Synthesis of 2-Aminobenzothiazole *via* $FeCl_3$-Catalyzed Tandem Reaction of 2-Iodoaniline with Isothiocyanate in Water

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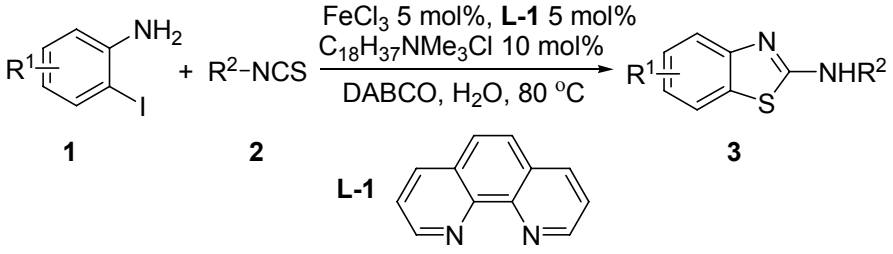
Supporting Information

General experimental methods:

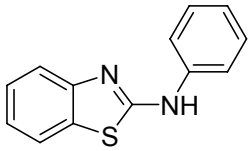
All reactions were performed in test tubes. Flash column chromatography was performed using silica gel (200-300 mesh). Analytical thin–layer chromatography was performed using glass plates pre-coated with 0.25 mm 230–400 mesh silica gel impregnated with a fluorescent indicator (254 nm). Thin layer chromatography plates were visualized by exposure to ultraviolet light. Organic solutions were concentrated on rotary evaporators at 25–35 °C. Commercial reagents and solvents were used as received. Proton (^{1}H NMR) and carbon (^{13}C NMR) nuclear magnetic resonance spectra were recorded on Bruker AV 400 at 400 MHz respectively 100 MHz at 293 K. The chemical shifts are given in parts per million (ppm) on the delta scale (δ) and are referenced to tetramethylsilane (0 ppm).

General procedure for $FeCl_3$-catalyzed tandem reaction of 2-iodoaniline 1 with isothiocyanate 2 in water:

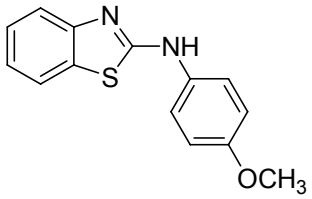


A mixture of 2-iodoaniline **1** (0.3 mmol), isothiocyanate **2** (0.45 mmol, 1.5 equiv.), DABCO (0.6 mmol, 2.0 equiv.), $FeCl_3$ (0.015 mmol, 5 mol %), and 1,10-phenanthroline **L-1** (0.015 mmol, 5 mol %), and octadecyltrimethylammonium chloride **PTC-4** (0.03 mmol, 10 mol%) was stirred in water (3 mL) at 80 °C. After completion of the reaction as indicated by TLC, the mixture was cooled to room

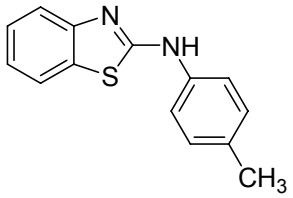
temperature. The mixture was washed with saturated brine, and extracted with ethyl acetate. The organic layers were dried with anhydrous $MgSO_4$ and evaporated the solvent under vacuum, and the residue was purified by flash column chromatography on silica gel to provide the corresponding pure product **3**.



N-phenylbenzo[*d*]thiazol-amine (**3a)**[1] white solid, mp 158-160 ^{o}C (lit. mp 157.2-159.4 ^{o}C); IR (prism, KBr, cm^{-1}) 3468, 1627; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.13-7.19 (m, 2H), 7.32 (t, *J* = 7.6 Hz, 1H), 7.41 (t, *J* = 8.4 Hz, 2H), 7.50 (d, *J* = 8.0 Hz, 2H), 7.56 (d, *J* = 8.0 Hz, 1H), 7.63 (d, *J* = 8.0 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 118.7, 119.9, 120.4, 121.9, 123.9, 125.6, 129.1, 129.3, 139.4, 150.7, 164.5.

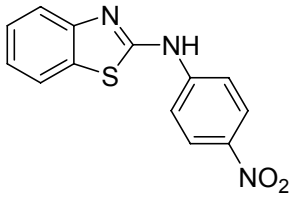


N-(4-methoxyphenyl)benzo[*d*]thiazol-2-amine **(3b)**[2] white solid, mp 153-155 ^{o}C (lit. mp 154-155 ^{o}C); IR (prism, KBr, cm^{-1}) 3428, 1621; ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.84 (s, 3H), 6.96 (d, *J* = 8.8 Hz, 2H), 7.09 (t, *J* = 7.6 Hz, 1H), 7.27 (t, *J* = 7.2 Hz, 1H), 7.38-7.44 (m, 3H), 7.57 (d, *J* = 8.0 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 55.5, 114.8, 118.8, 120.8, 121.9, 124.2, 126.0, 129.7, 133.0, 151.6, 157.4, 167.3.

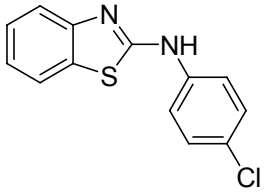


N-*p*-tolylbenzo[*d*]thiazol-2-amine (**3c)**[3] white solid, mp 178-179 ^{o}C (lit. mp 177-178

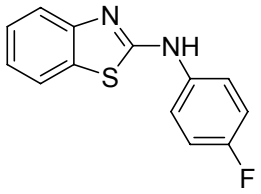
^{o}C); IR (prism, KBr, cm^{-1}) 3430, 1625; ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.37 (s, 3H), 7.12 (d, *J* = 8.4 Hz, 1H), 7.21 (d, *J* = 8.0 Hz, 2H), 7.30 (t, *J* = 8.0 Hz, 1H), 7.37 (d, *J* = 8.4 Hz, 2H), 7.51 (d, *J* = 7.6 Hz, 1H), 7.60 (d, *J* = 8.0 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 20.9, 119.1, 120.8, 121.2, 122.1, 126.0, 129.8, 130.1, 134.6, 137.4, 151.5, 165.9.



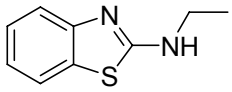
N-(4-nitrophenyl)benzo[*d*]thiazol-2-amine (**3d**)[4] yellow solid, mp 230-231 ^{o}C (lit. mp 225-227 ^{o}C); IR (prism, KBr, cm^{-1}) 3438, 1612; ^{1}H NMR (400 MHz, DMSO) δ 7.24 (t, *J* = 7.6 Hz, 1H), 7.39 (t, *J* = 7.6 Hz, 1H), 7.71 (d, *J* = 8.0 Hz, 1H), 7.90 (d, *J* = 7.6 Hz, 1H), 8.10 (d, *J* = 9.2 Hz, 2H), 8.27 (d, *J* = 9.2 Hz, 2H), 11.2 (br, 1H); ^{13}C NMR (100 MHz, DMSO) δ 117.7, 120.5, 121.8, 123.7, 125.9, 126.7, 130.8, 141.5, 146.9, 161.2.



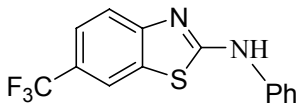
N-(4-chlorophenyl)benzo[*d*]thiazol-2-amine (**3e**)[5] white solid, mp 208-209 ^{o}C (lit. mp 206-207 ^{o}C); IR (prism, KBr, cm^{-1}) 3435, 1622; ^{1}H NMR (400 MHz, DMSO) δ 7.19 (t, *J* = 8.4 Hz, 1H), 7.36 (d, *J* = 8.0 Hz, 1H), 7.43 (d, *J* = 8.8 Hz, 2H), 7.63 (d, *J* = 8.0 Hz, 1H), 7.83 (d, *J* = 8.4 Hz, 2H); ^{13}C NMR (100 MHz, DMSO) δ 119.1, 119.3, 121.0, 122.4, 125.4, 125.9, 128.8, 129.9, 139.5, 151.9, 162.2.



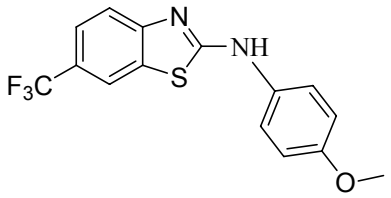
N-(4-fluorophenyl)benzo[*d*]thiazol-2-amine (**3f**)[5] white solid, mp 216-217 ^{o}C; IR (prism, KBr, cm^{-1}) 3467, 1626; ^{1}H NMR (400 MHz, DMSO) δ 7.14-7.22 (m, 3H), 7.33 (t, *J* = 7.6 Hz, 1H), 7.59 (d, *J* = 8.4 Hz, 1H), 7.77-7.82 (m, 3H), 10.40(br, 1H); ^{13}C NMR (100 MHz, DMSO) δ 115.5 (d, $^{2}J_{CF}$ = 22 Hz), 119.1 (d, $^{2}J_{CF}$ = 18 Hz), 119.2, 121.0, 122.3, 125.9, 129.9, 136.9, 151.9, 157.3 (d, $^{1}J_{CF}$ = 237 Hz), 161.5.



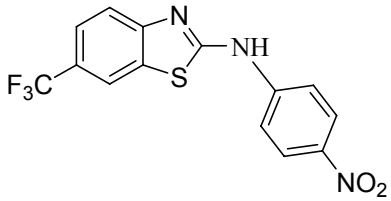
N-ethylbenzo[*d*]thiazol-2-amine (**3g**)[6] white solid, mp 114-116 ^{o}C IR (prism, KBr, cm^{-1}) 3436, 1611; ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.33 (t, *J* = 7.2 Hz, 3H), 3.46 (q, *J* = 7.2 Hz, 2H), 5.85 (br, 1H), 7.08 (t, *J* = 7.6 Hz, 1H), 7.29 (t, *J* = 7.6 Hz, 1H), 7.53 (d, *J* = 8.0 Hz, 1H), 7.59 (d, *J* = 7.6 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 14.9, 40.4, 118.7, 120.8, 121.4, 126.0, 130.2, 152.3, 167.7.



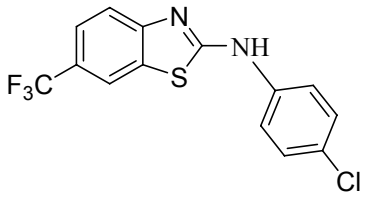
N-phenyl-6-(trifluoromethyl)benzo[*d*]thiazol-2-amine (**3h**)[6] white solid, mp 163-165 ^{o}C IR (prism, KBr, cm^{-1}) 3440, 1624; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.24 (t, *J* = 8.0 Hz, 1H), 7.44 (t, *J* = 8.0 Hz, 2H), 7.50 (d, *J* = 8.0 Hz, 2H), 7.54 (s, 2H), 7.86 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 118.3, 118.9, 121.0, 123.4 (q, $^{2}J_{CF}$ = 31.5 Hz), 125.7 (q, $^{1}J_{CF}$ = 270.8 Hz), 125.8, 129.8, 129.9, 139.3, 153.9, 167.4. 139.2, 153.9.



N-(4-methoxyphenyl)-6-(trifluoromethyl)benzo[*d*]thiazol-2-amine (**3i**)[4] white solid, mp 200-201 °C IR (prism, KBr, cm^{-1}) 3419, 1628; ^1H NMR (400 MHz, $CDCl_3$) δ 3.86 (s, 3H), 6.99 (d, *J* = 8.4 Hz, 2H), 7.41 (d, *J* = 8.8 Hz, 2H), 7.43 (d, *J* = 8.4 Hz, 1H), 7.51 (d, *J* = 8.4 Hz, 1H), 7.82 (s, 2H), 9.47 (br, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 55.5, 115.0, 118.3, 118.6, 123.7, 124.3 (q, $^2J_{CF}$ = 32 Hz), 124.6, 125.8 (q, $^1J_{CF}$ = 270 Hz), 130.0, 132.1, 154.3, 158.0, 169.3.

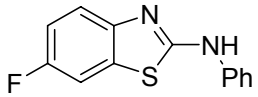


N-(4-nitrophenyl)-6-(trifluoromethyl)benzo[*d*]thiazol-2-amine (**3j**)[6] yellow solid, mp 253-254 °C IR (prism, KBr, cm^{-1}) 3437, 1619; ^1H NMR (400 MHz, DMSO) δ 7.70 (d, *J* = 8.0 Hz, 2H), 7.86 (d, *J* = 8.0 Hz, 1H), 8.03 (d, *J* = 9.2 Hz, 2H), 8.29 (d, *J* = 9.2 Hz, 2H), 8.36 (s, 1H); ^{13}C NMR (100 MHz, DMSO) δ 118.0, 119.6, 120.6, 123.8 (q, $^2J_{CF}$ = 33 Hz), 125.1 (q, $^1J_{CF}$ = 270 Hz), 125.8, 131.4, 141.8, 146.2, 154.7, 163.9.

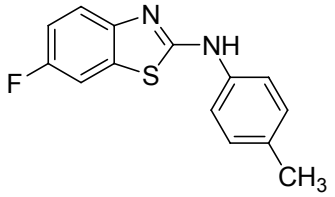


N-(4-chlorophenyl)-6-(trifluoromethyl)benzo[*d*]thiazol-2-amine (**3k**)[4] white solid, mp 193-194 °C (lit. mp 191-192 °C); IR (prism, KBr, cm^{-1}) 3435, 1623; ^1H NMR (400 MHz, DMSO) δ 7.45 (d, *J* = 8.8 Hz, 2H), 7.65 (d, *J* = 8.8 Hz, 1H), 7.77 (d, *J* = 8.4 Hz, 1H), 7.86 (d, *J* = 8.8 Hz, 2H), 8.30 (s, 1H), 10.93 (br, 1H); ^{13}C NMR (100 MHz,

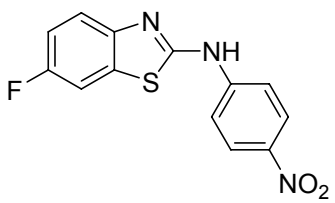
DMSO) δ 119.3, 119.8, 120.0, 123.3 (q, J_{CF} = 20 Hz), 125.4 (q, $^{1}J_{CF}$ = 270 Hz), 126.4, 126.6, 129.3, 131.1, 139.3, 155.2, 164.4.



6-fluoro-*N*-phenylbenzo[*d*]thiazol-2-amine (**3l**)[7] white solid, mp 158-160 °C (lit. mp 152-157 °C); IR (prism, KBr, cm^{-1}) 3437, 1630; ^{1}H NMR (400 MHz, $CDCl_3$) δ ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.01 (dt, *J* = 2.4, 8.8 Hz, 1H), 7.21 (d, *J* = 8.0 Hz, 2H), 7.29 (dd, *J* = 2.4, 8.0 Hz, 1H), 7.35 (d, *J* = 8.4 Hz, 2H), 7.41 (dd, *J* = 4.8, 8.8 Hz, 1H), 9.08 (br, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 107.6 (d, $^{2}J_{C-F}$ = 27 Hz), 113.8 (d, $^{2}J_{C-F}$ = 24 Hz), 119.6, 121.2, 130.2, 130.6, 134.7, 137.1, 148.0, 158.6 (d, $^{1}J_{C-F}$ = 239 Hz), 162.1.

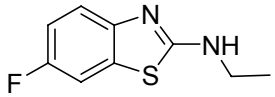


6-fluoro-*N*-p-tolylbenzo[*d*]thiazol-2-amine (**3m**)[4] white solid, mp 168-169 °C (lit. mp 174-175 °C); IR (prism, KBr, cm^{-1}) 3437, 1627; ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.37 (s, 3H), 7.10 (dt, *J* = 2.4, 8.8 Hz, 1H), 7.22 (d, *J* = 8.0 Hz, 2H), 7.30 (dd, *J* = 2.4, 8.0 Hz, 1H), 7.35 (d, *J* = 8.4 Hz, 2H), 7.40 (dd, *J* = 4.8, 8.8 Hz, 1H), 9.08 (br, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 20.9, 107.5 (d, $^{2}J_{C-F}$ = 27 Hz), 113.8 (d, $^{2}J_{C-F}$ = 24 Hz), 119.6, 121.1, 130.2, 130.6, 134.7, 137.1, 148.0, 158.6 (d, $^{1}J_{C-F}$ = 240 Hz), 162.5.

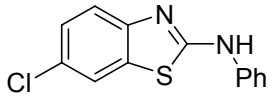


6-fluoro-*N*-(4-nitrophenyl)benzo[*d*]thiazol-2-amine (**3n**)[4] white solid, mp 262-263 °C

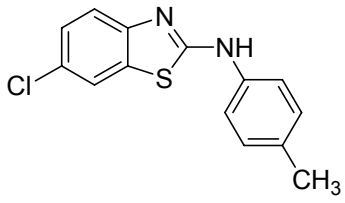
(lit. mp 259-260 °C); IR (prism, KBr, cm^{-1}) 3337, 1613; ^1H NMR (400 MHz, DMSO) δ 7.21-7.25 (m, 1H), 7.71 (dd, *J* = 4.8, 8.4 Hz, 1H), 7.77 (dd, *J* = 2.4, 8.4 Hz, 1H), 7.98 (d, *J* = 9.2 Hz, 2H), 8.26 (d, *J* = 9.2 Hz, 2H), 11.12 (br, 1H); ^{13}C NMR (100 MHz, DMSO) δ 108.2 (d, $^2J_{CF}$ = 27 Hz), 113.9 (d, $^2J_{CF}$ = 24 Hz), 117.0, 120.9, 125.4, 131.4, 140.9, 146.1, 148.0, 158.4 (d, $^1J_{CF}$ = 237 Hz), 160.4.



6-fluoro-*N*-phenylbenzo[*d*]thiazol-2-amine (**3o)** IR (prism, KBr, cm^{-1}) 3437, 1622; ^1H NMR (400 MHz, $CDCl_3$) δ 1.32 (t, *J* = 7.2 Hz, 3H), 3.44 (q, *J* = 7.2 Hz, 2H), 5.70 (br, 1H) 6.97-7.03 (m, 1H), 7.26-7.30 (m, 1H), 7.43 (dd, *J* = 4.8, 8.8 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 14.8, 40.3. 107.6 (d, $^2J_{CF}$ = 27 Hz), 113.5 (d, $^2J_{CF}$ = 24 Hz), 119.0, 130.9, 143.7, 158.1(d, $^1J_{CF}$ = 239 Hz), 167.2; HRMS calcd for $C_9H_{10}FN_2S^+$ $[M+H]^+$: 197.0500; Found: 197.0546.

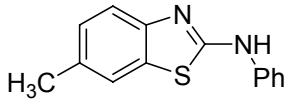


6-chloro-*N*-phenylbenzo[*d*]thiazol-2-amine (**3p)**[7] white solid, mp 187-189 °C (lit. mp 188-189 °C); IR (prism, KBr, cm^{-1}) 3445, 1624; ^1H NMR (400 MHz, $CDCl_3$) δ 7.11 (t, *J* = 7.2 Hz, 1H), 7.20 (d, *J* = 8.8 Hz, 1H), 7.34 (t, *J* = 7.6 Hz, 2H), 7.41 (d, *J* = 7.6 Hz, 3H), 7.51 (s, 1H), 8.20 (br, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 120.2, 120.5, 124.6, 126.7, 127.7, 129.6, 131.3, 139.4, 150.3, 164.4.

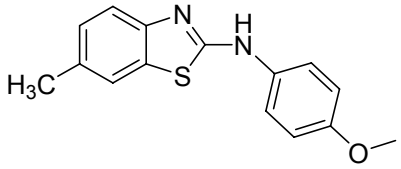


6-chloro-*N*-*p*-tolylbenzo[*d*]thiazol-2-amine (**3q)**[4] white solid, mp 198-200 °C (lit. mp

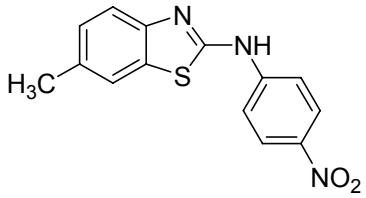
209-211 °C); IR (prism, KBr, cm^{-1}) 3434, 1627; ^1H NMR (400 MHz, DMSO) δ 2.37 (s, 3H), 7.10 (d, *J* = 8.0 Hz, 1H), 7.22 (d, *J* = 7.6 Hz, 2H), 7.25 (s, 1H), 7.35 (d, *J* = 7.6 Hz, 2H), 7.41 (d, *J* = 7.6 Hz, 1H), 8.50 (br, 1H); ^{13}C NMR (100 MHz, DMSO) δ 20.8, 118.5, 118.6, 120.4, 121.1, 126.3, 126.4, 129.8, 131.9, 132.1, 138.2, 151.5, 162.8.



6-methyl-*N*-phenylbenzo[*d*]thiazol-2-amine (**3r**)[7] white solid, mp 165-167 °C; IR (prism, KBr, cm^{-1}) 3436, 1626; ^1H NMR (400 MHz, $CDCl_3$) δ 2.41 (s, 1H), 7.14 (t, *J* = 8.8 Hz, 2H), 7.37-7.49 (m, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 21.3, 118.9, 120.2, 120.9, 124.2, 127.4, 129.5, 129.9, 132.2, 140.1, 149.1, 164.2.

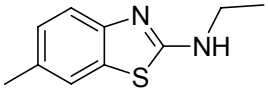


N-(4-methoxyphenyl)-6-methylbenzo[*d*]thiazol-2-amine (**3s**)[6] white solid, mp 154-156 °C; IR (prism, KBr, cm^{-1}) 3442, 1611; ^1H NMR (400 MHz, $CDCl_3$) δ 2.38 (s, 3H), 3.84 (s, 3H), 6.94 (d, *J* = 8.8 Hz, 2H), 7.07 (d, *J* = 8.0 Hz, 1H), 7.32 (d, *J* = 8.4 Hz, 1H), 7.36-7.40 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 21.3, 55.6, 114.8, 118.4, 120.9, 124.4, 127.2, 129.8, 131.7, 133.2, 149.5, 157.2, 166.5.



6-methyl-*N*-(4-nitrophenyl)benzo[*d*]thiazol-2-amine (**3t**)[6] yellow solid, mp 271-273 °C; IR (prism, KBr, cm^{-1}) 3440, 1611; ^1H NMR (400 MHz, DMSO) δ 2.36 (s, 3H),

7.19 (d, J = 8.0 Hz, 2H), 7.58 (d, J = 8.0 Hz, 1H), 7.65 (s, 1H), 7.97 (d, J = 8.0 Hz, 2H), 8.24 (d, J = 8.8 Hz, 2H); ^{13}C NMR (100 MHz, DMSO) δ 20.8, 117.0, 119.6, 121.0, 125.2, 127.3, 130.4, 132.7, 140.9, 146.4, 149.3, 159.7.



N-ethyl-6-methylbenzo[*d*]thiazol-2-amine (**3u**)[6] white solid, mp 104-106 ^{o}C; IR (prism, KBr, cm^{-1}) 3436, 1627; ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.31 (t, J = 7.2 Hz, 3H), 2.38 (s, 1H), 3.41-3.46 (q, J = 7.2 Hz, 2H), 5.78 (br, 1H), 7.09 (d, J = 8.0 Hz, 1H), 7.38 (s, 1H), 7.40 (d, J = 8.0 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 14.9, 21.2, 40.3, 118.2, 120.9, 127.1, 130.1, 131.2, 150.0, 167.0.

Reference:

1. D. Fajkusova and P. Pazdera *Synthesis*, 2008, 1297.

2. M. H. Nettekoven and S. Roever, *U.S. Pat. Appl. Publ.*, 2004, 35.

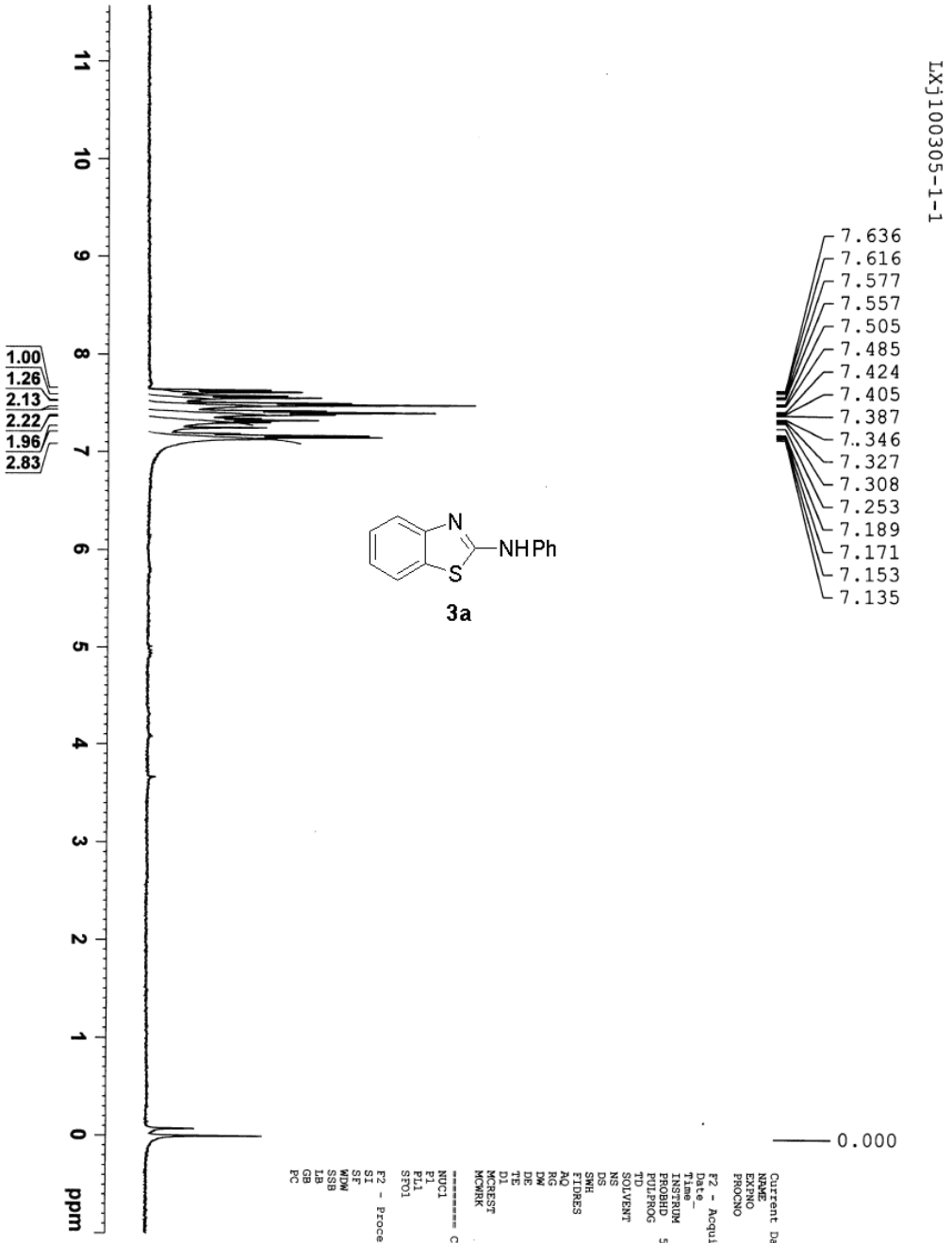
3. L. Gerrit, *J. Hetero. Chem*., 1990, **27**, 923.

