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Supporting Information

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Rhodium-catalyzed Propargylic Substitution: A Divergent Approach to Propargylic and Allenyl Sulfonamides

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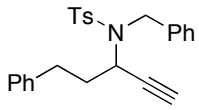


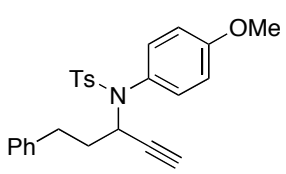
***N*-Benzyl-*N*-1[1-(2-phenylethyl)prop-2-yn-1-yl]-4-methylbenzenesulfonamide (2a).**

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.69 (d, *J* = 8.4 Hz, 2H), 7.46 (d, *J* = 7.2 Hz, 2H), 7.31-7.05 (m, 8H), 6.79 (d, *J* = 6.8 Hz, 2H), 4.75 (dt, *J* = 8.8, 2.1 Hz, 1H), 4.67 (d, A of AB, J_{AB} = 15.6 Hz, 1H), 4.13 (d, B of AB, J_{AB} = 15.6 Hz, 1H), 2.51 (t, *J* = 8.0 Hz, 2H), 2.38 (s, 3H), 2.17 (d, *J* = 2.3 Hz, 1H), 1.70-1.55 (m, 2H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 143.48 (e), 140.62 (e), 137.86 (e), 136.06 (e), 129.48 (o), 128.47 (o), 128.28 (o), 128.20 (o), 127.65 (o), 125.85 (o), 79.82 (e), 74.85 (o), 51.25 (o), 48.81 (e), 37.43 (e), 32.22 (e), 21.51 (o).

IR (neat) 3289 (s), 3029 (s), 2928 (s), 1599 (s), 1496 (s), 1455 (s), 1337 (s) cm^{-1}.

HRMS (CI, $M+H^+$) calcd for $C_{25}H_{26}NO_2S$ 404.1679, found 404.1671.



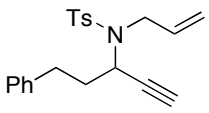
***N*-(4-Methoxyphenyl)-4-methyl-*N*-[1-phenylethyl)prop-2-yn-1-yl]benzenesulfonamide (2ab).**

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.56 (d, *J* = 8.4 Hz, 2H), 7.28-7.13 (m, 9H), 6.79 (d, *J* = 9.0 Hz, 2H), 5.11 (dt, *J* = 7.6, 2.3 Hz, 1H), 3.78 (s, 3H), 2.76 (t, *J* = 7.9 Hz, 2H), 2.40 (s, 3H), 2.25 (d, *J* = 2.3 Hz, 1H), 1.91-1.70 (m, 2H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 159.71 (e), 143.31 (e), 140.61 (e), 136.48 (e), 132.52 (o), 129.06 (o), 128.46 (e), 128.15 (o), 126.13 (o), 113.94 (o), 81.91 (e), 74.47 (o), 55.32 (o), 50.62 (o), 36.53 (e), 32.18 (e), 21.54 (o).

IR (neat) 3288 (s), 2933 (s), 1737 (m), 1602 (s), 1506 (s) cm^{-1}.

HRMS (CI, $M+H^+$) calcd for $C_{25}H_{26}NO_3S$ 420.1628, found 420.1616.



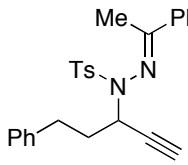
***N*-Allyl-4-nitro-*N*-[1-(2-phenethyl)prop-2-yn-1-yl]benzenesulfonamide (2ac).**

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.33 (d, *J* = 9.0 Hz, 2H), 8.00 (*J* = 9.0 Hz, 2H), 7.33–7.19 (m, 5H), 5.94 (dddd, *J* = 17.5, 10.2, 7.4, 4.8 Hz, 1H), 5.30 (d, *J* = 17.2 Hz, 1H), 5.19 (d, *J* = 10.2 Hz, 1H), 4.73 (dt, *J* = 7.7, 2.2 Hz, 1H), 3.96 (dd, A of ABX, J_{AB} = 16.2 Hz, J_{AX} = 4.7 Hz, 1H), 3.80 (dd, B of ABX, J_{AB} = 16.2 Hz, J_{BX} = 7.6 Hz, 1H), 2.78 (t, *J* = 7.8 Hz, 2H), 2.21 (d, *J* = 2.3 Hz, 1H), 2.14–2.00 (m, 2H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 150.05 (e), 144.85 (e), 140.21 (e), 134.61 (o), 128.85 (o), 128.52 (o), 128.42 (o) 126.28 (o), 124.06 (o), 118.38 (e), 79.55 (e), 74.84 (o), 50.80 (o), 47.92 (e), 37.01 (e), 32.05 (e).

IR (neat) 3278 (m), 2933 (m), 1531 (s), 1350 (s), 1166 (s) cm^{-1}.

HRMS (CI, $M+H^+$) calcd for $C_{20}H_{21}N_2O_4S$ 385.1217, found 385.1220.



4-Methyl-*N′*-(1-phenylethylidene)-*N*-[1-(2-phenethyl)prop-2-yn-1-yl]benzenesulfonahydrazide (2ad).

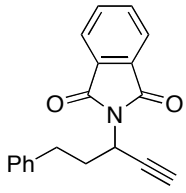
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.91 (d, *J* = 7.2 Hz, 2H), 7.67 (d, *J* = 8.2 Hz, 2H), 7.50–7.39 (m, 3H), 7.34–7.10 (m, 7H), 4.75 (dt, *J* = 7.4, 2.2 Hz, 1H), 2.82–2.65 (m, 2H), 2.64

(s, 3H), 2.41 (s, 3H), 1.90 (d, J = 2.2 Hz, 1H), 1.81 (q, J = 7.7 Hz, 1H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 178.93 (e), 143.99 (e), 140.76 (e), 137.11 (e), 133.89 (e), 131.13 (o), 129.28 (o), 128.97 (o), 128.49 (o), 128.44 (o), 128.41 (o), 127.46 (o), 126.11 (o), 79.41 (e), 74.00 (o), 52.88 (o), 36.16 (e), 32.24 (e), 21.61 (o), 18.11 (o).

IR (neat) 3292 (m), 3028 (m), 1599 (m), 1495 (m), 1354 (s), 1164 (s) cm^{-1}.

HRMS (CI, M+H$^+$) calcd for $C_{26}H_{27}N_2O_2S$ 431.1788, found 431.1775.



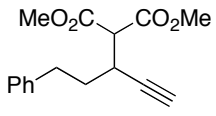
2-[1-(Phenylethyl)prop-2-yn-1-yl]-1-*H*-isoindole-1,3(2*H*)-dione (2ae).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.83–7.79 (m, 2H), 7.71–7.67 (m, 2H), 7.24–7.08 (m, 5H), 5.04 (dt, J = 7.8, 2.5 Hz, 1H), 2.80 (ddd, A of ABMX, J_{AB} = 14.5 Hz, J_{AM} = 8.7 Hz, J_{AX} = 5.8 Hz, 1H), 2.66 (ddd, B of ABMX, J_{AB} = 15.0 Hz, J_{BM} = 7.8 Hz, J_{BX} = 7.4 Hz, 1H), 2.50–2.34 (m, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 166.95 (e), 140.08 (e), 134.07 (o), 131.68 (e), 128.40 (o), 128.32 (o), 126.08 (o), 123.38 (o), 79.97 (e), 72.25 (o), 41.16 (o), 34.55 (e), 32.54 (e).

IR (neat) 3475 (s), 3281 (s), 2929 (s), 2255 (m), 1771 (s), 1614 (s), 1385 (s) cm^{-1}.

HRMS (CI, M+H$^+$) calcd for $C_{19}H_{16}NO_2$ 290.1176, found 290.1174.



Dimethyl [1-(2-phenylethyl)prop-2-yn-1-yl]malonate (2af).

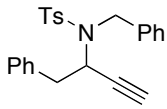
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.36–7.31 (m, 2H), 7.26–7.23 (m, 3H), 3.81 (s, 3H), 3.78 (s, 3H), 3.58 (d, J = 9.2 Hz, 1H), 3.25–3.18 (m, 1H), 2.99 (ddd, A of ABMX, J_{AB} = 14.3 Hz, J_{AM} = 9.3 Hz, J_{AX} = 5.0 Hz, 1H), 2.78 (ddd, B of ABMX, J_{AB} = 13.8

Hz, J_{BM} = 9.5 Hz, J_{BX} = 7.2 Hz, 1H), 2.27 (d, J = 2.0 Hz, 1H), 1.95–1.80 (m, 2H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 167.74 (e), 167.66 (e), 141.03 (e), 128.44 (o), 128.43 (o), 126.06 (o), 82.91 (e), 71.89 (o), 56.04 (o), 52.70 (o), 52.67 (o), 34.11 (e), 33.21 (e), 31.28 (o).

IR (neat) 3287 (s), 2955 (s), 1733 (s), 1435 (s) cm^{-1}.

HRMS (CI, $M+H^+$) calcd for $C_{16}H_{19}O_4$ 275.1278, found 275.1278.



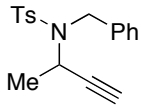
***N*-Benzyl-*N*-{1-benzylprop-2-yn-1-yl}-4-methyl benzenesulfonamide (2b).**

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.73 (d, J = 7.9 Hz, 2H), 7.48 (d, J = 7.3 Hz, 2H), 7.37–7.21 (m, 8H), 7.08 (d, J = 7.0 Hz, 2H), 5.03–5.00 (m, 1H), 4.76 (d, A of AB, J_{AB} = 15.6 Hz, 1H), 4.29 (d, B of AB, J_{AB} = 15.6 Hz, 1H), 2.84 (dd, A of ABX, J_{AB} = 13.2 Hz, J_{AX} = 5.3 Hz, 1H), 2.50 (dd, B of ABX, J_{AB} = 13.2 Hz, J_{BX} = 10.4 Hz, 1H), 2.44 (s, 3H), 2.22 (d, J = 1.3 Hz, 1H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 143.47 (e), 137.63 (e), 136.58 (e), 136.28 (e), 129.49 (o), 129.38 (o), 128.55 (o), 128.43 (o), 128.22 (o), 127.64 (o), 127.59 (o), 126.80 (o), 79.39 (e), 75.78 (o), 53.09 (o), 48.99 (e), 42.95 (e), 21.51 (o).

IR (neat) 3288 (m), 3031 (m), 1738 (m), 1599 (m), 1496 (s), 1455 (s), 1343 (s) cm^{-1}.

HRMS (EI, $M-H^+$) calcd for $C_{24}H_{22}NO_2S$ 388.1366, found 388.1359.



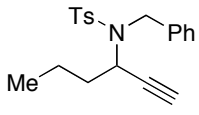
***N*-Benzyl-*N*-(1-methylprop-2-yn-1-yl)-4-methyl benzenesulfonamide (2c).**

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.69 (d, J = 8.2 Hz, 2H), 7.39 (d, J = 7.4 Hz, 2H), 7.28–7.19 (m, 5H), 4.91 (dq, J = 7.1, 2.3 Hz, 1H), 4.63 (d, A of AB, J_{AB} = 16.0 Hz, 1H), 4.15 (d, B of AB, J_{AB} = 15.6 Hz, 1H), 2.38 (s, 3H), 2.12 (d, J = 2.1 Hz, 1H), 1.11 (d, J = 7.0 Hz, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 143.44 (e), 138.24 (e), 136.22 (e), 129.48 (o), 128.35 (o), 127.97 (o), 127.61 (o), 127.39 (o), 80.93 (e), 73.82 (o), 48.43 (e), 46.61 (o), 22.99 (o), 21.52 (o).

IR (neat) 3263 (m), 2923 (w), 1599 (w), 1456 (m), 1334 (s), 1162 (s) cm^{-1}.

HRMS (EI, M^+) calcd for $C_{18}H_{19}NO_2S$ 313.1131, found 313.1142.



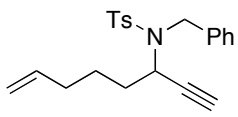
***N*-Benzyl-*N*-(1-propylprop-2-yn-1-yl)-4-methyl benzenesulfonamide (2d).**

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.72 (d, *J* = 8.2 Hz, 2H), 7.42 (d, *J* = 7.1 Hz, 2H), 7.30–7.21 (m, 5H), 4.75–4.72 (m, 1H), 4.64 (d, A of AB, J_{AB} = 15.7 Hz, 1H), 4.11 (d, B of AB, J_{AB} = 15.7 Hz, 1H), 2.40 (s, 3H), 2.14 (d, *J* = 2.2 Hz, 1H), 1.34–1.18 (m, 4H), 0.66 (t, *J* = 7.0 Hz, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 143.37 (e), 137.89 (e), 136.24 (e), 129.43 (o), 128.25 (o), 127.62 (o), 127.42 (o), 80.24 (e), 74.36 (o), 51.21 (o), 48.70 (e), 37.79 (e), 21.50 (o), 19.11 (e), 13.05 (o).

IR (neat) 3294 (s), 2962 (s), 2257 (w), 1599 (s), 1496 (s), 1456 (s), 1339 (s) cm^{-1}.

HRMS (CI, $M+H^+$) calcd for $C_{20}H_{24}NO_2S$ 342.1522, found 342.1512.



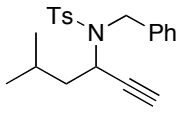
***N*-Benzyl-*N*-(1-ethynylhex-5-en-1-yl)-4-methyl benzenesulfonamide (2e).**

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.69 (d, *J* = 8.2 Hz, 2H), 7.40 (d, *J* = 7.0 Hz, 2H), 7.28–7.19 (m, 5H), 5.51 (ddt, *J* = 17.0, 10.5, 6.6 Hz, 1H), 4.83–4.79 (m, 2H), 4.74–4.66 (m, 1H), 4.63 (d, A of AB, J_{AB} = 15.6 Hz, 1H), 4.08 (d, B of AB, J_{AB} = 15.6 Hz, 1H), 2.38 (s, 3H), 2.13 (d, *J* = 2.2 Hz, 1H), 1.74–1.52 (m, 2H), 1.33–1.27 (m, 4H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 143.41 (e), 137.97 (o), 137.83 (e), 136.23 (e), 129.46 (o), 128.36 (o), 128.30 (o), 127.64 (o), 127.48 (o), 114.72 (e), 80.14 (e), 74.49 (o), 51.34 (o), 48.71 (e), 35.22 (e), 32.74 (e), 25.10 (e), 21.52 (o).

IR (neat) 3292 (s), 2926 (s), 1641 (s), 1599 (s), 1496 (s), 1455 (s), 1338 (s) cm^{-1}.

HRMS (CI, $M+H^+$) calcd for $C_{22}H_{26}NO_2S$ 368.1679, found 368.1675.



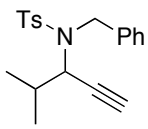
***N*-Benzyl-*N*-(1-isobutylprop-2-yn-1-yl)-4-methyl benzenesulfonamide (2f).**

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.58 (d, J = 8.2 Hz, 2H), 7.27 (d, J = 7.2 Hz, 2H), 7.15–7.05 (m, 5H), 4.66 (ddd, J = 8.8, 6.8, 2.0 Hz, 1H), 4.48 (d, A of AB, J_{AB} = 15.6 Hz, 1H), 3.94 (d, B of AB, J_{AB} = 15.8 Hz, 1H), 2.25 (s, 3H), 1.97 (d, J = 2.3 Hz, 1H), 1.46–1.36 (m, 1H), 1.14–1.07 (m, 1H), 1.01–0.83 (m, 1H), 0.66 (d, J = 6.6 Hz, 3H), 0.36 (d, J = 6.8 Hz, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 143.40 (e), 137.96 (e), 136.17 (e), 129.44 (o), 128.32 (o), 128.30 (o), 127.72 (o), 127.43 (o), 80.45 (e), 74.19 (o), 49.73 (o), 48.68 (e), 44.45 (e), 24.04 (o), 21.78 (o), 21.71 (o), 21.52 (o).

IR (neat) 3296 (s), 2959 (s), 2258 (w), 1599 (m), 1496 (m), 1338 (s) cm^{-1}.

HRMS (EI, M^+) calcd for $C_{21}H_{25}NO_2S$ 355.1601, found 355.1600.



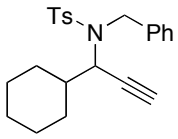
***N*-Benzyl-*N*-(1-isopropylprop-2-yn-1-yl)-4-methyl benzenesulfonamide (2g).**

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.74 (d, J = 8.2 Hz, 2H), 7.47 (d, J = 6.8 Hz, 2H), 7.31–7.26 (m, 5H), 4.66 (d, A of AB, J_{AB} = 15.4 Hz, 1H), 4.35 (dd, J = 10.6, 2.2 Hz, 1H), 4.12 (d, B of AB, J_{AB} = 15.4 Hz, 1H), 2.44 (s, 3H), 2.32 (d, J = 2.2 Hz, 1H), 1.41–1.22 (m, 1H), 0.91 (d, J = 6.6 Hz, 3H), 0.80 (d, J = 6.4 Hz, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 143.33 (e), 137.28 (e), 136.19 (e), 129.41 (o), 128.90 (o), 128.21 (o), 127.66 (o), 127.55 (o), 79.52 (e), 75.43 (o), 58.56 (o), 49.10 (e), 32.33 (o), 21.50 (o), 20.00 (o), 19.43 (o).

IR (neat) 3292 (s), 2964 (s), 1599 (m), 1496 (s), 1456 (s), 1337 (s) cm^{-1}.

HRMS (EI, M-$C_3H_7^+$) calcd for $C_{17}H_{16}NO_2S$ 298.0896, found 298.0897.



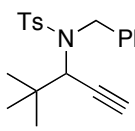
***N*-Benzyl-*N*-(1-cyclohexylprop-2-yn-1-yl)-4-methyl benzenesulfonamide (2h).**

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.71 (d, *J* = 7.7 Hz, 2H), 7.44 (d, *J* = 7.3 Hz, 2H), 7.28-7.22 (m, 5H), 4.65 (d, A of AB, J_{AB} = 15.2 Hz, 1H), 4.41 (d, *J* = 10.3 Hz, 1H), 4.07 (d, B of AB, J_{AB} = 15.2 Hz, 1H), 2.41 (s, 3H), 2.20-2.19 (m, 1H), 1.84 (d, *J* = 12.1 Hz, 1H), 1.76 (d, *J* = 12.6 Hz, 1H), 1.62-1.44 (m, 3H), 1.05-0.75 (m, 5H), 0.53-0.44 (m, 1H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 143.27 (e), 137.23 (e), 136.36 (e), 129.41 (o), 129.03 (o), 128.15 (o), 127.62 (o), 127.57 (o), 79.28 (e), 75.60 (o), 57.23 (o), 49.06 (e), 40.94 (o), 30.31 (e), 29.94 (e), 26.06 (e), 25.81 (e), 25.14 (e), 21.51 (o).

IR (neat) 3303 (s), 2923 (s), 1600 (s), 1496 (s), 1455 (s), 1336 (s) cm^{-1}.

HRMS (CI, M+H^+) calcd for $C_{23}H_{28}NO_2S$ 382.1835, found 382.1821.



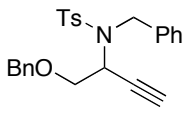
***N*-Benzyl-*N*-(1-*tert*-butylprop-2-yn-1-yl)-4-methyl benzenesulfonamide (2i).**

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.73 (d, *J* = 6.4 Hz, 2H), 7.48 (d, *J* = 7.5 Hz, 2H), 7.36-7.24 (m, 5H), 4.66 (t, *J* = 2.3 Hz, 1H), 4.49 (d, A of AB, J_{AB} = 17.2 Hz, 1H), 2.29 (d, B of AB, J_{AB} = 17.2 Hz, 1H), 2.45 (s, 3H), 2.22 (t, *J* = 2.5 Hz, 1H), 0.97 (d, *J* = 2.2 Hz, 9H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 143.48 (e), 138.18 (e), 135.24 (e), 129.39 (o), 128.14 (o), 128.02 (o), 127.66 (o), 126.89 (o), 78.60 (e), 75.82 (o), 61.90 (o), 50.62 (e), 36.32 (e), 26.84 (o), 21.51 (o).

IR (neat) 3303 (s), 2965 (s), 2257 (w), 1600 (s), 1496 (s), 1338 (s) cm^{-1}.

HRMS (CI, $M+H^+$) calcd for $C_{21}H_{26}NO_2S$ 356.1679, found 356.1683.



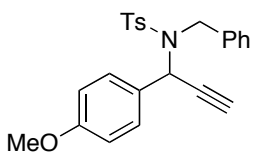
***N*-Benzyl-*N*-{1-[(benzyloxy)methyl]prop-2-yn-1-yl}-4-methylbenzenesulfonamide (2j).**

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.72 (d, J = 8.4 Hz, 2H), 7.38–7.36 (m, 2H), 7.30–7.22 (m, 8H), 7.18–7.16 (m, 2H), 5.06 (dt, J = 7.2, 2.2 Hz, 1H), 4.66 (d, A of AB, J_{AB} = 15.8 Hz, 1H), 4.25 (d, A of AB, J_{AB} = 11.9 Hz, 1H), 4.21 (d, B of AB, J_{AB} = 11.9 Hz, 1H), 4.19 (d, B of AB, J_{AB} = 15.6 Hz, 1H), 3.25 (dd, A of ABX, J_{AB} = 9.8 Hz, J_{AX} = 7.2 Hz, 1H), 3.18 (dd, B of ABX, J_{AB} = 9.8 Hz, J_{BX} = 7.0 Hz, 1H), 2.40 (s, 3H), 2.23 (d, J = 2.3 Hz, 1 H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 143.47 (e), 137.57 (e), 137.45 (e), 136.29 (e), 129.48 (o), 128.30 (o), 128.25 (o), 127.61 (o), 127.55 (o), 78.04 (e), 75.29 (o), 72.78 (e), 71.33 (e), 50.67 (o), 48.90 (e), 21.52 (o).

IR (neat) 3286 (s), 2864 (s), 2117 (w), 1599 (s), 1496 (s), 1455 (s), 1337 (s) cm^{-1}.

HRMS (CI, $M+H^+$) calcd for $C_{25}H_{26}NO_3S$ 420.1628, found 420.1633.



***N*-Benzyl-*N*-[1-(4-methoxyphenyl)prop-2-yn-1-yl]-4-methylbenzenesulfonamide (2k).**

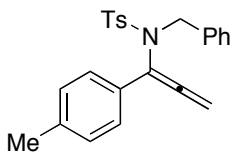
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.78 (d, J = 8.2 Hz, 2H), 7.34 (d, J = 8.6 Hz, 2H), 7.32 (d, J = 7.9 Hz, 2H), 7.05–6.98 (m, 5H), 6.68 (d, J = 8.6 Hz, 2H), 6.13 (d, J = 2.0 Hz, 1H), 4.48 (d, A of AB, J_{AB} = 15.6 Hz, 1H), 4.15 (d, B of AB, J_{AB}

= 15.4 Hz, 1H), 3.75 (s, 3H), 2.47 (s, 3H), 2.43 (d, *J* = 2.4 Hz, 1H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 159.34 (e), 143.41 (e), 136.55 (e), 136.36 (e), 129.44 (o), 129.42 (o), 128.44 (o), 127.76 (o), 127.62 (o), 126.75 (o), 113.42 (o), 78.33 (e), 76.63 (o), 55.26 (o), 53.24 (o), 48.80 (e), 21.53 (o).

IR (neat) 3260 (m), 2924 (m), 2113 (w), 1599 (m), 1512 (s), 1337 (s) cm^{-1}.

HRMS (CI, $M+H^+$) calcd for $C_{24}H_{24}NO_3S$ 406.1471, found 406.1469.



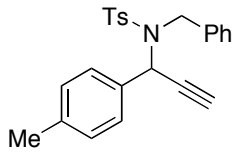
***N*-Benzyl-4-methyl-*N*-[1-(4-methylphenyl)propa-1,2-dien-1-yl]benzenesulfonamide (3l).**

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.71 (d, *J* = 8.2 Hz, 2H), 7.32–7.18 (m, 9H), 7.04 (d, *J* = 8.0 Hz, 2H), 5.00 (s, 2H), 4.39 (s, 2H), 2.44 (s, 3H), 2.27 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 208.66 (e), 143.61 (e), 137.40 (e), 135.49 (e), 134.06 (e), 131.34 (e), 129.27 (o), 129.10 (o), 128.79 (o), 128.24 (o), 128.16 (o), 127.76 (o), 125.83 (o), 112.88 (e), 84.77 (e), 54.40 (e), 21.55 (o), 21.08 (o).

IR (neat) 3031 (s), 2923 (s), 1934 (m), 1598 (s), 1512 (s), 1496 (s), 1456 (s), 1348 (s) cm^{-1}.

HRMS (CI, M^+) calcd for $C_{24}H_{23}NO_2S$ 389.1444, found 389.1440.



***N*-Benzyl-*N*-[1-(4-methylphenyl)prop-2-yn-1-yl]-4-methylbenzenesulfonamide (2l).**

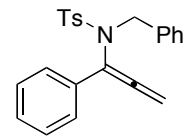
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.76 (d, *J* = 8.2 Hz, 2H), 7.32–7.29 (m, 4H), 7.05–6.95 (m, 7H), 6.14 (d, *J* = 1.4 Hz, 1H), 4.45 (d, A of AB, J_{AB} = 15.4 Hz, 1H), 4.16 (d, B of AB, J_{AB} = 15.4 Hz, 1H), 2.45 (s, 3H), 2.42 (d, *J* = 2.6 Hz, 1H), 2.26 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 143.38 (e), 137.78 (e), 136.46 (e), 136.36 (e), 132.47 (e), 129.37 (o), 128.68 (o), 128.47 (o),

128.06 (o), 127.74 (o), 127.55 (o), 126.65 (o), 78.27 (e), 76.62 (o), 53.49 (o), 48.87 (e), 21.50 (o), 20.92 (o).

IR (neat) 3289 (m), 2924 (m), 2119 (w), 1599 (m), 1339 (s), 1162 (s) cm^{-1}.

HRMS (CI, $M+H^+$) calcd for $C_{24}H_{24}NO_2S$ 390.1522, found 390.1519.



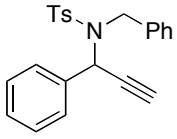
***N*-Benzyl-4-methyl-*N*-(1-phenylpropa-1,2-dien-1-yl)benzenesulfonamide (3m).**

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.75 (d, *J* = 8.2 Hz, 2H), 7.40-7.17 (m, 12H), 5.06 (s, 2H), 4.44 (s, 2H), 2.48 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 208.88 (e), 143.70 (e), 135.40 (e), 134.23 (e), 134.09 (e), 129.33 (o), 129.15 (o), 128.27 (o), 128.19 (o), 128.02 (o), 127.83 (o), 127.58 (o), 125.93 (o), 112.89 (e), 84.86 (e), 54.49 (e), 21.58 (o).

IR (neat) 3033 (s), 2924 (s), 2256 (m), 1935 (m), 1599 (s), 1348 (s) cm^{-1}.

HRMS (CI, $M+H^+$) calcd for $C_{23}H_{22}NO_2S$ 376.1366, found 376.1369.



***N*-Benzyl-4-methyl-*N*-(1-phenylprop-2-yn-1-yl)benzene sulfonamide (2m).** Trimethyl phosphite (12 μL, 0.10 mmol) was added directly to a red solution of Wilkinson's catalyst (23.1 mg, 0.025 mmol) in anhydrous THF (1.0 mL), under an atmosphere of argon. The catalyst was allowed to form over *ca.* 5 min resulting in a light yellow homogeneous solution, which was then added *via* Teflon® cannula to a stirred suspension of *p*-toluenesulfonyl benzylamine (0.132 g, 0.5 mmol) and potassium carbonate (69.1 mg, 0.5 mmol) in anhydrous THF. The propargylic carbonate **1m** (58.0 mg, 0.25 mmol), was then added dropwise, *via* a tared 250 μL syringe, and the mixture was heated to 30 °C for *ca.* 15 h (t.l.c. control). The reaction mixture was then quenched with saturated aqueous NH_4Cl solution (2 mL) and partitioned

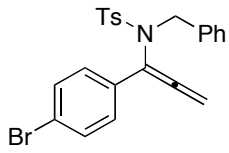
between diethyl ether and saturated aqueous NH_4Cl solution. The aqueous phase was washed with diethyl ether and the organic layers were combined, dried (Na_2SO_4), filtered, and concentrated *in vacuo* to afford a crude oil. Purification by flash chromatography (eluting with 5% ethyl acetate/hexanes) furnished the propargylic sulfonamide **2m** as a colorless oil (71.9 mg, 74%).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.77 (d, J = 8.2 Hz, 2H), 7.44 (m, 4H), 7.15 (m, 8H), 6.17 (d, J = 2.1 Hz, 1H), 4.50 (d, A of AB, J_{AB} = 15.2 Hz, 1H), 4.15 (d, B of AB, J_{AB} = 15.4 Hz, 1H), 2.45 (s, 3H), 2.44 (d, J = 2.5 Hz, 1H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 143.52 (e), 136.30 (e), 135.52 (e), 129.48 (o), 128.56 (o), 128.13 (o), 128.04 (o), 127.81 (o), 127.64 (o), 126.86 (o), 77.99 (e), 77.00 (o), 53.74 (o), 49.02 (e), 21.57 (o).

IR (neat) 3290 (s), 3031 (s), 2122 (m), 1739 (s), 1599 (s), 1495 (s), 1456 (s) cm^{-1}.

HRMS (CI, M+H$^+$) calcd for $C_{23}H_{22}NO_2S$ 376.1366, found 376.1367.



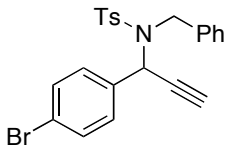
***N*-Benzyl-*N*-[1-(4-bromophenyl)propa-1,2-dien-1-yl)methylbenzenesulfonamide (3n).**

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.71 (d, J = 8.2 Hz, 2H), 7.35-7.33 (m, 4H), 7.26-7.22 (m, 7H), 5.04 (s, 2H), 4.37 (s, 2H), 2.47 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 208.57 (e), 143.91 (e), 135.14 (e), 133.70 (e), 133.50 (e), 131.15 (o), 129.42 (o), 129.14 (o), 128.37 (o), 128.21 (o), 127.99 (o), 127.47 (o), 121.57 (e), 85.47 (e), 54.68 (e), 21.61 (o).

IR (neat) 3032 (m), 2924 (m), 1933 (w), 1597 (m), 1486 (s), 1349 (s) cm^{-1}.

HRMS (CI, M+H$^+$) calcd for $C_{23}H_{21}{}^{79}BrNO_2S$ 454.0471, found 454.0471.



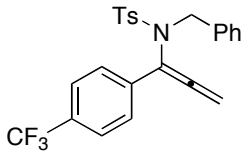
***N*-Benzyl-*N*-[1-(4-bromophenyl)prop-2-yn-1-yl]-4-methylbenzenesulfonamide (2n).**

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.77 (d, J = 8.4 Hz, 2H), 7.33 (d, J = 8.2 Hz, 2H), 7.26–7.18 (m, 4H), 7.07–6.95 (m, 5H), 6.10 (d, J = 2.1 Hz, 1H), 4.58 (d, A of AB, J_{AB} = 15.2 Hz, 1H), 4.08 (d, B of AB, J_{AB} = 15.0 Hz, 1H), 2.47–2.46 (m, 1H), 2.46 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 143.91 (e), 136.30 (e), 136.06 (e), 134.99 (e), 131.18 (o), 129.95 (o), 129.78 (o), 128.93 (o), 127.98 (o), 127.96 (o), 127.23 (o), 122.28 (e), 77.76 (e), 77.54 (o), 53.33 (o), 49.37 (e), 21.80 (o).

IR (neat) 3255 (m), 3032 (w), 2114 (w), 1598 (w), 1487 (m), 1349 (s), 1163 (s) cm^{-1}.

HRMS (CI, $M+H^+$) calcd for $C_{23}H_{21}{}^{79}BrNO_2S$ 454.0471, found 454.0478.



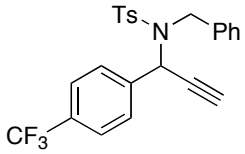
***N*-Benzyl-4-methyl-*N*-{1-[4-(trifluoromethyl) phenyl]propa1,2-dien-1-yl}benzenesulfonamide (3o).**

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.51 (d, J = 8.2 Hz, 2H), 7.26 (s, 4H), 7.14 (d, J = 8.0 Hz, 2H), 7.07–7.00 (m, 5H), 4.90 (s, 2H), 4.19 (s, 2H), 2.26 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 208.89 (e), 144.09 (e), 138.38 (e), 134.96 (e), 133.33 (e), 129.44 (o), 129.21 (e, q, J_{C-F} = 32.3 Hz), 129.10 (o), 128.36 (o), 128.13 (o), 127.99 (o), 126.02 (o), 124.89 (o, d, J_{C-F} = 3.1 Hz), 124.08 (e, q, J_{C-F} = 271.8 Hz), 112.16 (e), 85.72 (e), 54.72 (e), 21.48 (o).

IR (neat) 3665 (m), 2927 (s), 2257 (s), 1932 (s), 1733 (s), 1615 (s) cm^{-1}.

HRMS (CI, $M+H^+$) calcd for $C_{24}H_{21}F_3NO_2S$ 444.1240, found 444.1234.



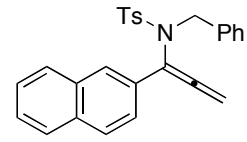
***N*-Benzyl-4-methyl-*N*-{1-[4-(trifluoromethyl) phenyl]prop-2-yn-1-yl}benzenesulfonamide (2o).**

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.11 (d, J = 8.2 Hz, 2H), 7.78 (d, J = 8.0 Hz, 2H), 7.67-7.57 (m, 4H), 7.32-7.23 (m, 5H), 6.51 (s, 1H), 4.97 (d, A of AB, J_{AB} = 15.0 Hz, 1H), 4.38 (d, B of AB, J_{AB} = 14.9 Hz, 1H), 2.81 (d, J = 2.3 Hz, 1H), 2.78 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 143.79 (e), 139.64 (e), 135.85 (e), 135.46 (e), 129.79 (e, q, J_{C-F} = 32.2 Hz), 129.58 (o), 128.77 (o), 128.29 (o), 127.65 (o), 127.07 (o), 124.61 (o, d, J_{C-F} = 3.8 Hz), 123.82 (e, q, J_{C-F} = 272.2 Hz), 78.09 (o), 76.68 (e), 53.08 (o), 49.20 (e), 21.47 (o).

