Organic Syntheses

A Publication
of Reliable Methods
for the Preparation
of Organic Compounds

Working with Hazardous Chemicals

The procedures in *Organic Syntheses* are intended for use only by persons with proper training in experimental organic chemistry. All hazardous materials should be handled using the standard procedures for work with chemicals described in references such as "Prudent Practices in the Laboratory" (The National Academies Press, Washington, D.C., 2011; the full text can be accessed free of charge at http://www.nap.edu/catalog.php?record_id=12654). All chemical waste should be disposed of in accordance with local regulations. For general guidelines for the management of chemical waste, see Chapter 8 of Prudent Practices.

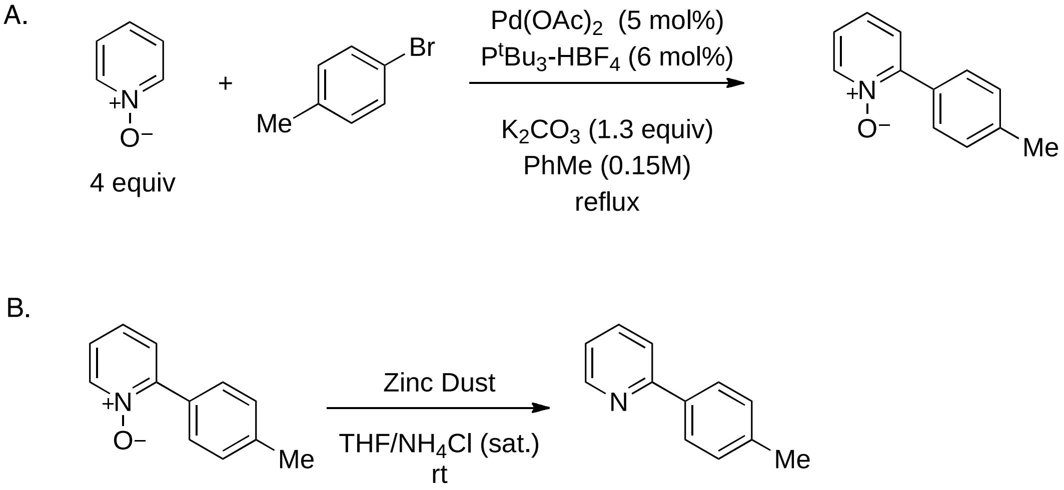
In some articles in *Organic Syntheses*, chemical-specific hazards are highlighted in red “Caution Notes” within a procedure. It is important to recognize that the absence of a caution note does not imply that no significant hazards are associated with the chemicals involved in that procedure. Prior to performing a reaction, a thorough risk assessment should be carried out that includes a review of the potential hazards associated with each chemical and experimental operation on the scale that is planned for the procedure. Guidelines for carrying out a risk assessment and for analyzing the hazards associated with chemicals can be found in Chapter 4 of Prudent Practices.

The procedures described in *Organic Syntheses* are provided as published and are conducted at one's own risk. *Organic Syntheses, Inc.*, its Editors, and its Board of Directors do not warrant or guarantee the safety of individuals using these procedures and hereby disclaim any liability for any injuries or damages claimed to have resulted from or related in any way to the procedures herein.

September 2014: The paragraphs above replace the section “Handling and Disposal of Hazardous Chemicals” in the originally published version of this article. The statements above do not supersede any specific hazard caution notes and safety instructions included in the procedure.

Copyright © 2011 Organic Syntheses, Inc. All Rights Reserved

SYNTHESIS OF 2-ARYL PYRIDINES BY PALLADIUM-CATALYZED DIRECT ARYLATION OF PYRIDINE N-OXIDES



Submitted by Louis-Charles Campeau[1] and Keith Fagnou.[2]
Checked by Adnan Ganić and Andreas Pfaltz.

1. Procedure

A. *2-(4'-Methylphenyl)-pyridine N-oxide.* A 1-L, three-necked round-bottomed flask is equipped with a magnetic stir bar (cylindrical, 4 × 1 cm), two glass stoppers and a reflux condenser with a gas bubbler on the top and connection to the argon line (Note 1). Pd(OAc)_2 (0.560 g, 2.50 mmol, 5 mol%), $\text{P}^t\text{Bu}_3\cdot\text{HBF}_4$ (0.870 g, 3.00 mmol, 6 mol%) (Notes 2, 3), potassium carbonate powder (K_2CO_3, 8.97 g, 65.0 mmol, 1.3 equiv) (Note 4), and pyridine *N*-oxide (19.0 g, 200 mmol, 4 equiv) (Note 5) are weighed in air and placed inside the flask. The whole setup is then evacuated (0.4 mmHg) and refilled with argon four times (Note 6).

A solution of 4-bromotoluene (8.55 g, 50 mmol, 1 equiv) (Note 7) in toluene (300 mL) (Note 8) is added under a steady flow of argon to the reaction mixture, and the glassware is rinsed with degassed toluene (30 mL) (Note 9). The obtained brown-orange suspension is immersed in the oil bath. Stirring (700 rpm) is commenced and the heating source is turned on (set to 125 °C). The mixture starts to reflux after approximately 45 min (Note 10).

