Supporting Information for

Palladium(0)-Catalyzed Intramolecular Dearomative Arylation of Pyrroles

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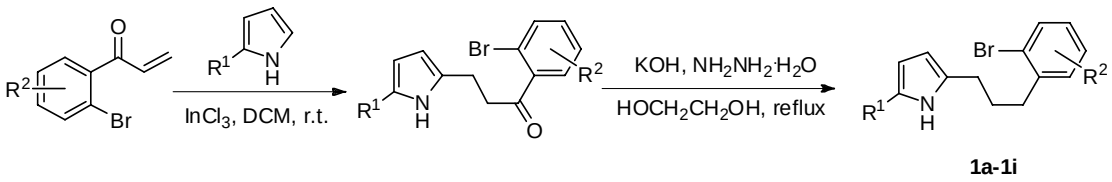
Table of Contents

General Methods. Unless stated otherwise, all reactions were carried out in flame-dried glassware under a dry argon atmosphere. All solvents were purified and dried according to standard methods prior to use. ^{1}H and ^{13}C NMR spectra were recorded on a Varian instrument (300 MHz and 75 MHz, 400 MHz and 100 MHz, respectively) and internally referenced to tetramethylsilane signal or residual protio solvent signals. ^{19}F NMR spectra was recorded on a Varian instrument (376 MHz and 282 MHz respectively) and internally referenced to trichlorofluoromethane signal. Data for ^{1}H NMR are recorded as follows: chemical shift (δ, ppm), multiplicity (s = singlet, d = doublet, t = triplet, m = multiplet or unresolved, br = broad singlet, coupling constant(s) in Hz, integration). Data for ^{13}C NMR and ^{19}F NMR are reported in terms of chemical shift (δ, ppm).

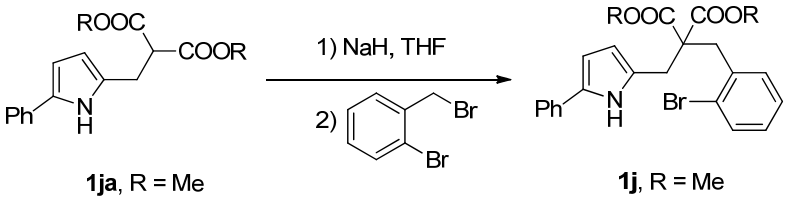
General procedure for synthesis of substrates 1a-1i.



1a-1i

Substrates **1a-1i** were synthesized from their corresponding *o*-bromoaryl vinyl ketones[1] *via* $InCl_3$ catalyzed Friedel-Crafts type Michael addition[2] and Wolff-Kishner-Huang reduction[3].

General method for synthesis of substrates 1j-1l.

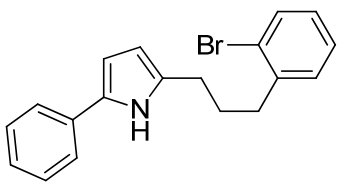


1ja, R = Me
1ka, R = Et
1la, R = ^{t}Bu

1j, R = Me
1k, R = Et
1l, R = ^{t}Bu

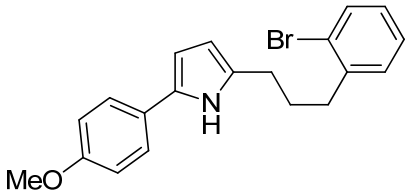
To a 50 mL flask cooled with an ice-bath containing **1ja**[4] (1.43 g, 5.0 mmol) in THF (10.0 mL), NaH (144 mg, 6.0 mmol) was added in several portions. After stirred for 20 min at room temperature, the flask was cooled with an ice-bath and *o*-bromo benzylbromide (1.50 g, 6.0 mmol) was added in one portion. The reaction mixture was stirred at room temperature for 16 h until the consumption of **1ja** (monitored by TLC), then quenched with water and extracted with EtOAc (3 X 30 mL). The combined organic layers were washed with brine, dried with Na_2SO_4, filtered and concentrated *in vacuo*. The residue was purified by silica gel column chromatography (petroleum ether/ethyl acetate = 5/1) to afford compound **1j** (1.51 g, 66% yield).

Syntheses of **1k** and **1l** were carried out according to the procedure above.



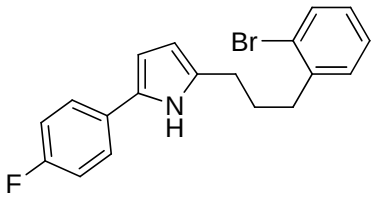
1a

1a, pink solid. ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.08 (s, 1H), 7.51 (d, *J* = 8.1 Hz, 1H), 7.38 (d, *J* = 7.5 Hz, 2H), 7.29 (t, *J* = 7.2 Hz, 2H), 7.20-7.10 (m, 3H), 7.04-6.99 (m, 1H), 6.41 (appt. *J* = 3.0 Hz, 1H), 6.00 (s, 1H), 2.78 (t, *J* = 7.5 Hz, 2H), 2.66 (t, *J* = 7.5 Hz, 2H), 2.00-1.90 (m, 2H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 141.2, 133.3, 132.8, 132.7, 130.5, 130.4, 128.7, 127.6, 127.3, 125.6, 124.4, 123.3, 107.1, 106.0, 35.6, 29.4, 27.3; IR (film): ν_{max} (cm^{-1}) = 3430, 2929, 2860, 1603, 1565, 1512, 1470, 1456, 1438, 1348, 1300, 1263, 1211, 1144, 1109, 1042, 1020, 895, 754, 692, 659, 518; ESI-MS (m/z): 340 ($M+H^+$, 100); HRMS (ESI): Exact mass calcd. for $C_{19}H_{19}NBr$ $[M+H]^+$: 340.0695. Found: 340.0688.



1b

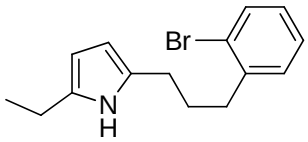
1b, pink solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.03 (s, 1H), 7.52 (d, *J* = 8.4 Hz, 1H), 7.34 (d, *J* = 9.2 Hz, 2H), 7.22-7.20 (m, 2H), 7.07-7.02 (m, 1H), 6.88 (d, *J* = 8.8 Hz, 2H), 6.29 (t, *J* = 2.8 Hz, 1H), 5.99 (t, *J* = 2.4 Hz, 1H), 3.79 (s, 3H), 2.81 (t, *J* = 7.6 Hz, 2H), 2.69 (t, *J* = 7.6 Hz, 2H), 2.02-1.94 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 157.8, 141.3, 132.8, 132.6, 130.7, 130.4, 127.6, 127.4, 126.1, 124.8, 124.4, 114.2, 106.9, 104.8, 55.3, 35.7, 29.5, 27.3; IR (film): ν_{max} (cm^{-1}) = 3433, 2934, 2860, 2834, 2040, 1882, 1614, 1522, 1470, 1438, 1386, 1250, 1180, 1113, 1027, 831, 767, 657, 537; EI-MS (m/z): 371 (9), 290 (12), 186 (100), 171 (8), 143 (15); HRMS (EI): Exact mass calcd. for $C_{20}H_{20}NOBr$ $[M]^+$: 369.0728. Found: 369.0724.



1c

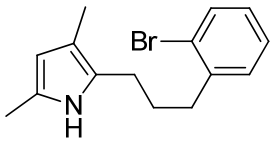
1c, pink oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.05 (s, 1H), 7.53 (d, *J* = 7.6 Hz, 1H), 7.37 (dd, *J* = 5.2, 9.2 Hz, 2H), 7.24-7.22 (m, 2H), 7.08-7.00 (m, 3H), 6.34 (t, *J* = 3.2 Hz, 1H), 6.00 (t, *J* = 3.2 Hz, 1H), 2.82 (t, *J* = 8.0 Hz, 2H), 2.71 (t, *J* = 7.6 Hz, 2H), 2.03-1.95 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 161.2 (d, *J* = 243.5 Hz), 141.2,

133.4, 132.8, 130.4, 129.9, 129.3 (d, J = 3.0 Hz), 127.6, 127.4, 125.0 (d, J = 7.8 Hz), 124.4, 115.7 (d, J = 21.2 Hz), 107.2, 105.9, 35.7, 29.6, 27.4; ^{19}F NMR (376 MHz, $CDCl_3$) δ -117.0 (m); IR (film): ν_{max} (cm^{-1}) = 3443, 3054, 2934, 2860, 1578, 1522, 1518, 1482, 1471, 1439, 1231, 1158, 1098, 1039, 831, 769, 753, 658, 522; EI-MS (m/z): 357 (9), 278 (18), 187 (13), 174 (100); HRMS (EI): Exact mass calcd. for $C_{19}H_{17}NFBr$ $[M]^+$: 357.0528. Found: 357.0532.



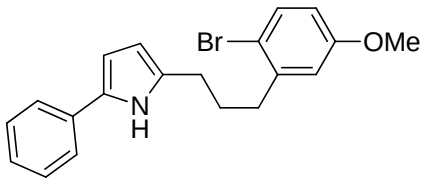
1d

1d, yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.61 (brs, 1H), 7.51 (d, J = 8.4 Hz, 1H), 7.21-7.20 (m, 2H), 7.05-7.01 (m, 1H), 5.82 (t, J = 3.2 Hz, 1H), 5.79 (t, J = 2.8 Hz, 1H), 2.78 (t, J = 8.0 Hz, 2H), 2.62 (t, J = 7.6 Hz, 2H), 2.57 (q, J = 7.6 Hz, 2H), 1.97-1.89 (m, 2H), 1.22 (t, J = 7.6 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 141.4, 132.7, 130.4, 127.5, 127.3, 124.4, 104.8, 103.9, 35.7, 29.6, 27.3, 20.8, 13.6; IR (film): ν_{max} (cm^{-1}) = 3435, 3367, 2964, 2931, 2863, 1682, 1590, 1567, 1511, 1471, 1439, 1326, 1179, 1023, 941, 750, 658, 515, 444; EI-MS (m/z): 291 (5), 276 (3), 212 (24), 108 (100), 106 (20), 93 (18); HRMS (EI): Exact mass calcd. for $C_{15}H_{18}NBr$ $[M]^+$: 291.0623. Found: 291.0620.



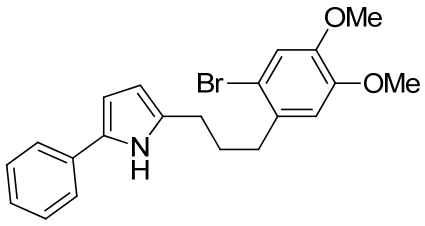
1e

1e, dark-brown oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.51 (d, J = 7.6 Hz, 1H), 7.38 (brs, 1H), 7.23-7.18 (m, 2H), 7.03 (dt, J = 2.4, 8.0 Hz, 1H), 5.64 (s, 1H), 2.75 (t, J = 8.0 Hz, 2H), 2.57 (t, J = 8.0 Hz, 2H), 2.18 (s, 3H), 1.98 (s, 3H), 1.89-1.81 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 141.4, 132.8, 130.2, 127.5, 127.3, 126.0, 124.9, 124.4, 114.1, 107.7, 35.8, 30.2, 25.4, 12.9, 10.8; IR (film): ν_{max} (cm^{-1}) = 3438, 3367, 2925, 2859, 1683, 1604, 1567, 1540, 1471, 1438, 1397, 1383, 1148, 1104, 1024, 788, 751, 658, 636, 518, 447; ESI-MS (m/z): 292 ($M+H^+$, 100); HRMS (ESI): Exact mass calcd. for $C_{15}H_{19}NBr$ $[M+H]^+$: 292.0695. Found: 292.0697.



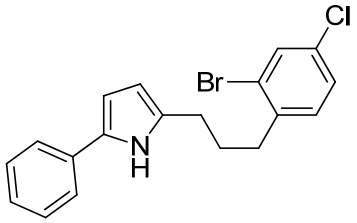
1f

1f, pale yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.14 (brs, 1H), 7.43-7.39 (m, 3H), 7.32 (t, *J* = 7.6 Hz, 2H), 7.15 (t, *J* = 7.2 Hz, 1H), 6.76 (d, *J* = 3.2 Hz, 1H), 6.62 (dd, *J* = 2.8, 8.4 Hz, 1H), 6.42 (t, *J* = 3.2 Hz, 1H), 6.01 (t, *J* = 2.8 Hz, 1H), 3.76 (s, 3H), 2.78 (t, *J* = 7.2 Hz, 2H), 2.71 (t, *J* = 7.6 Hz, 2H), 2.02-1.95 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.9, 142.2, 133.34, 133.28, 132.9, 130.7, 128.8, 125.7, 123.3, 116.1, 114.9, 113.1, 107.2, 106.1, 55.4, 35.9, 29.5, 27.4; IR (film): ν_{max} (cm^{-1}) = 3432, 2935, 2862, 2835, 1684, 1604, 1571, 1514, 1472, 1415, 1278, 1240, 1162, 1043, 1012, 803, 756, 693, 600, 518; ESI-MS (m/z): 370 ($M+H^+$, 100); HRMS (ESI): Exact mass calcd. for $C_{20}H_{21}NOBr$ $[M+H]^+$: 370.0801. Found: 370.0791.



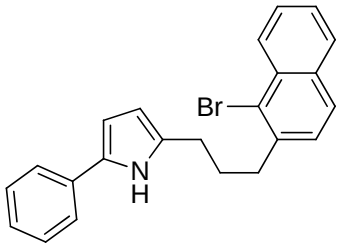
1g

1g, pale yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.19 (brs, 1H), 7.43 (dd, *J* = 1.2, 8.4 Hz, 2H), 7.32 (t, *J* = 7.2 Hz, 2H), 7.15 (t, *J* = 7.2 Hz, 1H), 7.00 (s, 1H), 6.69 (s, 1H), 6.42 (t, *J* = 3.2 Hz, 1H), 6.02 (t, *J* = 2.8 Hz, 1H), 3.83 (s, 3H), 3.82 (s, 3H), 2.75 (t, *J* = 7.6 Hz, 2H), 2.71 (t, *J* = 7.6 Hz, 2H), 2.01-1.93 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 148.2, 147.8, 133.4, 133.2, 132.8, 130.6, 128.8, 125.6, 123.3, 115.5, 114.0, 113.0, 107.2, 106.0, 56.1, 56.0, 35.3, 29.8, 27.3; IR (film): ν_{max} (cm^{-1}) = 3378, 2934, 2840, 1604, 1509, 1439, 1383, 1338, 1256, 1215, 1162, 1073, 1031, 855, 780, 757, 736, 694, 592, 517; ESI-MS (m/z): 400 ($M+H^+$, 100); HRMS (ESI): Exact mass calcd. for $C_{21}H_{23}NO_2Br$ $[M+H]^+$: 400.0907. Found: 400.0895.



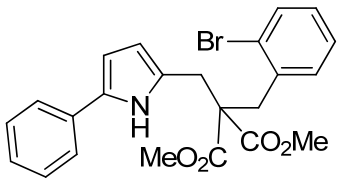
1h

1h, yellow solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.14 (brs, 1H), 7.55 (d, *J* = 2.0 Hz, 1H), 7.43 (d, *J* = 7.2 Hz, 2H), 7.34 (t, *J* = 7.6 Hz, 2H), 7.21 (dt, *J* = 2.0, 8.0 Hz, 1H), 7.17-7.14 (m, 2H), 6.43 (t, *J* = 2.8 Hz, 1H), 6.02 (t, *J* = 3.2 Hz, 1H), 2.80 (t, *J* = 7.6 Hz, 2H), 2.72 (t, *J* = 7.6 Hz, 2H), 2.01-1.94 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 139.8, 133.1, 132.9, 132.3, 131.0, 130.8, 128.8, 128.4, 127.6, 125.7, 124.6, 123.4, 107.3, 106.1, 35.1, 29.5, 27.3; IR (film): ν_{max} (cm^{-1}) = 3440, 3055, 2935, 2862, 1605, 1585, 1557, 1514, 1470, 1396, 1212, 1098, 1040, 867, 811, 755, 692, 517; EI-MS (m/z): 375 (4), 294 (9), 169 (10), 156 (100), 84 (42); HRMS (EI): Exact mass calcd. for $C_{19}H_{17}NClBr$ $[M]^+$: 373.0233. Found: 373.0226.



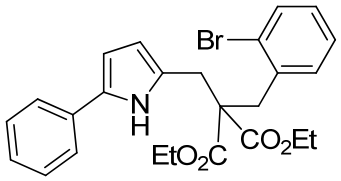
1i

1i, dark-brown solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.32 (d, *J* = 8.4 Hz, 1H), 8.12 (brs, 1H), 7.78 (d, *J* = 7.6 Hz, 1H), 7.72 (d, *J* = 8.4 Hz, 1H), 7.57 (dt, *J* = 1.2, 7.2 Hz, 1H), 7.47 (dt, *J* = 0.8, 7.2 Hz, 1H), 7.41 (d, *J* = 7.2 Hz, 2H), 7.34-7.30 (m, 3H), 7.15 (t, *J* = 7.2 Hz, 1H), 6.42 (t, *J* = 2.8 Hz, 1H), 6.03 (t, *J* = 2.8 Hz, 1H), 3.07 (t, *J* = 7.6 Hz, 2H), 2.75 (t, *J* = 7.6 Hz, 2H), 2.12-2.04 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 139.5, 133.4, 133.2, 132.9, 132.6, 130.7, 128.8, 128.1, 128.0, 127.6, 127.3, 127.2, 125.9, 125.7, 123.7, 123.4, 107.3, 106.1, 36.9, 29.8, 27.5; IR (film): ν_{max} (cm^{-1}) = 3417, 3042, 2924, 1679, 1604, 1514, 1455, 1400, 1328, 1253, 1041, 968, 912, 899, 818, 767, 754, 742, 691, 545, 527; EI-MS (m/z): 389 (2), 310 (69), 174 (11), 169 (16), 156 (100), 141 (16); HRMS (EI): Exact mass calcd. for $C_{23}H_{20}NBr$ $[M]^+$: 389.0779. Found: 389.0776.



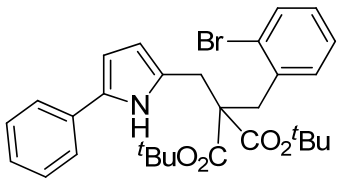
1j

1j, yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.04 (brs, 1H), 7.54 (d, *J* = 7.6 Hz, 1H), 7.42 (dd, *J* = 1.2, 8.4 Hz, 2H), 7.35-7.31 (m, 2H), 7.24-7.21 (m, 2H), 7.16 (t, *J* = 7.2 Hz, 1H), 7.11-7.07 (m, 1H), 6.34 (t, *J* = 3.2 Hz, 1H), 5.95 (t, *J* = 3.2 Hz, 1H), 3.64 (s, 6H), 3.58 (s, 2H), 3.21 (s, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 171.9, 136.1, 133.0, 132.9, 131.6, 131.2, 128.8, 128.6, 127.6, 127.4, 126.2, 125.7, 123.3, 110.2, 105.4, 60.7, 52.7, 39.5, 33.3; IR (film): v_{max} (cm^{-1}) = 3439, 3064, 2951, 2842, 1724, 1605, 1512, 1474, 1436, 1337, 1263, 1205, 1177, 1071, 1044, 950, 909, 859, 756, 733, 693; ESI-MS (m/z): 456 ($M+H^+$, 100); HRMS (ESI): Exact mass calcd. for $C_{23}H_{23}NO_4Br$ $[M+H]^+$: 456.0805. Found: 456.0797.



1k

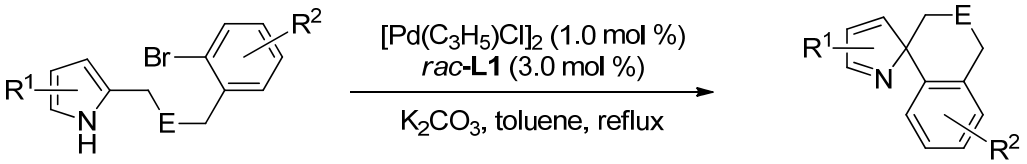
1k, yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.14 (brs, 1H), 7.53 (dd, *J* = 1.2, 8.4 Hz, 1H), 7.41 (d, *J* = 6.8 Hz, 2H), 7.32 (t, *J* = 7.6 Hz, 2H), 7.28 (dd, *J* = 2.0, 8.0 Hz, 1H), 7.21 (dt, *J* = 1.2, 7.2 Hz, 1H), 7.17-7.13 (m, 1H), 7.07 (dt, *J* = 1.6, 7.6 Hz, 1H), 6.32 (t, *J* = 3.2 Hz, 1H), 5.95 (t, *J* = 3.2 Hz, 1H), 4.14-4.04 (m, 4H), 3.58 (s, 2H), 3.20 (s, 2H), 1.07 (t, *J* = 7.6 Hz, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 171.7, 136.4, 133.1, 132.9, 131.6, 131.3, 128.7, 128.4, 127.8, 127.3, 126.3, 125.6, 123.4, 110.4, 105.3, 61.7, 60.5, 39.4, 33.3, 13.6; IR (film): v_{max} (cm^{-1}) = 3435, 3065, 2981, 2936, 1717, 1605, 1513, 1474, 1441, 1368, 1333, 1260, 1194, 1071, 1044, 907, 861, 779, 756, 693; ESI-MS (m/z): 484 ($M+H^+$, 100); HRMS (ESI): Exact mass calcd. for $C_{25}H_{27}NO_4Br$ $[M+H]^+$: 484.1118. Found: 484.1112.



1l

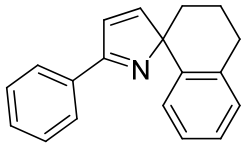
1l, yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.31 (brs, 1H), 7.54 (d, *J* = 8.0 Hz, 1H), 7.40 (d, *J* = 7.2 Hz, 2H), 7.37 (dd, *J* = 1.6, 8.0 Hz, 1H), 7.32 (t, *J* = 7.6 Hz, 2H), 7.21 (t, *J* = 7.6 Hz, 1H), 7.14 (t, *J* = 7.6 Hz, 1H), 7.07 (dt, *J* = 1.6, 7.6 Hz, 1H), 6.34 (t, *J* = 3.2 Hz, 1H), 5.94 (t, *J* = 3.2 Hz, 1H), 3.54 (s, 2H), 3.13 (s, 2H), 1.33 (s, 18H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 171.1, 137.1, 133.2, 132.9, 131.4, 131.2, 128.7, 128.4, 128.2, 127.1, 126.4, 125.4, 123.2, 110.7, 105.0, 82.3, 61.1, 39.5, 33.4, 27.6; IR (film): ν_{max} (cm^{-1}) = 3435, 2978, 2932, 1713, 1605, 1585, 1514, 1474, 1393, 1368, 1338, 1273, 1218, 1145, 1071, 1028, 910, 845, 756, 692, 592; ESI-MS (m/z): 540 ($M+H^+$, 100); HRMS (ESI): Exact mass calcd. for $C_{29}H_{35}NO_4Br$ $[M+H]^+$: 540.1744. Found: 540.1754.

General procedure for Pd-catalyzed dearomative arylation reaction (1a as an example).



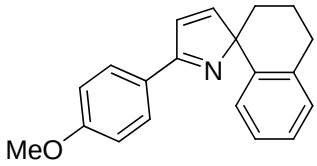
1 **2**

To a dry 25 mL Schlenk flask was added $[Pd(C_3H_5)Cl]_2$ (1.5 mg, 0.004 mmol), *rac*-**L1** (6.5 mg, 0.012 mmol) and K_2CO_3 (82.9 mg, 0.6 mmol) under argon. A solution of **1a** (136.0 mg, 0.4 mmol) in toluene (2.0 mL) was added. The resulting mixture was heated to reflux (at 120 ^{o}C) and stirred until the consumption of the starting material (monitored by TLC). The reaction mixture was cooled down to room temperature, filtered through a pad of celite, washed with EtOAc. The filtrate was concentrated and the residue was purified by silica gel column chromatography (petroleum ether/ethyl acetate = 10/1) to afford product **2a**.



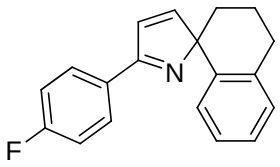
2a

2a, viscous colorless oil, 93.3 mg, 90% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.03-8.01 (m, 2H), 7.62 (d, *J* = 4.8 Hz, 1H), 7.47-7.45 (m, 3H), 7.16 (t, *J* = 7.2 Hz, 1H), 7.12 (t, *J* = 7.2 Hz, 1H), 6.96 (t, *J* = 7.6 Hz, 1H), 6.89 (d, *J* = 5.2 Hz, 1H), 6.62 (d, *J* = 8.0 Hz, 1H), 3.03-2.94 (m, 2H), 2.32-2.29 (m, 1H), 2.21-2.14 (m, 1H), 2.04-2.00 (m, 1H), 1.89 (ddd, *J* = 2.4, 8.0, 12.8 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 171.2, 162.8, 137.0, 133.9, 132.1, 130.5, 129.8, 128.6, 127.8, 127.2, 126.0, 125.8, 123.7, 84.0, 32.1, 30.0, 21.9; IR (film): v_{max} (cm^{-1}) = 3059, 2934, 2864, 1604, 1597, 1575, 1516, 1489, 1447, 1359, 1275, 1024, 907, 880, 750, 725, 694; ESI-MS (m/z): 260 ($M+H^+$, 100); HRMS (ESI): Exact mass calcd. for $C_{19}H_{18}N$ $[M+H]^+$: 260.1434. Found: 260.1439.



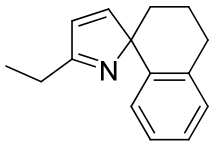
2b

2b, viscous colorless oil, 107.6 mg, 93% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.90 (d, *J* = 8.8 Hz, 2H), 7.51 (d, *J* = 4.8 Hz, 1H), 7.07 (t, *J* = 7.6 Hz, 1H), 7.04 (t, *J* = 7.2 Hz, 1H), 6.90-6.86 (m, 3H), 6.78 (d, *J* = 5.2 Hz, 1H), 6.54 (d, *J* = 8.0 Hz, 1H), 3.77 (s, 3H), 2.97-2.84 (m, 2H), 2.23-2.18 (m, 1H), 2.09 (ddd, *J* = 2.8, 10.0, 12.8 Hz, 1H), 1.95-1.89 (m, 1H), 1.80 (ddd, *J* = 2.4, 8.0, 12.4 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 170.6, 162.3, 161.5, 137.0, 132.4, 129.8, 129.4, 127.1, 126.5, 126.0, 125.8, 123.6, 114.0, 83.7, 55.3, 32.2, 29.9, 21.9; IR (film): v_{max} (cm^{-1}) = 3059, 3015, 2932, 2837, 1608, 1574, 1503, 1448, 1360, 1307, 1254, 1173, 1026, 839, 759; ESI-MS (m/z): 290 ($M+H^+$, 100); HRMS (ESI): Exact mass calcd. for $C_{20}H_{20}NO$ $[M+H]^+$: 290.1539. Found: 290.1530.



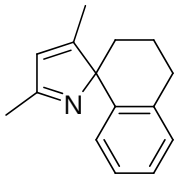
2c

2c, viscous colorless oil, 100.4 mg, 91% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.01 (dd, *J* = 5.2, 8.8 Hz, 2H), 7.62 (d, *J* = 4.8 Hz, 1H), 7.18-7.11 (m, 4H), 6.96 (t, *J* = 6.8 Hz, 1H), 6.85 (d, *J* = 4.8 Hz, 1H), 6.60 (d, *J* = 8.0 Hz, 1H), 3.07-2.92 (m, 2H), 2.32-2.25 (m, 1H), 2.17-2.11 (m, 1H), 2.05-1.95 (m, 1H), 1.90 (ddd, *J* = 2.4, 4.2, 12.8 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 170.1, 164.2 (d, *J* = 249.0 Hz), 163.0, 137.0, 132.0, 130.1 (d, *J* = 3.0 Hz), 129.89, 129.88, 129.81, 127.2, 125.9 (d, *J* = 7.1 Hz), 123.5, 115.7 (d, *J* = 21.5 Hz), 84.1, 32.1, 29.9, 21.8; ^{19}F NMR (376 MHz, $CDCl_3$) δ -109.8 (m); IR (film): ν_{max} (cm^{-1}) = 3061, 2933, 2865, 1603, 1585, 1520, 1502, 1448, 1412, 1352, 1261, 1225, 1156, 1098, 1014, 844, 809, 758, 617; ESI-MS (m/z): 278 ($M+H^+$, 100); HRMS (ESI): Exact mass calcd. for $C_{19}H_{17}FN$ $[M+H]^+$: 278.1340. Found: 278.1332.



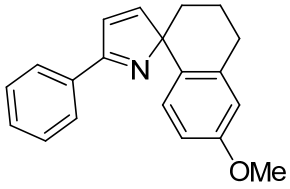
2d

2d, viscous colorless oil, 35.3 mg, 84% yield. ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.42 (d, *J* = 4.8 Hz, 1H), 7.12-7.08 (m, 2H), 6.96 (t, *J* = 6.6 Hz, 1H), 6.54 (d, *J* = 7.8 Hz, 1H), 6.33 (d, *J* = 4.5 Hz, 1H), 2.98-2.91 (m, 2H), 2.64 (q, *J* = 7.8 Hz, 2H), 2.25-2.19 (m, 1H), 2.03-1.95 (m, 2H), 1.85-1.79 (m, 1H), 1.28 (t, *J* = 7.8 Hz, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 176.7, 161.8, 137.1, 132.2, 129.7, 127.0, 125.9, 125.7, 125.6, 82.8, 31.8, 29.9, 26.0, 21.8, 11.4; IR (film): ν_{max} (cm^{-1}) = 3061, 2934, 2868, 1698, 1611, 1526, 1488, 1449, 1360, 1272, 1204, 1101, 1017, 904, 880, 759, 727; ESI-MS (m/z): 212 ($M+H^+$, 100); HRMS (ESI): Exact mass calcd. for $C_{15}H_{18}N$ $[M+H]^+$: 212.1434. Found: 212.1432.



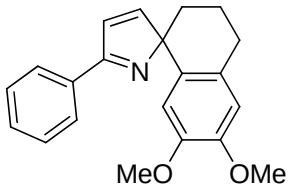
2e

2e, viscous colorless oil, 30.8 mg, 73% yield (Xphos was used as the ligand). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.14-7.08 (m, 2H), 7.00-6.96 (m, 1H), 6.46 (d, *J* = 8.0 Hz, 1H), 6.09 (q, *J* = 1.6 Hz, 1H), 2.98-2.93 (m, 1H), 2.89 (dd, *J* = 5.6, 11.2 Hz, 1H), 2.37-2.27 (m, 2H), 2.22 (s, 3H), 2.03-1.97 (m, 1H), 1.85 (d, *J* = 1.2 Hz, 3H), 1.52-1.47 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 172.4, 171.0, 137.7, 133.1, 129.6, 127.0, 126.1, 125.8, 125.6, 83.0, 32.3, 30.1, 21.0, 18.8, 13.4; IR (film): v_{max} (cm^{-1}) = 3384, 3058, 3018, 2933, 2864, 1634, 1556, 1489, 1438, 1380, 1331, 1272, 1214, 1181, 1003, 939, 907, 879, 827, 790, 763, 735, 599; ESI-MS (m/z): 212 ($M+H^+$, 100); HRMS (ESI): Exact mass calcd. for $C_{15}H_{18}N$ $[M+H]^+$: 212.1434. Found: 212.1439.



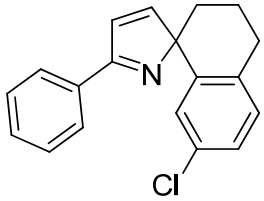
2f

2f, viscous colorless oil, 103 mg, 89% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.96-7.93 (m, 2H), 7.52 (d, *J* = 4.4 Hz, 1H), 7.40-7.38 (m, 3H), 6.80 (d, *J* = 4.8 Hz, 1H), 6.62 (s, 1H), 6.47 (s, 2H), 3.68 (s, 3H), 2.98-2.84 (m, 2H), 2.25-2.19 (m, 1H), 2.06 (ddd, *J* = 2.4, 9.6, 12.4 Hz, 1H), 1.96-1.91 (m, 1H), 1.82 (ddd, *J* = 2.4, 8.4, 12.8 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 170.9, 162.8, 158.6, 138.5, 133.9, 130.4, 128.6, 127.8, 127.2, 124.2, 123.5, 114.0, 112.5, 83.7, 55.2, 32.2, 30.4, 21.9; IR (film): v_{max} (cm^{-1}) = 3060, 2933, 2863, 2836, 1606, 1575, 1498, 1447, 1358, 1324, 1278, 1256, 1241, 1174, 1133, 1039, 881, 811, 755, 694; ESI-MS (m/z): 290 ($M+H^+$, 100); HRMS (ESI): Exact mass calcd. for $C_{20}H_{20}NO$ $[M+H]^+$: 290.1539. Found: 290.1530.