IR (neat) 3305 (s), 2927 (s), 2122 (w), 1621 (s), 1599 (s), 1496 (s), 1326 (s) cm^{-1}.

HRMS (CI, $M+H^+$) calcd for $C_{24}H_{21}F_3NO_2S$ 444.1240, found 444.1230.



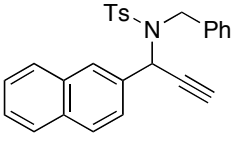
***N*-Benzyl-4-methyl-*N*-(1-napthylpropa-1,2-dien-1-yl)benzenesulfonamide (3p).**

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.85-7.70 (m, 6H), 7.48-7.20 (m, 10H), 5.13 (s, 2H), 4.53 (s, 2H), 2.48 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 209.59 (e), 143.73 (e), 135.45 (e), 134.35 (e), 133.18 (e), 132.89 (e), 131.44 (e), 129.37 (o), 129.19 (o), 128.33 (o), 128.28 (o), 128.23 (o), 127.88 (o), 127.63 (o), 127.46 (o), 126.01 (o), 125.94 (o), 125.07 (o), 123.89 (o), 112.98 (e), 84.97 (e), 54.64 (e), 21.60 (o).

IR (neat) 3060 (m), 2924 (m), 2256 (m), 1930 (m), 1598 (s), 1349 (s) cm^{-1}.

HRMS (CI, $M+H^+$) calcd for $C_{27}H_{24}NO_2S$ 426.1522, found 426.1516.



***N*-Benzyl-4-methyl-*N*-[1-(2-napthnyl)prop-2-yn-1-yl]benzenesulfonamide (2p).**

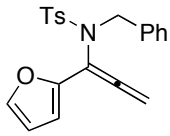
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.86-7.80 (m, 3H), 7.74-

7.69 (m, 2H), 7.61 (d, J = 8.6 Hz, 1H), 7.51 (d, J = 8.6 Hz, 1H), 7.46-7.41 (m, 2H), 7.33 (d, J = 8.2 Hz, 2H), 6.96-6.83 (m, 5H), 6.32 (s, 1H), 4.52 (d, A of AB, J_{AB} = 15.2 Hz, 1H), 4.19 (d, B of AB, J_{AB} = 15.2 Hz, 1H), 2.53 (d, J = 2.3 Hz, 1H), 2.47 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 143.53 (e), 136.28 (e), 136.11 (e), 132.90 (e), 132.86 (e), 132.64 (e), 129.48 (o), 128.57 (o), 128.00 (o), 127.92 (o), 127.82 (o), 127.44 (o), 127.41 (o), 127.18 (o), 126.74 (o), 126.23 (o), 125.98 (o), 125.90 (o), 77.97 (e), 77.21 (o), 53.91 (o), 49.09 (e), 21.56 (o).

IR (neat) 3293 (m), 3062 (m), 1599 (m), 1339 (s), 1162 (s) cm^{-1}.

HRMS (CI, M+H$^+$) calcd for $C_{27}H_{24}NO_2S$ 426.1522, found 426.1511.



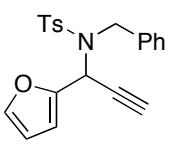
***N*-Benzyl-*N*-[1-(2-furyl)propa-1,2-dien-1-yl]-4-methylbenzenesulfonamide (3q).**

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.71 (d, J = 8.2 Hz, 2H), 7.30 (d, J = 8.0 Hz, 2H), 7.24-7.19 (m, 6H), 6.32-6.29 (m, 2H), 5.08 (s, 2H), 4.38 (s, 2H), 2.43 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 208.34 (e), 147.80 (e), 143.79 (e), 142.20 (o), 135.40 (e), 134.20 (e), 129.39 (o), 128.92 (o), 128.26 (o), 128.19 (o), 127.84 (o), 111.65 (o), 109.36 (o), 105.62 (e), 85.86 (e), 54.43 (e), 21.59 (o).

IR (neat) 3403 (m), 2925 (s), 1796 (s), 1731 (s), 1599 (s), 1496 (s), 1456 (s), 1343 (s) cm^{-1}.

HRMS (CI, M+H$^+$) calcd for $C_{21}H_{20}NO_3S$ 366.1158, found 366.1156.



***N*-Benzyl-*N*-[1-(2-furyl)prop-2-yn-1-yl]-4-methylbenzenesulfonamide (2q).**

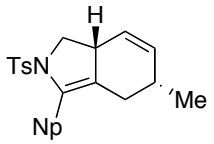
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.75 (d, J = 8.2 Hz, 2H), 7.29 (d, J = 8.2 Hz, 2H), 7.15-7.07 (m, 6H), 6.23 (d, J = 3.1 Hz, 1H), 6.14 (d, J = 1.6 Hz, 1H), 6.08-6.06 (m, 1H), 4.50 (d,

A of AB, J_{AB} = 15.7 Hz, 1H), 4.22 (d, B of AB, J_{AB} = 15.7 Hz, 1H), 2.44 (s, 3H), 2.34 (d, J = 2.4 Hz, 1H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 148.51 (e), 143.50 (e), 143.01 (o), 136.41 (e), 129.40 (o), 127.90 (o), 127.78 (o), 126.83 (o), 110.35 (o), 110.21 (o), 76.68 (e), 75.02 (o), 48.69 (e), 47.90 (o), 21.54 (o).

IR (neat) 3291 (m), 3033 (w), 2925 (m), 2124 (w), 1599 (m), 1497 (m), 1339 (s), 1163 (s) cm^{-1}.

HRMS (CI, M+H$^+$) calcd for $C_{21}H_{20}NO_3S$ 366.1158, found 366.1156.



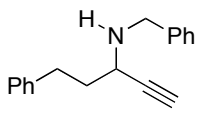
5-Methyl-2-[(4-methylphenyl)sulfonyl]-3-(2-naphthyl)-2,4,5,7a-tetrahydro-1*H*-isoindole (5).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.85–7.77 (m, 4H), 7.64–7.59 (m, 3H), 7.49–7.44 (m, 2H), 7.24 (d, J = 6.8 Hz, 2H), 5.66–5.63 (m, 1H), 5.40 (dd, J = 9.9, 2.1 Hz, 1H), 4.32 (dd, J = 12.3, 8.3 Hz, 1H), 3.42 (t, J = 12.3 Hz, 1H), 2.76 (t, J = 10.0 Hz, 1H), 2.45–2.42 (m, 1H), 2.40 (s, 3H), 2.34–2.24 (m, 2H), 0.61 (d, J = 6.8 Hz, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 143.62 (e), 136.86 (e), 134.72 (e), 133.94 (o), 133.16 (e), 132.98 (e), 130.41 (e), 130.32 (e), 129.37 (o), 128.06 (o), 127.79 (o), 127.48 (o), 127.22 (o), 126.12 (o), 125.99 (o), 125.67 (o), 56.79 (e), 40.93 (o), 31.43 (o), 29.48 (e), 21.61 (o), 21.01 (o).

IR (neat) 2956 (w), 1598 (w), 1455 (w), 1352 (s), 1166 (s) cm^{-1}.

HRMS (CI, M+H$^+$) calcd for $C_{26}H_{26}NO_2S$ 416.1679, found 416.1679.



***N*-Allyl-[1-(2-phenylethyl)prop-2-yn-1-yl]amine (7).**

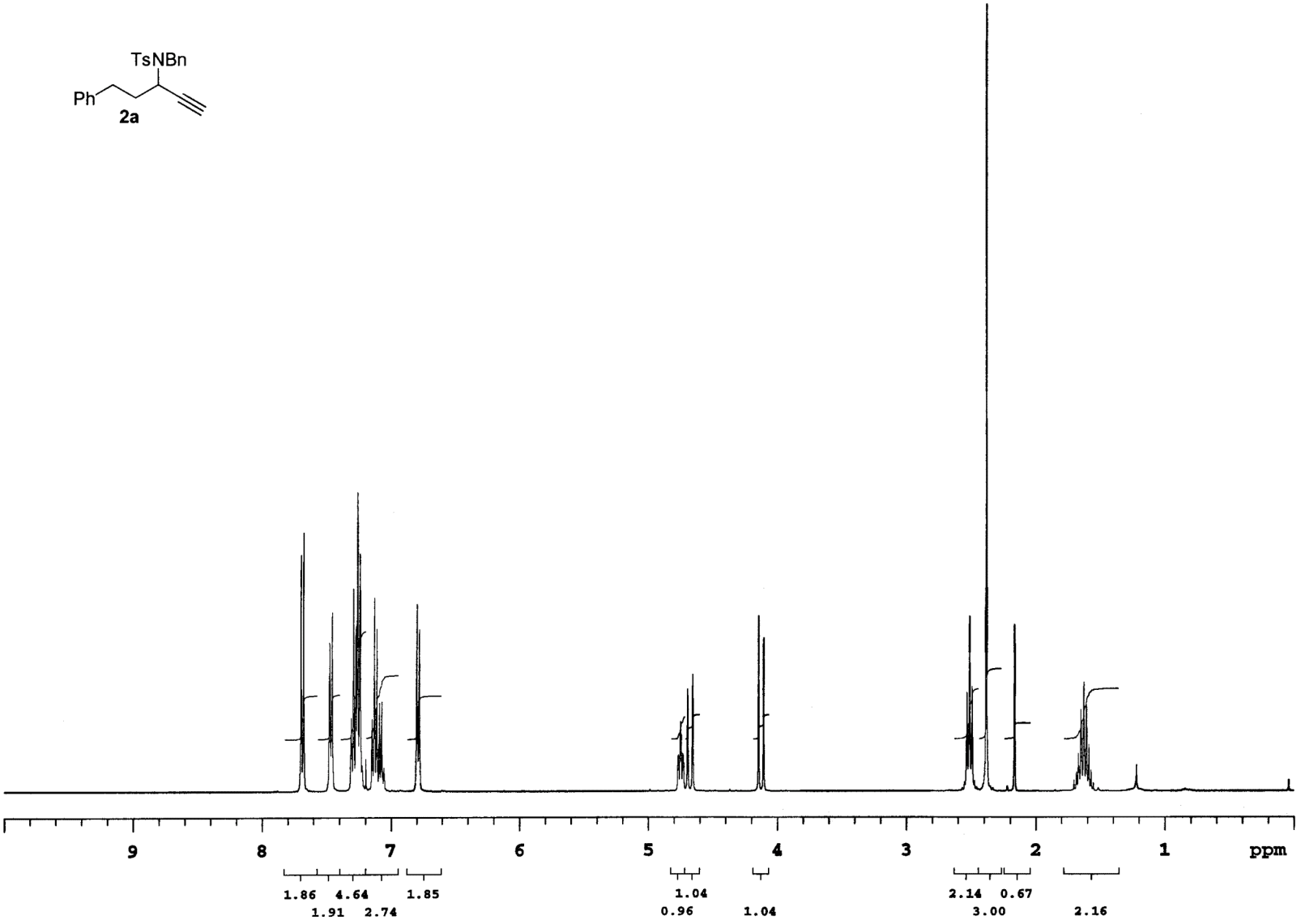
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.31–7.18 (m, 5H), 5.91 (ddt, J = 16.4, 10.6, 6.2 Hz, 1H), 5.22 (dq, J = 17.2, 1.7 Hz, 1H), 5.11 (dd, J = 10.4, 1.6 Hz, 1H), 3.50 (ddt, A of ABMX, J_{AB}

= 13.7, J_{AM} = 5.8, J_{AX} = 1.5 Hz, 1H), 3.39 (ddd, J = 8.0, 6.1, 2.1 Hz, 1H), 3.26 (ddt, B of ABMX, J_{AB} = 13.7, J_{BM} = 6.4, J_{BX} = 1.3 Hz, 1H), 2.86 (ddd, A of ABMX, J_{AB} = 13.8, J_{AM} = 9.1, J_{AX} = 6.3 Hz, 1H), 2.80 (ddd, B of ABMX, J_{AB} = 13.8, J_{BM} = 9.1, J_{BX} = 6.9 Hz, 1H), 2.35 (d, J = 2.2 Hz, 1H), 2.03–1.89 (m, 2H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 141.47 (e), 136.30 (o), 128.46 (o), 128.34 (o), 125.88 (o), 116.25 (e), 85.09 (e), 71.88 (o), 49.90 (e), 48.80 (o), 37.50 (e), 32.14 (e).

IR (neat) 3299 (s), 2925 (m), 1644 (w), 1603 (w), 1497 (m), 1455 (s) cm^{-1}.

HRMS (CI, $M+H^+$) calcd for $C_{14}H_{18}N$ 200.1434, found 200.1430.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9
8
7
6
5
4
3
2
1
ppm
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1.85
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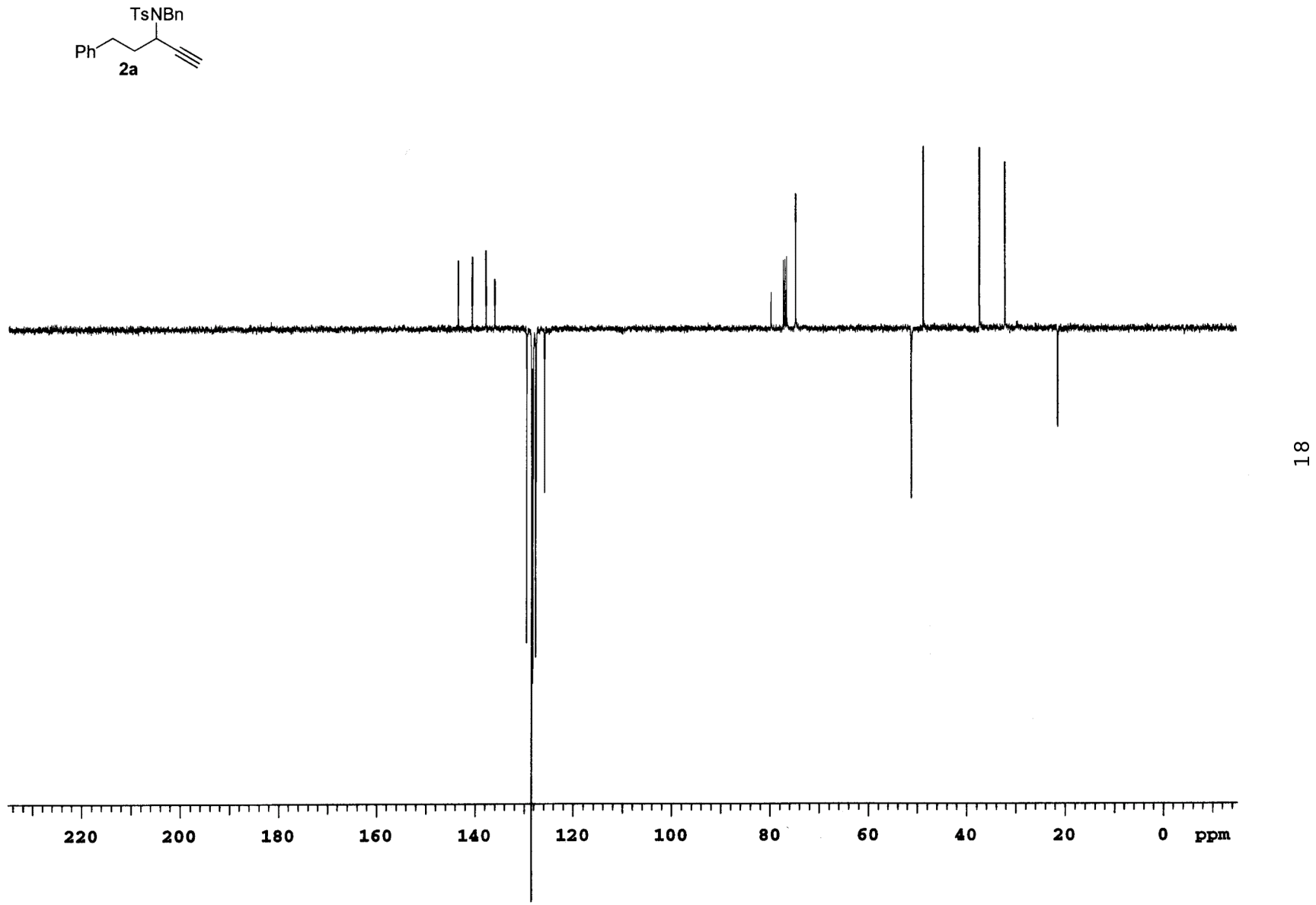
2.74
1.04
0.96
1.04
2.14
0.67
3.00
2.16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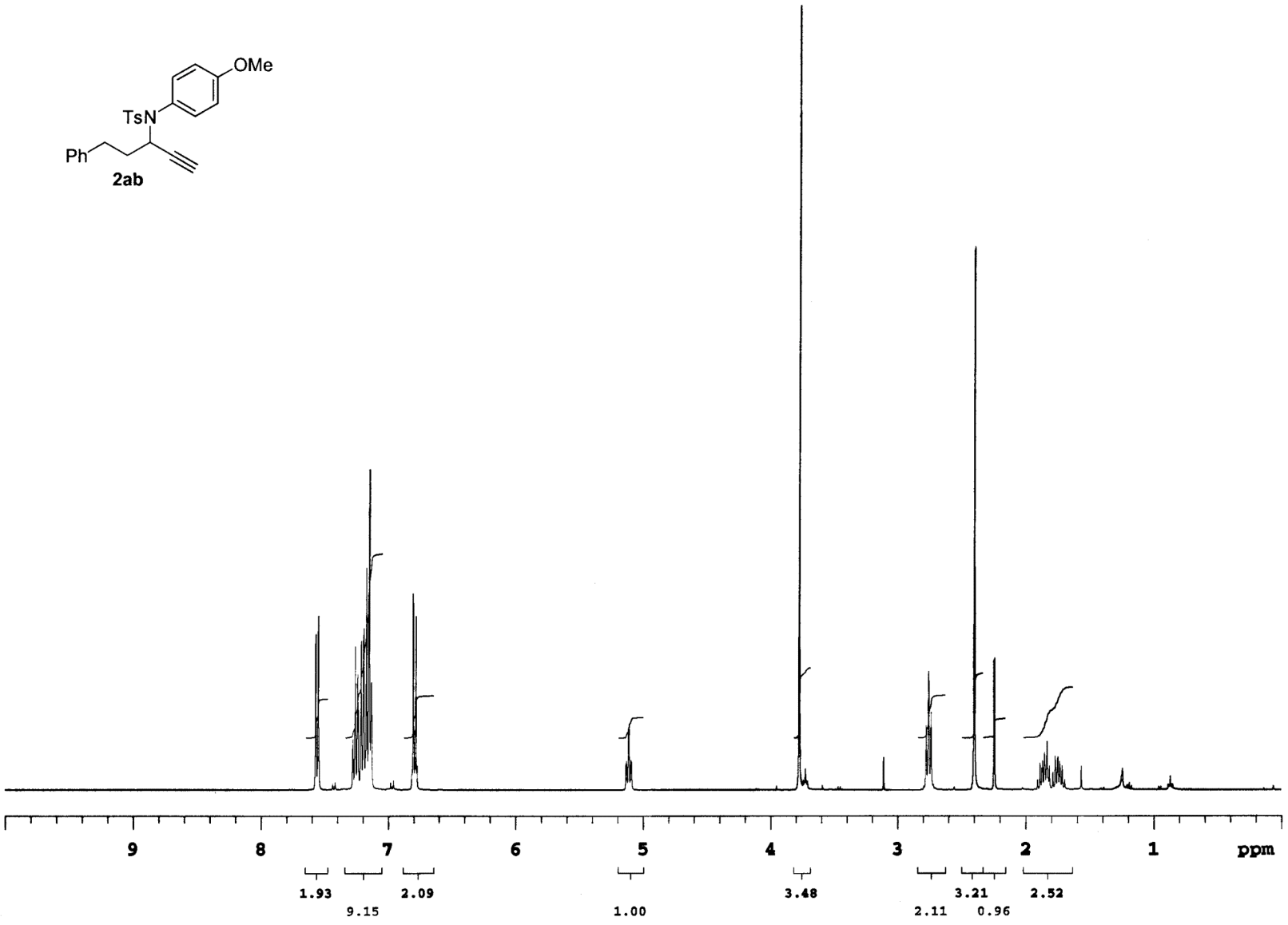
Ph
2a
220
200
180
160
140
120
100
80
60
40
20
0
ppm


OMe
TsN
Ph
2ab
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8
7
6
5
4
3
2
1
ppm
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9.15
2.09
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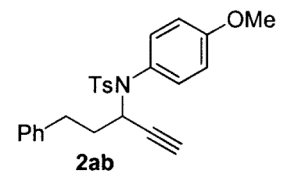
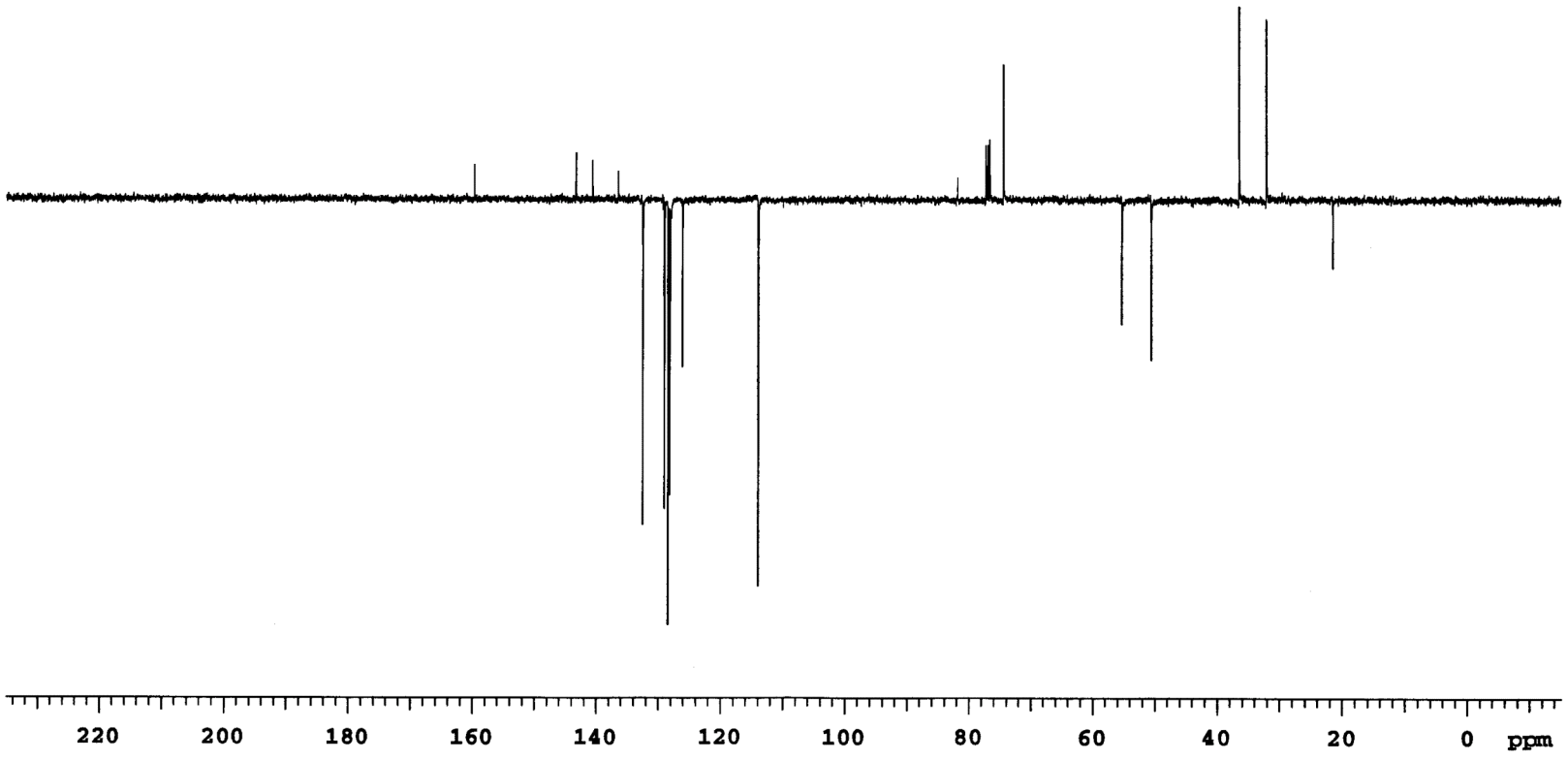
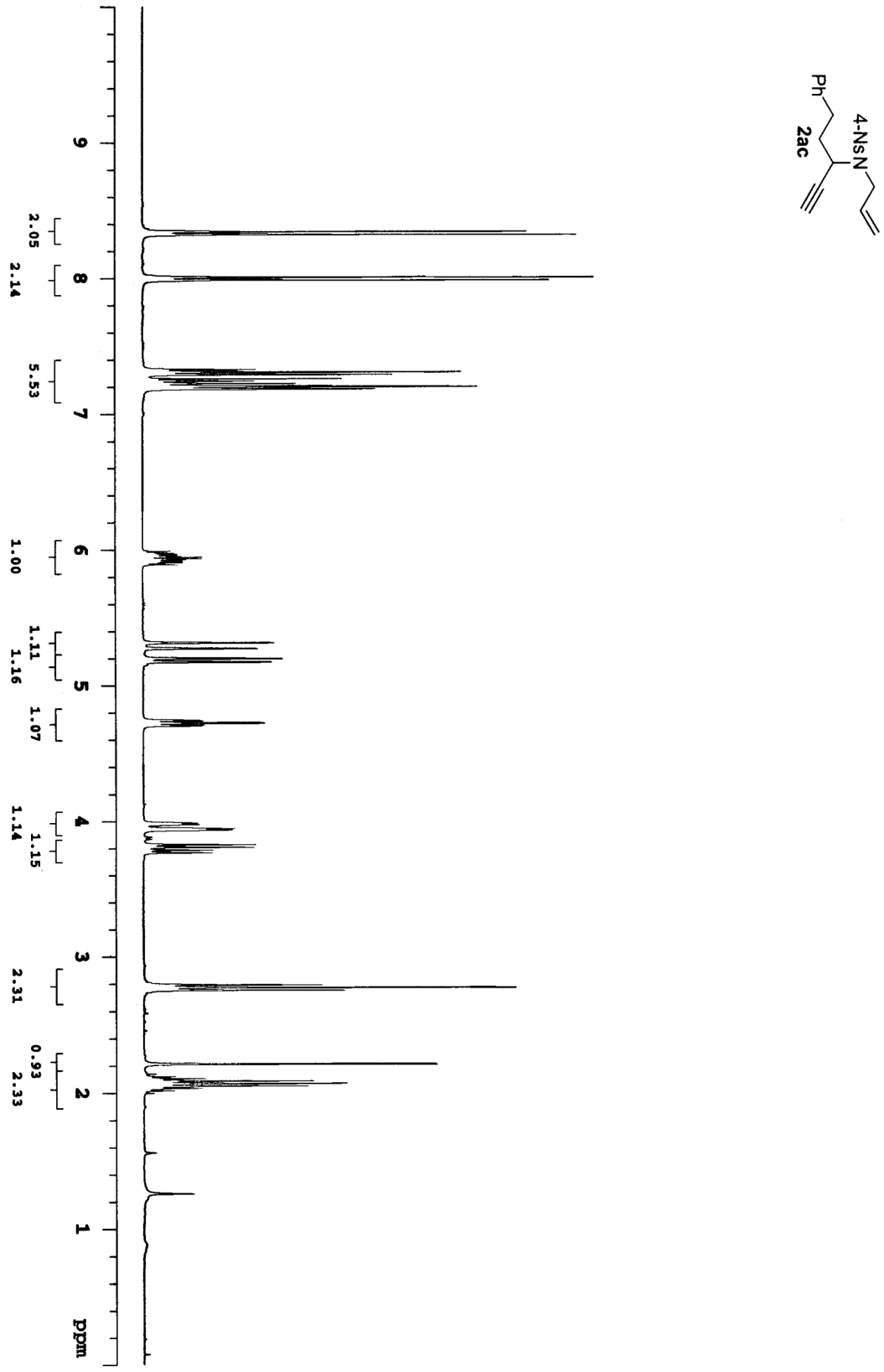
3.48
2.11
3.21
0.96
2.52



2ab

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Ph
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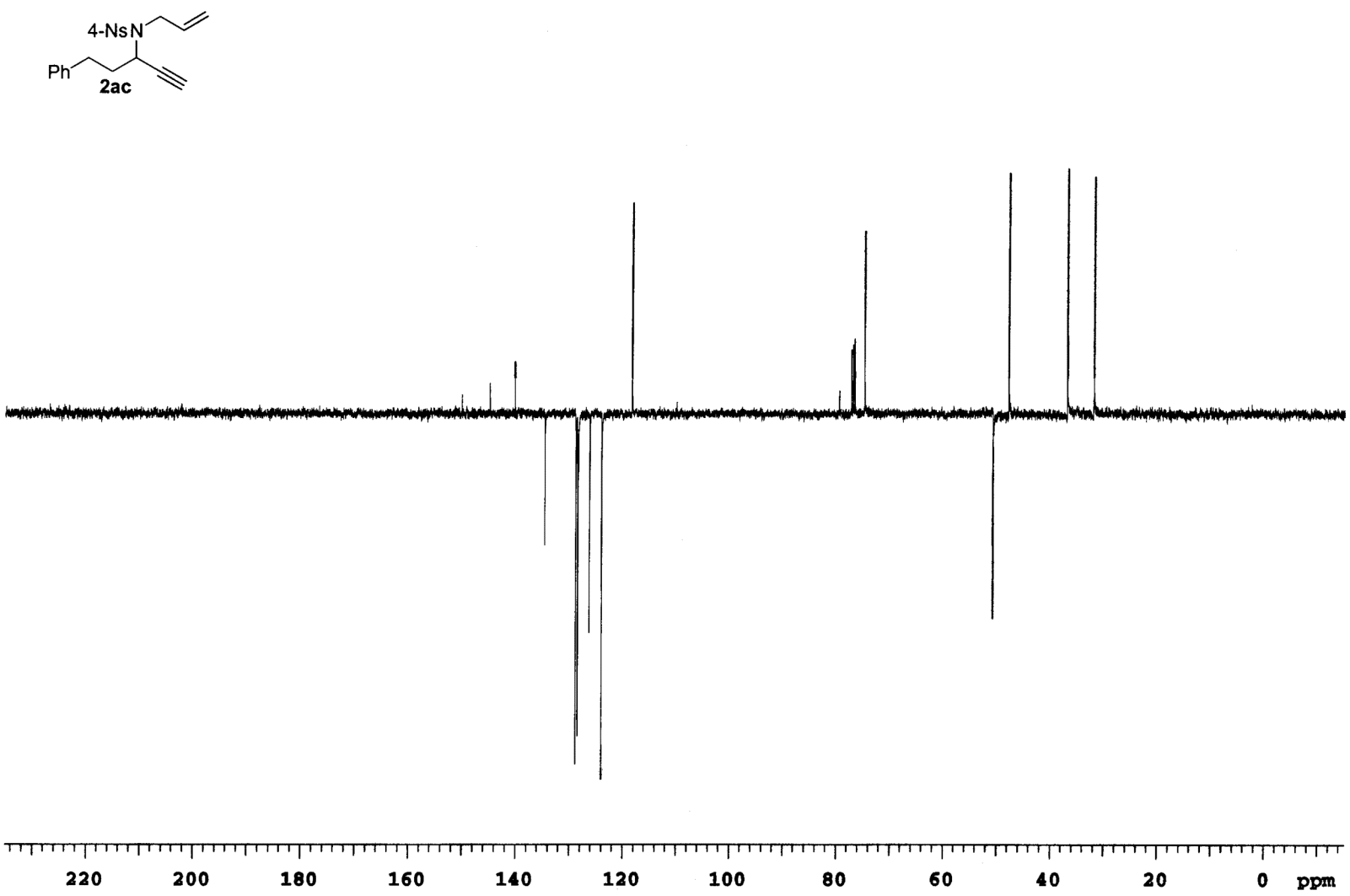
8
7
6
5
4
3
2
1
ppm
2.05
2.14
5.53
1.00
1.11
1.16
1.07
1.14
1.15
2.31
0.93
2.33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Ph
2ac
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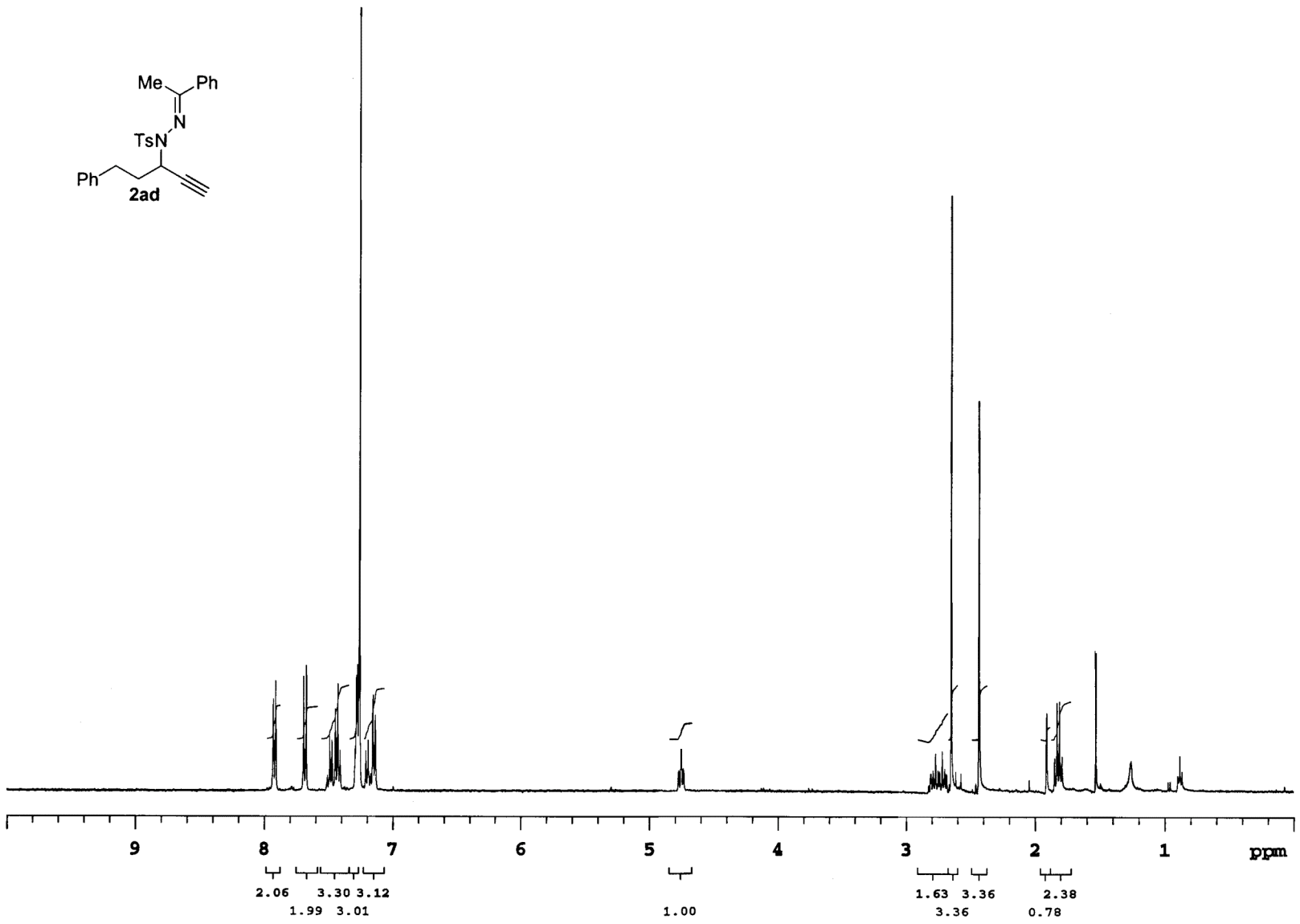
140
120
100
80
60
40
20
0
ppm


