

Supporting information for:

Polystyrene-Supported Triphenylarsine Reagents and Their Use in Suzuki Cross-Coupling Reactions

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General Procedures. All reagents were obtained from either the Aldrich, Lancaster, or Acros chemical companies and used as received. All moisture sensitive reactions were carried out in dried glassware under either a nitrogen or argon atmosphere. Tetrahydrofuran was distilled under an inert atmosphere over sodium and benzophenone. All other solvents were used as received. Silica gel 60 (230-400 mesh) was used for chromatography. Thin layer chromatography analysis was performed using silica gel 60 F₂₅₄. NMR spectra were recorded on either a Bruker 300 DRX spectrometer or an AV400 spectrometer operating at 300 or 400 MHz, respectively for ¹H and 75 or 100 MHz, respectively for ¹³C. All spectra were calibrated at δ 7.26 or δ 77.00 ppm (residual CHCl₃) for ¹H and ¹³C spectra, respectively. IR spectra were recorded using a Bio-Rad FTS 165 spectrometer. Melting points were determined using a Carl Zeiss apparatus. Elemental analyses to determine arsenic content were conducted by Galbraith Laboratories, Knoxville, TN.

Coupling reaction product characterization data.

The following products were identified by comparison with previously reported spectroscopic data: 2-phenyl-2-cyclohexen-1-one,¹ 2-(4-methoxyphenyl)-2-cyclohexen-1-one,² 2-(3-methoxyphenyl)-2-cyclohexen-1-one,¹ 2-(3,4-dimethoxyphenyl)-2-cyclohexen-1-one,³ biphenyl,⁴ and 4-methoxybiphenyl,⁴ 4'-methoxy-2,4,6-trimethylbiphenyl.⁵

2-Phenyl-2-cyclohexen-1-one: ¹H NMR (300 MHz, CDCl₃): 2.09-2.16 (m, 2H), 2.51-2.63 (m, 4H), 7.03 (t, 1H, *J* = 4.3 Hz), 7.28-7.38 (m, 5H).

2-(4-Methoxyphenyl)-2-cyclohexen-1-one: ¹H NMR (400 MHz, CDCl₃): 2.09-2.13 (m, 2H), 2.51-2.62 (m, 4H), 3.81 (s, 3H), 6.84-6.90 (m, 3H), 7.04 (t, 1H, *J* = 4.3 Hz), 7.26 (td, 1H, *J* = 7.5, 1.1 Hz).

2-(3-Methoxyphenyl)-2-cyclohexen-1-one: ¹H NMR (300 MHz, CDCl₃): 2.05-2.10 (m, 2H), 2.47-2.59 (m, 4H), 3.79 (s, 3H), 6.87 (d, 2H, *J* = 8.6 Hz), 6.97 (t, 1H, *J* = 4.3 Hz), 7.25 (d, 2H, *J* = 8.6 Hz).

2-(3,4-Dimethoxyphenyl)-2-cyclohexen-1-one: ¹H NMR (400 MHz, CDCl₃): 2.06-2.13 (m, 2H), 2.53 (td, 2H, *J* = 6.0, 4.4 Hz), 2.58 (t, 2H, *J* = 7.0 Hz), 3.87 (s, 3H), 3.88 (s, 3H), 6.83-6.89 (m, 3H), 7.01 (t, 1H, *J* = 4.3 Hz).

Biphenyl: ¹H NMR (400 MHz, CDCl₃): 7.31-7.36 (m, 2H), 7.40-7.46 (m, 4H), 7.57-7.61 (m, 4H).

4-Methoxybiphenyl: ¹H NMR (400 MHz, CDCl₃): 3.85 (s, 3H), 6.96-7.00 (m, 2H), 7.30 (tt, 1H, *J* = 7.4, 1.2 Hz), 7.39-7.43 (m, 2H), 7.51-7.57 (m, 4H).

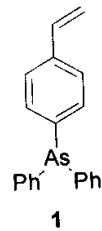
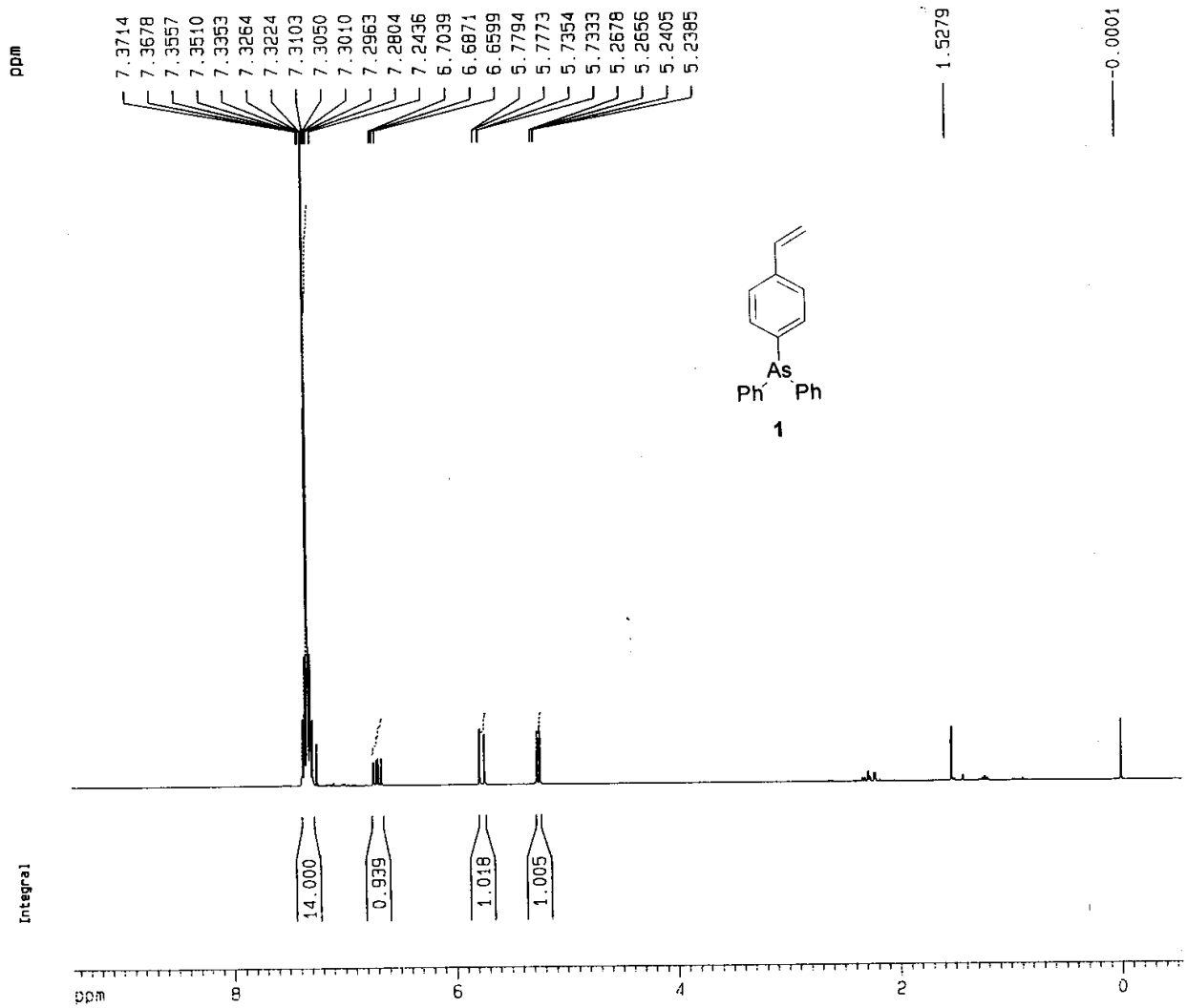
3-Methoxybiphenyl: ¹H NMR (400 MHz, CDCl₃): 3.82 (s, 3H), 6.88 (dd, 1H, *J* = 8.2, 2.5 Hz), 7.12 (s, 1H), 7.16 (d, 1H, *J* = 8.0 Hz), 7.30-7.35 (m, 2H), 7.41 (t, 2H, *J* = 7.8 Hz), 7.58 (d, 2H, *J* = 8.0 Hz). ¹³C NMR (100 MHz, CDCl₃): 55.5, 113.0, 113.2, 120.0, 127.4, 127.5, 127.7, 129.0, 130.1, 141.4, 143.1, 160.3. IR (CH₂Cl₂, cm⁻¹): 3068, 2838, 1599, 1574, 1480, 1468, 1456, 1444, 1421, 1323. HR EI-MS: calcd for C₁₃H₁₂O, 184.0888; found, 184.0879.