Heating and stirring under a steady flow or argon is maintained for 16 h (overnight). The now black reaction mixture is allowed to cool to room temperature and transferred to 1-L round-bottomed flask. The reaction flask is rinsed with toluene (50 mL) (Note 11), and the solvent is removed under reduced pressure (40 °C, 40 mmHg) on a rotary evaporator. A saturated aqueous solution of NH_4Cl (150 mL) and DCM (200 mL) are sequentially added to the dark slurry. The mixture is filtered through a *Celite*® pad (Note 12). The glassware is washed with water (50 mL) and DCM (2 × 50 mL). The resulting yellow biphasic solution is transferred into a 1-L separatory funnel and the layers are separated. The aqueous layer is washed with DCM (2 × 100 mL).The combined organic layers are dried over $MgSO_4$ (4 g) (Note 13), filtered and washed with DCM (2 × 50 mL). The solvent is removed under reduced pressure (40 °C, 500 mmHg). The resulting yellow solid (Note 14) is then dissolved in eluent (20 mL) (Note 15), charged on a column (7 × 8.5 cm) of silica gel (Note 16) and eluted with DCM/acetone/MeOH 90:8:2 mixture (3.5 L). After the first 300 mL of eluent, fraction collection (20-mL fractions) is started. The desired product is obtained from fractions 18-120 as beige solid (6.51 g, 35.1 mmol, 70%) (Note 17).

The solid obtained after column chromatography is placed in a 250-mL round-bottomed flask equipped with a magnetic stir bar (egg shaped, 2 × 1 cm) and a reflux condenser. Heptane (40 mL) and toluene (20 mL) are added, and the suspension is heated to 115 °C (700 rpm). Toluene is added in 5 mL portions through the reflux condenser over 20-30 30 min until a clear solution is obtained (the total volume of toluene used is 40 mL). A gas bubbler is placed on top of the condenser and connected to the argon line. The heating source is turned off and the clear (yellow solution) is allowed to cool down to rt overnight (14 h) under argon, while stirring is maintained. The obtained suspension is cooled down to 0 ºC with the help of an ice bath and stirred for 1 h. The resulting solid is collected by filtration using a 50-mL Büchner funnel under a stream of nitrogen and washed with ice-cold heptane (3 × 20 mL). The obtained solid is transferred to a 100-mL round-bottomed flask and dried overnight (>12 h) at 0.1 mbar to provide the title compound as a white solid (5.98 g, 32.3 mmol, 65%) (Notes 18, 19).

B. 2-(4'-Methylphenyl)-pyridine. A three-necked, 500-mL round-bottomed flask equipped with a condenser, a thermometer, a glass stopper and a magnetic stirrer (egg shaped, 3 × 1.5 cm) (Note 20) is charged with 2-(4'-methylphenyl)-pyridine *N*-oxide (5.98 g, 32.3 mmol, 1 equiv). Tetrahydrofuran (120 mL) (Note 21) is added, followed by saturated aqueous NH_4Cl solution (120 mL). This addition caused a slight increase of the reaction temperature from 22 °C up to 28 °C, and a white solid is formed in the aqueous layer. Zinc dust (Note 22) is added in 4 portions (10.6 g, 161 mmol, 5 equiv) within 10 min under stirring (700 rpm) to this biphasic mixture. Again, an increase of the reaction temperature from 25 ºC up to 38 ºC over a period of 15 min is observed. The reaction mixture is stirred for 20 min until TLC analysis reveals complete consumption of the starting material (Note 23). The mixture is filtered through a *Celite*® pad (Note 25) and is washed with MTBE (250 mL). The filtrate is transferred to a 1-L separatory funnel, and the layers are separated. The aqueous layer is back-extracted with MTBE (125 mL) using a second 250-mL separatory funnel. The organic layers are consecutively washed with half-saturated aqueous $NaHCO_3$ solution (125 mL) and with brine (125 mL). The combined organic layers are then dried over $MgSO_4$ (3 g), filtered and concentrated (40 °C, 250 mmHg) to afford the title compound as yellow liquid (5.47 g, 32.3 mmol, 100%). Purification by Kugelrohr distillation (150 °C, 0.3 mmHg) gives the title compound as a colorless liquid (5.35 g, 31.6 mmol, 98%) (Notes 25, 26).

2. Notes

1. Submitters setup: a 1-L pear-shaped flask is fitted with a Teflon sleeve and a cylindrical (4 × 1 cm) stir bar with a condenser.
2. Palladium (II) acetate (46-1780) and phosphonium salt (15-6000) were purchased from *Strem* and used without any purification.
3. By using 10 mol% of the phosphonium salt the checkers did not observe any increase in yield (70%).
4. Purchased from *Aldrich* (347825) and used as is.
5. Purchased from *Aldrich* (131652), particles greater than 1 cm^3 are crushed using a mortar. Pyridine *N*-oxide is a highly deliquescent solid,[3] and an undetermined amount of water is incorporated into the reaction mixture. The influence of water on the reaction was studied by the submitters. It is reported that the reaction occurs even when 5 equiv of water are added to the reaction mixture without affecting the yield.[4] An excess of this reagent is used to increase the yield of the reaction. The identical procedure can be performed with 1.5 equiv of pyridine *N*-oxide resulting in yields ranging from 65-70% (checkers: 58%). During the extraction protocol the excess *N*-oxide can be recovered from the aqueous phase by evaporation of water and chromatography of the residue with 10% MeOH in DCM.

6. The submitters used a rubber septum on the top of the condenser, which allows connection to the vacuum line. The submitters added argon from a balloon. The checkers used argon from an argon line.

