Suzuki-Miyaura Cross-Coupling of Benzylic Phosphates with Arylboronic Acids

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Supporting Information

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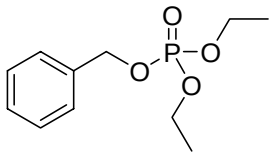
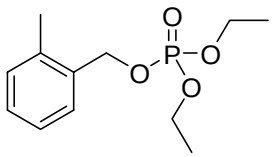
General considerations: All reactions were conducted under a nitrogen atmosphere in 8 mL vials equipped with magnetic stir-bars and septa. HPLC grade solvents were used with no additional purification/drying. NMR spectra were recorded using a Bruker DPX-400 spectrometer; ^{1}H NMR recorded at 400 MHz and ^{13}C recorded at 100 MHz. TLC was performed using 2.5 cm × 7.5 cm EMD glass-backed plates (silica gel 60, F_{254}, 250 μm thickness). Flash column chromatography was performed using EMD silica gel 60, 230-400 mesh. HPLC was performed on an Agilent 1100 Series machine using an Agilent Zorbax (Eclipse XDB C8) column (4.6 mm × 150 mm), 1 mL/min flowrate, 210 nm detection, 30 °C column temperature; mobile phase MeCN/0.1% aq. H_3PO_4 20/80 to 85/15 over 20 min then 85/15 for a further 2 min.

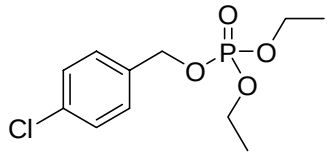
General procedure for the preparation of benzylic phosphates: To a flask charged with the requisite benzyl alcohol (20.0 mmol), triethylamine (4.18 mL, 30.0 mmol, 150 mol%), DMAP (244 mg, 2.0 mmol, 10 mol%) and THF (5 mL) was added neat diethyl chlorophosphate (2.88 mL, 20.0 mmol, 100 mol%) over a 30 min period at room temperature. An exotherm was observed, generally raising the internal temperature to 30-35 °C. The resultant white, heterogeneous mixture was stirred for 16 h before it was poured into a mixture of 2 M $KHSO_4$ (20 mL) and water (30 mL). The separated organic phase was then washed with satd. aq. $NaHCO_3$ (30 mL) and brine (30 mL), before it was dried over $MgSO_4$, filtered and concentrated to leave a crude oil. The crude oil was purified over a short pad of silica using appropriate mixtures of EtOAc/hexane (determined by TLC analysis) to elute any unreacted benzyl alcohol followed by the desired benzylic phosphate.



Diethyl benzyl phosphate (1)[1]**:** Following the general procedure, **1** was obtained as a pale yellow oil (4.45 g, 91%): ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.32 (t, J = 7.1 Hz, 6H), 4.03-4.14 (m, 4H), 5.07 (d, J = 8.1 Hz, 2H), 7.32-7.43 (m, 5H); ^{13}C {^{1}H} NMR (100 MHz, $CDCl_3$) δ 16.1 (d, J_{CP} = 10.1 Hz), 63.8 (d, J_{CP} = 10.0 Hz), 69.0 (d, J_{CP} = 10.0 Hz), 127.8, 128.4, 128.5, 136.1 (d, J_{CP} = 10.0 Hz).

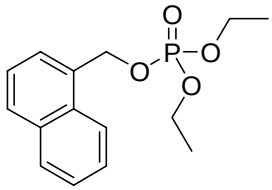


Diethyl 2-methylbenzyl phosphate (18)[2]**:** Following the general procedure, **18** was obtained as a pale yellow oil (4.39 g, 85%): ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.29 (t, J = 7.1 Hz, 6H), 2.37 (s, 3H), 4.01-4.12 (m, 4H), 5.08 (d, J = 7.4 Hz), 7.14-7.28 (m, 3H), 7.37 (d, J = 7.0 Hz, 1H); ^{13}C {^{1}H} NMR (100 MHz, $CDCl_3$) δ 16.1 (d, J_{CP} = 7.0 Hz), 18.8, 63.8 (d, J_{CP} = 6.0 Hz), 67.5 (d, J_{CP} = 5.0 Hz), 126.1, 128.8, 128.9, 130.4, 134.1 (d, J_{CP} = 7.0 Hz), 136.8.

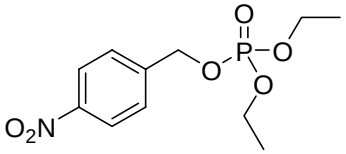


Diethyl 4-chlorobenzyl phosphate (19)[3]**:** Following the general procedure, **19** was obtained as a pale yellow oil (4.97 g, 89%): ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.31 (t, J = 7.1 Hz, 6H), 4.03-4.15 (m, 4H), 5.02 (d, J = 8.3 Hz, 2H), 7.30-7.38 (m, 4H); ^{13}C {^{1}H} NMR (100 MHz, $CDCl_3$) δ 16.1 (d, J_{CP} = 7.0 Hz), 63.9 (d, J_{CP} = 6.0 Hz), 68.2 (d, J_{CP} = 5.0 Hz), 128.8, 129.2, 134.4, 134.7 (d, J_{CP} = 7.0 Hz).

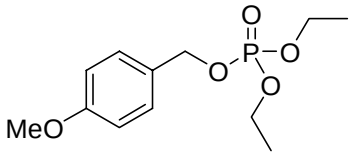
[1] Givens, R. S.; Matuszewski, B.; Athey, P. S.; Stoner, M. S. *J. Am. Chem. Soc.* **1990**, *112*, 6016-6021.
[2] Hammerschmidt, F.; Hanniger, A. *Chem. Ber.* **1995**, *128*, 823-830.
[3] Suh, Y. S.; Lee, J.-S.; Kim, S.-H.; Reike, R. D. *J. Organomet. Chem.* **2003**, *684*, 20-36.



Diethyl naphthalen-1-ylmethyl phosphate (20)[4]**:** Following the general procedure, **20** was obtained as a pale yellow oil (4.20 g, 71%): ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.26 (t, *J* = 7.1 Hz, 6H), 3.99-4.11 (m, 4H), 5.53 (d, *J* = 7.7 Hz, 2H), 7.45 (dd, *J* = 8.2, 7.0 Hz, 1H), 7.50-7.59 (m, 3H), 7.87 (dd, *J* = 8.2, 7.0 Hz, 2H), 8.11 (d, *J* = 8.2 Hz, 1H); ^{13}C {^{1}H} NMR (100 MHz, $CDCl_3$) δ 16.1 (d, J_{CP} = 7.0 Hz), 63.9 (d, J_{CP} = 6.0 Hz), 67.6 (d, J_{CP} = 6.0 Hz), 123.6, 125.3, 126.1, 126.7, 127.2, 128.7, 129.6, 131.4, 131.7, 133.8.



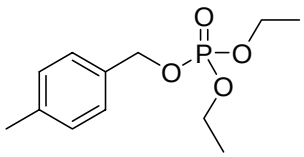
Diethyl 4-nitrobenzyl phosphate (21): Following the general procedure, **21** was obtained as a pale yellow oil (5.18 g, 90%): ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.31 (t, *J* = 7.1 Hz, 6H), 4.04-4.16 (m, 4H), 5.13 (d, *J* = 8.0 Hz, 2H), 7.53 (d, *J* = 8.6 Hz, 2H), 8.20 (d, *J* = 8.6 Hz, 2H); ^{13}C {^{1}H} NMR (100 MHz, $CDCl_3$) δ 16.1 (d, J_{CP} = 6.0 Hz), 64.2 (d, J_{CP} = 6.0 Hz), 67.4 (d, J_{CP} = 5.0 Hz), 123.8, 127.9, 143.4 (d, J_{CP} = 7.0 Hz), 147.8. HRMS calcd. for $C_{11}H_{16}NO_6P$ $[M+H]^+$ 290.07880, found 290.07957.



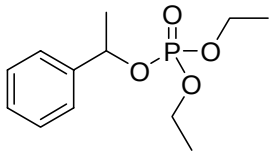
Diethyl 4-methoxybenzyl phosphate (22)[1]**:** Following the general procedure, **22** was obtained as a pale yellow oil (4.83 g, 88%): ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.28 (t, *J* = 7.1 Hz, 6H), 3.79 (s, 3H), 4.01-4.10 (m, 4H), 4.98 (d, *J* = 8.4 Hz, 2H), 6.87 (d, *J* = 8.7 Hz,

[4] Givens, R. S.; Matuszewski, B. *J. Am. Chem. Soc.* **1984,** *106*, 6860-6861.

2H), 7.31 (d, J = 8.7 Hz, 2H); ^{13}C {^{1}H} NMR (100 MHz, $CDCl_3$) δ 16.1 (d, J_{CP} = 7.0 Hz), 55.3, 63.7 (d, J_{CP} = 5.0 Hz), 69.0 (d, J_{CP} = 6.0 Hz), 114.0, 128.3 (d, J_{CP} = 6.0 Hz), 129.9, 159.9.



Diethyl 4-methylbenzyl phosphate (23)[1]: Following the general procedure, **23** was obtained as a pale yellow oil (4.66 g, 90%): ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.30 (t, J = 7.1 Hz, 6H), 2.35 (s, 3H), 4.02-4.14 (m, 4H), 5.20 (d, J = 8.1 Hz, 2H), 7.17 (d, J = 7.9 Hz, 2H), 7.27 (d, J = 7.9 Hz, 2H); ^{13}C {^{1}H} NMR (100 MHz, $CDCl_3$) δ 16.1 (d, J_{CP} = 6.4 Hz), 21.2, 63.8 (d, J_{CP} = 5.6 Hz), 69.0 (d, J_{CP} = 5.6 Hz), 128.1, 129.3, 133.2 (d, J_{CP} = 7.2 Hz), 138.4.

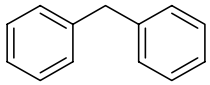


Diethyl phenethylphosphate (27)[5]: Following the general procedure, **22** was obtained as a pale yellow oil (1.56 g, 30%): ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.18 (t, J = 7.0 Hz, 3H), 1.28 (t, J = 7.0 Hz, 3H), 1.63 (d, J = 6.5 Hz, 3H), 3.87-4.11 (m, 4H), 5.42-5.49 (m, 1H), 7.25-7.38 (m, 5H); ^{13}C {^{1}H} NMR (100 MHz, $CDCl_3$) δ 16.0 (d, J_{CP} = 8.8 Hz), 16.1 (d, J_{CP} = 8.8 Hz), 24.2 (d, J_{CP} = 4.8 Hz), 63.5_8 (d, J_{CP} = 5.6 Hz), 63.6_0 (d, J_{CP} = 6.4 Hz), 76.7 (d, J_{CP} = 5.6 Hz), 125.9, 128.1, 128.5, 141.8 (d, J_{CP} = 4.8 Hz).

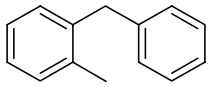
General procedure for Suzuki-Miyaura cross-coupling: The catalyst precursor (1 μmol, 1 mol%) and ligand (4 μmol, 4 mol%) were weighed into a small vial, dissolved in the reaction solvent (3 mL) and transferred into an 8 mL vial containing the benzylic

[5] Crich, D.; Xiao, X. Y. *J. Am. Chem. Soc.* **1996,** *118,* 6666-6670.

phosphate (1.0 mmol, 100 mol%), arylboronic acid (1.1 mmol, 110 mol%), inorganic base (1.1 mmol, 110 mol%) and a stir-bar. The reaction vial was closed with a cap fitted with a septum, then purged briefly with nitrogen. The vigorously stirred mixture was heated in an aluminum multi-reaction block to the desired temperature for 16 h. For screening reactions, the assay yield was determined by diluting the entire reaction mixture to a known volume with MeOH, followed by quantitative HPLC analysis of an aliquot against a pure standard. For reactions in which the cross-coupled product was isolated, the mixture was subjected to aqueous work-up using water then brine, with MTBE as the extraction solvent. Crude products were purified by silica flash column chromatography using appropriate mixtures of EtOAc/hexane (determined by TLC analysis) as the eluent.



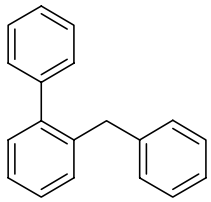
Diphenylmethane (3)[6]: Following the general procedure, diethyl benzyl phosphate **1** (244 mg, 1.0 mmol) was reacted with phenylboronic acid **2** (134 mg, 1.1 mmol) to afford **3** as a colorless oil (167 mg, 99%): ^{1}H NMR (400 MHz, $CDCl_3$) δ 4.14 (s, 2H), 7.24–7.30 (m, 6H), 7.43 (t, *J* = 7.5 Hz, 4H); ^{13}C {^{1}H} NMR (100 MHz, $CDCl_3$) δ 42.2, 126.3, 128.7, 129.2, 141.3.



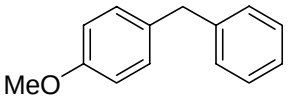
2-Benzyltoluene (11)[6]: Following the general procedure, diethyl benzyl phosphate **1** (244 mg, 1.0 mmol) was reacted with *o*-tolylboronic acid **4** (150 mg, 1.1 mmol) to afford **11** as a colorless oil (151 mg, 83%): ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.33 (s, 3H), 4.07 (s, 2H), 7.14–7.29 (m, 7H), 7.33 (t, *J* = 7.4 Hz, 2H); ^{13}C {^{1}H} NMR (100 MHz, CDCl3) δ 19.8, 39.6, 126.0, 126.1, 126.6, 128.5, 128.9, 130.0, 130.4, 136.8, 139.1, 140.5.

[6] Kuwano, R.; Yokogi, M. *Org Lett.* **2005**, *7*, 945-947.

Also prepared following the general procedure using diethyl 2-methylbenzyl phosphate **18** (258 mg, 1.0 mmol) and phenylboronic acid **2** (134 mg, 1.1 mmol) to afford **11** as a colorless oil (164 mg, 90%): analytical data as previous.

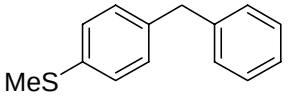


2-Benzylbiphenyl (12)[6]**:** Following the general procedure, diethyl benzyl phosphate **1** (244 mg, 1.0 mmol) was reacted with 2-biphenylboronic acid **5** (218 mg, 1.1 mmol) to afford **12** as a colorless oil (239 mg, 98%): ^{1}H NMR (400 MHz, $CDCl_3$) δ 4.09 (s, 2H), 7.11 (d, *J* = 7.6 Hz, 2H), (m, 12H); ^{13}C {^{1}H} NMR (100 MHz, $CDCl_3$) δ 39.2, 126.0, 126.4, 127.1, 127.7, 128.2, 128.4, 129.1, 129.5, 130.3, 130.5, 138.4, 141.4, 141.6, 142.5.

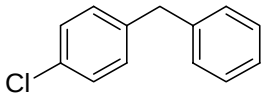


4-Benzylanisole (13)[6]**:** Following the general procedure, diethyl benzyl phosphate **1** (244 mg, 1.0 mmol) was reacted with 4-methoxyphenylboronic acid **6** (167 mg, 1.1 mmol) to afford **13** as a colorless oil (174 mg, 88%): ^{1}H NMR (400 MHz, $CDCl_3$, TMS) δ 3.84 (s, 3H), 4.01 (s, 2H), 6.91 (d, *J* = 8.5 Hz, 2H), 7.18 (d, *J* = 8.5 Hz, 2H), 7.24-7.28 (m, 3H), 7.34 (t, *J* = 7.3 Hz, 2H); ^{13}C {^{1}H} NMR (100 MHz, $CDCl_3$) δ 41.2, 55.4, 114.0, 126.1, 128.6, 129.0, 130.0, 133.4, 141.7, 158.1.

Also prepared following the general procedure using diethyl 4-methoxybenzyl phosphate **22** (274 mg, 1.0 mmol) and phenylboronic acid **2** (134 mg, 1.1 mmol) to afford **13** as a colorless oil (160 mg, 81%): analytical data as previous.

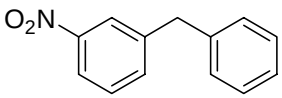


4-Benzylthioanisole (14): Following the general procedure, diethyl benzyl phosphate **1** (244 mg, 1.0 mmol) was reacted with 4-methylthiophenylboronic acid **7** (150 mg, 1.1 mmol) to afford **14** as a colorless oil (195 mg, 91%): ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.50 (s, 3H), 3.99 (s, 2H), 7.16 (d, *J* = 8.4 Hz, 2H), 7.20-7.28 (m, 5H), 7.30-7.36 (m, 2H); ^{13}C {^{1}H} NMR (100 MHz, $CDCl_3$) δ 16.3, 41.5, 126.2, 127.3, 128.6, 129.0, 129.6, 135.9, 138.3, 141.1. Anal. calcd. for $C_{14}H_{14}S$: C, 78.46; H, 6.58. Found: C, 78.16; H, 6.64.



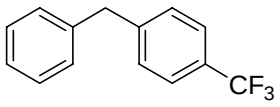
4-Benzyl-1-chlorobenzene (15)[6]: Following the general procedure, diethyl benzyl phosphate **1** (244 mg, 1.0 mmol) was reacted with 4-chlorophenylboronic acid **8** (172 mg, 1.1 mmol) to afford **15** as a colorless oil (177 mg, 87%): ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.94 (s, 2H), 7.17 (d, *J* = 8.4 Hz, 2H), 7.23 (d, *J* = 7.6 Hz, 2H), 7.25-7.39 (m, 5H); ^{13}C {^{1}H} NMR (100 MHz, $CDCl_3$) δ 41.4, 126.4, 127.3, 128.7, 129.0, 130.4, 132.0, 139.7, 140.7.

Also prepared following the general procedure using diethyl 4-chlorobenzyl phosphate **19** (279 mg, 1.0 mmol) and phenylboronic acid **2** (134 mg, 1.1 mmol) to afford **15** as a colorless oil (162 mg, 80%): analytical data as previous.

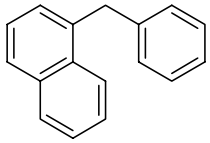


3-Benzyl-1-nitrobenzene (16)[6]: Following the general procedure, diethyl benzyl phosphate **1** (244 mg, 1.0 mmol) was reacted with 3-nitrophenylboronic acid **9** (184 mg, 1.1 mmol) to afford **16** as a colorless oil (144 mg, 67%): ^{1}H NMR (400 MHz, $CDCl_3$) δ 4.10 (s, 2H), 7.18 (d, *J* = 7.1 Hz, 2H), 7.24 (t, *J* = 7.3 Hz, 1H), 7.32 (t, *J* = 7.3 Hz, 2H), 7.41–7.47 (m, 1H), 7.51 (d, *J* = 7.6 Hz, 1H), 8.04–8.08 (m, 2H); ^{13}C {^{1}H} NMR (100

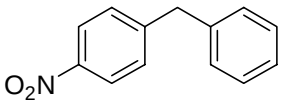
MHz, $CDCl_3$) δ 41.6, 121.4, 123.8, 126.8, 128.9, 129.0, 129.4, 135.1, 139.4, 143.3, 148.5.



4-Benzyl-1-(trifluoromethyl)benzene (17)[6]: Following the general procedure, diethyl benzyl phosphate **1** (244 mg, 1.0 mmol) was reacted with 4-trifluoromethylphenylboronic acid **10** (209 mg, 1.1 mmol) to afford **17** as a colorless oil (222 mg, 94%): ^{1}H NMR (400 MHz, $CDCl_3$) δ 4.09 (s, 2H), 7.16-7.42 (m, 7H), 7.59 (d, *J* = 8.1 Hz, 2H); ^{13}C {^{1}H} NMR (100 MHz, $CDCl_3$) δ 41.7, 124.4 (q, *J* = 272 Hz), 125.4 (q, *J* = 4 Hz), 126.5, 128.5 (q, *J* = 33 Hz), 128.6, 128.9, 129.2, 140.0, 145.3.