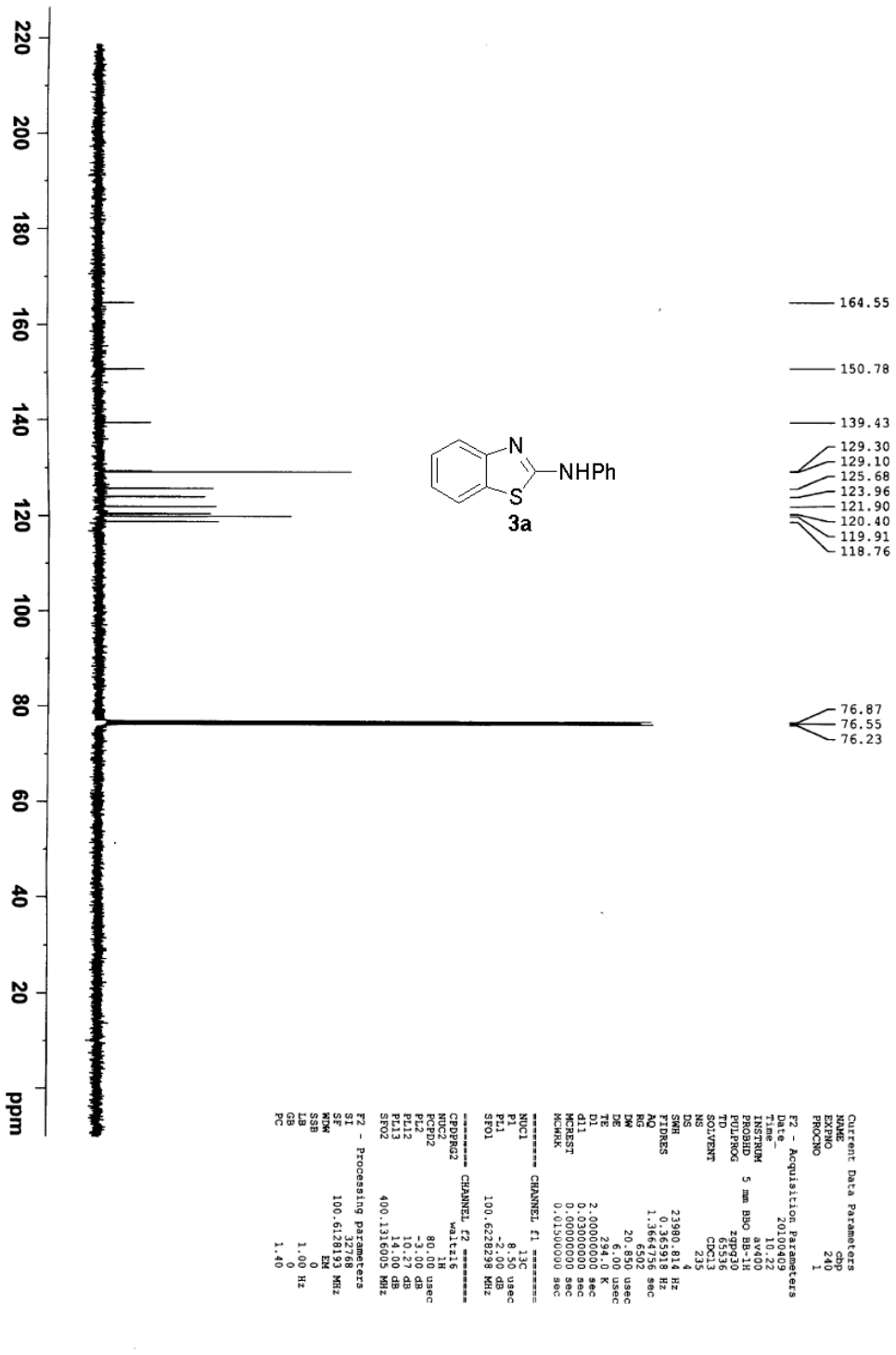
4. J. Qiu, X. Zhang, R. Tang, P. Zhong and J. Li, *Adv. Synth. Catal.*, 2009, **351**, 2319-2323.

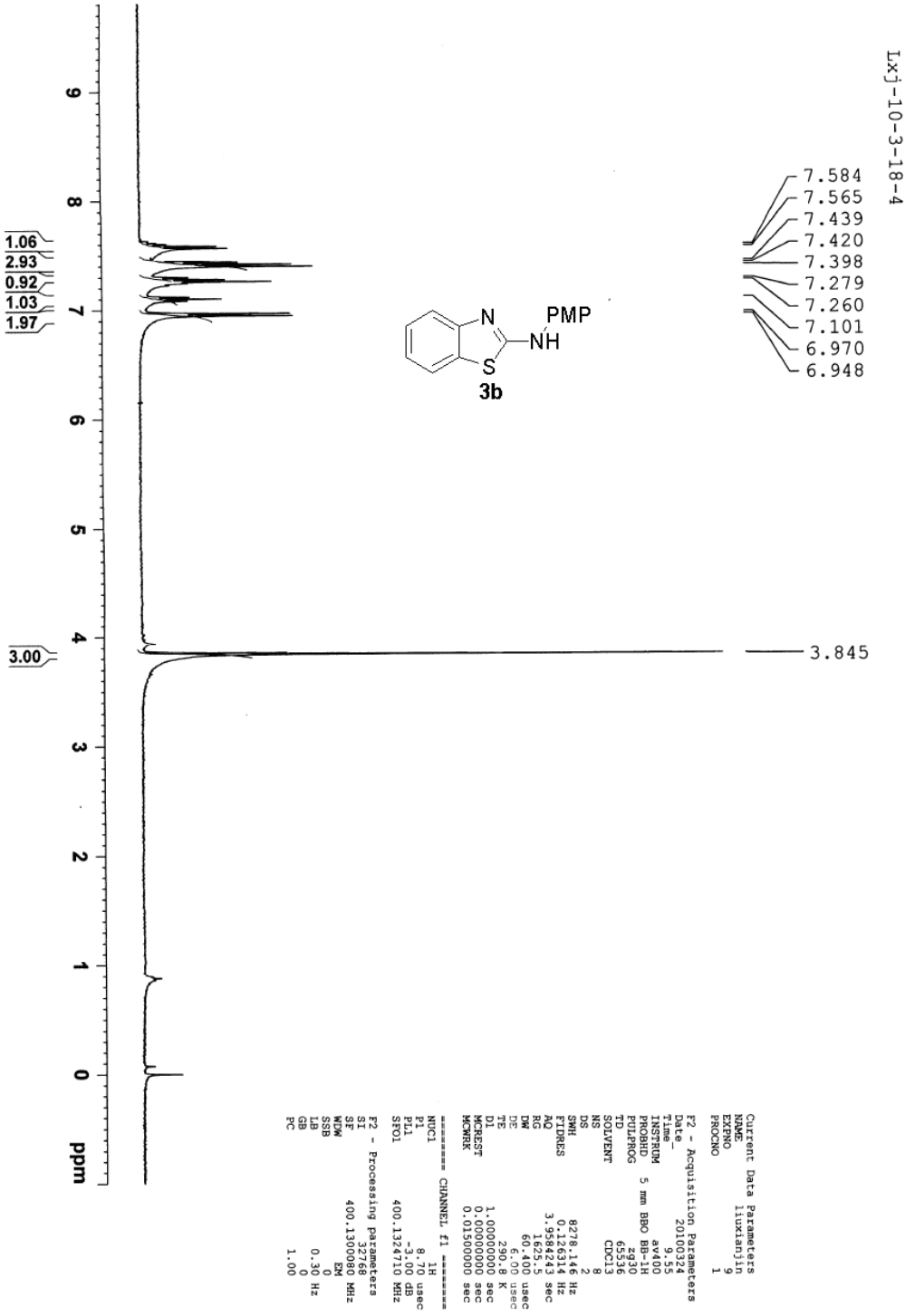
5. H. F. Motiwala, *Austr. J. Chem*., 2007, **60**, 369-374.

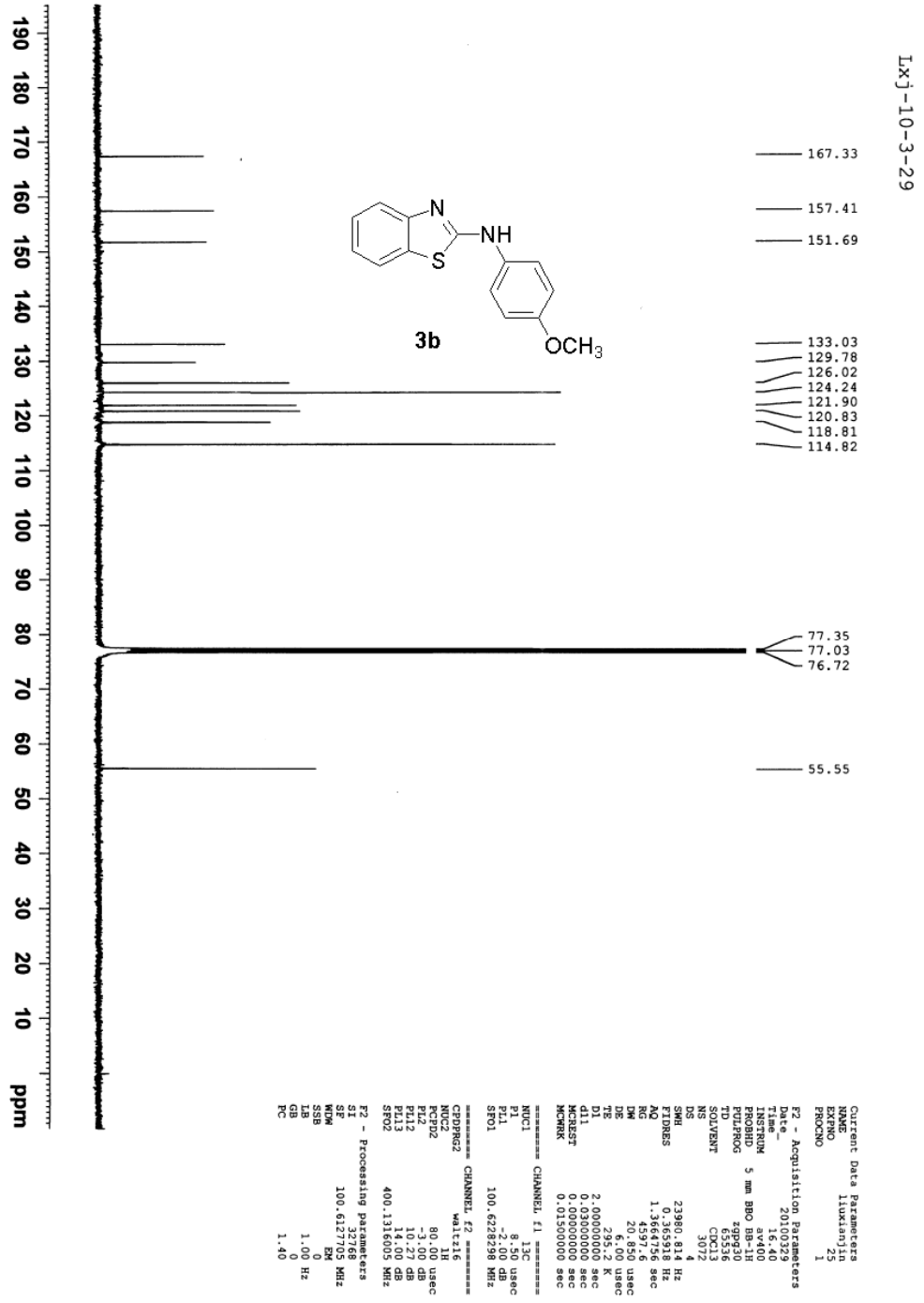
6. Q. Ding, X. He and J. Wu, *J. Comb. Chem.*, 2009, **11**, 587-591.

7. Y. Guo, R. Tang, P. Zhong and J. Li, *Tetrahedron Lett.* 2010, **51**, 649-652.


LXj100305-1-1
7.636
7.616
7.577
7.557
7.505
7.485
7.424
7.405
7.387
7.346
7.327
7.308
7.253
7.189
7.171
7.153
7.135
0.000
1.00
1.26
2.13
2.22
1.96
2.83
N
NHPh
S
3a
ppm
Current Data Parameters
NAME cbp
EXPNO 215
PROCNO 1
F2 - Acquisition Parameters
Date_ 20100310
Time 13.28
INSTRUM av400
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 2
SWH 8278.146 Hz
FIDRES 0.126314 Hz
AQ 3.9584243 sec
RG 1149.4
DW 60.400 usec
DE 6.00 usec
TE 298.1 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 8.70 usec
PL1 -3.00 dB
SFO1 400.1324710 MHz
F2 - Processing parameters
SI 32768
SF 400.1300092 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00


220
200
180
160
140
120
100
80
60
40
20
ppm
N
S
NHPh
3a
164.55
150.78
139.43
129.30
129.10
125.68
123.96
121.90
120.40
119.91
118.76
76.87
76.55
76.23
Current Data Parameters
NAME cdp
EXPNO 241
PROCNO 1
F2 - Acquisition Parameters
Date_ 20100409
Time 10.22
INSTRUM av400
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 233
DS 4
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 6502
DW 20.850 usec
DE 6.00 usec
TE 294.0 K
D1 2.00000000 sec
D11 0.03000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 8.50 usec
PL1 -2.00 dB
SFO1 100.622829 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -3.00 dB
PL12 10.27 dB
PL13 14.00 dB
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 32768
SF 100.6128193 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40


Lxj-10-3-18-4
7.584
7.565
7.439
7.420
7.398
7.279
7.260
7.101
6.970
6.948
3.845
1.06
2.93
0.92
1.03
1.97
3.00
PMP
NH
N
S
3b
ppm
Current Data Parameters
NAME liuxianjin
EXPNO 9
PROCNO 1
F2 - Acquisition Parameters
Date_ 20100325
Time 9.55
INSTRUM av400
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 2
SWH 8278.146 Hz
FIDRES 0.126314 Hz
AQ 3.9584243 sec
RG 1625.5
DW 60.400 usec
DE 6.00 usec
TE 298.0 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 8.70 usec
PL1 -3.00 dB
SFO1 400.1324710 MHz
F2 - Processing parameters
SI 32768
SF 400.1300084 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00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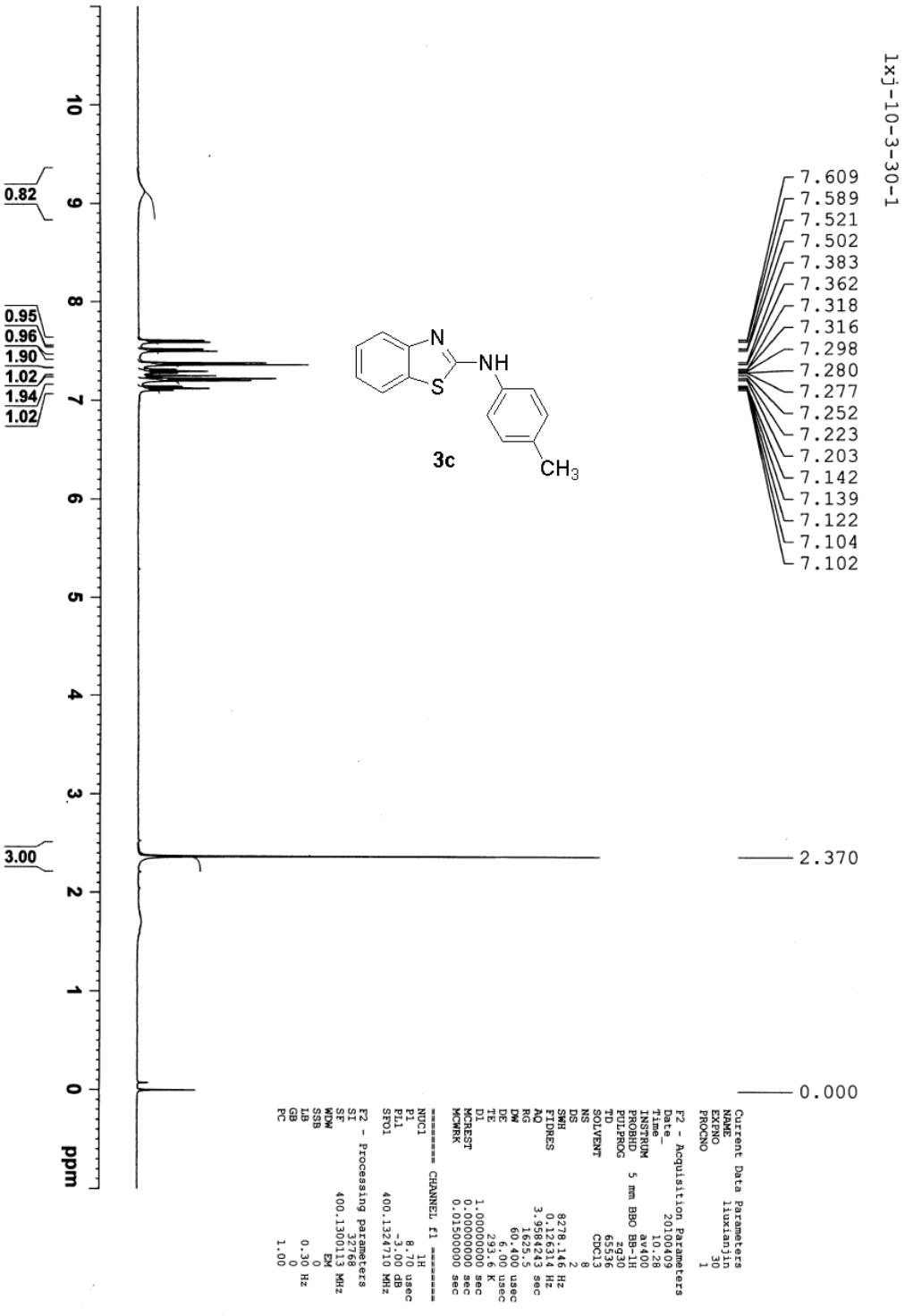
167.33
157.41
151.69
133.03
129.78
126.02
124.24
121.90
120.83
118.81
114.82
77.35
77.03
76.72
55.55
N
NH
S
OCH3
3b
ppm
Current Data Parameters
NAME liuxianjin
EXPNO 25
PROCNO 1
F2 - Acquisition Parameters
Date_ 20100329
Time 16.40
INSTRUM av400
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 3072
DS 4
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 4597.6
DW 20.850 usec
DE 6.00 usec
TE 295.2 K
D1 2.00000000 sec
D11 0.03000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 8.50 usec
PL1 -2.00 dB
SFO1 100.6228298 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -3.00 dB
PL12 10.27 dB
PL13 14.00 dB
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 32768
SF 100.6127705 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40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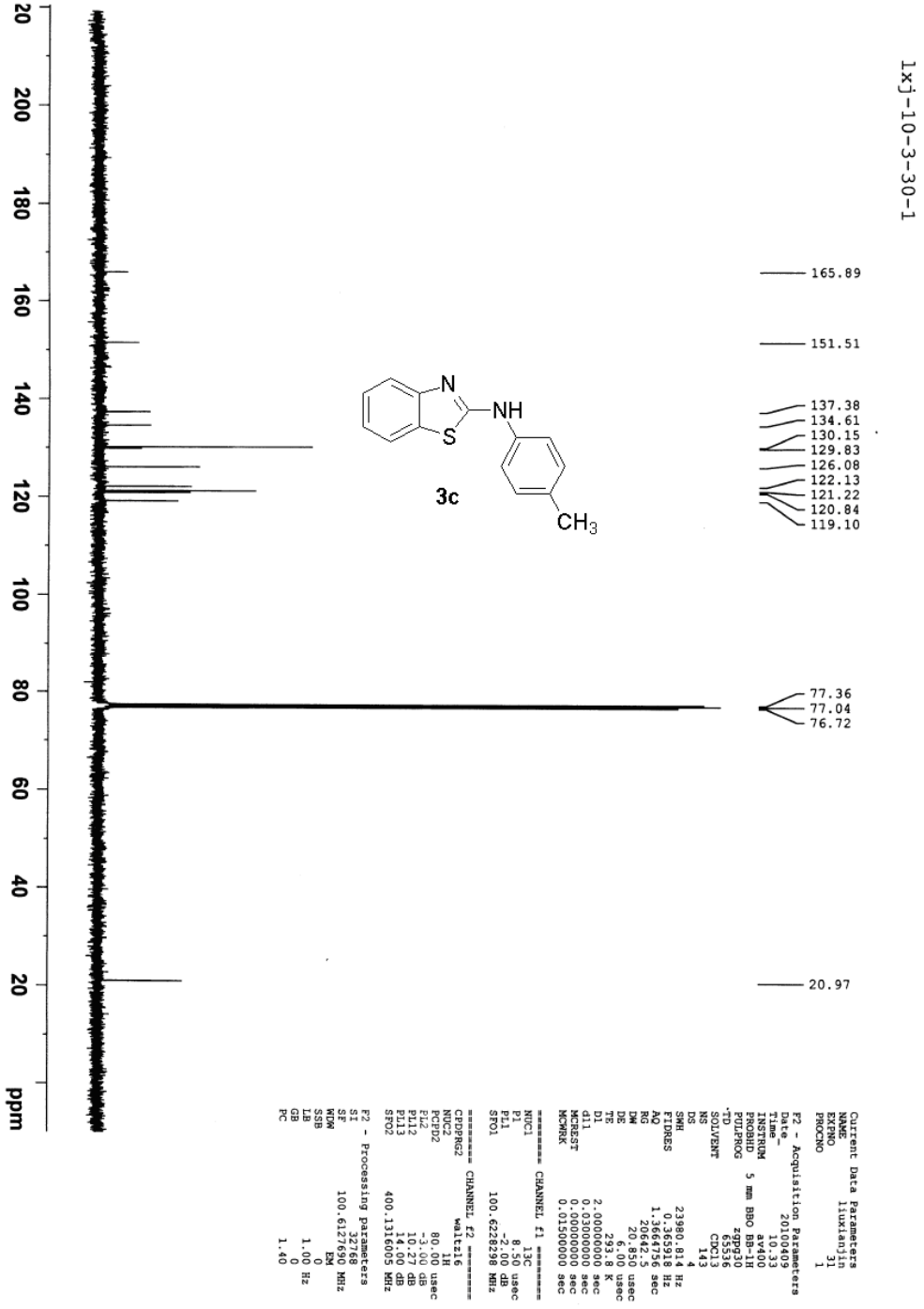
7.589
7.521
7.502
7.383
7.362
7.318
7.316
7.298
7.280
7.277
7.252
7.223
7.203
7.142
7.139
7.122
7.104
7.102
2.370
0.000
0.82
0.95
0.96
1.90
1.02
1.94
1.02
3.00
ppm
N
NH
S
CH3
3c
Current Data Parameters
NAME liuxianjin
EXPNO 30
PROCNO 1
F2 - Acquisition Parameters
Date_ 20100409
Time_ 10.28
INSTRUM av400
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 2
SWH 8278.146 Hz
FIDRES 0.126314 Hz
AQ 3.9584213 sec
RG 1625.5
DW 60.400 usec
DE 6.00 usec
TE 293.6 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 8.70 usec
PL1 -3.00 dB
SFO1 400.1324710 MHz
F2 - Processing parameters
SI 32768
SF 400.1300113 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00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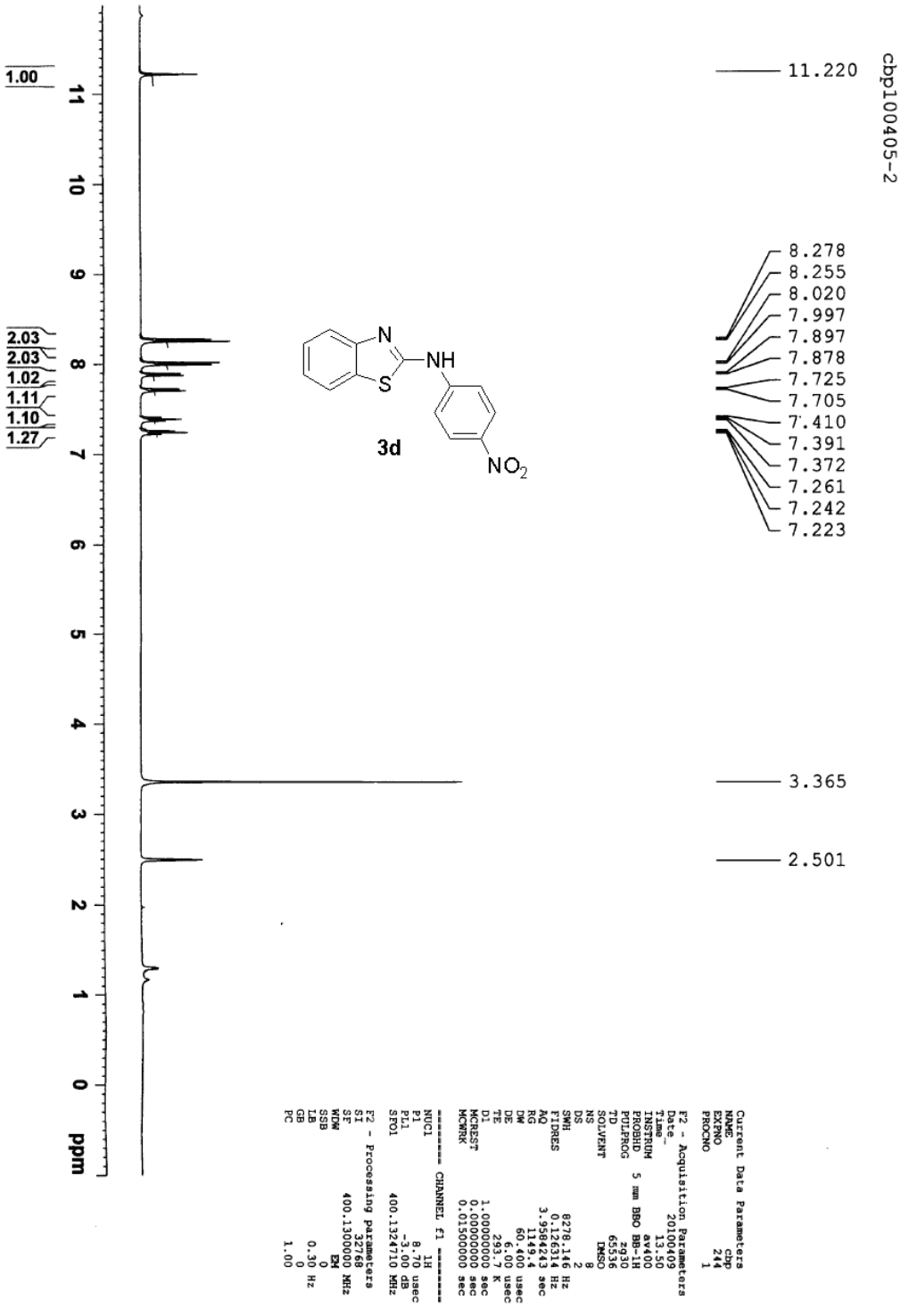
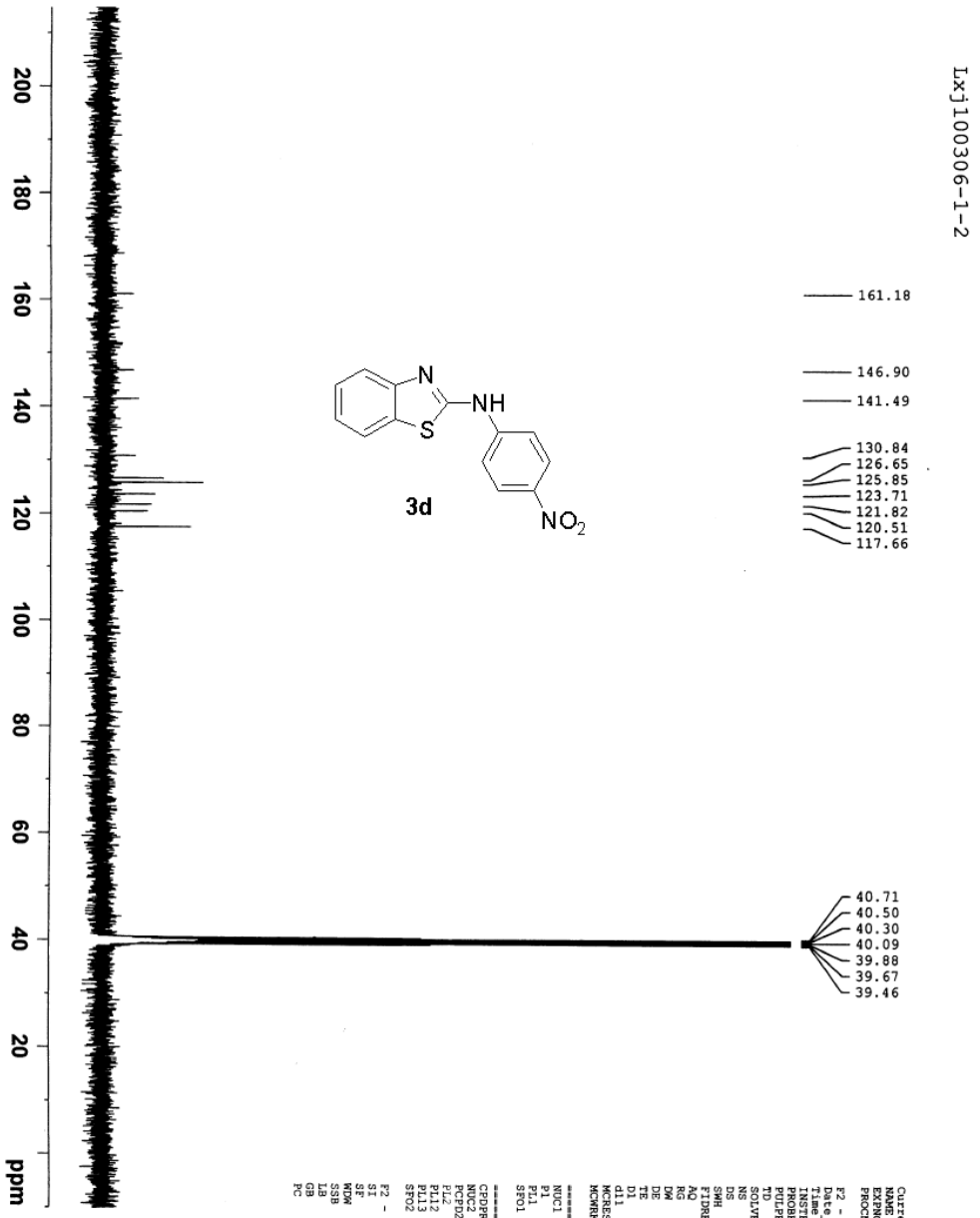
165.89
151.51
137.38
134.61
130.15
129.83
126.08
122.13
121.22
120.84
119.10
77.36
77.04
76.72
20.97
N
NH
S
CH3
3c
ppm
20
200
180
160
140
120
100
80
60
40
20
Current Data Parameters
NAME liuxian)1n
EXPNO 31
PROCNO 1
F2 - Acquisition Parameters
Date_ 20100409
Time 10.33
INSTRUM av400
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 143
DS 4
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 20642.5
DW 20.850 usec
DE 6.00 usec
TE 293.8 K
D1 2.00000000 sec
D11 0.03000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 8.50 usec
PL1 -2.00 dB
SFO1 100.6228298 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL12 -3.00 dB
PL12 10.27 dB
PL13 14.00 dB
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 1.00
LB 0 Hz
GB 0
PC 1.40


