Generation of diverse 2-pyrones via palladium-catalyzed site-selective Suzuki-Miyaura couplings of 3-bromo-4-tosyloxy-2-pyrone

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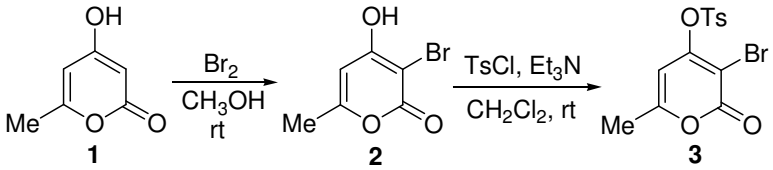
Supporting Information

General experimental methods

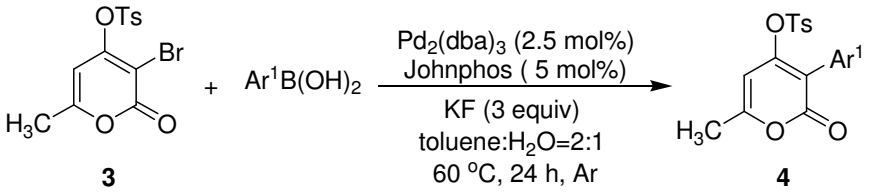
Unless otherwise stated, all commercial reagents and solvents were used without additional purification. All solvents were dried and distilled according to standard procedures. All reactions were performed in reaction tubes under Ar. The Flash column chromatography was performed using silica gel (60-Å pore size, 32–63 μm, standard grade). 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 ~20 Torr (house vacuum) at 25-35°C. Nuclear magnetic resonance (NMR) spectra are recorded in parts per million from internal tetramethylsilane (TMS) on the δ scale.

Synthesis of 3-bromo-6-methyl-4-tosyloxy-2-pyrone ***3*****:**[1]



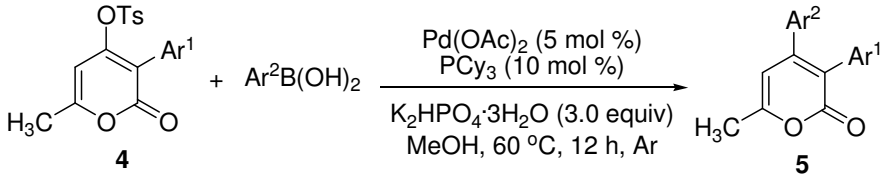
Br_2 (1.0 equiv) was added dropwise into a solution of 4-hydroxy-6-methyl-2-pyrone (8.0 mmol) in methanol at 0 °C. The resulting white solid was appeared in the process of addition of Br_2. After completion of the reaction as monitored by TLC, the mixture was then concentrated under reduced pressure to yield the crude 3-bromo-4-hydroxy-6- methyl-2-pyrone **2**. Without purification, the crude was dissolved in CH_2Cl_2. Then Et_3N (3.0 equiv) and TsCl (1.2 equiv) were added to the suspension of compound **2** at 0 °C. The mixture was stirred at room temperature until the reaction was completed. After the solvent was evaporated under reduced pressure, the mixture was purified by flash column chromatography on silica gel to afford the desiring product **3** in 86% yield.

General procedure for the reaction of compound ***3*** *with arylboronic acids (Scheme 2)*:



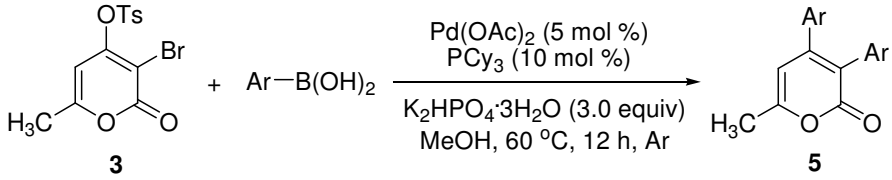
A mixture of compound **3** (0.3 mmol), arylboronic acid (1.5 equiv), $Pd_2(dba)_3$ (2.5 mol %), Johnphos (5 mol %), and KF (3.0 equiv) in 3.0 mL of toluene/H_2O (v/v:2/1) was stirred at 60 °C for 24 h. After completion of the reaction as indicated by TLC, the solvent was evaporated under reduced pressure and the residue was purified by column chromatography on silica gel to produce the corresponding product **4**.

*General procedure for the reaction of compound **4** with arylboronic acids (Table 3):*

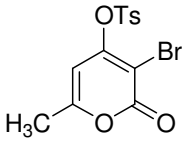


A mixture of substrate **4** (0.3 mmol), arylboronic acid (1.5 equiv), $Pd(OAc)_2$ (5 mol %), PCy_3 (10 mol %), and $K_2HPO_4{\cdot}3H_2O$ (3.0 equiv) in methanol (2.0 mL) was stirred at 60 °C for 12 h. After completion of the reaction as indicated by TLC, the solvent was evaporated under reduced pressure and the residue was purified by column chromatography on silica gel to produce the corresponding product **5**.

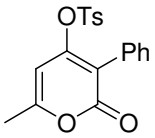
*General procedure for the Synthesis of symmetrically 3,4-diarylated 2-pyrones **5** (Scheme 3)***:**



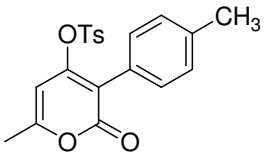
Following the same procedure above (increasing the amount of arylboronic acid to 3.0 equiv).



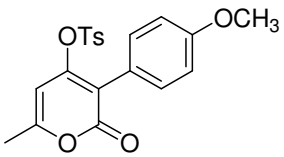
3-bromo-6-methyl-4-(4-methylbenzenesulfonyloxy)-2-pyrone **3**. White solid (86% yield), mp: 165.3-166.2 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.88 (d, *J* = 8.4 Hz, 2H), 7.40 (d, *J* = 8.0 Hz, 2H), 6.44 (s, 1H), 2.49 (s, 3H), 2.29 (s, 3H); ^{13}C NMR (400 MHz, $CDCl_3$) δ 161.9, 160.2, 158.8, 147.0, 131.9, 130.2, 128.5, 101.5, 99.8, 21.8, 19.9; HRMS (ESI) Calcd for $C_{13}H_{11}BrO_5SNa$ (M+Na), 380.9408; Found, 380.9408.



6-methyl-4-(4-methylbenzenesulfonyloxy)-3-phenyl-2-pyrone **4a**. White solid (92% yield), mp: 125.7-127.0 °C. ^{1}H NMR (400 MHz, $CDCl_3$) *δ* 7.30 (d, *J* = 7.2 Hz, 2H), 7.26-7.18 (m, 3H), 7.08-7.05 (m, *J* = 8 Hz, 4 Hz, 4H), 6.45 (s, 1H), 2.39 (s, 3H), 2.34 (s, 3H); ^{13}C NMR (400 MHz, $CDCl_3$) *δ* 163.2, 161.8, 156.4, 145.8, 131.5, 130.0, 129.7, 128.5, 128.1, 127.9, 127.7, 116.1, 102.3, 21.69, 20.1; HRMS (ESI) Calcd for $C_{19}H_{16}O_5SNa$ ($M+Na^+$), 379.0616; Found, 379.0622.

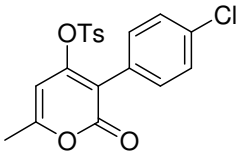


6-methyl-4-(4-methylbenzenesulfonyloxy)-3-(4-methylphenyl)-2-pyrone **4b**. Yellow oil (83% yield). ^{1}H NMR (400 MHz, $CDCl_3$) *δ* 7.32 (d, *J* = 8.0 Hz, 2H), 7.06-6.96 (m, 6H), 6.42 (s, 1H), 2.39 (s, 3H), 2.33 (s, 3H), 2.32 (s, 3H); ^{13}C NMR (400 MHz, $CDCl_3$) *δ* 163.4, 161.5, 156.2, 145.8, 138.1, 131.6, 129.9, 129.5, 128.4, 127.9, 126.0, 116.2, 102.4, 21.74, 21.34, 20.09; HRMS (ESI) Calcd for $C_{20}H_{18}O_5SH$ ($M+H^+$) 371.0953; Found, 371.0951.

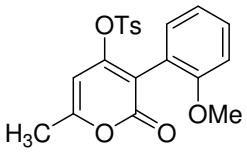


3-(4-methoxylphenyl)-6-methyl-4-(4-methylbenzenesulfonyloxy)-2-pyrone **4c**. Yellow oil (62% yield). ^{1}H NMR (400 MHz, $CDCl_3$) *δ* 7.35 (d, *J* = 8.0 Hz, 2H), 7.09

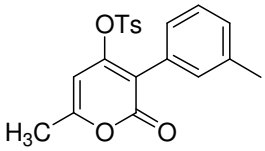
(d, *J* = 8.0 Hz, 2H), 7.04 (d, *J* = 8.4 Hz, 2H), 6.74 (d, *J* = 8.4 Hz, 2H), 6.43 (s, 1H), 3.81 (s, 3H), 2.39 (s, 3H), 2.33 (s, 3H); ^{13}C NMR (400 MHz, $CDCl_3$) δ 163.2, 161.2, 159.4, 155.9, 145.7, 131.3, 129.6, 127.9, 121.1, 115.1, 113.2, 102.5, 55.2, 21.7, 20.0; HRMS (ESI) Calcd for $C_{20}H_{18}O_6SNa$ ($M+Na^+$) 409.0722; Found, 409.0714.



3-(4-chlorophenyl)-6-methyl-4-(4-methylbenzenesulfonyloxy)-2-pyrone **4d**. Yellow solid (59% yield), mp: 108.1-109.3 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.34 (d, *J* = 8.4 Hz, 2H), 7.16 (d, *J* = 8.4 Hz, 2H), 7.12 (d, *J* = 8.0 Hz, 2H), 7.03 (d, *J* = 8.4 Hz, 2H), 6.43 (s, 1H), 2.34 (s, 3H), 2.23 (s, 3H); ^{13}C NMR (400 MHz, $CDCl_3$) *δ* 163.0, 162.3, 156.8, 146.2, 134.3, 131.5, 129.7, 127.9, 127.8, 127.5, 114.9, 102.7, 21.7, 20.2; HRMS (ESI) Calcd for $C_{19}H_{15}ClO_5Na$ (M+Na), 413.0226; Found, 413.0219.

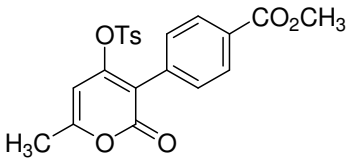


3-(2-Methoxyphenyl)-6-methyl-2-oxo-2H-pyran-4-yl 4-methylbenzenesulfonate **4e**. Yellow solid (66% yield), mp: 134.9-136.2 °C. ^{1}H NMR (400 MHz, $CDCl_3$) *δ* 7.37 (d, *J* = 8.0 Hz, 2H), 7.27 (d, J = 12.0 Hz, 1H), 7.13 (d, *J* = 8.0 Hz, 2H), 6.84 (d, *J* = 8.0 Hz, 2H), 6.77 (d, *J* = 8.0 Hz, 2H), 6.44 (s, 1H), 3.65 (s, 3H), 2.42 (s, 3H), 2.34 (s, 3H); ^{13}C NMR (400 MHz, $CDCl_3$) *δ* 162.8, 161.8, 157.1, 157.0, 145.5, 132.0, 131.3, 130.3, 130.0, 129.7, 128.4, 127.9, 120.1, 118.3, 113.5, 110.8, 101.8, 55.4, 21.7, 20.1; HRMS (ESI) Calcd for $C_{20}H_{18}NaO_6S$ (M+Na), 409.0722; Found, 409.0710.

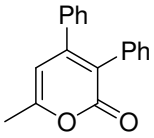


6-Methyl-2-oxo-3-*m*-tolyl-2H-pyran-4-yl 4-methylbenzenesulfonate **4f**. Yellow oil (85% yield). ^{1}H NMR (400 MHz, $CDCl_3$) *δ* 7.32 (d, *J* = 8.0 Hz, 2H), 7.12-7.04 (m, 4H), 6.91 (d, *J* = 4.0 Hz, 1H), 6.81 (s, 1H), 6.45 (s, 1H), 2.39 (s, 3H), 2.33 (s, 3H), 2.24 (s, 3H); ^{13}C NMR (400 MHz, $CDCl_3$) *δ* 163.3, 161.7, 156.3, 145.7, 137.3, 131.6, 130.4, 129.6, 128.9, 128.5, 127.9, 127.7, 127.2, 116.3, 102.4, 21.7, 21.3, 20.1; HRMS

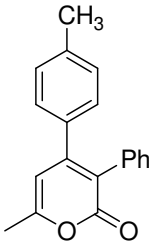
(ESI) Calcd for $C_{20}H_{19}O_5S$ (M+H), 371.0953; Found, 371.0958.



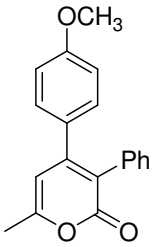
Methyl 4-(6-methyl-2-oxo-4-(tosyloxy)-2*H*-pyran-3-yl)benzoate **4g**. Yellow solid (95% yield), mp: 152.1-153.8 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.86 (d, J = 8.0 Hz, 2H), 7.33 (d, J = 8.0 Hz, 2H), 7.17 (d, J = 8.0 Hz, 2H), 7.06 (d, J = 8.0 Hz, 2H), 6.47 (s, 1H), 3.94 (s, 3H), 2.39 (s, 3H), 2.35 (s, 3H); ^{13}C NMR (400 MHz, $CDCl_3$) δ 166.6, 162.8, 162.7, 157.1, 146.2, 133.9, 131.3, 130.1, 129.8, 129.6, 128.8, 127.8, 115.0, 102.5, 52.2, 21.6, 20.2; HRMS (ESI) Calcd for $C_{21}H_{18}NaO_7S$ (M+Na), 437.0671; Found, 437.0678.



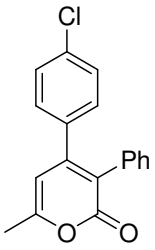
3,4-diphenyl-6-methyl-2-pyrone **5a**. Yellow solid (89% yield), mp: 130.1-130.7 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.24-7.20 (m, 6H), 7.14-7.12 (m, 2H), 7.09-7.07 (m, 2H), 6.17 (s, 1H), 2.33 (s, 3H); ^{13}C NMR (400 MHz, $CDCl_3$) δ 160.1, 152.6, 137.5, 133.8, 130.8, 128.7, 128.6, 128.2, 127.9, 127.5, 122.0, 107.1, 19.9; HRMS (ESI) Calcd for $C_{18}H_{14}NaO_2$ (M+Na) 285.0891; Found, 285.0895.



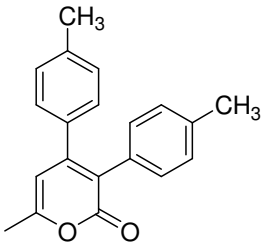
6-methyl-4-(4-methylphenyl)-3-phenyl-2-pyrone **5b**. Yellow solid (95% yield), mp: 109.2-110.7 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.22-7.15 (m, 3H), 7.15-7.13 (m, 2H), 7.02-6.96 (m, 4H), 6.16 (s, 1H), 2.31 (s, 3H), 2.28 (s, 3H); ^{13}C NMR (400 MHz, $CDCl_3$) δ 163.7, 159.9, 152.7, 138.8, 134.5, 134.2, 130.8, 128.9, 128.7, 128.0, 127.4, 121.6, 107.2, 21.3, 19.9; HRMS (ESI) Calcd for $C_{19}H_{16}O_2Na$ (M+Na^+) 299.1048; Found, 299.1044.



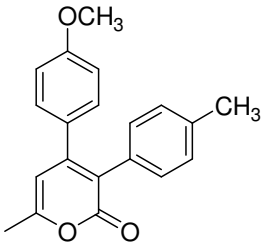
4-(4-methoxylphenyl)-6-methyl-3-phenyl-2-pyrone **5c**. Yellow solid (94% yield), mp: 109.3-110.0 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.24-7.22 (m, 3H), 7.16 (d, *J* = 8.8 Hz, 2H), 7.03 (d, *J* = 8.8 Hz, 2H), 6.72 (d, J = 8.8 Hz, 2H), 6.17 (s, 1H), 3.75 (s, 3H), 2.31 (s, 3H); ^{13}C NMR (400 MHz, $CDCl_3$) *δ* 163.7, 159.9, 152.2, 134.3, 130.9, 130.4, 129.5, 128.1, 127.5, 121.1, 113.7, 107.1, 55.2, 19.9; HRMS (ESI) Calcd for $C_{19}H_{16}O_3Na$ (M+Na) 315.0997; Found, 315.0997.



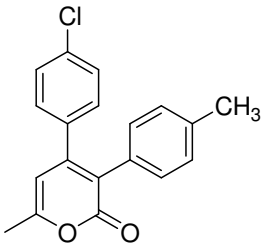
4-(4-chlorophenyl)-6-methyl-3-phenyl-2-pyrone **5d**. Yellow solid (73% yield), mp: 120.9-122.0 °C. ^{1}H NMR (400 MHz, $CDCl_3$) *δ* 7.26-7.11 (m, 8H), 7.03-7.01 (m, 1H), 6.13 (s, 1H), 2.33 (s, 3H); ^{13}C NMR (400 MHz, $CDCl_3$) *δ* 163.1， 160.4, 151.4, 135.9, 134.8, 133.5, 130.8, 130.1, 128.6, 128.2, 127.8, 122.2, 106.7, 19.9; HRMS (ESI) Calcd for $C_{18}H_{13}ClO_2Na$ (M+Na^+) 319.0502; Found, 319.0495.



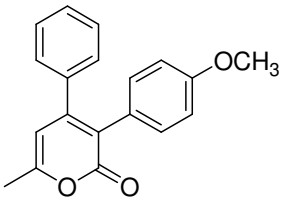
3,4-di(4-methylphenyl)-6-methyl-2-pyrone **5e**. Yellow oil (82% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.03-6.97 (m, 8H), 6.14 (s, 1H), 2.30 (s, 3H), 2.29 (s, 3H), 2.28 (s, 3H); ^{13}C NMR (400 MHz, $CDCl_3$) *δ* 163.8, 159.6, 152.3, 138.7, 137.2, 134.7, 131.1, 130.6, 128.9, 128.8, 128.6, 121.6, 107.2, 21.3, 19.9; HRMS (ESI) Calcd for $C_{20}H_{18}NO_2Na$ (M+Na^+) 313.1204; Found, 313.1204.



4-(4-methoxylphenyl)-6-methyl-3-(4-methylphenyl)-2-pyrone **5f**. Yellow solid (70% yield), mp: 135.7-137.1 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.05-7.29 (m，6H), 6.72 (d, J = 8.8 Hz, 2H), 6.15 (s, 1H), 3.76 (s, 3H), 2.30 (s, 3H), 2.29 (s, 3H); ^{13}C NMR (400 MHz, $CDCl_3$) δ 163.9, 159.8, 159.6, 151.8, 137.1, 131.2, 130.7, 130.3, 129.8, 128.8, 121.2, 113.7, 107.1, 55.2, 21.3, 19.9; HRMS (ESI) Calcd for $C_{20}H_{18}O_3Na$ ($M+Na^+$) 329.1154; Found, 329.1160.

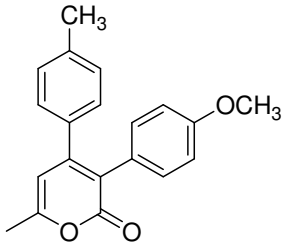


4-(4-chlorophenyl)-6-methyl-3-(4-methylphenyl)-2-pyrone **5g**. White solid (64% yield), mp: 131.6-132.6^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.20 (d, J = 8.4 Hz, 2H), 7.05-7.03 (m, 4H), 7.01(d, J = 8.0 Hz, 2H), 6.11 (s, 1H), 2.32 (s, 3H), 2.29 (s, 3H); ^{13}C NMR (400 MHz, $CDCl_3$) δ 163.5, 160.1, 150.9, 137.6, 136.1, 134.7, 130.6, 130.4, 130.1, 128.9, 128.6, 122.2, 106.7, 21.3, 19.9; HRMS (ESI) Calcd for $C_{19}H_{15}ClO_2Na$ ($M+Na^+$) 333.0658; Found, 333.0664.

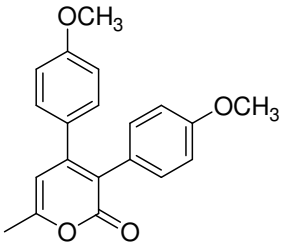


3-(4-methoxylphenyl)-6-methyl-4-phenyl-2-pyrone **5h**. Yellow oil (55% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.24-7.22 (m, 3H), 7.11-7.05 (m, 4H), 6.75 (d, J = 8.8 Hz, 2H), 6.15 (s, 1H), 3.75 (s, 3H), 2.32 (s, 3H); ^{13}C NMR (400 MHz, $CDCl_3$) δ 163.8, 159.6, 158.8, 152.1, 137.8, 132.0, 128.6, 128.5, 128.3, 125.9, 113.5, 107.1, 55.1, 19.8;

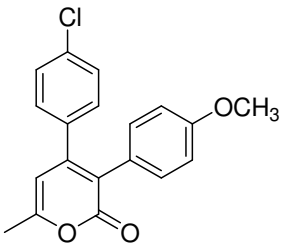
HRMS (ESI) Calcd for $C_{19}H_{17}O_3$ ($M+H^+$) 293.1178; Found, 293.1170.



3-(4-methoxylphenyl)-6-methyl-4-(4-methylphenyl)-2-pyrone **5i**. Yellow oil (67% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.08-6.98 (m, 6H), 6.76 (d, J = 8.4 Hz, 2H), 6.13 (s, 1H), 3.76 (s, 3H), 2.30 (s, 3H), 2.29 (s, 3H); ^{13}C NMR (400 MHz, $CDCl_3$) δ 163.9, 159.4, 158.8, 152.1, 138.6, 134.8, 132.0, 129.0, 128.6, 126.2, 121.2, 113.5, 107.2, 55.1, 21.2, 19.8; HRMS (ESI) Calcd for $C_{20}H_{19}O_3$ ($M+H^+$) 307.1334; Found, 307.1329.

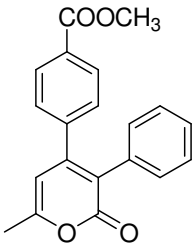


3,4-di(4-methoxylphenyl)-6-methyl-2-pyrone **5j**. Yellow oil (80% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.09 (d, J = 8.4 Hz, 2H), 7.05 (d, J = 8.8 Hz, 2H), 6.78 (d, J = 8.8 Hz, 2H), 6.75 (d, J = 8.8 Hz, 2H) 6.30 (s, 1H), 3.77 (s, 6H), 2.30 (s, 3H); ^{13}C NMR (400 MHz, $CDCl_3$) δ 163.7, 161.8, 158.7, 151.70, 132.0, 130.3, 128.2, 126.4, 120.8, 114.6, 113.7, 107.1, 103.2, 55.5, 55.2, 19.9. HRMS (ESI) Calcd for $C_{20}H_{18}O_4Na$ ($M+Na^+$), 345.1103; Found, 345.1088.

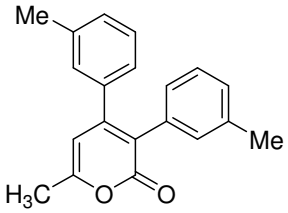


4-(4-chlorophenyl)-3-(4-methoxylphenyl)-6-methyl-2-pyrone **5k**. Yellow oil (80% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.21 (d, J = 8.8 Hz, 2H), 7.06-7.03 (m, 4H), 6.78 (d, J = 8.8 Hz, 2H), 6.10 (s, 1H), 3.76 (s, 3H), 2.31 (s, 3H); ^{13}C NMR (400 MHz,

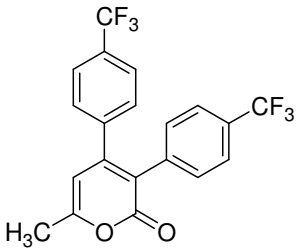
$CDCl_3$) δ 163.6, 159.9, 159.0, 150.8, 136.2, 134.6, 132.0, 130.1, 128.6, 125.6, 121.8, 113.7, 106.7, 55.2, 19.9; HRMS (ESI) Calcd for $C_{19}H_{15}ClO_3Na$ ($M+Na^+$) 349.0607; Found, 349.0601.



Methyl 4-(6-methyl-2-oxo-3-phenyl-2H-pyran-4-yl)benzoate **5l**. Yellow solid (66% yield), mp: 195.0-196.1 ^oC. ^1H NMR (400 MHz, $CDCl_3$) δ 7.90 (d, J = 8.0 Hz, 2H), 7.22 (t, J = 4.0 Hz, 2H), 7.17 (d, J = 8.0 Hz, 2H), 7.13 (d, J = 4.0 Hz, 2H), 6.17 (s, 1H), 3.89 (s, 3H), 2.35 (s, 3H); ^{13}C NMR (400 MHz, $CDCl_3$) δ 166.4, 163.2, 160.5, 151.5, 142.1, 133.3, 130.7, 130.1, 129.5, 128.7, 128.1, 127.8, 122.6, 106.5, 52.2, 19.9; HRMS (ESI) Calcd for $C_{20}H_{16}NaO_4$ ($M+Na^+$) 343.0946; Found, 343.0931.

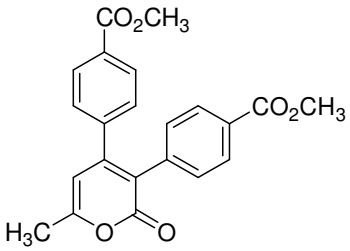


6-Methyl-3,4-di*m*-tolyl-2*H*-pyran-2-one **5m**. Yellow oil (71% yield). ^1H NMR (400 MHz, $CDCl_3$) δ 7.07-7.00 (m, 5H), 6.93 (s, 1H), 6.88-6.82 (m, 2H), 6.16 (s, 1H), 2.31 (s, 3H), 2.23 (s, 3H); ^{13}C NMR (400 MHz, $CDCl_3$) δ 163.7, 159.8, 152.7, 137.8, 137.4, 137.3, 133.8, 131.3, 129.3, 129.2, 128.3, 128.0, 127.9, 127.8, 125.8, 122.0, 107.1, 21.4, 21.3, 19.9; HRMS (ESI) Calcd for $C_{20}H_{18}NaO_2$ ($M+Na^+$) 313.1204; Found, 313.1215.