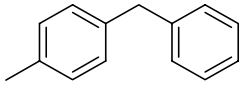


1-Benzylnaphthalene (24)[6]: Following the general procedure, diethyl naphthylmethyl phosphate **20** (294 mg, 1.0 mmol) was reacted with phenylboronic acid **2** (134 mg, 1.1 mmol) to afford **24** as a colorless oil (196 mg, 90%): ^{1}H NMR (400 MHz, $CDCl_3$) δ 4.53 (s, 2H), 7.24-7.31 (m, 3H), 7.32-7.40 (m, 3H), 7.47-7.56 (m, 3H), 7.85 (d, *J* = 8.4 Hz, 1H), 7.91-7.97 (m, 1H), 8.05-8.12 (m, 1H); ^{13}C {^{1}H} NMR (100 MHz, $CDCl_3$) δ 39.2, 124.4, 125.7, 126.1, 126.2, 127.5, 127.5, 128.6, 128.8, 128.9, 132.3, 134.1, 136.8, 140.8.



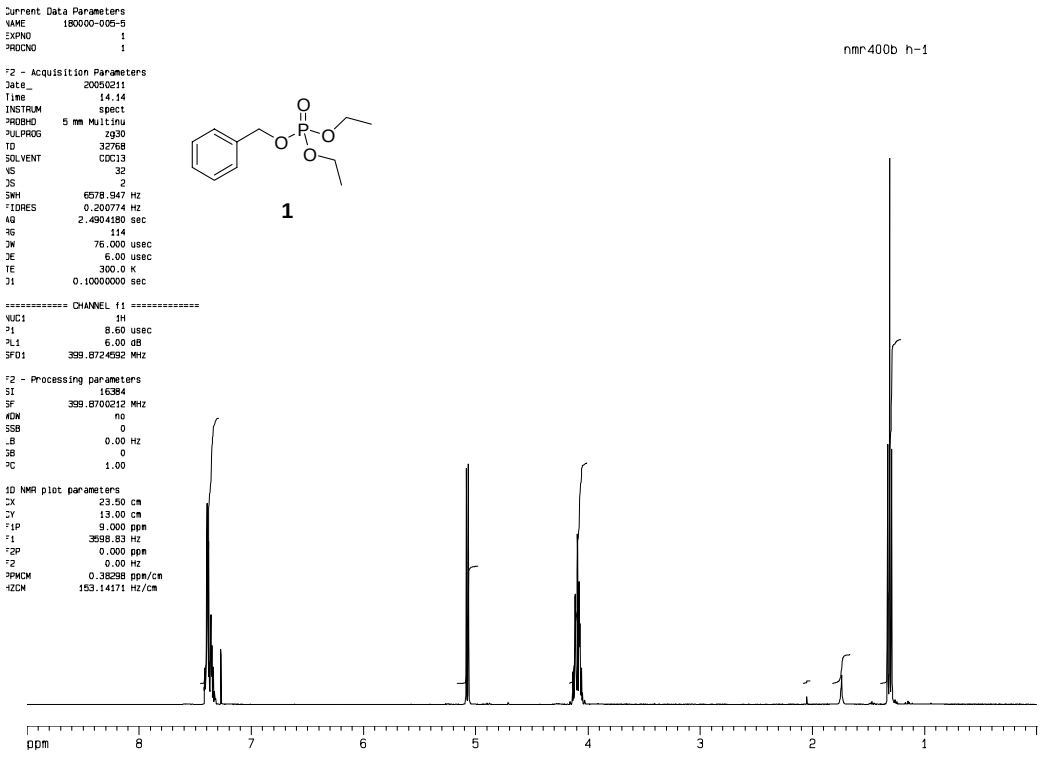
4-Benzyl-1-nitrobenzene (25): Following the general procedure, diethyl 4-nitrobenzyl phosphate **21** (289 mg, 1.0 mmol) was reacted with phenylboronic acid **2** (134 mg, 1.1 mmol) to afford **25** as a colorless oil (177 mg, 83%): ^{1}H NMR (400 MHz, $CDCl_3$) δ 4.10 (s, 2H), 7.20 (d, *J* = 7.0 Hz, 2H), 7.27 (t, *J* = 7.3 Hz, 1H), 7.35 (t, *J* = 7.3 Hz, 4H), 8.15

(d, J = 8.7 Hz, 2H); ^{13}C {^{1}H} NMR (100 MHz, $CDCl_3$) δ 41.8, 123.8, 126.8, 128.9, 129.1, 129.7, 139.3, 146.6, 149.9. Anal. calcd. for $C_{13}H_{11}NO_2$: C, 73.23; H, 5.20; N, 6.57. Found: C, 72.95; H, 5.18; N, 6.53.



4-Benzyltoluene (26)[7]**:** Following the general procedure, diethyl 4-methylbenzyl phosphate **23** (258 mg, 1.0 mmol) was reacted with phenylboronic acid **2** (134 mg, 1.1 mmol) to afford **26** as a colorless oil (178 mg, 98%): ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.43 (s, 3H), 4.06 (s, 2H), 7.18-7.24 (m, 4H), 7.28-7.33 (m, 3H), 7.37-7.43 (m, 2H); ^{13}C {^{1}H} NMR (100 MHz, $CDCl_3$) δ 21.2, 41.7, 126.2, 128.6, 129.0, 129.1, 129.3, 135.7, 138.3, 141.6.

[7] Gordon, P. E.; Fry, A. J. *Tetrahedron Lett.* **2001**, *42*, 831-834.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Time 14.14
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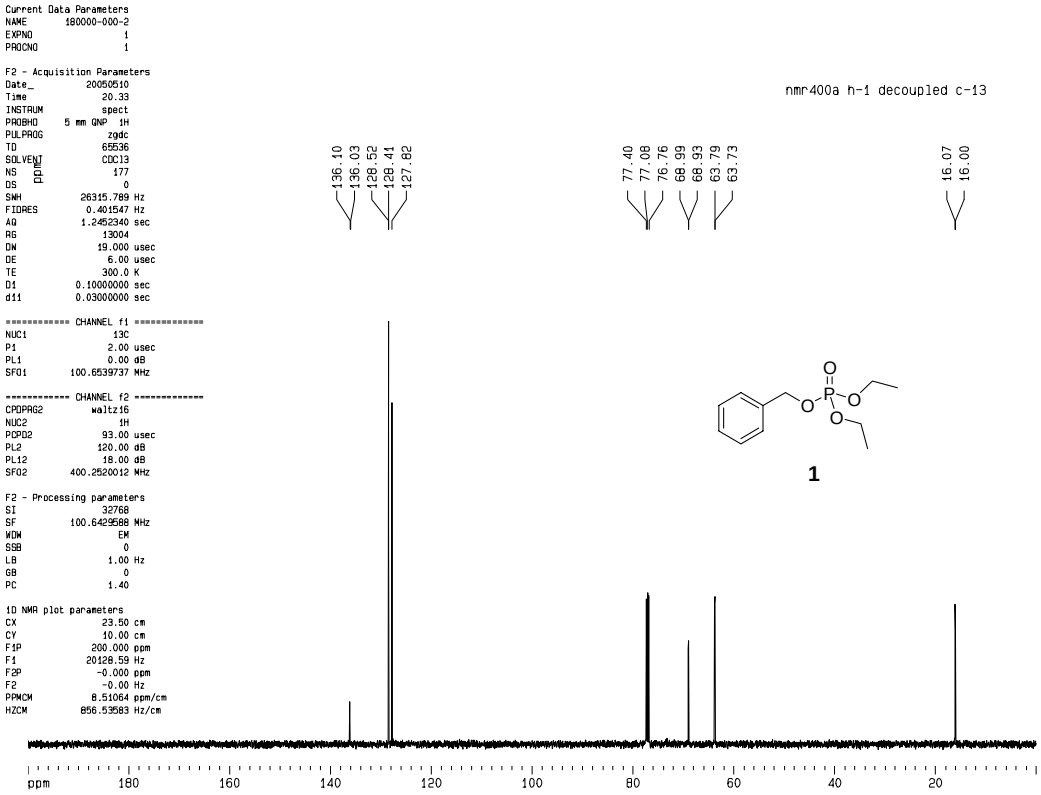
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 32
DS 2
SWH 6578.947 Hz
FIDRES 0.200774 Hz
AQ 2.4904180 sec
RG 114
DW 76.000 usec
DE 6.00 usec
TE 300.0 K
D1 0.10000000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 8.60 usec
PL1 6.00 dB
SFO1 399.8724592 MHz
F2 - Processing parameters
SI 16384
SF 399.8700212 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 23.50 cm
CY 13.00 cm
F1P 9.000 ppm
F1 3598.83 Hz
F2P 0.000 ppm
F2 0.00 Hz
PPMCM 0.38298 ppm/cm
HZCM 153.14171 Hz/cm
nmr400b h-1
1
ppm
8
7
6
5
4
3
2
1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EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20050510
Time 20.33
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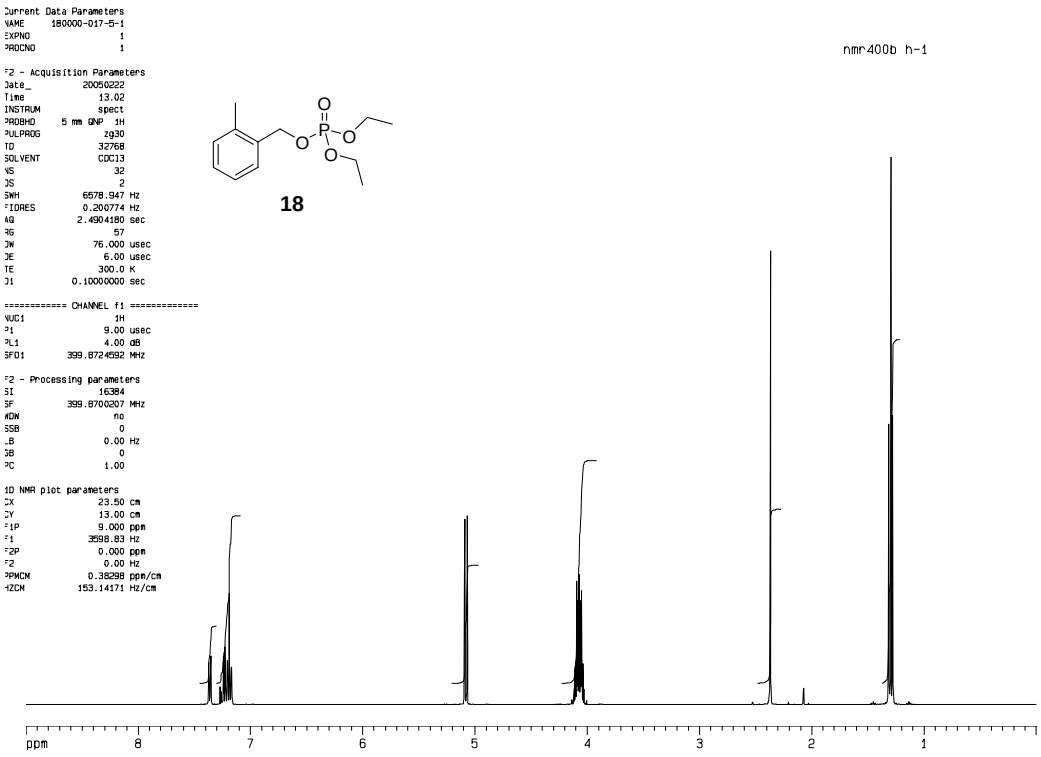
PULPROG zgdc
TD 65536
SOLVENT CDCl3
NS 177
DS 0
SWH 26315.789 Hz
FIDRES 0.401547 Hz
AQ 1.2452340 sec
RG 13004
DW 19.000 usec
DE 6.00 usec
TE 300.0 K
D1 0.10000000 sec
d11 0.03000000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 2.00 usec
PL1 0.00 dB
SFO1 100.6539737 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 93.00 usec
PL2 120.00 dB
PL12 18.00 dB
SFO2 400.2520012 MHz
F2 - Processing parameters
SI 32768
SF 100.6429588 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
1D NMR plot parameters
CX 23.50 cm
CY 10.00 cm
F1P 200.000 ppm
F1 20128.59 Hz
F2P -0.000 ppm
F2 -0.00 Hz
PPMCM 8.51064 ppm/cm
HZCM 856.53583 Hz/cm
nmr400a h-1 decoupled c-13
136.10
136.03
128.52
128.41
127.82
77.40
77.08
76.76
68.99
68.93
63.79
63.73
16.07
16.00
1
ppm
180
160
140
120
100
80
60
40
20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EXPNO 1
PROCNO 1
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Date_ 20050222
Time 13.02
INSTRUM spect
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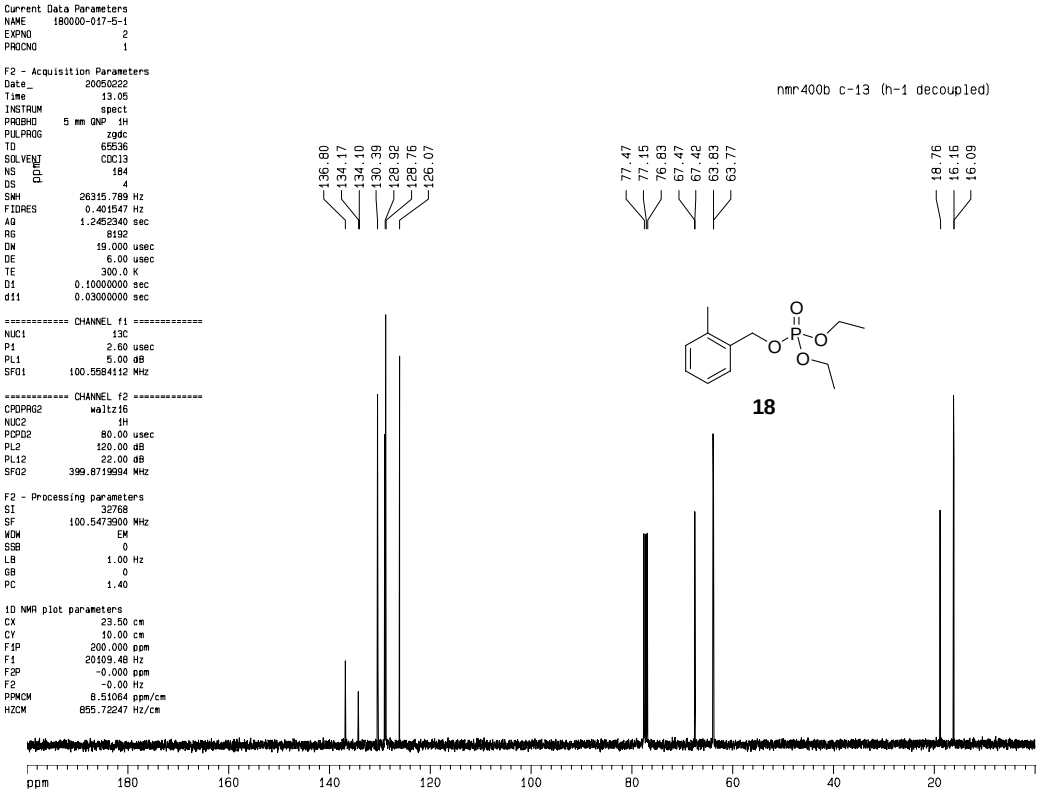
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 32
DS 2
SWH 6578.947 Hz
FIDRES 0.200774 Hz
AQ 2.4904180 sec
RG 57
DW 76.000 usec
DE 6.00 usec
TE 300.0 K
D1 0.10000000 sec
========== CHANNEL f1 ==========
NUC1 1H
P1 9.00 usec
PL1 4.00 dB
SFO1 399.8724592 MHz
F2 - Processing parameters
SI 16384
SF 399.8700207 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 23.50 cm
CY 13.00 cm
F1P 9.000 ppm
F1 3598.83 Hz
F2P 0.000 ppm
F2 0.00 Hz
PPMCM 0.38298 ppm/cm
HZCM 153.14171 Hz/cm
nmr400b h-1
18
ppm
8
7
6
5
4
3
2
1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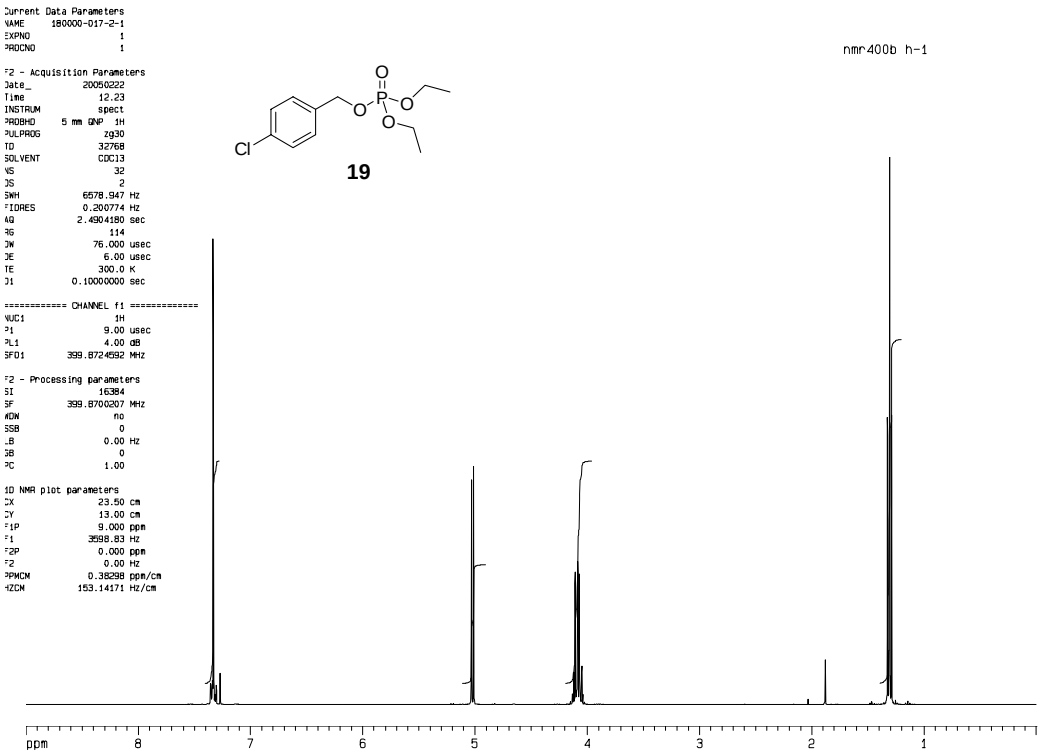
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20050222
Time 13.05
INSTRUM spect
PROBHD 5 mm QNP 1H
PULPROG zgdc
TD 65536
SOLVENT CDCl3
NS 184
DS 4
SWH 26315.789 Hz
FIDRES 0.401547 Hz
AQ 1.2452340 sec
RG 8192
DW 19.000 usec
DE 6.00 usec
TE 300.0 K
D1 0.10000000 sec
d11 0.03000000 sec
========== CHANNEL f1 ==========
NUC1 13C
P1 2.60 usec
PL1 5.00 dB
SFO1 100.5584112 MHz
========== CHANNEL f2 ==========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 120.00 dB
PL12 22.00 dB
SFO2 399.8719994 MHz
F2 - Processing parameters
SI 32768
SF 100.5473900 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
1D NMR plot parameters
CX 23.50 cm
CY 10.00 cm
F1P 200.000 ppm
F1 20109.48 Hz
F2P -0.000 ppm
F2 -0.00 Hz
PPMCM 8.51064 ppm/cm
HZCM 855.72247 Hz/cm
nmr400b c-13 (h-1 decoupled)
136.80
134.17
134.10
130.39
128.92
128.76
126.07
77.47
77.15
76.83
67.47
67.42
63.83
63.77
18.76
16.16
16.09
18
ppm
180
160
140
120
100
80
60
40
20


