Electronic Supplementary Material (ESI) for ChemComm.

Supporting Information

Gold-catalyzed Oxidative Couplings of Two Indoles with One Aryldiazo Cyanide under Oxidant-free Conditions

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Contents:

Experimental Section:

General Information

Unless otherwise noted, 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, Toluene 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. ^1H NMR and ^{13}C NMR spectra were recorded on a Varian 400 MHz, Bruker 400 and 600 MHz Spectrometers using chloroform-d ($CDCl_3$) and CD_2Cl_2 as the internal standards. Compounds ***1b-1d***, ***1f-1o*** *and* ***1q*** have been prepared in literatures.

1a, 1e and **s2** is commercially available compound.[r1-r3]

[r1] (a) S. Xu, X. Huang, X. Hong, B. Xu, *Org. Lett*. **2012**, *14*, 4614; (b) J. B. Ernst, A. Rìhling, B. Wibbeling, F. Glorius, *Chem. Eur. J.* **2016**, *22*, 4400-4404; c) L. Yu, P. Lia, L. Wang, *Chem. Commun*. **2013**, *49*, 2368-2370; d) Z. -L. Xu, H. -X. Li, Z. -G. Ren, W. -Y. Du, W. -C. Xu, J. -P. Lang, *Tetrahedron* **2011**, 67, 5282-5288; e) F. Diness, D. P. Fairlie, *Angew. Chem. Int. Ed.* **2012**, *51*, 8012-8016; f) R. F. Alamdari, M. G. Haqiqib, N. Zekria, *New J. Chem.*, **2016**, *40*, 1287 -1296; g) B. S. Lane, M. A. Brown, D. Sames, *J. Am. Chem. Soc*. **2005**, *127*, 8050-8057; h) P. Y. Choy, C. P. Lau, F. Y. Kwong, *J. Org. Chem.* **2011**, *76*, 80-84.

[r2] a) for first step diazo preparation: J. P. Graham, N. Langlade, J. M. Northall, A. J. Roberts, A. J. Whitehead, *Organic Process Research & Development* **2011**, *15*, 44-48; b) For second and third step diazo preparation: R. Breslow, C. Yuan, *J. Am. Chem. Soc*. **1958**, *80(22)*, 5991-5994.

[r3] a) T. Abe, S. Nakamura, R. Yanada, T. Choshi, S. Hibino, M. Ishikura, *Org. Lett.* **2013**, *15*, 3622; b) J. Xiang, J. Wang, M. Wang, X. Meng, A. Wu, *Org. Biomol. Chem*., **2015**, *13*, 4240; c) D. E. Gillespie, S. F. Brady, A. D. Bettermann, N. P. Cianciotto, M. R. Liles, M. R. Rondon, J. Clardy, R. M. Goodman, J. Handelsman, *Appl. Environ. Microbiol.* **2002**, *68*, 4301; d) N. Y. Tomomi, T. Masashi, A. Hiroshi, H. Yuichi, *Chem. Pharm. Bull.*, **2009**, *57*, 536; e) K. V. Sashidhara, M. Kumar, R. Sonkar, B. S. Singh, A. K. Khanna, G. Bhatia, *J. Med. Chem.*, **2012**, *55*, 2769.

[r4] a) M. Nambo, M.Yar, J. D. Smith and C. M, Crudden, *Org. Lett.*, **2015**, *17*, 50;

2] Naturally Occurring bioactive molecule with BIMs moiety[s3]**:**

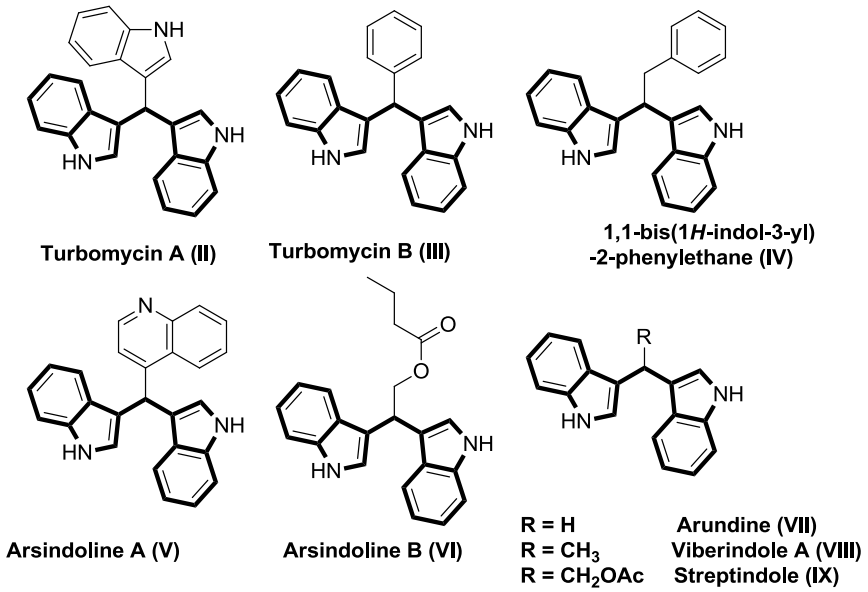
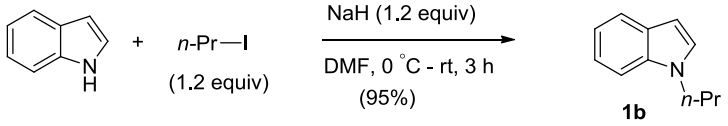


Figure s1. List of BIMs with biological activity.

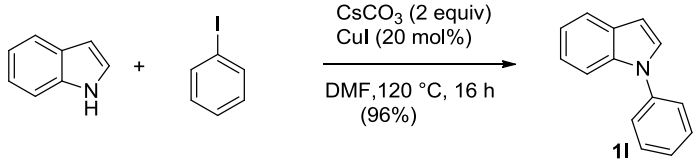
3] Representative Synthetic Procedures:

(a) Preparation of 1-propyl-1*H*-indole (1b):



Indole (1.0 g, 0.009 mol) was dissolved in anhydrous DMF before cooling to 0 °C. Sodium hydride (60% dispersion in mineral oil, (0.41g, 0.010 mol) was added in small portions over a period of 10-15 min. Once addition was complete, the reaction mixture was stirred at 0 °C for 30 min before *n*-propyl iodide (1.74g, 0.010 mol) was added. The solution was continued to stir it at room temperature until completion. The reaction was monitored by TLC before it was quenched by a dropwise addition of water. The solution was extracted with ether, washed with water, brine and dried over $MgSO_4$. After filtration, the filtrates was concentrated to afford the crude product which was purified by flash column chromatography on silica gel to afford **3b** (1.29 g, 0.008 mmol) in 95% yield.

(b) Preparation of *N*-phenyl Indole (1l):



Indole (500 mg, 0.0042 mol), iodobenzene (0.87g, 4.3 mmol), copper(I) iodide (82 mg, 0.0004 mol) and cesium carbonate (1.67 g, mmol) were stirred for 16 h at 120 °C in DMF (10 mL). After cooling to room temperature, the reaction mixture was diluted with EtOAc (30 mL) and washed with water (2 x 20 mL). The combined aqueous layer was extracted with EtOAc (2 x 20 mL). The combined organic layer was dried over $MgSO_4$, filtered and concentrated in vacuum. Purification by silica-gel chromatography afforded the product **1l** as colorless oil (790 mg, 4.1 mmol, 96%).

*All other derivative **1b-1o, 1q** were prepared according to the above reported procedure and their spectral data have been reported previouslyr [r1].*

(c) Preparation of 2-diazo-2-phenylacetonitrile compound (2a-2h):

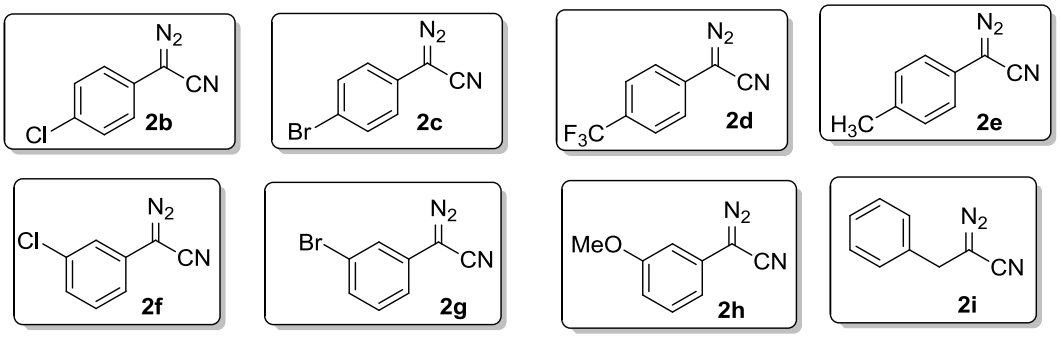
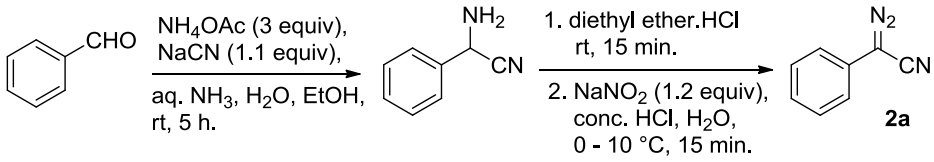


Figure s2. List of diazo substrates

To an aqueous solution (40 mL) of ammonium acetate (21.8 g, 282.9 mmol) and sodium cyanide (5.2 g, 103.7 mmol), aqueous ammonia (35% w/w; 29 mL) and ethanol (40 mL) was added benzaldehyde (10 g, 94.3 mmol); the resulting solution was stirred at 25 °C for 5 h. The solution was extracted with diethyl



ether, dried over $MgSO_4$, filtered and concentrated at 20-30 °C under reduced pressure; the crude material was used immediately for the next step. (Caution: Aqueous layer was cooled in ice and treated by sodium hypochlorite solution, NaClO).

To the crude 2-amino-2-phenylacetonitrile was added Et_2O.HCl (80 mL); and the mixture was stirred for 15 min. at room temperature. The pale yellow precipitates were collected, and washed with cold diethyl ether (2 x 10 mL). This solid residue was dissolved in water (100 mL), and treated with diethyl ether (100 mL). The aqueous layer was separated from ether and used for the next reaction. The aqueous solution of 2-amino-2-phenylacetonitrile hydrochloride (100 mL) and diethyl ether (100 mL) was cooled to 0 °C, and to this solution was treated with an aqueous solution (25 mL) of $NaNO_2$ (7.8 g, 113.1 mmol). To this mixture was added concentrated HCl (0.20 mL); and the reaction mixture was stirred for additional 5 min. The solution was extracted with diethyl ether (50 mL), and the ether extracts were washed with 10% aqueous Na_2CO_3. The extract was dried over $MgSO_4$, filtered and concentrated under reduced pressure. The crude product was purified on a silica column with 15% dichloromethane/*n*-pentane to afford 2-diazo-2-phenylacetonitrile **2a** as red viscous oil (2 g, 13.98 mmol, 14.8 % overall yield).

All other diazo derivative **2b** to **2h** were prepared according to the above procedure.

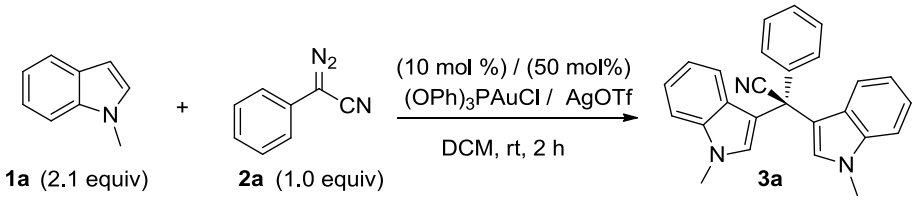
(d) Preparation of 2-diazo-3-phenylpropanenitrile compound (2i):

A flask was charged with sodium bisulfite (6.5 g, 62.0 mmol) and water (17 mL). To this solution was added slowly a THF solution (14 mL) of phenylacetaldehyde (5.0 g, 4.0 mmol). The resulting suspension was stirred at room temperature for 40 min before treatment with ammonium hydroxide solution (4.85 mL). The resulting solution was stirred at 60 ^oC for 1 h and kept on stirring at room temperature for 12 h. The solution was cooled at 0-5 ^oC and aqueous sodium cyanide (2.42 g, 49.0 mmol) in 14 mL water was slowly added over 5 min. The resulting solution was stirred at room temperature for 18 h and then extracted with ether. The combined organic layer was dried over $MgSO_4$ and evaporated to afford aniline derivative. The crude material was used immediately for the next step.

The next two steps are similar to the above procedure followed for preparation of **2a**-**2h**.

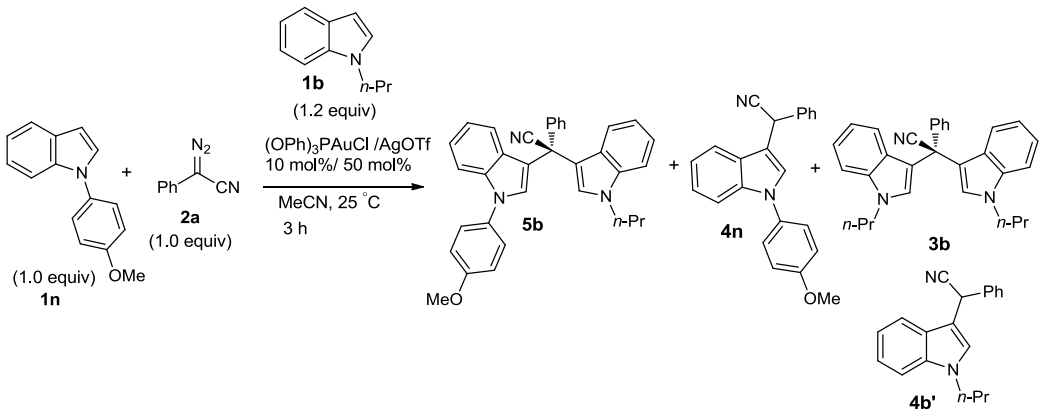
4] Standard Catalytic Procedure:

(a) Synthesis of 2,2-bis(1-methyl-*1H*-indol-3-yl)-2-phenylacetonitrile (3a):



A reaction tube was charged with (chlorotriphenoxyphosphoranyl)gold(I) (38.0 mg, 0.0698 mmol) and silver(I) trifluoromethanesulfonate (AgOTf) (89.0 mg, 0.349 mmol). To the above mixture was added a dry DCM (1.0 mL), and the mixture was stirred at room temperature under an argon atmosphere for 5 min. To this solution was added a dry DCM solution (2 mL) of *N*-methyl Indole **1a** (191 mg, 1.47 mmol) and 2-diazo-2-phenylacetonitrile **2a** (100 mg, 0.070 mmol) with syringe in a period of 25 minute. The mixture was kept stirring at 25 °C for 2 h before it was filtered over a short silica bed. The solvent was concentrated, and the crude product was chromatographed through a silica gel column to afford compound **3a** (178 mg, 0.47 mmol, 68% yield) as light yellow semisolid.

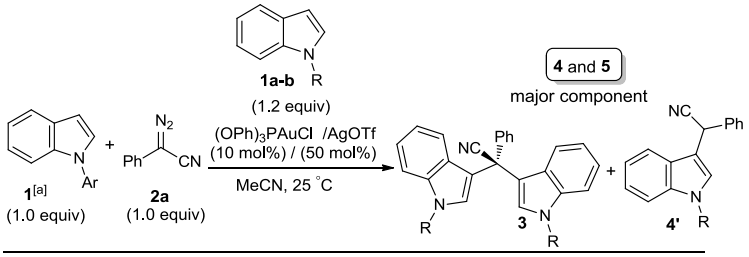
(b) Synthesis of 2,2-bis(1-methyl-*1H*-indol-3-yl)-2-phenylacetonitrile (5b):

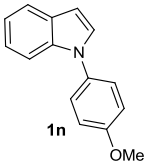
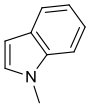
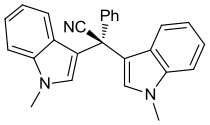
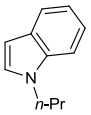
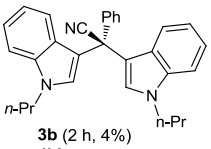
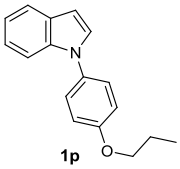
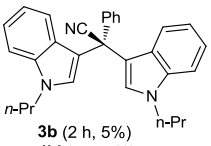
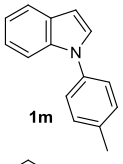
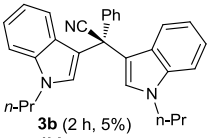
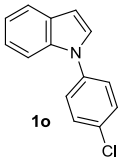
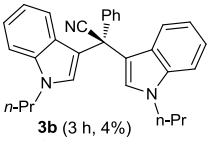
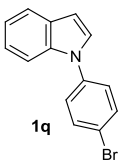
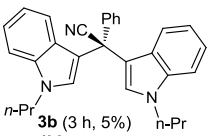


A reaction tube was charged with (chlorotriphenoxyphosphoranyl)gold(I) (38.0 mg, 0.0698 mmol) and silver(I) trifluoromethanesulfonate (AgOTf) (89.0 mg, 0.349 mmol). To the above mixture a dry acetonitrile solution (1.0 mL) was added, and the mixture stirred at room temperature under an argon atmosphere for 5 min. To this solution was added a dry acetonitrile solution (2 mL) of 2-diazo-2-phenylacetonitrile **2a** (100 mg, 0.07 mmol), 1-(4-methoxyphenyl)-1*H*-indole **1n** (155 mg, 0.07 mmol) and 1-propyl-1*H*-indole

1b (133 mg, 0.08 mmol) with a syringe in a period of 5 minute. The mixture was kept stirring at 25 °C for 3 h before it was filtered over a short silica bed. The solution was concentrated, and the crude product was chromatographed through a silica gel column with EA/Hexane (3/97) to afford compound **5b** (180 mg, 0.036 mmol, 52%, R_f = 0.43, yellowish semisolid), major byproduct **4n** (43 mg, 0.012 mmol, 18%, R_f = 0.52), homo-coupling compounds **3b** (7.0 mg, 0.016 mmol, 4%, R_f = 0.40) and **4b'** (2.5 mg, 0.009 mmol, 2%, R_f = 0.42).

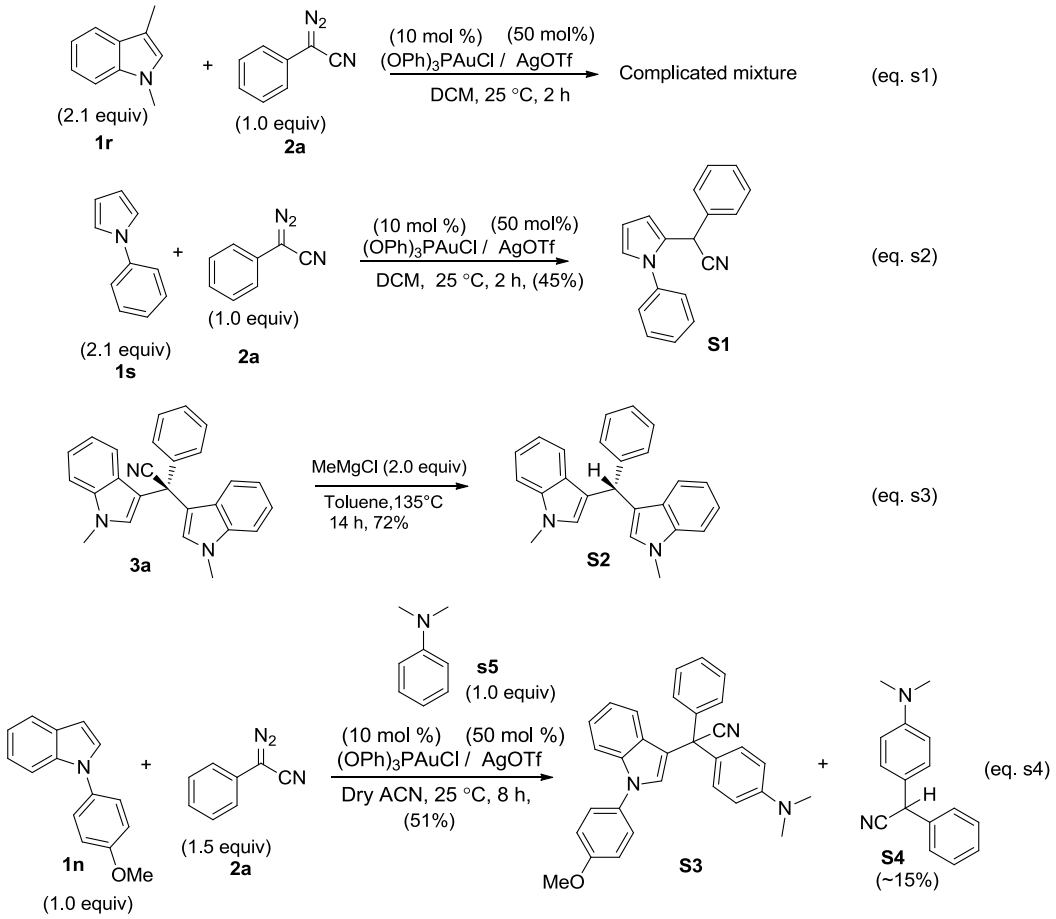
Table s1. Minor products for double indolylations with two different indoles.



Entry	1	1	Minor product (3) and (4a')
1)			 **3a** (1.8 h, 5%)[b] **4a'** (1.8 h, 4%)
2)	**1n**		 **3b** (2 h, 4%) **4b'** (2 h, 2%)
3)		**1b**	 **3b** (2 h, 5%) **4b'** (2 h, 3%)
4)		**1b**	 **3b** (2 h, 5%) **4b'** (2 h, 4%)
5)		**1b**	 **3b** (3 h, 4%) **4b'** (3 h, 3%)
6)		**1b**	 **3b** (3 h, 5%) **4b'** (3 h, 3%)

[a] **1** = 0.02 M. [b] Product yields are reported after purification using a silica column.

(c) Reaction of 2-diazo-2-phenylacetonitrile (2a) with other reaction partner.

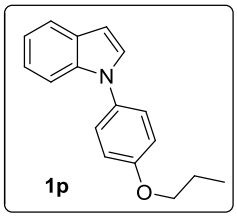


***Scheme S1* :** Testing of various other electron rich reaction partner.

Note: Experimental procedure for eq. s1 and eq. s2 same as **3a** and experimental procedure for eq. s4 is same as **5b** and Experimental procedure for eq. s3 follwed from reference r4.

5] Spectral data:

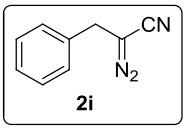
Spectral data for 1-(4-propoxyphenyl)-1*H*-indole (1p).



Red liquid; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.66 (d, *J* = 7.4 Hz, 1H), 7.44 (d, *J* = 8.0 Hz, 1H), 7.39 ~ 7.36 (m, 2H), 7.26 ~ 7.23 (m, 1H), 7.20 ~ 7.11 (m, 2H), 7.02 ~ 6.99 (m, 2H), 6.64 ~ 662 (m, 1H), 3.99 ~ 3.95 (m, 2H), 1.87 ~ 1.81 (m, 2H), 1.08 ~ 1.04

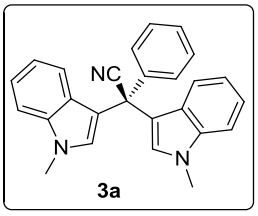
(m, 3H), ; ^{13}C NMR (150 MHz, $CDCl_3$): δ 157.8, 136.3, 132.6, 128.9, 128.3, 125.9, 122.1, 121.0, 120.0, 115.2, 110.4, 102.8, 69.9, 22.6, 10.5.

Spectral data for 2-diazo-3-phenylpropanenitrile (2i).



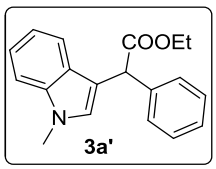
Pale yellow liquid; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.41 ~ 7.34 (m, 2H), 7.32 ~ 7.30 (m, 1H), 7.25 ~ 7.23 (m, 2H), 3.55 (s, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 134.8, 129.1, 128.3, 127.9, 113.8, 31.5.

Spectral data for 2,2-bis(1-methyl-*1H*-indol-3-yl)-2-phenylacetonitrile (3a).



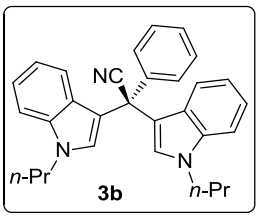
Light yellow Semisolid; ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.52 ~ 7.51 (m, 2H), 7.47 (d, *J* = 8.1 Hz, 2H), 7.35 ~ 7.31 (m, 5H), 7.24 ~ 7.22 (m, 2H), 7.05 ~ 7.02 (m, 2H), 6.53 (s, 2H), 3.67 (s, 6H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 139.8, 137.7, 129.2, 128.5, 127.8, 125.8, 122.1, 121.8, 120.8, 119.7, 114.1, 109.4, 44.4, 32.8; ESI-MS calcd. for $C_{26}H_{21}N_3$: 375.1735; found: 376.1808 [M+H].

Spectral data for ethyl 2-(1-methyl-1H-indol-3-yl)-2-phenylacetate (3a').



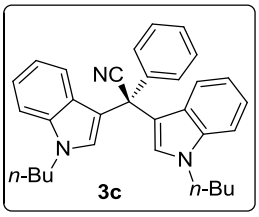
Colorless liquid; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.47 ~ 7.42 (m, 3H), 7.33 ~ 7.12 (m, 5H), 7.05 ~ 7.04 (m, 2H), 5.24 (s, 1H), 4.09 (q, *J* = 7.2, 5.2 Hz, 2H), 3.74 (s, 3H), 1.26 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 173.0, 138.9, 137.0, 128.6, 128.5, 128.4, 127.8, 127.1, 121.8, 119.2, 119.1, 112.2, 109.3, 61.1, 48.9, 32.8, 14.2; ESI-MS calcd. for $C_{19}H_{19}NO_2$: 293.1416; found: 294.1418 [M+H].

Spectral data for 2-phenyl-2,2-bis(1-propyl-1*H*-indol-3-yl)acetonitrile (3b).



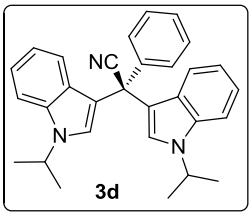
Yellow viscous solid; ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.51 ~ 7.49 (m, 2H), 7.45 ~ 7.44 (m, 2H), 7.35 ~ 7.30 (m, 5H), 7.20 (t, *J* = 7.3 Hz, 2H), 7.00 (t, *J* = 7.4 Hz, 2H), 6.58 (s, 2H), 3.97 (t, *J* = 7.2 Hz, 4H), 1.81 ~ 1.75 (m, 4H), 0.85 (t, *J* = 7.3, 6H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 139.9, 137.0, 128.5, 128.4, 127.9, 127.8, 125.9, 121.9, 120.9, 120.7, 119.5, 113.9, 109.7, 48.2, 44.8, 23.4, 11.4; ESI-MS calcd. for $C_{30}H_{29}N_3$: 431.2361; found: 454.2254 [M+Na].

Spectral data for 2,2-bis(1-butyl-*1H*-indol-3-yl)-2-phenylacetonitrile (3c).



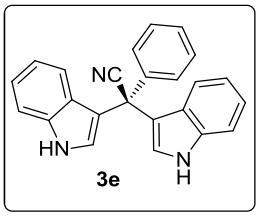
Light yellow liquid; ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.51 ~ 7.49 (m, 2H), 7.44 ~ 7.43 (m, 2H), 7.35 ~ 7.29 (m, 5H), 7.21 ~ 7.18 (m, 2H), 7.02 ~ 6.99 (m, 2H), 6.57 (s, 2H), 4.00 (t, *J* = 6.2 Hz, 4H), 1.75 ~ 1.70 (m, 4H), 1.28 ~ 1.18 (m, 4H), 0.87 (t, *J* = 4.8, 6H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 139.8, 137.0, 128.4, 127.8, 127.7, 125.9, 121.9, 121.8, 120.9, 119.5, 113.9, 109.6, 46.2, 44.8, 32.2, 20.1, 13.7; HRMS calcd. for $C_{32}H_{33}N_3$: 459.2674; found: 482.2560 [M+Na].

Spectral data for 2,2-bis(1-isopropyl-*1H*-indol-3-yl)-2-phenylacetonitrile (3d).



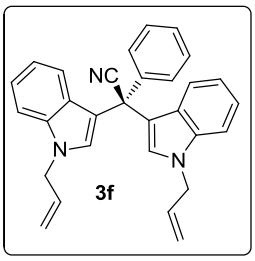
Light brown semisolid; ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.51 ~ 7.49 (m, 2H), 7.39 ~ 7.35 (m, 4H), 7.33 ~ 7.29 (m, 3H), 7.19 ~ 7.17 (m, 2H), 6.99 ~ 6.97 (m, 2H), 6.72 (s, 2H), 4.62 ~ 4.56 (m, 2H), 1.42 ~ 1.41 (m, 12H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 139.9, 136.6, 128.4, 127.9, 127.7, 126.0, 124.5, 122.1, 121.7, 120.9, 119.5, 114.1, 109.7, 47.3, 45.2, 22.7; ESI-MS calcd. for $C_{30}H_{29}N_3$: 431.2361; found: 454.2254 [M+Na].

Spectral data for 2,2-di(*1H*-indol-3-yl)-2-phenylacetonitrile (3e).



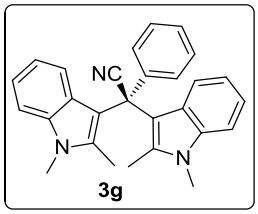
Yellow semisolid; ^{1}H NMR (600 MHz, $CDCl_3$): δ 8.01 (s, 2H), 7.51 ~ 7.47 (m, 4H), 7.38 ~ 7.32 (m, 5H), 7.20 (t, *J* = 7.4 Hz, 2H), 7.01 (t, *J* = 7.7 Hz, 2H), 6.65 (s, 2H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 139.4, 136.9, 128.5, 127.9, 127.8, 125.3, 124.9, 122.6, 121.6, 120.7, 120.2, 115.7, 111.3, 44.8; ESI-MS calcd. for $C_{24}H_{17}N_3$: 347.1422; found: 370.1315 [M+Na].

Spectral data for 2,2-bis(1-allyl-*1H*-indol-3-yl)-2-phenylacetonitrile (3f).



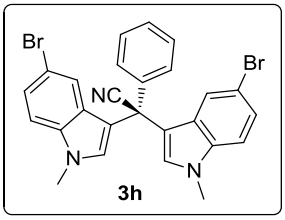
Colorless liquid; ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.51 ~ 7.50 (m, 2H), 7.45 ~ 7.43 (m, 2H), 7.34 ~ 7.29 (m, 5H), 7.20 ~ 7.18 (m, 2H), 7.03 ~ 7.00 (m, 2H), 6.58 (s, 2H), 5.99 ~ 5.88 (m, 2H), 5.14 (dd, *J* = 10.2, 1.2, 2H), 5.02 (dd, *J* = 16.8, 1.2, 2H), 4.63 ~ 4.61 (m, 4H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 139.6, 137.1, 133.1, 128.5, 128.4, 127.8, 125.6, 122.1, 121.8, 120.9, 119.8, 117.2, 114.4, 109.8, 48.8, 45.1; ESI-MS calcd. for $C_{30}H_{25}N_3$: 427.2048; found: 450.1941 [M+Na].

Spectral data for 2,2-bis(1,2-dimethyl-*1H*-indol-3-yl)-2-phenylacetonitrile (3g).



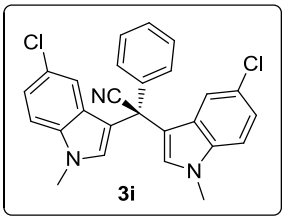
White semisolid; ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.52 (d, *J* = 7.1 Hz, 2H), 7.37 ~ 7.35 (m, 3H), 7.28 (d, *J* = 8.2 Hz, 2H), 7.01 (t, *J* = 7.4 Hz, 2H), 6.73 (t, *J* = 8.4 Hz, 2H), 6.16 (d, *J* = 8.2 Hz, 2H), 3.68 (s, 6H), 2.13 (s, 6H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 140.4, 136.3, 135.6, 128.9, 128.6, 128.1, 126.5, 123.1, 120.6, 119.6, 119.4, 109.4, 108.7, 45.9, 29.6, 11.6; ESI-MS calcd. for $C_{28}H_{25}N_3$: 403.2048; found: 426.1941 [M+Na].

Spectral data for 2,2-bis(5-bromo-1-methyl-1*H*-indol-3-yl)-2-phenylacetonitrile (3h).



Yellow semisolid; ^{1}H NMR (700 MHz, $CDCl_3$): δ 7.53 (s, 2H), 7.43 (t, *J* = 4.2 Hz, 2H), 7.35 (d, *J* = 4.2 Hz, 3H), 7.31 (d, *J* = 9.1 Hz, 2H), 7.18 (d, *J* = 9.2 Hz, 2H), 6.53 (s, 2H), 3.68 (s, 6H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 139.0, 136.2, 130.4, 128.7, 128.2, 127.6, 126.5, 125.8, 122.8, 121.3, 120.0, 113.5, 110.7, 44.4, 33.2; ESI-MS calcd. for $C_{26}H_{19}Br_2N_3$: 530.9946; found: 553.9838 [M+H].

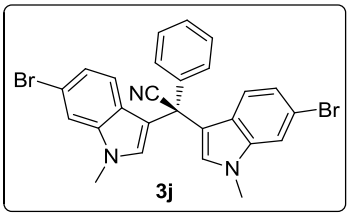
Spectral data for 2,2-bis(5-chloro-1-methyl-1*H*-indol-3-yl)-2-phenylacetonitrile (3i).



3i

Yellow semisolid; ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.45 ~ 7.44 (m, 2H), 7.37 (d, *J* = 1.9 Hz, 2H), 7.36 ~ 7.34 (m, 3H), 7.23 (*J* = 8.8 Hz, 2H), 7.18 ~ 7.17 (m, 2H), 6.53 (s, 2H), 3.68 (s, 6H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 139.0, 136.2, 130.4, 128.7, 128.2, 127.6, 126.5, 125.8, 122.8, 121.3, 120.0, 113.5, 110.7, 44.4, 33.2; HRMS calcd. for $C_{26}H_{19}Cl_2N_3$: 443.0956; found: 443.0956 [M+H].

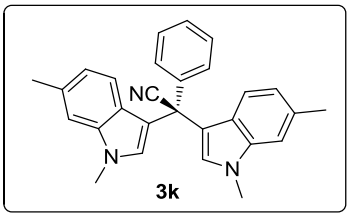
Spectral data for 2,2-bis(6-bromo-1-methyl-1*H*-indol-3-yl)-2-phenylacetonitrile (3j).



3j

Brownish jelly; ^{1}H NMR (700 MHz, $CDCl_3$): δ 7.54 (s, 2H), 7.43 (t, *J* = 4.2 Hz, 2H), 7.35 (d, *J* = 4.2 Hz, 3H), 7.31 (d, *J* = 9.1 Hz, 2H), 7.18 (d, *J* = 9.2 Hz, 2H), 6.53 (s, 2H), 3.68 (s, 6H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 139.0, 136.2, 130.4, 128.7, 128.2, 127.6, 126.5, 125.8, 122.8, 121.3, 120.0, 113.5, 110.7, 44.4, 33.2; ESI-MS calcd. for $C_{26}H_{19}Br_2N_3$: 530.9946; found: 553.9838 [M+H].

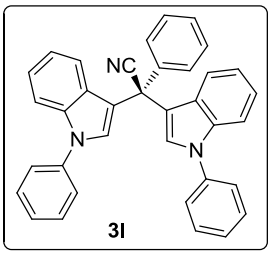
Spectral data for 2,2-bis(1,6-dimethyl-1*H*-indol-3-yl)-2-phenylacetonitrile (3k).



3k

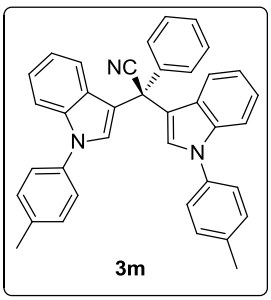
White semisolid; ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.51 ~ 7.50 (m, 2H), 7.35 ~ 7.31 (m, 5H), 7.10 (s, 2H), 6.88 ~ 6.86 (m, 2H), 6.47 (s, 2H), 3.64 (s, 6H), 2.47 (s, 6H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 139.9, 138.1, 131.9, 128.7, 128.4, 127.8, 127.7, 123.7, 121.9, 121.4, 120.4, 114.0, 109.4, 44.7, 32.8, 21.8; ESI-MS calcd. for $C_{28}H_{25}N_3$: 403.2048; found: 404.2052 [M+H].

Spectral data for 2-phenyl-2,2-bis(1-phenyl-*1H*-indol-3-yl)acetonitrile (3l).



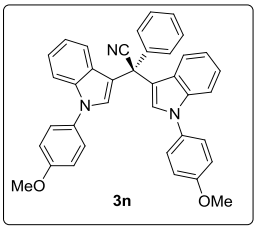
Colorless viscous solid; ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.62 ~ 7.59 (m, 3H), 7.54 ~ 7.53 (m, 2H), 7.46 ~ 7.44 (m, 3H), 7.40 ~ 7.28 (m, 11H), 7.24 ~ 7.22 (m, 2H), 7.13 ~7.10 (m, 2H), 6.85 (s, 2H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 139.1, 137.0, 131.2, 129.6, 129.4, 128.7, 128.1, 127.9, 126.8, 124.6, 123.0, 121.4, 121.0, 120.8, 116.8, 116.3, 110.8, 44.8; ESI-MS calcd. for $C_{36}H_{25}N_3$: 499.2048; found: 522.1931 [M+Na].

Spectral data for 2-phenyl-2,2-bis(1-(p-tolyl)-*1H*-indol-3-yl)acetonitrile (3m).



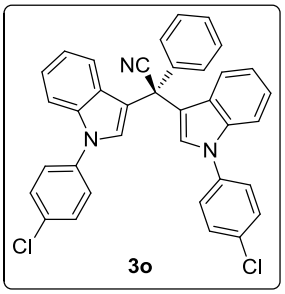
White semisolid; ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.62 (d, *J* = 9.0 Hz, 2H), 7.57 (d, *J* = 8.4 Hz, 2H), 7.49 (d, *J* = 7.8 Hz, 2H), δ 7.36 ~ 7.20 (m, 13H), 7.09 (t, *J* = 7.8 Hz, 2H), 6.82 (s, 2H), 2.38 (s, 6H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 139.2, 137.1, 136.8, 136.6, 131.1, 130.1, 129.4, 129.2, 128.7, 127.9, 126.3, 124.5, 122.8, 120.9, 120.6, 116.8, 115.9, 110.8, 44.8, 20.9; ESI-MS calcd. for $C_{38}H_{29}N_3$: 527.2361; found: 550.2254 [M+Na].

Spectral data for 2,2-bis(1-(4-methoxyphenyl)-1*H*-indol-3-yl)-2-phenylacetonitrile (3n).



White semisolid; ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.61 (d, *J* = 7.7 Hz, 2H), 7.57 (d, *J* = 8.1 Hz, 2H), 7.41 (d, *J* = 8.4 Hz, 2H), 7.36 ~ 7.32 (m, 3H), 7.29 (d, *J* = 8.8 Hz, 4H), 7.20 (t, *J* = 7.3 Hz, 2H), 7.08 (t, *J* = 7.8 Hz, 2H), 6.95 (d, *J* = 8.8 Hz, 4H), 6.80 (s, 2H), 3.83 (s, 6H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 158.5, 139.3, 137.5, 132.1, 128.9, 128.6, 128.0, 127.9, 126.2, 126.1, 122.8, 121.5, 120.9, 120.5, 115.8, 114.7, 110.7, 55.6, 44.9; ESI-MS calcd. for $C_{38}H_{29}N_3O_2$: 559.2260; found: 560.233 [M+H].

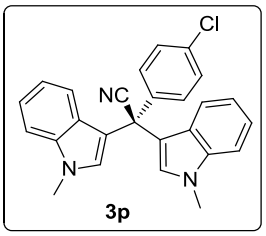
Spectral data for 2,2-bis(1-(4-chlorophenyl)-1*H*-indol-3-yl)-2-phenylacetonitrile (3o).



3o

Yellow semisolid; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.59 (t, *J* = 6.8 Hz, 4H), 7.48 (d, *J* = 8.0 Hz, 2H), δ 7.43 ~ 7.32 (m, 11H), 7.25 (t, *J* = 8.0 Hz, 2H), 7.12 (t, *J* = 7.6 Hz, 2H), 6.80 (s, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 138.8, 137.6, 136.9, 132.5, 129.8, 128.8, 128.2, 127.8, 126.5, 125.7, 123.4, 121.1, 121.0, 116.8, 110.6, 44.8; ESI-MS calcd. for $C_{36}H_{23}Cl_2N_3$: 567.1269; found: 590.1167 [M+Na].

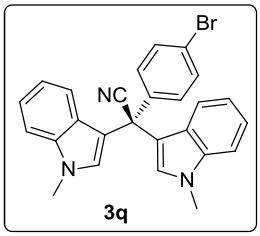
Spectral data for 2-(4-chlorophenyl)-2,2-bis(1-methyl-*1H*-indol-3-yl)acetonitrile (3p).



3p

Light yellow solid; ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.44 (d, *J* = 8.2 Hz, 4H), 7.33 ~ 7.29 (m, 4H), 7.26 ~ 7.24 (m, 2H), 7.05 (t, *J* = 8.0 Hz, 2H), 6.50 (s, 2H), 3.70 (s, 6H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 138.5, 137.7, 133.8, 129.3, 129.2, 128.7, 125.6, 122.3, 121.5, 120.7, 119.9, 113.6, 109.5, 44.3, 32.9; HRMS calcd. for $C_{26}H_{20}ClN_3$: 409.1346; found: 432.1238 [M+Na].

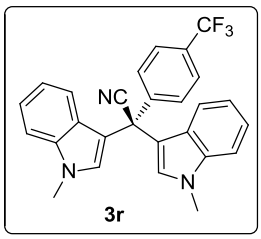
Spectral data for 2-(4-bromophenyl)-2,2-bis(1-methyl-*1H*-indol-3-yl)acetonitrile (3q).



3q

White solid; ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.47 ~ 7.43 (m, 4H), 7.39 ~ 7.36 (m, 2H), 7.32 (d, *J* = 8.0 Hz, 2H), 7.26 ~ 7.23 (m, 2H), 7.05 (t, *J* = 7.5 Hz, 2H), 6.54 (s, 2H), 3.69 (s, 6H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 139.0, 137.7, 131.6, 129.6, 129.3, 125.6, 122.3, 121.9, 121.4, 120.7, 119.9, 113.5, 109.5, 44.4, 32.9, 21.0; ESI-MS calcd. for $C_{26}H_{20}BrN_3$: 453.0841; found: 476.0738 [M+Na].

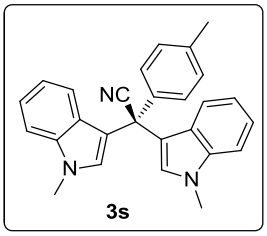
Spectral data for 2,2-bis(1-methyl-*1H*-indol-3-yl)-2-(4-(trifluoromethyl)phenyl) acetonitrile (3r).



3r

Brown semisolid; ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.66 (d, *J* = 8.2 Hz, 2H), 7.59 (d, *J* = 7.8 Hz, 2H), 7.44 (d, *J* = 7.5 Hz, 2H), 7.34 (d, *J* = 8.1 Hz, 2H), 7.27 ~ 7.24 (m, 2H), 7.06 (t, *J* = 7.6 Hz, 2H), 6.55 (s, 2H), 3.70 (s, 6H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 143.9, 137.8, 130.2, 130.0, 129.3, 128.3, 125.5, 124.9, 122.4, 121.2, 120.6, 119.9, 113.2, 109.6, 44.7, 32.9; HRMS calcd. for $C_{27}H_{20}F_3N_3$: 443.1609; found: 466.1507 [M+Na].

Spectral data for 2,2-bis(1-methyl-*1H*-indol-3-yl)-2-(p-tolyl)acetonitrile (3s).

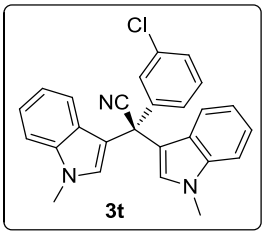


3s

Colorless semisolid; ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.49 ~ 7.47 (m, 2H), 7.38 (d, *J* = 8.1 Hz, 2H), 7.33 ~ 7.31 (m, 2H), 7.26 ~ 7.23 (m, 2H), 7.13 (d, *J* = 8.0 Hz, 2H), 7.06 ~ 7.03 (m, 2H), 6.55 (s, 2H), 3.69 (s, 6H), 2.35 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$):

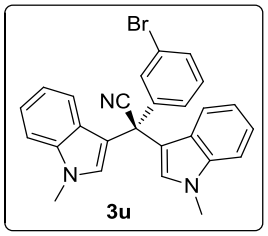
δ 137.7, 137.4, 136.9, 129.3, 129.1, 127.7, 125.8, 122.1, 121.9, 120.8, 119.7, 114.3, 109.4, 44.4, 32.9, 21.1; HRMS calcd. for $C_{27}H_{23}N_3$: 389.1892; found: 412.1784 [M+Na].

Spectral data for 2-(3-chlorophenyl)-2,2-bis(1-methyl-*1H*-indol-3-yl)acetonitrile (3t).



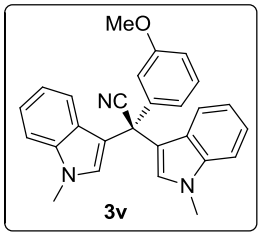
Yellow solid; ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.49 ~ 7.40 (m, 4H), 7.32 ~ 7.23 (m, 6H), 7.07 ~ 7.04 (m, 2H), 6.54 (s, 2H), 3.69 (s, 6H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 141.9, 137.7, 134.5, 129.7, 129.3, 128.2, 128.0, 126.1, 125.6, 122.3, 121.3, 120.6, 119.9, 113.4, 109.6, 44.6, 32.9; HRMS calcd. for $C_{26}H_{20}ClN_3$: 409.1346; found: 432.1238 [M+Na].

Spectral data for 2-(3-bromophenyl)-2,2-bis(1-methyl-*1H*-indol-3-yl)acetonitrile (3u).



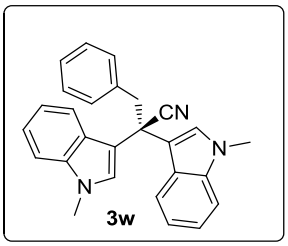
White semisolid; ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.67 (t, *J* = 7.8 Hz, 1H), 7.45 (d, *J* = 8.1 Hz, 4H), 7.32 (d, *J* = 7.9 Hz, 2H), 7.26 ~ 7.20 (m, 3H), 7.07 ~ 7.04 (m, 2H), 6.53 (s, 2H), 3.69 (s, 6H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 142.2, 137.7, 131.1, 130.8, 129.9, 129.3, 126.5, 125.6, 122.7, 122.3, 121.2, 120.6, 119.9, 113.4, 109.6, 44.5, 32.9; HRMS calcd. for $C_{26}H_{20}BrN_3$: 453.0841; found: 476.0733 [M+Na].

Spectral data for 2-(3-methoxyphenyl)-2,2-bis(1-methyl-*1H*-indol-3-yl)acetonitril -e (3v).



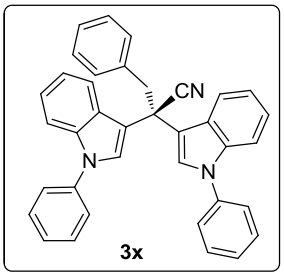
White semisolid; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.49 (d, *J* = 8.4 Hz, 2H), 7.31 (d, *J* = 8.1 Hz, 2H), 7.26 ~ 7.21 (m, 4H), 7.08 ~ 7.02 (m, 3H), 6.87 ~ 6.84 (m, 1H), 6.54 (s, 2H), 3.73 (s, 3H), 3.68 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 159.7, 141.4, 137.7, 129.4, 129.3, 125.8, 122.1, 121.7, 120.8, 120.3, 119.7, 114.0, 113.9, 112.9, 109.4, 55.3, 44.7, 32.9; HRMS calcd. for $C_{27}H_{23}N_3O$: 405.1841; found: 405.1899 [M+H].

Spectral data for 2,2-bis(1-methyl-1*H*-indol-3-yl)-3-phenylpropanenitrile (3w).



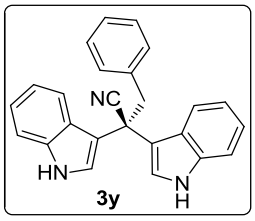
Colorless liquid; ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.52 (d, *J* = 8.1 Hz, 2H), 7.30 (d, *J* = 8.2 Hz, 2H), 7.21 ~ 7.14 (m, 3H), 7.09 (t, *J* = 8.1 Hz, 2H), 7.02 ~ 6.99 (m, 4H), 6.85 (d, *J* = 7.7 Hz, 2H), 3.87 (s, 2H), 3.67 (s, 6H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 137.8, 135.8, 130.4, 128.4, 127.9, 127.1, 125.5, 121.9, 121.5, 120.4, 119.4, 112.6, 109.6, 43.8, 42.4, 32.9; ESI-MS calcd. for $C_{27}H_{23}N_3$: 389.1892; found: 390.1895 [M+H].

Spectral data for 3-phenyl-2,2-bis(1-phenyl-1*H*-indol-3-yl)propanenitrile (3x).



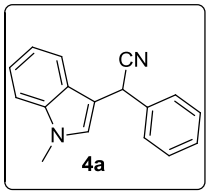
Colorless viscous solid; ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.62 ~ 7.59 (m, 3H), 7.54 ~ 7.53 (m, 2H), 7.46 ~ 7.44 (m, 3H), 7.40 ~ 7.28 (m, 11H), 7.24 ~ 7.22 (m, 2H), 7.13 ~7.10 (m, 2H), 6.85 (s, 2H), 3.46 (s, 2H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 139.1, 137.0, 131.2, 129.6, 129.4, 128.7, 128.1, 127.9, 126.8, 124.6, 123.0, 121.4, 121.0, 120.8, 116.8, 116.3, 110.8, 44.8, 43.5; ESI-MS calcd. for $C_{37}H_{27}N_3$: 513.2205; found: 536.2105 [M+Na].

Spectral data for 2,2-di(1*H*-indol-3-yl)-3-phenylpropanenitrile (3y).



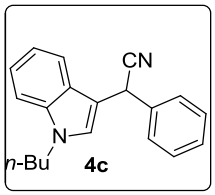
White semisolid; ^{1}H NMR (600 MHz, $CDCl_3$): δ 8.09 (s, 2H), 7.48 (d, *J* = 8.1 Hz, 2H), 7.35 (d, *J* = 8.3 Hz, 2H), 7.18 ~ 7.14 (m, 5H), 7.09 (t, *J* = 7.7 Hz, 2H), 6.98 (t, *J* = 7.2 Hz, 2H), 6.84 (d, *J* = 7.1 Hz, 2H), 3.89 (s, 2H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 136.9, 135.6, 130.4, 127.7, 127.0, 125.0, 123.2, 122.5, 121.3, 120.2, 119.9, 114.3, 111.5, 43.5, 42.4, 26.5; ESI-MS calcd. for $C_{25}H_{19}N_3$: 361.1579; found: 362.1575 [M+H].

Spectral data for 2-(1-methyl-*1H*-indol-3-yl)-2-phenylacetonitrile (4a).



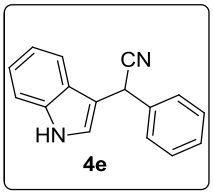
Colorless liquid; ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.45 ~ 7.43 (m, 3H), 7.36 ~ 7.34 (m, 2H), 7.32 ~ 7.24 (m, 3H), 7.10 ~ 7.08 (m, 1H), 7.00 (s, 1H), 5.37 (s, 1H), 3.76 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 137.4, 135.7, 129.9, 128.9, 128.1, 127.9, 127.6, 125.8, 122.4, 121.2, 119.8, 118.8, 109.6, 109.4, 34.4, 32.8. ESI-MS calcd. for $C_{17}H_{14}N_2$: 246.1157; found: 247.1238 [M+H].

Spectral data for 2-(1-butyl-*1H*-indol-3-yl)-2-phenylacetonitrile (4c).



Light yellow liquid; ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.48 ~ 7.41 (m, 3H), 7.38 ~ 7.29 (m, 4H), 7.24 ~ 7.21 (m, 1H), 7.10 ~ 7.05 (m, 2H), 5.37 (s, 1H), 4.09 (q, *J* = 12.5, 7.4 Hz, 2H), 1.83 ~ 1.78 (m, 2H), 1.34 ~ 1.25 (m, 2H), 0.97 ~ 0.85 (m, 3H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 136.7, 135.7, 128.9, 128.0, 127.7, 126.7, 125.8, 122.2, 119.9, 119.7, 118.9, 109.8, 109.1, 46.3, 34.4, 32.2, 20.1, 13.7.

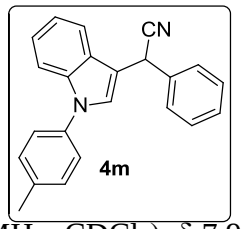
Spectral data for 2-(*1H*-indol-3-yl)-2-phenylacetonitrile (4e).



Colorless liquid; ^{1}H NMR (600 MHz, $CDCl_3$): δ 8.20 (s, 1H), 7.44 ~ 7.31 (m, 6H), 7.24 ~ 7.01 (m, 4H), 5.38 (s, 1H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 136.6, 135.4, 129.0,

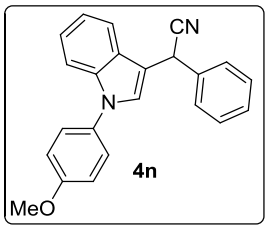
128.1, 127.7, 125.3, 123.2, 122.9, 120.3, 119.8, 118.8, 111.5, 110.1, 34.5. ESI-MS calcd. for $C_{16}H_{12}N_2$: 232.1000; found: 2255.0900 [M+Na].

Spectral data for 2-phenyl-2-(1-(p-tolyl)-1*H*-indol-3-yl)acetonitrile (4m).



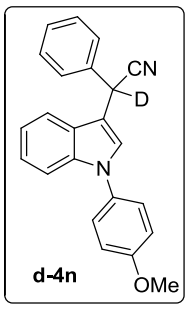
Colorless liquid; ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.97 (d, *J* = 8.4 Hz, 1H), 7.76 (d, *J* = 8.3 Hz, 2H), 7.55 (s, 1H), 7.36 ~ 7.30 (m, 7H), 7.23 (d, *J* = 8.0 Hz, 2H), 7.17 (t, *J* = 7.4 Hz, 1H), 5.25 (s, 1H), 2.34 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 145.4, 135.4, 134.8, 133.6, 130.0, 129.3, 128.6, 127.9, 127.6, 126.9, 125.4, 124.9, 123.6, 119.5, 118.6, 117.3, 113.9, 34.2, 21.6; ESI-MS calcd. for $C_{23}H_{18}N_2$: 322.1470; found: 323.1475 [M+H].

Spectral data for 2-(1-(4-methoxyphenyl)-1*H*-indol-3-yl)-2-phenylacetonitrile (4n).



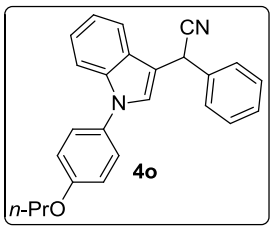
Colorless liquid; ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.51 ~ 7.48 (m, 2H), 7.41 (d, *J* = 8.3 Hz, 1H), 7.38 ~ 7.32 (m, 6H), 7.23 ~ 7.20 (m, 2H), 7.14 ~ 7.11 (m, 1H), 7.03 ~ 7.00 (m, 2H), 5.43 (s, 1H), 3.87 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 158.6, 137.1, 135.3, 132.0, 129.1, 128.2, 127.8, 127.6, 127.2, 126.2, 123.1, 120.6, 119.7, 118.9, 114.8, 111.3, 110.9, 55.6, 34.5; ESI-MS calcd. for $C_{23}H_{18}N_2O$: 338.1419; found: 339.1492 [M+H].

Spectral data for 2-(1-(4-mthoxyphenyl)-1*H*-indol-3-yl)-2-phenylacetonitrile (d-4n) with deuterium.



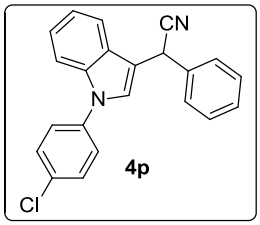
Colorless liquid; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.51 ~ 7.46 (m, 2H), 7.43 ~ 7.28 (m, 6H), 7.24 ~ 7.19 (m, 2H), 7.14 ~ 7.10 (m, 1H), 7.04 ~ 7.00 (m, 2H), 5.42 (s, 0.14H), 3.86 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 158.6, 137.1, 135.3, 132.0, 129.1, 128.2, 127.8, 127.6, 127.2, 126.1, 123.1, 120.6, 119.7, 119.0, 114.8, 111.3, 110.9, 55.6, 34.5; ESI-MS calcd. for $C_{23}H_{18}DN_2O$: 339.1482ound: 340.1555 [M+H].

Spectral data for 2-phenyl-2-(1-(4-propoxyphenyl)-1*H*-indol-3-yl)acetonitrile (4o)



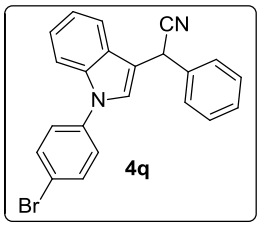
Light yellow liquid; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.51 ~ 7.45 (m, 3H), 7.43 ~ 7.31 (m, 7H), 7.23 ~ 7.18 (m, 1H), 7.14 ~ 7.10 (m, 1H), 7.03 ~ 6.99 (m, 2H), 5.42 (s, 1H), 3.96 (t, *J* = 6.8 Hz, 2H), 1.88 ~ 1.81 (m, 2H), 1.08 (d, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 158.2, 137.2, 135.3, 131.8, 129.1, 128.2, 127.8, 127.3, 126.2, 126.0, 123.0, 120.6, 119.7, 118.9, 115.4, 111.2, 110.9, 69.9, 34.5, 22.6, 10.5; ESI-MS calcd. for $C_{25}H_{22}N_2O$: 366.1732; found: 367.11728 [M+H].

Spectral data for 2-(1-(4-chlorophenyl)-1*H*-indol-3-yl)-2-phenylacetonitrile (4p).



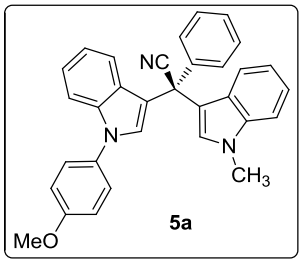
Yellow liquid; ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.51 ~ 7.47 (m, 6H), 7.42 ~ 7.37 (m, 4H), 7.34 ~ 7.33 (m, 1H), 7.24 ~ 7.23 (m, 2H), 7.15 (d, *J* = 7.1 Hz, 1H), 5.42 (s, 1H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 137.6, 136.5, 134.9, 132.6, 129.9, 129.1, 128.3, 127.7, 126.6, 126.5, 125.6, 123.5, 121.1, 119.5, 119.3, 112.4, 110.7, 34.4.

Spectral data for 2-(1-(4-bromophenyl)-1*H*-indol-3-yl)-2-phenylacetonitrile (4q).



Brownish liquid; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.51 ~ 7.48 (m, 6H), 7.42 ~ 7.32 (m, 6H), 7.24 ~ 7.23 (m, 1H), 7.16 ~ 7.12 (m, 1H), 5.42 (s, 1H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 137.6, 136.5, 134.9, 132.6, 129.9, 129.1, 128.3, 127.7, 126.6, 126.5, 125.6, 123.5, 121.1, 119.5, 119.3, 112.4, 110.7, 34.4. ESI-MS calcd. for $C_{22}H_{15}BrN_2$: 386.0419; found: 387.0423 [M+H].

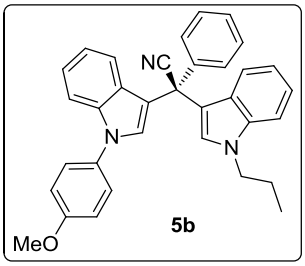
Spectral data for (S)-2-(1-(4-methoxyphenyl)-1H-indol-3-yl)-2-(1-methyl-1H-indo-l-3-yl)-2-phenylacetonitrile (5a).



5a

White semisolid; ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.56 ~ 7.55 (m, 2H), 7.53 ~ 7.50 (m, 2H), 7.41 (d, *J* = 8.4 Hz, 1H), 7.36 ~ 7.28 (m, 6H), 7.23 ~ 7.18 (m, 2H), 7.09 ~ 7.03 (m, 2H), 6.95 (d, *J* = 8.2 Hz, 2H), 6.75 (s, 1H), 6.58 (s, 1H), 3.82 (s, 3H), 3.69 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 158.5, 139.6, 137.7, 137.5, 132.1, 129.3, 128.8, 128.6, 127.9, 127.8, 126.2, 126.1, 125.8, 122.8, 122.2, 121.7, 121.0, 120.8, 120.5, 119.8, 116.0, 114.7, 113.9, 110.6, 109.5, 55.6, 44.8, 32.9; ESI-MS calcd. for $C_{32}H_{25}N_3O$: 467.1988; found: 490.1890 [M+Na].

Spectral data for (S)-2-(1-(4-methoxyphenyl)-1*H*-indol-3-yl)-2-phenyl-2-(1-propy-l-1*H*-indol-3-yl)acetonitrile (5b).

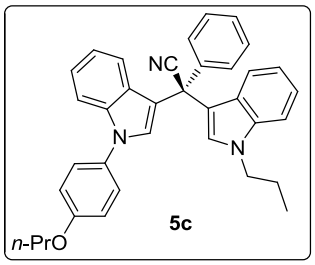


5b

White semisolid; ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.56 (d, *J* = 8.4 Hz, 2H), 7.53 ~ 7.48 (m, 1H), 7.41 (d, *J* = 8.1 Hz, 1H), 7.36 ~ 7.28 (m, 7H), 7.20 (t, *J* = 7.3 Hz, 2H), 7.07 (t, *J* = 7.3 Hz, 1H), 7.03 (t, *J* = 7.4 Hz, 1H), 6.96 (d, *J* = 7.3 Hz, 2H), 6.73 (s, 1H), 6.65 (s, 1H), 3.98 (t, *J* = 7.0 Hz, 2H), 3.83 (s, 3H), 1.80 ~ 1.76 (m, 2H), 0.86 (t, *J* = 7.4, 3H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 158.5, 139.6, 137.5, 137.1, 132.1, 128.8, 128.6, 128.5, 127.9, 126.2, 126.1, 125.9, 122.7, 121.9, 121.7, 121.0, 120.8, 120.4,

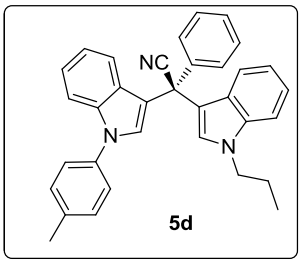
119.7, 116.1, 114.8, 114.7, 113.5, 110.6, 109.7, 55.6, 48.1, 44.8, 23.4, 11.4; HRMS calcd. for $C_{34}H_{29}N_3O$: 495.2311; found: 518.2203 [M+Na].

Spectral data for(S)-2-phenyl-2-(1-(4-propoxyphenyl)-1*H*-indol-3-yl)-2-(1-propyl -1*H*-indol-3-yl)acetonitrile (5c).



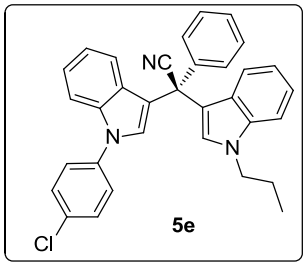
Brownish semisolid; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.54 (d, *J* = 8.0 Hz, 2H), 7.52 ~ 7.47 (m, 2H), 7.41 (d, *J* = 8.8 Hz, 1H), 7.34 ~ 7.26 (m, 6H), 7.19 (t, *J* = 7.6 Hz, 2H), 7.01 ~ 7.00 (m, 2H), 6.94 (d, *J* = 8.8 Hz, 2H), 6.72 (s, 1H), 6.64 (s, 1H), 3.98 (t, *J* = 7.2 Hz, 2H), 3.92 (t, *J* = 7.4 Hz, 2H), 1.85 ~ 1.73 (m, 4H), 1.03 (t, *J* = 7.4, 3H), 0.85 (t, *J* = 7.4, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 158.0, 139.6, 137.5, 137.1, 131.9, 128.8, 128.6, 128.5, 127.9, 126.2, 126.1, 125.9, 122.7, 121.9, 121.7, 121.0, 120.8, 120.4, 119.7, 116.1, 115.3, 113.5, 110.7, 109.7, 69.9, 48.1, 44.8, 23.4, 22.5, 11.4, 10.5; HRMS calcd. for $C_{36}H_{33}N_3O$: 523.2624; found: 523.2626.

Spectral data for (S)-2-phenyl-2-(1-propyl-1H-indol-3-yl)-2-(1-(p-tolyl)-1H- indol -3-yl)acetonitrile (5d).



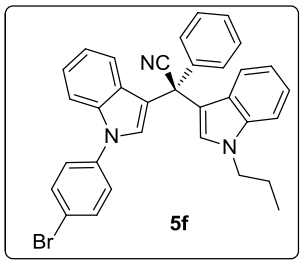
White semisolid; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.57 ~ 7.52 (m, 3H), 7.49 (d, *J* = 8.0 Hz, 2H), 7.37 ~ 7.25 (m, 6H), 7.23 ~ 7.18 (m, 4H), 7.07 (t, *J* = 7.2 Hz, 1H), 7.03 (t, *J* = 7.6 Hz, 1H), 6.75 (s, 1H), 6.65 (s, 1H), 3.98 (t, *J* = 7.2 Hz, 2H), 2.38 (s, 3H), 1.81 ~ 1.76 (m, 2H), 0.86 (t, *J* = 7.2, 3H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 139.6, 137.1, 136.7, 136.6, 130.1, 129.4, 129.2, 128.6, 128.5, 127.9, 127.8, 126.4, 125.9, 124.5, 122.8, 122.0, 121.7, 121.1, 120.8, 120.5, 119.7, 113.5, 110.8, 109.7, 48.1, 44.8, 23.4, 21.0, 11.4; HRMS calcd. for $C_{34}H_{29}N_3$: 479.2361; found: 502.2259.

Spectral data for (S)-2-(1-(4-chlorophenyl)-1*H*-indol-3-yl)- 2-phenyl-2-(1-propyl -1*H*-indol-3-yl)acetonitrile (5e).



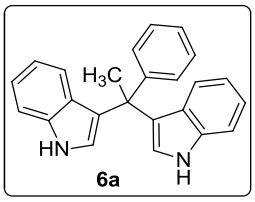
Yellow semisolid ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.56 ~ 7.50 (m, 3H), 7.49 ~ 7.47 (m, 2H), 7.42 (d, *J* = 6.8 Hz, 2H), 7.37 ~ 7.29 (m, 6H), 7.26 ~ 7.19 (m, 2H), 7.09 (t, *J* = 8.0 Hz, 1H), 7.04 (t, *J* = 8.2 Hz, 1H), 6.75 (s, 1H), 6.63 (s, 1H), 3.99 (t, *J* = 7.2 Hz, 2H), 1.83 ~ 1.74 (m, 2H), 0.86 (t, *J* = 7.2, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 139.3, 137.7, 137.1, 136.9, 132.4, 129.8, 128.6, 128.5, 128.2, 128.0, 127.8, 126.6, 125.8, 125.7, 123.2, 122.1, 121.6, 121.3, 120.9, 120.8, 119.7, 117.3, 113.3, 110.5, 109.8, 48.1, 44.8, 23.4, 11.4; HRMS calcd. for $C_{33}H_{26}ClN_3$: 499.1815; found: 499.1815.

Spectral data for (S)-2-(1-(4-bromophenyl)-1*H*-indol-3-yl)-2-phenyl-2-(1-propyl -1*H*-indol-3-yl)acetonitrile (5f).



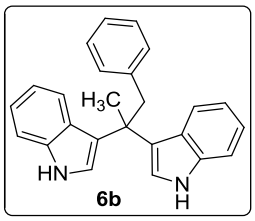
Light brown semisolid; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.56 ~ 7.50 (m, 3H), 7.49 ~ 7.47 (m, 2H), 7.42 (d, *J* = 6.8 Hz, 2H), 7.37 ~ 7.29 (m, 6H), 7.26 ~ 7.19 (m, 2H), 7.09 (t, *J* = 8.0 Hz, 1H), 7.04 (t, *J* = 8.2 Hz, 1H), 6.75 (s, 1H), 6.63 (s, 1H), 3.99 (t, *J* = 7.2 Hz, 2H), 1.83 ~ 1.74 (m, 2H), 0.86 (t, *J* = 7.2, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 139.3, 137.7, 137.1, 136.9, 132.4, 129.8, 128.6, 128.5, 128.2, 128.0, 127.8, 126.6, 125.8, 125.7, 123.2, 122.1, 121.6, 121.3, 120.9, 120.8, 119.7, 117.3, 113.3, 110.5, 109.8, 48.1, 44.8, 23.4, 11.4; HRMS calcd. for $C_{33}H_{26}BrN_3$: 543.1310; found: 543.1314.

Spectral data for 3,3'-(1-phenylethane-1,1-diyl)bis(1*H*-indole) (6a).



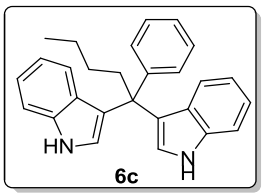
White semisolid; ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.79 (s, 2H), 7.39 (d, *J* = 7.5 Hz, 2H), 7.31(d, *J* = 8.5 Hz, 4H), 7.24 (t, *J* = 7.0 Hz, 2H), 7.18 (t, *J* = 7.0 Hz, 1H), 7.12 (t, *J* = 8.0 Hz, 2H), 6.93 (t, *J* = 7.0 Hz, 2H), 6.59 (d, *J* = 2.0 Hz, 2H), 2.36 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 148.0, 137.1, 128.0, 127.8, 126.5, 125.8, 124.7, 123.3, 122.1, 121.5, 118.9, 111.1, 43.7, 28.7; ESI-MS calcd. for $C_{24}H_{20}N_2$: 336.1626; found: 337.1630 [M+H].

Spectral data for 3,3'-(1-phenylpropane-2,2-diyl)bis(1*H*-indole) (6b).



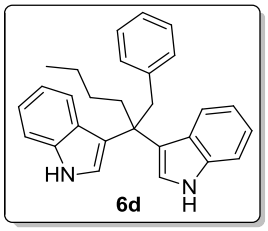
White Semisolid; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.88 (s, 2H), 7.36 ~ 7.30 (m, 4H), 7.09 ~ 7.00 (m, 5H), 6.95 (d, *J* = 2.3 Hz, 2H), 6.84 (t, *J* = 7.6 Hz, 2H), 6.58 (d, *J* = 8.0 Hz, 2H), 3.68 (s, 2H), 1.67 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 138.6, 137.0, 130.7, 127.0, 126.5, 125.7, 123.6, 121.4, 121.3, 121.1, 118.8, 111.0, 45.7, 39.2, 26.5; ESI-MS calcd. for $C_{25}H_{22}N_2$: 350.1783; found: 351.1780 [M+H].

Spectral data for 3,3'-(1-phenylpentane-1,1-diyl)bis(1H-indole) (6c).



