Electronic Supplementary Material (ESI) for Chemical Communications.


# *Supporting Information*

## Sulfonamides-directed Gold-catalyzed [2+2+2]-Cycloadditions of Nitriles with Two Discrete Ynamides to Construct 2,4-Diaminopyridine cores

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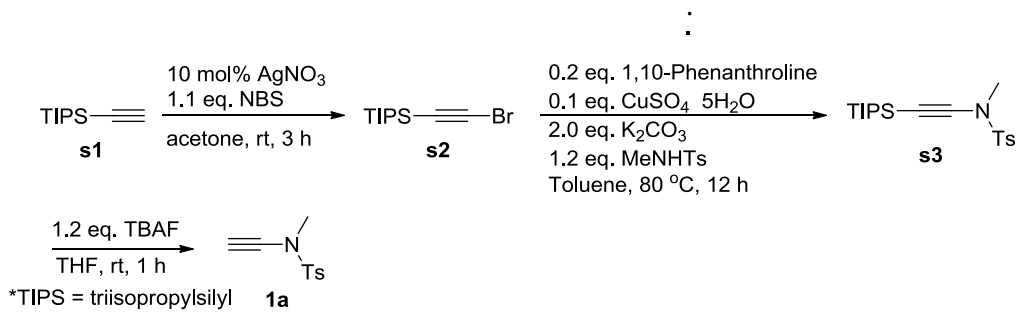
## (I) Representative Synthetic Procedures:

### (a) General procedure:

Unless otherwise noted, all the reactions for the preparation of the substrates were performed in oven-dried glassware under nitrogen atmosphere with freshly distilled solvents. The catalytic reactions were performed under Nitrogen atmosphere. DCE, DCM and $CH_3CN$ were distilled from $CaH_2$ under nitrogen. THF were distilled from Na metal under nitrogen. All other commercial reagents were used without further purification, unless otherwise indicated. Reactions were magnetically stirred and monitored by thin layer chromatography carried out on 0.25 mm E. Merck silica gel plate (60f- 254) using UV light as visualizing agents and alkaline $KMnO_4$ and heat as developing agents. $^1H$ NMR and $^{13}C$ NMR spectra were recorded on a Varian 400 MHz, Bruker 400, Bruker 500 and 600 MHz Spectrometers using chloroform-*d* ($CDCl_3$), Dimethyl sulfoxide-*d* (DMSO) and Acetone-$d^6$ as the internal standards.

### (b) Preparation of ynamide (1a).




### Synthesis of 1-(2-bromoethynyl)triisopropylsilane (s2).

To a solution of triisopropylsilyl acetylene (**s1**) (500 mg, 2.74 mmol) in acetone (50 mL) was added NBS (536 mg, 3.01 mmol) and $AgNO_3$ (46.5 mg, 0.274 mmol) the resulting mixture was stirred under nitrogen for 3 h at room temperature. After removing excess acetone, the reaction was quenched with water, and the organic layer was extracted with pentane (30 mL×3), organic layer was dried over MgSO4, and concentrated under reduced pressure to obtain pure colorless oil of 1-(2-bromoethynyl)triisopropylsilane (**s2**) (637 mg, 89%).

**Synthesis of *N*,4-dimethyl-*N*- ((triisopropylsilyl)ethynyl)benzenesulfonamide (s3).**

To a dried flask was added *N*,4-dimethylbenzenesulfonamide (680 mg, 3.67 mmol), $CuSO_4 \cdot 5H_2O$ (76.4 mg, 0.306 mmol), 1,10-phenanthroline (110 mg, 0.612 mmol) and $K_2CO_3$ (846 mg, 6.12 mmol); this mixture was subsequently treated with anhydrous toluene (3 mL) and (bromoethynyl)triisopropylsilane **(s2)** (800 mg, 3.06 mmol). The reaction mixture was caped under a blanket of nitrogen, and heated in an oil bath at 70-80 $^oC$ for 12h. After complete conversion of starting material, the reaction mixture was cooled to room temperature, filtered through Celite$^{TM}$, and concentrated in vacuo. Purification of the crude residue using silica gel flash column chromatography gave the pure ynamide **s3** as pale yellow oil (996 mg, 89%).

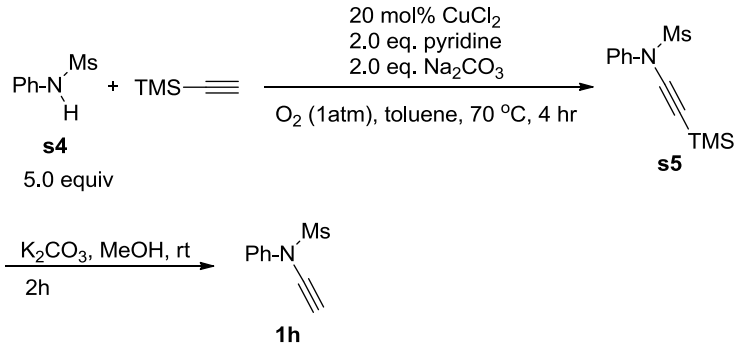
**Synthesis of *N*-ethynyl-*N*,4-dimethylbenzenesulfonamide (1a)**.

To a THF (20 mL) solution of *N*,4-dimethyl-*N*-((triisopropylsilyl) ethynyl) benzenesulfonamide **s3** (500 mg, 1.36 mmol) was added *n*-tetrabutyl ammonium fluoride (1.0 M in THF, 2.05 mL, 2.05 mmol) at 0 °C, and the resulting mixture was stirred at rt for 1h. Then reaction mixture was quenched with $H_2O$ (10 ml) and extracted with ethyl acetate (3x 30 mL), Organic layer was dried over $MgSO_4$ and concentrated under reduced pressure. Crude material was purified on a silica gel using (ethyl acetate : hexane = 3:97) to afford compound **1a** (267 mg, 94%) as a yellow solid.[s1]

The experimental procedure for the preparation of compounds **1b, 1c, 1f, 1g** is similar to **1a**.

[s1]Y. Zhang, R. P. Hsung, M. R. Tracey, K. C. M. Kurtz and E. L. Vera, *Org. Lett*., 2004, **6**, 1151-1154.

**(b) Preparation of ynamide (1h).**



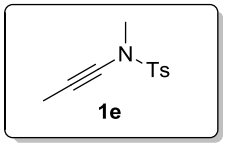
$CuCl_2$ (0.6 mmol), **s4** (15 mmol) and $Na_2CO_3$ (6 mmol) were added to a 500 mL three-necked round-bottomed flask. The reaction flask was vacuumed for 15 minute. A solution of pyridine (6 mmol) in dry toluene (15 mL) was added. A balloon filled with oxygen was connected to the flask and the stirred mixture was heated at 70℃. After 15 min, a solution of Trimethylsilylacetylene (3 mmol) in dry toluene (15 mL) was added by droping funnel over 4 h. The mixture was allowed to stir at 70℃ for another 4h and was then cooled to room temperature. The reaction mixture was filtered through a short plug of silica gel. The solution of crude was concentrated, and purified by flash chromatography (*n*-Hexane/ ethylacetate = 20:1) to give product **s5** (85%).

$K_2CO_3$ (3 equiv.) was added to a solution of the ynamide **s5** (3 mmol) in MeOH (8 mL), the resulting solution was stirred for 2 h (depend on TLC analysis) at room temperature. The reaction mixture was filtered through a short plug of silica gel. After evaporation of the solvent, the residue was purified by column chromatography on silica gel to afford the corresponding product **1h** (76%).

The experimental procedure for the preparation of compounds **1d**[s2] is similar to **1h**

[s2]L. -Q. Yang, K.-B. Wang and C.-Y. Li, *Eur. J. Org. Chem.* 2013, 2775.

**(c) *N*,4-dimethyl-*N*-(prop-1-yn-1-yl)benzenesulfonamide (1e).**

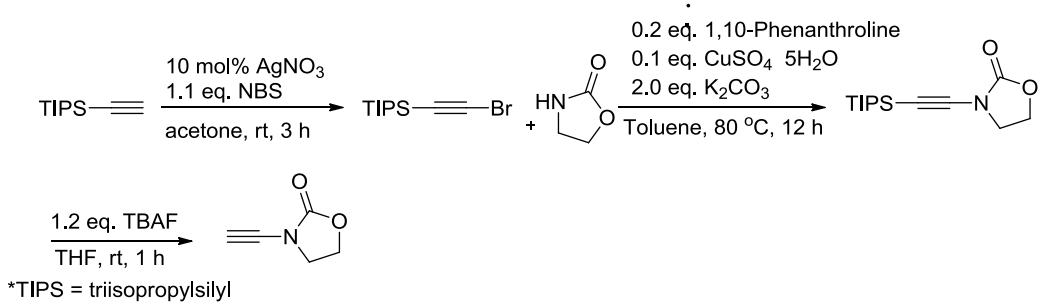


1e

Synthesized according to the reported literature procedure.[s3]

[s3] X. Y. Mak, A. L. Crombie and R. L. Danheiser, *J. Org. Chem.*, 2011, **76**, 1852.

**(d) Preparation of ynamide 3-ethynyloxazolidin-2-one (4a)**

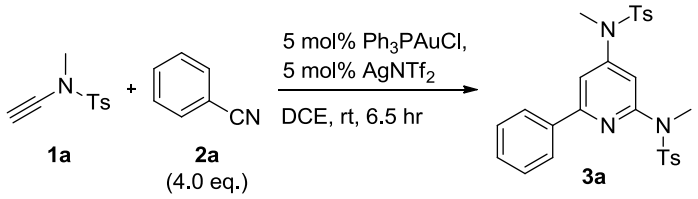



The experimental procedure for the preparation of compounds **4a** similar to **1a.**

The experimental procedure for the preparation of compounds **4b**[s4] and **4c** is similar to **4a.**

[s4]N. Riddell, K. Villeneuve and W. Tam, *Org. Lett.*, 2005, **7**, 3681.

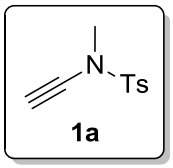
## (II) Standard procedure for gold(I) catalyzed [2+2+2]-cycloaddition reactions.




A two-necked flask was charged with chloro(triphenylphosphine)gold (I) (11.8 mg, 0.0239 mmol) and silver bis(trifluoromethanesulfonyl)imide (9.28 mg, 0.0239 mmol), and to this mixture was added dry DCE (1.0 mL). The resulting mixture was stirred at room temperature for 5 min. To this mixture was added a dry DCE solution (2 mL) of compound **1a** (100 mg, 0.478 mmol) and Benzonitrile (197 mg, 1.913 mmol). After stirring at 25 °C for 6.5 h, the reaction mixture was filtered over a short celite bed. The filtrate was concentrated under reduced pressure. The residue was eluted through a silica gel column to give the desired *N*,*N'*-(6-phenylpyridine-2,4-diyl)bis(*N*,4-dimethylbenzenesulfonamide) **3a** (92 mg, 0.177 mmol, 88 %) as white solid.

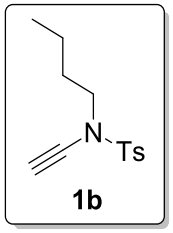
## (III) Spectral Data for Key Compounds:

***N*-ethynyl-*N*,4-dimethylbenzenesulfonamide (1a).**



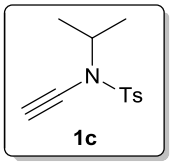

White solid; $^{1}$H NMR (500 MHz, $CDCl_3$): δ 7.78 (d, *J* = 8 Hz, 2 H), 7.35 (d, *J* = 8 Hz, 2 H), 3.04 (s, 3 H), 2.66 (s, 1 H), 2.44 (s, 3 H); $^{13}$C NMR (125 MHz, $CDCl_3$): δ 144.9, 133.1, 129.8, 127.8 77.5, 57.4, 38.8, 21.6.

***N*-butyl-*N*-ethynyl-4-methylbenzenesulfonamide (1b).**



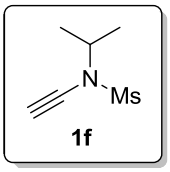

White solid; $^{1}$H NMR (500 MHz, $CDCl_3$): δ 7.76 (d, *J* = 8 Hz, 2 H), 7.32 (d, *J* = 8 Hz, 2 H), 3.26 (t, *J* = 7.3 Hz, 2 H), 2.70 (s, 1 H), 2.41 (s, 3 H), 1.62 ~ 1.56 (m, 2 H), 1.34 ~ 1.27 (m, 2 H), 0.87 (t, *J* = 7.3 Hz, 3 H); $^{13}$C NMR (125 MHz, $CDCl_3$): δ 144.6, 134.5, 129.7, 127.5, 76.0, 58.9, 50.8, 29.6, 21.6, 19.3, 13.4.

***N*-ethynyl-*N*-isopropyl-4-methylbenzenesulfonamide** (**1c**).



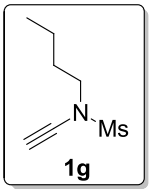

White solid; $^{1}$H NMR (600 MHz, $CDCl_3$): δ 7.79 (d, *J* = 8.4 Hz, 2 H), 7.32 (d, *J* = 7.8 Hz, 2 H), 4.14 ~ 4.08 (m, 1 H), 2.78 (s, 1 H), 2.43 (s, 3 H), 1.09 (d, *J* = 6 Hz, 6 H); $^{13}$C NMR (150 MHz, $CDCl_3$): δ 144.5, 135.9, 129.8, 127.4, 73.0, 61.0, 52.1, 21.6, 20.5.

***N*-ethynyl-*N*-isopropylmethanesulfonamide (1f).**



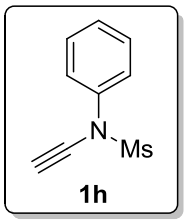

White solid; $^{1}$H NMR (600 MHz, $CDCl_3$): δ 4.20 ~ 4.14 (m, 1 H), 3.07 (s, 3 H), 2.85 (s, 1 H), 1.29 (d, *J* = 6.6 Hz, 6 H); $^{13}$C NMR (150 MHz, $CDCl_3$): δ 72.5, 61.8, 52.0, 39.4, 20.9; HRMS calcd. for $C_6H_{11}NO_2S$: 161.0510; found: 161.0507.

***N*-butyl-*N*-ethynylmethanesulfonamide (1g).**



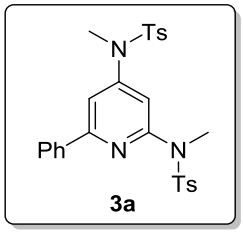

Yelliw oil; $^{1}$H NMR (600 MHz, $CDCl_3$): δ 3.41 (t, *J* = 7.2 Hz, 2 H), 3.05 (s, 3 H), 2.78 (s, 1 H), 1.71 ~ 1.66 (m, 2 H), 1.40 ~ 1.34 (m, 2 H), 0.92 (t, *J* = 7.5 Hz, 3 H); $^{13}$C NMR (150 MHz, $CDCl_3$): δ 75.5, 59.5, 50.9, 38.0, 30.0, 19.3, 13.4.

***N*-ethynyl-*N*-phenylmethanesulfonamide (1h)**



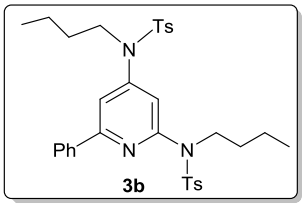

Yellow oil; $^{1}$H NMR (400 MHz, $CDCl_3$): δ 7.51 ~ 7.49 (m, 2 H), 7.44 ~ 7.40 (m, 2 H), 7.37 ~ 7.33 (m, 1 H), 3.10 (s, 3 H), 2.94 (d, *J* = 0.4 Hz, 1 H); $^{13}$C NMR (150 MHz, $CDCl_3$): δ 144.1, 129.5, 128.6, 125.6, 75.8, 59.7, 36.7.

***N*,*N*'-(6-phenylpyridine-2,4-diyl)bis(*N*,4-dimethylbenzenesulfonamide) (3a)**



White solid; $^{1}$H NMR (500 MHz, $CDCl_3$): δ 7.78 ~ 7.77 (m, 2 H), 7.66 (d, *J* = 1.5 Hz, 1 H), 7.54 (d, *J* = 8.5 Hz, 2 H), 7.45 (d, *J* = 8 Hz, 2 H), 7.39 ~ 7.37 (m, 3 H), 7. 27 ~ 7.25 (m, 3 H), 7.19 (d, *J* = 8.5 Hz, 2 H), 3.31 (s, 3 H), 3.28 (s, 3 H), 2.39 (s, 3 H), 2.37 (s, 3 H); $^{13}$C NMR (125 MHz, $CDCl_3$): δ 155.9, 154.1, 151.0, 144.4, 143.9, 138.1, 134.3, 133.7, 129.8, 129.5, 129.4, 128.6, 127.5 (x 2), 126.8, 113.1, 111.3, 36.9, 35.6, 21.6, 21.5; ESI-MS calcd. for $C_{27}H_{27}N_3O_4S_2$: 521.1443; found: 521.1441.

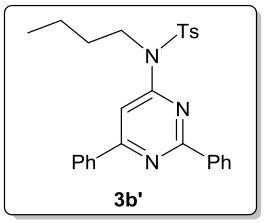
***N, N'*-(6-phenylpyridine-2,4-diyl)bis(*N*-butyl-4-methylbenzenesulfonamide) (3b).**



**3b**

White solid; $^{1}$H NMR (500 MHz, $CDCl_3$): δ 7.77 ~ 7.75 (m, 2 H), 7.67 (d, *J* = 1.5 Hz, 1 H), 7.49 (d, *J* = 8.5 Hz, 2 H), 7.44 (d, *J* = 8 Hz, 2 H), 7.39 ~ 7.38 (m, 3 H), 7.25 (d, *J* = 8 Hz, 2 H), 7.19 (d, *J* = 8 Hz, 2 H), 6.99 (d, *J* = 1.0 Hz, 1 H), 3.80 (t, *J* = 7 Hz, 2 H), 3.61 (t, *J* = 7 Hz, 2 H) , 2.39 (s, 3 H), 2.36 (s, 3 H), 1.51 ~ 1.41 (m, 4 H), 1.38 ~ 1.24 (m, 4 H), 0.88 ~ 0.84 (m, 6 H); $^{13}$C NMR (125 MHz, $CDCl_3$): δ 156.3, 152.9, 149.3, 144.1, 143.5, 137.9, 135.5, 134.6, 129.7, 129.5, 129.4, 128.6, 127.5, 127.4, 126.8, 117.6, 116.7, 48.8, 47.8, 30.5, 29.9, 21.6, 21.5, 19.8, 19.6, 13.7, 13.5; ESI-MS calcd. for $C_{33}H_{39}N_3O_4S_2$: 605.2382; found: 605.2385.

***N*-butyl-*N*-(2, 6-diphenylpyrimidin-4-yl)-4-methylbenzenesulfonamide (3b')**

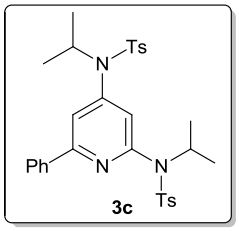


**3b'**

White solid; $^{1}$H NMR (500 MHz, $CDCl_3$): δ 8.45 ~ 8.43 (m, 2 H), 8.17 ~ 8.15 (m, 2 H), 7.93 (s, 1 H), 7.69 (d, *J* = 8.5 Hz, 2 H), 7.52 ~ 7.51 (m, 3 H), 7.47 ~ 7.46 (m, 3 H), 7.23 (d, *J* = 8.5 Hz, 2 H), 4.21 (t, *J* = 7.5 Hz, 2 H), 2.35 (s, 3 H), 1.82 ~ 1.76 (m, 2 H), 1.50 ~ 1.42 (m, 2 H), 0.96 (t, *J* = 7.5 Hz, 3 H); $^{13}$C NMR (125 MHz, $CDCl_3$): δ 164.8, 163.6, 159.8, 144.3, 137.6, 137.2, 136.2,

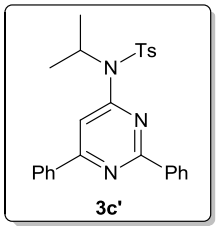
130.8 (x 2), 129.8, 128.9, 128.4, 128.2, 127.3, 127.1, 106.1, 47.2, 31.1, 21.5, 20.1, 13.8; ESI-MS calcd. for $C_{27}H_{27}N_3O_2S$: 457.1824; found: 457.1821.

**_N_,_N_'-(6-phenylpyridine-2,4-diyl)bis(_N_-isopropyl-4-methylbenzenesulfonamide) (3c)**



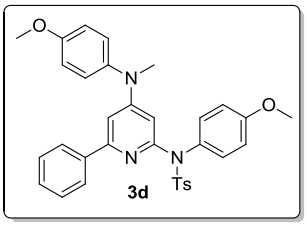

White solid; $^1$H NMR (600 MHz, $CDCl_3$): δ 7.84 ~ 7.82 (m, 2 H), 7.71 (d, *J* = 8 Hz, 2 H), 7.64 (d, *J* = 8 Hz, 2 H), 7.59 (d, *J* = 1.2 Hz, 1 H), 7.43 ~ 7.41 (m, 3 H), 7.28 ~ 7.22 (m, 4 H), 6.86 (d, *J* = 1.6 Hz, 1 H), 4.67 ~ 4.57 (m, 1 H), 4.48 ~ 4.38 (m, 1 H), 2.42 (s, 3 H), 2.41 (s, 3 H), 1.13 ~ 1.10 (m, 12 H); $^{13}$C NMR (150 MHz, $CDCl_3$): δ 157.1, 151.6, 146.3, 143.7, 143.2, 138.4, 137.8, 137.6, 129.8, 129.7, 129.3, 128.7, 127.9, 127.4, 126.9, 126.8, 122.9, 52.3, 52.1, 22.2, 21.9, 21.5 (one carbon merge with others); ESI-MS calcd. for $C_{31}H_{35}N_3O_4S_2$: 577.2069; found: 577.2071.

**_N_-(2,6-diphenylpyrimidin-4-yl)-_N_-isopropyl-4-methylbenzenesulfonamide (3c')**




White solid; $^1$H NMR (600 MHz, $CDCl_3$): δ 8.45 ~ 8.44 (m, 2 H), 8.17 ~ 8.15 (m, 2 H), 7.79 (d, *J* = 8.4 Hz, 2 H), 7.74 (s, 1 H), 7.52 ~ 7.47 (m, 6 H), 7.27 ~ 7.26 (m, 2 H), 4.80 ~ 4.74 (m, 1 H), 2.39 (s, 3 H), 1.47 (d, *J* = 6.6 Hz, 6 H); $^{13}$C NMR (150 MHz, $CDCl_3$): δ 165.2, 163.9, 160.4, 143.9, 137.8, 137.6, 137.0, 131.0, 130.8, 129.7, 128.9, 128.5, 128.3, 127.6, 127.4, 111.0, 53.2, 21.9, 21.6; ESI-MS calcd. for $C_{26}H_{25}N_3O_4S$: 443.1667; found: 443.1667.

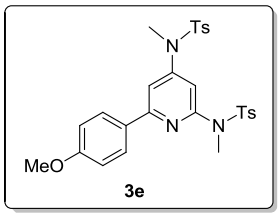
**_N_-(4-methoxyphenyl)-_N_-(4-((4-methoxyphenyl)(methyl)amino)-6-phenylpyridin-2-yl)-4-methylbenzenesulfonamide (3d)**



3d

Viscous oil; $^{1}$H NMR (400 MHz, $CDCl_3$): δ 7.77 (d, *J* = 8.0 Hz, 2 H), 7.63 ~ 7.62 (m, 2 H), 7.43 (d, *J* = 8.4 Hz, 2 H), 7.36 ~ 7.35 (m, 3 H), 7.23 ~ 7.14 (m, 6 H), 7.05 ~ 7.02 (m, 3 H), 6.92 (d, *J* = 8.4 Hz, 2 H), 6.85 (d, *J* = 8.8 Hz, 2 H), 6.63 (s, 1 H), 3.85 (s, 3 H), 3.82 (s, 3 H), 2.39 (s, 3 H), 2.36 (s, 3 H); $^{13}$C NMR (100 MHz, $CDCl_3$): δ 159.9, 159.7, 156.5, 155.6, 151.6, 144.4, 143.4, 138.6, 137.5, 136.3, 131.8, 131.6, 131.4, 131.1, 129.8, 129.1, 129.0, 128.7, 128.4, 127.8, 127.2, 114.9, 114.6, 109.4, 107.3, 55.5, 21.6, 21.6 (one carbon merge with others); EI-MS calcd. for $C_{39}H_{35}N_3O_6S_2$: 705.1967; found: 705.1964.

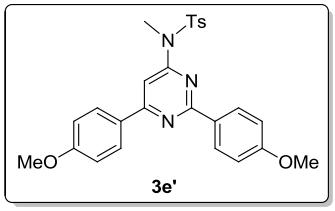
***N*,*N*'-(6-(4-methoxyphenyl)pyridine-2,4-diyl)bis(*N*,4-dimethylbenzenesulfonamide) (3e).**



3e

White solid; $^{1}$H NMR (600 MHz, $CDCl_3$): δ 7.73 (d, *J* = 9 Hz, 2 H), 7.58 (d, *J* = 1.8 Hz, 1 H), 7.54 (d, *J* = 8.4 Hz, 2 H), 7.46 (d, *J* = 8.4 Hz, 2 H), 7.25 (d, *J* = 7.8 Hz, 2 H), 7. 20 ~ 7.18 (m, 3 H), 6.89 (d, *J* = 8.4 Hz, 2 H), 3.82 (s, 3 H), 3.30 (s, 3 H), 3.26 (s, 3 H), 2.39 (s, 3 H), 2.36 (s, 3 H); $^{13}$C NMR (150 MHz, $CDCl_3$): δ 160.8, 155.7, 154.0, 151.0, 144.3, 143.8, 134.5, 133.8, 130.8, 129.8, 129.5, 128.2, 127.5 (x 2), 114.0,112.3, 110.6, 55.4, 36.9, 35.5, 21.6, 21.5; ESI-MS calcd. for $C_{28}H_{29}N_3O_5S_2$: 551.1549; found: 551.1549.

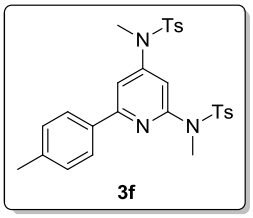
***N*-(2,6-bis(4-methoxyphenyl)pyrimidin-4-yl)-*N*,4-dimethylbenzenesulfonamide (3e')**



3e'

White solid; $^{1}$H NMR (600 MHz, $CDCl_3$): δ 8.38 (d, *J* = 9 Hz, 2 H), 8.16 (d, *J* = 8.4 Hz, 2 H), 7.92 (s, 1 H), 7.67 (d, *J* = 8.4 Hz, 2 H), 7. 23 ~ 7.22 (m, 2 H), 7.02 (d, *J* = 9 Hz, 2 H), 6.94 (d, *J* = 9 Hz, 2 H), 3.88 (s, 3 H), 3.85 (s, 3 H), 3.55 (s, 3 H), 2.34 (s, 3 H); $^{13}$C NMR (150 MHz, $CDCl_3$): δ 164.2, 163.3, 161.9, 161.9, 160.4, 144.4, 135.4, 130.5, 129.9, 129.8, 128.9, 127.2, 114.2, 113.7, 103.8, 55.4, 55.4, 34.5, 21.5, one carbon merge with others; ESI-MS calcd. for $C_{26}H_{25}N_3O_4S$: 475.1566; found: 475.1567.

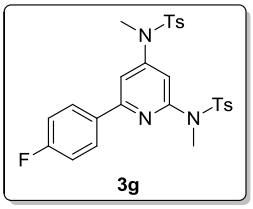
***N, N'*-(6-(p-tolyl) pyridine-2, 4-diyl)bis(*N*,4-dimethylbenzenesulfonamide) (3f)**



**3f**

White solid; $^{1}$H NMR (500 MHz, $CDCl_3$): δ 7.67 (d, *J* = 8 Hz, 2 H), 7.62 (s, 1 H), 7.54 (d, *J* = 8 Hz, 2 H), 7.46 (d, *J* = 8 Hz, 2 H), 7.25 (d, *J* = 8.5 Hz, 3 H), 7. 20 ~ 7.17 (m, 4 H), 3.30 (s, 3 H), 3.27 (s, 3 H), 2.39 (s, 3 H), 2.36 (s, 6 H); $^{13}$C NMR (125 MHz, $CDCl_3$): δ 156.0, 154.0, 151.0, 144.4, 143.8, 139.5, 135.3, 134.3, 133.7, 129.8, 129.5, 129.3, 127.5 (x 2), 126.7, 112.8, 111.1, 36.9, 35.5, 21.6, 21.5, 21.3; ESI-MS calcd. for $C_{28}H_{29}ClN_3O_4S_2$: 535.1599; found: 535.1602.

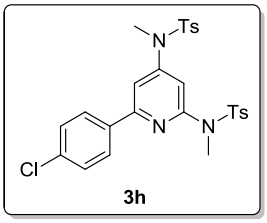
***N*,*N*'-(6-(4-fluorophenyl)pyridine-2,4-diyl)bis(*N*,4-dimethylbenzenesulfonamide) (3g)**



**3g**

White solid; $^{1}$H NMR (600 MHz, $CDCl_3$): δ 7. 78 ~ 7.75 (m, 2 H), 7.63 (d, *J* = 1.8 Hz, 1 H), 7. 55 ~ 7.54 (m, 2 H), 7. 46 ~ 7.45 (m, 2 H), 7. 27 ~ 7.26 (m, 2 H), 7.24 (d, *J* = 1.8 Hz, 1 H), 7.20 ~ 7.19 (m, 2 H), 7. 07 ~ 7.04 (m, 2 H), 3.30 (s, 3 H), 3.27 (s, 3 H), 2.40 (s, 3 H), 2.37 (s, 3 H); $^{13}$C NMR (150 MHz, $CDCl_3$): δ 163.7 (d, *J* = 247.5 Hz), 155.0, 154.2, 151.2, 144.5, 143.9, 134.6, 134.3, 133.9, 129.8, 129.5, 128.7 (d, *J* = 9 Hz), 127.5, 127.5, 115.6 (d, *J* = 22.5 Hz), 112.8, 111.0, 36.9, 35.5, 21.6, 21.5; ESI-MS calcd. for $C_{27}H_{26}FN_3O_4S_2$: 539.1349; found: 539.1350.

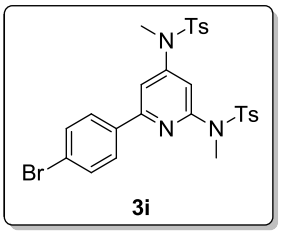
***N*,*N*'-(6-(4-chlorophenyl)pyridine-2,4-diyl)bis(*N*,4-dimethylbenzenesulfonamide) (3h)**



**3h**

White solid; $^{1}$H NMR (500 MHz, $CDCl_3$): δ 7.71 (d, *J* = 8.5 Hz, 2 H), 7.65 (d, *J* = 1 Hz, 1 H), 7.54 (d, *J* = 8.5 Hz, 2 H), 7.45 (d, *J* = 8 Hz, 2 H), 7.34 (d, *J* = 8.5 Hz, 2 H), 7. 27 ~ 7.25 (m, 3 H), 7.19 (d, *J* = 8.5 Hz, 2 H), 3.30 (s, 3 H), 3.27 (s, 3 H), 2.40 (s, 3 H), 2.37 (s, 3 H); $^{13}$C NMR (125 MHz, $CDCl_3$): δ 154.7, 154.2, 151.2, 144.5, 144.0, 136.5, 135.5, 134.3, 133.6, 129.9, 129.5, 128.8, 128.1, 127.5 (x 2), 113.0, 111.3, 36.8, 35.5, 21.6 (x 2); ESI-MS calcd. for $C_{27}H_{26}ClN_3O_4S_2$: 555.1053; found: 555.1055.

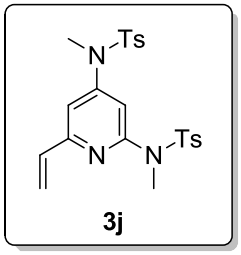
***N*,*N*'-(6-(4-bromophenyl)pyridine-2,4-diyl)bis(*N*,4-dimethylbenzenesulfonamide) (3i)**



**3i**

White solid; $^{1}$H NMR (500 MHz, $CDCl_3$): δ 7. 64 ~ 7.62 (m, 3 H), 7.52 (d, *J* = 8 Hz, 2 H), 7.48 (d, *J* = 8.5 Hz, 2 H), 7.43 (d, *J* = 8.5 Hz, 2 H), 7. 26 ~ 7.22 (m, 3 H), 7.18 (d, *J* = 8 Hz, 2 H), 3.28 (s, 3 H), 3.25 (s, 3 H), 2.38 (s, 3 H), 2.35 (s, 3 H); $^{13}$C NMR (125 MHz, $CDCl_3$): δ 154.7, 154.2, 151.2, 144.5, 144.0, 137.0, 134.3, 133.6, 131.8, 129.9, 129.5, 128.4, 127.5, 127.5, 123.9, 112.9, 111.4, 36.8, 35.5, 21.6, 21.6; ESI-MS calcd. for $C_{27}H_{26}BrN_3O_4S_2$: 599.0548; found: 599.0547.

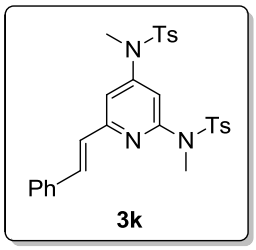
***N*,*N*'-(6-vinylpyridine-2,4-diyl)bis(*N*,4-dimethylbenzenesulfonamide) (3j)**




**3j**

White solid; $^{1}$H NMR (500 MHz, $CDCl_3$): δ 7.52 (d, *J* = 8 Hz, 2 H), 7.45 (d, *J* = 8 Hz, 2 H), 7. 26 ~ 7.19 (m, 5 H), 7.15 (d, *J* = 1.5 Hz, 1 H), 6.60 ~ 6.55 (m, 1 H), 6.05 ~ 6.01 (m, 1 H), 5.36 (d, *J* = 11 Hz, 1 H), 3.24 (s, 3 H), 3.22 (s, 3 H), 2.39 (s, 3 H), 2.38 (s, 3 H); $^{13}$C NMR (125 MHz, $CDCl_3$): δ 154.4, 154.0, 150.7, 144.4, 143.9, 135.8, 134.5, 133.7, 129.8, 129.5, 127.5 (x 2), 119.1, 114.4, 111.5, 36.8, 35.4, 21.6 (x 2); ESI-MS calcd. for $C_{23}H_{25}BrN_3O_4S_2$: 471.1286; found: 471.1287.

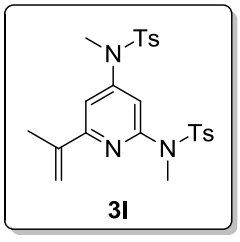
**(E)-*N*,*N*'-(6-styrylpyridine-2,4-diyl)bis(*N*,4-dimethylbenzenesulfonamide) (3k)**




**3k**

White solid; $^{1}$H NMR (600 MHz, $CDCl_3$): δ 7.54 (d, *J* = 8.4 Hz, 2 H), 7. 49 ~ 7.46 (m, 4 H), 7.38 ~ 7.33 (m, 3 H), 7.29 ~ 7.25 (m, 3 H), 7.23 ~ 7.19 (m, 4 H), 6.94 (d, *J* = 15.6 Hz, 1 H), 3.30 (s, 3 H), 3.24 (s, 3 H), 2.39 (s, 3 H), 2.37 (s, 3 H); $^{13}$C NMR (150 MHz, $CDCl_3$): δ 154.5, 154.2, 150.8, 144.4, 143.8, 136.3, 134.7, 133.9, 133.7, 129.8, 129.5, 128.7, 128.6, 127.6, 127.5, 127.1 (x 2), 115.0, 111.1, 36.8, 35.5, 21.6, 21.5; HRMS calcd. for $C_{29}H_{29}N_3O_4S_2$: 547.1599; found: 547.1601.

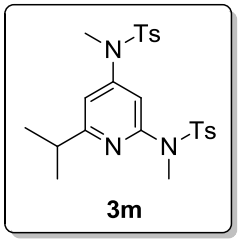
***N*,*N*'-(6-(prop-1-en-2-yl)pyridine-2,4-diyl)bis(*N*,4-dimethylbenzenesulfonamide) (3l)**




**3l**

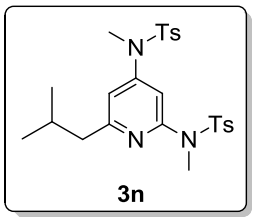
White solid; $^{1}$H NMR (600 MHz, $CDCl_3$): δ 7.52 (d, *J* = 8.4 Hz, 2 H), 7.43 (d, *J* = 8.4 Hz, 2 H), 7.35 (d, *J* = 1.8 Hz, 1 H), 7.26 (d, *J* = 7.8 Hz, 2 H), 7.20 ~ 7.19 (m, 3 H), 5.71 (s, 1 H), 5.19 ~ 5.19 (m, 1 H), 3.22 (s, 6 H), 2.39 (s, 3 H), 2.37 (s, 3 H), 2.00 (s, 3 H); $^{13}$C NMR (150 MHz, $CDCl_3$): δ 156.9, 153.4, 150.7, 144.3, 143.8, 142.2, 134.4, 133.8, 129.8, 129.4, 127.5, 116.3, 112.8, 111.6, 36.9, 35.4, 21.6, 21.5, 20.0; ESI-MS calcd. for $C_{24}H_{27}N_3O_4S_2$: 485.1443; found: 485.1443.

***N*,*N*'-(6-isopropylpyridine-2,4-diyl)bis(*N*,4-dimethylbenzenesulfonamide) (3m)**




White solid; $^{1}$H NMR (600 MHz, $CDCl_3$): δ 7.52 (d, *J* = 8.4 Hz, 2 H), 7.38 (d, *J* = 7.8 Hz, 2 H), 7. 26 ~ 7.24 (m, 2 H), 7. 18 ~ 7.16 (m, 2 H), 7.08 (d, *J* = 2.4 Hz, 1 H), 7.02 (d, *J* = 1.8 Hz, 1 H), 3.21 (s, 3 H), 3.19 (s, 3 H), 2.84 ~ 2.77 (m, 1 H), 2.38 (s, 3 H), 2.36 (s, 3 H), 1.06 (d, *J* = 7.2 Hz, 6 H); $^{13}$C NMR (150 MHz, $CDCl_3$): δ 166.5, 153.8, 150.5, 144.2, 143.6, 134.5, 134.0, 129.7, 129.3, 127.6, 127.5, 113.8, 111.1, 36.8, 36.0, 35.5, 22.1, 21.5 (x 2); ESI-MS calcd. for $C_{24}H_{29}N_3O_4S_2$: 487.1599; found: 487.1600.

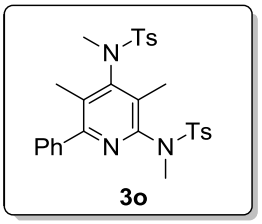
***N*,*N*'-(6-isobutylpyridine-2,4-diyl)bis(*N*,4-dimethylbenzenesulfonamide) (3n)**




White solid; $^{1}$H NMR (600 MHz, $CDCl_3$): δ 7.50 (d, *J* = 8.4 Hz, 2 H), 7.38 (d, *J* = 8.4 Hz, 2 H), 7.25 ~ 7.24 (m, 2 H), 7.17 (d, *J* = 8.4 Hz, 2 H), 7.10 (d, *J* = 1.8 Hz, 1 H), 6.99 (d, *J* = 1.8 Hz, 1 H), 3.21 (s, 3 H), 3.19 (s, 3 H), 2.41 (d, *J* = 7.2 Hz, 2 H), 2.38 (s, 3 H), 2.37 (s, 3 H), 1.85 ~ 1.78 (m, 1 H), 0.75 (d, *J* = 6.6 Hz, 6 H); $^{13}$C NMR (150 MHz, $CDCl_3$): δ 160.8, 153.8, 150.1, 144.3,

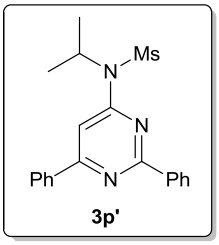
143.6, 134.4, 133.8, 129.7, 129.3, 127.5, 127.5, 116.2, 110.9, 47.0, 36.8, 35.5, 28.7, 22.2, 21.6, 21.5; ESI-MS calcd. for $C_{25}H_{31}N_3O_4S_2$: 501.1756; found: 501.1755.

**_N_,_N'_-(3,5-dimethyl-6-phenylpyridine-2,4-diyl)bis(_N_,4-dimethylbenzenesulfonamide) (3o)**



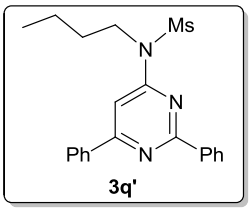

Sticky solid; $^1$H NMR (600 MHz, $CDCl_3$): δ 7.74 (d, *J* = 8.3 Hz, 2 H), 7.61 (d, *J* = 8.2 Hz, 2 H), 7.35 ~ 7.33 (m, 5 H), 7.25 ~ 7.23 (m, 4 H), 3.18 (s, 3 H), 3.05 (s, 3 H), 2.45 (s, 3 H), 2.42 (s, 3 H), 2.27 (s, 3 H), 2.10 (s, 3 H); $^{13}$C NMR (150 MHz, $CDCl_3$): δ 156.5, 152.1, 149.9, 143.9, 143.4, 139.6, 137.2, 134.5, 132.5, 132.1, 129.9, 129.2, 129.2, 128.7, 128.1, 127.8, 127.4, 37.4, 36.7, 21.6, 21.5, 16.9, 14.4; ESI-MS calcd. for $C_{29}H_{32}N_3O_4S_2$ (M + H): 550.18342; found: 550.18355.

**_N_-(2,6-diphenylpyrimidin-4-yl)-_N_-isopropylmethanesulfonamide (3p')**




White solid; $^1$H NMR (600 MHz, $CDCl_3$): δ 8.15 ~ 8.13 (m, 2 H), 7.83 ~ 7.81 (m, 2 H), 7.16 ~ 7.13 (m, 6 H), 6.87 (s, 1 H), 4.37 ~ 4.30 (m, 1 H), 2.90 (s, 3 H), 1.16 (d, *J* = 6.6 Hz, 6 H); $^{13}$C NMR (150 MHz, $CDCl_3$): δ 165.9, 164.3, 160.7, 137.4, 136.8, 131.1, 131.0, 129.0, 128.6, 128.4, 127.4, 110.7, 53.2, 42.1, 22.1; ESI-MS calcd. for $C_{20}H_{21}N_3O_2S$: 367.1354; found: 367.1355.

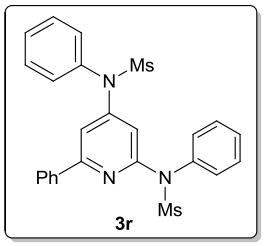
**_N_-butyl-_N_-(2,6-diphenylpyrimidin-4-yl)methanesulfonamide (3q')**



**3q'**

Yellow oil; $^{1}$H NMR (600 MHz, $CDCl_3$): δ 8.53 ~ 8.52 (m, 2 H), 8.18 ~ 8.17 (m, 2 H), 7.65 (s, 1 H), 7.53 ~ 7.50 (m, 6 H), 4.16 (t, *J* = 7.5 Hz, 2 H), 3.25 (s, 3 H), 1.80 ~ 1.75 (m, 2 H), 1.49 ~ 1.42 (m, 2 H), 0.98 (t, *J* = 7.5 Hz, 3 H); $^{13}$C NMR (150 MHz, $CDCl_3$): δ 165.6, 163.9, 160.2, 137.5, 137.2, 130.9, 128.9, 128.5, 128.4, 127.4, 104.1, 47.0, 40.8, 31.0, 20.1, 13.7 (one carbon merge with others); ESI-MS calcd. for $C_{21}H_{23}N_3O_2S$: 381.1511; found: 381.1513.

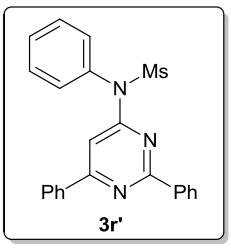
***N*,*N*'-(6-phenylpyridine-2,4-diyl)bis(*N*-phenylmethanesulfonamide) (3r)**



**3r**

Yellow oil; $^{1}$H NMR (400 MHz, $CDCl_3$): δ 7.89 ~ 7.87 (m, 2 H), 7.46 ~ 7.37 (m, 11 H), 7.29 (d, J = 1.2 Hz, 1 H), 7.27 ~ 7.25 (m, 2 H), 6.40 (s, 1 H), 3.56 (s, 3 H), 3.13 (s, 3 H); $^{13}$C NMR (150 MHz, $CDCl_3$): δ 157.1, 156.2, 151.6, 139.0, 138.4, 138.2, 130.2, 129.7, 1296, 129.6, 129.5, 128.8, 128.8, 127.1, 108.8, 107.6, 41.4, 39.8 (one carbon merge with others); ESI-MS calcd. for $C_{25}H_{23}N_3O_4S_2$: 493.1130; found: 493.1131.

***N*-(2,6-diphenylpyrimidin-4-yl)-*N*-phenylmethanesulfonamide (3r')**

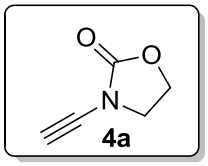


**3r'**

Yellow oil; $^{1}$H NMR (600 MHz, $CDCl_3$): δ 8.56 ~ 8.54 (m, 2 H), 7.93 ~ 7.92 (m, 2 H), 7.54 ~

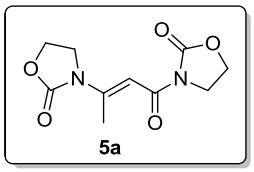
7.51 (m, 6 H), 7.44 ~ 7.41 (m, 5 H), 6.59 (s, 1 H), 3.71 (s, 3 H); $^{13}$C NMR (150 MHz, $CDCl_3$): δ 165.3, 163.7, 162.5, 137.5, 137.2, 137.0, 131.0, 130.9, 130.2, 130.2, 129.8, 128.8, 128.6, 128.6, 127.2, 103.4, 42.5; ESI-MS calcd. for $C_{23}H_{19}N_3O_2S$: 401.1198; found: 401.1198.

**3-ethynyloxazolidin-2-one (4a)**



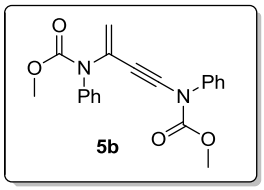

Semi solid; $^1$H NMR (600 MHz, $CDCl_3$): δ 4.43 (t, *J* = 7.8 Hz, 2 H), 3.92 (t, *J* = 7.8 Hz, 2 H), 2.83 (s, 1 H); $^{13}$C NMR (150 MHz, $CDCl_3$): δ 72.3, 63.1, 59.8, 46.4.

**(*E*)-3,3'-(but-2-enoyl)bis(oxazolidin-2-one) (5a)**




White solid; $^1$H NMR (600 MHz, $CDCl_3$): δ 6.60 (s, 1 H), 4.41 ~ 4.36 (m, 4 H), 4.06 (t, *J* = 7.8 Hz, 2 H), 3.94 (t, *J* = 7.8 Hz, 2 H), 2.77 (s, 1 H); $^{13}$C NMR (150 MHz, $CDCl_3$): δ 164.8, 155.3, 154.0, 153.8, 100.0, 61.7, 61.1, 45.6, 42.8, 16.0.