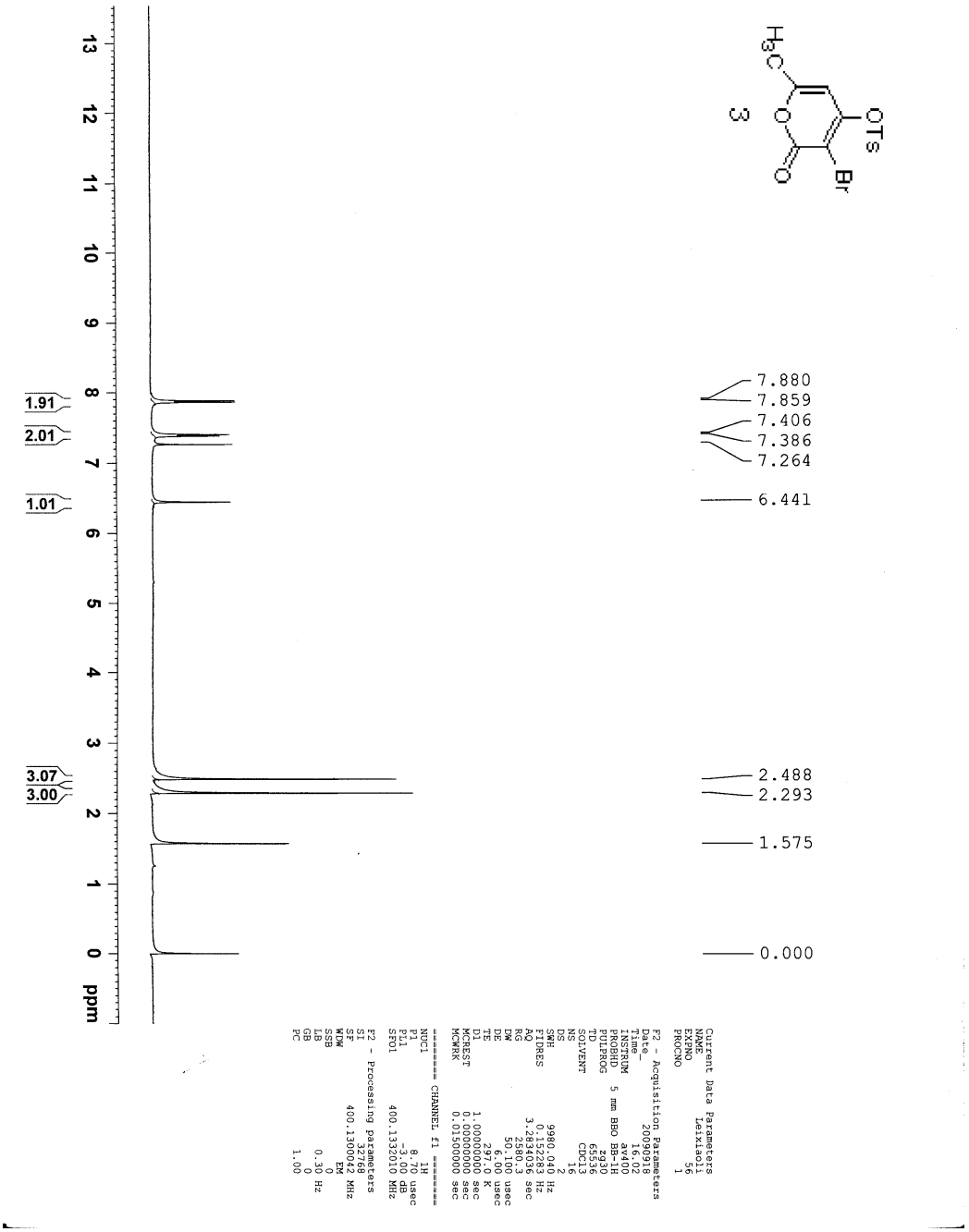


6-Methyl-3,4-bis(4-(trifluoromethyl)phenyl)-2*H*-pyran-2-one **5n**. White crystal (60%

yield), mp: 125.8-126.8 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.54-7.49 (m, 4H), 7.25 (d, J = 8.0 Hz, 2H), 7.22 (d, J = 8.0 Hz, 2H), 6.18 (s, 1H), 2.37 (s, 3H); ^{13}C NMR (400 MHz, $CDCl_3$) δ 162.6, 161.6, 152.0, 140.6, 137.0, 131.5, 130.9, 129.7, 128.9, 125.6 (dd), 125.2 (dd), 122.5, 122.2, 121.2, 106.6, 20.0; HRMS (ESI) Calcd for $C_{20}H_{12}F_6NaO_2$ ($M+Na^+$) 421.0639; Found, 421.0651.



6-Methyl-2-pyrone **5o**. Yellow solid (60% yield), mp: 54.9-55.9 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.90-7.87 (m, 4H), 7.22 (d, J = 8.0 Hz, 2H), 7.16 (d, J = 8.0 Hz, 2H), 6.20 (s, 1H), 3.89 (s, 3H), 3.88 (s, 3H), 2.36 (s, 3H); ^{13}C NMR (400 MHz, $CDCl_3$) δ 166.6, 166.2, 162.6, 161.3, 152.4, 141.5, 138.3, 130.9, 130.4, 129.6, 129.3, 129.2, 128.6, 121.5, 106.6, 52.2, 52.1, 20.0; HRMS (ESI) Calcd for $C_{22}H_{18}NaO_6$ ($M+Na^+$) 401.1001; Found, 401.1012.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Br
O
O
H3C
3
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7.859
7.406
7.386
7.264
6.441
2.488
2.293
1.575
0.000
1.91
2.01
1.01
3.07
3.00
ppm
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NAME Lei Xiaoli
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
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Time 11.12.12
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PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 65536
SOLVENT CDCl3
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DS 2
SWH 9980.040 Hz
FIDRES 0.152283 Hz
AQ 3.2834036 sec
RG 256.03
DW 50.100 usec
DE 6.00 usec
TE 297.0 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
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PL1 -3.00 dB
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F2 - Processing parameters
SI 32768
SF 400.1300022 MHz
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LB 0.30 Hz
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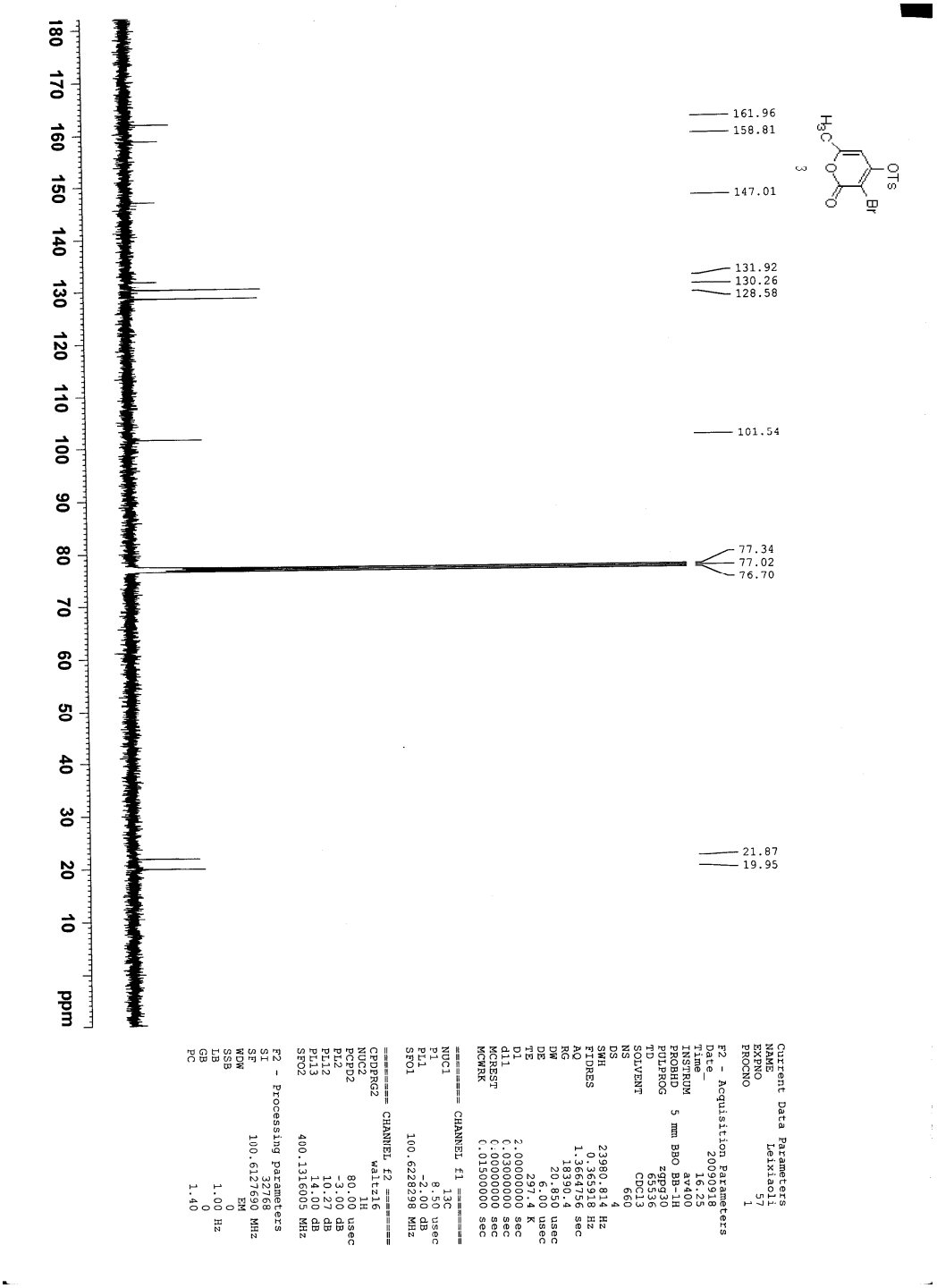
PC 1.00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158.81
147.01
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130.26
128.58
101.54
77.34
77.02
76.70
21.87
19.95
OTs
Br
O
O
O
3
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EXPNO 57
PROCNO 1
F2 - Acquisition Parameters
Date_ 20090918
Time 16.25
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PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 660
DS 4
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 18390.4
DW 20.850 usec
DE 6.00 usec
TE 297.4 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
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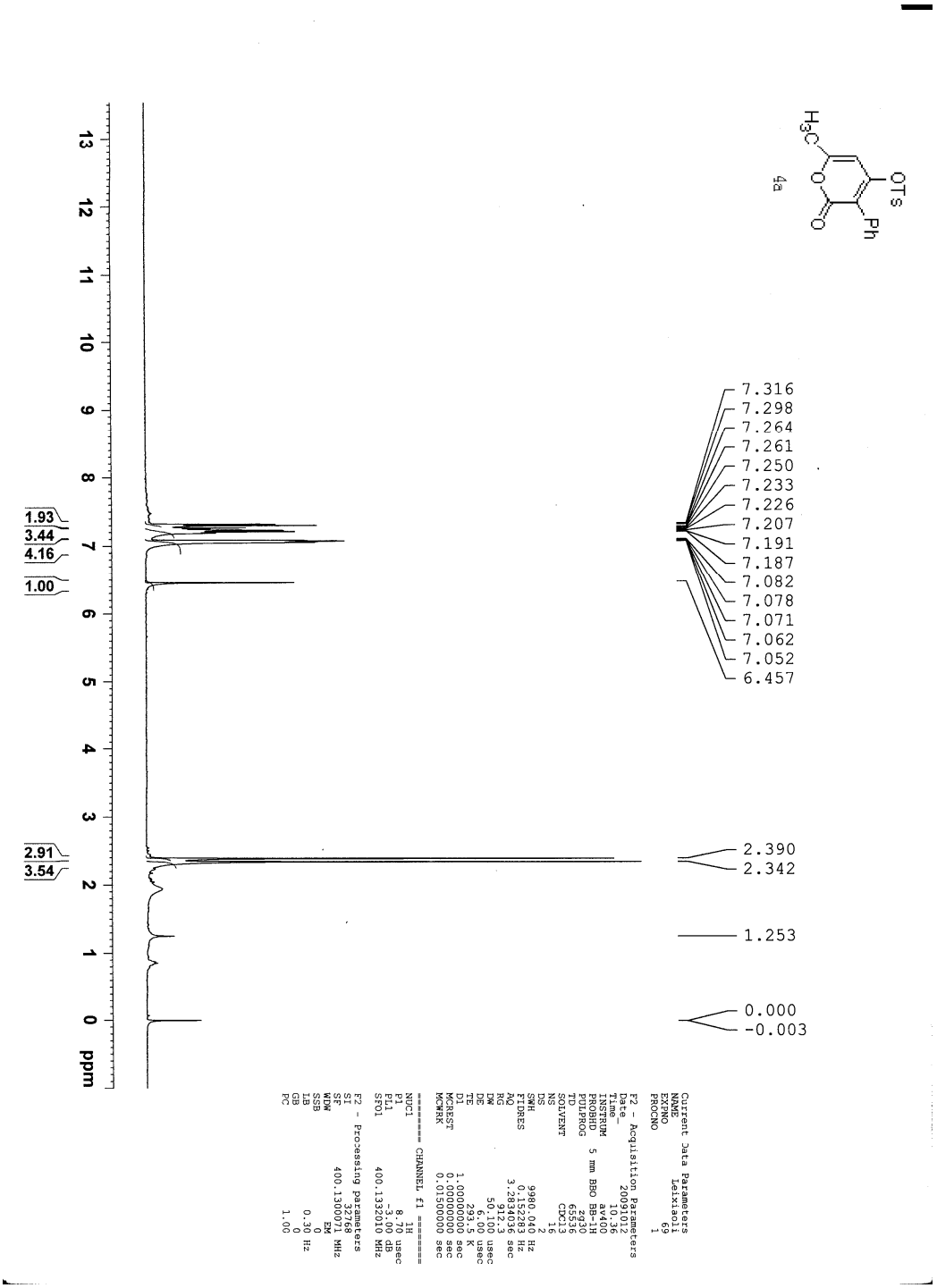
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40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7.264
7.261
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7.207
7.191
7.187
7.082
7.078
7.071
7.062
7.052
6.457
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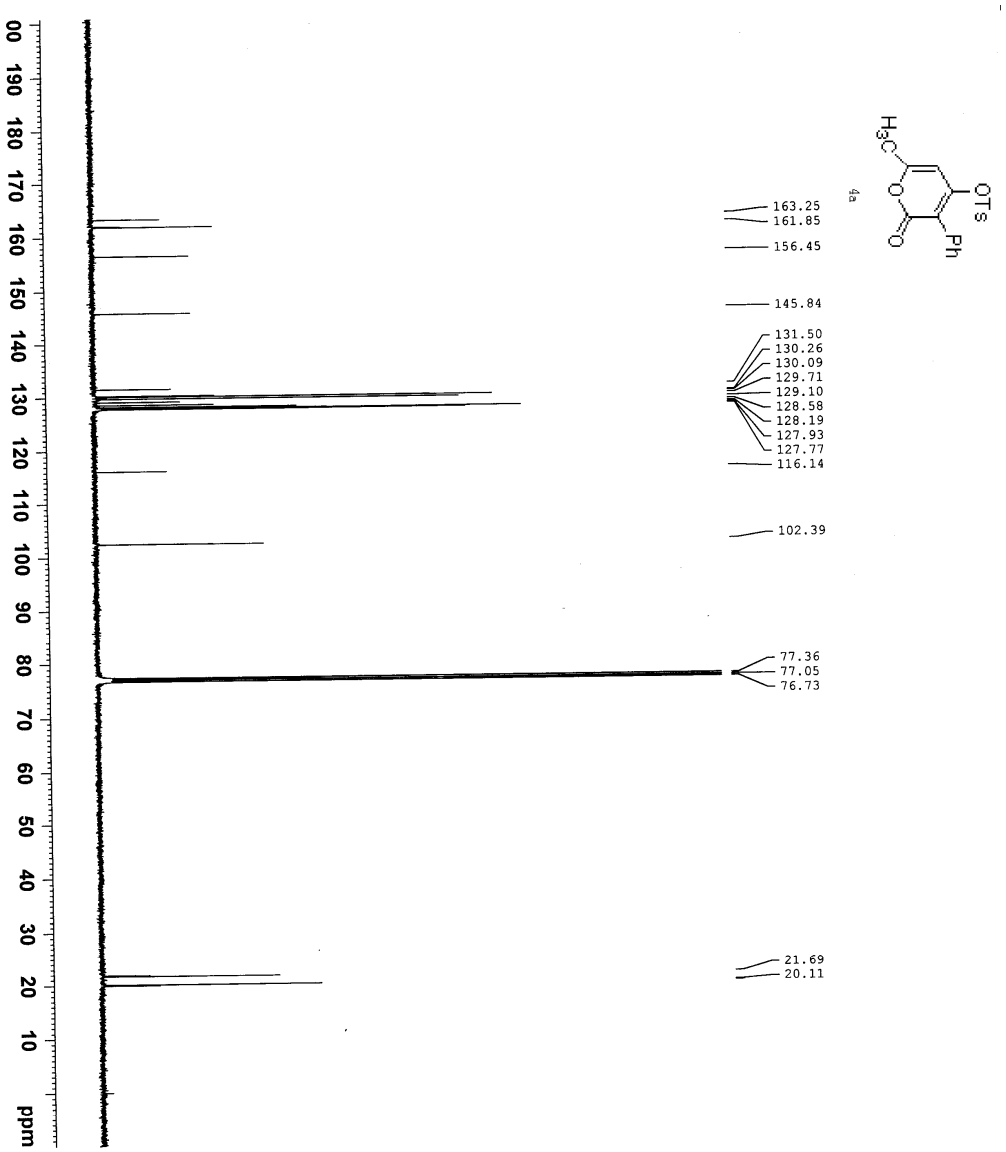
3.44
4.16
1.00
2.91
3.54
ppm

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EXPNO                        74
PROCNO                        1

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Time_                    9.14
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PULPROG             zgpg30
TD                       65536
SOLVENT                CDCl3
NS                        2048
DS                           4
SWH                23980.814 Hz
FIDRES                0.365918 Hz
AQ                    1.3664756 sec
RG                      1032.13
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
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SF            100.6127691 MHz
WDW                       EM
SSB                        0
LB                      1.00 Hz
GB                         0
PC                      1.40
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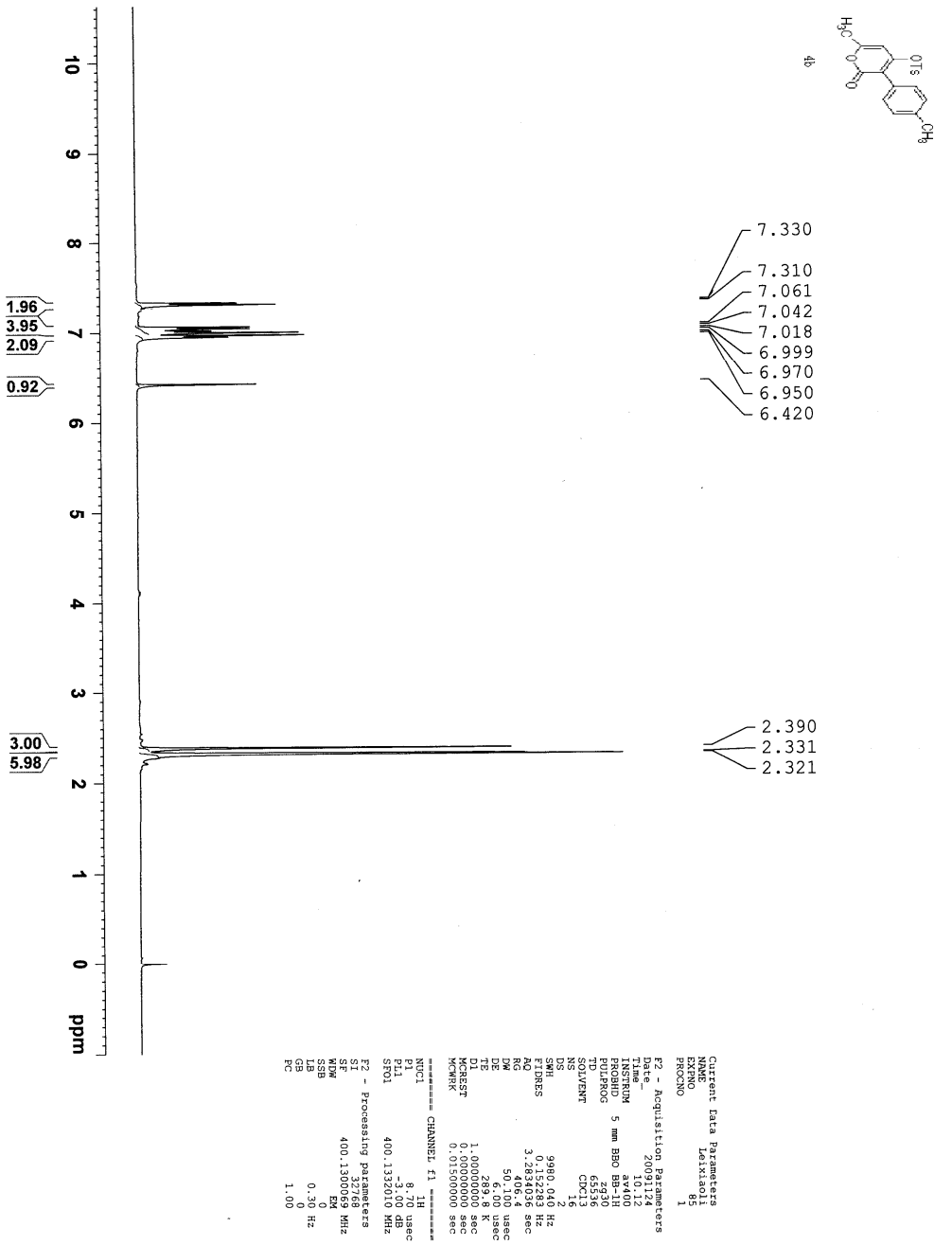
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7.310
7.061
7.042
7.018
6.999
6.970
6.950
6.420
2.390
2.331
2.321
1.96
3.95
2.09
0.92
3.00
5.98
ppm
Current Data Parameters
NAME leixiaoli
EXPNO 85
PROCNO 1
F2 - Acquisition Parameters
Date_ 20091124
Time_ 10.12
INSTRUM av400
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 9980.040 Hz
FIDRES 0.152283 Hz
AQ 3.2834036 sec
RG 406.4
DW 50.100 usec
DE 6.00 usec
TE 289.8 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
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P1 8.70 usec
PL1 -3.00 dB
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F2 - Processing parameters
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SF 400.1300069 MHz
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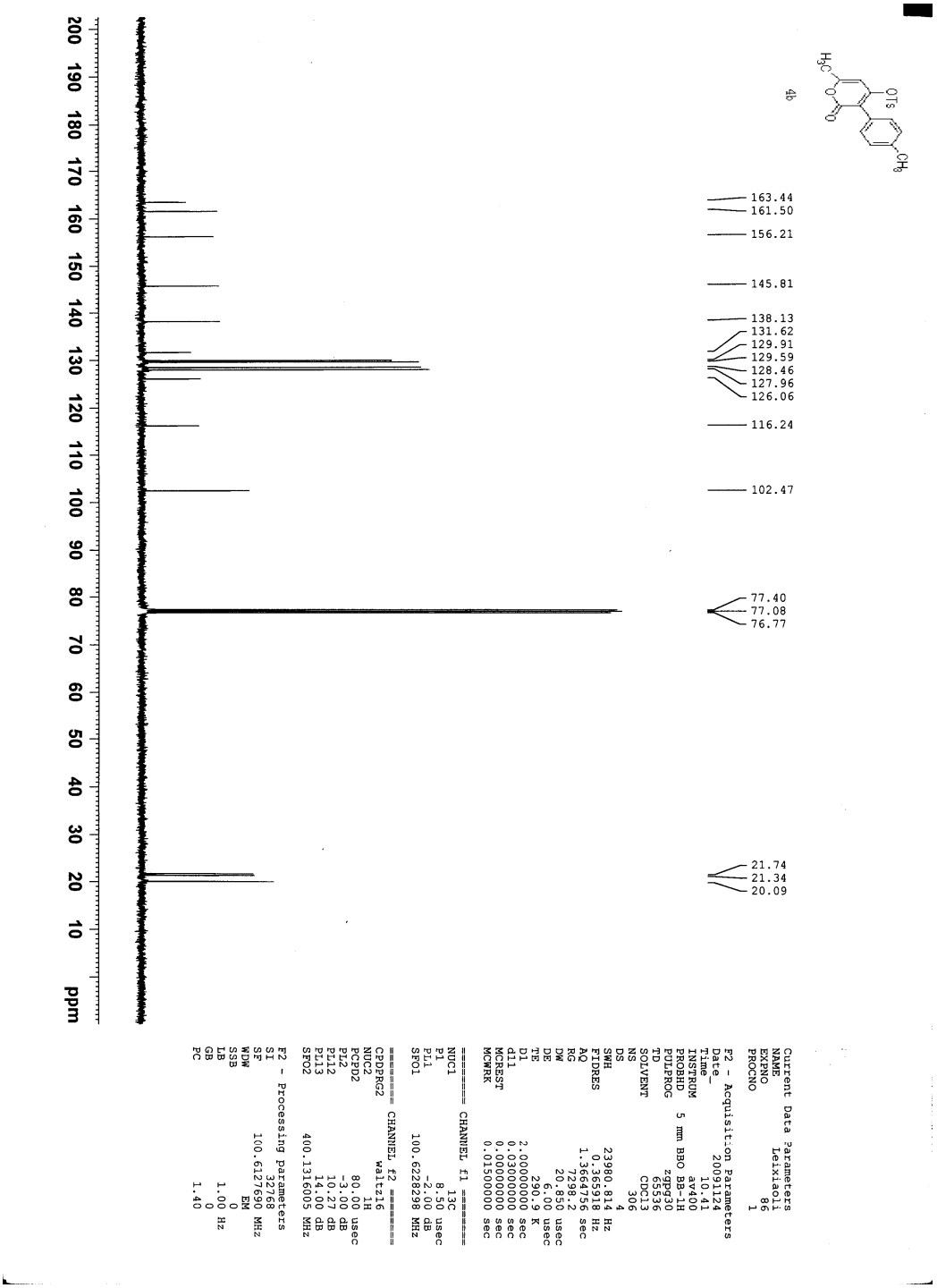
PC 1.00