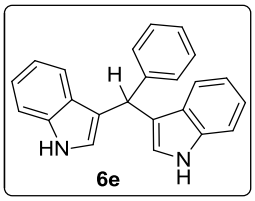
Yellow Semisolid; ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.88 (s, 2H), 7.45 ~ 7.44 (m, 2H), 7.32 ~ 7.30 (m, 4H), 7.18 (t, *J* = 6.6 Hz, 2H), 7.11 ~ 7.08 (m, 3H), 6.89 ~ 6.87 (m, 4H), 2.76 ~ 2.73 (m, 2H), 1.31 ~ 1.26 (m, 2H), 1.18 ~ 1.13 (m, 2H), 0.78 (t, *J* = 7.3 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 147.3, 136.9, 128.4, 127.6, 126.8, 125.5, 123.5, 122.5, 122.3, 121.4, 118.8, 110.9, 47.9, 40.6, 28.3, 23.3, 14.0; HRMS calcd. for $C_{27}H_{26}N_2$: 378.2096; found: 378.2098.

Spectral data for 3,3'-(1-phenylhexane-2,2-diyl)bis(1*H*-indole) (6d).



Yellow Semisolid; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.92 (s, 2H), 7.30 (d, *J* = 7.2 Hz, 2H), 7.21 (d, *J* = 8.4 Hz, 2H), 7.09 ~ 6.99 (m, 7H), 6.77 ~ 6.74 (m, 2H), 6.49 (d, *J* = 6.8 Hz, 2H), 2.03 (d, *J* = 2.1 Hz, 2H), 1.22 ~ 1.18 (m, 4H), 0.78 (t, *J* = 6.4 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 138.6, 136.9, 130.5, 127.0, 126.8, 125.6, 122.5, 121.8, 121.3, 121.1, 118.7, 110.8, 42.7, 42.2, 35.4, 26.5, 23.1, 14.2; HRMS calcd. for $C_{28}H_{28}N_2$: 392.2252; found: 392.2256.

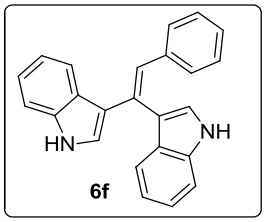
Spectral data for 3,3'-(phenylmethylene)bis(1*H*-indole) or Turbomycin B (6e).



6e

White Solid; ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.76 (s, 2H), 7.39 (d, *J* = 7.7 Hz, 2H), 7.35 ~ 7.22 (m, 7H), 7.17 (t, *J* = 7.3 Hz, 2H), 7.01 (t, *J* = 7.5 Hz, 2H), 6.58 (s, 2H), 5.87 (s, 1H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 143.9, 136.6, 128.7, 128.2, 127.0, 126.1, 123.6, 121.9, 119.9, 119.6, 119.2, 111.0, 40.2; ESI-MS calcd. for $C_{23}H_{17}N_2$: 322.1470; found: 321.1387 [M^{+}-H].

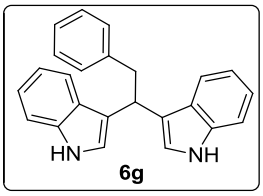
Spectral data for 3,3'-(2-phenylethene-1,1-diyl)bis(1*H*-indole) (6f).



6f

Light yellow liquid; ^{1}H NMR (600 MHz, $CDCl_3$): δ 8.08 (s, 1H), 7.99 (s, 1H), 7.78 (d, *J* = 6.6 Hz, 1H), 7.38 ~ 7.35 (m, 2H), 7.22 ~ 7.16 (m, 3H), 7.15 ~ 7.14 (m, 3H), 7.11 (t, *J* = 7.9 Hz, 1H), 7.07 (t, *J* = 7.7 Hz, 2H), 7.04 ~ 7.00 (m, 2H), 6.97 (d, *J* = 2.4 Hz, 1H), 6.92 (t, *J* = 7.8 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 138.7, 136.8, 136.1, 128.8, 127.8, 126.8, 125.8, 125.7, 125.6, 124.9, 124.6, 122.2, 121.9, 121.2, 120.9, 120.8, 120.1, 119.6, 116.4, 111.3, 110.9; ESI-MS calcd. for $C_{24}H_{18}N_2$: 334.1470; found: 335.1472 [M+H].

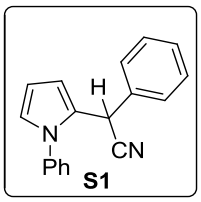
Spectral data for 3,3'-(2-phenylethane-1,1-diyl)bis(1*H*-indole) (6g).



6g

White Semisolid; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.80 (s, 2H), 7.56 (d, *J* = 8.0 Hz, 2H), 7.30 (d, *J* = 8.0 Hz, 2H), 7.16 ~ 7.08 (m, 7H), 7.02 (t, *J* = 7.2 Hz, 2H), 6.91 (d, *J* = 2.0 Hz, 2H), 4.79 (t, *J* = 7.6 Hz, 1H), 3.53 (d, *J* = 7.6 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 141.3, 136.6, 129.0, 128.0, 127.0, 125.7, 121.9, 121.7, 119.7, 119.4, 119.1, 111.0, 41.7, 36.2; HRMS calcd. for $C_{24}H_{20}N_2$: 336.1626; found: 336.1625.

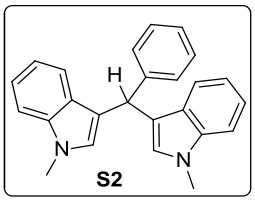
Spectral data for 2-phenyl-2-(1-phenyl-1H-pyrrol-2-yl)acetonitrile (S1).



S1

Yellowish Semisolid; ^{1}H NMR (600 MHz, $CDCl_3$): δ 7 .38 ~ 7.36 (m, 3H), 7.26 ~ 7.24 (m, 3H), 7.14 ~ 7.10 (m, 4H), 6.78 ~ 6.77 (m, 1H), 6.33 ~ 6.32 (m, 1H), 6.26 (t, *J* = 3.5 Hz, 1H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 138.80, 132.8, 129.3, 128.8, 128.3, 128.1, 127.5, 126.8, 126.6, 124.2, 118.9, 110.5, 108.6, 35.1; ESI-MS calcd. for $C_{18}H_{14}N_2$: 258.1157; found: 259.1162. [M+H].

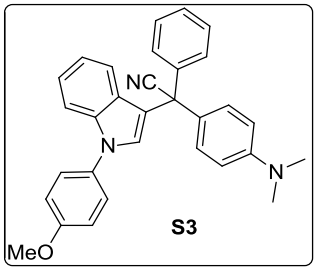
Spectral data for 3,3'-(phenylmethylene)bis(1-methyl-1*H*-indole) (S2).



S2

White Semisolid; ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.36 (d, *J* = 8.4 Hz, 2H), 7.33 (d, *J* = 7.9 Hz, 2H), 7.27 (d, *J* = 7.8 Hz, 2H), 7.21 ~ 7.18 (m, 5H), 7.00 (t, *J* = 7.3 Hz, 2H), 6.49 (s, 2H), 5.82 (s, 1H), 3.67 (s, 6H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 143.5, 137.4, 131.3, 130.4, 128.2, 127.2, 121.5, 119.9, 119.8, 118.7, 117.6, 109.1, 39.5, 32.7; ESI-MS calcd. for $C_{25}H_{22}N_2$: 350.1783; found: 351.1817.

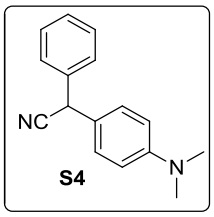
Spectral data for 2-(4-(dimethylamino)phenyl)-2-(1-(4-methoxyphenyl)- 1*H*-indol -3-yl)-2-phenylacetonitrile (S3).



S3

Yellow Semisolid; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.44 ~ 7.36 (m, 4H), 7.33 ~ 7.29 (m, 5H), 7.23 ~ 7.17 (m, 3H), 7.06 (t, *J* = 5.6 Hz, 1H), 6.96 (dd, *J* = 8.8, 1.2 Hz, 2H), 6.45 (d, *J* = 8.8 Hz, 2H), 6.54 (s, 1H), 3.84 (s, 3H), 2.94 (s, 6H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 158.7, 149.9, 140.6, 137.7, 132.3, 129.3, 129.1, 128.5, 128.3, 127.8, 126.5, 126.3, 122.9, 122.8, 121.2, 120.5, 117.5, 114.8, 112.3, 110.6, 55.6, 50.6, 40.4, 29.7; ESI-MS calcd. for $C_{31}H_{27}N_3O$: 457.2154; found: 458.2160 [M+H].

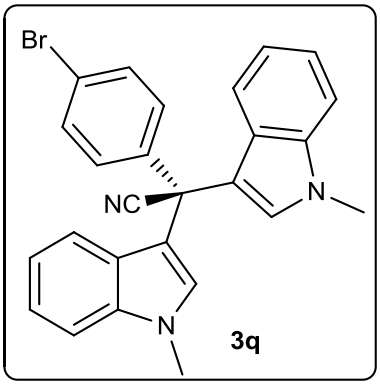
Spectral data for 2-(4-(dimethylamino)phenyl)-2-phenylacetonitrile (S4).



Colorless liquid; ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.33 ~ 7.23 (m, 5H), 7.15 (d, *J* = 8.8 Hz, 2H), 6.66 (d, *J* = 8.6 Hz, 2H), 5.04 (s, 1H), 2.92 (s, 6H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 150.2, 136.7, 129.2, 129.0, 128.5, 127.9, 127.6, 120.2, 112.6, 41.7, 40.4 ;

X-ray crystallographic structure and data

X-ray data for compound 3q :



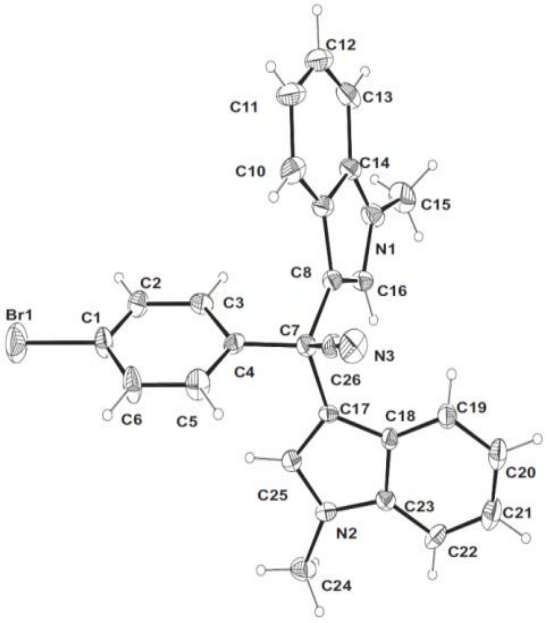


Table 1. Crystal data and structure refinement for ch18209.

Identification code ch18209

Empirical formula C_{26} H_{20} Br N_3

Formula weight 454.36

Temperature 296(2) K

Wavelength 0.71073 Å

Crystal system Triclinic

Space group P -1

Unit cell dimensions a = 9.542(5) Å □= 105.75(2)°.

b = 11.051(6) Å □= 108.68(2)°.

c = 11.500(7) Å □ = 95.23(2)°.

Volume 1084.4(10) Å3

Z 2

Density (calculated) 1.392 Mg/m3

Absorption coefficient 1.913 mm-1

F(000) 464

Crystal size 0.29 x 0.04 x 0.01 mm3

Theta range for data collection 1.97 to 25.09°.

Index ranges -10<=h<=11, -13<=k<=13, -13<=l<=13

Reflections collected 9487

Independent reflections 3787 [R(int) = 0.1022]

Completeness to theta = 25.09° 98.2 %

Absorption correction multi-scan

Max. and min. transmission 0.9811 and 0.6070

Refinement method Full-matrix least-squares on F2

Data / restraints / parameters 3787 / 0 / 267

Goodness-of-fit on F2 0.923

Final R indices [I>2sigma(I)] R1 = 0.0685, wR2 = 0.1448

R indices (all data) R1 = 0.2308, wR2 = 0.2086

Largest diff. peak and hole 0.261 and -0.451 e.Å-3

Table 2. Atomic coordinates (x 104) and equivalent isotropic displacement parameters (Å2x 103)

for ch18209. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
C(1)	8089(9)	3898(7)	2915(8)	58(2)
C(2)	6937(10)	4511(7)	2695(7)	60(2)
C(3)	6910(8)	5435(6)	2093(7)	48(2)
C(4)	8087(8)	5758(6)	1695(7)	42(2)
C(5)	9259(8)	5092(7)	1941(8)	64(2)
C(6)	9253(9)	4167(8)	2525(9)	77(3)
C(7)	8036(8)	6757(7)	973(7)	42(2)
C(8)	7002(9)	7673(7)	1262(8)	48(2)
C(9)	7149(10)	8493(7)	2533(9)	50(2)
C(10)	8194(10)	8749(8)	3766(10)	64(2)
C(11)	7986(13)	9584(8)	4806(10)	90(3)
C(12)	6701(13)	10127(9)	4569(11)	90(3)
C(13)	5617(11)	9902(7)	3354(11)	78(3)
C(14)	5856(11)	9063(7)	2304(11)	59(3)
C(15)	3542(10)	8990(8)	380(9)	93(3)
C(16)	5686(10)	7786(7)	382(8)	56(2)

C(17)	7594(7)	6098(7)	-478(7)	37(2)
C(18)	7581(8)	6670(7)	-1445(7)	39(2)
C(19)	8010(8)	7911(7)	-1414(8)	53(2)
C(20)	7888(9)	8140(9)	-2542(10)	63(2)
C(21)	7354(10)	7158(10)	-3708(10)	72(3)
C(22)	6918(8)	5914(8)	-3778(8)	56(2)
C(23)	7062(8)	5683(7)	-2633(8)	41(2)
C(24)	6263(9)	3282(7)	-3365(7)	65(2)
C(25)	7105(7)	4806(7)	-1096(8)	43(2)
C(26)	9604(10)	7547(7)	1459(8)	48(2)
N(1)	4974(9)	8619(6)	1003(9)	66(2)
N(2)	6766(6)	4549(6)	-2403(6)	46(2)
N(3)	10757(8)	8138(7)	1805(7)	72(2)
Br(1)	8047(1)	2627(1)	3692(1)	110(1)

Table 3. Bond lengths [Å] and angles [°] for ch18209.

C(1)-C(2)	1.335(10)
C(1)-C(6)	1.362(10)
C(1)-Br(1)	1.863(7)
C(2)-C(3)	1.379(9)
C(2)-H(2)	0.9300
C(3)-C(4)	1.394(9)
C(3)-H(3)	0.9300
C(4)-C(5)	1.391(9)

C(4)-C(7)	1.547(9)
C(5)-C(6)	1.367(9)
C(5)-H(5)	0.9300
C(6)-H(6)	0.9300
C(7)-C(26)	1.508(11)
C(7)-C(17)	1.526(9)
C(7)-C(8)	1.522(9)
C(8)-C(16)	1.378(9)
C(8)-C(9)	1.450(10)
C(9)-C(10)	1.382(10)
C(9)-C(14)	1.419(10)
C(10)-C(11)	1.381(10)
C(10)-H(10)	0.9300
C(11)-C(12)	1.395(13)
C(11)-H(11)	0.9300
C(12)-C(13)	1.387(12)
C(12)-H(12)	0.9300
C(13)-C(14)	1.406(11)
C(13)-H(13)	0.9300
C(14)-N(1)	1.381(10)
C(15)-N(1)	1.478(10)
C(15)-H(15A)	0.9600
C(15)-H(15B)	0.9600
C(15)-H(15C)	0.9600
C(16)-N(1)	1.374(8)

C(16)-H(16) 0.9300

C(17)-C(25) 1.370(9)

C(17)-C(18) 1.417(9)

C(18)-C(19) 1.383(9)

C(18)-C(23) 1.400(9)

C(19)-C(20) 1.359(9)

C(19)-H(19) 0.9300

C(20)-C(21) 1.381(10)

C(20)-H(20) 0.9300

C(21)-C(22) 1.373(10)

C(21)-H(21) 0.9300

C(22)-C(23) 1.375(9)

C(22)-H(22) 0.9300

C(23)-N(2) 1.373(8)

C(24)-N(2) 1.453(8)

C(24)-H(24A) 0.9600

C(24)-H(24B) 0.9600

C(24)-H(24C) 0.9600

C(25)-N(2) 1.372(8)

C(25)-H(25) 0.9300

C(26)-N(3) 1.115(8)

C(2)-C(1)-C(6) 120.1(7)

C(2)-C(1)-Br(1) 119.4(6)

C(6)-C(1)-Br(1) 120.5(6)

C(1)-C(2)-C(3) 121.1(7)

C(1)-C(2)-H(2)	119.4
C(3)-C(2)-H(2)	119.4
C(2)-C(3)-C(4)	120.9(7)
C(2)-C(3)-H(3)	119.6
C(4)-C(3)-H(3)	119.6
C(5)-C(4)-C(3)	115.9(7)
C(5)-C(4)-C(7)	122.8(6)
C(3)-C(4)-C(7)	121.2(7)
C(6)-C(5)-C(4)	122.2(7)
C(6)-C(5)-H(5)	118.9
C(4)-C(5)-H(5)	118.9
C(1)-C(6)-C(5)	119.8(7)
C(1)-C(6)-H(6)	120.1
C(5)-C(6)-H(6)	120.1
C(26)-C(7)-C(17)	107.3(6)
C(26)-C(7)-C(8)	107.3(6)
C(17)-C(7)-C(8)	111.7(6)
C(26)-C(7)-C(4)	107.9(6)
C(17)-C(7)-C(4)	110.8(5)
C(8)-C(7)-C(4)	111.6(6)
C(16)-C(8)-C(9)	107.7(7)
C(16)-C(8)-C(7)	126.1(7)
C(9)-C(8)-C(7)	125.9(8)
C(10)-C(9)-C(14)	121.6(9)
C(10)-C(9)-C(8)	134.0(9)

C(14)-C(9)-C(8) 104.4(8)

C(11)-C(10)-C(9) 119.6(9)

C(11)-C(10)-H(10) 120.2

C(9)-C(10)-H(10) 120.2

C(10)-C(11)-C(12) 118.2(11)

C(10)-C(11)-H(11) 120.9

C(12)-C(11)-H(11) 120.9

C(13)-C(12)-C(11) 124.6(10)

C(13)-C(12)-H(12) 117.7

C(11)-C(12)-H(12) 117.7

C(12)-C(13)-C(14) 116.5(10)

C(12)-C(13)-H(13) 121.8

C(14)-C(13)-H(13) 121.8

N(1)-C(14)-C(13) 130.3(9)

N(1)-C(14)-C(9) 110.1(8)

C(13)-C(14)-C(9) 119.5(10)

N(1)-C(15)-H(15A) 109.5

N(1)-C(15)-H(15B) 109.5

H(15A)-C(15)-H(15B) 109.5

N(1)-C(15)-H(15C) 109.5

H(15A)-C(15)-H(15C) 109.5

H(15B)-C(15)-H(15C) 109.5

N(1)-C(16)-C(8) 110.2(7)

N(1)-C(16)-H(16) 124.9

C(8)-C(16)-H(16) 124.9

C(25)-C(17)-C(18) 106.7(7)

C(25)-C(17)-C(7) 125.2(7)

C(18)-C(17)-C(7) 128.1(6)

C(19)-C(18)-C(23) 119.0(7)

C(19)-C(18)-C(17) 133.7(8)

C(23)-C(18)-C(17) 107.2(6)

C(20)-C(19)-C(18) 119.0(8)

C(20)-C(19)-H(19) 120.5

C(18)-C(19)-H(19) 120.5

C(19)-C(20)-C(21) 121.2(8)

C(19)-C(20)-H(20) 119.4

C(21)-C(20)-H(20) 119.4

C(20)-C(21)-C(22) 121.5(8)

C(20)-C(21)-H(21) 119.3

C(22)-C(21)-H(21) 119.3

C(23)-C(22)-C(21) 117.2(8)

C(23)-C(22)-H(22) 121.4

C(21)-C(22)-H(22) 121.4

N(2)-C(23)-C(22) 130.0(8)

N(2)-C(23)-C(18) 107.9(6)

C(22)-C(23)-C(18) 122.1(7)

N(2)-C(24)-H(24A) 109.5

N(2)-C(24)-H(24B) 109.5

H(24A)-C(24)-H(24B) 109.5

N(2)-C(24)-H(24C) 109.5

H(24A)-C(24)-H(24C) 109.5

H(24B)-C(24)-H(24C) 109.5

N(2)-C(25)-C(17) 109.7(6)

N(2)-C(25)-H(25) 125.1

C(17)-C(25)-H(25) 125.1

N(3)-C(26)-C(7) 179.1(9)

C(16)-N(1)-C(14) 107.6(7)

C(16)-N(1)-C(15) 125.9(9)

C(14)-N(1)-C(15) 126.5(8)

C(25)-N(2)-C(23) 108.4(6)

C(25)-N(2)-C(24) 125.6(6)

C(23)-N(2)-C(24) 126.0(7)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters (Å2x 103)for ch18209. The anisotropic

displacement factor exponent takes the form: -2□2[h2a*2U11 + ... + 2 h k a* b* U12]

U11 U22 U33 U23 U13 U12

C(1)	49(6)	64(5)	84(7)	49(5)	30(5)	23(5)
C(2)	67(7)	54(5)	73(7)	27(5)	43(5)	1(5)
C(3)	31(5)	56(5)	59(6)	13(4)	23(4)	18(4)
C(4)	36(5)	49(4)	43(5)	11(4)	22(4)	3(4)

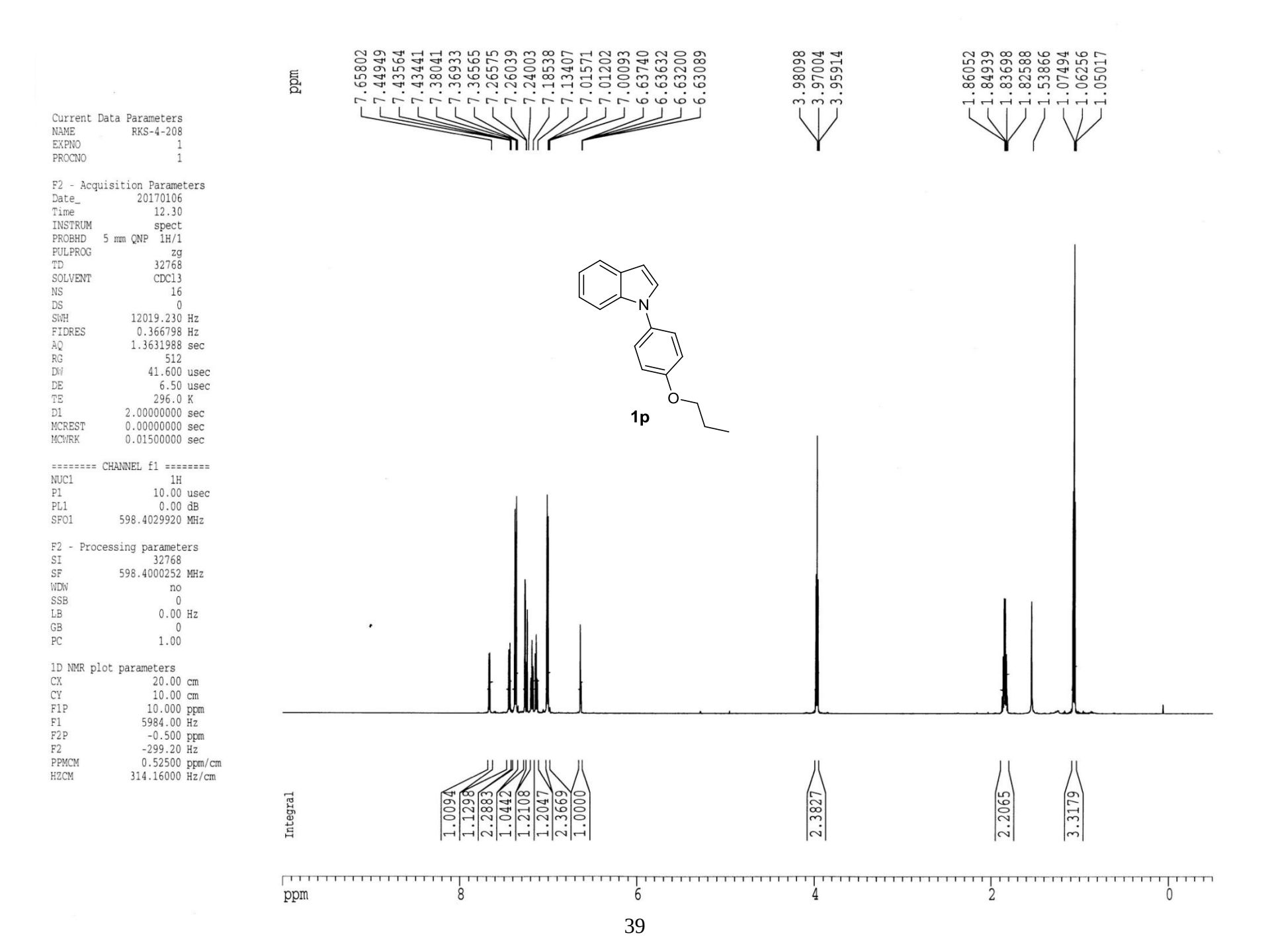
C(5)	31(5)	89(6)	101(7)	51(6)	40(5)	26(5)
C(6)	58(6)	94(7)	136(9)	88(7)	57(6)	48(5)
C(7)	35(5)	44(4)	51(6)	15(4)	19(5)	12(4)
C(8)	56(6)	43(5)	55(6)	16(5)	35(5)	13(5)
C(9)	55(7)	40(5)	62(7)	8(5)	37(6)	-1(5)
C(10)	64(7)	63(6)	57(7)	10(5)	25(6)	-10(5)
C(11)	134(10)	55(5)	85(5)	-7(4)	77(7)	-19(5)
C(12)	134(10)	55(5)	85(5)	-7(4)	77(7)	-19(5)
C(13)	89(8)	43(5)	136(10)	24(6)	89(8)	16(5)
C(14)	69(7)	44(5)	86(8)	15(6)	61(7)	8(5)
C(15)	77(7)	106(7)	140(9)	61(7)	63(7)	70(6)
C(16)	67(7)	50(5)	63(6)	16(5)	40(6)	21(5)
C(17)	34(5)	40(5)	40(5)	9(4)	20(4)	15(4)
C(18)	36(5)	44(5)	51(6)	27(5)	22(4)	19(4)
C(19)	57(6)	51(5)	70(6)	31(5)	35(5)	20(4)
C(20)	59(6)	74(7)	79(7)	52(6)	29(6)	20(5)
C(21)	67(7)	97(8)	76(8)	60(7)	30(6)	23(6)
C(22)	51(6)	87(6)	46(6)	32(5)	27(5)	18(5)
C(23)	33(5)	42(5)	52(6)	14(5)	19(5)	10(4)
C(24)	65(6)	56(5)	60(6)	0(5)	22(5)	2(5)
C(25)	29(5)	49(5)	59(6)	21(4)	25(5)	11(4)
C(26)	48(6)	52(5)	53(6)	21(5)	27(5)	13(5)
N(1)	68(6)	54(4)	93(7)	20(5)	52(6)	19(4)
N(2)	46(4)	51(4)	42(5)	9(4)	21(4)	13(3)
N(3)	43(5)	80(5)	83(6)	22(4)	20(5)	-10(4)

Br(1)	129(1)	110(1)	151(1)	94(1)	82(1)	38(1)

Table 5. Hydrogen coordinates (x 104) and isotropic displacement parameters (Å2x 103)

for ch18209.

	x	y	z	U(eq)
H(2)	6140	4311	2952	72
H(3)	6095	5849	1950	57
H(5)	10074	5282	1701	77
H(6)	10042	3723	2655	93
H(10)	9032	8362	3894	77
H(11)	8683	9778	5641	108
H(12)	6562	10679	5276	108
H(13)	4777	10287	3240	93
H(15A)	3259	8670	-543	140
H(15B)	3669	9907	656	140
H(15C)	2766	8633	624	140
H(16)	5331	7359	-505	67
H(19)	8376	8579	-634	63
H(20)	8169	8973	-2528	76
H(21)	7288	7344	-4464	86
H(22)	6542	5256	-4565	68
H(24A)	5238	3194	-3919	98
H(24B)	6324	2642	-2938	98
H(24C)	6895	3172	-3874	98
H(25)	7016	4195	-691	51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SOLVENT CDCl3
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FIDRES 0.366798 Hz
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RG 512
DW 41.600 usec
DE 6.50 usec
TE 296.0 K
D1 2.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
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PL1 0.00 dB
SFO1 598.4029920 MHz
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SSB 0
LB 0.00 Hz
GB 0
PC 1.00
1D NMR plot parameters
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CY 10.00 cm
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F1 5984.00 Hz
F2P -0.500 ppm
F2 -299.20 Hz
PPMCM 0.52500 ppm/cm
HZCM 314.16000 Hz/cm
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7.44949
7.43564
7.43441
7.38041
7.36933
7.36565
7.26575
7.26039
7.24003
7.18538
7.13407
7.01571
7.01202
7.00093
6.63740
6.63632
6.63200
6.63089
3.98098
3.97004
3.95914
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1.82588
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1.07494
1.06256
1.05017
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Integral
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4
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PROCNO                1

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SOLVENT           CDCl3
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DS                    0
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FIDRES         1.374666 Hz
AQ            0.3637748 sec
RG                 4096
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DE                6.50 usec
TE               296.2 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        150.4843515 MHz

======== CHANNEL f2 ========
CPDPRG2         waltz16
NUC2                1H
PCPD2             92.00 usec
PL2              120.00 dB
PL12               9.00 dB
PL13              14.00 dB
SFO2        598.4029920 MHz

F2 - Processing parameters
SI                 65536
SF          150.4678043 MHz
WDW                   EM
SSB                    0
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GB                     0
PC                 1.00

1D NMR plot parameters
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CY                 4.00 cm
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F2               0.00 Hz
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HZCM         1504.67798 Hz/cm
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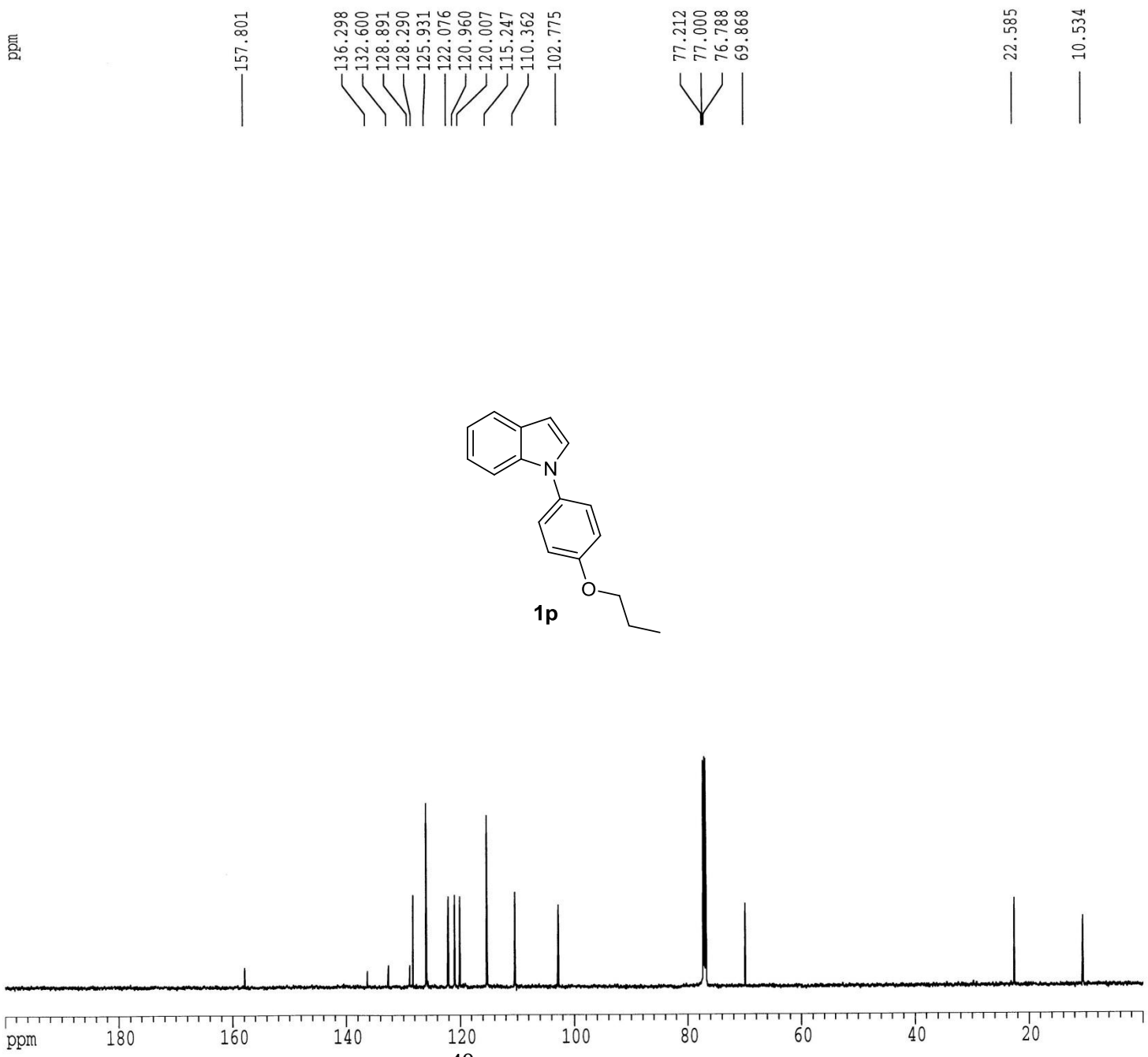

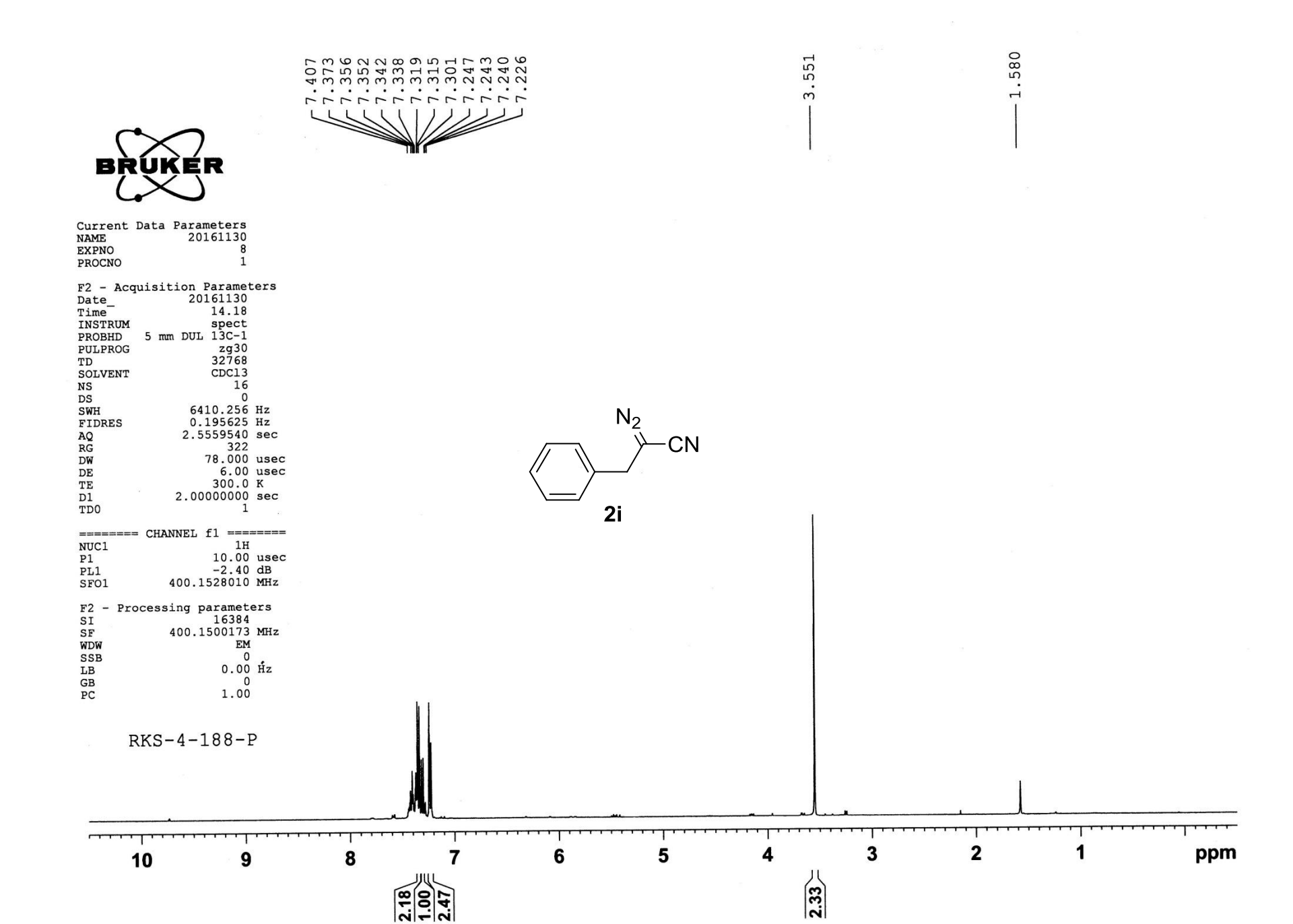
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7.240
7.226
3.551
1.580
BRUKER
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EXPNO 8
PROCNO 1
F2 - Acquisition Parameters
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PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 6410.256 Hz
FIDRES 0.195625 Hz
AQ 2.5559540 sec
RG 322
DW 78.000 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
TD0 1
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NUC1 1H
P1 10.00 usec
PL1 -2.40 dB
SFO1 400.1528010 MHz
F2 - Processing parameters
SI 16384
SF 400.1500173 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
N2
CN
2i
RKS-4-188-P
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8
7
6
5
4
3
2
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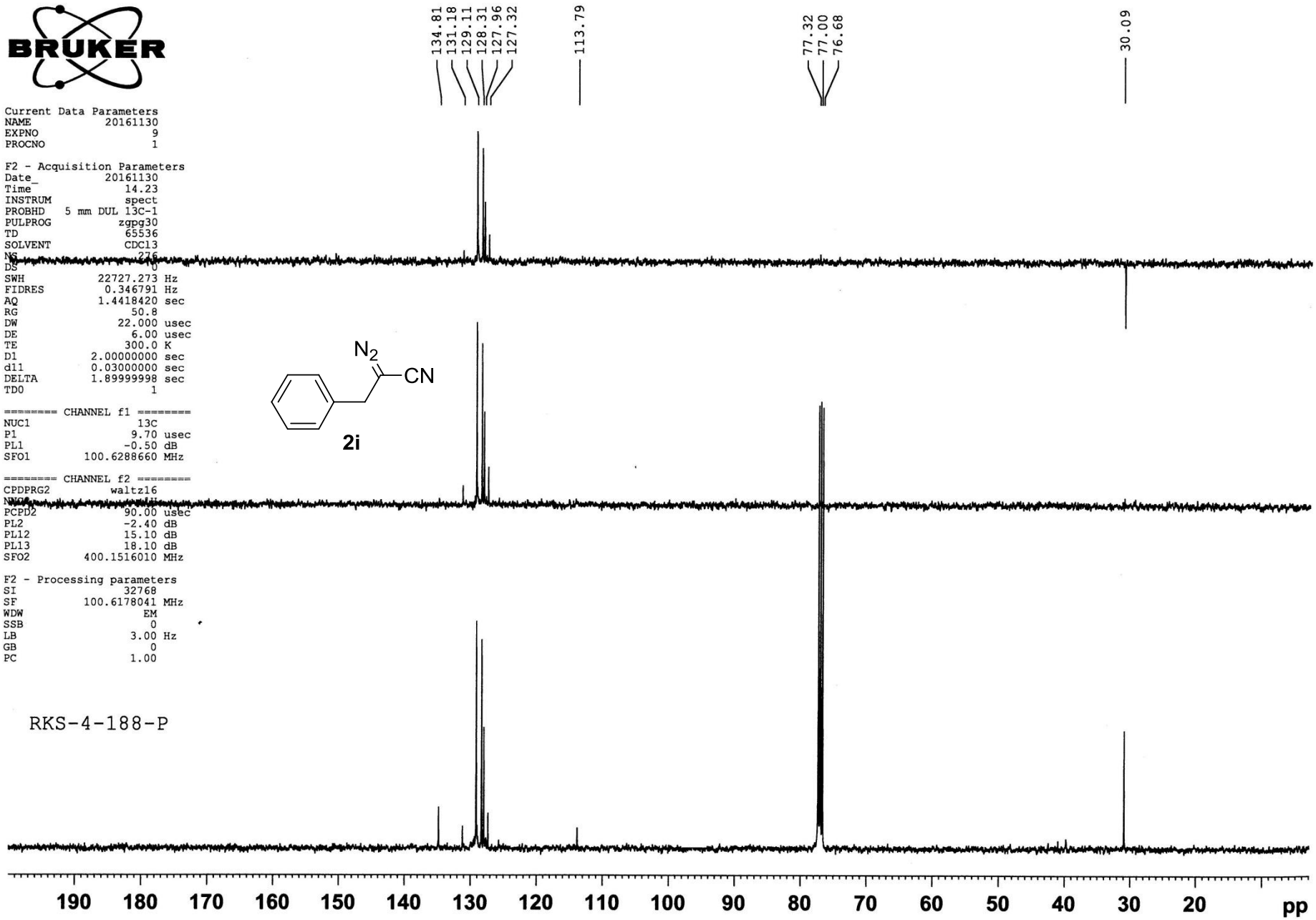
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EXPNO 9
PROCNO 1
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Time 14.23
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PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 276
DS 4
SWH 22727.273 Hz
FIDRES 0.346791 Hz
AQ 1.4418420 sec
RG 50.8
DW 22.000 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
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NUC1 13C
P1 9.70 usec
PL1 -0.50 dB
SFO1 100.6288660 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
PCPD2 90.00 usec
PL2 -2.40 dB
PL12 15.10 dB
PL13 18.10 dB
SFO2 400.1516010 MHz
F2 - Processing parameters
SI 32768
SF 100.6178041 MHz
WDW EM
SSB 0
LB 3.00 Hz
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N2
CN
2i
RKS-4-188-P
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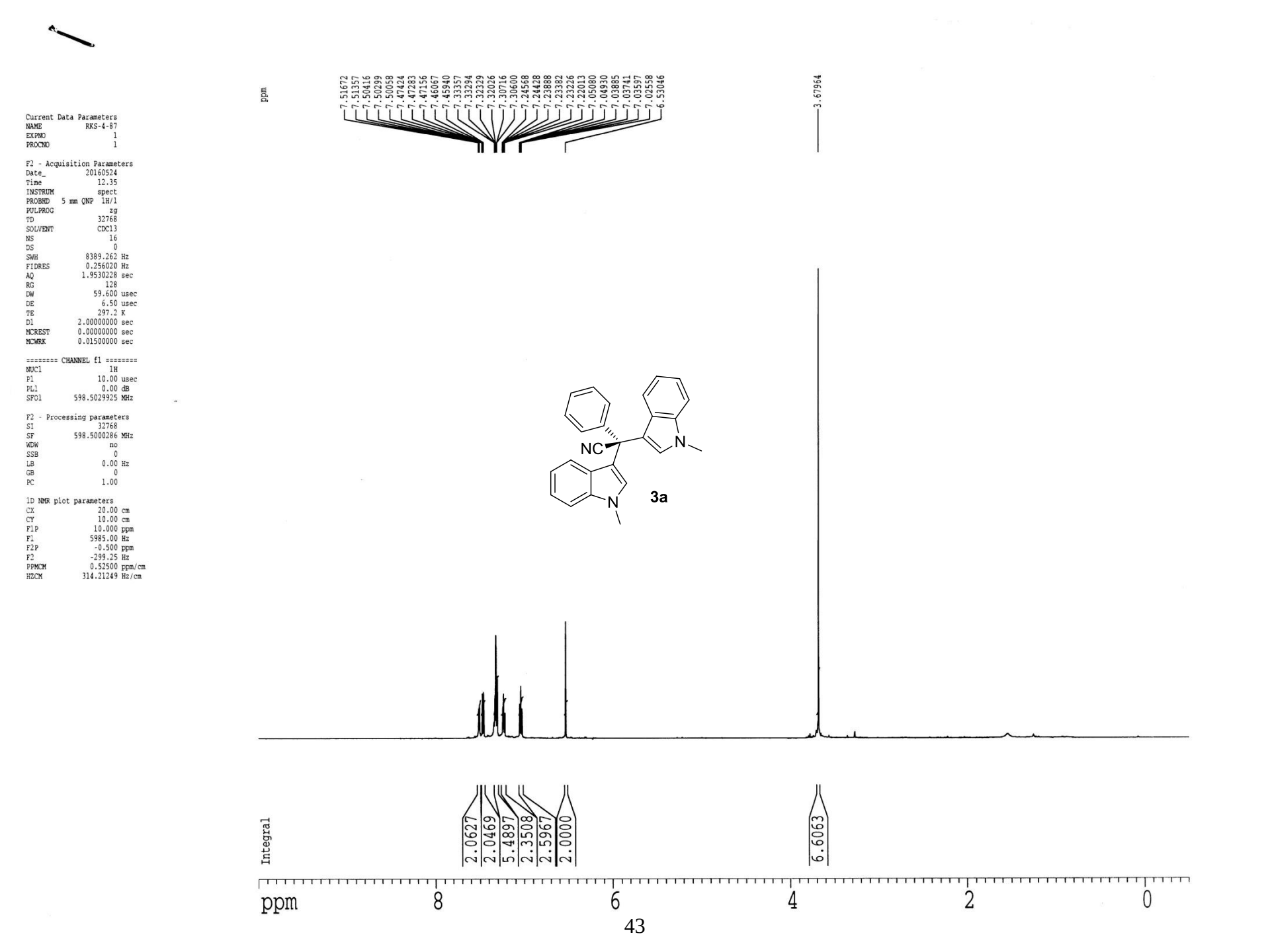
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PULPROG zg
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 8389.262 Hz
FIDRES 0.256020 Hz
AQ 1.9530228 sec
RG 128
DW 59.600 usec
DE 6.50 usec
TE 297.2 K
D1 2.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
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NUC1 1H
P1 10.00 usec
PL1 0.00 dB
SFO1 598.5029925 MHz
F2 - Processing parameters
SI 32768
SF 598.5000286 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
1D NMR plot parameters
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CY 10.00 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
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7.51357
7.50416
7.50299
7.50058
7.47424
7.47283
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7.45940
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N
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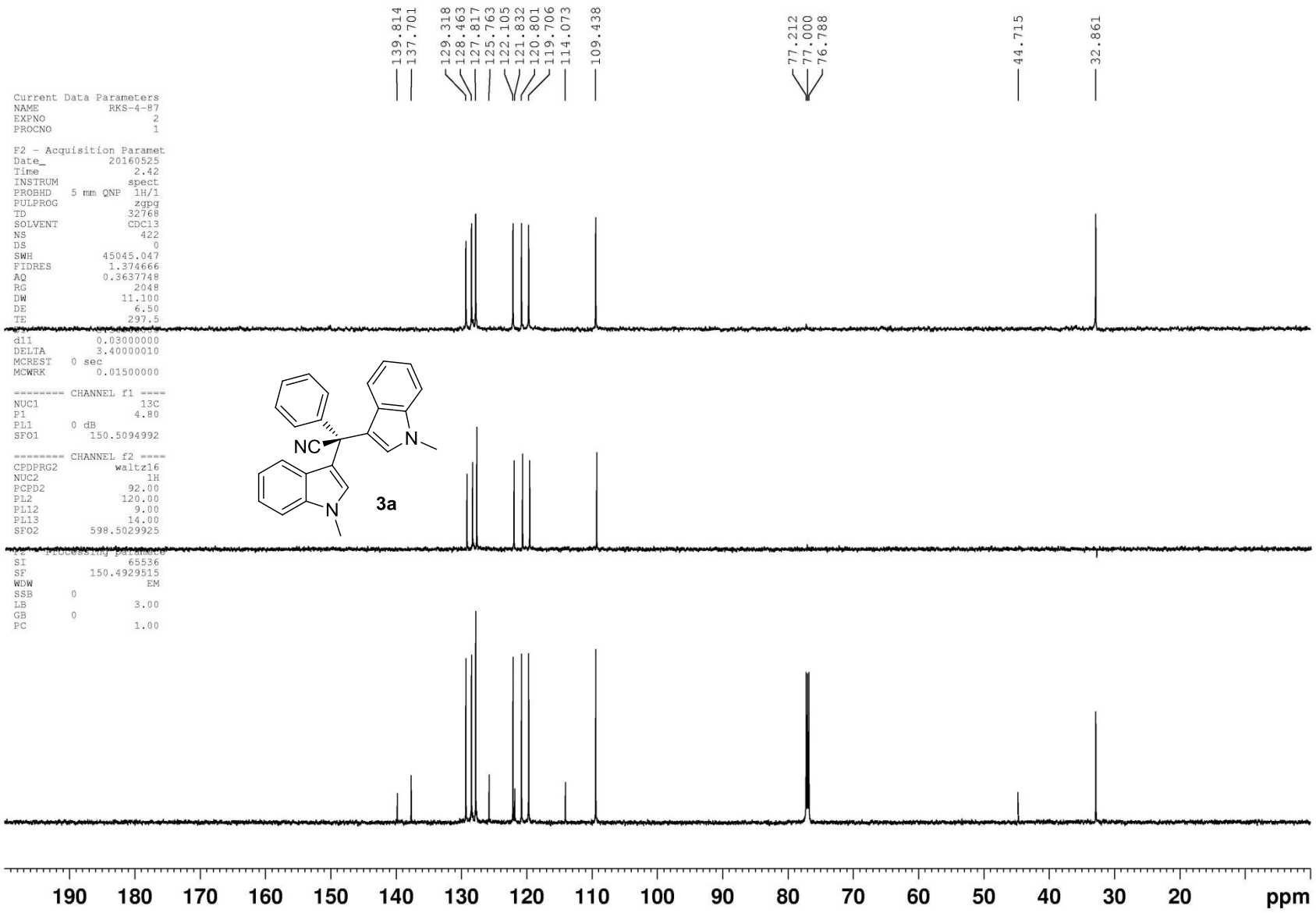
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PROCNO 1
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Time 2.42
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PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 422
DS 0
SWH 45045.047
FIDRES 1.374666
AQ 0.3637748
RG 2048
DW 11.100
DE 6.50
TE 297.5
d11 0.03000000
DELTA 3.40000010
MCREST 0 sec
MCWRK 0.01500000
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NUC1 13C
P1 4.80
PL1 0 dB
SFO1 150.5094992
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CPDPRG2 waltz16
NUC2 1H
PCPD2 92.00
PL2 120.00
PL12 9.00
PL13 14.00
SFO2 598.5029925
F2 - Processing parameters
SI 65536
SF 150.4929515
WDW EM
SSB 0
LB 3.00
GB 0
PC 1.00
NC
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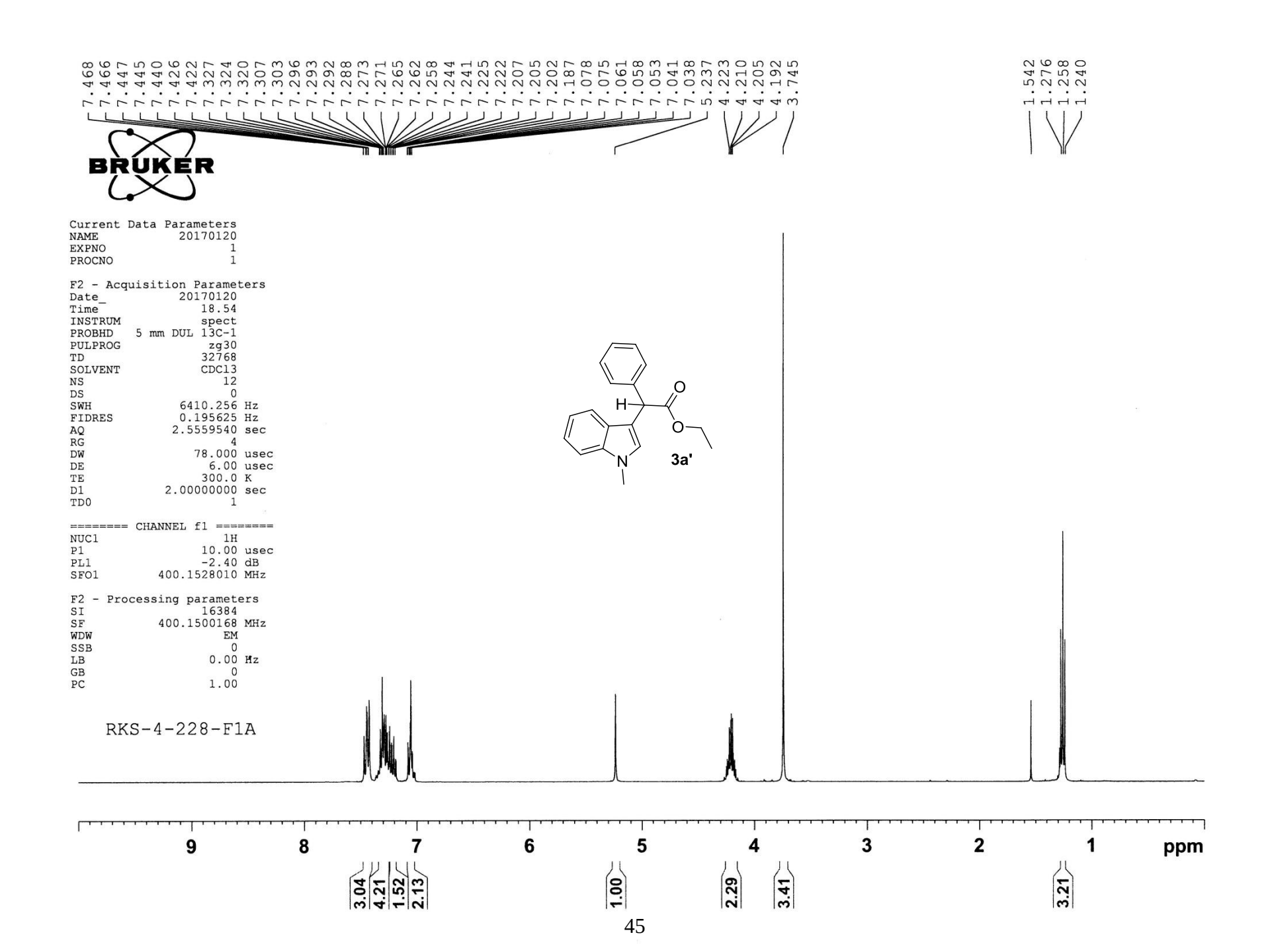
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7.262
7.258
7.244
7.241
7.225
7.222
7.207
7.205
7.202
7.187
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7.075
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7.058
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BRUKER
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PULPROG zg30
TD 32768
SOLVENT CDCl3
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FIDRES 0.195625 Hz
AQ 2.5559540 sec
RG 4
DW 78.000 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
TD0 1
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NUC1 1H
P1 10.00 usec
PL1 -2.40 dB
SFO1 400.1528010 MHz
F2 - Processing parameters
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SSB 0
LB 0.00 Hz
GB 0
PC 1.00
O
H
O
N
3a'
RKS-4-228-F1A
9
8
7
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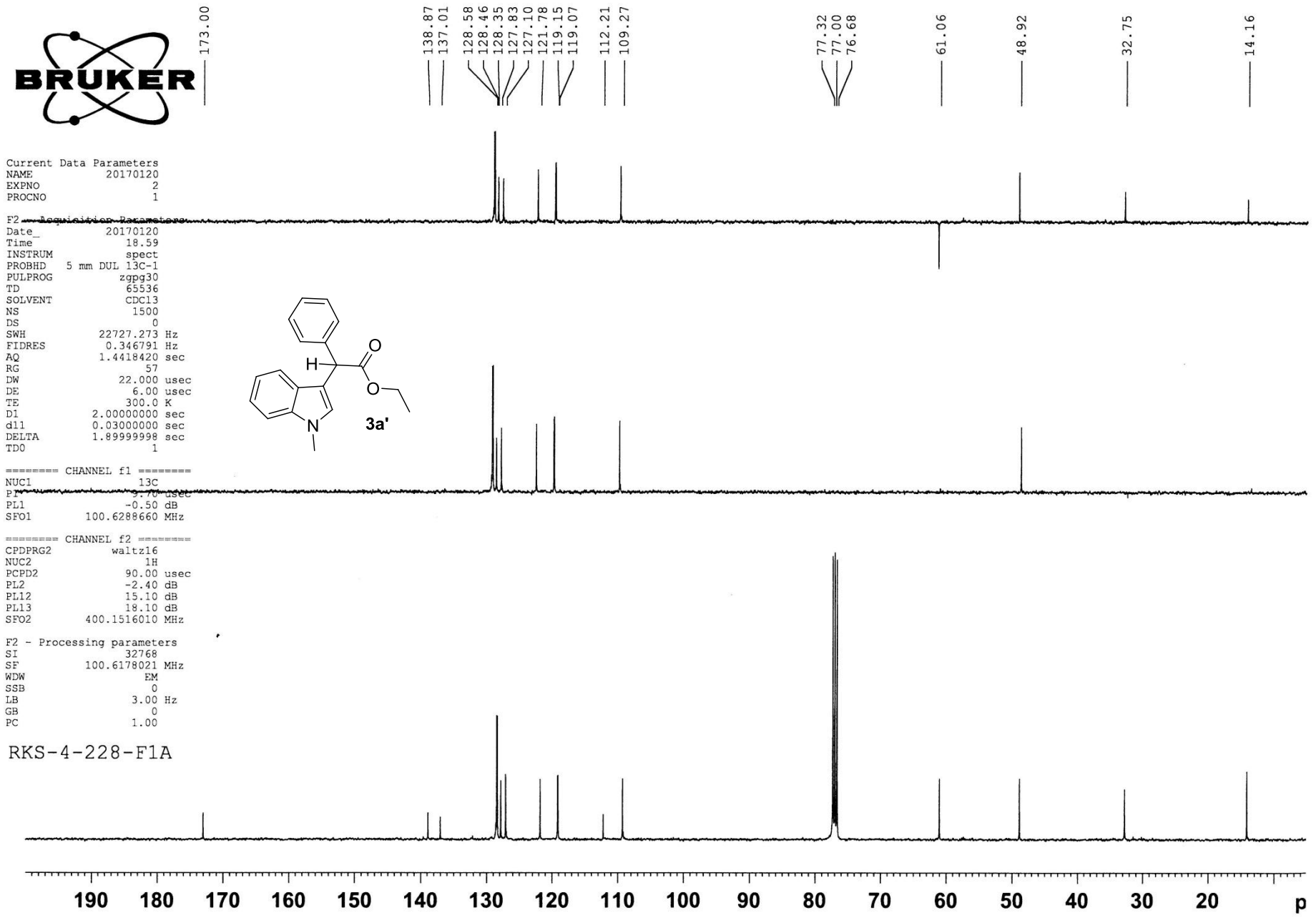
BRUKER
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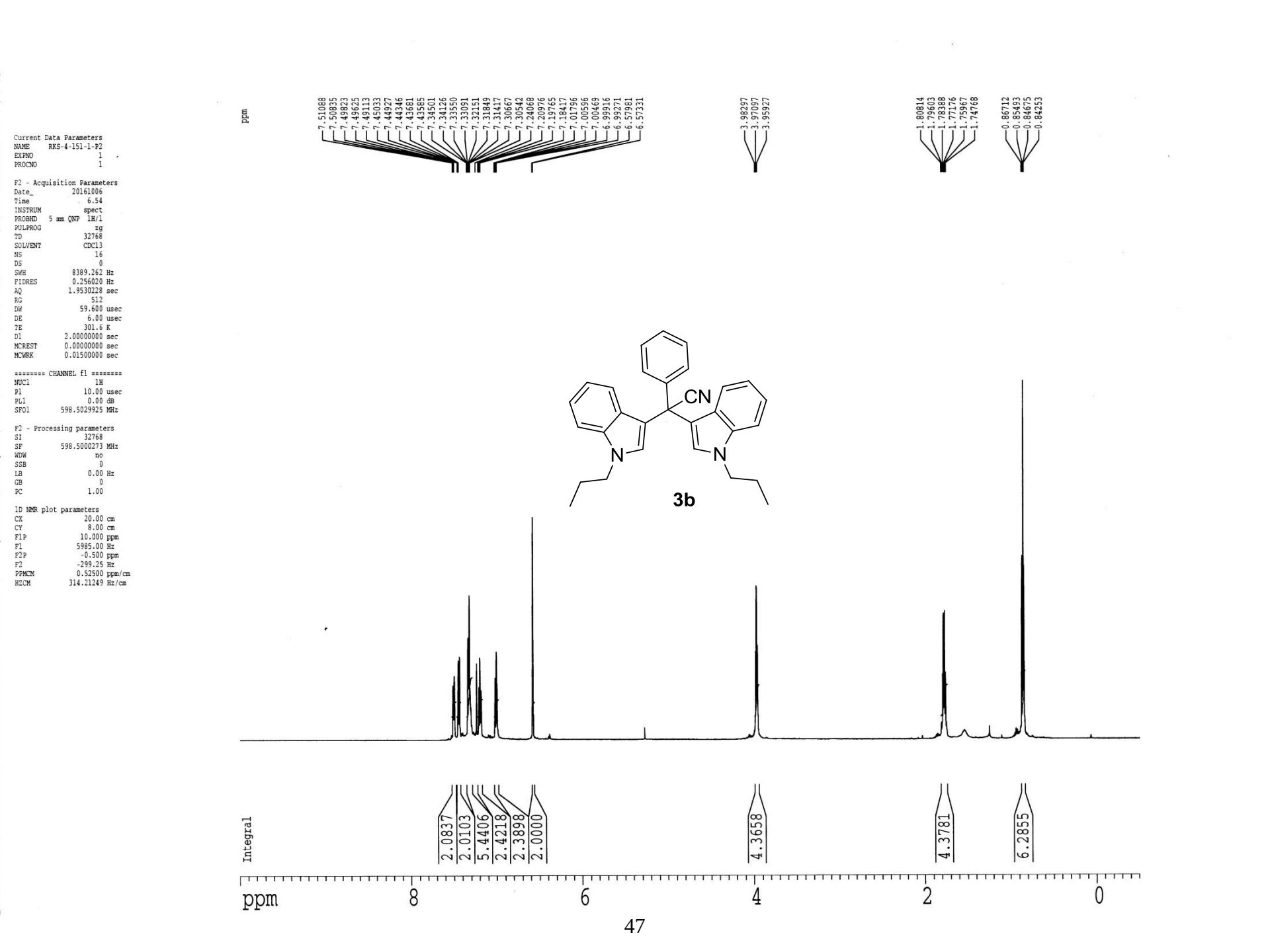
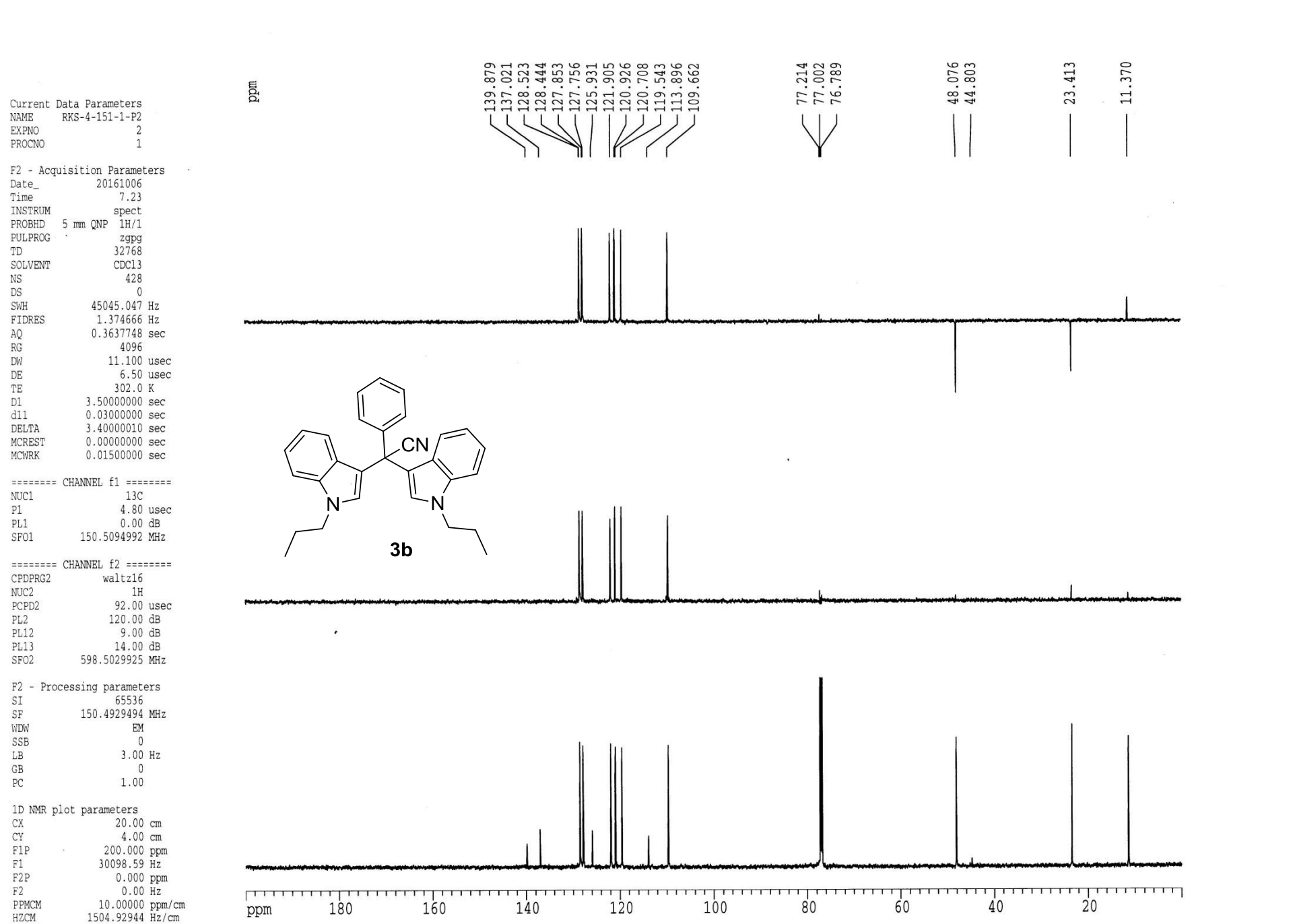
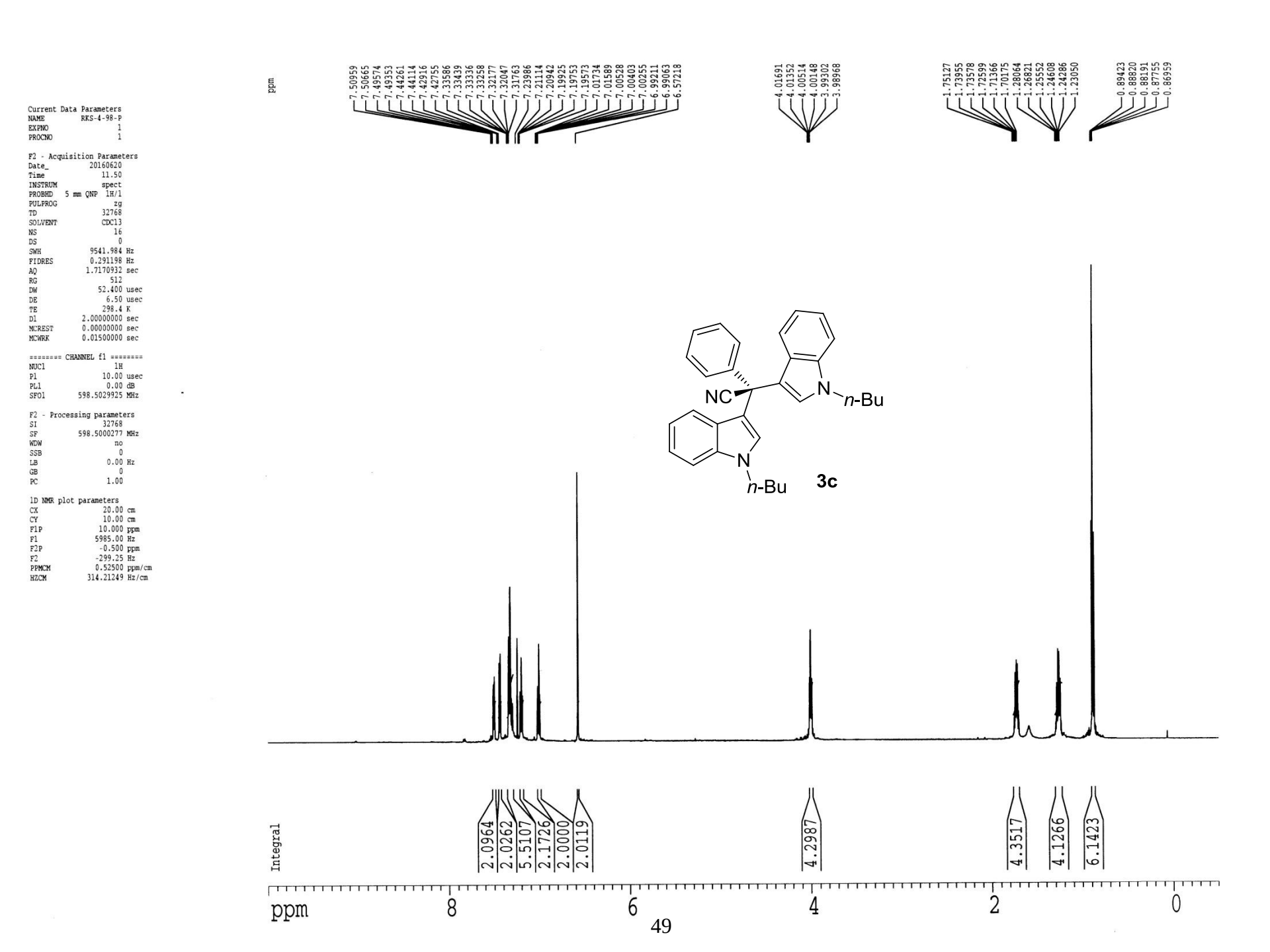
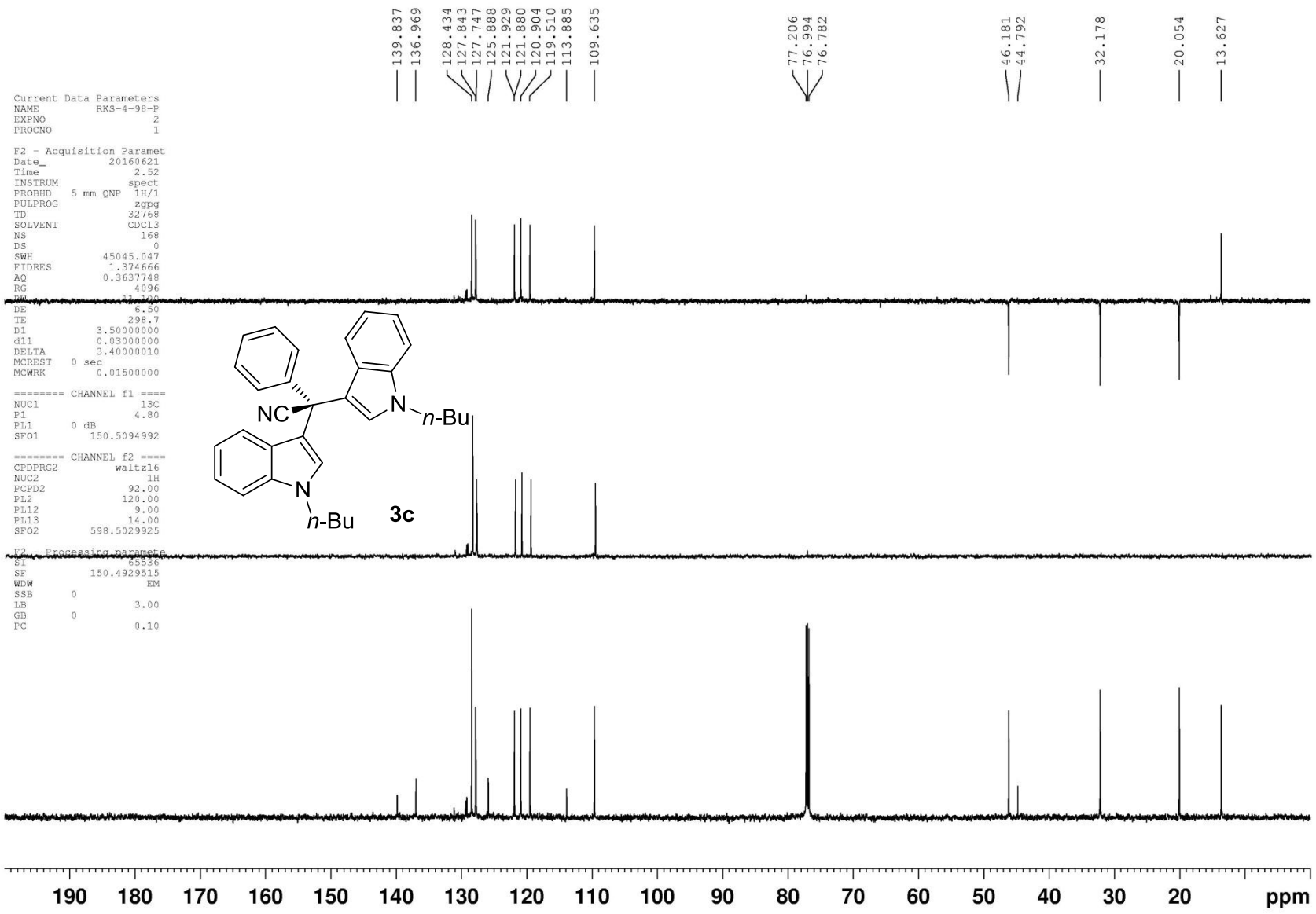
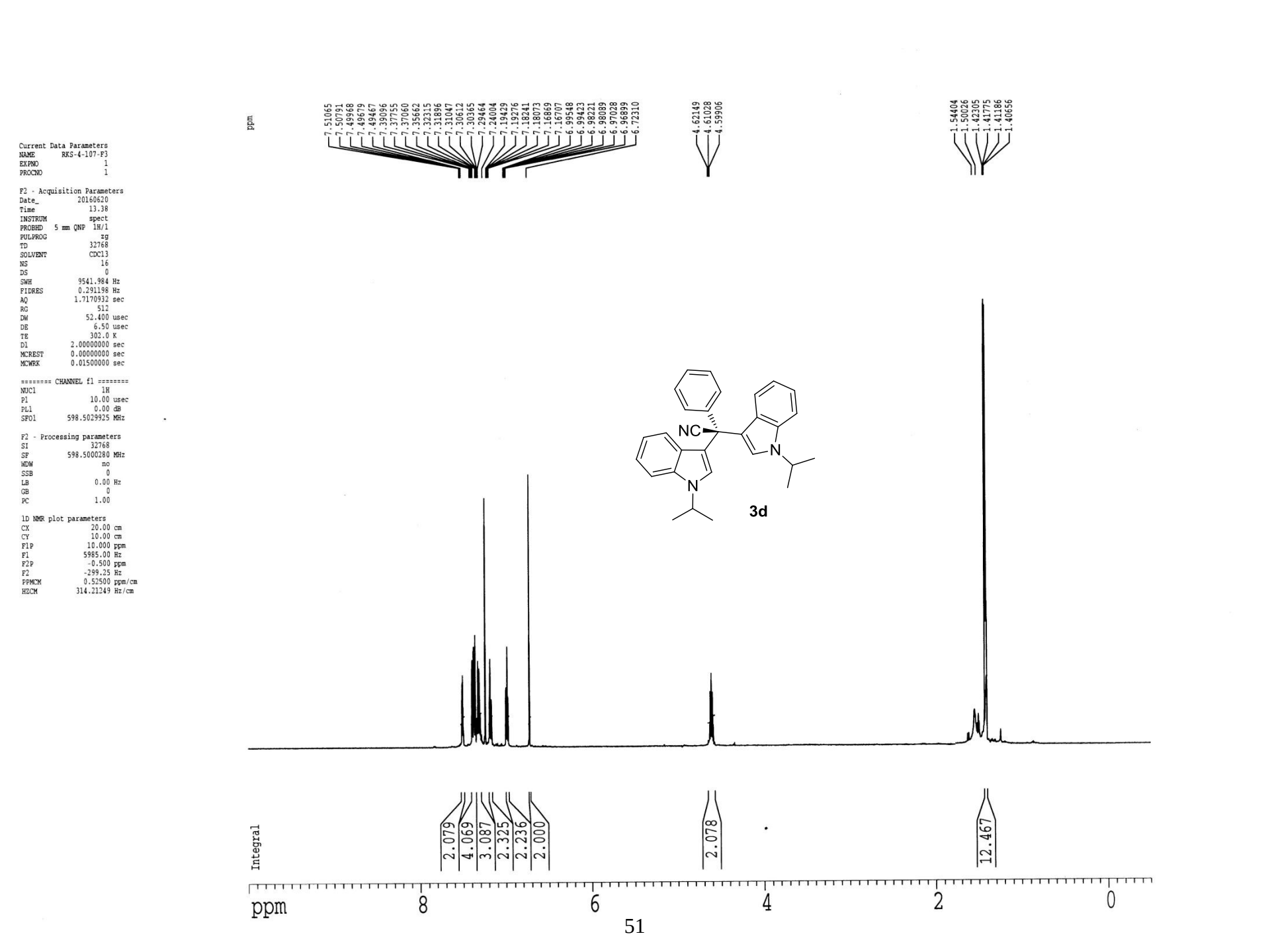
128.35
127.83
127.10
121.78
119.15
119.07
112.21
109.27
77.32
77.00
76.68
61.06
48.92
32.75
14.16
Current Data Parameters
NAME 20170120
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170120
Time 18.59
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1500
DS 0
SWH 22727.273 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
TD0 1
======== CHANNEL f1 ========
NUC1 13C
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
SFO2 400.1516010 MHz
F2 - Processing parameters
SI 32768
SF 100.6178021 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
RKS-4-228-F1A
O
H
O
N
3a'
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
p

