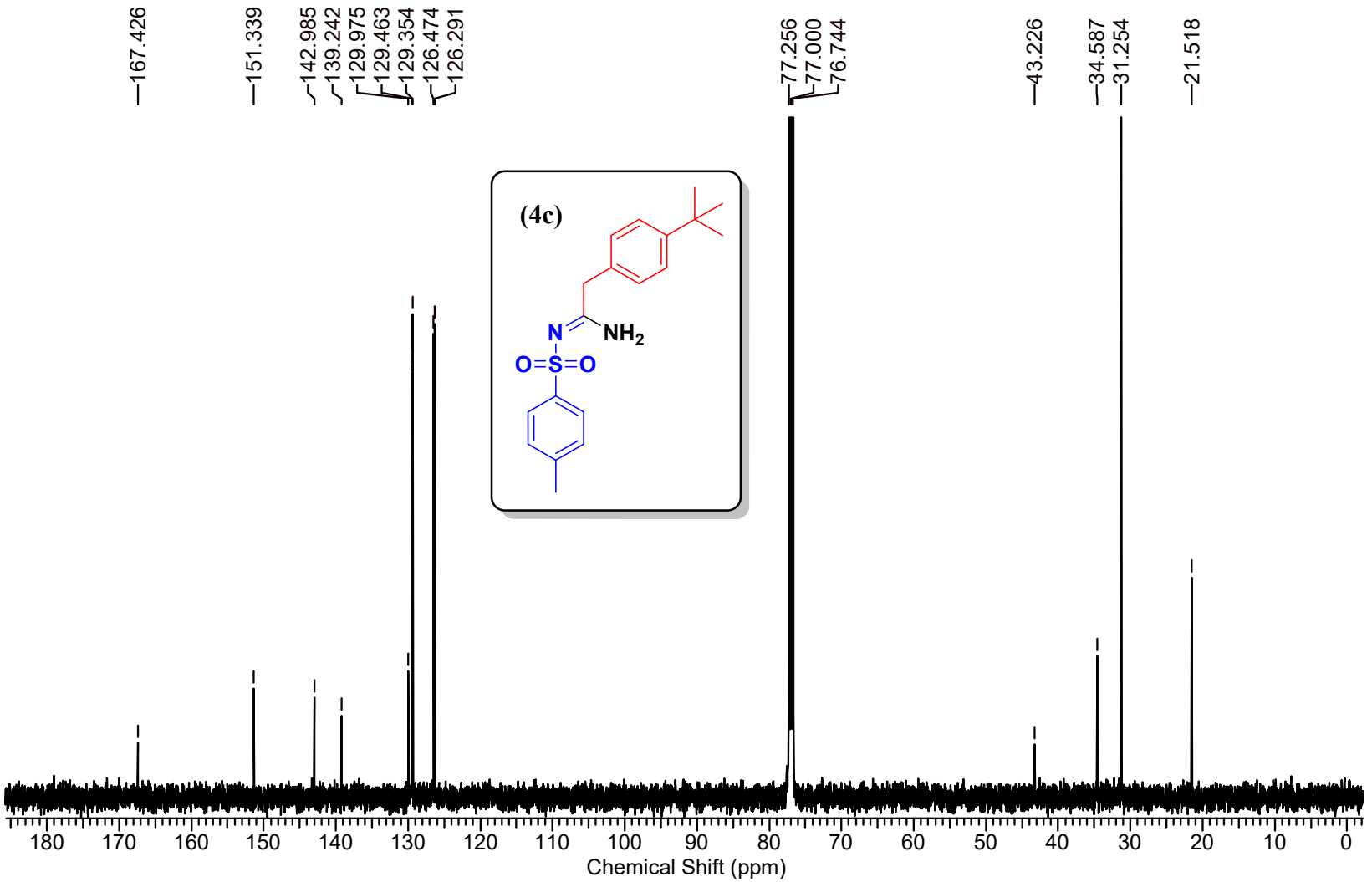
0.81
1.87
3.01
9.04
9 8 7 6 5 4 3 2 1 0
Chemical Shift (ppm)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142.985
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126.291
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77.000
76.744
43.226
34.587
31.254
21.518
(4c)
N
NH2
O=S=O
180
170
160
150
140
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120
110
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70
60
50
40
30
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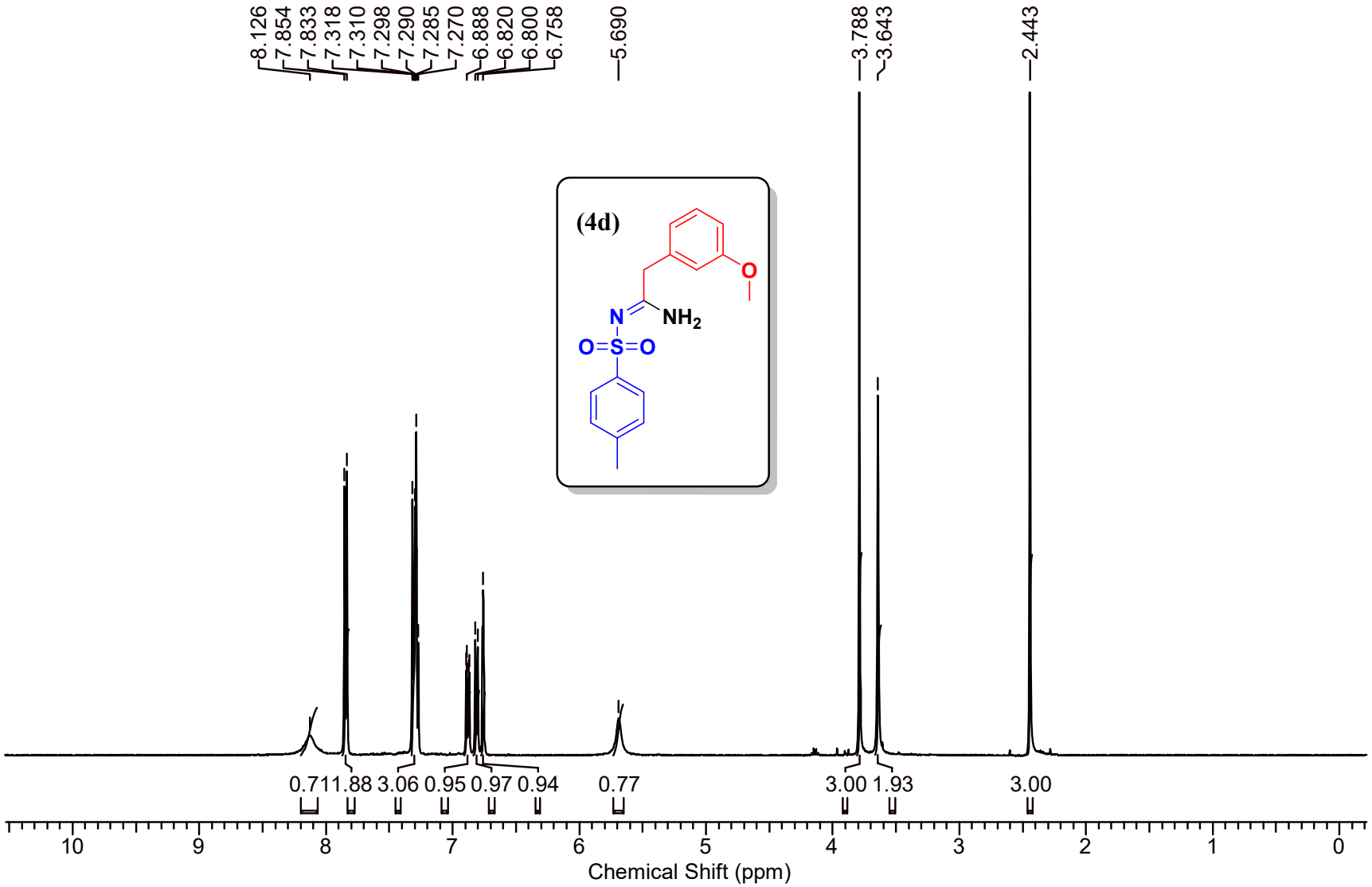
Chemical Shift (ppm)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7.285
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6.820
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5.690
3.788
3.643
2.443
(4d)
O
N
NH2
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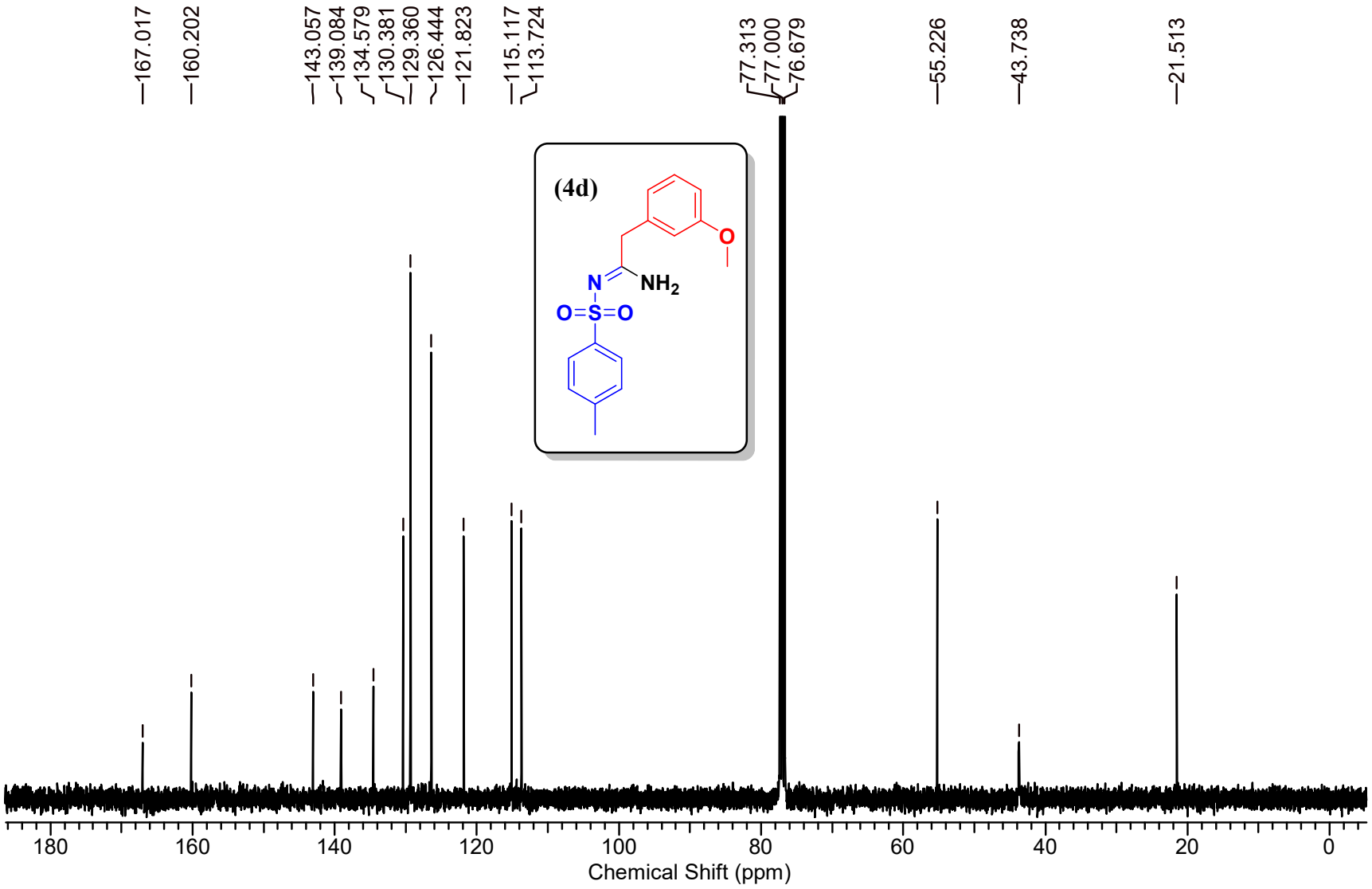
Chemical Shift (ppm)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77.000
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55.226
43.738
21.513
(4d)
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NH2
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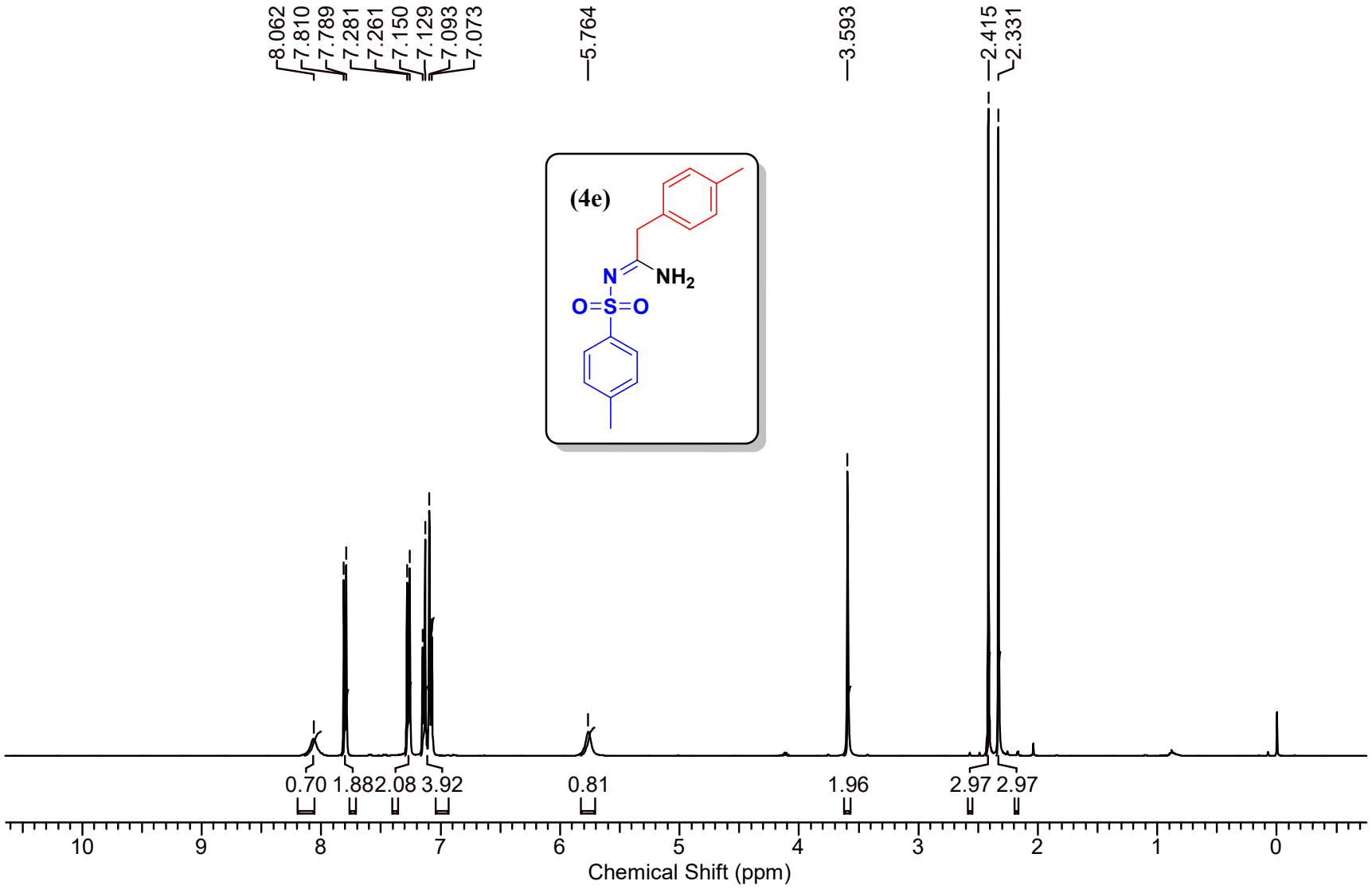
160
140
120
100
80
60
40
20
0
Chemical Shift (ppm)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7.093
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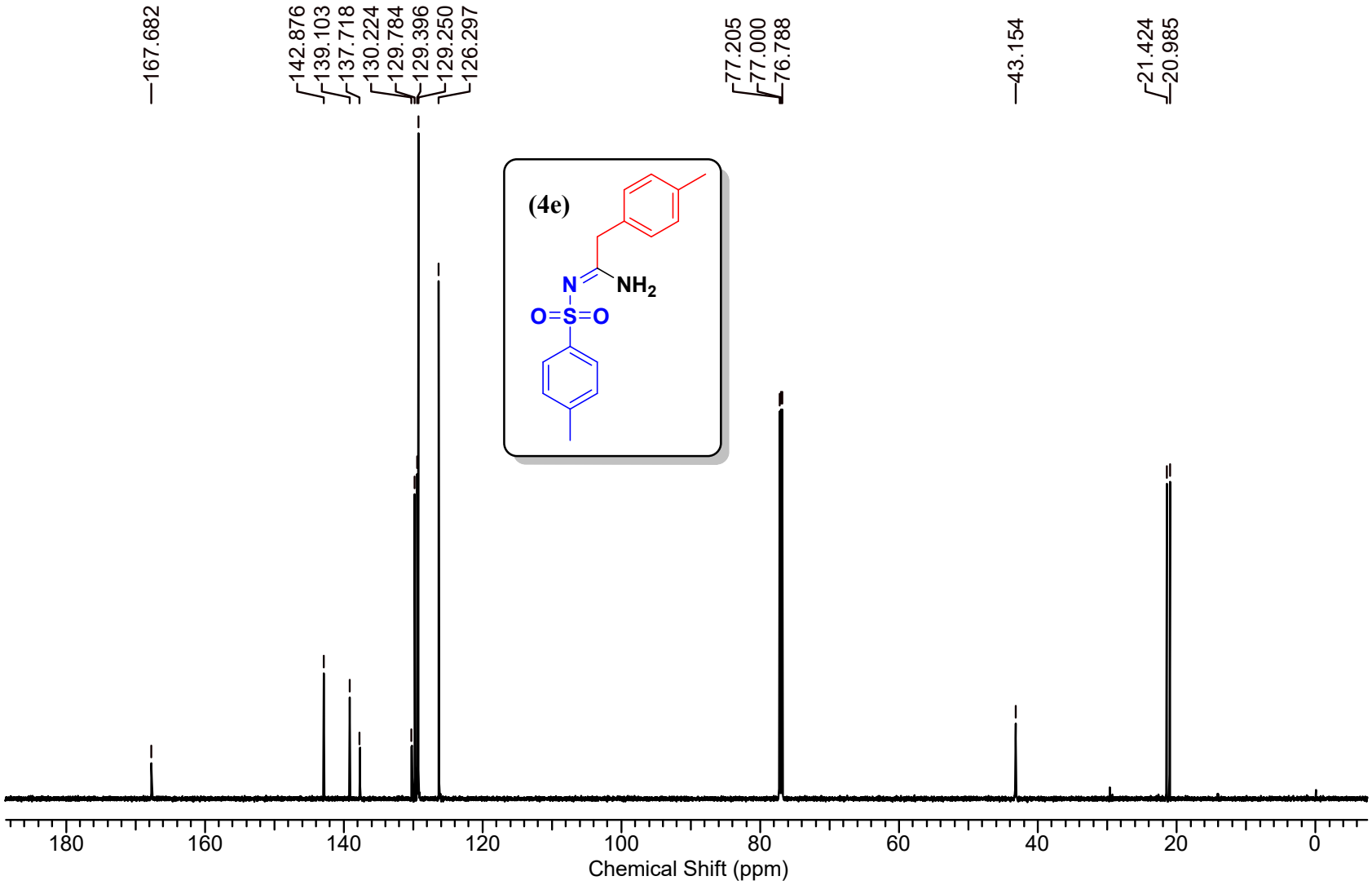
3.593
2.415
2.331
(4e)
N
NH2
O=S=O
0.70
1.88
2.08
3.92
0.81
1.96
2.97
2.97
10
9
8
7
6
5
4
3
2
1
0
Chemical Shift (ppm)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129.396
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77.205
77.000
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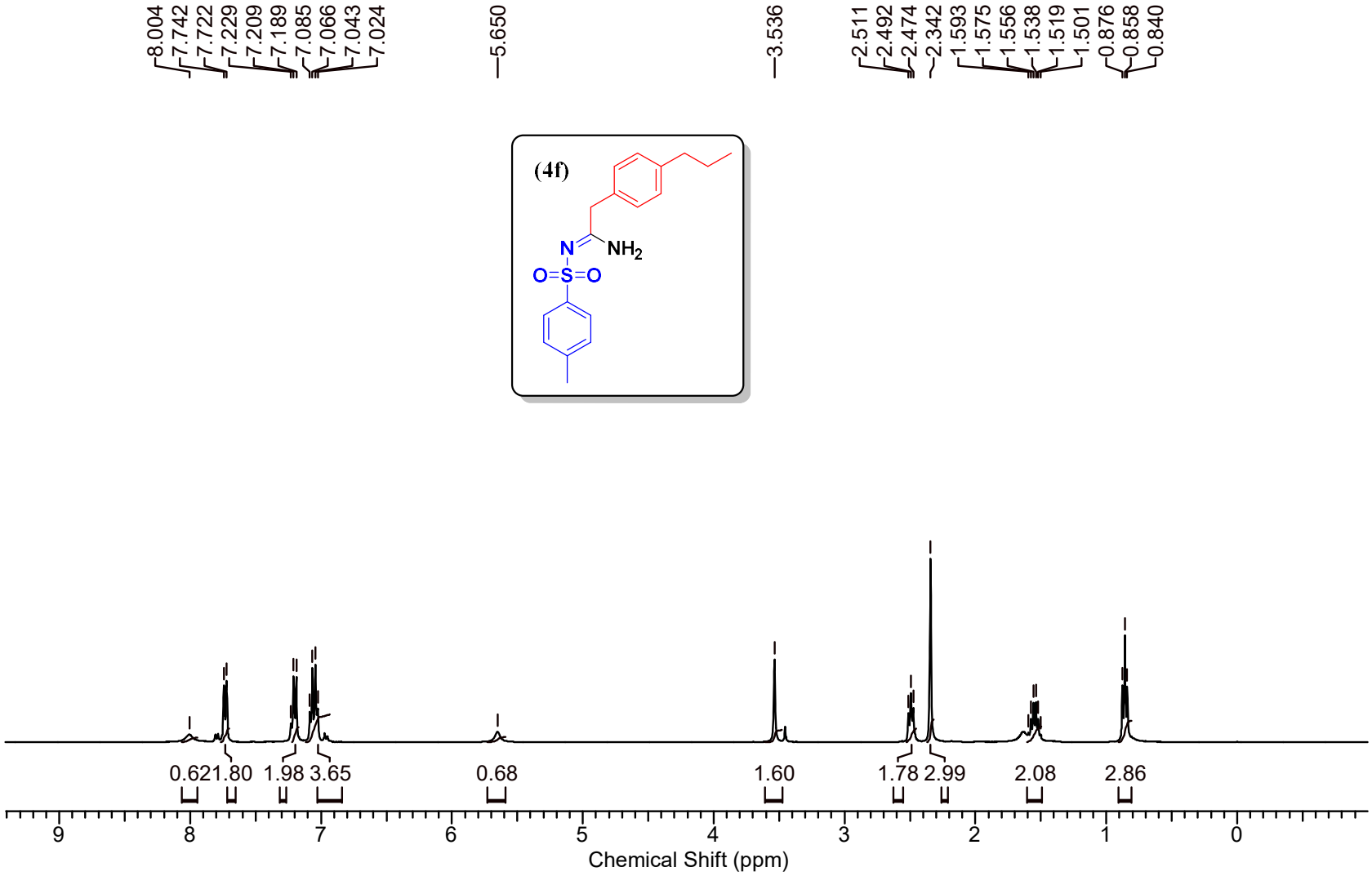
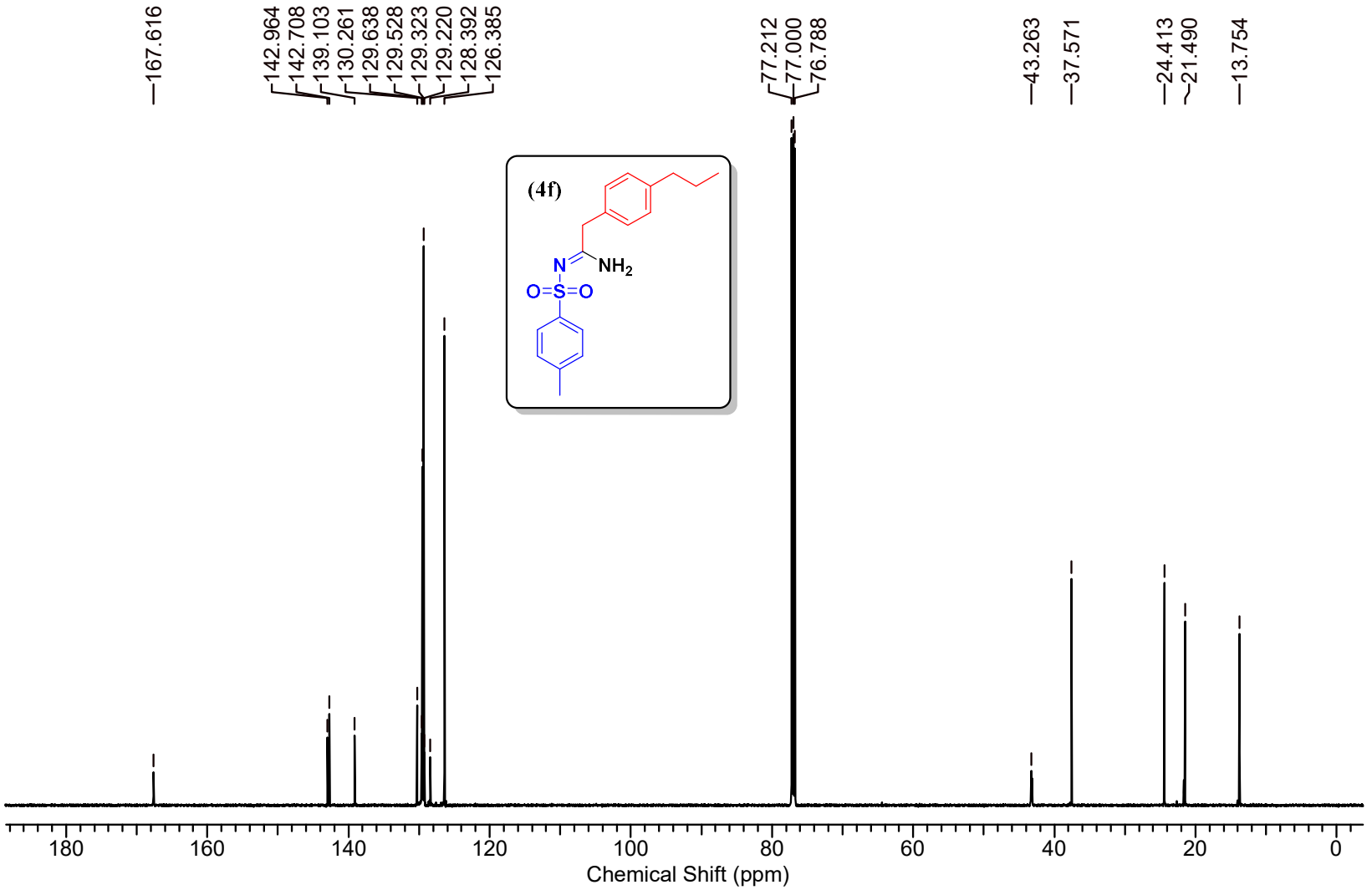
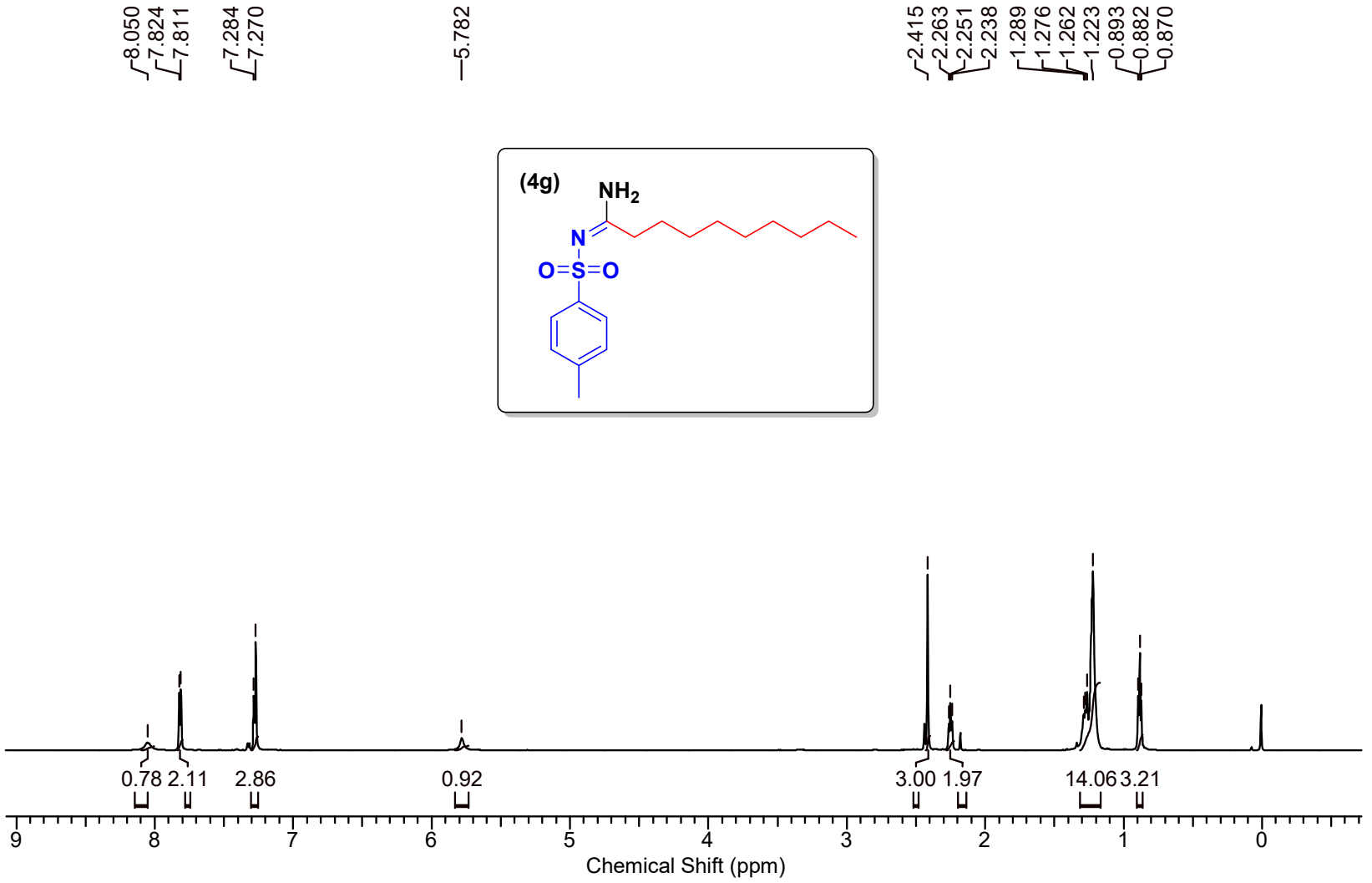
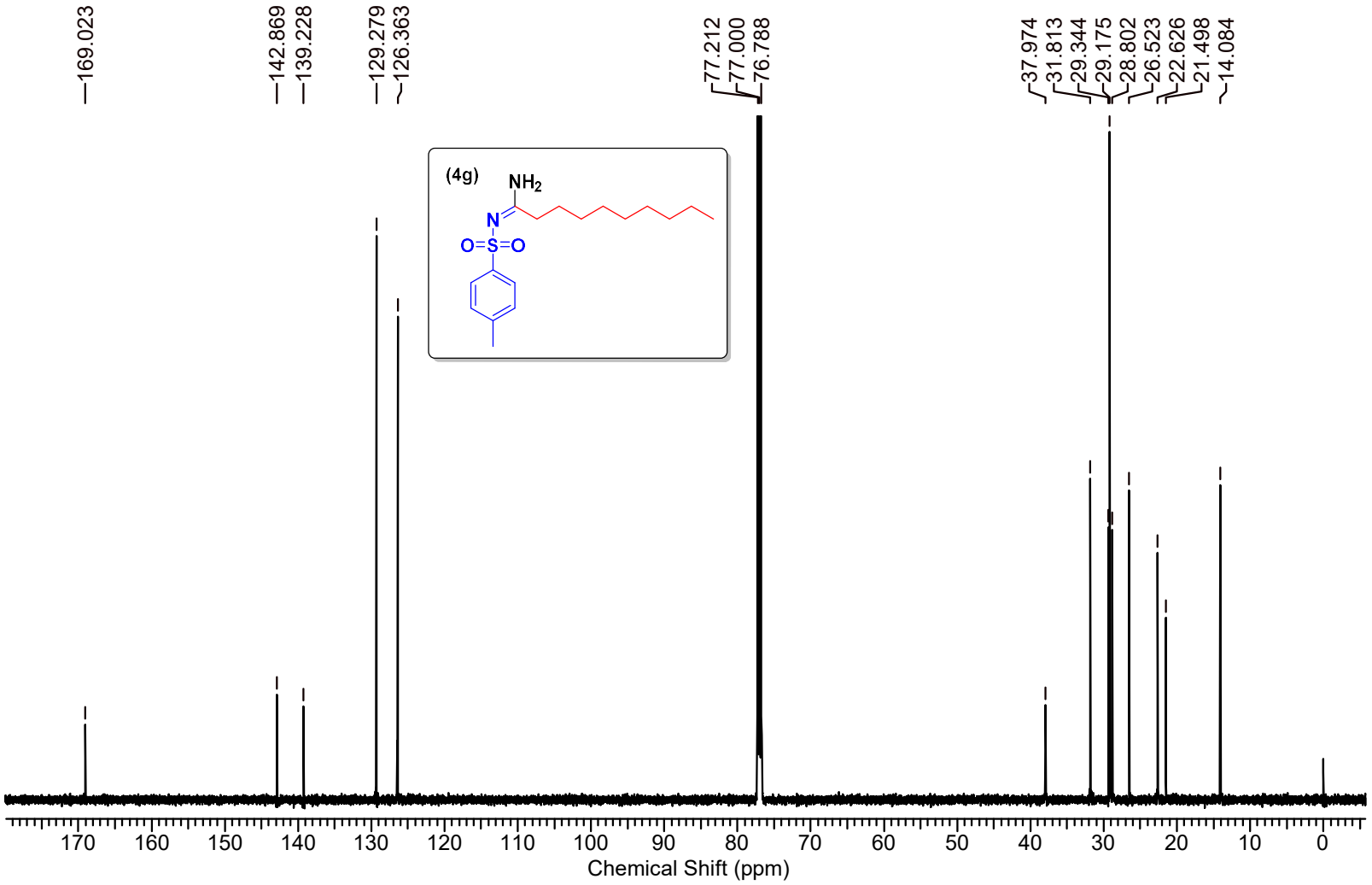
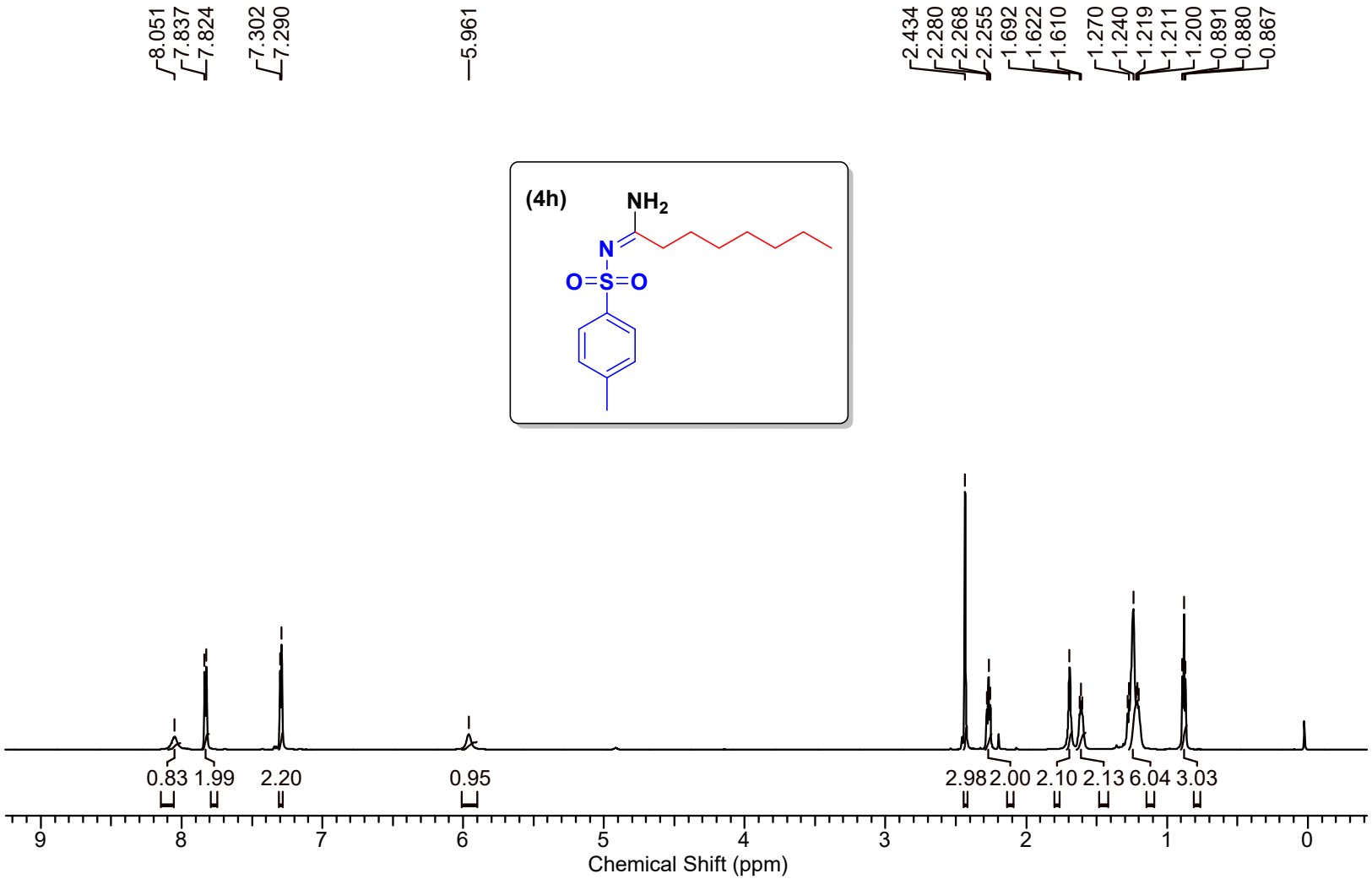
43.154
21.424
20.985
(4e)
N
NH2
O=S=O
180
160
140
120
100
80
60
40
20
0
Chemical Shift (ppm)