3,4-Dimethoxybiphenyl: Mp 66-67 °C. ¹H NMR (400 MHz, CDCl₃): 3.92(s, 3H), 3.95(s, 3H), 6.94 (d, 1H, *J* = 8.2 Hz), 7.10-7.16 (m, 2H), 7.31 (t, 1H, *J* = 7.4 Hz), 7.42 (t, 2H, *J* = 7.8 Hz), 7.55 (d, 2H, *J* = 7.5 Hz). ¹³C NMR (100 MHz, CDCl₃): 55.9, 110.5, 111.5, 119.4, 126.8, 128.7, 134.2, 141.0, 148.6, 149.1. IR (CH₂Cl₂, cm⁻¹): 3064, 2837, 1606, 1574, 1522, 1443, 1408, 1325. HR EI-MS: calcd for C₁₄H₁₄O₂, 214.0994; found, 214.0990.

4'-Methoxy-2,4,6-trimethyl-biphenyl: ¹H NMR (300 MHz, CDCl₃): 2.01(s, 6H), 2.32(s, 3H), 3.84(s, 3H), 6.92-6.96(m, 4H), 7.03-7.06 (m, 2H).

References:

1. Majetich, G.; Liu, S.; Fang, J.; Siesel, D.; Zhang, Y. *J. Org. Chem.* **1997**, *60*, 6928.
2. Ruel, F. S.; Braun, M. P.; Johnson, C. R. *Org. Syn.* **1998**, *75*, 69.
3. Iwamatsu, S.; Matsubara, K., Nagashima, H. *J. Org. Chem.* **1999**, *64*, 9625.
4. Rao, M. S. C.; Rao, G. S. K. *Synthesis* **1987**, 231.
5. Molander, G. A.; Biolatto, B. *J. Org. Chem.* **2003**, *68*, 4302.



