Electronic Supplementary Material (ESI) for ChemComm.

Supporting Information

Gold-catalyzed [3+2]-Annulations of α-Aryl Diazonitriles with Ynamides and Allenamides to Yield 1-Amino-1*H*-Indenes

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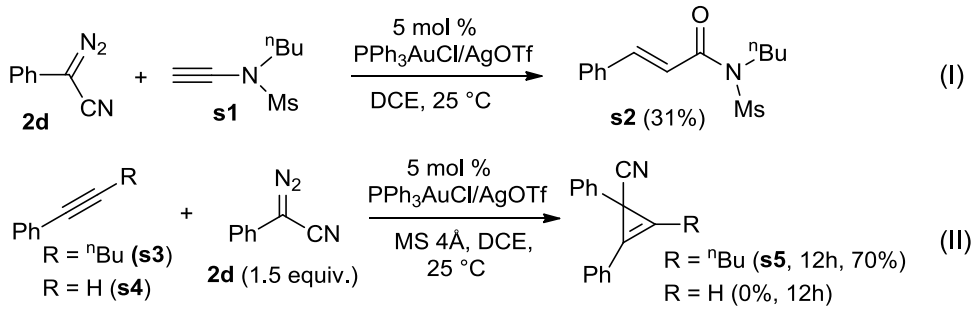
1. Reaction of diazonitrile 2d with terminal ynamide or alkyne:

The gold-catalyzed reaction of terminal ynamide **s1** with diazonitrile **2d** afforded unsaturated amide **s2** in 31% yield (eq I). To probe the electronic effect of a sulfonamide, we tested the reaction of an unactivated alkyne **s3** with diazonitrile **2d** to give a typical cycloproprenation product **s5** in 70% yields, whereas terminal alkyne **s4** gave products in a complicated mixture (eq II). Unlike other cyclopropene species, cyclopropene compound **8c** remained intact even in the presence of PPh_3AuX (X = OTf and Tf_2) and $Rh_2(OAc)_4$ in hot DCE (70 ℃, 12 h). An effective coordination of a nitrile to a metal complex likely impedes a cyclopropene cleavage through alkenylmetal carbene intermediates.[1]



2. Representative synthetic procedures:

(a) General procedure:

Unless otherwise noted, all reactions were carried out under a nitrogen atmosphere in oven-dried glassware using standard syringe, cannula and septa apparatus. The Catalytic reactions were performed under Argon atmosphere. Tetrahydrofuran and hexanes were dried with sodium, benzophenone and distilled before use. 1,2-Dichloroethane (DCE), dichloromethane (DCM) and toluene were dried over CaH_2 and distilled before use. Reagents were purchased from commercial sources and used without purification. Reactions were magnetically stirred and monitored by thin layer chromatography. ^1H and ^{13}C NMR spectra were recorded on a Bruker 400, Varian 500, Varian 600 and Varian 700 MHz NMR spectrometers using $CDCl_3$, CD_3COCD_3, CD_2Cl_2 and C_6D_6 as internal standards. Ynamides[3] **1a-1o**, **9** and **11a** and allenamides **5a-5d**[2] were prepared according to literature procedures; diazo compounds **2d-2j** according to literature procedures[4] and DFT theoretical calculation with references [5].

[1] See selected examples: a) C. Li, Y. Zeng, J. Wang, *Tetrahedron Lett.*, 2009, **50**, 2956-2959; b) Zhu, Z.-B.; Shi, M. *Chem. Eur. J.*, 2008, **14**, 10219-10222.

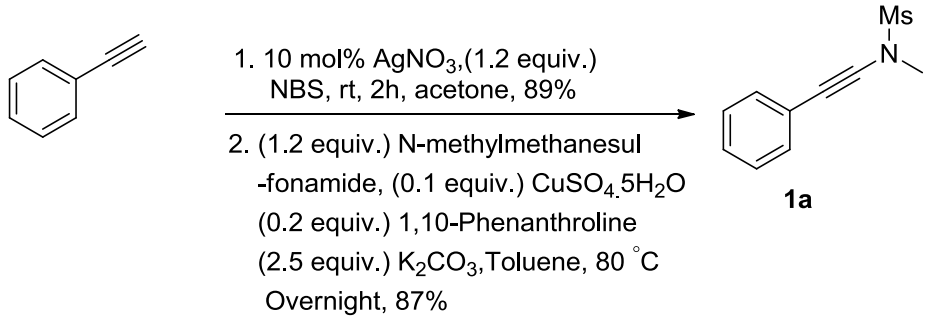
[2] a) Compounds **1a-1g**, **1i-1j**, **1n-1o**: A. Mukherjee, R. B. Dateer, R. Chaudhari, S. Bhunia, S. N. Karad, R.-S. Liu, *J. Am. Chem. Soc*. **2011**, *133*, 15372-15375; b) Compounds **1h, 1l**: R. B. Dateer, B. S. Shaibu, R.-S. Liu, *Angew. Chem. Int. Ed.* **2012**, *51*, 113-117; c) Compound **1m**: B. Yao, Z. Liang, T. Niu, Y. Zhang, *J. Org. Chem.* **2009**, *74*, 4630-4633; d) Compound **5**: Y. L. Chen, P. Sharma, R.-S. Liu, *Chem Commun*. **2016**, *52*, 3187-3190; e) Compound **7a**: M. Bakherad, A. Keivanloo, S. Samangooei, *Tetrahedron letters* **2012**, *53*, 5773-5776.

[3] a) Compound **5a** : L.-L. Wei, J. A. Mulder, H. Xiong, C. A. Zificsak, C. J. Douglas, R. P. Hsung; *Tetrahedron*, **2001**, *57*, 459-466; b) Compound **5b**: S. H. Faustino, F. Lopez, L. Castedoa, J. L. Mascarenas, *Chem. Sci.*, **2011**, *2*, 633; M. R. Tracey, T. Grebe, J. A. Mulder, R. P. Hsung, *Organic Syntheses*, **2005**, *81*, 147-151; c) Compounds **5c** and **5d**: B. M. Trost, D. T. Stiles, *Org. Lett*., **2005**, *7*, 2117-2120.

[4] a) for first step: 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: R. Breslow, C. Yuan, *J. Am. Chem. Soc*. **1958**, *80(22)*, 5991-5994.

(b) Preparation of substrates

(b1) Preparation of ynamides (1a)



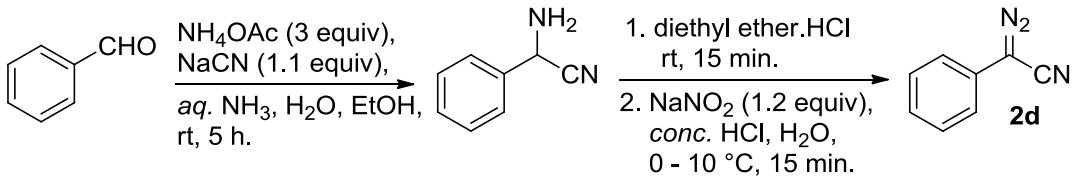
To a solution of phenylacetylene (400.0 mg, 3.92 mmol) in acetone (50 mL) was added NBS (837.2 mg, 4.70 mmol) and $AgNO_3$ (66.2 mg, 0.39 mmol); the resulting mixture was stirred under nitrogen at room temperature for 2 hours. The solution was concentrated before it was

extracted with pentane (40 mL x 2), dried over $MgSO_4$ and evaporated to dryness to afford a pure colorless oil of (bromoethynyl)benzene (630.9 mg, 89%).

To a dried flask was added *N*-methymethanesulfonamide (363.9 mg, 3.34 mmol), $CuSO_4 \cdot 5H_2O$ (68.02 mg, 0.28 mmol), 1,10-phenanthroline (100.1 mg, 0.56 mmol) and K_2CO_3 (960.1 mg, 8.35 mmol), and this mixture was subsequently treated with anhydrous toluene (3 mL) and (bromoethynyl)benzene (500 mg, 2.78 mmol). The flask was charged with nitrogen, and the solution was heated at 80 ℃ for eight hours. After completion, the crude reaction mixture was cooled to room temperature, filtered through CeliteTM, and concentrated in rota evaporator. Purification of the crude residue using silica gel flash column chromatography gave the pure *N*-methyl-*N*-(phenylethynyl)methanesulfonamide **1a** as a white solid 505.8 mg (2.41 mmol, 87%).

All the ynamide substrates were prepared by using the procedures reported in [s2].

(b2) Preparation of 2-diazo-2-phenylacetonitrile (2d)



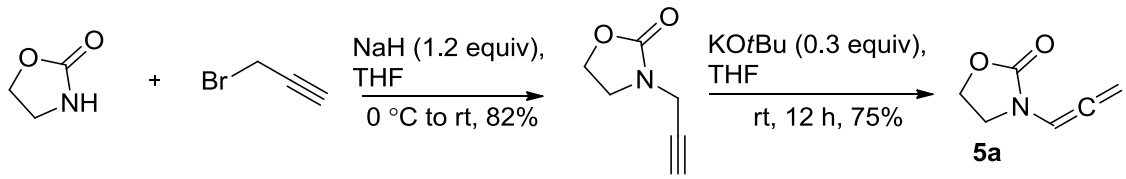
To an aqueous solution (40 mL) of ammonium acetate (21.8 g, 282.9 mmol) and sodium cyanide (5.2 g, 103.7 mmol), aqueous ammonia (35% w/w; 29 mL) and ethanol (40 mL) was added benzaldehyde (10 g, 94.3 mmol); the resulting solution was stirred at 25 ℃ for 5 h. The solution was extracted with diethyl ether, dried over $MgSO_4$, and filtered. The solution was concentrated at 20-30 ℃ under reduced pressure; the crude material was used immediately for the next step. (Aq. Layer was cooled in ice and treated by sodium hypochlorite solution (NaClO).

To the crude 2-amino-2-phenylacetonitrile was added excess of acidic ether (Et_2O.HCl, 80 mL); 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 ℃, 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 **2d** as red viscous oil (2 g, 13.98 mmol, 14.8 % overall yield).

***Note*:** All the diazo compound is highly unstable to light and environment so it was immediately cover with alluminium foil and stored in deep freezer.

(b3) Preparation of 3-(propa-1,2-dien-1-yl)oxazolidin-2-one (5a)

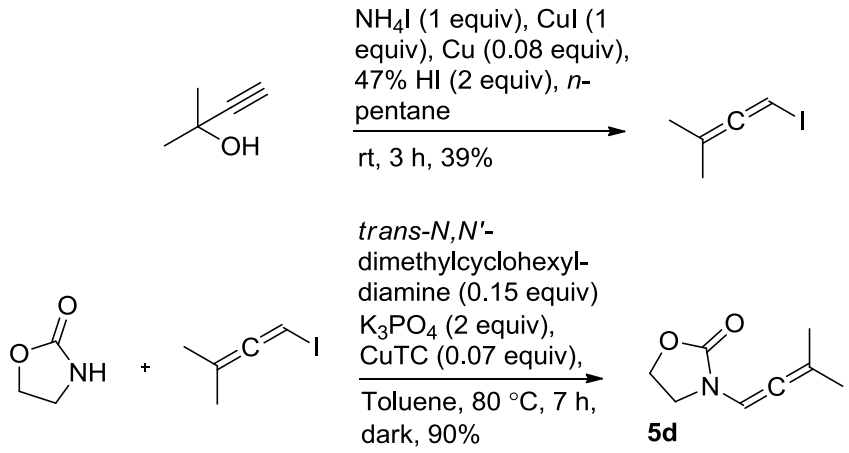


To a solution of oxazolidin-2-one (5 g, 57.4 mmol) and THF (100 mL) was added NaH (60 wt% in mineral oil, 2.76 g, 68.9 mmol); stirred this solution at rt for 0.5 h before an addition of propargyl bromide (80% solution in toluene, 17.1 mL). The resulting solution was stirred at room temperature for 12 h. The solution was filtered through a celiteTM and washed with diethyl ether (50 mL). The solution was concentrated under reduced pressure. The crude product was purified on a neutral alumina column with 15% ethylacetate/*n*-hexane to afford 3-(prop-2-yn-1-yl)oxazolidin-2-one as pale yellow viscous oil (5.9 g, 47.1 mmol, 82 % yield)

To the solution of 3-(prop-2-yn-1-yl)oxazolidin-2-one (5 g, 40 mmol) and THF (100 mL) was added KO*t*Bu (1.3 g, 12 mmol); the reaction mixture was stirred for 12 h. The solution was filtered through a celiteTM and washed with diethyl ether (25 mL X 2). The solution was concentrated under reduced pressure. The crude product was purified on a neutral alumina column with 12% ethylacetate/*n*-hexane to afford 3-(propa-1,2-dien-1-yl)oxazolidin-2-one **5a** as pale yellow viscous oil (3.75 g, 30 mmol, 75 % yield)

The compounds **5b** and **5c** were synthesized using the same synthetic procedures.

(b4) Preparation of 3-(3-methylbuta-1,2-dien-1-yl)oxazolidin-2-one (5d)

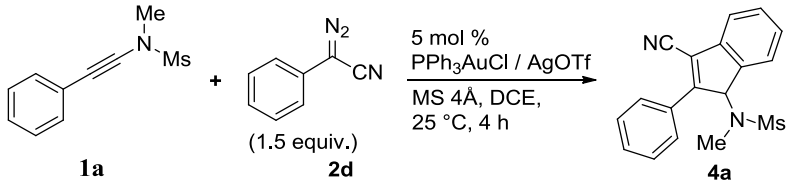


To the solution of ammonium iodide (9.93 g, 68.5 mmol), copper(I) iodide (13.04 g, 68.5 mmol), copper metal (340 mg, 5.34 mmol), and 47% hydroiodic acid (24.9 mL, 37.3 g, 137 mmol) was added 2-methy-3-butyn-2-ol (6.64 mL, 5.76 g, 68.5 mmol) in 15 mL of *n*-pentane slowly over 0.5 h. After stirring for 3 h, the biphasic mixture was filtered through celiteTM. The layers were separated and the aqueous layer was extracted with *n*-pentane (2 x 25 mL). The organic extracts were combined, washed with water (2 x 15 mL), dried over magnesium sulfate, filtered through a plug of silica gel, and concentrated under reduced pressure to give the allenyl iodide (5.27 g, 27.1 mmol, 39 % yield).

To a dry sealed tube, 2-oxazolidinone (1.3 g, 14.9 mmol), CuTC (200 mg, 1.04 mmol), and K_3PO_4 (6.3 g, 29.8 mmol) were added. After flushing with nitrogen 3 times, 50 mL of toluene was added, followed by *trans-N,N'*-dimethylcyclohexyldiamine (320 mg, 2.23 mmol), and 1-iodo-3-methylbuta-1,2-diene (5.0 g, 25.4 mmol). The flask was covered with aluminum foil and heated to 85 ℃ for 7 h. The reaction was cooled to room temperature and added to 100 mL of water, then extracted with ethyl acetate (3 x 50 mL), washed with brine, dried over magnesium sulfate, and concentrated under reduced pressure. The crude product was purified by column chromatography on neutral alumina to afford 3-(3-methylbuta-1,2-dien-1-yl)oxazolidin-2-one **5d** (4.0 g, 26.1 mmol, 75.8 %) as a viscous solid.

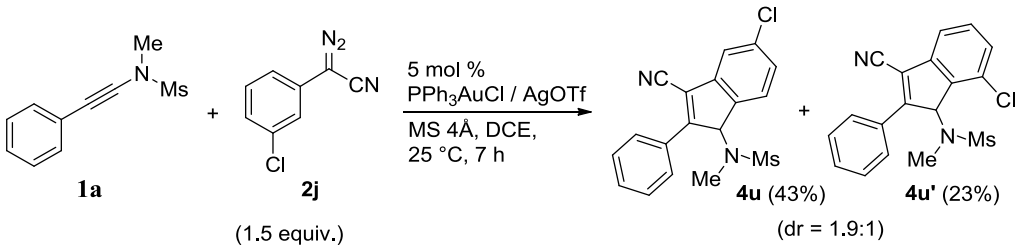
(c) Standard procedures for catalytic operations

(c-1) Standard Catalytic Procedure for synthesis of *N*-(3-cyano-2-phenyl-1*H*-inden-1-yl)-*N*-methylmethanesulfonamide (4a).



A reaction tube containing powdered MS 4Å was charged with (triphenylphosphine) gold(I) chloride (11.8 mg, 0.0239 mmol) and Silver(I) trifluoromethanesulfonate (AgOTf) (6.14 mg, 0.0239 mmol). To the above mixture dry DCE (1.0 mL) was added and stirred at room temperature under an argon atmosphere for 5 min. To this solution was added a dry DCE solution (2 mL) of *N*-methyl-*N*-(phenylethynyl)methanesulfonamide **1a** (100 mg, 0.48 mmol) and 2-diazo-2-phenylacetonitrile **2d** (89 mg, 0.63 mmol) with syringe in the duration of 5 minute. The mixture was kept stirring at 25 ℃ for 4 h before it was filtered over a short silica bed. The solvent was evaporated, and the crude product was chromatographed through a silica gel column to afford compound **4a** as white solid (115 mg, 0.35 mmol, 74% yield).

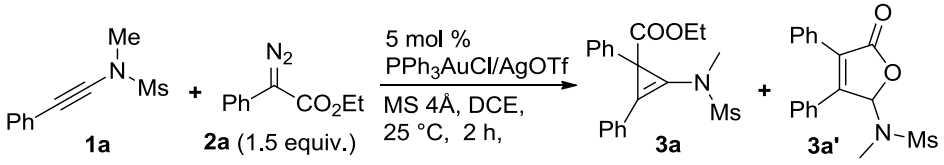
(c-2) Standard Catalytic Procedure for synthesis of *N*-(5-chloro-3-cyano-2-phenyl-1*H*-inden-1-yl)-*N*-methylmethanesulfonamide.



A reaction tube containing powdered MS 4Å was charged with (triphenylphosphine) gold(I) chloride (11.8 mg, 0.0239 mmol) and Silver(I) trifluoromethanesulfonate (AgOTf) (6.14 mg, 0.0239 mmol). To the above mixture dry DCE (1.0 mL) was added and stirred at room temperature under an argon atmosphere for 5 min. To this solution was added a dry DCE solution (2 mL) of *N*-methyl-*N*-(phenylethynyl)methanesulfonamide **1a** (100 mg, 0.48 mmol) and 2-(3-chlorophenyl)-2-diazoacetonitrile **2j** (111 mg, 0.62 mmol) with syringe in the duration

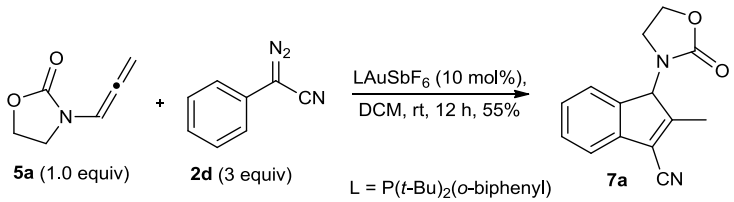
of 5 minute. The mixture was kept stirring at 25 °C for 7 h before it was filtered over a short silica bed. The solvent was evaporated, and the crude product was chromatographed through a silica gel column to afford compound **4u** (74 mg, 0.21 mmol, 43% yield) as yellow viscous liquid and **4u'** (39 mg, 0.11 mmol, 23% yield) as yellow viscous liquid.

(c-3) Standard Catalytic Procedure for synthesis of ethyl 2-(*N*-methylmethylsulfonamido) -1,3-diphenylcycloprop-2-enecarboxylate



A reaction tube containing powdered MS 4Å was charged with (triphenylphosphine) gold(I) chloride (11.8 mg, 0.0239 mmol) and Silver(I) trifluoromethanesulfonate (AgOTf) (6.14 mg, 0.0239 mmol). To the above mixture dry DCE (1.0 mL) was added and stirred at room temperature under an argon atmosphere for 5 min. To this solution was added a dry DCE solution (2 mL) of *N*-methyl-*N*-(phenylethynyl)methanesulfonamide **1a** (100 mg, 0.48 mmol) and ethyl 2-diazo-2-phenylacetate **2a** (136 mg, 0.72 mmol) with syringe in the duration of 5 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 (**115 mg, 0.31 mmol, 65% yield) as a white solid and **3a' (**36 mg, 0.11 mmol, 22% yield) as white solid.

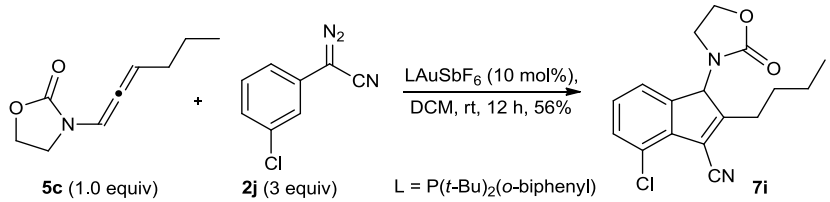
(c-4) Standard procedures for synthesis of compound 2-methyl-1-(2-oxooxazolidin-3-yl)-1*H*-indene-3-carbonitrile 7a



To a DCM solution (1 mL) of AuCl(*t*-Bu)$_2$P(*o*-biphenyl) (42 mg, 10 mole %), silver hexafluoroantimonate (27 mg, 10 mole %) was added a DCM solution (3 mL) of 3-(propa-1,2-dien-1-yl)oxazolidin-2-one **5a** (100 mg, 0.80 mmol) and 2-diazo-2-phenylacetonitrile **2d** (343

mg, 23.98 mmol) at 28 ℃ dropwise over 5 min.; the resulting solution was stirred at rt for 12 h before it was filtered over a short celite bed, concentrated and eluted through a neutral alumina column (15% ethylacetate/hexane, R_f = 0.3 in 30 % ethylacetate/hexane system) to afford compound **7a** (105 mg, 0.44 mmol, 55 %) as a white solid.

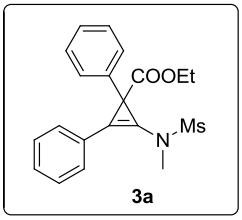
(c-5) Standard procedures for synthesis of compound 2-butyl-4-chloro-1-(2-oxooxazolidin-3-yl)-1*H*-indene-3-carbonitrile 7i



To a DCM solution (1 mL) of AuCl(t-Bu)$_2$P(o-biphenyl) (32 mg, 10 mole %), silver hexafluoroantimonate (20 mg, 10 mole %) was added a DCM solution (3 mL) of 3-(propa-1,2-dien-1-yl)oxazolidin-2-one **5c** (100 mg, 0.59 mmol) and 2-(3-chlorophenyl)-2-diazoacetonitrile **2j** (318 mg, 1.79 mmol) at 28 ℃ dropwise over 5 min.; the resulting solution was stirred at rt for 12 h before it was filtered over a short celite bed, concentrated and eluted through a neutral alumina column (15% ethylacetate/hexane, R_f = 0.3 in 30 % ethylacetate/hexane system) to afford compound **7i** (106 mg, 0.33 mmol, 56 %) as a pale yellow oil.

3. Spectral data of key compounds.

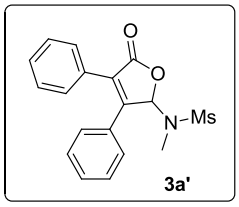
Spectral data for ethyl 2-(*N*-methylmethylsulfonamido)-1,3-diphenylcycloprop-2-ene carboxylate (3a).



White solid; mp: 221-222 $^{\circ}$C; IR (neat, cm^{-1}): 2366, 2323, 1750, 1680, 1520, 1430, 1178, 958, 763; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.28 (s, 5 H), 7.24 ~ 7.14 (m, 5 H), 4.23 (q, J = 7.0 Hz, 2 H), 3.20 (s, 3 H), 2.82 (s, 3 H), 1.36 (t, J = 7.2 Hz, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 153.0,

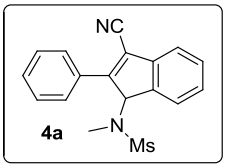
133.6, 131.1, 131.0, 129.3, 128.9, 128.3, 128.0, 127.6, 126.0, 123.2, 102.1, 68.4, 38.7, 38.6, 15.1; ESI-MS: calcd. for $C_{20}H_{21}NO_4S$: 371.1191; found: 372.1274 [M+H].

Spectral data for *N*-methyl-*N*-(5-oxo-3,4-diphenyl-2,5-dihydrofuran-2-yl)methanesulfonamide (3a').



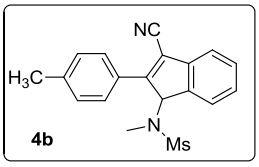
White solid; mp: 215-2166 °C; IR (neat, cm^{-1}): 2364, 1716, 1660, 1594, 1418, 1222, 1065, 786, 641; ^1H NMR (600 MHz, $CDCl_3$): δ 7.42 ~ 7.33 (m, 10 H), 7.05 (s, 1 H), 3.07 (s, 3 H), 2.62 (s, 3 H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 169.9, 153.0, 131.1, 129.5, 129.3, 129.0, 128.8, 128.5, 87.2, 38.5, 27.7; ESI-MS: calcd. for $C_{18}H_{17}NO_4S$: 343.0878; Found: 344.0960 [M+H].

Spectral data for *N*-(3-cyano-2-phenyl-1*H*-inden-1-yl)-*N*-methylmethanesulfonamide (4a).



White solid; mp: 172-173 °C; IR (neat, cm^{-1}): 2366, 2119, 1680, 1447, 758, 693; ^1H NMR (400 MHz, $CDCl_3$): δ 7.79 (d, *J* = 10.2 Hz, 2 H), 7.57 ~ 7.44 (m, 6 H), 7.37 (d, *J* = 7.4 Hz, 1 H), 6.31 (s, 1 H), 2.87 (s, 3 H), 2.21 (s, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 157.8, 139.0, 138.9, 131.1, 130.7, 129.7, 129.1, 128.3, 128.1, 124.5, 120.8, 114.5, 110.8, 64.6, 40.0, 29.1; ESI-MS: calcd. for $C_{18}H_{16}N_2O_2S$: 324.0932; Found: 347.0827 [M+Na].

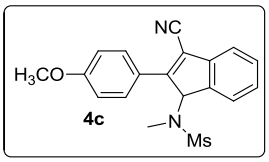
Spectral data for *N*-(3-cyano-2-(*p*-tolyl)-1*H*-inden-1-yl)-*N*-methylmethanesulfonamide (4b).



White viscous liquid; IR (neat, cm^{-1}): 2960, 2367, 2220, 1670, 1623, 1435, 1018, 870, 704; ^1H NMR (600 MHz, $CDCl_3$): δ 7.71 (d, *J* = 8.2 Hz, 2 H), 7.55 (d, *J* = 7.5 Hz, 1 H), 7.52 (d, *J* = 7.5 Hz, 1 H), 7.45 (t, *J* = 7.4 Hz, 1 H), 7.37 (t, *J* = 7.5 Hz, 1 H), 7.32 (d, *J* = 8.5 Hz, 2 H), 6.30 (s, 1 H), 2.91 (s, 3 H), 2.41 (s, 3 H), 2.21 (s, 3 H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 157.9, 141.4, 139.2,

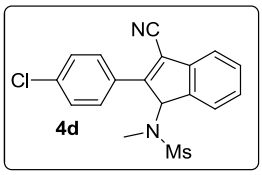
138.9, 129.9, 129.7, 128.3, 127.9, 124.5, 120.7, 114.8, 110.9, 64.6, 40.0, 29.1, 21.5; ESI-MS: calcd. for $C_{19}H_{18}N_2O_2S$: 338.1089; Found: 338.1089.

Spectral data for *N*-(3-cyano-2-(4-methoxyphenyl)-1*H*-inden-1-yl)-*N*-methylmethane sulfonamide (4c).



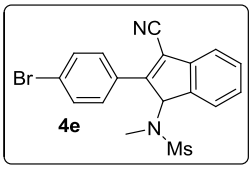
Light yellow viscous liquid; IR (neat, cm^{-1}): 2366, 2320, 2221, 1748, 1652, 1318, 1260, 736; ^1H NMR (600 MHz, $CDCl_3$): δ 7.82 (d, *J* = 8.8 Hz, 2 H), 7.52 (dd, *J* = 15, 7.5 Hz, 2 H), 7.44 (t, *J* = 7.3 Hz, 1 H), 7.34 (t, *J* = 7.5 Hz, 1 H), 7.02 (d, *J* = 8.5 Hz, 2 H), 6.27 (s, 1 H), 3.86 (s, 3 H), 2.95 (s, 3 H), 2.20 (s, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 161.6, 157.3, 139.3, 138.6, 130.0, 129.6, 127.7, 124.4, 123.5, 120.5, 115.1, 114.6, 109.5, 64.4, 55.4, 40.0 29.1; ESI-MS: calcd. for $C_{19}H_{18}N_2O_3S$: 354.1038; Found: 354.1110 [M+H].

Spectral data for *N*-(2-(4-chlorophenyl)-3-cyano-1*H*-inden-1-yl)-*N*-methylmethanesulfonamide (4d).



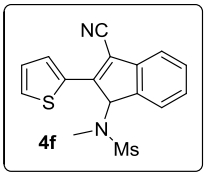
Yellow viscous liquid; IR (neat, cm^{-1}): 2366, 2222, 1670, 1652, 1387, 1138, 736; ^1H NMR (400 MHz, $CDCl_3$): δ 7.77 (d, *J* = 8.3 Hz, 2 H), 7.55 ~ 7.45 (m, 5 H), 7.39 (t, *J* = 7.4 Hz, 1 H), 6.28 (s, 1 H), 2.96 (s, 3 H), 2.21 (s, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 156.3, 138.8, 138.7, 136.9, 129.8, 129.6, 129.4, 128.3, 124.4, 120.9, 114.4, 112.1, 64.5, 40.1 29.2; ESI-MS: calcd. for $C_{18}H_{15}ClN_2O_2S$: 358.0543; Found: 381.0439 [M+Na].

Spectral data for *N*-(2-(4-bromophenyl)-3-cyano-1*H*-inden-1-yl)-*N*-methylmethanesulfonamide (4e).



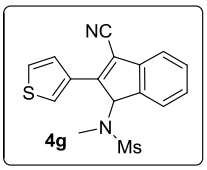
Light yellow solid; mp: 135-136 °C; IR (neat, cm^{-1}): 2363, 2221, 1698, 1623, 1457, 1150, 964, 883, 762; ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.70 (d, *J* = 5.8 Hz, 2 H), 7.64 (d, *J* = 6.8 Hz, 2 H), 7.55 ~ 7.43 (m, 2 H), 7.47 (t, *J* = 7.5 Hz, 1 H), 7.40 (t, *J* = 7.5 Hz, 1 H), 6.28 (s, 1 H), 2.96 (s, 3 H), 2.21 (s, 3 H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 156.3, 138.8, 138.7, 134.2, 132.5, 129.8, 129.7, 128.4, 125.4, 124.4, 121.0, 114.4, 112.2, 64.5, 40.1 29.2; ESI-MS: calcd. for $C_{18}H_{15}BrN_2O_2S$: 402.0038; Found: 403.0041 [M+H].

Spectral data for *N*-(2-cyano-2-(thiophen-3-yl)-1*H*-inden-1-yl)-*N*-methylmethanesulfonamide (4f).



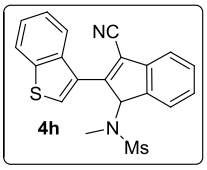
Brownish viscous liquid; IR (neat, cm^{-1}): 2364, 2216, 1771, 1541, 1507, 1405, 1260, 1132, 761; ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.97 (d, *J* = 3.8 Hz, 1 H), 7.57 ~ 7.55 (m, 2 H), 7.49 (d, *J* = 16 Hz, 1 H), 7.44 (t, *J* = 7.4 Hz, 1 H), 7.35 (t, *J* = 7.4 Hz, 1 H), 7.20 ~ 7.19 (m, 1 H), 6.14 (s, 1 H), 3.17 (s, 3 H), 2.35 (s, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 149.3, 139.0, 138.2, 133.6, 130.1, 130.0, 129.8, 128.4, 127.9, 124.4, 120.6, 114.9, 108.6, 65.3, 40.1 29.5; ESI-MS: calcd. for $C_{16}H_{14}N_2O_2S_2$: 330.0497; Found: 353.0388 [M+Na].

Spectral data for *N*-(3-cyano-2-(thiophen-3-yl)-1*H*-inden-1-yl)-*N*-methylmethanesulfonamide (4g).



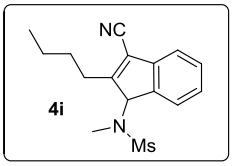
Brownish viscous liquid; IR (neat, cm^{-1}): 2364, 2216, 1771, 1647, 1540, 1418, 1265, 736; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.97 (d, *J* = 3.8 Hz, 1 H), 7.56 (t, *J* = 5.1 Hz, 2 H), 7.51 (d, *J* = 16 Hz, 1 H), 7.46 (t, *J* = 9.4 Hz, 1 H), 7.35 (t, *J* = 7.4 Hz, 1 H), 7.19 (t, *J* = 8.8 Hz, 1 H), 6.13 (s, 1 H), 3.17 (s, 3 H), 2.32 (s, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 149.3, 139.0, 138.2, 133.6, 130.1, 130.0, 129.8, 128.4, 127.9, 124.4, 120.6, 114.9, 108.6, 65.3, 40.1 29.5; ESI-MS: calcd. for $C_{16}H_{14}N_2O_2S_2$: 330.0497; Found: 331.0567 [M+H].

Spectral data for *N*-(2-(benzo[b]thiophen-3-yl)-3-cyano-1*H*-inden-1-yl)-*N*-methylmethane-sulfonamide (4h).



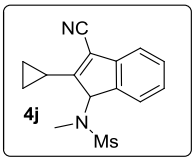
Light yellow solid; mp: 182-183 °C; IR (neat, cm^{-1}): 2365, 2222, 1623, 1541, 1473, 1396, 1185, 963, 883, 736; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.99 (d, *J* = 7.6 Hz, 1 H), 7.93 (d, *J* = 6.4 Hz, 1 H), 7.88 (s, 1 H), 7.60 (t, *J* = 6.4 Hz, 2 H), 7.54 ~ 7.40 (m, 4 H), 6.46 (s, 1 H), 2.55 (s, 3 H), 2.28 (s, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 153.2, 140.5, 139.2, 138.7, 136.2, 129.8, 129.6, 128.3, 127.9, 125.5, 125.2, 124.5, 123.3, 123.0, 120.9, 114.1, 113.6, 66.4, 39.7, 29.4; ESI-MS: calcd. for $C_{20}H_{16}N_2O_2S_2$: 380.0653; Found: 381.0651 [M+H].

Spectral data for *N*-(2-butyl-3-cyano-1*H*-inden-1-yl)-*N*-methylmethanesulfonamide (4i).



White viscous liquid; IR (neat, cm^{-1}): 2956, 2931, 2873, 2364, 2224, 1662, 1594, 1396, 1340, 964, 728; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.42 ~ 7.38 (m, 3 H), 7.32 ~ 7.28 (m, 1 H), 5.58 (s, 1 H), 3.12 (s, 3 H), 2.78 ~ 2.70 (m, 1 H), 2.52 ~ 2.45 (m, 1 H), 2.34 (s, 3 H), 1.74 ~ 1.57 (m, 2 H), 1.46 ~ 1.23 (m, 2 H), 0.95 (t, *J* = 7.3 Hz, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 164.4, 138.8, 138.7, 129.5, 127.3, 123.9, 120.4, 113.8, 113.7, 65.0, 40.0 30.8, 29.6, 28.1, 22.5, 13.6; ESI-MS: calcd. for $C_{16}H_{20}N_2O_2S$: 304.1245; Found: 305.1319 [M+H].

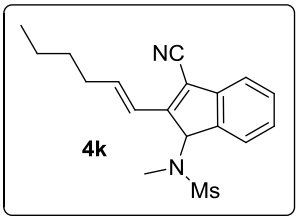
Spectral data for *N*-(3-cyano-2-cyclopropyl-1*H*-inden-1-yl)-*N*-methylmethanesulfonamide (4j).



Yellowish viscous liquid; IR (neat, cm^{-1}): 2366, 2220, 1652, 1489, 1387, 1261, 858, 763; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.38 ~ 7.34 (m, 3 H), 7.28 ~ 7.25 (m, 1 H), 5.58 (s, 1 H), 3.12 (s, 3 H), 2.40 (s, 3 H), 1.99 ~ 1.94 (m, 1 H), 1.44 ~ 1.41 (m, 1 H), 1.33 ~ 1.23 (m, 2 H), 1.16 ~ 1.11 (m, 1 H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 164.9, 139.1, 138.2, 129.5, 127.0, 123.6, 120.0, 113.9,

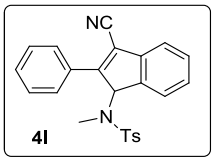
109.7, 66.1, 40.0, 29.7, 12.3, 10.6, 9.3; ESI-MS: calcd. for $C_{15}H_{16}N_2O_2S$: 288.0932, Found: 311.0821 [M+Na].

Spectral data for *N*-(3-cyano-2-(hex-1-en-1-yl)-1*H*-inden-1-yl)-*N*-methylmethanesulfonamide (4k).



Light yellow viscous liquid; IR (neat, cm^{-1}): 2365, 2223, 1844, 1670, 1647, 1387, 1265, 1153, 936, 736; ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.44 ~ 7.38 (m, 3 H), 7.31 (t, *J* = 7.3 Hz, 1 H), 6.74 ~ 6.70 (m, 1 H), 6.56 (d, *J* = 15.9 Hz, 1 H), 5.89 (s, 1 H), 3.12 (s, 3 H), 2.32 ~ 2.27 (m, 5 H), 1.52 ~ 1.45 (m, 2 H), 1.38 ~ 1.35 (m, 2 H), 0.92 (t, *J* = 7.3 Hz, 3 H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 155.8, 143.4, 139.1, 138.9, 129.6, 127.7, 124.1, 121.4, 120.6, 114.0, 111.2, 63.4, 40.3, 33.6, 30.9, 29.2, 22.3, 13.8; ESI-MS: calcd. for $C_{18}H_{22}N_2O_2S$: 330.1402; Found: 331.1474 [M+H].

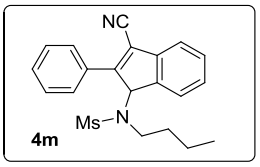
Spectral data for *N*-(3-cyano-2-phenyl-1*H*-inden-1-yl)-*N*,4-dimethylbenzenesulfonamide (4l).



White solid; mp: 190-191 °C; IR (neat, cm^{-1}): 2366, 2221, 1684, 1652, 1362, 1318, 1088, 867, 760; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.85 ~ 7.83 (m, 2 H), 7.73 (d, *J* = 8.4 Hz, 2 H), 7.50 (d, *J* = 7.6 Hz, 1 H), 7.46 ~ 7.45 (m, 3 H), 7.40 (t, *J* = 8.4 Hz, 1 H), 7.29 (d, *J* = 8.4 Hz, 2 H), 7.25 ~ 7.21 (m, 1 H), 7.08 (d, *J* = 7.2 Hz, 1 H), 6.36 (s, 1 H), 2.44 (s, 3 H), 2.14 (s, 3 H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 158.0, 144.0, 138.9, 138.6, 136.3, 130.8, 130.5, 129.8, 129.4, 128.9, 128.5, 127.8, 127.7, 124.7, 120.6, 114.7, 111.5, 64.5, 29.4, 21.5; ESI-MS: calcd. for $C_{24}H_{20}N_2O_2S$: 400.1245; Found: 401.1327 [M+H].

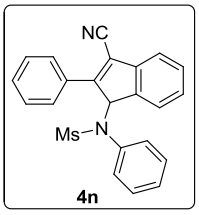
Spectral data for *N*-butyl-*N*-(3-cyano-2-phenyl-1*H*-inden-1-yl)methanesulfonamide (4m).

White viscous liquid; IR (neat, cm^{-1}): 2364, 2222, 1617, 1608, 1489, 1396, 962, 787; ^{1}H NMR



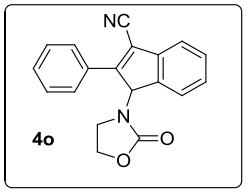
(600 MHz, $CDCl_3$): δ 7.78 (d, *J* = 7.2 Hz, 2 H), 7.56 ~ 7.46 (m, 6 H), 7.38 (t, *J* = 8.8 Hz, 1 H), 6.37 (s, 1 H), 3.00 (s, 3 H), 2.86 ~ 2.79 (m, 1 H), 2.47 ~ 2.42 (m, 1 H), 0.92 ~ 0.73 (m, 4 H), 0.54 (t, *J* = 7.3 Hz, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 158.9, 140.0, 138.6, 131.6, 130.6, 129.5, 129.2, 128.4, 128.0, 124.6, 120.8, 114.7, 111.5, 64.8, 45.5, 41.8, 31.3, 19.9, 13.3; ESI-MS: calcd. for $C_{21}H_{22}N_2O_2S$: 366.1402; Found: 367.1482 [M+H].

Spectral data for *N*-(3-cyano-2-phenyl-1*H*-inden-1-yl)-*N*-phenylmethanesulfonamide (4n).



White viscous liquid; IR (neat, cm^{-1}): 2367, 2221, 1670, 1623, 1473, 1225, 981, 762, 737; ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.87 (d, *J* = 6.7 Hz, 1 H), 7.80 (d, *J* = 7.4 Hz, 2 H), 7.58 ~ 7.51 (m, 3 H), 7.43 ~ 7.35 (m, 3 H), 7.15 (t, *J* = 7.4 Hz, 1 H), 7.00 (t, *J* = 7.7 Hz, 2 H), 6.73 (s, 1 H), 6.53 (d, *J* = 7.7 Hz, 2 H), 2.90 (s, 3 H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 157.0, 140.0, 138.8, 134.5, 131.7, 130.6, 130.4, 129.5, 129.2, 128.8, 128.5, 127.9, 124.9, 120.6, 114.6, 111.7, 65.4, 40.5; ESI-MS: calcd. for $C_{23}H_{18}N_2O_2S$: 386.1089; Found: 409.0994 [M+Na].

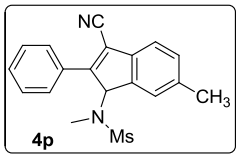
Spectral data for 1-(2-oxooxazolidin-3-yl)-2-phenyl-1*H*-indene-3-carbonitrile (4o).



Yellowish viscous liquid; IR (neat, cm^{-1}): 2366, 2217, 1748, 1670, 1457, 1085, 757, 704; ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.88 (dd, *J* = 1.3, 6.9 Hz, 2 H), 7.55 (d, *J* = 7.2 Hz, 1 H), 7.52 ~ 7.46 (m, 5 H), 7.37 (t, *J* = 7.2 Hz, 1 H), 6.28 (s, 1 H), 4.21 ~ 4.07 (m, 2 H), 2.96 ~ 2.80 (m, 2 H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 158.6, 156.7, 139.3, 138.3, 131.0,130.5, 129.9, 129.5, 128.1, 128.0,

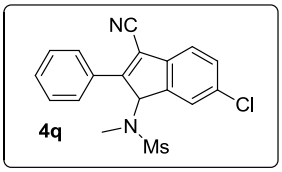
124.0, 120.8, 114.8, 111.1, 62.1, 60.4, 39.9; ESI-MS: calcd. for $C_{19}H_{14}N_2O_2$: 302.1055; Found: 303.1132 [M+H].

Spectral data for *N*-(3-cyano-6-methyl-2-phenyl-1*H*-inden-1-yl)-*N*-methylmethanesulfonamide (4p).



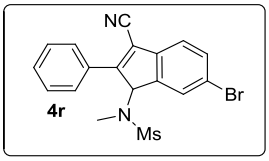
White viscous liquid; IR (neat, cm^{-1}): 2357, 2222, 1683, 1557, 1473, 1318, 736; ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.77 (d, *J* = 7.3 Hz, 2 H), 7.50 (t, *J* = 7.1 Hz, 2 H), 7.45 (t, *J* = 7.2 Hz, 1 H), 7.39 (d, *J* = 7.7 Hz, 1 H), 7.36 (s, 1 H), 7.25 (d, *J* = 8.0 Hz, 1 H), 6.23 (s, 1 H), 2.86 (s, 3 H), 2.41 (s, 3 H), 2.22 (s, 3 H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 156.7, 139.2, 138.5, 136.3, 131.3, 130.5, 130.3, 129.1, 128.2, 125.2, 120.4, 114.6, 111.8, 64.5, 40.0, 29.0, 21.5; ESI-MS: calcd. for $C_{19}H_{18}N_2O_2S$: 338.1089; Found: 339.1160 [M+H].

Spectral data for *N*-(6-chloro-3-cyano-2-phenyl-1*H*-inden-1-yl)-*N*-methylmethanesulfonamide (4q).



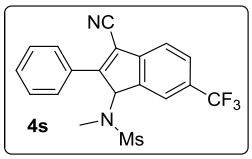
Yellow viscous liquid; IR (neat, cm^{-1}): 2367, 2223, 1683, 1670, 1558, 1338, 1178, 764, 686; ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.76 (d, *J* = 7.2 Hz, 2 H), 7.54 ~ 7.48 (m, 4 H), 7.43 (s, 2 H), 6.30 (s, 1 H), 2.88 (s, 3 H), 2.23 (s, 3 H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 158.1, 140.8, 137.3, 134.5, 130.9, 130.7, 129.9, 129.2, 128.2, 124.9, 121.6, 114.1, 110.9, 64.4, 40.0 29.1; ESI-MS: calcd. for $C_{18}H_{15}ClN_2O_2S$: 358.0543; Found: 381.0445 [M+Na].

Spectral data for *N*-(6-bromo-3-cyano-2-phenyl-1*H*-inden-1-yl)-*N*-methylmethanesulfonamide (4r).



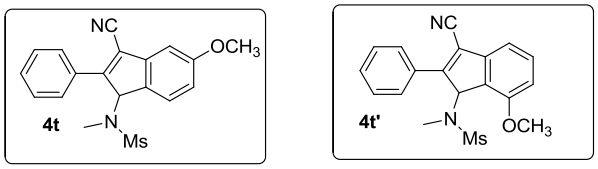
Light yellow solid; mp: 177-178 °C; IR (neat, cm^{-1}): 2367, 2222, 1683, 1623, 1558, 1230, 1060, 876, 695; ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.76 (d, *J* = 7.2 Hz, 2 H), 7.70 (s, 1 H), 7.60 (d, *J* = 8.0 Hz, 1 H), 7.53 ~ 7.39 (m, 3 H), 7.39 (d, 8.0 Hz, 1 H), 6.29 (s, 1 H), 2.87 (s, 3 H), 2.24 (s, 3 H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 158.0, 141.1, 137.8, 132.9, 131.0, 130.8, 129.3, 128.3, 127.8, 122.5, 121.9, 114.1, 111.2, 64.5, 40.0, 29.2; ESI-MS: calcd. for $C_{18}H_{15}BrN_2O_2S$: 402.0038; Found: 424.9929 [M+Na].

Spectral data for *N*-(3-cyano-2-phenyl-6-(trifluoromethyl)-1*H*-inden-1-yl)-*N*-methyl-methanesulfonamide (4s).



Yellow viscous liquid; IR (neat, cm^{-1}): 2364, 2222, 1698, 167, 1473, 1132, 964, 762; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.82 ~ 7.80 (m, 3 H), 7.76 (d, *J* = 8.0 Hz, 1 H), 7.65 (d, *J* = 8.0 Hz, 1 H), 7.58 ~ 7.75 (m, 3 H), 6.40 (s, 1 H), 2.89 (s, 3 H), 2.24 (s, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 160.6, 142.2, 139.8, 131.5, 130.6, 130.3, 129.4, 128.5, 127.3, 125.2, 121.4, 121.1, 114.0, 111.0, 64.7, 40.0 29.3; ESI-MS: calcd. for $C_{19}H_{15}F_3N_2O_2S$: 392.0806; Found: 415.0700 [M+Na].

Spectral data for *N*-(3-cyano-5-methoxy-2-phenyl-1*H*-inden-1-yl)-*N*-methylmethanesulfonamide (4t), (4t').

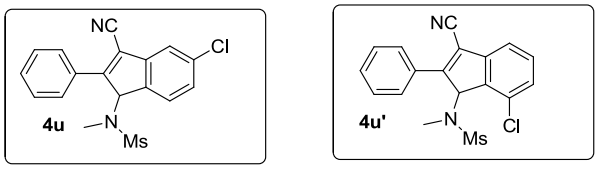


White viscous liquid; IR (neat, cm^{-1}): 2367, 2221, 1748, 1684, 1670, 1265, 736; ^{1}H NMR (600 MHz, $CDCl_3$):major isomer **4t**: δ 7.79 (d, *J* = 9.1 Hz, 2 H), 7.53 ~ 7.48 (m, 3 H), 7.44 (d, *J* = 8.3 Hz, 1 H), 7.05 (d, *J* = 2.3 Hz, 1 H), 6.89 (dd, *J* = 8.3, 2.3 Hz, 1 H), 6.27 (s, 1 H), 3.86 (s, 3 H), 2.87 (s, 3 H), 2.22 (s, 3 H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 161.3, 159.1, 140.4, 131.2, 130.8, 130.5, 129.2, 128.3, 125.4, 114.6, 114.3, 111.7, 106.1, 64.1, 55.7, 40.0, 29.0; ESI-MS: calcd. for $C_{19}H_{18}N_2O_3S$: 354.1038; Found: 377.0935 [M+Na].

White viscous liquid; IR (neat, cm^{-1}): 2365, 2221, 1748, 1685, 1670, 1290, 736; ^{1}H NMR (400 MHz, $CDCl_3$): minor isomer **4t'**: δ 7.86 (d, *J* = 7.2 Hz, 2 H), 7.53 ~ 7.43 (m, 4 H), 7.17 (d, *J* =

7.6 Hz, 1 H), 6.89 (d, *J* = 8.4 Hz, 1 H), 6.44 (s, 1 H), 3.91 (s, 3 H), 2.90 (s, 3 H), 2.24 (s, 3 H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 159.6, 156.0, 140.9, 131.7, 130.8, 129.1, 128.6, 124.1, 114.8, 113.6, 111.2, 110.5, 63.4, 55.3, 39.2, 29.7, 28.8; ESI-MS: calcd. for $C_{19}H_{18}N_2O_3S$: 354.1038; Found: 377.0935 [M+Na].

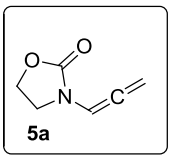
Spectral data for *N*-(5-chloro-3-cyano-2-phenyl-1*H*-inden-1-yl)-*N*-methylmethanesulfonamide (4u), (4u').



Yellow viscous liquid; IR (neat, cm^{-1}): 2366, 2222, 1716, 1670, 1652, 1473, 1338, 1265, 965, 789; ^{1}H NMR (400 MHz, $CDCl_3$): major isomer: δ 7.79 (dd, *J* = 8.0, 1.6 Hz, 2 H), 7.56 ~ 7.50 (m, 3 H), 7.44 ~ 7.42 (m, 2 H), 7.33 ~ 7.31 (m, 1 H), 6.54 (s, 1 H), 2.64 (s, 3 H), 2.26 (s, 3 H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 159.9, 141.1, 135.1, 131.7, 131.4, 131.2, 130.9, 129.3, 129.0, 128.7, 119.3, 114.0, 111.6, 64.8, 39.7, 28.7; ESI-MS: calcd. for $C_{18}H_{15}ClN_2O_2S$: 358.0543; Found: 381.0438 [M+Na].

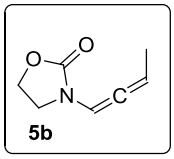
Yellow viscous liquid; minor isomer, IR (neat, cm^{-1}): 2366, 2222, 1716, 1670, 1652, 1473, 1338, 1265, 965, 789; ^{1}H NMR (600 MHz, $CDCl_3$): (Minor): δ 7.78 (dd, *J* = 8.0, 1.6 Hz, 2 H), 7.54 ~ 7.49 (m, 5 H), 7.35 (dd, *J* = 8.0, 1.6 Hz, 1 H), 6.31 (s, 1 H), 2.87 (s, 3 H), 2.22 (s, 3 H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 159.4, 140.6, 137.2, 135.9, 131.2, 130.8, 129.3, 128.4, 128.2, 125.6, 121.2, 114.1, 111.6, 110.8, 64.2, 39.9, 29.1; ESI-MS: calcd. for $C_{18}H_{15}ClN_2O_2S$: 358.0543; Found: 381.0438 [M+Na].

Spectral data for 3-(propa-1,2-dien-1-yl)oxazolidin-2-one (5a).



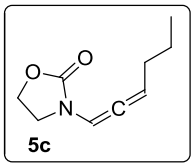
Colorless liquid; IR (neat, cm^{-1}): 2984, 2914, 1965, 1764, 1486, 1433, 1393, 1310, 1251, 1082, 1035, 757, 666 cm^{-1}; ^{1}H NMR (600 MHz, CDCl3): δ 6.87 ~ 6.85 (td, *J* = 1.7, 8.3 Hz, 1H), 5.42 (d, *J* = 6.4 Hz, 2H), 4.41 ~ 4.38 (td, *J* = 1.0, 7.8 Hz, 2H), 3.58 (t, *J* = 8.3 Hz, 2H). ^{13}C NMR (150 MHz, $CDCl_3$): δ 201.4, 155.2, 97.0, 87.8, 62.2, 43.1.

Spectral data for 3-(buta-1,2-dien-1-yl)oxazolidin-2-one (5b).



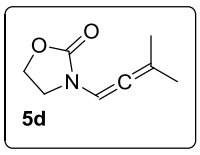
Colorless liquid; IR (neat, cm^{-1}): 2981, 2913, 1965, 1766, 1486, 1431, 1392, 1310, 1250, 1082, 1033, 758, 669 cm^{-1}; ^{1}H NMR (600 MHz, C_6D_6): δ 6.95 ~ 6.93 (m, 1H), 5.47 ~ 5.43 (m, 1H), 3.32 ~ 3.29 (m, 2H), 2.54 ~ 2.44 (m, 2H), 1.48 ~ 1.46 (m, 3H). ^{13}C NMR (150 MHz, C_6D_6): δ 195.9, 155.0, 98.2, 96.9, 61.5, 42.6, 16.4.

Spectral data for 3-(hexa-1,2-dien-1-yl)oxazolidin-2-one (5c).



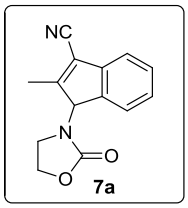
Colorless liquid; IR (neat, cm^{-1}): 2984, 2914, 1966, 1764, 1488, 1433, 1393, 1311, 1251, 1082, 1035, 759, 670 cm^{-1}; ^{1}H NMR (600 MHz, C_6D_6): δ 7.02 ~ 6.99 (m, 1H), 5.53 (q, *J* = 6.4 Hz, 1H), 3.28 (t, *J* = 8.1 Hz, 2H), 2.54 ~ 2.50 (m, 2H), 1.85 ~ 1.80 (m, 2H), 1.31 ~ 1.24 (m, 2H), 0.82 ~ 0.81 (m, 3H). ^{13}C NMR (150 MHz, C_6D_6): δ 194.9, 154.8, 103.2, 97.3, 61.2, 42.4, 32.6, 21.9, 13.5.

Spectral data for 3-(3-methylbuta-1,2-dien-1-yl)oxazolidin-2-one (5d).



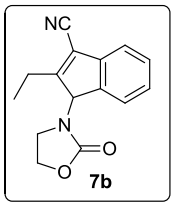
Colorless liquid; IR (neat, cm^{-1}): 2984, 2914, 1965, 1764, 1486, 1433, 1393, 1310, 1251, 1082, 1035, 757, 666 cm^{-1}; ^{1}H NMR (600 MHz, $CDCl_3$): δ 6.57 (m, 1H), 4.35 (d, *J* = 8.0 Hz, 2H), 3.51 (d, *J* = 8.2 Hz, 2H), 1.76 (d, *J* = 2.4 Hz). ^{13}C NMR (150 MHz, $CDCl_3$): δ 191.2, 155.5, 108.8, 94.1, 62.1, 43.2, 22.2.

Spectral data for 2-methyl-1-(2-oxooxazolidin-3-yl)-1*H*-indene-3-carbonitrile (7a).



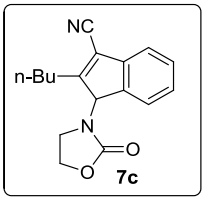
White solid; mp: 149-150 °C; IR (neat, cm^{-1}): 2359, 2225, 1747, 1541, 1418, 1233, 1033, 762, 697; ^1H NMR (600 MHz, $CDCl_3$): δ 7.39 ~ 7.36 (m, 3H), 7.30 ~ 7.27 (m, 1H), 5.55 (s, 1H), 4.38 ~ 4.32 (m, 2H), 3.03 ~ 2.97 (m, 2H), 2.25 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 159.2, 158.8, 138.7, 138.1, 129.5, 127.3, 123.9, 120.2, 114.5, 113.4, 62.6, 62.2, 40.4, 14.2; HRMS calcd for $C_{14}H_{12}N_2O_2$: 240.0899; found: 240.0896.

Spectral data for 2-ethyl-1-(2-oxooxazolidin-3-yl)-1*H*-indene-3-carbonitrile (7b).



Yellow viscous liquid; IR (neat, cm^{-1}): 2977, 2225, 1748, 1541, 1420, 1229, 1030, 761, 703; ^1H NMR (600 MHz, $CDCl_3$): δ 7.42 ~ 7.37 (m, 3H), 7.31 ~ 7.29 (m, 1H), 5.68 (s, 1H), 4.35 ~ 4.32 (m, 2H), 3.02 ~ 2.97 (m, 2H), 2.79 ~ 2.77 (m, 1H), 2.44 ~ 2.41 (m, 1H), 1.30 (t, *J* = 7.6 Hz, 3H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 164.7, 158.7, 138.8, 138.2, 129.6, 127.4, 123.9, 120.4, 113.5, 62.2, 60.8, 40.5, 22.1, 13.3 (one aromatic quaternary carbon merged); HRMS calcd for $C_{15}H_{14}N_2O_2$: 254.1055; found: 254.1054.

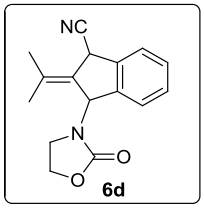
Spectral data for 2-butyl-1-(2-oxooxazolidin-3-yl)-1*H*-indene-3-carbonitrile (7c).



Pale yellow oil; IR (neat, cm^{-1}): 2961, 2360, 2230, 1749, 1542, 1419, 1243, 1040, 761, 699; ^1H NMR (600 MHz, $CDCl_3$): δ 7.42 ~ 7.36 (m, 3H), 7.31 ~ 7.29 (m, 1H), 5.66 (s, 1H), 4.36 ~ 4.31 (m, 2H), 3.01 ~ 2.96 (m, 2H), 2.76 ~ 2.72 (m, 1H), 2.41 ~ 2.37 (m, 1H), 1.72 ~ 1.70 (m, 1H),

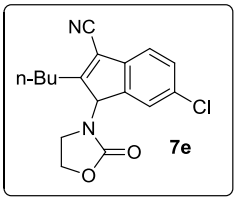
1.63 ~ 1.61 (m, 1H), 1.43 ~ 1.38 (m, 2H), 0.94 (t, *J* = 7.4 Hz, 3H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 163.7, 158.7, 138.8, 138.3, 129.6, 127.4, 123.9, 120.4, 114.1, 113.6, 62.2, 61.0, 40.5, 30.8, 28.4, 22.5, 13.6; ESI-MS: calcd. for $C_{17}H_{18}N_2O_2$: 282.1368; found: 283.1449 [M+Na].

Spectral data for 3-(2-oxooxazolidin-3-yl)-2-(propan-2-ylidene)-2,3-dihydro-1*H*-indene-1-carbonitrile (6d).



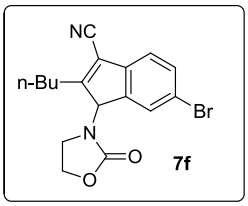
White solid; mp: 161 -162 °C; IR (neat, cm^{-1}): 2908, 2360, 2230, 1734, 1533, 1419, 1250, 1032, 759, 696; ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.46 ~ 7.38 (m, 4H), 6.03 (s, 1H), 4.68 (s, 1H), 4.31 ~ 4.27 (m, 1H), 4.24 ~ 4.19 (m, 1H), 3.38 ~ 3.34 (m, 1H), 3.02 ~ 2.98 (m, 1H), 2.00 (s, 3H), 1.89 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 157.6, 140.1, 139.9, 136.4, 130.1, 130.0, 125.9, 124.9, 118.8, 62.1, 58.1, 40.4, 36.4, 22.1, 21.2 (one aromatic quaternary carbon merged); HRMS calcd for $C_{16}H_{16}N_2O_2$: 268.1212; found: 268.1214.

Spectral data for 2-butyl-6-chloro-1-(2-oxooxazolidin-3-yl)-1*H*-indene-3-carbonitrile (7e).



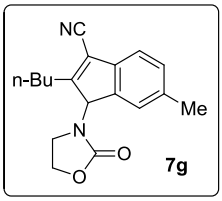
Colorless oil; IR (neat, cm^{-1}): 2960, 2360, 2225, 1749, 1542, 1418, 1234, 1033, 761, 715; ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.39 (dd, *J* = 1.8, 8.1 Hz, 1H), 7.37 (s, 1H), 7.34 (d, *J* = 8.1 Hz, 1H), 5.65 (s, 1H), 4.36 (t, *J* = 7.8 Hz, 2H), 3.04 ~ 2.98 (m, 2H), 2.76 ~ 2.70 (m, 1H), 2.39 ~ 2.31 (m, 1H), 1.73 ~ 1.69 (m, 1H), 1.62 ~ 1.58 (m, 1H), 1.44 ~ 1.23 (m, 2H), 0.94 (t, *J* = 7.4 Hz, 3H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 164.1, 158.5, 140.1, 137.2, 133.9, 129.9, 124.5, 121.2, 113.5, 113.2, 62.5, 60.8, 40.5, 30.8, 28.5, 22.5, 13.6; HRMS calcd for $C_{17}H_{17}ClN_2O_2$: 316.0979, found: 316.0973.

Spectral data for 6-bromo-2-butyl-1-(2-oxooxazolidin-3-yl)-1*H*-indene-3-carbonitrile (7f).