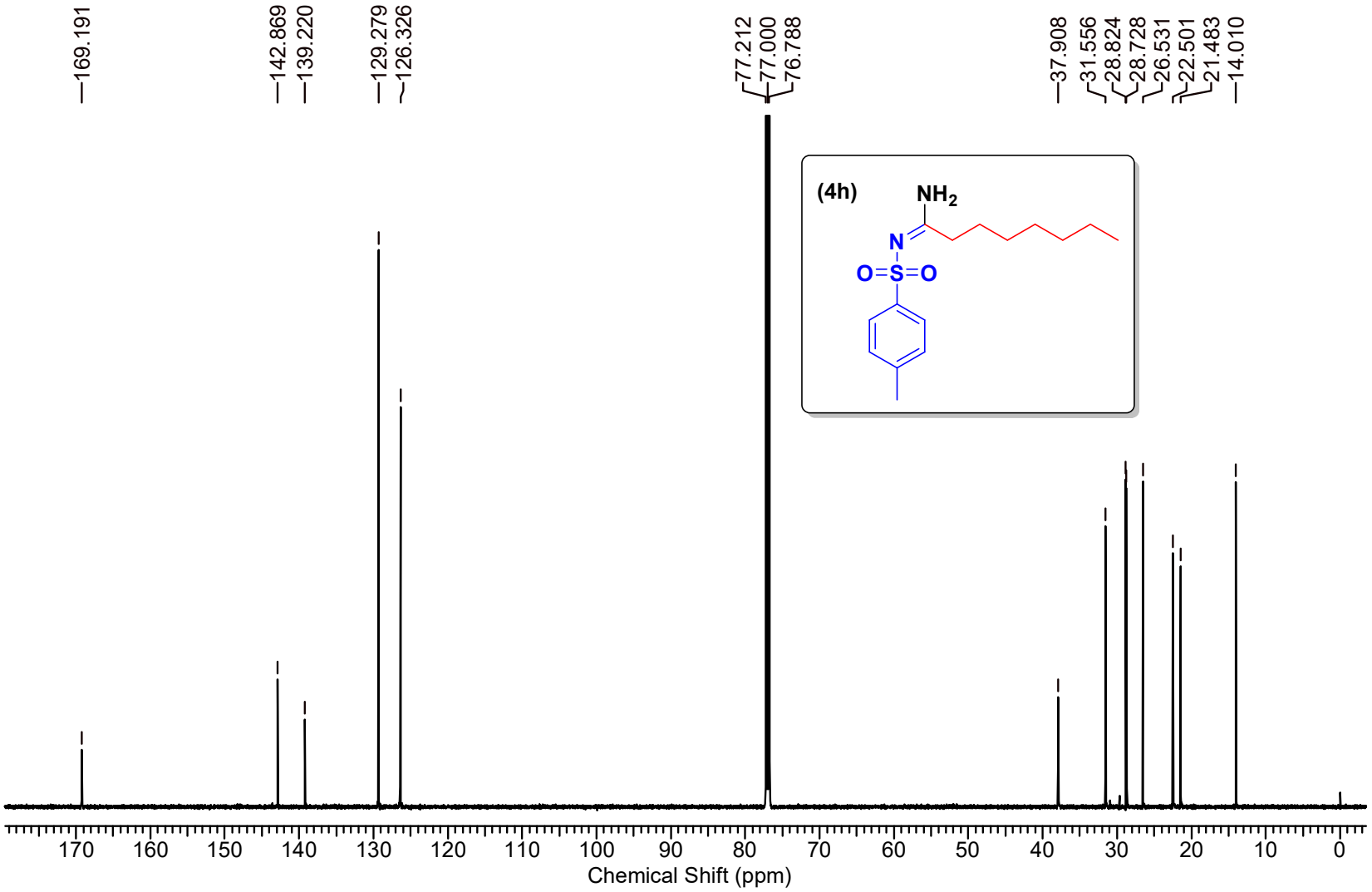

8.004
7.742
7.722
7.229
7.209
7.189
7.085
7.066
7.043
7.024
5.650
3.536
2.511
2.492
2.474
2.342
1.593
1.575
1.556
1.538
1.519
1.501
0.876
0.858
0.840
(4f)
N
NH2
O=S=O
0.62
1.80
1.98
3.65
0.68
1.60
1.78
2.99
2.08
2.86
9
8
7
6
5
4
3
2
1
0
Chemical Shift (ppm)

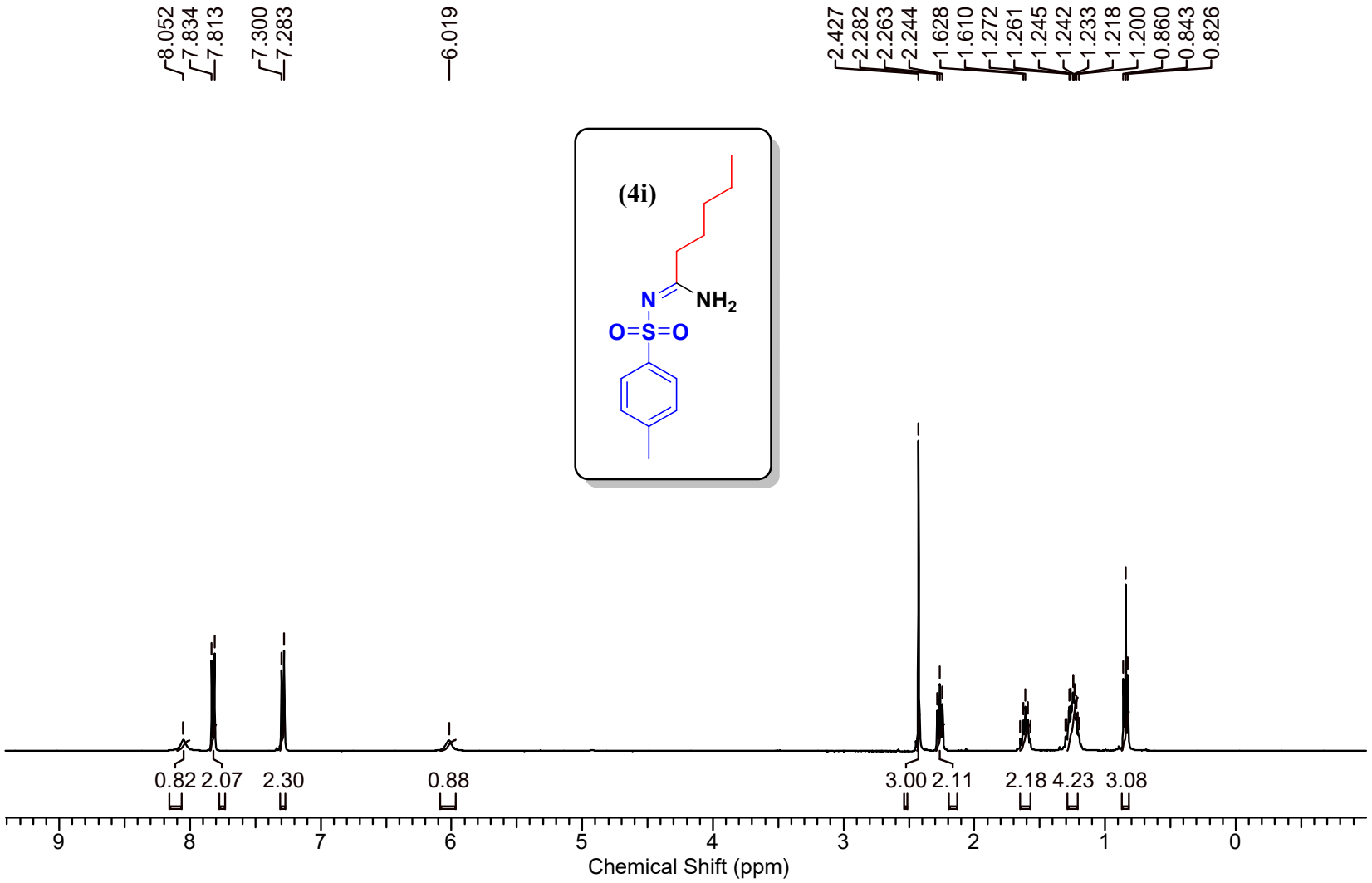

167.616
142.964
142.708
139.103
130.261
129.638
129.528
129.323
129.220
128.392
126.385
77.212
77.000
76.788
43.263
37.571
24.413
21.490
13.754
(4f)
N
NH2
O=S=O
180
160
140
120
100
80
60
40
20
0
Chemical Shift (ppm)