4b
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161.50
156.21
145.81
138.13
131.62
129.91
129.59
128.46
127.96
126.06
116.24
102.47
77.40
77.08
76.77
21.74
21.34
20.09
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm
Current Data Parameters
NAME Leixiaoli
EXPNO 86
PROCNO 1
F2 - Acquisition Parameters
Date_ 20091124
Time_ 10.41
INSTRUM av400
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 306
DS 4
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 7298.2
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DE 6.00 usec
TE 290.9 K
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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
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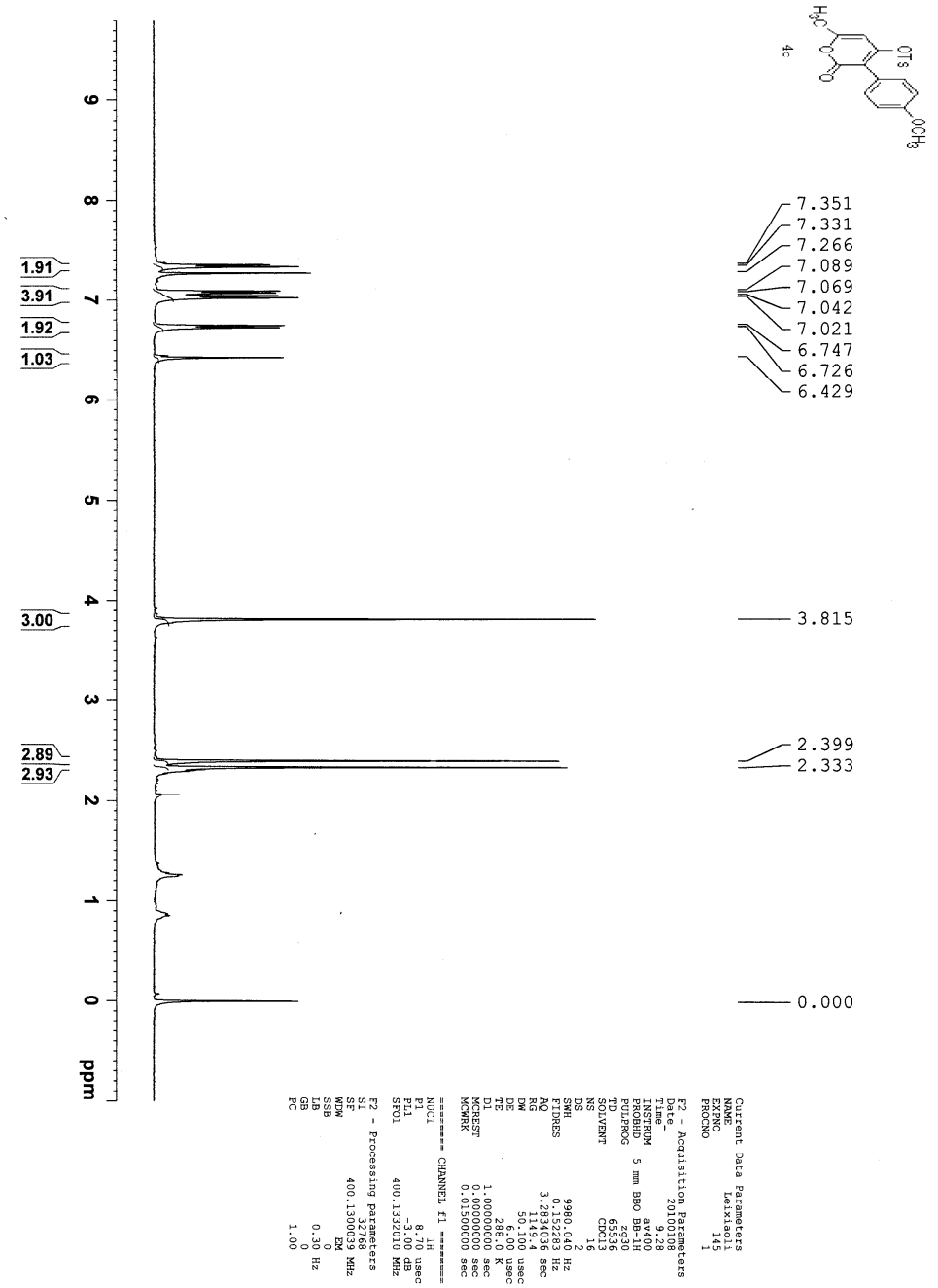
SSB 0
LB 1.00 Hz
GB 0
PC 1.40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7.266
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7.069
7.042
7.021
6.747
6.726
6.429
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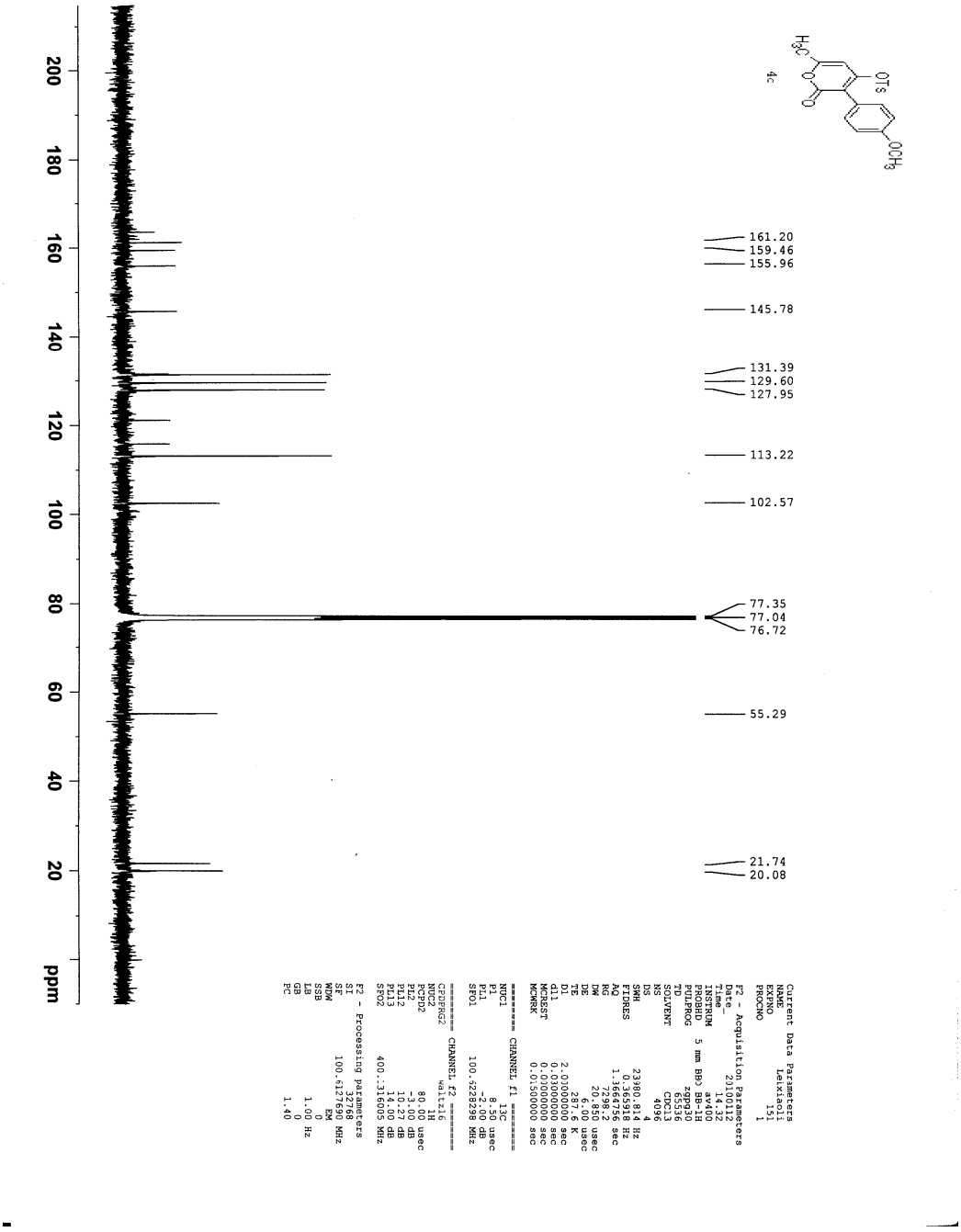
2.333
0.000
1.91
3.91
1.92
1.03
3.00
2.89
2.93
ppm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155.96
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127.95
113.22
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77.35
77.04
76.72
55.29
21.74
20.08
ppm
Current Data Parameters
NAME Leixiaoli
EXPNO 151
PROCNO 1
F2 - Acquisition Parameters
Date_ 20100112
Time 14.32
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 4096
DS 4
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 228.2
DW 20.850 usec
DE 6.00 usec
TE 287.6 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 100.6228398 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 1.00 dB
PL12 13.00 dB
PL13 14.00 dB
SFO2 400.1316005 MHz
F2 - Processing parameters
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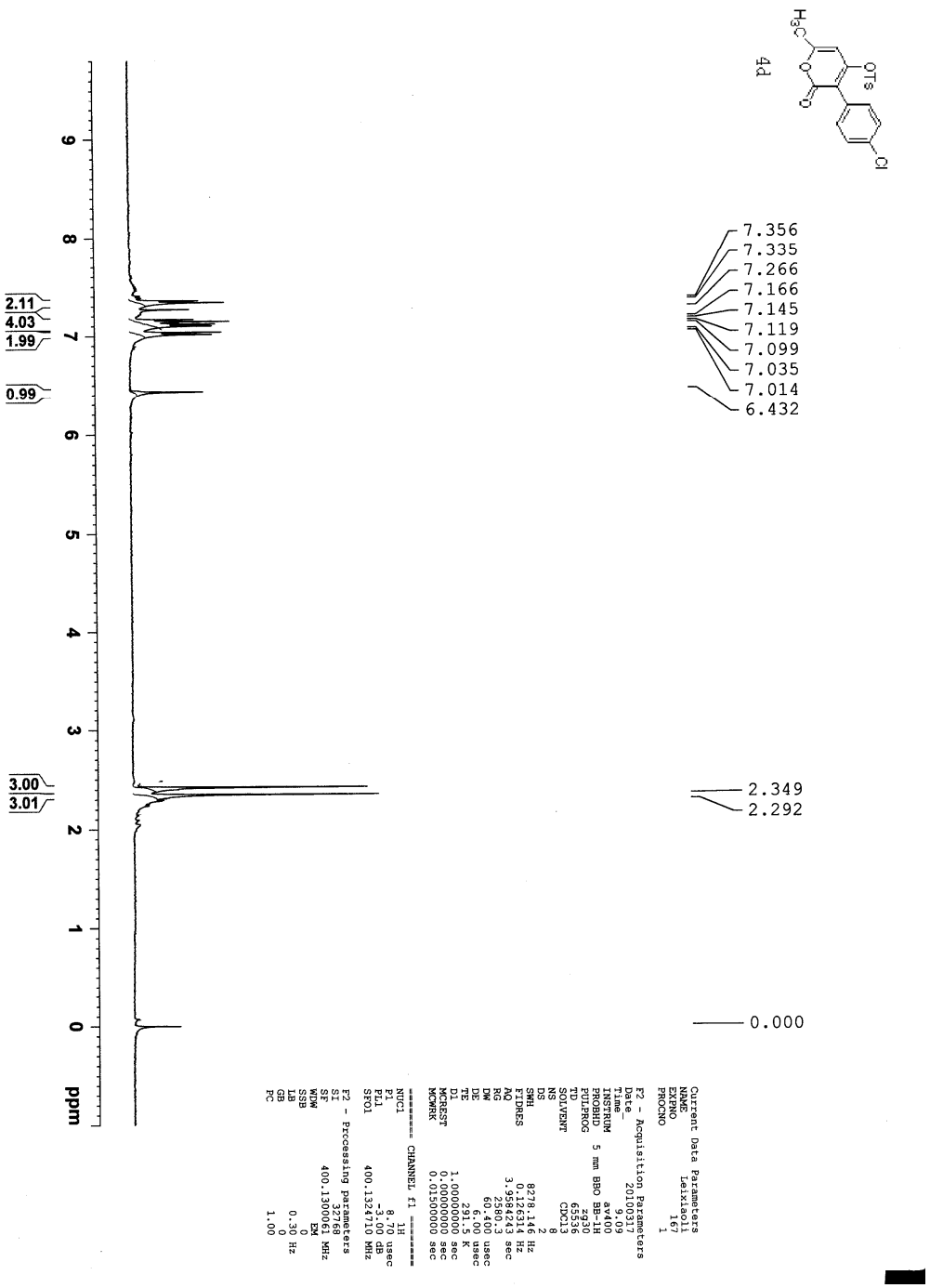
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40


4d
OTs
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7.166
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7.119
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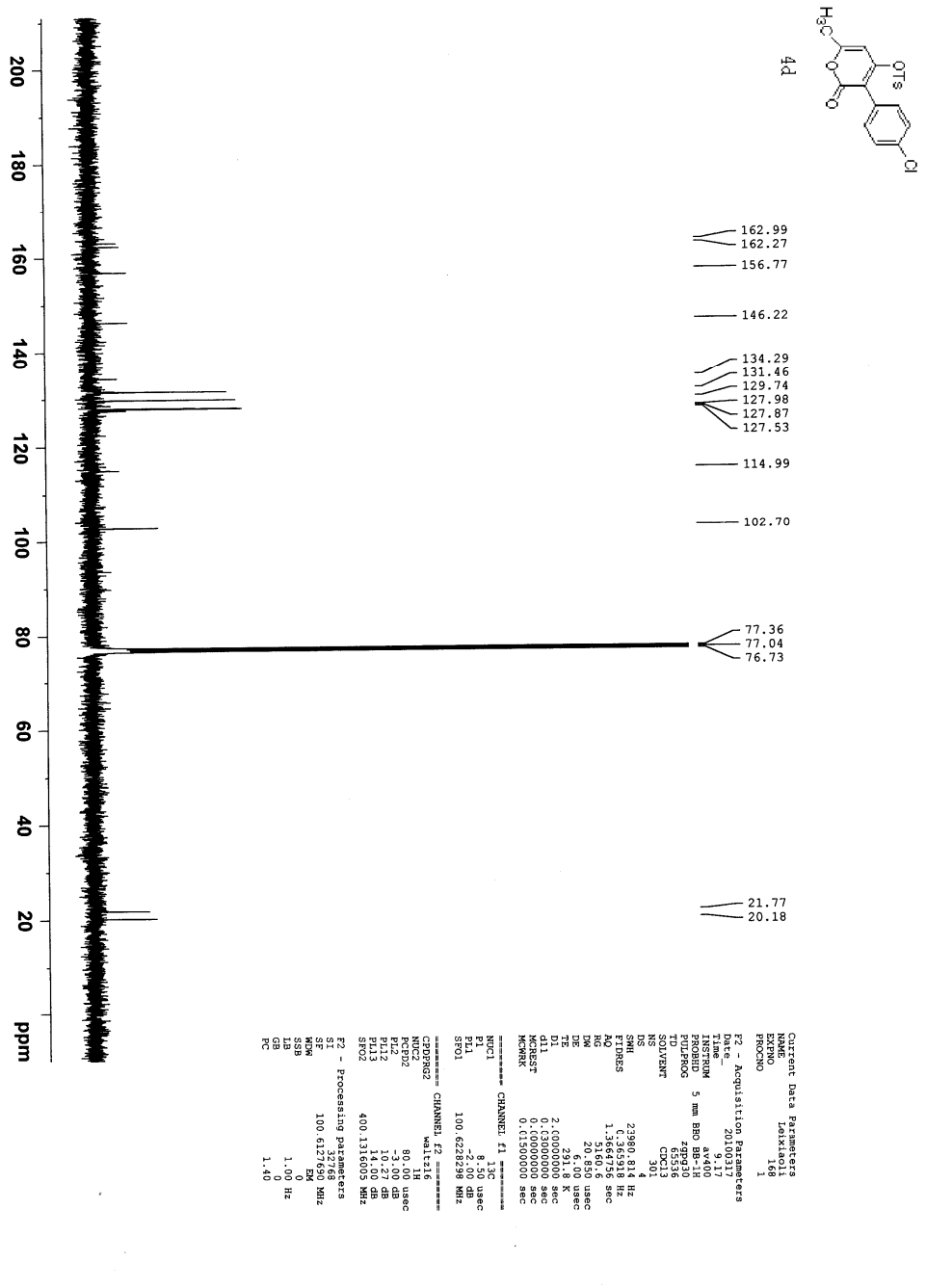
ppm


4d
OTs
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134.29
131.46
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127.98
127.87
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114.99
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76.73
21.77
20.18
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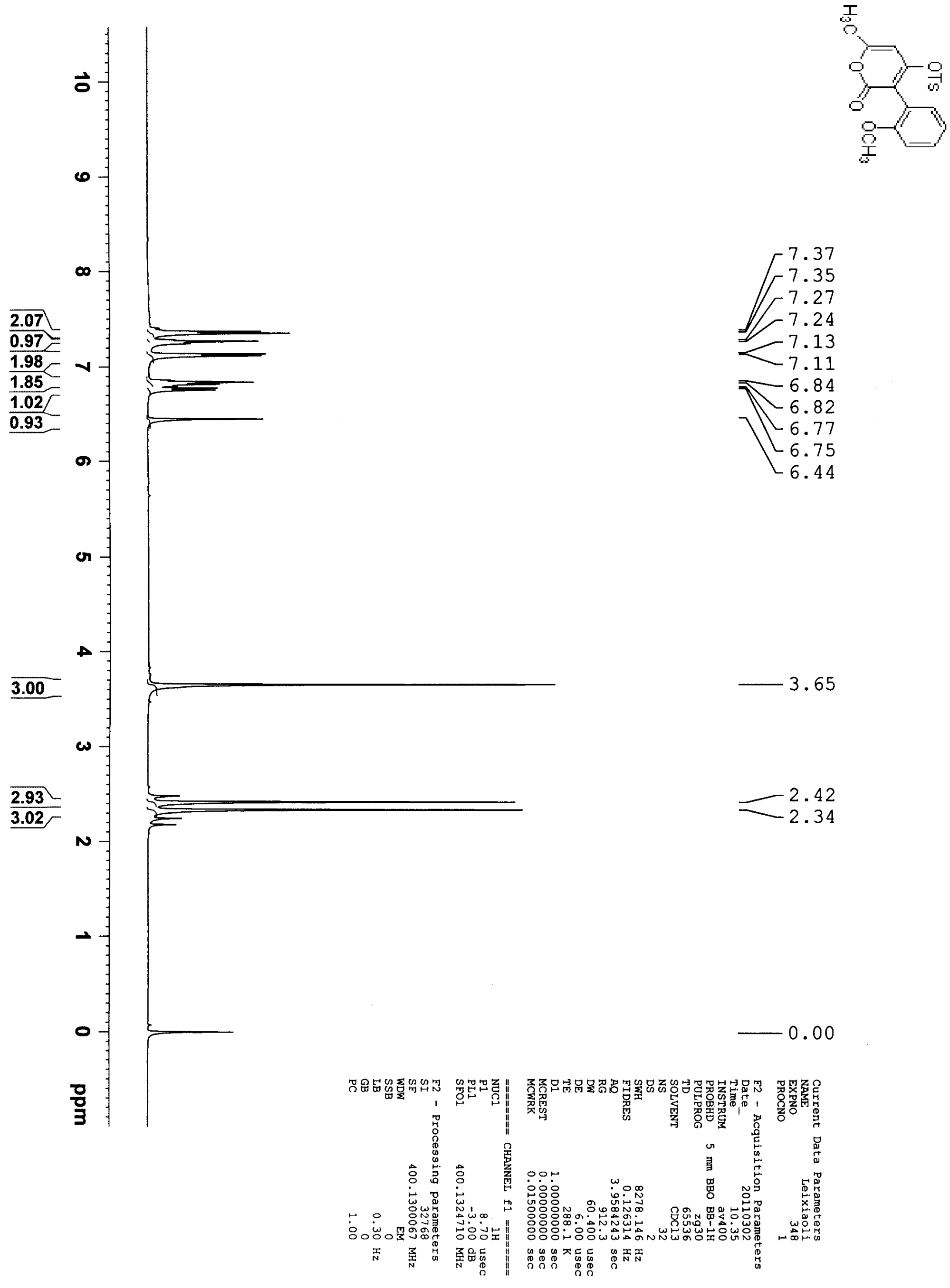
140
120
100
80
60
40
20
ppm


OTs
OCH3
H3C
O
O
7.37
7.35
7.27
7.24
7.13
7.11
6.84
6.82
6.77
6.75
6.44
3.65
2.42
2.34
0.00
2.07
0.97
1.98
1.85
1.02
0.93
3.00
2.93
3.02
ppm
Current Data Parameters
NAME Leixiaoli
EXPNO 348
PROCNO 1
F2 - Acquisition Parameters
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Time 10.35
INSTRUM av400
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PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 32
DS 2
SWH 8278.146 Hz
FIDRES 0.126314 Hz
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RG 912.3
DW 60.400 usec
DE 6.00 usec
TE 288.1 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
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P1 8.70 usec
PL1 -3.00 dB
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F2 - Processing parameters
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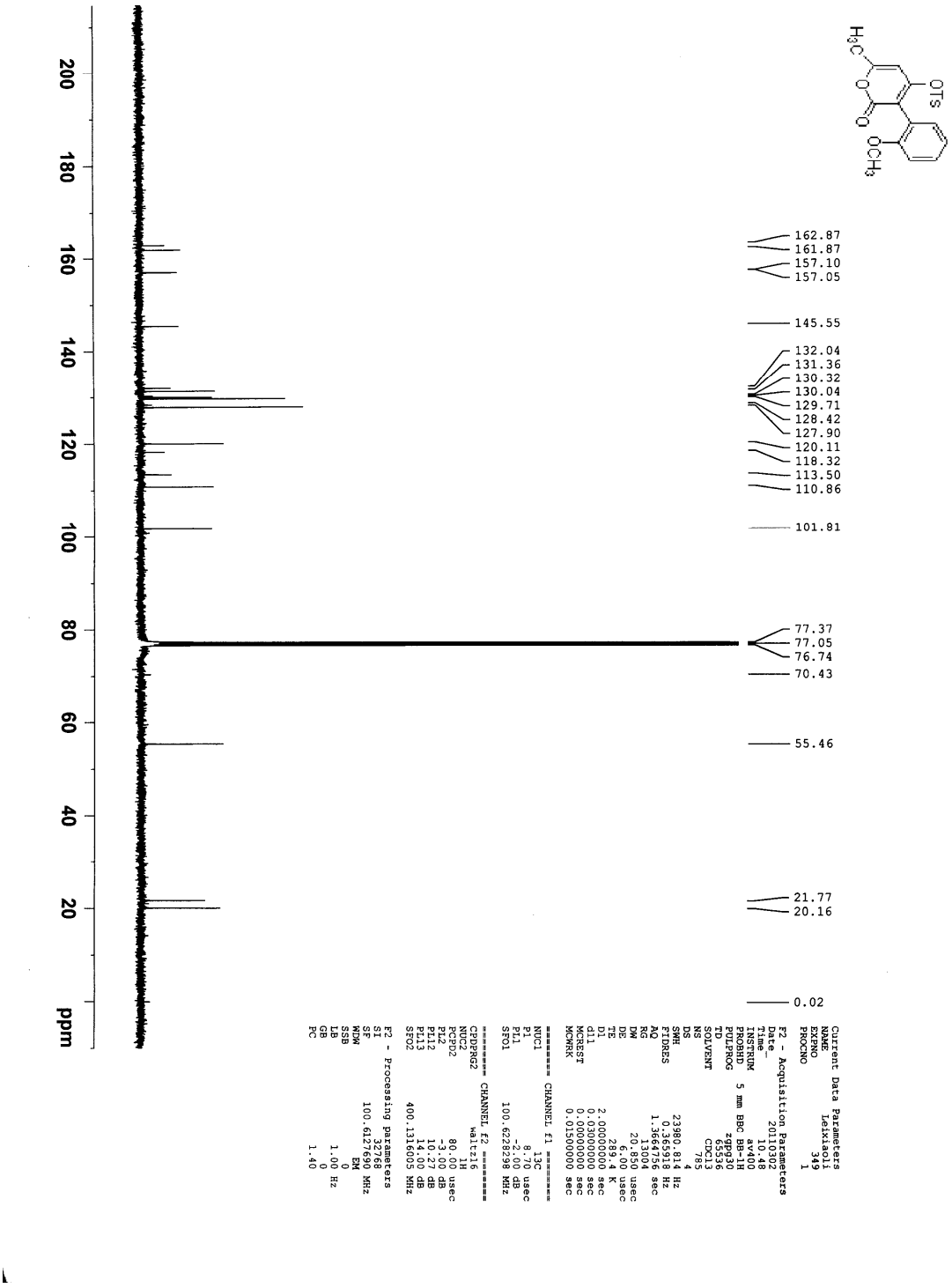
GB 0
PC 1.00