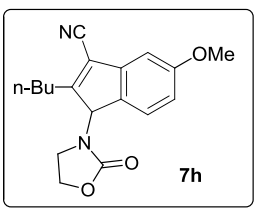
Colorless oil; IR (neat, cm^{-1}): 2961, 2369, 2225, 1748, 1542, 1419, 1233, 1034, 759, 699; ^1H NMR (600 MHz, $CDCl_3$): δ 7.55 (dd, *J* = 1.8, 8.1 Hz, 1H), 7.52 (s, 1H), 7.28 (d, *J* = 8.1 Hz, 1H), 5.65 (s, 1H), 4.36 (t, *J* = 8.0 Hz, 2H), 3.06 ~ 2.98 (m, 2H), 2.75 ~ 2.70 (m, 1H), 2.39 ~ 2.34 (m, 1H), 1.73 ~ 1.69 (m, 1H), 1.62 ~ 1.58 (m, 1H), 1.42 ~ 1.36 (m, 2H), 0.94 (t, *J* = 7.4 Hz, 3H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 164.0, 158.5, 140.4, 137.7, 132.8, 127.4, 121.7, 121.6, 113.6, 113.2, 62.2, 60.8, 40.5, 30.8, 28.5, 22.6, 13.6; HRMS calcd for $C_{17}H_{17}BrN_2O_2$: 360.0473, found: 360.0474.

Spectral data for 2-butyl-6-methyl-1-(2-oxooxazolidin-3-yl)-1*H*-indene-3-carbonitrile (7g).



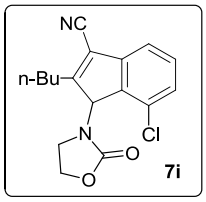
Pale yellow oil; IR (neat, cm^{-1}): 2958, 2360, 2223, 1749, 1541, 1419, 1244, 1034, 761, 701; ^1H NMR (600 MHz, $CDCl_3$): δ 7.29 (d, *J* = 7.7 Hz, 1H), 7.20 ~ 7.18 (m, 2H), 5.61 (s, 1H), 4.35 ~ 4.32 (m, 2H), 3.02 ~ 2.97 (m, 2H), 2.74 ~ 2.69 (m, 1H), 2.39 ~ 2.34 (m, 4H, CH_3 group merged), 1.74 ~ 1.71 (m, 1H), 1.63 ~ 1.59 (m, 1H), 1.40 ~ 1.38 (m, 2H), 0.93 (t, *J* = 7.4 Hz, 3H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 162.5, 158.7, 138.6, 137.7, 136.2, 130.1, 124.8, 120.0, 113.9, 113.8, 62.2, 60.8, 40.5, 30.9, 28.4, 22.5, 21.4, 13.6; HRMS calcd for $C_{18}H_{20}N_2O_2$: 296.1525, found: 296.1524.

Spectral data for 2-butyl-5-methoxy-1-(2-oxooxazolidin-3-yl)-1*H*-indene-3-carbonitrile (7h).



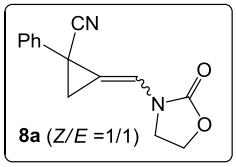
Pale yellow oil; IR (neat, cm^{-1}): 2958, 2360, 2223, 1749, 1542, 1419, 1223, 1033, 761, 705; ^1H NMR (600 MHz, $CDCl_3$): δ 7.25 (s, 1H), 6.94 (d, *J* = 2.3 Hz, 1H), 6.89 (dd, *J* = 2.3, 8.2 Hz, 1H), 5.59 (s, 1H), 4.35 ~ 4.29 (m, 2H), 3.83 (s, 3H), 3.02 ~ 2.99 (m, 1H), 2.97 ~ 2.94 (m, 1H), 2.73 ~ 2.71 (m, 1H), 2.39 ~ 2.36 (m, 1H), 1.73 ~ 1.68 (m, 1H), 1.61 ~ 1.58 (m, 1H), 1.40 ~ 1.33 (m, 2H), 0.93 (t, *J* = 7.4 Hz, 3H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 165.1, 161.2, 158.7, 140.3, 129.8, 124.8, 113.9, 113.6, 113.2, 106.0, 62.2, 60.4, 55.7, 40.4, 30.8, 28.5, 22.5, 13.6; HRMS calcd for $C_{18}H_{20}N_2O_3$: 312.1474; Found: 312.1478.

Spectral data for 2-butyl-7-chloro-1-(2-oxooxazolidin-3-yl)-1*H*-indene-3-carbonitrile (7i).



Pale yellow oil; IR (neat, cm^{-1}): 2966, 2360, 2228, 1749, 1542, 1419, 1227, 1031, 760, 698; ^1H NMR (600 MHz, $CDCl_3$): δ 7.37 (t, *J* = 7.8 Hz, 1H), 7.32 (dd, *J* = 0.8, 7.8 Hz, 1H), 7.24 ~ 7.23 (m, 1H, merged with $CDCl_3$ peak), 5.75 (s, 1H), 4.38 ~ 4.32 (m, 2H), 3.02 ~ 2.98 (m, 2H), 2.76 ~ 2.70 (m, 1H), 2.46 ~ 2.41 (m, 1H), 1.74 ~ 1.71 (m, 1H), 1.63 ~ 1.58 (m, 1H), 1.41 ~ 1.37 (m, 2H), 0.93 (t, *J* = 7.4 Hz, 3H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 165.1, 158.2, 140.9, 134.5, 131.3, 131.1, 127.9, 118.9, 113.2, 113.0, 62.2, 61.0, 40.6, 30.7, 28.3, 22.5, 13.6; HRMS calcd for $C_{17}H_{17}ClN_2O_2$: 316.0979, found: 316.0978.

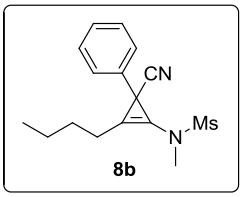
Spectral data for 2-((2-oxooxazolidin-3-yl)methylene)-1-phenylcyclopropanecarbonitrile (8a - *Z/E*:1/1).



first isomer: Pale yellow oil; IR (neat, cm^{-1}): 2960, 2360, 2225, 1749, 1542, 1418, 1231, 1037, 761, 699; ^1H NMR (400 MHz, $CDCl_3$): δ 7.40 ~ 7.37 (m, 2H), 7.32 ~ 7.29 (m, 4H), 4.40 ~ 4.34 (m, 1H), 4.29 ~ 4.24 (m, 1H), 4.01 ~ 3.95 (m, 1H), 3.58 ~ 3.52 (m, 1H), 2.59 ~ 2.56 (dd, *J* = 2.0, 8.7 Hz, 1H), 1.94 ~ 1.92 (dd, *J* = 2.0, 8.7 Hz, 1H); ^{13}C NMR (175 MHz, $CDCl_3$): δ 155.1, 136.4, 129.1, 127.8, 124.8, 120.5, 118.3, 103.6, 62.5, 42.8, 23.6, 17.9; HRMS calcd for $C_{14}H_{12}N_2O_2$:

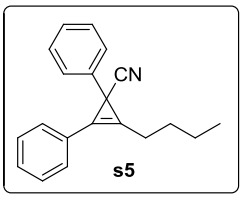
240.0899, found: 240.0893. second isomer: Pale yellow oil; ^{1}H NMR (600 MHz, $CDCl_3$): 7.26 ~ 7.22 (m, 2H), 7.12 ~ 7.07 (m, 4H), 3.28 ~ 3.23 (m, 2H), 2.25 ~ 2.22 (m, 1H), 2.19 ~ 2.16 (m, 1H), 1.83 ~ 1.81 (dd, *J* = 2.4, 8.3 Hz, 1H), 1.16 ~ 1.14 (dd, *J* = 2.0, 8.3 Hz, 1H), ^{13}C NMR (100 MHz, $CDCl_3$): δ 154.6, 135.9, 129.1, 128.6, 126.3, 120.3, 120.0, 102.7, 61.6, 41.3, 23.3, 16.8; HRMS calcd for $C_{14}H_{12}N_2O_2$: 240.0899, found: 240.0893.

Spectral data for *N*-(2-butyl-3-cyano-3-phenylcycloprop-1-en-1-yl)-*N*-methylmethane-sulfonamide (8b).



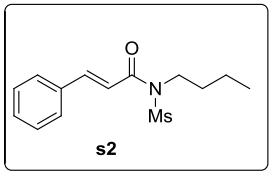
White semisolid; IR (neat, cm^{-1}): 2367, 2220, 1636, 1559, 1170, 735; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.46 ~ 7.41 (m, 3 H), 7.40 ~ 7.36 (m, 2 H), 3.39 (s, 3 H), 3.35 (s, 3 H), 2.51 (t, *J* = 8.0 Hz, 2 H), 1.46 ~ 1.40 (m, 2 H), 1.27 ~ 1.22 (m, 2 H), 0.80 (t, *J* = 7.6 Hz, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 168.3, 155.6, 131.1, 129.7, 129.1, 128.6, 117.5, 112.0, 40.6, 32.8, 31.6, 29.5, 22.5, 13.5; ESI-MS: calcd. for $C_{16}H_{20}N_2O_2S$: 304.1245; Found: 305.1318 [M+H].

Spectral data for 2-butyl-1,3-diphenylcycloprop-2-enecarbonitrile (s5).



White viscous liquid; IR (neat, cm^{-1}): 2358, 2220, 1683, 1647, 1594, 1265, 737; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.50 ~ 7.48 (m, 2 H), 7.43 ~ 7.38 (m, 3 H), 7.31 ~ 7.29 (m, 4 H), 7.24 ~ 7.21 (m, 1 H), 2.73 (t, *J* = 7.6 Hz, 2 H), 1.79 ~ 1.72 (m, 2 H), 1.50 ~ 1.43 (m, 2 H), 0.94 (t, *J* = 7.2 Hz, 3 H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 138.1, 129.8, 129.5, 129.4, 129.2, 129.1, 128.6, 126.8, 125.2, 124.3, 122.1, 111.7, 105.6, 29.1, 23.6, 22.5, 13.7; HR-MS: calcd. for $C_{20}H_{19}N$: 273.1517; Found: 273.1519.

Spectral data for *N*-butyl-*N*-(methylsulfonyl)cinnamamide (s2).



s2

Colorless liquid; IR (neat, cm^{-1}): 2963, 2935, 1670, 1617, 1350, 1265, 1163, 964, 763; ^1H NMR (600 MHz, $CDCl_3$): δ 7.82 (d, *J* = 15.4 Hz, 1 H), 7.55 ~ 7.54 (m, 2 H), 7.41 ~ 7.39 (m, 3 H), 7.14 (d, *J* = 15.4 Hz, 1 H), 3.85 (t, 7.8 Hz, 2 H), 3.27 (s, 3 H), 1.72 ~ 1.68 (m, 2 H), 1.41 ~ 1.37 (m, 2 H), 0.96 (t, *J* = 7.4 Hz, 3 H) ; ^{13}C NMR (150 MHz, $CDCl_3$): δ 166.3, 146.9, 134.3, 130.8, 129.0, 128.4, 117.1, 46.2, 42.9, 32.3, 20.0, 13.6; ESI-MS: calcd. for $C_{14}H_{19}NO_3S$: 281.1086; Found: 304.0980 [M+Na].

4. Theoretical Calculation

Quantum-chemical simulations were performed with the density functional theory (DFT) method, as implemented in Gaussian09 program. All geometries were optimized by using the PBE1PBE density functional with SDD basis set for Au and 6-31$^+$G* for all other atoms. Harmonic vibrational frequencies were calculated with the optimized geometries to characterize the stationary points as minima.

Figure-S1

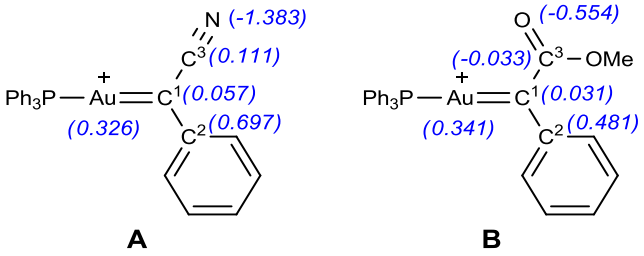


Table-S1

compound	bond distance (Å) (Au-C)	charge (Au)	charge (C^1)	charge (C^2)	charge (C^3)	charge (N)	charge (O)

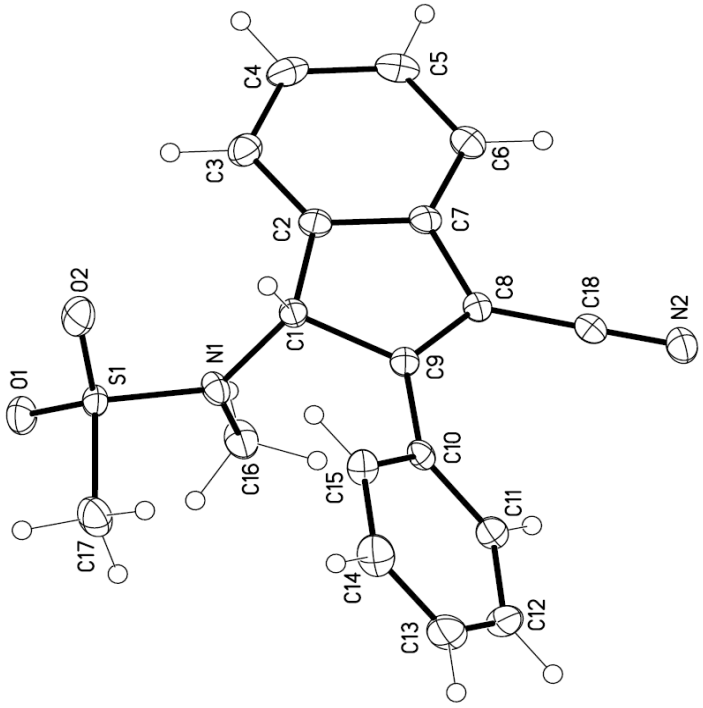
A	2.040	0.326	0.057	0.697	0.111	-1.383	---
B	2.033	0.341	0.031	0.481	-0.033	---	-0.554

References :

[5] a) C. Adamo, V. Barone, *J. Chem. Phys.* **1999**, *110*, 6158-6170. b) Q. Zhou, Y. Li, *J. Am. Chem. Soc*. **2014**, *136*, 1505-1513.

5. x-ray crystallographic structure and data

(5.1) x-ray data for compound 4a :



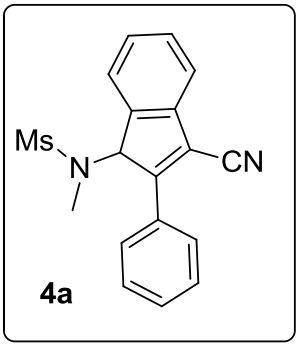


Table 1. Crystal data and structure refinement for 150722LT_a.

Identification code	150722LT_a	
Empirical formula	C18 H16 N2 O2 S	
Formula weight	324.39	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 21/c	
Unit cell dimensions	a = 8.4209(5) Å	α= 90°.

	b = 28.5775(16) Å	β= 101.544(2)°.
	c = 6.9049(4) Å	γ = 90°.
Volume	1628.04(16) Å^3	
Z	4	
Density (calculated)	1.323 Mg/m^3	
Absorption coefficient	0.210 mm^{-1}	
F(000)	680	
Crystal size	0.15 x 0.12 x 0.12 mm^3	
Theta range for data collection	1.425 to 26.408°.	
Index ranges	-9<=h<=10, -25<=k<=35, -8<=l<=6	
Reflections collected	14968	
Independent reflections	3346 [R(int) = 0.0276]	
Completeness to theta = 25.242°	99.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9485 and 0.8991	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3346 / 0 / 210	
Goodness-of-fit on F^2	1.138	
Final R indices [I>2sigma(I)]	R1 = 0.0341, wR2 = 0.0965	
R indices (all data)	R1 = 0.0405, wR2 = 0.1087	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.576 and -0.710 e.Å^{-3}	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å ^{2}x 10^3) for 150722LT_a. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	4594(2)	6188(1)	5171(2)	14(1)
C(2)	3213(2)	6538(1)	4879(2)	16(1)
C(3)	1696(2)	6514(1)	3664(2)	20(1)
C(4)	616(2)	6882(1)	3730(2)	22(1)
C(5)	1054(2)	7262(1)	4984(2)	21(1)
C(6)	2592(2)	7289(1)	6191(2)	18(1)
C(7)	3657(2)	6923(1)	6113(2)	15(1)
C(8)	5326(2)	6844(1)	7204(2)	13(1)

C(9)	5896(2)	6427(1)	6705(2)	13(1)
C(10)	7493(2)	6215(1)	7403(2)	14(1)
C(11)	8901(2)	6485(1)	7747(2)	18(1)
C(12)	10399(2)	6274(1)	8367(2)	24(1)
C(13)	10506(2)	5793(1)	8651(2)	26(1)
C(14)	9111(2)	5523(1)	8296(3)	25(1)
C(15)	7614(2)	5730(1)	7679(2)	18(1)
C(16)	5811(2)	6474(1)	2359(2)	22(1)
C(17)	6754(2)	5286(1)	2742(3)	25(1)
C(18)	6195(2)	7164(1)	8626(2)	15(1)
N(1)	5197(2)	6083(1)	3367(2)	16(1)
N(2)	6885(2)	7420(1)	9777(2)	20(1)
O(1)	4516(1)	5670(1)	160(2)	23(1)
O(2)	3758(1)	5328(1)	3143(2)	25(1)
S(1)	4891(1)	5584(1)	2248(1)	16(1)

Table 3. Bond lengths [Å] and angles [°] for 150722LT_a.

C(1)-N(1)	1.4676(18)
C(1)-C(2)	1.516(2)
C(1)-C(9)	1.525(2)
C(1)-H(1)	1.0000
C(2)-C(3)	1.383(2)
C(2)-C(7)	1.396(2)
C(3)-C(4)	1.398(2)
C(3)-H(3)	0.9500
C(4)-C(5)	1.391(2)
C(4)-H(4)	0.9500
C(5)-C(6)	1.395(2)
C(5)-H(5)	0.9500
C(6)-C(7)	1.386(2)
C(6)-H(6)	0.9500
C(7)-C(8)	1.473(2)
C(8)-C(9)	1.354(2)
C(8)-C(18)	1.431(2)

C(9)-C(10)	1.465(2)
C(10)-C(11)	1.395(2)
C(10)-C(15)	1.400(2)
C(11)-C(12)	1.387(2)
C(11)-H(11)	0.9500
C(12)-C(13)	1.388(3)
C(12)-H(12)	0.9500
C(13)-C(14)	1.386(2)
C(13)-H(13)	0.9500
C(14)-C(15)	1.381(2)
C(14)-H(14)	0.9500
C(15)-H(15)	0.9500
C(16)-N(1)	1.4646(18)
C(16)-H(16A)	0.9800
C(16)-H(16B)	0.9800
C(16)-H(16C)	0.9800
C(17)-S(1)	1.7561(16)
C(17)-H(17A)	0.9800
C(17)-H(17B)	0.9800
C(17)-H(17C)	0.9800
C(18)-N(2)	1.149(2)
N(1)-S(1)	1.6195(12)
O(1)-S(1)	1.4341(12)
O(2)-S(1)	1.4352(12)

N(1)-C(1)-C(2)	114.07(12)
N(1)-C(1)-C(9)	110.95(11)
C(2)-C(1)-C(9)	102.87(11)
N(1)-C(1)-H(1)	109.6
C(2)-C(1)-H(1)	109.6
C(9)-C(1)-H(1)	109.6
C(3)-C(2)-C(7)	120.76(14)
C(3)-C(2)-C(1)	129.69(14)
C(7)-C(2)-C(1)	109.54(13)
C(2)-C(3)-C(4)	118.09(15)
C(2)-C(3)-H(3)	121.0

C(4)-C(3)-H(3)	121.0
C(5)-C(4)-C(3)	120.98(15)
C(5)-C(4)-H(4)	119.5
C(3)-C(4)-H(4)	119.5
C(4)-C(5)-C(6)	120.91(14)
C(4)-C(5)-H(5)	119.5
C(6)-C(5)-H(5)	119.5
C(7)-C(6)-C(5)	117.73(14)
C(7)-C(6)-H(6)	121.1
C(5)-C(6)-H(6)	121.1
C(6)-C(7)-C(2)	121.52(14)
C(6)-C(7)-C(8)	130.89(14)
C(2)-C(7)-C(8)	107.58(13)
C(9)-C(8)-C(18)	125.31(14)
C(9)-C(8)-C(7)	110.86(13)
C(18)-C(8)-C(7)	123.81(13)
C(8)-C(9)-C(10)	128.97(13)
C(8)-C(9)-C(1)	109.13(12)
C(10)-C(9)-C(1)	121.88(12)
C(11)-C(10)-C(15)	119.24(14)
C(11)-C(10)-C(9)	121.31(13)
C(15)-C(10)-C(9)	119.43(13)
C(12)-C(11)-C(10)	120.06(14)
C(12)-C(11)-H(11)	120.0
C(10)-C(11)-H(11)	120.0
C(11)-C(12)-C(13)	120.29(15)
C(11)-C(12)-H(12)	119.9
C(13)-C(12)-H(12)	119.9
C(14)-C(13)-C(12)	119.86(15)
C(14)-C(13)-H(13)	120.1
C(12)-C(13)-H(13)	120.1
C(15)-C(14)-C(13)	120.31(15)
C(15)-C(14)-H(14)	119.8
C(13)-C(14)-H(14)	119.8
C(14)-C(15)-C(10)	120.24(15)
C(14)-C(15)-H(15)	119.9

C(10)-C(15)-H(15)	119.9
N(1)-C(16)-H(16A)	109.5
N(1)-C(16)-H(16B)	109.5
H(16A)-C(16)-H(16B)	109.5
N(1)-C(16)-H(16C)	109.5
H(16A)-C(16)-H(16C)	109.5
H(16B)-C(16)-H(16C)	109.5
S(1)-C(17)-H(17A)	109.5
S(1)-C(17)-H(17B)	109.5
H(17A)-C(17)-H(17B)	109.5
S(1)-C(17)-H(17C)	109.5
H(17A)-C(17)-H(17C)	109.5
H(17B)-C(17)-H(17C)	109.5
N(2)-C(18)-C(8)	179.52(16)
C(16)-N(1)-C(1)	117.56(11)
C(16)-N(1)-S(1)	118.95(10)
C(1)-N(1)-S(1)	122.40(10)
O(1)-S(1)-O(2)	119.25(7)
O(1)-S(1)-N(1)	108.04(7)
O(2)-S(1)-N(1)	107.37(7)
O(1)-S(1)-C(17)	106.68(8)
O(2)-S(1)-C(17)	108.39(8)
N(1)-S(1)-C(17)	106.47(7)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x 10^3$) for 150722LT_a. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2} U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	15(1)	14(1)	14(1)	-1(1)	4(1)	-1(1)
C(2)	16(1)	16(1)	15(1)	2(1)	5(1)	-1(1)
C(3)	18(1)	24(1)	17(1)	0(1)	4(1)	-4(1)
C(4)	13(1)	31(1)	21(1)	5(1)	2(1)	-1(1)
C(5)	18(1)	25(1)	23(1)	6(1)	8(1)	6(1)

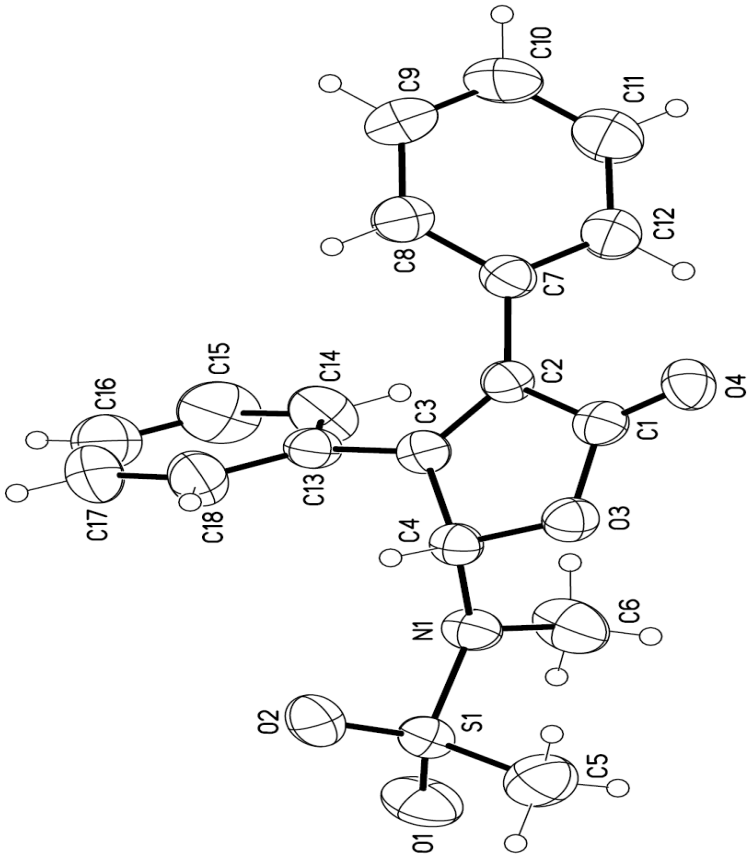
C(6)	21(1)	17(1)	17(1)	2(1)	7(1)	1(1)
C(7)	15(1)	17(1)	13(1)	2(1)	5(1)	0(1)
C(8)	16(1)	12(1)	12(1)	1(1)	4(1)	-1(1)
C(9)	16(1)	13(1)	12(1)	1(1)	4(1)	-2(1)
C(10)	17(1)	16(1)	10(1)	-1(1)	3(1)	2(1)
C(11)	19(1)	19(1)	18(1)	-2(1)	5(1)	-1(1)
C(12)	16(1)	34(1)	22(1)	-4(1)	3(1)	-2(1)
C(13)	19(1)	35(1)	23(1)	-3(1)	-1(1)	11(1)
C(14)	28(1)	20(1)	23(1)	0(1)	-1(1)	7(1)
C(15)	21(1)	16(1)	16(1)	-1(1)	1(1)	1(1)
C(16)	31(1)	18(1)	20(1)	-1(1)	11(1)	-7(1)
C(17)	27(1)	23(1)	24(1)	-6(1)	1(1)	7(1)
C(18)	18(1)	13(1)	14(1)	2(1)	6(1)	2(1)
N(1)	23(1)	12(1)	16(1)	-2(1)	8(1)	-3(1)
N(2)	24(1)	18(1)	19(1)	-4(1)	5(1)	-1(1)
O(1)	23(1)	26(1)	16(1)	-6(1)	0(1)	0(1)
O(2)	29(1)	18(1)	30(1)	-7(1)	9(1)	-10(1)
S(1)	16(1)	14(1)	16(1)	-5(1)	2(1)	-1(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å ^{2}x 10 ^{3}) for 150722LT_a.

	x	y	z	U(eq)
H(1)	4247	5891	5734	17
H(3)	1396	6254	2810	24
H(4)	-432	6873	2907	26
H(5)	295	7506	5018	26
H(6)	2899	7549	7039	22
H(11)	8834	6814	7556	22
H(12)	11356	6459	8598	29
H(13)	11533	5650	9088	32
H(14)	9186	5193	8479	29
H(15)	6663	5542	7440	22

H(16A)	4897	6658	1643	33
H(16B)	6445	6353	1424	33
H(16C)	6501	6674	3337	33
H(17A)	7065	5223	4162	38
H(17B)	7587	5480	2328	38
H(17C)	6650	4990	2011	38

(5.2) X-ray data for compound 3a':



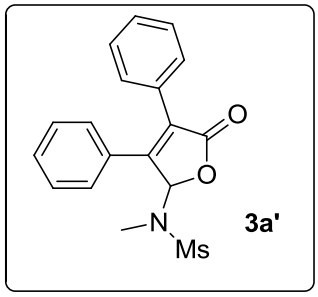


Table 1. Crystal data and structure refinement for 160104_0M_A.

Identification code	160104_0m_a
Empirical formula	C18 H17 N O4 S
Formula weight	343.38
Temperature	296(2) K
Wavelength	0.71073 Å
Crystal system	Triclinic

Space group	P -1	
Unit cell dimensions	a = 6.5556(3) Å	α= 113.781(3)°.
	b = 11.4813(6) Å	β= 98.198(3)°.
	c = 12.6356(7) Å	γ = 93.092(3)°.
Volume	854.85(8) Å^3	
Z	2	
Density (calculated)	1.334 Mg/m^3	
Absorption coefficient	0.210 mm^{-1}	
F(000)	360	
Crystal size	0.12 x 0.10 x 0.09 mm^3	
Theta range for data collection	1.790 to 26.414°.	
Index ranges	-8<=h<=6, -14<=k<=14, -15<=l<=15	
Reflections collected	12221	
Independent reflections	3495 [R(int) = 0.0363]	
Completeness to theta = 25.242°	100.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9485 and 0.9039	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3495 / 0 / 219	
Goodness-of-fit on F^2	1.126	
Final R indices [I>2sigma(I)]	R1 = 0.0454, wR2 = 0.1305	
R indices (all data)	R1 = 0.0685, wR2 = 0.1637	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.301 and -0.335 e.Å^{-3}	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å ^{2}x 10^3) for 160104_0M_A. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	2519(3)	9682(2)	4726(2)	36(1)
C(2)	2624(3)	8288(2)	4353(2)	35(1)
C(3)	3131(3)	7819(2)	3283(2)	35(1)
C(4)	3420(3)	8888(2)	2897(2)	34(1)
C(5)	2850(5)	10774(3)	1391(3)	66(1)
C(6)	-139(3)	8489(3)	1734(2)	63(1)

C(7)	2376(3)	7637(2)	5131(2)	40(1)
C(8)	3898(4)	6938(3)	5358(2)	51(1)
C(9)	3687(5)	6320(3)	6076(3)	65(1)
C(10)	1959(5)	6373(3)	6559(3)	75(1)
C(11)	418(6)	7037(4)	6335(3)	89(1)
C(12)	625(5)	7683(3)	5631(3)	69(1)
C(13)	3435(3)	6500(2)	2530(2)	38(1)
C(14)	1927(4)	5489(2)	2296(2)	55(1)
C(15)	2203(5)	4253(3)	1571(3)	71(1)
C(16)	3946(5)	4013(3)	1104(3)	66(1)
C(17)	5473(5)	5007(3)	1344(3)	66(1)
C(18)	5193(4)	6243(3)	2041(2)	53(1)
N(1)	2123(2)	8654(2)	1798(2)	38(1)
O(1)	1688(3)	8500(2)	-218(2)	65(1)
O(2)	5178(2)	8970(2)	979(2)	56(1)
O(3)	2956(2)	10011(1)	3849(1)	38(1)
O(4)	2202(2)	10478(2)	5638(1)	42(1)
S(1)	3038(1)	9142(1)	892(1)	40(1)

Table 3. Bond lengths [Å] and angles [°] for 160104_0M_A.

C(1)-O(4)	1.202(3)
C(1)-O(3)	1.367(3)
C(1)-C(2)	1.484(3)
C(2)-C(3)	1.337(3)
C(2)-C(7)	1.476(3)
C(3)-C(13)	1.471(3)
C(3)-C(4)	1.505(3)
C(4)-N(1)	1.436(3)
C(4)-O(3)	1.448(3)
C(4)-H(4)	0.9800
C(5)-S(1)	1.737(3)
C(5)-H(5A)	0.9600
C(5)-H(5B)	0.9600
C(5)-H(5C)	0.9600

C(6)-N(1)	1.472(3)
C(6)-H(6A)	0.9600
C(6)-H(6B)	0.9600
C(6)-H(6C)	0.9600
C(7)-C(12)	1.381(3)
C(7)-C(8)	1.382(3)
C(8)-C(9)	1.375(3)
C(8)-H(8)	0.9300
C(9)-C(10)	1.354(4)
C(9)-H(9)	0.9300
C(10)-C(11)	1.362(5)
C(10)-H(10)	0.9300
C(11)-C(12)	1.384(4)
C(11)-H(11)	0.9300
C(12)-H(12)	0.9300
C(13)-C(18)	1.375(3)
C(13)-C(14)	1.388(3)
C(14)-C(15)	1.383(4)
C(14)-H(14)	0.9300
C(15)-C(16)	1.351(4)
C(15)-H(15)	0.9300
C(16)-C(17)	1.381(4)
C(16)-H(16)	0.9300
C(17)-C(18)	1.374(4)
C(17)-H(17)	0.9300
C(18)-H(18)	0.9300
N(1)-S(1)	1.6305(18)
O(1)-S(1)	1.4267(18)
O(2)-S(1)	1.4225(17)

O(4)-C(1)-O(3)	121.1(2)
O(4)-C(1)-C(2)	130.1(2)
O(3)-C(1)-C(2)	108.80(19)
C(3)-C(2)-C(7)	129.1(2)
C(3)-C(2)-C(1)	108.00(19)
C(7)-C(2)-C(1)	122.73(19)

C(2)-C(3)-C(13)	129.5(2)
C(2)-C(3)-C(4)	109.37(19)
C(13)-C(3)-C(4)	121.08(19)
N(1)-C(4)-O(3)	111.61(17)
N(1)-C(4)-C(3)	113.43(17)
O(3)-C(4)-C(3)	104.63(17)
N(1)-C(4)-H(4)	109.0
O(3)-C(4)-H(4)	109.0
C(3)-C(4)-H(4)	109.0
S(1)-C(5)-H(5A)	109.5
S(1)-C(5)-H(5B)	109.5
H(5A)-C(5)-H(5B)	109.5
S(1)-C(5)-H(5C)	109.5
H(5A)-C(5)-H(5C)	109.5
H(5B)-C(5)-H(5C)	109.5
N(1)-C(6)-H(6A)	109.5
N(1)-C(6)-H(6B)	109.5
H(6A)-C(6)-H(6B)	109.5
N(1)-C(6)-H(6C)	109.5
H(6A)-C(6)-H(6C)	109.5
H(6B)-C(6)-H(6C)	109.5
C(12)-C(7)-C(8)	118.3(2)
C(12)-C(7)-C(2)	121.6(2)
C(8)-C(7)-C(2)	120.09(19)
C(9)-C(8)-C(7)	120.9(2)
C(9)-C(8)-H(8)	119.6
C(7)-C(8)-H(8)	119.6
C(10)-C(9)-C(8)	120.1(3)
C(10)-C(9)-H(9)	119.9
C(8)-C(9)-H(9)	119.9
C(9)-C(10)-C(11)	120.3(3)
C(9)-C(10)-H(10)	119.9
C(11)-C(10)-H(10)	119.9
C(10)-C(11)-C(12)	120.2(3)
C(10)-C(11)-H(11)	119.9
C(12)-C(11)-H(11)	119.9

C(7)-C(12)-C(11)	120.1(3)
C(7)-C(12)-H(12)	119.9
C(11)-C(12)-H(12)	119.9
C(18)-C(13)-C(14)	118.8(2)
C(18)-C(13)-C(3)	121.1(2)
C(14)-C(13)-C(3)	120.0(2)
C(15)-C(14)-C(13)	119.8(3)
C(15)-C(14)-H(14)	120.1
C(13)-C(14)-H(14)	120.1
C(16)-C(15)-C(14)	120.7(3)
C(16)-C(15)-H(15)	119.7
C(14)-C(15)-H(15)	119.7
C(15)-C(16)-C(17)	120.1(3)
C(15)-C(16)-H(16)	120.0
C(17)-C(16)-H(16)	120.0
C(18)-C(17)-C(16)	119.7(3)
C(18)-C(17)-H(17)	120.1
C(16)-C(17)-H(17)	120.1
C(17)-C(18)-C(13)	120.8(2)
C(17)-C(18)-H(18)	119.6
C(13)-C(18)-H(18)	119.6
C(4)-N(1)-C(6)	117.48(17)
C(4)-N(1)-S(1)	118.96(13)
C(6)-N(1)-S(1)	118.81(16)
C(1)-O(3)-C(4)	109.16(16)
O(2)-S(1)-O(1)	119.15(12)
O(2)-S(1)-N(1)	106.86(10)
O(1)-S(1)-N(1)	106.59(10)
O(2)-S(1)-C(5)	108.22(14)
O(1)-S(1)-C(5)	108.10(14)
N(1)-S(1)-C(5)	107.37(12)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for 160104_0M_A. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	28(1)	42(1)	37(1)	16(1)	1(1)	2(1)
C(2)	34(1)	37(1)	34(1)	16(1)	6(1)	5(1)
C(3)	32(1)	35(1)	36(1)	15(1)	5(1)	2(1)
C(4)	31(1)	37(1)	35(1)	16(1)	6(1)	2(1)
C(5)	91(2)	53(2)	66(2)	33(2)	21(2)	18(2)
C(6)	31(1)	106(2)	52(2)	36(2)	3(1)	-2(1)
C(7)	48(1)	38(1)	35(1)	16(1)	11(1)	8(1)
C(8)	49(1)	63(2)	53(2)	34(1)	14(1)	15(1)
C(9)	76(2)	72(2)	64(2)	45(2)	12(2)	25(2)
C(10)	105(2)	80(2)	73(2)	56(2)	39(2)	27(2)
C(11)	102(3)	111(3)	109(3)	82(3)	68(2)	47(2)
C(12)	81(2)	79(2)	86(2)	58(2)	49(2)	41(2)
C(13)	46(1)	36(1)	32(1)	15(1)	7(1)	5(1)
C(14)	64(2)	42(2)	52(2)	12(1)	18(1)	-4(1)
C(15)	97(2)	39(2)	68(2)	15(2)	14(2)	-8(2)
C(16)	104(2)	42(2)	48(2)	12(1)	19(2)	21(2)
C(17)	80(2)	63(2)	59(2)	23(2)	32(2)	30(2)
C(18)	56(1)	48(2)	58(2)	20(1)	23(1)	9(1)
N(1)	31(1)	50(1)	36(1)	21(1)	3(1)	0(1)
O(1)	73(1)	82(2)	31(1)	18(1)	0(1)	2(1)
O(2)	45(1)	75(1)	60(1)	36(1)	24(1)	16(1)
O(3)	42(1)	34(1)	39(1)	16(1)	6(1)	4(1)
O(4)	40(1)	42(1)	36(1)	8(1)	6(1)	7(1)
S(1)	43(1)	47(1)	34(1)	19(1)	10(1)	9(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for 160104_0M_A.

	x	y	z	U(eq)
H(4)	4877	9017	2828	41

H(5A)	3424	11098	891	99
H(5B)	3606	11212	2181	99
H(5C)	1418	10912	1377	99
H(6A)	-451	8139	2275	95
H(6B)	-793	7916	950	95
H(6C)	-651	9306	1937	95
H(8)	5080	6886	5020	61
H(9)	4733	5864	6230	78
H(10)	1823	5955	7045	90
H(11)	-777	7056	6657	106
H(12)	-418	8150	5495	83
H(14)	735	5643	2626	66
H(15)	1179	3580	1403	85
H(16)	4118	3178	620	79
H(17)	6685	4841	1035	79
H(18)	6206	6913	2183	64

(5.3) X-ray crystallographic structure and data for compound 7a

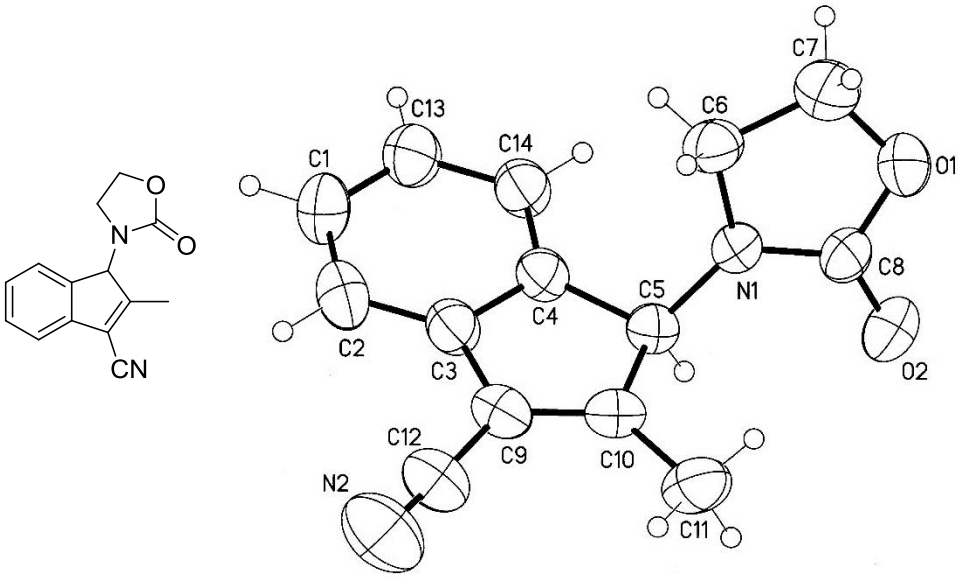


Table 1. Crystal data and structure refinement for 150830_0m.

Identification code	150830_0m

Empirical formula	C14 H12 N2 O2	
Formula weight	240.26	
Temperature	296(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P -1	
Unit cell dimensions	a = 6.0661(4) Å	α= 91.070(4)°.
	b = 7.8841(5) Å	β= 94.098(4)°.
	c = 12.8564(8) Å	γ = 97.330(3)°.
Volume	608.04(7) $Å^3$	
Z	2	
Density (calculated)	1.312 Mg/m^3	
Absorption coefficient	0.090 mm^{-1}	
F(000)	252	
Crystal size	0.20 x 0.20 x 0.15 mm^3	
Theta range for data collection	1.589 to 26.404°.	
Index ranges	-7<=h<=7, -9<=k<=8, -16<=l<=15	
Reflections collected	8386	
Independent reflections	2424 [R(int) = 0.0249]	
Completeness to theta = 25.242°	97.1 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9485 and 0.8740	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	2424 / 0 / 164	

Goodness-of-fit on F^2	1.127
Final R indices [I>2sigma(I)]	R1 = 0.0460, wR2 = 0.1350
R indices (all data)	R1 = 0.0609, wR2 = 0.1556
Extinction coefficient	n/a
Largest diff. peak and hole	0.311 and -0.307 e.$Å^{-3}$

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for 150830_0m. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
O(1)	10234(2)	7498(2)	5760(1)	61(1)
O(2)	12608(2)	5534(2)	5749(1)	64(1)
N(1)	9560(2)	5228(2)	6719(1)	44(1)
N(2)	9962(4)	1926(3)	10736(1)	90(1)
C(1)	4036(3)	56(3)	7513(2)	63(1)
C(2)	5650(3)	528(3)	8312(2)	59(1)
C(3)	7456(3)	1699(2)	8109(1)	47(1)
C(4)	7668(3)	2352(2)	7117(1)	43(1)
C(5)	9817(2)	3556(2)	7120(1)	43(1)
C(6)	7716(3)	6166(2)	6901(1)	51(1)
C(7)	8191(3)	7677(3)	6220(2)	74(1)
C(8)	10946(3)	6011(2)	6057(1)	46(1)
C(9)	9395(3)	2499(2)	8783(1)	49(1)
C(10)	10749(3)	3580(2)	8249(1)	48(1)

C(11)	12870(3)	4620(3)	8616(2)	65(1)
C(12)	9731(4)	2173(3)	9867(1)	61(1)
C(13)	4230(3)	722(2)	6535(2)	57(1)
C(14)	6050(3)	1878(2)	6325(1)	49(1)

Table 3. Bond lengths [Å] and angles [°] for 150830_0m.

O(1)-C(8)	1.353(2)
O(1)-C(7)	1.432(2)
O(2)-C(8)	1.210(2)
N(1)-C(8)	1.342(2)
N(1)-C(5)	1.447(2)
N(1)-C(6)	1.447(2)
N(2)-C(12)	1.140(2)
C(1)-C(2)	1.378(3)
C(1)-C(13)	1.378(3)
C(1)-H(1)	0.9300
C(2)-C(3)	1.383(3)
C(2)-H(9)	0.9300
C(3)-C(4)	1.393(2)
C(3)-C(9)	1.475(2)
C(4)-C(14)	1.374(2)
C(4)-C(5)	1.511(2)
C(5)-C(10)	1.519(2)

C(5)-H(10)	0.9800
C(6)-C(7)	1.503(3)
C(6)-H(11)	0.9700
C(6)-H(12)	0.9700
C(7)-H(2)	0.9700
C(7)-H(3)	0.9700
C(9)-C(10)	1.339(2)
C(9)-C(12)	1.428(2)
C(10)-C(11)	1.476(3)
C(11)-H(4)	0.9600
C(11)-H(5)	0.9600
C(11)-H(6)	0.9600
C(13)-C(14)	1.385(3)
C(13)-H(8)	0.9300
C(14)-H(7)	0.9300

C(8)-O(1)-C(7)	109.30(14)
C(8)-N(1)-C(5)	122.41(13)
C(8)-N(1)-C(6)	112.63(14)
C(5)-N(1)-C(6)	124.74(13)
C(2)-C(1)-C(13)	120.85(17)
C(2)-C(1)-H(1)	119.6
C(13)-C(1)-H(1)	119.6
C(1)-C(2)-C(3)	118.26(17)

C(1)-C(2)-H(9)	120.9
C(3)-C(2)-H(9)	120.9
C(2)-C(3)-C(4)	120.85(16)
C(2)-C(3)-C(9)	131.86(16)
C(4)-C(3)-C(9)	107.29(15)
C(14)-C(4)-C(3)	120.53(16)
C(14)-C(4)-C(5)	130.31(14)
C(3)-C(4)-C(5)	109.16(14)
N(1)-C(5)-C(4)	114.38(12)
N(1)-C(5)-C(10)	114.31(13)
C(4)-C(5)-C(10)	103.30(13)
N(1)-C(5)-H(10)	108.2
C(4)-C(5)-H(10)	108.2
C(10)-C(5)-H(10)	108.2
N(1)-C(6)-C(7)	101.34(14)
N(1)-C(6)-H(11)	111.5
C(7)-C(6)-H(11)	111.5
N(1)-C(6)-H(12)	111.5
C(7)-C(6)-H(12)	111.5
H(11)-C(6)-H(12)	109.3
O(1)-C(7)-C(6)	106.88(15)
O(1)-C(7)-H(2)	110.3
C(6)-C(7)-H(2)	110.3
O(1)-C(7)-H(3)	110.3

C(6)-C(7)-H(3)	110.3
H(2)-C(7)-H(3)	108.6
O(2)-C(8)-N(1)	127.86(17)
O(2)-C(8)-O(1)	122.39(16)
N(1)-C(8)-O(1)	109.75(15)
C(10)-C(9)-C(12)	125.14(17)
C(10)-C(9)-C(3)	111.27(15)
C(12)-C(9)-C(3)	123.58(17)
C(9)-C(10)-C(11)	129.00(17)
C(9)-C(10)-C(5)	108.91(14)
C(11)-C(10)-C(5)	122.05(16)
C(10)-C(11)-H(4)	109.5
C(10)-C(11)-H(5)	109.5
H(4)-C(11)-H(5)	109.5
C(10)-C(11)-H(6)	109.5
H(4)-C(11)-H(6)	109.5
H(5)-C(11)-H(6)	109.5
N(2)-C(12)-C(9)	178.7(2)
C(1)-C(13)-C(14)	121.10(18)
C(1)-C(13)-H(8)	119.5
C(14)-C(13)-H(8)	119.5
C(4)-C(14)-C(13)	118.39(16)
C(4)-C(14)-H(7)	120.8
C(13)-C(14)-H(7)	120.8

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x 10^3$) for 150830_0m. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2} U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
O(1)	54(1)	49(1)	77(1)	18(1)	1(1)	-5(1)
O(2)	43(1)	77(1)	73(1)	13(1)	16(1)	2(1)
N(1)	35(1)	45(1)	54(1)	10(1)	6(1)	7(1)
N(2)	127(2)	91(2)	52(1)	9(1)	-5(1)	21(1)
C(1)	59(1)	53(1)	76(1)	10(1)	11(1)	-8(1)
C(2)	68(1)	54(1)	56(1)	14(1)	14(1)	2(1)
C(3)	51(1)	43(1)	48(1)	8(1)	7(1)	10(1)
C(4)	45(1)	38(1)	47(1)	5(1)	5(1)	8(1)
C(5)	40(1)	44(1)	47(1)	7(1)	5(1)	10(1)
C(6)	43(1)	50(1)	63(1)	2(1)	3(1)	12(1)
C(7)	59(1)	60(1)	105(2)	21(1)	5(1)	15(1)
C(8)	36(1)	49(1)	51(1)	5(1)	-3(1)	-5(1)
C(9)	56(1)	49(1)	45(1)	6(1)	1(1)	15(1)
C(10)	42(1)	51(1)	51(1)	4(1)	-2(1)	14(1)
C(11)	48(1)	74(1)	72(1)	3(1)	-10(1)	8(1)
C(12)	77(1)	58(1)	50(1)	6(1)	-2(1)	15(1)
C(13)	55(1)	49(1)	65(1)	4(1)	-2(1)	-2(1)

C(14)	53(1)	45(1)	49(1)	5(1)	1(1)	4(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å ^{2}x 10 ^{3}) for 150830_0m.

	x	y	z	U(eq)
H(1)	2801	-722	7635	76
H(9)	5527	70	8970	71
H(10)	10831	3030	6690	52
H(11)	7729	6517	7629	62
H(12)	6296	5498	6687	62
H(2)	6989	7694	5682	88
H(3)	8338	8734	6632	88
H(4)	13094	4557	9360	98
H(5)	12818	5788	8430	98
H(6)	14078	4190	8296	98
H(8)	3119	390	6008	69
H(7)	6175	2324	5664	59

(5.4) x-ray crystallographic structure and data for compound 6d

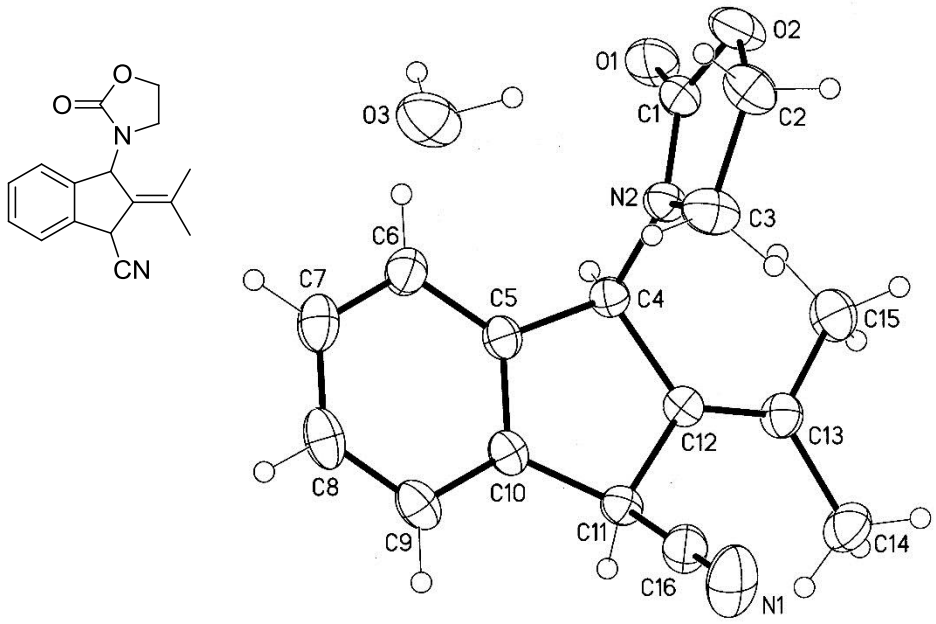


Table 1. Crystal data and structure refinement for 151232_0M_A.

Identification code	151232_0m_a	
Empirical formula	C16 H16 N2 O2	
Formula weight	268.31	
Temperature	296(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P -1	
Unit cell dimensions	a = 9.2837(4) Å	α= 92.401(2)°.
	b = 9.9699(4) Å	β= 112.162(2)°.
	c = 9.9836(4) Å	γ = 116.147(2)°.
Volume	743.75(6) $Å^3$	
Z	2	
Density (calculated)	1.198 Mg/m^3	

Absorption coefficient	0.080 mm^{-1}
F(000)	284
Crystal size	0.20 x 0.20 x 0.15 mm^3
Theta range for data collection	2.275 to 26.382°.
Index ranges	-11<=h<=11, -12<=k<=12, -12<=l<=12
Reflections collected	11208
Independent reflections	3018 [R(int) = 0.0236]
Completeness to theta = 25.242°	99.4 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9485 and 0.8826
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3018 / 0 / 192
Goodness-of-fit on F^2	1.091
Final R indices [I>2sigma(I)]	R1 = 0.0490, wR2 = 0.1503
R indices (all data)	R1 = 0.0601, wR2 = 0.1634
Extinction coefficient	n/a
Largest diff. peak and hole	0.387 and -0.399 e.$Å^{-3}$

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for 151232_0M_A. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	3032(2)	7820(2)	7170(2)	46(1)

C(2)	3556(3)	7759(2)	9580(2)	63(1)
C(3)	4588(3)	7131(3)	9176(2)	60(1)
C(4)	4656(2)	6618(2)	6668(2)	36(1)
C(5)	3994(2)	4911(2)	6471(2)	39(1)
C(6)	2230(2)	3734(2)	5908(2)	50(1)
C(7)	1892(3)	2244(2)	5865(2)	58(1)
C(8)	3278(3)	1913(2)	6363(2)	60(1)
C(9)	5031(3)	3072(2)	6900(2)	51(1)
C(10)	5379(2)	4586(2)	6960(2)	40(1)
C(11)	7175(2)	6055(2)	7541(2)	40(1)
C(12)	6688(2)	7332(2)	7301(2)	37(1)
C(13)	7835(2)	8812(2)	7513(2)	44(1)
C(14)	9812(2)	9415(2)	8102(2)	58(1)
C(15)	7234(3)	9986(2)	7156(2)	59(1)
C(16)	8267(2)	6224(2)	9119(2)	54(1)
N(1)	9080(3)	6330(2)	10334(2)	88(1)
N(2)	4078(2)	7177(1)	7629(1)	40(1)
O(1)	2409(2)	8037(2)	5946(2)	64(1)
O(2)	2783(2)	8278(2)	8316(2)	68(1)
O(3)	856(2)	5703(2)	3191(2)	85(1)

Table 3. Bond lengths [Å] and angles [°] for 151232_0M_A.