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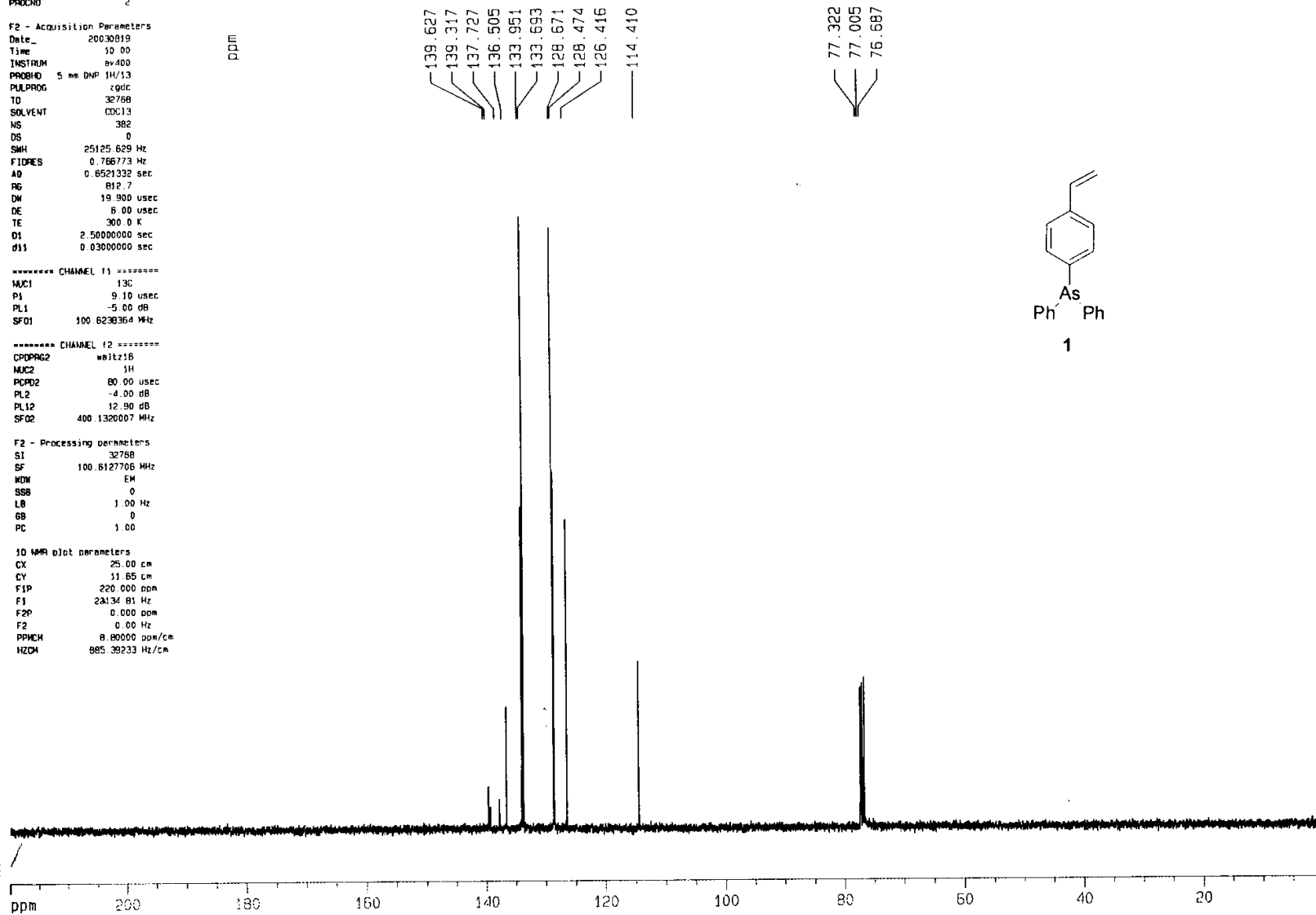
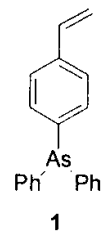
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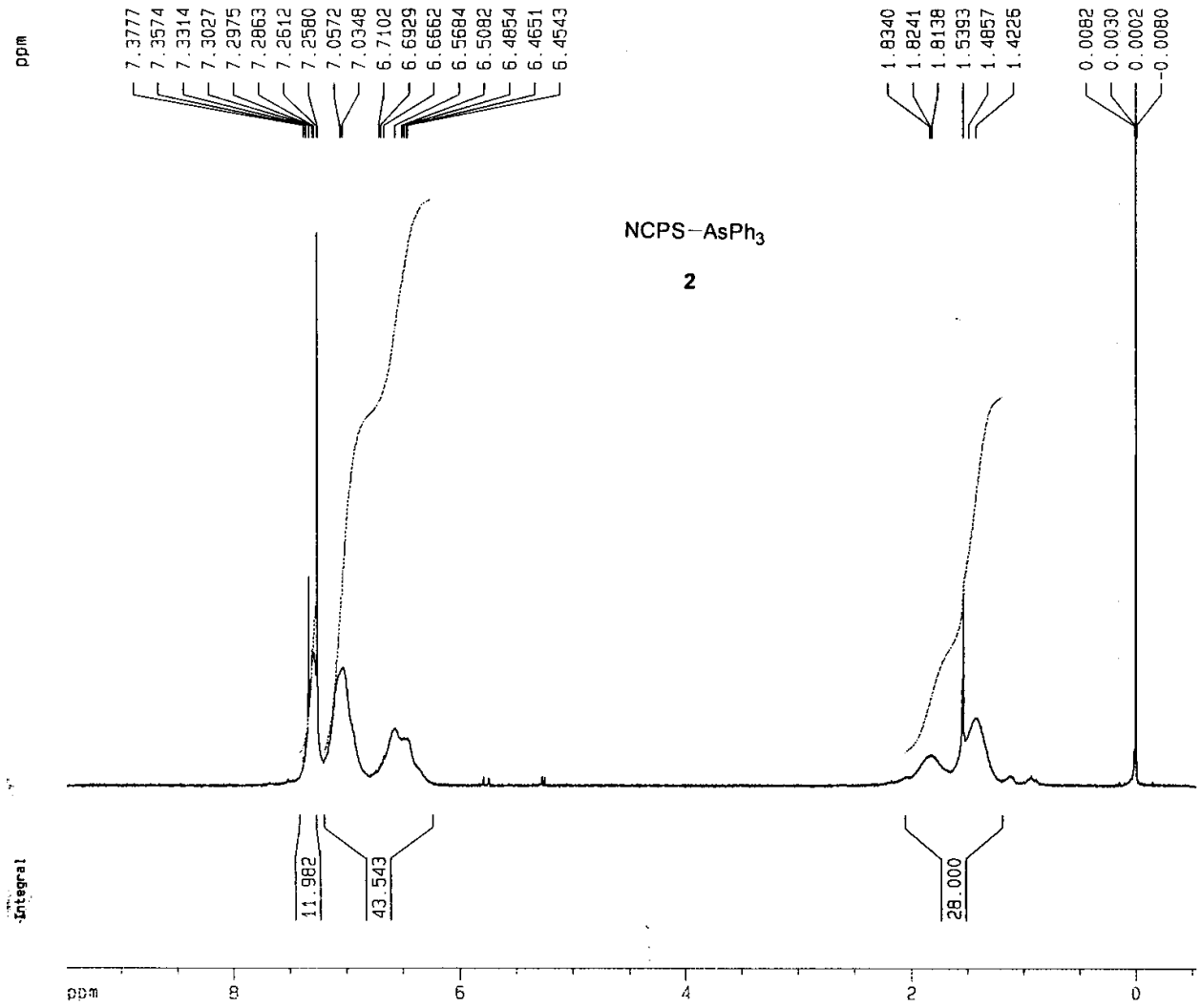
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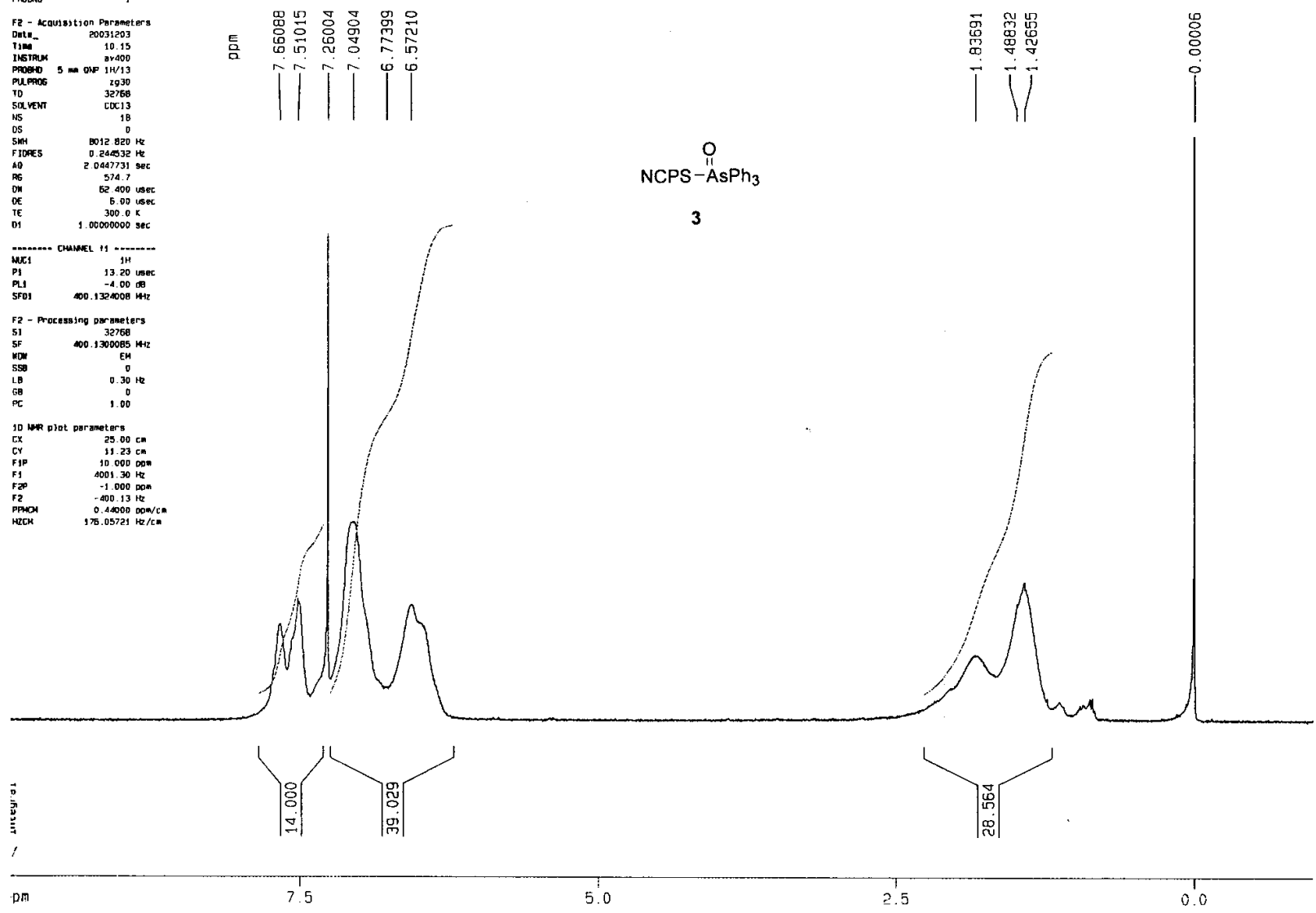
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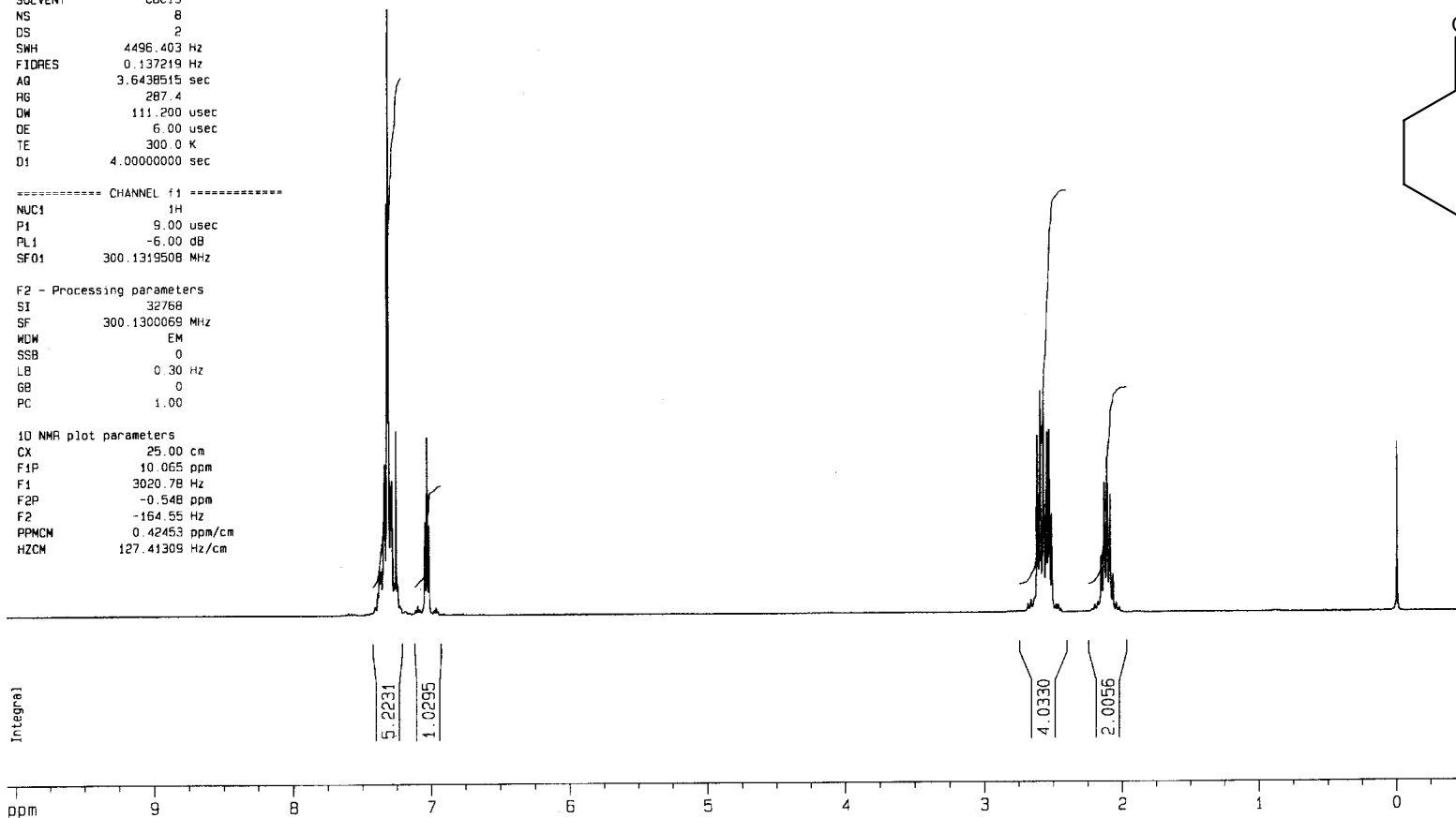