7. Purchased from *Aldrich* (B82200). 4-Bromotoluene is a low melting solid (mp 30 °C*)*. The submitters reported that it was stored in the freezer before use to facilitate its weighing as a solid. Alternatively, one could add it as a stock solution in toluene or as a liquid if heated. If it is added as a stock solution or a liquid, it should be added with the solvent. The checkers melted it using a water bath (40 °C) and weighed it as a liquid.

8. The submitters used certified A.C.S. Grade toluene purchased from *Fisher Scientific* (T324) and degassed it with argon (10 min) before use. The checkers used *J. T. Baker* (Baker analyzed) toluene and degassed the solution by bubbling argon for 15 min prior to its use.

9. Submitters reaction setup: Toluene (330 mL) is added in 50 mL portions under a steady flow of argon. After addition of the first 50 mL, the reaction is immersed in the oil bath. Stirring (400 rpm) is commenced and the heating source is turned on (set to 125 ºC). After the remaining toluene has been added the reaction is kept under an argon atmosphere and the stirring speed is raised to 700 rpm.

10. The submitters report that the mixture starts to reflux after approximately 20 min and the color of the mixture pales to off-white after 30-40 min, which was not observed by the checkers. The reaction mixture remains heterogeneous, but slowly turns from brown-orange into a dark suspension.

11. Not all material is dissolved in toluene, and therefore the reaction flask is rinsed with DCM and sat. aq. NH_4Cl solution, which is added to the dark slurry.

12. *Celite*® (10 g) is weighed dry and packed using DCM (50 mL) in a 75-mL coarse fritted Büchner funnel. 20 g of sand is added to the top of the *Celite*® layer.

13. The submitters used 15 g of $MgSO_4$.

14. In some cases a yellow oil is obtained which can be reduced to a yellow solid under high vacuum or longer time on rotary evaporator.

15. The submitters used 20-35 mL of eluent for dissolving the material and report that sonication or heating with heat gun was necessary to fully dissolve the solid. The checkers dissolved the solid in 20 mL of eluent by stirring on a rotary evaporator without additional heating.

16. The submitters used 175 g of *Silicycle* (R10030B) silica gel on a 8.5 cm diameter column. 200 mL is collected in an Erlenmeyer flask followed by 15-mL fractions. The majority of the product was obtained from fractions 20-48. The product tailed off past fraction 55 but resulted only in a 2% increase in yield when collected. The checkers used silica gel (175 g) from *Fluka* (89943) and a sand (50 g) layer on the top. The fractions between 121-160 contained product that was contaminated with unreacted starting material.

17. The submitters report yields ranging from 79-83% (>97% purity by HPLC; contamination with <1% of tri-*tert*-butylphosphine oxide; mp 129–131 °C). This material was usually carried through to further transformations, although analytically pure material could be obtained by recrystallization. Submitters HPLC conditions: Zorbax SB C18, RRHT, 1.8 micron (50 × 4.6 mm) 0.1% H_3PO_4 in water / MeCN start 90:10, ramp to 50:50 over 8 min, ramp to 5:95 over 4 min. Total: 12 min, 2 mL/min, 35 ºC, 215 nm, 5 uL. Retention times: Free base: 1.699 min, *N*-oxide: 3.250 min. The checkers obtained yields in the 68-70% range (99% purity by HPLC; mp 141–143 °C). Checkers HPLC conditions: Reprosil 100 C18, 3 micron (125 × 3 mm), 0.1% H_3PO_4 in water/MeCN start 80:20, ramp to 50:50 over 15 min, ramp to 15:85 over 15 min, total: 30 min, 0.5 mL/min, 35 ºC, 254 nm, 1 mg/mL, 5 μL; retention time: 7.50 min.

18. The checkers obtained yields after recrystallization in the 62-65% range (>99% purity by HPLC). Analytical data: mp 144–145 °C (lit.[5] mp 145–146 °C; TLC (SiO_2, DCM/Acetone/MeOH 90:8:2): $R_f = 0.19$; ^1H NMR (400 MHz, $CDCl_3$) δ: 2.41 (s, 3 H), 7.14–7.23 (m, 1 H), 7.24–7.32 (m, 3 H), 7.41 (dd, *J* = 7.8, 1.7 Hz, 1 H), 7.72 (d, *J* = 6.6 Hz, 2 H), 8.32 (d, *J* = 6.4 Hz, 1 H); ^{13}C NMR (101 MHz, $CDCl_3$) δ: 21.6, 124.3, 125.7, 127.3, 129.1, 129.3, 129.8, 139.9, 139.9, 140.7; IR (ATR) $\tilde{\nu}$: 3064, 3043, 1478, 1430, 1403, 1328, 1237, 1186, 1144, 1110, 1028, 1011, 948, 842, 817, 798, 735, 713, 694, 573, 526 cm^{-1}; MS (EI, 70 eV, 150 °C) *m/z* (%): 185 (M^+, 63), 184 ($M-H^+$, 100), 169 (10), 156 (13), 117 (25), 78 (12); Anal. calcd. for $C_{12}H_{11}NO$: C, 77.81; H, 5.99; N, 7.56; found: C, 77.92; H, 6.22; N, 7.53.