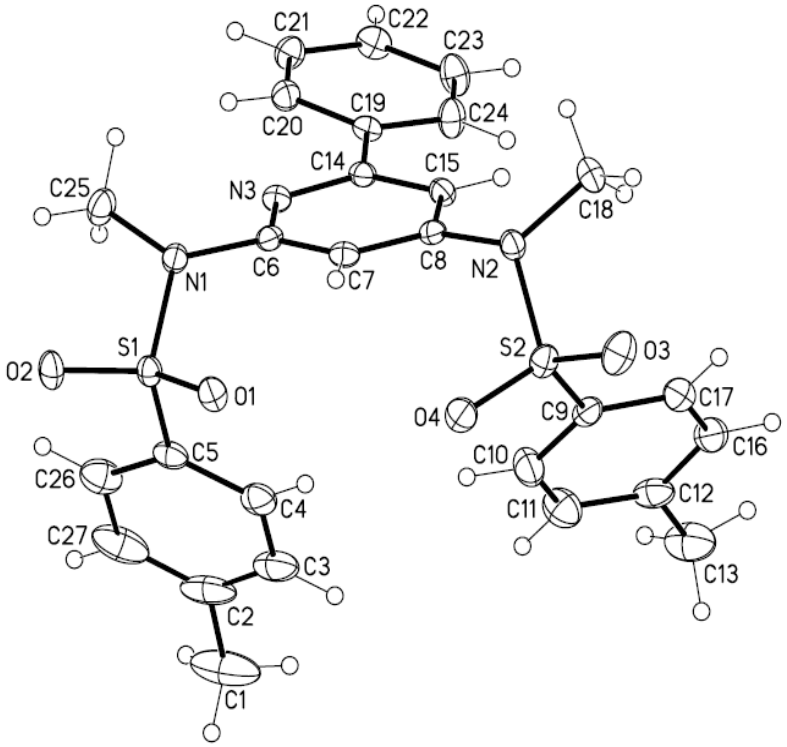
**dimethyl but-3-en-1-yne-1,3-diylbis(phenylcarbamate) (5b)**




Sticky solid; $^1$H NMR (400 MHz, $CDCl_3$): δ 7.35 ~ 7.22 (m, 10 H), 5.45 (d, *J* = 8.4 Hz, 2 H), 3.81 (s, 3 H), 3.72 (s, 3 H); $^{13}$C NMR (100 MHz, $CDCl_3$): δ 154.5, 154.4, 141.0, 138.9, 129.3, 128.9, 128.8, 127.0, 126.8, 124.3, 118.1, 82.6, 67.8, 54.3, 53.2 (one cabon merge with others).

## (IV) X-ray crystallographic data

## (a) compound 3a (CCDC 1437539).



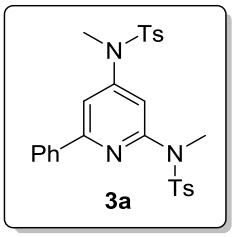




Table 1. Crystal data and structure refinement for 131005lt_0m.

| | | |
|---|---|---|
| Identification code | 131005lt_0m | |
| Empirical formula | C27 H27 N3 O4 S2 | |
| Formula weight | 521.64 | |
| Temperature | 100(2) K | |
| Wavelength | 0.71073 Å | |
| Crystal system | Triclinic | |
| Space group | P -1 | |
| Unit cell dimensions | a = 9.8347(3) Å | α= 77.323(2)°. |
| | b = 10.7763(4) Å | β= 76.332(2)°. |
| | c = 13.3710(4) Å | γ = 67.333(2)°. |
| Volume | 1257.50(7) $Å^3$ | |
| Z | 2 | |
| Density (calculated) | 1.378 $Mg/m^3$ | |

| | |
|---|---|
| Absorption coefficient | 0.251 $mm^{-1}$ |
| F(000) | 548 |
| Crystal size | 0.30 x 0.26 x 0.15 $mm^3$ |
| Theta range for data collection | 1.58 to 26.44°. |
| Index ranges | -12<=h<=12, -13<=k<=13, -16<=l<=16 |
| Reflections collected | 19210 |
| Independent reflections | 5143 [R(int) = 0.0389] |
| Completeness to theta = 26.44° | 99.2 % |
| Absorption correction | Semi-empirical from equivalents |
| Max. and min. transmission | 0.9486 and 0.8843 |
| Refinement method | Full-matrix least-squares on $F^2$ |
| Data / restraints / parameters | 5143 / 0 / 329 |
| Goodness-of-fit on $F^2$ | 1.203 |
| Final R indices [I>2sigma(I)] | R1 = 0.0405, wR2 = 0.1182 |
| R indices (all data) | R1 = 0.0540, wR2 = 0.1518 |
| Largest diff. peak and hole | 0.438 and -0.519 e.$Å^{-3}$ |

Table 2. Atomic coordinates ( x $10^4$) and equivalent isotropic displacement parameters ($Å^2$x $10^3$) for 131005lt_0m. U(eq) is defined as one third of the trace of the orthogonalized $U^{ij}$ tensor.

| | x | y | z | U(eq) |
|---|---|---|---|---|
| S(1) | 2207(1) | 3160(1) | 7012(1) | 15(1) |
| S(2) | 5802(1) | 6121(1) | 7194(1) | 19(1) |
| O(1) | 1963(2) | 4566(1) | 6951(1) | 19(1) |
| O(2) | 1073(2) | 2785(2) | 6795(1) | 21(1) |
| O(3) | 5998(2) | 7407(2) | 6898(1) | 28(1) |
| O(4) | 4332(2) | 6061(2) | 7485(1) | 23(1) |
| N(1) | 3730(2) | 2496(2) | 6178(1) | 16(1) |
| N(2) | 6657(2) | 5277(2) | 6191(1) | 16(1) |
| N(3) | 6268(2) | 1503(2) | 6286(1) | 15(1) |
| C(1) | 3415(3) | 541(4) | 11344(2) | 56(1) |
| C(2) | 3187(3) | 1161(3) | 10243(2) | 38(1) |
| C(3) | 3452(3) | 2343(3) | 9793(2) | 34(1) |
| C(4) | 3161(2) | 2953(3) | 8809(2) | 25(1) |
| C(5) | 2589(2) | 2358(2) | 8259(2) | 20(1) |

| | | | | |
|---|---|---|---|---|
| C(6) | 5092(2) | 2659(2) | 6239(2) | 15(1) |
| C(7) | 5152(2) | 3929(2) | 6200(2) | 15(1) |
| C(8) | 6515(2) | 3983(2) | 6259(2) | 15(1) |
| C(9) | 6795(2) | 5195(2) | 8221(2) | 19(1) |
| C(10) | 6285(3) | 4269(2) | 8934(2) | 26(1) |
| C(11) | 7046(3) | 3545(3) | 9746(2) | 31(1) |
| C(12) | 8329(2) | 3712(2) | 9855(2) | 26(1) |
| C(13) | 9098(3) | 2967(3) | 10767(2) | 39(1) |
| C(14) | 7601(2) | 1568(2) | 6309(1) | 14(1) |
| C(15) | 7758(2) | 2793(2) | 6319(2) | 16(1) |
| C(16) | 8844(3) | 4623(3) | 9110(2) | 28(1) |
| C(17) | 8082(2) | 5377(2) | 8300(2) | 25(1) |
| C(18) | 8132(2) | 5374(2) | 5704(2) | 20(1) |
| C(19) | 8883(2) | 265(2) | 6336(2) | 15(1) |
| C(20) | 8748(2) | -895(2) | 6136(2) | 18(1) |
| C(21) | 9944(2) | -2118(2) | 6164(2) | 20(1) |
| C(22) | 11282(2) | -2211(2) | 6388(2) | 20(1) |
| C(23) | 11428(2) | -1070(2) | 6583(2) | 24(1) |
| C(24) | 10239(2) | 158(2) | 6564(2) | 21(1) |
| C(25) | 3915(3) | 1203(2) | 5864(2) | 23(1) |
| C(26) | 2321(3) | 1164(2) | 8682(2) | 29(1) |
| C(27) | 2625(3) | 568(3) | 9678(2) | 40(1) |

Table 3. Bond lengths [Å] and angles [°] for 131005lt_0m.

| | |
|---|---|
| S(1)-O(1) | 1.4265(15) |
| S(1)-O(2) | 1.4290(15) |
| S(1)-N(1) | 1.6535(17) |
| S(1)-C(5) | 1.756(2) |
| S(2)-O(3) | 1.4292(17) |
| S(2)-O(4) | 1.4288(15) |
| S(2)-N(2) | 1.6573(17) |
| S(2)-C(9) | 1.765(2) |
| N(1)-C(6) | 1.440(3) |
| N(1)-C(25) | 1.475(3) |
| N(2)-C(8) | 1.435(3) |

| | |
|---|---|
| N(2)-C(18) | 1.477(3) |
| N(3)-C(6) | 1.336(3) |
| N(3)-C(14) | 1.347(3) |
| C(1)-C(2) | 1.506(4) |
| C(1)-H(1A) | 0.9800 |
| C(1)-H(1B) | 0.9800 |
| C(1)-H(1C) | 0.9800 |
| C(2)-C(3) | 1.378(4) |
| C(2)-C(27) | 1.402(4) |
| C(3)-C(4) | 1.378(3) |
| C(3)-H(3) | 0.9500 |
| C(4)-C(5) | 1.396(3) |
| C(4)-H(4) | 0.9500 |
| C(5)-C(26) | 1.383(3) |
| C(6)-C(7) | 1.381(3) |
| C(7)-C(8) | 1.386(3) |
| C(7)-H(7) | 0.9500 |
| C(8)-C(15) | 1.392(3) |
| C(9)-C(10) | 1.377(3) |
| C(9)-C(17) | 1.385(3) |
| C(10)-C(11) | 1.383(3) |
| C(10)-H(10) | 0.9500 |
| C(11)-C(12) | 1.385(3) |
| C(11)-H(11) | 0.9500 |
| C(12)-C(16) | 1.388(3) |
| C(12)-C(13) | 1.498(3) |
| C(13)-H(13A) | 0.9800 |
| C(13)-H(13B) | 0.9800 |
| C(13)-H(13C) | 0.9800 |
| C(14)-C(15) | 1.390(3) |
| C(14)-C(19) | 1.483(3) |
| C(15)-H(15) | 0.9500 |
| C(16)-C(17) | 1.386(3) |
| C(16)-H(16) | 0.9500 |
| C(17)-H(17) | 0.9500 |
| C(18)-H(18A) | 0.9800 |

| | |
|---|---|
| C(18)-H(18B) | 0.9800 |
| C(18)-H(18C) | 0.9800 |
| C(19)-C(24) | 1.394(3) |
| C(19)-C(20) | 1.394(3) |
| C(20)-C(21) | 1.388(3) |
| C(20)-H(20) | 0.9500 |
| C(21)-C(22) | 1.379(3) |
| C(21)-H(21) | 0.9500 |
| C(22)-C(23) | 1.376(3) |
| C(22)-H(22) | 0.9500 |
| C(23)-C(24) | 1.388(3) |
| C(23)-H(23) | 0.9500 |
| C(24)-H(24) | 0.9500 |
| C(25)-H(25A) | 0.9800 |
| C(25)-H(25B) | 0.9800 |
| C(25)-H(25C) | 0.9800 |
| C(26)-C(27) | 1.393(4) |
| C(26)-H(26) | 0.9500 |
| C(27)-H(27) | 0.9500 |

| | |
|---|---|
| O(1)-S(1)-O(2) | 118.91(9) |
| O(1)-S(1)-N(1) | 108.18(9) |
| O(2)-S(1)-N(1) | 105.88(9) |
| O(1)-S(1)-C(5) | 107.88(10) |
| O(2)-S(1)-C(5) | 108.56(10) |
| N(1)-S(1)-C(5) | 106.84(9) |
| O(3)-S(2)-O(4) | 120.03(10) |
| O(3)-S(2)-N(2) | 106.03(9) |
| O(4)-S(2)-N(2) | 107.59(9) |
| O(3)-S(2)-C(9) | 108.90(10) |
| O(4)-S(2)-C(9) | 107.66(10) |
| N(2)-S(2)-C(9) | 105.78(9) |
| C(6)-N(1)-C(25) | 115.48(16) |
| C(6)-N(1)-S(1) | 118.61(13) |
| C(25)-N(1)-S(1) | 116.64(14) |
| C(8)-N(2)-C(18) | 116.30(16) |

| | |
|---|---|
| C(8)-N(2)-S(2) | 117.02(13) |
| C(18)-N(2)-S(2) | 114.98(14) |
| C(6)-N(3)-C(14) | 118.29(18) |
| C(2)-C(1)-H(1A) | 109.5 |
| C(2)-C(1)-H(1B) | 109.5 |
| H(1A)-C(1)-H(1B) | 109.5 |
| C(2)-C(1)-H(1C) | 109.5 |
| H(1A)-C(1)-H(1C) | 109.5 |
| H(1B)-C(1)-H(1C) | 109.5 |
| C(3)-C(2)-C(27) | 118.8(2) |
| C(3)-C(2)-C(1) | 121.3(3) |
| C(27)-C(2)-C(1) | 119.8(3) |
| C(4)-C(3)-C(2) | 121.3(3) |
| C(4)-C(3)-H(3) | 119.3 |
| C(2)-C(3)-H(3) | 119.3 |
| C(3)-C(4)-C(5) | 119.2(2) |
| C(3)-C(4)-H(4) | 120.4 |
| C(5)-C(4)-H(4) | 120.4 |
| C(26)-C(5)-C(4) | 121.2(2) |
| C(26)-C(5)-S(1) | 120.28(18) |
| C(4)-C(5)-S(1) | 118.51(18) |
| N(3)-C(6)-C(7) | 124.26(19) |
| N(3)-C(6)-N(1) | 114.36(18) |
| C(7)-C(6)-N(1) | 121.30(18) |
| C(6)-C(7)-C(8) | 117.07(19) |
| C(6)-C(7)-H(7) | 121.5 |
| C(8)-C(7)-H(7) | 121.5 |
| C(7)-C(8)-C(15) | 119.90(19) |
| C(7)-C(8)-N(2) | 119.58(18) |
| C(15)-C(8)-N(2) | 120.40(18) |
| C(10)-C(9)-C(17) | 120.4(2) |
| C(10)-C(9)-S(2) | 119.05(17) |
| C(17)-C(9)-S(2) | 120.55(17) |
| C(9)-C(10)-C(11) | 119.6(2) |
| C(9)-C(10)-H(10) | 120.2 |
| C(11)-C(10)-H(10) | 120.2 |

| | |
|---|---|
| C(10)-C(11)-C(12) | 121.5(2) |
| C(10)-C(11)-H(11) | 119.2 |
| C(12)-C(11)-H(11) | 119.2 |
| C(11)-C(12)-C(16) | 117.8(2) |
| C(11)-C(12)-C(13) | 120.7(2) |
| C(16)-C(12)-C(13) | 121.5(2) |
| C(12)-C(13)-H(13A) | 109.5 |
| C(12)-C(13)-H(13B) | 109.5 |
| H(13A)-C(13)-H(13B) | 109.5 |
| C(12)-C(13)-H(13C) | 109.5 |
| H(13A)-C(13)-H(13C) | 109.5 |
| H(13B)-C(13)-H(13C) | 109.5 |
| N(3)-C(14)-C(15) | 121.59(18) |
| N(3)-C(14)-C(19) | 116.50(18) |
| C(15)-C(14)-C(19) | 121.91(19) |
| C(14)-C(15)-C(8) | 118.80(19) |
| C(14)-C(15)-H(15) | 120.6 |
| C(8)-C(15)-H(15) | 120.6 |
| C(17)-C(16)-C(12) | 121.6(2) |
| C(17)-C(16)-H(16) | 119.2 |
| C(12)-C(16)-H(16) | 119.2 |
| C(9)-C(17)-C(16) | 119.1(2) |
| C(9)-C(17)-H(17) | 120.5 |
| C(16)-C(17)-H(17) | 120.5 |
| N(2)-C(18)-H(18A) | 109.5 |
| N(2)-C(18)-H(18B) | 109.5 |
| H(18A)-C(18)-H(18B) | 109.5 |
| N(2)-C(18)-H(18C) | 109.5 |
| H(18A)-C(18)-H(18C) | 109.5 |
| H(18B)-C(18)-H(18C) | 109.5 |
| C(24)-C(19)-C(20) | 118.34(19) |
| C(24)-C(19)-C(14) | 121.63(19) |
| C(20)-C(19)-C(14) | 120.04(19) |
| C(21)-C(20)-C(19) | 120.2(2) |
| C(21)-C(20)-H(20) | 119.9 |
| C(19)-C(20)-H(20) | 119.9 |

| | |
|---|---|
| C(22)-C(21)-C(20) | 120.9(2) |
| C(22)-C(21)-H(21) | 119.5 |
| C(20)-C(21)-H(21) | 119.5 |
| C(23)-C(22)-C(21) | 119.3(2) |
| C(23)-C(22)-H(22) | 120.4 |
| C(21)-C(22)-H(22) | 120.4 |
| C(22)-C(23)-C(24) | 120.5(2) |
| C(22)-C(23)-H(23) | 119.8 |
| C(24)-C(23)-H(23) | 119.8 |
| C(23)-C(24)-C(19) | 120.8(2) |
| C(23)-C(24)-H(24) | 119.6 |
| C(19)-C(24)-H(24) | 119.6 |
| N(1)-C(25)-H(25A) | 109.5 |
| N(1)-C(25)-H(25B) | 109.5 |
| H(25A)-C(25)-H(25B) | 109.5 |
| N(1)-C(25)-H(25C) | 109.5 |
| H(25A)-C(25)-H(25C) | 109.5 |
| H(25B)-C(25)-H(25C) | 109.5 |
| C(5)-C(26)-C(27) | 118.4(2) |
| C(5)-C(26)-H(26) | 120.8 |
| C(27)-C(26)-H(26) | 120.8 |
| C(26)-C(27)-C(2) | 121.0(3) |
| C(26)-C(27)-H(27) | 119.5 |
| C(2)-C(27)-H(27) | 119.5 |

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for 131005lt_0m. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

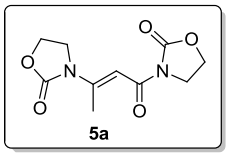
| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{23}$ | $U^{13}$ | $U^{12}$ |
|---|---|---|---|---|---|---|
| S(1) | 13(1) | 14(1) | 19(1) | -3(1) | -3(1) | -4(1) |
| S(2) | 16(1) | 16(1) | 24(1) | -6(1) | -5(1) | -2(1) |
| O(1) | 16(1) | 14(1) | 27(1) | -4(1) | -2(1) | -4(1) |
| O(2) | 15(1) | 22(1) | 31(1) | -5(1) | -6(1) | -8(1) |

| | | | | | | |
|---|---|---|---|---|---|---|
| O(3) | 33(1) | 15(1) | 36(1) | -5(1) | -12(1) | -6(1) |
| O(4) | 13(1) | 26(1) | 30(1) | -12(1) | -3(1) | -2(1) |
| N(1) | 15(1) | 16(1) | 18(1) | -5(1) | -3(1) | -6(1) |
| N(2) | 14(1) | 16(1) | 19(1) | -3(1) | -2(1) | -6(1) |
| N(3) | 15(1) | 16(1) | 15(1) | -2(1) | -2(1) | -4(1) |
| C(1) | 39(2) | 75(2) | 22(1) | 3(1) | 2(1) | 5(2) |
| C(2) | 21(1) | 51(2) | 20(1) | -6(1) | 3(1) | 7(1) |
| C(3) | 19(1) | 52(2) | 21(1) | -11(1) | 0(1) | -3(1) |
| C(4) | 14(1) | 34(1) | 24(1) | -8(1) | -1(1) | -4(1) |
| C(5) | 14(1) | 23(1) | 17(1) | -3(1) | 0(1) | -2(1) |
| C(6) | 15(1) | 19(1) | 13(1) | -5(1) | -2(1) | -6(1) |
| C(7) | 14(1) | 16(1) | 14(1) | -3(1) | -1(1) | -2(1) |
| C(8) | 17(1) | 17(1) | 11(1) | -3(1) | -1(1) | -7(1) |
| C(9) | 18(1) | 21(1) | 18(1) | -8(1) | -4(1) | -4(1) |
| C(10) | 22(1) | 31(1) | 28(1) | -2(1) | -4(1) | -14(1) |
| C(11) | 30(1) | 32(1) | 28(1) | 2(1) | -4(1) | -12(1) |
| C(12) | 20(1) | 31(1) | 20(1) | -9(1) | -2(1) | 1(1) |
| C(13) | 30(1) | 50(2) | 27(1) | -4(1) | -7(1) | -2(1) |
| C(14) | 14(1) | 17(1) | 12(1) | -2(1) | -1(1) | -5(1) |
| C(15) | 13(1) | 18(1) | 16(1) | -2(1) | -1(1) | -6(1) |
| C(16) | 18(1) | 43(2) | 26(1) | -12(1) | -4(1) | -9(1) |
| C(17) | 23(1) | 32(1) | 22(1) | -6(1) | -2(1) | -12(1) |
| C(18) | 16(1) | 22(1) | 22(1) | 0(1) | -3(1) | -9(1) |
| C(19) | 14(1) | 14(1) | 13(1) | -1(1) | 0(1) | -4(1) |
| C(20) | 17(1) | 18(1) | 20(1) | -5(1) | -2(1) | -6(1) |
| C(21) | 23(1) | 16(1) | 22(1) | -5(1) | -3(1) | -7(1) |
| C(22) | 19(1) | 15(1) | 23(1) | -2(1) | -2(1) | -2(1) |
| C(23) | 16(1) | 20(1) | 33(1) | 0(1) | -8(1) | -6(1) |
| C(24) | 20(1) | 13(1) | 32(1) | -3(1) | -7(1) | -6(1) |
| C(25) | 21(1) | 19(1) | 31(1) | -11(1) | -5(1) | -6(1) |
| C(26) | 30(1) | 23(1) | 26(1) | -1(1) | 2(1) | -6(1) |
| C(27) | 34(2) | 28(1) | 33(1) | 8(1) | 8(1) | 1(1) |

Table 5. Hydrogen coordinates ( x $10^4$) and isotropic displacement parameters ($Å^2$x $10^3$) for 131005lt_0m.

| | x | y | z | U(eq) |
|---|---|---|---|---|
| H(1A) | 4262 | 695 | 11492 | 85 |
| H(1B) | 3619 | -437 | 11429 | 85 |
| H(1C) | 2510 | 964 | 11826 | 85 |
| H(3) | 3842 | 2745 | 10168 | 40 |
| H(4) | 3348 | 3768 | 8508 | 30 |
| H(7) | 4296 | 4730 | 6136 | 19 |
| H(10) | 5416 | 4128 | 8867 | 32 |
| H(11) | 6680 | 2918 | 10242 | 37 |
| H(13A) | 8529 | 3393 | 11387 | 59 |
| H(13B) | 10108 | 3002 | 10625 | 59 |
| H(13C) | 9160 | 2017 | 10886 | 59 |
| H(15) | 8696 | 2818 | 6365 | 19 |
| H(16) | 9740 | 4732 | 9156 | 34 |
| H(17) | 8439 | 6011 | 7806 | 30 |
| H(18A) | 8837 | 4915 | 6193 | 30 |
| H(18B) | 8037 | 6332 | 5522 | 30 |
| H(18C) | 8501 | 4939 | 5073 | 30 |
| H(20) | 7834 | -849 | 5981 | 22 |
| H(21) | 9840 | -2903 | 6027 | 24 |
| H(22) | 12094 | -3053 | 6407 | 25 |
| H(23) | 12348 | -1124 | 6732 | 28 |
| H(24) | 10351 | 936 | 6707 | 25 |
| H(25A) | 4657 | 1051 | 5227 | 34 |
| H(25B) | 2956 | 1244 | 5737 | 34 |
| H(25C) | 4254 | 456 | 6420 | 34 |
| H(26) | 1939 | 761 | 8301 | 35 |
| H(27) | 2449 | -252 | 9979 | 48 |

## (b) compound 5a (CCDC 1446058)



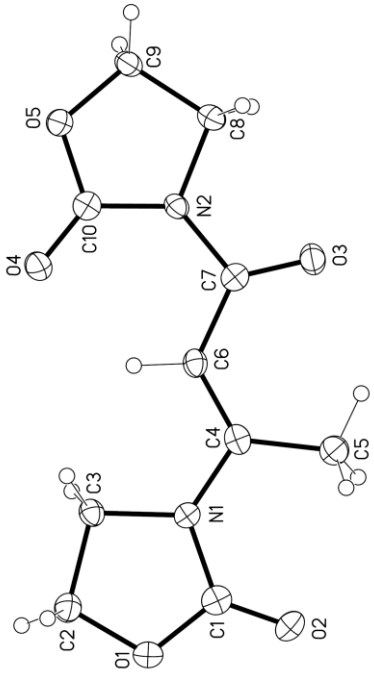




Table 1. Crystal data and structure refinement for 150416LT_a.

| | | |
|---|---|---|
| Identification code | 150416LT_a | |
| Empirical formula | C10 H12 N2 O5 | |
| Formula weight | 240.22 | |
| Temperature | 100(2) K | |
| Wavelength | 0.71073 Å | |
| Crystal system | Orthorhombic | |
| Space group | P n a 21 | |
| Unit cell dimensions | a = 13.782(4) Å | α= 90°. |
| | b = 18.539(5) Å | β= 90°. |
| | c = 3.9890(12) Å | γ = 90°. |
| Volume | 1019.2(5) $Å^3$ | |
| Z | 4 | |
| Density (calculated) | 1.566 $Mg/m^3$ | |
| Absorption coefficient | 0.127 $mm^{-1}$ | |

| | |
|---|---|
| F(000) | 504 |
| Crystal size | 0.30 x 0.01 x 0.01 $mm^3$ |
| Theta range for data collection | 1.841 to 26.645°. |
| Index ranges | -17<=h<=17, -22<=k<=23, -4<=l<=3 |
| Reflections collected | 5305 |
| Independent reflections | 1680 [R(int) = 0.0412] |
| Completeness to theta = 25.242° | 99.3 % |
| Absorption correction | Semi-empirical from equivalents |
| Max. and min. transmission | 0.9485 and 0.7676 |
| Refinement method | Full-matrix least-squares on $F^2$ |
| Data / restraints / parameters | 1680 / 1 / 156 |
| Goodness-of-fit on $F^2$ | 1.034 |
| Final R indices [I>2sigma(I)] | R1 = 0.0397, wR2 = 0.0837 |
| R indices (all data) | R1 = 0.0503, wR2 = 0.0880 |
| Absolute structure parameter | -1(2) |
| Extinction coefficient | n/a |
| Largest diff. peak and hole | 0.179 and -0.186 e.$Å^{-3}$ |

Table 2. Atomic coordinates ( x $10^4$) and equivalent isotropic displacement parameters ($Å^2$x $10^3$) for 150416LT_a. U(eq) is defined as one third of the trace of the orthogonalized $U^{ij}$ tensor.

| | x | y | z | U(eq) |
|---|---|---|---|---|
| C(1) | 6329(2) | 1023(2) | 316(8) | 18(1) |
| C(2) | 4692(2) | 1029(2) | 1488(9) | 21(1) |
| C(3) | 5106(2) | 1747(1) | 2647(9) | 17(1) |
| C(4) | 6842(2) | 2131(2) | 3429(8) | 16(1) |
| C(5) | 7894(2) | 1931(2) | 3069(10) | 23(1) |
| C(6) | 6500(2) | 2737(2) | 4862(8) | 17(1) |
| C(7) | 7086(2) | 3316(2) | 6295(9) | 16(1) |
| C(8) | 7103(2) | 4477(1) | 9403(9) | 18(1) |
| C(9) | 6275(2) | 4964(2) | 10544(9) | 19(1) |
| C(10) | 5594(2) | 3882(2) | 8959(9) | 16(1) |
| N(1) | 6156(2) | 1631(1) | 2265(7) | 16(1) |
| N(2) | 6564(2) | 3871(1) | 7917(7) | 15(1) |
| O(1) | 5480(1) | 692(1) | -364(6) | 22(1) |

| | | | | |
|---|---|---|---|---|
| O(2) | 7087(1) | 800(1) | -742(7) | 23(1) |
| O(3) | 7971(1) | 3386(1) | 6168(7) | 22(1) |
| O(4) | 4964(1) | 3445(1) | 8473(6) | 22(1) |
| O(5) | 5437(1) | 4487(1) | 10761(7) | 20(1) |

Table 3. Bond lengths [Å] and angles [°] for 150416LT_a.

| | |
|---|---|
| C(1)-O(2) | 1.201(3) |
| C(1)-O(1) | 1.349(3) |
| C(1)-N(1) | 1.389(4) |
| C(2)-O(1) | 1.455(3) |
| C(2)-C(3) | 1.521(4) |
| C(2)-H(2A) | 0.9900 |
| C(2)-H(2B) | 0.9900 |
| C(3)-N(1) | 1.471(3) |
| C(3)-H(3A) | 0.9900 |
| C(3)-H(3B) | 0.9900 |
| C(4)-C(6) | 1.345(4) |
| C(4)-N(1) | 1.403(4) |
| C(4)-C(5) | 1.504(4) |
| C(5)-H(5A) | 0.9800 |
| C(5)-H(5B) | 0.9800 |
| C(5)-H(5C) | 0.9800 |
| C(6)-C(7) | 1.460(4) |
| C(6)-H(6) | 0.9500 |
| C(7)-O(3) | 1.228(3) |
| C(7)-N(2) | 1.414(4) |
| C(8)-N(2) | 1.471(4) |
| C(8)-C(9) | 1.525(4) |
| C(8)-H(8A) | 0.9900 |
| C(8)-H(8B) | 0.9900 |
| C(9)-O(5) | 1.458(3) |
| C(9)-H(9A) | 0.9900 |
| C(9)-H(9B) | 0.9900 |
| C(10)-O(4) | 1.204(3) |
| C(10)-O(5) | 1.350(4) |

| | |
|---|---|
| C(10)-N(2) | 1.400(4) |

| | |
|---|---|
| O(2)-C(1)-O(1) | 121.8(3) |
| O(2)-C(1)-N(1) | 128.7(3) |
| O(1)-C(1)-N(1) | 109.4(2) |
| O(1)-C(2)-C(3) | 104.5(2) |
| O(1)-C(2)-H(2A) | 110.9 |
| C(3)-C(2)-H(2A) | 110.9 |
| O(1)-C(2)-H(2B) | 110.9 |
| C(3)-C(2)-H(2B) | 110.9 |
| H(2A)-C(2)-H(2B) | 108.9 |
| N(1)-C(3)-C(2) | 102.1(2) |
| N(1)-C(3)-H(3A) | 111.4 |
| C(2)-C(3)-H(3A) | 111.4 |
| N(1)-C(3)-H(3B) | 111.4 |
| C(2)-C(3)-H(3B) | 111.4 |
| H(3A)-C(3)-H(3B) | 109.2 |
| C(6)-C(4)-N(1) | 117.2(2) |
| C(6)-C(4)-C(5) | 125.7(3) |
| N(1)-C(4)-C(5) | 117.1(2) |
| C(4)-C(5)-H(5A) | 109.5 |
| C(4)-C(5)-H(5B) | 109.5 |
| H(5A)-C(5)-H(5B) | 109.5 |
| C(4)-C(5)-H(5C) | 109.5 |
| H(5A)-C(5)-H(5C) | 109.5 |
| H(5B)-C(5)-H(5C) | 109.5 |
| C(4)-C(6)-C(7) | 125.9(2) |
| C(4)-C(6)-H(6) | 117.0 |
| C(7)-C(6)-H(6) | 117.0 |
| O(3)-C(7)-N(2) | 116.5(3) |
| O(3)-C(7)-C(6) | 127.7(3) |
| N(2)-C(7)-C(6) | 115.7(2) |
| N(2)-C(8)-C(9) | 101.2(2) |
| N(2)-C(8)-H(8A) | 111.5 |
| C(9)-C(8)-H(8A) | 111.5 |
| N(2)-C(8)-H(8B) | 111.5 |

| | |
|---|---|
| C(9)-C(8)-H(8B) | 111.5 |
| H(8A)-C(8)-H(8B) | 109.3 |
| O(5)-C(9)-C(8) | 104.5(2) |
| O(5)-C(9)-H(9A) | 110.8 |
| C(8)-C(9)-H(9A) | 110.8 |
| O(5)-C(9)-H(9B) | 110.8 |
| C(8)-C(9)-H(9B) | 110.8 |
| H(9A)-C(9)-H(9B) | 108.9 |
| O(4)-C(10)-O(5) | 122.0(3) |
| O(4)-C(10)-N(2) | 129.2(3) |
| O(5)-C(10)-N(2) | 108.8(2) |
| C(1)-N(1)-C(4) | 127.2(2) |
| C(1)-N(1)-C(3) | 110.3(2) |
| C(4)-N(1)-C(3) | 122.1(2) |
| C(10)-N(2)-C(7) | 129.2(2) |
| C(10)-N(2)-C(8) | 110.6(2) |
| C(7)-N(2)-C(8) | 118.9(2) |
| C(1)-O(1)-C(2) | 110.5(2) |
| C(10)-O(5)-C(9) | 110.2(2) |

Symmetry transformations used to generate equivalent atoms:

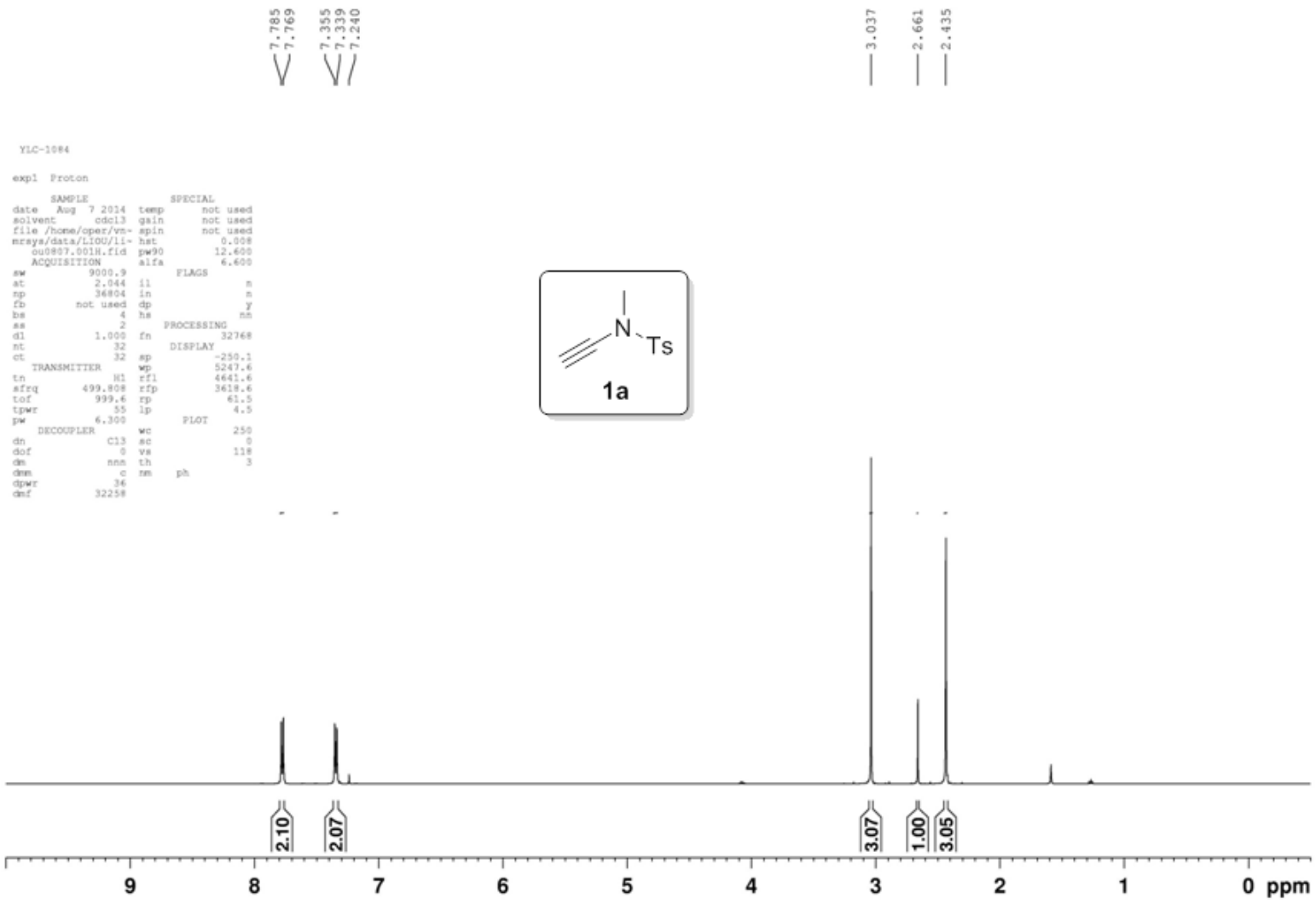
Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for 150416LT_a. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{23}$ | $U^{13}$ | $U^{12}$ |
|---|---|---|---|---|---|---|
| C(1) | 23(2) | 18(1) | 13(2) | 5(1) | -2(1) | 2(1) |
| C(2) | 18(1) | 21(1) | 23(2) | 0(2) | 2(1) | 0(1) |
| C(3) | 15(1) | 20(2) | 15(2) | 0(1) | -2(1) | -1(1) |
| C(4) | 17(1) | 19(1) | 11(2) | 7(1) | 1(1) | -2(1) |
| C(5) | 21(2) | 24(2) | 24(2) | -4(2) | -2(1) | 1(1) |
| C(6) | 14(1) | 21(2) | 15(2) | 1(1) | 1(1) | -1(1) |
| C(7) | 20(1) | 16(1) | 11(2) | 4(1) | 0(1) | 1(1) |
| C(8) | 19(1) | 18(1) | 17(2) | -1(1) | -1(1) | -4(1) |
| C(9) | 18(1) | 19(1) | 20(2) | -3(2) | -1(1) | -4(1) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C(10) | 20(2) | 18(1) | 11(2) | 4(1) | -2(1) | 1(1) |
| N(1) | 17(1) | 16(1) | 16(2) | 0(1) | 1(1) | 1(1) |
| N(2) | 14(1) | 17(1) | 15(2) | -1(1) | -1(1) | -2(1) |
| O(1) | 22(1) | 20(1) | 24(1) | -5(1) | -1(1) | -1(1) |
| O(2) | 23(1) | 23(1) | 23(1) | -3(1) | 4(1) | 4(1) |
| O(3) | 16(1) | 26(1) | 23(1) | -1(1) | 0(1) | -1(1) |
| O(4) | 18(1) | 23(1) | 24(2) | -3(1) | 2(1) | -4(1) |
| O(5) | 18(1) | 20(1) | 21(1) | -3(1) | 3(1) | -1(1) |

Table 5. Hydrogen coordinates ( x $10^4$) and isotropic displacement parameters ($Å^2$x $10^3$) for 150416LT_a.