Current Data Parameters
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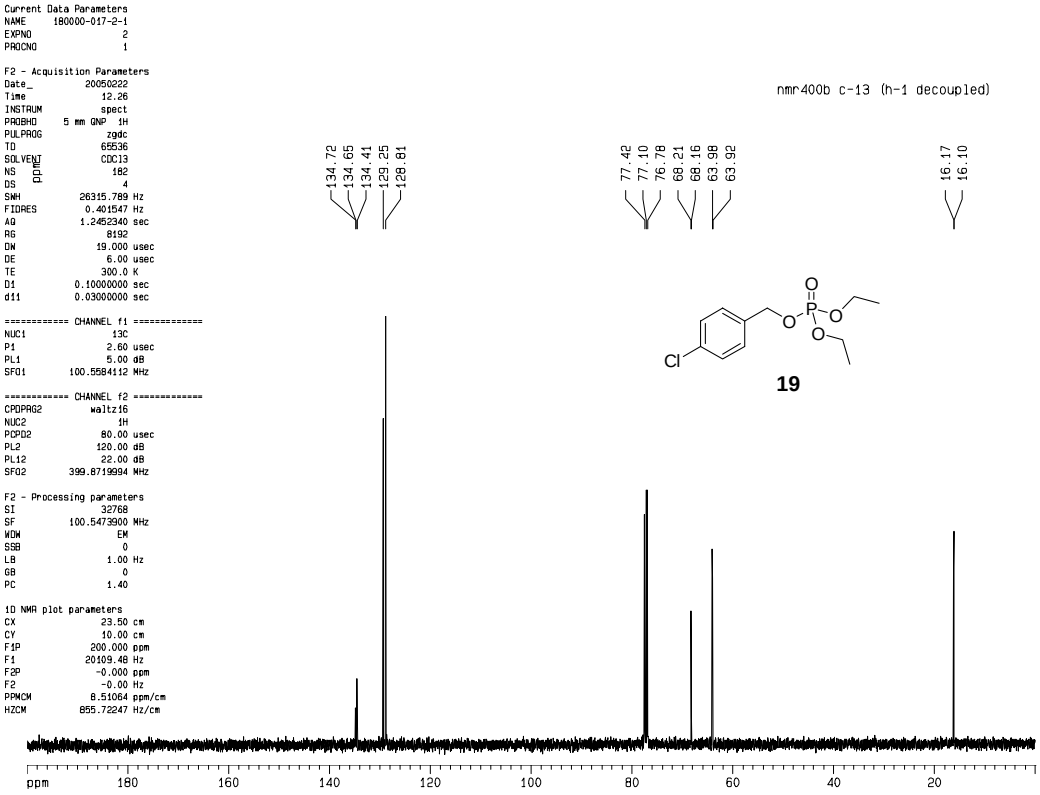
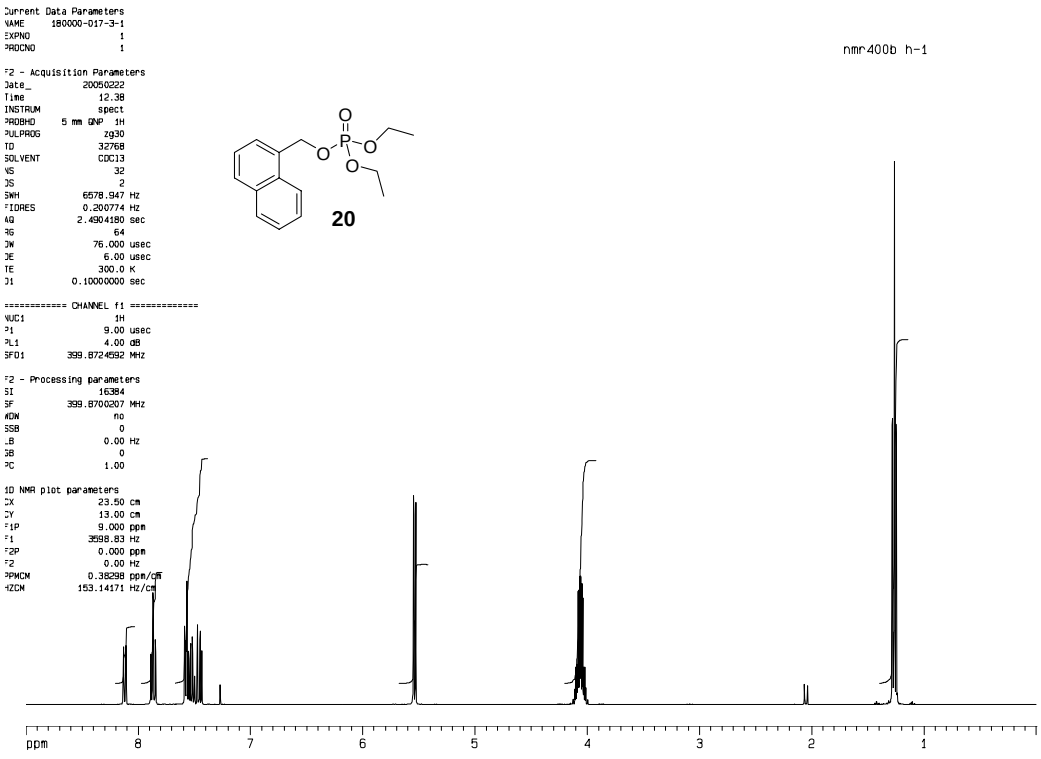
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20050222
Time 12.23
INSTRUM spect
PROBHD 5 mm QNP 1H
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 32
DS 2
SWH 6578.947 Hz
FIDRES 0.200774 Hz
AQ 2.4904180 sec
RG 114
DW 76.000 usec
DE 6.00 usec
TE 300.0 K
D1 0.10000000 sec
========== CHANNEL f1 ==========
NUC1 1H
P1 9.00 usec
PL1 4.00 dB
SFO1 399.8724592 MHz
F2 - Processing parameters
SI 16384
SF 399.8700207 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 23.50 cm
CY 13.00 cm
F1P 9.000 ppm
F1 3598.83 Hz
F2P 0.000 ppm
F2 0.00 Hz
PPMCM 0.38298 ppm/cm
HZCM 153.14171 Hz/cm
nmr400b h-1
Cl
O
P
O
O
O
19
ppm
8
7
6
5
4
3
2
1


Current Data Parameters
NAME 180000-017-2-1
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20050222
Time 12.26
INSTRUM spect
PROBHD 5 mm QNP 1H
PULPROG zgdc
TD 65536
SOLVENT CDCl3
NS 182
DS 4
SWH 26315.789 Hz
FIDRES 0.401547 Hz
AQ 1.2452340 sec
RG 8192
DW 19.000 usec
DE 6.00 usec
TE 300.0 K
D1 0.10000000 sec
d11 0.03000000 sec
========== CHANNEL f1 ==========
NUC1 13C
P1 2.60 usec
PL1 5.00 dB
SFO1 100.5584112 MHz
========== CHANNEL f2 ==========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 120.00 dB
PL12 22.00 dB
SFO2 399.8719994 MHz
F2 - Processing parameters
SI 32768
SF 100.5473900 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
1D NMR plot parameters
CX 23.50 cm
CY 10.00 cm
F1P 200.000 ppm
F1 20109.48 Hz
F2P -0.000 ppm
F2 -0.00 Hz
PPMCM 8.51064 ppm/cm
HZCM 855.72247 Hz/cm
nmr400b c-13 (h-1 decoupled)
134.72
134.65
134.41
129.25
128.81
77.42
77.10
76.78
68.21
68.16
63.98
63.92
16.17
16.10
Cl
O
P
O
O
O
19
ppm
180
160
140
120
100
80
60
40
20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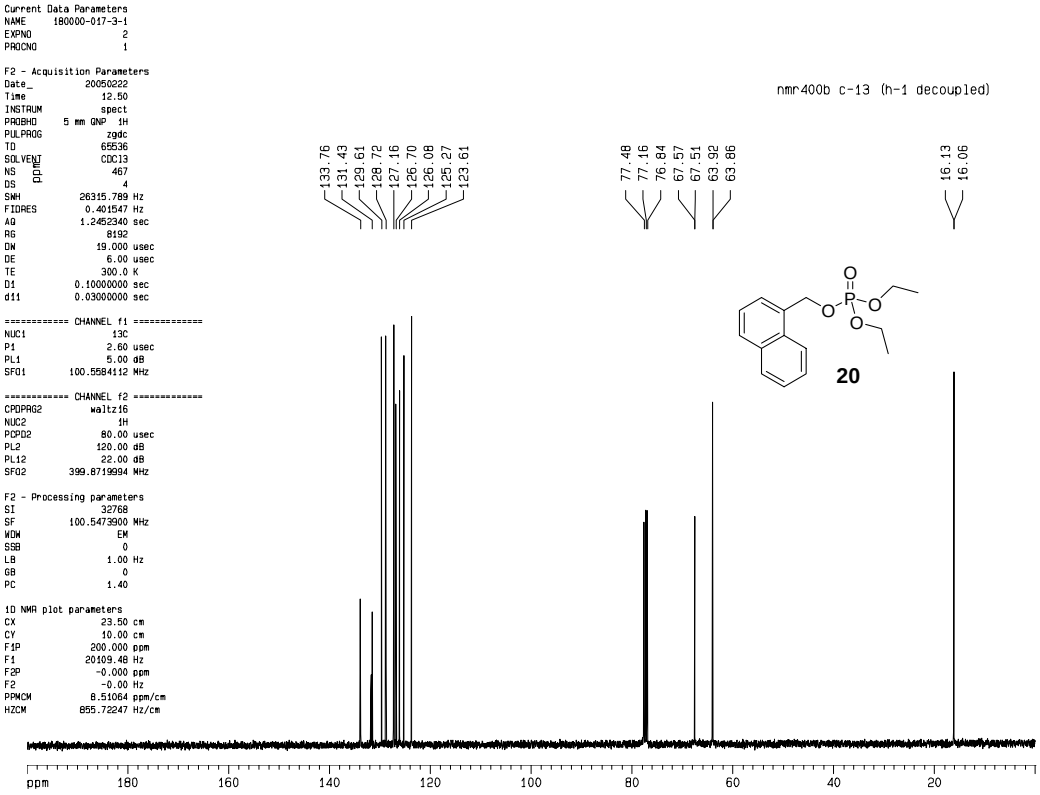
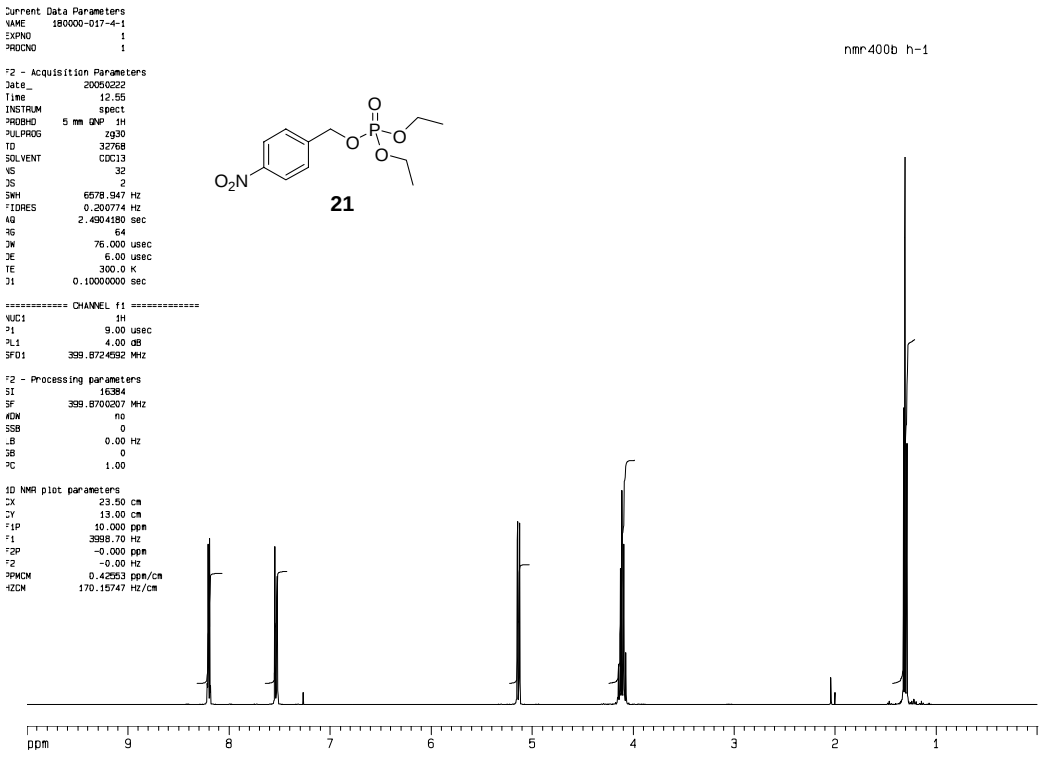
NAME 180000-017-3-1
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20050222
Time 12.38
INSTRUM spect
PROBHD 5 mm QNP 1H
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 32
DS 2
SWH 6578.947 Hz
FIDRES 0.200774 Hz
AQ 2.4904180 sec
RG 64
DW 76.000 usec
DE 6.00 usec
TE 300.0 K
D1 0.10000000 sec
========== CHANNEL f1 ==========
NUC1 1H
P1 9.00 usec
PL1 4.00 dB
SFO1 399.8724592 MHz
F2 - Processing parameters
SI 16384
SF 399.8700207 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 23.50 cm
CY 13.00 cm
F1P 9.000 ppm
F1 3598.83 Hz
F2P 0.000 ppm
F2 0.00 Hz
PPMCM 0.38298 ppm/cm
HZCM 153.14171 Hz/cm
nmr400b h-1
20
ppm
8
7
6
5
4
3
2
1