Me
Ph
N
TsN
Ph
2ad
9
8
7
6
5
4
3
2
1
ppm
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3.30
3.12
1.99
3.01
1.00
1.63
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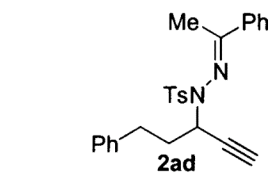
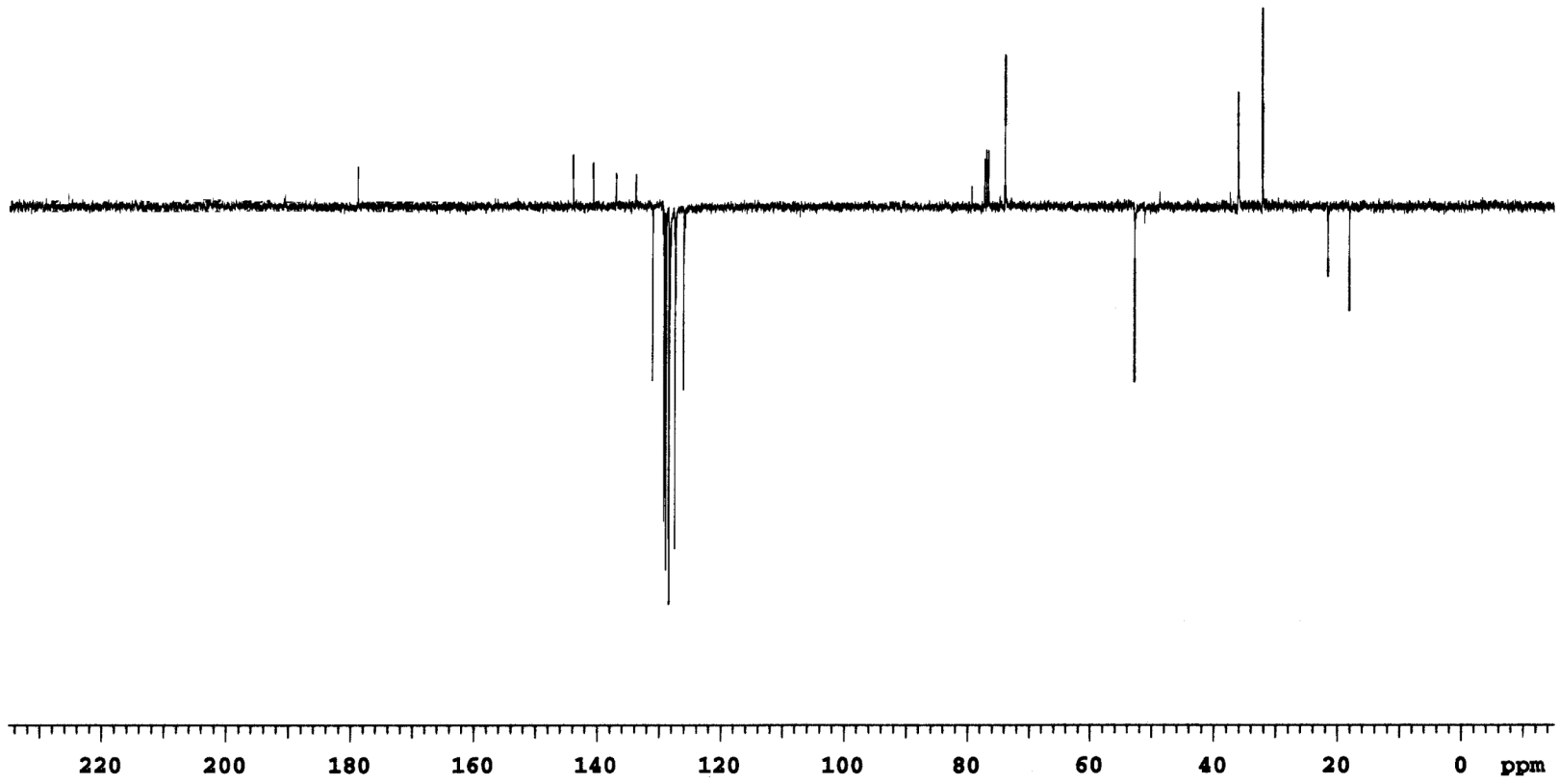
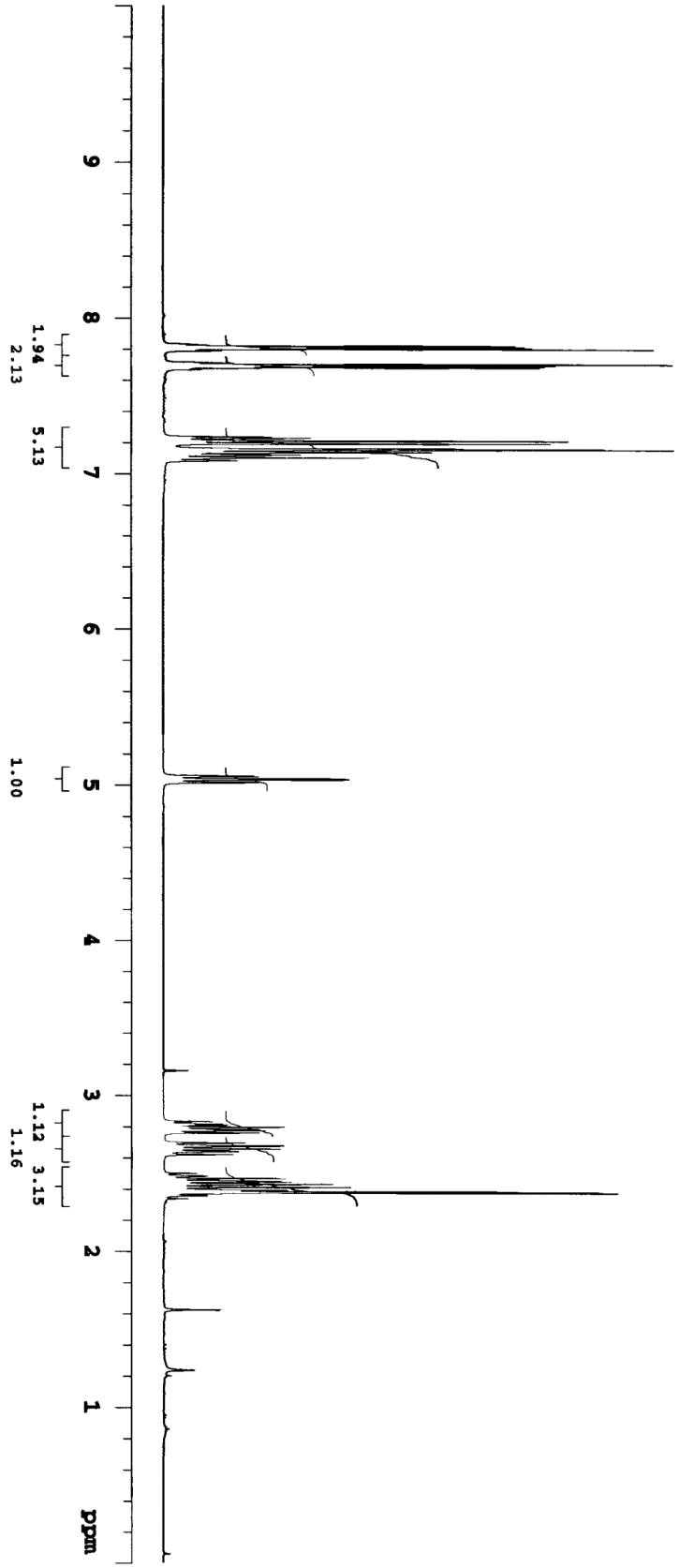
2.38
3.36
0.78



2ad

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8
7
6
5
4
3
2
1
ppm
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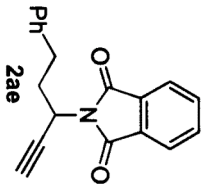
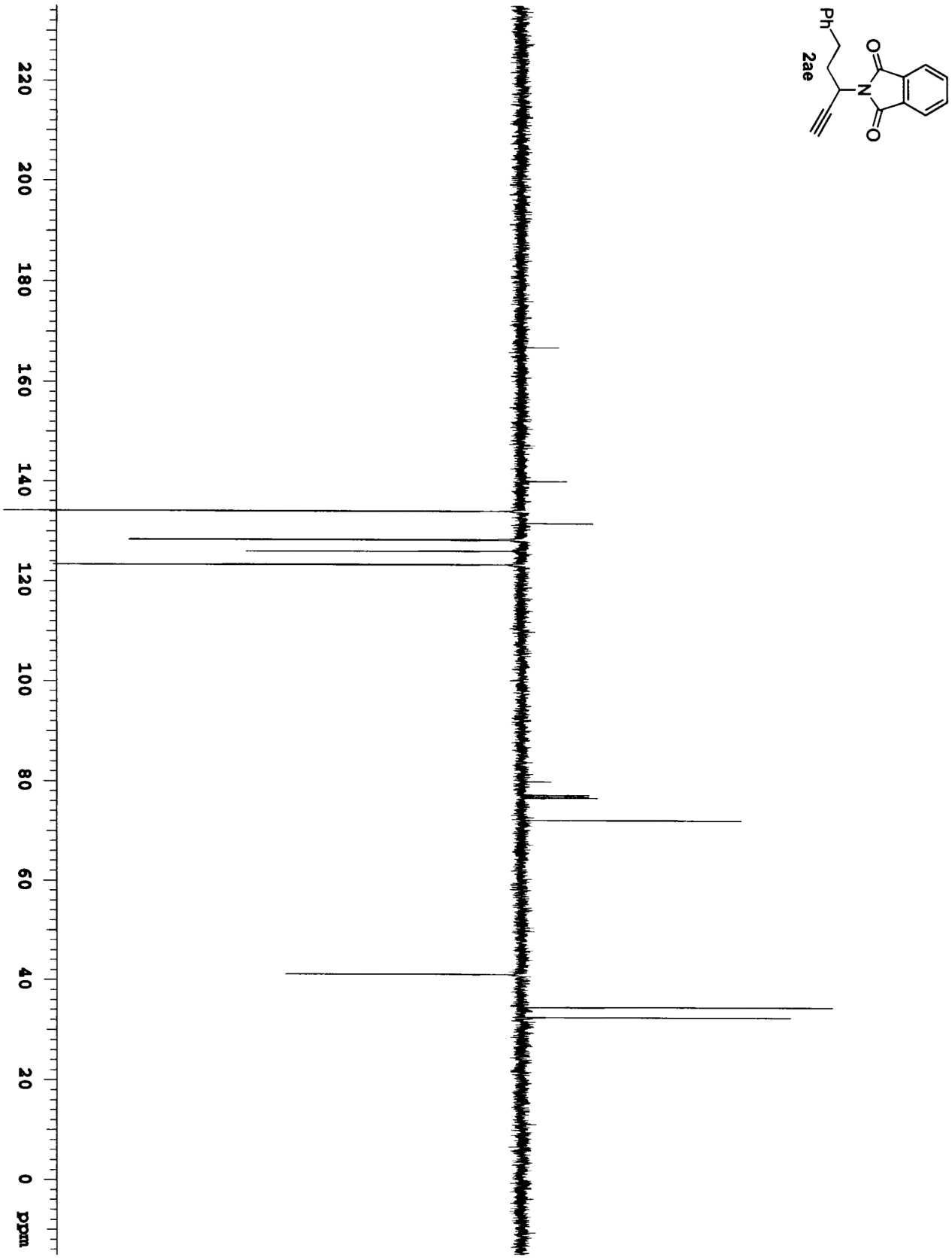
2.13
5.13
1.00
1.12
1.16
3.15


Ph
2ae
O
N
O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N
O
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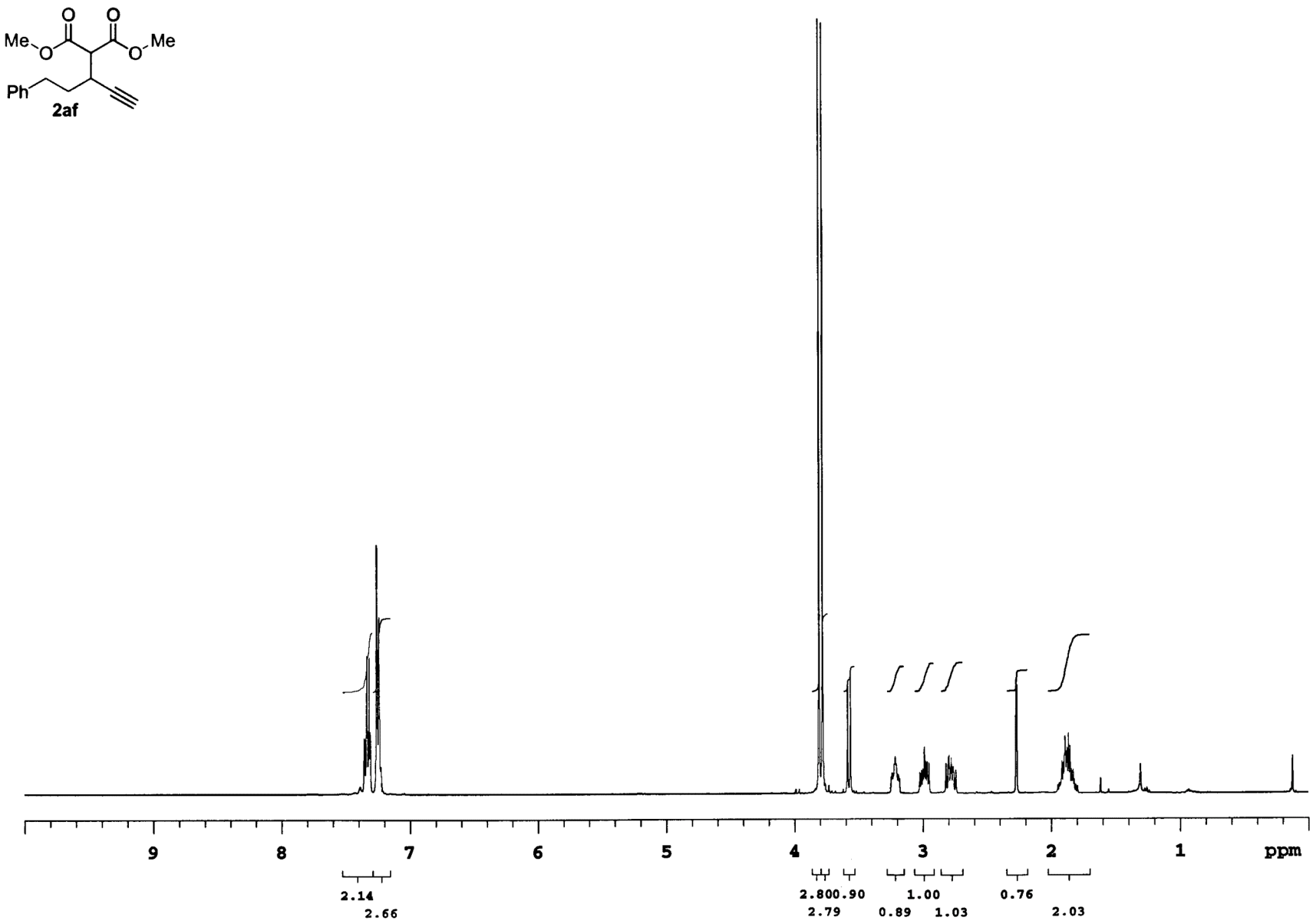
140
120
100
80
60
40
20
0
ppm


Me
O
O
O
O
Me
Ph
2af
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8
7
6
5
4
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2
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ppm
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2.80
2.79
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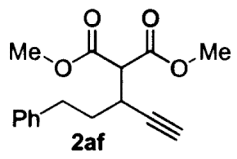
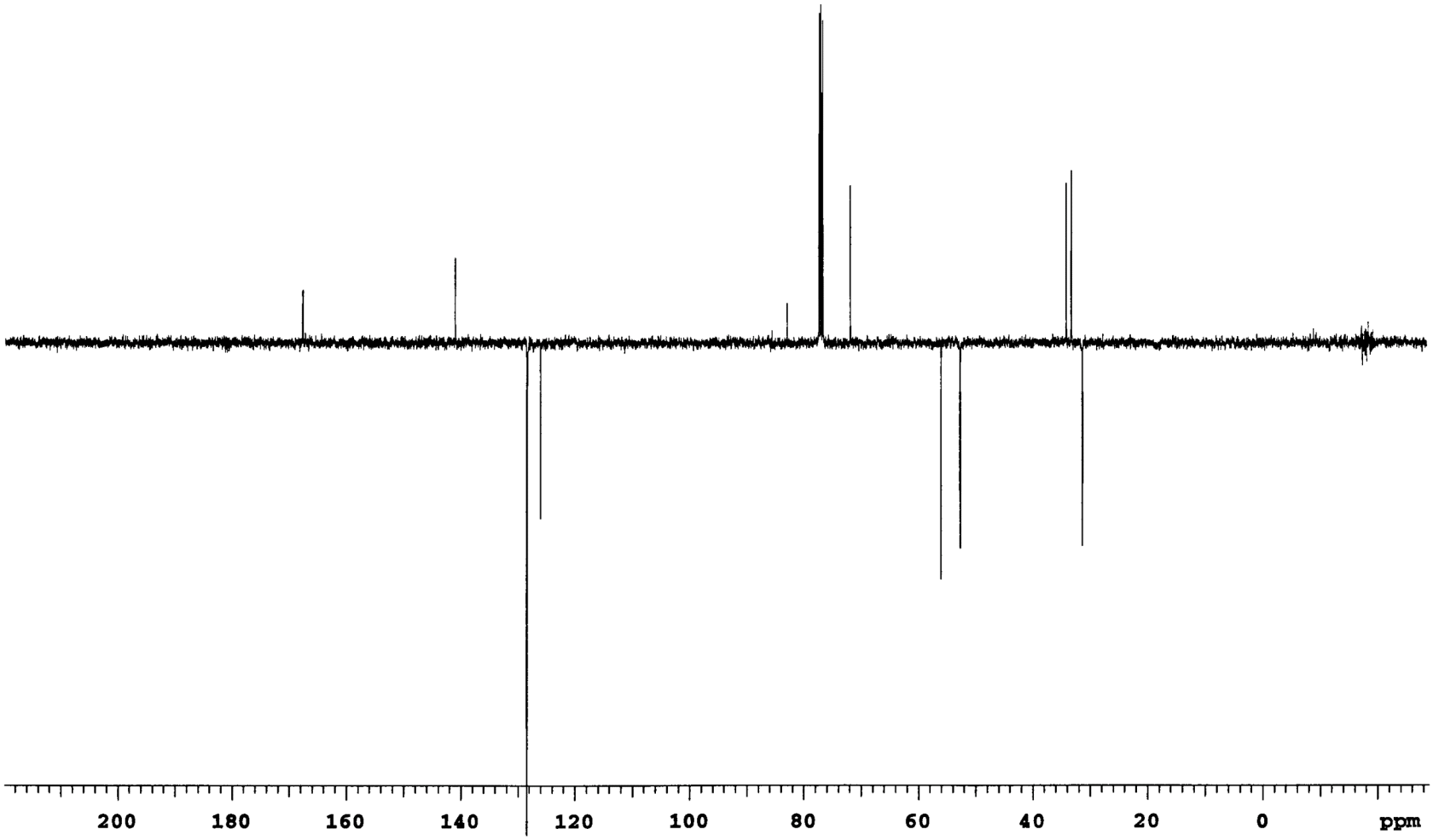
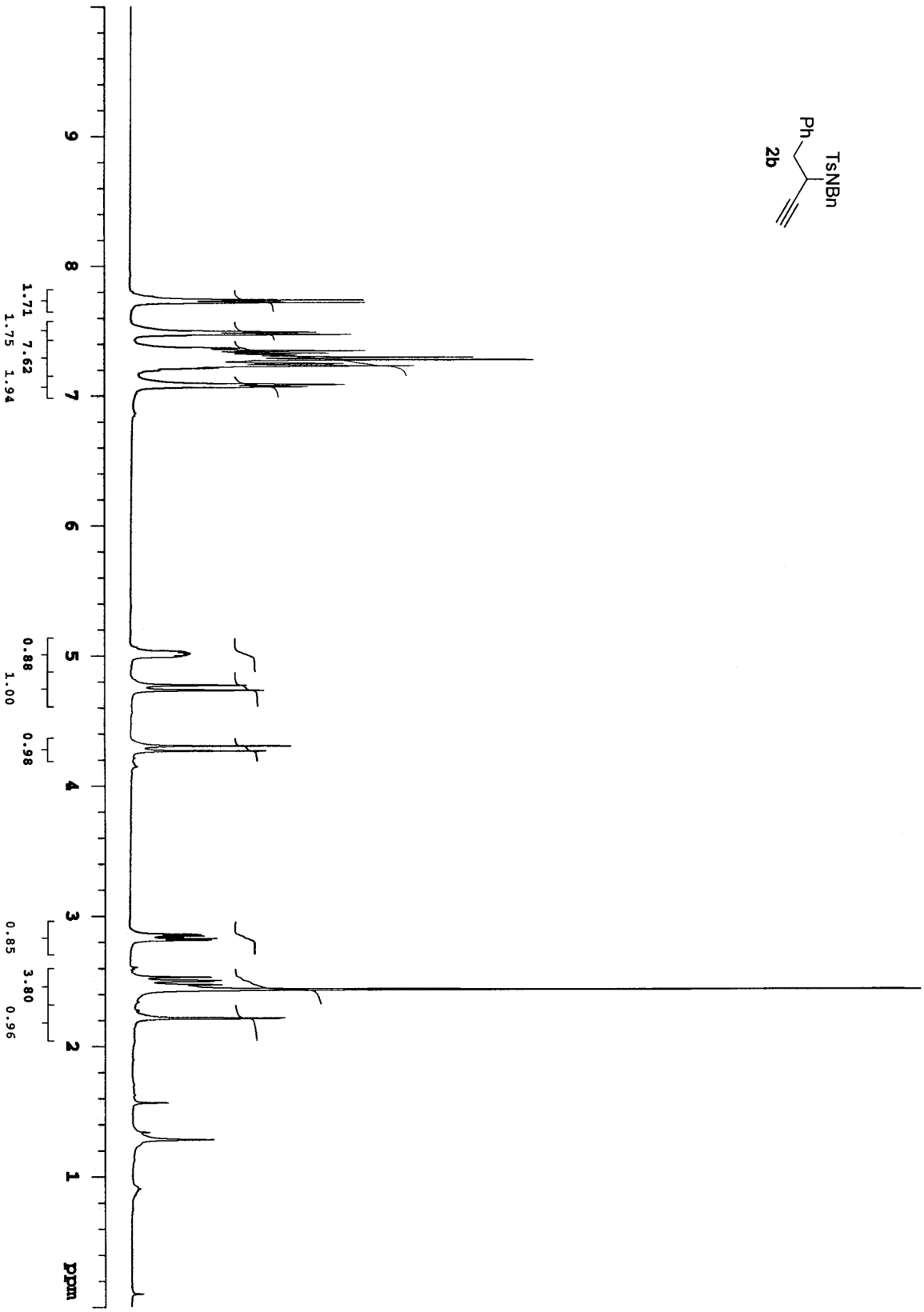
1.03
0.76
2.03



