Supplementary Material

Smiles rearrangement for the synthesis of diarylamines

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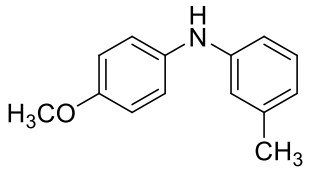
1. General remarks

^{1}H NMR and. ^{13}C NMR spectra were recorded in $CDCl_3$ (300 MHz for ^{1}H NMR and 75 MHz for. ^{13}C NMR, respectively) with tetramethylsilane as the internal reference on Bruker Advance 300 FT spectrometer. Chemical shifts were reported in parts per million. Mass spectra (MS) were measured by ESI. $CDCl_3$ were used as delivered from Sigma-Aldrich. Silica gel (70-230 mesh) was used for flash column chromatography. All the reactions were monitored by TLC using 0.25 mm silica gel plates (Merck 60F254) with UV indicator. The microwave-assisted reaction time is the hold time at the final temperature. Unless otherwise noted, other reagents were obtained from commercial suppliers and used without further purification.

2. General Procedure for the Smiles Rearrangement for the Synthesis of Diarylamines (3)

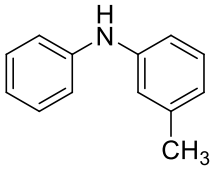
To a magnetically stirred solution of the appropriate arylamine **2** (1.0 mmol) and Cs_2CO_3 (3.2 mmol) in dry DMF cooled by ice bath were added chloroacetyl chloride (1.2 mmol) and substituted phenol **1** (1.0 mmol). The reaction mixture was then stirred for 30 min at room temperature and placed into microwave oven (600W, 150 ^oC) and irradiated for 30-80 min. The solvent was removed under vacuum and water (20 mL) was added into the residue. The mixture was then extracted by ethyl acetate (4 x 30 mL). The combined organic layers were dried over anhydrous $MgSO_4$ and evaporated under vacuum to give the crude product. Pure product was obtained by column chromatography on silica gel.

3. Synthesis and analytical data of (3a-u)



Scheme S1. *N*-(4-Methoxyphenyl)-3-methylbenzenamine **3a.**[1]

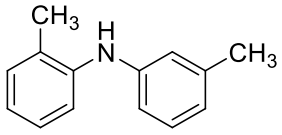
Following the general procedure, the crude product was purified over a silica gel column using petroleum ether to give a gray solid. Mp 72-75 ^oC (lit.[1] 75-76 ^oC). ^1H NMR (300 MHz, $CDCl_3$): δ 2.28 (s, 3H; CH_3), 3.80 (s, 3H; OCH_3), 5.45 (s, br, 1H; NH), 6.64-7.24 (m, 8H; Ar*H*) ppm. ^{13}C NMR (75 MHz, $CDCl_3$): δ 21.5 (CH_3), 55.6 (OCH_3), 112.8 (CH), 114.2 (CH), 114.6 (CH), 116.3 (CH), 120.5 (CH), 122.2 (CH), 129.1 (CH), 135.9 (C), 139.1 (C), 145.1 (C), 155.2 (C) ppm.



Scheme S2. 3-Methyl-*N*-phenylbenzenamine **3b.**[2]

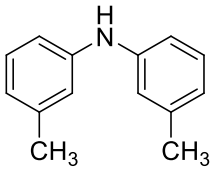
Following the general procedure, the crude product was purified over a silica gel

column using petroleum ether to give a yellow liquid. ^{1}H NMR (300 MHz, $CDCl_3$): δ 2.29 (s, 3H; CH_3), 5.58 (s, 1H; NH), 6.85-7.28 (m, 9H; Ar*H*) ppm. ^{13}C NMR (75 MHz, $CDCl_3$): δ 20.7 (CH_3), 116.8 (CH), 117.8 (CH), 118.9 (CH), 120.2 (CH), 120.9 (CH), 129.3 (CH), 129.8 (CH), 130.9 (CH), 140.2 (C), 143.9 (C) ppm.



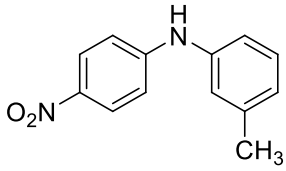
Scheme S3. 3-Methyl-*N*-*o*-tolylbenzenamine **3c.**[3]

Following the general procedure, the crude product was purified over a silica gel column using petroleum ether to give a yellow liquid. ^{1}H NMR (300 MHz, $CDCl_3$): δ 2.22 (s, 3H; CH_3), 2.28 (s, 3H; CH_3), 5.29 (s, br, 1H; NH), 6.69-7.23 (m, 9H; Ar*H*) ppm. ^{13}C NMR (75 MHz, $CDCl_3$): δ 17.8 (CH_3), 21.45 (CH_3), 114.5 (CH), 118.1 (CH), 118.8 (CH), 121.3 (CH), 121.8 (CH), 126.7 (CH), 128.1 (C), 129.1 (CH), 130.8 (CH), 139.1 (C), 141.2 (C), 143.8 (C) ppm.



Scheme S4. di*m*-Tolylamine **3d.**[4]

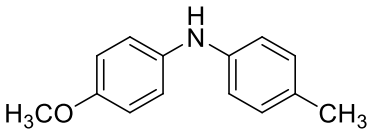
Following the general procedure, the crude product was purified over a silica gel column using petroleum ether to give a colorless liquid. ^{1}H NMR (300 MHz, $CDCl_3$): δ 2.25 (s, 6H; CH_3), 5.46 (s, br, 1H; NH), 6.69 (d, *J* = 7.2 Hz, 2H; Ar*H*), 6.79-6.83 (m, 4H; Ar*H*), 7.07-7.12 (m, 2H; Ar*H*). ppm. ^{13}C NMR (75 MHz, $CDCl_3$): δ 21.4 (CH_3), 114.8 (CH), 118.5 (CH), 121.6 (CH), 129.0 (CH), 139.0 (C), 143.1 (C) ppm.



Scheme S5. 3-Methyl-*N*-(4-nitrophenyl)benzenamine **3e.**

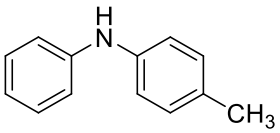
Following the general procedure, the crude product was purified over a silica gel column using petroleum ether to give a brown solid. Mp 130-133 ºC. ^{1}H NMR (300

MHz, $CDCl_3$): δ 2.37 (s, 3H; CH_3), 6.29 (s, br, 1H; NH), 6.92 (d, *J* = 8.7 Hz, 2H; Ar*H*), 6.97-7.02 (m, 3H; Ar*H*), 7.25-7.27 (m, 1H, Ar*H*), 8.11 (d, *J* = 8.5 Hz, 2H; Ar*H*) ppm. ^{13}C NMR (75 MHz, $CDCl_3$): δ 21.4 (CH_3), 113.6 (CH), 119.0 (CH), 122.6 (CH), 125.5 (CH), 126.2 (CH), 129.5 (C), 139.4 (C), 139.6 (C), 139.7 (C), 150.3 (C) ppm. MS (ESI, m/z)(%): 229 (8) [M+1], 212 (57), 182 (74), 167 (100).



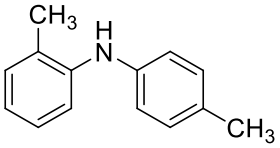
Scheme S6. *N*-(4-Methoxyphenyl)-4-methylbenzenamine **3f.**[5]

Following the general procedure, the crude product was purified over a silica gel column using petroleum ether to give a gray solid. Mp 80-82 °C (lit.[5] 82 °C). ^1H NMR (300 MHz, $CDCl_3$): δ 2.27 (s, 3H; CH_3), 3.78 (s, 3H; OCH_3), 5.38 (s, br, 1H; NH), 6.83-6.85 (m, 4H; Ar*H*), 7.00-7.04 (m, 4H; Ar*H*) ppm. ^{13}C NMR (75 MHz, $CDCl_3$): δ 20.5 (CH_3), 55.6 (OCH_3), 114.6 (CH), 116.5 (CH), 121.1 (CH), 129.3 (C), 129.8 (CH), 136.6 (C), 142.4 (C), 154.7 (C) ppm.



Scheme S7. 4-Methyl-*N*-phenylbenzenamine **3g.**[6]

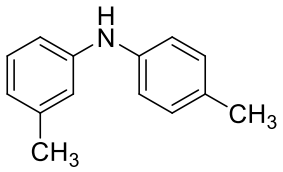
Following the general procedure, the crude product was purified over a silica gel column using petroleum ether to give a white solid. Mp 85-87 °C (lit.[6] 87 °C). ^1H NMR (300 MHz, $CDCl_3$): δ 2.24 (s, 3H; CH_3), 5.49 (s, br, 1H; NH), 6.54-7.22 (m, 9H; Ar*H*) ppm.



Scheme S8. 4-Methyl-*N*-*o*-tolylbenzenamine **3h.**[7]

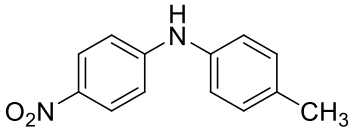
Following the general procedure, the crude product was purified over a silica gel column using petroleum ether to give a yellow viscous oil. ^1H NMR (300 MHz, $CDCl_3$): δ 2.25 (s, 3H; CH_3), 2.30 (s, 3H; CH_3), 5.29 (s, br, 1H; NH), 6.85-6.95 (m, 3H; Ar*H*), 7.06-7.24 (m, 5H; Ar*H*) ppm. ^{13}C NMR (75 MHz, $CDCl_3$): δ 17.8 (CH_3),

20.6 (CH_3), 117.2 (CH), 118.6 (CH), 121.0 (CH), 126.7 (CH), 126.9 (C), 129.8 (CH), 130.4 (C), 130.8 (CH), 141.0 (C), 142.0 (C) ppm.



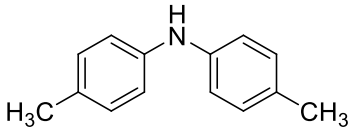
Scheme S8. 4-Methyl-*N*-*m*-tolylbenzenamine **3i.**[8]

Following the general procedure, the crude product was purified over a silica gel column using petroleum ether to give a yellow viscous oil. ^{1}H NMR (300 MHz, $CDCl_3$): δ 2.27 (d, 6H; CH_3), 5.49 (s, br, 1H; NH), 6.68 (d, *J* = 7.2 Hz, 1H; Ar*H*), 6.80 -7.21 (m, 7H; Ar*H*) ppm. ^{13}C NMR (75 MHz, $CDCl_3$): δ 20.6 (CH_3), 21.5 (CH_3), 113.9 (CH), 117.5 (CH), 118.8 (CH), 121.1 (CH), 129.1 (CH), 129.8 (CH), 130.7 (C), 139.1 (C), 140.3 (C), 143.8 (C) ppm.



Scheme S9. 4-Methyl-*N*-(4-nitrophenyl)benzenamine **3j.**[9]

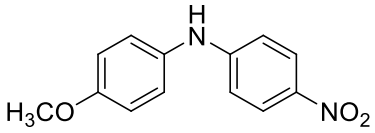
Following the general procedure, the crude product was purified over a silica gel column using petroleum ether to give a brown solid. Mp 132-135 ºC (lit.[9] 137 ºC). ^{1}H NMR (300 MHz, $CDCl_3$): δ 2.36 (s, 6H; CH_3), 6.29 (s, br, 1H; NH), 6.86 (d, *J* = 9.0 Hz, 2H; Ar*H*), 7.11 (d, *J* = 8.1 Hz, 2H; Ar*H*), 7.19 (d, *J* = 8.0 Hz, 2H; Ar*H*), 8.08 (d, *J* = 9.0 Hz, 2H; Ar*H*) ppm. ^{13}C NMR (75 MHz, $CDCl_3$): δ 20.9 (CH_3), 113.1 (CH), 122.6 (CH), 126.2 (CH), 130.2 (CH), 134.8 (C), 136.6 (C), 139.2 (C), 150.8 (C) ppm.



Scheme S10. di*p*-Tolylamine **3k.**[10]

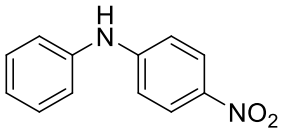
Following the general procedure, the crude product was purified over a silica gel column using petroleum ether to give a light yellow solid. Mp 74-77 ºC (lit.[10] 73-75 ºC). ^{1}H NMR (300 MHz, $CDCl_3$): δ 2.28 (s, 6H; CH_3), 5.49 (s, br, 1H; NH), 6.93 (d, *J* = 8.0 Hz, 4H; Ar*H*), 7.05 (d, *J* = 8.0 Hz, 4H; Ar*H*) ppm. ^{13}C NMR (75 MHz, $CDCl_3$):

δ 20.6 (CH_3), 117.9 (CH), 129.8 (CH), 130.1 (C), 141.1 (C) ppm.



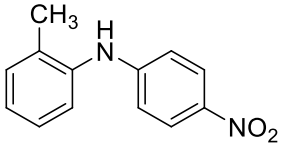
Scheme S11. *N*-(4-Methoxyphenyl)-4-nitrobenzenamine **3l.**[11]

Following the general procedure, the crude product was purified over a silica gel column using petroleum ether to give a brown solid. Mp 149-152 °C (lit.[11] 152-153 °C). ^{1}H NMR (300 MHz, $CDCl_3$): δ 3.84 (s, 3H; OCH_3), 6.16 (s, 1H; NH), 6.76 (d, *J* = 8.8 Hz, 2H; Ar*H*), 6.94 (d, *J* = 8.4 Hz, 2H; Ar*H*), 7.16 (d, *J* = 8.4 Hz, 2H; Ar*H*), 8.08 (d, *J* = 8.8 Hz, 2H; Ar*H*) ppm. ^{13}C NMR (75 MHz, $CDCl_3$): δ 55.5 (OCH_3), 112.6 (CH), 114.9 (CH), 125.5 (CH), 126.3 (CH), 131.9 (C), 139.0 (C), 151.7 (C), 157.4 (C) ppm.



Scheme S12. 4-Nitro-*N*-phenylbenzenamine **3m.**[12]

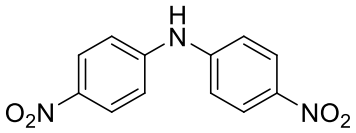
4Following the general procedure, the crude product was purified over a silica gel column using petroleum ether to give a brown solid. Mp 131-133 °C (lit.[12] 131 °C). ^{1}H NMR (300 MHz, $CDCl_3$): δ 6.40 (s, 1H; NH), 6.94 (d, *J* = 9.0 Hz, 2H; Ar*H*), 7.14-7.42 (m, 5H; Ar*H*), 8.11 (d, *J* = 9.0 Hz, 2H; Ar*H*) ppm. ^{13}C NMR (75 MHz, $CDCl_3$): δ 113.6 (CH), 121.9 (CH), 124.6 (C), 126.2 (CH), 139.4 (C), 139.6 (C), 150.2 (C) ppm.



Scheme S13. 4-Nitro-*N*-*o*-tolylbenzenamine **3n.**

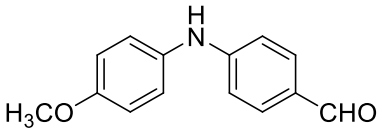
Following the general procedure, the crude product was purified over a silica gel column using petroleum ether to give a brown solid. Mp 130-133 °C. ^{1}H NMR (300 MHz, $CDCl_3$): δ 2.25 (s, 3H; CH_3), 6.10 (s, 1H; NH), 6.72 (d, *J* = 8.9 Hz, 2H; Ar*H*), 7.18-7.31 (m, 4H; Ar*H*), 8.08 (d, *J* = 8.9 Hz, 2H; Ar*H*) ppm. ^{13}C NMR (75 MHz, $CDCl_3$): δ 17.8 (CH_3), 113.0 (CH), 124.7 (CH), 126.1 (CH), 126.2 (CH), 127.1 (CH),

131.4 (CH), 133.2 (C), 137.5 (C), 139.1 (C), 151.3 (C) ppm. MS (ESI, *m/z*)(%): 229 (9) [M+1], 212 (100), 182 (77), 168 (94).



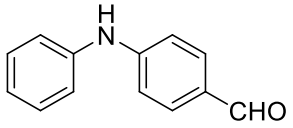
Scheme S14. 3-methyl-*N*-(3-nitrophenyl)benzenamine **3o.**[13]

Following the general procedure, the crude product was purified over a silica gel column using petroleum ether to give a yellow solid. Mp 145-147 ºC (lit.[13] 146 ºC); ^{1}H NMR (300 MHz, $CDCl_3$): δ4.36 (s, br, 1H; NH), 6.63 (d, *J* = 8.9 Hz, 2H; Ar*H*), 7.21-7.26 (m, 3H; Ar*H*), 8.1 (d, *J* = 8.8 Hz, 1H; Ar*H*), 8.2 (d, *J*=8.9 Hz, 2H; Ar*H*) ppm. ^{13}C NMR (75 MHz, $CDCl_3$): δ113.2 (CH), 117.2 (CH), 125.9 (CH), 126.2 (C) ppm.



Scheme S15. 4-(4-methoxyphenylamino)benzaldehyde **3p.**[14]

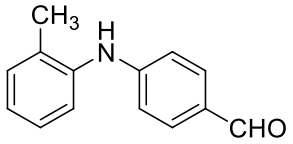
Following the general procedure, the crude product was purified over a silica gel column using petroleum ether to give a brown solid. Mp 108-111 ºC (lit.[14] 113 ºC). ^{1}H NMR (300 MHz, $CDCl_3$): δ 3.83 (s, 3H; OCH_3), 6.08 (s, 1H; NH), 6.85 (d, *J* = 8.4 Hz, 2H; Ar*H*), 6.92 (d, *J* = 8.7 Hz, 2H; Ar*H*), 7.16 (d, *J* = 8.7 Hz, 2H; Ar*H*), 7.70 (d, *J* = 8.4 Hz, 2H; Ar*H*), 9.75 (s, 1H; CHO) ppm. ^{13}C NMR (75 MHz, $CDCl_3$): δ 55.5 (OCH_3), 113.4 (CH), 114.8 (CH), 125.1 (CH), 127.8 (C), 132.2 (CH), 132.6 (C), 151.4 (C), 157.0 (C), 190.2 (CHO) ppm.



Scheme S16. 4-(phenylamino)benzaldehyde **3q.**[15]

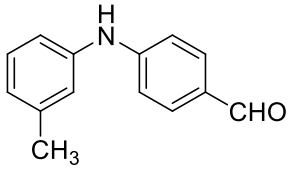
Following the general procedure, the crude product was purified over a silica gel column using petroleum ether to give a brown solid. Mp 94-97 ºC (lit.[15] 95-97 ºC). ^{1}H NMR (300 MHz, $CDCl_3$): δ 6.38 (s, 1H; NH), 7.02 (d, *J* = 8.2 Hz, 2H; Ar*H*), 7.09-7.39 (m, 5H; Ar*H*), 7.74 (d, *J* = 8.2 Hz, 2H; Ar*H*), 9.78 (s, 1H; CHO) ppm. ^{13}C NMR (75 MHz, $CDCl_3$): δ 114.4 (CH), 121.3 (CH), 123.8 (CH), 128.4 (C), 129.5

(CH), 132.1 (CH), 140.0 (C), 149.8 (C), 190.4 (CHO) ppm.