Current Data Parameters
NAME 180000-017-3-1
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20050222
Time 12.50
INSTRUM spect
PROBHD 5 mm QNP 1H
PULPROG zgdc
TD 65536
SOLVENT CDCl3
NS 467
DS 4
SWH 26315.789 Hz
FIDRES 0.401547 Hz
AQ 1.2452340 sec
RG 8192
DW 19.000 usec
DE 6.00 usec
TE 300.0 K
D1 0.10000000 sec
d11 0.03000000 sec
========== CHANNEL f1 ==========
NUC1 13C
P1 2.60 usec
PL1 5.00 dB
SFO1 100.5584112 MHz
========== CHANNEL f2 ==========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 120.00 dB
PL12 22.00 dB
SFO2 399.8719994 MHz
F2 - Processing parameters
SI 32768
SF 100.5473900 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
1D NMR plot parameters
CX 23.50 cm
CY 10.00 cm
F1P 200.000 ppm
F1 20109.48 Hz
F2P -0.000 ppm
F2 -0.00 Hz
PPMCM 8.51064 ppm/cm
HZCM 855.72247 Hz/cm
nmr400b c-13 (h-1 decoupled)
133.76
131.43
129.61
128.72
127.16
126.70
126.08
125.27
123.61
77.48
77.16
76.84
67.57
67.51
63.92
63.86
16.13
16.06
20
ppm
180
160
140
120
100
80
60
40
20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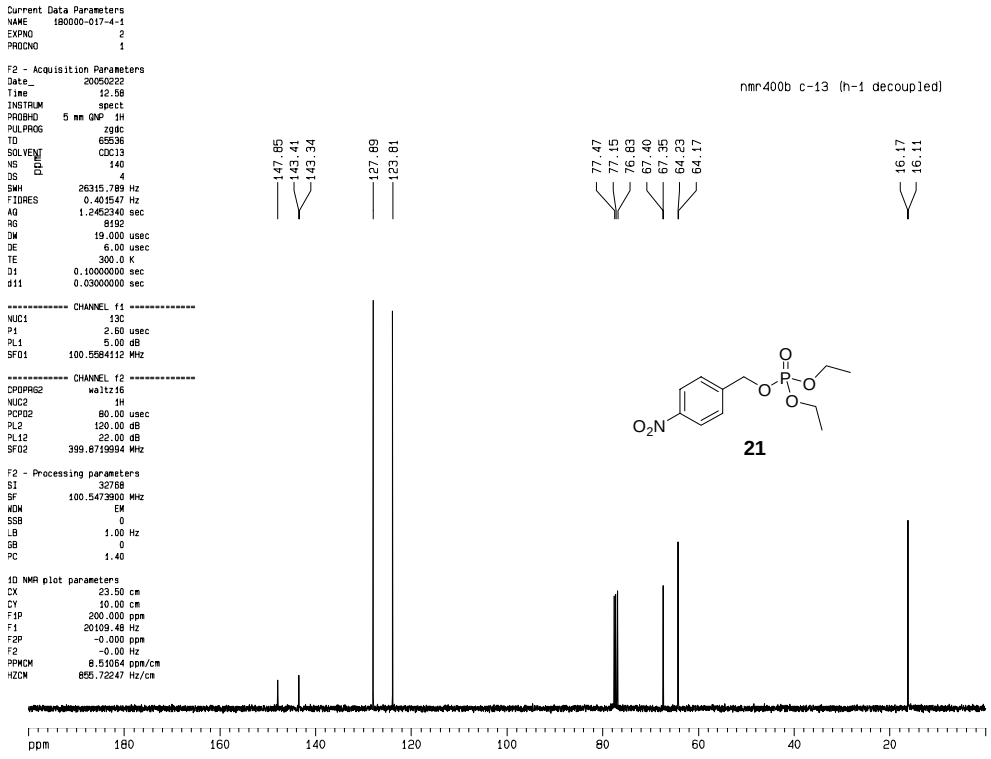
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20050222
Time 12.55
INSTRUM spect
PROBHD 5 mm GNP 1H
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 32
DS 2
SWH 6578.947 Hz
FIDRES 0.200774 Hz
AQ 2.4904180 sec
RG 64
DW 76.000 usec
DE 6.00 usec
TE 300.0 K
D1 0.10000000 sec
========== CHANNEL f1 ==========
NUC1 1H
P1 9.00 usec
PL1 4.00 dB
SFO1 399.8724592 MHz
F2 - Processing parameters
SI 16384
SF 399.8700207 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 23.50 cm
CY 13.00 cm
F1P 10.000 ppm
F1 3998.70 Hz
F2P -0.000 ppm
F2 -0.00 Hz
PPMCM 0.42553 ppm/cm
HZCM 170.15747 Hz/cm
O2N
O
P
O
O
O
21
nmr400b h-1
ppm
9
8
7
6
5
4
3
2
1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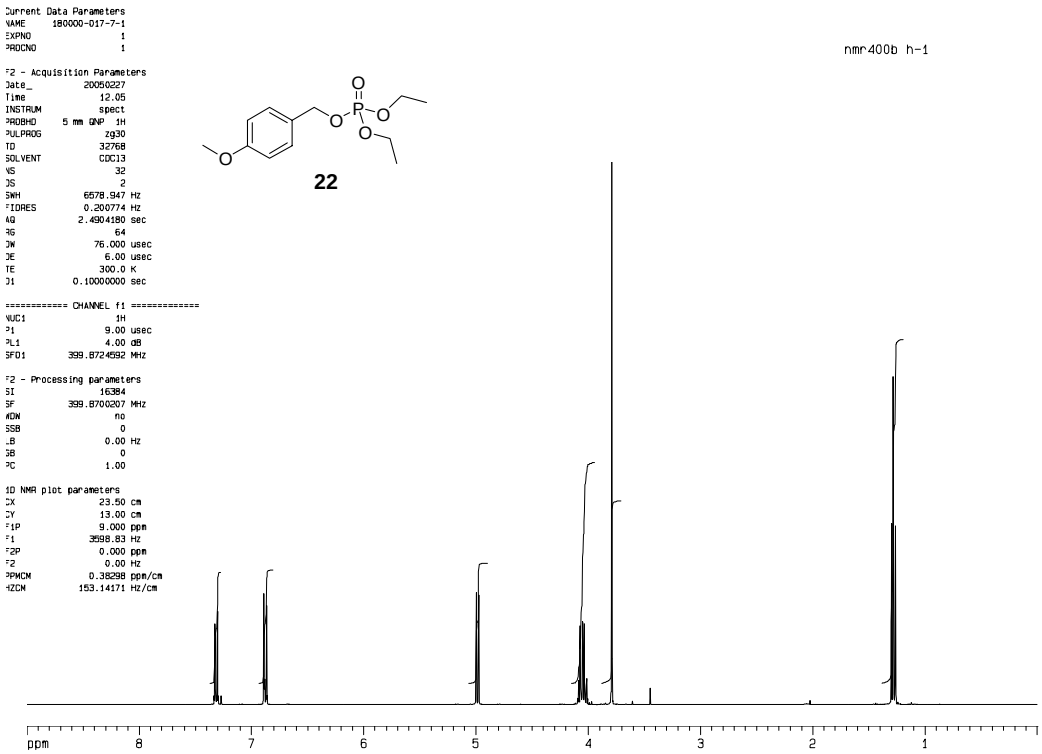
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20050222
Time 12.58
INSTRUM spect
PROBHD 5 mm GNP 1H
PULPROG zgpg
TD 65536
SOLVENT CDCl3
NS 140
DS 4
SWH 26315.789 Hz
FIDRES 0.401547 Hz
AQ 1.2452340 sec
RG 8192
DW 19.000 usec
DE 6.00 usec
TE 300.0 K
D1 0.10000000 sec
d11 0.03000000 sec
========== CHANNEL f1 ==========
NUC1 13C
P1 2.60 usec
PL1 5.00 dB
SFO1 100.5584112 MHz
========== CHANNEL f2 ==========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 120.00 dB
PL12 22.00 dB
SFO2 399.8719994 MHz
F2 - Processing parameters
SI 32768
SF 100.5473900 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
1D NMR plot parameters
CX 23.50 cm
CY 10.00 cm
F1P 200.000 ppm
F1 20109.48 Hz
F2P -0.000 ppm
F2 -0.00 Hz
PPMCM 8.51064 ppm/cm
HZCM 855.72247 Hz/cm
ppm
147.85
143.41
143.34
127.89
123.81
77.47
77.15
76.83
67.40
67.35
64.23
64.17
16.17
16.11
O2N
O
P
O
O
O
21
nmr400b c-13 (h-1 decoupled)
ppm
180
160
140
120
100
80
60
40
20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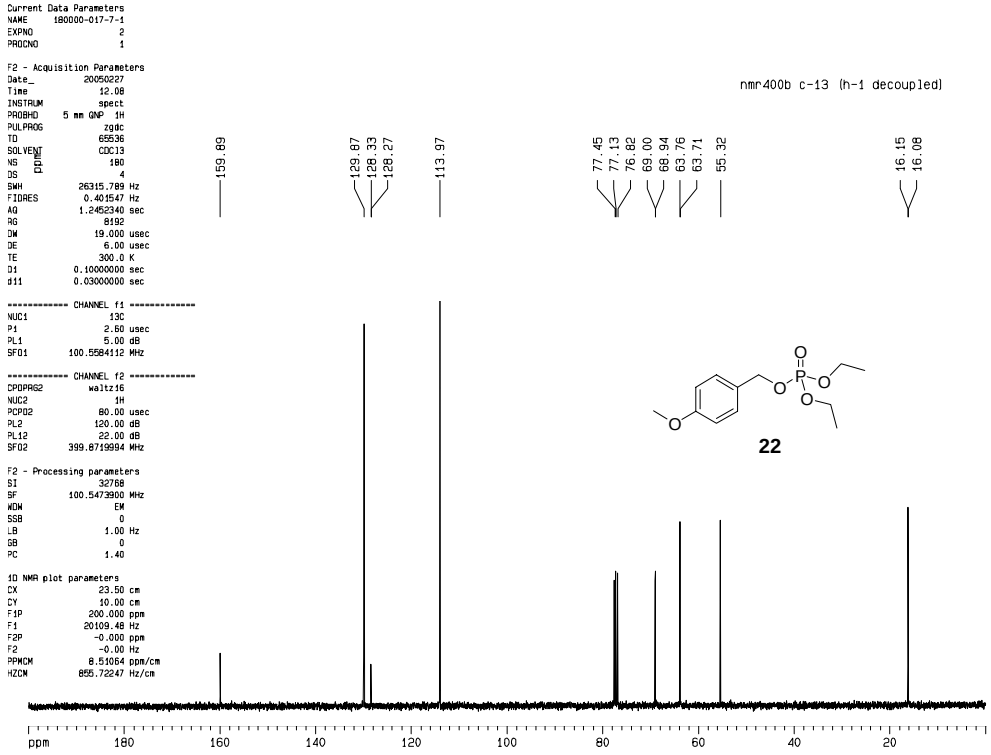
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20050227
Time 12.05
INSTRUM spect
PROBHD 5 mm GNP 1H
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 32
DS 2
SWH 6578.947 Hz
FIDRES 0.200774 Hz
AQ 2.4904180 sec
RG 64
DW 76.000 usec
DE 6.00 usec
TE 300.0 K
D1 0.10000000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 9.00 usec
PL1 4.00 dB
SFO1 399.8724592 MHz
F2 - Processing parameters
SI 16384
SF 399.8700207 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 23.50 cm
CY 13.00 cm
F1P 9.000 ppm
F1 3598.83 Hz
F2P 0.000 ppm
F2 0.00 Hz
PPMCM 0.38298 ppm/cm
HZCM 153.14171 Hz/cm
nmr400b h-1
22
ppm
8
7
6
5
4
3
2
1


Current Data Parameters
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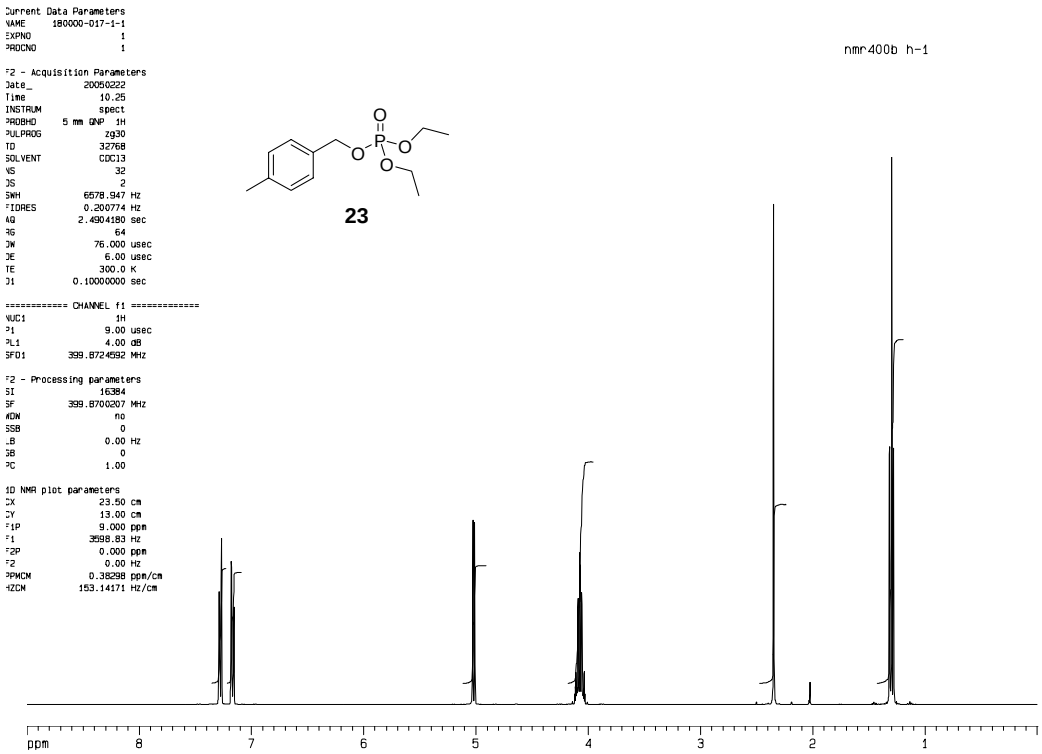
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20050227
Time 12.08
INSTRUM spect
PROBHD 5 mm GNP 1H
PULPROG zgpg
TD 65536
SOLVENT CDCl3
NS 180
DS 4
SWH 26315.789 Hz
FIDRES 0.401547 Hz
AQ 1.2452340 sec
RG 8192
DW 19.000 usec
DE 6.00 usec
TE 300.0 K
D1 0.10000000 sec
d11 0.03000000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 2.60 usec
PL1 5.00 dB
SFO1 100.5584112 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 120.00 dB
PL12 22.00 dB
SFO2 399.8719994 MHz
F2 - Processing parameters
SI 32768
SF 100.5473900 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
1D NMR plot parameters
CX 23.50 cm
CY 10.00 cm
F1P 200.000 ppm
F1 20109.48 Hz
F2P -0.000 ppm
F2 -0.00 Hz
PPMCM 8.51064 ppm/cm
HZCM 855.72247 Hz/cm
nmr400b c-13 (h-1 decoupled)
159.89
129.87
128.33
128.27
113.97
77.45
77.13
76.82
69.00
68.94
63.76
63.71
55.32
16.15
16.08
22
ppm
180
160
140
120
100
80
60
40
20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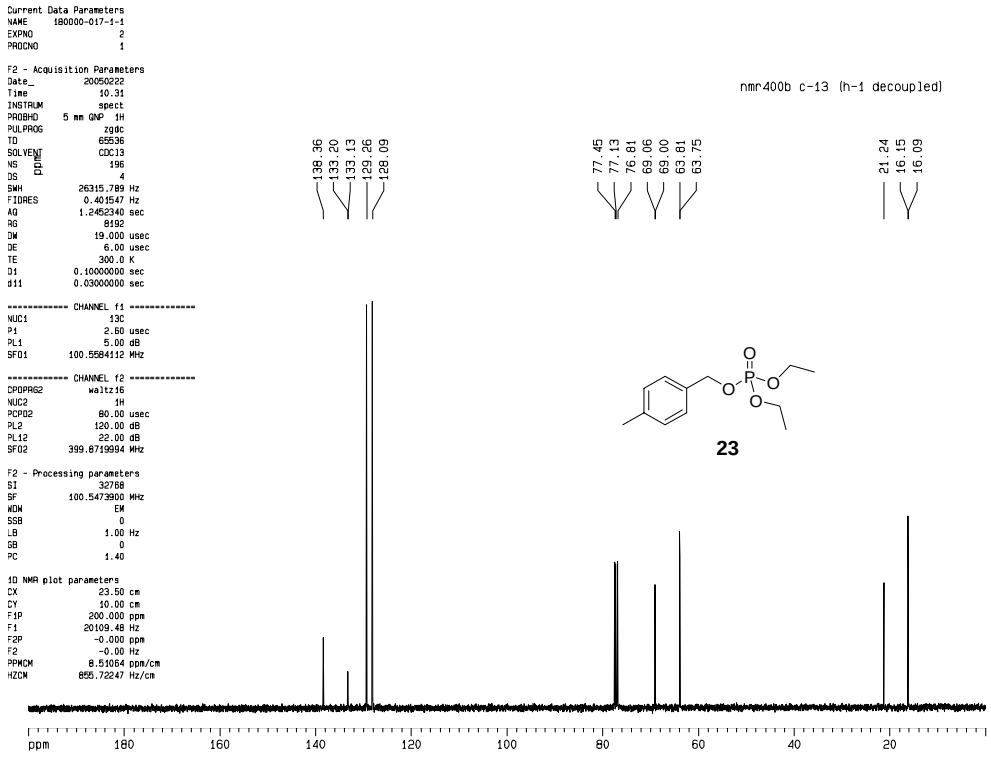
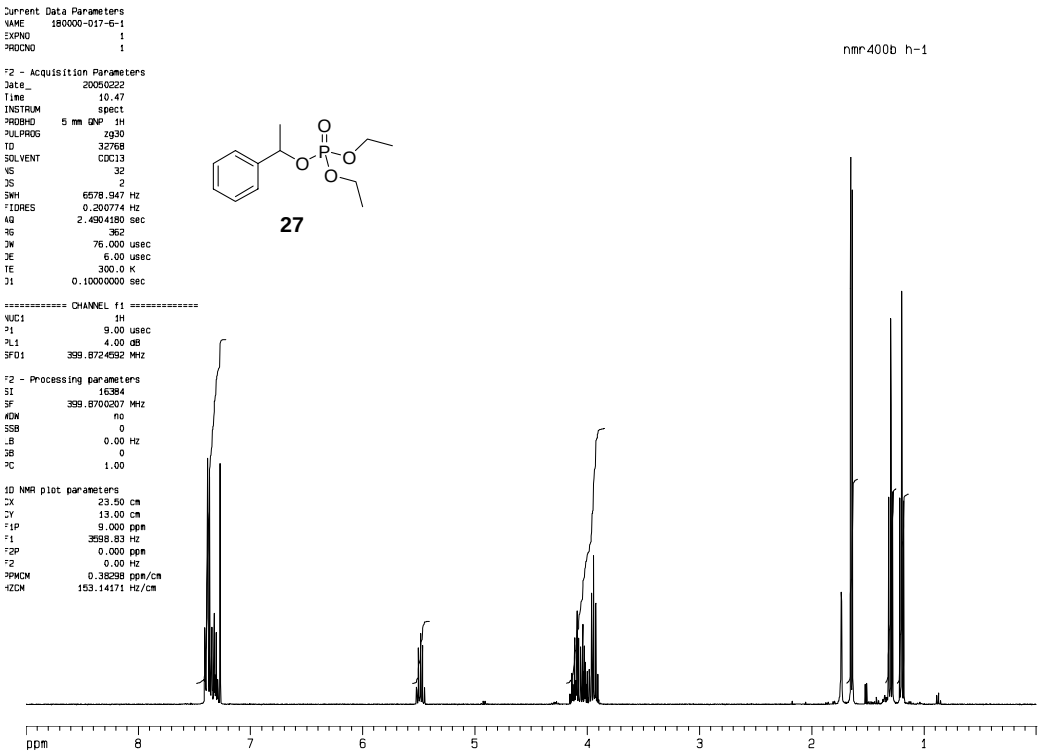
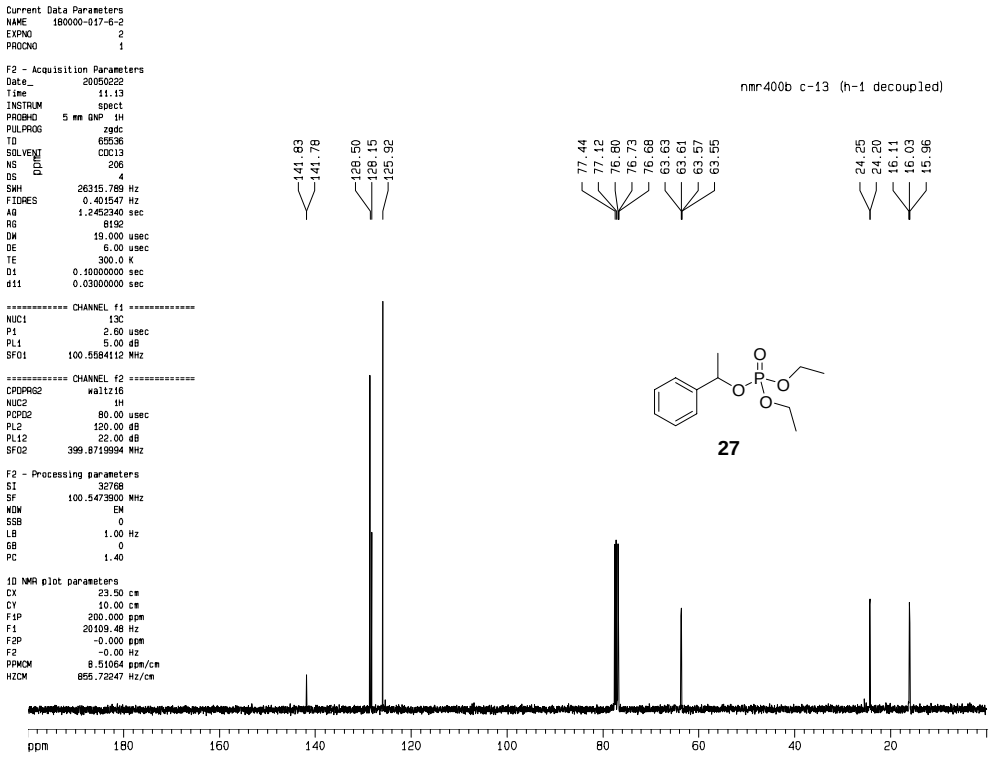
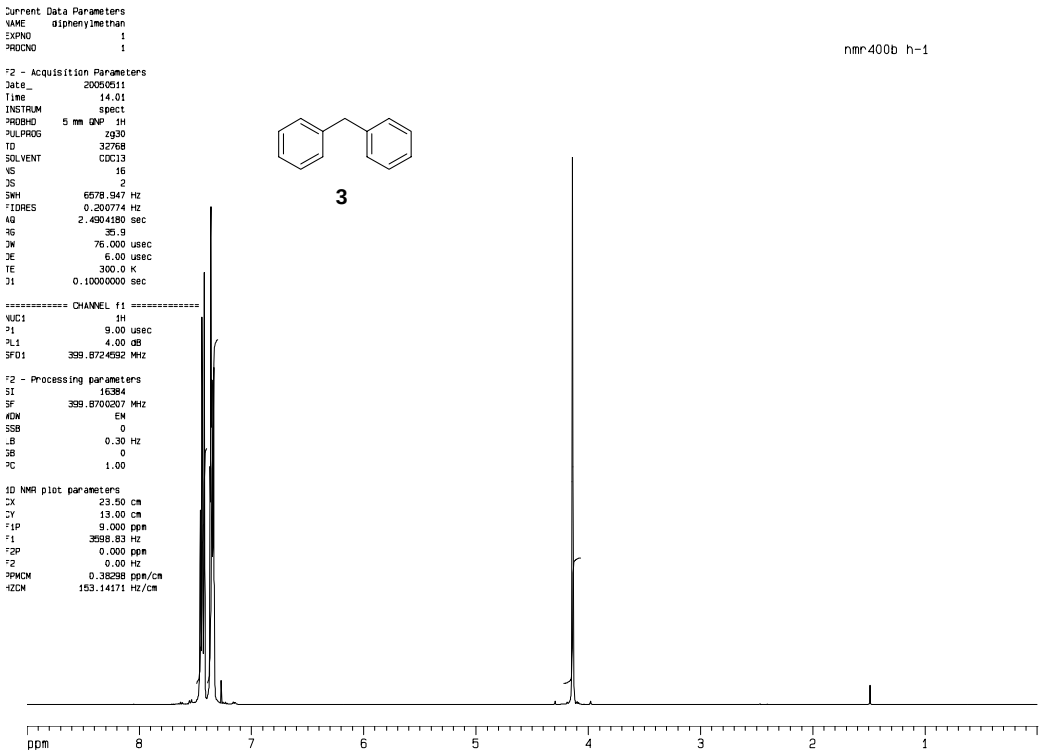
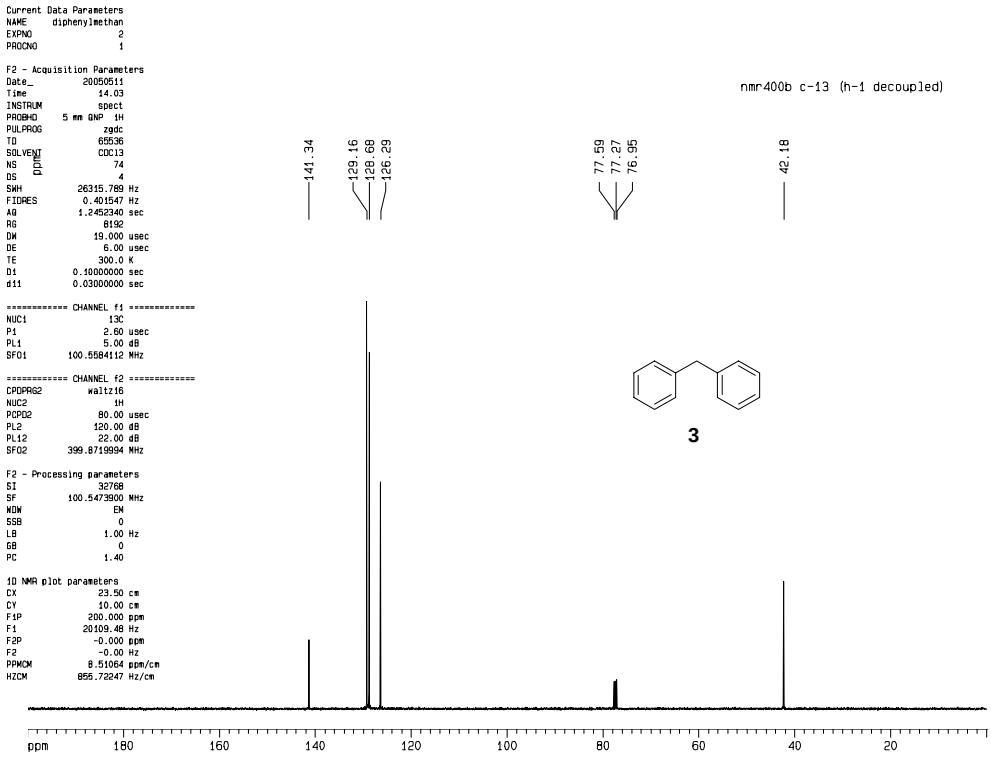
NAME 180000-017-1-1
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20050222
Time 10.25
INSTRUM spect
PROBHD 5 mm GNP 1H
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 32
DS 2
SWH 6578.947 Hz
FIDRES 0.200774 Hz
AQ 2.4904180 sec
RG 64
DW 76.000 usec
DE 6.00 usec
TE 300.0 K
D1 0.10000000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 9.00 usec
PL1 4.00 dB
SFO1 399.8724592 MHz
F2 - Processing parameters
SI 16384
SF 399.8700207 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 23.50 cm
CY 13.00 cm
F1P 9.000 ppm
F1 3598.83 Hz
F2P 0.000 ppm
F2 0.00 Hz
PPMCM 0.38298 ppm/cm
HZCM 153.14171 Hz/cm
nmr400b h-1
23
ppm
8
7
6
5
4
3
2
1