OTs
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157.10
157.05
145.55
132.04
131.36
130.32
130.04
129.71
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120.11
118.32
113.50
110.86
101.81
77.37
77.05
76.74
70.43
55.46
21.77
20.16
0.02
ppm
Current Data Parameters
NAME Leikiaoli
EXPNO 34
PROCNO 1
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Time 10.48
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PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 785
DS 4
SWH 23980.814 Hz
FIDRES 0.365718 Hz
AQ 1.3664768 sec
RG 113004
DW 20.850 usec
DE 6.00 usec
TE 289.4 K
D1 2.00000000 sec
d11 0.03000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 8.70 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 11.00 dB
SFO2 400.1316005 MHz
F2 - Processing parameters
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SF 100.6127690 MHz
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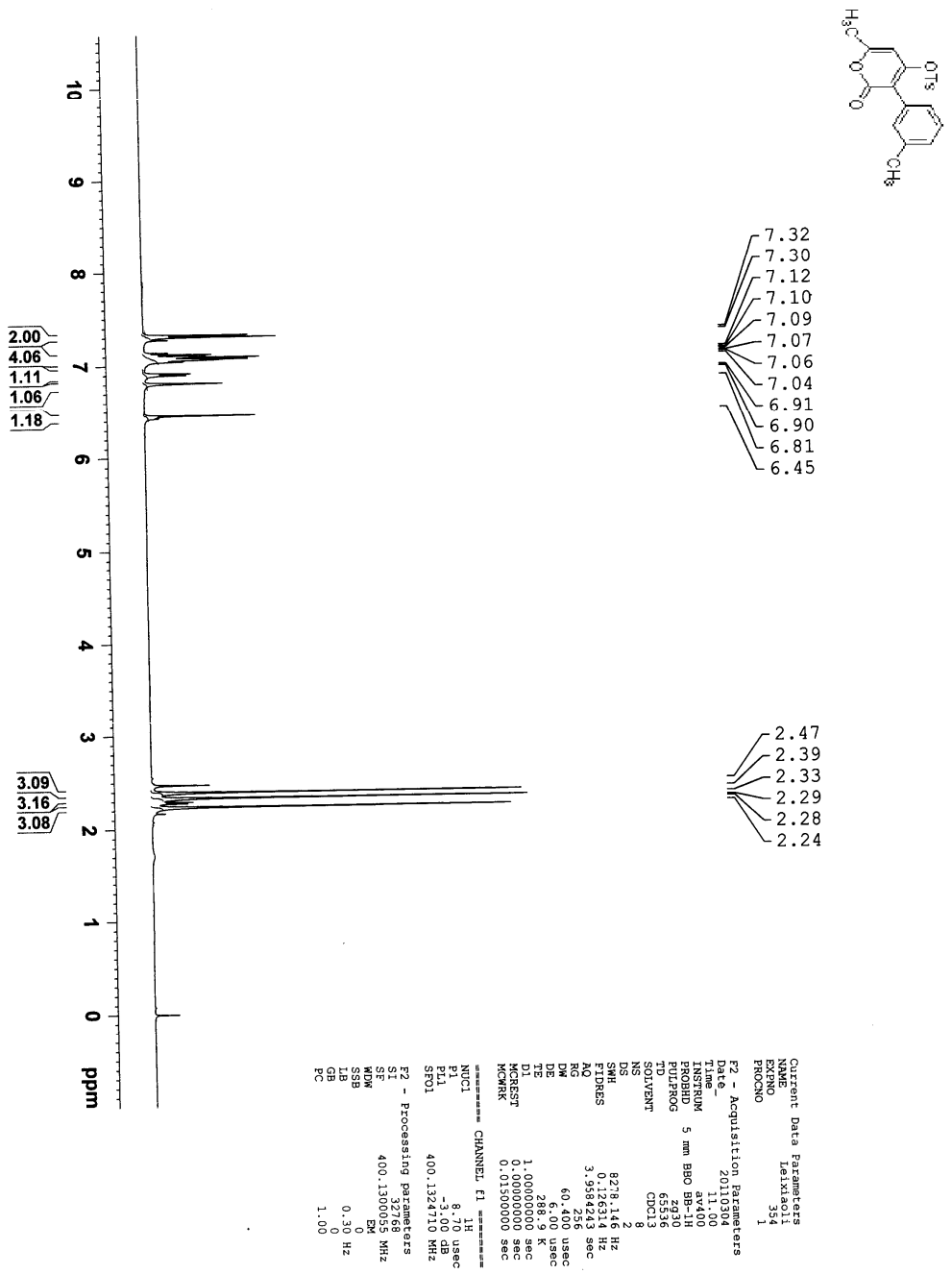
SSB 0
LB 1.00 Hz
GB 0
PC 1.40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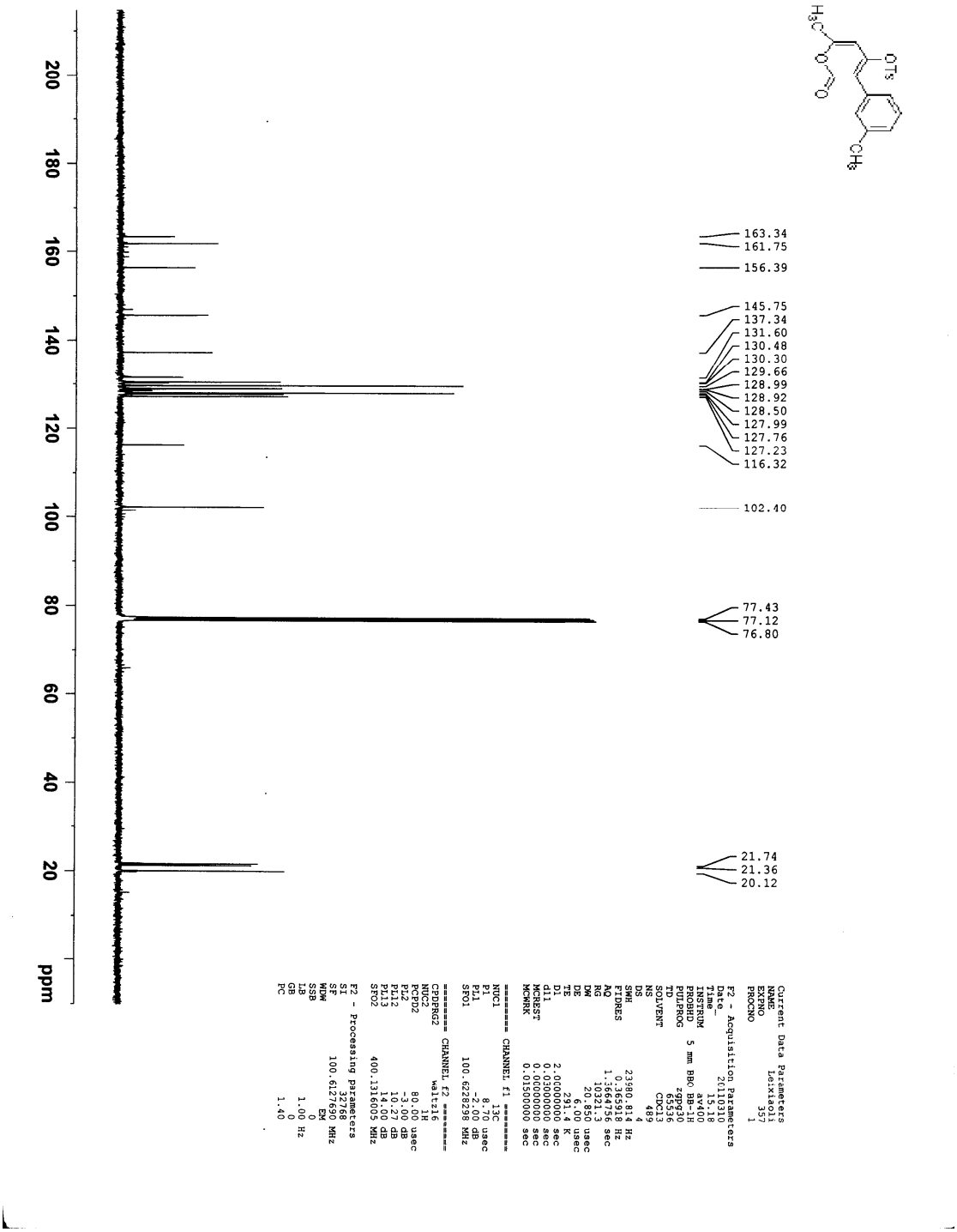
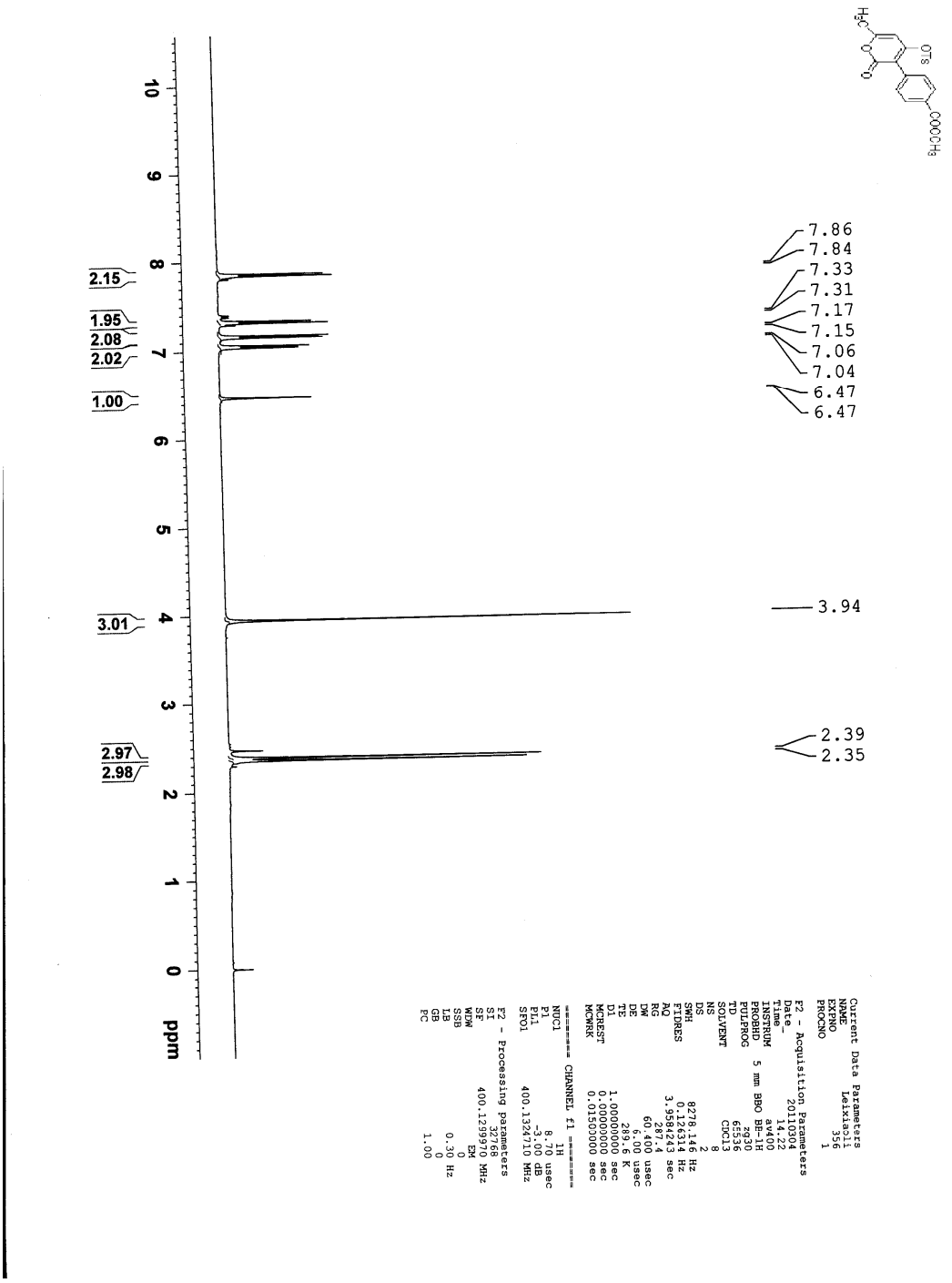
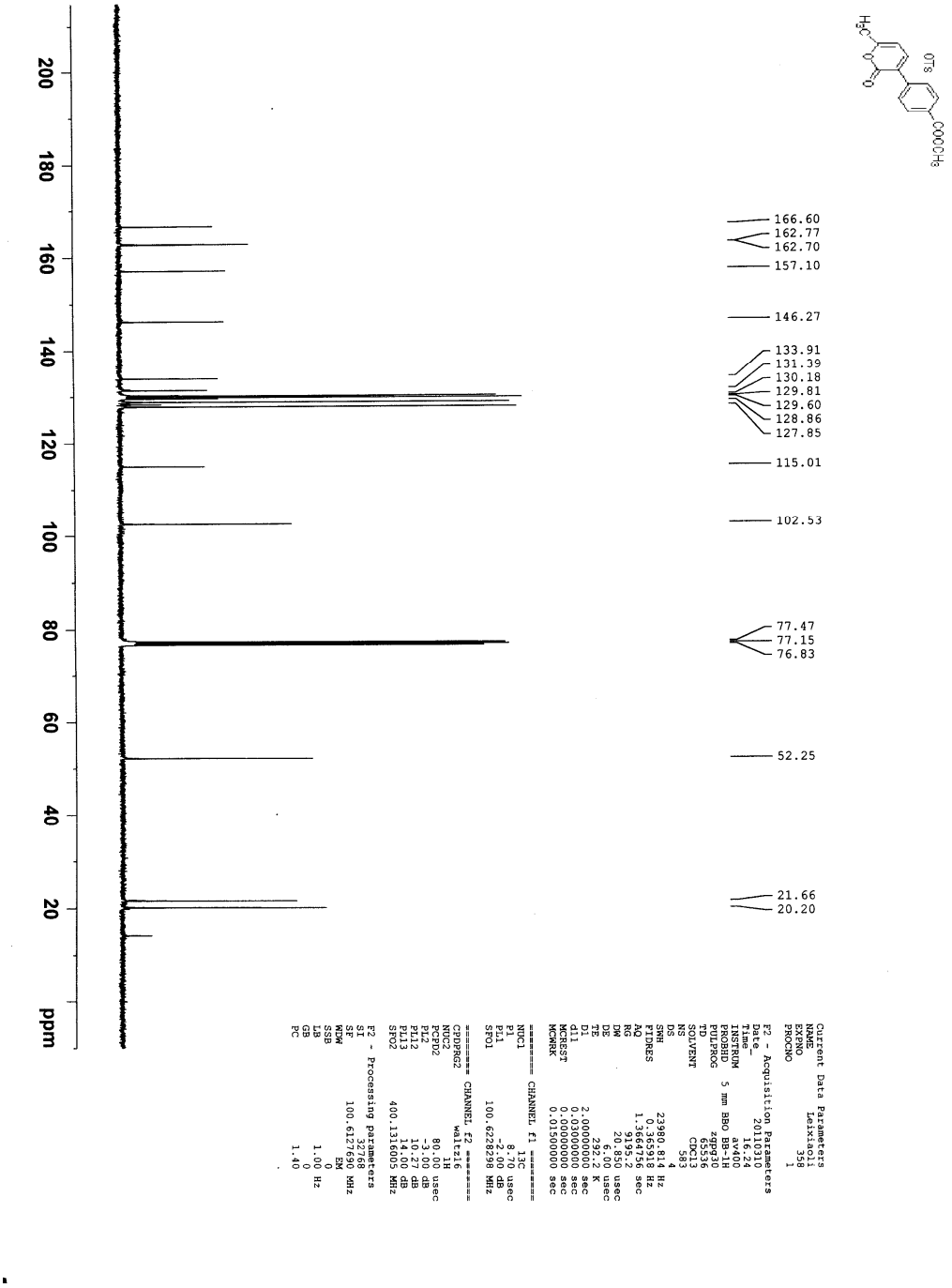
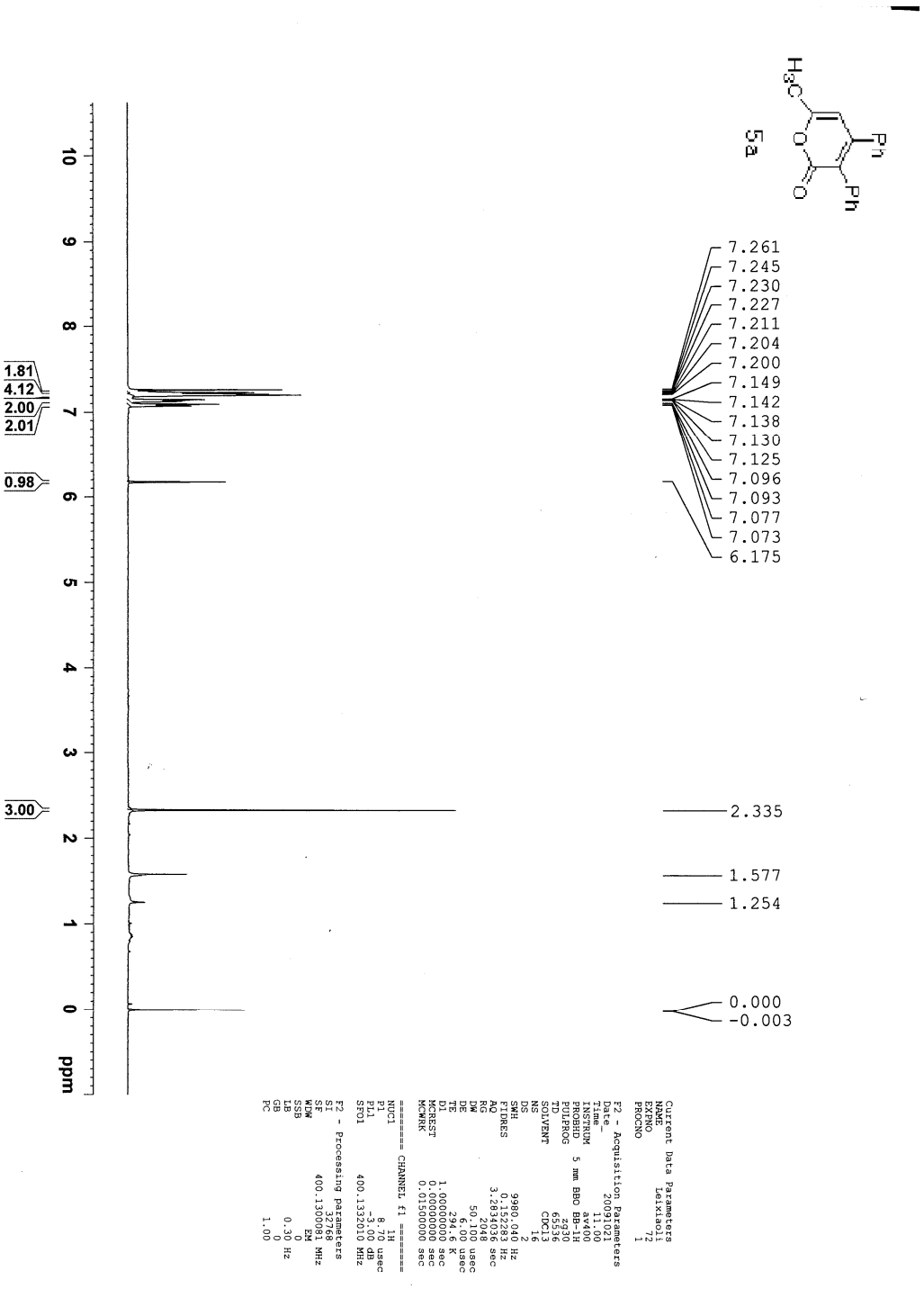
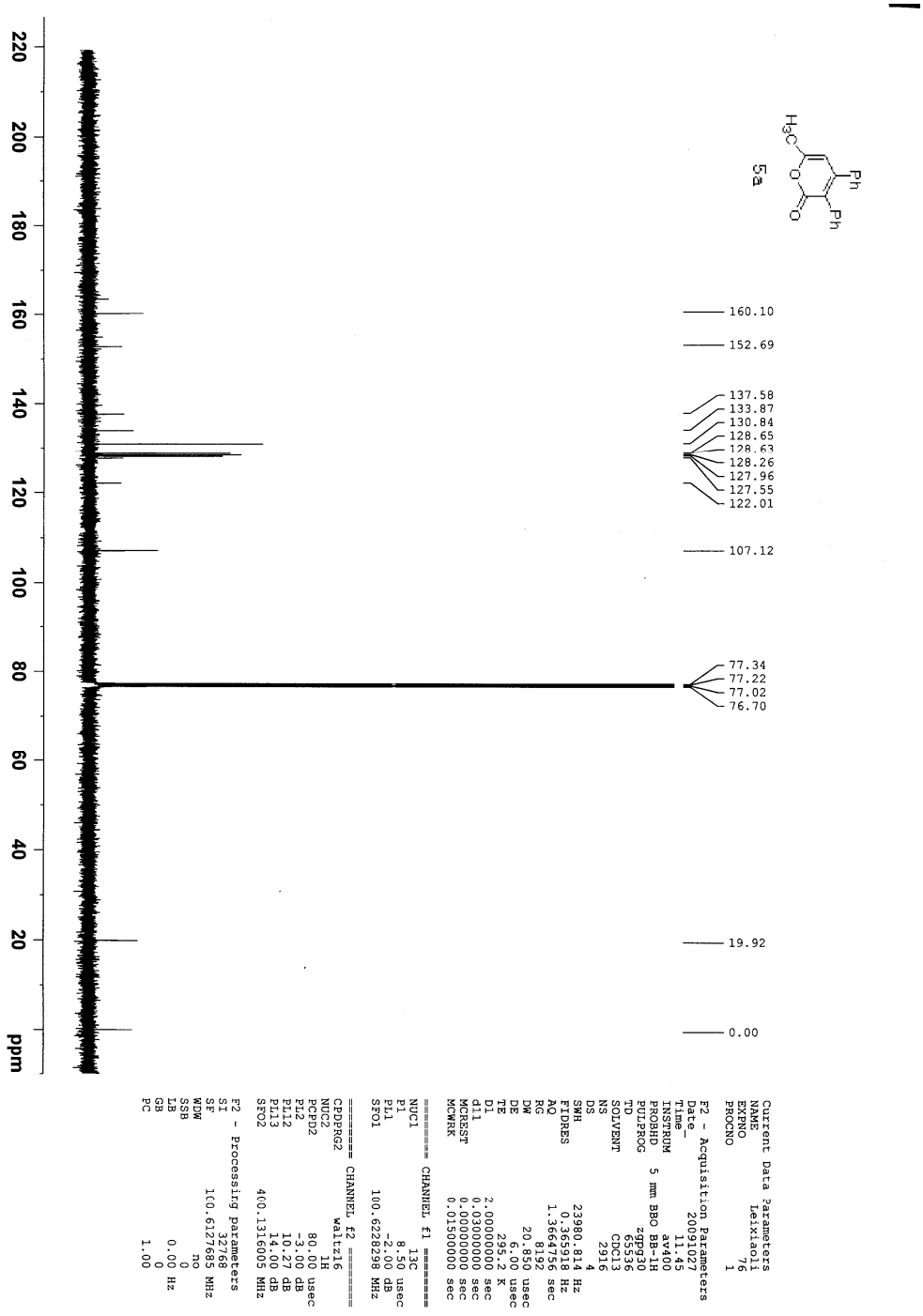
OTs
O
O
CH3
7.32
7.30
7.12
7.10
7.09
7.07
7.06
7.04
6.91
6.90
6.81
6.45
2.47
2.39
2.33
2.29
2.28
2.24
2.00
4.06
1.11
1.06
1.18
3.09
3.16
3.08
10
9
8
7
6
5
4
3
2
1
0
ppm
Current Data Parameters
NAME Leixiaoli
EXPNO 354
PROCNO 1
F2 - Acquisition Parameters
Date_ 20110304
Time 11.00
INSTRUM spect
PROBHD 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 256
DW 60.400 usec
DE 6.00 usec
TE 288.9 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 400.1300055 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

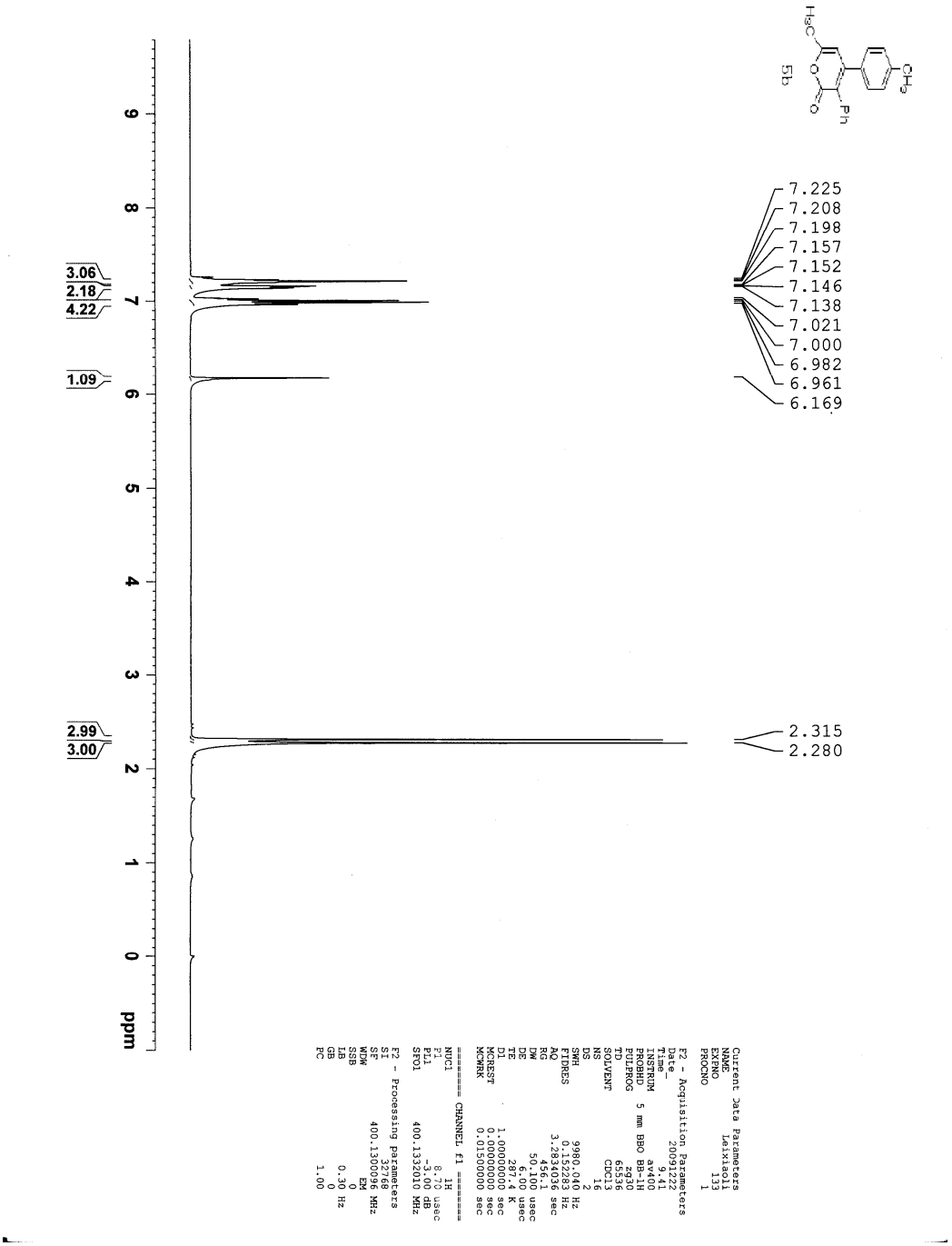

OTs
CH3
163.34
161.75
156.39
145.75
137.34
131.60
130.48
130.30
129.66
128.99
128.92
128.50
127.99
127.76
127.23
116.32
102.40
77.43
77.12
76.80
21.74
21.36
20.12
ppm
200
180
160
140
120
100
80
60
40
20

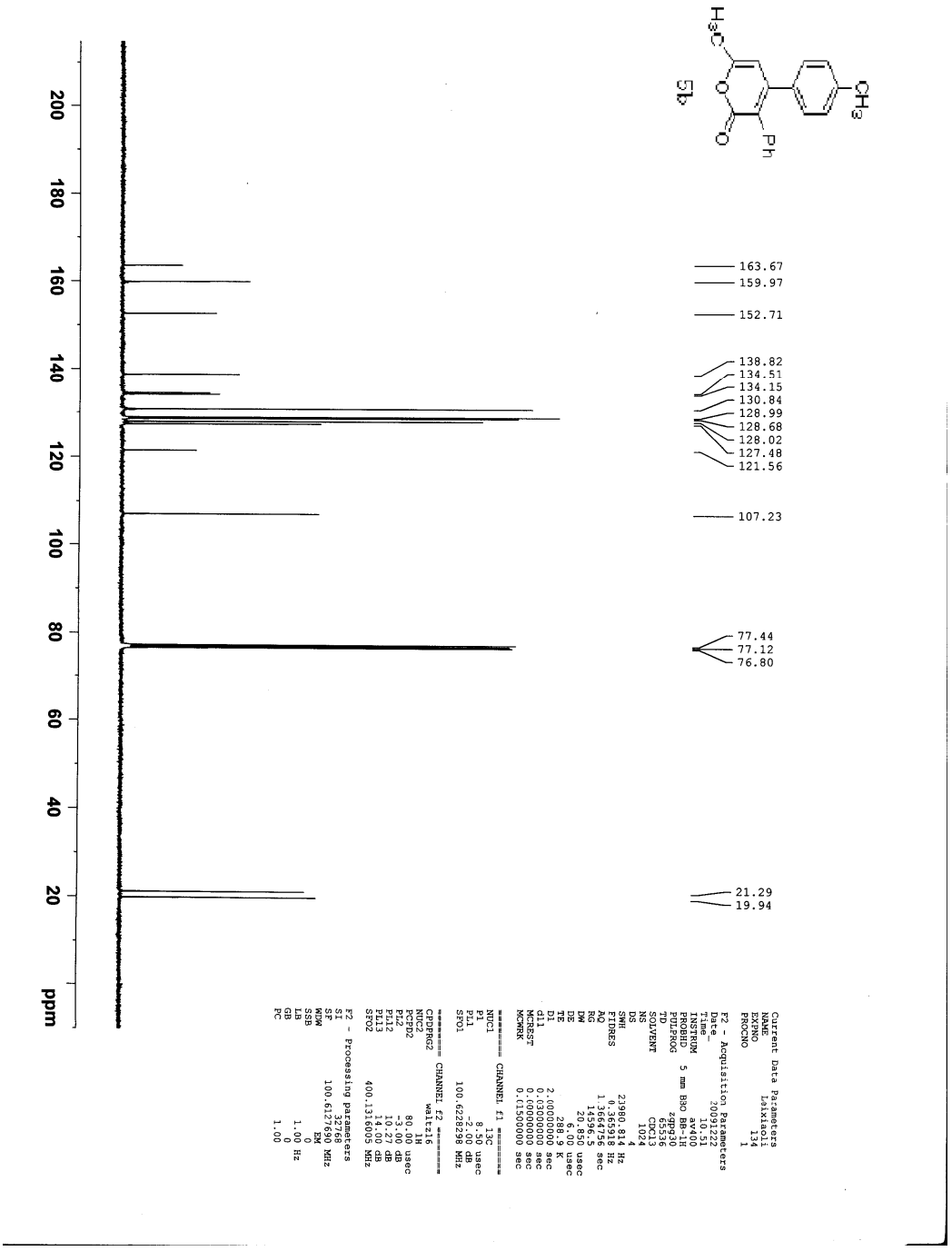

7.86
7.84
7.33
7.31
7.17
7.15
7.06
7.04
6.47
6.47
3.94
2.39
2.35
2.15
1.95
2.08
2.02
1.00
3.01
2.97
2.98
ppm
Current Data Parameters
NAME Leixiaoli
EXPNO 356
PROCNO 1
F2 - Acquisition Parameters
Date_ 20110924
Time 14.22
INSTRUM av400
PROBHD 5 mm BBO BF-1H
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 2
SWH 8278.146 Hz
FIDRES 0.126314 Hz
AQ 3.9584243 sec
RG 287.4
DW 60.400 usec
DE 6.00 usec
TE 299.6 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 400.1299970 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