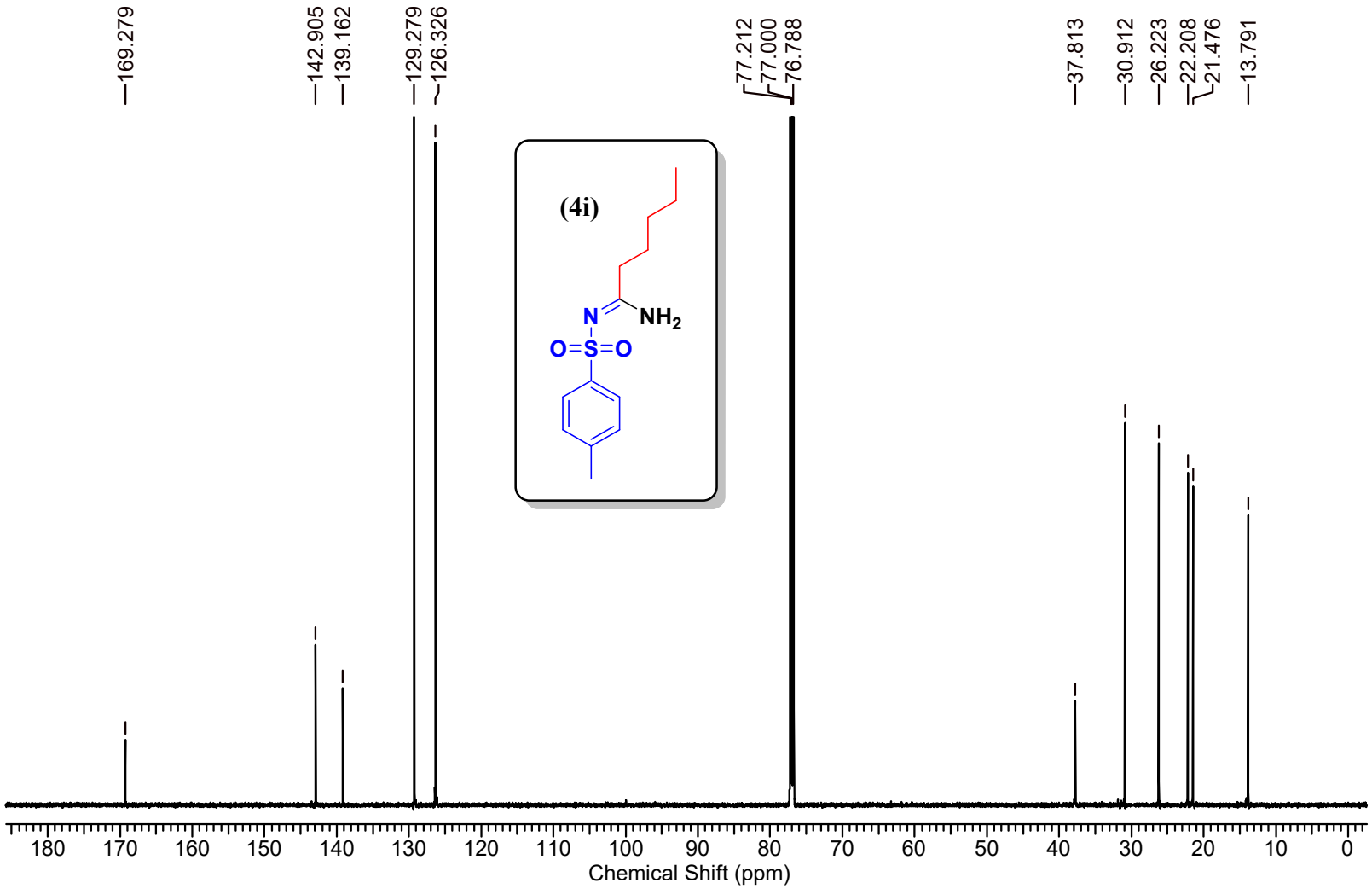

8.050
7.824
7.811
7.284
7.270
5.782
2.415
2.263
2.251
2.238
1.289
1.276
1.262
1.223
0.893
0.882
0.870
(4g)
NH2
N
O=S=O
0.78
2.11
2.86
0.92
3.00
1.97
14.06
3.21
9
8
7
6
5
4
3
2
1
0
Chemical Shift (ppm)

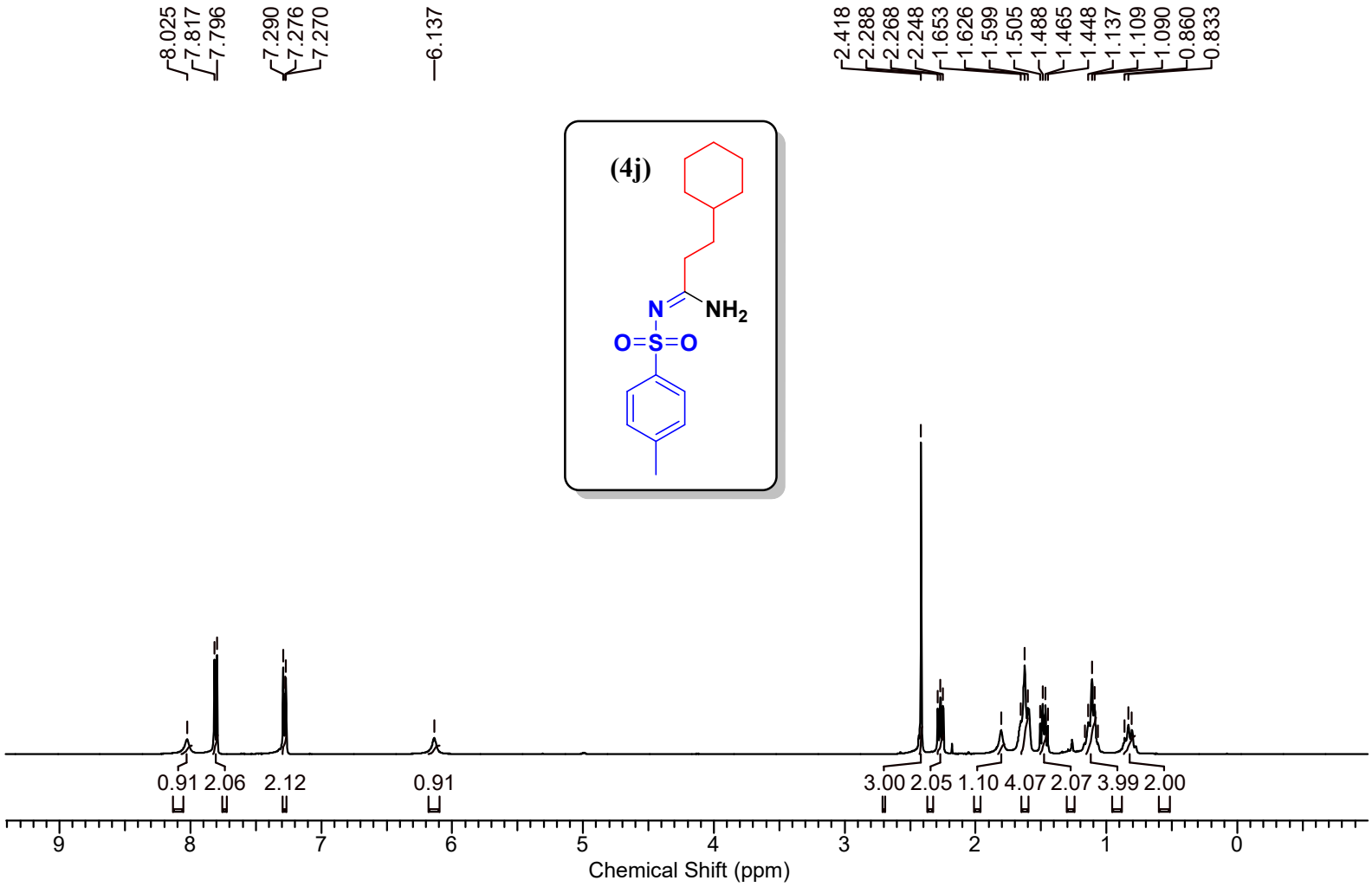

169.023
142.869
139.228
129.279
126.363
77.212
77.000
76.788
37.974
31.813
29.344
29.175
28.802
26.523
22.626
21.498
14.084
(4g)
NH2
N
O=S=O
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
Chemical Shift (ppm)

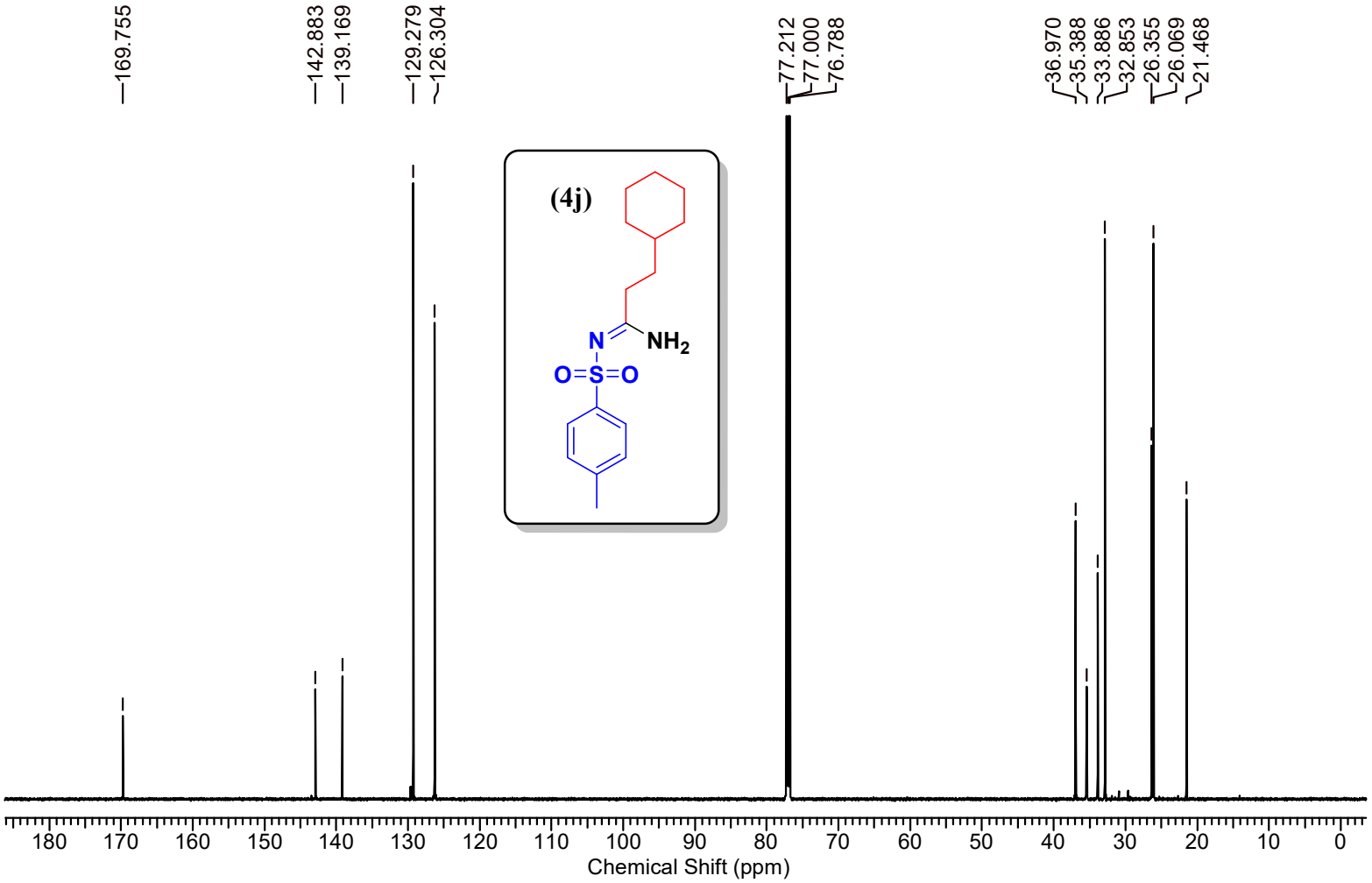

8.051
7.837
7.824
7.302
7.290
5.961
2.434
2.280
2.268
2.255
1.692
1.622
1.610
1.270
1.240
1.219
1.211
1.200
0.891
0.880
0.867
(4h)
NH2
N
O=S=O
0.83
1.99
2.20
0.95
2.98
2.00
2.10
2.13
6.04
3.03
9
8
7
6
5
4
3
2
1
0
Chemical Shift (ppm)

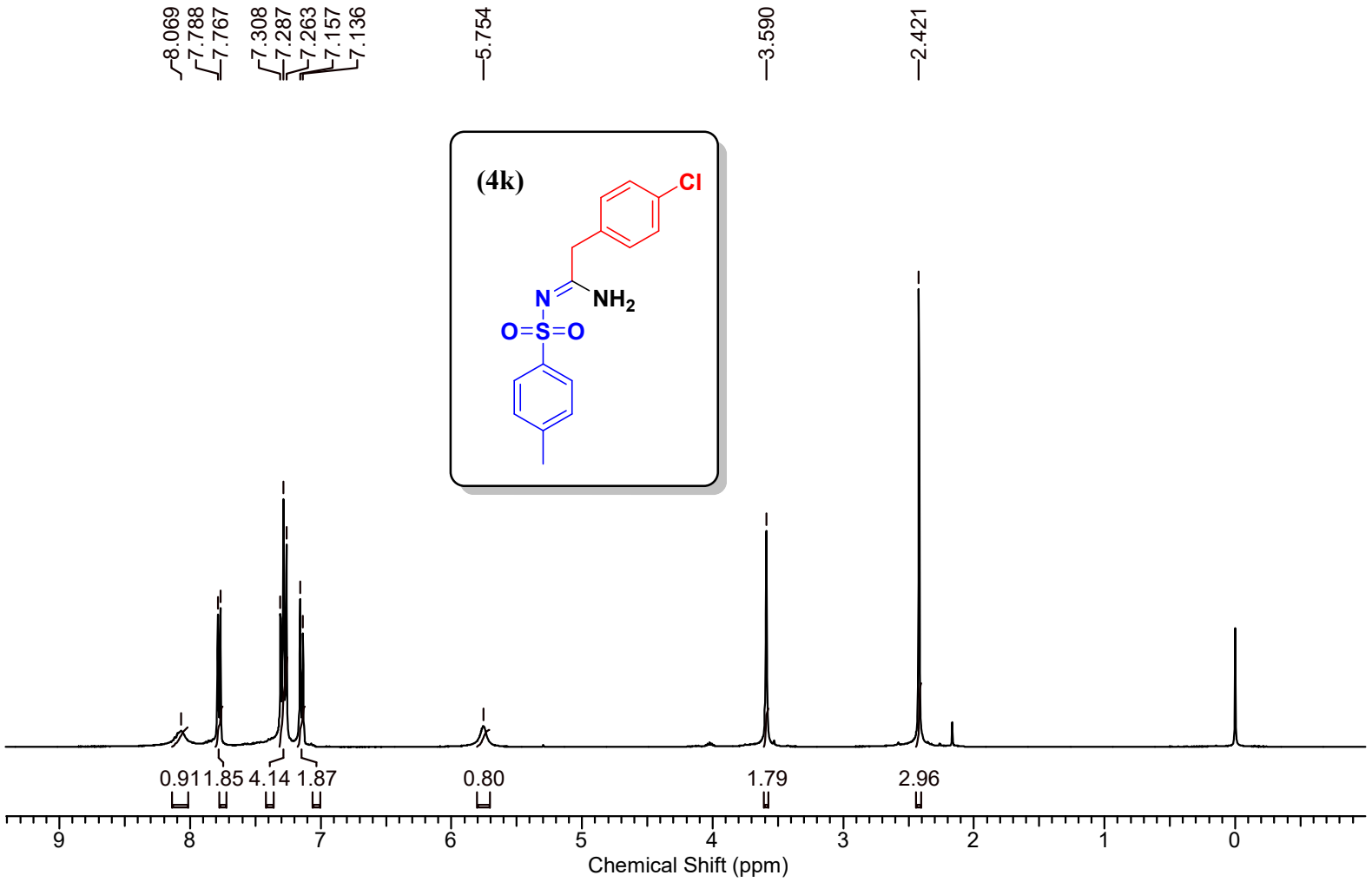

169.191
142.869
139.220
129.279
126.326
77.212
77.000
76.788
37.908
31.556
28.824
28.728
26.531
22.501
21.483
14.010
(4h)
NH2
N
O=S=O
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
Chemical Shift (ppm)

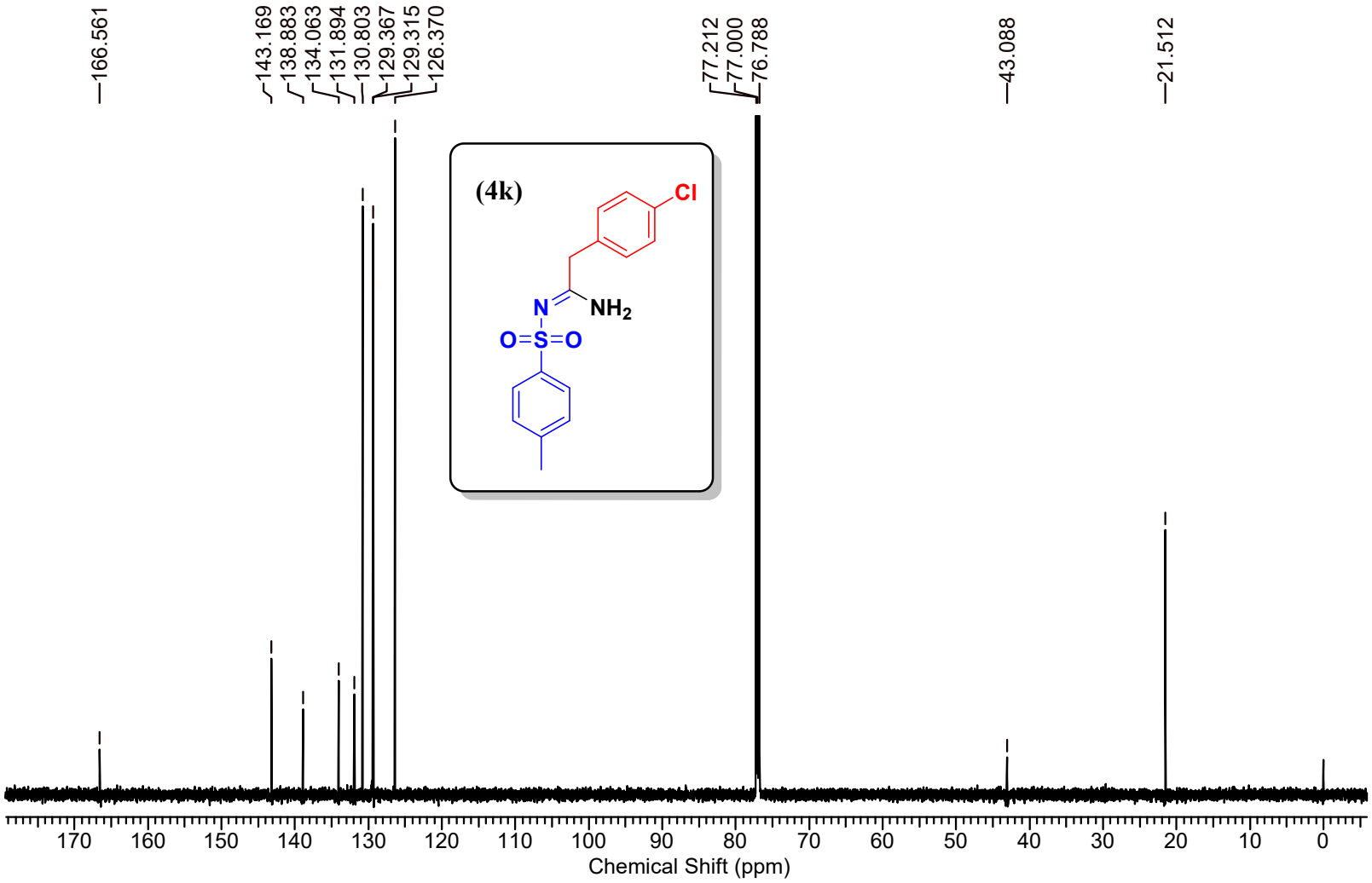

8.052
7.834
7.813
7.300
7.283
6.019
2.427
2.282
2.263
2.244
1.628
1.610
1.272
1.261
1.245
1.242
1.233
1.218
1.200
0.860
0.843
0.826
(4i)
N
NH2
O=S=O
0.82
2.07
2.30
0.88
3.00
2.11
2.18
4.23
3.08
9
8
7
6
5
4
3
2
1
0
Chemical Shift (ppm)

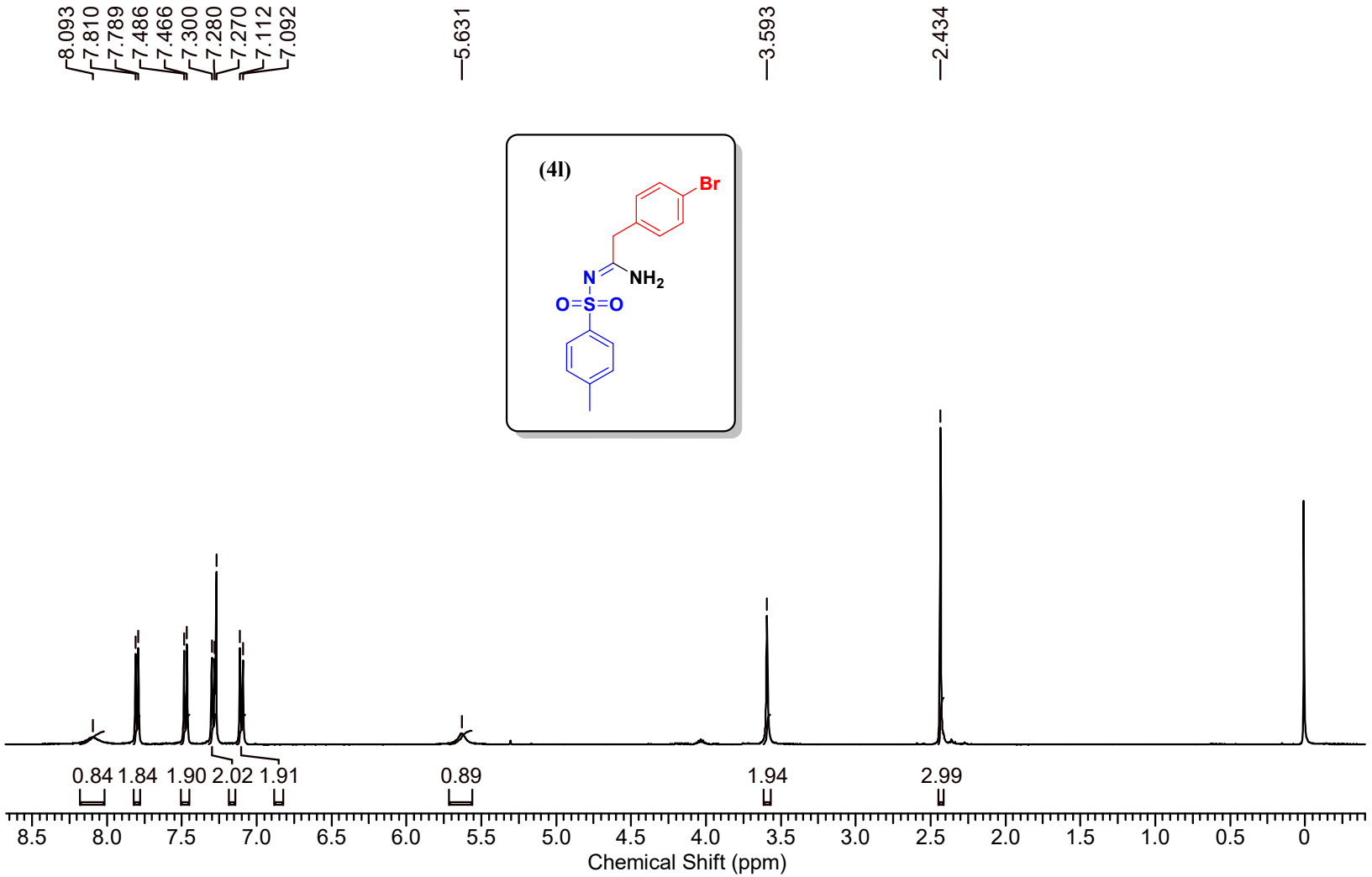

169.279
142.905
139.162
129.279
126.326
77.212
77.000
76.788
37.813
30.912
26.223
22.208
21.476
13.791
(4i)
N
NH2
O=S=O
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
Chemical Shift (ppm)

