Electronic Supplementary Material (ESI) for Chemical Communications

Supporting Information for

Iron-catalyzed oxidative coupling of arylboronic acids with benzene derivatives through homolytic aromatic substitution mechanism

Nanase Uchiyama, Eiji Shirakawa,* Ryo Nishikawa, and Tamio Hayashi*

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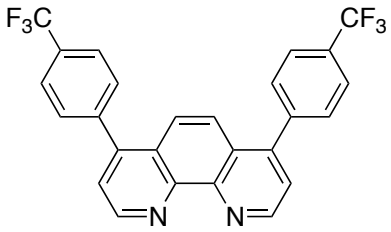
General Remarks. All manipulations of oxygen- and moisture-sensitive materials were conducted with a standard Schlenk technique under a nitrogen atmosphere. Nuclear magnetic resonance spectra were taken on a JEOL JNM LA500 spectrometer (^{1}H, 500 MHz) or a JEOL JNM LA600 spectrometer (^{13}C, 150 MHz) using tetramethylsilane (^{1}H and ^{13}C) as an internal standard. GC spectra were taken on Shimazu GC-18A. GC-MS spectra were taken on Shimazu GCMS-QP5050A. High-resolution mass spectra were obtained with a Bruker Daltonics microTOF-Q spectrometer (ESI). Di-*tert*-butyl hyponitrite was prepared according to a literature procedure.[1] Unless otherwise noted, reagents were commercially available and used without further purification. ^{1}H NMR analysis using *p*-dimethoxybenzene as an internal standard showed that arylboronic acids used are free from the corresponding boroxines in DMSO-d_6 and the molar amounts of the arylboron moieties are within a margin of error of plus or minus 5% compared with those calculated on the assumption that the arylboronic acids are pure.

Preparation of 4,7-Bis[4-(trifluoromethyl)phenyl]-1,10-phenanthroline (L3). The title compound was prepared according to a literature method for the coupling of 4,7-dibromo-1,10-phenanthroline with 4-methoxy-3,5-dimethylphenylzinc chloride with a slight modification.[2] To a solution of 1-bromo-4-(trifluoromethyl)benzene (339 mg, 1.50 mmol) in THF (10 mL) at –78 °C was added *n*-BuLi (0.94 mL, 1.6 M solution in hexane, 1.5 mmol). To this mixture was added at –78 °C a solution of $ZnCl_2$ (204 mg, 1.50 mmol) in THF (5 mL), cooled by ice bath, via cannula. It was allowed to warm to room temperature and a suspension of 4,7-dichloro-1,10-phenanthroline (125 mg, 0.500 mmol) and $Pd(PPh_3)_4$ (28.9 mg, 0.0250 mmol) in THF (10 mL) was added to the organozinc intermediate using a large gauge cannula. The mixture was heated at reflux for 12 h, cooled to room temperature, quenched with sat. NH_4Cl aq. (15 mL), and neutralized with sat. $NaHCO_3$ aq. (30 mL). After extraction with EtOAc (30 mL x 3) and washing with brine, the organic layer was dried over $MgSO_4$ and concentrated. The residue was subjected to SiO_2 column chromatography (EtOAc then CH_2Cl_2/MeOH/NH_3 aq. = 93/5/2) to give 4,7-bis[4-(trifluoromethyl)phenyl]-1,10-phenanthroline (**L3**: 161 mg, 59% yield).

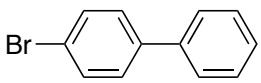
4,7-Bis[4-(trifluoromethyl)phenyl]-1,10-phenanthroline (L3).



A white solid. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.61 (d, *J* = 4.4 Hz, 2 H), 7.66 (d, *J* = 8.3 Hz, 4 H), 7.78 (s, 2 H), 7.82 (d, *J* = 8.3 Hz, 4 H), 9.30 (d, *J* = 4.4 Hz, 2 H). ^{13}C NMR (150 MHz, $CDCl_3$) δ123.6, 124.03, 124.04 (q, *J* = 274 Hz), 125.8 (q, *J* = 2.9 Hz), 126.2, 130.1, 130.9 (q, *J* = 32 Hz), 141.5, 146.9, 147.0, 150.1. HRMS (ESI) Calcd for $C_{26}H_{14}F_6N_2$: $[M+Na]^+$, 491.0959. Found: m/z 491.0962.

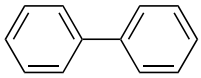
Iron-Catalyzed Oxidative Coupling of 4-Bromophenylboronic Acid with Benzene (Table 1): General Procedure. To a partial suspension of an iron complex (0.0120 mmol) and 4-bromophenylboronic acid (**1a**: 24.1 mg, 0.120 mmol) in benzene (**2o**: 1.07 mL, 12.0 mmol) in a 20 mL Schlenk tube was added a ligand (0.012 mmol) and *t*-BuO*t*-Bu (**3**: 44.0 μL, 0.240 mmol). After stirring at 80 °C for the time specified in Table 1, nonane as an internal standard was added. An aliquot of the solution was subjected to GC analysis. The rest of the solution was poured into brine (20 mL) and extracted with Et_2O (25 mL x 3). The organic layer was dried over $MgSO_4$, filtered, and concentrated. The residue was subjected to ^{1}H NMR

analysis using $MeNO_2$ as an internal standard.

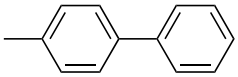


4-Bromobiphenyl (4ao).[3] A white solid. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.37 (t, *J* = 6.9 Hz, 1 H), 7. 44 (t, *J* = 7.6 Hz, 2 H), 7.46 (d, *J* = 8.5 Hz, 2 H), 7.55 (d, *J* = 7.6 Hz, 2 H), 7.57 (d, *J* = 8.5 Hz, 2 H).

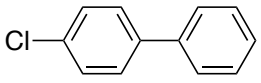
Iron-Catalyzed Oxidative Coupling of Arylboronic Acids with Arenes (Table 2 and Scheme 1). General Procedure. To a partial suspension of $Fe(OTf)_3$ (10.1 mg, 0.0200 mmol), 4,7-bis[4-(trifluoromethyl)phenyl]-1,10-phenanthroline (**L3**: 9.4 mg, 0.020 mmol) and an arylboronic acid (**1**: 0.200 mmol) in an arene (**2**: 20.0 mmol) in a 20 mL Schlenk tube was added *t*-BuO*O*t-Bu (**3**: 73.0 μL, 0.400 mmol). After stirring at 80 °C for the time specified in Table 2 or Scheme 1, the resulting solution was poured into brine (20 mL) and extracted with Et_2O (25 mL x 3). The organic layer was dried over $MgSO_4$, filtered, and concentrated. The residue was subjected to SiO_2 chromatography (PTLC) to give the corresponding coupling product (**4**).



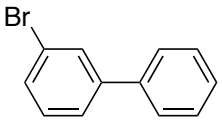
Biphenyl (4bo).[4] A white solid. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.35 (t, *J* = 7.6 Hz, 2 H), 7.44 (t, *J* = 7.6 Hz, 4 H), 7.60 (d, *J* = 8.4 Hz, 4 H).



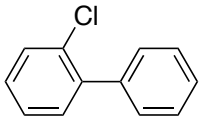
4-Methylbiphenyl (4co).[5] A white solid. ^{1}H NMR (500 MHz, $CDCl_3$) δ 2.40 (s, 3 H), 7.25 (d, *J* = 8.2 Hz, 2 H), 7.32 (t, *J* = 7.4 Hz, 1 H), 7.42 (t, *J* = 7.7 Hz, 2 H), 7.50 (d, *J* = 8.2 Hz, 2 H), 7.59 (d, *J* = 7.2 Hz, 2 H).



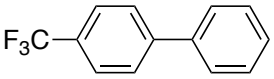
4-Chlorobiphenyl (4do).[6] A white solid. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.36 (t, *J* = 7.7 Hz, 1 H), 7.41 (d, *J* = 8.5 Hz, 2 H), 7.44 (t, *J* = 7.8 Hz, 2 H), 7.52 (d, *J* = 8.5 Hz, 2 H), 7.55 (d, *J* = 7.2 Hz, 2 H).



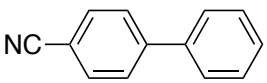
3-Bromobiphenyl (4eo).[7] A colorless oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.31 (t, *J* = 7.9 Hz, 1 H), 7.38 (t, *J* = 7.4 Hz, 1 H), 7.45 (t, *J* = 7.9 Hz, 2 H), 7.46–7.50 (m, 1 H), 7.52 (d, *J* = 7.7 Hz, 1 H), 7.56 (d, *J* = 7.1 Hz, 2 H), 7.74 (t, *J* = 1.8 Hz, 1 H).



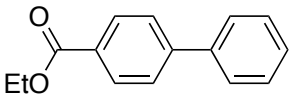
2-Chlorobiphenyl (4fo).[8] A pale yellow oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.26–7.42 (m, 4 H), 7.42–7.46 (m, 4 H), 7.48 (dd, *J* = 7.6, 1.5 Hz, 1 H).



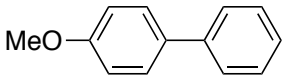
4-(Trifluoromethyl)biphenyl (4go).[9] A white solid. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.41 (t, *J* = 7.4 Hz, 1 H), 7.48 (t, *J* = 7.6 Hz, 2 H), 7.60 (d, *J* = 7.4 Hz, 2 H), 7.70 (s, 4 H).



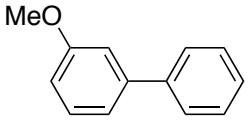
4-Cyanobiphenyl (4ho).[10] A white solid. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.43 (t, *J* = 7.3 Hz, 1 H), 7.49 (t, *J* = 7.5 Hz, 2 H), 7.59 (d, *J* = 7.1 Hz, 2 H), 7.69 (d, *J* = 8.2 Hz, 2 H), 7.73 (d, *J* = 8.2 Hz, 2 H).



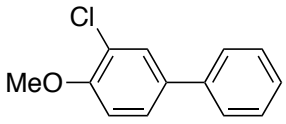
4-Ethoxycarbonylbiphenyl (4io).[11] A white solid. ^{1}H NMR (500 MHz, $CDCl_3$) δ 1.42 (t, *J* = 7.1 Hz, 3 H), 4.41 (q, *J* = 7.1 Hz, 2 H), 7.39 (t, *J* = 7.4 Hz, 1 H), 7.47 (t, *J* = 7.6 Hz, 2 H), 7.63 (d, *J* = 7.2 Hz, 2 H), 7.66 (d, *J* = 8.2 Hz, 2 H), 8.12 (d, *J* = 8.2 Hz, 2 H).



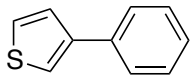
4-Methoxylbiphenyl (4jo).[4] A white solid. ^{1}H NMR (500 MHz, $CDCl_3$) δ 3.86 (s, 3 H), 6.98 (d, *J* = 8.4 Hz, 2 H), 7.30 (t, *J* = 7.4 Hz, 1 H), 7.42 (t, *J* = 7.6 Hz, 2 H), 7.53 (d, *J* = 8.4 Hz, 2 H), 7.55 (d, *J* = 7.2 Hz, 2 H).



3-Methoxybiphenyl (4ko).[4] A colorless oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ 3.87 (s, 3 H), 6.91 (dd, *J* = 8.2, 2.6 Hz, 1 H), 7.14 (t, *J* = 2.0 Hz, 1 H), 7.19 (d, *J* = 7.6 Hz, 1 H), 7.33–7.38 (m, 2 H), 7.44 (t, *J* = 7.8 Hz, 2 H), 7.59 (d, *J* = 7.2 Hz, 2 H).

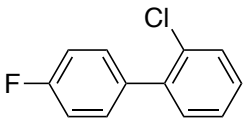


3-Chloro-4-methoxybiphenyl (4lo).[12] A white solid. ^{1}H NMR (500 MHz, $CDCl_3$) δ 3.95 (s, 3 H), 7.00 (d, *J* = 8.6 Hz, 1 H), 7.33 (t, *J* = 7.4 Hz, 1 H), 7.42 (t, *J* = 7.8 Hz, 2 H), 7.45 (dd, *J* = 8.6, 2.3 Hz, 1 H), 7.53 (d, *J* = 7.1 Hz, 2 H), 7.62 (d, *J* = 2.3 Hz, 1 H).

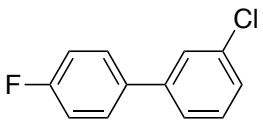


3-Phenylthiophene (4mo).[13] A white solid. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.30 (t, *J* = 7.4 Hz, 1 H), 7.38–7.43 (m, 4 H), 7.46 (dd, *J* = 2.6, 1.8 Hz, 1 H), 7.61 (d, *J* = 8.2 Hz, 2 H).

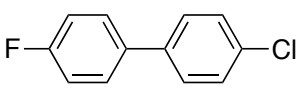
A mixture of three isomers of (4-fluorophenyl)chlorobenzene (*o*/*m*/*p* = 64/20/16) (4np). A colorless oil. The ratio of *o*/*m*/*p* was determined as follows. ^{1}H NMR showed that the peaks of the ortho isomer are the largest and those of the para isomer are the smallest, determined mainly from the integral the triplets (2 H, ortho to F) that appear at 7.1209 ppm (the ortho isomer), 7.135 (meta) and 7.1265 (para). However, the determination of the exact isomer ratio was difficult because of overlap of the peaks. The ratio of *o*/*m*/*p* was estimated by the integral on GC to be 64/20/16.



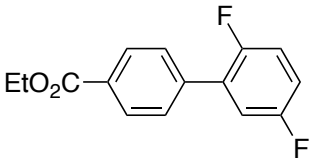
2-Chloro-4'-fluorobiphenyl.[14] ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.12 (t, *J* = 8.7 Hz, 2 H), 7.25–7.33 (m, 3 H), 7.38–7.43 (m, 2 H), 7.44–7.48 (m, 1 H).



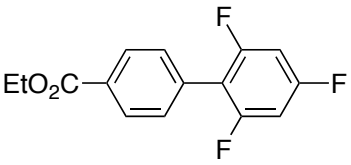
3-Chloro-4'-fluorobiphenyl.[8] ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.13 (t, *J* = 8.7 Hz, 2 H), 7.31 (m, 1 H), 7.36 (t, *J* = 7.8 Hz, 1 H), 7.39–7.43 (m, 1 H), 7.45–7.54 (m, 3 H).



4-Chloro-4'-fluorobiphenyl.[8] ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.13 (t, *J* = 8.8 Hz, 2 H), 7.39–7.43 (m, 2 H), 7.45–7.48 (m, 2 H), 7.49–7.54 (m, 2 H).

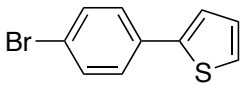


4'-(Ethoxycarbonyl)-2,5-difluorobiphenyl (4iq).[15] A white solid. ^{1}H NMR (500 MHz, $CDCl_3$) δ 1.42 (t, *J* = 7.2 Hz, 3 H), 4.41 (q, *J* = 7.2 Hz, 2 H), 7.02–7.07 (m, 1 H), 7.11–7.19 (m, 2 H), 7.61 (d, *J* = 8.7 Hz, 2 H), 8.13 (d, *J* = 8.7 Hz, 2 H).