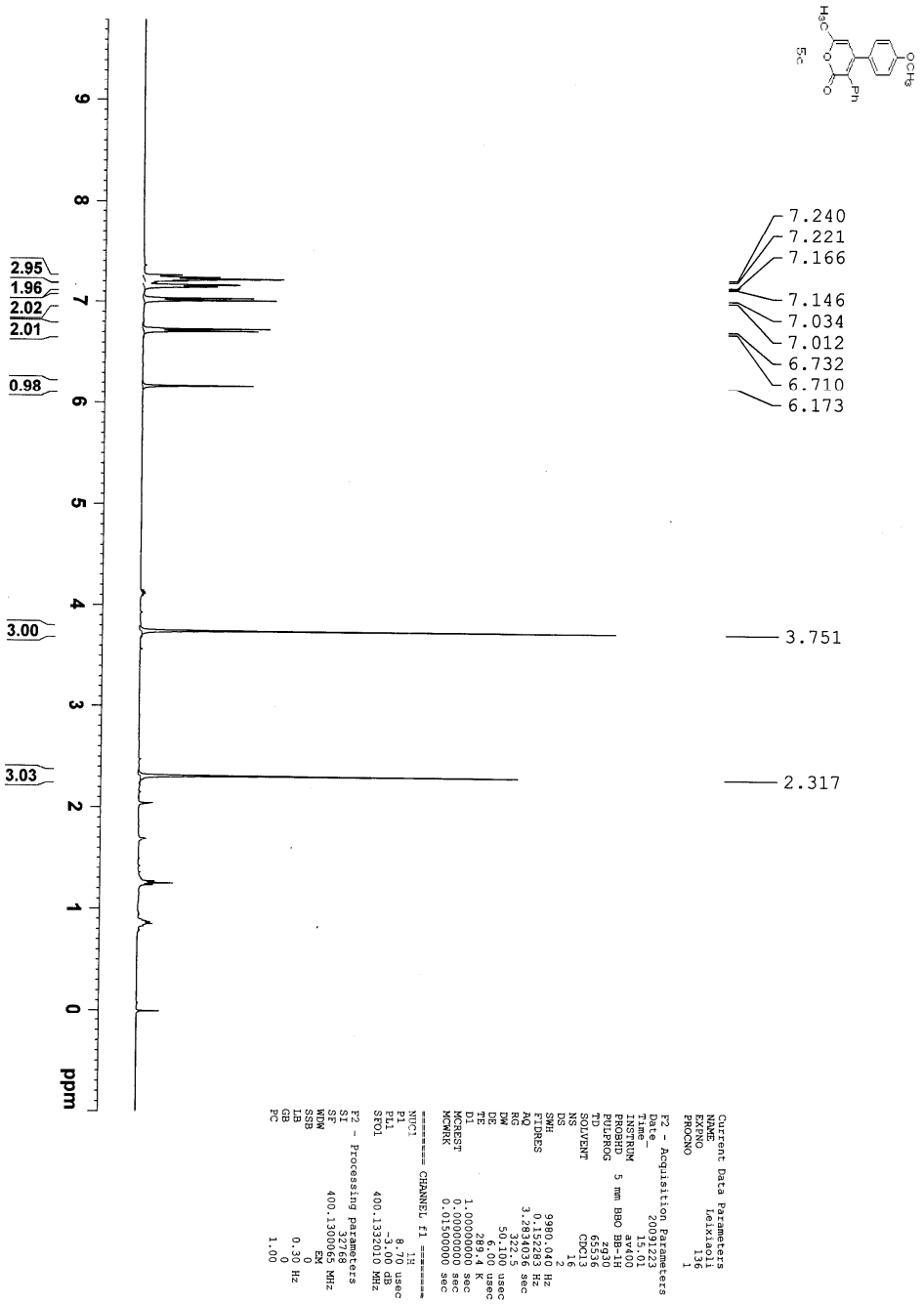

166.60
162.77
162.70
157.10
146.27
133.91
131.39
130.18
129.81
129.60
128.86
127.85
115.01
102.53
77.47
77.15
76.83
52.25
21.66
20.20
200
180
160
140
120
100
80
60
40
20
ppm
Current Data Parameters
NAME Leixiaoli
EXPNO 350
PROCNO 1
F2 - Acquisition Parameters
Date_ 20110310
Time 16.24
INSTRUM spect
PROBHD 5 mm BBO BB-H
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 583
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 292.2 K
D1 2.00000000 sec
D11 0.03000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 8.70 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

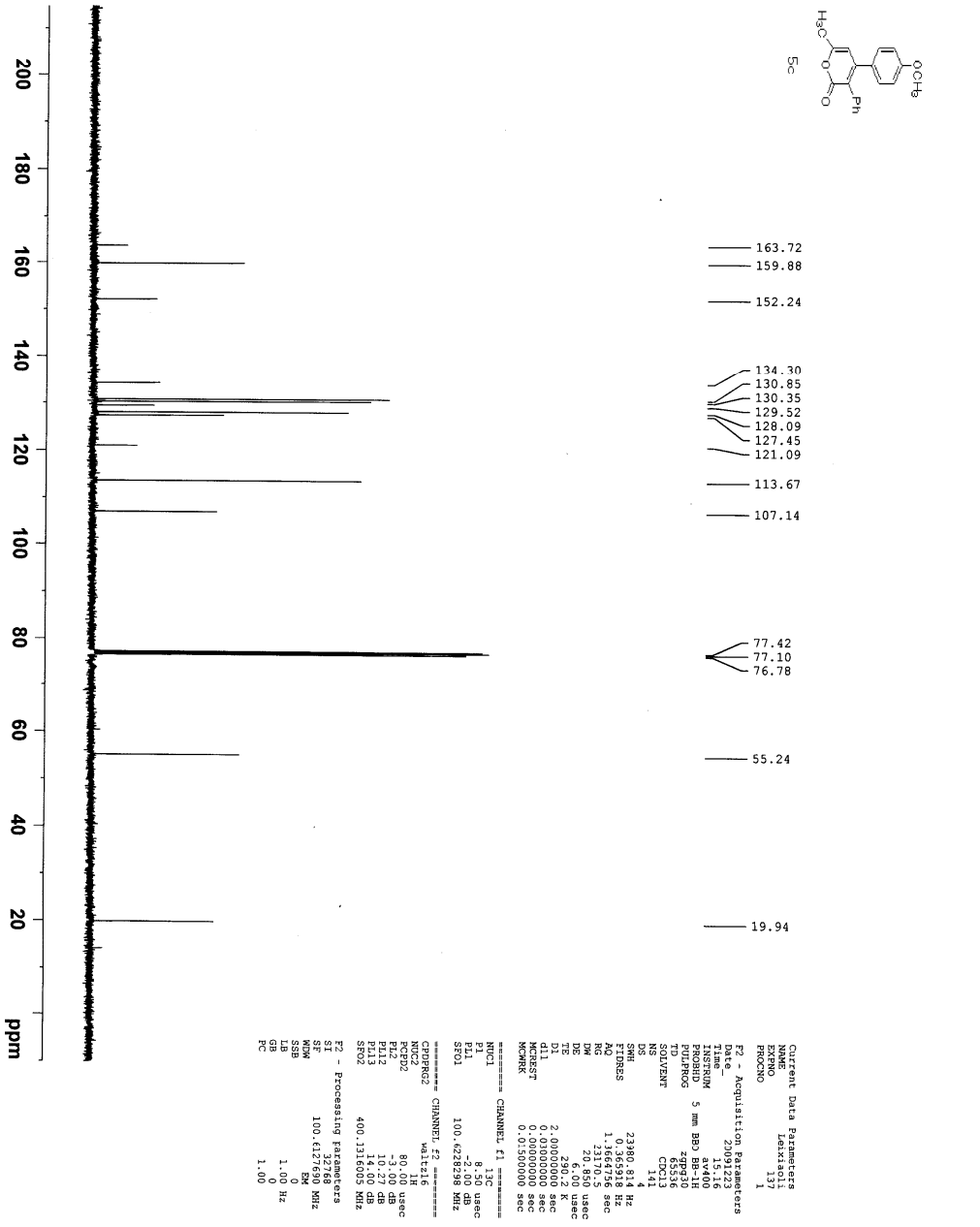

5a
7.261
7.245
7.230
7.227
7.211
7.204
7.200
7.149
7.142
7.138
7.130
7.125
7.096
7.093
7.077
7.073
6.175
2.335
1.577
1.254
0.000
-0.003
1.81
4.12
2.00
2.01
0.98
3.00
ppm

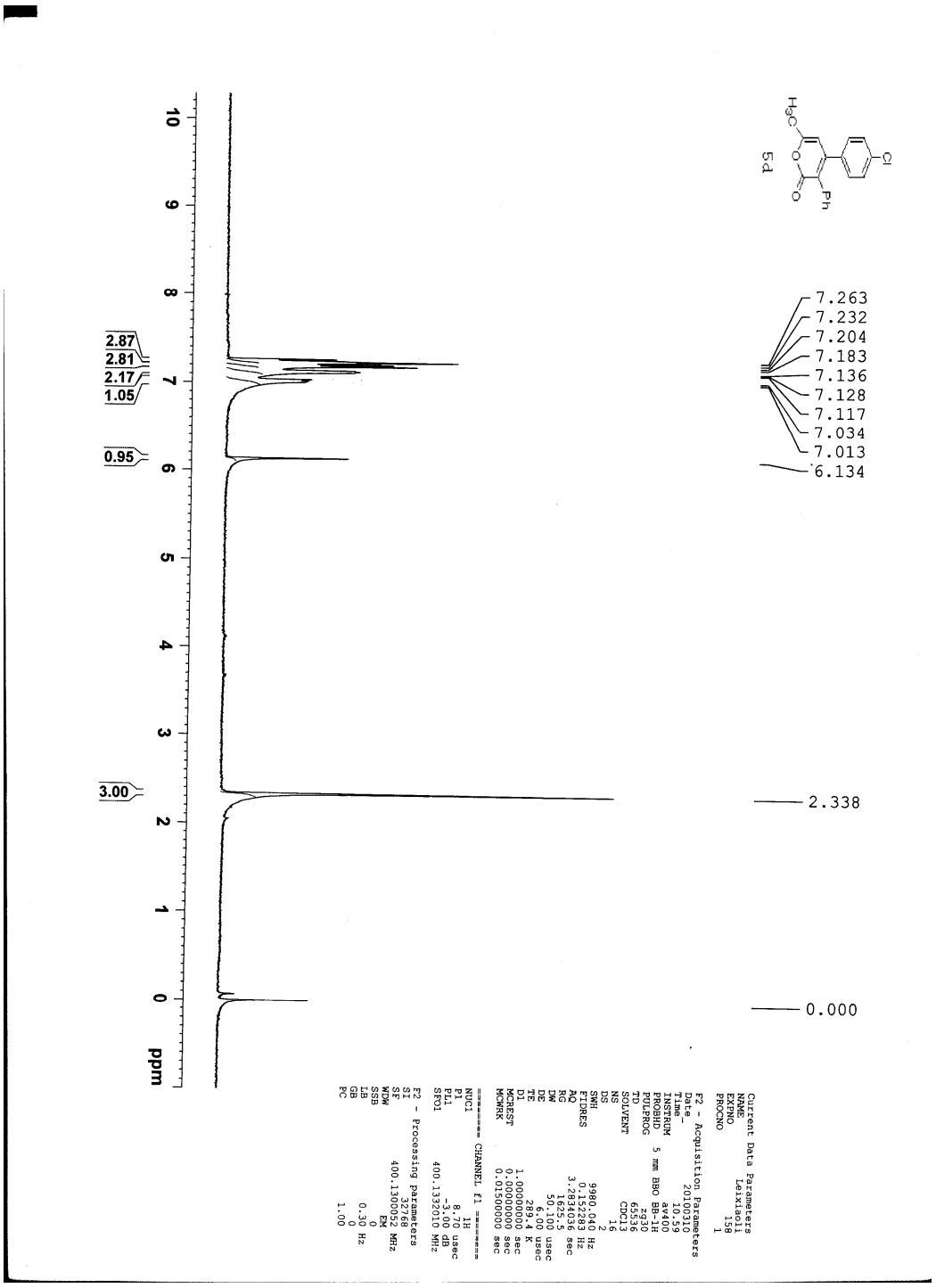

5a
160.10
152.69
137.58
133.87
130.84
128.65
128.63
128.26
127.96
127.55
122.01
107.12
77.34
77.22
77.02
76.70
19.92
0.00
ppm
Current Data Parameters
NAME lexiaoli
EXPNO 76
PROCNO 1
F2 - Acquisition Parameters
Date_ 20051027
Time 11.45
INSTRUM av400
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 2916
DS 4
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 8192
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 100.6127685 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00

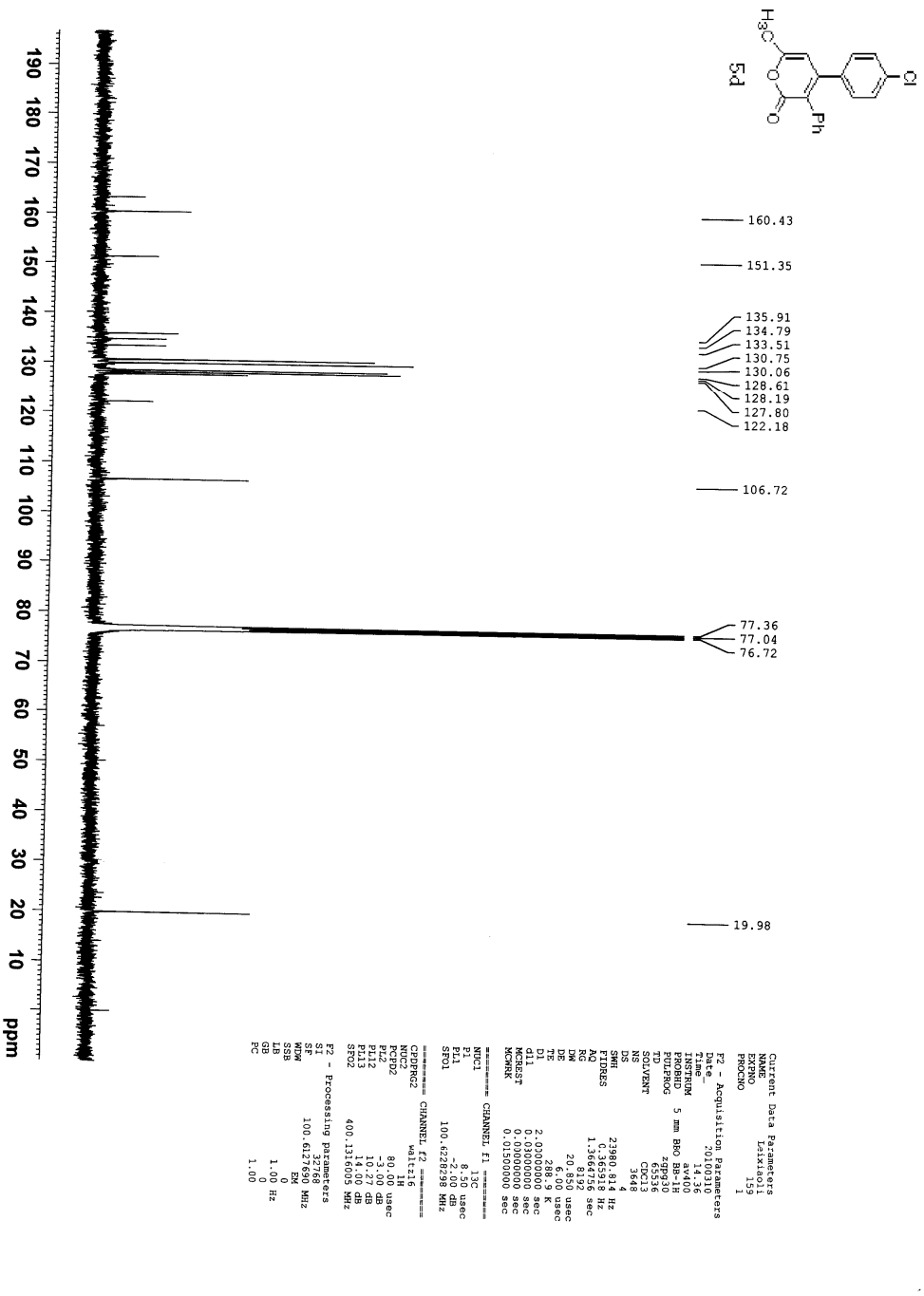

H3C
Sb
O
O
Ph
CH3
7.225
7.208
7.198
7.157
7.152
7.146
7.138
7.021
7.000
6.982
6.961
6.169
2.315
2.280
3.06
2.18
4.22
1.09
2.99
3.00
ppm
Current Data Parameters
NAME Lexiao111
EXPNO 133
PROCNO 1
F2 - Acquisition Parameters
Date_ 20091222
Time 9.11
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 9980.040 Hz
FIDRES 0.152283 Hz
AQ 3.2834036 sec
RG 456.1
DW 50.100 usec
DE 6.00 usec
TE 287.4 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 400.1332010 MHz
F2 - Processing parameters
SI 32768
SF 400.1300096 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

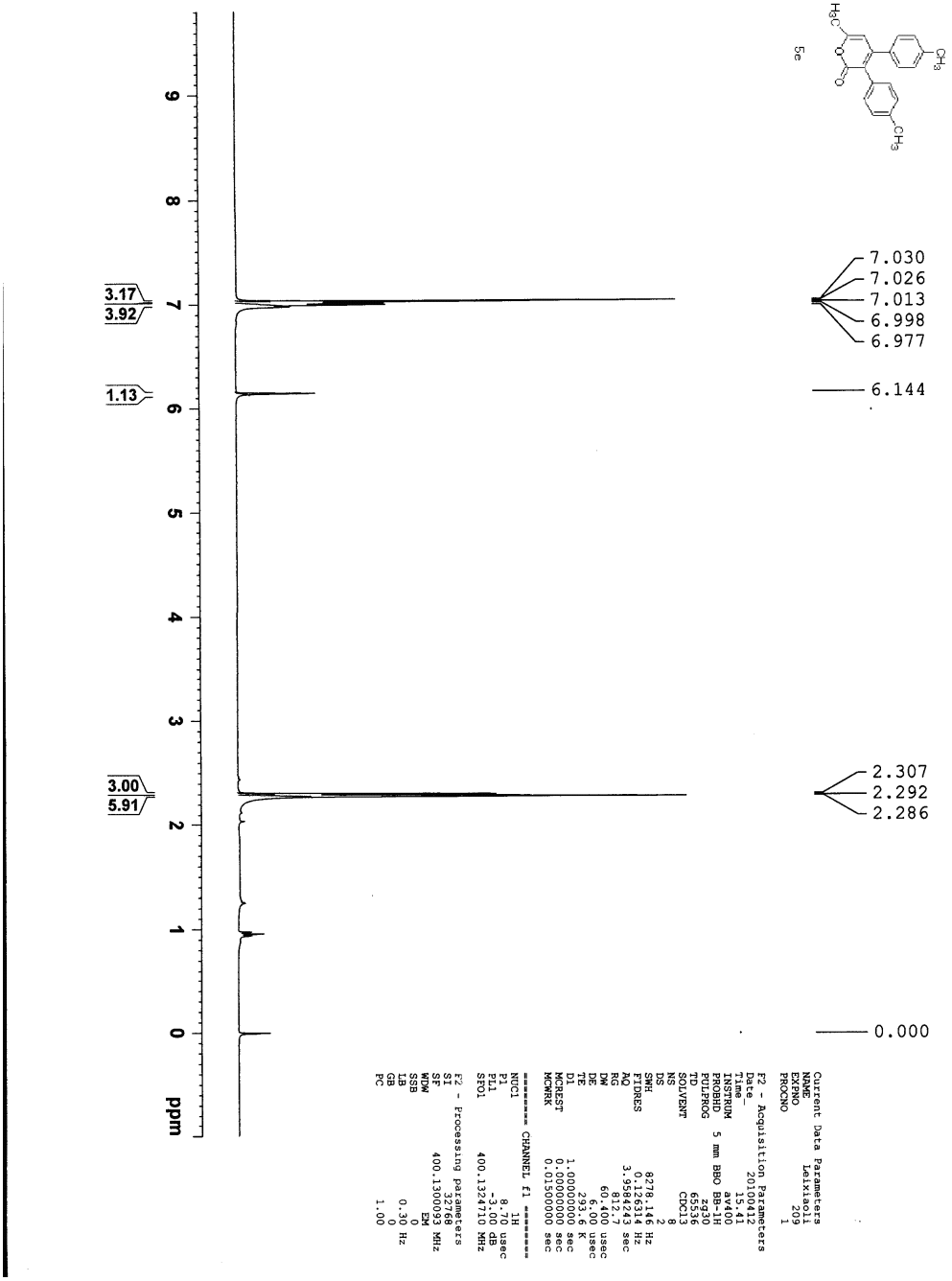

5b
163.67
159.97
152.71
138.82
134.51
134.15
130.84
128.99
128.68
128.02
127.48
121.56
107.23
77.44
77.12
76.80
21.29
19.94
ppm
Current Data Parameters
NAME laixiaoli
EXPNO 134
PROCNO 1
F2 - Acquisition Parameters
Date_ 20111221
Time 10.51
INSTRUM av400
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1024
DS 4
SWH 21980.814 Hz
FIDRES 0.335514 Hz
AQ 1.4864756 sec
RG 14596.5
DW 20.850 usec
DE 6.00 usec
TE 298.5 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
PL13 10.27 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 1.00

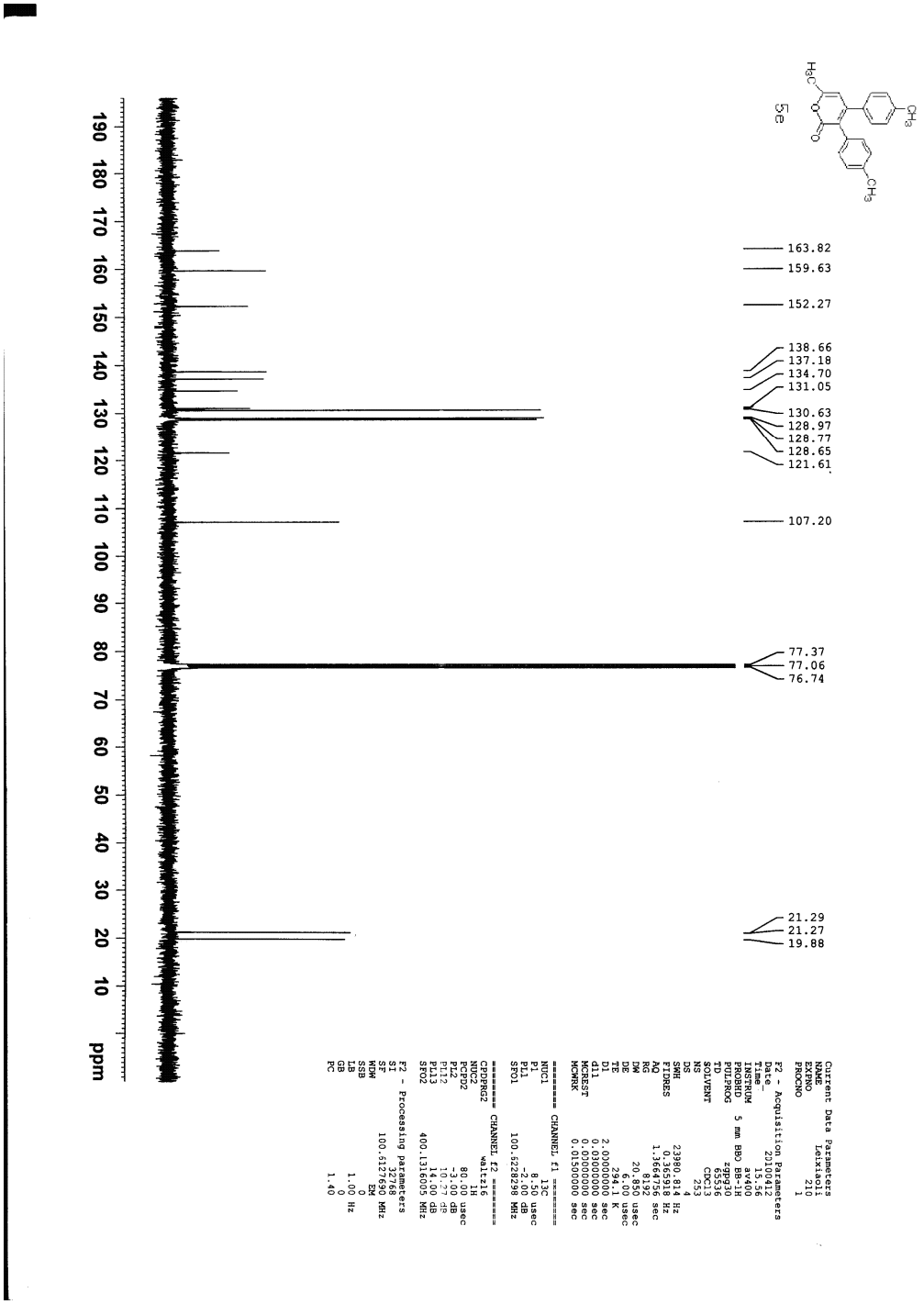

5c
7.240
7.221
7.166
7.146
7.034
7.012
6.732
6.710
6.173
3.751
2.317
2.95
1.96
2.02
2.01
0.98
3.00
3.03
ppm

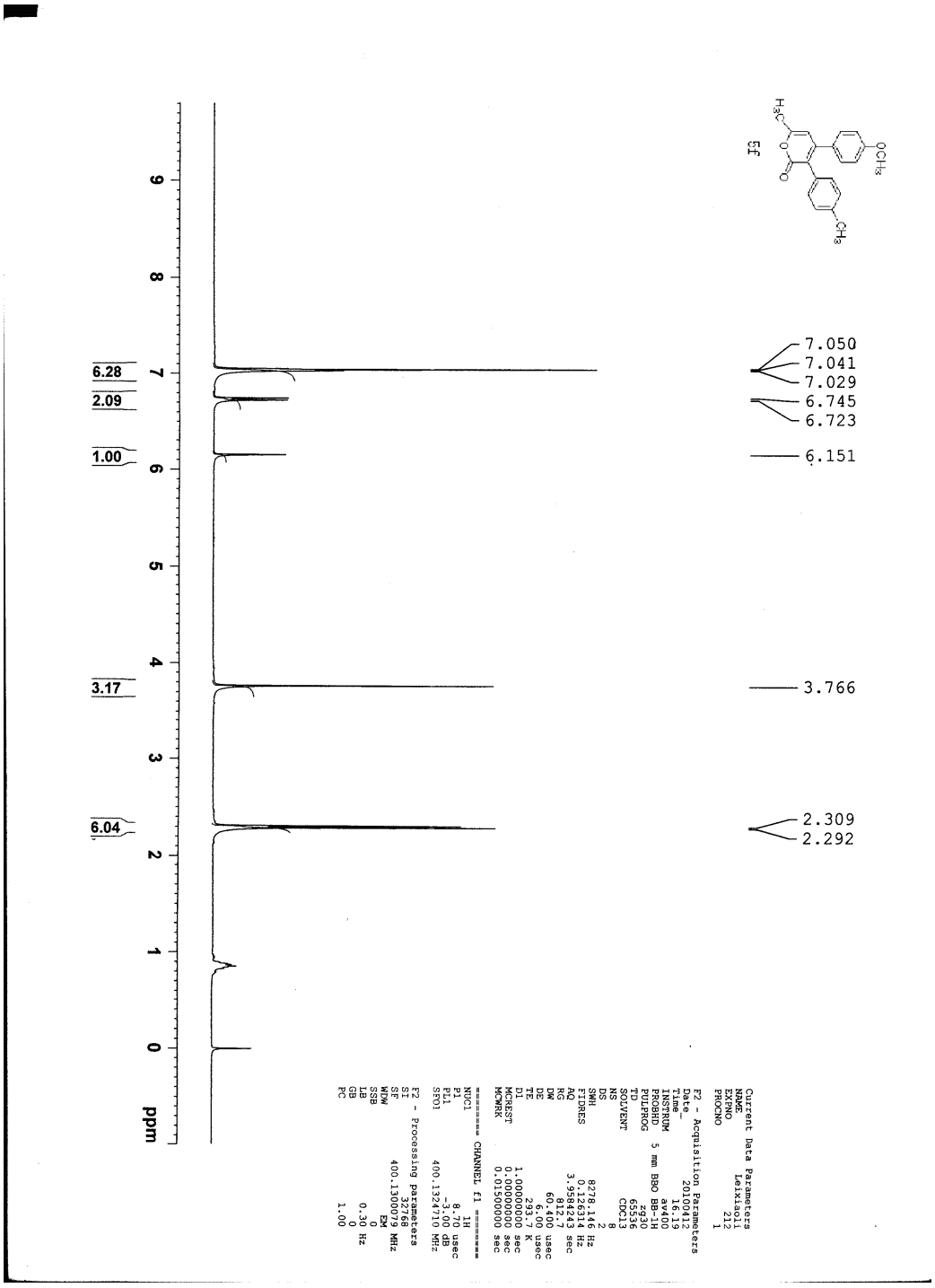

5c
H3C
O
O
Ph
OCH3
163.72
159.88
152.24
134.30
130.85
130.35
129.52
128.09
127.45
121.09
113.67
107.14
77.42
77.10
76.78
55.24
19.94
ppm
200
180
160
140
120
100
80
60
40
20
Current Data Parameters
NAME
EXPNO
PROCNO
1
F2 - Acquisition Parameters
Date_
Time
INSTRUM
PROBHD
PULPROG
TD
SOLVENT
NS
DS
SWH
FIDRES
AQ
RG
DW
DE
TE
D1
d11
MCREST
MCWRK
CDCl3
141
23980.814 Hz
0.365918 Hz
1.1664756 sec
23170.5
20.850 usec
6.00 usec
298.2 K
2.00000000 sec
0.01000000 sec
0.00000000 sec
0.03500000 sec
CHANNEL f1
NUC1
P1
PL1
SFO1
13C
8.50 usec
-2.00 dB
100.622898 MHz
CHANNEL f2
CPDPRG2
NUC2
PCPD2
PL2
PL12
PL13
SFO2
waltz16
1H
80.00 usec
-3.00 dB
10.27 dB
14.00 dB
400.1316005 MHz
F2 - Processing parameters
SI
SF
WDW
SSB
LB
GB
PC
32768
100.6127690 MHz
EM
0
1.00 Hz
0
1.00