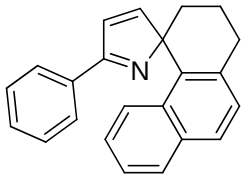
2g

2g, viscous colorless oil, 120 mg, 94% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.05-8.03 (m, 2H), 7.61 (d, *J* = 5.2 Hz, 1H), 7.48-7.47 (m, 3H), 6.90 (d, *J* = 4.8 Hz, 1H), 6.65 (s, 1H), 6.08 (s, 1H), 3.84 (s, 3H), 3.62 (s, 3H), 2.96-2.86 (m, 2H), 2.30-2.26 (m, 1H), 2.15-2.09 (m, 1H), 2.02-1.98 (m, 1H), 1.87 (ddd, *J* = 2.8, 8.8, 12.8 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 171.0, 162.9, 148.3, 147.2, 133.8, 130.5, 129.5, 128.6, 127.8, 123.9, 123.6, 112.1, 108.5, 83.8, 55.78, 55.76, 32.2, 29.6, 22.1; IR (film): v_{max} (cm^{-1}) = 3061, 2998, 2934, 2847, 1605, 1575, 1513, 1464, 1447, 1358, 1256, 1219, 1129, 1030, 952, 882, 856, 778, 755, 696; ESI-MS (m/z): 320 ($M+H^+$, 100); HRMS (ESI): Exact mass calcd. for $C_{21}H_{22}NO_2$ $[M+H]^+$: 320.1645. Found: 320.1635.



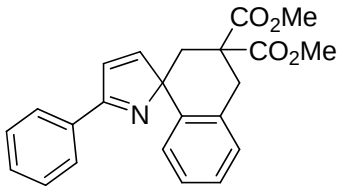
2h

2h, viscous colorless oil, 102 mg, 87% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.04-8.01 (m, 2H), 7.58 (d, *J* = 5.2 Hz, 1H), 7.48-7.47 (m, 3H), 7.09 (s, 2H), 6.92 (d, *J* = 4.8 Hz, 1H), 6.58 (s, 1H), 3.00-2.88 (m, 2H), 2.31-2.25 (m, 1H), 2.14 (ddd, *J* = 2.4, 9.6, 12.4 Hz, 1H), 2.03-1.96 (m, 1H), 1.86 (ddd, *J* = 2.4, 8.0, 12.8 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 171.7, 162.1, 135.4, 134.2, 133.5, 131.3, 131.1, 130.7, 128.7, 127.9, 127.3, 125.8, 124.3, 83.6, 31.8, 29.4, 21.7; IR (film): v_{max} (cm^{-1}) = 3063, 2936, 2865, 1693, 1604, 1575, 1517, 1485, 1447, 1358, 1262, 1186, 1168, 1092, 1024, 882, 864, 811, 799, 754, 693, 645; ESI-MS (m/z): 294 ($M+H^+$, 100); HRMS (ESI): Exact mass calcd. for $C_{19}H_{17}NCl$ $[M+H]^+$: 294.1044. Found: 294.1038.



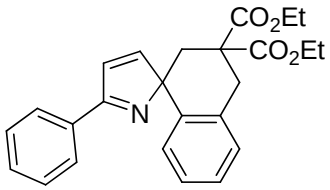
2i

2i, viscous colorless oil, 193 mg, 79% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.08-8.05 (m, 2H), 7.91 (d, *J* = 4.8 Hz, 1H), 7.67 (d, *J* = 8.4 Hz, 2H), 7.48-7.46 (m, 3H), 7.28 (d, *J* = 8.4 Hz, 2H), 7.24 (d, *J* = 8.4 Hz, 2H), 7.11 (d, *J* = 4.8 Hz, 1H), 3.18-3.12 (m, 2H), 2.32-2.27 (m, 1H), 1.99-1.97 (m, 1H), 1.78 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 171.4, 166.4, 136.7, 134.2, 133.4, 132.7, 130.5, 128.7, 128.6, 128.4, 128.2, 127.8, 125.8, 124.5, 124.4, 124.3, 85.0, 38.8, 32.4, 22.7; IR (film): ν_{max} (cm^{-1}) = 3060, 2933, 2864, 1694, 1603, 1502, 1448, 1412, 1352, 1261, 1225, 1156, 1099, 1013, 907, 881, 844, 810, 758, 728; ESI-MS (m/z): 310 ($M+H^+$, 100); HRMS (ESI): Exact mass calcd. for $C_{23}H_{20}N$ $[M+H]^+$: 310.1590. Found: 310.1587.



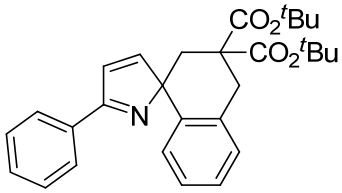
2j

2j, viscous colorless oil, 139 mg, 93% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.97-7.95 (m, 2H), 7.45-7.43 (m, 4H), 7.27-7.25 (m, 1H), 7.18 (dt, *J* = 1.2, 7.6 Hz, 1H), 7.02-6.98 (m, 2H), 6.63 (d, *J* = 7.6 Hz, 1H), 3.76 (s, 3H), 3.74 (s, 3H), 3.67 (AB, J_{AB} = 16.4 Hz, 1H), 3.30 (BA, J_{BA} = 16.8 Hz, 1H), 2.66 (AB, J_{AB} = 14.4 Hz, 1H), 2.53 (BA, J_{BA} = 13.2 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 172.1, 171.2, 170.3, 160.8, 134.0, 133.6, 130.6, 130.5, 129.4, 128.6, 127.9, 126.5, 125.7, 125.4, 82.3, 52.80, 52.78, 52.6, 35.8, 34.9; IR (film): ν_{max} (cm^{-1}) = 3060, 3028, 2952, 1736, 1604, 1575, 1519, 1493, 1447, 1360, 1328, 1256, 1216, 1119, 1043, 759, 695, 614; ESI-MS (m/z): 376 ($M+H^+$, 100); HRMS (ESI): Exact mass calcd. for $C_{23}H_{22}NO_4$ $[M+H]^+$: 376.1543. Found: 376.1535.



2k

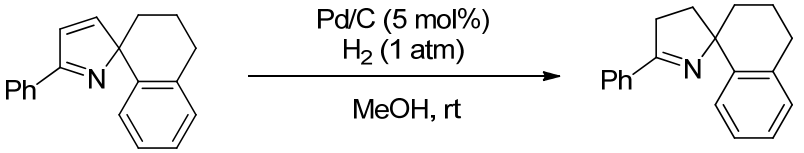
2k, viscous colorless oil, 148 mg, 92% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.98-7.95 (m, 2H), 7.47-7.43 (m, 4H), 7.26-7.24 (m, 1H), 7.17 (dt, J = 1.2, 7.6 Hz, 1H), 7.01-6.96 (m, 2H), 6.63 (d, J = 7.6 Hz, 1H), 4.31-4.14 (m, 4H), 3.63 (AB, J_{AB} = 16.8 Hz, 1H), 3.32 (BA, J_{BA} = 16.4 Hz, 1H), 2.63 (AB, J_{AB} = 13.6 Hz, 1H), 2.57 (BA, J_{BA} = 14.0 Hz, 1H), 1.25 (t, J = 7.2 Hz, 3H), 1.16 (t, J = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 171.7, 170.9, 170.5, 161.0, 134.1, 133.6, 130.63, 130.59, 129.4, 128.5, 127.8, 126.4, 125.6, 125.1, 82.4, 61.6, 61.5, 52.7, 35.7, 34.9, 14.0, 13.9; IR (film): ν_{max} (cm^{-1}) = 3061, 2980, 2935, 1732, 1605, 1576, 1519, 1492, 1447, 1360, 1324, 1252, 1213, 1191, 1155, 1118, 1043, 1018, 862, 758, 695; ESI-MS (m/z): 404 ($M+H^+$, 100); HRMS (ESI): Exact mass calcd. for $C_{25}H_{26}NO_4$ $[M+H]^+$: 404.1856. Found: 404.1845.



2l

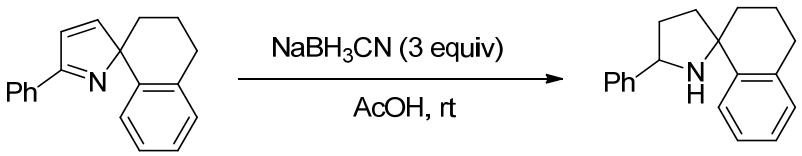
2l, viscous colorless oil, 159 mg, 87% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.01-7.99 (m, 2H), 7.55 (d, J = 4.8 Hz, 1H), 7.46 (d, J = 2.0 Hz, 2H), 7.45 (d, J = 2.0 Hz, 1H), 7.23 (d, J = 7.2 Hz, 1H), 7.15 (dt, J = 1.2, 7.2 Hz, 1H), 6.99 (t, J = 6.8 Hz, 1H), 6.87 (d, J = 4.8 Hz, 1H), 6.62 (d, J = 7.2 Hz, 1H), 3.39 (s, 2H), 2.77 (AB, J_{AB} = 13.6 Hz, 1H), 2.40 (BA, J_{BA} = 14.0 Hz, 1H), 1.45 (s, 9H), 1.44 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 171.4, 170.9, 170.2, 161.4, 134.6, 133.7, 131.1, 130.5, 129.2, 128.6, 128.0, 127.6, 126.3, 125.3, 123.8, 82.8, 81.7, 81.5, 54.0, 35.4, 35.0, 27.9, 27.8; IR (film): ν_{max} (cm^{-1}) = 3061, 2977, 2926, 2851, 2360, 1728, 1606, 1576, 1519, 1492, 1449, 1393, 1368, 1326, 1275, 1257, 1168, 1118, 1077, 1025, 980, 910, 847, 756, 694; ESI-MS (m/z): 460 ($M+H^+$, 100); HRMS (ESI): Exact mass calcd. for $C_{29}H_{34}NO_4$ $[M+H]^+$: 460.2482. Found: 460.2486.

Transformation of product 2a.



2a **3a**, 61% yield

Under argon, to a 25 mL round-bottom flask was added **2a** (52.0 mg, 0.2 mmol), MeOH (2.0 mL) and Pd/C (10 mg, 0.01 mmol). The resulting mixture was stirred under H_2 atmosphere at room temperature until the consumption of the starting material (monitored by TLC), filtered through a pad of celite and then washed with EtOAc. The filtrate was concentrated and the residue was purified by silica gel column chromatography (petroleum ether/ethyl acetate = 30/1) to afford viscous colorless oil **3a** (31.5 mg, 61% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.94 (dd, J = 1.6, 7.2 Hz, 1H), 7.44-7.42 (m, 3H), 7.13-7.09 (m, 3H), 7.02-6.99 (m, 1H), 3.19-3.10 (m, 2H), 2.93-2.86 (m, 2H), 2.30 (ddd, J = 4.4, 9.2, 13.2 Hz, 1H), 2.13-2.05 (m, 3H), 1.95-1.87 (m, 1H), 1.79-1.75 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 171.6, 142.6, 136.1, 134.6, 130.5, 128.8, 128.4, 127.9, 127.1, 126.4, 126.2, 78.0, 38.8, 35.3, 35.0, 29.6, 20.7; IR (film): ν_{max} (cm^{-1}) = 3058, 3025, 2931, 2863, 1954, 1814, 1614, 1575, 1489, 1448, 1342, 1328, 1210, 1075, 1024, 1009, 758, 726, 693, 556; ESI-MS (m/z): 262 ($M+H^+$, 100); HRMS (ESI): Exact mass calcd. for $C_{19}H_{20}N$ $[M+H]^+$: 262.1590. Found: 262.1587.



2a **3b**, 58% yield, > 20:1 dr

To a 25 mL round-bottom flask was added **2a** (52.0 mg, 0.2 mmol) and AcOH (2.0 mL). The resulting solution was stirred at room temperature, and then $NaBH_3CN$ (36 mg, 0.6 mmol) was added in portions. The reaction mixture was stirred until the consumption of the starting material (monitored by TLC), quenched by saturated aqueous Na_2CO_3 solution and then extracted with EtOAc (3 X 10 mL). The combined organic layers were dried over anhydrous Na_2SO_4, filtered and concentrated *in vacuo*.

The residue was purified by silica gel column chromatography (petroleum ether/dichloromethane = 30/1 then petroleum ether/ethyl acetate = 50/1) to afford viscous colorless oil **3b** (30.2 mg, 58% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.83 (d, *J* = 7.6 Hz, 1H), 7.52 (d, *J* = 7.6 Hz, 2H), 7.34 (t, *J* = 7.2 Hz, 2H), 7.26-7.20 (m, 2H), 7.12 (dt, *J* = 1.6, 7.6 Hz, 1H), 7.04 (d, *J* = 7.6 Hz, 1H), 4.44 (dd, *J* = 7.2, 8.4 Hz, 1H), 2.83-2.78 (m, 2H), 2.34-2.27 (m, 1H), 2.12-2.02 (m, 3H), 1.98-1.86 (m, 2H), 1.84-1.77 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 145.03, 145.00, 136.7, 128.5, 128.3, 127.4, 126.8, 126.7, 126.2, 126.1, 62.5, 61.1, 41.9, 37.9, 35.7, 29.8, 20.8; IR (film): v_{max} (cm^{-1}) = 3331, 3059, 3024, 2927, 2863, 1947, 1602, 1486, 1448, 1394, 1341, 1293, 1233, 1155, 1086, 1066, 1027, 941, 908, 878, 753, 697, 644; ESI-MS (m/z): 264 ($M+H^+$, 100); HRMS (ESI): Exact mass calcd. for $C_{19}H_{22}N$ $[M+H]^+$: 264.1747. Found: 264.1744.

Experimental References:

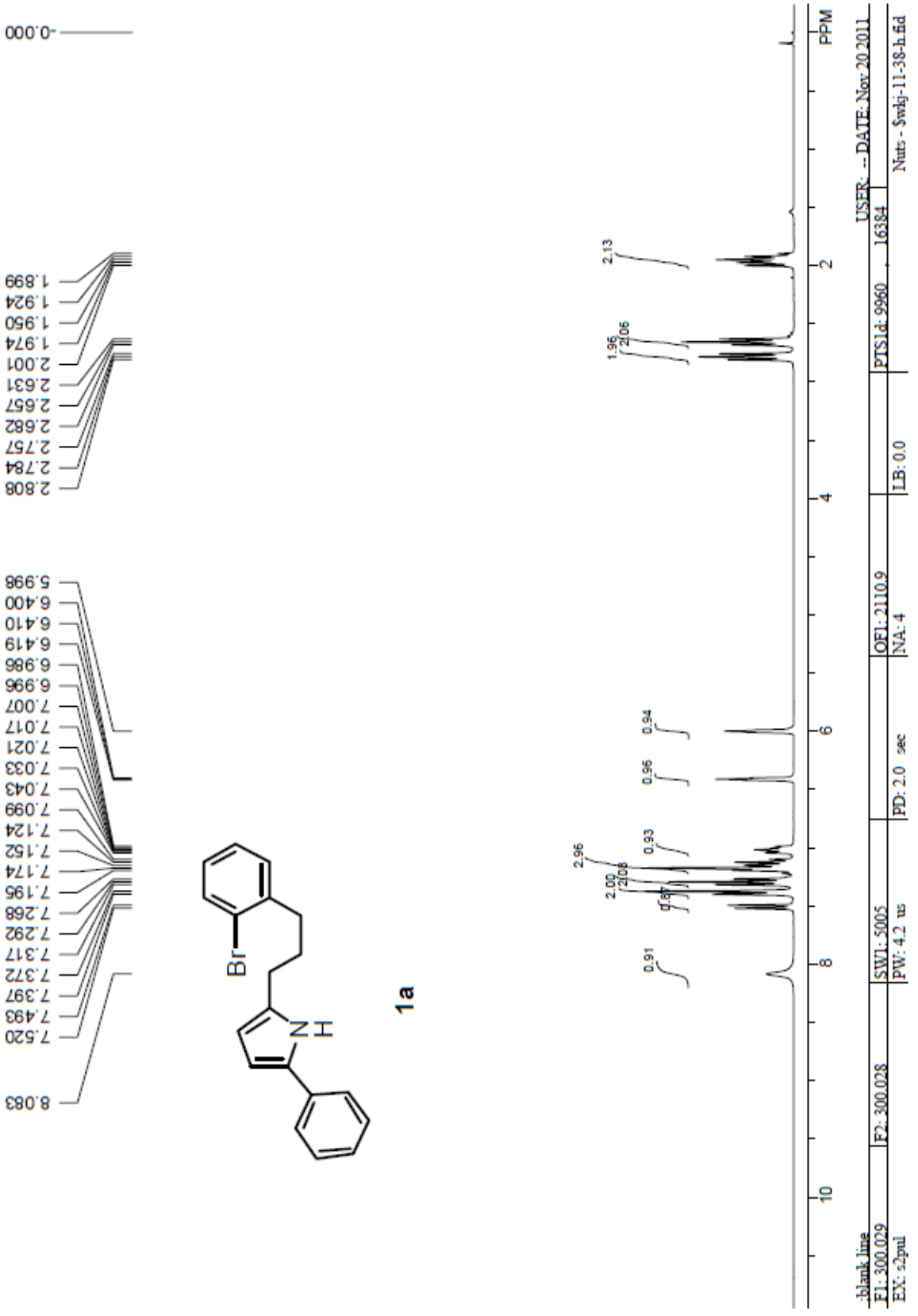
(1) Jautze, S.; Peters, R. *Angew. Chem., Int. Ed.* **2008**, *47*, 9284.

(2) Yadav, J. S.; Abraham, S.; Reddy, B. V. S.; Sabitha, G. *Synthesis* **2001**, *14*, 2165.

(3) Huang, M. *J. Am. Chem. Soc.* **1946**, *68*, 2487.

(4) Bandini, M.; Eichholzer, A. *Angew. Chem., Int. Ed.* **2009**, *48*, 9533.