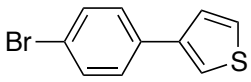


4'-(Ethoxycarbonyl)-2,4,6-trifluorobiphenyl (4ir). A white solid. ^{1}H NMR (500 MHz, $CDCl_3$) δ 1.41 (t, *J* = 7.1 Hz, 3 H), 4.41 (q, *J* = 7.1 Hz, 2 H), 6.78 (t, *J* = 8.2 Hz, 2 H), 7.50 (d, *J* = 8.2 Hz, 2 H), 8.13 (d, *J* = 8.2 Hz, 2 H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 14.4, 61.2, 100.8 (td, *J* = 24, 7.2 Hz), 114.2 (t, *J* = 22 Hz), 129.6, 130.36, 130.43, 133.0, 160.3 (ddd, *J* = 250, 15, 10 Hz), 162.3 (dt, *J* = 250, 16 Hz), 166.3. Anal. Calcd for $C_{15}H_{11}F_3O_2$: C, 64.29; H, 3.96. Found: C, 64.33; H, 3.79.

A mixture of two isomers of (4-bromophenyl)thiophene (2-/3- = 84/16) (4as). A pale yellow solid. The isomer ratio was determined by GC and confirmed by ^{1}H NMR.

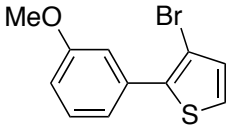


2-(4-Bromophenyl)thiophene.[16] ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.08 (t, *J* = 4.3 Hz, 1 H), 7.30 (d, *J* = 4.3 Hz, 2 H), 7.47 (d, *J* = 9.0 Hz, 2 H), 7.50 (d, *J* = 9.0 Hz, 2 H).

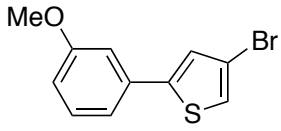


3-(4-Bromophenyl)thiophene.[17] ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.35 (dd, *J* = 5.0, 1.3 Hz, 1 H), 7.40 (dd, *J* = 5.0, 2.9 Hz, 1 H), 7.44 (dd, *J* = 2.9, 1.3 Hz, 1 H), 7.45–7.53 (m, 4 H).

A mixture of two isomers of (3-methoxyphenyl)-3-bromothiophene (2-/5- = 75/25) (4kt). A colorless oil. The isomer ratio was determined by GC and confirmed by ^{1}H NMR.



3-Bromo-2-(3-methoxyphenyl)thiophene.[18] ^{1}H NMR (500 MHz, $CDCl_3$) δ 3.86 (s, 3 H), 6.93 (dd, *J* = 8.3, 2.6 Hz, 1 H), 7.05 (d, *J* = 5.3 Hz, 1 H), 7.21–7.24 (m, 2 H), 7.28 (d, *J* = 5.3 Hz, 1 H), 7.34 (t, *J* = 8.2 Hz, 1 H).



4-Bromo-2-(3-methoxyphenyl)thiophene.[18] ^{1}H NMR (500 MHz, $CDCl_3$) δ 3.85 (s, 3 H), 6.87 (dd, *J* = 8.3, 2.5 Hz, 1 H), 7.08 (t, *J* = 2.1 Hz, 1 H), 7.15 (d, *J* = 7.7 Hz, 1 H), 7.17 (d, *J* = 1.4 Hz, 1 H), 7.20 (d, *J* = 1.4 Hz, 1 H) 7.30 (t, *J* = 8.0 Hz, 1 H).

ICP-MS (Inductively Coupled Plasma-Mass Spectrometry) of Fe(OTf)$_3$ (Footnote 15). A sample was prepared by diluting $Fe(OTf)_3$ with 1-methyl-2-pyrrolidone in 10,000-fold. Analysis was conducted on Agilent 7500cs using XSTC-7, 13B (SPEX) as a standard solution for calibration curve. The contents are shown in Table S1.

Table S1 ICP-MS analysis on the contents (ppm) of elements in $Fe(OTf)_3$

Co	Ni	Cu	Ru	Rh	Pd	Ag	Ir	Pt	Au
<5	26	29	<5	<5	<5	<5	<5	<5	<5

Reaction of 4-Bromophenylboronic Acid with Di-tert-butyl Hyponitrite and $CDCl_3$ (Scheme 2). A solution of 4-bromophenylboronic acid (**1a**: 24.1 mg, 0.120 mmol) and di-*tert*-butyl hyponitrite (25.1 mg, 0.144 mmol) in $CDCl_3$ (1.0 mL) was stirred at 60 °C for 12 h. After adding $MeNO_2$ as an internal standard, the resulting solution was subjected to ^1H NMR analysis to determine the yield of 1-bromo-4-deuteriobenzene (**6**) and its deuteration ratio.

Reaction of Iron Complexes with Di-tert-butyl Peroxide in the Presence of 4-Bromophenylboronic Acid and $CDCl_3$ (Scheme 3): General Procedure. To a partial suspension of $Fe(OTf)_3$ (30.2 mg, 0.0600 mmol), a ligand (0.060 mmol), and 4-bromophenylboronic acid (**1a**: 12.0 mg, 0.0600 mmol) in 0.60 mL of $CDCl_3$ in a 20 mL Schlenk tube was added *t*-BuOO*t*-Bu (**3**: 11 μL, 0.059 mmol). After stirring at 60 °C for the time specified in Scheme 3, nonane as an internal standard was added to the resulting solution. An aliquot of the solution was subjected to GC analysis to determine the yield of 1-bromo-4-deuteriobenzene (**6**) and the conversion of **3**. After concentration, the residue was subjected to SiO_2 chromatography (PTLC) to obtain **6** for determination of its deuteration ratio by ^1H NMR.

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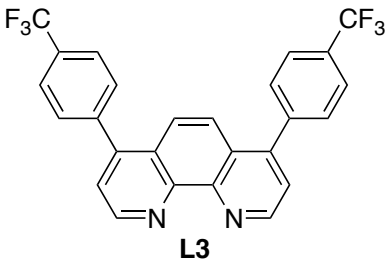
^{1}H and ^{13}C NMR Spectra of a Ligand and the Coupling Products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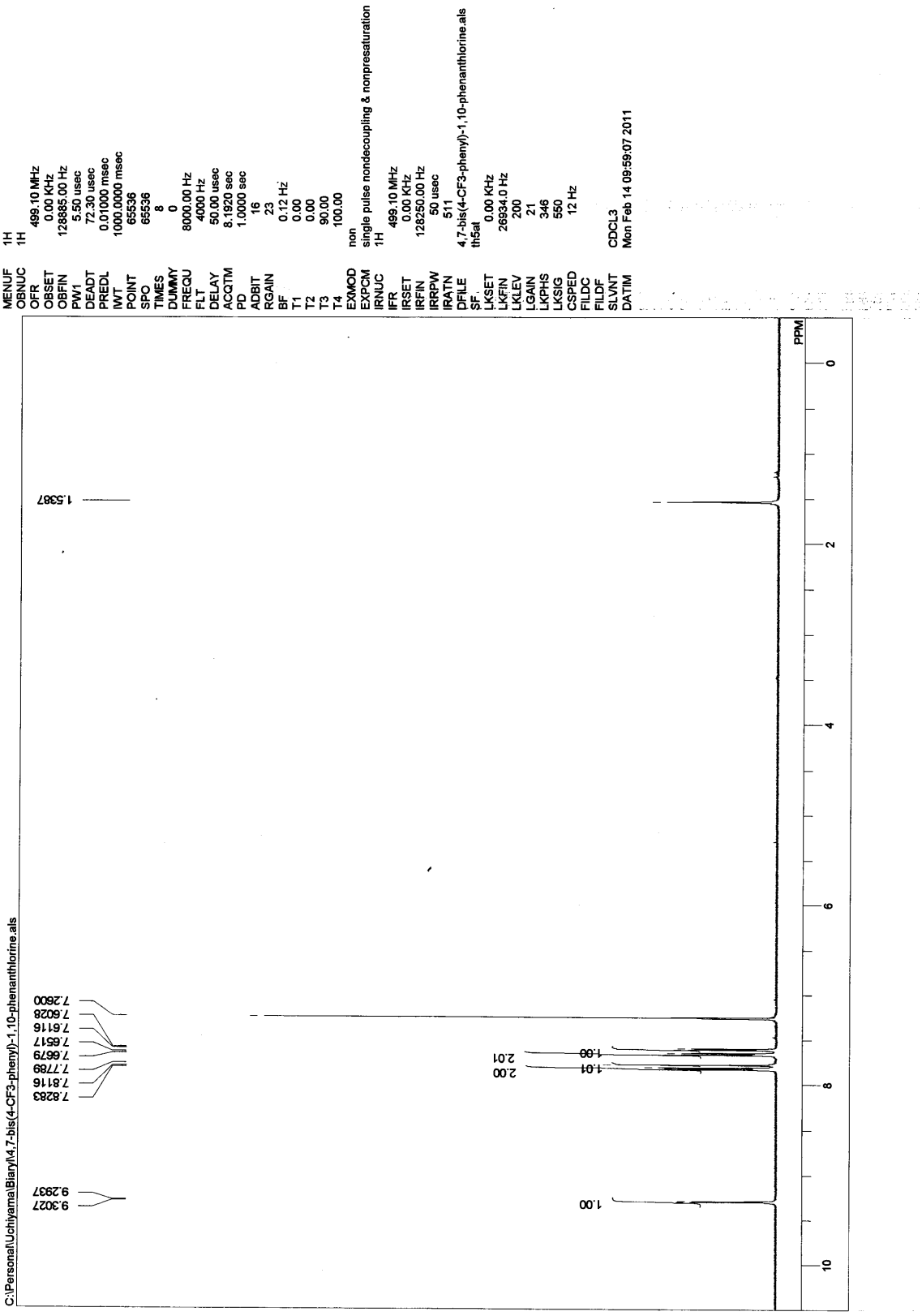
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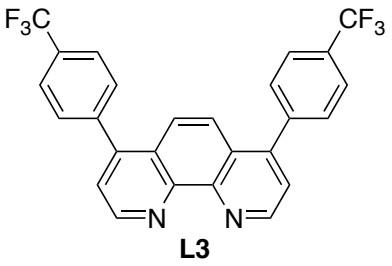
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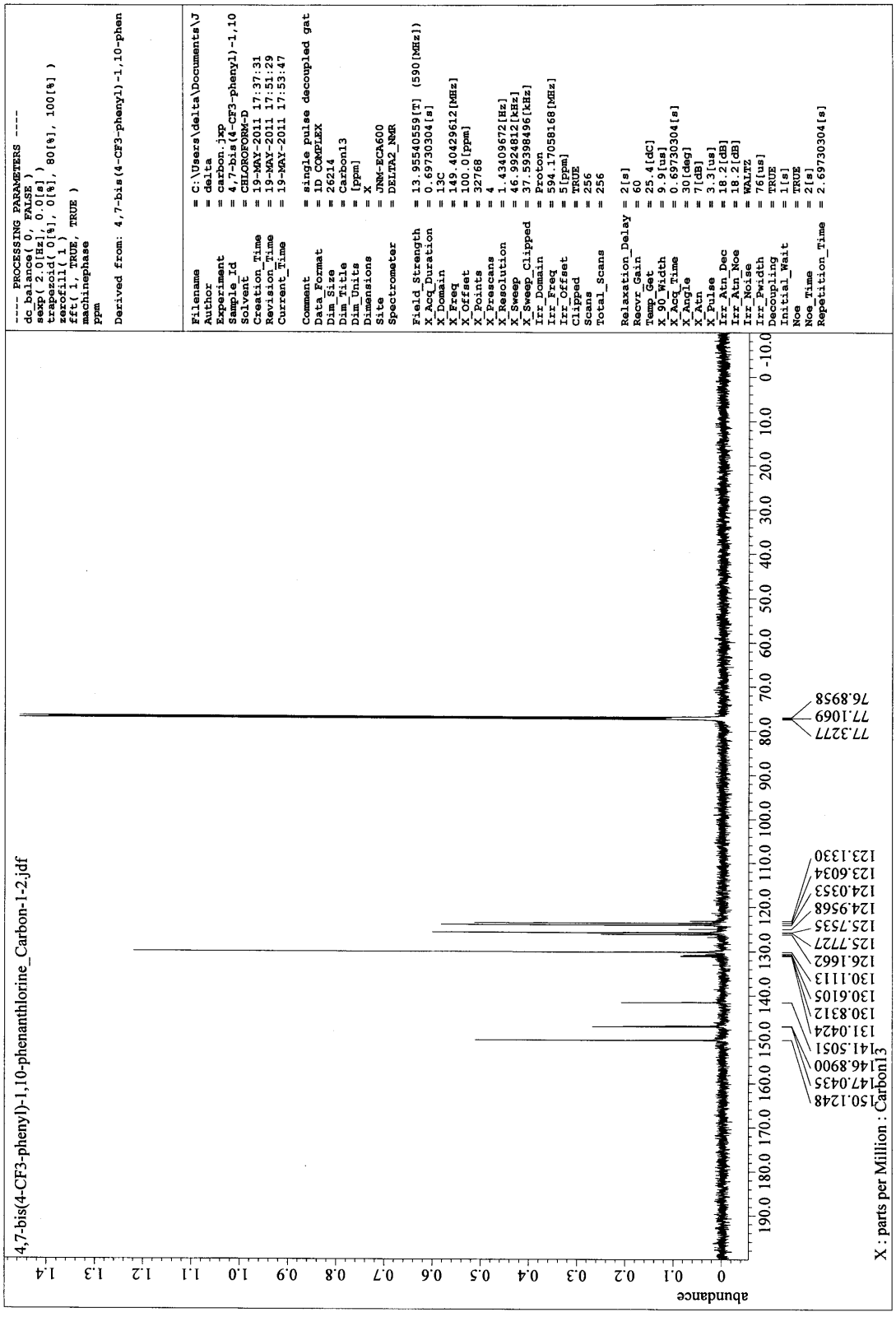
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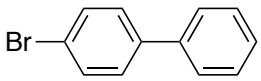
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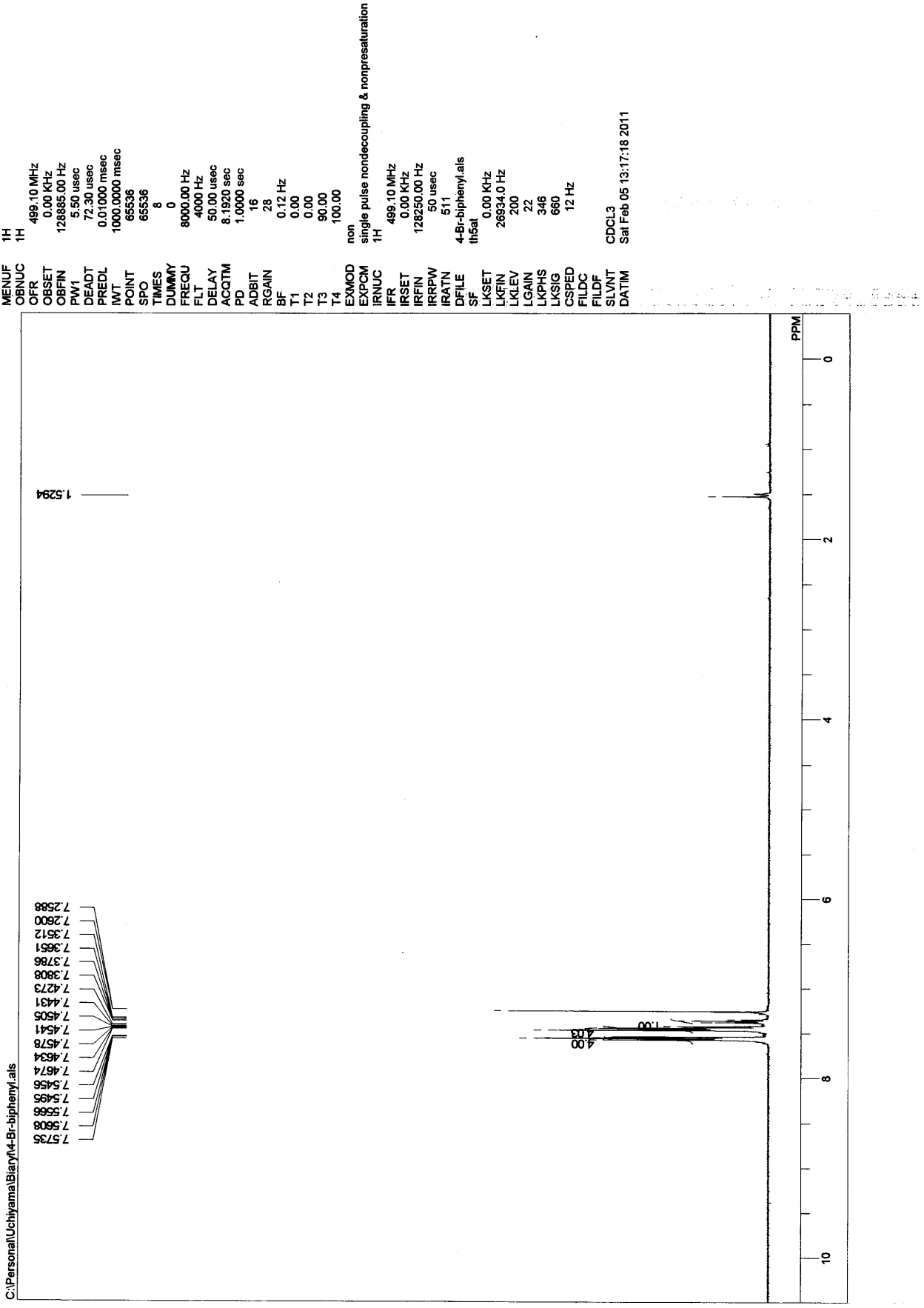
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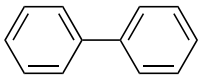