2af

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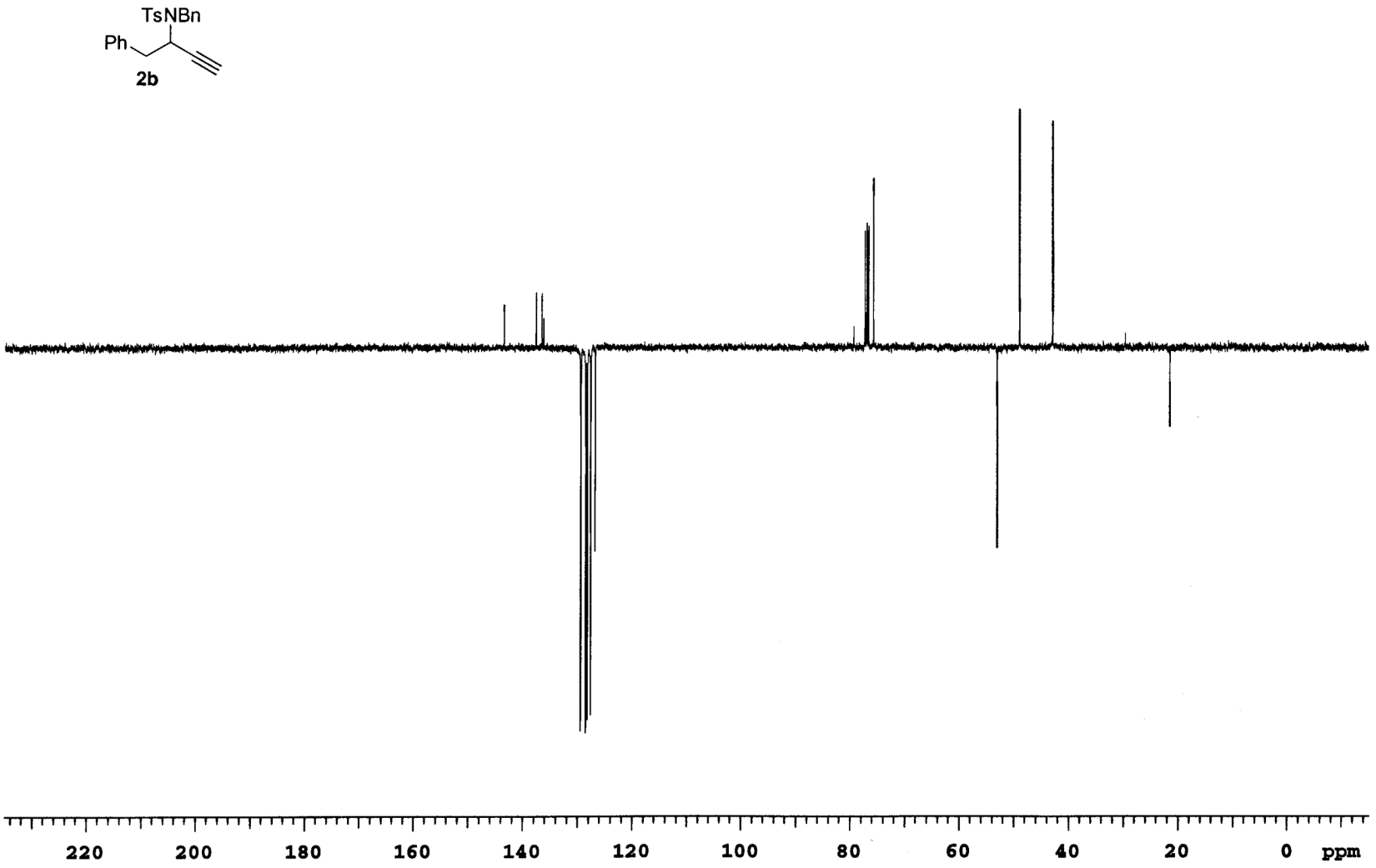
3.80
0.96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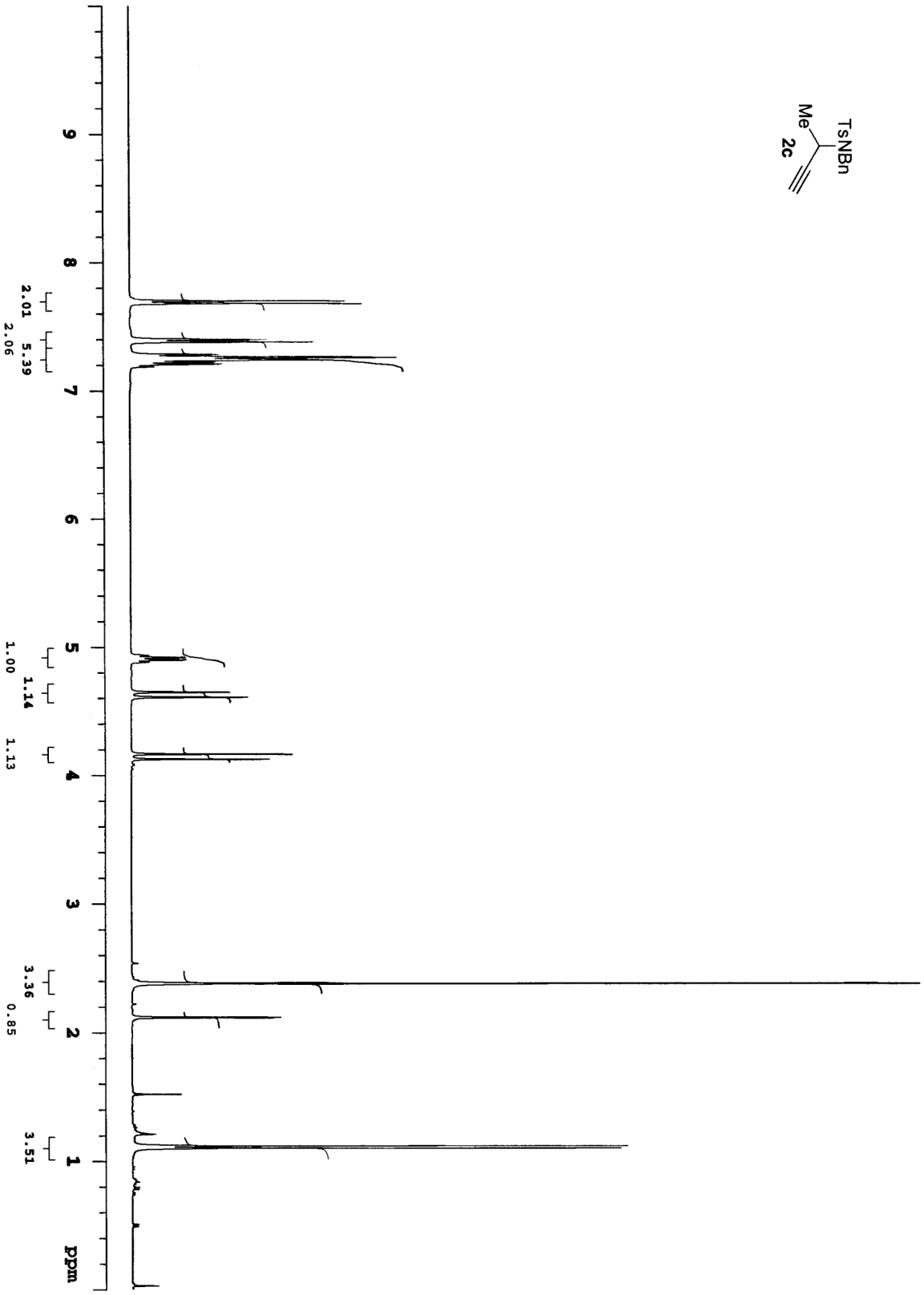
0
ppm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Me
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7
6
5
4
3
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1
ppm
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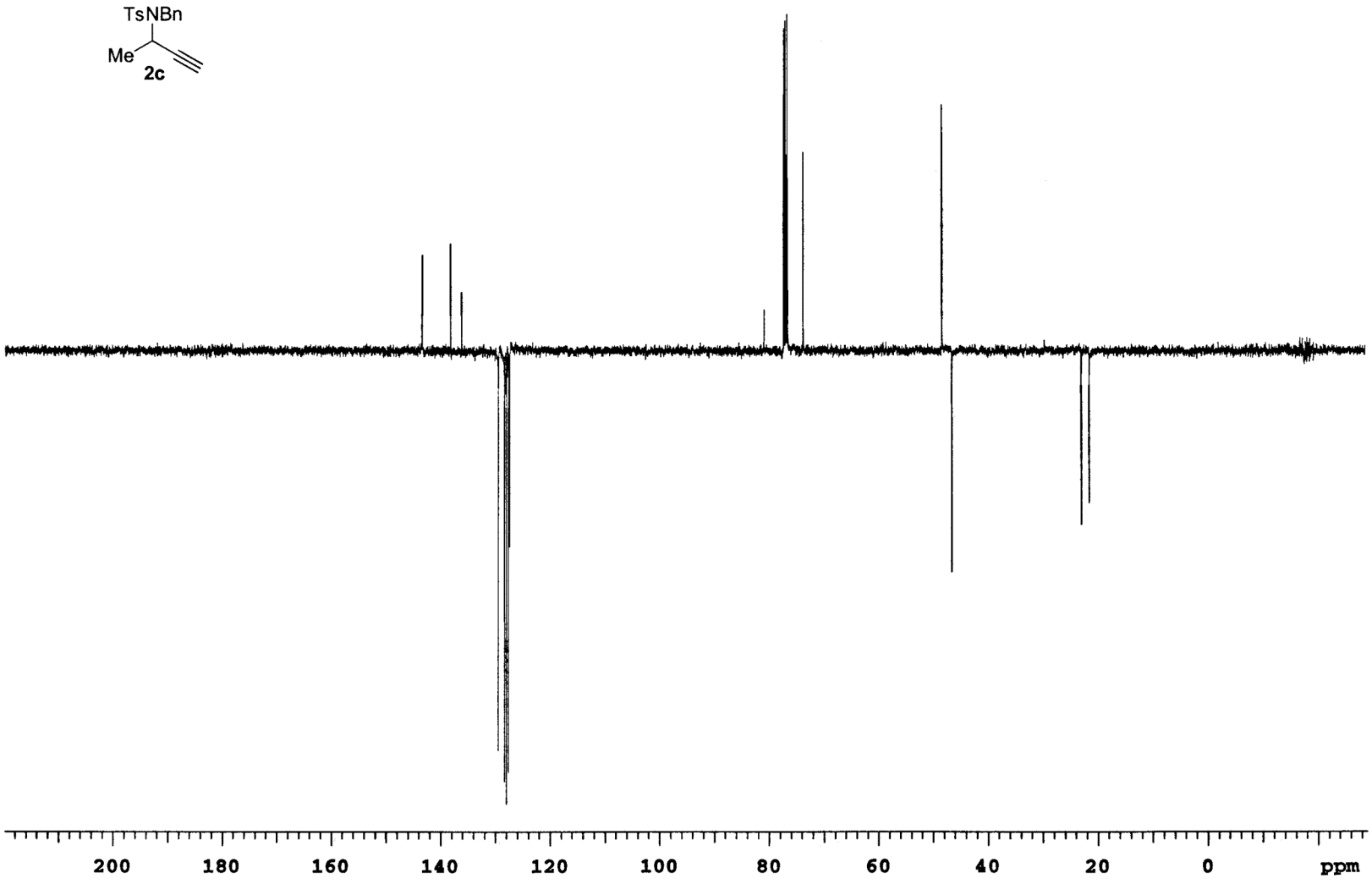
3.51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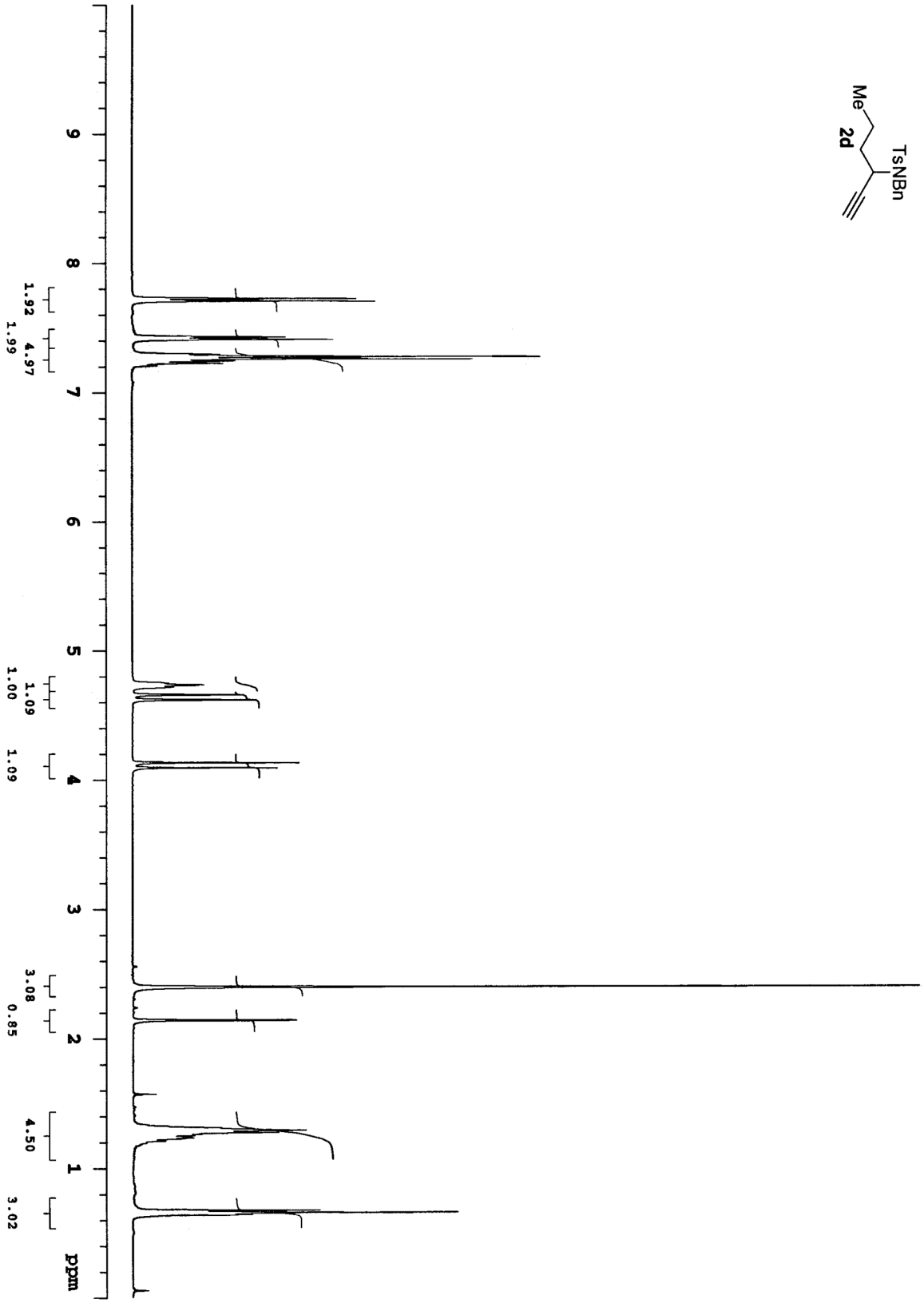
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6
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1.09
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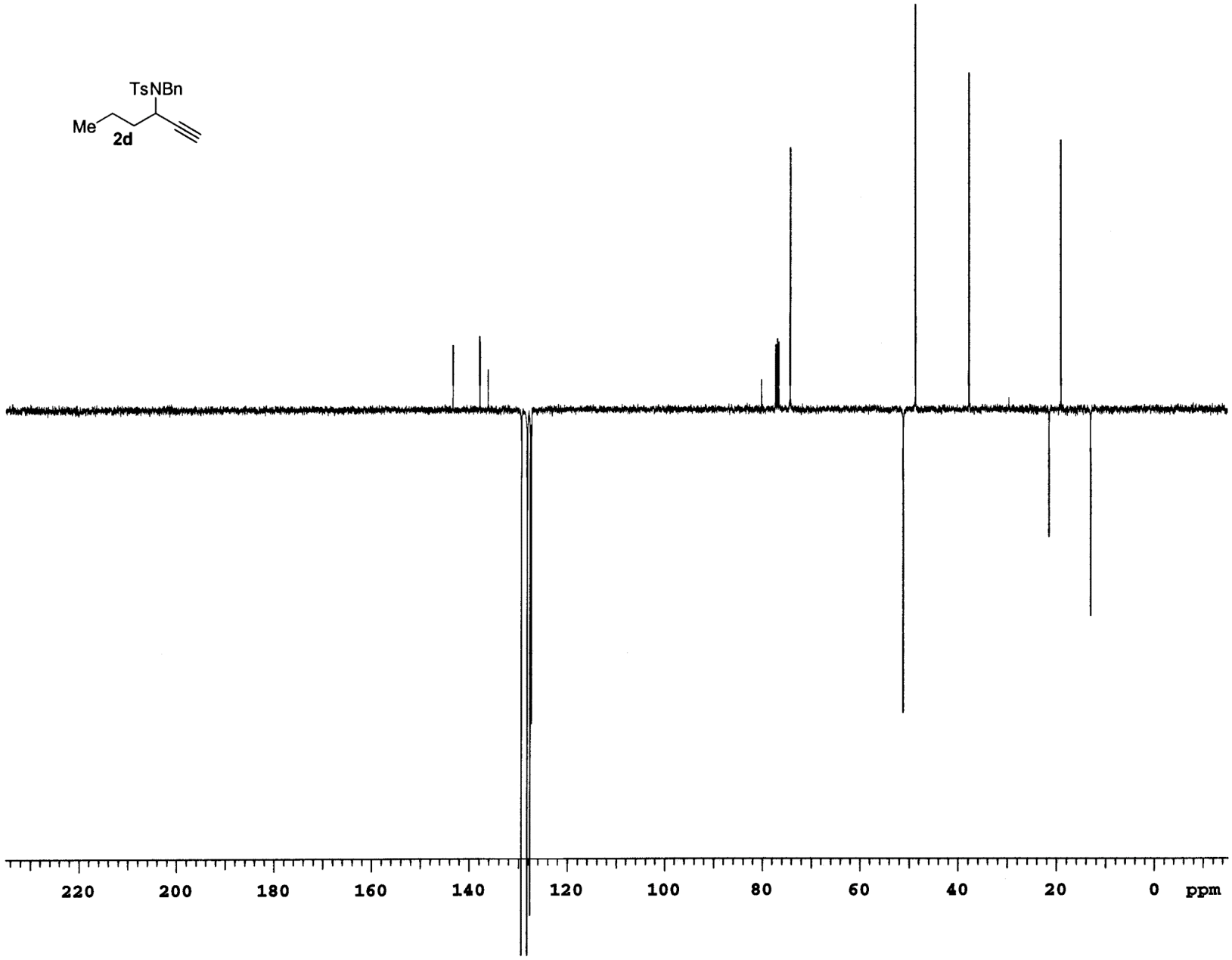
4.50
3.02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0
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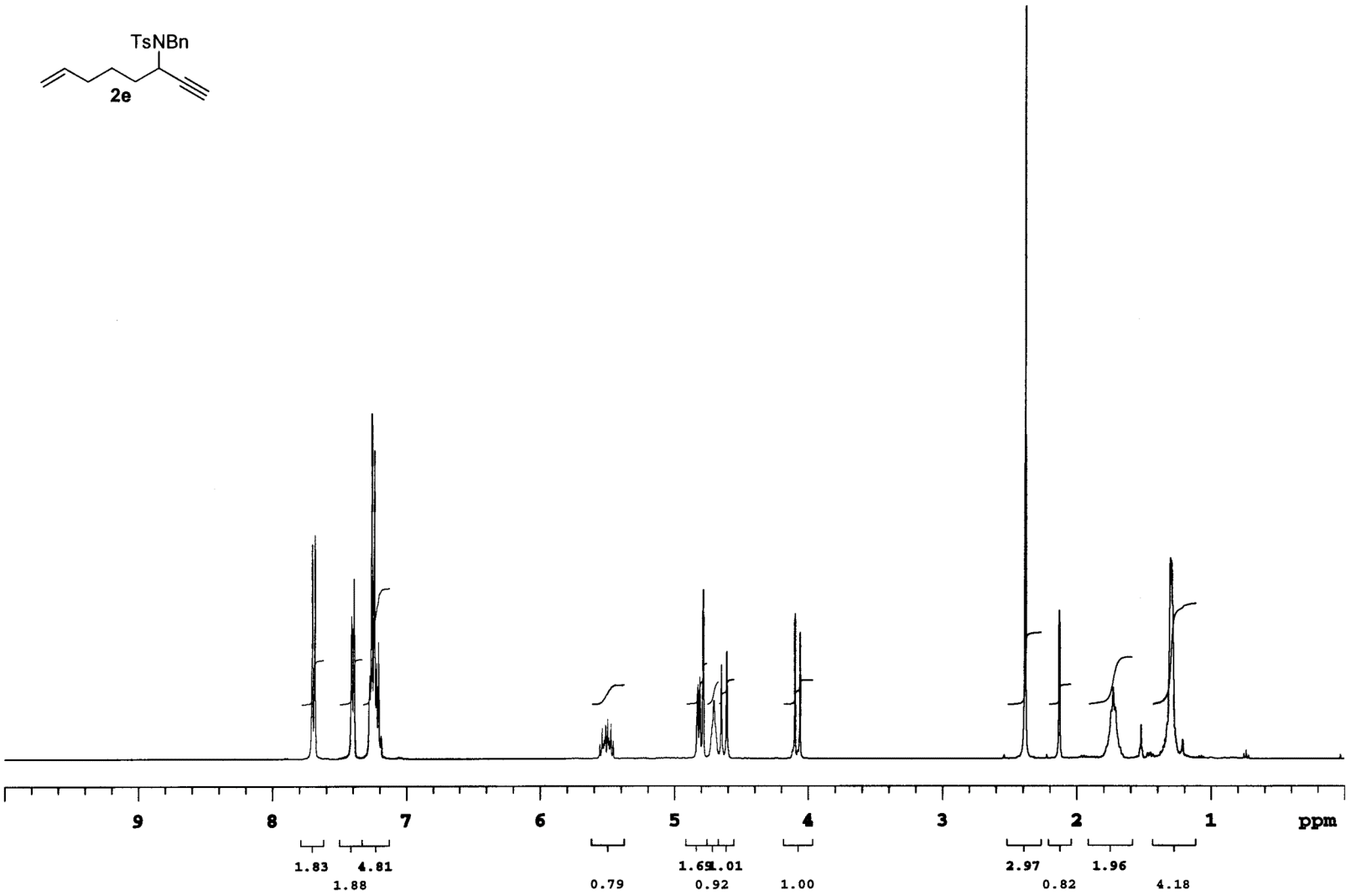
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ppm
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1.01
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1.00
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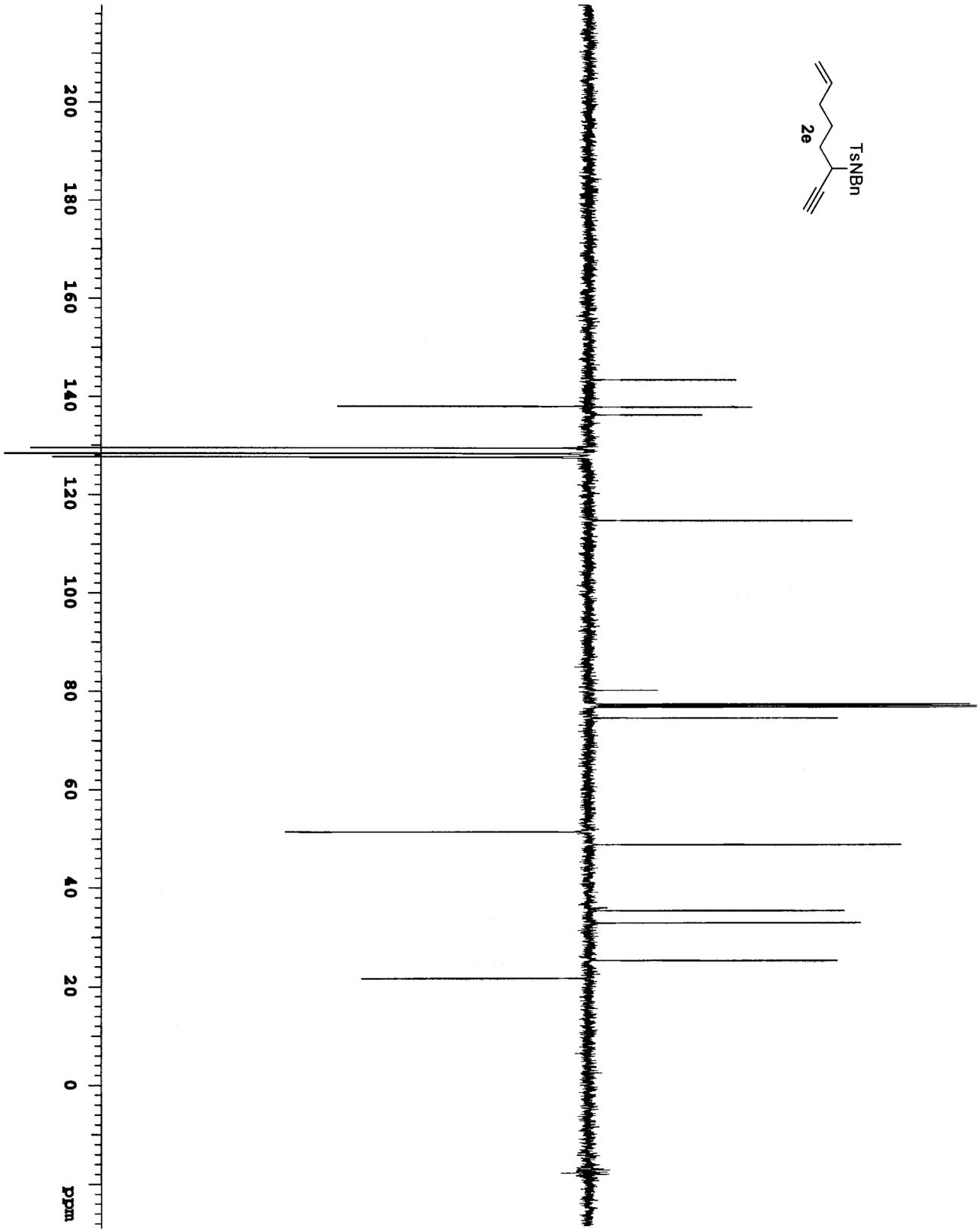
4.18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120
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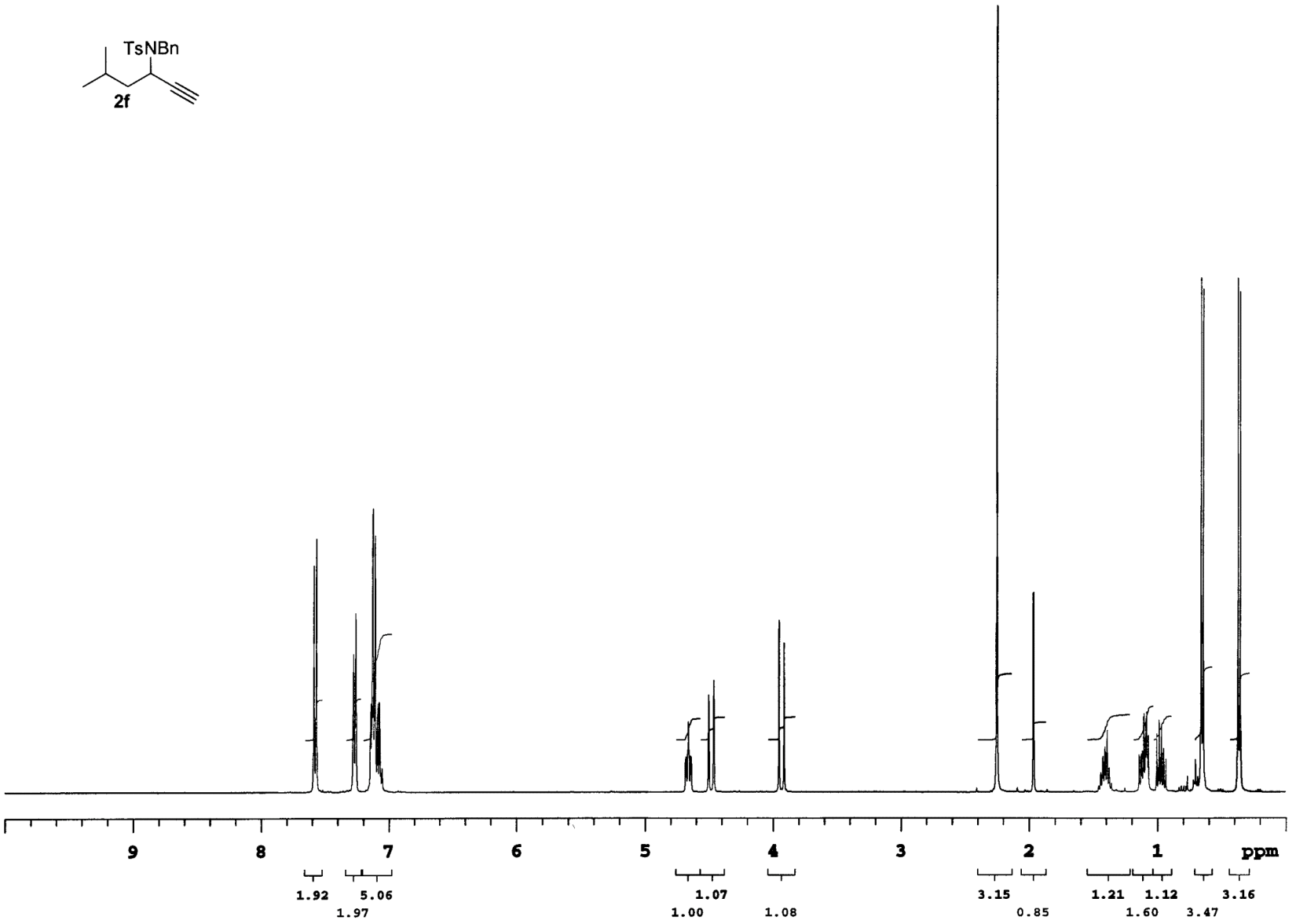
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4
3
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ppm
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1.08
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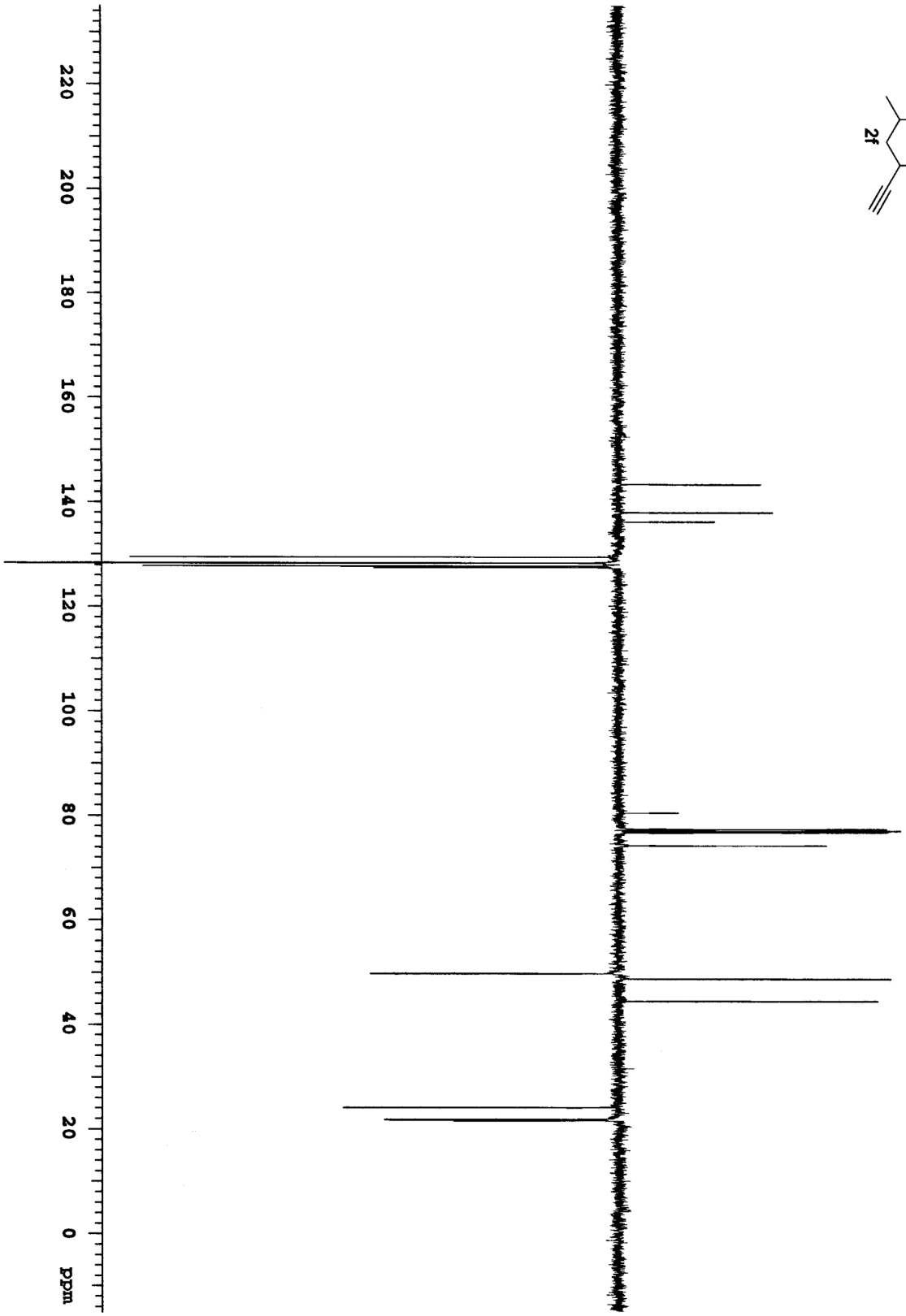
3.16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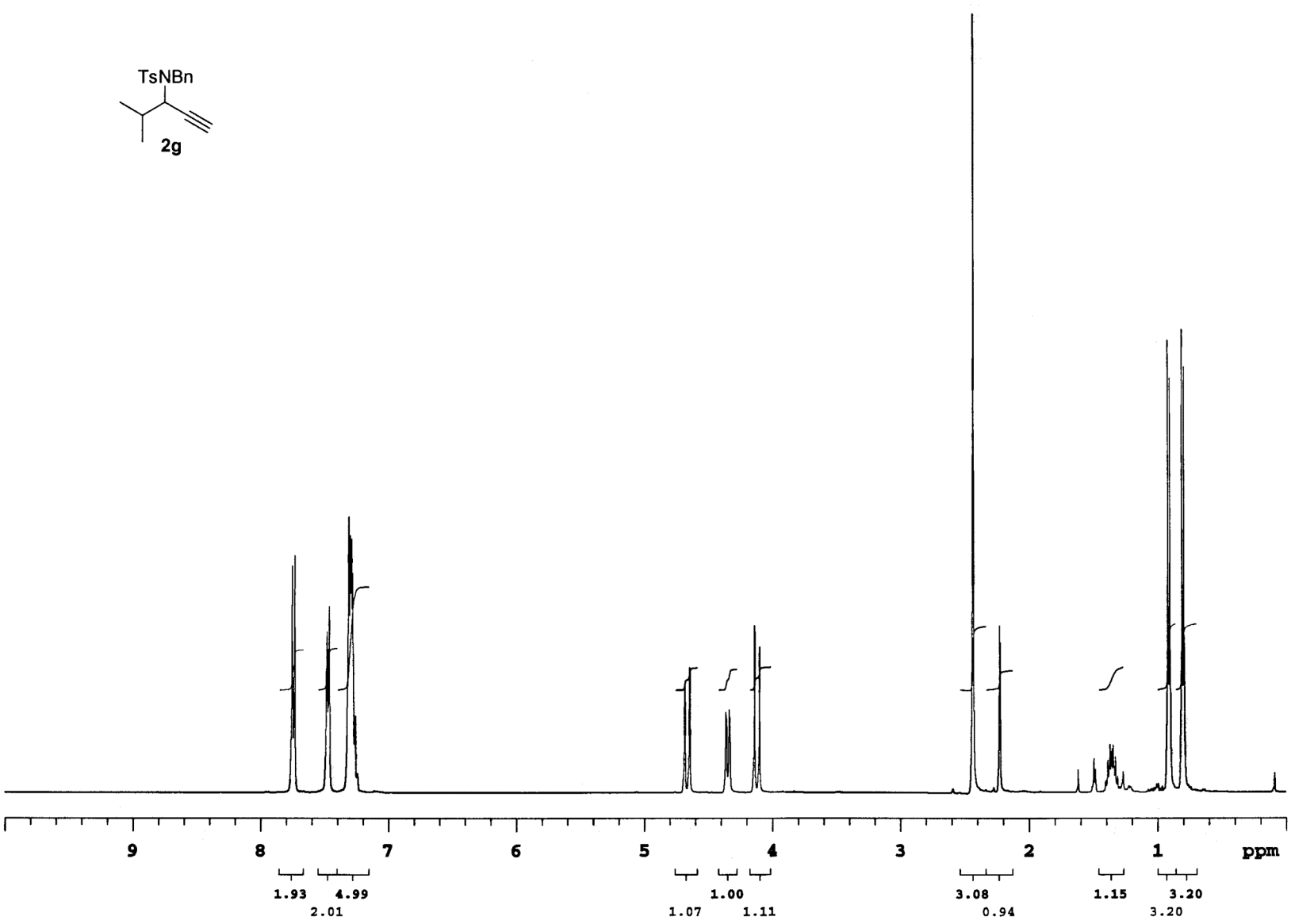
ppm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7
6
5
4
3
2
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ppm
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1.07
1.00
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3.08
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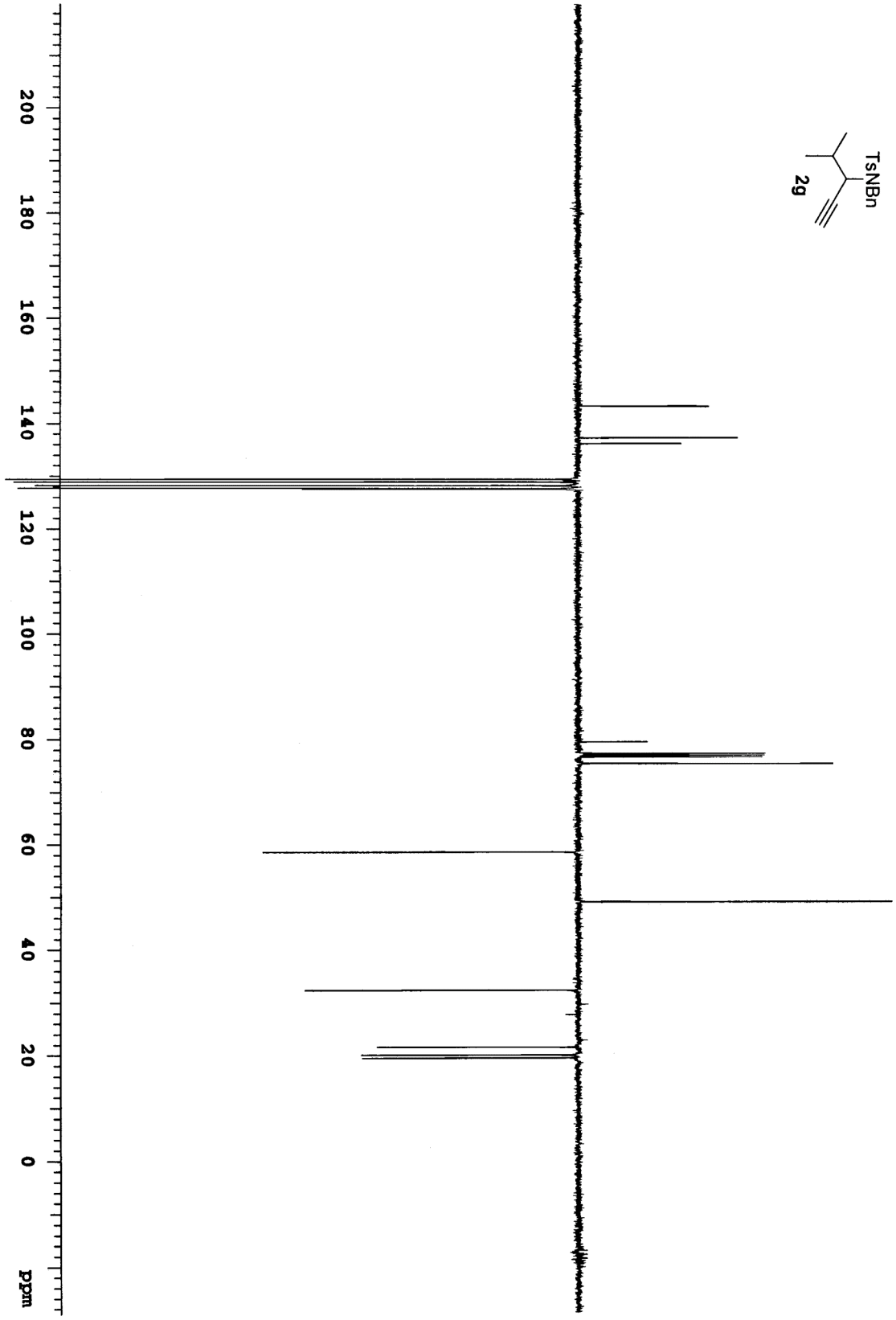
3.20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40
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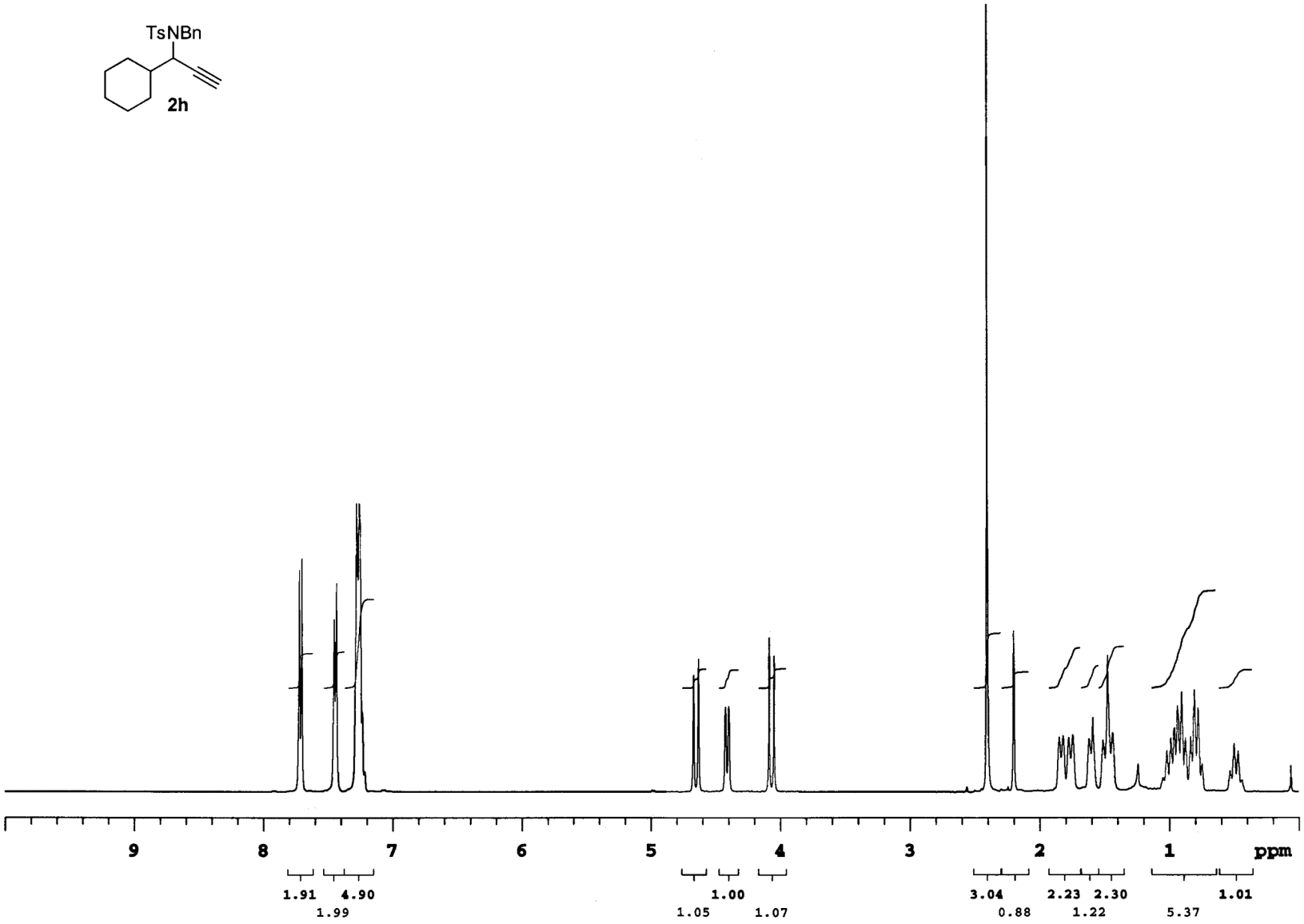
ppm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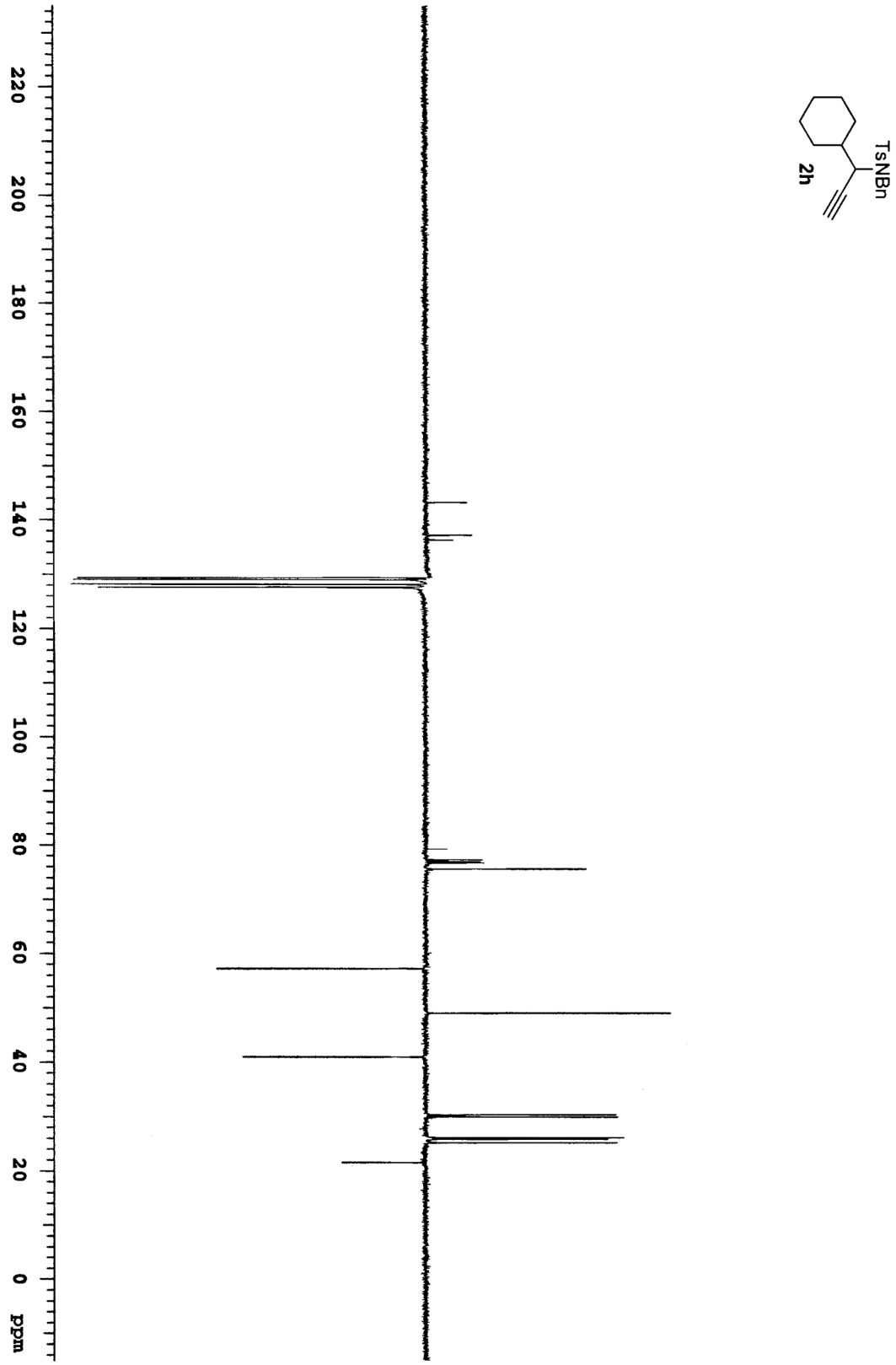
1.01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2h
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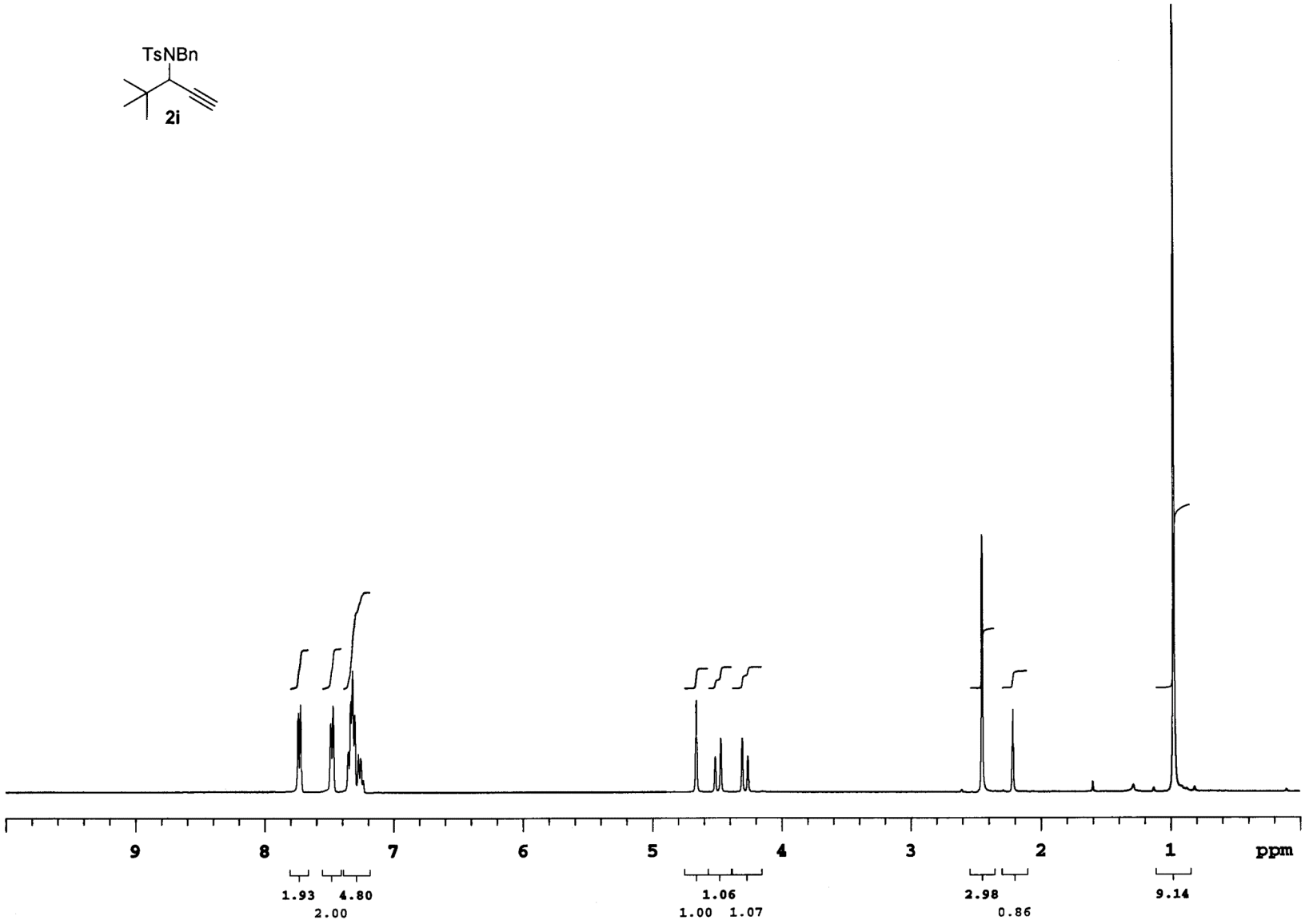
ppm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2i
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8
7
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1.00
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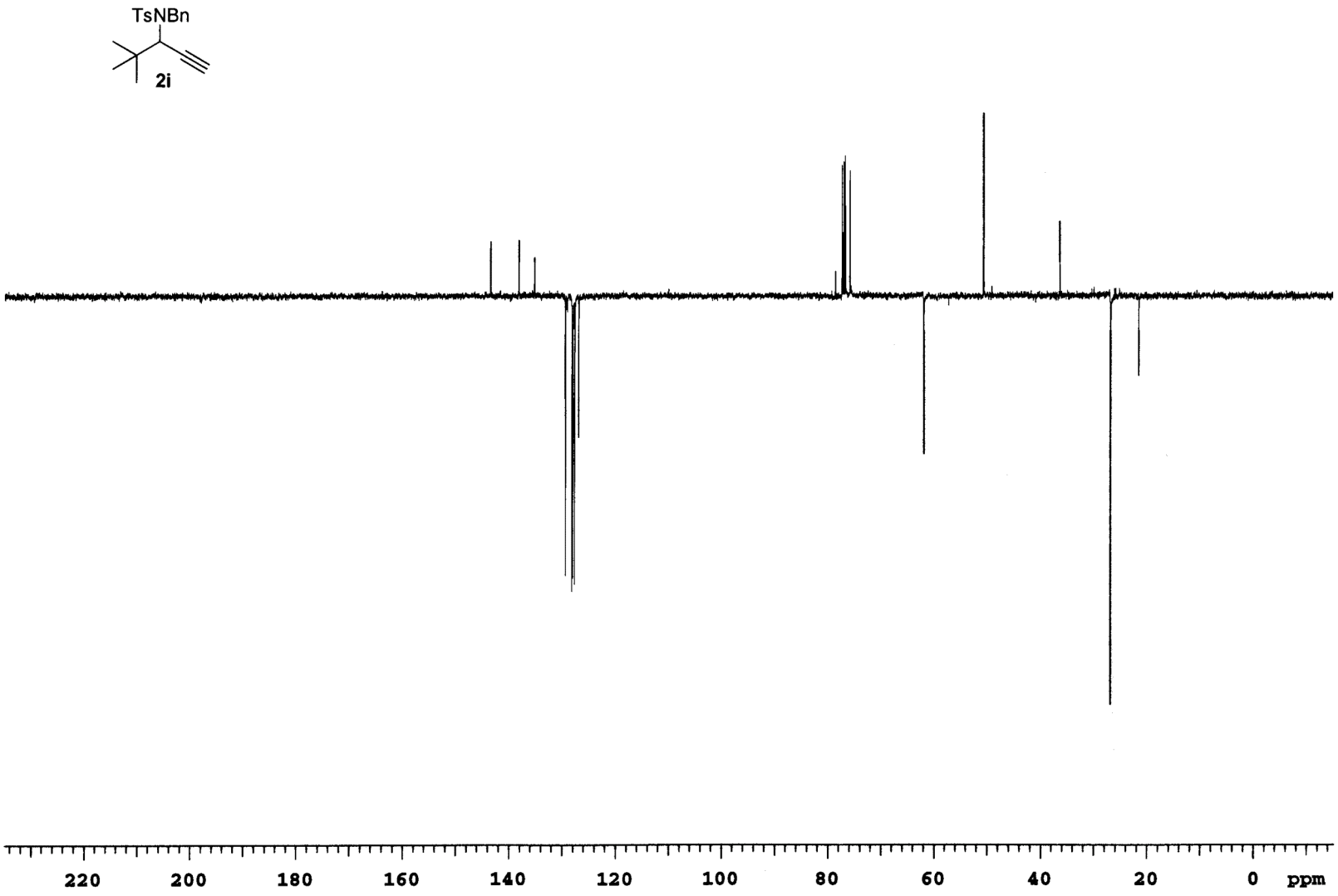
9.14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2i
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200
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40
20
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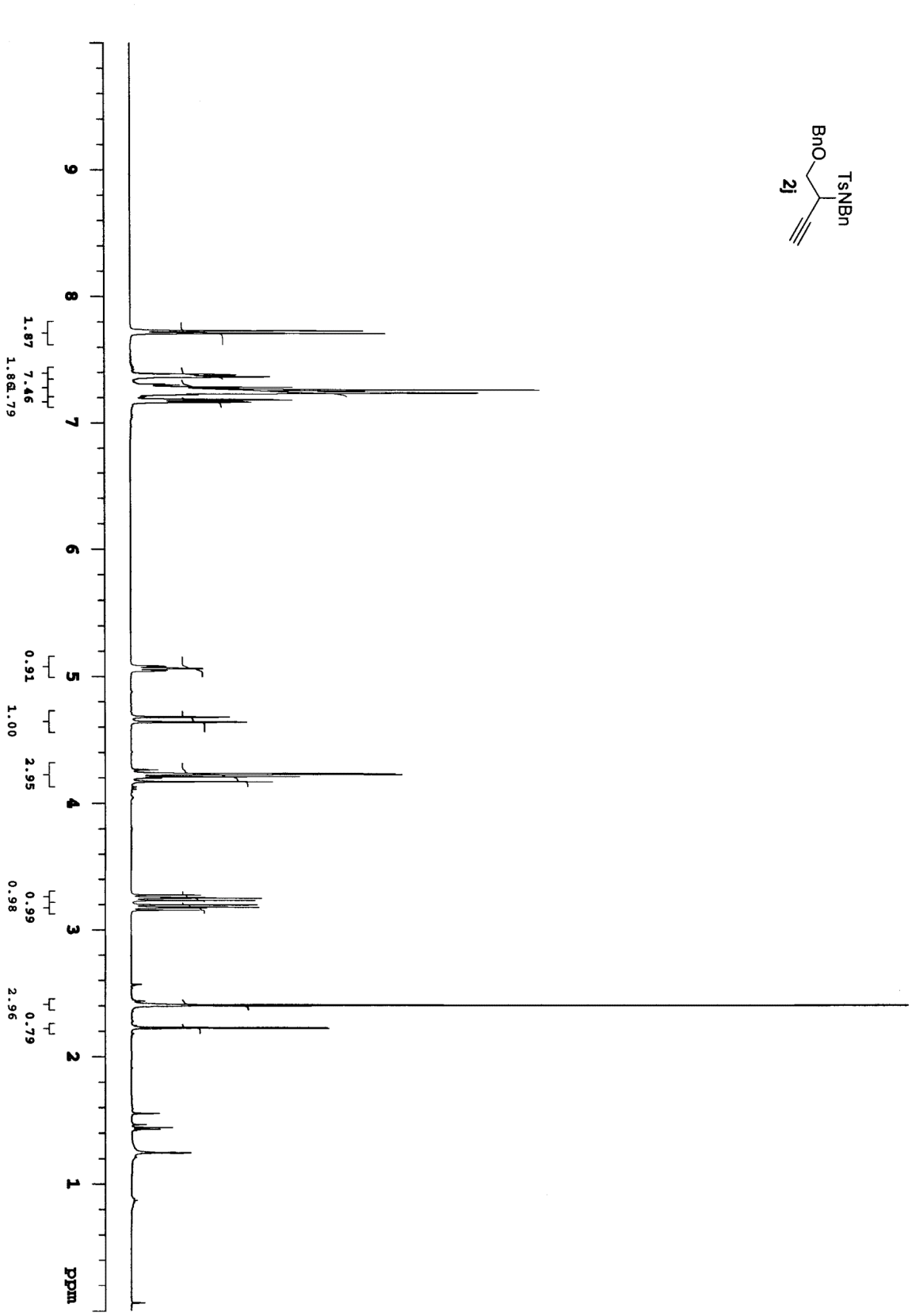
ppm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BnO
2j
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5
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0.91
1.00
2.95
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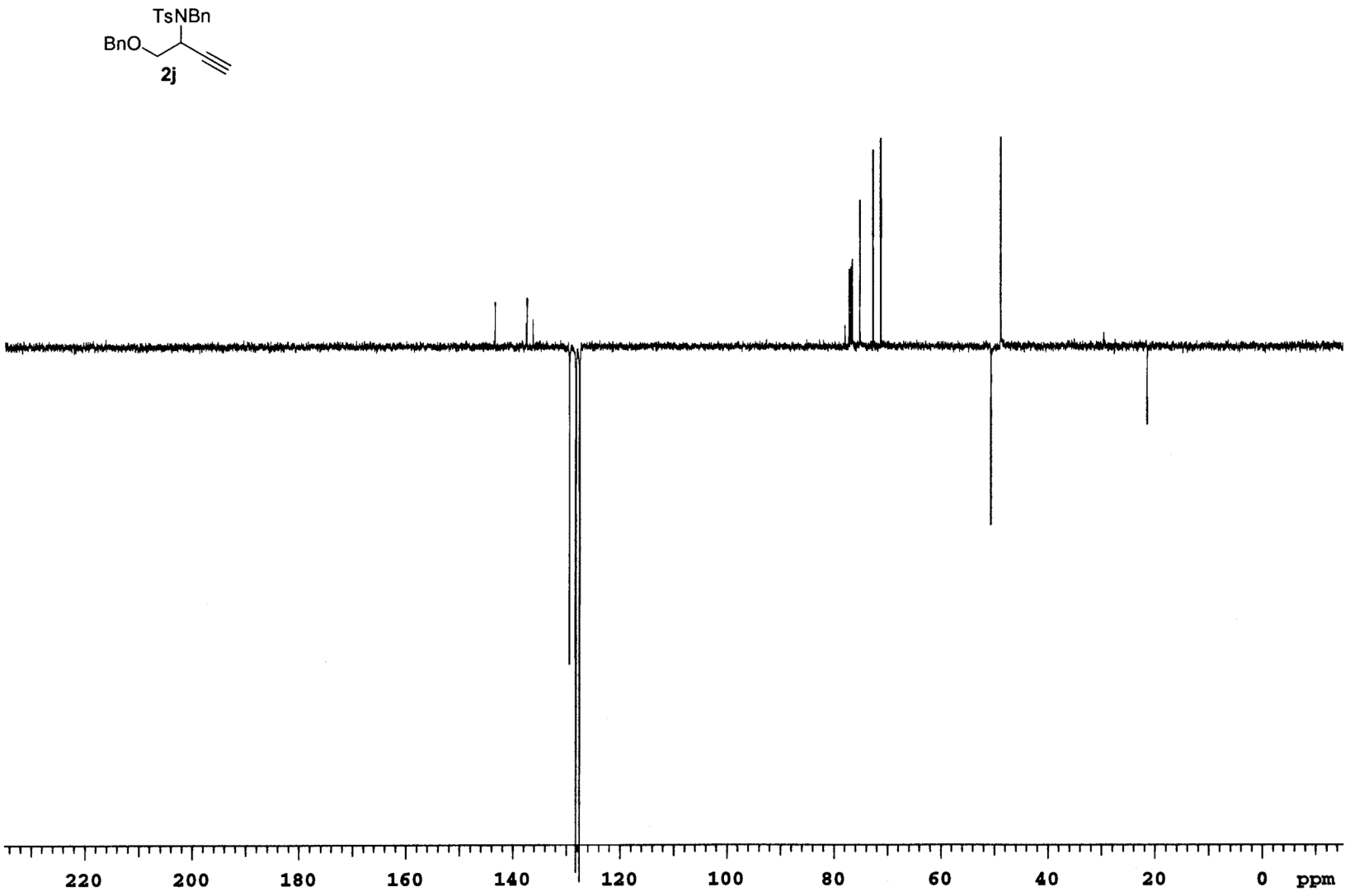
0.79
2.96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BnO
2j
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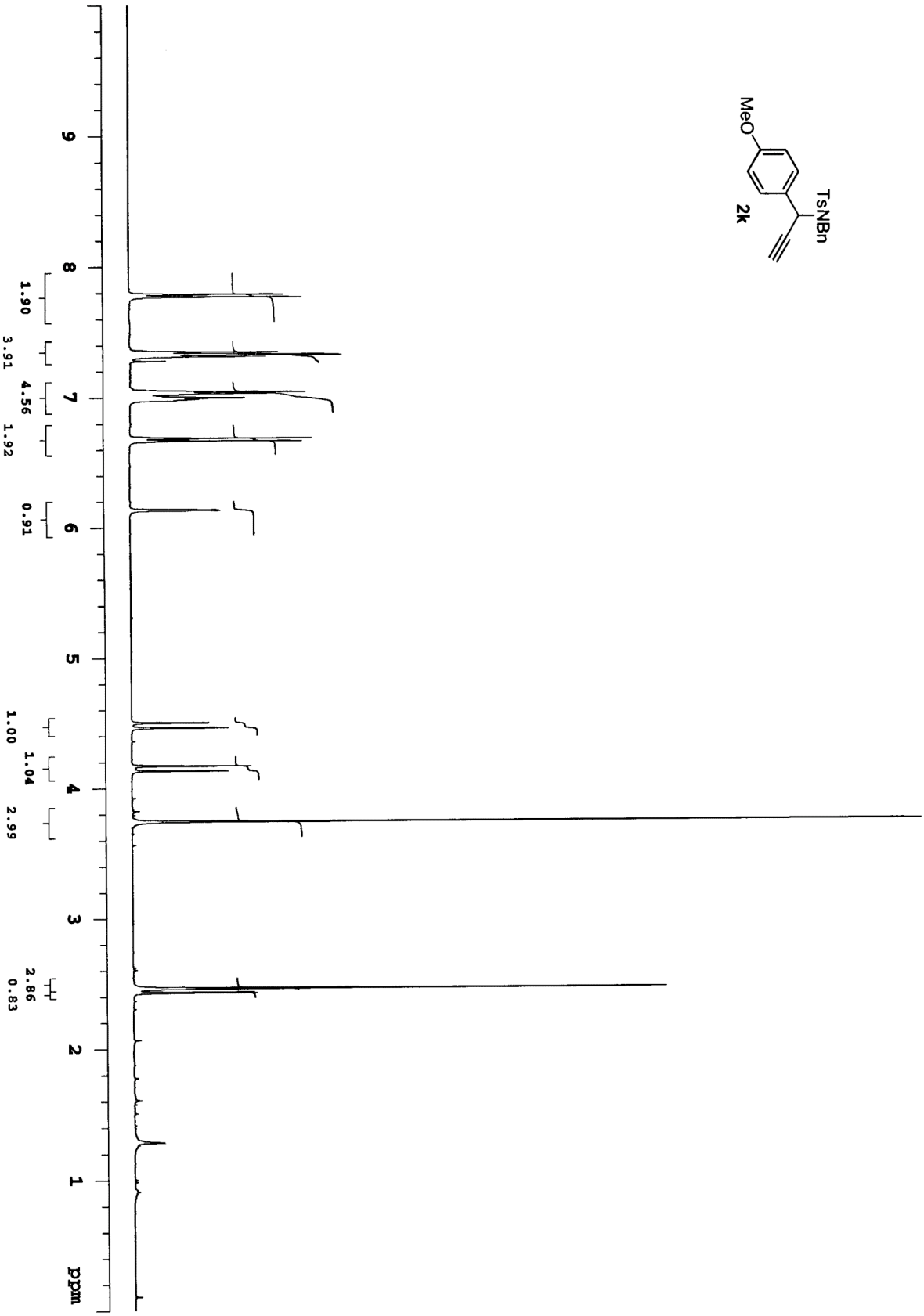
200
180
160
140
120
100
80
60
40
20
0
ppm