cbp100405-2
11.220
8.278
8.255
8.020
7.997
7.897
7.878
7.725
7.705
7.410
7.391
7.372
7.261
7.242
7.223
3.365
2.501
1.00
2.03
2.03
1.02
1.11
1.10
1.27
ppm
N
NH
S
NO2
3d
Current Data Parameters
NAME cbp
EXPNO 244
PROCNO 1
F2 - Acquisition Parameters
Date_ 20100409
Time 13.50
INSTRUM av400
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 2
DS 2
SWH 8278.146 Hz
FIDRES 0.126314 Hz
AQ 3.9584243 sec
RG 1149.4
DW 60.400 usec
DE 6.00 usec
TE 293.7 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
---------- CHANNEL f1 ----------
NUC1 1H
P1 8.70 usec
PL1 -3.00 dB
SFO1 400.1324710 MHz
F2 - Processing parameters
SI 32768
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00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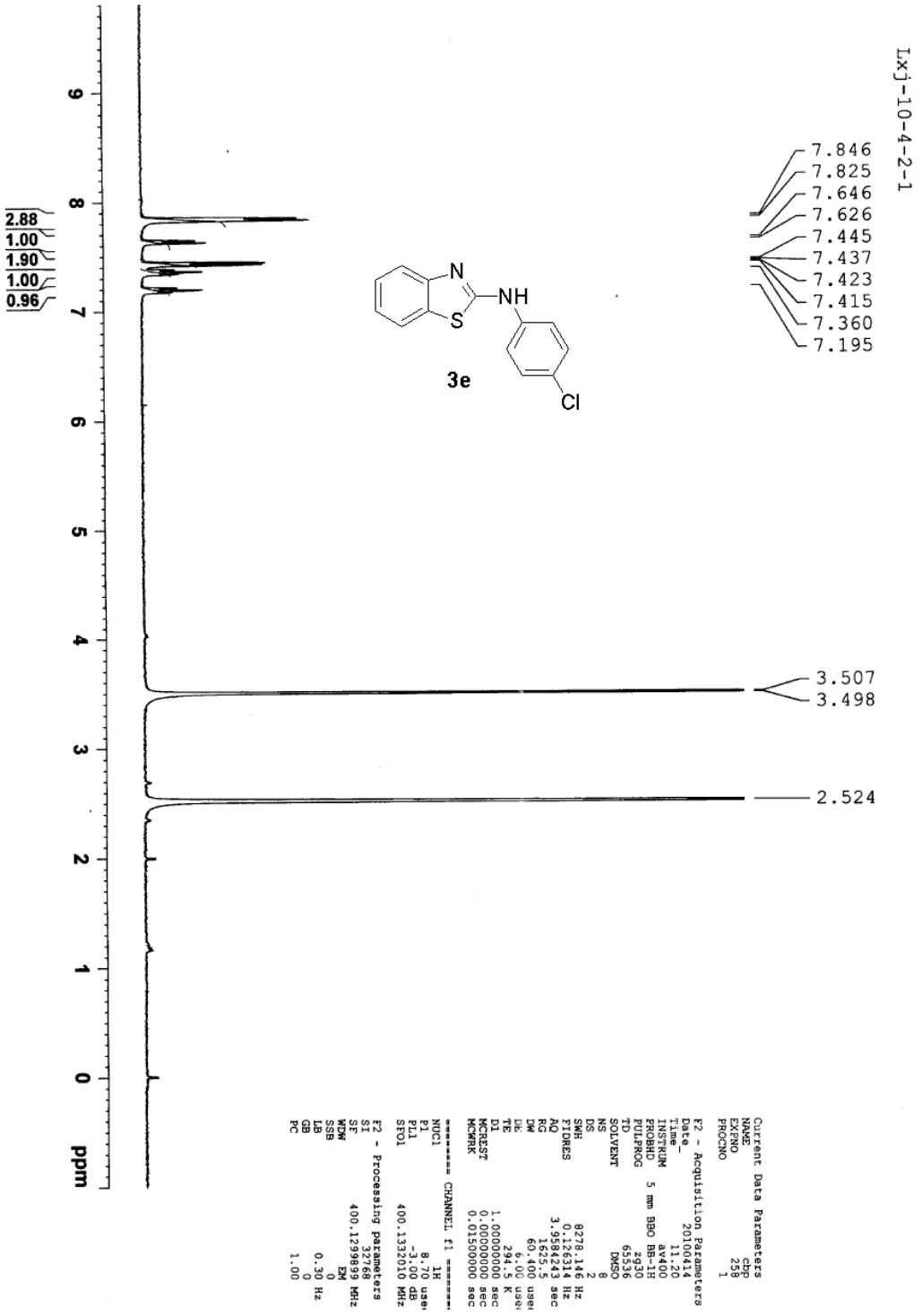
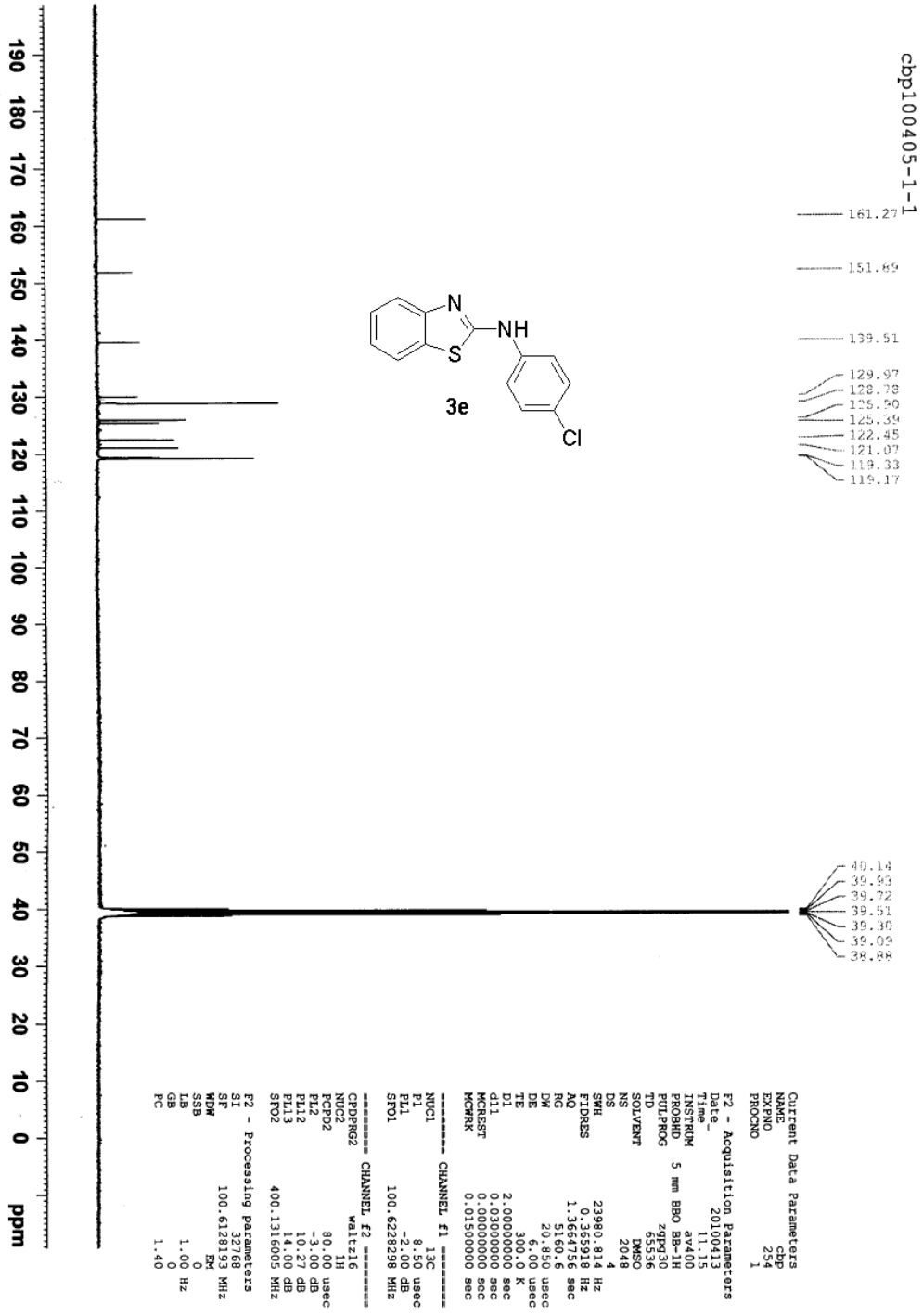
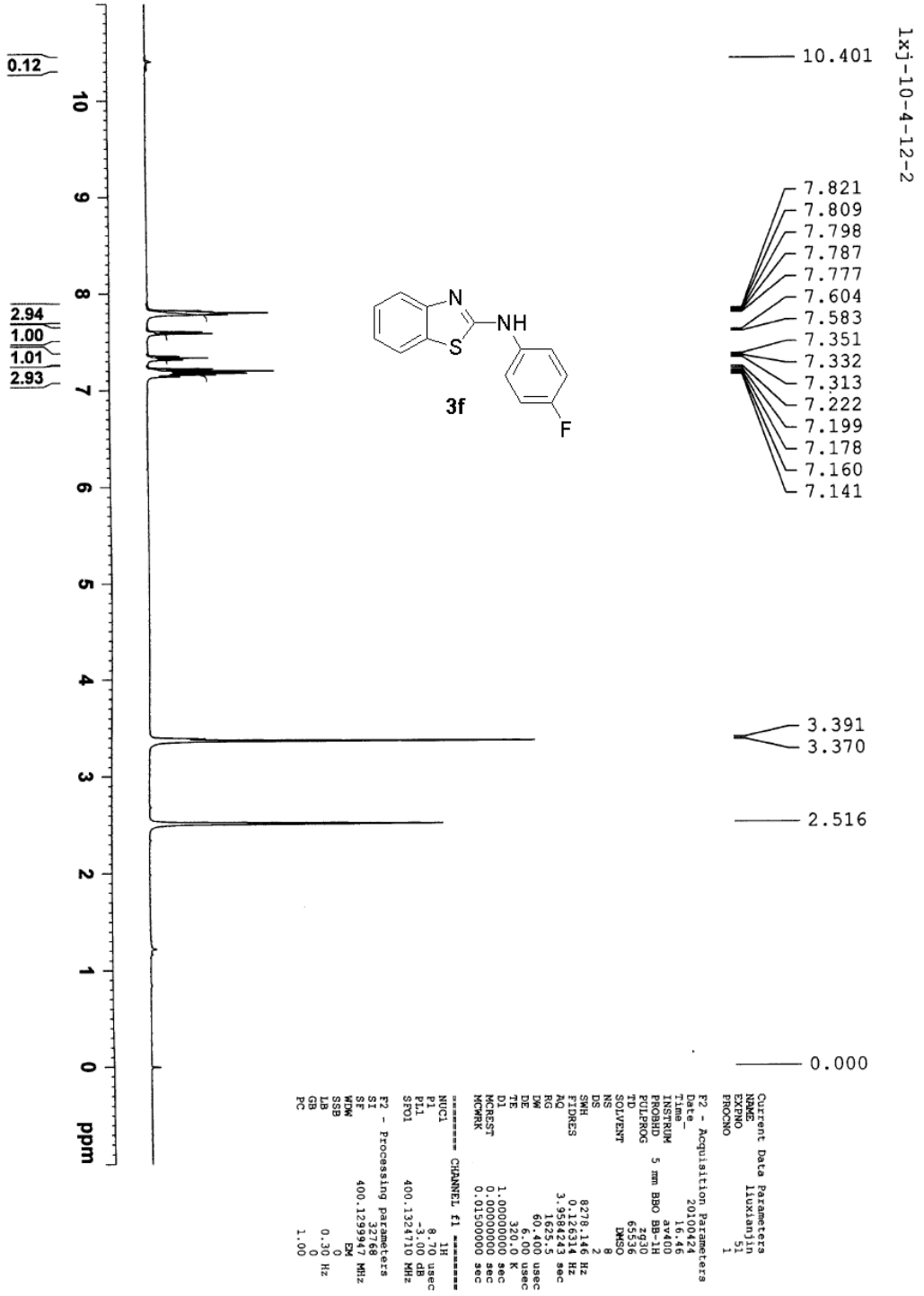
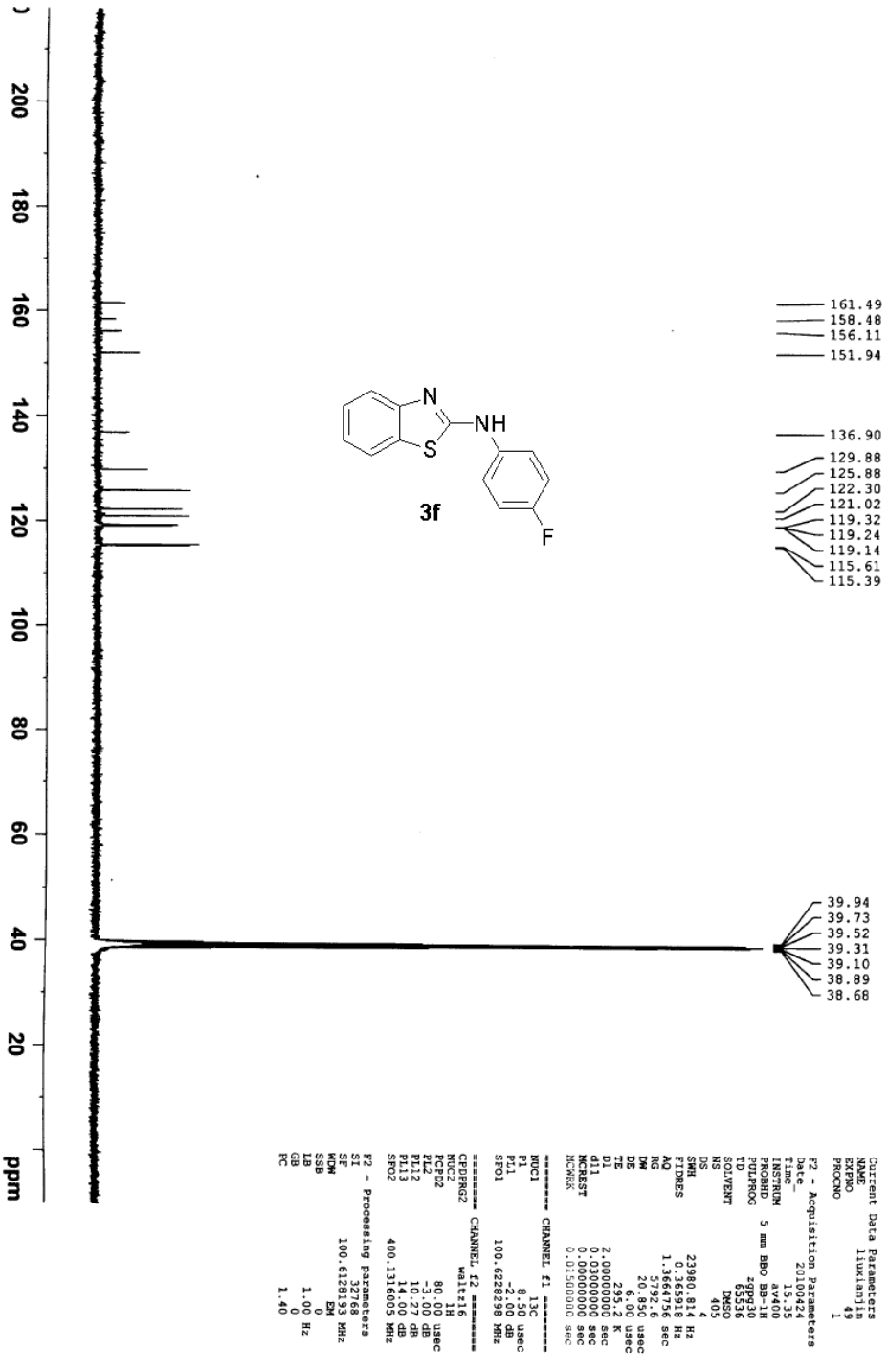
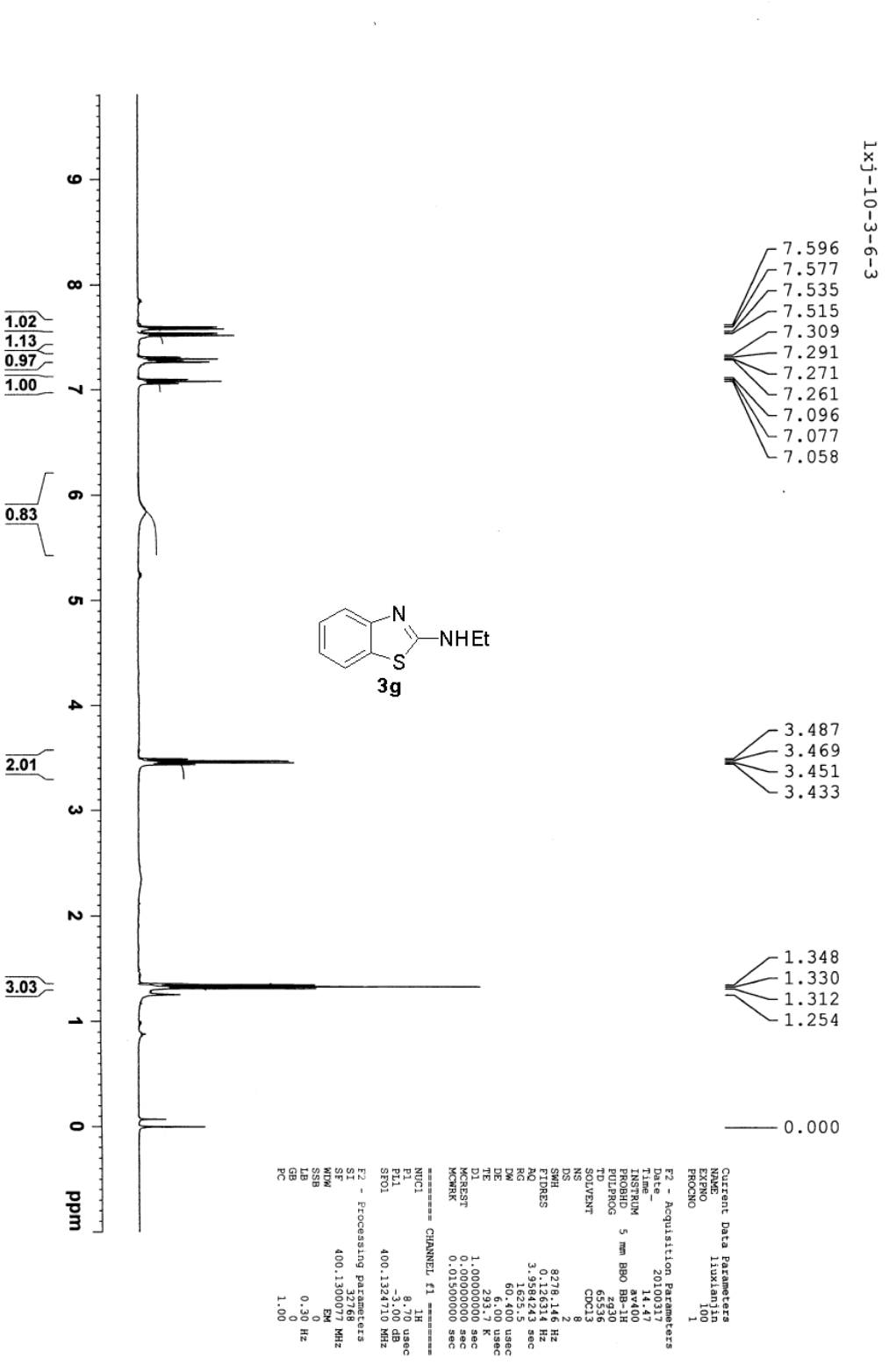
161.18
146.90
141.49
130.84
126.65
125.85
123.71
121.82
120.51
117.66
40.71
40.50
40.30
40.09
39.88
39.67
39.46
N
NH
S
NO2
3d
200
180
160
140
120
100
80
60
40
20
ppm
Current Data Parameters
NAME liuxianjin
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20100315
Time_ 10.30
INSTRUM av400
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 324
DS 4
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 4096
DW 20.850 usec
DE 6.00 usec
TE 310.0 K
D1 2.00000000 sec
d11 0.03000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 8.50 usec
PL1 -2.00 dB
SFO1 100.6228298 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -3.00 dB
PL12 10.27 dB
PL13 14.00 dB
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40