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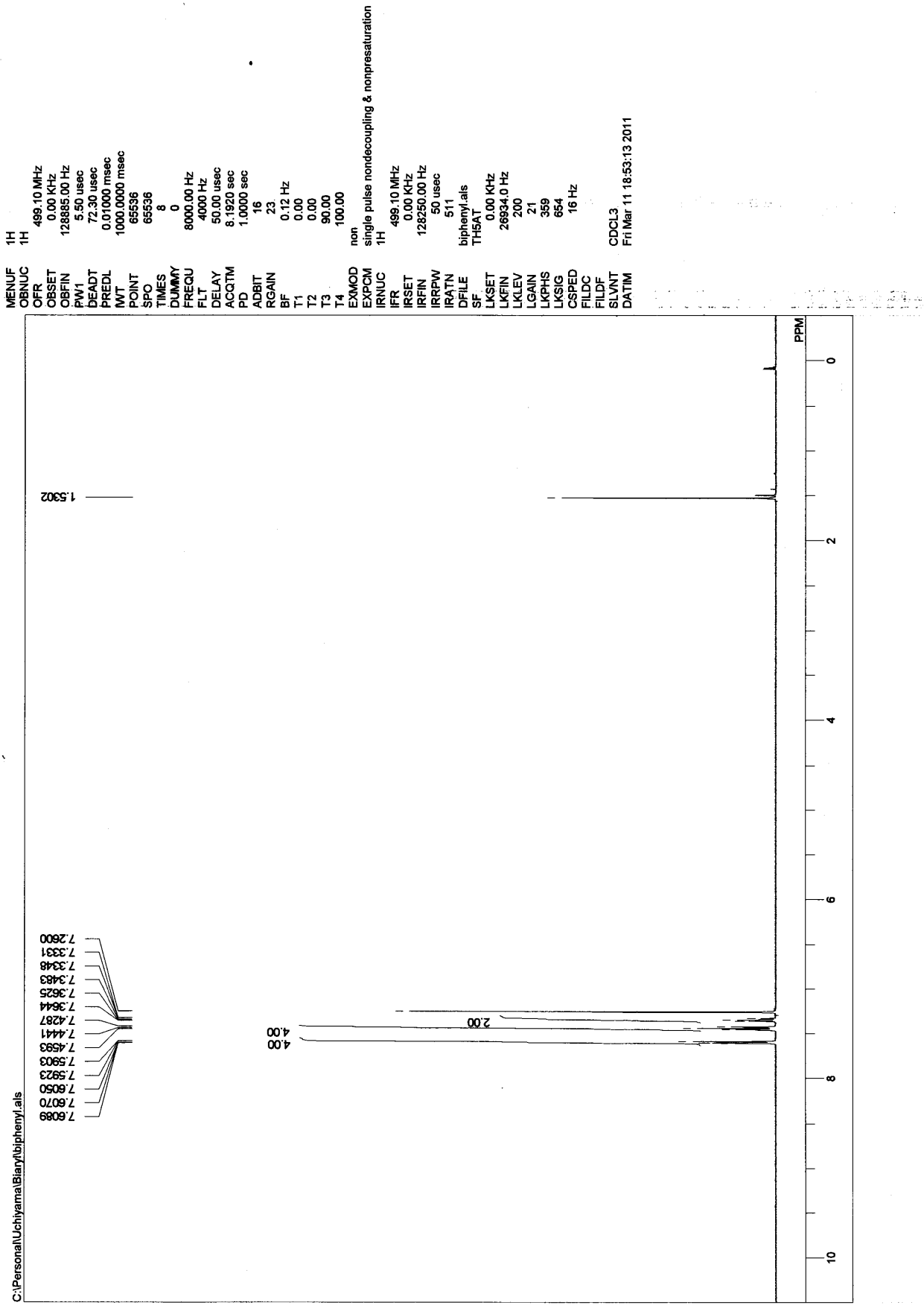
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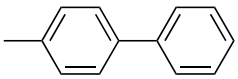