19. Submitters' recrystallization conditions: *N*-oxide was suspended in 6 mL/g of heptane in a three-necked flask fitted with a reflux condenser and a mechanical stirrer. The suspension is heated to 95 °C in an oil bath and toluene is added (in 1 mL/g portions) until all solids dissolve (typically ~6 mL/g). The heat source on the oil bath is turned off and mixture is allowed to cool in the oil bath overnight. In the morning, the suspension is

immersed in an ice bath for 30 min and then filtered on a fritted Büchner funnel. The solid collected is then washed with 10 mL/g of heptane, and the solid is dried under a stream of N_2 and collected as a fluffy white solid which is >99% pure (Note 17). Recovery for this procedure is typically from 88-95%.

20. The Submitters used a mechanical stirrer.

21. The submitters used ACS Grade THF with BHT over sieves from *A&C*, which is used as is. The checkers use *J. T. Baker* (Baker analyzed) material.

22. Both submitters and checkers purchased zinc dust from *Aldrich* (20,998-8) and used as received.

23. The submitters stirred the reaction mixture for 40 min, and the reaction progress was checked by HPLC analysis. The checkers used TLC analysis (SiO_2, DCM/acetone/MeOH 90:8:2; R_f 0.87) to monitor the reaction progress.

24. The submitters used *Solka floc*®. They weighed Solka floc dry (15 g) and packed it using MTBE in a 60-mL coarse fritted Büchner funnel. The checkers used *Celite*® (10 g), which was weighed dry and packed using MTBE in a 75-mL coarse fritted Büchner funnel, adding 10 g of sand to the top of the *Celite*® layer.

25. HPLC analysis shows >99% purity (for conditions, see Note 18; retention time 4.19 min). Analytical data: ^{1}H NMR (400 MHz, $CDCl_3$) δ: 2.41 (s, 3 H), 7.20 (ddd, *J* = 6.6, 4.8, 2.1 Hz, 1 H), 7.29 (d, *J* = 7.9 Hz, 2 H), 7.64–7.78 (m, 2 H), 7.86–7.93 (m, 2 H), 8.65–8.71 (m, 1 H); ^{13}C NMR (101 MHz, $CDCl_3$) δ: 22.4, 120.4, 121.9, 126.9, 129.6, 136.7, 136.8, 139.1, 149.8, 157.6; IR (ATR) $\tilde{\upsilon}$: 3006, 2918, 1613, 1586, 1562, 1514, 1464, 1432, 1298, 1185, 1152, 1016, 829, 772, 741, 566, 529 cm^{-1}; MS (EI, 70 eV, rt) *m*/*z* (%): 169 (M^+, 100), 168 (49), 167 (16); Anal. calcd. for $C_{12}H_{11}N$: C, 85.17; H, 6.55; N, 8.28, found: C, 85.13; H, 6.84; N, 8.15.

26. In the submitters' procedure the product was not purified by distillation. It was stated that the isolated product was >98% pure (HPLC and exhibited identical spectral data as a commercial sample available from *Aldrich* (98870). Storing of the obtained material is recommended under inert atmosphere, because the obtained product turns yellow under air at rt.

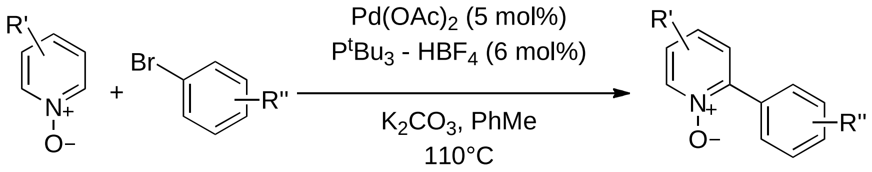
Waste Disposal Information

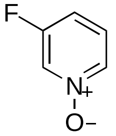
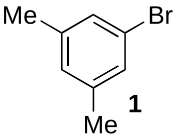
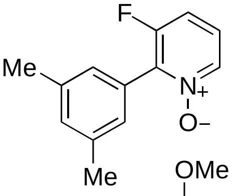
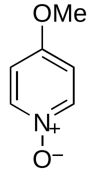
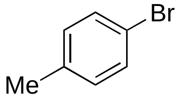
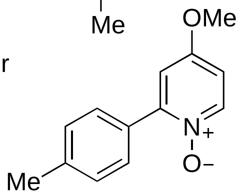
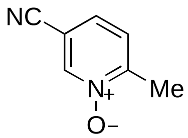
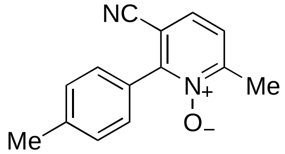
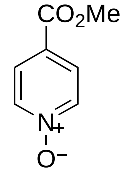
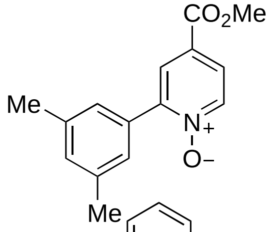
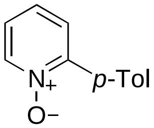
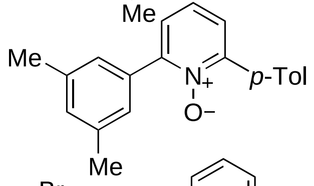
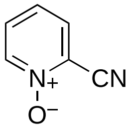
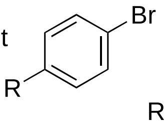
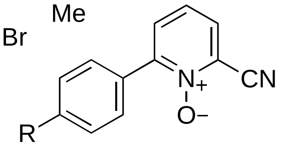
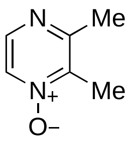
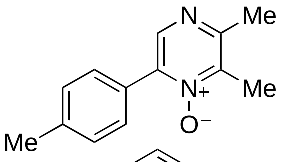
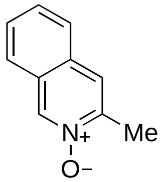
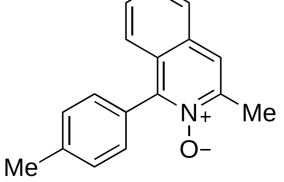
All hazardous materials should be handled and disposed of in accordance with “Prudent Practices in the Laboratory”; National Academy Press; Washington, DC, 1995