Lxj-10-4-2-1
7.846
7.825
7.646
7.626
7.445
7.437
7.423
7.415
7.360
7.195
3.507
3.498
2.524
2.88
1.00
1.90
1.00
0.96
N
NH
S
Cl
3e
ppm
Current Data Parameters
NAME
EXPNO 258
PROCNO 1
F2 - Acquisition Parameters
Date_ 20100414
Time 11.20
INSTRUM av400
PROBHD 5 mm BBO BB-1H
PULPROG 2930
TD 65536
SOLVENT DMSO
NS 2
DS 2
SWH 8278.146 Hz
FIDRES 0.126314 Hz
AQ 3.9584243 sec
RG 1625.5
DW 60.400 use
DE 6.00 use
TE 294.5 K
D1 1.00000000 sec
D11 0.00000000 sec
MCREST 0.01500000 sec
MCWRK sec
======== CHANNEL f1 ========
NUC1 1H
P1 8.70 use
PL1 -3.00 dB
SFO1 400.1332010 MHz
F2 - Processing parameters
SI 32768
SF 400.1299899 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00


cbp100405-1-1
161.27
151.89
139.51
129.97
128.78
125.50
125.39
122.45
121.07
119.33
119.17
40.14
39.93
39.72
39.51
39.30
39.09
38.88
N
NH
S
Cl
3e
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm
Current Data Parameters
NAME cbp
EXPNO 254
PROCNO 1
F2 - Acquisition Parameters
Date_ 20100413
Time_ 11.15
INSTRUM av400
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 2048
DS 4
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 5160.6
DW 20.850 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 8.50 usec
PL1 -2.00 dB
SFO1 100.6228298 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -3.00 dB
PL12 10.27 dB
PL13 14.00 dB
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 32768
SF 100.6128193 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40


lxj-10-4-12-2
10.401
7.821
7.809
7.798
7.787
7.777
7.604
7.583
7.351
7.332
7.313
7.222
7.199
7.178
7.160
7.141
3.391
3.370
2.516
0.000
0.12
2.94
1.00
1.01
2.93
ppm
N
NH
S
F
3f
Current Data Parameters
NAME liuxianjin
EXPNO 51
PROCNO 1
F2 - Acquisition Parameters
Date_ 20100424
Time_ 16.46
INSTRUM av400
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 8
DS 2
SWH 8278.146 Hz
FIDRES 0.126314 Hz
AQ 3.9568243 sec
RG 1625.5
DW 60.400 usec
DE 6.00 usec
TE 320.0 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 8.70 usec
PL1 -3.00 dB
SFO1 400.1324710 MHz
F2 - Processing parameters
SI 32768
SF 400.1299947 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00


161.49
158.48
156.11
151.94
136.90
129.88
125.88
122.30
121.02
119.32
119.24
119.14
115.61
115.39
39.94
39.73
39.52
39.31
39.10
38.89
38.68
N
NH
S
F
3f
ppm
200
180
160
140
120
100
80
60
40
20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7.596
7.577
7.535
7.515
7.309
7.291
7.271
7.261
7.096
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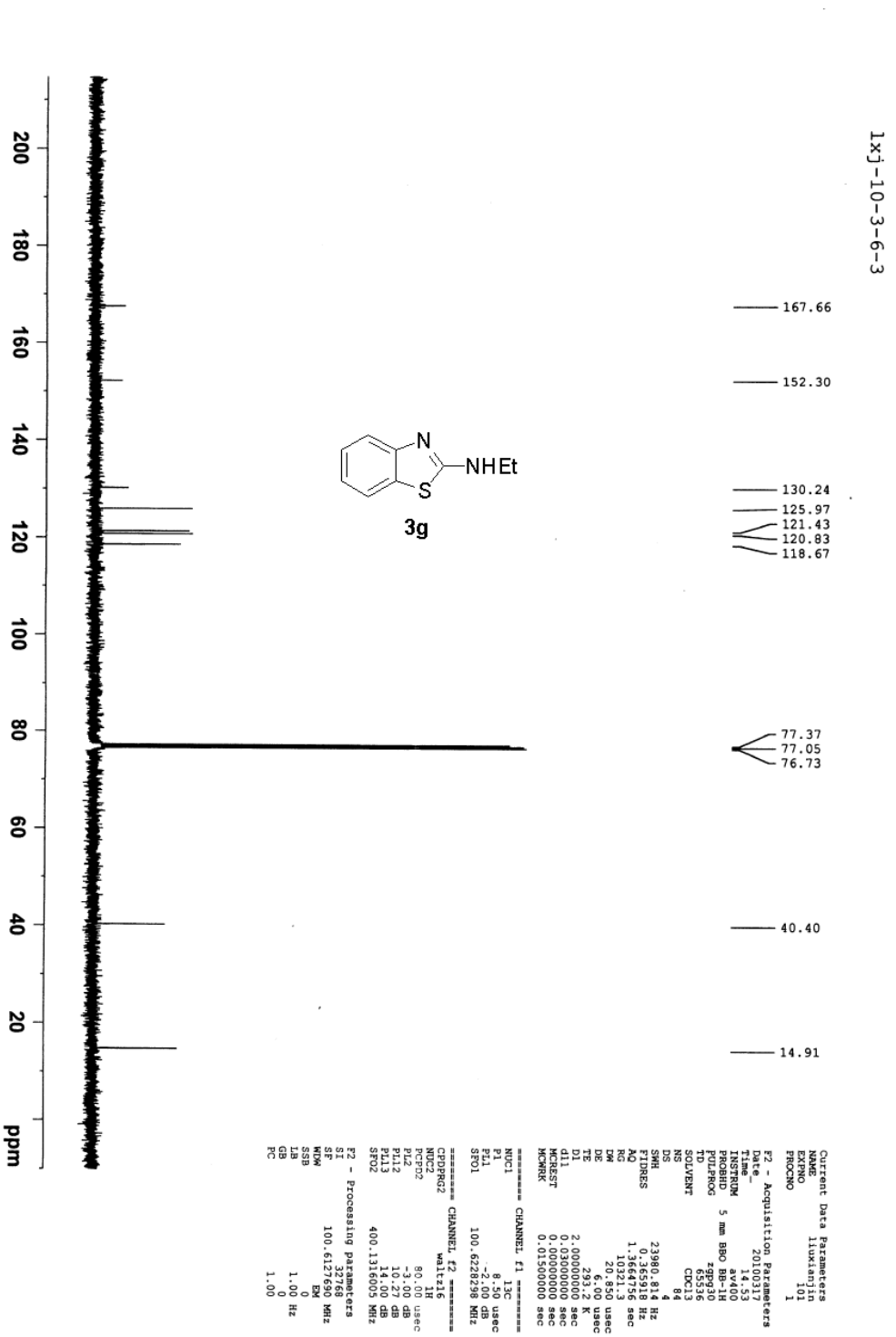
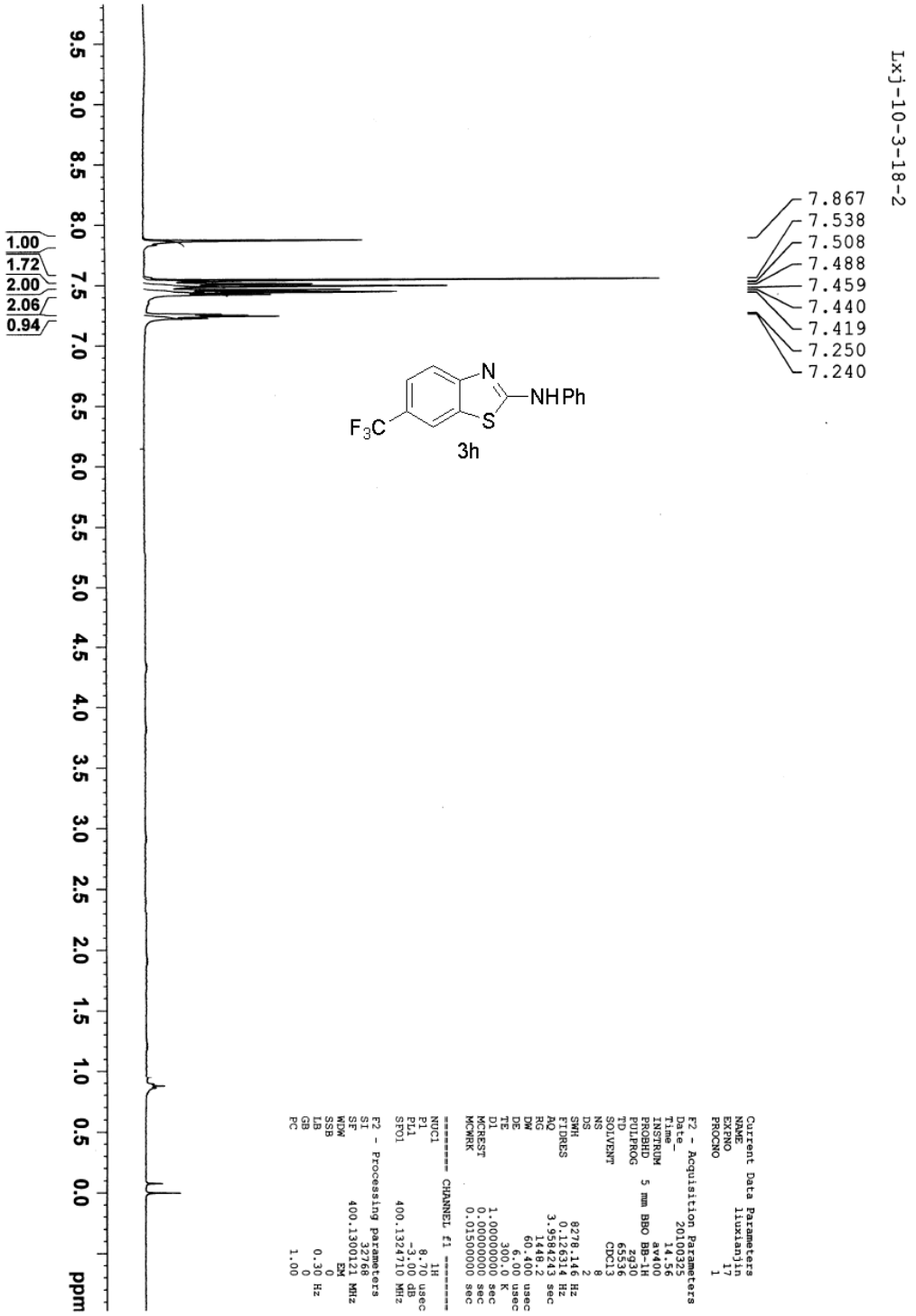
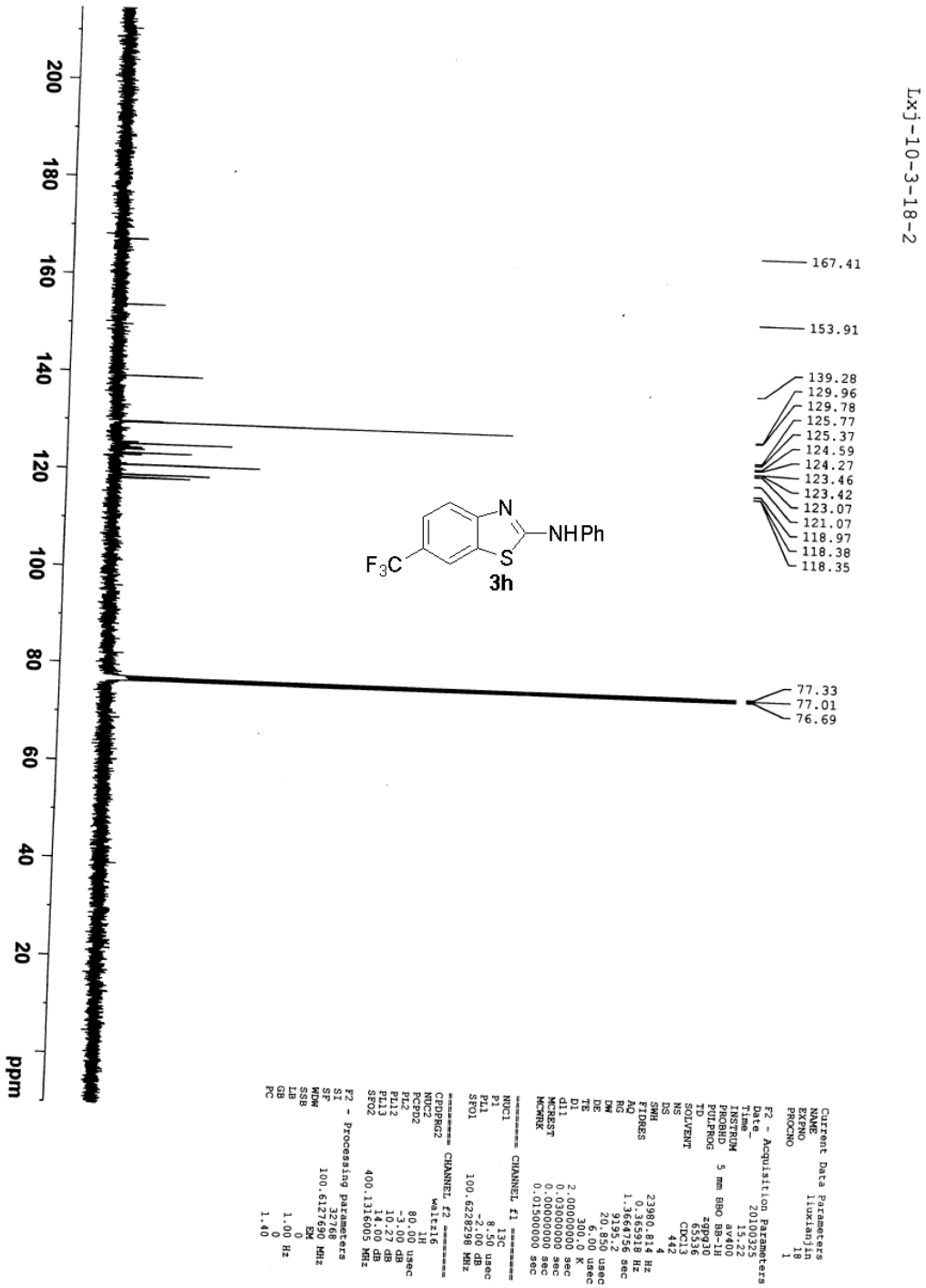
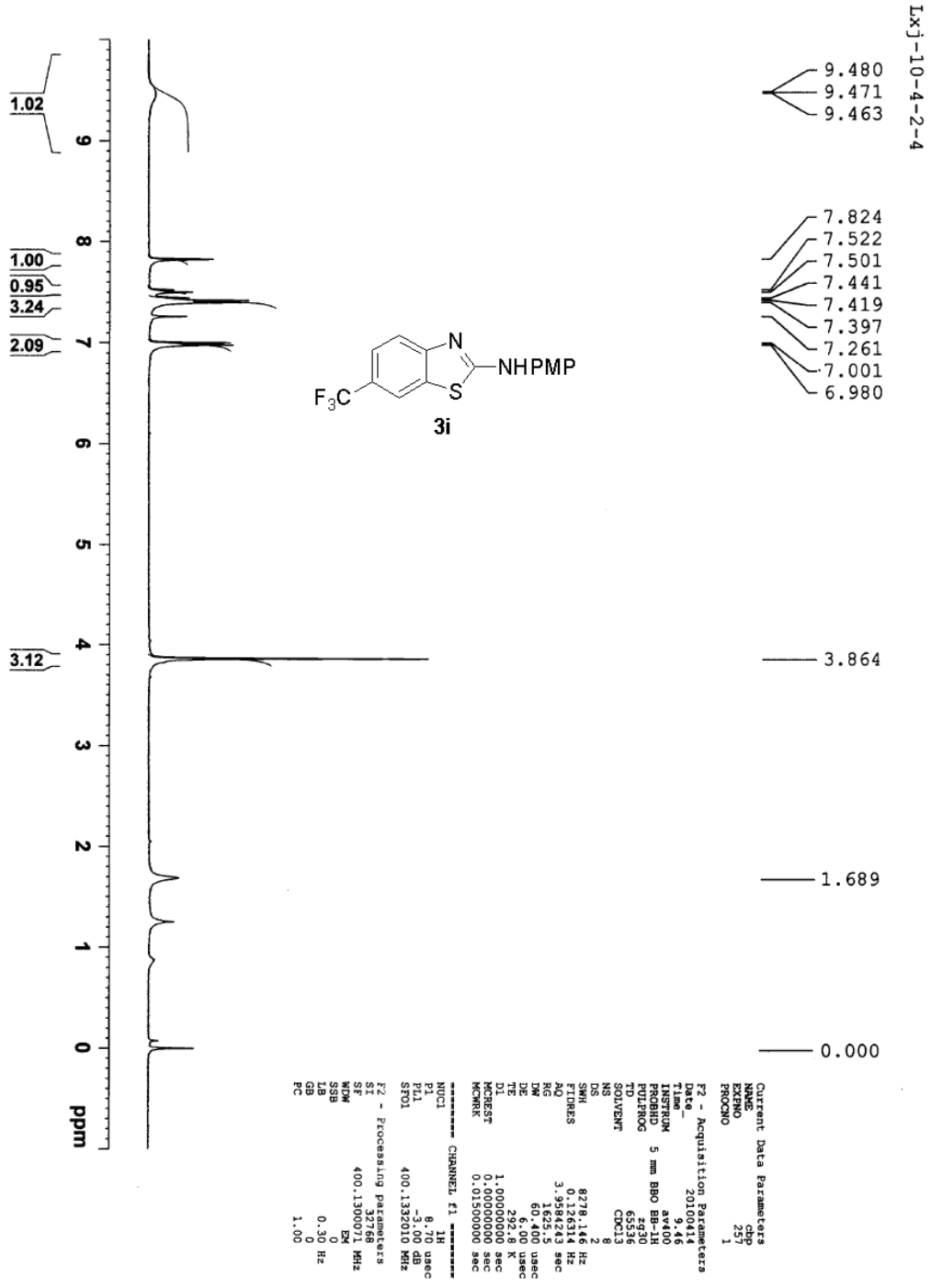
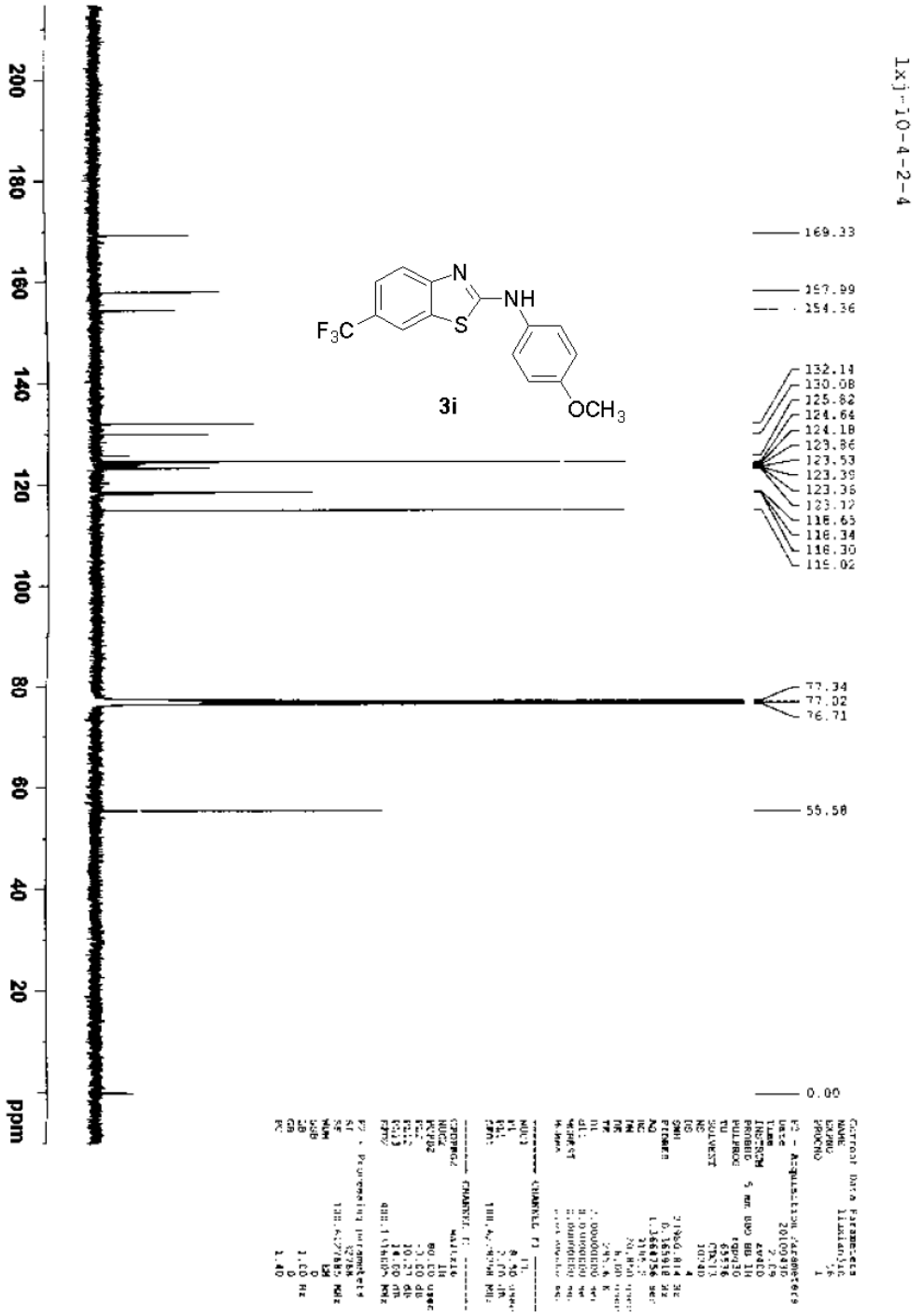
7.058
3.487
3.469
3.451
3.433
1.348
1.330
1.312
1.254
0.000
1.02
1.13
0.97
1.00
0.83
2.01
3.03
ppm
N
NHEt
S
3g