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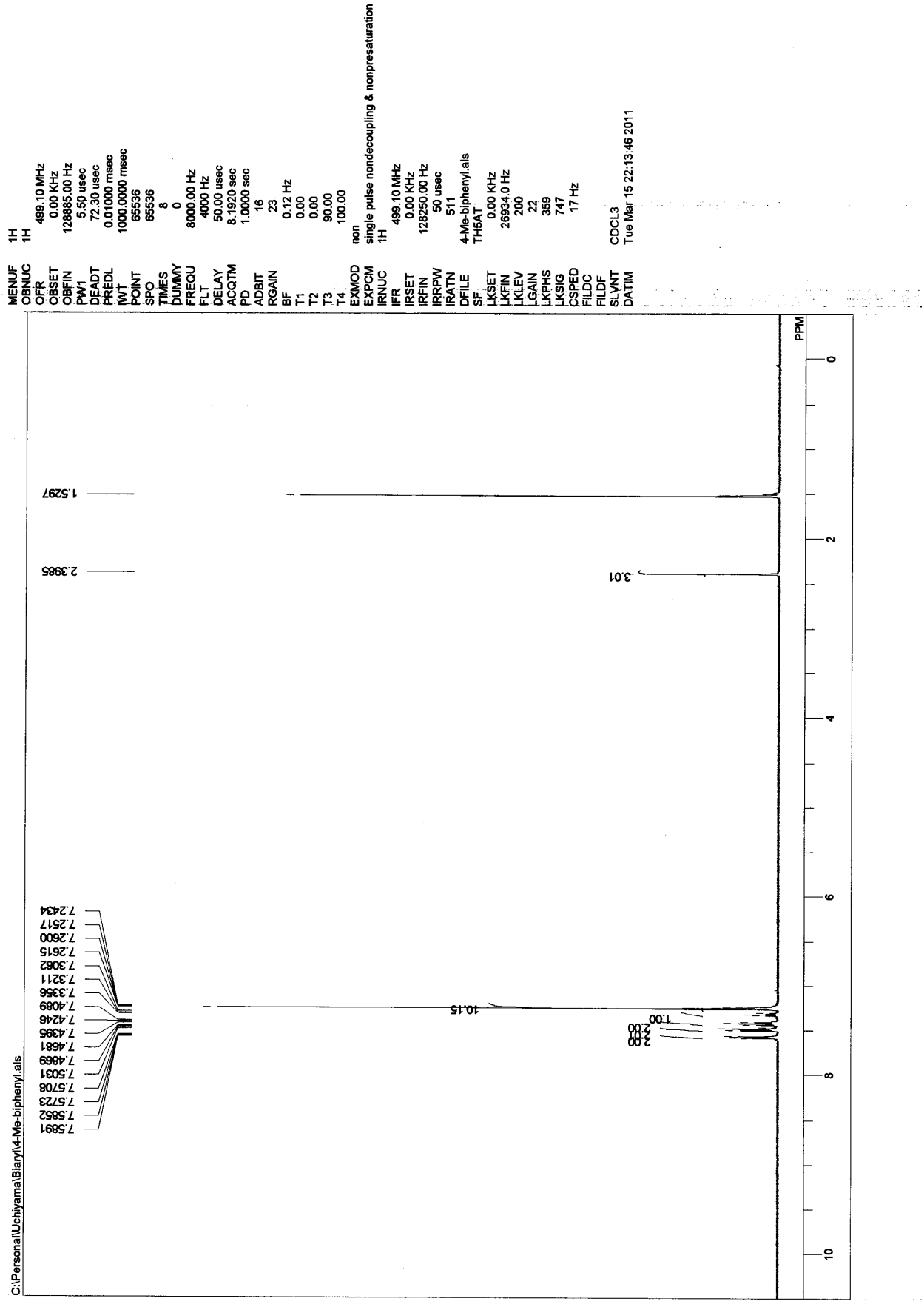
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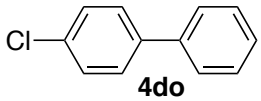
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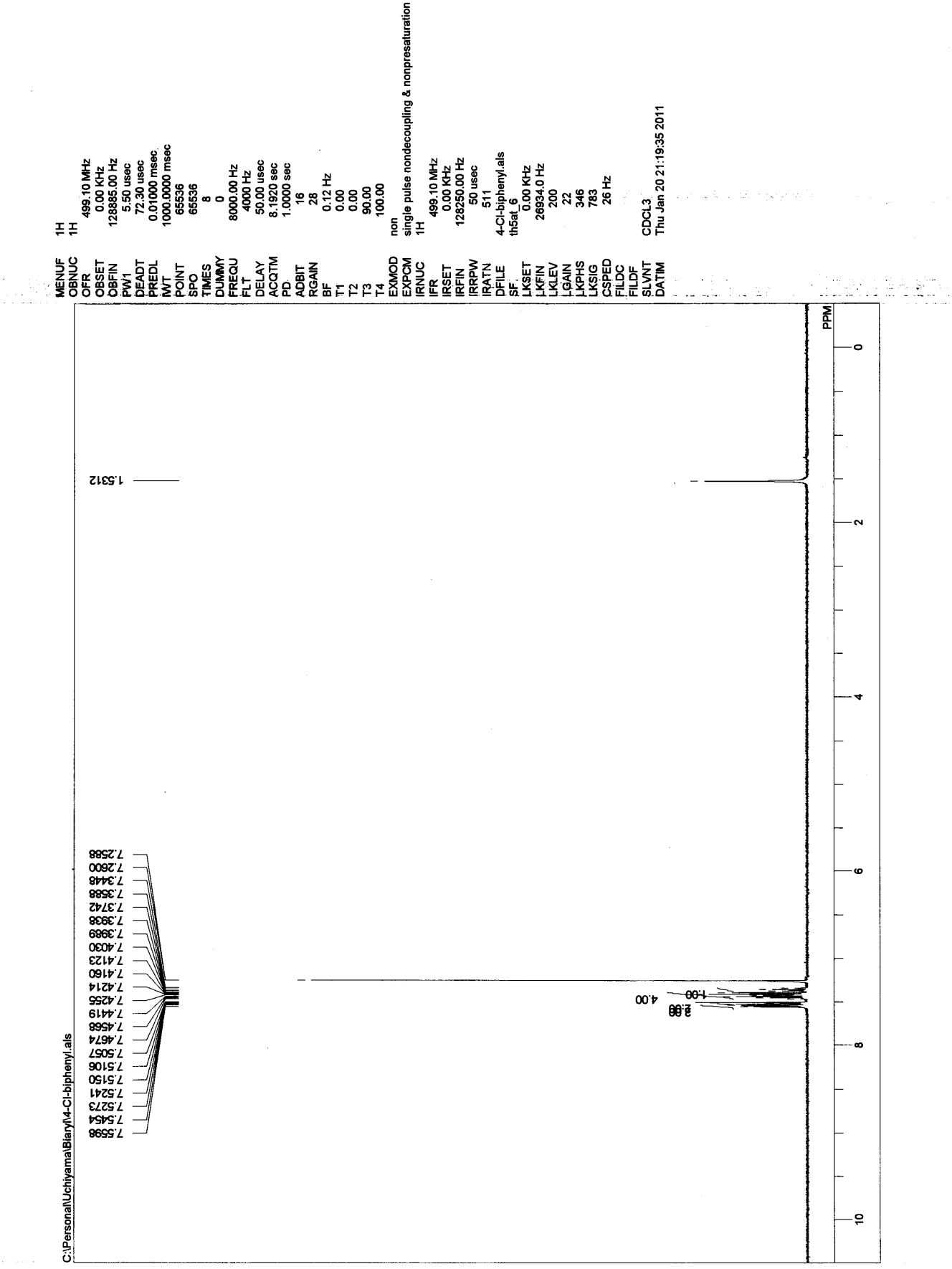
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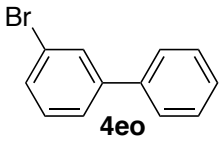
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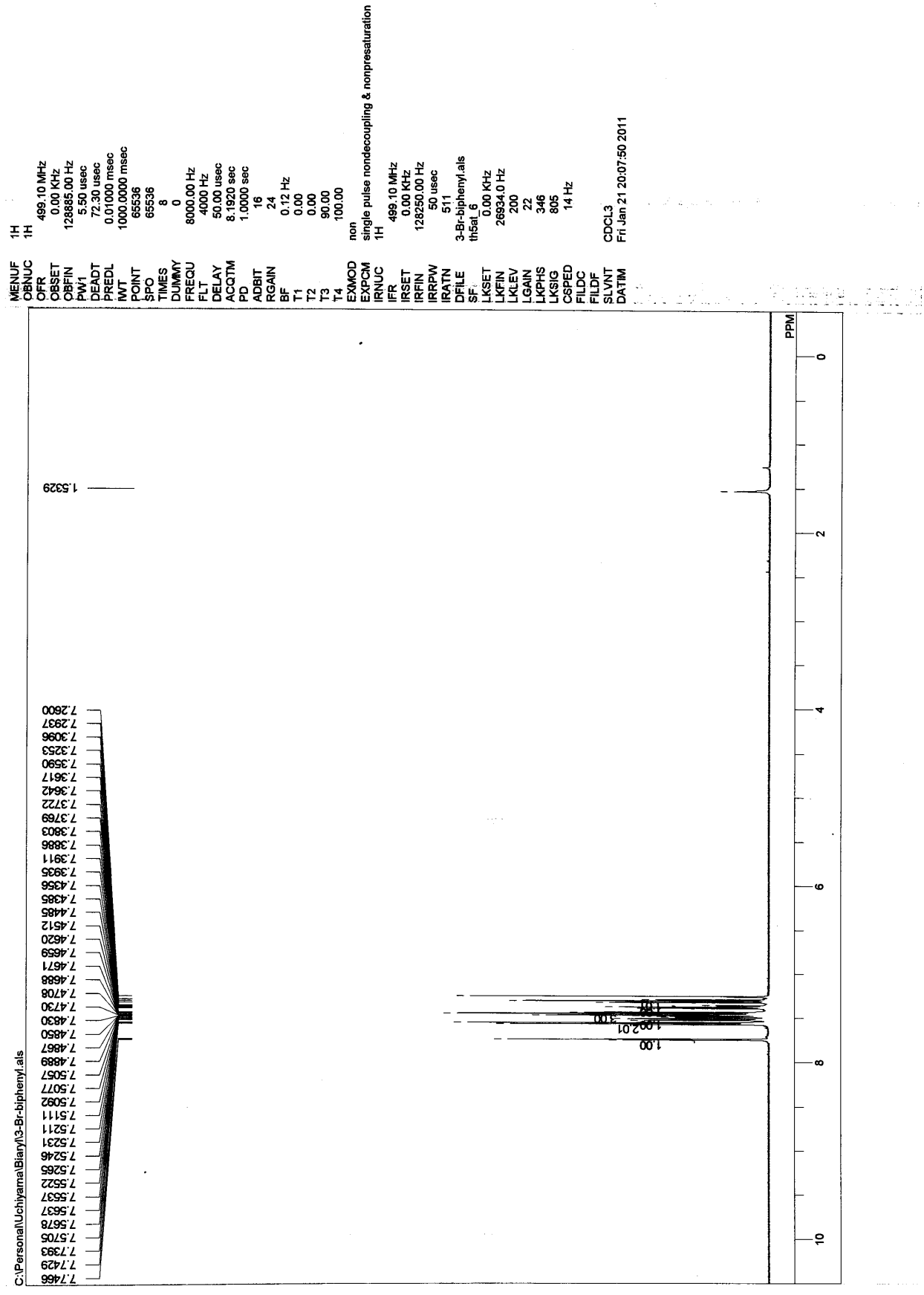
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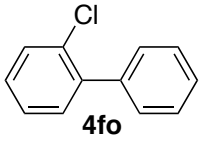
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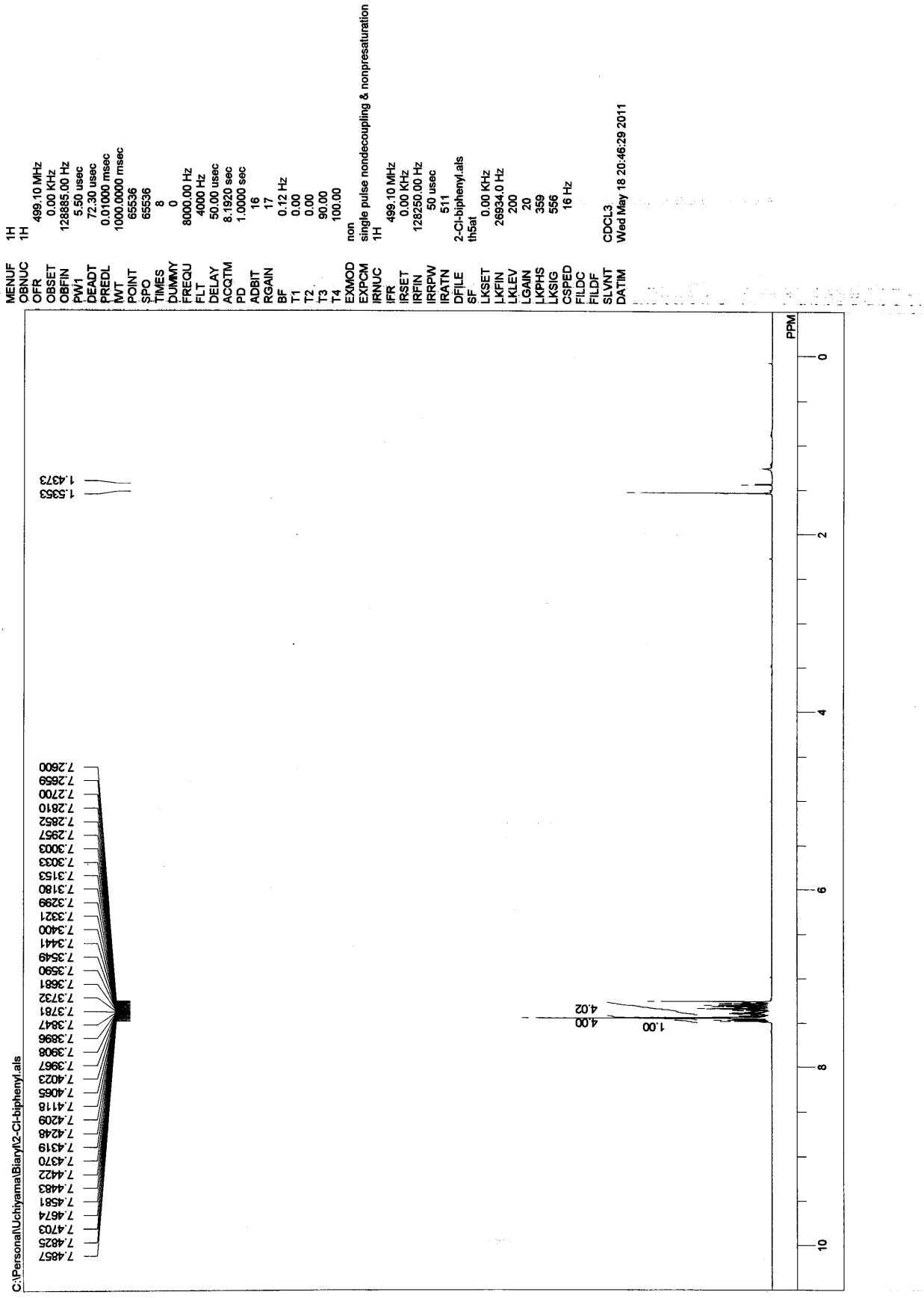
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RGAIN
BF
T1
T2
T3
T4
EXMOD
EXPCM
IRNUC
IFR
IRSET
IRFIN
IRRPW
IRATN
DFILE
SF
LKSET
LKFIN
LKLEV
LGAIN
LKPHS
LKSIG
CSPED
FILDC
FILDF
SLVNT
DATIM
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7.3781
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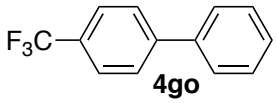
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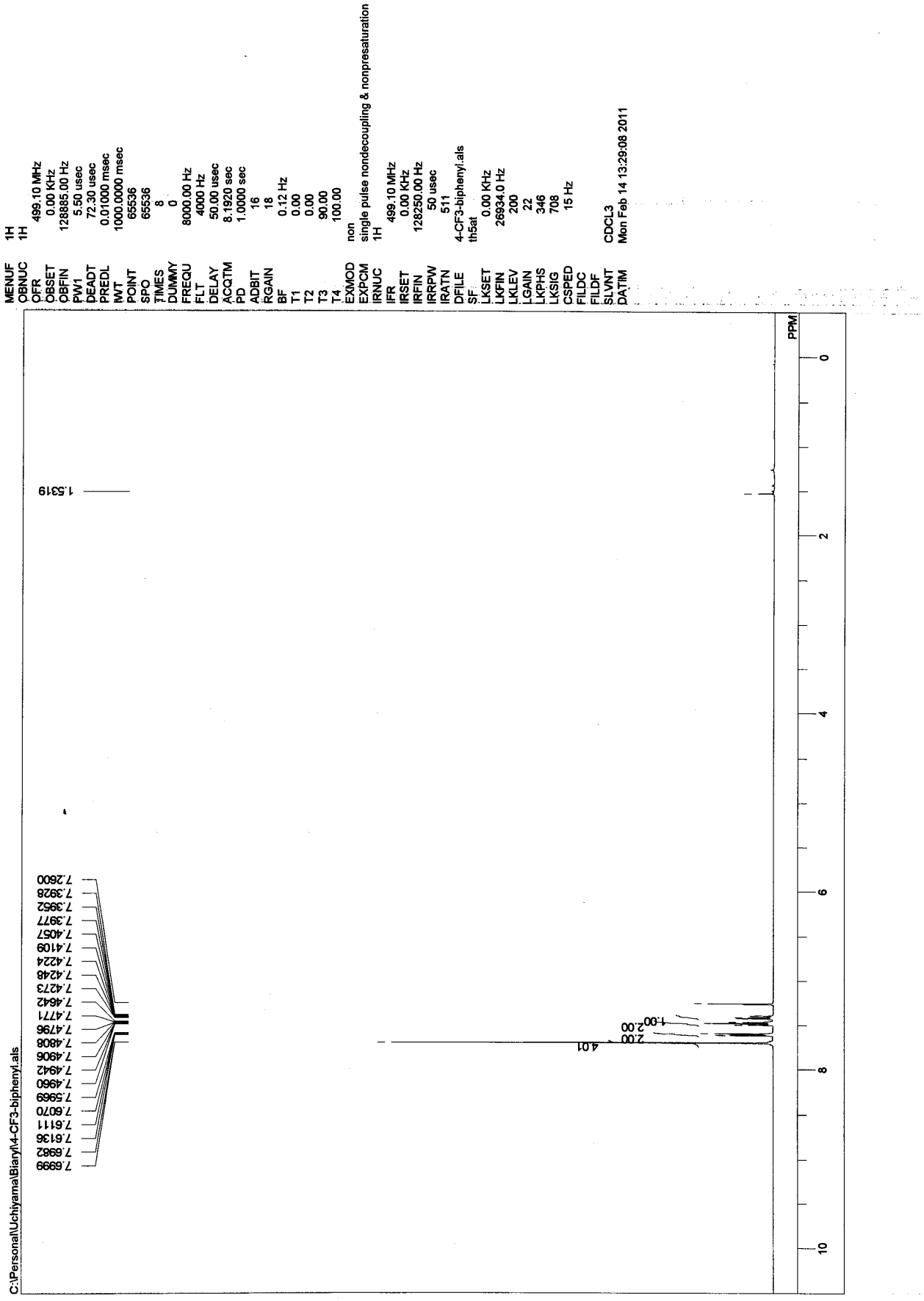
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1000.0000 msec
65536
65536
8
0
8000.00 Hz
4000 Hz
50.00 usec
8.1920 sec
1.0000 sec
16
18
0.12 Hz
0.00
0.00
90.00
100.00
non
single pulse nondecoupling & nonpresaturation
1H
499.10 MHz
0.00 KHz
128250.00 Hz
50 usec
511
4-CF3-biphenyl.als
th5at
0.00 KHz
26934.0 Hz
200
22
346
708
15 Hz
CDCL3
Mon Feb 14 13:29:08 2011
MENUF
OBNUC
OFR
OBSET
OBFIN
PW1
DEADT
PREDL
IWT
POINT
SPO
TIMES
DUMMY
FREQU
FLT
DELAY
ACQTM
PD
ADBIT
RGAIN
BF
T1
T2
T3
T4
EXMOD
EXPCM
IRNUC
IFR
IRSET
IRFIN
IRRPW
IRATN
DFILE
SF
LKSET
LKFIN
LKLEV
LGAIN
LKPHS
LKSIG
CSPED
FILDC
FILDF
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DATIM
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7.3952
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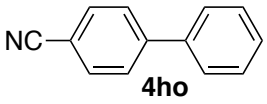
C:\Personal\Uchiyama\Biaryl\4-CF3-biphenyl.als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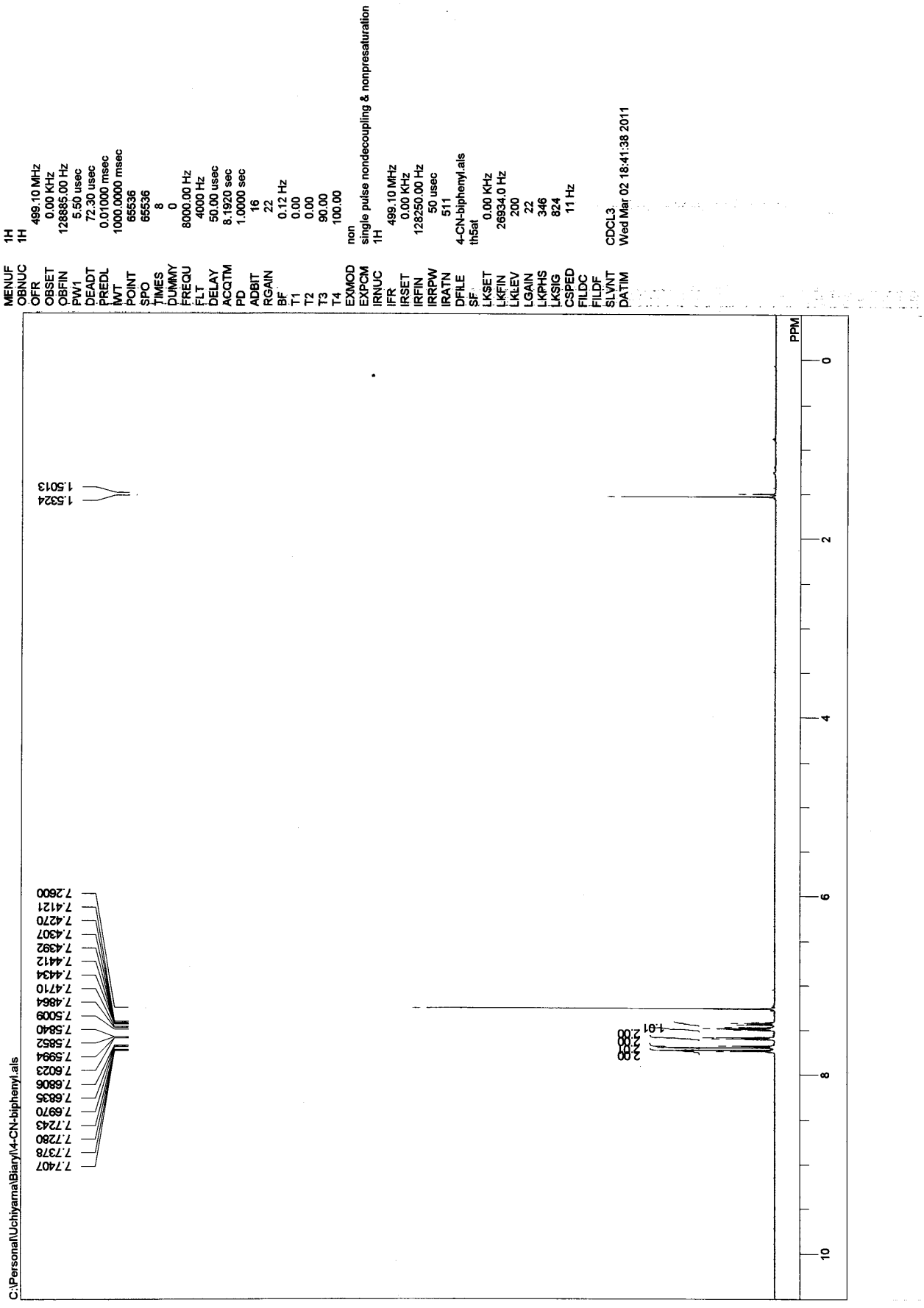
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5.50 usec
72.30 usec
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1000.0000 msec
65536
65536
8
0
8000.00 Hz
4000 Hz
50.00 usec
8.1920 sec
1.0000 sec
16
22
0.12 Hz
0.00
0.00
90.00
100.00
non
single pulse nondecoupling & nonpresaturation
1H
499.10 MHz
0.00 KHz
128250.00 Hz
50 usec
511
4-CN-biphenyl.als
th5at
0.00 KHz
26934.0 Hz
200
22
346
824
11 Hz
CDCL3
Wed Mar 02 18:41:38 2011
MENUF
OBNUC
OFR
OBSET
OBFIN
PW1
DEADT
PREDL
IWT
POINT
SPO
TIMES
DUMMY
FREQU
FLT
DELAY
ACQTM
PD
ADBIT
RGAIN
BF
T1
T2
T3
T4
EXMOD
EXPCM
IRNUC
IFR
IRSET
IRFIN
IRRPW
IRATN
DFILE
SF
LKSET
LKFIN
LKLEV
LGAIN
LKPHS
LKSIG
CSPED
FILDC
FILDF
SLVNT
DATIM
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7.4270
7.4307
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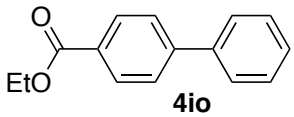
C:\Personal\Uchiyama\Biaryl\4-CN-biphenyl.als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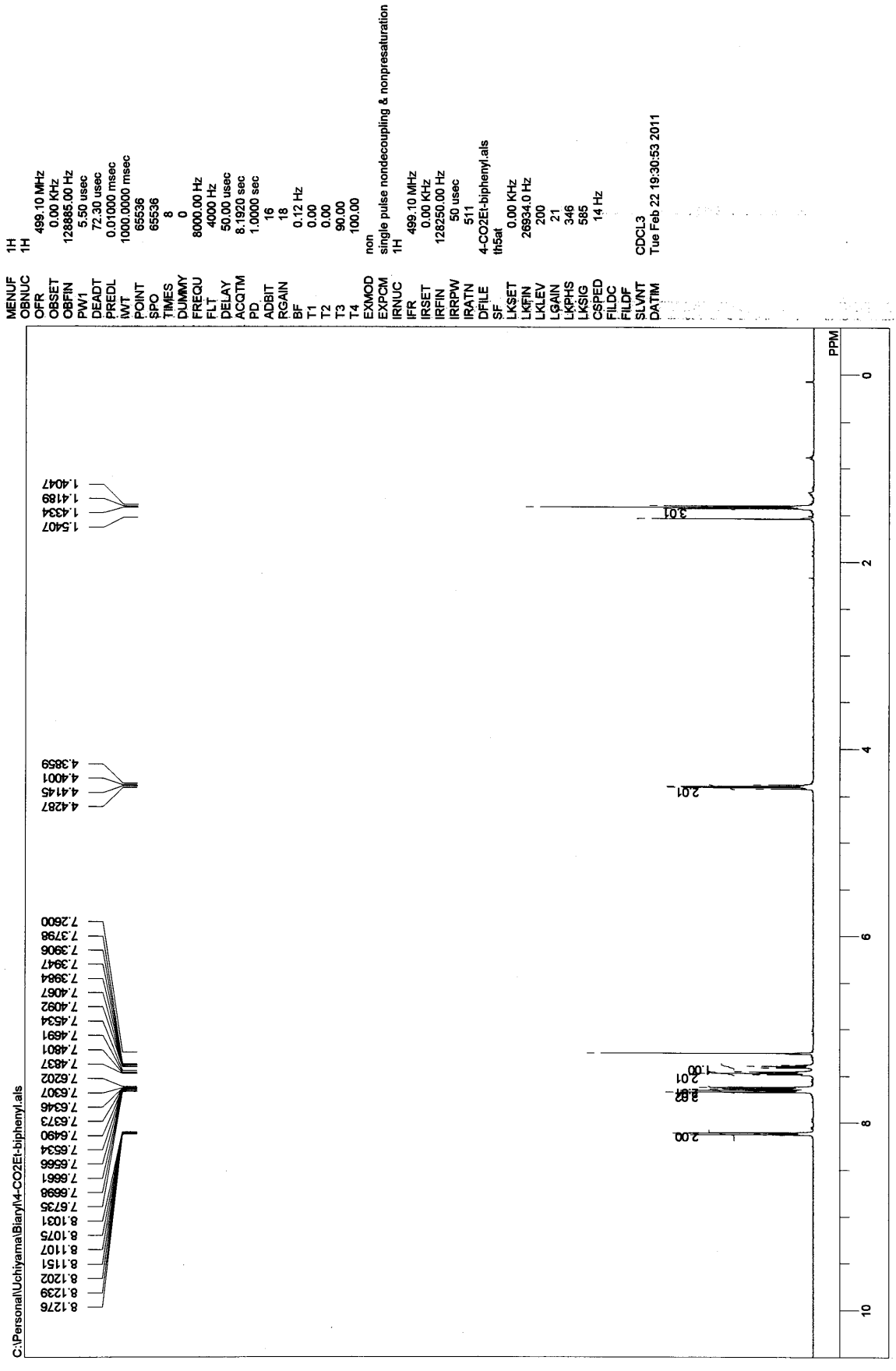