MeO
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2k
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6
5
4
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2
1
ppm
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1.00
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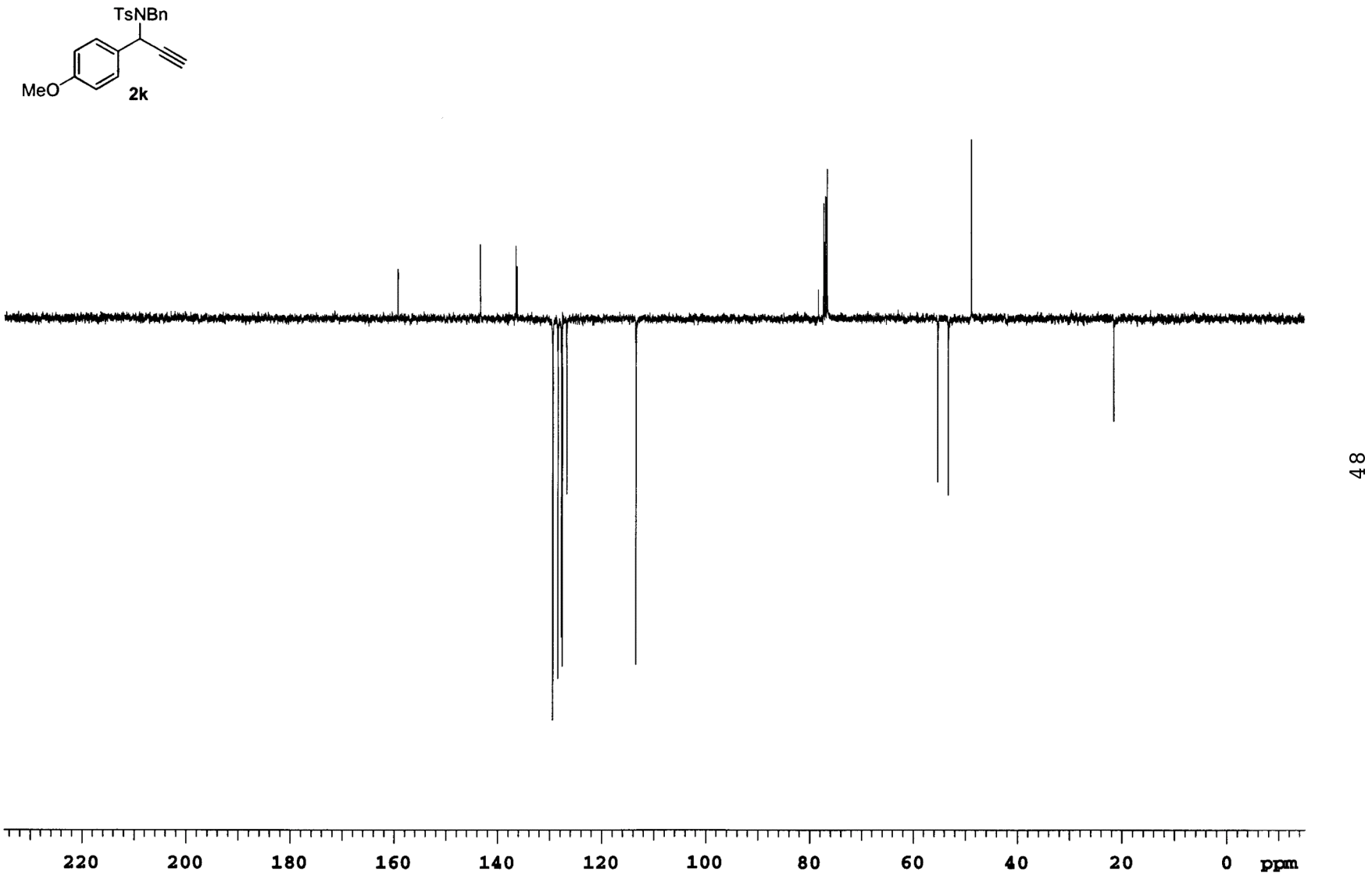
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MeO
2k
220
200
180
160
140
120
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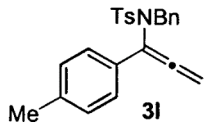

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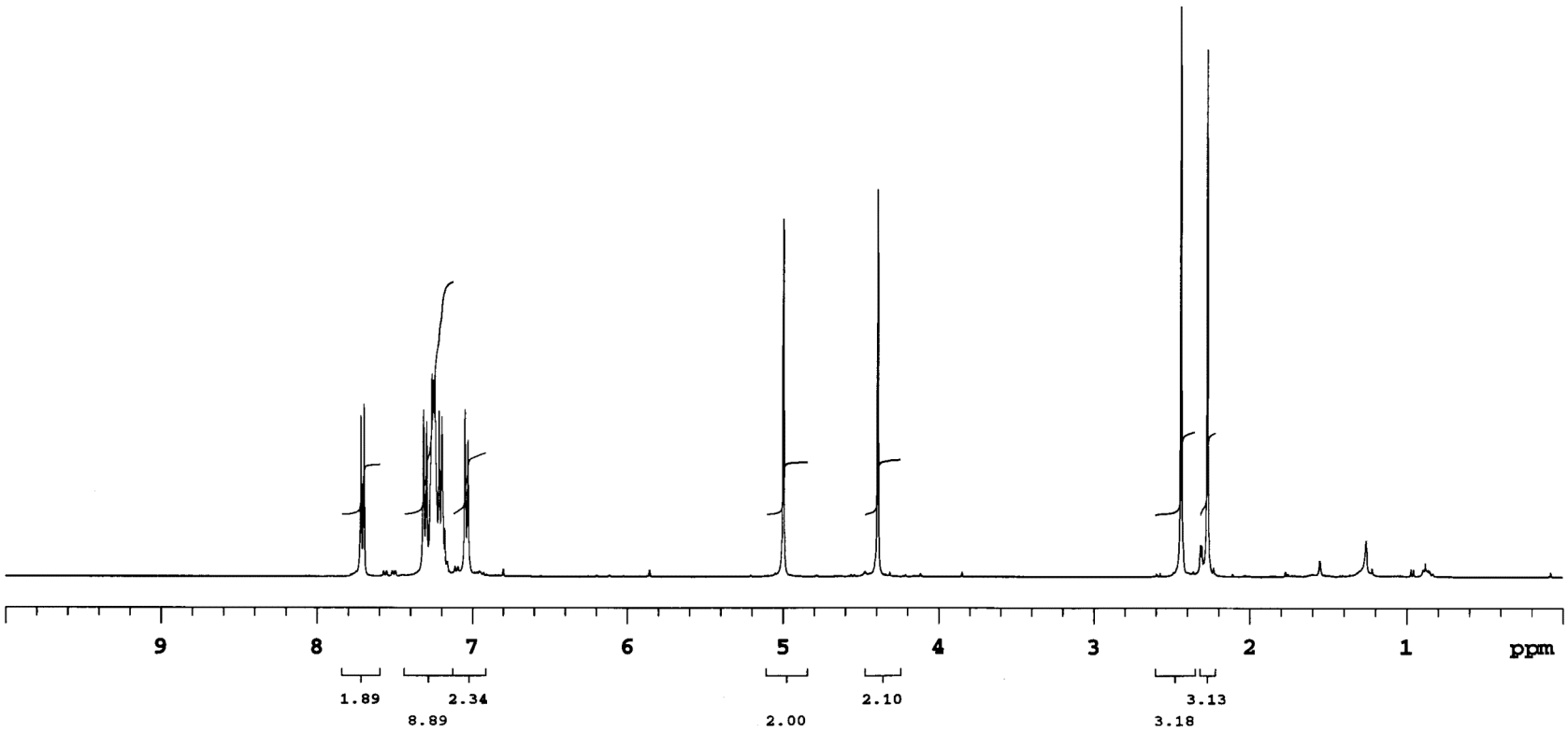