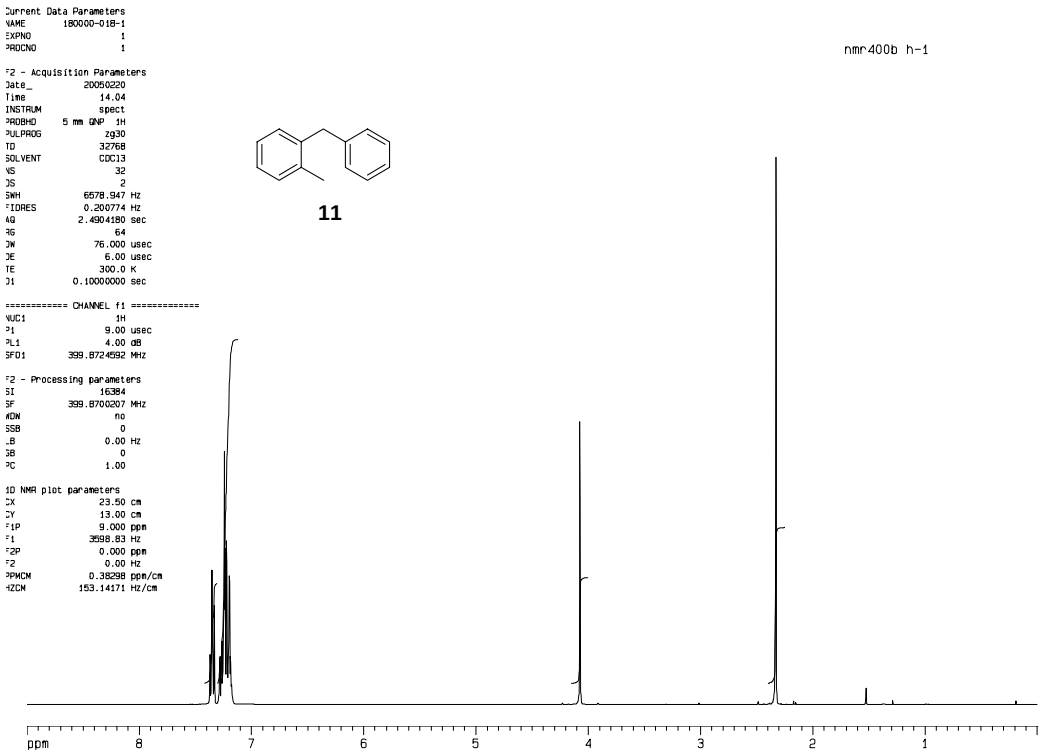

Current Data Parameters
NAME 180000-017-1-1
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20050222
Time 10.31
INSTRUM spect
PROBHD 5 mm GNP 1H
PULPROG zgpg
TD 65536
SOLVENT CDCl3
NS 196
DS 4
SWH 26315.789 Hz
FIDRES 0.401547 Hz
AQ 1.2452340 sec
RG 8192
DW 19.000 usec
DE 6.00 usec
TE 300.0 K
D1 0.10000000 sec
D11 0.03000000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 2.60 usec
PL1 5.00 dB
SFO1 100.5584112 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 120.00 dB
PL12 22.00 dB
SFO2 399.8719994 MHz
F2 - Processing parameters
SI 32768
SF 100.5473900 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
1D NMR plot parameters
CX 23.50 cm
CY 10.00 cm
F1P 200.000 ppm
F1 20109.48 Hz
F2P -0.000 ppm
F2 -0.00 Hz
PPMCM 8.51064 ppm/cm
HZCM 855.72247 Hz/cm
nmr400b c-13 (h-1 decoupled)
138.36
133.20
133.13
129.26
128.09
77.45
77.13
76.81
69.06
69.00
63.81
63.75
21.24
16.15
16.09
23
ppm
180
160
140
120
100
80
60
40
20

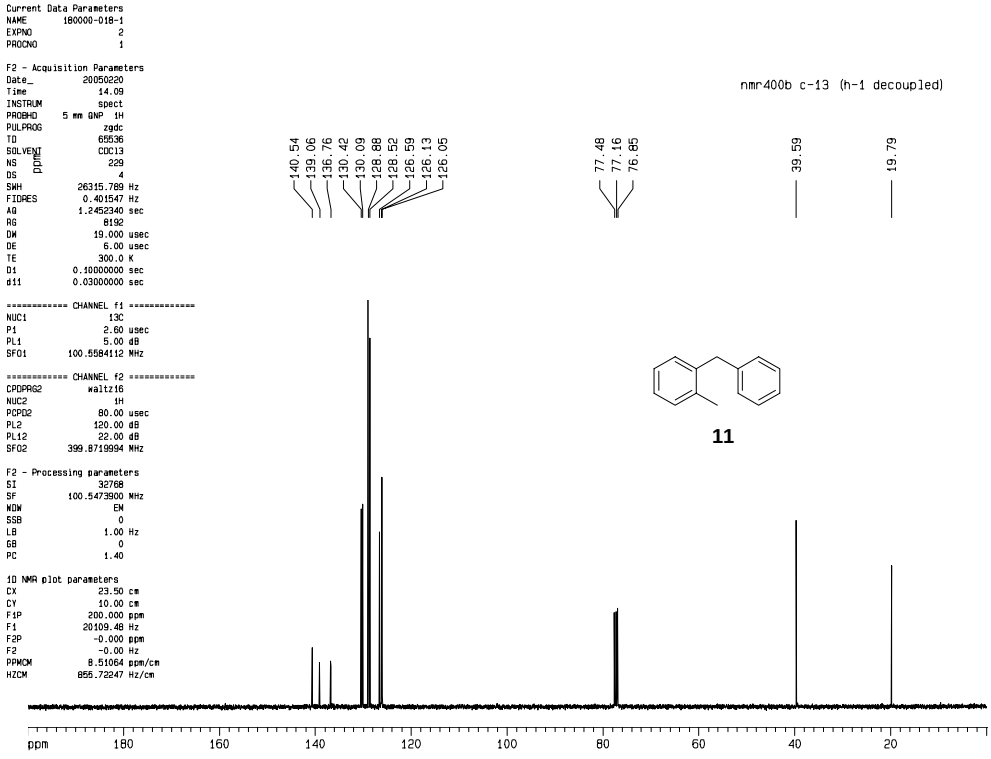

Current Data Parameters
NAME 180000-017-6-1
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20050222
Time 10.47
INSTRUM spect
PROBHD 5 mm GNP 1H
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 32
DS 2
SWH 6578.947 Hz
FIDRES 0.200774 Hz
AQ 2.4904180 sec
RG 362
DW 76.000 usec
DE 6.00 usec
TE 300.0 K
D1 0.10000000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 9.00 usec
PL1 4.00 dB
SFO1 399.8724592 MHz
F2 - Processing parameters
SI 16384
SF 399.8700207 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 23.50 cm
CY 13.00 cm
F1P 9.000 ppm
F1 3598.83 Hz
F2P 0.000 ppm
F2 0.00 Hz
PPMCM 0.38298 ppm/cm
HZCM 153.14171 Hz/cm
nmr400b h-1
27
ppm
8
7
6
5
4
3
2
1

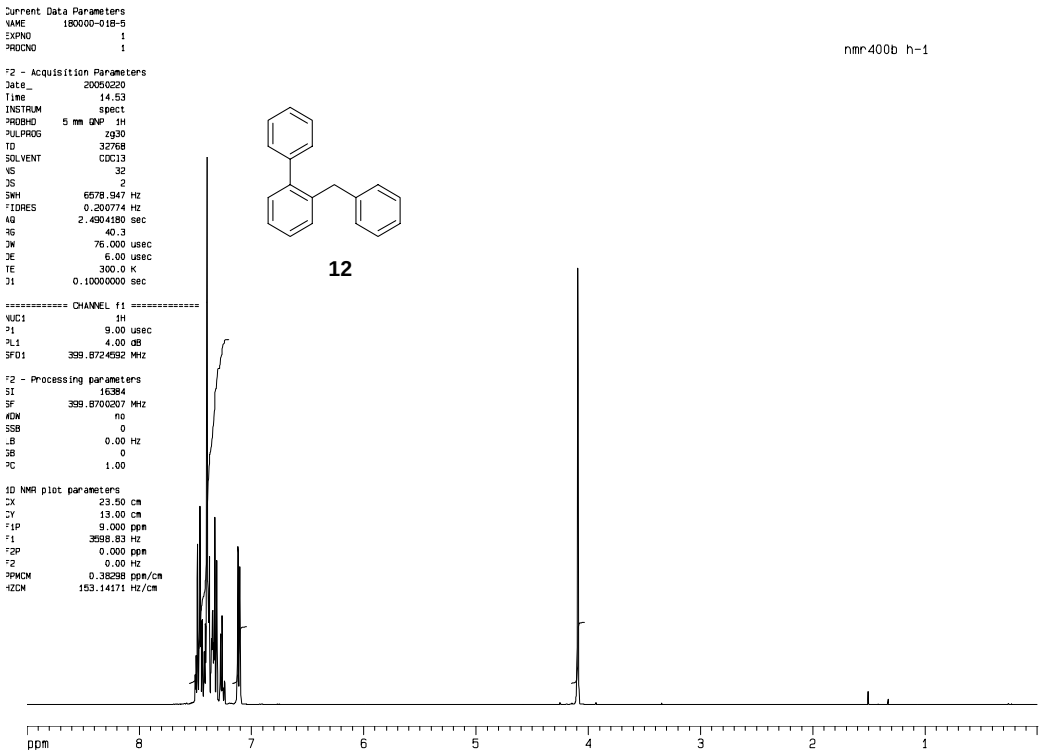

Current Data Parameters
NAME 180000-017-6-2
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20050222
Time 11.13
INSTRUM spect
PROBHD 5 mm GNP 1H
PULPROG zgdc
TD 65536
SOLVENT CDCl3
NS 206
DS 4
SWH 26315.789 Hz
FIDRES 0.401547 Hz
AQ 1.2452340 sec
RG 8192
DW 19.000 usec
DE 6.00 usec
TE 300.0 K
D1 0.10000000 sec
d11 0.03000000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 2.60 usec
PL1 5.00 dB
SFO1 100.5584112 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 120.00 dB
PL12 22.00 dB
SFO2 399.8719994 MHz
F2 - Processing parameters
SI 32768
SF 100.5473900 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
1D NMR plot parameters
CX 23.50 cm
CY 10.00 cm
F1P 200.000 ppm
F1 20109.48 Hz
F2P -0.000 ppm
F2 -0.00 Hz
PPMCM 8.51064 ppm/cm
HZCM 855.72247 Hz/cm
nmr400b c-13 (h-1 decoupled)
141.83
141.78
128.50
128.15
125.92
77.44
77.12
76.80
76.73
76.68
63.63
63.61
63.57
63.55
24.25
24.20
16.11
16.03
15.96
27
ppm
180
160
140
120
100
80
60
40
20

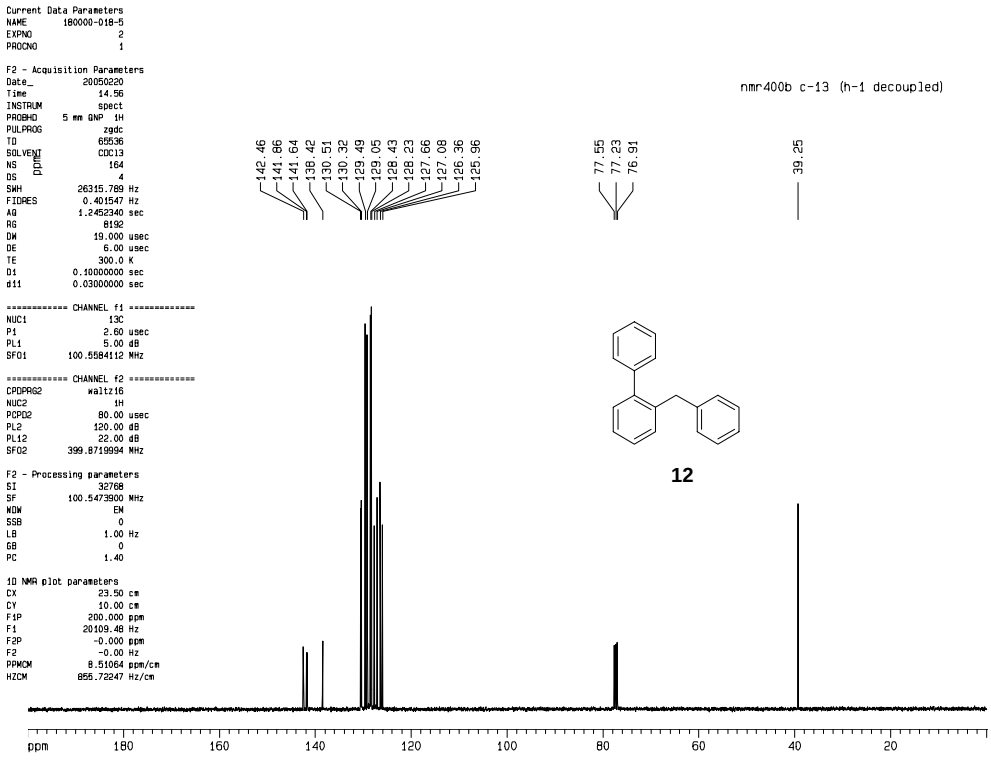

Current Data Parameters
NAME diphenylmethan
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20050511
Time 14.01
INSTRUM spect
PROBHD 5 mm GNP 1H
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 2
SWH 6578.947 Hz
FIDRES 0.200774 Hz
AQ 2.4904180 sec
RG 35.9
DW 76.000 usec
DE 6.00 usec
TE 300.0 K
D1 0.10000000 sec
========== CHANNEL f1 ==========
NUC1 1H
P1 9.00 usec
PL1 4.00 dB
SFO1 399.8724592 MHz
F2 - Processing parameters
SI 16384
SF 399.8700207 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 23.50 cm
CY 13.00 cm
F1P 9.000 ppm
F1 3598.83 Hz
F2P 0.000 ppm
F2 0.00 Hz
PPMCM 0.38298 ppm/cm
HZCM 153.14171 Hz/cm
nmr400b h-1
3
ppm
8
7
6
5
4
3
2
1

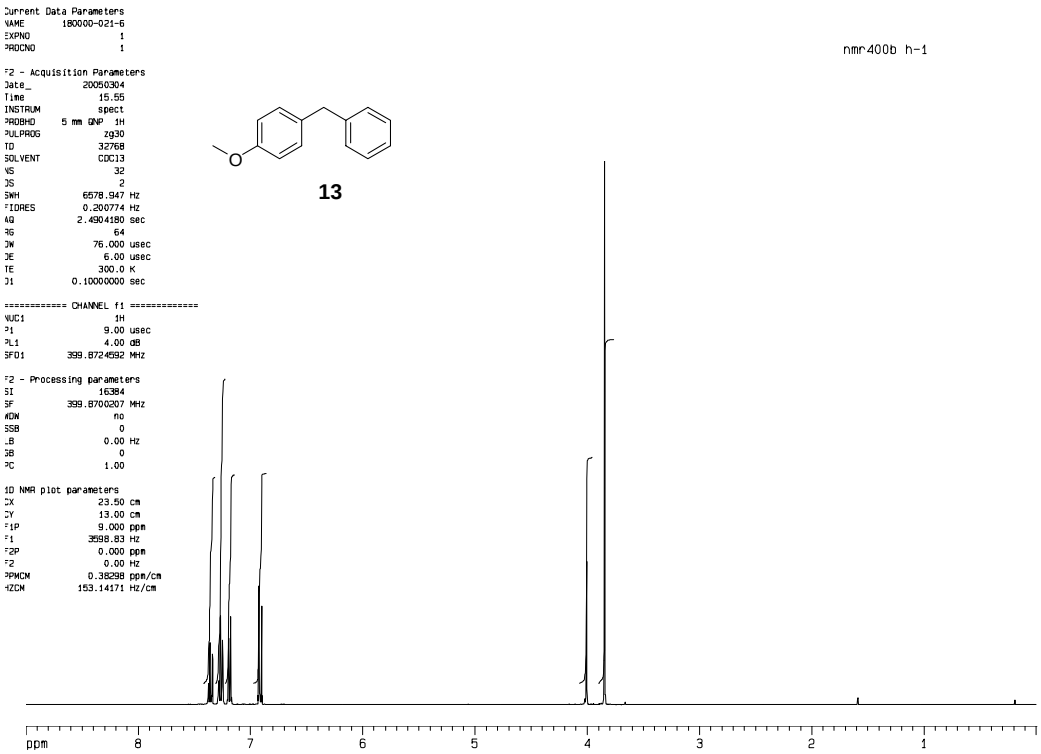

Current Data Parameters
NAME diphenylmethan
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20050511
Time 14.03
INSTRUM spect
PROBHD 5 mm GNP 1H
PULPROG zgdc
TD 65536
SOLVENT CDCl3
NS 74
DS 4
SWH 26315.789 Hz
FIDRES 0.401547 Hz
AQ 1.2452340 sec
RG 8192
DW 19.000 usec
DE 6.00 usec
TE 300.0 K
D1 0.10000000 sec
d11 0.03000000 sec
========== CHANNEL f1 ==========
NUC1 13C
P1 2.60 usec
PL1 5.00 dB
SFO1 100.5584112 MHz
========== CHANNEL f2 ==========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 120.00 dB
PL12 22.00 dB
SFO2 399.8719994 MHz
F2 - Processing parameters
SI 32768
SF 100.5473900 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
1D NMR plot parameters
CX 23.50 cm
CY 10.00 cm
F1P 200.000 ppm
F1 20109.48 Hz
F2P -0.000 ppm
F2 -0.00 Hz
PPMCM 8.51064 ppm/cm
HZCM 855.72247 Hz/cm
nmr400b c-13 (h-1 decoupled)
141.34
129.16
128.68
126.29
77.59
77.27
76.95
42.18
3
ppm
180
160
140
120
100
80
60
40
20