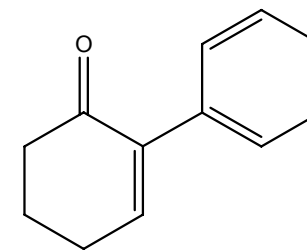
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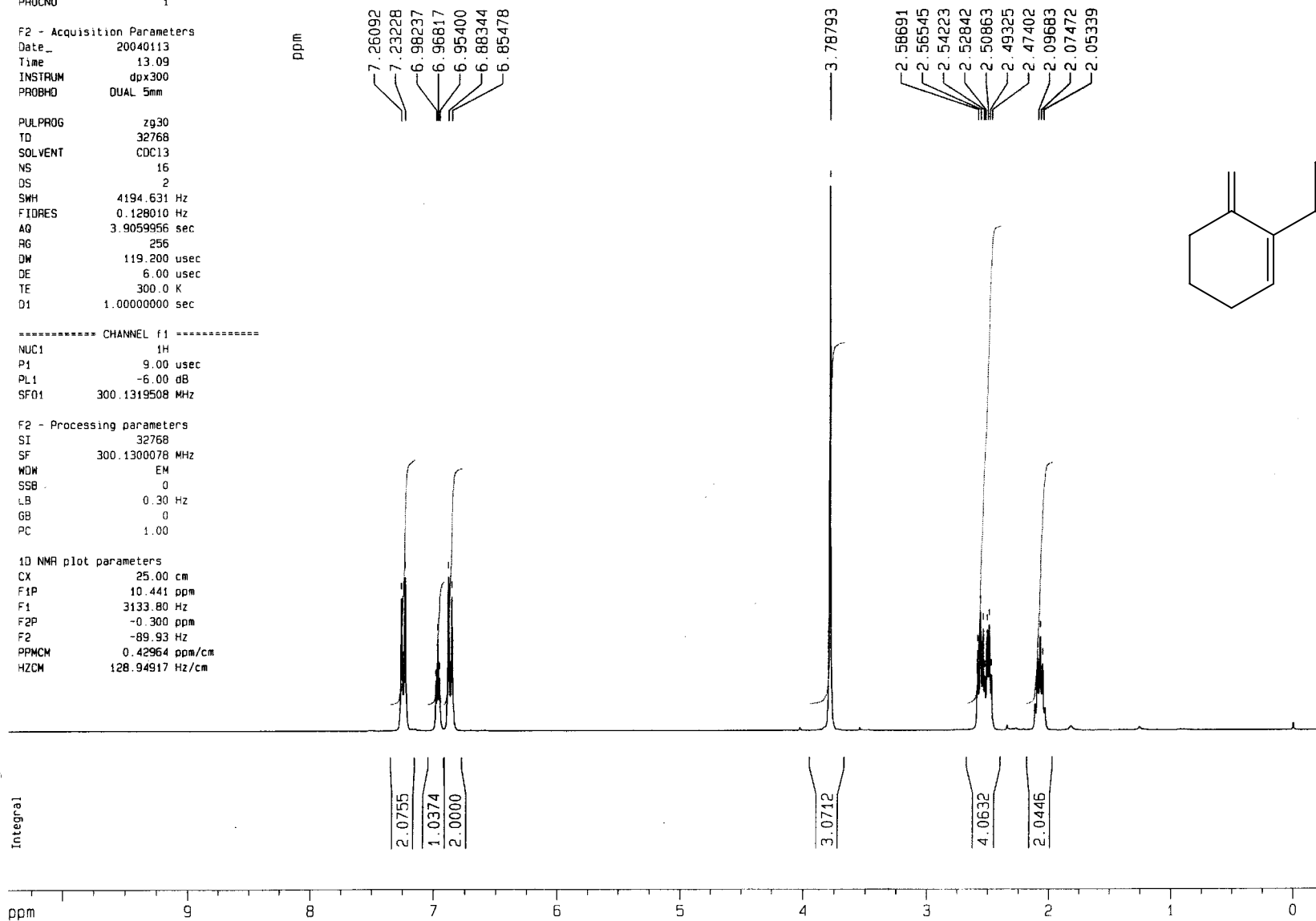
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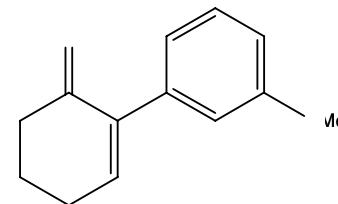
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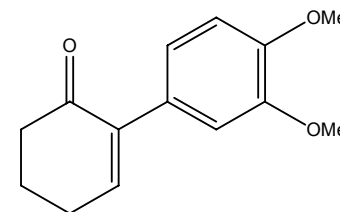
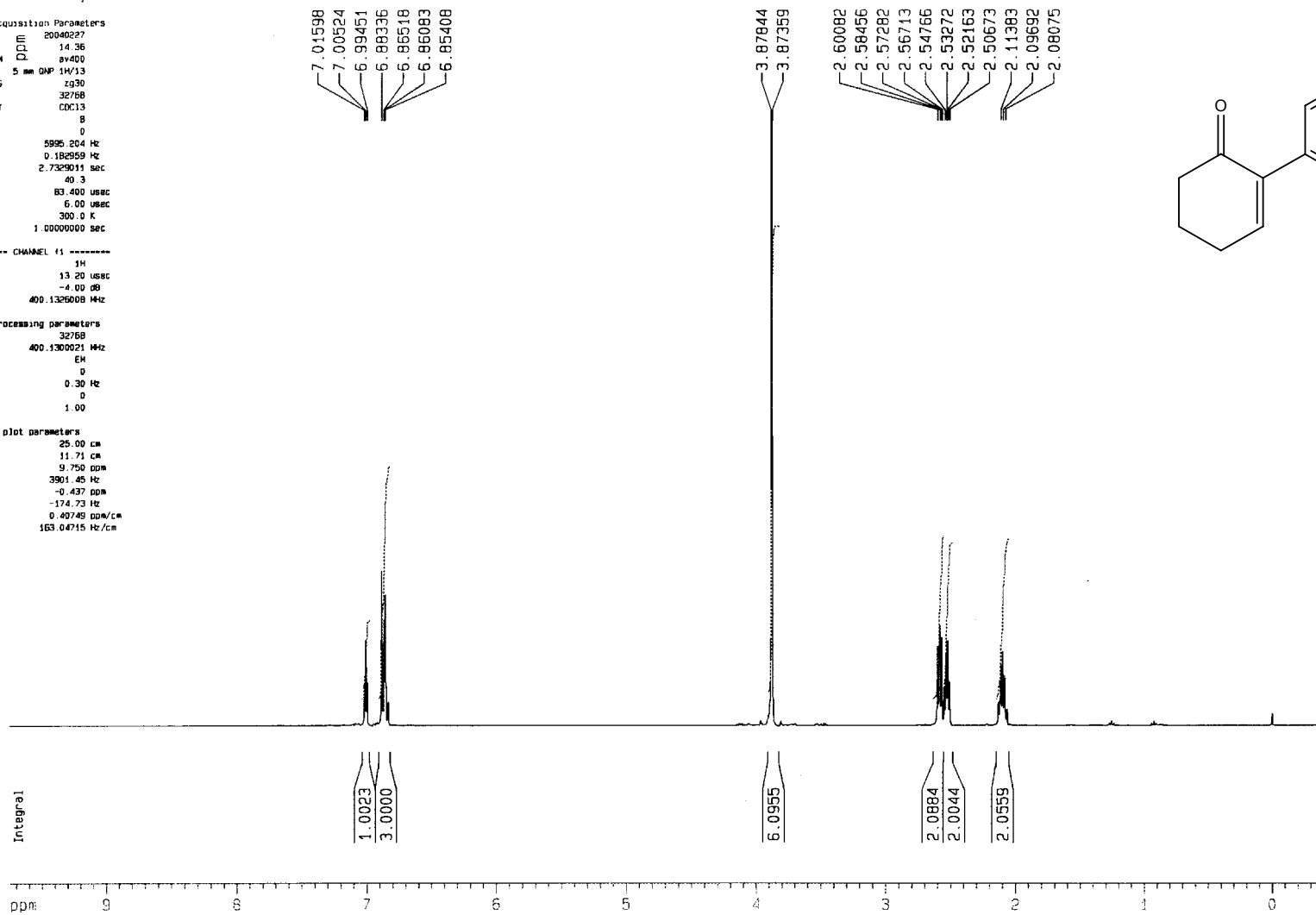