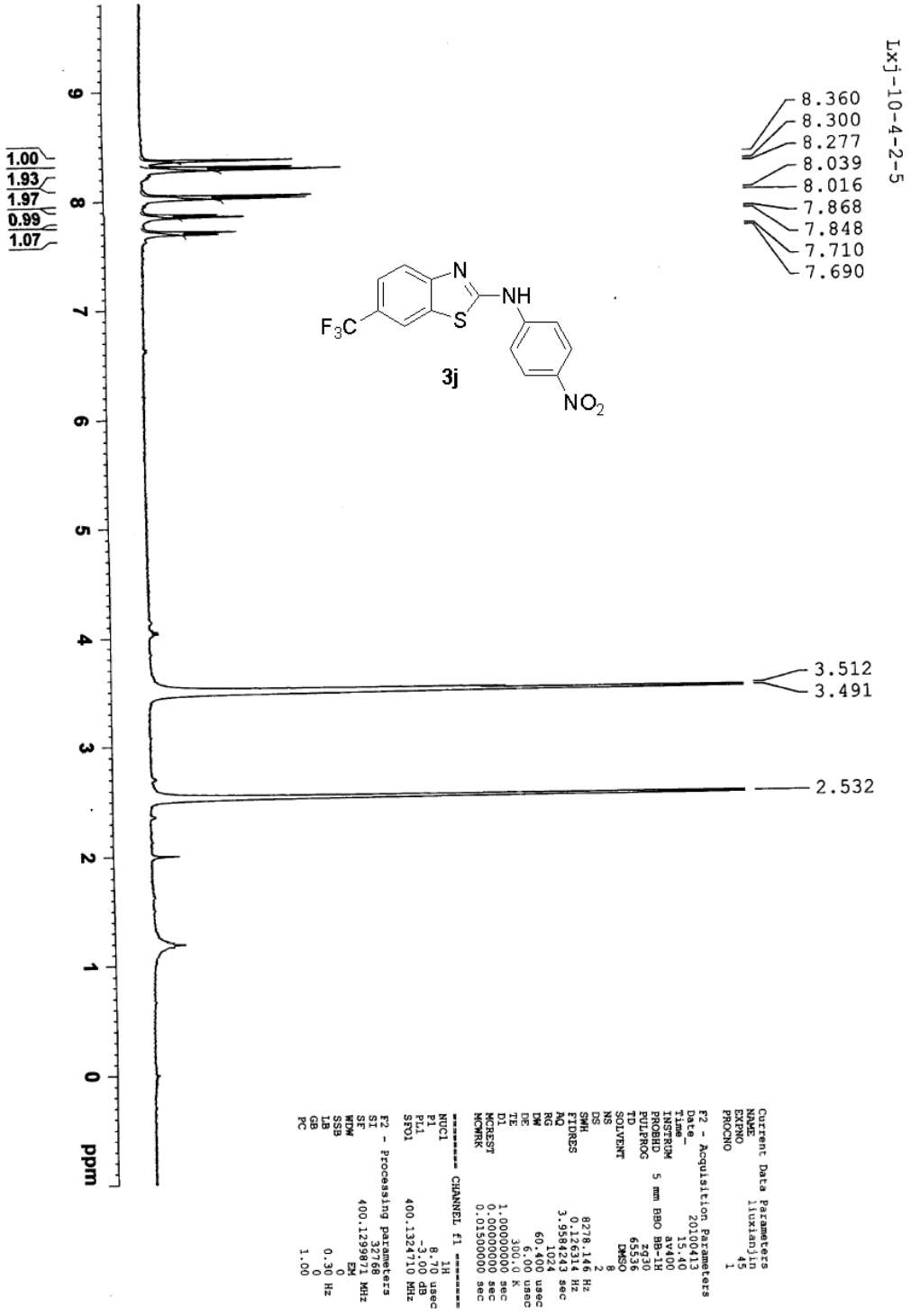

1xj-10-3-6-3
167.66
152.30
130.24
125.97
121.43
120.83
118.67
77.37
77.05
76.73
40.40
14.91
N
NHEt
S
3g
200
180
160
140
120
100
80
60
40
20
ppm

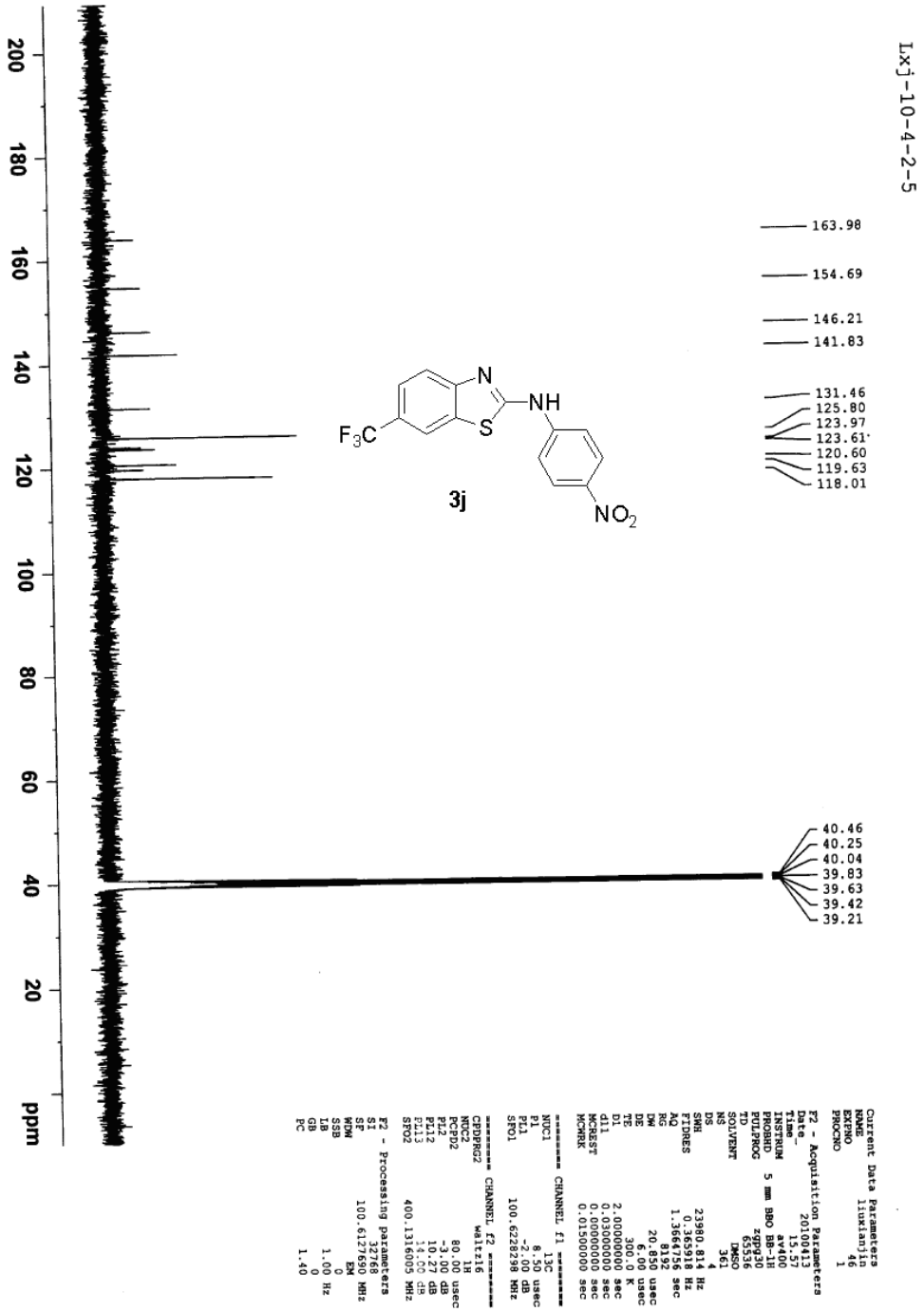

Lxj-10-3-18-2
7.867
7.538
7.508
7.488
7.459
7.440
7.419
7.250
7.240
1.00
1.72
2.00
2.06
0.94
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 ppm
N
NHPh
S
F3C
3h
Current Data Parameters
NAME liuxianjin
EXPNO 17
PROCNO 1
F2 - Acquisition Parameters
Date_ 20100325
Time 14.56
INSTRUM av400
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 2
SWH 8278.146 Hz
FIDRES 0.126314 Hz
AQ 3.9584243 sec
RG 1448.2
DW 60.400 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 8.70 usec
PL1 -3.00 dB
SFO1 400.1324710 MHz
F2 - Processing parameters
SI 32768
SF 400.1300121 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

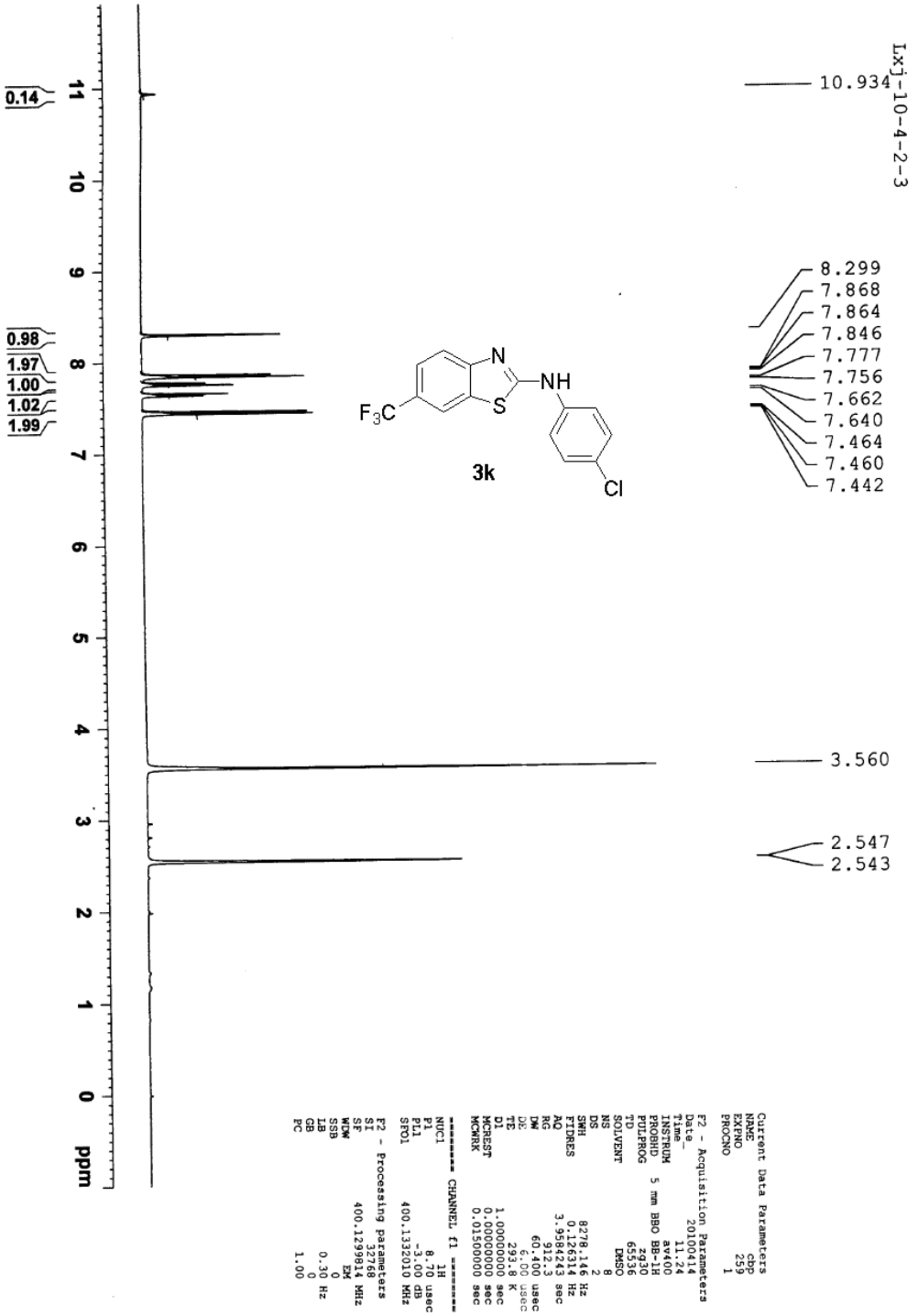

Lxj-10-3-18-2
167.41
153.91
139.28
129.96
129.78
125.77
125.37
124.59
124.27
123.46
123.42
123.07
121.07
118.97
118.38
118.35
77.33
77.01
76.69
N
NHPh
S
F3C
3h
ppm
200
180
160
140
120
100
80
60
40
20
Current Data Parameters
NAME liuxianjin
EXPNO 18
PROCNO 1
F2 - Acquisition Parameters
Date_ 20100325
Time 15.22
INSTRUM av400
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 442
DS 4
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 9195.2
DW 20.850 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 8.50 usec
PL1 -2.00 dB
SFO1 100.6228298 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -3.00 dB
PL12 10.27 dB
PL13 14.00 dB
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

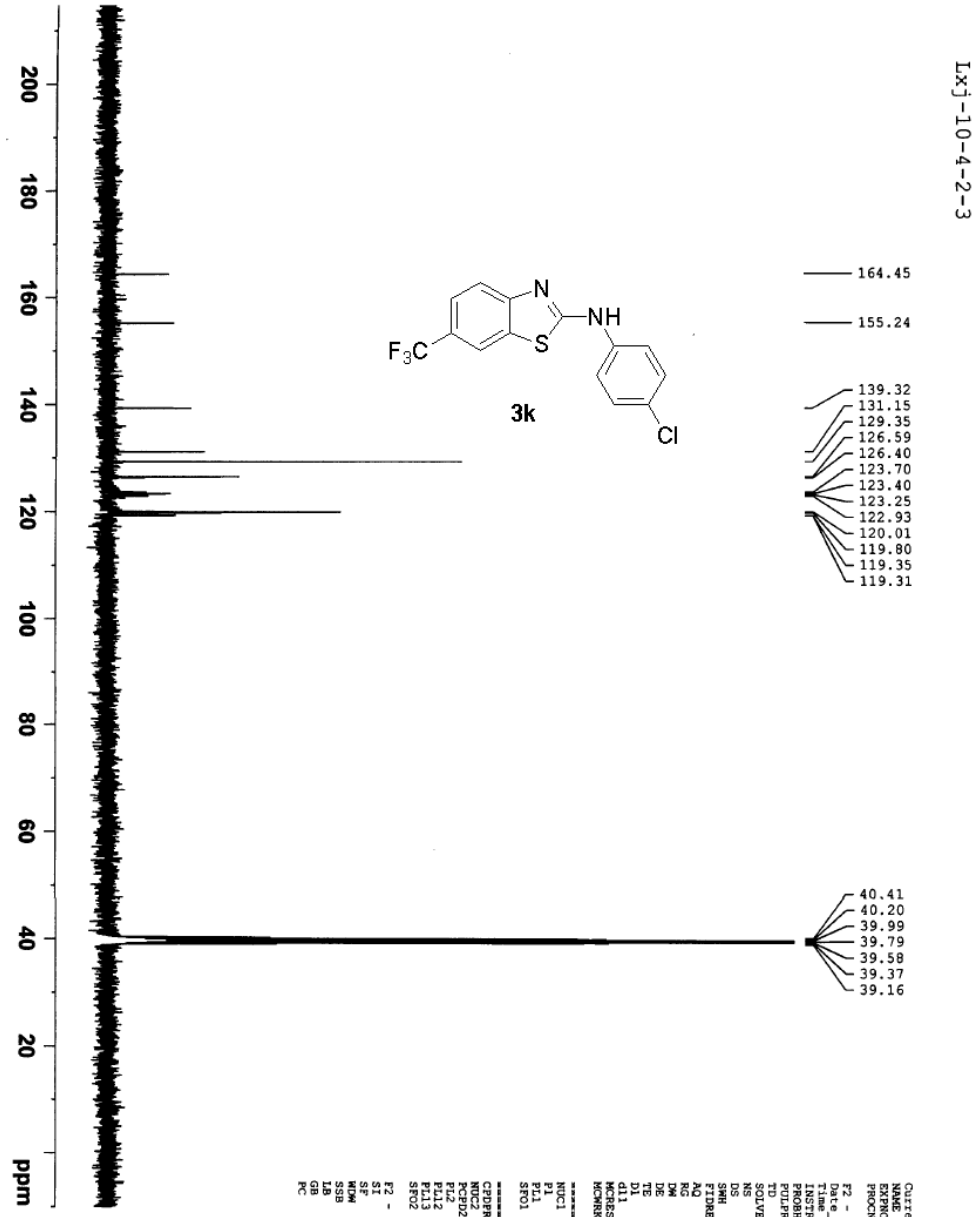

Lxj-10-4-2-4
9.480
9.471
9.463
7.824
7.522
7.501
7.441
7.419
7.397
7.261
7.001
6.980
3.864
1.689
0.000
1.02
1.00
0.95
3.24
2.09
3.12
ppm
N
NHPMP
S
F3C
3i
Current Data Parameters
NAME
EXPNO
PROCNO
F2 - Acquisition Parameters
Date_
Time
INSTRUM
PROBHD
PULPROG
TD
SOLVENT
NS
DS
SWH
FIDRES
AQ
RG
DW
DE
TE
D1
MCREST
MCWRK
CHANNEL f1
NUC1
P1
PL1
SFO1
F2 - Processing parameters
SI
SF
WDW
SSB
LB
GB
PC

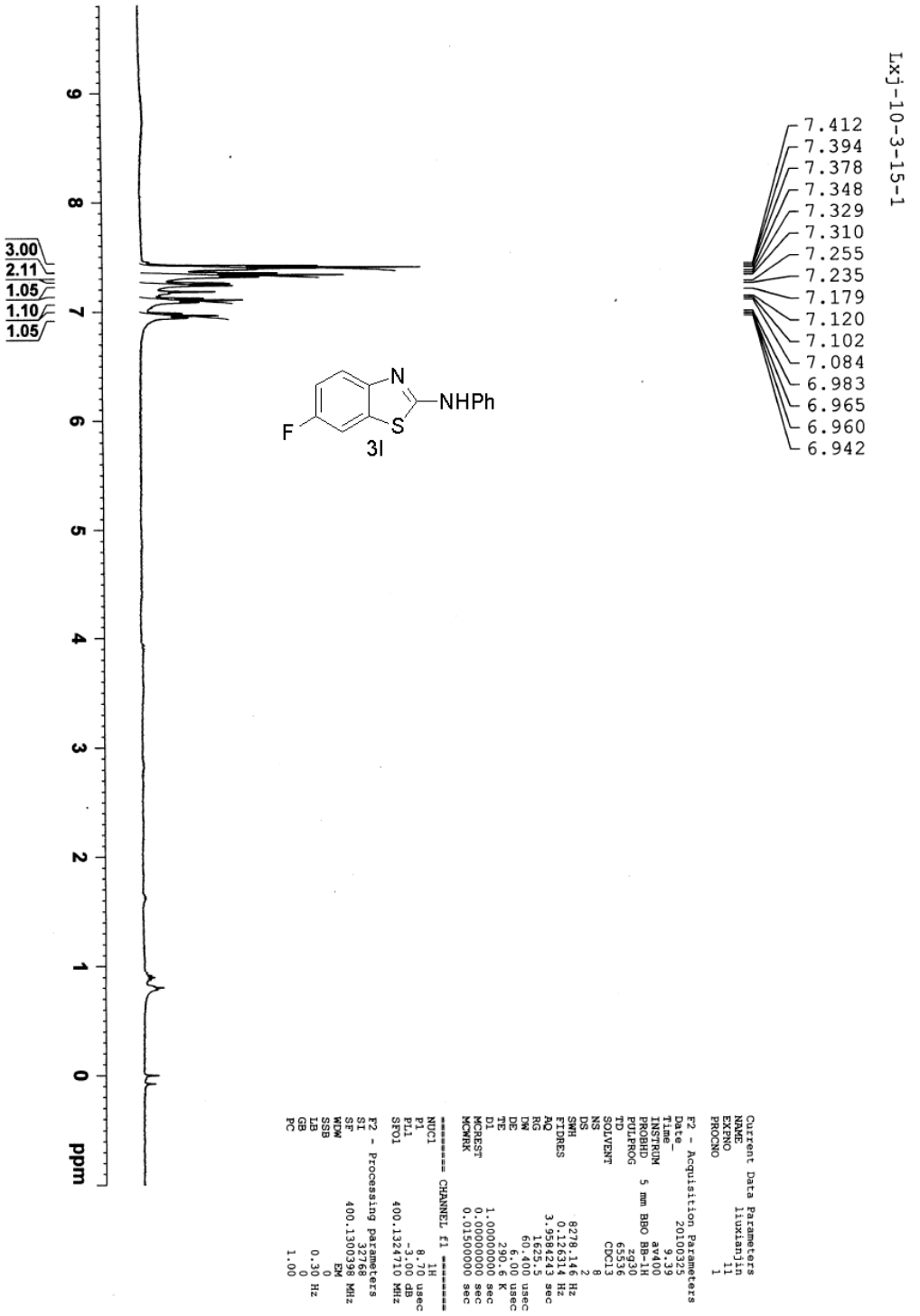

lxj-10-4-2-4
169.33
157.99
154.36
132.14
130.08
125.82
124.64
124.18
123.86
123.53
123.39
123.36
123.12
118.65
118.34
118.30
115.02
77.34
77.02
76.71
55.58
0.00
200
180
160
140
120
100
80
60
40
20
ppm
N
NH
S
F3C
OCH3
3i

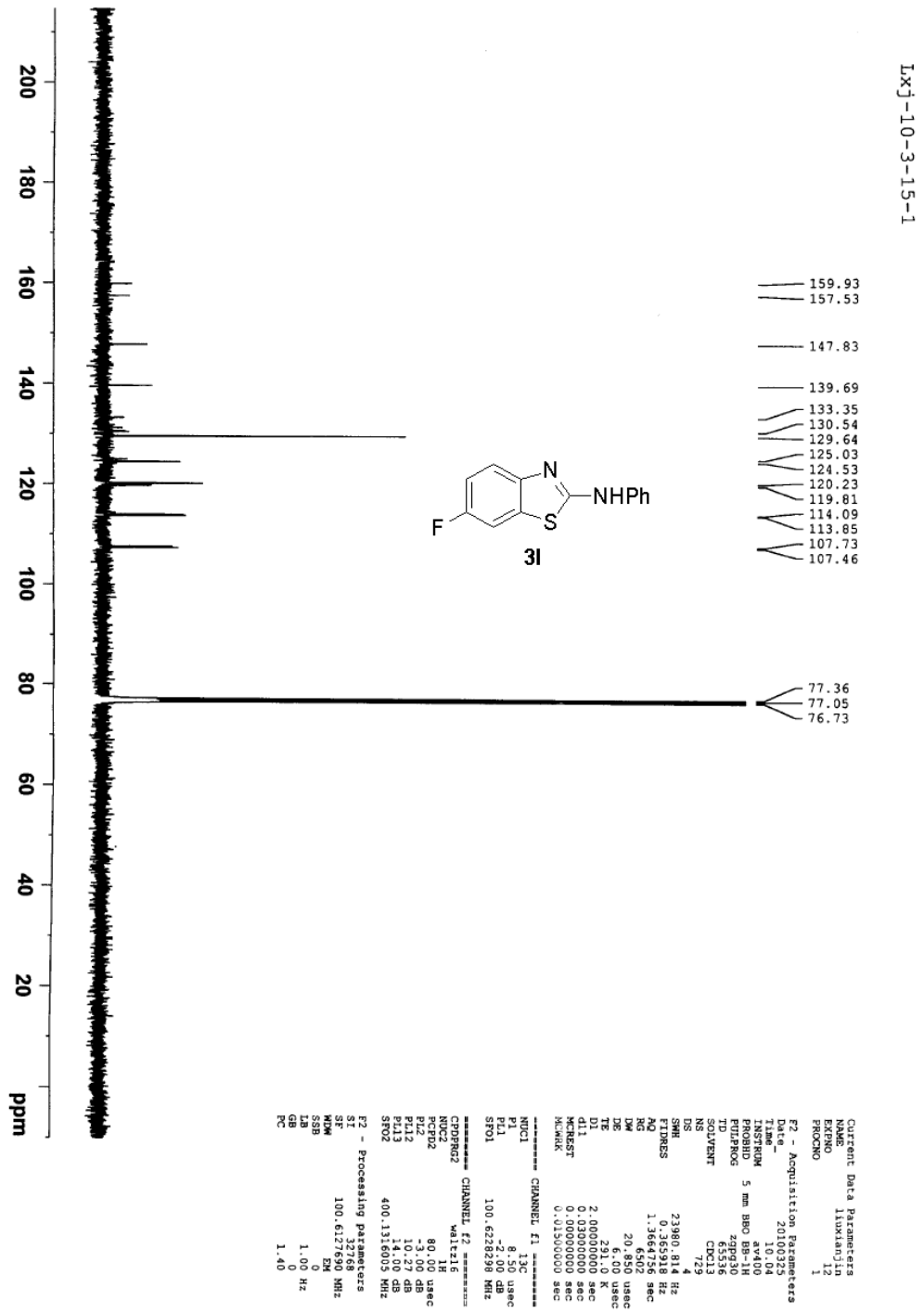

Lxj-10-4-2-5
8.360
8.300
8.277
8.039
8.016
7.868
7.848
7.710
7.690
1.00
1.93
1.97
0.99
1.07
3.512
3.491
2.532
3j
ppm