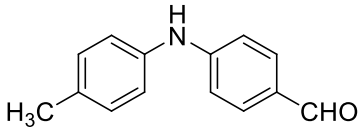
Scheme S17. 4-(*o*-toluidino)benzaldehyde **3r.**

Following the general procedure, the crude product was purified over a silica gel column using petroleum ether to give a brown solid. Mp 85-87 ºC. ^{1}H NMR (300 MHz, $CDCl_3$): δ 2.25 (s, 3H; CH_3), 6.00 (s, 1H; NH), 6.82 (d, *J* = 8.4 Hz, 2H; Ar*H*), 7.13-7.27 (m, 4H; Ar*H*), 7.71 (d, *J* = 8.4 Hz, 2H; Ar*H*), 9.76 (s, 1H; CHO) ppm. ^{13}C NMR (75 MHz, $CDCl_3$): δ 17.9 (CH_3), 113.8 (CH), 124.1 (CH), 125.4 (CH), 127.0 (CH), 127.9 (C), 131.3 (CH), 132.1 (CH), 132.6 (C), 138.0 (C), 151.0 (C), 190.3 (CHO) ppm. MS (ESI, *m/z*)(%): 212 (28) [M+1], 184 (12), 183 (9), 182 (14), 169 (52), 168 (24), 103 (48), 88 (100), 75 (11), 60 (10).



Scheme S18. 4-(*m*-toluidino)benzaldehyde **3s.**

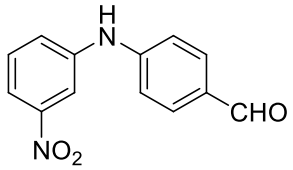
Following the general procedure, the crude product was purified over a silica gel column using petroleum ether to give a brown solid. Mp 117-119 ºC. ^{1}H NMR (300 MHz, $CDCl_3$): δ 2.34 (s, 3H; CH_3), 6.37 (s, 1H; NH), 6.92-7.24 (m, 6H; Ar*H*), 7.71-7.74 (d, *J* = 8.3 Hz, 2H; Ar*H*), 9.77 (s, 1H; CHO) ppm. ^{13}C NMR (75 MHz, $CDCl_3$): δ 21.4 (CH_3), 114.4 (CH), 118.3 (CH), 121.9 (CH), 124.7 (CH), 128.2 (C), 129.3 (CH), 132.1 (CH), 139.5 (C), 139.9 (C), 150.0 (C), 190.4 (CHO) ppm. MS (ESI, *m/z*)(%): 212 (33) [M+1], 183 (21), 169 (69), 103 (81), 88 (100), 75 (34), 73 (6), 60 (21).



Scheme S19. 4-(*p*-toluidino)benzaldehyde **3t.**

Following the general procedure, the crude product was purified over a silica gel

column using petroleum ether to give a brown solid. Mp 85-88 ºC. ^{1}H NMR (300 MHz, $CDCl_3$): δ 2.35 (s, 3H; CH_3), 6.20 (s, 1H; NH), 6.95 (d, *J* = 8.4 Hz, 2H; Ar*H*), 7.10 (d, *J* = 8.1 Hz, 2H; Ar*H*), 7.18 (d, *J* = 8.1 Hz, 2H; Ar*H*), 7.72 (d, *J* = 8.4 Hz, 2H; Ar*H*), 9.77 (s, 1H; CHO) ppm. ^{13}C NMR (75 MHz, $CDCl_3$): δ 20.8 (CH_3), 113.9 (CH), 122.1 (CH), 128.1 (C), 130.1 (CH), 132.1 (CH), 134.0 (C), 137.2 (C), 150.5 (C), 190.3 (CHO) ppm.



Scheme S20. 4-(3-nitrophenylamino)benzaldehyde **3u.**

Following the general procedure, the crude product was purified over a silica gel column using petroleum ether to give a yellow solid. Mp 152-155 ºC. ^{1}H NMR (300 MHz, $CDCl_3$): δ 6.35 (s, 1H; NH), 7.13 (d, *J* = 8.1 Hz, 2H; Ar*H*), 7.49-7.52 (m, 2H; Ar*H*), 7.83 (d, *J* = 8.1 Hz, 2H; Ar*H*), 7.87-8.04 (m, 2H; Ar*H*), 9.87 (s, 1H; CHO) ppm. ^{13}C NMR (75 MHz, $CDCl_3$): δ 114.1 (CH), 116.1 (CH), 117.6 (CH), 122.3 (C), 125.2 (C), 130.4 (C), 132.1 (CH), 142.1 (C), 147.6 (C), 148.5 (C), 190.3 (CHO) ppm. MS (ESI, *m/z*)(%): 243 (16) [M+1], 197 (42), 168 (80), 167 (100).

4. References

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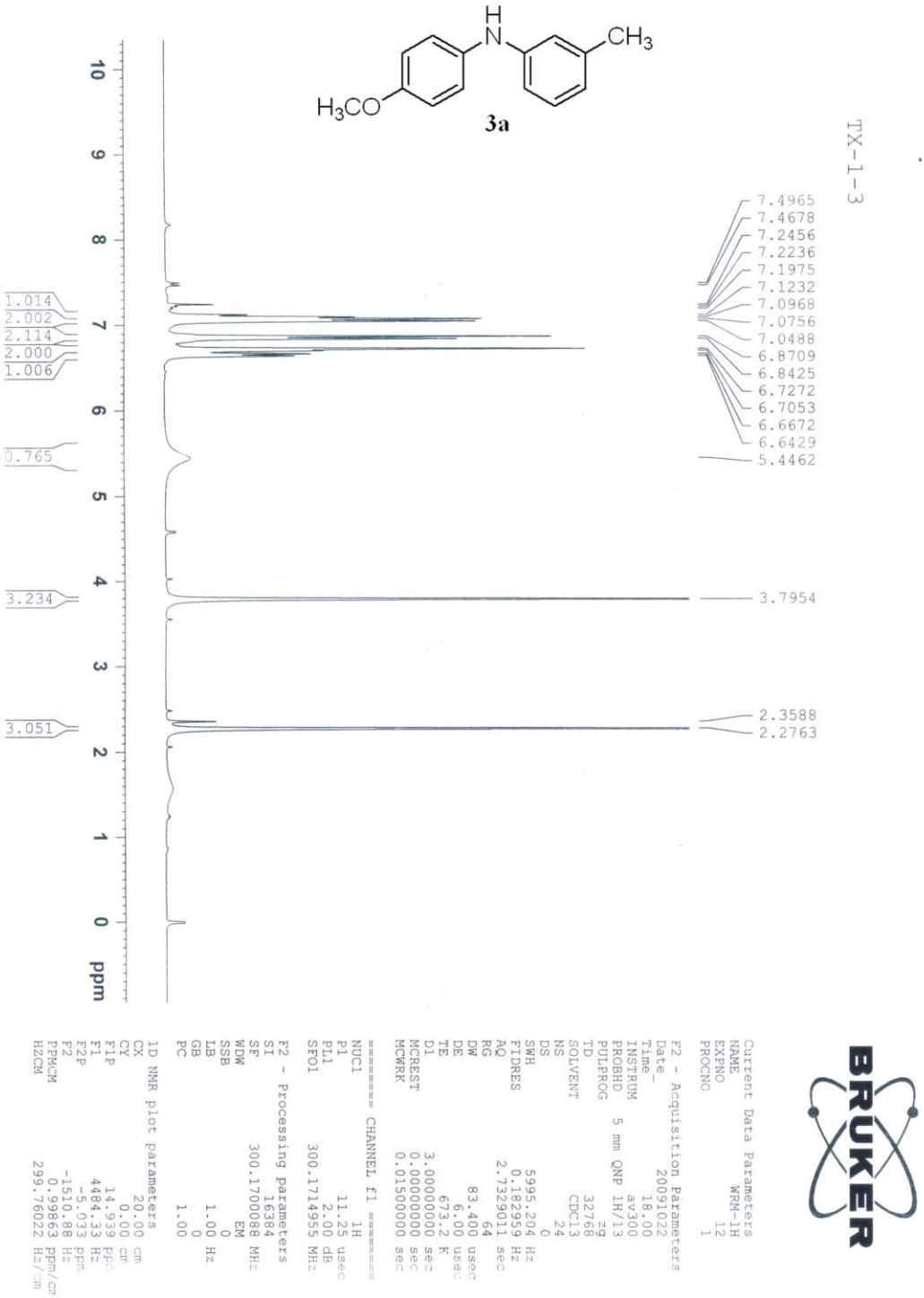
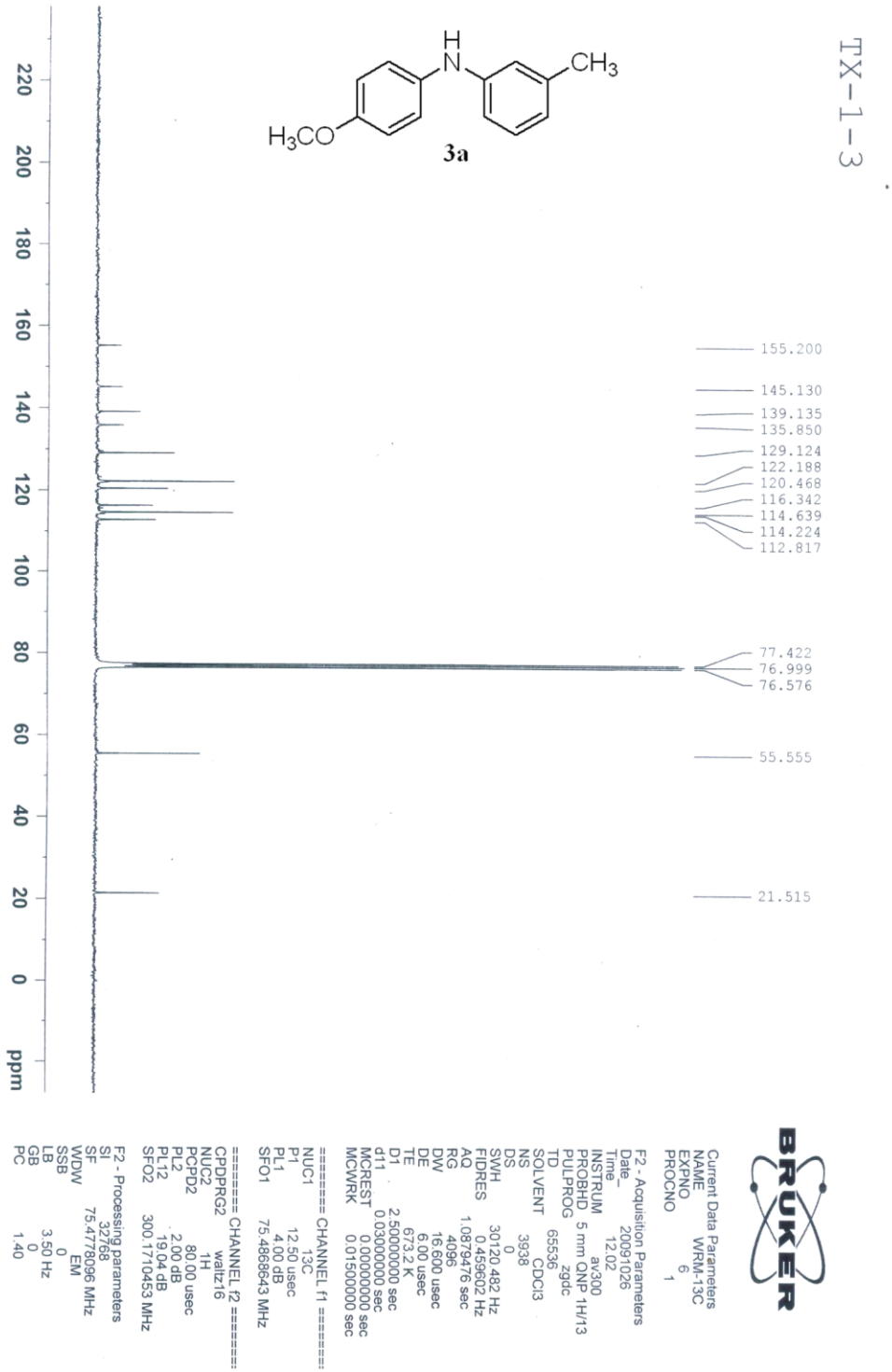
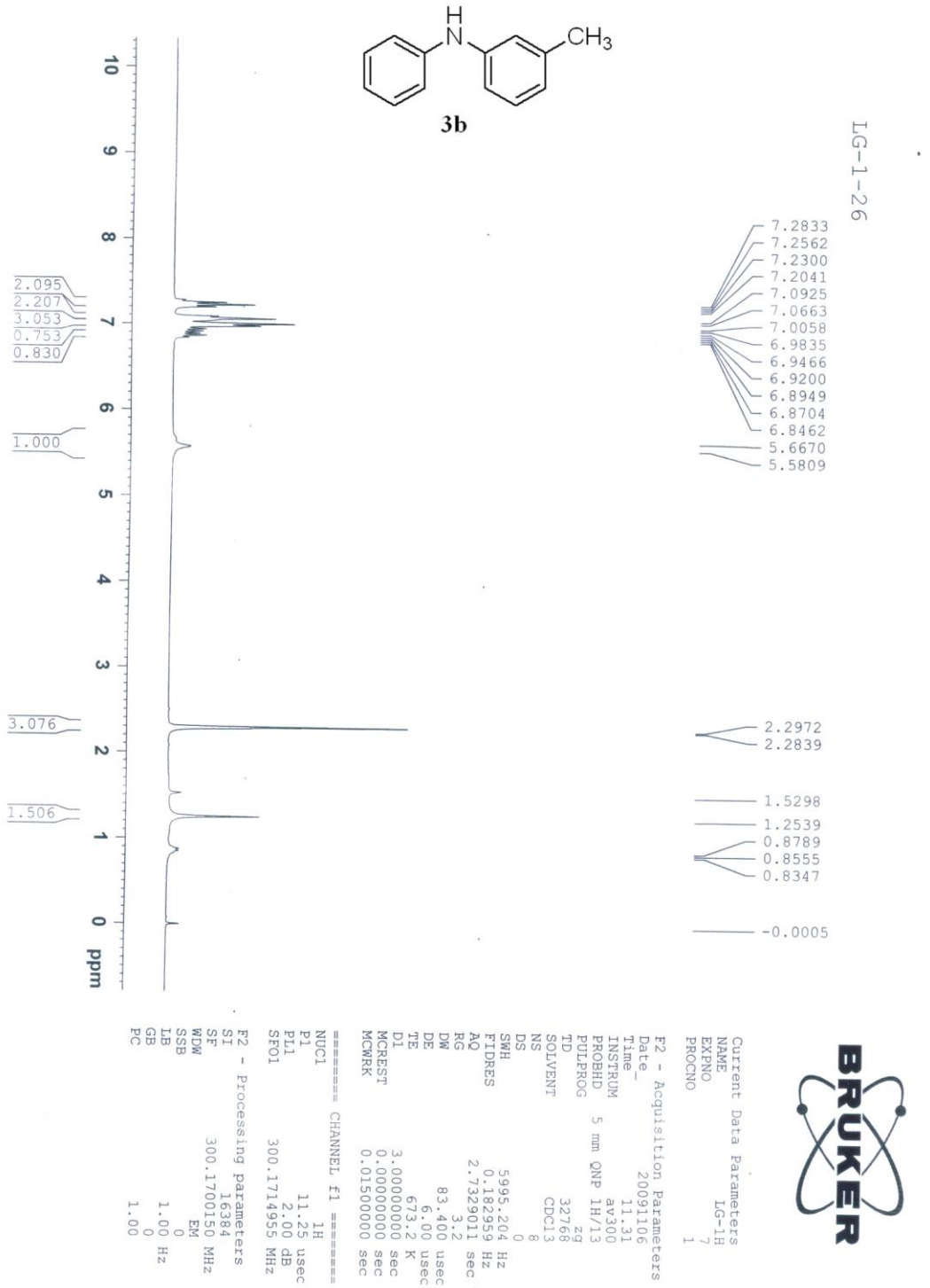
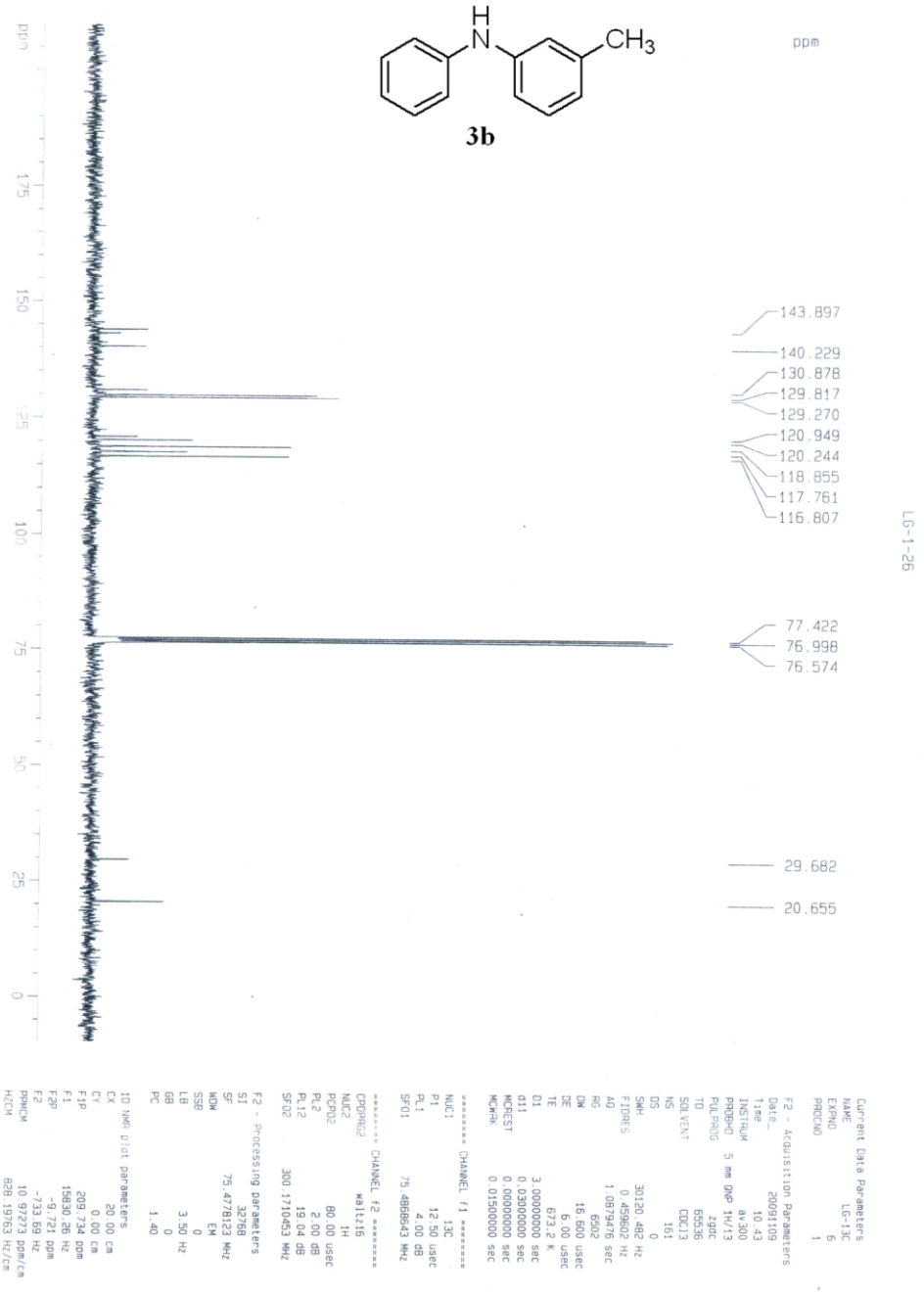
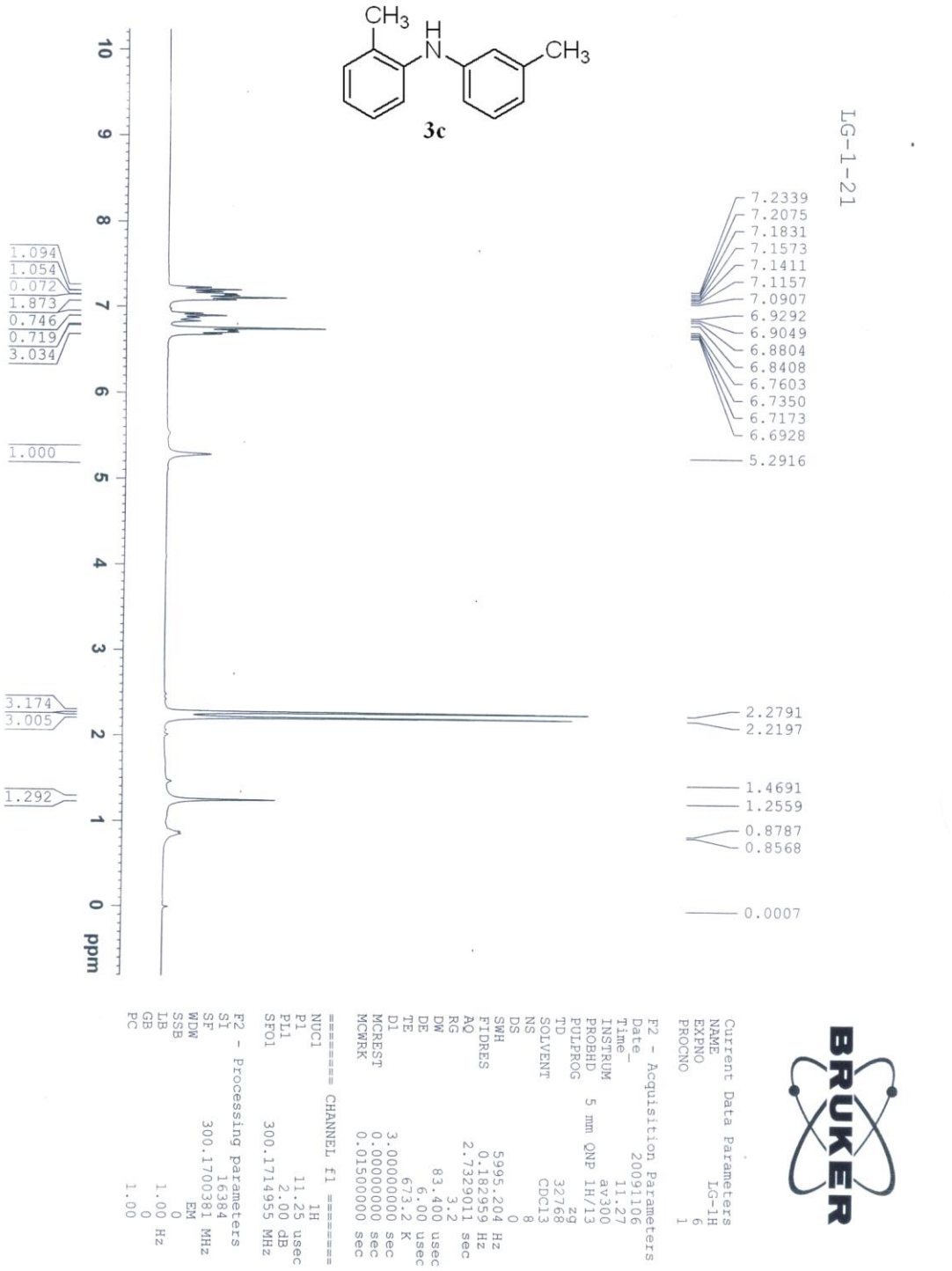
5. Copies of NMR and MS spectra for compounds