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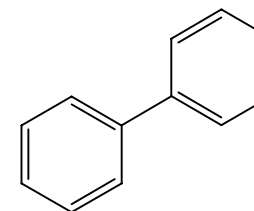
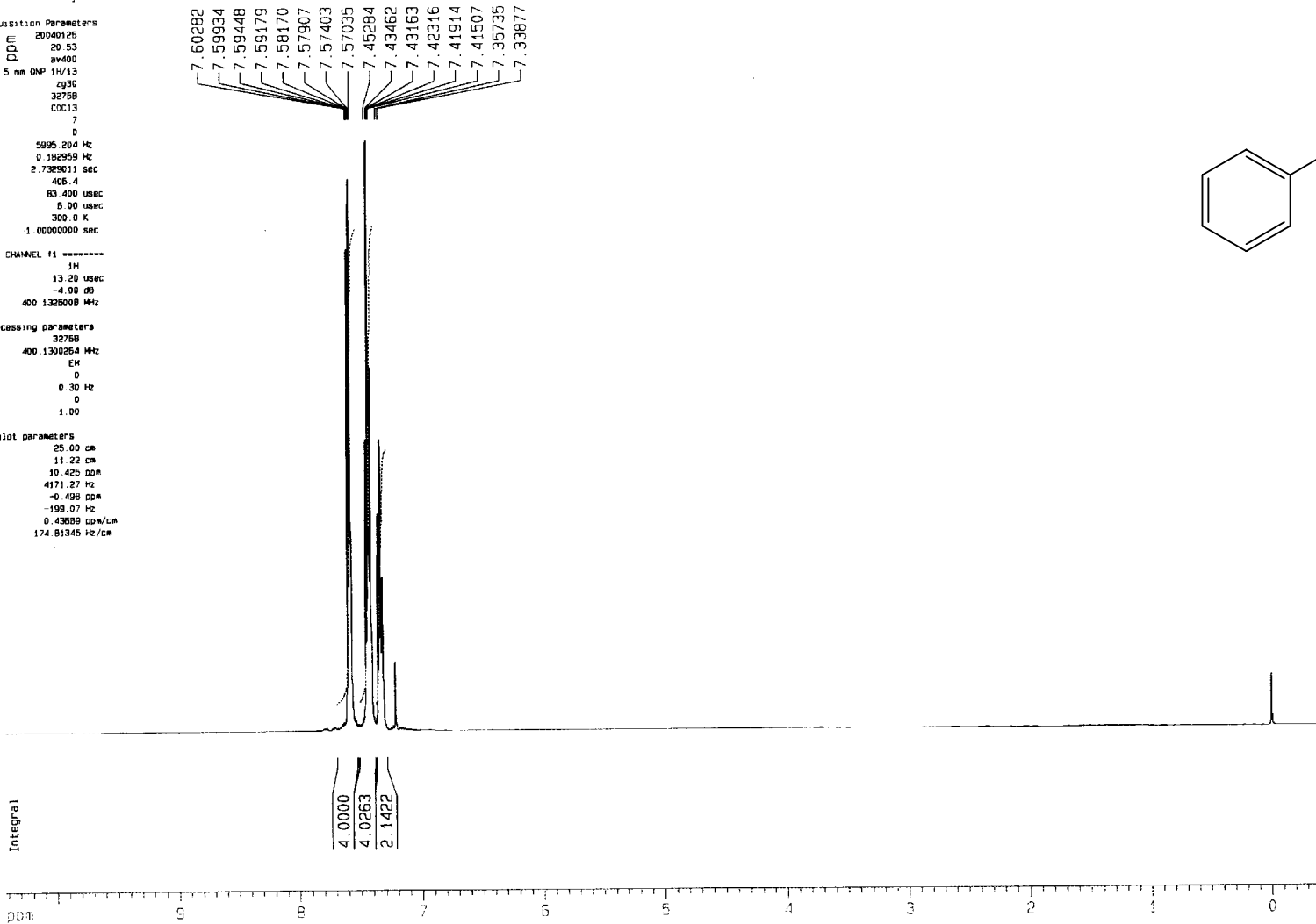
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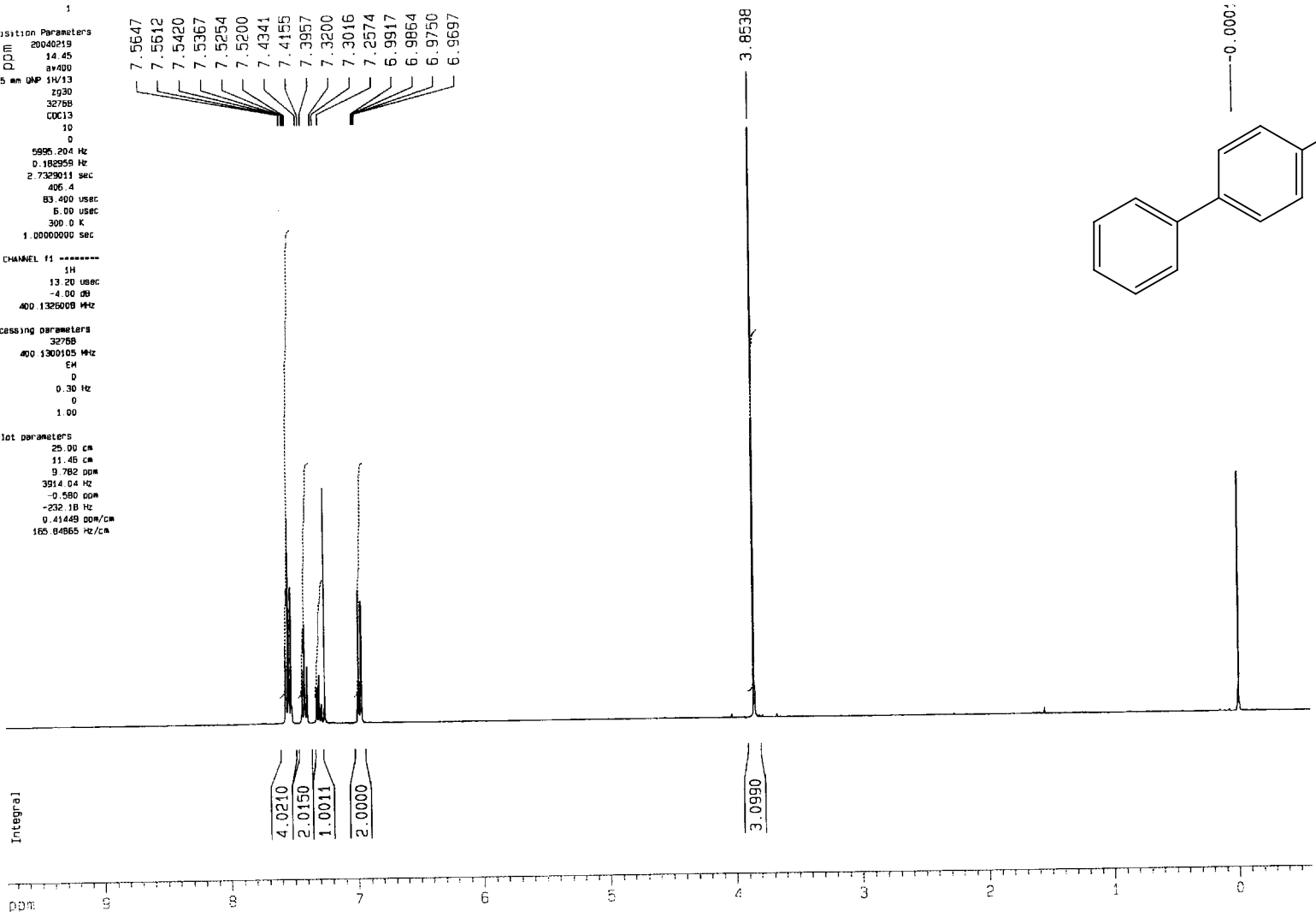
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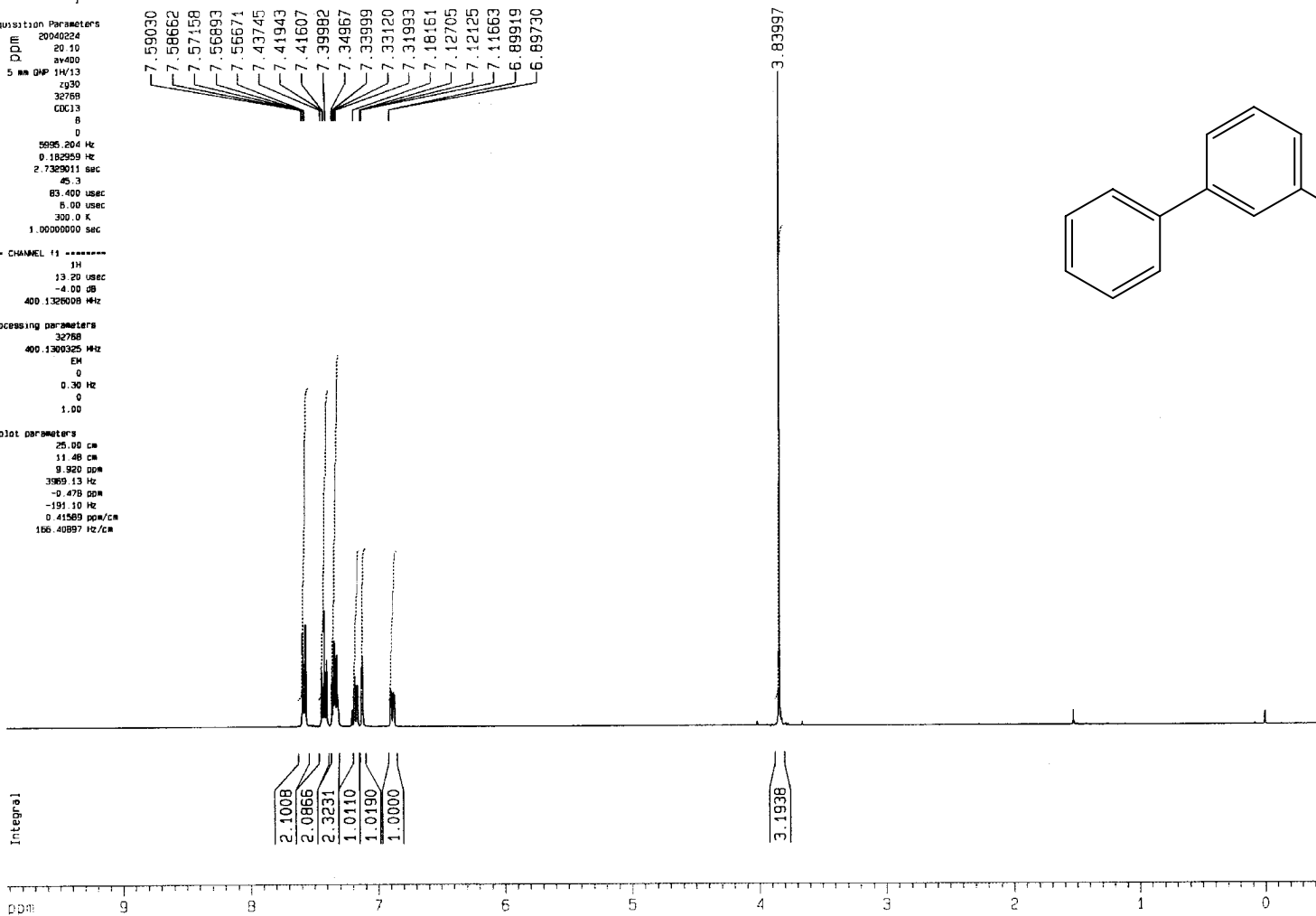
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EXPNO 2
PROCNO 1