| | x | y | z | U(eq) |
|---|---|---|---|---|
| H(2A) | 4499 | 728 | 3429 | 25 |
| H(2B) | 4119 | 1103 | 29 | 25 |
| H(3A) | 4877 | 2149 | 1217 | 20 |
| H(3B) | 4932 | 1848 | 5009 | 20 |
| H(5A) | 8295 | 2284 | 4259 | 34 |
| H(5B) | 8070 | 1927 | 689 | 34 |
| H(5C) | 8002 | 1450 | 4024 | 34 |
| H(6) | 5816 | 2793 | 4948 | 20 |
| H(8A) | 7520 | 4719 | 7724 | 22 |
| H(8B) | 7507 | 4317 | 11318 | 22 |
| H(9A) | 6421 | 5183 | 12752 | 23 |
| H(9B) | 6160 | 5355 | 8898 | 23 |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7.240
3.037
2.661
2.435
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expl Proton
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at 2.044
np 36804
fb not used
bs 4
ss 2
dl 1.000
nt 32
ct 32
TRANSMITTER
tn H1
sfrq 499.808
tof 999.6
tpwr 55
pw 6.300
DECOUPLER
dn C13
dof 0
dm nnn
dmm c
dpwr 36
dmf 32258
SPECIAL
temp not used
gain not used
spin not used
hst 0.008
pw90 12.600
alfa 6.600
FLAGS
il n
in n
dp y
hs nn
PROCESSING
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DISPLAY
sp -250.1
wp 5247.6
rfl 4641.6
rfp 3618.6
rp 41.5
lp 4.5
PLOT
wc 250
sc 0
vs 118
th 3
nm ph
N
Ts
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3.07
1.00
3.05
9
8
7
6
5
4
3
2
1
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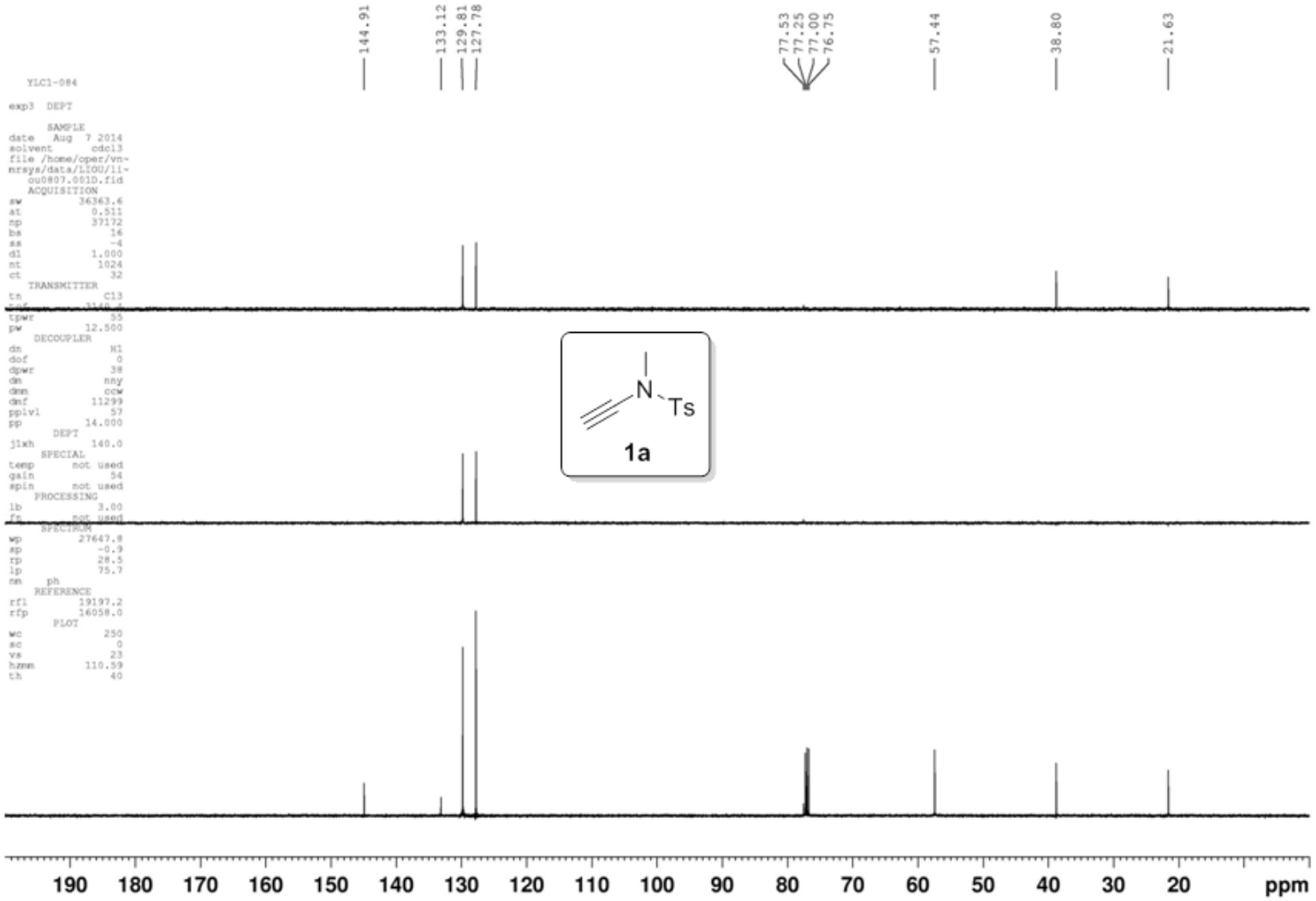
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77.25
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76.75
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38.80
21.63
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date Aug 7 2014
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at 0.511
np 37172
bs 16
ss -4
d1 1.000
nt 1024
ct 32
TRANSMITTER
tn C13
tpwr 55
pw 12.500
DECOUPLER
dn H1
dof 0
dpwr 38
dm nny
dmm ccw
dmf 11299
pplvl 57
pp 14.000
DEPT
j1xh 140.0
SPECIAL
temp not used
gain 54
spin not used
PROCESSING
lb 3.00
fn not used
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wp 27647.8
sp -0.9
rp 28.5
lp 75.7
nm ph
REFERENCE
rfl 19197.2
rfp 16058.0
PLOT
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vs 23
hzmm 110.59
th 40
N
Ts
1a
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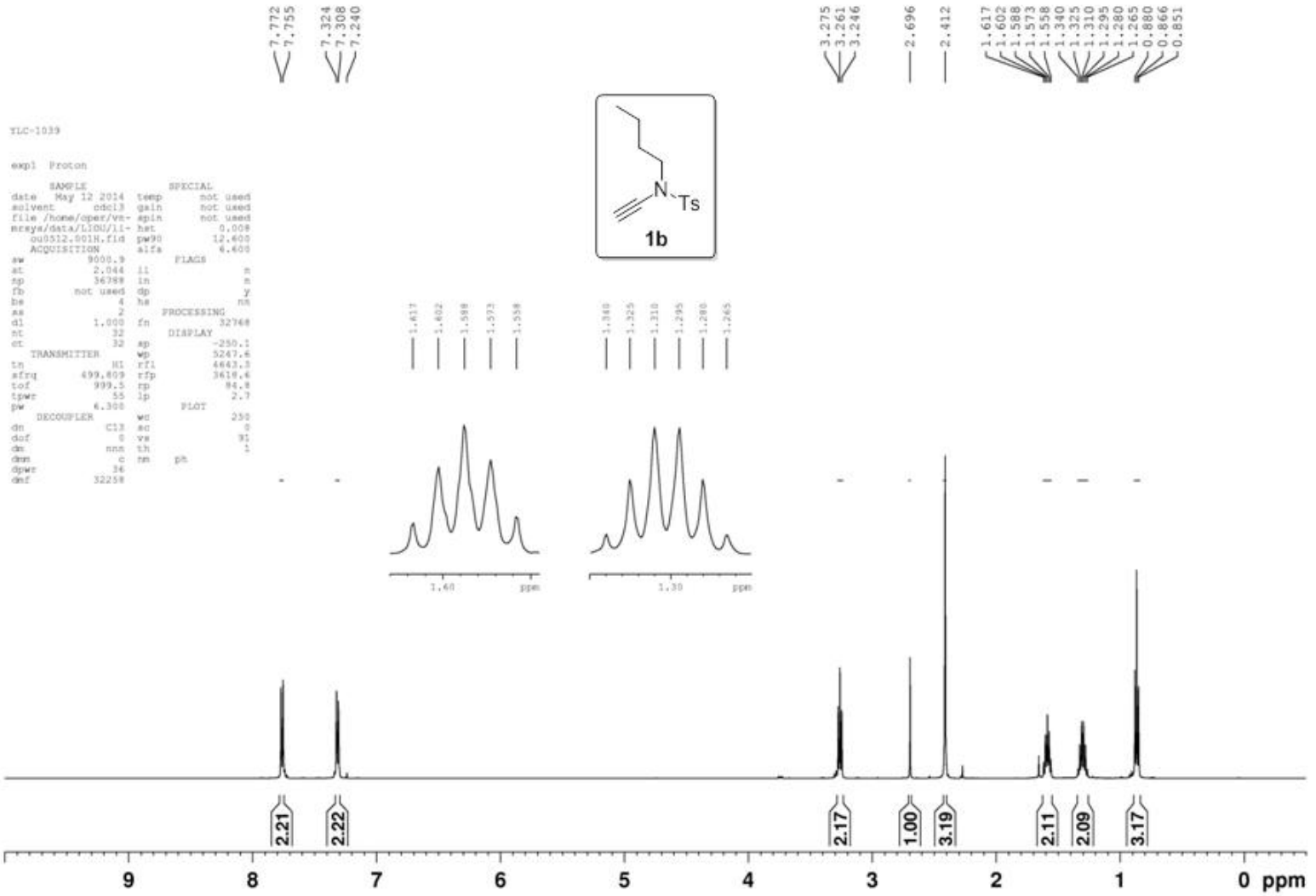
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3.261
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2.412
1.617
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1.588
1.573
1.558
1.340
1.325
1.310
1.295
1.280
1.265
0.880
0.866
0.851
1b
TLC-1039
expl Proton
SAMPLE
date May 12 2014
solvent cdcl3
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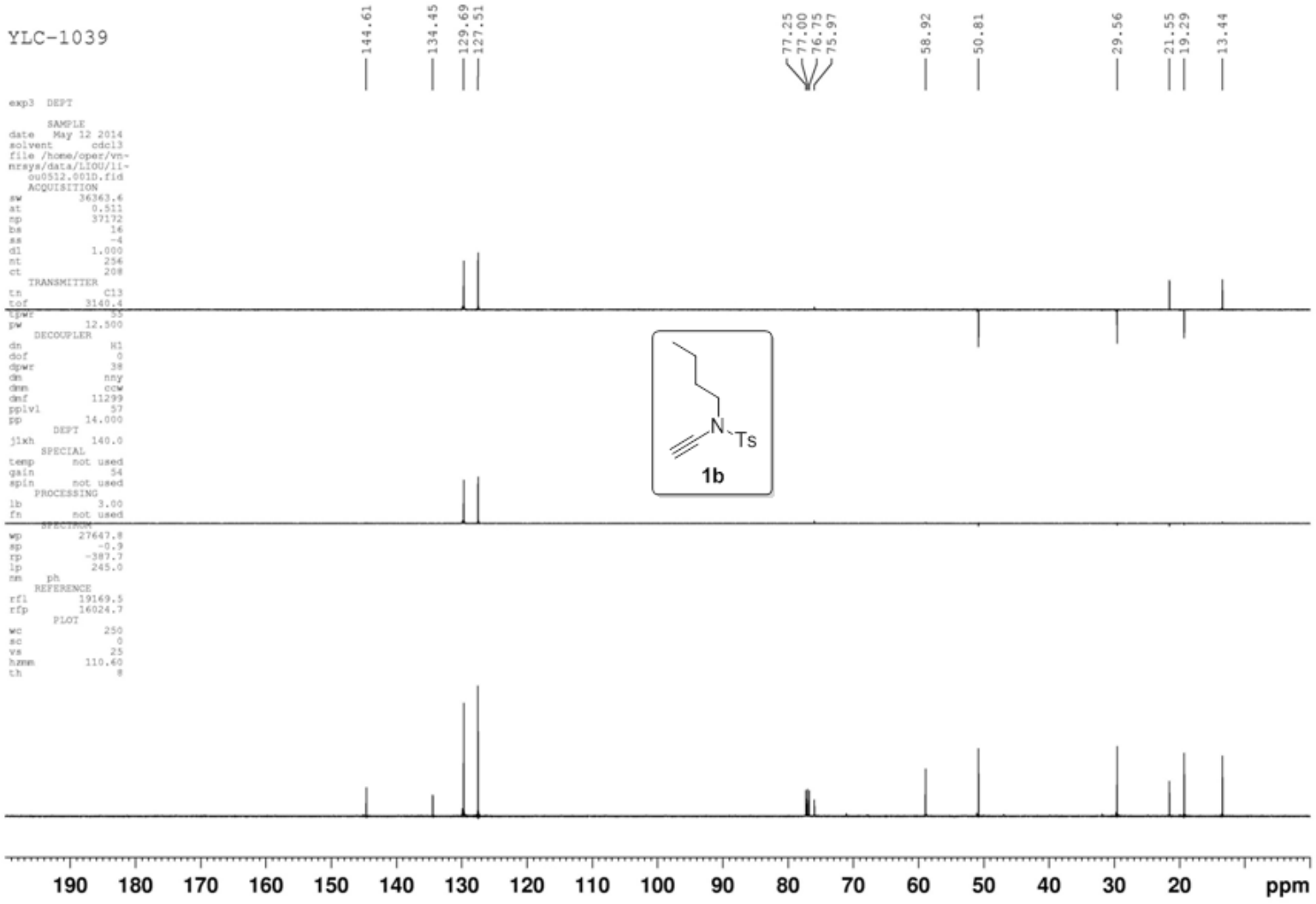
at 2.044
np 36788
fb not used
bs 4
ss 2
d1 1.000
nt 32
ct 32
TRANSMITTER
tn H1
sfrq 499.809
tof 999.5
tpwr 55
pw 6.300
DECOUPLER
dn C13
dof 0
dm nnn
dmm c
dpwr 36
dmf 32258
SPECIAL
temp not used
gain not used
spin not used
hst 0.008
pw90 12.400
alfa 6.400
FLAGS
ll n
in n
dp y
hs nn
PROCESSING
fn 32768
DISPLAY
sp -250.1
wp 5247.6
rfl 4643.3
rfp 3618.4
rp 94.4
lp 2.7
PLOT
wc 250
sc 0
vs 91
th 1
nn ph
1.40
ppm
1.30
ppm
2.21
2.22
2.17
1.00
3.19
2.11
2.09
3.17
9
8
7
6
5
4
3
2
1
0 ppm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134.45
129.69
127.51
77.25
77.00
76.75
75.97
58.92
50.81
29.56
21.55
19.29
13.44
exp3 DEPT
SAMPLE
date May 12 2014
solvent cdcl3
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np 37172
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ss -4
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nt 256
ct 208
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tn C13
tof 3140.4
tpwr 55
pw 12.500
DECOUPLER
dn H1
dof 0
dpwr 38
dm nny
dmm ccw
dmf 11299
pplvl 57
pp 14.000
DEPT
j1xh 140.0
SPECIAL
temp not used
gain 54
spin not used
PROCESSING
lb 3.00
fn not used
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sp -0.9
rp -387.7
lp 245.0
ph
REFERENCE
rfl 19169.5
rfp 16024.7
PLOT
wc 250
sc 0
vs 25
hzmm 110.60
th 8
N
Ts
1b
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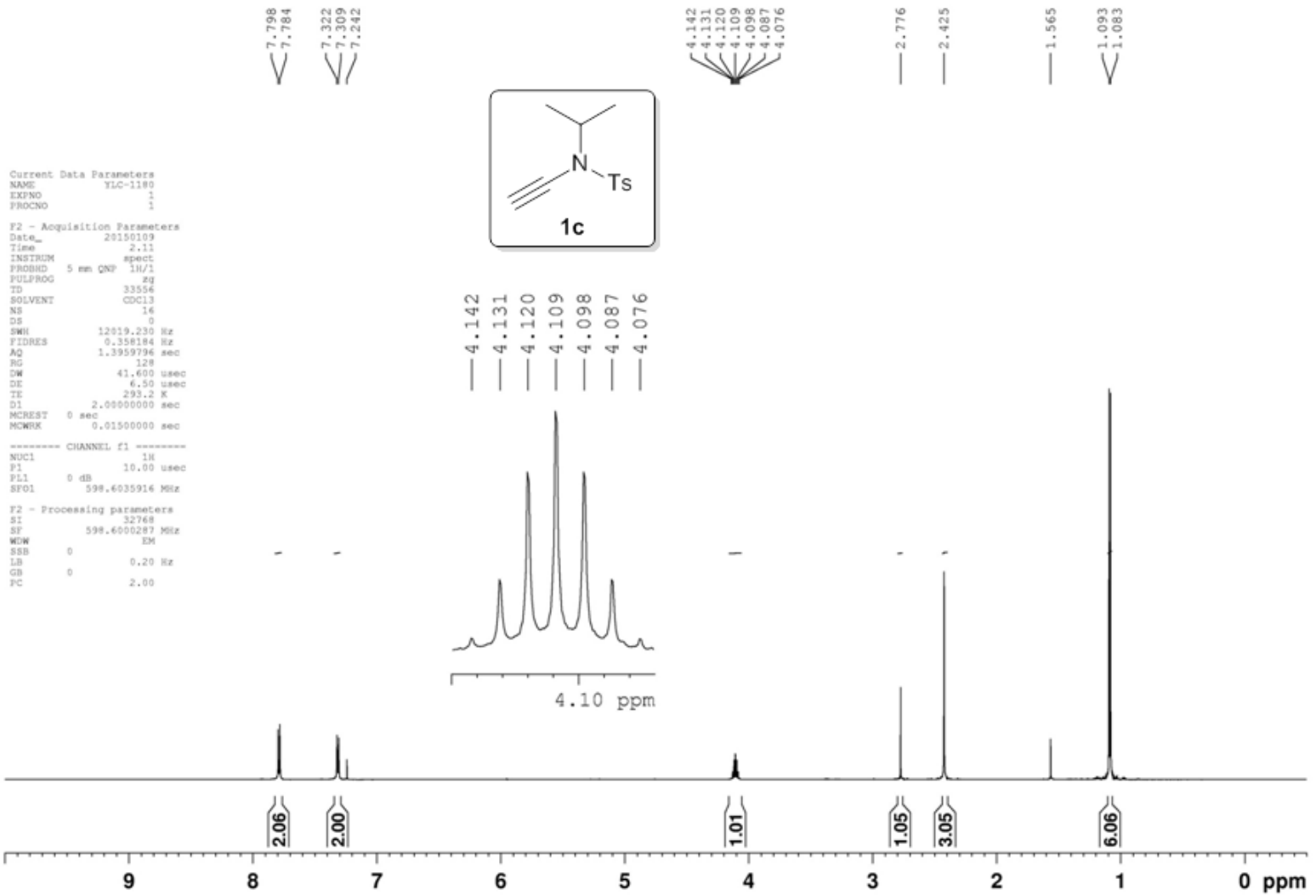
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm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7.322
7.309
7.242
4.142
4.131
4.120
4.109
4.098
4.087
4.076
2.776
2.425
1.565
1.093
1.083
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PROCNO 1
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Time 2.11
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg
TD 33556
SOLVENT CDCl3
NS 16
DS 0
SWH 12019.230 Hz
FIDRES 0.358184 Hz
AQ 1.3959796 sec
RG 128
DW 41.600 usec
DE 6.50 usec
TE 293.2 K
D1 2.00000000 sec
MCREST 0 sec
MCWRK 0.01500000 sec
-------- CHANNEL f1 --------
NUC1 1H
P1 10.00 usec
PL1 0 dB
SFO1 598.6035916 MHz
F2 - Processing parameters
SI 32768
SF 598.6000287 MHz
WDW EM
SSB 0
LB 0.20 Hz
GB 0
PC 2.00
N
Ts
1c
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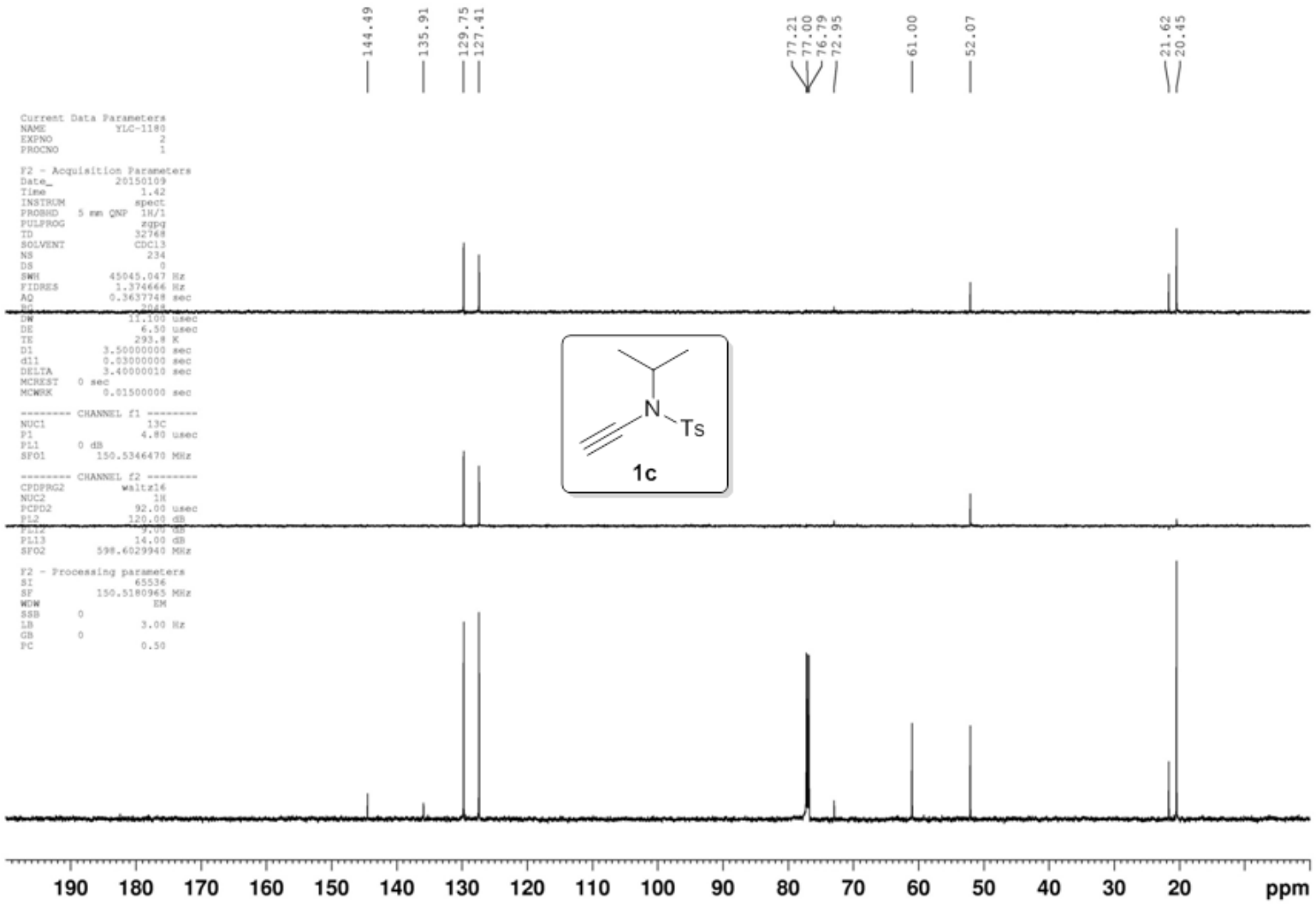
2.00
1.01
1.05
3.05
6.06
9
8
7
6
5
4
3
2
1
0 ppm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TD 32768
SOLVENT CDCl3
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FIDRES 1.374666 Hz
AQ 0.3637748 sec
RG 2048
DW 11.100 usec
DE 6.50 usec
TE 293.8 K
D1 3.50000000 sec
d11 0.03000000 sec
DELTA 3.40000010 sec
MCREST 0 sec
MCWRK 0.01500000 sec
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NUC1 13C
P1 4.80 usec
PL1 0 dB
SFO1 150.5346470 MHz
-------- CHANNEL f2 --------
CPDPRG2 waltz16
NUC2 1H
PCPD2 92.00 usec
PL2 120.00 dB
PL12 9.00 dB
PL13 14.00 dB
SFO2 598.6029940 MHz
F2 - Processing parameters
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SF 150.5180965 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 0.50
N
Ts
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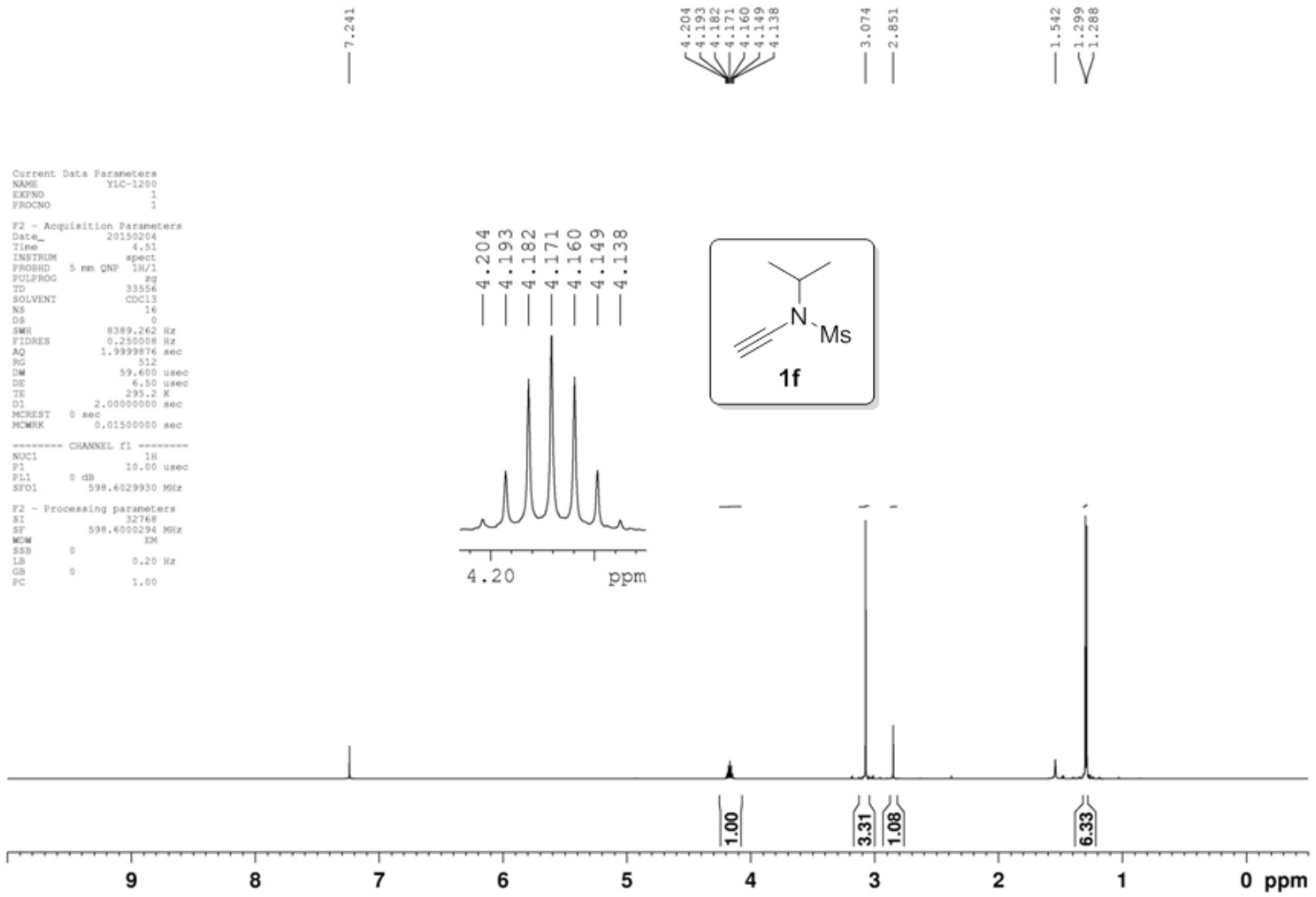
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm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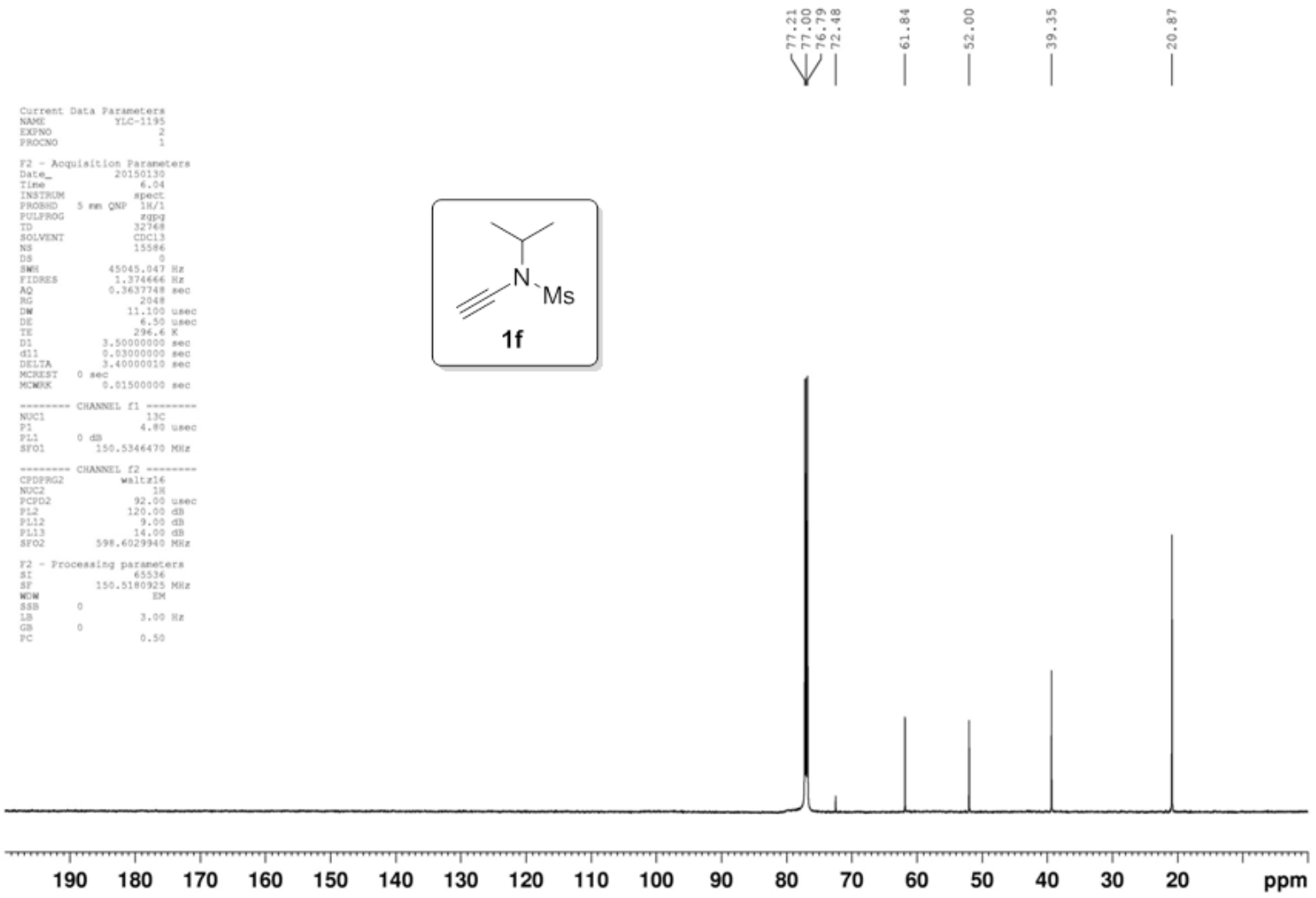
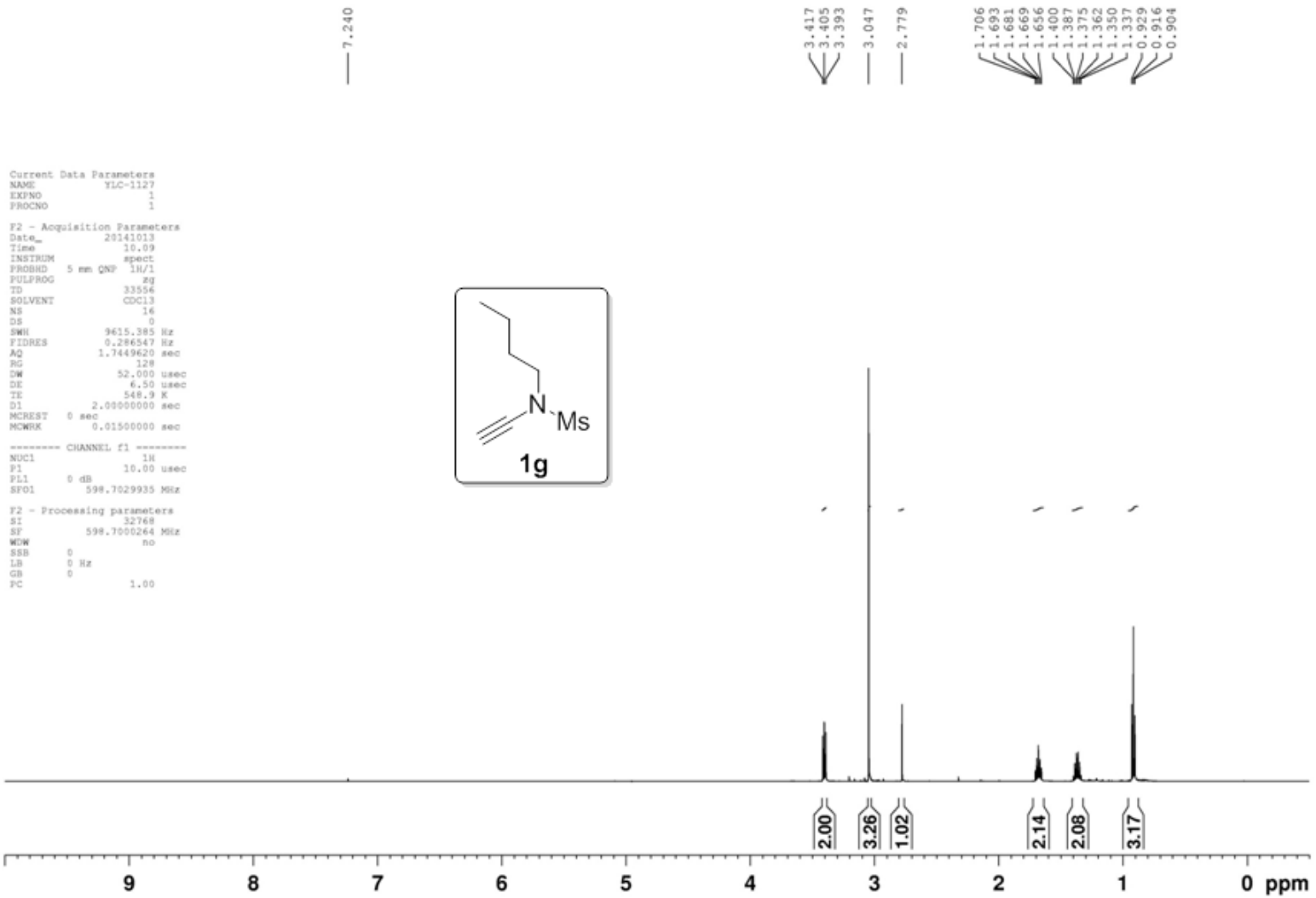
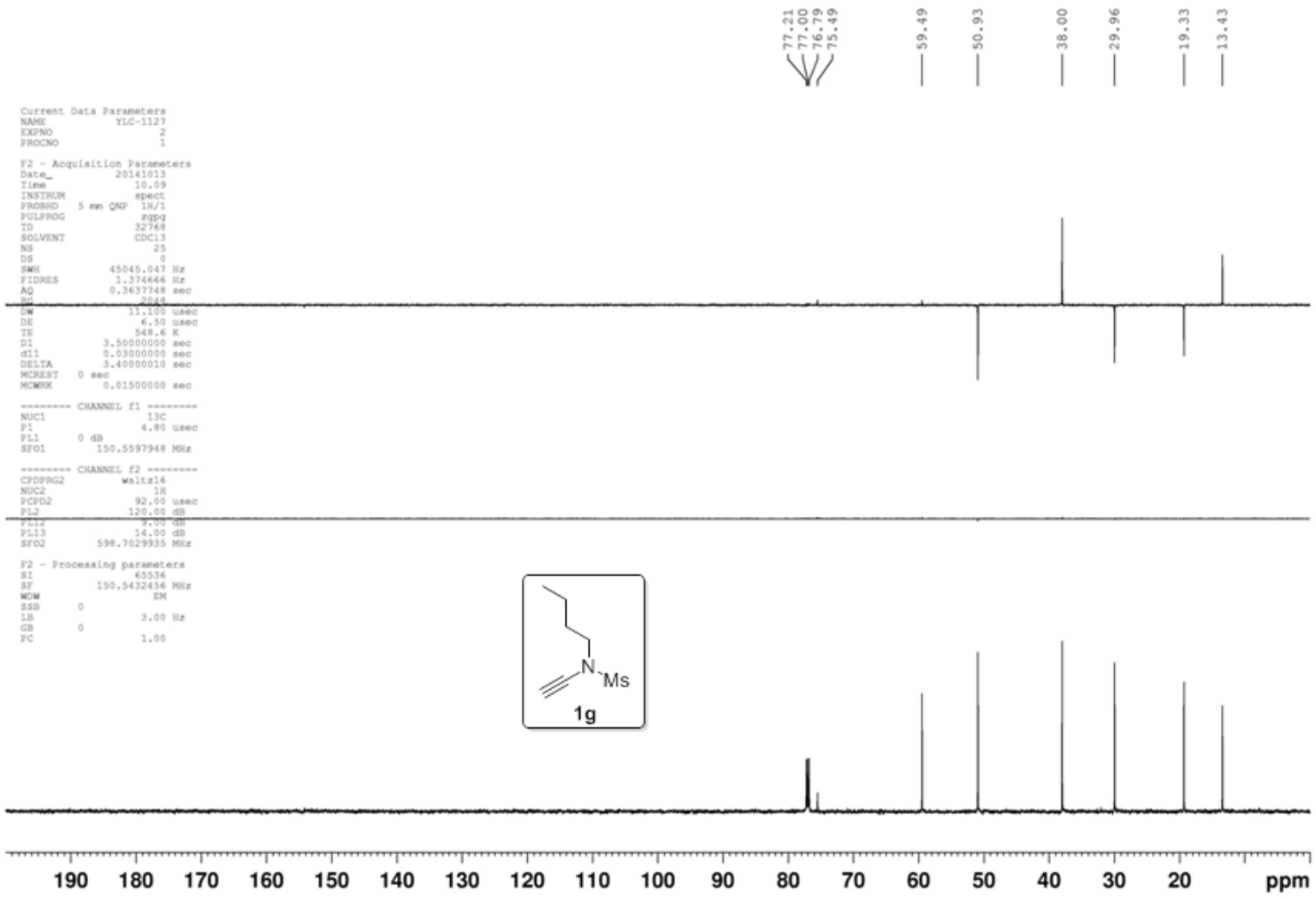
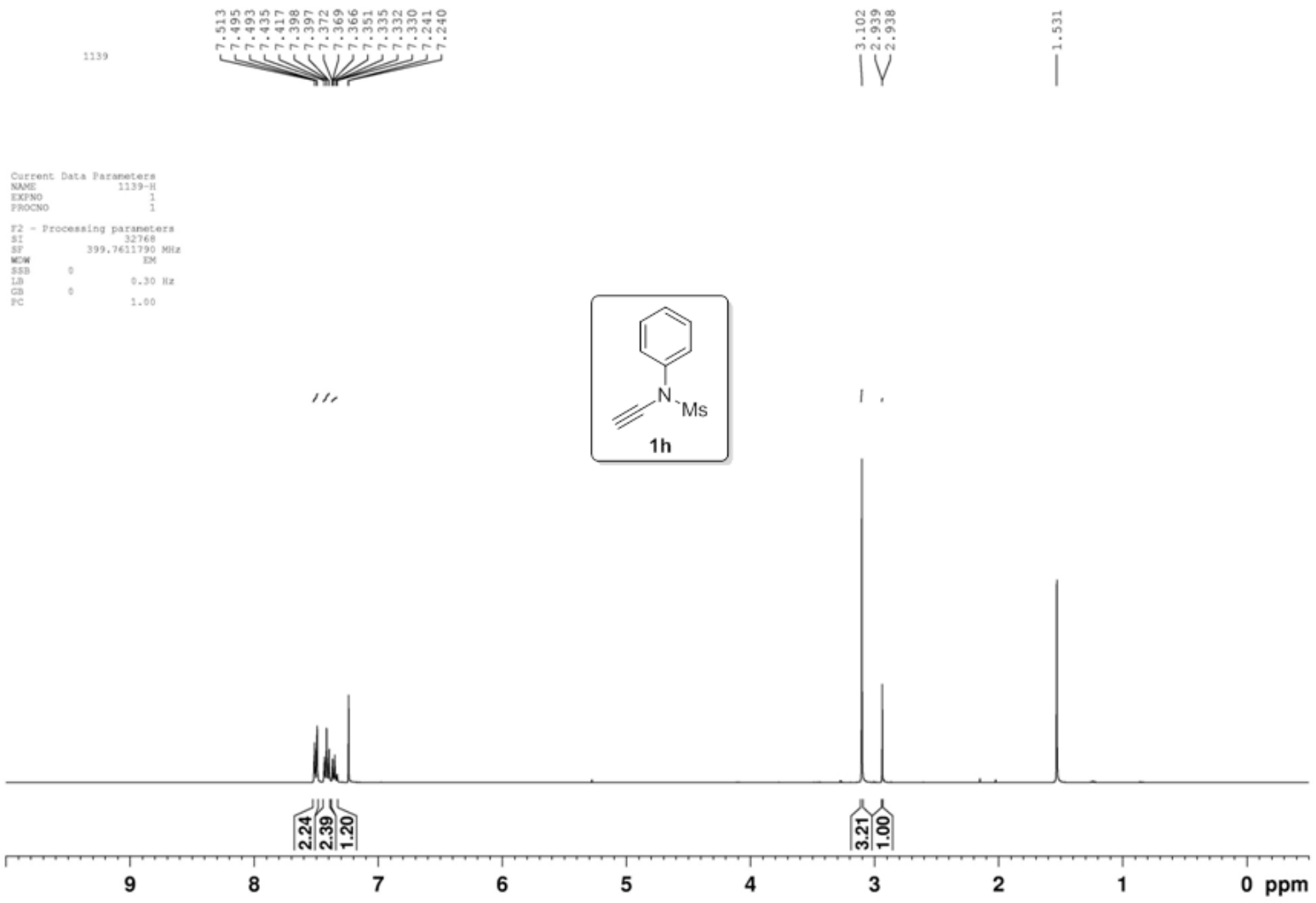
DS 0
SWH 8389.262 Hz
FIDRES 0.250008 Hz
AQ 1.9999876 sec
RG 512
DW 59.600 usec
DE 6.50 usec
TE 295.2 K
D1 2.00000000 sec
MCREST 0 sec
MCWRK 0.01500000 sec
-------- CHANNEL f1 --------
NUC1 1H
P1 10.00 usec
PL1 0 dB
SFO1 598.6029930 MHz
F2 - Processing parameters
SI 32768
SF 598.6000294 MHz
WDW EM
SSB 0
LB 0.20 Hz
GB 0
PC 1.00
4.20
ppm
N
Ms
1f
1.00
3.31
1.08
6.33
9
8
7
6
5
4
3
2
1
0 ppm

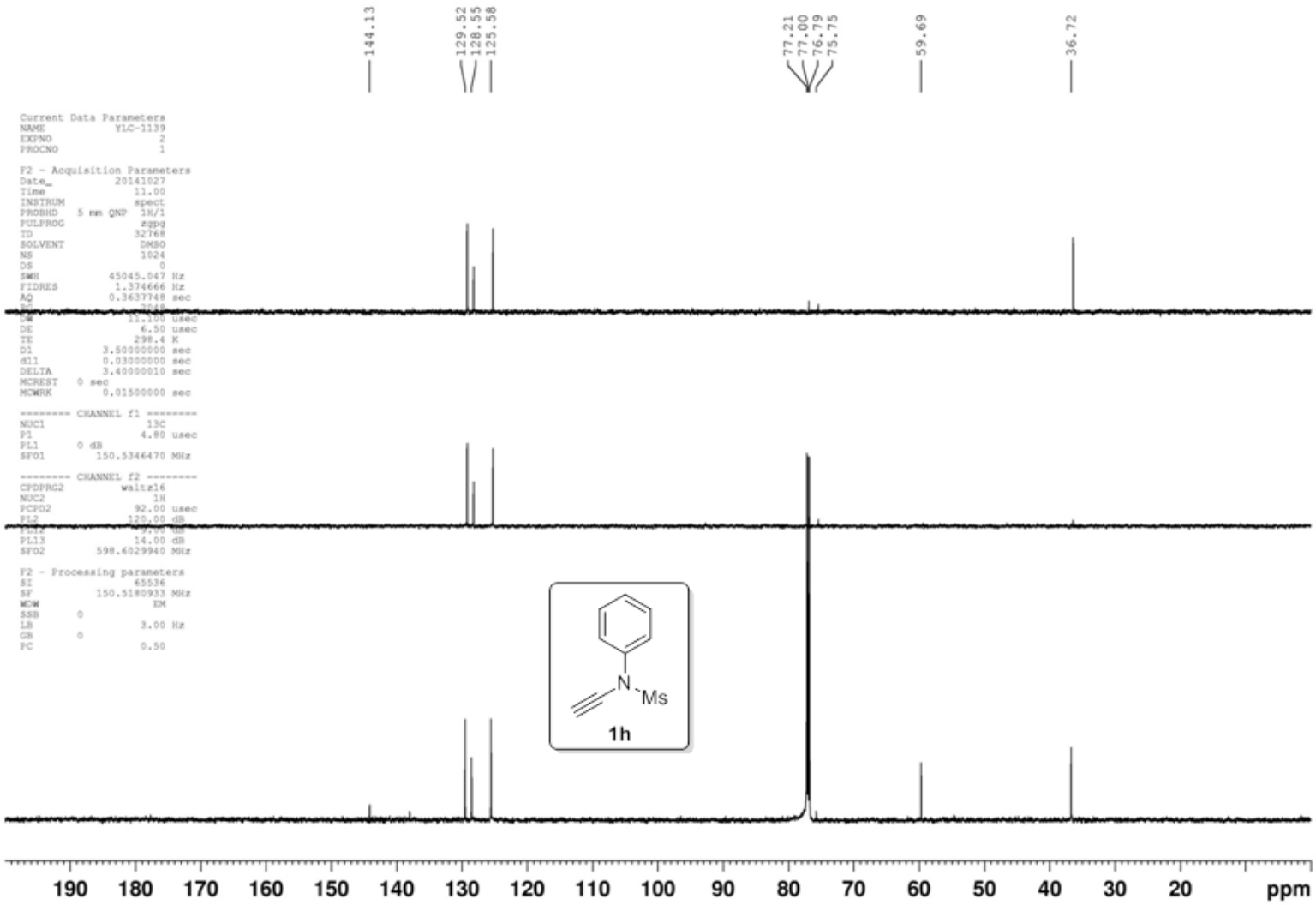


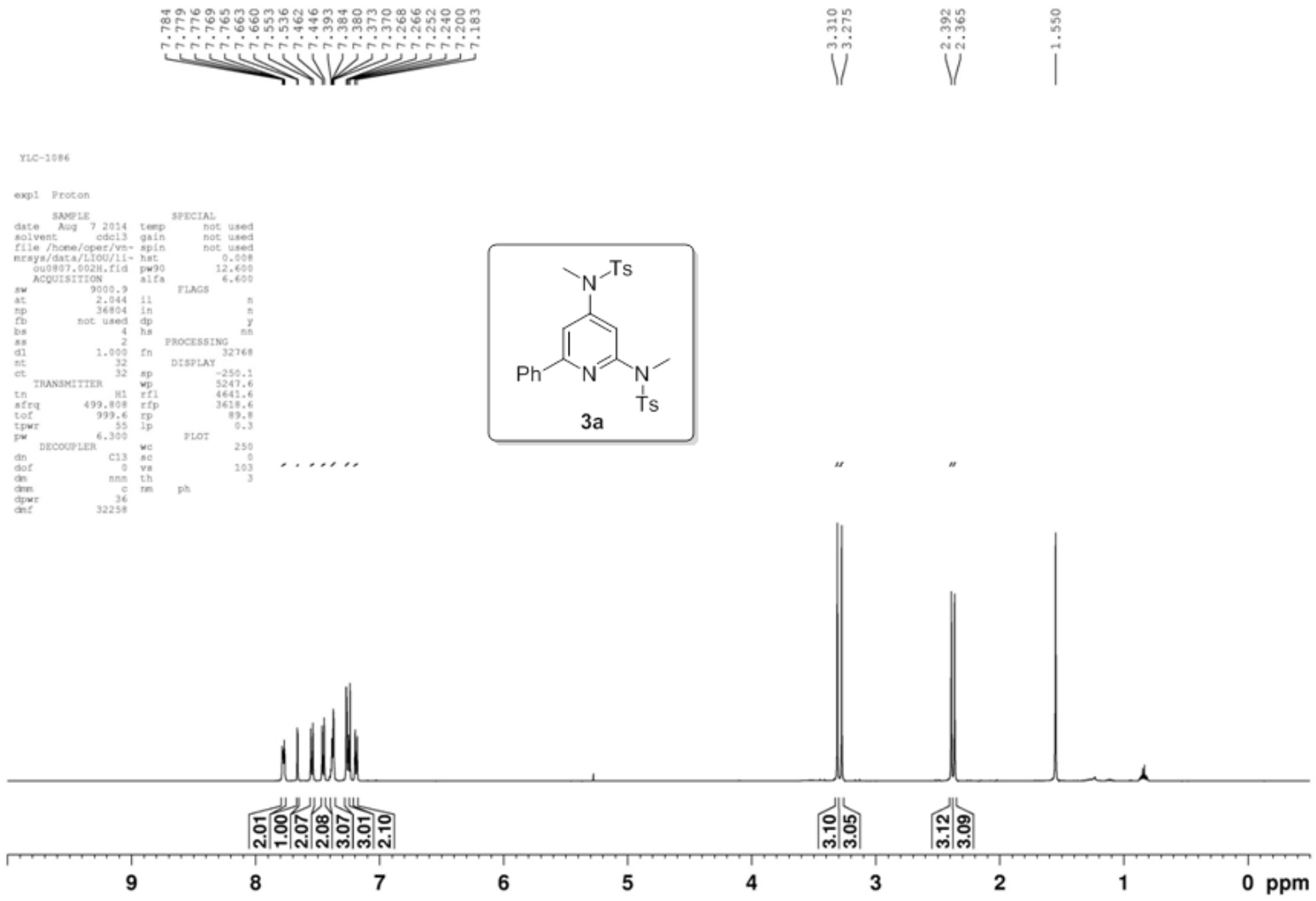

```
Current Data Parameters
NAME            YLC-1195
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20150130
Time                6.04
INSTRUM             spect
PROBHD   5 mm QNP  1H/1
PULPROG             zgpg
TD                 32768
SOLVENT            CDCl3
NS                 15586
DS                     0
SWH           45045.047 Hz
FIDRES         1.374666 Hz
AQ            0.3637748 sec
RG                  2048
DW               11.100 usec
DE                6.50 usec
TE              296.6 K
D1           3.50000000 sec
d11          0.03000000 sec
DELTA        3.40000010 sec
MCREST   0 sec
MCWRK        0.01500000 sec

======== CHANNEL f1 ========
NUC1                13C
P1                 4.80 usec
PL1       0 dB
SFO1        150.5346470 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                1H
PCPD2             92.00 usec
PL2              120.00 dB
PL12               9.00 dB
PL13              14.00 dB
SFO2        598.6029940 MHz

F2 - Processing parameters
SI                 65536
SF          150.5180925 MHz
WDW                   EM
SSB       0
LB                 3.00 Hz
GB        0
PC                 0.50
```

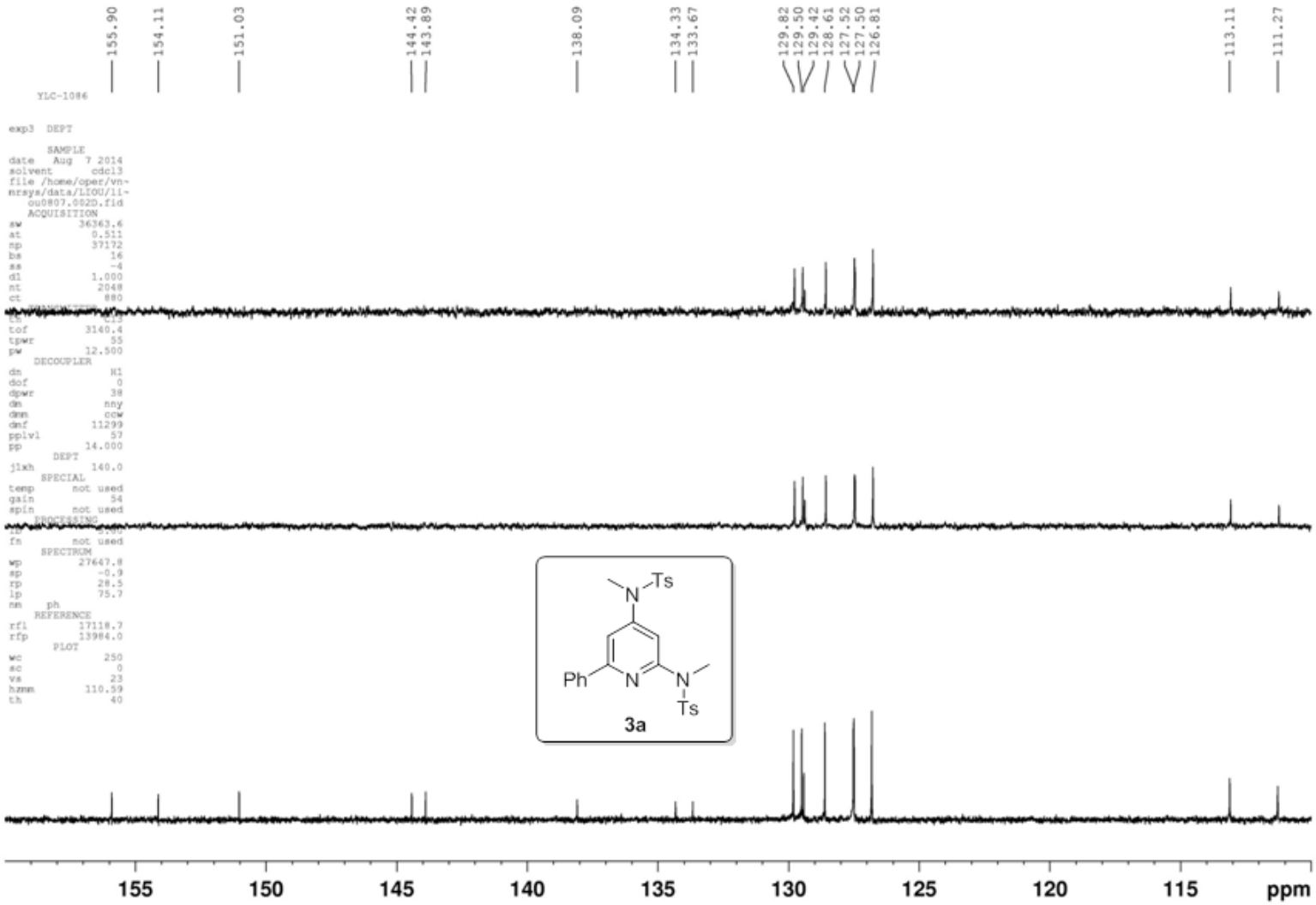

7.240
3.417
3.405
3.393
3.047
2.779
1.706
1.693
1.681
1.669
1.656
1.400
1.387
1.375
1.362
1.350
1.337
0.929
0.916
0.904
Current Data Parameters
NAME YLC-1127
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20141013
Time 10.09
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg
TD 33556
SOLVENT CDCl3
NS 16
DS 0
SWH 9615.385 Hz
FIDRES 0.286547 Hz
AQ 1.7449620 sec
RG 128
DW 52.000 usec
DE 6.50 usec
TE 548.9 K
D1 2.00000000 sec
MCREST 0 sec
MCWRK 0.01500000 sec
-------- CHANNEL f1 --------
NUC1 1H
P1 10.00 usec
PL1 0 dB
SFO1 598.7029935 MHz
F2 - Processing parameters
SI 32768
SF 598.7000264 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 1.00
N
Ms
1g
2.00
3.26
1.02
2.14
2.08
3.17
9
8
7
6
5
4
3
2
1
0 ppm