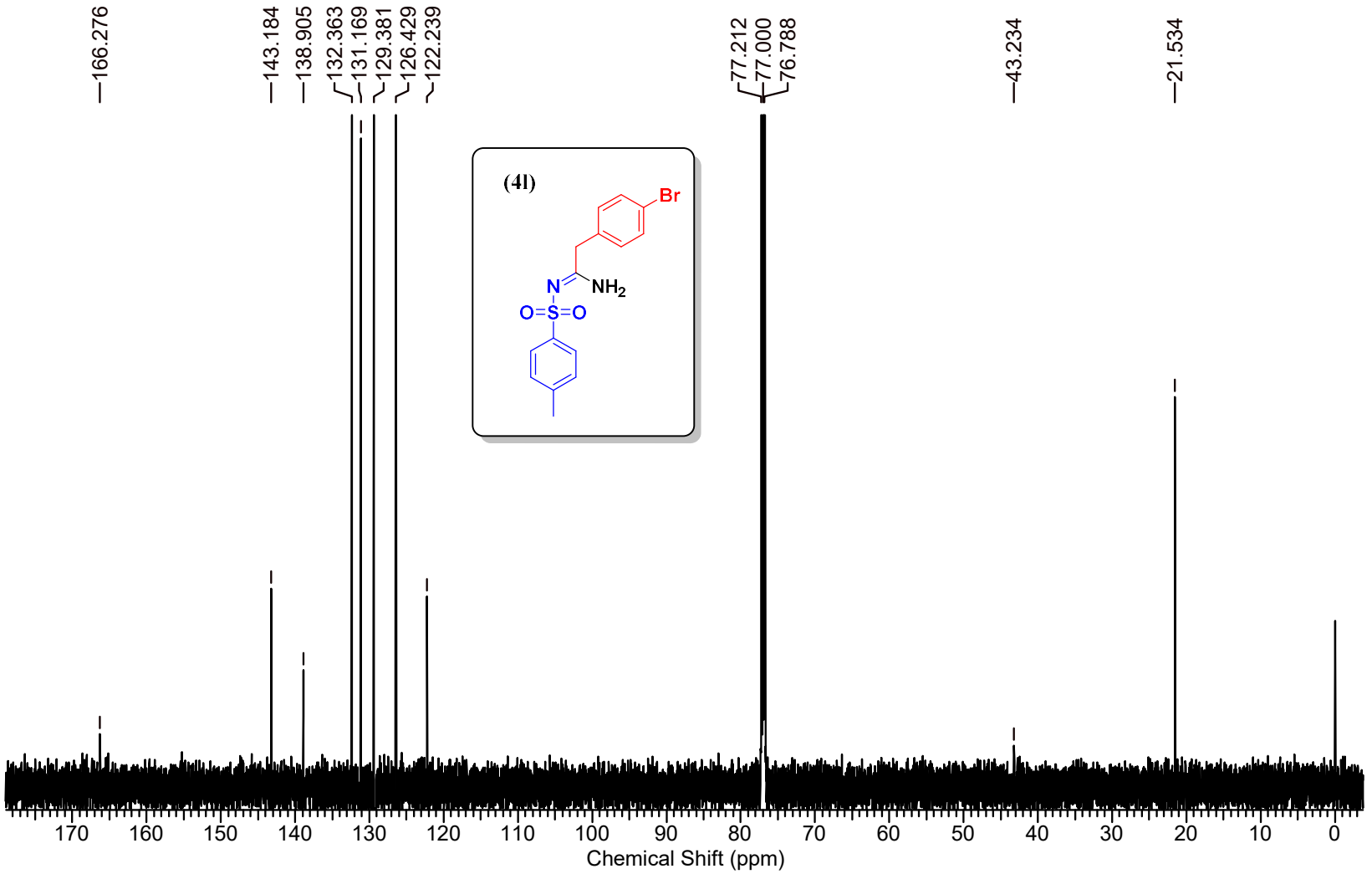

8.025
7.817
7.796
7.290
7.276
7.270
6.137
2.418
2.288
2.268
2.248
1.653
1.626
1.599
1.505
1.488
1.465
1.448
1.137
1.109
1.090
0.860
0.833
(4j)
N
NH2
O=S=O
0.91 2.06 2.12 0.91
3.00 2.05 1.10 4.07 2.07 3.99 2.00
9 8 7 6 5 4 3 2 1 0
Chemical Shift (ppm)

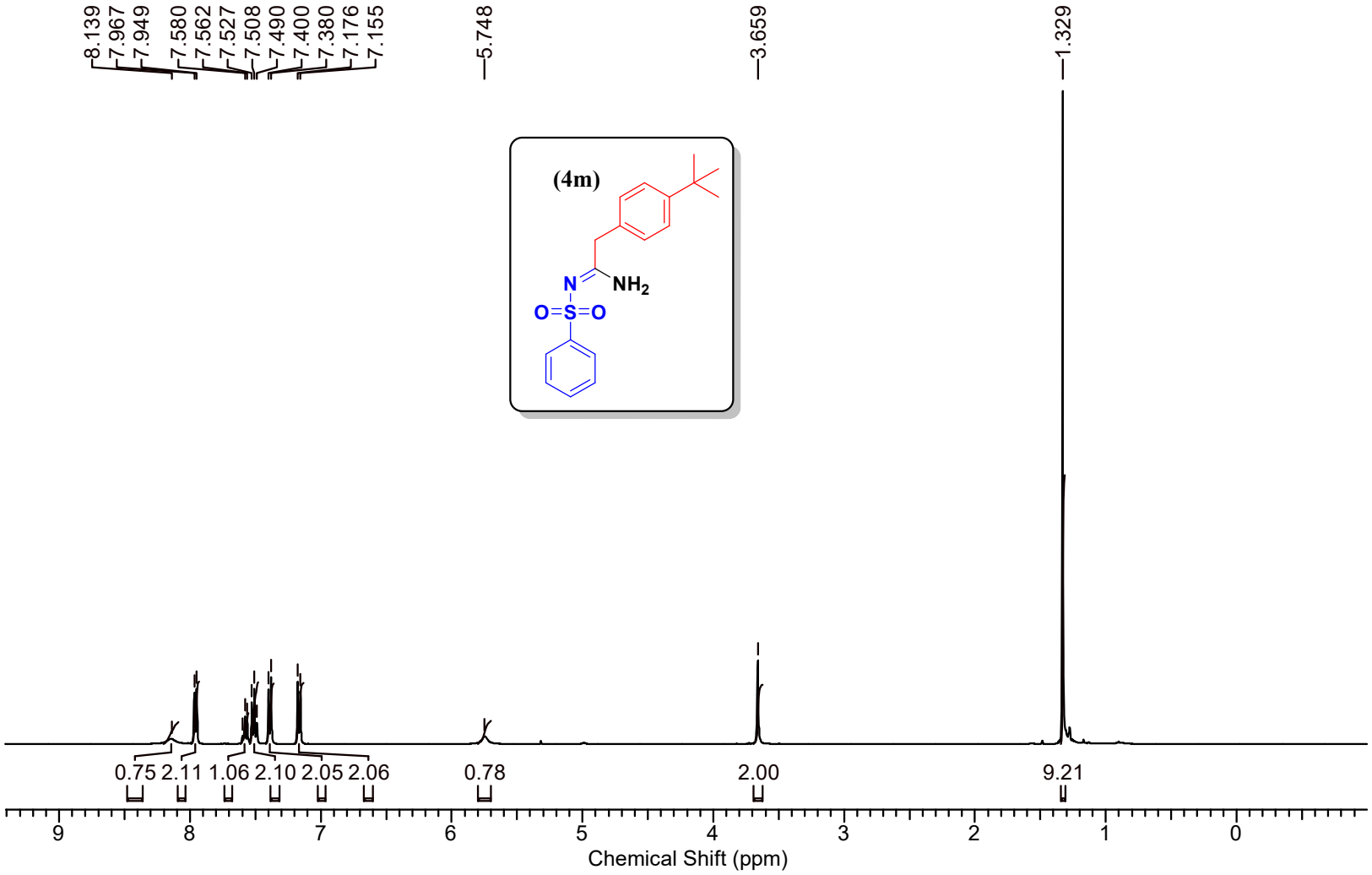

169.755
142.883
139.169
129.279
126.304
77.212
77.000
76.788
36.970
35.388
33.886
32.853
26.355
26.069
21.468
(4j)
N
NH2
O=S=O
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
Chemical Shift (ppm)

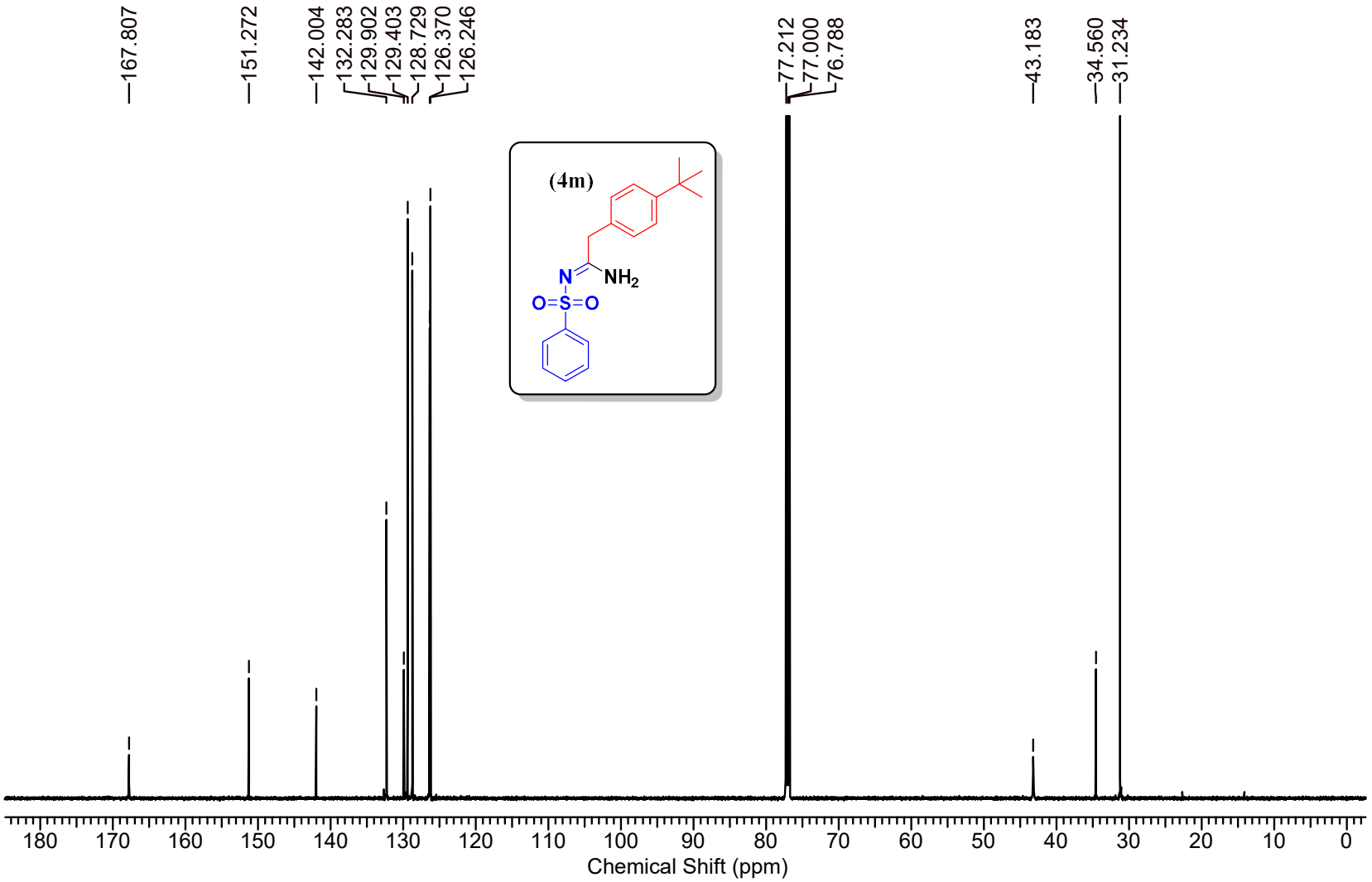

8.069
7.788
7.767
7.308
7.287
7.263
7.157
7.136
5.754
3.590
2.421
(4k)
Cl
N
NH2
O=S=O
0.91
1.85
4.14
1.87
0.80
1.79
2.96
9
8
7
6
5
4
3
2
1
0
Chemical Shift (ppm)

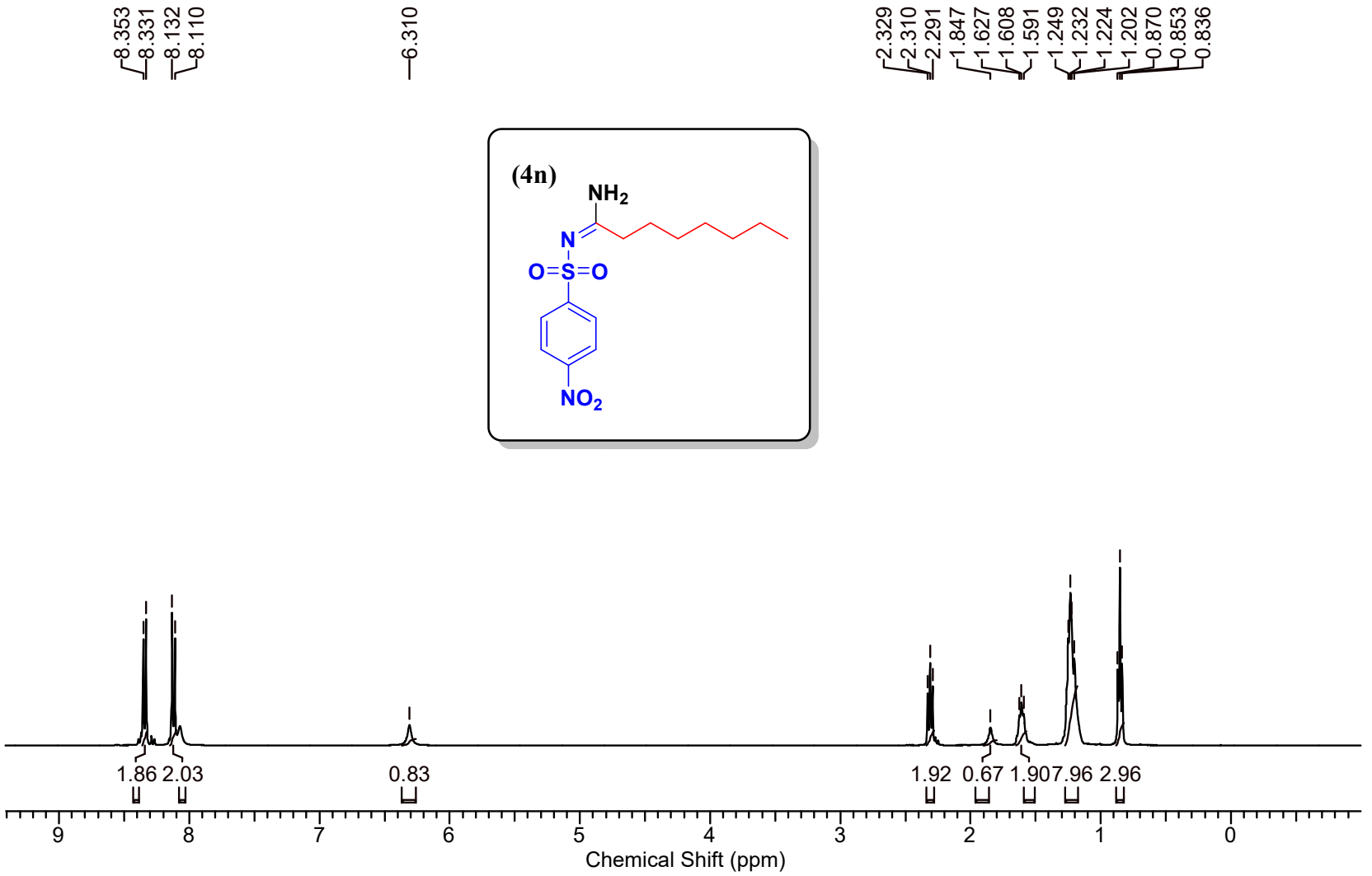

166.561
143.169
138.883
134.063
131.894
130.803
129.367
129.315
126.370
77.212
77.000
76.788
43.088
21.512
(4k)
Cl
N
NH2
O=S=O
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
Chemical Shift (ppm)

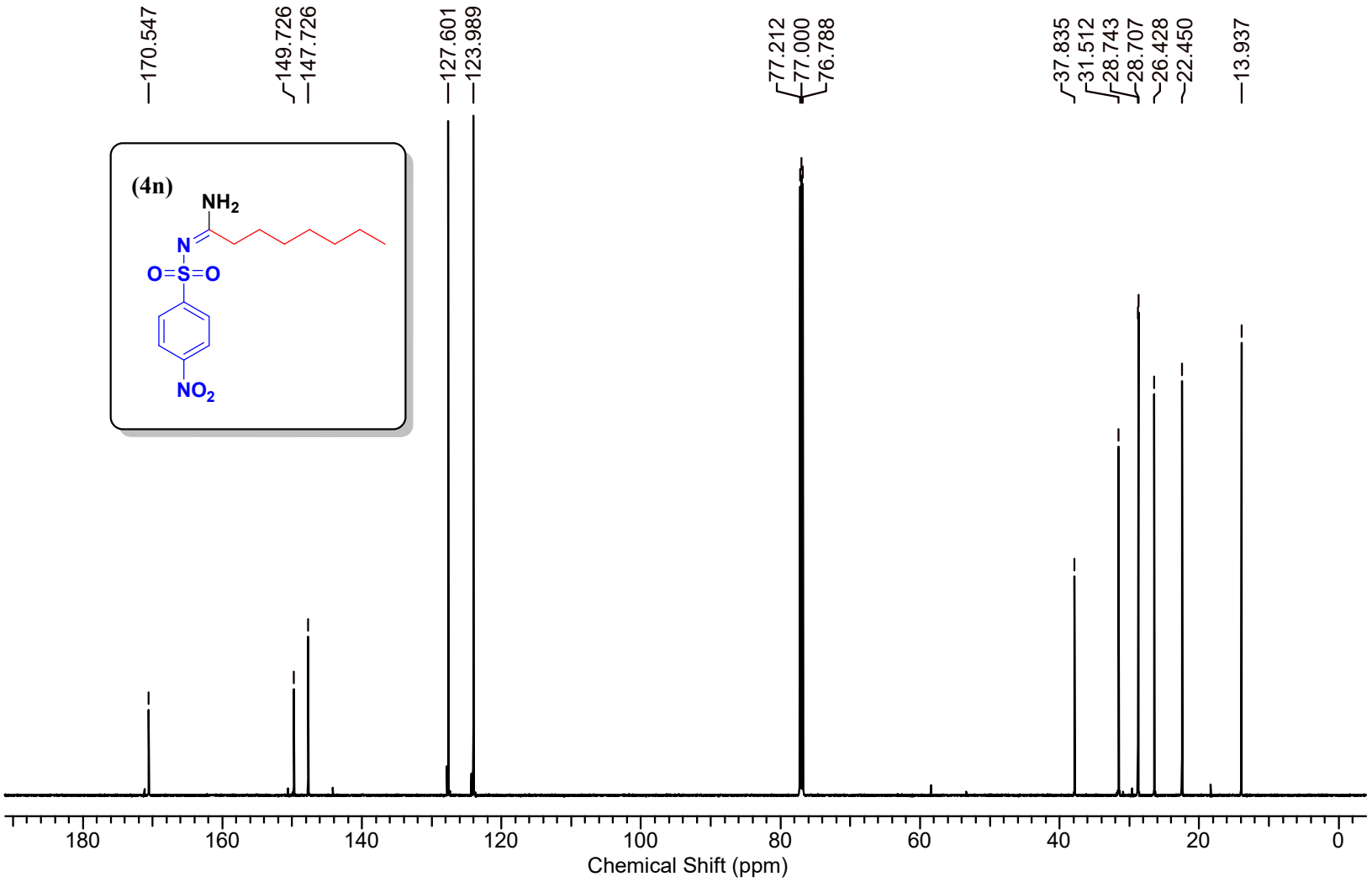

8.093
7.810
7.789
7.486
7.466
7.300
7.280
7.270
7.112
7.092
5.631
3.593
2.434
(4l)
Br
N
NH2
O=S=O
0.84 1.84 1.90 2.02 1.91
0.89
1.94
2.99
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0
Chemical Shift (ppm)

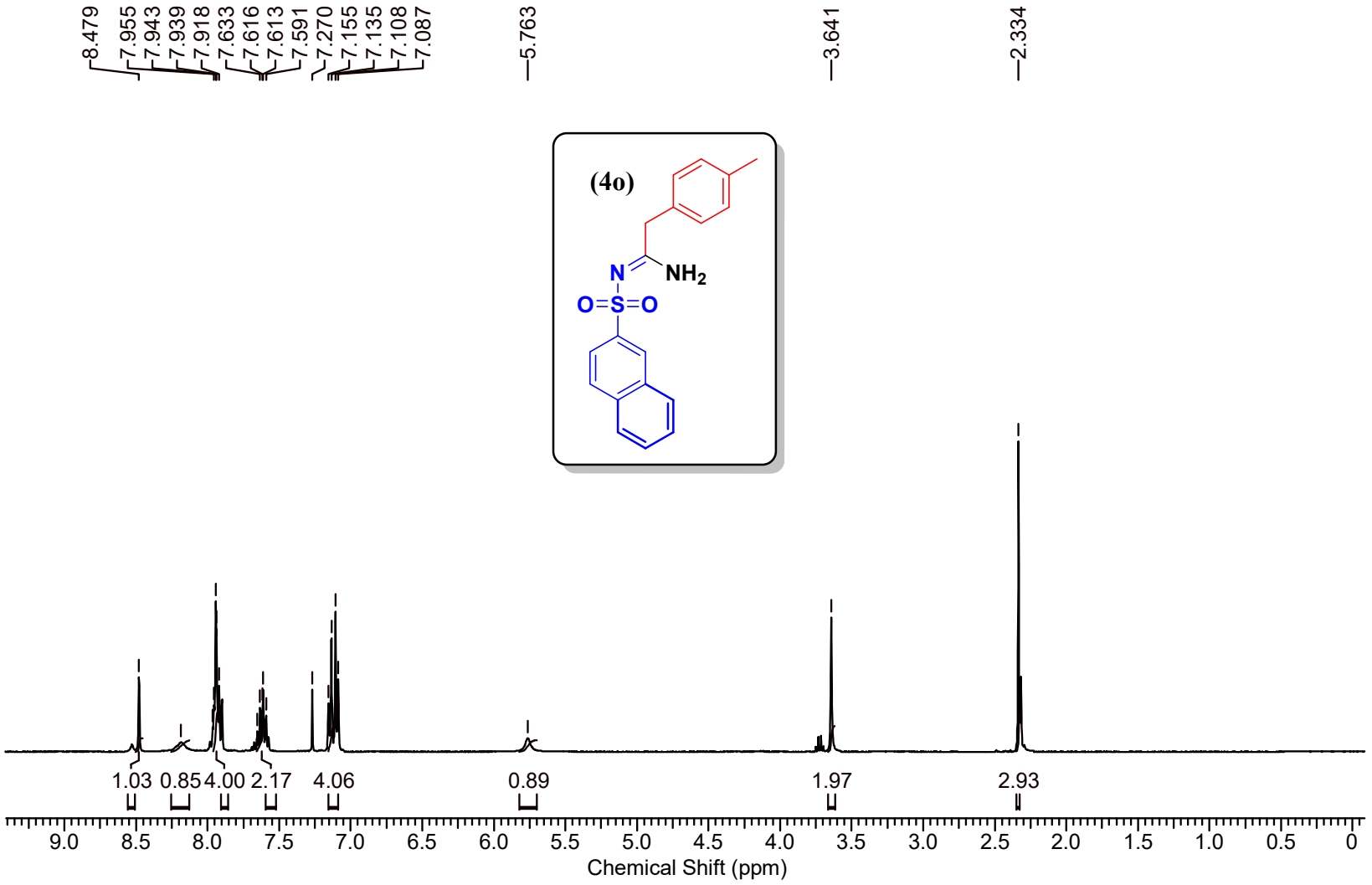

166.276
143.184
138.905
132.363
131.169
129.381
126.429
122.239
77.212
77.000
76.788
43.234
21.534
(4l)
Br
N
NH2
O=S=O
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
Chemical Shift (ppm)