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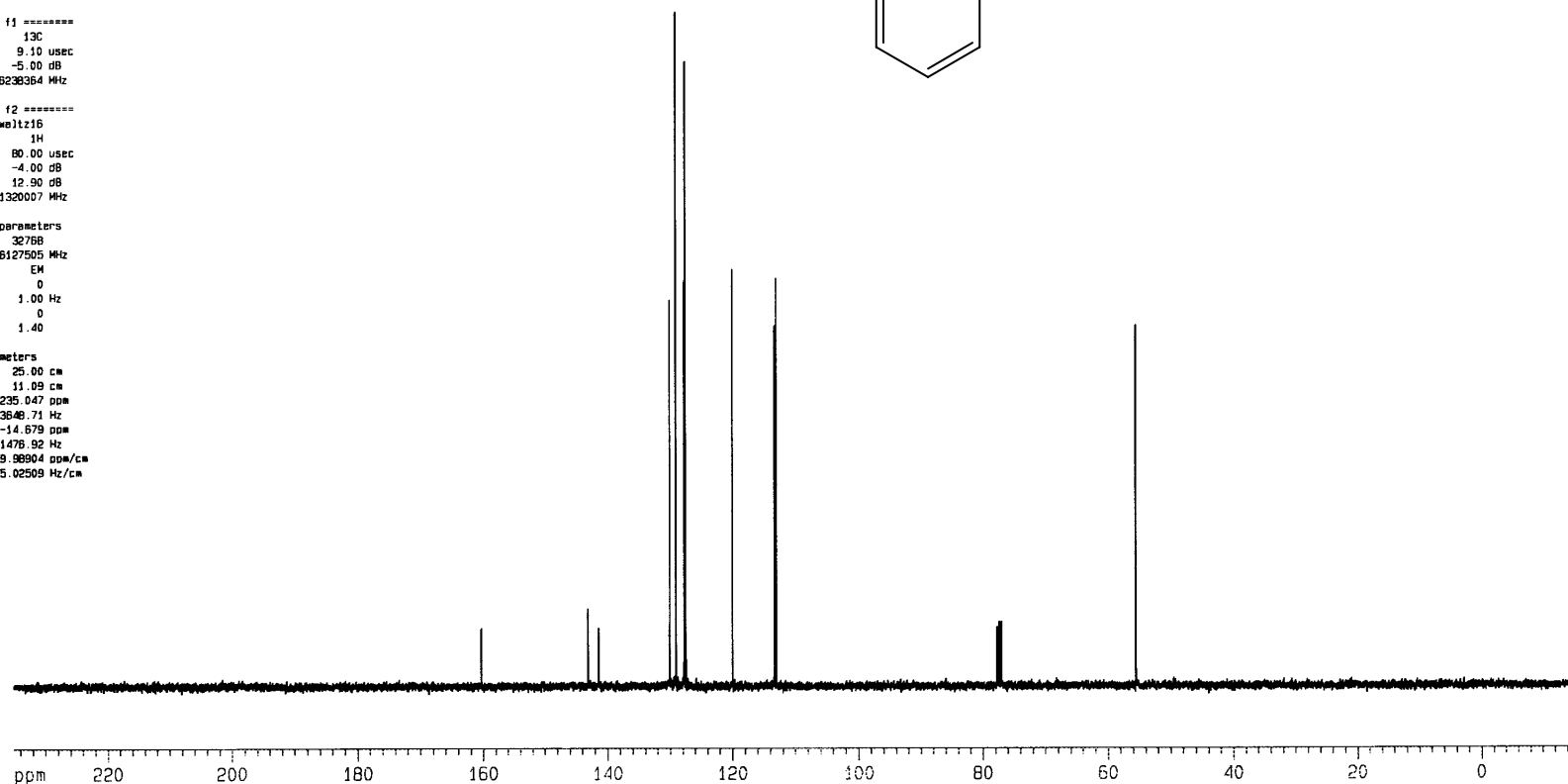
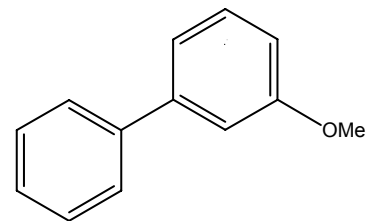
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F1 23646.71 Hz
F2P -14.679 ppm
F2 -1478.92 Hz
PPMCH 9.98904 ppm/cm
HZCM 1005.02509 Hz/cm