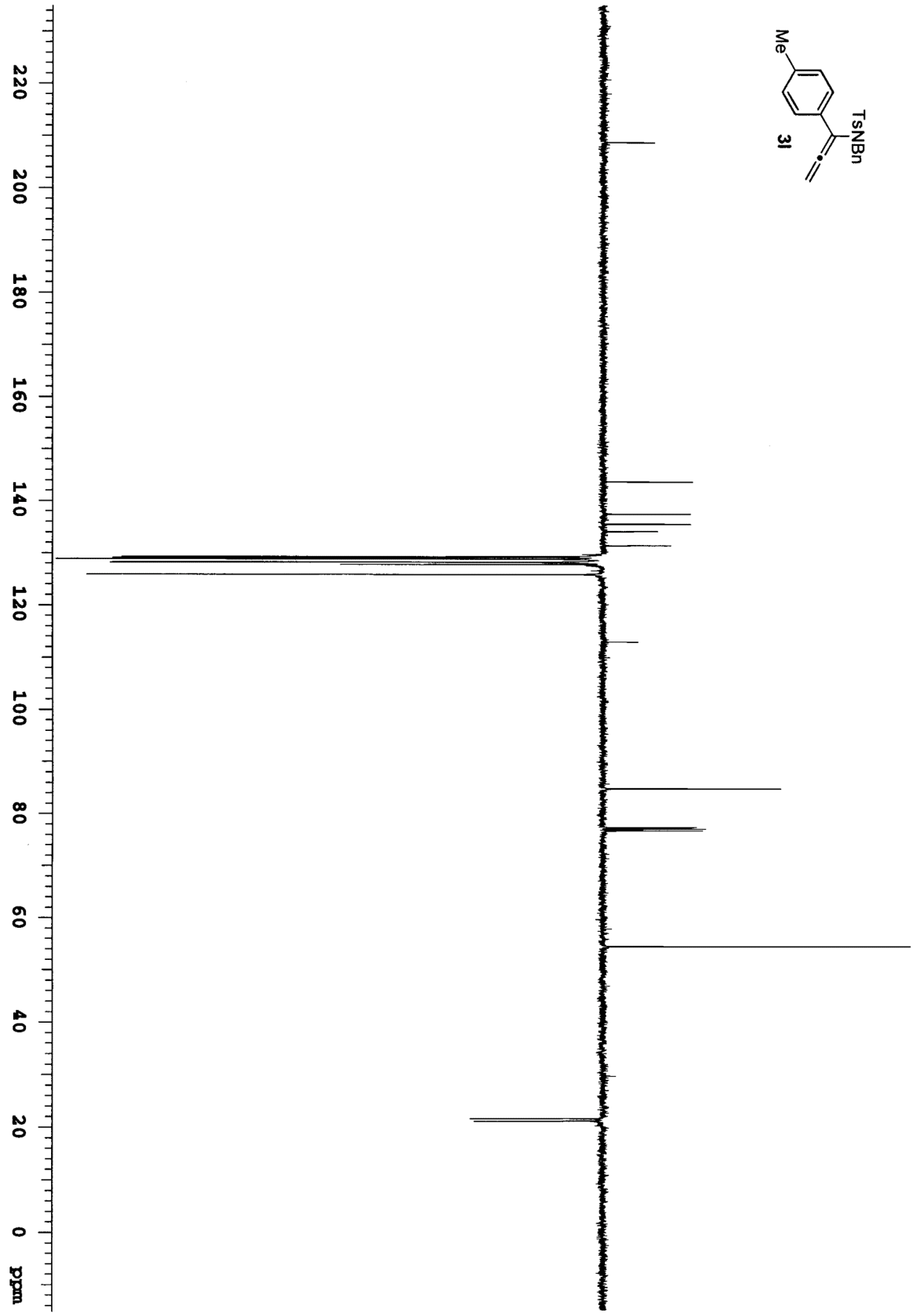
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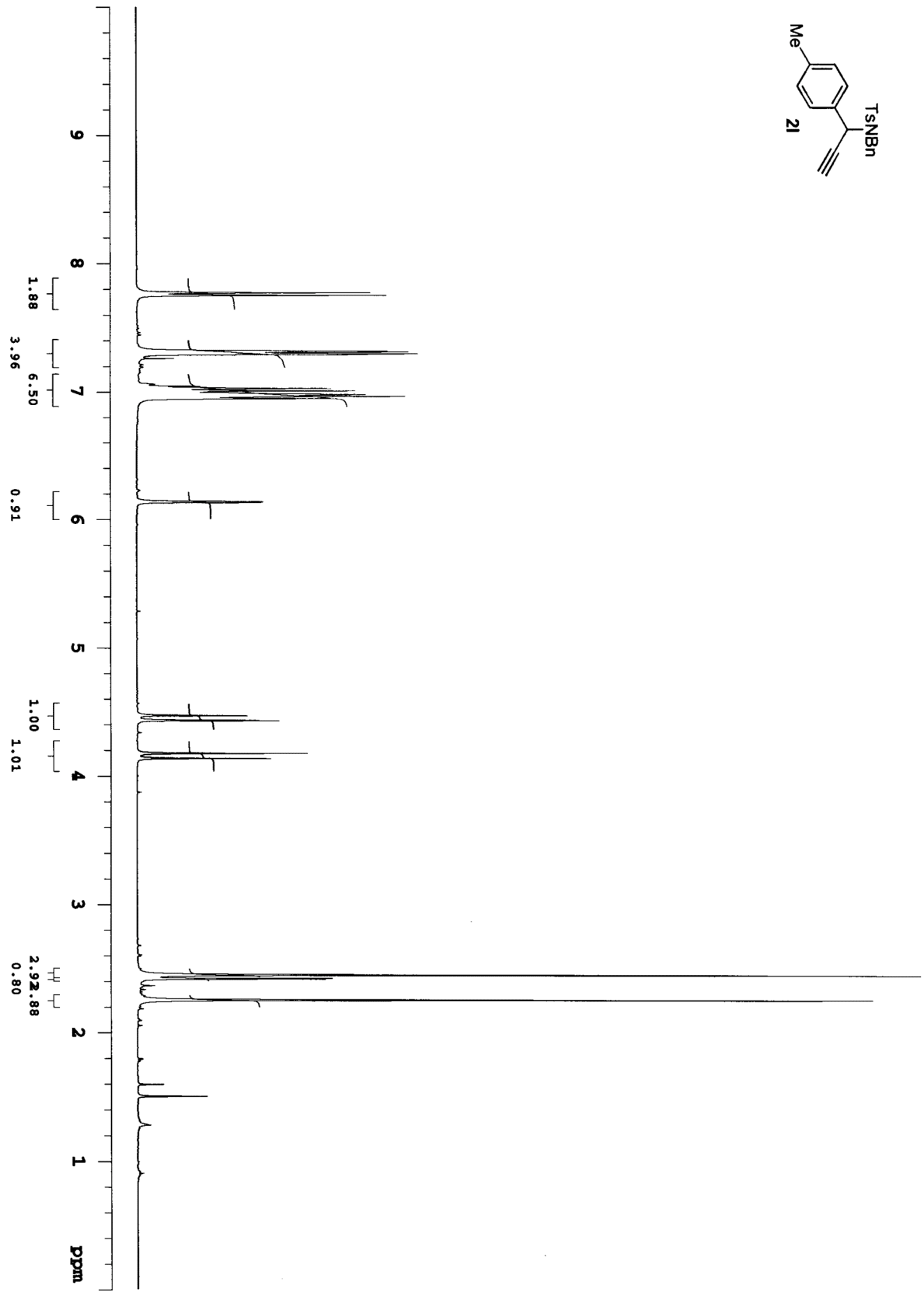
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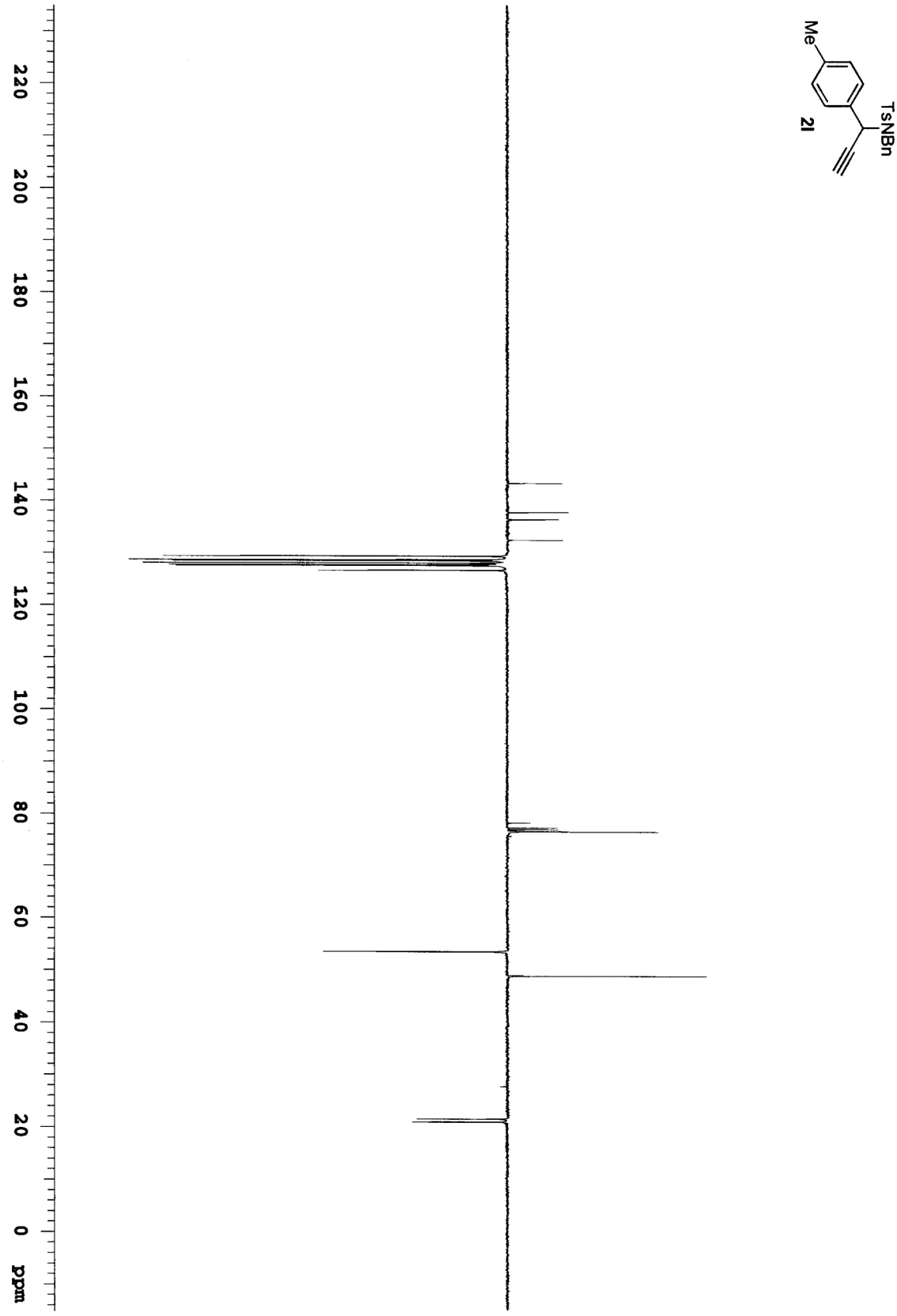
2.88
0.80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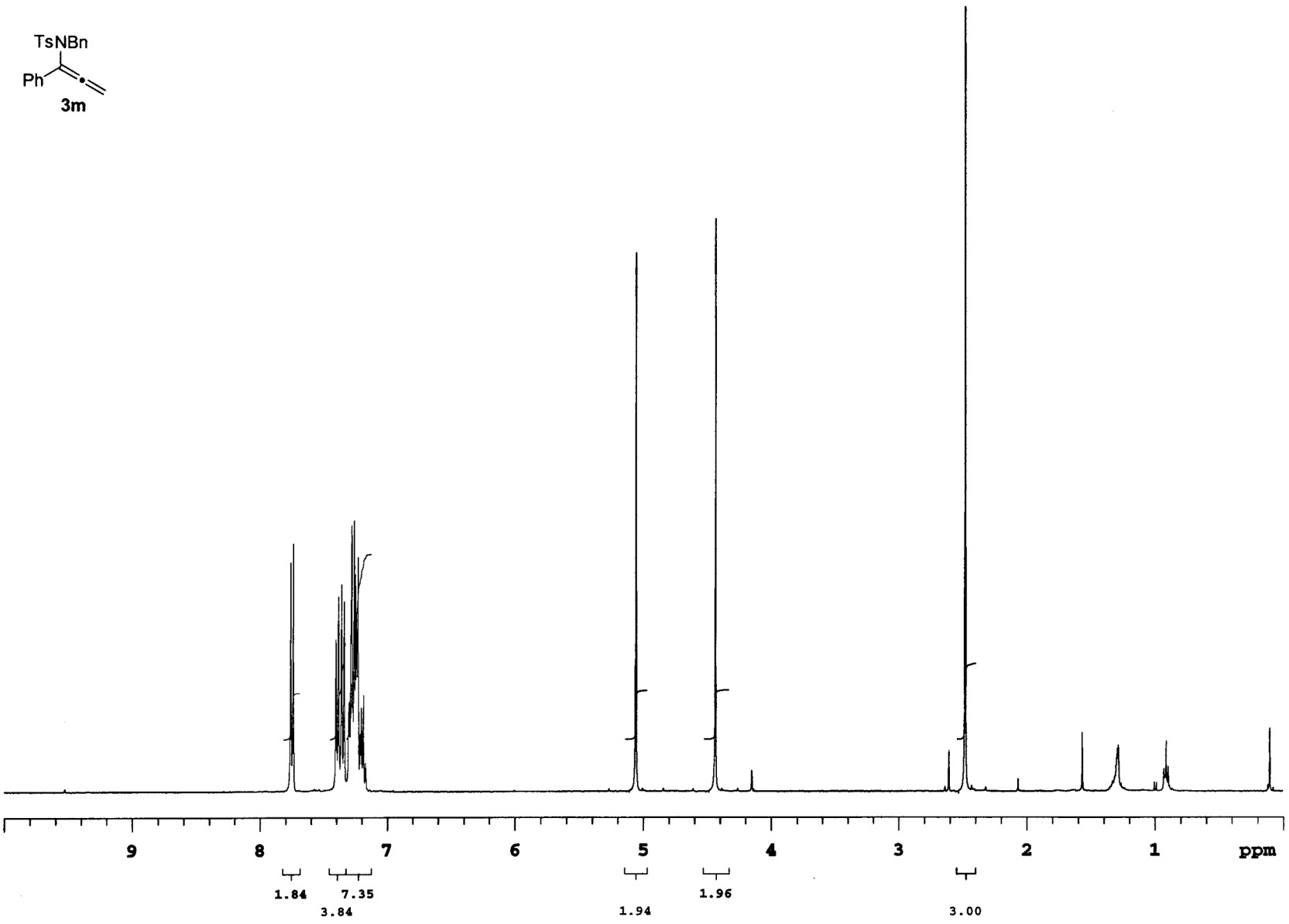
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Ph
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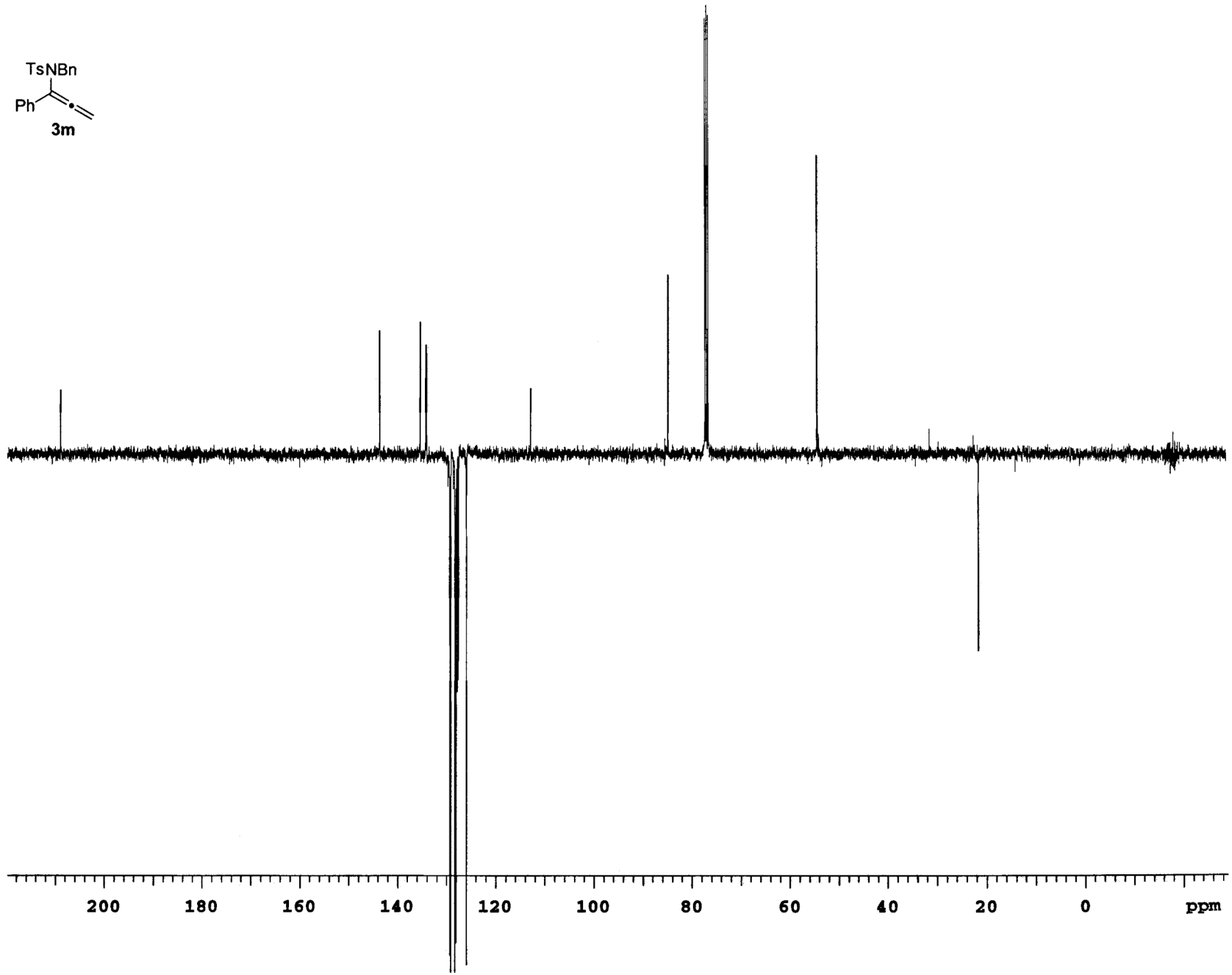
3.00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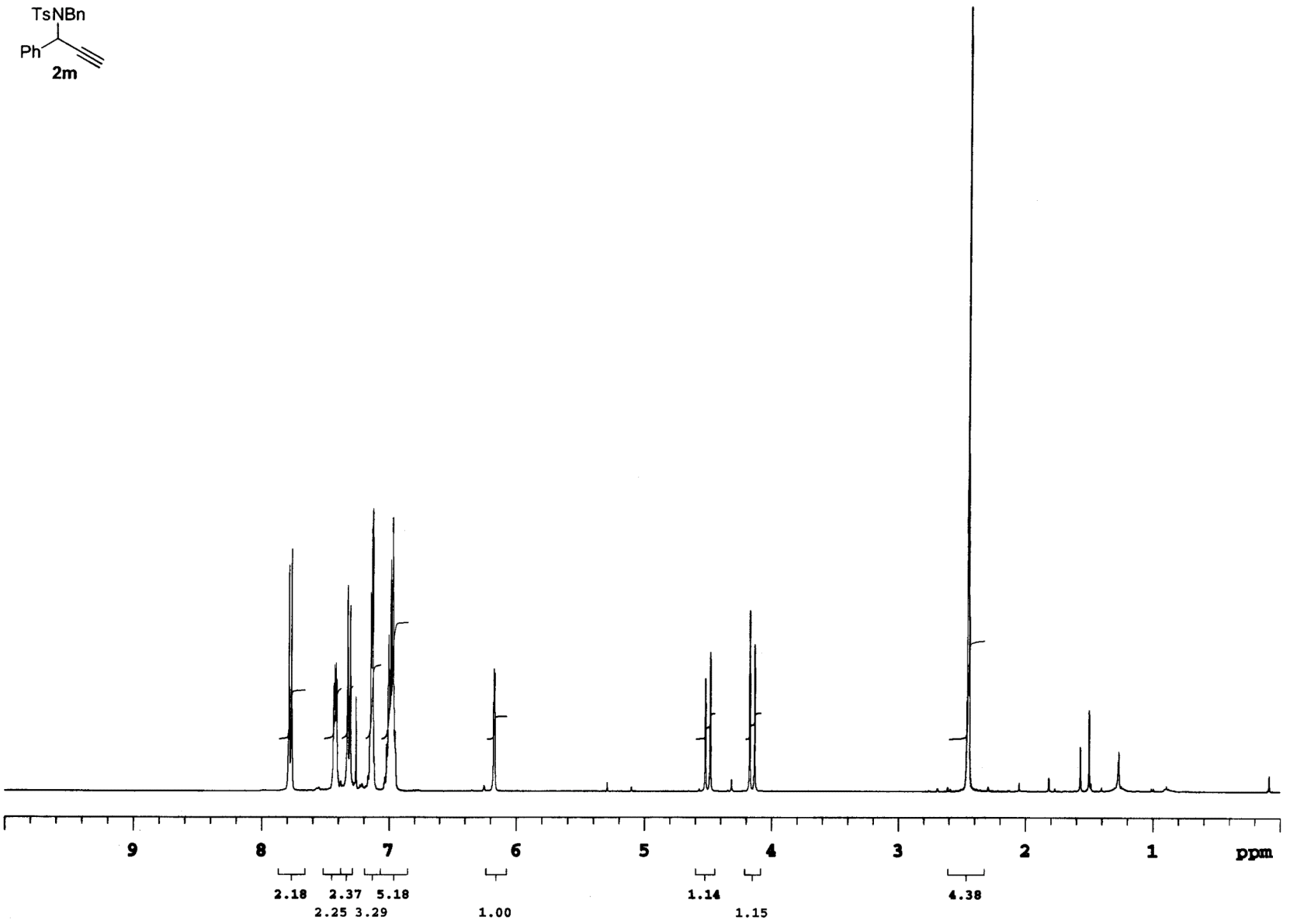
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Ph
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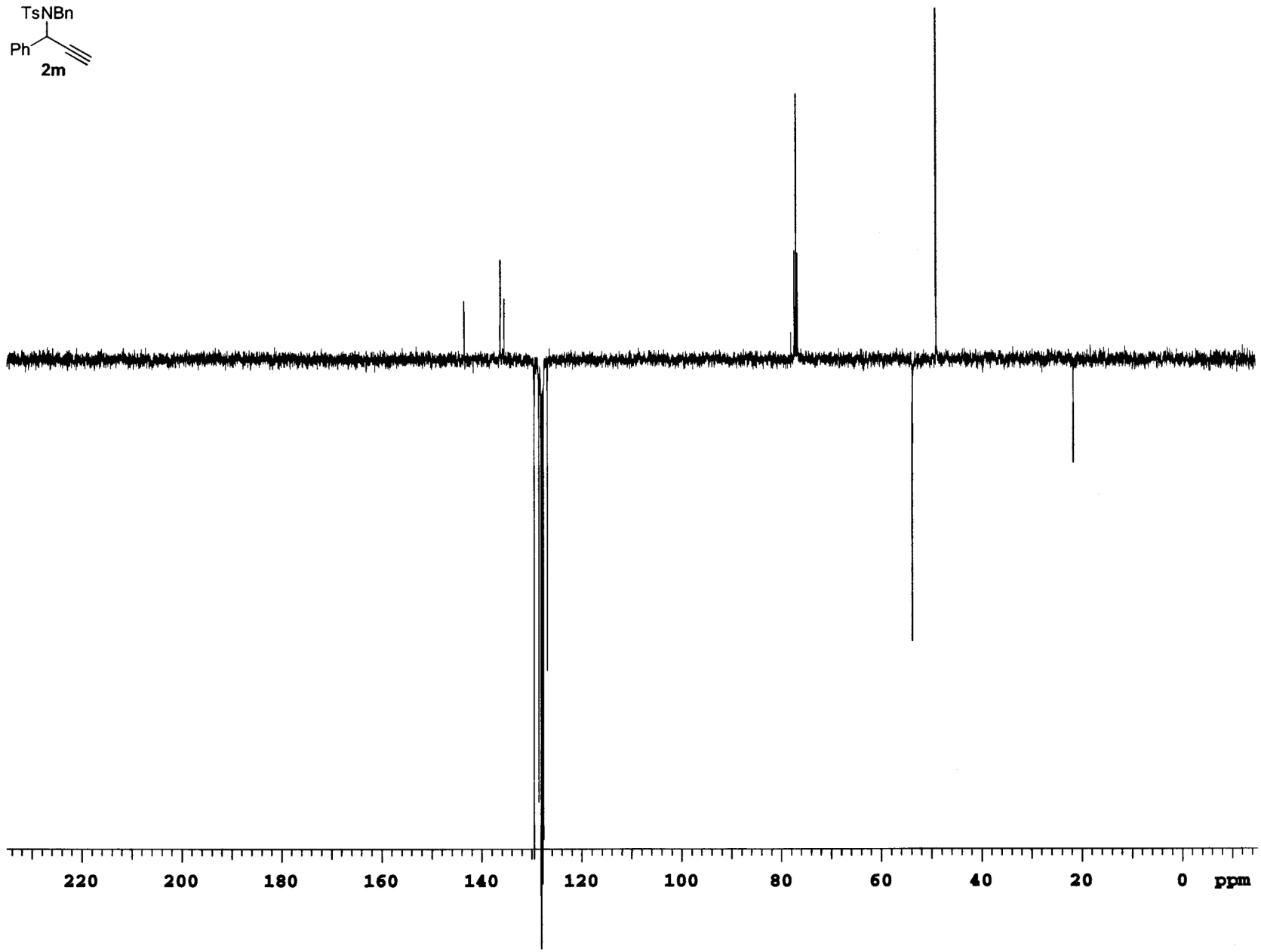
1.15
4.38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Ph
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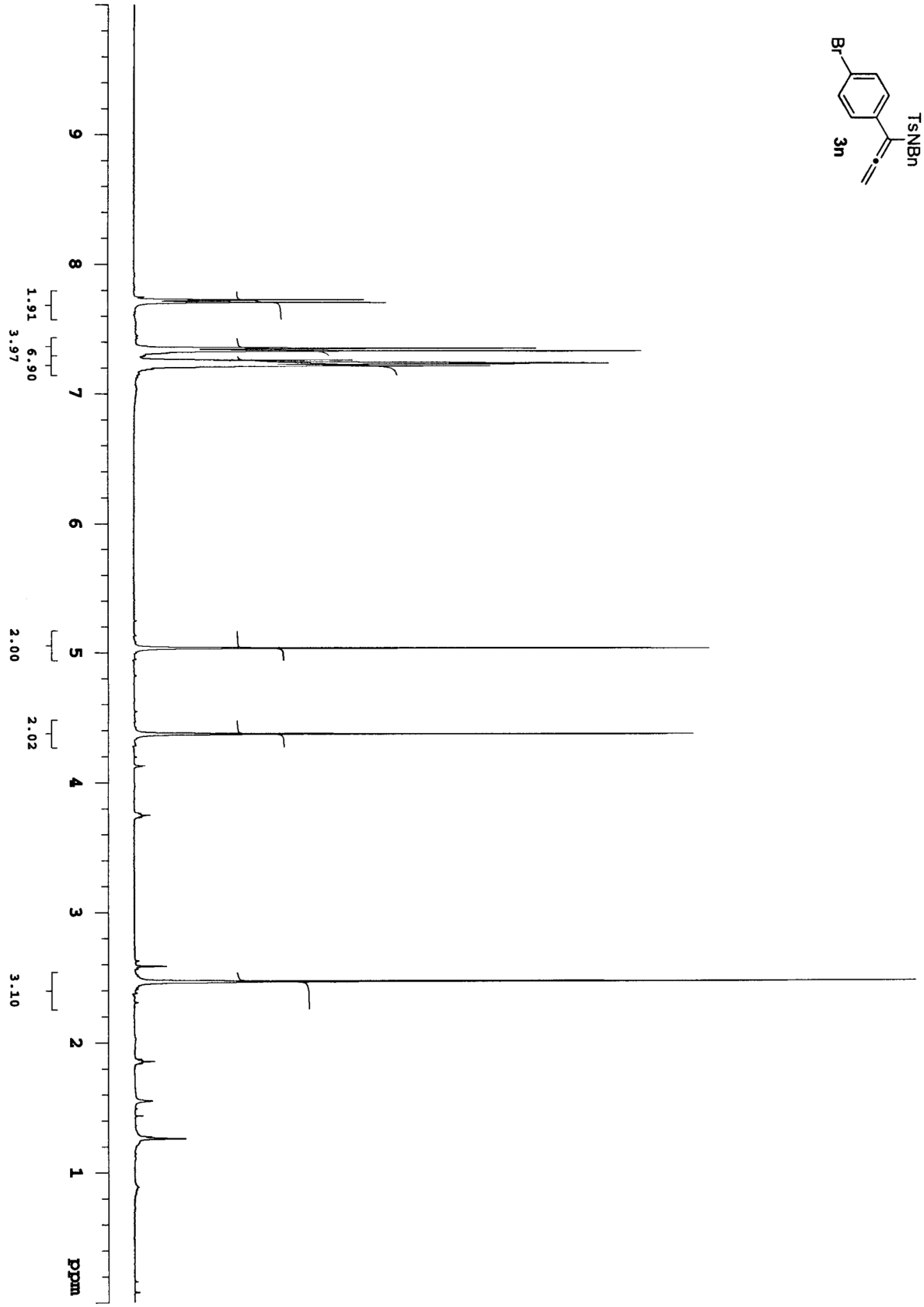
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TsNBn
3n
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5
4
3
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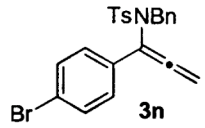
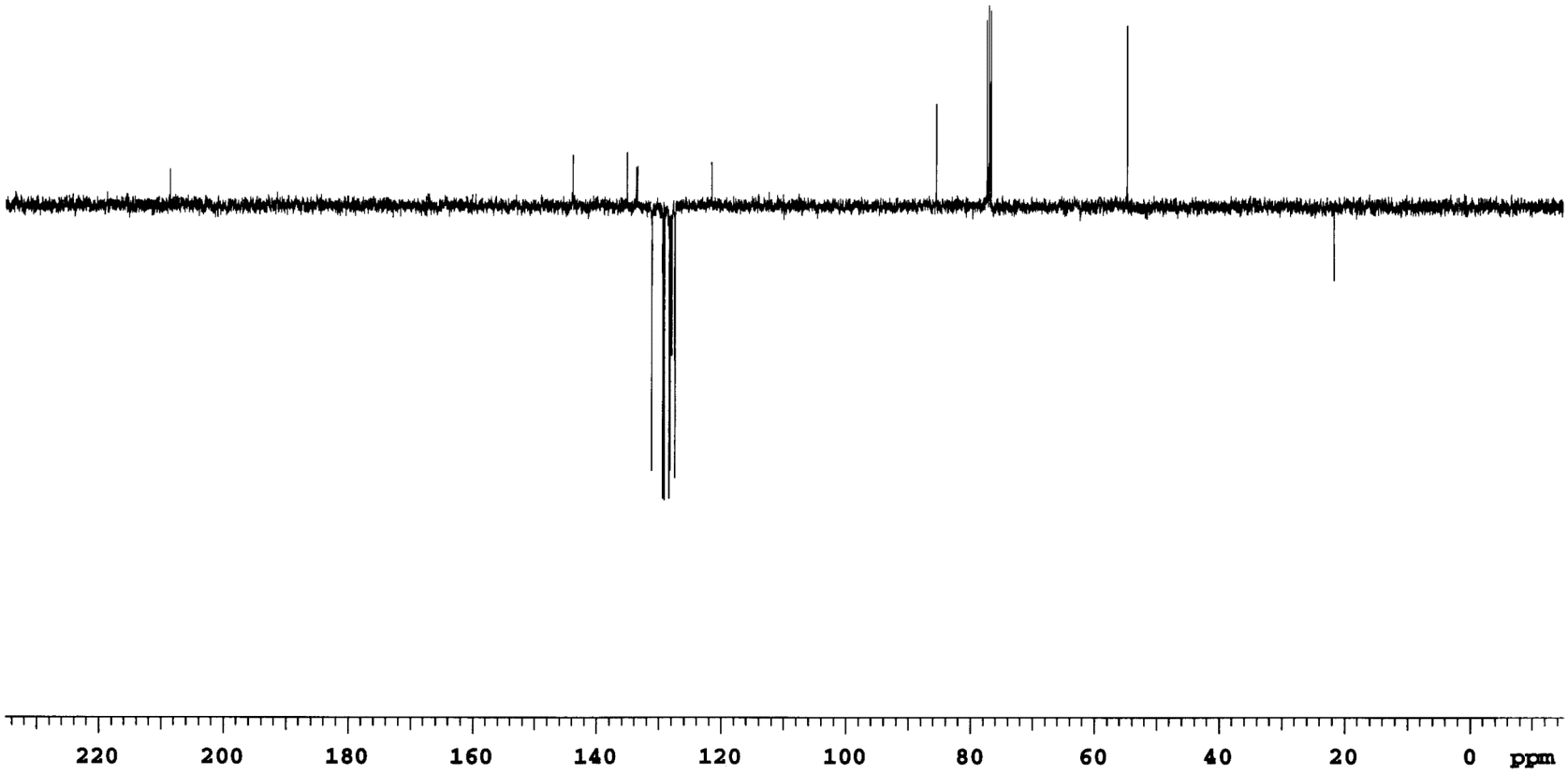
2.02
3.10


TsNBn
Br
3n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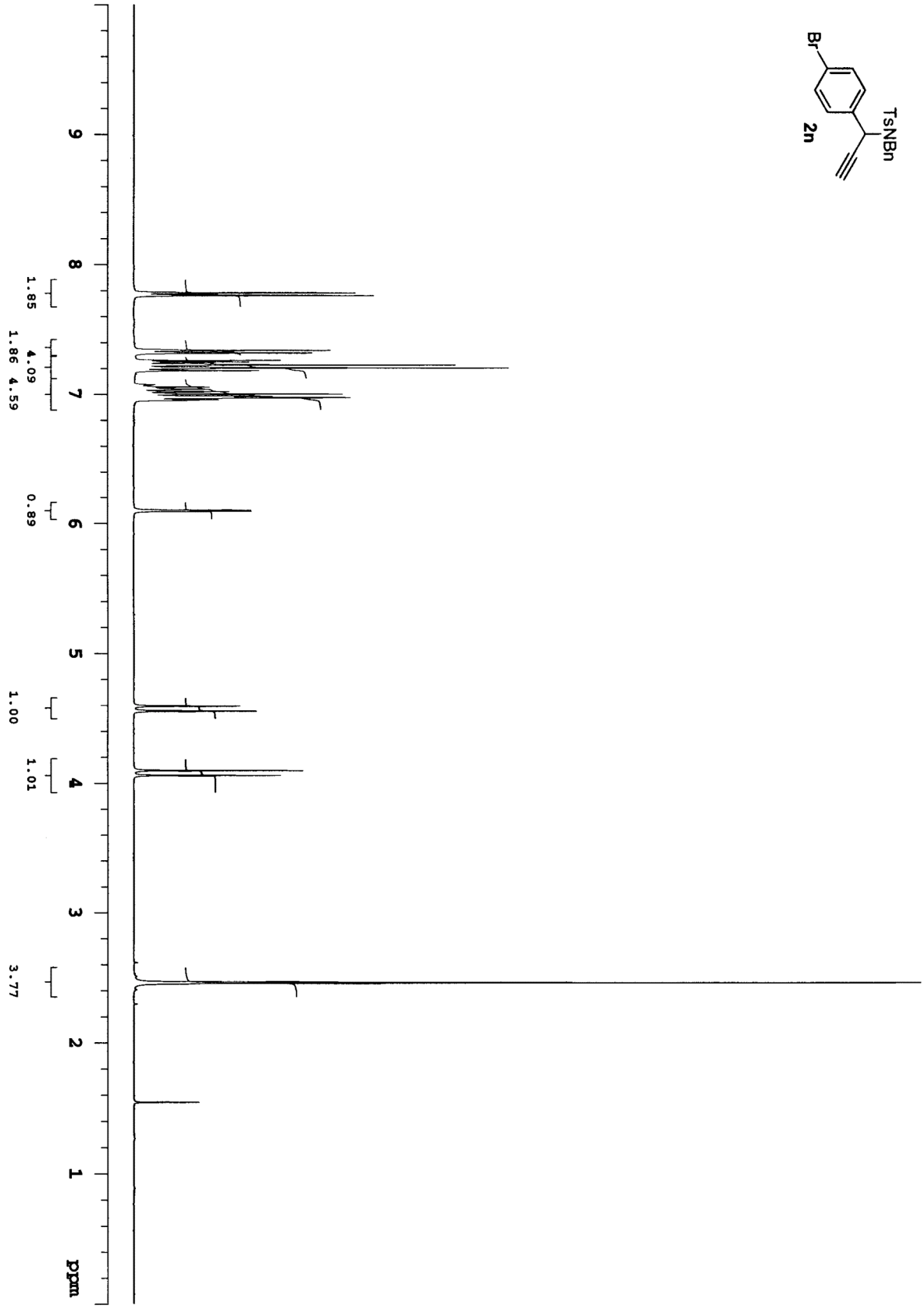
60
40
20
0
ppm