C(1)-O(1)	1.214(2)
C(1)-N(2)	1.342(2)
C(1)-O(2)	1.350(2)
C(2)-O(2)	1.440(3)
C(2)-C(3)	1.508(3)
C(2)-H(2A)	0.9700
C(2)-H(2B)	0.9700
C(3)-N(2)	1.444(2)
C(3)-H(3A)	0.9700
C(3)-H(3B)	0.9700
C(4)-N(2)	1.4582(19)
C(4)-C(5)	1.507(2)
C(4)-C(12)	1.531(2)
C(4)-H(4)	0.9800
C(5)-C(10)	1.379(2)
C(5)-C(6)	1.390(2)
C(6)-C(7)	1.372(3)
C(6)-H(6)	0.9300
C(7)-C(8)	1.385(3)
C(7)-H(7)	0.9300
C(8)-C(9)	1.380(3)
C(8)-H(8)	0.9300

C(9)-C(10)	1.391(2)
C(9)-H(9)	0.9300
C(10)-C(11)	1.519(2)
C(11)-C(16)	1.469(2)
C(11)-C(12)	1.528(2)
C(11)-H(11)	0.9800
C(12)-C(13)	1.332(2)
C(13)-C(14)	1.503(2)
C(13)-C(15)	1.506(2)
C(14)-H(14A)	0.9600
C(14)-H(14B)	0.9600
C(14)-H(14C)	0.9600
C(15)-H(15A)	0.9600
C(15)-H(15B)	0.9600
C(15)-H(15C)	0.9600
C(16)-N(1)	1.132(2)
O(3)-H(3C)	1.0601
O(3)-H(3D)	1.0006
O(1)-C(1)-N(2)	128.19(16)
O(1)-C(1)-O(2)	122.08(15)
N(2)-C(1)-O(2)	109.70(14)
O(2)-C(2)-C(3)	105.95(15)
O(2)-C(2)-H(2A)	110.5
C(3)-C(2)-H(2A)	110.5

O(2)-C(2)-H(2B)	110.5
C(3)-C(2)-H(2B)	110.5
H(2A)-C(2)-H(2B)	108.7
N(2)-C(3)-C(2)	101.57(15)
N(2)-C(3)-H(3A)	111.5
C(2)-C(3)-H(3A)	111.5
N(2)-C(3)-H(3B)	111.5
C(2)-C(3)-H(3B)	111.5
H(3A)-C(3)-H(3B)	109.3
N(2)-C(4)-C(5)	111.43(11)
N(2)-C(4)-C(12)	113.83(11)
C(5)-C(4)-C(12)	103.80(12)
N(2)-C(4)-H(4)	109.2
C(5)-C(4)-H(4)	109.2
C(12)-C(4)-H(4)	109.2
C(10)-C(5)-C(6)	120.71(15)
C(10)-C(5)-C(4)	112.09(13)
C(6)-C(5)-C(4)	127.18(14)
C(7)-C(6)-C(5)	118.71(17)
C(7)-C(6)-H(6)	120.6
C(5)-C(6)-H(6)	120.6
C(6)-C(7)-C(8)	120.79(17)
C(6)-C(7)-H(7)	119.6
C(8)-C(7)-H(7)	119.6

C(9)-C(8)-C(7)	120.82(16)
C(9)-C(8)-H(8)	119.6
C(7)-C(8)-H(8)	119.6
C(8)-C(9)-C(10)	118.52(17)
C(8)-C(9)-H(9)	120.7
C(10)-C(9)-H(9)	120.7
C(5)-C(10)-C(9)	120.44(15)
C(5)-C(10)-C(11)	111.01(13)
C(9)-C(10)-C(11)	128.54(15)
C(16)-C(11)-C(10)	109.92(13)
C(16)-C(11)-C(12)	113.04(13)
C(10)-C(11)-C(12)	103.98(12)
C(16)-C(11)-H(11)	109.9
C(10)-C(11)-H(11)	109.9
C(12)-C(11)-H(11)	109.9
C(13)-C(12)-C(11)	125.41(14)
C(13)-C(12)-C(4)	125.42(14)
C(11)-C(12)-C(4)	109.02(11)
C(12)-C(13)-C(14)	122.19(15)
C(12)-C(13)-C(15)	122.26(15)
C(14)-C(13)-C(15)	115.54(15)
C(13)-C(14)-H(14A)	109.5
C(13)-C(14)-H(14B)	109.5
H(14A)-C(14)-H(14B)	109.5

C(13)-C(14)-H(14C)	109.5
H(14A)-C(14)-H(14C)	109.5
H(14B)-C(14)-H(14C)	109.5
C(13)-C(15)-H(15A)	109.5
C(13)-C(15)-H(15B)	109.5
H(15A)-C(15)-H(15B)	109.5
C(13)-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(11)	178.6(2)
C(1)-N(2)-C(3)	112.63(14)
C(1)-N(2)-C(4)	123.22(13)
C(3)-N(2)-C(4)	124.14(13)
C(1)-O(2)-C(2)	109.41(13)
H(3C)-O(3)-H(3D)	104.7

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x 10^3$) for 151232_0M_A. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2} U^{11} + ... + 2 h k a^* b^* U^{12}]$

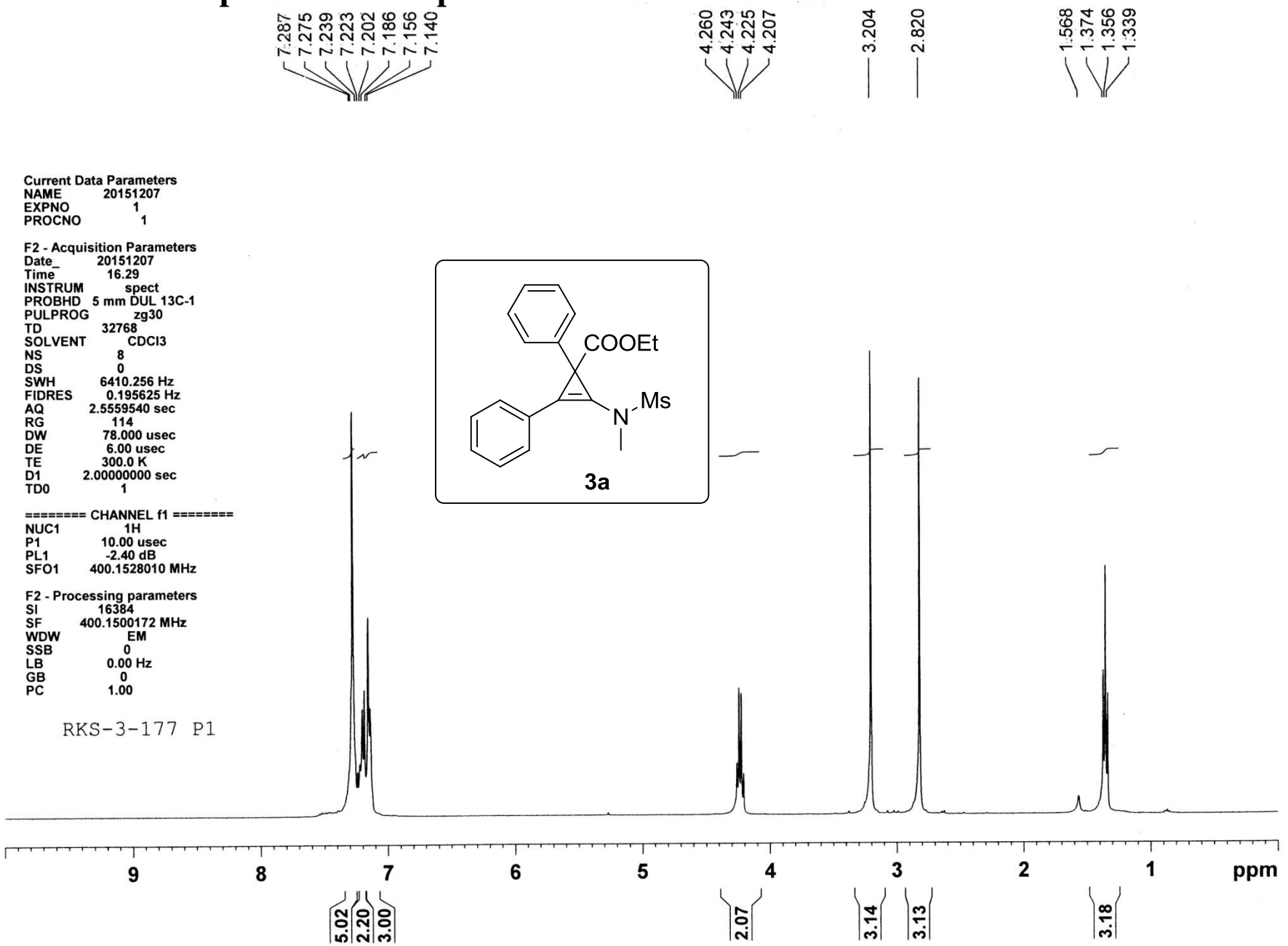
	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	45(1)	38(1)	54(1)	8(1)	17(1)	24(1)
C(2)	80(1)	66(1)	63(1)	16(1)	40(1)	43(1)

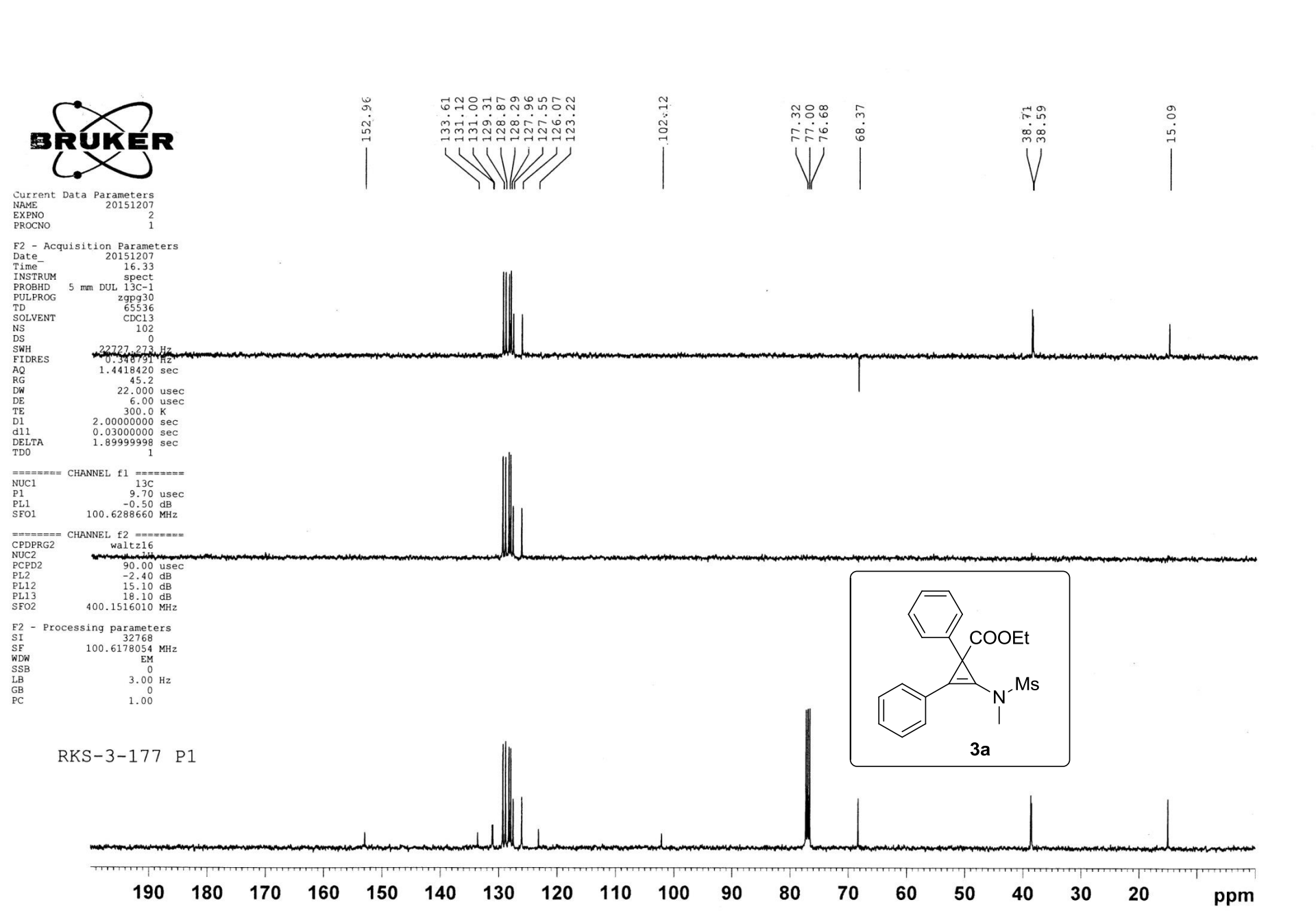
C(3)	72(1)	85(1)	47(1)	23(1)	31(1)	53(1)
C(4)	38(1)	36(1)	36(1)	11(1)	16(1)	20(1)
C(5)	44(1)	36(1)	36(1)	9(1)	19(1)	19(1)
C(6)	44(1)	45(1)	50(1)	8(1)	19(1)	16(1)
C(7)	59(1)	40(1)	60(1)	8(1)	28(1)	10(1)
C(8)	83(1)	32(1)	57(1)	12(1)	32(1)	22(1)
C(9)	70(1)	45(1)	46(1)	14(1)	25(1)	35(1)
C(10)	50(1)	37(1)	34(1)	10(1)	19(1)	22(1)
C(11)	42(1)	41(1)	40(1)	11(1)	18(1)	24(1)
C(12)	40(1)	37(1)	37(1)	12(1)	18(1)	20(1)
C(13)	44(1)	41(1)	45(1)	13(1)	22(1)	18(1)
C(14)	44(1)	56(1)	66(1)	12(1)	27(1)	15(1)
C(15)	63(1)	41(1)	72(1)	20(1)	30(1)	24(1)
C(16)	53(1)	46(1)	53(1)	13(1)	11(1)	27(1)
N(1)	91(1)	69(1)	57(1)	16(1)	-6(1)	33(1)
N(2)	42(1)	42(1)	42(1)	12(1)	18(1)	25(1)
O(1)	69(1)	65(1)	64(1)	21(1)	17(1)	48(1)
O(2)	80(1)	77(1)	74(1)	15(1)	37(1)	57(1)
O(3)	101(1)	105(1)	66(1)	22(1)	24(1)	76(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å ^{2}x 10^3) for 151232_0M_A.

	x	y	z	U(eq)
H(2A)	2628	6961	9768	76
H(2B)	4345	8609	10468	76
H(3A)	5867	7778	9779	72
H(3B)	4231	6085	9286	72
H(4)	4195	6823	5688	44
H(6)	1296	3953	5566	59
H(7)	718	1446	5498	70
H(8)	3024	897	6334	72
H(9)	5959	2846	7215	61
H(11)	7799	6022	6948	48
H(14A)	10051	8572	8201	88
H(14B)	10427	10131	9060	88
H(14C)	10220	9930	7420	88
H(15A)	5961	9466	6567	88
H(15B)	7808	10599	6606	88
H(15C)	7551	10642	8068	88
H(3C)	1433	6624	4130	80
H(3D)	221	6021	2323	80

^{1}H and ^{13}C NMR spectras of compounds

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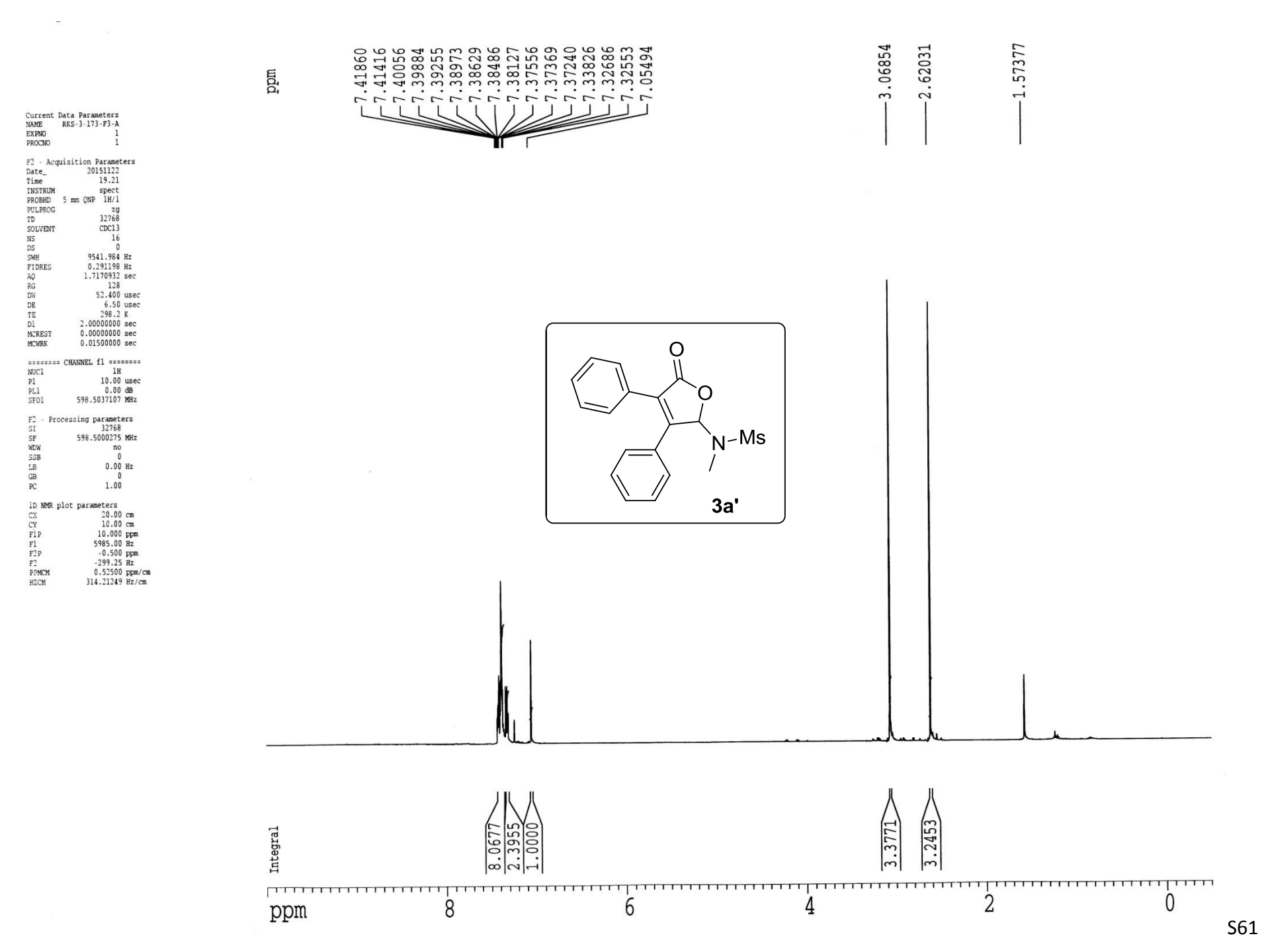
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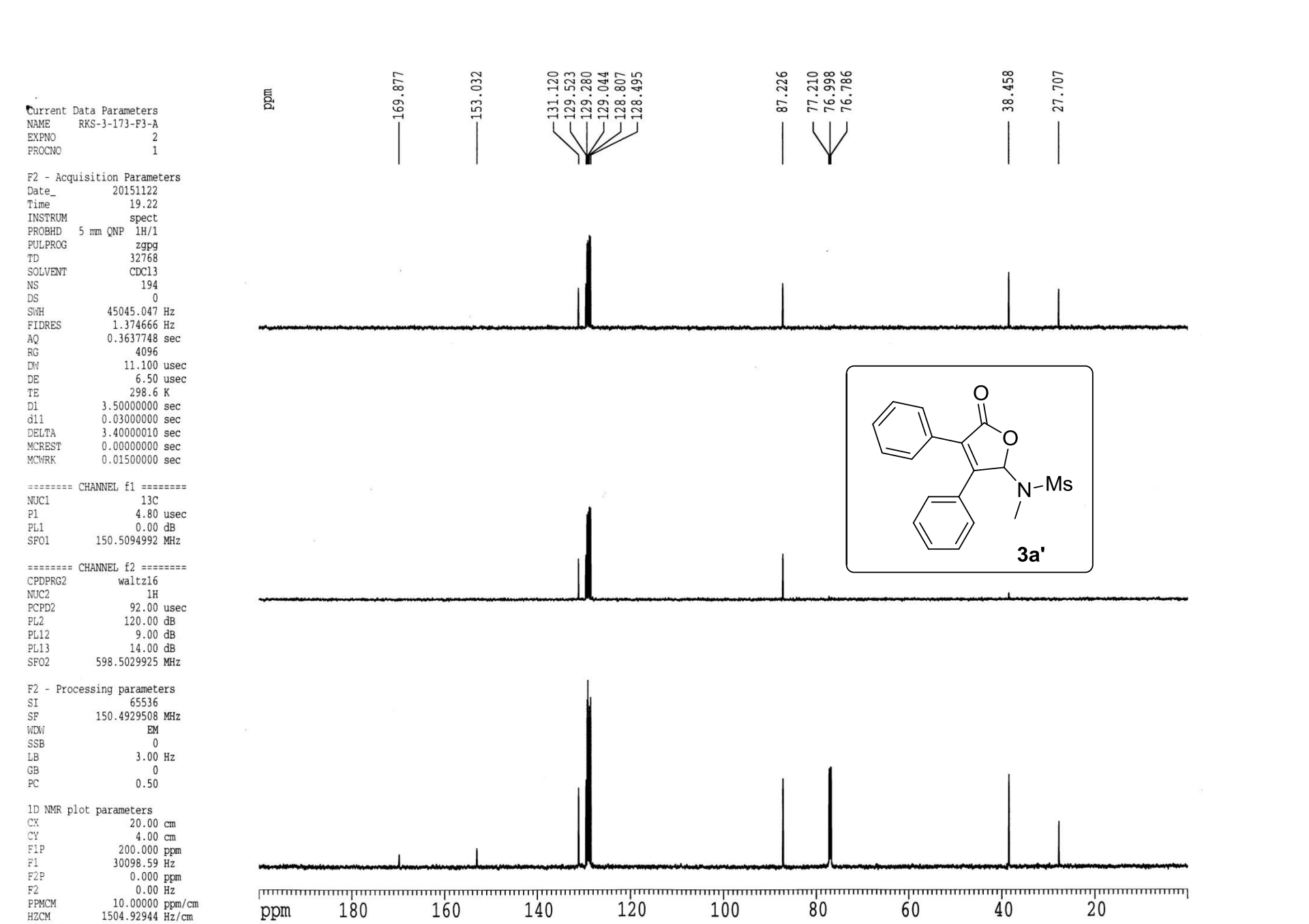
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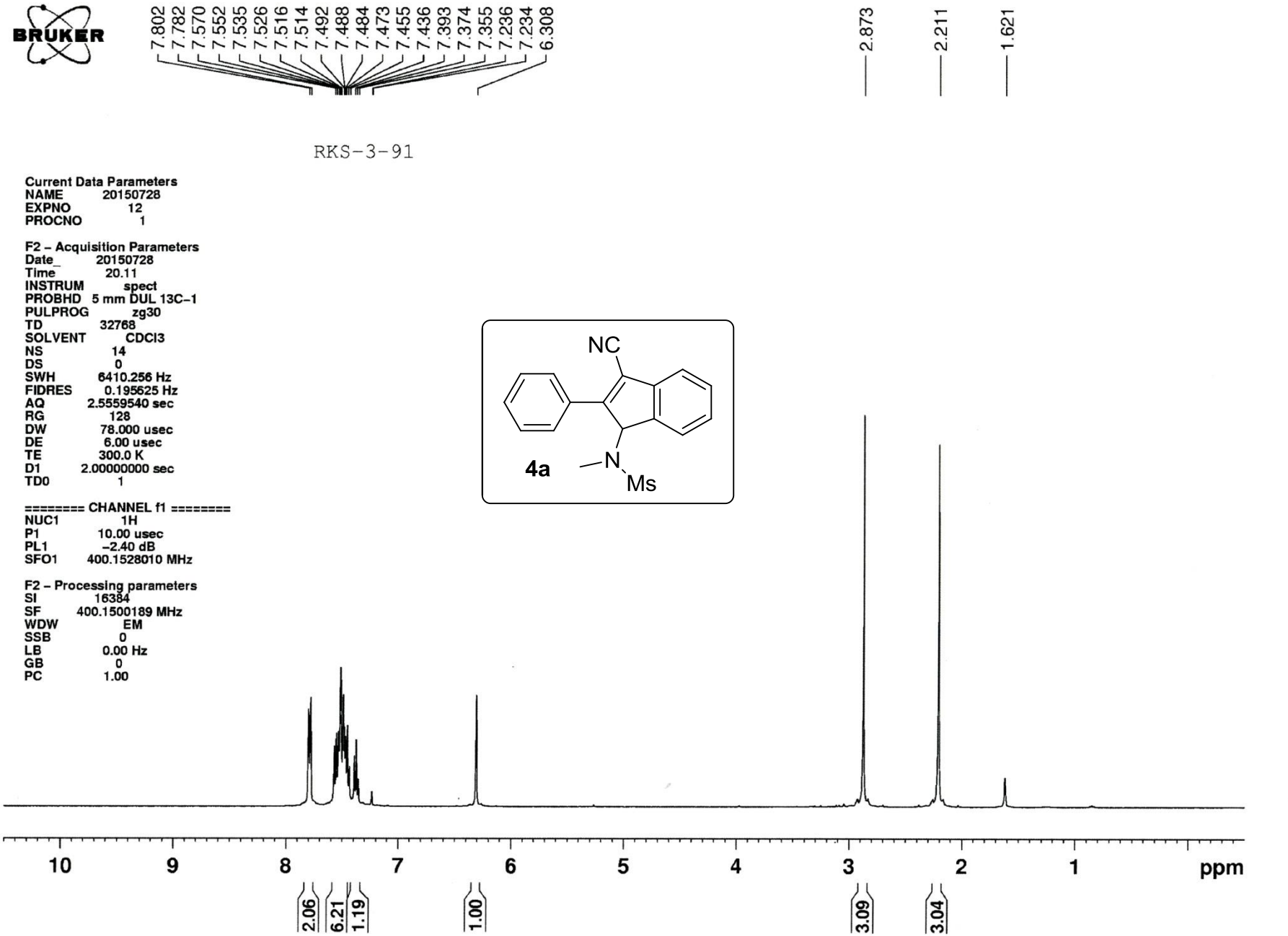
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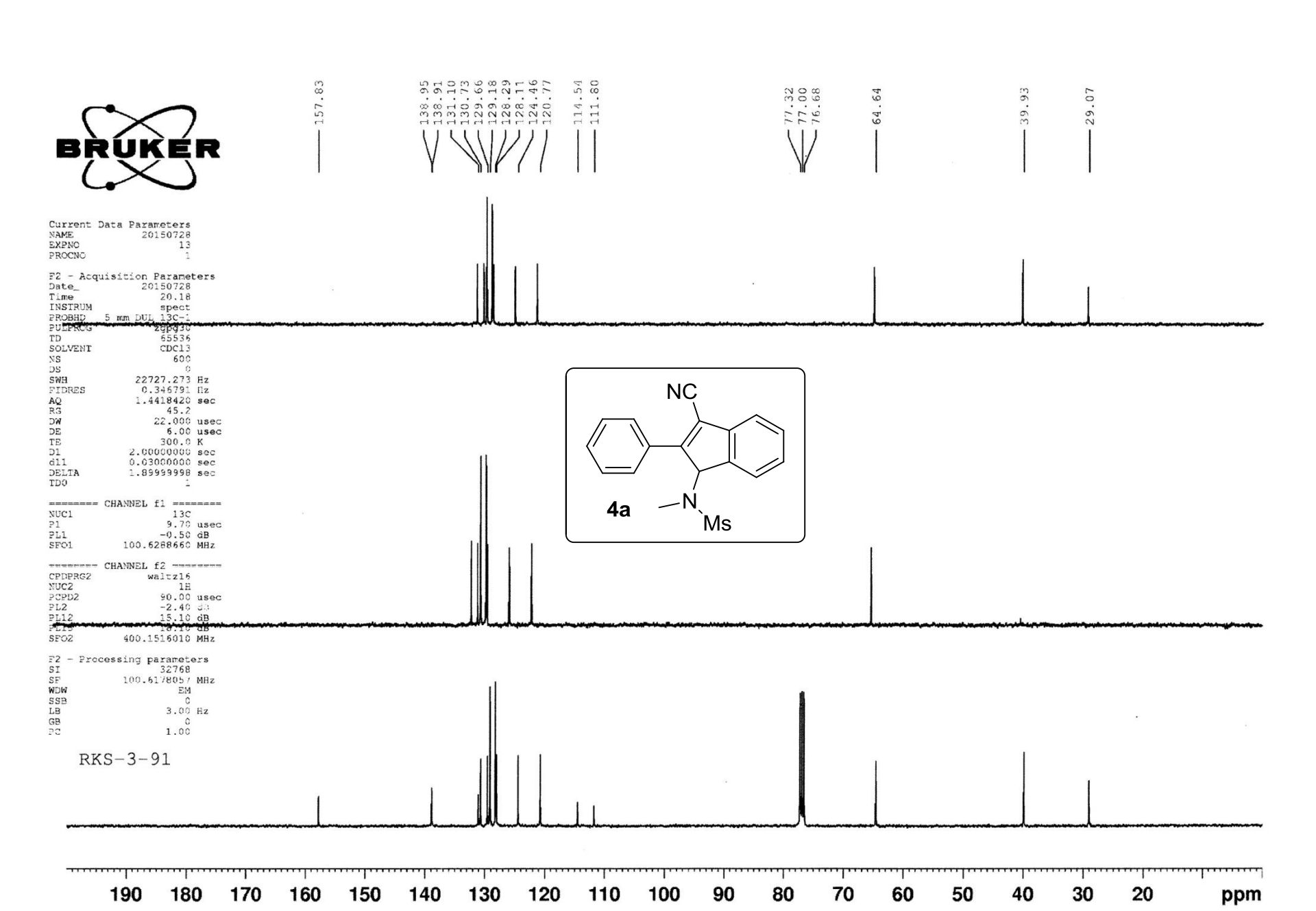
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RG 45.2
DW 22.000 usec
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TE 300.0 K
D1 2.00000000 sec
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DELTA 1.89999998 sec
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NUC2 1H
PCPD2 90.00 usec
PL2 -2.40 dB
PL12 15.10 dB
PL13 28.10 dB
SFO2 400.1516010 MHz
F2 - Processing parameters
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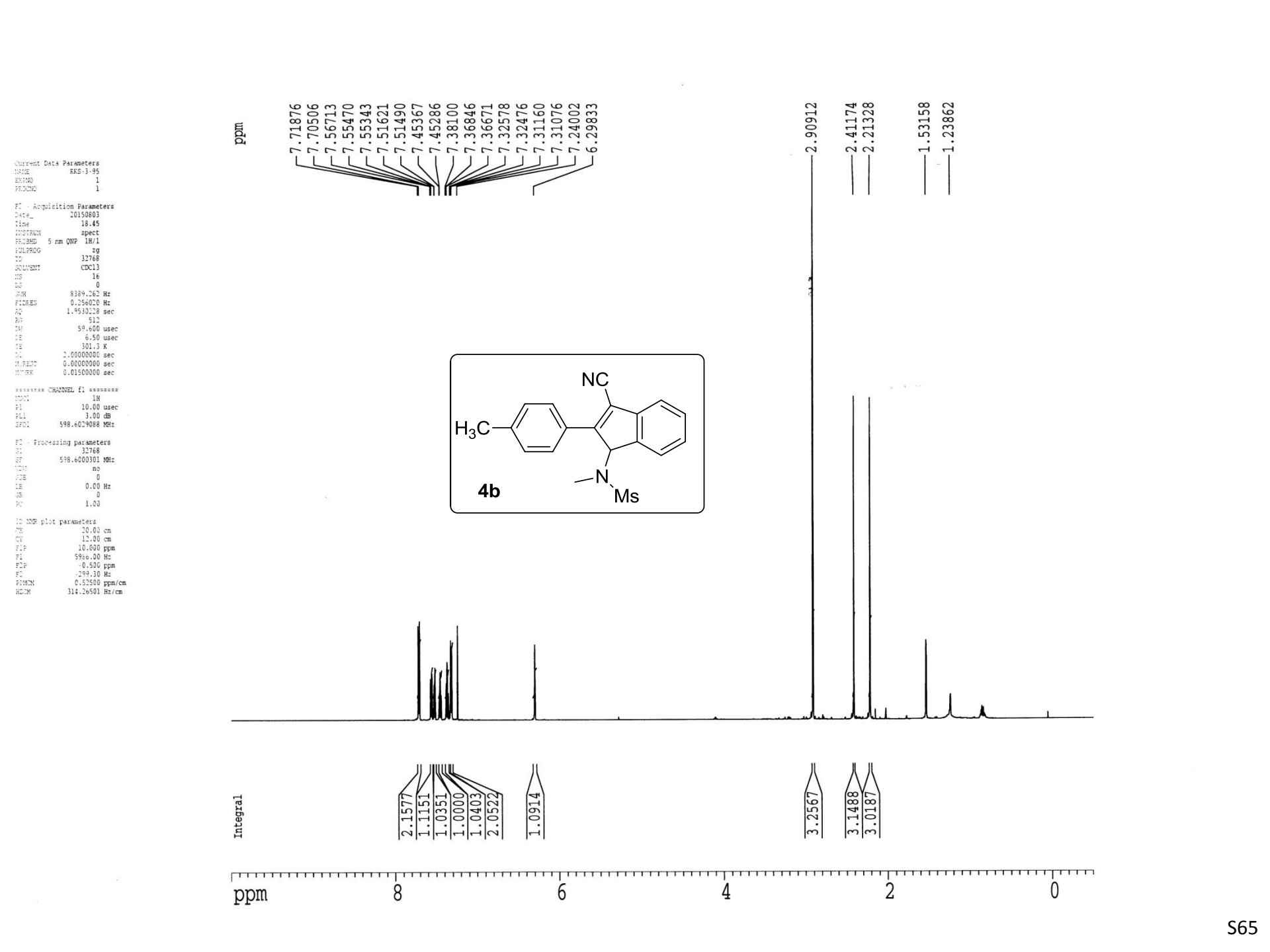
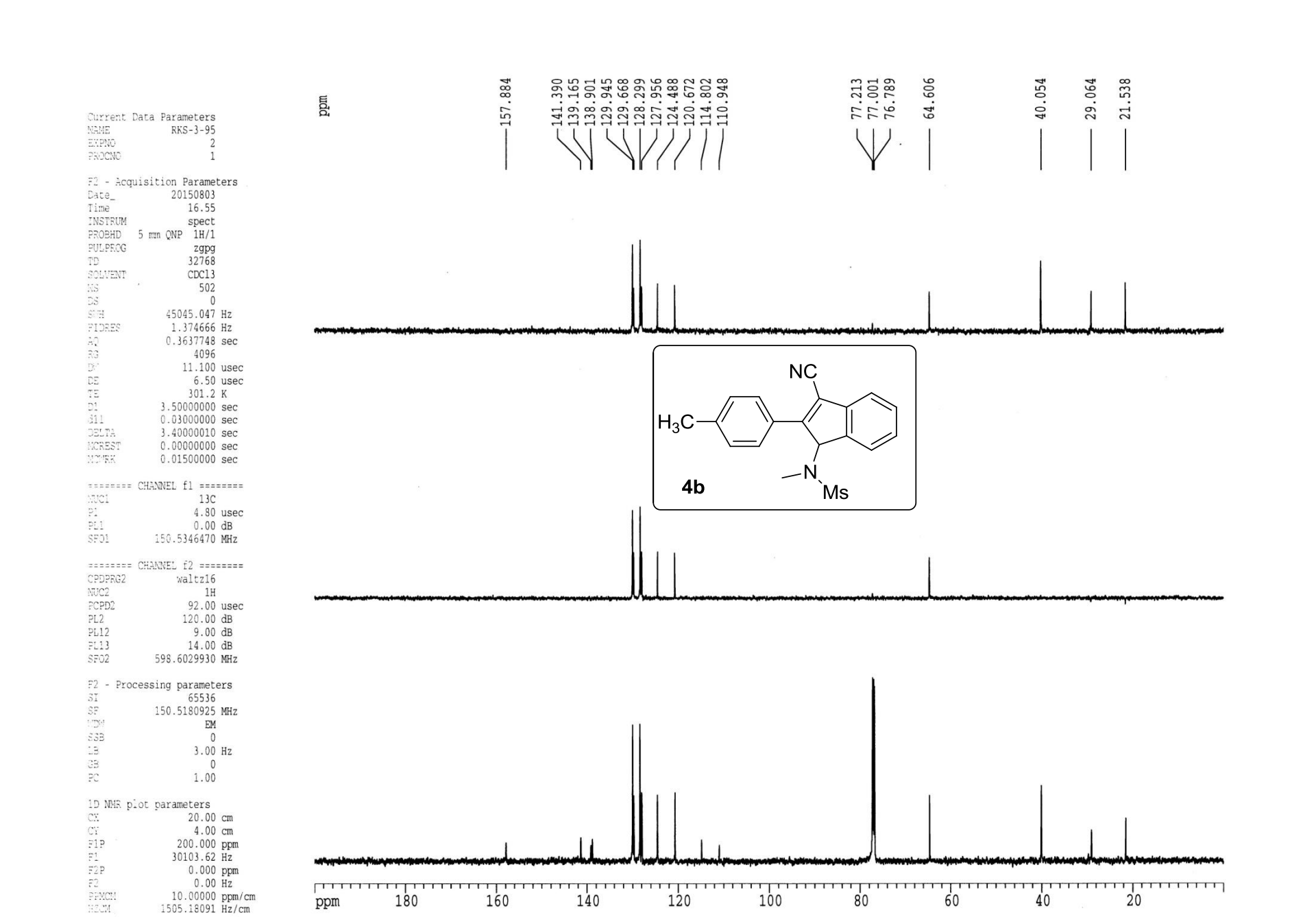
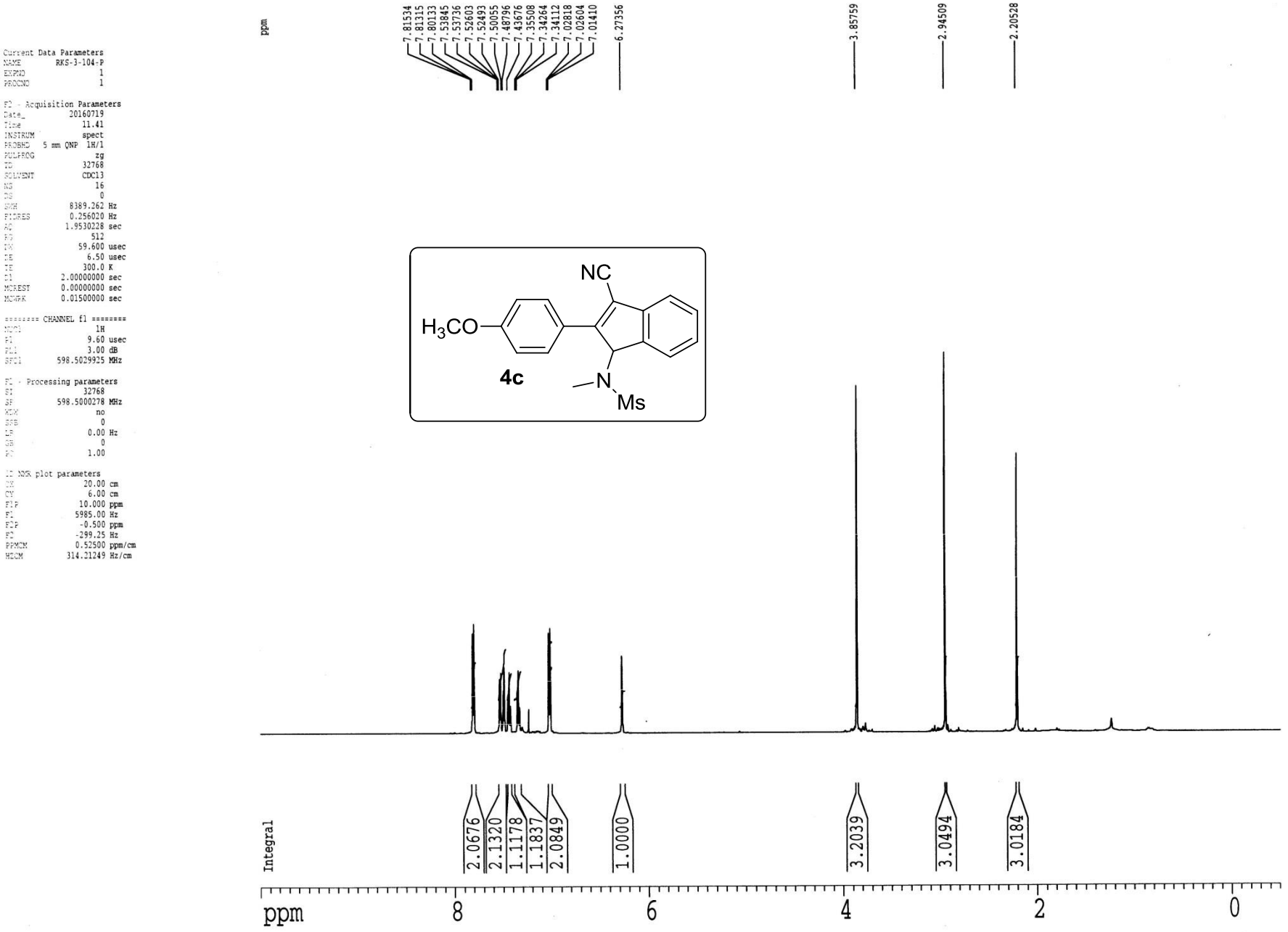
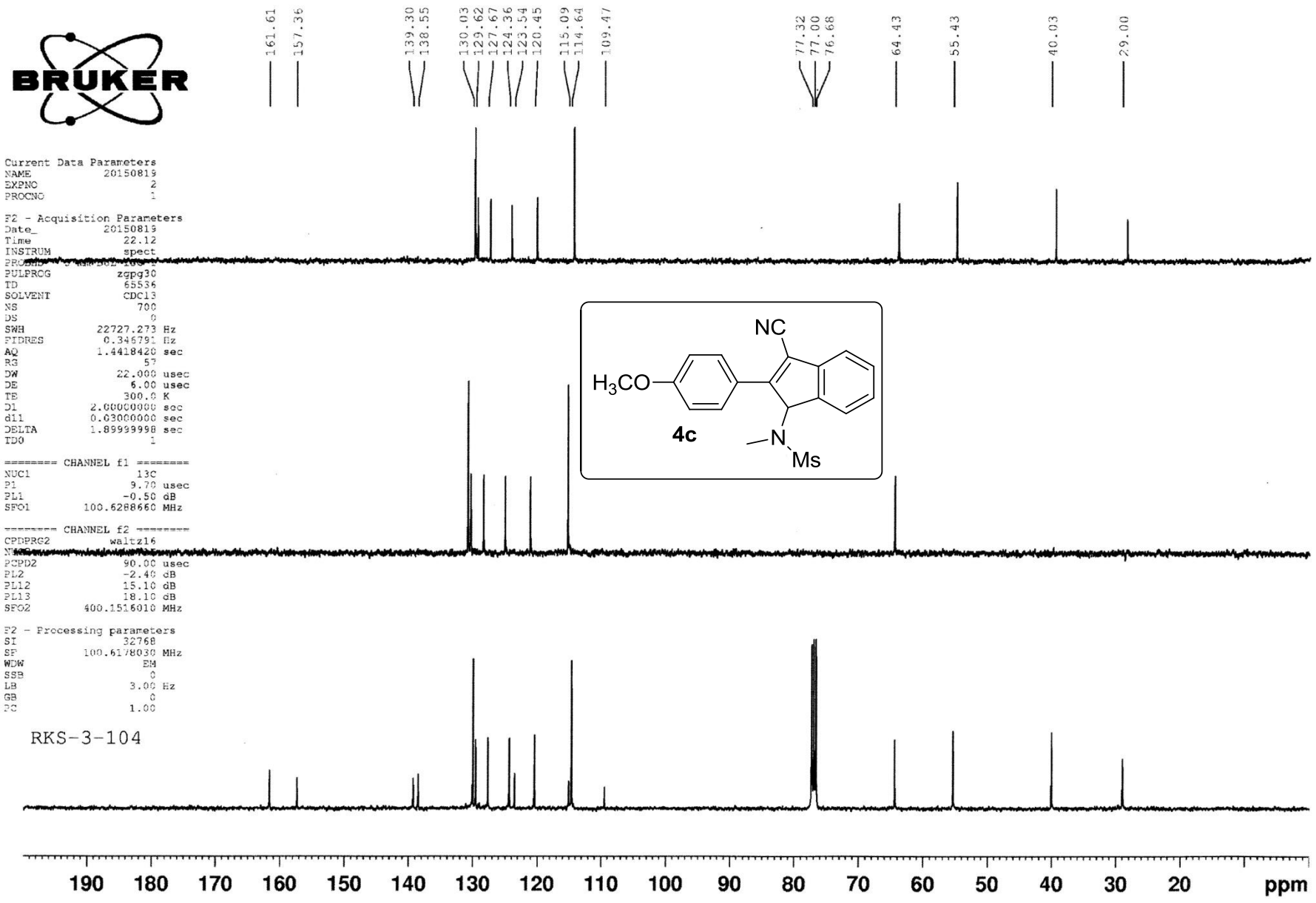
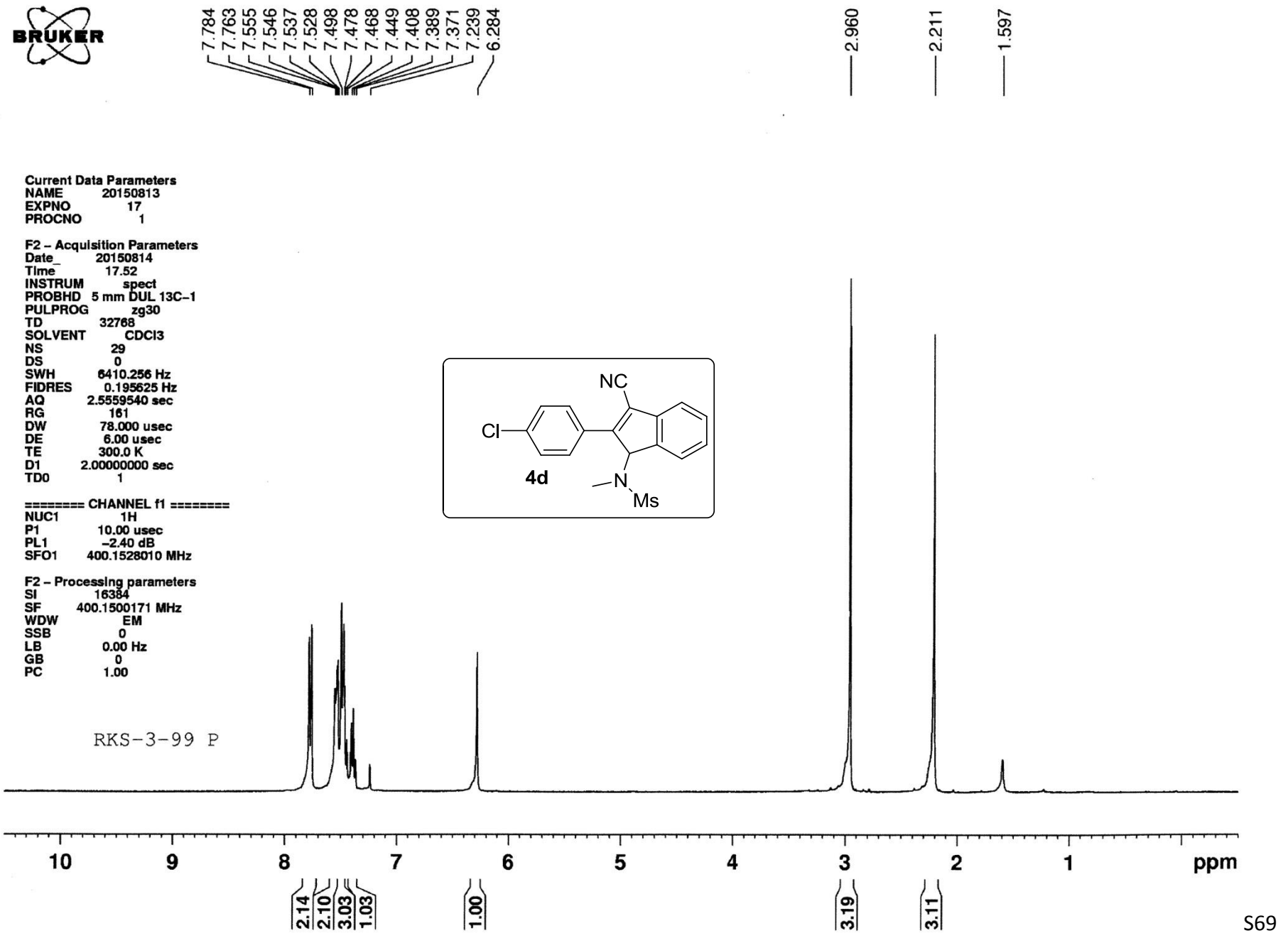
RKS-3-91
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

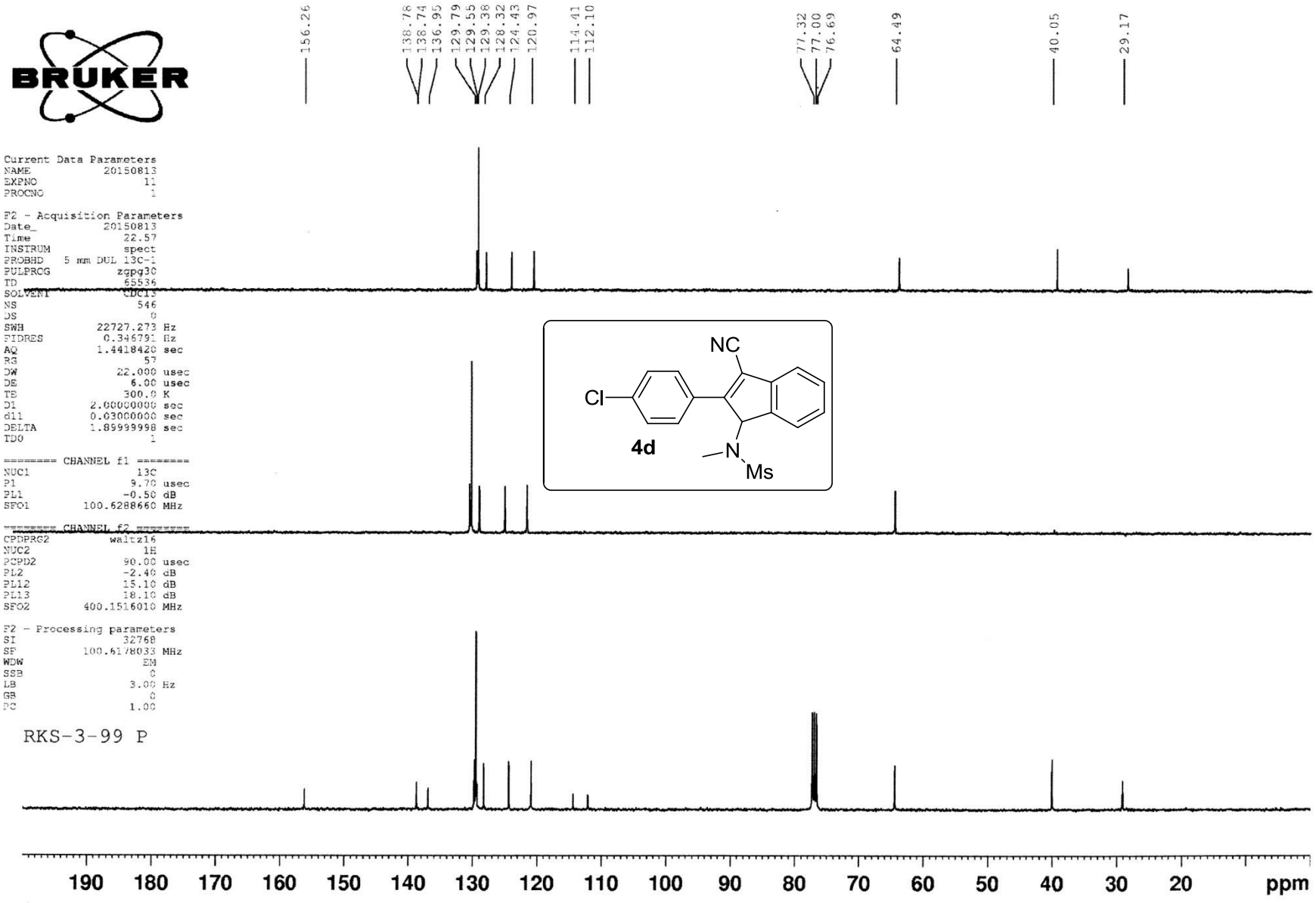

Current Data Parameters
NAME RKS-3-95
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20150803
Time 18.45
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 8389.262 Hz
FIDRES 0.256020 Hz
AQ 1.9530128 sec
RG 512
DW 59.600 usec
DE 6.50 usec
TE 301.3 K
D1 2.00000000 sec
D11PLRDT 0.00000000 sec
D11PLRW 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 3.00 dB
SFO1 598.6029088 MHz
F2 - Processing parameters
SI 32768
SF 598.6000301 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 5986.00 Hz
F2P -0.500 ppm
F2 -299.30 Hz
PPMCM 0.52500 ppm/cm
HZCM 314.26501 Hz/cm
ppm
7.71876
7.70506
7.56713
7.55470
7.55343
7.51621
7.51490
7.45367
7.45286
7.38100
7.36846
7.36671
7.32578
7.32476
7.31160
7.31076
7.24002
6.29833
2.90912
2.41174
2.21328
1.53158
1.23862
NC
H3C
N
Ms
4b
Integral
2.1577
1.1151
1.0351
1.0000
1.0403
2.0522
1.0914
3.2567
3.1488
3.0187
ppm
8
6
4
2
0

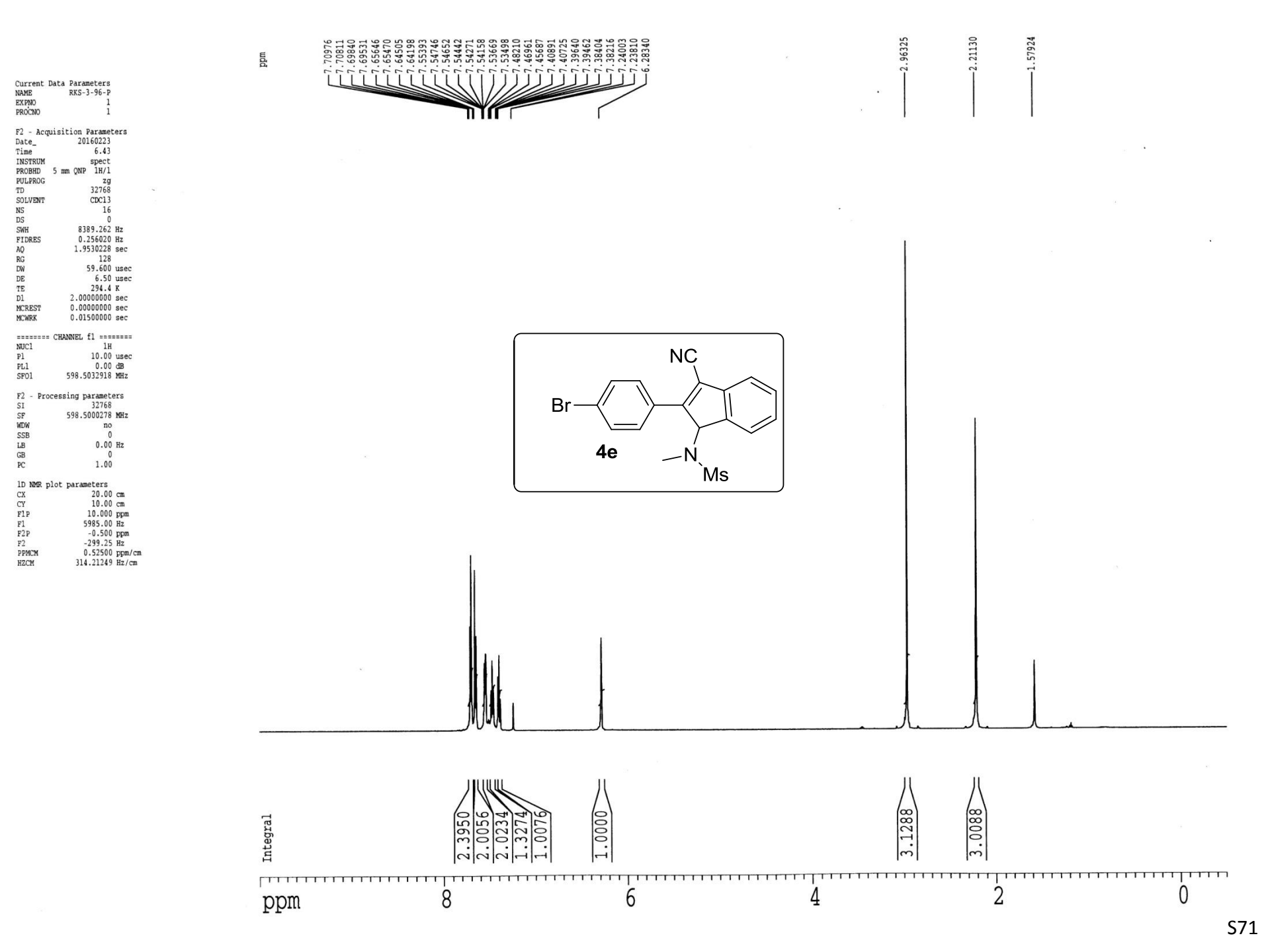

Current Data Parameters
NAME RKS-3-95
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20150803
Time 16.55
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 502
DS 0
SWH 45045.047 Hz
FIDRES 1.374666 Hz
AQ 0.3637748 sec
RG 4096
DW 11.100 usec
DE 6.50 usec
TE 301.2 K
D1 3.50000000 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 150.5346470 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 150.5180925 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 30103.62 Hz
F2P 0.000 ppm
F2 0.00 Hz
PPMCM 10.00000 ppm/cm
HZCM 1505.18091 Hz/cm
ppm
157.884
141.390
139.165
138.901
129.945
129.668
128.299
127.956
124.488
120.672
114.802
110.948
77.213
77.001
76.789
64.606
40.054
29.064
21.538
NC
H3C
N
Ms
4b
ppm
180
160
140
120
100
80
60
40
20

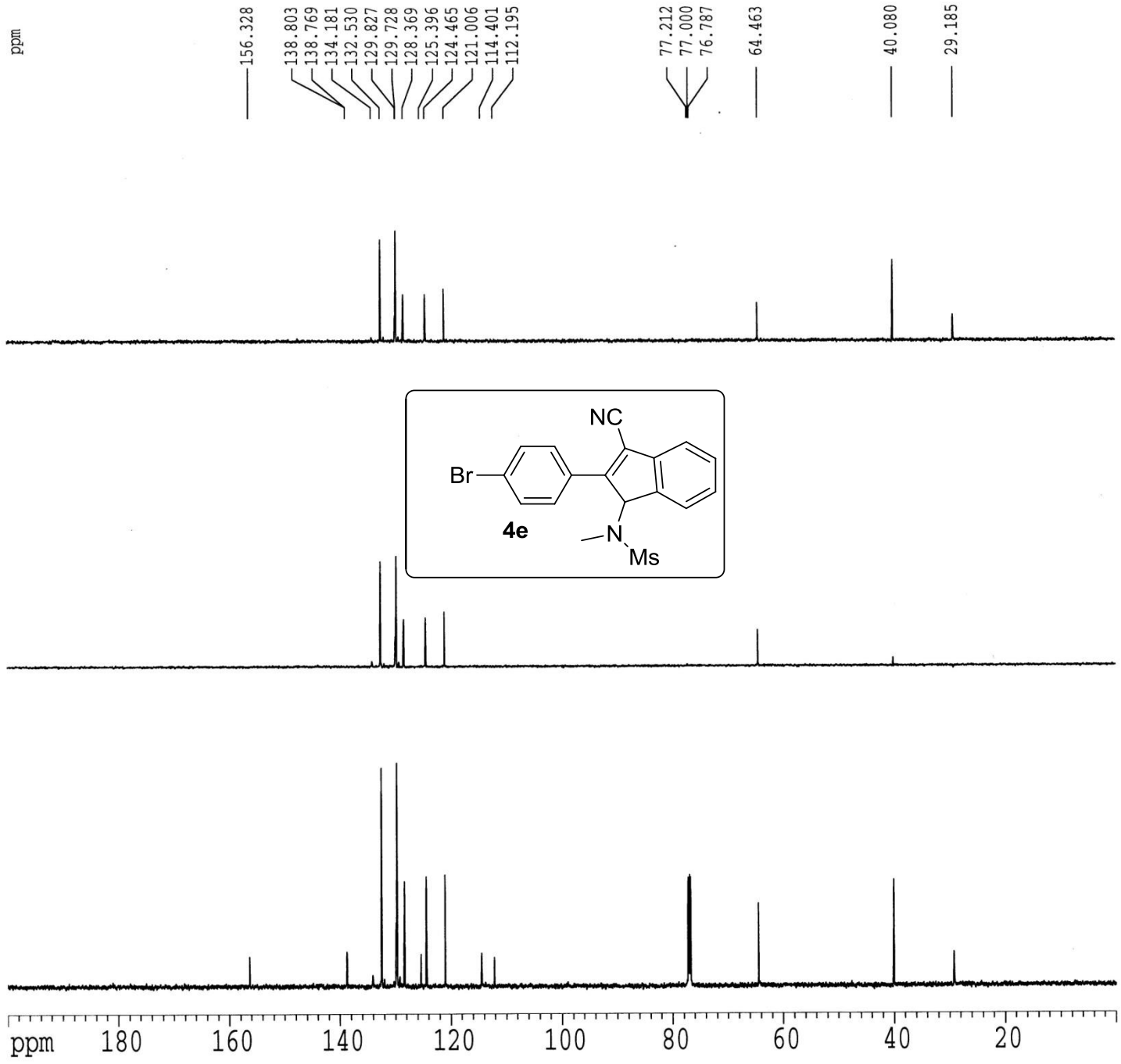

Current Data Parameters
NAME RKS-3-104-P
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20160719
Time 11.41
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 8389.262 Hz
FIDRES 0.256020 Hz
AQ 1.9530228 sec
RG 512
DW 59.600 usec
DE 6.50 usec
TE 300.0 K
D1 2.00000000 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
F1 - 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
ppm
7.81534
7.81315
7.80133
7.53845
7.53736
7.52603
7.52493
7.50055
7.48796
7.43676
7.35508
7.34264
7.34112
7.02818
7.02604
7.01410
6.27356
3.85759
2.94509
2.20528
NC
H3CO
4c
N
Ms
Integral
2.0676
2.1320
1.1178
1.1837
2.0849
1.0000
3.2039
3.0494
3.0184
ppm
8
6
4
2
0


161.61
157.36
139.30
138.55
130.03
129.62
127.67
124.36
123.54
120.45
115.09
114.64
109.47
77.32
77.00
76.68
64.43
55.43
40.03
29.00
Current Data Parameters
NAME 20150819
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20150819
Time 22.12
INSTRUM spect
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 700
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
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 100.6178030 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
RKS-3-104
NC
H3CO
4c
N
Ms
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm


7.784
7.763
7.555
7.546
7.537
7.528
7.498
7.478
7.468
7.449
7.408
7.389
7.371
7.239
6.284
2.960
2.211
1.597
Current Data Parameters
NAME 20150813
EXPNO 17
PROCNO 1
F2 – Acquisition Parameters
Date_ 20150814
Time 17.52
INSTRUM spect
PROBHD 5 mm DUL 13C–1
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 29
DS 0
SWH 6410.256 Hz
FIDRES 0.195625 Hz
AQ 2.5559540 sec
RG 161
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 400.1500171 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
NC
Cl
4d
N
Ms
RKS-3-99 P
10
9
8
7
6
5
4
3
2
1
ppm
2.14
2.10
3.03
1.03
1.00
3.19
3.11


156.26
138.76
138.74
136.95
129.79
129.55
129.38
128.32
124.43
120.97
114.41
112.10
77.32
77.00
76.69
64.49
40.05
29.17
Current Data Parameters
NAME 20150813
EXPNO 11
PROCNO 1
F2 - Acquisition Parameters
Date_ 20150813
Time 22.57
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 546
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 100.6178033 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
RKS-3-99 P
NC
Cl
4d
N
Ms
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm


Current Data Parameters
NAME RKS-3-96-P
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20160223
Time 6.43
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 294.4 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 598.5032918 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
7.70976
7.70811
7.69840
7.69531
7.65646
7.65470
7.64505
7.64198
7.55393
7.54746
7.54652
7.54442
7.54271
7.54158
7.53669
7.53498
7.48210
7.46961
7.45687
7.40891
7.40725
7.39640
7.39462
7.38404
7.38216
7.24003
7.23810
6.28340
2.96325
2.21130
1.57924
NC
Br
4e
N
Ms
Integral
2.3950
2.0056
2.0234
1.3274
1.0076
1.0000
3.1288
3.0088
ppm
8
6
4
2
0



Current Data Parameters
NAME RKS-3-96-P
EXPNO 2
PROCNO 1

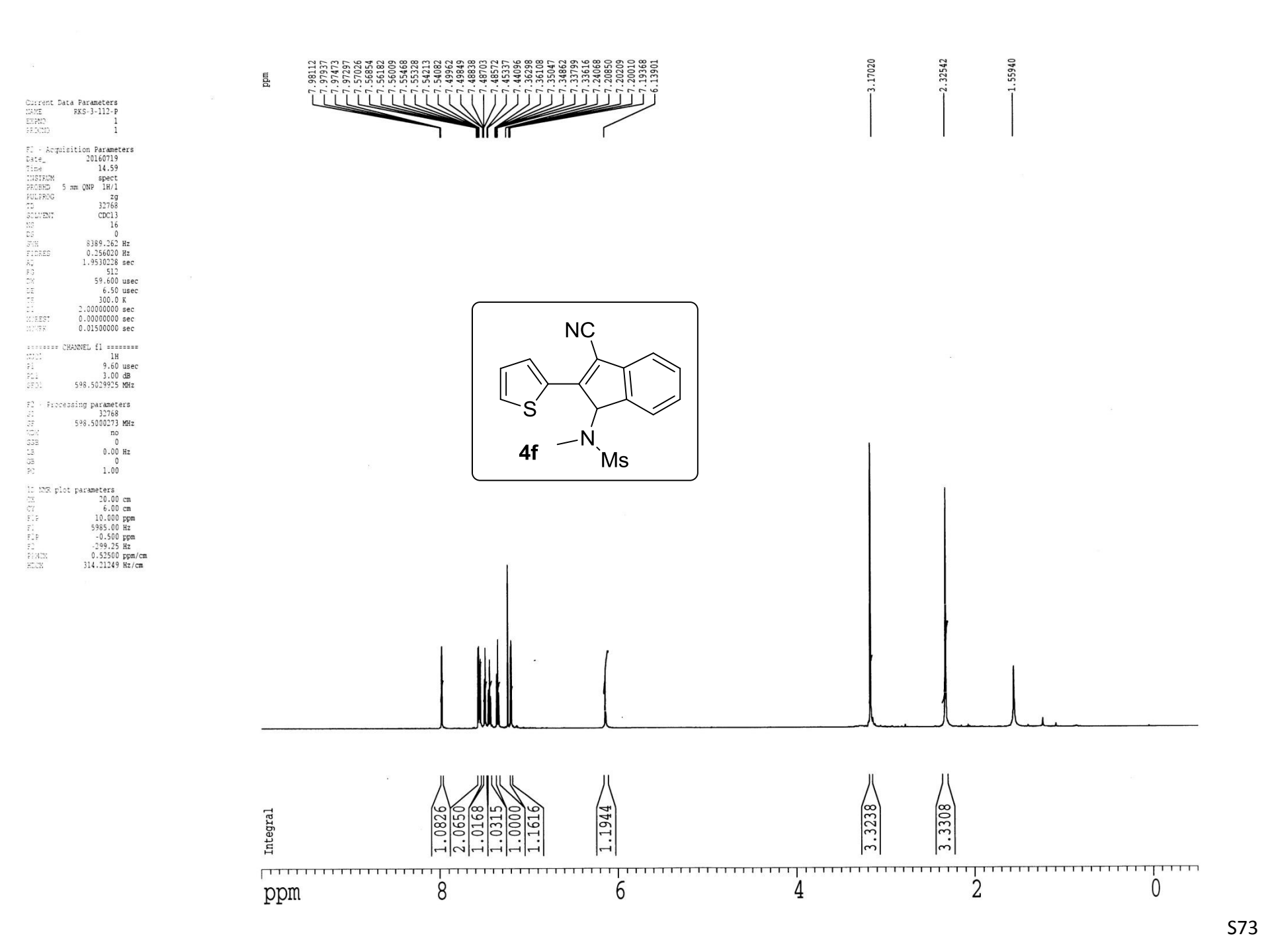
F2 - Acquisition Parameters
Date_ 20160223
Time 6.56
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 208
DS 0
SWH 45045.047 Hz
FIDRES 1.374666 Hz
AQ 0.3637748 sec
RG 4096
DW 11.100 usec
DE 6.50 usec
TE 296.5 K
D1 3.50000000 sec
d11 0.03000000 sec
DELTA 3.40000010 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