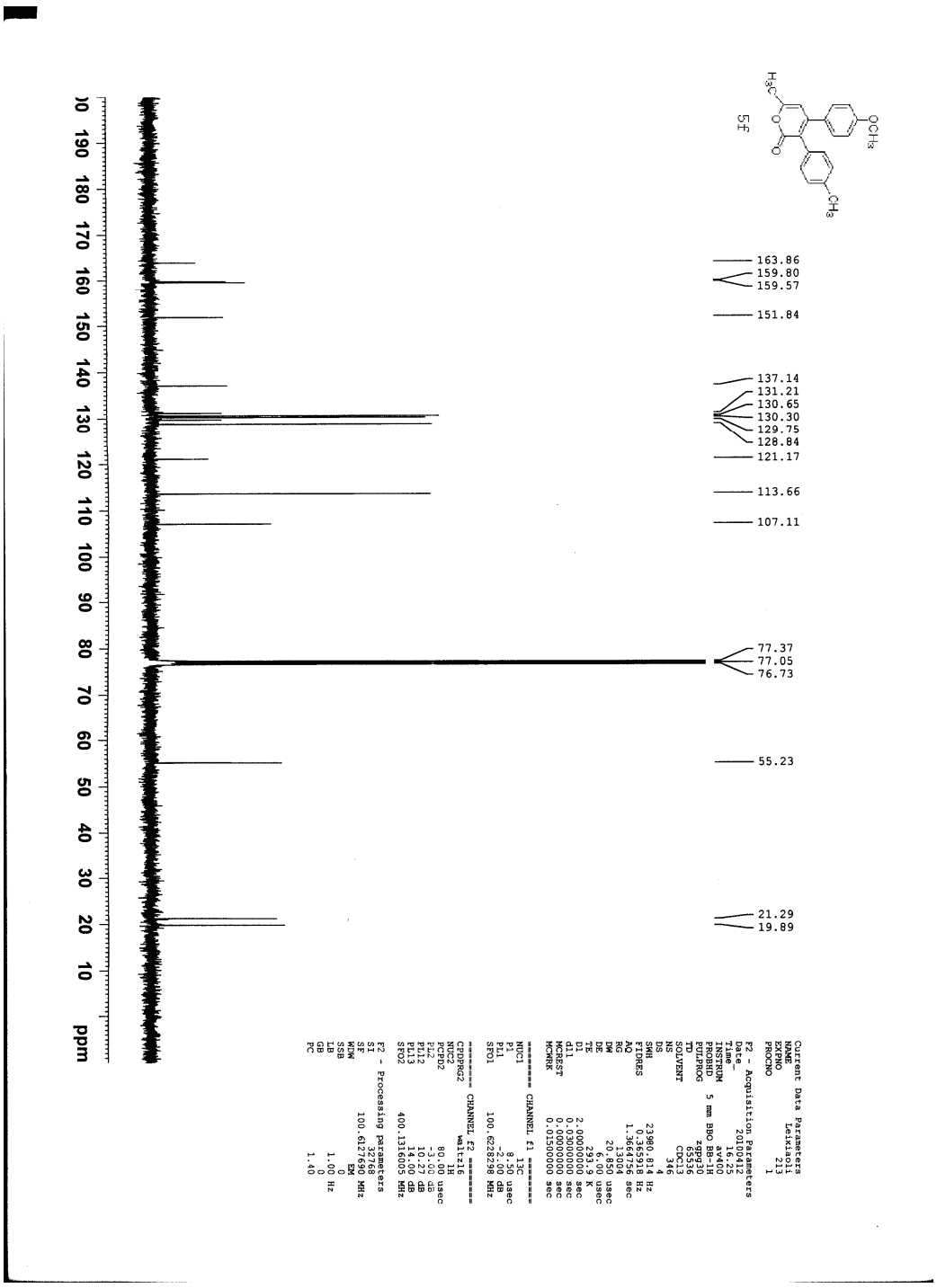

5d
7.263
7.232
7.204
7.183
7.136
7.128
7.117
7.034
7.013
6.134
2.338
0.000
2.87
2.81
2.17
1.05
0.95
3.00
ppm

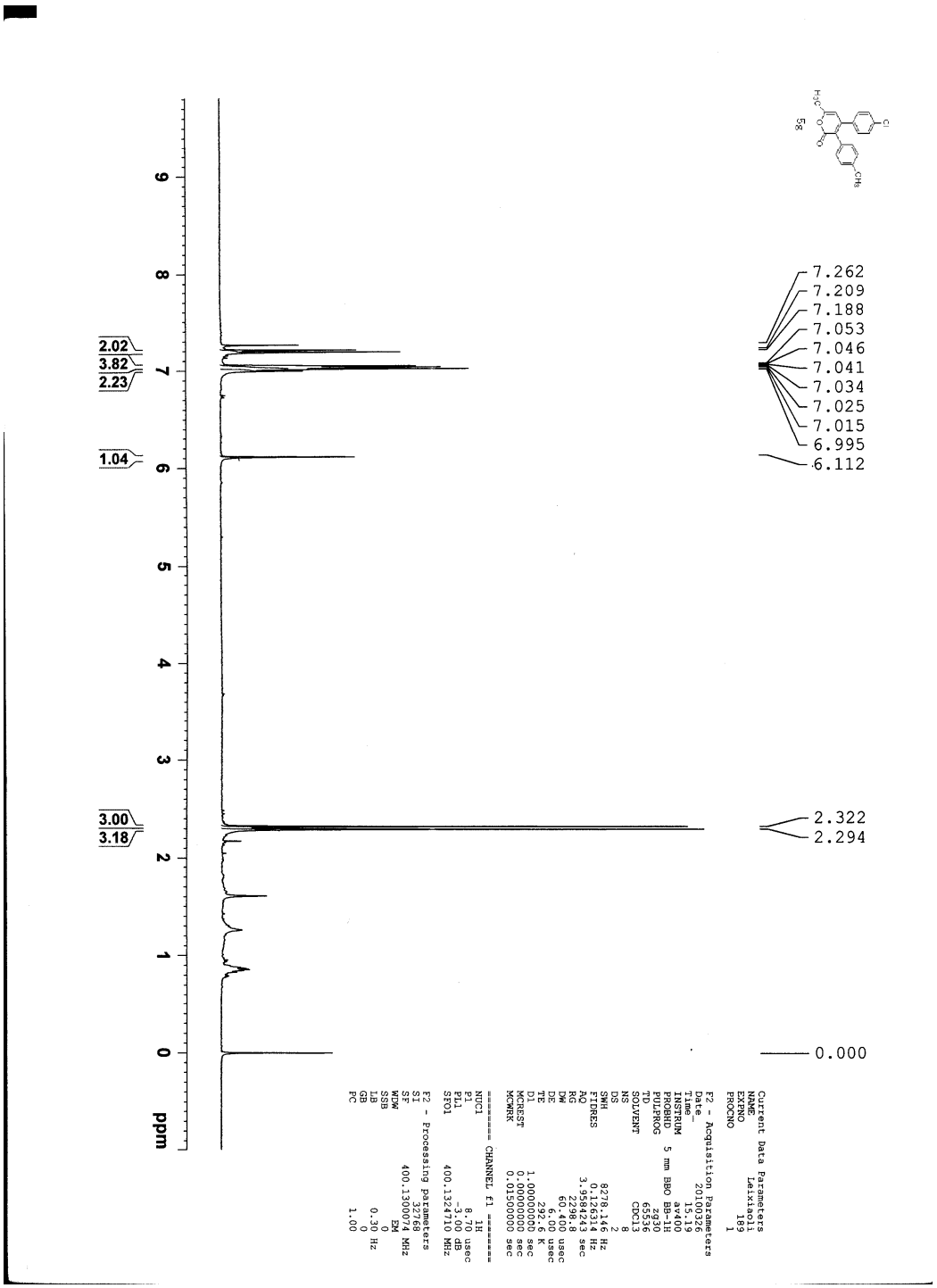

5d
160.43
151.35
135.91
134.79
133.51
130.75
130.06
128.61
128.19
127.80
122.18
106.72
77.36
77.04
76.72
19.98
ppm

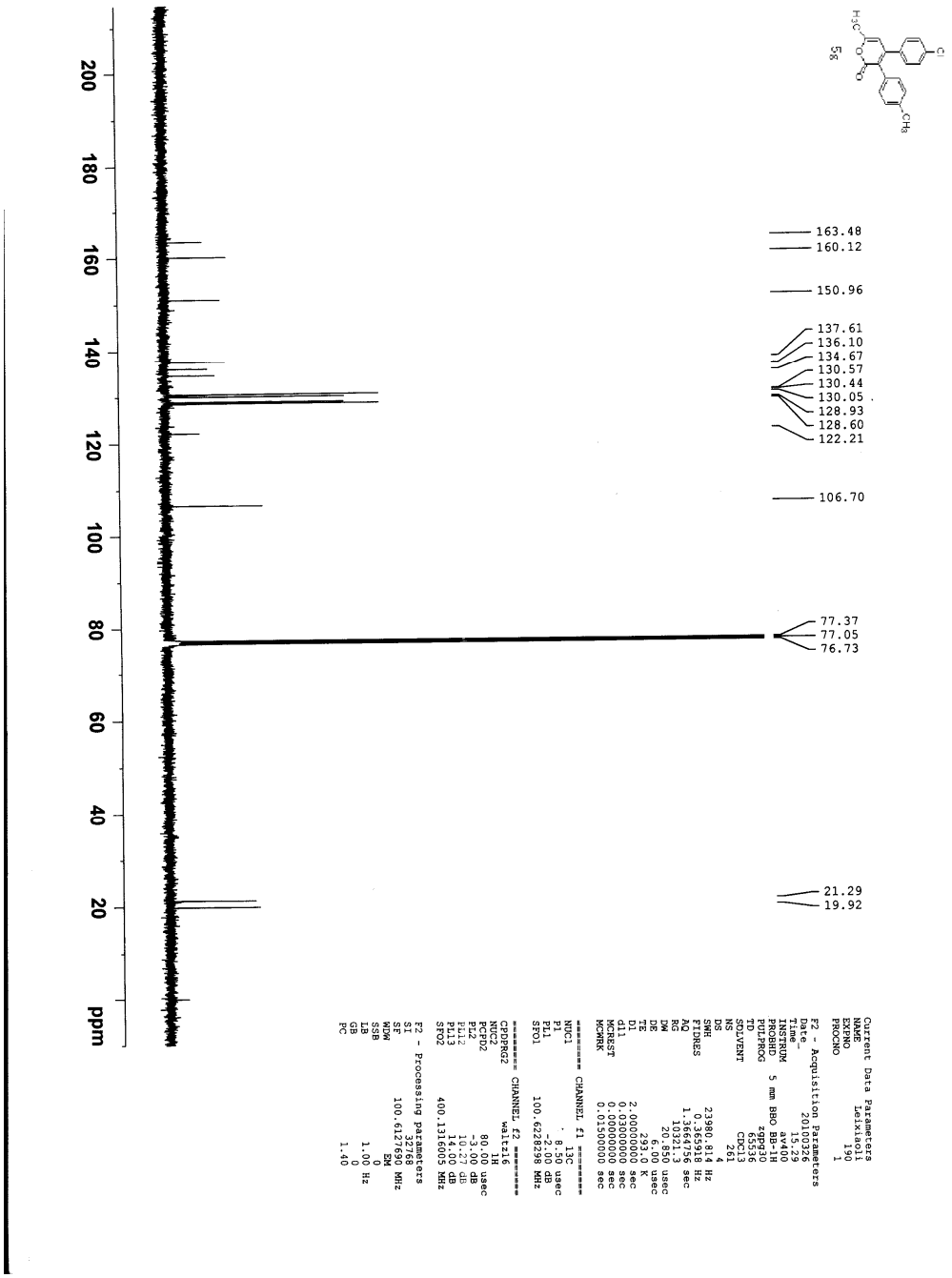

5e
7.030
7.026
7.013
6.998
6.977
6.144
2.307
2.292
2.286
0.000
3.17
3.92
1.13
3.00
5.91
ppm
Current Data Parameters
NAME Lelx1a201
EXPNO 201
PROCNO 1
F2 - Acquisition Parameters
Date_ 20100412
Time 15.40
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 2
SWH 8278.146 Hz
FIDRES 0.126314 Hz
AQ 3.9584243 sec
RG 812.7
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 400.1300093 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

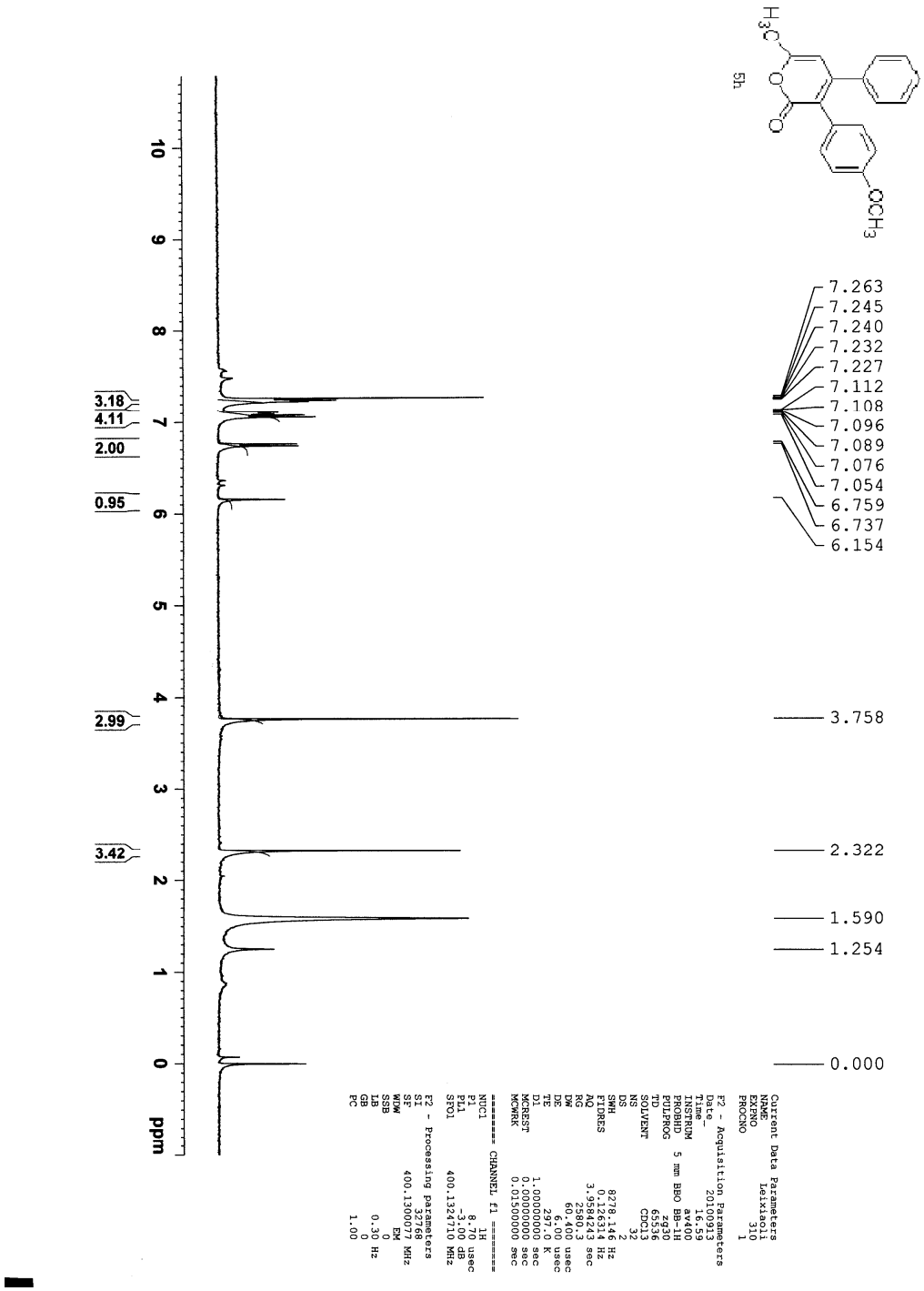

5e
163.82
159.63
152.27
138.66
137.18
134.70
131.05
130.63
128.97
128.77
128.65
121.61
107.20
77.37
77.06
76.74
21.29
21.27
19.88
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm
Current Data Parameters
NAME Leixiaoli
EXPNO 210
PROCNO 1
F2 - Acquisition Parameters
Date_ 22100412
Time 15.56
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 29
DS 4
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3664736 sec
RG 8192
DW 20.850 usec
DE 6.00 usec
TE 294.1 K
D1 2.00000000 sec
D11 0.03000000 sec
MCREST 0.01500000 sec
MCWRK
======== 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 -5.00 dB
PL13 10.27 dB
PL13 14.00 dB
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 32768
SF 100.5127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

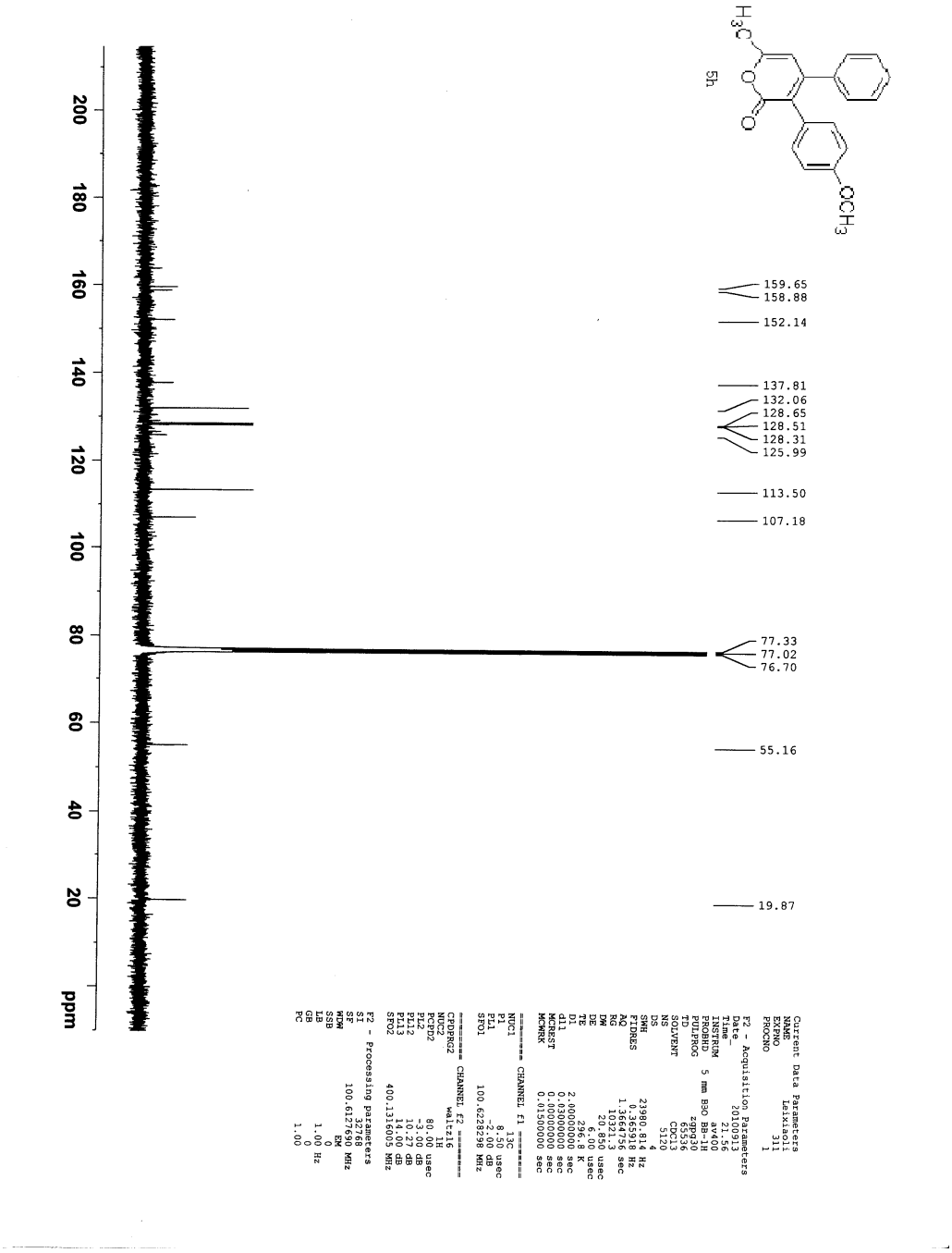

5f
7.050
7.041
7.029
6.745
6.723
6.151
3.766
2.309
2.292
6.28
2.09
1.00
3.17
6.04
ppm

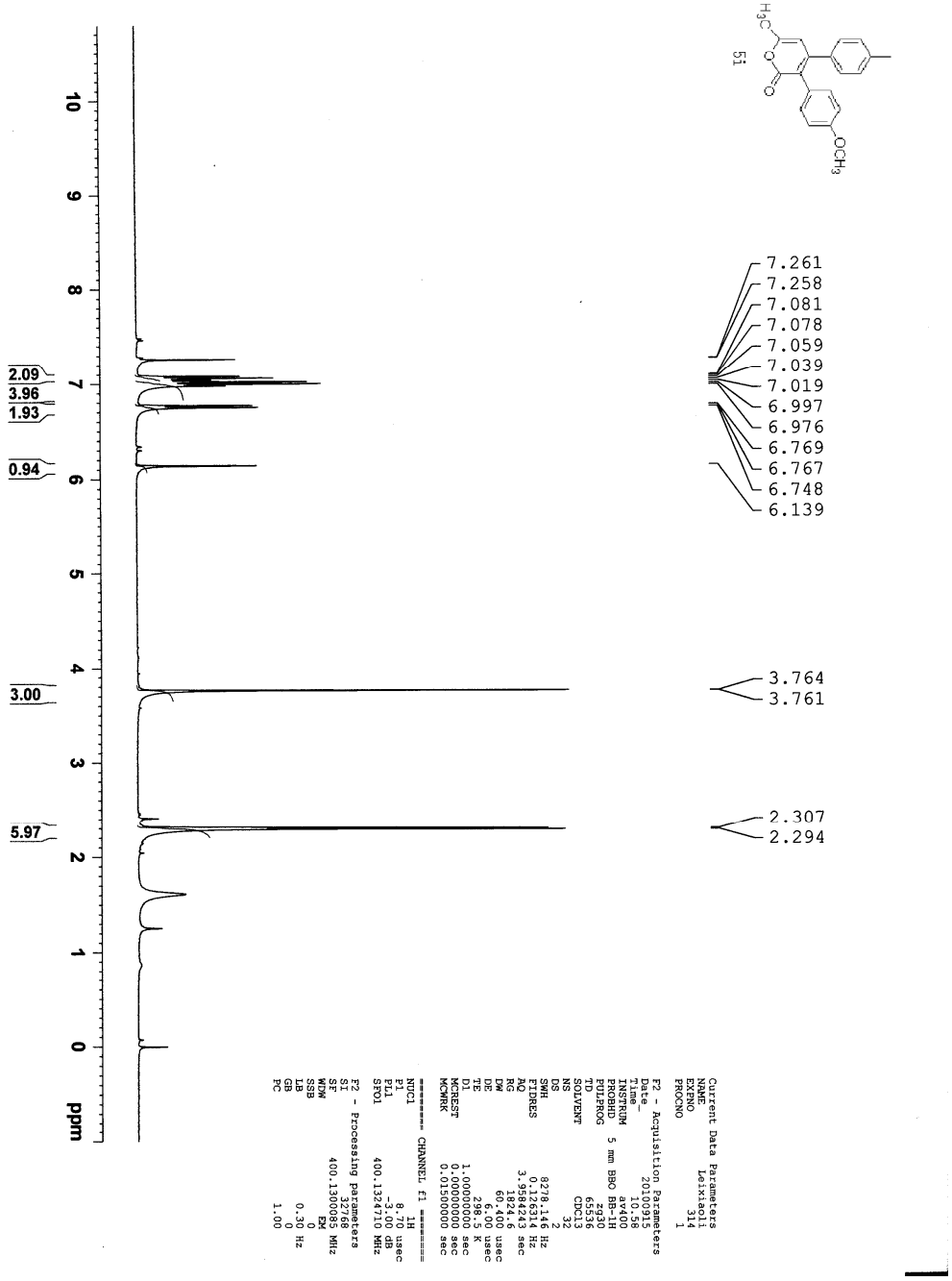

5f
163.86
159.80
159.57
151.84
137.14
131.21
130.65
130.30
129.75
128.84
121.17
113.66
107.11
77.37
77.05
76.73
55.23
21.29
19.89
ppm

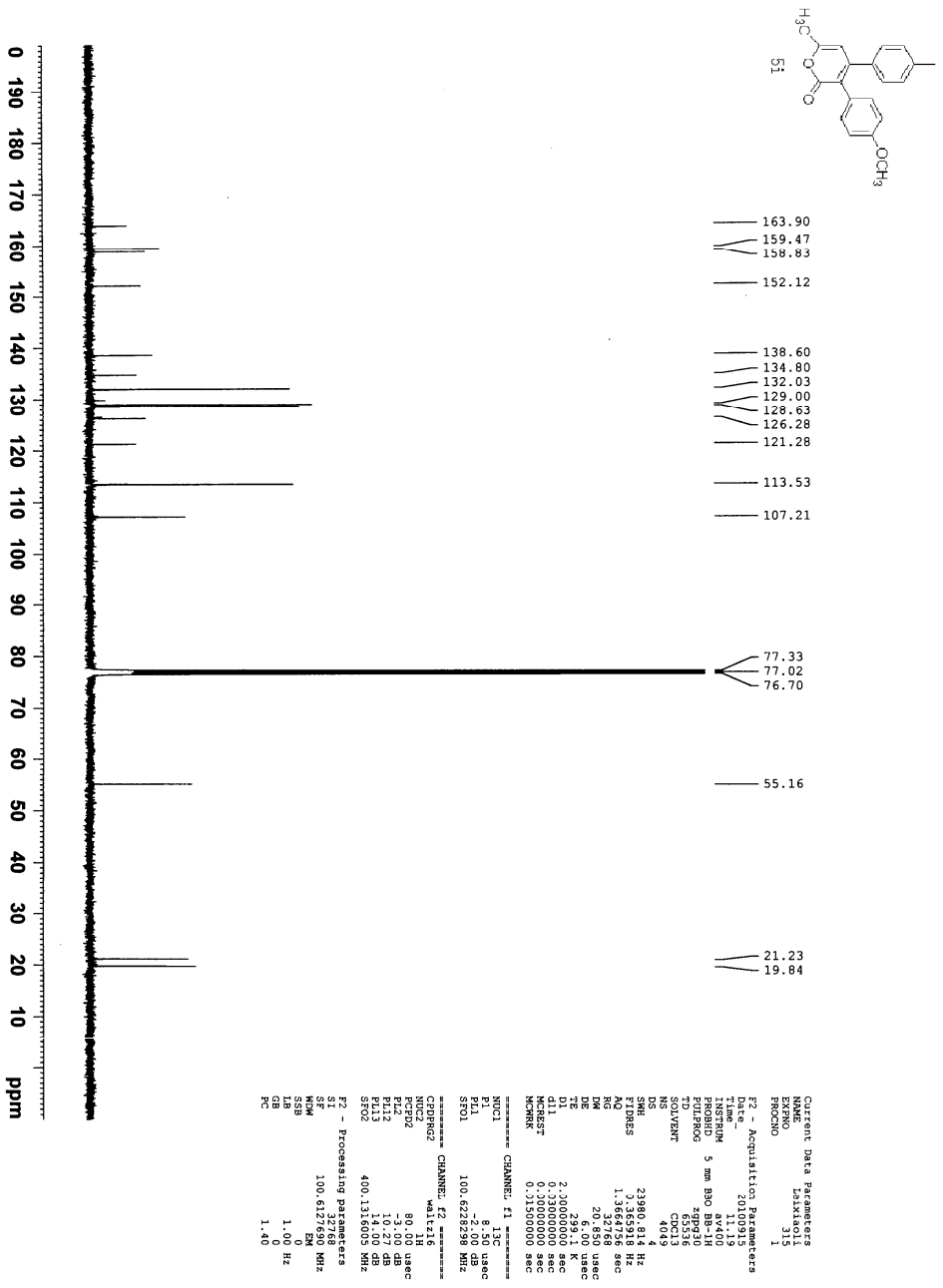

5g
7.262
7.209
7.188
7.053
7.046
7.041
7.034
7.025
7.015
6.995
6.112
2.322
2.294
0.000
2.02
3.82
2.23
1.04
3.00
3.18
ppm
Current Data Parameters
NAME Lexiaoli
EXPNO 103
PROCNO 1
F2 - Acquisition Parameters
Date_ 20100326
Time 15:19
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 2
SWH 8278.146 Hz
FIDRES 0.126314 Hz
AQ 3.9584243 sec
RG 2298.8
DW 60.400 usec
DE 6.00 usec
TE 282.0 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 131072
SF 400.1300074 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