NMR Spectra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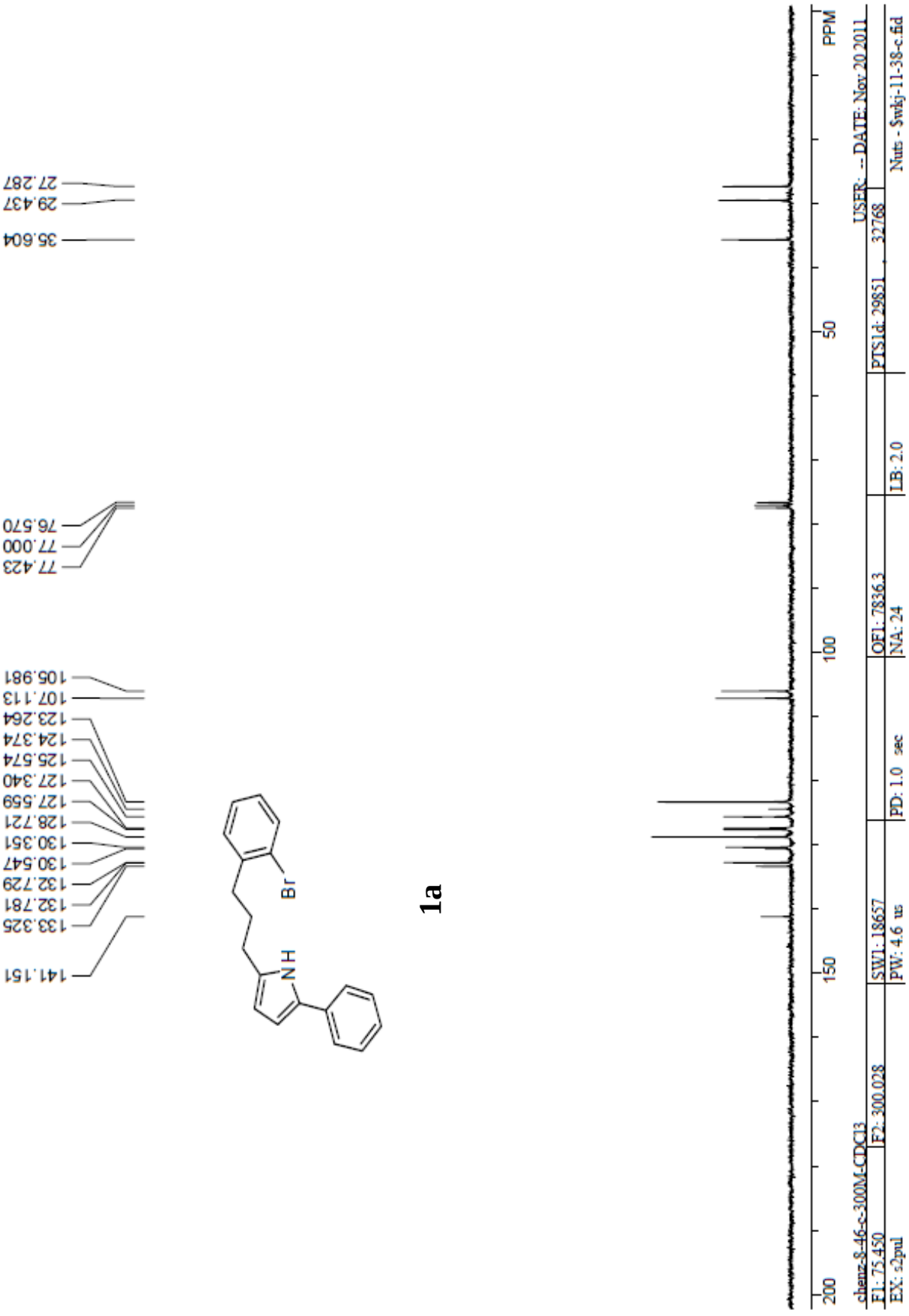
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128.721
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130.547
132.729
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Br
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150
100
50
PPM
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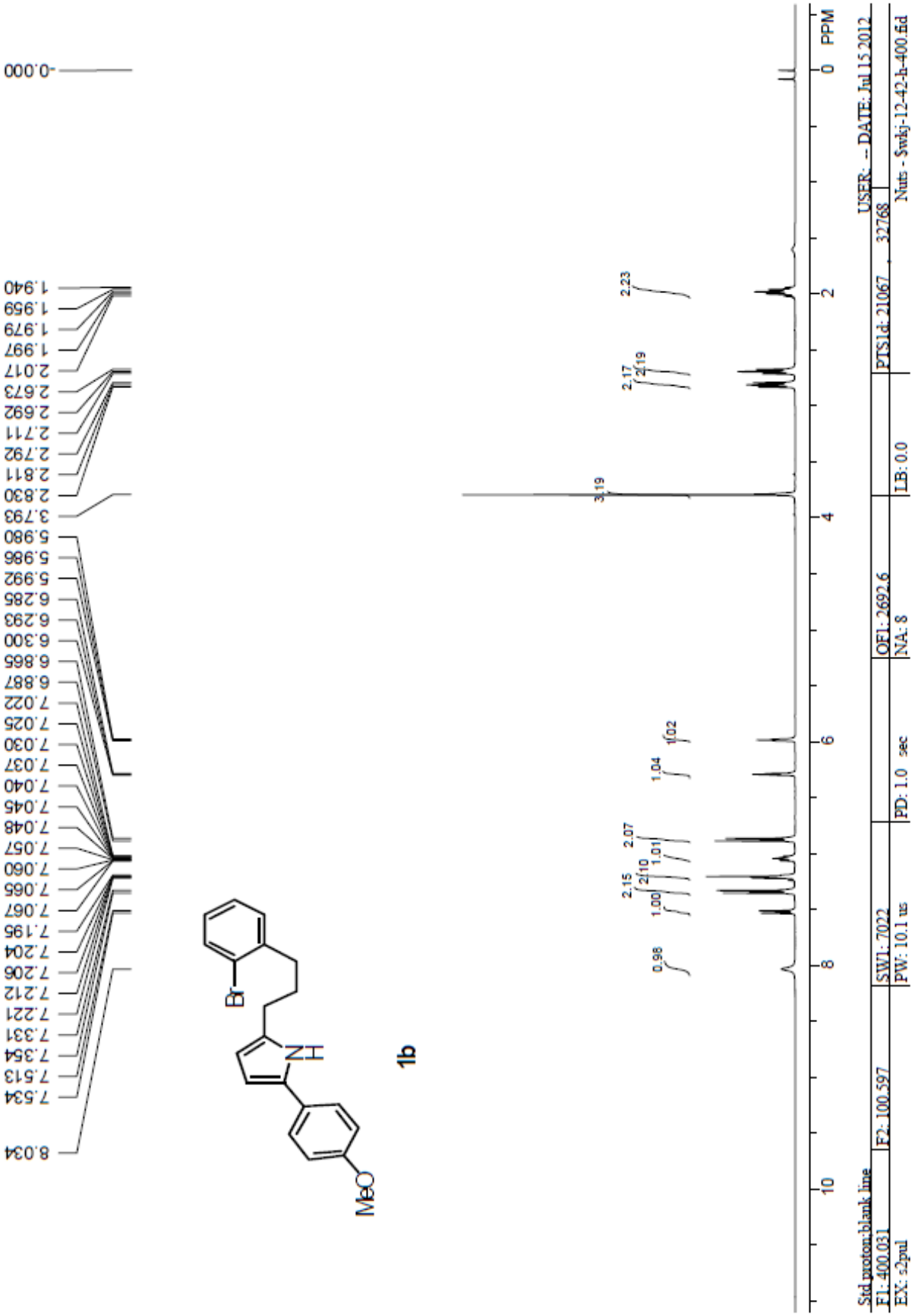
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7.025
7.030
7.037
7.040
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NH
MeO
1b
3.19
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2.17
2.19
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2.10
2.07
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1.01
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1.02
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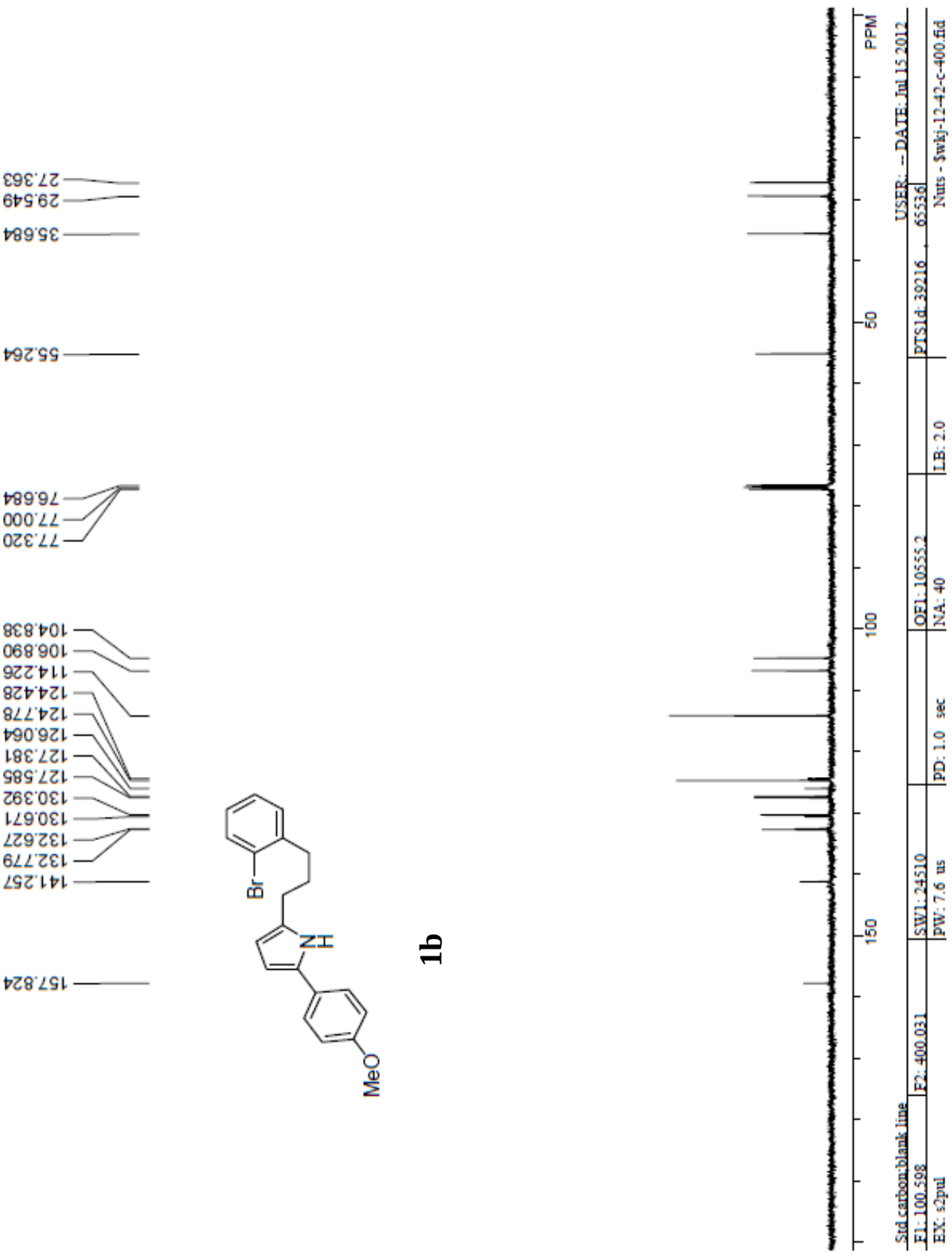
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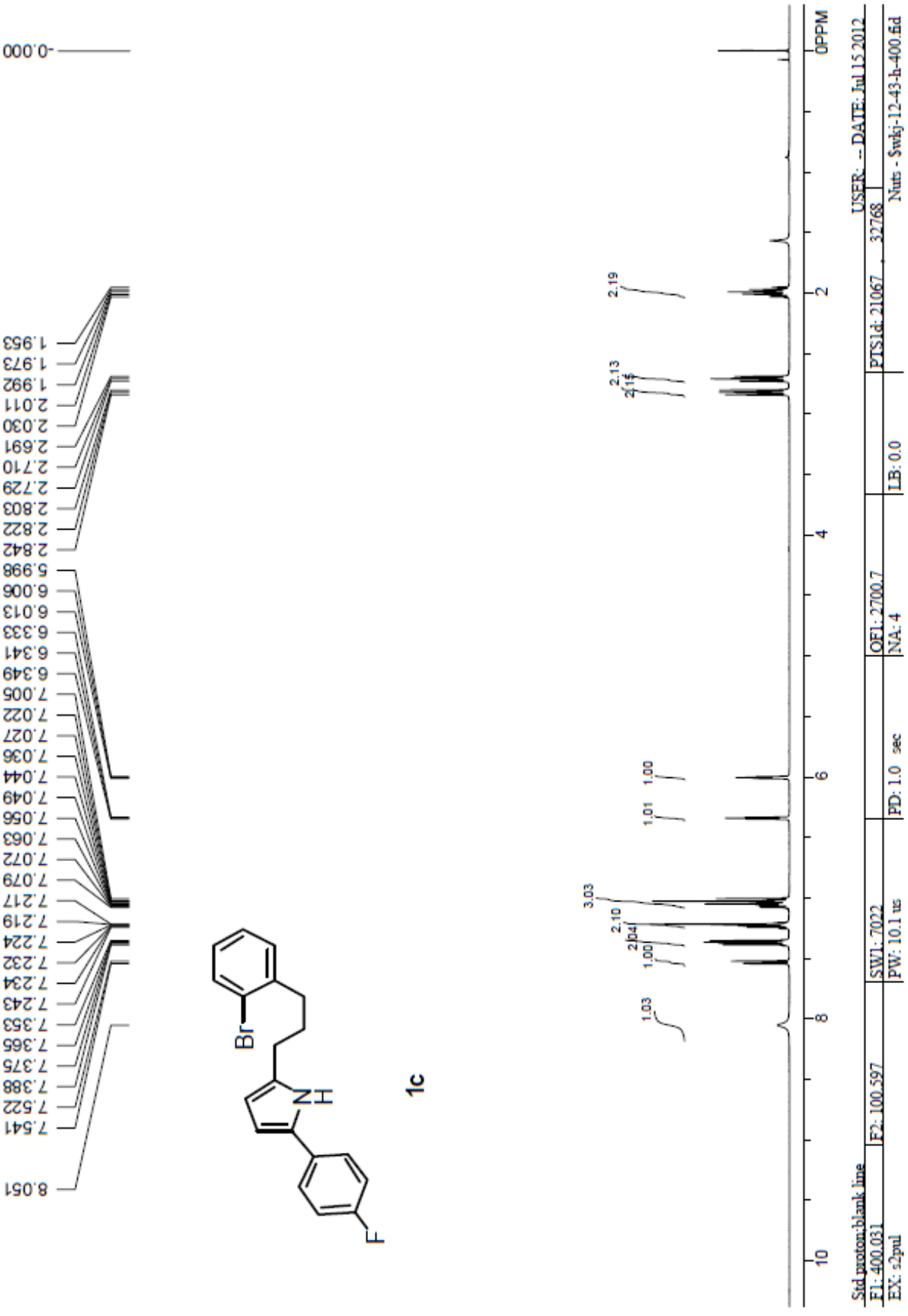
1b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H
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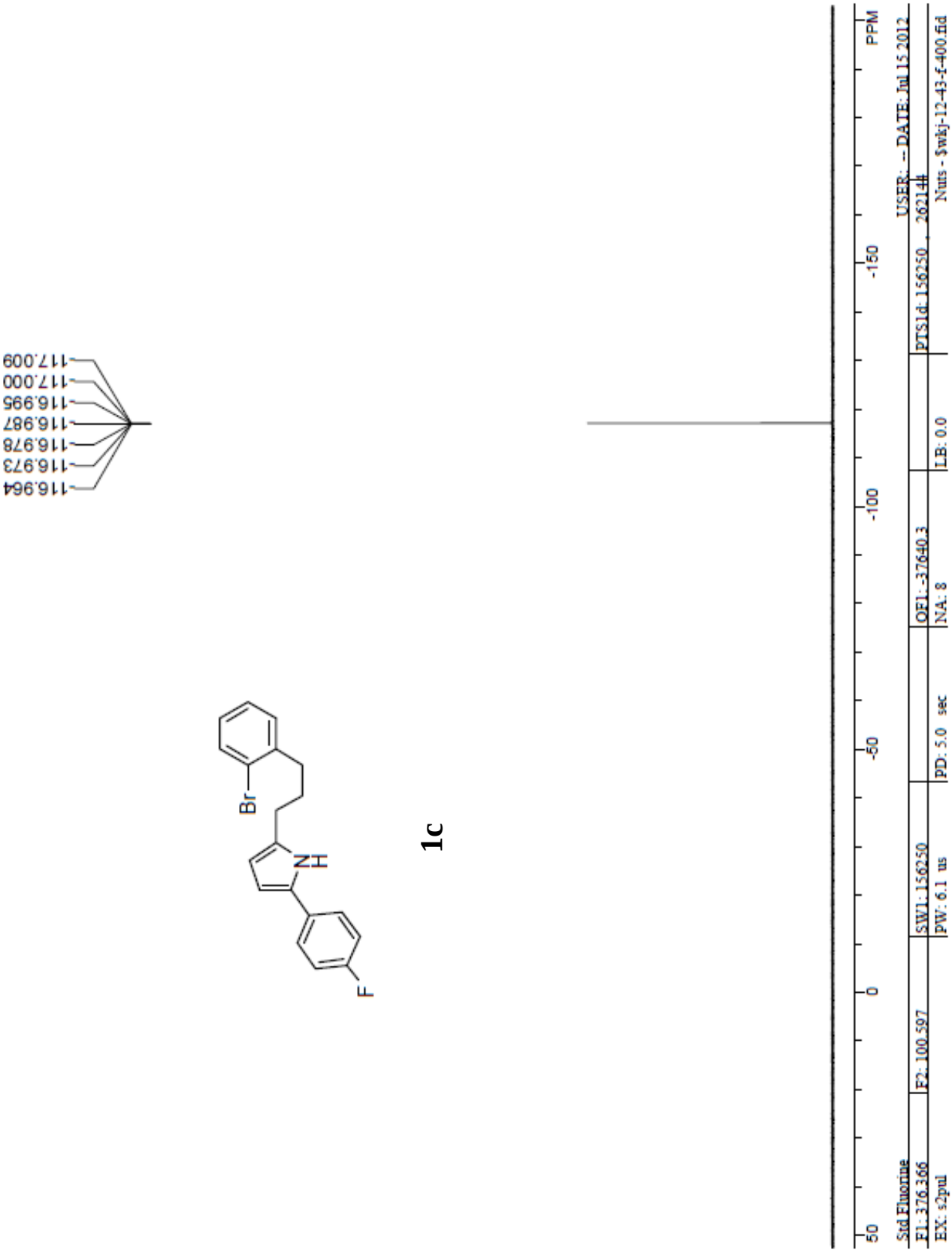
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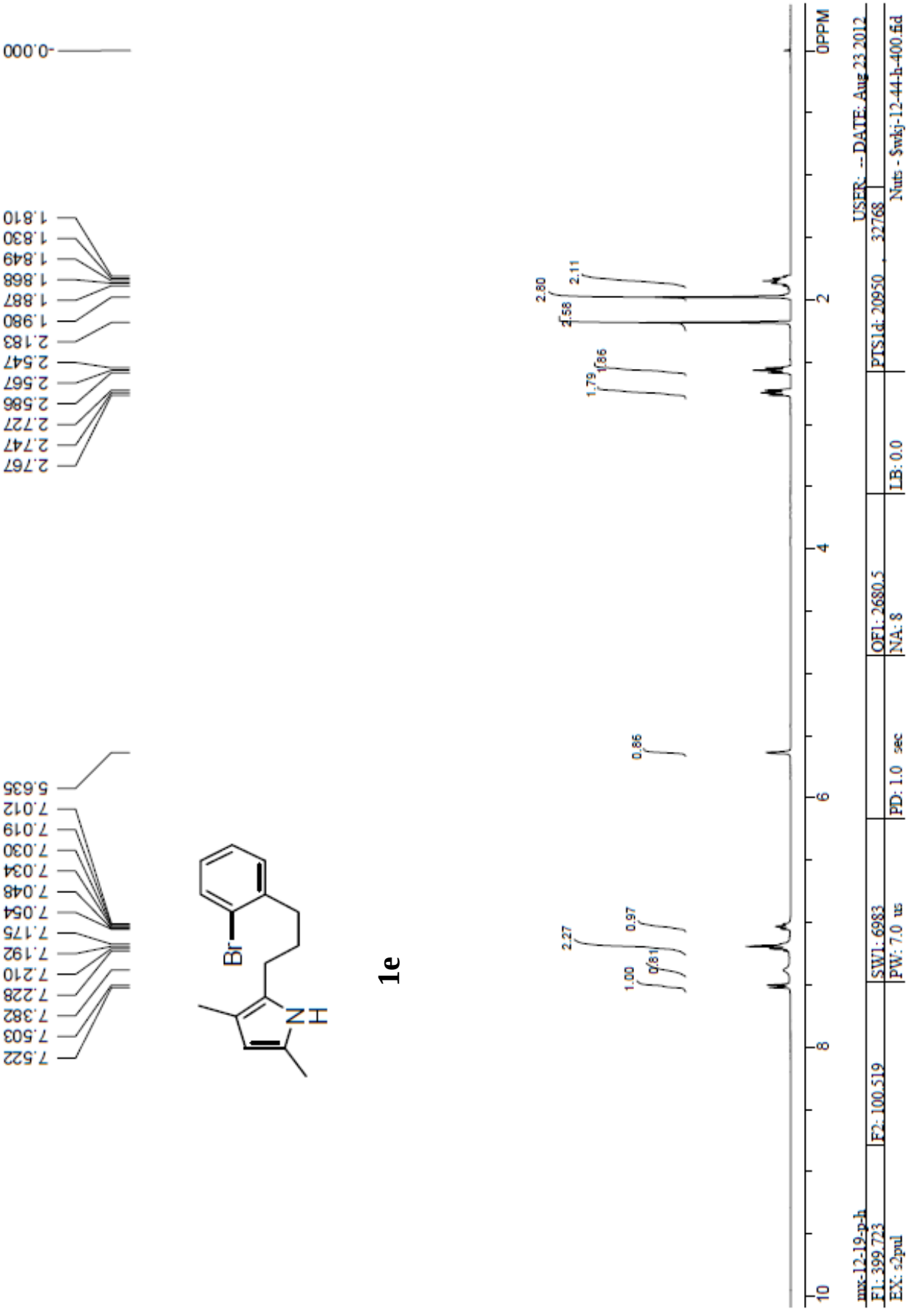
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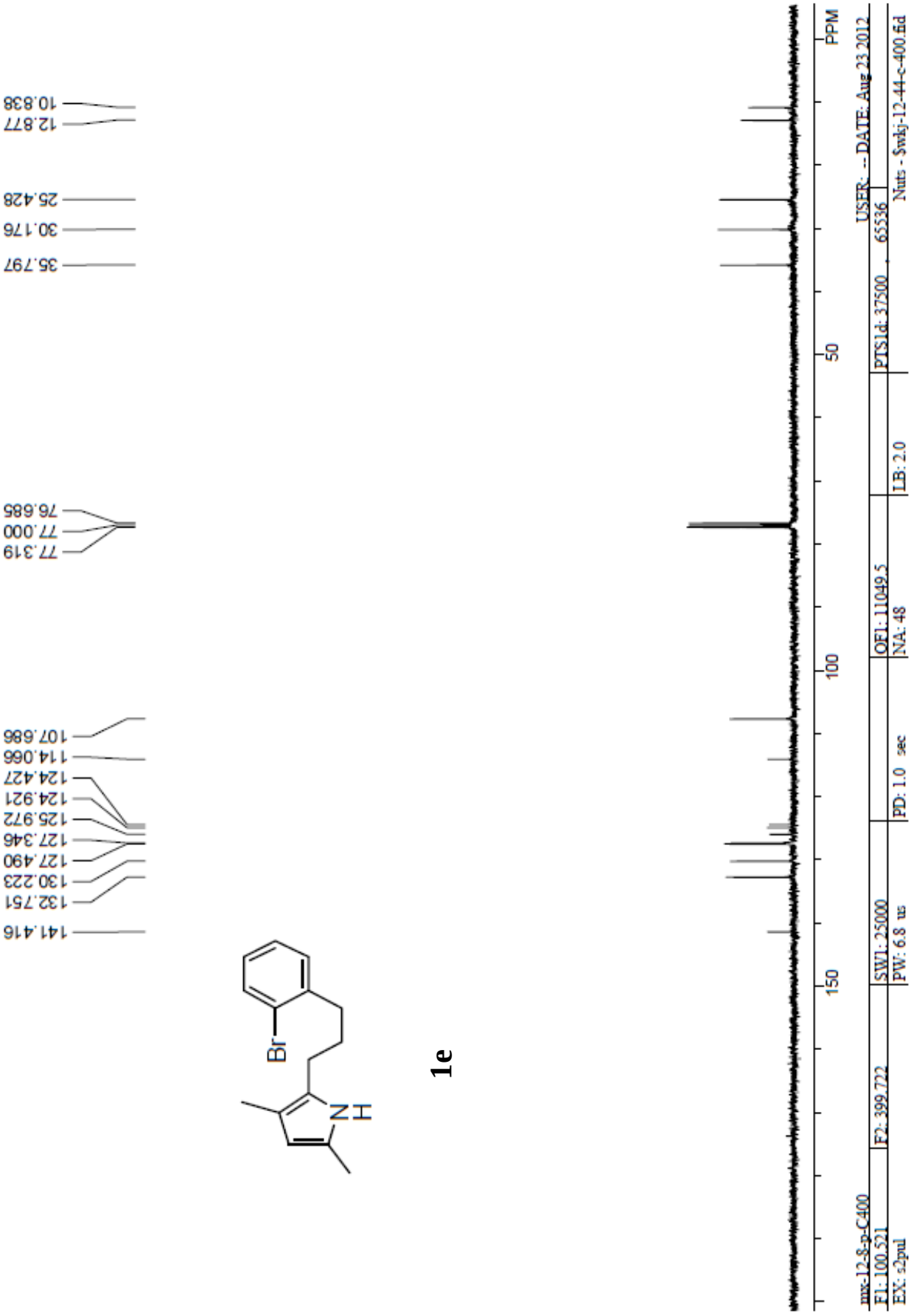
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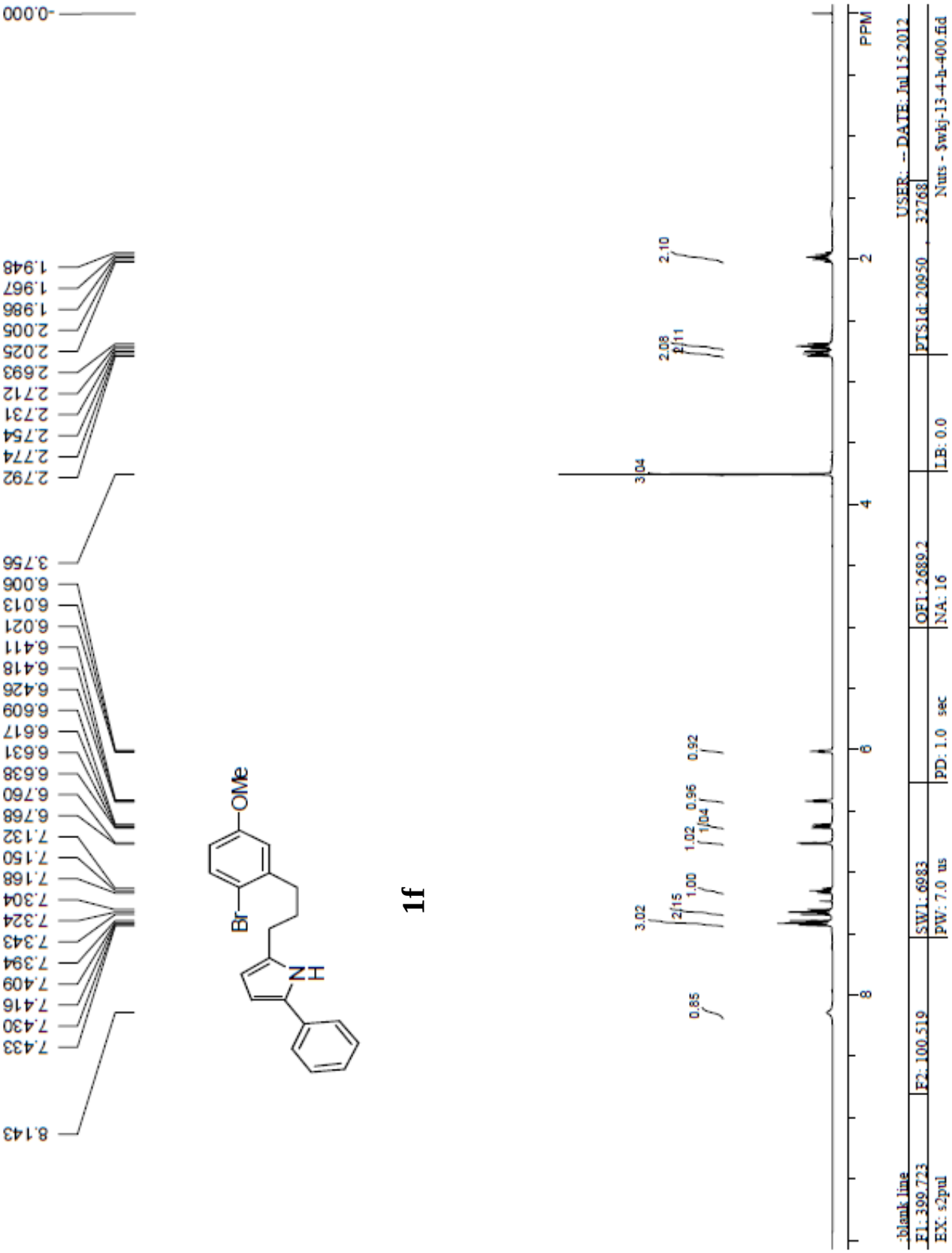
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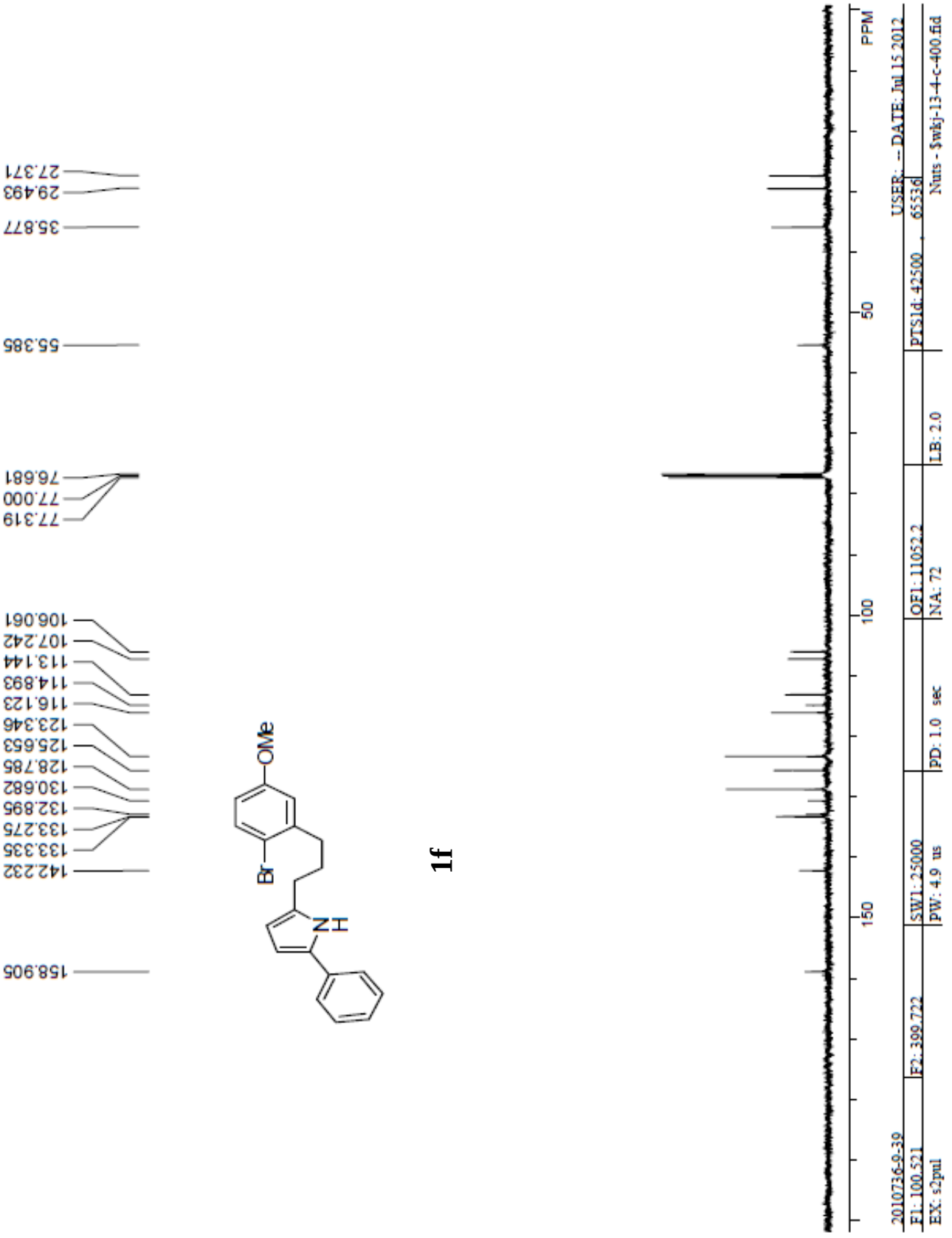
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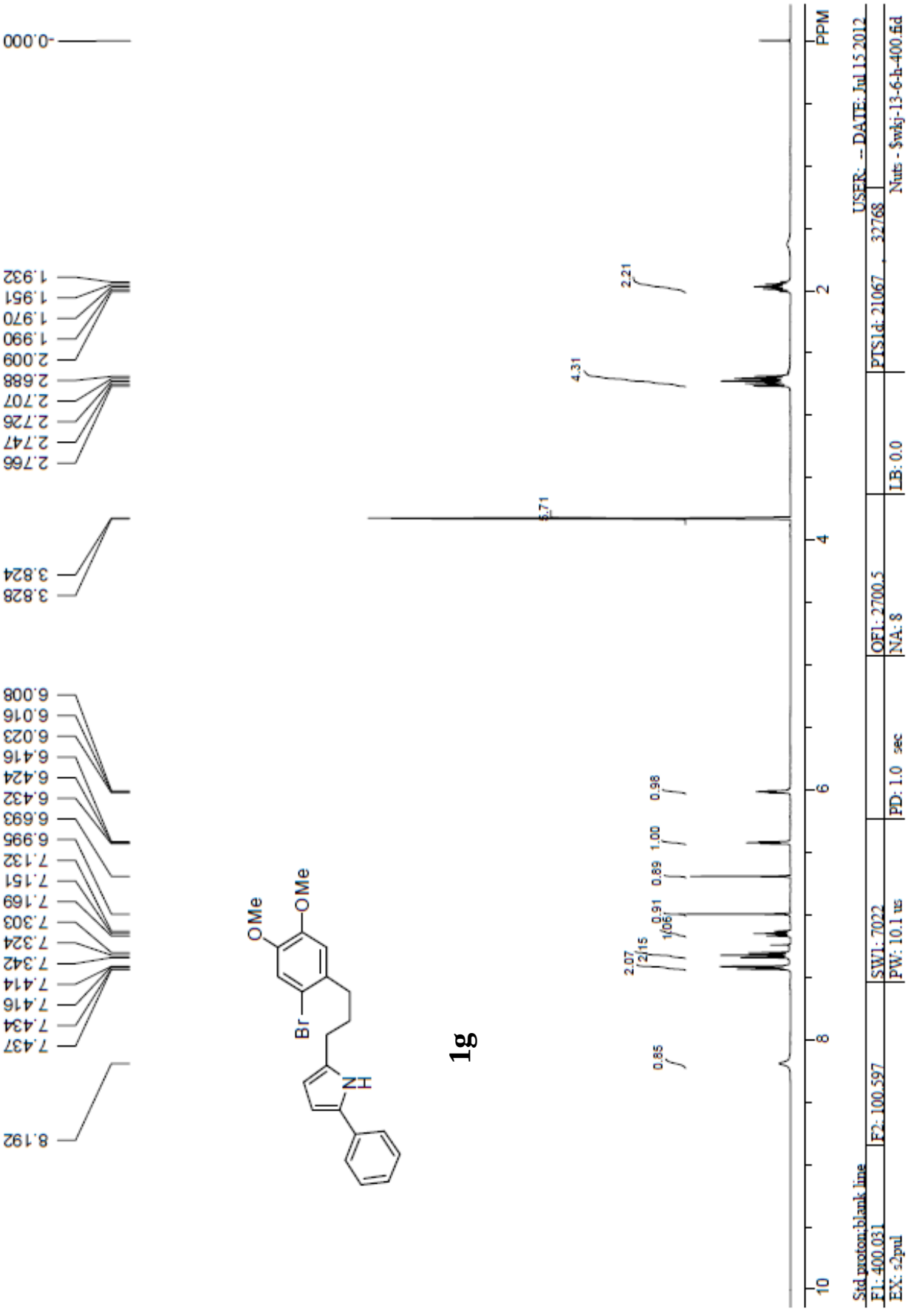
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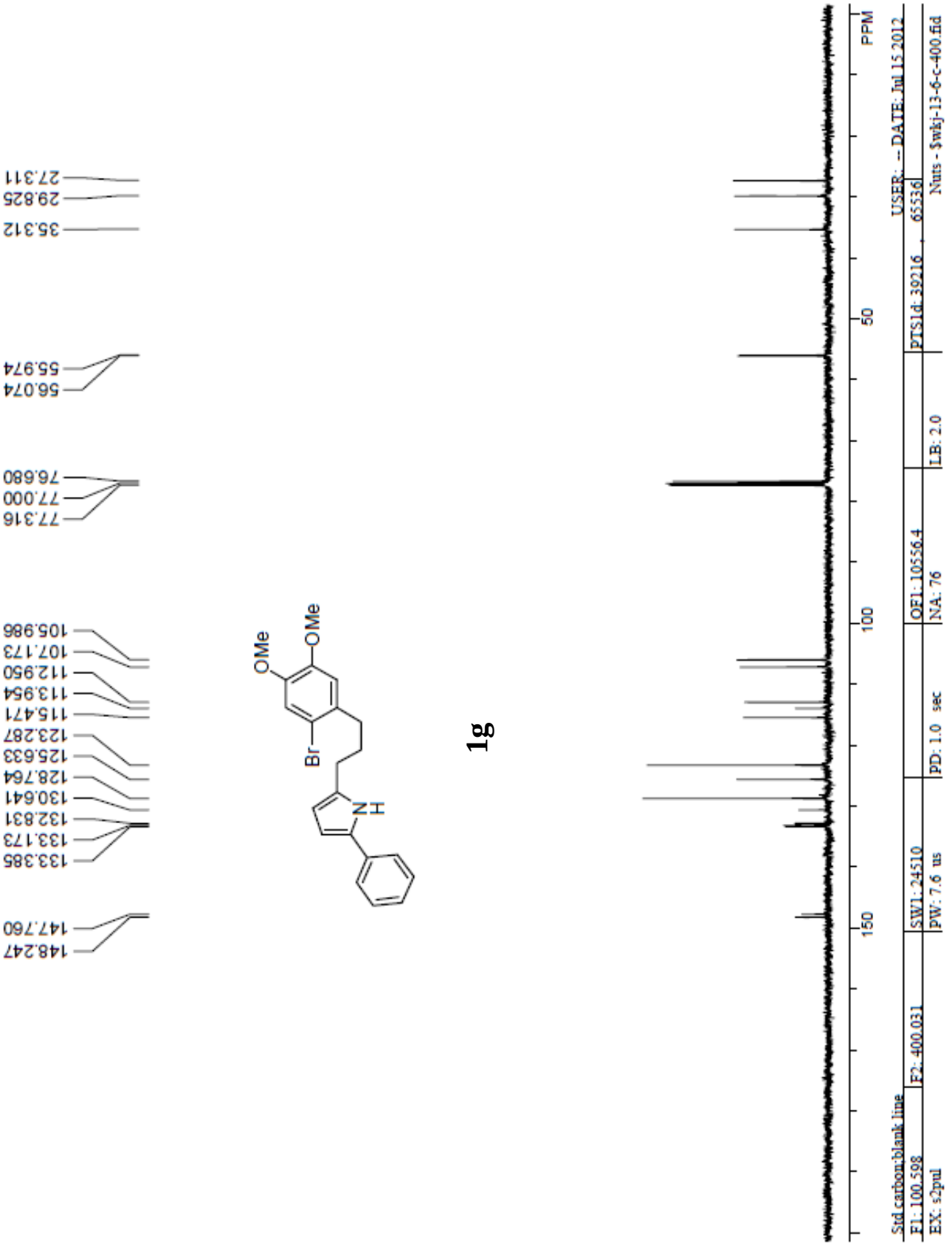
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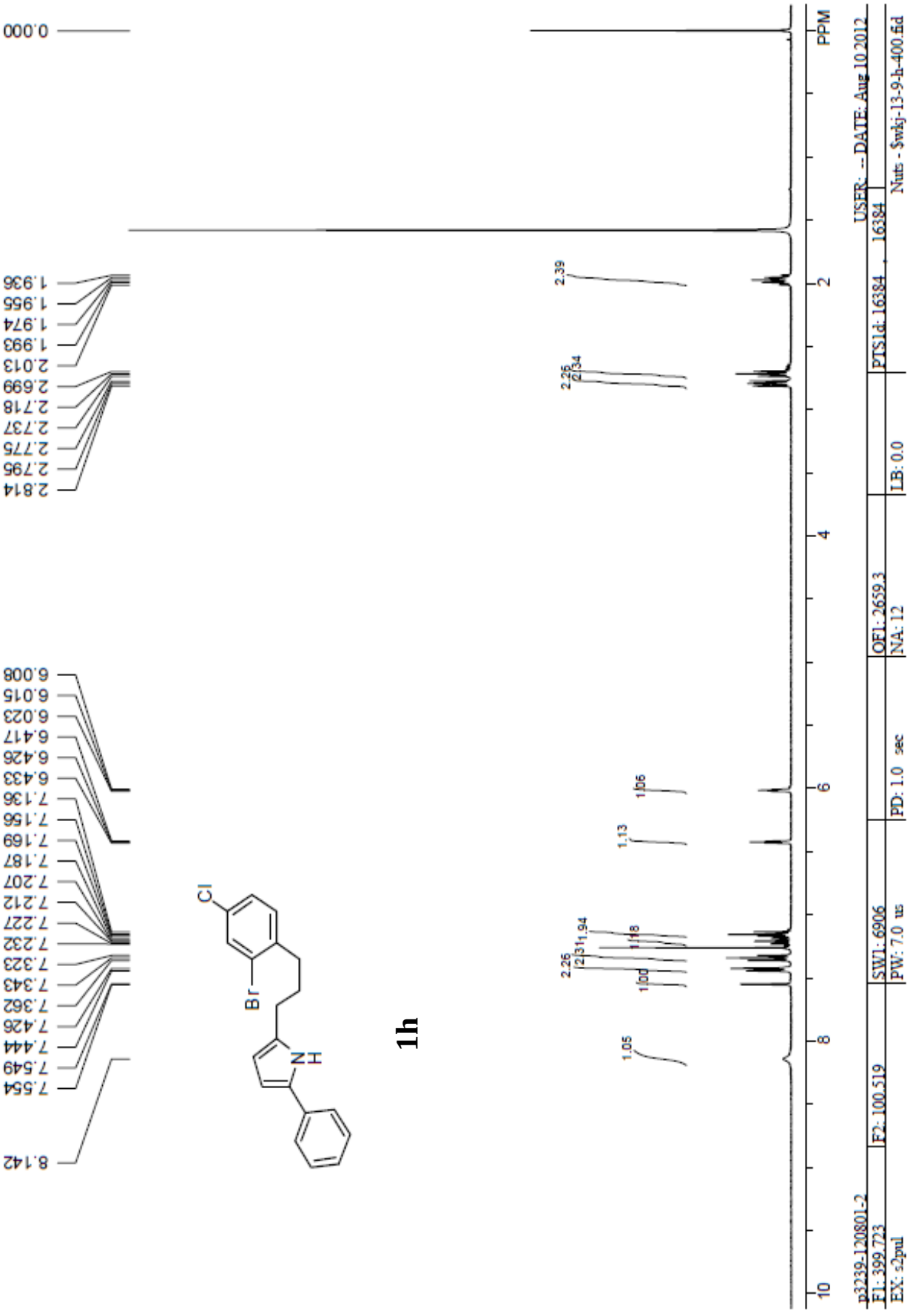
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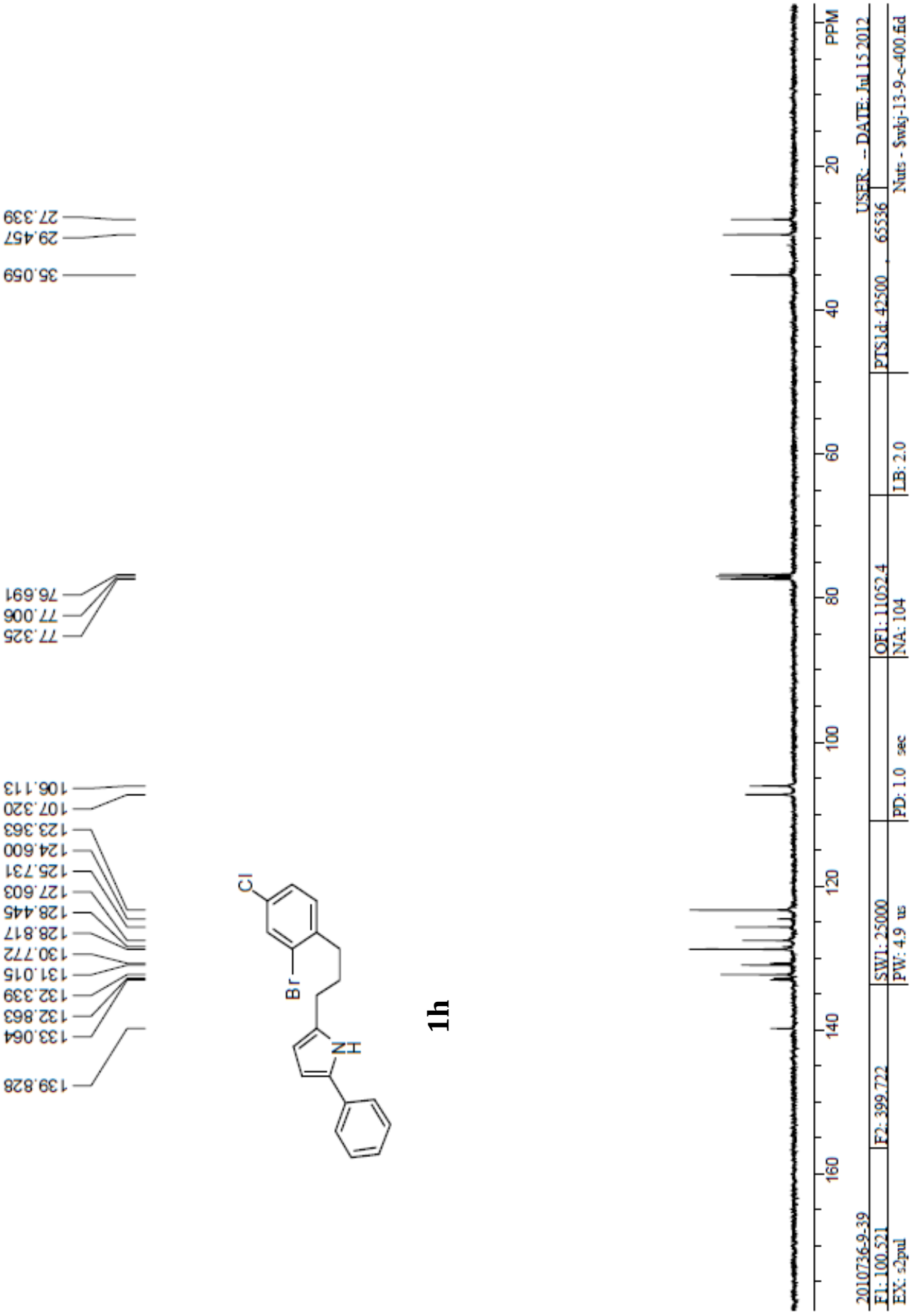
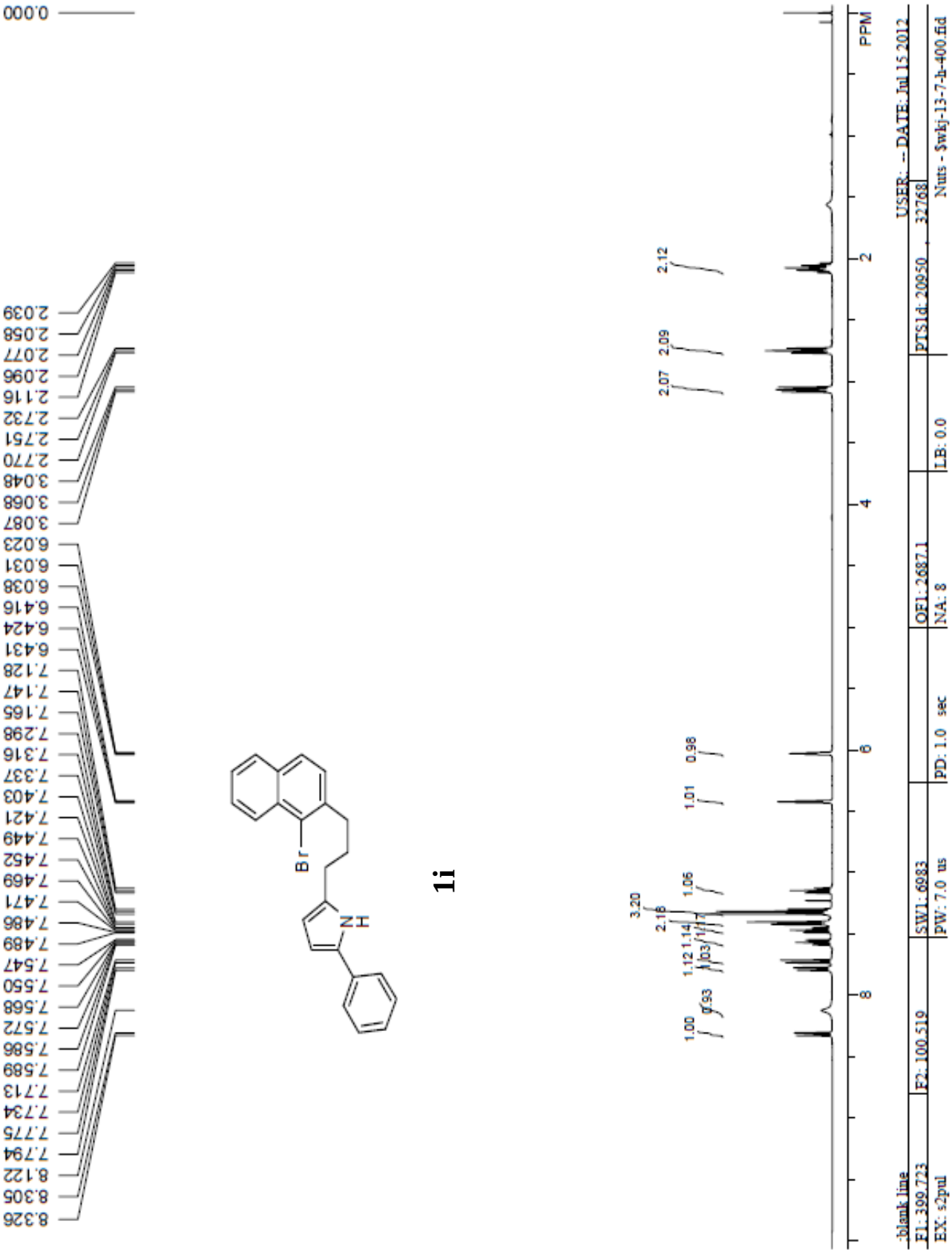
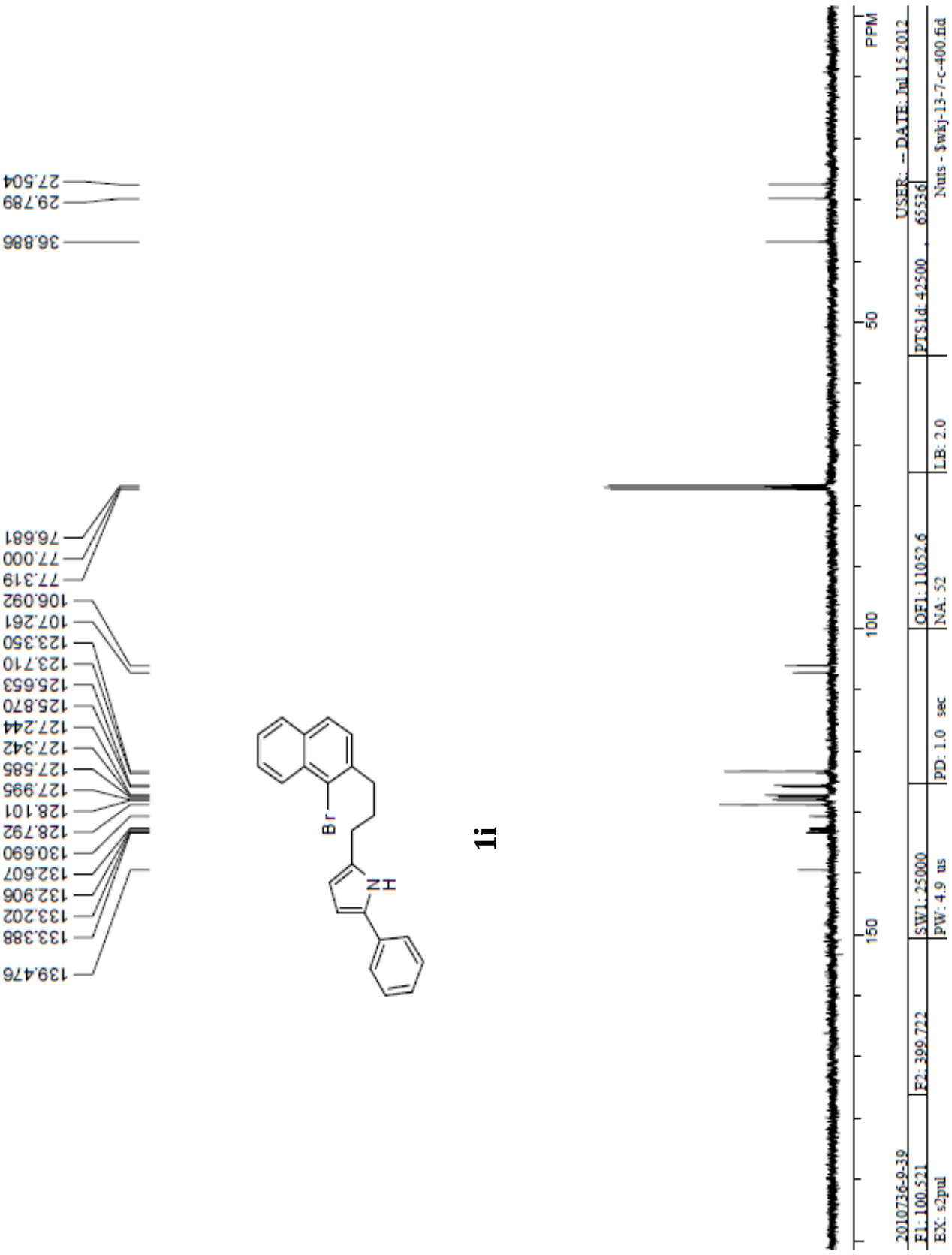
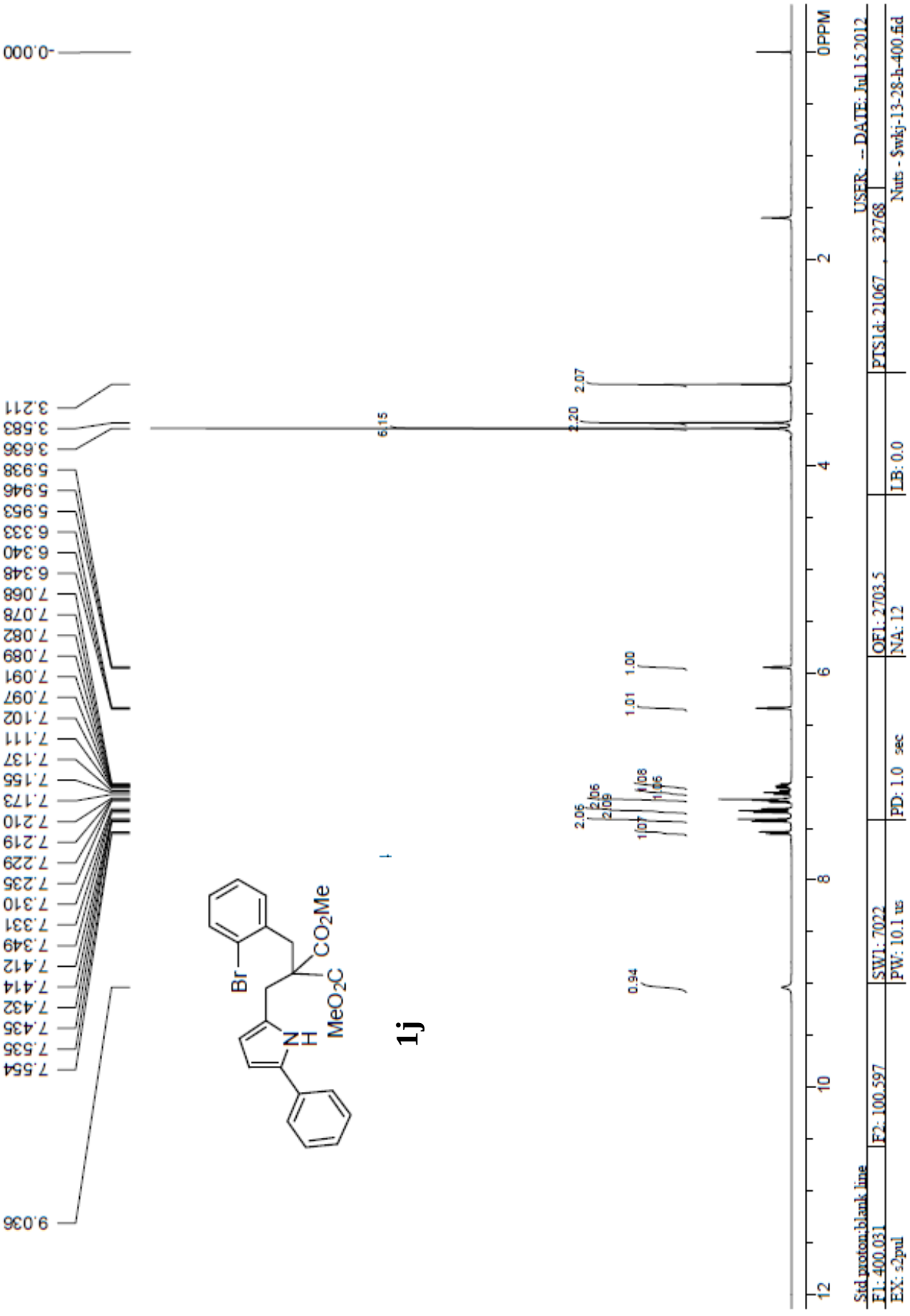
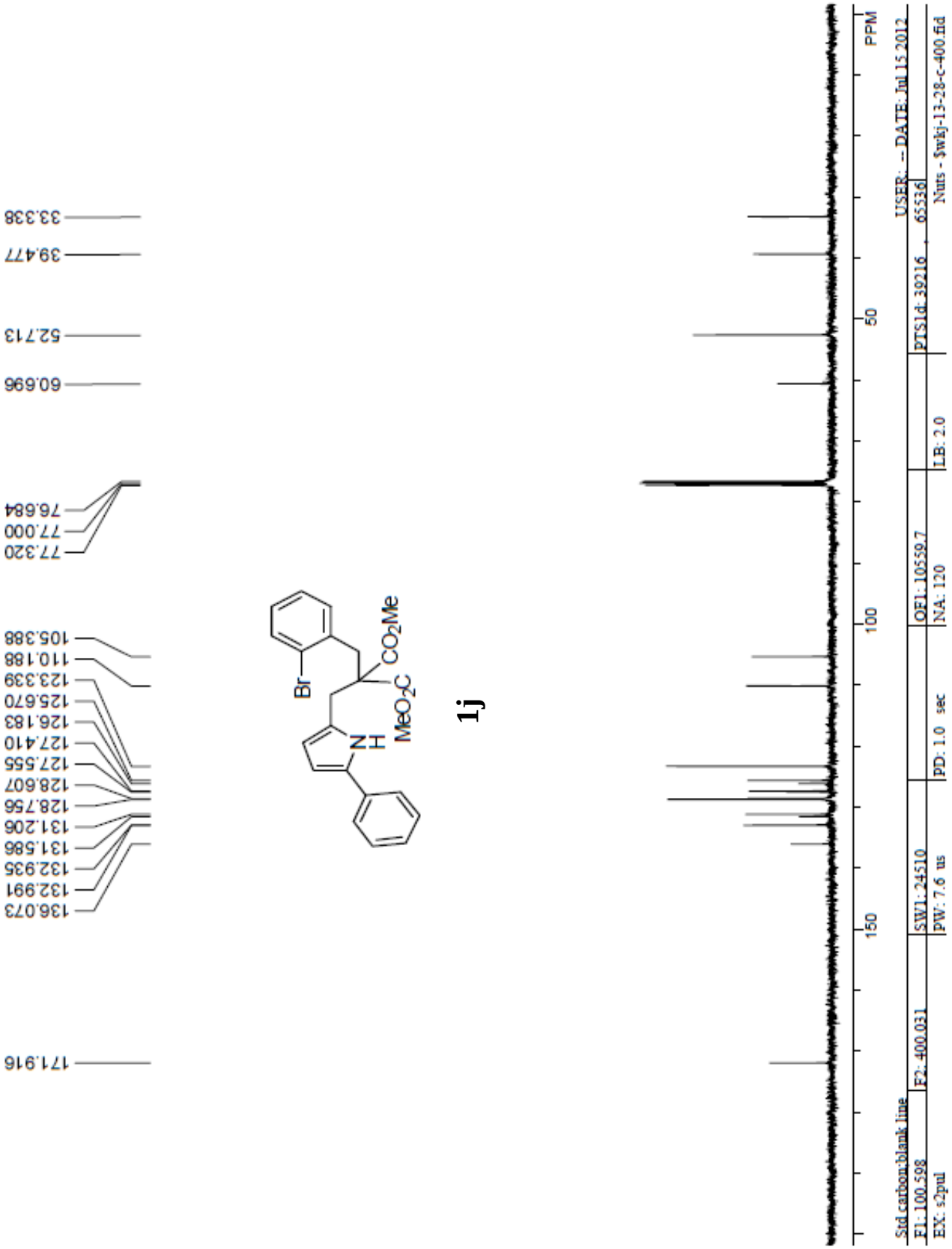
F1: 399.723
EX: s2pul
p3239-120801-2