160.271
143.062
141.404
130.051
129.032
127.707
127.520
127.486
119.969
113.215
112.976
77.677
77.359
77.040
55.530



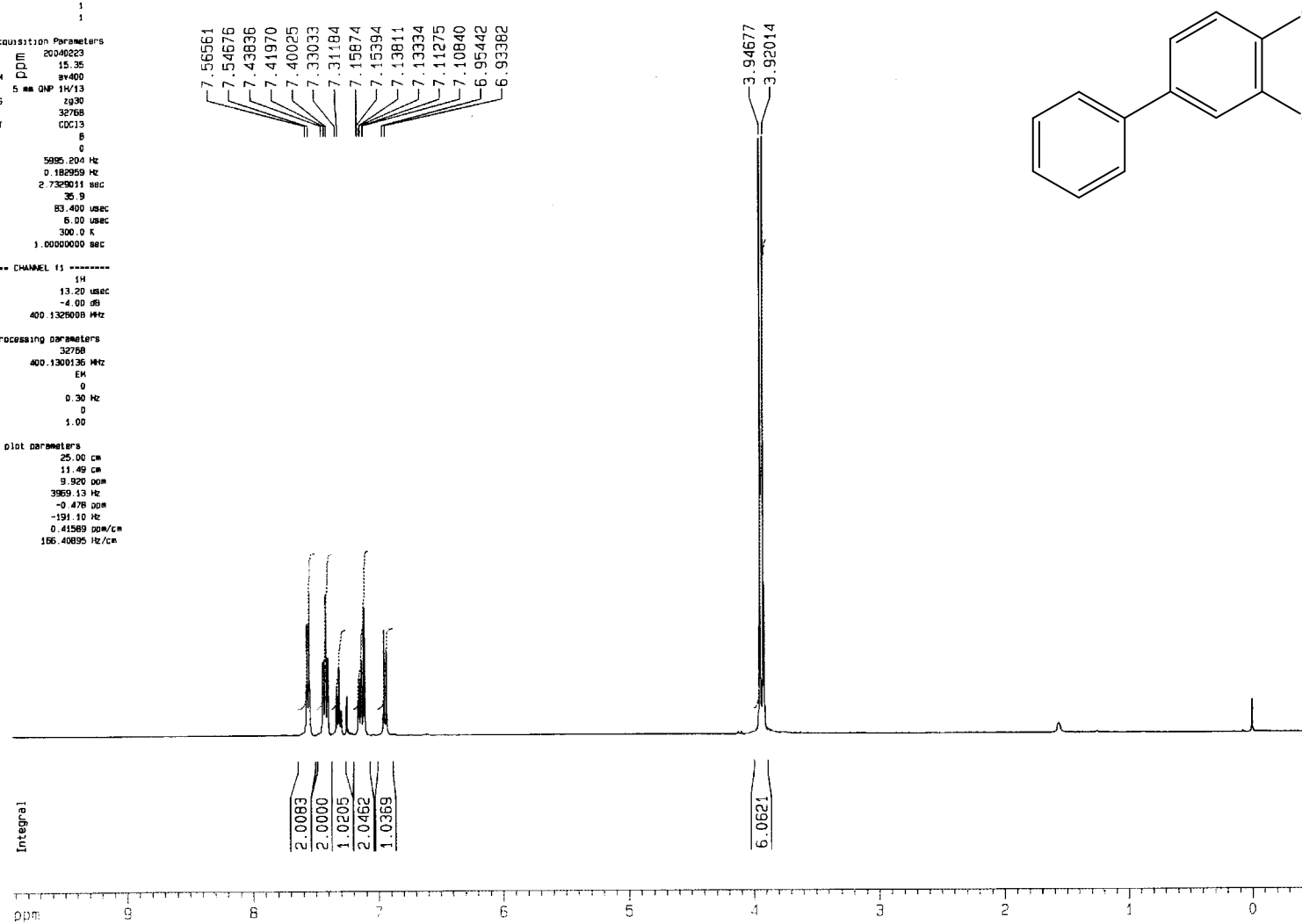
Current Data Parameters
 NAME SK-68-P
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20040223
 Time 15.35
 INSTRUM av400
 P1 5.00
 PULPROG zg30
 TD 32768
 SOLVENT CDC13
 NS 8
 DS 0
 SWH 5895.204 Hz
 FIDRES 0.182959 Hz
 AQ 2.7329011 sec
 RG 35.9
 DM 83.400 usec
 DE 6.00 usec
 TE 300.0 K
 D1 1.00000000 sec