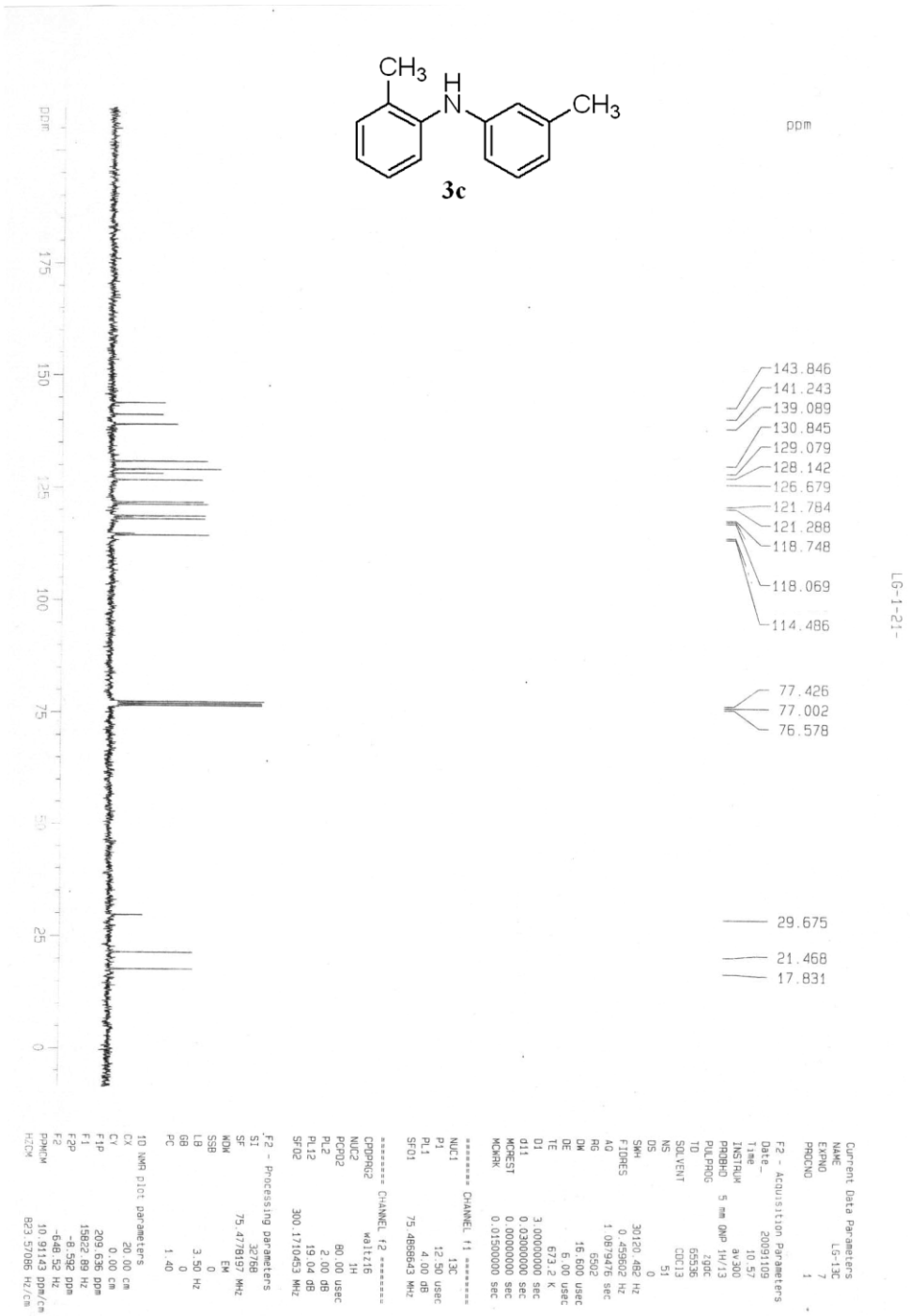


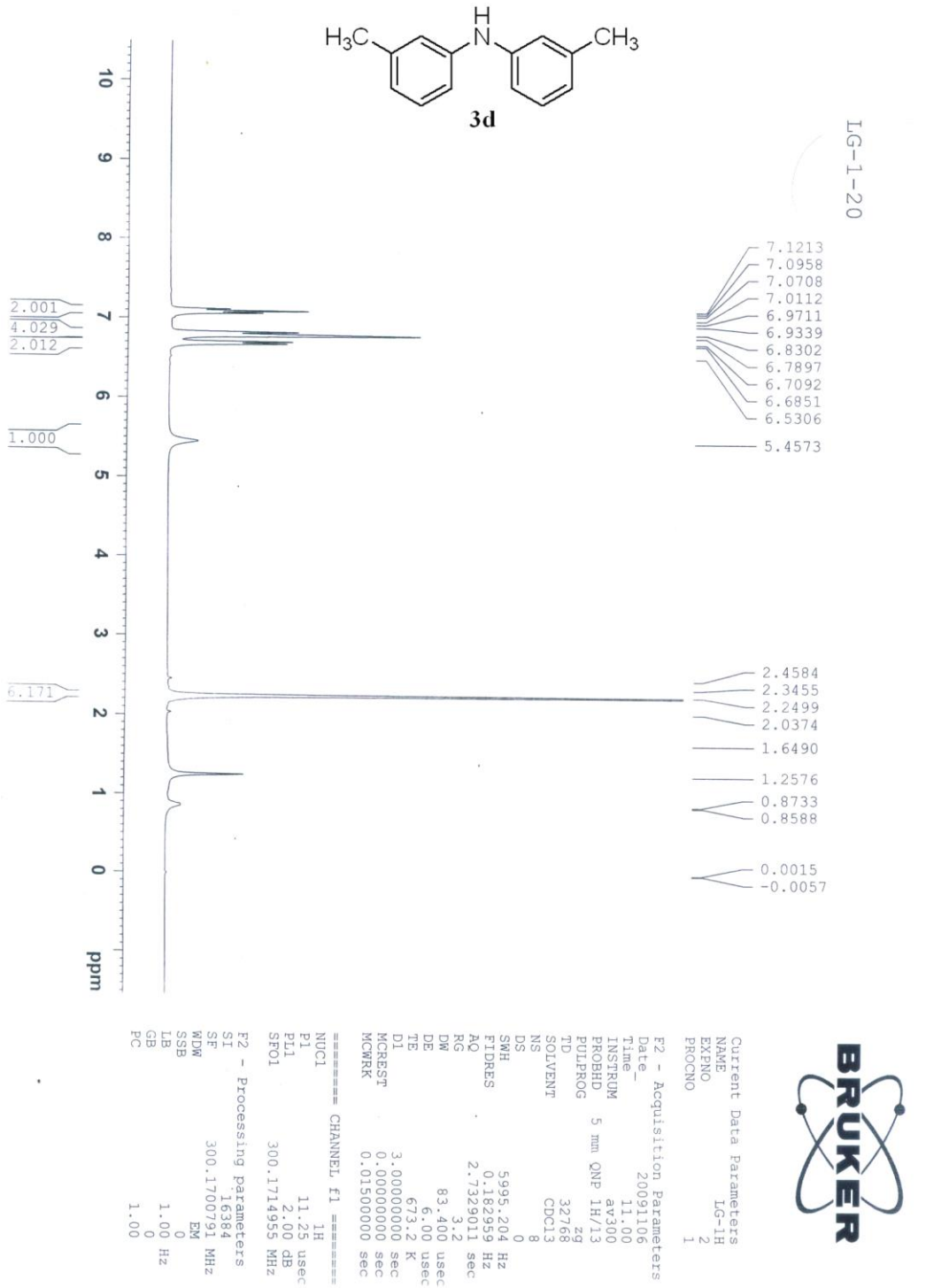


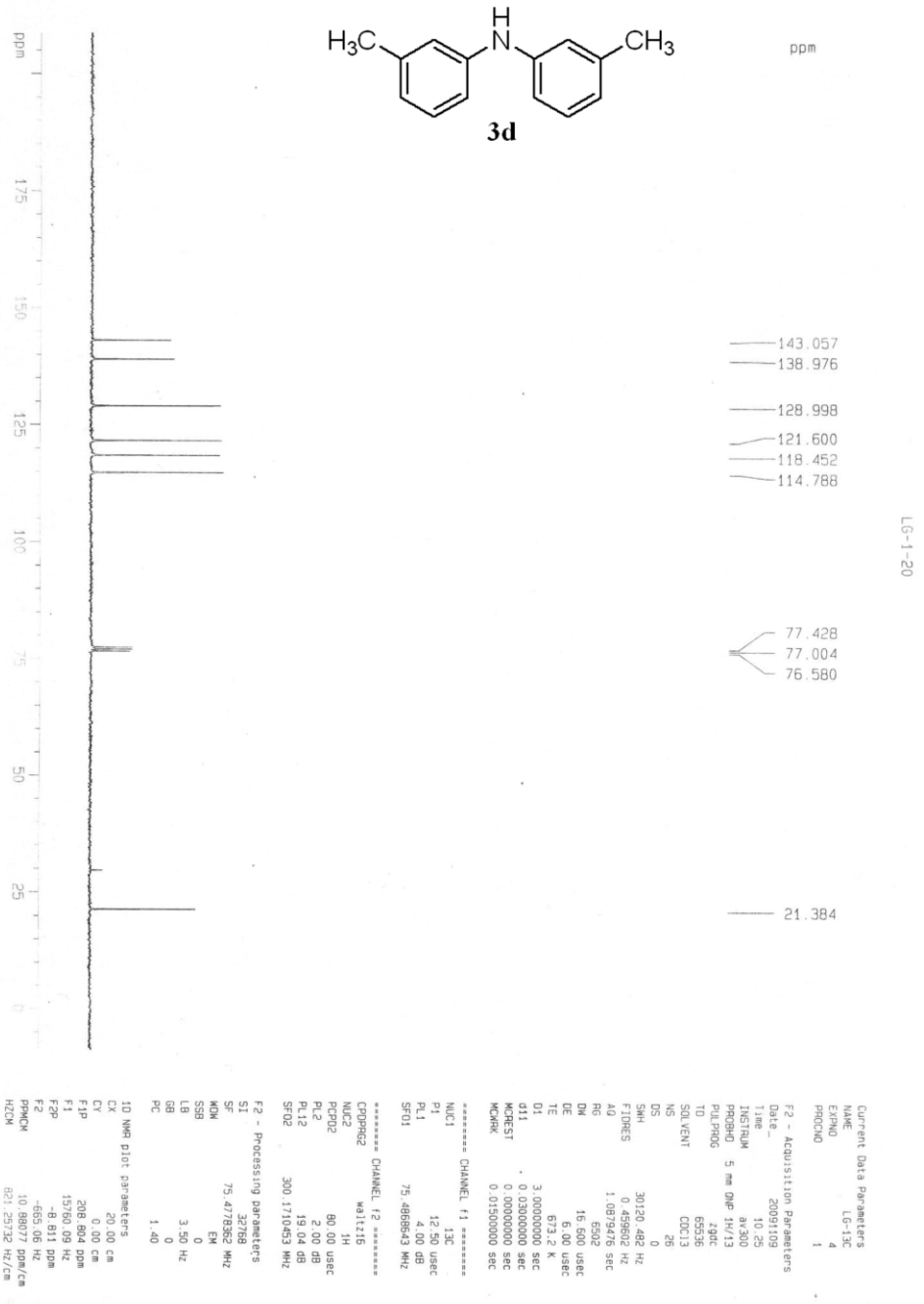


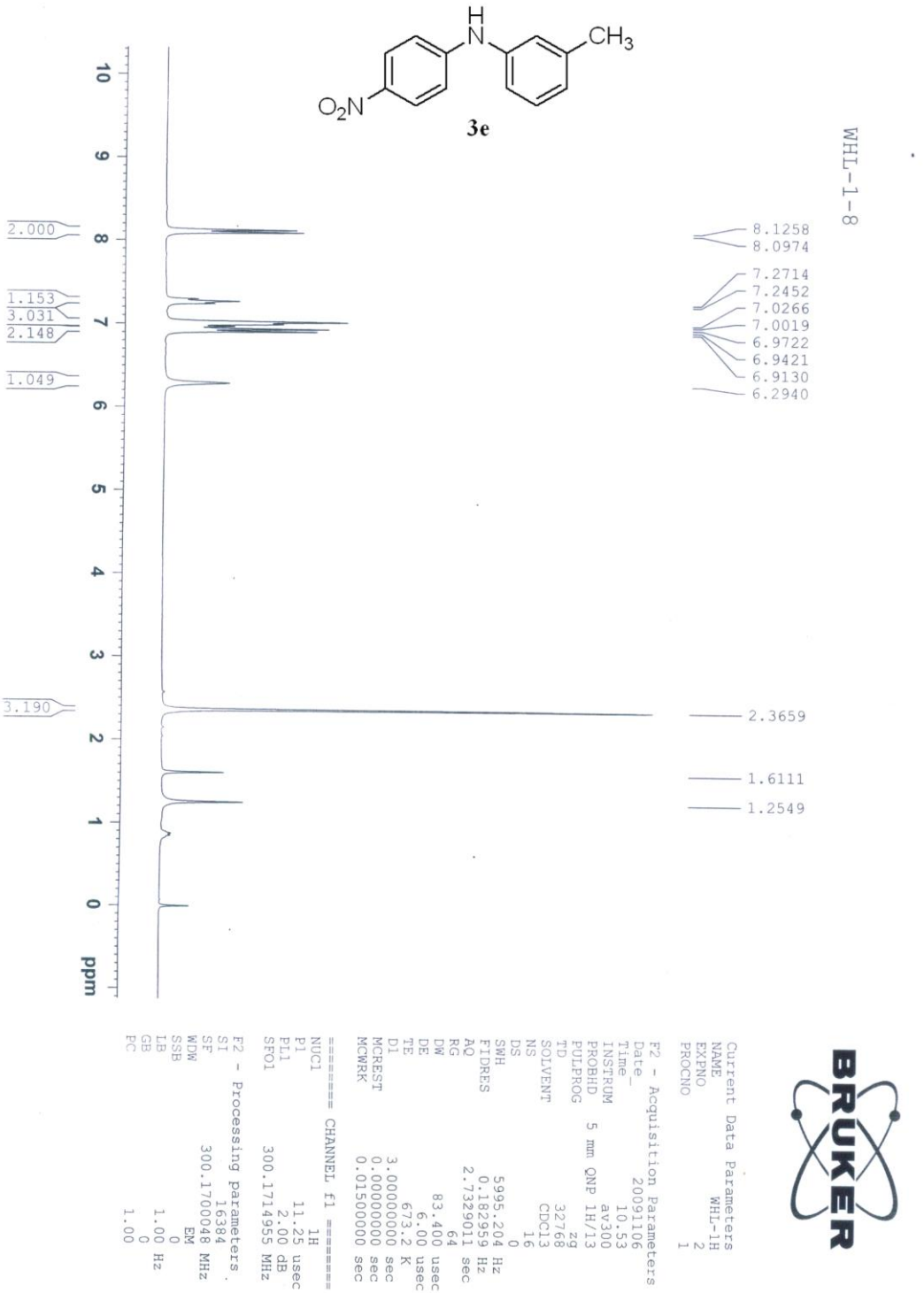


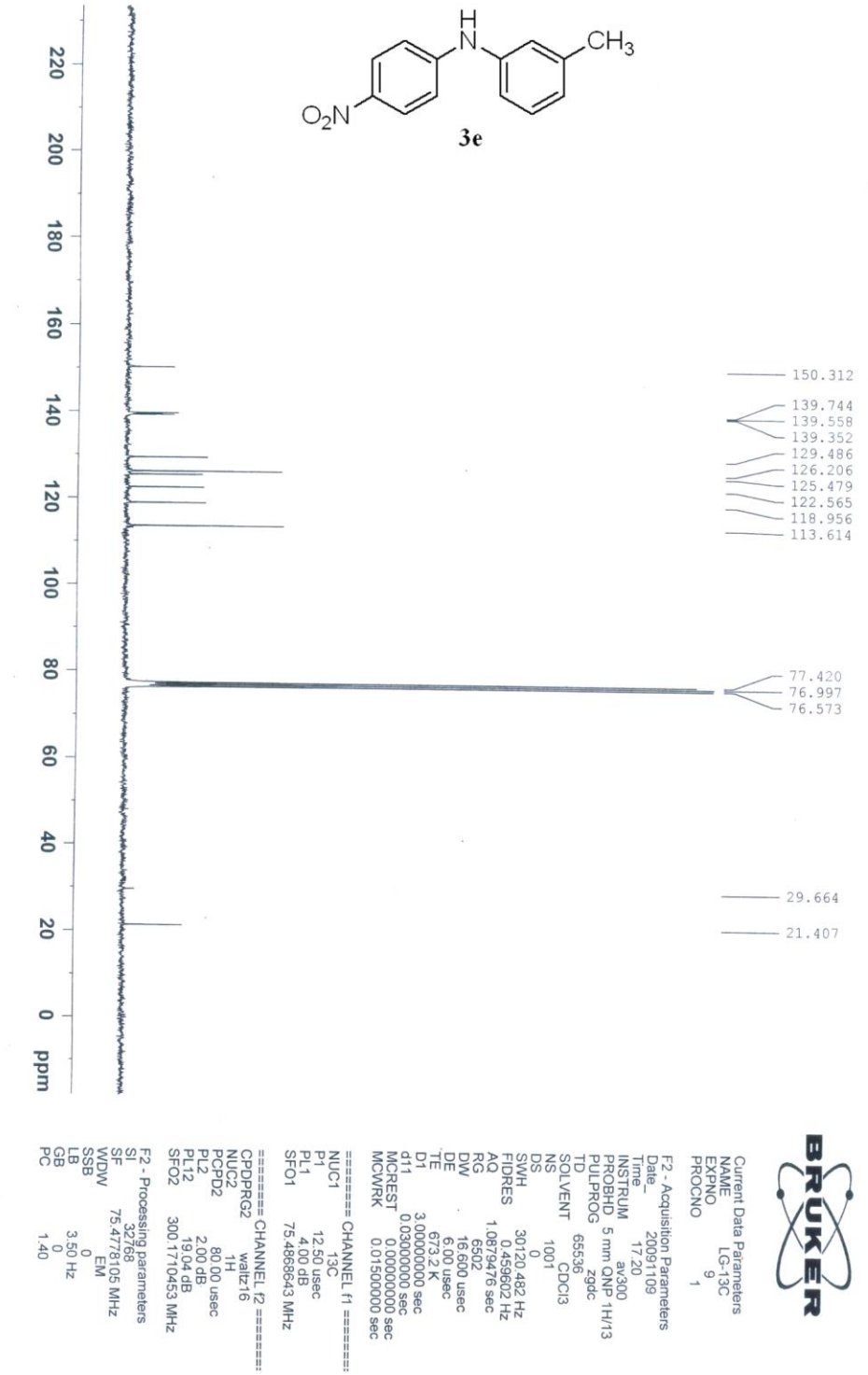