3. Discussion

The limited number of successful metal-catalyzed cross-coupling protocols using 2-metallapyridines has fueled the investigations of methods that do not require their use.[6] One strategy is to use direct arylation methodology, where a simple arene replaces the organometallic component.[7] In 2005, we reported that pyridine *N*-oxide was a good substitute for 2-metallapyridine in cross-coupling reactions.[4,8] The 2-aryl pyridine *N*-oxide products can easily be converted to the corresponding 2-aryl pyridines under mild conditions and in high yield.[9] This protocol therefore allows for the rapid and easy synthesis of 2-aryl pyridines. More recently a full account describing optimized reaction conditions and reaction scope was reported.[10] The reaction tolerates a broad range of substitution patterns on both coupling partners. Substitution in the *ortho*, *meta* and *para* position is well tolerated for alkyl and both electron-donating and electron-withdrawing substituents. The pyridyl moiety can be substituted at the 2-, 3- or 4-position allowing for a broad range of potential products. The reaction also proceeds with other azines such as isoquinoline and pyrazine. The procedure is convenient and makes use of cheap, readily available and air stable reagents. No precautions in the storage or the purification of the starting materials were taken. The 2-aryl pyridines obtained via this procedure are found in a number of biologically active compounds and are of value as organic synthesis building blocks. Furthermore, the *N*-oxide moiety can serve as a useful handle in further elaboration of the pyridine core.

Table 1. Direct Arylation of Azine *N*-Oxides



Entry	*N*-Oxide	Aryl Halide	Product	Yield[b]
1		 **1**		78*d*
2		 **2**		80
3		**2**		74
4		**1**		97
5		**1**		74
6		$R=CO_2Et$ 		81[c]
7		R=OMe		81[c]
8		**2**		89
9		**2**		90[d]

[a]Conditions: Aryl halide (1 equiv), pyridine *N*-oxide (2-4 equiv), K_2CO_3 (2 equiv), $Pd(OAc)_2$ (0.05 equiv) and P^tBu_3 - HBF_4 (0.06 equiv) in toluene (0.15M) at 110 °C overnight. [b]Isolated yields. [c]With 4 equiv of *N*-oxide and 15 mol% P^tBu_3 - HBF_4. [d]With 1.1 equiv of *N*-oxide.

1. Current address: Department of Process Research and Development, Merck Frosst Canada, 16711 Trans Canada Hwy, Kirkland, Quebec, H9H 3L1.
2. Department of Chemistry, University of Ottawa, 10 Marie Curie, Ottawa, Ontario, K1N 5N6.
3. Mosher H. S.; Turner L. Carlsmith A. *Org. Synth.* **1953**, *33*, 79–81; *Org. Synth. Coll. Vol.* **1963**, *4*, 828–830.
4. Campeau, L.-C.; Rousseaux, S.; Fagnou, K. *J. Am. Chem. Soc.* **2005**, *127*, 18020–18021.
5. Butler D. E.; Bass P.; Nordin I. C.; Hauck, Jr. F. P.; L'Italien Y. J. *J. Med. Chem.* **1971**, *14*, 575–579.
6. Campeau, L.-C.; Fagnou, K. *Chem. Soc. Rev.* **2007**, *36*, 1058–1068.
7. For recent reviews, see: (a) Alberico, D.; Scott M. E.; Lautens, M. *Chem. Rev.* **2007**, *107*, 174–238. (b) Campeau, L.-C.; Fagnou, K. *Chem. Commun.* **2006**, 1253–1264. (c) Campeau, L.-C.; Stuart, D.R.; Fagnou, K. *Aldrich. Chim. Acta.* **2007**, *40*, 35–41. (d) Zhao, D.; Wang, W.; Yang, F.; Lan, J.; Yang, L.; Gao, G.; You, J. *Angew. Chem. Int. Ed.* **2009**, *48*, 3296–3300.
8. ***!!Caution!!:*** Pyridine *N*-oxides have been shown to exothermically decompose at very high temperature. Uncontrolled heating of the reaction media should be avoided. DSC analysis of this particular 2-arylpyridine *N*-oxide as well as others have revealed no exotherms at temperature up to 250 °C. Examples of exothermic onset temperatures (*T*o) for pyridine *N*-oxide, 288 °C; 2,6-lutidine *N*-oxide, 288 °C; nicotinic acid *N*-oxide, 302 °C; picoline *N*-oxide, 285 °C; picolinic acid *N*-oxide, 307 °C, from: Ando, T.; Fujimoto, Y.; Morisaki, S. *J. Haz. Mater.* **1991**, *28*, 251–280.
9. (a) Pd/C: Balicki, R. *Synthesis* **1989**, 645–646. (b) Zinc: Aoyagi, Y.; Abe, T.; Ohta, A. *Synthesis* **1997**, 891–894.
10. Campeau, L.-C; Stuart, D. R.; Leclerc, J.-P.; Bertrand-Laperle, M.; Villemeure, E.; Sun, H.-Y; Guimond, N.; Lasserre, S.; Lecavellier, M.; Fagnou, K. *J. Am. Chem. Soc.* **2009**, *131*, 3291–3306.