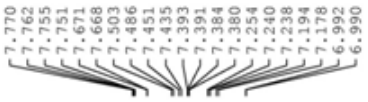

77.21
77.00
76.79
75.49
59.49
50.93
38.00
29.96
19.33
13.43
Current Data Parameters
NAME YLC-1127
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20141013
Time 10.09
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 25
DS 0
SWH 45045.047 Hz
FIDRES 1.374666 Hz
AQ 0.3637748 sec
RG 2048
DW 11.100 usec
DE 6.50 usec
TE 548.6 K
D1 3.50000000 sec
d11 0.03000000 sec
DELTA 3.40000010 sec
MCREST 0 sec
MCWRK 0.01500000 sec
-------- CHANNEL f1 --------
NUC1 13C
P1 4.80 usec
PL1 0 dB
SFO1 150.5597948 MHz
-------- CHANNEL f2 --------
CPDPRG2 waltz16
NUC2 1H
PCPD2 92.00 usec
PL2 120.00 dB
PL12 9.00 dB
PL13 14.00 dB
SFO2 598.7029935 MHz
F2 - Processing parameters
SI 65536
SF 150.5432456 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
N
Ms
1g
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

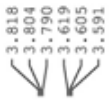

1139
7.513
7.495
7.493
7.435
7.417
7.398
7.397
7.372
7.369
7.366
7.351
7.335
7.332
7.330
7.241
7.240
3.102
2.939
2.938
1.531
Current Data Parameters
NAME 1139-H
EXPNO 1
PROCNO 1
F2 - Processing parameters
SI 32768
SF 399.7611790 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
N
Ms
1h
2.24
2.39
1.20
3.21
1.00
9
8
7
6
5
4
3
2
1
0 ppm

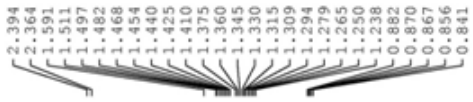

144.13
129.52
128.55
125.58
77.21
77.00
76.79
75.75
59.69
36.72
Current Data Parameters
NAME YLC-1139
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20141027
Time 11.00
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT DMSO
NS 1024
DS 0
SWH 45045.047 Hz
FIDRES 1.374666 Hz
AQ 0.3637748 sec
RG 2048
DW 11.100 usec
DE 6.50 usec
TE 298.4 K
D1 3.50000000 sec
d11 0.03000000 sec
DELTA 3.40000010 sec
MCREST 0 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 4.80 usec
PL1 0 dB
SFO1 150.5346470 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 92.00 usec
PL2 120.00 dB
PL12 16.00 dB
PL13 14.00 dB
SFO2 598.6029940 MHz
F2 - Processing parameters
SI 65536
SF 150.5180933 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 0.50
N
Ms
1h
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm


7.784
7.779
7.776
7.769
7.765
7.663
7.660
7.553
7.536
7.462
7.446
7.393
7.384
7.380
7.373
7.370
7.268
7.266
7.252
7.240
7.200
7.183
3.310
3.275
2.392
2.365
1.550
YLC-1086
exp1 Proton
SAMPLE
date Aug 7 2014
solvent cdcl3
file /home/oper/vn-mrsys/data/LIOU/li-ou0807.002H.fid
ACQUISITION
sw 9000.9
at 2.044
np 36804
fb not used
bs 4
ss 2
d1 1.000
nt 32
ct 32
TRANSMITTER
tn H1
sfrq 499.808
tof 999.6
tpwr 55
pw 6.300
DECOUPLER
dn C13
dof 0
dm nnn
dmm c
dpwr 36
dmf 32258
SPECIAL
temp not used
gain not used
spin not used
hst 0.008
pw90 12.600
alfa 6.600
FLAGS
il n
in n
dp y
hs nn
PROCESSING
fn 32768
DISPLAY
sp -250.1
wp 5247.6
rf1 4641.6
rfp 3618.6
rp 89.8
lp 0.3
PLOT
wc 250
sc 0
vs 103
th 3
nm ph
N
Ts
Ph
N
N
Ts
3a
2.01
1.00
2.07
2.08
3.07
3.01
2.10
3.10
3.05
3.12
3.09
9
8
7
6
5
4
3
2
1
0 ppm


155.90
154.11
151.03
144.42
143.89
138.09
134.33
133.67
129.82
129.50
129.42
128.61
127.52
127.50
126.81
113.11
111.27
YLC-1086
exp3 DEPT
SAMPLE
date Aug 7 2014
solvent cdcl3
file /home/oper/vnmrsys/data/LIOU/liou0807.002D.fid
ACQUISITION
sw 36363.6
at 0.511
np 37172
bs 16
ss -4
d1 1.000
nt 2048
ct 880
tof 3140.4
tpwr 55
pw 12.500
DECOUPLER
dn H1
dof 0
dpwr 38
dn nny
dmm ccw
dmf 11299
pplvl 57
pp 14.000
DEPT
jlxh 140.0
SPECIAL
temp not used
gain 54
spin not used
PROCESSING
fn not used
SPECTRUM
wp 27647.8
sp -0.9
rp 28.5
lp 75.7
nn ph
REFERENCE
rfl 17118.7
rfp 13984.0
PLOT
wc 250
sc 0
vs 23
hzmm 110.59
th 40
N
Ts
Ph
N
N
Ts
3a
155
150
145
140
135
130
125
120
115
ppm



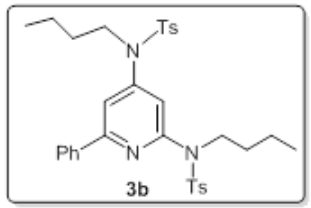



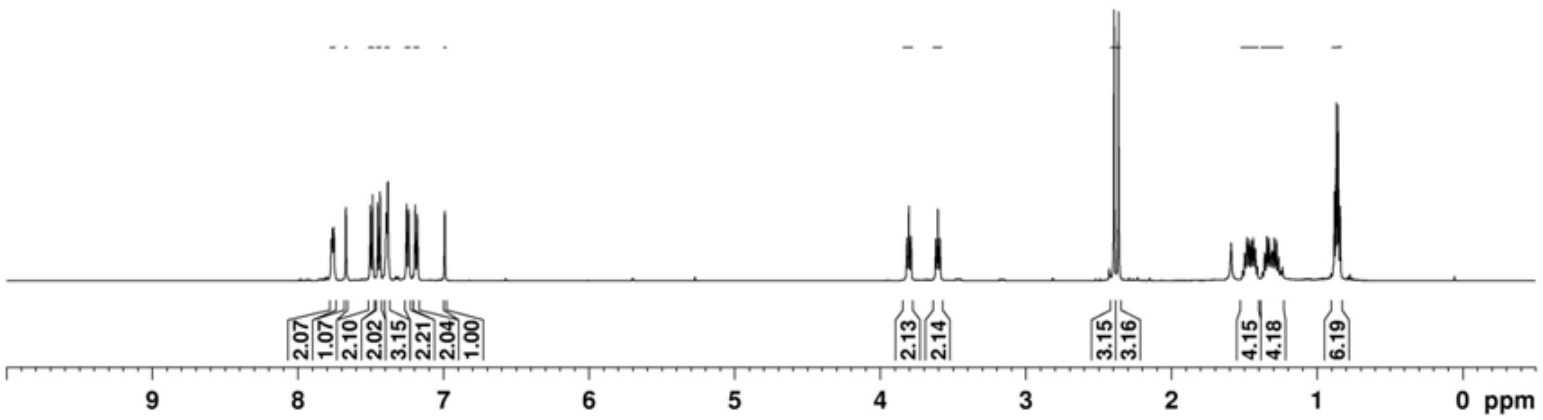

YLC-1041-2

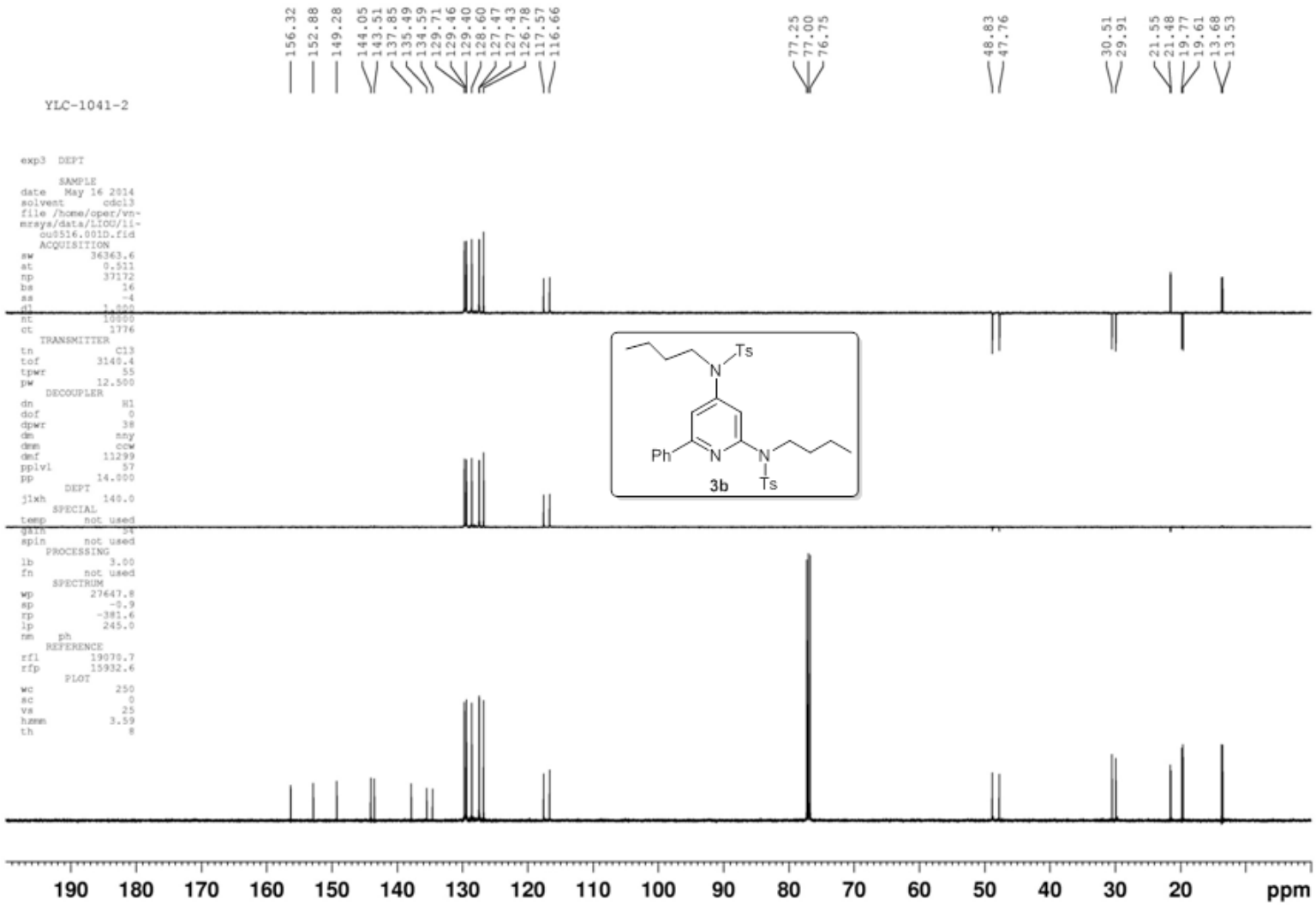
exp1 Proton

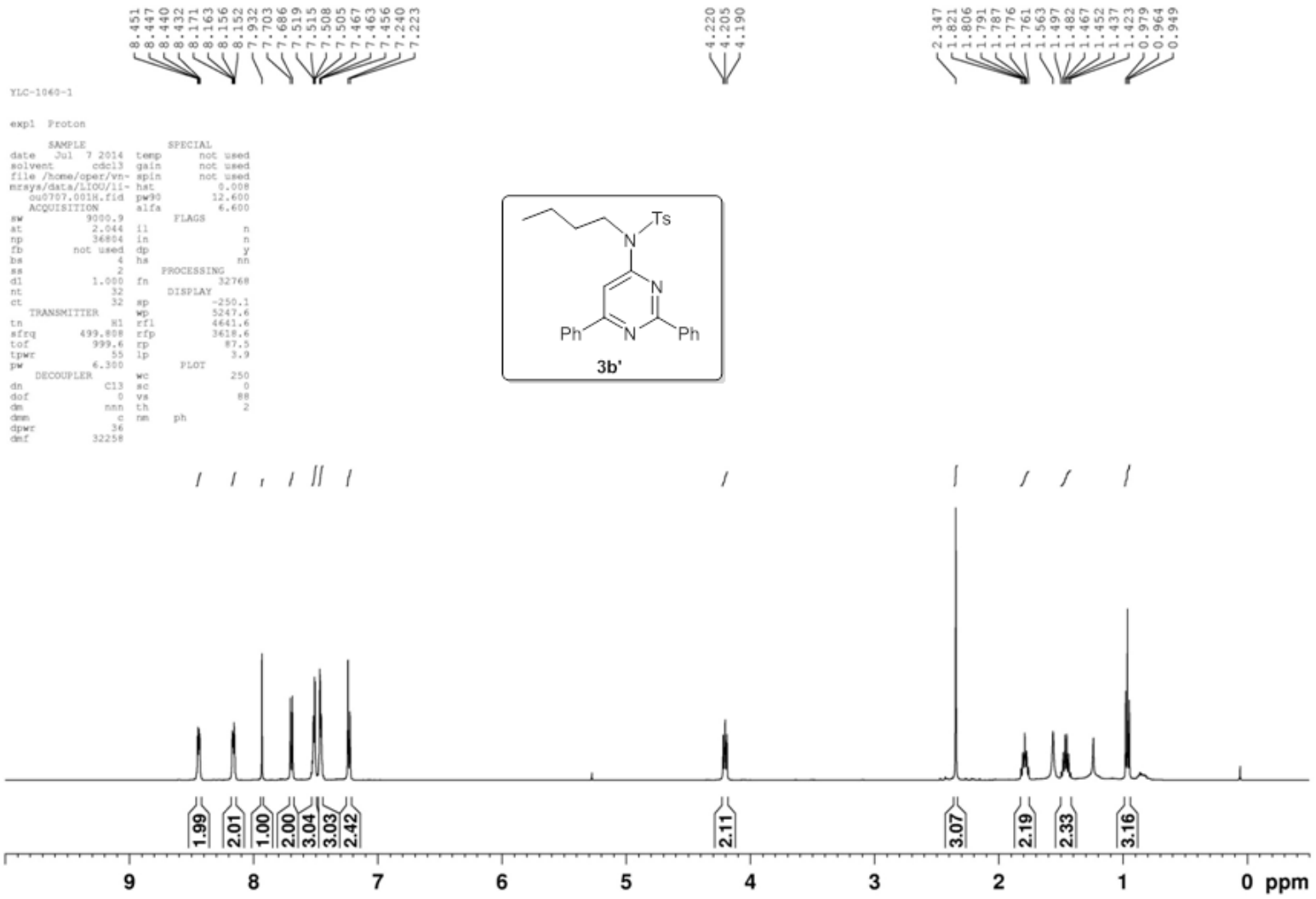
| SAMPLE | | SPECIAL | |
|---|---|---|---|
| date | May 12 2014 | temp | not used |
| solvent | cdcl3 | gain | not used |
| file | /home/oper/vn-mrsys/data/LIOU/li-ou0512.001H.fid | spin | not used |
| | | hst | 0.008 |
| ACQUISITION | | pw90 | 12.600 |
| | | alfa | 6.600 |
| sw | 9000.9 | FLAGS | |
| at | 2.044 | il | n |
| np | 36788 | in | n |
| fb | not used | dp | y |
| bs | 4 | hs | nn |
| ss | 2 | PROCESSING | |
| dl | 1.000 | fn | 32768 |
| nt | 32 | DISPLAY | |
| ct | 32 | sp | -250.1 |
| TRANSMITTER | | wp | 5247.6 |
| tn | H1 | rf1 | 4643.3 |
| sfrq | 499.809 | rfp | 3618.6 |
| tof | 999.5 | rp | 84.3 |
| tpwr | 55 | lp | 2.7 |
| pw | 6.300 | PLOT | |
| DECOUPLER | | wc | 250 |
| dn | C13 | sc | 0 |
| dof | 0 | vs | 91 |
| dm | nnn | th | 1 |
| dmm | c | nm | ph |
| dpwr | 36 | | |
| dmf | 32258 | | |

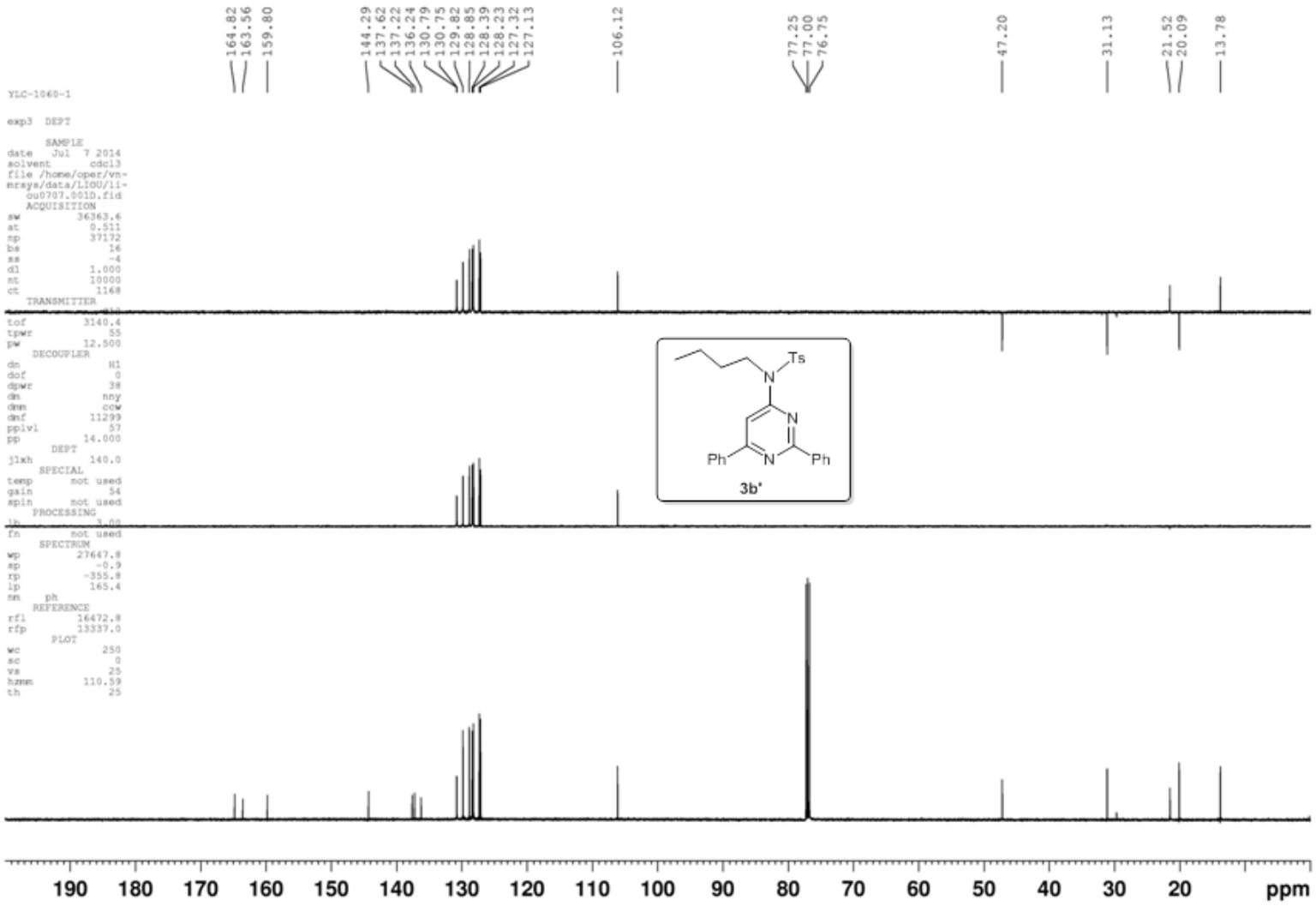


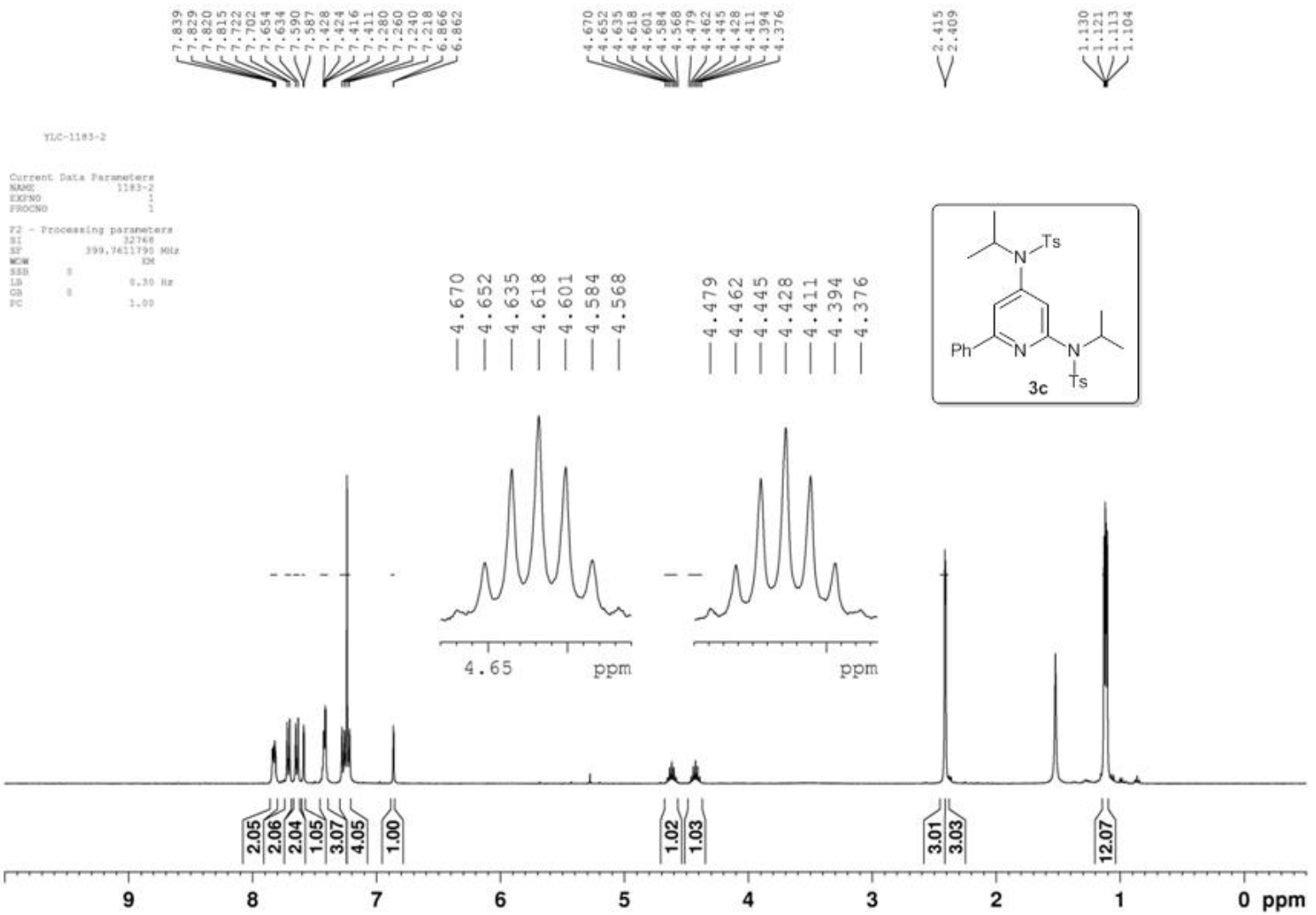

3b

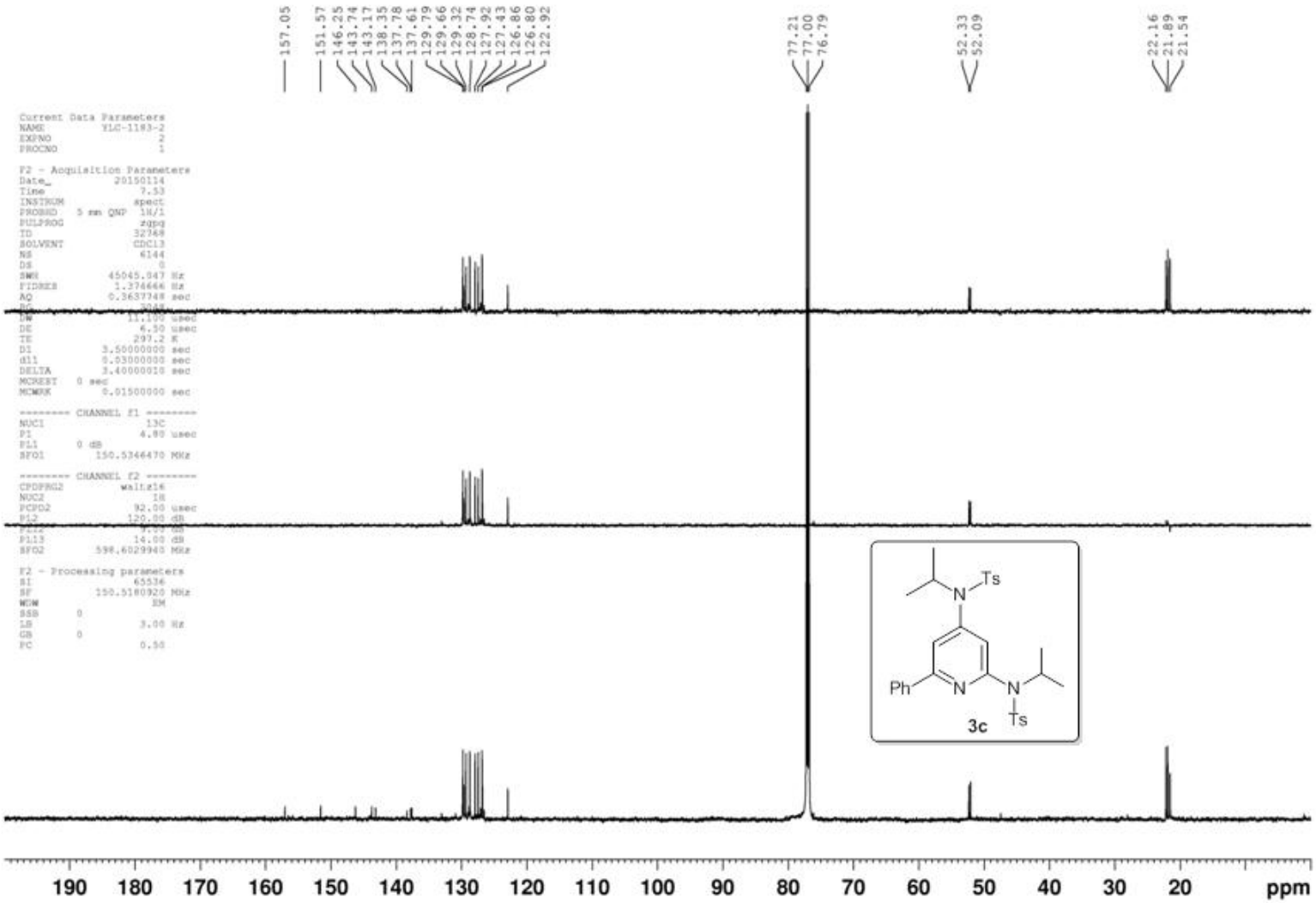


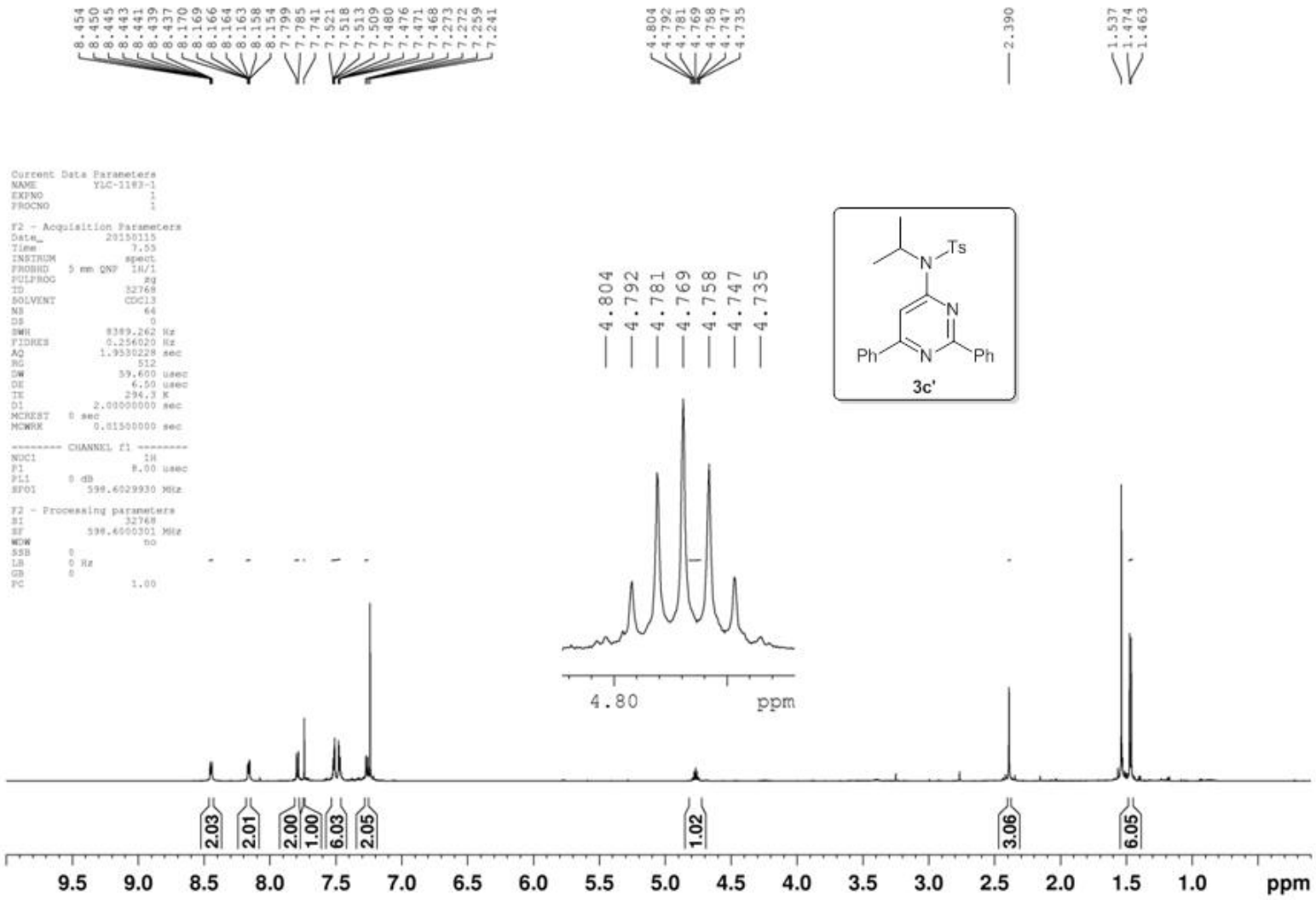

156.32
152.88
149.28
144.05
143.51
137.85
135.49
134.59
129.71
129.46
129.40
128.60
127.47
127.43
126.78
117.57
116.66
77.25
77.00
76.75
48.83
47.76
30.51
29.91
21.55
21.48
19.77
19.61
13.68
13.53
YLC-1041-2
exp3 DEPT
SAMPLE
date May 16 2014
solvent cdcl3
file /home/oper/vnmrsys/data/LIOU/liou516.001D.fid
ACQUISITION
sw 36363.6
at 0.511
np 37172
bs 16
as -4
d1 1.000
nt 10000
ct 1776
TRANSMITTER
tn C13
tof 3140.4
tpwr 55
pw 12.500
DECOUPLER
dn H1
dof 0
dpwr 38
dm nny
dmm ccw
dmf 11299
pplvl 57
pp 14.000
DEPT
j1xh 140.0
SPECIAL
temp not used
gain -- 54
spin not used
PROCESSING
lb 3.00
fn not used
SPECTRUM
wp 27647.8
sp -0.9
rp -381.6
lp 245.0
nm ph
REFERENCE
rf1 19079.7
rfp 15932.6
PLOT
wc 250
sc 0
vs 25
hzmm 3.59
th 8
N
Ts
Ph
N
N
Ts
3b
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

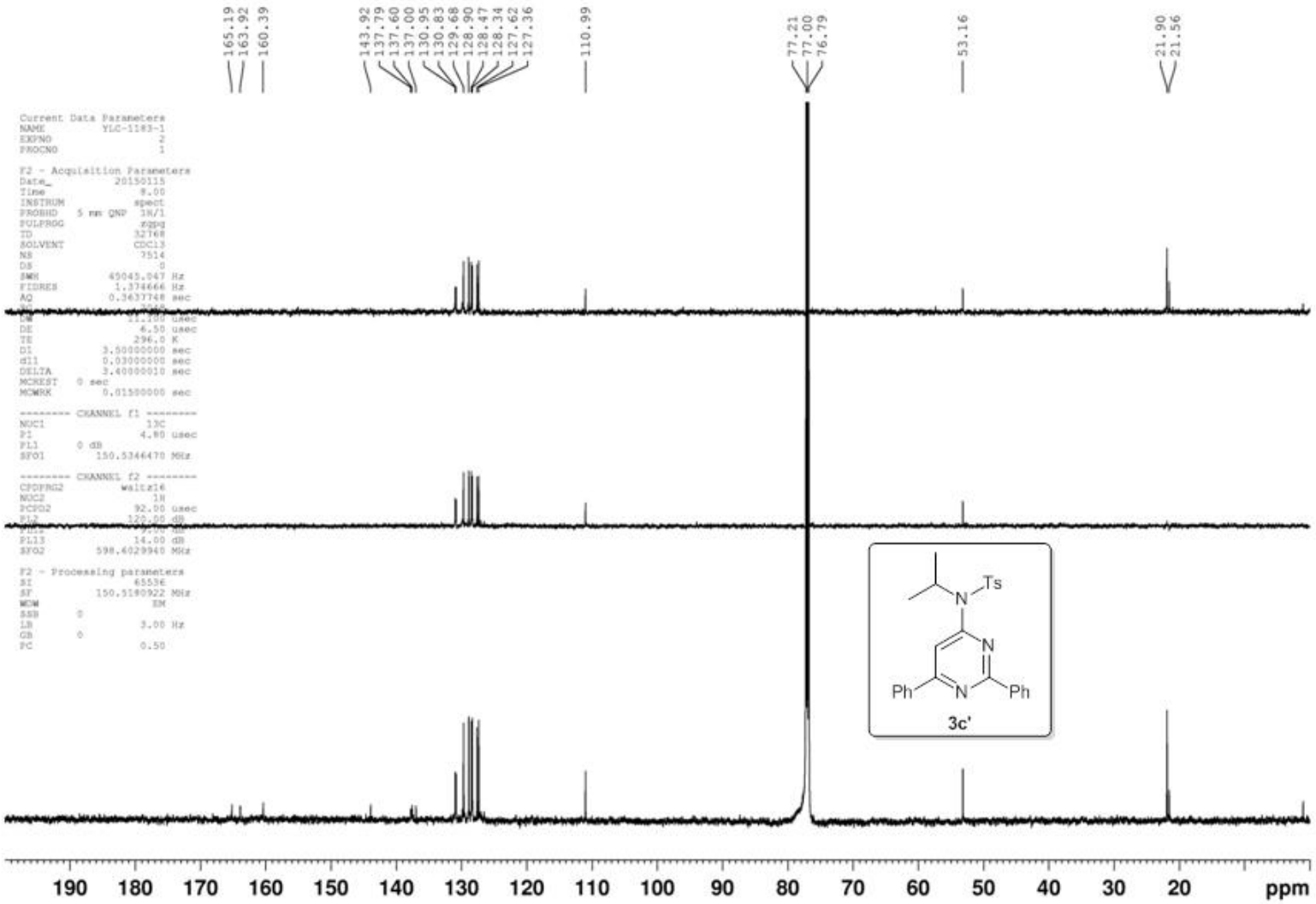

8.451
8.447
8.440
8.432
8.171
8.163
8.156
8.152
7.932
7.703
7.686
7.519
7.515
7.508
7.505
7.467
7.463
7.456
7.240
7.223
4.220
4.205
4.190
2.347
1.821
1.806
1.791
1.787
1.776
1.761
1.563
1.497
1.482
1.467
1.452
1.437
1.423
0.979
0.964
0.949
YLC-1060-1
expl Proton
SAMPLE
date Jul 7 2014
solvent cdcl3
file /home/oper/vn-mrsys/data/LIOU/li-ou0707.001H.fid
ACQUISITION
sw 9000.9
at 2.044
np 36804
fb not used
bs 4
ss 2
d1 1.000
nt 32
ct 32
TRANSMITTER
tn H1
sfrq 499.808
tof 999.6
tpwr 55
pw 6.300
DECOUPLER
dn C13
dof 0
dm nnn
dmm c
dpwr 36
dmf 32258
SPECIAL
temp not used
gain not used
spin not used
hst 0.008
pw90 32.600
alfa 6.600
FLAGS
il n
in n
dp y
hs nn
PROCESSING
fn 32768
DISPLAY
sp -250.1
wp 5247.6
rfl 4641.6
rfp 3618.6
rp 87.5
lp 3.9
PLOT
wc 250
sc 0
vs 88
th 2
nm ph
Ts
N
N
Ph
N
Ph
3b'
1.99
2.01
1.00
2.00
3.04
3.03
2.42
2.11
3.07
2.19
2.33
3.16
9
8
7
6
5
4
3
2
1
0 ppm

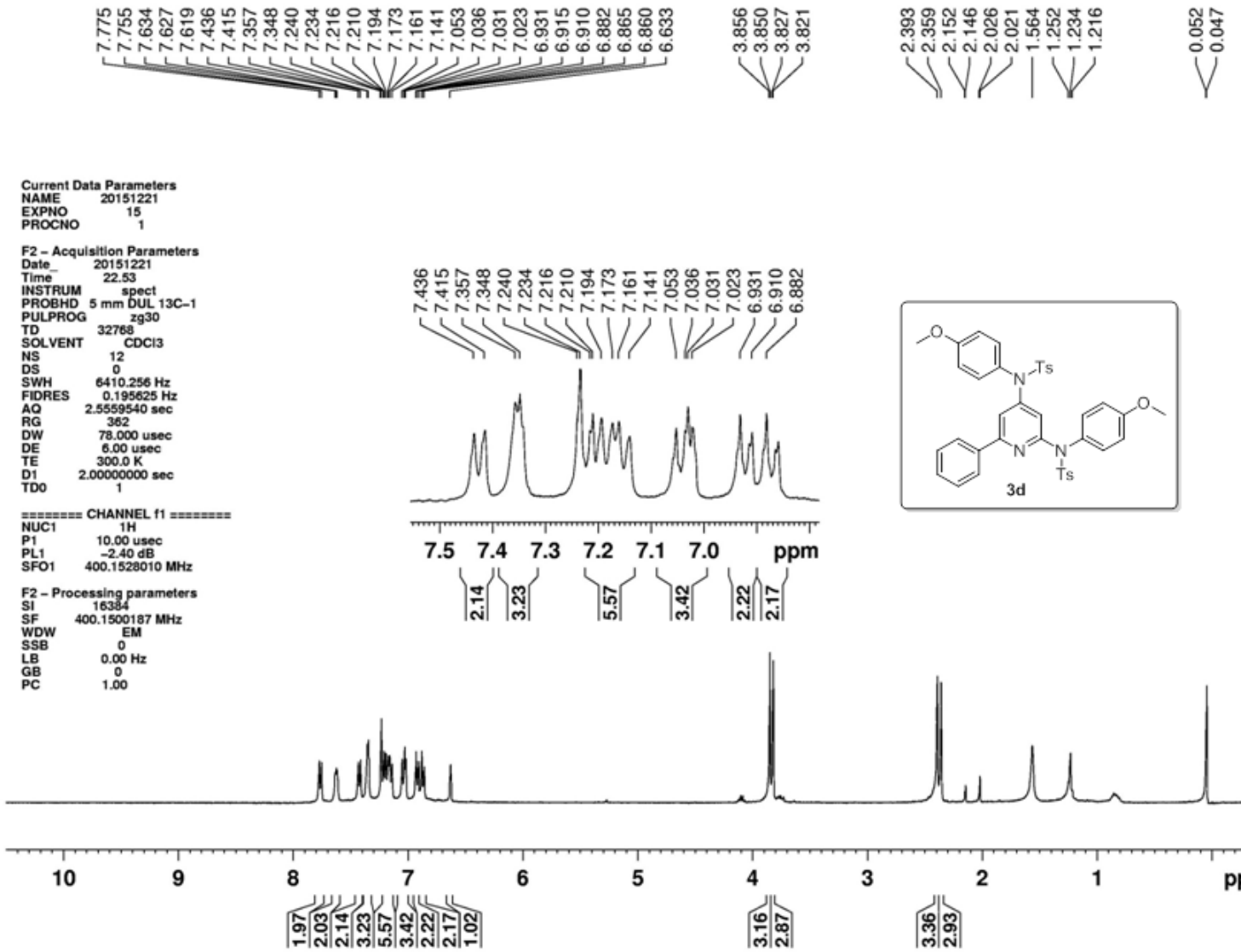

164.82
163.56
159.80
144.29
137.62
137.22
136.24
130.79
130.75
129.82
128.85
128.39
128.23
127.32
127.13
106.12
77.25
77.00
76.75
47.20
31.13
21.52
20.09
13.78
YLC-1060-1
exp3 DEPT
SAMPLE
date Jul 7 2014
solvent cdcl3
file /home/oper/vnmrsys/data/LIOU/liou0707.001D.fid
ACQUISITION
sw 36363.6
at 0.511
np 37172
bs 16
ss -4
d1 1.000
nt 10000
ct 1168
TRANSMITTER
tof 3140.4
tpwr 55
pw 12.500
DECOUPLER
dn H1
dof 0
dpwr 38
dn nny
dmm ccw
dmf 11299
pplvl 57
pp 14.000
DEPT
jlxh 140.0
SPECIAL
temp not used
gain 54
spin not used
PROCESSING
lb 3.00
fn not used
SPECTRUM
wp 27647.8
sp -0.9
rp -355.8
lp 165.4
nn ph
REFERENCE
rfl 16472.8
rfp 13337.0
PLOT
wc 250
sc 0
vs 25
hzmm 110.59
th 25
Ts
N
N
Ph
N
Ph
3b'
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

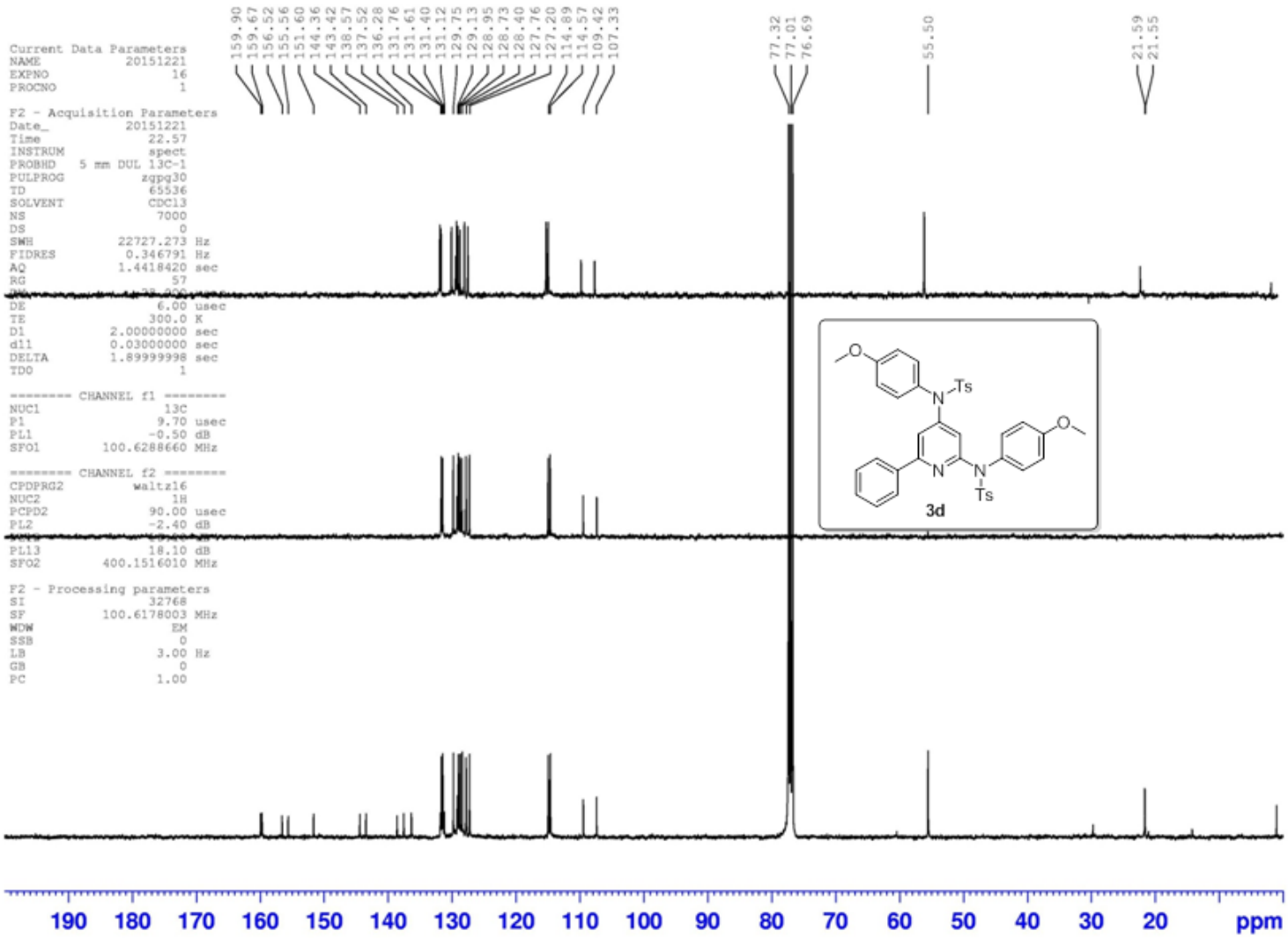

7.839
7.829
7.820
7.815
7.722
7.702
7.654
7.634
7.590
7.587
7.428
7.424
7.416
7.411
7.280
7.260
7.240
7.218
6.866
6.862
4.670
4.652
4.635
4.618
4.601
4.584
4.568
4.479
4.462
4.445
4.428
4.411
4.394
4.376
2.415
2.409
1.130
1.121
1.113
1.104
YLC-1183-2
Current Data Parameters
NAME 1183-2
EXPNO 1
PROCNO 1
F2 - Processing parameters
SI 32768
SF 399.7611790 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
4.65 ppm
ppm
Ts
N
Ph
3c
2.05
2.06
2.04
1.05
3.07
4.05
1.00
1.02
1.03
3.01
3.03
12.07
9
8
7
6
5
4
3
2
1
0 ppm