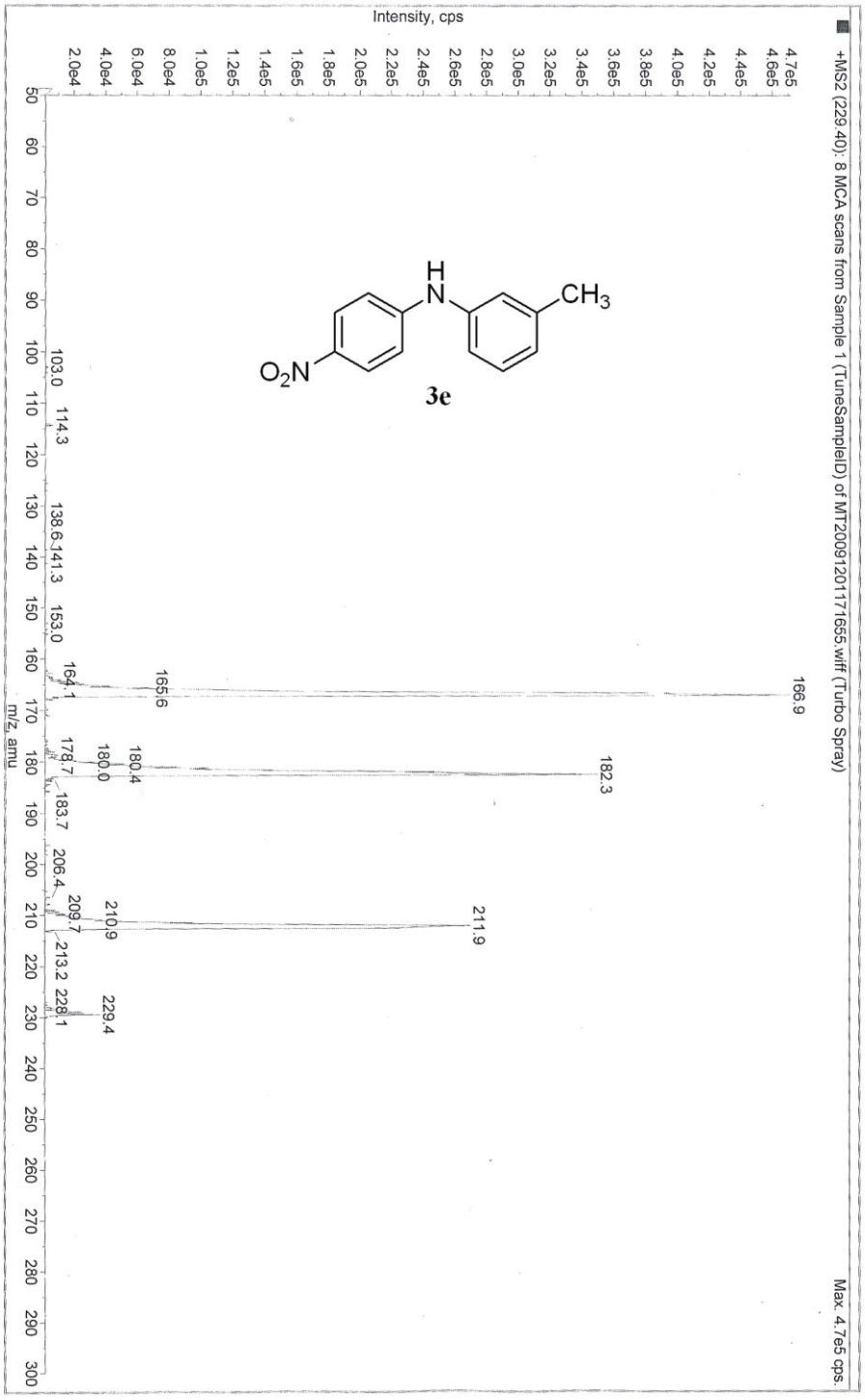


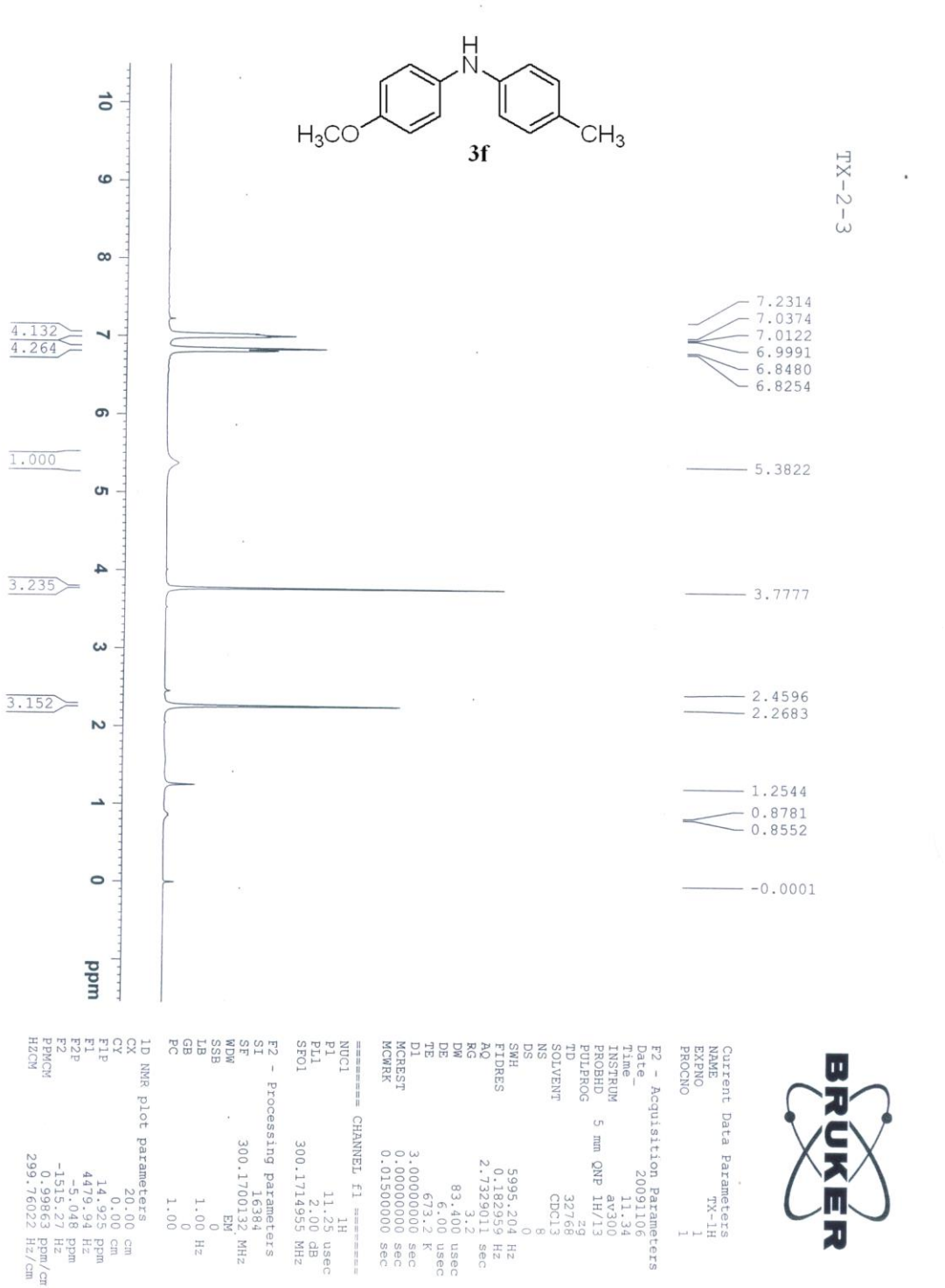


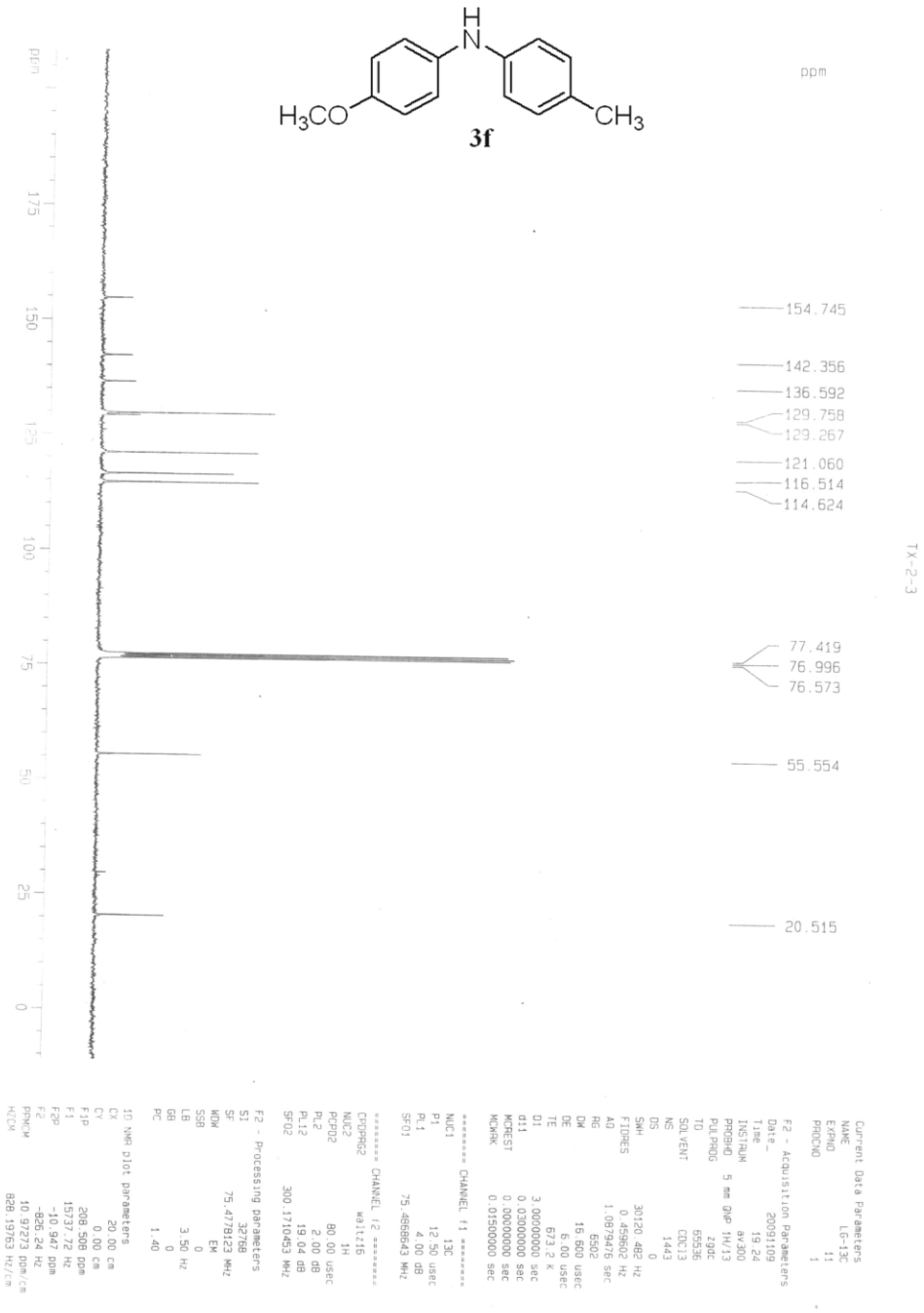


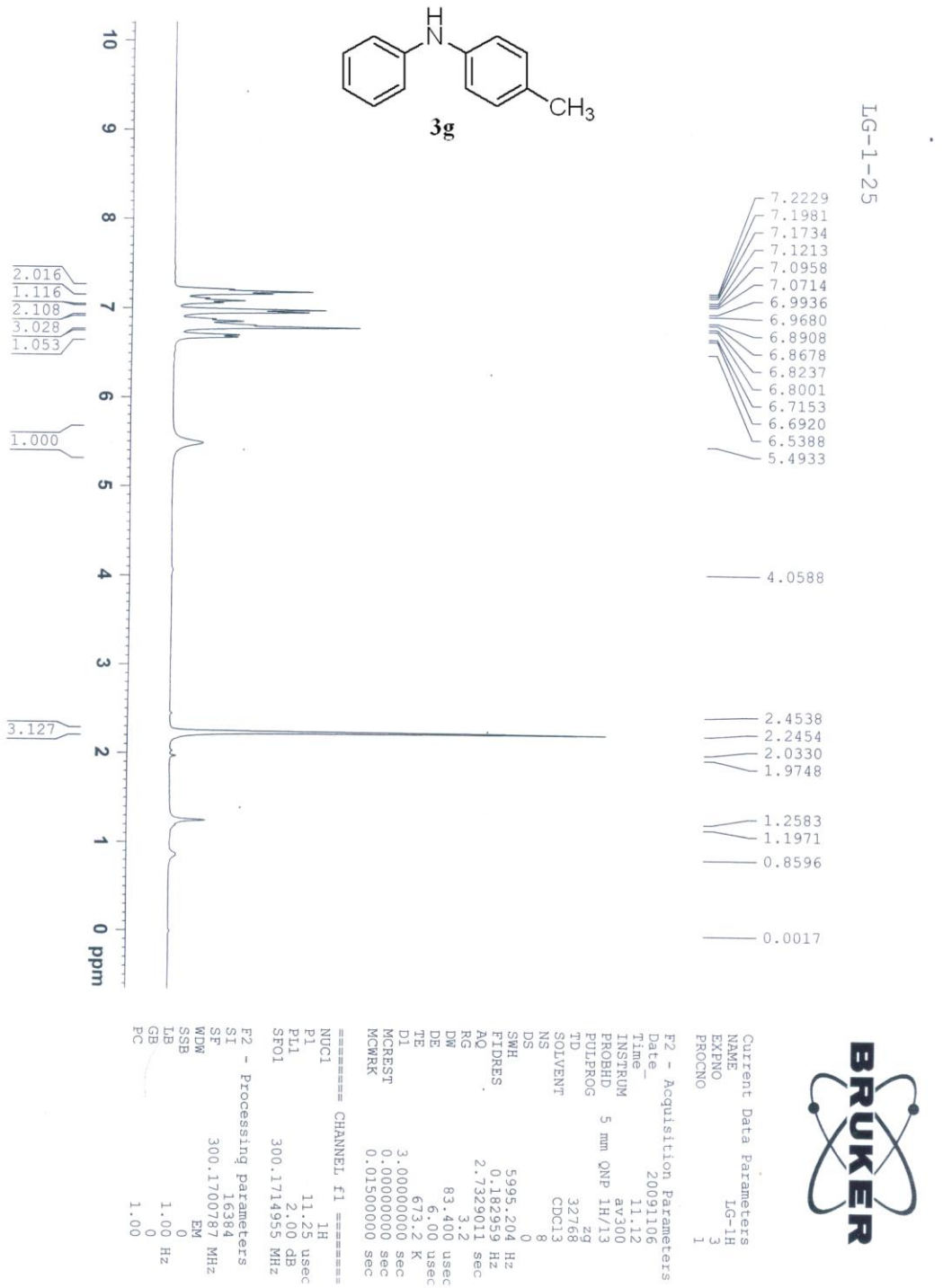


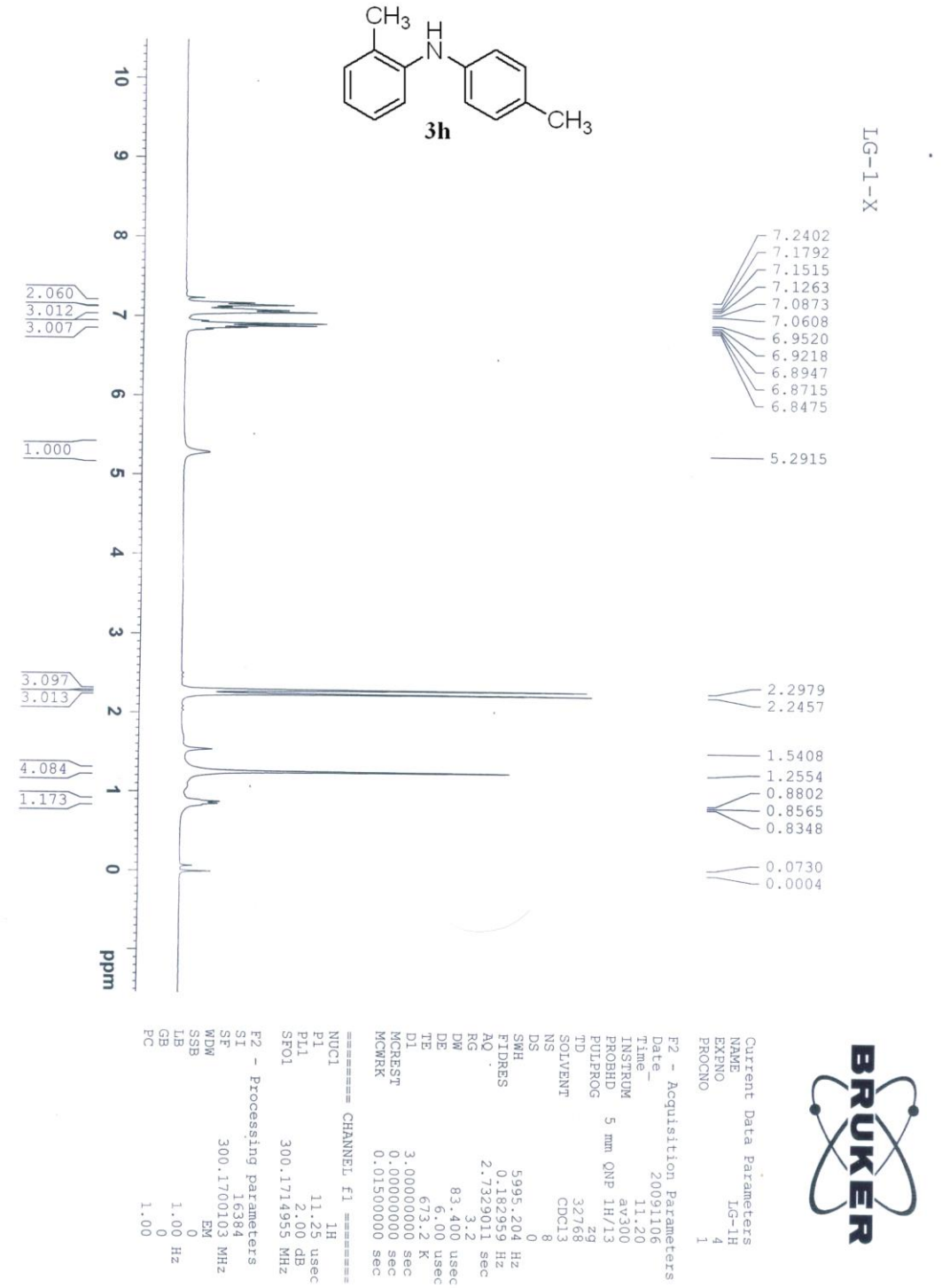