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OBFIN 128885.00 Hz
PW1 5.50 usec
DEADT 72.30 usec
PREDL 0.01000 msec
IWT 1000.0000 msec
POINT 65536
SPO 65536
TIMES 8
DUMMY 0
FREQU 8000.00 Hz
FLT 4000 Hz
DELAY 50.00 usec
ACQTM 8.1920 sec
PD 1.0000 sec
ADBIT 16
RGAIN 18
BF 0.12 Hz
T1 0.00
T2 0.00
T3 90.00
T4 100.00
EXMOD non
EXPCM single pulse nondecoupling & nonpresaturation
IRNUC 1H
IFR 499.10 MHz
IRSET 0.00 KHz
IRFIN 128250.00 Hz
IRRPW 50 usec
IRATN 511
DFILE 4-CO2Et-biphenyl.als
SF th5at
LKSET 0.00 KHz
LKFIN 26934.0 Hz
LKLEV 200
LKGAIN 21
LKPHS 346
LKSIG 585
CSPED 14 Hz
FILDC
FILDF
SLVNT CDCL3
DATIM Tue Feb 22 19:30:53 2011
C:\Personal\Uchiyama\Biaryl\4-CO2Et-biphenyl.als
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7.6373
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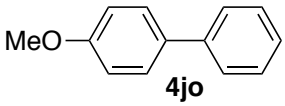
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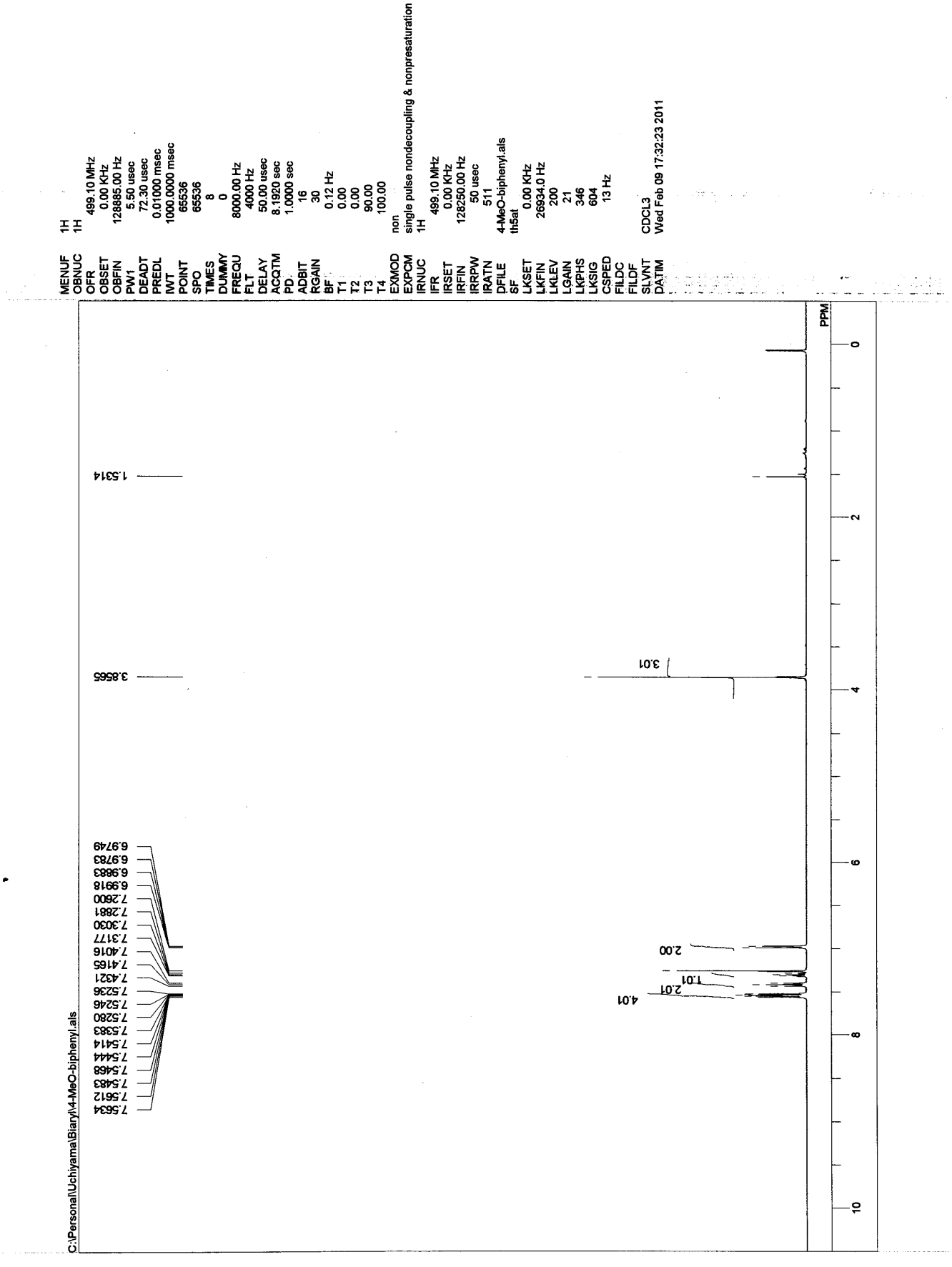
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72.30 usec
0.01000 msec
1000.0000 msec
65536
65536
8
0
8000.00 Hz
4000 Hz
50.00 usec
8.1920 sec
1.0000 sec
16
30
0.12 Hz
0.00
0.00
90.00
100.00
non
single pulse nondecoupling & nonpresaturation
1H
499.10 MHz
0.00 KHz
128250.00 Hz
50 usec
511
4-MeO-biphenyl.als
th5at
0.00 KHz
26934.0 Hz
200
21
346
604
13 Hz
CDCL3
Wed Feb 09 17:32:23 2011
MENUF
OBNUC
OFR
OBSET
OBFIN
PW1
DEADT
PREDL
IWT
POINT
SPO
TIMES
DUMMY
FREQU
FLT
DELAY
ACQTM
PD
ADBIT
RGAIN
BF
T1
T2
T3
T4
EXMOD
EXPCM
IRNUC
IFR
IRSET
IRFIN
IRRPW
IRATN
DFILE
SF
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LKFIN
LKLEV
LGAIN
LKPHS
LKSIG
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7.5634
3.01
2.00
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PPM
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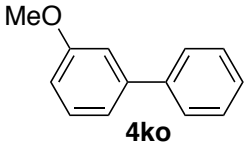
4
6
8
10
C:\Personal\Uchiyama\Biaryl\4-MeO-biphenyl.als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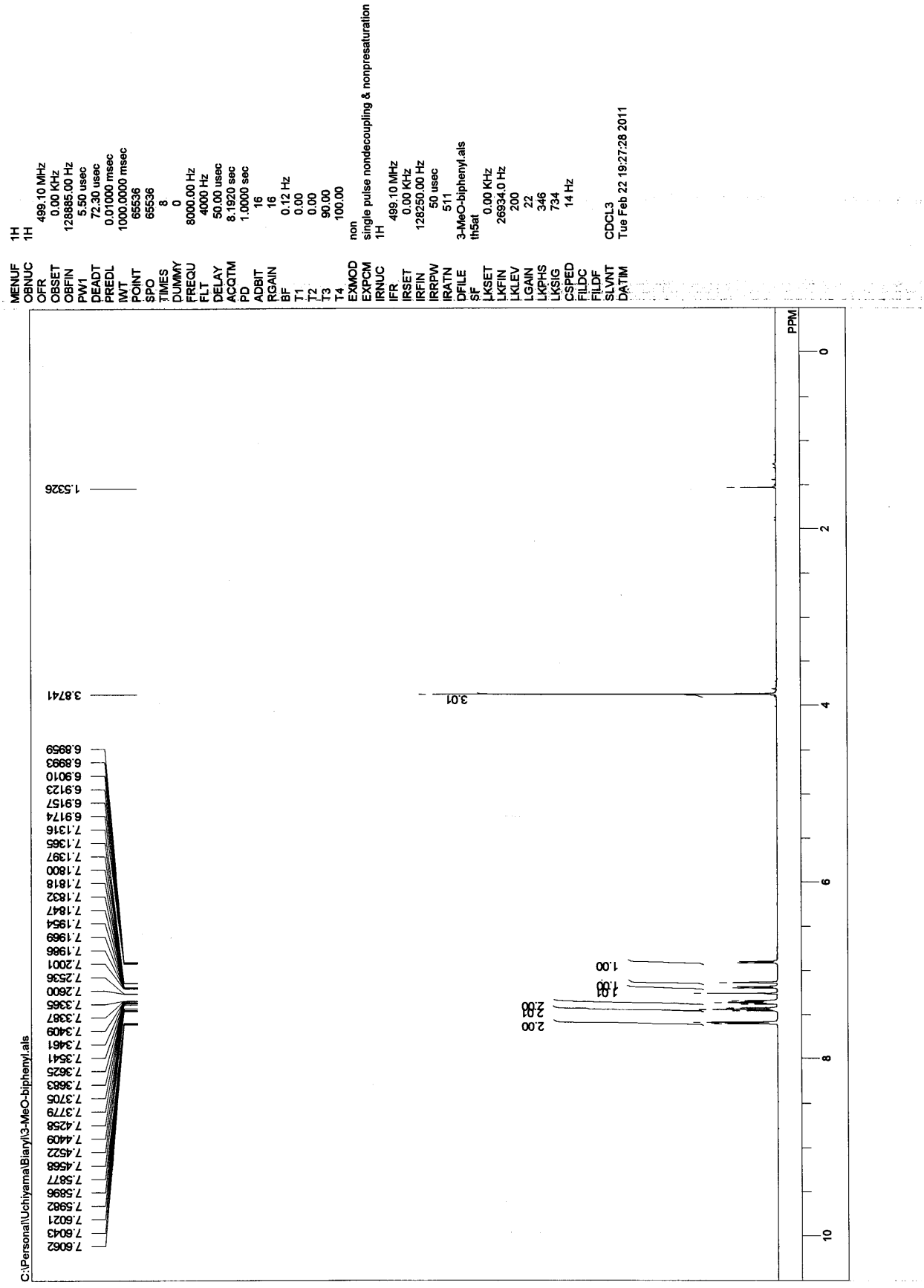
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72.30 usec
0.01000 msec
1000.0000 msec
65536
65536
8
0
8000.00 Hz
4000 Hz
50.00 usec
8.1920 sec
1.0000 sec
16
16
0.12 Hz
0.00
0.00
90.00
100.00
non
single pulse nondecoupling & nonpresaturation
1H
499.10 MHz
0.00 KHz
128250.00 Hz
50 usec
511
3-MeO-biphenyl.als
th5at
0.00 KHz
26934.0 Hz
200
22
346
734
14 Hz
CDCL3
Tue Feb 22 19:27:28 2011
MENUF
OBNUC
OFR
OBSET
OBFIN
PW1
DEADT
PREDL
IWT
POINT
SPO
TIMES
DUMMY
FREQU
FLT
DELAY
ACQTM
PD
ADBIT
RGAIN
BF
T1
T2
T3
T4
EXMOD
EXPCM
IRNUC
IFR
IRSET
IRFIN
IRRPW
IRATN
DFILE
SF
LKSET
LKFIN
LKLEV
LGAIN
LKPHS
LKSIG
CSPED
FILDC
FILDF
SLVNT
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7.3683
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7.6021
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C:\Personal\UchiyamaBiaryl\3-MeO-biphenyl.als
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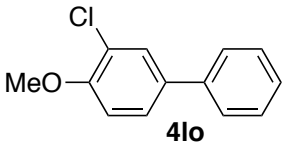
Cl
MeO