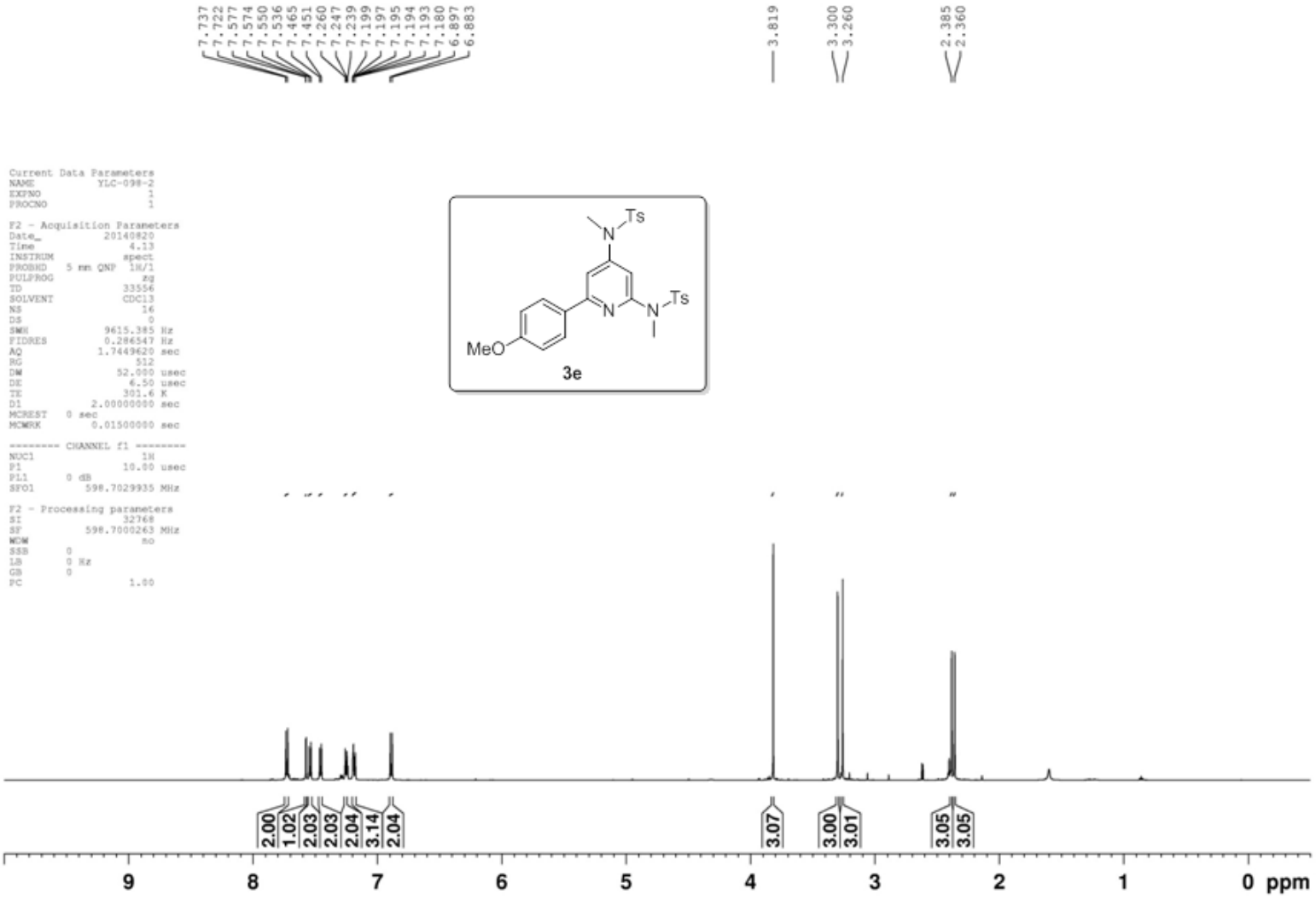

157.05
151.57
146.25
143.74
143.17
138.35
137.78
137.61
129.79
129.66
129.32
128.74
127.92
127.43
126.86
126.80
122.92
77.21
77.00
76.79
52.33
52.09
22.16
21.89
21.54
Current Data Parameters
NAME YLC-1183-2
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20150114
Time 7.53
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 6144
DS 0
SWH 45045.047 Hz
FIDRES 1.374666 Hz
AQ 0.3637748 sec
DW 11.100 usec
DE 6.50 usec
TE 297.2 K
D1 3.50000000 sec
d11 0.03000000 sec
DELTA 3.40000010 sec
MCREST 0 sec
MCWRK 0.01500000 sec
-------- CHANNEL f1 --------
NUC1 13C
P1 4.80 usec
PL1 0 dB
SFO1 150.5366470 MHz
-------- CHANNEL f2 --------
CPDPRG2 waltz16
NUC2 1H
PCPD2 92.00 usec
PL2 120.00 dB
PL12 14.00 dB
PL13 14.00 dB
SFO2 598.6029940 MHz
F2 - Processing parameters
SI 65536
SF 150.5180920 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 0.50
Ph
N
Ts
3c
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

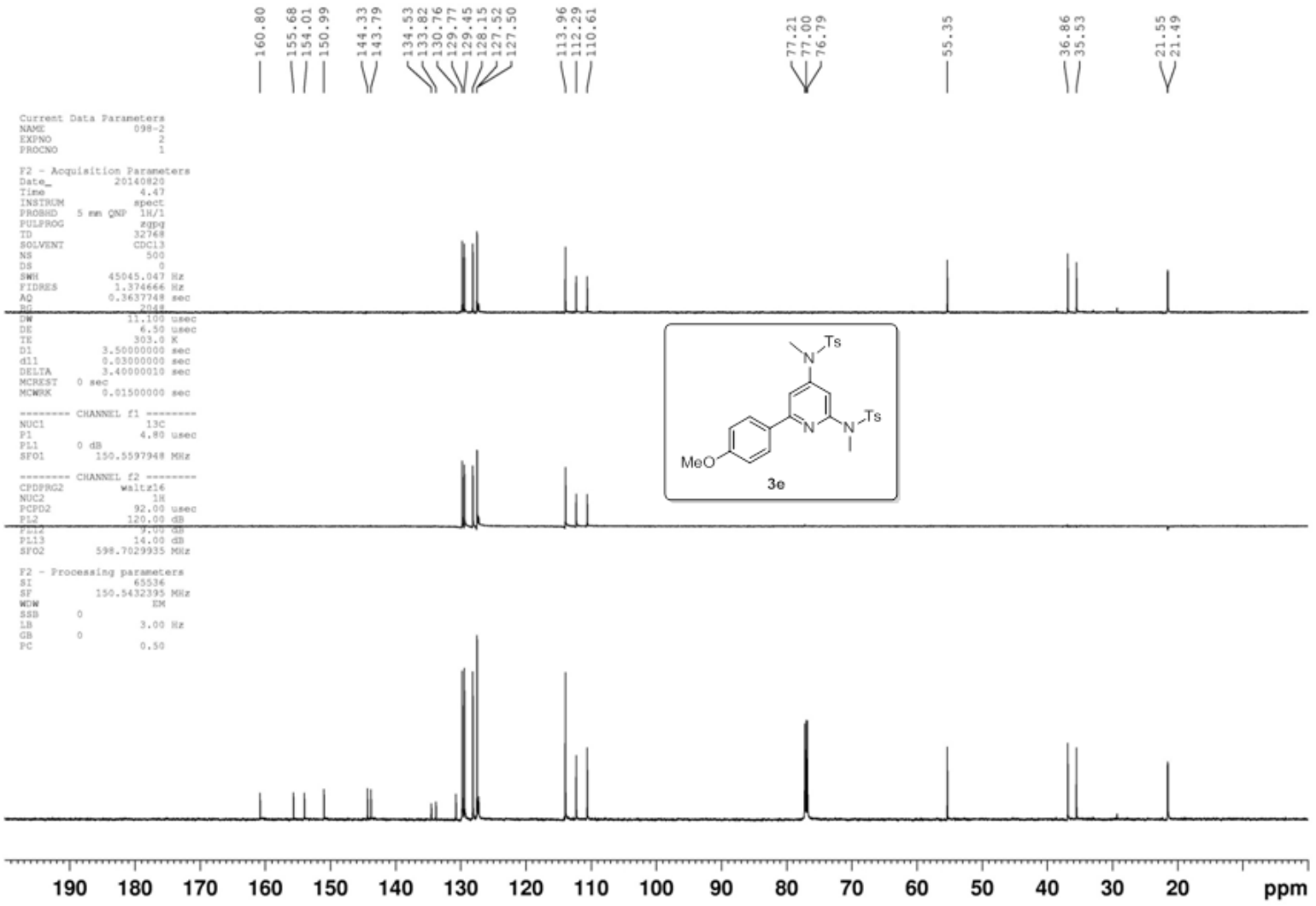

8.454
8.450
8.445
8.443
8.441
8.439
8.437
8.170
8.169
8.166
8.164
8.163
8.158
8.154
7.799
7.785
7.741
7.521
7.518
7.513
7.509
7.480
7.476
7.471
7.468
7.273
7.272
7.259
7.241
4.804
4.792
4.781
4.769
4.758
4.747
4.735
2.390
1.537
1.474
1.463
Current Data Parameters
NAME YLC-1183-1
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20150115
Time 7.55
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 64
DS 0
SWH 8389.262 Hz
FIDRES 0.256020 Hz
AQ 1.9530228 sec
RG 512
DW 59.600 usec
DE 6.50 usec
TE 294.3 K
D1 2.00000000 sec
MCREST 0 sec
MCWRK 0.01500000 sec
-------- CHANNEL f1 --------
NUC1 1H
P1 8.00 usec
PL1 0 dB
SFO1 598.6029930 MHz
F2 - Processing parameters
SI 32768
SF 598.6000301 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 1.00
4.804
4.792
4.781
4.769
4.758
4.747
4.735
4.80
ppm
Ph
N
Ts
N
Ph
3c'
2.03
2.01
2.00
1.00
6.03
2.05
1.02
3.06
6.05
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
ppm

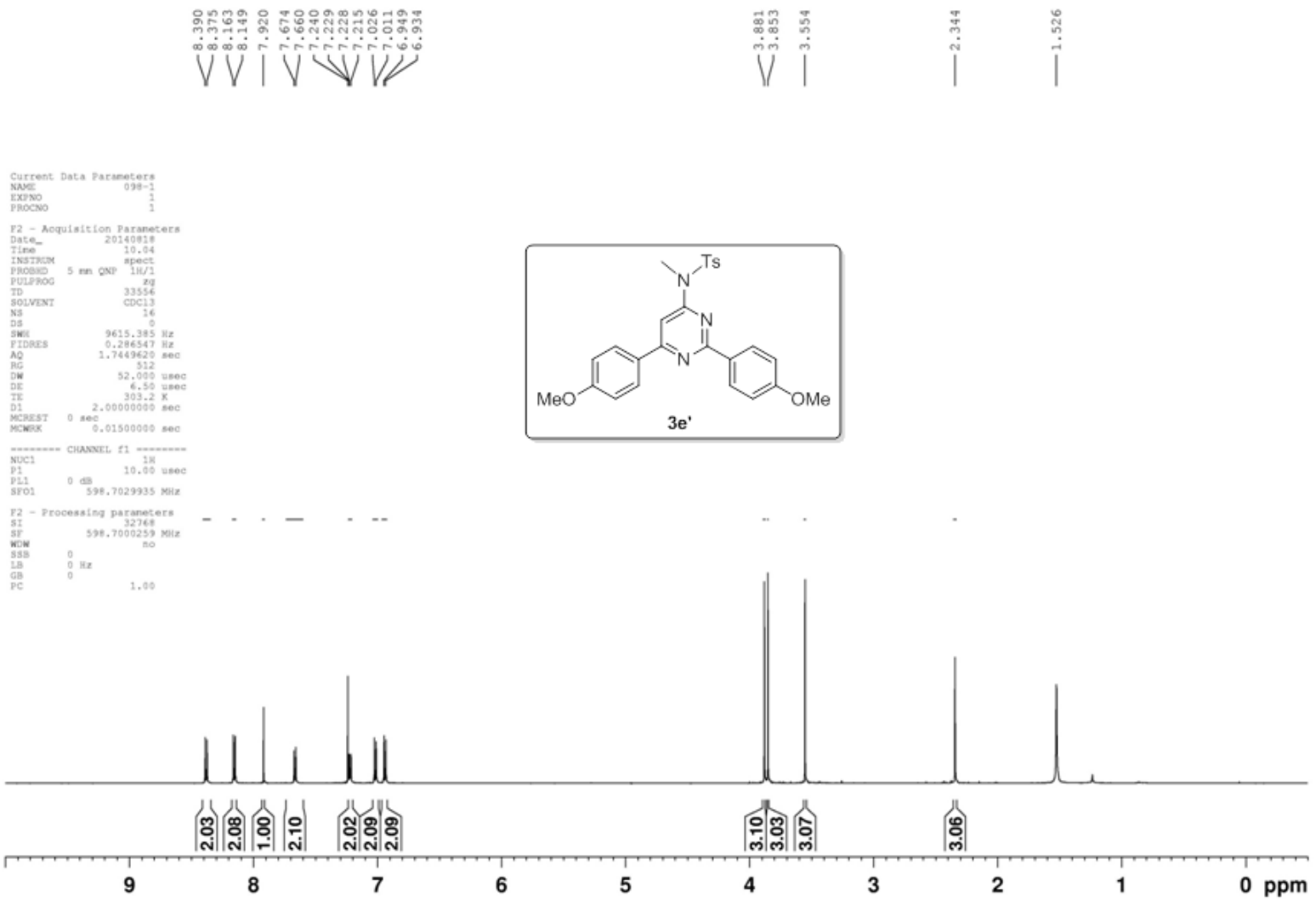

165.19
163.92
160.39
143.92
137.79
137.60
137.00
130.95
130.83
129.68
128.90
128.47
128.34
127.62
127.36
110.99
77.21
77.00
76.79
53.16
21.90
21.56
Current Data Parameters
NAME YLC-1183-1
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20150115
Time 8.00
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 7514
DS 0
SWH 45045.047 Hz
FIDRES 1.374666 Hz
AQ 0.3637748 sec
DW 11.100 usec
DE 4.50 usec
TE 296.0 K
D1 3.50000000 sec
d11 0.03000000 sec
DELTA 3.40000010 sec
MCREST 0 sec
MCWRK 0.01500000 sec
-------- CHANNEL f1 --------
NUC1 13C
P1 4.80 usec
PL1 0 dB
SFO1 150.5344470 MHz
-------- CHANNEL f2 --------
CPDPRG2 waltz16
NUC2 1H
PCPD2 92.00 usec
PL2 120.00 dB
PL12 16.00 dB
PL13 14.00 dB
SFO2 598.4029940 MHz
F2 - Processing parameters
SI 65536
SF 150.5180922 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 0.50
N
Ts
N
Ph
N
Ph
3c'
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

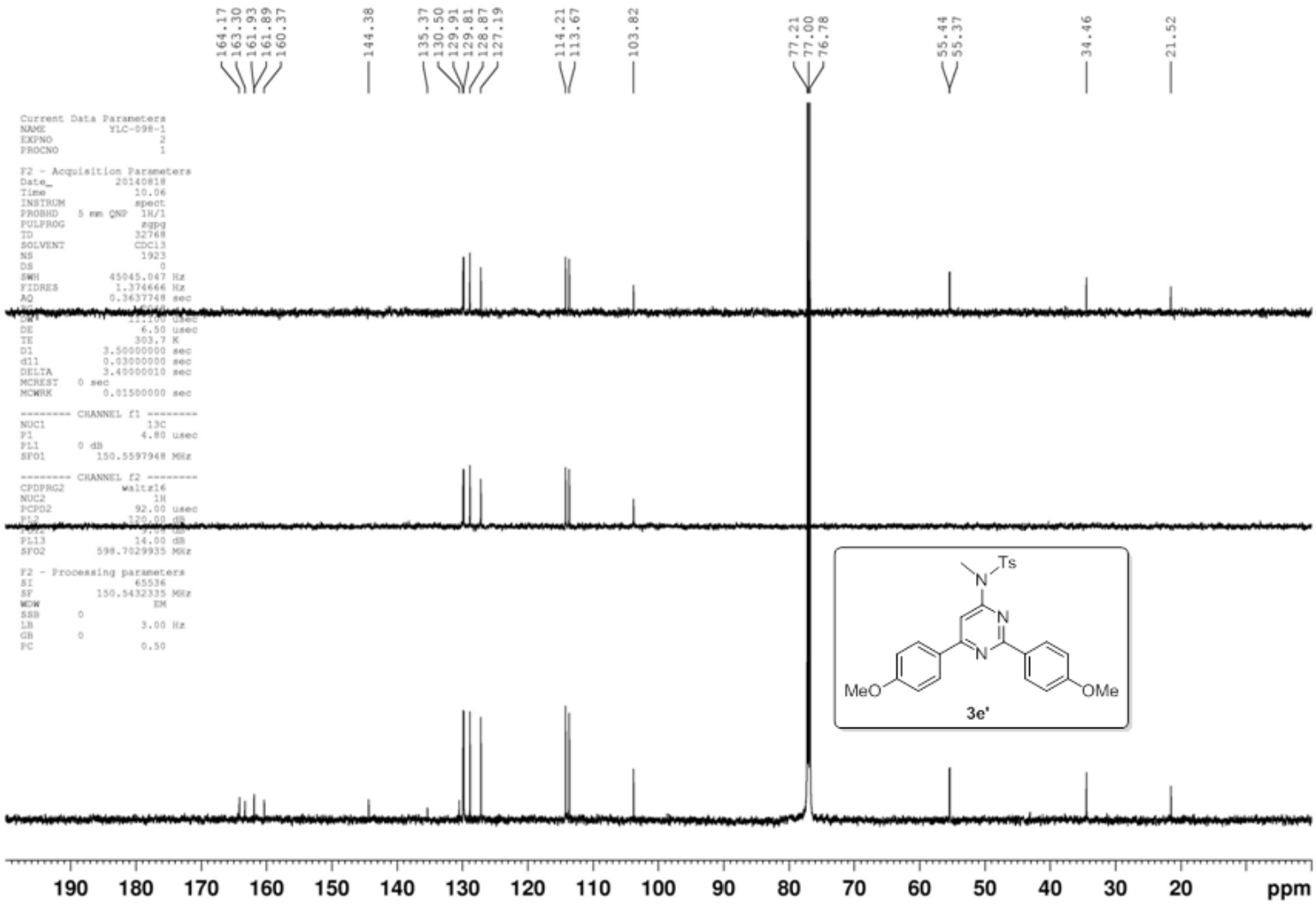

7.775
7.755
7.634
7.627
7.619
7.436
7.415
7.357
7.348
7.240
7.234
7.216
7.210
7.194
7.173
7.161
7.141
7.053
7.036
7.031
7.023
6.931
6.915
6.910
6.882
6.865
6.860
6.633
3.856
3.850
3.827
3.821
2.393
2.359
2.152
2.146
2.026
2.021
1.564
1.252
1.234
1.216
0.052
0.047
Current Data Parameters
NAME 20151221
EXPNO 15
PROCNO 1
F2 – Acquisition Parameters
Date_ 20151221
Time 22.53
INSTRUM spect
PROBHD 5 mm DUL 13C–1
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 12
DS 0
SWH 6410.256 Hz
FIDRES 0.195625 Hz
AQ 2.5559540 sec
RG 362
DW 78.000 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 –2.40 dB
SFO1 400.1528010 MHz
F2 – Processing parameters
SI 16384
SF 400.1500187 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
7.436
7.415
7.357
7.348
7.240
7.234
7.216
7.210
7.194
7.173
7.161
7.141
7.053
7.036
7.031
7.023
6.931
6.910
6.882
7.5
7.4
7.3
7.2
7.1
7.0
ppm
2.14
3.23
5.57
3.42
2.22
2.17
Ts
N
O
3d
10
9
8
7
6
5
4
3
2
1
ppm
1.97
2.03
2.14
3.23
5.57
3.42
2.22
2.17
1.02
3.16
2.87
3.36
2.93

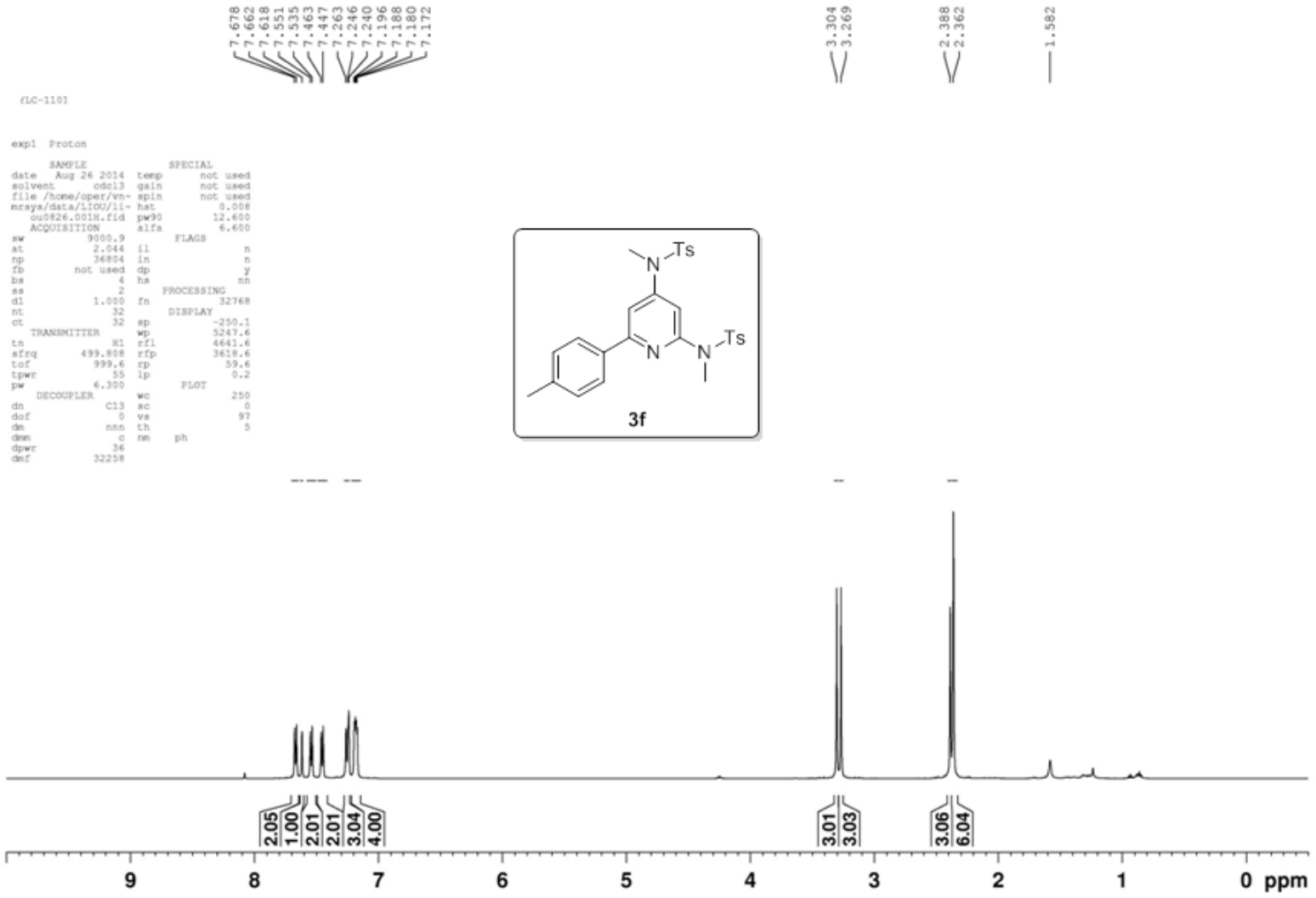

159.90
159.67
156.52
155.56
151.60
144.36
143.42
138.57
137.52
136.28
131.76
131.61
131.40
131.12
129.75
129.13
128.95
128.73
128.40
127.76
127.20
114.89
114.57
109.42
107.33
77.32
77.01
76.69
55.50
21.59
21.55
Current Data Parameters
NAME 20151221
EXPNO 16
PROCNO 1
F2 - Acquisition Parameters
Date_ 20151221
Time 22.57
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 7000
DS 0
SWH 22727.273 Hz
FIDRES 0.346791 Hz
AQ 1.4418420 sec
RG 57
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.70 usec
PL1 -0.50 dB
SFO1 100.6288660 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -2.40 dB
PL13 18.10 dB
SFO2 400.1516010 MHz
F2 - Processing parameters
SI 32768
SF 100.6178003 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
O
N
Ts
N
N
Ts
O
3d
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

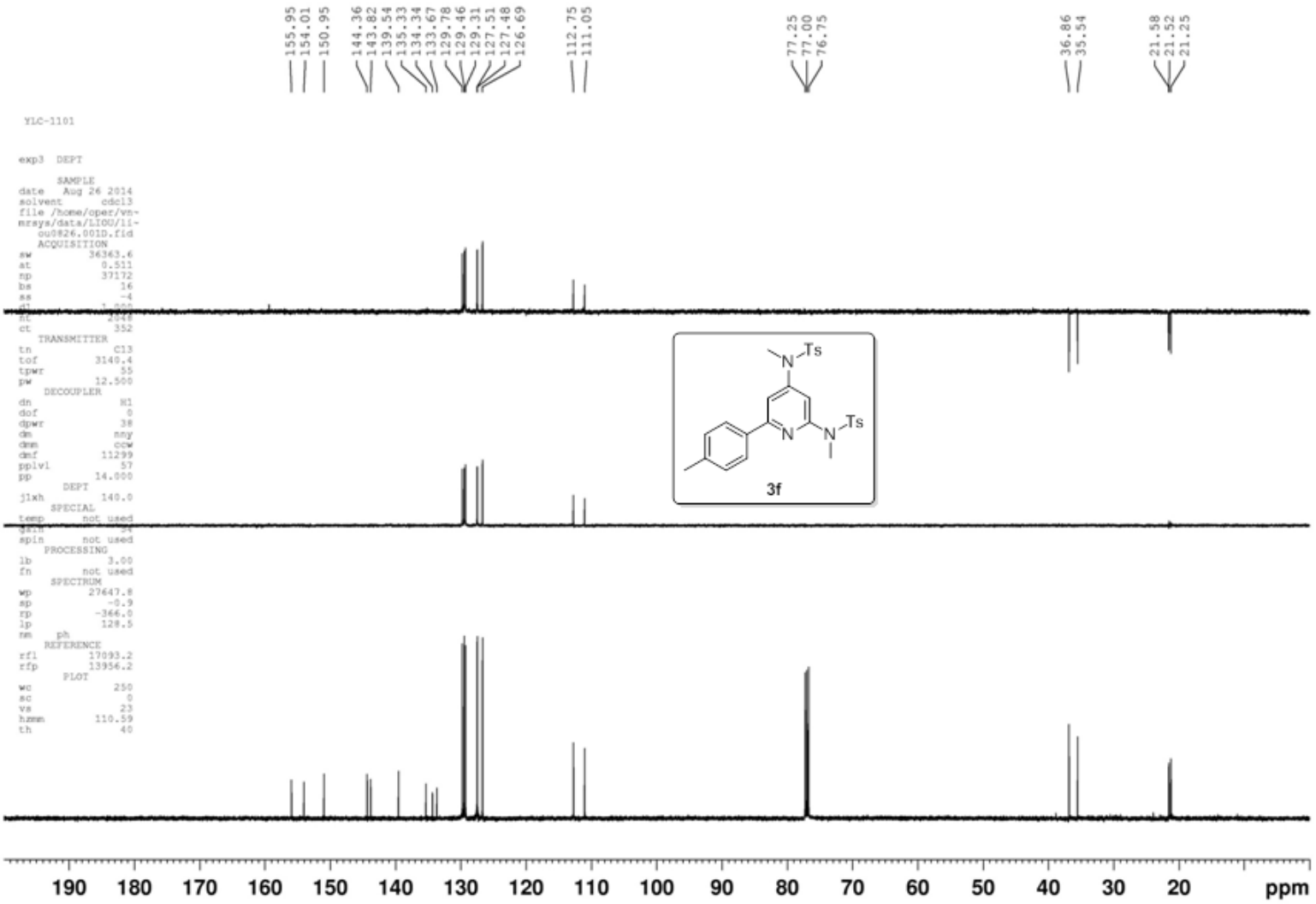

7.737
7.722
7.577
7.574
7.550
7.536
7.465
7.451
7.260
7.247
7.239
7.199
7.197
7.195
7.194
7.193
7.180
6.897
6.883
3.819
3.300
3.260
2.385
2.360
Current Data Parameters
NAME YLC-098-2
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20140820
Time 4.13
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg
TD 33556
SOLVENT CDCl3
NS 16
DS 0
SWH 9615.385 Hz
FIDRES 0.286547 Hz
AQ 1.7449620 sec
RG 512
DW 52.000 usec
DE 6.50 usec
TE 301.6 K
D1 2.00000000 sec
MCREST 0 sec
MCWRK 0.01500000 sec
-------- CHANNEL f1 --------
NUC1 1H
P1 10.00 usec
PL1 0 dB
SFO1 598.7029935 MHz
F2 - Processing parameters
SI 32768
SF 598.7000263 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 1.00
Ts
N
Ts
N
N
MeO
3e
2.00
1.02
2.03
2.03
2.04
3.14
2.04
3.07
3.00
3.01
3.05
3.05
9
8
7
6
5
4
3
2
1
0 ppm

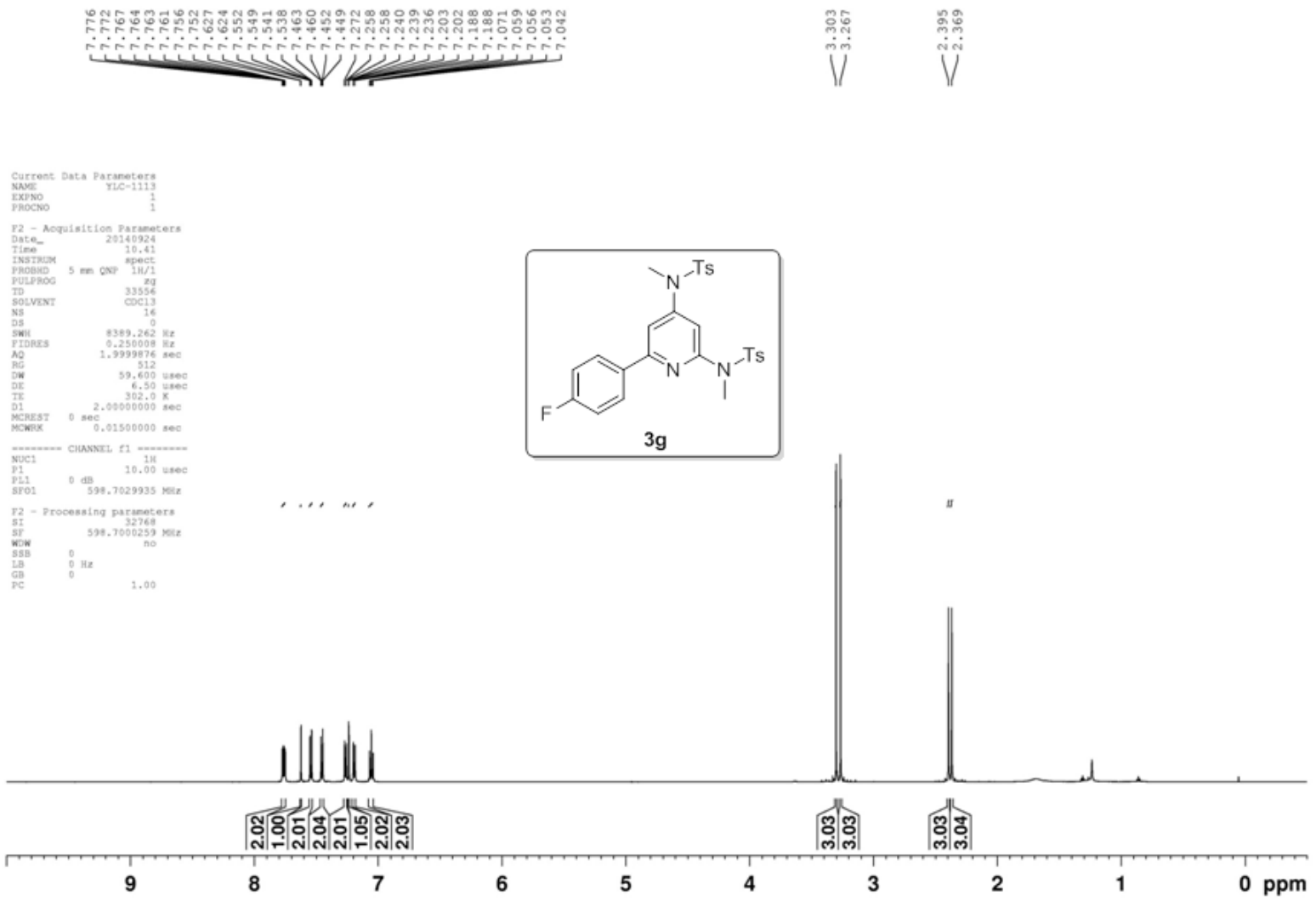

160.80
155.68
154.01
150.99
144.33
143.79
134.53
133.82
130.76
129.77
129.45
128.15
127.52
127.50
113.96
112.29
110.61
77.21
77.00
76.79
55.35
36.86
35.53
21.55
21.49
Current Data Parameters
NAME 098-2
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20140820
Time 4.47
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 500
DS 0
SWH 45045.047 Hz
FIDRES 1.374666 Hz
AQ 0.3637748 sec
RG 2048
DW 11.100 usec
DE 6.50 usec
TE 303.0 K
D1 3.50000000 sec
d11 0.03000000 sec
DELTA 3.40000010 sec
MCREST 0 sec
MCWRK 0.01500000 sec
-------- CHANNEL f1 --------
NUC1 13C
P1 4.80 usec
PL1 0 dB
SFO1 150.5597948 MHz
-------- CHANNEL f2 --------
CPDPRG2 waltz16
NUC2 1H
PCPD2 92.00 usec
PL2 120.00 dB
PL12 9.00 dB
PL13 14.00 dB
SFO2 598.7029935 MHz
F2 - Processing parameters
SI 65536
SF 150.5432395 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 0.50
Ts
N
Ts
N
N
MeO
3e
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

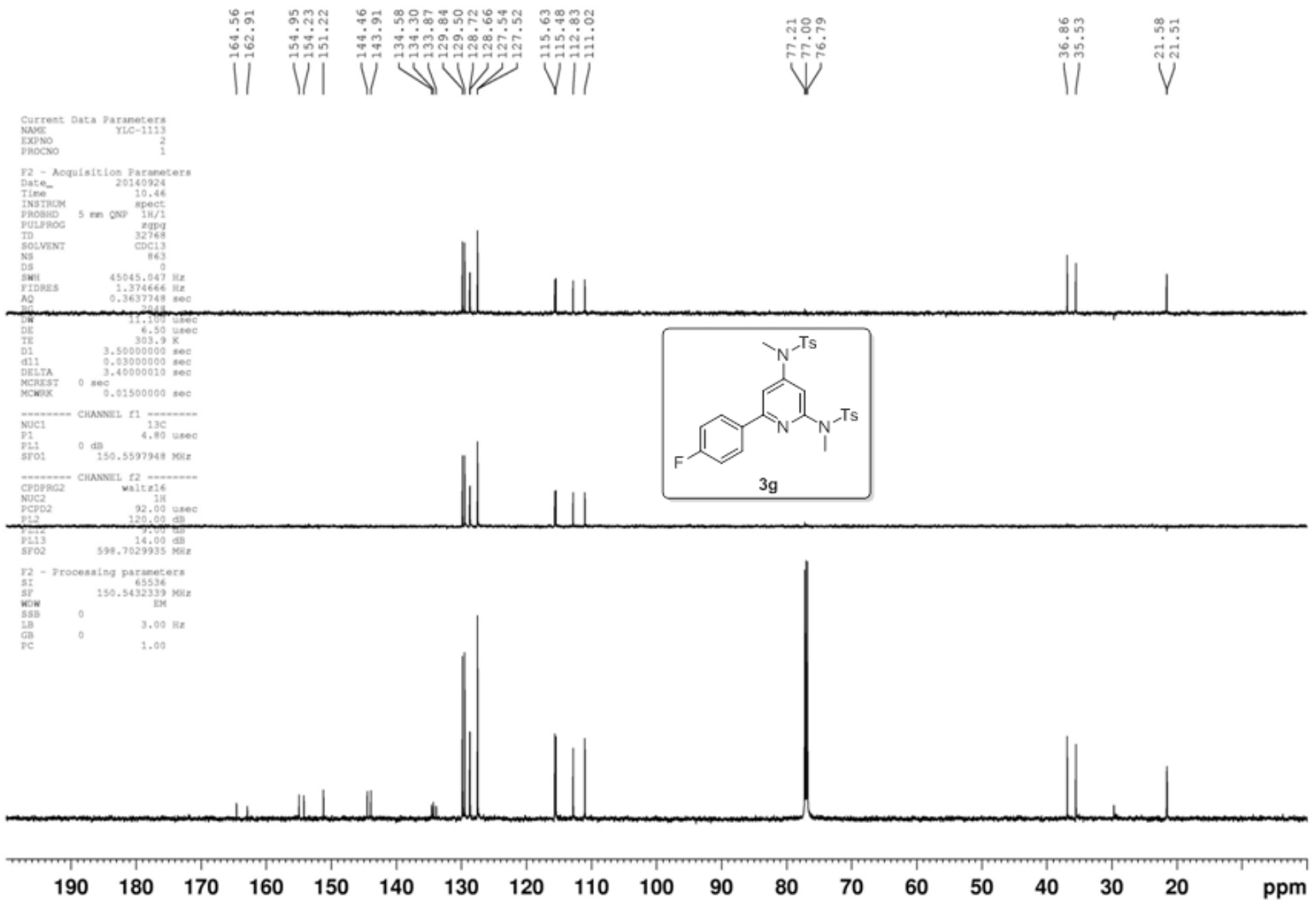

8.390
8.375
8.163
8.149
7.920
7.674
7.660
7.240
7.229
7.228
7.215
7.026
7.011
6.949
6.934
3.881
3.853
3.554
2.344
1.526
Current Data Parameters
NAME 098-1
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20140818
Time 10.04
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg
TD 33554
SOLVENT CDCl3
NS 16
DS 0
SWH 9615.385 Hz
FIDRES 0.286547 Hz
AQ 1.7449620 sec
RG 512
DW 52.000 usec
DE 6.50 usec
TE 303.2 K
D1 2.00000000 sec
MCREST 0 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 0 dB
SFO1 598.7029935 MHz
F2 - Processing parameters
SI 32768
SF 598.7000259 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 1.00
Ts
N
N
N
MeO
OMe
3e'
2.03
2.08
1.00
2.10
2.02
2.09
2.09
3.10
3.03
3.07
3.06
9
8
7
6
5
4
3
2
1
0 ppm

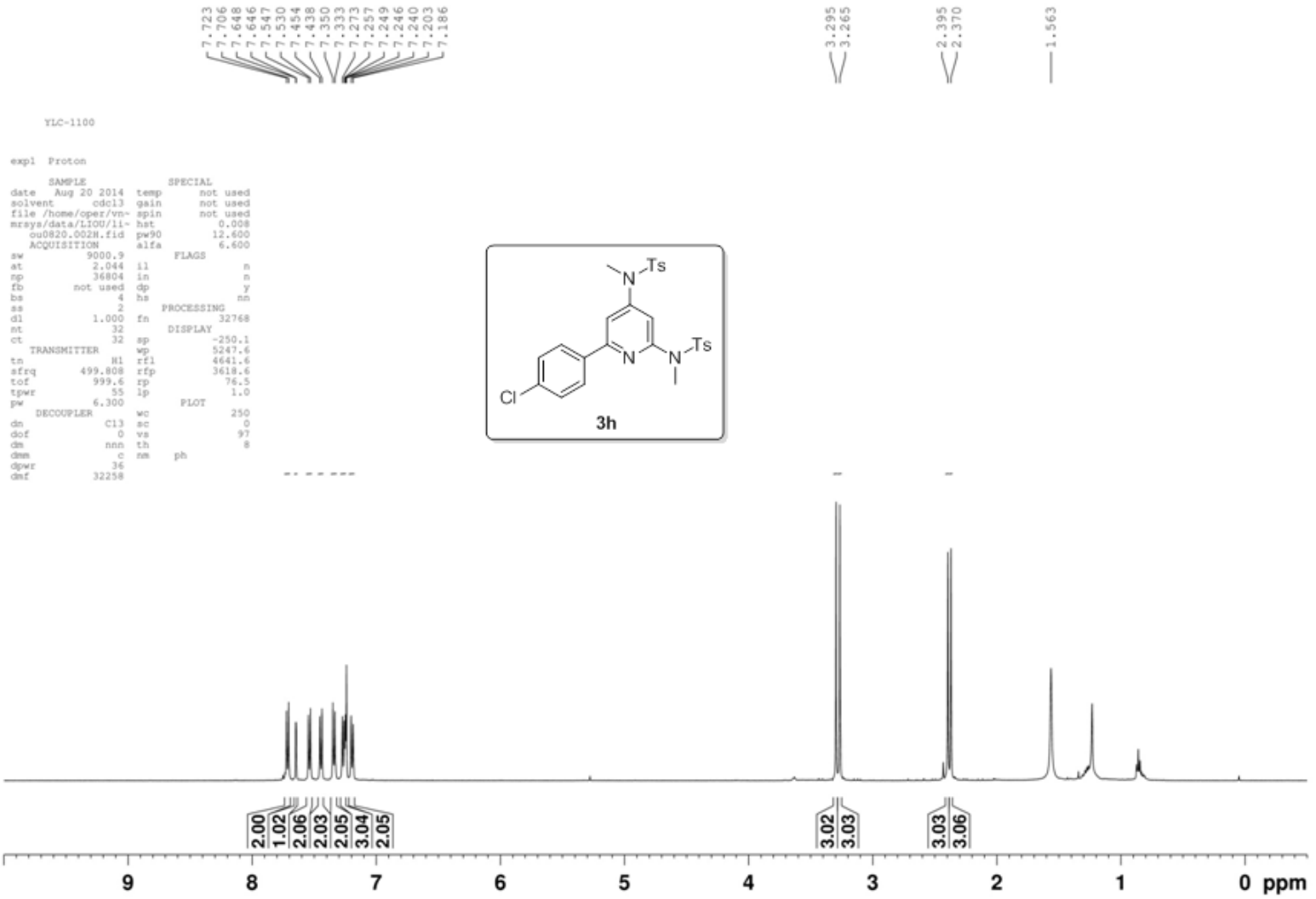

164.17
163.30
161.93
161.89
160.37
144.38
135.37
130.50
129.91
129.81
128.87
127.19
114.21
113.67
103.82
77.21
77.00
76.78
55.44
55.37
34.46
21.52
Current Data Parameters
NAME YLC-098-1
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20140818
Time 10.06
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 1923
DS 0
SWH 45045.047 Hz
FIDRES 1.374666 Hz
AQ 0.3637748 sec
DW 11.100 usec
DE 6.50 usec
TE 303.7 K
D1 3.50000000 sec
d11 0.03000000 sec
DELTA 3.40000010 sec
MCREST 0 sec
MCWRK 0.01500000 sec
-------- CHANNEL f1 --------
NUC1 13C
P1 4.80 usec
PL1 0 dB
SFO1 150.5597948 MHz
-------- CHANNEL f2 --------
CPDPRG2 waltz16
NUC2 1H
PCPD2 92.00 usec
PL13 14.00 dB
SFO2 598.7029935 MHz
F2 - Processing parameters
SI 65536
SF 150.5432335 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 0.50
N
Ts
N
N
MeO
OMe
3e'
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