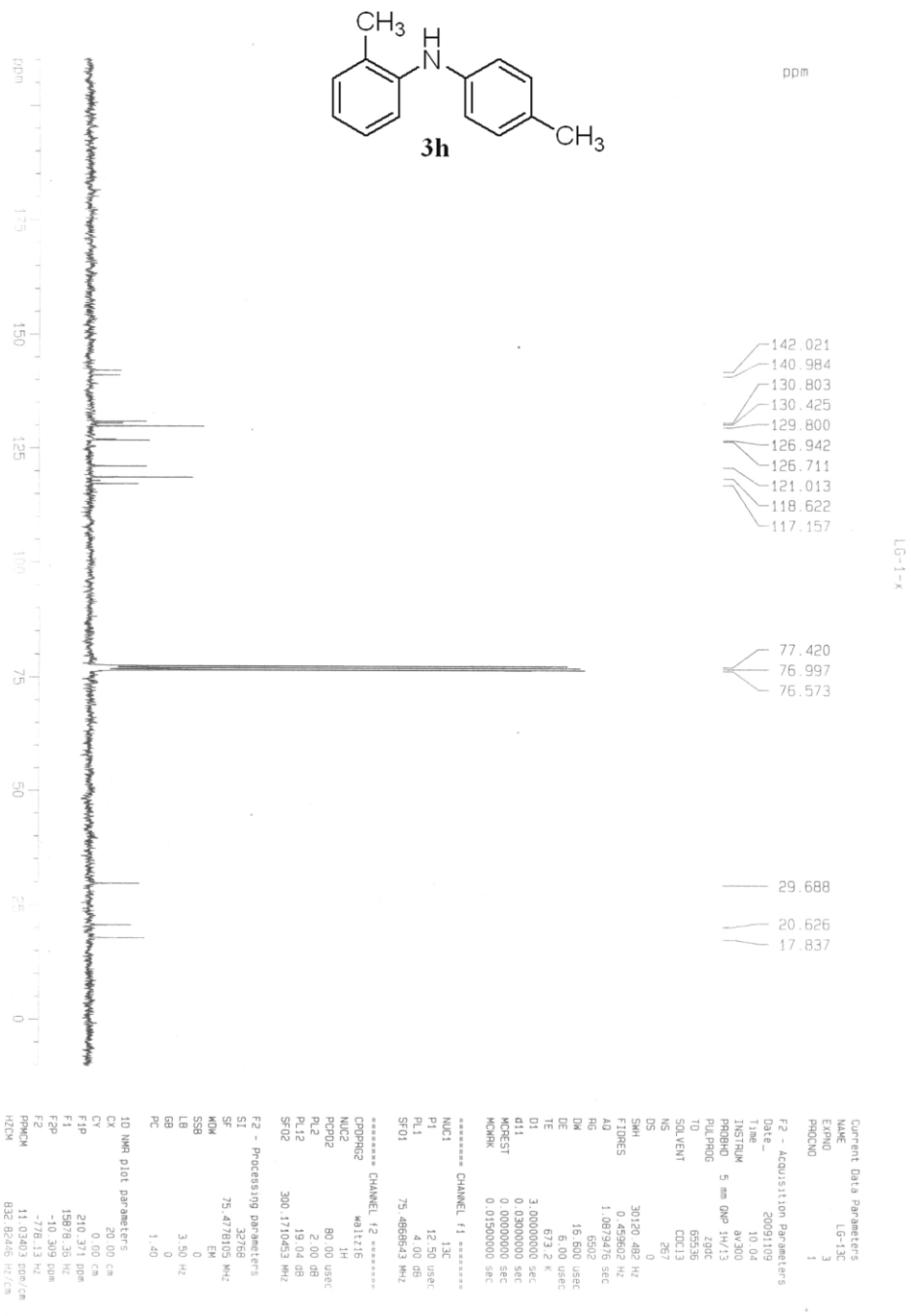


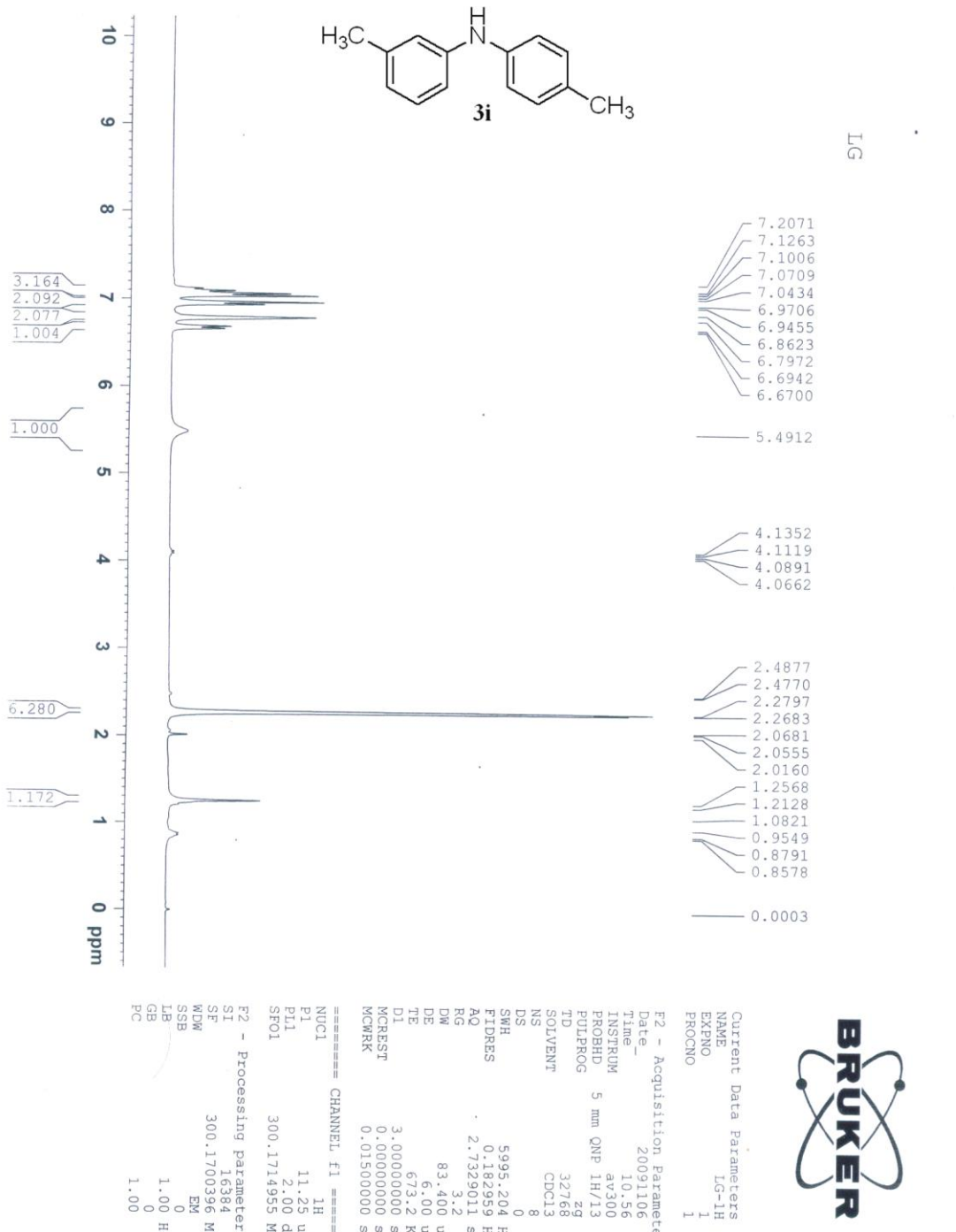


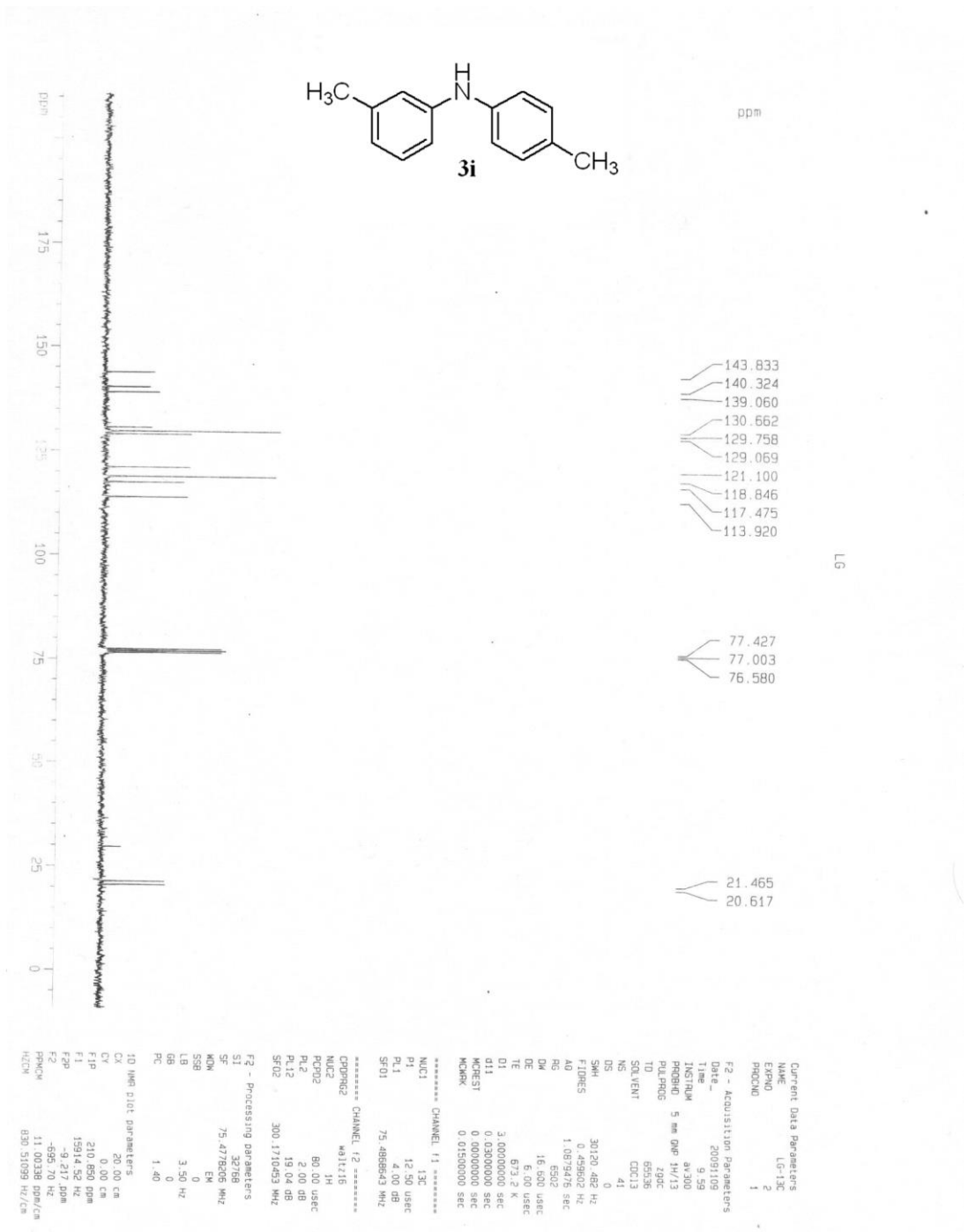


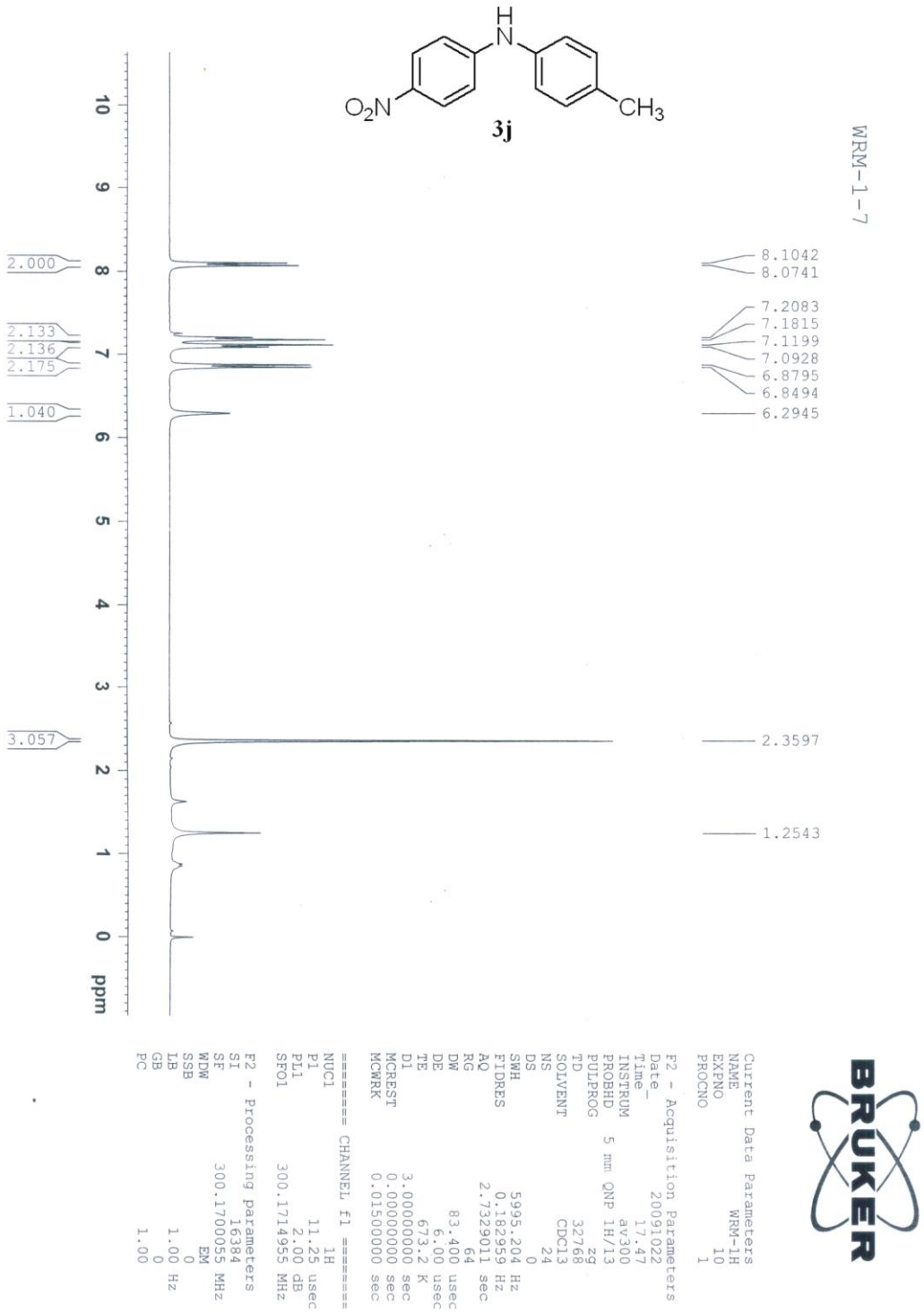


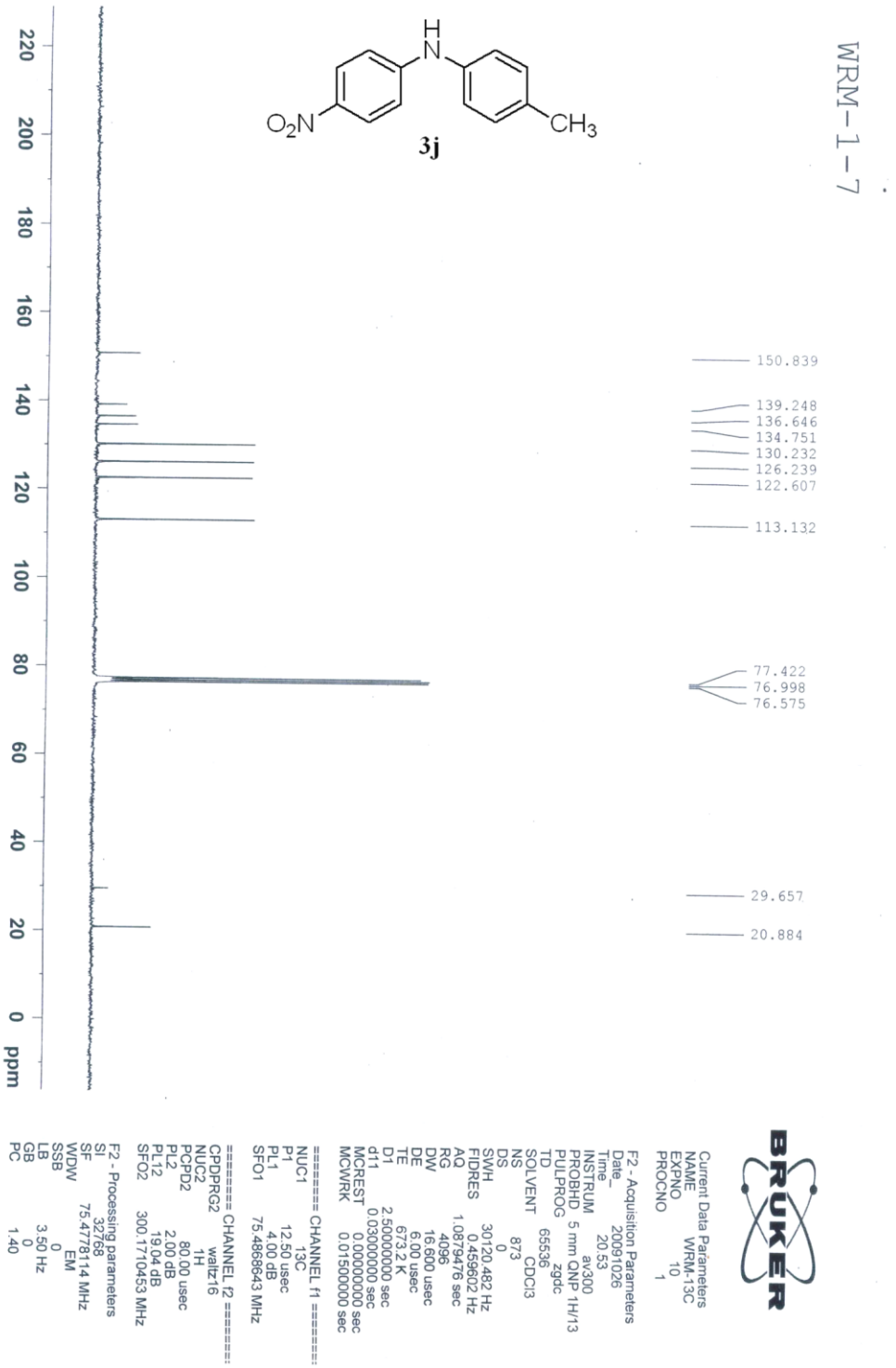