Br
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2n
9
8
7
6
5
4
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1
ppm
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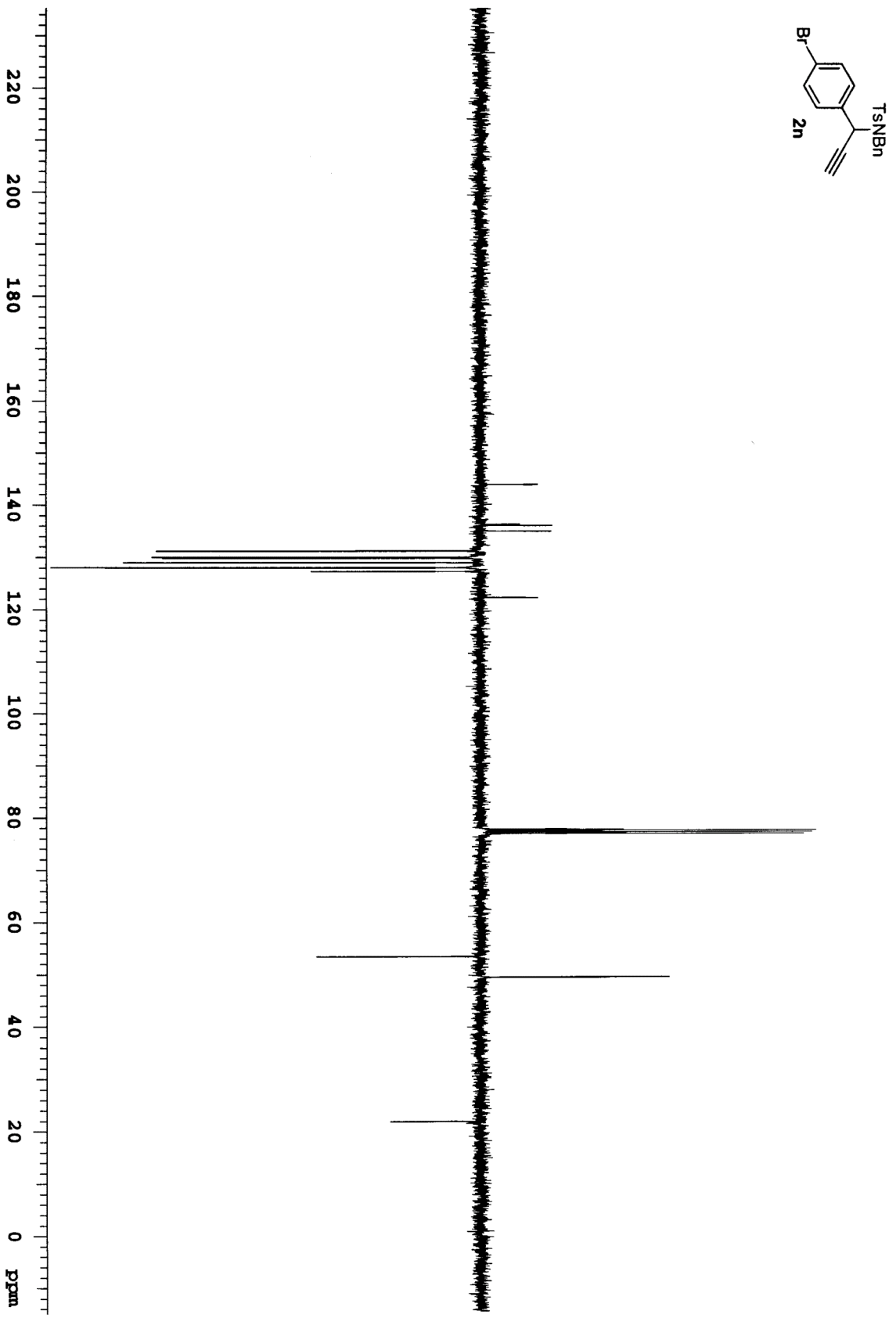
4.59
0.89
1.00
1.01
3.77


Br
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2n
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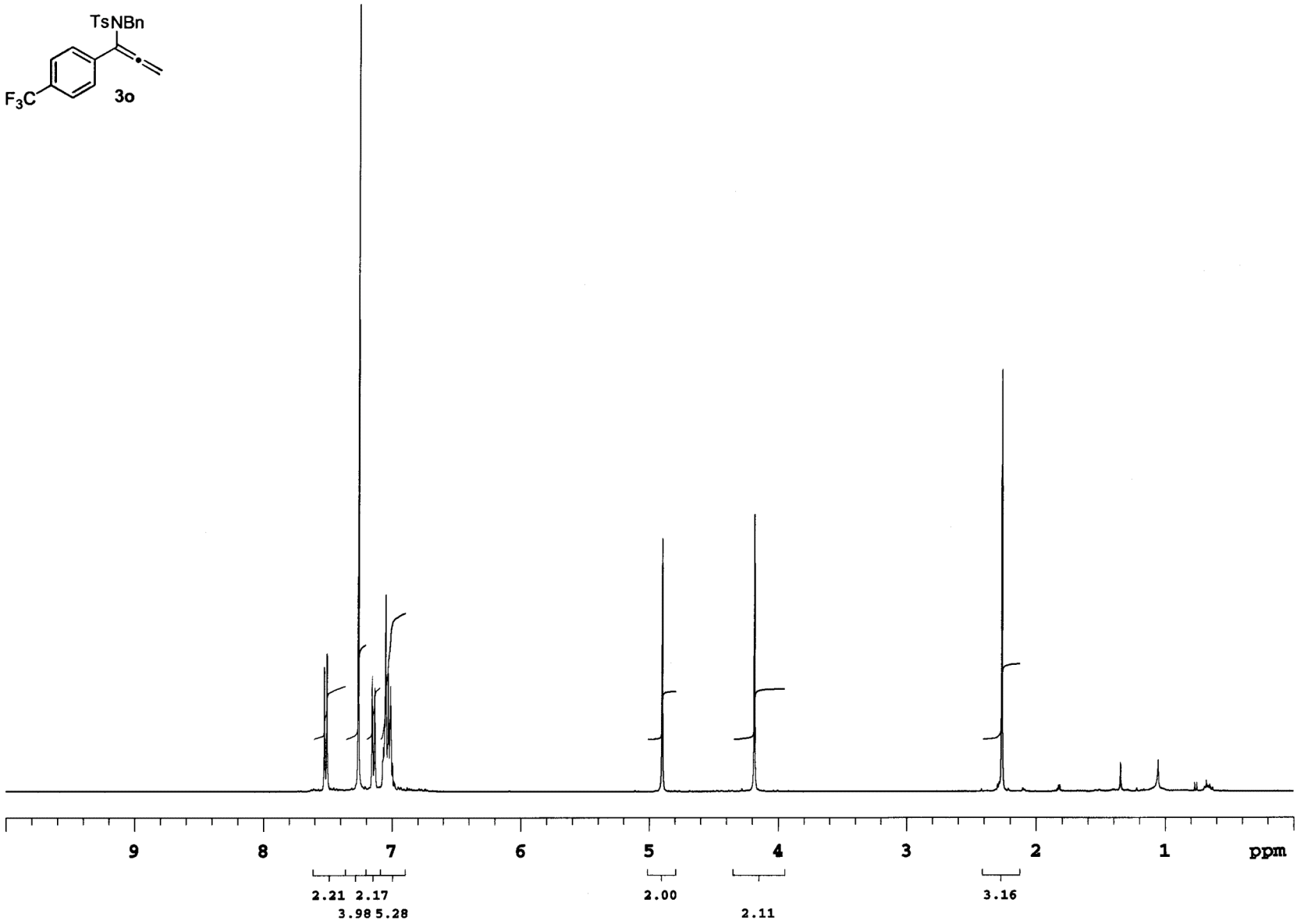
ppm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3
2
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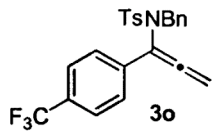
3.16



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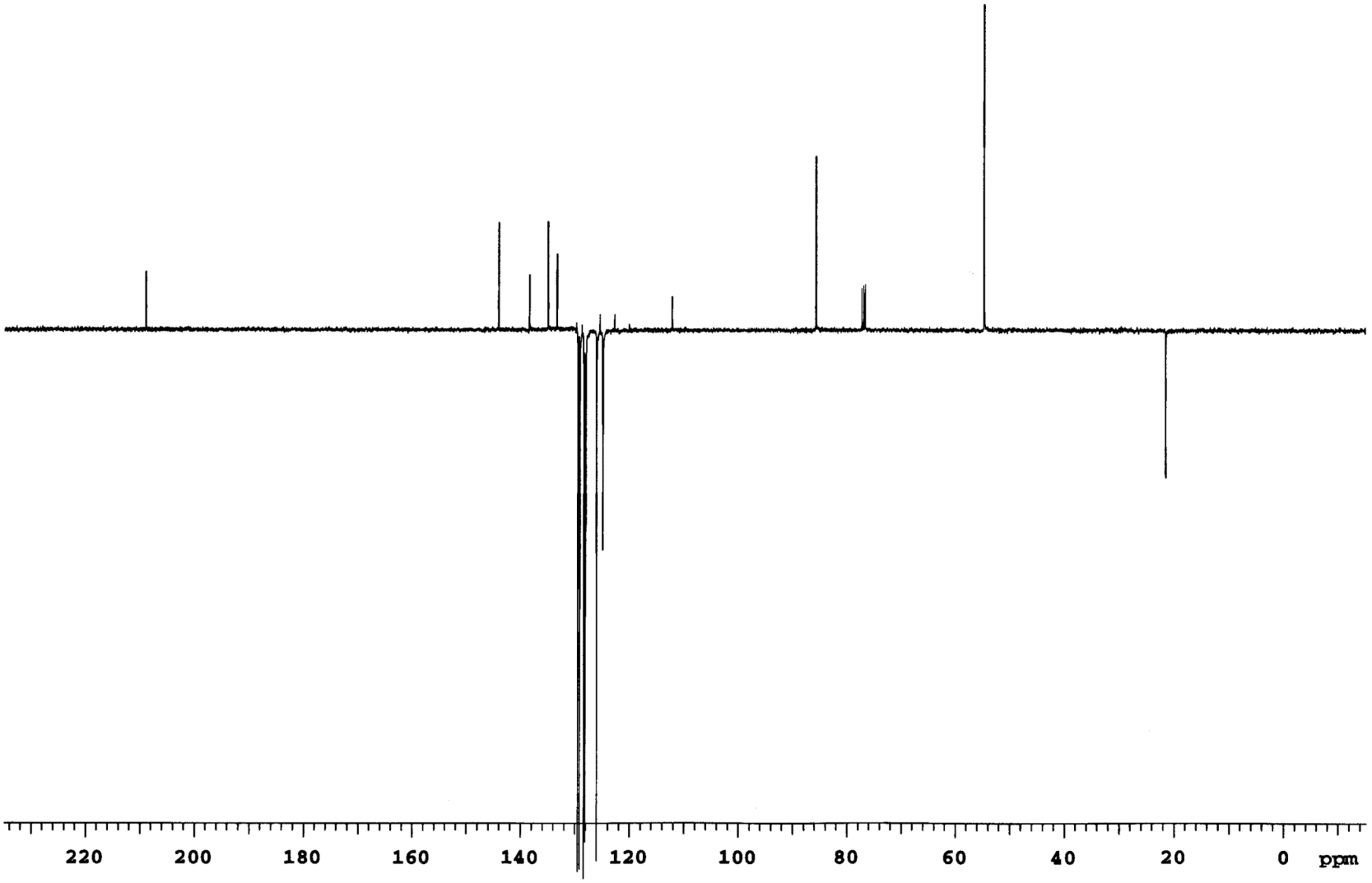

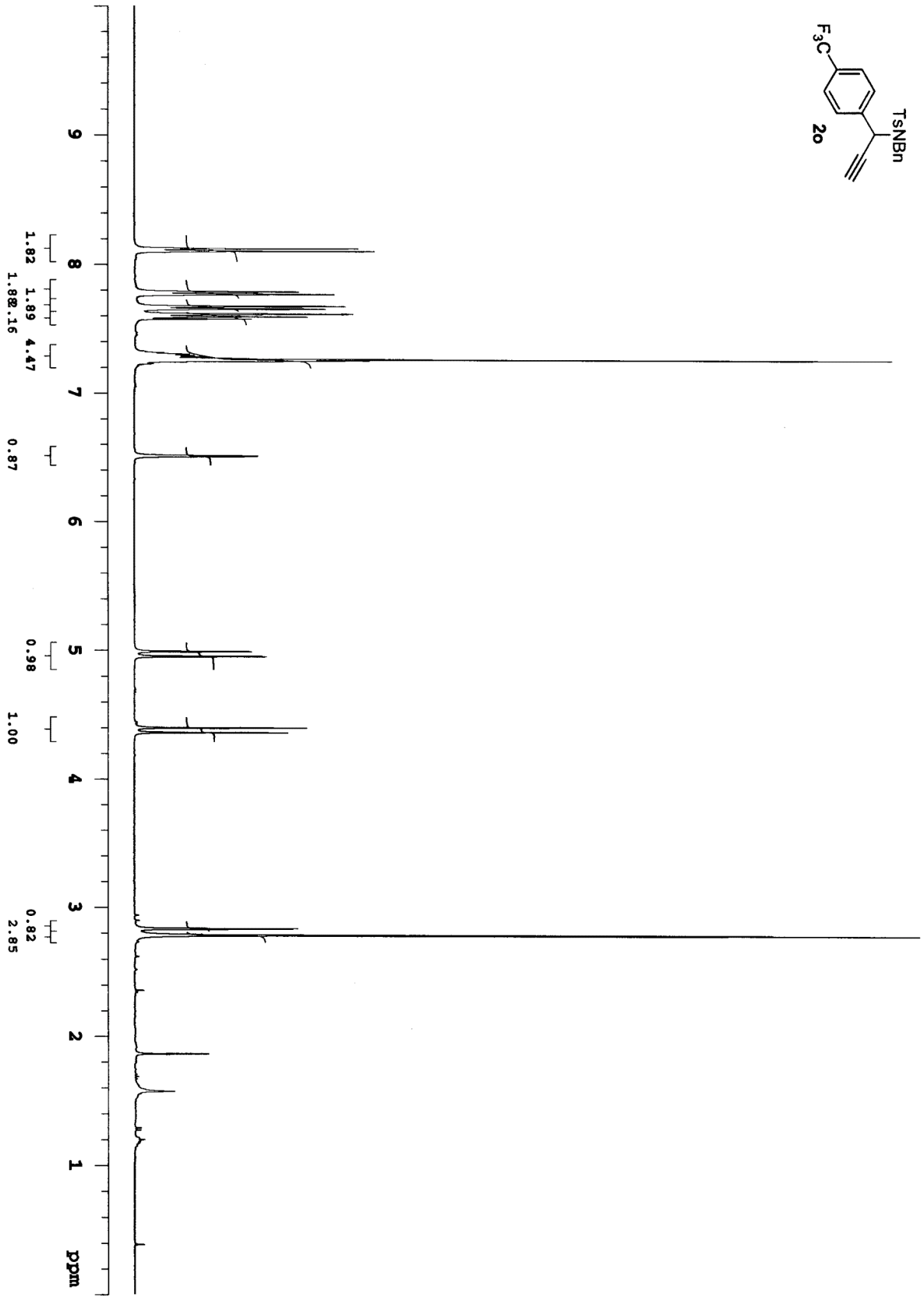
F3C
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2o
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7
6
5
4
3
2
1
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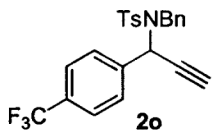
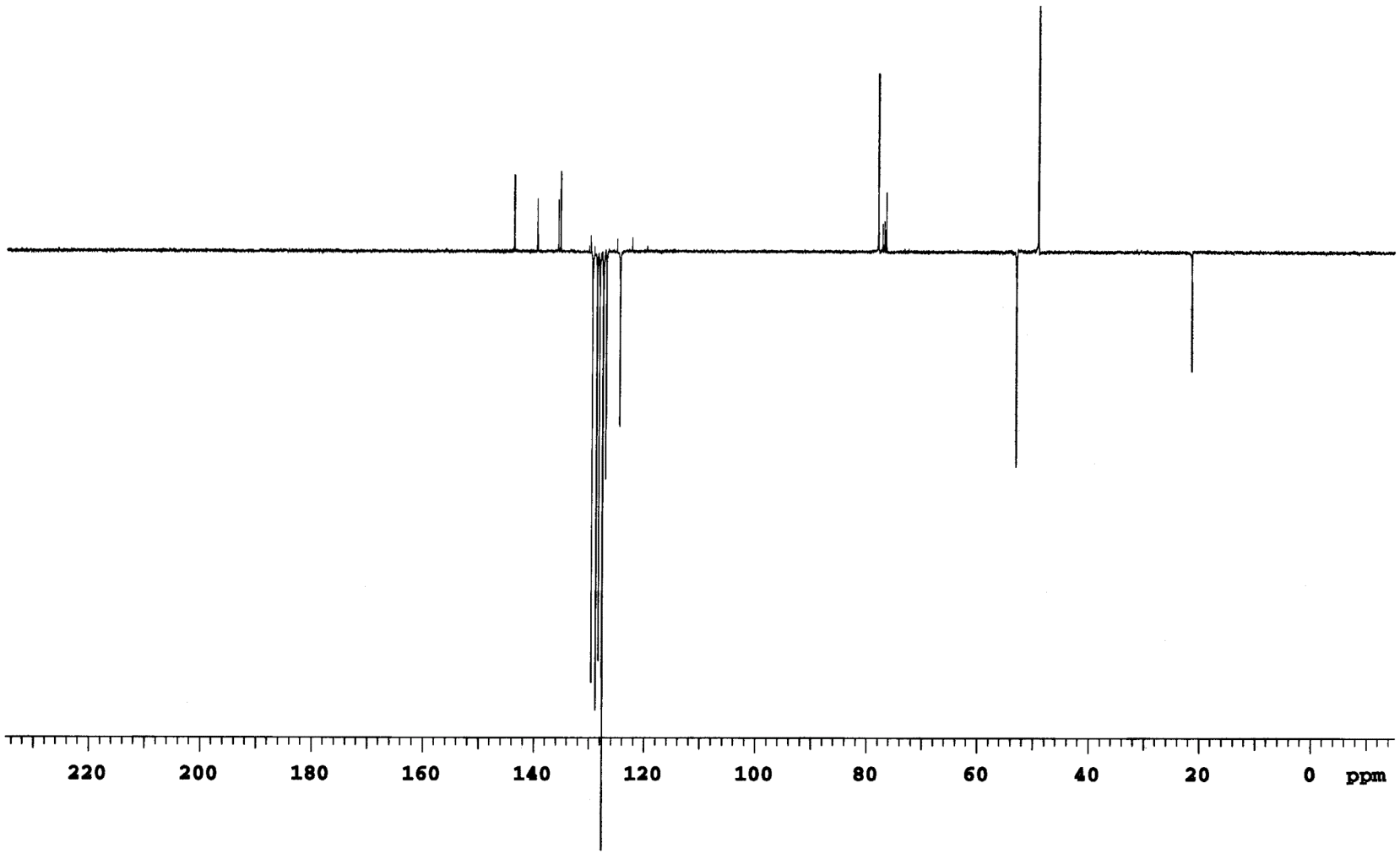
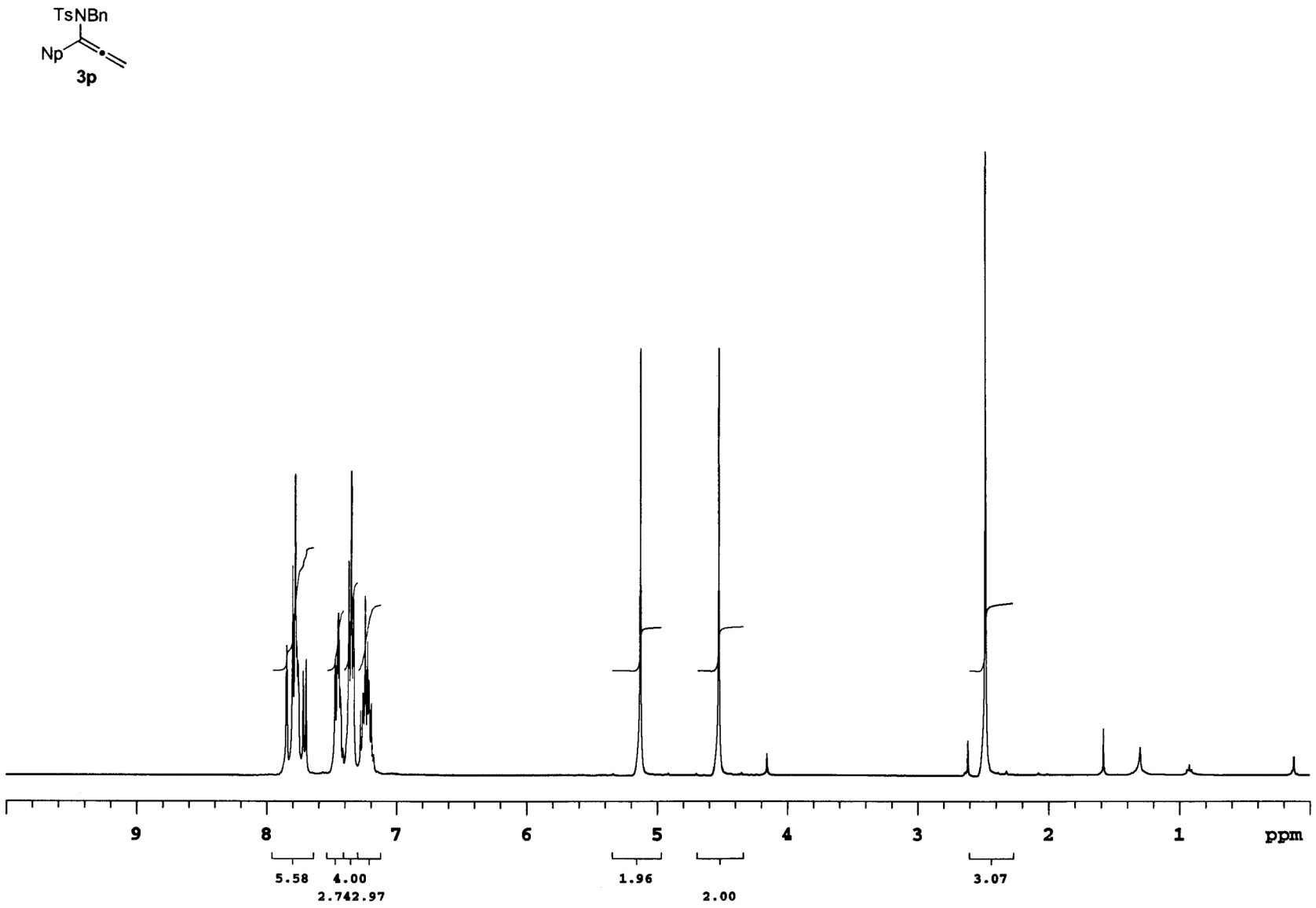
0.82
2.85



2o

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3p
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2
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ppm
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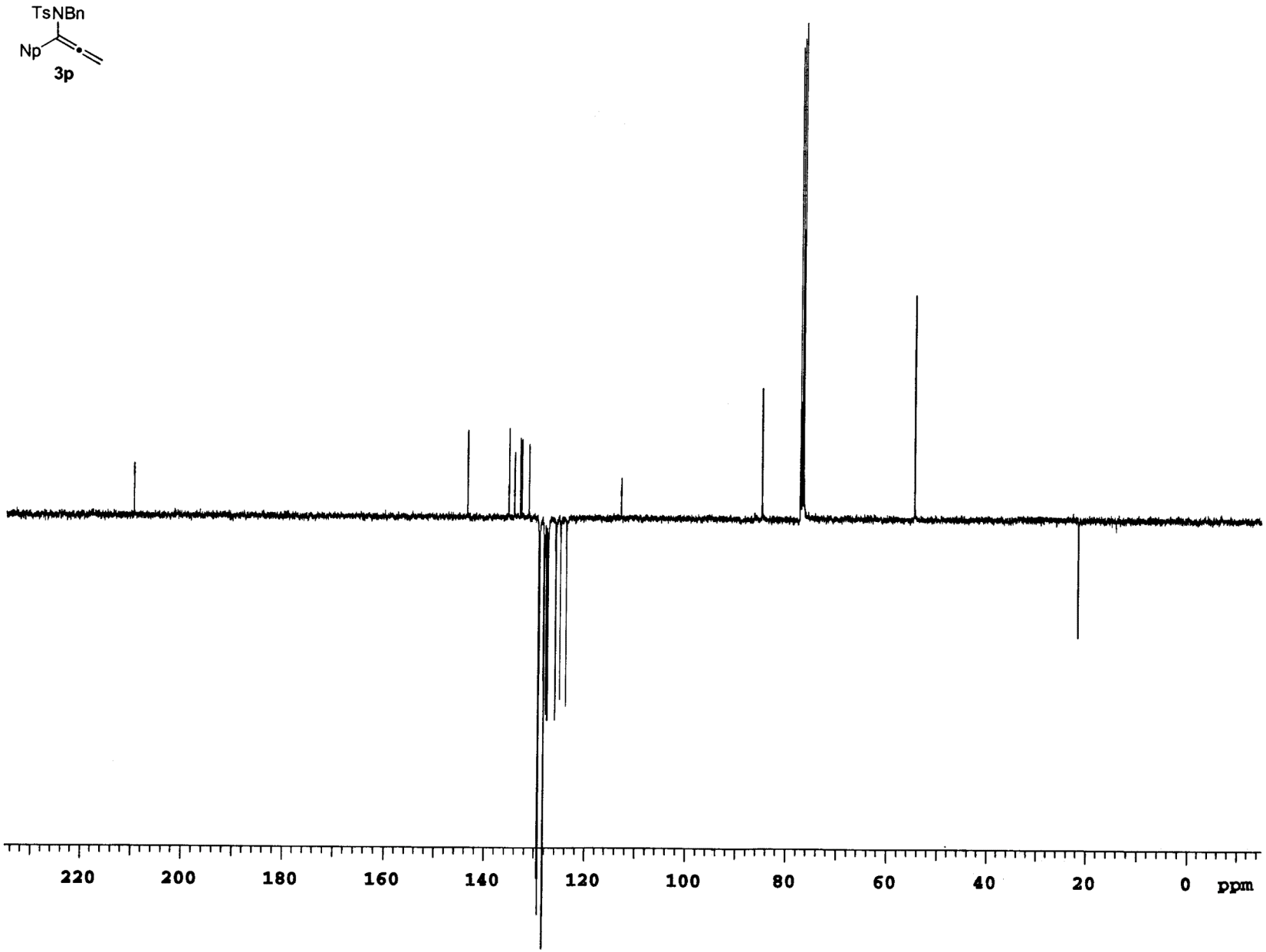
3.07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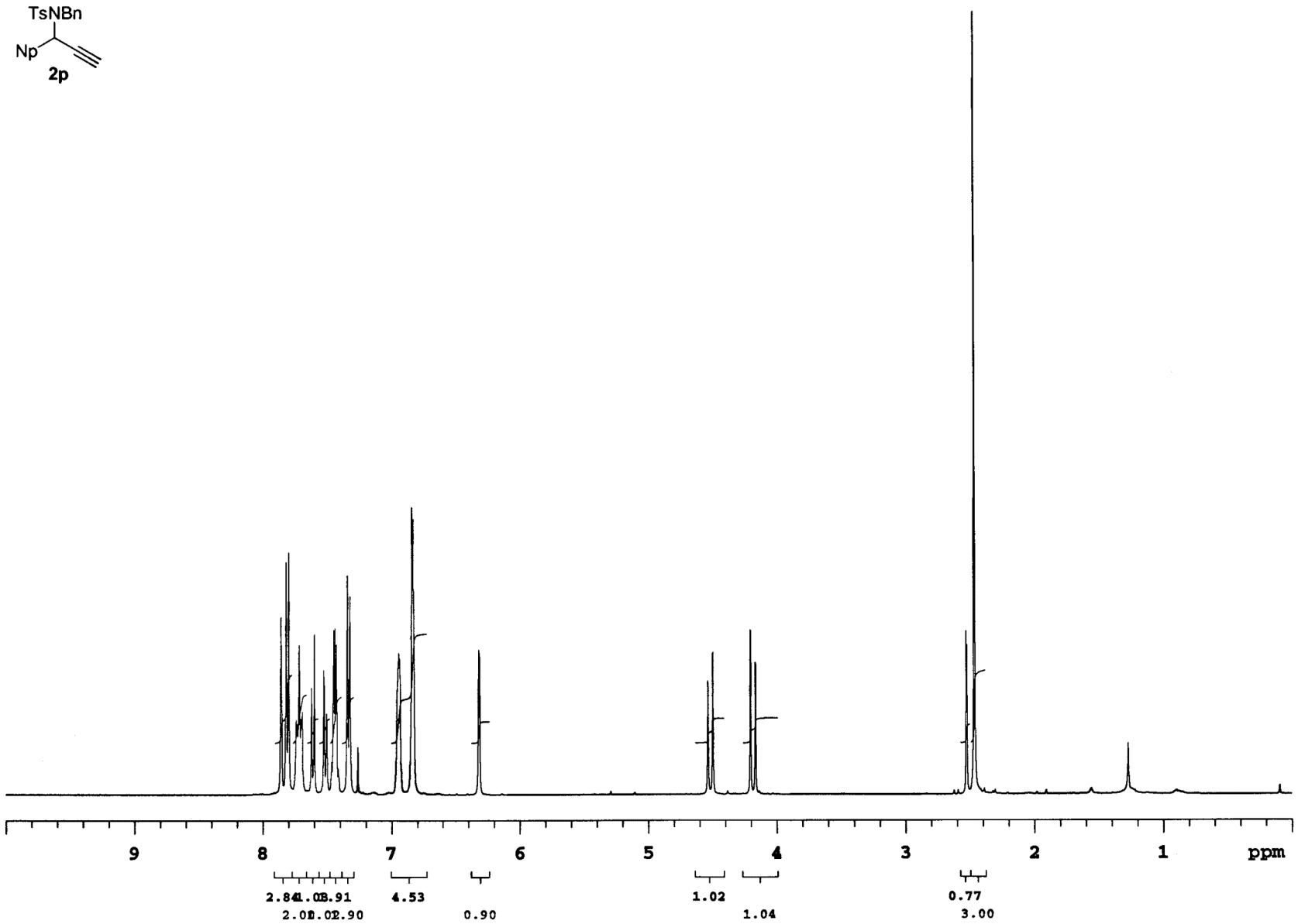
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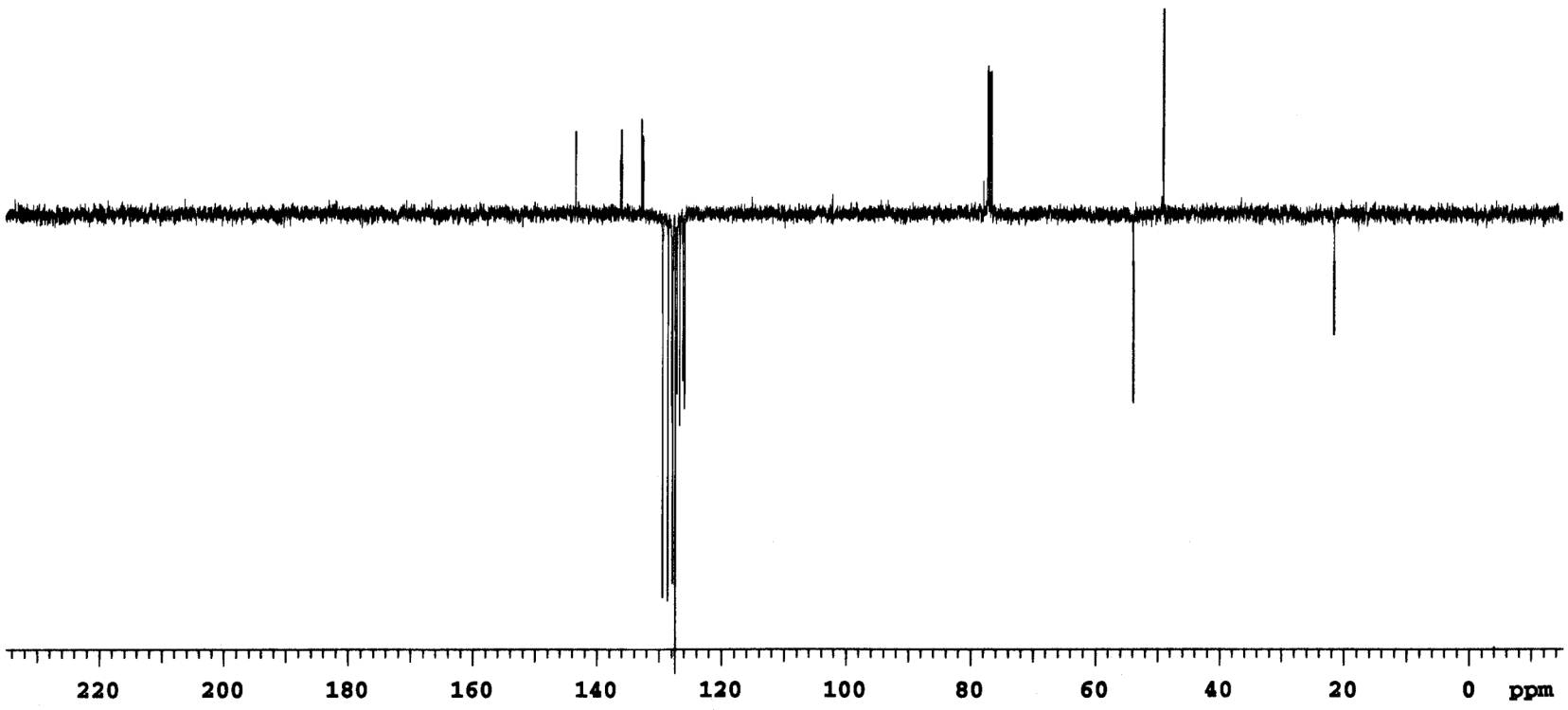
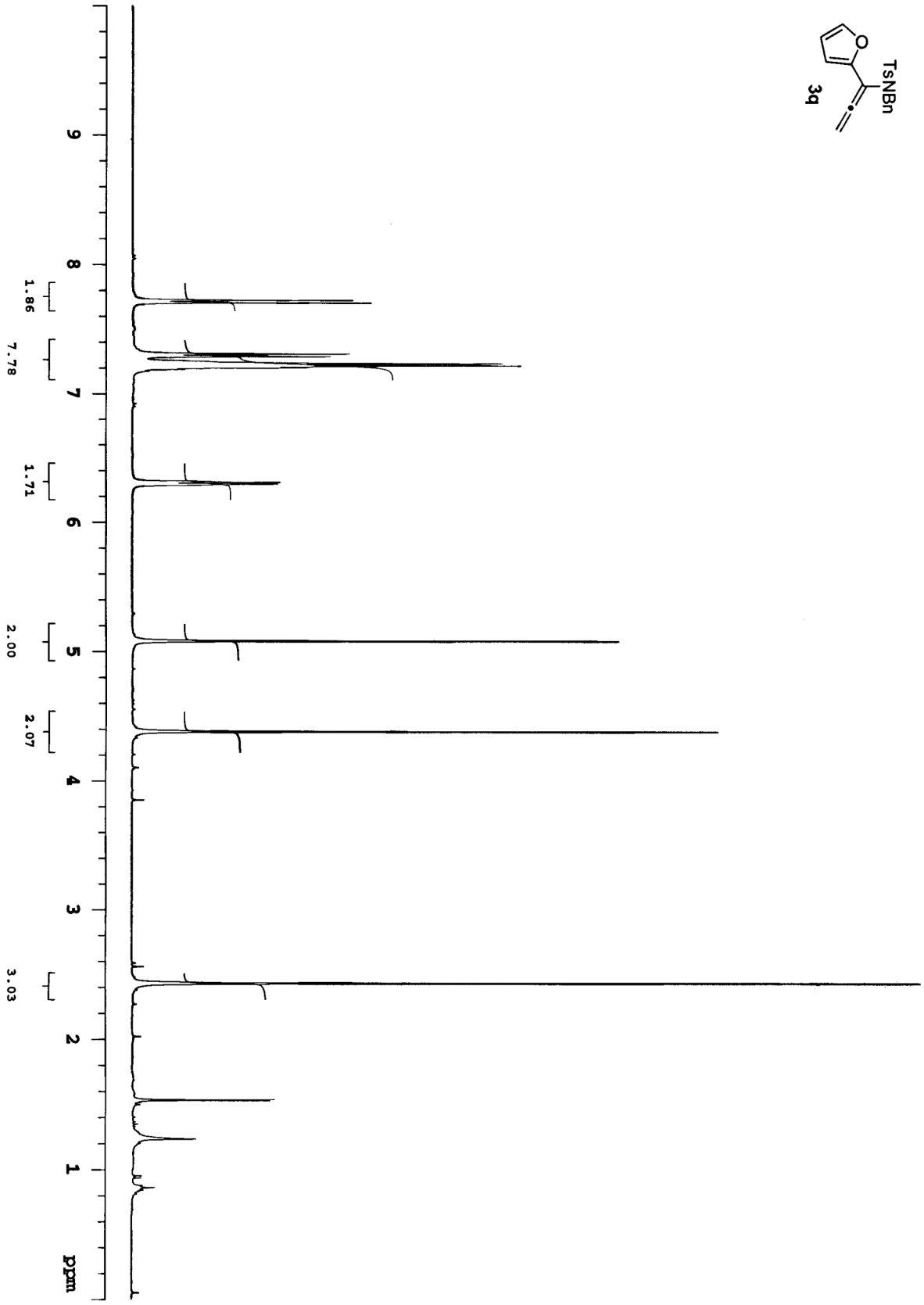
2p