----- CHANNEL f1 -----
 NU1 1H
 P1 13.20 usec
 PL1 -4.00 dB
 SFO1 400.1326009 MHz

F2 - Processing parameters
 SI 32768
 SF 400.1300136 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 25.00 cm
 CY 11.49 cm
 F1 9.920 ppm
 F1 3989.13 Hz
 F2 -0.478 ppm
 F2 -191.10 Hz
 PPMCH 0.41589 ppm/cm
 HZCH 166.40895 Hz/cm



Current Data Parameters
NAME SK-GB-P-C
EXPNO 2
PROCNO 1

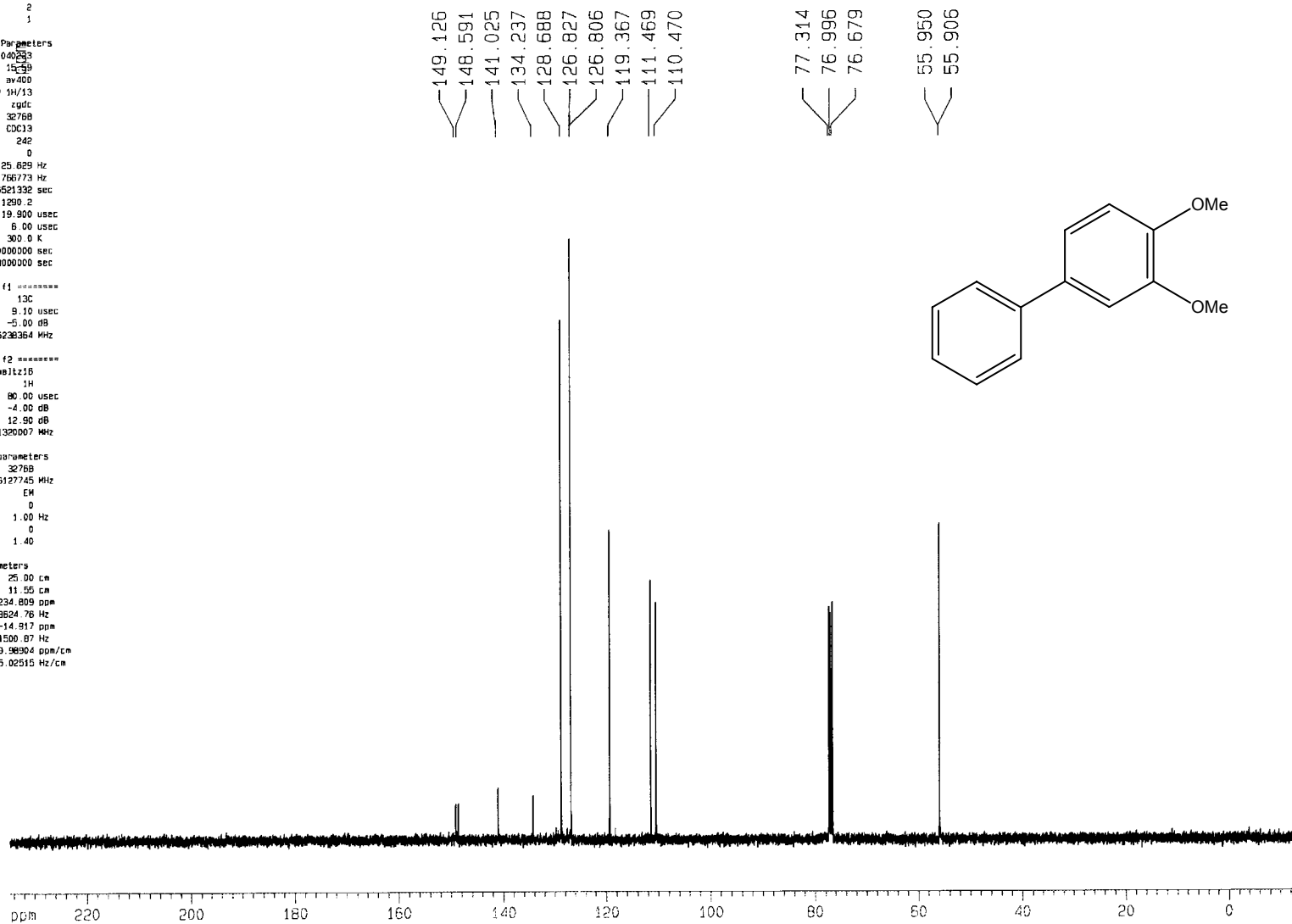
F2 - Acquisition Parameters
Date_ 20040523
Time 15:59
INSTRUM av400
PROBHD 5 mm DNP 1H/13
PULPROG zgdc
TD 32768
SOLVENT CDCl3
NS 242
DS 0
SWH 25125.829 Hz
FIDRES 0.766773 Hz
AQ 0.6521332 sec
RG 1290.2
DM 19.900 usec
DE 6.00 usec
TE 300.0 K
D1 3.0000000 sec
d11 0.0300000 sec

===== CHANNEL f1 =====
NUC1 13C
P1 9.10 usec
PL1 -5.00 dB
SFO1 100.626364 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -4.00 dB
PL12 12.90 dB
SFO2 400.132007 MHz

F2 - Processing parameters
SI 32768
SF 100.6127745 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

1D NMR plot parameters
CX 25.00 cm
CY 11.55 cm
F1P 234.809 ppm
F1 23824.76 Hz
F2P -14.917 ppm
F2 -1500.87 Hz
PPMCM 9.98904 ppm/cm
HZCM 1005.02515 Hz/cm



Current Data Parameters
NAME SK-118-P
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20040706
Time 11.13
INSTRUM dpx300
PROBHD DUAL 5mm

PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 4
DS 2
SWH 4496.403 Hz
FIDRES 0.137219 Hz
AQ 3.6438515 sec
RG 114
DW 111.200 usec
DE 6.00 usec
TE 300.0 K
D1 4.0000000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 9.00 usec
PL1 -6.00 dB
SF01 300.1319508 MHz

F2 - Processing parameters
SI 32768
SF 300.1300207 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 25.00 cm
F1P 10.168 ppm
F1 3051.82 Hz
F2P -0.434 ppm
F2 -130.32 Hz
PPMCM 0.42410 ppm/cm
HZCM 127.28575 Hz/cm