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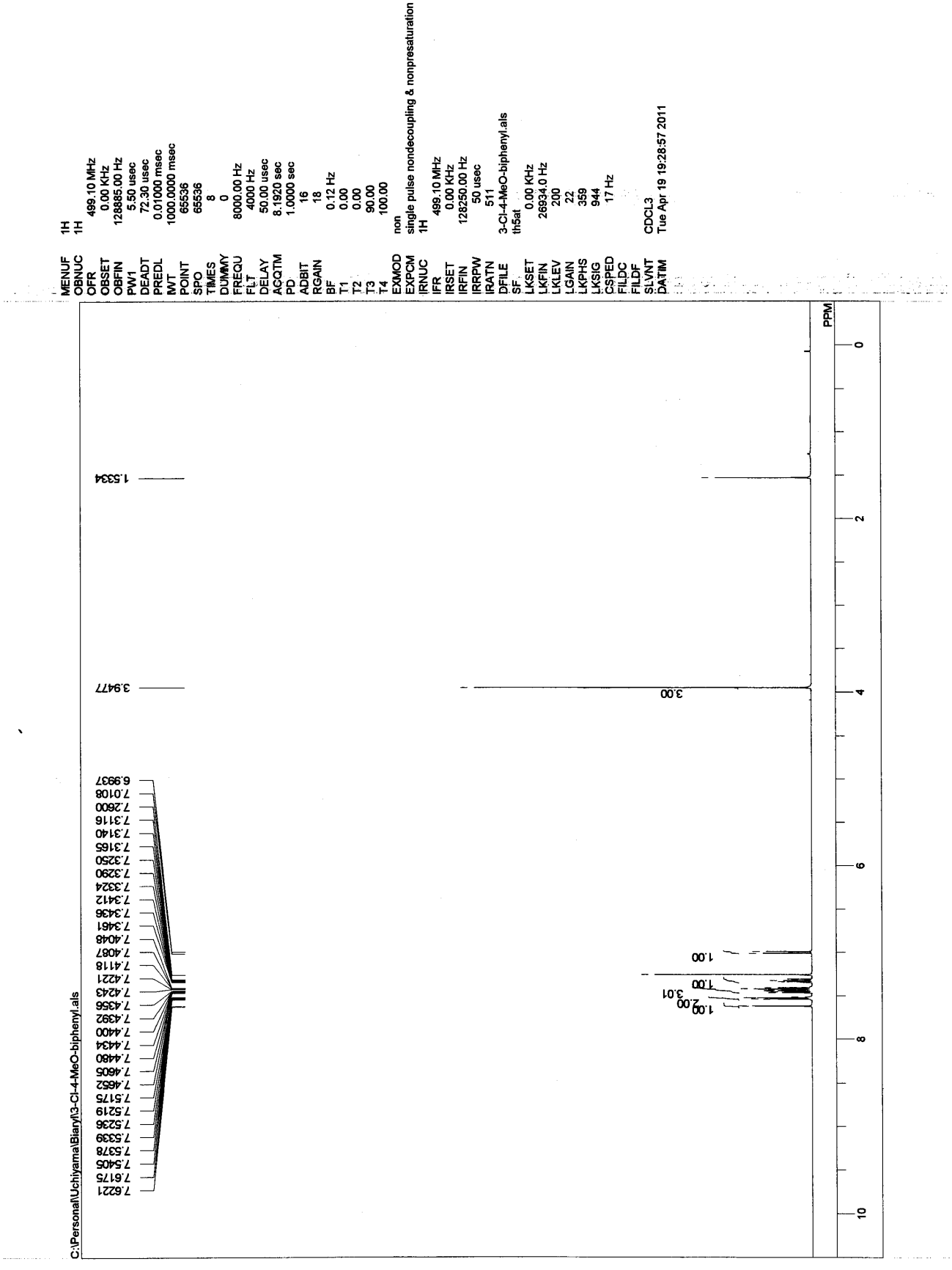
1H
1H
MENUF
OBNUC
OFR
OBSET
OBFIN
PW1
DEADT
PREDL
IVT
POINT
SPO
TIMES
DUMMY
FREQU
FLT
DELAY
ACQTM
PD
ADBIT
RGAIN
BF
T1
T2
T3
T4
EXMOD
EXPCM
IRNUC
IFR
IRSET
IRFIN
IRRPW
IRATN
DFILE
SF
LKSET
LKFIN
LKLEV
LGAIN
LKPHS
LKSIG
CSPED
FILDC
FILDF
SLVNT
DATIM
499.10 MHz
0.00 KHz
128885.00 Hz
5.50 usec
72.30 usec
0.01000 msec
1000.0000 msec
65536
65536
8
0
8000.00 Hz
4000 Hz
50.00 usec
8.1920 sec
1.0000 sec
16
18
0.12 Hz
0.00
0.00
90.00
100.00
non
single pulse nondecoupling & nonpresaturation
1H
499.10 MHz
0.00 KHz
128250.00 Hz
50 usec
511
3-Cl-4-MeO-biphenyl.als
th5at
0.00 KHz
26934.0 Hz
200
22
359
944
17 Hz
CDCL3
Tue Apr 19 19:28:57 2011
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C:\Personal\Uchiyama\Biaryl\3-Cl-4-MeO-biphenyl.als
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4
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8
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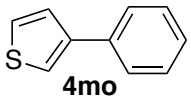
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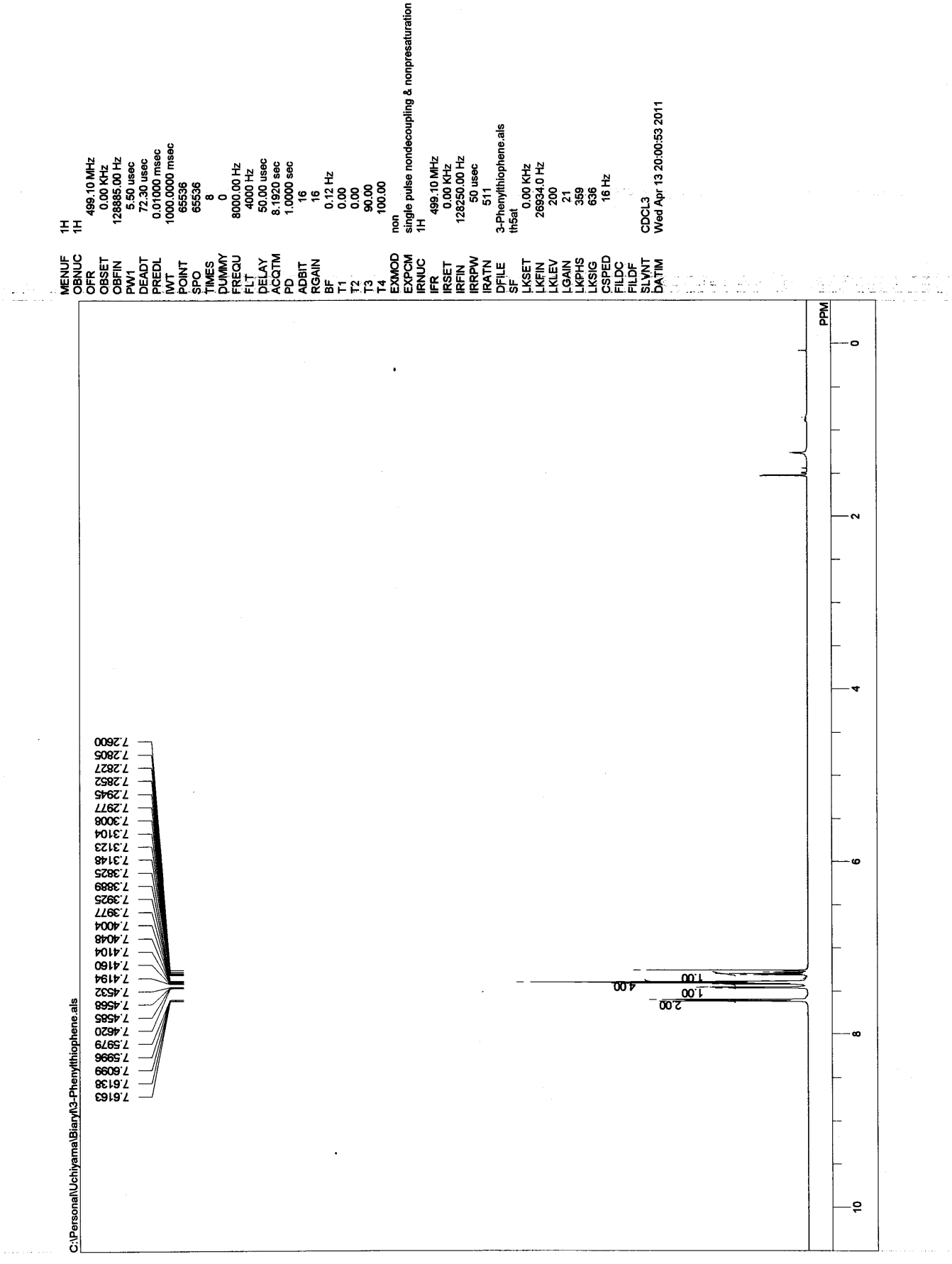
MENUF 1H
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OBFIN 128885.00 Hz
PW1 5.50 usec
DEADT 72.30 usec
PREDL 0.01000 msec
IWT 1000.0000 msec
POINT 65536
SPO 65536
TIMES 8
DUMMY 0
FREQU 8000.00 Hz
FLT 4000 Hz
DELAY 50.00 usec
ACQTM 8.1920 sec
PD 1.0000 sec
ADBIT 16
RGAIN 16
BF 0.12 Hz
T1 0.00
T2 0.00
T3 90.00
T4 100.00
EXMOD non
EXPCM single pulse nondecoupling & nonpresaturation
IRNUC 1H
IFR 499.10 MHz
IRSET 0.00 KHz
IRFIN 128250.00 Hz
IRRPW 50 usec
IRATN 511
DFILE 3-Phenylthiophene.als
SF tfi5at
LKSET 0.00 KHz
LKFIN 26934.0 Hz
LKLEV 200
LGAIN 21
LKPHS 359
LKSIG 636
CSPED 16 Hz
FILDC
FILDF
SLVNT CDCL3
DATIM Wed Apr 13 20:00:53 2011
C:\Personal\Uchiyama\Biaryl\3-Phenylthiophene.als
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PPM
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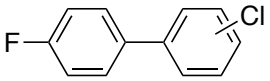
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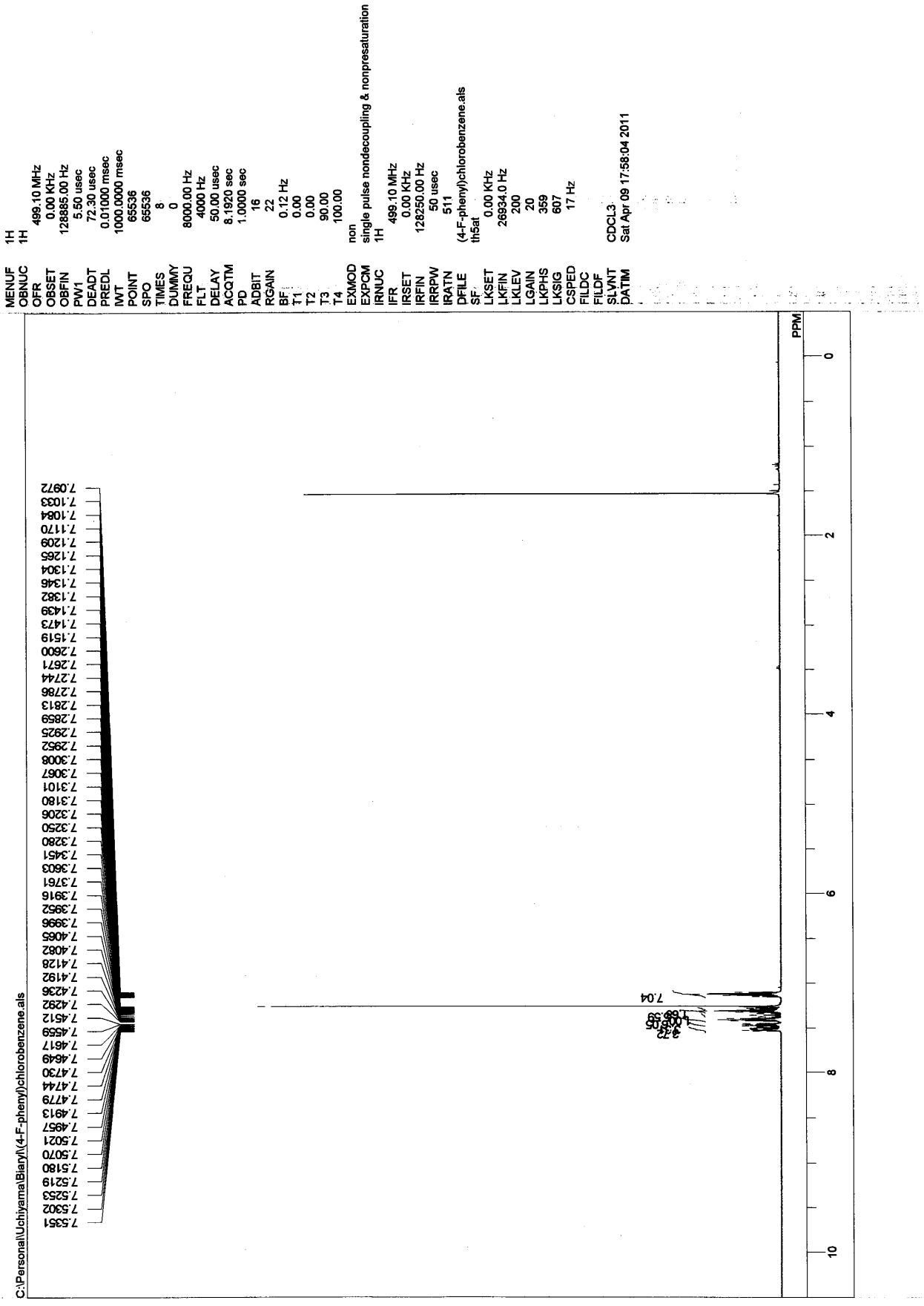
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OFR 499.10 MHz
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OBFIN 128885.00 Hz
PW1 5.50 usec
DEADT 72.30 usec
PREDL 0.01000 msec
IVT 1000.0000 msec
POINT 65536
SPO 65536
TIMES 8
DUMMY 0
FREQU 8000.00 Hz
FLT 4000 Hz
DELAY 50.00 usec
ACQTM 8.1920 sec
PD 1.0000 sec
ADBIT 16
RGAIN 22
BF 0.12 Hz
T1 0.00
T2 0.00
T3 90.00
T4 100.00
EXMOD non
EXPCM single pulse nondecoupling & nonpresaturation
IRNUC 1H
IFR 499.10 MHz
IRSET 0.00 KHz
IRFIN 128250.00 Hz
IRRPW 50 usec
IRATN 511
DFILE (4-F-phenyl)chlorobenzene.als
SF th5at
LKSET 0.00 KHz
LKFIN 26934.0 Hz
LKLEV 200
LGAIN 20
LKPHS 359
LKSIG 607
CSPED 17 Hz
FILDC
FILDF
SLVNT CDCL3
DATIM Sat Apr 09 17:58:04 2011
C:\Personal\Uchiyama\Biaryl\(4-F-phenyl)chlorobenzene.als
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7.1382
7.1439
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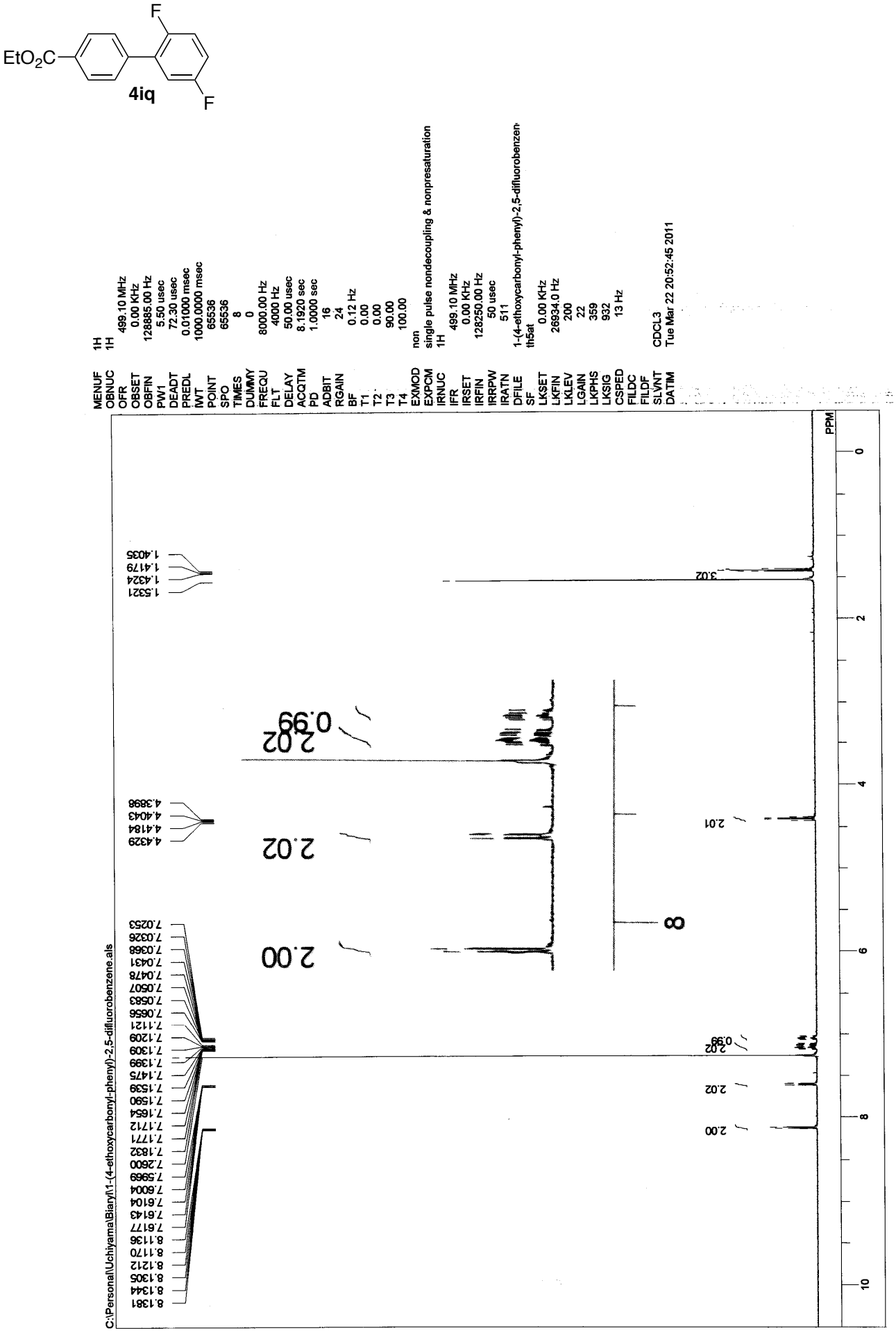
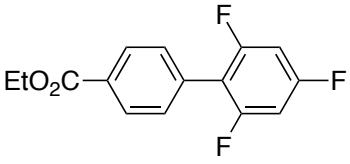
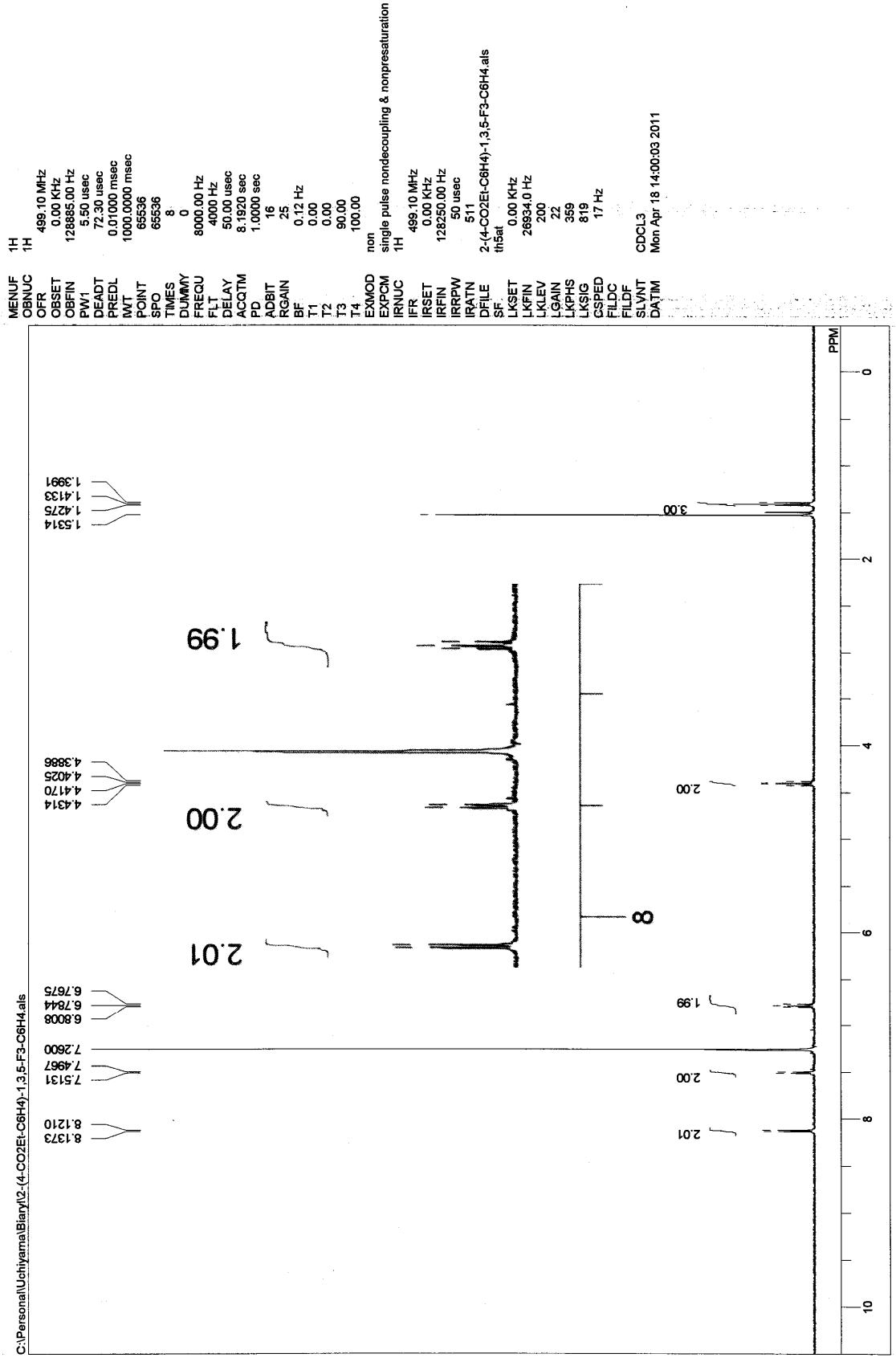
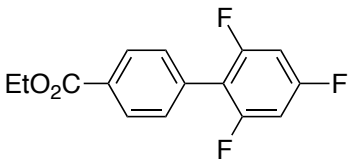