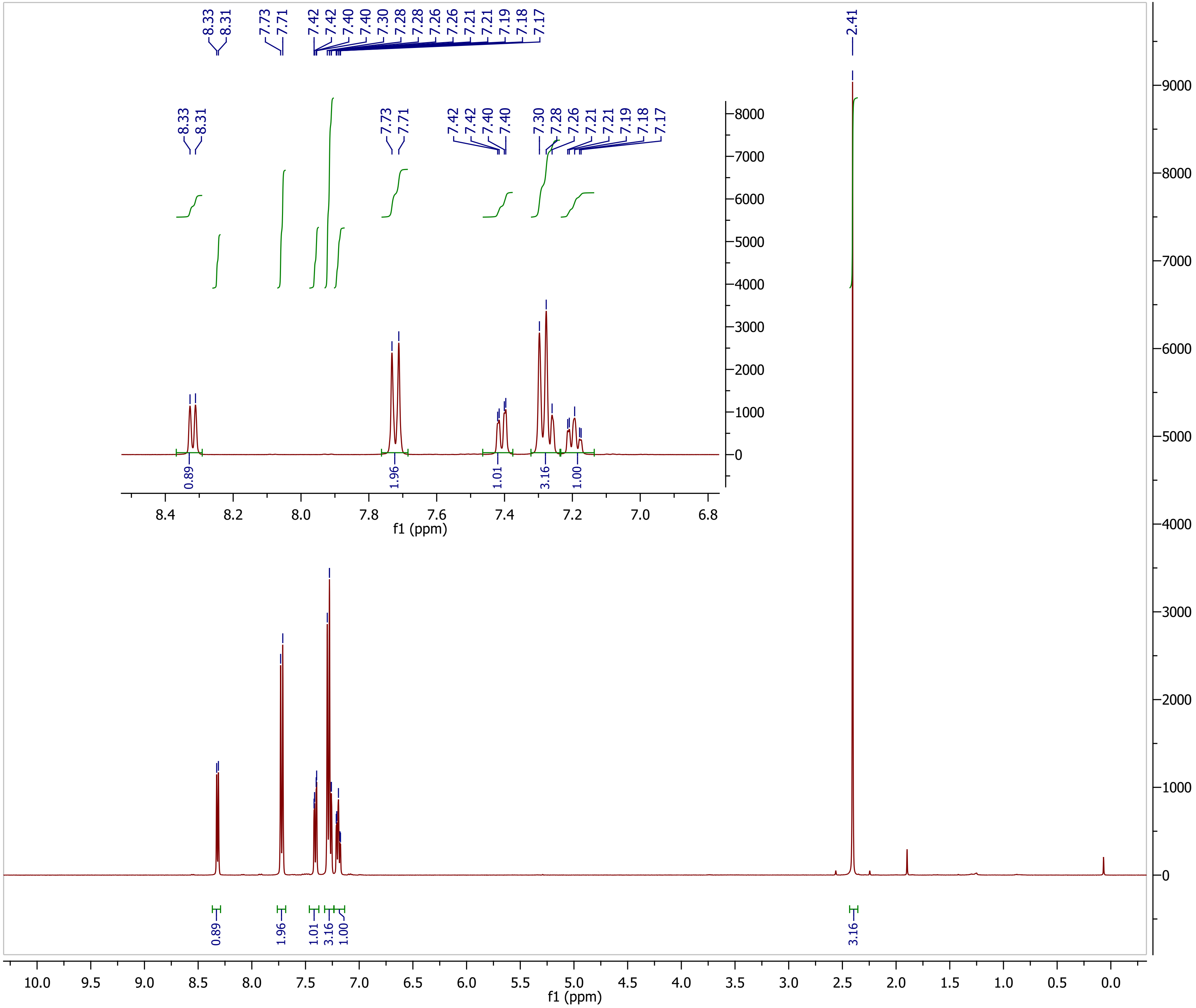
Appendix
Chemical Abstracts Nomenclature; (Registry Number)

Palladium acetate: $Pd(OAc)_2$; (3375-31-3)
$P^tBu_3 \cdot HBF_4$: Phosphine, tris(1,1-dimethylethyl)-, tetrafluoroborate(1-) (1:1); (155026-77-0)
Pyridine *N*-oxide: Pyridine, 1-oxide; (694-59-7)
4-Bromotoluene: Benzene, 1-bromo-4-methyl-: (106-38-7)
Potassium carbonate; (584-08-7)
Zinc; (7440-66-6)
2-(4’-Methylphenyl)-pyridine; (4467-06-5)

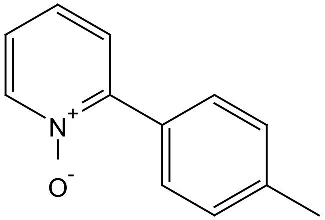
Keith Fagnou was born in 1971 in Saskatoon, Saskatchewan, Canada. He received a Bachelor of education (B.Ed.) degree with distinction from the University of Saskatchewan in 1995 and, after teaching at the high school level for a short period of time, he continued his studies in chemistry at the University of Toronto. In 2000, he received an M.Sc. degree and, in 2002, completed his Ph.D. requirements under the supervision of Mark Lautens. He then joined the chemistry faculty at the University of Ottawa, and had initiated research programs focusing on the development of new catalytic reactions for use in organic synthesis. Most recently, he was awarded the OMCOS Award, as well as the Rutherford Memorial Medal, for outstanding research contributions to the field. Keith Fagnou passed away suddenly after a short illness in November 2009.