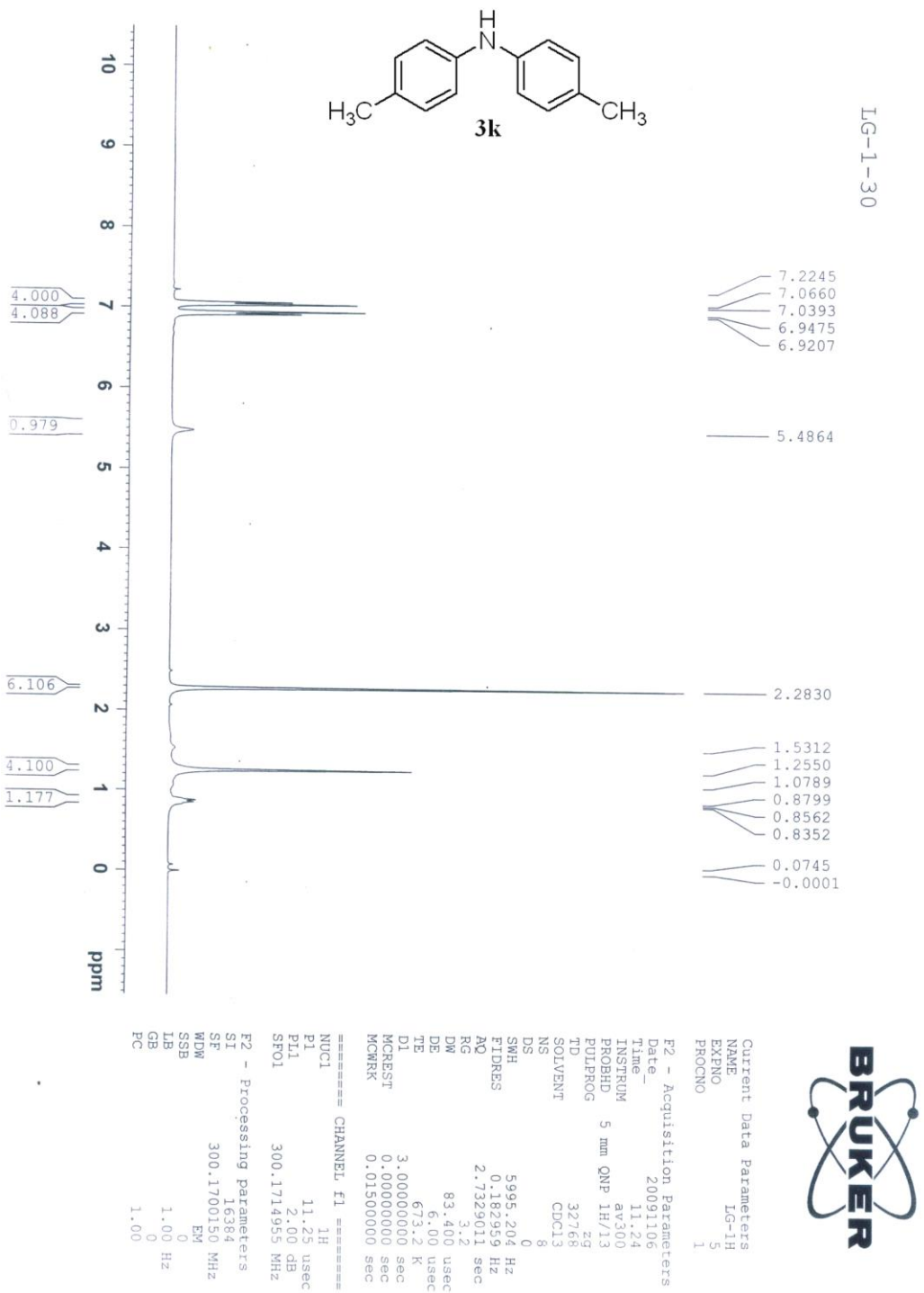


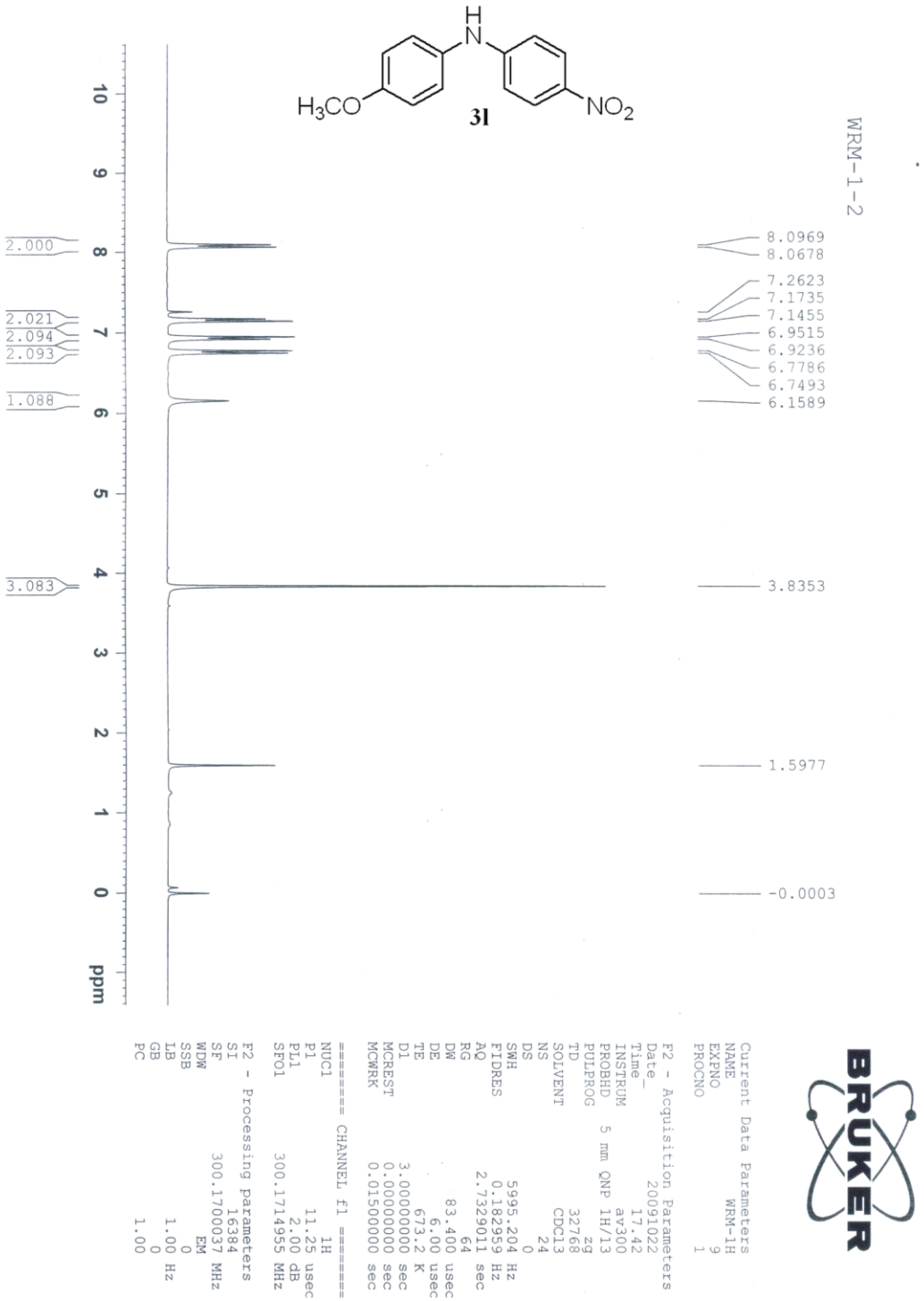


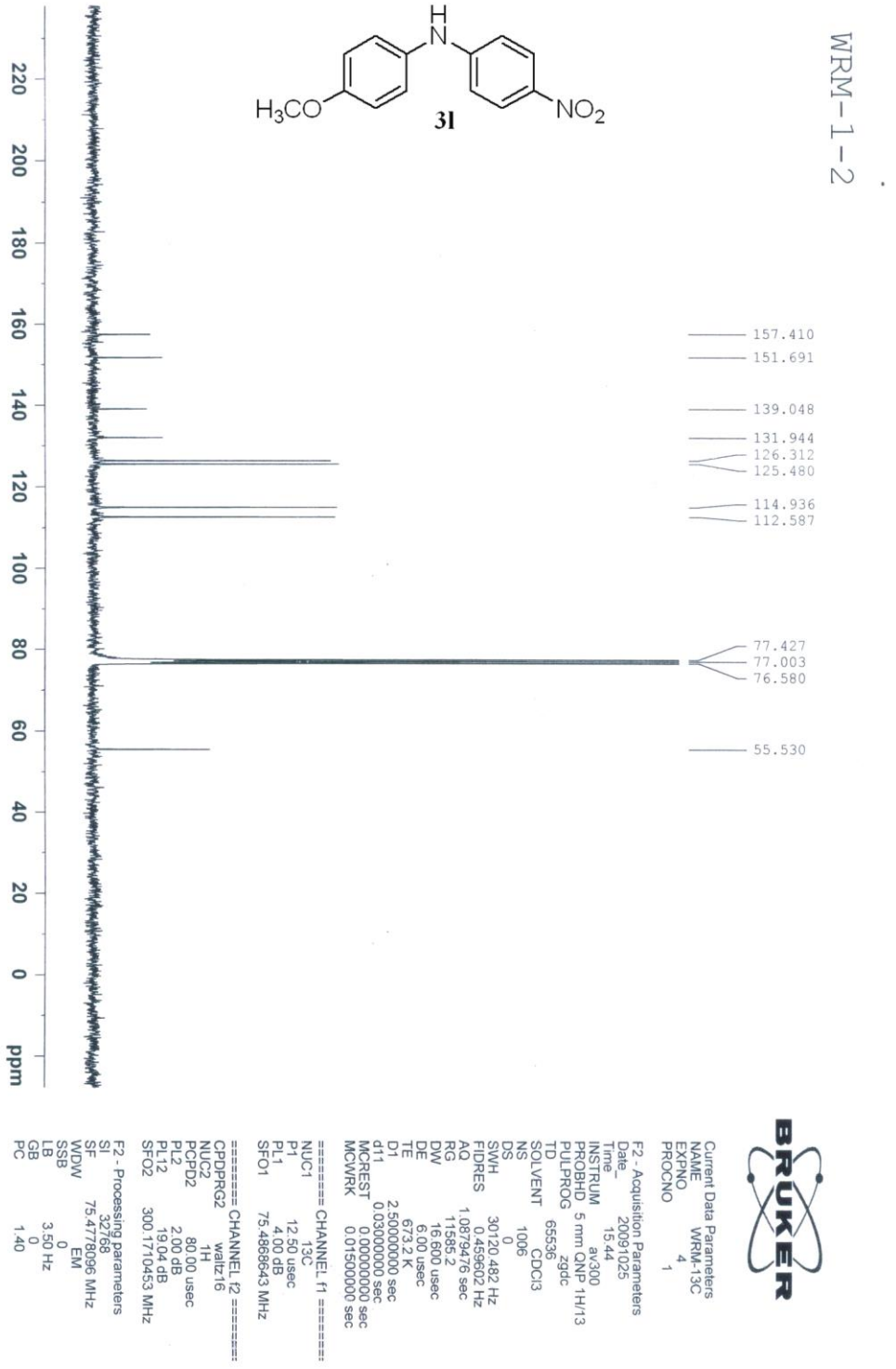


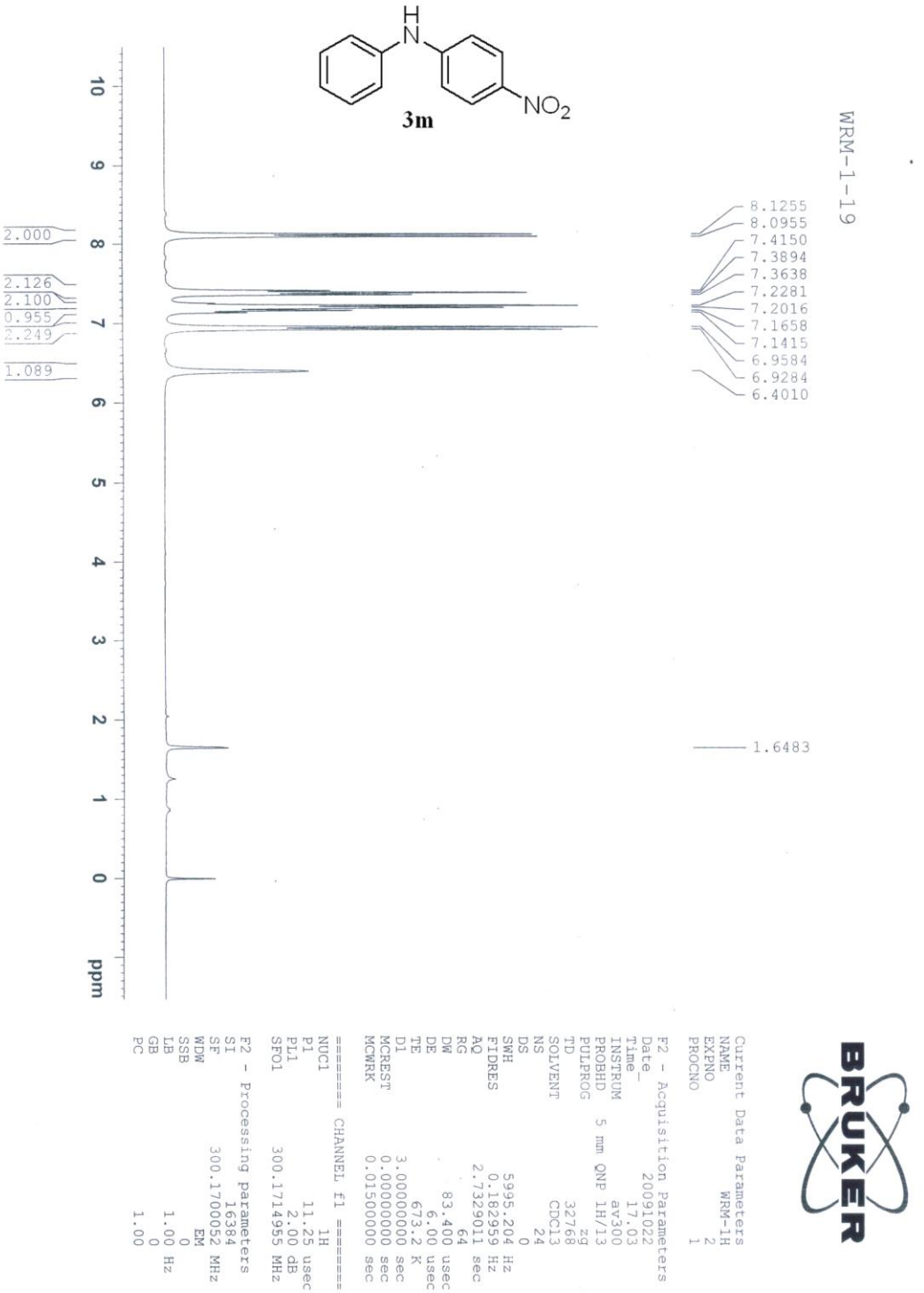


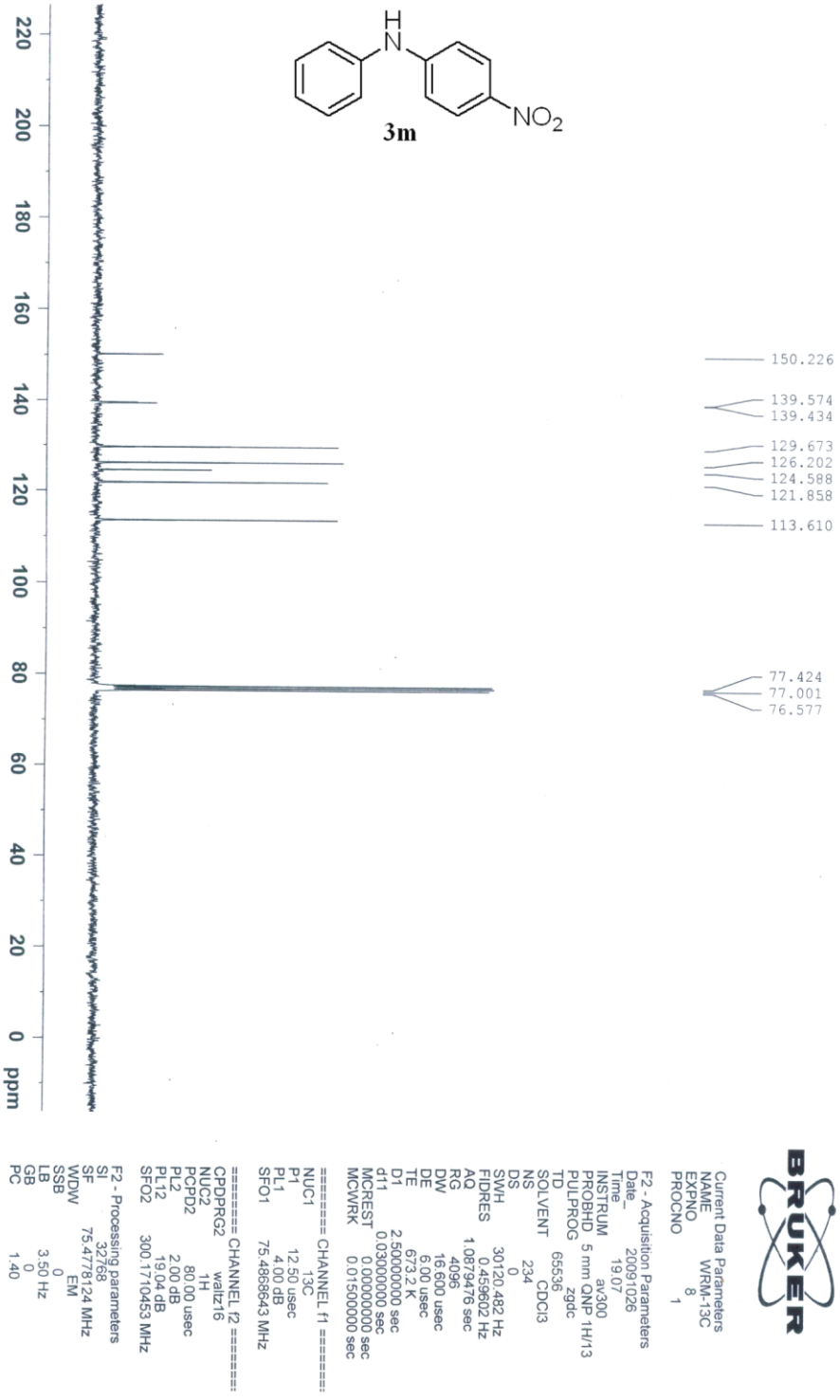