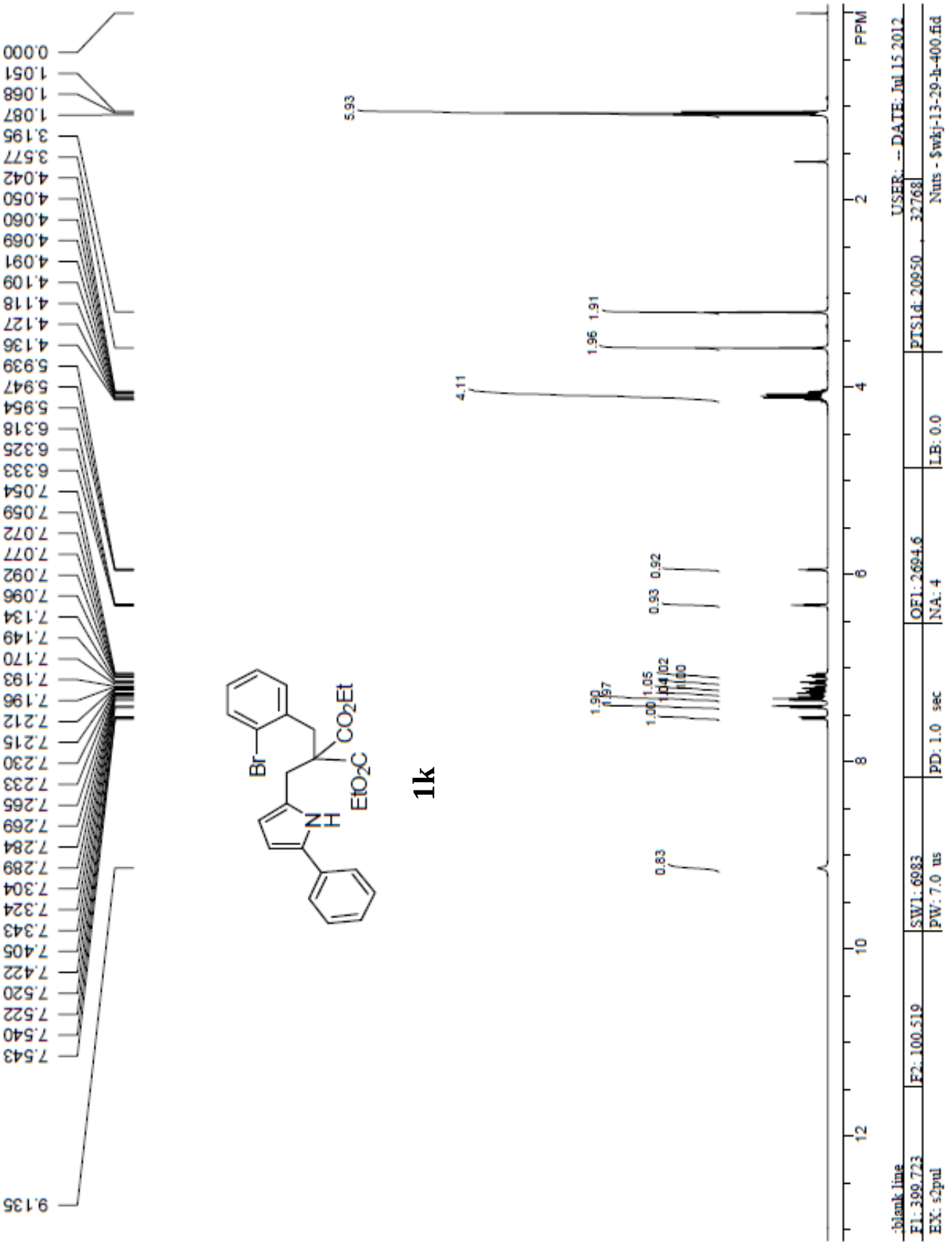

27.339
29.457
35.059
76.691
77.006
77.325
106.113
107.320
123.363
124.600
125.731
127.603
128.445
128.817
130.772
131.015
132.339
132.863
133.064
139.828
Cl
Br
NH
1h
PPM
USER: -- DATE: Jul 15 2012
2010736-9-39
F1: 100.521
F2: 399.722
SW1: 25000
OF1: 11052.4
PTS1d: 42500
65536
EX: s2pul
PW: 4.9 us
PD: 1.0 sec
NA: 104
LB: 2.0
Nuts - $wkj-13-9-c-400.fid

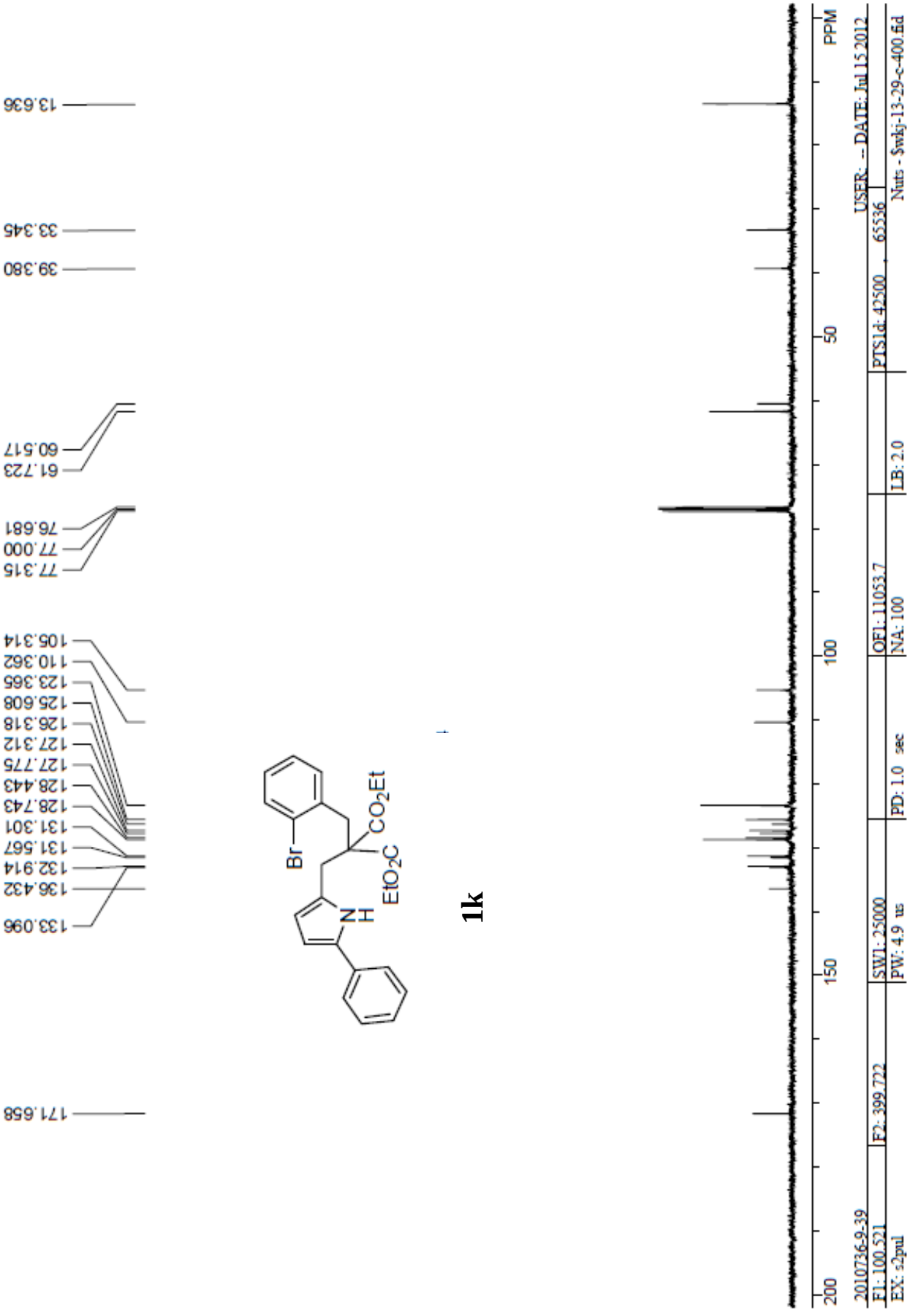

0.000
2.039
2.058
2.077
2.096
2.116
2.732
2.751
2.770
3.048
3.068
3.087
6.023
6.031
6.038
6.416
6.424
6.431
7.128
7.147
7.165
7.298
7.316
7.337
7.403
7.421
7.449
7.452
7.469
7.471
7.486
7.489
7.547
7.550
7.568
7.572
7.586
7.589
7.713
7.734
7.775
7.794
8.122
8.305
8.326
Br
N
H
1i
3.20
2.16
1.12
1.14
1.06
1.01
0.98
1.00
0.93
3.03
2.12
2.09
2.07
PPM
blank line
F1: 399.723
F2: 100.519
SW1: 6983
OF1: 2687.1
PTS1d: 20950
32768
USER: -- DATE: Jul 15 2012
EX: s2pul
PW: 7.0 us
PD: 1.0 sec
NA: 8
LB: 0.0
Nuts - $wkj-13-7-h-400.fid

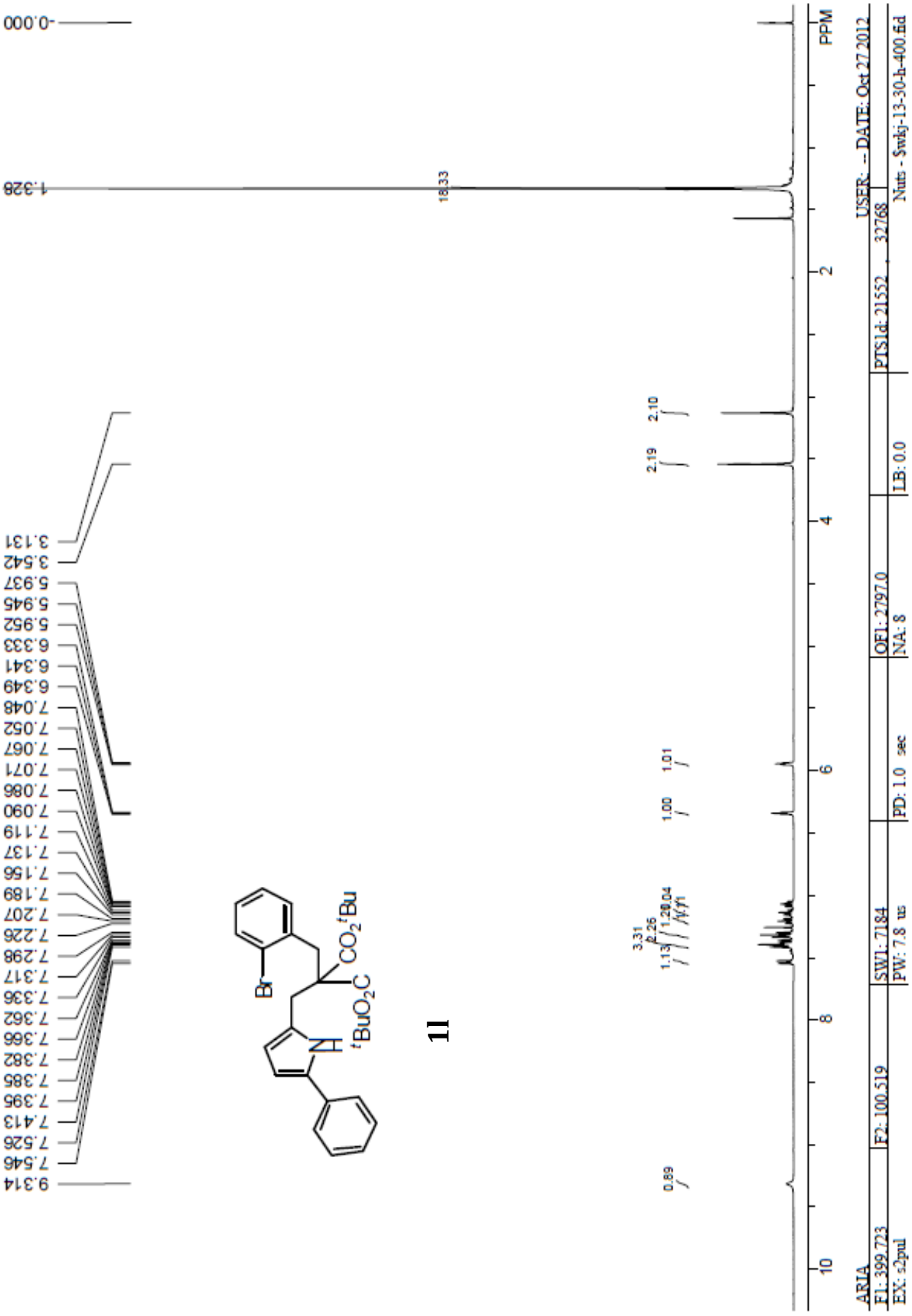

27.504
29.789
36.886
76.681
77.000
77.319
106.092
107.261
123.350
123.710
125.653
125.870
127.244
127.342
127.585
127.995
128.101
128.792
130.690
132.607
132.906
133.202
133.388
139.476
Br
N
H
1i
PPM
50
100
150
2010736-9-39
F1: 100.521
EX: s2pul
F2: 399.722
SW1: 25000
PW: 4.9 us
PD: 1.0 sec
OF1: 11052.6
NA: 52
LB: 2.0
PTS1d: 42500
65536
USER: -- DATE: Jul 15 2012
Nuts - $wkj-13-7-c-400.fid


1j
Br
CO2Me
MeO2C
NH
9.036
7.554
7.535
7.435
7.432
7.414
7.412
7.349
7.331
7.310
7.235
7.229
7.219
7.210
7.173
7.155
7.137
7.111
7.102
7.097
7.091
7.089
7.082
7.078
7.068
6.348
6.340
6.333
5.953
5.946
5.938
3.636
3.583
3.211
6.15
2.20
2.07
2.06
2.06
2.09
1.08
1.06
1.07
1.01
1.00
0.94
0PPM
Std proton:blank_line
F1: 400.031
F2: 100.597
EX: s2pul
SW1: 7022
PW: 10.1 us
PD: 1.0 sec
QF1: 2703.5
NA: 12
LB: 0.0
PTS1d: 21067 32768
USER: -- DATE: Jul 15 2012
Nuts - $wkj-13-28-h-400.fid

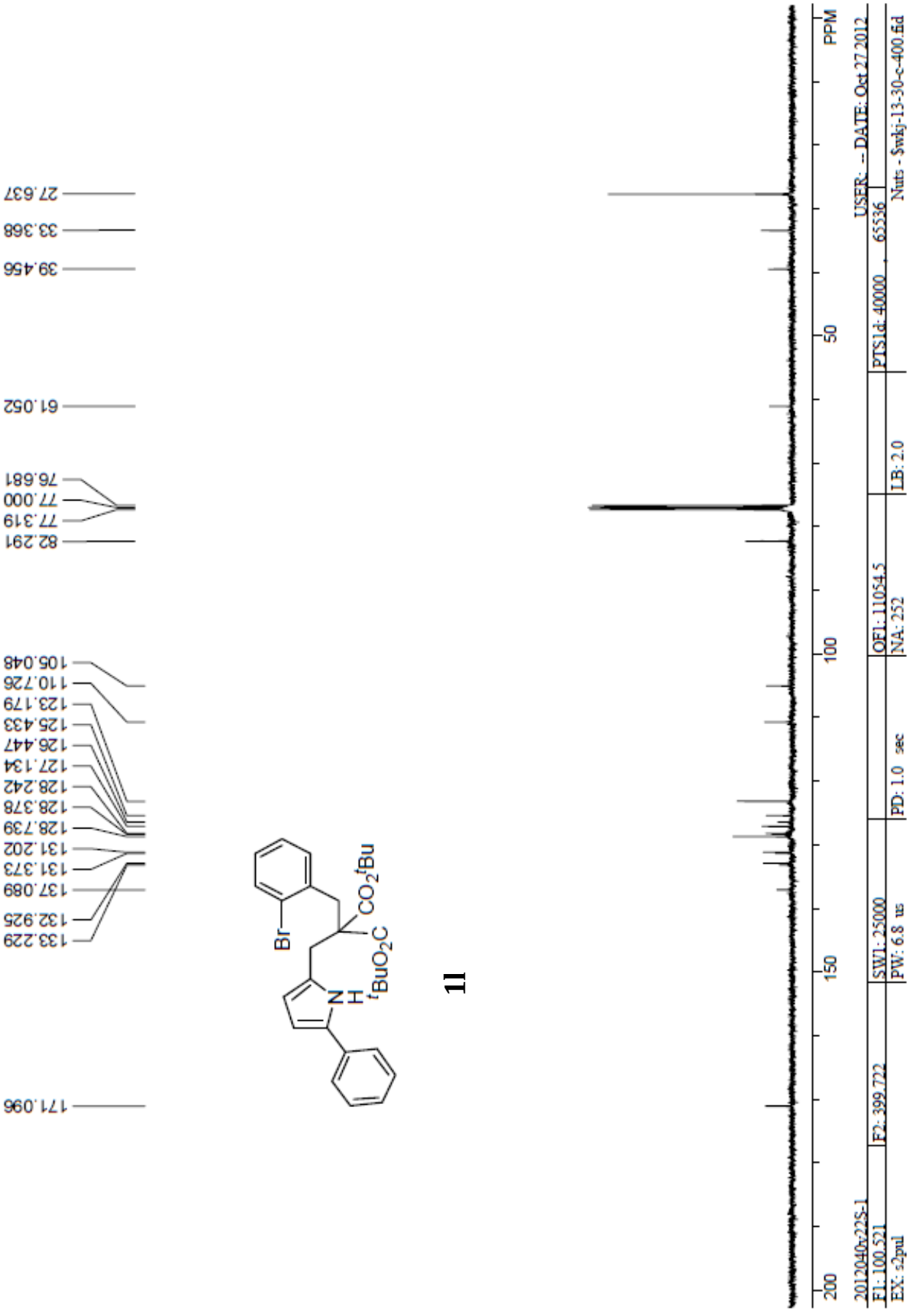

33.338
39.477
52.713
60.696
76.684
77.000
77.320
105.388
110.188
123.339
125.670
126.183
127.410
127.555
128.607
128.756
131.206
131.586
132.935
132.991
136.073
171.916
Br
CO2Me
MeO2C
N
H
1j
PPM
50
100
150
USER: -- DATE: Jul 15 2012
PTS1d: 39216 , 65536
Nuts - $wkj-13-28-c-400.fid
OF1: 10559.7
LB: 2.0
NA: 120
SW1: 24510
PW: 7.6 us
PD: 1.0 sec
F2: 400.031
F1: 100.598
EX: s2pul
Std carbon blank line