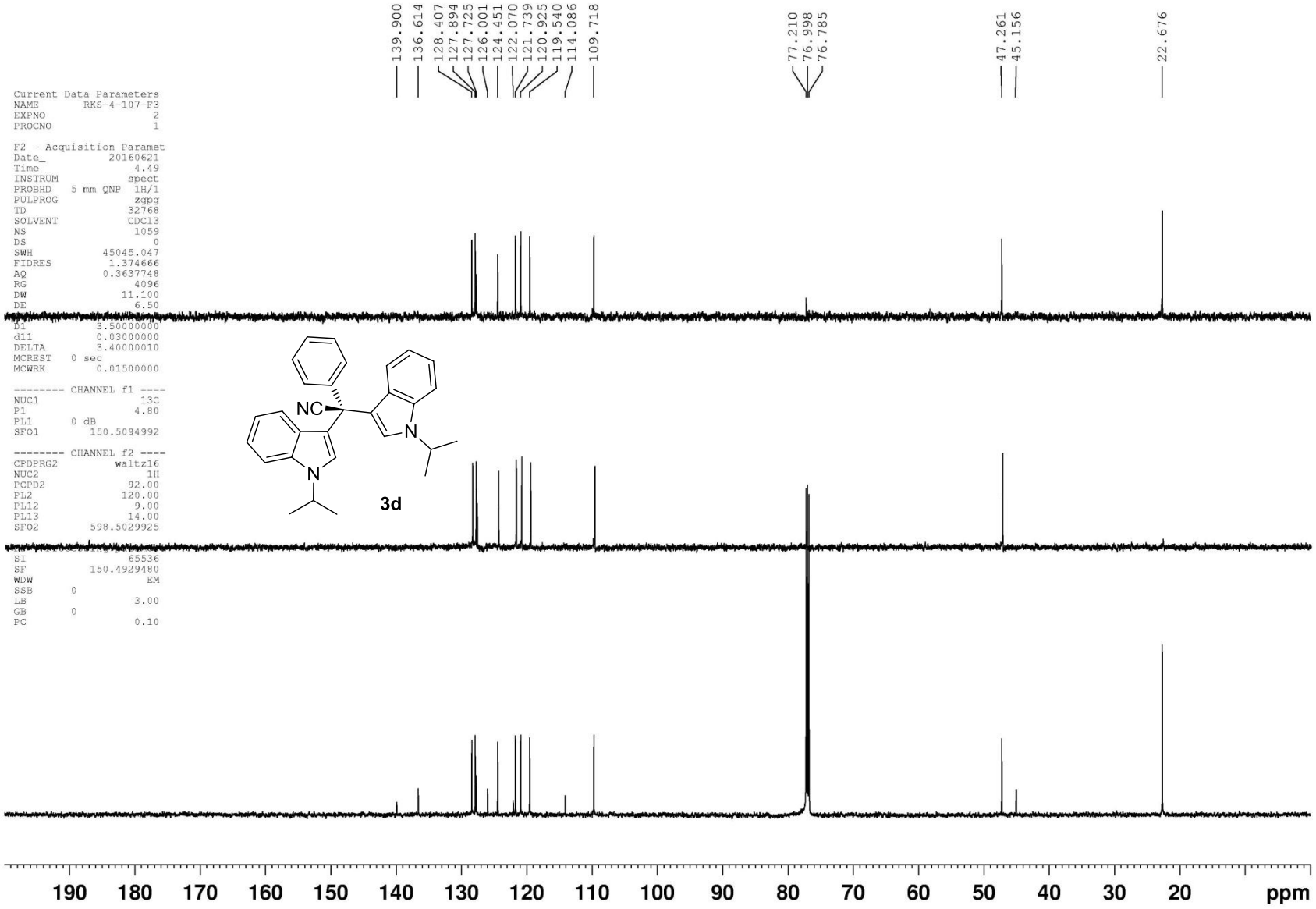

Current Data Parameters
NAME RKS-4-151-1-P2
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20161006
Time 6.54
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 8389.262 Hz
FIDRES 0.256020 Hz
AQ 1.9530228 sec
RG 512
DW 59.600 usec
DE 6.00 usec
TE 301.6 K
D1 2.00000000 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 598.5000273 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 20.00 cm
CY 8.00 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
7.51088
7.50835
7.49823
7.49625
7.49113
7.45033
7.44927
7.44346
7.43681
7.43585
7.34501
7.34126
7.33550
7.33091
7.32151
7.31849
7.31417
7.30667
7.30542
7.24068
7.20976
7.19765
7.18417
7.01796
7.00596
7.00469
6.99916
6.99271
6.57981
6.57331
3.98297
3.97097
3.95927
1.80814
1.79603
1.78388
1.77176
1.75967
1.74768
0.86712
0.85493
0.84675
0.84253
CN
N
N
3b
Integral
2.0837
2.0103
5.4406
2.4218
2.3898
2.0000
4.3658
4.3781
6.2855
ppm
8
6
4
2
0

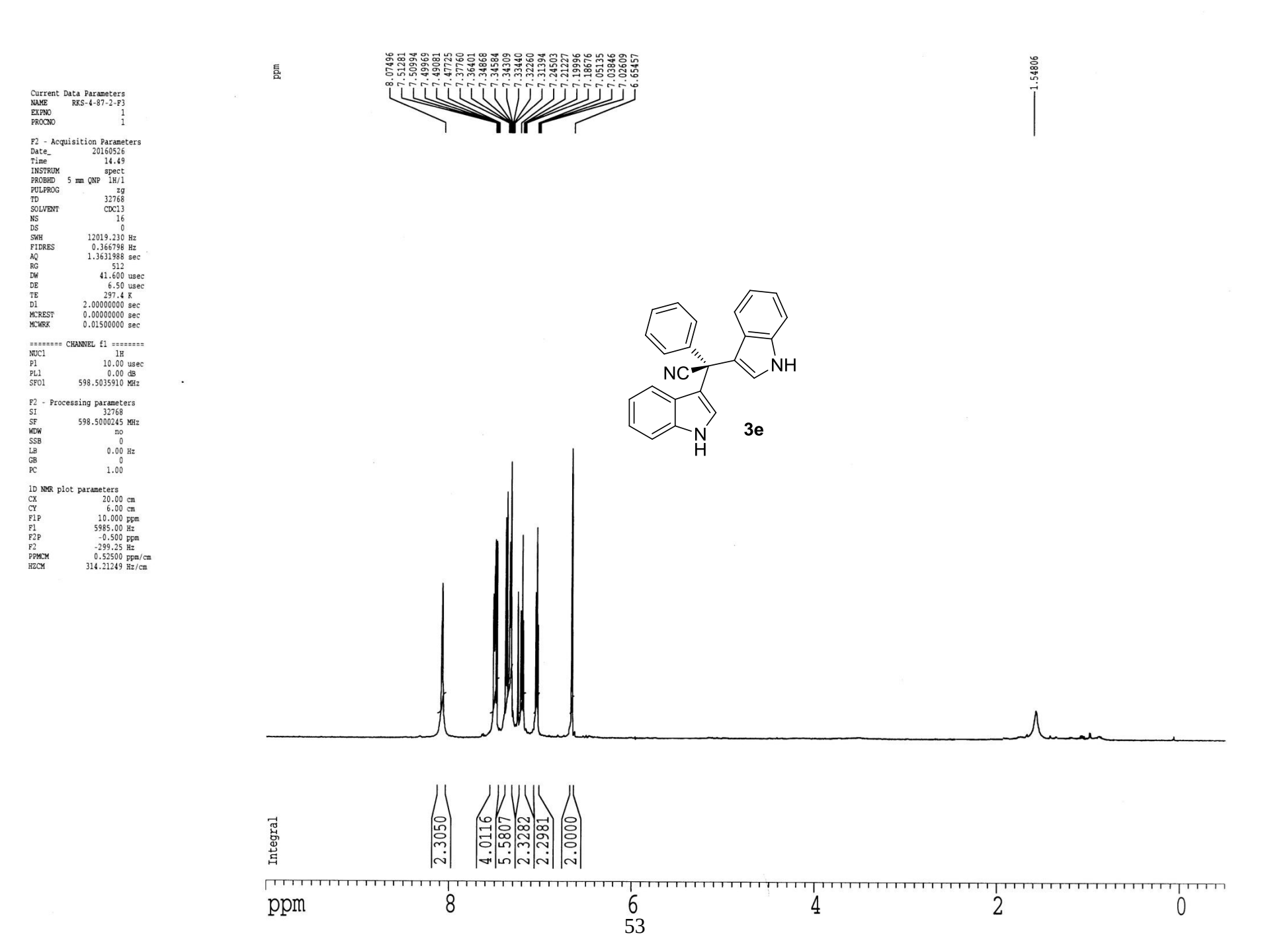

Current Data Parameters
NAME RKS-4-151-1-P2
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20161006
Time 7.23
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 428
DS 0
SWH 45045.047 Hz
FIDRES 1.374666 Hz
AQ 0.3637748 sec
RG 4096
DW 11.100 usec
DE 6.50 usec
TE 302.0 K
D1 3.50000000 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 150.4929494 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 20.00 cm
CY 4.00 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
139.879
137.021
128.523
128.444
127.853
127.756
125.931
121.905
120.926
120.708
119.543
113.896
109.662
77.214
77.002
76.789
48.076
44.803
23.413
11.370
CN
N
N
3b
ppm
180
160
140
120
100
80
60
40
20


Current Data Parameters
NAME RKS-4-98-P
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20160620
Time 11.50
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 298.4 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 598.5000277 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 20.00 cm
CY 10.00 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
7.50959
7.50665
7.49574
7.49353
7.44261
7.44114
7.42916
7.42755
7.33586
7.33439
7.33336
7.33258
7.32177
7.32047
7.31763
7.23986
7.21114
7.20942
7.19925
7.19753
7.19573
7.01734
7.01589
7.00528
7.00403
7.00255
6.99211
6.99063
6.57218
4.01691
4.01352
4.00514
4.00148
3.99302
3.98968
1.75127
1.73955
1.73578
1.72599
1.71366
1.70175
1.28064
1.26821
1.25552
1.24608
1.24286
1.23050
0.89423
0.88820
0.88191
0.87755
0.86959
NC
N
n-Bu
N
n-Bu
3c
Integral
2.0964
2.0262
5.5107
2.1726
2.0000
2.0119
4.2987
4.3517
4.1266
6.1423
ppm
8
6
4
2
0


139.837
136.969
128.434
127.843
127.747
125.888
121.929
121.880
120.904
119.510
113.885
109.635
77.206
76.994
76.782
46.181
44.792
32.178
20.054
13.627
Current Data Parameters
NAME RKS-4-98-P
EXPNO 2
PROCNO 1
F2 - Acquisition Paramet
Date_ 20160621
Time 2.52
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 168
DS 0
SWH 45045.047
FIDRES 1.374666
AQ 0.3637748
RG 4096
DW 11.100
DE 6.50
TE 298.7
D1 3.50000000
d11 0.03000000
DELTA 3.40000010
MCREST 0 sec
MCWRK 0.01500000
======== CHANNEL f1 ====
NUC1 13C
P1 4.80
PL1 0 dB
SFO1 150.5094992
======== CHANNEL f2 ====
CPDPRG2 waltz16
NUC2 1H
PCPD2 92.00
PL2 120.00
PL12 9.00
PL13 14.00
SFO2 598.5029925
F2 - Processing paramete
SI 65536
SF 150.4929515
WDW EM
SSB 0
LB 3.00
GB 0
PC 0.10
NC
N
n-Bu
N
n-Bu
3c
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm


Current Data Parameters
NAME RKS-4-107-F3
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20160620
Time 13.38
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 302.0 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 598.5000280 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 20.00 cm
CY 10.00 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
7.51065
7.50791
7.49968
7.49679
7.49467
7.39096
7.37755
7.37060
7.35662
7.32315
7.31896
7.31047
7.30612
7.30365
7.29464
7.24004
7.19429
7.19276
7.18241
7.18073
7.16869
7.16707
6.99548
6.99423
6.98221
6.98089
6.97028
6.96899
6.72310
4.62149
4.61028
4.59906
1.54404
1.50026
1.42305
1.41775
1.41186
1.40656
NC
N
N
3d
Integral
2.079
4.069
3.087
2.325
2.236
2.000
2.078
12.467
ppm
8
6
4
2
0


139.900
136.614
128.407
127.894
127.725
126.001
124.451
122.070
121.739
120.925
119.540
114.086
109.718
77.210
76.998
76.785
47.261
45.156
22.676
Current Data Parameters
NAME RKS-4-107-F3
EXPNO 2
PROCNO 1
F2 - Acquisition Paramet
Date_ 20160621
Time 4.49
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDC13
NS 1059
DS 0
SWH 45045.047
FIDRES 1.374666
AQ 0.3637748
RG 4096
DW 11.100
DE 6.50
D1 3.50000000
d11 0.03000000
DELTA 3.40000010
MCREST 0 sec
MCWRK 0.01500000
======== CHANNEL f1 ====
NUC1 13C
P1 4.80
PL1 0 dB
SFO1 150.5094992
======== CHANNEL f2 ====
CPDPRG2 waltz16
NUC2 1H
PCPD2 92.00
PL2 120.00
PL12 9.00
PL13 14.00
SFO2 598.5029925
SI 65536
SF 150.4929480
WDW EM
SSB 0
LB 3.00
GB 0
PC 0.10
NC
N
N
3d
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm


Current Data Parameters
NAME RKS-4-87-2-F3
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20160526
Time 14.49
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 12019.230 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 512
DW 41.600 usec
DE 6.50 usec
TE 297.4 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 598.5035910 MHz
F2 - Processing parameters
SI 32768
SF 598.5000245 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 20.00 cm
CY 6.00 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
8.07496
7.51281
7.50994
7.49969
7.49081
7.47725
7.37760
7.36401
7.34868
7.34584
7.34309
7.33440
7.32260
7.31394
7.24503
7.21227
7.19996
7.18676
7.05135
7.03846
7.02609
6.65457
1.54806
NC
NH
N
H
3e
Integral
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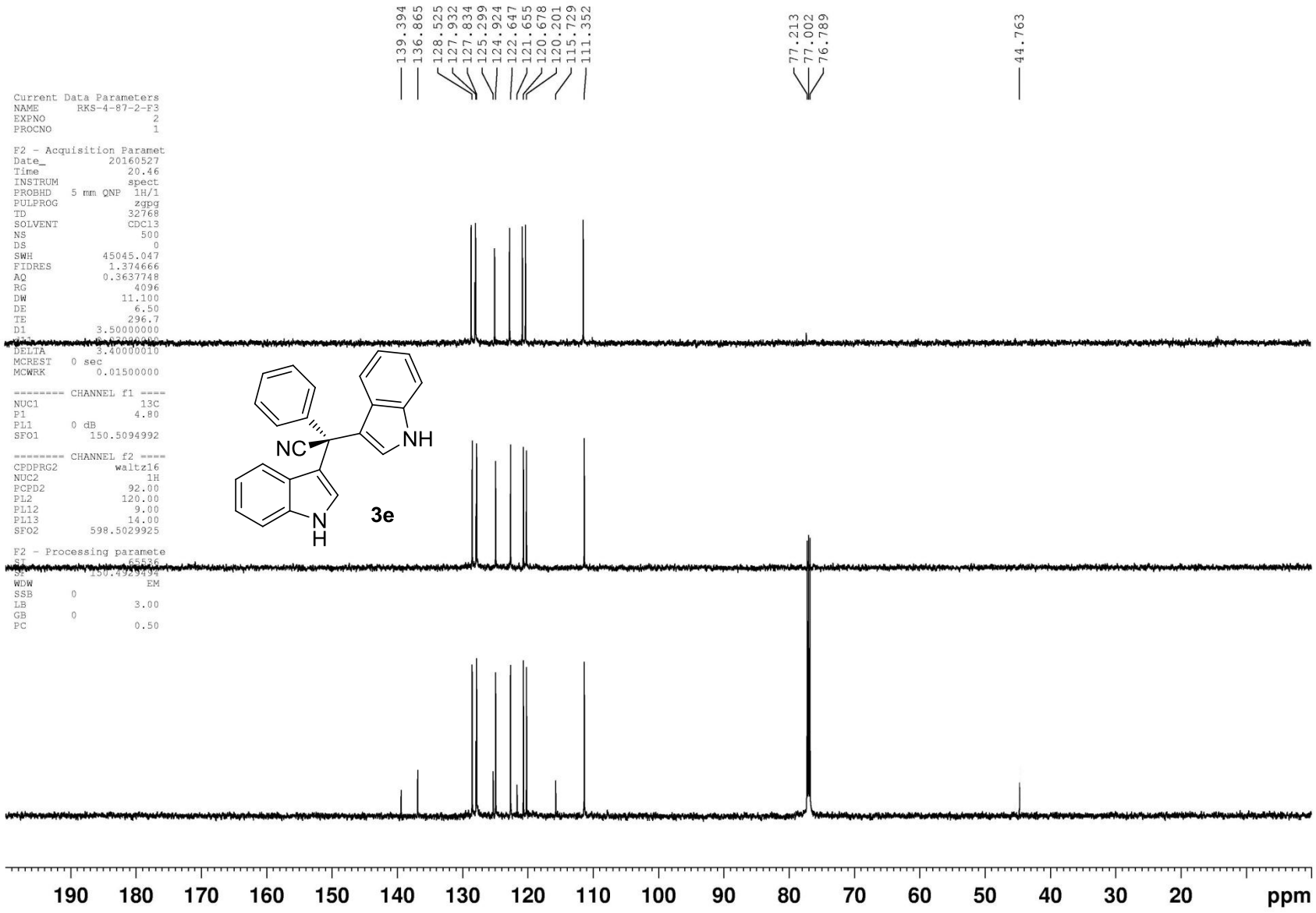
4.0116
5.5807
2.3282
2.2981
2.0000
ppm
8
6
4
2
0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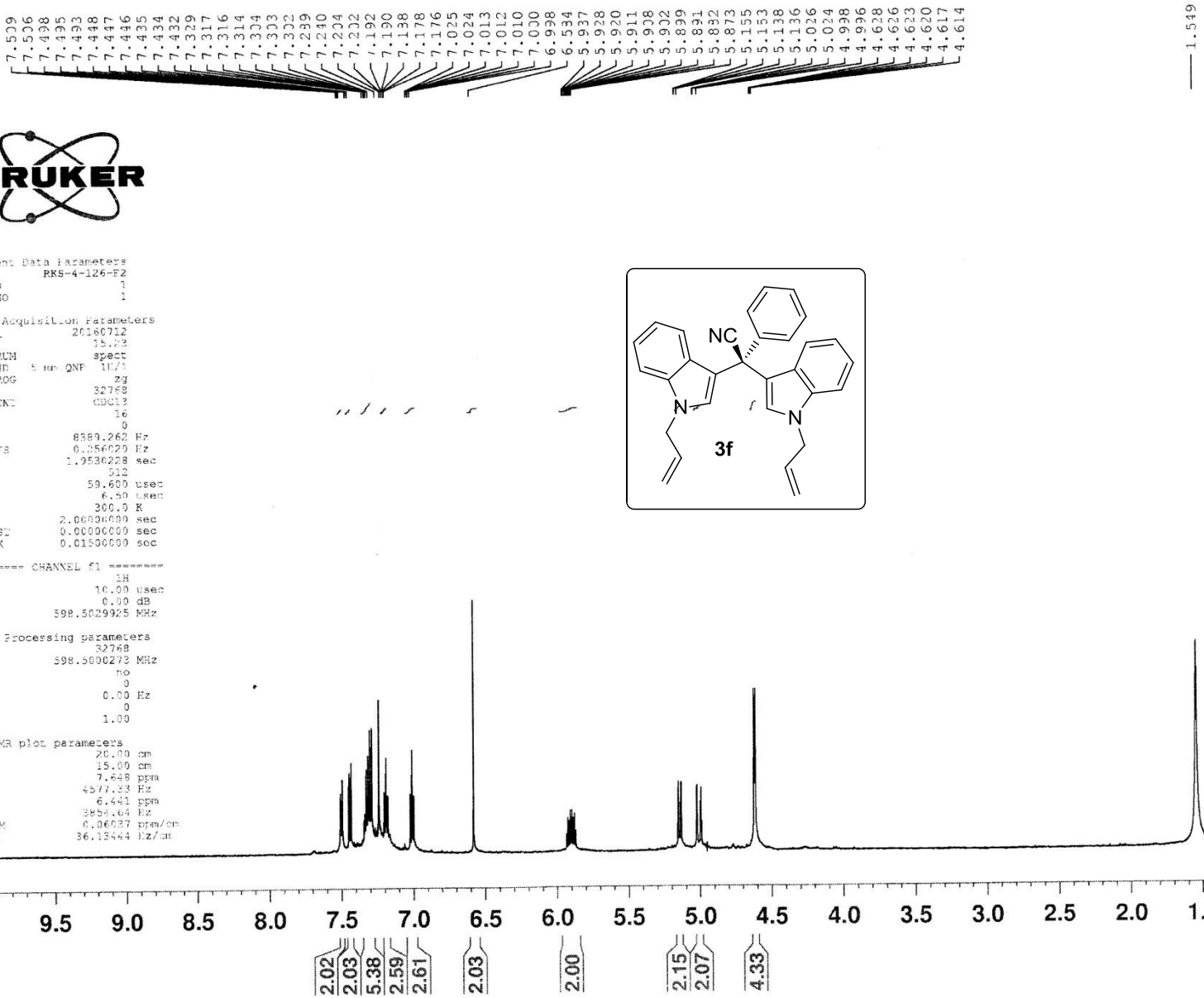
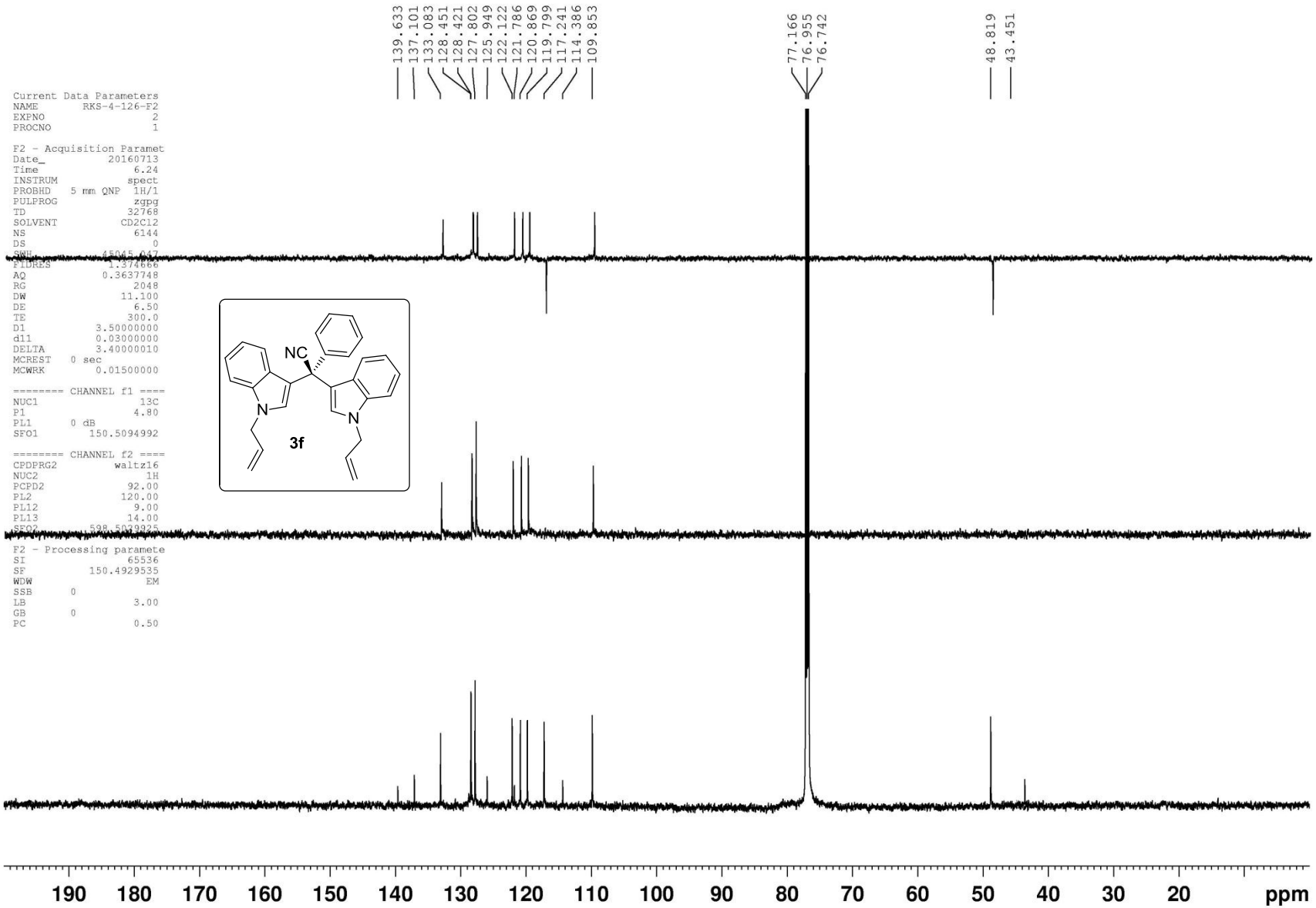
124.924
122.647
121.655
120.678
120.201
115.729
111.352
77.213
77.002
76.789
44.763
Current Data Parameters
NAME RKS-4-87-2-F3
EXPNO 2
PROCNO 1
F2 - Acquisition Paramet
Date_ 20160527
Time 20.46
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 500
DS 0
SWH 45045.047
FIDRES 1.374666
AQ 0.3637748
RG 4096
DW 11.100
DE 6.50
TE 296.7
D1 3.50000000
DELTA 3.40000010
MCREST 0 sec
MCWRK 0.01500000
======== CHANNEL f1 ====
NUC1 13C
P1 4.80
PL1 0 dB
SFO1 150.5094992
======== CHANNEL f2 ====
CPDPRG2 waltz16
NUC2 1H
PCPD2 92.00
PL2 120.00
PL12 9.00
PL13 14.00
SFO2 598.5029925
F2 - Processing paramete
WDW EM
SSB 0
LB 3.00
GB 0
PC 0.50
NC
NH
N
H
3e
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm


7.599
7.596
7.498
7.495
7.493
7.448
7.447
7.446
7.435
7.434
7.432
7.329
7.317
7.316
7.314
7.304
7.303
7.302
7.239
7.240
7.204
7.202
7.192
7.190
7.138
7.178
7.176
7.025
7.024
7.013
7.012
7.010
7.000
6.998
6.534
5.937
5.928
5.920
5.911
5.908
5.902
5.899
5.891
5.832
5.873
5.155
5.153
5.138
5.136
5.026
5.024
4.998
4.996
4.628
4.626
4.623
4.620
4.617
4.614
1.549
BRUKER
Current Data Parameters
NAME RKS-4-126-F2
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20160712
Time 15.23
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 8389.262 Hz
FIDRES 0.256029 Hz
AQ 1.9530228 sec
RG 512
DW 59.600 usec
DE 6.50 usec
TE 300.0 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 598.5000273 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 20.00 cm
CY 15.00 cm
F1P 7.648 ppm
F1 4577.33 Hz
F2P 6.441 ppm
F2 3854.64 Hz
PPMCM 0.06027 ppm/cm
HZCM 36.13444 Hz/cm
NC
N
N
3f
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
2.02
2.03
5.38
2.59
2.61
2.03
2.00
2.15
2.07
4.33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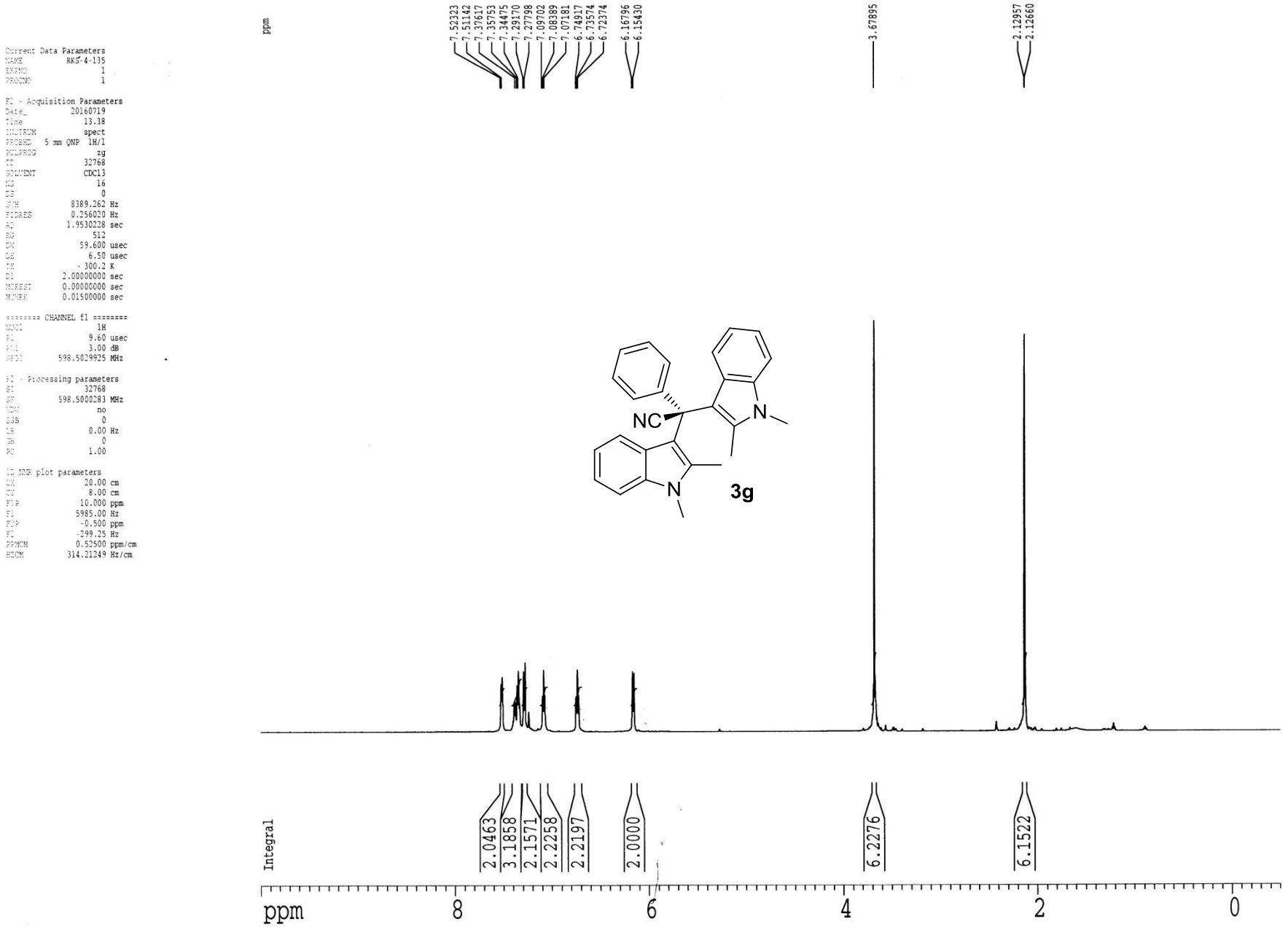
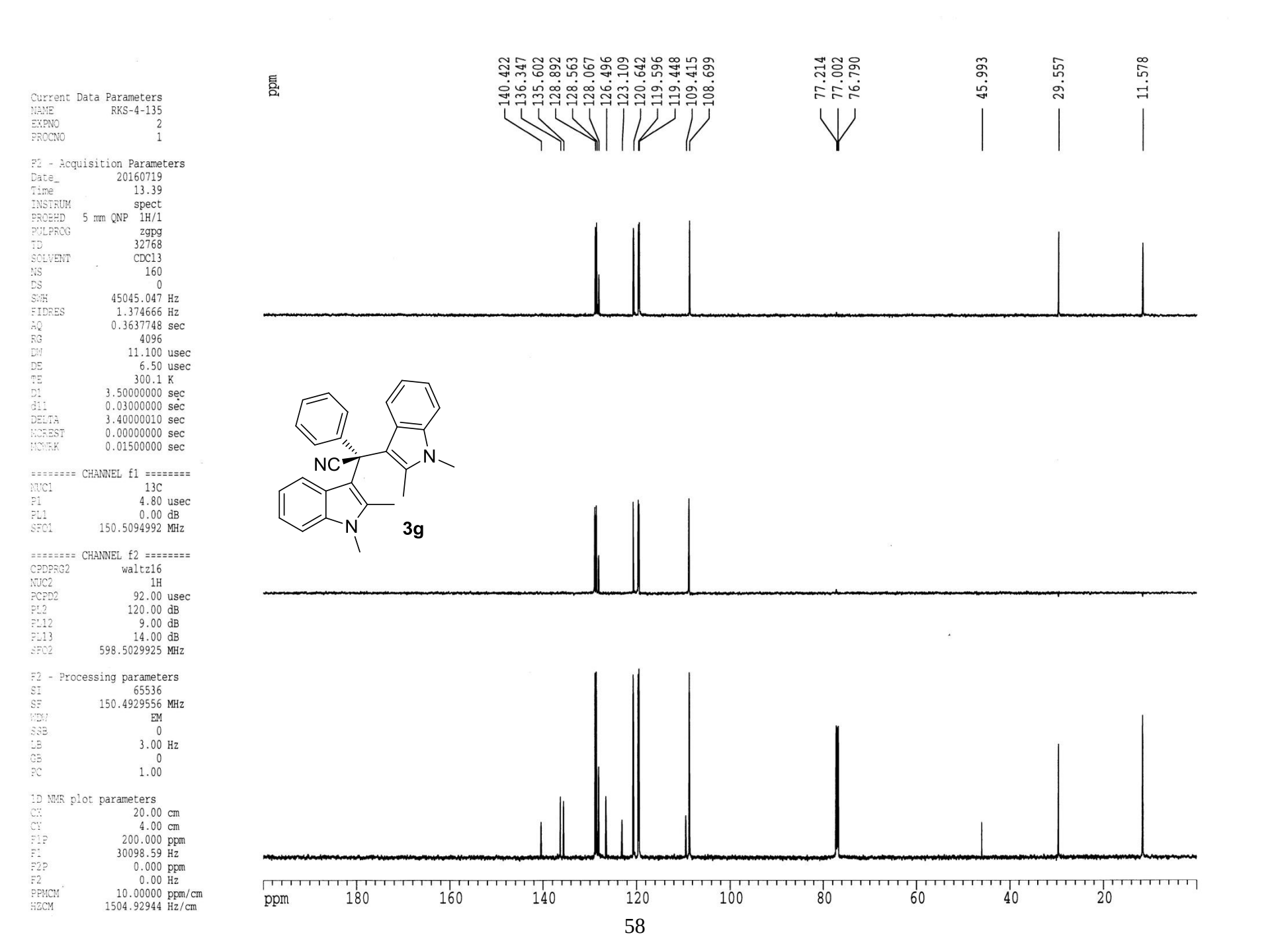
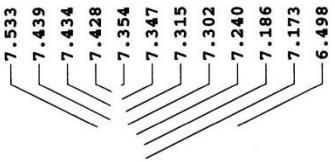
137.101
133.083
128.451
128.421
127.802
125.949
122.122
121.786
120.869
119.799
117.241
114.386
109.853
77.166
76.955
76.742
48.819
43.451
Current Data Parameters
NAME RKS-4-126-F2
EXPNO 2
PROCNO 1
F2 - Acquisition Paramet
Date_ 20160713
Time 6.24
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CD2Cl2
NS 6144
DS 0
SWH 45045.045
FIDRES 1.374666
AQ 0.3637748
RG 2048
DW 11.100
DE 6.50
TE 300.0
D1 3.50000000
d11 0.03000000
DELTA 3.40000010
MCREST 0 sec
MCWRK 0.01500000
======== CHANNEL f1 ====
NUC1 13C
P1 4.80
PL1 0 dB
SFO1 150.5094992
======== CHANNEL f2 ====
CPDPRG2 waltz16
NUC2 1H
PCPD2 92.00
PL2 120.00
PL12 9.00
PL13 14.00
F2 - Processing paramete
SI 65536
SF 150.4929535
WDW EM
SSB 0
LB 3.00
GB 0
PC 0.50
NC
N
N
3f
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm


Current Data Parameters
NAME RKS-4-135
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20160719
Time 13.38
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 300.2 K
D1 2.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 9.60 usec
PL1 3.00 dB
SFO1 598.5029925 MHz
F2 - Processing parameters
SI 32768
SF 598.5000283 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
1C NMR plot parameters
CX 20.00 cm
CY 8.00 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
7.52323
7.51142
7.37617
7.35753
7.34475
7.29170
7.27798
7.09702
7.08389
7.07181
6.74917
6.73574
6.72374
6.16796
6.15430
3.67895
2.12957
2.12660
NC
N
N
3g
Integral
2.0463
3.1858
2.1571
2.2258
2.2197
2.0000
6.2276
6.1522
ppm
8
6
4
2
0

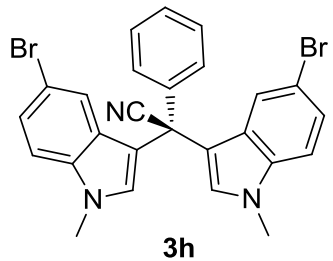

Current Data Parameters
NAME RKS-4-135
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20160719
Time 13.39
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 160
DS 0
SWH 45045.047 Hz
FIDRES 1.374666 Hz
AQ 0.3637748 sec
RG 4096
DW 11.100 usec
DE 6.50 usec
TE 300.1 K
D1 3.50000000 sec
d11 0.03000000 sec
DELTA 3.40000010 sec
NOREST 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 150.4929556 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 20.00 cm
CY 4.00 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
140.422
136.347
135.602
128.892
128.563
128.067
126.496
123.109
120.642
119.596
119.448
109.415
108.699
77.214
77.002
76.790
45.993
29.557
11.578
NC
N
N
3g
ppm
180
160
140
120
100
80
60
40
20

RKS-4-147-P3

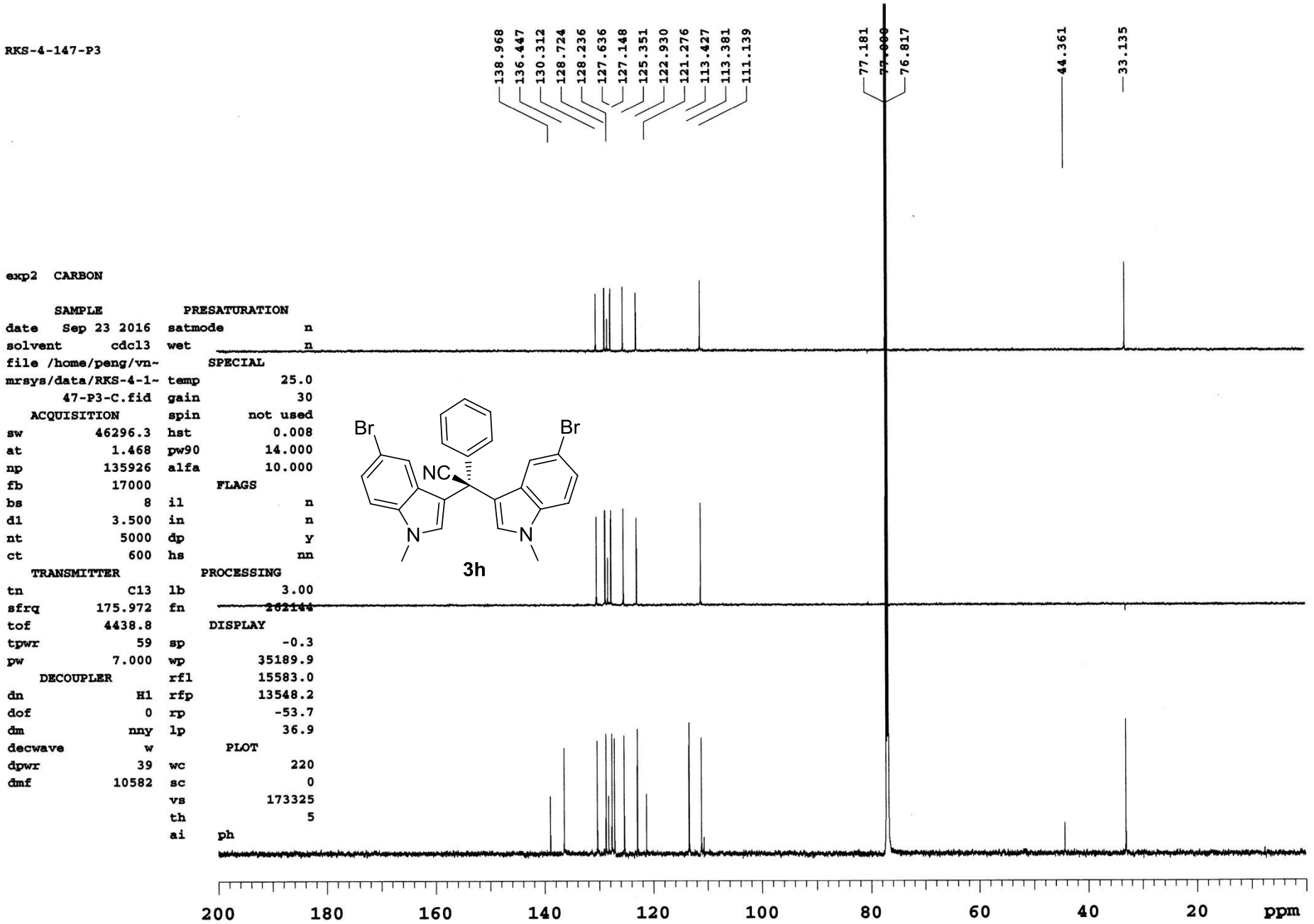


exp1 PROTON

SAMPLE		PRESATURATION	
date	Sep 23 2016	satmode	n
solvent	cdcl3	wet	n
file	exp	SPECIAL	
ACQUISITION		temp	25.0
sw	11904.8	gain	12
at	2.753	spin	not used
np	65536	hst	0.008
fb	4000	pw90	6.500
bs	8	alfa	10.000
d1	2.000	FLAGS	
nt	16	il	n
ct	16	in	n
TRANSMITTER		dp	y
tn	H1	hs	nn
sfrq	699.749	PROCESSING	
tof	349.9	fn	not used
tpwr	62	DISPLAY	
pw	3.250	sp	-0.2
DECOUPLER		wp	6997.2
dn	C13	rfl	7179.3
dof	0	rfp	5066.2
dm	nnn	rp	-62.4
decwave	W40_Cold	lp	0
dpwr	40	PLOT	
dmf	38462	wc	200
		sc	0
		vs	334
		th	5
		ai cdc ph	



3h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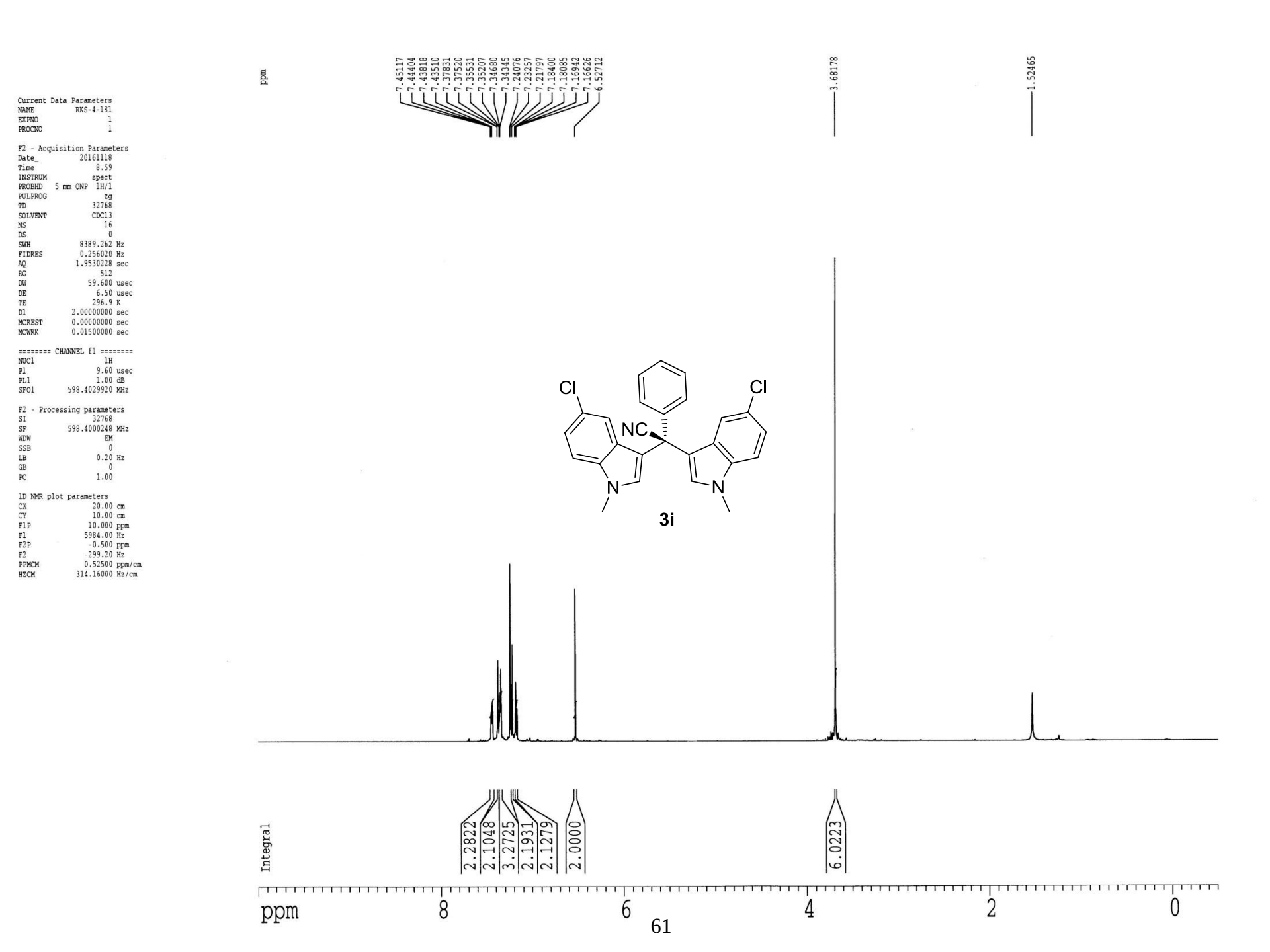
138.968
136.447
130.312
128.724
128.236
127.636
127.148
125.351
122.930
121.276
113.427
113.381
111.139
77.181
77.000
76.817
44.361
33.135
exp2 CARBON
SAMPLE
date Sep 23 2016
solvent cdcl3
file /home/peng/vn~
mrsys/data/RKS-4-1~
47-P3-C.fid
ACQUISITION
sw 46296.3
at 1.468
np 135926
fb 17000
bs 8
d1 3.500
nt 5000
ct 600
TRANSMITTER
tn C13
sfrq 175.972
tof 4438.8
tpwr 59
pw 7.000
DECOUPLER
dn H1
dof 0
dm nny
decwave w
dpwr 39
dmf 10582
PRESATURATION
satmode n
wet n
SPECIAL
temp 25.0
gain 30
spin not used
hst 0.008
pw90 14.000
alfa 10.000
FLAGS
il n
in n
dp y
hs nn
PROCESSING
lb 3.00
fn 262144
DISPLAY
sp -0.3
wp 35189.9
rf1 15583.0
rfp 13548.2
rp -53.7
lp 36.9
PLOT
wc 220
sc 0
vs 173325
th 5
ai ph
Br
Br
NC
N
N
3h
200
180
160
140
120
100
80
60
40
20
ppm


Current Data Parameters
NAME RKS-4-181
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20161118
Time 8.59
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 296.9 K
D1 2.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 9.60 usec
PL1 1.00 dB
SFO1 598.4029920 MHz
F2 - Processing parameters
SI 32768
SF 598.4000248 MHz
WDW EM
SSB 0
LB 0.20 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 20.00 cm
CY 10.00 cm
F1P 10.000 ppm
F1 5984.00 Hz
F2P -0.500 ppm
F2 -299.20 Hz
PPMCM 0.52500 ppm/cm
HZCM 314.16000 Hz/cm
ppm
7.45117
7.44404
7.43818
7.43510
7.37831
7.37520
7.35531
7.35207
7.34680
7.34345
7.24076
7.23257
7.21797
7.18400
7.18085
7.16942
7.16626
6.52712
3.68178
1.52465
Cl
Cl
NC
N
N
3i
Integral
2.2822
2.1048
3.2725
2.1931
2.1279
2.0000
6.0223
ppm
8
6
4
2
0

Current Data Parameters
NAME RKS-4-181
EXPNO 2
PROCNO 1

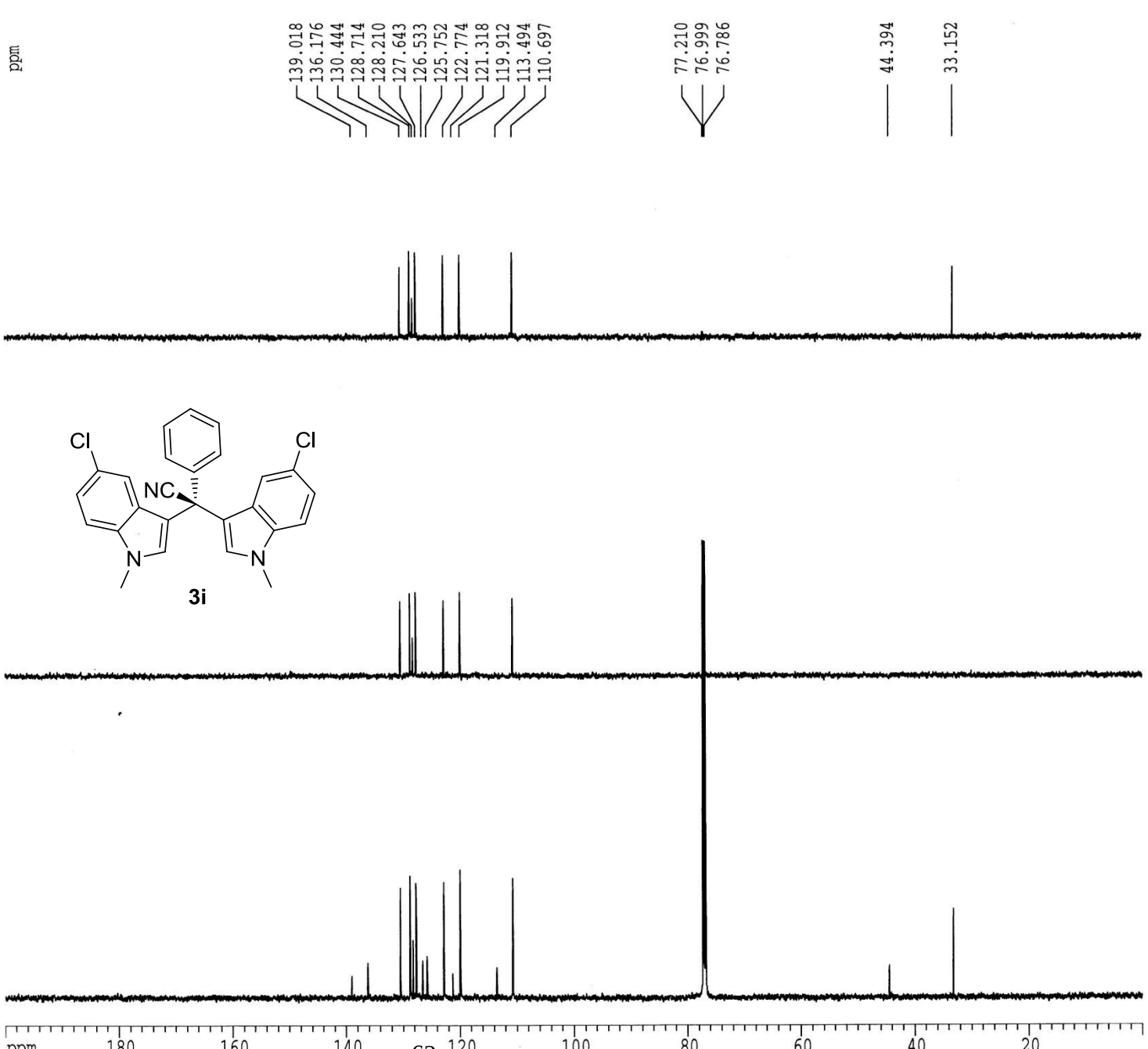
F2 - Acquisition Parameters
Date_ 20161118
Time 9.01
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 858
DS 0
SWH 45045.047 Hz
FIDRES 1.374666 Hz
AQ 0.3637748 sec
RG 4096
DW 11.100 usec
DE 6.50 usec
TE 296.9 K
D1 3.50000000 sec
d11 0.03000000 sec
DELTA 3.40000010 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

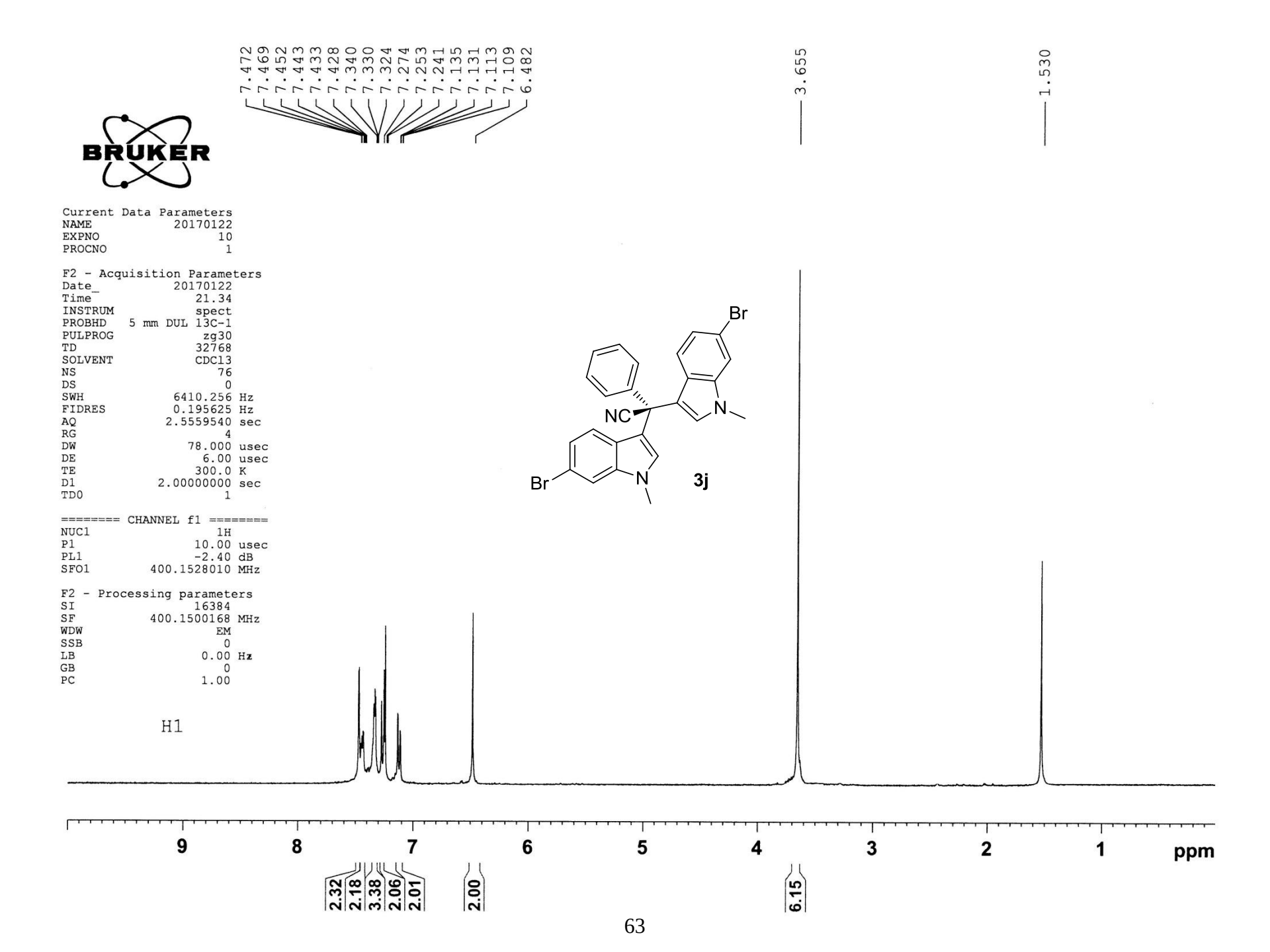
======== CHANNEL f1 ========
NUC1 13C
P1 4.80 usec
PL1 0.00 dB
SFO1 150.4843515 MHz

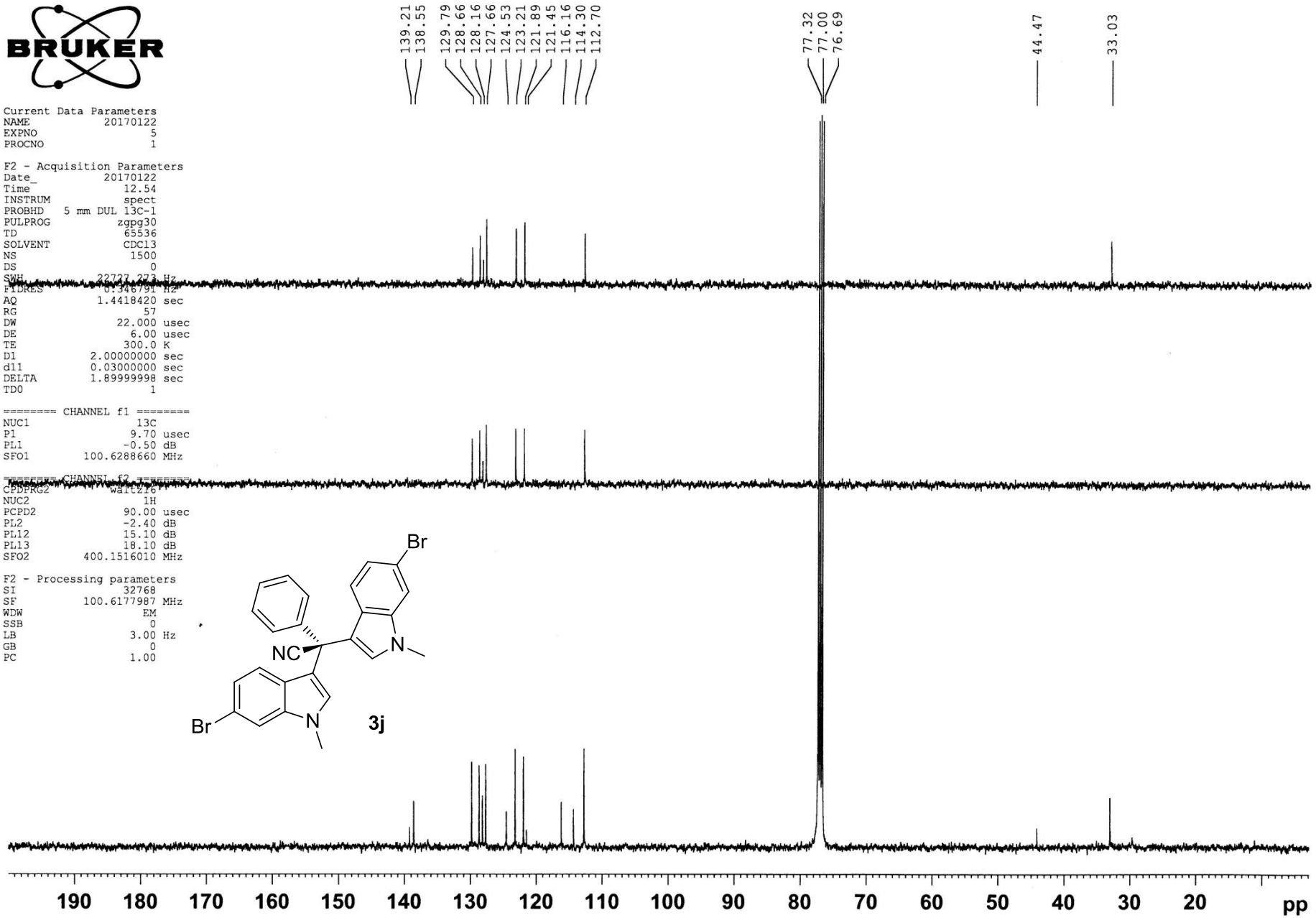
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 92.00 usec
PL2 120.00 dB
PL12 9.00 dB
PL13 14.00 dB
SFO2 598.4029920 MHz

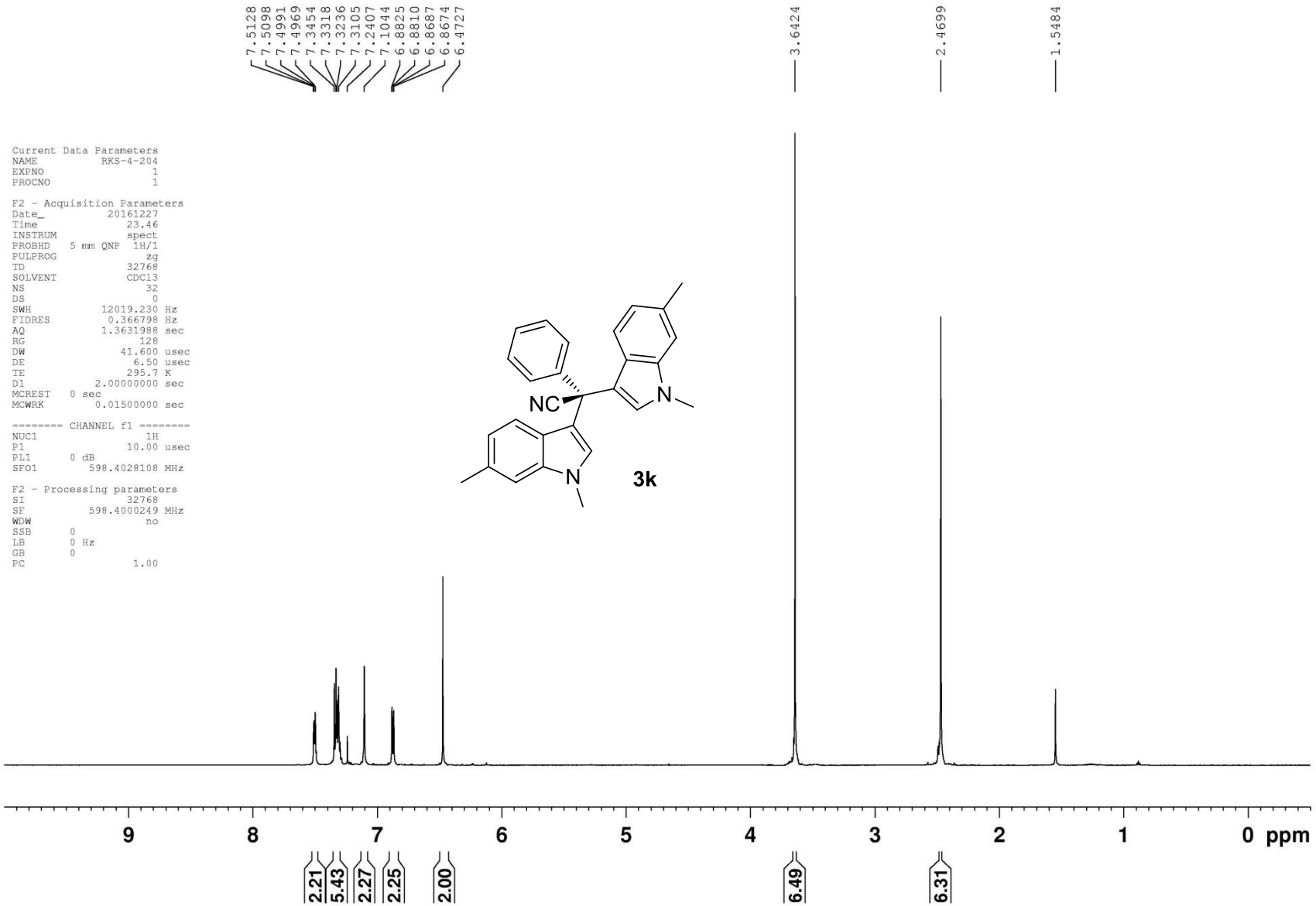
F2 - Processing parameters
SI 65536
SF 150.4678043 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00