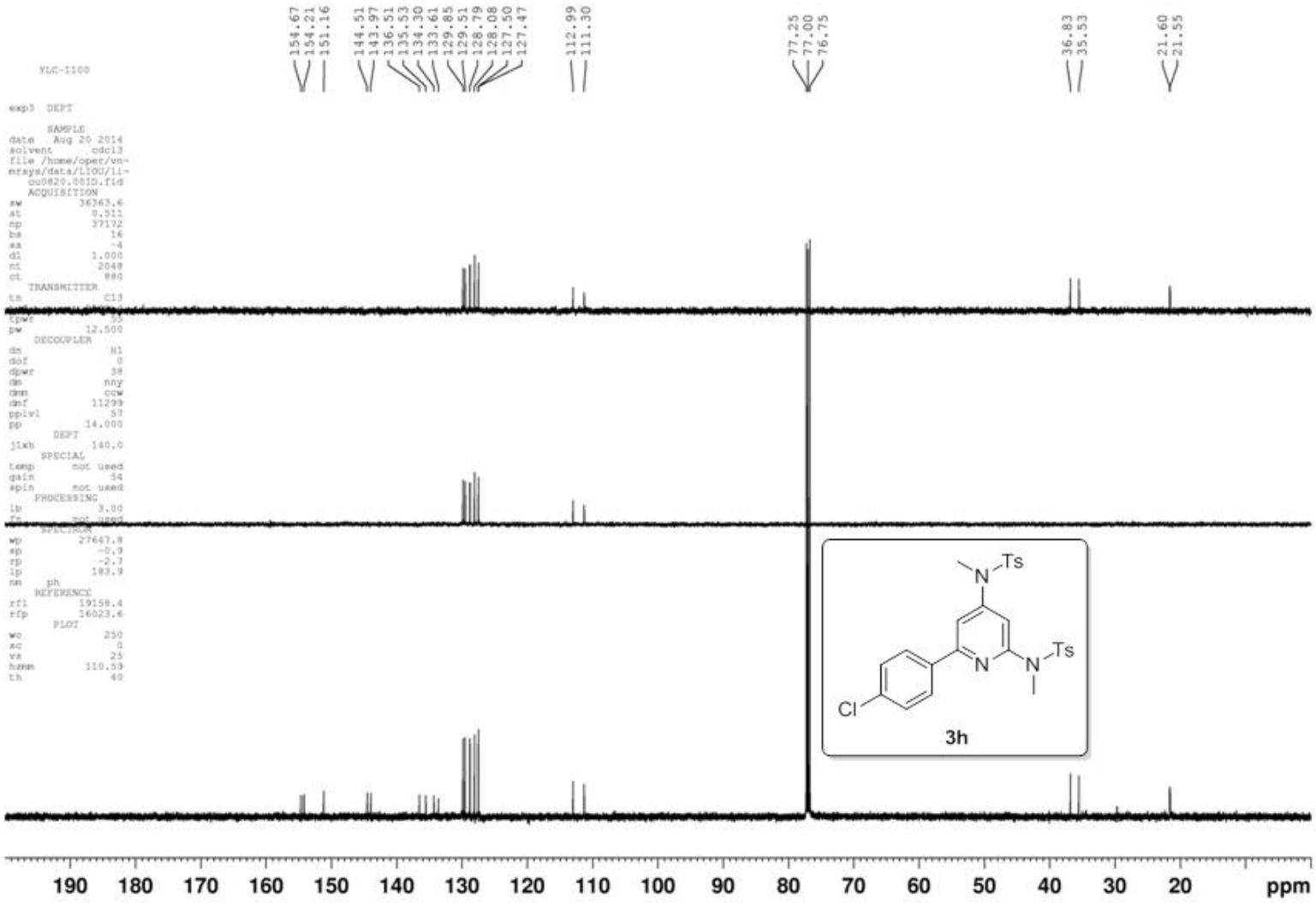

7.678
7.662
7.618
7.551
7.535
7.463
7.447
7.263
7.246
7.240
7.196
7.188
7.180
7.172
3.304
3.269
2.388
2.362
1.582
rLC-1101
exp1 Proton
SAMPLE
date Aug 26 2014
solvent cdcl3
file /home/oper/vn-
mrsys/data/LIOU/li-
ou0826.001H.fid
ACQUISITION
sw 9000.9
at 2.044
np 36804
fb not used
bs 4
ss 2
d1 1.000
nt 32
ct 32
TRANSMITTER
tn H1
sfrq 499.808
tof 999.6
tpwr 55
pw 6.300
DECOUPLER
dn C13
dof 0
dm nnn
dmm c
dpwr 36
dmf 32258
SPECIAL
temp not used
gain not used
spin not used
hst 0.008
pw90 12.600
alfa 6.600
FLAGS
il n
in n
dp y
hs nn
PROCESSING
fn 32768
DISPLAY
sp -250.1
wp 5247.6
rfl 4641.6
rfp 3618.6
rp 59.6
lp 0.2
PLOT
wc 250
sc 0
vs 97
th 5
nm ph
Ts
N
Ts
N
N
3f
2.05
1.00
2.01
2.01
3.04
4.00
3.01
3.03
3.06
6.04
9
8
7
6
5
4
3
2
1
0 ppm

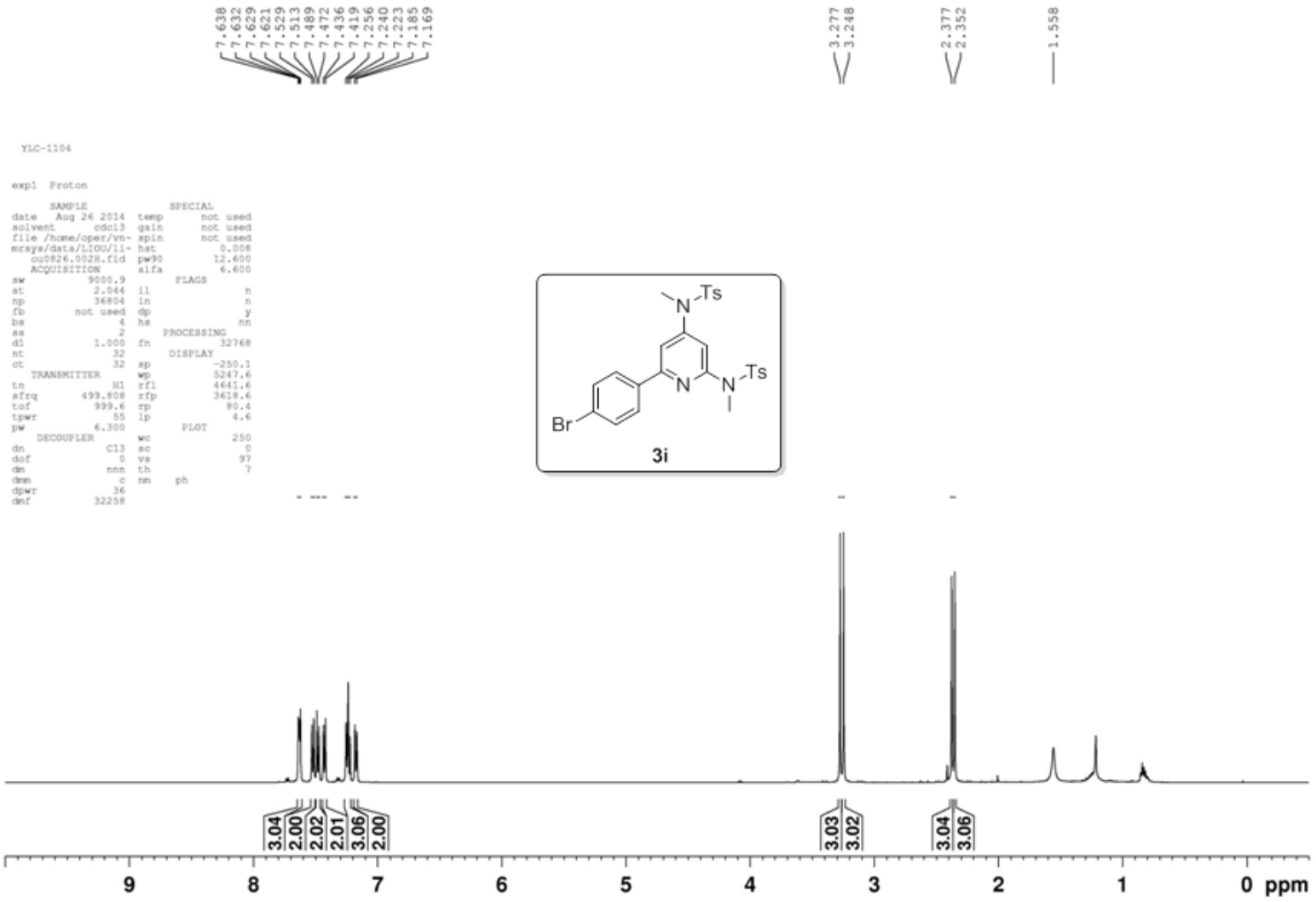

155.95
154.01
150.95
144.36
143.82
139.54
135.33
134.34
133.67
129.78
129.46
129.31
127.51
127.48
126.69
112.75
111.05
77.25
77.00
76.75
36.86
35.54
21.58
21.52
21.25
YLC-1101
exp3 DEPT
SAMPLE
date Aug 26 2014
solvent cdcl3
file /home/oper/vn-mrsys/data/LIOU/li-ou0826.001D.fid
ACQUISITION
sw 36363.6
at 0.511
np 37172
bs 16
ss -4
d1 1.000
fb 2048
ct 352
TRANSMITTER
tn C13
tof 3140.4
tpwr 55
pw 12.500
DECOUPLER
dn H1
dof 0
dpwr 38
dm nny
dmm ccw
dmf 11299
pplvl 57
pp 14.000
DEPT
jlxh 140.0
SPECIAL
temp not used
gain 24
spin not used
PROCESSING
lb 3.00
fn not used
SPECTRUM
wp 27647.8
sp -0.9
rp -366.0
lp 128.5
nm ph
REFERENCE
rf1 17093.2
rfp 13956.2
PLOT
wc 250
sc 0
vs 23
hmm 110.59
th 40
Ts
N
Ts
N
N
3f
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

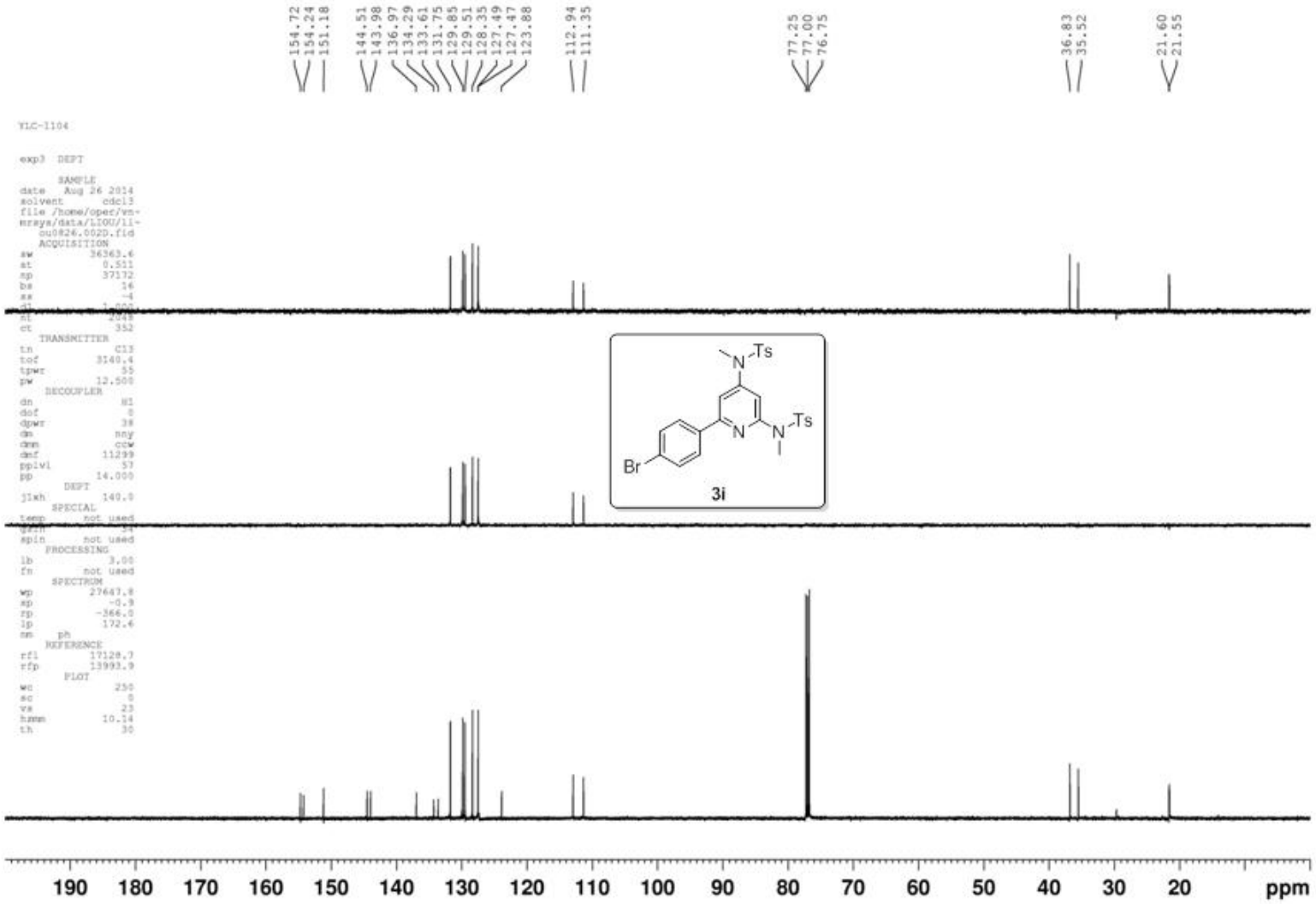

7.776
7.772
7.767
7.764
7.763
7.761
7.756
7.752
7.627
7.624
7.552
7.549
7.541
7.538
7.463
7.460
7.452
7.449
7.272
7.258
7.258
7.240
7.239
7.236
7.203
7.202
7.188
7.188
7.071
7.059
7.056
7.053
7.042
3.303
3.267
2.395
2.369
Current Data Parameters
NAME YLC-1113
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20140924
Time 10.41
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg
TD 33556
SOLVENT CDCl3
NS 16
DS 0
SWH 8389.262 Hz
FIDRES 0.250008 Hz
AQ 1.9999876 sec
RG 512
DW 59.600 usec
DE 6.50 usec
TE 302.0 K
D1 2.00000000 sec
MCREST 0 sec
MCWRK 0.01500000 sec
-------- CHANNEL f1 --------
NUC1 1H
P1 10.00 usec
PL1 0 dB
SFO1 598.7029935 MHz
F2 - Processing parameters
SI 32768
SF 598.7000259 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 1.00
N
Ts
N
N
Ts
F
3g
2.02
1.00
2.01
2.04
2.01
1.05
2.02
2.03
3.03
3.03
3.03
3.04
9
8
7
6
5
4
3
2
1
0 ppm

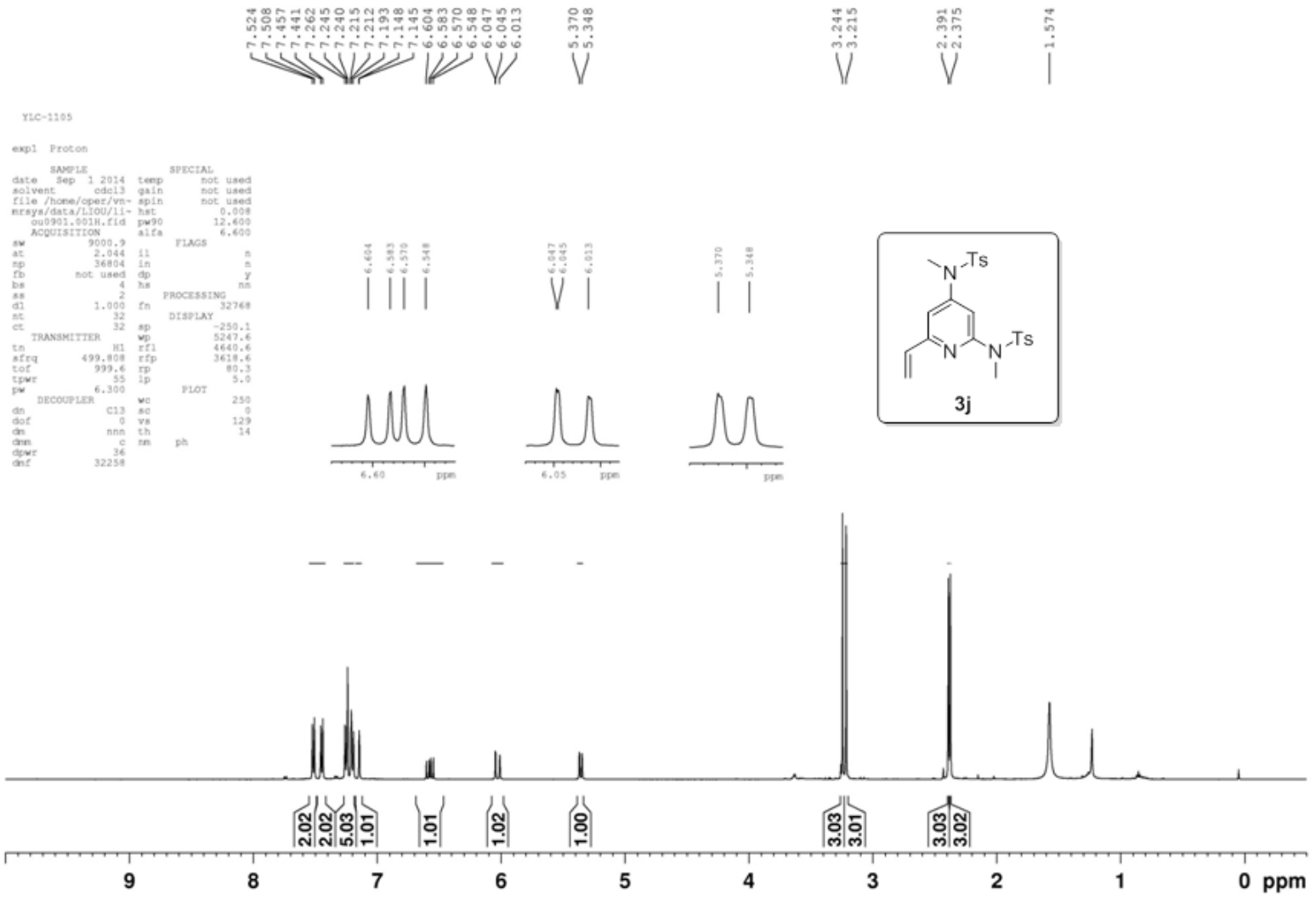

164.56
162.91
154.95
154.23
151.22
144.46
143.91
134.58
134.30
133.87
129.84
129.50
128.72
128.66
127.54
127.52
115.63
115.48
112.83
111.02
77.21
77.00
76.79
36.86
35.53
21.58
21.51
Current Data Parameters
NAME YLC-1113
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20140924
Time 10.46
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 863
DS 0
SWH 45045.047 Hz
FIDRES 1.374666 Hz
AQ 0.3637748 sec
DW 11.100 usec
DE 6.50 usec
TE 303.9 K
D1 3.50000000 sec
d11 0.03000000 sec
DELTA 3.40000010 sec
MCREST 0 sec
MCWRK 0.01500000 sec
-------- CHANNEL f1 --------
NUC1 13C
P1 4.80 usec
PL1 0 dB
SFO1 150.5597948 MHz
-------- CHANNEL f2 --------
CPDPRG2 waltz16
NUC2 1H
PCPD2 92.00 usec
PL2 120.00 dB
PL12 17.00 dB
PL13 14.00 dB
SFO2 598.7029935 MHz
F2 - Processing parameters
SI 65536
SF 150.5432339 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
N
Ts
N
Ts
F
3g
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

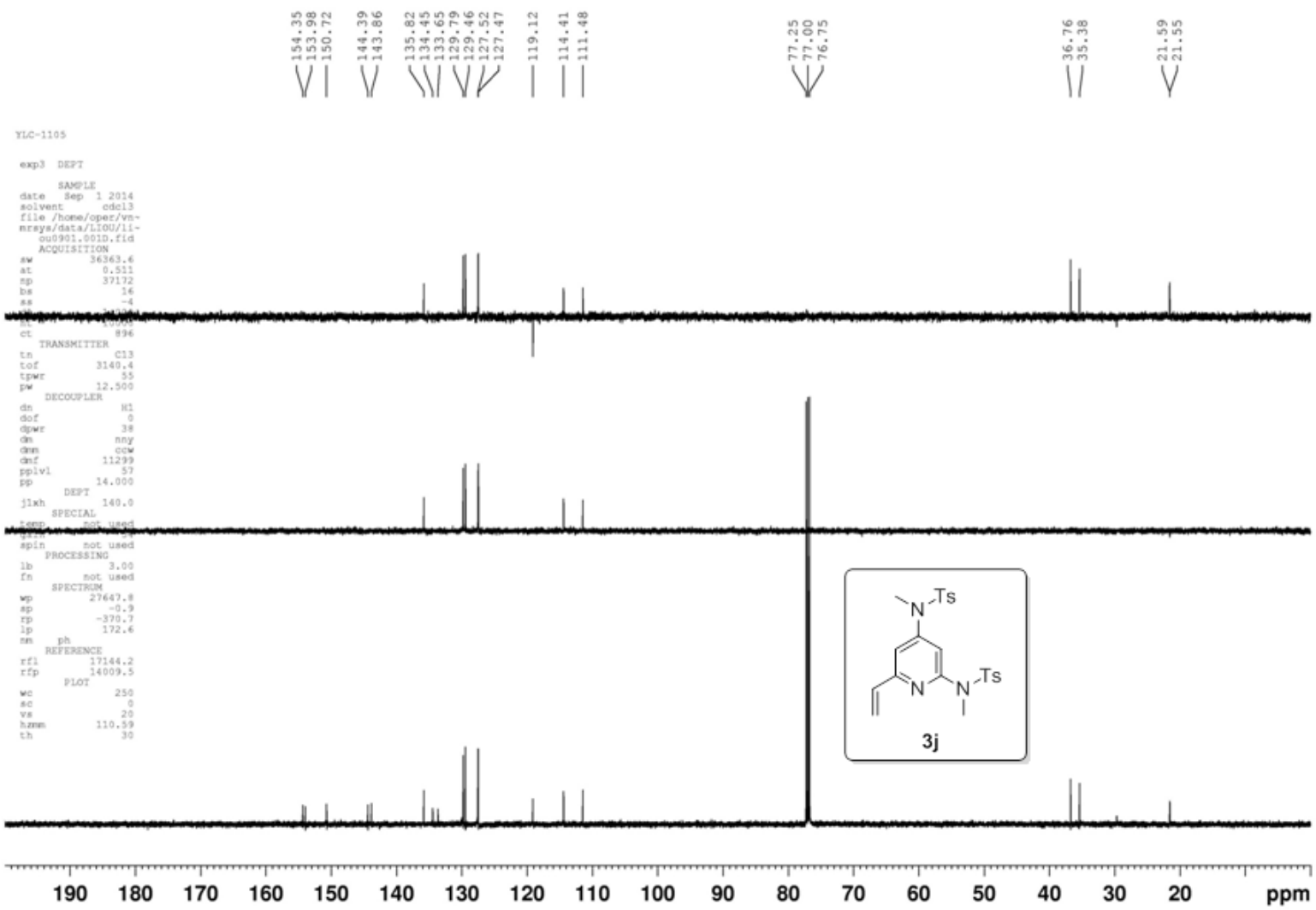

7.723
7.706
7.648
7.646
7.547
7.530
7.454
7.438
7.350
7.333
7.273
7.257
7.249
7.246
7.240
7.203
7.186
3.295
3.265
2.395
2.370
1.563
YLC-1100
expl Proton
SAMPLE
date Aug 20 2014
solvent cdcl3
file /home/oper/vn-
mrsys/data/LIOU/li-
ou0820.002N.fid
ACQUISITION
sw 9000.9
at 2.044
np 36804
fb not used
bs 4
ss 2
d1 1.000
nt 32
ct 32
TRANSMITTER
tn H1
sfrq 499.808
tof 999.6
tpwr 55
pw 6.300
DECOUPLER
dn C13
dof 0
dm nnn
dmm c
dpwr 36
dmf 32258
SPECIAL
temp not used
gain not used
spin not used
hst 0.008
pw90 12.600
alfa 6.600
FLAGS
il n
in n
dp y
hs nn
PROCESSING
fn 32768
DISPLAY
sp -250.1
wp 5247.6
rfl 4641.6
rfp 3618.6
rp 76.5
lp 1.0
PLOT
wc 250
sc 0
vs 97
th 8
nm ph
N
Ts
N
Ts
Cl
3h
2.00
1.02
2.06
2.03
2.05
3.04
2.05
3.02
3.03
3.03
3.06
9
8
7
6
5
4
3
2
1
0 ppm

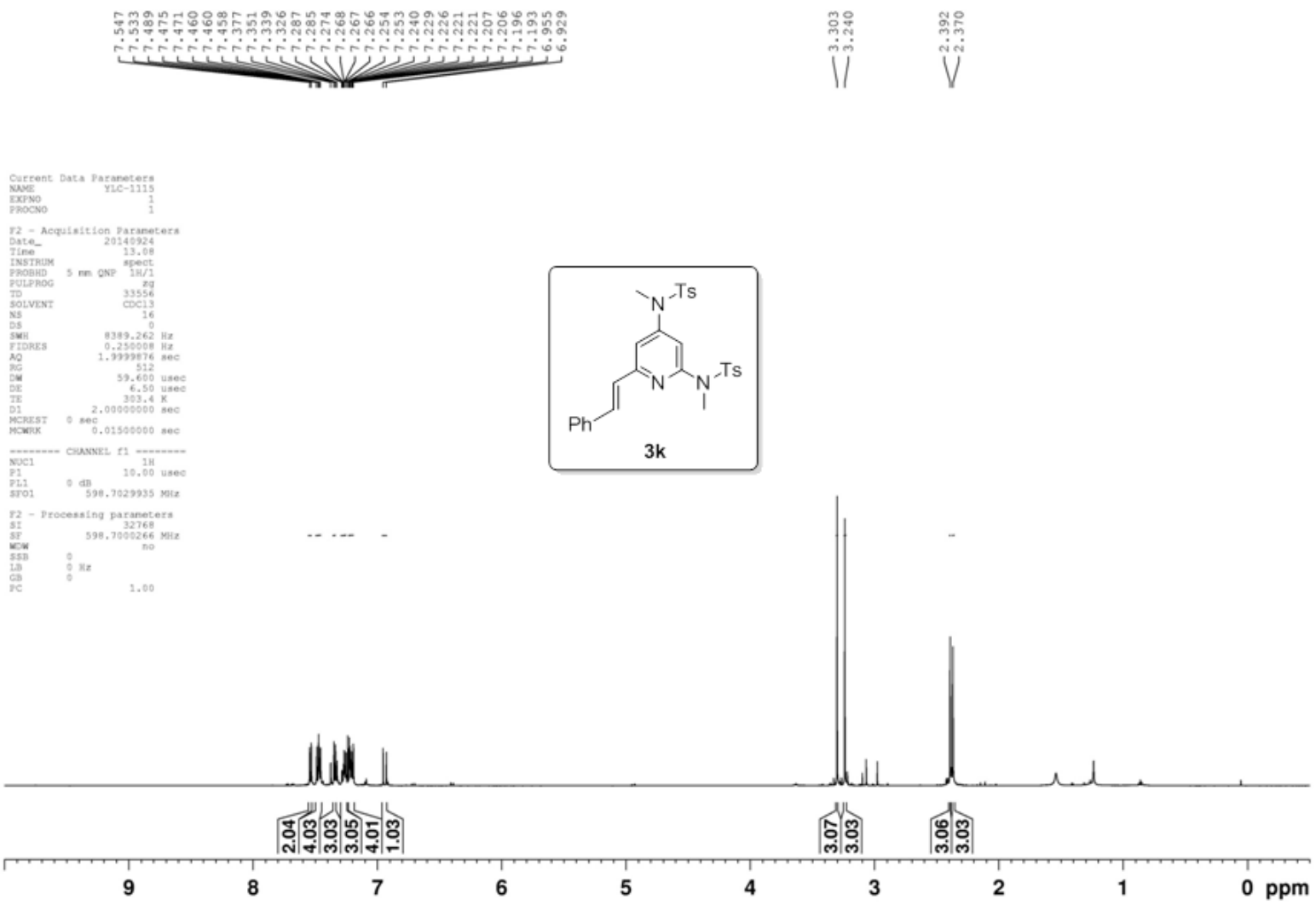

154.67
154.21
151.16
144.51
143.97
136.51
135.53
134.30
133.61
129.85
129.51
128.79
128.08
127.50
127.47
112.99
111.30
77.25
77.00
76.75
36.83
35.53
21.60
21.55
YLC-1100
exp3 DEPT
SAMPLE
date Aug 20 2014
solvent odcl3
file /home/oper/vnmrsys/data/LIOU/li-ou0820.001S.fid
ACQUISITION
sw 36363.6
at 0.511
np 37132
bs 16
as -4
dl 1.000
nt 2048
ct 880
TRANSMITTER
tn C13
tpwr 55
pw 12.500
DECOUPLER
dn H1
dof 0
dpwr 38
dm nny
dmm ccw
dmf 11299
pplvl 57
pp 14.000
DEPT
jlxh 140.0
SPECIAL
temp not used
gain 54
spin not used
PROCESSING
lb 3.00
fn not used
SPECTRUM
wp 27647.8
sp -0.9
rp -2.7
lp 183.9
nn ph
REFERENCE
rfl 19158.4
rfp 16023.6
PLOT
wc 250
sc 0
vs 25
hzmm 110.59
th 40
N
Ts
N
Ts
Cl
3h
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

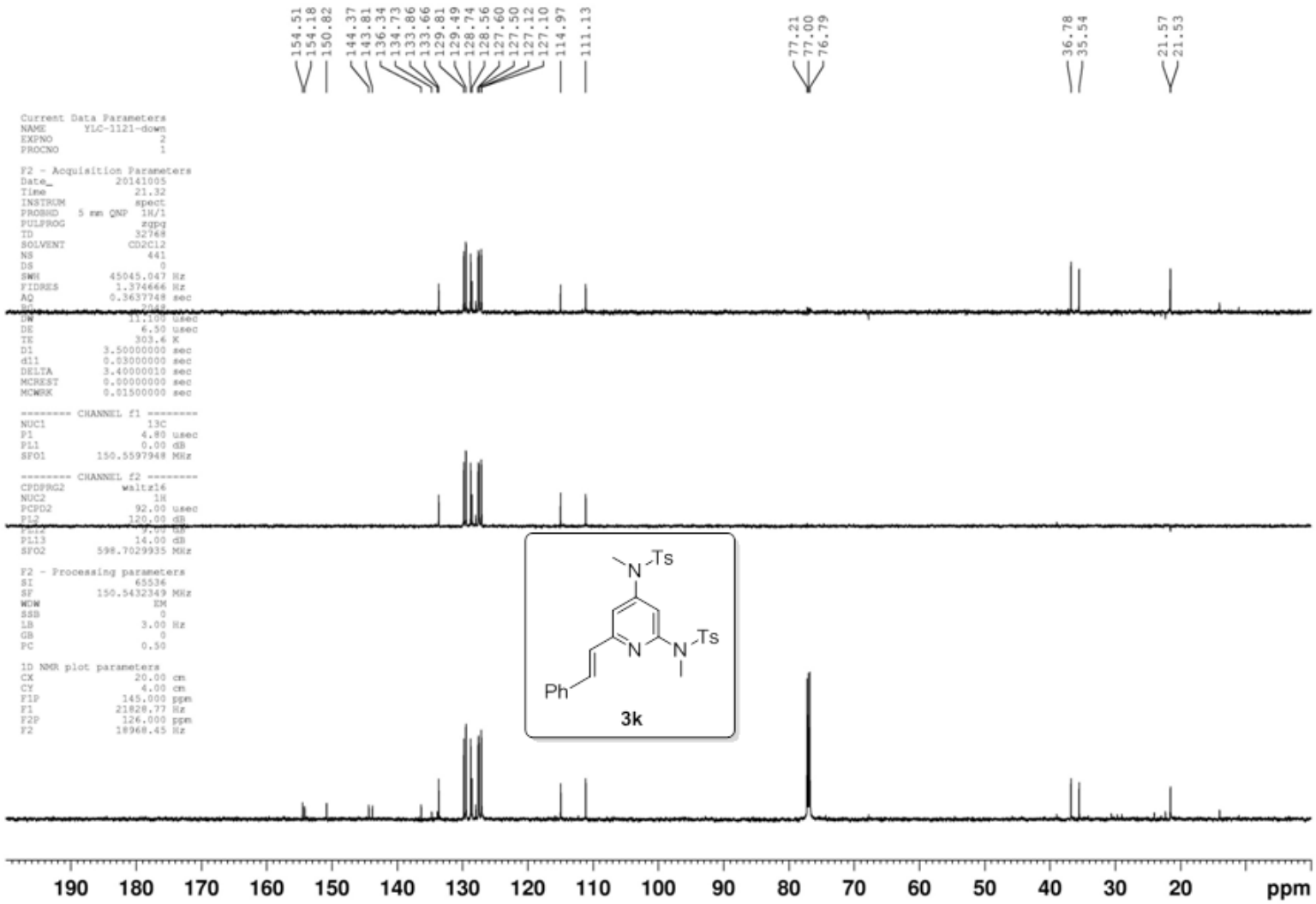

7.638
7.632
7.629
7.621
7.529
7.513
7.489
7.472
7.436
7.419
7.256
7.240
7.223
7.185
7.169
3.277
3.248
2.377
2.352
1.558
YLC-1104
expl Proton
SAMPLE
date Aug 26 2014
solvent cdcl3
file /home/oper/vn-mrsys/data/LIOU/li-ou0826.002N.fid
ACQUISITION
sw 9000.9
at 2.044
np 36804
fb not used
bs 4
ss 2
d1 1.000
nt 32
ct 32
TRANSMITTER
tn H1
sfrq 499.808
tof 999.6
tpwr 55
pw 6.300
DECOUPLER
dn C13
dof 0
dm nnn
dmm c
dpwr 36
dmf 32258
SPECIAL
temp not used
gain not used
spin not used
hst 0.008
pw90 12.600
alfa 6.600
FLAGS
il n
in n
dp y
hs nn
PROCESSING
fn 32768
DISPLAY
sp -250.1
wp 5247.6
rfl 4641.6
rfp 3618.6
rp 80.4
lp 4.6
PLOT
wc 250
sc 0
vs 97
th 7
nn ph
Ts
N
Br
3i
3.04
2.00
2.02
2.01
3.06
2.00
3.03
3.02
3.04
3.06
9
8
7
6
5
4
3
2
1
0 ppm

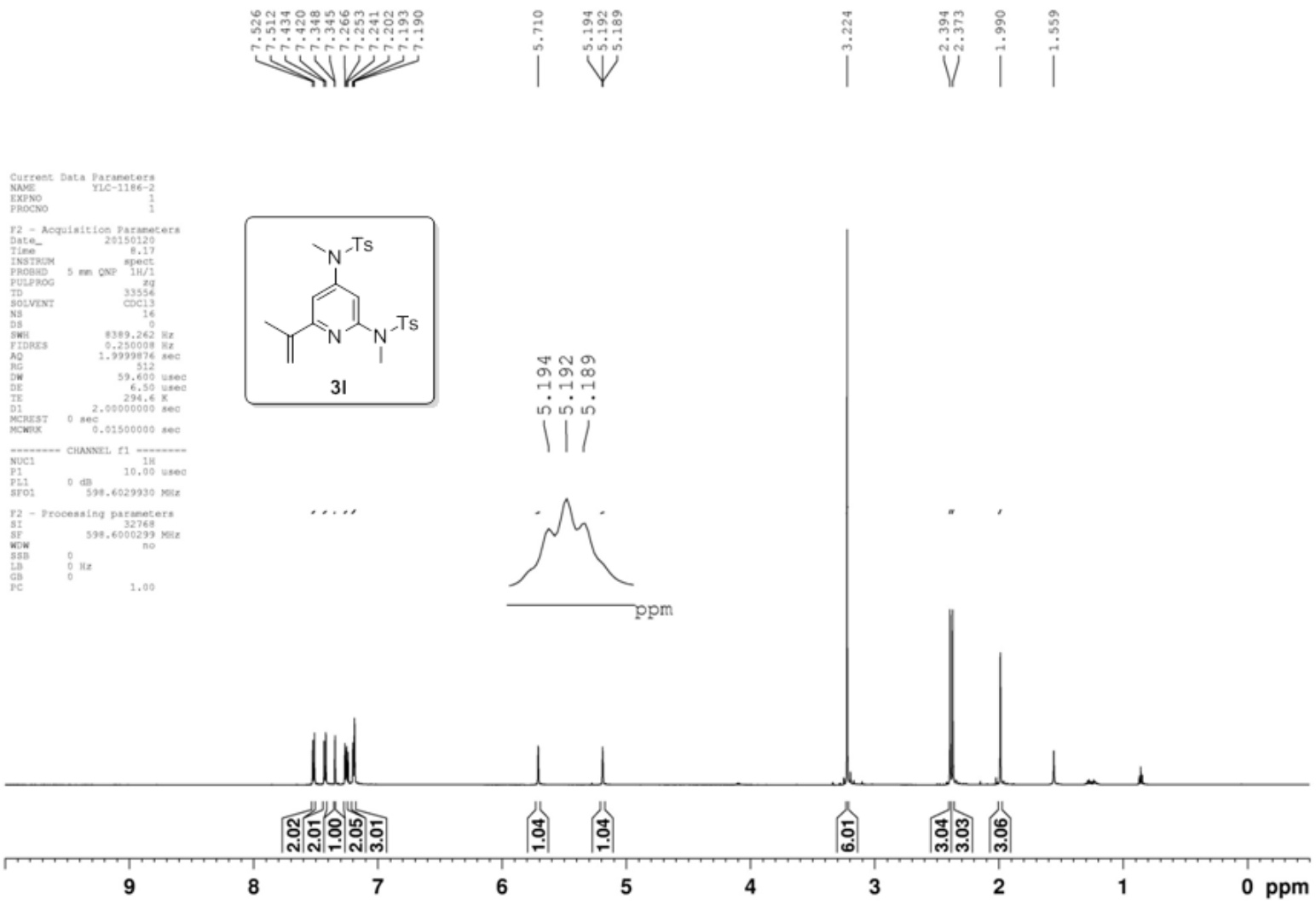

154.72
154.24
151.18
144.51
143.98
136.97
134.29
133.61
131.75
129.85
129.51
128.35
127.49
127.47
123.88
112.94
111.35
77.25
77.00
76.75
36.83
35.52
21.60
21.55
YLC-1104
exp3 DEPT
SAMPLE
date Aug 26 2014
solvent cdcl3
file /home/opec/vn-mrsys/data/LIOU/li-ou0826.002D.fid
ACQUISITION
sw 36363.6
at 0.511
np 37132
bs 16
ss -4
d1 1.000
nt 2048
ct 352
TRANSMITTER
tn C13
tof 3140.4
tpwr 55
pw 12.500
DECOUPLER
dn H1
dof 0
dpwr 38
dm nny
dmm ccw
dmf 11299
pplvl 57
pp 14.000
DEPT
jlkh 140.0
SPECIAL
temp not used
spin not used
PROCESSING
lb 3.00
fn not used
SPECTROM
wp 27647.8
sp -0.9
rp -366.0
lp 172.6
nm ph
REFERENCE
rfl 17128.7
rfp 13993.9
PLOT
wc 250
sc 0
vs 23
hzmm 10.14
th 30
N
Ts
N
Ts
Br
3i
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

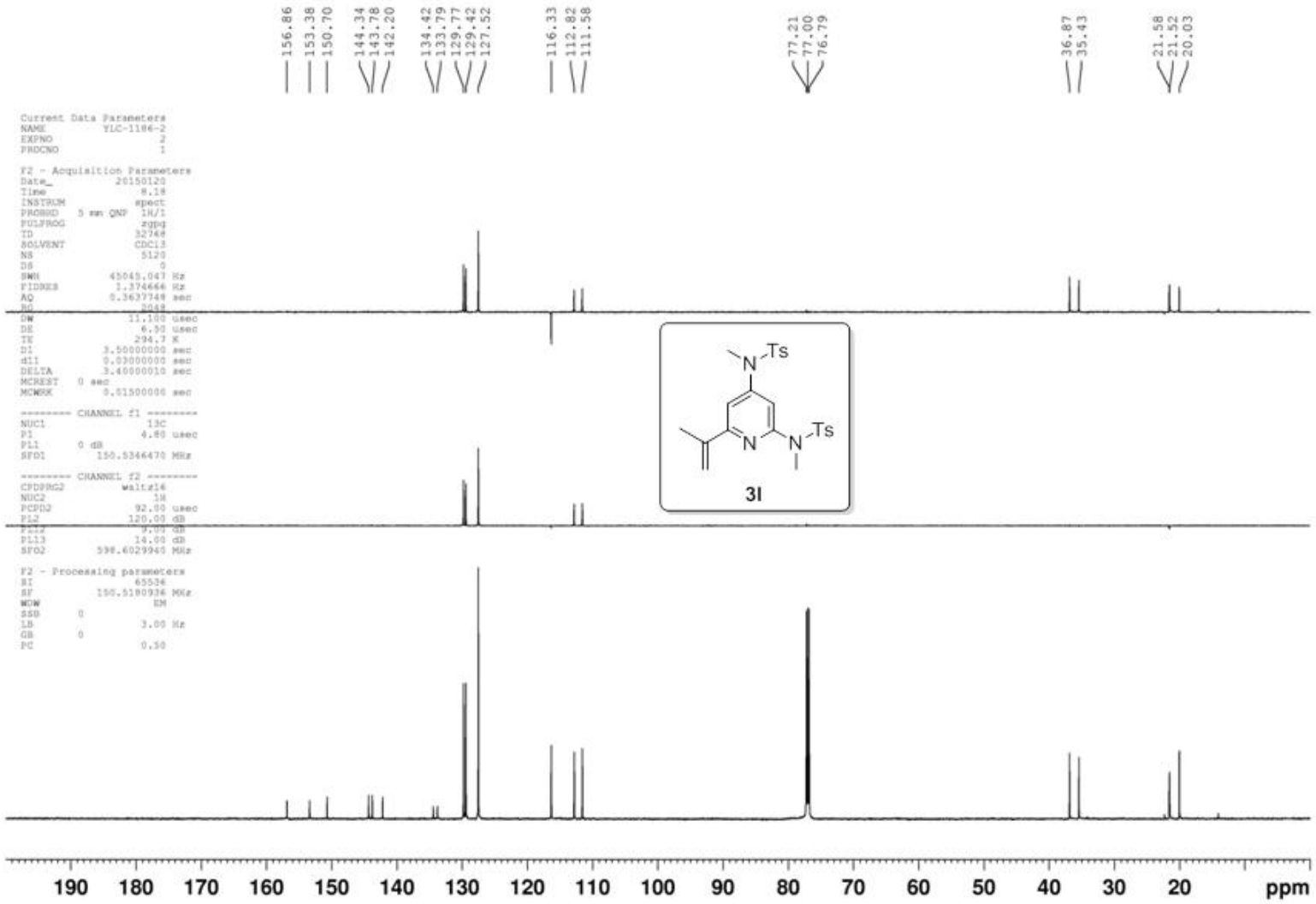

7.524
7.508
7.457
7.441
7.262
7.245
7.240
7.215
7.212
7.193
7.148
7.145
6.604
6.583
6.570
6.548
6.047
6.045
6.013
5.370
5.348
3.244
3.215
2.391
2.375
1.574
YLC-1105
expl Proton
SAMPLE
date Sep 1 2014
solvent cdcl3
file /home/oper/vn-mrsys/data/LIOU/li-ou0901.001N.fid
ACQUISITION
sw 9000.9
at 2.044
np 36804
fb not used
bs 4
ss 2
d1 1.000
nt 32
ct 32
TRANSMITTER
tn H1
sfrq 499.808
tof 999.6
tpwr 55
pw 6.300
DECOUPLER
dn C13
dof 0
dn nnn
dmm c
dpwr 36
dmf 32258
SPECIAL
temp not used
gain not used
spin not used
hst 0.008
pw90 12.600
alfa 6.600
FLAGS
il n
in n
dp y
hs nn
PROCESSING
fn 32768
DISPLAY
sp -250.1
wp 5247.6
rfl 4640.6
rfp 3618.6
rp 80.3
lp 5.0
PLOT
wc 250
sc 0
vs 129
th 14
ph
6.60
ppm
6.05
ppm
ppm
3j
2.02
2.02
5.03
1.01
1.01
1.02
1.00
3.03
3.01
3.03
3.02
9
8
7
6
5
4
3
2
1
0 ppm

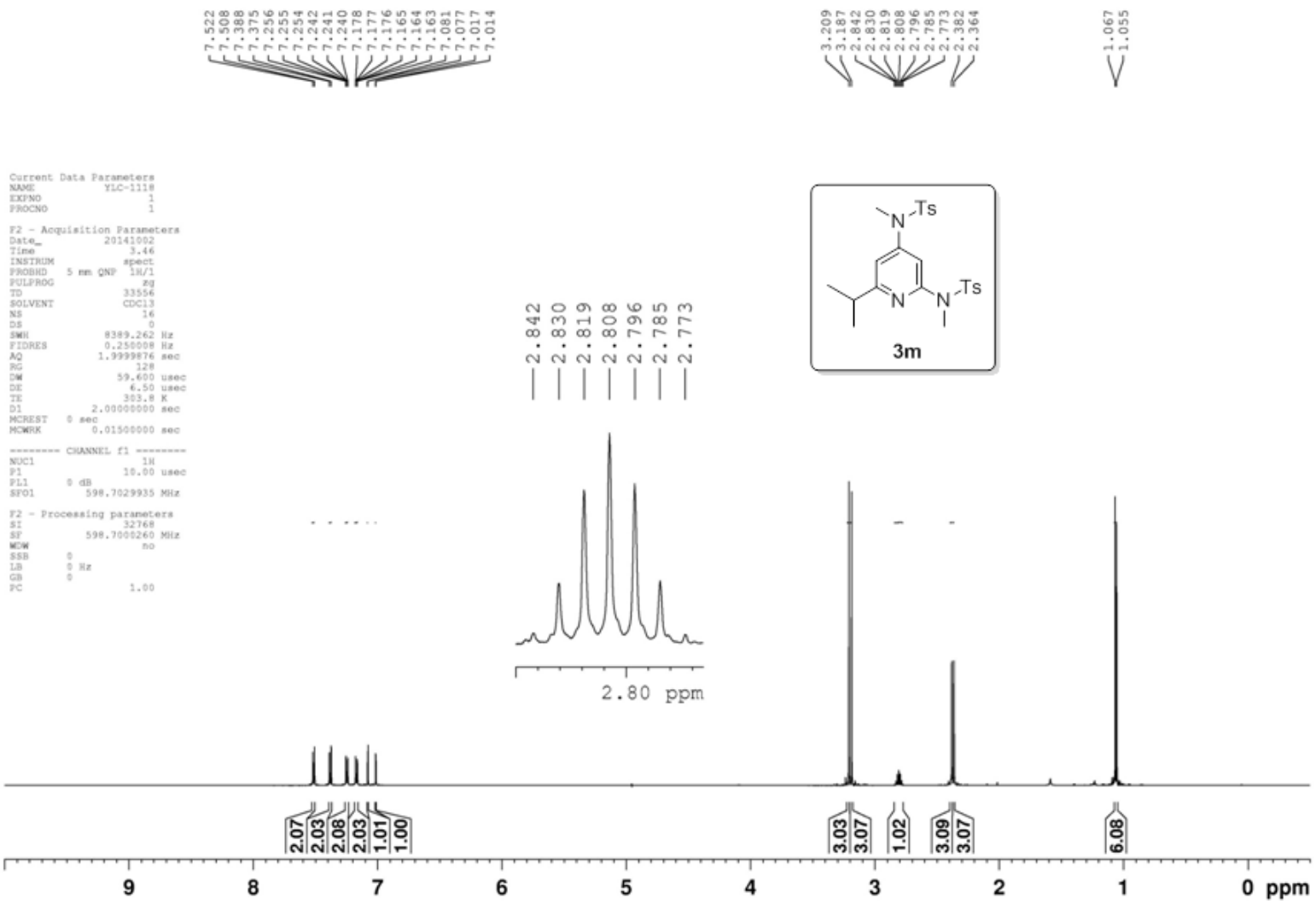

154.35
153.98
150.72
144.39
143.86
135.82
134.45
133.65
129.79
129.46
127.52
127.47
119.12
114.41
111.48
77.25
77.00
76.75
36.76
35.38
21.59
21.55
YLC-1105
exp3 DEPT
SAMPLE
date Sep 1 2014
solvent cdcl3
file /home/oper/vn-
nrsys/data/LIOU/li-
ou0901.001D.fid
ACQUISITION
sw 36363.6
at 0.511
np 37172
bs 16
ss -4
ct 896
TRANSMITTER
tn C13
tof 3140.4
tpwr 55
pw 12.500
DECOUPLER
dn H1
dof 0
dpwr 38
dm nny
dmm ccw
dmf 11299
pplvl 57
pp 14.000
DEPT
jlxh 140.0
SPECIAL
spin not used
PROCESSING
lb 3.00
fn not used
SPECTRUM
wp 27647.8
sp -0.9
rp -370.7
lp 172.6
nm ph
REFERENCE
rfl 17144.2
rfp 14009.5
PLOT
wc 250
sc 0
vs 20
hzmm 110.59
th 30
Ts
N
Ts
N
N
3j
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