F
EtO2C
4iq
F
1H
1H
499.10 MHz
0.00 KHz
128885.00 Hz
5.50 usec
72.30 usec
0.01000 msec
1000.0000 msec
65536
65536
8
0
8000.00 Hz
4000 Hz
50.00 usec
8.1920 sec
1.0000 sec
16
24
0.12 Hz
0.00
0.00
90.00
100.00
non
single pulse nondecoupling & nonpresaturation
1H
499.10 MHz
0.00 KHz
128250.00 Hz
50 usec
511
1-(4-ethoxycarbonyl-phenyl)-2,5-difluorobenzen
th5at
0.00 KHz
26934.0 Hz
200
22
359
932
13 Hz
CDCl3
Tue Mar 22 20:52:45 2011
MENUF
OBNUC
OFR
OBSET
OBFIN
PW1
DEADT
PREDL
IWT
POINT
SPO
TIMES
DUMMY
FREQU
FLT
DELAY
ACQTM
PD
ADBIT
RGAIN
BF
T1
T2
T3
T4
EXMOD
EXPCM
IRNUC
IFR
IRSET
IRFIN
IRRPW
IRATN
DFILE
SF
LKSET
LKFIN
LKLEV
LGAIN
LKPHS
LKSIG
CSPED
FILDC
FILDF
SLVNT
DATIM
C:\Personal\Uchiyama\Biaryl\1-(4-ethoxycarbonyl-phenyl)-2,5-difluorobenzene.als
8.1381
8.1344
8.1305
8.1212
8.1170
8.1136
7.6177
7.6143
7.6104
7.6004
7.5969
7.2600
7.1832
7.1771
7.1712
7.1654
7.1590
7.1539
7.1475
7.1399
7.1309
7.1209
7.1121
7.0656
7.0583
7.0507
7.0478
7.0431
7.0368
7.0326
7.0253
4.4329
4.4184
4.4043
4.3898
1.5321
1.4324
1.4179
1.4035
2.00
2.02
0.99
2.02
8
3.02
2.01
2.00
2.02
0.99
PPM
0
2
4
6
8
10