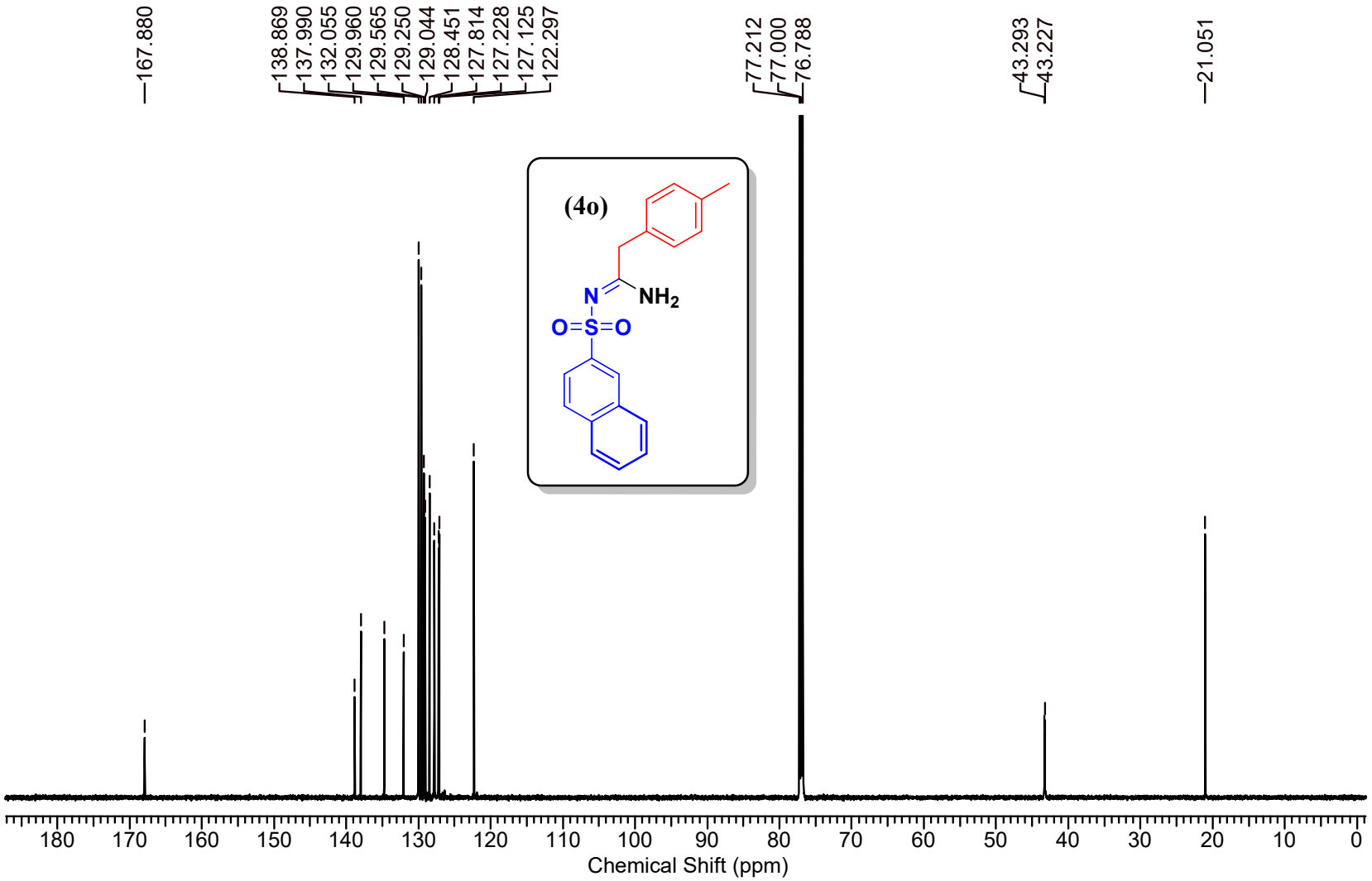

8.139
7.967
7.949
7.580
7.562
7.527
7.508
7.490
7.400
7.380
7.176
7.155
5.748
3.659
1.329
(4m)
N
NH2
O=S=O
0.75 2.11 1.06 2.10 2.05 2.06
0.78
2.00
9.21
9
8
7
6
5
4
3
2
1
0
Chemical Shift (ppm)

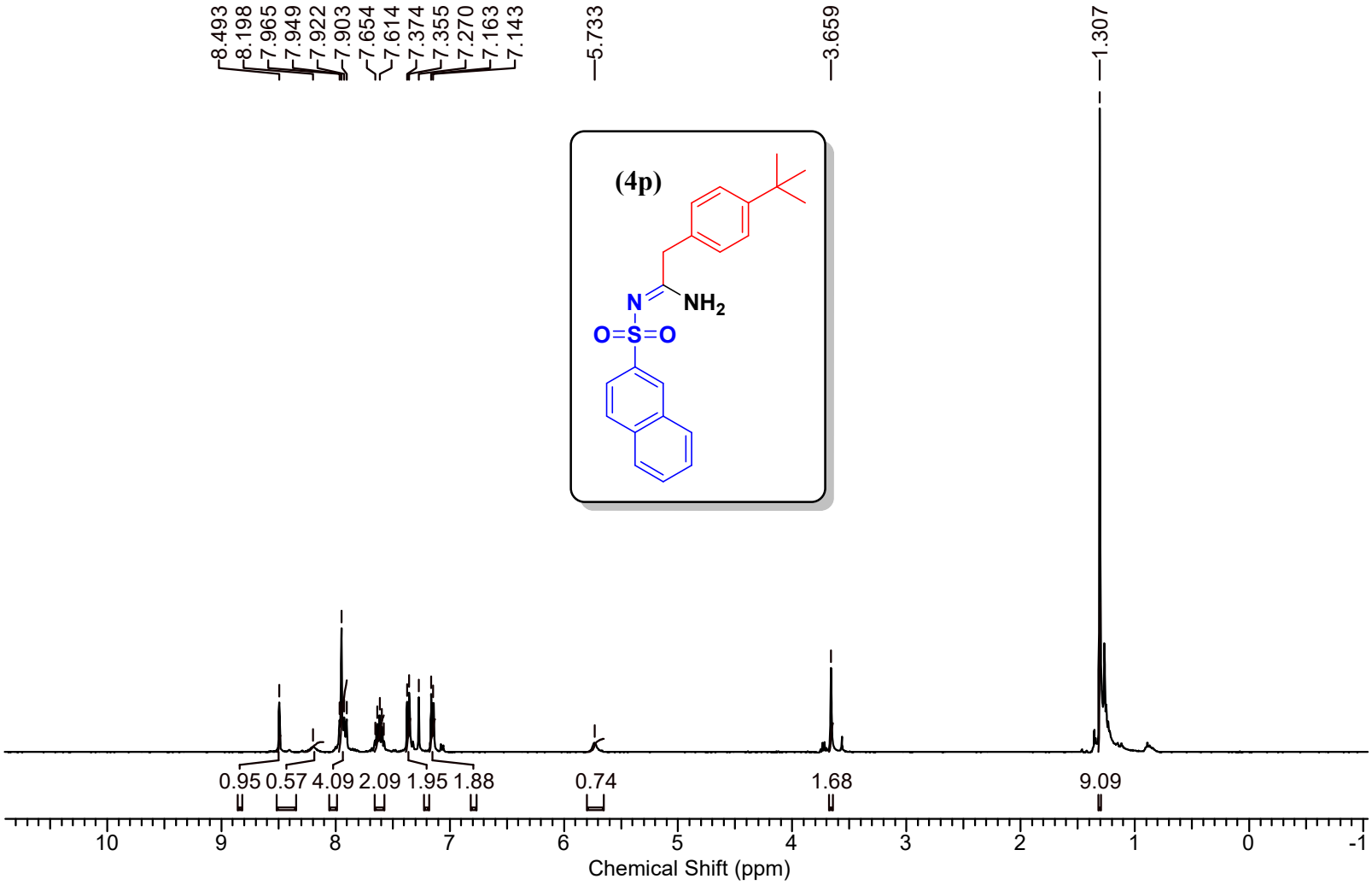

167.807
151.272
142.004
132.283
129.902
129.403
128.729
126.370
126.246
77.212
77.000
76.788
43.183
34.560
31.234
(4m)
NH2
O=S=O
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
Chemical Shift (ppm)

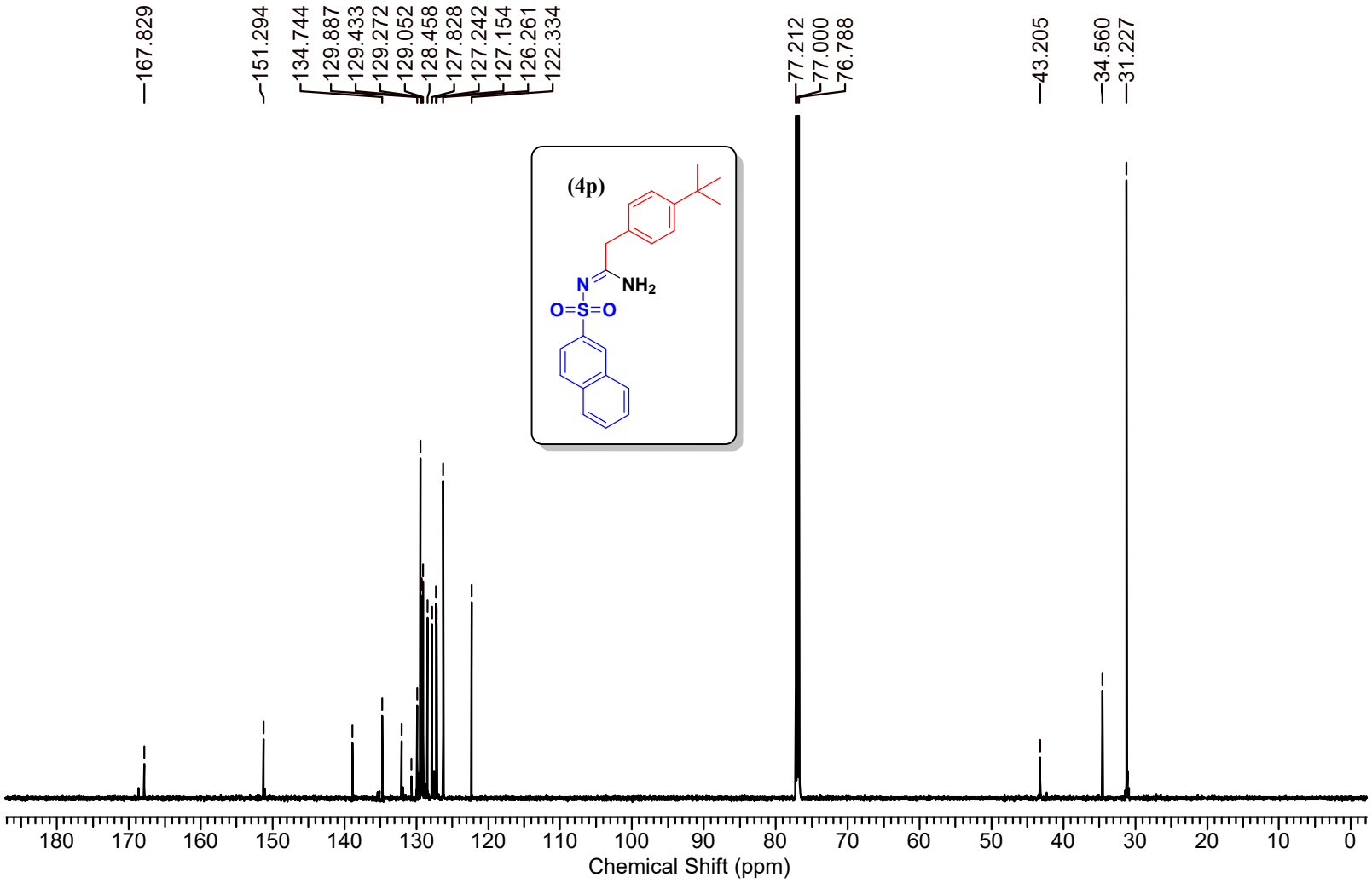

8.353
8.331
8.132
8.110
6.310
2.329
2.310
2.291
1.847
1.627
1.608
1.591
1.249
1.232
1.224
1.202
0.870
0.853
0.836
(4n)
NH2
N
O=S=O
NO2
1.86
2.03
0.83
1.92
0.67
1.90
7.96
2.96
9
8
7
6
5
4
3
2
1
0
Chemical Shift (ppm)

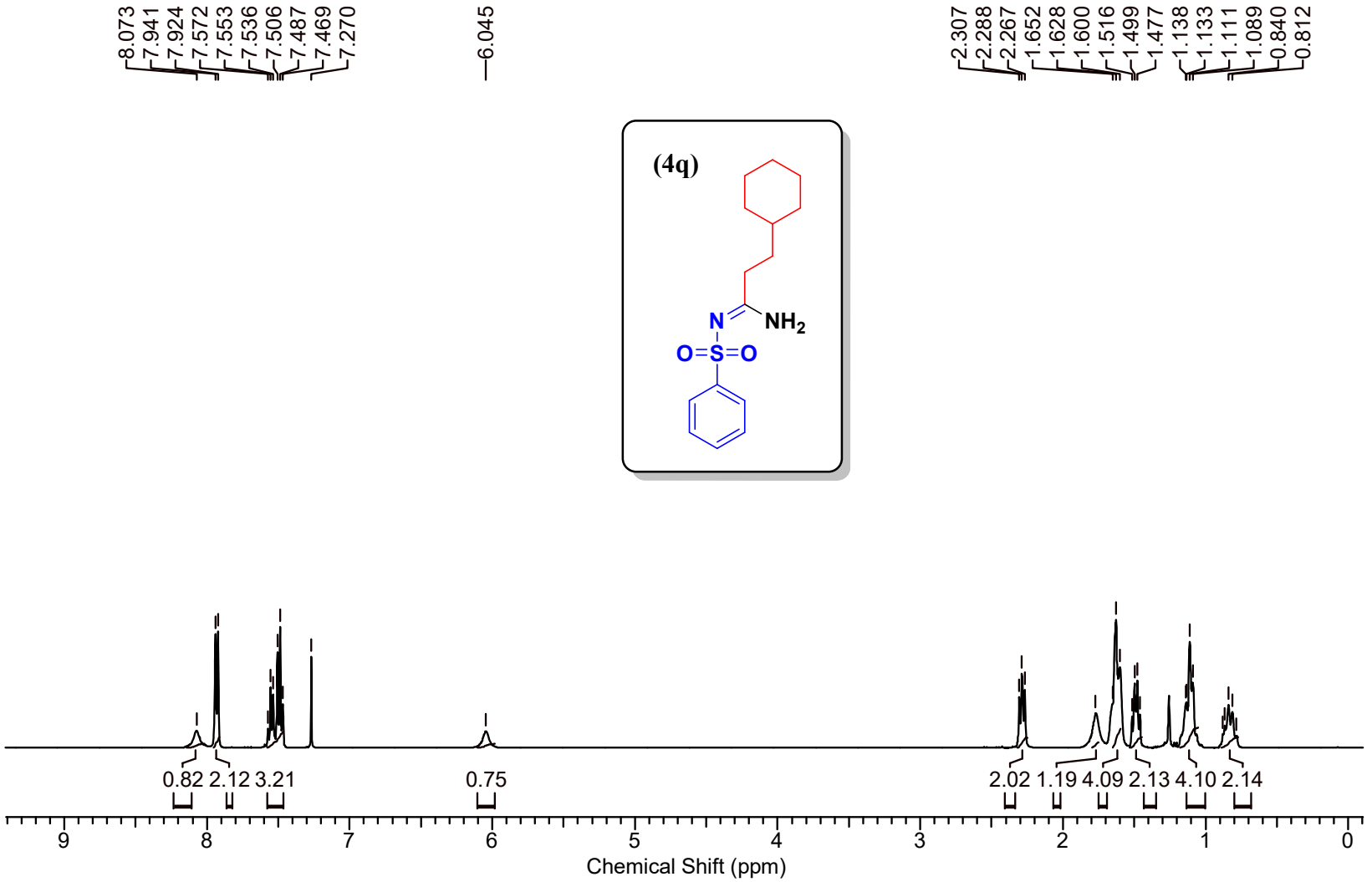

170.547
149.726
147.726
127.601
123.989
77.212
77.000
76.788
37.835
31.512
28.743
28.707
26.428
22.450
13.937
(4n)
NH2
N
O=S=O
NO2
180
160
140
120
100
80
60
40
20
0
Chemical Shift (ppm)

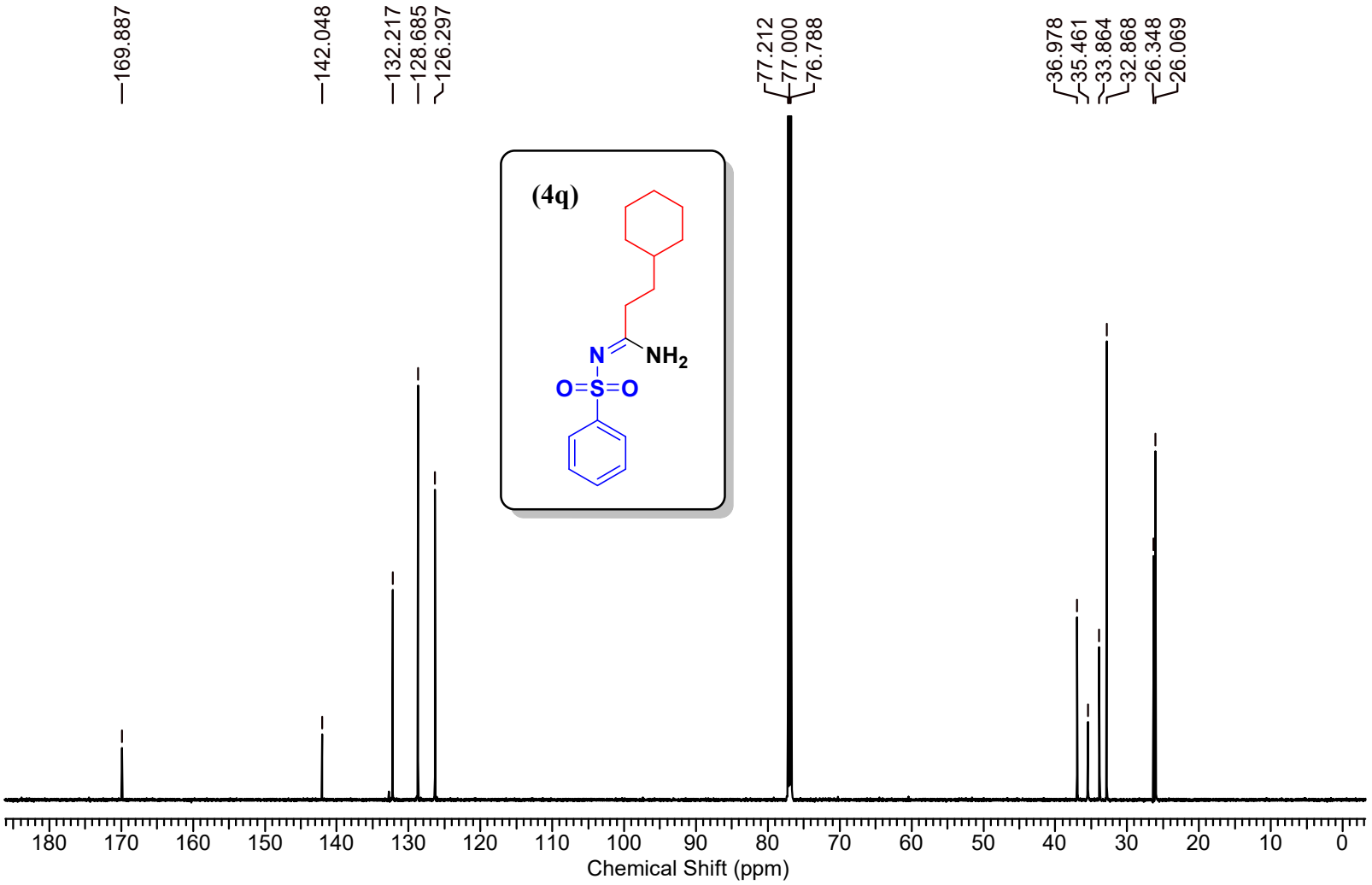

8.479
7.955
7.943
7.939
7.918
7.633
7.616
7.613
7.591
7.270
7.155
7.135
7.108
7.087
5.763
3.641
2.334
(4o)
N
NH2
O=S=O
1.03
0.85
4.00
2.17
4.06
0.89
1.97
2.93
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0
Chemical Shift (ppm)

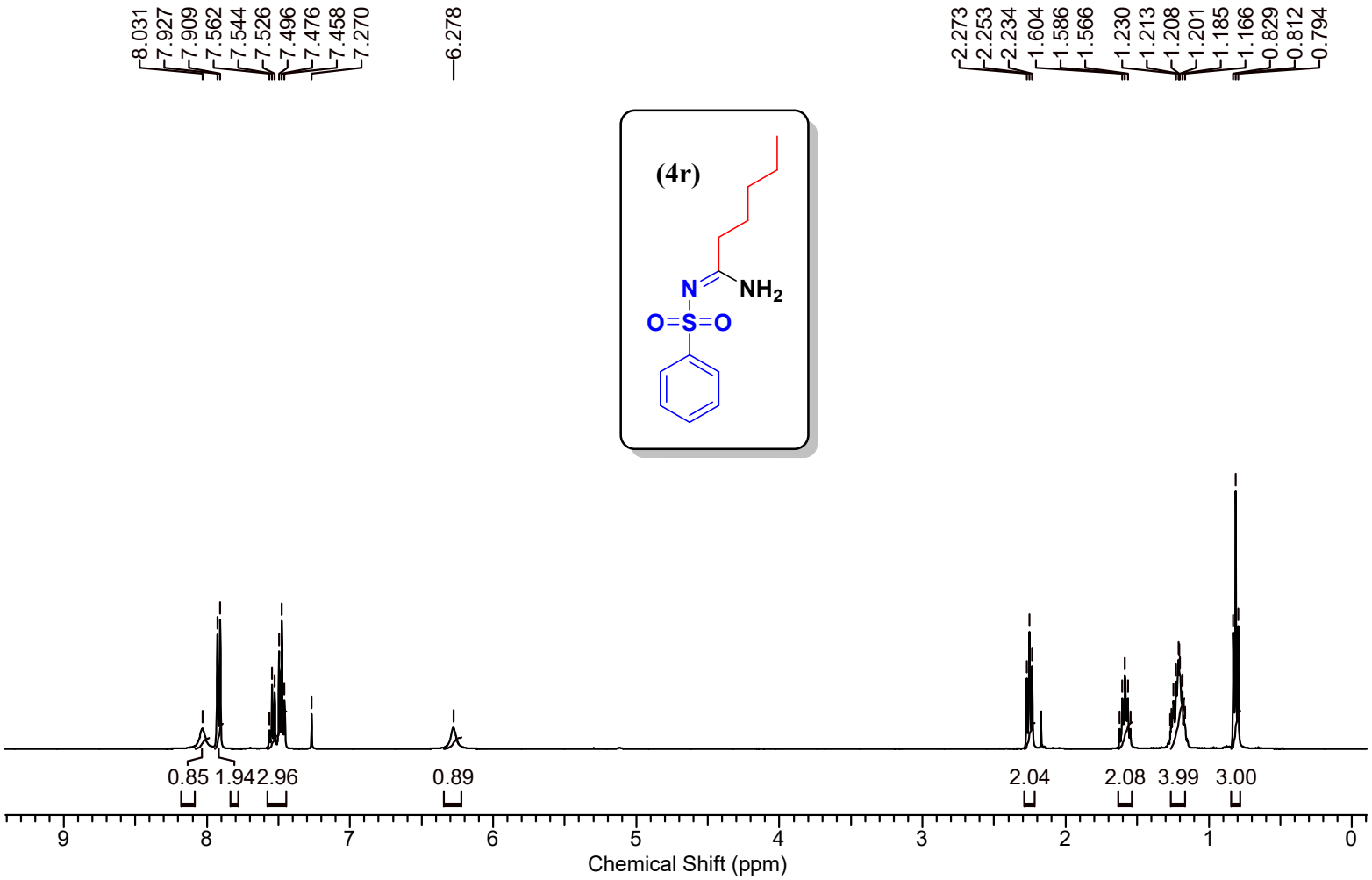

167.880
138.869
137.990
132.055
129.960
129.565
129.250
129.044
128.451
127.814
127.228
127.125
122.297
77.212
77.000
76.788
43.293
43.227
21.051
(4o)
N
NH2
O=S=O
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
Chemical Shift (ppm)