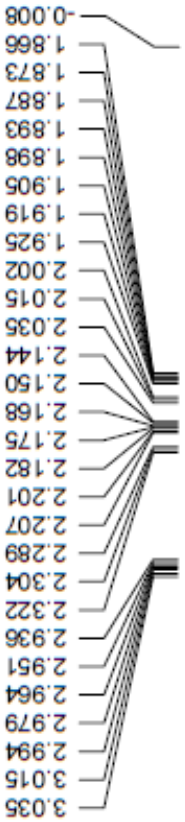

0.000
1.051
1.068
1.087
3.195
3.577
4.042
4.050
4.060
4.069
4.091
4.109
4.118
4.127
4.136
5.939
5.947
5.954
6.318
6.325
6.333
7.054
7.059
7.072
7.077
7.092
7.096
7.134
7.149
7.170
7.193
7.196
7.212
7.215
7.230
7.233
7.265
7.269
7.284
7.289
7.304
7.324
7.343
7.405
7.422
7.520
7.522
7.540
7.543
9.135
Br
CO2Et
EtO2C
N
H
1k
5.93
4.11
1.96
1.91
1.90
1.97
1.00
1.05
1.04
1.02
1.00
0.93
0.92
0.83
PPM
2
4
6
8
10
12
blank line
F1: 399.723
F2: 100.519
SW1: 6983
PW: 7.0 us
PD: 1.0 sec
OF1: 2694.6
NA: 4
LB: 0.0
PTS1d: 20950
32768
USER: -- DATE: Jul 15 2012
EX: s2pul
Nuts - $wkj-13-29-h-400.fid

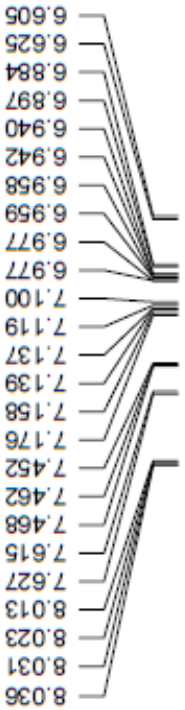

13.636
33.345
39.380
60.517
61.723
76.681
77.000
77.315
105.314
110.362
123.365
125.608
126.318
127.312
127.775
128.443
128.743
131.301
131.567
132.914
136.432
133.096
171.658
Br
CO2Et
EtO2C
N
H
1k
PPM
50
100
150
200
USER: -- DATE: Jul 15 2012
PTS1d: 42500 65536
LB: 2.0
OF1: 11053.7
NA: 100
PD: 1.0 sec
SW1: 25000
PW: 4.9 us
F2: 399.722
F1: 100.521
EX: s2pul
2010736-9-39
Nuts - $wkj-13-29-c-400.fid

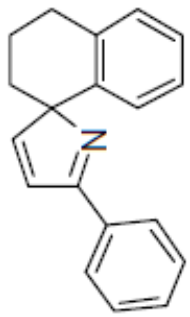

0.000
1.328
18.33
2.19
2.10
3.31
2.26
1.13
1.28
1.04
1.00
1.01
0.89
3.131
3.542
5.937
5.945
5.952
6.333
6.341
6.349
7.048
7.052
7.067
7.071
7.086
7.090
7.119
7.137
7.156
7.189
7.207
7.226
7.298
7.317
7.336
7.362
7.366
7.382
7.385
7.395
7.413
7.526
7.546
9.314
PPM
ARIA
F1: 399.723
EX: s2pul
F2: 100.519
SW1: 7184
PW: 7.8 us
PD: 1.0 sec
OF1: 2797.0
NA: 8
LB: 0.0
PTS1d: 21552
32768
USER: -- DATE: Oct 27 2012
Nuts - $wkj-13-30-h-400.fid
Br
$CO_2{}^tBu$
$^tBuO_2C$
N
H

11

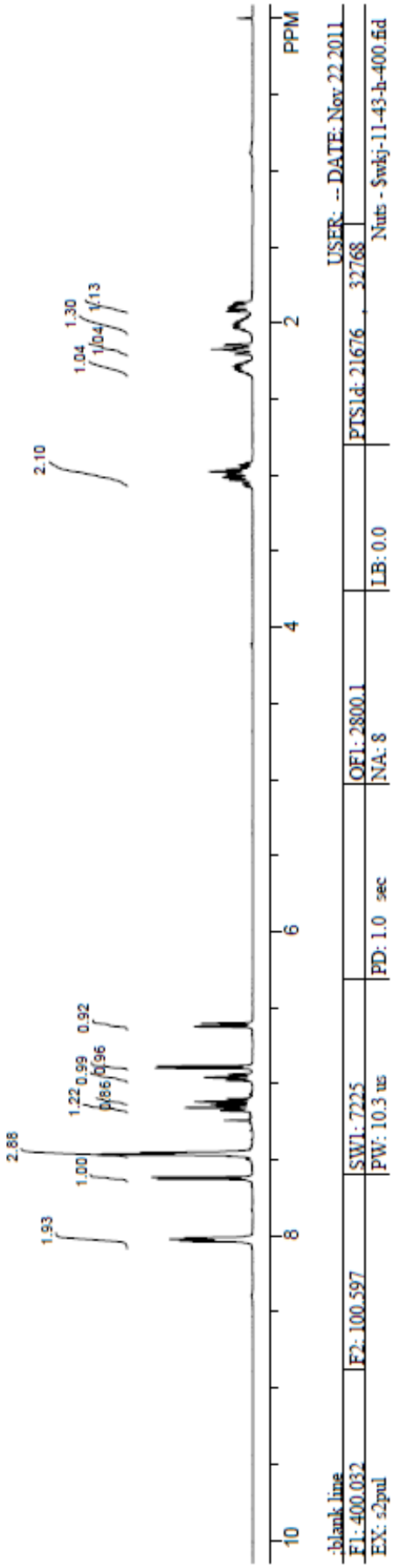

27.637
33.368
39.456
61.052
76.681
77.000
77.319
82.291
105.048
110.726
123.179
125.433
126.447
127.134
128.242
128.378
128.739
131.202
131.373
137.089
132.925
133.229
171.096
Br
CO2tBu
tBuO2C
N
H
11
PPM
200
150
100
50
USER: -- DATE: Oct 27 2012
2012040v222S-1
F1: 100.521
F2: 399.722
SW1: 25000
OF1: 11054.5
PTS1d: 40000
65536
EX: s2pul
PW: 6.8 us
PD: 1.0 sec
NA: 252
LB: 2.0
Nuts - $wkj-13-30-c-400.fid

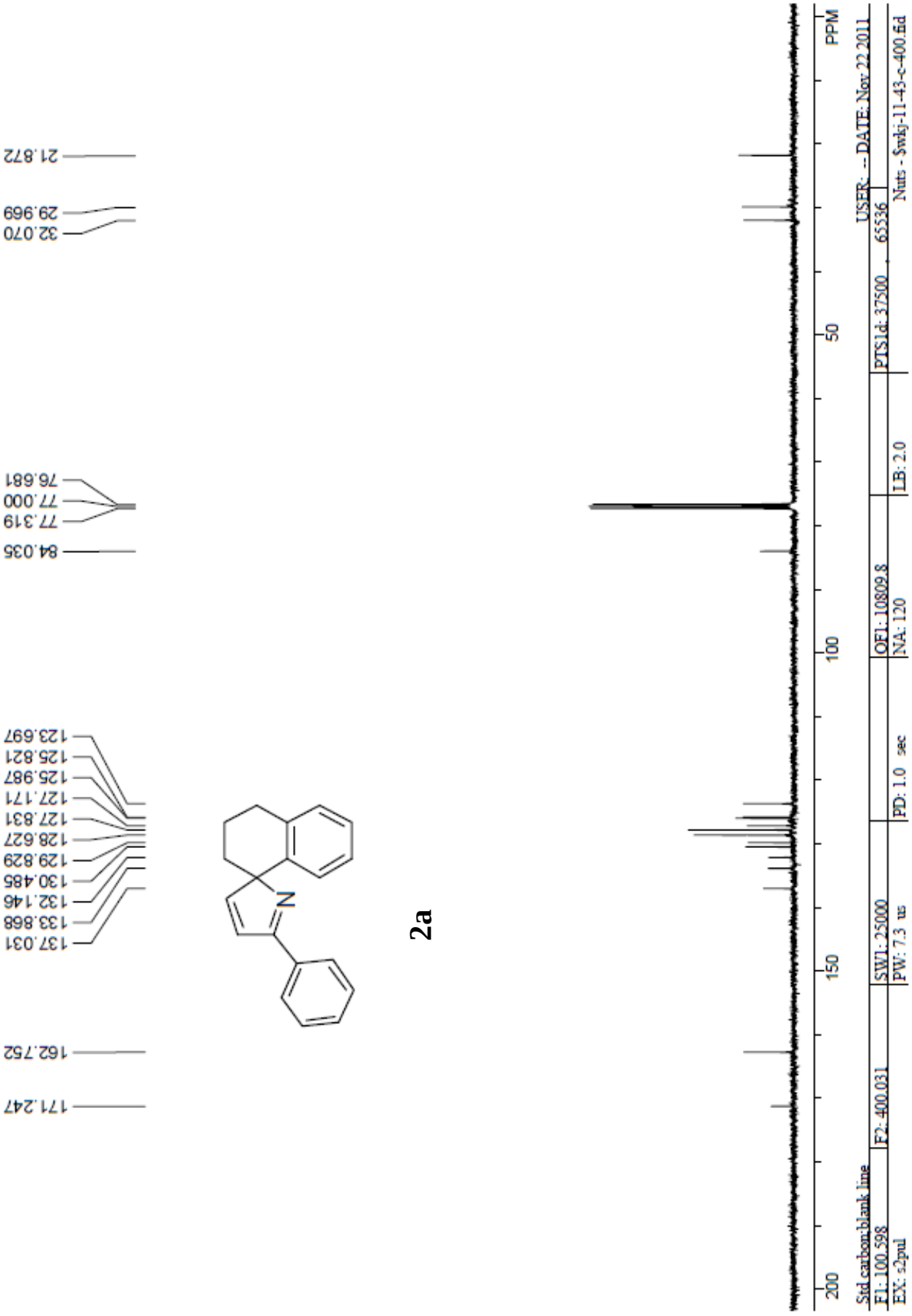

-0.008
1.866
1.873
1.887
1.893
1.898
1.905
1.919
1.925
2.002
2.015
2.035
2.144
2.150
2.168
2.175
2.182
2.201
2.207
2.289
2.304
2.322
2.936
2.951
2.964
2.979
2.994
3.015
3.035

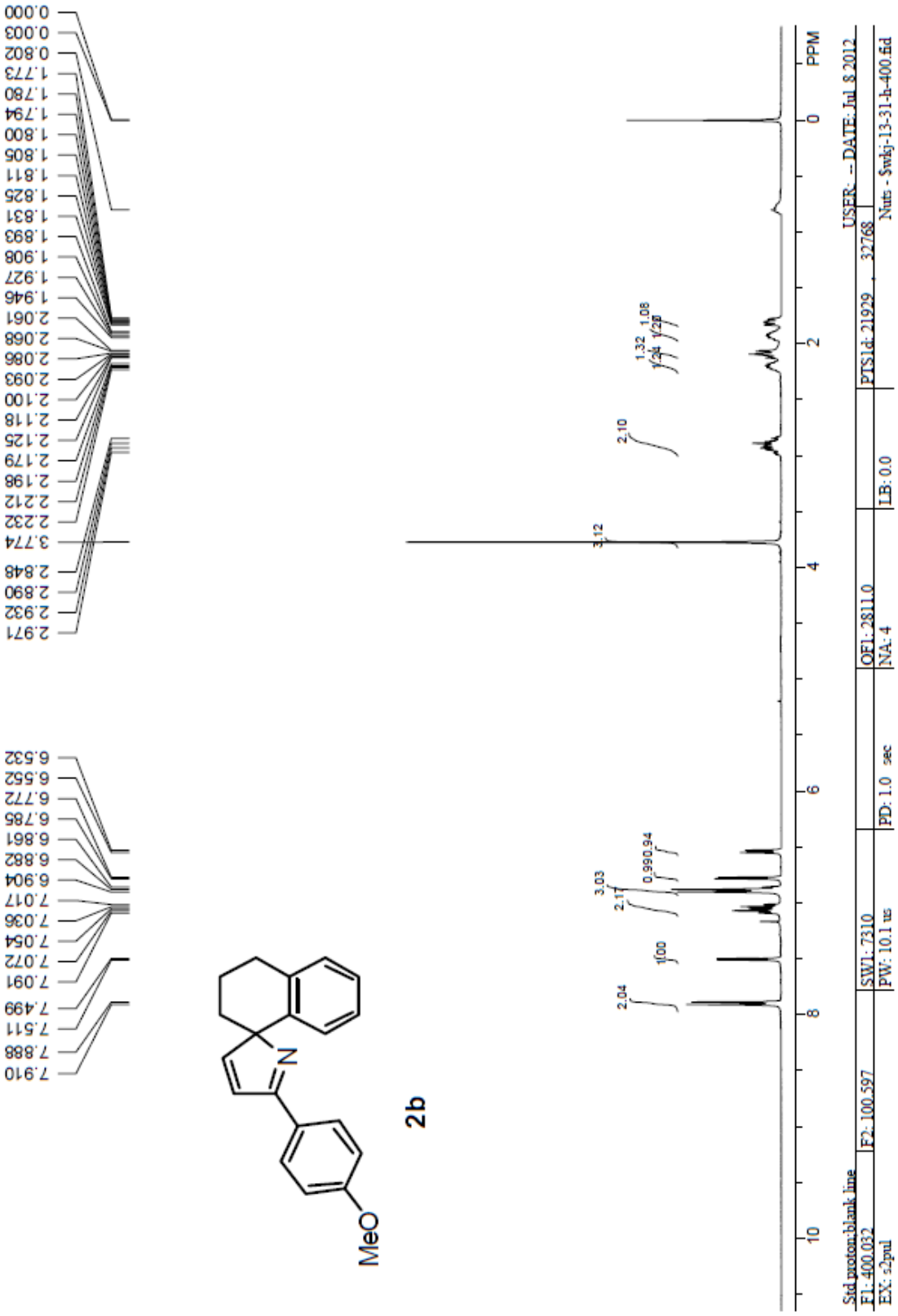

6.605
6.625
6.884
6.897
6.940
6.942
6.958
6.959
6.977
6.977
7.100
7.119
7.137
7.139
7.158
7.176
7.452
7.462
7.468
7.615
7.627
8.013
8.023
8.031
8.036

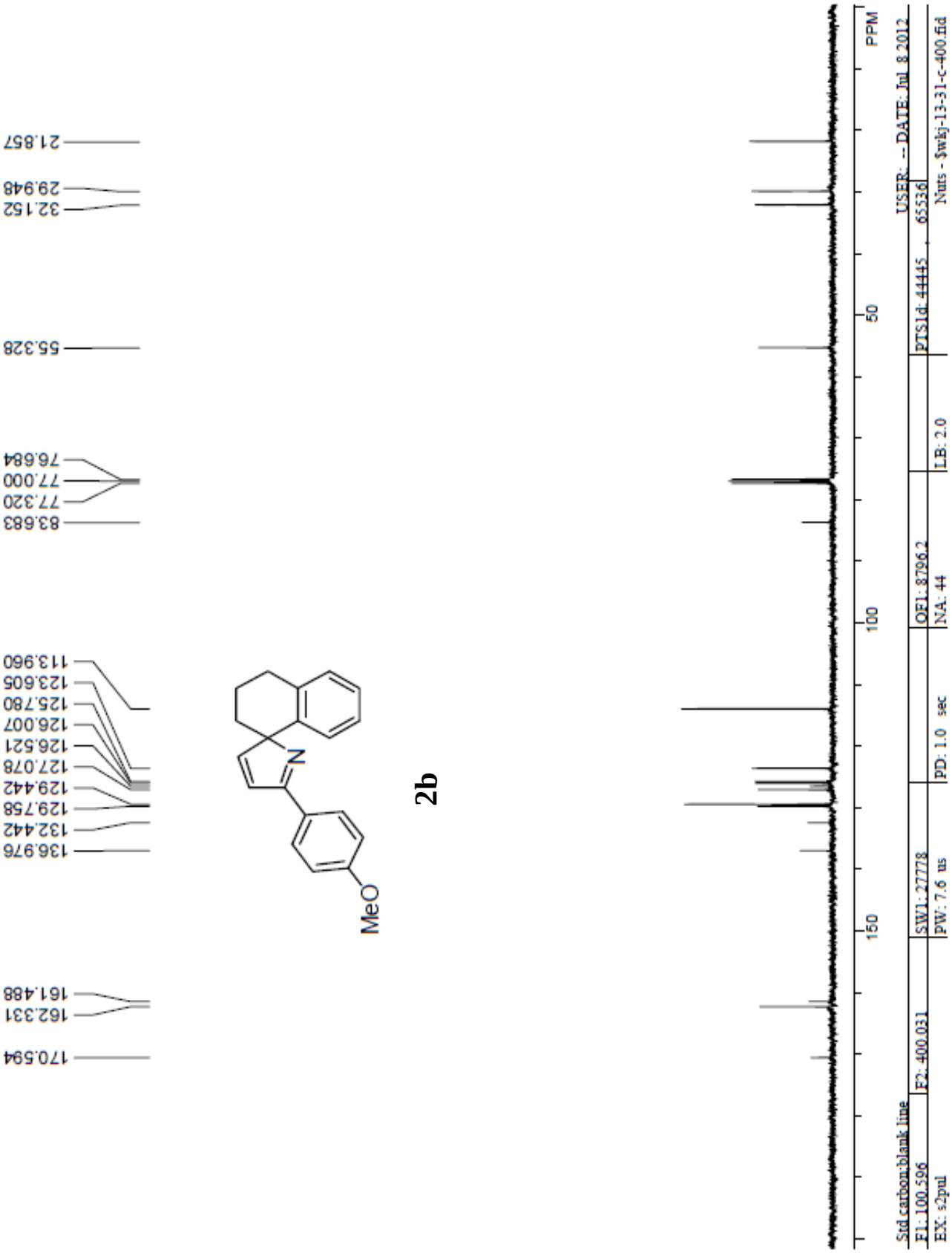

N

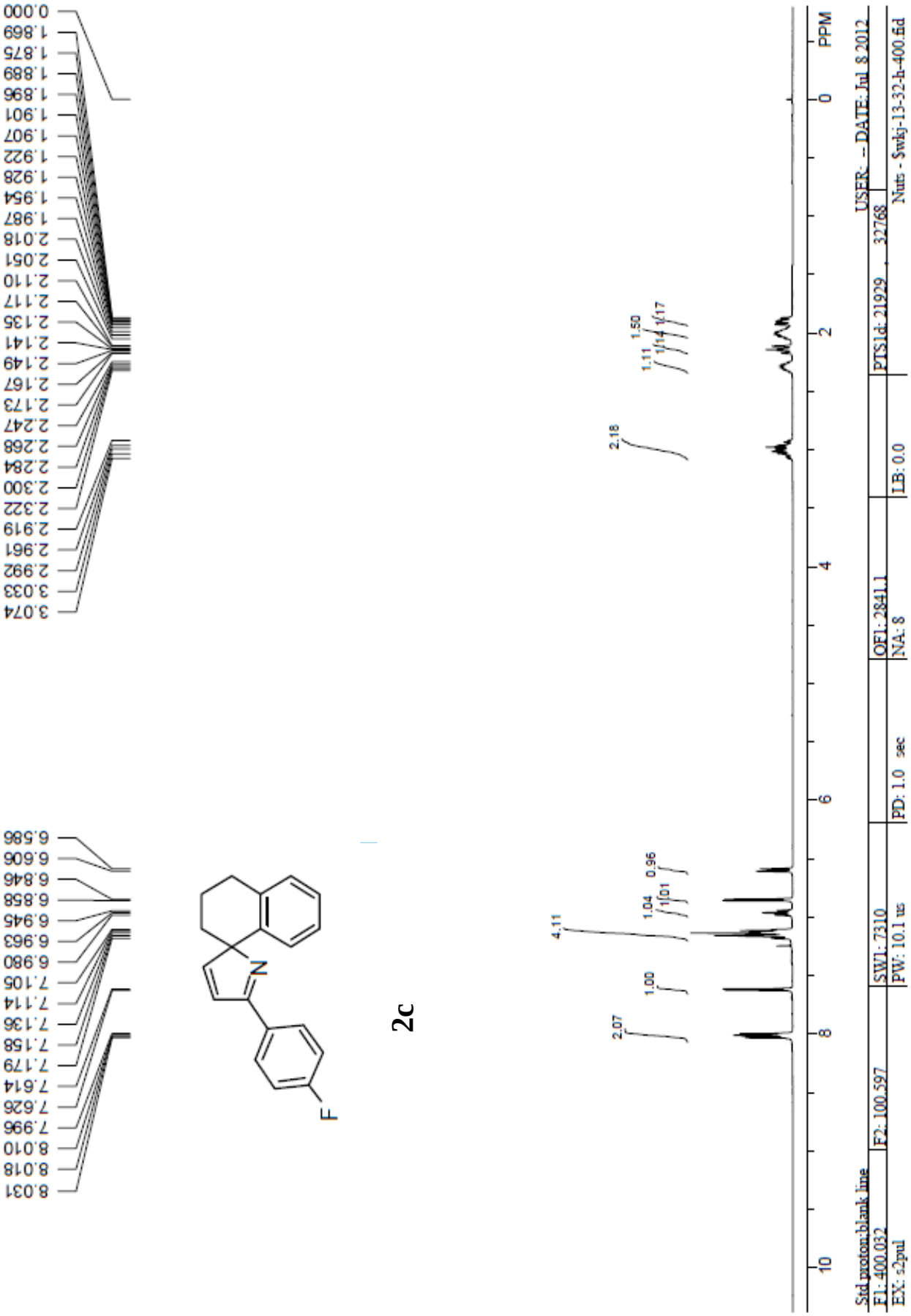
2a


2.88
1.93
1.00
1.22
0.99
0.86
0.96
0.92
2.10
1.04
1.30
1.04
1.13
10
8
6
4
2
PPM
blank line
F1: 400.032
EX: s2pul
F2: 100.597
SW1: 7225
PW: 10.3 us
PD: 1.0 sec
OF1: 2800.1
NA: 8
LB: 0.0
PTS1d: 21676 . 32768
USER: --DATE: Nov 22 2011
Nuts - $wkj-11-43-h-400.fid


21.872
29.969
32.070
76.681
77.000
77.319
84.035
123.697
125.821
125.987
127.171
127.831
128.627
129.829
130.485
132.146
133.868
137.031
162.752
171.247
N
2a
PPM
200
150
100
50
Std carbon:blank line
F1: 100.598
EX: s2pul
F2: 400.031
SW1: 25000
PW: 7.3 us
PD: 1.0 sec
OF1: 10809.8
NA: 120
LB: 2.0
PTS1d: 37500
65536
USER: --DATE: Nov 22 2011
Nuts - $wkj-11-43-c-400.fid

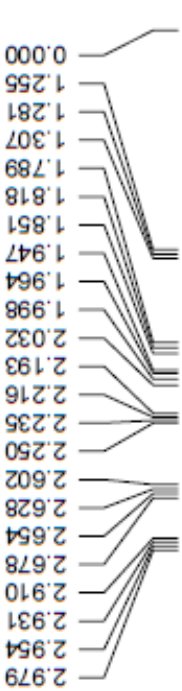

0.000
0.003
0.802
1.773
1.780
1.794
1.800
1.805
1.811
1.825
1.831
1.893
1.908
1.927
1.946
2.061
2.068
2.086
2.093
2.100
2.118
2.125
2.179
2.198
2.212
2.232
3.774
2.848
2.890
2.932
2.971
6.532
6.552
6.772
6.785
6.861
6.882
6.904
7.017
7.036
7.054
7.072
7.091
7.499
7.511
7.888
7.910
MeO
N
2b
3.12
2.10
1.32
1.08
3.03
2.17
0.990.94
1.00
2.04
PPM
Std proton.blank line
F1: 400.032
F2: 100.597
SW1: 7310
OF1: 2811.0
PTS1d: 21929
32768
EX: s2pul
PW: 10.1 us
PD: 1.0 sec
NA: 4
LB: 0.0
USER: -- DATE: Jul 8 2012
Nuts - $wkj-13-31-h-400.fid

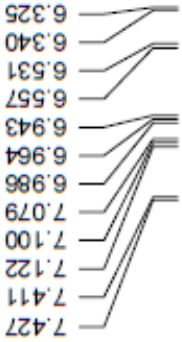

21.857
29.948
32.152
55.328
76.684
77.000
77.320
83.683
113.960
123.605
125.780
126.007
126.521
127.078
129.442
129.758
132.442
136.976
161.488
162.331
170.594
N
MeO
2b
PPM
150
100
50
Std carbon:blank line
F1: 100.596
F2: 400.031
SW1: 27778
PW: 7.6 us
PD: 1.0 sec
OF1: 8796.2
NA: 44
LB: 2.0
USER: -- DATE: Jul 8 2012
PTS1d: 44445 , 65536
EX: s2pul
Nuts - $wkj-13-31-c-400.fid

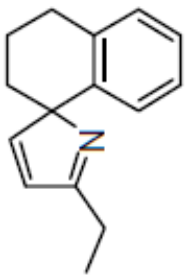

0.000
1.869
1.875
1.889
1.896
1.901
1.907
1.922
1.928
1.954
1.987
2.018
2.051
2.110
2.117
2.135
2.141
2.149
2.167
2.173
2.247
2.268
2.284
2.300
2.322
2.919
2.961
2.992
3.033
3.074
6.586
6.606
6.846
6.858
6.945
6.963
6.980
7.105
7.114
7.136
7.158
7.179
7.614
7.626
7.996
8.010
8.018
8.031
N
F
2c
2.07
1.00
4.11
1.04
1.01
0.96
2.18
1.11
1.14
1.17
1.50
PPM
Std proton:blank_line
F1: 400.032
EX: s2pul
F2: 100.597
SW1: 7310
PW: 10.1 us
PD: 1.0 sec
OF1: 2841.1
NA: 8
LB: 0.0
PTS1d: 21929
32768
USER: -- DATE: Jul 8 2012
Nuts - $wkj-13-32-h-400.fid


21.811
29.927
32.059
76.680
77.000
77.316
84.058
115.544
115.759
123.504
125.835
125.906
127.238
129.812
129.880
129.892
130.082
130.112
131.991
137.018
162.976
163.018
165.466
170.089
N
F
2c
PPM
200
150
100
50
Std carbon:blank line
F1: 100.596
EX: s2pul
F2: 400.031
SW1: 27778
PW: 7.6 us
PD: 1.0 sec
OF1: 8797.0
NA: 600
LB: 2.0
PTS1d: 44445
65536
USER: -- DATE: Jul 8 2012
Nuts - $wkj-13-32-c-400.fid

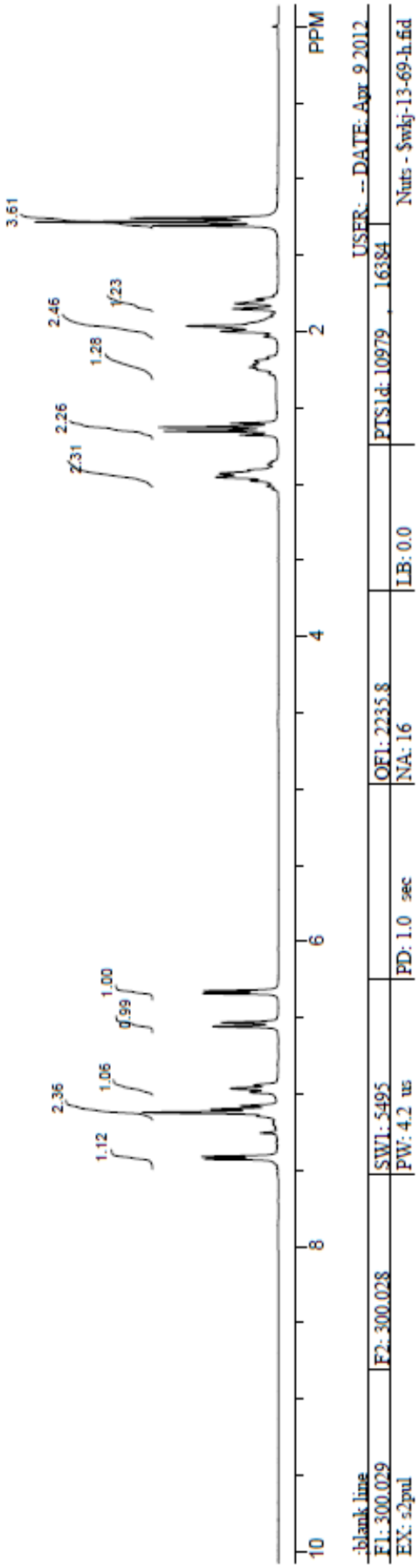

2c
N
F
109.819
109.827
109.833
109.841
109.849
109.855
109.863
PPM
-60
-80
-100
-120
-140
-160
-180
STANDARD 1H OBSERVE - profile
F1: 376.366
F2: 100.597
SW1: 156250
PW: 6.1 us
PD: 1.0 sec
OF1: -37640.3
NA: 4
PTS1d: 187500
LB: 0.0
USER: -- DATE: Jul 8 2012
EX: s2pul
Nuts - $wkj-13-32-f-400.fid

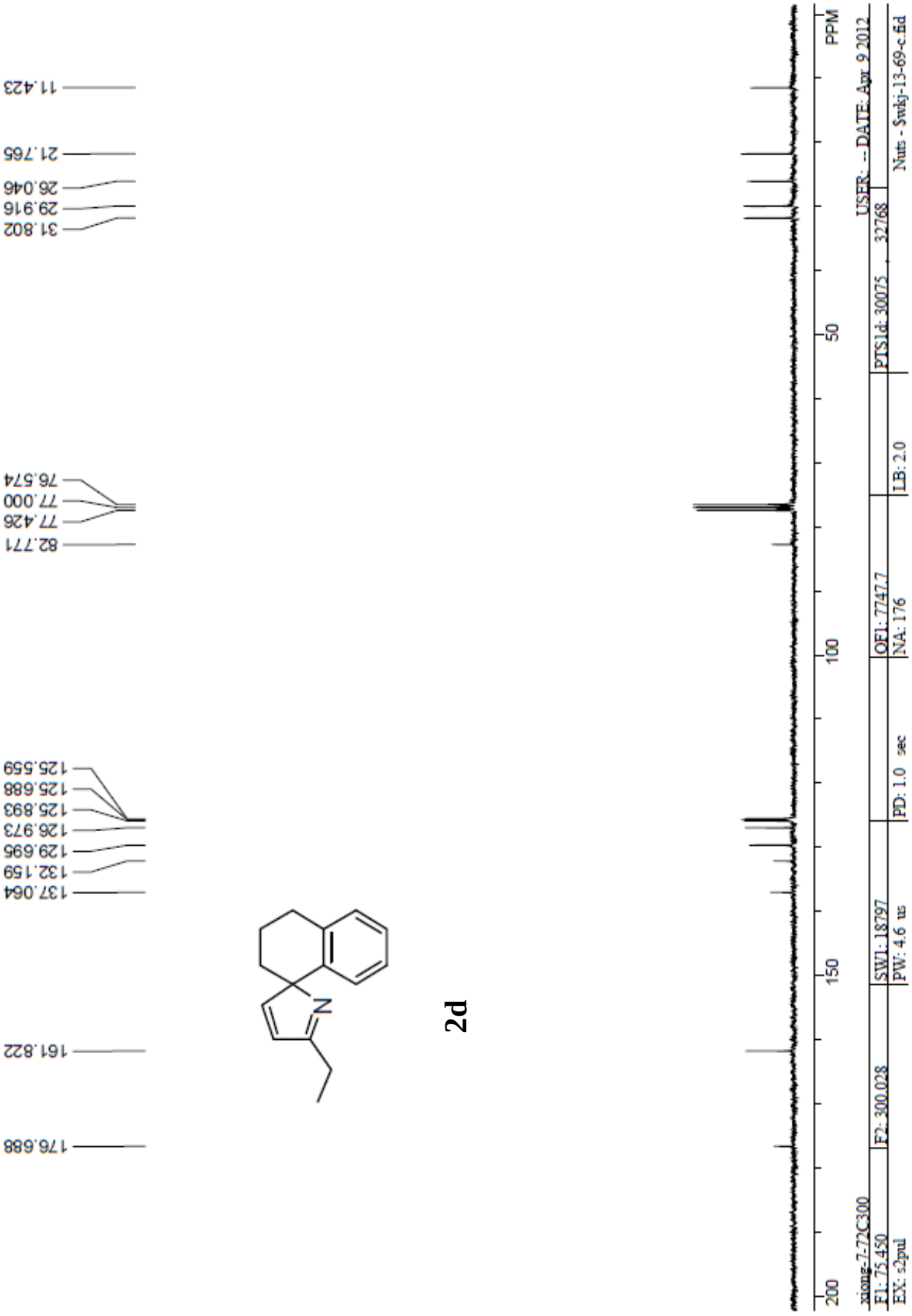

0.000
1.255
1.281
1.307
1.789
1.818
1.851
1.947
1.964
1.998
2.032
2.193
2.216
2.235
2.250
2.602
2.628
2.654
2.678
2.910
2.931
2.954
2.979