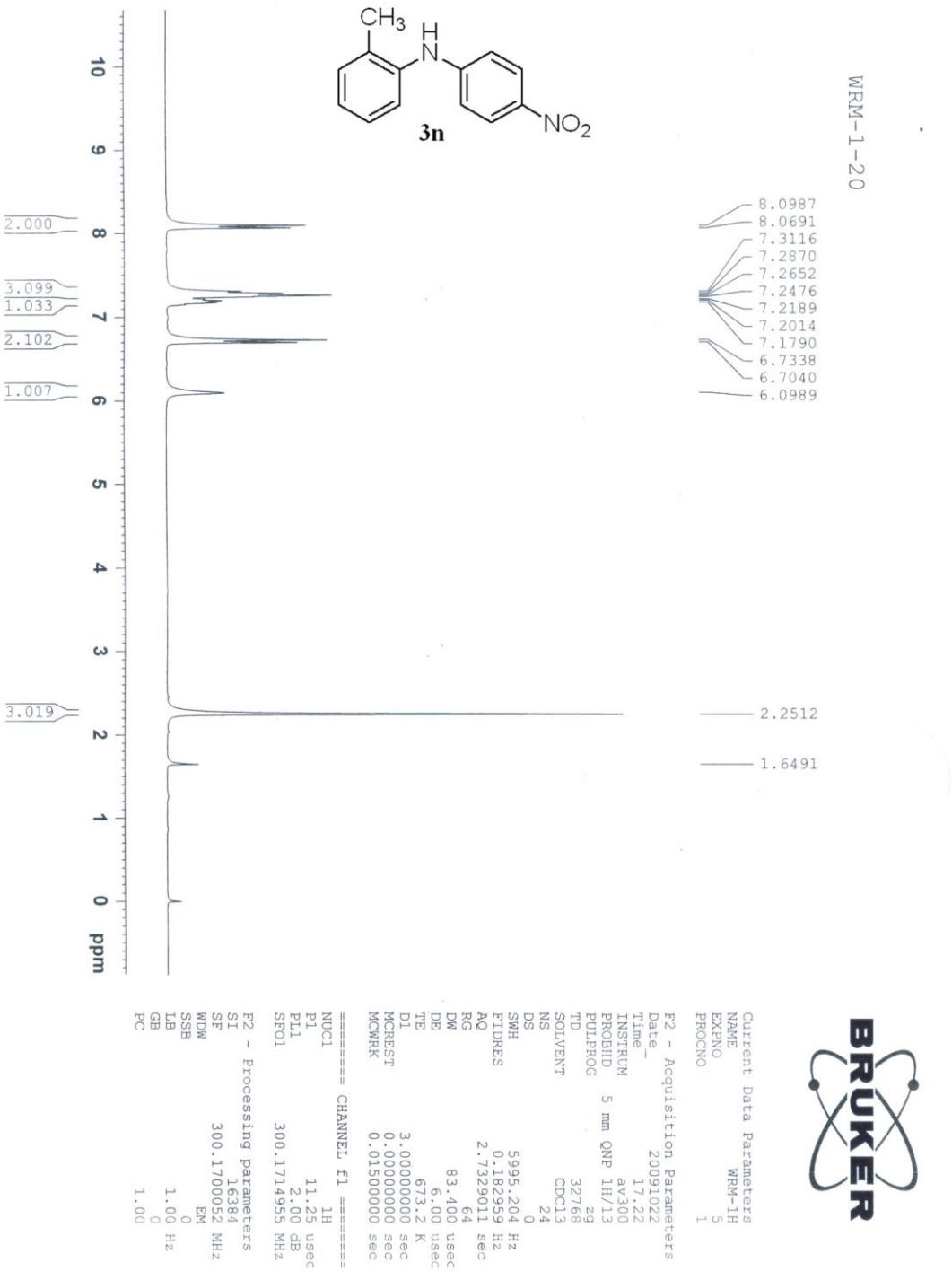


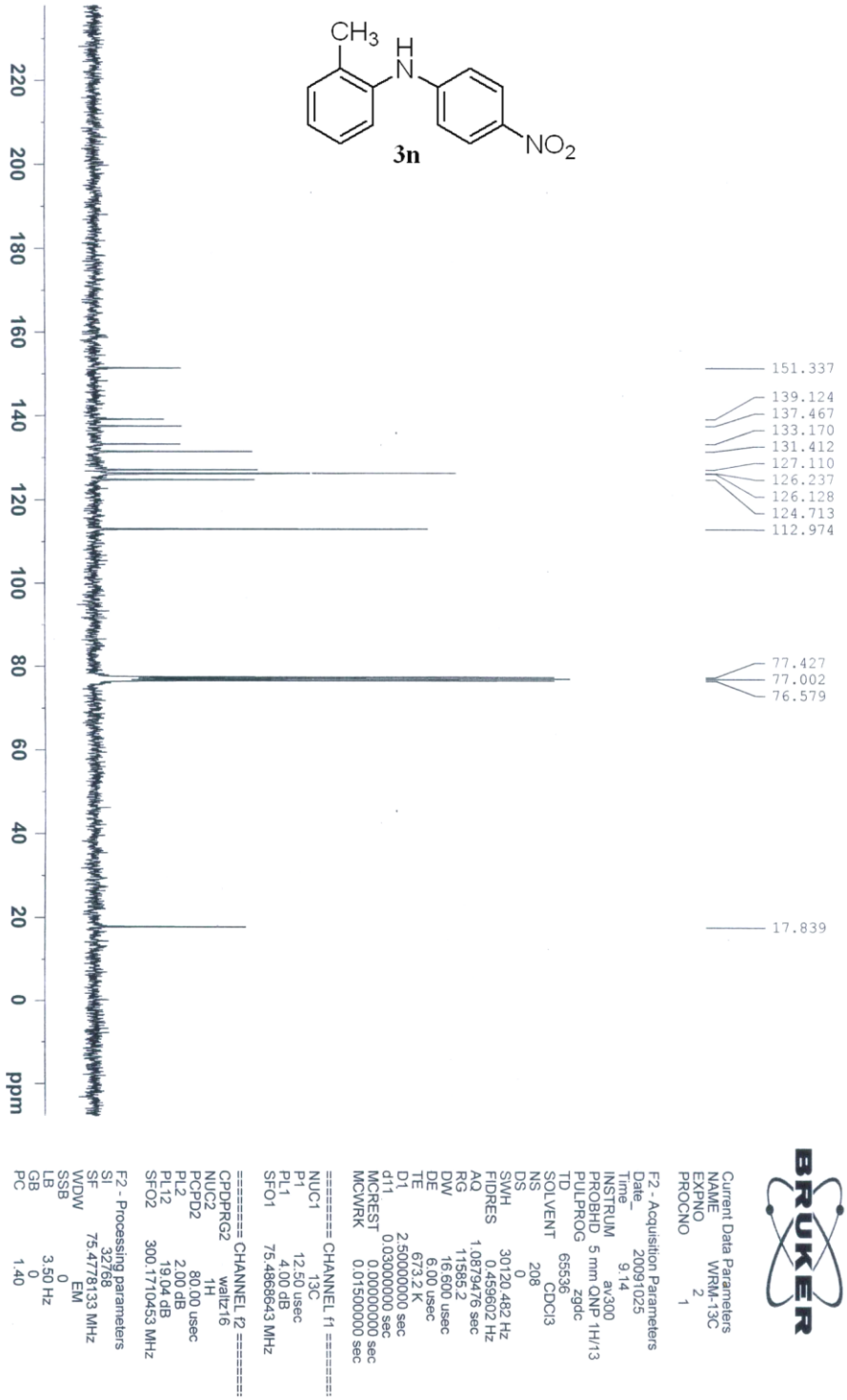


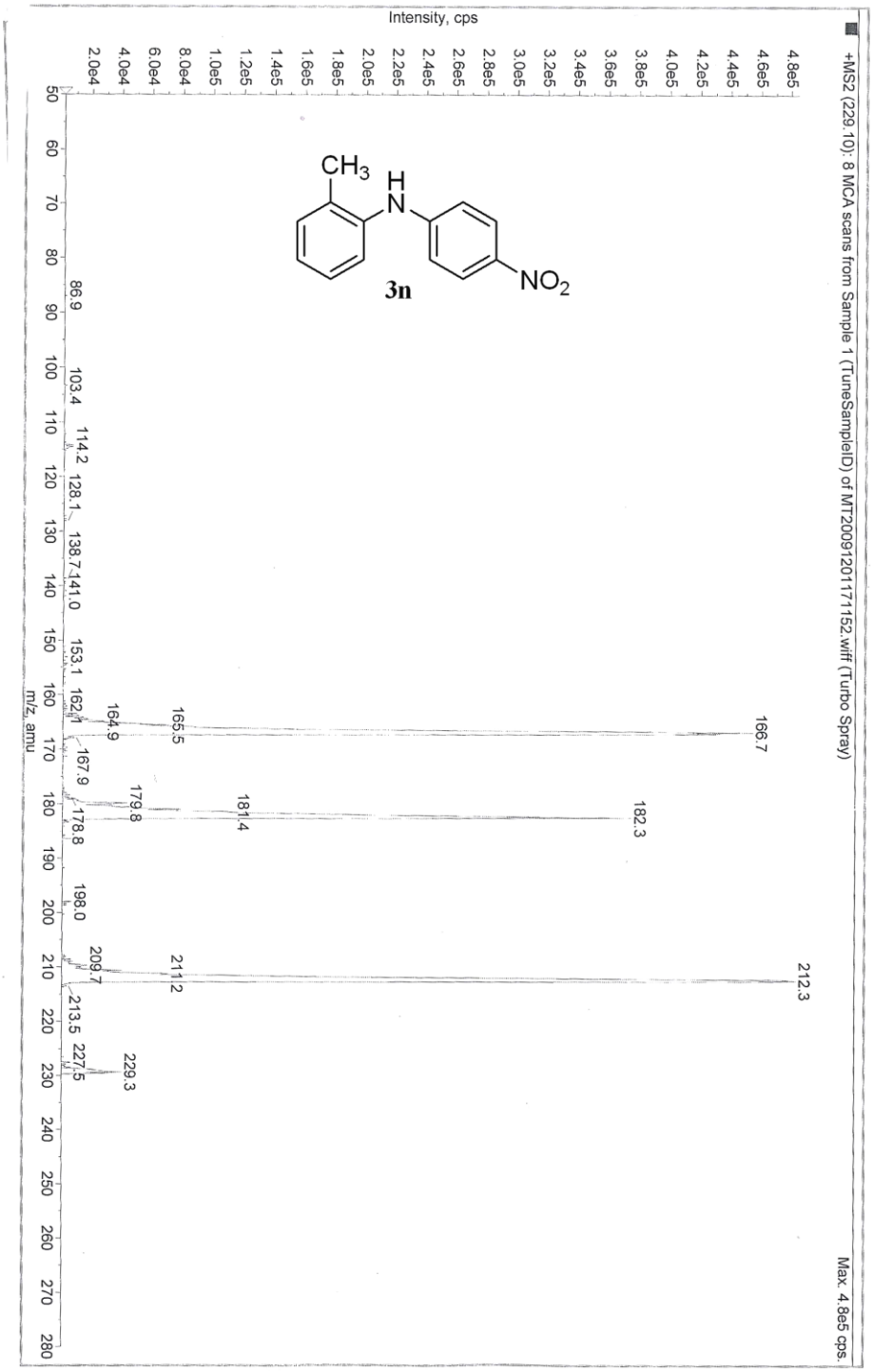


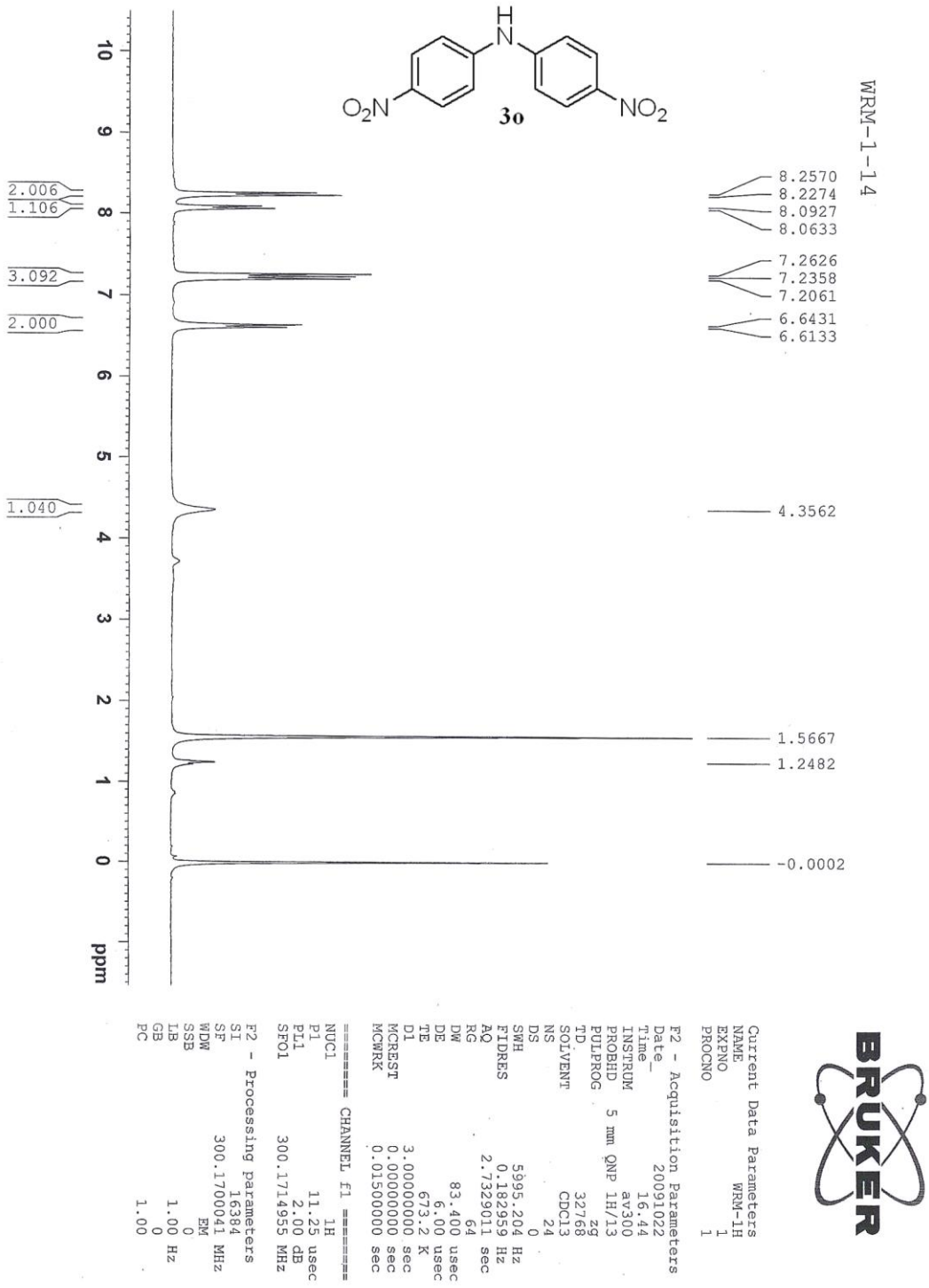


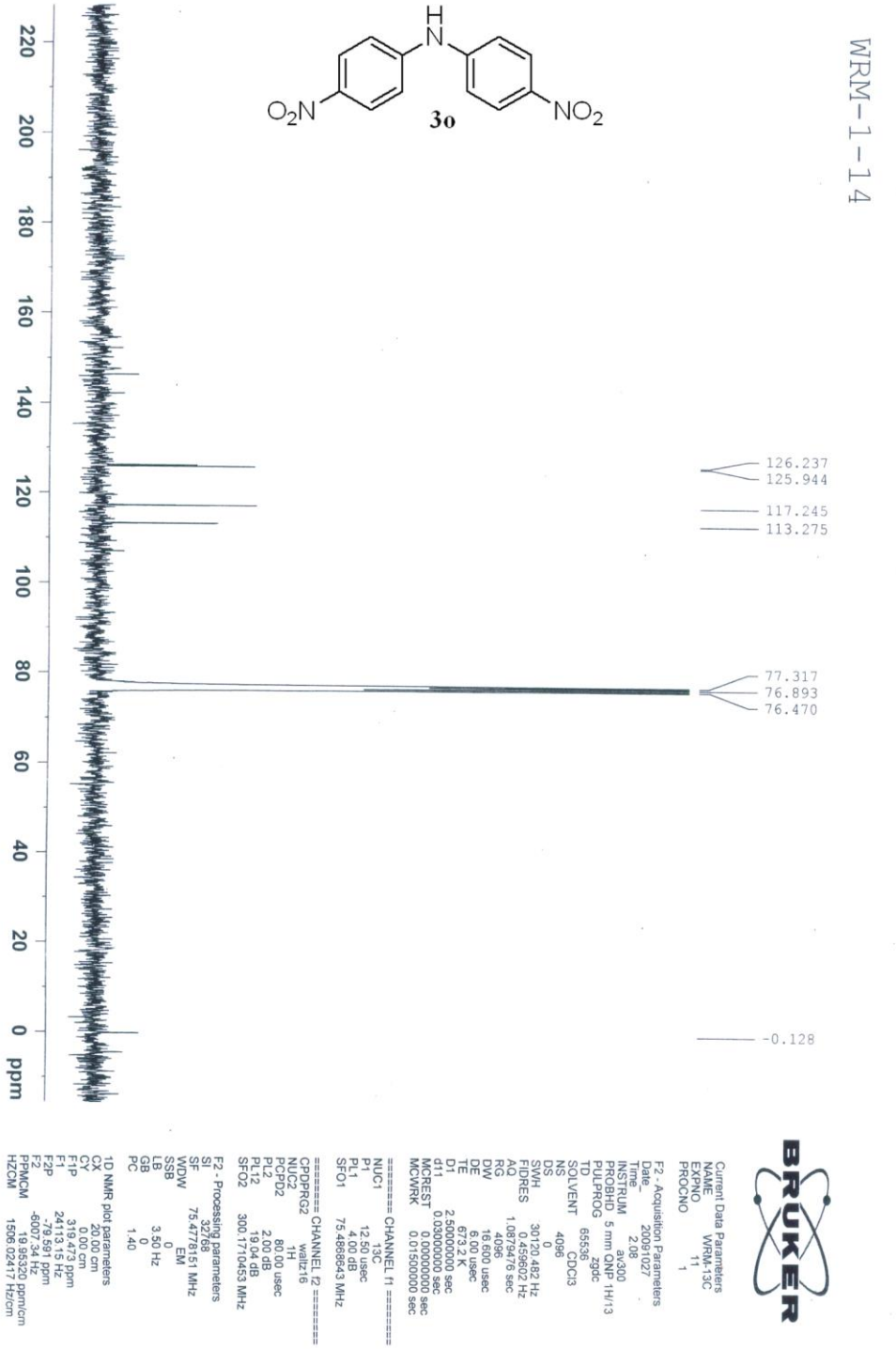