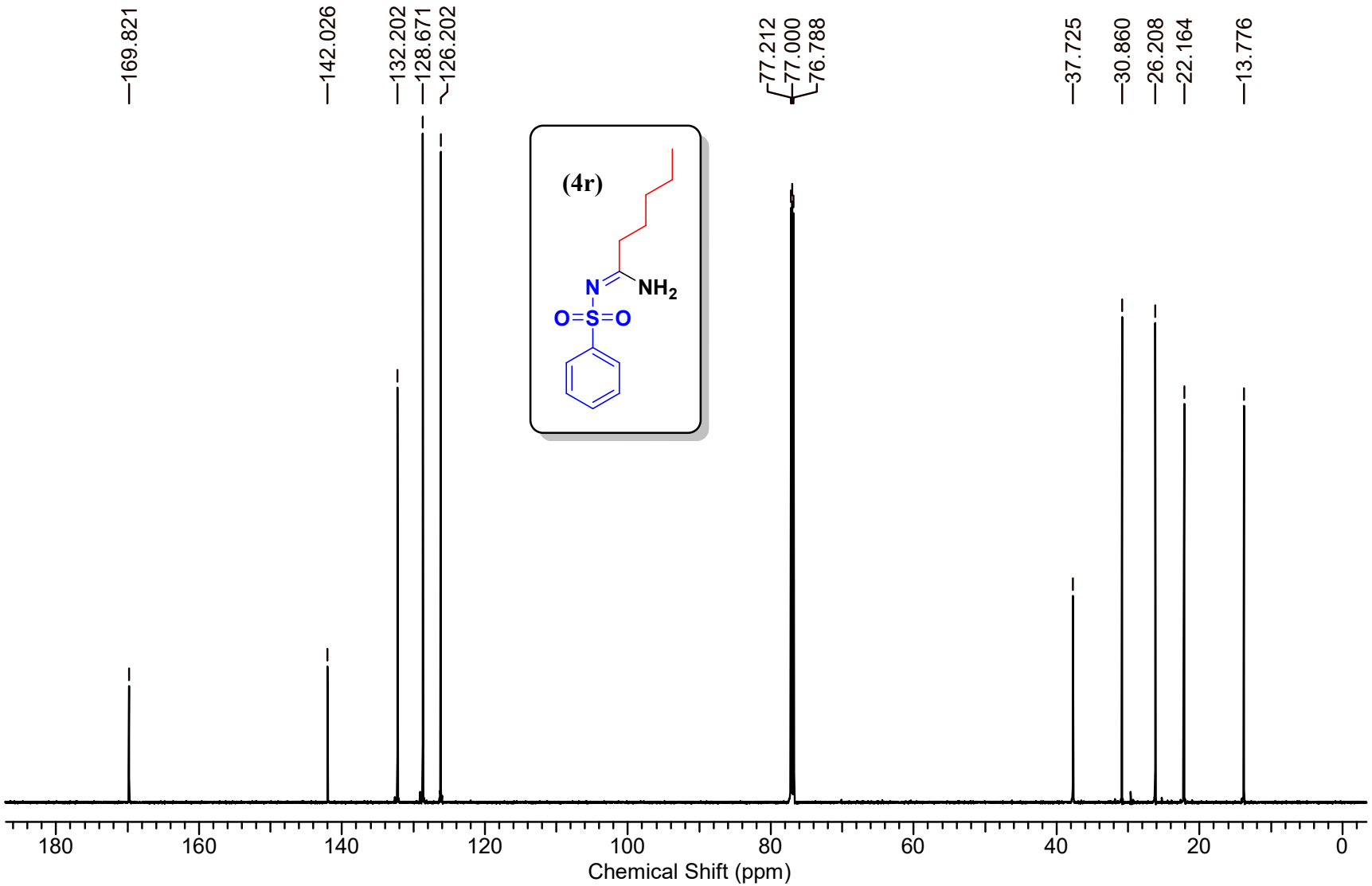

8.493
8.198
7.965
7.949
7.922
7.903
7.654
7.614
7.374
7.355
7.270
7.163
7.143
5.733
3.659
1.307
(4p)
N
NH2
O=S=O
0.95 0.57 4.09 2.09 1.95 1.88
0.74
1.68
9.09
10 9 8 7 6 5 4 3 2 1 0 -1
Chemical Shift (ppm)

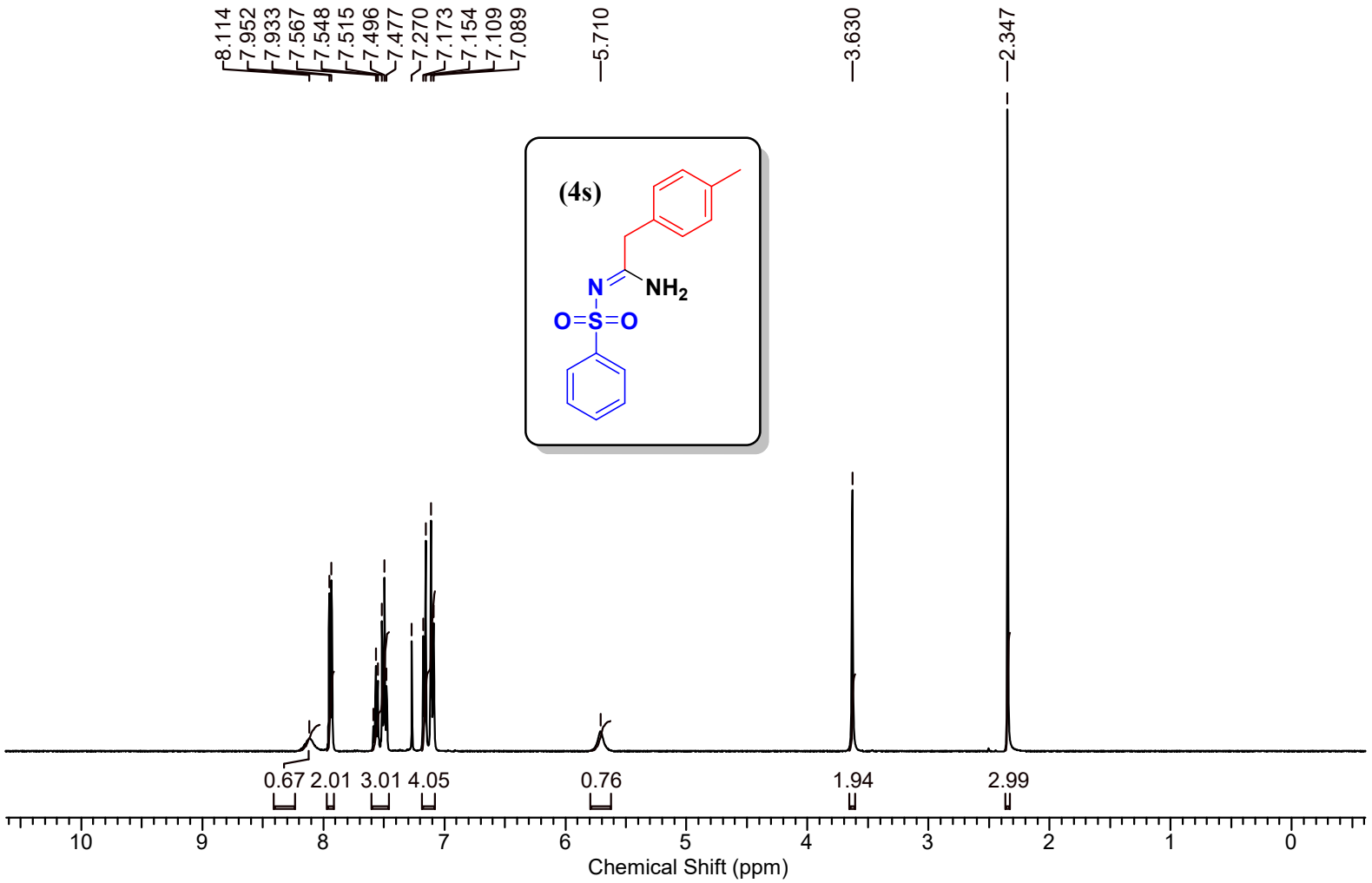

167.829
151.294
134.744
129.887
129.433
129.272
129.052
128.458
127.828
127.242
127.154
126.261
122.334
77.212
77.000
76.788
43.205
34.560
31.227
(4p)
N
NH2
O=S=O
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
Chemical Shift (ppm)

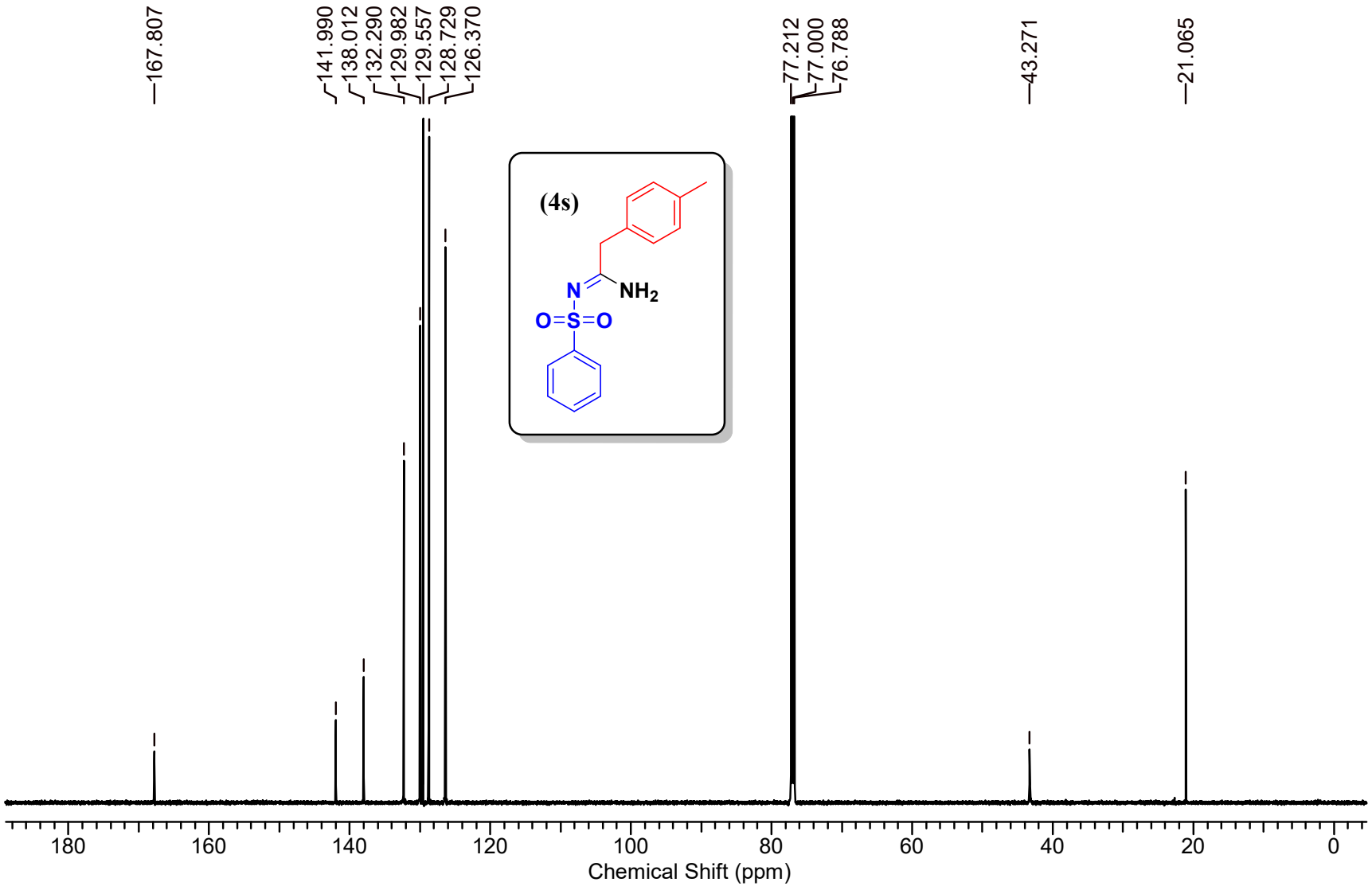

8.073
7.941
7.924
7.572
7.553
7.536
7.506
7.487
7.469
7.270
6.045
2.307
2.288
2.267
1.652
1.628
1.600
1.516
1.499
1.477
1.138
1.133
1.111
1.089
0.840
0.812
(4q)
N
NH2
O=S=O
0.82 2.12 3.21
0.75
2.02 1.19 4.09 2.13 4.10 2.14
9
8
7
6
5
4
3
2
1
0
Chemical Shift (ppm)

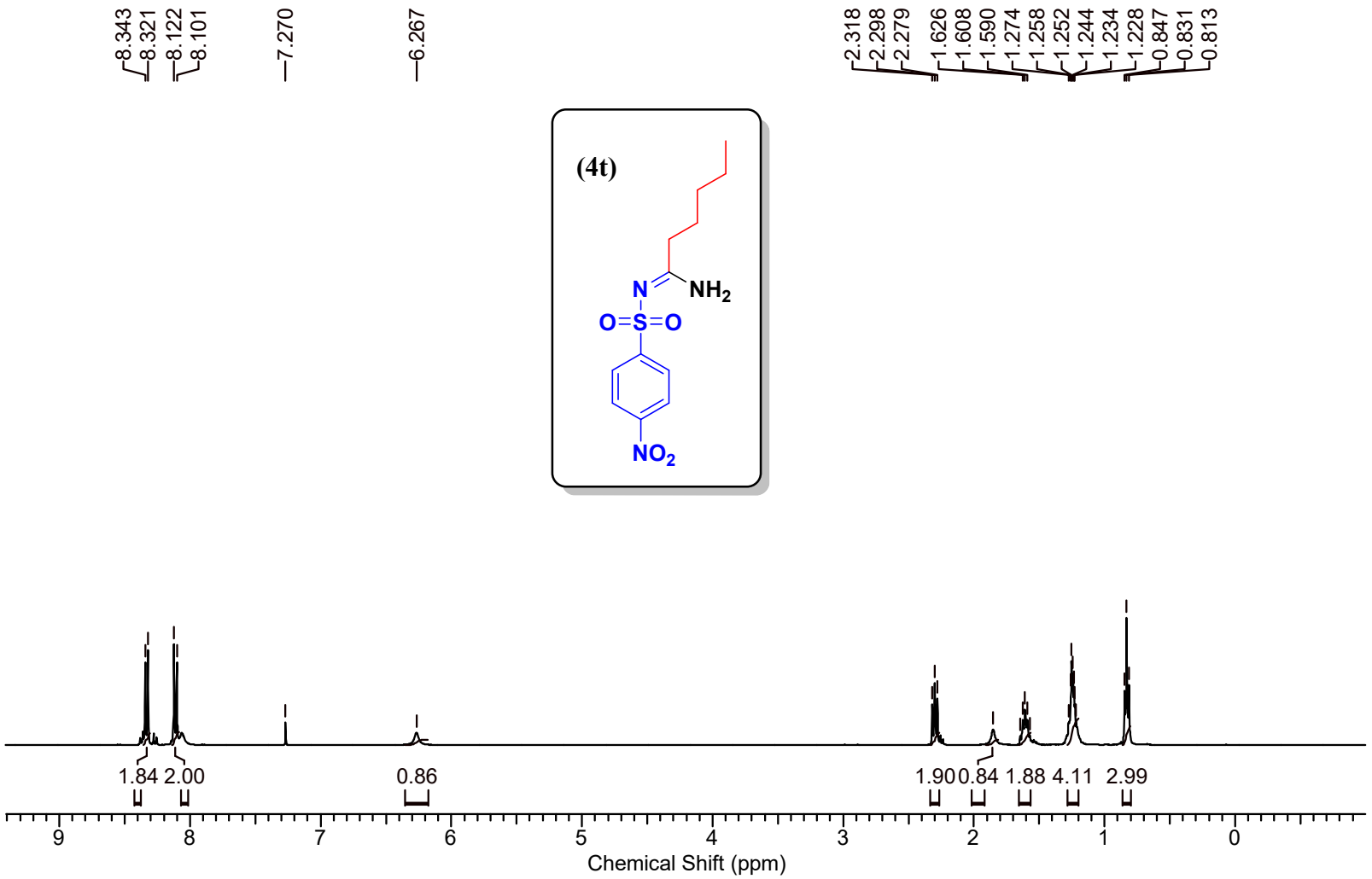

169.887
142.048
132.217
128.685
126.297
77.212
77.000
76.788
36.978
35.461
33.864
32.868
26.348
26.069
(4q)
N
NH2
O=S=O
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
Chemical Shift (ppm)

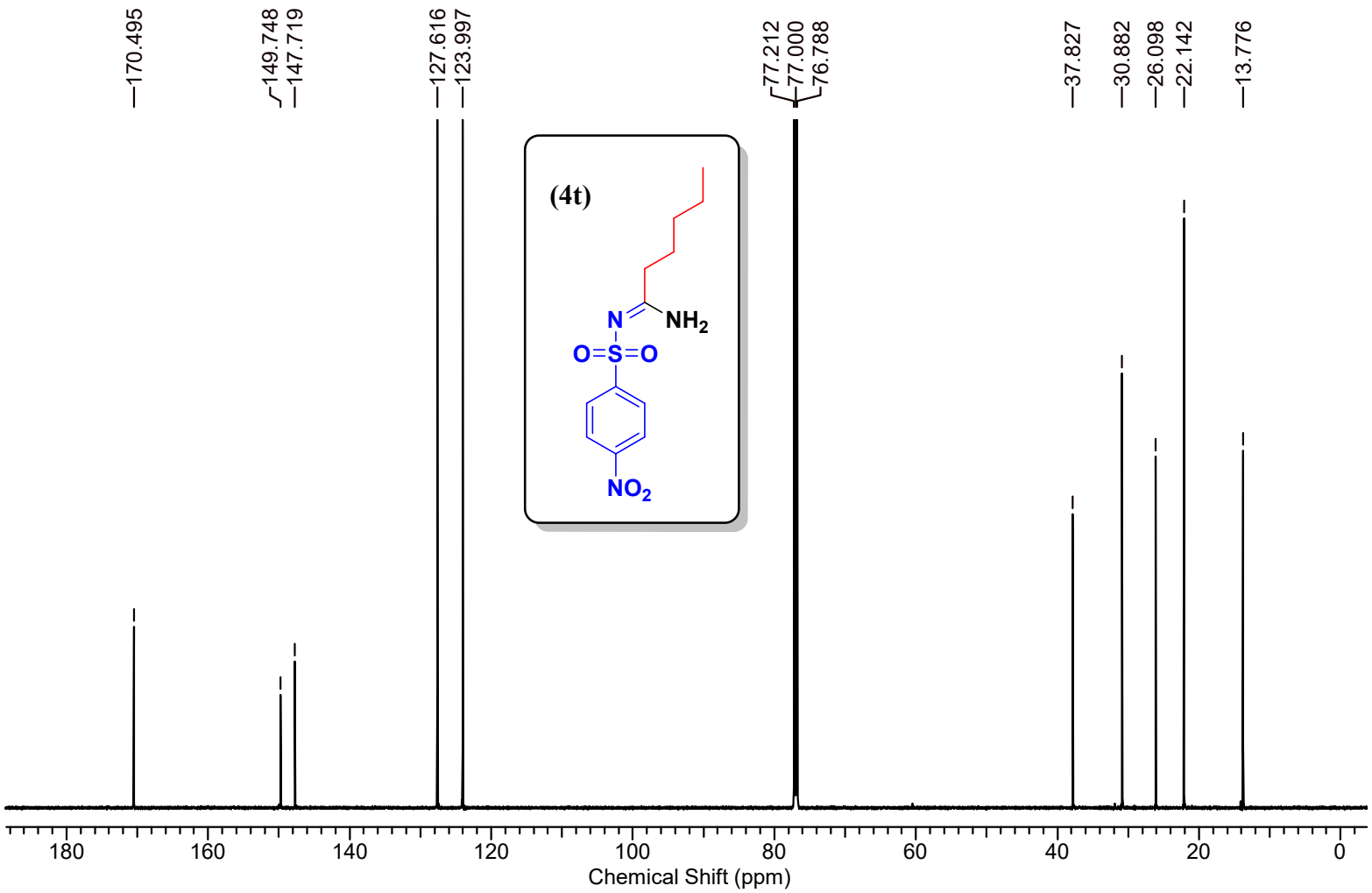

8.031
7.927
7.909
7.562
7.544
7.526
7.496
7.476
7.458
7.270
6.278
2.273
2.253
2.234
1.604
1.586
1.566
1.230
1.213
1.208
1.201
1.185
1.166
0.829
0.812
0.794
(4r)
N
NH2
O=S=O
0.85
1.94
2.96
0.89
2.04
2.08
3.99
3.00
9
8
7
6
5
4
3
2
1
0
Chemical Shift (ppm)

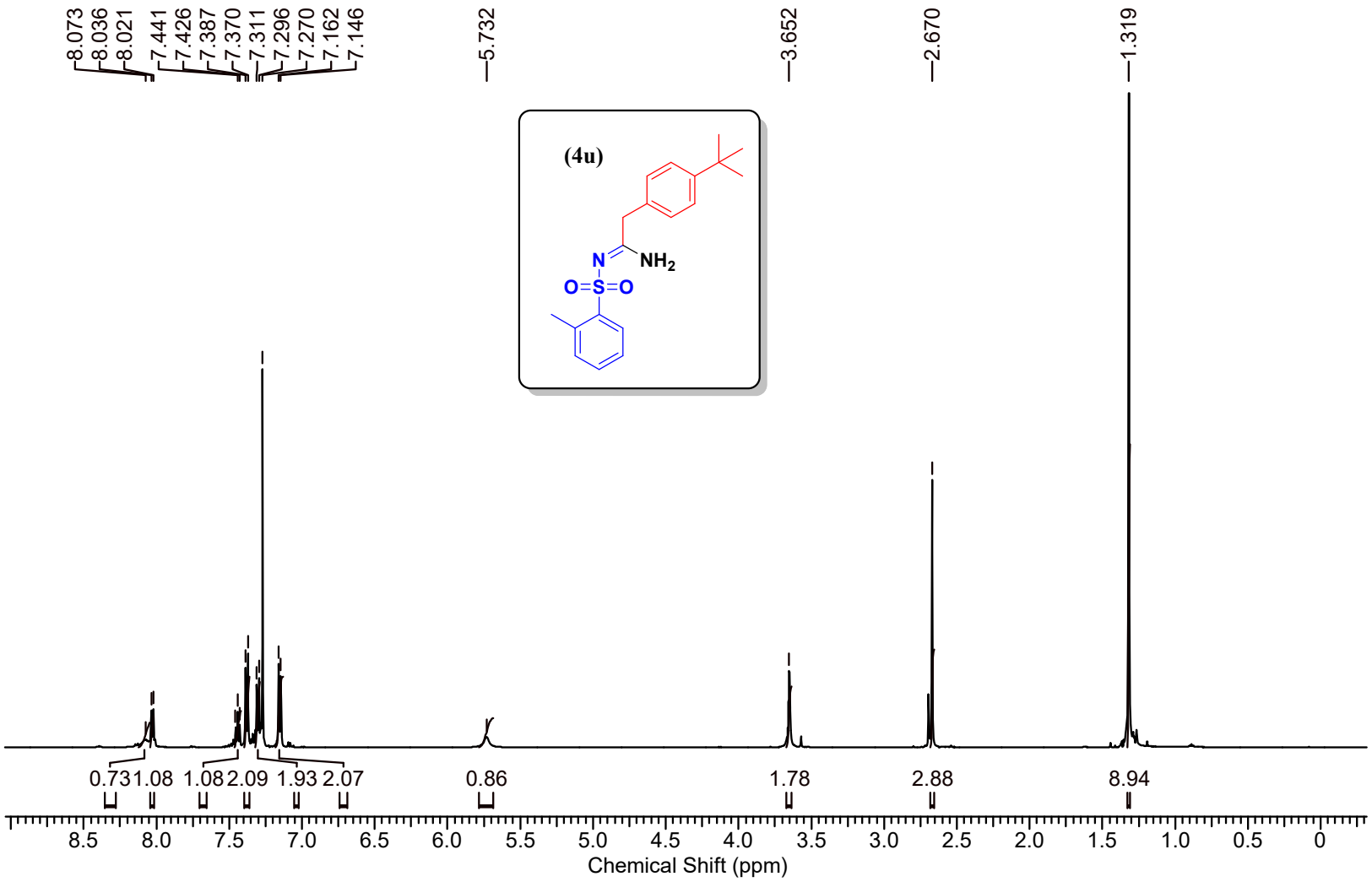

169.821
142.026
132.202
128.671
126.202
77.212
77.000
76.788
37.725
30.860
26.208
22.164
13.776
(4r)
N
NH2
O=S=O
180
160
140
120
100
80
60
40
20
0
Chemical Shift (ppm)