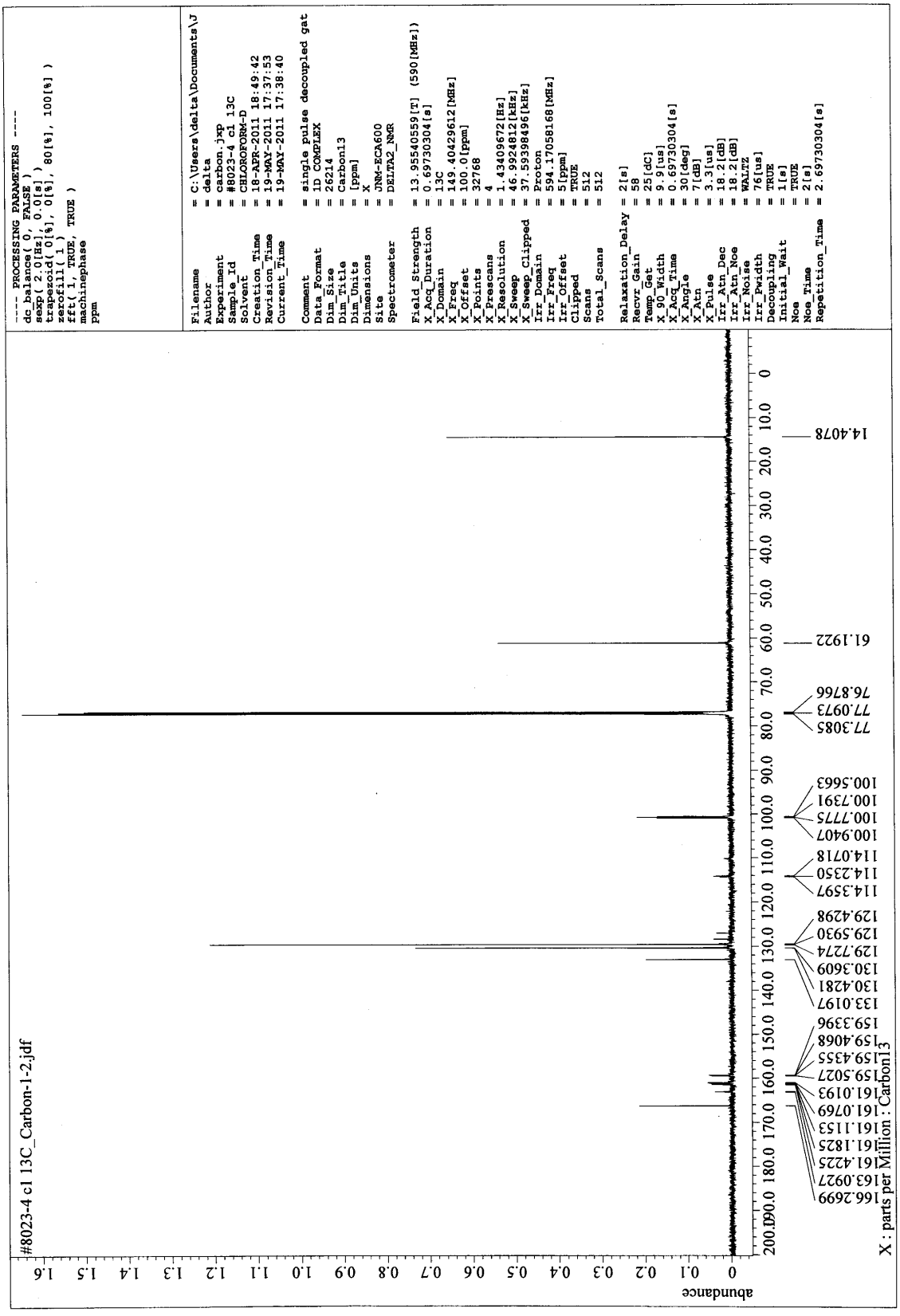

F
EtO2C
F
F

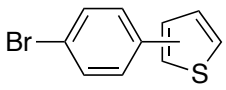
4ir


1H
1H
499.10 MHz
0.00 KHz
128885.00 Hz
5.50 usec
72.30 usec
0.01000 msec
1000.0000 msec
65536
65536
8
0
8000.00 Hz
4000 Hz
50.00 usec
8.1920 sec
1.0000 sec
16
25
0.12 Hz
0.00
0.00
90.00
100.00
non
single pulse nondecoupling & nonpresaturation
1H
499.10 MHz
0.00 KHz
128250.00 Hz
50 usec
511
2-(4-CO2Et-C6H4)-1,3,5-F3-C6H4.als
th5at
0.00 KHz
26934.0 Hz
200
22
359
819
17 Hz
CDCl3
Mon Apr 18 14:00:03 2011
MENUF
OBNUC
OFR
OBSET
OBFIN
PW1
DEADT
PREDL
IWT
POINT
SPO
TIMES
DUMMY
FREQU
FLT
DELAY
ACQTM
PD
ADBIT
RGAIN
BF
T1
T2
T3
T4
EXMOD
EXPCM
IRNUC
IFR
IRSET
IRFIN
IRRPW
IRATN
DFILE
SF
LKSET
LKFIN
LKLEV
LGAIN
LKPHS
LKSIG
GSPED
FILDC
FILDF
SLVNT
DATIM
C:\Personal\Uchiyama\Biaryl\2-(4-CO2Et-C6H4)-1,3,5-F3-C6H4.als
1.3991
1.4133
1.4275
1.5314
4.3886
4.4025
4.4170
4.4314
6.7675
6.7844
6.8008
7.2600
7.4967
7.5131
8.1210
8.1373
1.99
2.00
2.01
3.00
2.00
1.99
2.00
2.01
8
PPM
0
2
4
6
8
10

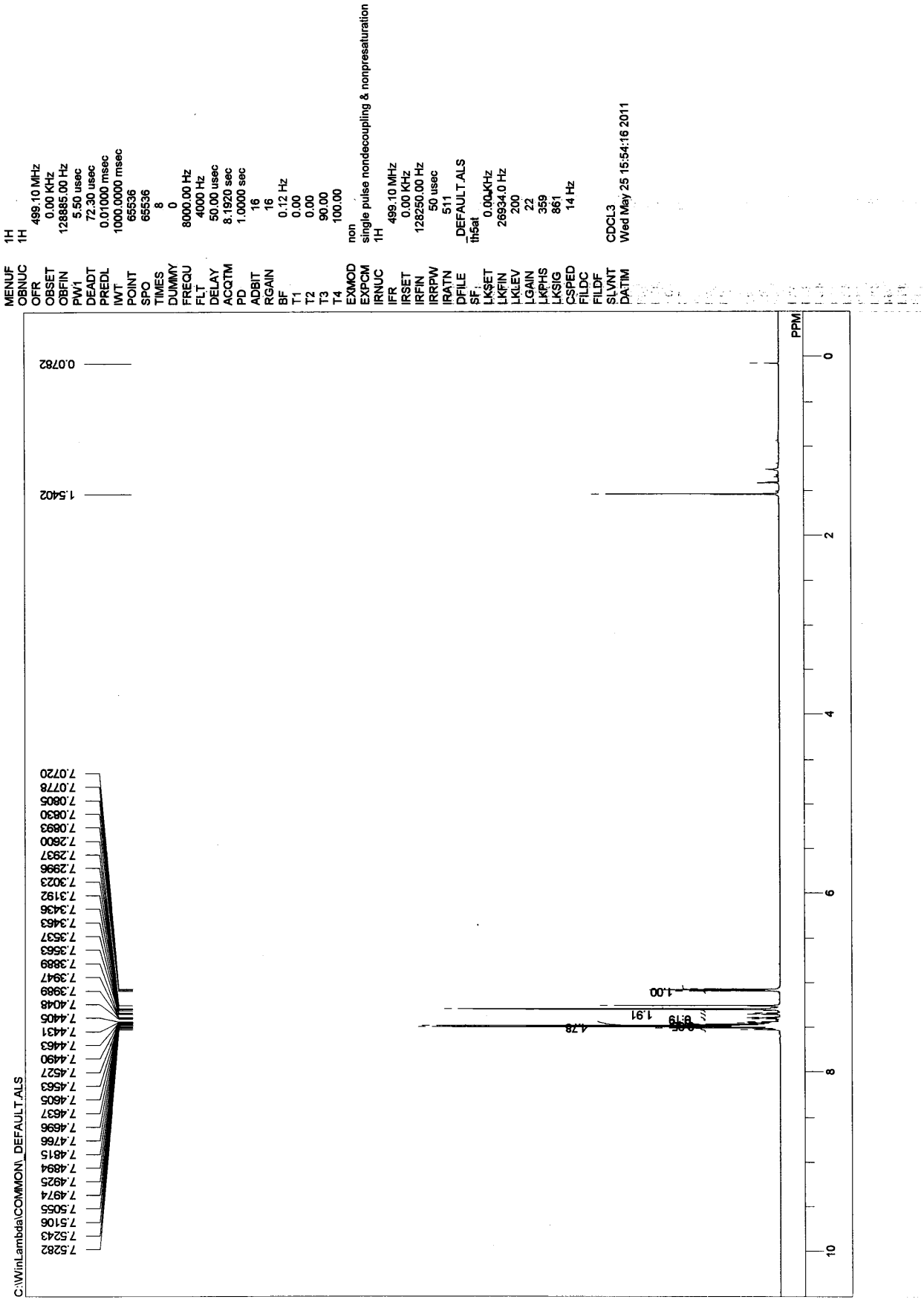

F
EtO2C
F
F

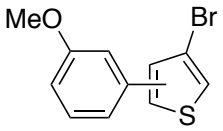
4ir


#8023-4 c1 13C_Carbon-1-2.jdf
X : parts per Million : Carbon13
abundance
14.4078
61.1922
76.8766
77.0973
77.3085
100.5663
100.7391
100.7775
100.9407
114.0718
114.2350
114.3597
129.4298
129.5930
129.7274
130.3609
130.4281
133.0197
159.3396
159.4068
159.4355
159.5027
161.0193
161.0769
161.1153
161.1825
161.4225
163.0927
166.2699

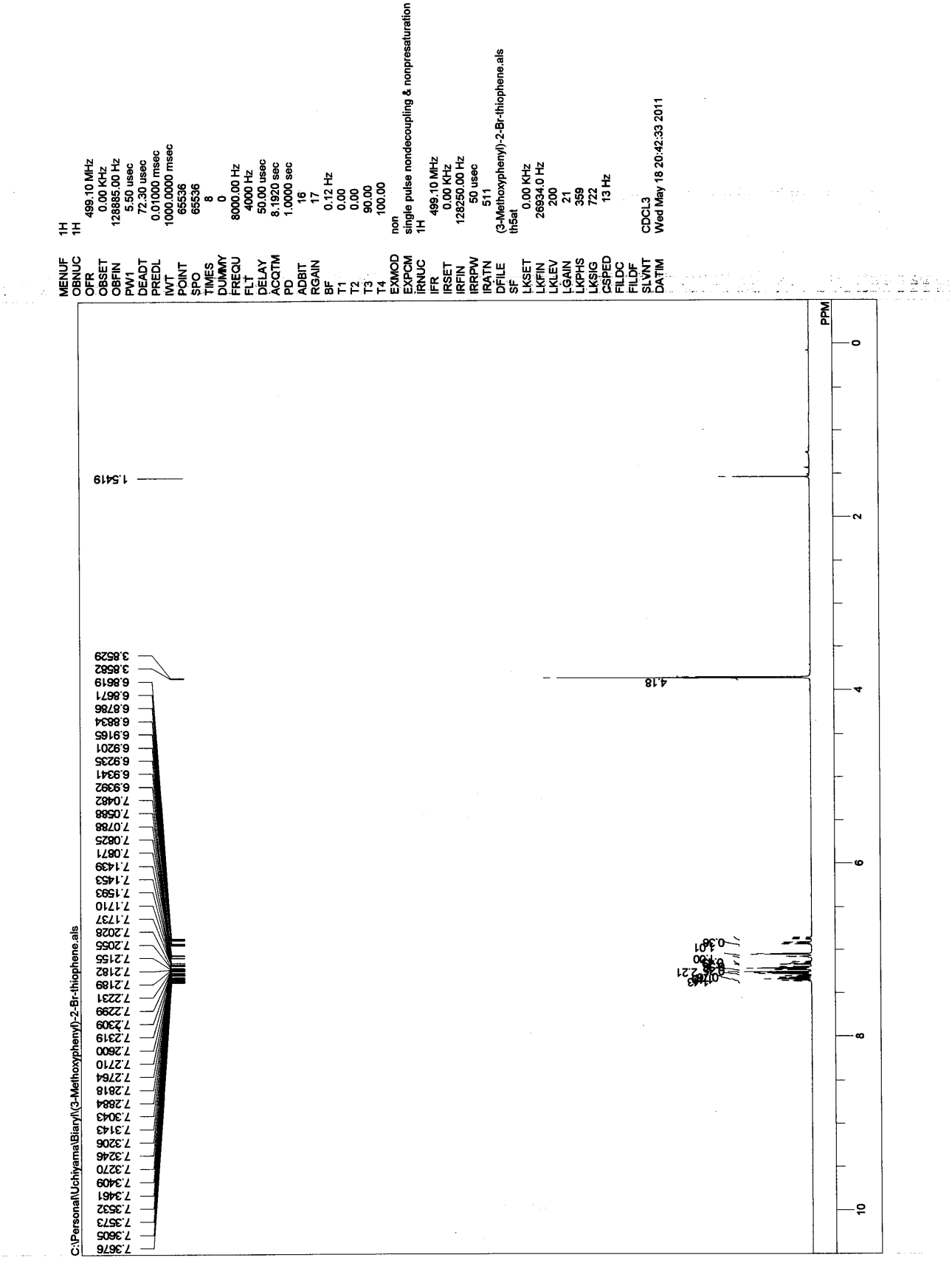

Br
S

4as


MENUF 1H
OBNUC 1H
OFR 499.10 MHz
OBSET 0.00 KHz
OBFIN 128885.00 Hz
PW1 5.50 usec
DEADT 72.30 usec
PREDL 0.01000 msec
IWT 1000.0000 msec
POINT 65536
SPO 65536
TIMES 8
DUMMY 0
FREQU 8000.00 Hz
FLT 4000 Hz
DELAY 50.00 usec
ACQTM 8.1920 sec
PD 1.0000 sec
ADBIT 16
RGAIN 16
BF 0.12 Hz
T1 0.00
T2 0.00
T3 90.00
T4 100.00
EXMOD non
EXPCM single pulse nondecoupling & nonpresaturation
IRNUC 1H
IFR 499.10 MHz
IRSET 0.00 KHz
IRFIN 128250.00 Hz
IRRPW 50 usec
IRATN 511
DFILE DEFAULT.ALS
SF th5at
LKSET 0.00 KHz
LKFIN 26934.0 Hz
LKLEV 200
LGAIN 22
LKPHS 359
LKSIG 861
CSPED 14 Hz
FILDC
FILDF
SLVNT CDCL3
DATIM Wed May 25 15:54:16 2011
0.0782
1.5402
7.0720
7.0778
7.0805
7.0830
7.0893
7.2600
7.2937
7.2996
7.3023
7.3192
7.3436
7.3463
7.3537
7.3563
7.3889
7.3947
7.3969
7.4048
7.4405
7.4431
7.4463
7.4490
7.4527
7.4563
7.4605
7.4637
7.4696
7.4766
7.4815
7.4894
7.4925
7.4974
7.5055
7.5106
7.5243
7.5282
1.00
1.91
4.78
C:\WinLambda\COMMON_DEFAULT.ALS
PPM
0
2
4
6
8
10


MeO
Br
S

4kt


MENUF 1H
OBNUC 1H
OFR 499.10 MHz
OBSET 0.00 KHz
OBFIN 128885.00 Hz
PW1 5.50 usec
DEADT 72.30 usec
PREDL 0.01000 msec
IVT 1000.0000 msec
POINT 65536
SPO 65536
TIMES 8
DUMMY 0
FREQU 8000.00 Hz
FLT 4000 Hz
DELAY 50.00 usec
ACQTM 8.1920 sec
PD 1.0000 sec
ADBIT 16
RGAIN 17
BF 0.12 Hz
T1 0.00
T2 0.00
T3 90.00
T4 100.00
EXMOD non
EXPCM single pulse nondecoupling & nonpresaturation
IRNUC 1H
IFR 499.10 MHz
IRSET 0.00 KHz
IRFIN 128250.00 Hz
IRRPW 50 usec
IRATN 511
DFILE (3-Methoxyphenyl)-2-Br-thiophene.als
SF th5at
LKSET 0.00 KHz
LKFIN 26934.0 Hz
LKLEV 200
LGAIN 21
LKPHS 359
LKSIG 722
GSPED 13 Hz
FILDC
FILDF
SLVNT CDCL3
DATIM Wed May 18 20:42:33 2011
1.5419
3.8529
3.8582
6.8619
6.8671
6.8786
6.8834
6.9165
6.9201
6.9235
6.9341
6.9392
7.0482
7.0588
7.0788
7.0825
7.0871
7.1439
7.1453
7.1593
7.1710
7.1737
7.2028
7.2055
7.2155
7.2182
7.2189
7.2231
7.2299
7.2309
7.2319
7.2600
7.2710
7.2764
7.2818
7.2884
7.3043
7.3143
7.3206
7.3246
7.3270
7.3409
7.3461
7.3532
7.3573
7.3605
7.3676
4.18
C:\Personal\Uchiyama\Biaryl\(3-Methoxyphenyl)-2-Br-thiophene.als
PPM
0
2
4
6
8
10