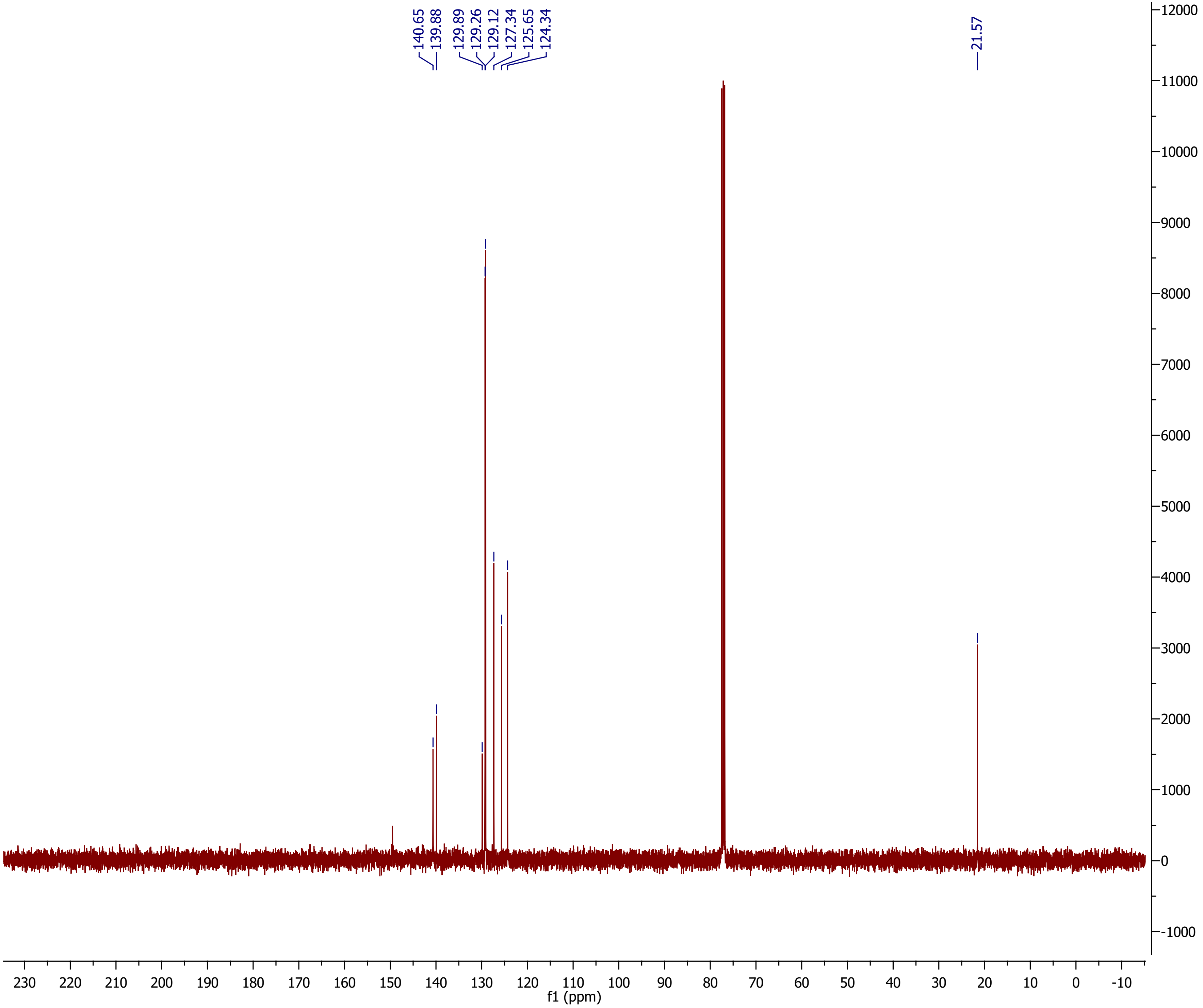
Louis-Charles Campeau was born in 1980 in Cornwall, Ontario, Canada. In 2003, he received his bachelor’s degree with distinction in biopharmaceutical sciences (medicinal chemistry option) from the University of Ottawa. He then joined the research group of Professor Keith Fagnou, where his Ph.D. research was directed towards the development of new transition-metal-catalyzed processes. Louis-Charles received the University's Pierre Laberge Thesis Prize for the Sciences. In the summer of 2007, he joined the process research group at Merck in Montreal. He then moved to Merck in Rahway NJ, in 2010.

Adnan Ganić was born in Travnik (Bosnia and Herzegovina) in 1980 and moved with his family to Switzerland in 1992. Fascinated by the world of chemistry during his apprenticeship in the F. Hoffmann-La Roche company he decided to study chemistry at University of Applied Science (Fachhochschule beider Basel) in Basel. After a half year industry internship again working for F. Hoffmann-La Roche Adnan continued his studies at the University of Basel. During this time he joined the group of Prof. Andreas Pfaltz, where he started his Ph.D. studies in March of 2008. His research interests include the development of new P,N-ligands for iridium catalyzed asymmetric hydrogenation and application of new substrates.