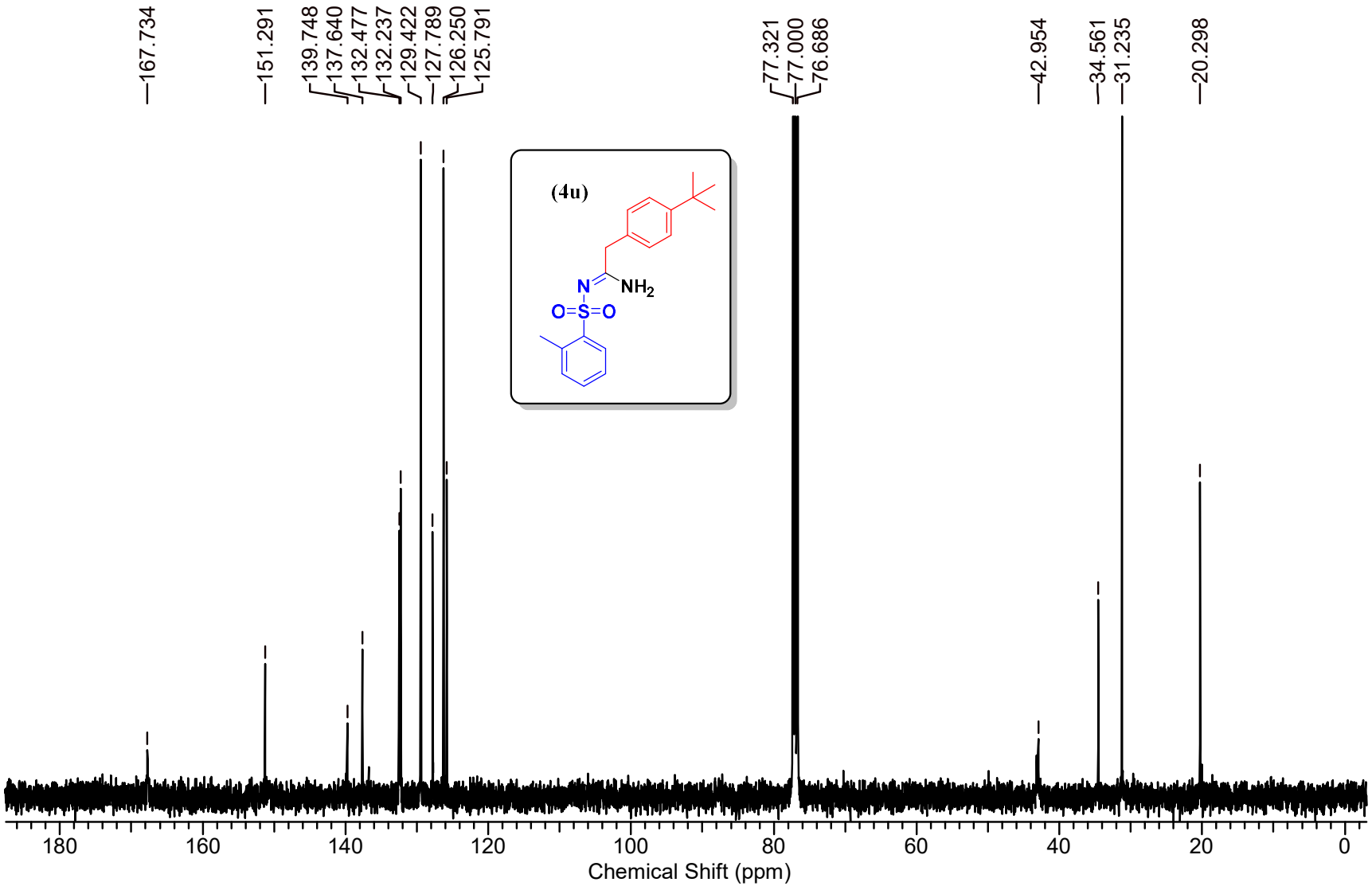

8.114
7.952
7.933
7.567
7.548
7.515
7.496
7.477
7.270
7.173
7.154
7.109
7.089
5.710
3.630
2.347
(4s)
N
NH2
O=S=O
0.67
2.01
3.01
4.05
0.76
1.94
2.99
10
9
8
7
6
5
4
3
2
1
0
Chemical Shift (ppm)

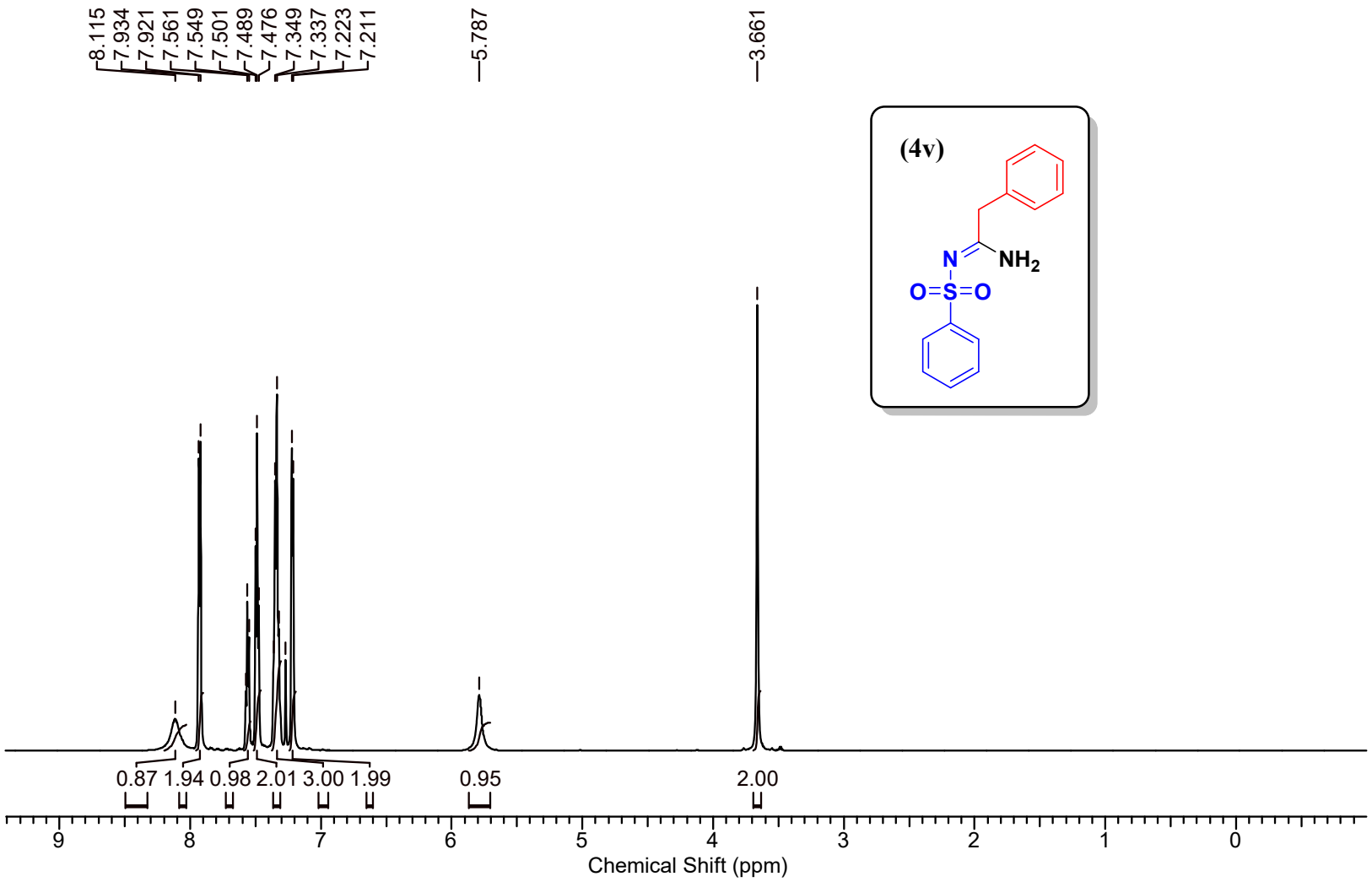

167.807
141.990
138.012
132.290
129.982
129.557
128.729
126.370
77.212
77.000
76.788
43.271
21.065
(4s)
N
NH2
O=S=O
180
160
140
120
100
80
60
40
20
0
Chemical Shift (ppm)

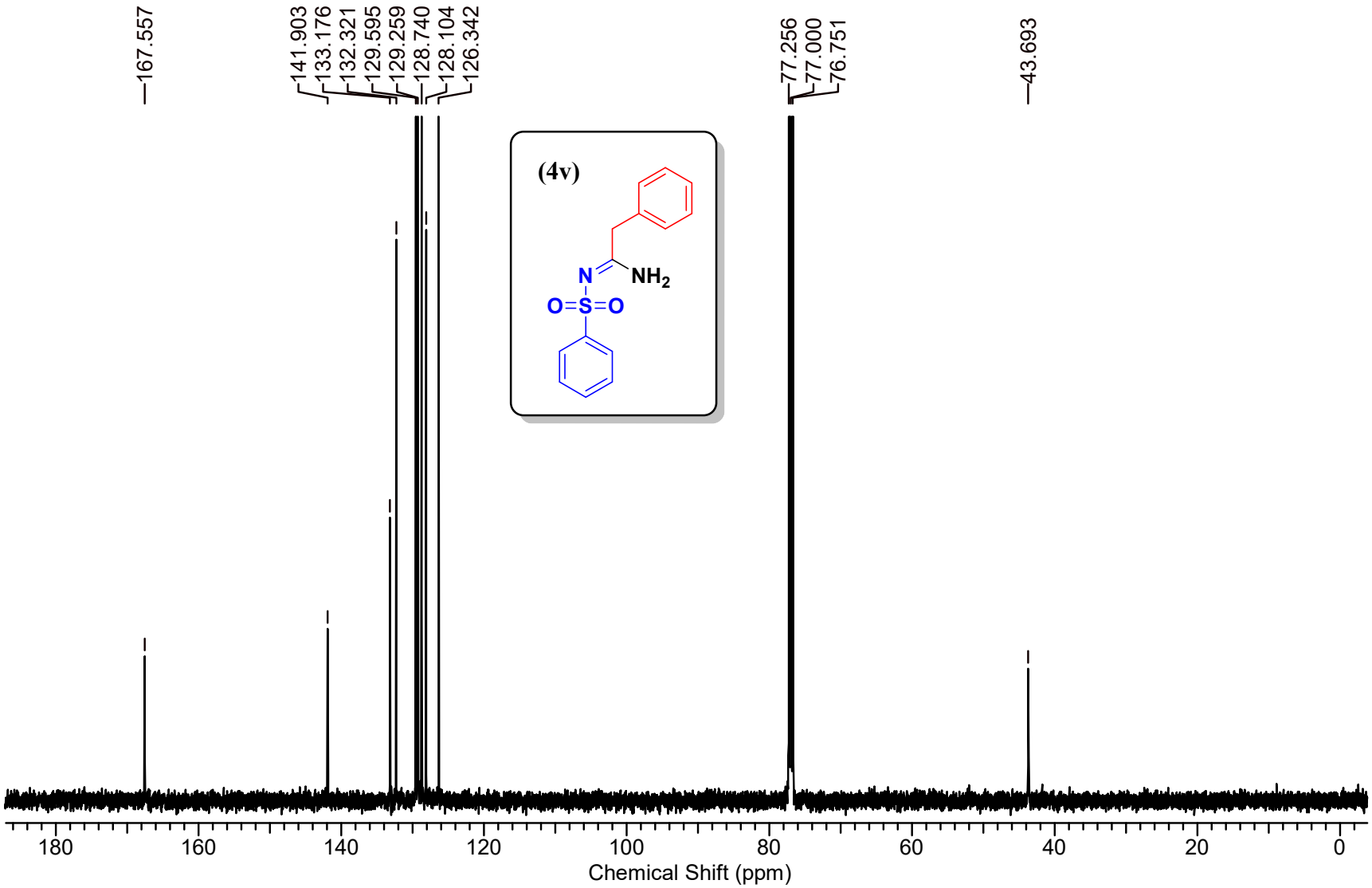

8.343
8.321
8.122
8.101
7.270
6.267
2.318
2.298
2.279
1.626
1.608
1.590
1.274
1.258
1.252
1.244
1.234
1.228
0.847
0.831
0.813
(4t)
N
NH2
O=S=O
NO2
1.84
2.00
0.86
1.90
0.84
1.88
4.11
2.99
9
8
7
6
5
4
3
2
1
0
Chemical Shift (ppm)

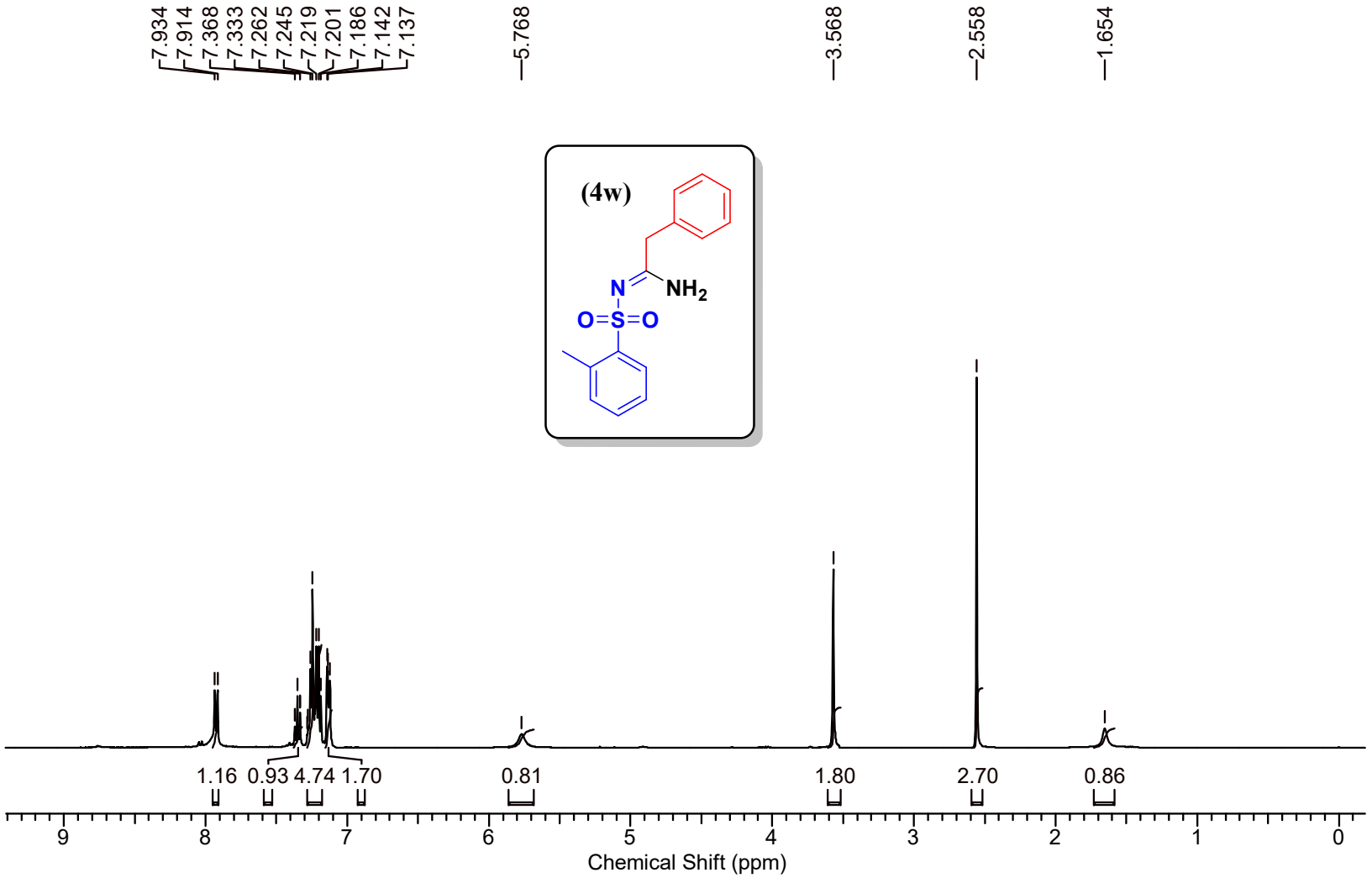

170.495
149.748
147.719
127.616
123.997
77.212
77.000
76.788
37.827
30.882
26.098
22.142
13.776
(4t)
N
NH2
O=S=O
NO2
180
160
140
120
100
80
60
40
20
0
Chemical Shift (ppm)

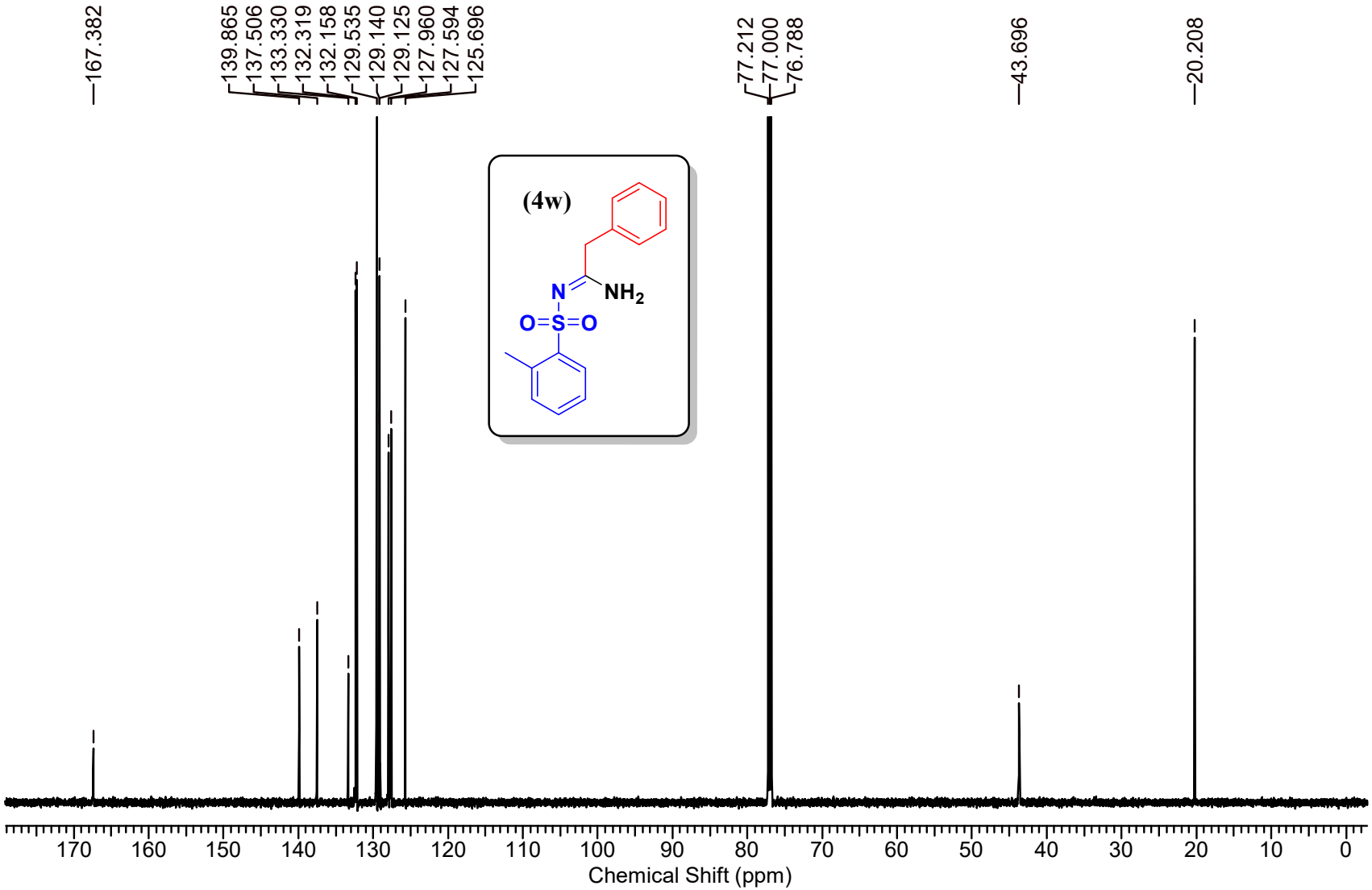

8.073
8.036
8.021
7.441
7.426
7.387
7.370
7.311
7.296
7.270
7.162
7.146
5.732
3.652
2.670
1.319
(4u)
N
NH2
O=S=O
0.73
1.08
1.08
2.09
1.93
2.07
0.86
1.78
2.88
8.94
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0
Chemical Shift (ppm)