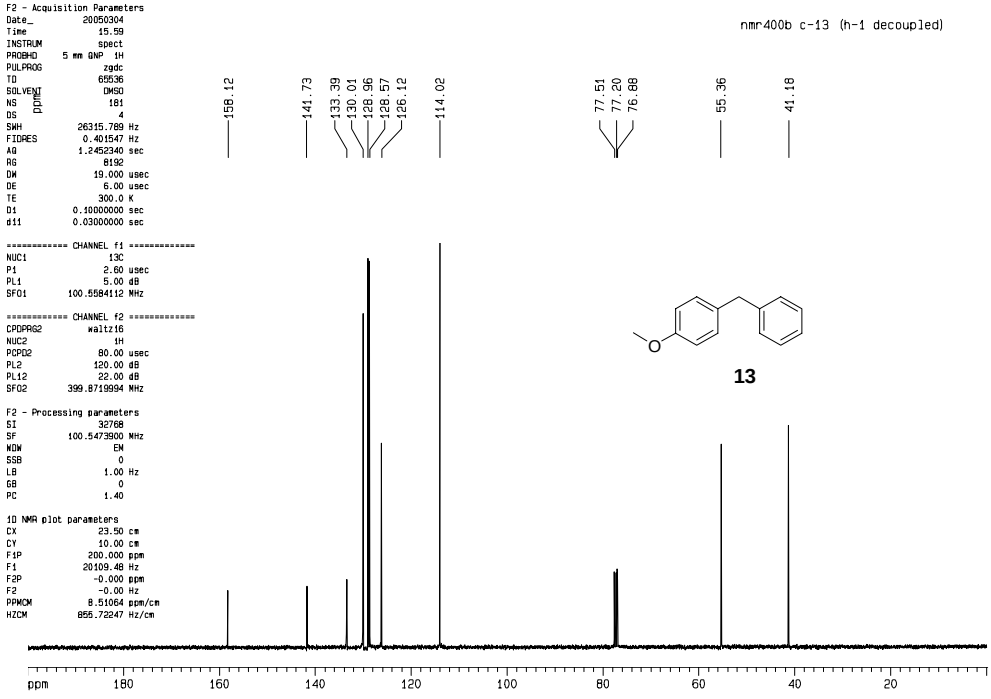

Current Data Parameters
NAME 180000-018-1
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20050220
Time 14.04
INSTRUM spect
PROBHD 5 mm QNP 1H
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 32
DS 2
SWH 6578.947 Hz
FIDRES 0.200774 Hz
AQ 2.4904180 sec
RG 64
DW 76.000 usec
DE 6.00 usec
TE 300.0 K
D1 0.10000000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 9.00 usec
PL1 4.00 dB
SFO1 399.8724592 MHz
F2 - Processing parameters
SI 16384
SF 399.8700207 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 23.50 cm
CY 13.00 cm
F1P 9.000 ppm
F1 3598.83 Hz
F2P 0.000 ppm
F2 0.00 Hz
PPMCM 0.38298 ppm/cm
HZCM 153.14171 Hz/cm
nmr400b h-1
11
ppm
8
7
6
5
4
3
2
1

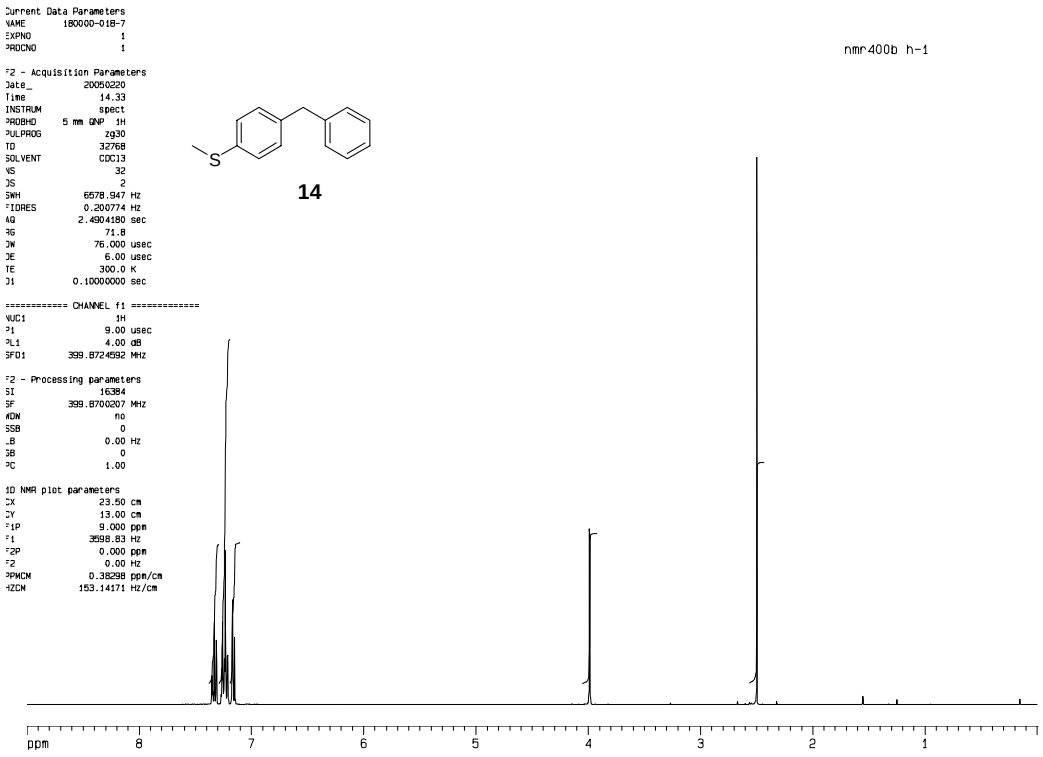

Current Data Parameters
NAME 180000-018-1
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20050220
Time 14.09
INSTRUM spect
PROBHD 5 mm QNP 1H
PULPROG zgdc
TD 65536
SOLVENT CDCl3
NS 229
DS 4
SWH 26315.789 Hz
FIDRES 0.401547 Hz
AQ 1.2452340 sec
RG 8192
DW 19.000 usec
DE 6.00 usec
TE 300.0 K
D1 0.10000000 sec
d11 0.03000000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 2.60 usec
PL1 5.00 dB
SFO1 100.5584112 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 120.00 dB
PL12 22.00 dB
SFO2 399.8719994 MHz
F2 - Processing parameters
SI 32768
SF 100.5473900 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
1D NMR plot parameters
CX 23.50 cm
CY 10.00 cm
F1P 200.000 ppm
F1 20109.48 Hz
F2P -0.000 ppm
F2 -0.00 Hz
PPMCM 8.51064 ppm/cm
HZCM 855.72247 Hz/cm
nmr400b c-13 (h-1 decoupled)
140.54
139.06
136.76
130.42
130.09
128.88
128.52
126.59
126.13
126.05
77.48
77.16
76.85
39.59
19.79
11
ppm
180
160
140
120
100
80
60
40
20

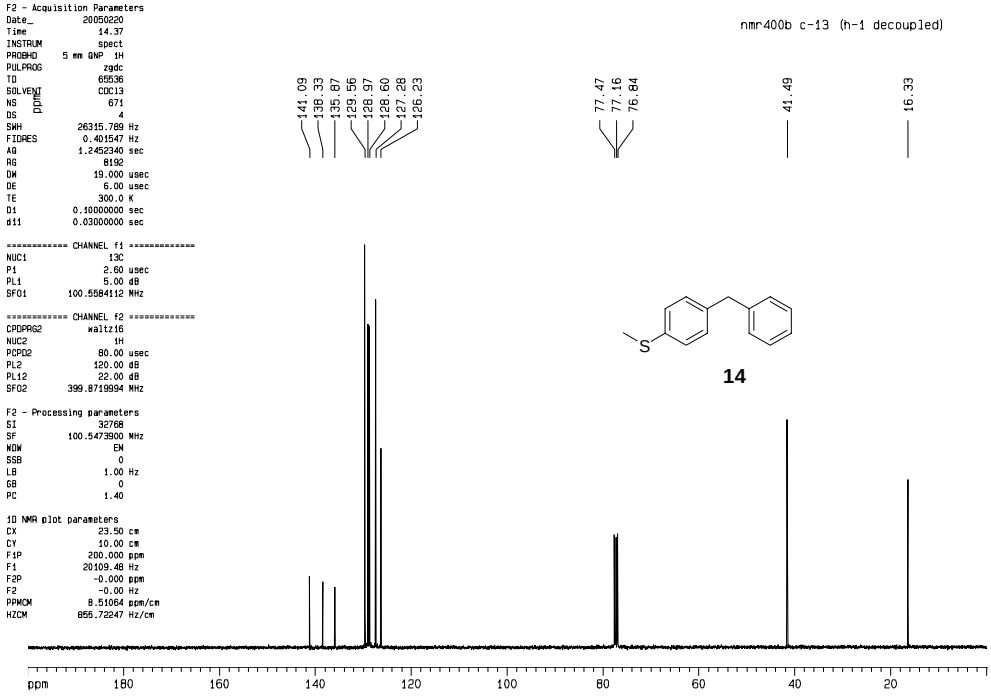

Current Data Parameters
NAME 180000-018-5
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20050220
Time 14.53
INSTRUM spect
PROBHD 5 mm QNP 1H
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 32
DS 2
SWH 6578.947 Hz
FIDRES 0.200774 Hz
AQ 2.4904180 sec
RG 40.3
DW 76.000 usec
DE 6.00 usec
TE 300.0 K
D1 0.10000000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 9.00 usec
PL1 4.00 dB
SFO1 399.8724592 MHz
F2 - Processing parameters
SI 16384
SF 399.8700207 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 23.50 cm
CY 13.00 cm
F1P 9.000 ppm
F1 3598.83 Hz
F2P 0.000 ppm
F2 0.00 Hz
PPMCM 0.38298 ppm/cm
HZCM 153.14171 Hz/cm
nmr400b h-1
12
ppm
8
7
6
5
4
3
2
1

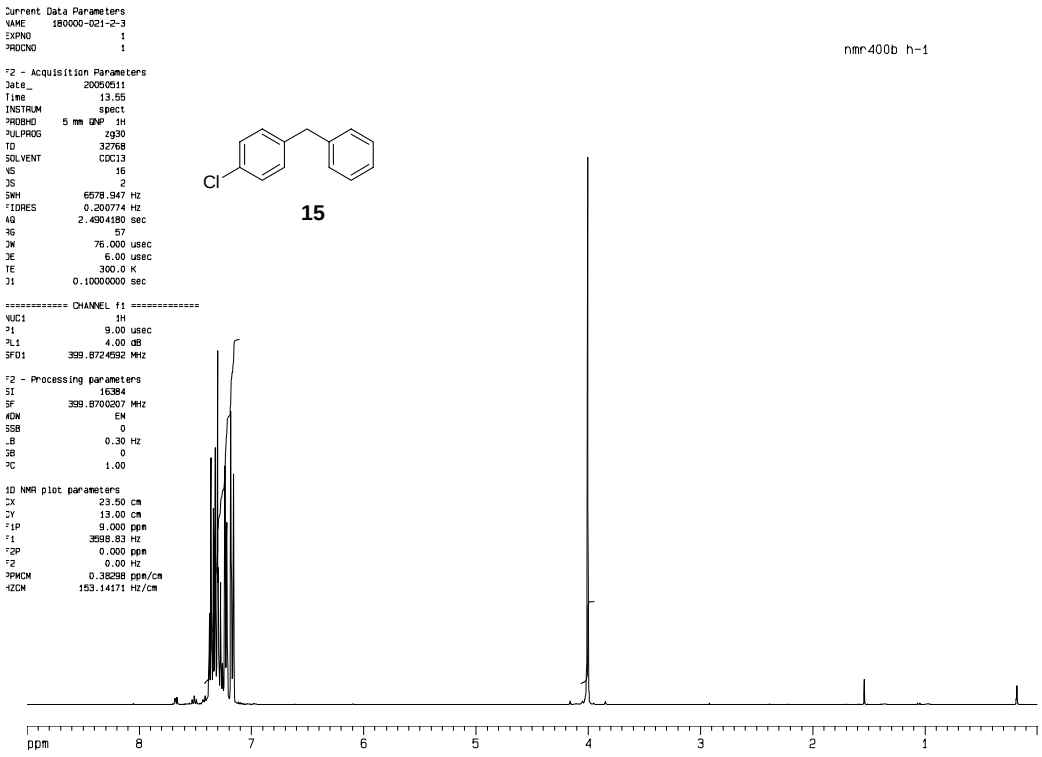

Current Data Parameters
NAME 180000-018-5
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20050220
Time 14.56
INSTRUM spect
PROBHD 5 mm QNP 1H
PULPROG zgdc
TD 65536
SOLVENT CDCl3
NS 164
DS 4
SWH 26315.789 Hz
FIDRES 0.401547 Hz
AQ 1.2452340 sec
RG 8192
DW 19.000 usec
DE 6.00 usec
TE 300.0 K
D1 0.10000000 sec
d11 0.03000000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 2.60 usec
PL1 5.00 dB
SFO1 100.5584112 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 120.00 dB
PL12 22.00 dB
SFO2 399.8719994 MHz
F2 - Processing parameters
SI 32768
SF 100.5473900 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
1D NMR plot parameters
CX 23.50 cm
CY 10.00 cm
F1P 200.000 ppm
F1 20109.48 Hz
F2P -0.000 ppm
F2 -0.00 Hz
PPMCM 8.51064 ppm/cm
HZCM 855.72247 Hz/cm
nmr400b c-13 (h-1 decoupled)
142.46
141.86
141.64
138.42
130.51
130.32
129.49
129.05
128.43
128.23
127.66
127.08
126.36
125.96
77.55
77.23
76.91
39.25
12
ppm
180
160
140
120
100
80
60
40
20

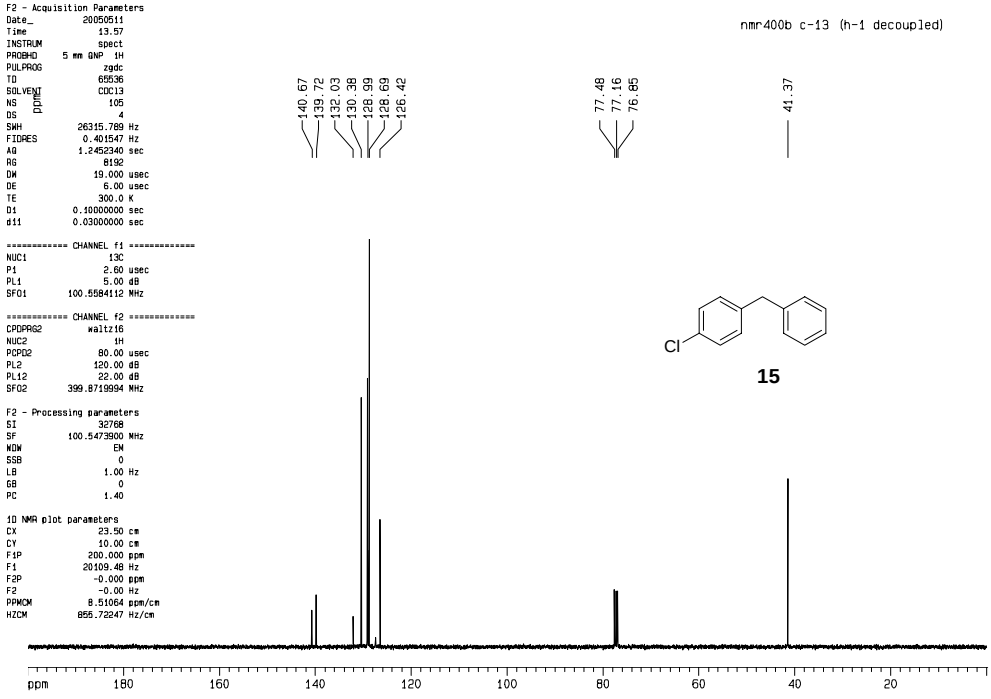

Current Data Parameters
NAME 180000-021-6
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20050304
Time 15.55
INSTRUM spect
PROBHD 5 mm QNP 1H
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 32
DS 2
SWH 6578.947 Hz
FIDRES 0.200774 Hz
AQ 2.4904180 sec
RG 64
DW 76.000 usec
DE 6.00 usec
TE 300.0 K
D1 0.10000000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 9.00 usec
PL1 4.00 dB
SFO1 399.8724592 MHz
F2 - Processing parameters
SI 16384
SF 399.8700207 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 23.50 cm
CY 13.00 cm
F1P 9.000 ppm
F1 3598.83 Hz
F2P 0.000 ppm
F2 0.00 Hz
PPMCM 0.38298 ppm/cm
HZCM 153.14171 Hz/cm
nmr400b h-1
13
ppm
8
7
6
5
4
3
2
1