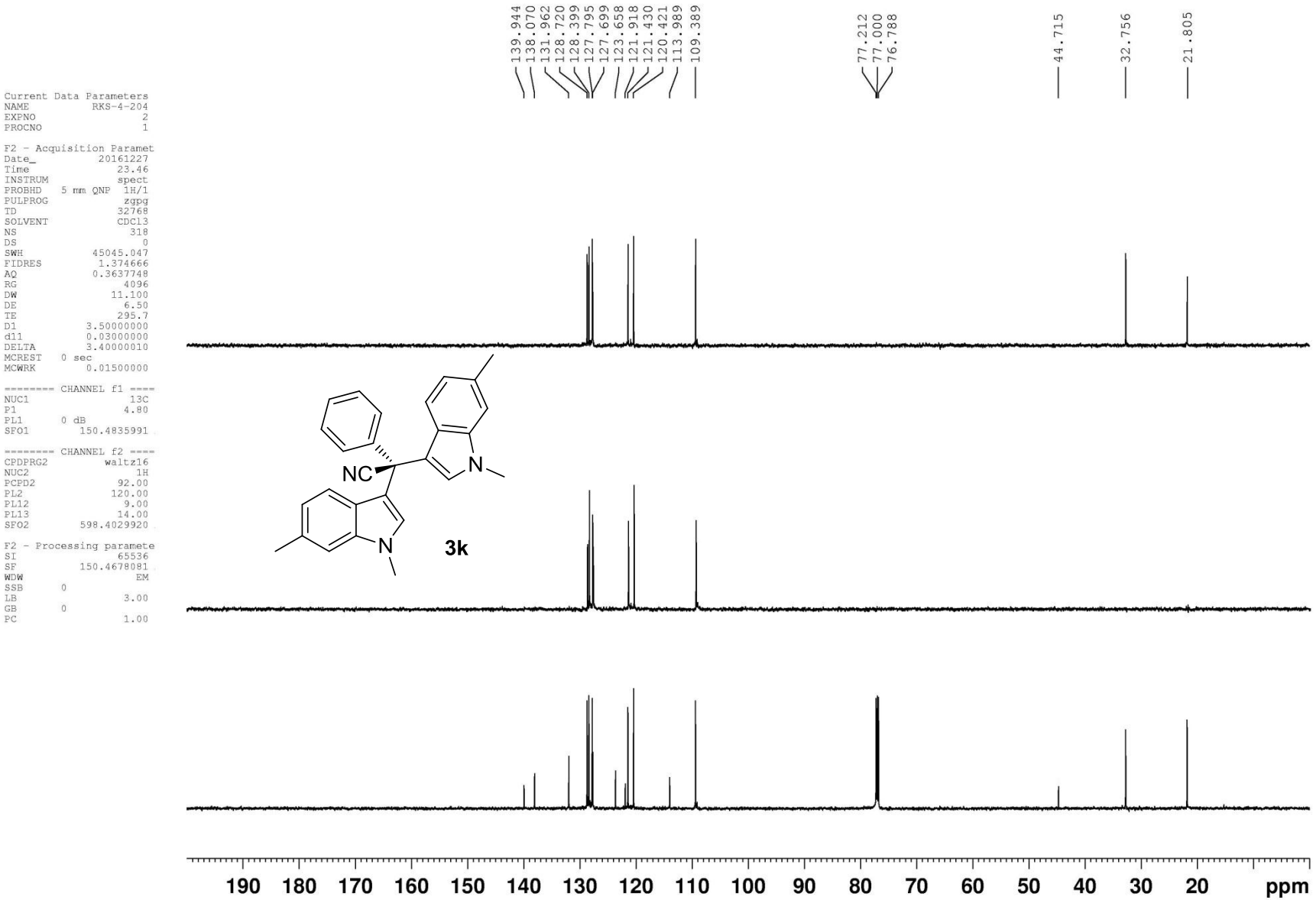
1D NMR plot parameters
CX 20.00 cm
CY 8.00 cm
F1P 200.000 ppm
F1 30093.56 Hz
F2P 0.000 ppm
F2 0.00 Hz
PPMCM 10.00000 ppm/cm
HZCM 1504.67798 Hz/cm

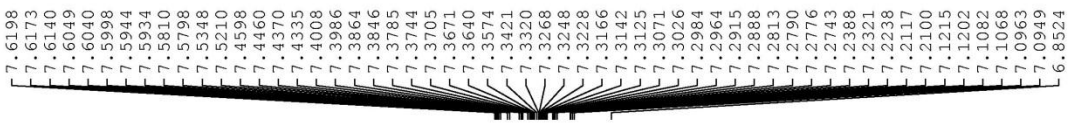



7.472
7.469
7.452
7.443
7.433
7.428
7.340
7.330
7.324
7.274
7.253
7.241
7.135
7.131
7.113
7.109
6.482
3.655
1.530
BRUKER
Current Data Parameters
NAME 20170122
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170122
Time 21.34
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 76
DS 0
SWH 6410.256 Hz
FIDRES 0.195625 Hz
AQ 2.5559540 sec
RG 4
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 400.1500168 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
Br
NC
N
Br
N
3j
H1
9
8
7
6
5
4
3
2
1
ppm
2.32
2.18
3.38
2.06
2.01
2.00
6.15


139.21
138.55
129.79
128.66
128.16
127.66
124.53
123.21
121.89
121.45
116.16
114.30
112.70
77.32
77.00
76.69
44.47
33.03
Current Data Parameters
NAME 20170122
EXPNO 5
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170122
Time 12.54
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1500
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
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
PL12 15.10 dB
PL13 18.10 dB
SFO2 400.1516010 MHz
F2 - Processing parameters
SI 32768
SF 100.6177987 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
Br
NC
N
Br
N
3j
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm


7.5128
7.5098
7.4991
7.4969
7.3454
7.3318
7.3236
7.3105
7.2407
7.1044
6.8825
6.8810
6.8687
6.8674
6.4727
3.6424
2.4699
1.5484
Current Data Parameters
NAME RKS-4-204
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20161227
Time 23.46
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 32
DS 0
SWH 12019.230 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 128
DW 41.600 usec
DE 6.50 usec
TE 295.7 K
D1 2.00000000 sec
MCREST 0 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 0 dB
SFO1 598.4028108 MHz
F2 - Processing parameters
SI 32768
SF 598.4000249 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 1.00
NC
N
N
3k
9
8
7
6
5
4
3
2
1
0 ppm
2.21
5.43
2.27
2.25
2.00
6.49
6.31


Current Data Parameters
NAME RKS-4-204
EXPNO 2
PROCNO 1
F2 - Acquisition Paramet
Date_ 20161227
Time 23.46
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 318
DS 0
SWH 45045.047
FIDRES 1.374666
AQ 0.3637748
RG 4096
DW 11.100
DE 6.50
TE 295.7
D1 3.50000000
d11 0.03000000
DELTA 3.40000010
MCREST 0 sec
MCWRK 0.01500000
======== CHANNEL f1 ====
NUC1 13C
P1 4.80
PL1 0 dB
SFO1 150.4835991
======== CHANNEL f2 ====
CPDPRG2 waltz16
NUC2 1H
PCPD2 92.00
PL2 120.00
PL12 9.00
PL13 14.00
SFO2 598.4029920
F2 - Processing paramete
SI 65536
SF 150.4678081
WDW EM
SSB 0
LB 3.00
GB 0
PC 1.00
139.944
138.070
131.962
128.720
128.399
127.795
127.699
123.658
121.918
121.430
120.421
113.989
109.389
77.212
77.000
76.788
44.715
32.756
21.805
NC
N
N
3k
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm




```
Current Data Parameters
NAME      RKS-4-128-P2-A
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20160824
Time                5.29
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               300.8 K
D1            2.00000000 sec
MCREST    0 sec
MCWRK         0.01500000 sec

======== CHANNEL f1 ========
NUC1                  1H
P1                 9.60 usec
PL1                3.00 dB
SFO1        598.5029925 MHz

F2 - Processing parameters
SI                 32768
SF          598.5000286 MHz
WDW                   no
SSB       0
LB        0 Hz
GB        0
PC                 1.00
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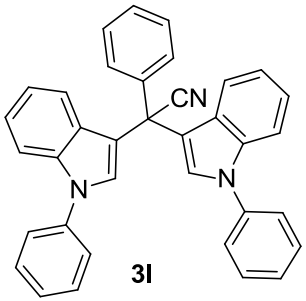

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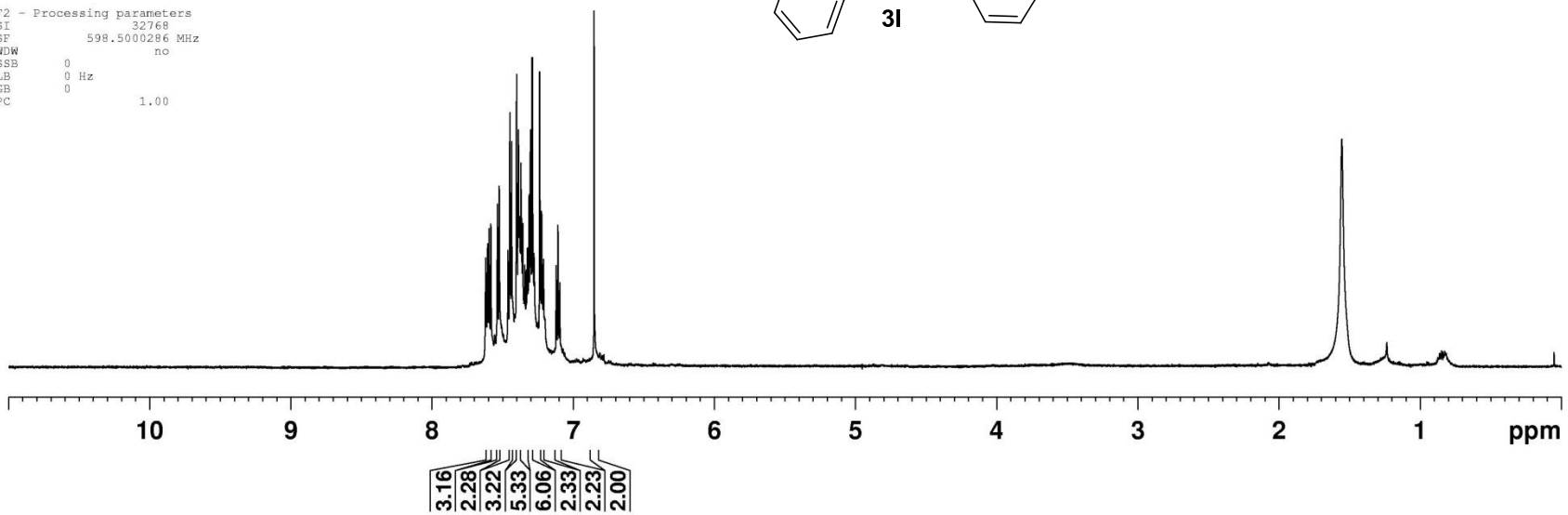

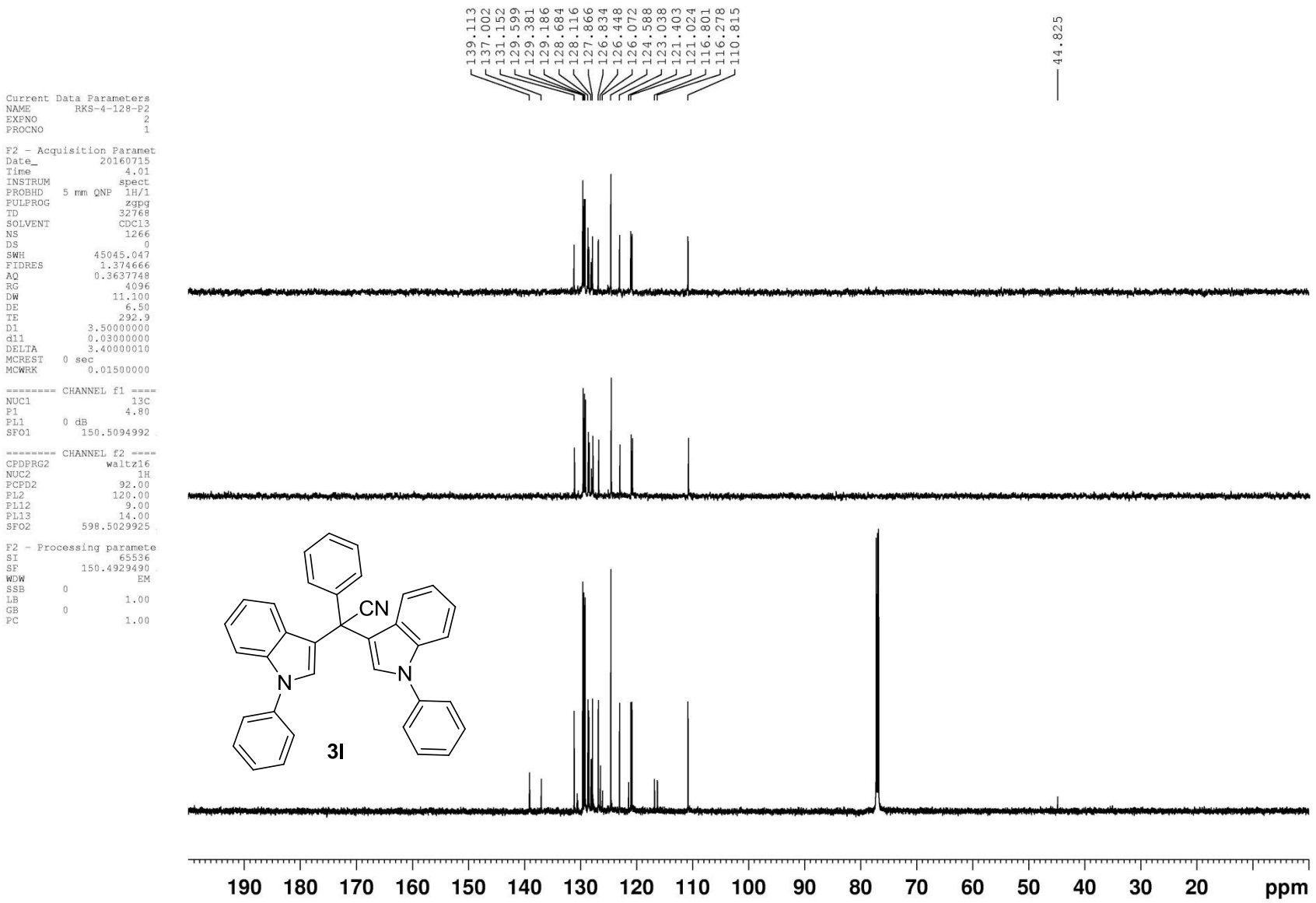
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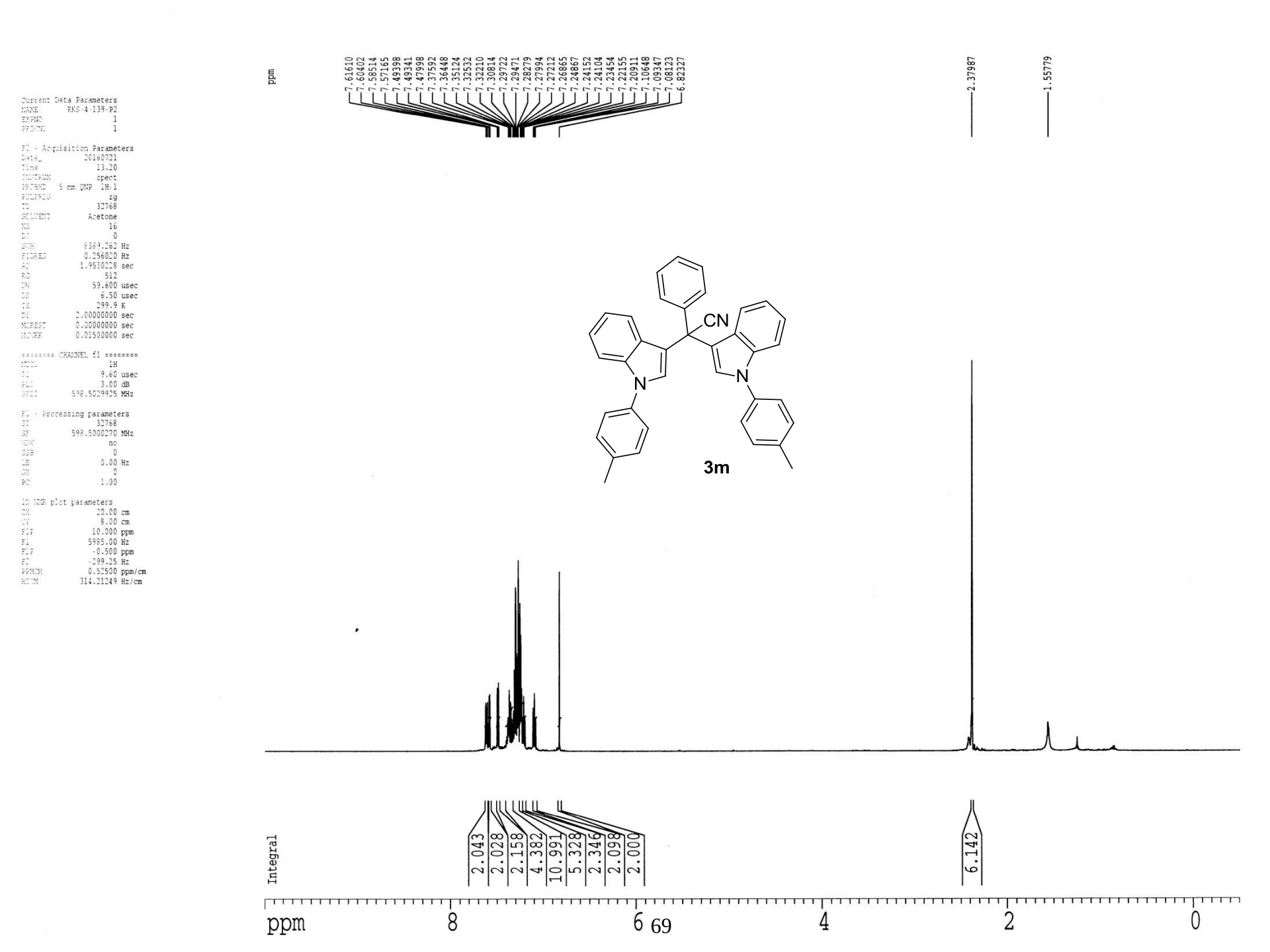
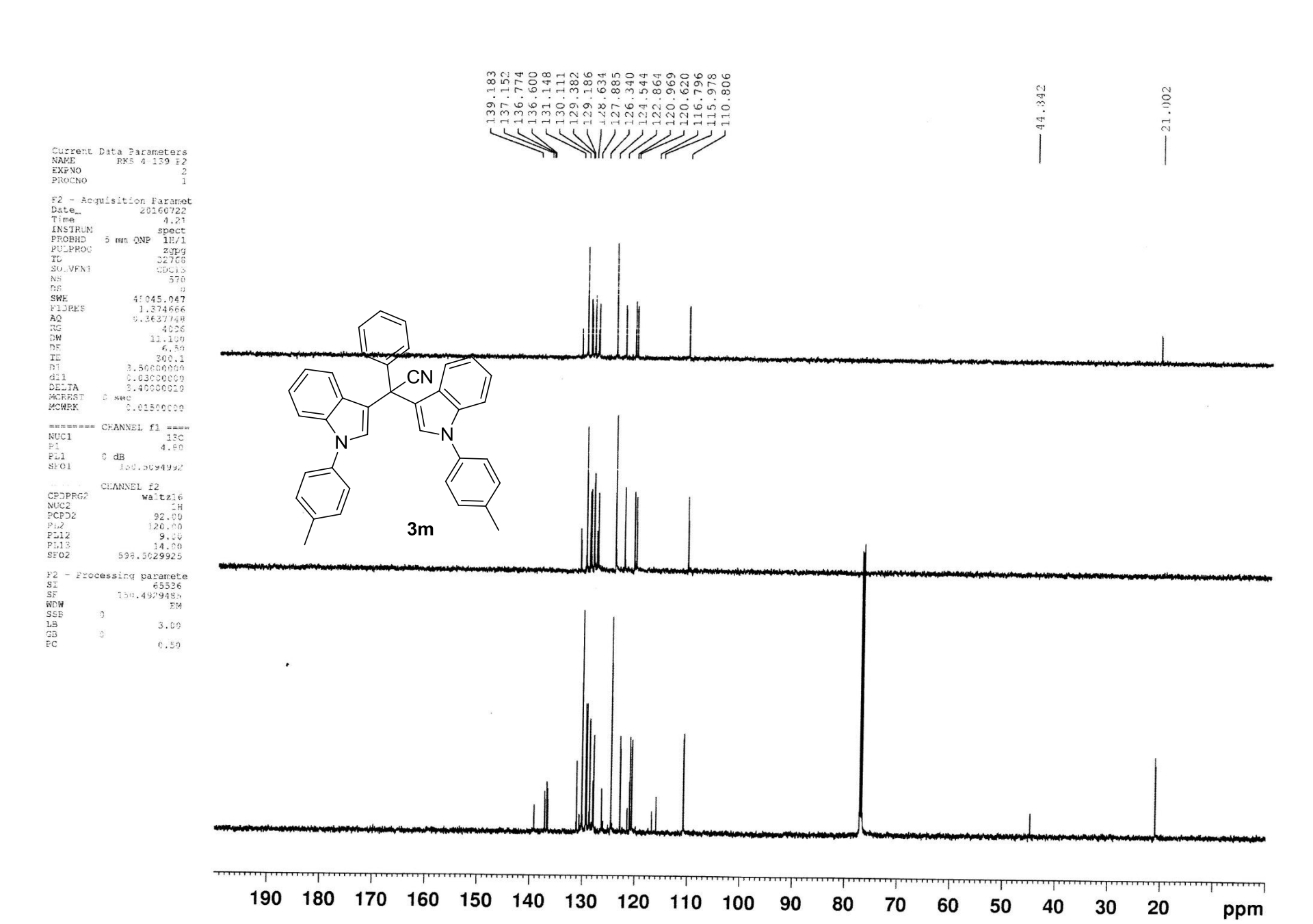
137.002
131.152
129.599
129.381
129.186
128.684
128.116
127.866
126.834
126.448
126.072
124.588
123.038
121.403
121.024
116.801
116.278
110.815
44.825
Current Data Parameters
NAME RKS-4-128-P2
EXPNO 2
PROCNO 1
F2 - Acquisition Paramet
Date_ 20160715
Time 4.01
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 1266
DS 0
SWH 45045.047
FIDRES 1.374666
AQ 0.3637748
RG 4096
DW 11.100
DE 6.50
TE 292.9
D1 3.50000000
d11 0.03000000
DELTA 3.40000010
MCREST 0 sec
MCWRK 0.01500000
======== CHANNEL f1 ====
NUC1 13C
P1 4.80
PL1 0 dB
SFO1 150.5094992
======== CHANNEL f2 ====
CPDPRG2 waltz16
NUC2 1H
PCPD2 92.00
PL2 120.00
PL12 9.00
PL13 14.00
SFO2 598.5029925
F2 - Processing paramete
SI 65536
SF 150.4929490
WDW EM
SSB 0
LB 1.00
GB 0
PC 1.00
CN
N
N
3l
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm


Current Data Parameters
NAME RKS-4-139-P2
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20160721
Time 13.20
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg
TD 32768
SOLVENT Acetone
NS 16
DS 0
SWH 8389.262 Hz
FIDRES 0.256020 Hz
AQ 1.9530028 sec
RG 512
DW 59.600 usec
DE 6.50 usec
TE 299.9 K
D1 2.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 9.60 usec
PL1 3.00 dB
SFO1 598.5029925 MHz
F2 - Processing parameters
SI 32768
SF 598.5000270 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 20.00 cm
CY 8.00 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
7.61610
7.60402
7.58514
7.57165
7.49398
7.49341
7.47998
7.37592
7.36448
7.35124
7.32532
7.32210
7.30814
7.29722
7.29471
7.28279
7.27994
7.27212
7.26865
7.24867
7.24152
7.24104
7.23454
7.22155
7.20911
7.10648
7.09347
7.08123
6.82327
2.37987
1.55779
CN
N
N
3m
Integral
2.043
2.028
2.158
4.382
10.991
5.329
2.346
2.098
2.000
6.142
ppm
8
6
4
2
0

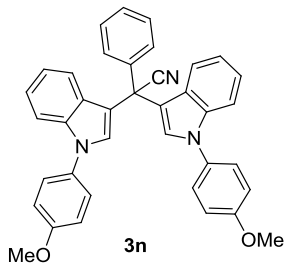

Current Data Parameters
NAME RKS 4 139 f2
EXPNO 2
PROCNO 1
F2 - Acquisition Paramet
Date_ 20160722
Time 4.21
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 570
DS 0
SWE 40045.047
FIDRES 1.374666
AQ 0.3637748
RG 4096
DW 11.100
DE 6.50
TE 300.1
D1 3.50000000
d11 0.03000000
DELTA 3.40000010
MCREST 0 sec
MCWRK 0.01500000
======== CHANNEL f1 ====
NUC1 13C
P1 4.90
PL1 0 dB
SFO1 150.5094992
CHANNEL f2
CPDPRG2 waltz16
NUC2 1H
PCPD2 92.00
PL2 120.00
PL12 9.00
PL13 14.00
SFO2 599.5029925
F2 - Processing paramete
SI 65536
SF 150.4979485
WDW EM
SSB 0
LB 3.00
GB 0
PC 0.50
139.183
137.152
136.774
136.600
131.148
130.111
129.382
129.186
128.634
127.885
126.340
124.544
122.864
120.969
120.620
116.796
115.978
110.806
44.342
21.002
CN
N
N
3m
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

RKS-4-142-P1

7.621 7.611 7.586 7.575 7.431 7.419 7.380 7.370 7.358 7.341 7.330 7.312 7.300 7.245 7.221 7.220 7.210 7.199 7.198 7.109 7.108 7.097 7.087 7.086 6.971 6.959 6.797 3.831

exp6 PROTON

SAMPLE		PRESATURATION	
date	Sep 23 2016	satmode	n
solvent	cdcl3	wet	n
file	/home/peng/vn~	SPECIAL	
mrsys/data/RKS-4-1~		temp	25.0
	42-P1-H.fid	gain	12
ACQUISITION		spin	not used
sw	11904.8	hst	0.008
at	2.753	pw90	6.500
np	65536	alfa	10.000
fb	4000	FLAGS	
bs	8	il	n
d1	2.000	in	n
nt	16	dp	y
ct	16	hs	nn
TRANSMITTER		PROCESSING	
tn	H1	fn	not used
sfrq	699.749	DISPLAY	
tof	349.9	sp	-0.1
tpwr	62	wp	6997.2
pw	3.250	rfl	2108.4
DECOUPLER		rfp	0
dn	C13	rp	-60.6
dof	0	lp	.0
dm	nnn	PLOT	
decwave	W40_Cold	wc	200
dpwr	40	sc	0
dmf	38462	vs	196
		th	4
		ai cdc ph	

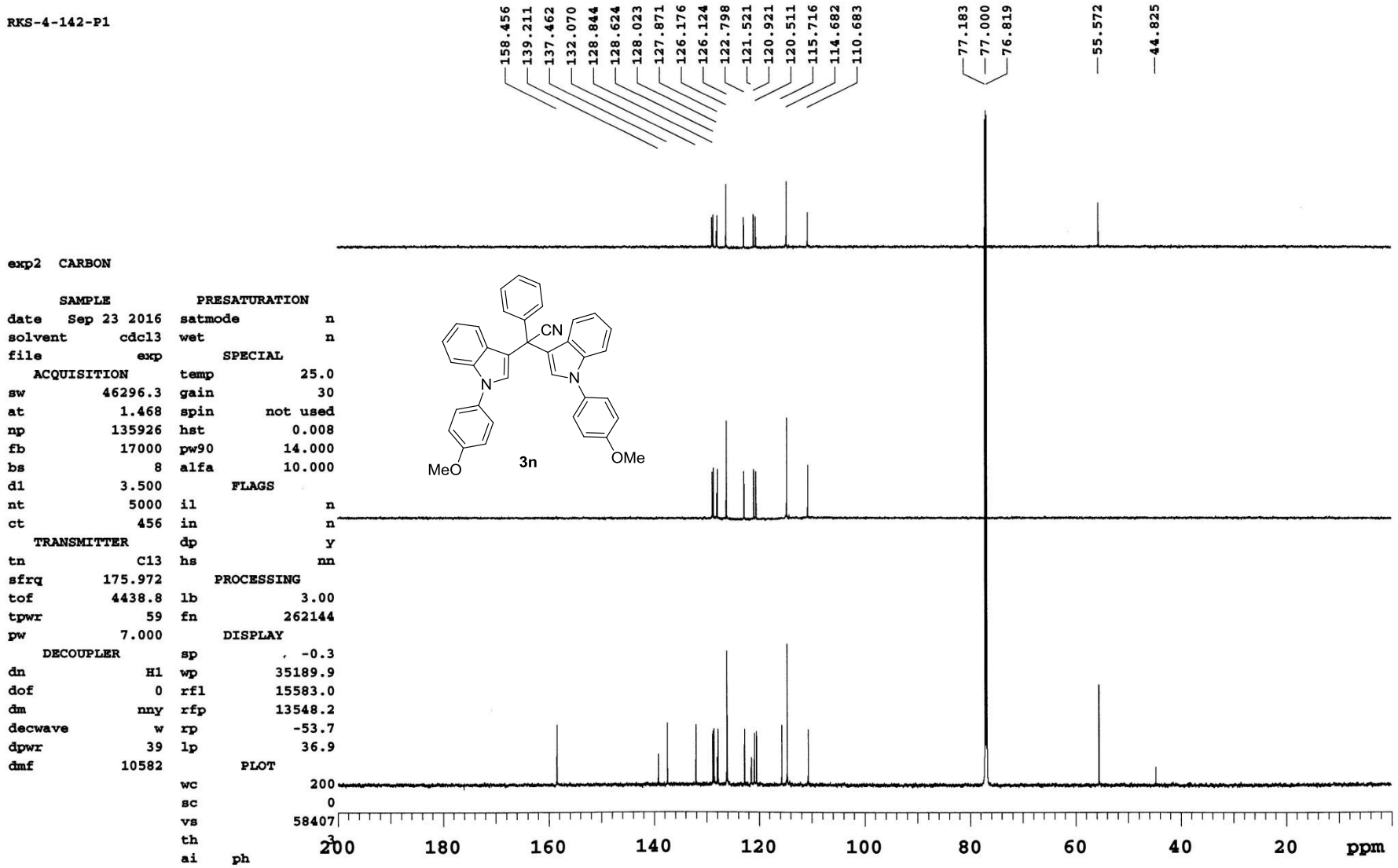


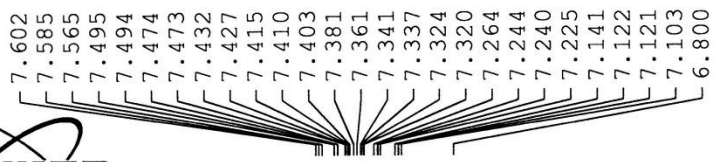
3n

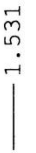
10 9 8 7 6 5 4 3 2 1 ppm

2.06 2.00 2.28 2.28 5.48 2.65 2.29 4.26 2.00

6.20


RKS-4-142-P1
158.456
139.211
137.462
132.070
128.844
128.624
128.023
127.871
126.176
126.124
122.798
121.521
120.921
120.511
115.716
114.682
110.683
77.183
77.000
76.819
55.572
44.825
exp2 CARBON
SAMPLE
date Sep 23 2016
solvent cdcl3
file exp
ACQUISITION
sw 46296.3
at 1.468
np 135926
fb 17000
bs 8
d1 3.500
nt 5000
ct 456
TRANSMITTER
tn C13
sfrq 175.972
tof 4438.8
tpwr 59
pw 7.000
DECOUPLER
dn H1
dof 0
dm nny
decwave w
dpwr 39
dmf 10582
PRESATURATION
satmode n
wet n
SPECIAL
temp 25.0
gain 30
spin not used
hst 0.008
pw90 14.000
alfa 10.000
FLAGS
il n
in n
dp y
hs nn
PROCESSING
lb 3.00
fn 262144
DISPLAY
sp -0.3
wp 35189.9
rfl 15583.0
rfp 13548.2
rp -53.7
lp 36.9
PLOT
wc 200
sc 0
vs 58407
th 3
ai ph
CN
N
N
MeO
OMe
3n
200
180
160
140
120
100
80
60
40
20
ppm



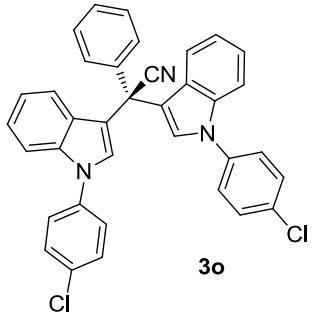



```
Current Data Parameters
NAME            20170106
EXPNO                  4
PROCNO                 1

F2 - Acquisition Parameters
Date_           20170106
Time                0.22
INSTRUM            spect
PROBHD   5 mm DUL 13C-1
PULPROG             zg30
TD                 32768
SOLVENT            CDCl3
NS                    14
DS                     0
SWH             6410.256 Hz
FIDRES          0.195625 Hz
AQ             2.5559540 sec
RG                  2050
DW                78.000 usec
DE                 6.00 usec
TE                300.0 K
D1           2.00000000 sec
TD0                    1

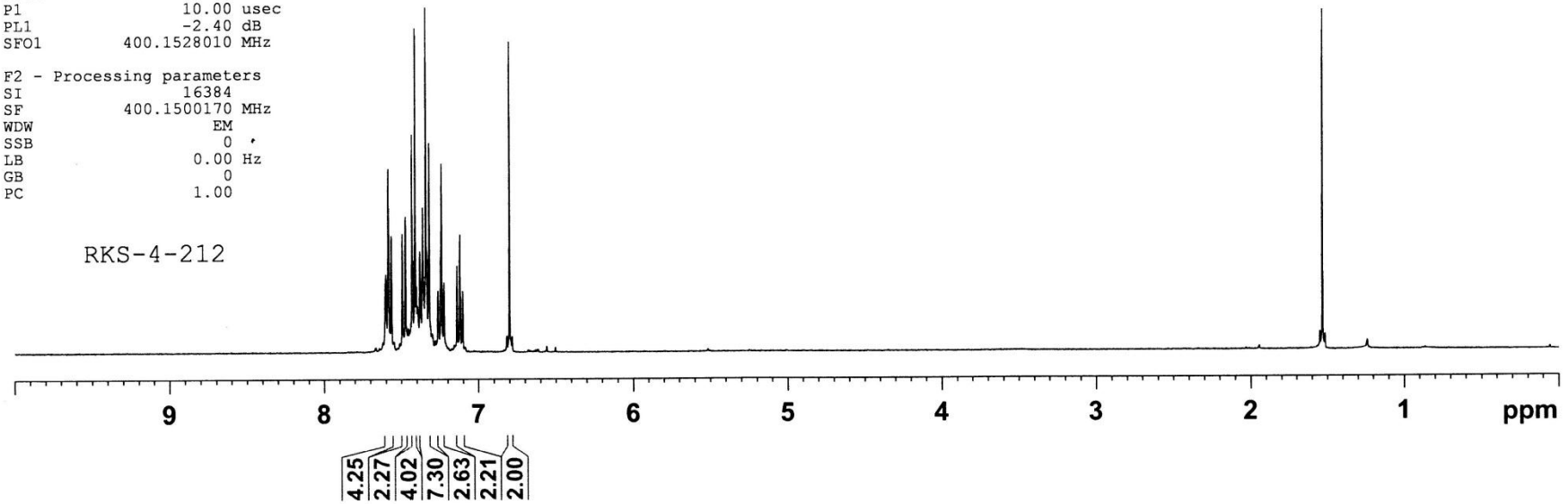
======== CHANNEL f1 ========
NUC1                  1H
P1                10.00 usec
PL1               -2.40 dB
SFO1         400.1528010 MHz

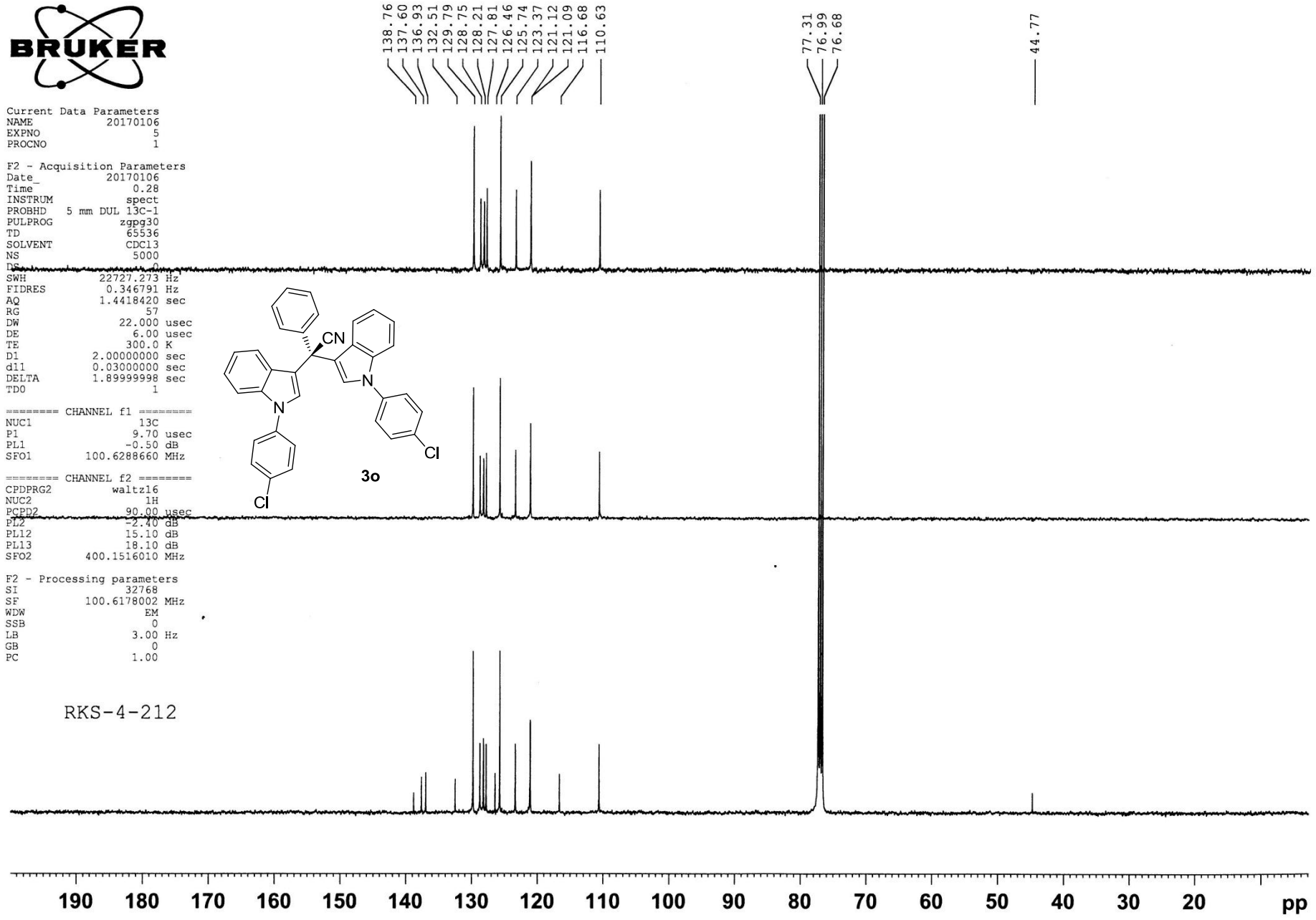
F2 - Processing parameters
SI                 16384
SF          400.1500170 MHz
WDW                   EM
SSB                    0
LB                  0.00 Hz
GB                     0
PC                  1.00
```

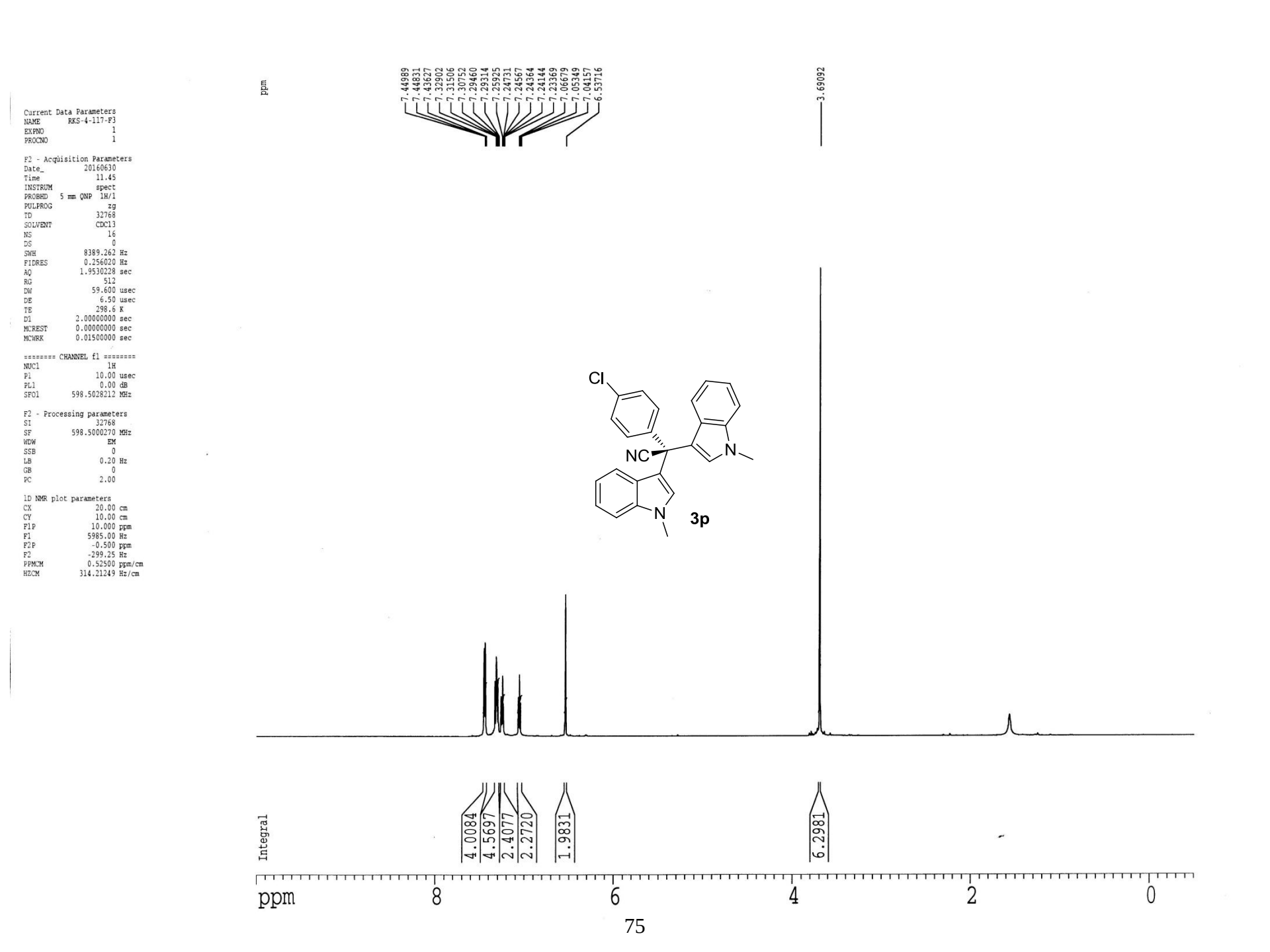


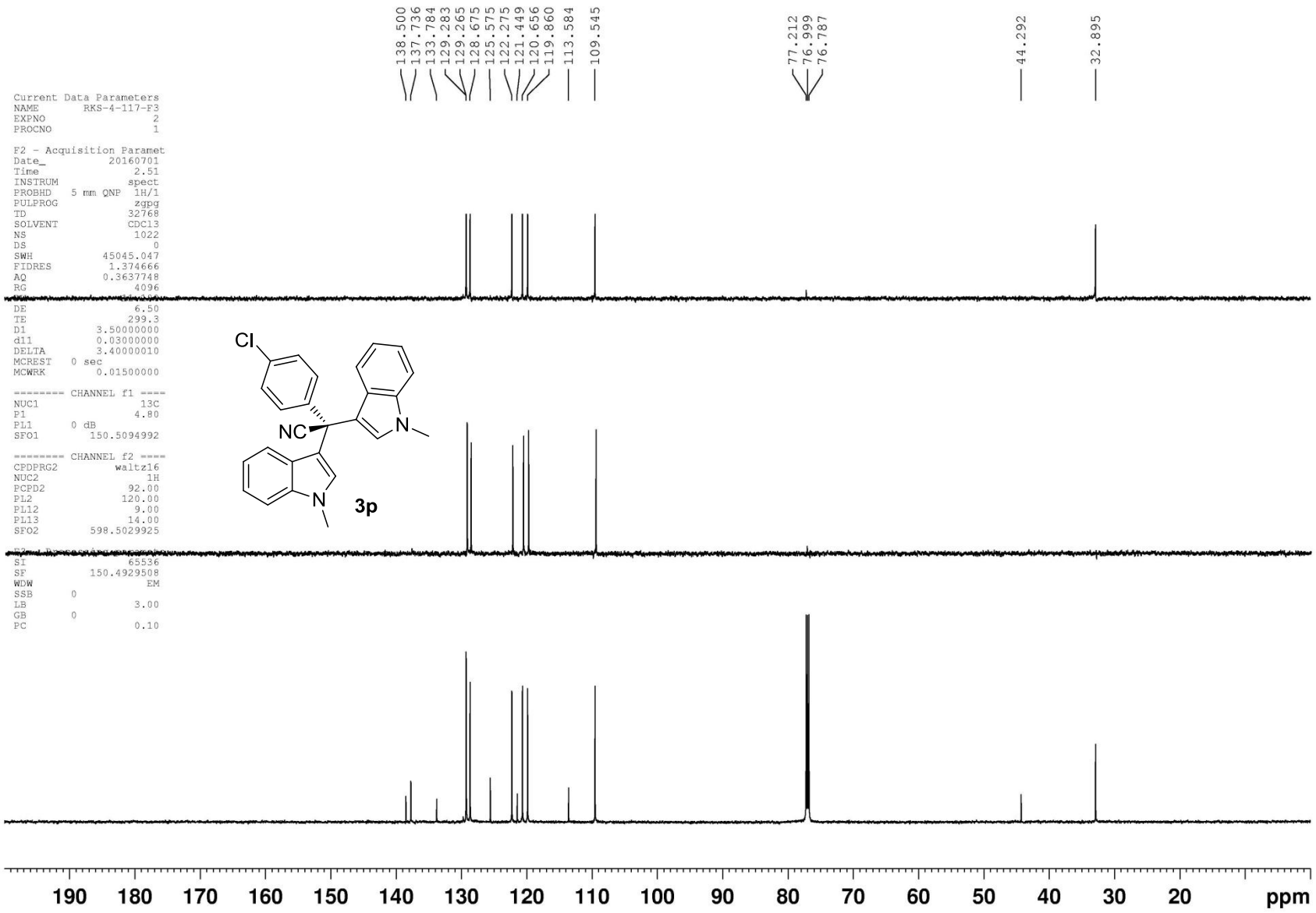
3o

RKS-4-212

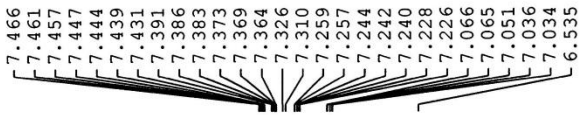



138.76
137.60
136.93
132.51
129.79
128.75
128.21
127.81
126.46
125.74
123.37
121.12
121.09
116.68
110.63
77.31
76.99
76.68
44.77
Current Data Parameters
NAME 20170106
EXPNO 5
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170106
Time 0.28
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 5000
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
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
PL12 15.10 dB
PL13 18.10 dB
SFO2 400.1516010 MHz
F2 - Processing parameters
SI 32768
SF 100.6178002 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
CN
N
N
Cl
Cl
3o
RKS-4-212
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
pp


Current Data Parameters
NAME RKS-4-117-F3
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20160630
Time 11.45
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 298.6 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 598.5028212 MHz
F2 - Processing parameters
SI 32768
SF 598.5000270 MHz
WDW EM
SSB 0
LB 0.20 Hz
GB 0
PC 2.00
1D NMR plot parameters
CX 20.00 cm
CY 10.00 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
7.44989
7.44831
7.43627
7.32902
7.31506
7.30752
7.29460
7.29314
7.25925
7.24731
7.24567
7.24364
7.24144
7.23369
7.06679
7.05349
7.04157
6.53716
3.69092
Cl
NC
N
N
3p
Integral
4.0084
4.5697
2.4077
2.2720
1.9831
6.2981
ppm
8
6
4
2
0


138.500
137.736
133.784
129.283
129.265
128.675
125.575
122.275
121.449
120.656
119.860
113.584
109.545
77.212
76.999
76.787
44.292
32.895
Current Data Parameters
NAME RKS-4-117-F3
EXPNO 2
PROCNO 1
F2 - Acquisition Paramet
Date_ 20160701
Time 2.51
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 1022
DS 0
SWH 45045.047
FIDRES 1.374666
AQ 0.3637748
RG 4096
DE 6.50
TE 299.3
D1 3.50000000
d11 0.03000000
DELTA 3.40000010
MCREST 0 sec
MCWRK 0.01500000
======== CHANNEL f1 ====
NUC1 13C
P1 4.80
PL1 0 dB
SFO1 150.5094992
======== CHANNEL f2 ====
CPDPRG2 waltz16
NUC2 1H
PCPD2 92.00
PL2 120.00
PL12 9.00
PL13 14.00
SFO2 598.5029925
SI 65536
SF 150.4929508
WDW EM
SSB 0
LB 3.00
GB 0
PC 0.10
Cl
NC
N
N
3p
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

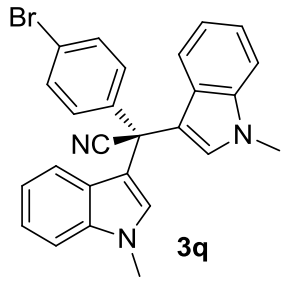
1H / RKS-4-119



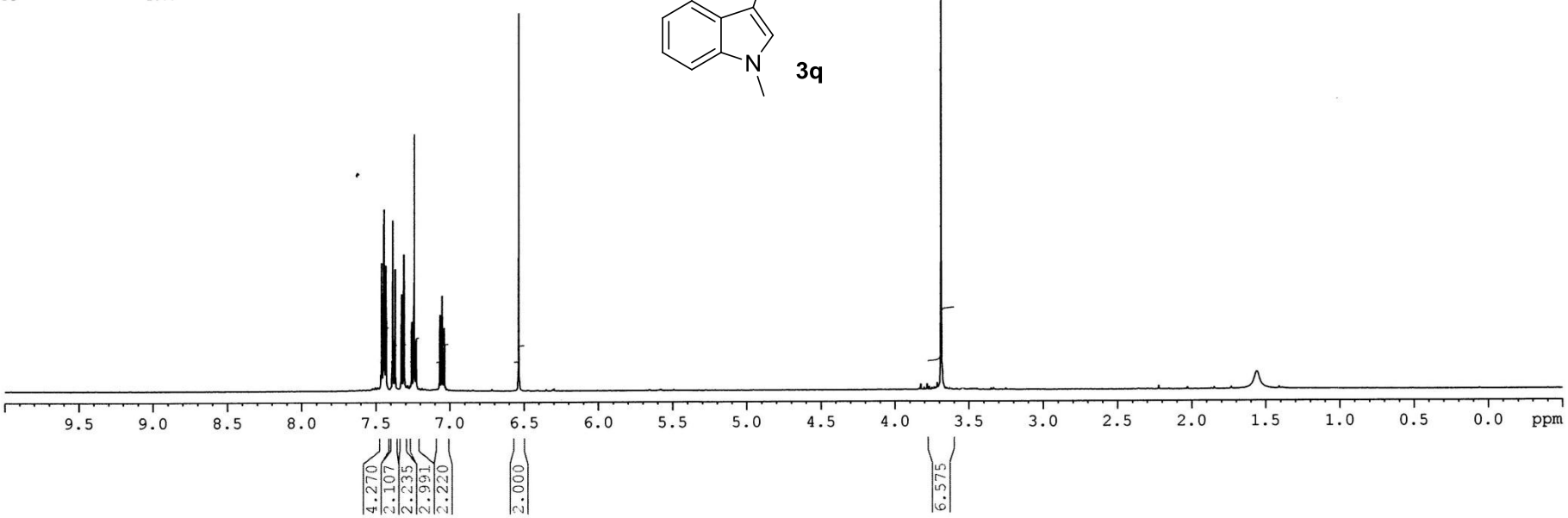

```
Current Data Parameters
NAME       liou0629.002
EXPNO                 1
PROCNO                1

F2 - Acquisition Parameters
Date_          20160629
Time             13.44 h
INSTRUM           spect
PROBHD   Z119470_0234 (
PULPROG            zg30
TD                32768
SOLVENT           CDCl3
NS                   32
DS                    0
SWH           10026.738 Hz
FIDRES         0.305992 Hz
AQ            1.6340309 sec
RG                89.22
DW               49.867 usec
DE                7.71 usec
TE               300.0 K
D1           2.00000000 sec
TD0                   1
SFO1        500.1630010 MHz
NUC1                1H
P1                10.00 usec
PLW1        22.69799995 W