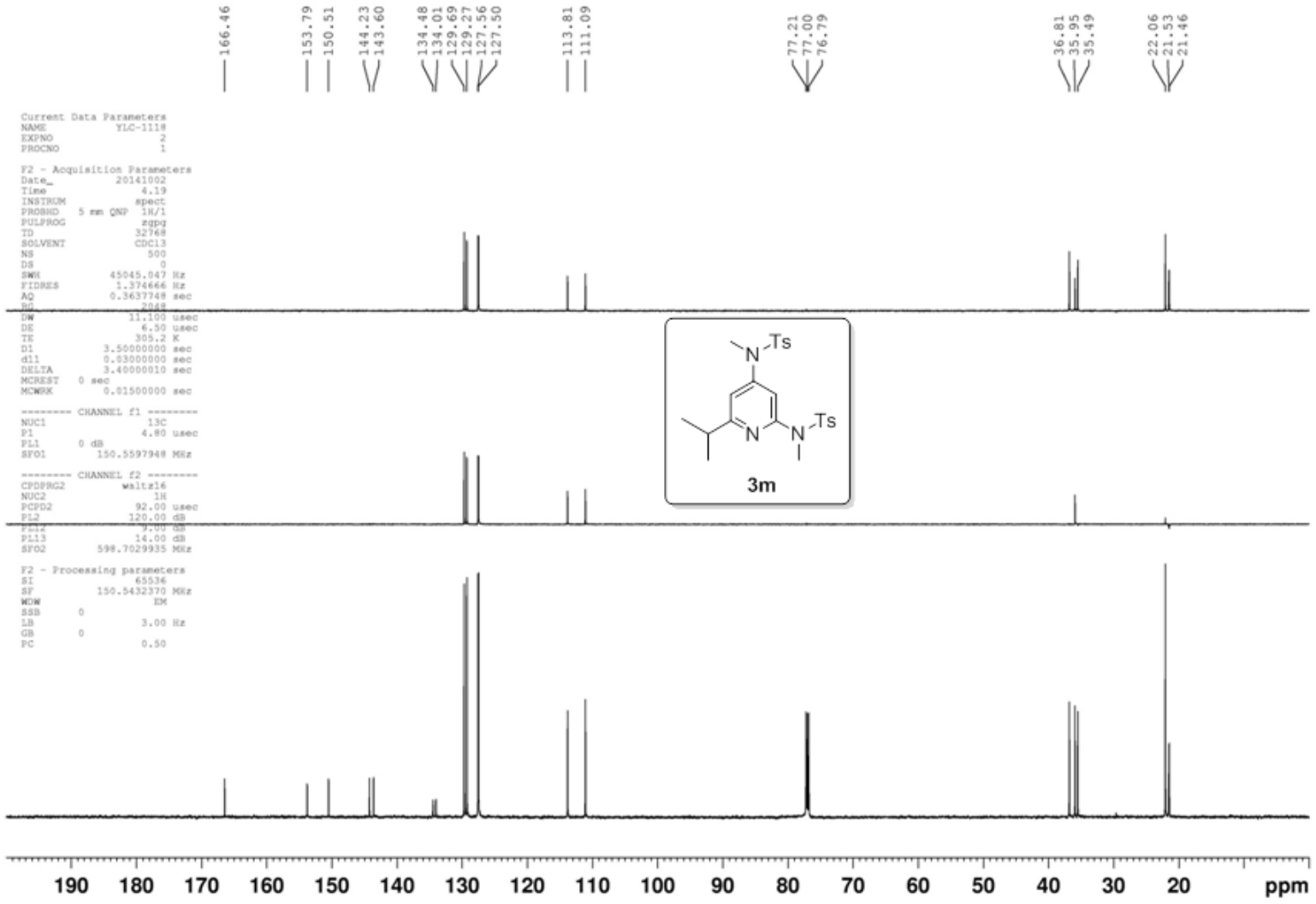

7.547
7.533
7.489
7.475
7.471
7.460
7.460
7.458
7.377
7.351
7.339
7.326
7.287
7.285
7.274
7.268
7.267
7.266
7.254
7.253
7.240
7.229
7.226
7.221
7.221
7.207
7.206
7.196
7.193
6.955
6.929
3.303
3.240
2.392
2.370
Current Data Parameters
NAME YLC-1115
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20140924
Time 13.08
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg
TD 33556
SOLVENT CDCl3
NS 16
DS 0
SWH 8389.262 Hz
FIDRES 0.250008 Hz
AQ 1.9999876 sec
RG 512
DW 59.600 usec
DE 6.50 usec
TE 303.4 K
D1 2.00000000 sec
MCREST 0 sec
MCWRK 0.01500000 sec
-------- CHANNEL f1 --------
NUC1 1H
P1 10.00 usec
PL1 0 dB
SFO1 598.7029935 MHz
F2 - Processing parameters
SI 32768
SF 598.7000266 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 1.00
N
Ts
N
N
Ts
Ph
3k
2.04
4.03
3.03
3.05
4.01
1.03
3.07
3.03
3.06
3.03
9
8
7
6
5
4
3
2
1
0 ppm

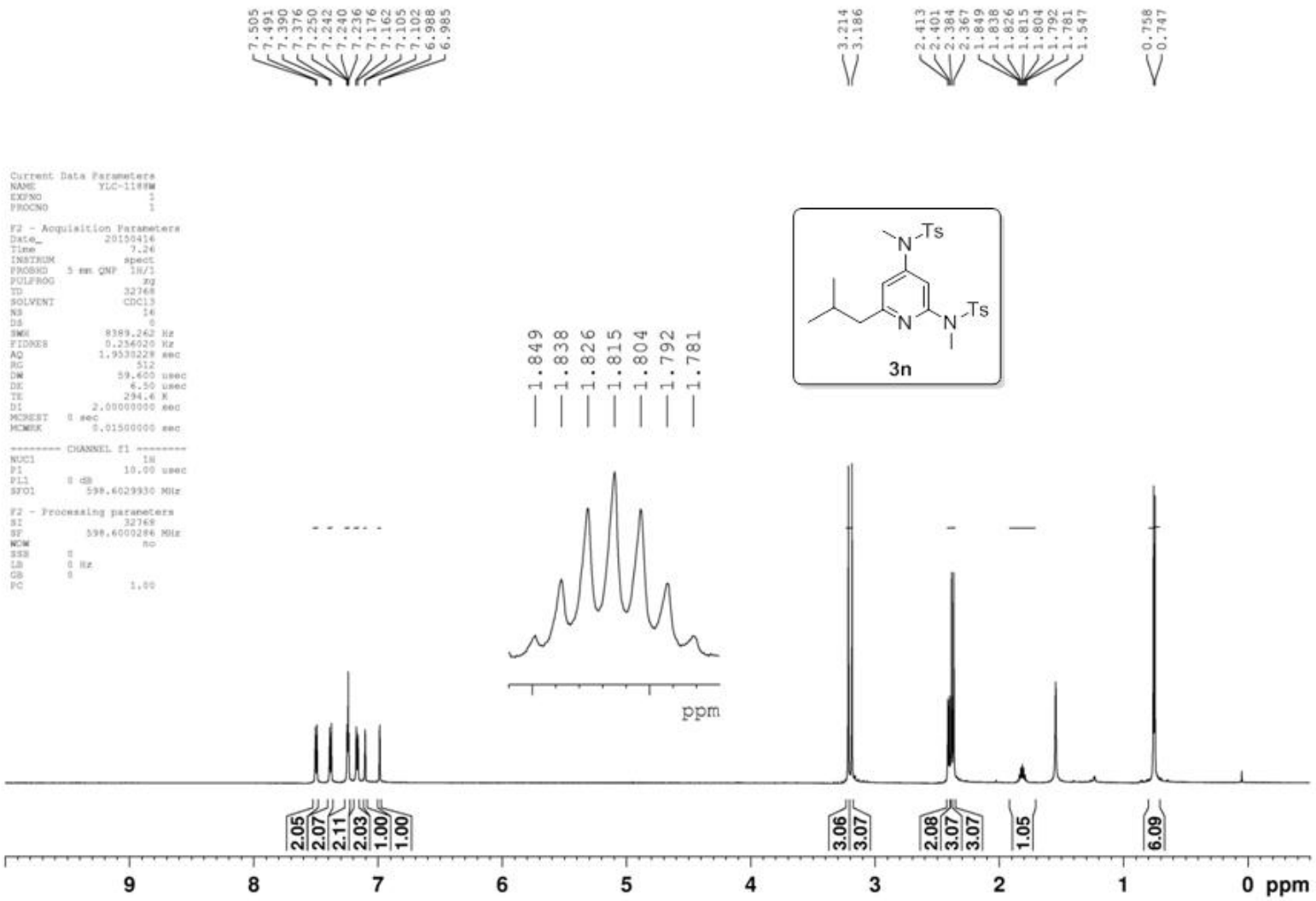

154.51
154.18
150.82
144.37
143.81
136.34
134.73
133.86
133.66
129.81
129.49
128.74
128.56
127.60
127.50
127.12
127.10
114.97
111.13
77.21
77.00
76.79
36.78
35.54
21.57
21.53
Current Data Parameters
NAME YLC-1121-down
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20141005
Time 21.32
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CD2Cl2
NS 441
DS 0
SWH 45045.047 Hz
FIDRES 1.374666 Hz
AQ 0.3637748 sec
RG 2048
DW 11.100 usec
DE 6.50 usec
TE 303.6 K
D1 3.50000000 sec
d11 0.03000000 sec
DELTA 3.40000010 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 4.80 usec
PL1 0.00 dB
SFO1 150.5597948 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 92.00 usec
PL2 120.00 dB
PL12 7.00 dB
PL13 14.00 dB
SFO2 598.7029935 MHz
F2 - Processing parameters
SI 65536
SF 150.5432349 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 0.50
1D NMR plot parameters
CX 20.00 cm
CY 4.00 cm
F1P 145.000 ppm
F1 21828.77 Hz
F2P 126.000 ppm
F2 18968.45 Hz
N
Ts
N
N
Ts
Ph
3k
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

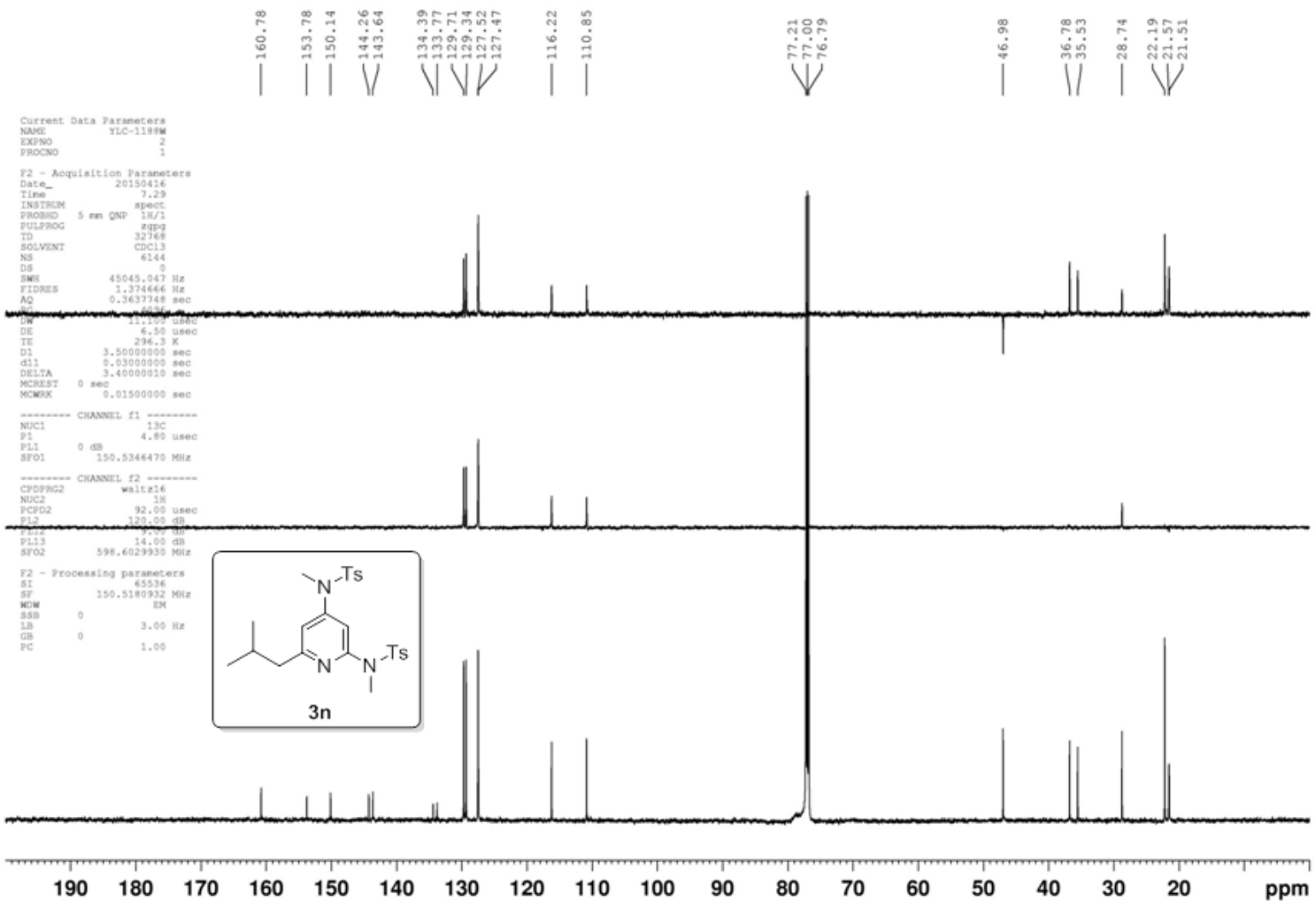

7.526
7.512
7.434
7.420
7.348
7.345
7.266
7.253
7.241
7.202
7.193
7.190
5.710
5.194
5.192
5.189
3.224
2.394
2.373
1.990
1.559
Current Data Parameters
NAME YLC-1186-2
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20150120
Time 8.17
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg
TD 33556
SOLVENT CDCl3
NS 16
DS 0
SWH 8389.262 Hz
FIDRES 0.250008 Hz
AQ 1.9999876 sec
RG 512
DW 59.600 usec
DE 6.50 usec
TE 294.6 K
D1 2.00000000 sec
MCREST 0 sec
MCWRK 0.01500000 sec
-------- CHANNEL f1 --------
NUC1 1H
P1 10.00 usec
PL1 0 dB
SFO1 598.6029930 MHz
F2 - Processing parameters
SI 32768
SF 598.6000299 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 1.00
Ts
N
Ts
N
N
3l
5.194
5.192
5.189
ppm
2.02
2.01
1.00
2.05
3.01
1.04
1.04
6.01
3.04
3.03
3.06
9
8
7
6
5
4
3
2
1
0 ppm

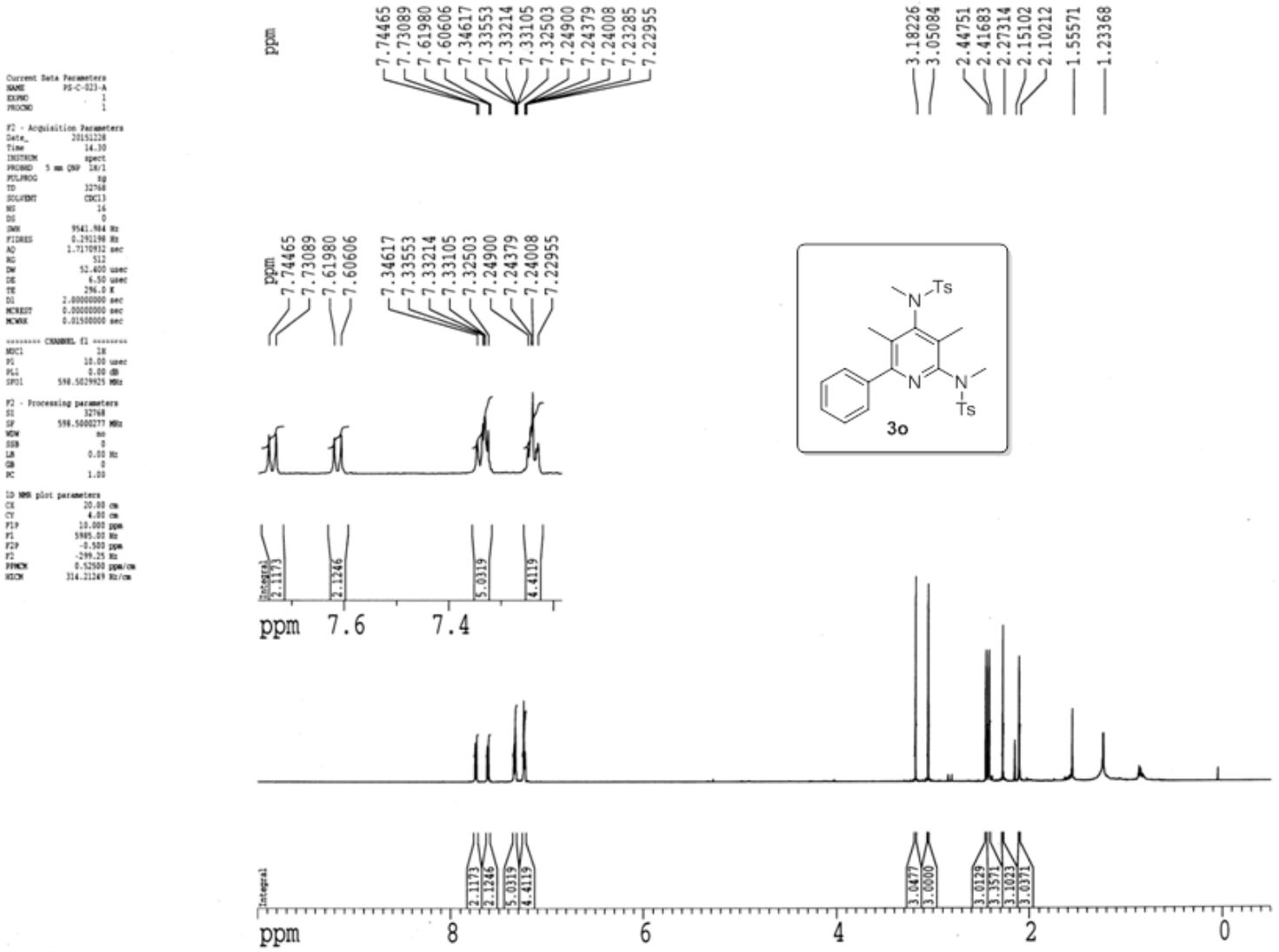

156.86
153.38
150.70
144.34
143.78
142.20
134.42
133.79
129.77
129.42
127.52
116.33
112.82
111.58
77.21
77.00
76.79
36.87
35.43
21.58
21.52
20.03
Current Data Parameters
NAME YLC-1186-2
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20150120
Time 8.18
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 5120
DS 0
SWH 45045.047 Hz
FIDRES 1.374666 Hz
AQ 0.3637748 sec
RG 2048
DW 11.100 usec
DE 6.50 usec
TE 294.7 K
D1 3.50000000 sec
d11 0.03000000 sec
DELTA 3.40000010 sec
MCREST 0 sec
MCWRK 0.01500000 sec
-------- CHANNEL f1 --------
NUC1 13C
P1 4.80 usec
PL1 0 dB
SFO1 150.5346470 MHz
-------- CHANNEL f2 --------
CPDPRG2 waltz16
NUC2 1H
PCPD2 92.00 usec
PL2 120.00 dB
PL12 9.00 dB
PL13 14.00 dB
SFO2 598.6029940 MHz
F2 - Processing parameters
SI 65536
SF 150.5180936 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 0.50
N
Ts
N
N
Ts
3l
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

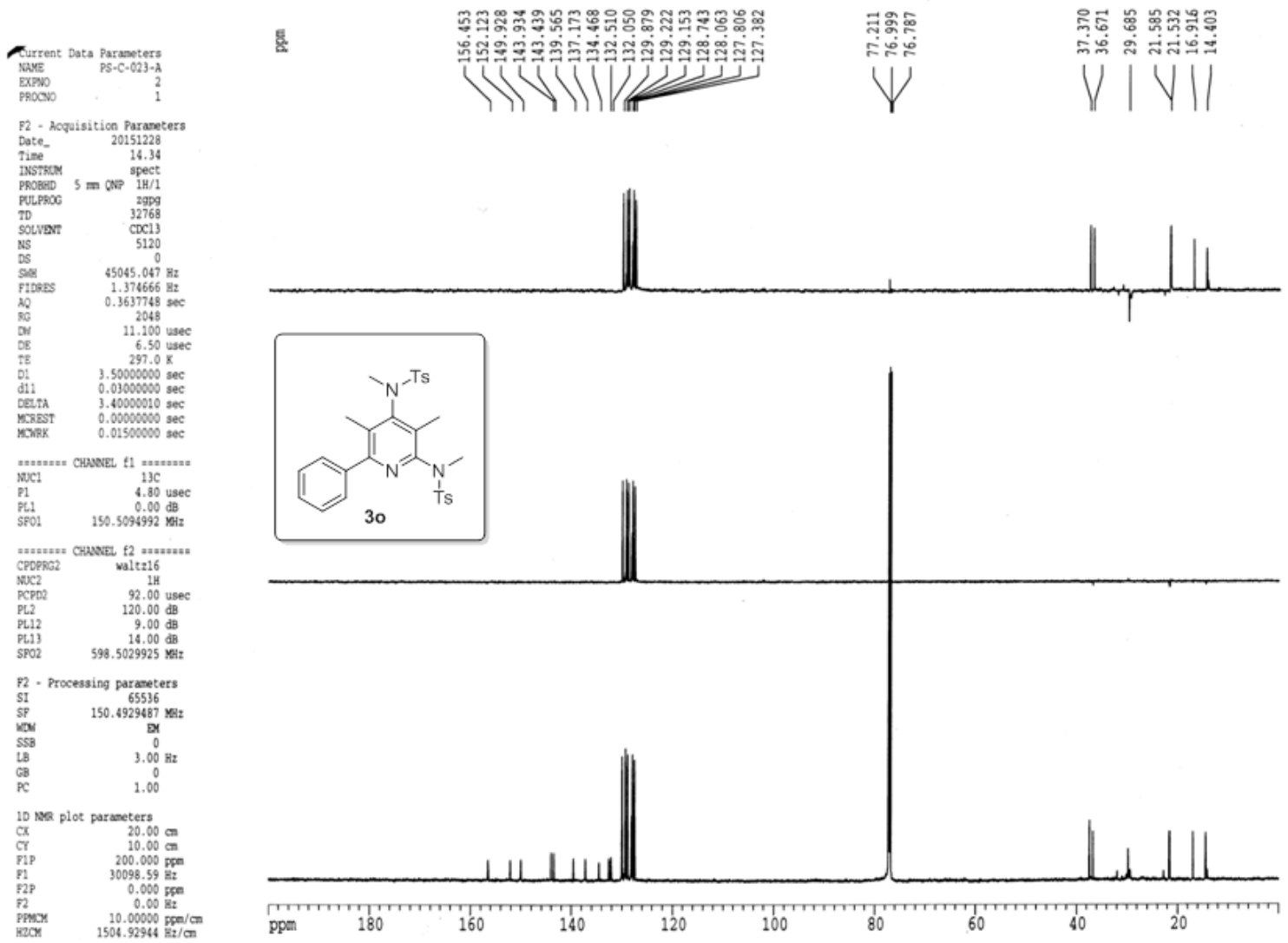

7.522
7.508
7.388
7.375
7.256
7.255
7.254
7.242
7.241
7.240
7.178
7.177
7.176
7.165
7.164
7.163
7.081
7.077
7.017
7.014
3.209
3.187
2.842
2.830
2.819
2.808
2.796
2.785
2.773
2.382
2.364
1.067
1.055
Current Data Parameters
NAME YLC-1118
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20141002
Time 3.46
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg
TD 33556
SOLVENT CDCl3
NS 16
DS 0
SWH 8389.262 Hz
FIDRES 0.250008 Hz
AQ 1.9999876 sec
RG 128
DW 59.600 usec
DE 6.50 usec
TE 303.8 K
D1 2.00000000 sec
MCREST 0 sec
MCWRK 0.01500000 sec
-------- CHANNEL f1 --------
NUC1 1H
P1 10.00 usec
PL1 0 dB
SFO1 598.7029935 MHz
F2 - Processing parameters
SI 32768
SF 598.7000260 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 1.00
2.842
2.830
2.819
2.808
2.796
2.785
2.773
2.80 ppm
Ts
N
Ts
N
N
3m
2.07
2.03
2.08
2.03
1.01
1.00
3.03
3.07
1.02
3.09
3.07
6.08
9
8
7
6
5
4
3
2
1
0 ppm

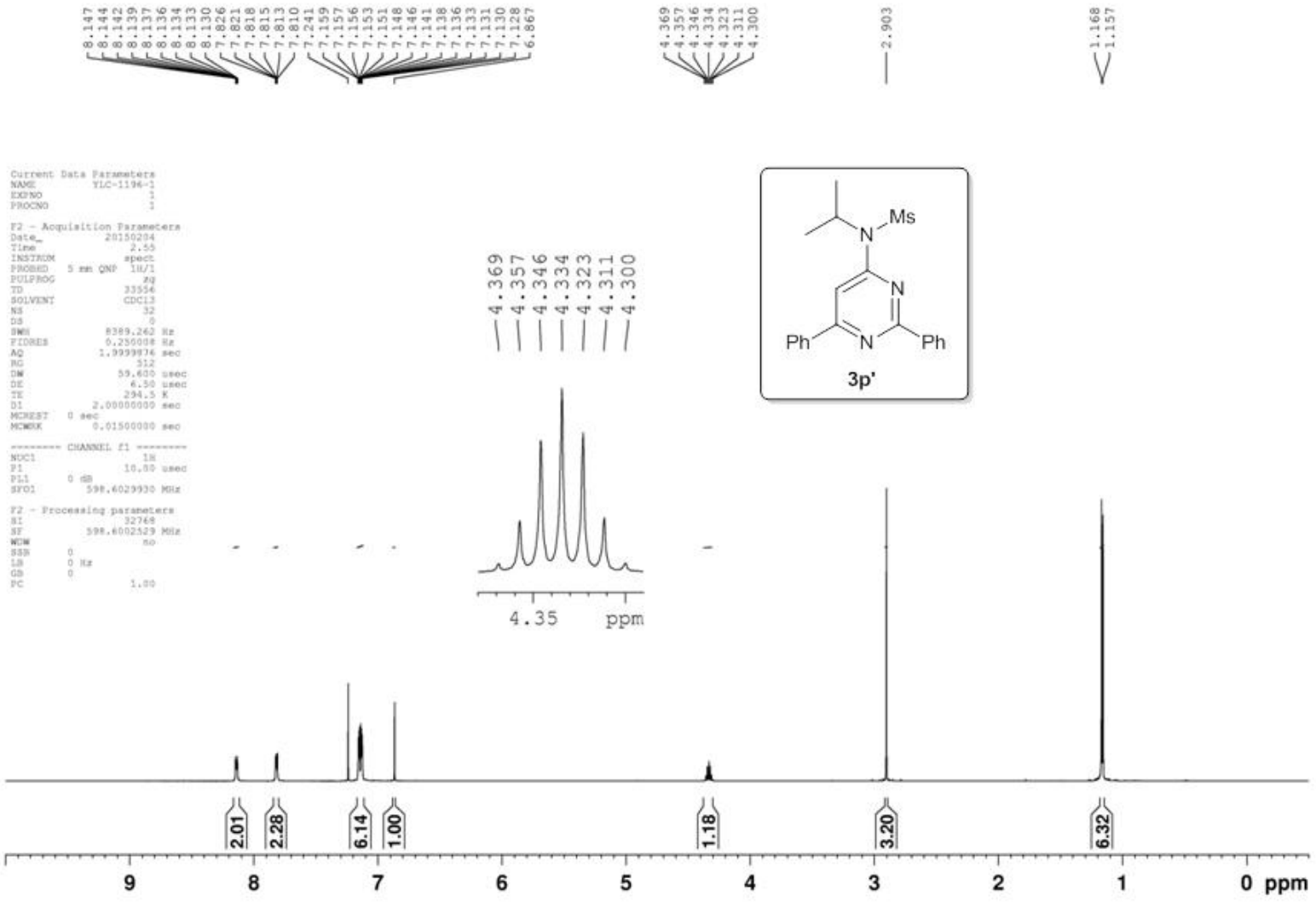

166.46
153.79
150.51
144.23
143.60
134.48
134.01
129.69
129.27
127.56
127.50
113.81
111.09
77.21
77.00
76.79
36.81
35.95
35.49
22.06
21.53
21.46
Current Data Parameters
NAME YLC-1118
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20141002
Time 4.19
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 500
DS 0
SWH 45045.047 Hz
FIDRES 1.374666 Hz
AQ 0.3637748 sec
RG 2048
DW 11.100 usec
DE 6.50 usec
TE 305.2 K
D1 3.50000000 sec
d11 0.03000000 sec
DELTA 3.40000010 sec
MCREST 0 sec
MCWRK 0.01500000 sec
-------- CHANNEL f1 --------
NUC1 13C
P1 4.80 usec
PL1 0 dB
SFO1 150.5597948 MHz
-------- CHANNEL f2 --------
CPDPRG2 waltz16
NUC2 1H
PCPD2 92.00 usec
PL2 120.00 dB
PL12 9.00 dB
PL13 14.00 dB
SFO2 598.7029935 MHz
F2 - Processing parameters
SI 65536
SF 150.5432370 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 0.50
N
Ts
N
N
Ts
3m
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

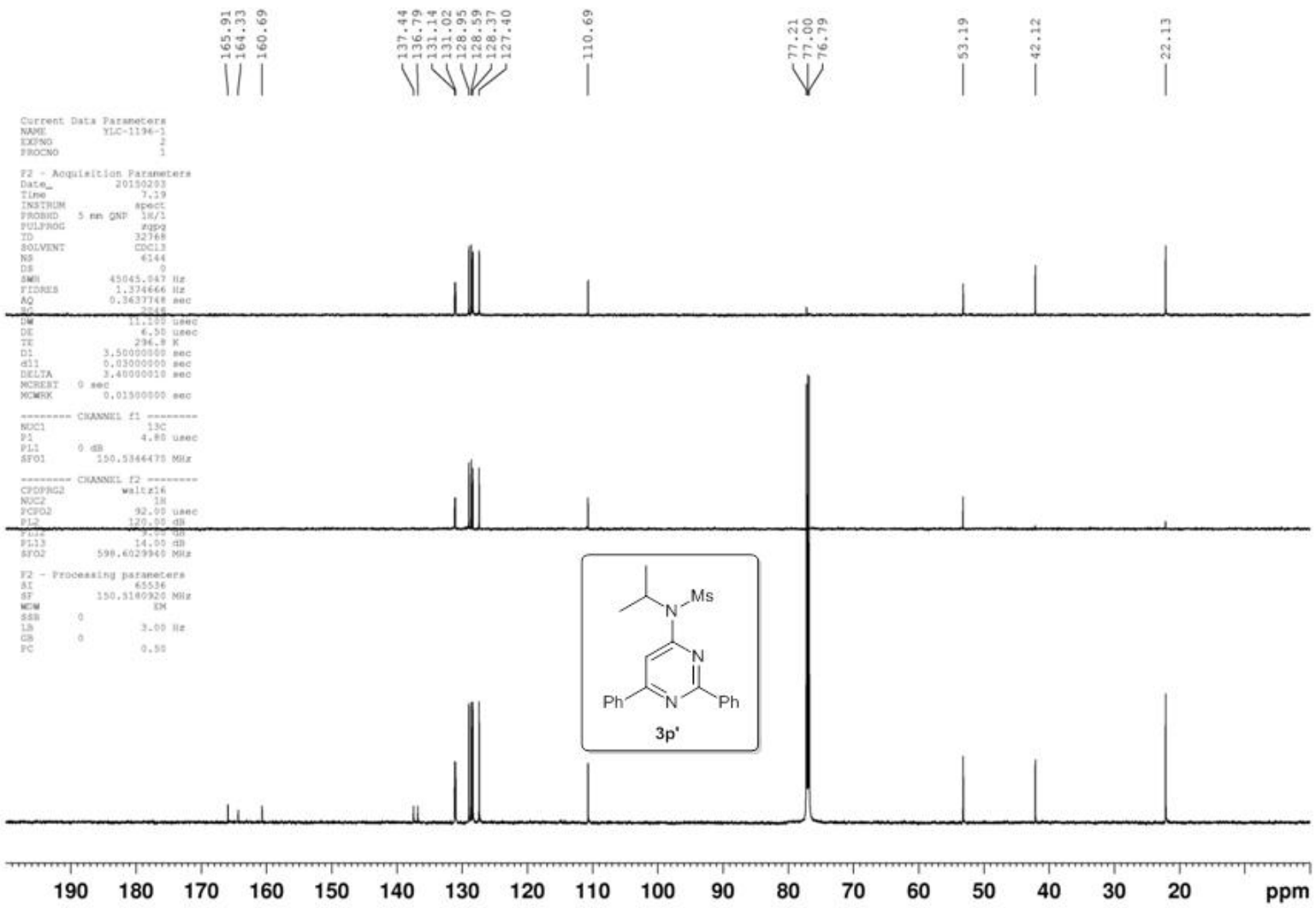

7.505
7.491
7.390
7.376
7.250
7.242
7.240
7.236
7.176
7.162
7.105
7.102
6.988
6.985
3.214
3.186
2.413
2.401
2.384
2.367
1.849
1.838
1.826
1.815
1.804
1.792
1.781
1.547
0.758
0.747
Current Data Parameters
NAME YLC-118BM
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20150416
Time 7.26
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 8389.262 Hz
FIDRES 0.256020 Hz
AQ 1.9530229 sec
RG 512
DW 59.600 usec
DE 6.50 usec
TE 294.6 K
D1 2.00000000 sec
MCREST 0 sec
MCWRK 0.01500000 sec
-------- CHANNEL f1 --------
NUC1 1H
P1 10.00 usec
PL1 0 dB
SFO1 598.6029930 MHz
F2 - Processing parameters
SI 32768
SF 598.6000286 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 1.00
1.849
1.838
1.826
1.815
1.804
1.792
1.781
ppm
3n
2.05
2.07
2.11
2.03
1.00
1.00
3.06
3.07
2.08
3.07
3.07
1.05
6.09
9
8
7
6
5
4
3
2
1
0 ppm

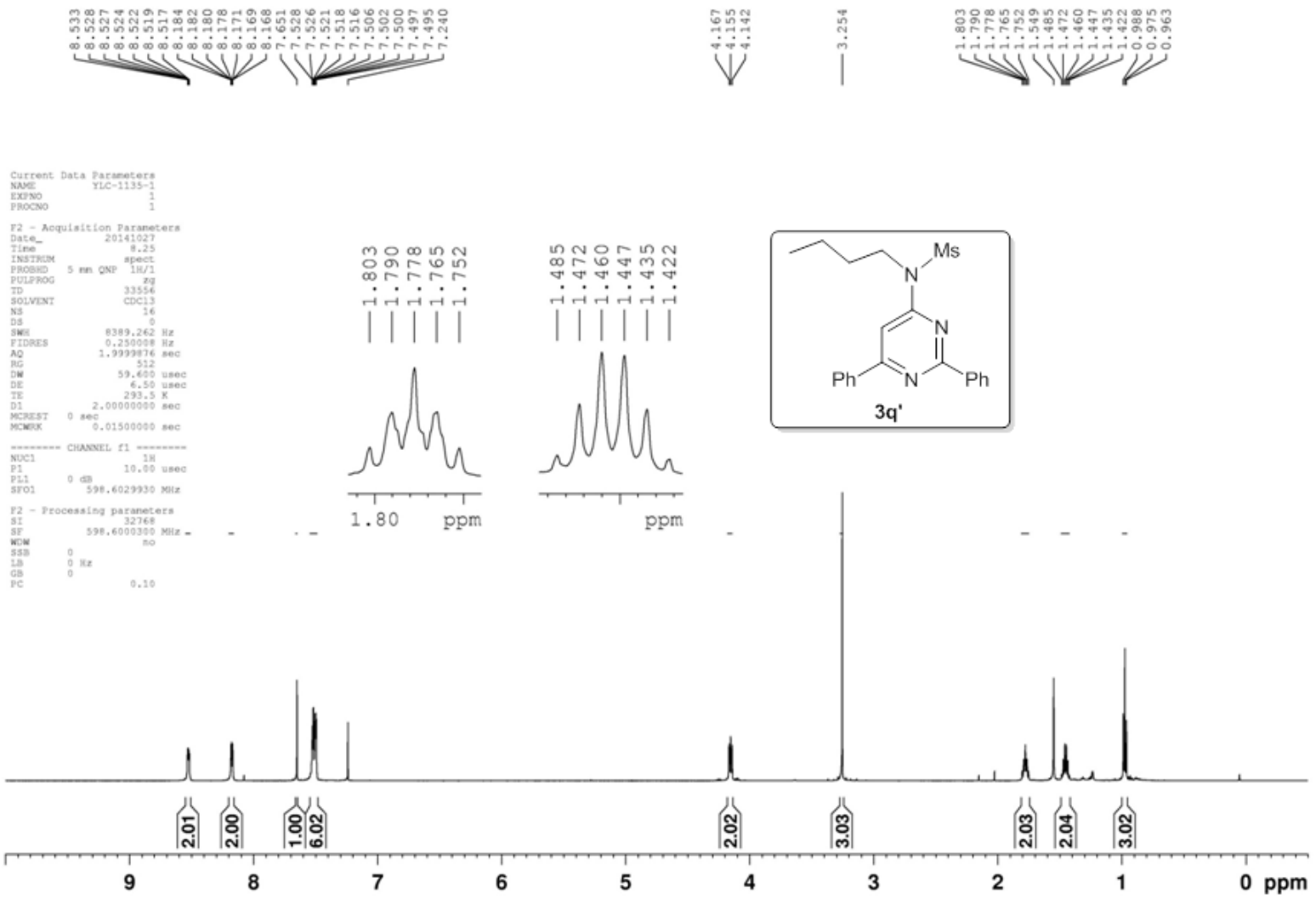

160.78
153.78
150.14
144.26
143.64
134.39
133.77
129.71
129.34
127.52
127.47
116.22
110.85
77.21
77.00
76.79
46.98
36.78
35.53
28.74
22.19
21.57
21.51
Current Data Parameters
NAME YLC-1188W
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20150416
Time 7.29
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 6144
DS 0
SWH 45045.047 Hz
FIDRES 1.374666 Hz
AQ 0.3637748 sec
DW 11.100 usec
DE 6.50 usec
TE 296.3 K
D1 3.50000000 sec
d11 0.03000000 sec
DELTA 3.40000010 sec
MCREST 0 sec
MCWRK 0.01500000 sec
-------- CHANNEL f1 --------
NUC1 13C
P1 4.80 usec
PL1 0 dB
SFO1 150.5346470 MHz
-------- CHANNEL f2 --------
CPDPRG2 waltz16
NUC2 1H
PCPD2 92.00 usec
PL2 120.00 dB
PL12 14.00 dB
PL13 14.00 dB
SFO2 598.6029930 MHz
F2 - Processing parameters
SI 65536
SF 150.5180932 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
Ts
N
Ts
N
N
3n
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

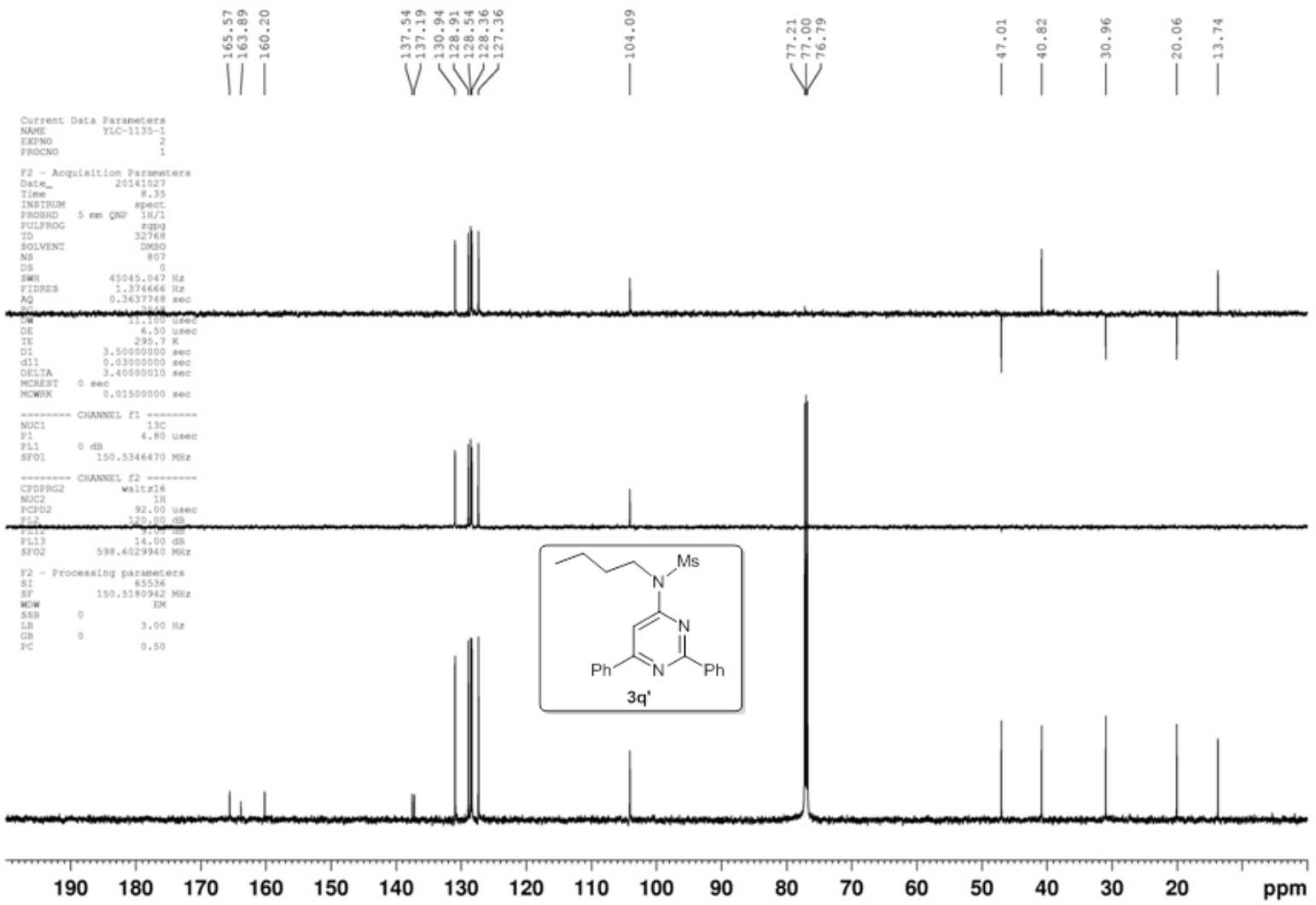

Current Data Parameters
NAME PS-C-023-A
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20151228
Time 14.30
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 9541.984 Hz
FIDRES 0.291198 Hz
AQ 1.7170932 sec
RG 512
DW 52.400 usec
DE 6.50 usec
TE 296.0 K
D1 2.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 0.00 dB
SFO1 598.5029925 MHz
F2 - Processing parameters
SI 32768
SF 598.5000279 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 20.00 cm
CY 4.00 cm
F1P 10.000 ppm
F1 5985.00 Hz
F2P -0.500 ppm
F2 -299.25 Hz
PPMCM 0.52500 ppm/cm
HZCM 314.21249 Hz/cm
ppm
7.74465
7.73089
7.61980
7.60606
7.34617
7.33553
7.33214
7.33105
7.32503
7.24900
7.24379
7.24008
7.23285
7.22955
3.18226
3.05084
2.44751
2.41683
2.27314
2.15102
2.10212
1.55571
1.23368
Integral
2.1173
2.1246
5.0319
4.4119
ppm 7.6 7.4
3o
3.0477
3.0000
3.0129
3.3571
3.1023
3.0371
ppm 8 6 4 2 0


Current Data Parameters
NAME PS-C-023-A
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20151228
Time 14.34
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 5120
DS 0
SWH 45045.047 Hz
FIDRES 1.374666 Hz
AQ 0.3637748 sec
RG 2048
DW 11.100 usec
DE 6.50 usec
TE 297.0 K
D1 3.50000000 sec
d11 0.03000000 sec
DELTA 3.40000010 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 4.80 usec
PL1 0.00 dB
SFO1 150.5094992 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 92.00 usec
PL2 120.00 dB
PL12 9.00 dB
PL13 14.00 dB
SFO2 598.5029925 MHz
F2 - Processing parameters
SI 65536
SF 150.4929487 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 20.00 cm
CY 10.00 cm
F1P 200.000 ppm
F1 30098.59 Hz
F2P 0.000 ppm
F2 0.00 Hz
PPMCM 10.00000 ppm/cm
HZCM 1504.92944 Hz/cm
ppm
156.453
152.123
149.928
143.934
143.439
139.565
137.173
134.468
132.510
132.050
129.879
129.222
129.153
128.743
128.063
127.806
127.382
77.211
76.999
76.787
37.370
36.671
29.685
21.585
21.532
16.916
14.403
Ts
N
N
Ts
3o
ppm
180
160
140
120
100
80
60
40
20

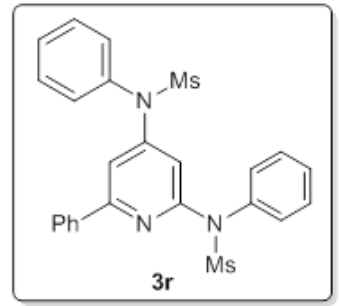

8.147
8.144
8.142
8.139
8.137
8.136
8.134
8.133
8.130
7.826
7.821
7.818
7.815
7.813
7.810
7.241
7.159
7.157
7.156
7.153
7.151
7.148
7.146
7.141
7.138
7.136
7.133
7.131
7.130
7.128
6.867
4.369
4.357
4.346
4.334
4.323
4.311
4.300
2.903
1.168
1.157
Current Data Parameters
NAME YLC-1196-1
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20150204
Time 2.55
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg
TD 33554
SOLVENT CDCl3
NS 32
DS 0
SWH 8389.262 Hz
FIDRES 0.250008 Hz
AQ 1.9999876 sec
RG 312
DW 59.600 usec
DE 6.50 usec
TE 294.5 K
D1 2.00000000 sec
MCREST 0 sec
MCWRK 0.01500000 sec
-------- CHANNEL f1 --------
NUC1 1H
P1 10.00 usec
PL1 0 dB
SFO1 598.6029930 MHz
F2 - Processing parameters
SI 32768
SF 598.6002529 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 1.00
4.35 ppm
N
Ms
N
N
Ph
Ph
3p'
2.01
2.28
6.14
1.00
1.18
3.20
6.32
9
8
7
6
5
4
3
2
1
0 ppm