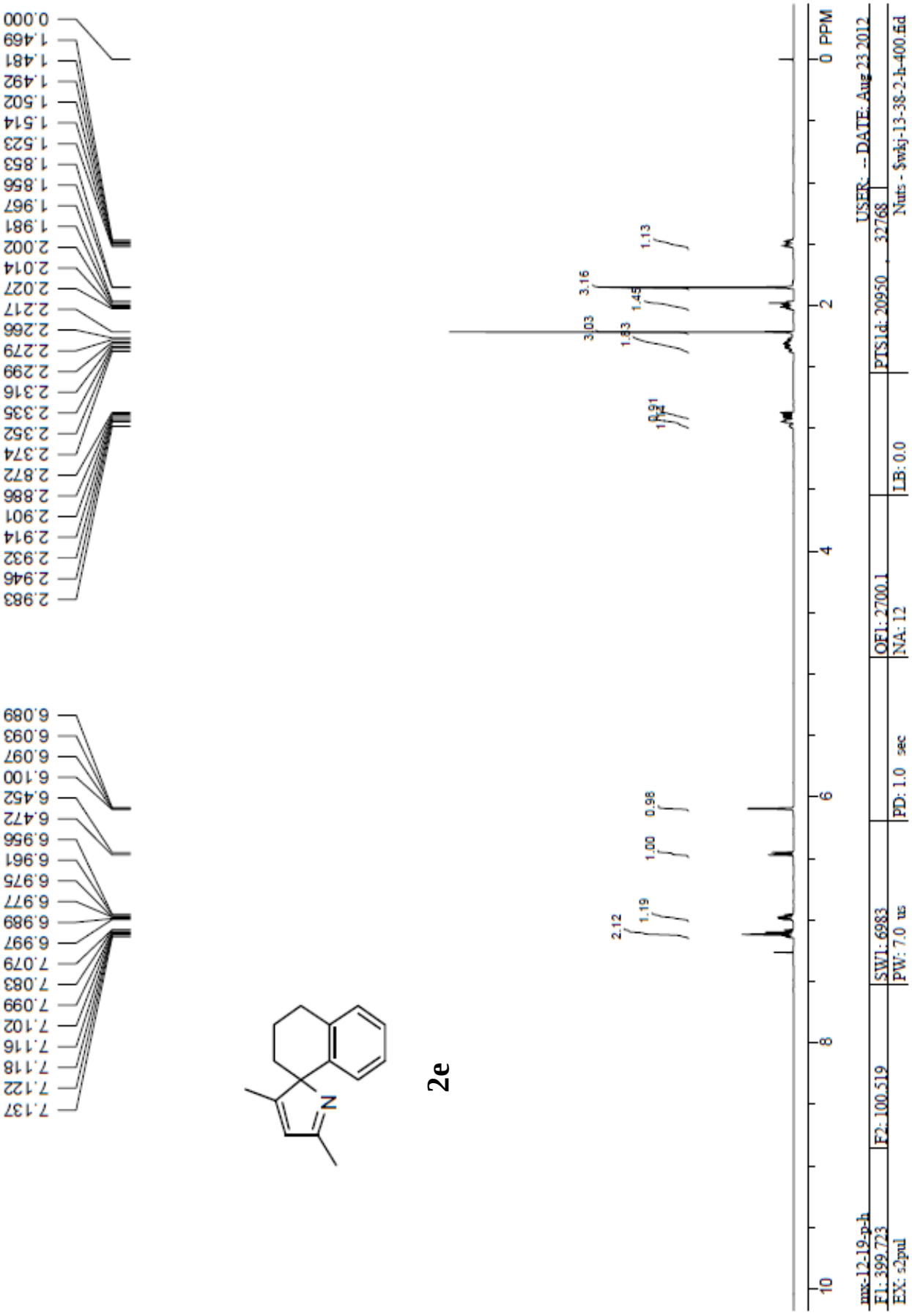

6.325
6.340
6.531
6.557
6.943
6.964
6.986
7.079
7.100
7.122
7.411
7.427

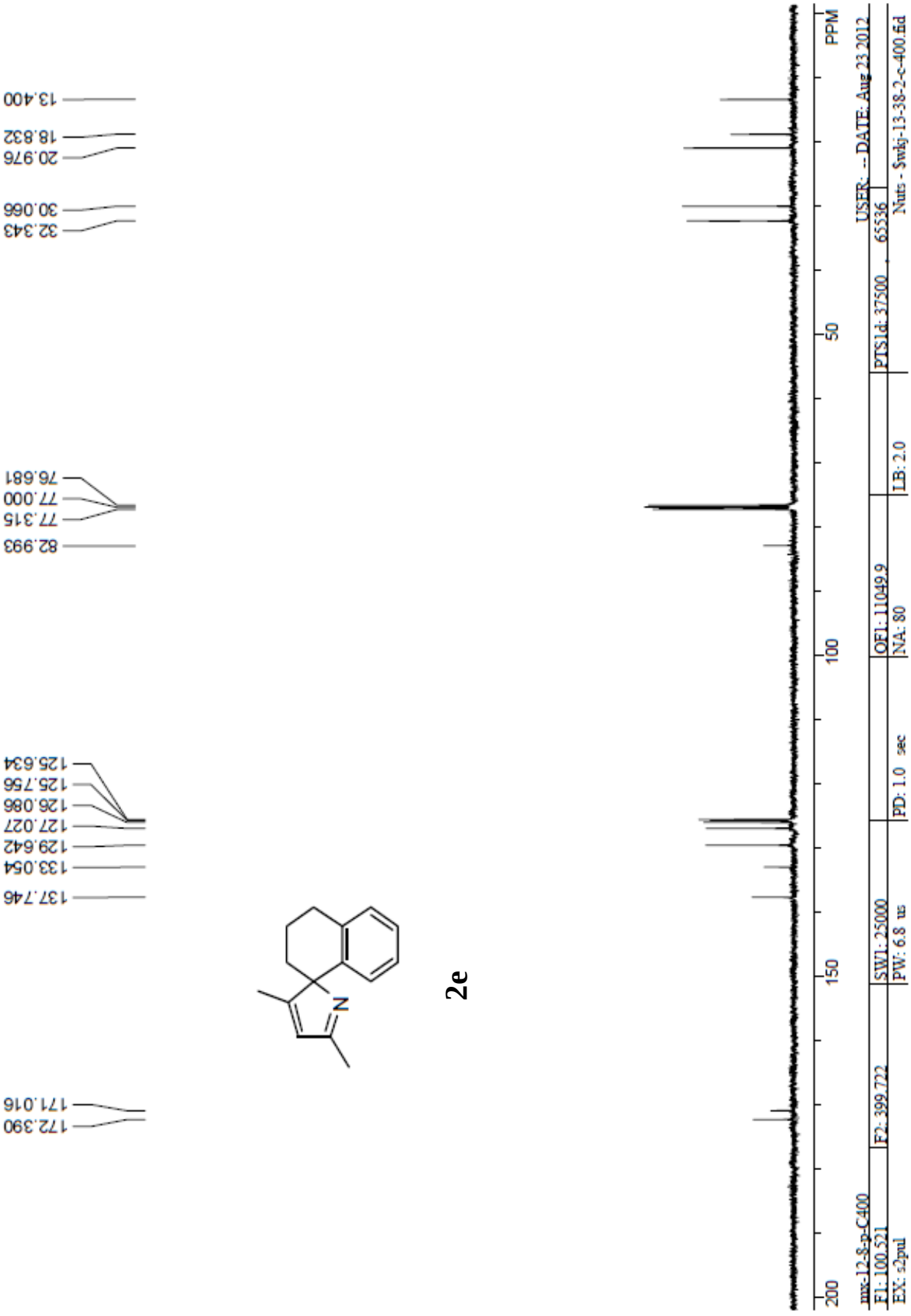

N

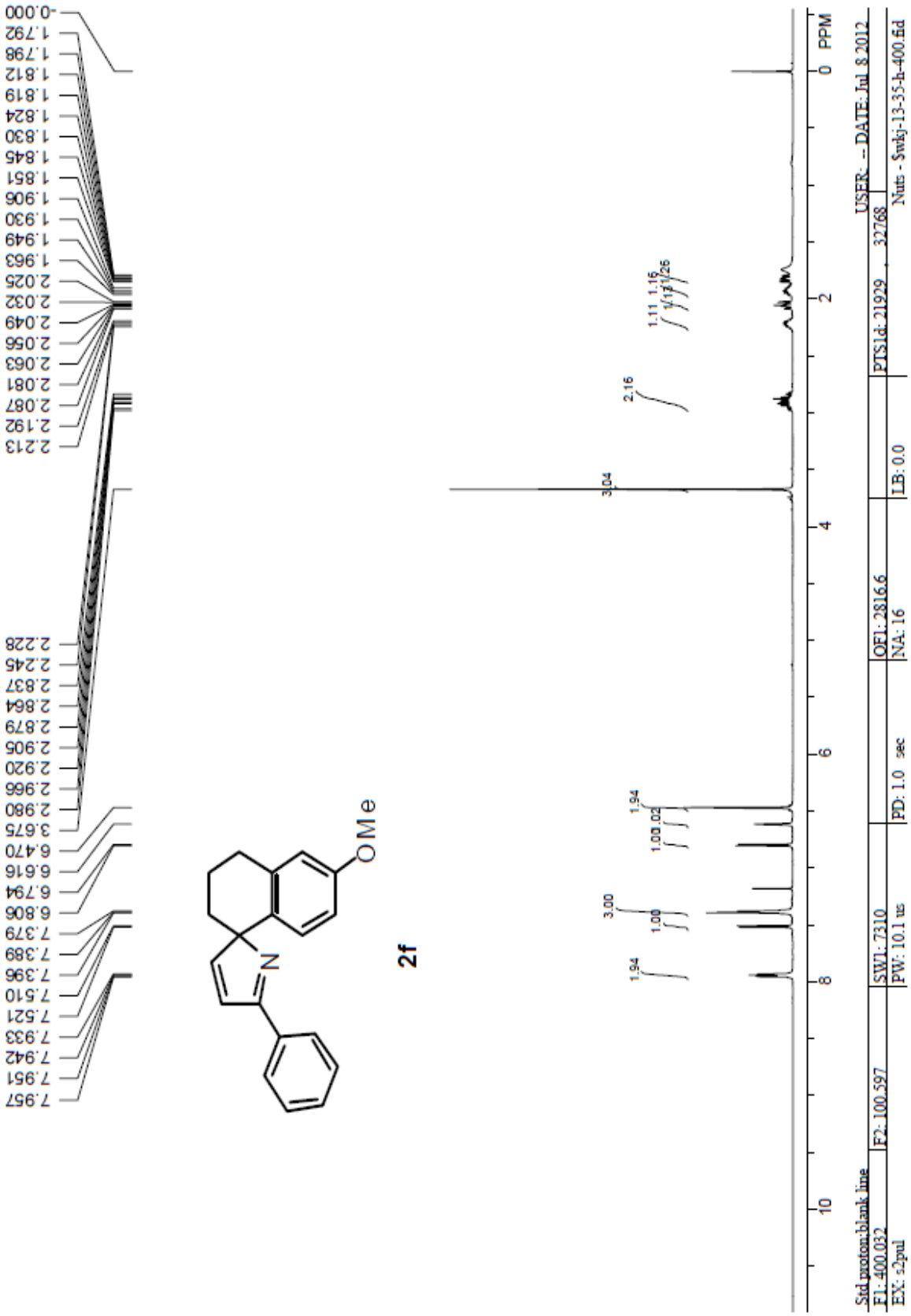
2d

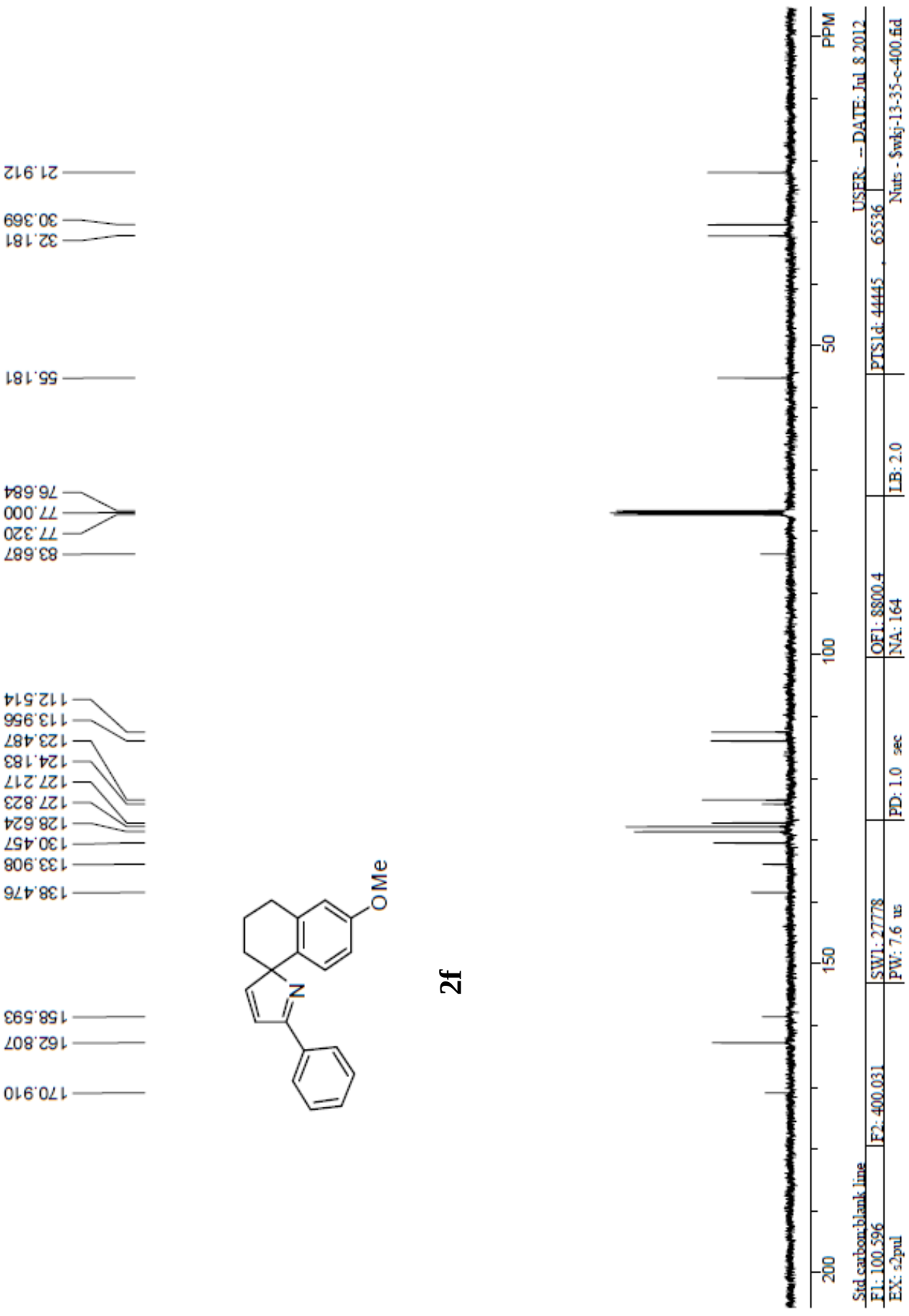

3.61
2.46
1.28
1.23
2.26
2.31
2.36
1.12
1.06
0.99
1.00
10
8
6
4
2
PPM
blank line
F1: 300.029
EX: s2pul
F2: 300.028
SW1: 5495
PW: 4.2 us
PD: 1.0 sec
OF1: 2235.8
NA: 16
LB: 0.0
USER: -- DATE: Apr 9 2012
PTS1d: 10979 , 16384
Nuts - $wkj-13-69-h.fid

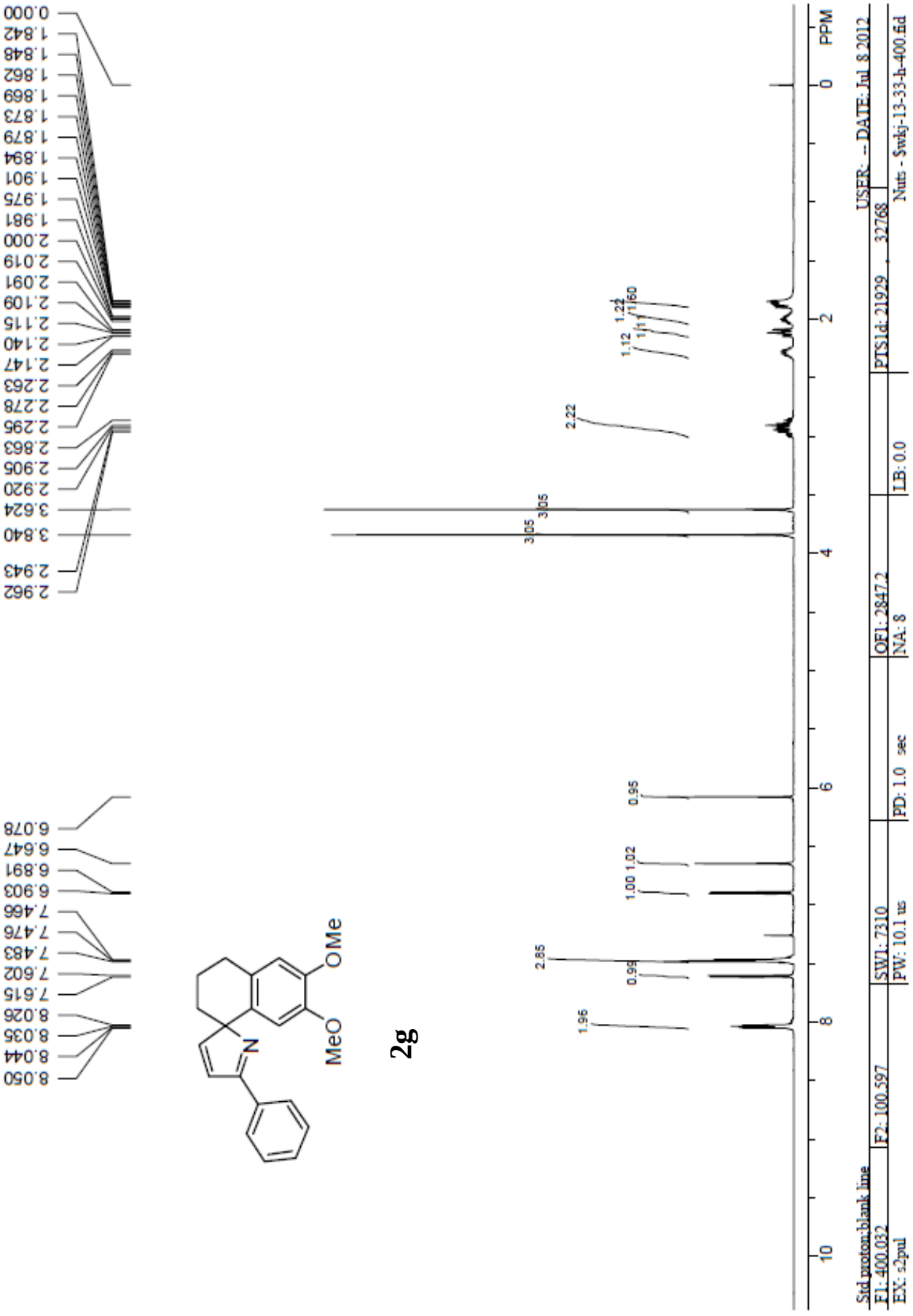

11.423
21.765
26.046
29.916
31.802
76.574
77.000
77.426
82.771
125.559
125.688
125.893
126.973
129.695
132.159
137.064
161.822
176.688
N
2d
PPM
200
150
100
50
xiong-7-72C300
F1: 75.450
EX: s2pul
F2: 300.028
SW1: 18797
PW: 4.6 us
PD: 1.0 sec
QF1: 7747.7
NA: 176
LB: 2.0
PTS1d: 30075
32768
USER: --DATE: Apr 9 2012
Nuts - $wkj-13-69-c.fid

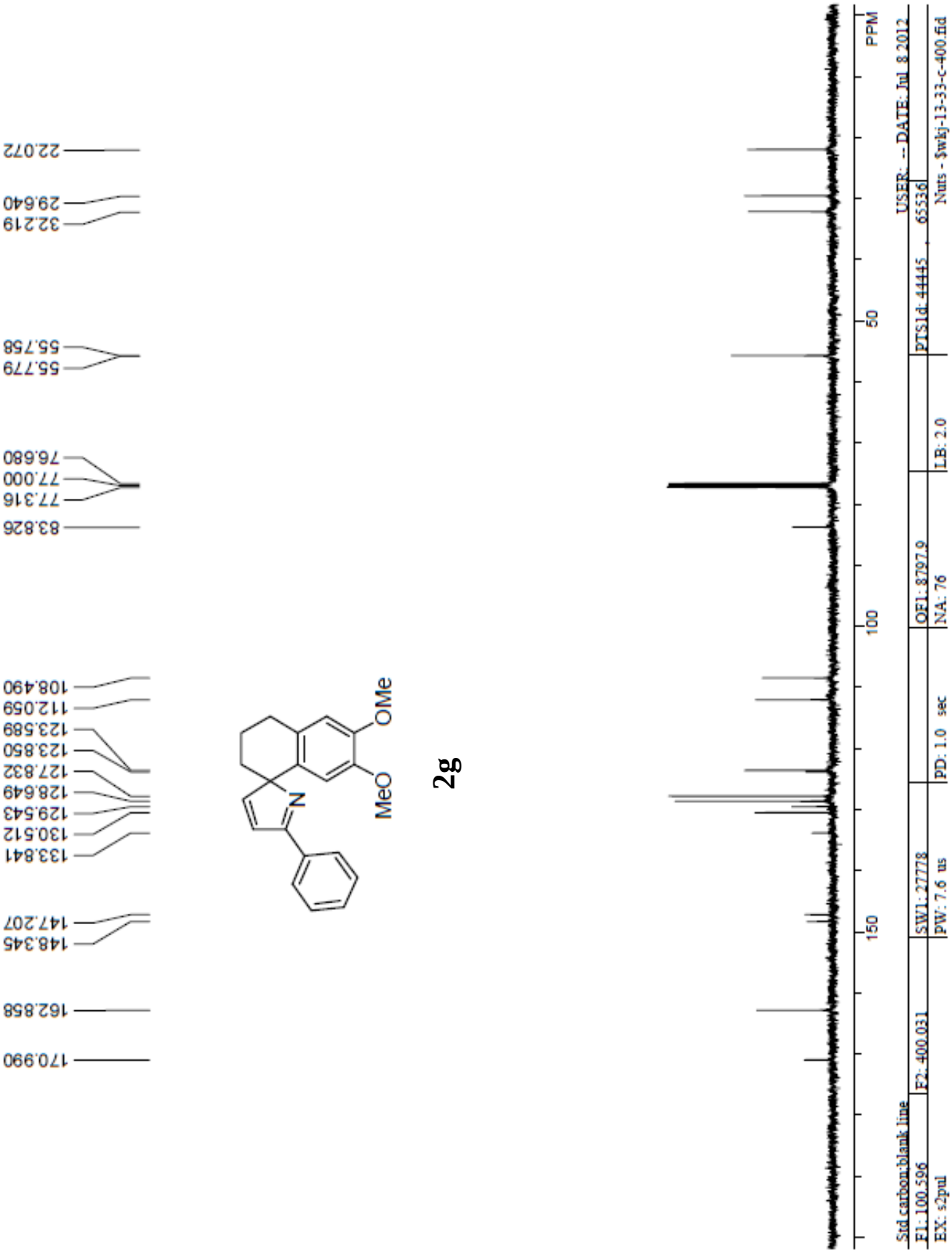

0.000
1.469
1.481
1.492
1.502
1.514
1.523
1.853
1.856
1.967
1.981
2.002
2.014
2.027
2.217
2.266
2.279
2.299
2.316
2.335
2.352
2.374
2.872
2.886
2.901
2.914
2.932
2.946
2.983
6.089
6.093
6.097
6.100
6.452
6.472
6.956
6.961
6.975
6.977
6.989
6.997
7.079
7.083
7.099
7.102
7.116
7.118
7.122
7.137
N
2e
2.12
1.19
1.00
0.98
0.91
3.03
1.83
3.16
1.45
1.13
0 PPM
2
4
6
8
10
mx-12-19-p-h
F1: 399.723
EX: s2pul
F2: 100.519
SW1: 6983
PW: 7.0 us
PD: 1.0 sec
OF1: 2700.1
NA: 12
LB: 0.0
PTS1d: 20950
32768
USER: --DATE: Aug 23 2012
Nuts - $wkj-13-38-2-h-400.fid

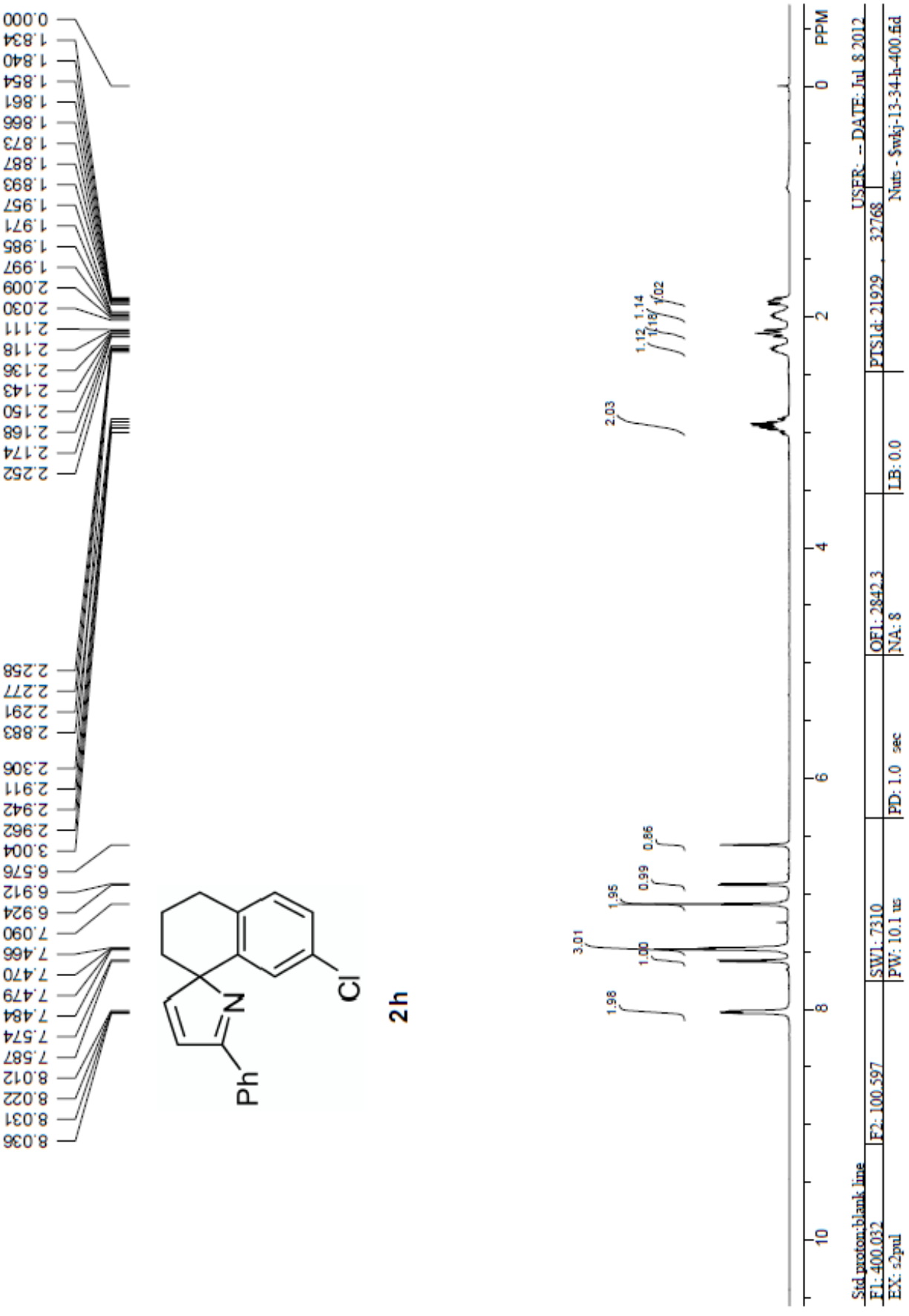

13.400
18.832
20.976
30.066
32.343
76.681
77.000
77.315
82.993
125.634
125.756
126.086
127.027
129.642
133.054
137.746
171.016
172.390
N
2e
PPM
200
150
100
50
mx-12-8-p-C400
F1: 100.521
EX: s2pul
F2: 399.722
SW1: 25000
PW: 6.8 us
PD: 1.0 sec
OF1: 11049.9
NA: 80
LB: 2.0
PTS1d: 37500 , 65536
USER: -- DATE: Aug 23 2012
Nuts - $wkj-13-38-2-c-400.fid