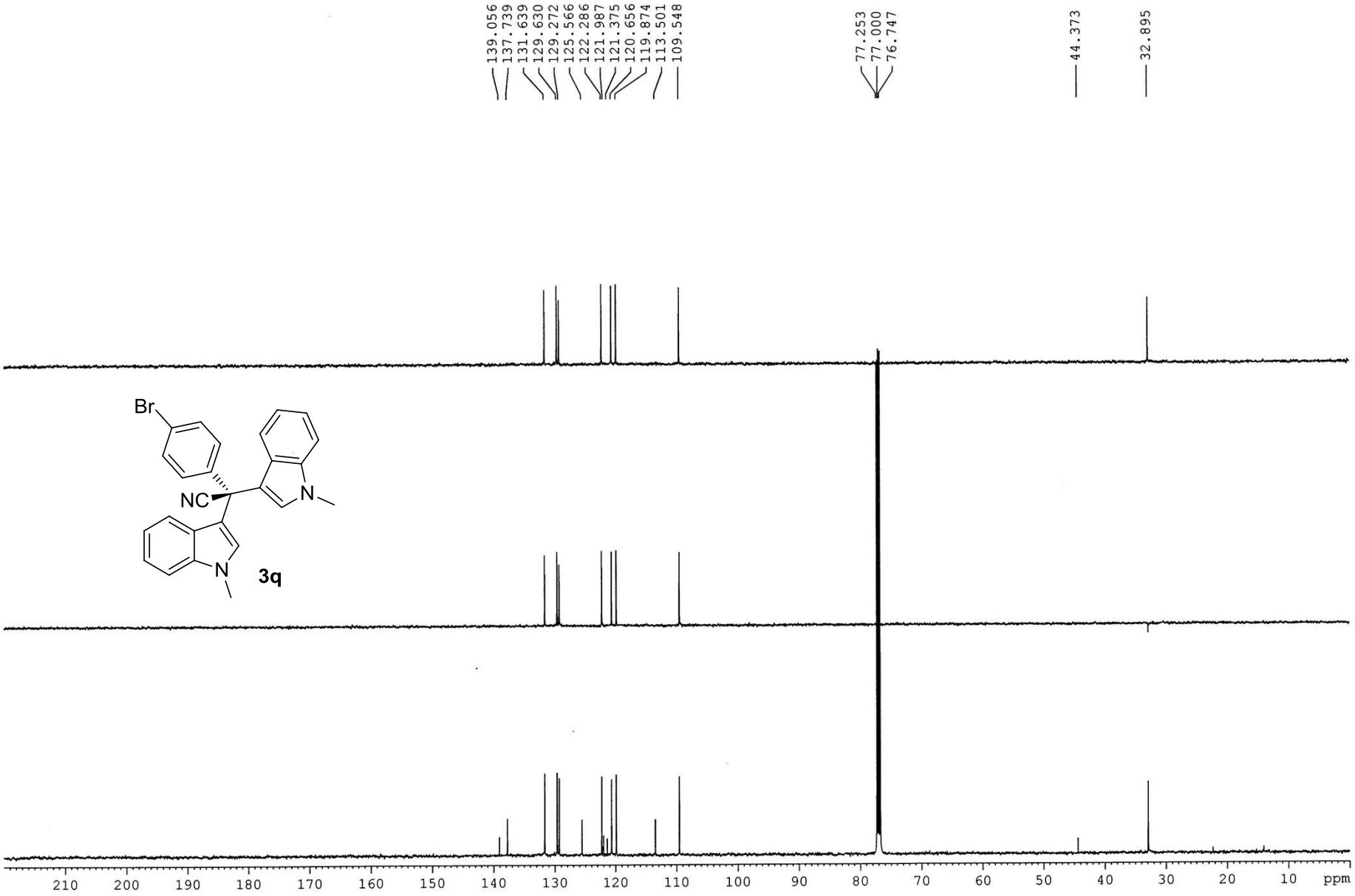
F2 - Processing parameters
SI                16384
SF          500.1600212 MHz
WDW                  EM
SSB       0
LB        0 Hz
GB        0
PC                1.00
```

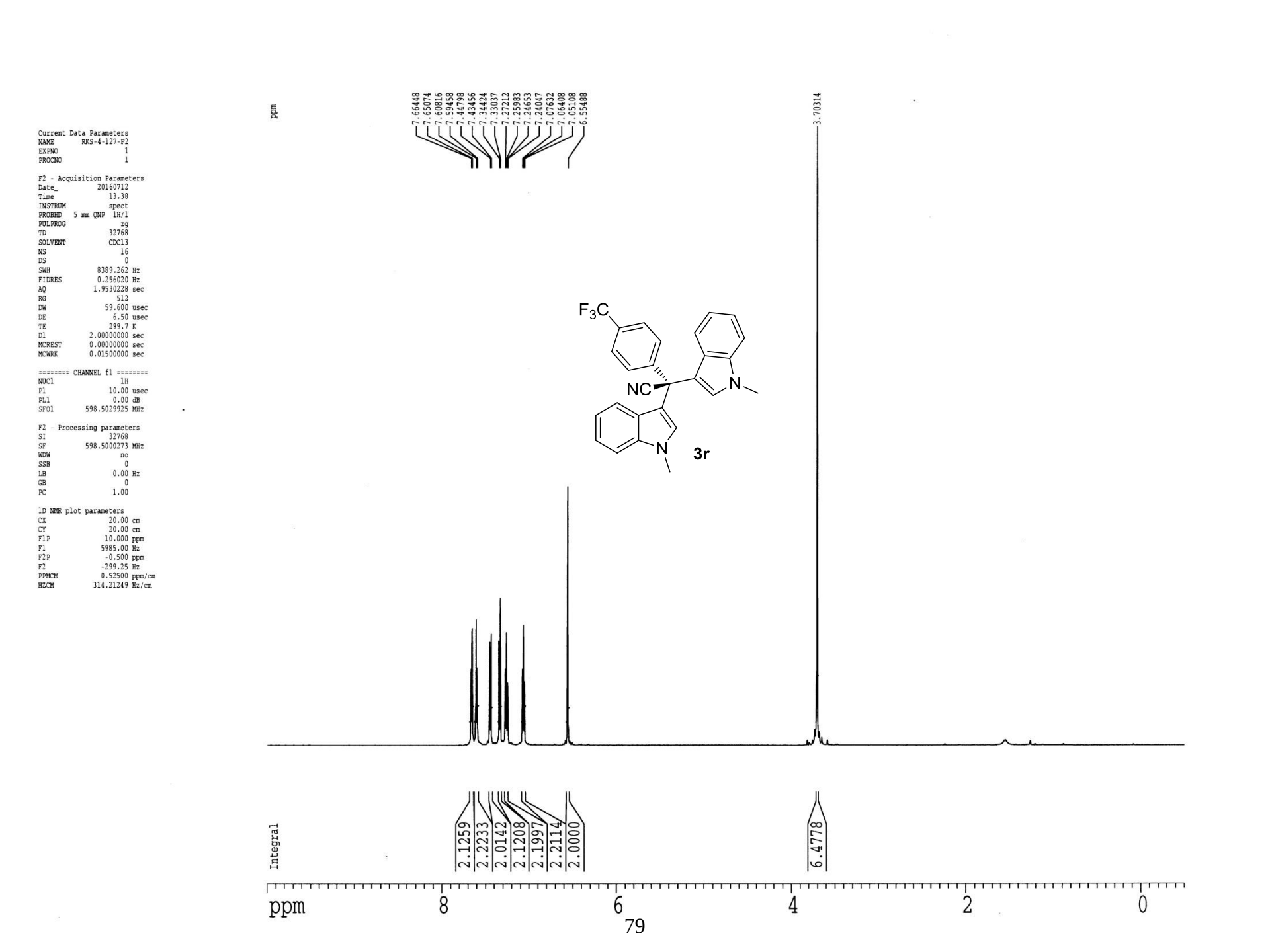


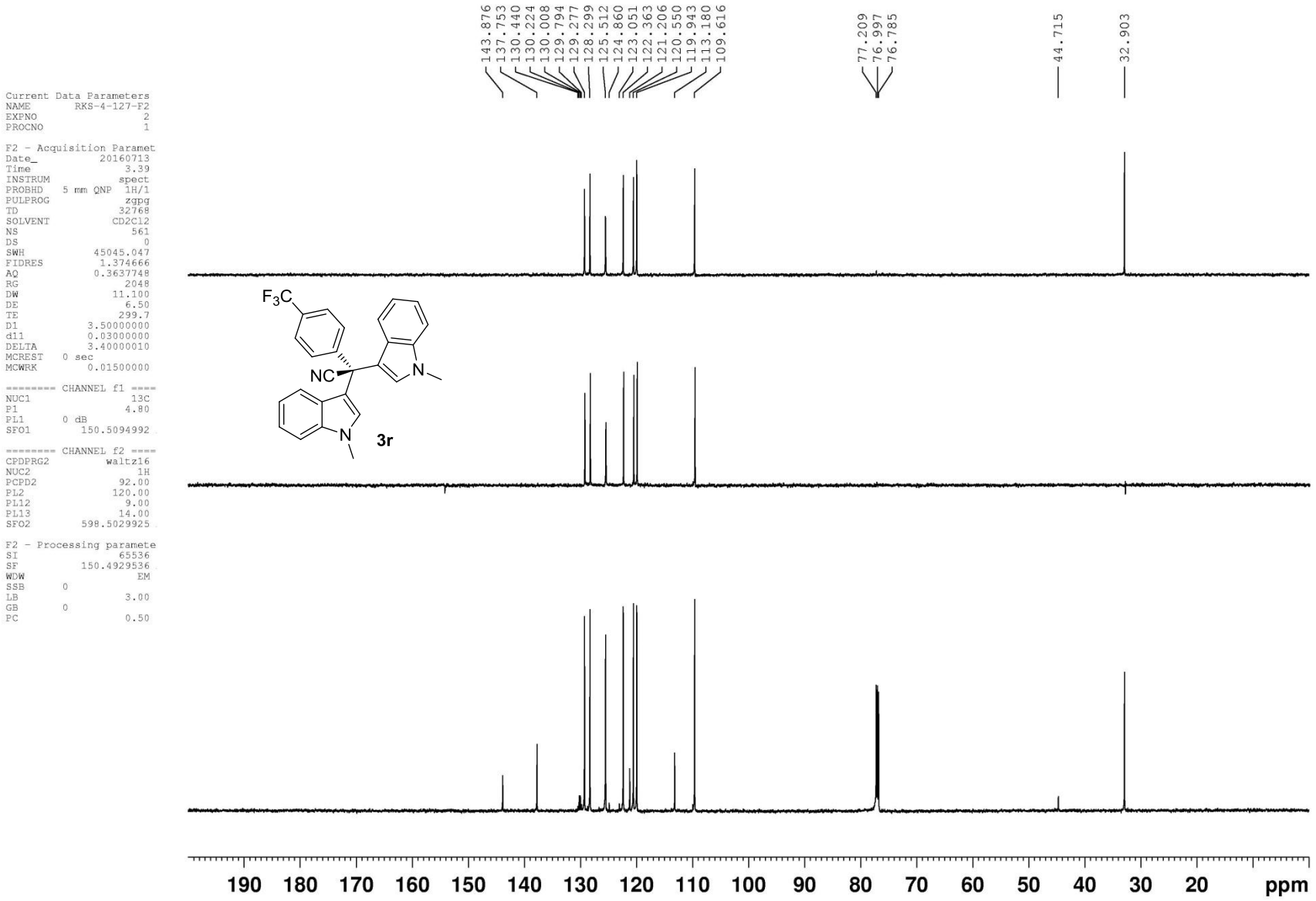
3q

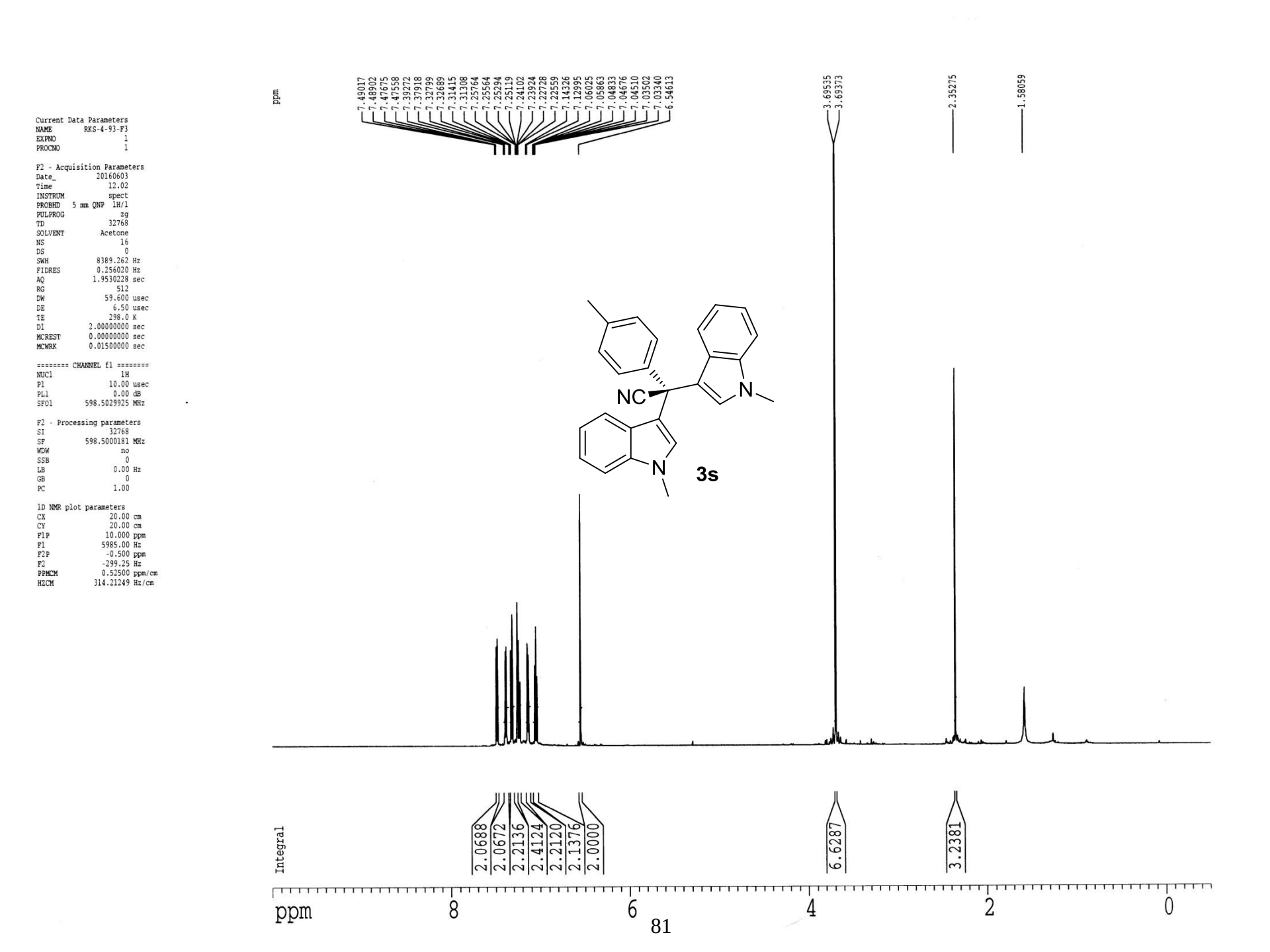


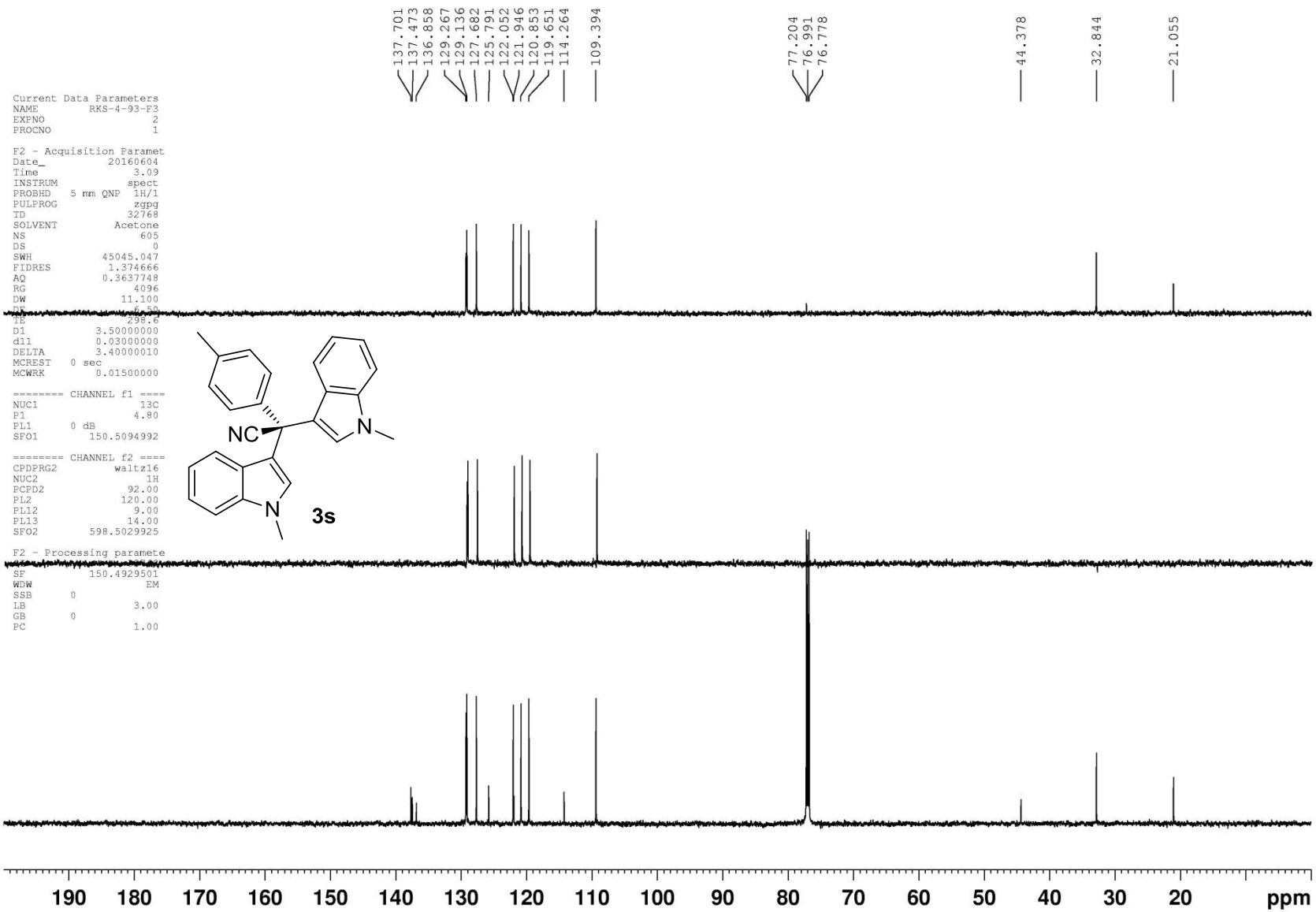
RKS-4-119

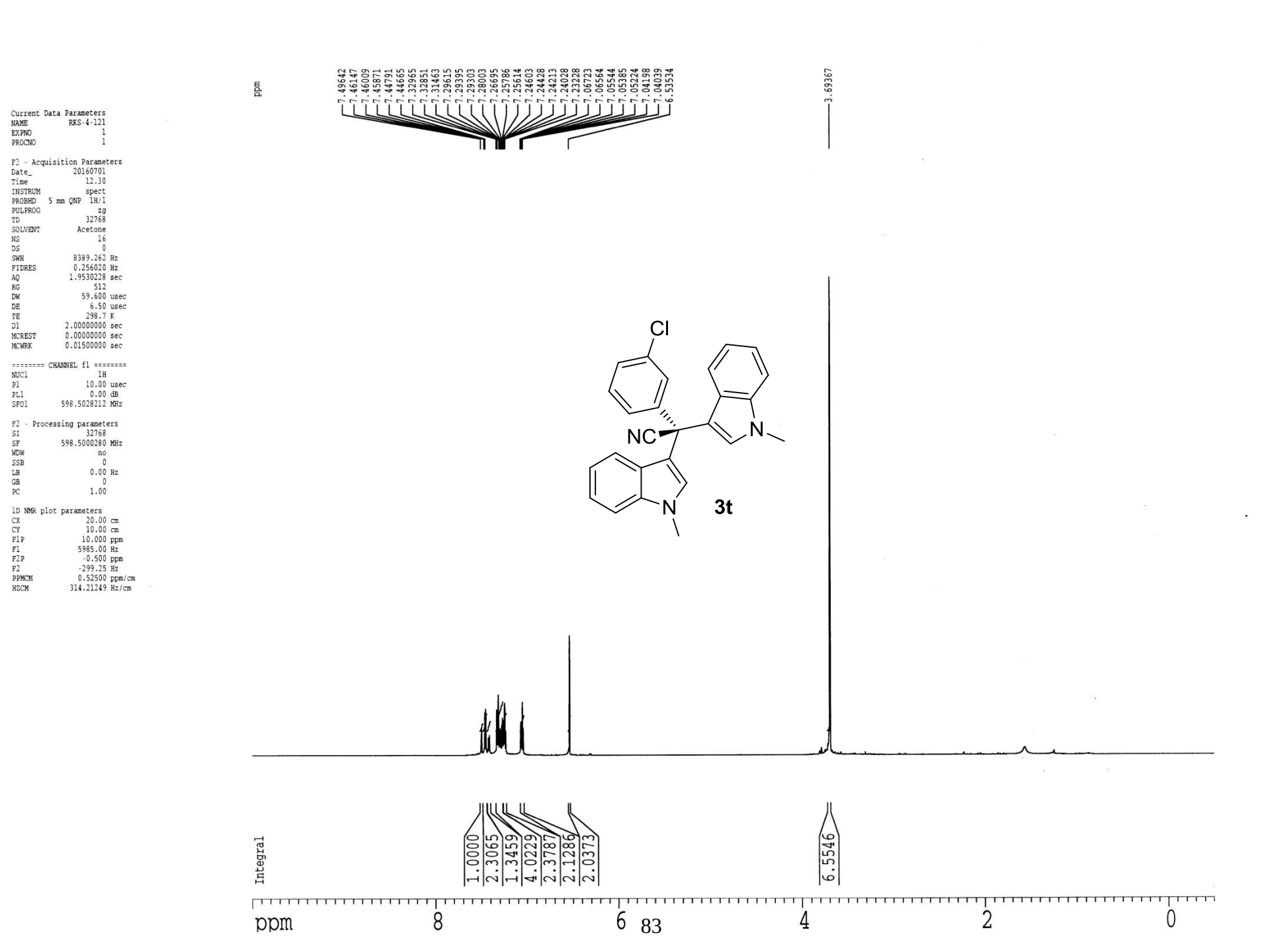

139.056
137.739
131.639
129.630
129.272
125.566
122.286
121.987
121.375
120.656
119.874
113.501
109.548
77.253
77.000
76.747
44.373
32.895
Br
NC
N
N
3q
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

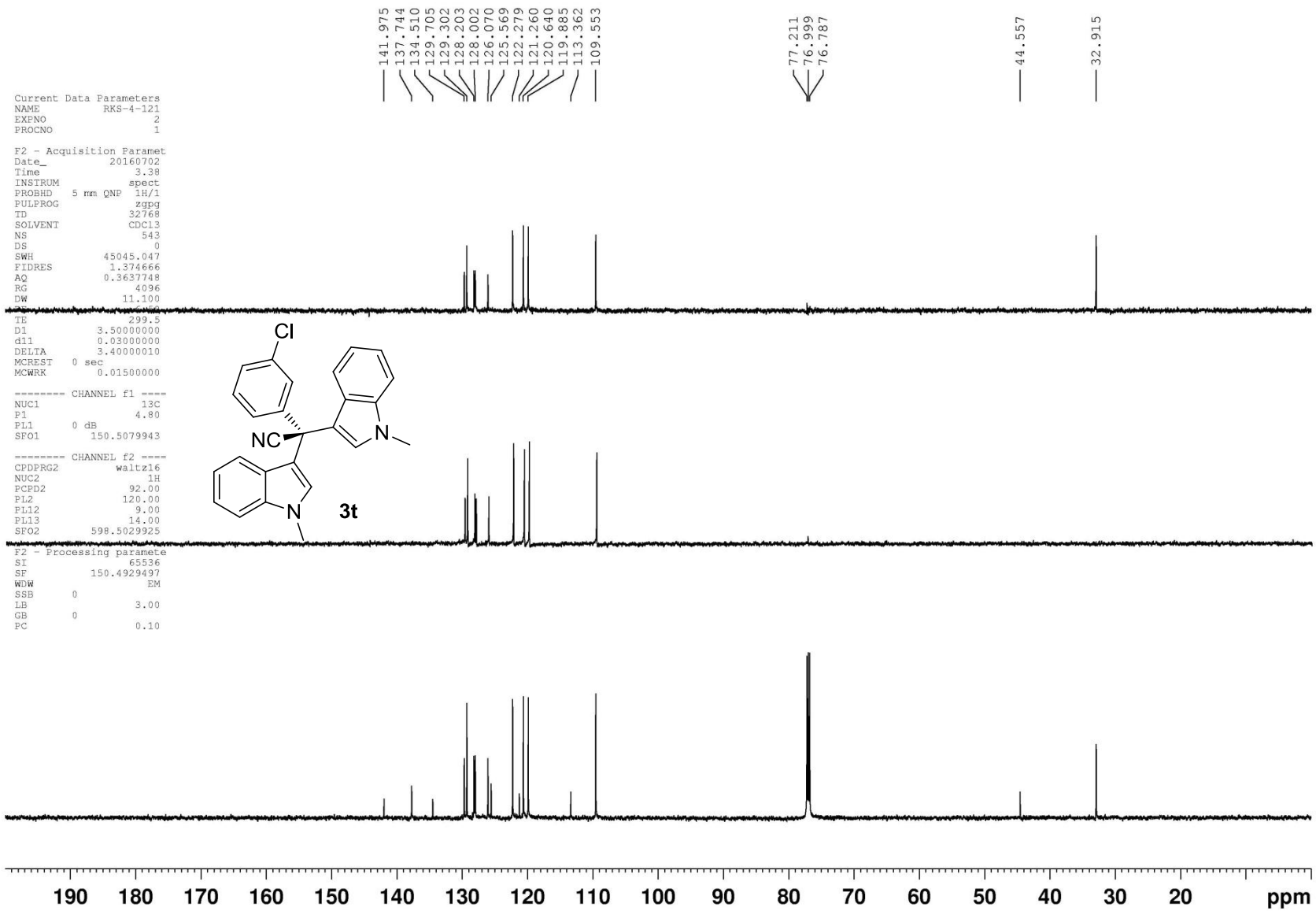

Current Data Parameters
NAME RKS-4-127-F2
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20160712
Time 13.38
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 8389.262 Hz
FIDRES 0.256020 Hz
AQ 1.9530228 sec
RG 512
DW 59.600 usec
DE 6.50 usec
TE 299.7 K
D1 2.00000000 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 598.5000273 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 20.00 cm
CY 20.00 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
7.66448
7.65074
7.60816
7.59458
7.44798
7.43456
7.34424
7.33037
7.27212
7.25983
7.24653
7.24047
7.07632
7.06408
7.05108
6.55488
3.70314
F3C
NC
N
N
3r
Integral
2.1259
2.2233
2.0142
2.1208
2.1997
2.2114
2.0000
6.4778
ppm
8
6
4
2
0

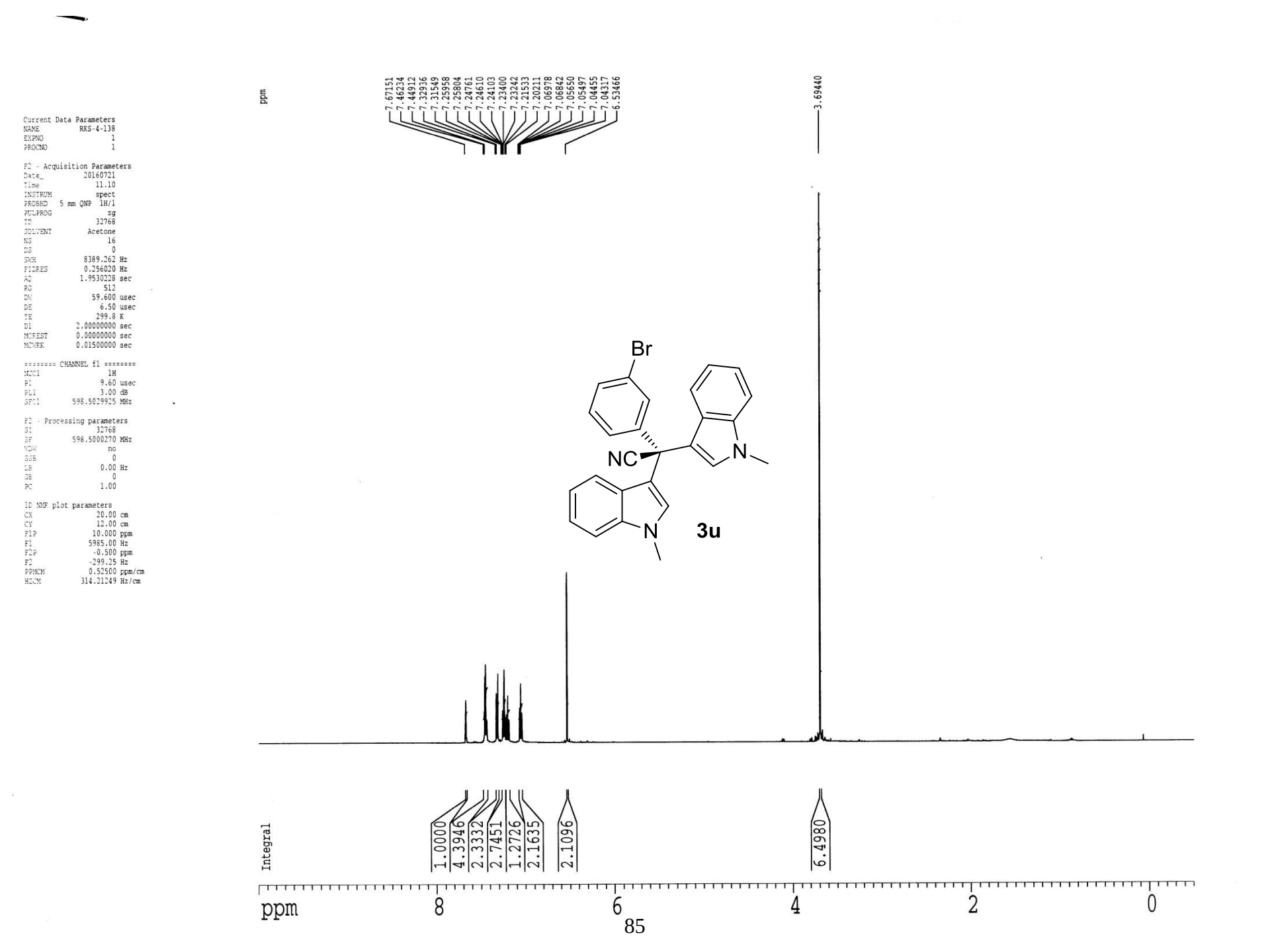

143.876
137.753
130.440
130.224
130.008
129.794
129.277
128.299
125.512
124.860
123.051
122.363
121.206
120.550
119.943
113.180
109.616
77.209
76.997
76.785
44.715
32.903
Current Data Parameters
NAME RKS-4-127-F2
EXPNO 2
PROCNO 1
F2 - Acquisition Paramet
Date_ 20160713
Time 3.39
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CD2Cl2
NS 561
DS 0
SWH 45045.047
FIDRES 1.374666
AQ 0.3637748
RG 2048
DW 11.100
DE 6.50
TE 299.7
D1 3.50000000
d11 0.03000000
DELTA 3.40000010
MCREST 0 sec
MCWRK 0.01500000
======== CHANNEL f1 ====
NUC1 13C
P1 4.80
PL1 0 dB
SFO1 150.5094992
======== CHANNEL f2 ====
CPDPRG2 waltz16
NUC2 1H
PCPD2 92.00
PL2 120.00
PL12 9.00
PL13 14.00
SFO2 598.5029925
F2 - Processing paramete
SI 65536
SF 150.4929536
WDW EM
SSB 0
LB 3.00
GB 0
PC 0.50
F3C
NC
N
N
3r
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm


Current Data Parameters
NAME RKS-4-93-F3
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20160603
Time 12.02
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg
TD 32768
SOLVENT Acetone
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 298.0 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 598.5000181 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 20.00 cm
CY 20.00 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
7.49017
7.48902
7.47675
7.47558
7.39272
7.37918
7.32799
7.32689
7.31415
7.31308
7.25764
7.25564
7.25294
7.25119
7.24102
7.23924
7.22728
7.22559
7.14326
7.12995
7.06025
7.05863
7.04833
7.04676
7.04510
7.03502
7.03340
6.54613
3.69535
3.69373
2.35275
1.58059
NC
N
N
3s
Integral
2.0688
2.0672
2.2136
2.4124
2.2120
2.1376
2.0000
6.6287
3.2381
ppm
8
6
4
2
0

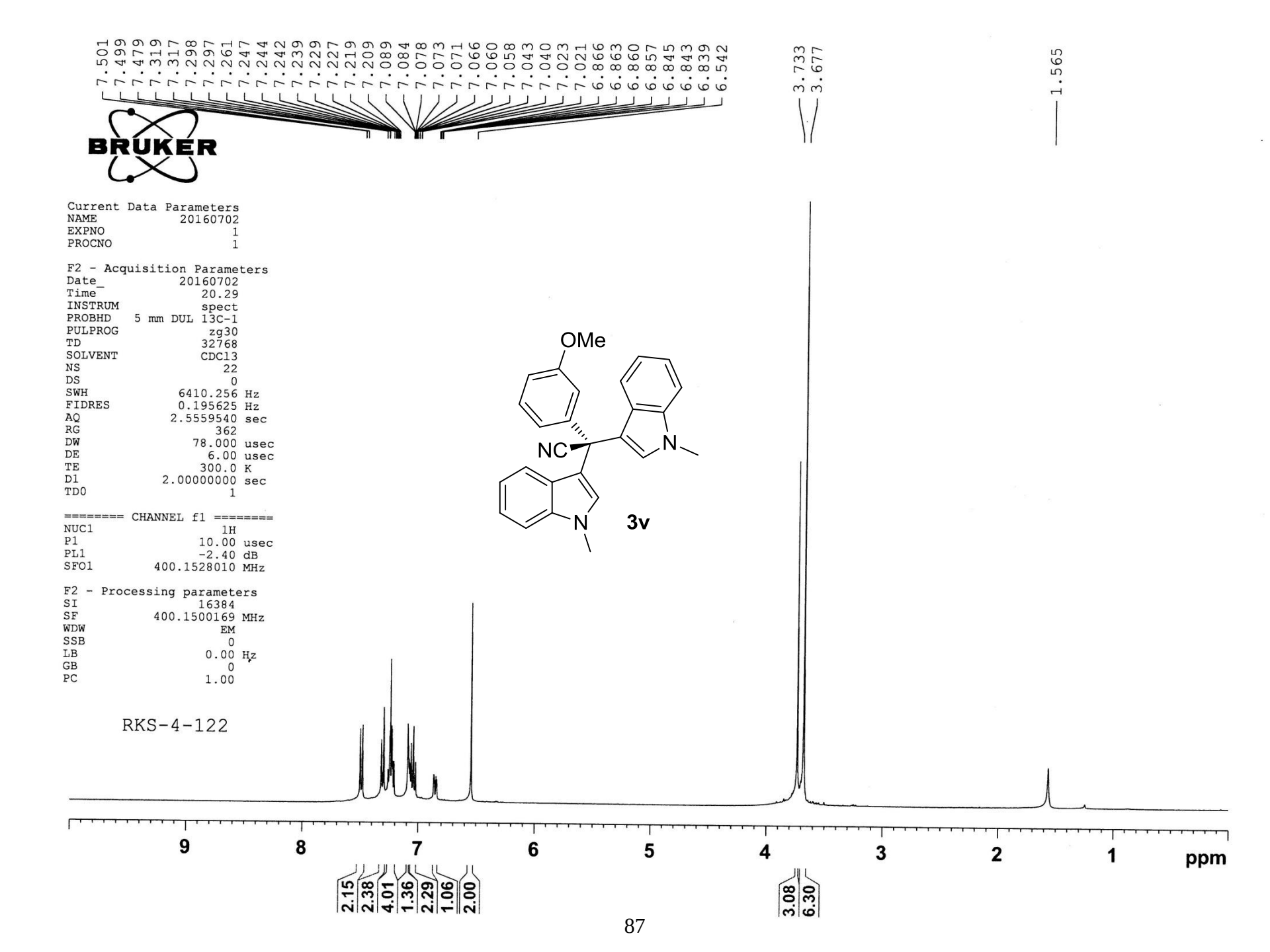

137.701
137.473
136.858
129.267
129.136
127.682
125.791
122.052
121.946
120.853
119.651
114.264
109.394
77.204
76.991
76.778
44.378
32.844
21.055
Current Data Parameters
NAME RKS-4-93-F3
EXPNO 2
PROCNO 1
F2 - Acquisition Paramet
Date_ 20160604
Time 3.09
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT Acetone
NS 605
DS 0
SWH 45045.047
FIDRES 1.374666
AQ 0.3637748
RG 4096
DW 11.100
TE 298.6
D1 3.50000000
d11 0.03000000
DELTA 3.40000010
MCREST 0 sec
MCWRK 0.01500000
======== CHANNEL f1 ====
NUC1 13C
P1 4.80
PL1 0 dB
SFO1 150.5094992
======== CHANNEL f2 ====
CPDPRG2 waltz16
NUC2 1H
PCPD2 92.00
PL2 120.00
PL12 9.00
PL13 14.00
SFO2 598.5029925
F2 - Processing paramete
SF 150.4929501
WDW EM
SSB 0
LB 3.00
GB 0
PC 1.00
NC
N
N
3s
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

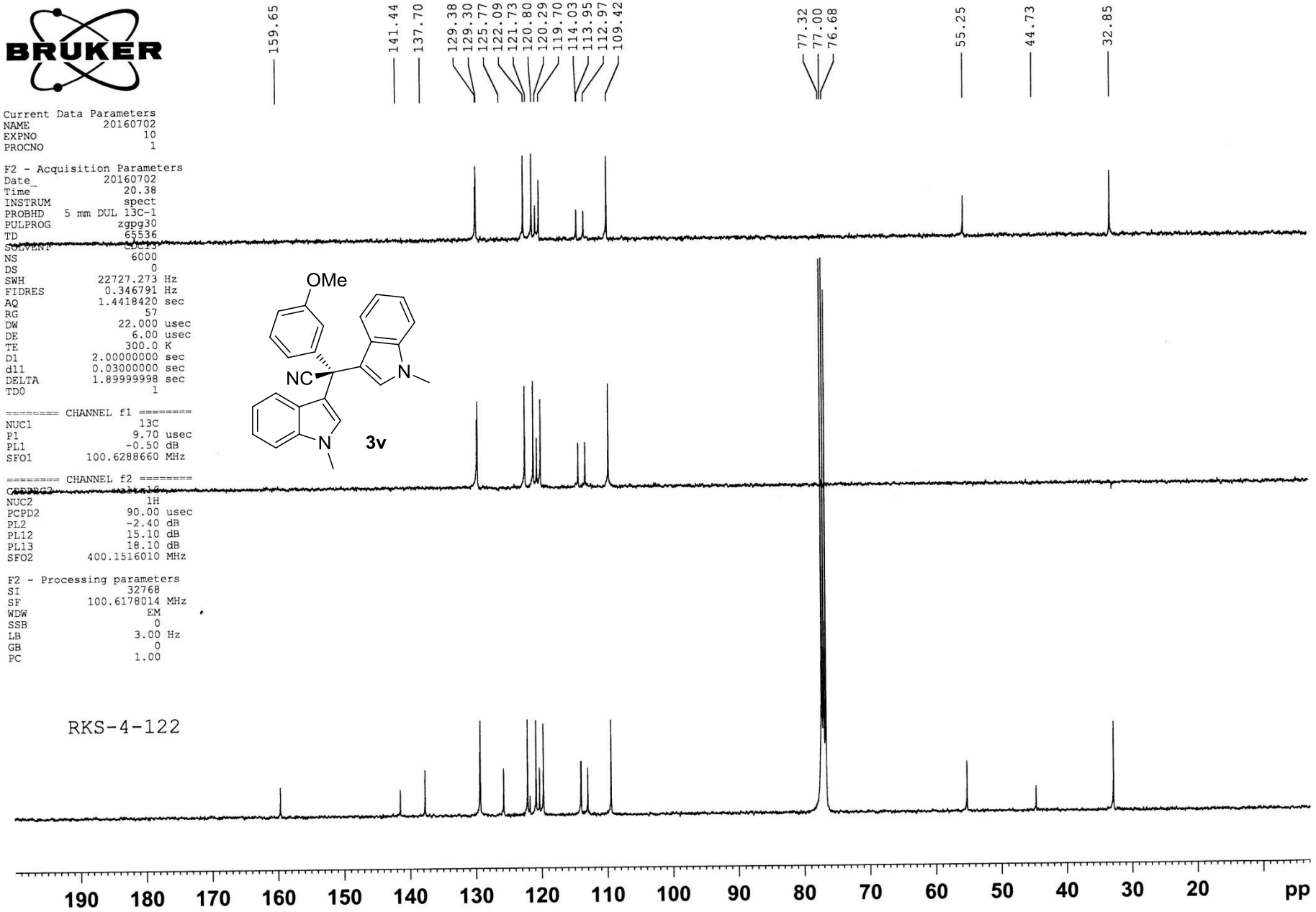

Current Data Parameters
NAME RKS-4-121
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20160701
Time 12.30
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg
TD 32768
SOLVENT Acetone
NS 16
DS 0
SWH 8389.262 Hz
FIDRES 0.256020 Hz
AQ 1.9530228 sec
RG 512
DW 59.600 usec
DE 6.50 usec
TE 298.7 K
D1 2.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 0.00 dB
SFO1 598.5028212 MHz
F2 - Processing parameters
SI 32768
SF 598.5000280 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 20.00 cm
CY 10.00 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
7.49642
7.46147
7.46009
7.45871
7.44791
7.44665
7.32965
7.32851
7.31463
7.29615
7.29395
7.29303
7.28003
7.26695
7.25786
7.25614
7.24603
7.24428
7.24213
7.24028
7.23228
7.06723
7.06564
7.05544
7.05385
7.05224
7.04198
7.04039
6.53534
3.69367
Cl
NC
N
N
3t
Integral
1.0000
2.3065
1.3459
4.0229
2.3787
2.1286
2.0373
6.5546
ppm
8
6
4
2
0

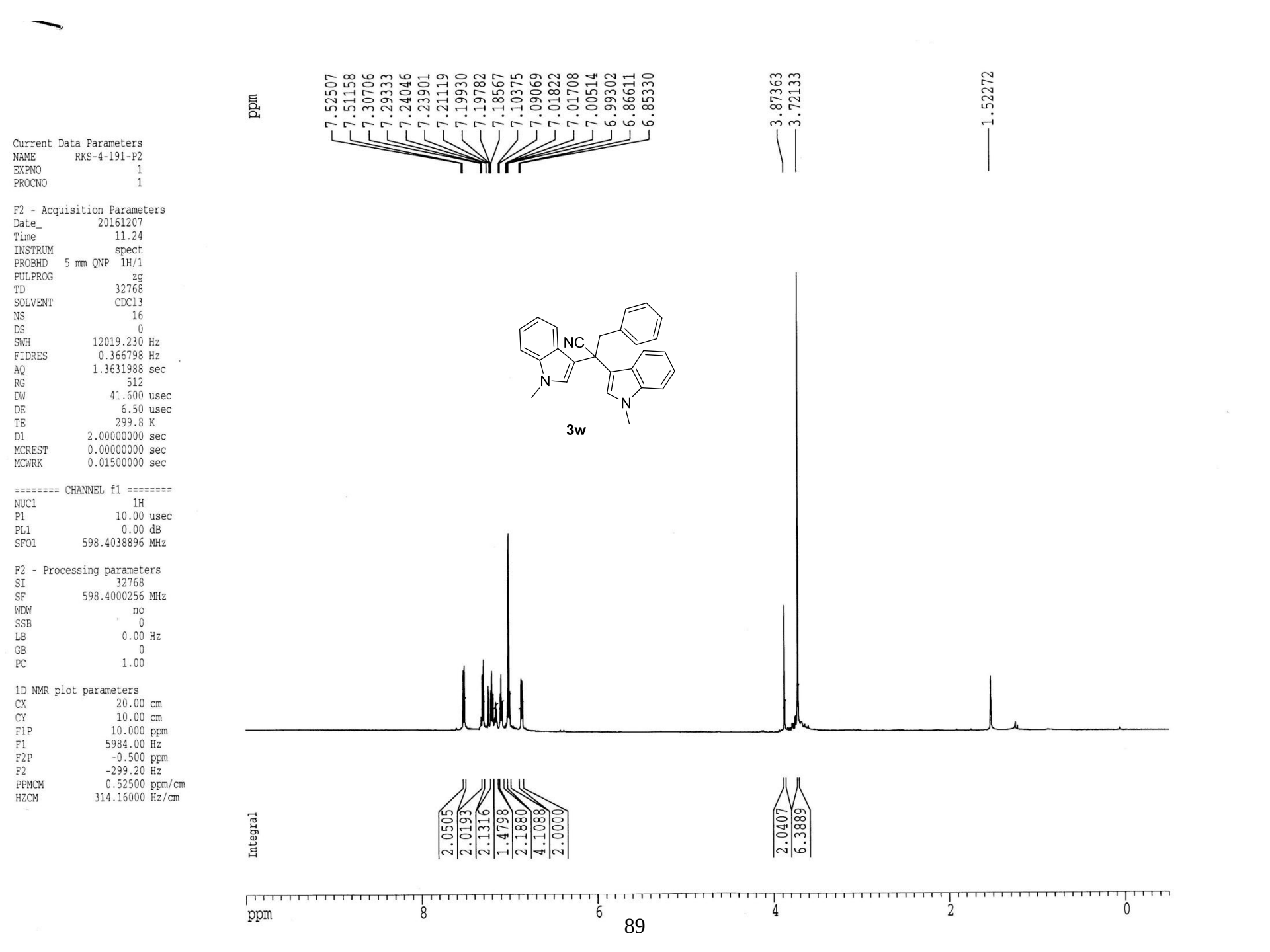

141.975
137.744
134.510
129.705
129.302
128.203
128.002
126.070
125.569
122.279
121.260
120.640
119.885
113.362
109.553
77.211
76.999
76.787
44.557
32.915
Current Data Parameters
NAME RKS-4-121
EXPNO 2
PROCNO 1
F2 - Acquisition Paramet
Date_ 20160702
Time 3.38
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 543
DS 0
SWH 45045.047
FIDRES 1.374666
AQ 0.3637748
RG 4096
DW 11.100
TE 299.5
D1 3.50000000
d11 0.03000000
DELTA 3.40000010
MCREST 0 sec
MCWRK 0.01500000
======== CHANNEL f1 ====
NUC1 13C
P1 4.80
PL1 0 dB
SFO1 150.5079943
======== CHANNEL f2 ====
CPDPRG2 waltz16
NUC2 1H
PCPD2 92.00
PL2 120.00
PL12 9.00
PL13 14.00
SFO2 598.5029925
F2 - Processing paramete
SI 65536
SF 150.4929497
WDW EM
SSB 0
LB 3.00
GB 0
PC 0.10
Cl
NC
N
N
3t
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

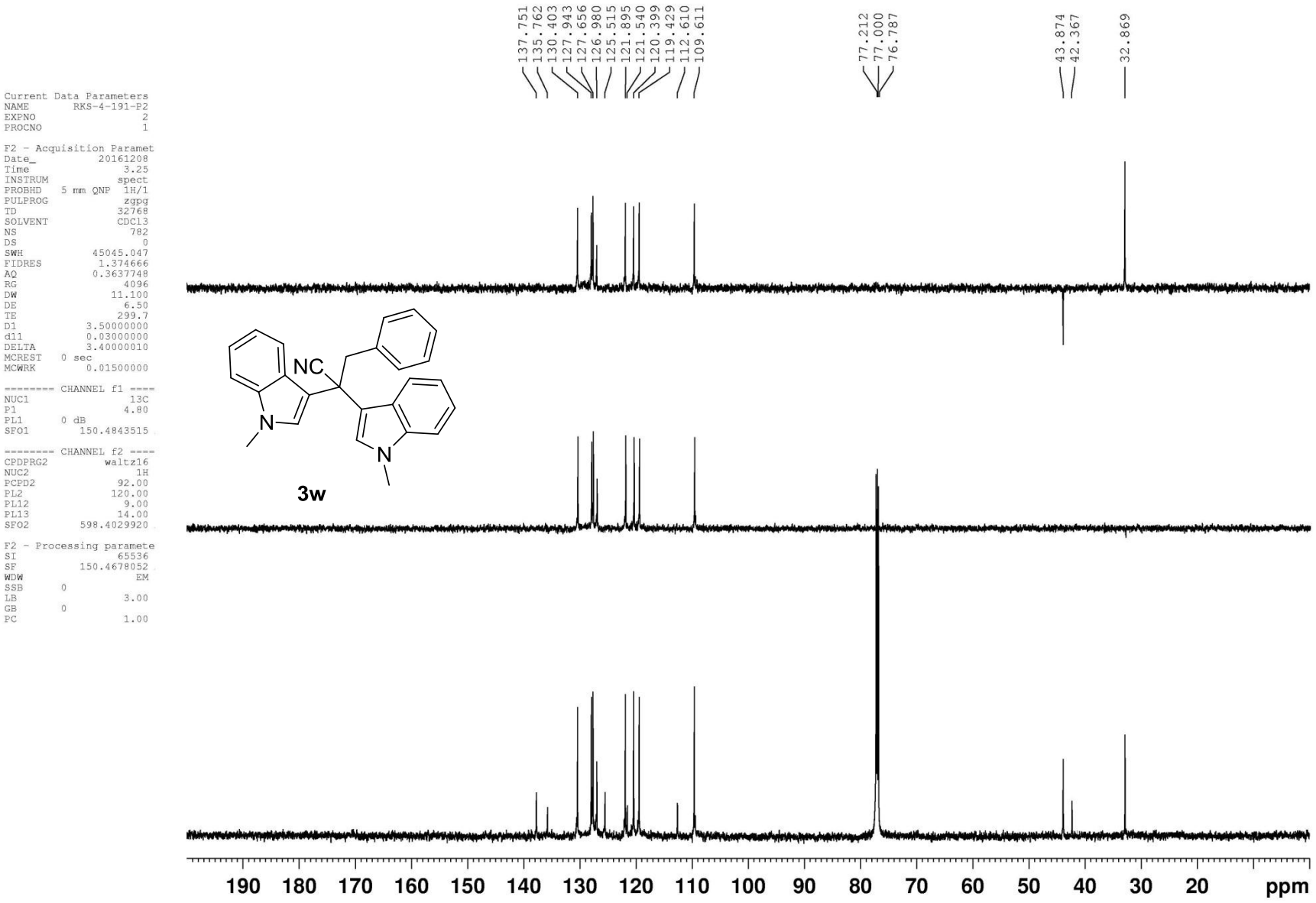

Current Data Parameters
NAME RKS-4-138
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20160721
Time 11.10
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg
TD 32768
SOLVENT Acetone
NS 16
DS 0
SWH 8389.262 Hz
FIDRES 0.256020 Hz
AQ 1.9530228 sec
RG 512
DW 59.600 usec
DE 6.50 usec
TE 299.8 K
D1 2.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 9.60 usec
PL1 3.00 dB
SFO1 598.5029925 MHz
F2 - Processing parameters
SI 32768
SF 598.5000270 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 20.00 cm
CY 12.00 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
7.67151
7.46234
7.44912
7.32936
7.31549
7.25958
7.25804
7.24761
7.24610
7.24103
7.23400
7.23242
7.21533
7.20211
7.06978
7.06842
7.05650
7.05497
7.04455
7.04317
6.53466
3.69440
Br
NC
N
N
3u
Integral
1.0000
4.3946
2.3332
2.7451
1.2726
2.1635
2.1096
6.4980
ppm
8
6
4
2
0

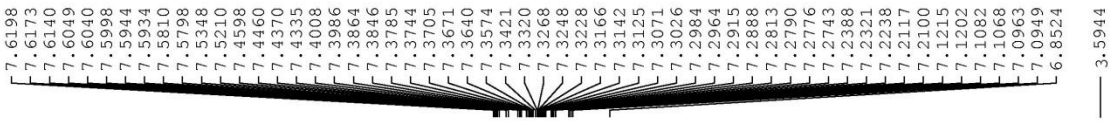
Current Data Parameters
NAME RKS-4-138
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20160721
Time 11.43
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 537
DS 0
SWH 45045.047 Hz
FIDRES 1.374666 Hz
AQ 0.3637748 sec
RG 4096
DW 11.100 usec
DE 6.50 usec
TE 300.5 K
D1 3.50000000 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 150.4929508 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 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
142.198
137.743
131.138
130.826
129.979
129.308
126.519
125.554
122.662
122.281
121.230
120.636
119.889
113.351
109.552
77.209
76.997
76.785
44.509
32.914
Br
NC
N
N
3u
ppm
180
160
140
120
100
80
60
40
20

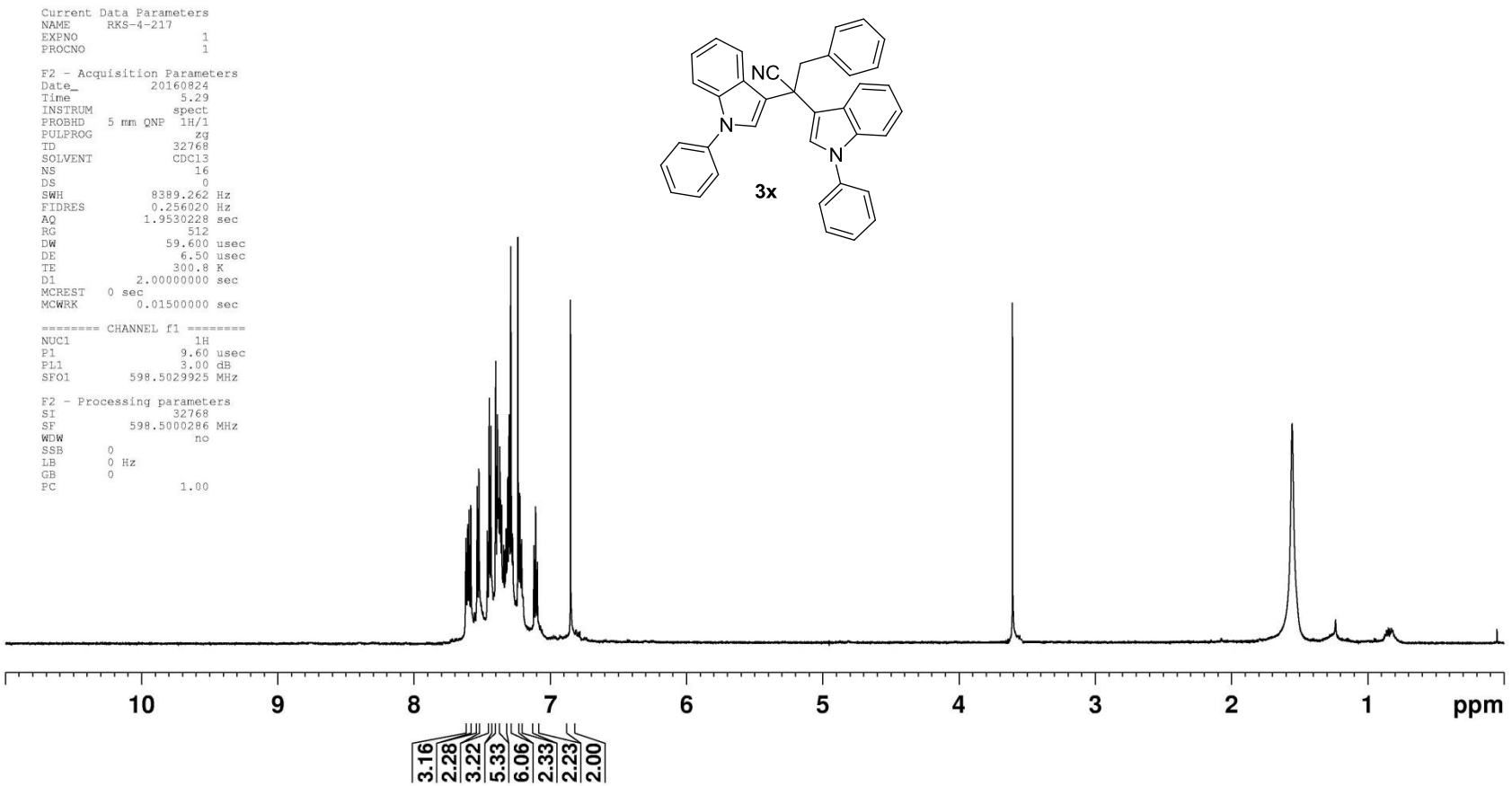

7.501
7.499
7.479
7.319
7.317
7.298
7.297
7.261
7.247
7.244
7.242
7.239
7.229
7.227
7.219
7.209
7.089
7.084
7.078
7.073
7.071
7.066
7.060
7.058
7.043
7.040
7.023
7.021
6.866
6.863
6.860
6.857
6.845
6.843
6.839
6.542
3.733
3.677
1.565
BRUKER
Current Data Parameters
NAME 20160702
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20160702
Time 20.29
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 22
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 400.1500169 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
OMe
NC
N
N
3v
RKS-4-122
9
8
7
6
5
4
3
2
1
ppm
2.15
2.38
4.01
1.36
2.29
1.06
2.00
3.08
6.30

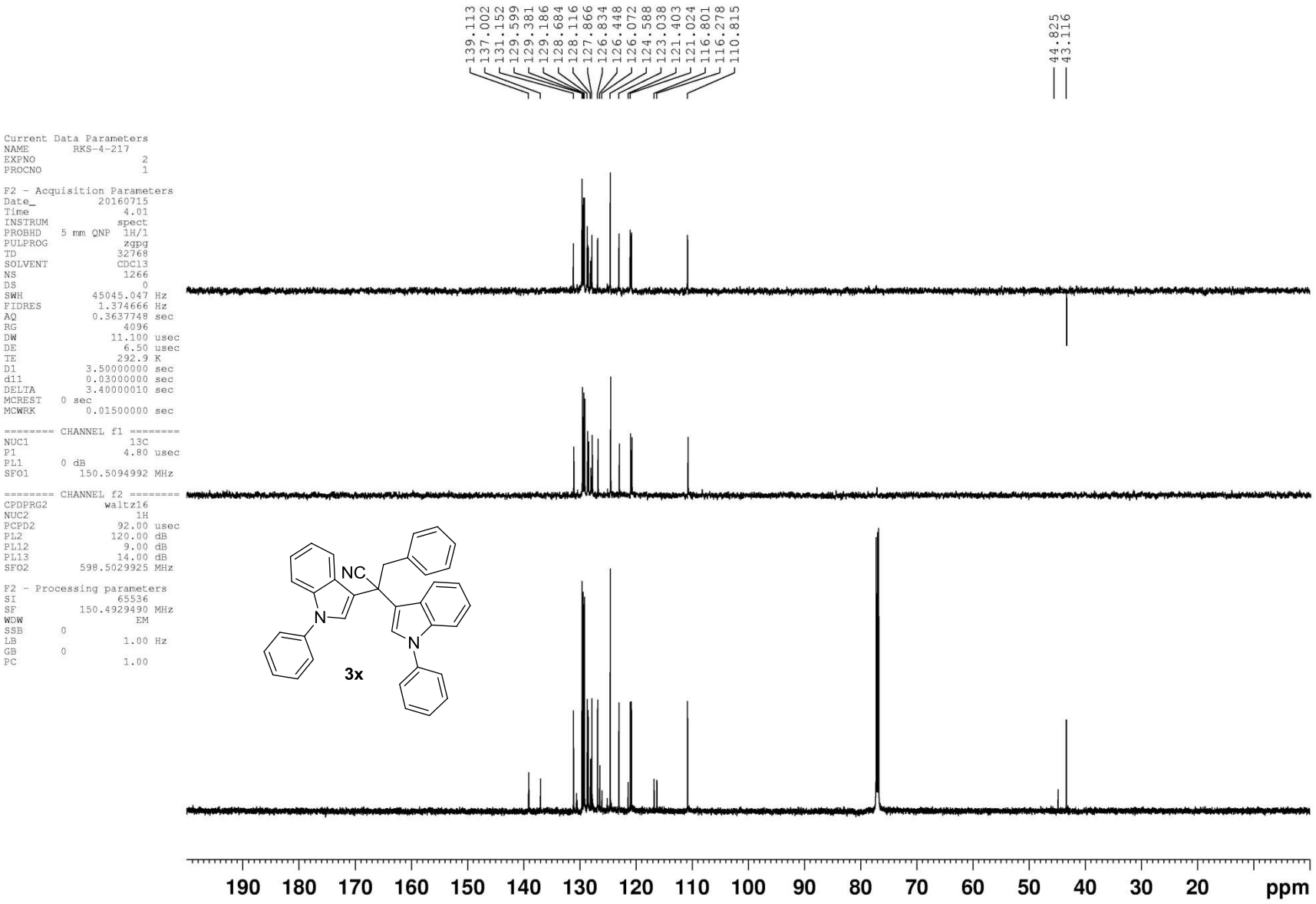

159.65
141.44
137.70
129.38
129.30
125.77
122.09
121.73
120.80
120.29
119.70
114.03
113.95
112.97
109.42
77.32
77.00
76.68
55.25
44.73
32.85
Current Data Parameters
NAME 20160702
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20160702
Time 20.38
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 6000
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
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.70 usec
PL1 -0.50 dB
SFO1 100.6288660 MHz
======== CHANNEL f2 ========
NUC2 1H
PCPD2 90.00 usec
PL2 -2.40 dB
PL12 15.10 dB
PL13 18.10 dB
SFO2 400.1516010 MHz
F2 - Processing parameters
SI 32768
SF 100.6178014 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
OMe
NC
N
N
3v
RKS-4-122
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

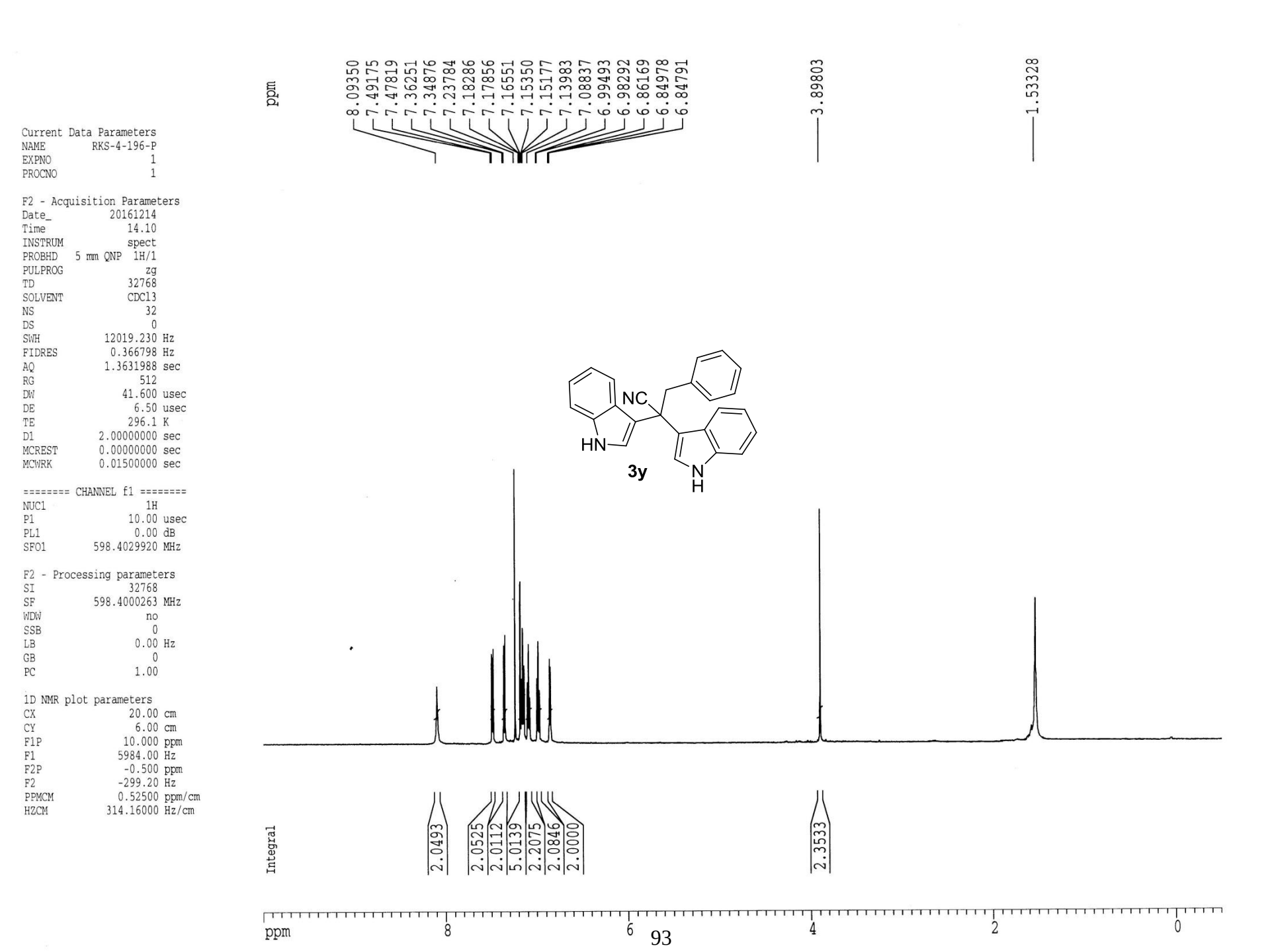

Current Data Parameters
NAME RKS-4-191-P2
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20161207
Time 11.24
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 12019.230 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 512
DW 41.600 usec
DE 6.50 usec
TE 299.8 K
D1 2.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 0.00 dB
SFO1 598.4038896 MHz
F2 - Processing parameters
SI 32768
SF 598.4000256 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 20.00 cm
CY 10.00 cm
F1P 10.000 ppm
F1 5984.00 Hz
F2P -0.500 ppm
F2 -299.20 Hz
PPMCM 0.52500 ppm/cm
HZCM 314.16000 Hz/cm
ppm
7.52507
7.51158
7.30706
7.29333
7.24046
7.23901
7.21119
7.19930
7.19782
7.18567
7.10375
7.09069
7.01822
7.01708
7.00514
6.99302
6.86611
6.85330
3.87363
3.72133
1.52272
NC
N
N
3w
Integral
2.0505
2.0193
2.1316
1.4798
2.1880
4.1088
2.0000
2.0407
6.3889
ppm
8
6
4
2
0

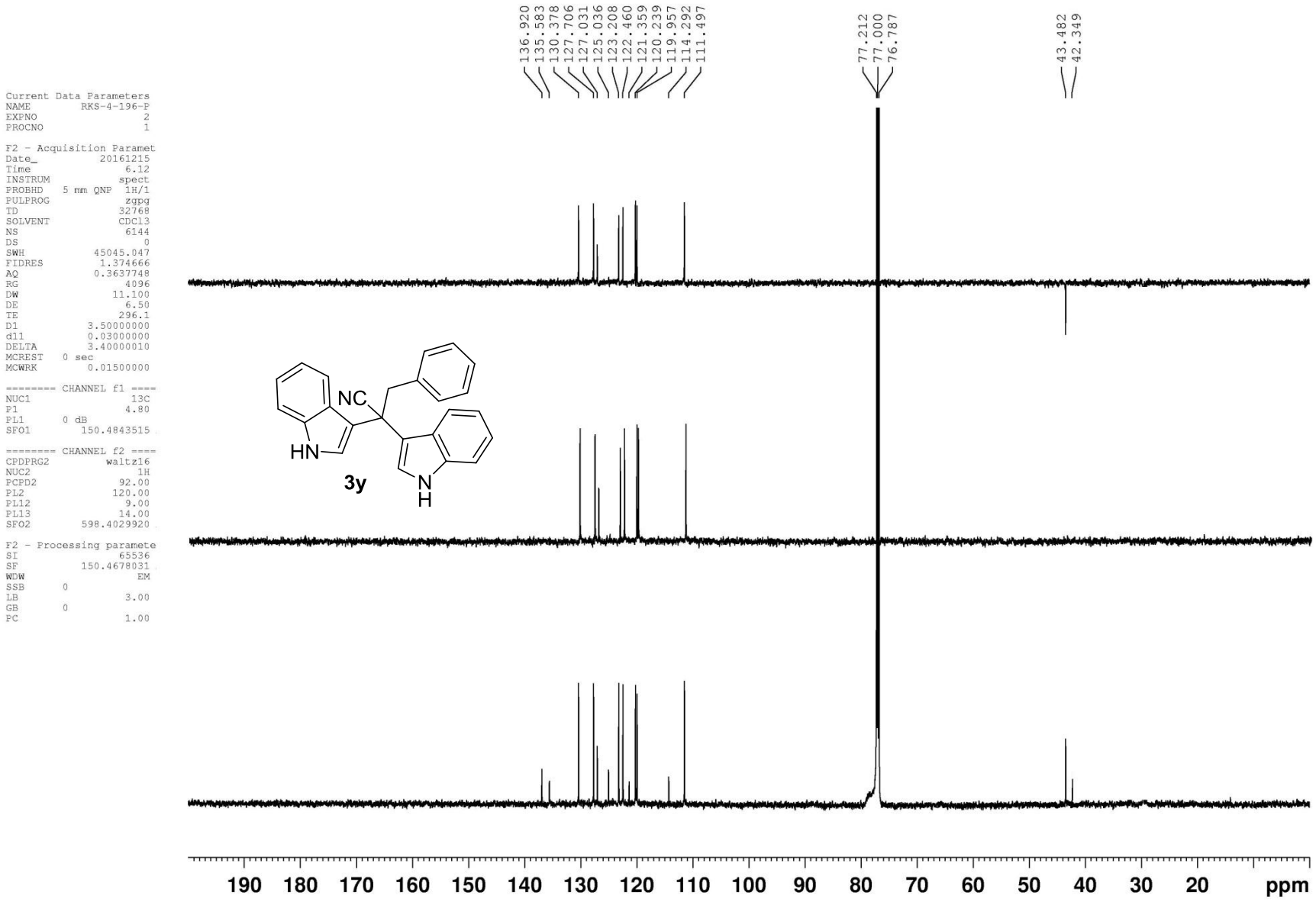

Current Data Parameters
NAME RKS-4-191-P2
EXPNO 2
PROCNO 1
F2 - Acquisition Paramet
Date_ 20161208
Time 3.25
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 782
DS 0
SWH 45045.047
FIDRES 1.374666
AQ 0.3637748
RG 4096
DW 11.100
DE 6.50
TE 299.7
D1 3.50000000
d11 0.03000000
DELTA 3.40000010
MCREST 0 sec
MCWRK 0.01500000
======== CHANNEL f1 ====
NUC1 13C
P1 4.80
PL1 0 dB
SFO1 150.4843515
======== CHANNEL f2 ====
CPDPRG2 waltz16
NUC2 1H
PCPD2 92.00
PL2 120.00
PL12 9.00
PL13 14.00
SFO2 598.4029920
F2 - Processing paramete
SI 65536
SF 150.4678052
WDW EM
SSB 0
LB 3.00
GB 0
PC 1.00
137.751
135.762
130.403
127.943
127.656
126.980
125.515
121.895
121.540
120.399
119.429
112.610
109.611
77.212
77.000
76.787
43.874
42.367
32.869
NC
N
N
3w
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm


7.6198
7.6173
7.6140
7.6049
7.6040
7.5998
7.5944
7.5934
7.5810
7.5798
7.5348
7.5210
7.4598
7.4460
7.4370
7.4335
7.4008
7.3986
7.3864
7.3846
7.3785
7.3744
7.3705
7.3671
7.3640
7.3574
7.3421
7.3320
7.3268
7.3248
7.3228
7.3166
7.3142
7.3125
7.3071
7.3026
7.2984
7.2964
7.2915
7.2888
7.2813
7.2790
7.2776
7.2743
7.2388
7.2321
7.2238
7.2117
7.2100
7.1215
7.1202
7.1082
7.1068
7.0963
7.0949
6.8524
3.5944
1.5550


Current Data Parameters
NAME RKS-4-217
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20160824
Time 5.29
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 300.8 K
D1 2.00000000 sec
MCREST 0 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 9.60 usec
PL1 3.00 dB
SFO1 598.5029925 MHz
F2 - Processing parameters
SI 32768
SF 598.5000286 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 1.00
NC
N
N
3x
10
9
8
7
6
5
4
3
2
1
ppm
3.16
2.28
3.22
5.33
6.06
2.33
2.23
2.00


139.113
137.002
131.152
129.599
129.381
129.186
128.684
128.116
127.866
126.834
126.448
126.072
124.588
123.038
121.403
121.024
116.801
116.278
110.815
44.825
43.116
Current Data Parameters
NAME RKS-4-217
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20160715
Time 4.01
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 1266
DS 0
SWH 45045.047 Hz
FIDRES 1.374666 Hz
AQ 0.3637748 sec
RG 4096
DW 11.100 usec
DE 6.50 usec
TE 292.9 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 150.5094992 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 150.4929490 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00
NC
N
N
3x
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm


ppm
8.09350
7.49175
7.47819
7.36251
7.34876
7.23784
7.18286
7.17856
7.16551
7.15350
7.15177
7.13983
7.08837
6.99493
6.98292
6.86169
6.84978
6.84791
3.89803
1.53328
Current Data Parameters
NAME RKS-4-196-P
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20161214
Time 14.10
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 32
DS 0
SWH 12019.230 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 512
DW 41.600 usec
DE 6.50 usec
TE 296.1 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 598.4029920 MHz
F2 - Processing parameters
SI 32768
SF 598.4000263 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 20.00 cm
CY 6.00 cm
F1P 10.000 ppm
F1 5984.00 Hz
F2P -0.500 ppm
F2 -299.20 Hz
PPMCM 0.52500 ppm/cm
HZCM 314.16000 Hz/cm
NC
HN
N
H
3y
Integral
2.0493
2.0525
2.0112
5.0139
2.2075
2.0846
2.0000
2.3533
ppm
8
6
4
2
0


136.920
135.583
130.378
127.706
127.031
125.036
123.208
122.460
121.359
120.239
119.957
114.292
111.497
77.212
77.000
76.787
43.482
42.349
Current Data Parameters
NAME RKS-4-196-P
EXPNO 2
PROCNO 1
F2 - Acquisition Paramet
Date_ 20161215
Time 6.12
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 6144
DS 0
SWH 45045.047
FIDRES 1.374666
AQ 0.3637748
RG 4096
DW 11.100
DE 6.50
TE 296.1
D1 3.50000000
d11 0.03000000
DELTA 3.40000010
MCREST 0 sec
MCWRK 0.01500000
======== CHANNEL f1 ====
NUC1 13C
P1 4.80
PL1 0 dB
SFO1 150.4843515
======== CHANNEL f2 ====
CPDPRG2 waltz16
NUC2 1H
PCPD2 92.00
PL2 120.00
PL12 9.00
PL13 14.00
SFO2 598.4029920
F2 - Processing paramete
SI 65536
SF 150.4678031
WDW EM
SSB 0
LB 3.00
GB 0
PC 1.00
NC
HN
N
H
3y
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

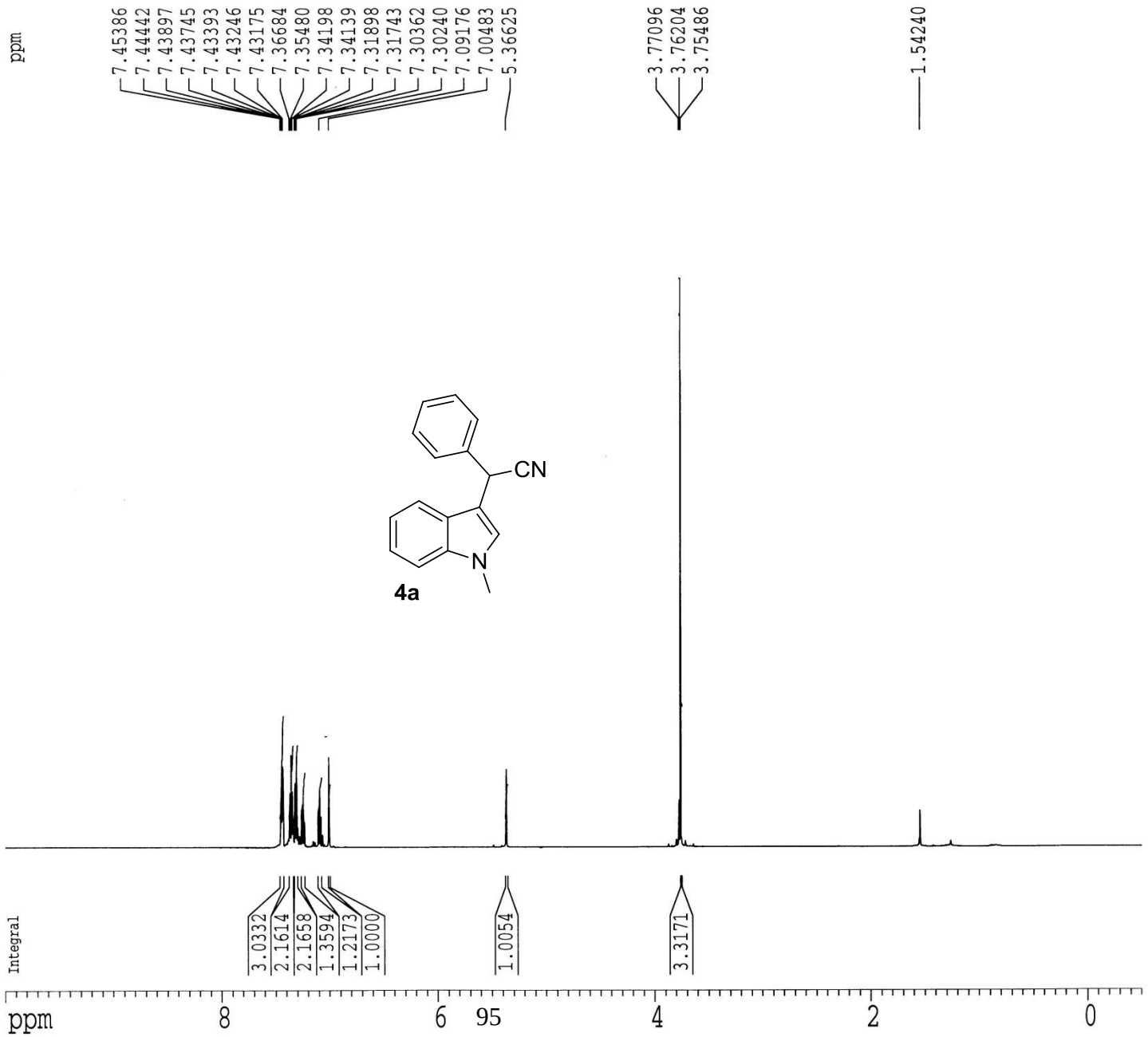
Current Data Parameters
NAME RKS-3-146-P
EXPNO 1
PROCNO 1

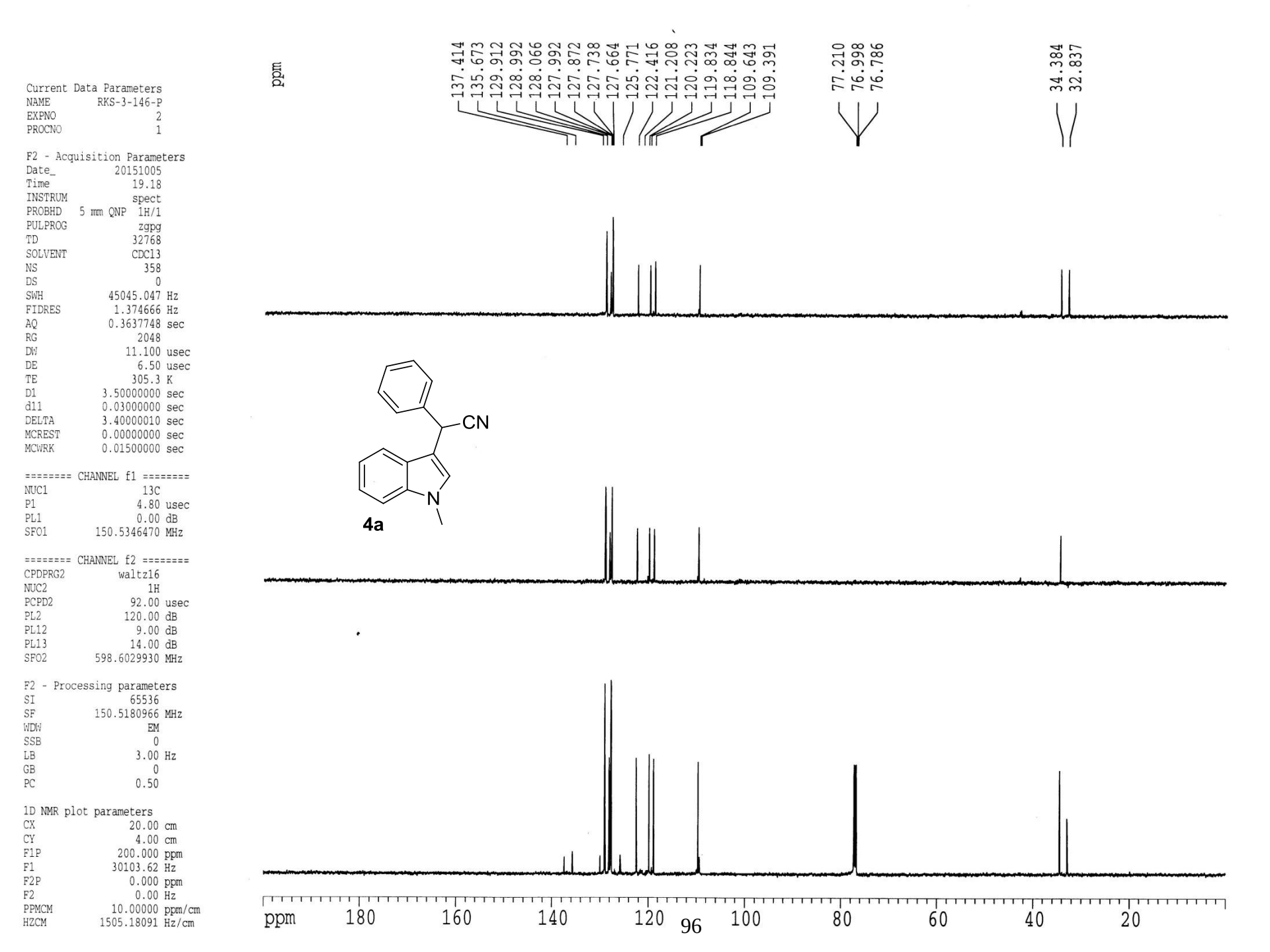
F2 - Acquisition Parameters
Date_ 20151005
Time 19.15
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 9541.984 Hz
FIDRES 0.291198 Hz
AQ 1.7170932 sec
RG 128
DW 52.400 usec
DE 6.50 usec
TE 304.4 K
D1 2.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

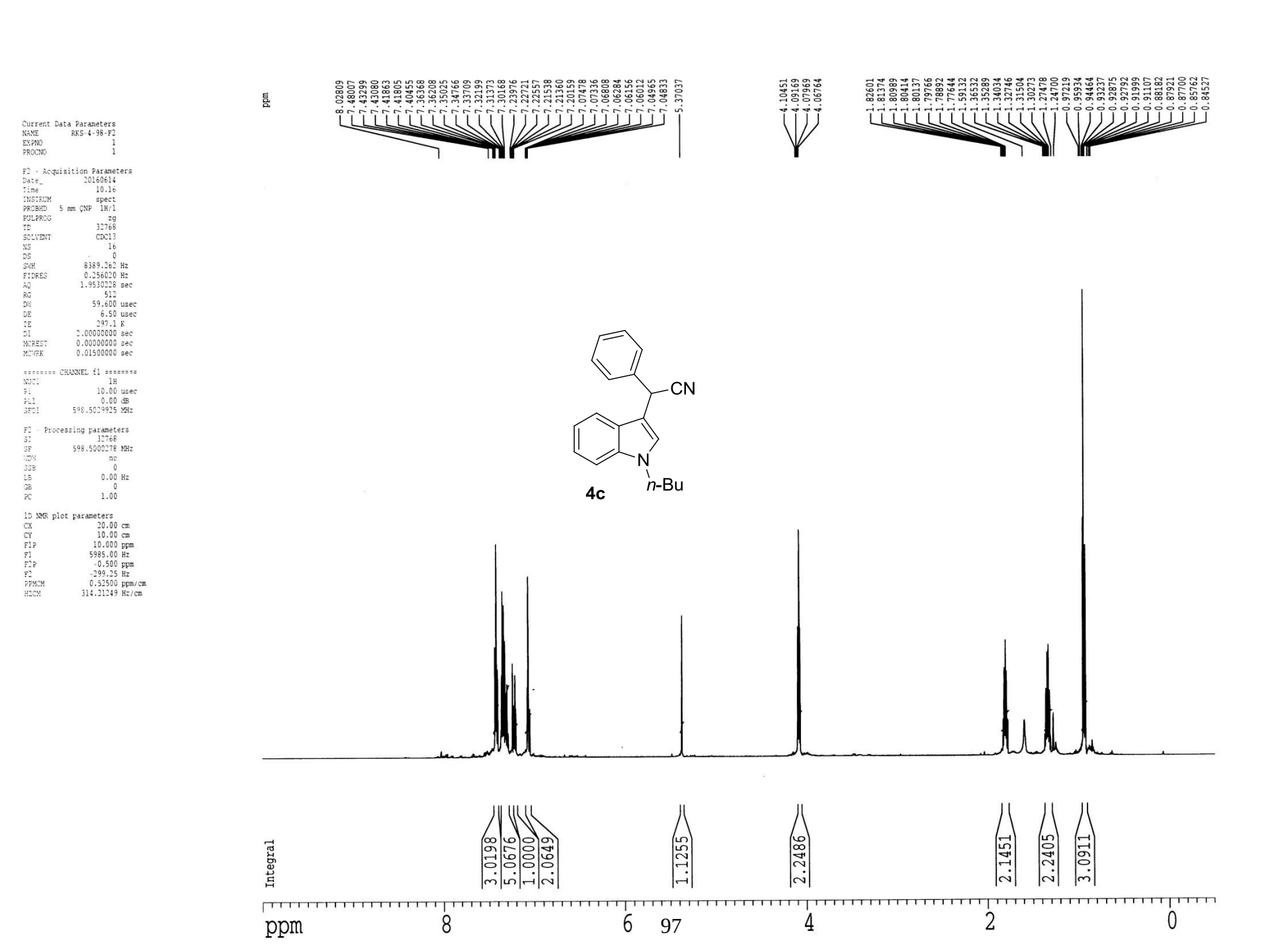
======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 0.00 dB
SFO1 598.6029930 MHz

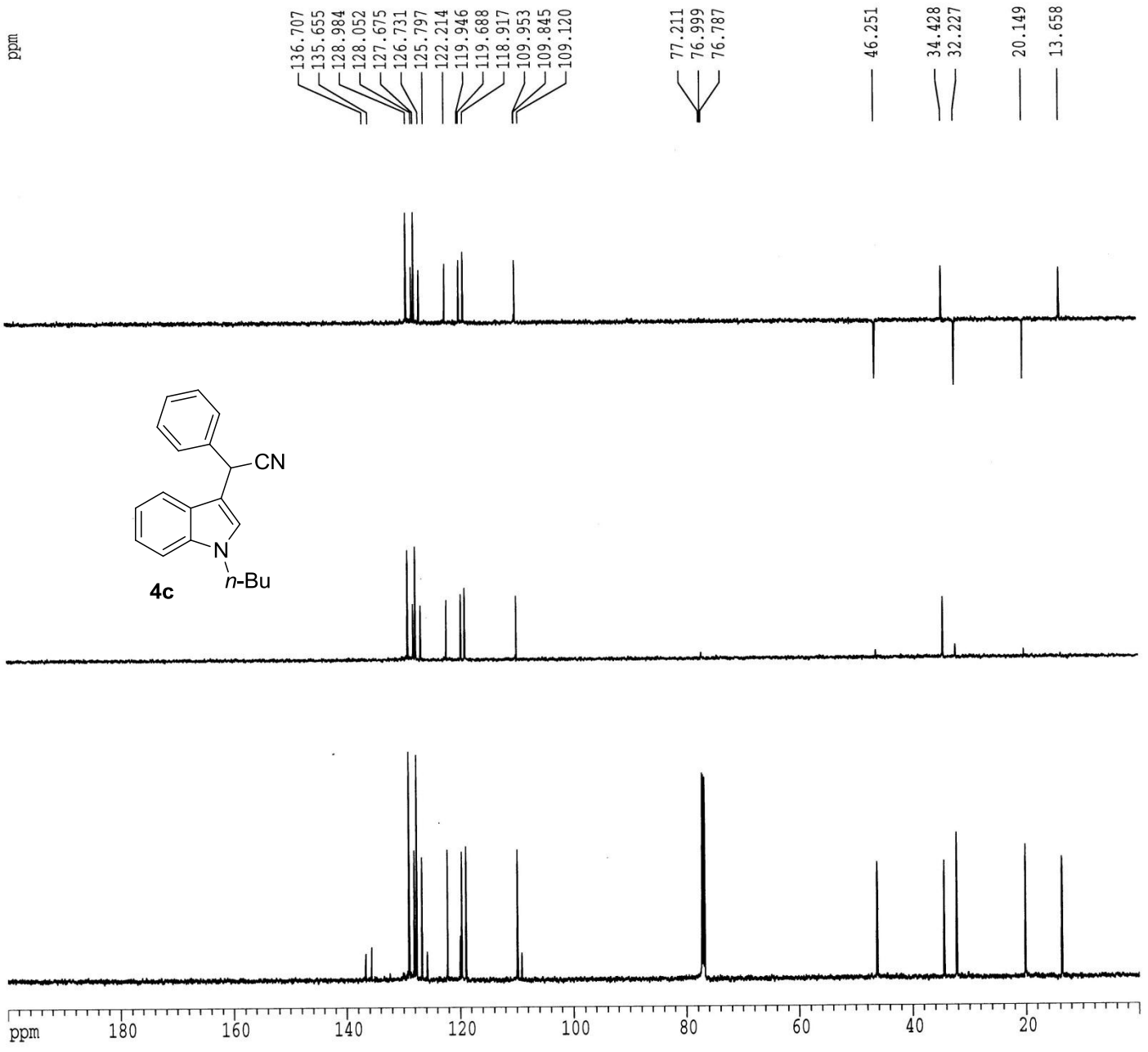
F2 - Processing parameters
SI 32768
SF 598.6000304 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 20.00 cm
CY 10.00 cm
F1P 10.000 ppm
F1 5986.00 Hz
F2P -0.500 ppm
F2 -299.30 Hz
PPMCM 0.52500 ppm/cm
HZCM 314.26501 Hz/cm




Current Data Parameters
NAME RKS-3-146-P
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20151005
Time 19.18
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 358
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 305.3 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 150.5346470 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 150.5180966 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 200.000 ppm
F1 30103.62 Hz
F2P 0.000 ppm
F2 0.00 Hz
PPMCM 10.00000 ppm/cm
HZCM 1505.18091 Hz/cm
ppm
137.414
135.673
129.912
128.992
128.066
127.992
127.872
127.738
127.664
125.771
122.416
121.208
120.223
119.834
118.844
109.643
109.391
77.210
76.998
76.786
34.384
32.837
CN
N
4a
ppm
180
160
140
120
100
80
60
40
20


Current Data Parameters
NAME RKS-4-98-F2
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20160614
Time 10.16
INSTRUM spect
PROBHD 5 mm CNP 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 297.1 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 598.5029935 MHz
F2 - Processing parameters
SI 32768
SF 598.5000278 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 20.00 cm
CY 10.00 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
8.02809
7.48007
7.43299
7.43080
7.41863
7.41805
7.40455
7.36368
7.36208
7.35025
7.34766
7.33709
7.32199
7.31373
7.30168
7.23976
7.22721
7.22557
7.21538
7.21360
7.20159
7.07478
7.07336
7.06808
7.06284
7.06156
7.06012
7.04965
7.04833
5.37037
4.10451
4.09169
4.07969
4.06764
1.82601
1.81374
1.80989
1.80414
1.80137
1.79766
1.78892
1.77644
1.59132
1.36532
1.35289
1.34034
1.32746
1.31504
1.30273
1.27478
1.24700
0.97219
0.95934
0.94464
0.93237
0.92875
0.92792
0.91999
0.91107
0.88182
0.87921
0.87700
0.85762
0.84527
CN
N
n-Bu
4c
Integral
3.0198
5.0676
1.0000
2.0649
1.1255
2.2486
2.1451
2.2405
3.0911
ppm
8
6
4
2
0



Current Data Parameters
NAME RKS-4-98-F2
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20160614
Time 10.39
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 359
DS 0
SWH 45045.047 Hz
FIDRES 1.374666 Hz
AQ 0.3637748 sec
RG 4096
DW 11.100 usec
DE 6.50 usec
TE 297.8 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 150.4929529 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 20.00 cm
CY 4.00 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

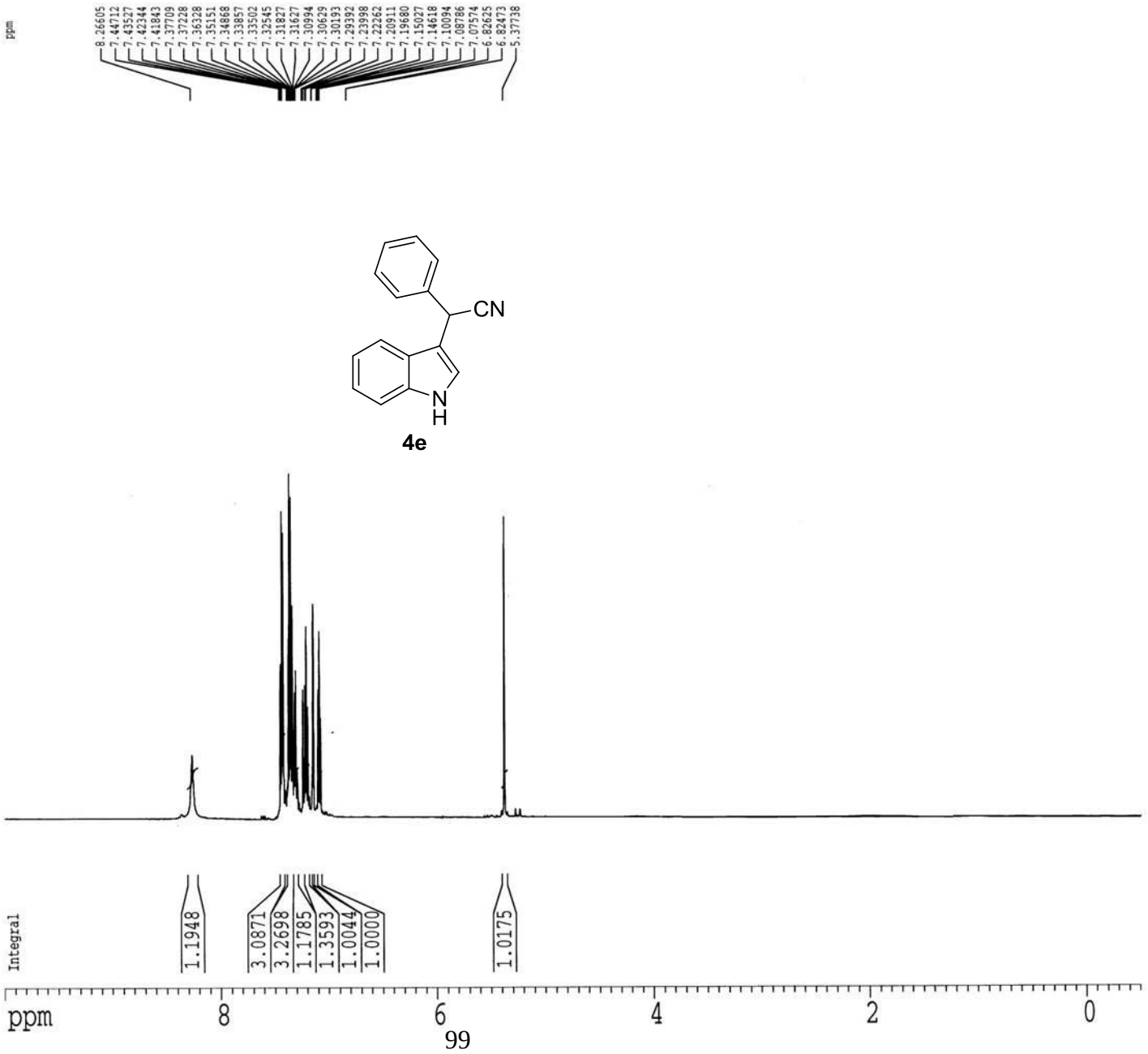
```
Current Data Parameters
NAME      RKS-4-87-2-f2
EXPNO              1
PROCNO             1