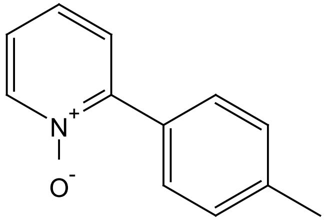


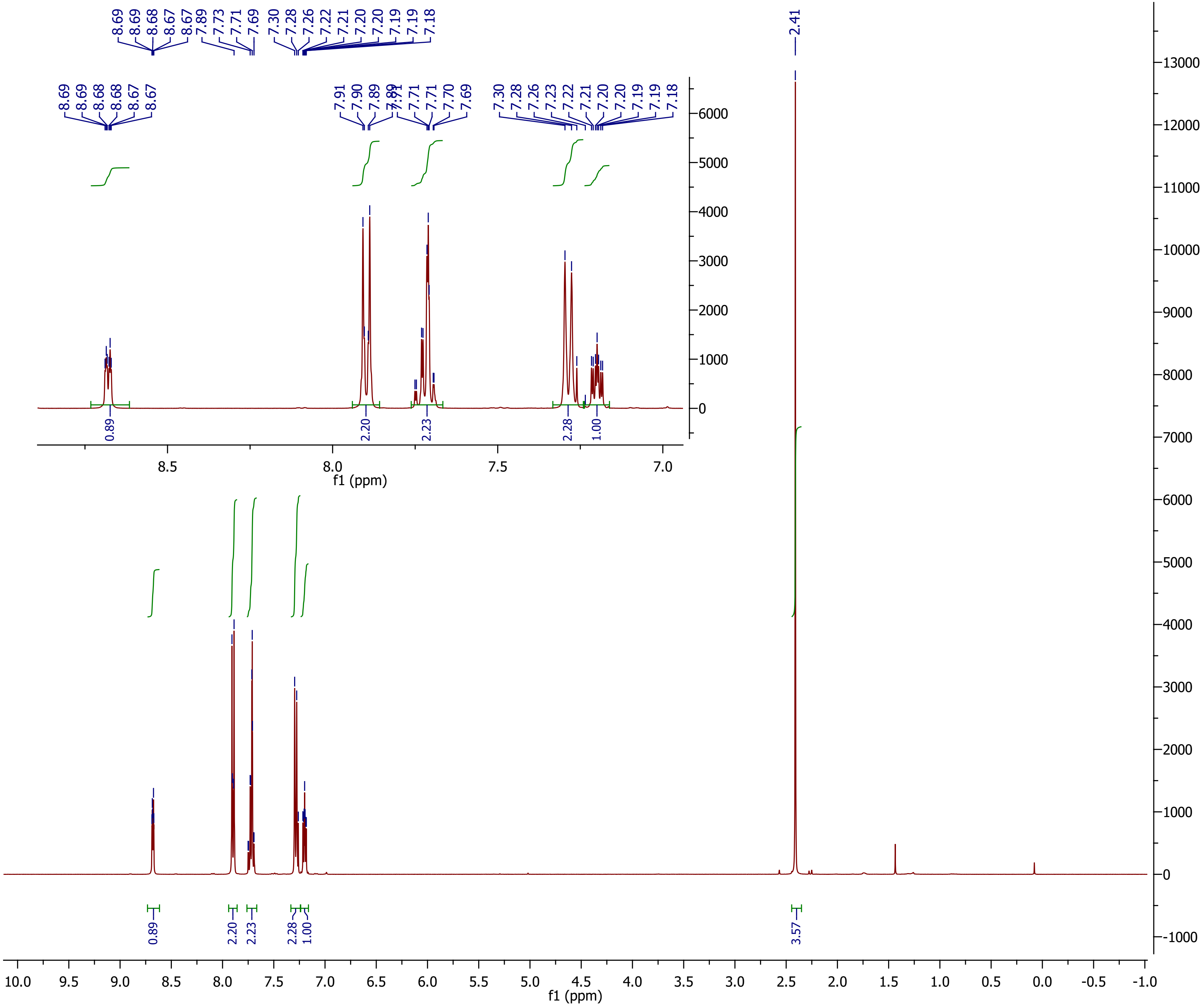
	Parameter	Value
1	Data File Name	D:/ UniBas/ Dissertation/ Projekte/ OrgSyn/ AG-OS-1-7/ adnanI.213/ 4/ fid
2	Title	adnanI.213
3	Solvent	CDCl3
4	Temperature	300.0
5	Number of Scans	16
6	Spectrometer Frequency	400.13
7	Nucleus	1H





Parameter	Value
1 Data File Name	D:/ UniBas/ Dissertation/ Projekte/ OrgSyn/ AG-OS-1-7/ adnanI.213/ 2/ fid
2 Title	adnanI.213
3 Solvent	CDCl3
4 Temperature	300.0
5 Number of Scans	384
6 Spectrometer Frequency	100.61
7 Nucleus	13C





Parameter	Value
1 Data File Name	D:/ UniBas/ Dissertation/ Projekte/ OrgSyn/ AG-OS-2-7/ adnanI.215/ 1/ fid
2 Title	adnanI.215
3 Solvent	CDCl3
4 Temperature	300.0
5 Number of Scans	16
6 Spectrometer Frequency	400.13
7 Nucleus	1H