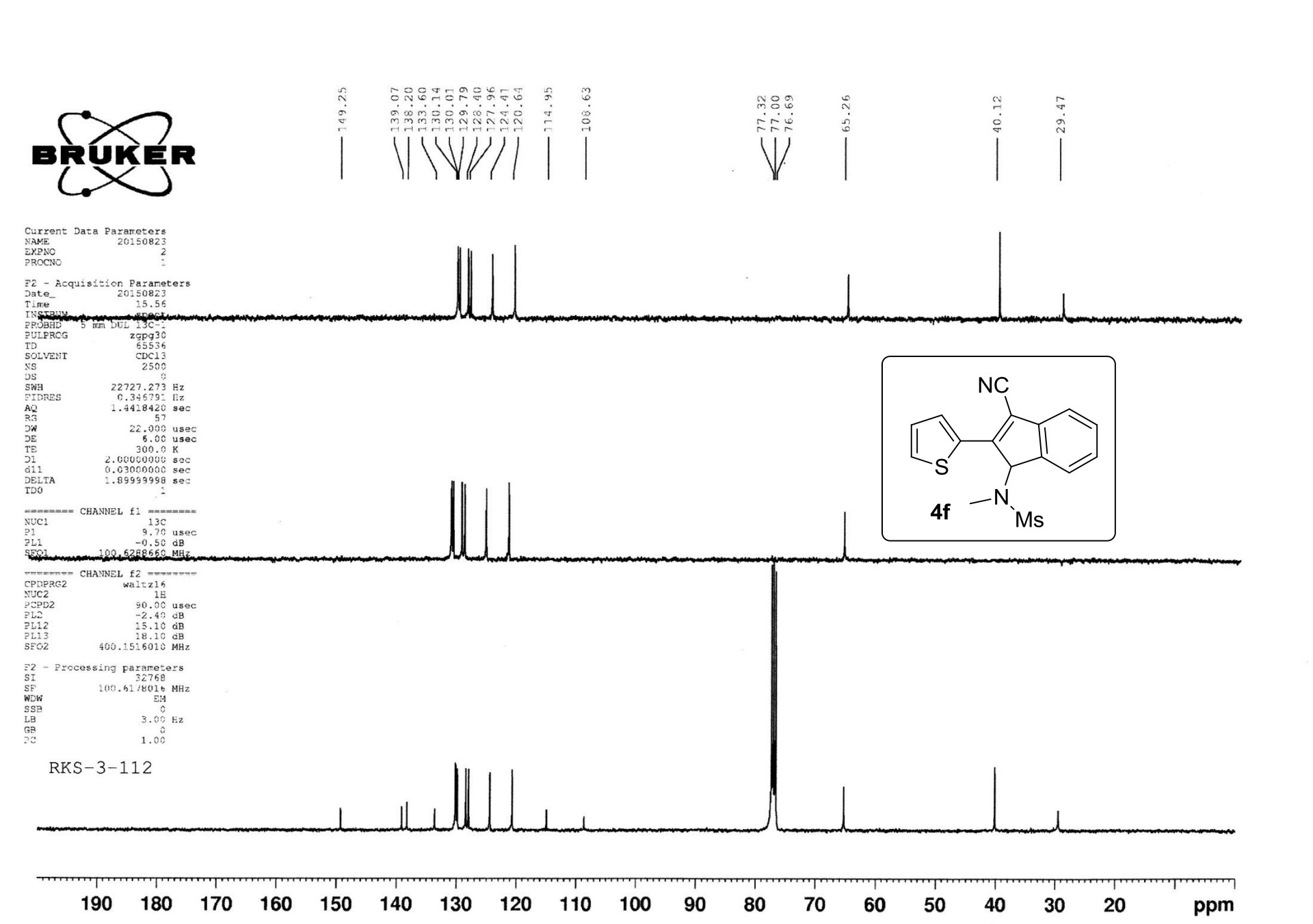
======== CHANNEL f1 ========
NUC1 13C
P1 4.80 usec
PL1 0.00 dB
SFO1 150.5094992 MHz

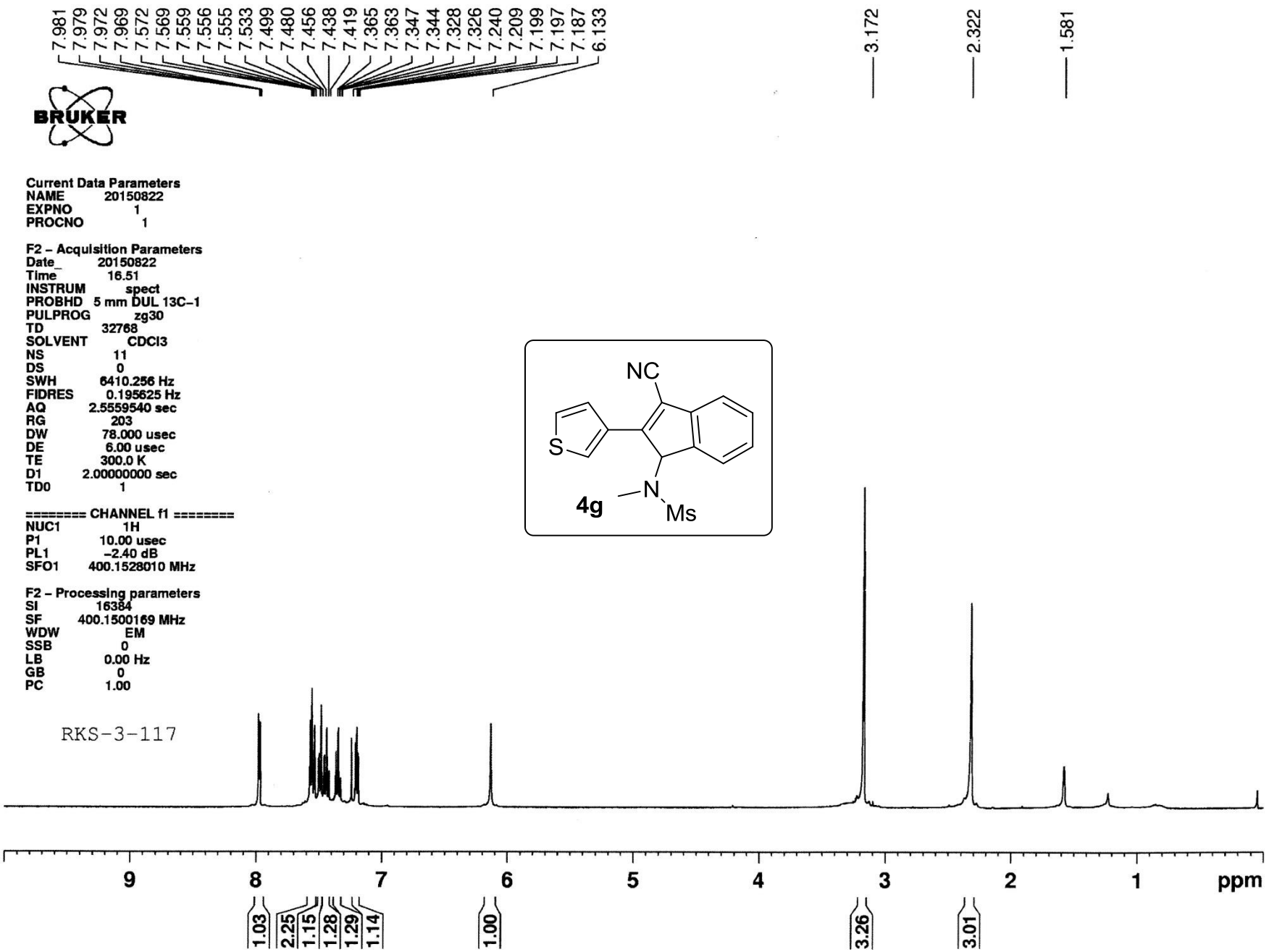
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 92.00 usec
PL2 120.00 dB
PL12 9.00 dB
PL13 14.00 dB
SFO2 598.5029925 MHz

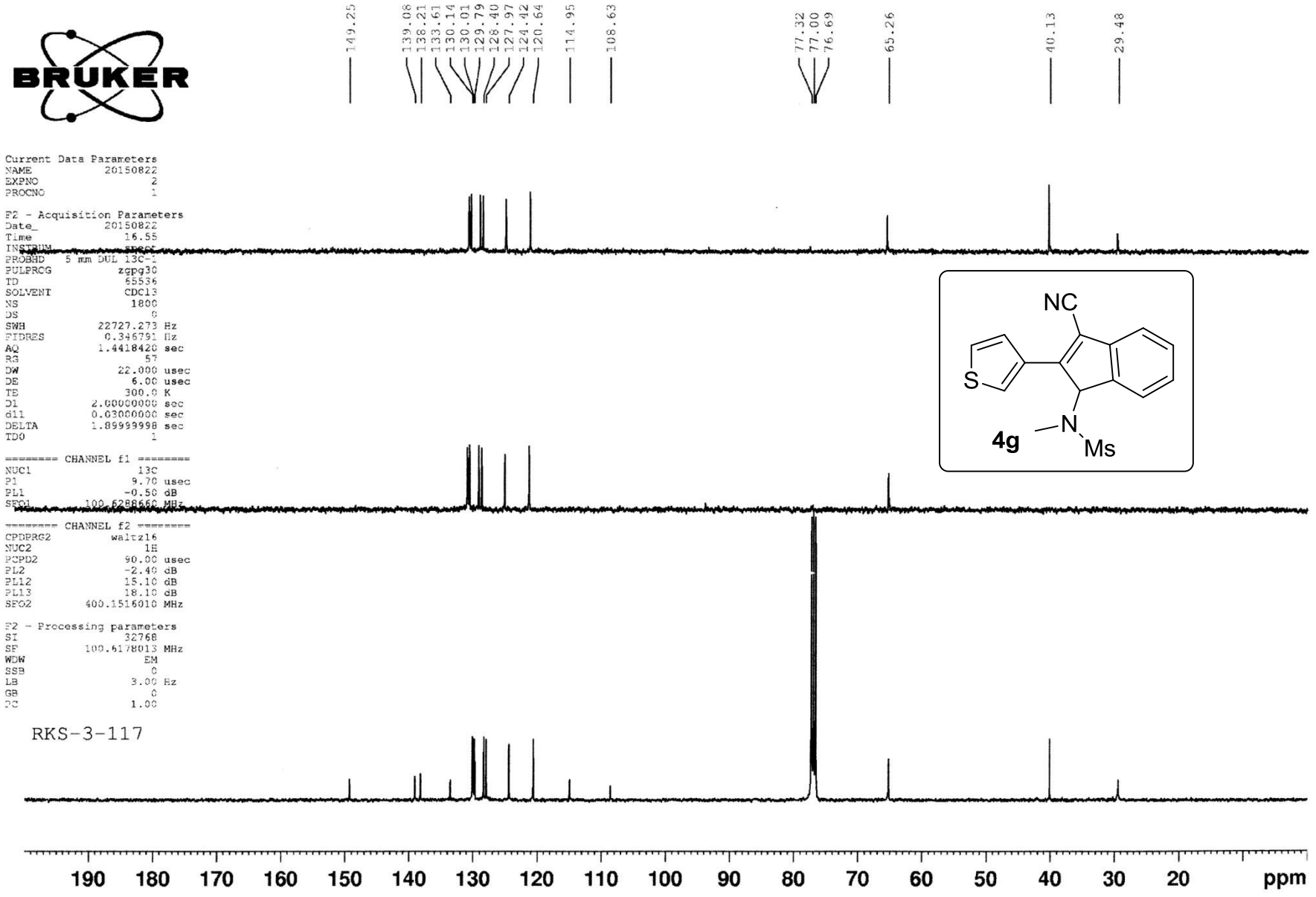
F2 - Processing parameters
SI 65536
SF 150.4929508 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00

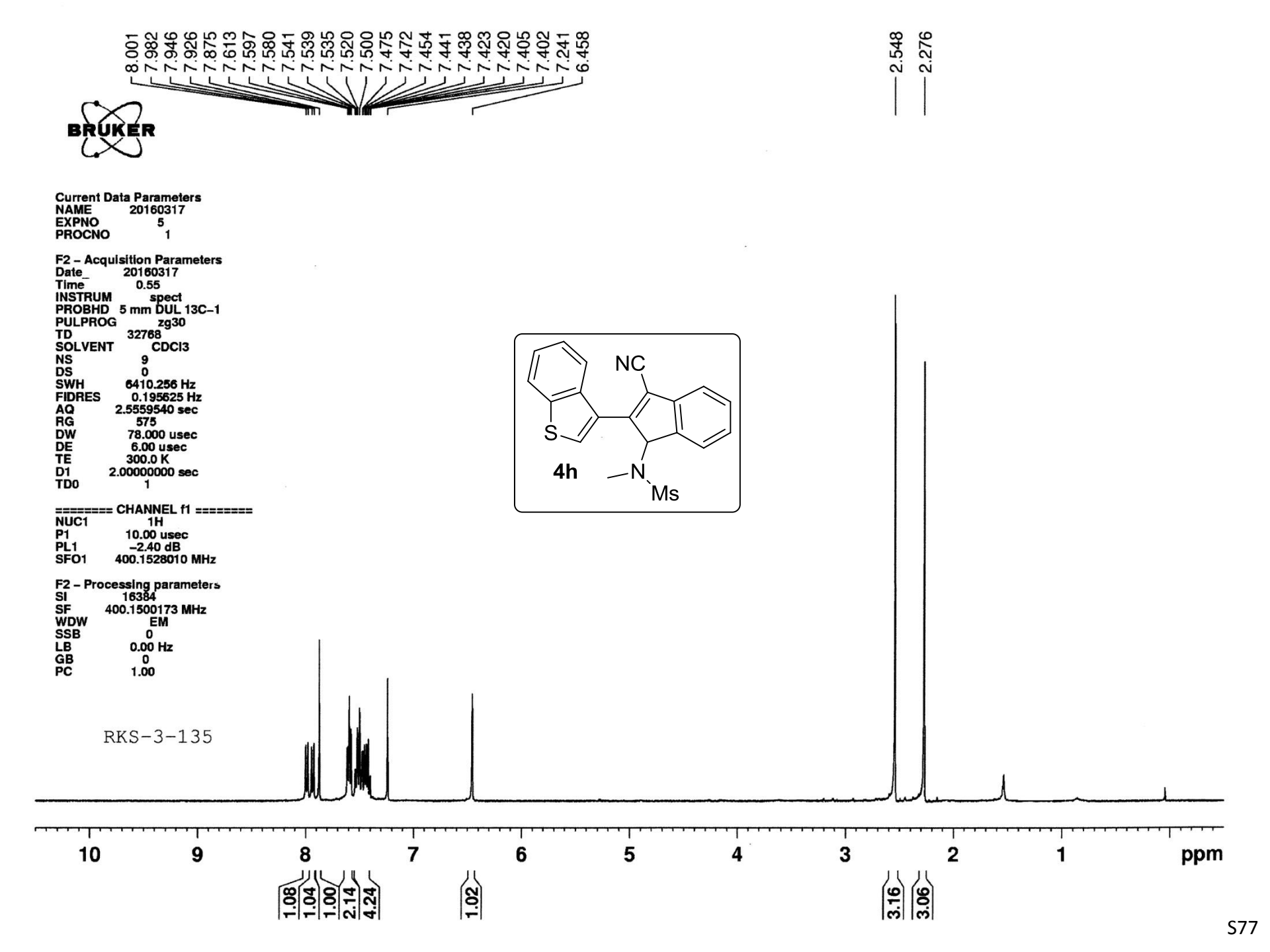
1D NMR plot parameters
CX 20.00 cm
CY 4.00 cm
F1P 200.000 ppm
F1 30098.59 Hz
F2P 0.000 ppm
F2 0.00 Hz
PPMCM 10.00000 ppm/cm
HZCM 1504.92944 Hz/cm

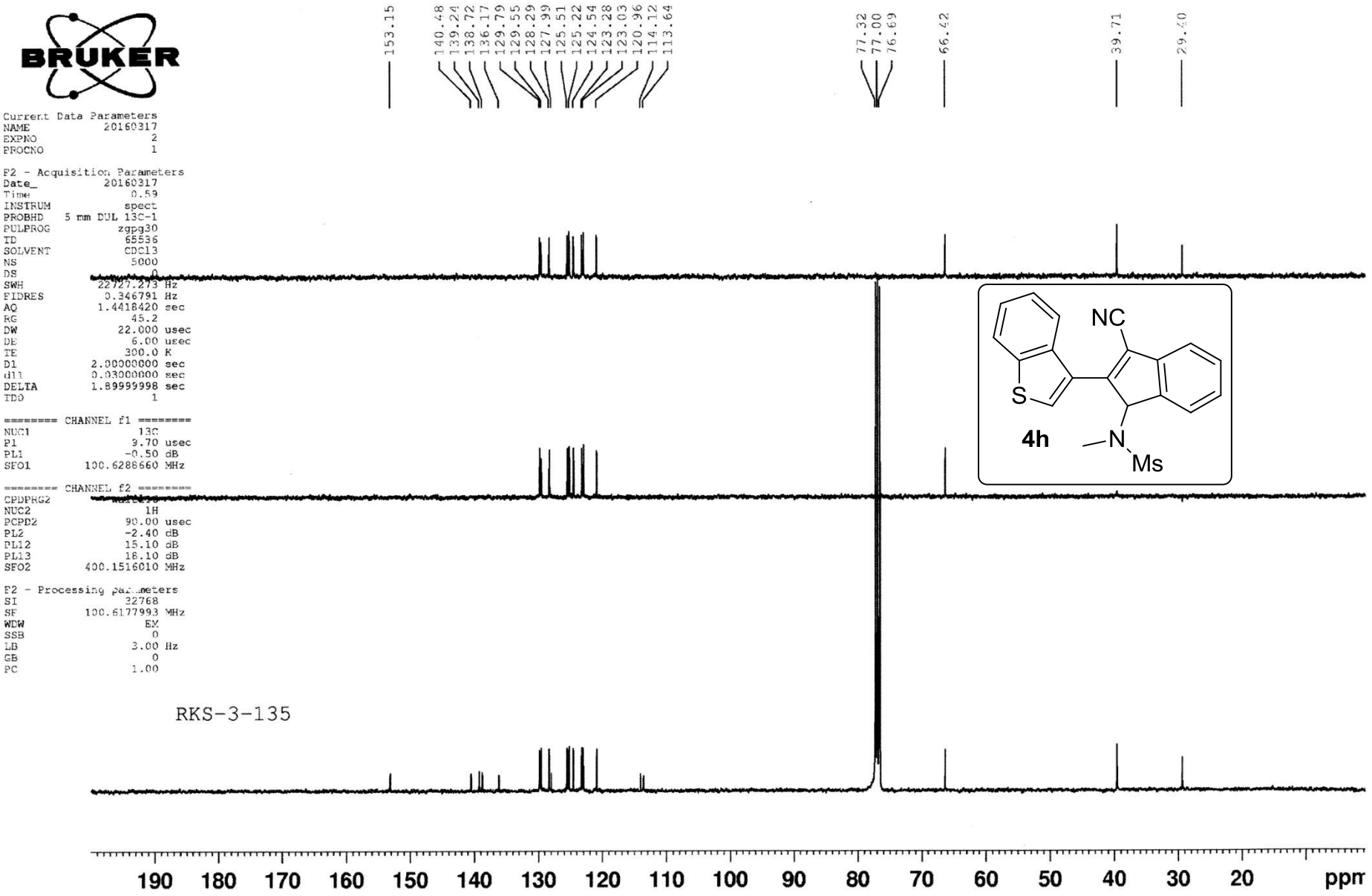

Current Data Parameters
NAME RKS-3-112-P
EXPNO 1
PROCNO 1
F1 - Acquisition Parameters
Date_ 20160719
Time 14.59
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 8389.262 Hz
FIDRES 0.256020 Hz
AQ 1.9530228 sec
RG 512
DW 59.600 usec
DE 6.50 usec
TE 300.0 K
D1 2.00000000 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 598.5000273 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 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
7.98112
7.97937
7.97473
7.97297
7.57026
7.56854
7.56182
7.56009
7.55468
7.55328
7.54213
7.54082
7.49962
7.49849
7.48838
7.48703
7.48572
7.45337
7.44096
7.36298
7.36108
7.35047
7.34862
7.33799
7.33616
7.24068
7.20850
7.20209
7.20010
7.19368
6.13901
3.17020
2.32542
1.55940
NC
S
N
Ms
4f
Integral
1.0826
2.0650
1.0168
1.0315
1.0000
1.1616
1.1944
3.3238
3.3308
ppm
8
6
4
2
0

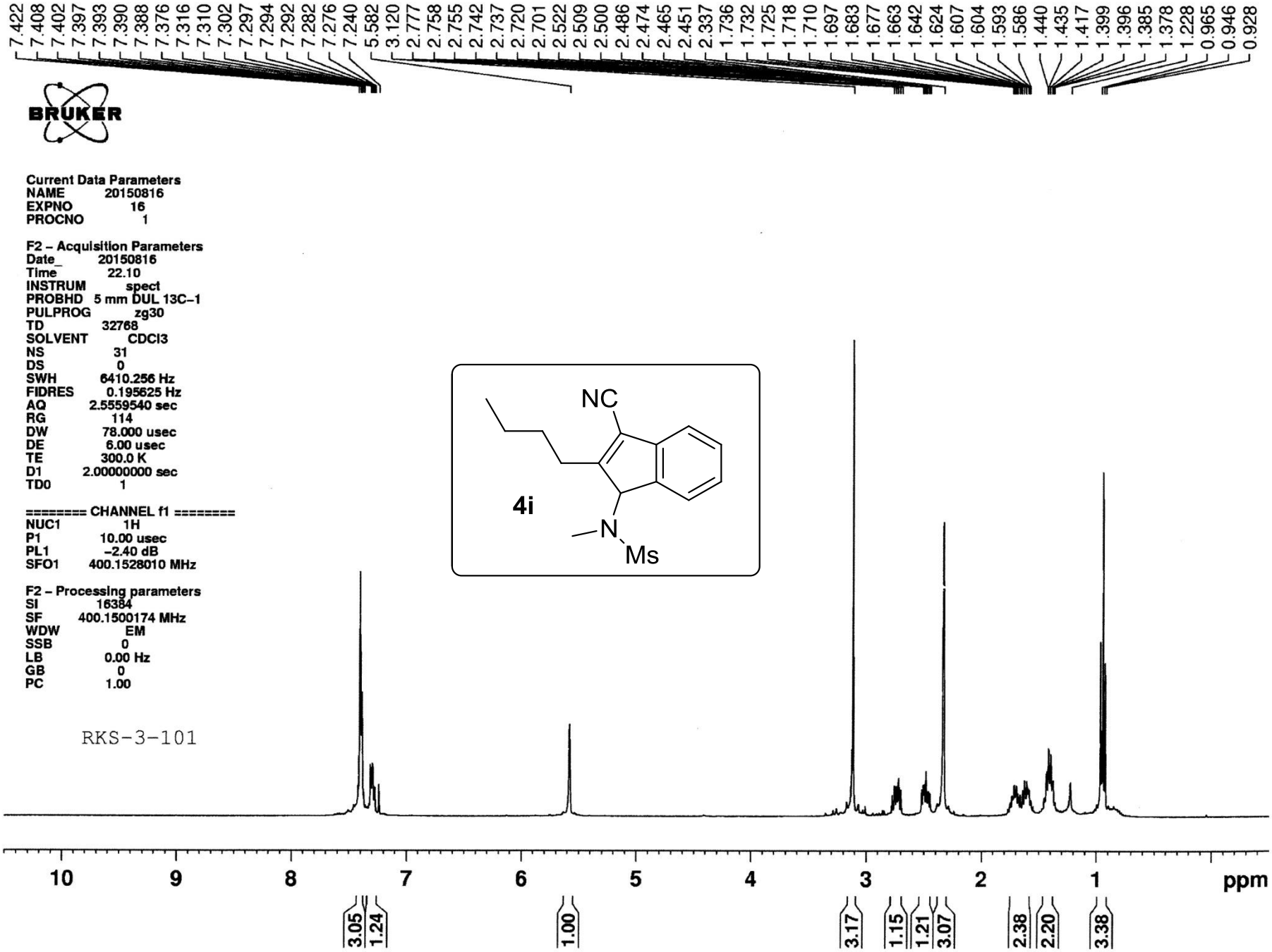

149.25
139.07
138.20
133.60
130.14
130.01
129.79
128.40
127.96
124.41
120.64
114.95
108.63
77.32
77.00
76.69
65.26
40.12
29.47
Current Data Parameters
NAME 20150823
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20150823
Time 15.56
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 2500
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 100.6178016 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
RKS-3-112
NC
S
N
Ms
4f
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

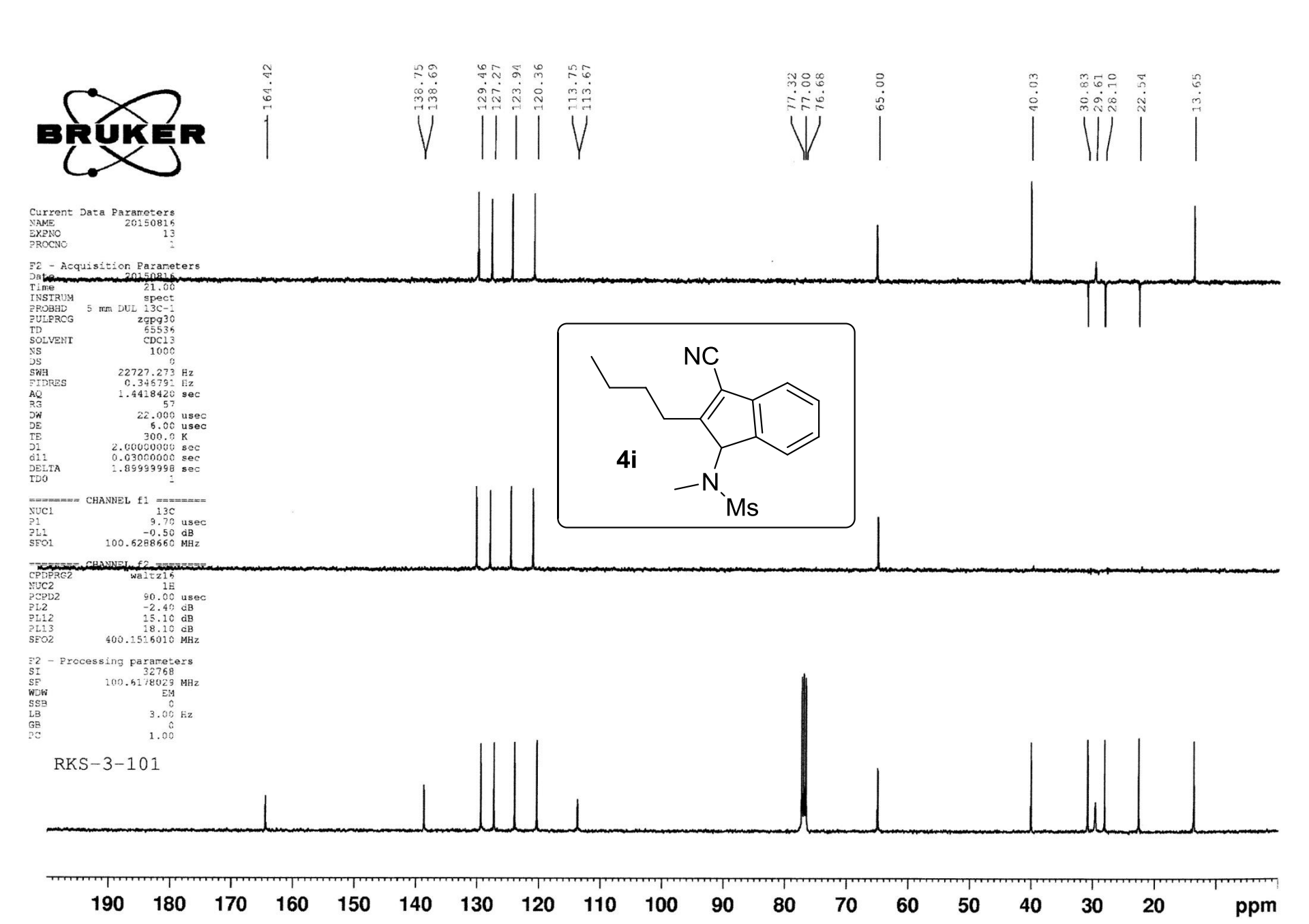

7.981
7.979
7.972
7.969
7.572
7.569
7.559
7.556
7.555
7.533
7.499
7.480
7.456
7.438
7.419
7.365
7.363
7.347
7.344
7.328
7.326
7.240
7.209
7.199
7.197
7.187
6.133
3.172
2.322
1.581
BRUKER
Current Data Parameters
NAME 20150822
EXPNO 1
PROCNO 1
F2 – Acquisition Parameters
Date_ 20150822
Time 16.51
INSTRUM 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 203
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
NC
S
N
Ms
4g
RKS-3-117
9
8
7
6
5
4
3
2
1
ppm
1.03
2.25
1.15
1.28
1.29
1.14
1.00
3.26
3.01

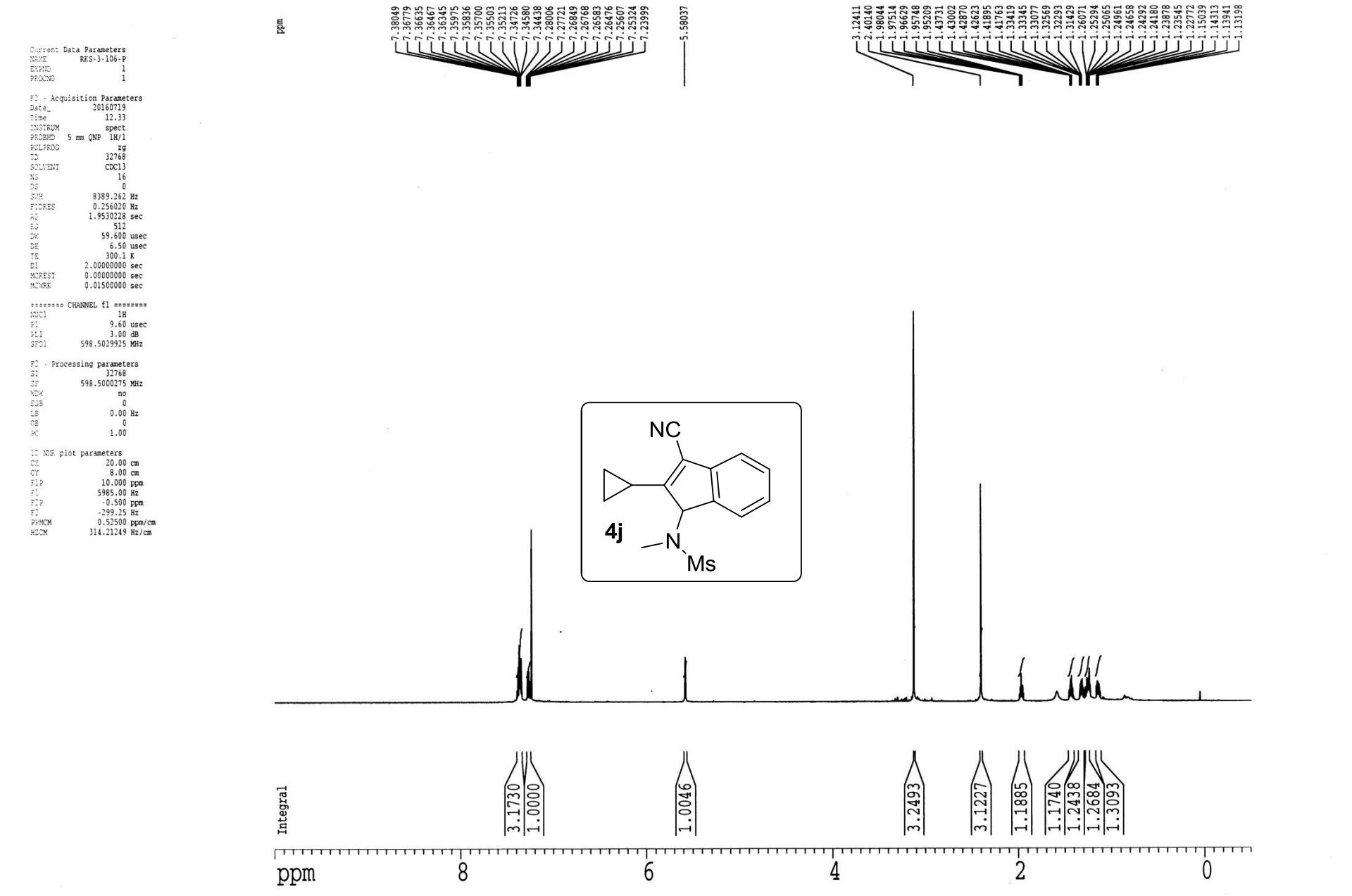

149.25
139.08
138.21
133.61
130.14
130.01
129.79
128.40
127.97
124.42
120.64
114.95
108.63
77.32
77.00
76.69
65.26
40.13
29.48
Current Data Parameters
NAME 20150822
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20150822
Time 16.55
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1800
DS 8
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 100.6178013 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
RKS-3-117
NC
S
N
Ms
4g
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

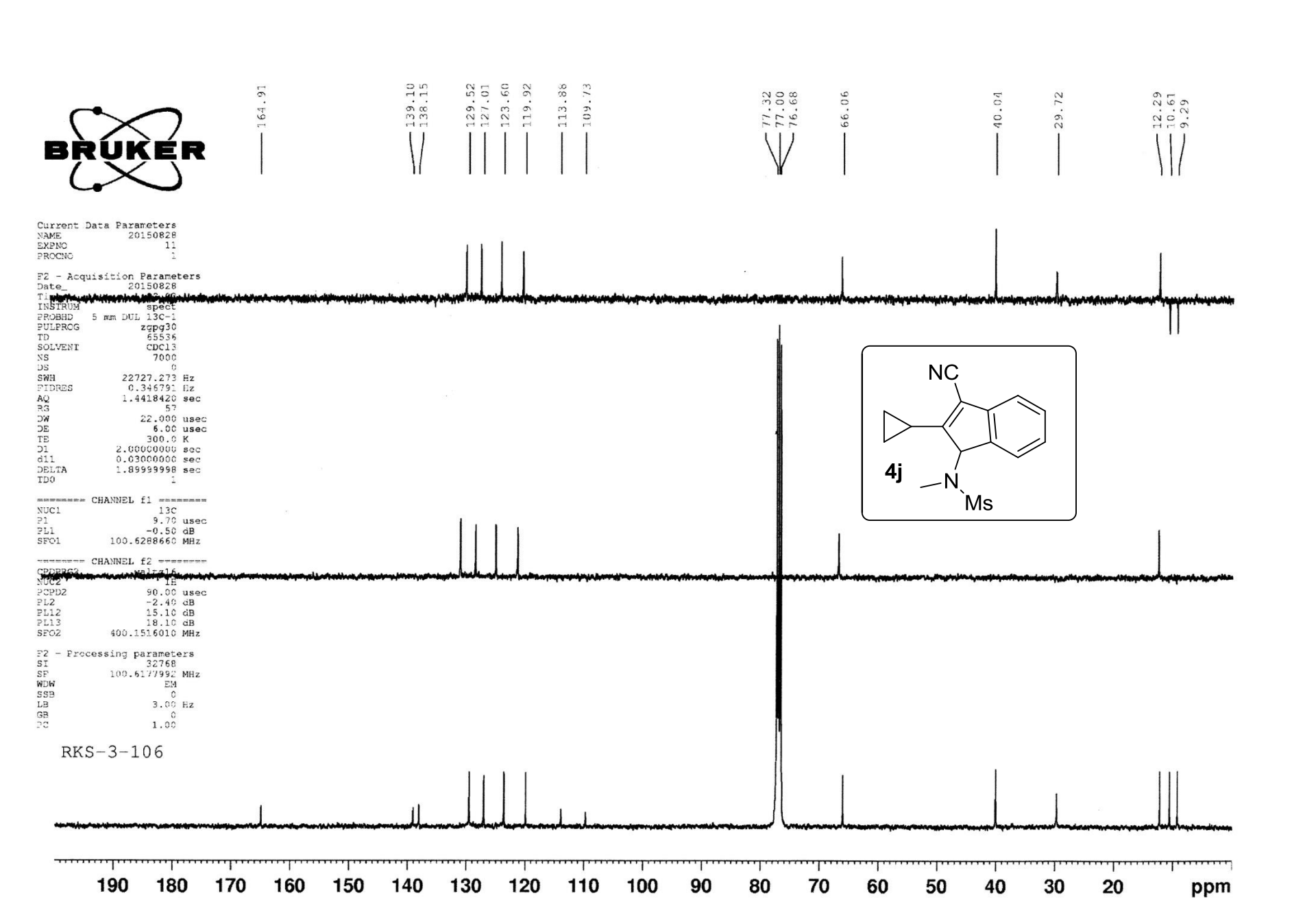

8.001
7.982
7.946
7.926
7.875
7.613
7.597
7.580
7.541
7.539
7.535
7.520
7.500
7.475
7.472
7.454
7.441
7.438
7.423
7.420
7.405
7.402
7.241
6.458
2.548
2.276
BRUKER
Current Data Parameters
NAME 20160317
EXPNO 5
PROCNO 1
F2 – Acquisition Parameters
Date_ 20160317
Time 0.55
INSTRUM spect
PROBHD 5 mm DUL 13C–1
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 9
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 400.1500173 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
NC
S
4h
N
Ms
RKS-3-135
10
9
8
7
6
5
4
3
2
1
ppm
1.08
1.04
1.00
2.14
4.24
1.02
3.16
3.06

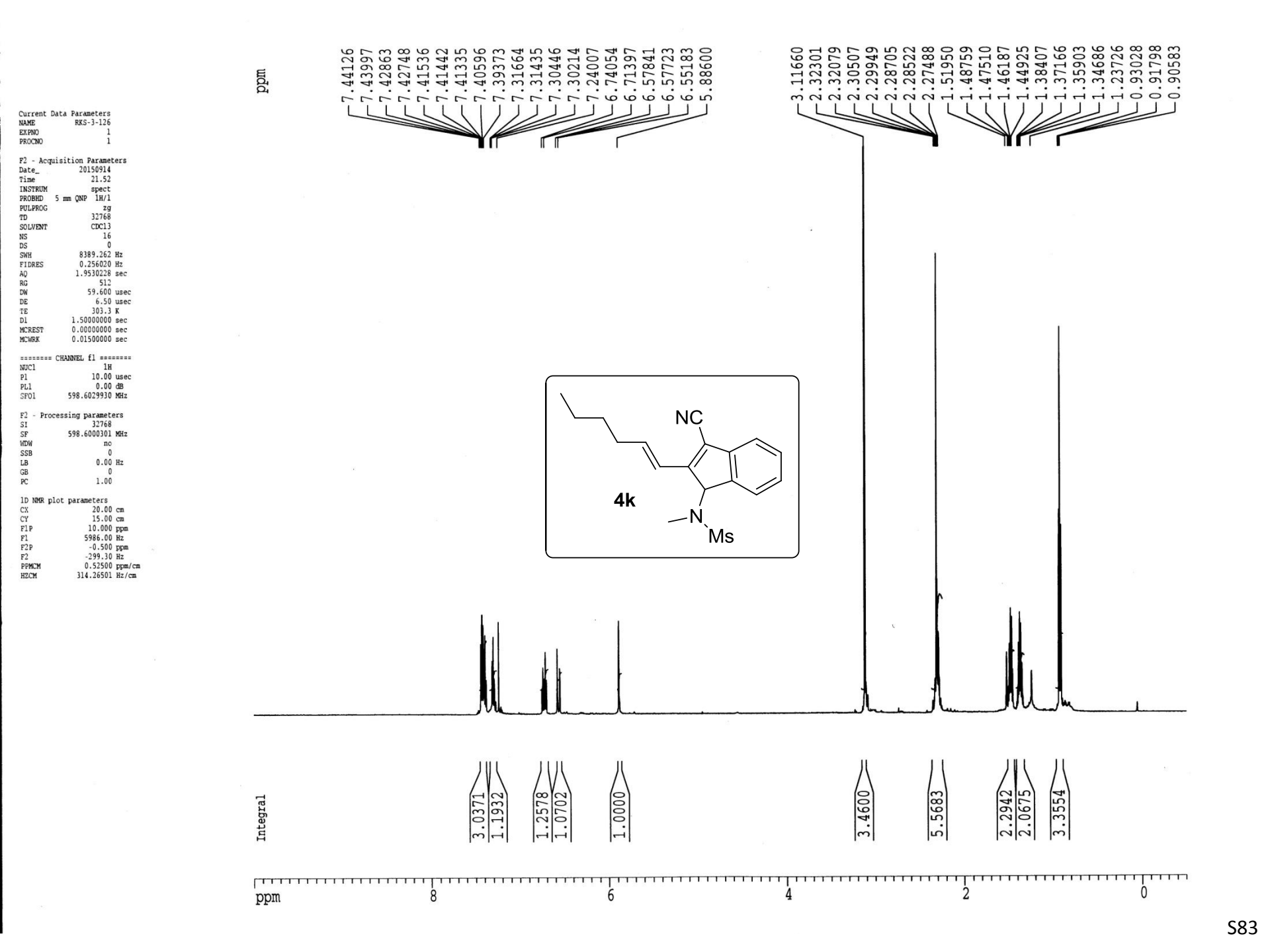

153.15
140.48
139.24
138.72
136.17
129.79
129.55
128.29
127.99
125.51
125.22
124.54
123.28
123.03
120.96
114.12
113.64
77.32
77.00
76.69
66.42
39.71
29.40
Current Data Parameters
NAME 20160317
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20160317
Time 0.59
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 5000
DS 0
SWH 22727.273 Hz
FIDRES 0.346791 Hz
AQ 1.4418420 sec
RG 45.2
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
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
RKS-3-135
NC
S
4h
N
Ms
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

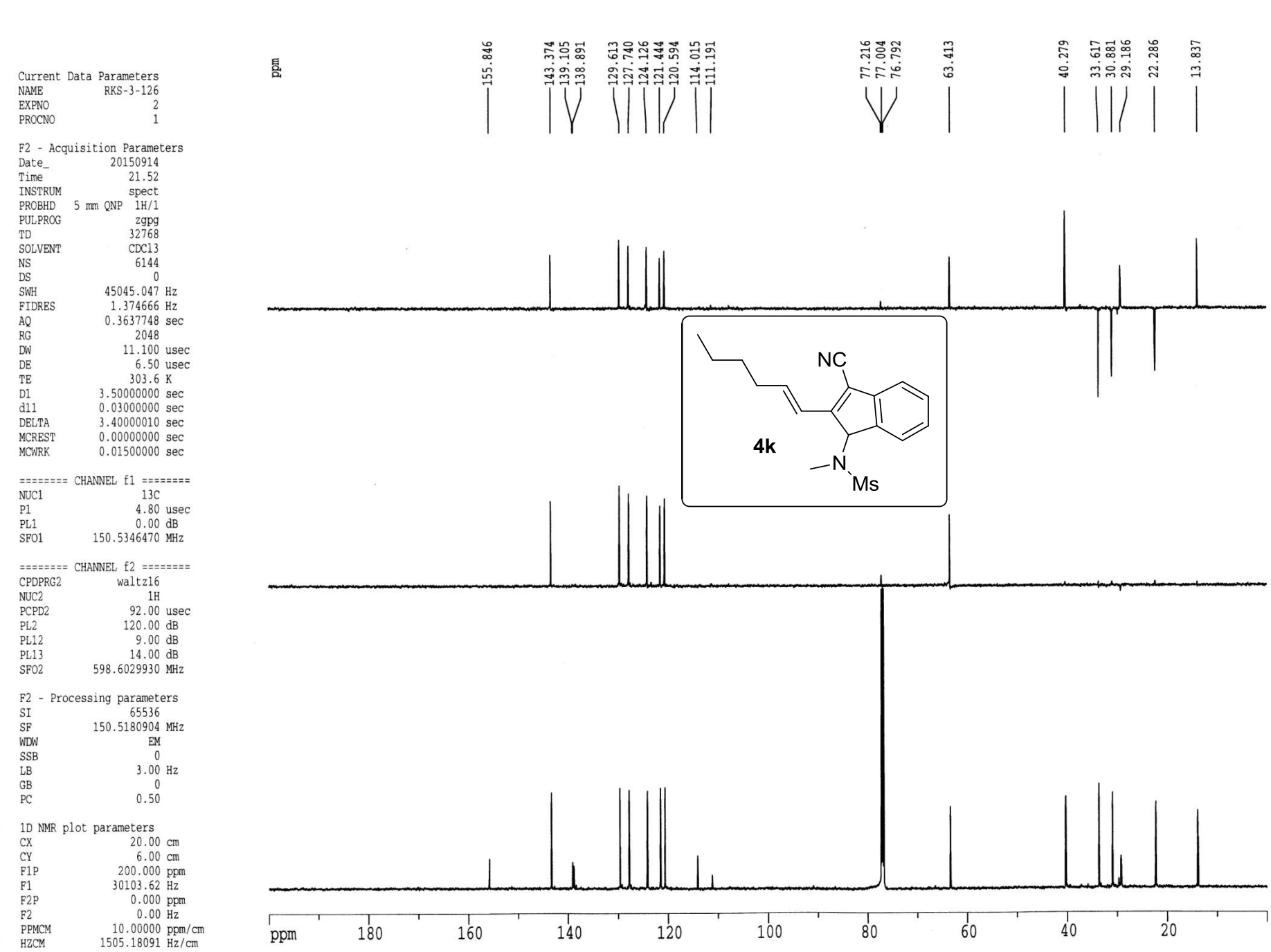

7.422 7.408 7.402 7.397 7.393 7.390 7.388 7.376 7.316 7.310 7.302 7.297 7.294 7.292 7.282 7.276 7.240 5.582 3.120 2.777 2.758 2.755 2.742 2.737 2.720 2.701 2.522 2.509 2.500 2.486 2.474 2.465 2.451 2.337 1.736 1.732 1.725 1.718 1.710 1.697 1.683 1.677 1.663 1.642 1.624 1.607 1.604 1.593 1.586 1.440 1.435 1.417 1.399 1.396 1.385 1.378 1.228 0.965 0.946 0.928
BRUKER
Current Data Parameters
NAME 20150816
EXPNO 16
PROCNO 1
F2 – Acquisition Parameters
Date_ 20150816
Time 22.10
INSTRUM spect
PROBHD 5 mm DUL 13C–1
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 31
DS 0
SWH 6410.256 Hz
FIDRES 0.195625 Hz
AQ 2.5559540 sec
RG 114
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 400.1500174 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
RKS-3-101
NC
4i
N
Ms
10 9 8 7 6 5 4 3 2 1 ppm
3.05 1.24 1.00 3.17 1.15 1.21 3.07 2.38 2.20 3.38

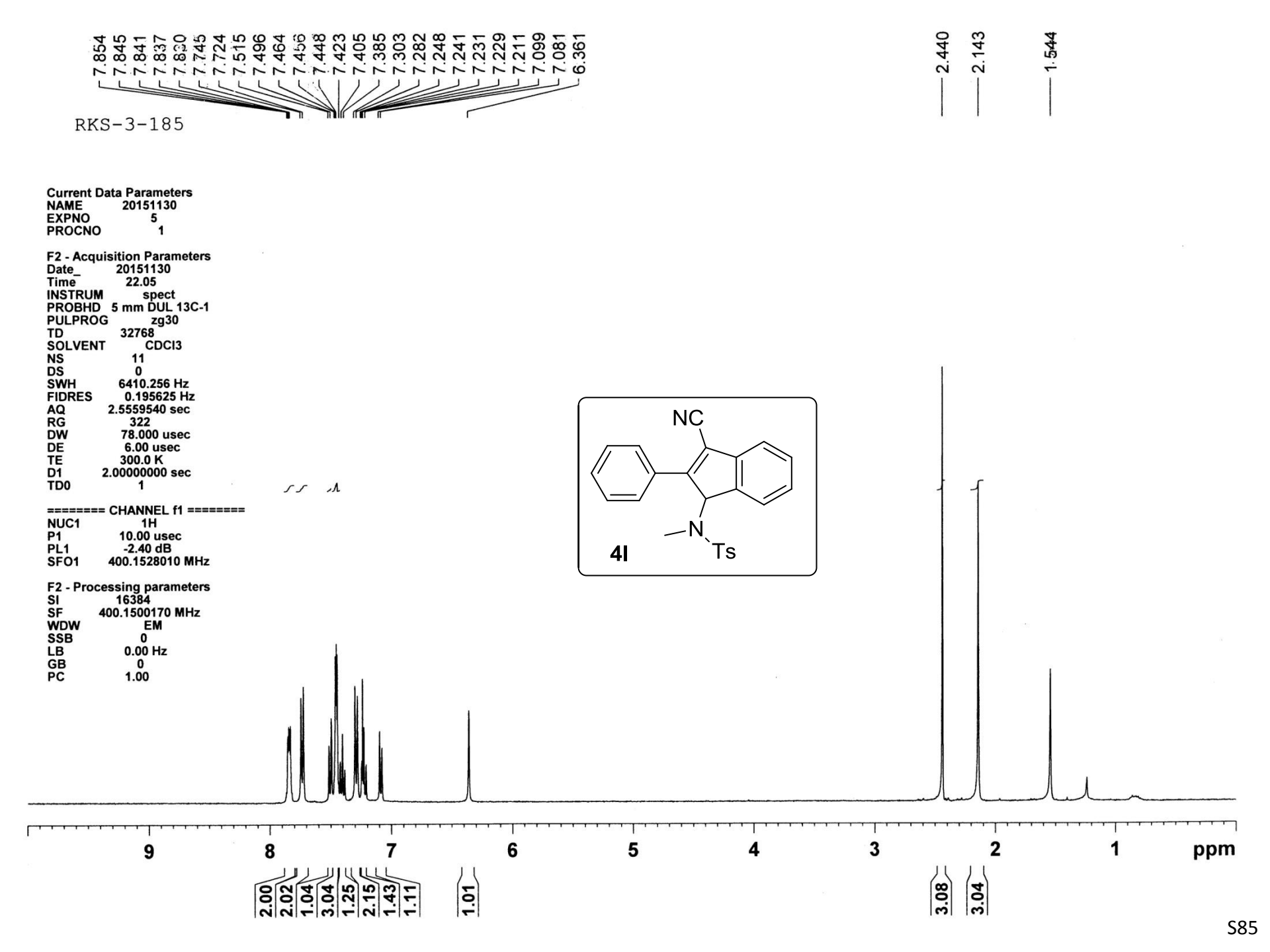

164.42
138.75
138.69
129.46
127.27
123.94
120.36
113.75
113.67
77.32
77.00
76.68
65.00
40.03
30.83
29.61
28.10
22.54
13.65
Current Data Parameters
NAME 20150816
EXPNO 13
PROCNO 1
F2 - Acquisition Parameters
Date_ 20150816
Time 21.00
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1000
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 100.6178029 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
NC
4i
N
Ms
RKS-3-101
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm


Current Data Parameters
NAME RKS-3-106-P
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20160719
Time 12.33
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 300.1 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 598.5000275 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
7.38049
7.36779
7.36635
7.36467
7.36345
7.35975
7.35836
7.35700
7.35503
7.35213
7.34726
7.34580
7.34438
7.28006
7.27721
7.26849
7.26768
7.26583
7.26476
7.25607
7.25324
7.23999
5.58037
3.12411
2.40140
1.98044
1.97514
1.96629
1.95748
1.95209
1.43731
1.43002
1.42870
1.42623
1.41895
1.41763
1.33419
1.33345
1.33077
1.32569
1.32293
1.31429
1.26071
1.25294
1.25065
1.24961
1.24658
1.24292
1.24180
1.23878
1.23545
1.22772
1.15039
1.14313
1.13941
1.13198
NC
4j
N
Ms
Integral
3.1730
1.0000
1.0046
3.2493
3.1227
1.1885
1.1740
1.2438
1.2684
1.3093
ppm
8
6
4
2
0


164.91
139.10
138.15
129.52
127.01
123.60
119.92
113.88
109.73
77.32
77.00
76.68
66.06
40.04
29.72
12.29
10.61
9.29
Current Data Parameters
NAME 20150828
EXPNO 11
PROCNO 1
F2 - Acquisition Parameters
Date_ 20150828
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 7000
DS 0
SWH 22727.273 Hz
FIDRES 0.346791 Hz
AQ 1.4418420 sec
RG 57
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 ========
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 100.6177992 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
RKS-3-106
NC
4j
N
Ms
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm


Current Data Parameters
NAME RKS-3-126
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20150914
Time 21.52
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 303.3 K
D1 1.50000000 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 598.6000301 MHz
WDW nc
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 20.00 cm
CY 15.00 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
ppm
7.44126
7.43997
7.42863
7.42748
7.41536
7.41442
7.41335
7.40596
7.39373
7.31664
7.31435
7.30446
7.30214
7.24007
6.74054
6.71397
6.57841
6.57723
6.55183
5.88600
3.11660
2.32301
2.32079
2.30507
2.29949
2.28705
2.28522
2.27488
1.51950
1.48759
1.47510
1.46187
1.44925
1.38407
1.37166
1.35903
1.34686
1.23726
0.93028
0.91798
0.90583
NC
4k
N
Ms
Integral
3.0371
1.1932
1.2578
1.0702
1.0000
3.4600
5.5683
2.2942
2.0675
3.3554
ppm
8
6
4
2
0


Current Data Parameters
NAME RKS-3-126
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20150914
Time 21.52
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 6144
DS 0
SWH 45045.047 Hz
FIDRES 1.374666 Hz
AQ 0.3637748 sec
RG 2048
DW 11.100 usec
DE 6.50 usec
TE 303.6 K
D1 3.50000000 sec
d11 0.03000000 sec
DELTA 3.40000010 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 4.80 usec
PL1 0.00 dB
SFO1 150.5346470 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 150.5180904 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 0.50
1D NMR plot parameters
CX 20.00 cm
CY 6.00 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
155.846
143.374
139.105
138.891
129.613
127.740
124.126
121.444
120.594
114.015
111.191
77.216
77.004
76.792
63.413
40.279
33.617
30.881
29.186
22.286
13.837
NC
4k
N
Ms
ppm
180
160
140
120
100
80
60
40
20


7.854
7.845
7.841
7.837
7.830
7.745
7.724
7.515
7.496
7.464
7.455
7.448
7.423
7.405
7.385
7.303
7.282
7.248
7.241
7.231
7.229
7.211
7.099
7.081
6.361
2.440
2.143
1.544
RKS-3-185
Current Data Parameters
NAME 20151130
EXPNO 5
PROCNO 1
F2 - Acquisition Parameters
Date_ 20151130
Time 22.05
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 32768
SOLVENT CDCI3
NS 11
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 400.1500170 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
NC
N
Ts
4l
9
8
7
6
5
4
3
2
1
ppm
2.00
2.02
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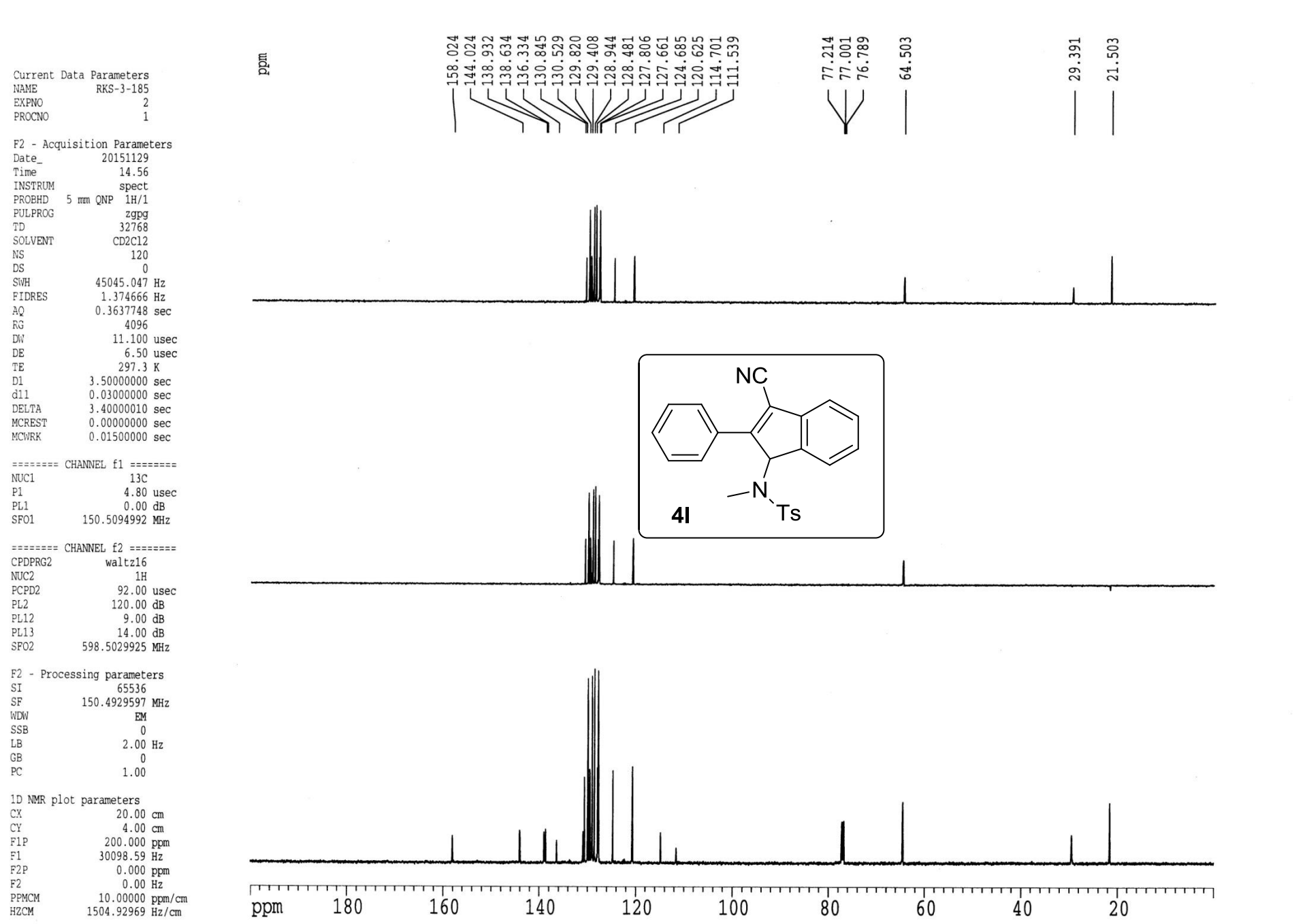
2.15
1.43
1.11
1.01
3.08
3.04



Current Data Parameters
NAME RKS-3-185
EXPNO 2
PROCNO 1

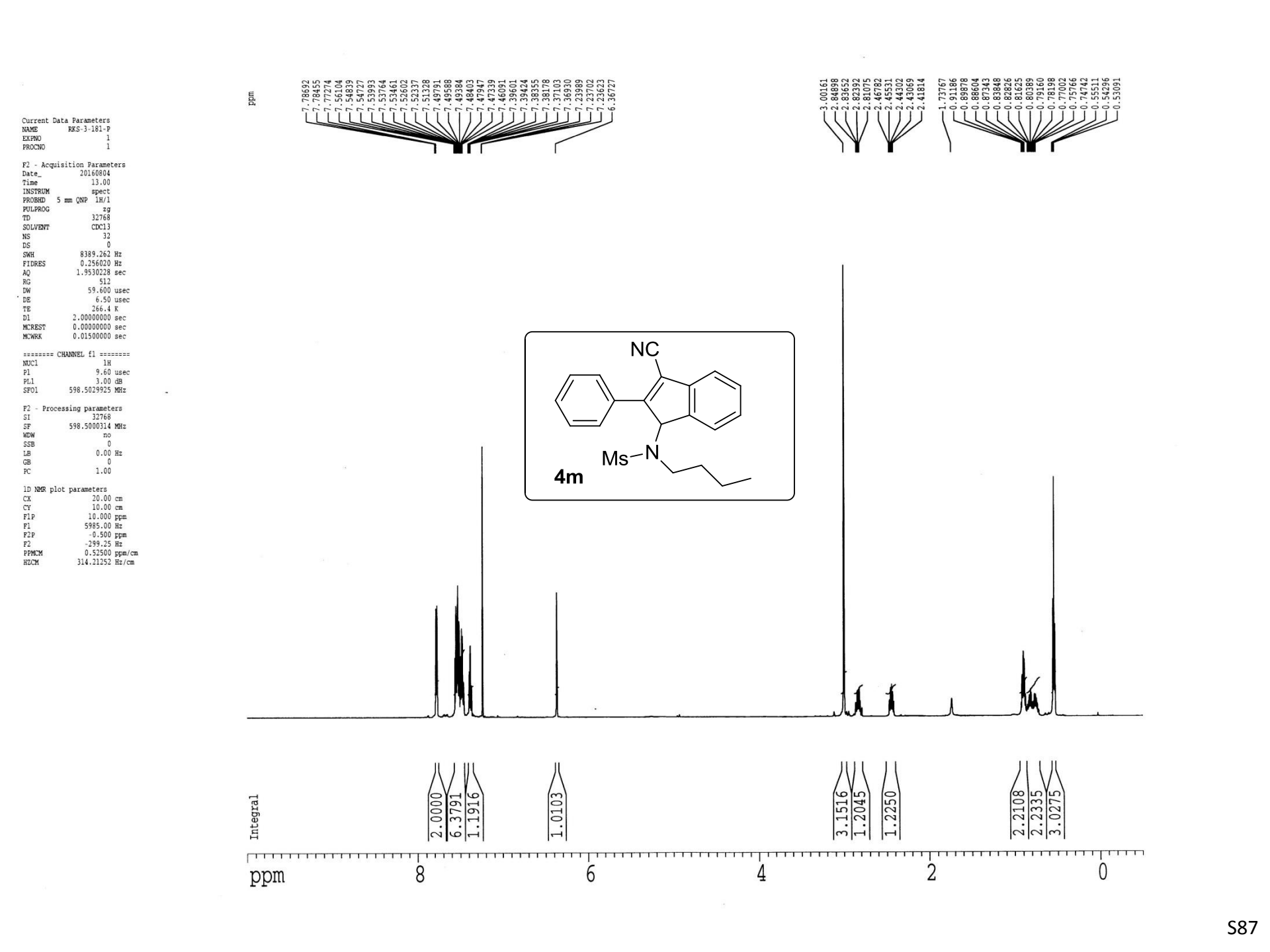
F2 - Acquisition Parameters
Date_ 20151129
Time 14.56
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CD2Cl2
NS 120
DS 0
SWH 45045.047 Hz
FIDRES 1.374666 Hz
AQ 0.3637748 sec
RG 4096
DW 11.100 usec
DE 6.50 usec
TE 297.3 K
D1 3.50000000 sec
d11 0.03000000 sec
DELTA 3.40000010 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

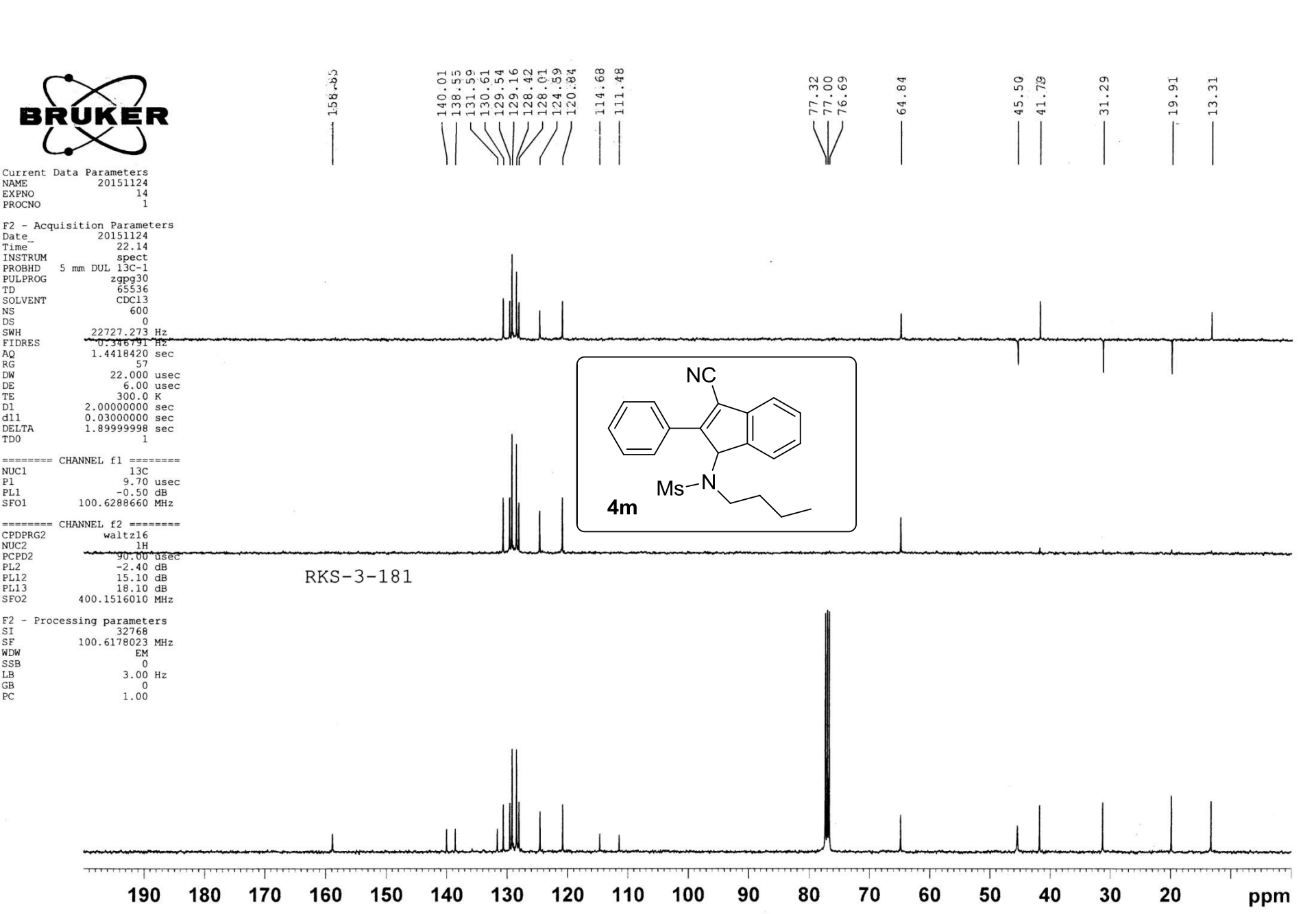
======== CHANNEL f1 ========
NUC1 13C
P1 4.80 usec
PL1 0.00 dB
SFO1 150.5094992 MHz

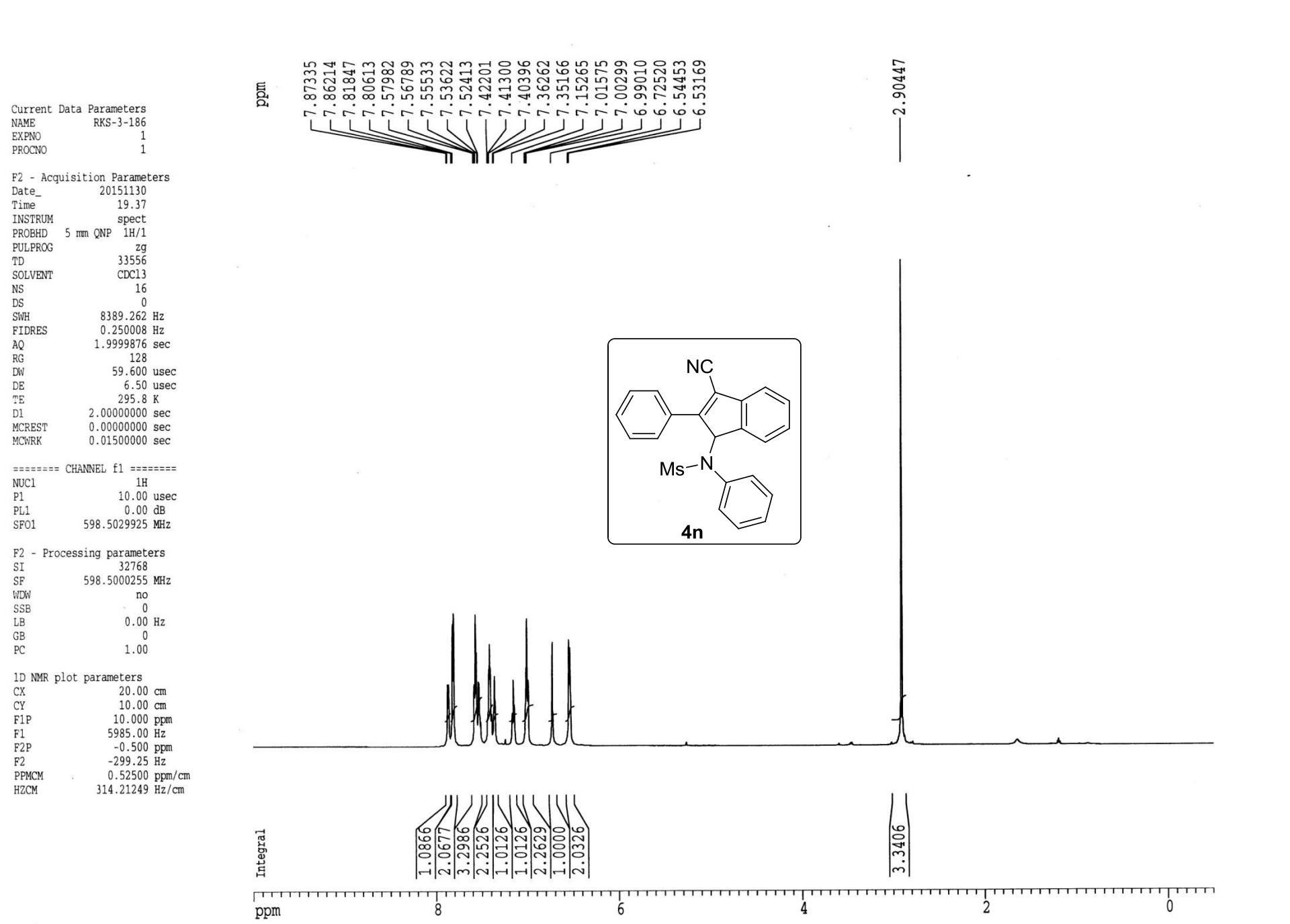
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 92.00 usec
PL2 120.00 dB
PL12 9.00 dB
PL13 14.00 dB
SFO2 598.5029925 MHz

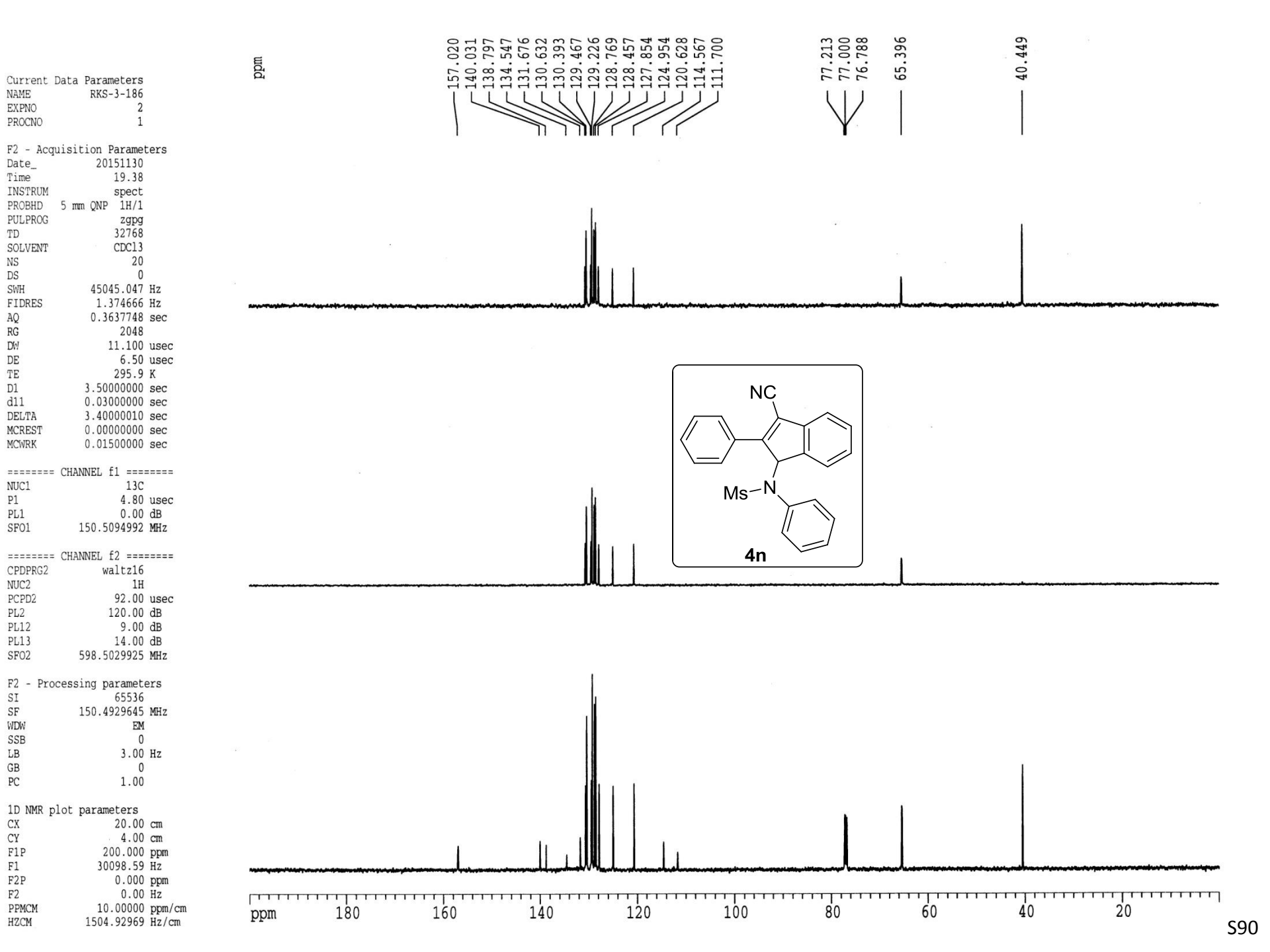
F2 - Processing parameters
SI 65536
SF 150.4929597 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.00

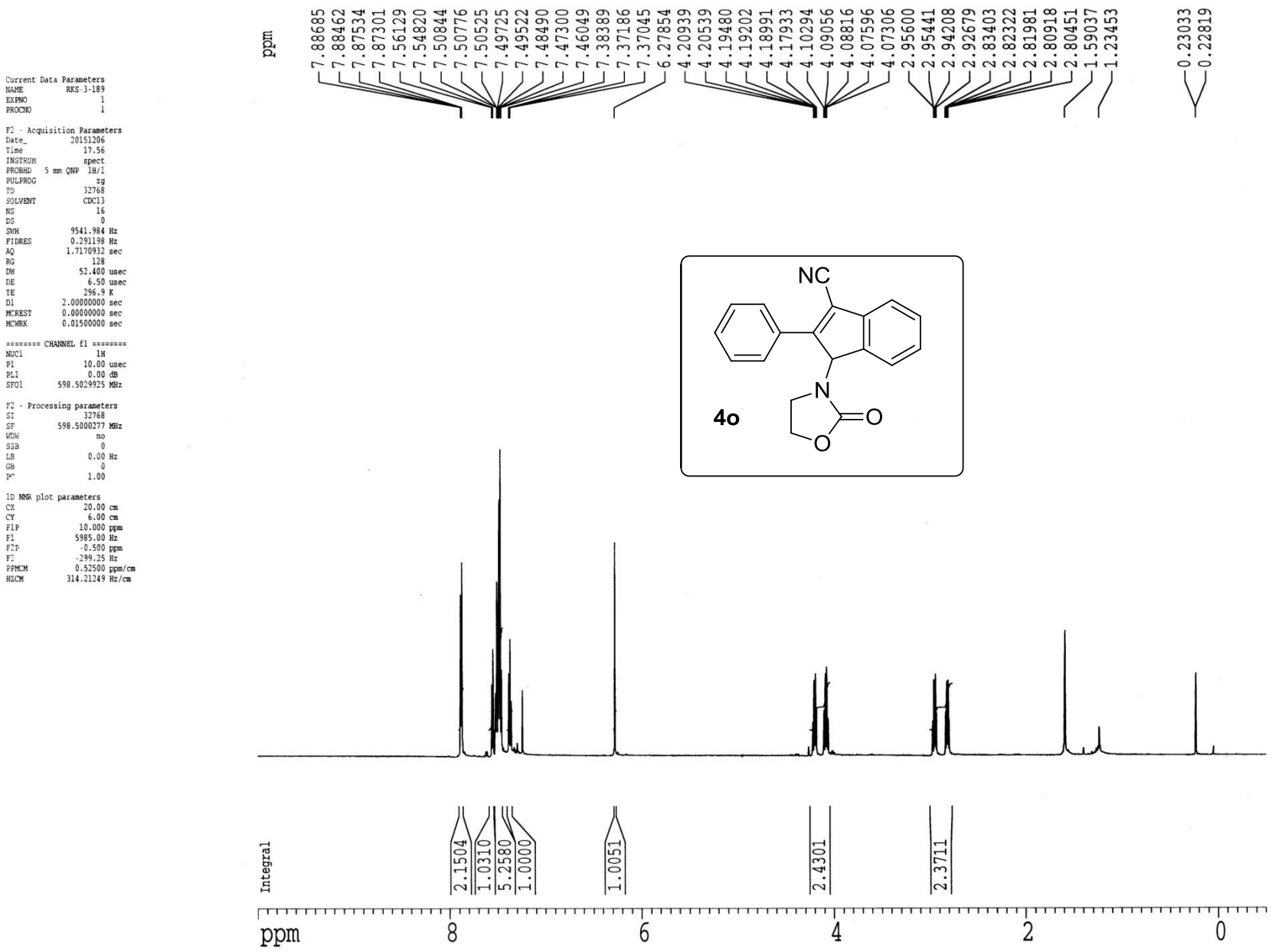
1D NMR plot parameters
CX 20.00 cm
CY 4.00 cm
F1P 200.000 ppm
F1 30098.59 Hz
F2P 0.000 ppm
F2 0.00 Hz
PPMCM 10.00000 ppm/cm
HZCM 1504.92969 Hz/cm

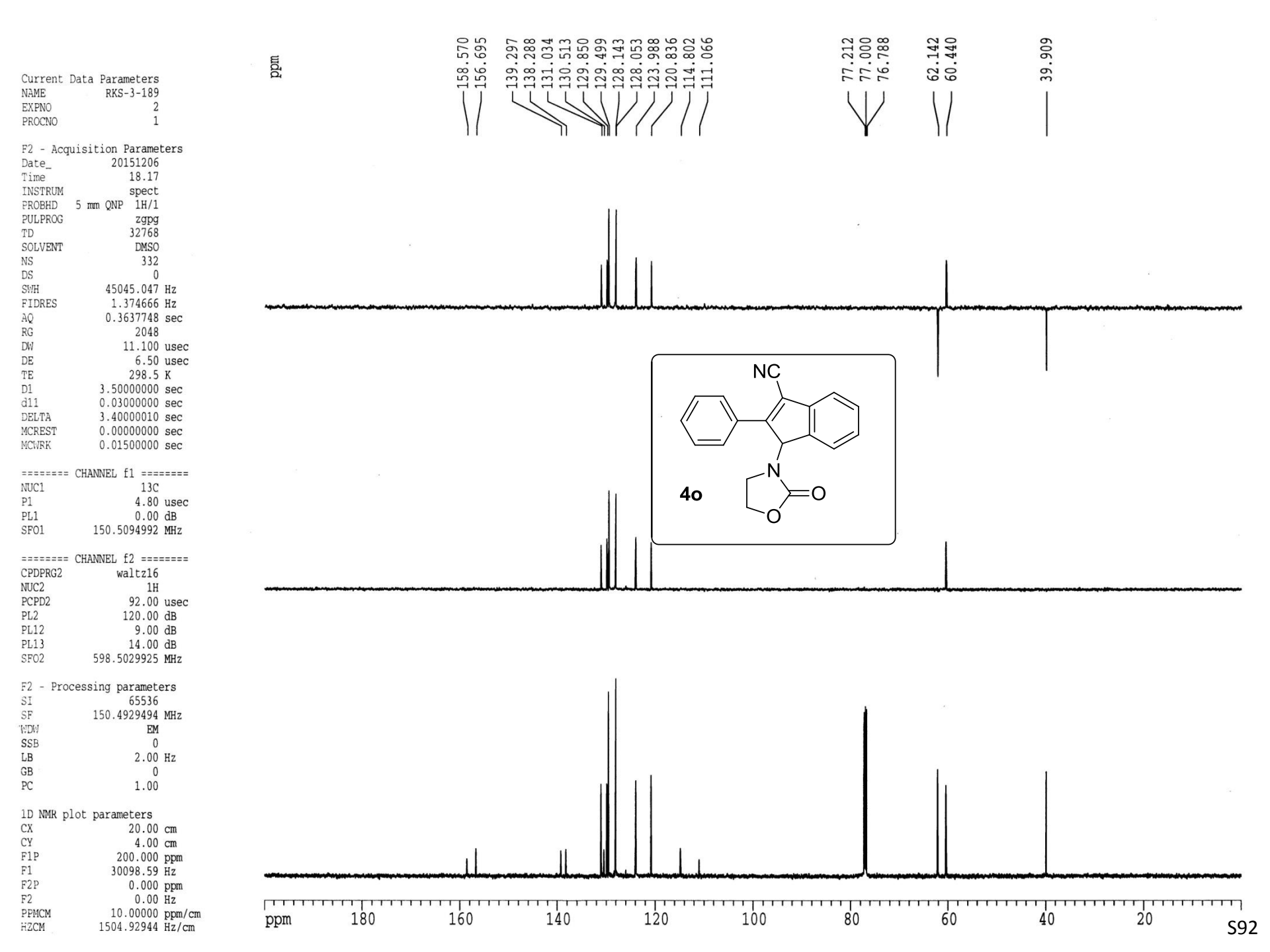

Current Data Parameters
NAME RKS-3-181-P
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20160804
Time 13.00
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 32
DS 0
SWH 8389.262 Hz
FIDRES 0.256020 Hz
AQ 1.9530228 sec
RG 512
DW 59.600 usec
DE 6.50 usec
TE 266.4 K
D1 2.00000000 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 598.5000314 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 314.21252 Hz/cm
ppm
7.78692
7.78455
7.77274
7.56104
7.54839
7.54727
7.53993
7.53764
7.53461
7.52602
7.52337
7.51328
7.49791
7.49588
7.49384
7.48403
7.47947
7.47339
7.46091
7.39601
7.39424
7.38355
7.38178
7.37103
7.36930
7.23989
7.23702
7.23623
6.36727
3.00161
2.84898
2.83652
2.82392
2.81075
2.46782
2.45531
2.44302
2.43069
2.41814
1.73767
0.91186
0.89878
0.88604
0.87343
0.83848
0.82826
0.81625
0.80389
0.79160
0.78198
0.77002
0.75766
0.74742
0.55511
0.54296
0.53091
NC
Ms
N
4m
Integral
2.0000
6.3791
1.1916
1.0103
3.1516
1.2045
1.2250
2.2108
2.2335
3.0275
ppm
8
6
4
2
0

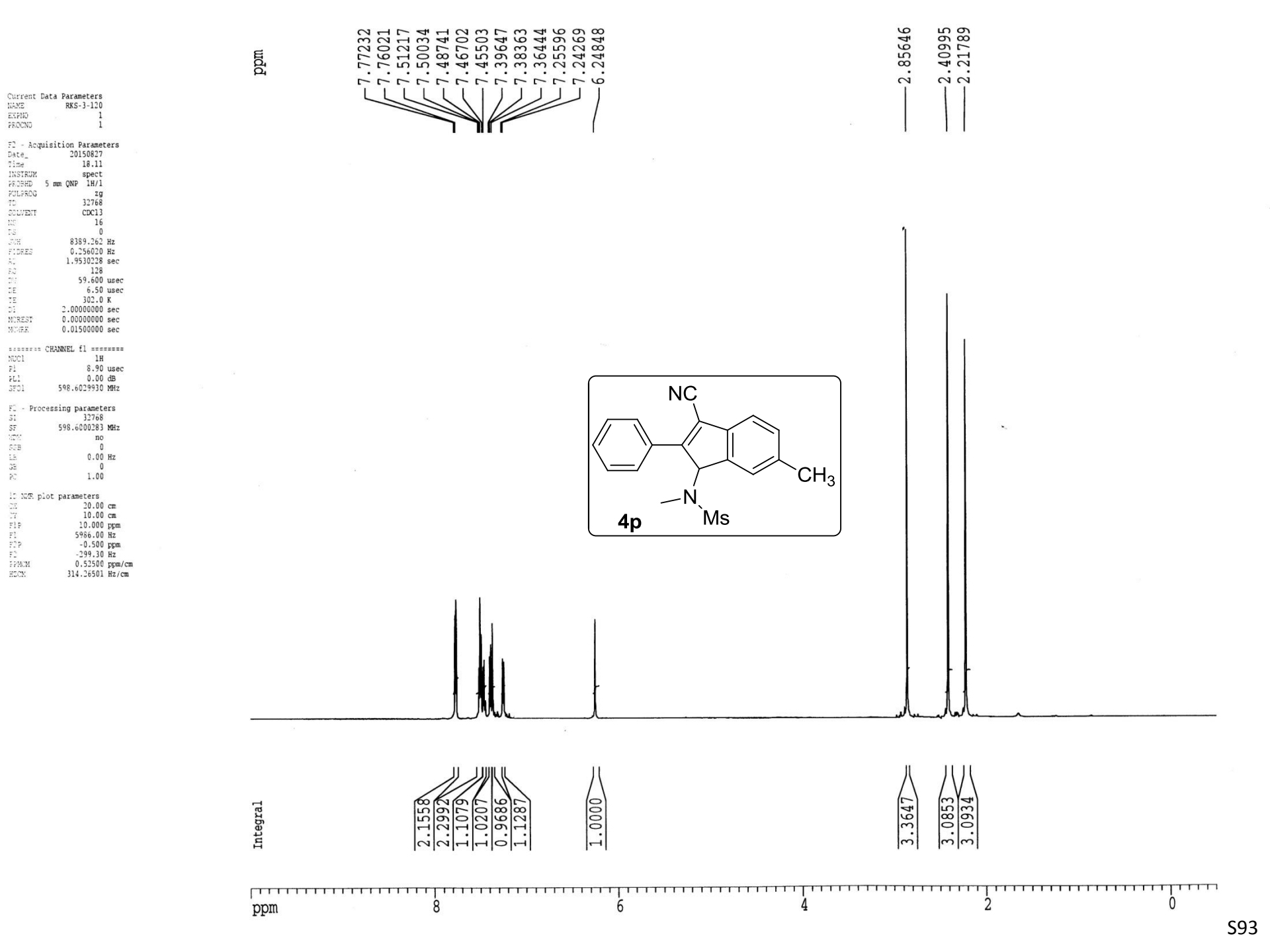

158.55
140.01
138.55
131.59
130.61
129.54
129.16
128.42
128.01
124.59
120.84
114.68
111.48
77.32
77.00
76.69
64.84
45.50
41.73
31.29
19.91
13.31
Current Data Parameters
NAME 20151124
EXPNO 14
PROCNO 1
F2 - Acquisition Parameters
Date_ 20151124
Time 22.14
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 600
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 100.6178023 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
NC
Ms
N
4m
RKS-3-181
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

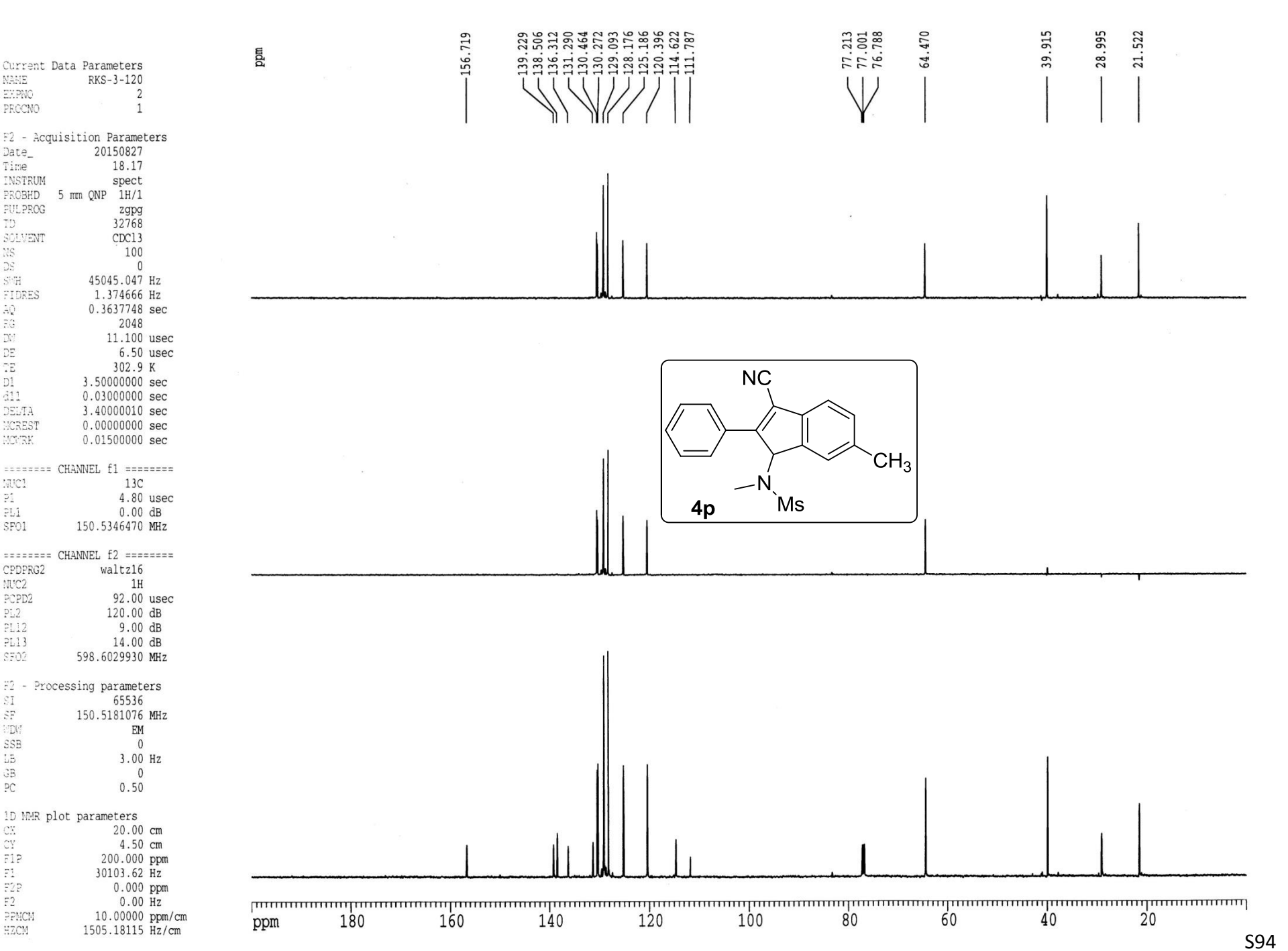

Current Data Parameters
NAME RKS-3-186
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20151130
Time 19.37
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg
TD 33556
SOLVENT CDCl3
NS 16
DS 0
SWH 8389.262 Hz
FIDRES 0.250008 Hz
AQ 1.9999876 sec
RG 128
DW 59.600 usec
DE 6.50 usec
TE 295.8 K
D1 2.00000000 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 598.5000255 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
7.87335
7.86214
7.81847
7.80613
7.57982
7.56789
7.55533
7.53622
7.52413
7.42201
7.41300
7.40396
7.36262
7.35166
7.15265
7.01575
7.00299
6.99010
6.72520
6.54453
6.53169
2.90447
NC
Ms–N
4n
Integral
1.0866
2.0677
3.2986
2.2526
1.0126
1.0126
2.2629
1.0000
2.0326
3.3406
ppm
8
6
4
2
0

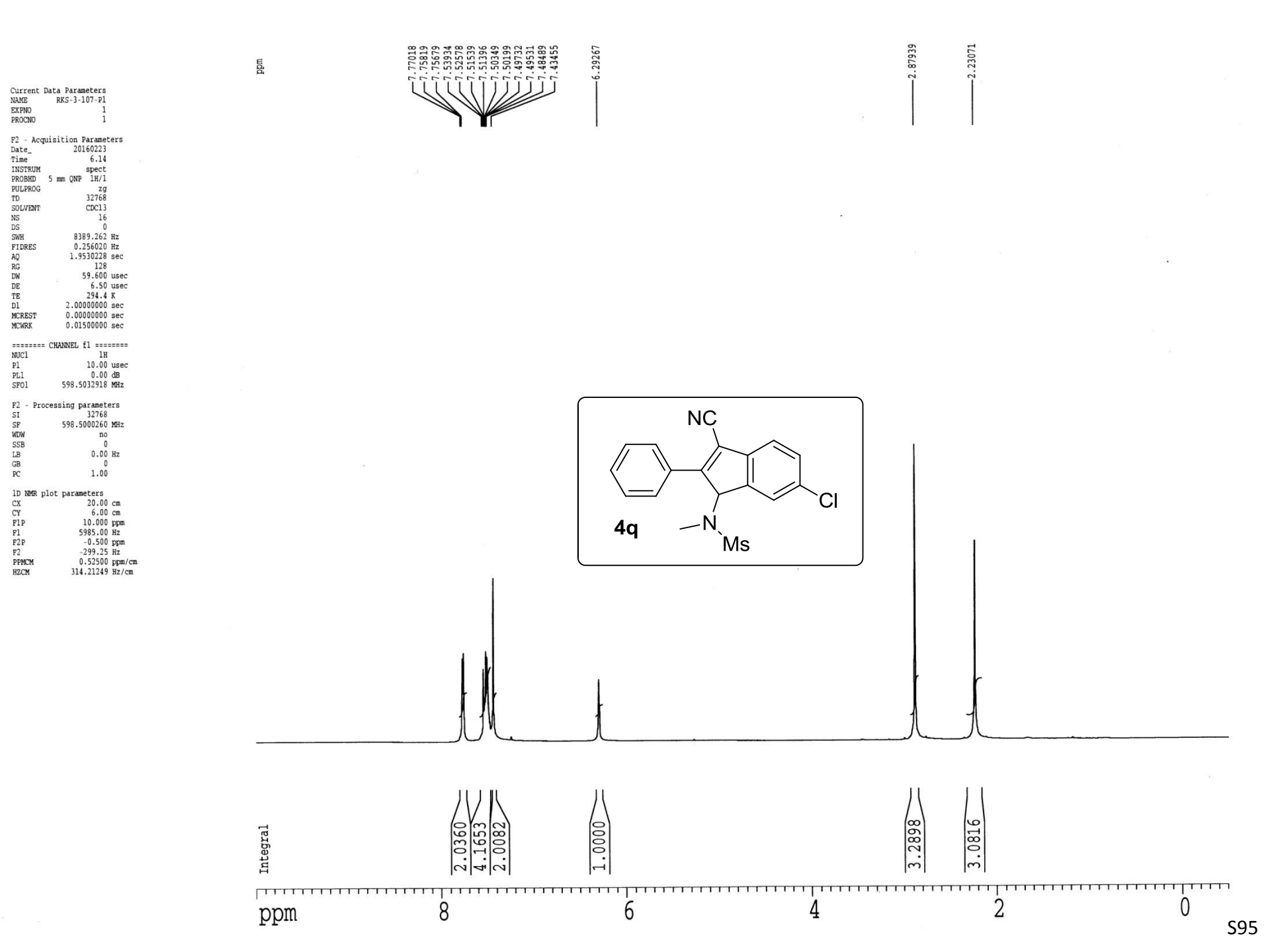

Current Data Parameters
NAME RKS-3-186
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20151130
Time 19.38
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 20
DS 0
SWH 45045.047 Hz
FIDRES 1.374666 Hz
AQ 0.3637748 sec
RG 2048
DW 11.100 usec
DE 6.50 usec
TE 295.9 K
D1 3.50000000 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 150.5094992 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 150.4929645 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 1504.92969 Hz/cm
ppm
157.020
140.031
138.797
134.547
131.676
130.632
130.393
129.467
129.226
128.769
128.457
127.854
124.954
120.628
114.567
111.700
77.213
77.000
76.788
65.396
40.449
NC
Ms–N
4n
ppm
180
160
140
120
100
80
60
40
20

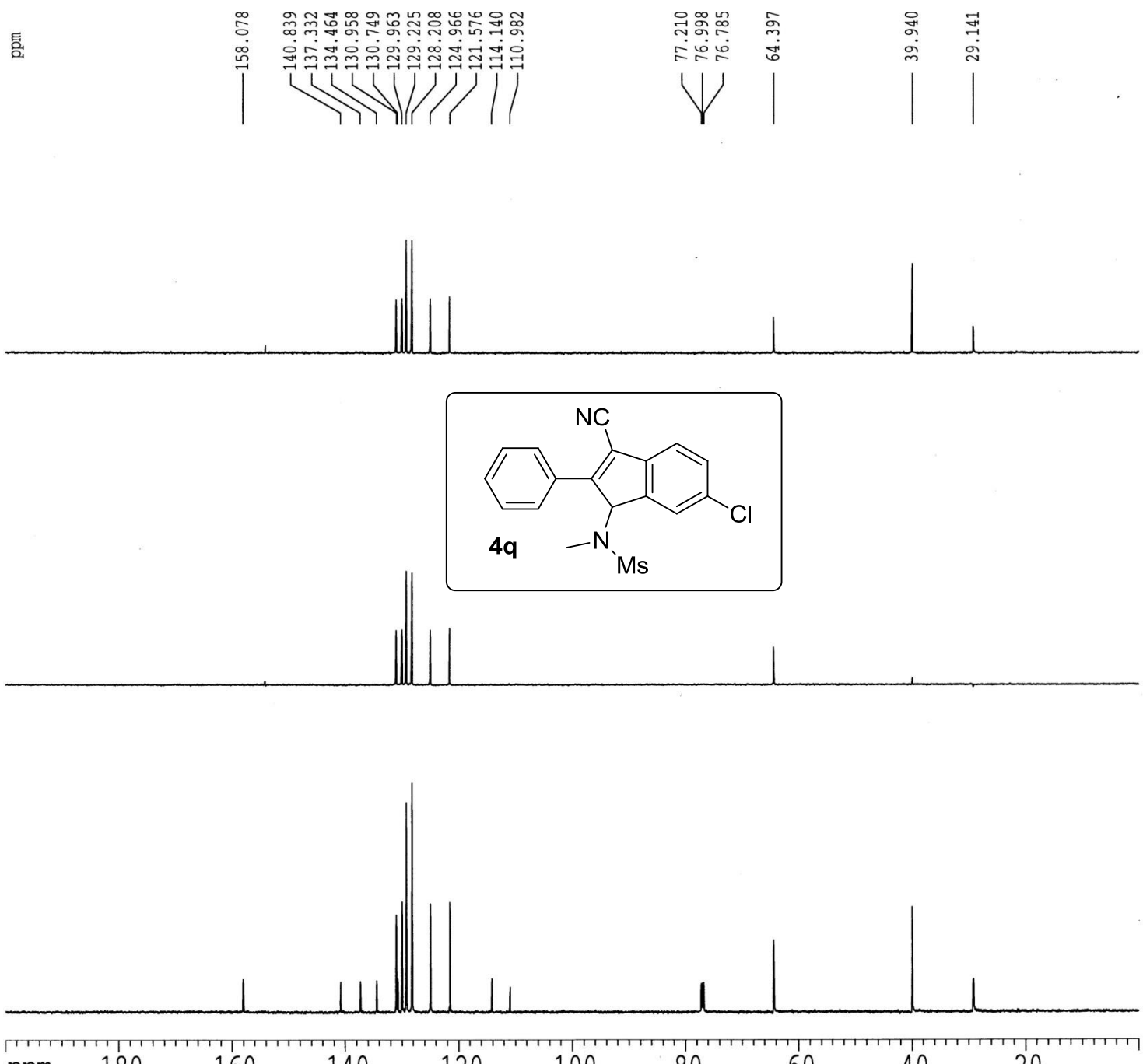

Current Data Parameters
NAME RKS-3-189
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20151206
Time 17.56
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 9541.984 Hz
FIDRES 0.291198 Hz
AQ 1.7170932 sec
RG 128
DW 52.400 usec
DE 6.50 usec
TE 296.9 K
D1 2.00000000 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 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
7.88685
7.88462
7.87534
7.87301
7.56129
7.54820
7.50844
7.50776
7.50525
7.49725
7.49522
7.48490
7.47300
7.46049
7.38389
7.37186
7.37045
6.27854
4.20939
4.20539
4.19480
4.19202
4.18991
4.17933
4.10294
4.09056
4.08816
4.07596
4.07306
2.95600
2.95441
2.94208
2.92679
2.83403
2.82322
2.81981
2.80918
2.80451
1.59037
1.23453
0.23033
0.22819
NC
N
O
O
4o
Integral
2.1504
1.0310
5.2580
1.0000
1.0051
2.4301
2.3711
ppm
8
6
4
2
0


Current Data Parameters
NAME RKS-3-189
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20151206
Time 18.17
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT DMSO
NS 332
DS 0
SWH 45045.047 Hz
FIDRES 1.374666 Hz
AQ 0.3637748 sec
RG 2048
DW 11.100 usec
DE 6.50 usec
TE 298.5 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 150.4929494 MHz
WDW EM
SSB 0
LB 2.00 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
158.570
156.695
139.297
138.288
131.034
130.513
129.850
129.499
128.143
128.053
123.988
120.836
114.802
111.066
77.212
77.000
76.788
62.142
60.440
39.909
NC
N
O
O
4o
ppm
180
160
140
120
100
80
60
40
20


Current Data Parameters
NAME RKS-3-120
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20150827
Time 18.11
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 302.0 K
D1 2.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 8.90 usec
PL1 0.00 dB
SFO1 598.6029930 MHz
F2 - Processing parameters
SI 32768
SF 598.6000283 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
ppm
7.77232
7.76021
7.51217
7.50034
7.48741
7.46702
7.45503
7.39647
7.38363
7.36444
7.25596
7.24269
6.24848
2.85646
2.40995
2.21789
NC
CH3
N
Ms
4p
Integral
2.1558
2.2992
1.1079
1.0207
0.9686
1.1287
1.0000
3.3647
3.0853
3.0934
ppm
8
6
4
2
0


Current Data Parameters
NAME RKS-3-120
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20150827
Time 18.17
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 2048
DW 11.100 usec
DE 6.50 usec
TE 302.9 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 150.5346470 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 150.5181076 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 0.50
1D NMR plot parameters
CX 20.00 cm
CY 4.50 cm
F1P 200.000 ppm
F1 30103.62 Hz
F2P 0.000 ppm
F2 0.00 Hz
PPMCM 10.00000 ppm/cm
HZCM 1505.18115 Hz/cm
ppm
156.719
139.229
138.506
136.312
131.290
130.464
130.272
129.093
128.176
125.186
120.396
114.622
111.787
77.213
77.001
76.788
64.470
39.915
28.995
21.522
NC
CH3
N
Ms
4p
ppm
180
160
140
120
100
80
60
40
20


Current Data Parameters
NAME RKS-3-107-P1
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20160223
Time 6.14
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 294.4 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 598.5032918 MHz
F2 - Processing parameters
SI 32768
SF 598.5000260 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
7.77018
7.75819
7.75679
7.53934
7.52578
7.51539
7.51396
7.50349
7.50199
7.49732
7.49531
7.48489
7.43455
6.29267
2.87939
2.23071
NC
Cl
4q
N
Ms
Integral
2.0360
4.1653
2.0082
1.0000
3.2898
3.0816
ppm
8
6
4
2
0



Current Data Parameters
NAME RKS-3-107-P1
EXPNO 2
PROCNO 1

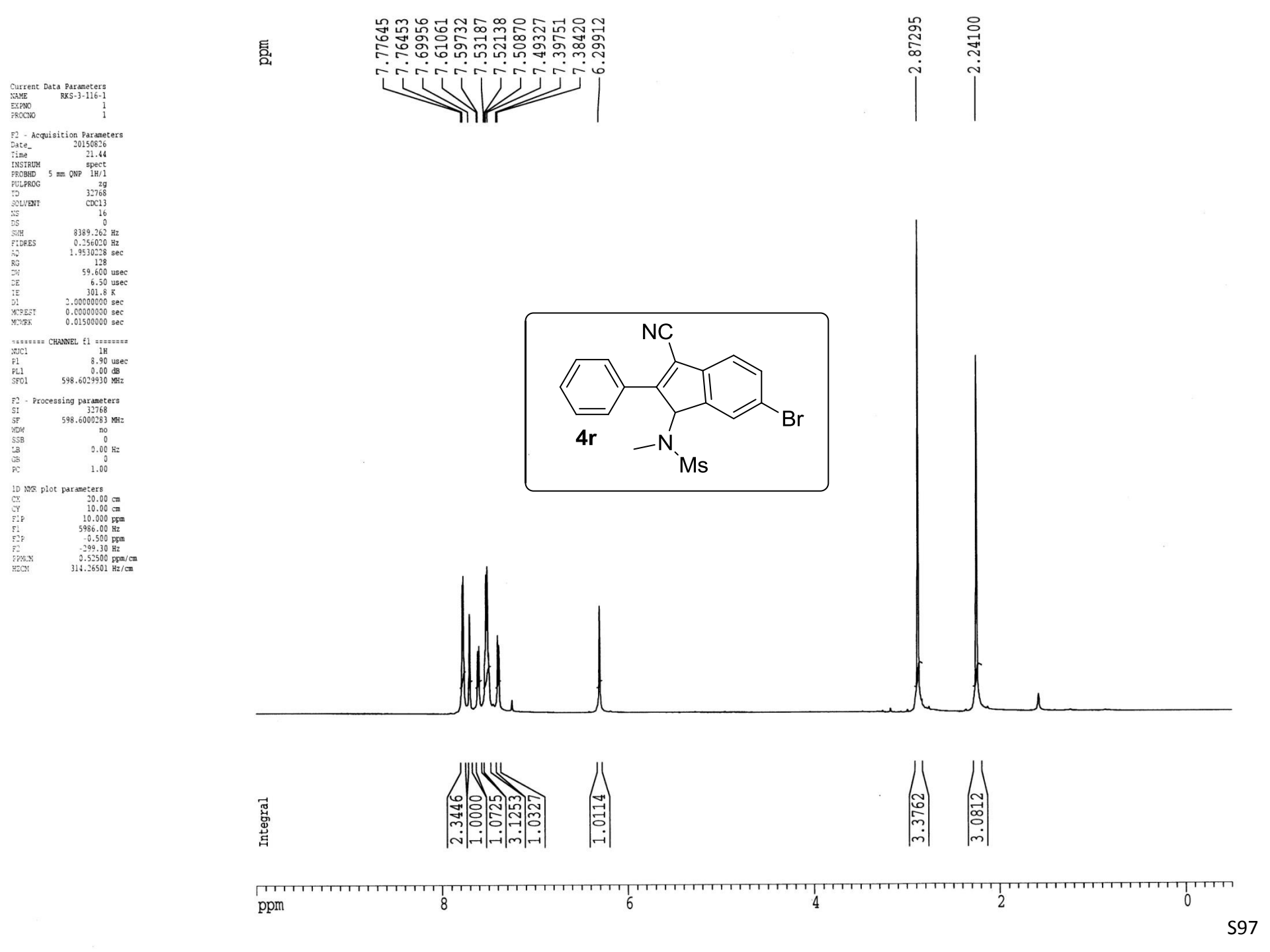
F2 - Acquisition Parameters
Date_ 20160223
Time 6.21
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 100
DS 0
SWH 45045.047 Hz
FIDRES 1.374666 Hz
AQ 0.3637748 sec
RG 4096
DW 11.100 usec
DE 6.50 usec
TE 296.6 K
D1 3.50000000 sec
d11 0.03000000 sec
DELTA 3.40000010 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

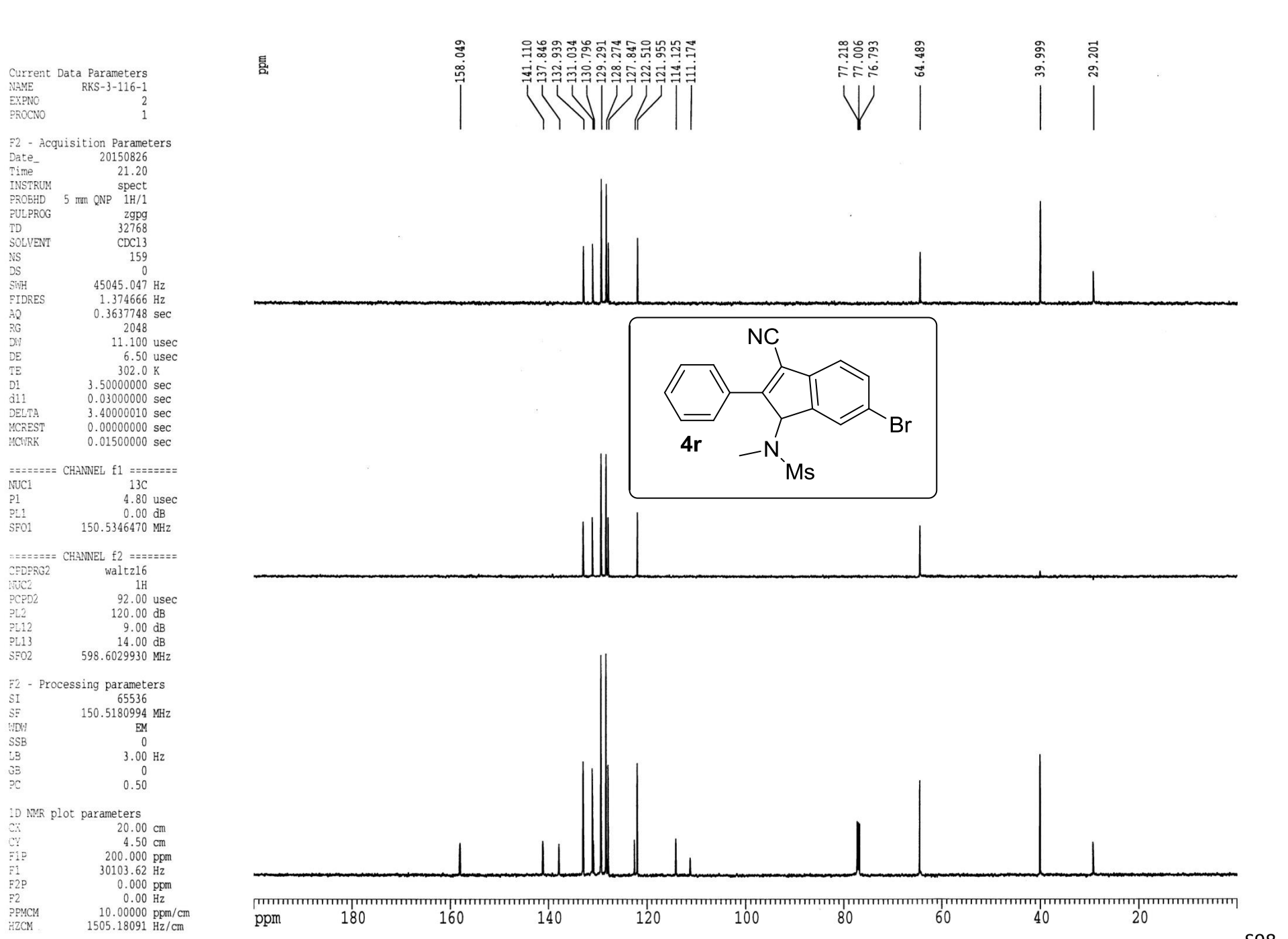
======== CHANNEL f1 ========
NUC1 13C
P1 4.80 usec
PL1 0.00 dB
SFO1 150.5094992 MHz

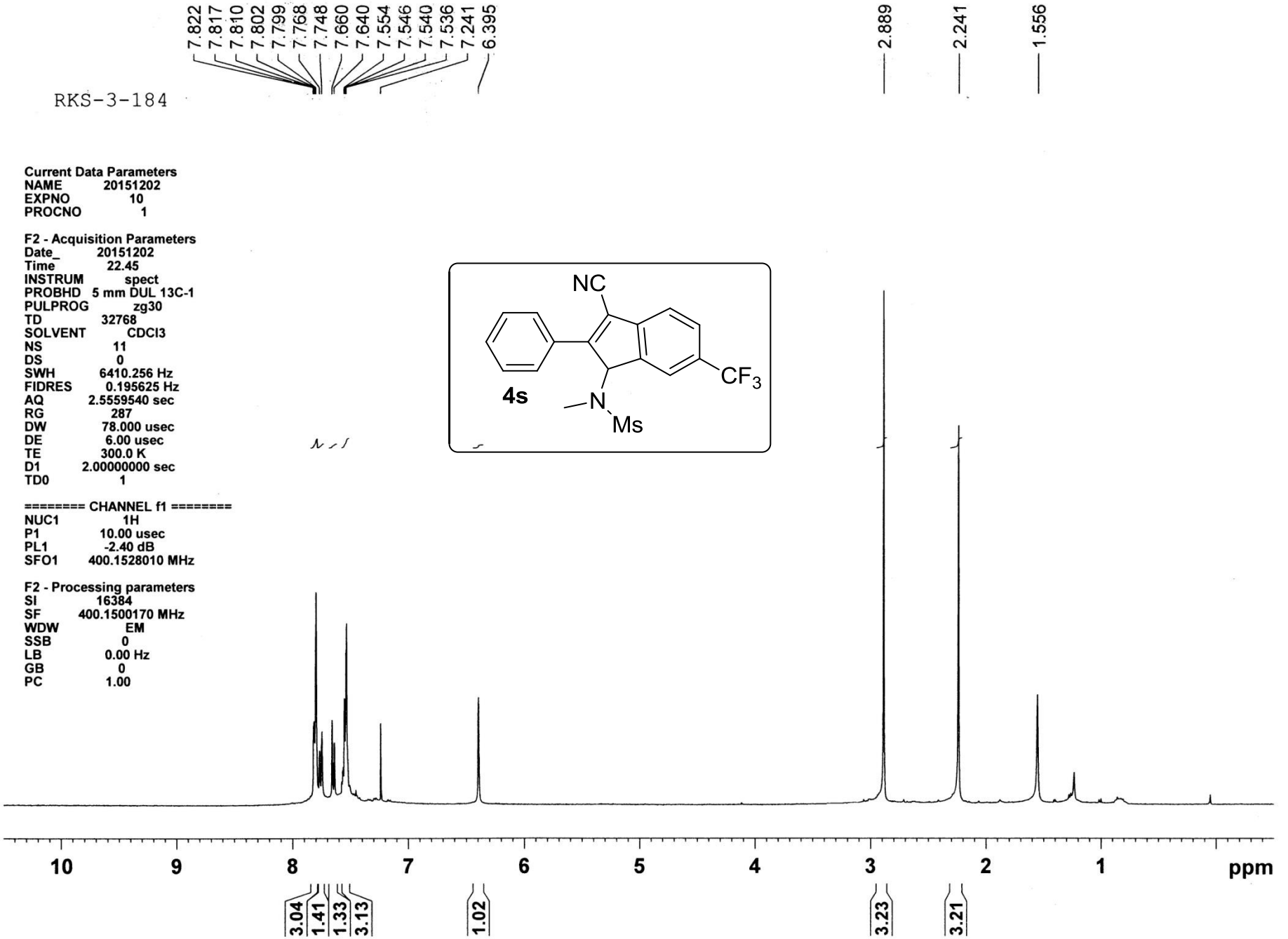
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 92.00 usec
PL2 120.00 dB
PL12 9.00 dB
PL13 14.00 dB
SFO2 598.5029925 MHz

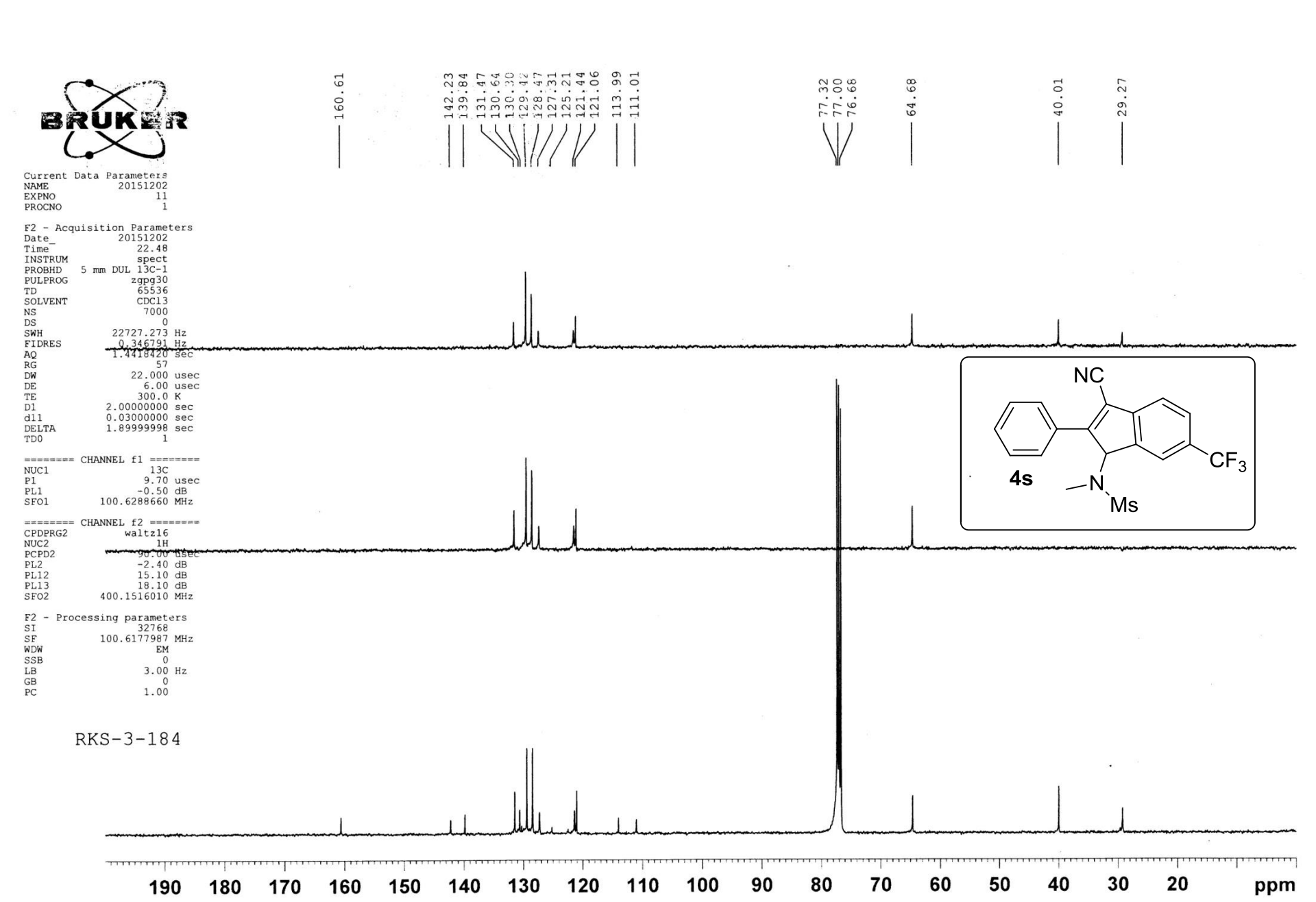
F2 - Processing parameters
SI 65536
SF 150.4929625 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00

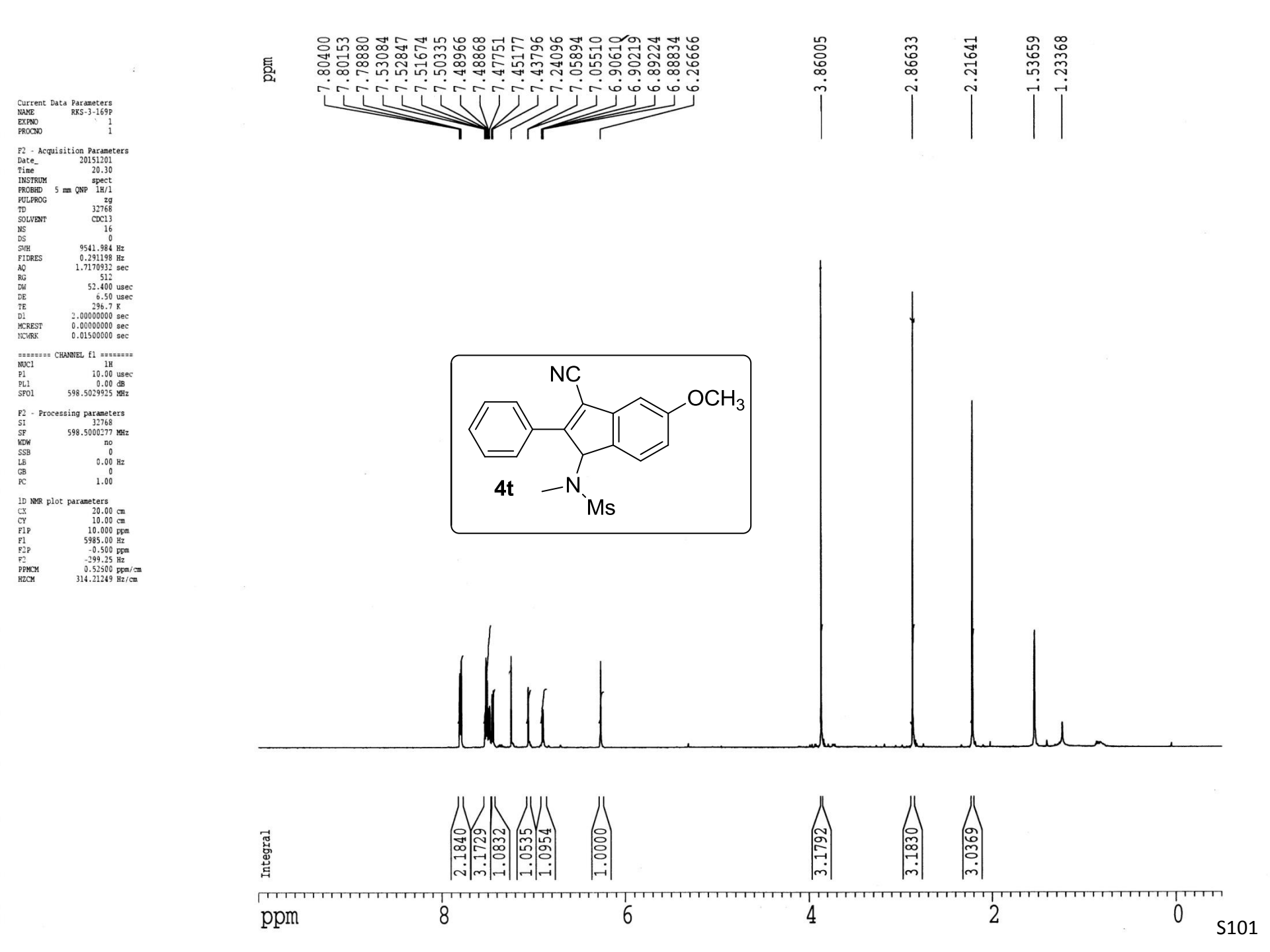
1D NMR plot parameters
CX 20.00 cm
CY 4.00 cm
F1P 200.000 ppm
F1 30098.59 Hz
F2P 0.000 ppm
F2 0.00 Hz
PPMCM 10.00000 ppm/cm
HZCM 1504.92969 Hz/cm

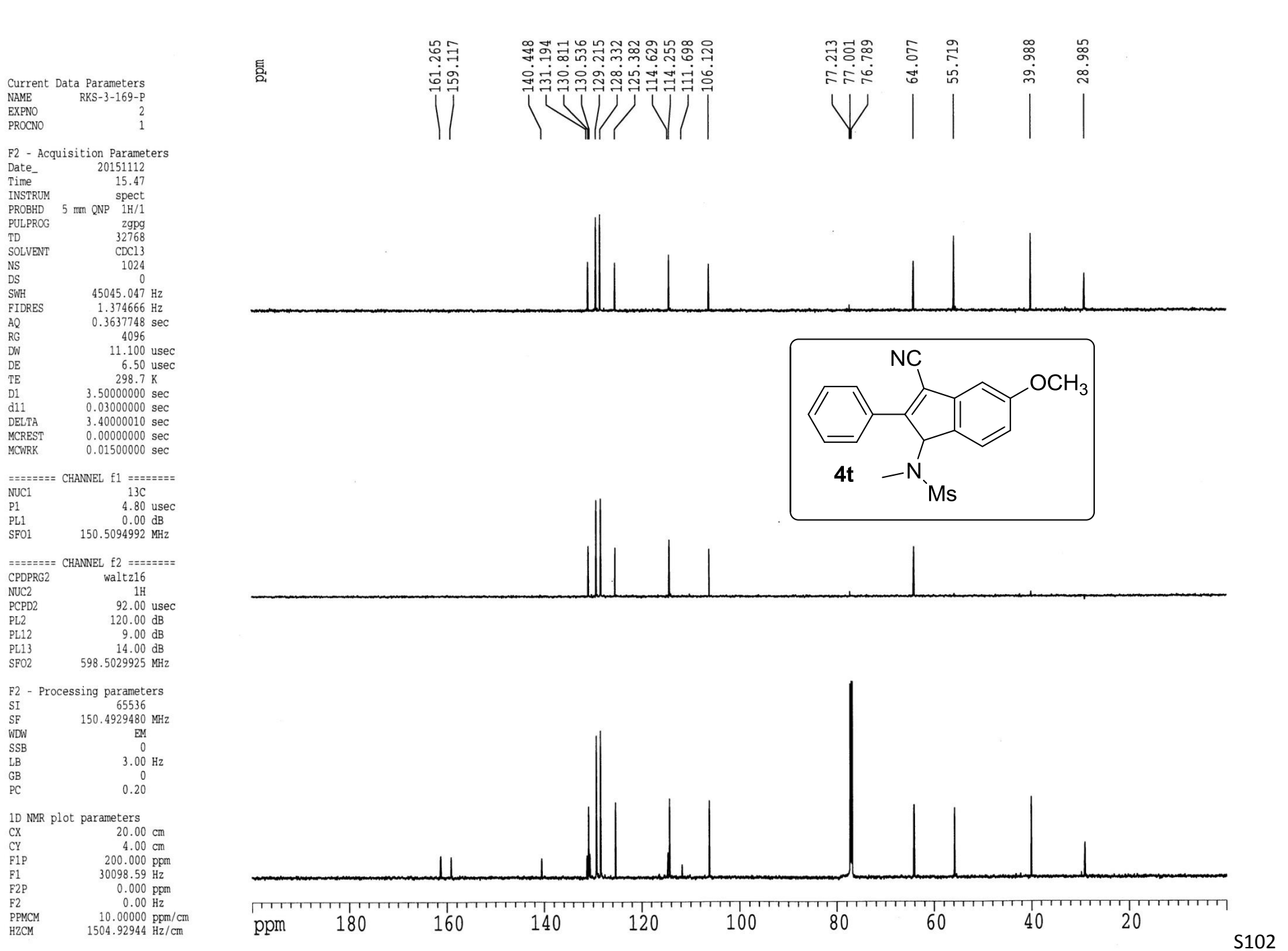

Current Data Parameters
NAME RKS-3-116-1
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20150826
Time 21.44
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 8389.262 Hz
FIDRES 0.256020 Hz
AQ 1.9530228 sec
RG 128
DW 59.600 usec
DE 6.50 usec
TE 301.8 K
D1 2.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 8.90 usec
PL1 0.00 dB
SFO1 598.6029930 MHz
F2 - Processing parameters
SI 32768
SF 598.6000283 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
ppm
7.77645
7.76453
7.69956
7.61061
7.59732
7.53187
7.52138
7.50870
7.49327
7.39751
7.38420
6.29912
2.87295
2.24100
NC
Br
4r
N
Ms
Integral
2.3446
1.0000
1.0725
3.1253
1.0327
1.0114
3.3762
3.0812
ppm
8
6
4
2
0


Current Data Parameters
NAME RKS-3-116-1
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20150826
Time 21.20
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 159
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 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 150.5346470 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 150.5180994 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 0.50
1D NMR plot parameters
CX 20.00 cm
CY 4.50 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
158.049
141.110
137.846
132.939
131.034
130.796
129.291
128.274
127.847
122.510
121.955
114.125
111.174
77.218
77.006
76.793
64.489
39.999
29.201
NC
Br
4r
N
Ms
ppm
180
160
140
120
100
80
60
40
20

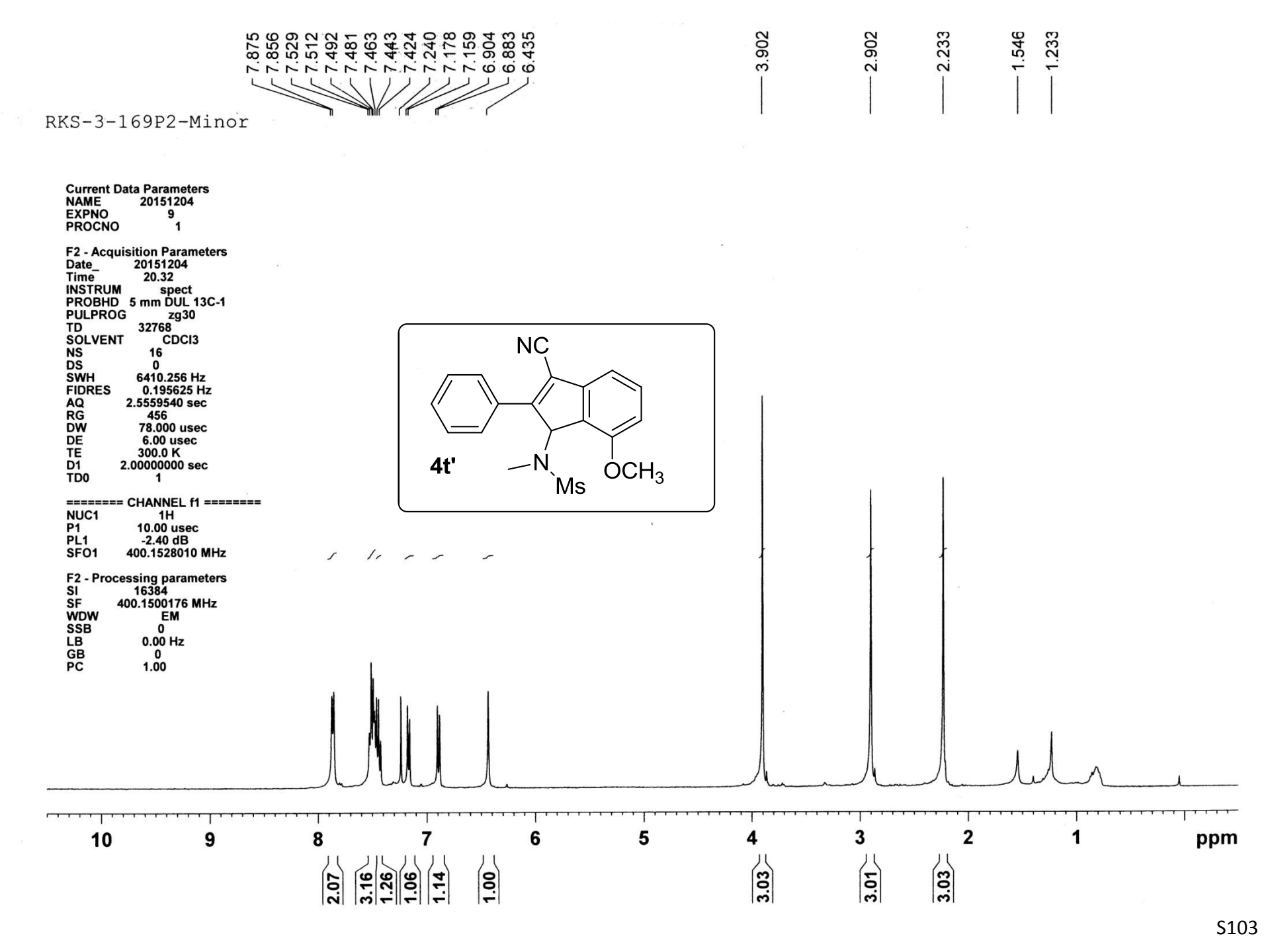

7.822
7.817
7.810
7.802
7.799
7.768
7.748
7.660
7.640
7.554
7.546
7.540
7.536
7.241
6.395
2.889
2.241
1.556
RKS-3-184
Current Data Parameters
NAME 20151202
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20151202
Time 22.45
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 11
DS 0
SWH 6410.256 Hz
FIDRES 0.195625 Hz
AQ 2.5559540 sec
RG 287
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
NC
CF3
4s
N
Ms
10
9
8
7
6
5
4
3
2
1
ppm
3.04
1.41
1.33
3.13
1.02
3.23
3.21

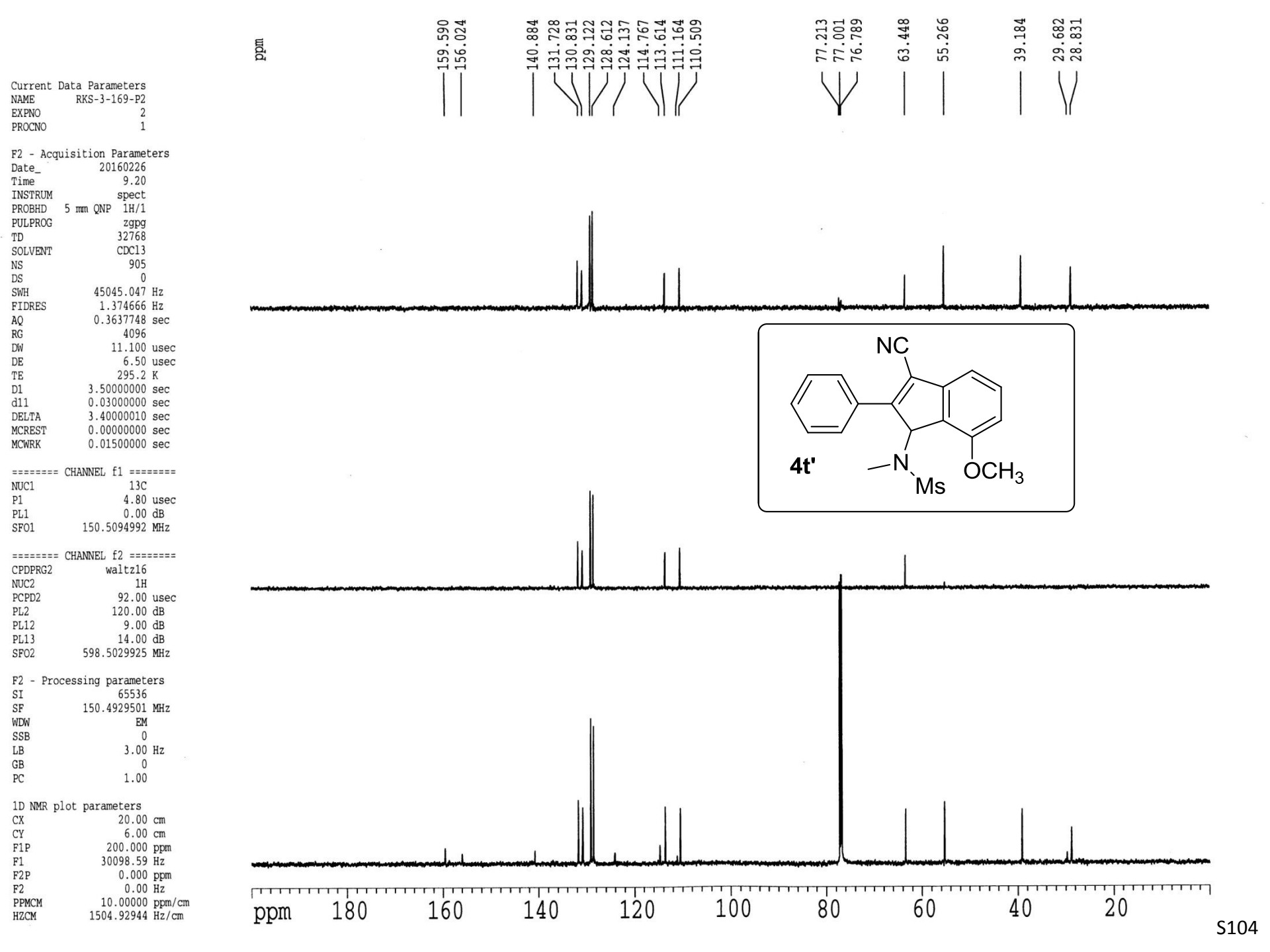

160.61
142.23
139.84
131.47
130.64
130.30
129.42
128.47
127.31
125.21
121.44
121.06
113.99
111.01
77.32
77.00
76.68
64.68
40.01
29.27
Current Data Parameters
NAME 20151202
EXPNO 11
PROCNO 1
F2 - Acquisition Parameters
Date_ 20151202
Time 22.48
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 7000
DS 0
SWH 22727.273 Hz
FIDRES 0.346791 Hz
AQ 1.4418420 sec
RG 57
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
RKS-3-184
NC
CF3
4s
N
Ms
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm


Current Data Parameters
NAME RKS-3-169P
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20151201
Time 20.30
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 9541.984 Hz
FIDRES 0.291198 Hz
AQ 1.7170932 sec
RG 512
DW 52.400 usec
DE 6.50 usec
TE 296.7 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 598.5000277 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
7.80400
7.80153
7.78880
7.53084
7.52847
7.51674
7.50335
7.48966
7.48868
7.47751
7.45177
7.43796
7.24096
7.05894
7.05510
6.90610
6.90219
6.89224
6.88834
6.26666
3.86005
2.86633
2.21641
1.53659
1.23368
NC
OCH3
4t
N
Ms
Integral
2.1840
3.1729
1.0832
1.0535
1.0954
1.0000
3.1792
3.1830
3.0369
ppm
8
6
4
2
0


Current Data Parameters
NAME RKS-3-169-P
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20151112
Time 15.47
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 298.7 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 150.4929480 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 0.20
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
161.265
159.117
140.448
131.194
130.811
130.536
129.215
128.332
125.382
114.629
114.255
111.698
106.120
77.213
77.001
76.789
64.077
55.719
39.988
28.985
NC
OCH3
4t
N
Ms
ppm
180
160
140
120
100
80
60
40
20

RKS-3-169P2-Minor





Current Data Parameters
NAME RKS-3-169-P2
EXPNO 2
PROCNO 1

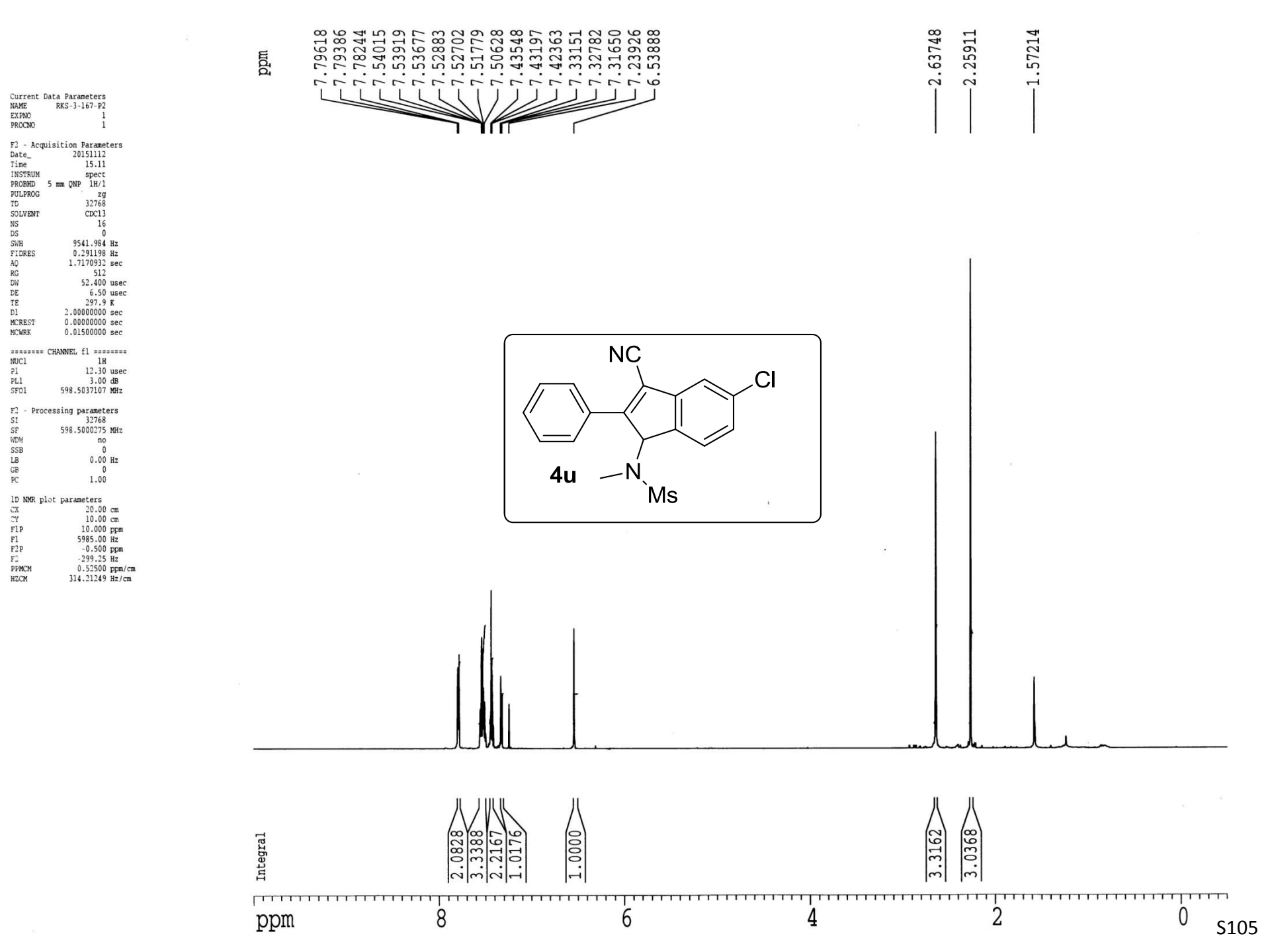
F2 - Acquisition Parameters
Date_ 20160226
Time 9.20
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 905
DS 0
SWH 45045.047 Hz
FIDRES 1.374666 Hz
AQ 0.3637748 sec
RG 4096
DW 11.100 usec
DE 6.50 usec
TE 295.2 K
D1 3.50000000 sec
d11 0.03000000 sec
DELTA 3.40000010 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

======== CHANNEL f1 ========
NUC1 13C
P1 4.80 usec
PL1 0.00 dB
SFO1 150.5094992 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 150.4929501 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-3-167-P2
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20151112
Time 15.11
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 297.9 K
D1 2.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 12.30 usec
PL1 3.00 dB
SFO1 598.5037107 MHz
F2 - Processing parameters
SI 32768
SF 598.5000275 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
7.79618
7.79386
7.78244
7.54015
7.53919
7.53677
7.52883
7.52702
7.51779
7.50628
7.43548
7.43197
7.42363
7.33151
7.32782
7.31650
7.23926
6.53888
2.63748
2.25911
1.57214
NC
Cl
4u
N
Ms
Integral
2.0828
3.3388
2.2167
1.0176
1.0000
3.3162
3.0368
ppm
8
6
4
2
0

Current Data Parameters
NAME RKS-3-167-P2
EXPNO 2
PROCNO 1

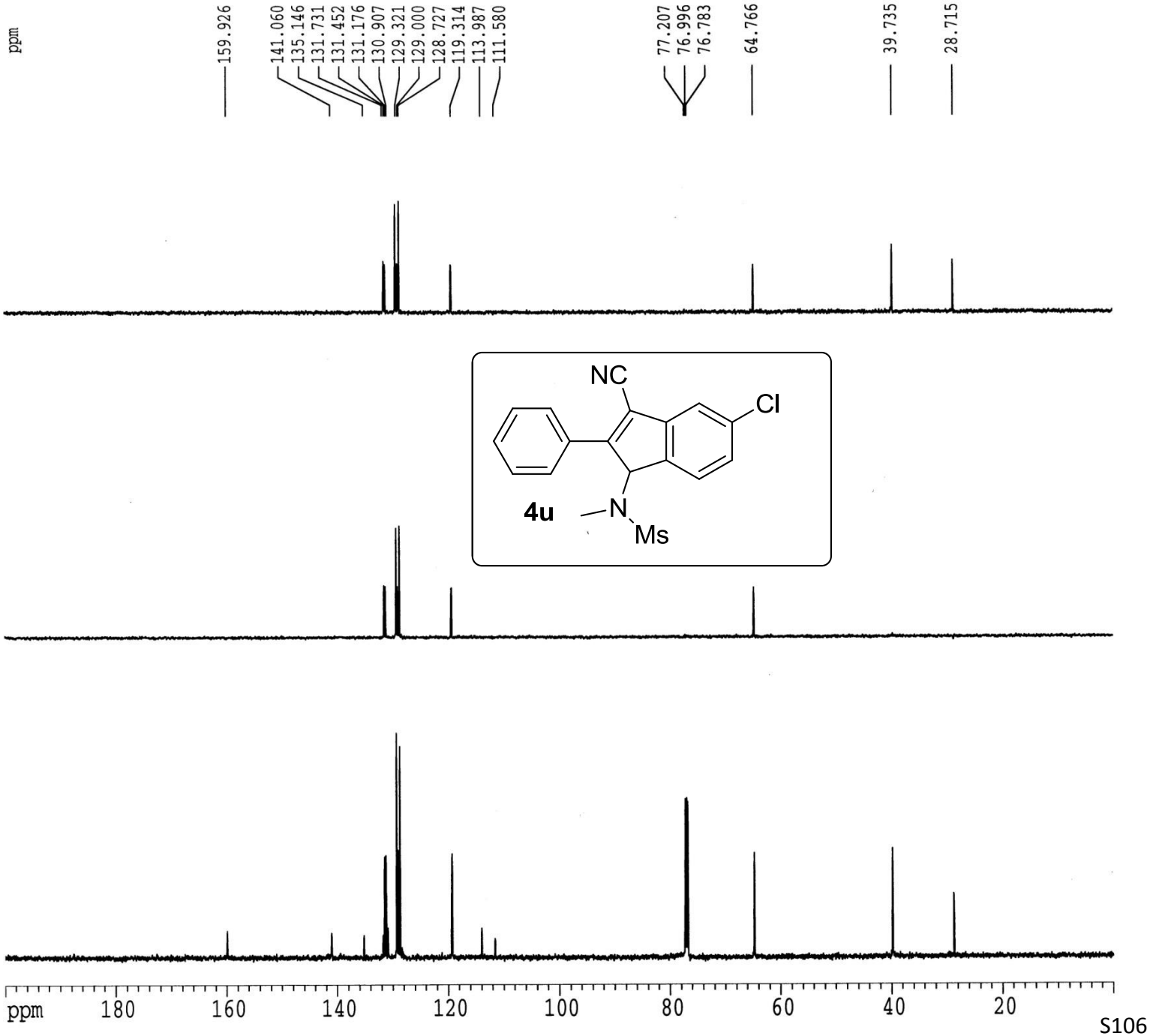
F2 - Acquisition Parameters
Date_ 20151112
Time 15.14
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 207
DS 0
SWH 45045.047 Hz
FIDRES 1.374666 Hz
AQ 0.3637748 sec
RG 4096
DW 11.100 usec
DE 6.50 usec
TE 298.7 K
D1 3.50000000 sec
d11 0.03000000 sec
DELTA 3.40000010 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

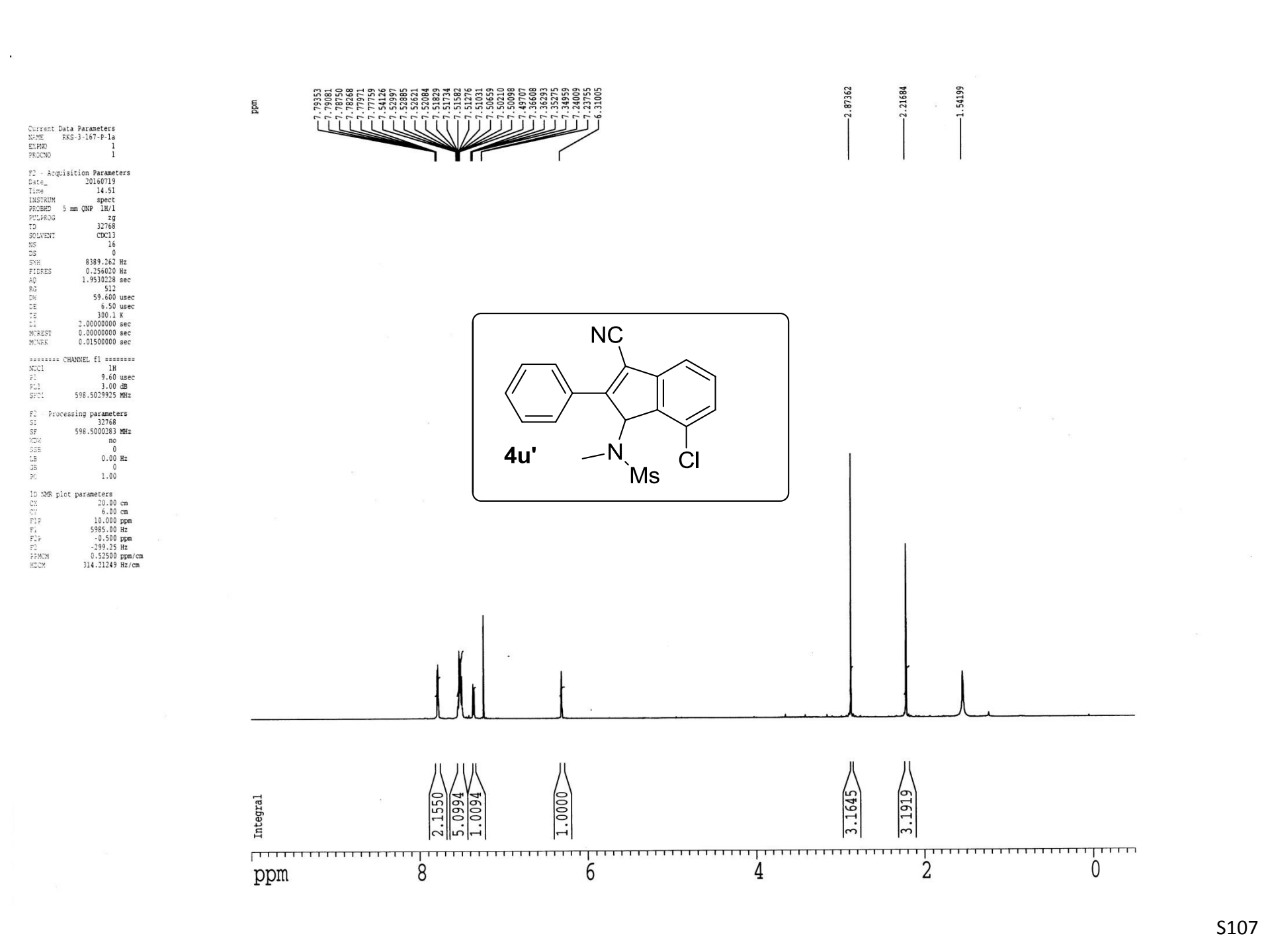
======== CHANNEL f1 ========
NUC1 13C
P1 4.80 usec
PL1 0.00 dB
SFO1 150.5094992 MHz

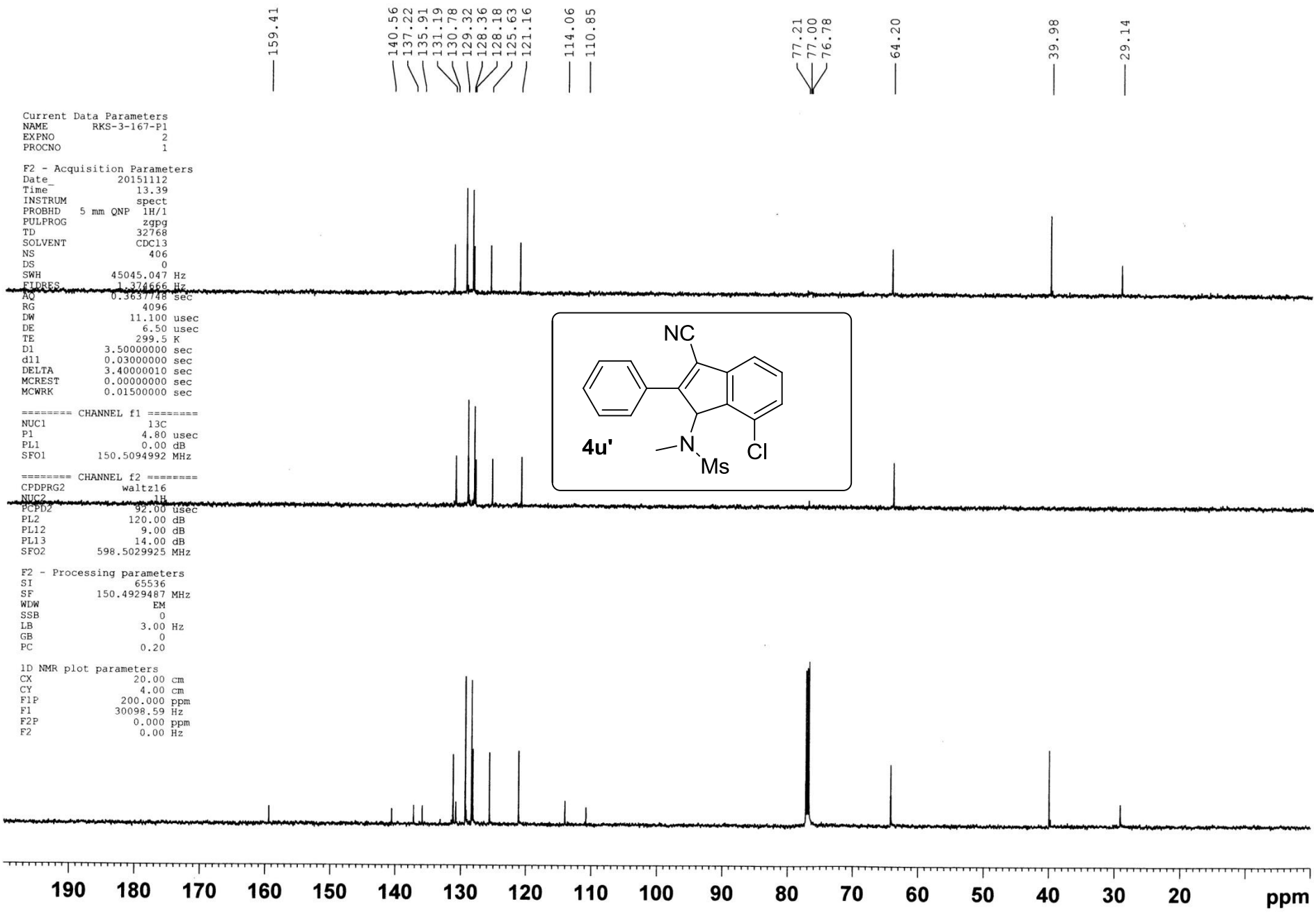
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 92.00 usec
PL2 120.00 dB
PL12 9.00 dB
PL13 14.00 dB
SFO2 598.5029925 MHz

F2 - Processing parameters
SI 65536
SF 150.4929515 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 0.20

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-3-167-P-1a
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20160719
Time 14.51
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 300.1 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
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
7.79353
7.79081
7.78750
7.78268
7.77971
7.77759
7.54126
7.52997
7.52885
7.52621
7.52084
7.51829
7.51734
7.51582
7.51276
7.51031
7.50659
7.50210
7.50098
7.49707
7.36608
7.36293
7.35275
7.34959
7.24009
7.23755
6.31005
2.87362
2.21684
1.54199
NC
4u'
N
Ms
Cl
Integral
2.1550
5.0994
1.0094
1.0000
3.1645
3.1919
ppm
8
6
4
2
0


159.41
140.56
137.22
135.91
131.19
130.78
129.32
128.36
128.18
125.63
121.16
114.06
110.85
77.21
77.00
76.78
64.20
39.98
29.14
Current Data Parameters
NAME RKS-3-167-P1
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20151112
Time 13.39
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 406
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 299.5 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 150.4929487 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 0.20
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
NC
4u'
N
Ms
Cl
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

```
Current Data Parameters
NAME          SKP-05-72
EXPNO                 1
PROCNO                1

F1 - Acquisition Parameters
Date_           20150319
Time              14.12
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                  128
DW               41.600 usec
DE                6.50 usec
TE               296.0 K
D1           2.00000000 sec
MCREST       0.00000000 sec
MCWRK        0.01500000 sec

======== CHANNEL f1 ========
NUC1                 1H
P1                10.00 usec
PL1                0.00 dB
SFO1        598.6035916 MHz

F2 - Processing parameters
SI                32768
SF          598.6000298 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              5986.00 Hz
F2P               0.500 ppm
F2              -299.30 Hz
PPMCM          0.52500 ppm/cm
HZCM          314.26501 Hz/cm
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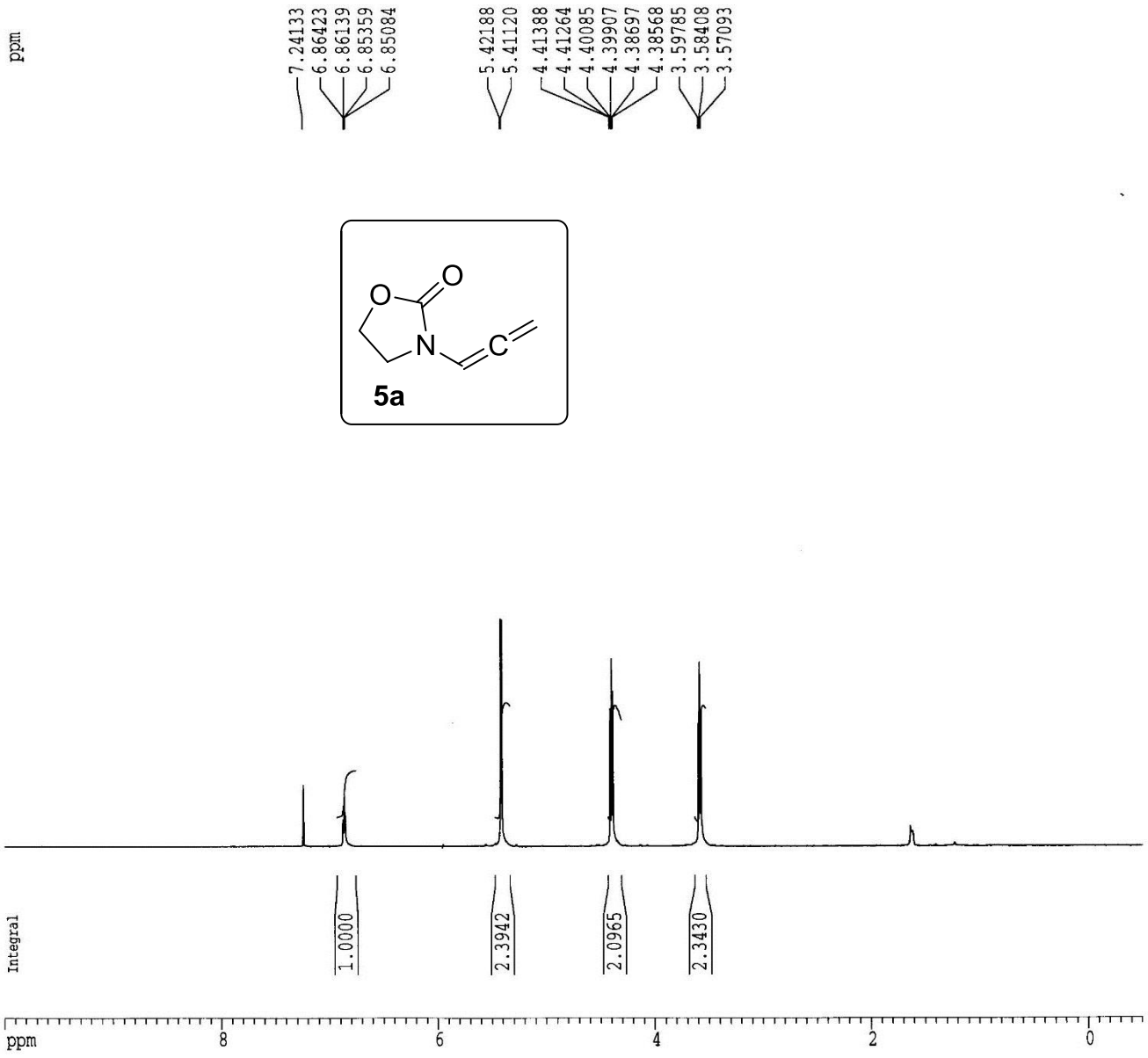


```
Current Data Parameters
NAME          SKP-05-72
EXPNO                 2
PROCNO                1

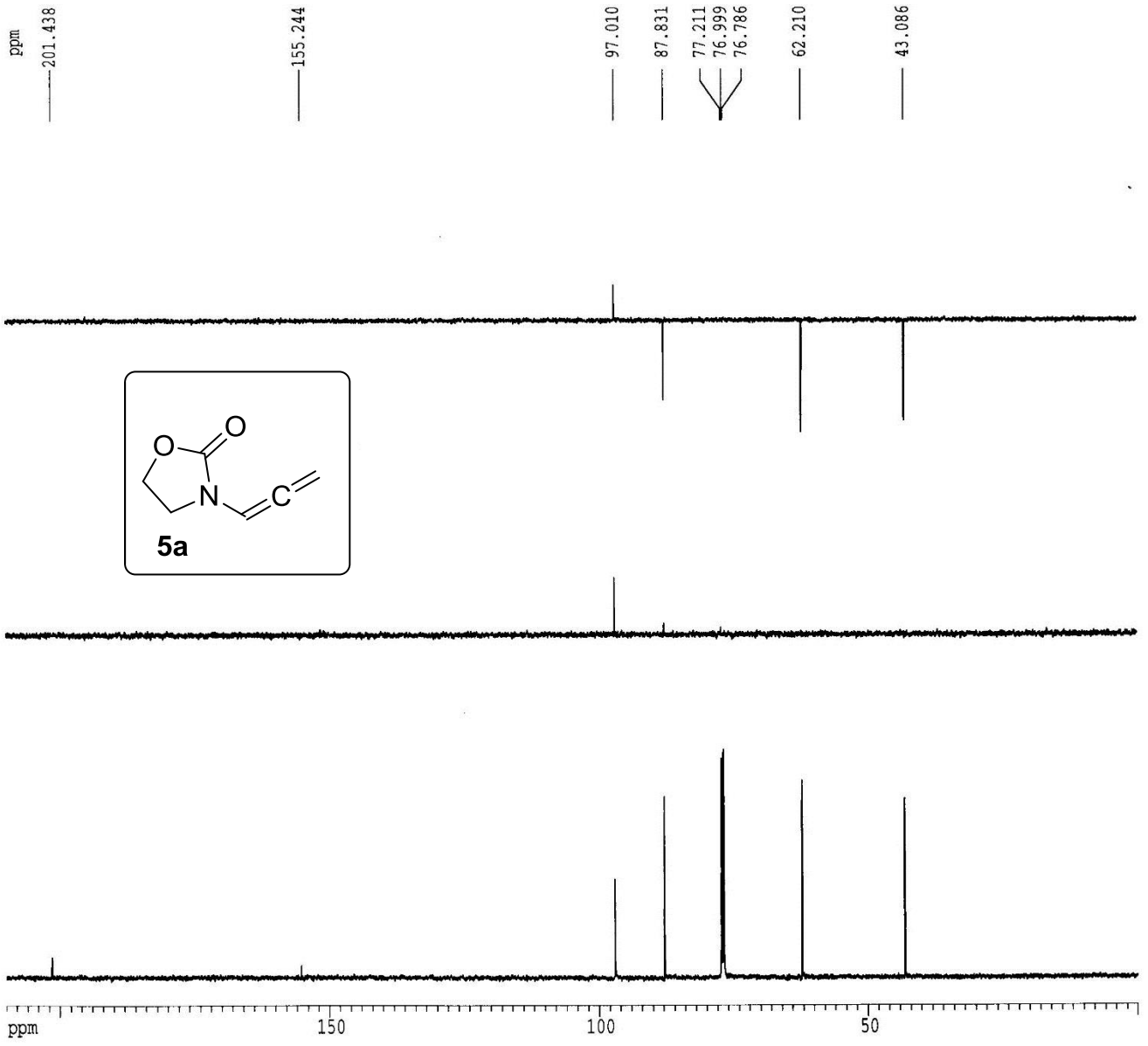
F2 - Acquisition Parameters
Date_          20150319
Time              14.14
INSTRUM           spect
PROBHD   5 mm QNP  1H/1
PULPROG           zgpg
TD               32768
SOLVENT          CDCl3
NS                 508
DS                   0
SWH          45045.047 Hz
FIDRES        1.374666 Hz
AQ           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

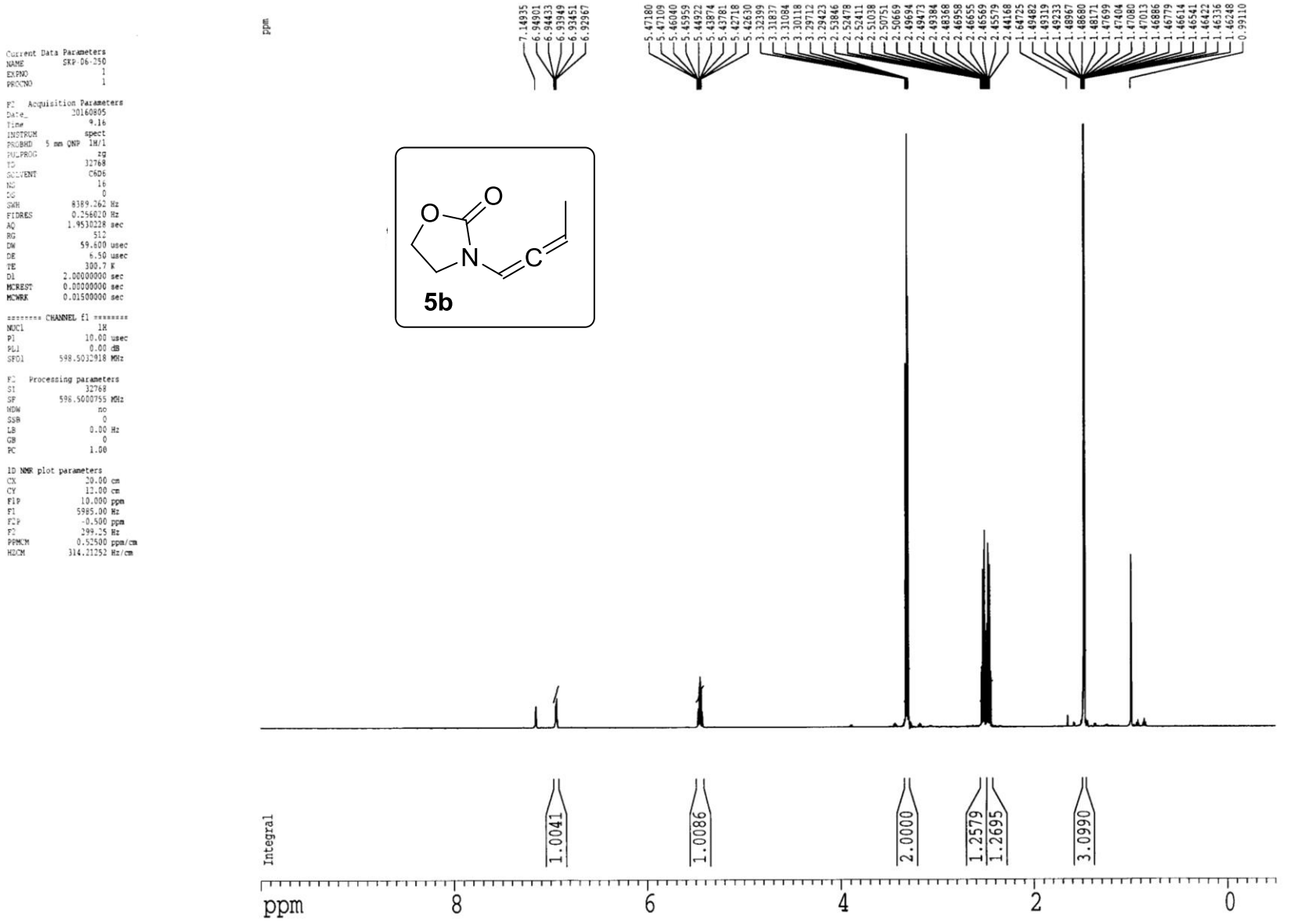
======== CHANNEL f1 ========
NUC1               13C
P1                4.80 usec
PL1               0.00 dB
SFO1       150.5346470 MHz

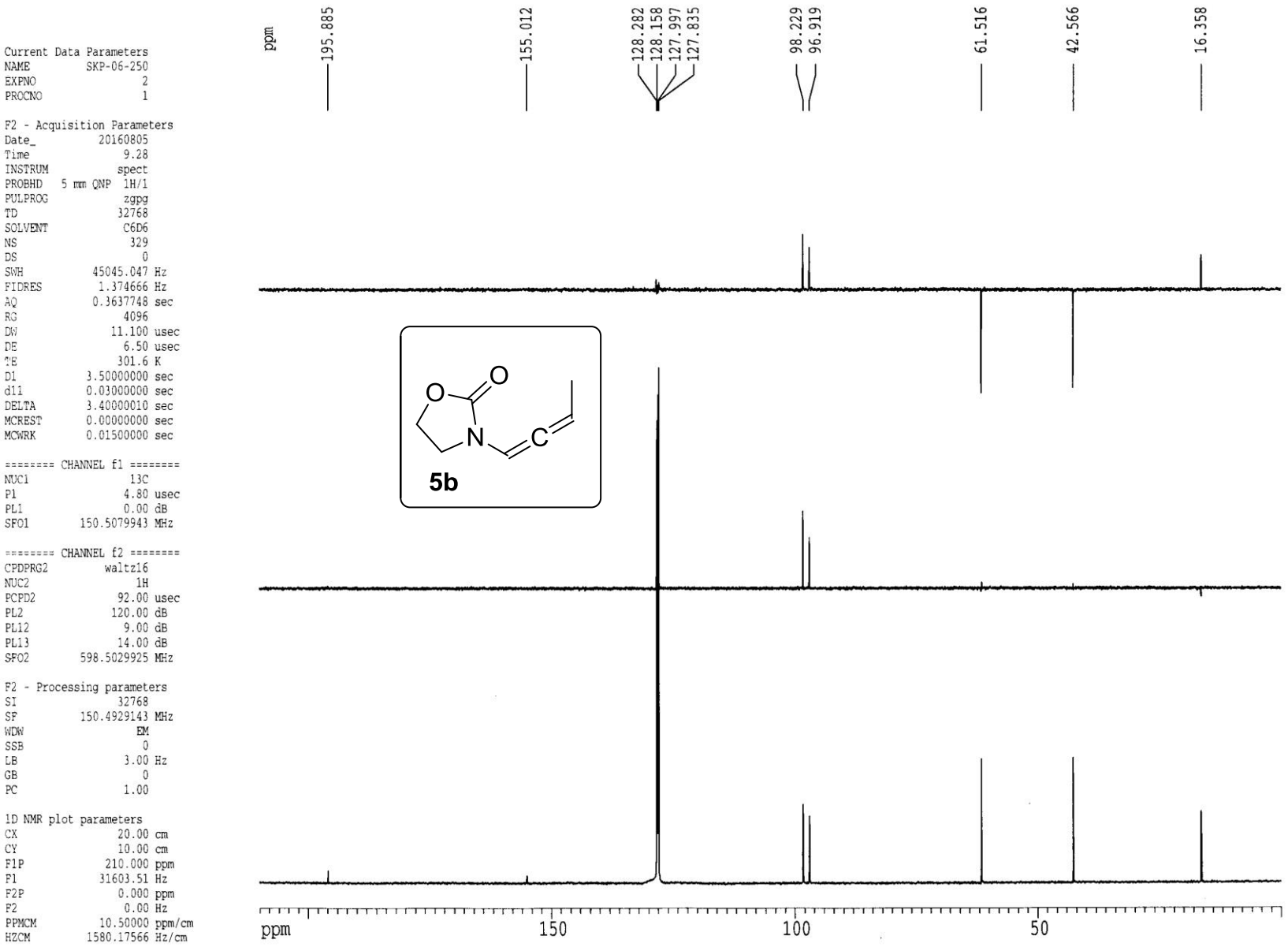
======== CHANNEL f2 ========
CPDPRG2        waltz16
NUC2               1H
PCPD2            92.00 usec
PL2              120.00 dB
PL12              9.00 dB
PL13             14.00 dB
SFO2       598.6029930 MHz

F2 - Processing parameters
SI                65536
SF         150.5180959 MHz
WDW                  EM
SSB                   0
LB                 3.00 Hz
GB                    0
PC                 1.00

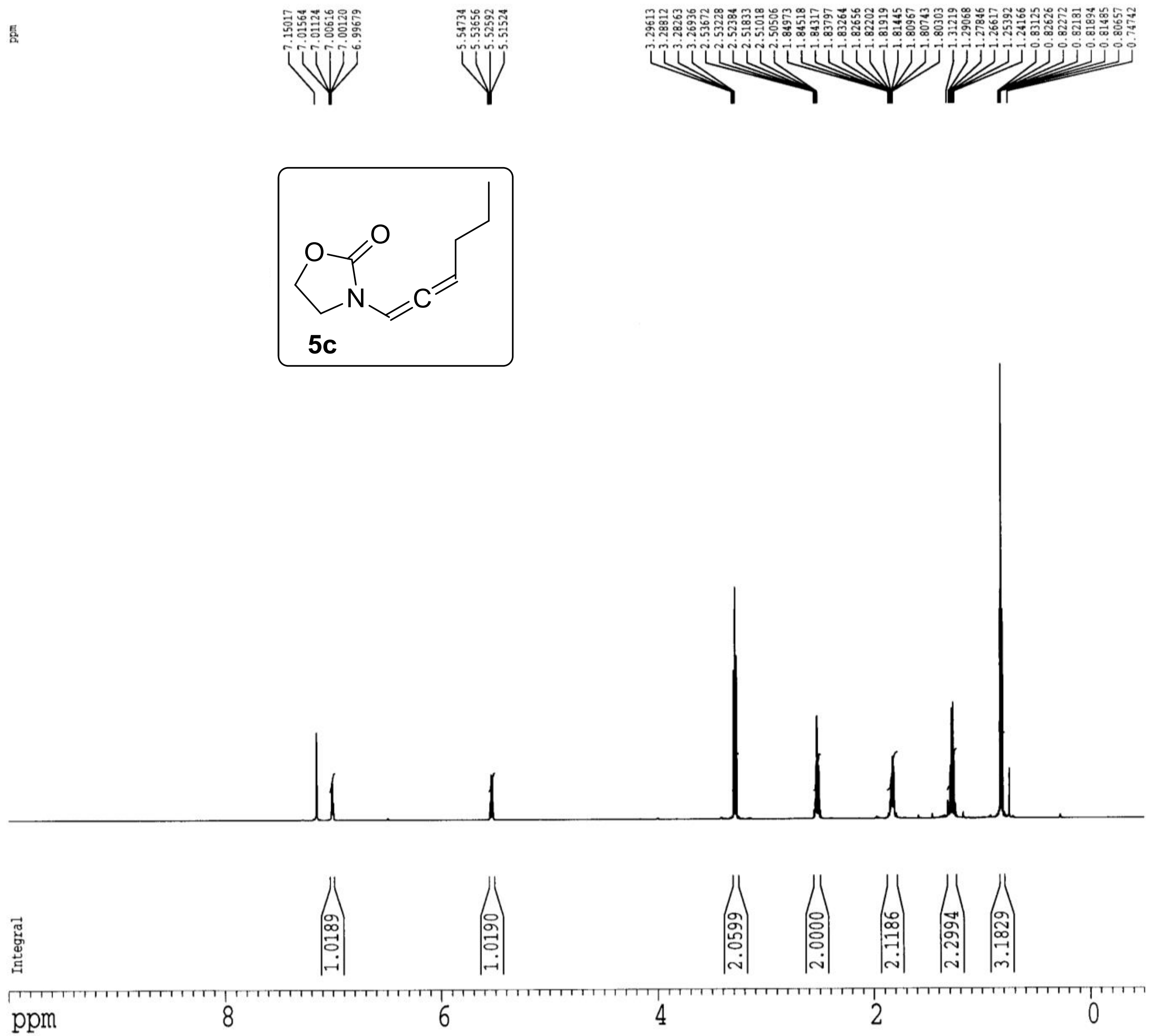
1D NMR plot parameters
CX                20.00 cm
CY                 4.00 cm
F1P              210.000 ppm
F1             31608.80 Hz
F2P                0.000 ppm
F2                 0.00 Hz
PPMCM          10.50000 ppm/cm
HZCM         1580.44006 Hz/cm
```

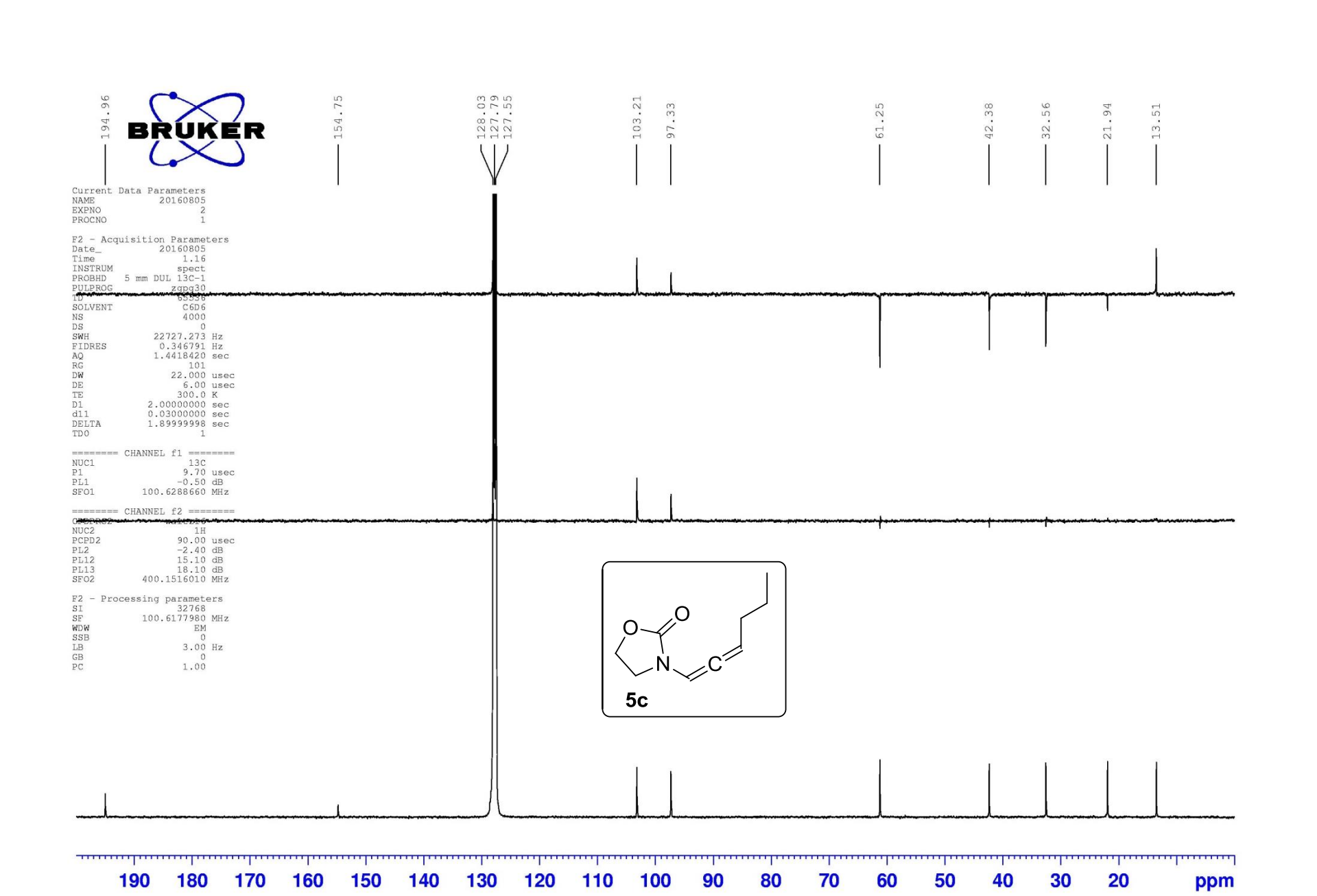



Current Data Parameters
NAME SKP-06-250
EXPNO 1
PROCNO 1
F1 Acquisition Parameters
Date_ 20160805
Time 9.16
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg
TD 32768
SOLVENT C6D6
NS 16
DS 0
SWH 8389.262 Hz
FIDRES 0.256020 Hz
AQ 1.9530228 sec
RG 512
DW 59.600 usec
DE 6.50 usec
TE 300.7 K
D1 2.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 0.00 dB
SFO1 598.5032918 MHz
F2 Processing parameters
SI 32768
SF 598.5000755 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 314.21252 Hz/cm
ppm
7.14935
6.94901
6.94433
6.93949
6.93451
6.92967
5.47180
5.47109
5.46040
5.45959
5.44922
5.43874
5.43781
5.42718
5.42630
3.32399
3.31837
3.31084
3.30118
3.29712
3.29423
2.53846
2.52478
2.52411
2.51038
2.50751
2.50669
2.49694
2.49473
2.49384
2.48368
2.46958
2.46655
2.46569
2.46579
2.44168
1.64725
1.49482
1.49319
1.49233
1.48967
1.48880
1.48171
1.47699
1.47404
1.47080
1.47013
1.46886
1.46779
1.46614
1.46541
1.46422
1.46336
1.46248
0.99110
O
O
N
C
5b
Integral
1.0041
1.0086
2.0000
1.2579
1.2695
3.0990
ppm
8
6
4
2
0


Current Data Parameters
NAME SKP-06-250
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20160805
Time 9.28
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT C6D6
NS 329
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 301.6 K
D1 3.50000000 sec
d11 0.03000000 sec
DELTA 3.40000010 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 4.80 usec
PL1 0.00 dB
SFO1 150.5079943 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 32768
SF 150.4929143 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 20.00 cm
CY 10.00 cm
F1P 210.000 ppm
F1 31603.51 Hz
F2P 0.000 ppm
F2 0.00 Hz
PPMCM 10.50000 ppm/cm
HZCM 1580.17566 Hz/cm
ppm
195.885
155.012
128.282
128.158
127.997
127.835
98.229
96.919
61.516
42.566
16.358
O
O
N
C
5b
ppm
150
100
50

Current Data Parameters	
NAME	SKP 06-240
EXPNO	1
PROCNO	1
F2 - Acquisition Parameters	
Date_	20160805
Time	7.36
INSTRUM	spect
PROBHD	5 mm QNP 1H/1
PULPROG	zg
TD	32768
SOLVENT	C6D6
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	300.6 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	598.5032918 MHz
F2 - Processing parameters	
SI	32768
SF	598.5000750 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	314.21252 Hz/cm




194.96
154.75
128.03
127.79
127.55
103.21
97.33
61.25
42.38
32.56
21.94
13.51
Current Data Parameters
NAME 20160805
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20160805
Time 1.16
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
SOLVENT C6D6
NS 4000
DS 0
SWH 22727.273 Hz
FIDRES 0.346791 Hz
AQ 1.4418420 sec
RG 101
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 100.6177980 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
O
O
N
C
5c
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

```
Current Data Parameters
NAME        SKP-05-Dime
EXPNO                 1
PROCNO                1

F2 - Acquisition Parameters
Date_          20151202
Time              19.29
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                   64
DW                52.400 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         598.5029925 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
```

```
Current Data Parameters
NAME        SKP-05-Dime
EXPNO                 2
PROCNO                1

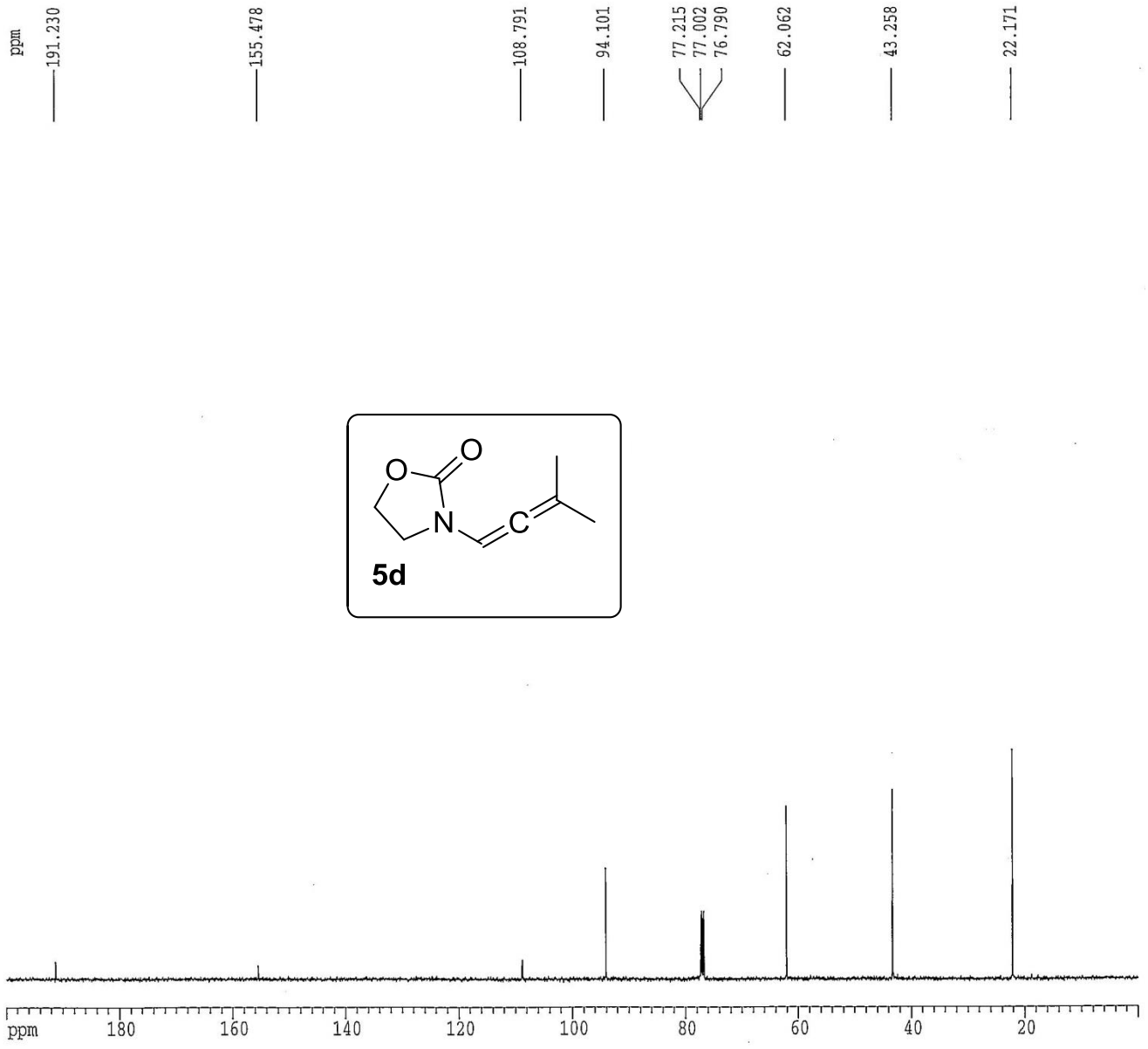
F2 - Acquisition Parameters
Date_          20151202
Time              19.33
INSTRUM           spect
PROBHD   5 mm QNP  1H/1
PULPROG           zgpg
TD                32768
SOLVENT           CDCl3
NS                   60
DS                    0
SWH           45045.047 Hz
FIDRES         1.374666 Hz
AQ             0.3637748 sec
RG                 2048
DW                11.100 usec
DE                 6.50 usec
TE                298.3 K
D1            3.50000000 sec
d11           0.03000000 sec
DELTA         3.40000010 sec
MCREST        0.00000000 sec
MCWRK         0.01500000 sec

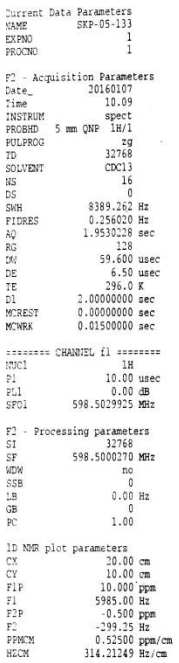
======== CHANNEL f1 ========
NUC1                13C
P1                 4.80 usec
PL1                0.00 dB
SFO1       150.5094992 MHz

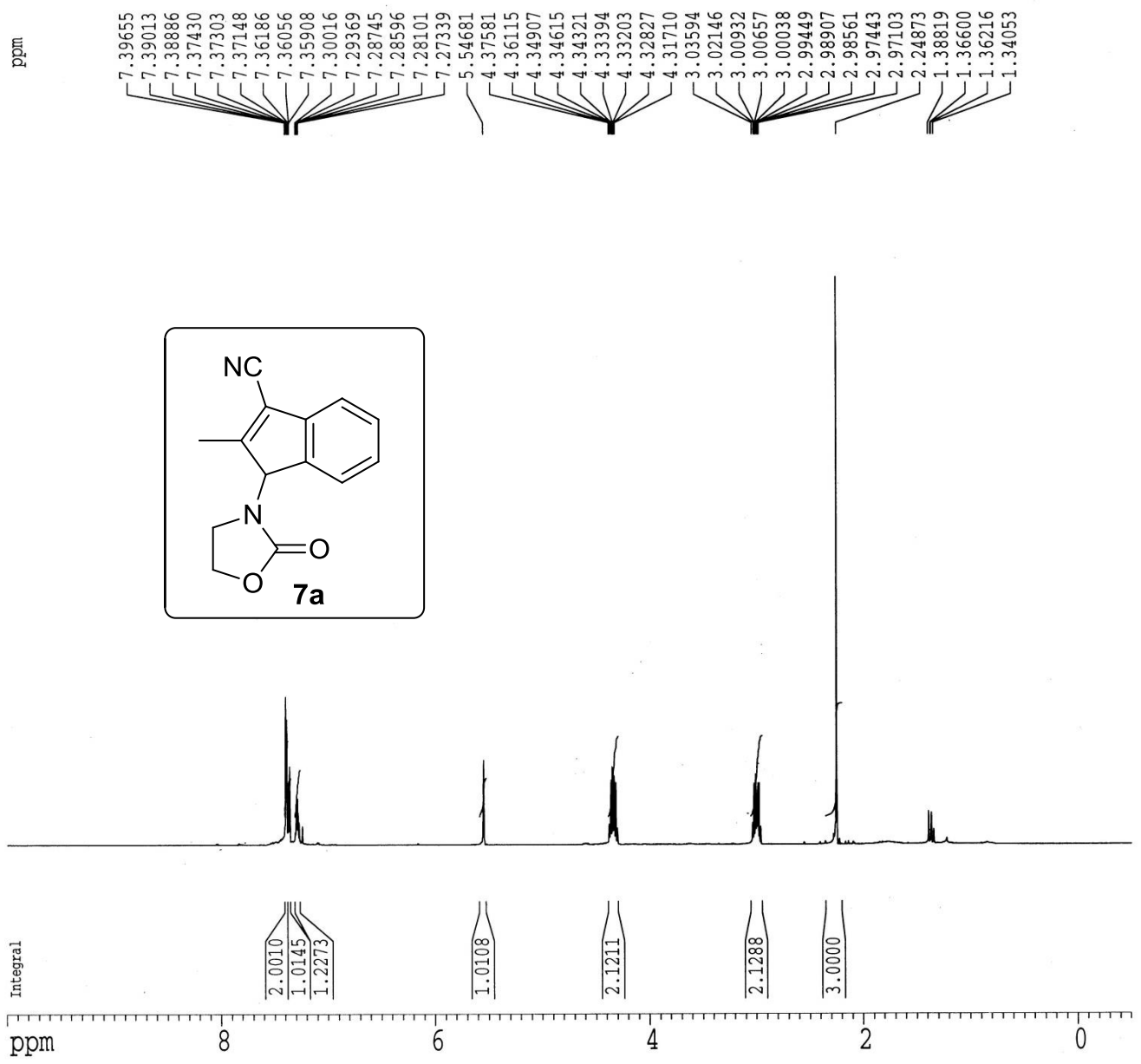
======== CHANNEL f2 ========
CPDPRG2         waltz16
NUC2                1H
PCPD2             92.00 usec
PL2              120.00 dB
PL12               9.00 dB
PL13              14.00 dB
SFO2       598.5029925 MHz

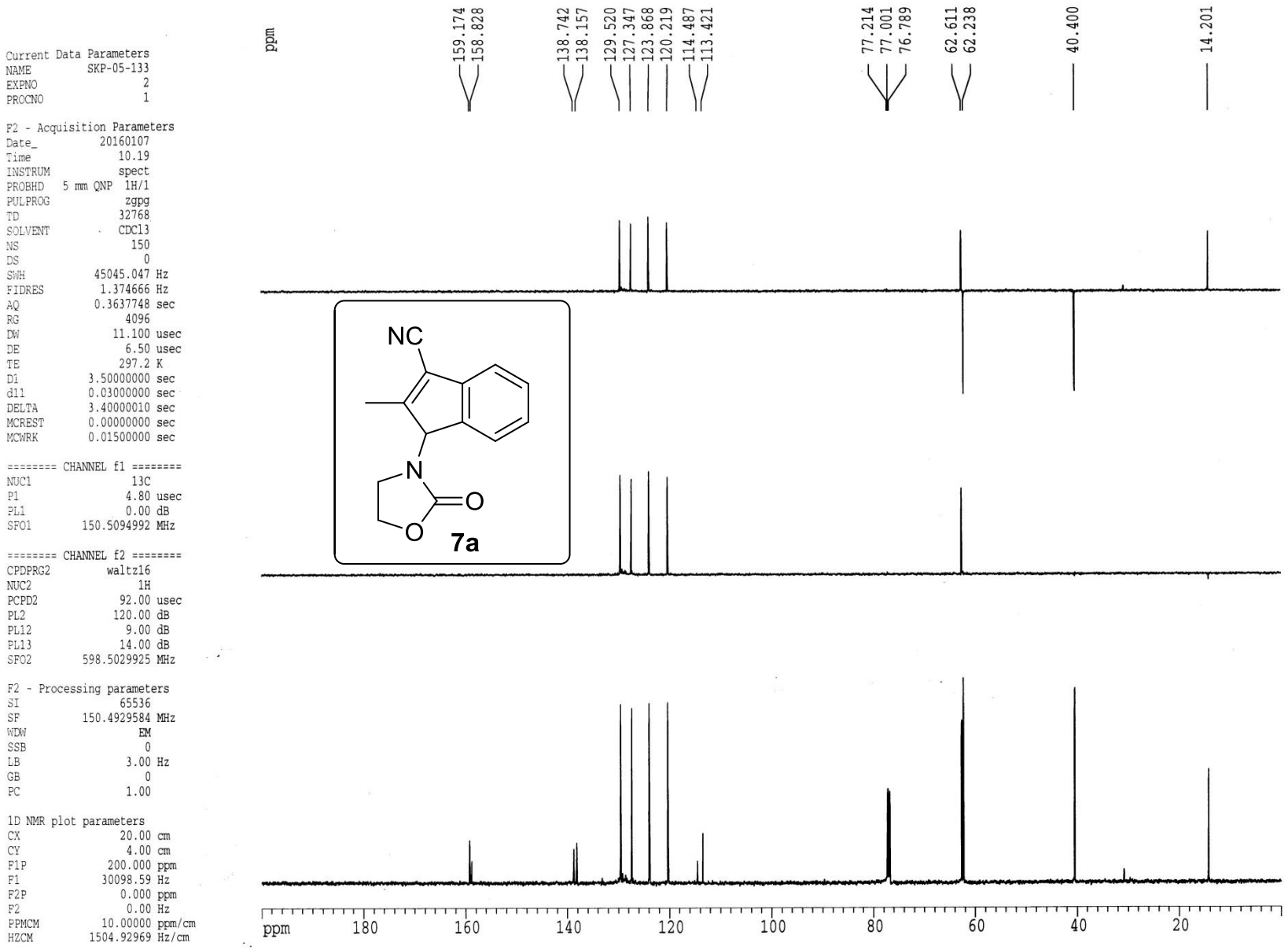
F2 - Processing parameters
SI                 65536
SF          150.4929570 MHz
WDW                   EM
SSB                    0
LB                  3.00 Hz
GB                     0
PC                  1.00

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 SKP-05-133
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20160107
Time 10.09
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 296.0 K
D1 2.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 0.00 dB
SFO1 598.5029925 MHz
F2 - Processing parameters
SI 32768
SF 598.5000270 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
7.39655
7.39013
7.38886
7.37430
7.37303
7.37148
7.36186
7.36056
7.35908
7.30016
7.29369
7.28745
7.28596
7.28101
7.27339
5.54681
4.37581
4.36115
4.34907
4.34615
4.34321
4.33394
4.33203
4.32827
4.31710
3.03594
3.02146
3.00932
3.00657
3.00038
2.99449
2.98907
2.98561
2.97443
2.97103
2.24873
1.38819
1.36600
1.36216
1.34053
NC
N
O
O
7a
Integral
2.0010
1.0145
1.2273
1.0108
2.1211
2.1288
3.0000
ppm
8
6
4
2
0


Current Data Parameters
NAME SKP-05-133
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20160107
Time 10.19
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 150
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 297.2 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 150.5094992 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 150.4929584 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 1504.92969 Hz/cm
ppm
159.174
158.828
138.742
138.157
129.520
127.347
123.868
120.219
114.487
113.421
77.214
77.001
76.789
62.611
62.238
40.400
14.201
NC
N
O
O
7a
ppm
180
160
140
120
100
80
60
40
20

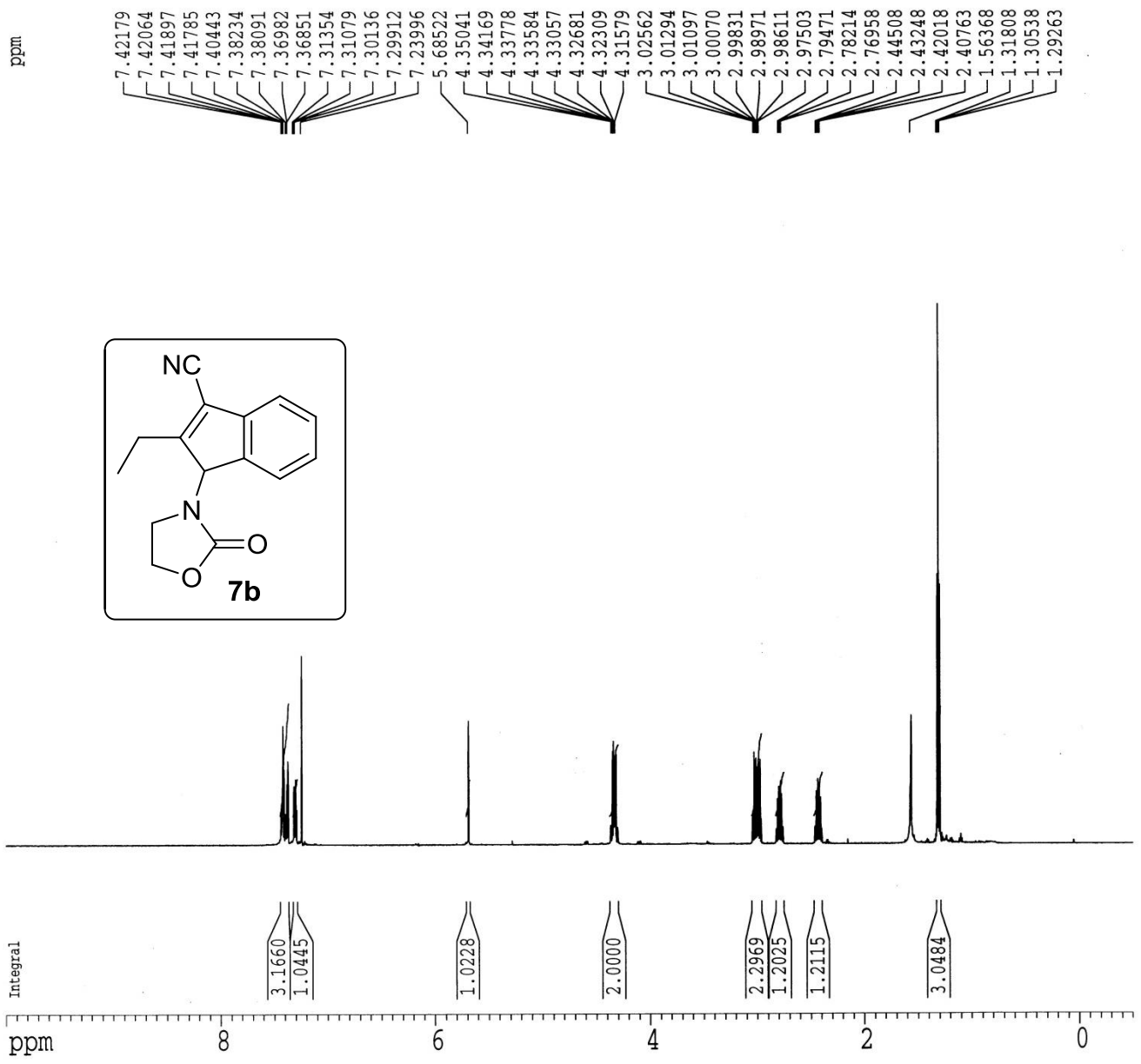
Current Data Parameters
NAME SKP-05-aMe
EXPNO 1
PROCNO 1

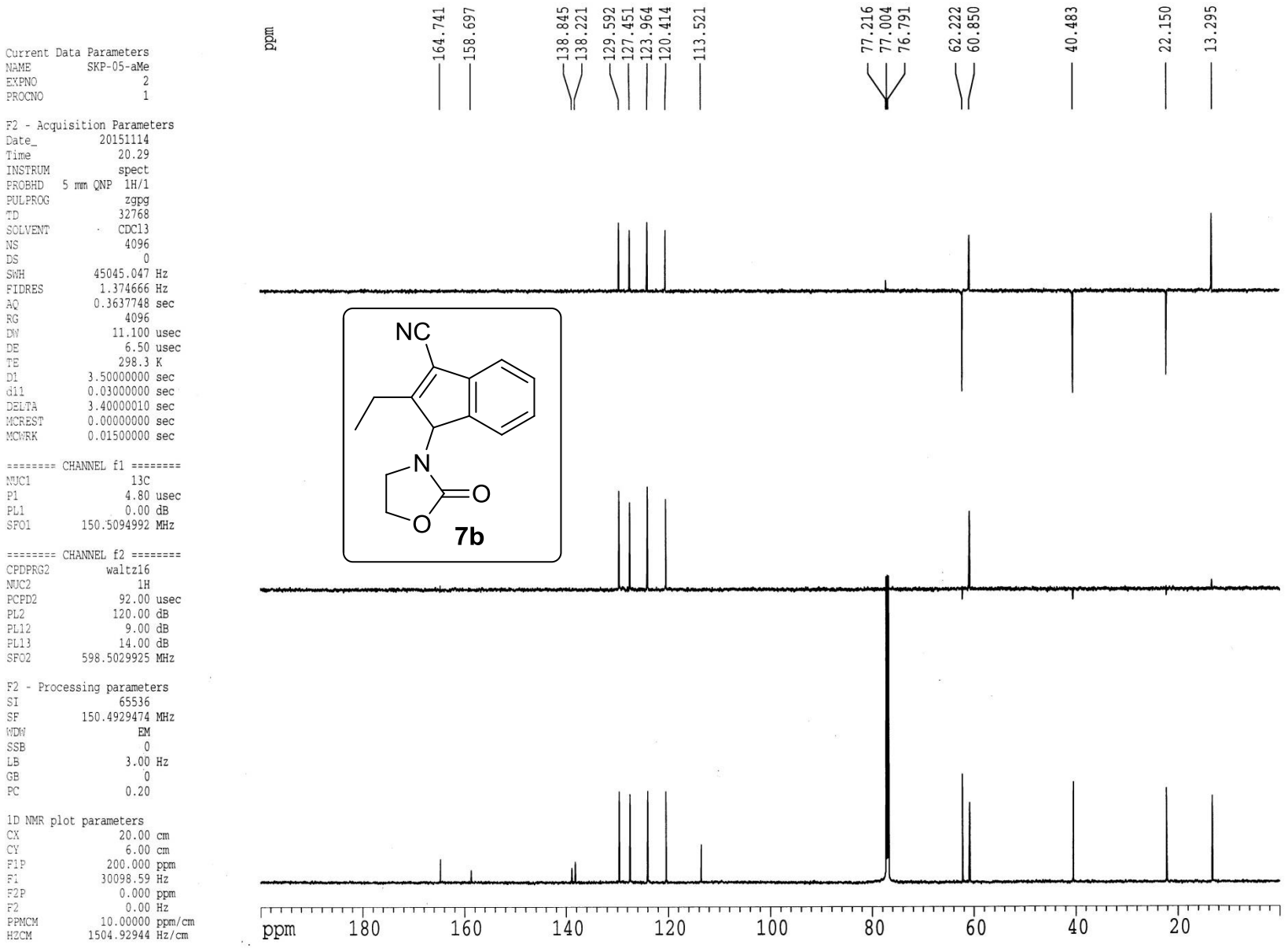
F2 - Acquisition Parameters
Date_ 20151114
Time 20.28
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 9541.984 Hz
FIDRES 0.291198 Hz
AQ 1.7170932 sec
RG 512
DW 52.400 usec
DE 6.50 usec
TE 298.3 K
D1 2.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

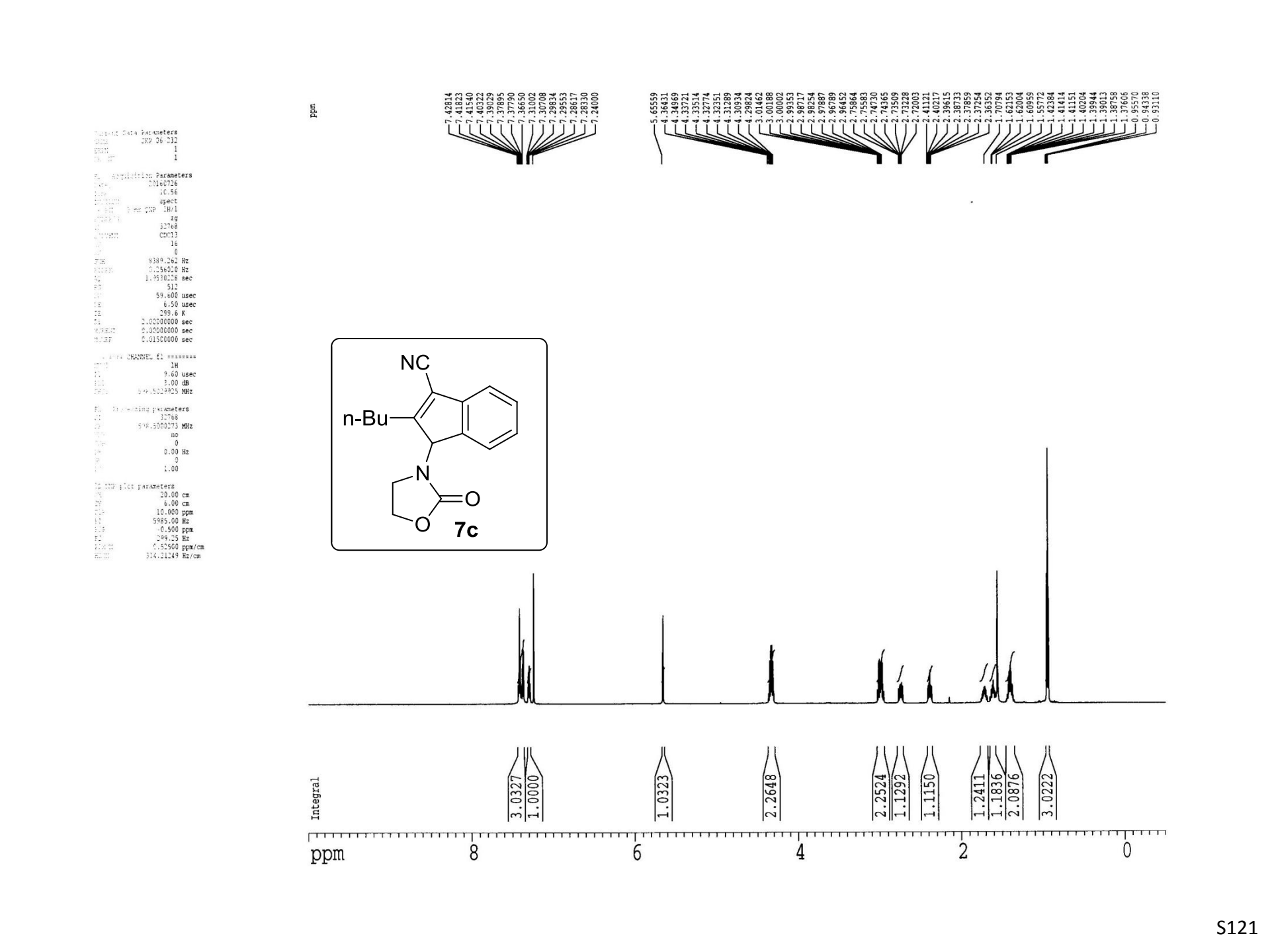
======== CHANNEL f1 ========
NUC1 1H
P1 12.30 usec
PL1 3.00 dB
SFO1 598.5037107 MHz

F2 - Processing parameters
SI 32768
SF 598.5000281 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 SKP-05-aMe
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20151114
Time 20.29
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 4096
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 298.3 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 150.5094992 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 150.4929474 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 0.20
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
ppm
164.741
158.697
138.845
138.221
129.592
127.451
123.964
120.414
113.521
77.216
77.004
76.791
62.222
60.850
40.483
22.150
13.295
NC
N
O
O
7b
ppm
180
160
140
120
100
80
60
40
20


ppm
7.42814
7.41823
7.41540
7.40322
7.39029
7.37895
7.37790
7.36650
7.31002
7.30708
7.29834
7.29553
7.28617
7.28330
7.24000
5.65559
4.36431
4.34969
4.33721
4.33514
4.32774
4.32351
4.31289
4.30934
4.29824
4.01462
3.00188
3.00002
2.99353
2.98717
2.98254
2.97887
2.96789
2.96452
2.75864
2.75583
2.74730
2.74365
2.73509
2.73228
2.72003
2.41121
2.40217
2.39615
2.38733
2.37859
2.37254
2.36352
1.70794
1.62153
1.62004
1.60959
1.55772
1.42384
1.41414
1.41151
1.40204
1.39944
1.39013
1.38758
1.37606
0.95570
0.94338
0.93110
NC
n-Bu
N
O
O
7c
Integral
3.0327
1.0000
1.0323
2.2648
2.2524
1.1292
1.1150
1.2411
1.1836
2.0876
3.0222
ppm
8
6
4
2
0

```
Current Data Parameters
NAME         SKP-06-232
EXPNO                 2
PROCNO                1

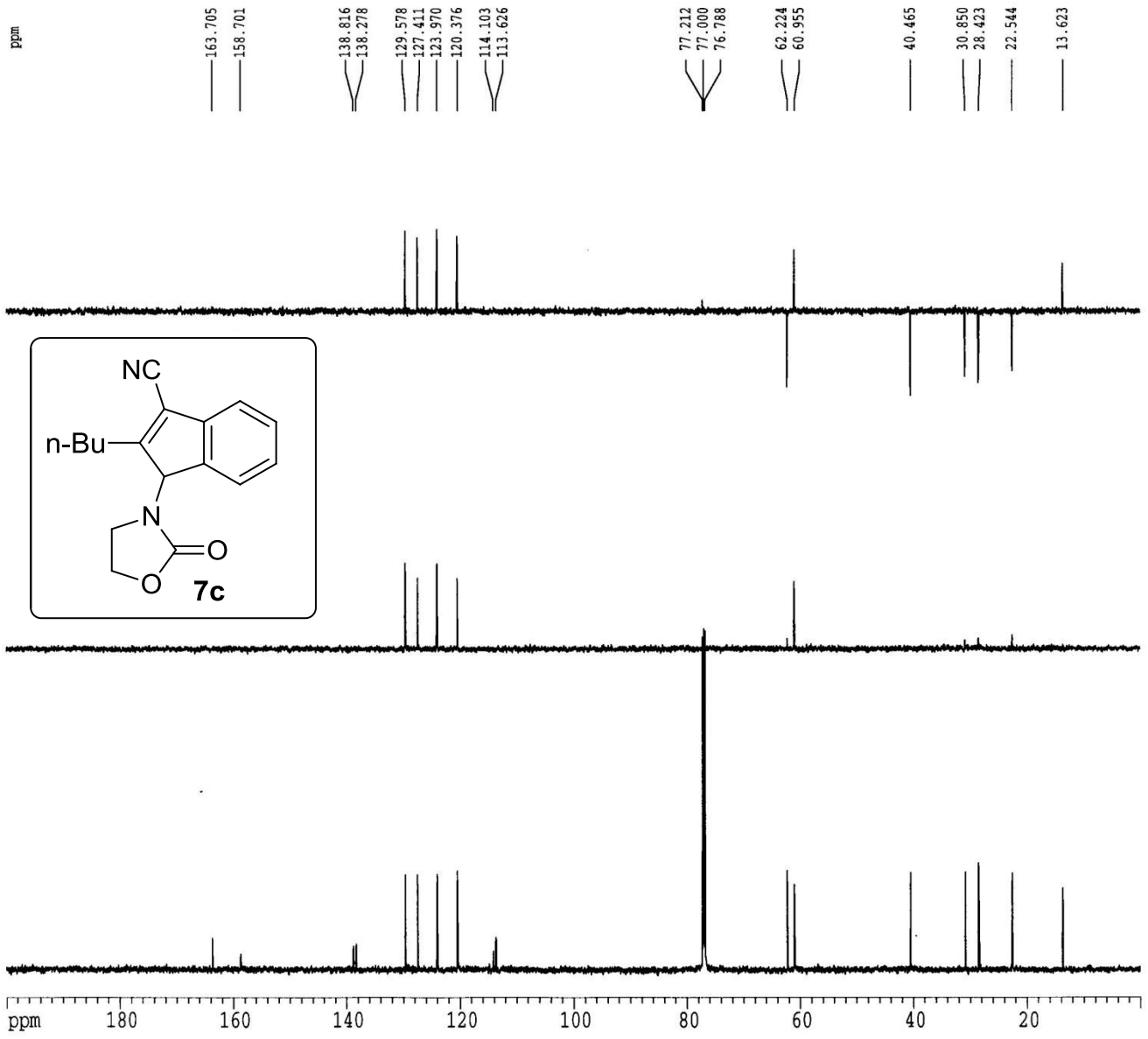
F2 - Acquisition Parameters
Date_          20160726
Time              10.57
INSTRUM           spect
PROBHD   5 mm QNP  1H/1
PULPROG           zgpg
TD               32768
SOLVENT           CDCl3
NS                  576
DS                    0
SWH           45045.047 Hz
FIDRES         1.374666 Hz
AQ            0.3637748 sec
RG                 4096
DW               11.100 usec
DE                6.50 usec
TE              299.6 K
D1           3.50000000 sec
D11          0.03000000 sec
TDLTA        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          150.4929480 MHz
WDW                  EM
SSB                   0
LB                 3.00 Hz
GB                    0
PC                 0.10

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
```



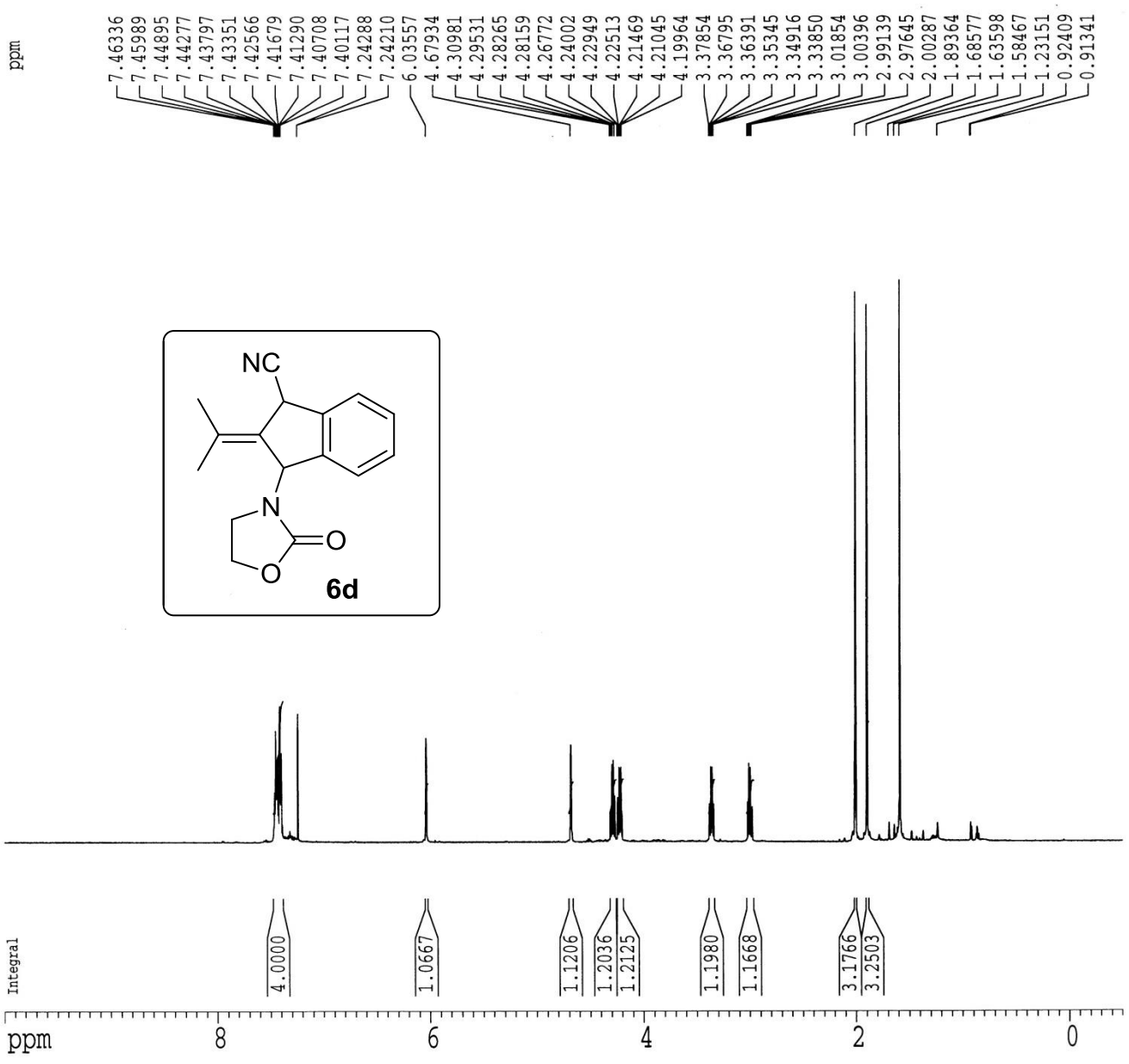
```
Current Data Parameters
NAME          SKP-06-054
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20151229
Time               10.59
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                295.4 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           598.5000262 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          SKP-06-054
EXPNO                  2
PROCNO                 1

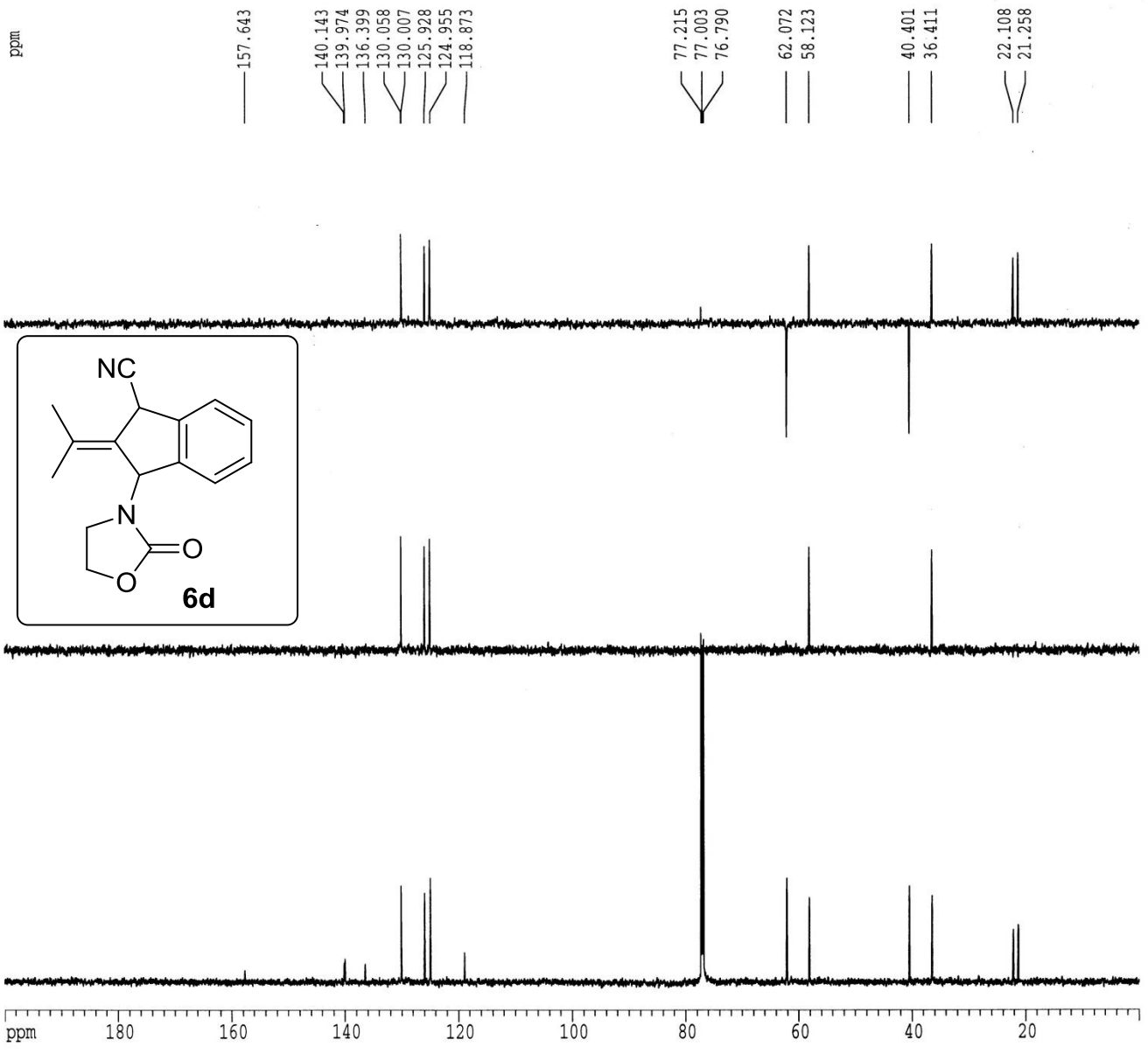
F2 - Acquisition Parameters
Date_           20160106
Time                4.51
INSTRUM            spect
PROBHD   5 mm QNP  1H/1
PULPROG             zgpg
TD                 32768
SOLVENT          Acetone
NS                   777
DS                     0
SWH            45045.047 Hz
FIDRES             1.374666 Hz
AQ                 0.3637748 sec
RG                    2048
DW                   11.100 usec
DE                    6.50 usec
TE                   296.6 K
D1             3.50000000 sec
d11            0.03000000 sec
DELTA          3.40000010 sec
MCREST         0.00000000 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                  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
```



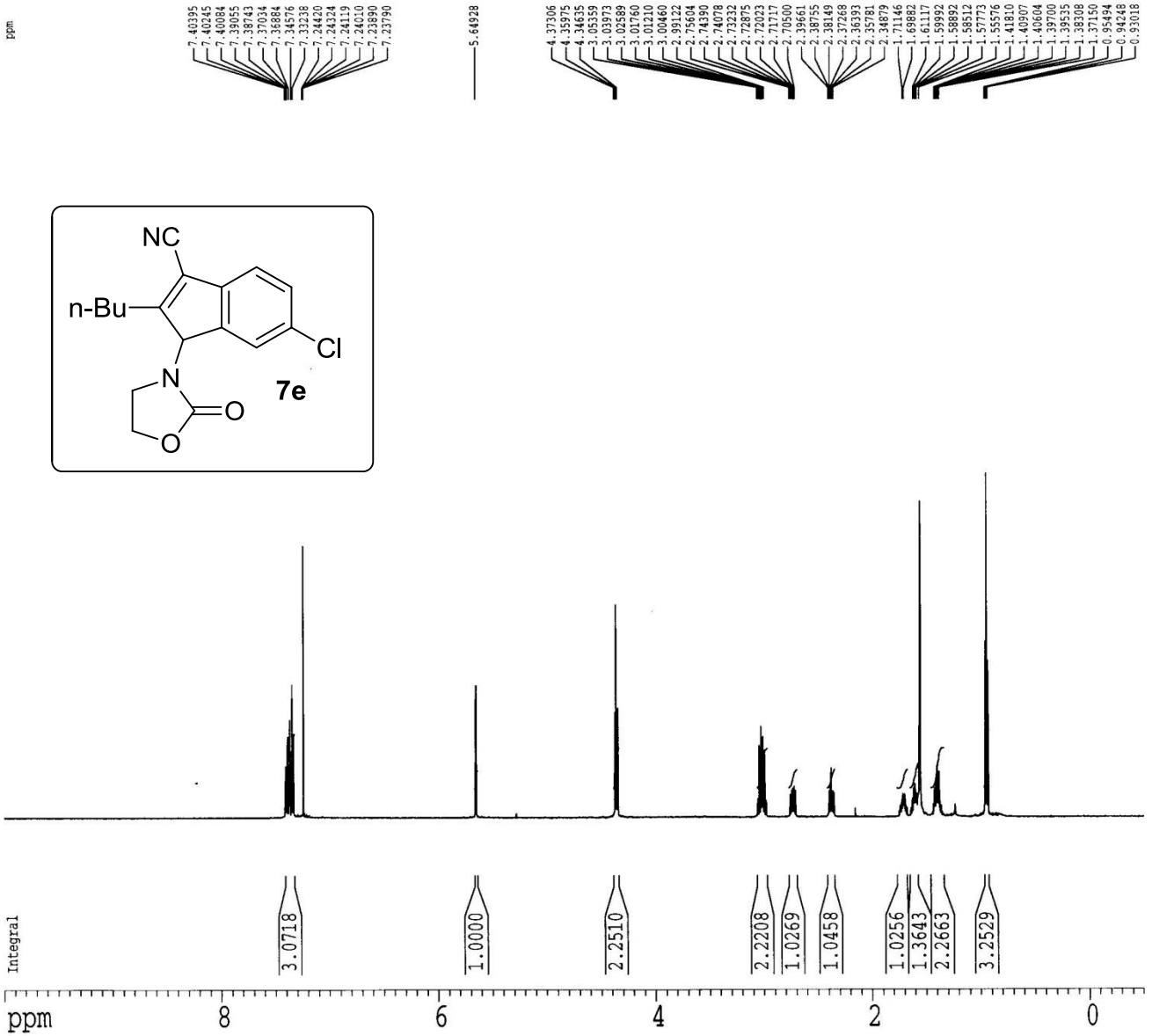
```
Current Data Parameters
NAME          SKP-06-233
EXPNO                  1
PROCNO                 1

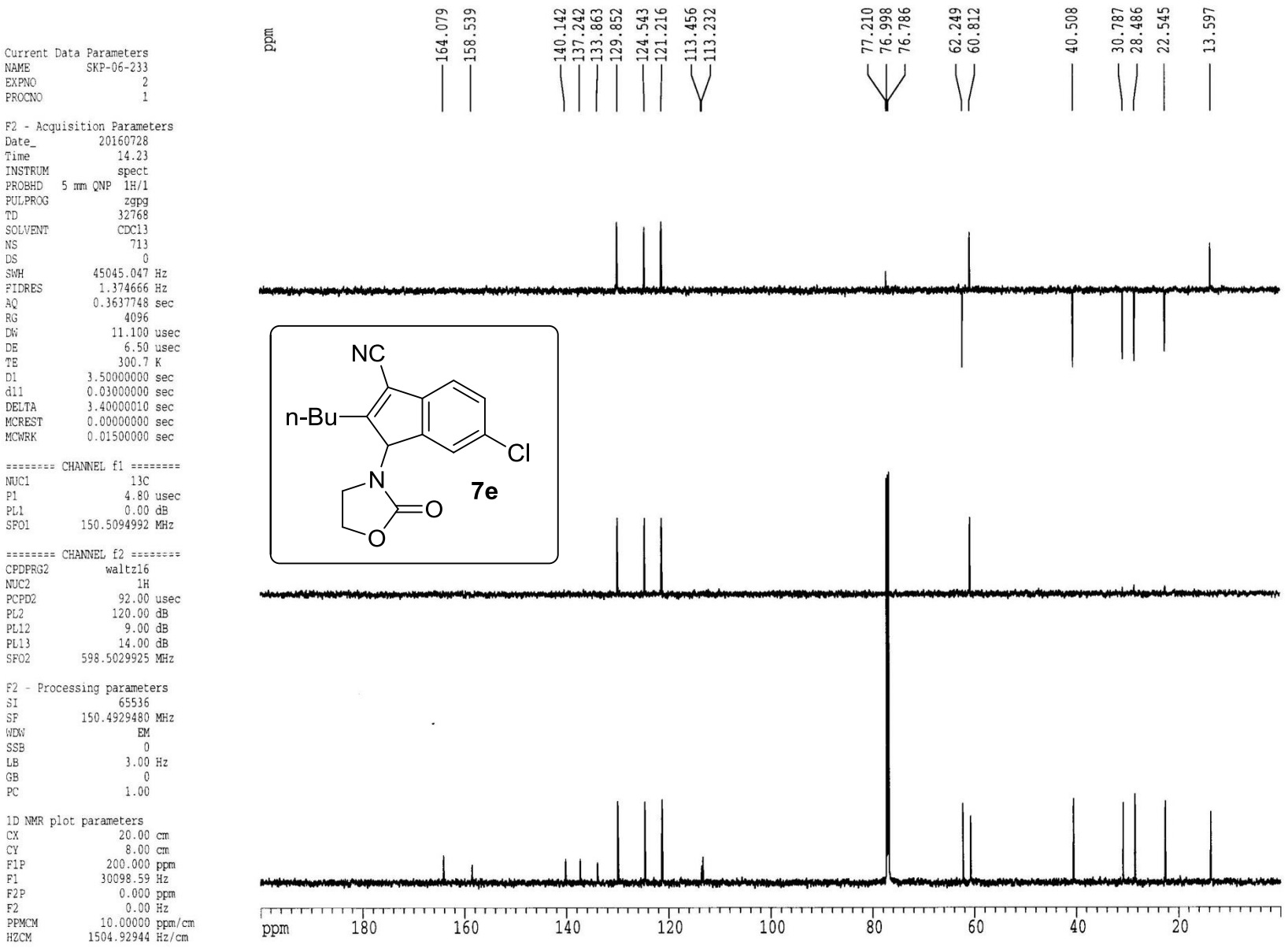
F2 - Acquisition Parameters
Date_           20160728
Time               14.14
INSTRUM            spect
PROBHD   5 mm QNP  1H/1
PULPROG              zg
TD                32768
SOLVENT           CDCl3
NS                   16
DS                    0
SWH            8389.262 Hz
FIDRES            0.256020 Hz
AQ             1.9530228 sec
RG                  512
DW               59.600 usec
DE                6.50 usec
TE                300.3 K
D1             2.00000000 sec
MCREST         0.00000000 sec
MCWRK          0.01500000 sec

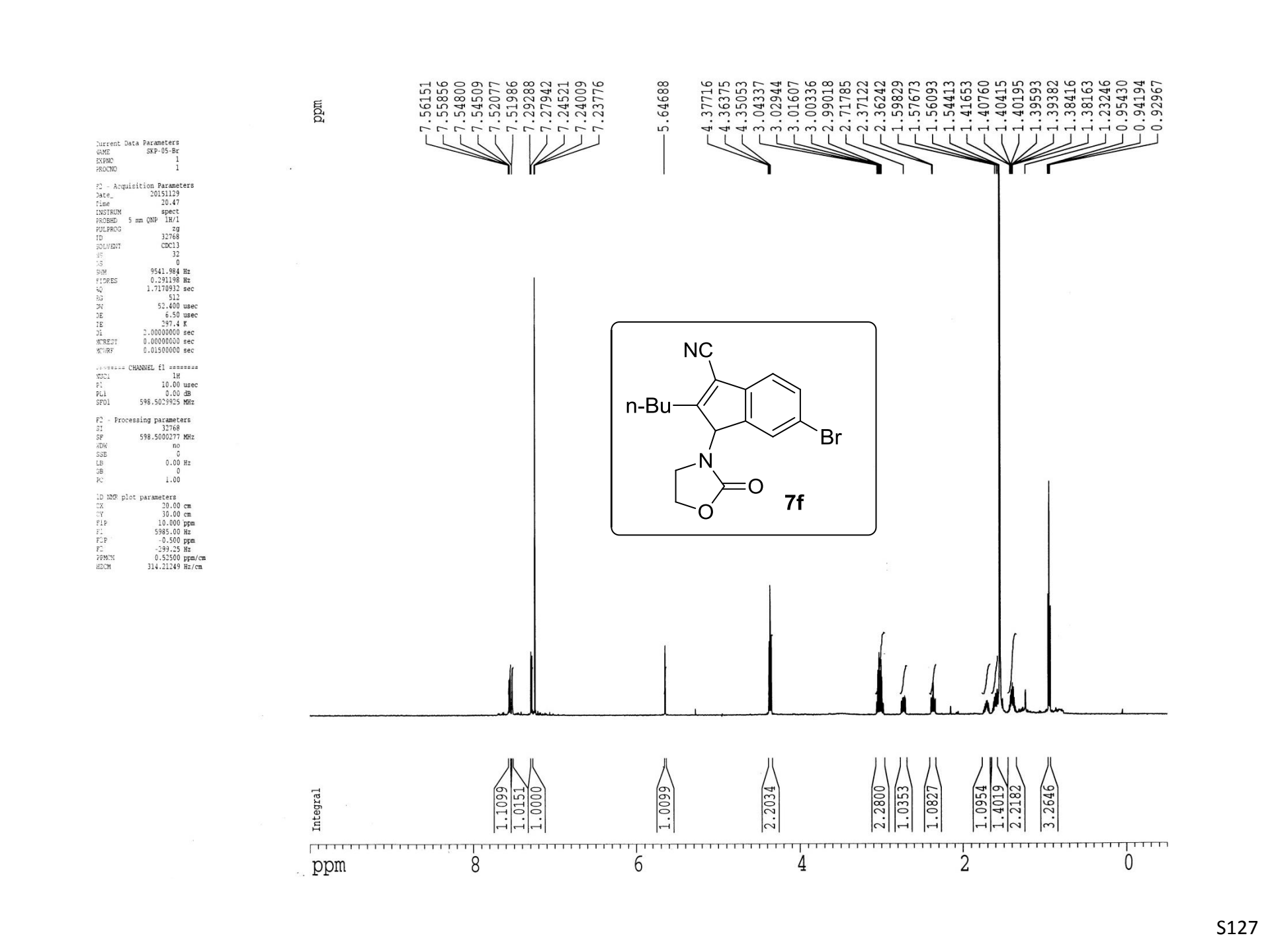
======== CHANNEL f1 ========
NUC1                 1H
P1                 9.60 usec
PL1                3.00 dB
SFO1        598.5029935 MHz

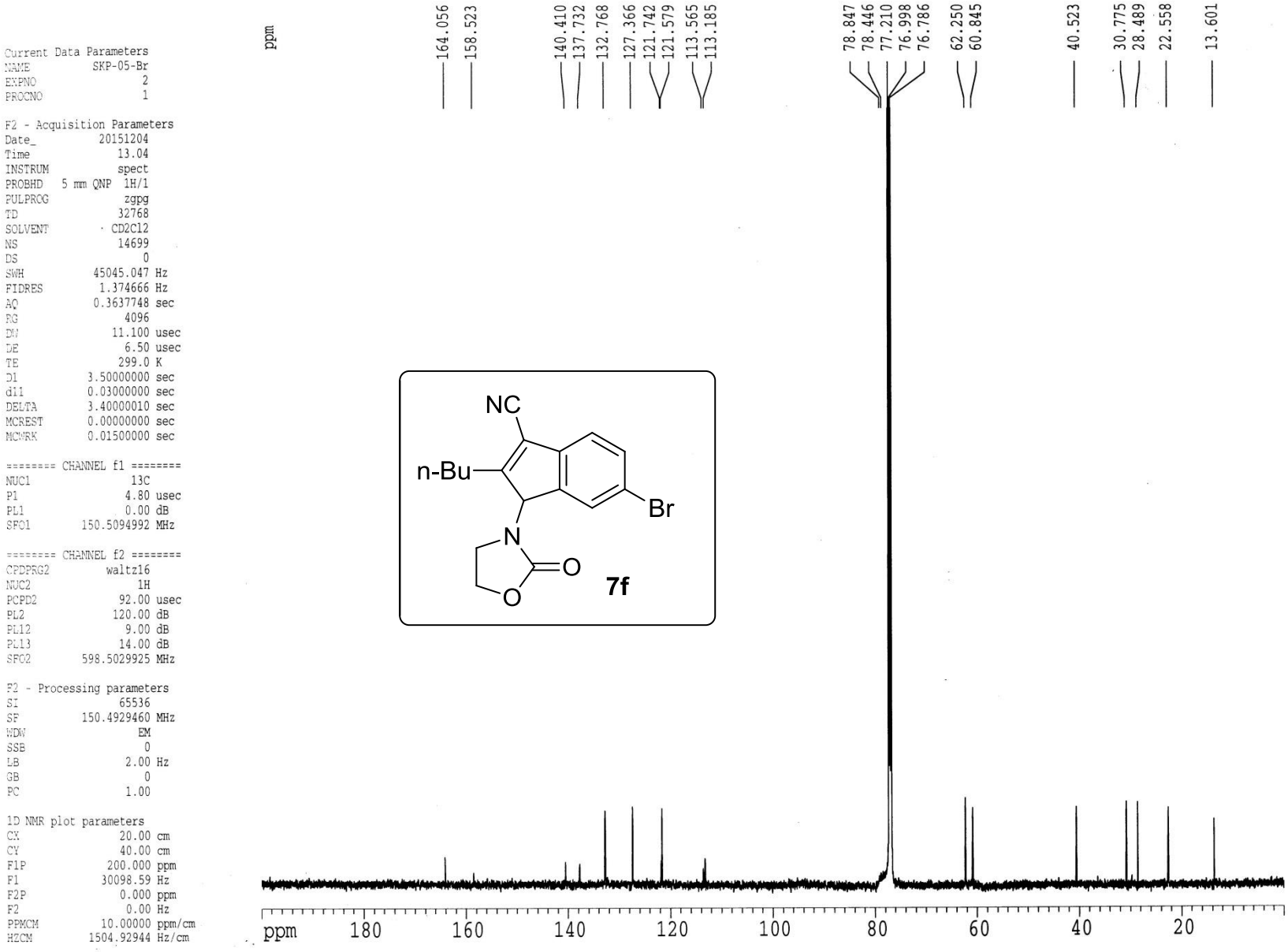
F2 - Processing parameters
SI                32768
SF          598.5000283 MHz
WDW                  no
SSB                   0
LB                 0.00 Hz
GB                    0
PC                 1.00

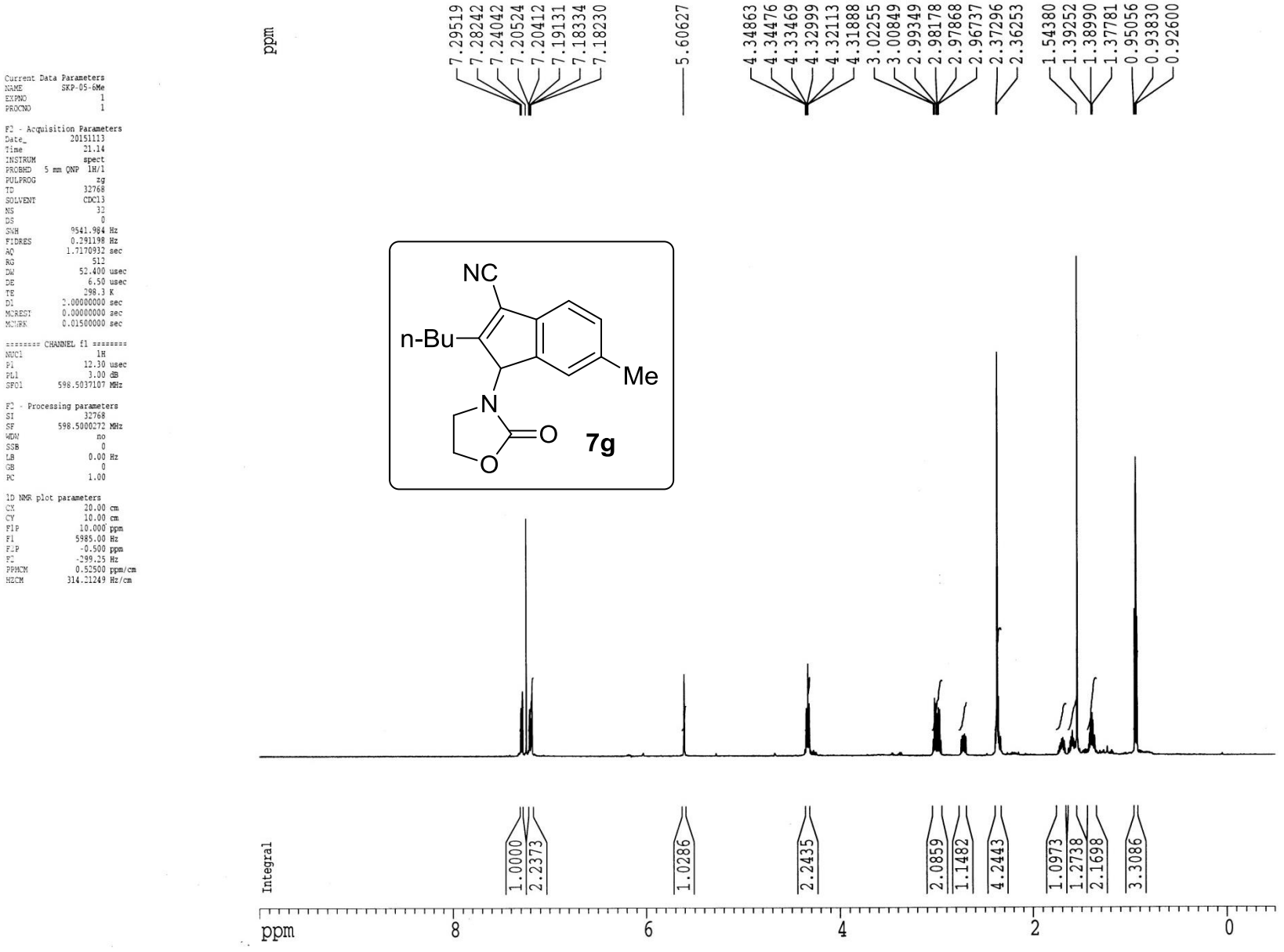
1D NMR plot parameters
CX                20.00 cm
CY                 6.00 cm
F1P              10.000 ppm
F1              5985.00 Hz
F2P              -0.500 ppm
F2              -299.25 Hz
PPMCM            0.52500 ppm/cm
HZCM           314.21249 Hz/cm
```




Current Data Parameters
NAME SKP-06-233
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20160728
Time 14.23
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 713
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 300.7 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 150.4929480 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 30098.59 Hz
F2P 0.000 ppm
F2 0.00 Hz
PPMCM 10.00000 ppm/cm
HZCM 1504.92944 Hz/cm
ppm
164.079
158.539
140.142
137.242
133.863
129.852
124.543
121.216
113.456
113.232
77.210
76.998
76.786
62.249
60.812
40.508
30.787
28.486
22.545
13.597
NC
n-Bu
Cl
N
O
O
7e
ppm
180
160
140
120
100
80
60
40
20


Current Data Parameters
NAME SKP-05-Br
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20151129
Time 20.47
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 512
DW 52.400 usec
DE 6.50 usec
TE 297.4 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRF 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 30.00 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
7.56151
7.55856
7.54800
7.54509
7.52077
7.51986
7.29288
7.27942
7.24521
7.24009
7.23776
5.64688
4.37716
4.36375
4.35053
3.04337
3.02944
3.01607
3.00336
2.99018
2.71785
2.37122
2.36242
1.59829
1.57673
1.56093
1.54413
1.41653
1.40760
1.40415
1.40195
1.39593
1.39382
1.38416
1.38163
1.23246
0.95430
0.94194
0.92967
NC
n-Bu
Br
N
O
O
7f
Integral
1.1099
1.0151
1.0000
1.0099
2.2034
2.2800
1.0353
1.0827
1.0954
1.4019
2.2182
3.2646
ppm
8
6
4
2
0