F2 - Acquisition Parameters
Date_          20160526
Time             10.54
INSTRUM          spect
PROBHD   5 mm QNP  1H/1
PULPROG            zg
TD              32768
SOLVENT         CDCl3
NS                16
DS                 0
SWH         12019.230 Hz
FIDRES       0.366798 Hz
AQ           1.3631988 sec
RG               512
DW              41.600 usec
DE               6.50 usec
TE              296.8 K
D1          2.00000000 sec
MCREST      0.00000000 sec
MCWRK       0.01500000 sec

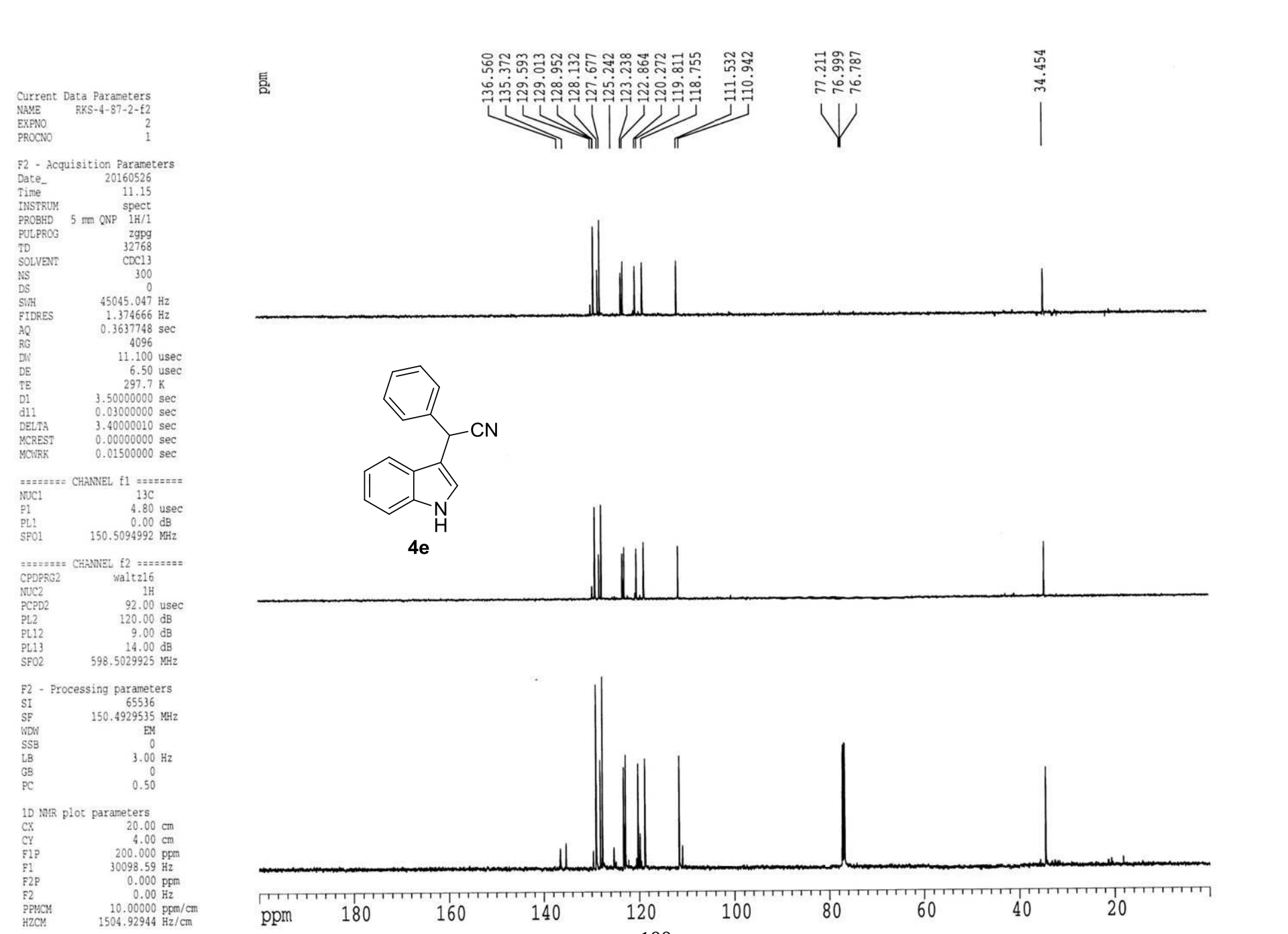
======== CHANNEL f1 ========
NUC1               1H
P1              10.00 usec
PL1              0.00 dB
SFO1       598.5035910 MHz

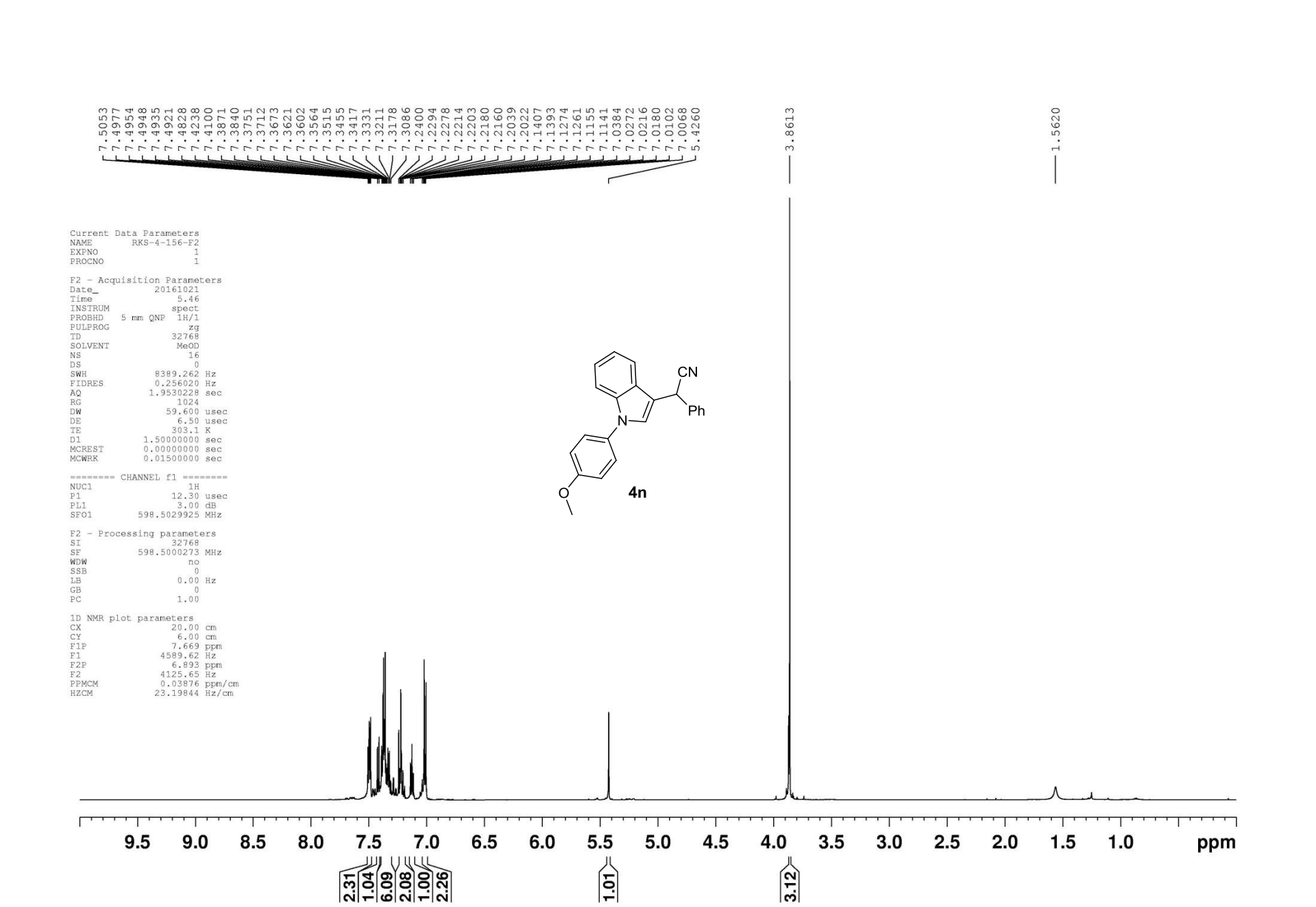
F2 - Processing parameters
SI              32768
SF         598.5000278 MHz
WDW                no
SSB                 0
LB               0.00 Hz
GB                  0
PC               1.00

1D NMR plot parameters
CX              20.00 cm
CY               6.00 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
```



4e


Current Data Parameters
NAME RKS-4-87-2-f2
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20160526
Time 11.15
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 300
DS 0
SWH 45045.047 Hz
FIDRES 1.374666 Hz
AQ 0.3637748 sec
RG 4096
DW 11.100 usec
DE 6.50 usec
TE 297.7 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 150.4929535 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 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
136.560
135.372
129.593
129.013
128.952
128.132
127.677
125.242
123.238
122.864
120.272
119.811
118.755
111.532
110.942
77.211
76.999
76.787
34.454
CN
N
H
4e
ppm
180
160
140
120
100
80
60
40
20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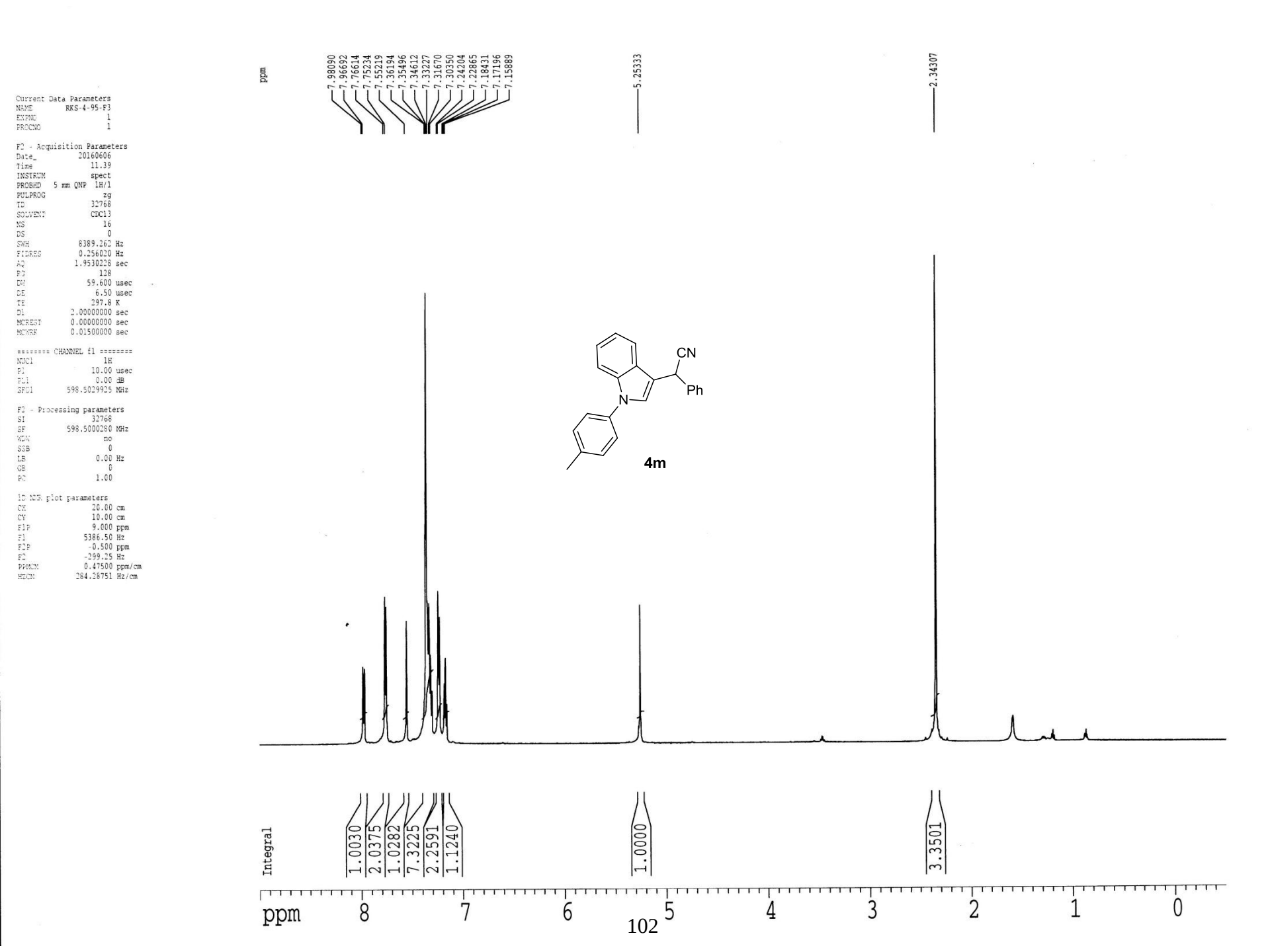
7.4977
7.4954
7.4948
7.4935
7.4921
7.4828
7.4238
7.4100
7.3871
7.3840
7.3751
7.3712
7.3673
7.3621
7.3602
7.3564
7.3515
7.3455
7.3417
7.3331
7.3211
7.3178
7.3086
7.2400
7.2294
7.2278
7.2214
7.2203
7.2180
7.2160
7.2039
7.2022
7.1407
7.1393
7.1274
7.1261
7.1155
7.1141
7.0384
7.0272
7.0216
7.0180
7.0102
7.0068
5.4260
3.8613
1.5620
Current Data Parameters
NAME RKS-4-156-F2
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20161021
Time 5.46
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg
TD 32768
SOLVENT MeOD
NS 16
DS 0
SWH 8389.262 Hz
FIDRES 0.256020 Hz
AQ 1.9530228 sec
RG 1024
DW 59.600 usec
DE 6.50 usec
TE 303.1 K
D1 1.50000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 12.30 usec
PL1 3.00 dB
SFO1 598.5029925 MHz
F2 - Processing parameters
SI 32768
SF 598.5000273 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 20.00 cm
CY 6.00 cm
F1P 7.669 ppm
F1 4589.62 Hz
F2P 6.893 ppm
F2 4125.65 Hz
PPMCM 0.03876 ppm/cm
HZCM 23.19844 Hz/cm
CN
Ph
N
O
4n
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
2.31
1.04
6.09
2.08
1.00
2.26
1.01
3.12


Current Data Parameters
NAME RKS-4-95-F3
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20160606
Time 11.39
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 128
DW 59.600 usec
DE 6.50 usec
TE 297.8 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 598.5000280 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 20.00 cm
CY 10.00 cm
F1P 9.000 ppm
F1 5386.50 Hz
F2P -0.500 ppm
F2 -299.25 Hz
PPMCM 0.47500 ppm/cm
HZCM 284.28751 Hz/cm
ppm
7.98090
7.96692
7.76614
7.75234
7.55219
7.36194
7.35496
7.34612
7.33227
7.31670
7.30350
7.24204
7.22865
7.18431
7.17196
7.15889
5.25333
2.34307
CN
Ph
N
4m
Integral
1.0030
2.0375
1.0282
7.3225
2.2591
1.1240
1.0000
3.3501
ppm
8
7
6
5
4
3
2
1
0

```
Current Data Parameters
NAME        RKS-4-95-F3
EXPNO                 2
PROCNO                1

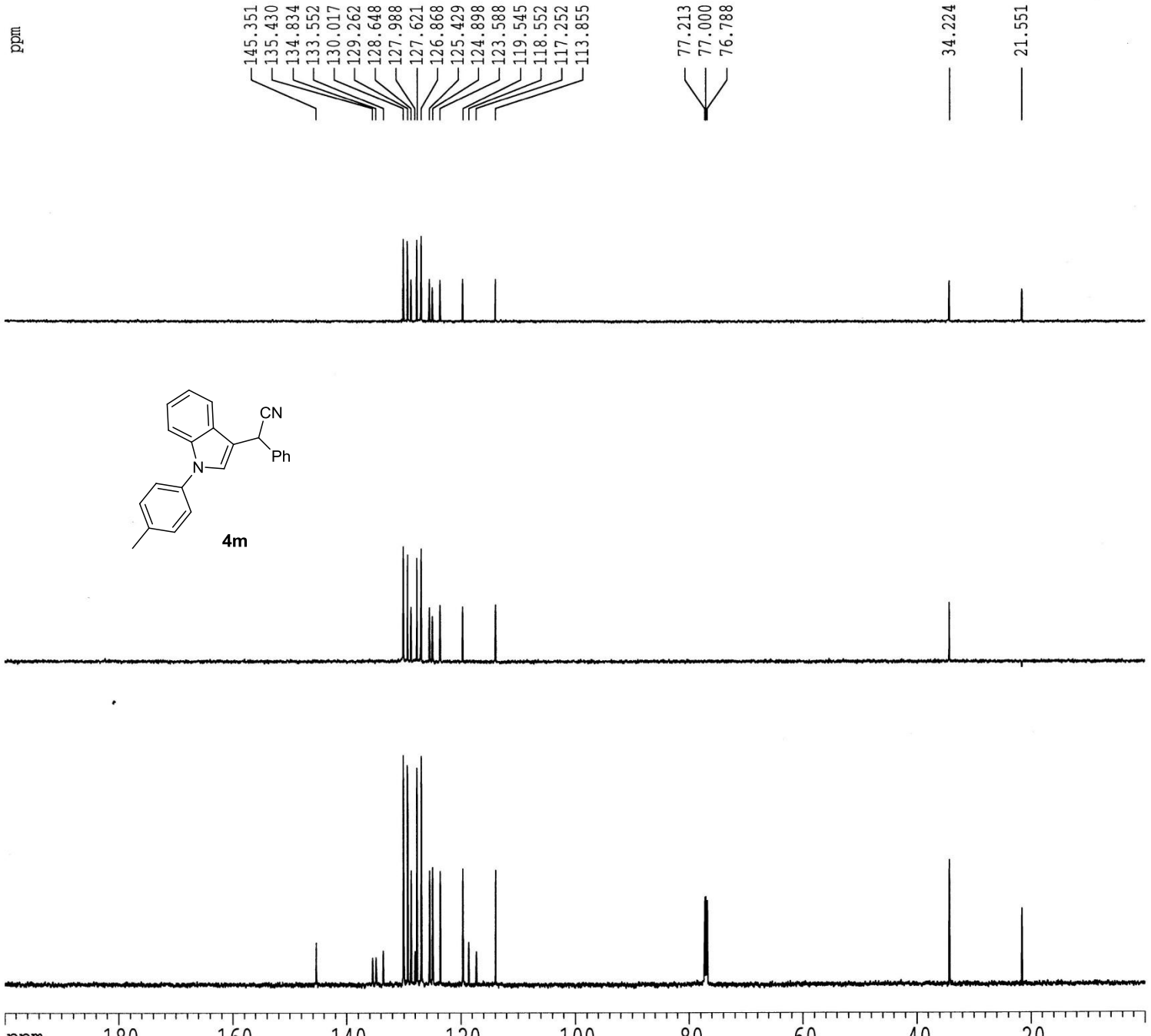
F2 - Acquisition Parameters
Date_          20160606
Time              11.25
INSTRUM           spect
PROBHD   5 mm QNP  1H/1
PULPROG           zgpg
TD               32768
SOLVENT        Acetone
NS                   83
DS                    0
SWH           45045.047 Hz
FIDRES         1.374666 Hz
AQ            0.3637748 sec
RG                 4096
DW               11.100 usec
DE                6.50 usec
TE               297.8 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

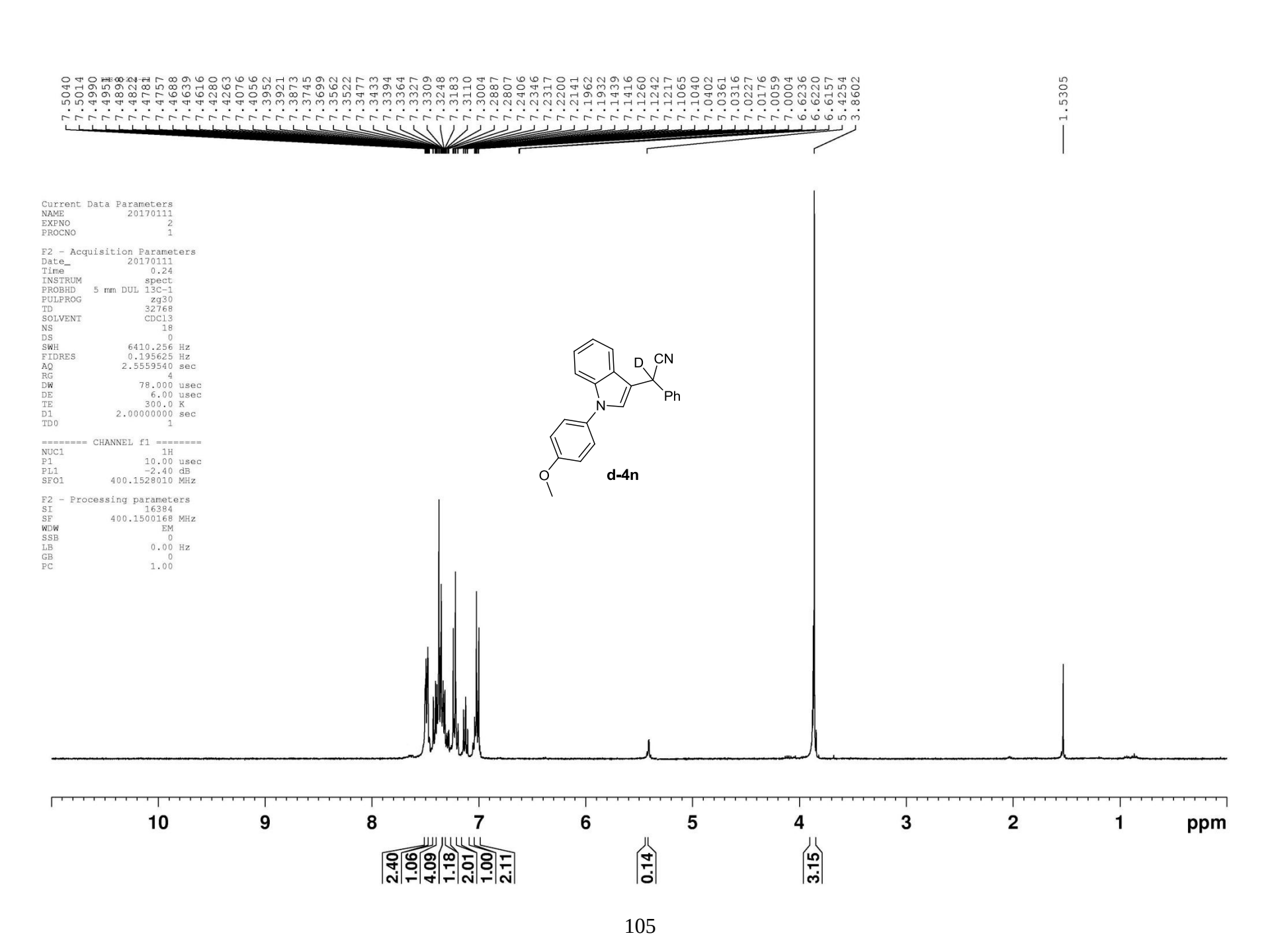
======== CHANNEL f2 ========
CPDPRG2         waltz16
NUC2                1H
PCPD2             92.00 usec
PL2              120.00 dB
PL12               9.00 dB
PL13              14.00 dB
SFO2        598.5029925 MHz

F2 - Processing parameters
SI                 65536
SF          150.4929563 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              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
```



158.595
137.134
135.299
132.020
129.076
128.197
127.755
127.612
127.215
126.085
123.057
120.582
119.691
118.994
114.810
111.279
110.863
77.211
76.999
76.787
55.594
34.450
Current Data Parameters
NAME RKS-4-156-F2
EXPNO 2
PROCNO 1
F2 - Acquisition Paramet
Date_ 20161021
Time 20.50
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 253
DS 0
SWH 45045.047
FIDRES 1.374666
AQ 0.3637748
RG 4096
DW 11.100
DE 6.50
TE 303.4
D1 3.50000000
d11 0.03000000
DELTA 3.40000010
MCREST 0 sec
MCWRK 0.01500000
======== CHANNEL f1 ====
NUC1 13C
P1 4.80
PL1 0 dB
SFO1 150.5094992
======== CHANNEL f2 ====
CPDPRG2 waltz16
NUC2 1H
PCPD2 92.00
PL2 120.00
PL12 9.00
PL13 14.00
SFO2 598.5029925
F2 - Processing paramete
SI 65536
SF 150.4929501
WDW EM
SSB 0
LB 3.00
GB 0
PC 1.00
CN
Ph
N
O
4n
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm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7.4990
7.4898
7.4822
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7.4757
7.4688
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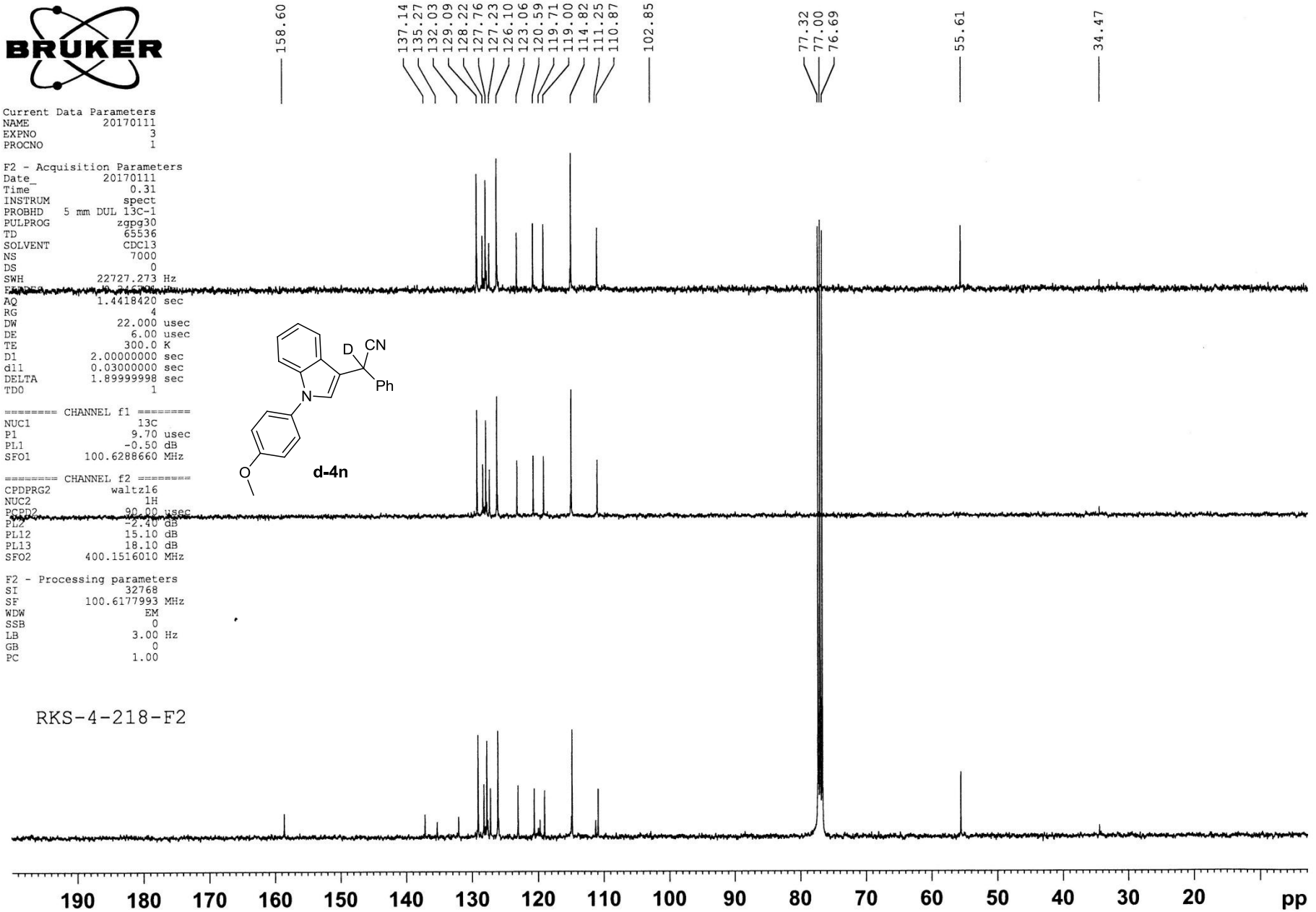
7.4263
7.4076
7.4056
7.3952
7.3921
7.3873
7.3745
7.3699
7.3562
7.3522
7.3477
7.3433
7.3394
7.3364
7.3327
7.3309
7.3248
7.3183
7.3110
7.3004
7.2887
7.2807
7.2406
7.2346
7.2317
7.2200
7.2141
7.1962
7.1932
7.1439
7.1416
7.1260
7.1242
7.1217
7.1065
7.1040
7.0402
7.0361
7.0316
7.0227
7.0176
7.0059
7.0004
6.6236
6.6220
6.6157
5.4254
3.8602
1.5305
Current Data Parameters
NAME 20170111
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170111
Time 0.24
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 18
DS 0
SWH 6410.256 Hz
FIDRES 0.195625 Hz
AQ 2.5559540 sec
RG 4
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 400.1500168 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
D
CN
Ph
N
O
d-4n
10
9
8
7
6
5
4
3
2
1
ppm
2.40
1.06
4.09
1.18
2.01
1.00
2.11
0.14
3.15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137.14
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132.03
129.09
128.22
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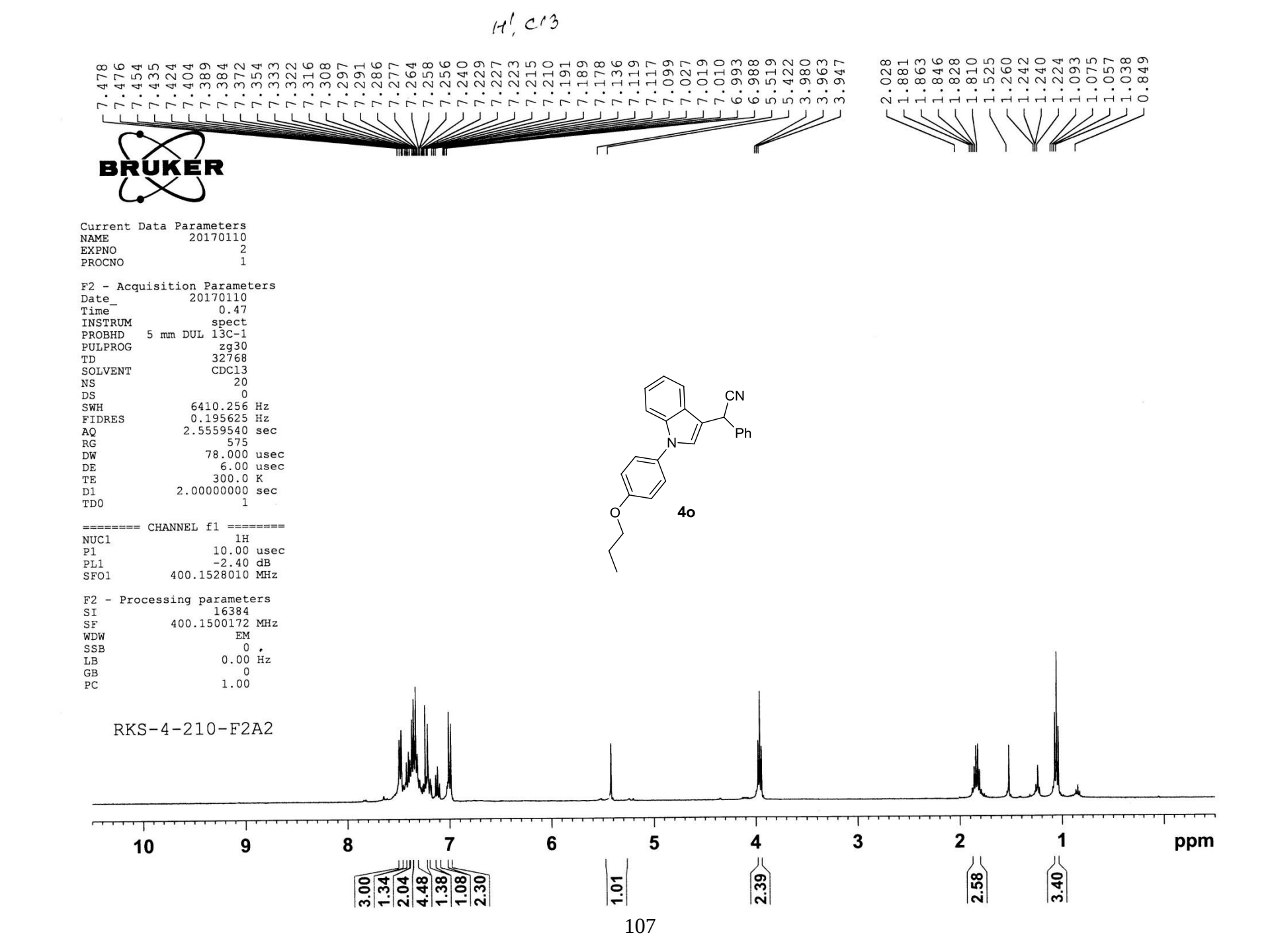
127.23
126.10
123.06
120.59
119.71
119.00
114.82
111.25
110.87
102.85
77.32
77.00
76.69
55.61
34.47
Current Data Parameters
NAME 20170111
EXPNO 3
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170111
Time 0.31
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 7000
DS 0
SWH 22727.273 Hz
AQ 1.4418420 sec
RG 4
DW 22.000 usec
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
PL12 15.10 dB
PL13 18.10 dB
SFO2 400.1516010 MHz
F2 - Processing parameters
SI 32768
SF 100.6177993 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
D
CN
Ph
N
O
d-4n
RKS-4-218-F2
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
pp


1H, C13
7.478
7.476
7.454
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7.424
7.404
7.389
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7.372
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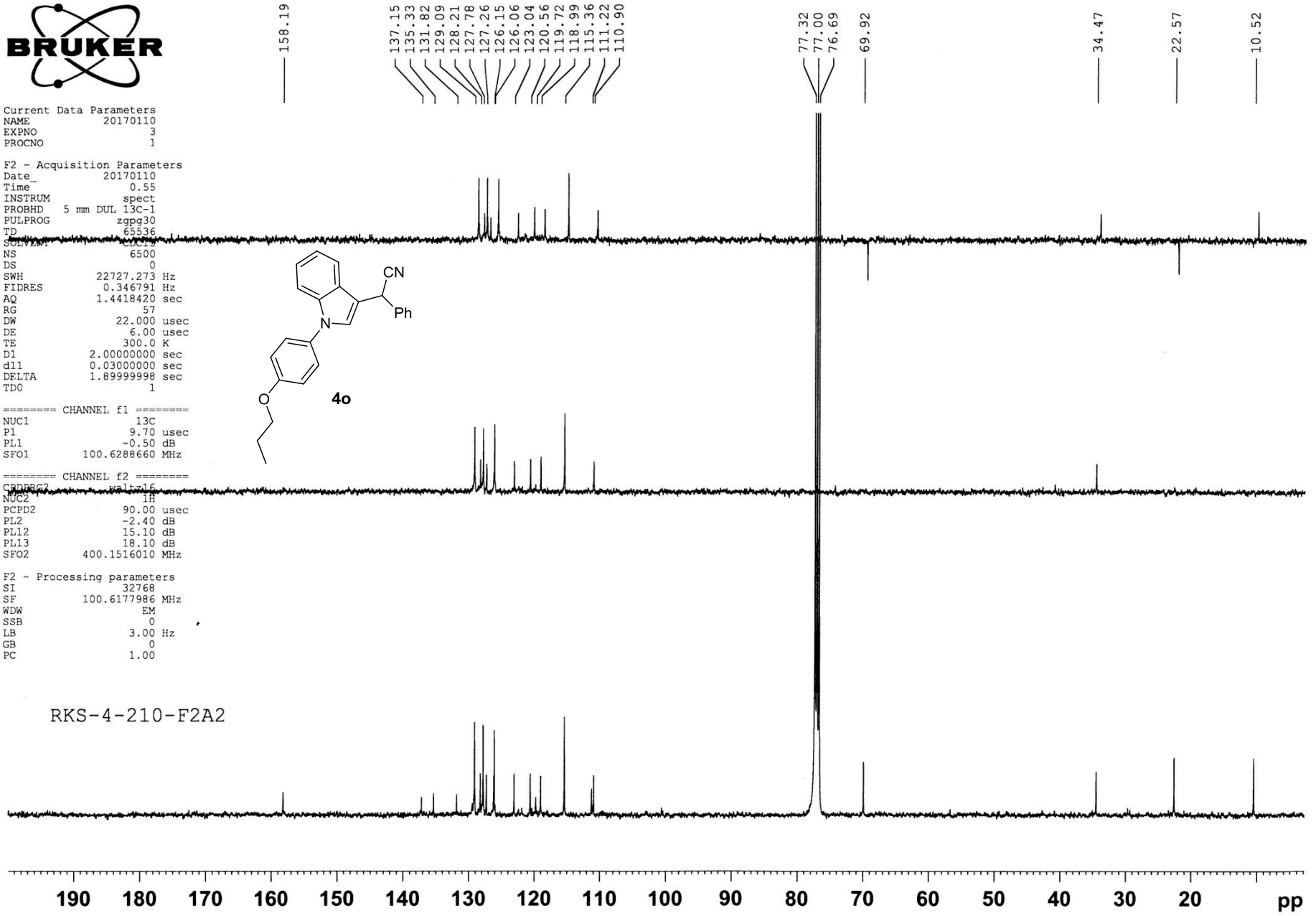
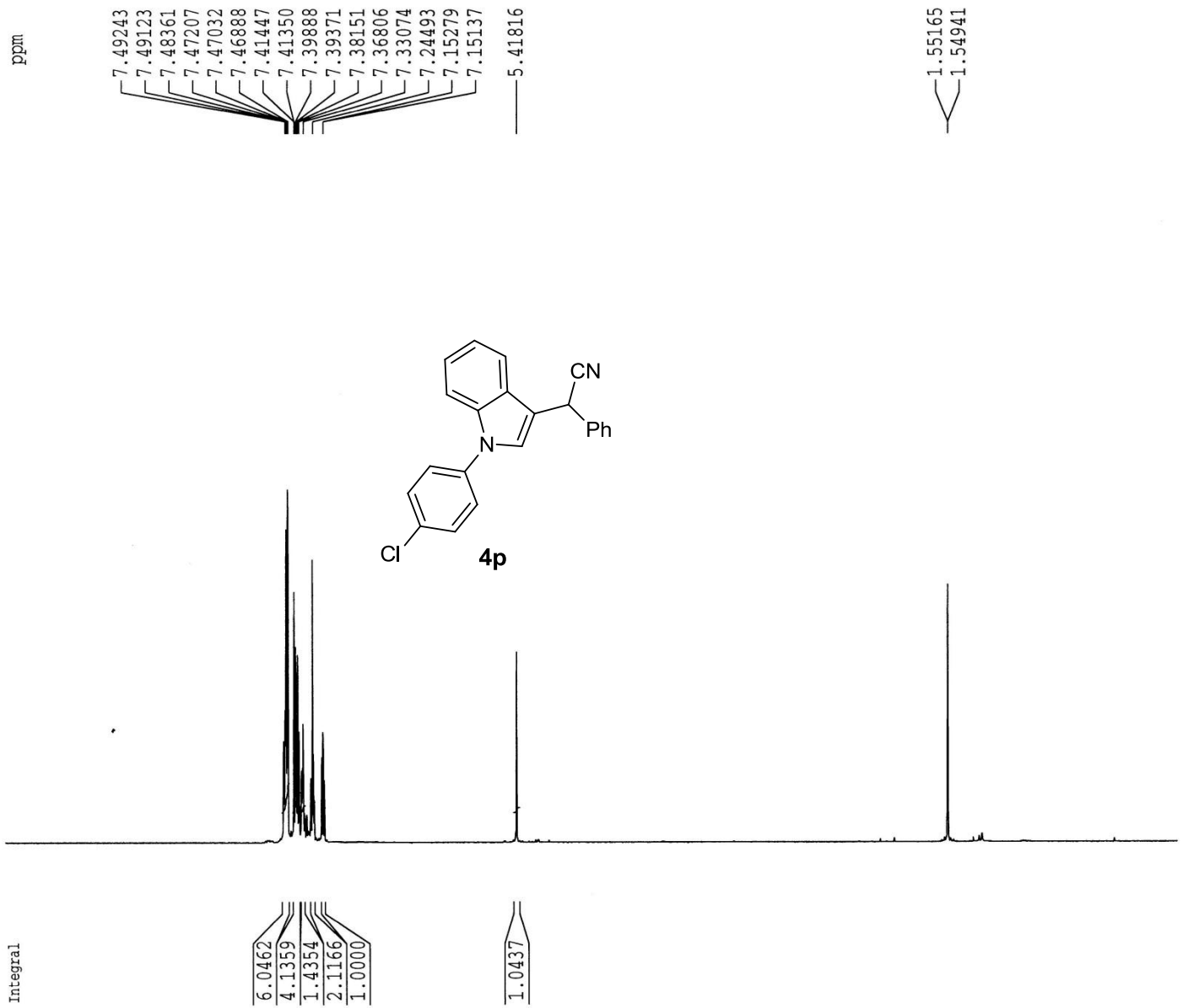
7.333
7.322
7.316
7.308
7.297
7.291
7.286
7.277
7.264
7.258
7.256
7.240
7.229
7.227
7.223
7.215
7.210
7.191
7.189
7.178
7.136
7.119
7.117
7.099
7.027
7.019
7.010
6.993
6.988
5.519
5.422
3.980
3.963
3.947
2.028
1.881
1.863
1.846
1.828
1.810
1.525
1.260
1.242
1.240
1.224
1.093
1.075
1.057
1.038
0.849
BRUKER
Current Data Parameters
NAME 20170110
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170110
Time 0.47
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 20
DS 0
SWH 6410.256 Hz
FIDRES 0.195625 Hz
AQ 2.5559540 sec
RG 575
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 400.1500172 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
CN
Ph
N
O
4o
RKS-4-210-F2A2
10
9
8
7
6
5
4
3
2
1
ppm
3.00
1.34
2.04
4.48
1.38
1.08
2.30
1.01
2.39
2.58
3.40


158.19
137.15
135.33
131.82
129.09
128.21
127.78
127.26
126.15
126.06
123.04
120.56
119.72
118.99
115.36
111.22
110.90
77.32
77.00
76.69
69.92
34.47
22.57
10.52
Current Data Parameters
NAME 20170110
EXPNO 3
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170110
Time 0.55
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 6500
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
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
PL12 15.10 dB
PL13 18.10 dB
SFO2 400.1516010 MHz
F2 - Processing parameters
SI 32768
SF 100.6177986 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
CN
Ph
N
O
4o
RKS-4-210-F2A2
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
pp



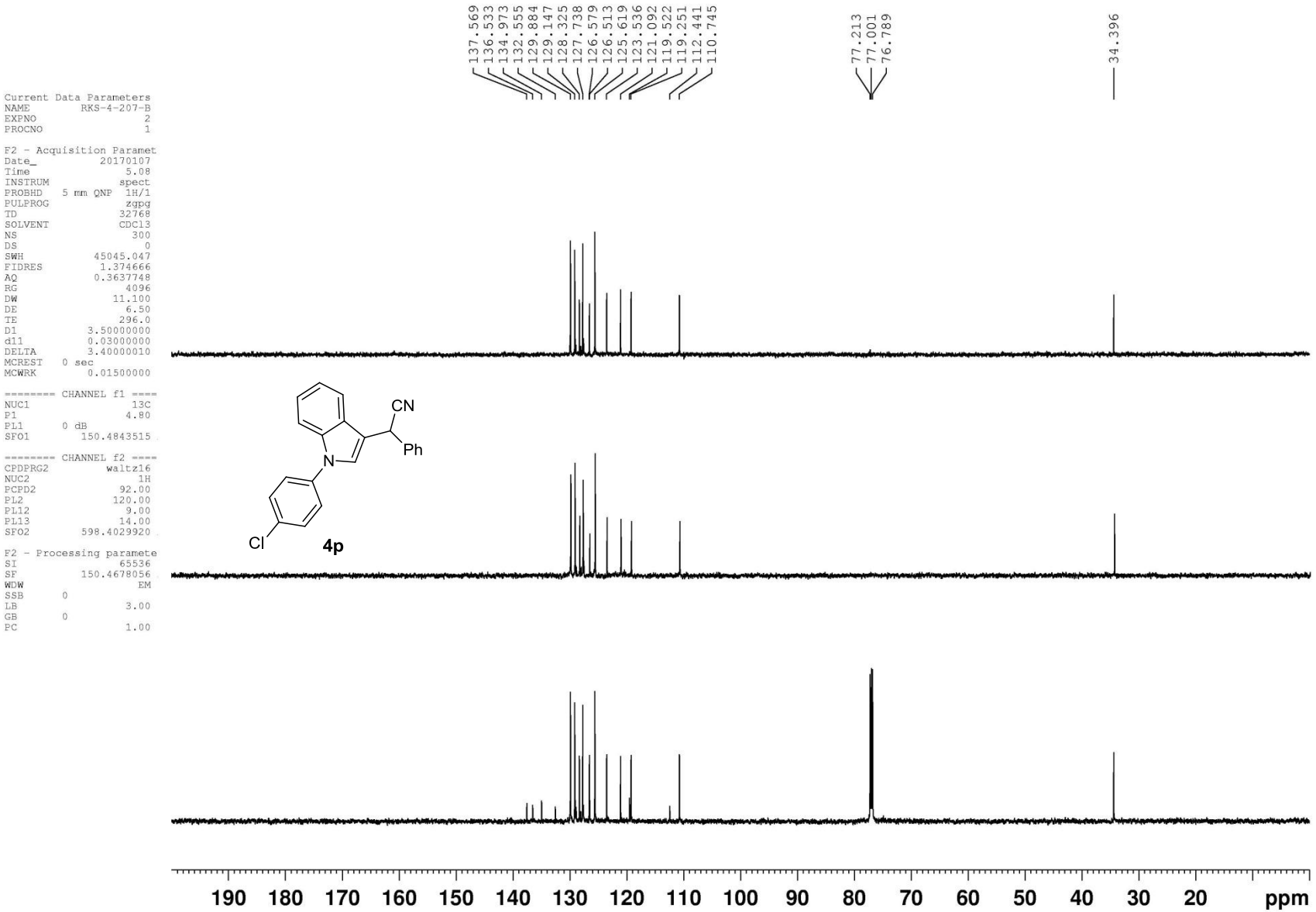
Current Data Parameters
NAME RKS-4-207-B
EXPNO 1
PROCNO 1

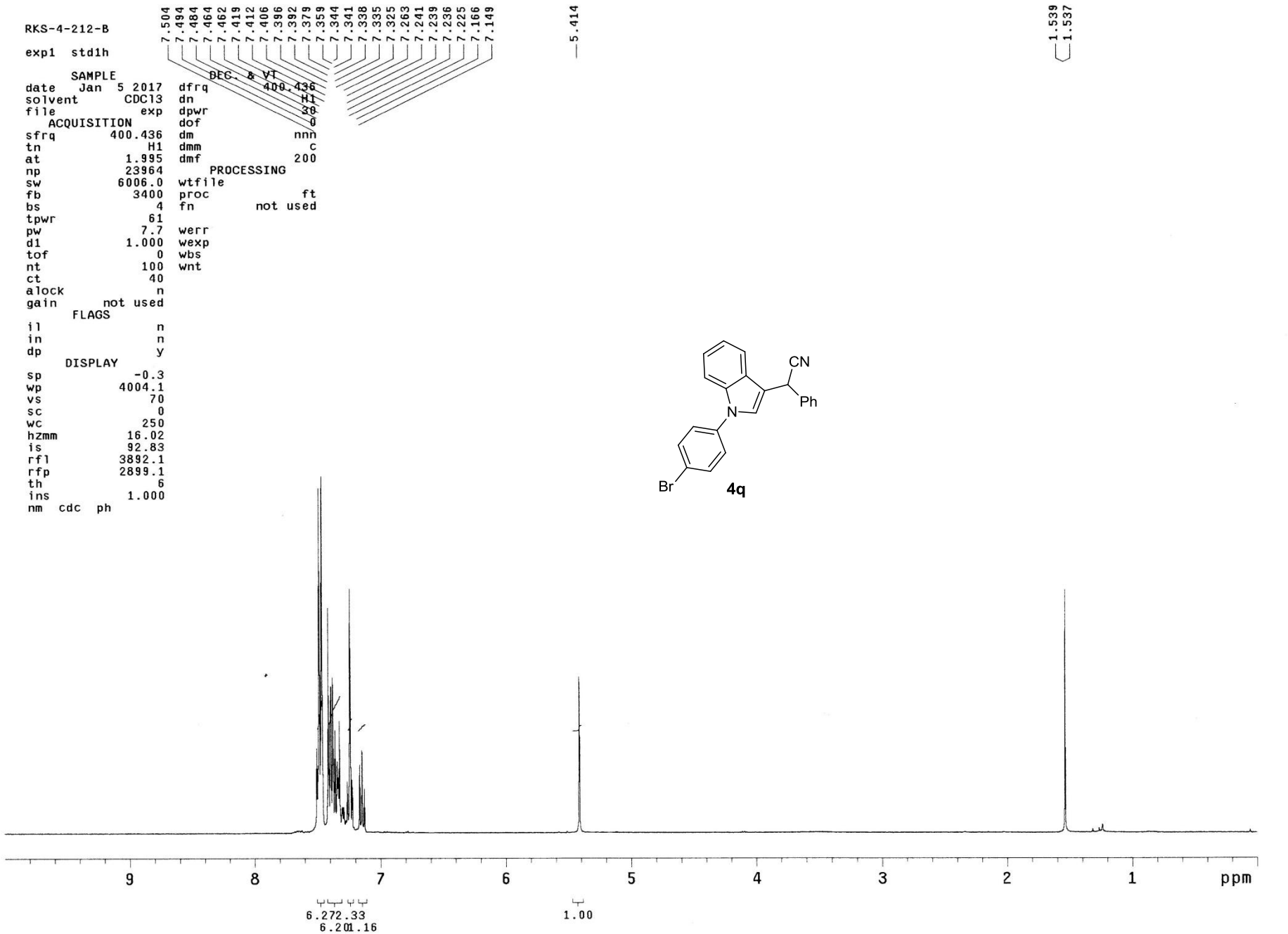
F2 - Acquisition Parameters
Date_ 20170106
Time 9.45
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 12019.230 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 512
DW 41.600 usec
DE 6.50 usec
TE 296.1 K
D1 2.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

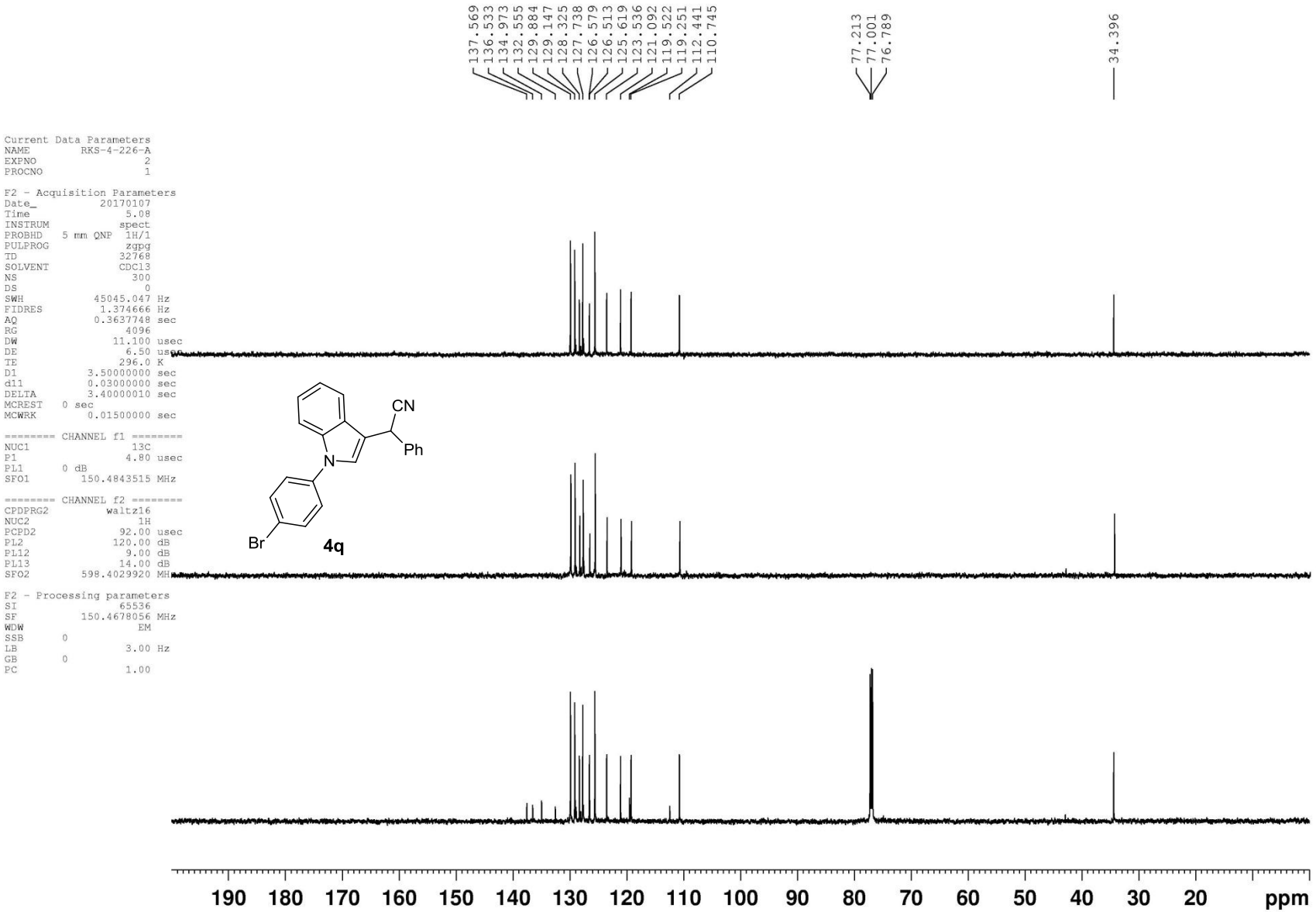
======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 0.00 dB
SFO1 598.4029920 MHz

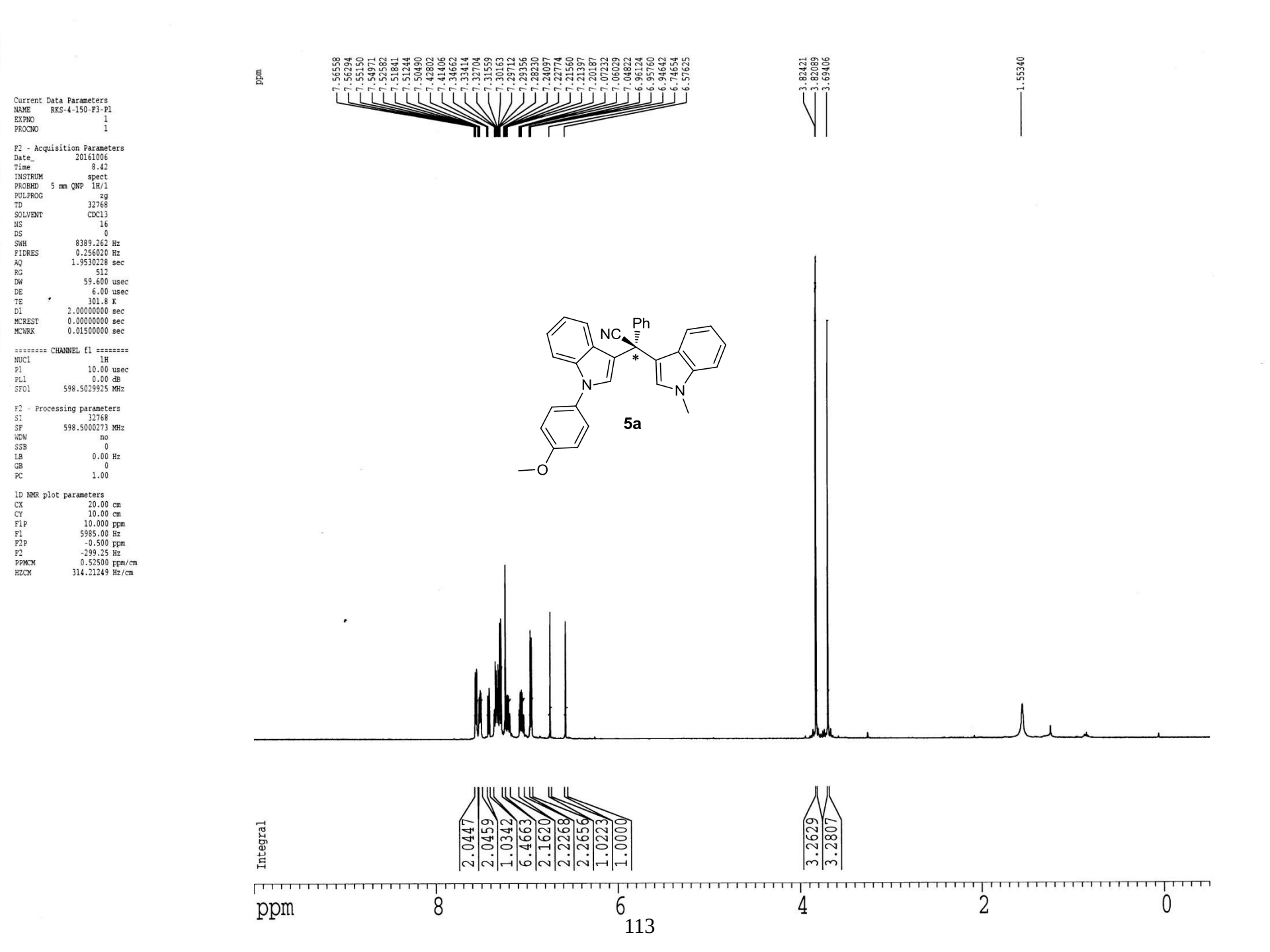
F2 - Processing parameters
SI 32768
SF 598.4000244 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 20.00 cm
CY 6.00 cm
F1P 10.000 ppm
F1 5984.00 Hz
F2P -0.500 ppm
F2 -299.20 Hz
PPMCM 0.52500 ppm/cm
HZCM 314.16000 Hz/cm


137.569
136.533
134.973
132.555
129.884
129.147
128.325
127.738
126.579
126.513
125.619
123.536
121.092
119.522
119.251
112.441
110.745
77.213
77.001
76.789
34.396
Current Data Parameters
NAME RKS-4-207-B
EXPNO 2
PROCNO 1
F2 - Acquisition Paramet
Date_ 20170107
Time 5.08
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 300
DS 0
SWH 45045.047
FIDRES 1.374666
AQ 0.3637748
RG 4096
DW 11.100
DE 6.50
TE 296.0
D1 3.50000000
d11 0.03000000
DELTA 3.40000010
MCREST 0 sec
MCWRK 0.01500000
======== CHANNEL f1 ====
NUC1 13C
P1 4.80
PL1 0 dB
SFO1 150.4843515
======== CHANNEL f2 ====
CPDPRG2 waltz16
NUC2 1H
PCPD2 92.00
PL2 120.00
PL12 9.00
PL13 14.00
SFO2 598.4029920
F2 - Processing paramete
SI 65536
SF 150.4678056
WDW EM
SSB 0
LB 3.00
GB 0
PC 1.00
CN
Ph
N
Cl
4p
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm


RKS-4-212-B
exp1 std1h
SAMPLE
date Jan 5 2017
solvent CDCl3
file exp
ACQUISITION
sfrq 400.436
tn H1
at 1.995
np 23964
sw 6006.0
fb 3400
bs 4
tpwr 61
pw 7.7
d1 1.000
tof 0
nt 100
ct 40
alock n
gain not used
FLAGS
il n
in n
dp y
DISPLAY
sp -0.3
wp 4004.1
vs 70
sc 0
wc 250
hzmm 16.02
is 92.83
rfl 3892.1
rfp 2899.1
th 6
ins 1.000
nm cdc ph
DEC. & VT
dfrq 400.436
dn H1
dpwr 30
dof 0
dm nnn
dmm c
dmf 200
PROCESSING
wtfile
proc ft
fn not used
werr
wexp
wbs
wnt
7.504
7.494
7.484
7.464
7.462
7.419
7.412
7.406
7.396
7.392
7.379
7.359
7.344
7.341
7.338
7.335
7.325
7.263
7.241
7.239
7.236
7.225
7.166
7.149
5.414
1.539
1.537
CN
Ph
N
Br
4q
9
8
7
6
5
4
3
2
1
ppm
6.27
2.33
6.20
1.16
1.00


137.569
136.533
134.973
132.555
129.884
129.147
128.325
127.738
126.579
126.513
125.619
123.536
121.092
119.522
119.251
112.441
110.745
77.213
77.001
76.789
34.396
Current Data Parameters
NAME RKS-4-226-A
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170107
Time 5.08
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 300
DS 0
SWH 45045.047 Hz
FIDRES 1.374666 Hz
AQ 0.3637748 sec
RG 4096
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 150.4843515 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 92.00 usec
PL2 120.00 dB
PL12 9.00 dB
PL13 14.00 dB
SFO2 598.4029920 MH
F2 - Processing parameters
SI 65536
SF 150.4678056 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
CN
Ph
N
Br
4q
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm


Current Data Parameters
NAME RKS-4-150-F3-P1
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20161006
Time 8.42
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 6.00 usec
TE 301.8 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 598.5000273 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 20.00 cm
CY 10.00 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
7.56558
7.56294
7.55150
7.54971
7.52582
7.51841
7.51244
7.50490
7.42802
7.41406
7.34662
7.33414
7.32704
7.31559
7.30163
7.29712
7.29356
7.28230
7.24097
7.22774
7.21560
7.21397
7.20187
7.07232
7.06029
7.04822
6.96124
6.95760
6.94642
6.74654
6.57625
3.82421
3.82089
3.69406
1.55340
NC
Ph
*
N
N
O
5a
Integral
2.0447
2.0459
1.0342
6.4663
2.1620
2.2268
2.2656
1.0223
1.0000
3.2629
3.2807
ppm
8
6
4
2
0

```
Current Data Parameters
NAME      RKS-4-150-F3-P1
EXPNO                  2
PROCNO                 1

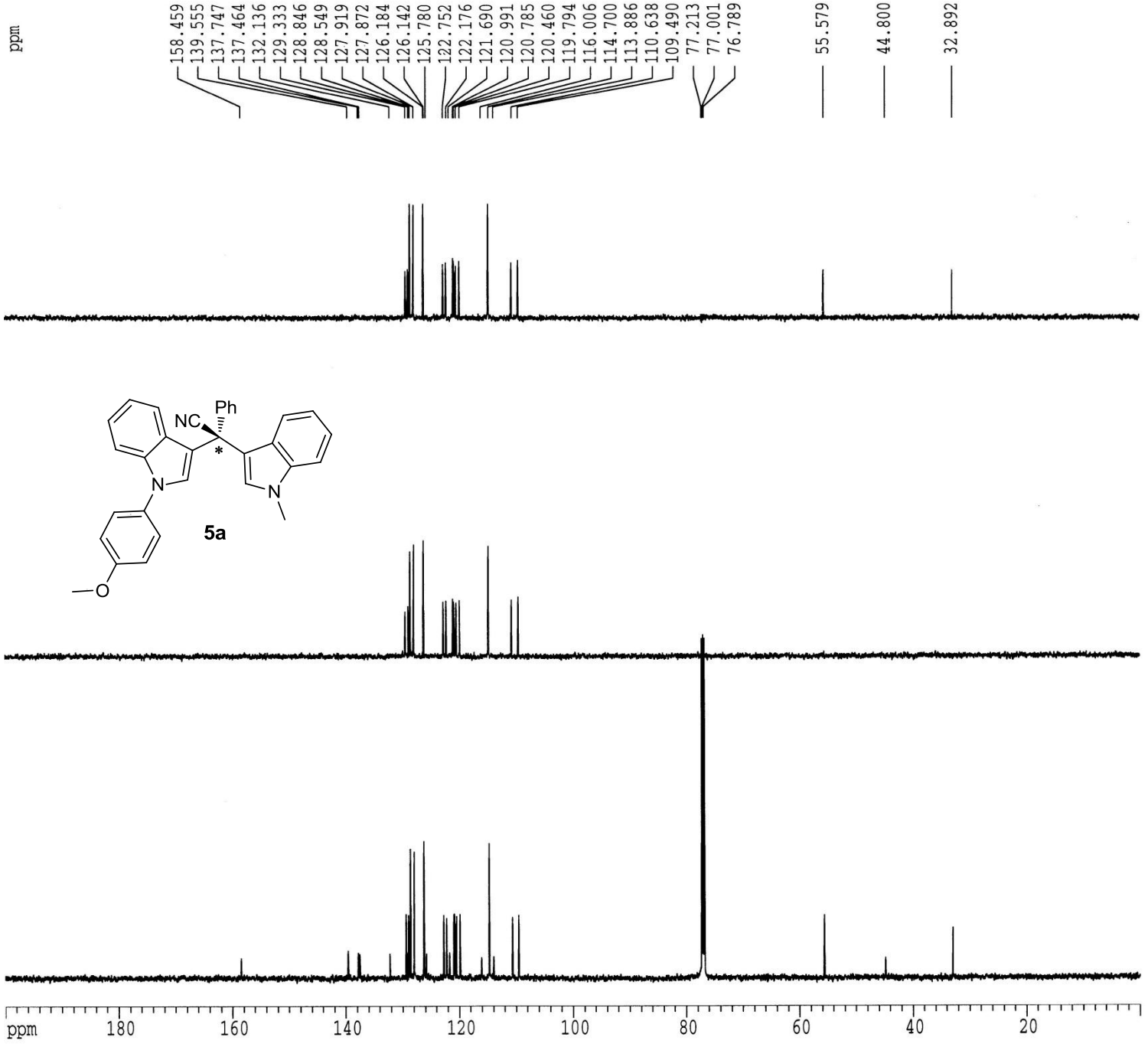
F2 - Acquisition Parameters
Date_           20161006
Time                8.42
INSTRUM            spect
PROBHD   5 mm QNP  1H/1
PULPROG            zgpg
TD                32768
SOLVENT           CDCl3
NS                 1024
DS                    0
SWH           45045.047 Hz
FIDRES         1.374666 Hz
AQ           0.3637748 sec
RG                 4096
DW               11.100 usec
DE                6.50 usec
TE               301.8 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          150.4929473 MHz
WDW                   EM
SSB                    0
LB                  3.00 Hz
GB                     0
PC                  1.00