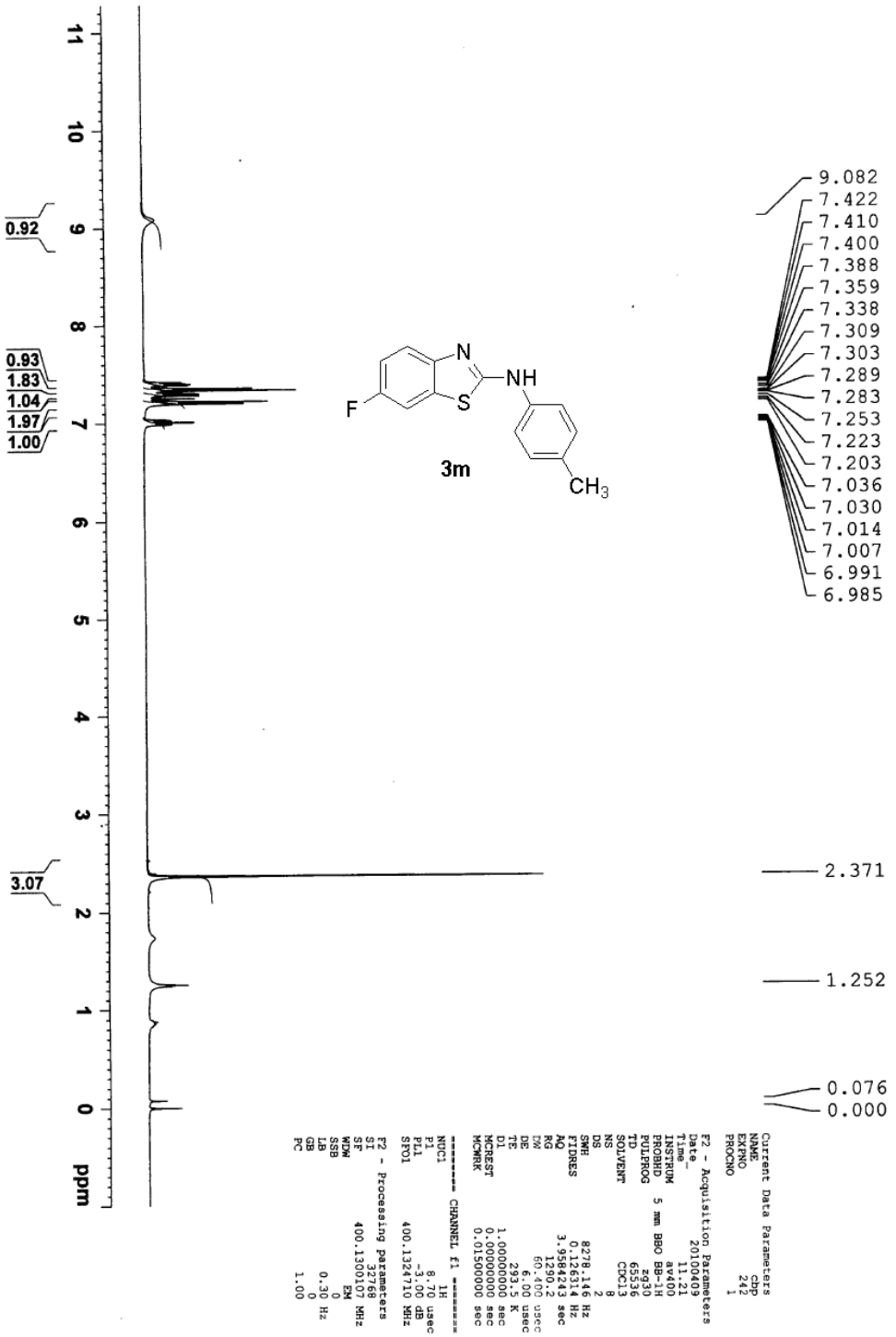

Lxj-10-4-2-5
163.98
154.69
146.21
141.83
131.46
125.80
123.97
123.61
120.60
119.63
118.01
40.46
40.25
40.04
39.83
39.63
39.42
39.21
3j
F3C
N
NH
S
NO2
200
180
160
140
120
100
80
60
40
20
ppm

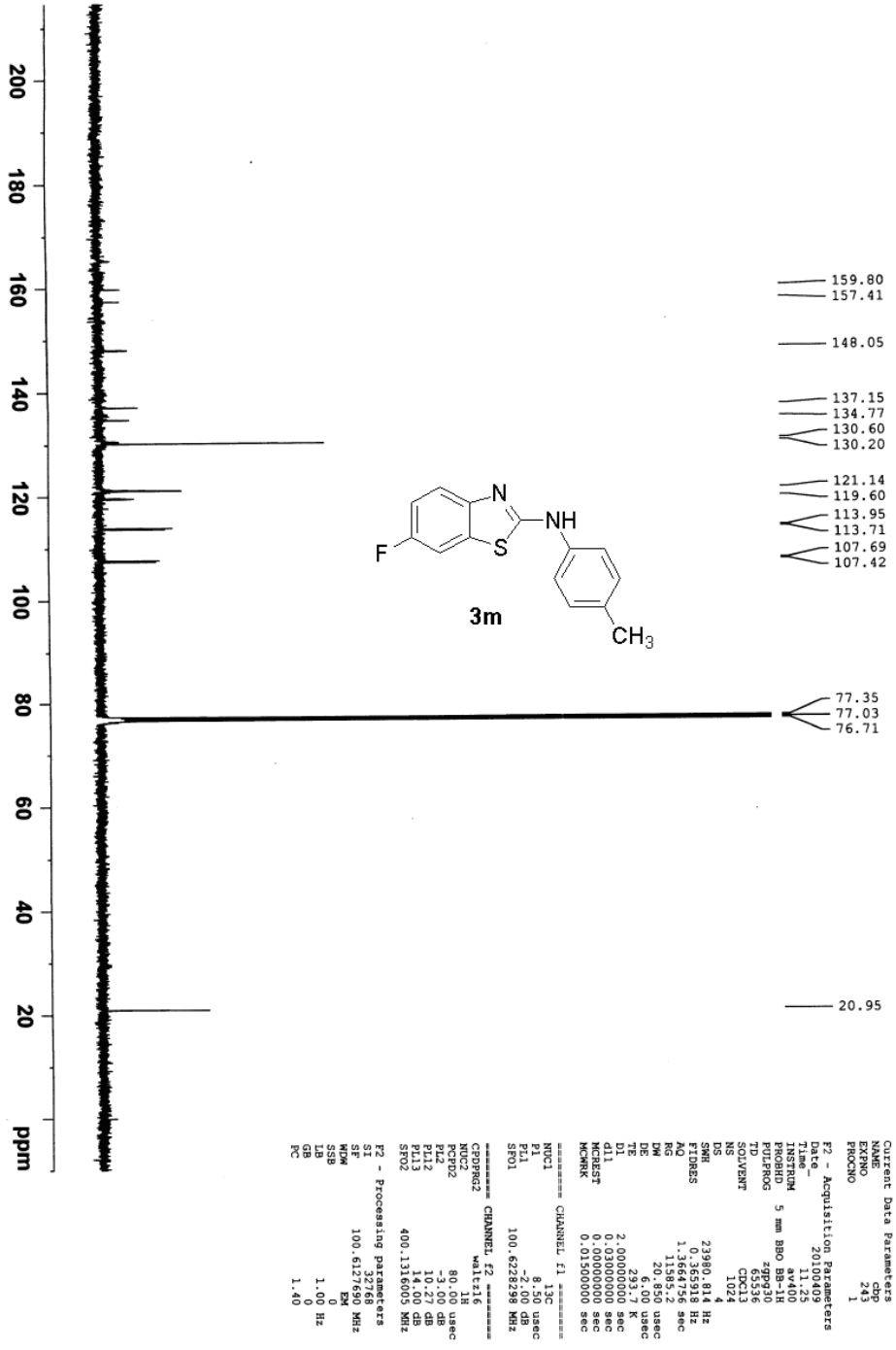

Lxj-10-4-2-3
10.934
8.299
7.868
7.864
7.846
7.777
7.756
7.662
7.640
7.464
7.460
7.442
3.560
2.547
2.543
0.14
0.98
1.97
1.00
1.02
1.99
ppm
3k
F3C
N
NH
S
Cl
Current Data Parameters
NAME Lxj-10-4-2-3
EXPNO 259
PROCNO 1
F2 - Acquisition Parameters
Date_ 20100414
Time_ 11.24
INSTRUM av400
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 8
DS 2
SWH 8278.146 Hz
FIDRES 0.126314 Hz
AQ 3.9584243 sec
RG 912.3
DW 60.400 usec
DE 6.00 usec
TE 293.8 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 8.30 usec
PL1 -3.00 dB
SFO1 400.1332010 MHz
F2 - Processing parameters
SI 32768
SF 400.1299814 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

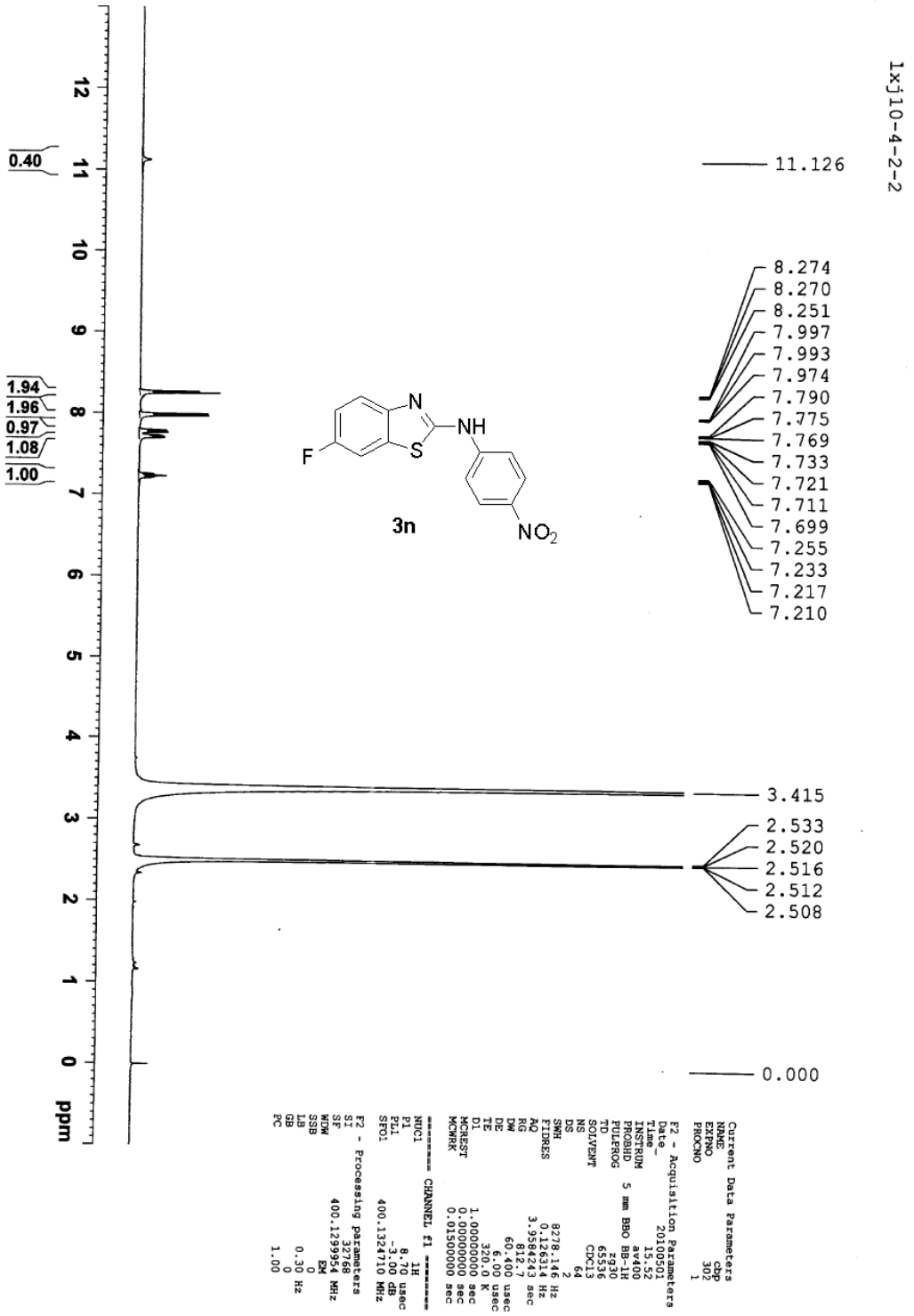

Lxj-10-4-2-3
164.45
155.24
139.32
131.15
129.35
126.59
126.40
123.70
123.40
123.25
122.93
120.01
119.80
119.35
119.31
40.41
40.20
39.99
39.79
39.58
39.37
39.16
N
NH
S
F3C
Cl
3k
200
180
160
140
120
100
80
60
40
20
ppm

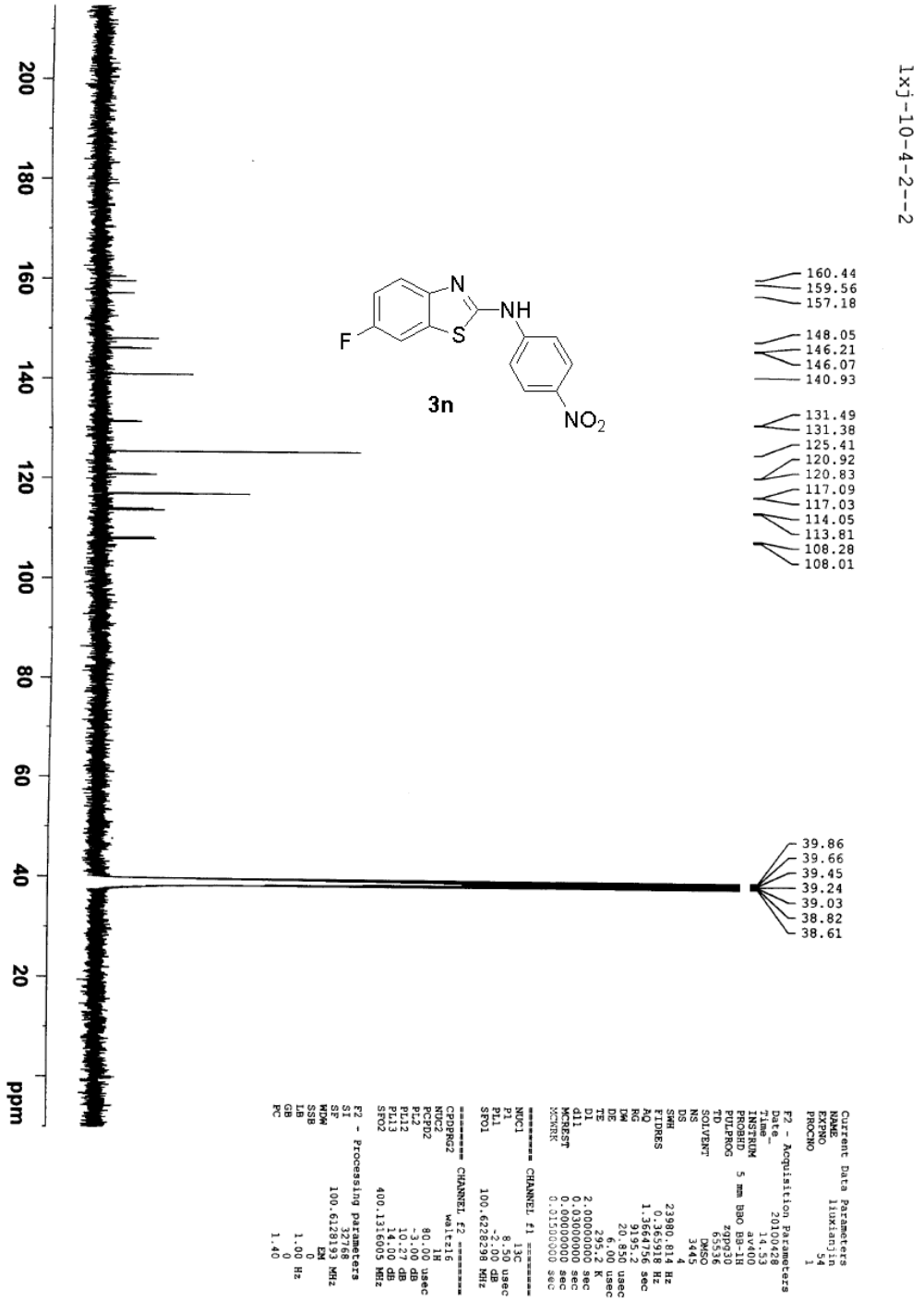

Lxj-10-3-15-1
7.412
7.394
7.378
7.348
7.329
7.310
7.255
7.235
7.179
7.120
7.102
7.084
6.983
6.965
6.960
6.942
3.00
2.11
1.05
1.10
1.05
N
NHPh
F
S
3l
ppm
Current Data Parameters
NAME liuxianjin
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20100325
Time_ 9.39
INSTRUM av400
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 2
SWH 8278.146 Hz
FIDRES 0.126314 Hz
AQ 3.958253 sec
RG 161.4
DW 60.400 usec
DE 6.00 usec
TE 290.6 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 8.70 usec
PL1 -3.00 dB
SFO1 400.1324710 MHz
F2 - Processing parameters
SI 32768
SF 400.1300396 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

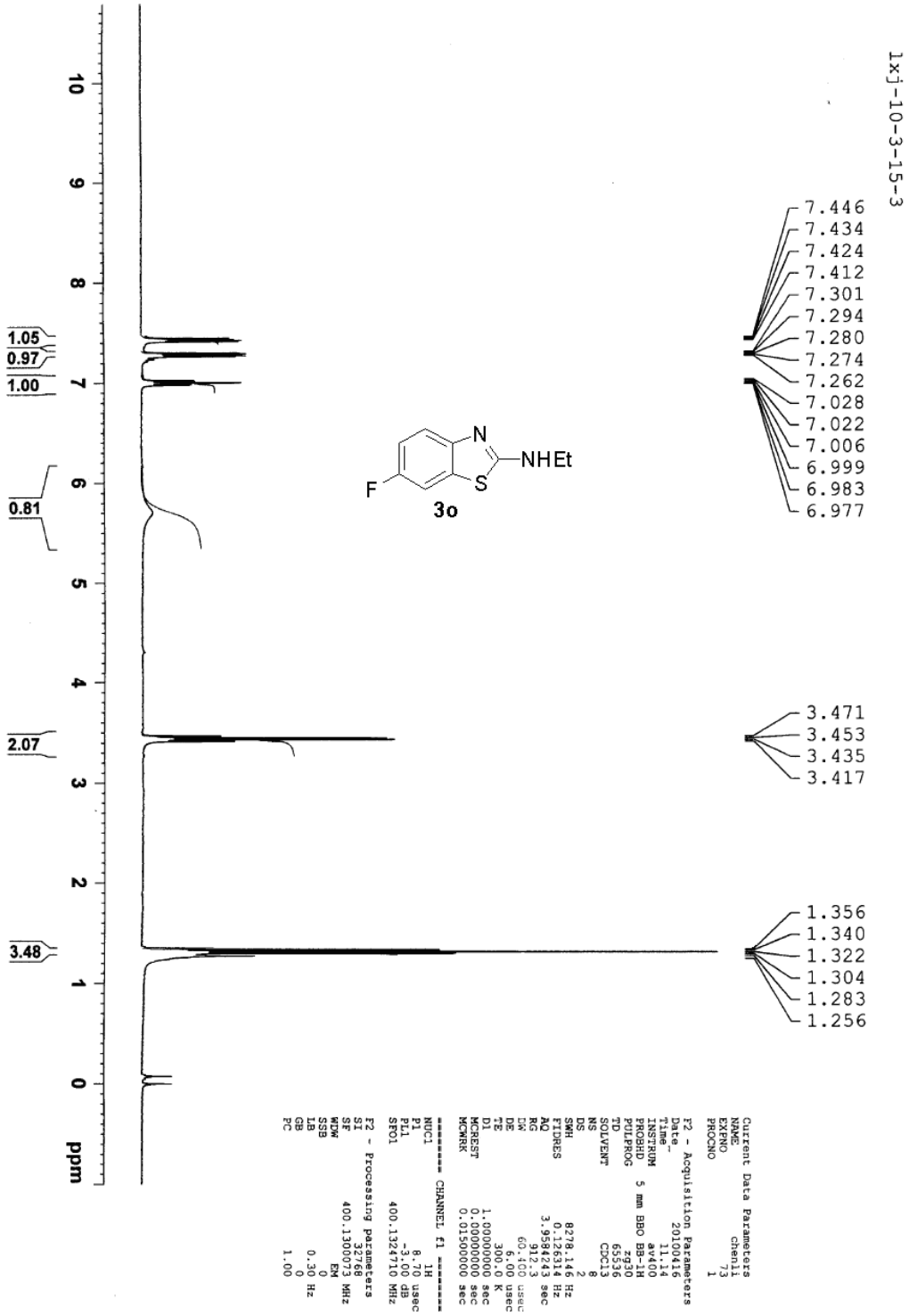

Lxj-10-3-15-1
159.93
157.53
147.83
139.69
133.35
130.54
129.64
125.03
124.53
120.23
119.81
114.09
113.85
107.73
107.46
77.36
77.05
76.73
N
NHPh
F
S
3l
200
180
160
140
120
100
80
60
40
20
ppm

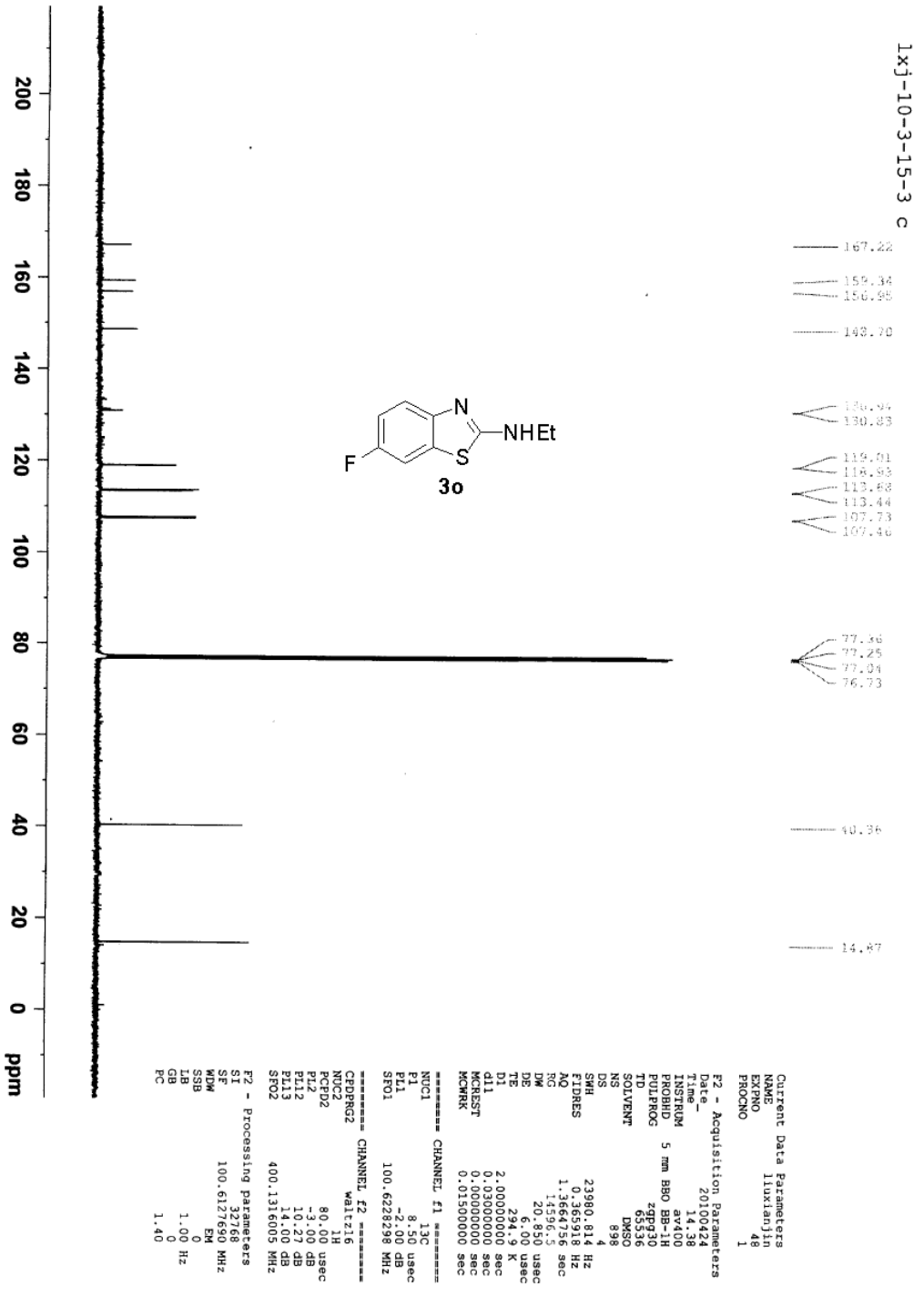

9.082
7.422
7.410
7.400
7.388
7.359
7.338
7.309
7.303
7.289
7.283
7.253
7.223
7.203
7.036
7.030
7.014
7.007
6.991
6.985
2.371
1.252
0.076
0.000
0.92
0.93
1.83
1.04
1.97
1.00
3.07
ppm
N
NH
S
F
CH3
3m