165.91
164.33
160.69
137.44
136.79
131.14
131.02
128.95
128.59
128.37
127.40
110.69
77.21
77.00
76.79
53.19
42.12
22.13
Current Data Parameters
NAME YLC-1196-1
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20150203
Time 7.19
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 4144
DS 0
SWH 45045.047 Hz
FIDRES 1.374666 Hz
AQ 0.3637748 sec
RG 2048
DW 11.100 usec
DE 6.50 usec
TE 296.8 K
D1 3.50000000 sec
d11 0.03000000 sec
DELTA 3.40000010 sec
MCREST 0 sec
MCWRK 0.01500000 sec
-------- CHANNEL f1 --------
NUC1 13C
P1 4.80 usec
PL1 0 dB
SFO1 150.5366475 MHz
-------- CHANNEL f2 --------
CPDPRG2 waltz16
NUC2 1H
PCPD2 92.00 usec
PL2 120.00 dB
PL12 19.00 dB
PL13 14.00 dB
SFO2 598.6029940 MHz
F2 - Processing parameters
SI 65536
SF 150.5180920 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 0.50
N
Ms
N
Ph
N
Ph
3p'
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

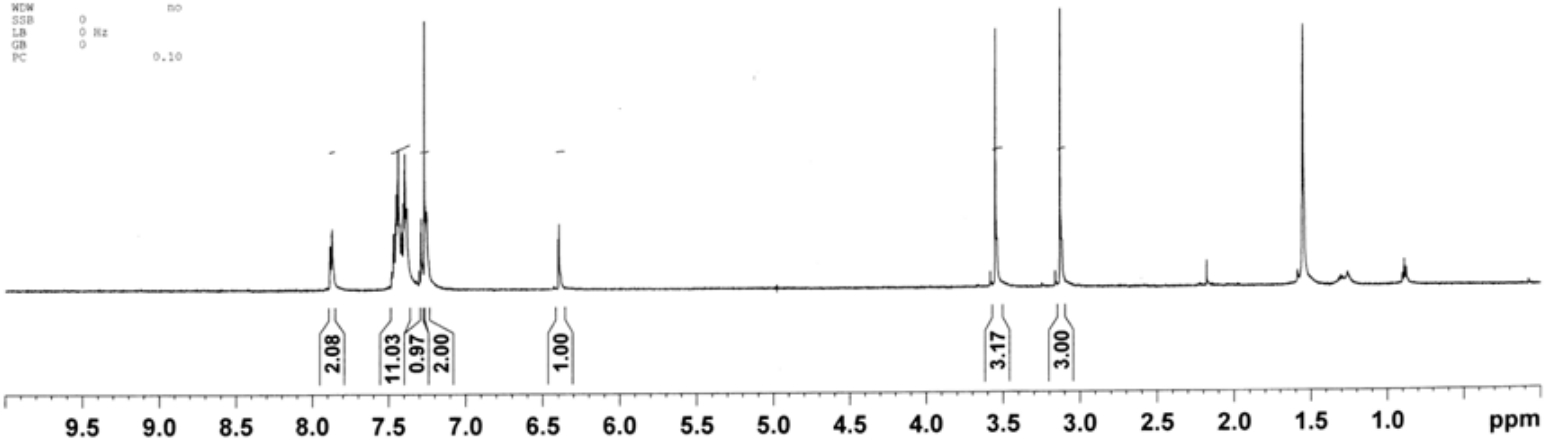

8.533
8.528
8.527
8.524
8.522
8.519
8.517
8.184
8.182
8.180
8.178
8.171
8.169
8.168
7.651
7.528
7.526
7.521
7.518
7.516
7.506
7.502
7.500
7.497
7.495
7.240
4.167
4.155
4.142
3.254
1.803
1.790
1.778
1.765
1.752
1.549
1.485
1.472
1.460
1.447
1.435
1.422
0.988
0.975
0.963
Current Data Parameters
NAME YLC-1135-1
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20141027
Time 8.25
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg
TD 33554
SOLVENT CDCl3
NS 16
DS 0
SWH 8389.262 Hz
FIDRES 0.250008 Hz
AQ 1.9999876 sec
RG 512
DW 59.600 usec
DE 6.50 usec
TE 293.5 K
D1 2.00000000 sec
MCREST 0 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 0 dB
SFO1 598.6029930 MHz
F2 - Processing parameters
SI 32768
SF 598.6000300 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 0.10
1.803
1.790
1.778
1.765
1.752
1.80 ppm
1.485
1.472
1.460
1.447
1.435
1.422
ppm
Ms
N
N
Ph
N
Ph
3q'
2.01
2.00
1.00
6.02
2.02
3.03
2.03
2.04
3.02
9
8
7
6
5
4
3
2
1
0 ppm

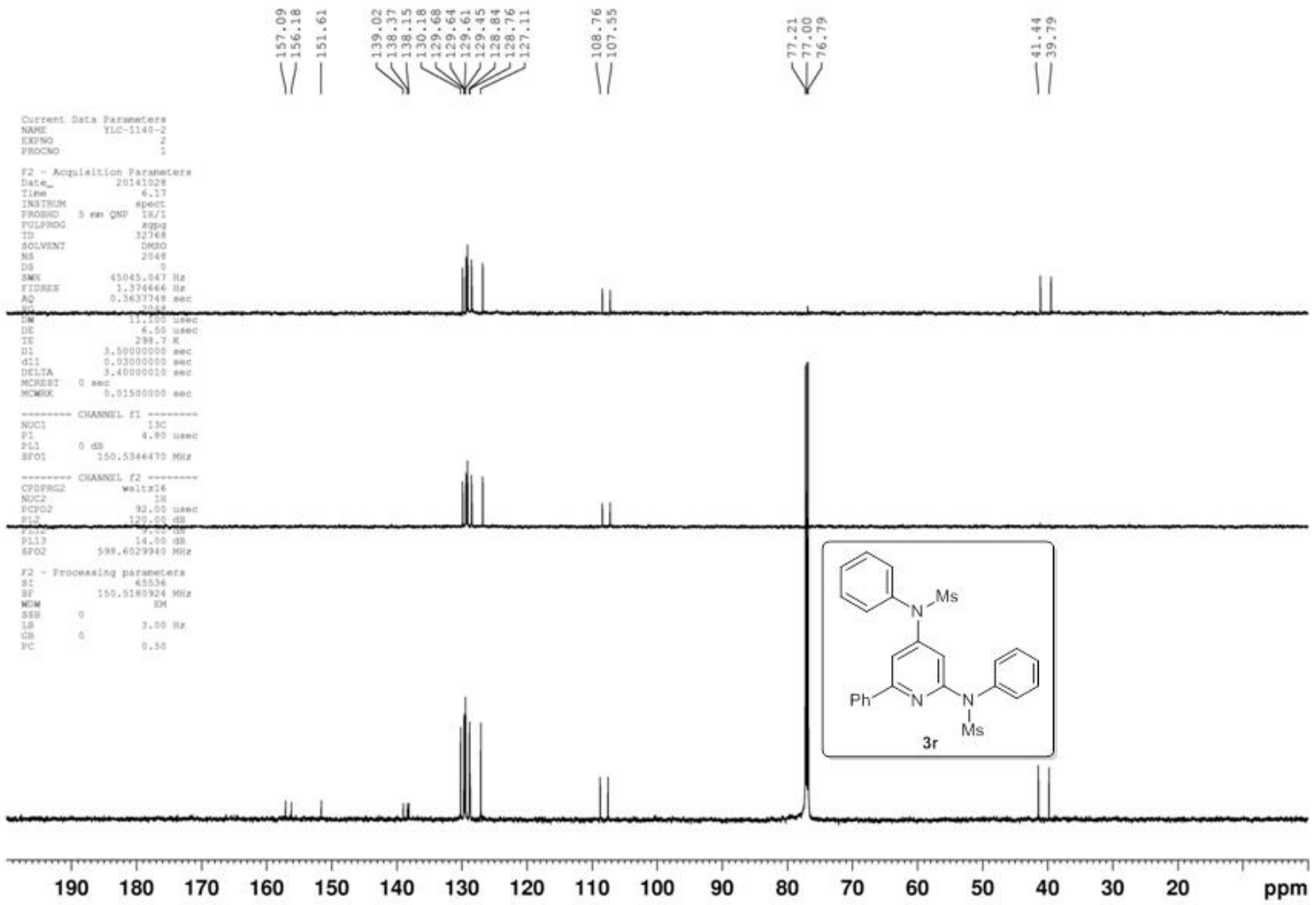

165.57
163.89
160.20
137.54
137.19
130.94
128.91
128.54
128.36
127.36
104.09
77.21
77.00
76.79
47.01
40.82
30.96
20.06
13.74
Current Data Parameters
NAME YLC-1135-1
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20141027
Time 8.35
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT DMSO
NS 807
DS 0
SWH 45045.047 Hz
FIDRES 1.374666 Hz
AQ 0.3637748 sec
RG 2048
DW 11.100 usec
DE 6.50 usec
TE 295.7 K
D1 3.50000000 sec
d11 0.03000000 sec
DELTA 3.40000010 sec
MCREST 0 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 4.80 usec
PL1 0 dB
SFO1 150.5346470 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 92.00 usec
PL2 120.00 dB
PL12 9.00 dB
PL13 14.00 dB
SFO2 598.6029940 MHz
F2 - Processing parameters
SI 65536
SF 150.5180942 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 0.50
Ms
N
N
Ph
N
Ph
3q'
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

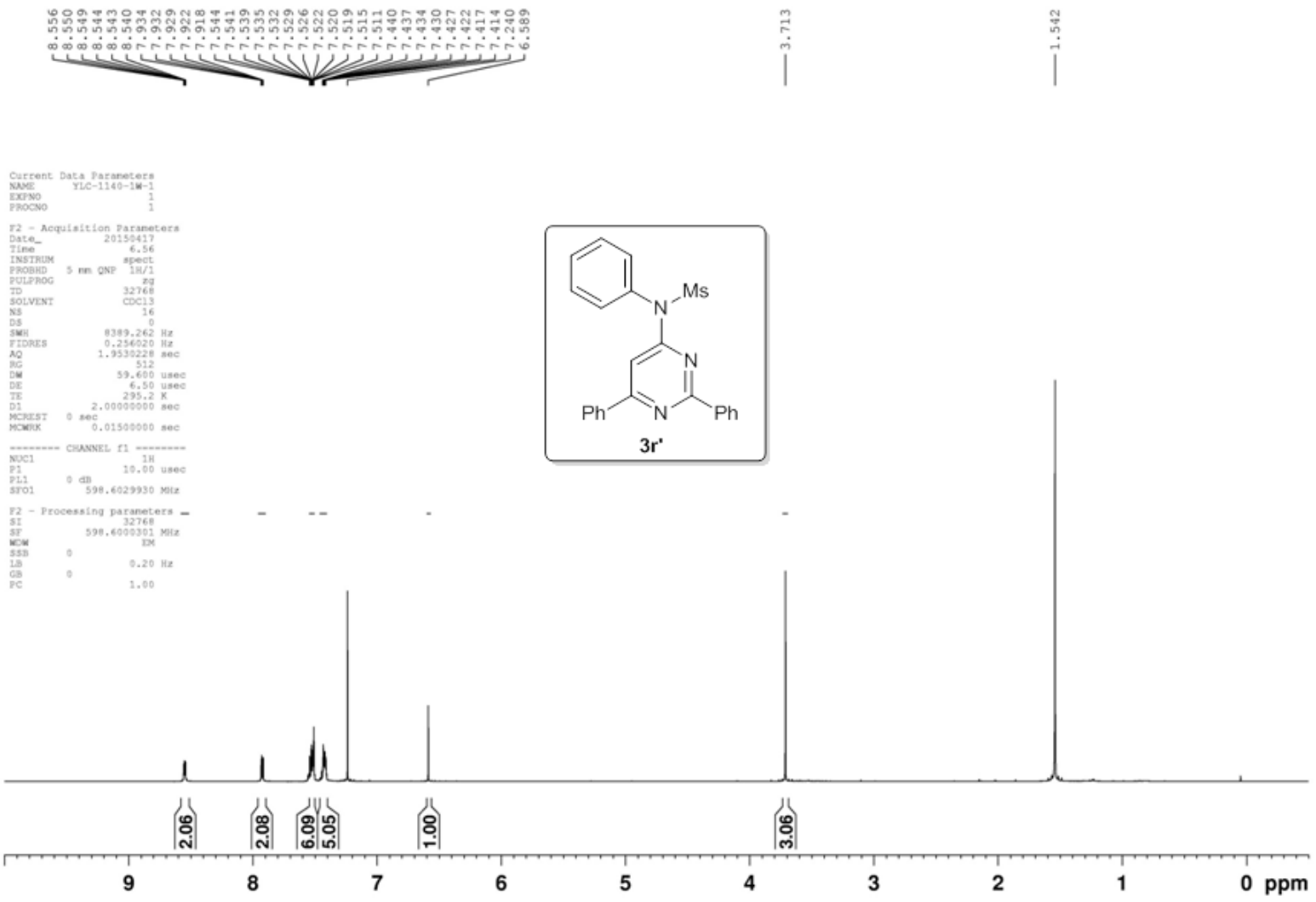

```
Current Data Parameters
NAME          YLC-1140-2
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20141028
Time               5.45
INSTRUM           spect
PROBHD   5 mm QNP  1H/1
PULPROG              zg
TD                33556
SOLVENT           CDCl3
NS                   16
DS                    0
SWH            8389.262 Hz
FIDRES         0.250008 Hz
AQ             1.9999876 sec
RG                 512
DW              59.600 usec
DE               6.50 usec
TE              297.4 K
D1              2.00000000 sec
MCREST   0 sec
MCWRK           0.01500000 sec

======== CHANNEL f1 ========
NUC1                  1H
P1                10.00 usec
PL1       0 dB
SFO1        598.6029930 MHz

F2 - Processing parameters
SI                32768
SF          598.6000140 MHz
WDW                  no
SSB       0
LB        0 Hz
GB        0
PC                 0.10
```

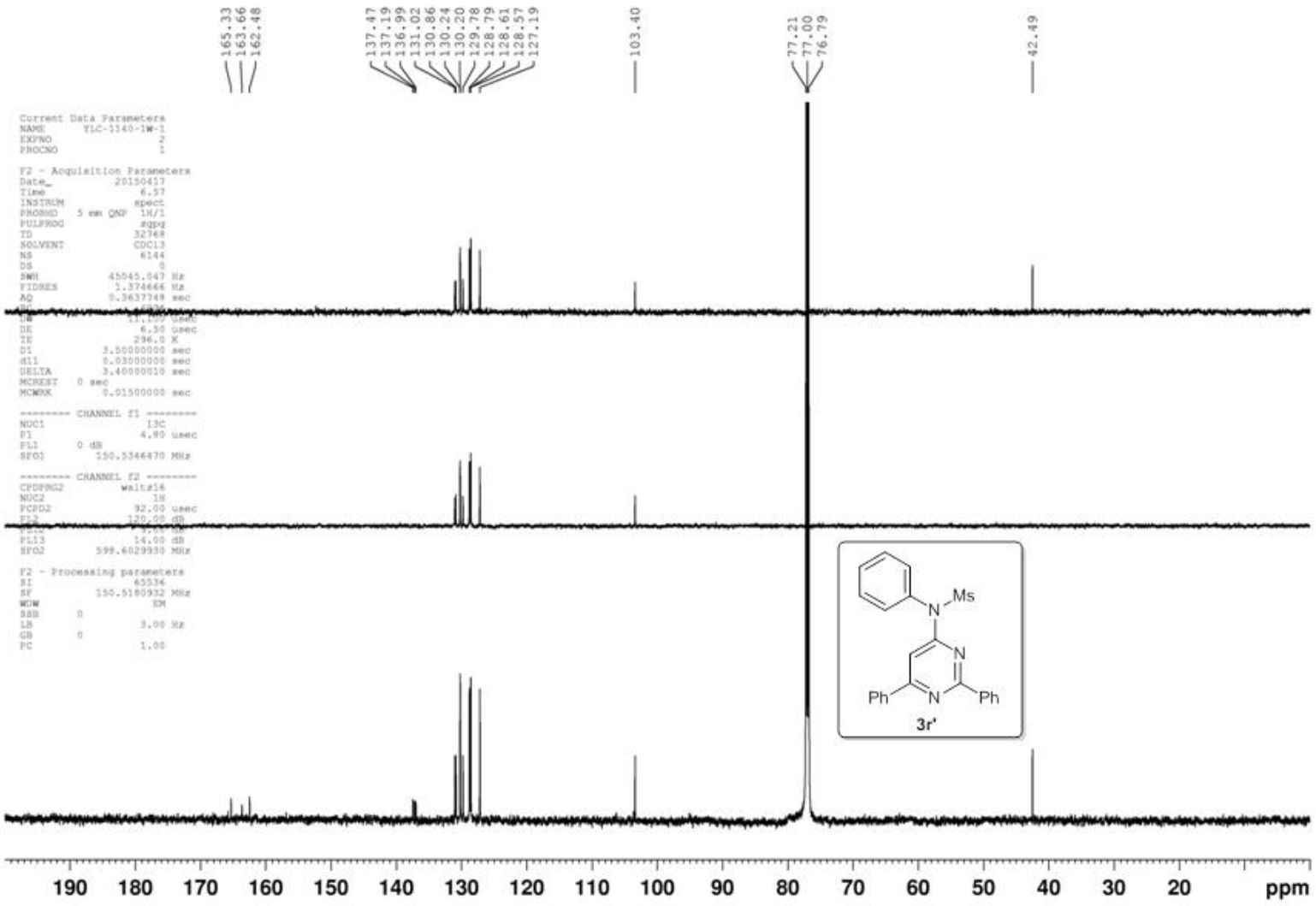


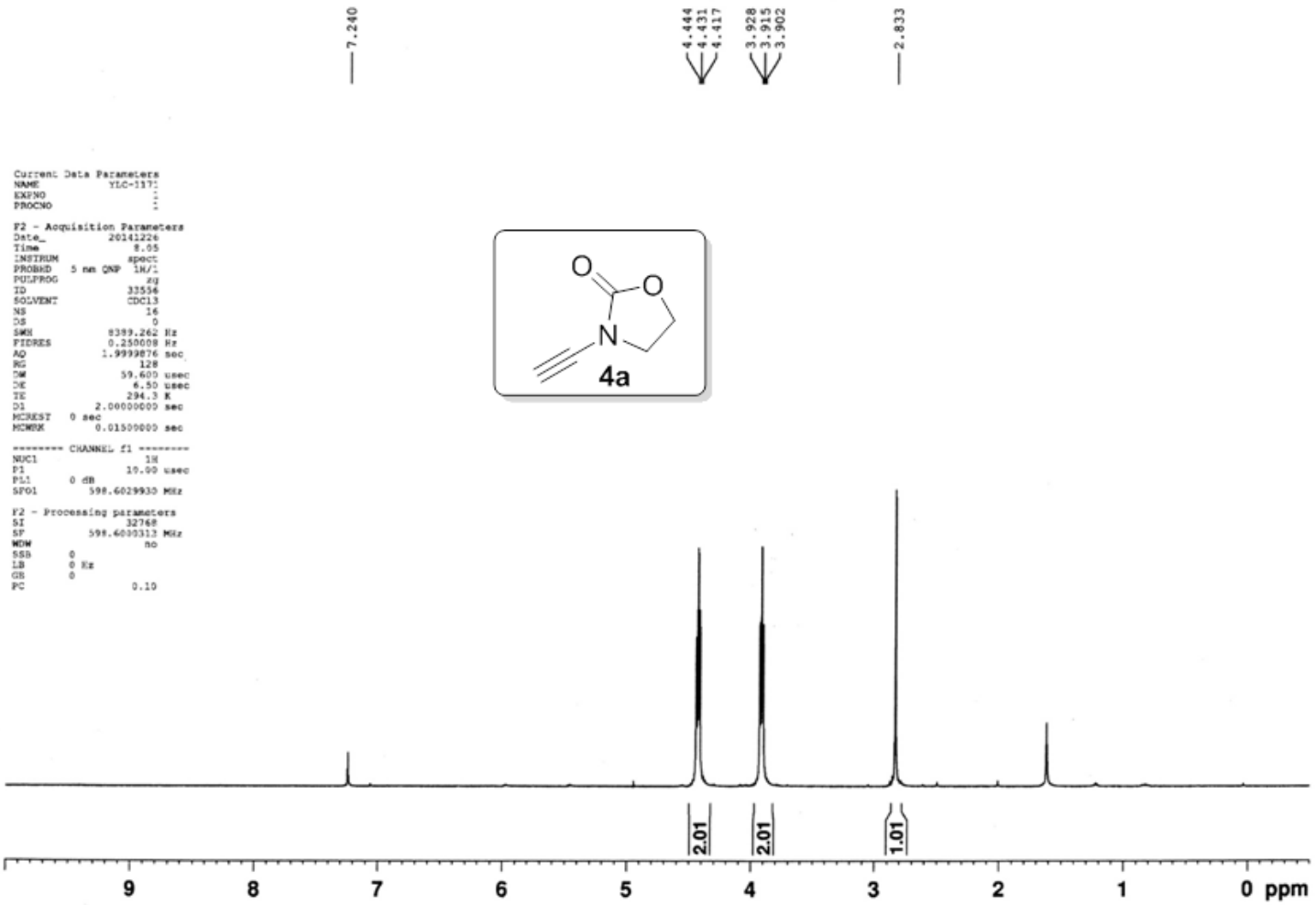

3r

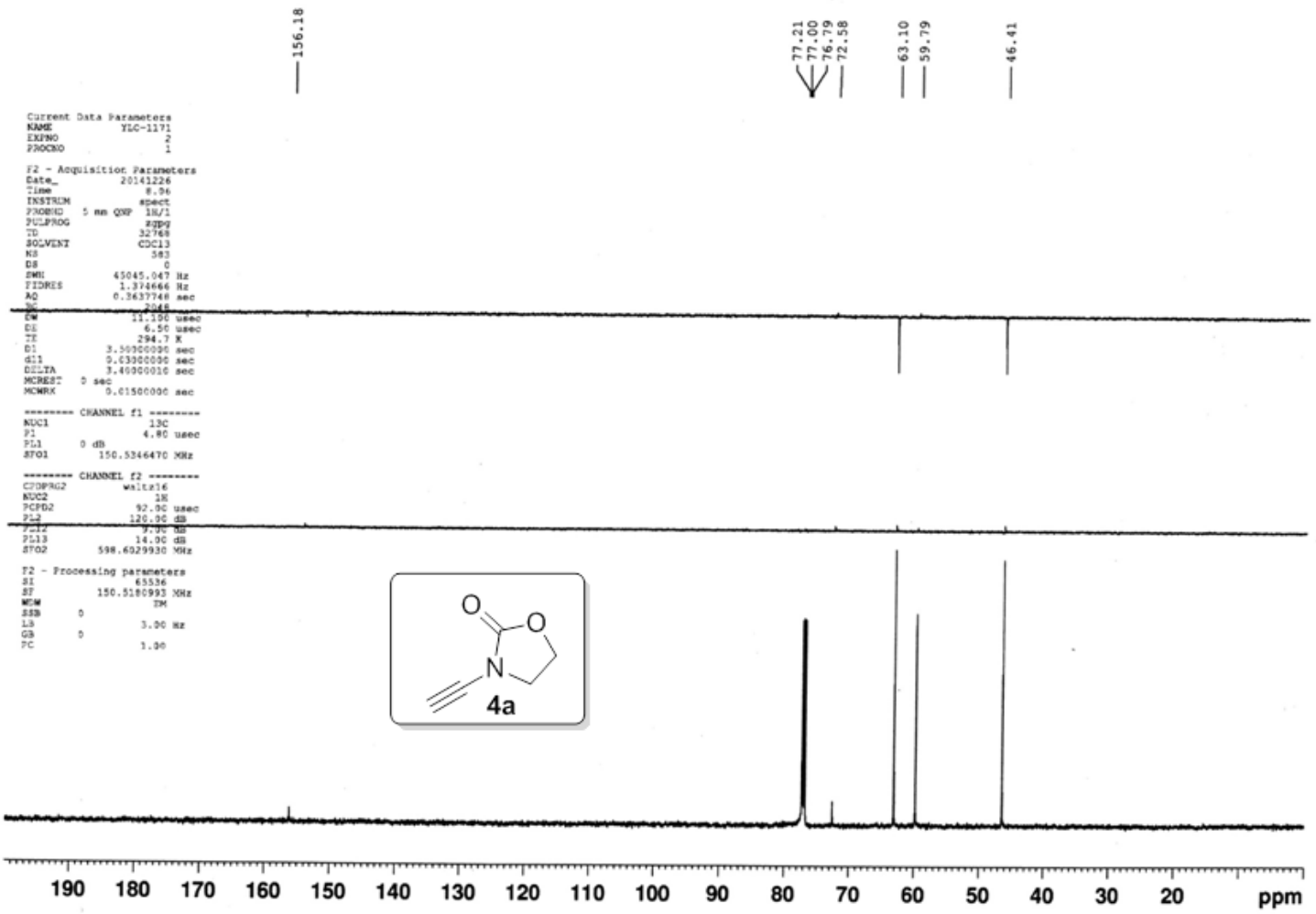


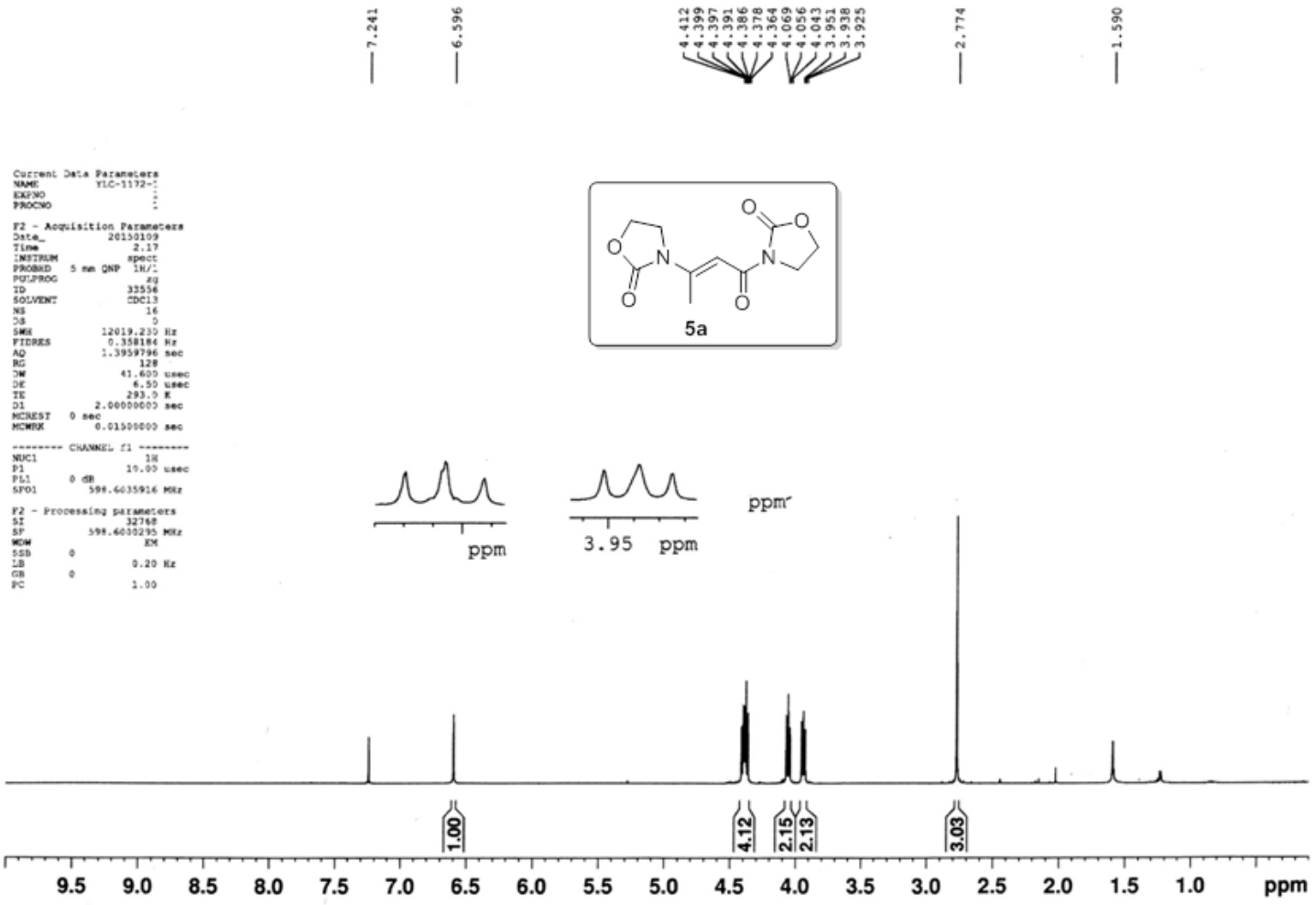

157.09
156.18
151.61
139.02
138.37
138.15
130.18
129.68
129.64
129.61
129.45
128.84
128.76
127.11
108.76
107.55
77.21
77.00
76.79
41.44
39.79
Current Data Parameters
NAME YLC-1140-2
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20141028
Time 6.17
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT DMSO
NS 2048
DS 0
SWH 65045.047 Hz
FIDRES 1.374666 Hz
AQ 0.3637748 sec
RG 2048
DW 11.100 usec
DE 6.50 usec
TE 298.7 K
D1 3.50000000 sec
d11 0.03000000 sec
DELTA 3.40000010 sec
MCREST 0 sec
MCWRK 0.01500000 sec
-------- CHANNEL f1 --------
NUC1 13C
P1 4.80 usec
PL1 0 dB
SFO1 150.5346470 MHz
-------- CHANNEL f2 --------
CPDPRG2 waltz16
NUC2 1H
PCPD2 92.00 usec
PL2 120.00 dB
PL12 20.00 dB
PL13 14.00 dB
SFO2 598.6029940 MHz
F2 - Processing parameters
SI 65536
SF 150.5180924 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 0.50
N
Ms
Ph
N
N
Ms
3r
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

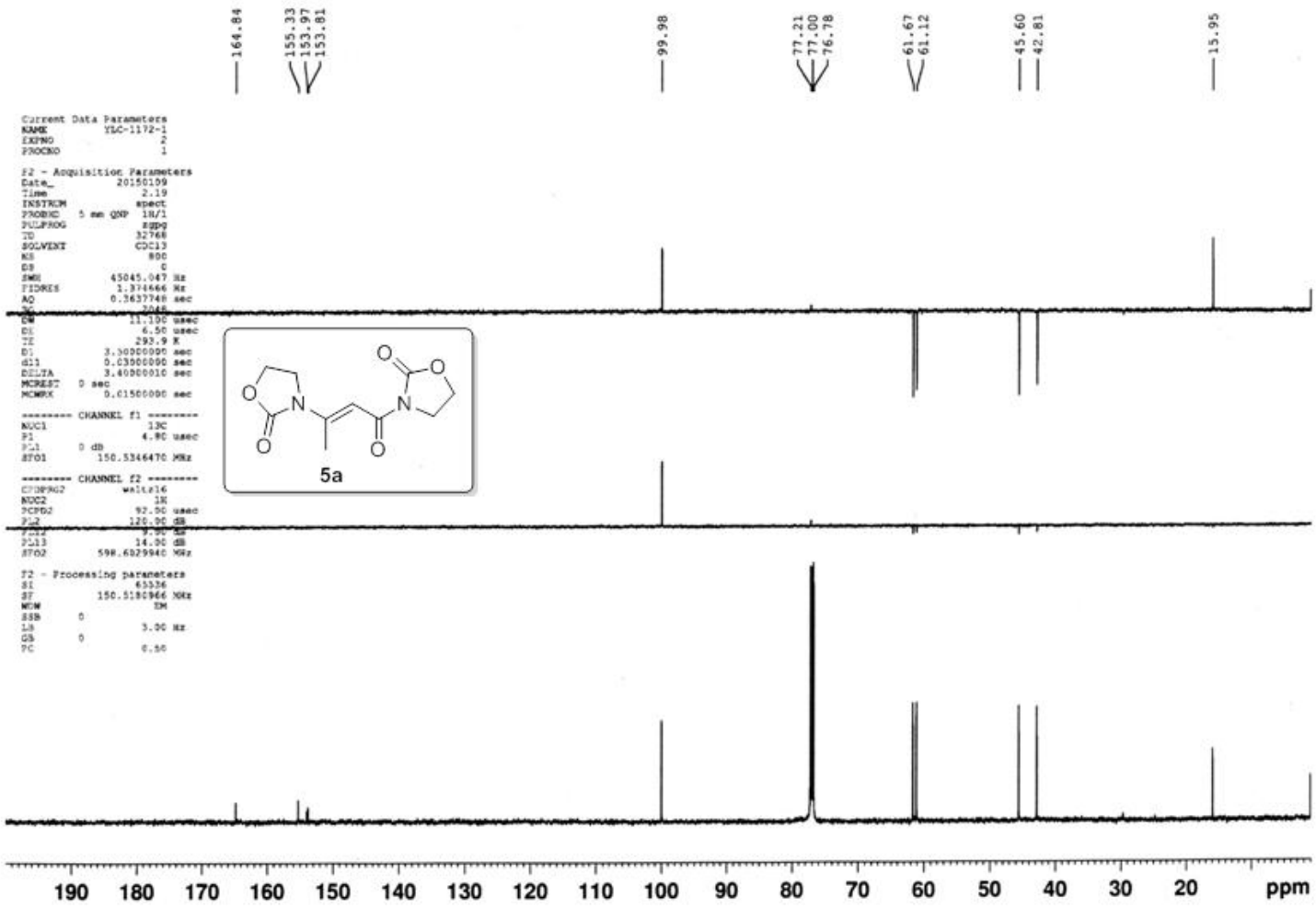

8.556
8.550
8.549
8.544
8.543
8.540
7.934
7.932
7.929
7.922
7.918
7.544
7.541
7.539
7.535
7.532
7.529
7.526
7.522
7.520
7.519
7.515
7.511
7.440
7.437
7.434
7.430
7.427
7.422
7.417
7.414
7.240
6.589
3.713
1.542
Current Data Parameters
NAME YLC-1140-1H-1
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20150417
Time 6.56
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 8389.262 Hz
FIDRES 0.256020 Hz
AQ 1.9530228 sec
RG 512
DW 59.600 usec
DE 6.50 usec
TE 295.2 K
D1 2.00000000 sec
MCREST 0 sec
MCWRK 0.01500000 sec
-------- CHANNEL f1 --------
NUC1 1H
P1 10.00 usec
PL1 0 dB
SFO1 598.6029930 MHz
F2 - Processing parameters
SI 32768
SF 598.6000301 MHz
WDW EM
SSB 0
LB 0.20 Hz
GB 0
PC 1.00
N
Ms
N
Ph
N
Ph
3r'
2.06
2.08
6.09
5.05
1.00
3.06
9
8
7
6
5
4
3
2
1
0 ppm

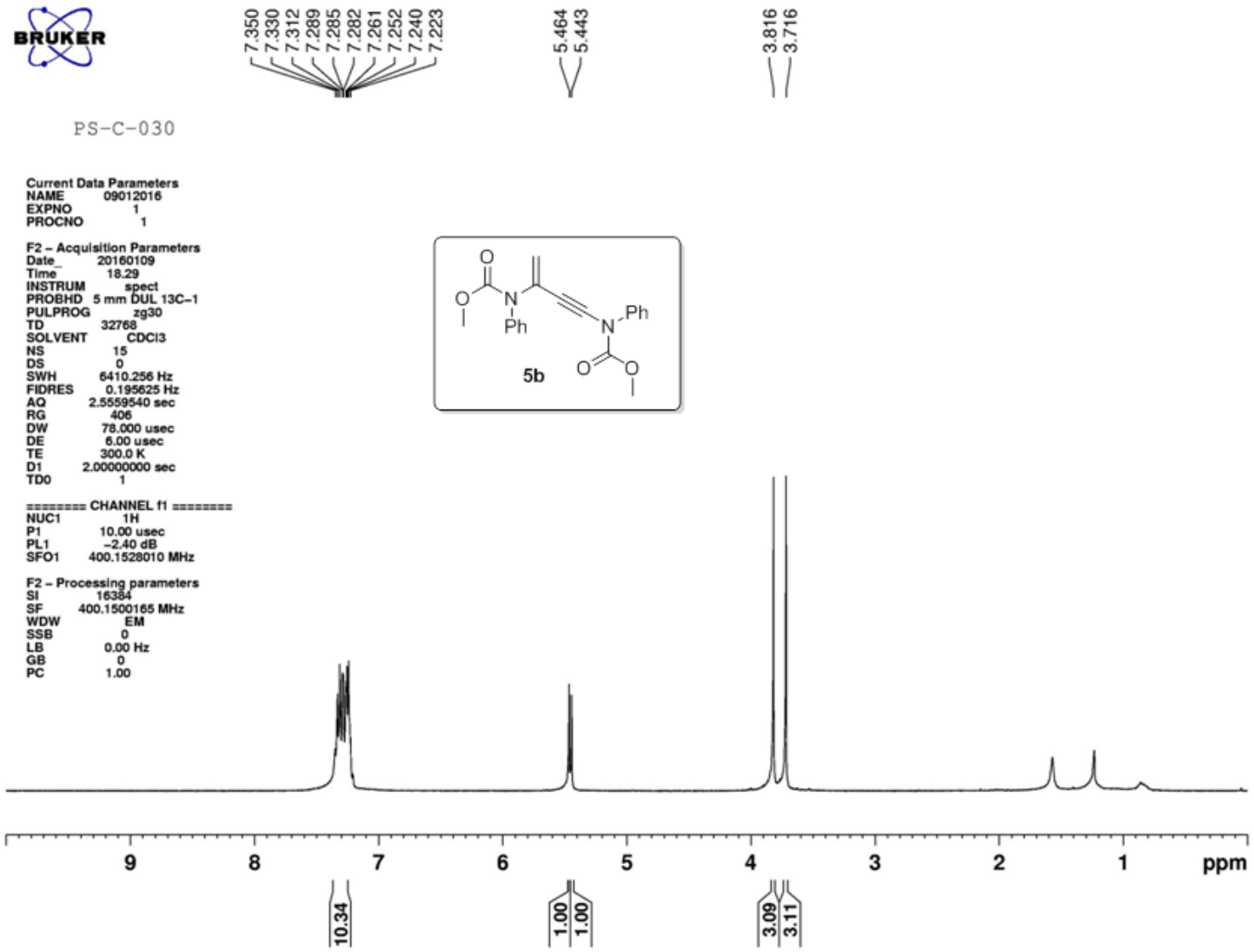

165.33
163.66
162.48
137.47
137.19
136.99
131.02
130.86
130.24
130.20
129.78
128.79
128.61
128.57
127.19
103.40
77.21
77.00
76.79
42.49
Current Data Parameters
NAME YLC-1140-1W-1
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20150417
Time 6.57
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 6144
DS 0
SWH 45045.047 Hz
FIDRES 1.374464 Hz
AQ 0.3637748 sec
DW 11.100 usec
DE 6.50 usec
TE 296.0 K
D1 3.50000000 sec
d11 0.03000000 sec
DELTA 3.40000010 sec
MCREST 0 sec
MCWRK 0.01500000 sec
-------- CHANNEL f1 --------
NUC1 13C
P1 4.80 usec
PL1 0 dB
SFO1 150.5346470 MHz
-------- CHANNEL f2 --------
CPDPRG2 waltz16
NUC2 1H
PCPD2 92.00 usec
PL2 120.00 dB
PL12 14.00 dB
PL13 14.00 dB
SFO2 599.6029930 MHz
F2 - Processing parameters
SI 65536
SF 150.5180932 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
Ms
N
N
Ph
N
Ph
3r'
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

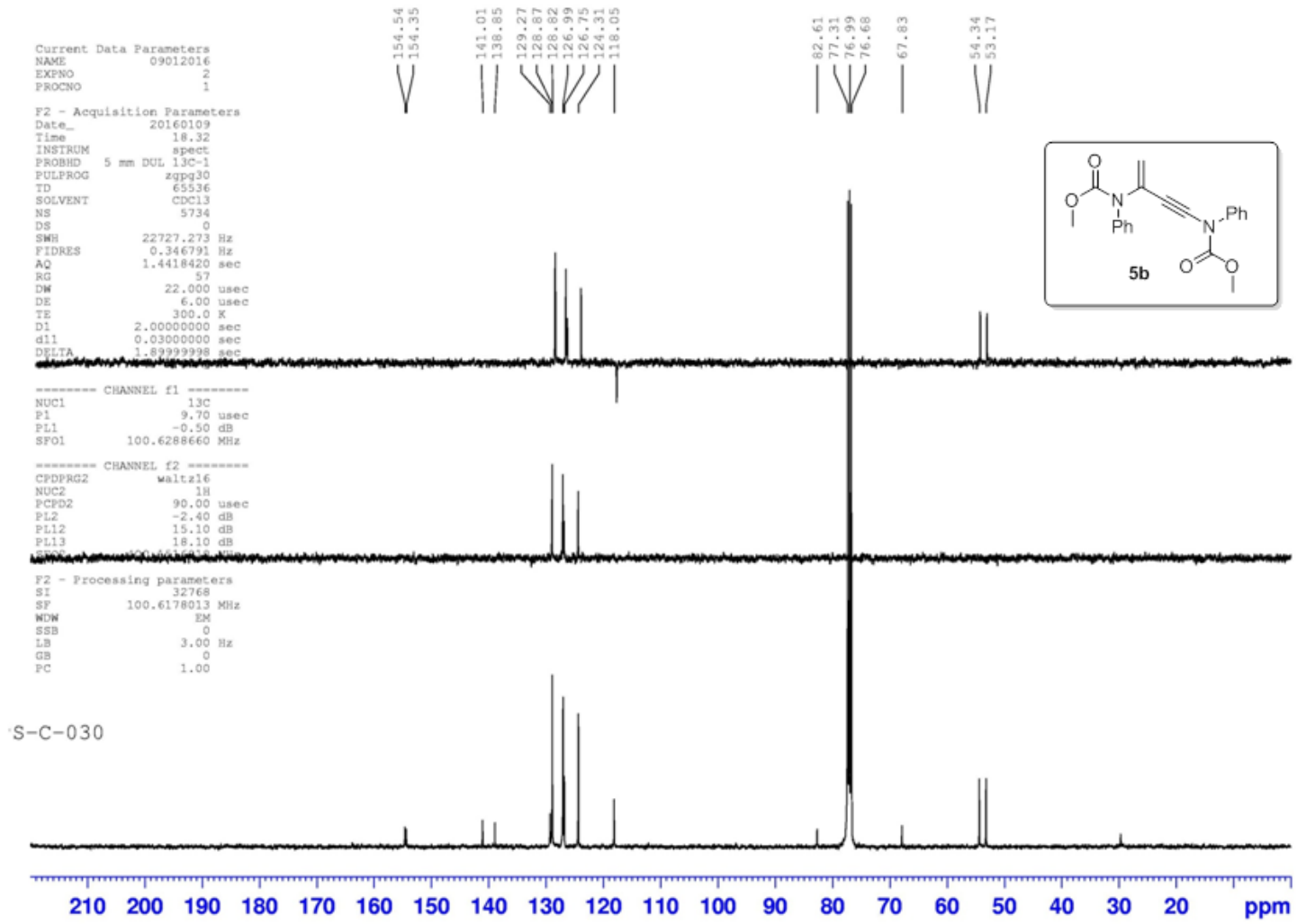

7.240
4.444
4.431
4.417
3.928
3.915
3.902
2.833
Current Data Parameters
NAME YLC-117
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20141226
Time 8.05
INSTRUM spect
PROBHD 5 mm QNP 1H/
PULPROG zg
TD 33536
SOLVENT CDCl3
NS 16
DS 0
SWH 8389.262 Hz
FIDRES 0.250008 Hz
AQ 1.9999876 sec
RG 128
DW 59.600 usec
DE 6.50 usec
TE 294.3 K
D1 2.00000000 sec
MCREST 0 sec
MCWRK 0.01500000 sec
-------- CHANNEL f1 --------
NUC1 1H
P1 10.00 usec
PL1 0 dB
SFO1 598.6029930 MHz
F2 - Processing parameters
SI 32768
SF 598.6000313 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 0.10
O
O
N
4a
2.01
2.01
1.01
9
8
7
6
5
4
3
2
1
0 ppm


156.18
77.21
77.00
76.79
72.58
63.10
59.79
46.41
Current Data Parameters
NAME YLC-1171
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20141226
Time 8.56
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 583
DS 0
SWH 45045.047 Hz
FIDRES 1.374666 Hz
AQ 0.3637748 sec
RG 2048
DW 11.100 usec
DE 6.50 usec
TE 294.7 K
D1 3.00000000 sec
d11 0.03000000 sec
DELTA 3.46000010 sec
MCREST 0 sec
MCWRK 0.01500000 sec
-------- CHANNEL f1 --------
NUC1 13C
P1 4.80 usec
PL1 0 dB
SFO1 150.5346470 MHz
-------- CHANNEL f2 --------
CPDPRG2 waltz16
NUC2 1H
PCPD2 92.00 usec
PL2 120.00 dB
PL12 9.00 dB
PL13 14.00 dB
SFO2 598.6029930 MHz
F2 - Processing parameters
SI 65536
SF 150.5180993 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
O
O
N
4a
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm


7.241
6.596
4.412
4.399
4.397
4.391
4.386
4.378
4.364
4.069
4.056
4.043
3.951
3.938
3.925
2.774
1.590
Current Data Parameters
F2 - Acquisition Parameters
F2 - Processing parameters
5a
ppm
3.95 ppm
1.00
4.12
2.15
2.13
3.03
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm


164.84
155.33
153.97
153.81
99.98
77.21
77.00
76.78
61.67
61.12
45.60
42.81
15.95
5a
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm


7.350
7.330
7.312
7.289
7.285
7.282
7.261
7.252
7.240
7.223
5.464
5.443
3.816
3.716
PS-C-030
Current Data Parameters
NAME 09012016
EXPNO 1
PROCNO 1
F2 – Acquisition Parameters
Date_ 20160109
Time 18.29
INSTRUM spect
PROBHD 5 mm DUL 13C–1
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 15
DS 0
SWH 6410.256 Hz
FIDRES 0.195625 Hz
AQ 2.5559540 sec
RG 406
DW 78.000 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 –2.40 dB
SFO1 400.1528010 MHz
F2 – Processing parameters
SI 16384
SF 400.1500165 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
5b
9
8
7
6
5
4
3
2
1
ppm
10.34
1.00
1.00
3.09
3.11


154.54
154.35
141.01
138.85
129.27
128.87
128.82
126.99
126.75
124.31
118.05
82.61
77.31
76.99
76.68
67.83
54.34
53.17
Current Data Parameters
NAME 09012016
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20160109
Time 18.32
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 5734
DS 0
SWH 22727.273 Hz
FIDRES 0.346791 Hz
AQ 1.4418420 sec
RG 57
DW 22.000 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
======== CHANNEL f1 ========
NUC1 13C
P1 9.70 usec
PL1 -0.50 dB
SFO1 100.6288660 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -2.40 dB
PL12 15.10 dB
PL13 18.10 dB
F2 - Processing parameters
SI 32768
SF 100.6178013 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
5b
S-C-030
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm