– Supporting Information –

Sequential Oxidative α-Cyanation/anti-Markovnikov Hydroalkoxylation of Allylamines

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1. General

All reactions were carried out under an atmosphere of dry nitrogen. ^{1}H (300 or 400 MHz) and ^{13}C (75.5 or 100.6 MHz) NMR spectra of solutions in $CDCl_3$ were recorded on 300 or 400 MHz NMR spectrometers. Chemical shifts are expressed in parts per million (ppm) downfield from tetramethylsilane and refer to the solvent signals (δ_H 7.26 and δ_C 77.16 ppm).[S1] Abbreviations for signal couplings are: s, singlet; d, doublet; t, triplet; q, quartet; m, multiplet. Signal assignments are based on gCOSY and gHSQC experiments. HRMS was performed on a Finnigan MAT 95Q mass spectrometer. Infrared spectra of neat substances were recorded on a Perkin-Elmer Spectrum BX II FT-IR spectrometer equipped with an ATR probe (diamond).

Materials. Triallylamine (Aldrich), iron(II) chloride (98 %, Aldrich), trimethylsilyl cyanide (98 %, Acros), *tert*.-butyl hydroperoxide (5.5 M solution in decane, purum, Aldrich) and d_4-methanol (99.80 % D, Euriso-Top) were purchased.

Allylanilines and allylamines were synthesized according to literature procedures.[S2,S3]

(S1) Fulmer, G. R.; Miller, A. J. M.; Sherden, N. H.; Gottlieb, H. E.; Nudelman, A.; Stoltz, B. M.; Bercaw, J. E.; Goldberg, K. I. *Organometallics* **2010**, *29*, 2176-2179.

(S2) Li, L.; Jones, W. D. *J. Am. Chem. Soc*. **2007**, *129*, 10707-10713.

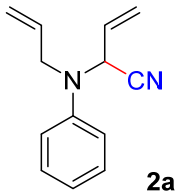
(S3) Bongartz, N. A.; Goodby, J. W. *Chem. Commun*. **2010**, *46*, 6452-6454.

2. Oxidative α-cyanation/hydroalkoxylation of tertiary allylamines

General Procedure. Under an atmosphere of dry N_2, a Schlenk flask was charged with iron(II) chloride (10 mol %, 13 mg). The tertiary allylamine (1.0 mmol), trimethylsilyl cyanide (2.0 mmol, 0.27 mL), and MeOH (2.0 mL) were added successively by syringe. To the mixture was added dropwise *t*BuOOH (2.5 mmol, 0.46 mL, 5.5 M solution in decane) over a period of 5 min. The mixture was stirred at room temperature for the indicated time. At the end of the reaction, the reaction mixture was poured into a saturated aqueous Na_2CO_3 solution (20 mL) and extracted with CH_2Cl_2 (3 × 20 mL). The organic phases were combined, dried ($MgSO_4$), and the volatile components were evaporated in a rotary evaporator. The crude product was purified by column chromatography on silica gel.

2-(Allyl(phenyl)amino)but-3-enenitrile (2a)

Following the *General Procedure*, *N*,*N*-diallylaniline **1a** (173 mg, 1.00 mmol) reacted with Me_3SiCN and *t*BuOOH for 4 h. The crude product was purified by column chromatography (SiO_2, pentane/CH_2Cl_2 = 3:2) to give **2a** (42 mg, 21 %) as a colorless liquid.



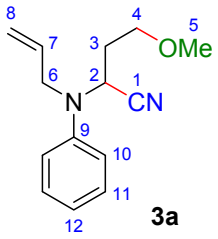
2a

^{1}H NMR (300 MHz, $CDCl_3$): δ = 3.77–3.90 (m, 2 H), 5.09–5.27 (m, 3 H), 5.41–5.45 (m, 1 H), 5.64–5.70 (m, 1 H), 5.75–5.90 (m, 2 H), 6.87–6.93 (m, 3 H), 7.20–7.26 (m, 2 H). **^{13}C NMR** (75.5 MHz, $CDCl_3$): δ = 52.2 (CH_2), 55.3 (CH), 116.4 (C), 117.56 (CH), 117.61 (CH_2), 120.4 (CH_2), 121.3 (CH), 129.4 (CH), 131.0 (CH), 134.5 (CH),

147.4 (C). **HRMS** (EI, 70 eV): *m*/*z* $[M]^{+\cdot}$ Calcd for $[C_{13}H_{14}N_2]^{+\cdot}$ 198.1152; Found 198.1147.

2-(Allyl(phenyl)amino)-4-methoxybutanenitrile (3a)

Following the *General Procedure*, *N*,*N*-diallylaniline **1a** (173 mg, 1.00 mmol) reacted with Me_3SiCN and *t*BuOOH for 16 h. The crude product was purified by column chromatography (SiO_2, pentane/CH_2Cl_2 = 3:2) to give **3a** (198 mg, 86 %) as a colorless liquid.



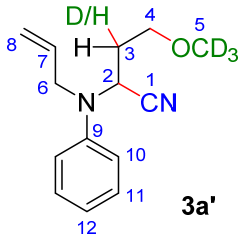
3a

^{1}H NMR (300 MHz, $CDCl_3$): δ = 2.03–2.18 (m, 2 H, 3-H), 3.36 (s, 3 H, 5-H), 3.51–3.55 (m, 2 H, 4-H), 3.85–4.00 (m, 2 H, 6-H), 4.76 (t, *J* = 7.7 Hz, 1 H, 2-H), 5.19–5.33 (m, 2 H, 8-H), 5.83–5.95 (m, 1 H, 7-H), 6.93–7.01 (m, 10-H and 12-H), 7.26–7.32 (m, 11-H). **^{13}C NMR** (75.5 MHz, $CDCl_3$): δ = 32.6 (CH_2, C-3), 49.9 (CH, C-2), 52.8 (CH_2, C-6), 58.9 (CH_3, C-5), 67.7 (CH_2, C-4), 117.5 (CH_2, C-8), 118.0 (CH, C-10), 118.6 (C, C-1), 121.3 (CH, C-12), 129.3 (CH, C-11), 134.6 (CH, C-7), 147.7 (C, C-9). *ν* (neat/ATR probe): 2959, 2929, 2874, 1495, 1453, 1363, 1189, 1116, 913, 731, 698 cm^{-1}. **HRMS** (EI, 70 eV): *m*/*z* $[M]^{+\cdot}$ Calcd for $[C_{14}H_{18}N_2O]^{+\cdot}$ 230.1414; Found 230.1414.

2-(Allyl(phenyl)amino)-4-(*d*$_3$-methoxy)butanenitrile (3a')

Following the *General Procedure* using CD_3OD as solvent, *N,N*-diallylaniline **1a** (173 mg, 1.00 mmol) reacted with Me_3SiCN and *t*BuOOH for 16 h. The crude product was

purified by column chromatography (SiO_2, pentane/CH_2Cl_2 = 3:2) to give **3a'** (205 mg, 88 %) as a colorless liquid.

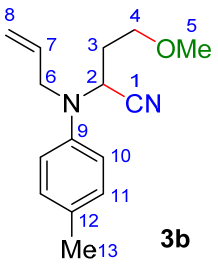


3a'

^{1}H NMR (300 MHz, $CDCl_3$): δ = 2.04–2.20 (m, 1.6 H, 3-H), 3.50–3.55 (m, 2 H, 4-H), 3.84–4.00 (m, 2 H, 6-H), 4.73–4.78 (m, 1 H, 2-H), 5.18–5.33 (m, 2 H, 8-H), 5.82–5.95 (m, 1 H, 7-H), 6.92–7.01 (m, 10-H and 12-H), 7.26–7.31 (m, 11-H). **^{2}H NMR** (61.4 MHz, $CDCl_3$): δ = 3.33 (s, 3 D, 5-D), ca. 2.13 (m, 0.4 D, 3-D). **^{13}C NMR** (100.6 MHz, $CDCl_3$): δ = 32.3 (t, $^1J_{C,D}$ = 20.0 Hz, CHD, C-3) and 32.6 (CH_2, C-3), 49.86/49.92 (CH, C-2), 52.79/52.80 (CH_2, C-6), 58.1 (sept, $^1J_{C,D}$ = 21.5 Hz, CD_3, C-5), 67.55/67.60 (CH_2, C-4), 117.5 (CH_2, C-8), 118.0 (CH, C-10), 118.6 (C, C-1), 121.3 (CH, C-12), 129.4 (CH, C-11), 134.6 (CH, C-7), 147.8 (C, C-9). **HRMS** (EI, 70 eV): *m*/*z* $[M]^{+\cdot}$ Calcd for $[C_{14}H_{15}{}^2H_3N_2O]^{+\cdot}$ 233.1602; Found 233.1617.

2-(Allyl(*p*-tolyl)amino)-4-methoxybutanenitrile (3b)

Following the *General Procedure*, *N,N*-diallyl-4-methylaniline **1b** (187 mg, 1.00 mmol) reacted with Me_3SiCN and *t*BuOOH in decane for 14 h. The crude product was purified by column chromatography (SiO_2, pentane/CH_2Cl_2 = 3:2) to give **3b** (208 mg, 85 %) as a colorless liquid.

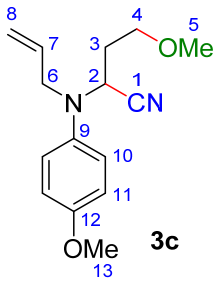


3b

^{1}H NMR (300 MHz, $CDCl_3$): δ = 1.98–2.20 (m, 2 H, 3-H), 2.30 (s, 3 H, 13-H), 3.36 (s, 3 H, 5-H), 3.47–3.60 (m, 2 H, 4-H), 3.80–3.95 (m, 2 H, 6-H), 4.64 (t, *J* = 7.7 Hz, 1 H, 2-H), 5.18–5.33 (m, 2 H, 8-H), 5.81–5.93 (m, 1 H, 7-H), 6.94–6.97 (m, 2 H, 10-H), 7.09–7.13 (m, 2 H, 11-H). **^{13}C NMR** (75.5 MHz, $CDCl_3$): δ = 20.6 (CH_3, C-13), 32.6 (CH_2, C-3), 50.6 (CH, C-2), 53.4 (CH_2, C-6), 58.9 (CH_3, C-5), 67.8 (CH_2, C-4), 117.6 (CH_2, C-8), 118.6 (C, C-1), 119.6 (CH, C-10), 129.9 (CH, C-11), 131.7 (C, C-12), 134.8 (CH, C-7), 145.4 (C, C-9). *ν* (neat/ATR probe): 2925, 2875, 1616, 1514, 1455, 1385, 1239, 1219, 1183, 1117, 990, 921, 866, 806, 727 cm^{-1}. **HRMS** (EI, 70 eV): *m*/*z* $[M]^{+\cdot}$ Calcd for $[C_{15}H_{20}N_2O]^{+\cdot}$ 244.1571; Found 244.1576.

2-(Allyl(4-methoxyphenyl)amino)-4-methoxybutanenitrile (3c)

Following the *General Procedure*, *N,N*-diallyl-4-methoxyaniline **1c** (203 mg, 1.00 mmol) reacted with Me_3SiCN and *t*BuOOH for 14 h. The crude product was purified by column chromatography (SiO_2, pentane/CH_2Cl_2 = 3:2) to give **3c** (242 mg, 93 %) as a colorless liquid.



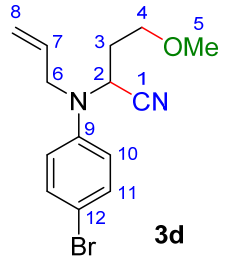
3c

^{1}H NMR (300 MHz, $CDCl_3$): δ = 1.88–2.14 (m, 2 H, 3-H), 3.35 (s, 3 H, 5-H), 3.45–3.60 (m, 2 H, 4-H), 3.68–3.85 (m, 2 H, 6-H), 3.78 (s superimposed with resonances of 6-H, 3 H, 13-H), 4.43 (t, *J* = 7.8 Hz, 1 H, 2-H), 5.14–5.31 (m, 2 H, 8-H), 5.75–5.88 (m, 1 H, 7-H), 6.83–6.86 and 7.06–7.09 (2 m, 2 × 2 H, 10-H and 11-H). **^{13}C NMR** (75.5 MHz, $CDCl_3$): δ = 32.6 (CH_2, C-3), 51.9 (CH, C-2), 54.9 (CH_2, C-6), 55.6 (CH_3, C-13), 58.9 (CH_3, C-5), 67.9 (CH_2, C-4), 114.5 (CH, C-10 or C-11), 118.0 (CH_2, C-8), 118.7 (C, C-1), 123.8 (CH, C-10 or C-11), 134.8 (CH, C-7), 141.1 (C, C-9), 156.3 (C,

C-12). ν (neat/ATR probe): 2931, 2834, 1509, 1462, 1244, 1214, 1181, 1117, 1036, 917, 866, 834, 731 cm^{-1}. **HRMS** (EI, 70 eV): *m*/*z* $[M]^{+\cdot}$ Calcd for $[C_{15}H_{20}N_2O_2]^{+\cdot}$ 260.1520; Found 260.1504.

2-(Allyl(4-bromophenyl)amino)-4-methoxybutanenitrile (3d)

Following the *General Procedure*, *N,N*-diallyl-4-bromoaniline **1d** (252 mg, 1.00 mmol) reacted with Me_3SiCN and *t*BuOOH for 19 h. The crude product was purified by column chromatography (SiO_2, pentane/CH_2Cl_2 = 3:2) to give **3d** (207 mg, 67 %) as a yellow liquid.

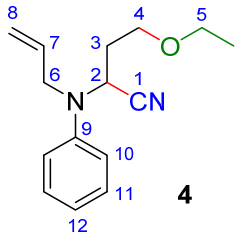


3d

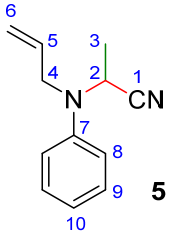
^{1}H NMR (300 MHz, $CDCl_3$): δ = 2.02–2.20 (m, 2 H, 3-H), 3.35 (s, 3 H, 5-H), 3.49–3.53 (m, 2 H, 4-H), 3.82–3.97 (m, 2 H, 6-H), 4.73 (t, *J* = 7.7 Hz, 1 H, 2-H), 5.19–5.30 (m, 2 H, 8-H), 5.78–5.91 (m, 1 H, 7-H), 6.83–6.86 (m, 2 H, 10-H), 7.35–7.38 (m, 2 H, 11-H). **^{13}C NMR** (75.5 MHz, $CDCl_3$): δ = 32.4 (CH_2, C-3), 49.7 (CH, C-2), 52.4 (CH_2, C-6), 58.9 (CH_3, C-5), 67.4 (CH_2, C-4), 113.5 (C, C-12), 117.8 (CH_2, C-8), 118.2 (C, C-1), 119.2 (CH, C-10), 132.1 (CH, C-11), 133.9 (CH, C-7), 146.6 (C, C-9). ν (neat/ATR probe): 2929, 2877, 2831, 1590, 1493, 1458, 1385, 1236, 1183, 1116, 1081, 998, 918, 866, 808, 731, 648 cm^{-1}. **HRMS** (EI, 70 eV): *m*/*z* $[M]^{+\cdot}$ Calcd for $[C_{14}H_{17}{}^{79}BrN_2O]^{+\cdot}$ 308.0519; Found 308.0522.

2-(Allyl(phenyl)amino)-4-ethoxybutanenitrile (4) and 2-(allyl(phenyl)amino)-propanenitrile (5)

Following the *General Procedure* using EtOH as solvent, *N,N*-diallylaniline **1a** (173 mg, 1.00 mmol) reacted with Me_3SiCN and *t*BuOOH for 16 h. The crude product was purified by column chromatography (SiO_2, pentane/CH_2Cl_2 = 3:2) to give **4** (166 mg, 68 %) as a colorless liquid and **5** (58 mg, 31 %) as a colorless liquid.



4



5

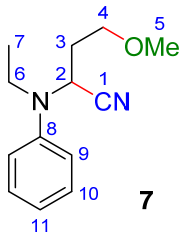
Analytical data for **4**: **^{1}H NMR** (300 MHz, $CDCl_3$): δ = 1.21 (t, *J* = 7.0 Hz, 3 H, 5-CH_3), 2.03–2.23 (m, 2 H, 3-H), 3.45–3.59 (m, 4 H, 4-H and 5-H), 3.85–4.01 (m, 2 H, 6-H), 4.79 (t, *J* = 7.7 Hz, 1 H, 2-H), 5.19–5.34 (m, 2 H, 8-H), 5.83–5.95 (m, 1 H, 7-H), 6.92–7.01 (m, 10-H and 12-H), 7.26–7.32 (m, 2 H, 11-H). **^{13}C NMR** (75.5 MHz, $CDCl_3$): δ = 15.1 (CH_3, 5-CH_3), 32.6 (CH_2, C-3), 49.8 (CH, C-2), 52.6 (CH_2, C-6), 65.3 (CH_2, C-4), 66.5 (CH_2, C-5), 117.4 (CH_2, C-8), 117.9 (CH, C-10), 118.6 (C, C-1), 121.1 (CH, C-12), 129.2 (CH, C-11), 134.5 (CH, C-7), 147.7 (C, C-9). *ν* (neat/ATR probe): 2975, 2930, 2867, 1598, 1502, 1377, 1236, 1172, 1110, 990, 915, 749, 732, 692 cm^{-1}. **HRMS** (EI, 70 eV): *m/z* $[M]^{+\cdot}$ Calcd for $[C_{15}H_{20}N_2O]^{+\cdot}$ 244.1570; Found 244.1569.

Analytical data for **5**: **^{1}H NMR** (300 MHz, $CDCl_3$): δ = 1.58 (d, *J* = 7.2, 3 H, 3-H), 3.85–4.00 (m, 2 H, 4-H), 4.56 (q, *J* = 7.2 Hz, 1 H, 2-H), 5.20–5.35 (m, 2 H, 6-H), 5.85–5.97 (m, 1 H, 5-H), 6.96–7.00 (m, 3 H, 8-H and 10-H), 7.26–7.33 (m, 2 H, 9-H). **^{13}C NMR** (75.5 MHz, $CDCl_3$): δ = 18.6 (CH_3, C-3), 47.4 (CH, C-2), 53.0 (CH_2, C-4), 117.4 (CH_2, C-6), 118.4 (CH, C-8), 119.3 (C, C-1), 121.7 (CH, C-10), 129.4 (CH, C-

9), 134.9 (CH, C-5), 147.7 (C, C-7). **HRMS** (EI, 70 eV): *m*/*z* $[M]^{+\cdot}$ Calcd for $[C_{12}H_{14}N_2]^{+\cdot}$ 186.1152; Found 186.1163.

2-(Ethyl(phenyl)amino)-4-methoxybutanenitrile (7)

Following the *General Procedure*, *N*-allyl-*N*-ethylaniline **6a** (161 mg, 1.00 mmol) reacted with Me_3SiCN and *t*BuOOH for 18 h. The crude product was purified by column chromatography (SiO_2, pentane/CH_2Cl_2 = 2:1) to give **7** (181 mg, 83 %) as a colorless liquid.



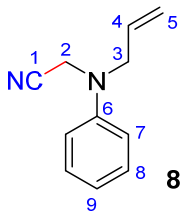
7

^{1}H NMR (300 MHz, $CDCl_3$): δ = 1.19 (t, *J* = 7.1 Hz, 3 H, 7-H), 2.02–2.19 (m, 2 H, 3-H), 3.26–3.43 (m, 2 H, 6-H), 3.36 (s superimposed with resonances of 6-H, 3 H, 5-H), 3.49–3.59 (m, 2 H, 4-H), 4.67 (t, *J* = 7.7 Hz, 1 H, 2-H), 6.94–7.02 (m, 3 H, 9-H and 11-H), 7.26–7.33 (m, 2 H, 10-H). **^{13}C NMR** (75.5 MHz, $CDCl_3$): δ = 13.7 (CH_3, C-7), 32.6 (CH_2, C-3), 43.7 (CH_2, C-6), 50.7 (CH, C-2), 59.0 (CH_3, C-5), 67.7 (CH_2, C-4), 118.7 (CH, C-9), 118.9 (C, C-1), 121.5 (CH, C-11), 129.5 (CH, C-10), 147.2 (C, C-8). ν (neat/ATR probe): 2977, 2929, 2875, 1598, 1502, 1385, 1248, 1190, 1116, 1014, 910, 862, 750, 730, 693, 647 cm^{-1}. **HRMS** (EI, 70 eV): *m*/*z* $[M]^{+\cdot}$ Calcd for $[C_{13}H_{18}N_2O]^{+\cdot}$ 218.1414; Found 218.1411.

2-(Allyl(phenyl)amino)acetonitrile (8)

Following the *General Procedure*, *N*-allyl-*N*-methylaniline **6b** (147 mg, 1.00 mmol) reacted with Me_3SiCN and *t*BuOOH for 18 h. The crude product was purified by column chromatography (SiO_2, pentane/CH_2Cl_2 = 2:1) to give **8** (128 mg, 74 %) as a

colorless liquid. Known compound, the NMR spectroscopic data agree with those given in ref[S4].

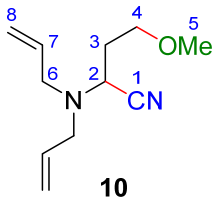


8

^{1}H NMR (400 MHz, $CDCl_3$): δ = 3.97 (d, *J* = 5.6 Hz, 2 H, 3-H), 4.15 (s, 2 H, 2-H), 5.28–5.38 (m, 2 H, 5-H), 5.85–5.95 (m, 1 H, 4-H), 6.89–6.95 (m, 3 H, 7-H and 9-H), 7.30–7.34 (m, 2 H, 8-H). **^{13}C NMR** (100.6 MHz, $CDCl_3$): δ = 39.4 (CH_2, C-3), 54.6 (CH_2, C-2), 115.3 (CH, C-7), 116.1 (C, C-1), 118.6 (CH_2, C-5), 120.3 (CH, C-9), 129.6 (C, C-8), 133.0 (CH, C-4), 147.5 (C, C-6).

2-(Diallylamino)-4-methoxybutanenitrile (10)

Following the *General Procedure*, triallylamine **9** (137 mg, 1.00 mmol) reacted with Me_3SiCN and *t*BuOOH for 40 h. The crude product was purified by column chromatography (SiO_2, pentane/CH_2Cl_2 = 2:3) to give **10** (161 mg, 83 %) as a colorless liquid.



10

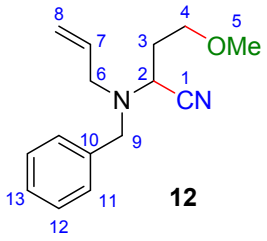
^{1}H NMR (300 MHz, $CDCl_3$): δ = 1.95–2.04 (m, 2 H, 3-H), 2.88–2.96 (m, 2 H, 6-H^a), 3.32–3.40 (m, 2 H, 6-H^b), 3.32 (s superimposed with resonances of 6-H^b, 3 H, 5-H), 3.42–3.55 (m, 2 H, 4-H), 3.98 (t, *J* = 7.8 Hz, 1 H, 2-H), 5.16–5.30 (m, 4 H, 8-H), 5.70–5.83 (m, 2 H, 7-H). **^{13}C NMR** (75.5 MHz, $CDCl_3$): δ = 31.9 (CH_2, C-3), 50.3 (CH,

(S4) Reddy, K. H. V.; Satish, G.; Reddy, V. P.; Kumar, B. S. P. A.; Nageswar, Y. V. D. *RSC Adv*. **2012**, *2*, 11084-11088.

C-2), 54.5 (CH_2, C-6), 58.9 (CH_3, C-5), 68.0 (CH_2, C-4), 117.8 (C, C-1), 118.5 (CH_2, C-8), 134.9 (CH, C-7). ν (neat/ATR probe): 3082, 2981, 2931, 2814, 1644, 1450, 1420, 1189, 1116, 994, 920, 732 cm^{-1}. **HRMS** (EI, 70 eV): *m*/*z* $[M-H]^-$ Calcd for $[C_{11}H_{17}N_2O]^-$ 193.1346; Found 193.1333.

2-(Allyl(benzyl)amino)-4-methoxybutanenitrile (12)

Following the *General Procedure*, *N,N*-diallyl-benzylamine **11** (187 mg, 1.00 mmol) reacted with Me_3SiCN and *t*BuOOH for 40 h. The crude product was purified by column chromatography (SiO_2, pentane/CH_2Cl_2 = 2:3) to give **12** (188 mg, 77 %) as a colorless liquid.



12

^{1}H NMR (400 MHz, $CDCl_3$): δ = 1.91–1.97 (m, 2 H, 3-H), 2.87–2.93 (m, 1 H, 6-H^a), 3.19 (s, 3 H, 5-H), 3.20–3.43 (m, 4 H, 4-H, 6-H^b and 9-H^a), 3.86–3.91 (m, 2 H, 2-H and 9-H^b), 5.12–5.15 (m, 2 H, 8-H), 5.21–5.26 (m, 1 H, 7-H), 7.18–7.29 (m, 5 H, 11-H, 12-H and 13-H). **^{13}C NMR** (100.6 MHz, $CDCl_3$): δ = 31.9 (CH_2, C-3), 50.3 (CH, C-2), 54.6 (CH_2, C-6), 55.5 (CH_2, C-9), 58.8 (CH_3, C-5), 68.0 (CH_2, C-4), 117.7 (C, C-1), 118.8 (CH_2, C-8), 127.6, 128.6, 128.7 (3 × CH, C-11, C-12 and C-13), 134.8 (CH, C-7), 138.1 (C, C-10). **HRMS** (EI, 70 eV): *m*/*z* $[M-H]^-$ Calcd for $[C_{15}H_{19}N_2O]^-$ 243.1503; Found 243.1490.

3. Preparation of tertiary allylamines 1a-d, 6a,b, and 11

According to a procedure reported in ref[S2]: In a 500 mL round-bottom flask equipped with a reflux condenser and a stir bar, aniline (50 mmol), allyl bromide (12.1 g, 100 mmol), and Na_2CO_3 (5.40 g, 51 mmol) were added to aqueous ethanol (200 mL, EtOH/H_2O = 4/1). The reaction mixture was refluxed overnight. The crude product was poured on saturated aq. $NaHCO_3$ (50 mL) and extracted with Et_2O (3 × 50 mL). The combined organic layers were washed with H_2O (2 × 50 mL), dried over $MgSO_4$, and the solvent was evaporated in the vacuum. The crude product was distilled over KOH to provide the corresponding diallylaniline.

***N,N*-Diallylaniline (1a):** 6.2 g (71 %). Known compound, the NMR spectroscopic data agree with those given in lit.[S5]: **^{1}H NMR** (300 MHz, $CDCl_3$): δ = 3.99-4.02 (m, 4 H), 5.22-5.30 (m, 4 H), 5.89-6.01 (m, 2 H), 6.77-6.81 (m, 3 H), 7.28-7.31 (m, 2 H). **^{13}C NMR** (75.5 MHz, $CDCl_3$): δ = 52.9, 112.5, 116.1, 116.4, 129.2, 134.2, 148.8.

***N,N*-Diallyl-4-methylaniline (1b):** 6.7 g (71 %). Known compound, the NMR spectroscopic data agree with those given in lit.[S5]: **^{1}H NMR** (300 MHz, $CDCl_3$): δ = 2.29 (s, 3 H), 3.93-3.95 (m, 4 H), 5.17-5.26 (m, 4 H), 5.84-5.97 (m, 2 H), 6.67-6.70 (m, 2 H), 7.05-7.08 (m, 2 H). **^{13}C NMR** (75.5 MHz, $CDCl_3$): δ = 20.3, 53.1, 112.8, 116.0, 125.6, 129.7, 134.4, 146.8.

***N,N*-Diallyl-4-methoxyaniline (1c):** 3.5 g (34 %). Known compound, the NMR spectroscopic data agree with those given in lit.[S5]: **^{1}H NMR** (300 MHz, $CDCl_3$): δ = 3.77 (s, 3 H), 3.88-3.89 (m, 4 H), 5.16-5.24 (m, 4 H), 5.82-5.93 (m, 2 H), 6.71-6.74

(S5) Chen, W.; Wang, J. *Organometallics* **2013**, *32*, 1958-1963.

(m, 2 H), 6.82-6.85 (m, 2 H). **^{13}C NMR** (75.5 MHz, $CDCl_3$): δ = 53.7, 55.9, 114.6, 114.8, 116.2, 134.7, 143.6, 151.7.

***N,N*-Diallyl-4-bromoaniline (1d):** 3.5 g (28 %). Known compound, the NMR spectroscopic data agree with those given in lit.[S5]: **^{1}H NMR** (300 MHz, $CDCl_3$): δ = 3.89-3.92 (m, 4 H), 5.14-5.20 (m, 4 H), 5.78-5.90 (m, 2 H), 6.56-6.59 (m, 2 H), 7.25-7.28 (m, 2 H). **^{13}C NMR** (75.5 MHz, $CDCl_3$): δ = 53.0, 108.2, 114.1, 116.3, 131.8, 133.5, 147.7.

***N*-Allyl-*N*-ethylaniline (6a)** from *N*-ethylaniline (6.1 g, 50 mmol), allyl bromide (4.8 mL, 40 mmol), and Na_2CO_3 (4.2 g, 40 mmol) as described above to the preparation of **1a**-**d**. The crude product was purified by vacuum distillation from CaH_2: 4.8 g (74 %). Known compound, the NMR spectroscopic data agree with those given in lit.[S6]: **^{1}H NMR** (300 MHz, $CDCl_3$): δ = 1.25 (t, *J* = 7.1 Hz, 3 H), 3.46 (q, *J* = 7.1 Hz, 2 H), 3.96-3.99 (m, 2 H), 5.19-5.29 (m, 2 H), 5.88-6.00 (m, 1 H), 6.74-6.79 (m, 3 H), 7.26-7.31 (m, 2 H). **^{13}C NMR** (75.5 MHz, $CDCl_3$): δ = 12.4, 44.8, 52.8, 112.2, 115.9, 116.0, 129.3, 134.6, 148.3.

***N*-Allyl-*N*-methylaniline (6b)** from *N*-methylaniline (5.4 g, 50 mmol), allyl bromide (4.8 mL, 40 mmol), and Na_2CO_3 (4.2 g, 40 mmol) as described above for the preparation of **1a**-**d**. The crude product was purified by vacuum distillation from CaH_2: 4.0 g (68 %). Known compound, the NMR spectroscopic data agree with those given in lit.[S6]: **^{1}H NMR** (400 MHz, $CDCl_3$): δ = 2.97 (s, 3 H), 3.94-3.96 (m, 2 H),

(S6) Yang, S.-H.; Hung, C.-W. *Synthesis* **1999**, 1747-1752.

5.16-5.23 (m, 2 H), 5.83-5.93 (m, 1 H), 6.73-6.78 (m, 3 H), 7.24-7.27 (m, 2 H). **^{13}C NMR** (100.6 MHz, $CDCl_3$): δ = 38.1, 55.4, 112.6, 116.3, 116.5, 129.2, 134.0, 149.6.

***N,N*-Diallyl-benzylamine (11)** from benzylamine as described above for the preparation of **1a**-**d**. The crude product was purified by vacuum distillation from CaH_2: 5.7 g (61 %). Known compound, the NMR spectroscopic data agree with those given in lit.[S5]: **^{1}H NMR** (300 MHz, $CDCl_3$, Me_4Si): δ = 3.00 (dt, *J* = 6.3 Hz, *J* = 1.4 Hz, 4 H), 3.49 (s, 2 H), 5.03-5.14 (m, 4 H), 5.73-5.87 (m, 2 H), 7.14-7.26 (m, 5 H). **^{13}C NMR** (75.5 MHz, $CDCl_3$): δ = 56.6, 57.7, 117.4, 126.9, 128.3, 129.0, 136.0, 139.6.

4. Theoretical studies

Following earlier theoretical work on the stabilitiy of N- and C-centered radicals[S7–S11] DFT calculations are employed for geometry optimizations and frequency calculations for open- and closed-shell systems at the unrestricted UB3LYP/6-31G(d) level and restricted B3LYP/6-31G(d) level, respectively.[S12,S13]All energies are reported for the structures in gas-phase at 298.15 K where thermal corrections to enthalpies have been calculated at the same level of theory using the rigid rotor/harmonic oscillator model and a scale factor of 0.9806 (in kJ/mol). Improved relative energies were obtained using single point calculations at the ROB2-PLYP/cc-pVTZ level of theory,[S14,S15] and using the G3(MP2)-RAD method developed by Radom et al. for open shell systems.[S16] For selected (smaller) systems more accurate energies were calculated using the G3B3 compound scheme.[S17] All the calculations were performed using the *Gaussian 09* software package.[S18]

(S7) Hioe, J.; Sakic, D.; Vrcek, V.; Zipse, H. *Org. Biomol. Chem.* **2015**, *13*, 157-169.

(S8) Achrainer, F.; Zipse, H. *Molecules* **2014**, *19*, 21489-21505.

(S9) Hioe, J.; Mosch, M.; Smith, D. M.; Zipse, H. *RSC Adv*. **2013**, *3*, 12403-12408.

(S10) Hioe, J.; Zipse, H. *Chem. Eur. J*. **2012**, *18*, 16463-16472.

(S11) Hioe, J.; Zipse, H. *Org. Biomol. Chem*. **2010**, *8*, 3609-3617.

(S12) Becke, A. D. *J. Chem. Phys*. **1993**, *98*, 5648-5652.

(S13) Hariharan, P. C.; Pople, J. A. *Theor. Chem. Acc*. **1973**, *28*, 213-222.

(S14) (a) Grimme, S. *J. Chem. Phys*. **2006**, *124*, 034108. (b) Graham, D. C.; Menon, A. S.; Goerigk, L.; Grimme, S.; Radom, L. *J. Phys. Chem. A* **2009**, *113*, 9861-9873.

(S15) Dunning, T. H., Jr. *J. Chem. Phys*. **1989**, *90*, 1007-1023.

(S16) (a) Henry, D. J.; Parkinson, C. J.; Radom, L. *J. Phys. Chem. A* **2002**, *106*, 7927-7936. (b) Henry, D. J.; Sullivan, M. B.; Radom, L. *J. Chem. Phys*. **2003**, *118*, 4849-4860.

(S17) Baboul, A. G.; Curtiss, L. A.; Redfern, P. C.; Raghavachari, K. *J. Chem. Phys*. **1999**, *110*, 7650-7657.

(S18) *Gaussian 09, Revision C.01*, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.;

The stability of radical **2a-rad** can be quantified through the reaction enthalpy for the hydrogen transfer reaction with methane/methyl radical shown in Figure S1.

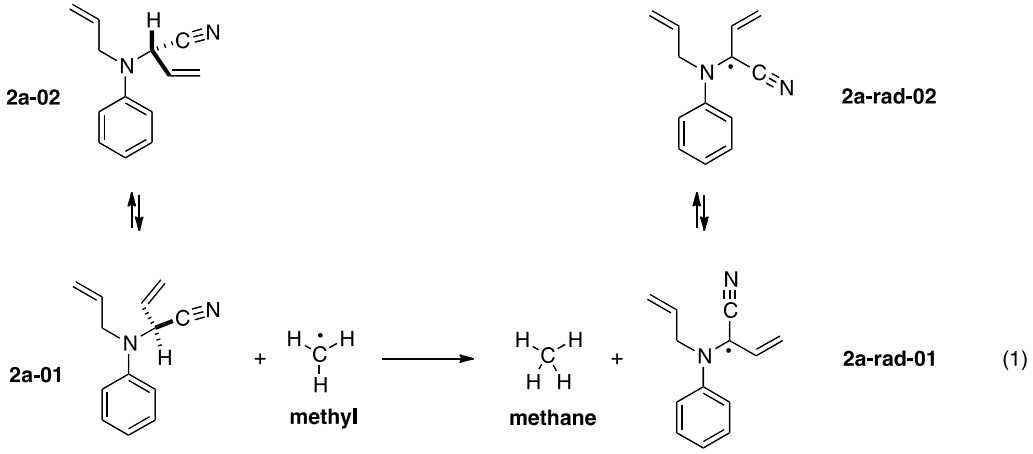


Figure S1. Isodesmic hydrogen transfer reaction between methane and radical **2a-rad**.

The most stable conformation of radical **2a-rad** points the cyano and vinyl substituents away from the phenyl group and contains a fully planar radical center. The alternative conformation **2a-rad-02** with the cyano group pointing towards the phenyl substituent is less stable by 8.6 kJ/mol (UB3LYP/6-31G(d)) or 6.8 kJ/mol (RO-B2PLYP/cc-pVTZ).

Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, J. A., Jr.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, J. M.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, Ö.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J., Gaussian, Inc., Wallingford CT, 2009.

Conformational preferences in the closed-shell parent **2a** are less clear and the conformations **2a-01** and **2a-02** are seperated by only 3.5 kJ/mol (both at B3LYP/6-31G(d) or B2PLYP/cc-pVTZ level). However, in both conformations significant stereoelectronic effects appear to exist between the aniline nitrogen lone pair electrons and the σ*(C-C(N)) bond. Reaction energies for the isodesmic reaction (1) and thus the radical stabilization energy (RSE) of radical **2a-rad** amount to –165.1 kJ/mol (UB3LYP/6-31G(d)), –146.7 kJ/mol (ROB2-PLYP/cc-pVTZ), or **–129.1 kJ/mol** (G3(MP2)-RAD). Important reference systems calculated at this latter level of theory include the allyl radical with RSE = –72.0 kJ/mol and the captodatively stabilized glycyl radical (•CH(NHCOCH$_3$)CONHCH$_3$) with RSE = –74.1 kJ/mol. This comparison illustrates that radical **2a-rad** is exceedingly well stabilized through the donor amino and the acceptor cyano groups as well as the additional vinyl substituent. Together with the BDE(C-H) energy of +439.3 kJ/mol in methane,[S19] the value of RSE(**2a-rad**) = –129.1 kJ/mol translates into a BDE(C-H) in parent **2a** of **+310.2 kJ/mol**. Aminonitrile **2a** is thus a more powerful hydrogen atom donor than thiophenol (BDE(S-H) = +349.4 ± 4.5 kJ/mol) or tri-n-butyltin hydride (HSnBu$_3$, BDE(Sn-H) = +328.9 kJ/mol).[S19,S20]

Radical **3a-rad** is significantly more flexible than **2a**, making the full exploration of conformational space rather time consuming. Starting conformations for geometry optimizations for **3a-rad** were therefore generated in two steps: for the best seven conformations of **2a-rad** all possible conformations for transforming the C-C double bond into the methoxyethyl side chain were generated and optimized; for

(S19) Luo, Y.-R. *Comprehensive Handbook of Chemical Bond Energies*; CRC Press: Boca Raton (FL), 2007.

(S20) Hioe, J.; Zipse, H. In *Encyclopedia of Radicals in Chemistry, Biology and Materials*; Chatgilialoglu, C., Studer, A., Eds.; Wiley: Chichester, 2012, pp 449-476.

all remaining conformations of **2a-rad** the methoxyethyl side chain was generated in an *all-trans* conformation and optimized. In a completely analogous fashion conformational searches were performed for the closed-shell parent **3a**.

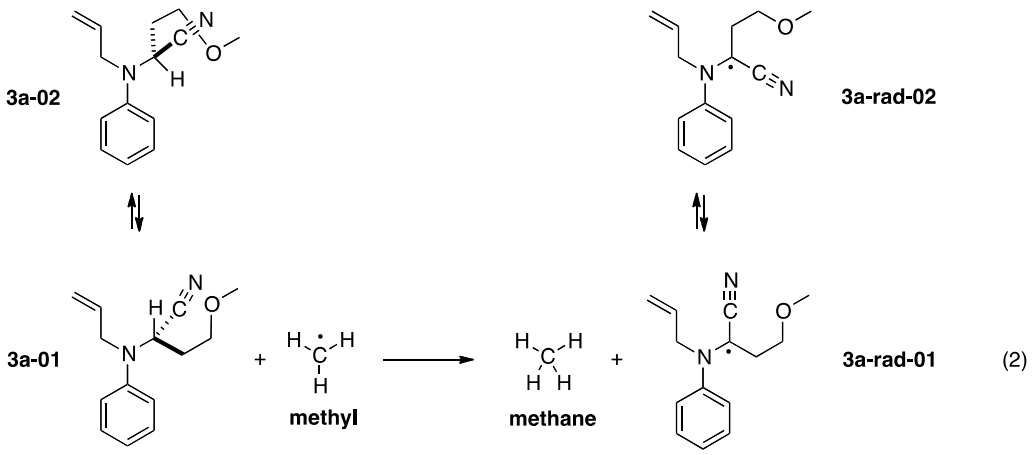


Figure S2. Isodesmic hydrogen transfer reaction between methane and radical **3a-rad**.

This latter system again orients the aniline nitrogen and cyano groups such as to allow for efficient donor/acceptor interactions. Conformations pointing the C-H bond at the chiral center away from the phenyl ring are 3.1 kJ/mol (UB3LYP/6-31G(d)) or 2.3 kJ/mol (RO-B2PLYP/cc-pVTZ) more favorable than those pointing the C-H bond downward. All low-energy conformations orient the methyoxyethyl side chain such as to allow for hydrogen-bonding interactions between the methoxy group oxygen and the chiral center C-H bond. Conformational preferences in radical **3a-rad** are similar to those on **2a-rad** in that upward orientation of the cyano substituent is preferred by 9.2 kJ/mol (UB3LYP/6-31G(d)) or 7.0 kJ/mol (RO-B2PLYP/cc-pVTZ) over the downward orentiation (as drawn in Figure S2). Reaction energies for isodesmic reaction (2) and thus the radical stabilization energy (RSE) of radical **3a-rad** amount

to –123.6 kJ/mol (UB3LYP/6-31G(d)), –109.4 kJ/mol (ROB2-PLYP/cc-pVTZ), or **–91.6 kJ/mol** (G3(MP2)-RAD).

Reaction energies for isodesmic reactions (1) and (2) can be combined to predict the reaction energy for hydrogen transfer reaction (3) between radical **3a-rad** and **2a** (Figure S3). This reaction is always exothermic, the reaction energy amounting to –41.4 kJ/mol (UB3LYP/6-31G(d)), –37.4 kJ/mol (ROB2-PLYP/cc-pVTZ), or **–37.5 kJ/mol** (G3(MP2)-RAD).

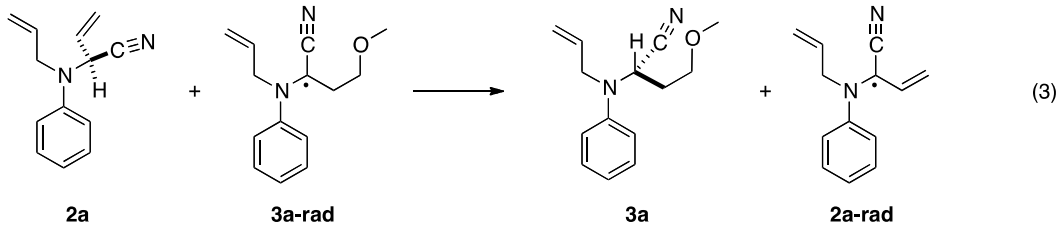


Figure S3. Isodesmic hydrogen transfer reaction between **2a** and radical **3a-rad**.

In order to elucidate further how substituents at the amine nitrogen and the radical center impact radical stability and C-H bond energies, additional smaller systems have been studied (Figure S4). The parent aminomethyl radical is stabilized by 46.7 kJ/mol, a value not influenced by the introduction of additional methyl substituents at the nitrogen atom. Higher stabilities are observed for the secondary 1-dimethylaminoethyl radical (RSE = -54.6 kJ/mol) and the 1-aminoallyl radical **13a-rad** (RSE = -111.3 kJ/mol). Introduction of an N-phenyl substituent in this latter system as in 14a-rad remains practically without consequence (RSE = -110.0 kJ/mol). Compared to this latter system, the donor-acceptor substituted substrate radical **2a-rad** is significantly more stable with RSE = -129.1 kJ/mol, while product radical **3a-rad** is less stable with RSE = -91.6 kJ/mol. All RSE values can, of course, be translated into BDE(C-H) values by addition of the experimentally measured C-H

bond energy in methane (BDE = +439.3 kJ/mol). In the reaction system used here two additional bond energy values merit note. The first is that of solvent methanol with BDE(C-H) = +405.8 kJ/mol (G3B3) or +401.9±0.6 kJ/mol (exp.). The second is that for *t*BuO_2H with BDE(O-H) = +356.9 kJ/mol (G3B3) or +352.8±8.3 kJ/mol (exp.). This latter value appears in Figure S4 as a large grey bar due to the large error margin of ±9 kJ/mol.

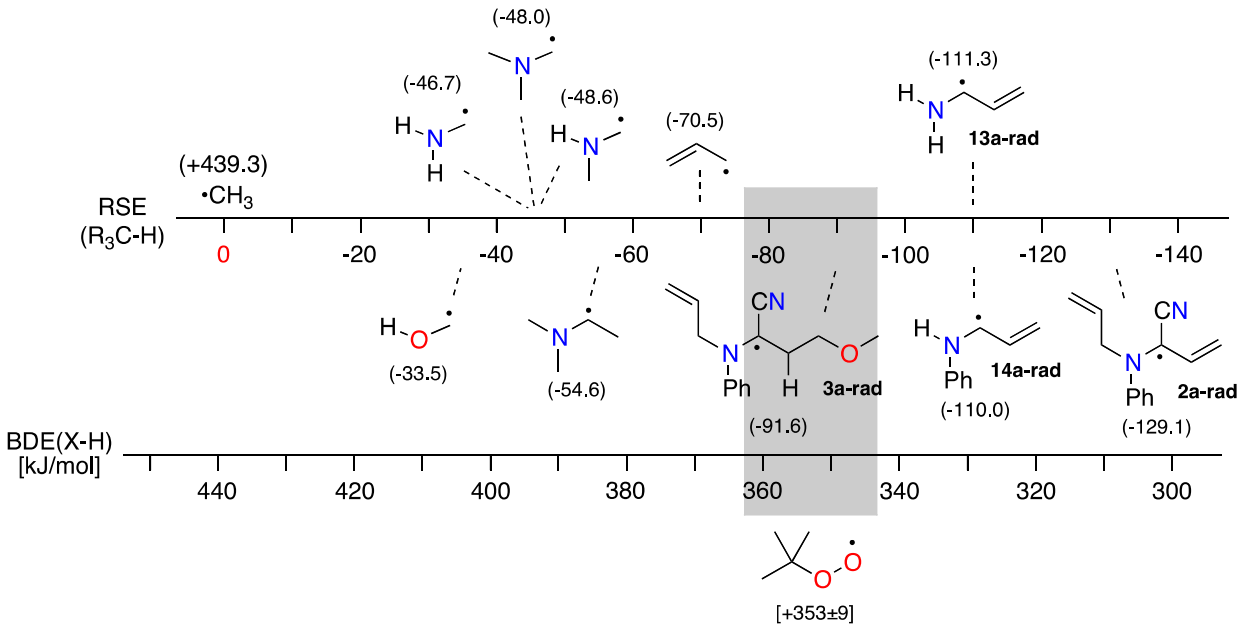
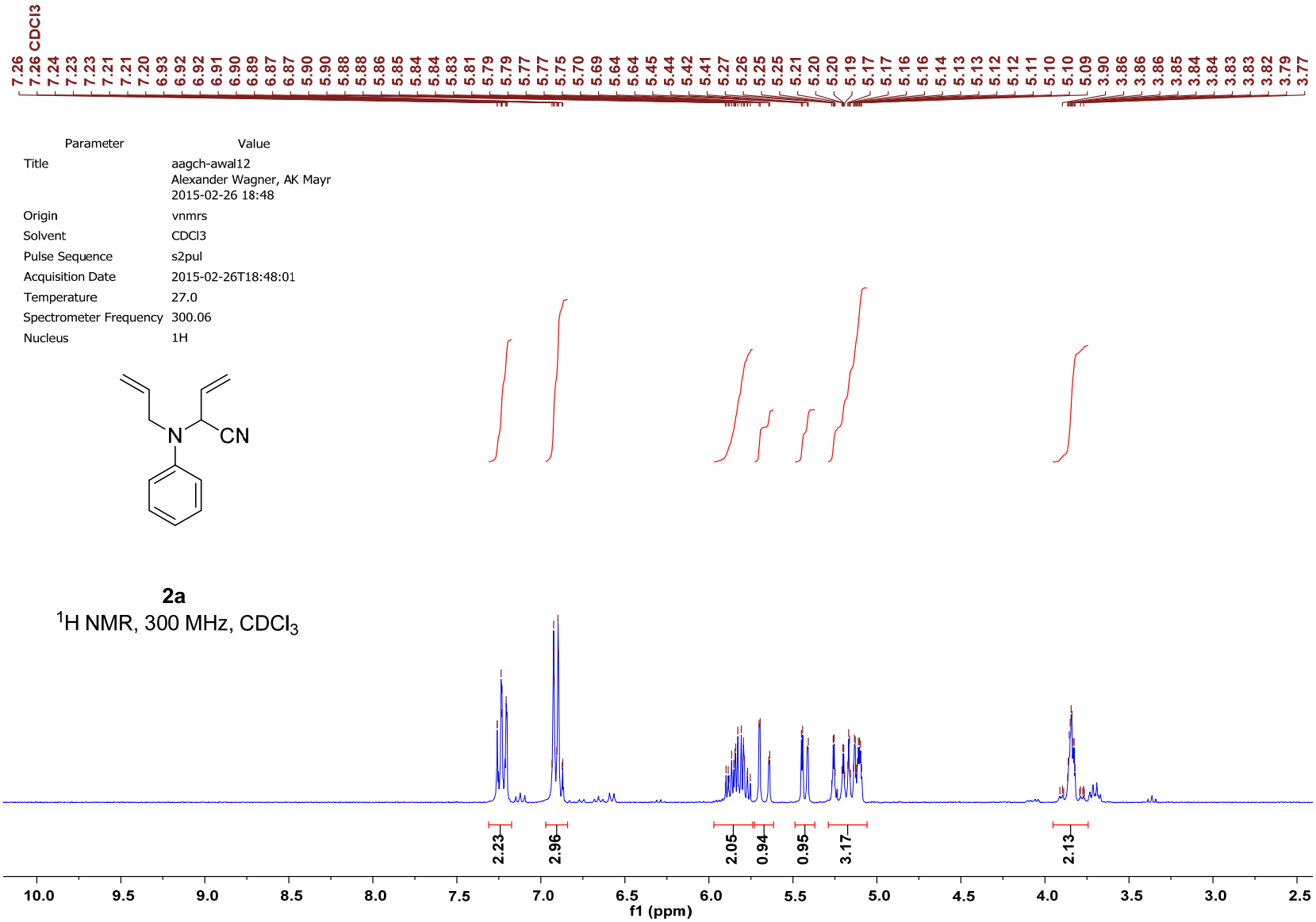


Figure S4. Radical stabilization energies (RSE) relative to methyl radical (•CH_3) and bond dissociation energies (BDE) of amino-substituted radicals and selected additional systems calculated at G3, G3B3, or G3(MP2)-RAD level of theory.

5. NMR and IR spectra of products 2–5, 7, 8, 10, and 12


7.26 CDCl3
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Alexander Wagner, AK Mayr
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CN
2a
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2.96
2.05
0.94
0.95
3.17
2.13
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f1 (ppm)

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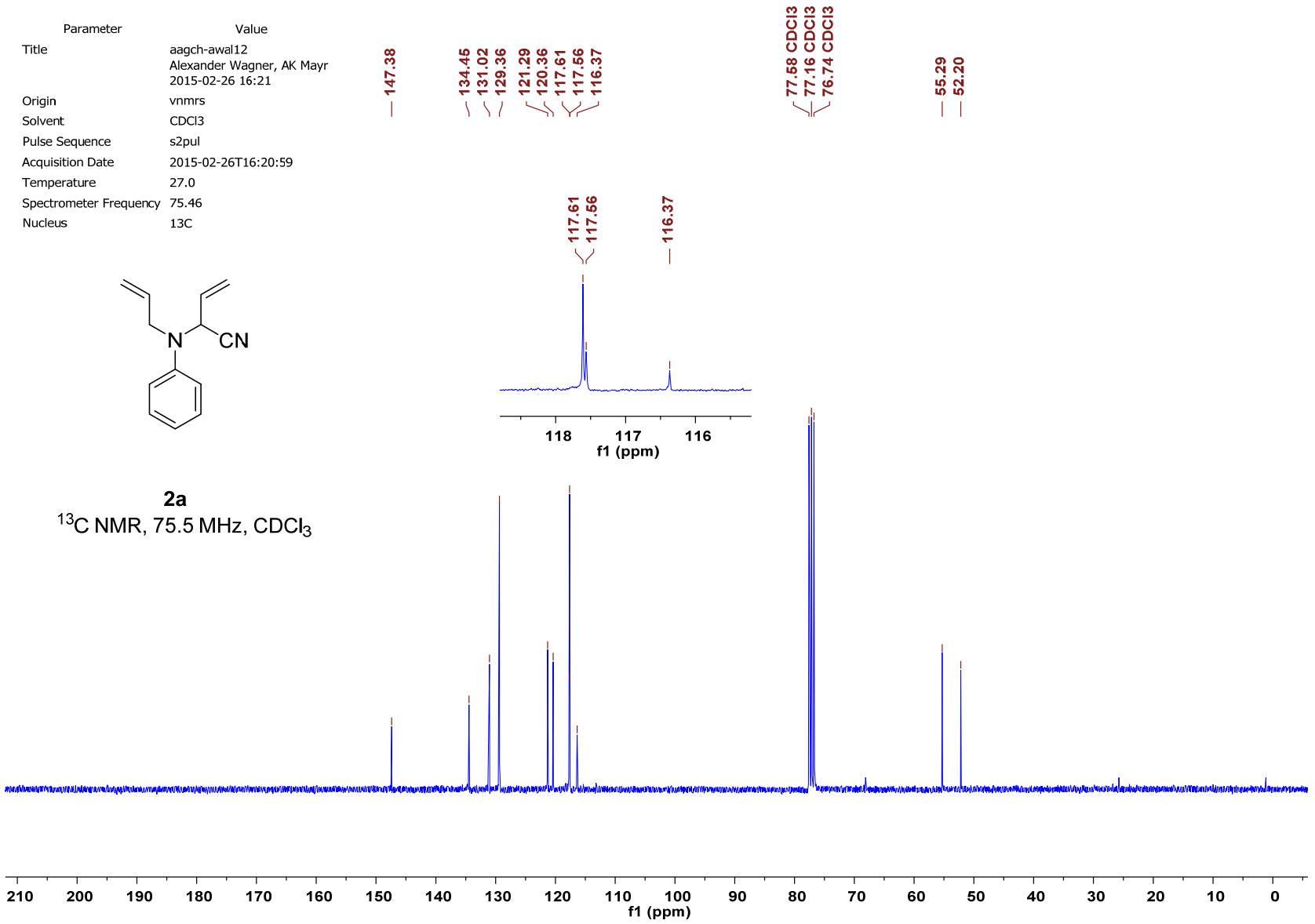

2a

^{13}C NMR, 75.5 MHz, $CDCl_3$

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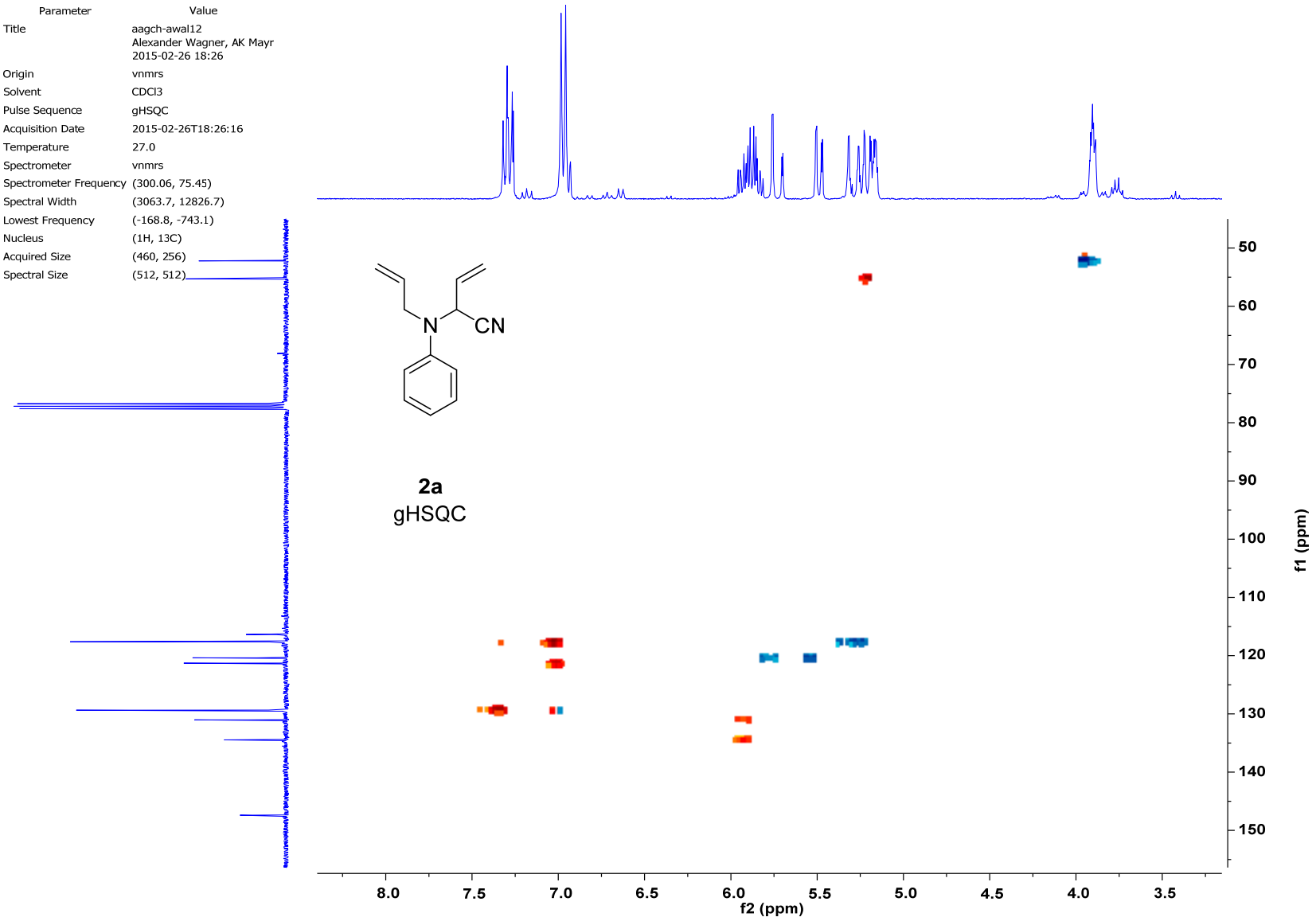
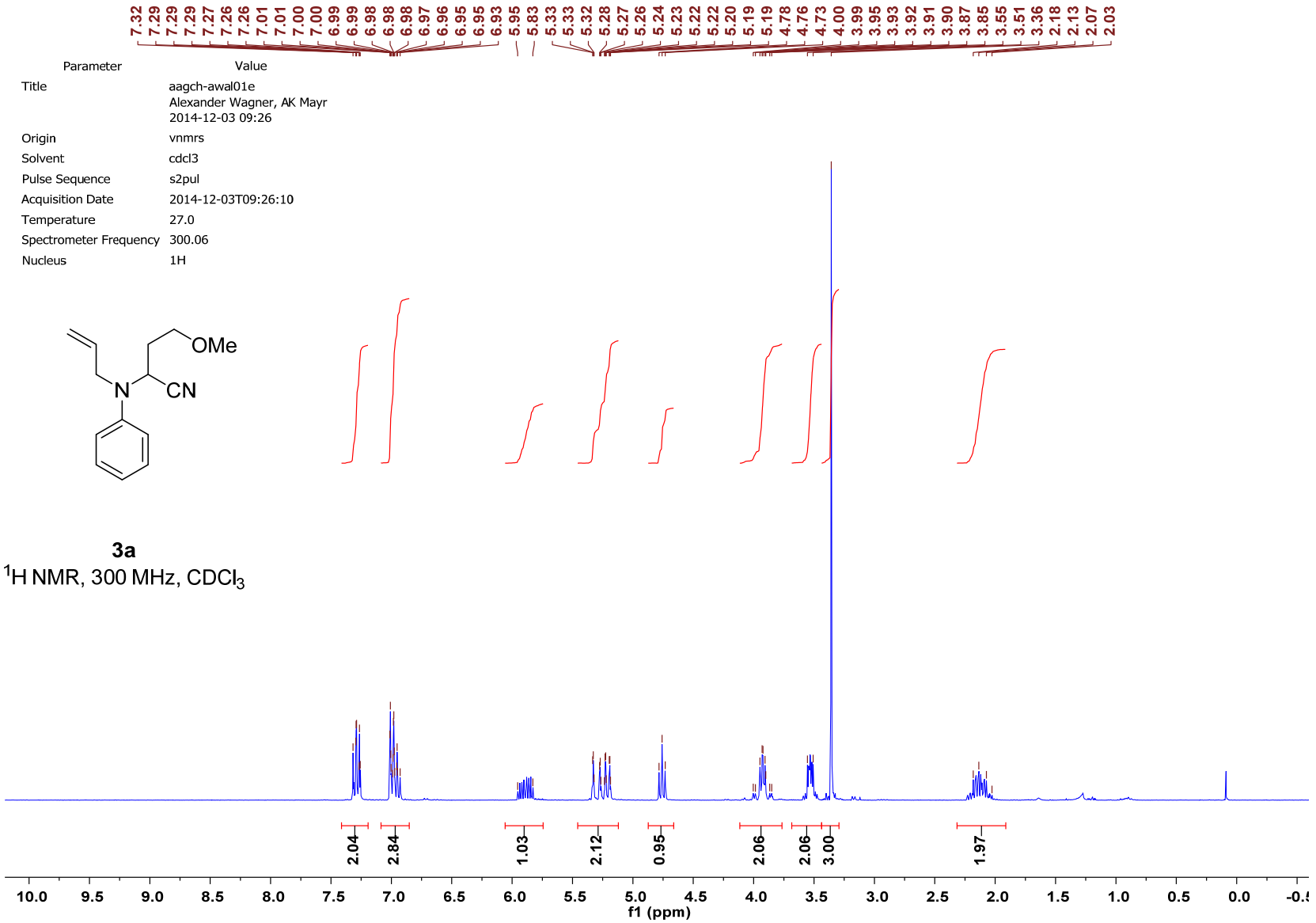
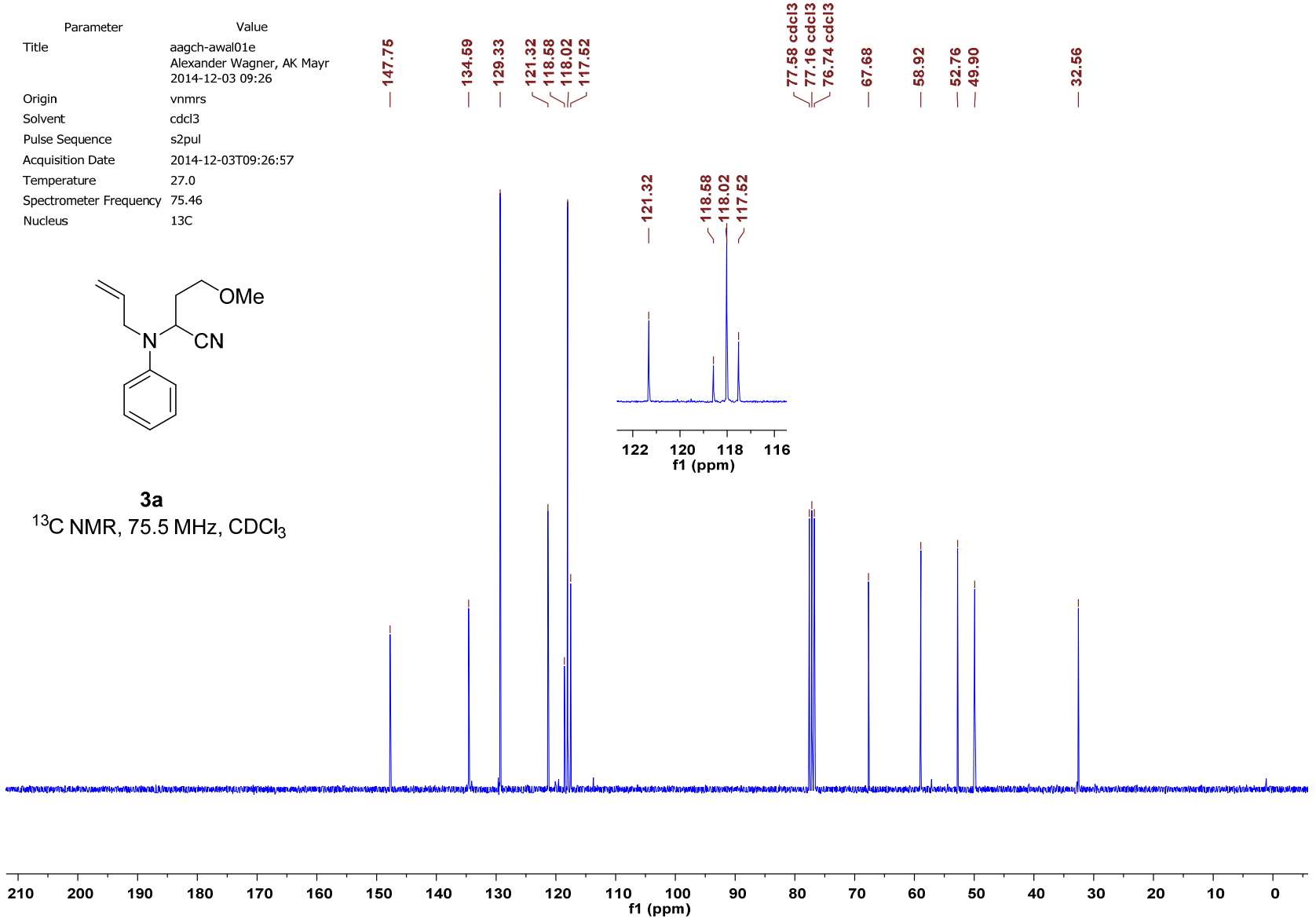




3a

^{1}H NMR, 300 MHz, $CDCl_3$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CN
3a
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f1 (ppm)

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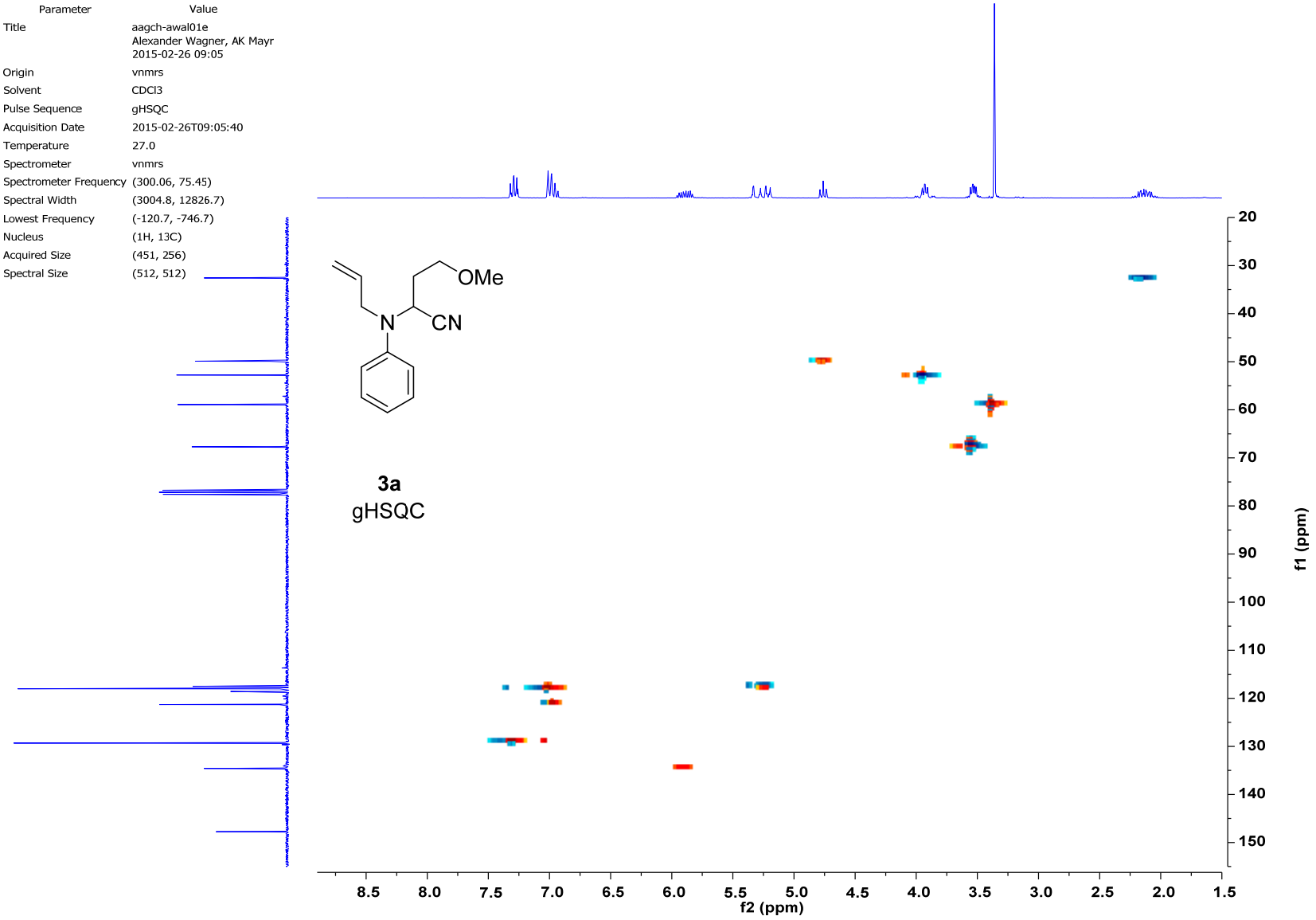

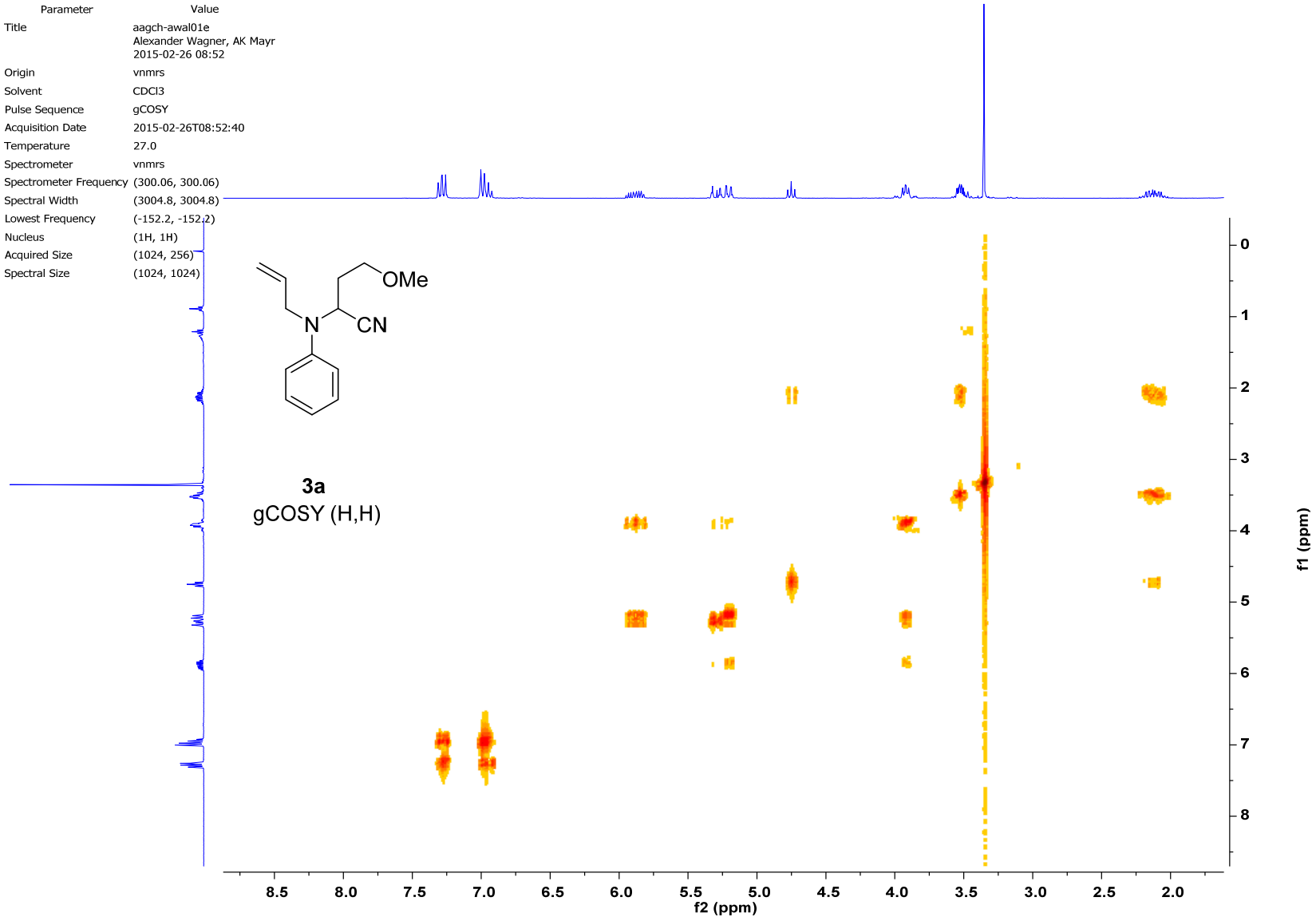
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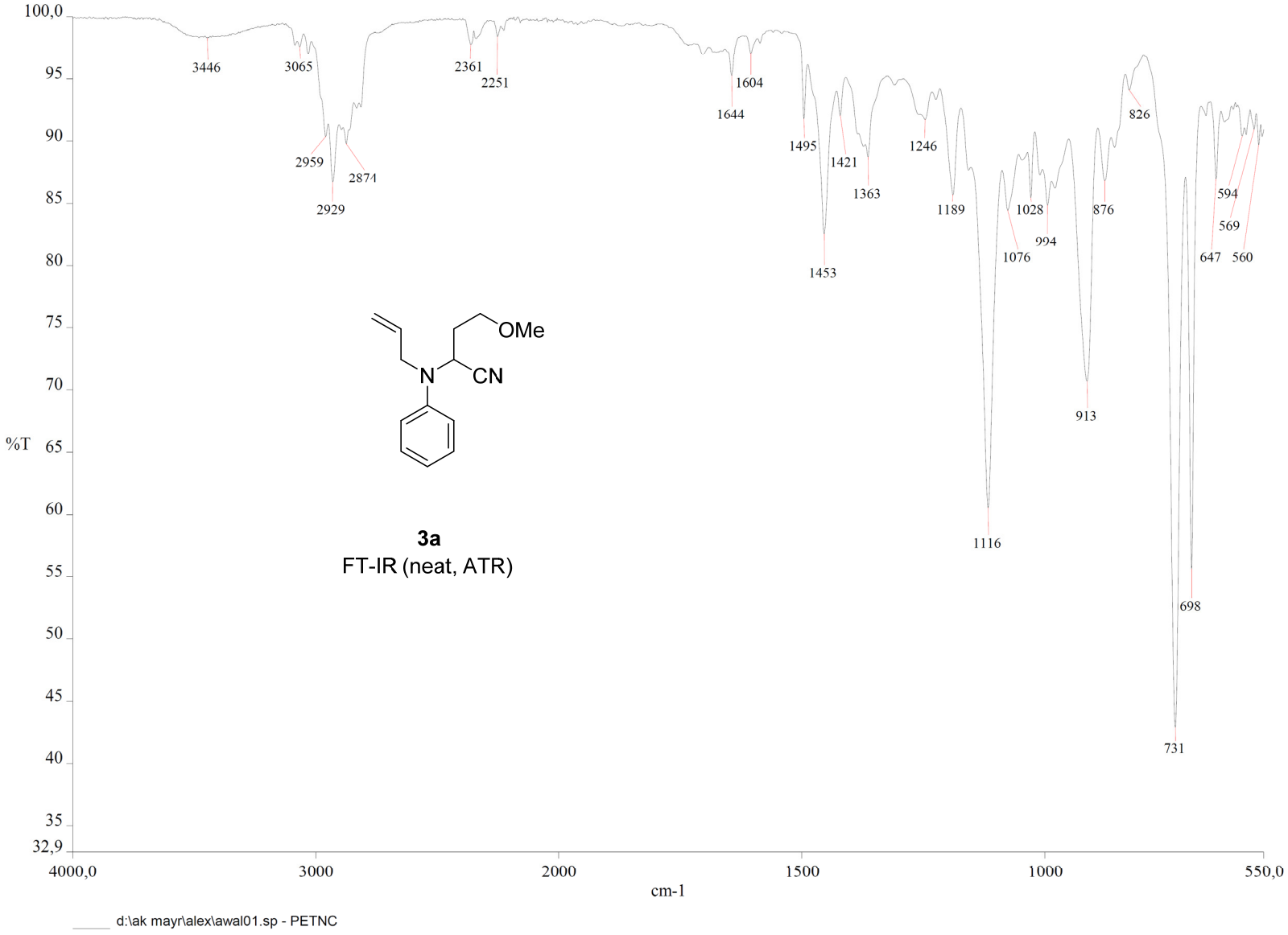
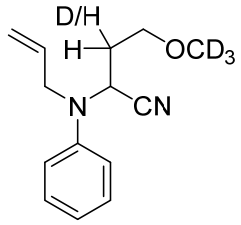
Alexander Wagner, AK Mayr
2015-02-26 08:52
Origin vnmrs
Solvent CDCl3
Pulse Sequence gCOSY
Acquisition Date 2015-02-26T08:52:40
Temperature 27.0
Spectrometer vnmrs
Spectrometer Frequency (300.06, 300.06)
Spectral Width (3004.8, 3004.8)
Lowest Frequency (-152.2, -152.2)
Nucleus (1H, 1H)
Acquired Size (1024, 256)
Spectral Size (1024, 1024)
OMe
N
CN
3a
gCOSY (H,H)
f2 (ppm)
f1 (ppm)



3a

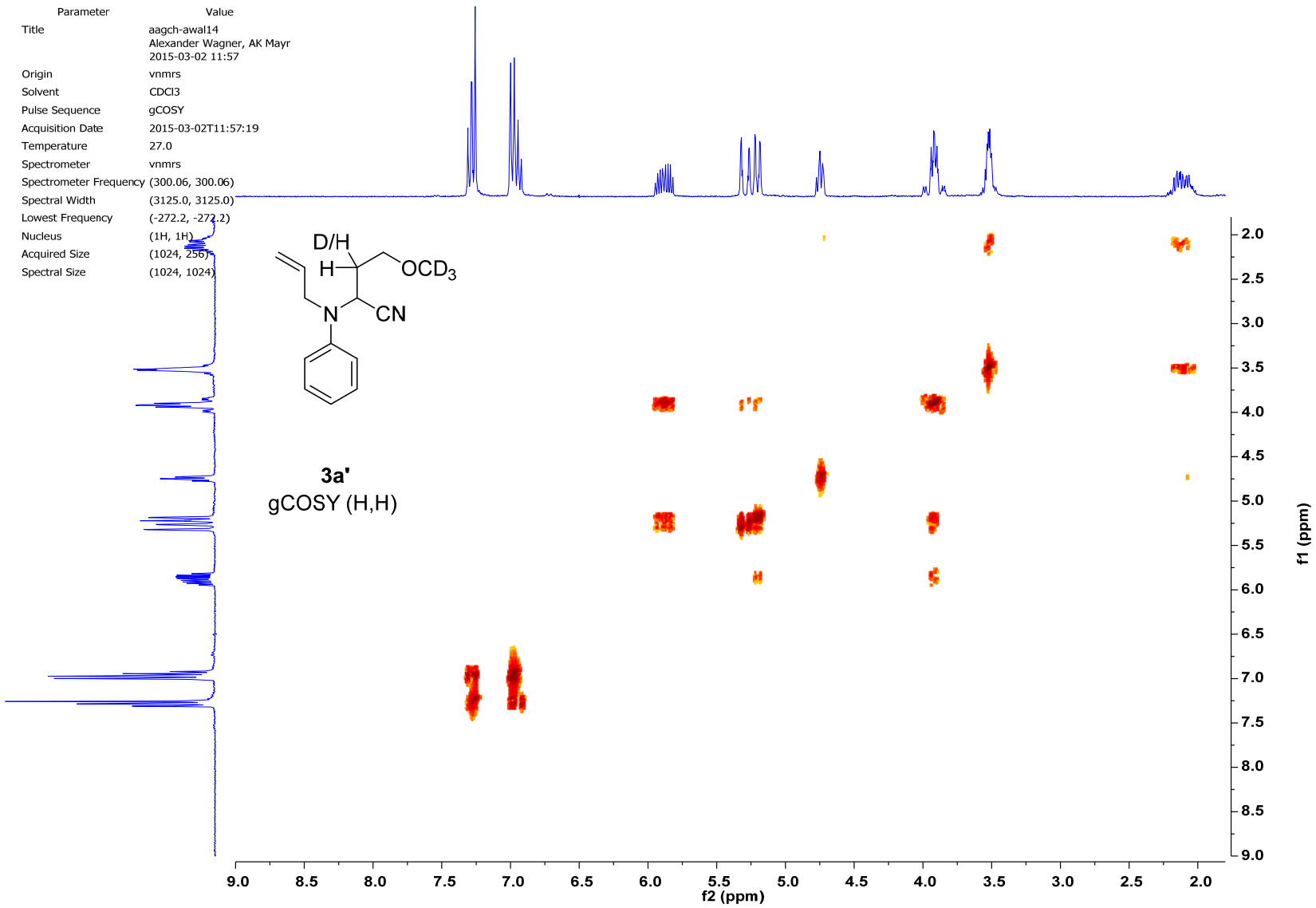
FT-IR (neat, ATR)

Parameter	Value
Title	aagch-awal14 Alexander Wagner, AK Mayr 2015-03-02 09:36
Origin	vnmrs
Solvent	CDCl3
Pulse Sequence	s2pul
Acquisition Date	2015-03-02T09:36:28
Temperature	27.0
Spectrometer Frequency	300.06
Nucleus	1H

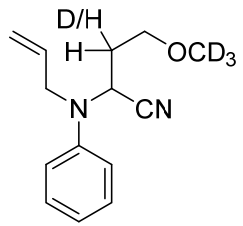


3a'

^{1}H NMR, 300 MHz, $CDCl_3$

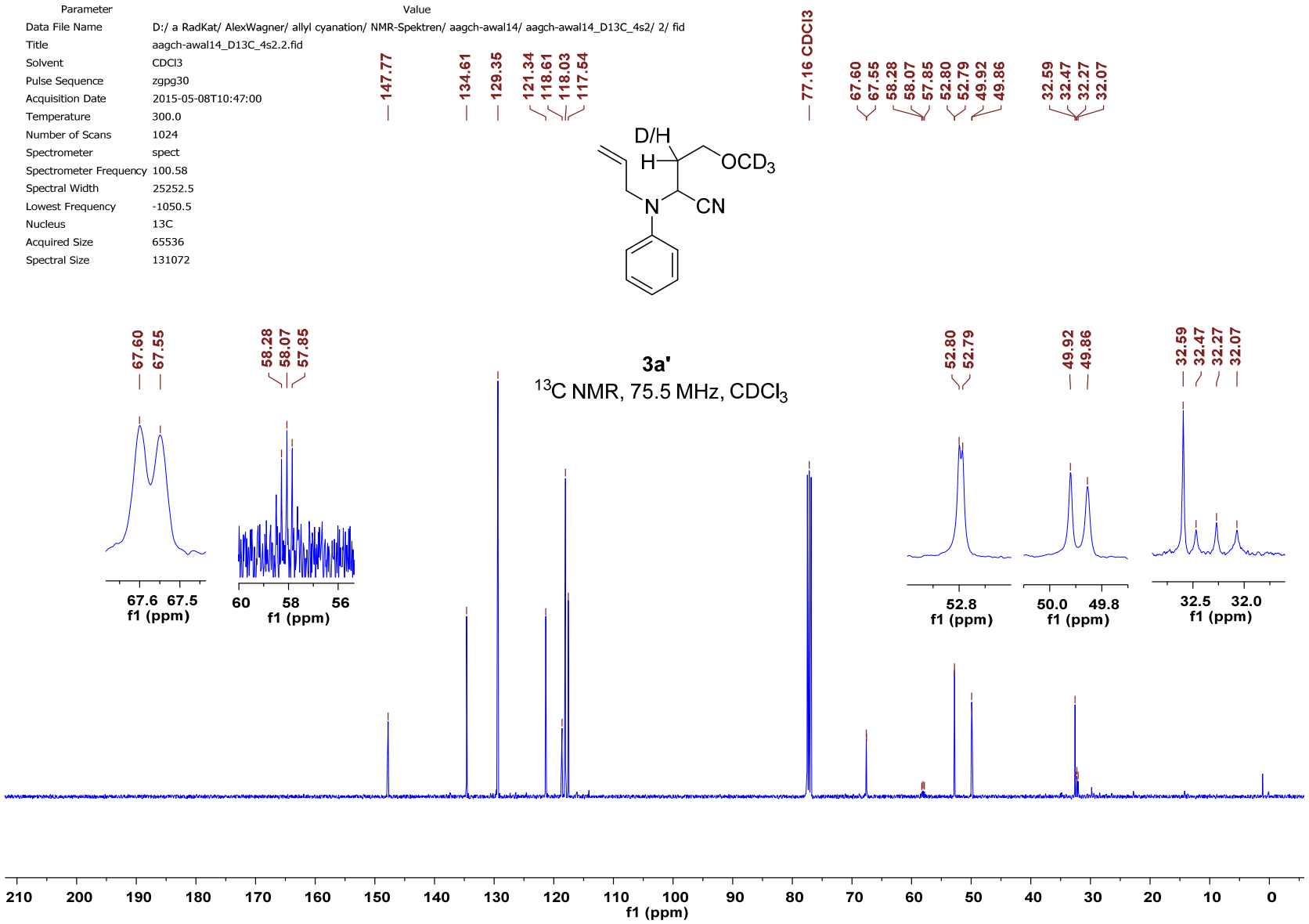

Parameter Value
Title aagch-awal14
Alexander Wagner, AK Mayr
2015-03-02 11:57
Origin vnmrs
Solvent CDCl3
Pulse Sequence gCOSY
Acquisition Date 2015-03-02T11:57:19
Temperature 27.0
Spectrometer vnmrs
Spectrometer Frequency (300.06, 300.06)
Spectral Width (3125.0, 3125.0)
Lowest Frequency (-272.2, -272.2)
Nucleus (1H, 1H)
Acquired Size (1024, 256)
Spectral Size (1024, 1024)
D/H
H
OCD3
N
CN
3a'
gCOSY (H,H)
f2 (ppm)
f1 (ppm)

Parameter	Value
Title	aagch-awal14 Alexander Wagner, AK Mayr 2015-03-20 09:46
Origin	vnmrs
Solvent	cdcl3
Pulse Sequence	s2pul
Acquisition Date	2015-03-20T09:55:43
Temperature	27.0
Spectrometer Frequency	61.39
Nucleus	Unknown

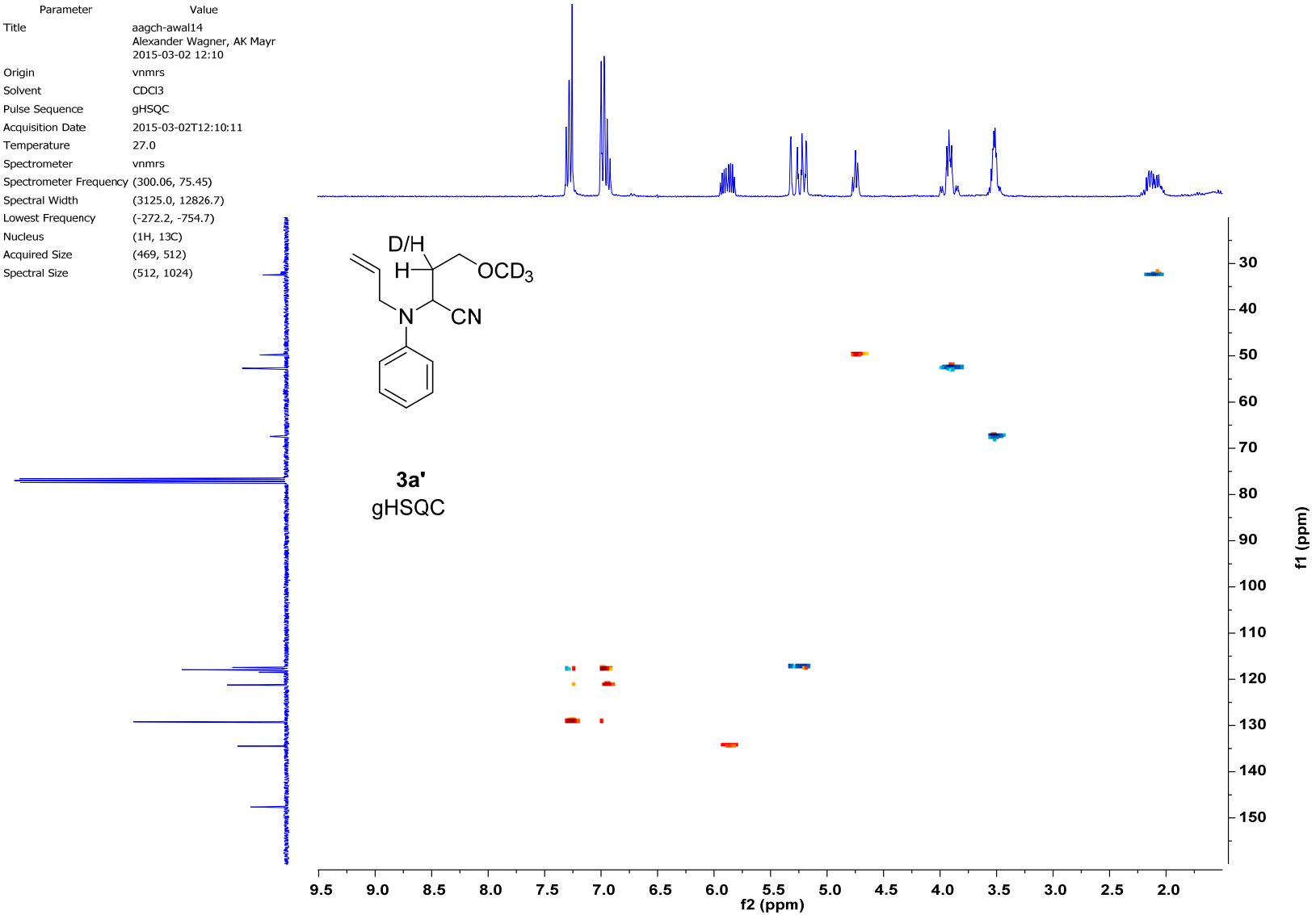


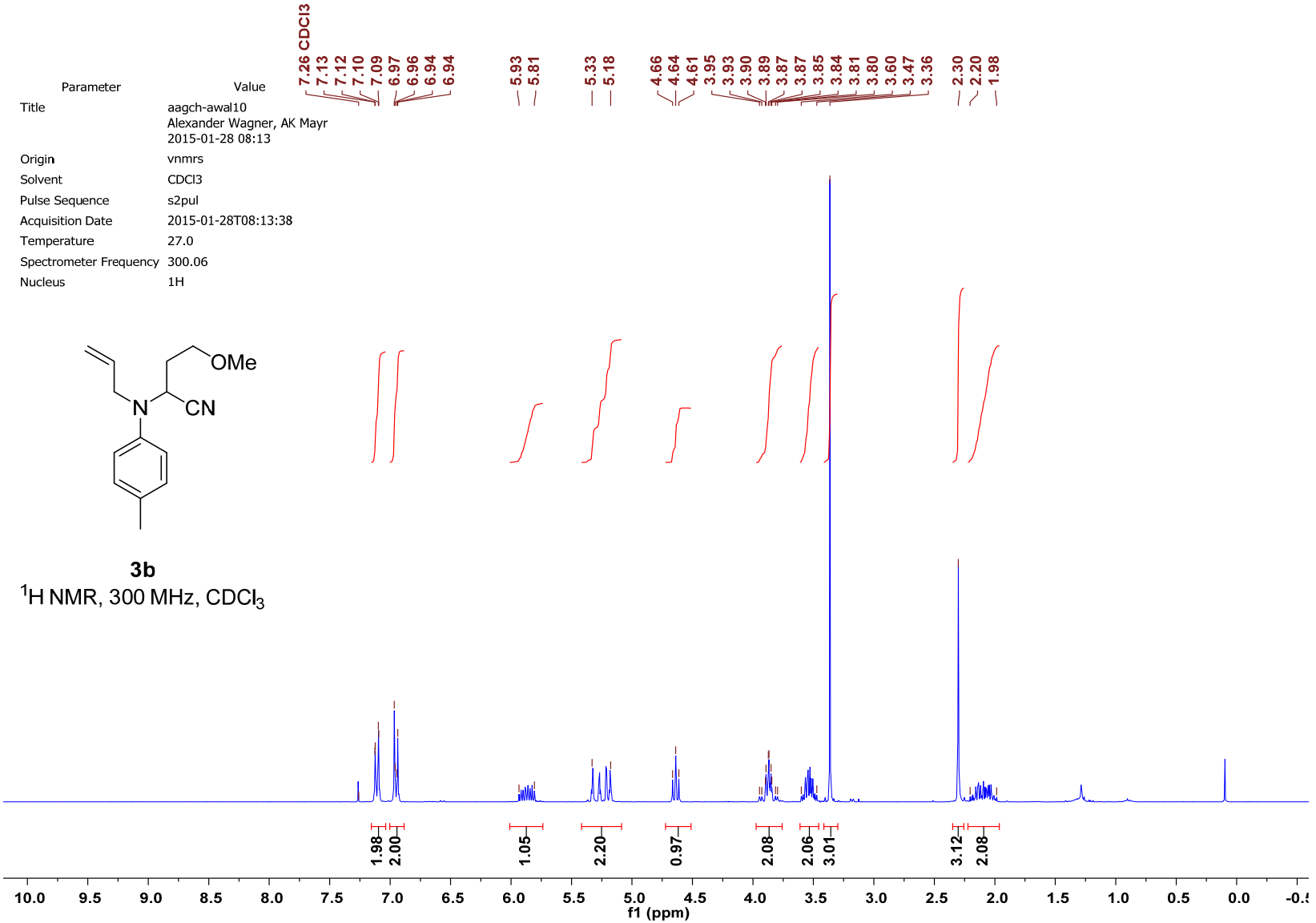
3a'

^{2}H NMR, 61.4 MHz, $CDCl_3$


Parameter Value
Data File Name D:/ a RadKat/ AlexWagner/ allyl cyanation/ NMR-Spektren/ aagch-awal14/ aagch-awal14_D13C_4s2/ 2/ fid
Title aagch-awal14_D13C_4s2.2.fid
Solvent CDCl3
Pulse Sequence zgpg30
Acquisition Date 2015-05-08T10:47:00
Temperature 300.0
Number of Scans 1024
Spectrometer spect
Spectrometer Frequency 100.58
Spectral Width 25252.5
Lowest Frequency -1050.5
Nucleus 13C
Acquired Size 65536
Spectral Size 131072
147.77
134.61
129.35
121.34
118.61
118.03
117.54
77.16 CDCl3
67.60
67.55
58.28
58.07
57.85
52.80
52.79
49.92
49.86
32.59
32.47
32.27
32.07
D/H
H
OCD3
N
CN
3a'
13C NMR, 75.5 MHz, CDCl3
f1 (ppm)

Parameter	Value
Title	aagch-awal14 Alexander Wagner, AK Mayr 2015-03-02 12:10
Origin	vnmrs
Solvent	CDCl3
Pulse Sequence	gHSQC
Acquisition Date	2015-03-02T12:10:11
Temperature	27.0
Spectrometer	vnmrs
Spectrometer Frequency	(300.06, 75.45)
Spectral Width	(3125.0, 12826.7)
Lowest Frequency	(-272.2, -754.7)
Nucleus	(1H, 13C)
Acquired Size	(469, 512)
Spectral Size	(512, 1024)

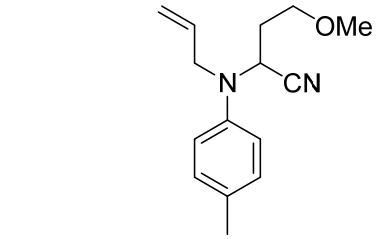




3b

^{1}H NMR, 300 MHz, $CDCl_3$

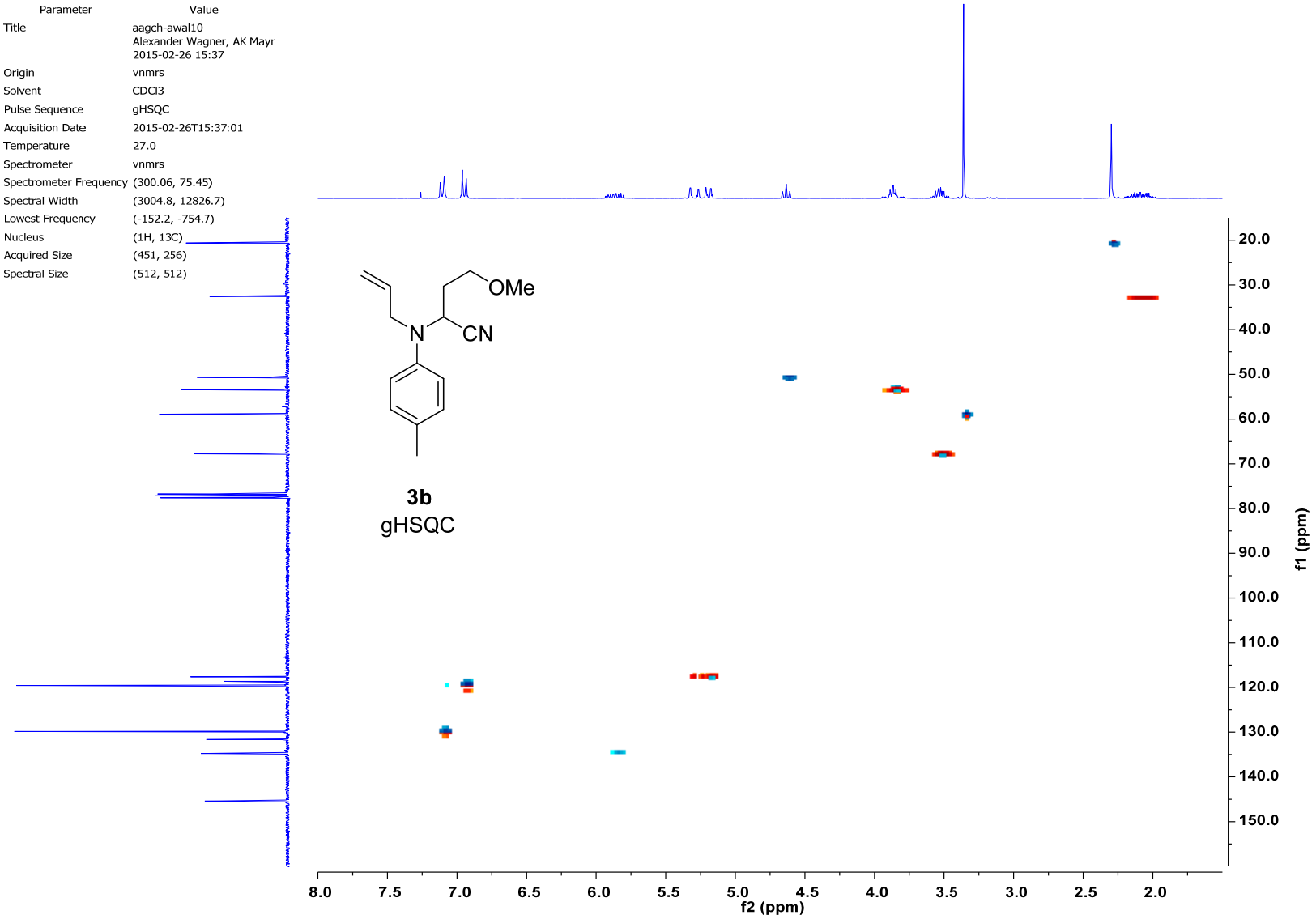
Parameter	Value
Title	aagch-awal10 Alexander Wagner, AK Mayr 2015-01-28 08:14
Origin	vnmrs
Solvent	CDCl3
Pulse Sequence	s2pul
Acquisition Date	2015-01-28T08:14:17
Temperature	27.0
Spectrometer Frequency	75.46
Nucleus	13C

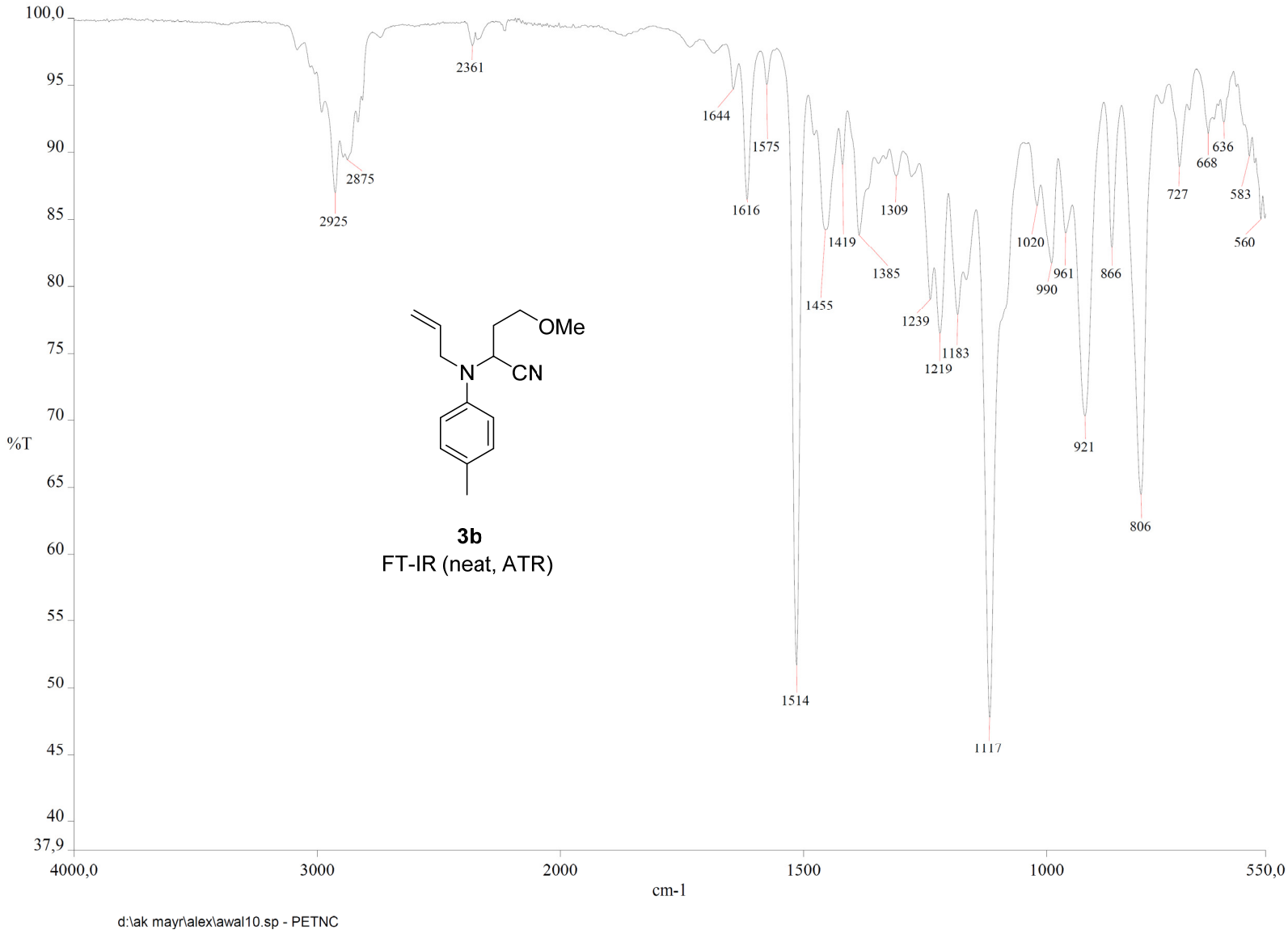


3b

^{13}C NMR, 75.5 MHz, $CDCl_3$

Parameter	Value
Title	aagch-awal10 Alexander Wagner, AK Mayr 2015-02-26 15:37
Origin	vnmrs
Solvent	CDCl3
Pulse Sequence	gHSQC
Acquisition Date	2015-02-26T15:37:01
Temperature	27.0
Spectrometer	vnmrs
Spectrometer Frequency	(300.06, 75.45)
Spectral Width	(3004.8, 12826.7)
Lowest Frequency	(-152.2, -754.7)
Nucleus	(1H, 13C)
Acquired Size	(451, 256)
Spectral Size	(512, 512)

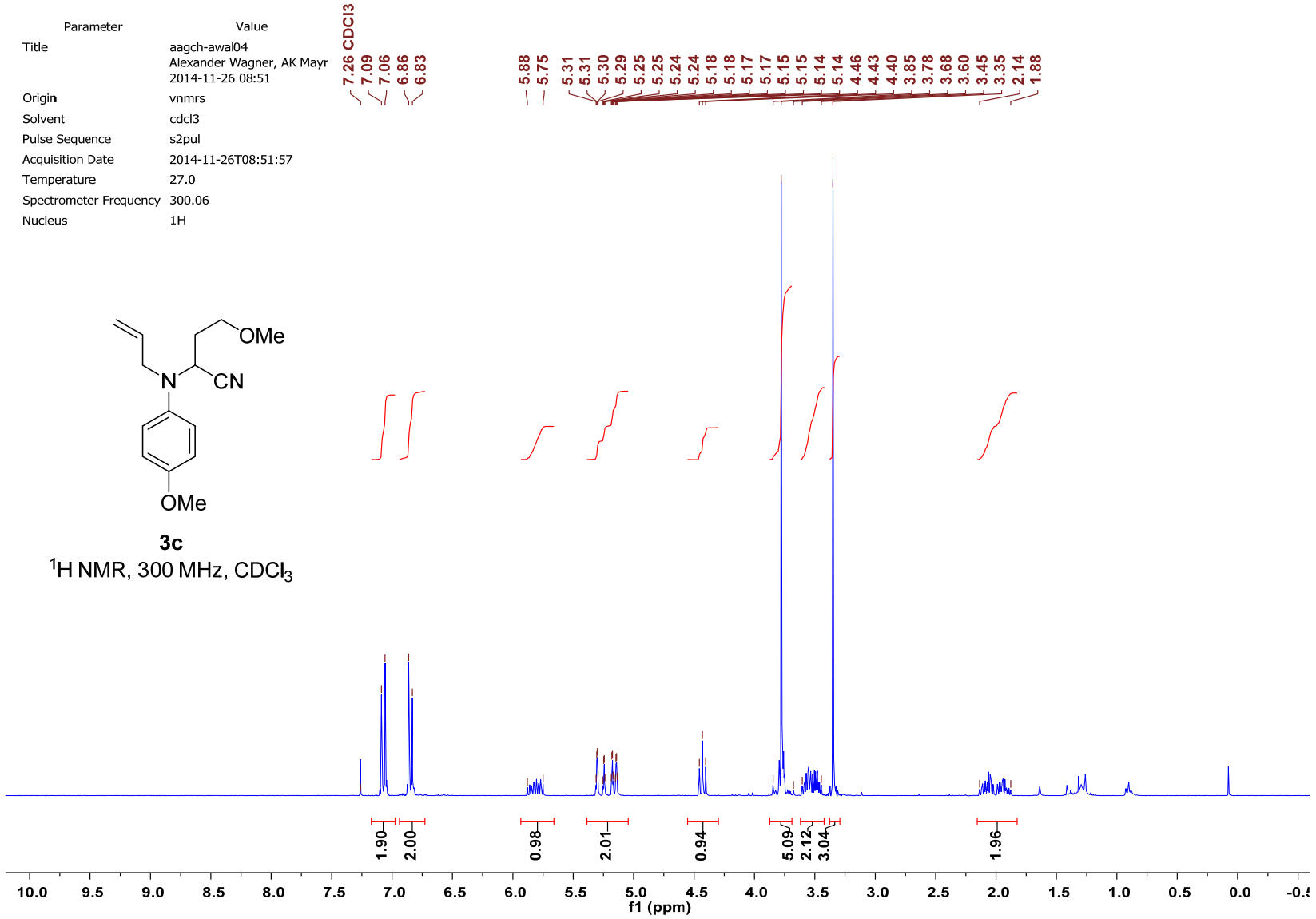




3b

FT-IR (neat, ATR)

Parameter	Value
Title	aagch-awal04 Alexander Wagner, AK Mayr 2014-11-26 08:51
Origin	vnmrs
Solvent	cdcl3
Pulse Sequence	s2pul
Acquisition Date	2014-11-26T08:51:57
Temperature	27.0
Spectrometer Frequency	300.06
Nucleus	1H

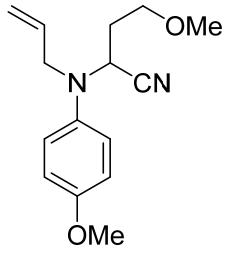


3c

^{1}H NMR, 300 MHz, $CDCl_3$

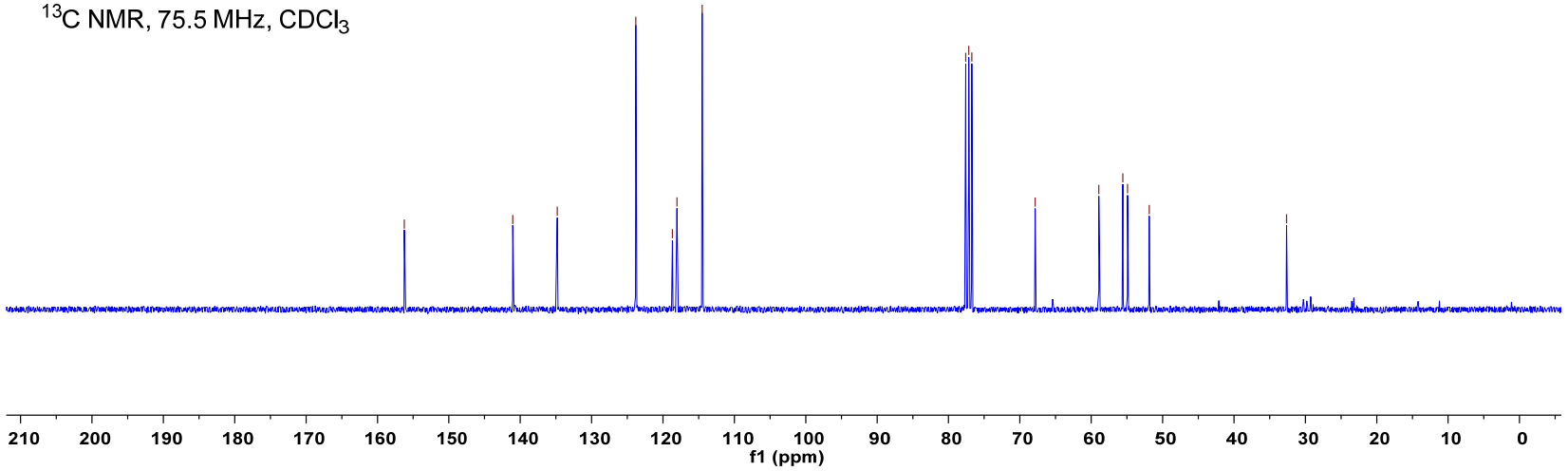
Parameter	Value
Title	aagch-awal04 Alexander Wagner, AK Mayr 2014-11-26 08:52
Origin	vnmrs
Solvent	cdcl3
Pulse Sequence	s2pul
Acquisition Date	2014-11-26T08:52:45
Temperature	27.0
Spectrometer Frequency	75.46
Nucleus	13C

156.25 141.06 134.81 123.82 118.68 118.03 114.51 77.58 cdcl3 77.16 cdcl3 76.74 cdcl3 67.86 58.93 55.58 54.92 51.87 32.63

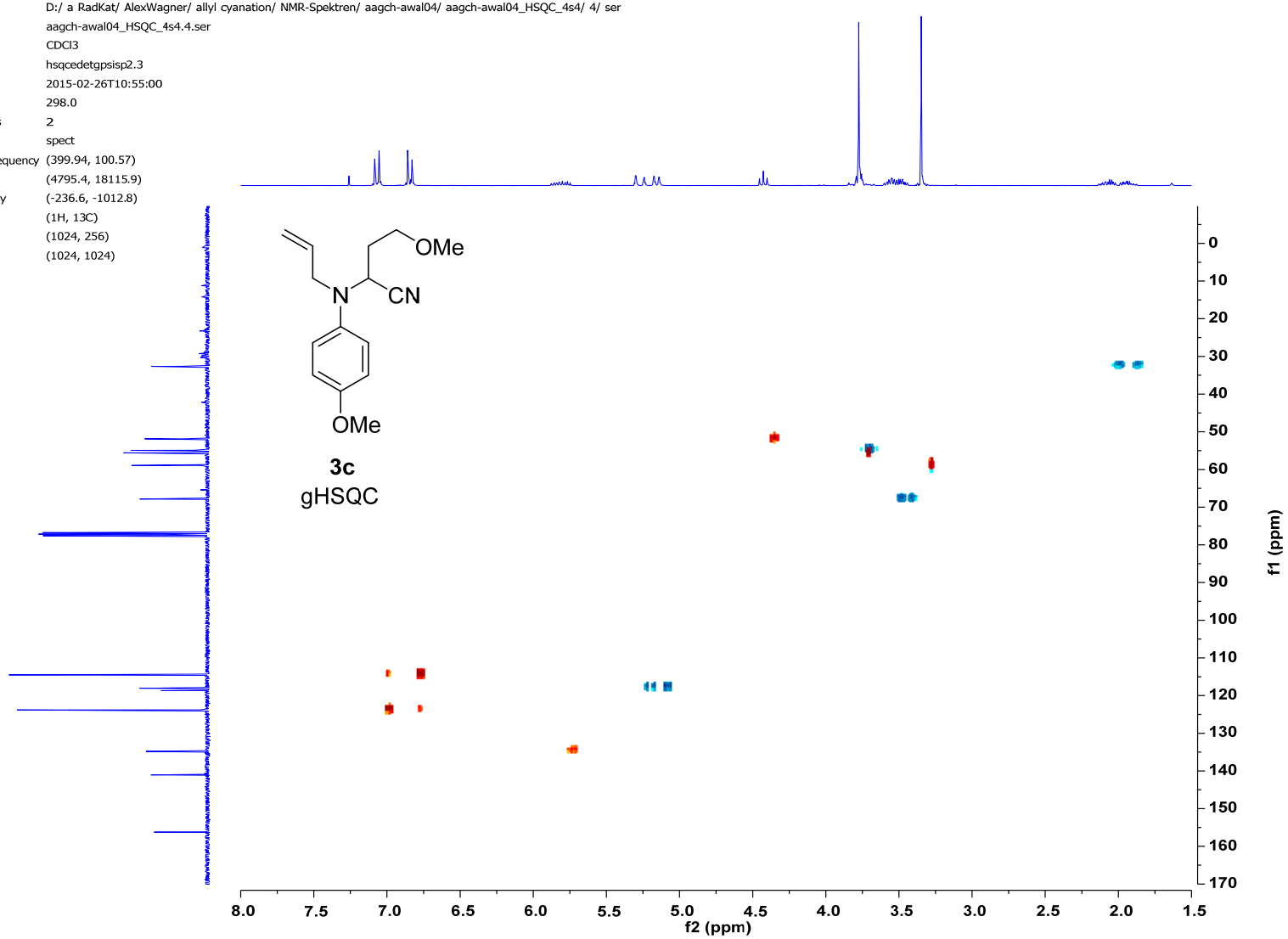


3c

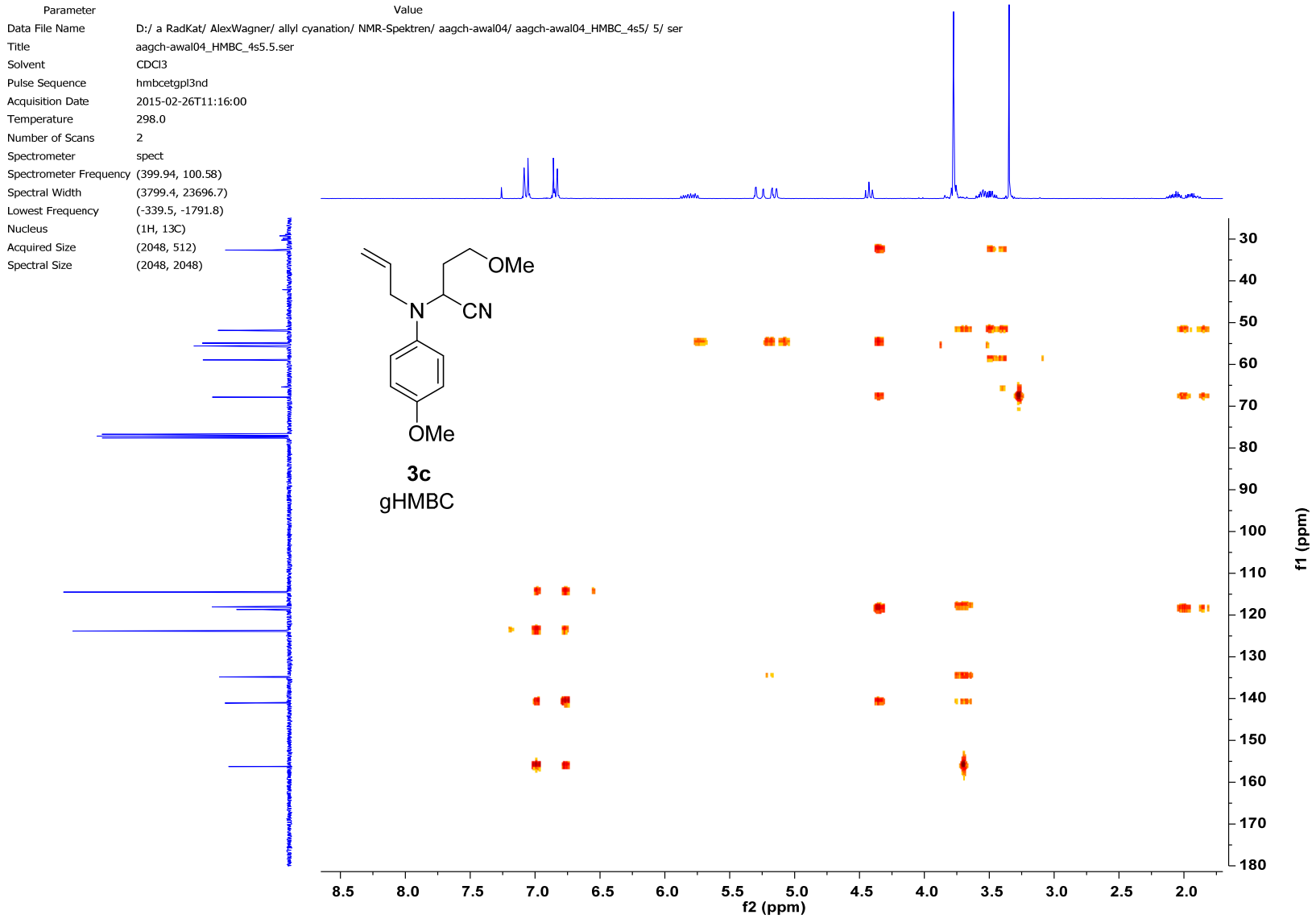
^{13}C NMR, 75.5 MHz, $CDCl_3$

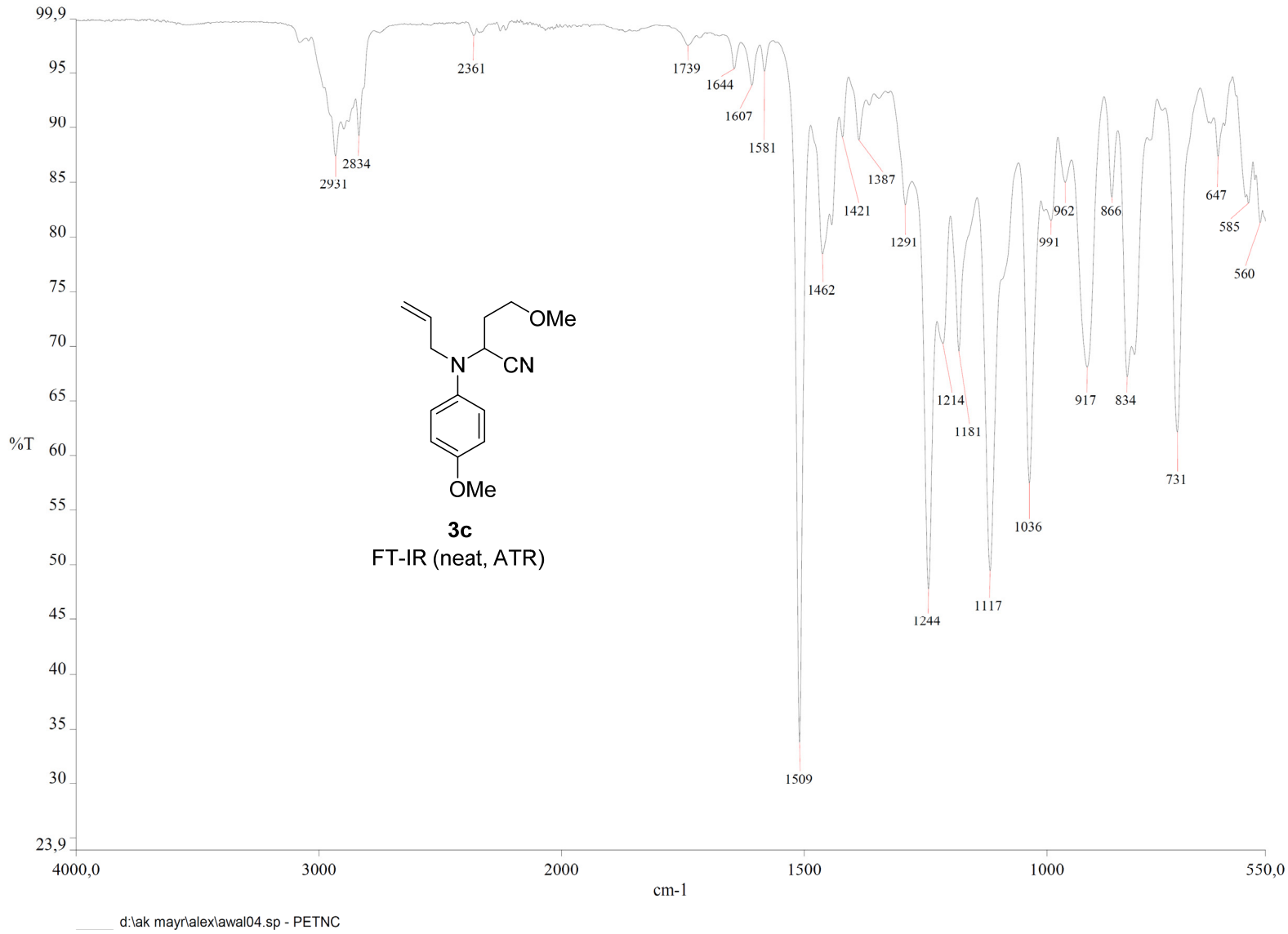


Parameter	Value
Data File Name	D:/ a RadKat/ AlexWagner/ allyl cyanation/ NMR-Spektren/ aagch-awal04/ aagch-awal04_HSQC_4s4/ 4/ ser
Title	aagch-awal04_HSQC_4s4.4.ser
Solvent	CDCl3
Pulse Sequence	hsqcedetgpsisp2.3
Acquisition Date	2015-02-26T10:55:00
Temperature	298.0
Number of Scans	2
Spectrometer	spect
Spectrometer Frequency	(399.94, 100.57)
Spectral Width	(4795.4, 18115.9)
Lowest Frequency	(-236.6, -1012.8)
Nucleus	(1H, 13C)
Acquired Size	(1024, 256)
Spectral Size	(1024, 1024)

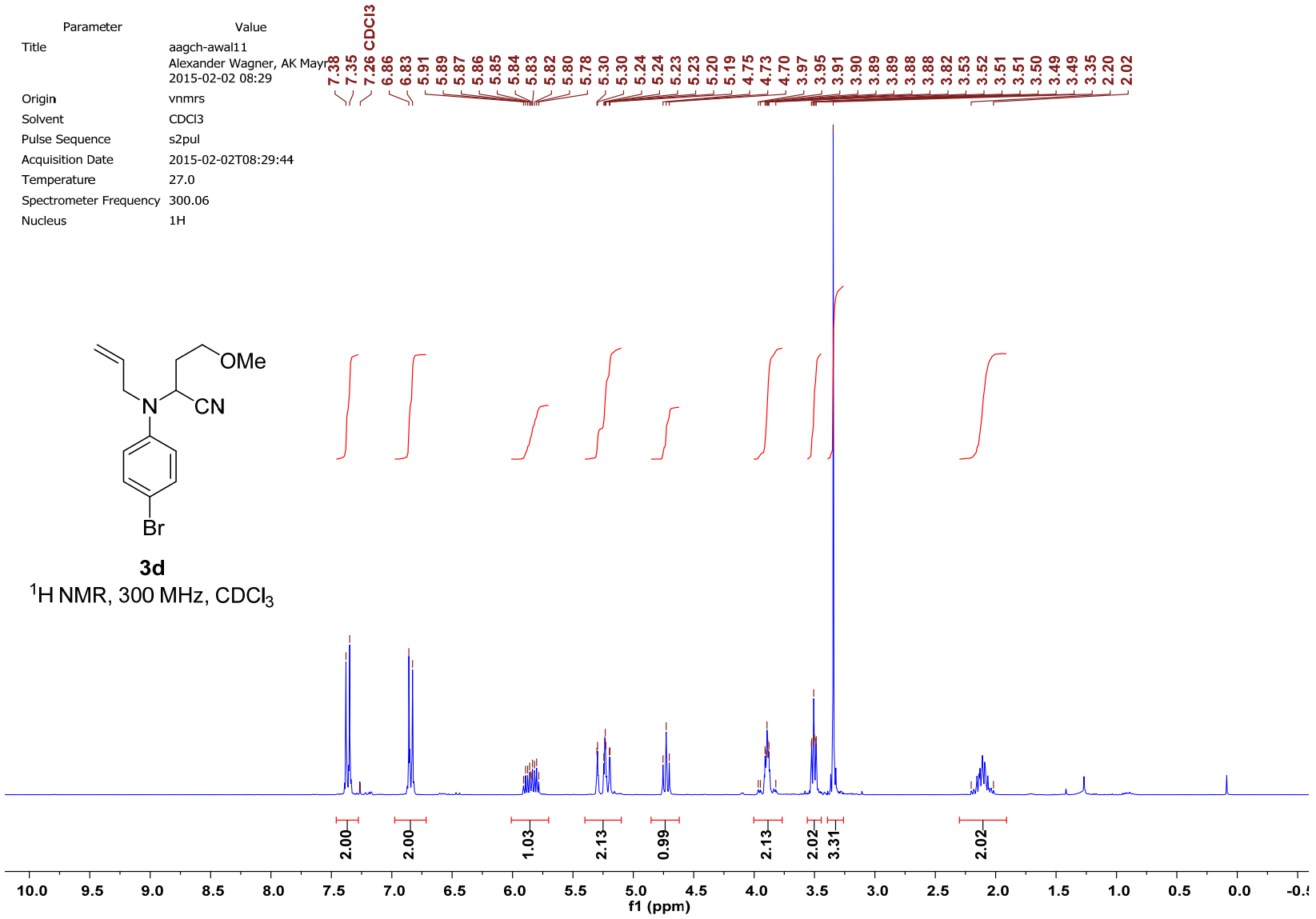


Parameter	Value
Data File Name	D:/ a RadKat/ AlexWagner/ allyl cyanation/ NMR-Spektren/ aagch-awal04/ aagch-awal04_HMBC_4s5/ 5/ ser
Title	aagch-awal04_HMBC_4s5.5.ser
Solvent	CDCl3
Pulse Sequence	hmbcetgpl3nd
Acquisition Date	2015-02-26T11:16:00
Temperature	298.0
Number of Scans	2
Spectrometer	spect
Spectrometer Frequency	(399.94, 100.58)
Spectral Width	(3799.4, 23696.7)
Lowest Frequency	(-339.5, -1791.8)
Nucleus	(1H, 13C)
Acquired Size	(2048, 512)
Spectral Size	(2048, 2048)




99,9
95
90
85
80
75
70
65
60
55
50
45
40
35
30
23,9
%T
4000,0
3000
2000
1500
1000
550,0
cm-1
2931
2834
2361
1739
1644
1607
1581
1509
1462
1421
1387
1291
1244
1214
1181
1117
1036
991
962
917
866
834
731
647
585
560
OMe
N
CN
OMe
3c
FT-IR (neat, ATR)
d:\ak mayr\alex\awal04.sp - PETNC

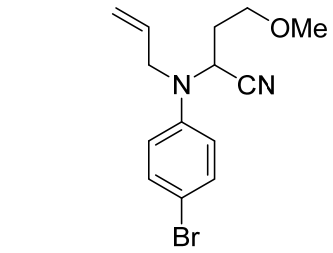
Parameter	Value
Title	aagch-awal11 Alexander Wagner, AK Mayr 2015-02-02 08:29
Origin	vnmrs
Solvent	CDCl3
Pulse Sequence	s2pul
Acquisition Date	2015-02-02T08:29:44
Temperature	27.0
Spectrometer Frequency	300.06
Nucleus	1H



3d

^{1}H NMR, 300 MHz, $CDCl_3$

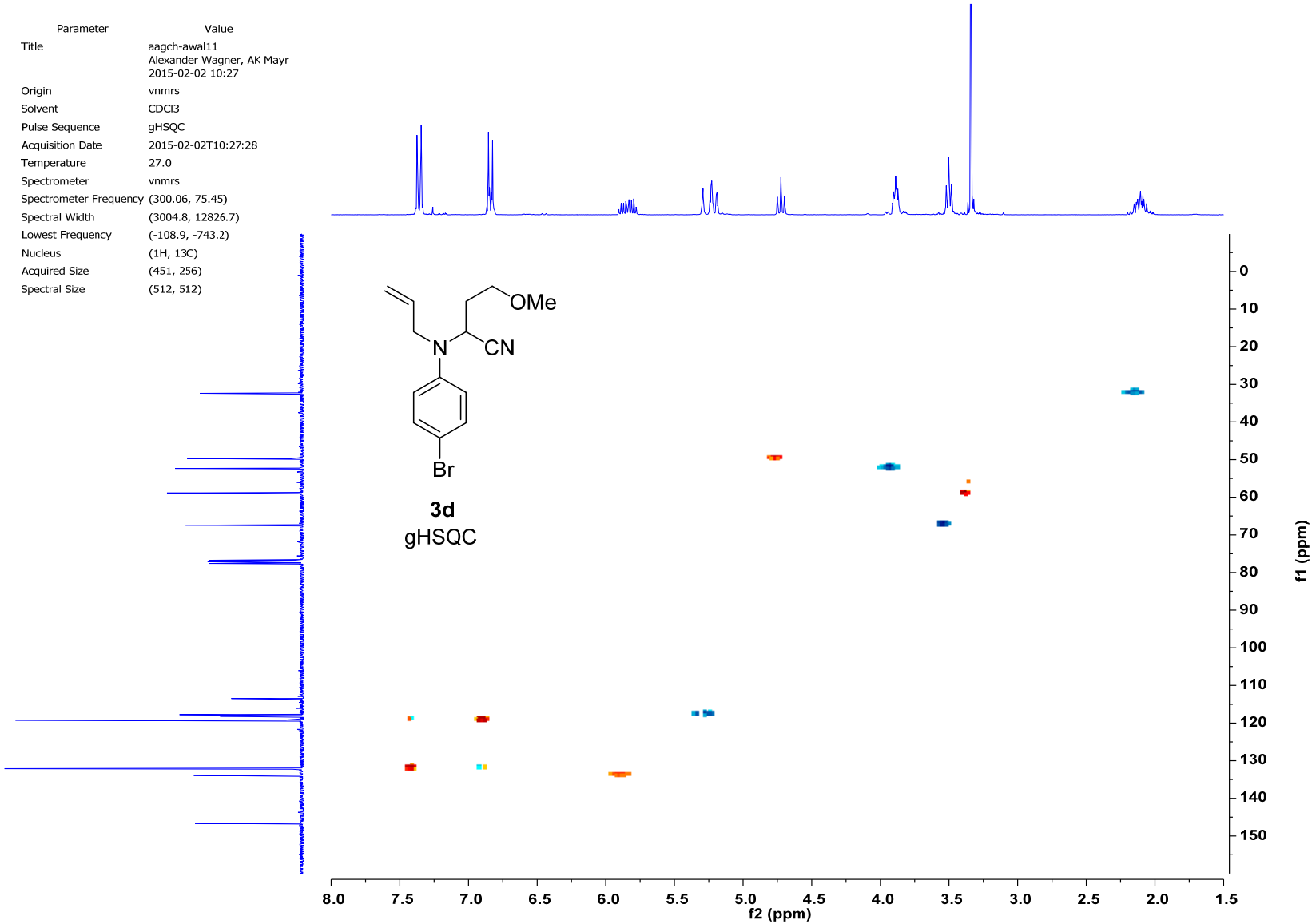
Parameter	Value
Title	aagch-awal11 Alexander Wagner, AK Mayr 2015-02-02 08:30
Origin	vnmrs
Solvent	CDCl3
Pulse Sequence	s2pul
Acquisition Date	2015-02-02T08:30:23
Temperature	27.0
Spectrometer Frequency	75.46
Nucleus	13C

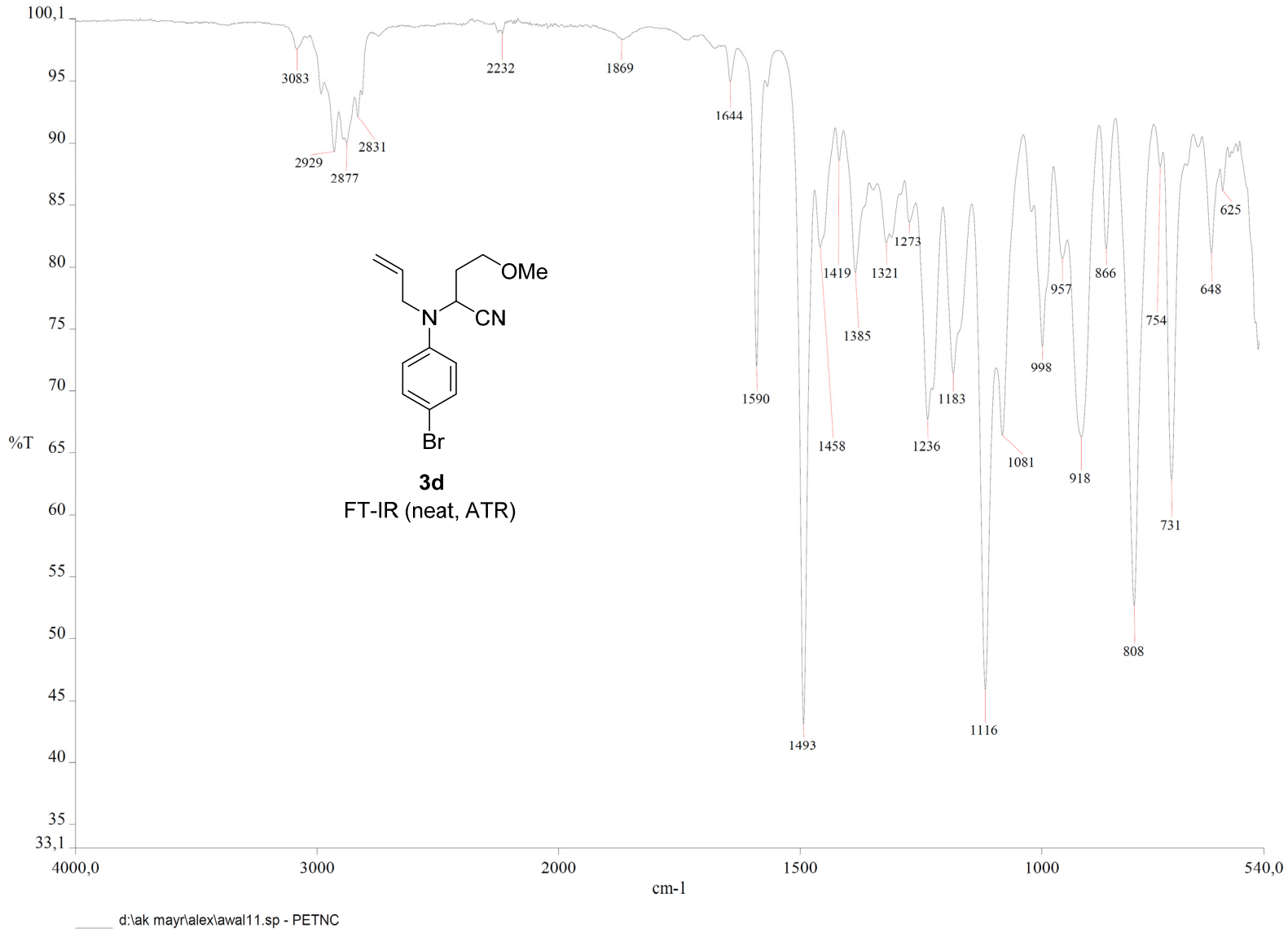


3d

^{13}C NMR, 75.5 MHz, $CDCl_3$

Parameter	Value
Title	aagch-awal11 Alexander Wagner, AK Mayr 2015-02-02 10:27
Origin	vnmrs
Solvent	CDCl3
Pulse Sequence	gHSQC
Acquisition Date	2015-02-02T10:27:28
Temperature	27.0
Spectrometer	vnmrs
Spectrometer Frequency	(300.06, 75.45)
Spectral Width	(3004.8, 12826.7)
Lowest Frequency	(-108.9, -743.2)
Nucleus	(1H, 13C)
Acquired Size	(451, 256)
Spectral Size	(512, 512)




100,1
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60
55
50
45
40
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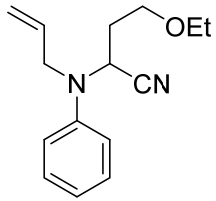
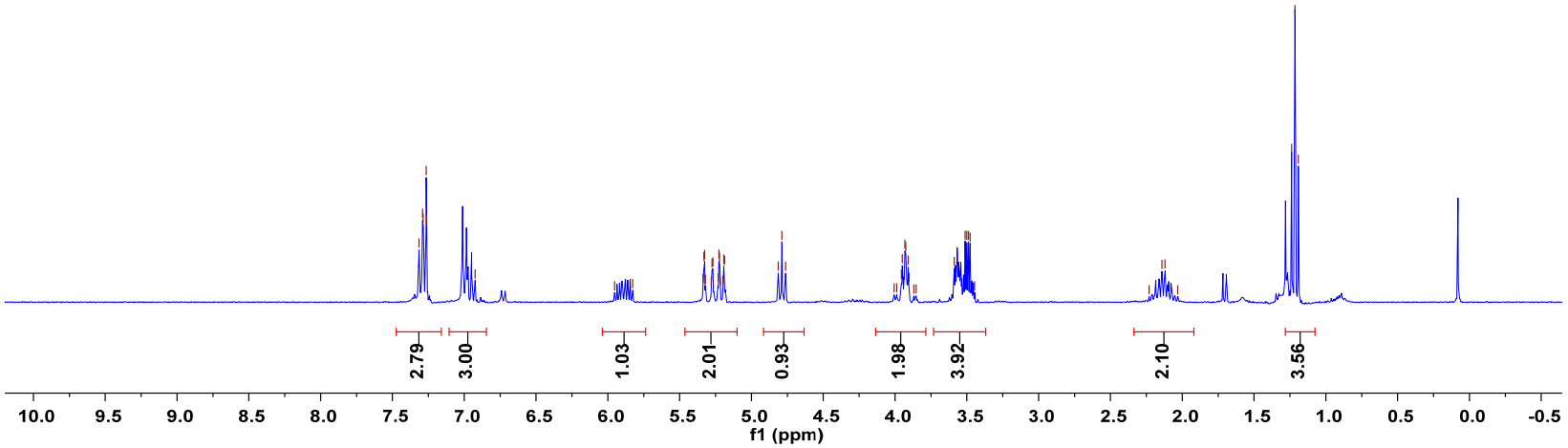
33,1
%T
4000,0
3000
2000
1500
1000
540,0
cm-1
3083
2929
2877
2831
2232
1869
1644
1590
1493
1458
1419
1385
1321
1273
1236
1183
1116
1081
998
957
918
866
808
754
731
648
625
OMe
CN
N
Br
3d
FT-IR (neat, ATR)
d:\ak mayr\alex\awal11.sp - PETNC

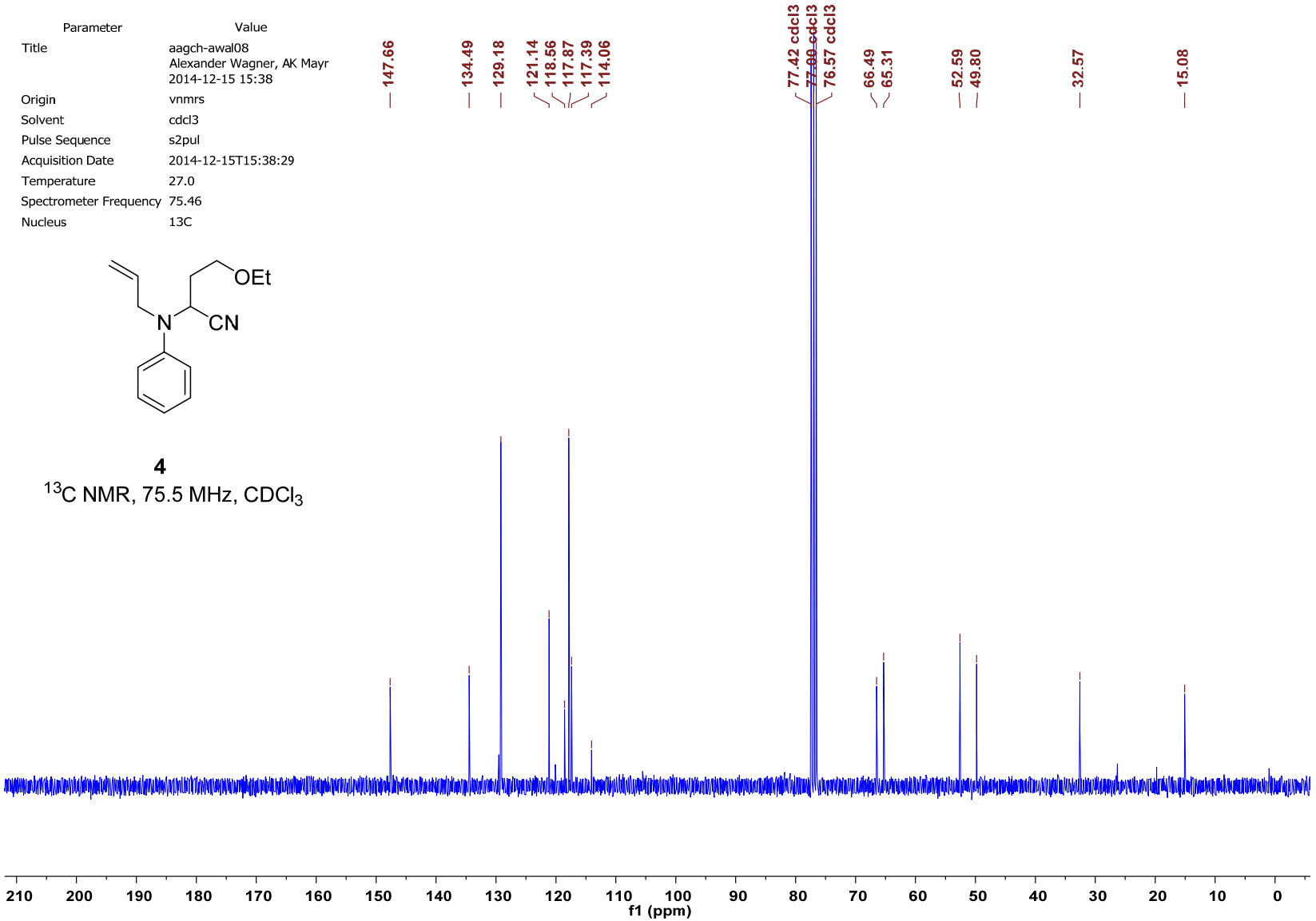
Parameter	Value
Title	aagch-awal08 Alexander Wagner, AK Mayr 2014-12-15 15:37
Origin	vnmrs
Solvent	cdcl3
Pulse Sequence	s2pul
Acquisition Date	2014-12-15T15:37:49
Temperature	27.0
Spectrometer Frequency	300.06
Nucleus	1H



4

^{1}H NMR, 300 MHz, $CDCl_3$

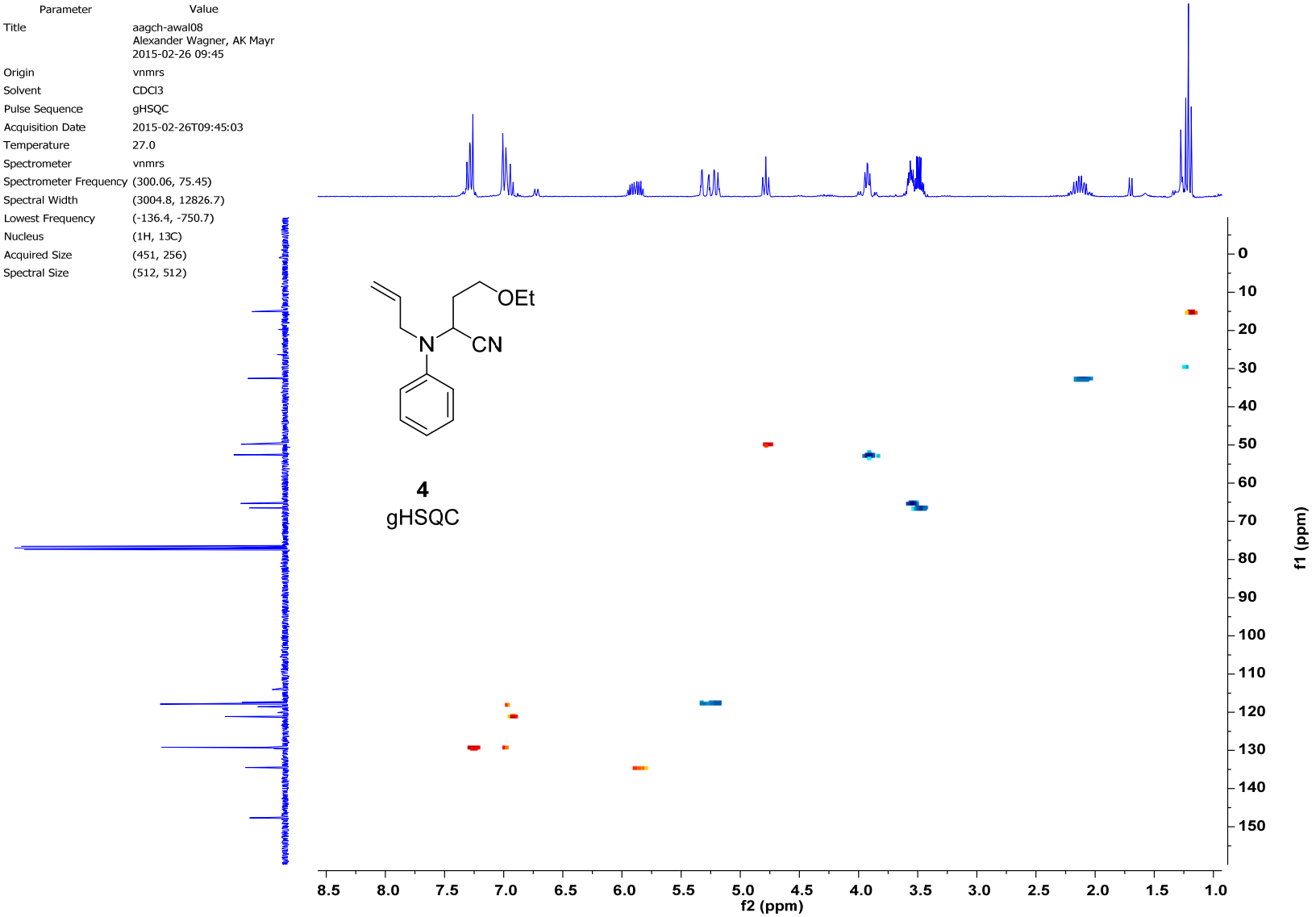


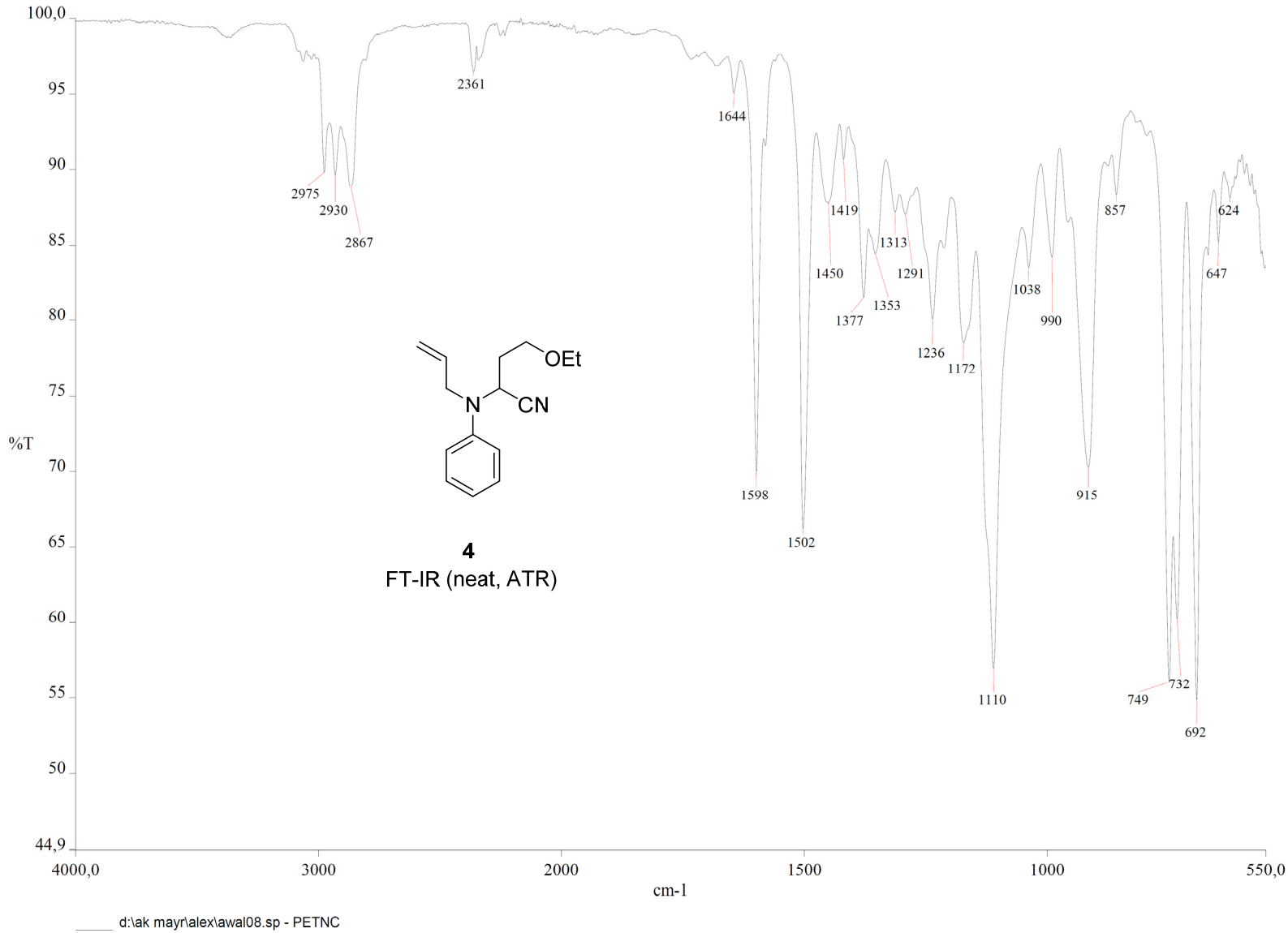


4

^{13}C NMR, 75.5 MHz, $CDCl_3$

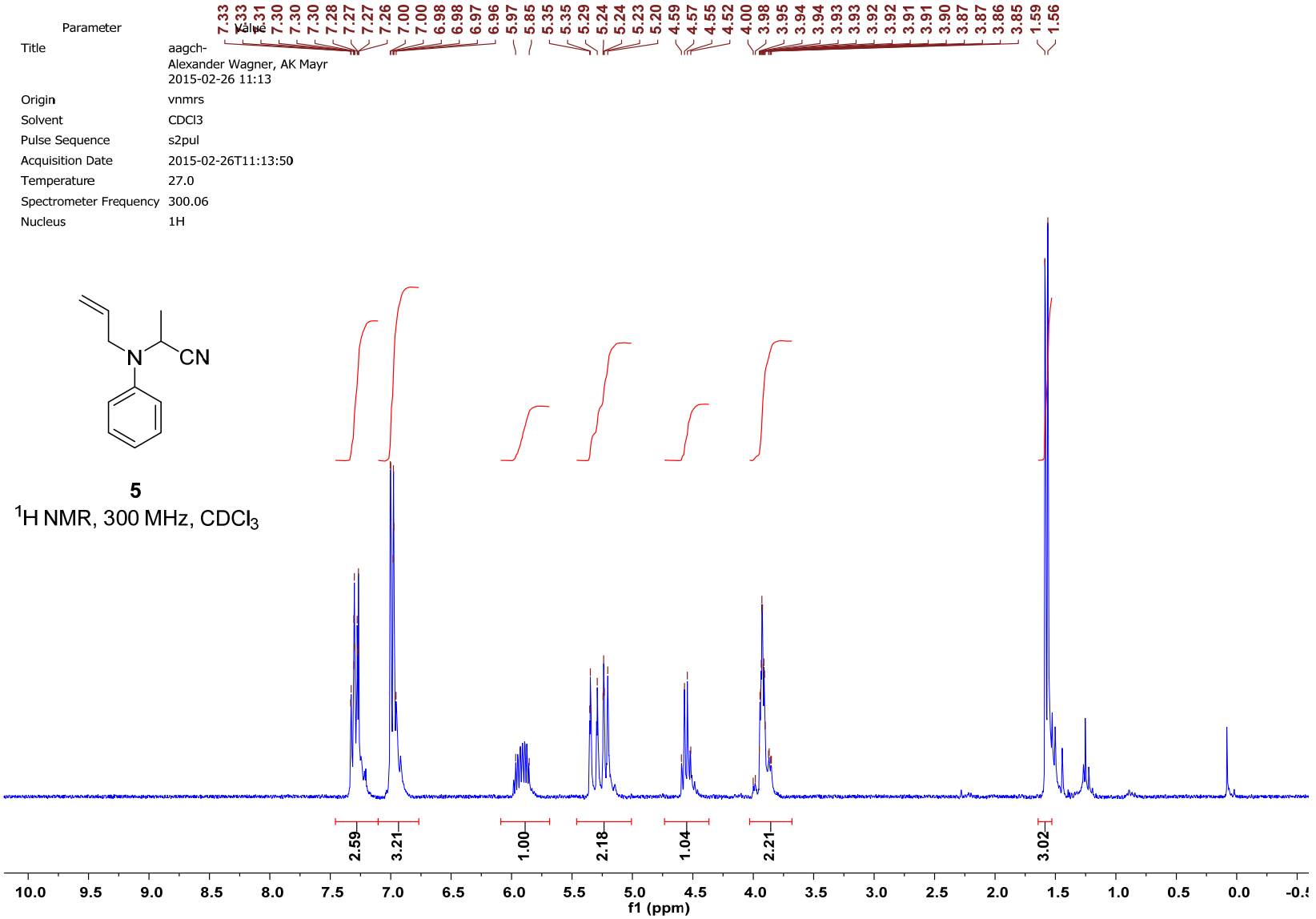
Parameter	Value
Title	aagch-awal08 Alexander Wagner, AK Mayr 2015-02-26 09:45
Origin	vnmrs
Solvent	CDCl3
Pulse Sequence	gHSQC
Acquisition Date	2015-02-26T09:45:03
Temperature	27.0
Spectrometer	vnmrs
Spectrometer Frequency	(300.06, 75.45)
Spectral Width	(3004.8, 12826.7)
Lowest Frequency	(-136.4, -750.7)
Nucleus	(1H, 13C)
Acquired Size	(451, 256)
Spectral Size	(512, 512)



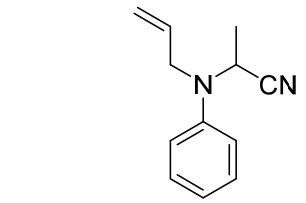


4

FT-IR (neat, ATR)


Parameter Value
Title aagch-
Alexander Wagner, AK Mayr
2015-02-26 11:13
Origin vnmrs
Solvent CDCl3
Pulse Sequence s2pul
Acquisition Date 2015-02-26T11:13:50
Temperature 27.0
Spectrometer Frequency 300.06
Nucleus 1H
7.33 7.33 7.31 7.30 7.30 7.30 7.28 7.27 7.27 7.26 7.00 7.00 6.98 6.98 6.97 6.96 5.97 5.85 5.35 5.35 5.29 5.24 5.24 5.23 5.20 4.59 4.57 4.55 4.52 4.00 3.98 3.95 3.94 3.94 3.93 3.93 3.92 3.92 3.91 3.91 3.90 3.87 3.87 3.86 3.85 1.59 1.56
N
CN
5
1H NMR, 300 MHz, CDCl3
2.59 3.21 1.00 2.18 1.04 2.21 3.02
10.0 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 0.5 0.0
f1 (ppm)

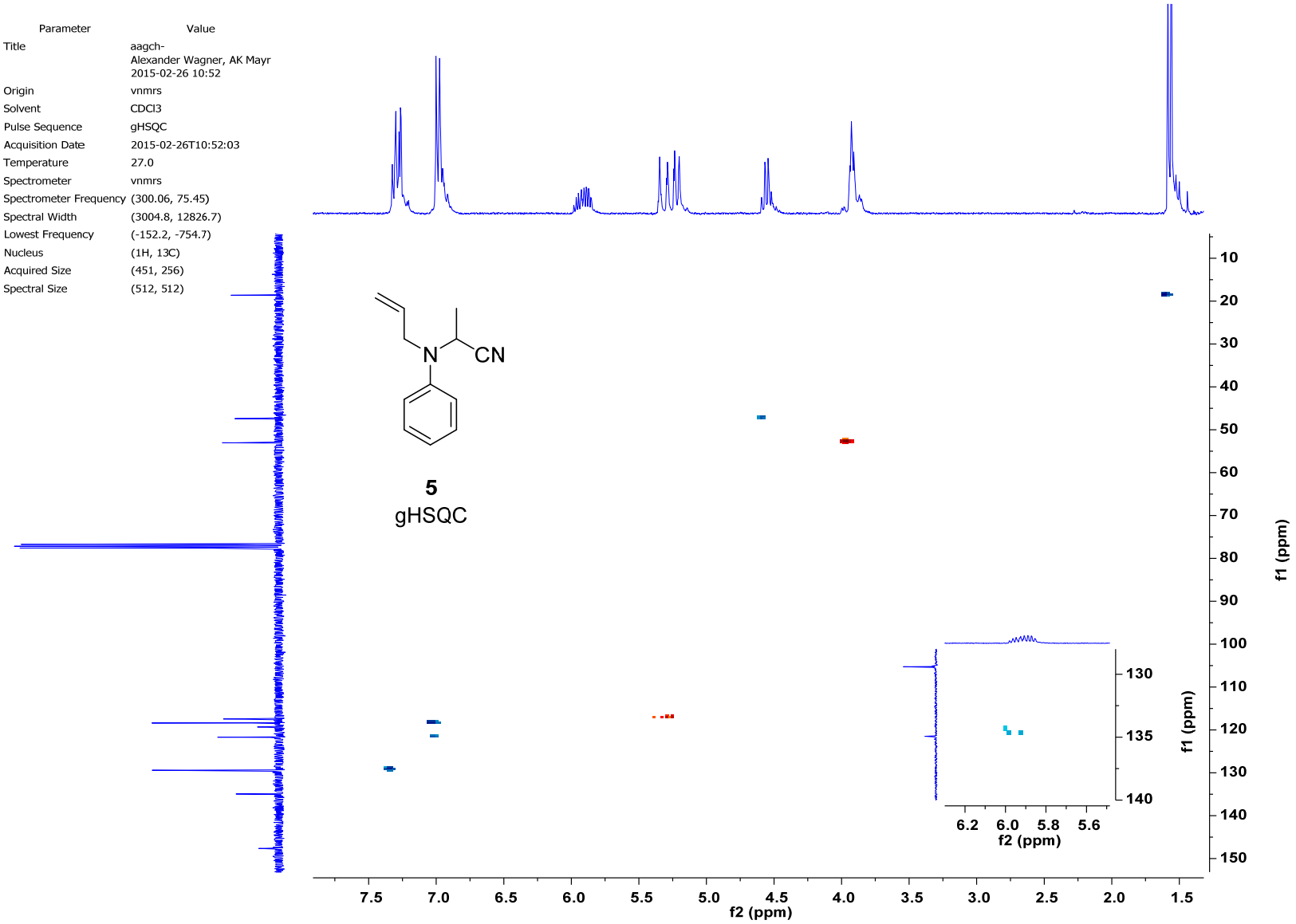
Parameter	Value
Title	aagch- Alexander Wagner, AK Mayr 2015-02-26 11:14
Origin	vnmrs
Solvent	CDCl3
Pulse Sequence	s2pul
Acquisition Date	2015-02-26T11:14:27
Temperature	27.0
Spectrometer Frequency	75.46
Nucleus	13C

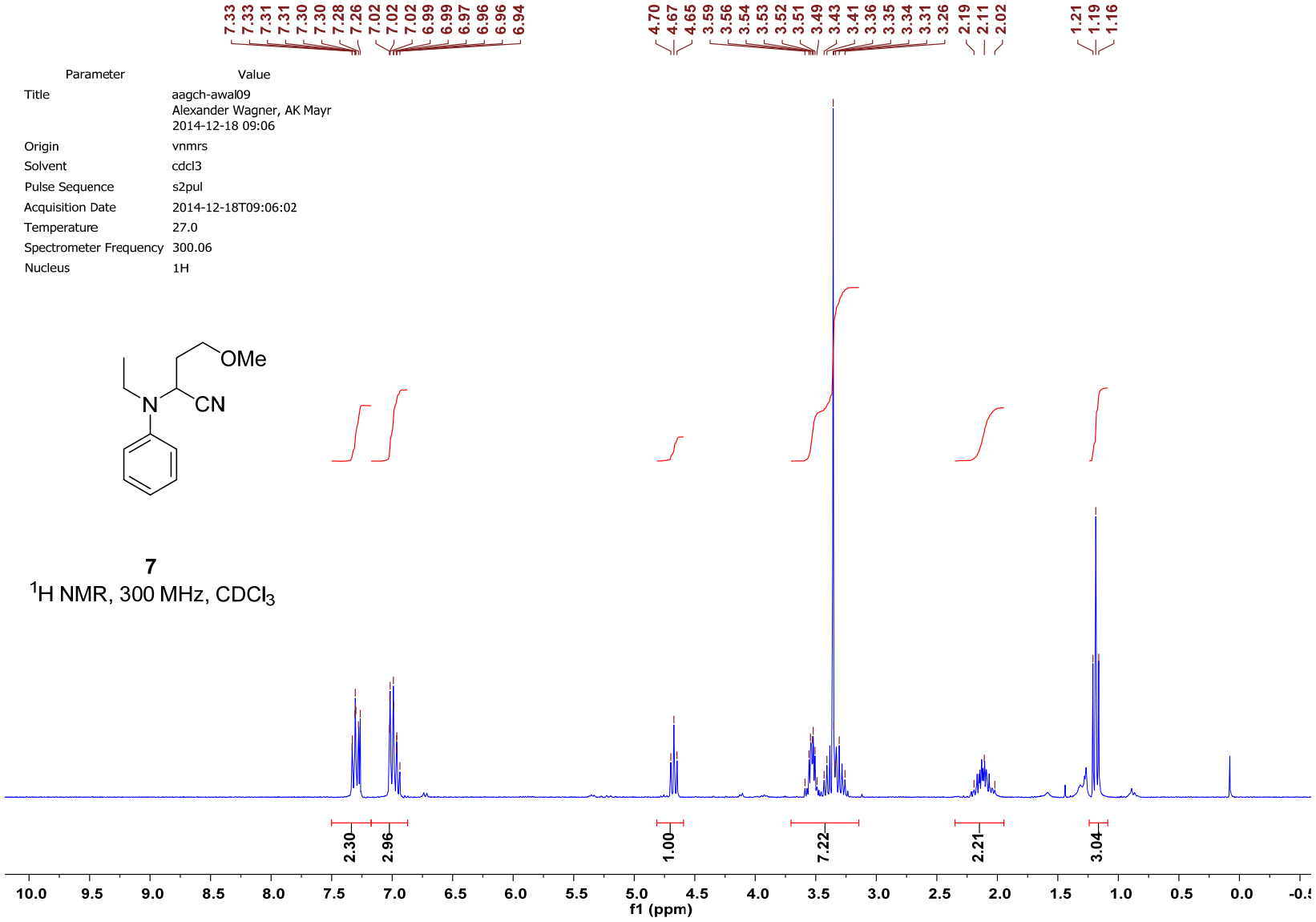


5

^{13}C NMR, 75.5 MHz, $CDCl_3$

Parameter	Value
Title	aagch- Alexander Wagner, AK Mayr 2015-02-26 10:52
Origin	vnmrs
Solvent	CDCl3
Pulse Sequence	gHSQC
Acquisition Date	2015-02-26T10:52:03
Temperature	27.0
Spectrometer	vnmrs
Spectrometer Frequency	(300.06, 75.45)
Spectral Width	(3004.8, 12826.7)
Lowest Frequency	(-152.2, -754.7)
Nucleus	(1H, 13C)
Acquired Size	(451, 256)
Spectral Size	(512, 512)

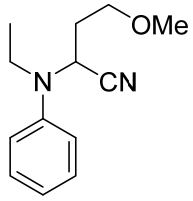




7

^{1}H NMR, 300 MHz, $CDCl_3$

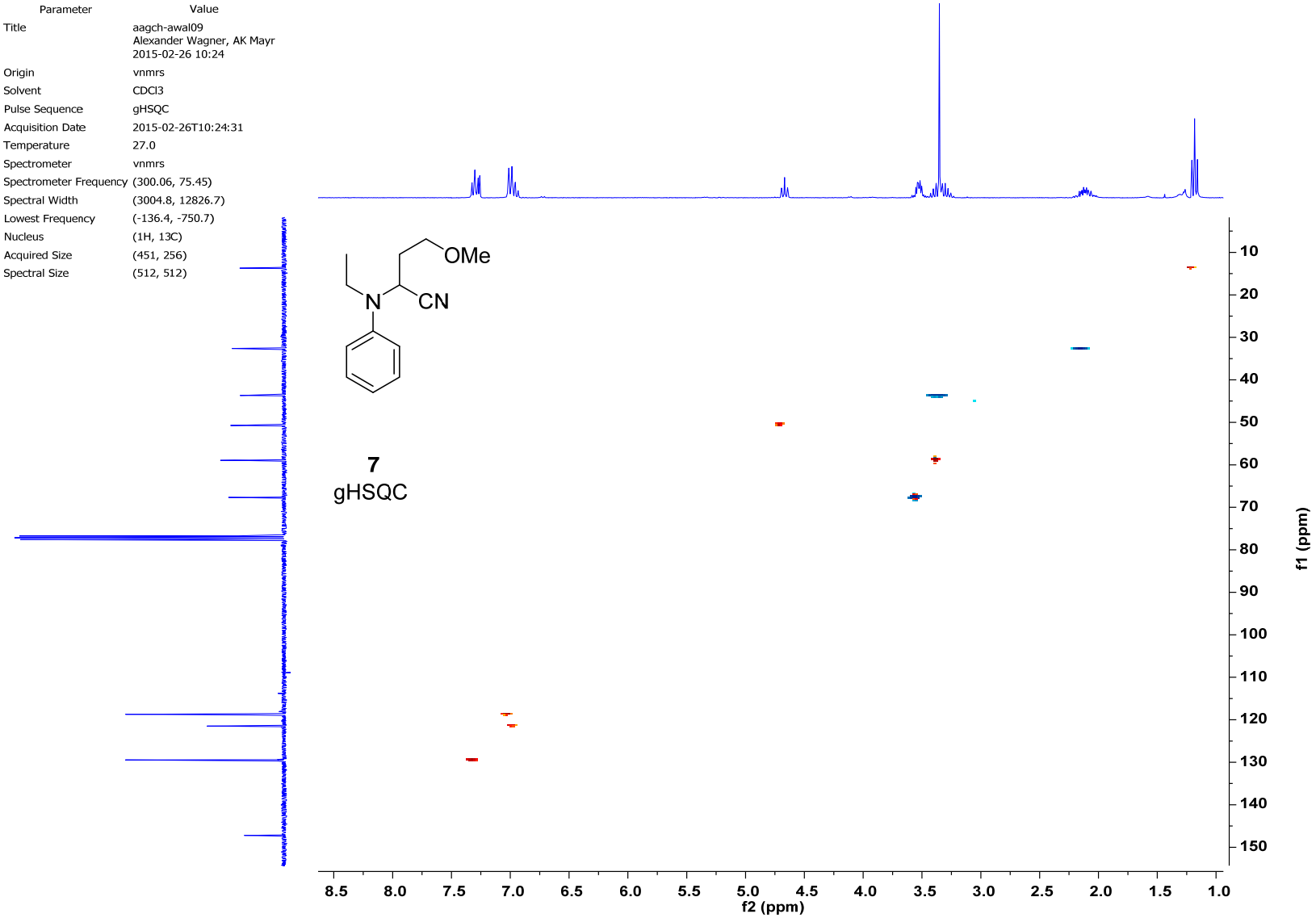
Parameter	Value
Title	aagch-awal09 Alexander Wagner, AK Mayr 2014-12-18 09:06
Origin	vnmrs
Solvent	cdcl3
Pulse Sequence	s2pul
Acquisition Date	2014-12-18T09:06:48
Temperature	27.0
Spectrometer Frequency	75.46
Nucleus	13C

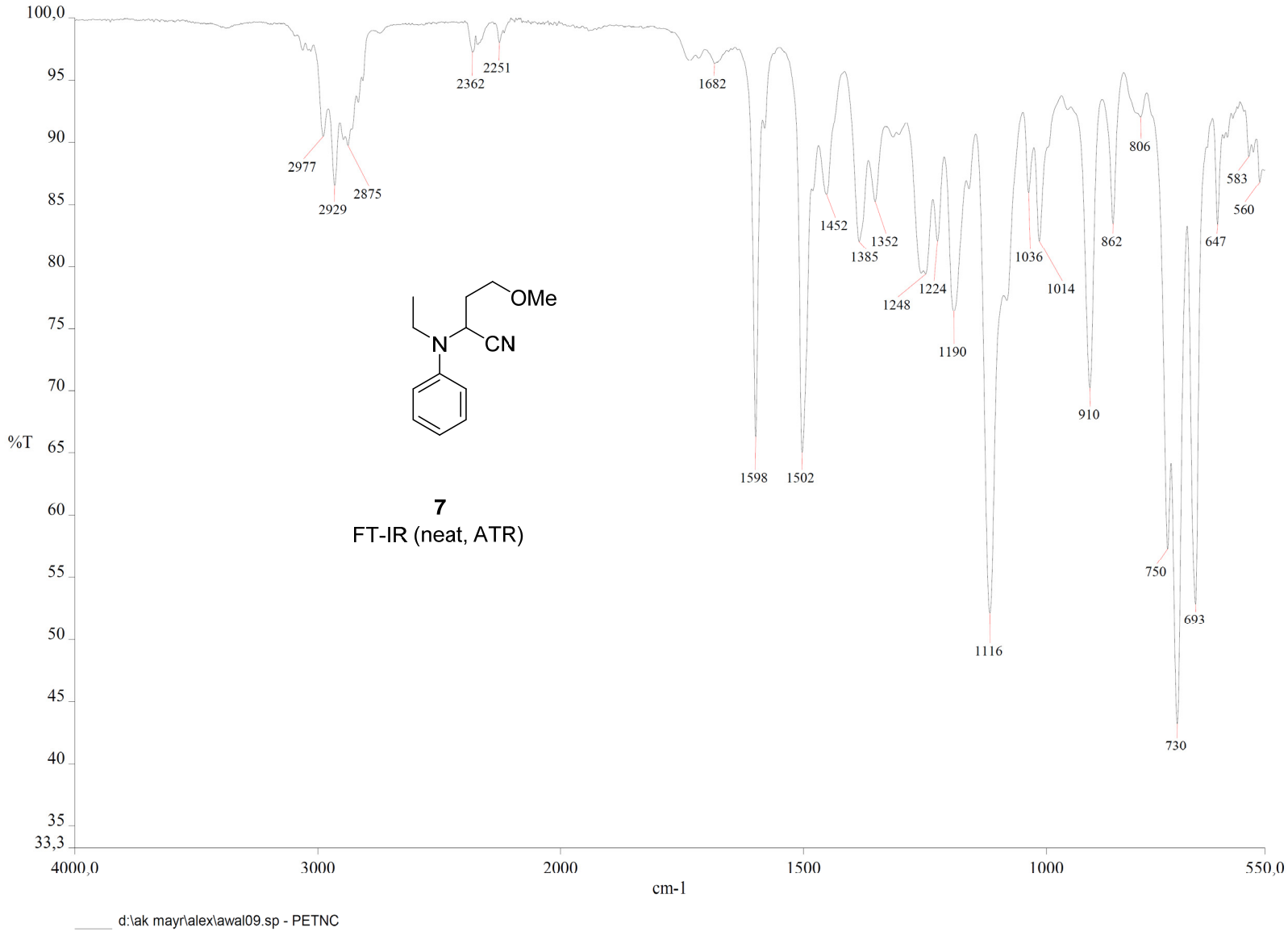


7

^{13}C NMR, 75.5 MHz, $CDCl_3$

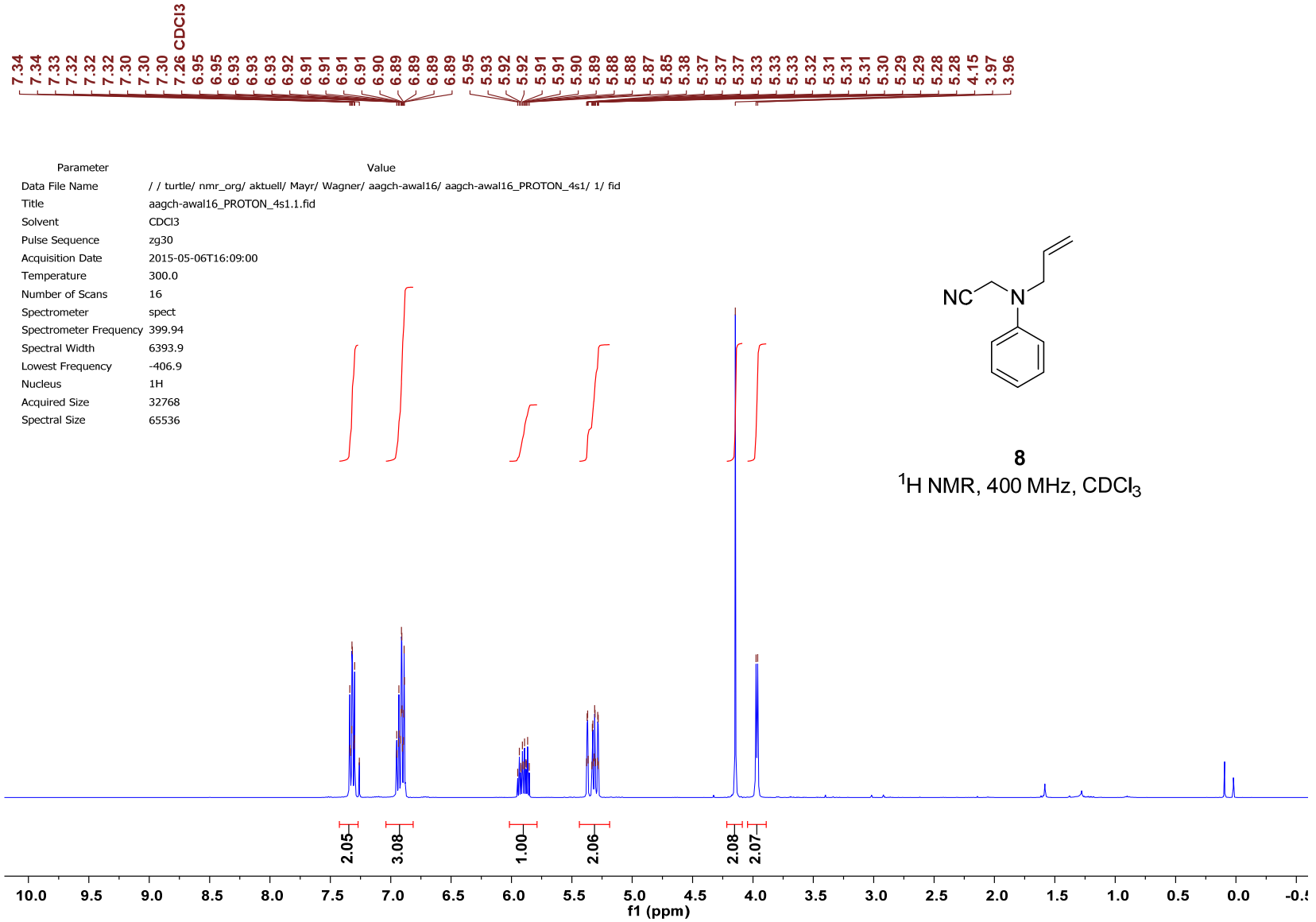
Parameter	Value
Title	aagch-awal09 Alexander Wagner, AK Mayr 2015-02-26 10:24
Origin	vnmrs
Solvent	CDCl3
Pulse Sequence	gHSQC
Acquisition Date	2015-02-26T10:24:31
Temperature	27.0
Spectrometer	vnmrs
Spectrometer Frequency	(300.06, 75.45)
Spectral Width	(3004.8, 12826.7)
Lowest Frequency	(-136.4, -750.7)
Nucleus	(1H, 13C)
Acquired Size	(451, 256)
Spectral Size	(512, 512)

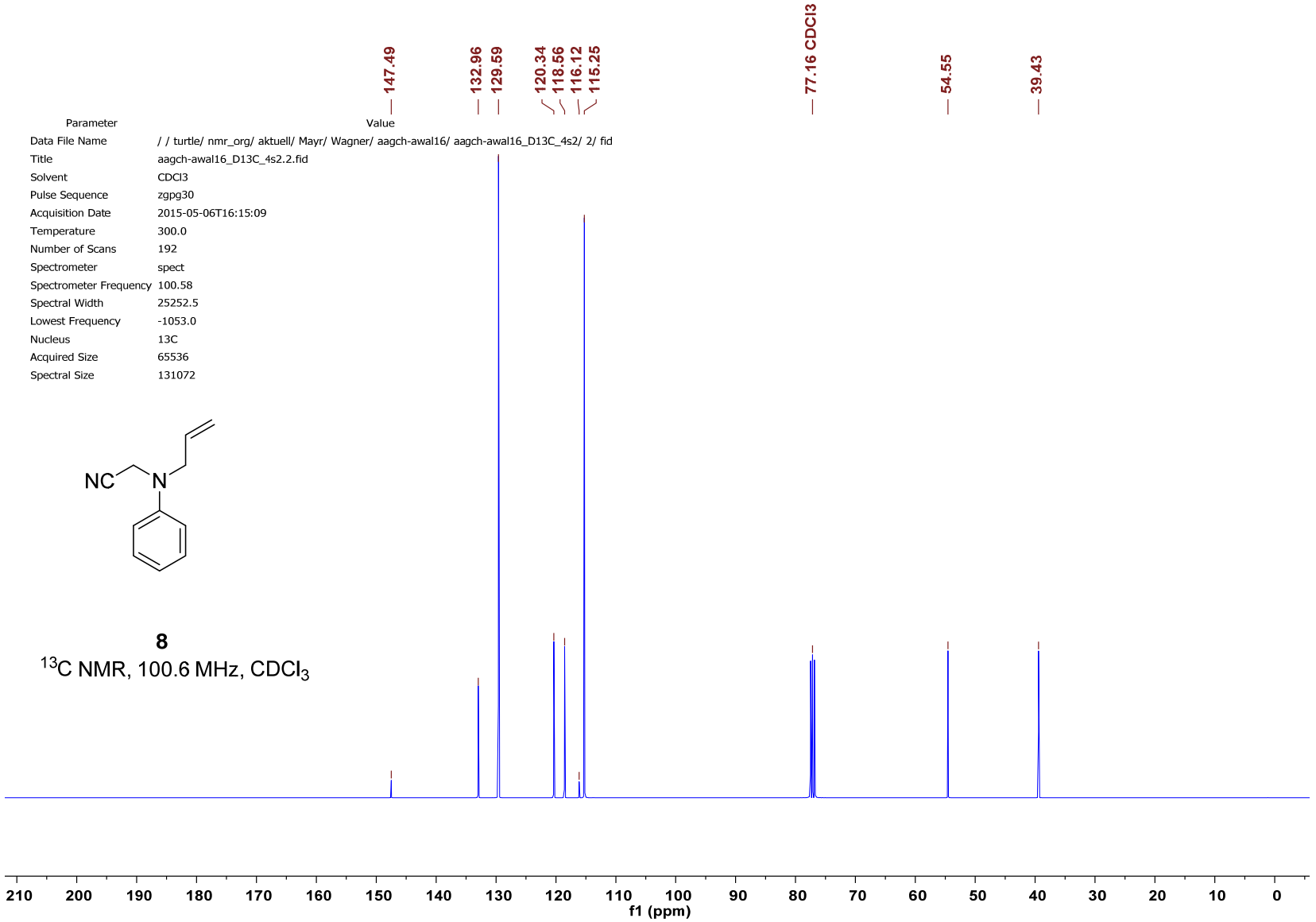




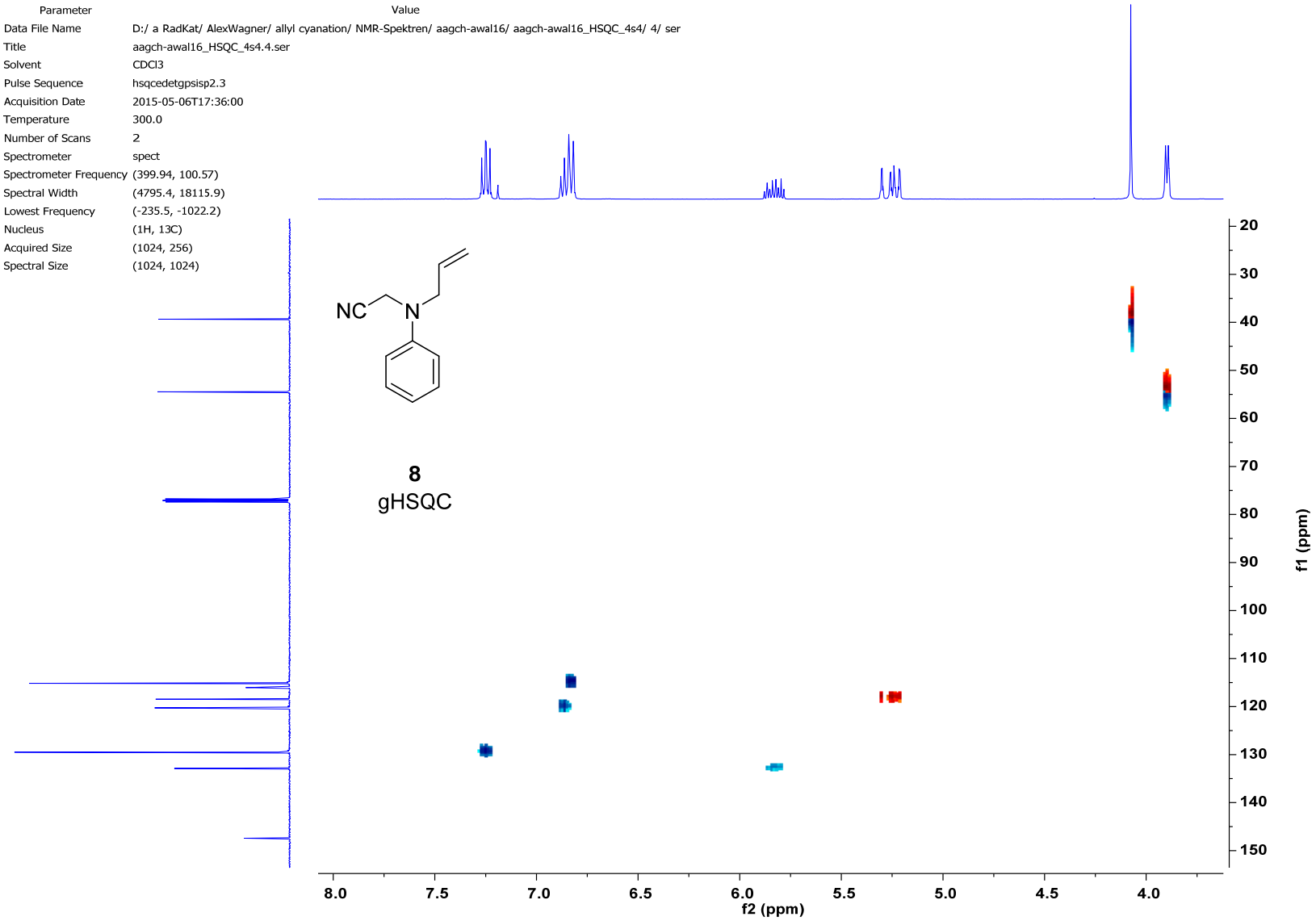
7

FT-IR (neat, ATR)

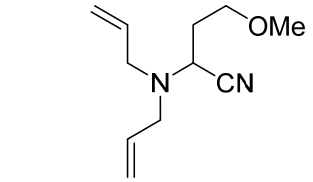

7.34 7.34 7.33 7.32 7.32 7.32 7.30 7.30 7.30 7.26 CDCl3 6.95 6.95 6.93 6.93 6.93 6.92 6.91 6.91 6.91 6.91 6.90 6.89 6.89 6.89 6.89 5.95 5.93 5.92 5.92 5.91 5.91 5.90 5.89 5.88 5.88 5.87 5.85 5.38 5.37 5.37 5.37 5.33 5.33 5.33 5.32 5.31 5.31 5.31 5.30 5.29 5.29 5.28 5.28 4.15 3.97 3.96
Parameter Value
Data File Name / / turtle/ nmr_org/ aktuell/ Mayr/ Wagner/ aagch-awal16/ aagch-awal16_PROTON_4s1/ 1/ fid
Title aagch-awal16_PROTON_4s1.1.fid
Solvent CDCl3
Pulse Sequence zg30
Acquisition Date 2015-05-06T16:09:00
Temperature 300.0
Number of Scans 16
Spectrometer spect
Spectrometer Frequency 399.94
Spectral Width 6393.9
Lowest Frequency -406.9
Nucleus 1H
Acquired Size 32768
Spectral Size 65536
NC
N
8
1H NMR, 400 MHz, CDCl3
2.05
3.08
1.00
2.06
2.08
2.07
10.0 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 0.5 0.0
f1 (ppm)


147.49
132.96
129.59
120.34
118.56
116.12
115.25
77.16 CDCl3
54.55
39.43
Parameter Value
Data File Name / / turtle/ nmr_org/ aktuell/ Mayr/ Wagner/ aagch-awal16/ aagch-awal16_D13C_4s2/ 2/ fid
Title aagch-awal16_D13C_4s2.2.fid
Solvent CDCl3
Pulse Sequence zgpg30
Acquisition Date 2015-05-06T16:15:09
Temperature 300.0
Number of Scans 192
Spectrometer spect
Spectrometer Frequency 100.58
Spectral Width 25252.5
Lowest Frequency -1053.0
Nucleus 13C
Acquired Size 65536
Spectral Size 131072
NC
N
8
13C NMR, 100.6 MHz, CDCl3
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

Parameter	Value
Data File Name	D:/ a RadKat/ AlexWagner/ allyl cyanation/ NMR-Spektren/ aagch-awal16/ aagch-awal16_HSQC_4s4/ 4/ ser
Title	aagch-awal16_HSQC_4s4.4.ser
Solvent	CDCl3
Pulse Sequence	hsqcedetgpsisp2.3
Acquisition Date	2015-05-06T17:36:00
Temperature	300.0
Number of Scans	2
Spectrometer	spect
Spectrometer Frequency	(399.94, 100.57)
Spectral Width	(4795.4, 18115.9)
Lowest Frequency	(-235.5, -1022.2)
Nucleus	(1H, 13C)
Acquired Size	(1024, 256)
Spectral Size	(1024, 1024)



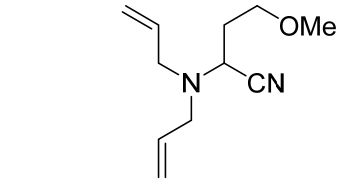
Parameter	Value
Title	aagch-awal06 Alexander Wagner, AK Mayr 2014-12-03 11:38
Origin	vnmrs
Solvent	cdcl3
Pulse Sequence	s2pul
Acquisition Date	2014-12-03T11:38:03
Temperature	27.0
Spectrometer Frequency	300.06
Nucleus	1H



10

^{1}H NMR, 300 MHz, $CDCl_3$

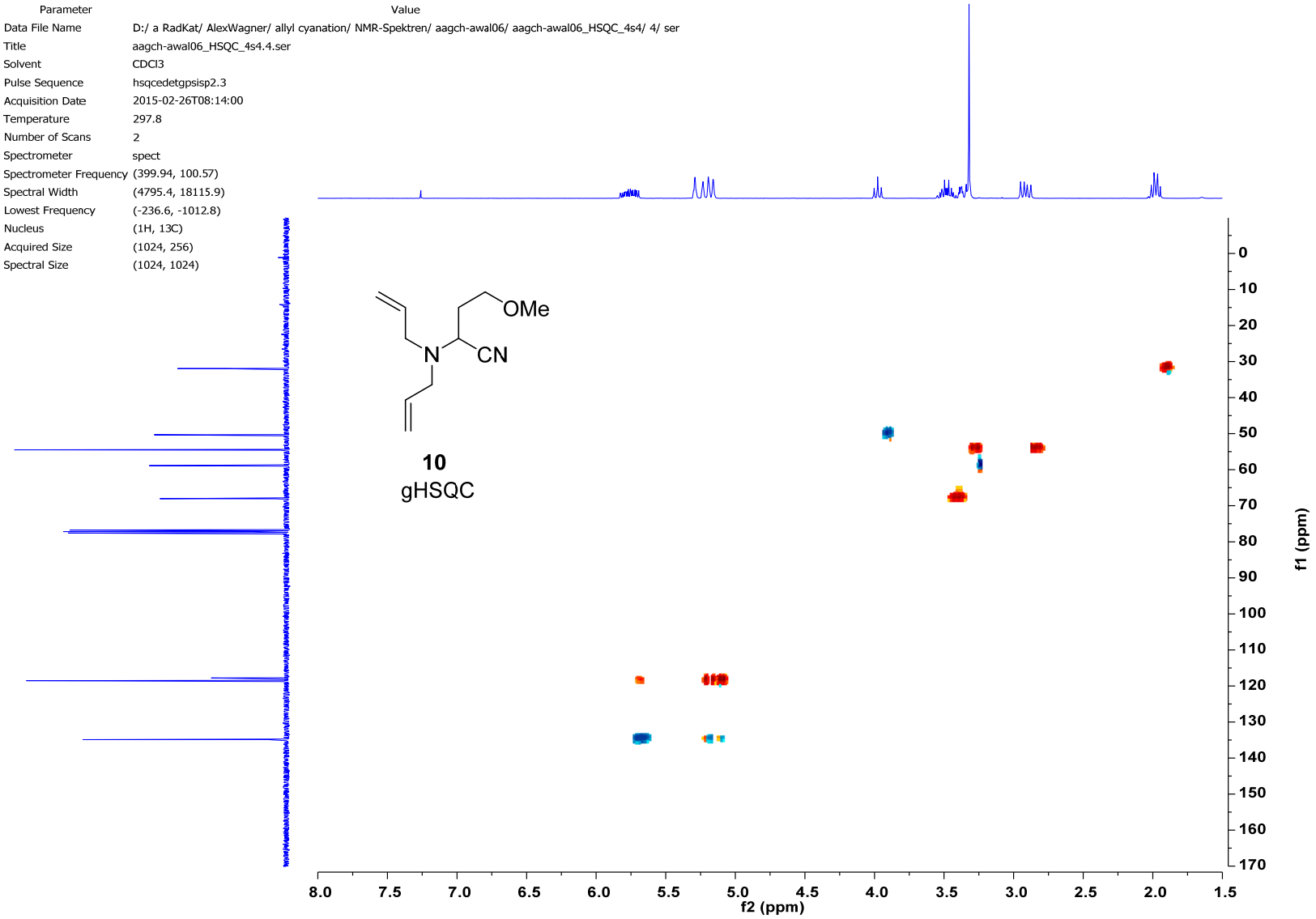
Parameter	Value
Title	aagch-awal06 Alexander Wagner, AK Mayr 2014-12-03 11:38
Origin	vnmrs
Solvent	cdcl3
Pulse Sequence	s2pul
Acquisition Date	2014-12-03T11:38:49
Temperature	27.0
Spectrometer Frequency	75.46
Nucleus	13C

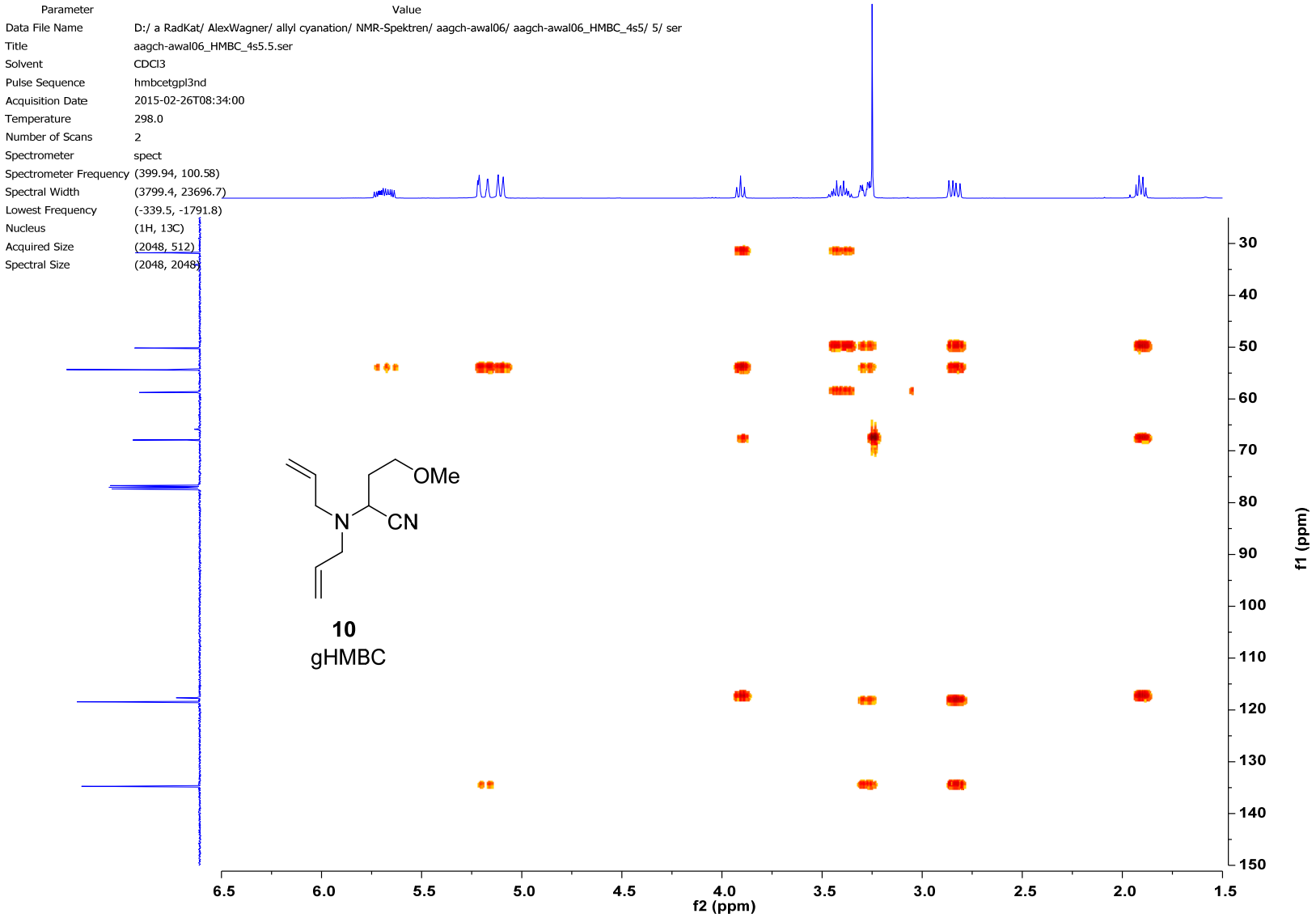


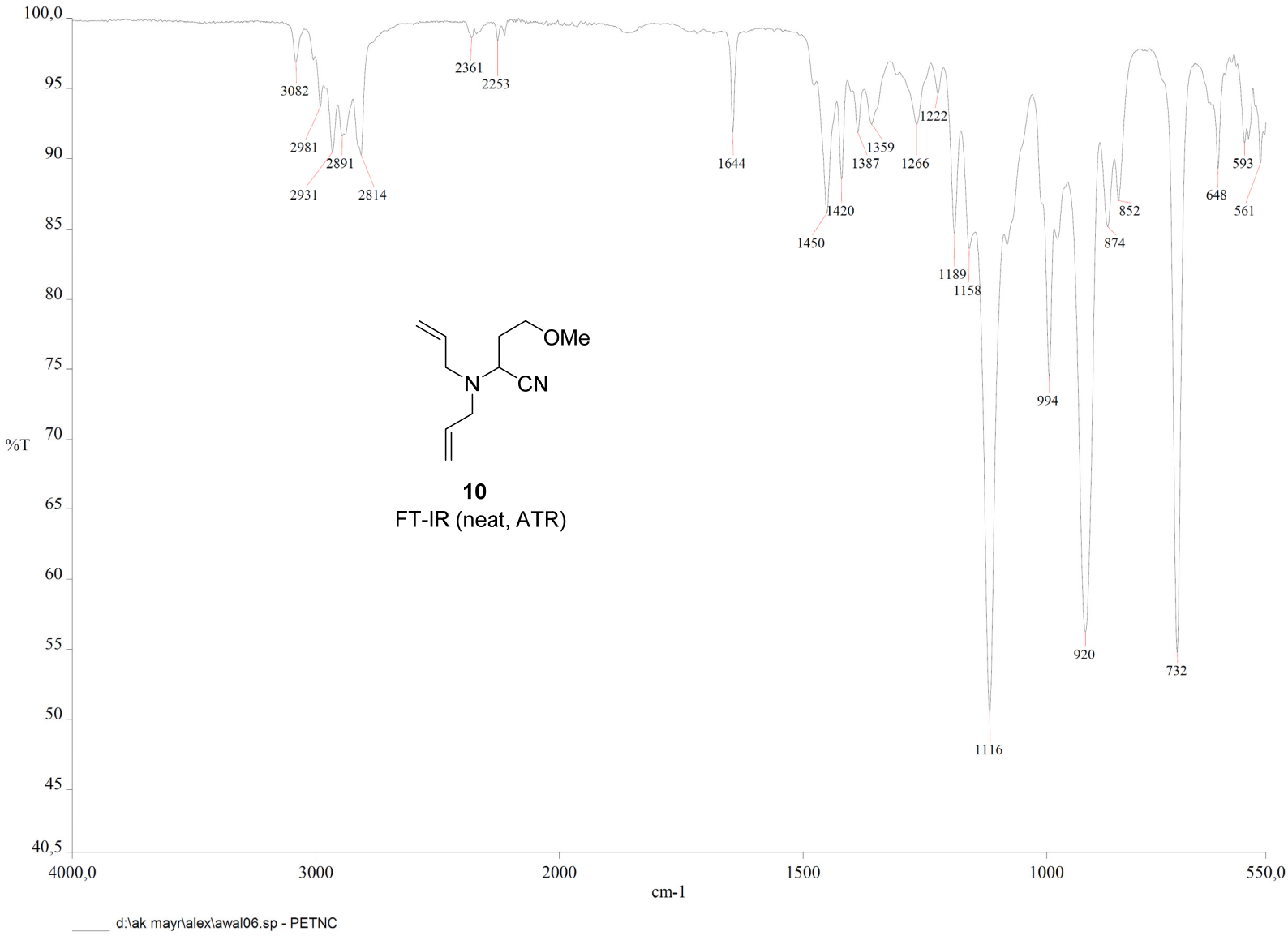
10

^{13}C NMR, 75.5MHz, $CDCl_3$

Parameter	Value
Data File Name	D:/ a RadKat/ AlexWagner/ allyl cyanation/ NMR-Spektren/ aagch-awal06/ aagch-awal06_HSQC_4s4/ 4/ ser
Title	aagch-awal06_HSQC_4s4.4.ser
Solvent	CDCl3
Pulse Sequence	hsqcedetgpsisp2.3
Acquisition Date	2015-02-26T08:14:00
Temperature	297.8
Number of Scans	2
Spectrometer	spect
Spectrometer Frequency	(399.94, 100.57)
Spectral Width	(4795.4, 18115.9)
Lowest Frequency	(-236.6, -1012.8)
Nucleus	(1H, 13C)
Acquired Size	(1024, 256)
Spectral Size	(1024, 1024)

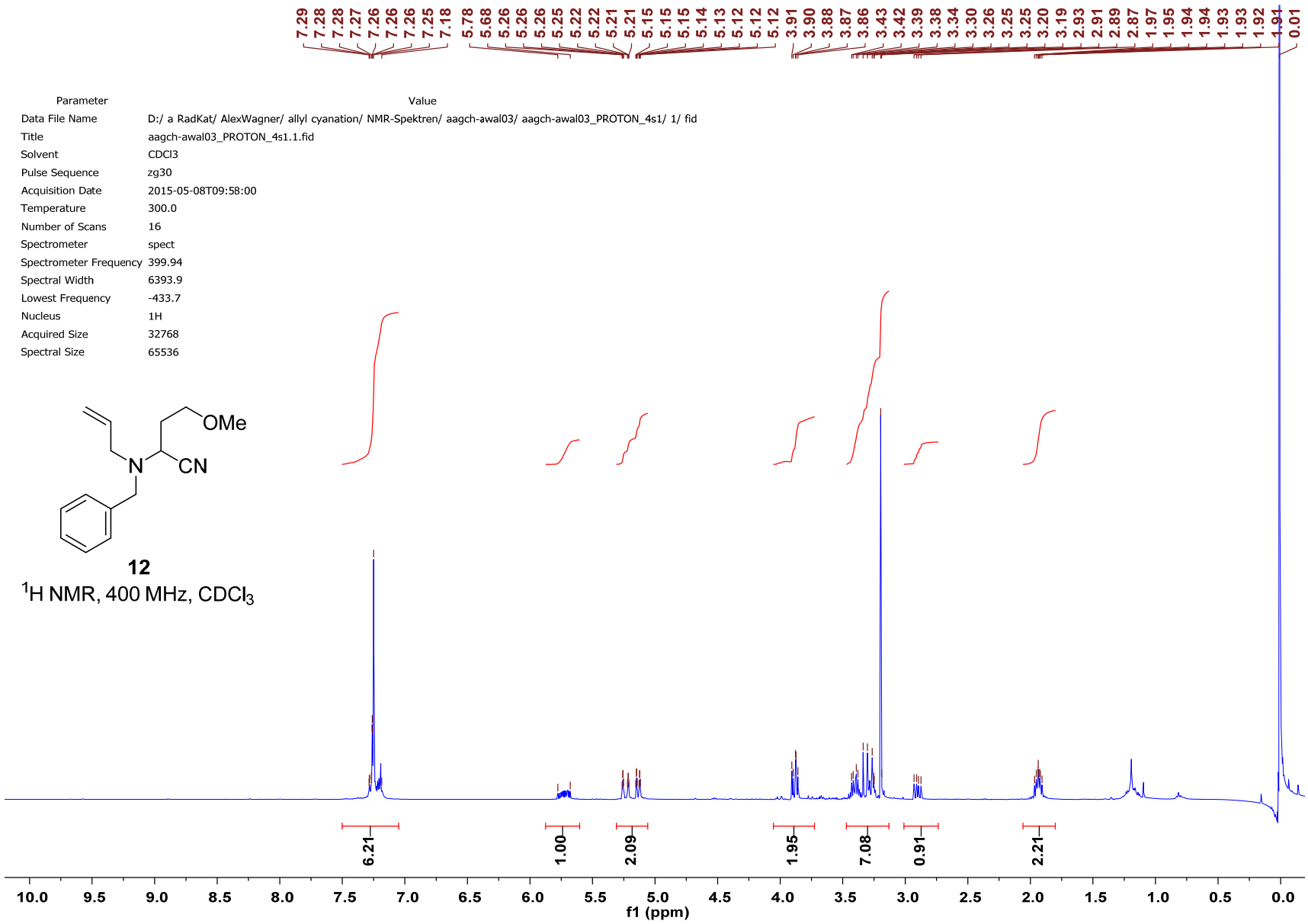



Parameter Value
Data File Name D:/ a RadKat/ AlexWagner/ allyl cyanation/ NMR-Spektren/ aagch-awal06/ aagch-awal06_HMBC_4s5/ 5/ ser
Title aagch-awal06_HMBC_4s5.5.ser
Solvent CDCl3
Pulse Sequence hmbcetgpl3nd
Acquisition Date 2015-02-26T08:34:00
Temperature 298.0
Number of Scans 2
Spectrometer spect
Spectrometer Frequency (399.94, 100.58)
Spectral Width (3799.4, 23696.7)
Lowest Frequency (-339.5, -1791.8)
Nucleus (1H, 13C)
Acquired Size (2048, 512)
Spectral Size (2048, 2048)
OMe
N
CN
10
gHMBC
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
f2 (ppm)
30
40
50
60
70
80
90
100
110
120
130
140
150
f1 (ppm)

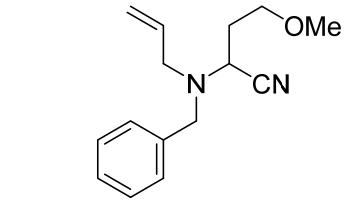


10

FT-IR (neat, ATR)


7.29 7.28 7.28 7.27 7.26 7.26 7.26 7.25 7.18
5.78 5.68 5.26 5.26 5.25 5.22 5.22 5.21 5.21 5.15 5.15 5.15 5.14 5.13 5.12 5.12 5.12
3.91 3.90 3.88 3.87 3.86 3.43 3.42 3.39 3.38 3.34 3.30 3.26 3.25 3.25 3.20 3.19 2.93 2.91 2.89 2.87 1.97 1.95 1.94 1.94 1.93 1.93 1.92 1.91 0.01
Parameter Value
Data File Name D:/ a RadKat/ AlexWagner/ allyl cyanation/ NMR-Spektren/ aagch-awal03/ aagch-awal03_PROTON_4s1/ 1/ fid
Title aagch-awal03_PROTON_4s1.1.fid
Solvent CDCl3
Pulse Sequence zg30
Acquisition Date 2015-05-08T09:58:00
Temperature 300.0
Number of Scans 16
Spectrometer spect
Spectrometer Frequency 399.94
Spectral Width 6393.9
Lowest Frequency -433.7
Nucleus 1H
Acquired Size 32768
Spectral Size 65536
OMe
N
CN
12
1H NMR, 400 MHz, CDCl3
6.21 1.00 2.09 1.95 7.08 0.91 2.21
10.0 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 0.5 0.0
f1 (ppm)

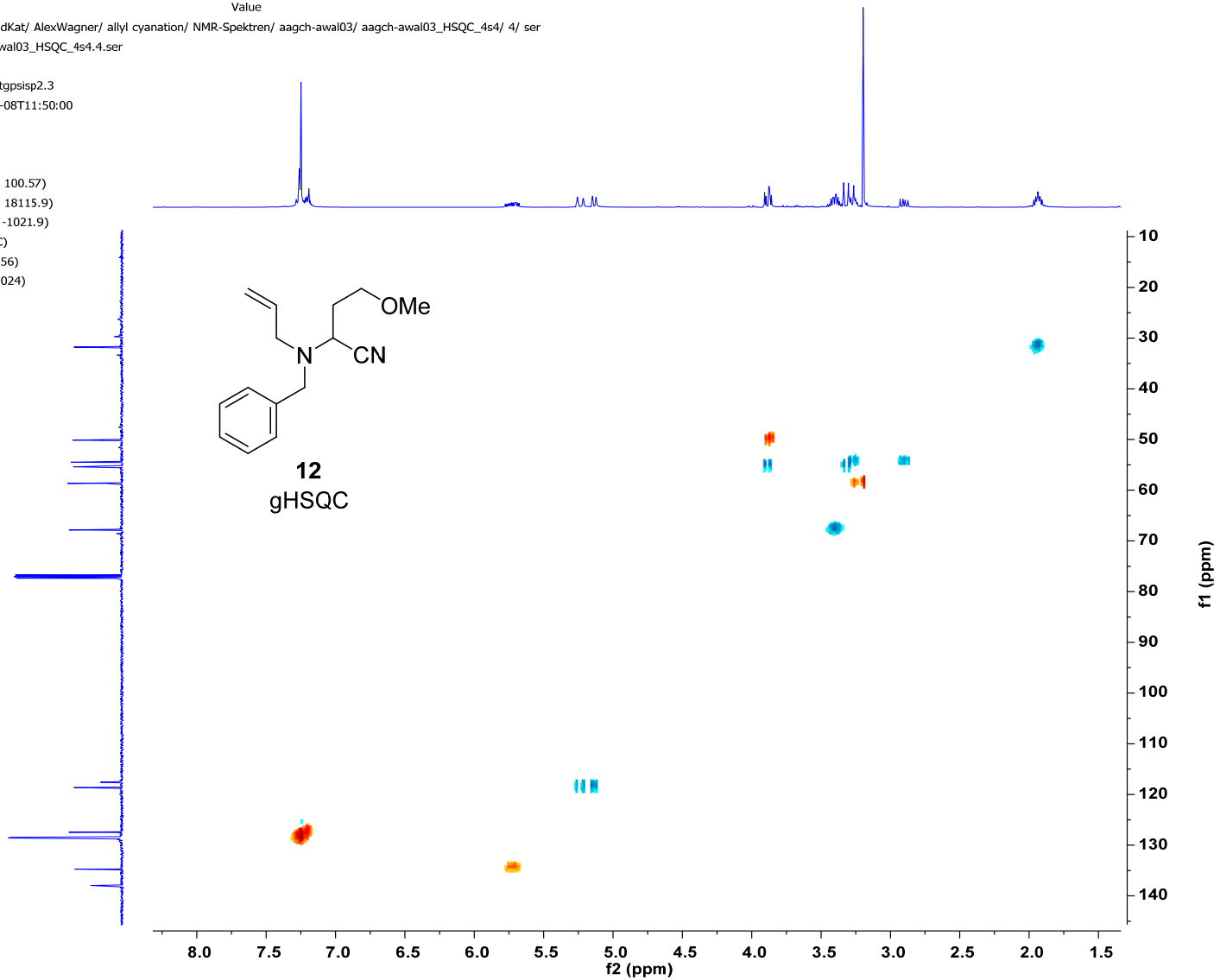
Parameter	Value
Data File Name	D:/ a RadKat/ AlexWagner/ allyl cyanation/ NMR-Spektren/ aagch-awal03/ aagch-awal03_D13C_4s2/ 2/ fid
Title	aagch-awal03_D13C_4s2.2.fid
Solvent	CDCl3
Pulse Sequence	zgpg30
Acquisition Date	2015-05-08T10:04:00
Temperature	300.0
Number of Scans	224
Spectrometer	spect
Spectrometer Frequency	100.58
Spectral Width	25252.5
Lowest Frequency	-1049.5
Nucleus	13C
Acquired Size	65536
Spectral Size	131072



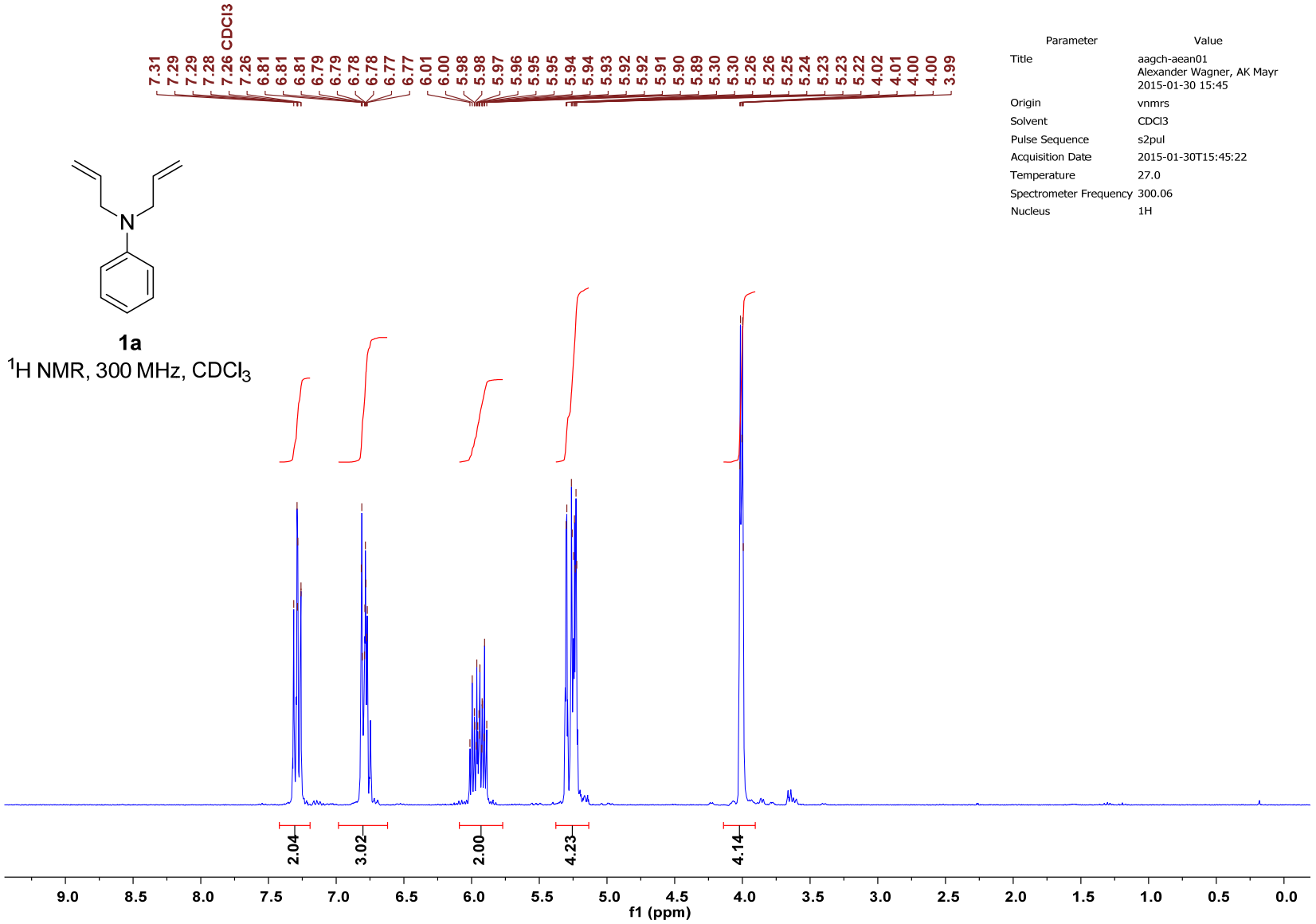
12

^{13}C NMR, 100.6 MHz, $CDCl_3$

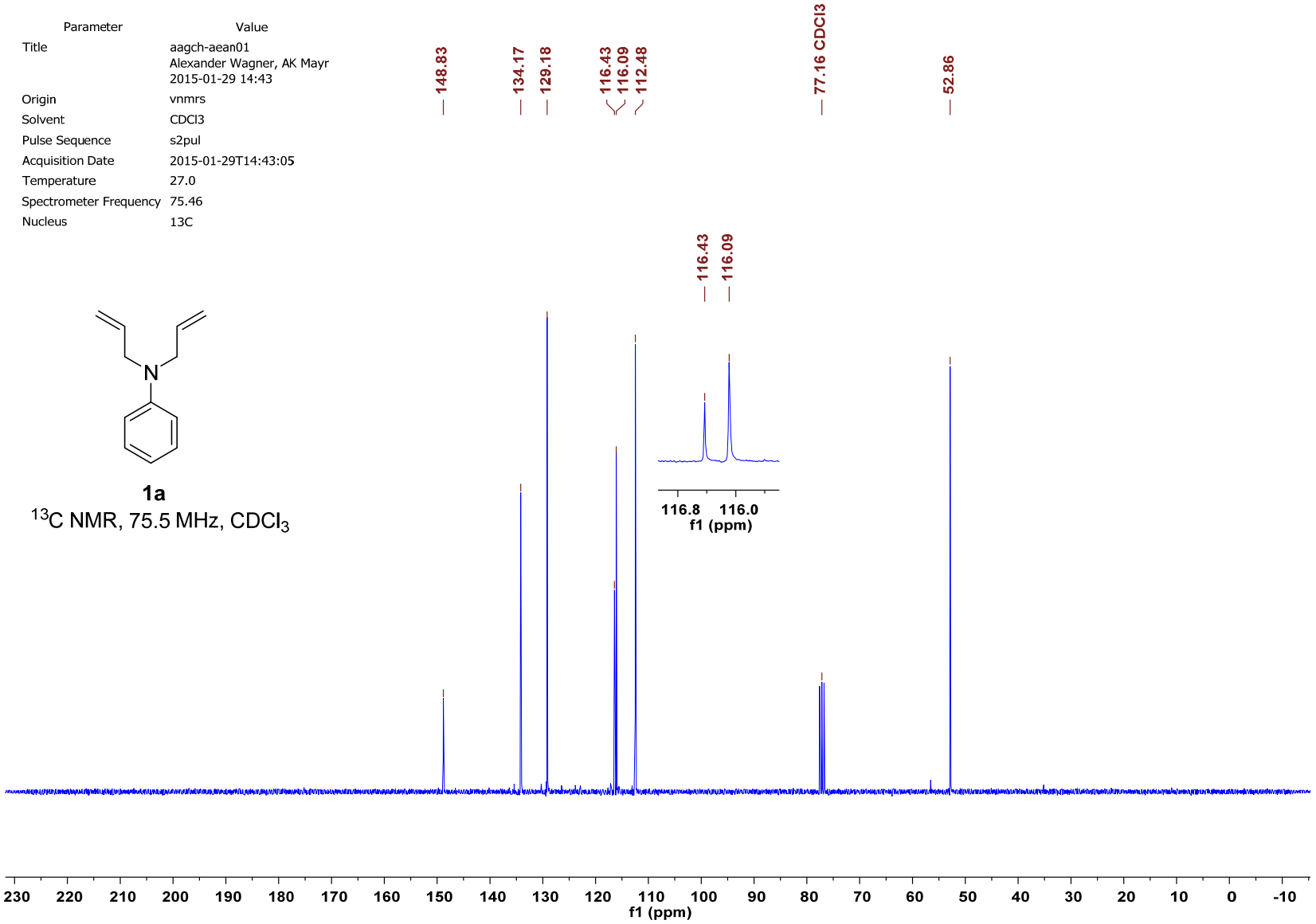
Parameter	Value
Data File Name	D:/ a RadKat/ AlexWagner/ allyl cyanation/ NMR-Spektren/ aagch-awal03/ aagch-awal03_HSQC_4s4/ 4/ ser
Title	aagch-awal03_HSQC_4s4.4.ser
Solvent	CDCl3
Pulse Sequence	hsqcedetgpsisp2.3
Acquisition Date	2015-05-08T11:50:00
Temperature	300.0
Number of Scans	2
Spectrometer	spect
Spectrometer Frequency	(399.94, 100.57)
Spectral Width	(4795.4, 18115.9)
Lowest Frequency	(-234.3, -1021.9)
Nucleus	(1H, 13C)
Acquired Size	(1024, 256)
Spectral Size	(1024, 1024)



6. NMR spectra of allylanilines and allylamines 1a-d, 6a,b, and 11

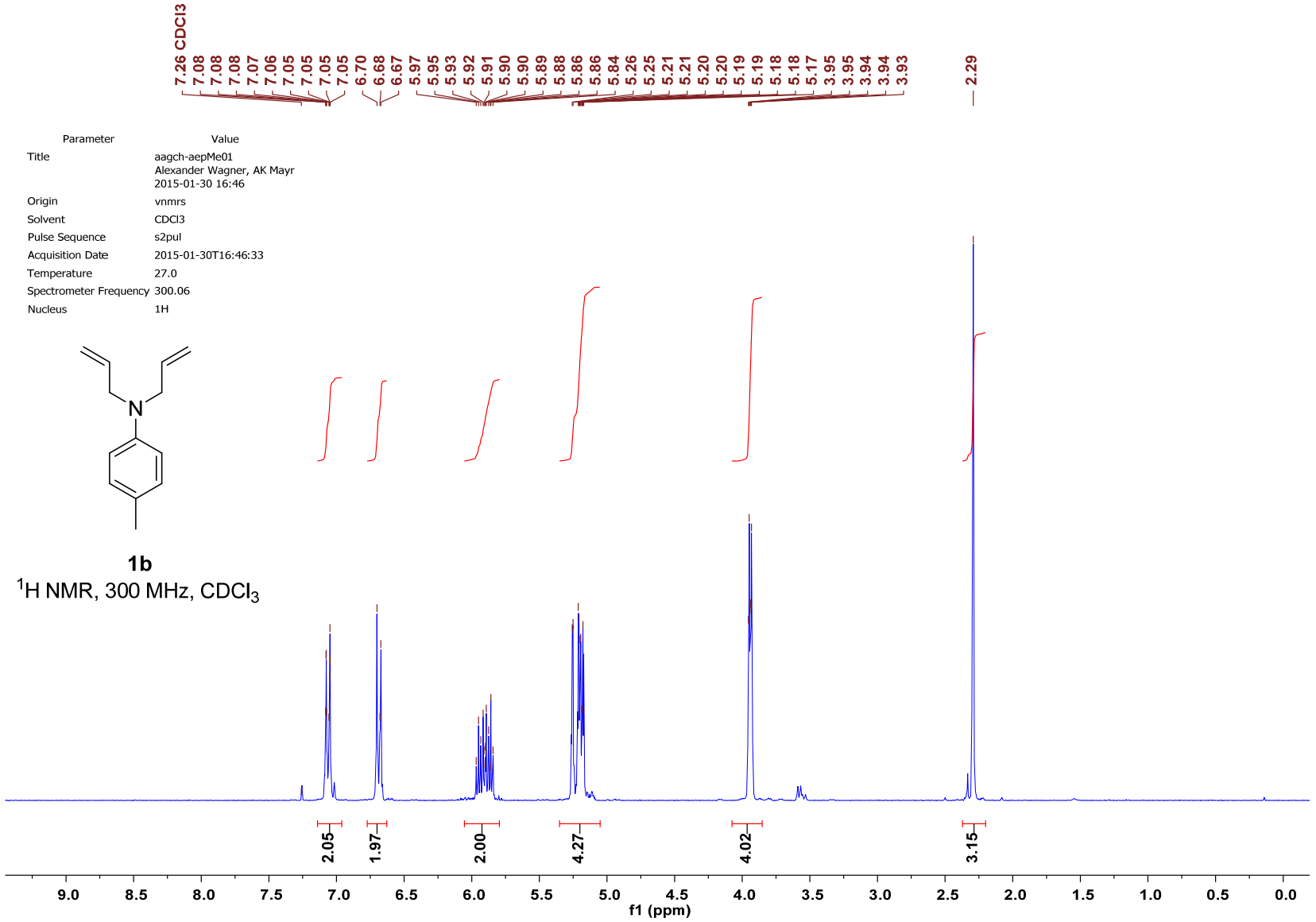

7.31 7.29 7.29 7.28 7.26 CDCl3 7.26 6.81 6.81 6.79 6.79 6.78 6.78 6.77 6.77 6.01 6.00 5.98 5.98 5.97 5.96 5.95 5.95 5.94 5.94 5.93 5.92 5.92 5.91 5.90 5.89 5.30 5.30 5.26 5.26 5.25 5.24 5.23 5.23 5.22 4.02 4.01 4.00 4.00 3.99
Parameter Value
Title aagch-aean01 Alexander Wagner, AK Mayr 2015-01-30 15:45
Origin vnmrs
Solvent CDCl3
Pulse Sequence s2pul
Acquisition Date 2015-01-30T15:45:22
Temperature 27.0
Spectrometer Frequency 300.06
Nucleus 1H
N
1a
1H NMR, 300 MHz, CDCl3
2.04
3.02
2.00
4.23
4.14
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 0.5 0.0
f1 (ppm)

Parameter	Value
Title	aagch-aean01 Alexander Wagner, AK Mayr 2015-01-29 14:43
Origin	vnmrs
Solvent	CDCl3
Pulse Sequence	s2pul
Acquisition Date	2015-01-29T14:43:05
Temperature	27.0
Spectrometer Frequency	75.46
Nucleus	13C

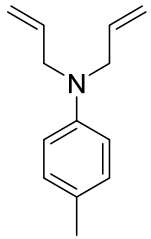


1a

^{13}C NMR, 75.5 MHz, $CDCl_3$


7.26 CDCl3
7.08
7.08
7.08
7.07
7.06
7.05
7.05
7.05
7.05
6.70
6.68
6.67
5.97
5.95
5.93
5.92
5.91
5.90
5.90
5.89
5.88
5.86
5.86
5.84
5.26
5.25
5.21
5.21
5.20
5.20
5.19
5.19
5.18
5.18
5.17
3.95
3.95
3.94
3.94
3.93
2.29
Parameter Value
Title aagch-aepMe01
Alexander Wagner, AK Mayr
2015-01-30 16:46
Origin vnmrs
Solvent CDCl3
Pulse Sequence s2pul
Acquisition Date 2015-01-30T16:46:33
Temperature 27.0
Spectrometer Frequency 300.06
Nucleus 1H
N
1b
1H NMR, 300 MHz, CDCl3
2.05
1.97
2.00
4.27
4.02
3.15
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
0.5
0.0
f1 (ppm)

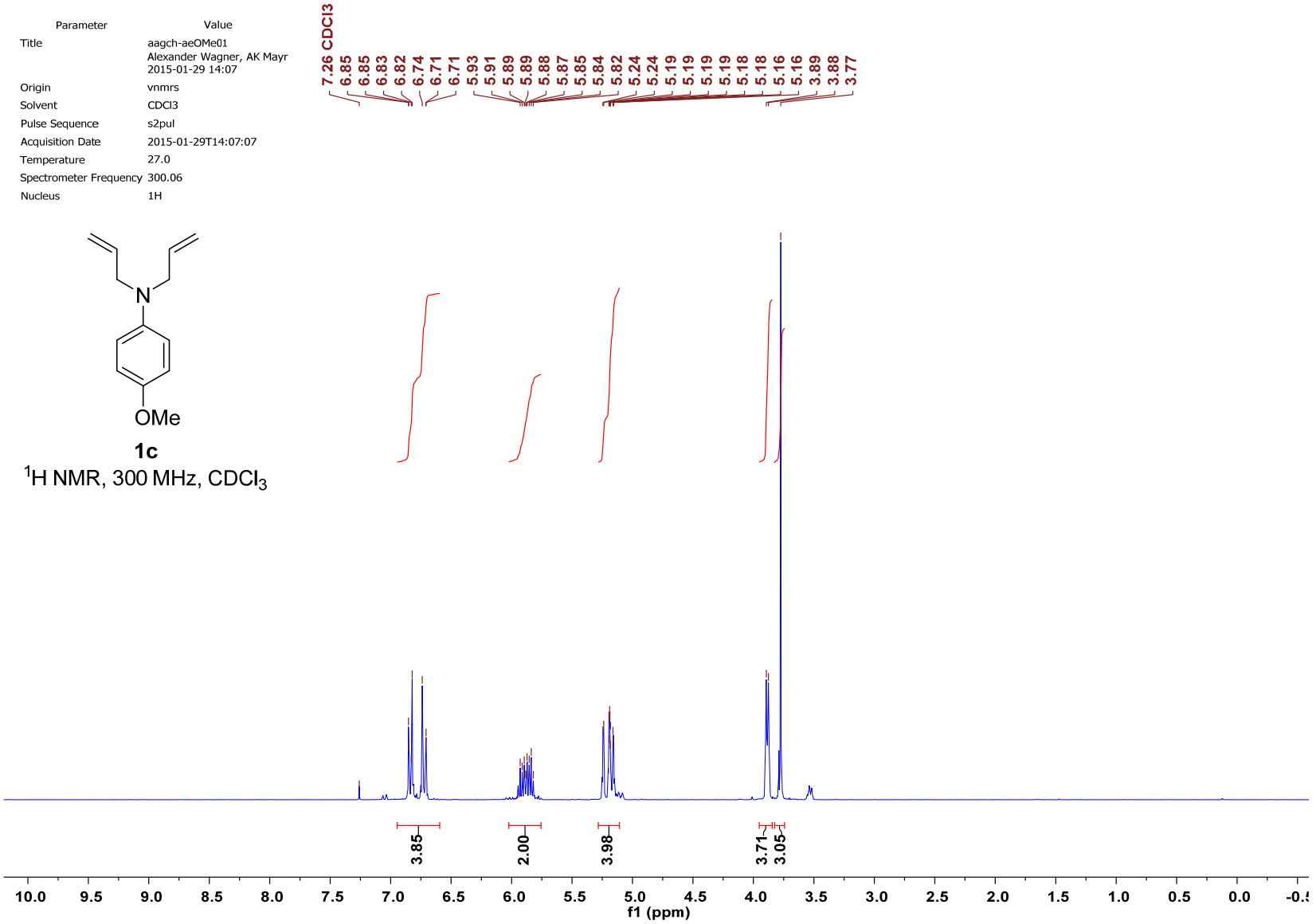
Parameter	Value
Title	aagch-aepMe01 Alexander Wagner, AK Mayr 2015-01-29 13:32
Origin	vnmrs
Solvent	CDCl3
Pulse Sequence	s2pul
Acquisition Date	2015-01-29T13:32:52
Temperature	27.0
Spectrometer Frequency	75.46
Nucleus	13C



1b

^{13}C NMR, 75.5 MHz, $CDCl_3$

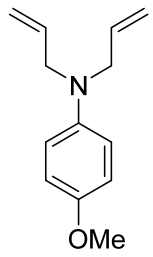
Parameter	Value
Title	aagch-aeOMe01 Alexander Wagner, AK Mayr 2015-01-29 14:07
Origin	vnmrs
Solvent	CDCl3
Pulse Sequence	s2pul
Acquisition Date	2015-01-29T14:07:07
Temperature	27.0
Spectrometer Frequency	300.06
Nucleus	1H



1c

^{1}H NMR, 300 MHz, $CDCl_3$

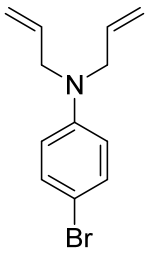
Parameter	Value
Title	aagch-aeOMe01 Alexander Wagner, AK Mayr 2015-01-29 14:07
Origin	vnmrs
Solvent	CDCl3
Pulse Sequence	s2pul
Acquisition Date	2015-01-29T14:07:46
Temperature	27.0
Spectrometer Frequency	75.46
Nucleus	13C



1c

^{13}C NMR, 75.5 MHz, $CDCl_3$

Parameter	Value
Title	aagch-aepBr01 Alexander Wagner, AK Mayr 2015-01-29 12:55
Origin	vnmrs
Solvent	CDCl3
Pulse Sequence	s2pul
Acquisition Date	2015-01-29T12:55:40
Temperature	27.0
Spectrometer Frequency	300.06
Nucleus	1H

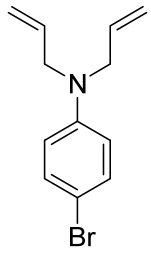


1d

^{1}H NMR, 300 MHz, $CDCl_3$

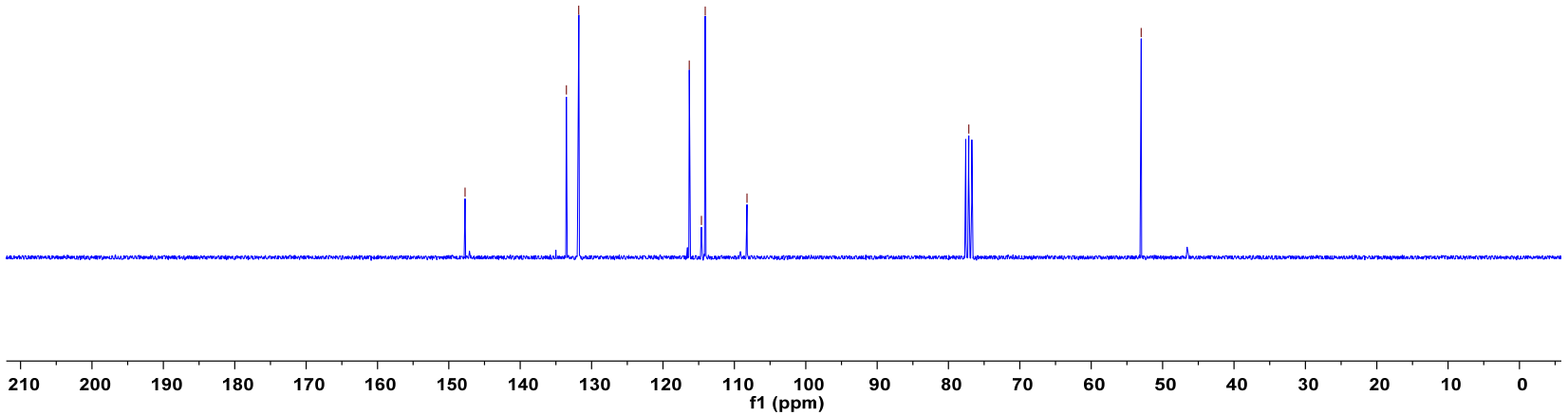
Parameter	Value
Title	aagch-aepBr01 Alexander Wagner, AK Mayr 2015-01-29 12:56
Origin	vnmrs
Solvent	CDCl3
Pulse Sequence	s2pul
Acquisition Date	2015-01-29T12:56:19
Temperature	27.0
Spectrometer Frequency	75.46
Nucleus	13C

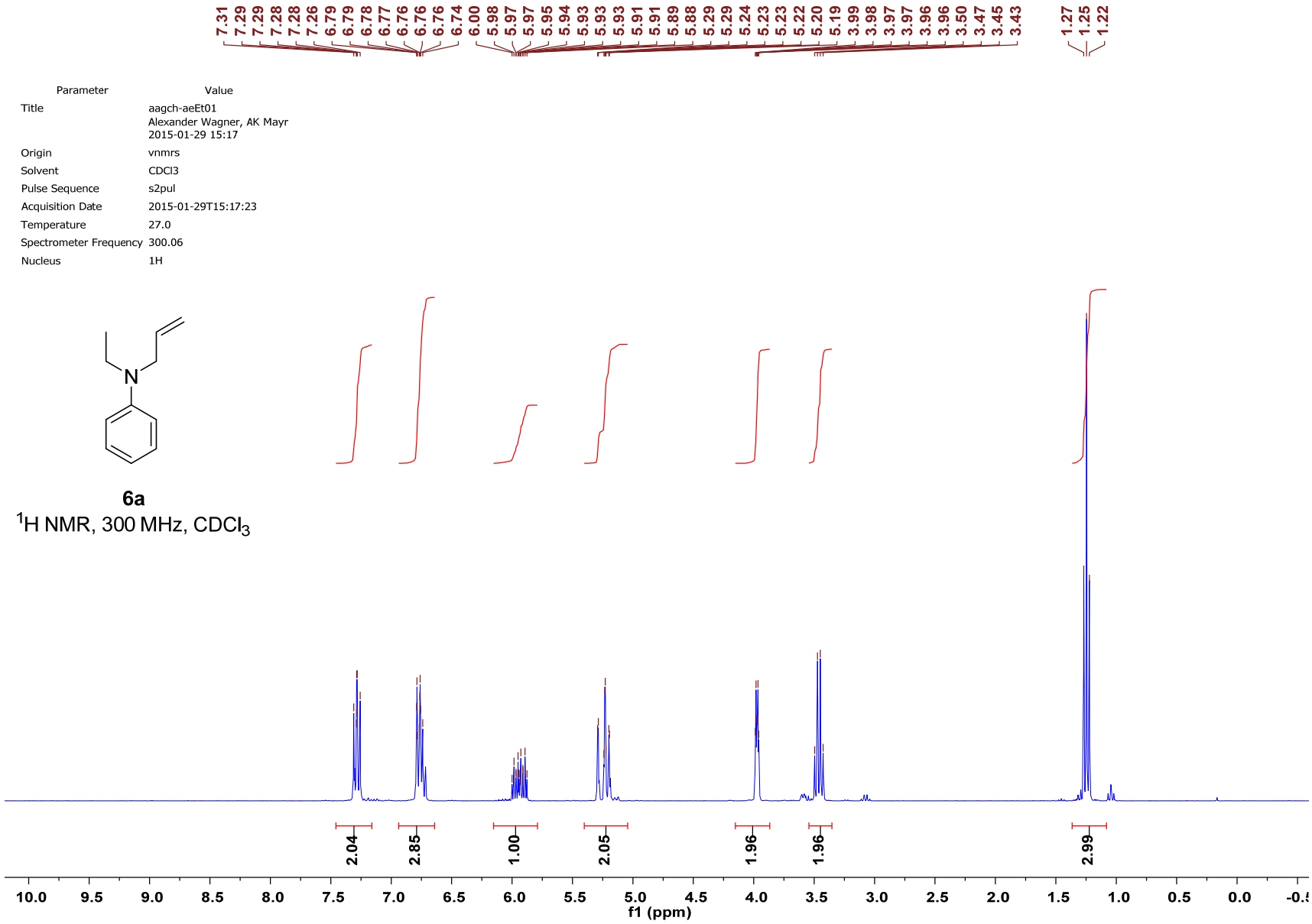
147.74
133.54
131.80
116.31
114.62
114.09
108.22
77.16 CDCl3
53.01



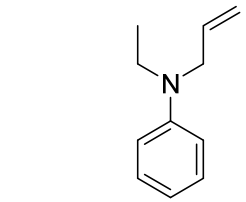
1d

^{13}C NMR, 75.5 MHz, $CDCl_3$



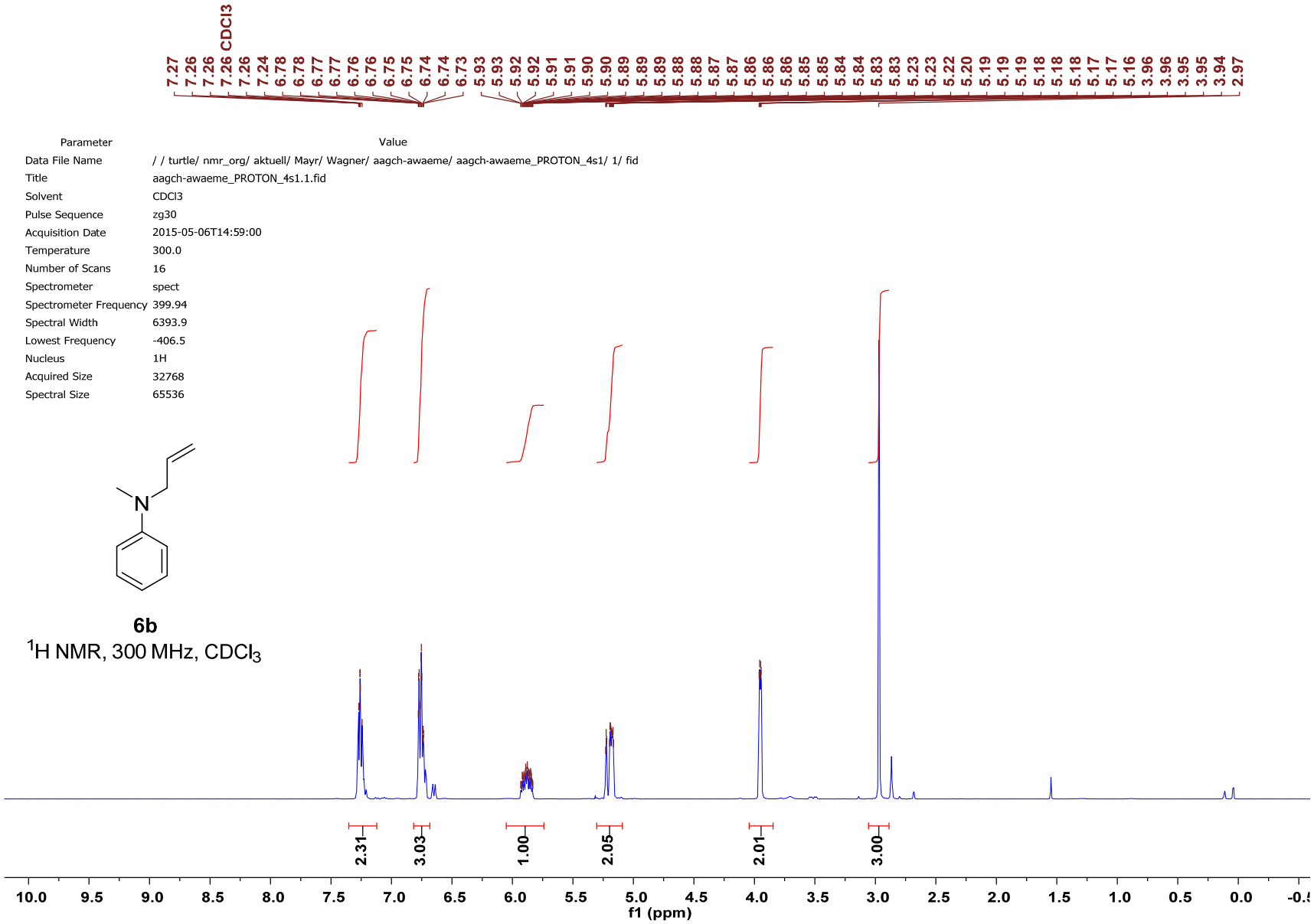

7.31 7.29 7.29 7.28 7.28 7.26 6.79 6.79 6.78 6.77 6.76 6.76 6.76 6.74
6.00 5.98 5.97 5.97 5.95 5.94 5.93 5.93 5.93 5.91 5.91 5.89 5.88 5.29 5.29 5.24 5.23 5.23 5.22 5.20 5.19 3.99 3.98 3.97 3.97 3.96 3.96 3.50 3.47 3.45 3.43
1.27 1.25 1.22
Parameter Value
Title aagch-aeEt01
Alexander Wagner, AK Mayr
2015-01-29 15:17
Origin vnmrs
Solvent CDCl3
Pulse Sequence s2pul
Acquisition Date 2015-01-29T15:17:23
Temperature 27.0
Spectrometer Frequency 300.06
Nucleus 1H
N
6a
1H NMR, 300 MHz, CDCl3
2.04 2.85 1.00 2.05 1.96 1.96 2.99
10.0 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 0.5 0.0
f1 (ppm)

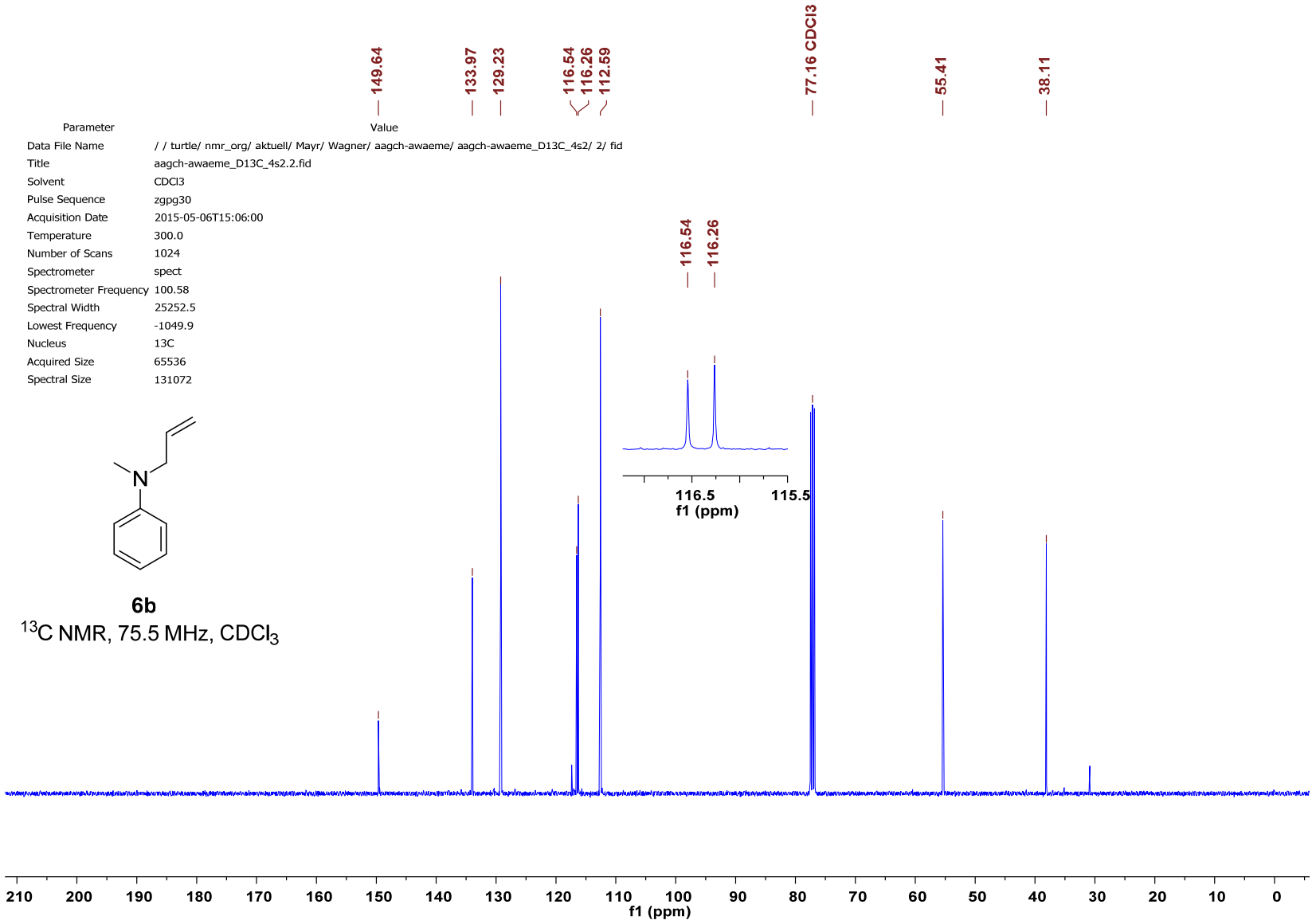
Parameter	Value
Title	aagch-aeEt01 Alexander Wagner, AK Mayr 2015-01-29 15:18
Origin	vnmrs
Solvent	CDCl3
Pulse Sequence	s2pul
Acquisition Date	2015-01-29T15:18:09
Temperature	27.0
Spectrometer Frequency	75.46
Nucleus	13C

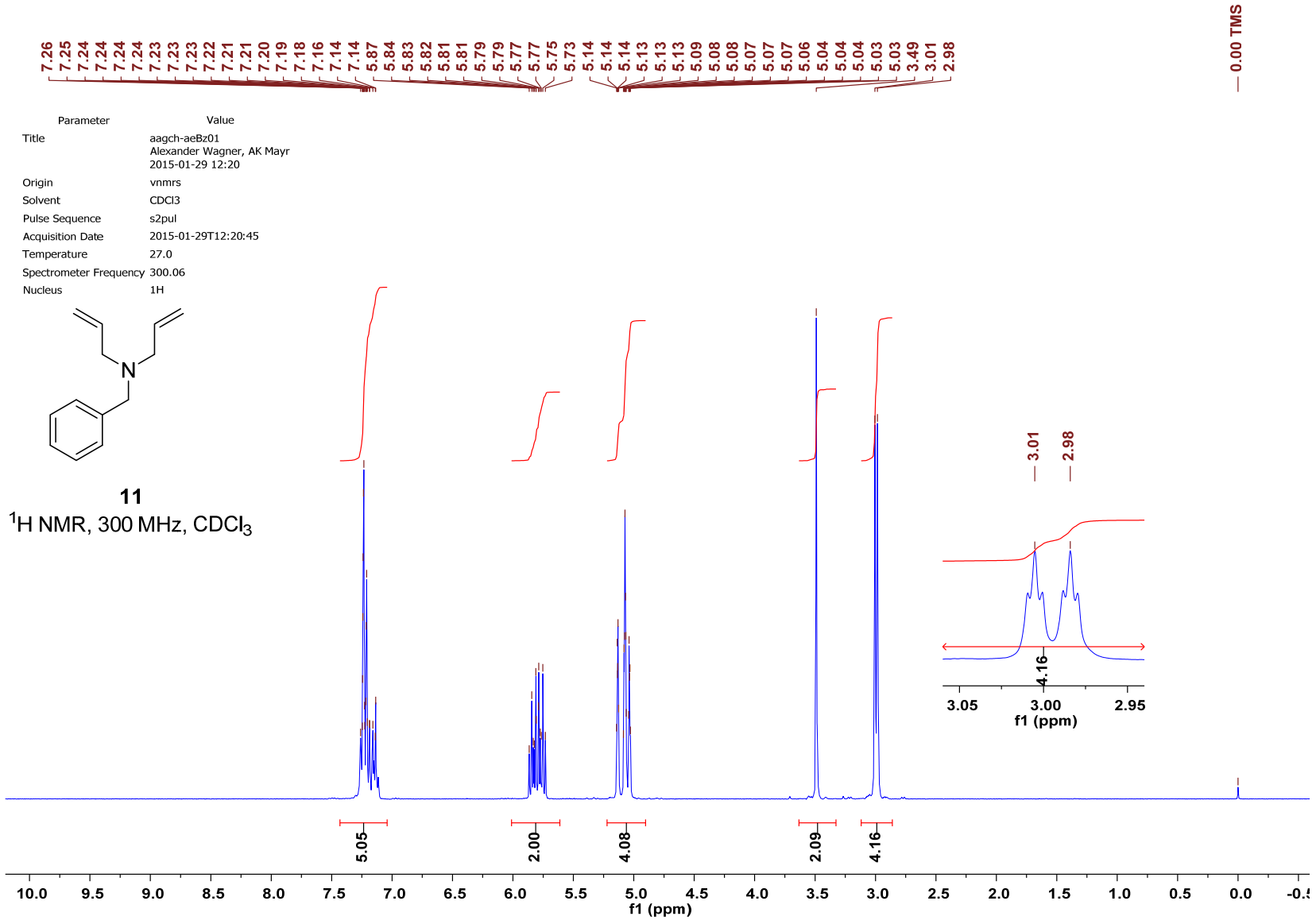


6a

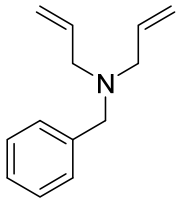
^{13}C NMR, 75.5 MHz, $CDCl_3$


CDCl3
7.27 7.26 7.26 7.26 7.24 6.78 6.78 6.77 6.77 6.76 6.76 6.75 6.75 6.74 6.74 6.73
5.93 5.93 5.92 5.92 5.91 5.91 5.90 5.90 5.89 5.89 5.89 5.88 5.88 5.87 5.87 5.86 5.86 5.86 5.85 5.85 5.84 5.84 5.83 5.83 5.23 5.23 5.22 5.20 5.19 5.19 5.19 5.18 5.18 5.18 5.17 5.17 5.16 3.96 3.96 3.95 3.95 3.94 2.97
Parameter Value
Data File Name / / turtle/ nmr_org/ aktuell/ Mayr/ Wagner/ aagch-awaeme/ aagch-awaeme_PROTON_4s1/ 1/ fid
Title aagch-awaeme_PROTON_4s1.1.fid
Solvent CDCl3
Pulse Sequence zg30
Acquisition Date 2015-05-06T14:59:00
Temperature 300.0
Number of Scans 16
Spectrometer spect
Spectrometer Frequency 399.94
Spectral Width 6393.9
Lowest Frequency -406.5
Nucleus 1H
Acquired Size 32768
Spectral Size 65536
N
6b
1H NMR, 300 MHz, CDCl3
2.31
3.03
1.00
2.05
2.01
3.00
10.0 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 0.5 0.0
f1 (ppm)


149.64
133.97
129.23
116.54
116.26
112.59
77.16 CDCl3
55.41
38.11
Parameter
Value
Data File Name / / turtle/ nmr_org/ aktuell/ Mayr/ Wagner/ aagch-awaeme/ aagch-awaeme_D13C_4s2/ 2/ fid
Title aagch-awaeme_D13C_4s2.2.fid
Solvent CDCl3
Pulse Sequence zgpg30
Acquisition Date 2015-05-06T15:06:00
Temperature 300.0
Number of Scans 1024
Spectrometer spect
Spectrometer Frequency 100.58
Spectral Width 25252.5
Lowest Frequency -1049.9
Nucleus 13C
Acquired Size 65536
Spectral Size 131072
N
6b
13C NMR, 75.5 MHz, CDCl3
116.54
116.26
116.5
115.5
f1 (ppm)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


7.26 7.25 7.24 7.24 7.24 7.24 7.23 7.23 7.23 7.22 7.21 7.21 7.20 7.19 7.18 7.16 7.14 7.14 5.87 5.84 5.83 5.82 5.81 5.81 5.79 5.79 5.77 5.77 5.75 5.73 5.14 5.14 5.14 5.13 5.13 5.13 5.09 5.08 5.08 5.07 5.07 5.07 5.06 5.04 5.04 5.04 5.03 5.03 3.49 3.01 2.98
0.00 TMS
Parameter Value
Title aagch-aeBz01
Alexander Wagner, AK Mayr
2015-01-29 12:20
Origin vnmrs
Solvent CDCl3
Pulse Sequence s2pul
Acquisition Date 2015-01-29T12:20:45
Temperature 27.0
Spectrometer Frequency 300.06
Nucleus 1H
N
11
1H NMR, 300 MHz, CDCl3
3.01
2.98
4.16
3.05 3.00 2.95
f1 (ppm)
5.05
2.00
4.08
2.09
4.16
10.0 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 0.5 0.0
f1 (ppm)

Parameter	Value
Title	aagch-aeBz01 Alexander Wagner, AK Mayr 2015-01-29 12:21
Origin	vnmrs
Solvent	CDCl3
Pulse Sequence	s2pul
Acquisition Date	2015-01-29T12:21:24
Temperature	27.0
Spectrometer Frequency	75.46
Nucleus	13C



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^{13}C NMR, 75.5 MHz, $CDCl_3$