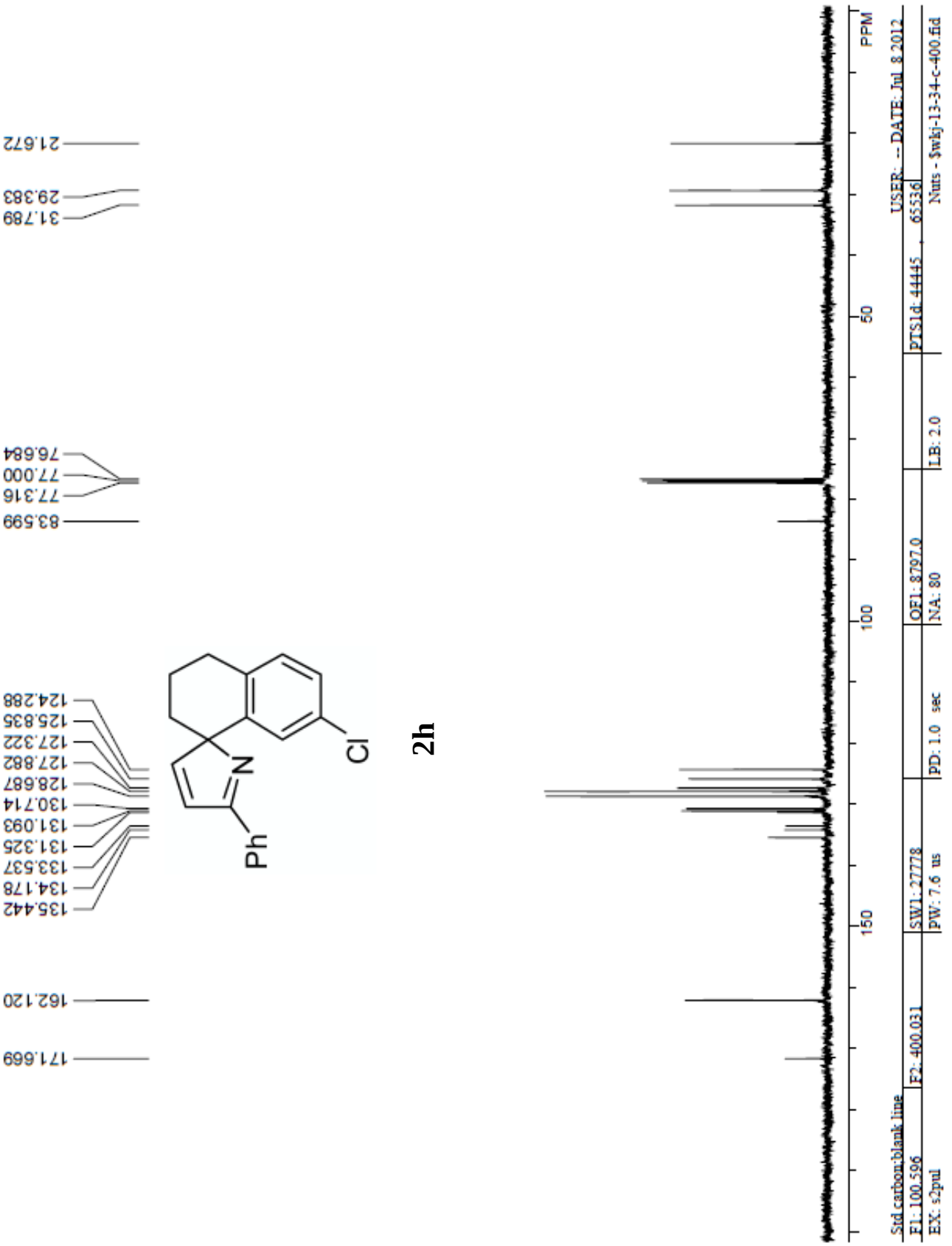

OMe
N
2f
7.957
7.951
7.942
7.933
7.521
7.510
7.396
7.389
7.379
6.806
6.794
6.616
6.470
3.675
2.980
2.966
2.920
2.905
2.879
2.864
2.837
2.245
2.228
2.213
2.192
2.087
2.081
2.063
2.056
2.049
2.032
2.025
1.963
1.949
1.930
1.906
1.851
1.845
1.830
1.824
1.819
1.812
1.798
1.792
0.000
3.04
2.16
1.11
1.16
1.26
1.94
1.00
3.00
1.94
1.00
1.02
10
8
6
4
2
0 PPM
Std proton.blank line
F1: 400.032
F2: 100.597
EX: s2pul
SW1: 7310
PW: 10.1 us
PD: 1.0 sec
OF1: 2816.6
NA: 16
LB: 0.0
PTS1d: 21929 , 32768
USER: -- DATE: Jul 8 2012
Nuts - $wkj-13-35-h-400.fid

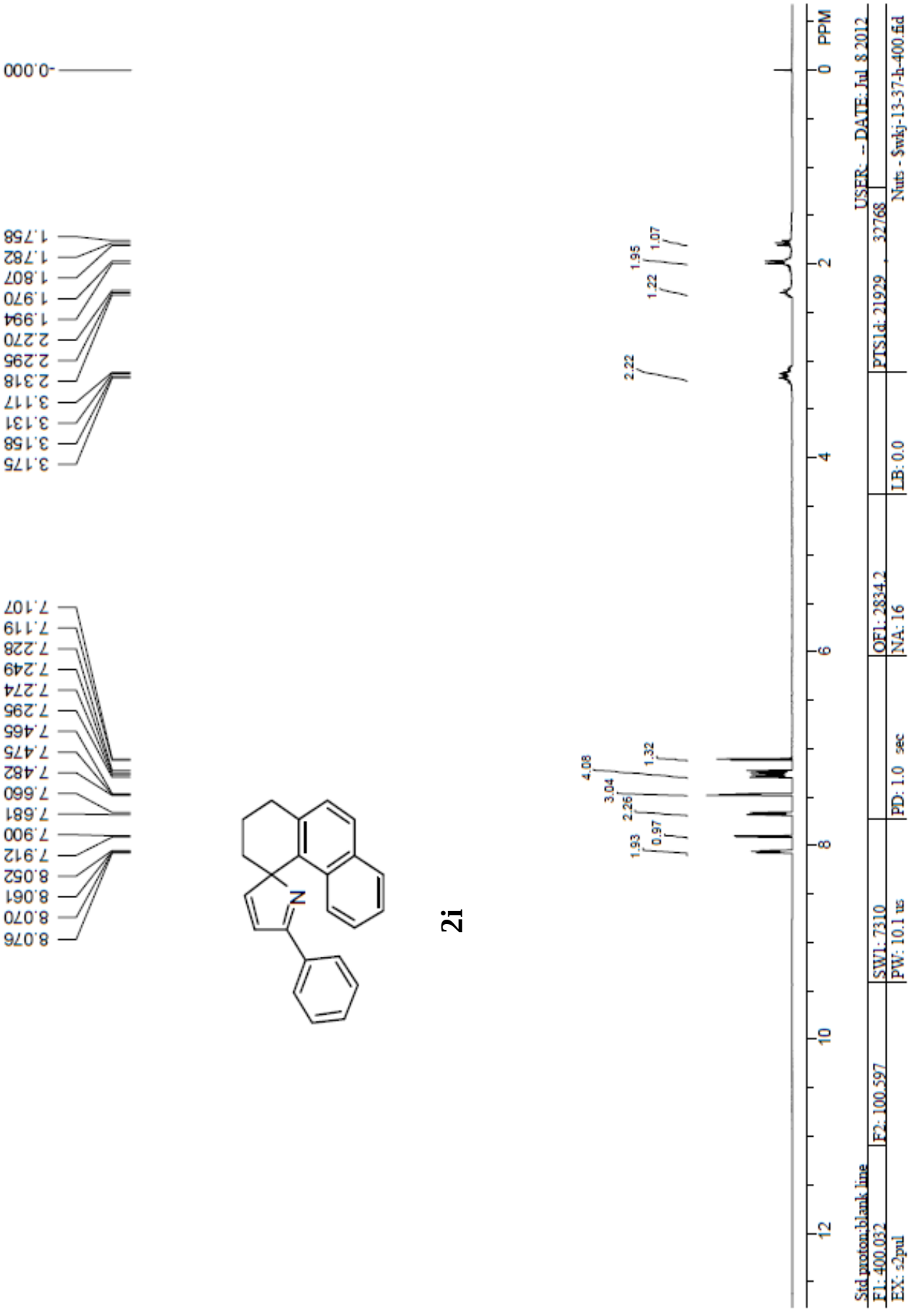

21.912
30.369
32.181
55.181
76.684
77.000
77.320
83.687
112.514
113.956
123.487
124.183
127.217
127.823
128.624
130.457
133.908
138.476
158.593
162.807
170.910
OMe
N
2f
PPM
200
150
100
50
Std carbon blank line
F1: 100.596
EX: s2pul
F2: 400.031
PW: 7.6 us
SW1: 27778
PD: 1.0 sec
OF1: 8800.4
NA: 164
LB: 2.0
PTS1d: 44445 , 65536
USER: -- DATE: Jul 8 2012
Nuts - $wkj-13-35-c-400.fid

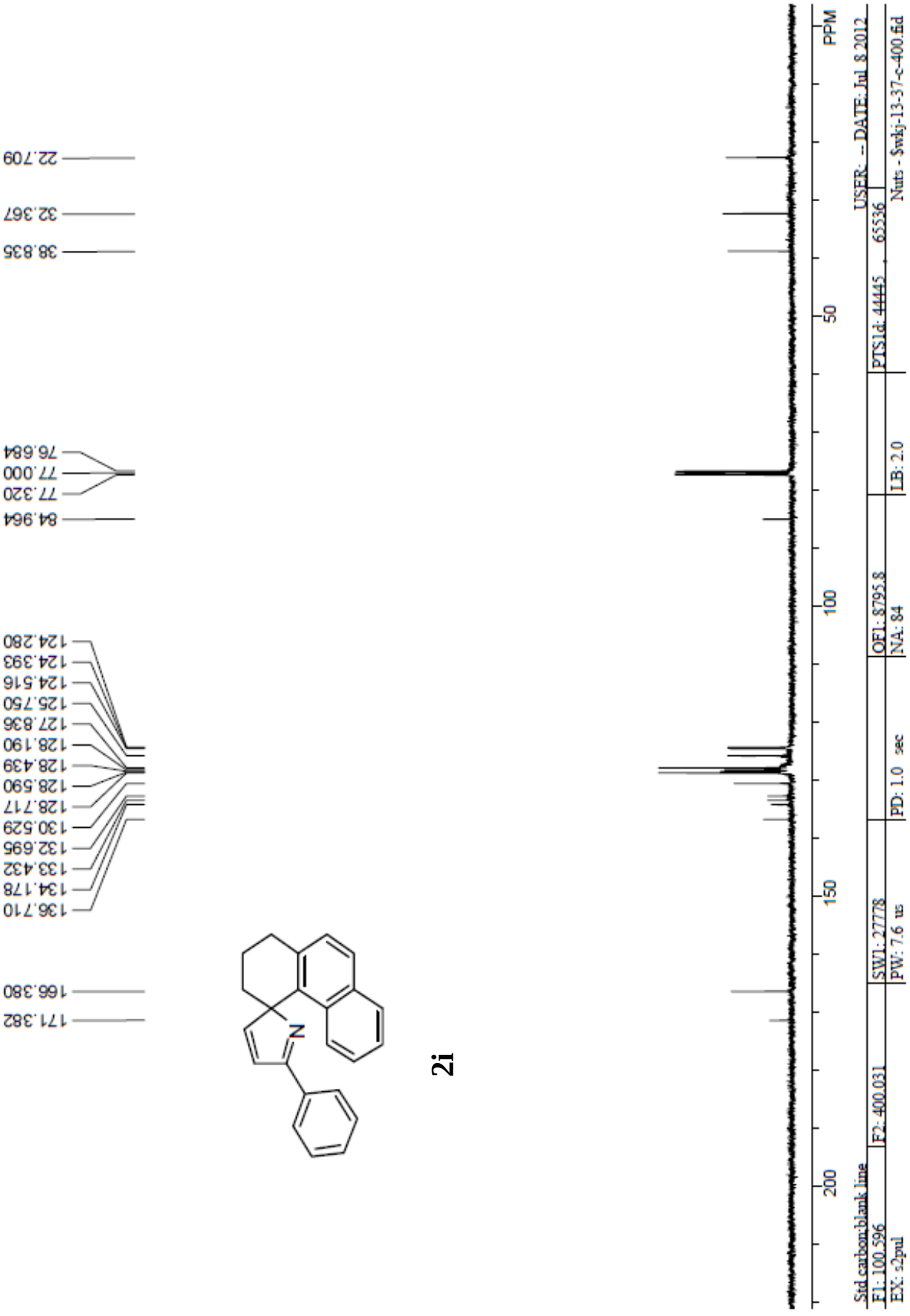

2g
OMe
MeO
N
0.000
1.842
1.848
1.862
1.869
1.873
1.879
1.894
1.901
1.975
1.981
2.000
2.019
2.091
2.109
2.115
2.140
2.147
2.263
2.278
2.295
2.863
2.905
2.920
3.624
3.840
2.943
2.962
6.078
6.647
6.891
6.903
7.466
7.476
7.483
7.602
7.615
8.026
8.035
8.044
8.050
3.05
3.05
2.22
1.12
1.11
1.22
1.60
0.95
1.00
1.02
2.85
0.99
1.96
PPM
Std proton:blank line
F1: 400.032
EX: s2pul
F2: 100.597
SW1: 7310
PW: 10.1 us
PD: 1.0 sec
OF1: 2847.2
NA: 8
LB: 0.0
PTS1d: 21929
32768
USER: -- DATE: Jul 8 2012
Nuts - $wkj-13-33-h-400.fid

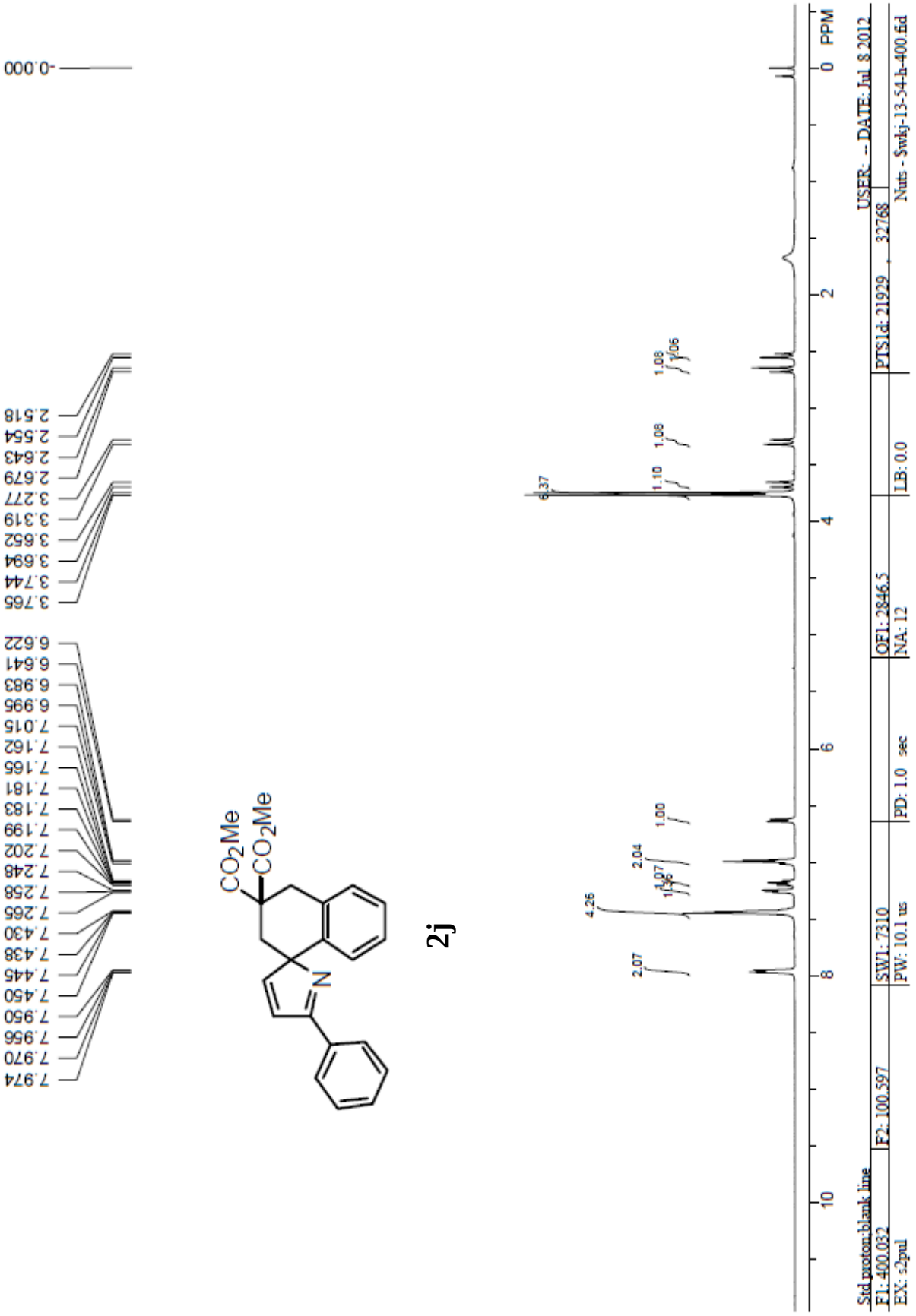

22.072
29.640
32.219
55.758
55.779
76.680
77.000
77.316
83.826
108.490
112.059
123.589
123.850
127.832
128.649
129.543
130.512
133.841
147.207
148.345
162.858
170.990
OMe
MeO
N
2g
PPM
50
100
150
Std carbon:blank line
F1: 100.596
F2: 400.031
SW1: 27778
PW: 7.6 us
PD: 1.0 sec
OF1: 8797.9
NA: 76
LB: 2.0
PTS1d: 44445 , 65536
USER: -- DATE: Jul 8 2012
EX: s2pul
Nuts - $wkj-13-33-c-400.fid

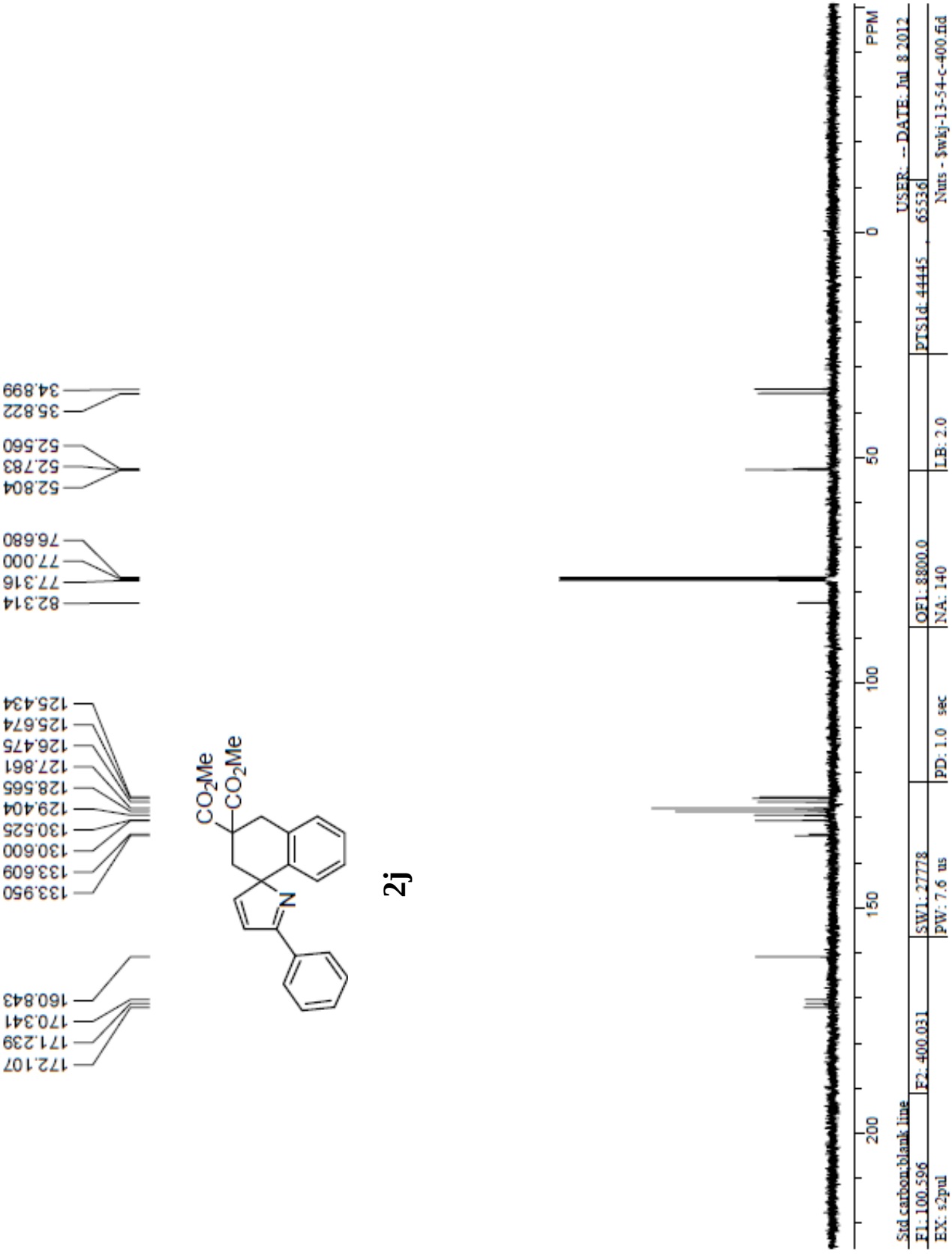

0.000
1.834
1.840
1.854
1.861
1.866
1.873
1.887
1.893
1.957
1.971
1.985
1.997
2.009
2.030
2.111
2.118
2.136
2.143
2.150
2.168
2.174
2.252
2.258
2.277
2.291
2.883
2.306
2.911
2.942
2.962
3.004
6.576
6.912
6.924
7.090
7.466
7.470
7.479
7.484
7.574
7.587
8.012
8.022
8.031
8.036
N
Ph
Cl
2h
2.03
1.12
1.14
1.16
1.02
3.01
1.98
1.95
1.00
0.99
0.86
10
8
6
4
2
0
PPM
Std proton:blank line
F1: 400.032
F2: 100.597
SW1: 7310
OF1: 2842.3
PTS1d: 21929
32768
EX: s2pul
PW: 10.1 us
PD: 1.0 sec
NA: 8
LB: 0.0
USER: -- DATE: Jul 8 2012
Nuts - $wkj-13-34-h-400.fid

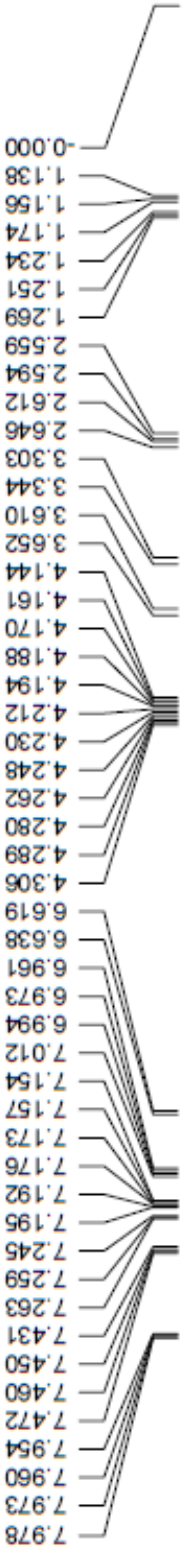

21.672
29.383
31.789
76.684
77.000
77.316
83.599
124.288
125.835
127.322
127.882
128.687
130.714
131.093
131.325
133.537
134.178
135.442
162.120
171.669
N
Cl
Ph
2h
PPM
50
100
150
Std carbon blank line
F1: 100.596
F2: 400.031
SW1: 27778
PW: 7.6 us
PD: 1.0 sec
OF1: 8797.0
NA: 80
LB: 2.0
EX: s2pul
PTS1d: 44445 , 65536
USER: -- DATE: Jul 8 2012
Nuts - $wkj-13-34-c-400.fid

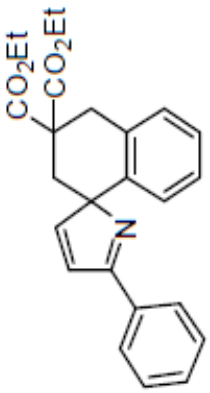

-0.000
1.758
1.782
1.807
1.970
1.994
2.270
2.295
2.318
3.117
3.131
3.158
3.175
7.107
7.119
7.228
7.249
7.274
7.295
7.465
7.475
7.482
7.660
7.681
7.900
7.912
8.052
8.061
8.070
8.076
N
2i
4.08
3.04
2.26
1.93
0.97
1.32
2.22
1.22
1.95
1.07
PPM
0
2
4
6
8
10
12
USER: -- DATE: Jul 8 2012
PTS1d: 21929 , 32768
Nuts - $wkj-13-37-h-400.fid
LB: 0.0
OF1: 2834.2
NA: 16
PD: 1.0 sec
SW1: 7310
PW: 10.1 us
F2: 100.597
Std proton:blank line
F1: 400.032
EX: s2pul


22.709
32.367
38.835
76.684
77.000
77.320
84.964
124.280
124.393
124.516
125.750
127.836
128.190
128.439
128.590
128.717
130.529
132.695
133.432
134.178
136.710
166.380
171.382
N
2i
PPM
50
100
150
200
Std carbon:blank line
F1: 100.596
F2: 400.031
SW1: 27778
PW: 7.6 us
PD: 1.0 sec
OF1: 8795.8
NA: 84
LB: 2.0
PTS1d: 44445 , 65536
USER: -- DATE: Jul 8 2012
EX: s2pul
Nuts - $wkj-13-37-c-400.fid

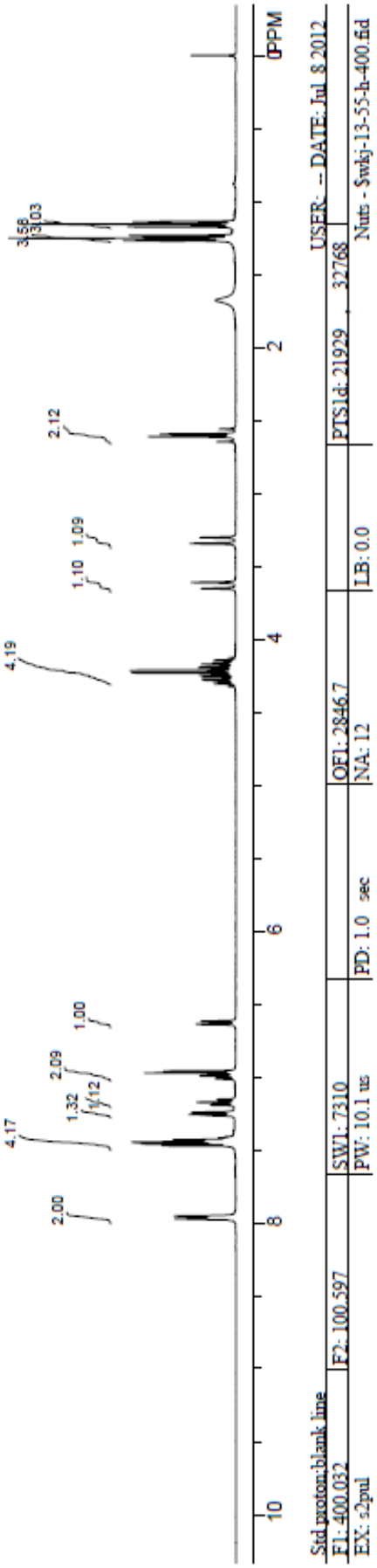

0.000
2.518
2.554
2.643
2.679
3.277
3.319
3.652
3.694
3.744
3.765
6.622
6.641
6.983
6.995
7.015
7.162
7.165
7.181
7.183
7.199
7.202
7.248
7.258
7.265
7.430
7.438
7.445
7.450
7.950
7.956
7.970
7.974
CO2Me
CO2Me
N
2j
6.37
1.10
1.08
1.08
1.06
1.06
4.26
2.07
2.04
1.07
1.06
1.00
0 PPM
2
4
6
8
10
Std proton:blank line
F1: 400.032
F2: 100.597
EX: s2pul
SW1: 7310
PW: 10.1 us
PD: 1.0 sec
OF1: 2846.5
NA: 12
PTS1d: 21929 , 32768
LB: 0.0
USER: -- DATE: Jul 8 2012
Nuts - $wkj-13-54-h-400.fid

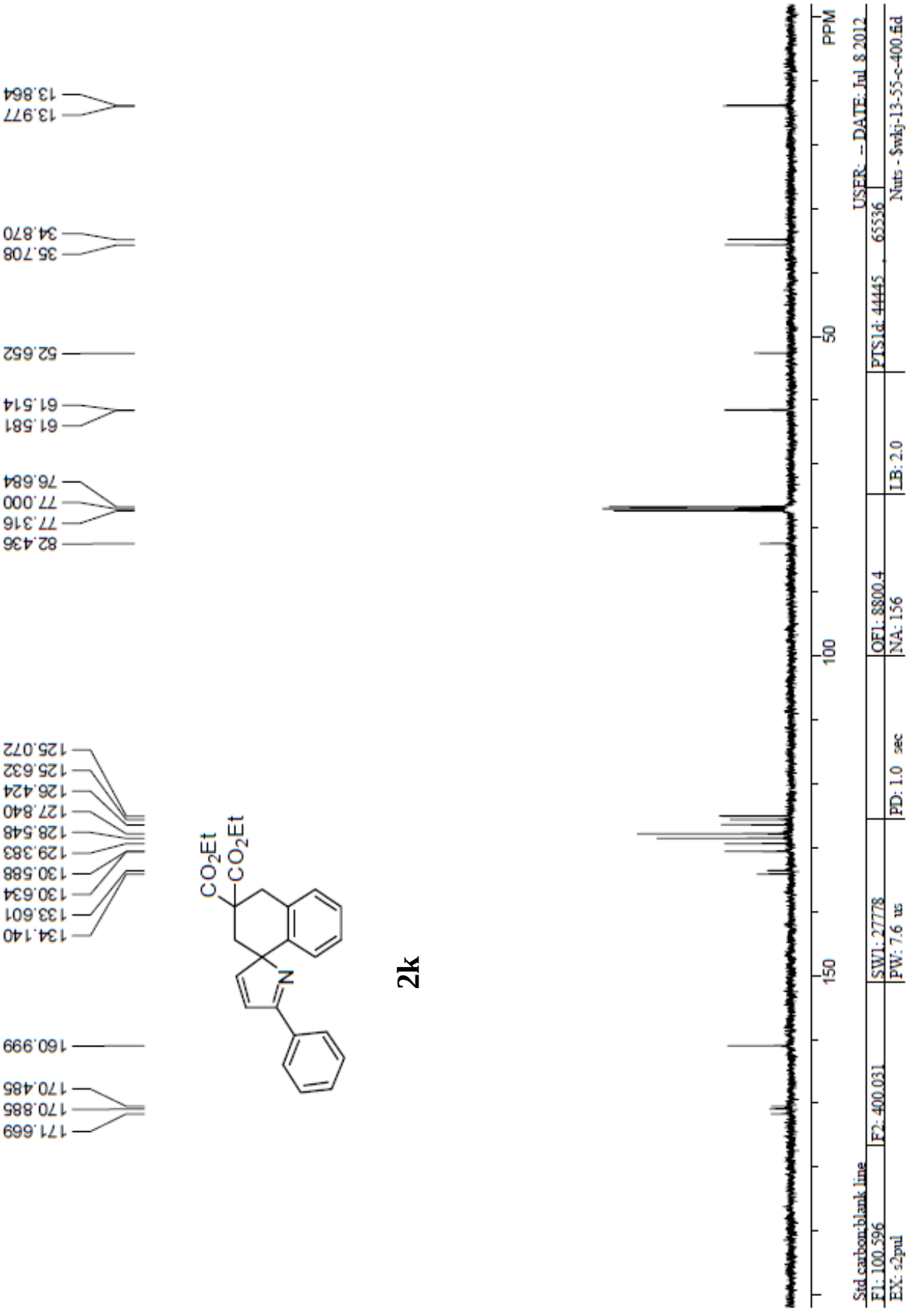

34.899
35.822
52.560
52.783
52.804
76.680
77.000
77.316
82.314
125.434
125.674
126.475
127.861
128.565
129.404
130.525
130.600
133.609
133.950
160.843
170.341
171.239
172.107
CO2Me
CO2Me
N
2j
PPM
0
50
100
150
200
Std carbon:blank line
F1: 100.596
F2: 400.031
SW1: 27778
PW: 7.6 us
PD: 1.0 sec
OF1: 8800.0
NA: 140
LB: 2.0
PTS1d: 44445 , 65536
USER: -- DATE: Jul 8 2012
EX: s2pul
Nuts - $wkj-13-54-c-400.fid