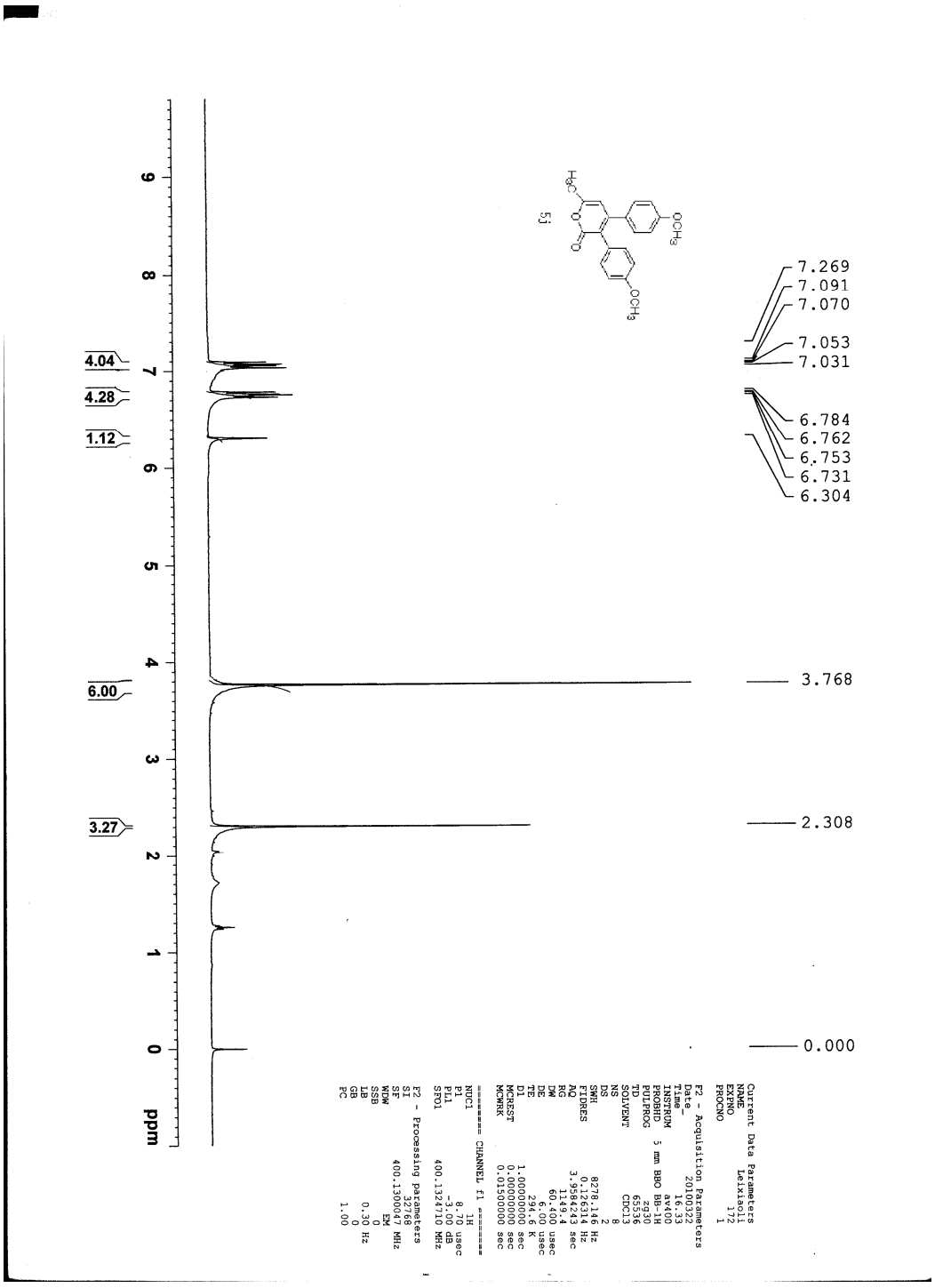

5s
163.48
160.12
150.96
137.61
136.10
134.67
130.57
130.44
130.05
128.93
128.60
122.21
106.70
77.37
77.05
76.73
21.29
19.92
200
180
160
140
120
100
80
60
40
20
ppm

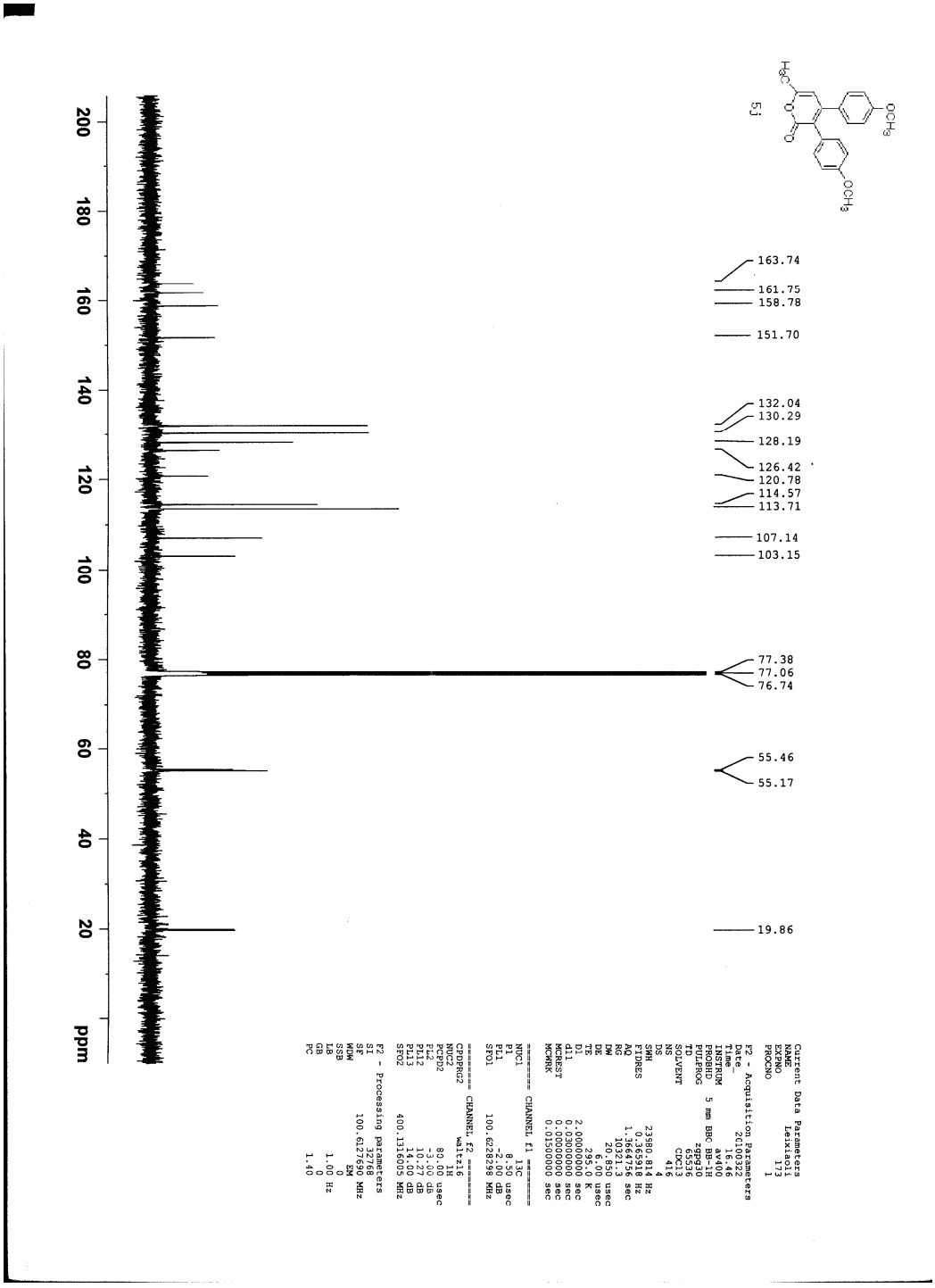

5h
7.263
7.245
7.240
7.232
7.227
7.112
7.108
7.096
7.089
7.076
7.054
6.759
6.737
6.154
3.758
2.322
1.590
1.254
0.000
3.18
4.11
2.00
0.95
2.99
3.42
ppm

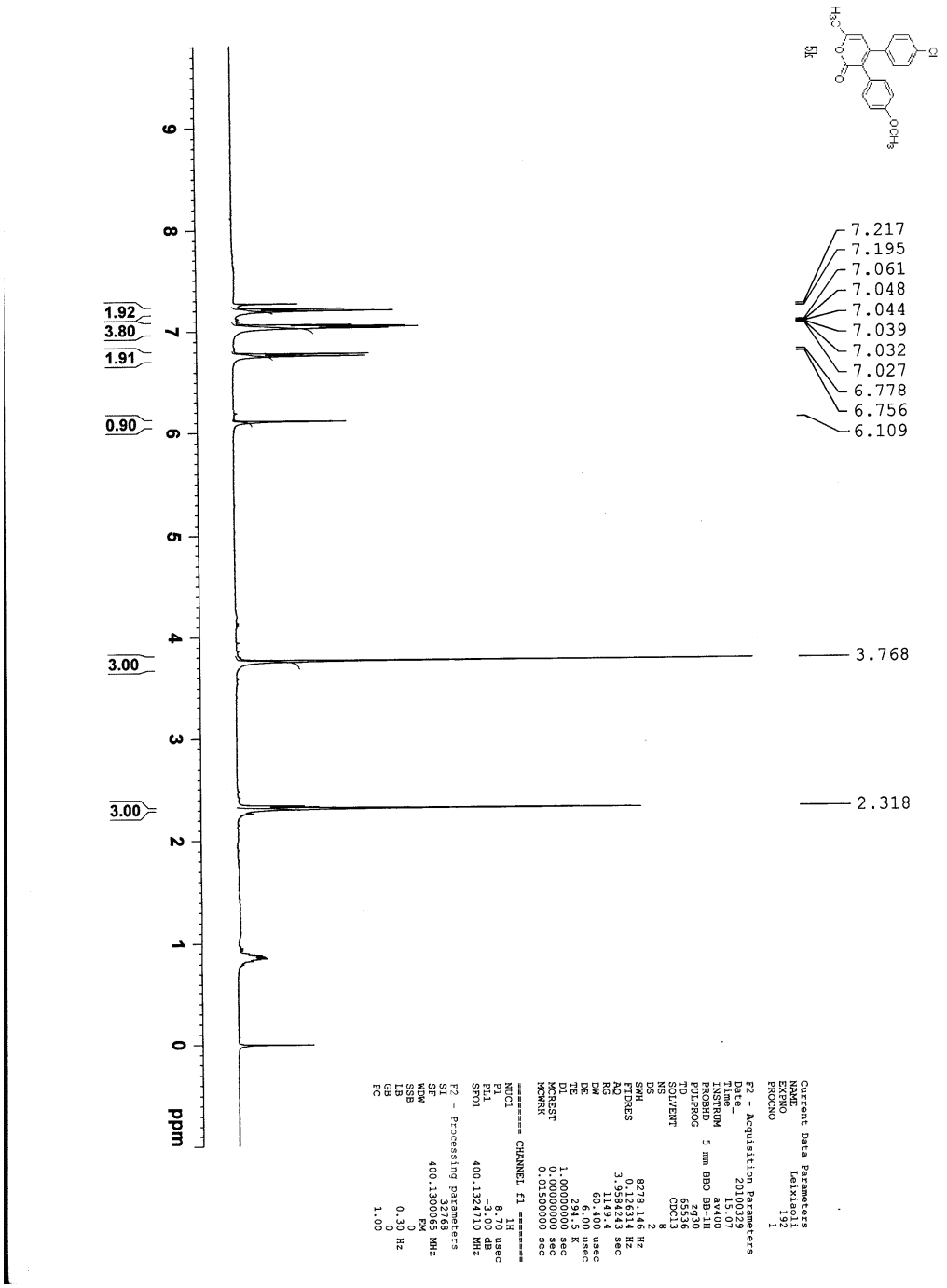

5h
159.65
158.88
152.14
137.81
132.06
128.65
128.51
128.31
125.99
113.50
107.18
77.33
77.02
76.70
55.16
19.87
ppm
Current Data Parameters
NAME Leixiaoli
EXPNO 311
PROCNO 1
F2 - Acquisition Parameters
Date_ 20100913
Time 21.56
INSTRUM av400
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 512
DS 4
SWH 23980.814 Hz
FIDRES 0.365910 Hz
AQ 1.3664755 sec
RG 101.71
DW 20.850 usec
DE 6.00 usec
TE 296.8 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
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 1.00

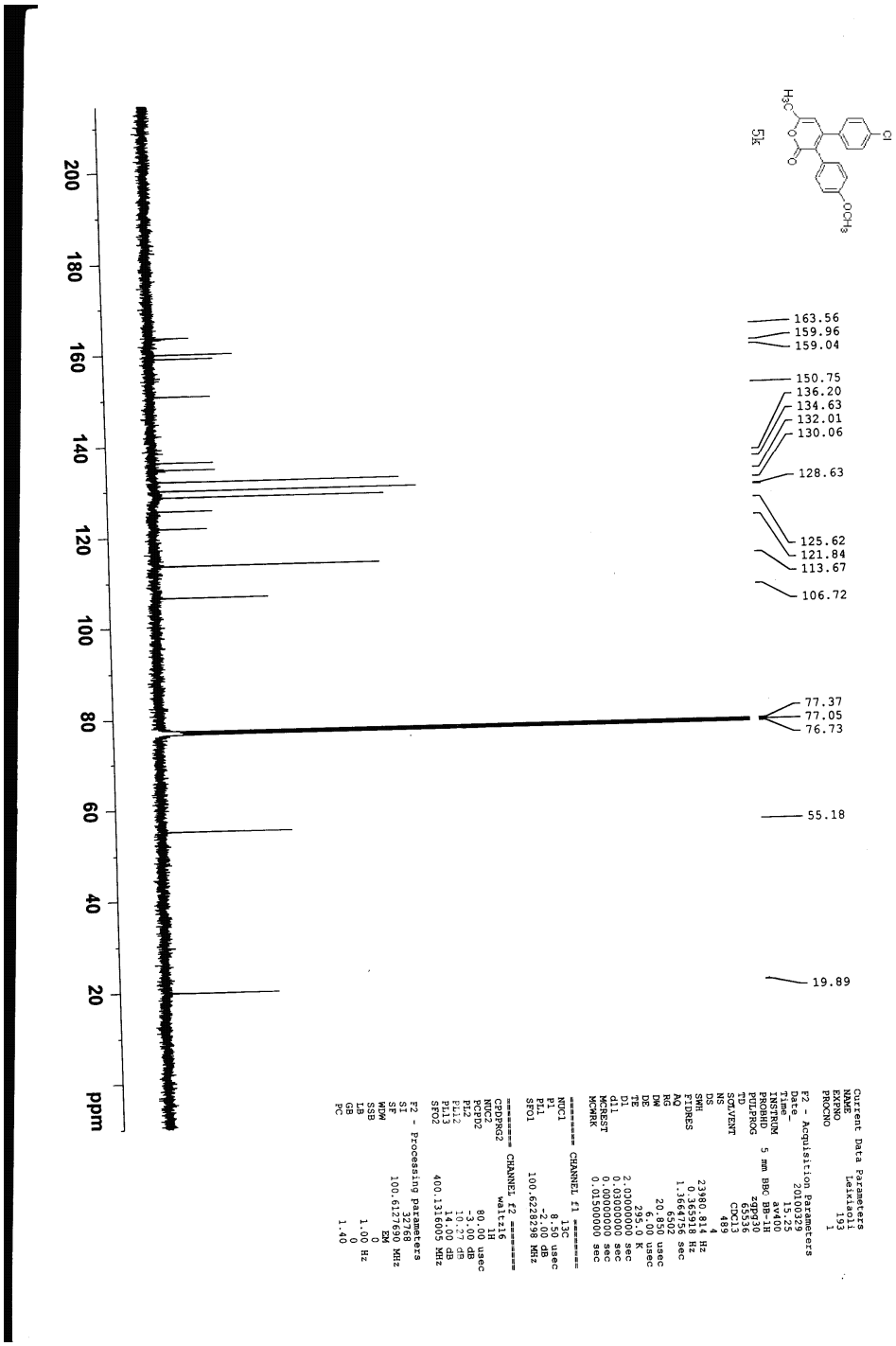

51
7.261
7.258
7.081
7.078
7.059
7.039
7.019
6.997
6.976
6.769
6.767
6.748
6.139
3.764
3.761
2.307
2.294
2.09
3.96
1.93
0.94
3.00
5.97
ppm
Current Data Parameters
NAME Leixiaoli
EXPNO 314
PROCNO 1
F2 - Acquisition Parameters
Date_ 20100915
Time_ 10.58
INSTRUM av400
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 32
DS 2
SWH 8278.146 Hz
FIDRES 0.126314 Hz
AQ 3.9582413 sec
RG 1824.6
DW 60.400 usec
DE 6.00 usec
TE 298.5 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 400.1300059 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

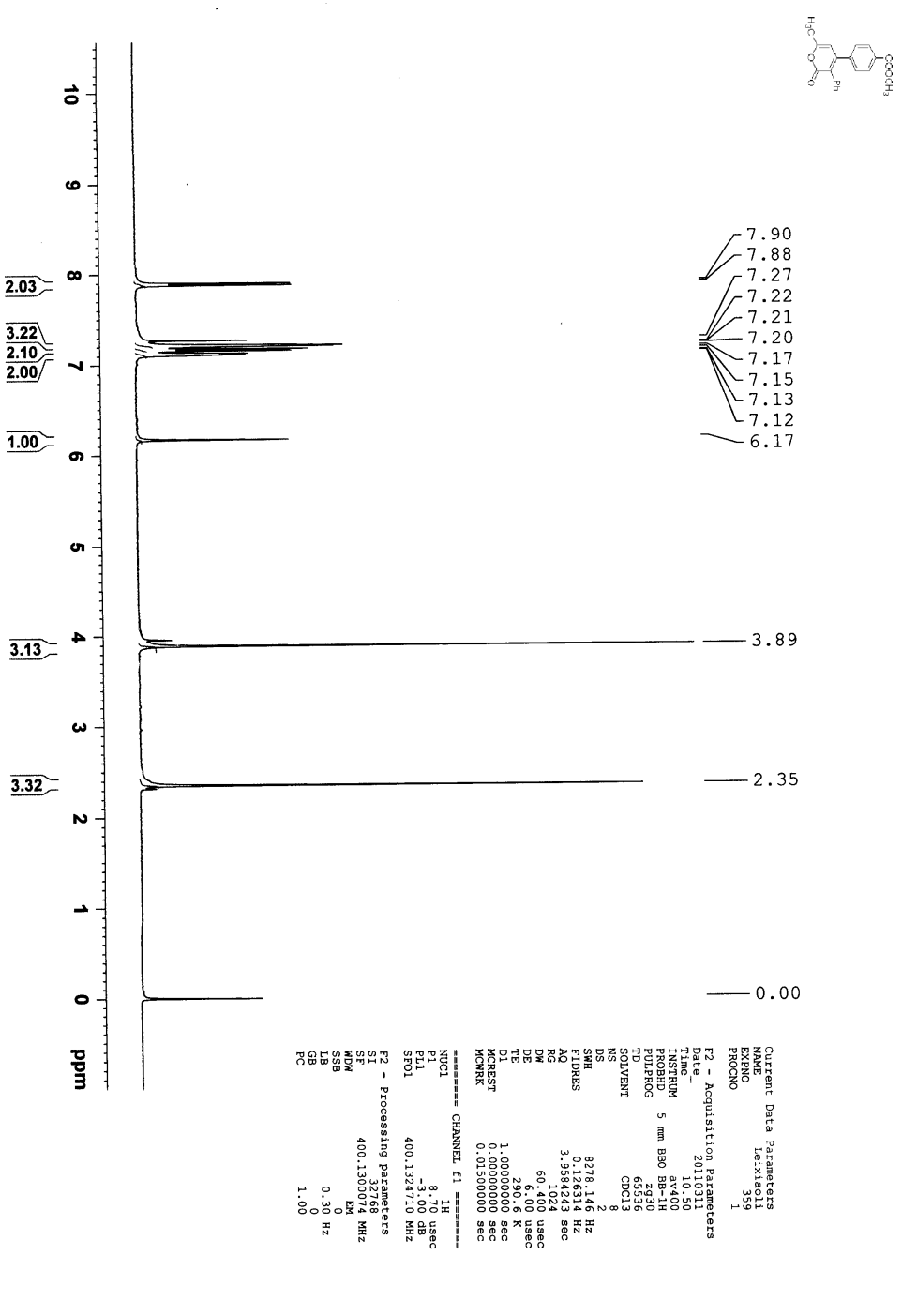

5i
163.90
159.47
158.83
152.12
138.60
134.80
132.03
129.00
128.63
126.28
121.28
113.53
107.21
77.33
77.02
76.70
55.16
21.23
19.84
0 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

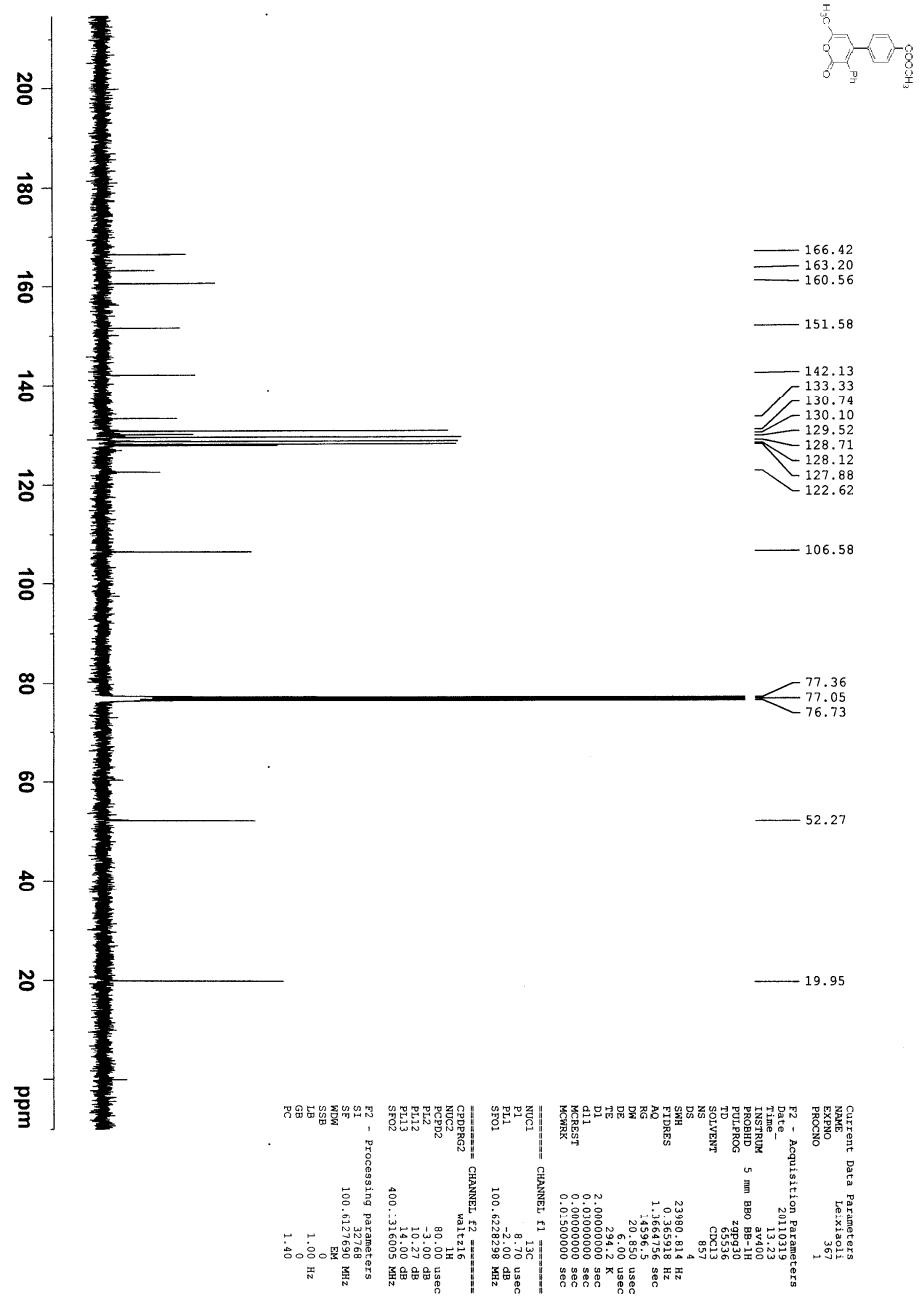

5j
7.269
7.091
7.070
7.053
7.031
6.784
6.762
6.753
6.731
6.304
3.768
2.308
0.000
4.04
4.28
1.12
6.00
3.27
ppm
Current Data Parameters
NAME Leixiaoli
EXPNO 172
PROCNO 1
F2 - Acquisition Parameters
Date_ 20110329
Time 16.33
INSTRUM av400
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 2
SWH 8278.146 Hz
FIDRES 0.126314 Hz
AQ 3.9584243 sec
RG 114.4
DW 60.400 usec
DE 6.00 usec
TE 294.6 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 400.1300047 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