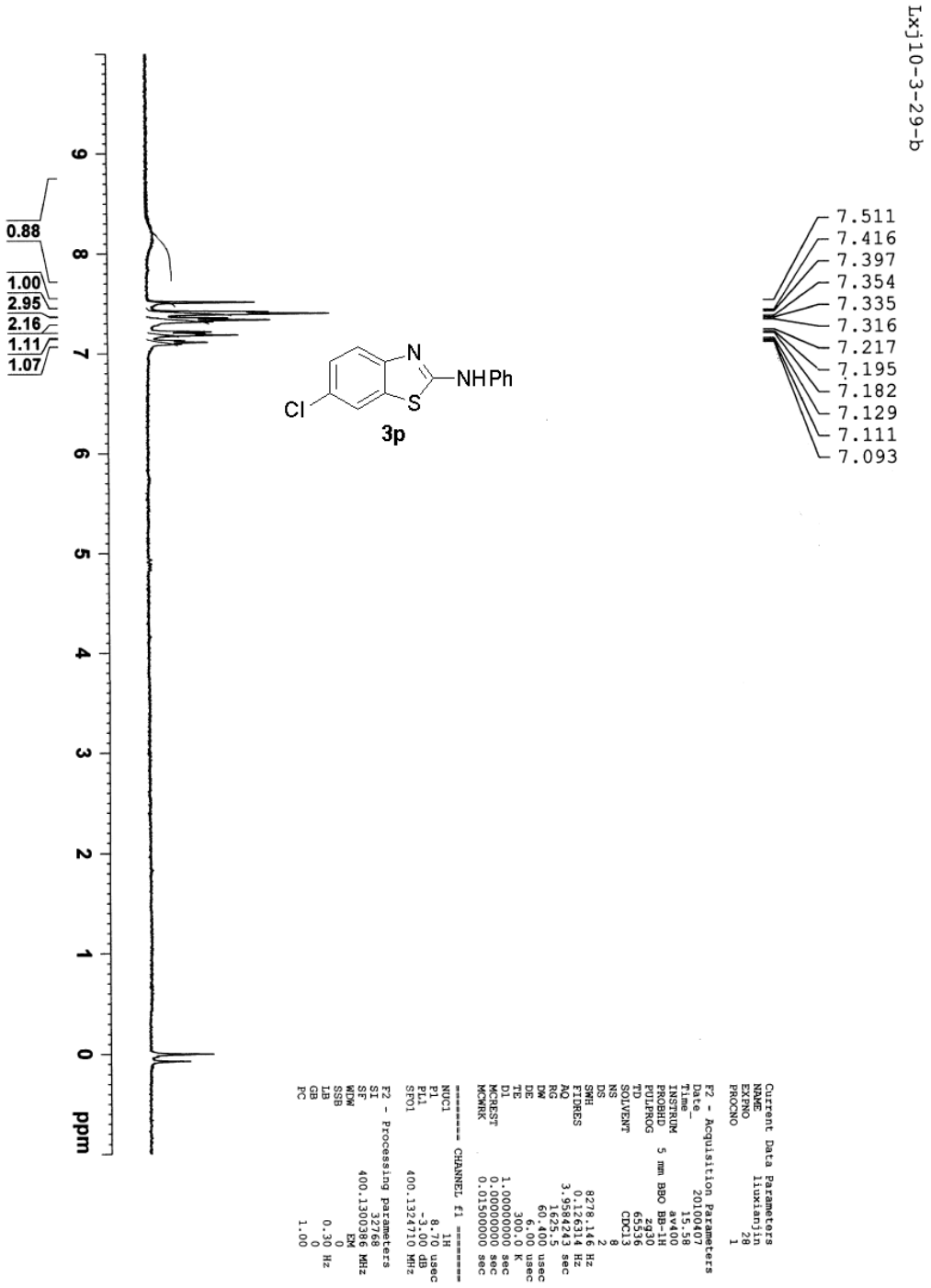

159.80
157.41
148.05
137.15
134.77
130.60
130.20
121.14
119.60
113.95
113.71
107.69
107.42
77.35
77.03
76.71
20.95
N
NH
F
S
CH3
3m
200
180
160
140
120
100
80
60
40
20
ppm
Current Data Parameters
NAME cbp
EXPNO 243
PROCNO 1
F2 - Acquisition Parameters
Date_ 20100409
Time_ 11.25
INSTRUM av400
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1024
DS 4
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 11585.2
DW 20.850 usec
DE 6.00 usec
TE 293.7 K
D1 2.00000000 sec
D11 0.03000000 sec
MAS1EST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 8.50 usec
PL1 -2.00 dB
SFO1 100.6228298 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -3.00 dB
PL12 10.27 dB
PL13 14.00 dB
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

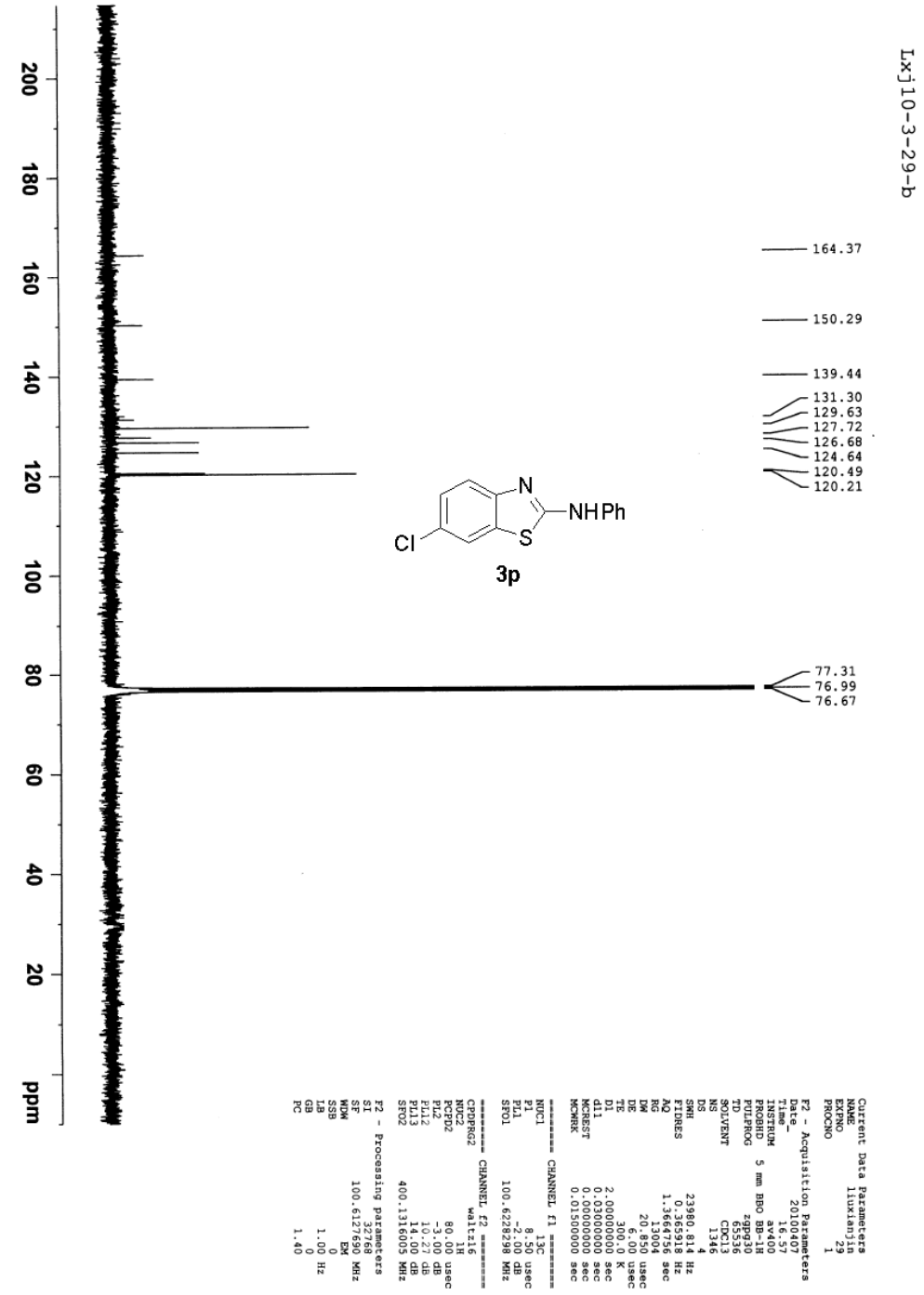

1xj10-4-2-2
11.126
8.274
8.270
8.251
7.997
7.993
7.974
7.790
7.775
7.769
7.733
7.721
7.711
7.699
7.255
7.233
7.217
7.210
3.415
2.533
2.520
2.516
2.512
2.508
0.000
0.40
1.94
1.96
0.97
1.08
1.00
ppm
3n
F
N
NH
S
NO2
Current Data Parameters
NAME 1xj10-4-2-2
EXPNO 302
PROCNO 1
F2 - Acquisition Parameters
Date_ 20100501
Time_ 15.52
INSTRUM av400
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 64
DS 2
SWH 8278.146 Hz
FIDRES 0.126314 Hz
AQ 3.9584243 sec
RG 812.7
DW 60.400 usec
DE 6.00 usec
TE 320.0 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
CHANNEL f1
NUC1 1H
P1 8.70 usec
PL1 -3.00 dB
SFO1 400.1324710 MHz
F2 - Processing parameters
SI 32768
SF 400.1299954 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

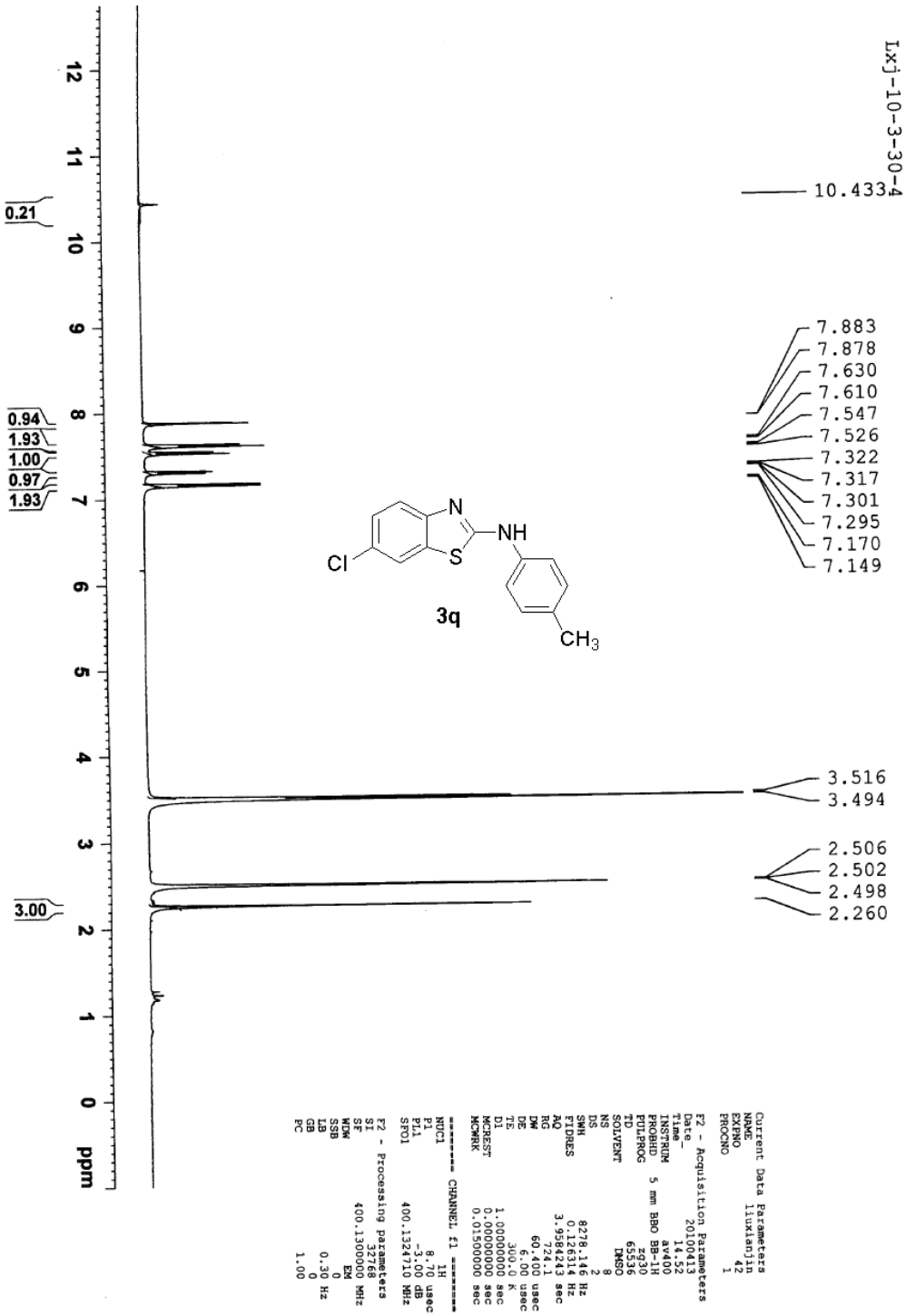

1xj-10-4-2--2
160.44
159.56
157.18
148.05
146.21
146.07
140.93
131.49
131.38
125.41
120.92
120.83
117.09
117.03
114.05
113.81
108.28
108.01
39.86
39.66
39.45
39.24
39.03
38.82
38.61
N
NH
F
S
NO2
3n
200
180
160
140
120
100
80
60
40
20
ppm

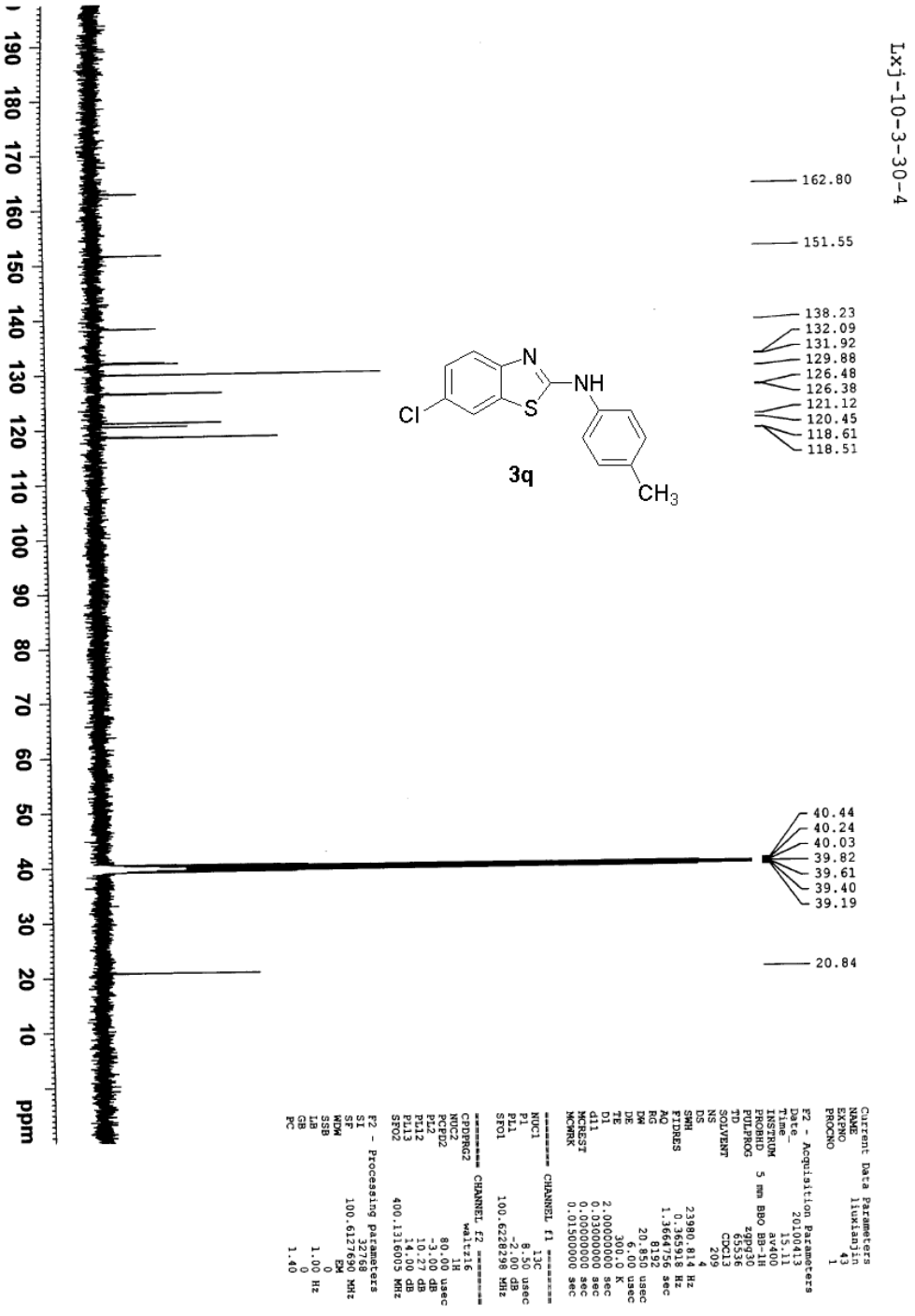

1xj-10-3-15-3
7.446
7.434
7.424
7.412
7.301
7.294
7.280
7.274
7.262
7.028
7.022
7.006
6.999
6.983
6.977
3.471
3.453
3.435
3.417
1.356
1.340
1.322
1.304
1.283
1.256
1.05
0.97
1.00
0.81
2.07
3.48
ppm
N
NHEt
F
S
3o

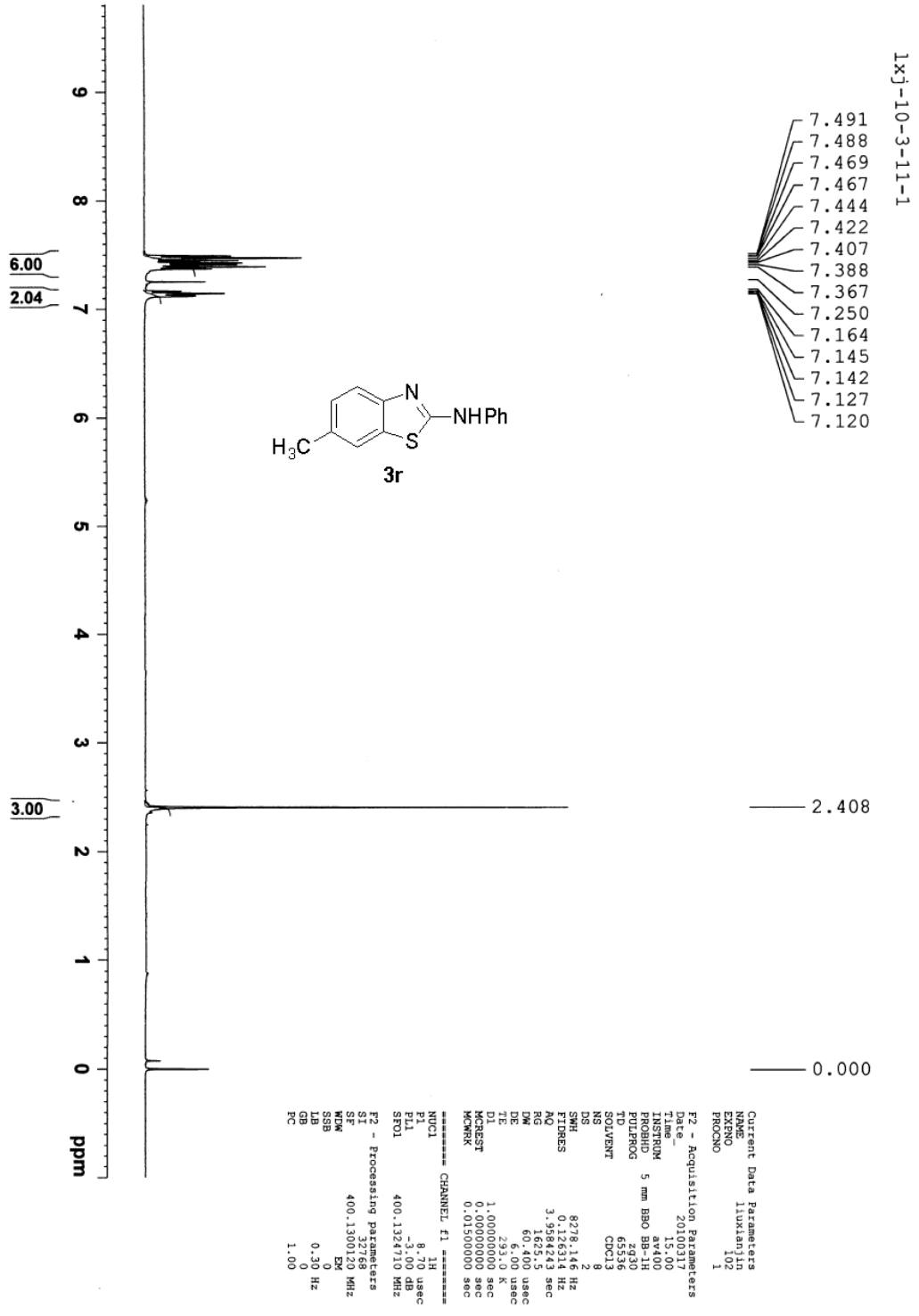

1xj-10-3-15-3 c
167.22
159.34
156.95
143.70
130.94
130.83
119.01
118.93
113.48
113.44
107.73
107.46
77.36
77.25
77.04
76.73
40.36
14.87
N
NHEt
S
F
3o
200
180
160
140
120
100
80
60
40
20
0
ppm
Current Data Parameters
NAME liuxianjin
EXPNO 48
PROCNO 1
F2 - Acquisition Parameters
Date_ 20100424
Time 14.38
INSTRUM av400
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 898
DS 4
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 1456.5
DW 20.850 usec
DE 6.00 usec
TE 294.9 K
D1 2.00000000 sec
D11 0.03000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 8.50 usec
PL1 -2.00 dB
SFO1 100.6228298 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -3.00 dB
PL12 10.27 dB
PL13 14.00 dB
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

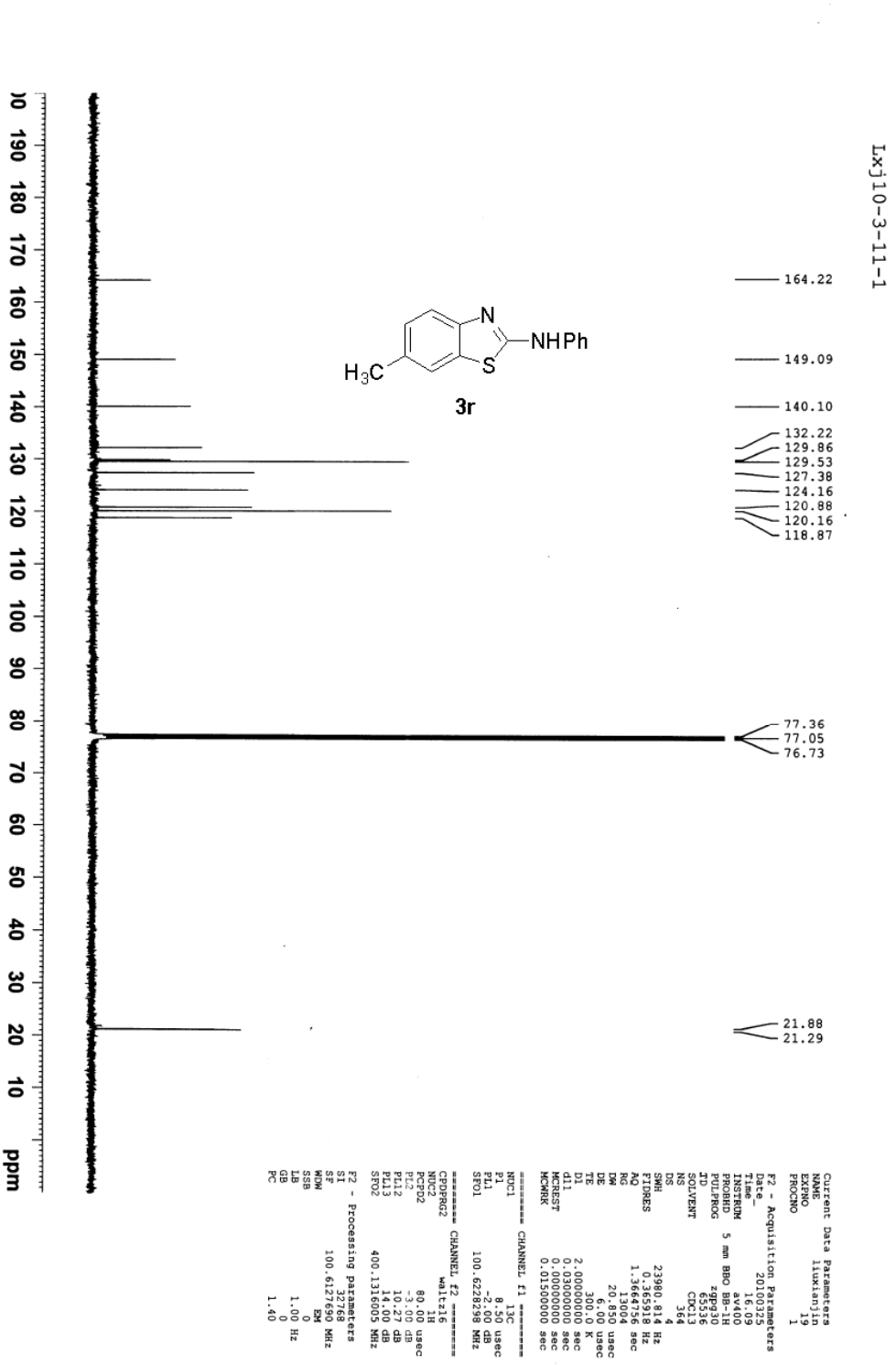

Lxj10-3-29-b
7.511
7.416
7.397
7.354
7.335
7.316
7.217
7.195
7.182
7.129
7.111
7.093
0.88
1.00
2.95
2.16
1.11
1.07
N
NH Ph
Cl
S
3p
ppm
Current Data Parameters
NAME liuxianjin
EXPNO 20
PROCNO 1
F2 - Acquisition Parameters
Date_ 20100407
Time 15.58
INSTRUM av400
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 2
SWH 8278.146 Hz
FIDRES 0.126314 Hz
AQ 3.9584243 sec
RG 16253
DW 60.400 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 8.70 usec
PL1 -3.00 dB
SFO1 400.1324710 MHz
F2 - Processing parameters
SI 32768
SF 400.1300396 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