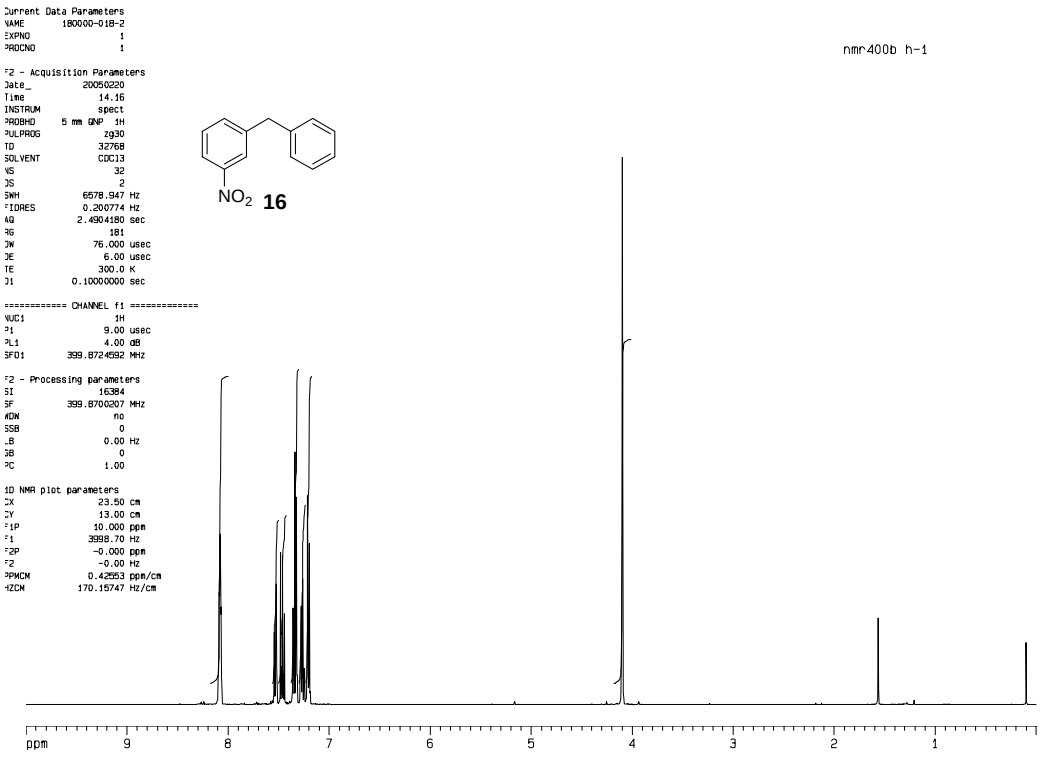

Current Data Parameters
NAME 180000-021-6
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20050304
Time 15.59
INSTRUM spect
PROBHD 5 mm QNP 1H
PULPROG zgdc
TD 65536
SOLVENT DMSO
NS 181
DS 4
SWH 26315.789 Hz
FIDRES 0.401547 Hz
AQ 1.2452340 sec
RG 8192
DW 19.000 usec
DE 6.00 usec
TE 300.0 K
D1 0.10000000 sec
d11 0.03000000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 2.60 usec
PL1 5.00 dB
SFO1 100.5584112 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 120.00 dB
PL12 22.00 dB
SFO2 399.8719994 MHz
F2 - Processing parameters
SI 32768
SF 100.5473900 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
1D NMR plot parameters
CX 23.50 cm
CY 10.00 cm
F1P 200.000 ppm
F1 20109.48 Hz
F2P -0.000 ppm
F2 -0.00 Hz
PPMCM 8.51064 ppm/cm
HZCM 855.72247 Hz/cm
nmr400b c-13 (h-1 decoupled)
ppm
158.12
141.73
133.39
130.01
128.96
128.57
126.12
114.02
77.51
77.20
76.88
55.36
41.18
13
ppm
180
160
140
120
100
80
60
40
20

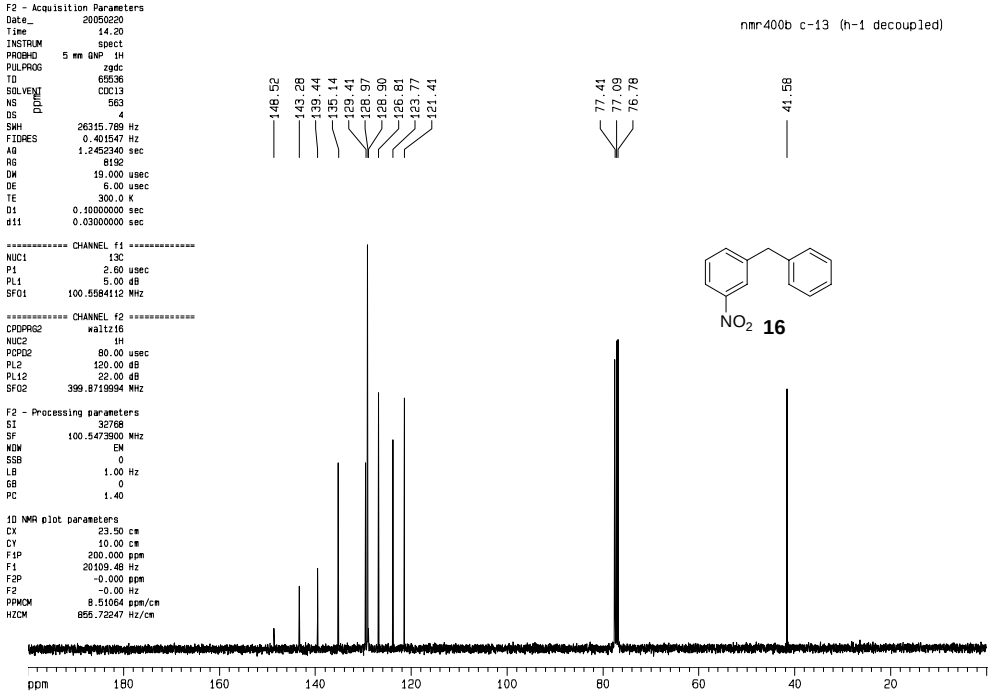

Current Data Parameters
NAME 180000-018-7
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20050220
Time 14.33
INSTRUM spect
PROBHD 5 mm QNP 1H
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 32
DS 2
SWH 6578.947 Hz
FIDRES 0.200774 Hz
AQ 2.4904180 sec
RG 71.8
DW 76.000 usec
DE 6.00 usec
TE 300.0 K
D1 0.10000000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 9.00 usec
PL1 4.00 dB
SFO1 399.8724592 MHz
F2 - Processing parameters
SI 16384
SF 399.8700207 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 23.50 cm
CY 13.00 cm
F1P 9.000 ppm
F1 3598.83 Hz
F2P 0.000 ppm
F2 0.00 Hz
PPMCM 0.38298 ppm/cm
HZCM 153.14171 Hz/cm
S
14
nmr400b h-1
ppm
8
7
6
5
4
3
2
1

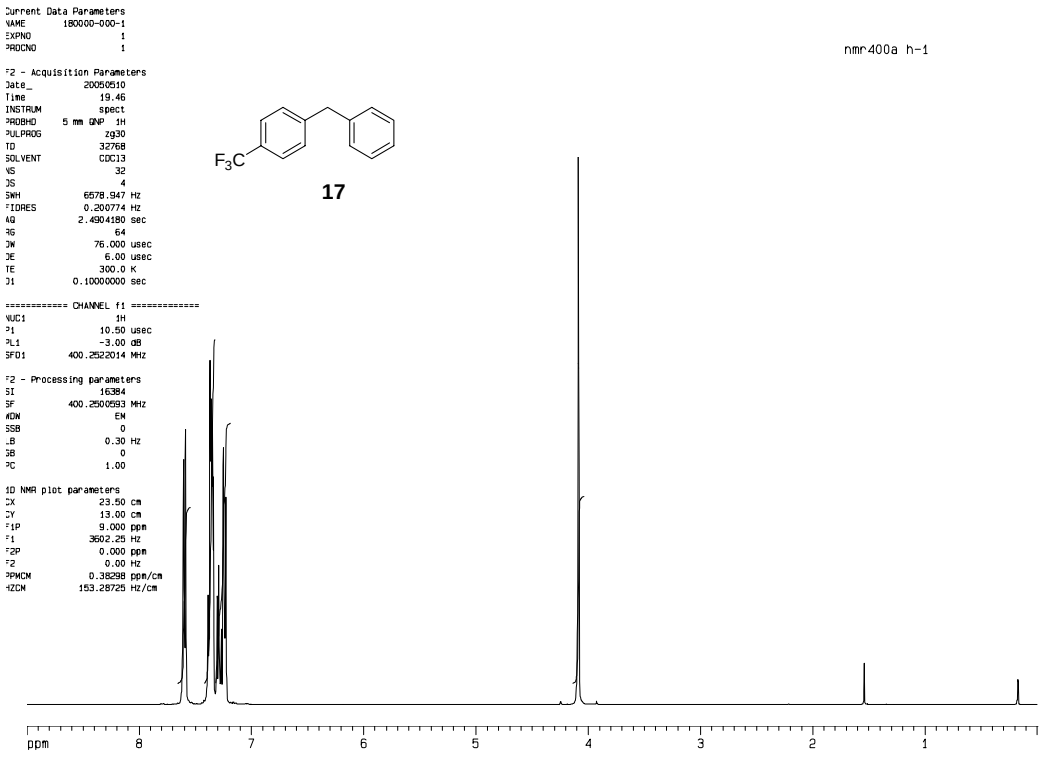

Current Data Parameters
NAME 180000-018-7
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20050220
Time 14.37
INSTRUM spect
PROBHD 5 mm QNP 1H
PULPROG zgdc
TD 65536
SOLVENT CDCl3
NS 671
DS 4
SWH 26315.789 Hz
FIDRES 0.401547 Hz
AQ 1.2452340 sec
RG 8192
DW 19.000 usec
DE 6.00 usec
TE 300.0 K
D1 0.10000000 sec
d11 0.03000000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 2.60 usec
PL1 5.00 dB
SFO1 100.5584112 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 120.00 dB
PL12 22.00 dB
SFO2 399.8719994 MHz
F2 - Processing parameters
SI 32768
SF 100.5473900 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
1D NMR plot parameters
CX 23.50 cm
CY 10.00 cm
F1P 200.000 ppm
F1 20109.48 Hz
F2P -0.000 ppm
F2 -0.00 Hz
PPMCM 8.51064 ppm/cm
HZCM 855.72247 Hz/cm
nmr400b c-13 (h-1 decoupled)
141.09
138.33
135.87
129.56
128.97
128.60
127.28
126.23
77.47
77.16
76.84
41.49
16.33
S
14
ppm
180
160
140
120
100
80
60
40
20

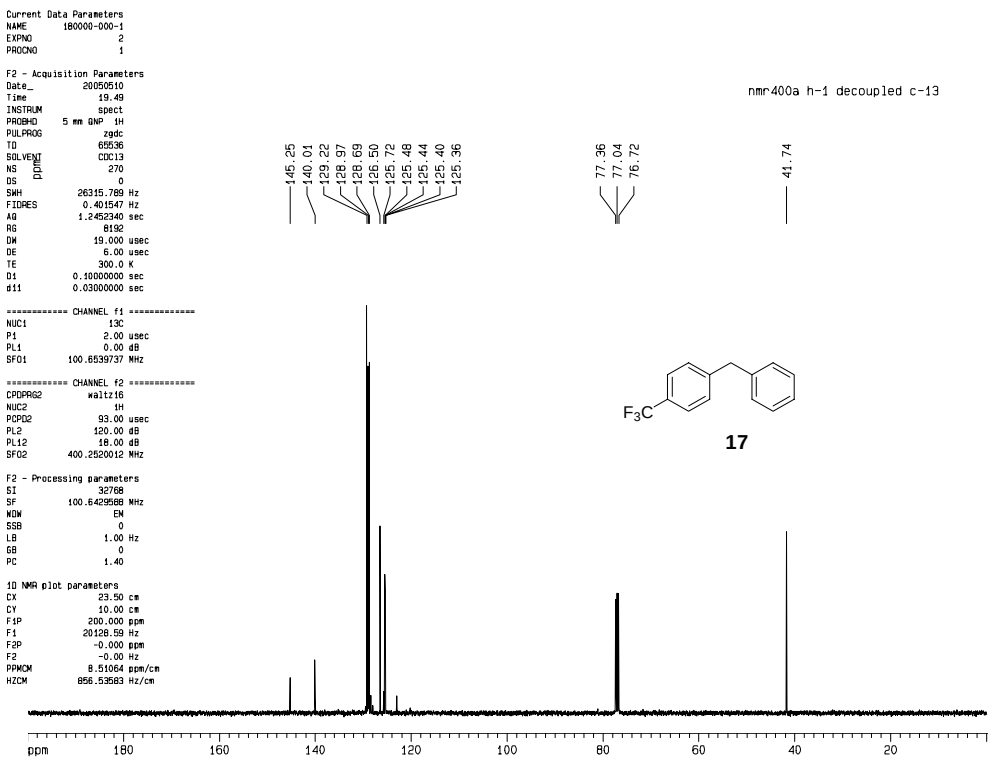

Current Data Parameters
NAME 180000-021-2-3
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20050511
Time 13.55
INSTRUM spect
PROBHD 5 mm QNP 1H
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 2
SWH 6578.947 Hz
FIDRES 0.200774 Hz
AQ 2.4904180 sec
RG 57
DW 76.000 usec
DE 6.00 usec
TE 300.0 K
D1 0.10000000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 9.00 usec
PL1 4.00 dB
SFO1 399.8724592 MHz
F2 - Processing parameters
SI 16384
SF 399.8700207 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 23.50 cm
CY 13.00 cm
F1P 9.000 ppm
F1 3598.83 Hz
F2P 0.000 ppm
F2 0.00 Hz
PPMCM 0.38298 ppm/cm
HZCM 153.14171 Hz/cm
nmr400b h-1
Cl
15
ppm
8
7
6
5
4
3
2
1

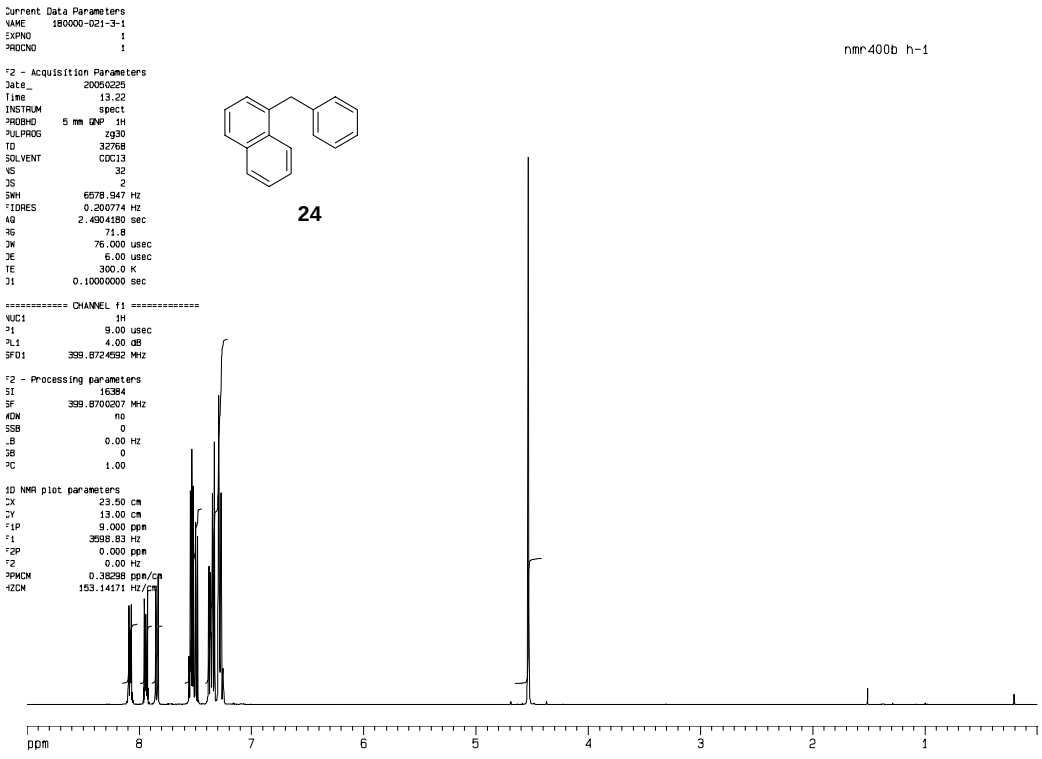

Current Data Parameters
NAME 180000-021-2-3
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20050511
Time 13.57
INSTRUM spect
PROBHD 5 mm QNP 1H
PULPROG zgdc
TD 65536
SOLVENT CDCl3
NS 105
DS 4
SWH 26315.789 Hz
FIDRES 0.401547 Hz
AQ 1.2452340 sec
RG 8192
DW 19.000 usec
DE 6.00 usec
TE 300.0 K
D1 0.10000000 sec
d11 0.03000000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 2.60 usec
PL1 5.00 dB
SFO1 100.5584112 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 120.00 dB
PL12 22.00 dB
SFO2 399.8719994 MHz
F2 - Processing parameters
SI 32768
SF 100.5473900 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
1D NMR plot parameters
CX 23.50 cm
CY 10.00 cm
F1P 200.000 ppm
F1 20109.48 Hz
F2P -0.000 ppm
F2 -0.00 Hz
PPMCM 8.51064 ppm/cm
HZCM 855.72247 Hz/cm
nmr400b c-13 (h-1 decoupled)
140.67
139.72
132.03
130.38
128.99
128.69
126.42
77.48
77.16
76.85
41.37
Cl
15
ppm
180
160
140
120
100
80
60
40
20

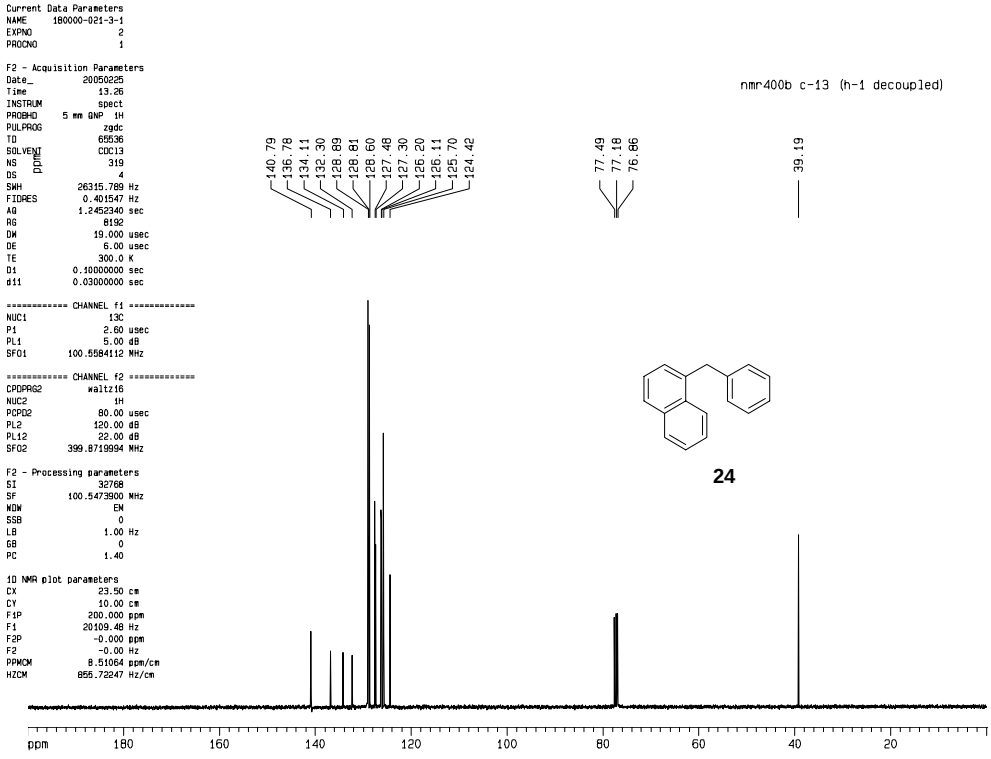

Current Data Parameters
NAME 180000-018-2
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20050220
Time 14.16
INSTRUM spect
PROBHD 5 mm QNP 1H
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 32
DS 2
SWH 6578.947 Hz
FIDRES 0.200774 Hz
AQ 2.4904180 sec
RG 181
DW 76.000 usec
DE 6.00 usec
TE 300.0 K
D1 0.10000000 sec
========== CHANNEL f1 ==========
NUC1 1H
P1 9.00 usec
PL1 4.00 dB
SFO1 399.8724592 MHz
F2 - Processing parameters
SI 16384
SF 399.8700207 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 23.50 cm
CY 13.00 cm
F1P 10.000 ppm
F1 3998.70 Hz
F2P -0.000 ppm
F2 -0.00 Hz
PPMCM 0.42553 ppm/cm
HZCM 170.15747 Hz/cm
NO2 16
nmr400b h-1
ppm 9 8 7 6 5 4 3 2 1