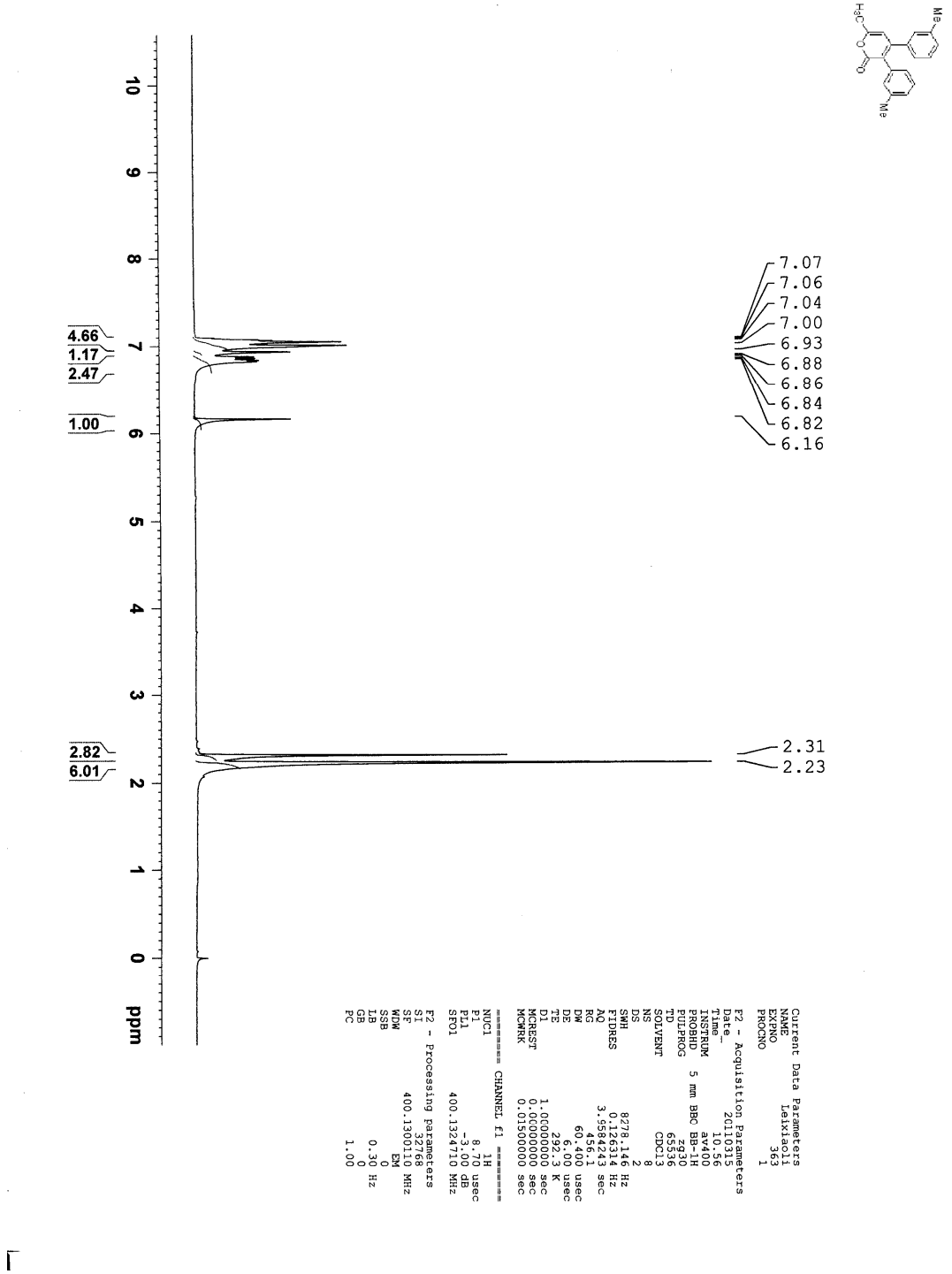

5j
163.74
161.75
158.78
151.70
132.04
130.29
128.19
126.42
120.78
114.57
113.71
107.14
103.15
77.38
77.06
76.74
55.46
55.17
19.86
200
180
160
140
120
100
80
60
40
20
ppm

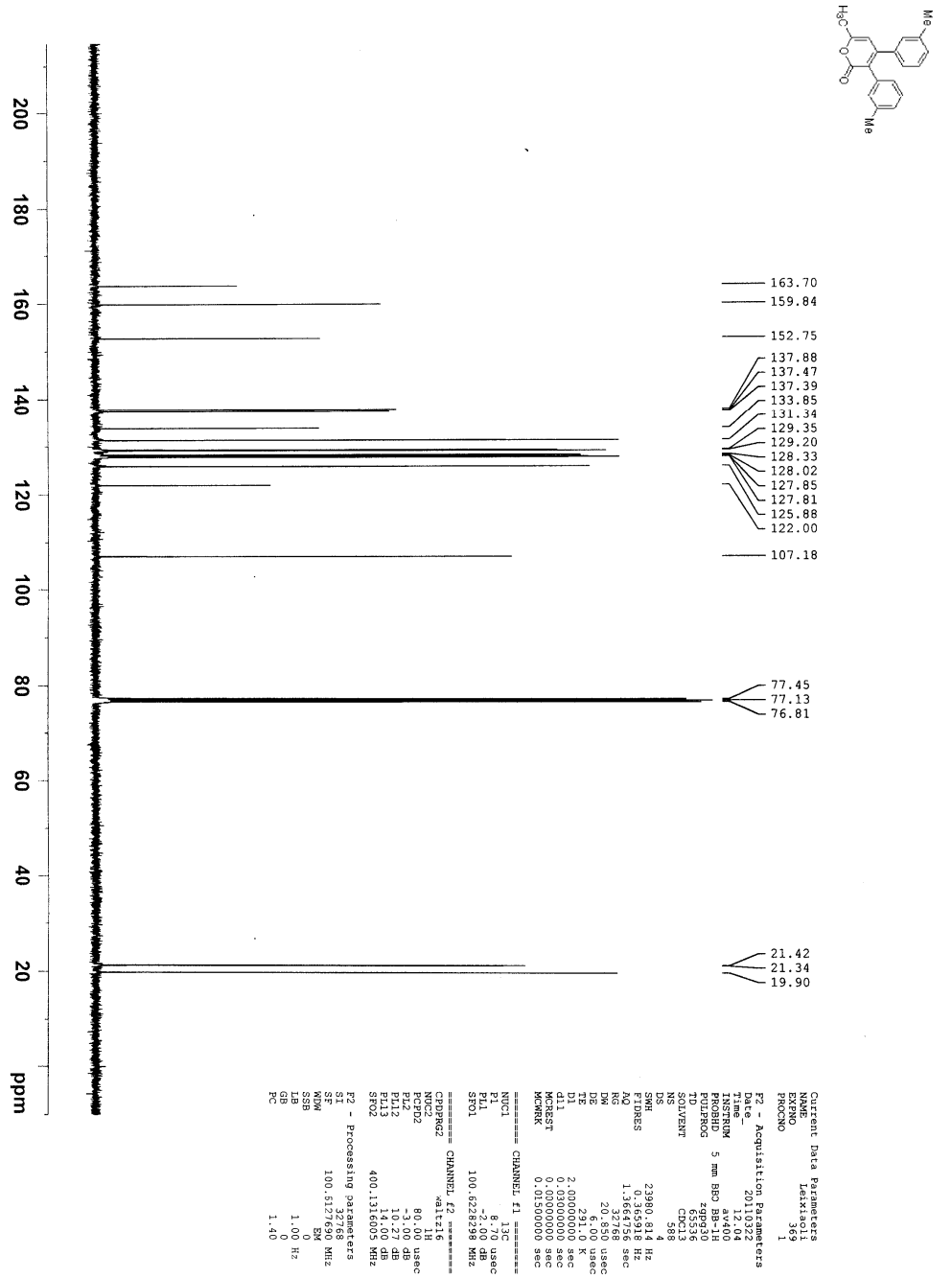

7.217
7.195
7.061
7.048
7.044
7.039
7.032
7.027
6.778
6.756
6.109
3.768
2.318
1.92
3.80
1.91
0.90
3.00
3.00
ppm
Current Data Parameters
NAME leixiaoli
EXPNO 192
PROCNO 1
F2 - Acquisition Parameters
Date_ 20100329
Time_ 15.07
INSTRUM av400
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 2
SWH 8278.146 Hz
FIDRES 0.126334 Hz
AQ 3.9584243 sec
RG 1149.4
DW 60.400 usec
DE 6.00 usec
TE 294.5 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 400.1300065 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

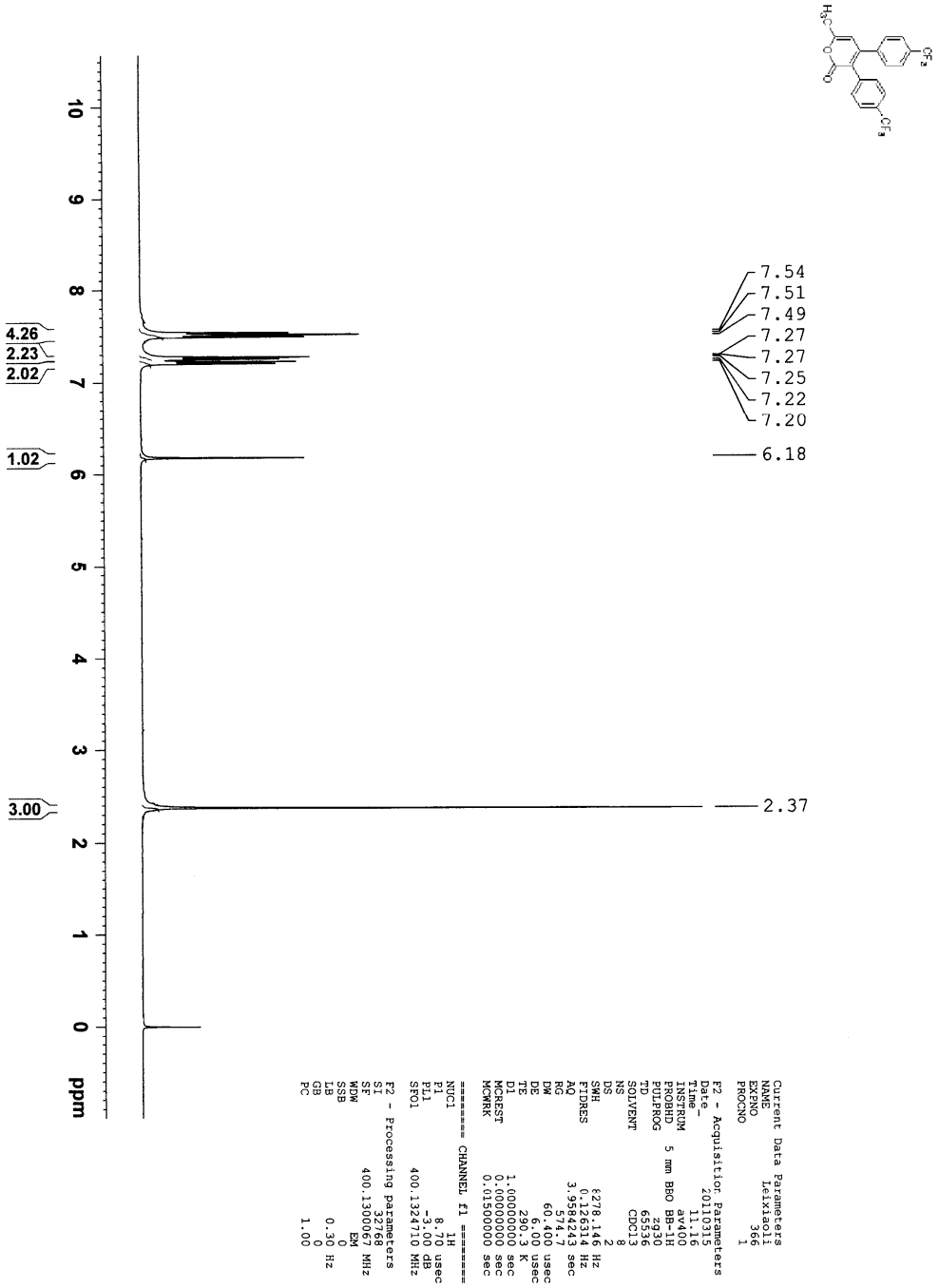

5k
163.56
159.96
159.04
150.75
136.20
134.63
132.01
130.06
128.63
125.62
121.84
113.67
106.72
77.37
77.05
76.73
55.18
19.89
200
180
160
140
120
100
80
60
40
20
ppm

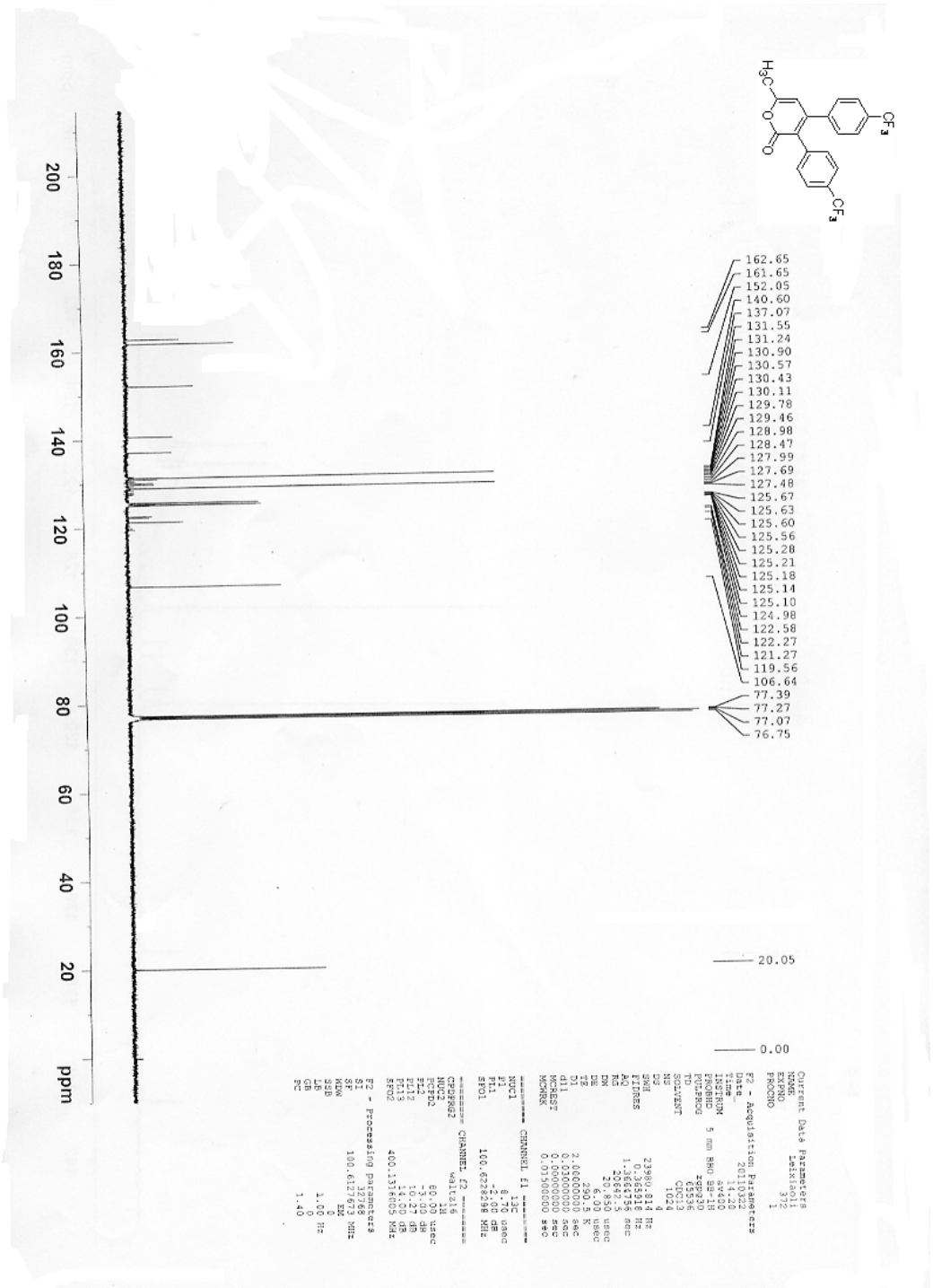


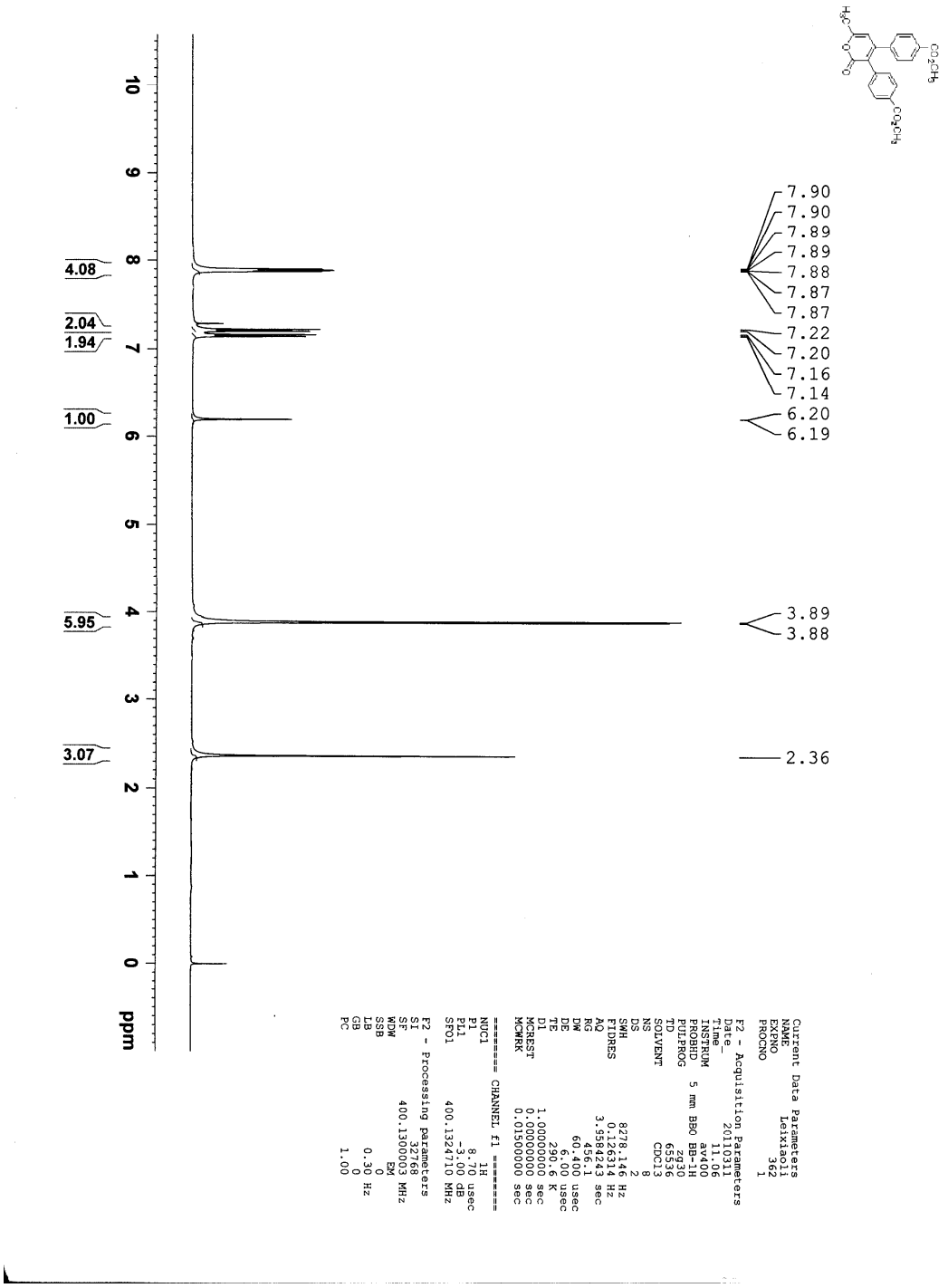

166.42
163.20
160.56
151.58
142.13
133.33
130.74
130.10
129.52
128.71
128.12
127.88
122.62
106.58
77.36
77.05
76.73
52.27
19.95
200
180
160
140
120
100
80
60
40
20
ppm
Current Data Parameters
NAME Le.Xiaoli
EXPNO 367
PROCNO 1
F2 - Acquisition Parameters
Date_ 20110319
Time_ 13.23
INSTRUM av400
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 857
DS 4
SWH 23980.814 Hz
FIDRES 1.465918 Hz
AQ 1.3664758 sec
RG 4596.5
DW 20.850 usec
DE 6.00 usec
TE 294.2 K
D1 2.00000000 sec
D11 0.01000000 sec
MCREST 0.00000000 sec
MCWRK 0.0:500000 sec
======== CHANNEL f1 ========
NUC1 13c
P1 8.70 usec
PL1 -2.00 dB
SFO1 100.622898 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 13.00 dB
PL12 10.27 dB
PL13 10.00 dB
SFO2 400.:316005 MHz
F2 - Processing parameters
SI 32768
SF 100.612768 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

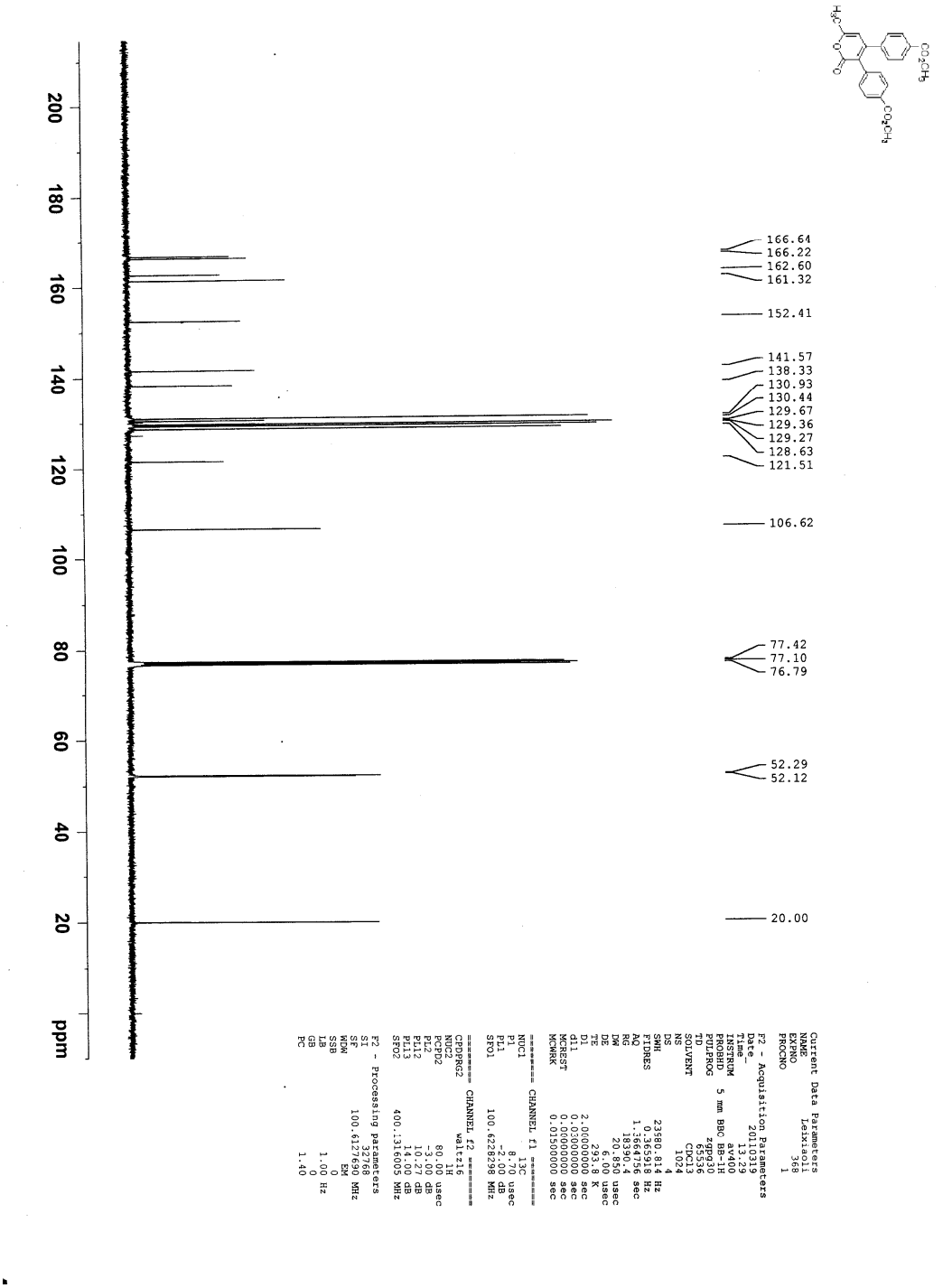

4.66
1.17
2.47
1.00
2.82
6.01
7.07
7.06
7.04
7.00
6.93
6.88
6.86
6.84
6.82
6.16
2.31
2.23
ppm
Current Data Parameters
NAME Leixiaoli
EXPNO 363
PROCNO 1
F2 - Acquisition Parameters
Date_ 20110315
Time_ 10.56
INSTRUM av400
PROBHD 5 mm BBC BB-1H
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 2
SWH 8778.146 Hz
FIDRES 0.126314 Hz
AQ 3.5584243 sec
RG 456.1
DW 60.400 usec
DE 6.00 usec
TE 292.3 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 400.1300110 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00


Me
H3C
O
O
Me
163.70
159.84
152.75
137.88
137.47
137.39
133.85
131.34
129.35
129.20
128.33
128.02
127.85
127.81
125.88
122.00
107.18
77.45
77.13
76.81
21.42
21.34
19.90
200
180
160
140
120
100
80
60
40
20
ppm
Current Data Parameters
NAME Leixiaoli
EXPNO 369
PROCNO 1
F2 - Acquisition Parameters
Date_ 20110322
Time_ 12.04
INSTRUM av400
PROBHD 5 mm BBO BB-1H
PULPROG zg530
TD 65536
SOLVENT CDCl3
NS 588
DS 4
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 32768
DW 20.850 usec
DE 6.00 usec
TE 295.1 K
D1 2.00000000 sec
d11 0.03000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 8.70 usec
PL1 -2.00 dB
SFO1 100.6228298 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 1.00 dB
PL12 13.20 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


7.54
7.51
7.49
7.27
7.27
7.25
7.22
7.20
6.18
2.37
4.26
2.23
2.02
1.02
3.00
ppm
Current Data Parameters
NAME Leikaioli
EXPNO 366
PROCNO 1
F2 - Acquisition Parameters
Date_ 20110315
TIme_ 11.16
INSTRUM av400
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 2
SWH 6278.146 Hz
FIDRES 0.126314 Hz
AQ 3.9584243 sec
RG 574.7
DW 60.400 usec
DE 6.00 usec
TE 296.3 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 400.1300069 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00


H3C
O
O
CF3
CF3
162.65
161.65
152.05
140.60
137.07
131.55
131.24
130.90
130.57
130.43
130.11
129.78
129.46
128.98
128.47
127.99
127.69
127.48
125.67
125.63
125.60
125.56
125.28
125.21
125.18
125.14
125.10
124.98
122.58
122.27
121.27
119.56
106.64
77.39
77.27
77.07
76.75
20.05
0.00
200
180
160
140
120
100
80
60
40
20
ppm


7.90
7.90
7.89
7.89
7.88
7.87
7.87
7.22
7.20
7.16
7.14
6.20
6.19
3.89
3.88
2.36
4.08
2.04
1.94
1.00
5.95
3.07
ppm
Current Data Parameters
NAME Leixiaoli
EXPNO 362
PROCNO 1
F2 - Acquisition Parameters
Date_ 20110311
Time_ 11.06
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 3.958241 sec
RG 456.1
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 dBm
SFO1 400.1324710 MHz
F2 - Processing parameters
SI 32768
SF 400.1300003 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00


166.64
166.22
162.60
161.32
152.41
141.57
138.33
130.93
130.44
129.67
129.36
129.27
128.63
121.51
106.62
77.42
77.10
76.79
52.29
52.12
20.00
200
180
160
140
120
100
80
60
40
20
ppm
Current Data Parameters
NAME Leixiaoli
EXPNO 368
PROCNO 1
F2 - Acquisition Parameters
Date_ 20110319
Time 13.29
INSTRUM av400
PROBHD BB-1H 5 mm BBO
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 1024
DS 4
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 18390.4
DW 20.850 usec
DE 6.00 usec
TE 295.8 K
D1 2.00000000 sec
d11 0.03000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13c
P1 8.70 usec
PL1 -2.00 dB
SFO1 100.6228298 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -3.00 dB
PL12 14.70 dB
PL13 14.70 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