1D NMR plot parameters
CX                 20.00 cm
CY                  6.00 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
```



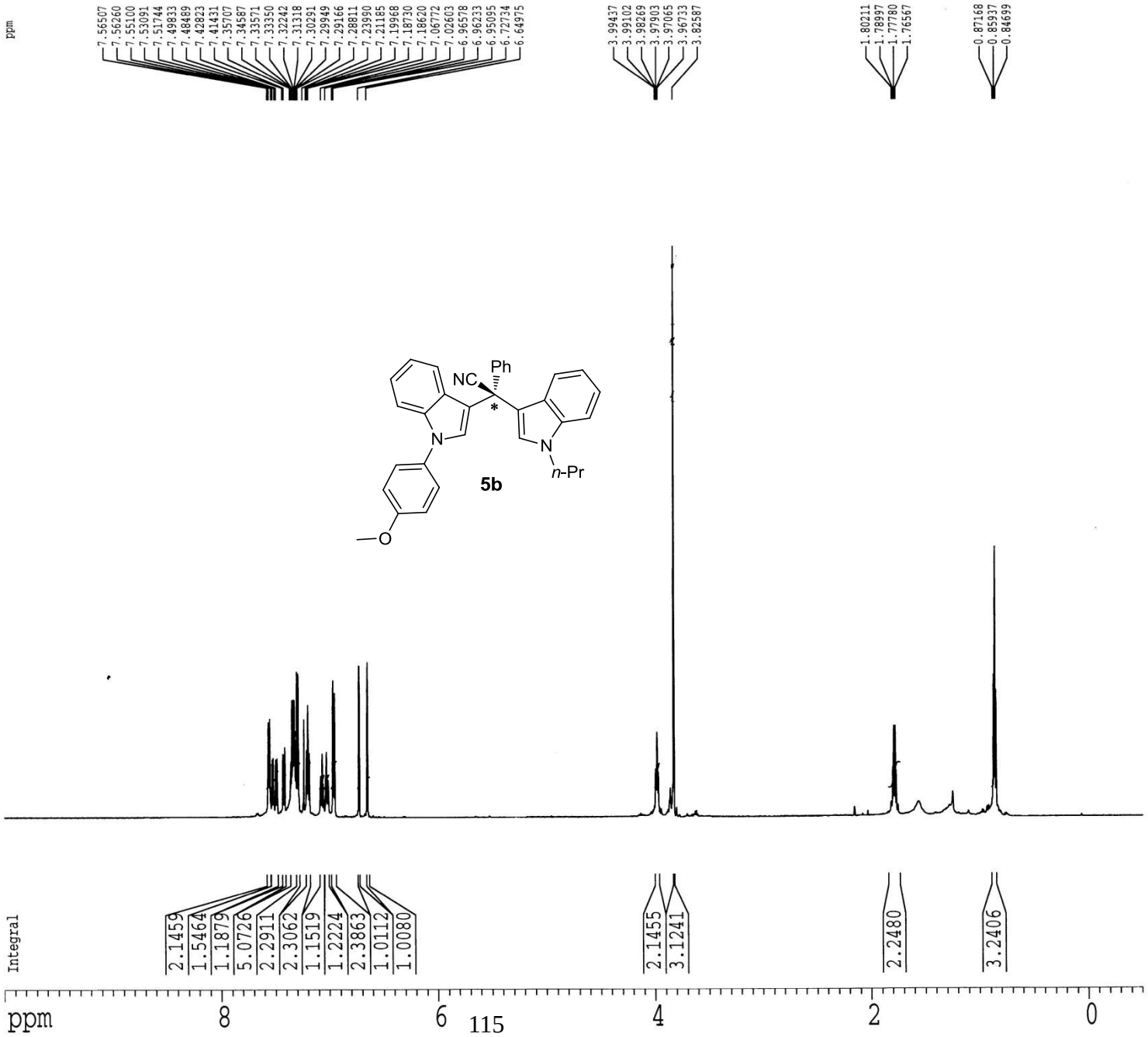
Current Data Parameters
NAME RKS-4-151-2-P2
EXPNO 1
PROCNO 1

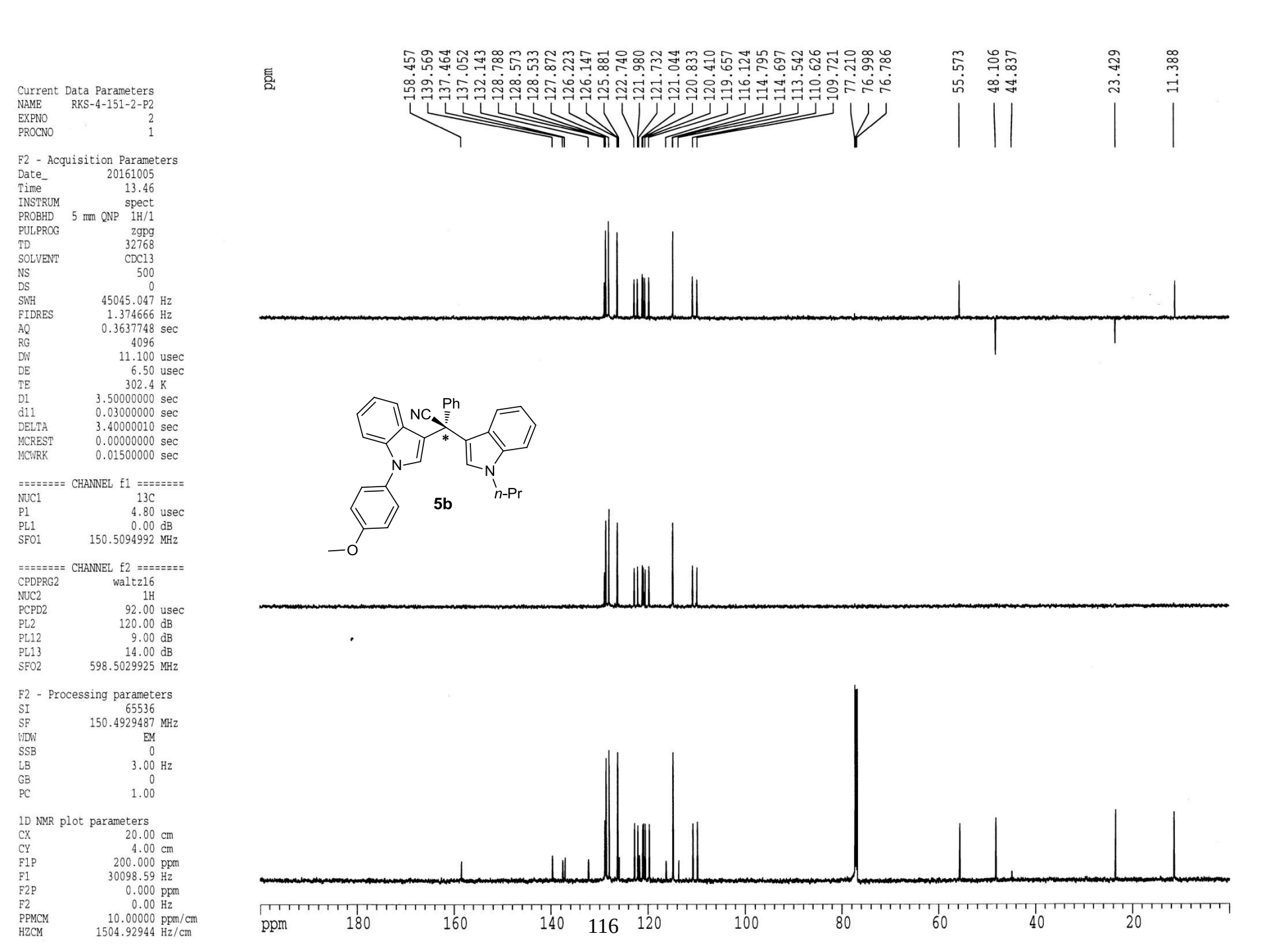
F2 - Acquisition Parameters
Date_ 20161005
Time 13.41
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 8389.262 Hz
FIDRES 0.256020 Hz
AQ 1.9530228 sec
RG 512
DW 59.600 usec
DE 6.00 usec
TE 302.1 K
D1 2.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

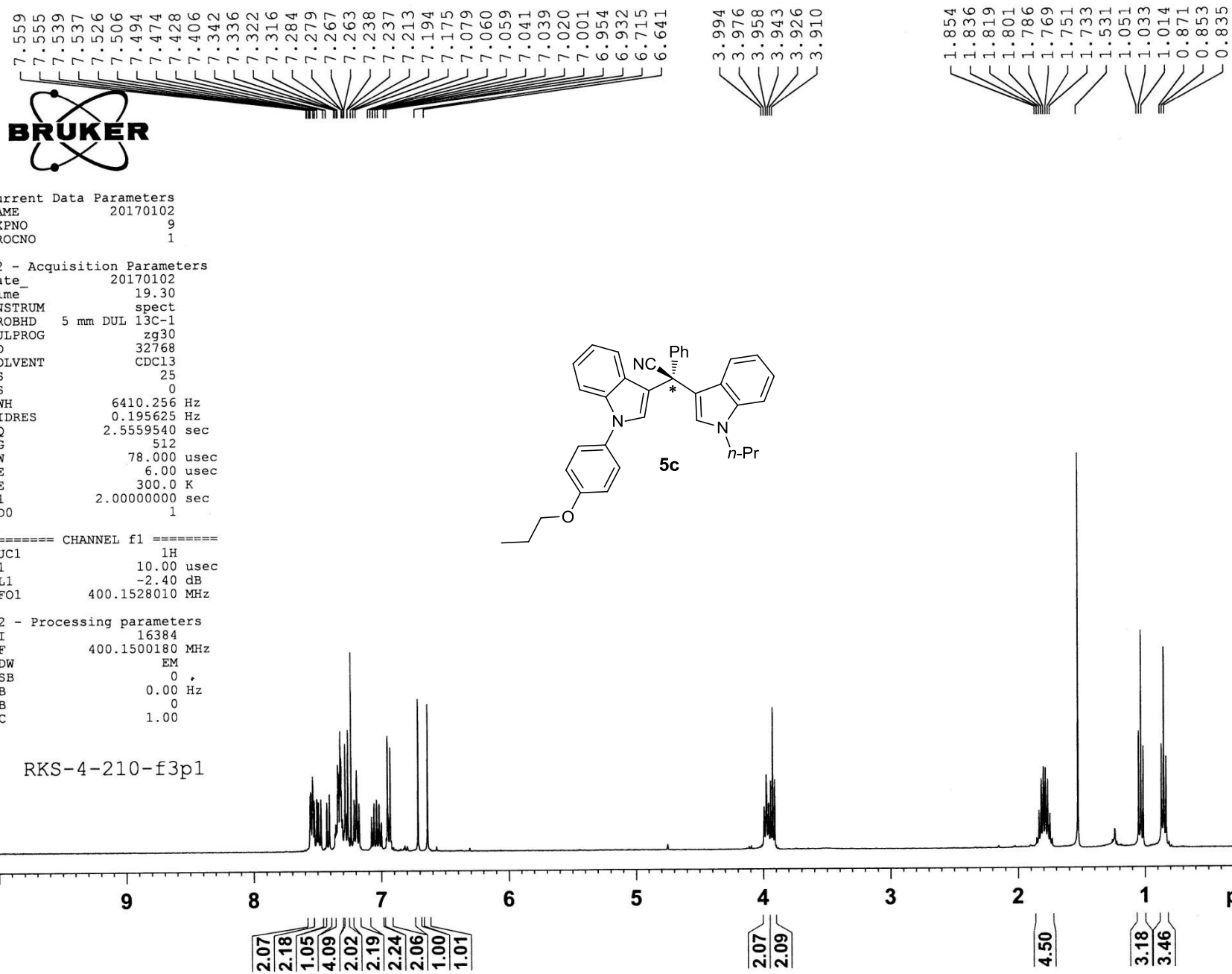
======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 0.00 dB
SFO1 598.5029925 MHz

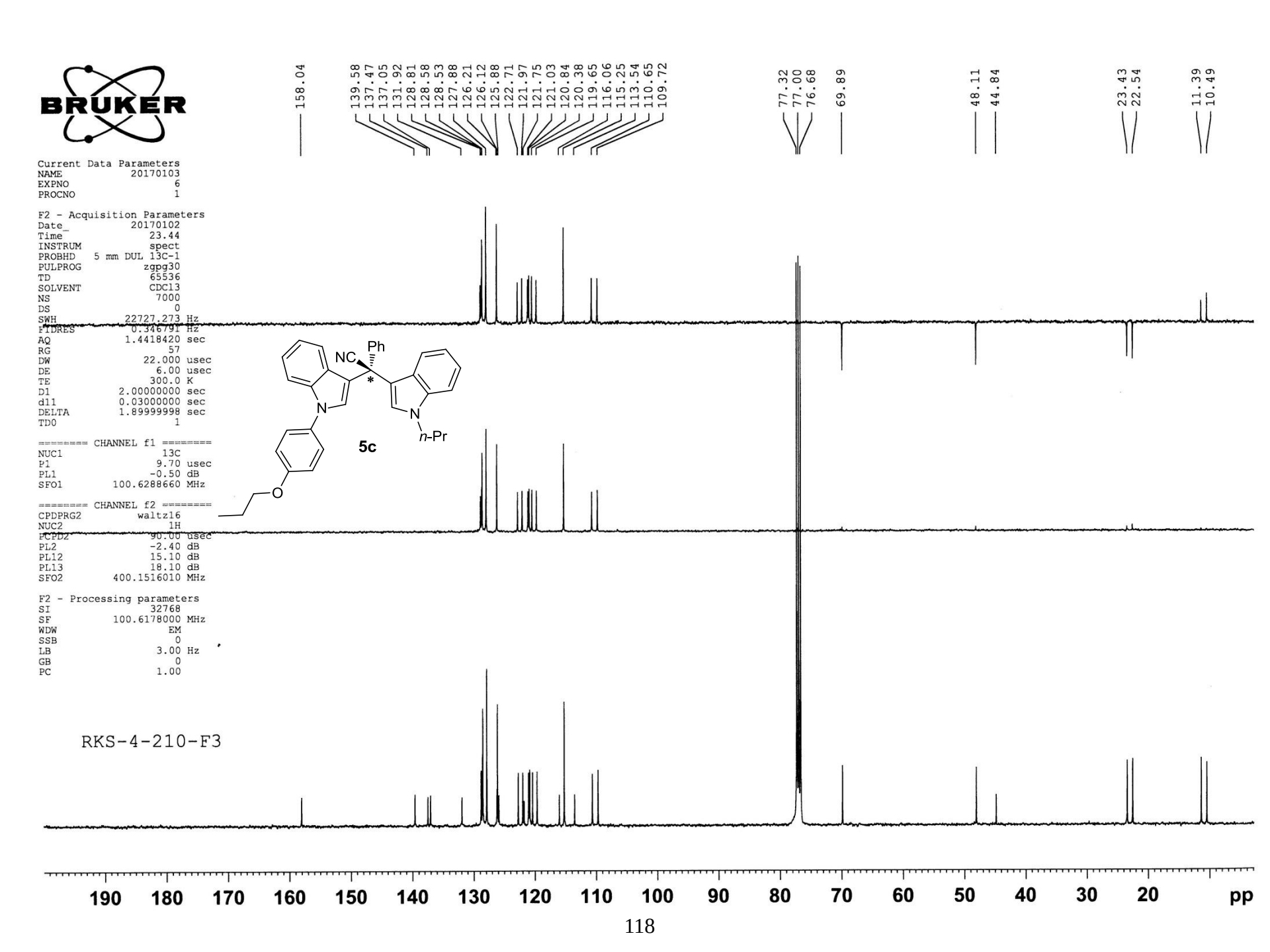
F2 - Processing parameters
SI 32768
SF 598.5000278 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 20.00 cm
CY 10.00 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




Current Data Parameters
NAME RKS-4-151-2-P2
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20161005
Time 13.46
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 4096
DW 11.100 usec
DE 6.50 usec
TE 302.4 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 4.00 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
158.457
139.569
137.464
137.052
132.143
128.788
128.573
128.533
127.872
126.223
126.147
125.881
122.740
121.980
121.732
121.044
120.833
120.410
119.657
116.124
114.795
114.697
113.542
110.626
109.721
77.210
76.998
76.786
55.573
48.106
44.837
23.429
11.388
NC
Ph
*
N
N
n-Pr
O
5b
ppm
180
160
140
120
100
80
60
40
20


7.559
7.555
7.539
7.537
7.526
7.506
7.494
7.474
7.428
7.406
7.342
7.336
7.322
7.316
7.284
7.279
7.267
7.263
7.238
7.237
7.213
7.194
7.175
7.079
7.060
7.059
7.041
7.039
7.020
7.001
6.954
6.932
6.715
6.641
3.994
3.976
3.958
3.943
3.926
3.910
1.854
1.836
1.819
1.801
1.786
1.769
1.751
1.733
1.531
1.051
1.033
1.014
0.871
0.853
0.835
BRUKER
Current Data Parameters
NAME 20170102
EXPNO 9
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170102
Time 19.30
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 25
DS 0
SWH 6410.256 Hz
FIDRES 0.195625 Hz
AQ 2.5559540 sec
RG 512
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 400.1500180 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
NC
Ph
*
N
N
n-Pr
O
5c
RKS-4-210-f3p1
9
8
7
6
5
4
3
2
1
ppm
2.07
2.18
1.05
4.09
2.02
2.19
2.24
2.06
1.00
1.01
2.07
2.09
4.50
3.18
3.46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131.92
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128.58
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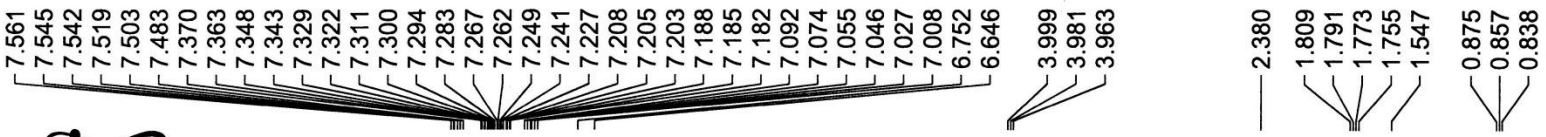
127.88
126.21
126.12
125.88
122.71
121.97
121.75
121.03
120.84
120.38
119.65
116.06
115.25
113.54
110.65
109.72
77.32
77.00
76.68
69.89
48.11
44.84
23.43
22.54
11.39
10.49
Current Data Parameters
NAME 20170103
EXPNO 6
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170102
Time 23.44
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 7000
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
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
PL12 15.10 dB
PL13 18.10 dB
SFO2 400.1516010 MHz
F2 - Processing parameters
SI 32768
SF 100.6178000 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
NC
Ph
*
N
N
n-Pr
O
5c
RKS-4-210-F3
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
pp



BRUKER

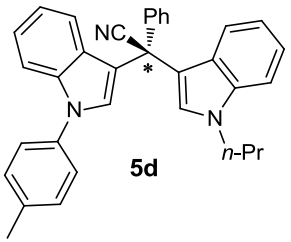
4-162-p2

Current Data Parameters
NAME 20161101
EXPNO 1
PROCNO 1

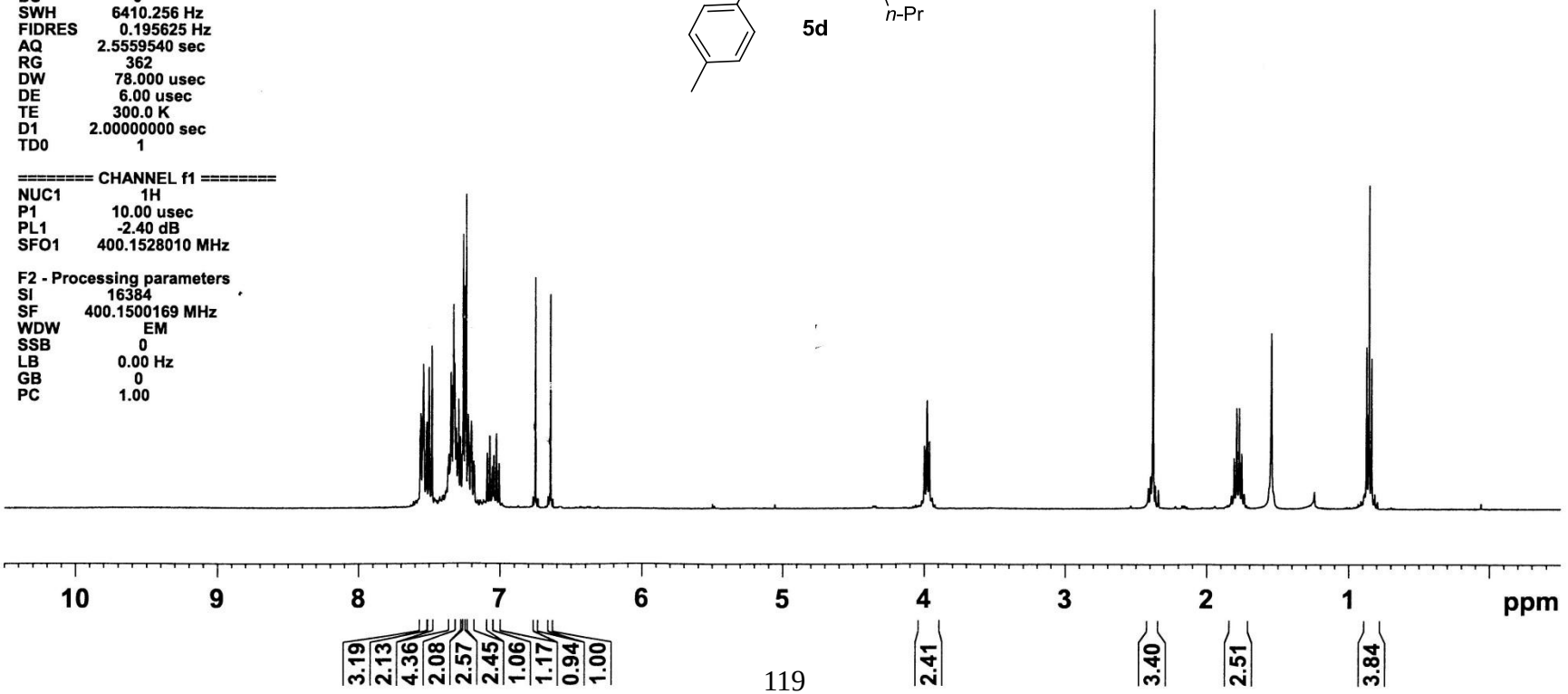
F2 - Acquisition Parameters
Date_ 20161101
Time 9.45
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 15
DS 0
SWH 6410.256 Hz
FIDRES 0.195625 Hz
AQ 2.5559540 sec
RG 362
DW 78.000 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
TD0 1

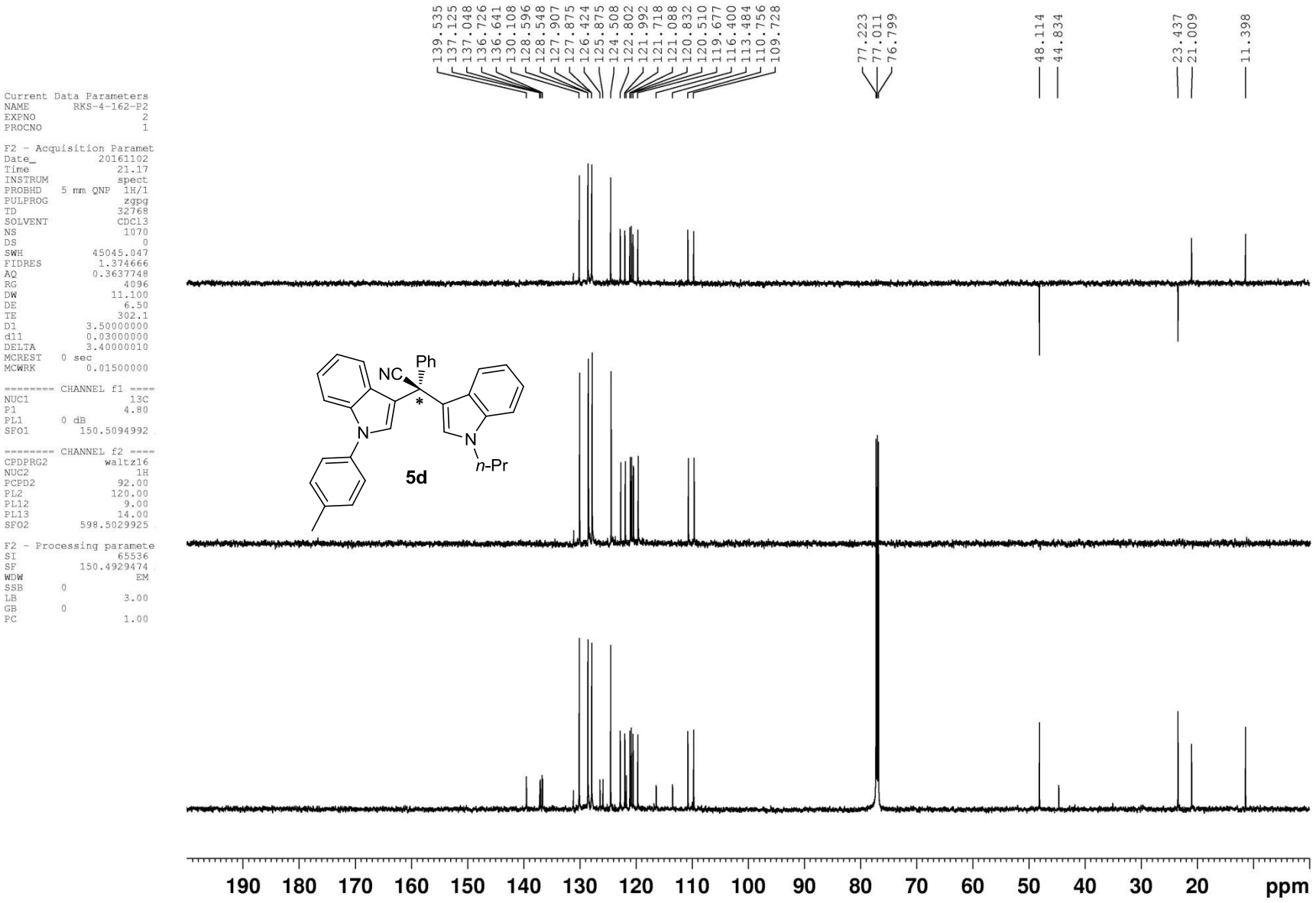
======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 -2.40 dB
SFO1 400.1528010 MHz

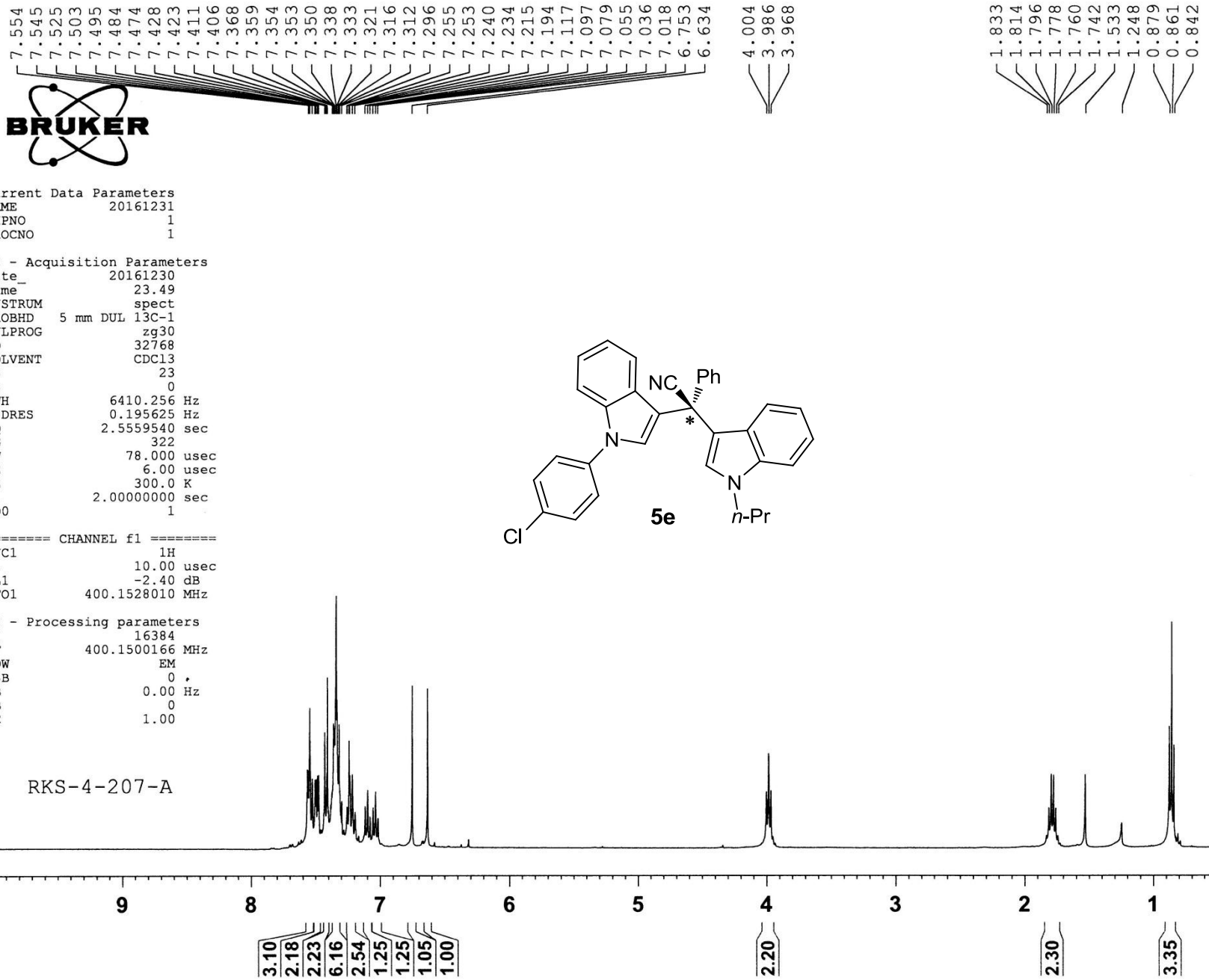
F2 - Processing parameters
SI 16384
SF 400.1500169 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 1.00

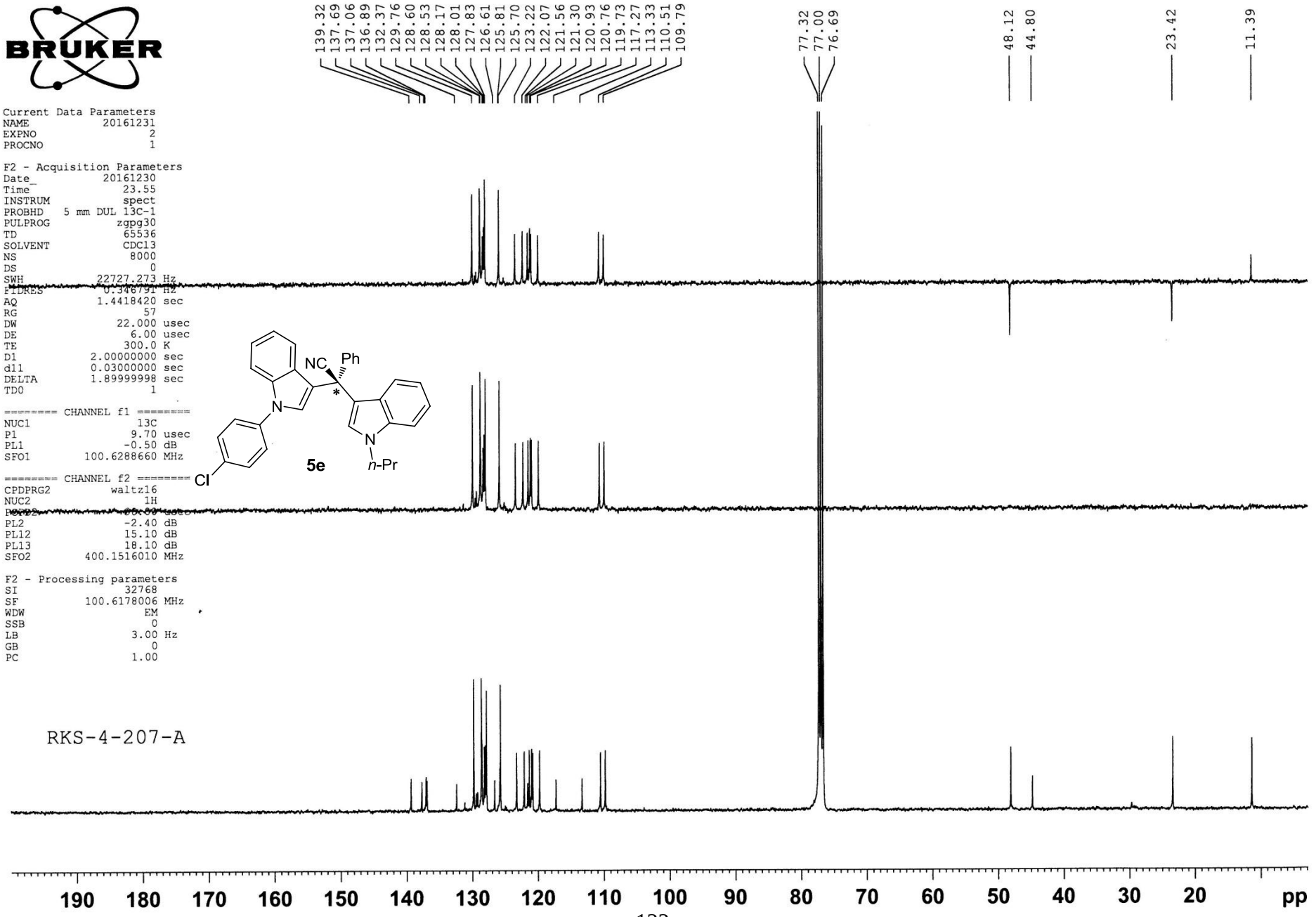


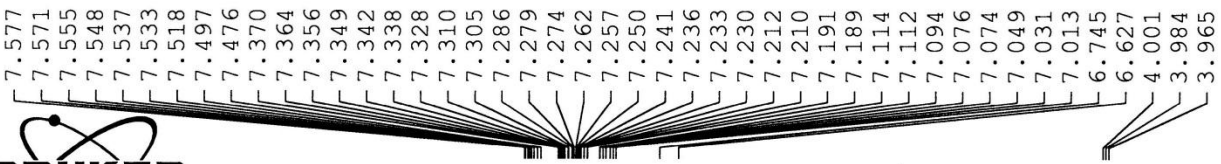
5d




Current Data Parameters
NAME RKS-4-162-P2
EXPNO 2
PROCNO 1
F2 - Acquisition Paramet
Date_ 20161102
Time 21.17
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 1070
DS 0
SWH 45045.047
FIDRES 1.374666
AQ 0.3637748
RG 4096
DW 11.100
DE 6.50
TE 302.1
D1 3.50000000
d11 0.03000000
DELTA 3.40000010
MCREST 0 sec
MCWRK 0.01500000
======== CHANNEL f1 ====
NUC1 13C
P1 4.80
PL1 0 dB
SFO1 150.5094992
======== CHANNEL f2 ====
CPDPRG2 waltz16
NUC2 1H
PCPD2 92.00
PL2 120.00
PL12 9.00
PL13 14.00
SFO2 598.5029925
F2 - Processing paramete
SI 65536
SF 150.4929474
WDW EM
SSB 0
LB 3.00
GB 0
PC 1.00
139.535
137.125
137.048
136.726
136.641
130.108
128.596
128.548
127.907
127.875
126.424
125.875
124.508
122.802
121.992
121.718
121.088
120.832
120.510
119.677
116.400
113.484
110.756
109.728
77.223
77.011
76.799
48.114
44.834
23.437
21.009
11.398
NC
Ph
*
N
N
n-Pr
5d
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm


7.554
7.545
7.525
7.503
7.495
7.484
7.474
7.428
7.423
7.411
7.406
7.368
7.359
7.354
7.353
7.350
7.338
7.333
7.321
7.316
7.312
7.296
7.255
7.253
7.240
7.234
7.215
7.194
7.117
7.097
7.079
7.055
7.036
7.018
6.753
6.634
4.004
3.986
3.968
1.833
1.814
1.796
1.778
1.760
1.742
1.533
1.248
0.879
0.861
0.842
BRUKER
Current Data Parameters
NAME 20161231
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20161230
Time 23.49
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 23
DS 0
SWH 6410.256 Hz
FIDRES 0.195625 Hz
AQ 2.5559540 sec
RG 322
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 400.1500166 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
NC
Ph
N
*
N
Cl
5e
n-Pr
RKS-4-207-A
9
8
7
6
5
4
3
2
1
ppm
3.10
2.18
2.23
6.16
2.54
1.25
1.25
1.05
1.00
2.20
2.30
3.35


BRUKER
139.32
137.69
137.06
136.89
132.37
129.76
128.60
128.53
128.17
128.01
127.83
126.61
125.81
125.70
123.22
122.07
121.56
121.30
120.93
120.76
119.73
117.27
113.33
110.51
109.79
77.32
77.00
76.69
48.12
44.80
23.42
11.39
Current Data Parameters
NAME 20161231
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20161230
Time 23.55
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 8000
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
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 65.00 usec
PL2 -2.40 dB
PL12 15.10 dB
PL13 18.10 dB
SFO2 400.1516010 MHz
F2 - Processing parameters
SI 32768
SF 100.6178006 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
NC
Ph
N
*
N
n-Pr
Cl
5e
RKS-4-207-A
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
pp



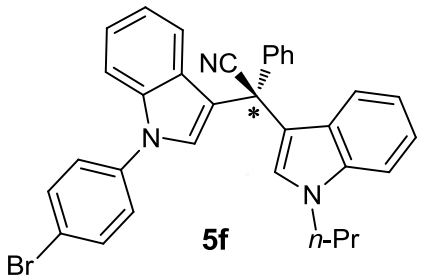
BRUKER

```
Current Data Parameters
NAME            20170117
EXPNO                 10
PROCNO                 1

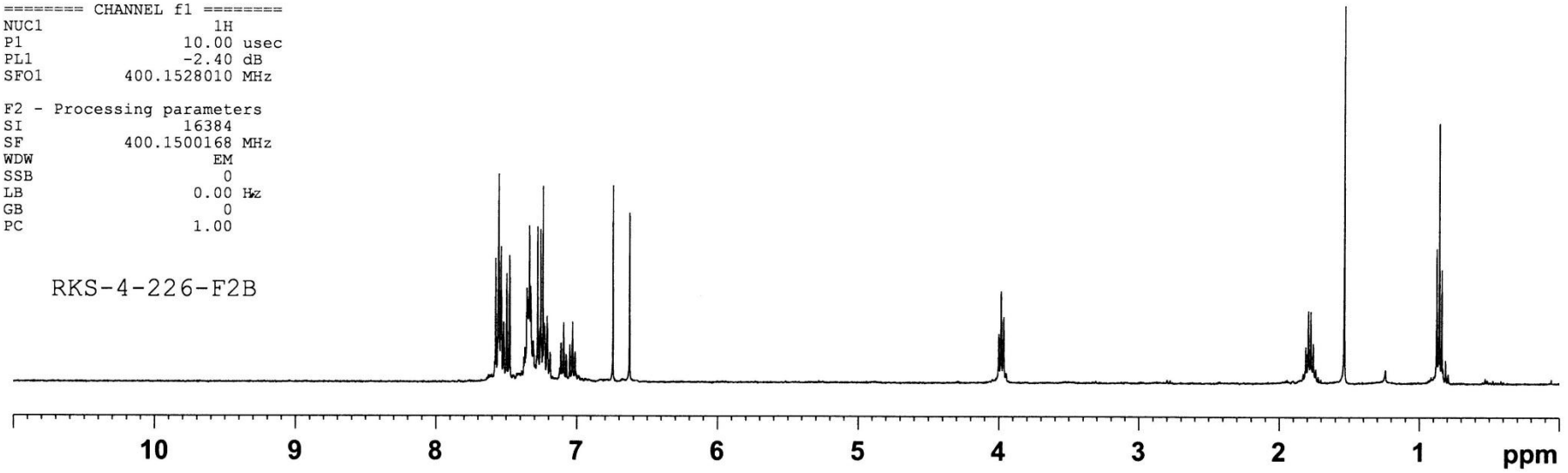
F2 - Acquisition Parameters
Date_           20170117
Time                23.16
INSTRUM             spect
PROBHD   5 mm DUL 13C-1
PULPROG              zg30
TD                  32768
SOLVENT             CDCl3
NS                     12
DS                      0
SWH               6410.256 Hz
FIDRES           0.195625 Hz
AQ               2.5559540 sec
RG                      4
DW                 78.000 usec
DE                  6.00 usec
TE                 300.0 K
D1            2.00000000 sec
TD0                     1

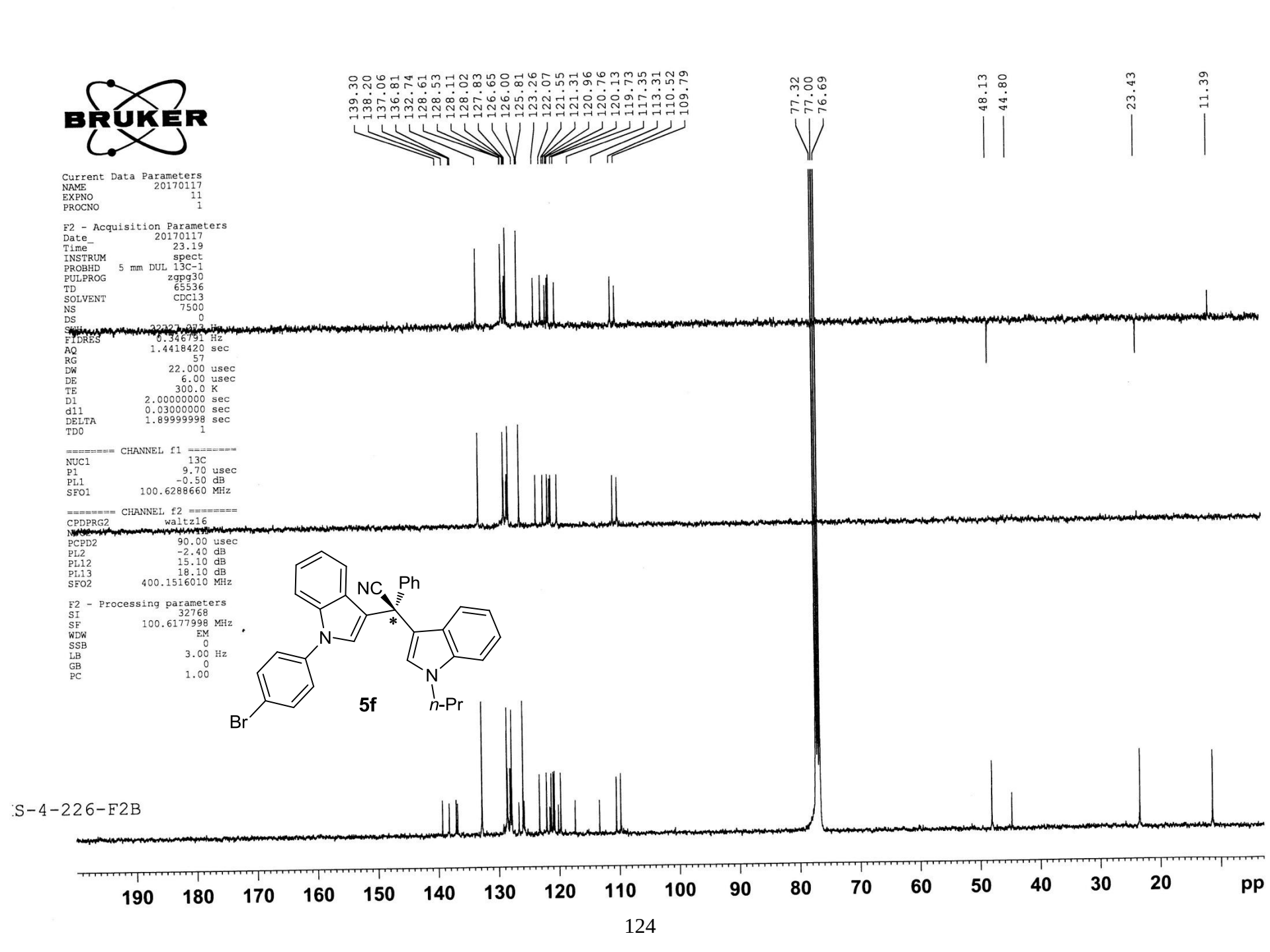
======== CHANNEL f1 ========
NUC1                   1H
P1                 10.00 usec
PL1                -2.40 dB
SFO1         400.1528010 MHz

F2 - Processing parameters
SI                  16384
SF           400.1500168 MHz
WDW                    EM
SSB                     0
LB                   0.00 Hz
GB                      0
PC                   1.00
```

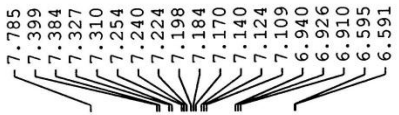


RKS-4-226-F2B




BRUKER
139.30
138.20
137.06
136.81
132.74
128.61
128.53
128.11
128.02
127.83
126.65
126.00
125.81
123.26
122.07
121.55
121.31
120.96
120.76
120.13
119.73
117.35
113.31
110.52
109.79
77.32
77.00
76.69
48.13
44.80
23.43
11.39
Current Data Parameters
NAME 20170117
EXPNO 11
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170117
Time 23.19
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 7500
DS 0
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
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.70 usec
PL1 -0.50 dB
SFO1 100.6288660 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
PCPD2 90.00 usec
PL2 -2.40 dB
PL12 15.10 dB
PL13 18.10 dB
SFO2 400.1516010 MHz
F2 - Processing parameters
SI 32768
SF 100.6177998 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
NC
Ph
*
N
N
Br
n-Pr
5f
S-4-226-F2B
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

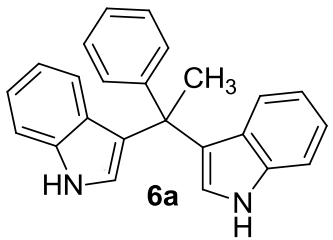
RKS-4-184-P /1H



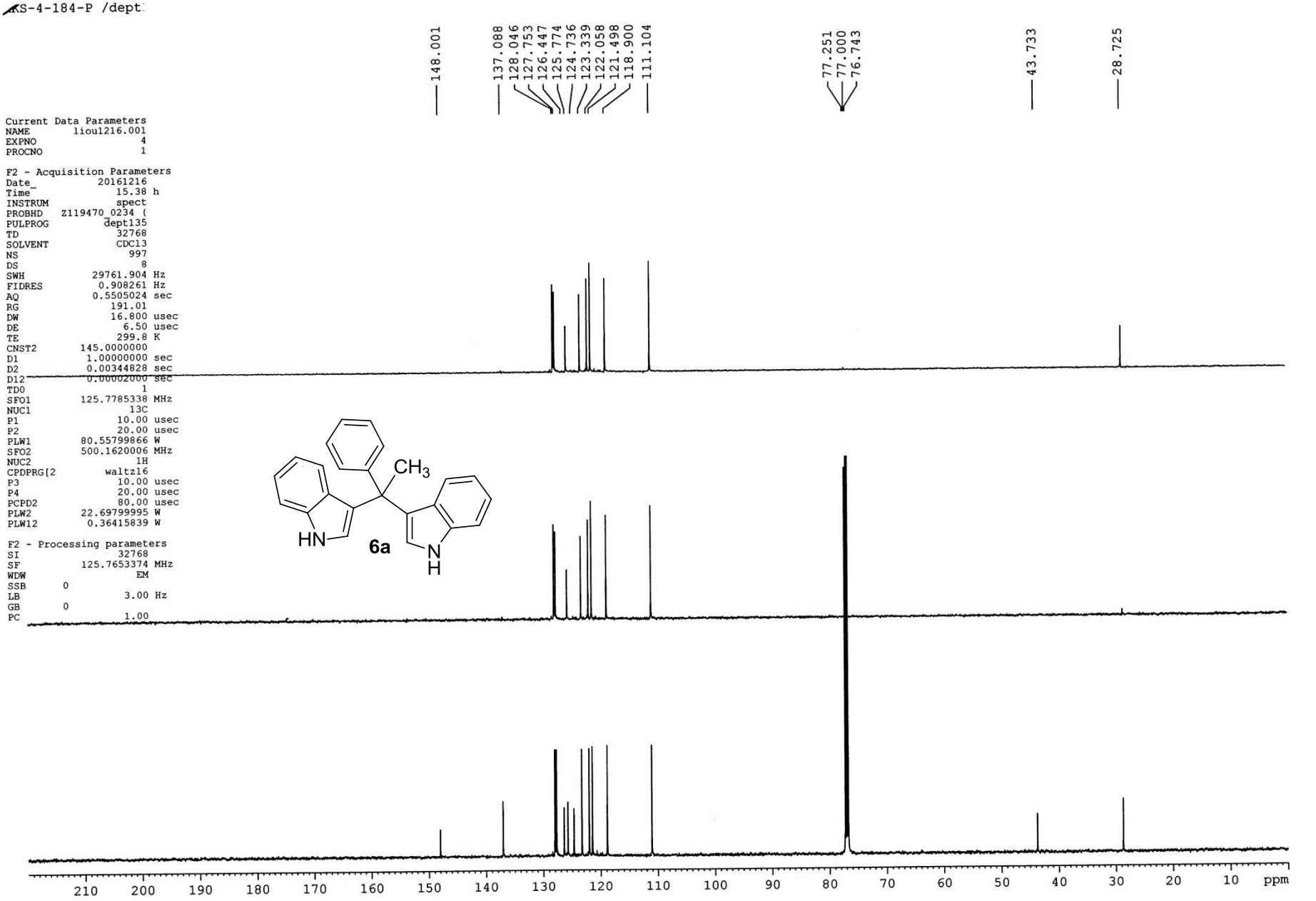

```
Current Data Parameters
NAME        liou1216.001
EXPNO                  1
PROCNO                 1

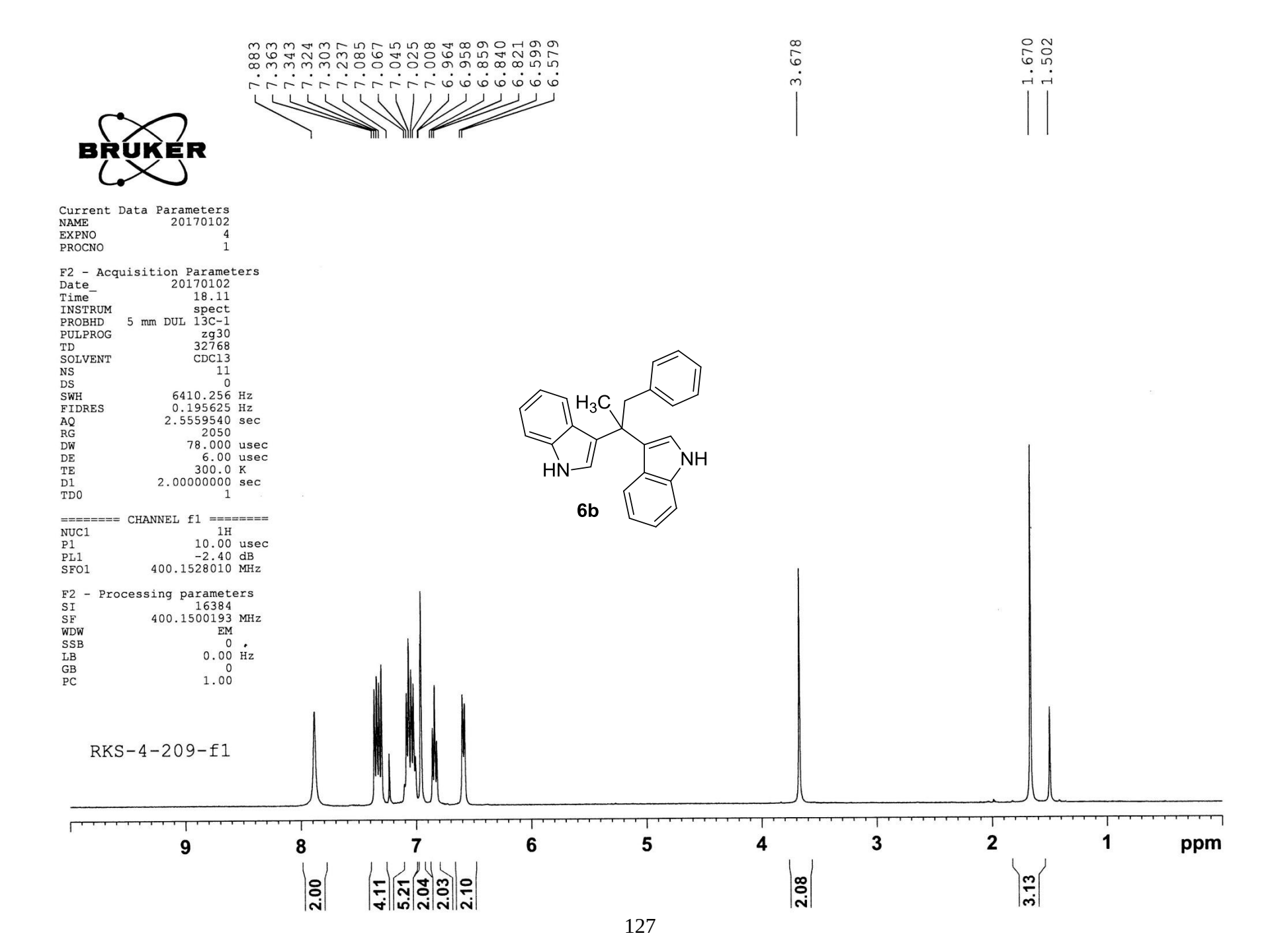
F2 - Acquisition Parameters
Date_           20161216
Time              15.02 h
INSTRUM            spect
PROBHD   Z119470_0234 (
PULPROG            zg30
TD                32768
SOLVENT           CDCl3
NS                   32
DS                    0
SWH           10026.738 Hz
FIDRES         0.305992 Hz
AQ            1.6340309 sec
RG                71.36
DW               49.867 usec
DE                7.71 usec
TE                303.0 K
D1           2.00000000 sec
TD0                   1
SFO1        500.1630010 MHz
NUC1                1H
P1                10.00 usec
PLW1        22.69799995 W