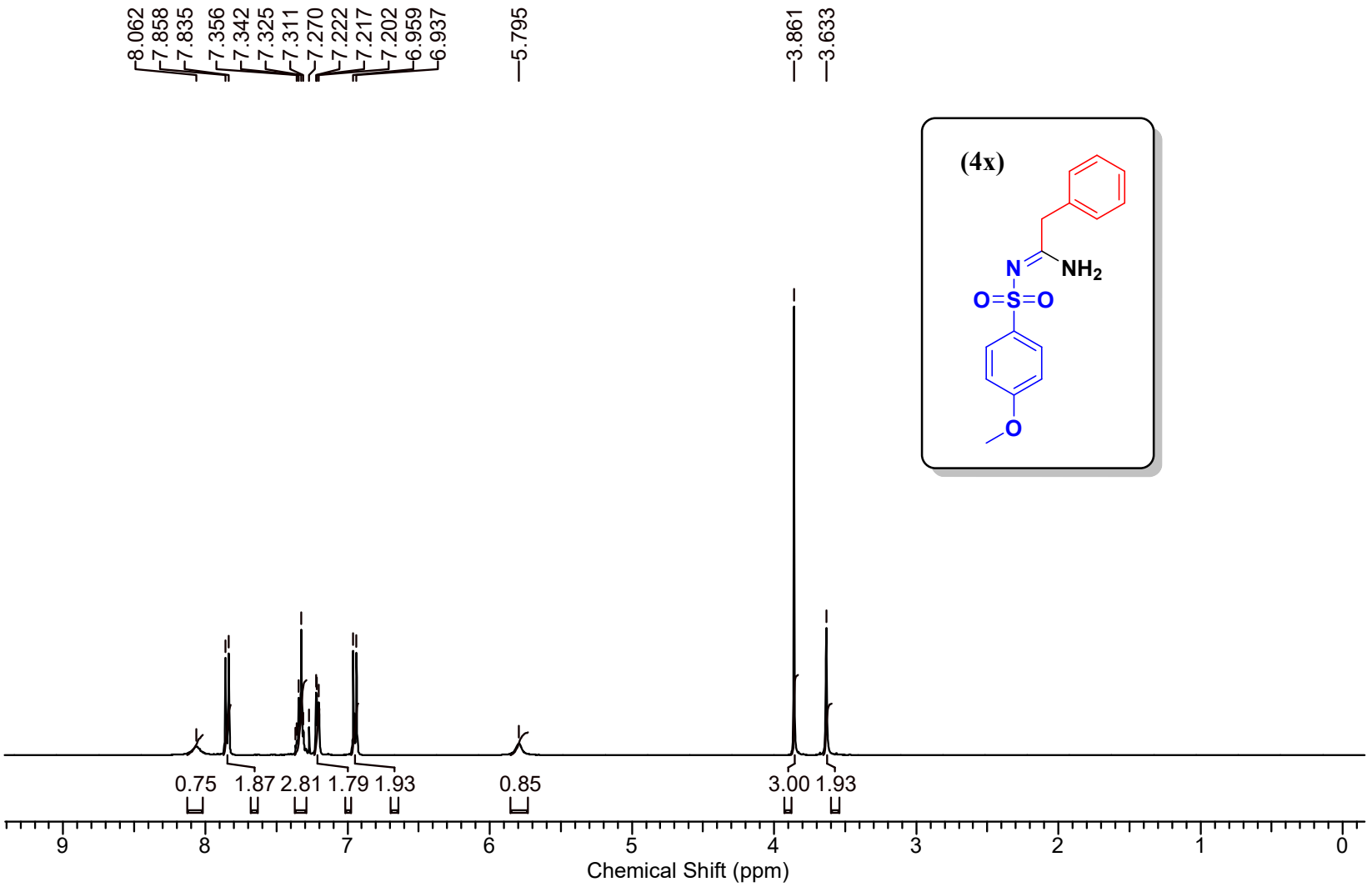

167.734
151.291
139.748
137.640
132.477
132.237
129.422
127.789
126.250
125.791
77.321
77.000
76.686
42.954
34.561
31.235
20.298
(4u)
N
NH2
O=S=O
180
160
140
120
100
80
60
40
20
0
Chemical Shift (ppm)

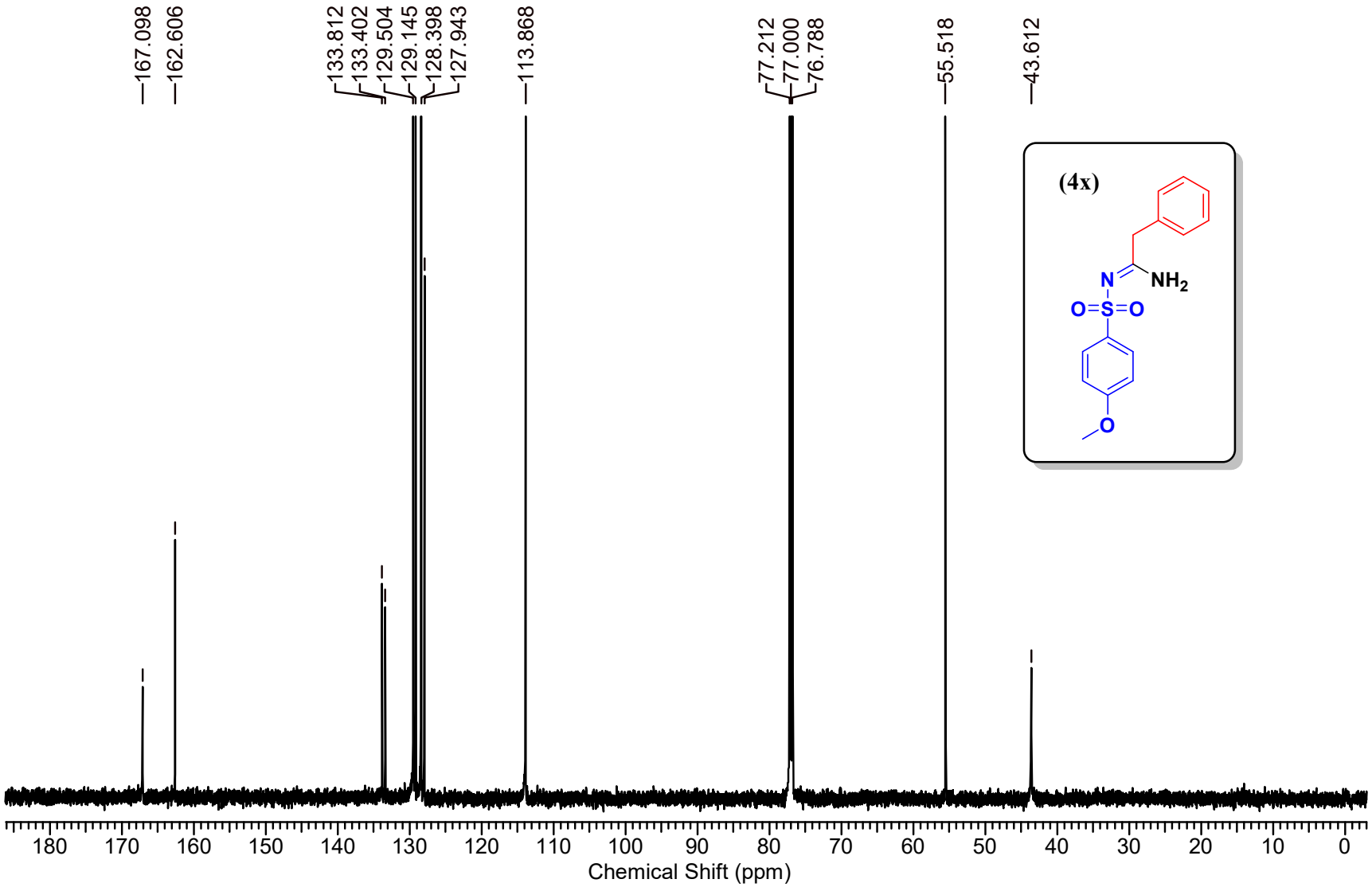

8.115
7.934
7.921
7.561
7.549
7.501
7.489
7.476
7.349
7.337
7.223
7.211
5.787
3.661
(4v)
N
NH2
O=S=O
0.87 1.94 0.98 2.01 3.00 1.99
0.95
2.00
9
8
7
6
5
4
3
2
1
0
Chemical Shift (ppm)

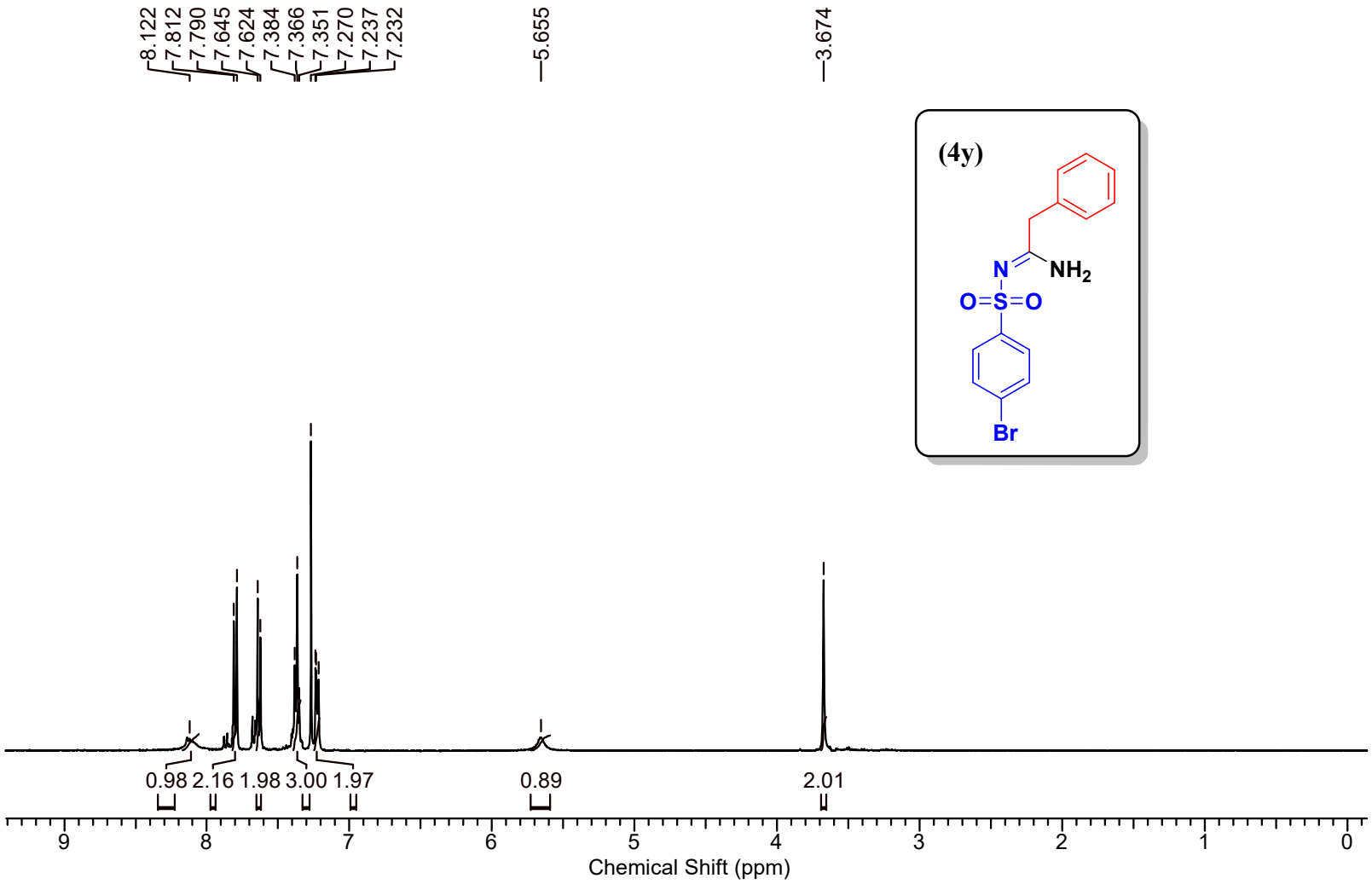

167.557
141.903
133.176
132.321
129.595
129.259
128.740
128.104
126.342
77.256
77.000
76.751
43.693
(4v)
N
NH2
O=S=O
180
160
140
120
100
80
60
40
20
0
Chemical Shift (ppm)

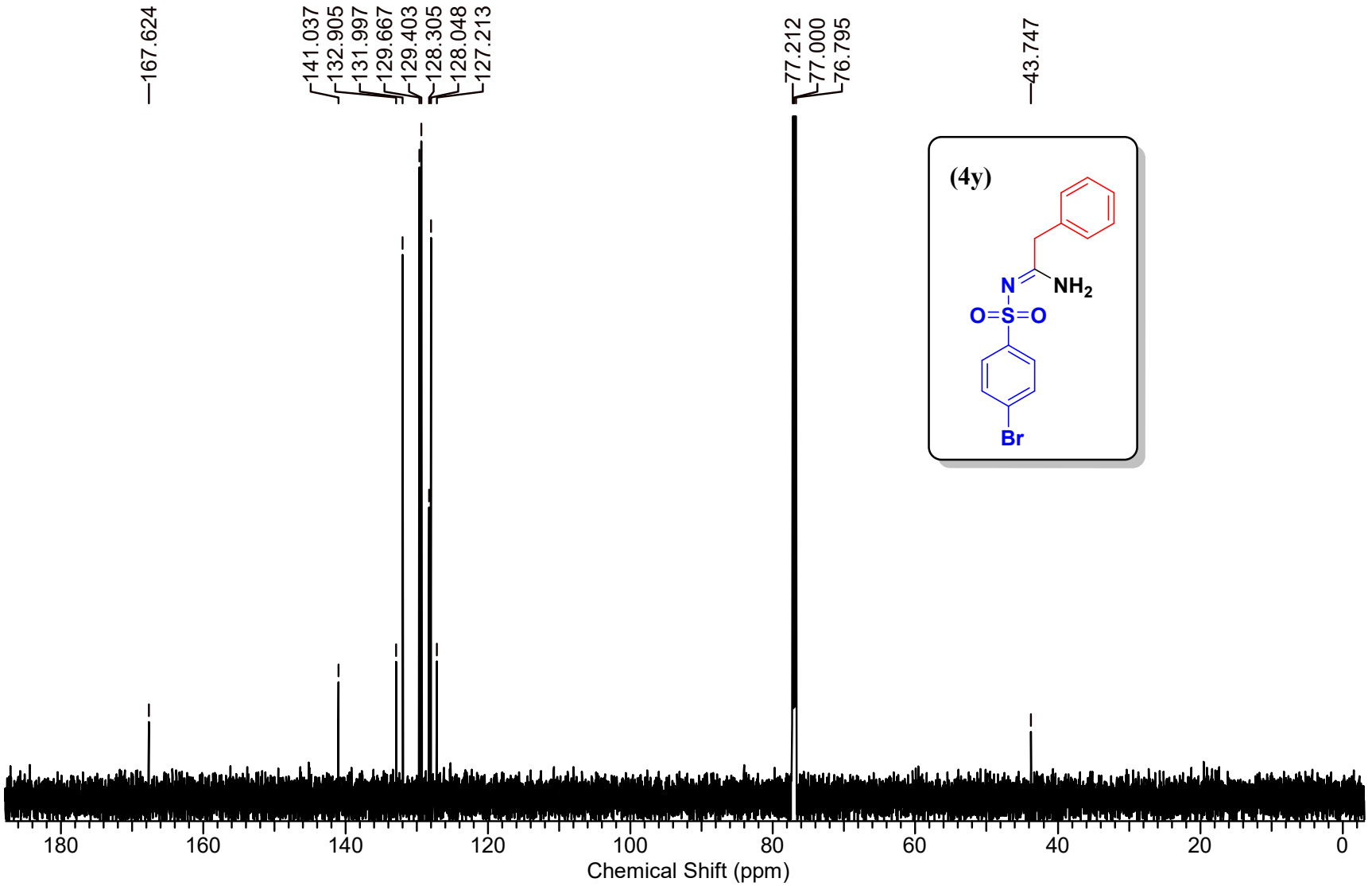

7.934
7.914
7.368
7.333
7.262
7.245
7.219
7.201
7.186
7.142
7.137
5.768
3.568
2.558
1.654
(4w)
N
NH2
O=S=O
1.16
0.93
4.74
1.70
0.81
1.80
2.70
0.86
9
8
7
6
5
4
3
2
1
0
Chemical Shift (ppm)

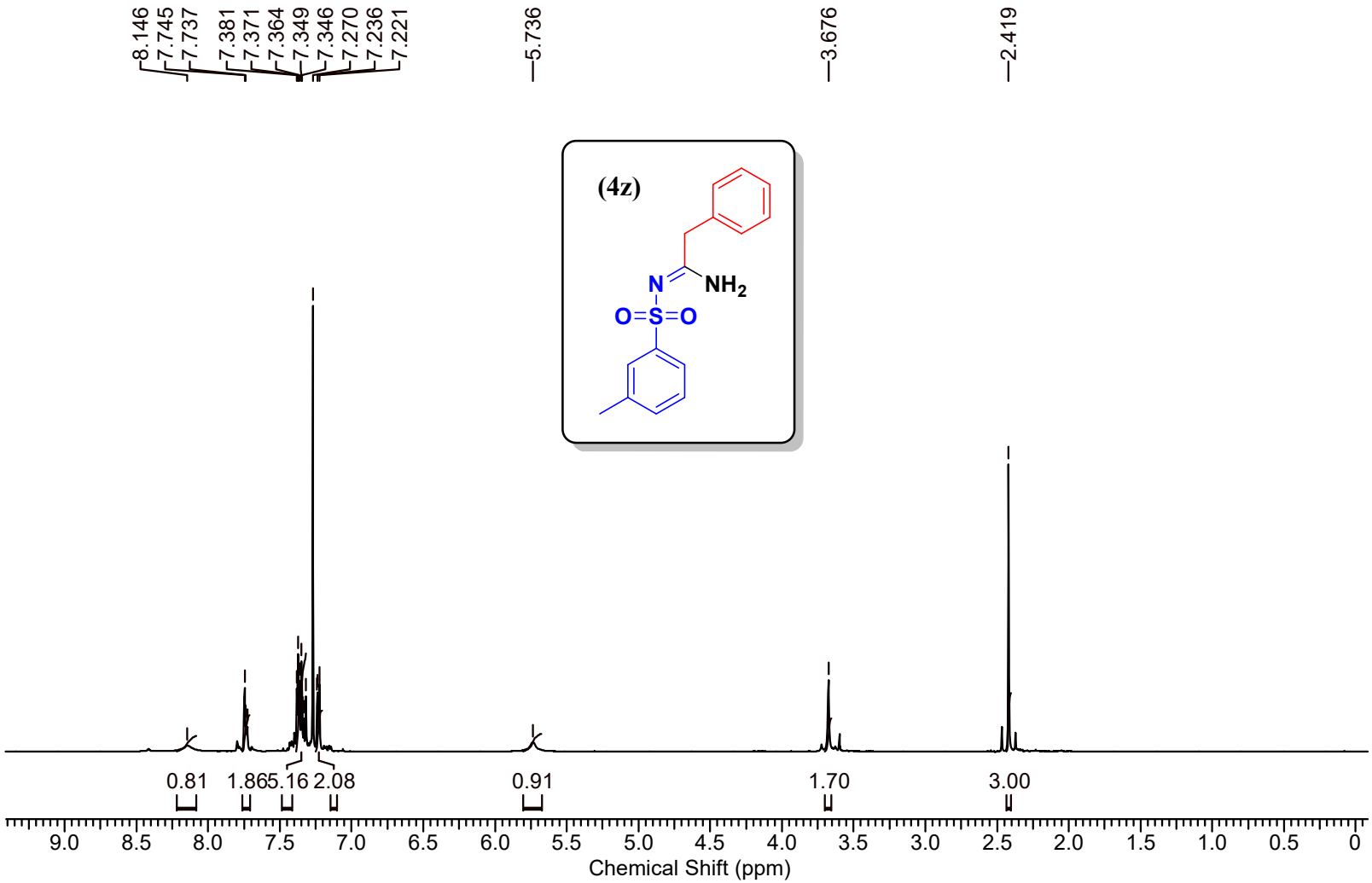

167.382
139.865
137.506
133.330
132.319
132.158
129.535
129.140
129.125
127.960
127.594
125.696
77.212
77.000
76.788
43.696
20.208
(4w)
N
NH2
O=S=O
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
Chemical Shift (ppm)

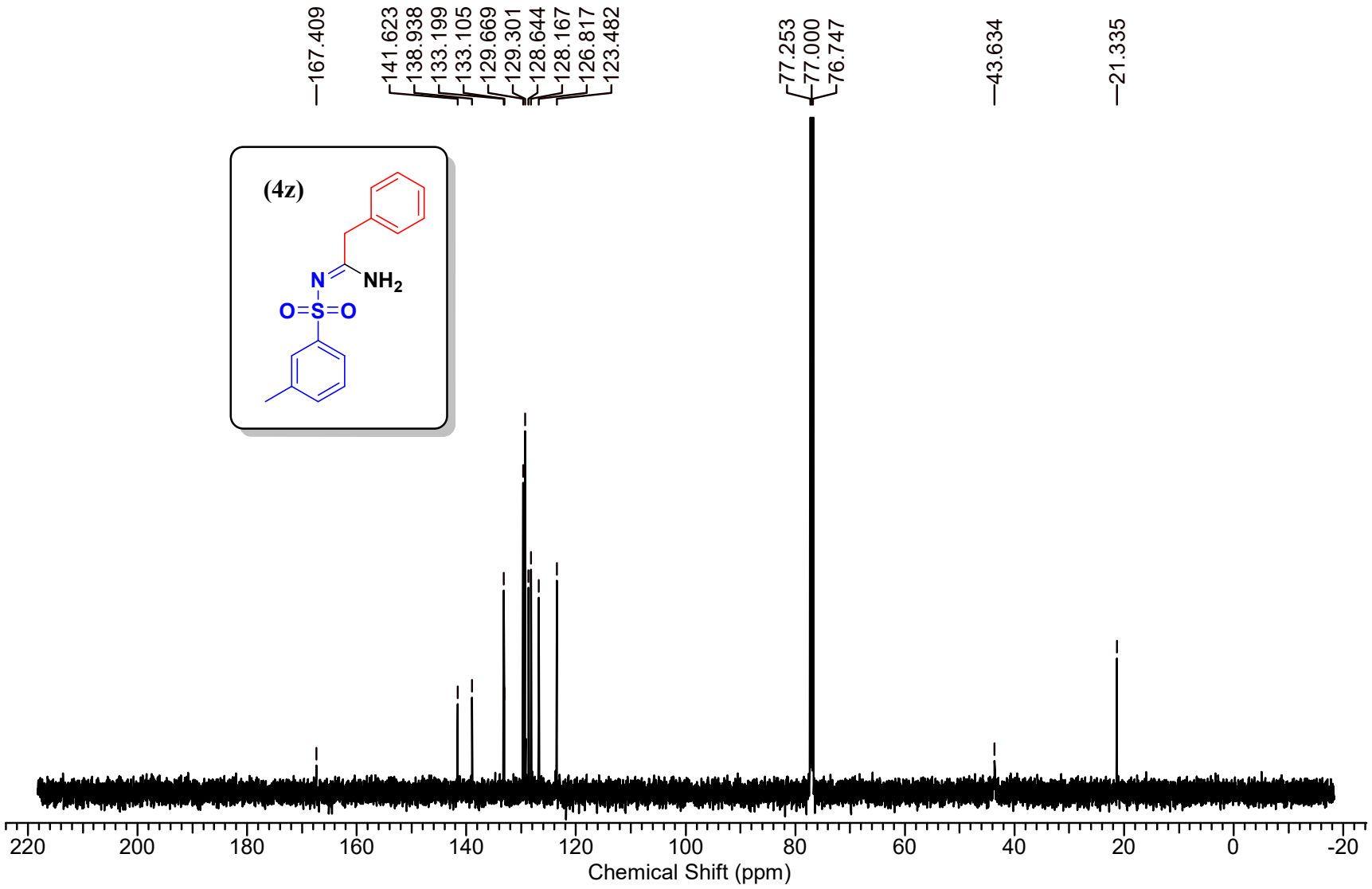

8.062
7.858
7.835
7.356
7.342
7.325
7.311
7.270
7.222
7.217
7.202
6.959
6.937
5.795
3.861
3.633
(4x)
N
NH2
O=S=O
O
0.75
1.87
2.81
1.79
1.93
0.85
3.00
1.93
9
8
7
6
5
4
3
2
1
0
Chemical Shift (ppm)


167.098
162.606
133.812
133.402
129.504
129.145
128.398
127.943
113.868
77.212
77.000
76.788
55.518
43.612
(4x)
N
NH2
O=S=O
O
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
Chemical Shift (ppm)


8.122
7.812
7.790
7.645
7.624
7.384
7.366
7.351
7.270
7.237
7.232
5.655
3.674
(4y)
N
NH2
O=S=O
Br
0.98 2.16 1.98 3.00 1.97
0.89
2.01
9
8
7
6
5
4
3
2
1
0
Chemical Shift (ppm)


167.624
141.037
132.905
131.997
129.667
129.403
128.305
128.048
127.213
77.212
77.000
76.795
43.747
(4y)
N
NH2
O=S=O
Br
180
160
140
120
100
80
60
40
20
0
Chemical Shift (ppm)


8.146
7.745
7.737
7.381
7.371
7.364
7.349
7.346
7.270
7.236
7.221
5.736
3.676
2.419
(4z)
N
NH2
O=S=O
0.81
1.86
5.16
2.08
0.91
1.70
3.00
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
Chemical Shift (ppm)


167.409
141.623
138.938
133.199
133.105
129.669
129.301
128.644
128.167
126.817
123.482
77.253
77.000
76.747
43.634
21.335
(4z)
N
NH2
O=S=O
220
200
180
160
140
120
100
80
60
40
20
0
-20
Chemical Shift (ppm)