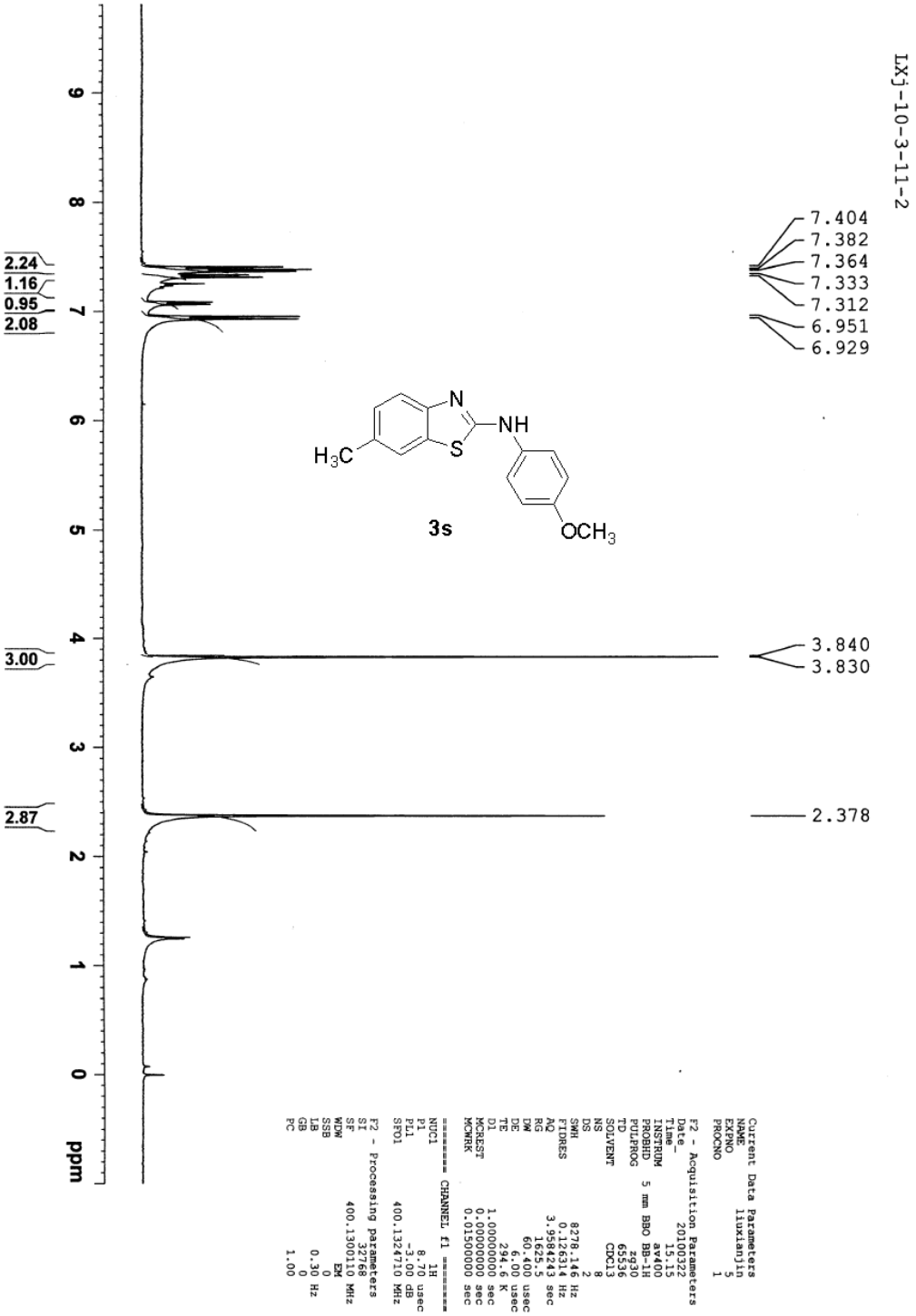

Lxj10-3-29-b
164.37
150.29
139.44
131.30
129.63
127.72
126.68
124.64
120.49
120.21
77.31
76.99
76.67
N
NHPh
Cl
S
3p
200
180
160
140
120
100
80
60
40
20
ppm

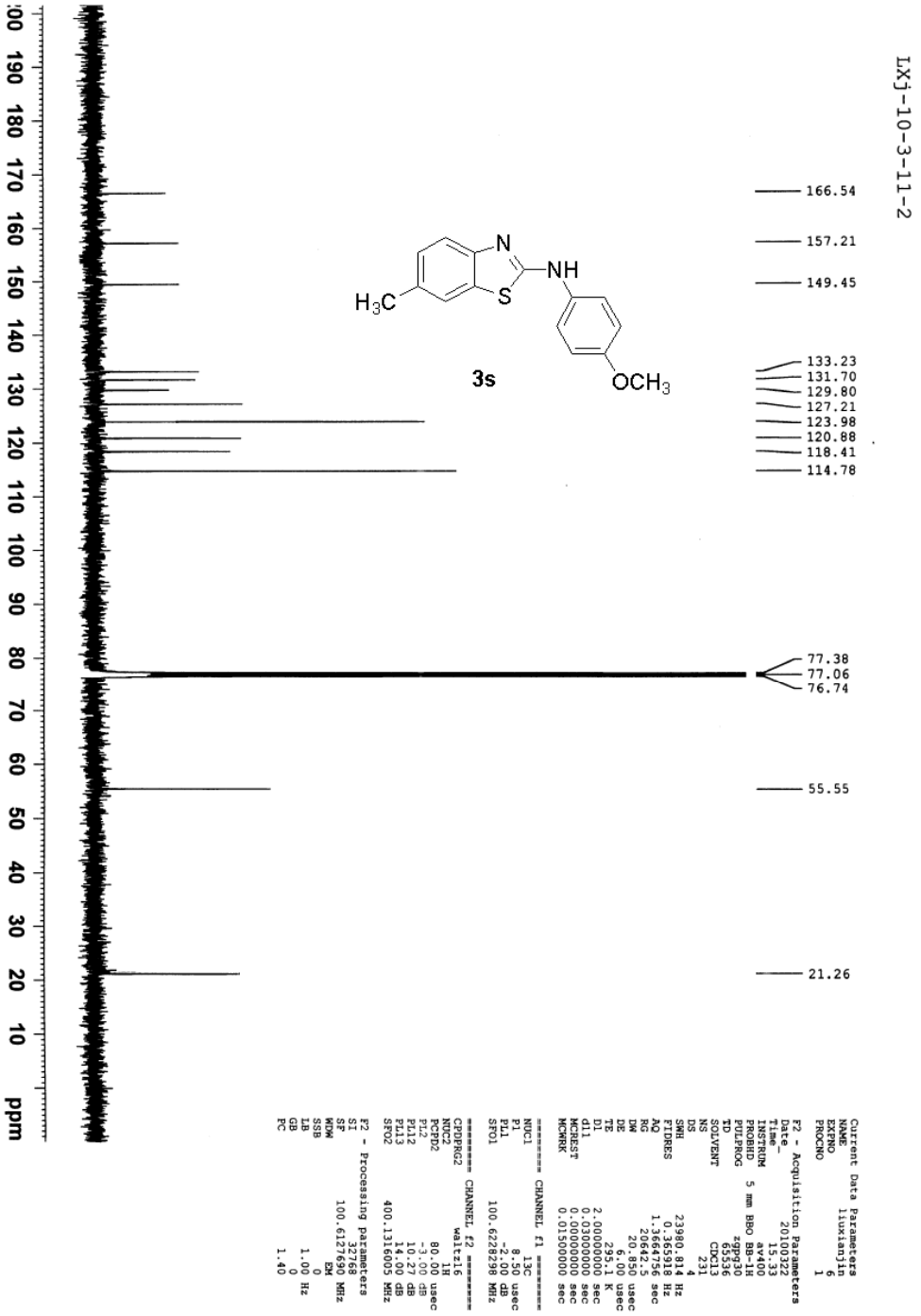

Lxj-10-3-30-4
10.433
7.883
7.878
7.630
7.610
7.547
7.526
7.322
7.317
7.301
7.295
7.170
7.149
3.516
3.494
2.506
2.502
2.498
2.260
0.21
0.94
1.93
1.00
0.97
1.93
3.00
ppm
N
NH
S
Cl
CH3
3q

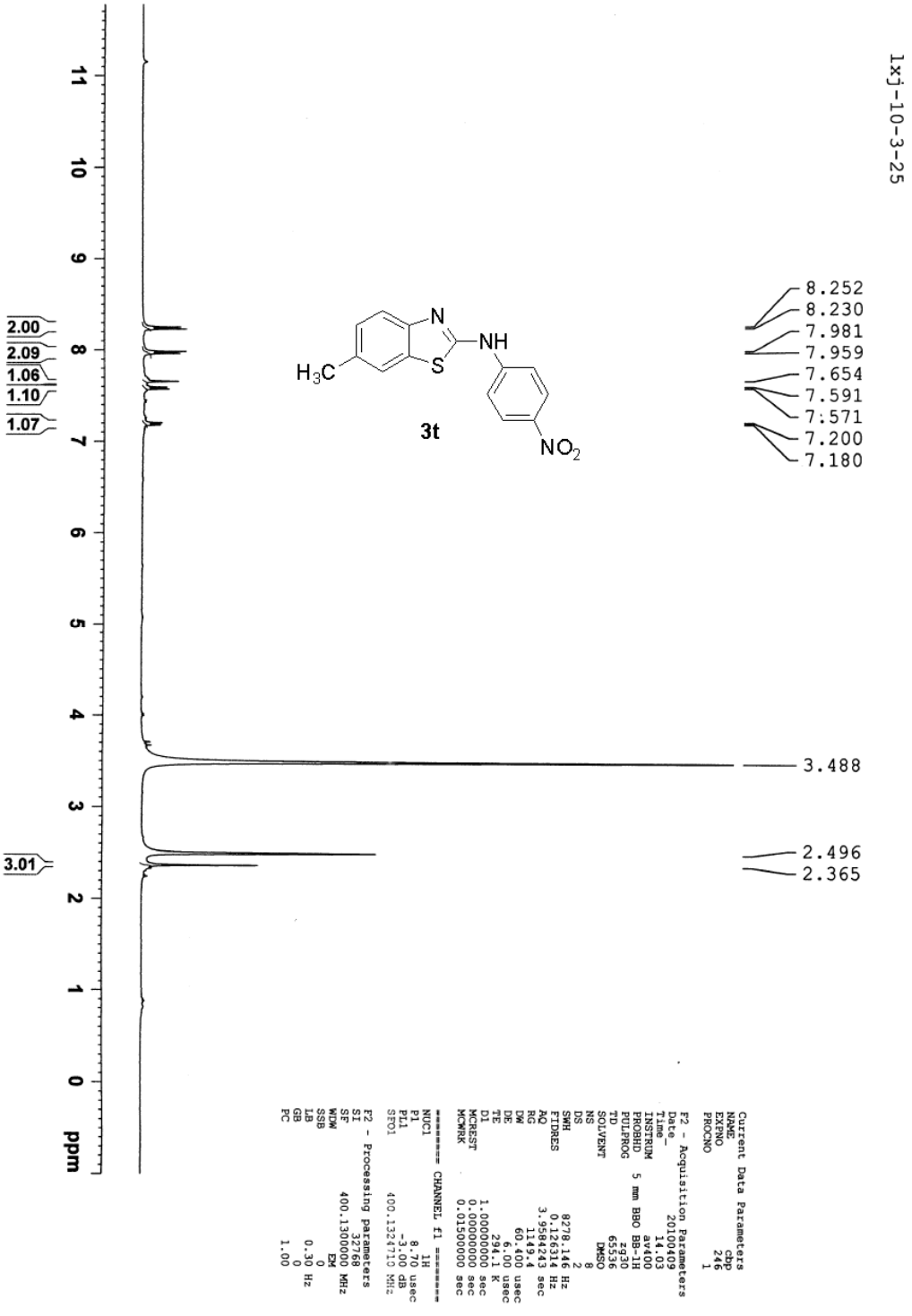

Lxj-10-3-30-4
162.80
151.55
138.23
132.09
131.92
129.88
126.48
126.38
121.12
120.45
118.61
118.51
40.44
40.24
40.03
39.82
39.61
39.40
39.19
20.84
ppm
3q

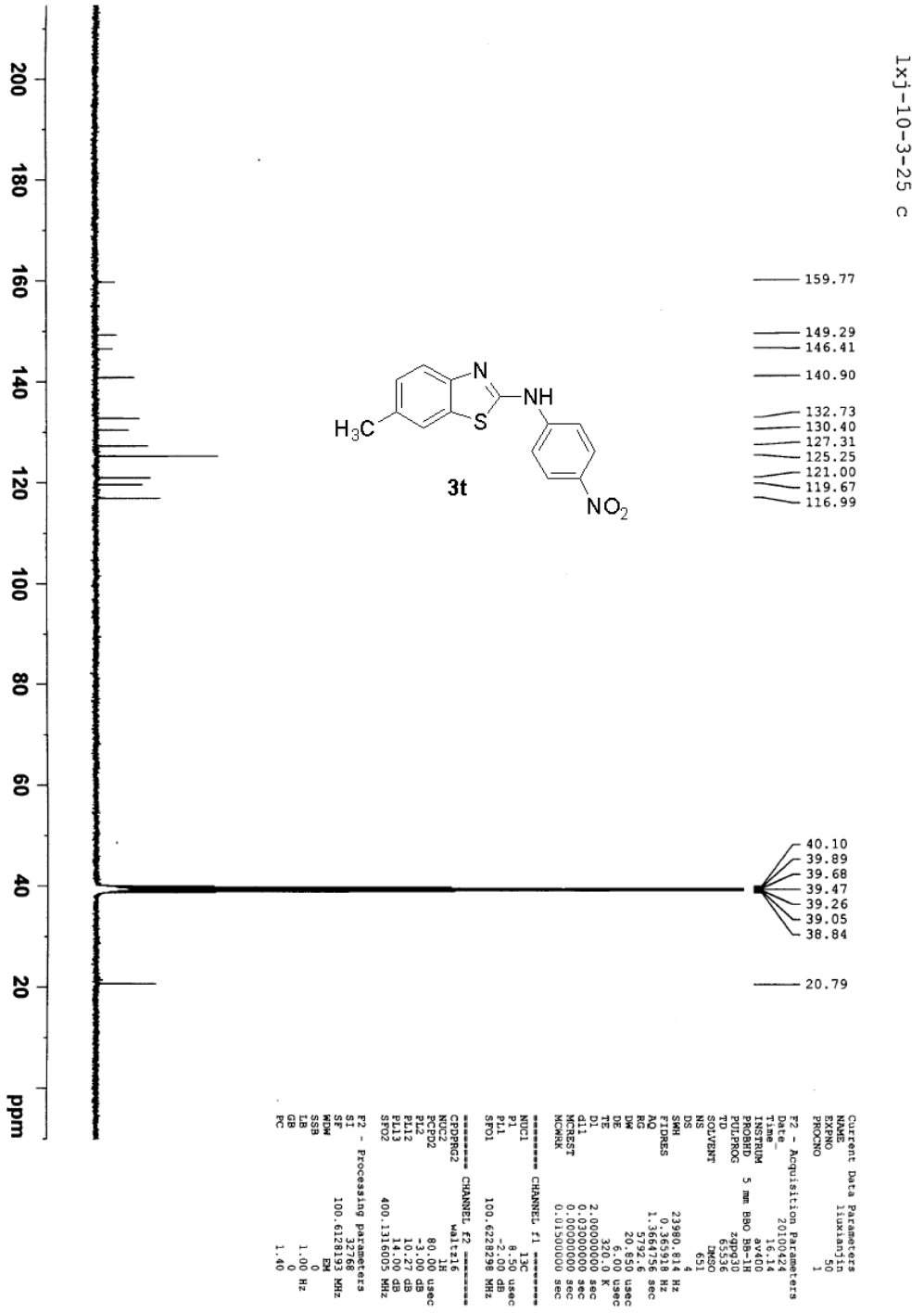

lxj-10-3-11-1
7.491
7.488
7.469
7.467
7.444
7.422
7.407
7.388
7.367
7.250
7.164
7.145
7.142
7.127
7.120
6.00
2.04
3.00
2.408
0.000
ppm
N
NHPh
S
H3C
3r
Current Data Parameters
NAME liuxianjin
EXPNO 102
PROCNO 1
F2 - Acquisition Parameters
Date_ 20100317
Time 15.40
INSTRUM av400
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 2
SWH 8278.146 Hz
FIDRES 0.126314 Hz
AQ 3.9584243 sec
RG 1625.5
DW 60.400 usec
DE 6.00 usec
TE 293.0 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 8.70 usec
PL1 -3.00 dB
SFO1 400.1324710 MHz
F2 - Processing parameters
SI 32768
SF 400.1300120 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

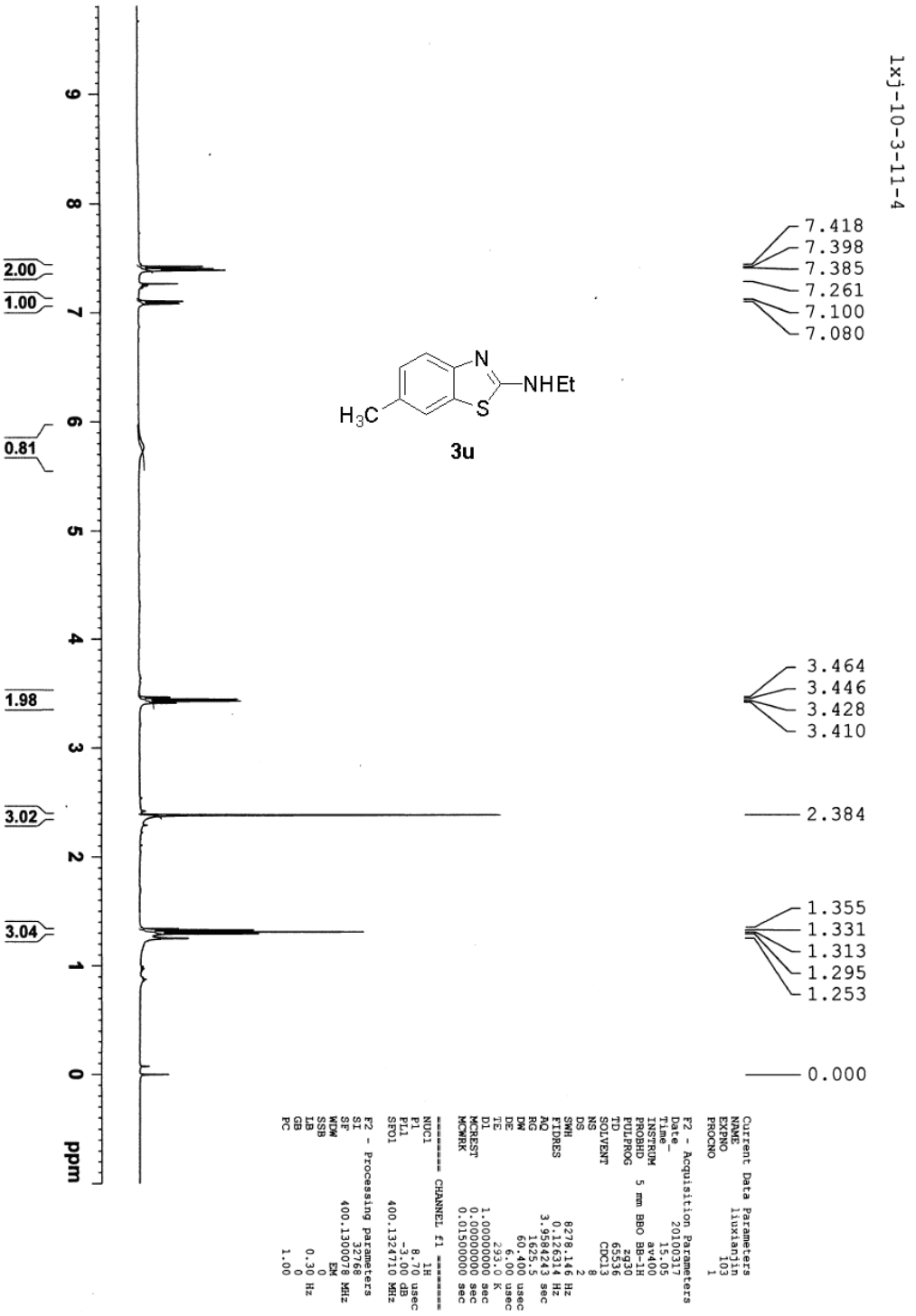

Lxj10-3-11-1
164.22
149.09
140.10
132.22
129.86
129.53
127.38
124.16
120.88
120.16
118.87
77.36
77.05
76.73
21.88
21.29
N
NHPh
S
H3C
3r
ppm

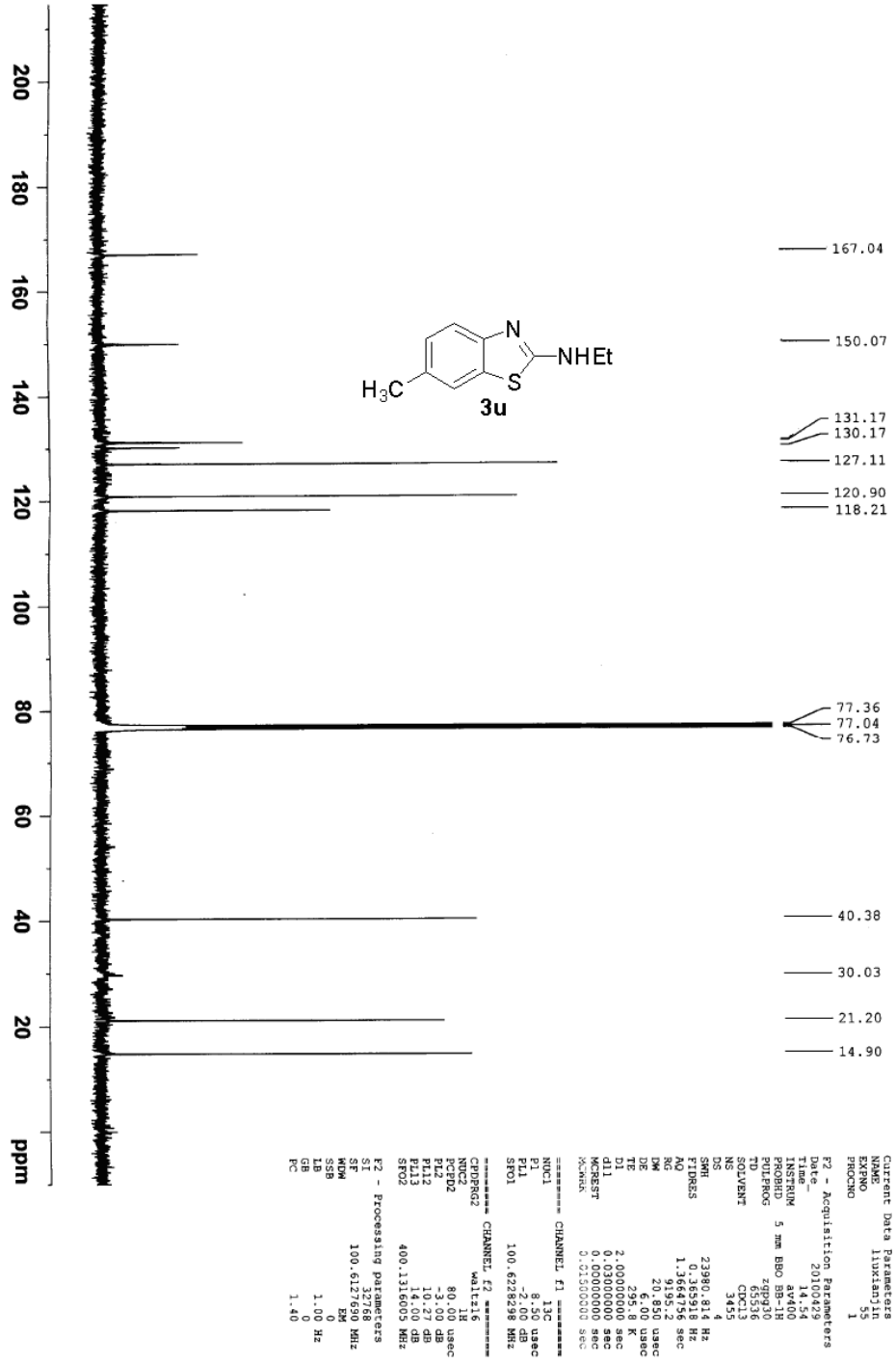

LXj-10-3-11-2
7.404
7.382
7.364
7.333
7.312
6.951
6.929
3.840
3.830
2.378
2.24
1.16
0.95
2.08
3.00
2.87
ppm
N
NH
S
H3C
OCH3
3s


LXj-10-3-11-2
166.54
157.21
149.45
133.23
131.70
129.80
127.21
123.98
120.88
118.41
114.78
77.38
77.06
76.74
55.55
21.26
ppm
3s
N
NH
S
H3C
OCH3


1xj-10-3-25
8.252
8.230
7.981
7.959
7.654
7.591
7.571
7.200
7.180
3.488
2.496
2.365
2.00
2.09
1.06
1.10
1.07
3.01
ppm
3t
N
NH
S
H3C
NO2
Current Data Parameters
NAME cbp
EXPNO 246
PROCNO 1
F2 - Acquisition Parameters
Date_ 20100409
Time 14.03
INSTRUM av400
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 8
DS 2
SWH 8278.146 Hz
FIDRES 0.126314 Hz
AQ 3.9584243 sec
RG 1149.4
DW 60.400 usec
DE 6.00 usec
TE 294.1 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 8.70 usec
PL1 -3.00 dB
SFO1 400.1324710 MHz
F2 - Processing parameters
SI 32768
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00


1xj-10-3-25 c
159.77
149.29
146.41
140.90
132.73
130.40
127.31
125.25
121.00
119.67
116.99
40.10
39.89
39.68
39.47
39.26
39.05
38.84
20.79
3t
ppm


lxj-10-3-11-4
7.418
7.398
7.385
7.261
7.100
7.080
3.464
3.446
3.428
3.410
2.384
1.355
1.331
1.313
1.295
1.253
0.000
2.00
1.00
0.81
1.98
3.02
3.04
ppm
N
NHEt
S
H3C
3u


167.04
150.07
131.17
130.17
127.11
120.90
118.21
77.36
77.04
76.73
40.38
30.03
21.20
14.90
ppm
N
NHEt
S
H3C
3u