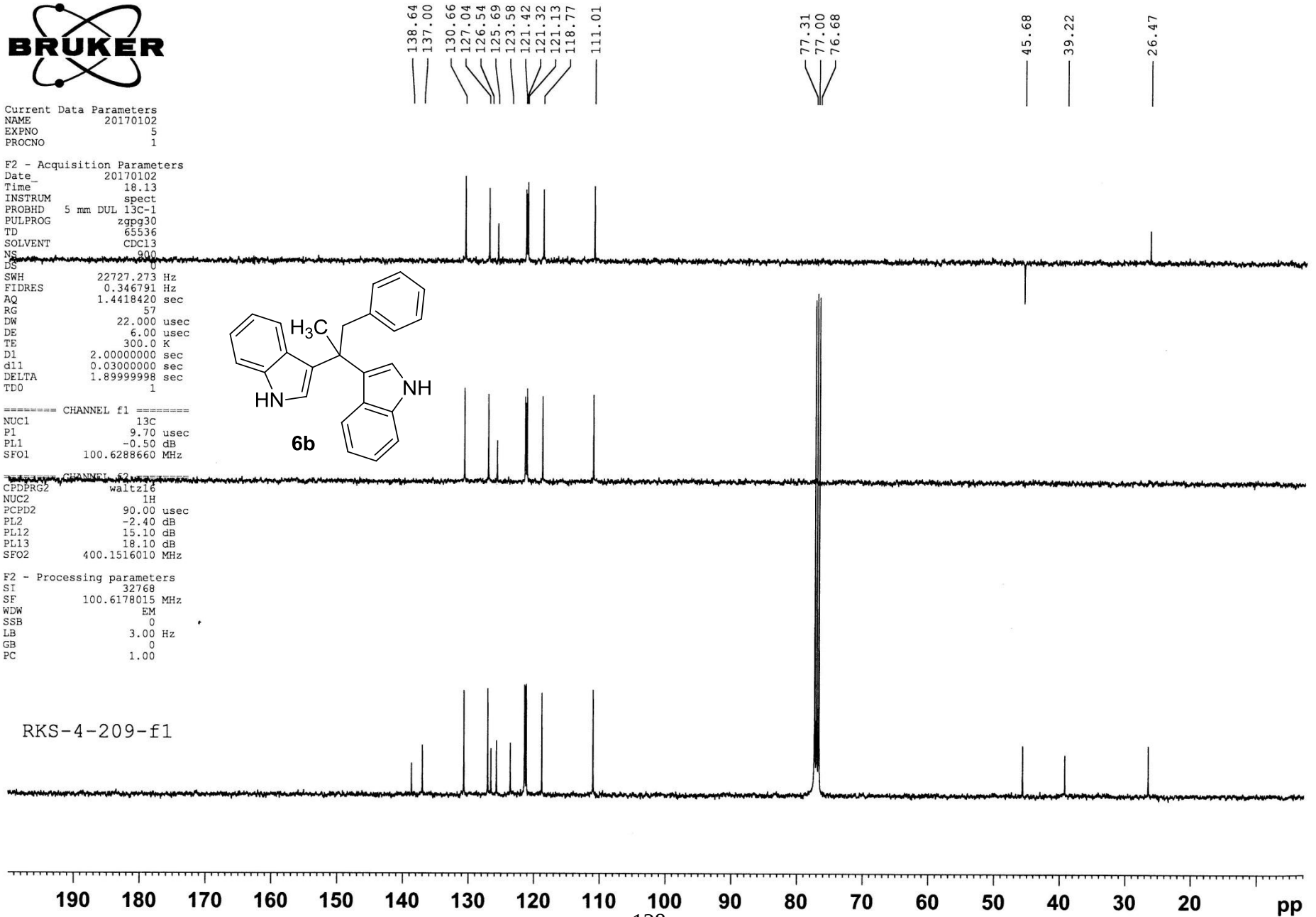
F2 - Processing parameters
SI                16384
SF          500.1600211 MHz
WDW                  EM
SSB       0
LB                0.30 Hz
GB        0
PC                1.00
```



6a


KS-4-184-P /dept
148.001
137.088
128.046
127.753
126.447
125.774
124.736
123.339
122.058
121.498
118.900
111.104
77.251
77.000
76.743
43.733
28.725
Current Data Parameters
NAME liou1216.001
EXPNO 4
PROCNO 1
F2 - Acquisition Parameters
Date_ 20161216
Time 15.38 h
INSTRUM spect
PROBHD Z119470_0234 (
PULPROG dept135
TD 32768
SOLVENT CDCl3
NS 997
DS 8
SWH 29761.904 Hz
FIDRES 0.908261 Hz
AQ 0.5505024 sec
RG 191.01
DW 16.800 usec
DE 6.50 usec
TE 299.8 K
CNST2 145.0000000
D1 1.00000000 sec
D2 0.00344828 sec
D12 0.00002000 sec
TD0 1
SFO1 125.7785338 MHz
NUC1 13C
P1 10.00 usec
P2 20.00 usec
PLW1 80.55799866 W
SFO2 500.1620006 MHz
NUC2 1H
CPDPRG[2 waltz16
P3 10.00 usec
P4 20.00 usec
PCPD2 80.00 usec
PLW2 22.69799995 W
PLW12 0.36415839 W
F2 - Processing parameters
SI 32768
SF 125.7653374 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
CH3
HN
N
H
6a
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm


7.883
7.363
7.343
7.324
7.303
7.237
7.085
7.067
7.045
7.025
7.008
6.964
6.958
6.859
6.840
6.821
6.599
6.579
3.678
1.670
1.502
BRUKER
Current Data Parameters
NAME 20170102
EXPNO 4
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170102
Time 18.11
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 11
DS 0
SWH 6410.256 Hz
FIDRES 0.195625 Hz
AQ 2.5559540 sec
RG 2050
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 400.1500193 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
H3C
HN
NH
6b
RKS-4-209-f1
9
8
7
6
5
4
3
2
1
ppm
2.00
4.11
5.21
2.04
2.03
2.10
2.08
3.13


138.64
137.00
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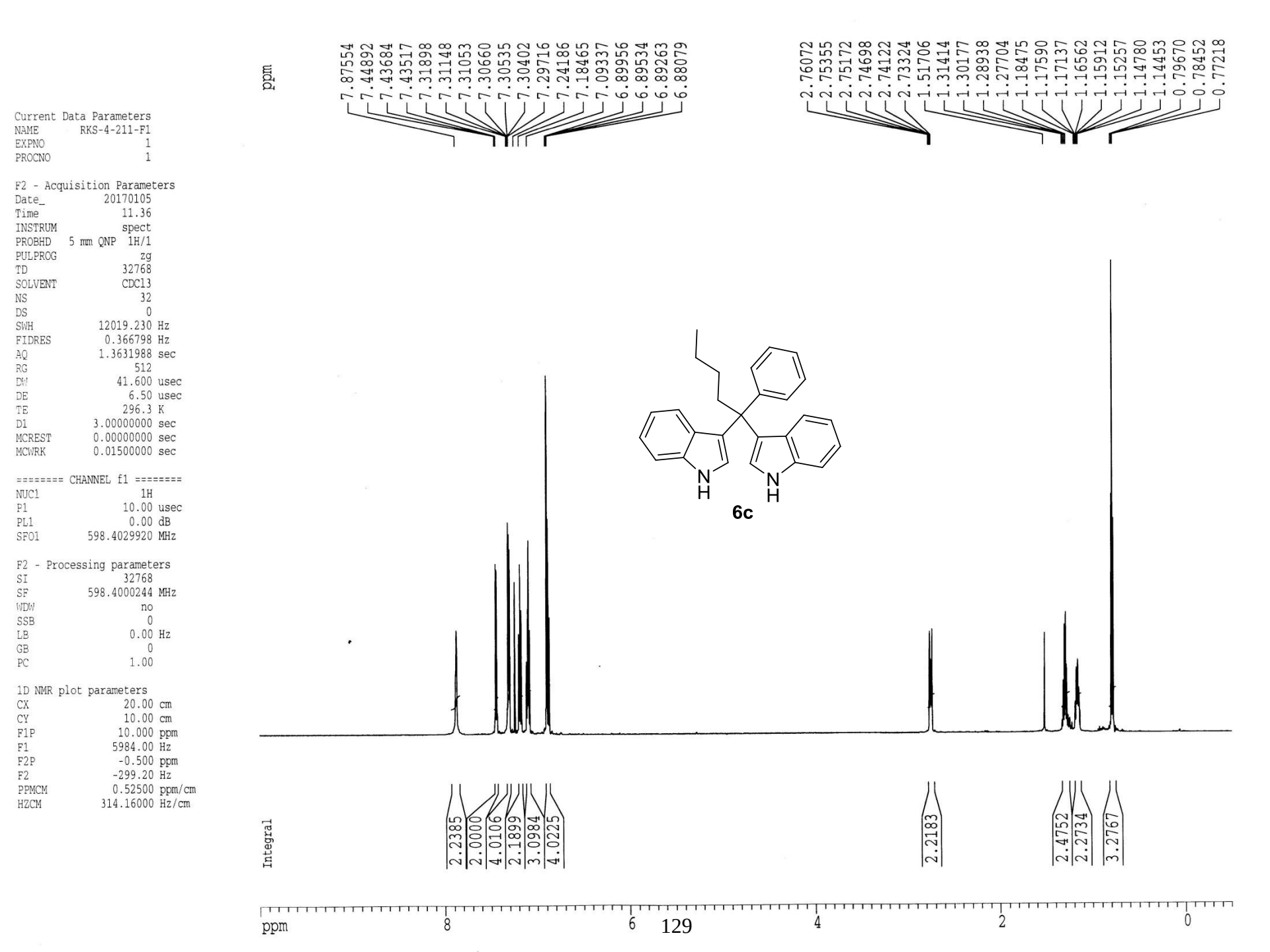
127.04
126.54
125.69
123.58
121.42
121.32
121.13
118.77
111.01
77.31
77.00
76.68
45.68
39.22
26.47
Current Data Parameters
NAME 20170102
EXPNO 5
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170102
Time 18.13
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 900
DS 0
SWH 22727.273 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
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.70 usec
PL1 -0.50 dB
SFO1 100.6288660 MHz
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -2.40 dB
PL12 15.10 dB
PL13 18.10 dB
SFO2 400.1516010 MHz
F2 - Processing parameters
SI 32768
SF 100.6178015 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
H3C
HN
NH
6b
RKS-4-209-f1
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 pp


Current Data Parameters
NAME RKS-4-211-F1
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170105
Time 11.36
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 32
DS 0
SWH 12019.230 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 512
DW 41.600 usec
DE 6.50 usec
TE 296.3 K
D1 3.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 0.00 dB
SFO1 598.4029920 MHz
F2 - Processing parameters
SI 32768
SF 598.4000244 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 20.00 cm
CY 10.00 cm
F1P 10.000 ppm
F1 5984.00 Hz
F2P -0.500 ppm
F2 -299.20 Hz
PPMCM 0.52500 ppm/cm
HZCM 314.16000 Hz/cm
ppm
7.87554
7.44892
7.43684
7.43517
7.31898
7.31148
7.31053
7.30660
7.30535
7.30402
7.29716
7.24186
7.18465
7.09337
6.89956
6.89534
6.89263
6.88079
2.76072
2.75355
2.75172
2.74698
2.74122
2.73324
1.51706
1.31414
1.30177
1.28938
1.27704
1.18475
1.17590
1.17137
1.16562
1.15912
1.15257
1.14780
1.14453
0.79670
0.78452
0.77218
N
H
N
H
6c
Integral
2.2385
2.0000
4.0106
2.1899
3.0984
4.0225
2.2183
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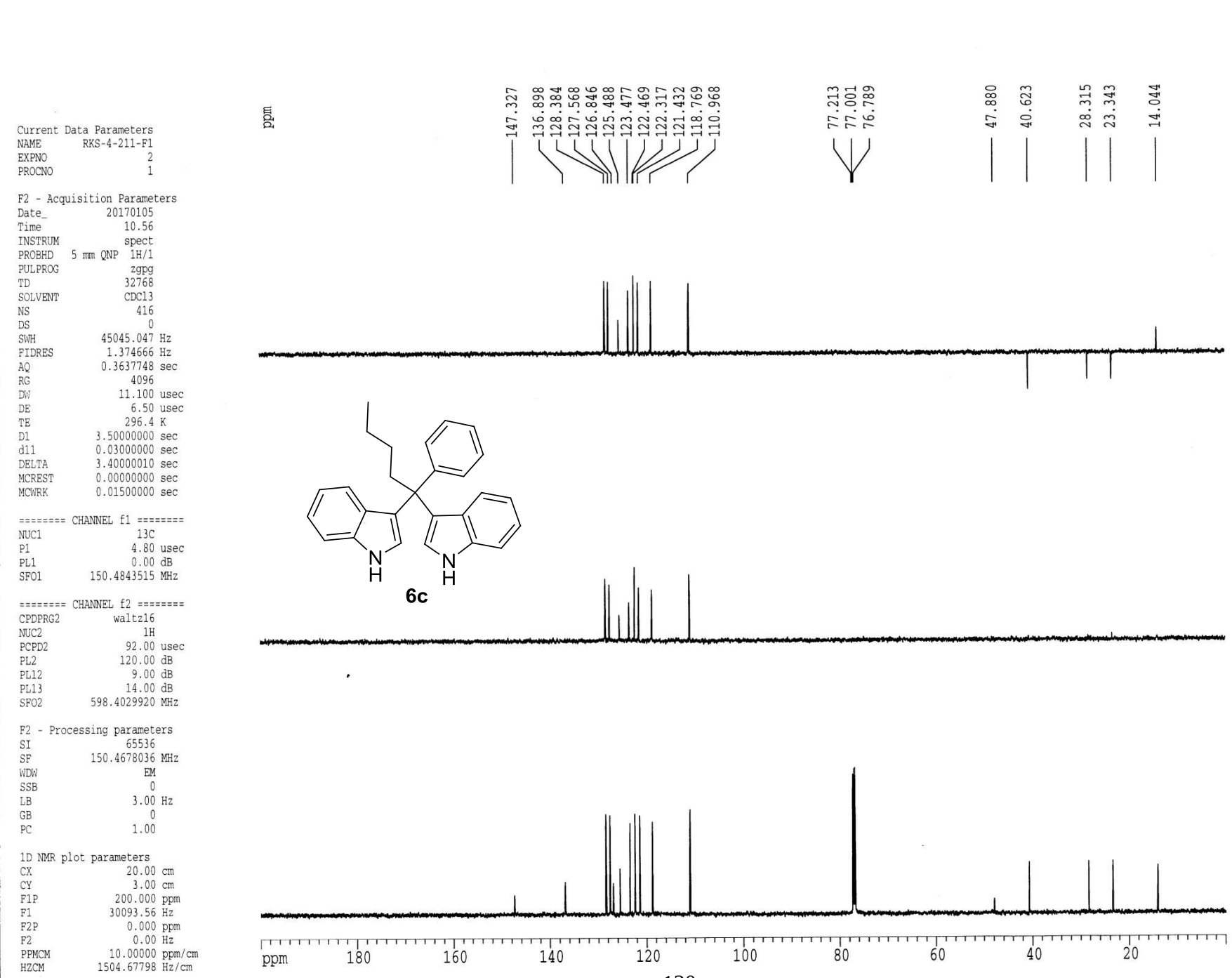
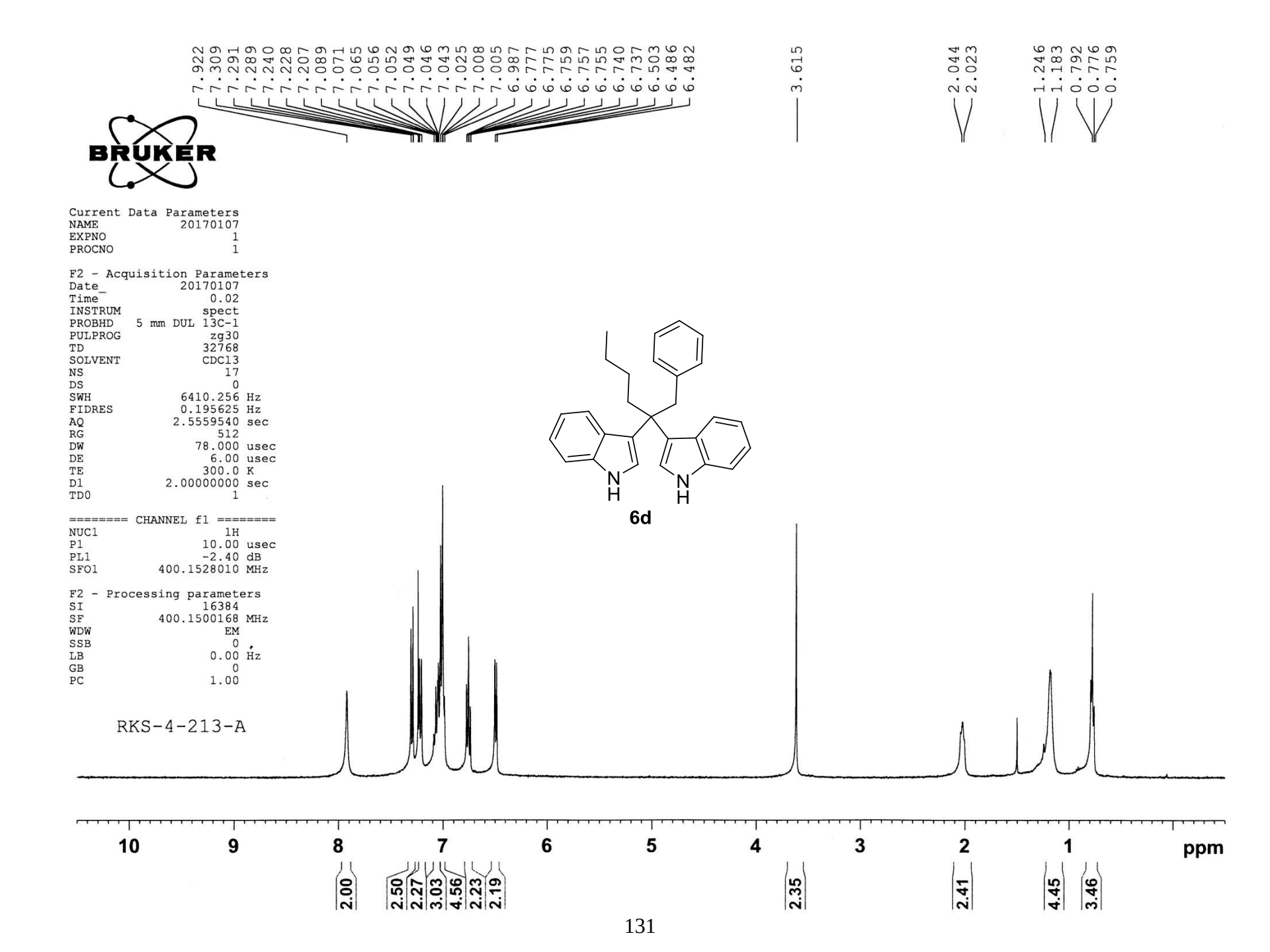
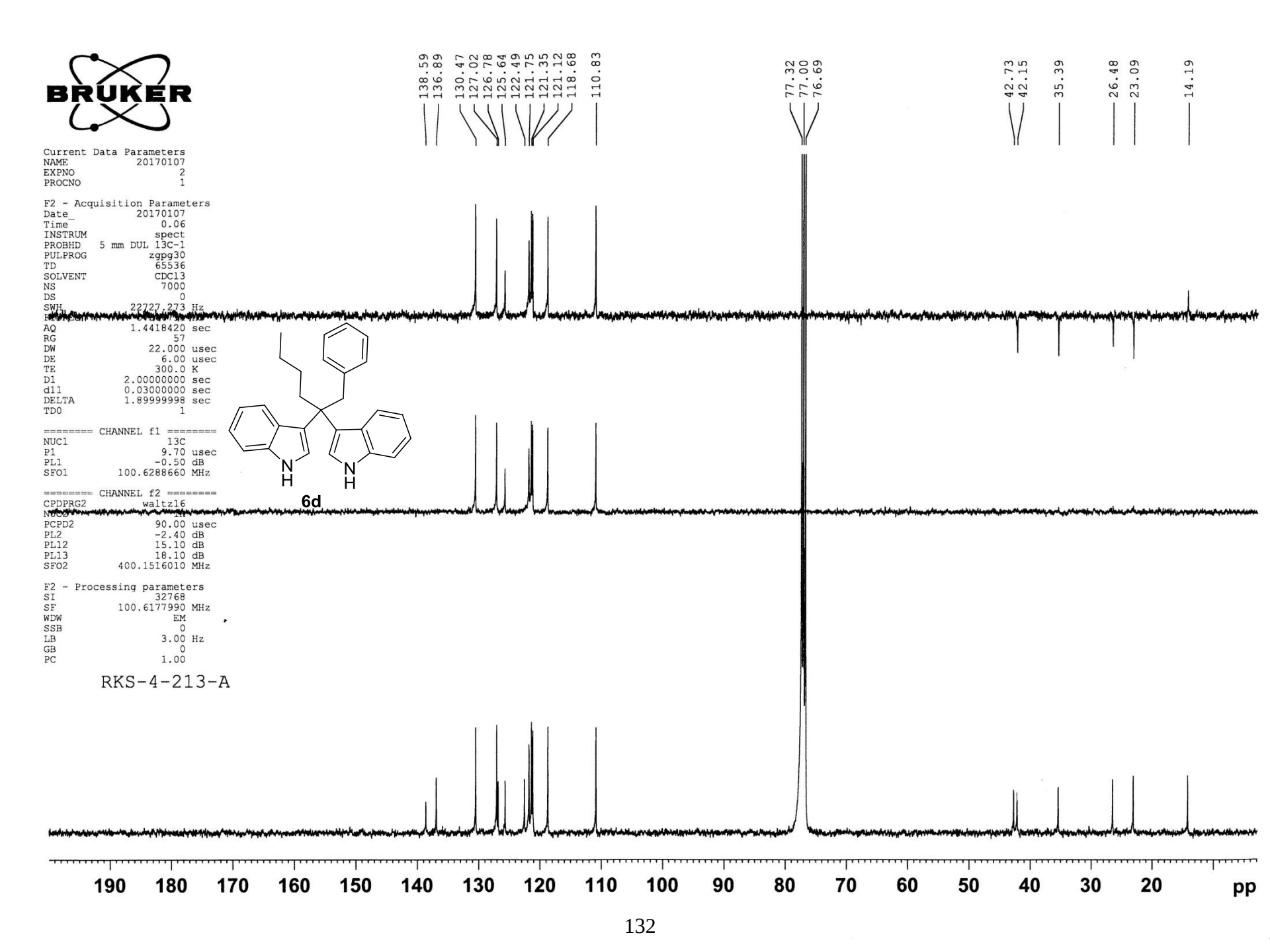
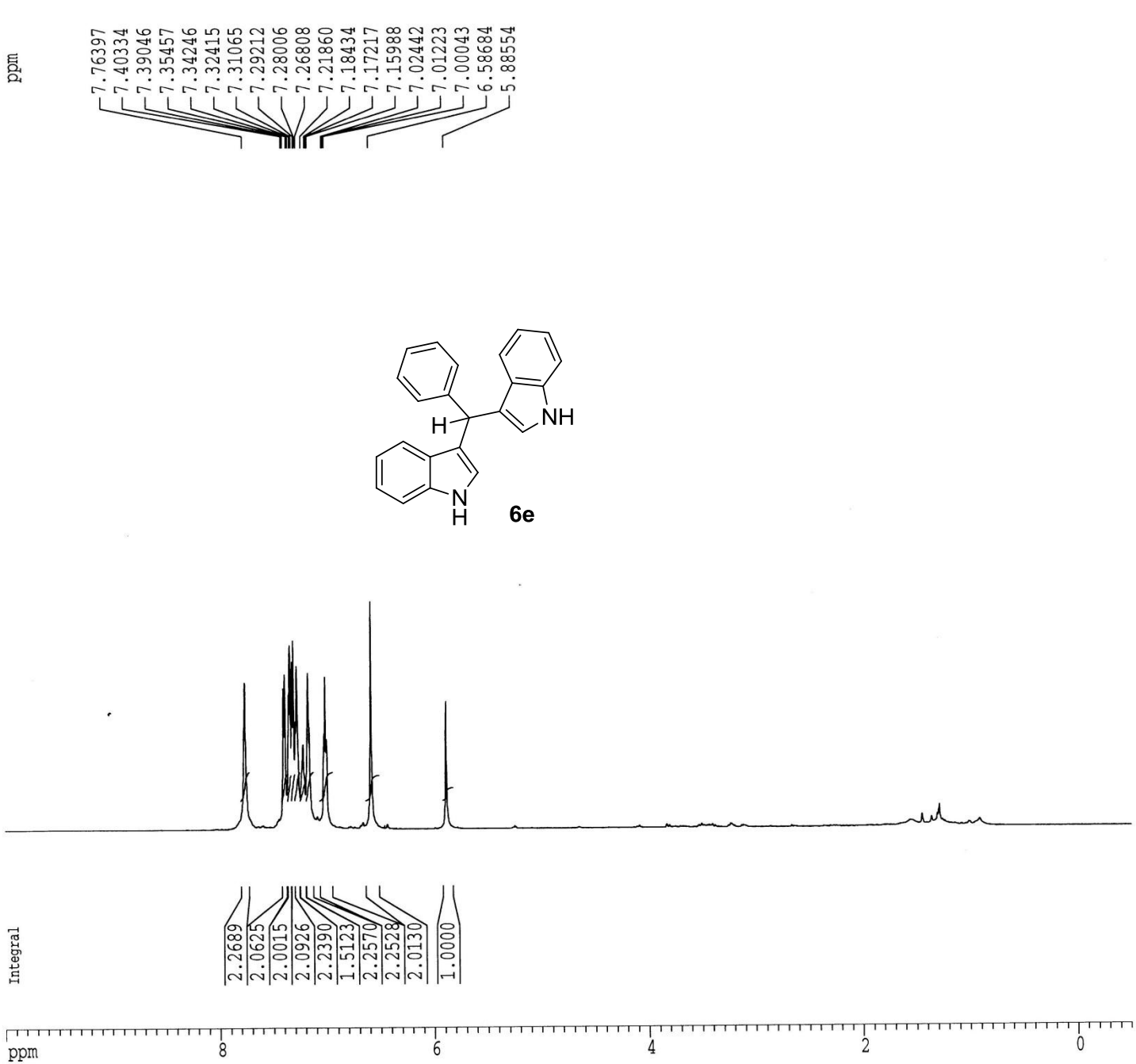
3.2767
ppm
8
6
4
2
0


Current Data Parameters
NAME RKS-4-211-F1
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170105
Time 10.56
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 416
DS 0
SWH 45045.047 Hz
FIDRES 1.374666 Hz
AQ 0.3637748 sec
RG 4096
DW 11.100 usec
DE 6.50 usec
TE 296.4 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 150.4843515 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 92.00 usec
PL2 120.00 dB
PL12 9.00 dB
PL13 14.00 dB
SFO2 598.4029920 MHz
F2 - Processing parameters
SI 65536
SF 150.4678036 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 20.00 cm
CY 3.00 cm
F1P 200.000 ppm
F1 30093.56 Hz
F2P 0.000 ppm
F2 0.00 Hz
PPMCM 10.00000 ppm/cm
HZCM 1504.67798 Hz/cm
ppm
147.327
136.898
128.384
127.568
126.846
125.488
123.477
122.469
122.317
121.432
118.769
110.968
77.213
77.001
76.789
47.880
40.623
28.315
23.343
14.044
N
H
N
H
6c
ppm
180
160
140
120
100
80
60
40
20


7.922
7.309
7.291
7.289
7.240
7.228
7.207
7.089
7.071
7.065
7.056
7.052
7.049
7.046
7.043
7.025
7.008
7.005
6.987
6.777
6.775
6.759
6.757
6.755
6.740
6.737
6.503
6.486
6.482
3.615
2.044
2.023
1.246
1.183
0.792
0.776
0.759
BRUKER
Current Data Parameters
NAME 20170107
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170107
Time 0.02
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 17
DS 0
SWH 6410.256 Hz
FIDRES 0.195625 Hz
AQ 2.5559540 sec
RG 512
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 400.1500168 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
N
H
N
H
6d
RKS-4-213-A
10
9
8
7
6
5
4
3
2
1
ppm
2.00
2.50
2.27
3.03
4.56
2.23
2.19
2.35
2.41
4.45
3.46


BRUKER
138.59
136.89
130.47
127.02
126.78
125.64
122.49
121.75
121.35
121.12
118.68
110.83
77.32
77.00
76.69
42.73
42.15
35.39
26.48
23.09
14.19
Current Data Parameters
NAME 20170107
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170107
Time 0.06
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 7000
DS 0
SWH 22727.273 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
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.70 usec
PL1 -0.50 dB
SFO1 100.6288660 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
PCPD2 90.00 usec
PL2 -2.40 dB
PL12 15.10 dB
PL13 18.10 dB
SFO2 400.1516010 MHz
F2 - Processing parameters
SI 32768
SF 100.6177990 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
N
H
N
H
6d
RKS-4-213-A
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
pp



Current Data Parameters
NAME RKS-4-193-P1
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20161207
Time 12.01
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 32
DS 0
SWH 12019.230 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 128
DW 41.600 usec
DE 6.50 usec
TE 298.4 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 598.4038896 MHz

F2 - Processing parameters
SI 32768
SF 598.4000256 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 5984.00 Hz
F2P -0.500 ppm
F2 -299.20 Hz
PPMCM 0.52500 ppm/cm
HZCM 314.16000 Hz/cm

Current Data Parameters
NAME RKS-4-193-P1
EXPNO 2
PROCNO 1

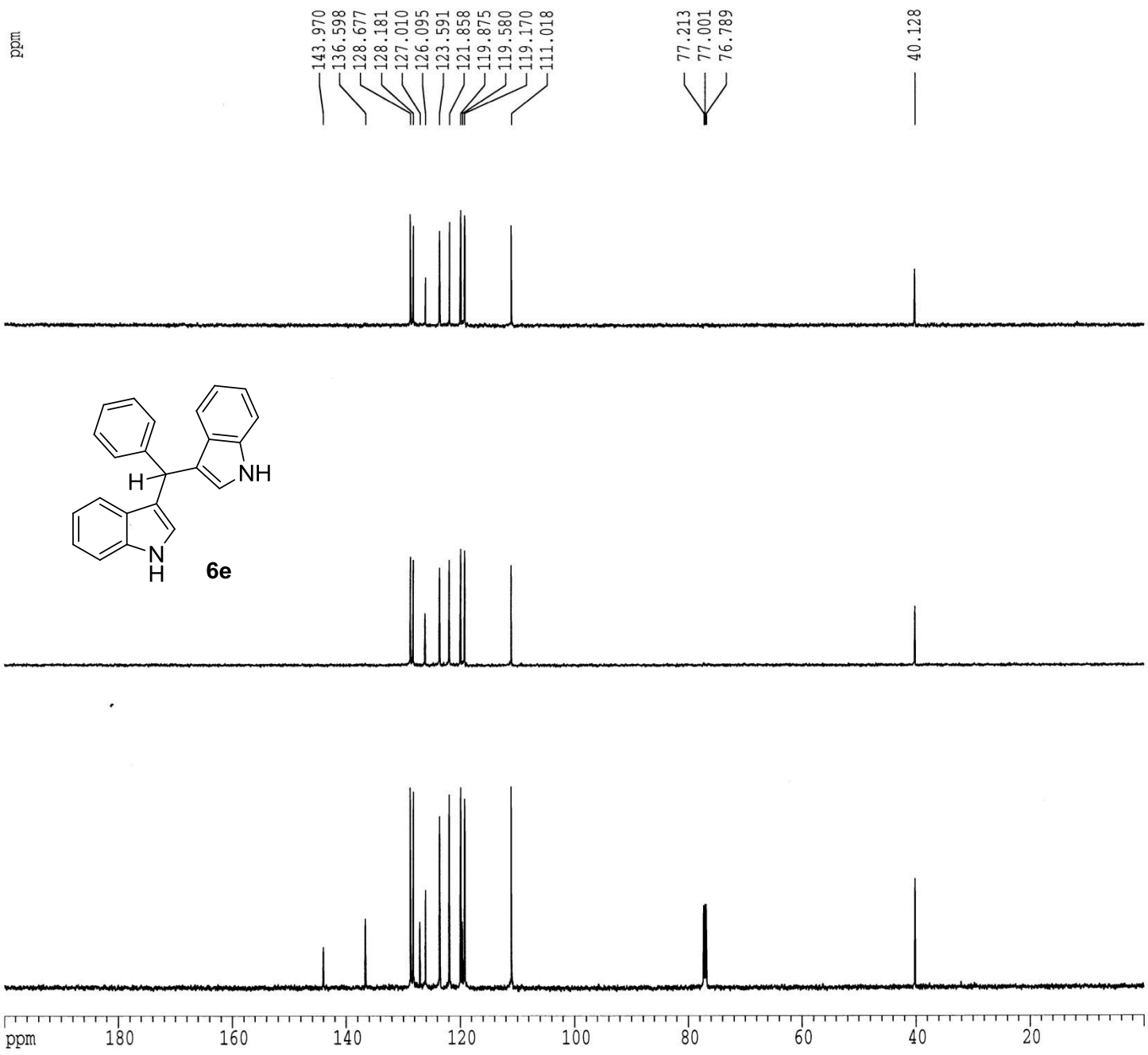
F2 - Acquisition Parameters
Date_ 20161207
Time 11.43
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 100
DS 0
SWH 45045.047 Hz
FIDRES 1.374666 Hz
AQ 0.3637748 sec
RG 4096
DW 11.100 usec
DE 6.50 usec
TE 299.0 K
D1 3.50000000 sec
d11 0.03000000 sec
DELTA 3.40000010 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

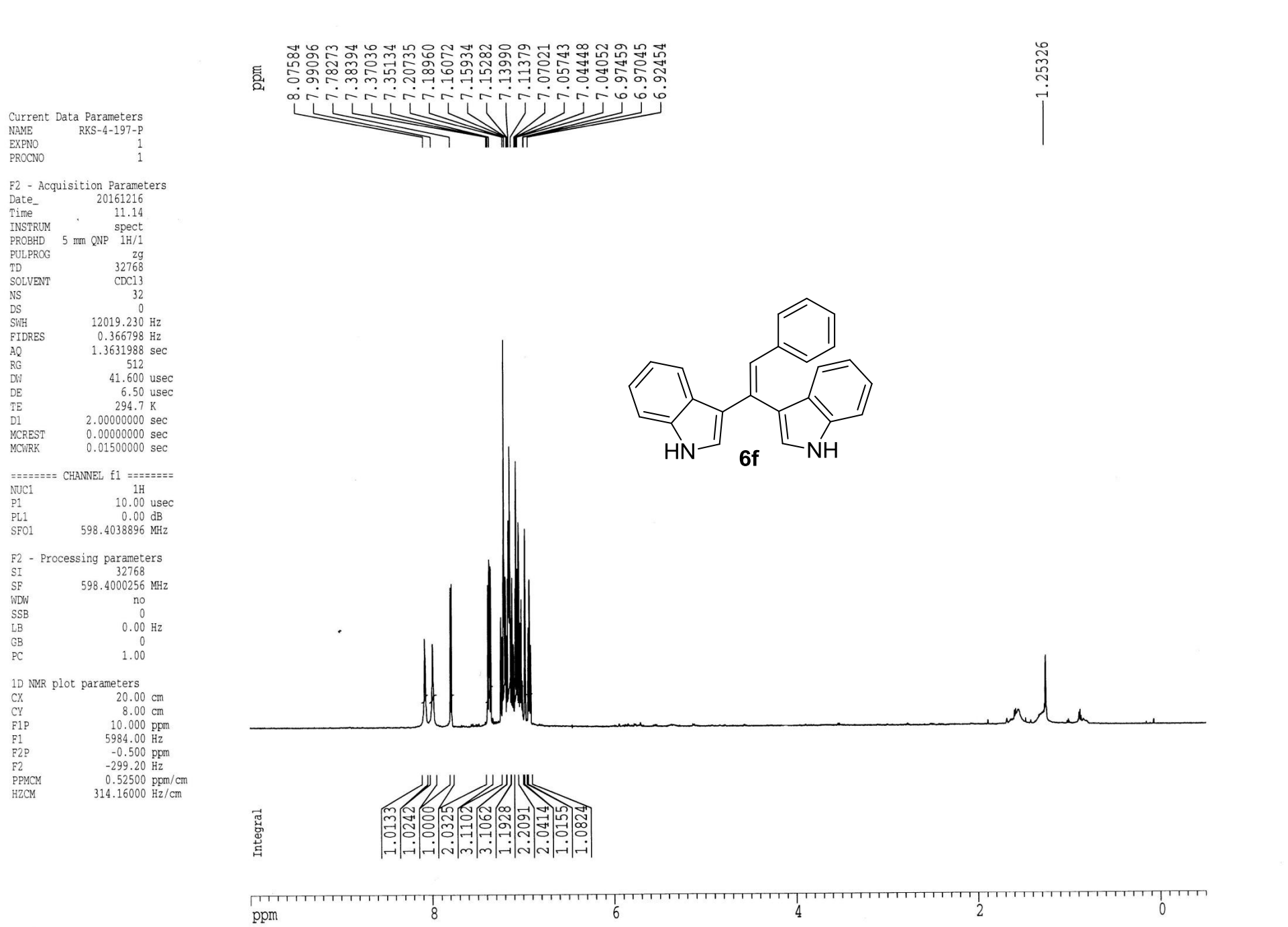
======== CHANNEL f1 ========
NUC1 13C
P1 4.80 usec
PL1 0.00 dB
SFO1 150.4843515 MHz

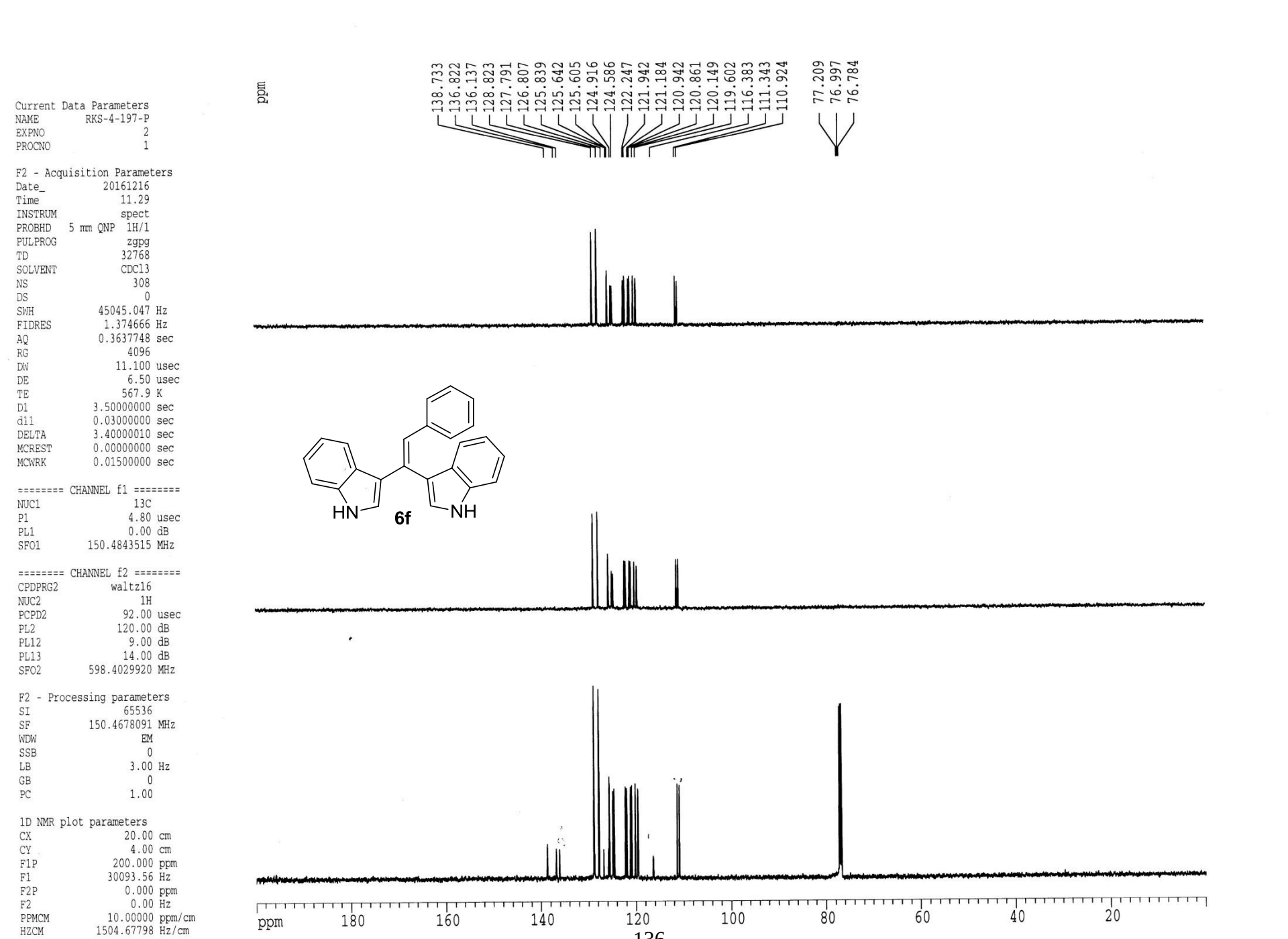
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 92.00 usec
PL2 120.00 dB
PL12 9.00 dB
PL13 14.00 dB
SFO2 598.4029920 MHz

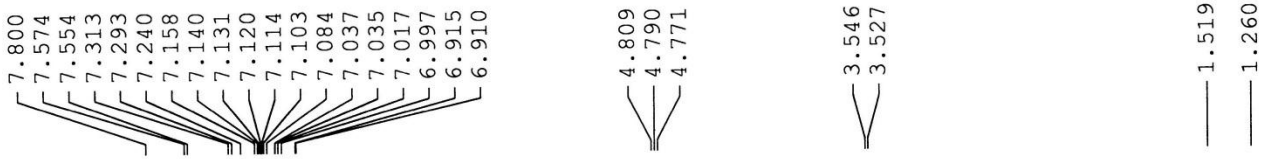
F2 - Processing parameters
SI 65536
SF 150.4678153 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 20.00 cm
CY 3.50 cm
F1P 200.000 ppm
F1 30093.56 Hz
F2P 0.000 ppm
F2 0.00 Hz
PPMCM 10.00000 ppm/cm
HZCM 1504.67822 Hz/cm




ppm
8.07584
7.99096
7.78273
7.38394
7.37036
7.35134
7.20735
7.18960
7.16072
7.15934
7.15282
7.13990
7.11379
7.07021
7.05743
7.04448
7.04052
6.97459
6.97045
6.92454
1.25326
Current Data Parameters
NAME RKS-4-197-P
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20161216
Time 11.14
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 32
DS 0
SWH 12019.230 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 512
DW 41.600 usec
DE 6.50 usec
TE 294.7 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 598.4038896 MHz
F2 - Processing parameters
SI 32768
SF 598.4000256 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 20.00 cm
CY 8.00 cm
F1P 10.000 ppm
F1 5984.00 Hz
F2P -0.500 ppm
F2 -299.20 Hz
PPMCM 0.52500 ppm/cm
HZCM 314.16000 Hz/cm
HN
NH
6f
Integral
1.0133
1.0242
1.0000
2.0325
3.1102
3.1062
1.1928
2.2091
2.0414
1.0155
1.0824
ppm
8
6
4
2
0


Current Data Parameters
NAME RKS-4-197-P
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20161216
Time 11.29
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 308
DS 0
SWH 45045.047 Hz
FIDRES 1.374666 Hz
AQ 0.3637748 sec
RG 4096
DW 11.100 usec
DE 6.50 usec
TE 567.9 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 150.4843515 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 92.00 usec
PL2 120.00 dB
PL12 9.00 dB
PL13 14.00 dB
SFO2 598.4029920 MHz
F2 - Processing parameters
SI 65536
SF 150.4678091 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 20.00 cm
CY 4.00 cm
F1P 200.000 ppm
F1 30093.56 Hz
F2P 0.000 ppm
F2 0.00 Hz
PPMCM 10.00000 ppm/cm
HZCM 1504.67798 Hz/cm
ppm
138.733
136.822
136.137
128.823
127.791
126.807
125.839
125.642
125.605
124.916
124.586
122.247
121.942
121.184
120.942
120.861
120.149
119.602
116.383
111.343
110.924
77.209
76.997
76.784
HN
NH
6f
ppm
180
160
140
120
100
80
60
40
20



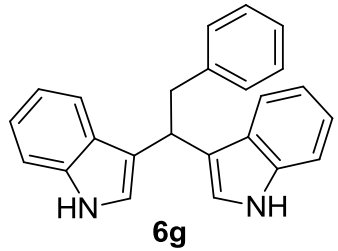
BRUKER

```
Current Data Parameters
NAME              20161230
EXPNO                   12
PROCNO                   1

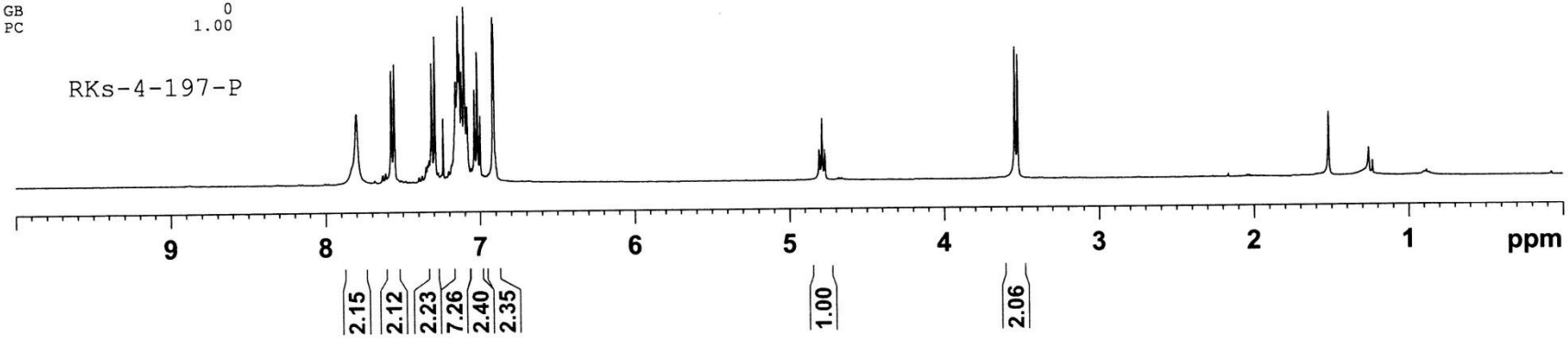
F2 - Acquisition Parameters
Date_             20161230
Time                 17.46
INSTRUM              spect
PROBHD   5 mm DUL 13C-1
PULPROG               zg30
TD                   32768
SOLVENT              CDCl3
NS                      12
DS                       0
SWH               6410.256 Hz
FIDRES            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

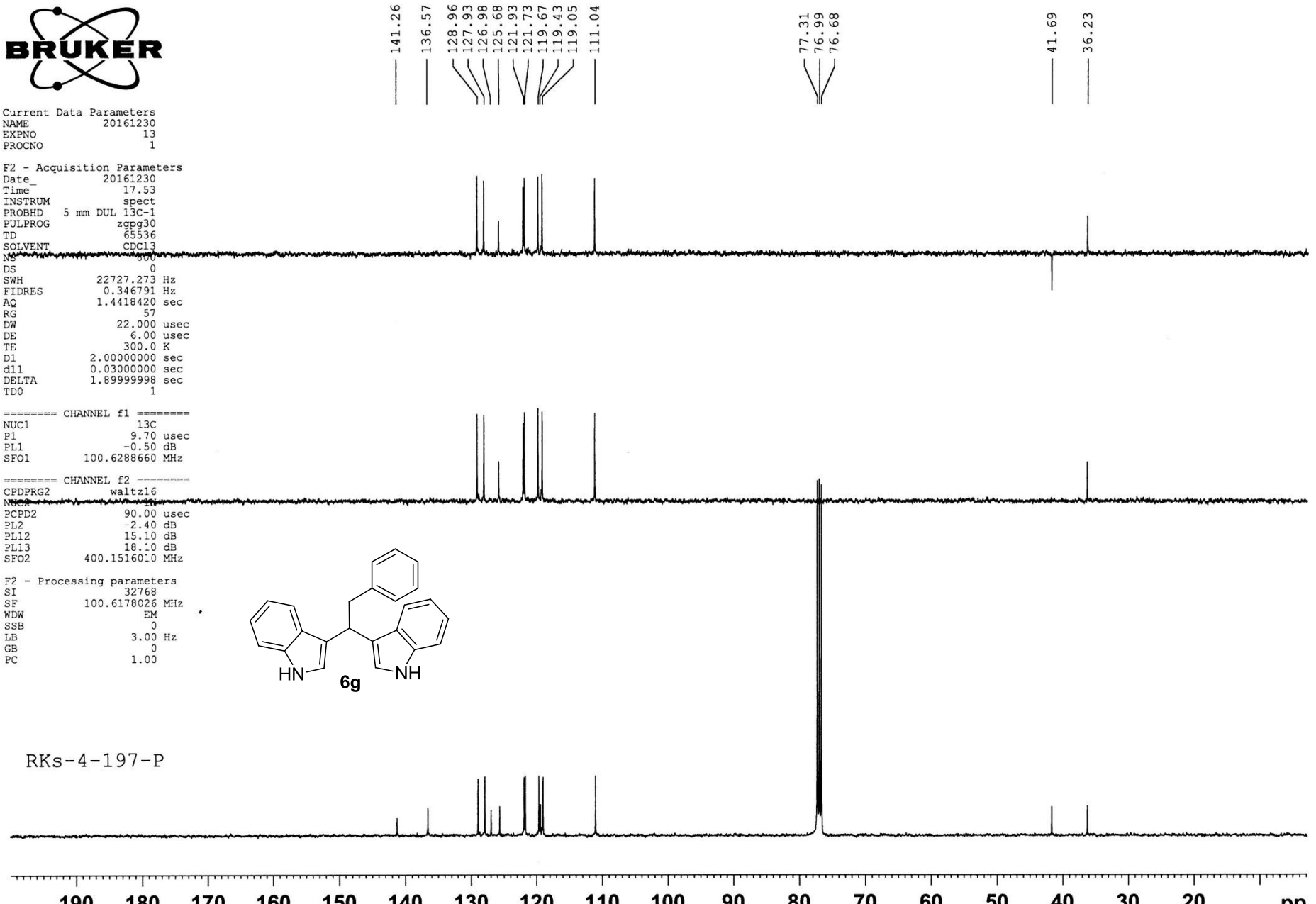
======== CHANNEL f1 ========
NUC1                    1H
P1                   10.00 usec
PL1                  -2.40 dB
SFO1          400.1528010 MHz

F2 - Processing parameters
SI                   16384
SF            400.1500172 MHz
WDW                     EM
SSB                      0
LB                    0.00 Hz
GB                       0
PC                    1.00
```



6g

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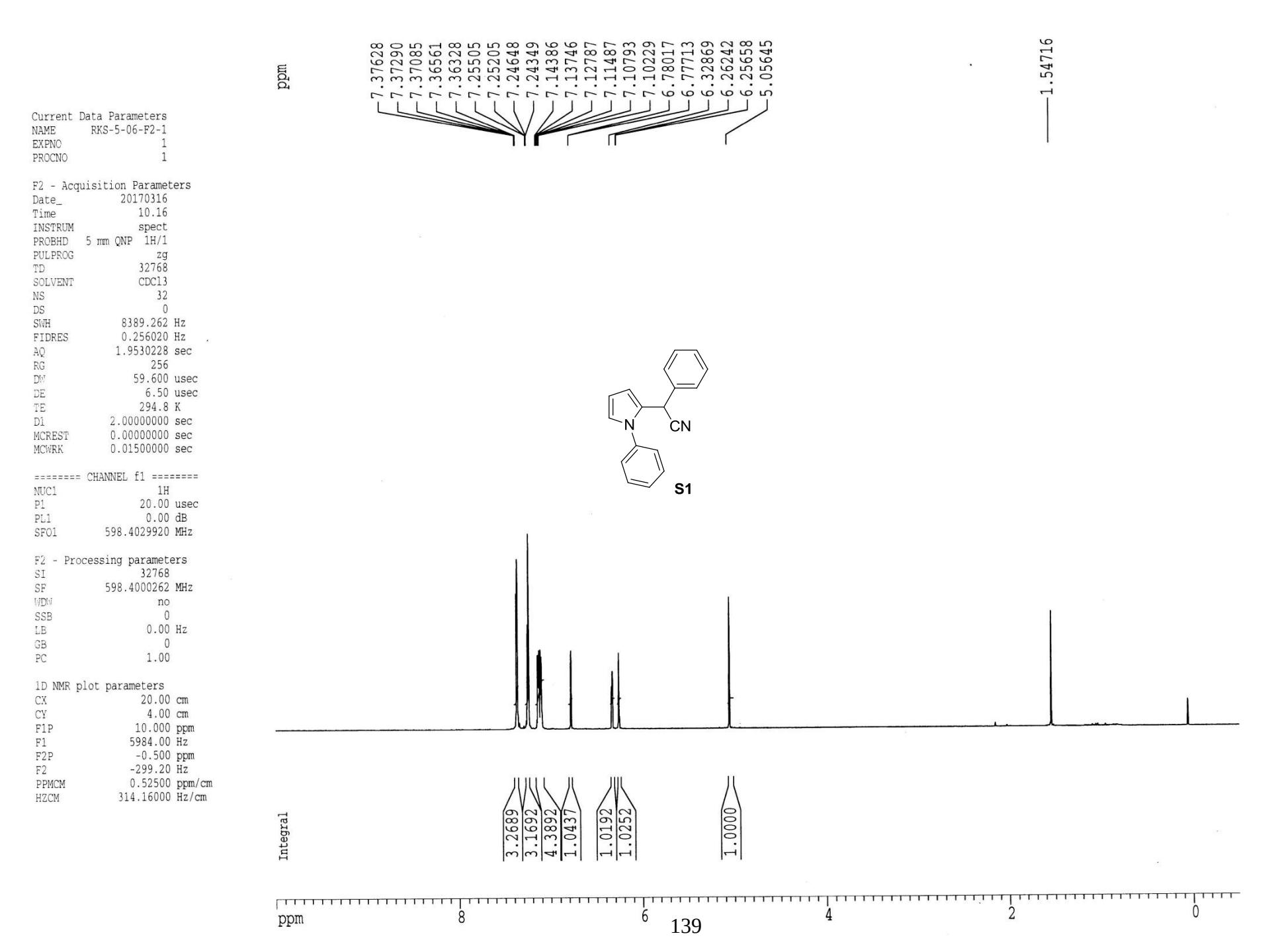
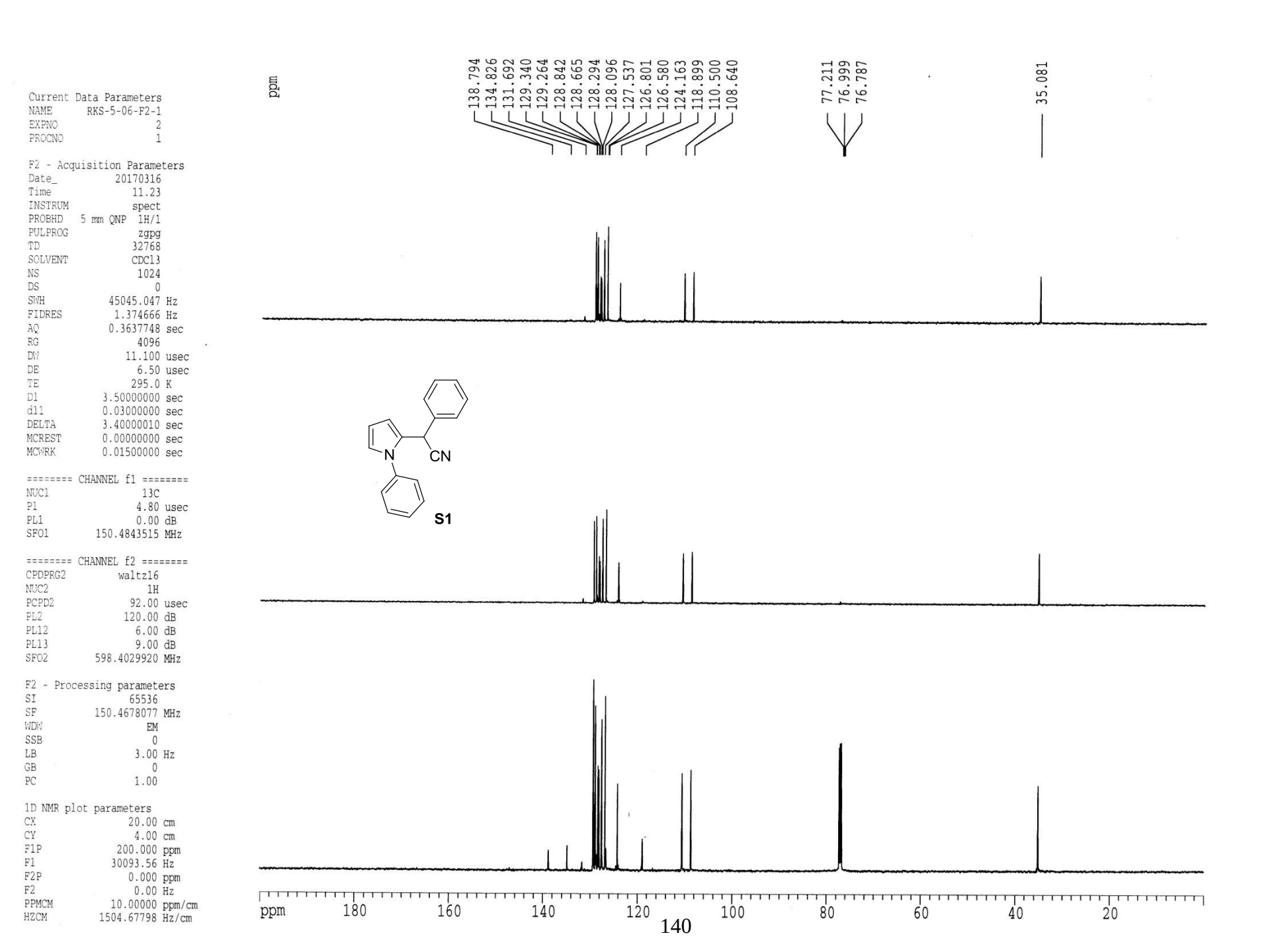
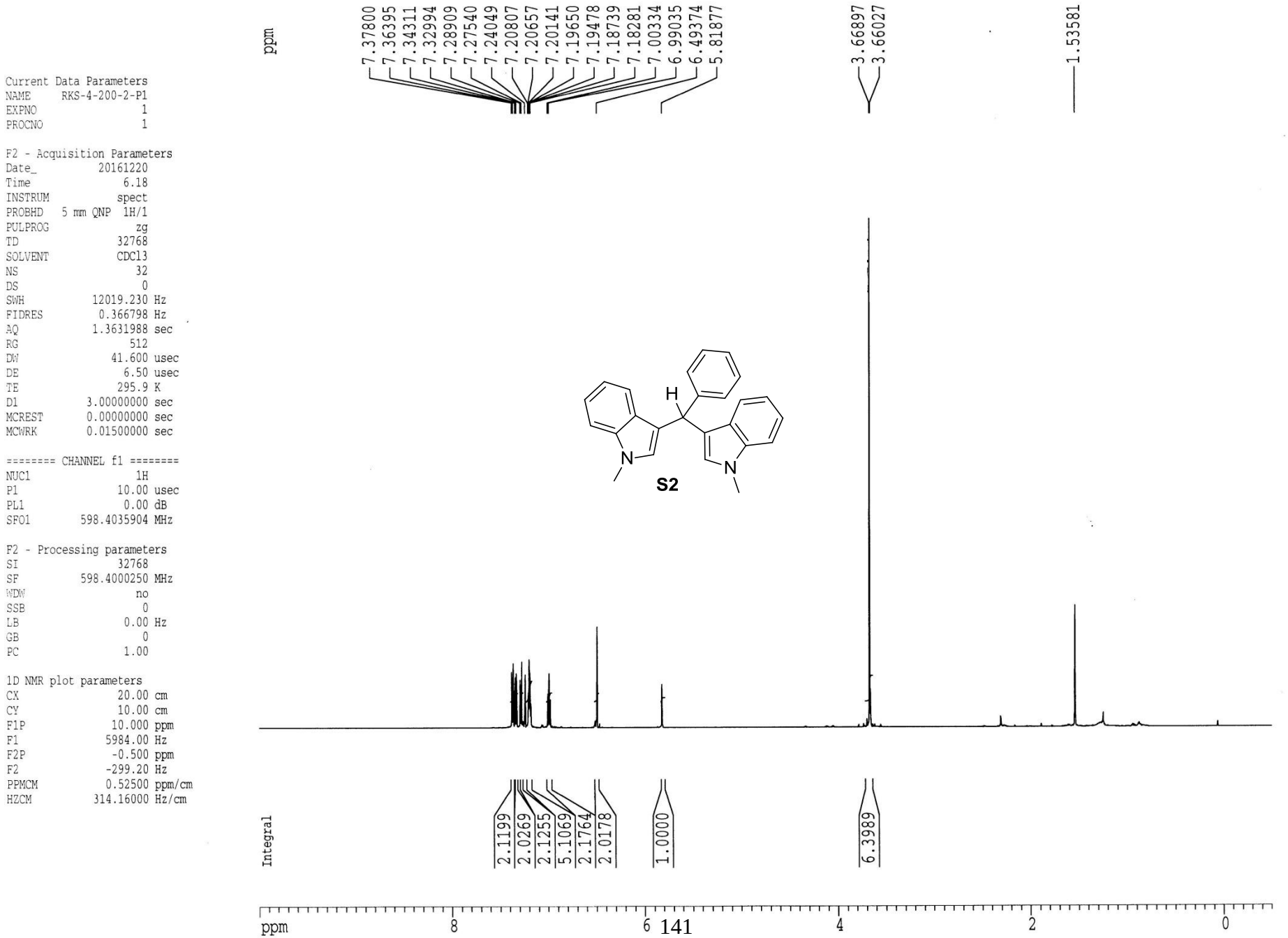
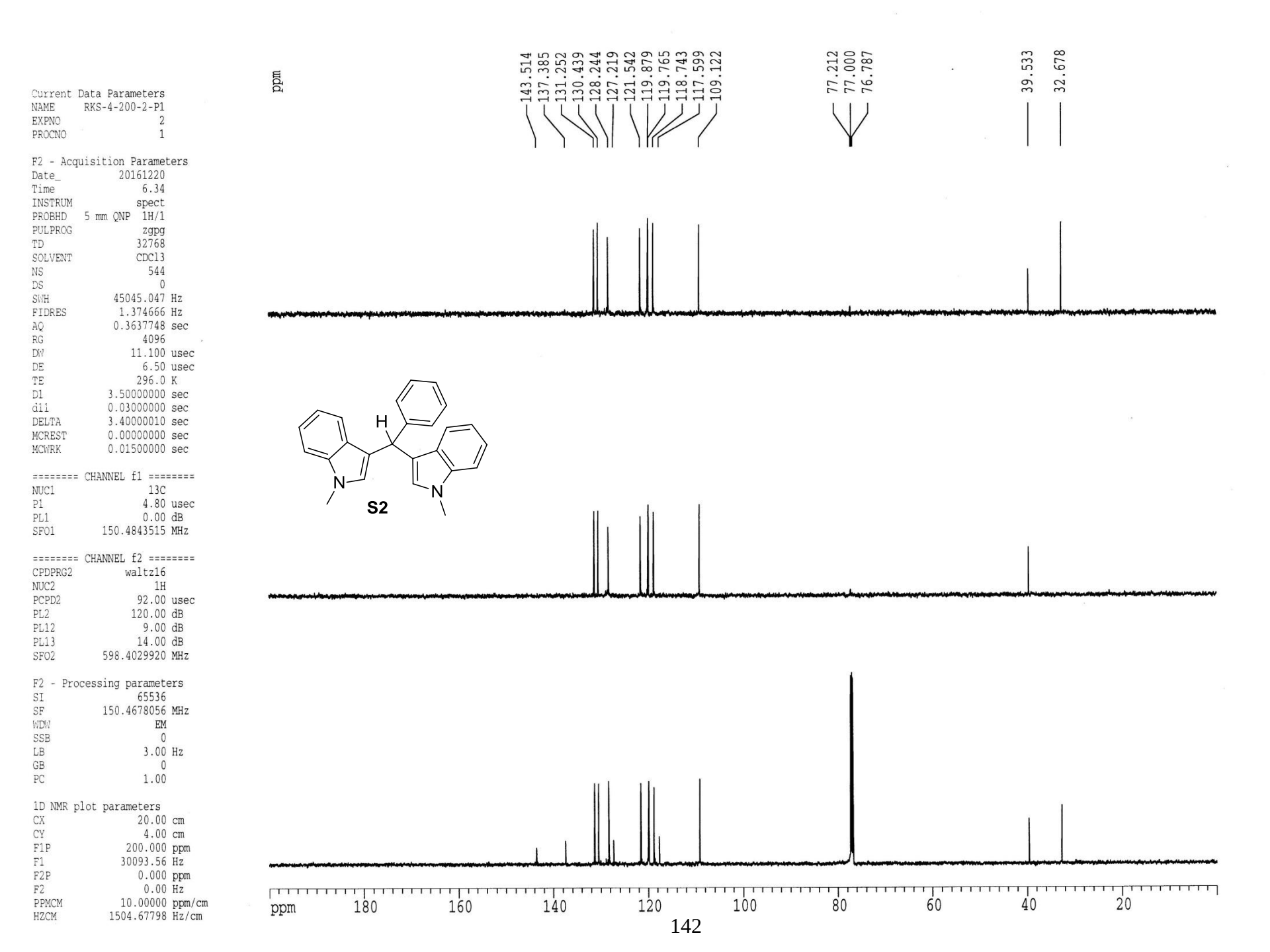
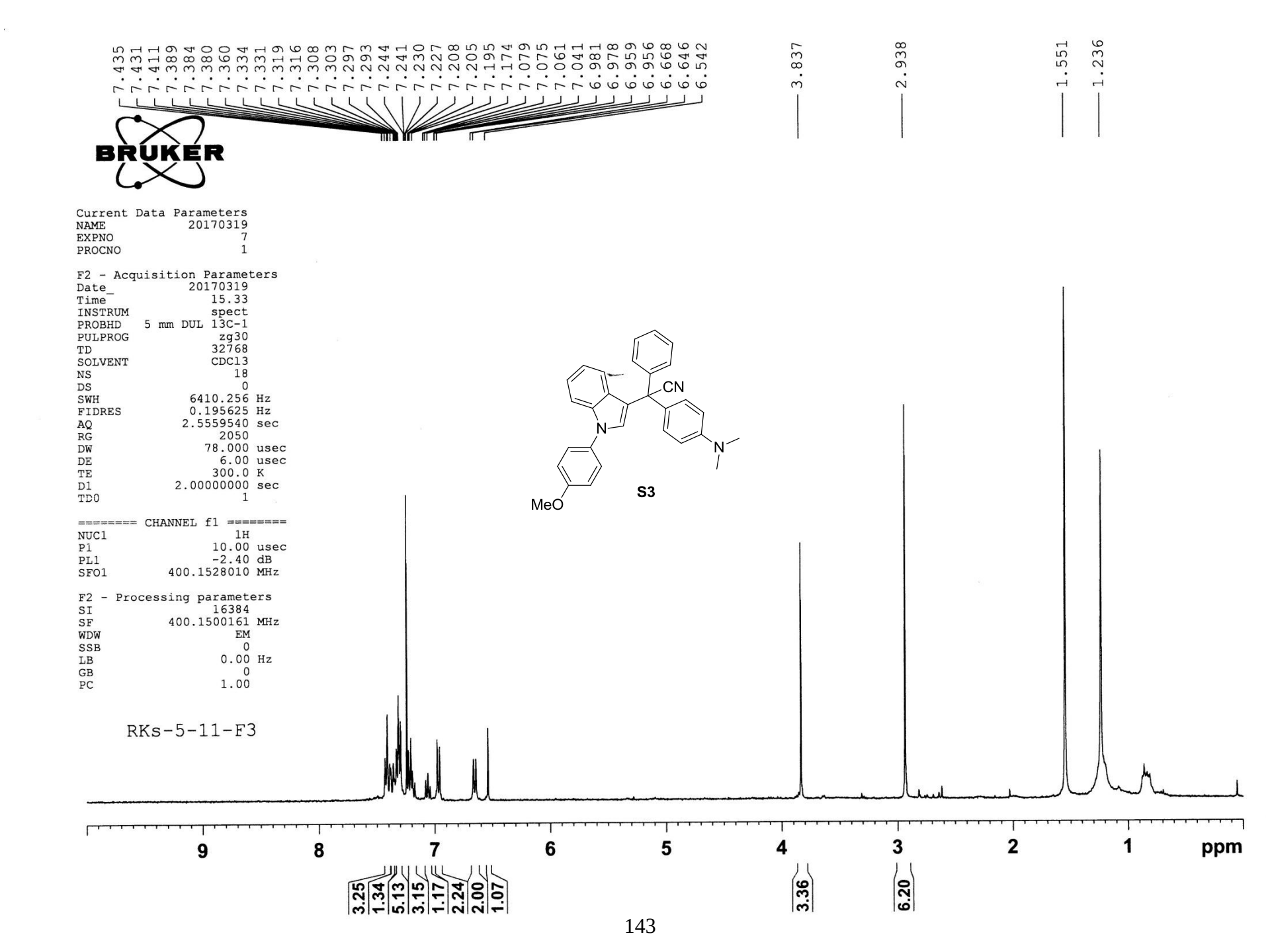
136.57
128.96
127.93
126.98
125.68
121.93
121.73
119.67
119.43
119.05
111.04
77.31
76.99
76.68
41.69
36.23
Current Data Parameters
NAME 20161230
EXPNO 13
PROCNO 1
F2 - Acquisition Parameters
Date_ 20161230
Time 17.53
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 800
DS 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
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
PL12 15.10 dB
PL13 18.10 dB
SFO2 400.1516010 MHz
F2 - Processing parameters
SI 32768
SF 100.6178026 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
HN
NH
6g
RKs-4-197-P
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
pp

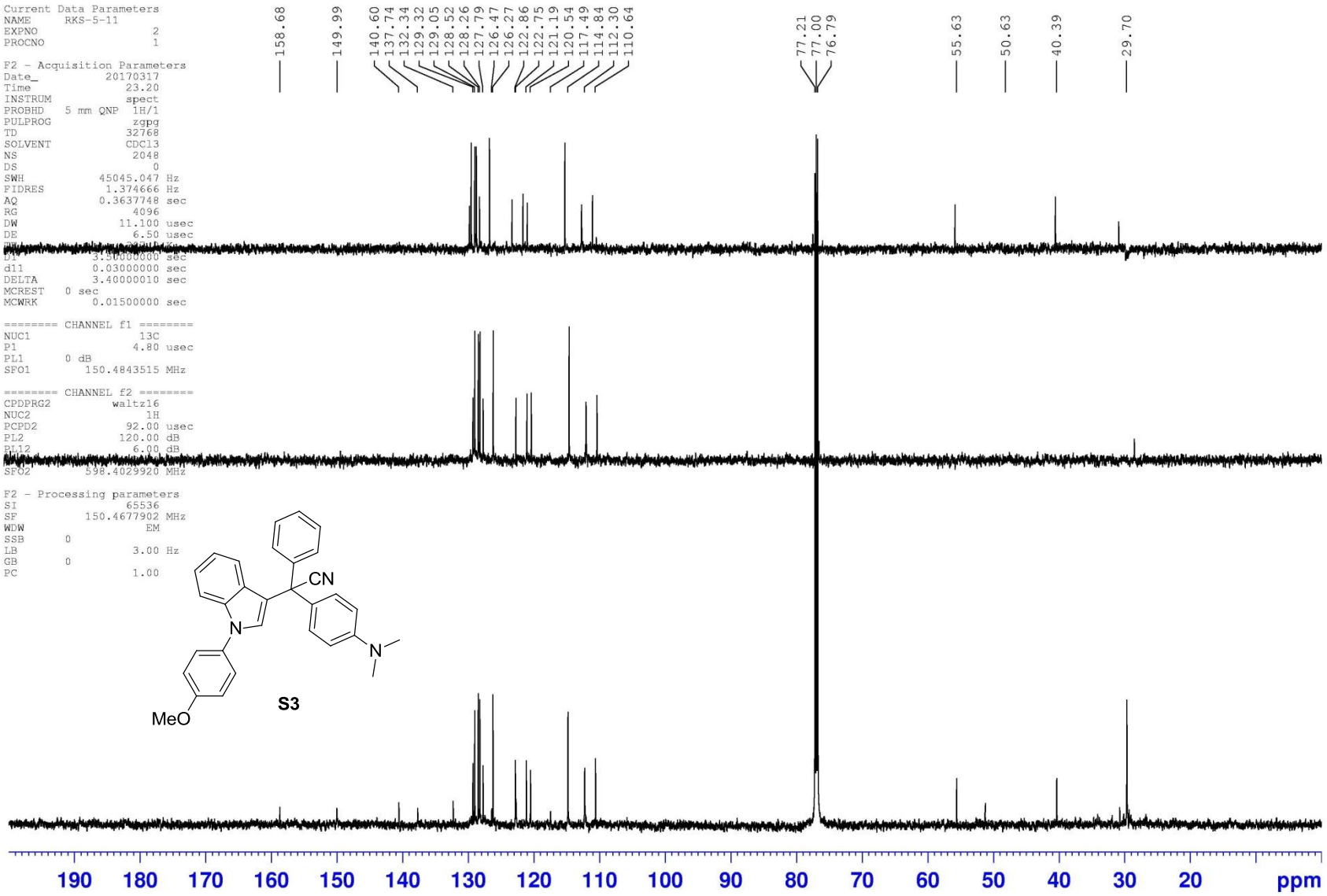

Current Data Parameters
NAME RKS-5-06-F2-1
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170316
Time 10.16
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 32
DS 0
SWH 8389.262 Hz
FIDRES 0.256020 Hz
AQ 1.9530228 sec
RG 256
DW 59.600 usec
DE 6.50 usec
TE 294.8 K
D1 2.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 20.00 usec
PL1 0.00 dB
SFO1 598.4029920 MHz
F2 - Processing parameters
SI 32768
SF 598.4000262 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 5984.00 Hz
F2P -0.500 ppm
F2 -299.20 Hz
PPMCM 0.52500 ppm/cm
HZCM 314.16000 Hz/cm
ppm
7.37628
7.37290
7.37085
7.36561
7.36328
7.25505
7.25205
7.24648
7.24349
7.14386
7.13746
7.12787
7.11487
7.10793
7.10229
6.78017
6.77713
6.32869
6.26242
6.25658
5.05645
1.54716
N
CN
S1
Integral
3.2689
3.1692
4.3892
1.0437
1.0192
1.0252
1.0000
ppm
8
6
4
2
0

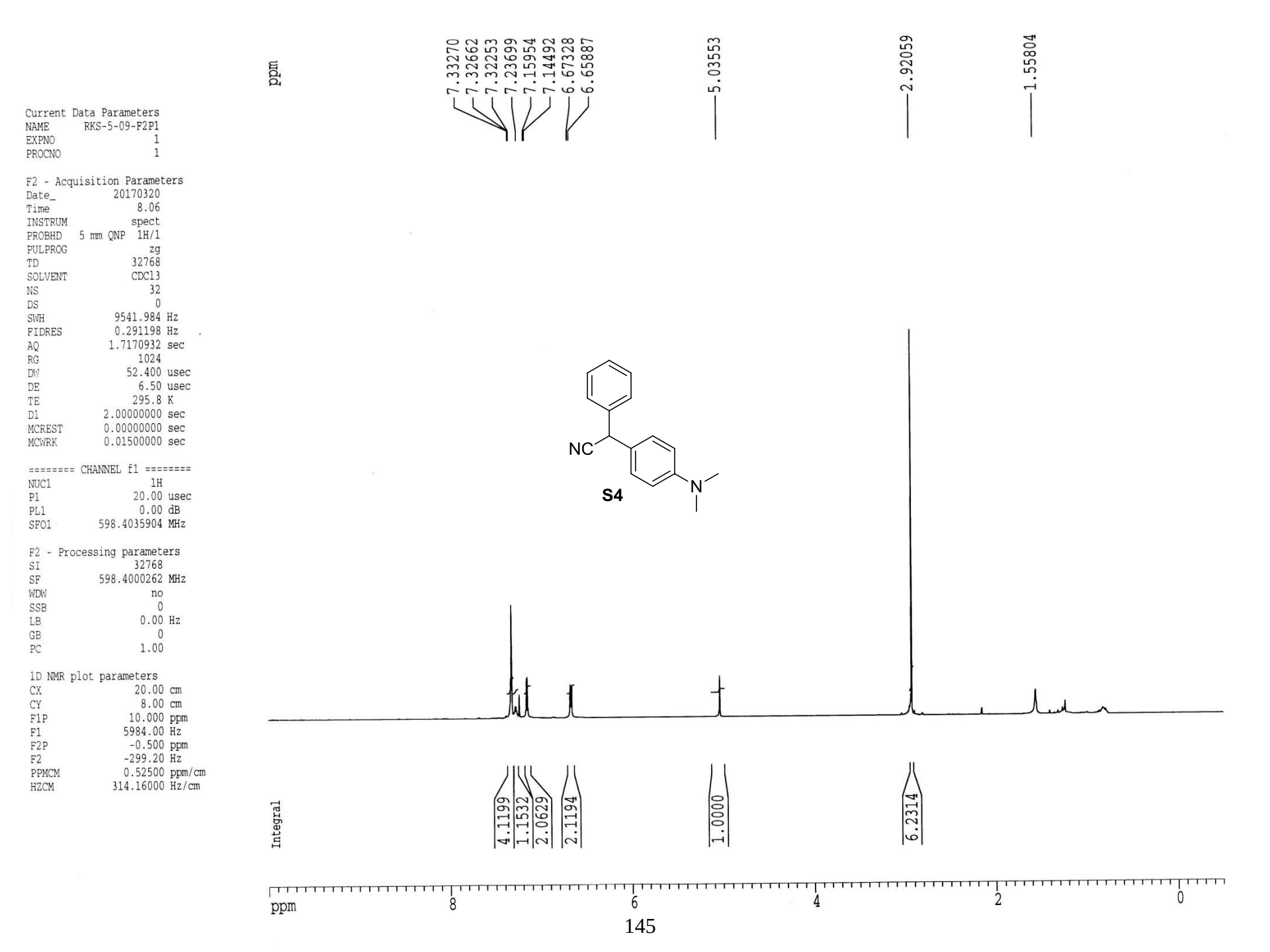

Current Data Parameters
NAME RKS-5-06-F2-1
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170316
Time 11.23
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 1024
DS 0
SWH 45045.047 Hz
FIDRES 1.374666 Hz
AQ 0.3637748 sec
RG 4096
DW 11.100 usec
DE 6.50 usec
TE 295.0 K
D1 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 150.4843515 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 92.00 usec
PL2 120.00 dB
PL12 6.00 dB
PL13 9.00 dB
SFO2 598.4029920 MHz
F2 - Processing parameters
SI 65536
SF 150.4678077 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 20.00 cm
CY 4.00 cm
F1P 200.000 ppm
F1 30093.56 Hz
F2P 0.000 ppm
F2 0.00 Hz
PPMCM 10.00000 ppm/cm
HZCM 1504.67798 Hz/cm
ppm
138.794
134.826
131.692
129.340
129.264
128.842
128.665
128.294
128.096
127.537
126.801
126.580
124.163
118.899
110.500
108.640
77.211
76.999
76.787
35.081
N
CN
S1
ppm
180
160
140
120
100
80
60
40
20

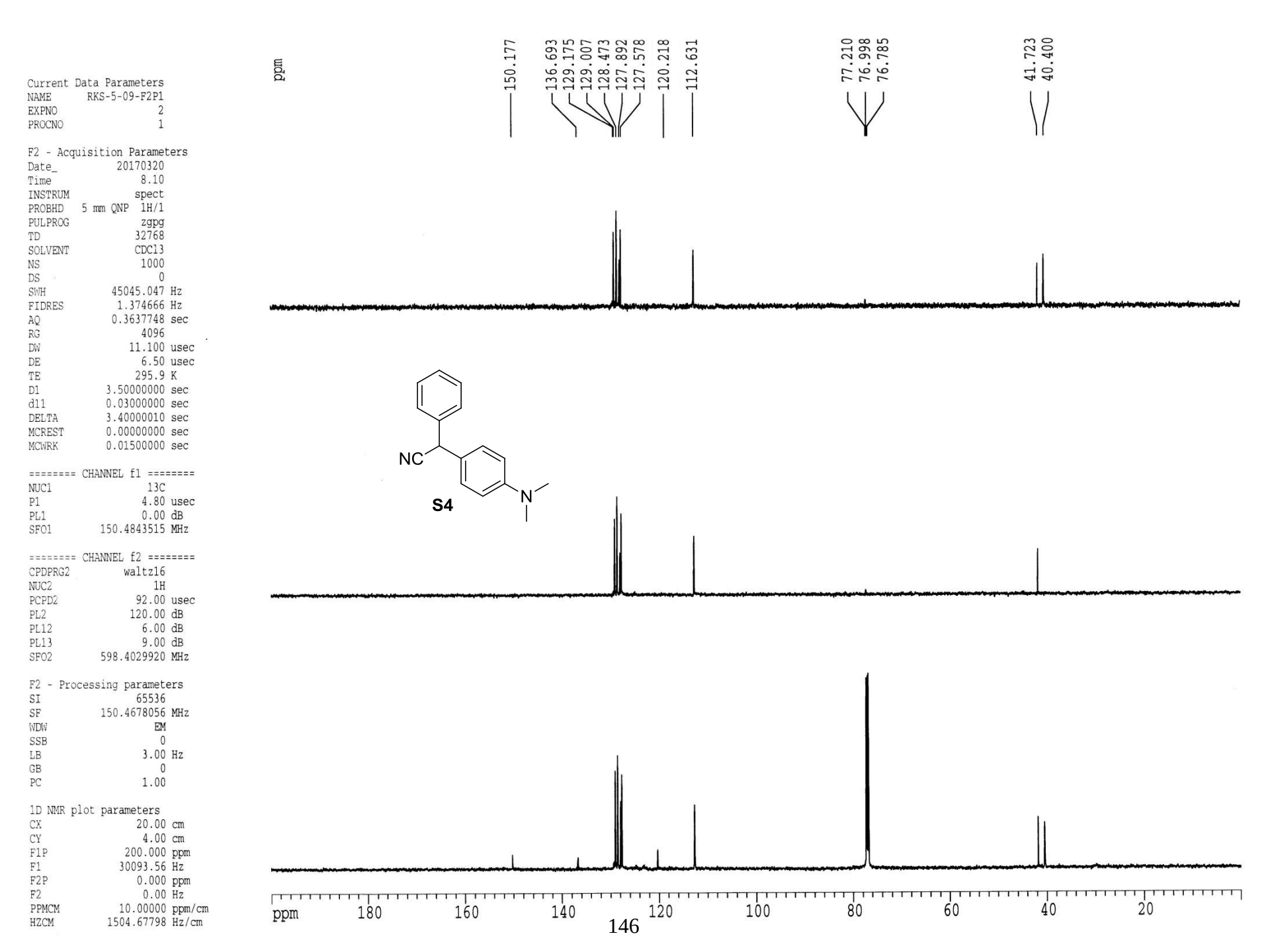

Current Data Parameters
NAME RKS-4-200-2-P1
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20161220
Time 6.18
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 32
DS 0
SWH 12019.230 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 512
DW 41.600 usec
DE 6.50 usec
TE 295.9 K
D1 3.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 0.00 dB
SFO1 598.4035904 MHz
F2 - Processing parameters
SI 32768
SF 598.4000250 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 20.00 cm
CY 10.00 cm
F1P 10.000 ppm
F1 5984.00 Hz
F2P -0.500 ppm
F2 -299.20 Hz
PPMCM 0.52500 ppm/cm
HZCM 314.16000 Hz/cm
ppm
7.37800
7.36395
7.34311
7.32994
7.28909
7.27540
7.24049
7.20807
7.20657
7.20141
7.19650
7.19478
7.18739
7.18281
7.00334
6.99035
6.49374
5.81877
3.66897
3.66027
1.53581
H
N
N
S2
Integral
2.1199
2.0269
2.1255
5.1069
2.1764
2.0178
1.0000
6.3989
ppm
8
6
4
2
0


Current Data Parameters
NAME RKS-4-200-2-P1
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20161220
Time 6.34
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 544
DS 0
SWH 45045.047 Hz
FIDRES 1.374666 Hz
AQ 0.3637748 sec
RG 4096
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 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 4.80 usec
PL1 0.00 dB
SFO1 150.4843515 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 92.00 usec
PL2 120.00 dB
PL12 9.00 dB
PL13 14.00 dB
SFO2 598.4029920 MHz
F2 - Processing parameters
SI 65536
SF 150.4678056 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 20.00 cm
CY 4.00 cm
F1P 200.000 ppm
F1 30093.56 Hz
F2P 0.000 ppm
F2 0.00 Hz
PPMCM 10.00000 ppm/cm
HZCM 1504.67798 Hz/cm
ppm
143.514
137.385
131.252
130.439
128.244
127.219
121.542
119.879
119.765
118.743
117.599
109.122
77.212
77.000
76.787
39.533
32.678
H
N
N
S2
ppm
180
160
140
120
100
80
60
40
20


7.435
7.431
7.411
7.389
7.384
7.380
7.360
7.334
7.331
7.319
7.316
7.308
7.303
7.297
7.293
7.244
7.241
7.230
7.227
7.208
7.205
7.195
7.174
7.079
7.075
7.061
7.041
6.981
6.978
6.959
6.956
6.668
6.646
6.542
3.837
2.938
1.551
1.236
BRUKER
Current Data Parameters
NAME 20170319
EXPNO 7
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170319
Time 15.33
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 18
DS 0
SWH 6410.256 Hz
FIDRES 0.195625 Hz
AQ 2.5559540 sec
RG 2050
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 400.1500161 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
CN
N
N
MeO
S3
RKs-5-11-F3
9
8
7
6
5
4
3
2
1
ppm
3.25
1.34
5.13
3.15
1.17
2.24
2.00
1.07
3.36
6.20


Current Data Parameters
NAME RKS-5-11
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170317
Time 23.20
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 2048
DS 0
SWH 45045.047 Hz
FIDRES 1.374666 Hz
AQ 0.3637748 sec
RG 4096
DW 11.100 usec
DE 6.50 usec
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 150.4843515 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 92.00 usec
PL2 120.00 dB
PL12 6.00 dB
SFO2 598.4029920 MHz
F2 - Processing parameters
SI 65536
SF 150.4677902 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
158.68
149.99
140.60
137.74
132.34
129.32
129.05
128.52
128.26
127.79
126.47
126.27
122.86
122.75
121.19
120.54
117.49
114.84
112.30
110.64
77.21
77.00
76.79
55.63
50.63
40.39
29.70
CN
N
N
MeO
S3
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm


Current Data Parameters
NAME RKS-5-09-F2P1
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170320
Time 8.06
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 32
DS 0
SWH 9541.984 Hz
FIDRES 0.291198 Hz
AQ 1.7170932 sec
RG 1024
DW 52.400 usec
DE 6.50 usec
TE 295.8 K
D1 2.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 20.00 usec
PL1 0.00 dB
SFO1 598.4035904 MHz
F2 - Processing parameters
SI 32768
SF 598.4000262 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 20.00 cm
CY 8.00 cm
F1P 10.000 ppm
F1 5984.00 Hz
F2P -0.500 ppm
F2 -299.20 Hz
PPMCM 0.52500 ppm/cm
HZCM 314.16000 Hz/cm
ppm
7.33270
7.32662
7.32253
7.23699
7.15954
7.14492
6.67328
6.65887
5.03553
2.92059
1.55804
NC
N
S4
Integral
4.1199
1.1532
2.0629
2.1194
1.0000
6.2314
ppm
8
6
4
2
0


Current Data Parameters
NAME RKS-5-09-F2P1
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170320
Time 8.10
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 1000
DS 0
SWH 45045.047 Hz
FIDRES 1.374666 Hz
AQ 0.3637748 sec
RG 4096
DW 11.100 usec
DE 6.50 usec
TE 295.9 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 150.4843515 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 92.00 usec
PL2 120.00 dB
PL12 6.00 dB
PL13 9.00 dB
SFO2 598.4029920 MHz
F2 - Processing parameters
SI 65536
SF 150.4678056 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 20.00 cm
CY 4.00 cm
F1P 200.000 ppm
F1 30093.56 Hz
F2P 0.000 ppm
F2 0.00 Hz
PPMCM 10.00000 ppm/cm
HZCM 1504.67798 Hz/cm
ppm
150.177
136.693
129.175
129.007
128.473
127.892
127.578
120.218
112.631
77.210
76.998
76.785
41.723
40.400
NC
N
S4
ppm
180
160
140
120
100
80
60
40
20