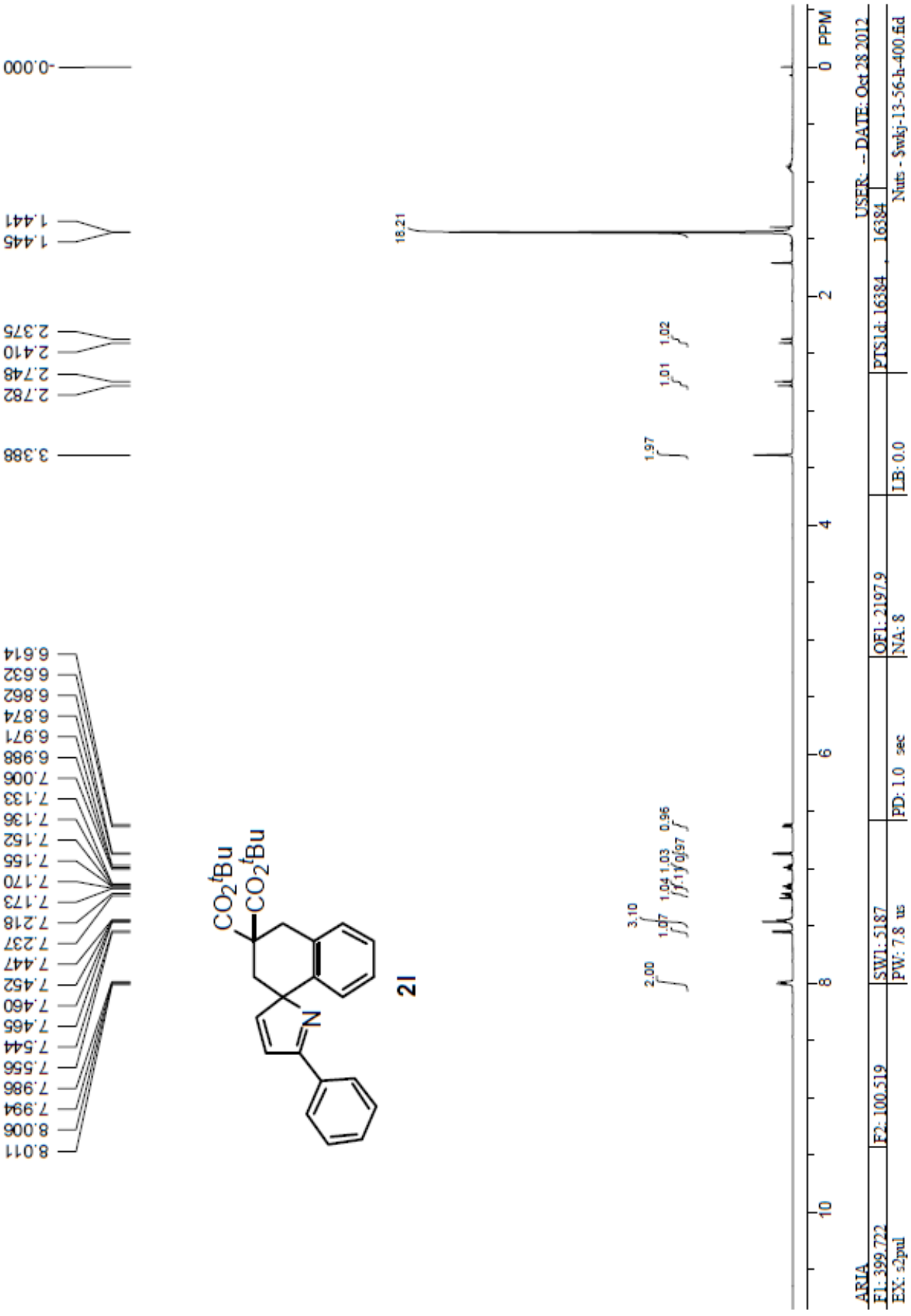

7.978
7.973
7.960
7.954
7.472
7.460
7.450
7.431
7.263
7.259
7.245
7.195
7.192
7.176
7.173
7.157
7.154
7.012
6.994
6.973
6.961
6.638
6.619
4.306
4.289
4.280
4.262
4.248
4.230
4.212
4.194
4.188
4.170
4.161
4.144
3.652
3.610
3.344
3.303
2.646
2.612
2.594
2.559
1.269
1.251
1.234
1.174
1.156
1.138
0.000

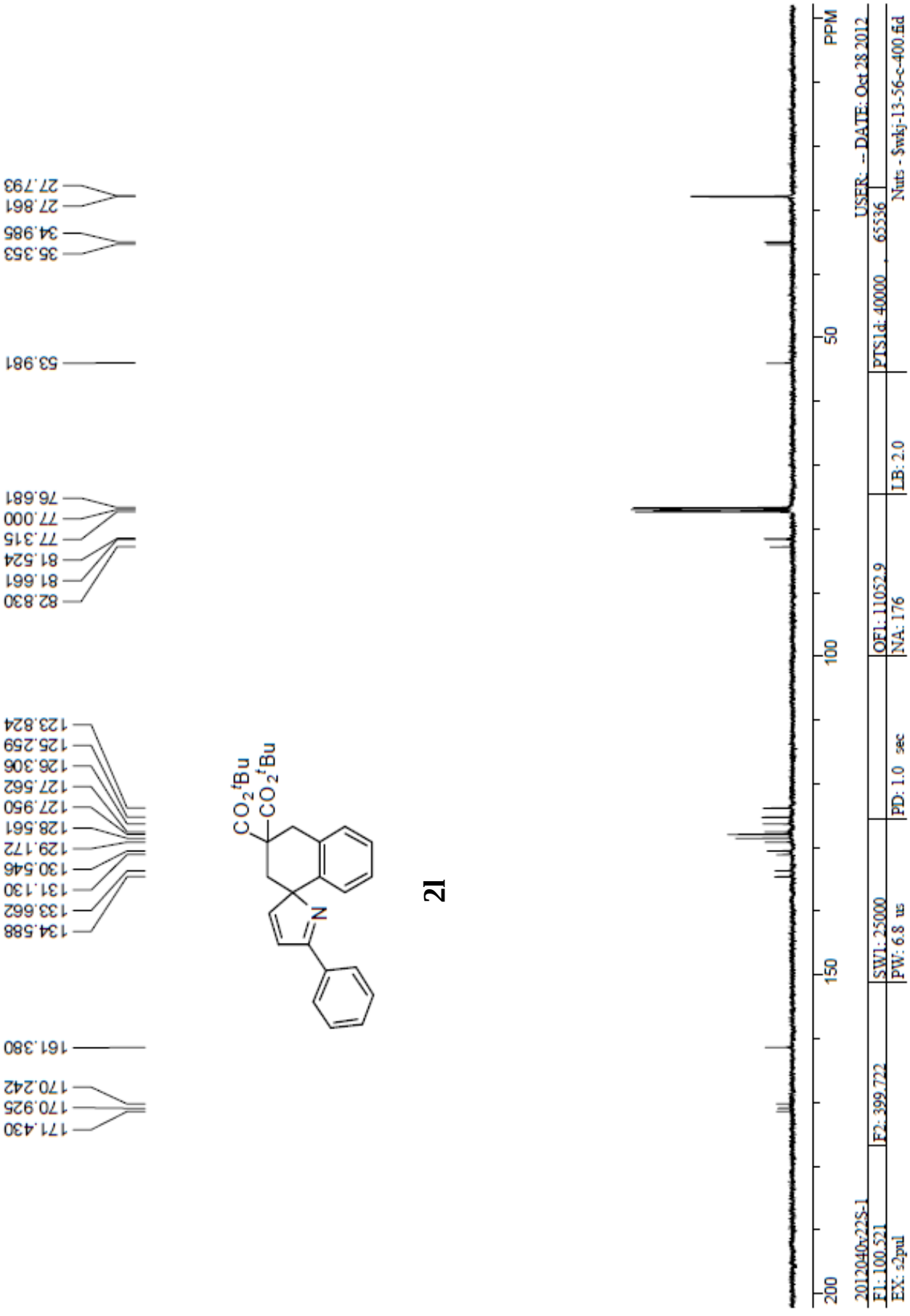

CO2Et
CO2Et
N

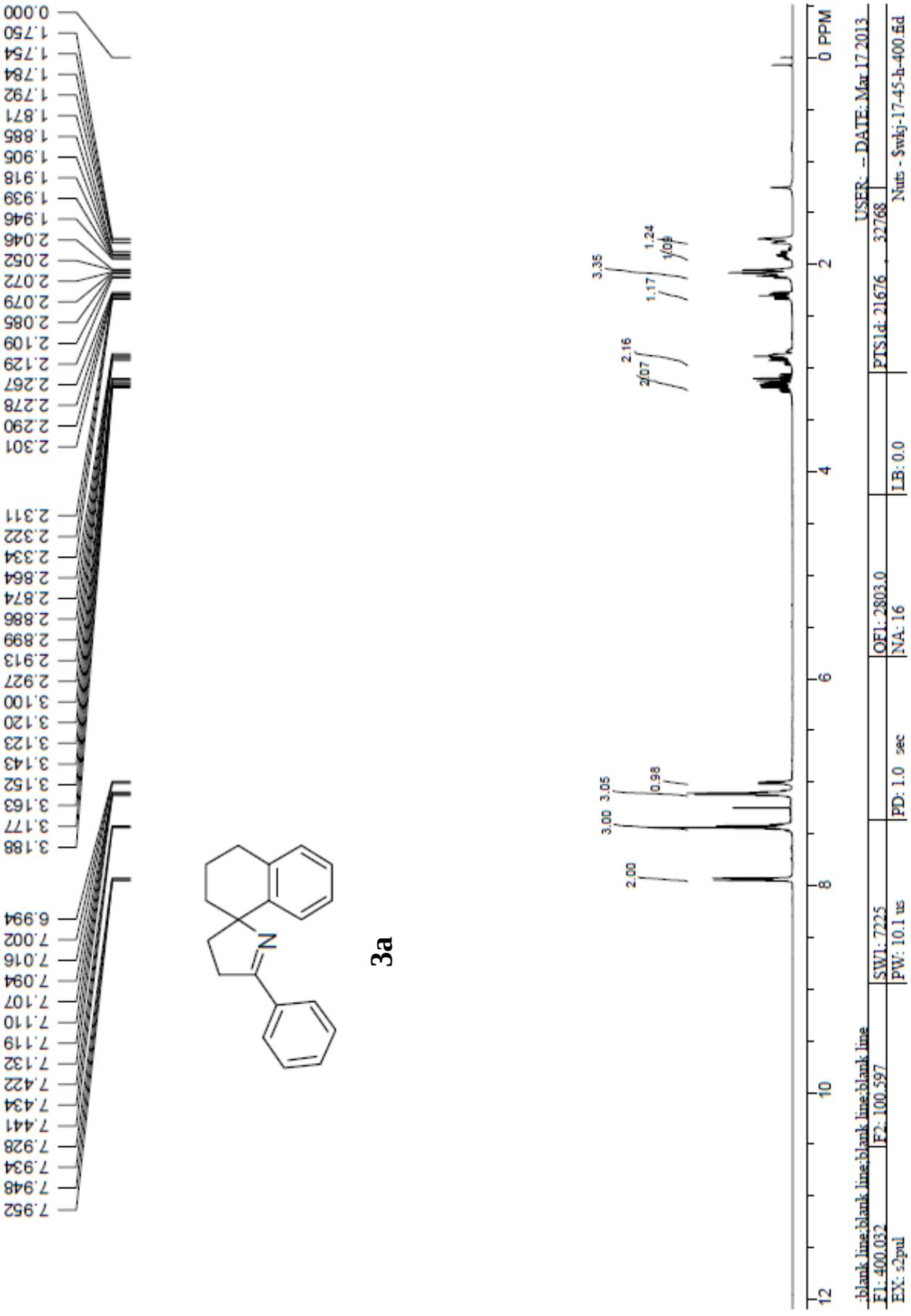
2k

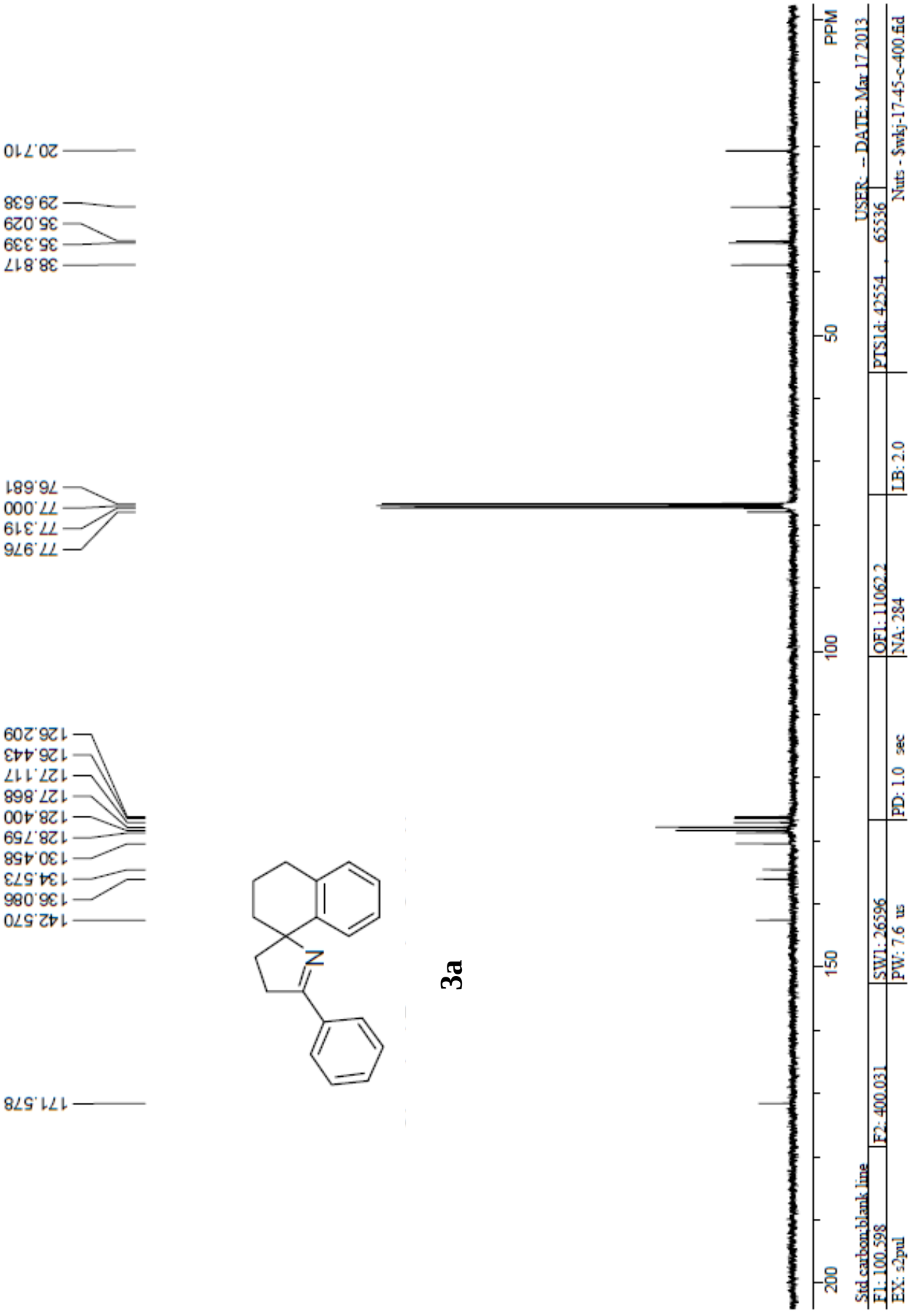

4.17
2.00
1.32
2.09
12
1.00
4.19
1.10
1.09
2.12
3.58
3.03
10
8
6
4
2
0PPM
Std proton:blank line
F1: 400.032
EX: s2pul
F2: 100.597
SW1: 7310
PW: 10.1 us
PD: 1.0 sec
OF1: 2846.7
NA: 12
LB: 0.0
PTS1d: 21929
32768
USER: -- DATE: Jul 8 2012
Nuts - $wkj-13-55-h-400.fid

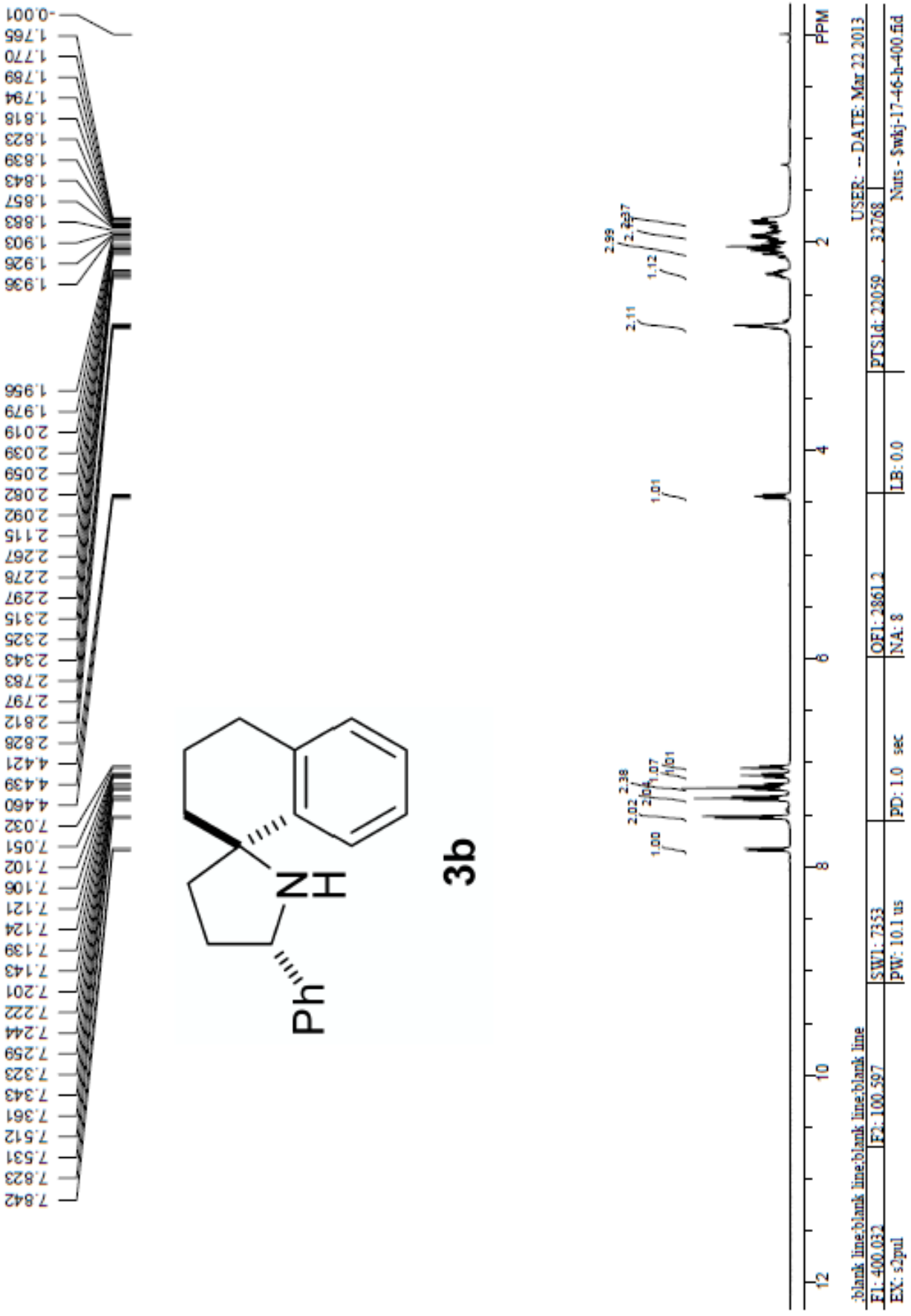

13.864
13.977
34.870
35.708
52.652
61.514
61.581
76.684
77.000
77.316
82.436
125.072
125.632
126.424
127.840
128.548
129.383
130.588
130.634
133.601
134.140
160.999
170.485
170.885
171.669
CO2Et
CO2Et
N
2k
PPM
50
100
150
Std carbon blank line
F1: 100.596
F2: 400.031
SW1: 27778
PW: 7.6 us
PD: 1.0 sec
OF1: 8800.4
NA: 156
LB: 2.0
PTS1d: 44445 , 65536
USER: -- DATE: Jul 8 2012
EX: s2pul
Nuts - $wkj-13-55-c-400.fid


0.000
1.441
1.445
2.375
2.410
2.748
2.782
3.388
6.614
6.632
6.862
6.874
6.971
6.988
7.006
7.133
7.136
7.152
7.155
7.170
7.173
7.218
7.237
7.447
7.452
7.460
7.465
7.544
7.556
7.986
7.994
8.006
8.011
CO2tBu
CO2tBu
N
2l
18.21
1.97
1.01
1.02
2.00
1.07
3.10
1.04
1.03
0.96
0 PPM
2
4
6
8
10
ARIA
F1: 399.722
F2: 100.519
SW1: 5187
PW: 7.8 us
PD: 1.0 sec
OF1: 2197.9
NA: 8
PTS1d: 16384
LB: 0.0
USER: -- DATE: Oct 28 2012
16384
Nuts - $wkj-13-56-h-400.fid
EX: s2pul


27.793
27.861
34.985
35.353
53.981
76.681
77.000
77.315
81.524
81.661
82.830
123.824
125.259
126.306
127.562
127.950
128.561
129.172
130.546
131.130
133.662
134.588
161.380
170.242
170.925
171.430
$CO_2{}^tBu$
$CO_2{}^tBu$
N
21
PPM
200
150
100
50
2012040v22S-1
F1: 100.521
EX: s2pul
F2: 399.722
SW1: 25000
PW: 6.8 us
PD: 1.0 sec
OF1: 11052.9
NA: 176
LB: 2.0
USER: -- DATE: Oct 28 2012
PTS1di: 40000 , 65536
Nuts - $wkj-13-56-c-400.fid


0.000
1.750
1.754
1.784
1.792
1.871
1.885
1.905
1.918
1.939
1.946
2.046
2.052
2.072
2.079
2.085
2.109
2.129
2.267
2.278
2.290
2.301
2.311
2.322
2.334
2.864
2.874
2.886
2.899
2.913
2.927
3.100
3.120
3.123
3.143
3.152
3.163
3.177
3.188
6.994
7.002
7.016
7.094
7.107
7.110
7.119
7.132
7.422
7.434
7.441
7.928
7.934
7.948
7.952
N
3a
3.35
1.24
1.17
2.16
2.07
3.00
3.05
0.98
2.00
0 PPM
2
4
6
8
10
12
USER: -- DATE: Mar 17 2013
blank line:blank line:blank line:blank line
F1: 400.032
F2: 100.597
SW1: 7225
PW: 10.1 us
PD: 1.0 sec
OF1: 2803.0
NA: 16
PTS1d: 21676 , 32768
LB: 0.0
EX: s2pul
Nuts - $wkj-17-45-h-400.fid


20.710
29.638
35.029
35.339
38.817
76.681
77.000
77.319
77.976
126.209
126.443
127.117
127.868
128.400
128.759
130.458
134.573
136.086
142.570
171.578
N
3a
PPM
200
150
100
50
Std carbon blank line
F1: 100.598
EX: s2pul
F2: 400.031
SW1: 26596
PW: 7.6 us
PD: 1.0 sec
OF1: 11062.2
NA: 284
LB: 2.0
PTS1d: 42554 , 65536
USER: -- DATE: Mar 17 2013
Nuts - $wkj-17-45-c-400.fid


-0.001
1.765
1.770
1.789
1.794
1.818
1.823
1.839
1.843
1.857
1.863
1.903
1.926
1.936
1.956
1.979
2.019
2.039
2.059
2.082
2.092
2.115
2.267
2.278
2.297
2.315
2.325
2.343
2.783
2.797
2.812
2.828
4.421
4.439
4.460
7.032
7.051
7.102
7.106
7.121
7.124
7.139
7.143
7.201
7.222
7.244
7.259
7.323
7.343
7.361
7.512
7.531
7.823
7.842
Ph
N
H
3b
2.99
2.97
2.11
1.12
1.01
2.38
2.02
2.07
1.00
PPM
USER: -- DATE: Mar 22 2013
blank line;blank line;blank line;blank line;blank line
F1: 400.032
F2: 100.597
SWH: 7353
PW: 10.1 us
PD: 1.0 sec
OF1: 2861.2
NA: 8
PTS1d: 22059
32768
LB: 0.0
EX: s2pul
Nuts - $wkj-17-46-h-400.fid

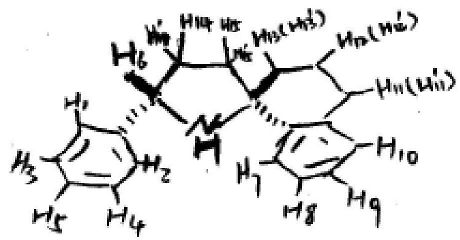

20.804
29.806
35.666
37.904
41.908
61.079
62.510
76.664
77.000
77.316
126.101
126.172
126.663
126.800
127.418
128.295
128.500
136.735
145.004
145.034
Ph
N
H
3b
200
150
100
50
PPM
Std carbon:blank line
F1: 100.598
F2: 400.031
SWH: 24510
PW: 7.6 us
PD: 1.0 sec
OF1: 10561.2
NA: 520
LB: 2.0
EX: s2pul
USER: -- DATE: Mar 22 2013
PTS1d: 39216 . 65536
Nuts - $wkj-17-46-c-400.fid

Archive directory: /export/home/omc/vnmrsys/data
Sample directory: wkj-17-46-thi-cosy_18Apr2013

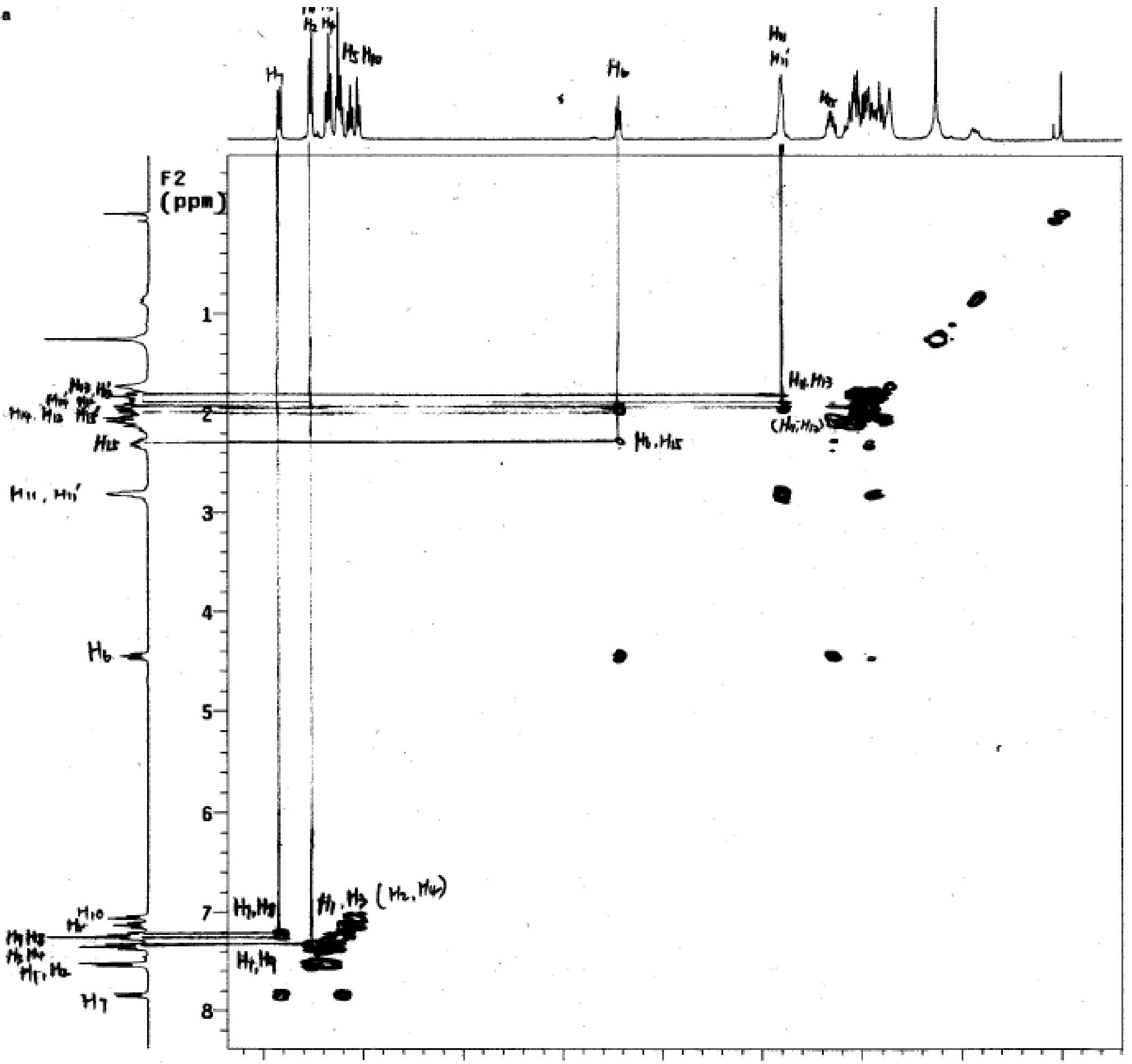
Pulse Sequence: gCOSY

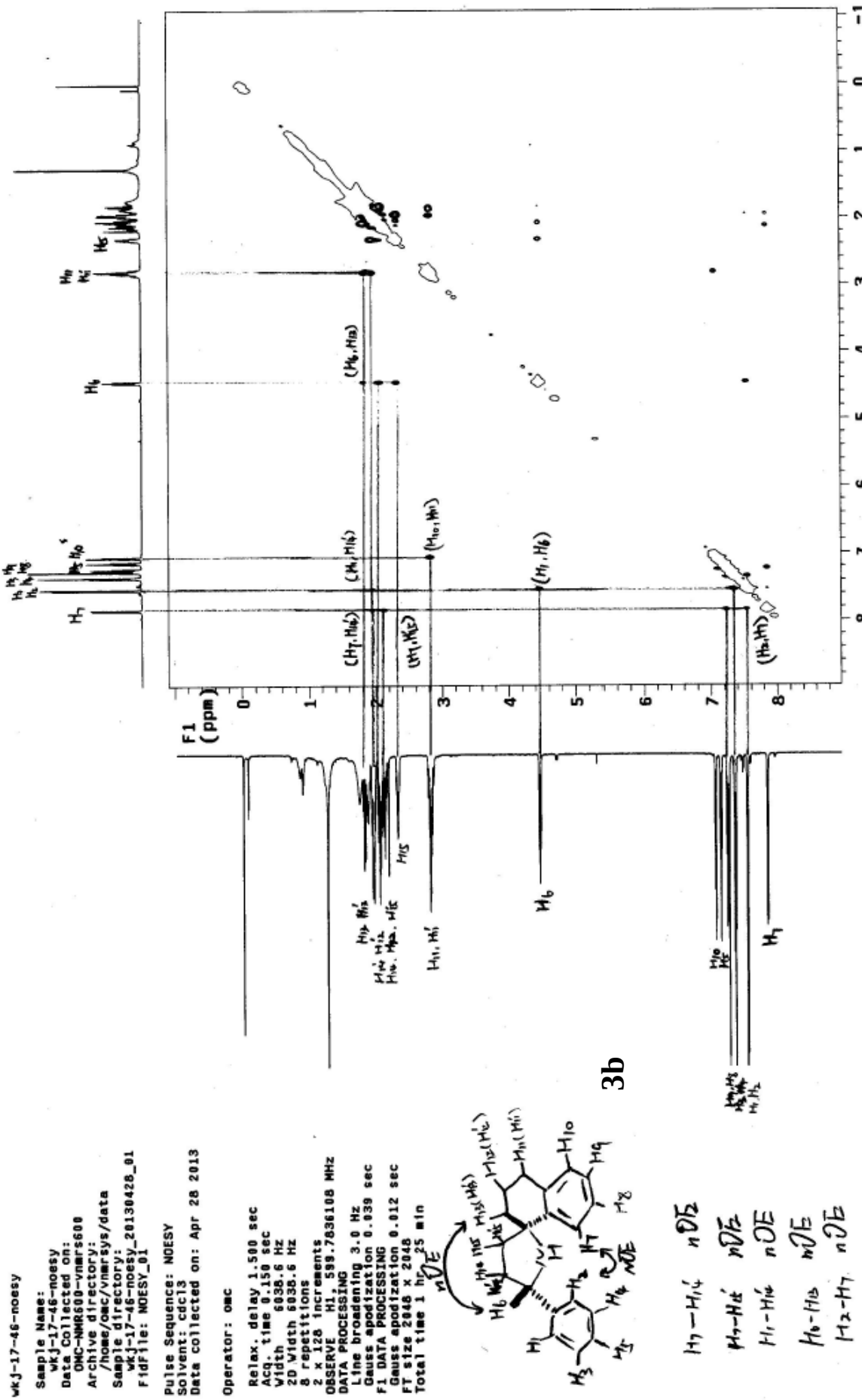
Operator: omc1
VNMRS-400 "Agilent-NMR"

Relax. delay 1.000 sec
Acq. time 0.142 sec
Width 3597.1 Hz
2D Width 3597.1 Hz
2 repetitions
128 increments
OBSERVE H1, 300.0268169 MHz
DATA PROCESSING
Sq. sine bell 0.071 sec
F1 DATA PROCESSING
Sq. sine bell 0.036 sec
FT size 1024 x 1024
Total time 5 min 16 sec



3b




wkj-17-46-noesy
Sample Name:
wkj-17-46-noesy
Data Collected on:
DMC-NMR600-vnmrs600
Archive directory:
/home/omc/vnmrsys/data
Sample directory:
wkj-17-46-noesy_20130428_01
FidFile: NOESY_01
Pulse Sequence: NOESY
Solvent: cdcl3
Data collected on: Apr 28 2013
Operator: omc
Relax. delay 1.500 sec
Acq. time 0.150 sec
Width 6038.6 Hz
2D Width 6038.6 Hz
8 repetitions
2 x 128 increments
OBSERVE H1, 599.7836108 MHz
DATA PROCESSING
Line broadening 3.0 Hz
Gauss apodization 0.039 sec
F1 DATA PROCESSING
Gauss apodization 0.012 sec
FT size 2048 x 2048
Total time 1 hr 25 min
F1 (ppm)
3b
H7-H14 nOE
H9-H8' nOE
H1-H14 nOE
H6-H5 nOE
H12-H7 nOE