Current Data Parameters
NAME SKP-05-Br
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20151204
Time 13.04
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CD2Cl2
NS 14699
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 150.5094992 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 150.4929460 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 20.00 cm
CY 40.00 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
164.056
158.523
140.410
137.732
132.768
127.366
121.742
121.579
113.565
113.185
78.847
78.446
77.210
76.998
76.786
62.250
60.845
40.523
30.775
28.489
22.558
13.601
NC
n-Bu
Br
N
O
O
7f
ppm
180
160
140
120
100
80
60
40
20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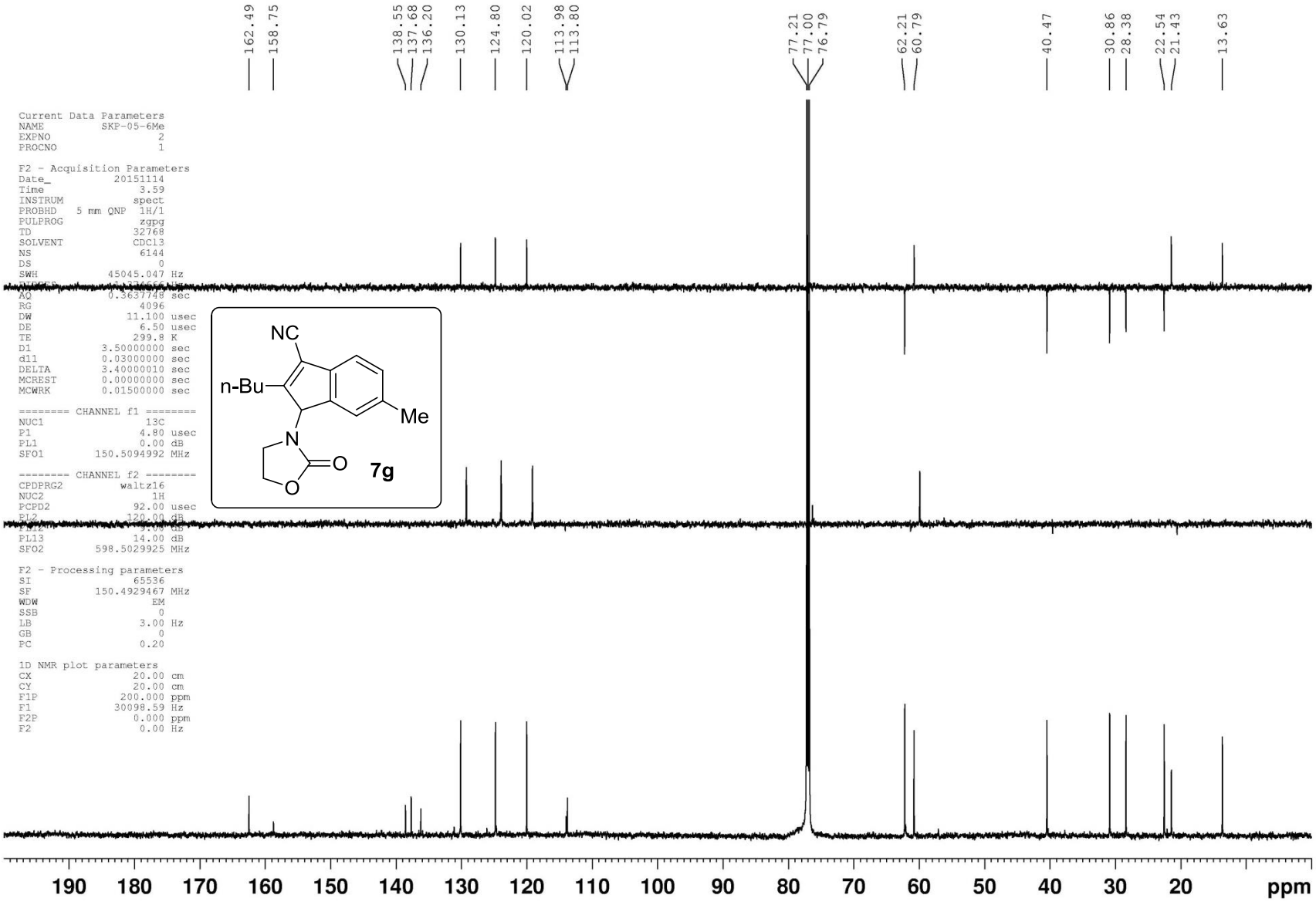
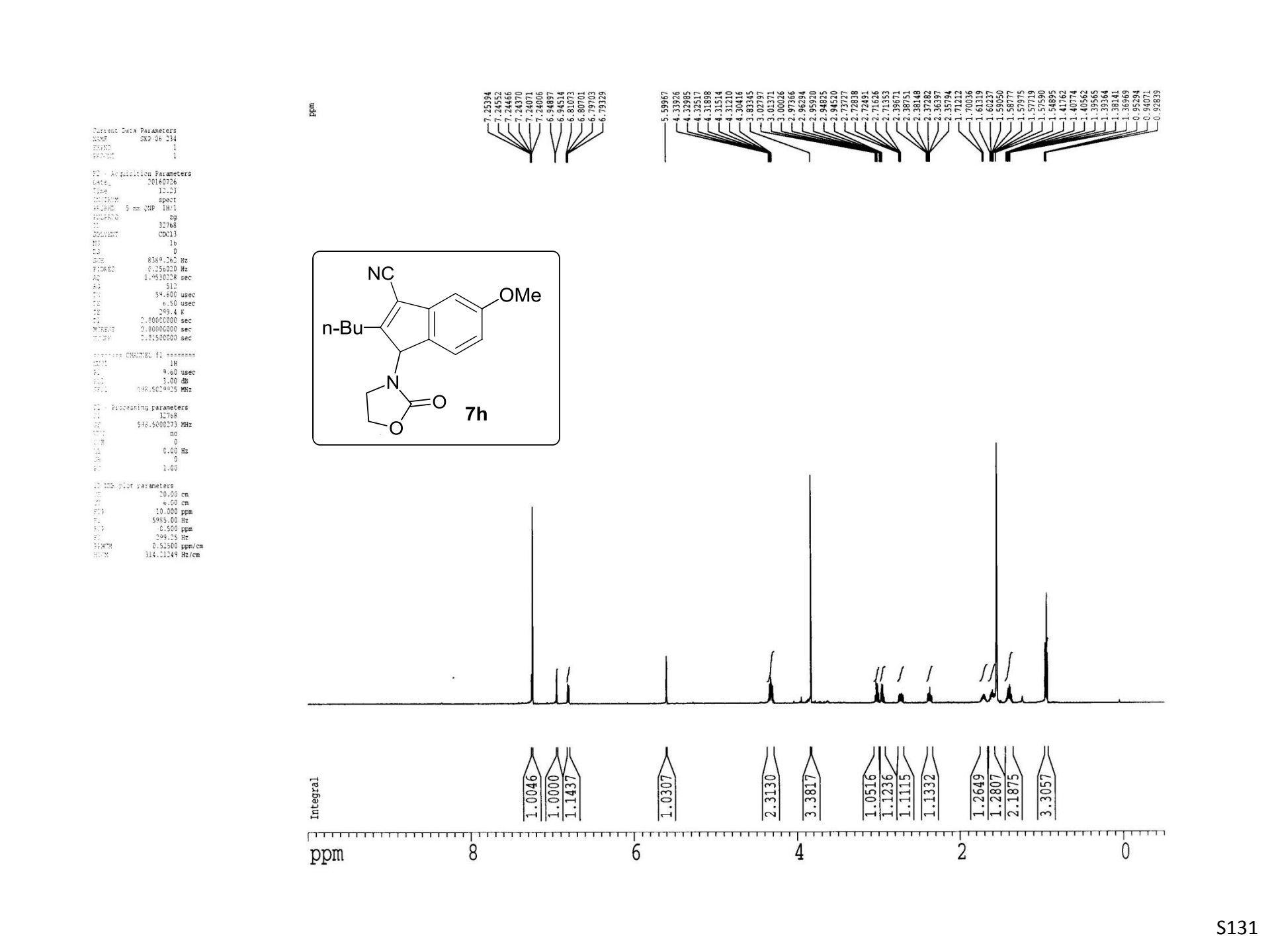
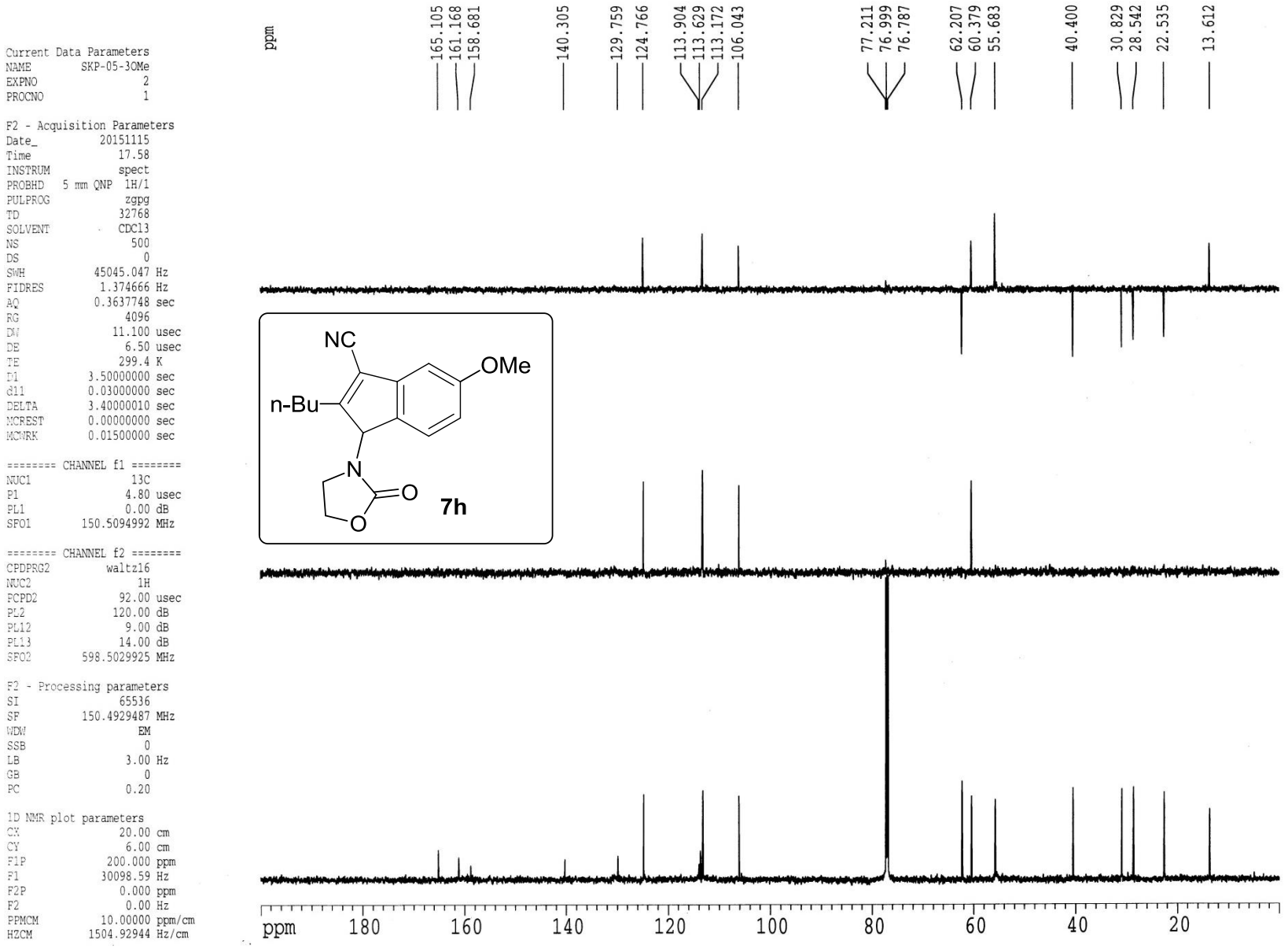
NAME SKP-05-6Me
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20151113
Time 21.14
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 32
DS 0
SWH 9541.984 Hz
FIDRES 0.291198 Hz
AQ 1.7170932 sec
RG 512
DW 52.400 usec
DE 6.50 usec
TE 298.3 K
D1 2.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 12.30 usec
PL1 3.00 dB
SFO1 598.5037107 MHz
F2 - Processing parameters
SI 32768
SF 598.5000272 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
7.29519
7.28242
7.24042
7.20524
7.20412
7.19131
7.18334
7.18230
5.60627
4.34863
4.34476
4.33469
4.32999
4.32113
4.31888
3.02255
3.00849
2.99349
2.98178
2.97868
2.96737
2.37296
2.36253
1.54380
1.39252
1.38990
1.37781
0.95056
0.93830
0.92600
NC
n-Bu
Me
N
O
O
7g
Integral
1.0000
2.2373
1.0286
2.2435
2.0859
1.1482
4.2443
1.0973
1.2738
2.1698
3.3086
ppm
8
6
4
2
0


162.49
158.75
138.55
137.68
136.20
130.13
124.80
120.02
113.98
113.80
77.21
77.00
76.79
62.21
60.79
40.47
30.86
28.38
22.54
21.43
13.63
Current Data Parameters
NAME SKP-05-6Me
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20151114
Time 3.59
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 6144
DS 0
SWH 45045.047 Hz
AQ 0.3637748 sec
RG 4096
DW 11.100 usec
DE 6.50 usec
TE 299.8 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
PL13 14.00 dB
SFO2 598.5029925 MHz
F2 - Processing parameters
SI 65536
SF 150.4929467 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 0.20
1D NMR plot parameters
CX 20.00 cm
CY 20.00 cm
F1P 200.000 ppm
F1 30098.59 Hz
F2P 0.000 ppm
F2 0.00 Hz
NC
n-Bu
Me
N
O
O
7g
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm


Current Data Parameters
NAME SKP-06-234
EXPNO 1
PROCNO 1
1H - Acquisition Parameters
Date_ 20160726
Time 12.23
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 8389.262 Hz
FIDRES 0.256020 Hz
AQ 1.9530224 sec
RG 512
DW 59.600 usec
DE 6.50 usec
TE 299.4 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 500.5079925 MHz
1H - Processing parameters
SI 32768
SF 500.5000273 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
1H NMR plot parameters
CX 20.00 cm
CY 6.00 cm
F1P 10.000 ppm
F1 5005.00 Hz
F2P 0.500 ppm
F2 249.25 Hz
PPMCM 0.52500 ppm/cm
HZCM 314.21249 Hz/cm
ppm
7.25394
7.24552
7.24466
7.24370
7.24071
7.24006
6.94897
6.94514
6.81073
6.80701
6.79703
6.79329
5.59967
4.33926
4.32985
4.32517
4.31898
4.31514
4.31210
4.30416
3.88345
3.02797
3.01371
3.00026
2.97366
2.96294
2.95920
2.94825
2.94520
2.73727
2.72838
2.72491
2.71626
2.71353
2.39671
2.38751
2.38148
2.37282
2.36397
2.35794
1.71212
1.70036
1.61319
1.60237
1.59050
1.58777
1.57975
1.57719
1.57590
1.54895
1.41762
1.40774
1.40562
1.39565
1.39364
1.38141
1.36969
0.95294
0.94071
0.92839
NC
OMe
n-Bu
N
O
O
7h
Integral
1.0046
1.0000
1.1437
1.0307
2.3130
3.3817
1.0516
1.1236
1.1115
1.1332
1.2649
1.2807
2.1875
3.3057
ppm
8
6
4
2
0


Current Data Parameters
NAME SKP-05-3OMe
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20151115
Time 17.58
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 299.4 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 0.20
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
ppm
165.105
161.168
158.681
140.305
129.759
124.766
113.904
113.629
113.172
106.043
77.211
76.999
76.787
62.207
60.379
55.683
40.400
30.829
28.542
22.535
13.612
NC
OMe
n-Bu
N
O
O
7h
ppm
180
160
140
120
100
80
60
40
20

```
Current Data Parameters
NAME        SKP-05-3Cl-A
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20151118
Time                17.29
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                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         598.5037107 MHz

F2 - Processing parameters
SI                 32768
SF           598.5000284 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
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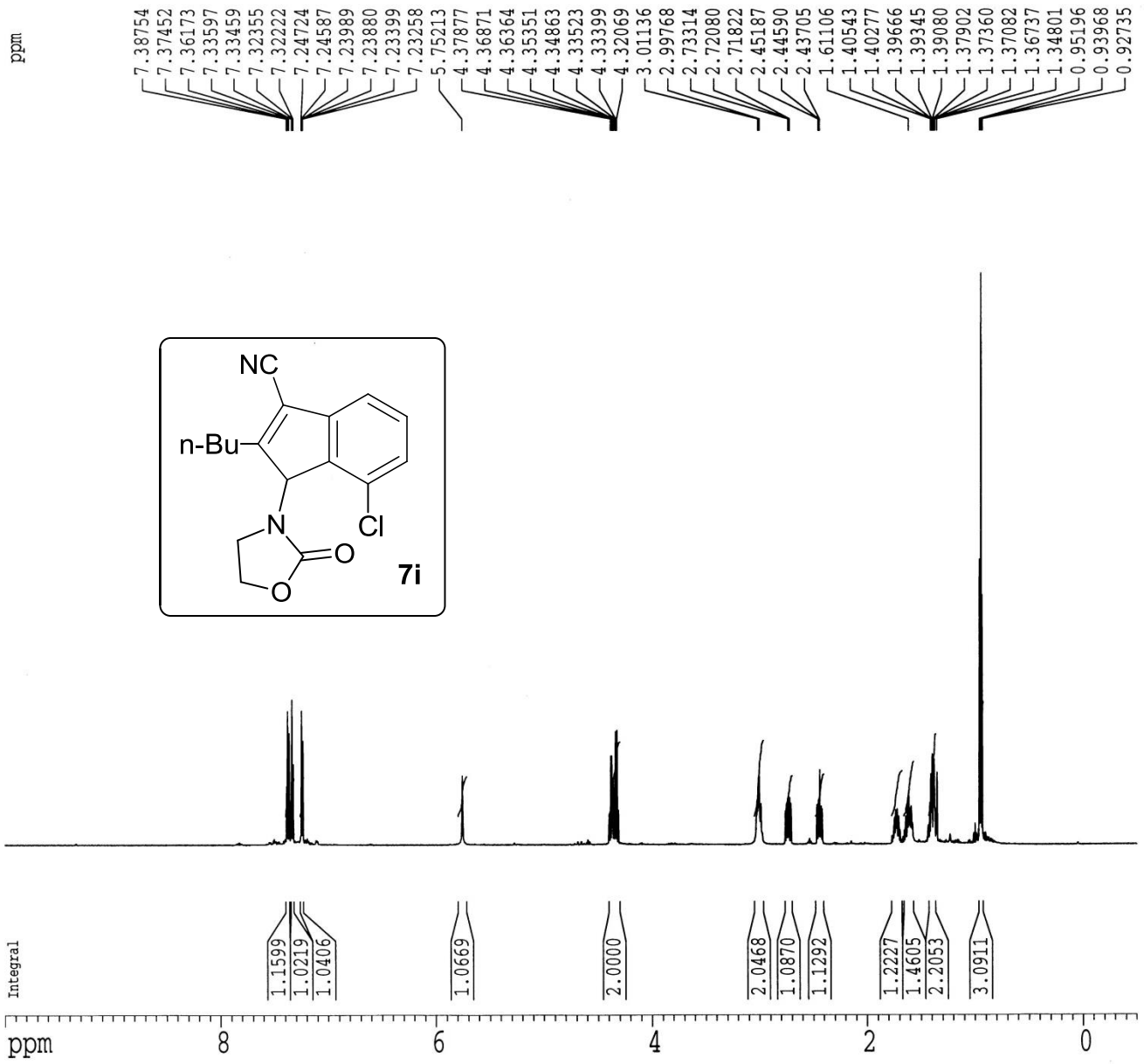
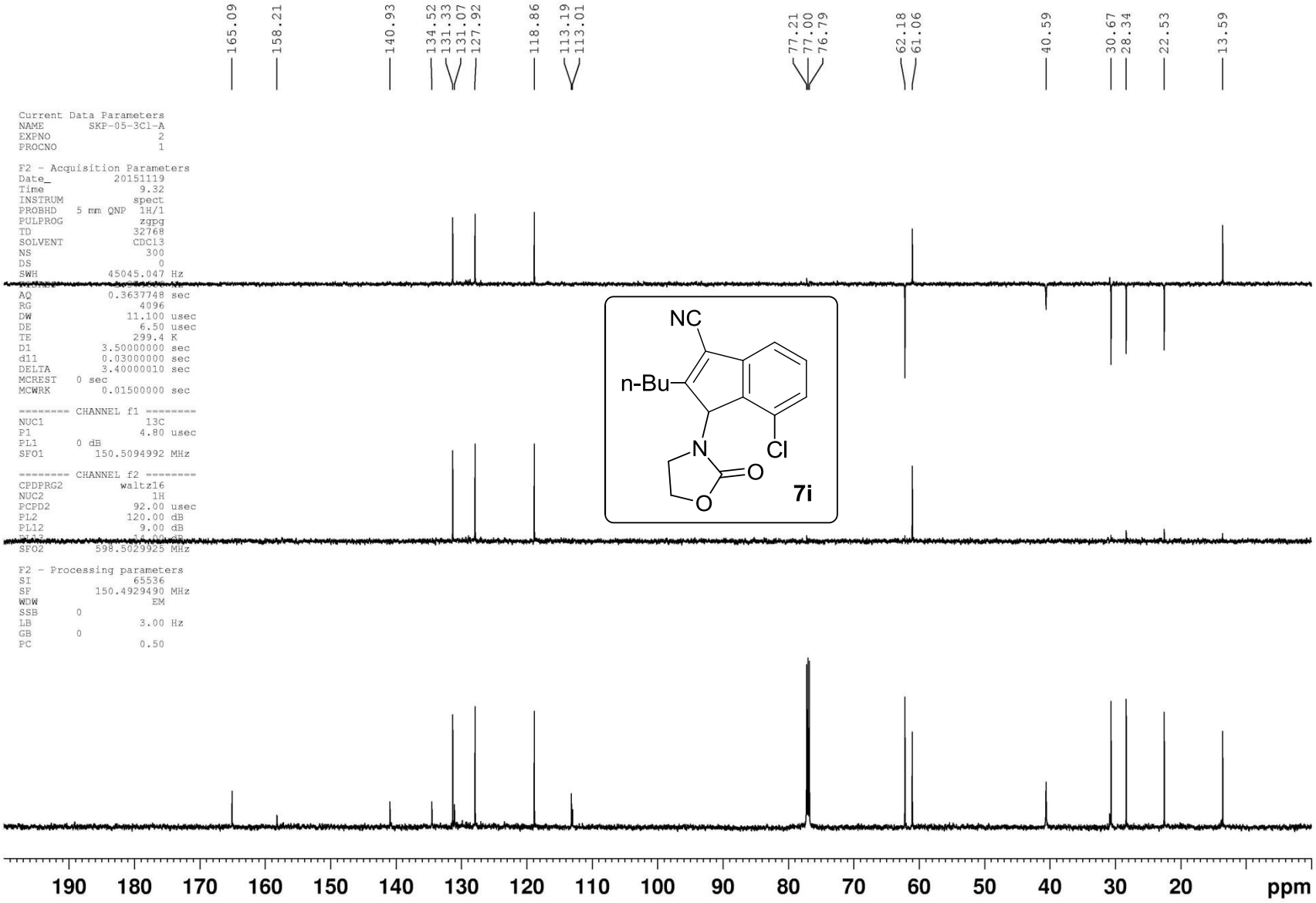
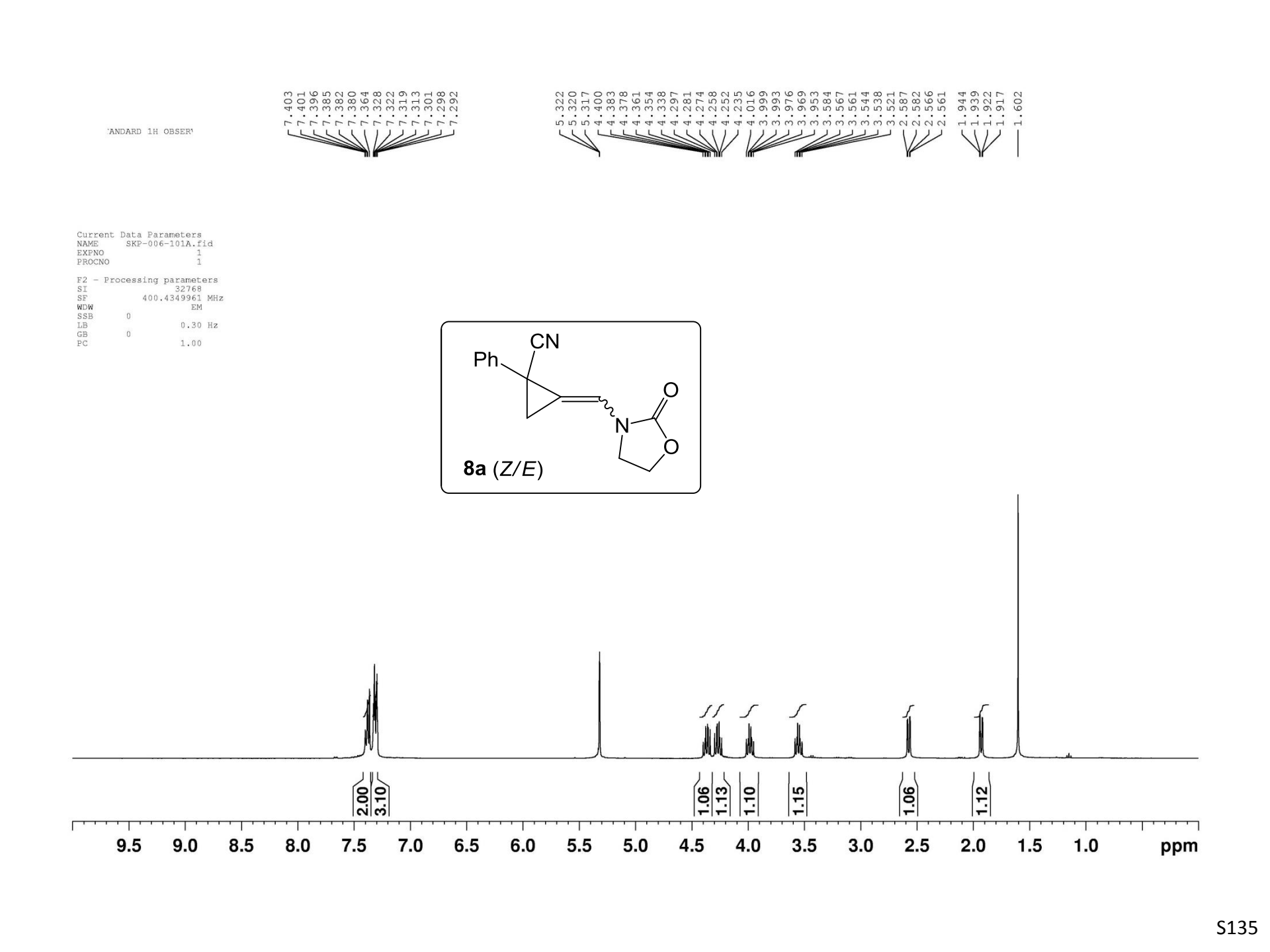
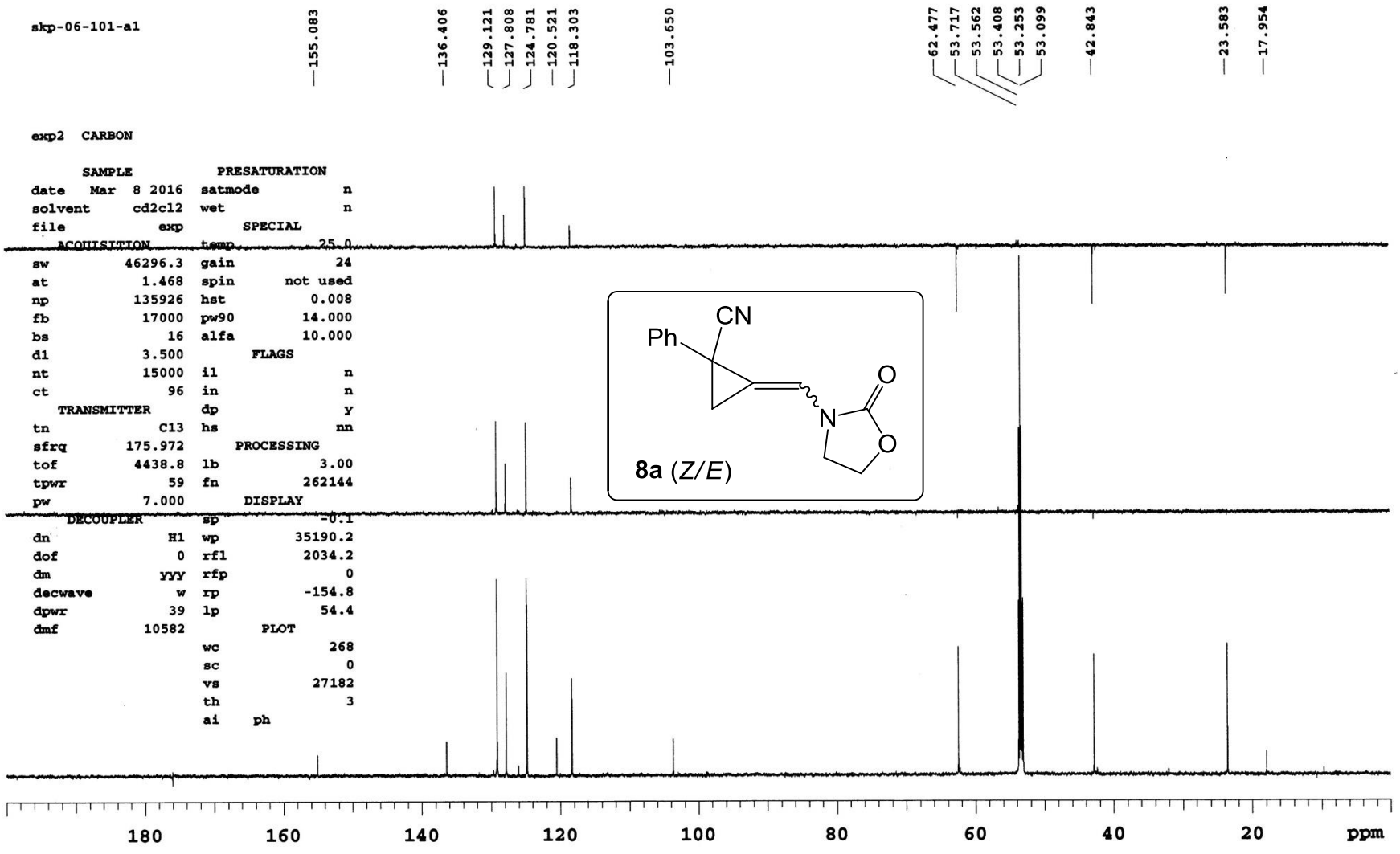



165.09
158.21
140.93
134.52
131.33
131.07
127.92
118.86
113.19
113.01
77.21
77.00
76.79
62.18
61.06
40.59
30.67
28.34
22.53
13.59
Current Data Parameters
NAME SKP-05-3Cl-A
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20151119
Time 9.32
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 300
DS 0
SWH 45045.047 Hz
AQ 0.3637748 sec
RG 4096
DW 11.100 usec
DE 6.50 usec
TE 299.4 K
D1 3.50000000 sec
d11 0.03000000 sec
DELTA 3.40000010 sec
MCREST 0 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 4.80 usec
PL1 0 dB
SFO1 150.5094992 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 92.00 usec
PL2 120.00 dB
PL12 9.00 dB
SFO2 598.5029925 MHz
F2 - Processing parameters
SI 65536
SF 150.4929490 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 0.50
NC
n-Bu
N
Cl
O
O
7i
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm


'ANDARD 1H OBSER'
7.403
7.401
7.396
7.385
7.382
7.380
7.364
7.328
7.322
7.319
7.313
7.301
7.298
7.292
5.322
5.320
5.317
4.400
4.383
4.378
4.361
4.354
4.338
4.297
4.281
4.274
4.258
4.252
4.235
4.016
3.999
3.993
3.976
3.969
3.953
3.584
3.567
3.561
3.544
3.538
3.521
2.587
2.582
2.566
2.561
1.944
1.939
1.922
1.917
1.602
Current Data Parameters
NAME SKP-006-101A.fid
EXPNO 1
PROCNO 1
F2 - Processing parameters
SI 32768
SF 400.4349961 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
CN
Ph
O
N
O
8a (Z/E)
2.00
3.10
1.06
1.13
1.10
1.15
1.06
1.12
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


skp-06-101-a1
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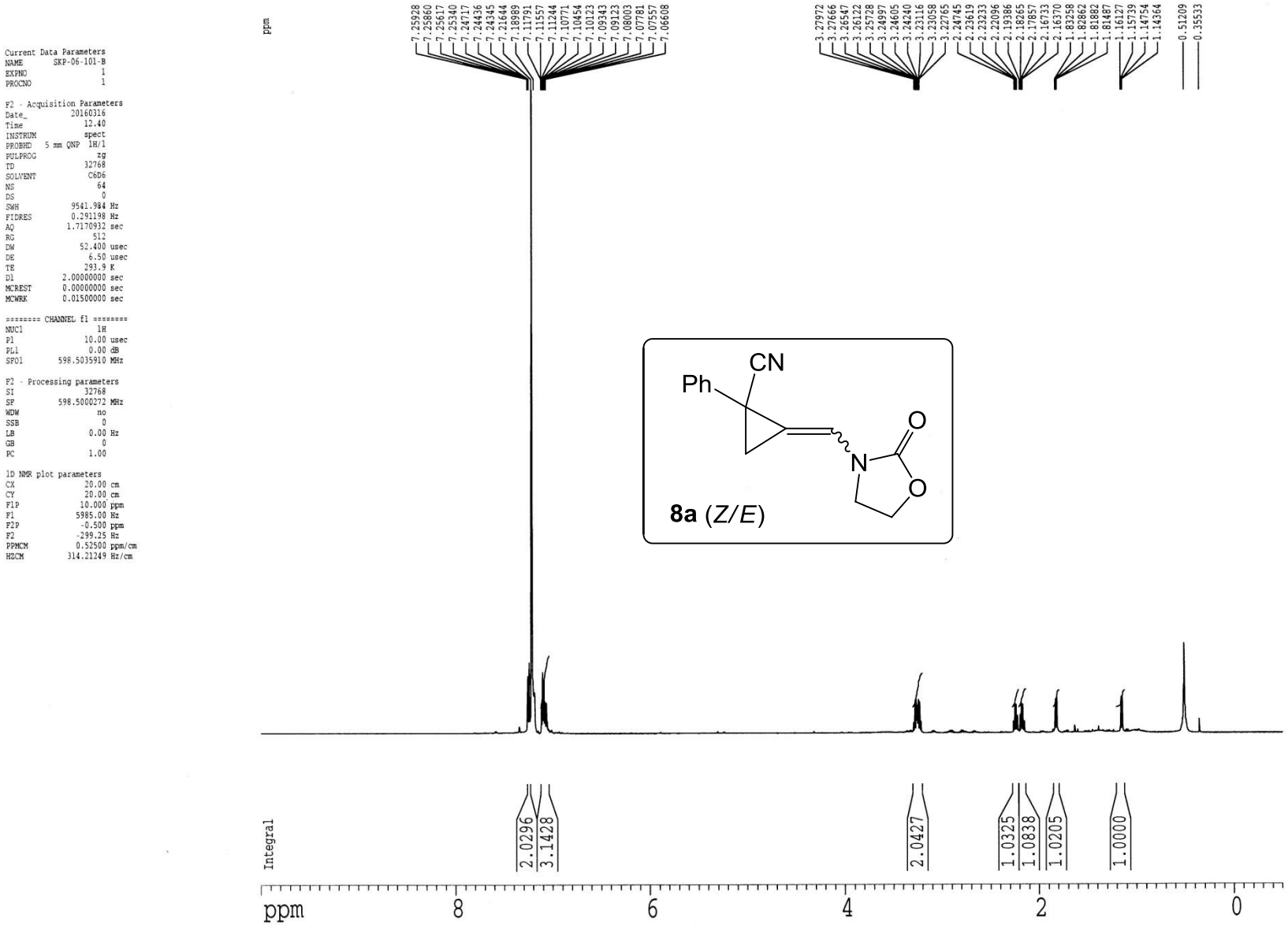
136.406
129.121
127.808
124.781
120.521
118.303
103.650
62.477
53.717
53.562
53.408
53.253
53.099
42.843
23.583
17.954
exp2 CARBON
SAMPLE
date Mar 8 2016
solvent cd2cl2
file exp
ACQUISITION
sw 46296.3
at 1.468
np 135926
fb 17000
bs 16
d1 3.500
nt 15000
ct 96
TRANSMITTER
tn C13
sfrq 175.972
tof 4438.8
tpwr 59
pw 7.000
DECOUPLER
dn H1
dof 0
dm yyy
decwave w
dpwr 39
dmf 10582
PRESATURATION
satmode n
wet n
SPECIAL
temp 25.0
gain 24
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 -0.1
wp 35190.2
rfl 2034.2
rfp 0
rp -154.8
lp 54.4
PLOT
wc 268
sc 0
vs 27182
th 3
ai ph
CN
Ph
O
N
O
8a (Z/E)
180
160
140
120
100
80
60
40
20
ppm


Current Data Parameters
NAME SKP-06-101-B
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20160316
Time 12.40
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg
TD 32768
SOLVENT C6D6
NS 64
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 293.9 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 598.5000272 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
7.25928
7.25860
7.25617
7.25340
7.24717
7.24436
7.24345
7.21644
7.18989
7.11791
7.11557
7.11244
7.10771
7.10454
7.10123
7.09343
7.09123
7.08003
7.07781
7.07557
7.06608
3.27972
3.27666
3.26547
3.26122
3.25728
3.24997
3.24605
3.24240
3.23116
3.23058
3.22765
2.24745
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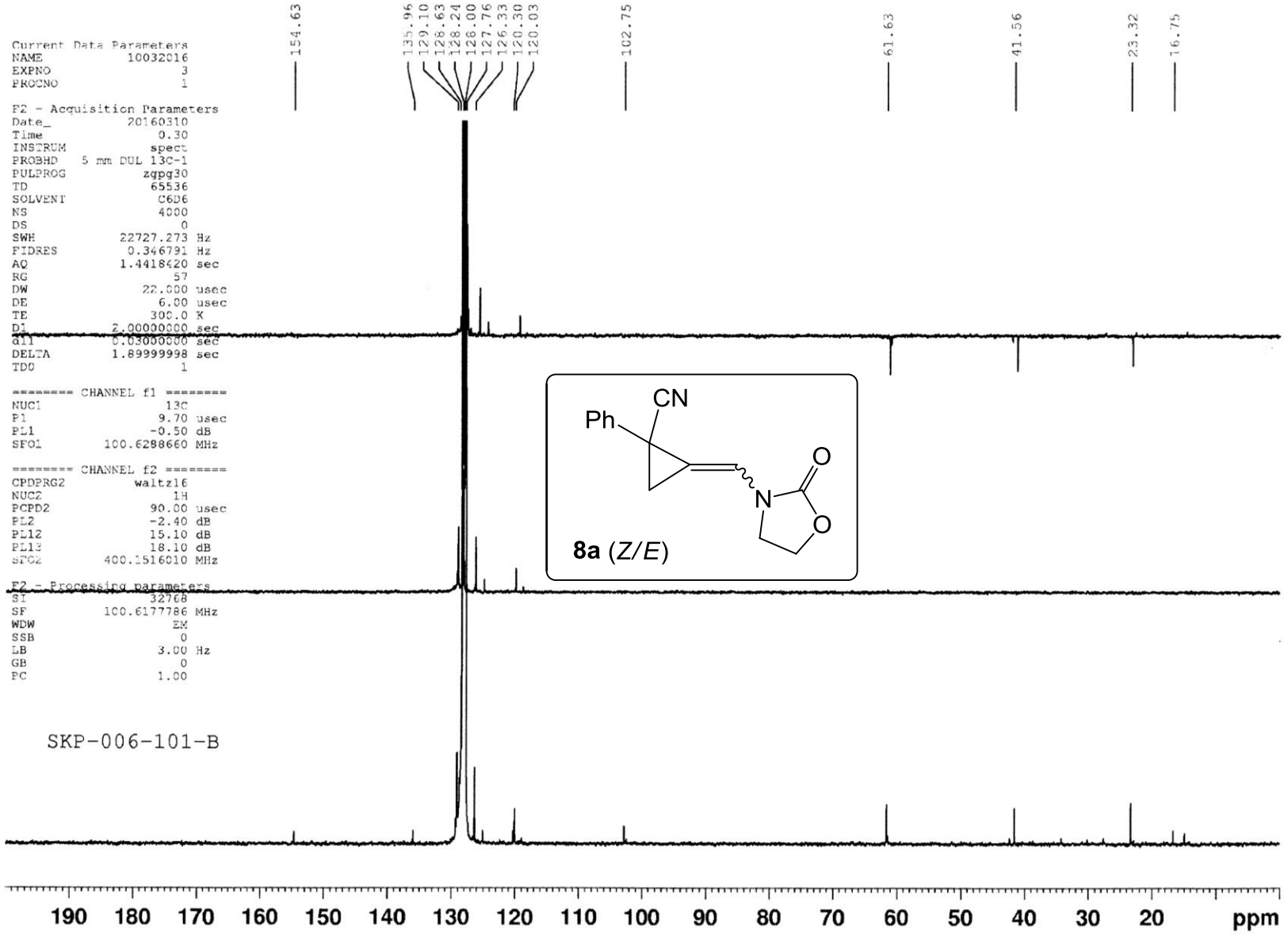
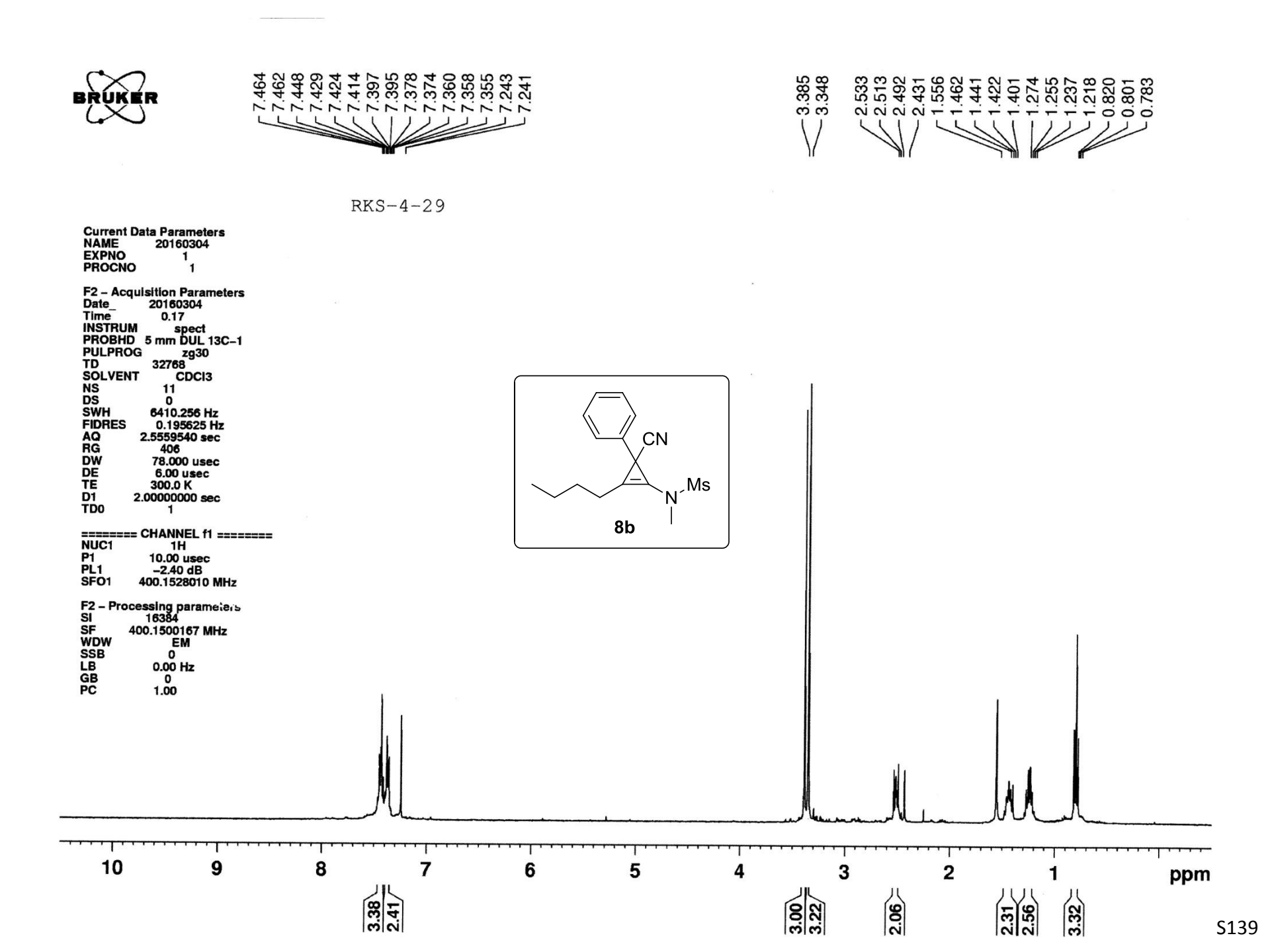
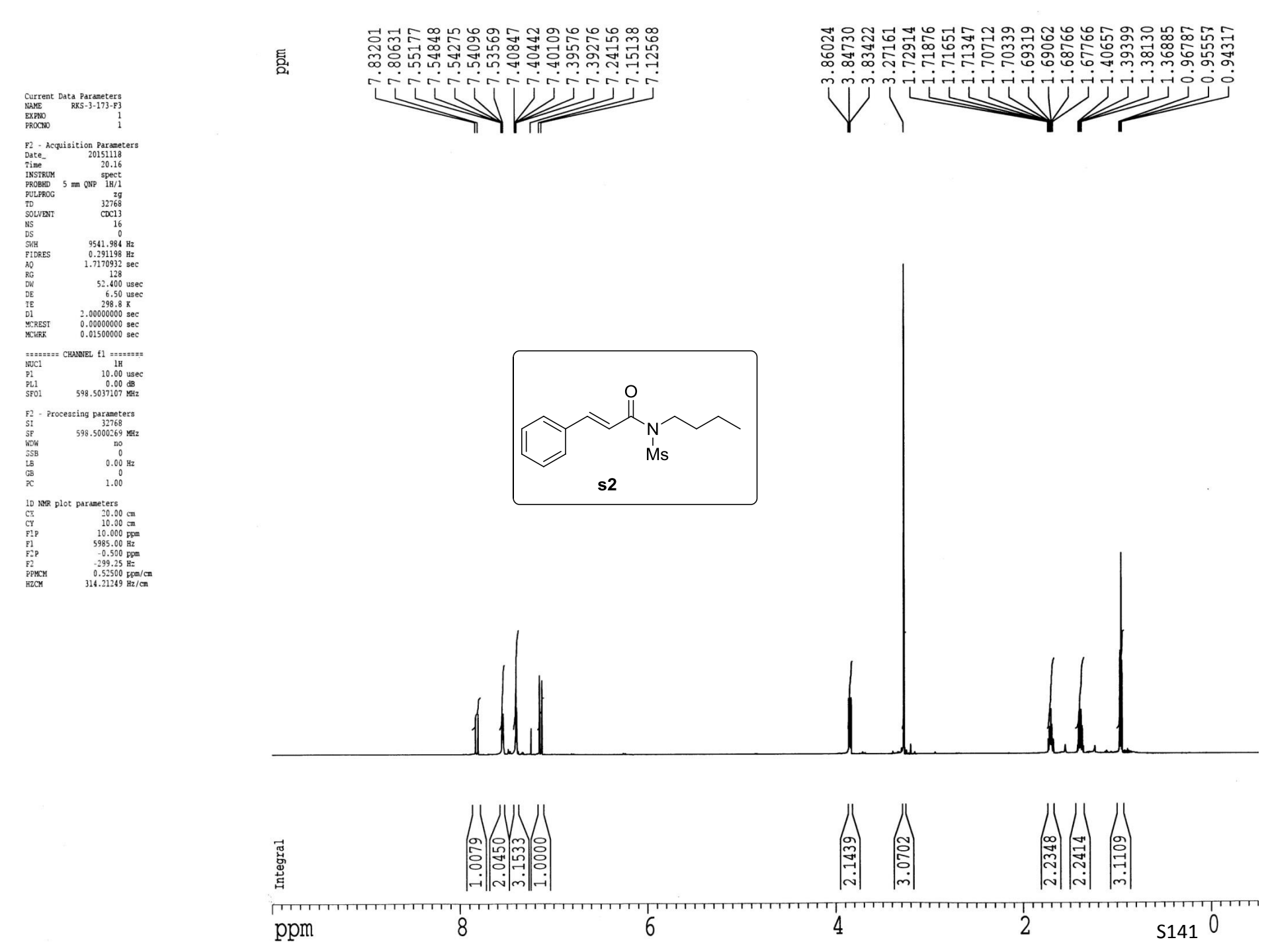
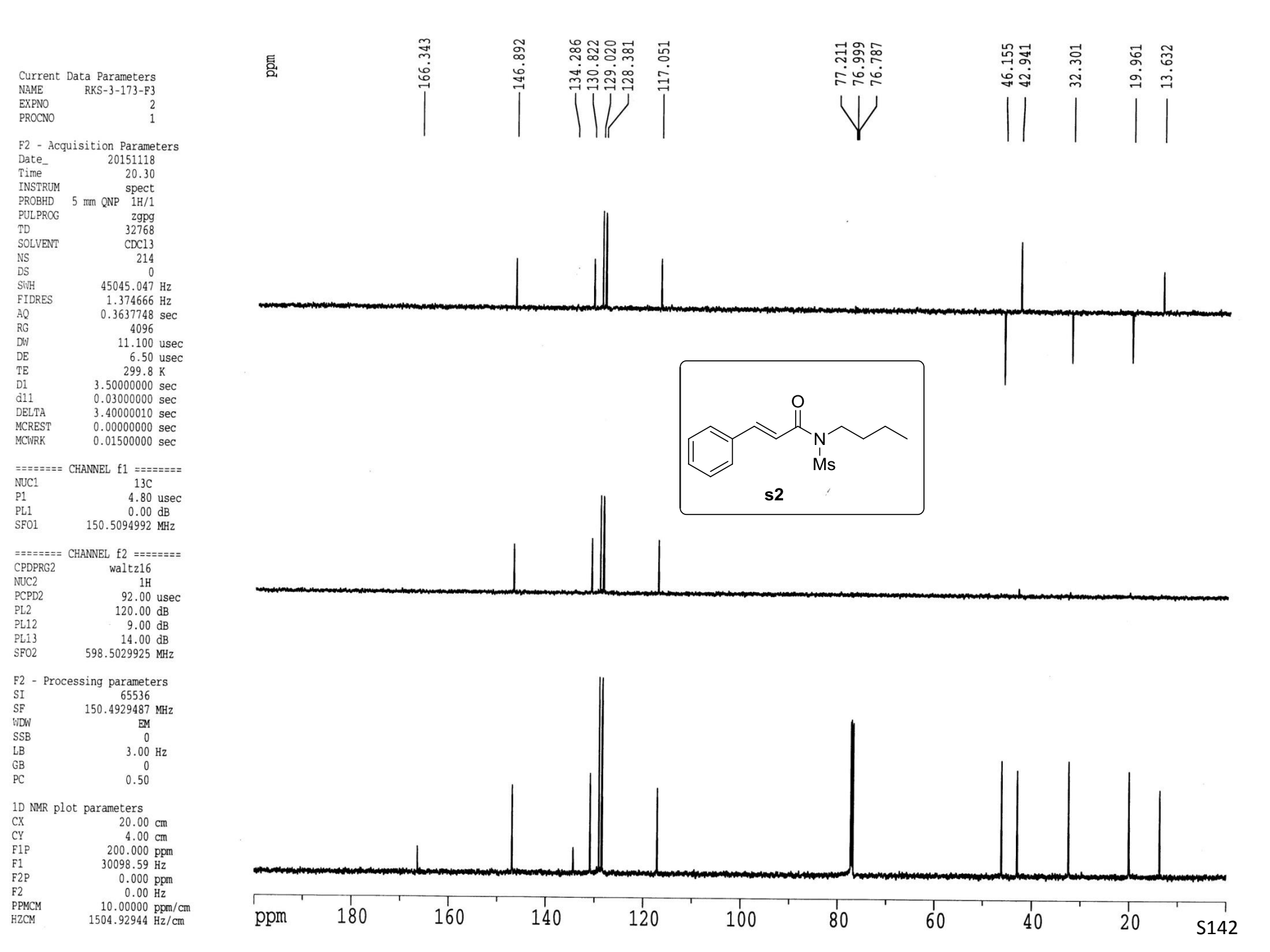
2.23233
2.22096
2.19386
2.18265
2.17857
2.16733
2.16370
1.83258
1.82862
1.81882
1.81487
1.16127
1.15739
1.14754
1.14364
0.51209
0.35533
CN
Ph
O
N
O
8a (Z/E)
Integral
2.0296
3.1428
2.0427
1.0325
1.0838
1.0205
1.0000
ppm
8
6
4
2
0

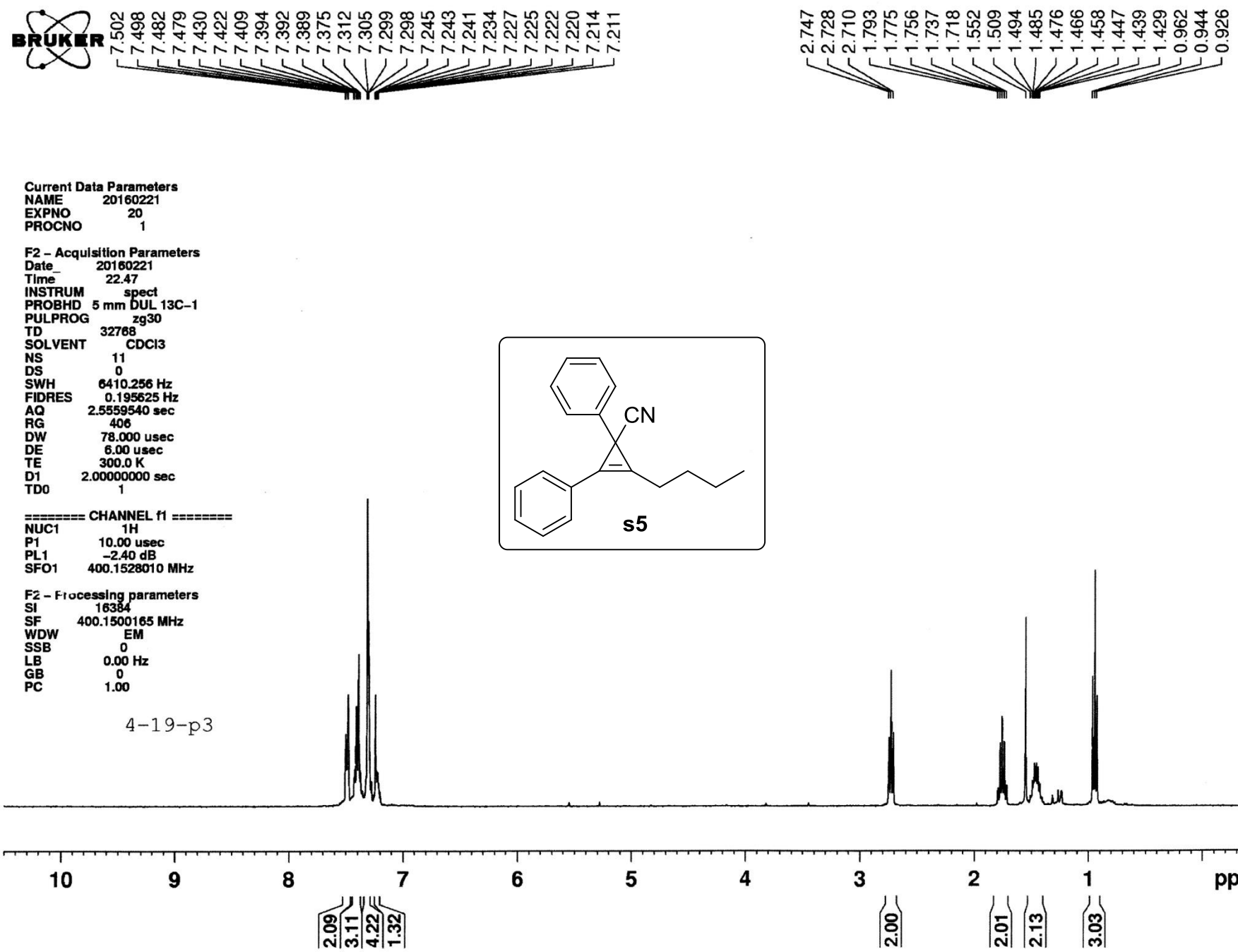

154.63
135.96
129.10
128.63
128.24
126.00
127.76
126.33
120.30
120.03
102.75
61.63
41.56
23.32
16.75
Current Data Parameters
NAME 10032016
EXPNO 3
PROCNO 1
F2 - Acquisition Parameters
Date_ 20160310
Time 0.30
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT C6D6
NS 4000
DS 0
SWH 22727.273 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 100.6177786 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
SKP-006-101-B
CN
Ph
O
N
O
8a (Z/E)
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

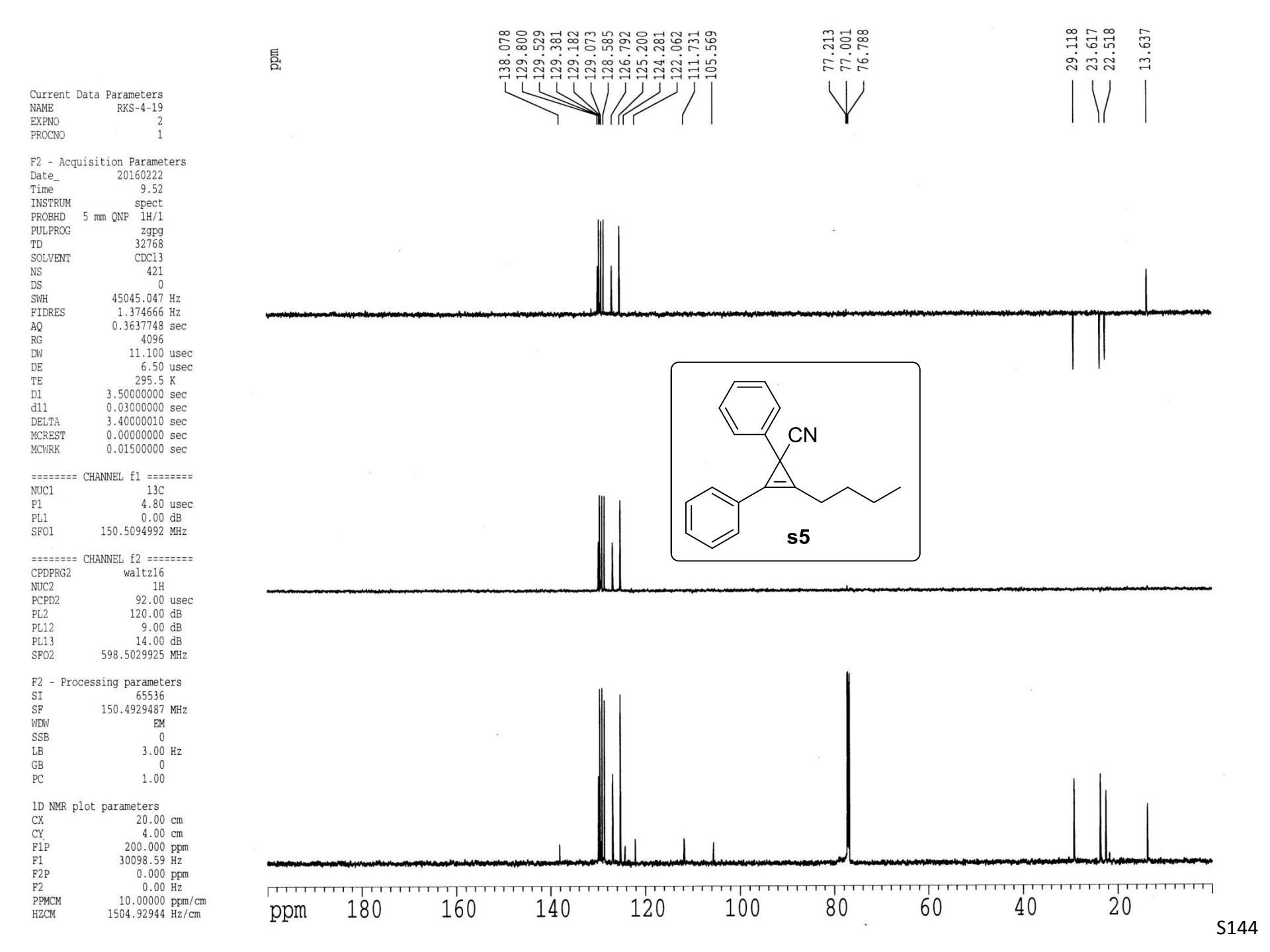

7.464
7.462
7.448
7.429
7.424
7.414
7.397
7.395
7.378
7.374
7.360
7.358
7.355
7.243
7.241
3.385
3.348
2.533
2.513
2.492
2.431
1.556
1.462
1.441
1.422
1.401
1.274
1.255
1.237
1.218
0.820
0.801
0.783
RKS-4-29
Current Data Parameters
NAME 20160304
EXPNO 1
PROCNO 1
F2 – Acquisition Parameters
Date_ 20160304
Time 0.17
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 406
DW 78.000 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 -2.40 dB
SFO1 400.1528010 MHz
F2 – Processing parameters
SI 16384
SF 400.1500167 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
CN
N
Ms
8b
10
9
8
7
6
5
4
3
2
1
ppm
3.38
2.41
3.00
3.22
2.06
2.31
2.56
3.32

168.29
155.64
131.11
129.69
129.11
128.62
117.53
112.04
77.32
77.00
76.68
40.59
32.76
31.57
29.47
22.52
13.52
Current Data Parameters
NAME 20160304
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20160304
Time 0.22
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 45.2
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
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 100.6177999 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
CN
N
Ms
8b
RKS-4-29
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20
ppm


Current Data Parameters
NAME RKS-3-173-F3
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20151118
Time 20.16
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 298.8 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 598.5037107 MHz
F2 - Processing parameters
SI 32768
SF 598.5000269 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
7.83201
7.80631
7.55177
7.54848
7.54275
7.54096
7.53569
7.40847
7.40442
7.40109
7.39576
7.39276
7.24156
7.15138
7.12568
3.86024
3.84730
3.83422
3.27161
1.72914
1.71876
1.71651
1.71347
1.70712
1.70339
1.69319
1.69062
1.68766
1.67766
1.40657
1.39399
1.38130
1.36885
0.96787
0.95557
0.94317
O
N
Ms
s2
Integral
1.0079
2.0450
3.1533
1.0000
2.1439
3.0702
2.2348
2.2414
3.1109
ppm
8
6
4
2
0


Current Data Parameters
NAME RKS-3-173-F3
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20151118
Time 20.30
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 214
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 299.8 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 150.4929487 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
166.343
146.892
134.286
130.822
129.020
128.381
117.051
77.211
76.999
76.787
46.155
42.941
32.301
19.961
13.632
O
N
Ms
s2
ppm
180
160
140
120
100
80
60
40
20


7.502
7.498
7.482
7.479
7.430
7.422
7.409
7.394
7.392
7.389
7.375
7.312
7.305
7.299
7.298
7.245
7.243
7.241
7.234
7.227
7.225
7.222
7.220
7.214
7.211
2.747
2.728
2.710
1.793
1.775
1.756
1.737
1.718
1.552
1.509
1.494
1.485
1.476
1.466
1.458
1.447
1.439
1.429
0.962
0.944
0.926
Current Data Parameters
NAME 20160221
EXPNO 20
PROCNO 1
F2 – Acquisition Parameters
Date_ 20160221
Time 22.47
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 406
DW 78.000 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 –2.40 dB
SFO1 400.1528010 MHz
F2 – Processing parameters
SI 16384
SF 400.1500165 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
4-19-p3
CN
s5
10
9
8
7
6
5
4
3
2
1
ppm
2.09
3.11
4.22
1.32
2.00
2.01
2.13
3.03



Current Data Parameters
NAME RKS-4-19
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20160222
Time 9.52
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 421
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 295.5 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 150.4929487 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