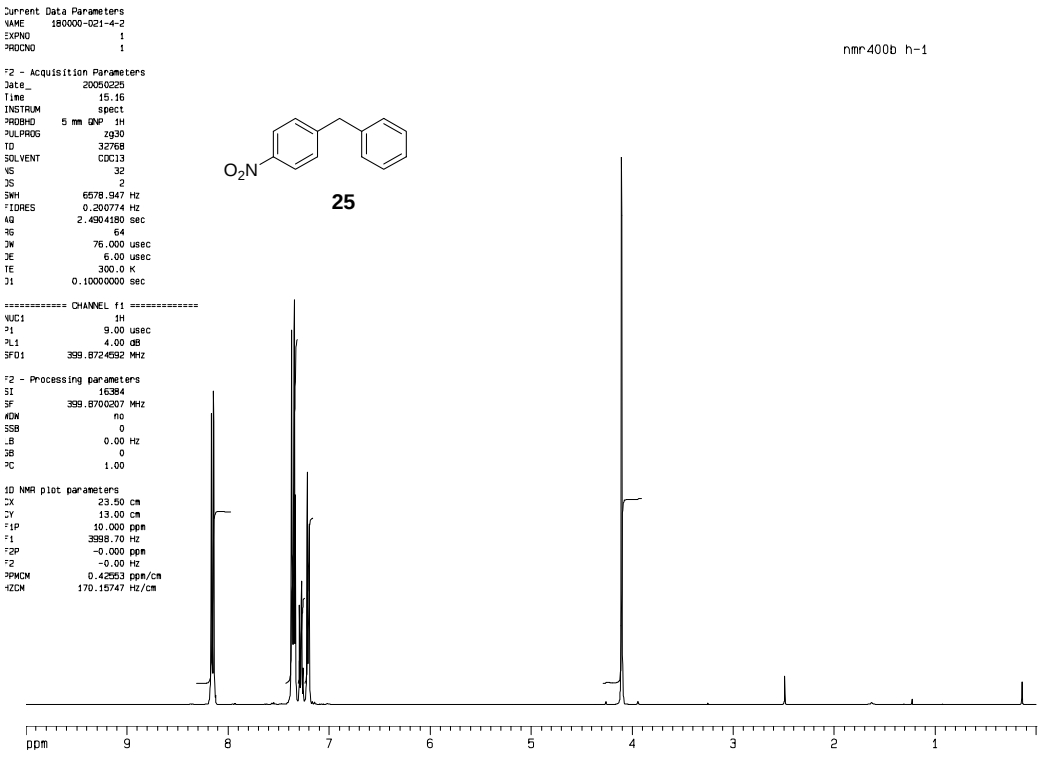

Current Data Parameters
NAME 180000-018-2
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20050220
Time 14.20
INSTRUM spect
PROBHD 5 mm QNP 1H
PULPROG zgdc
TD 65536
SOLVENT CDCl3
NS 563
DS 4
SWH 26315.789 Hz
FIDRES 0.401547 Hz
AQ 1.2452340 sec
RG 8192
DW 19.000 usec
DE 6.00 usec
TE 300.0 K
D1 0.10000000 sec
d11 0.03000000 sec
========== CHANNEL f1 ==========
NUC1 13C
P1 2.60 usec
PL1 5.00 dB
SFO1 100.5584112 MHz
========== CHANNEL f2 ==========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 120.00 dB
PL12 22.00 dB
SFO2 399.8719994 MHz
F2 - Processing parameters
SI 32768
SF 100.5473900 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
1D NMR plot parameters
CX 23.50 cm
CY 10.00 cm
F1P 200.000 ppm
F1 20109.48 Hz
F2P -0.000 ppm
F2 -0.00 Hz
PPMCM 8.51064 ppm/cm
HZCM 855.72247 Hz/cm
ppm
148.52
143.28
139.44
135.14
129.41
128.97
128.90
126.81
123.77
121.41
77.41
77.09
76.78
41.58
NO2 16
nmr400b c-13 (h-1 decoupled)
ppm 180 160 140 120 100 80 60 40 20

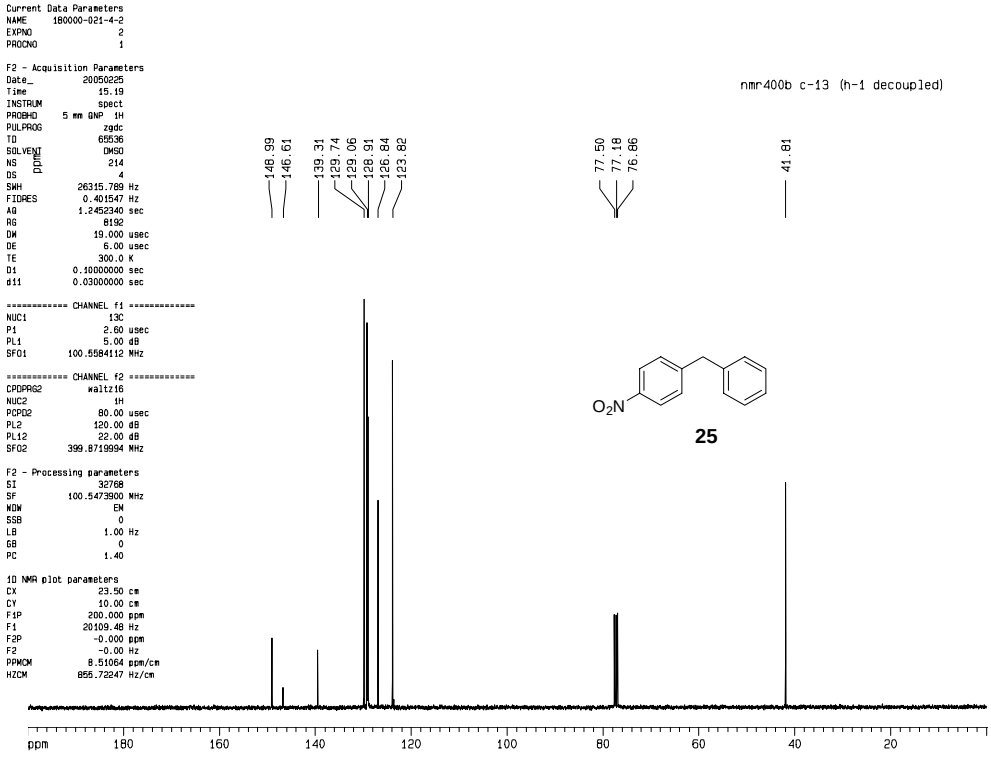

Current Data Parameters
NAME 180000-000-1
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20050510
Time 19.46
INSTRUM spect
PROBHD 5 mm QNP 1H
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 32
DS 4
SWH 6578.947 Hz
FIDRES 0.200774 Hz
AQ 2.4904180 sec
RG 64
DW 76.000 usec
DE 6.00 usec
TE 300.0 K
D1 0.10000000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 10.50 usec
PL1 -3.00 dB
SFO1 400.2522014 MHz
F2 - Processing parameters
SI 16384
SF 400.2500593 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 23.50 cm
CY 13.00 cm
F1P 9.000 ppm
F1 3602.25 Hz
F2P 0.000 ppm
F2 0.00 Hz
PPMCM 0.38298 ppm/cm
HZCM 153.28725 Hz/cm
nmr400a h-1
F3C
17
ppm
8
7
6
5
4
3
2
1

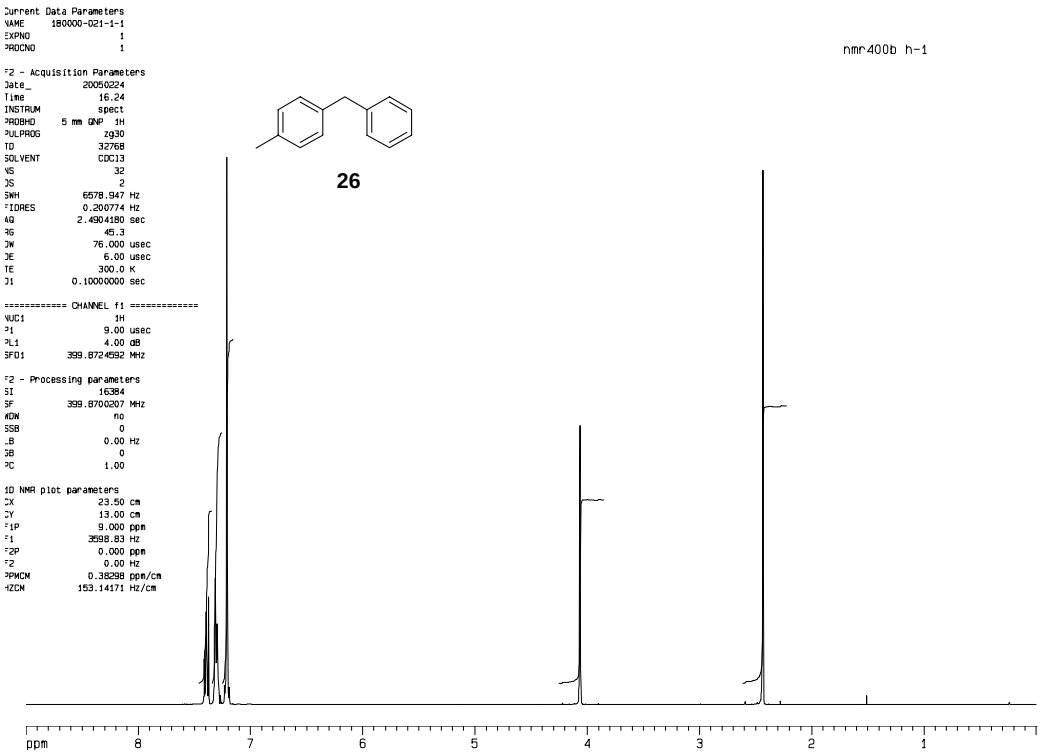

Current Data Parameters
NAME 180000-000-1
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20050510
Time 19.49
INSTRUM spect
PROBHD 5 mm QNP 1H
PULPROG zgdc
TD 65536
SOLVENT CDCl3
NS 270
DS 0
SWH 26315.789 Hz
FIDRES 0.401547 Hz
AQ 1.2452340 sec
RG 8192
DW 19.000 usec
DE 6.00 usec
TE 300.0 K
D1 0.10000000 sec
d11 0.03000000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 2.00 usec
PL1 0.00 dB
SFO1 100.6539737 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 93.00 usec
PL2 120.00 dB
PL12 18.00 dB
SFO2 400.2520012 MHz
F2 - Processing parameters
SI 32768
SF 100.6429588 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
1D NMR plot parameters
CX 23.50 cm
CY 10.00 cm
F1P 200.000 ppm
F1 20128.59 Hz
F2P -0.000 ppm
F2 -0.00 Hz
PPMCM 8.51064 ppm/cm
HZCM 856.53583 Hz/cm
nmr400a h-1 decoupled c-13
145.25
140.01
129.22
128.97
128.69
126.50
125.72
125.48
125.44
125.40
125.36
77.36
77.04
76.72
41.74
F3C
17
ppm
180
160
140
120
100
80
60
40
20

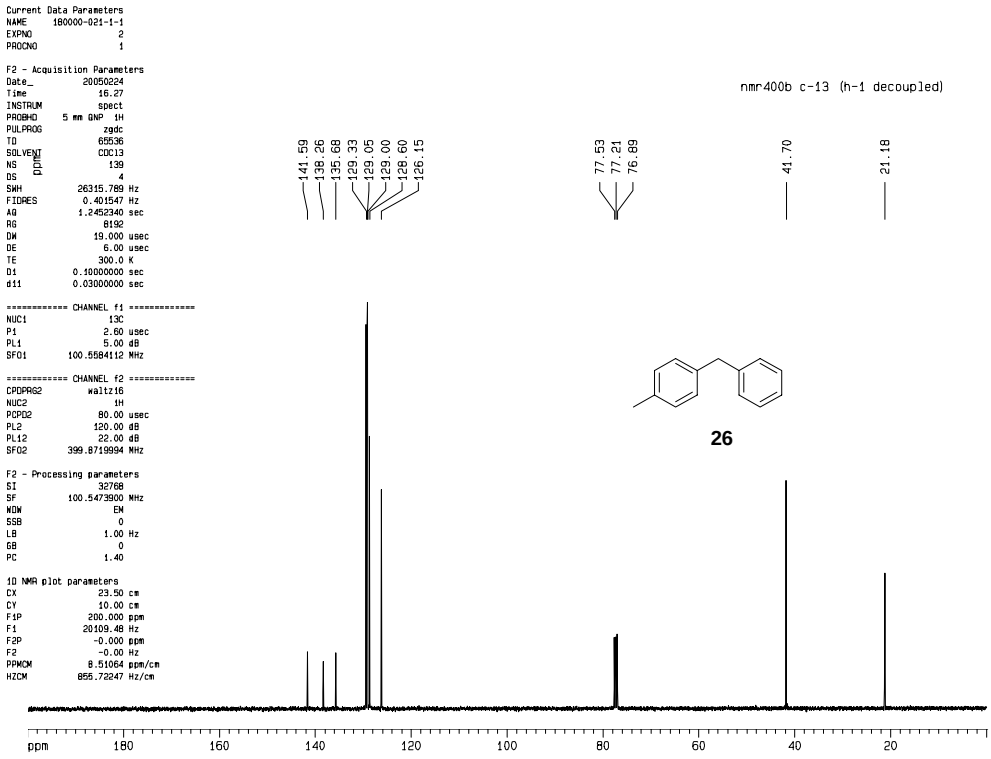

Current Data Parameters
NAME 180000-021-3-1
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20050225
Time 13.22
INSTRUM spect
PROBHD 5 mm QNP 1H
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 32
DS 2
SWH 6578.947 Hz
FIDRES 0.200774 Hz
AQ 2.4904180 sec
RG 71.8
DW 76.000 usec
DE 6.00 usec
TE 300.0 K
D1 0.10000000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 9.00 usec
PL1 4.00 dB
SFO1 399.8724592 MHz
F2 - Processing parameters
SI 16384
SF 399.8700207 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 23.50 cm
CY 13.00 cm
F1P 9.000 ppm
F1 3598.83 Hz
F2P 0.000 ppm
F2 0.00 Hz
PPMCM 0.38298 ppm/cm
HZCM 153.14171 Hz/cm
nmr400b h-1
24
ppm
8
7
6
5
4
3
2
1


Current Data Parameters
NAME 180000-021-3-1
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20050225
Time 13.26
INSTRUM spect
PROBHD 5 mm QNP 1H
PULPROG zgdc
TD 65536
SOLVENT CDCl3
NS 319
DS 4
SWH 26315.789 Hz
FIDRES 0.401547 Hz
AQ 1.2452340 sec
RG 8192
DW 19.000 usec
DE 6.00 usec
TE 300.0 K
D1 0.10000000 sec
d11 0.03000000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 2.60 usec
PL1 5.00 dB
SFO1 100.5584112 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 120.00 dB
PL12 22.00 dB
SFO2 399.8719994 MHz
F2 - Processing parameters
SI 32768
SF 100.5473900 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
1D NMR plot parameters
CX 23.50 cm
CY 10.00 cm
F1P 200.000 ppm
F1 20109.48 Hz
F2P -0.000 ppm
F2 -0.00 Hz
PPMCM 8.51064 ppm/cm
HZCM 855.72247 Hz/cm
nmr400b c-13 (h-1 decoupled)
140.79
136.78
134.11
132.30
128.89
128.81
128.60
127.48
127.30
126.20
126.11
125.70
124.42
77.49
77.18
76.86
39.19
24
ppm
180
160
140
120
100
80
60
40
20


Current Data Parameters
NAME 180000-021-4-2
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20050225
Time 15.16
INSTRUM spect
PROBHD 5 mm GNP 1H
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 32
DS 2
SWH 6578.947 Hz
FIDRES 0.200774 Hz
AQ 2.4904180 sec
RG 64
DW 76.000 usec
DE 6.00 usec
TE 300.0 K
D1 0.10000000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 9.00 usec
PL1 4.00 dB
SFO1 399.8724592 MHz
F2 - Processing parameters
SI 16384
SF 399.8700207 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 23.50 cm
CY 13.00 cm
F1P 10.000 ppm
F1 3998.70 Hz
F2P -0.000 ppm
F2 -0.00 Hz
PPMCM 0.42553 ppm/cm
HZCM 170.15747 Hz/cm
nmr400b h-1
O2N
25
ppm
9
8
7
6
5
4
3
2
1


Current Data Parameters
NAME 180000-021-4-2
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20050225
Time 15.19
INSTRUM spect
PROBHD 5 mm GNP 1H
PULPROG zgdc
TD 65536
SOLVENT DMSO
NS 214
DS 4
SWH 26315.789 Hz
FIDRES 0.401547 Hz
AQ 1.2452340 sec
RG 8192
DW 19.000 usec
DE 6.00 usec
TE 300.0 K
D1 0.10000000 sec
d11 0.03000000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 2.60 usec
PL1 5.00 dB
SFO1 100.5584112 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 120.00 dB
PL12 22.00 dB
SFO2 399.8719994 MHz
F2 - Processing parameters
SI 32768
SF 100.5473900 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
1D NMR plot parameters
CX 23.50 cm
CY 10.00 cm
F1P 200.000 ppm
F1 20109.48 Hz
F2P -0.000 ppm
F2 -0.00 Hz
PPMCM 8.51064 ppm/cm
HZCM 855.72247 Hz/cm
nmr400b c-13 (h-1 decoupled)
148.99
146.61
139.31
129.74
129.06
128.91
126.84
123.82
77.50
77.18
76.86
41.81
O2N
25
ppm
180
160
140
120
100
80
60
40
20


Current Data Parameters
NAME 180000-021-1-1
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20050224
Time 16.24
INSTRUM spect
PROBHD 5 mm GNP 1H
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 32
DS 2
SWH 6578.947 Hz
FIDRES 0.200774 Hz
AQ 2.4904180 sec
RG 45.3
DW 76.000 usec
DE 6.00 usec
TE 300.0 K
D1 0.10000000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 9.00 usec
PL1 4.00 dB
SFO1 399.8724592 MHz
F2 - Processing parameters
SI 16384
SF 399.8700207 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 23.50 cm
CY 13.00 cm
F1P 9.000 ppm
F1 3598.83 Hz
F2P 0.000 ppm
F2 0.00 Hz
PPMCM 0.38298 ppm/cm
HZCM 153.14171 Hz/cm
nmr400b h-1
26
ppm
8
7
6
5
4
3
2
1


Current Data Parameters
NAME 180000-021-1-1
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20050224
Time 16.27
INSTRUM spect
PROBHD 5 mm GNP 1H
PULPROG zgdc
TD 65536
SOLVENT CDCl3
NS 139
DS 4
SWH 26315.789 Hz
FIDRES 0.401547 Hz
AQ 1.2452340 sec
RG 8192
DW 19.000 usec
DE 6.00 usec
TE 300.0 K
D1 0.10000000 sec
d11 0.03000000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 2.60 usec
PL1 5.00 dB
SFO1 100.5584112 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 120.00 dB
PL12 22.00 dB
SFO2 399.8719994 MHz
F2 - Processing parameters
SI 32768
SF 100.5473900 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
1D NMR plot parameters
CX 23.50 cm
CY 10.00 cm
F1P 200.000 ppm
F1 20109.48 Hz
F2P -0.000 ppm
F2 -0.00 Hz
PPMCM 8.51064 ppm/cm
HZCM 855.72247 Hz/cm
nmr400b c-13 (h-1 decoupled)
141.59
138.26
135.68
129.33
129.05
129.00
128.60
126.15
77.53
77.21
76.89
41.70
21.18
26
ppm
180
160
140
120
100
80
60
40
20