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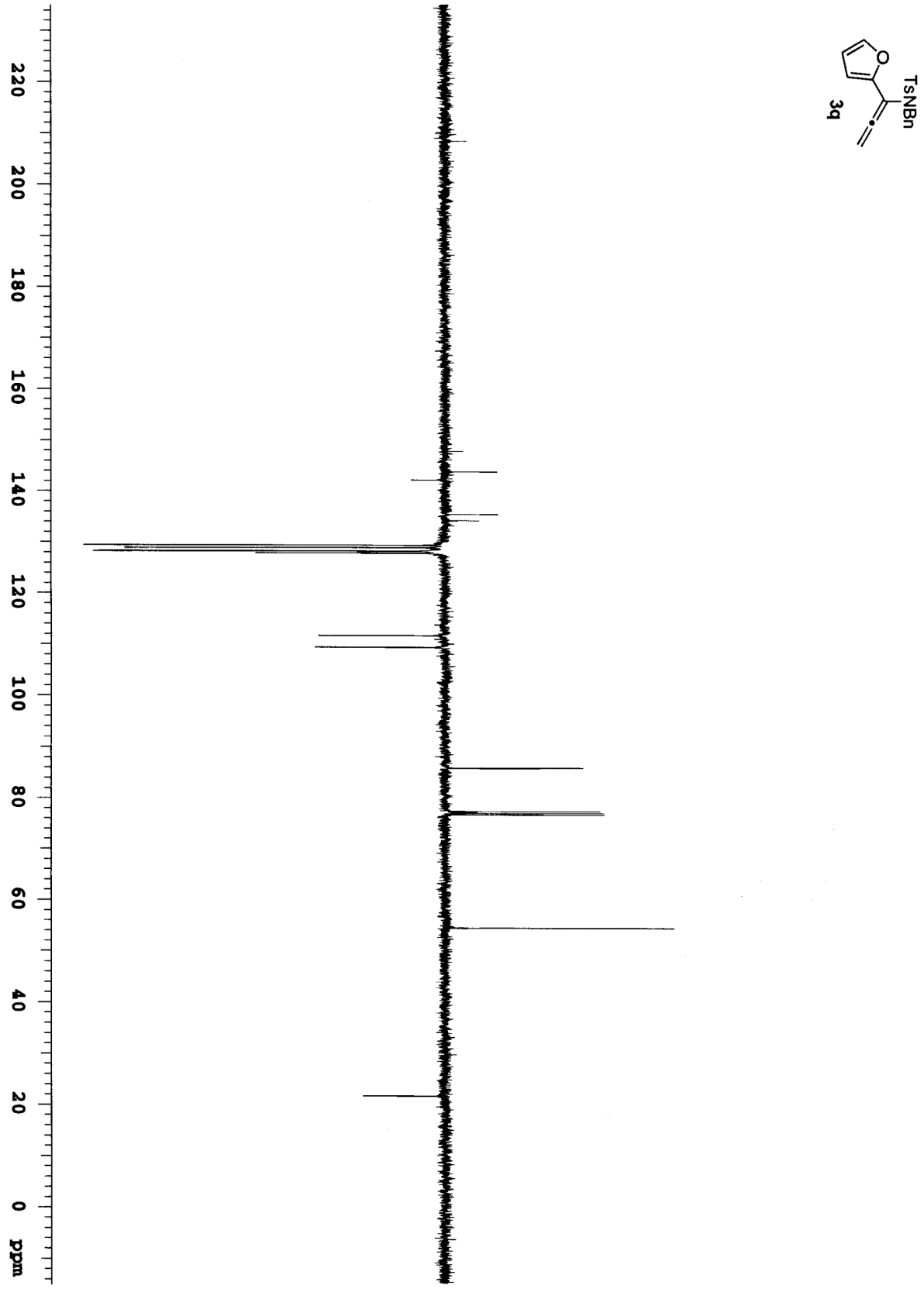
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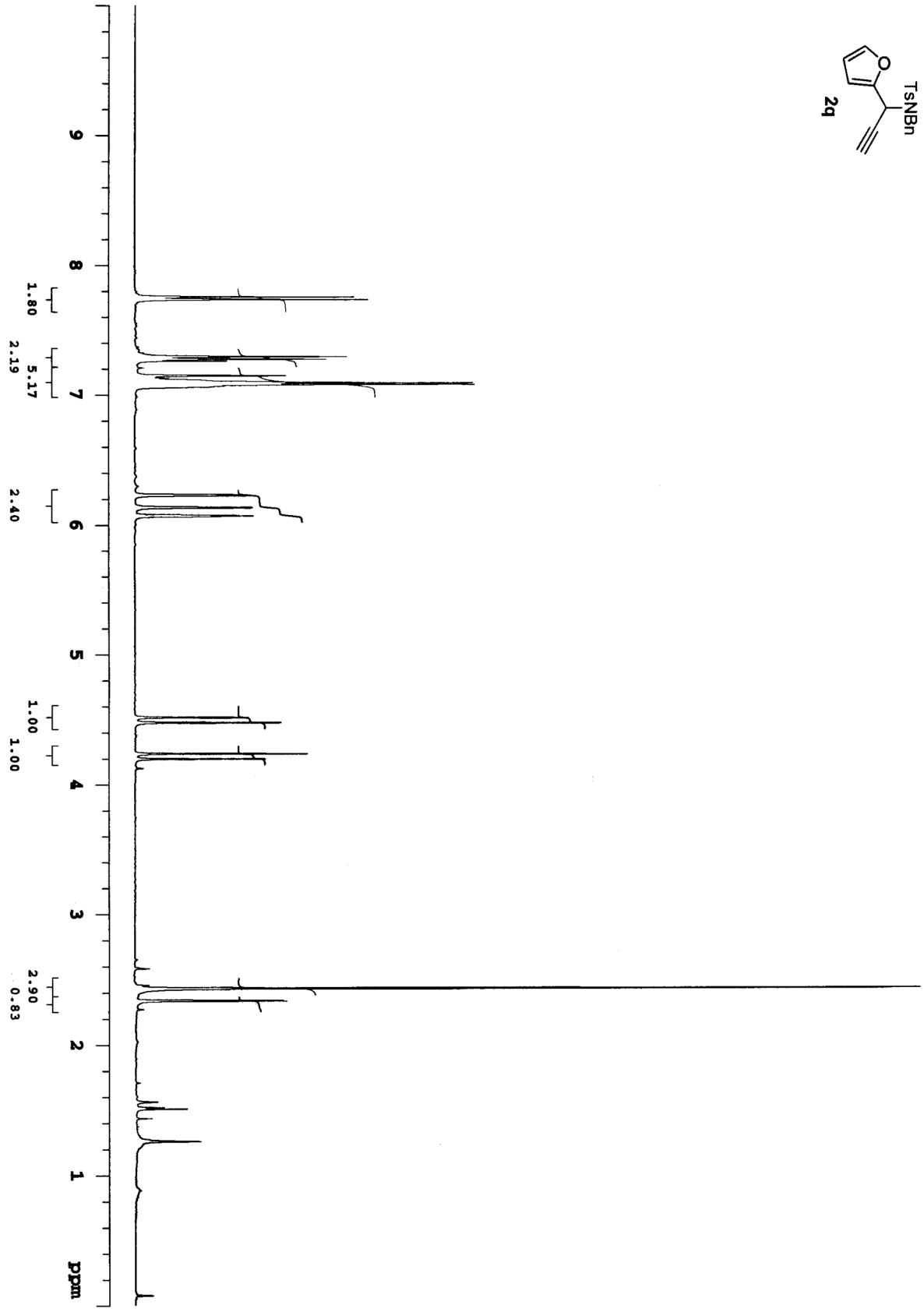
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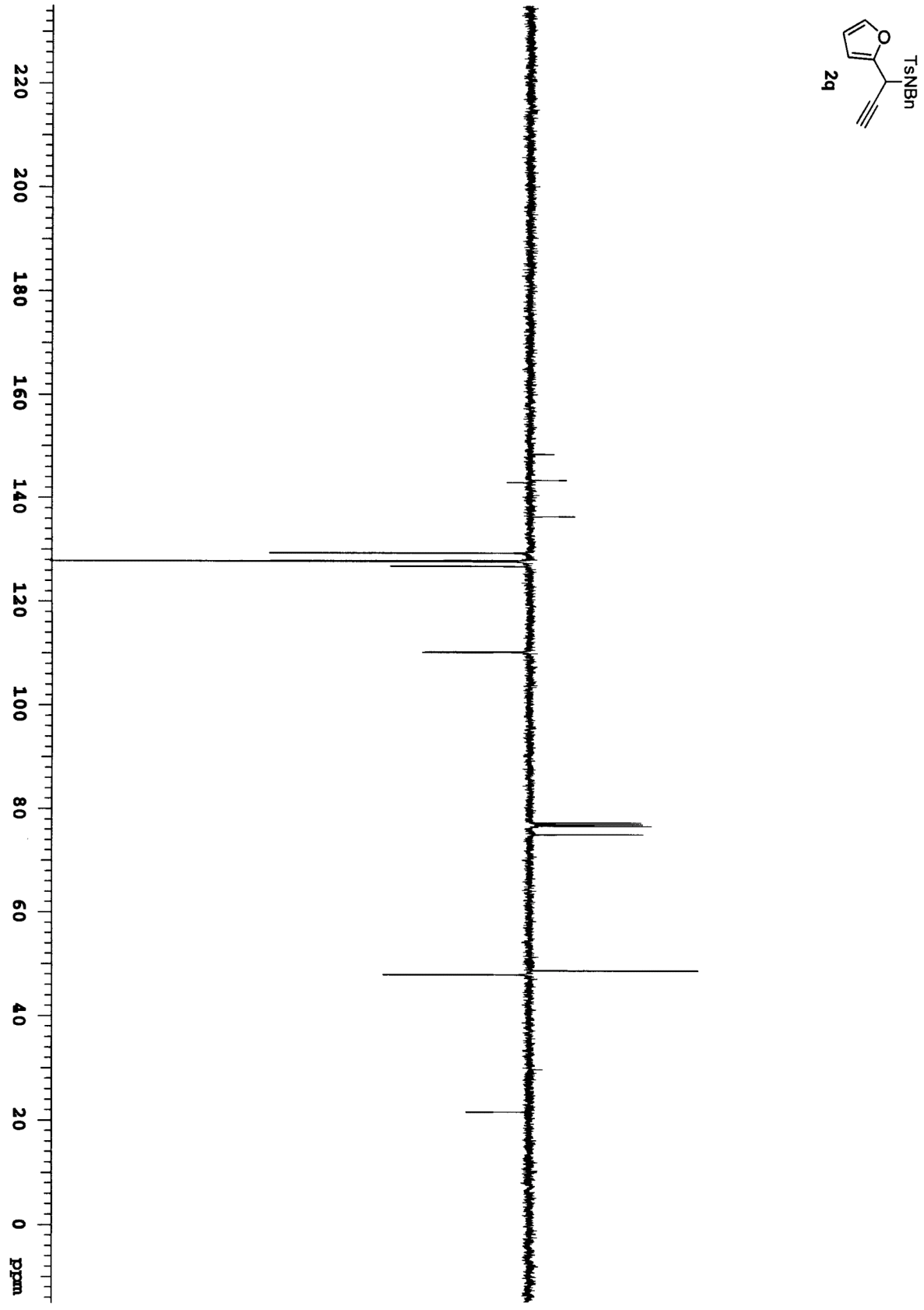
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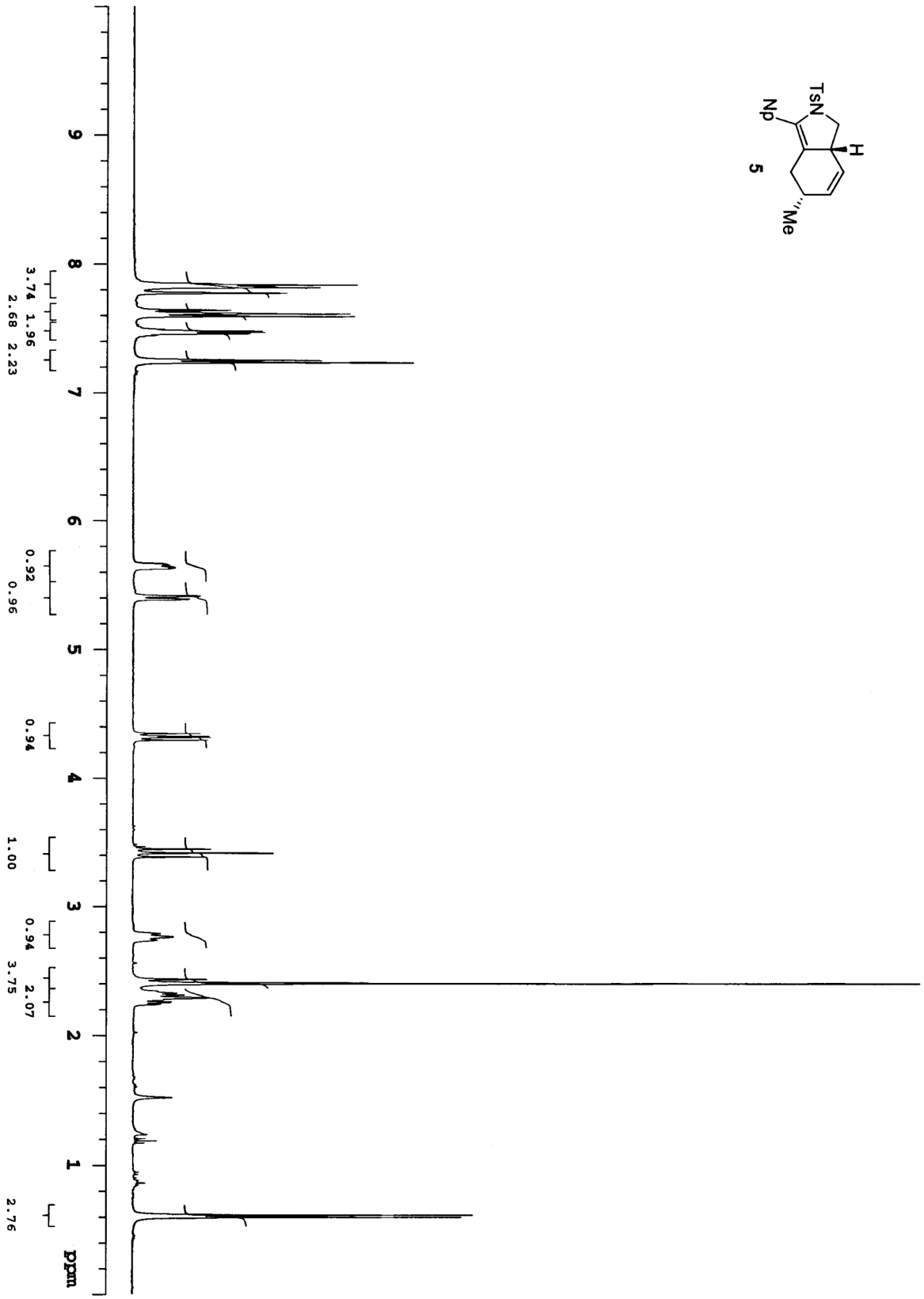
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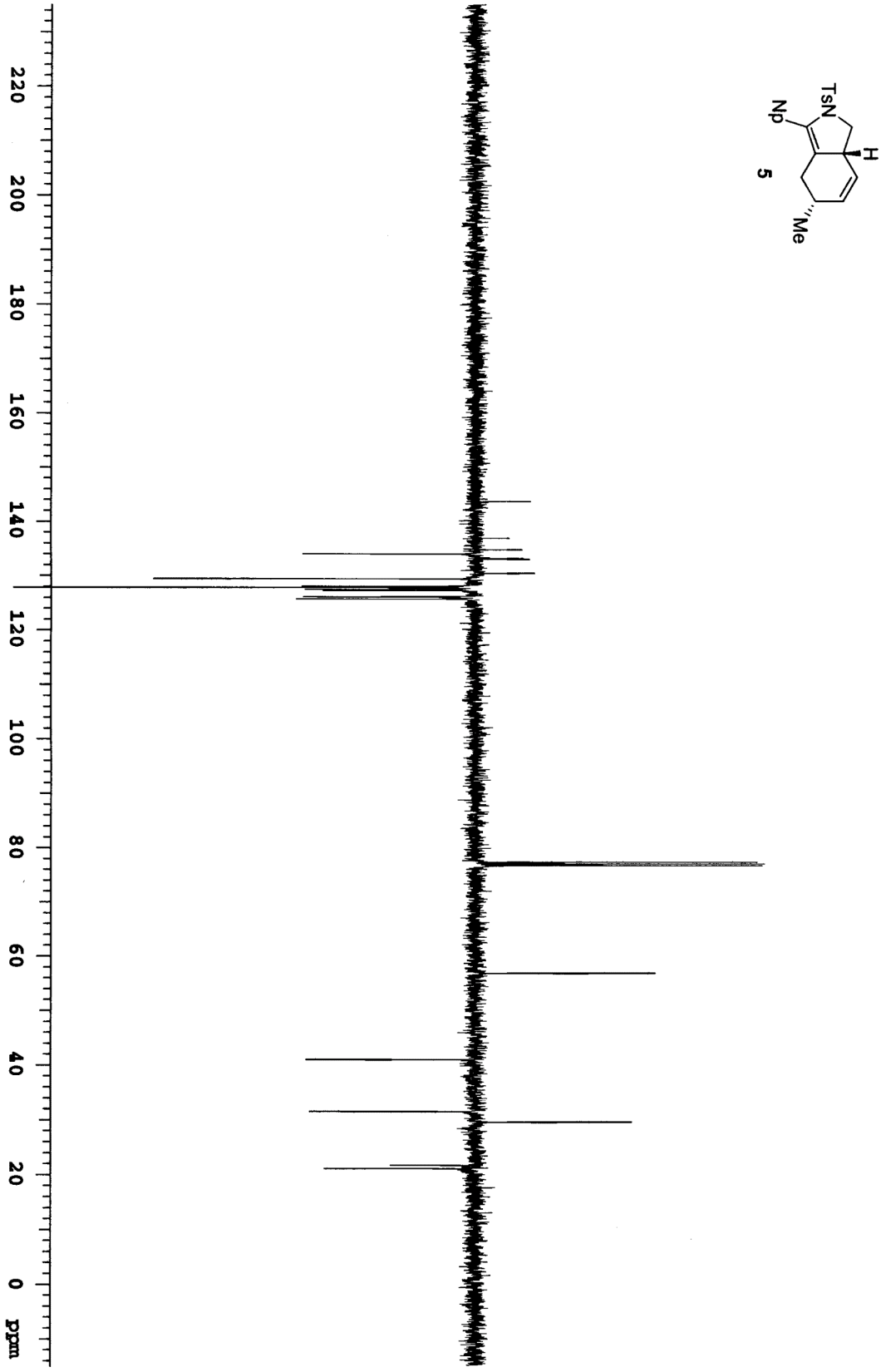
2.76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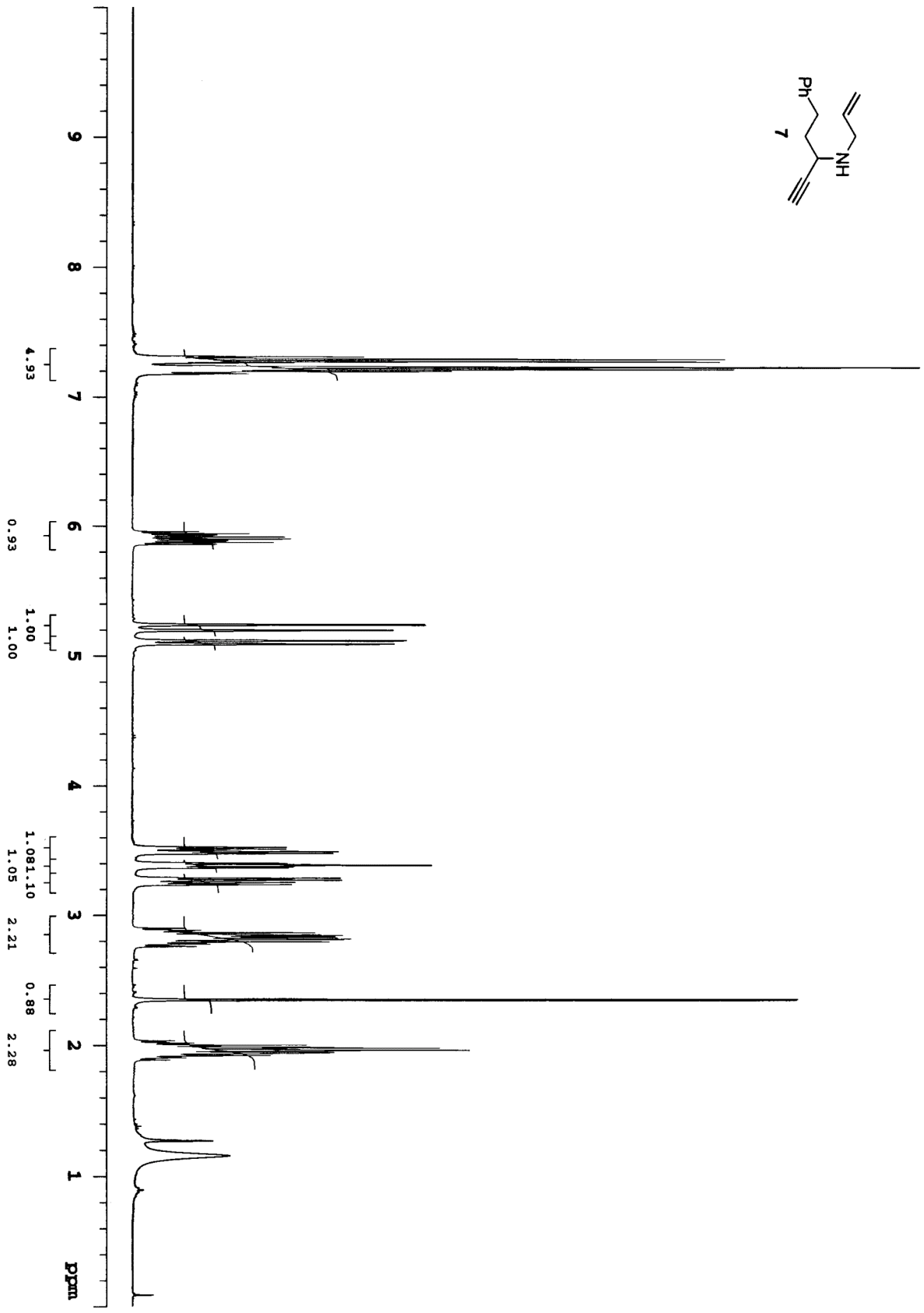
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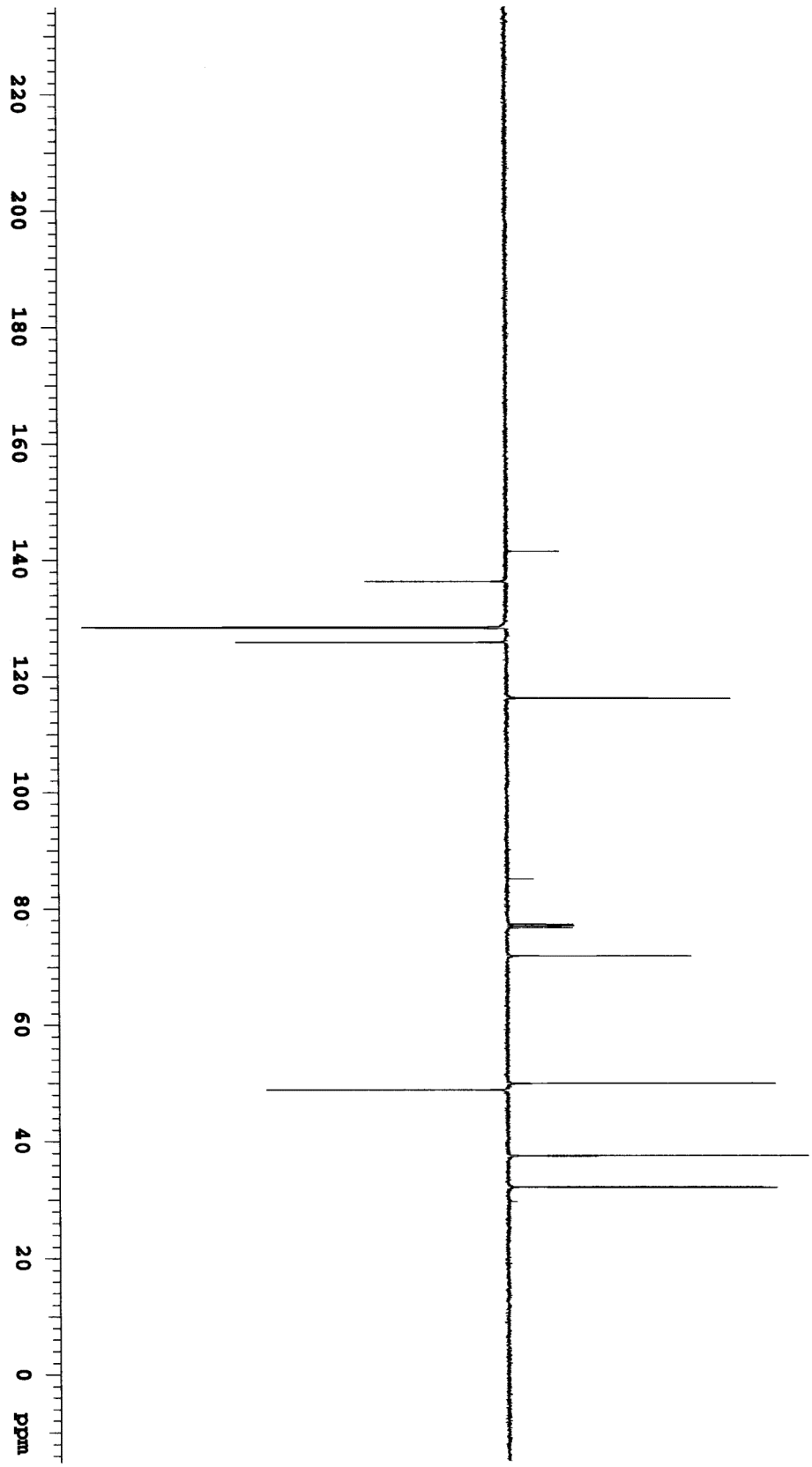
2.28

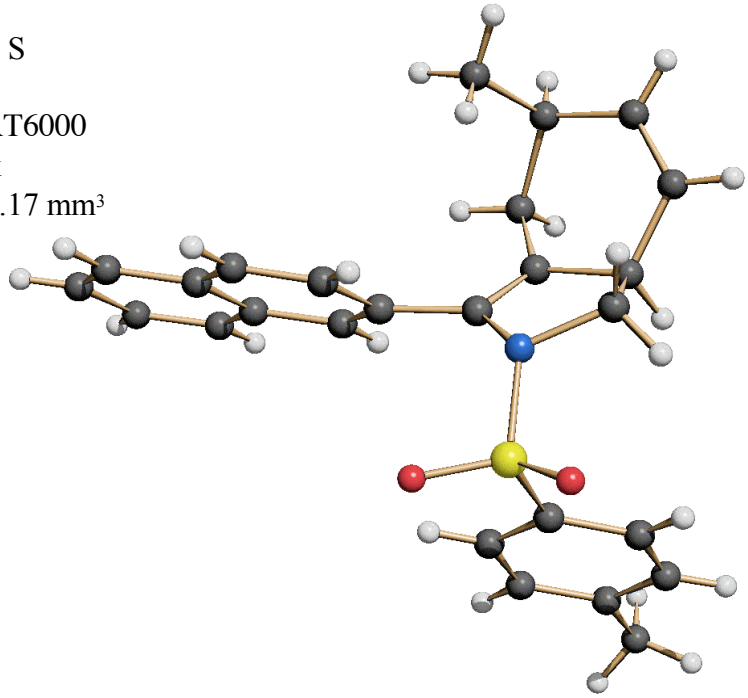

Ph
NH
7
220
200
180
160
140
120
100
80
60
40
20
0
ppm

Indiana University Molecular Structure Center

Report 05270:

Maren Pink
September 16, 2005

Empirical Formula	C26 H25 N O2 S
Molecular Weight	415.53
Instrument	IUMSC SMART6000
Crystal color, habit	Colorless block
Crystal size	0.23 × 0.20 × 0.17 mm^3
Crystal System	Monoclinic
Space Group	C2/c
Cell Dimensions (130 K)	
a =	22.5029(10) Å
b =	9.0115(4) Å
c =	22.8456(10) Å
α =	90°
β =	109.8390(10)°
γ =	90°
Volume	4357.8(3) $Å^3$
Z (Molecules/Cell)	8
Calculated Density	1.267 Mg/m^3
Absorption Coefficient	0.171 mm^{-1}
Final Residuals	
R1, observed data	0.0361
wR2, all data	0.1017



The sample was submitted by Michael J. Lawler (research group of P. A. Evans, Department of Chemistry, Indiana University).

A preliminary set of cell constants was calculated from reflections harvested from three sets of 20 frames. These initial sets of frames were oriented such that orthogonal wedges of reciprocal space were surveyed. This produced initial orientation matrices determined from 184 reflections. The data collection was carried out using Mo Kα radiation (graphite monochromator) with a frame time of 15 seconds and a detector distance of 5.0 cm. A randomly oriented region of reciprocal space was surveyed to the extent of a sphere. Four major sections of frames were collected with 0.30° steps in ω at different ϕ settings and a detector position of −43° in 2θ. An additional set of 50 frames was collected in order to model decay. Data to a resolution of 0.77 Å were considered in the reduction. Final cell constants were calculated from the xyz centroids of 8328 strong reflections from the actual data collection after integration. The intensity data were corrected for absorption.

The structure was found as proposed. Non-classical hydrogen bonds were observed between the oxygen atom and the aryl hydrogens.

Complete data are available at http://bl-chem-iumsc110.chem.indiana.edu/recipnet/