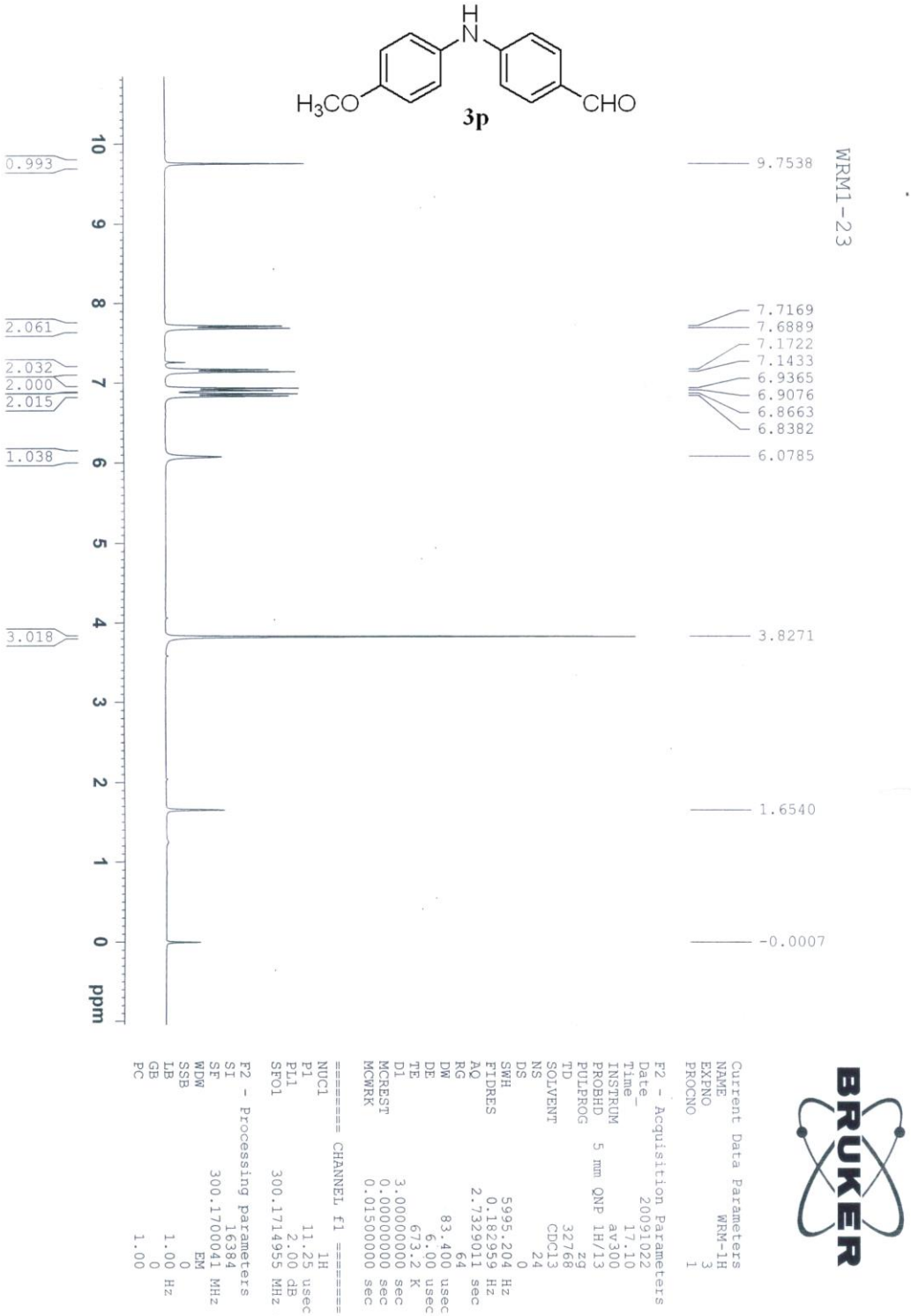


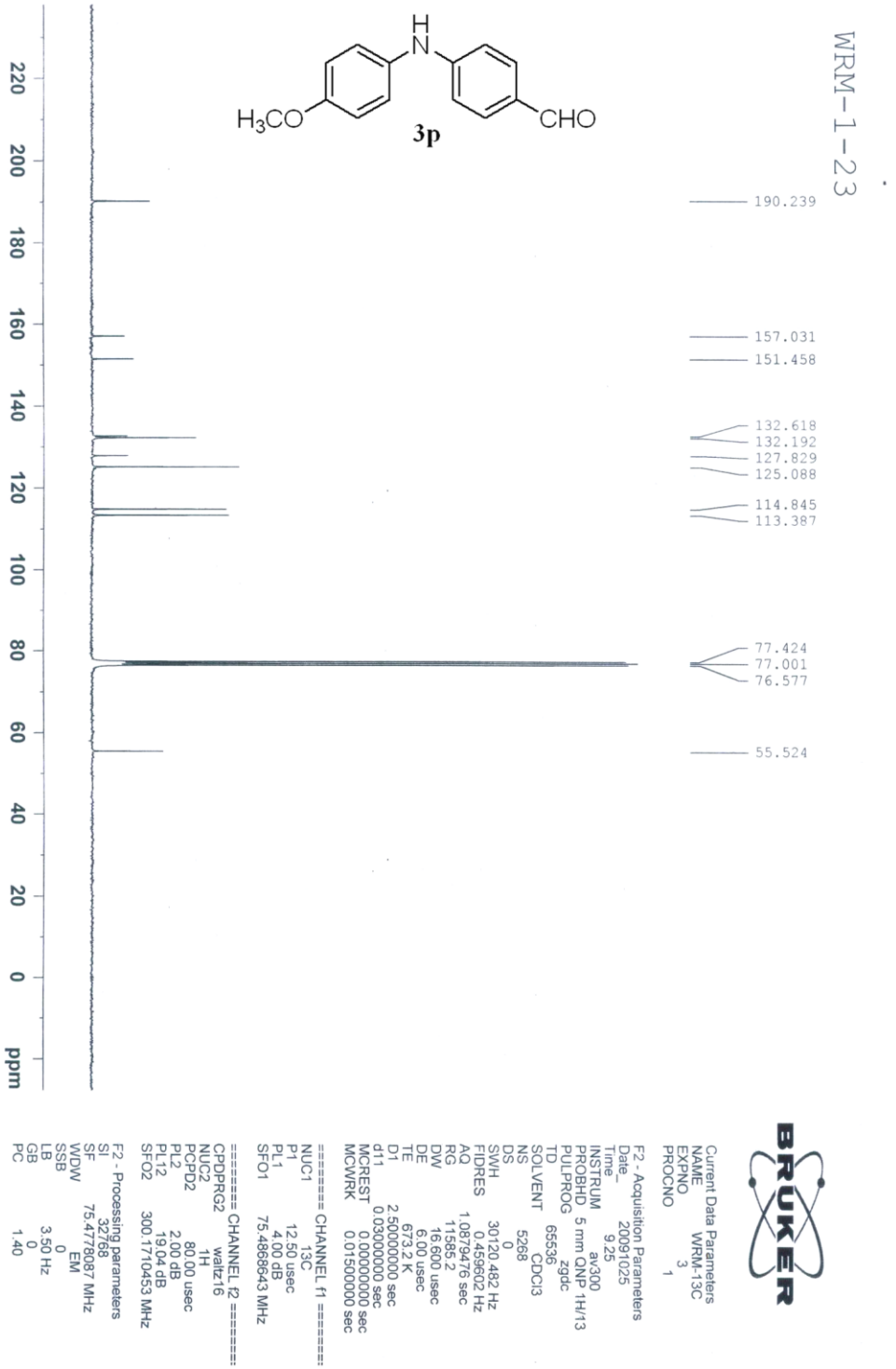


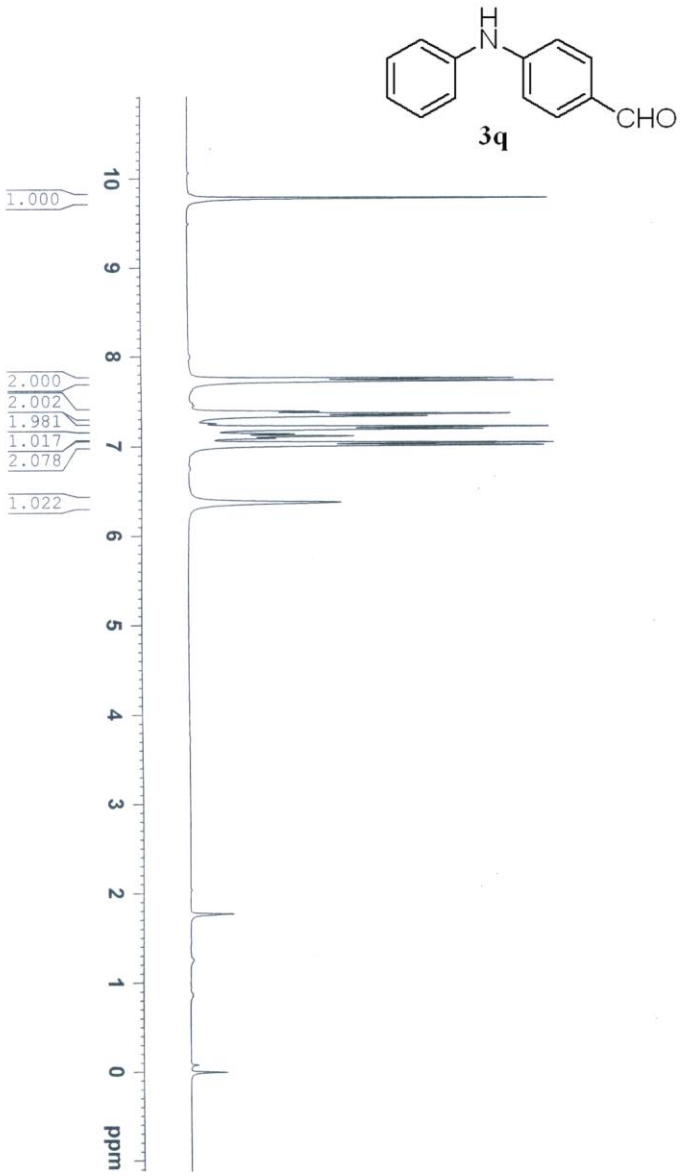










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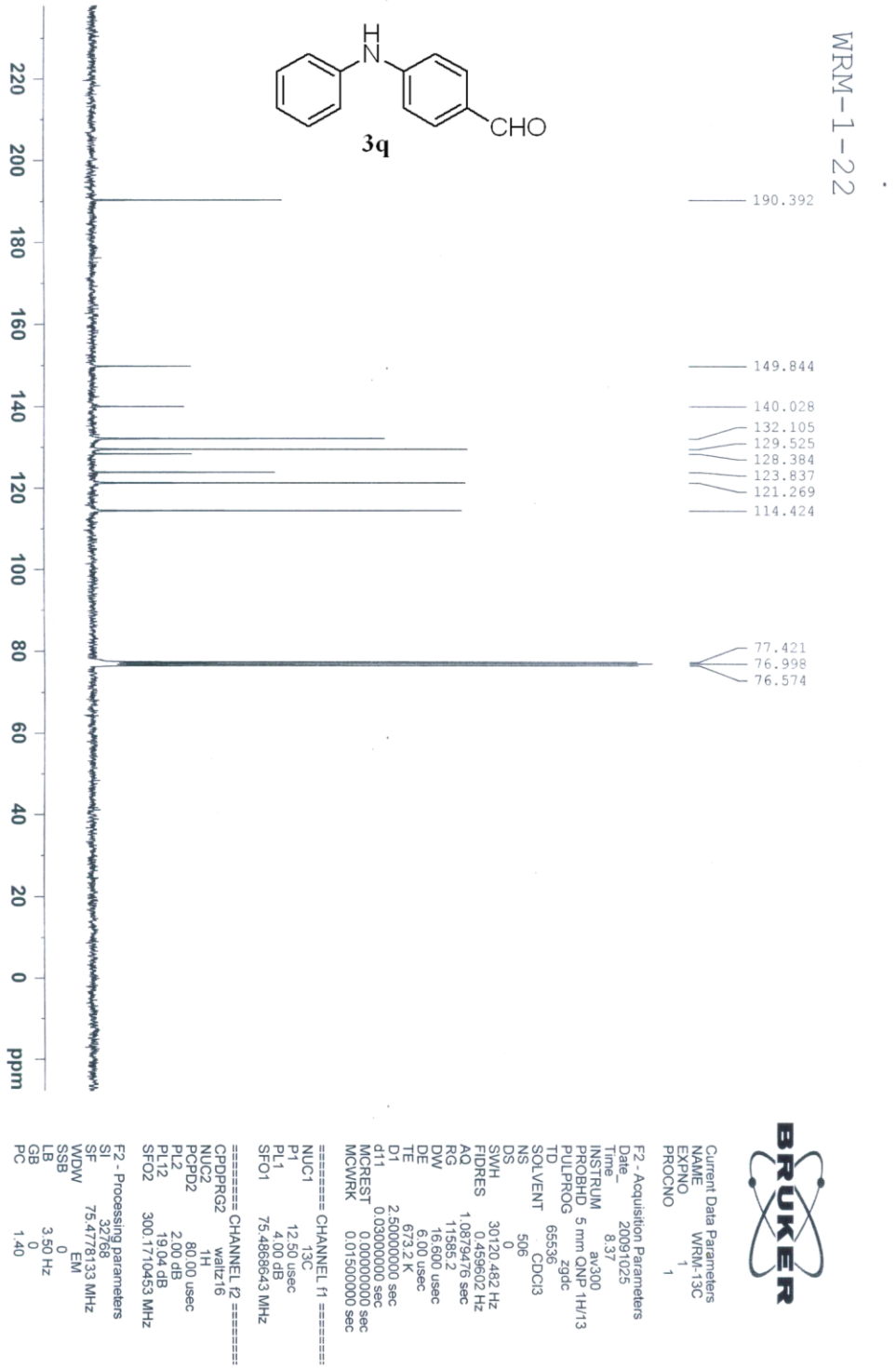

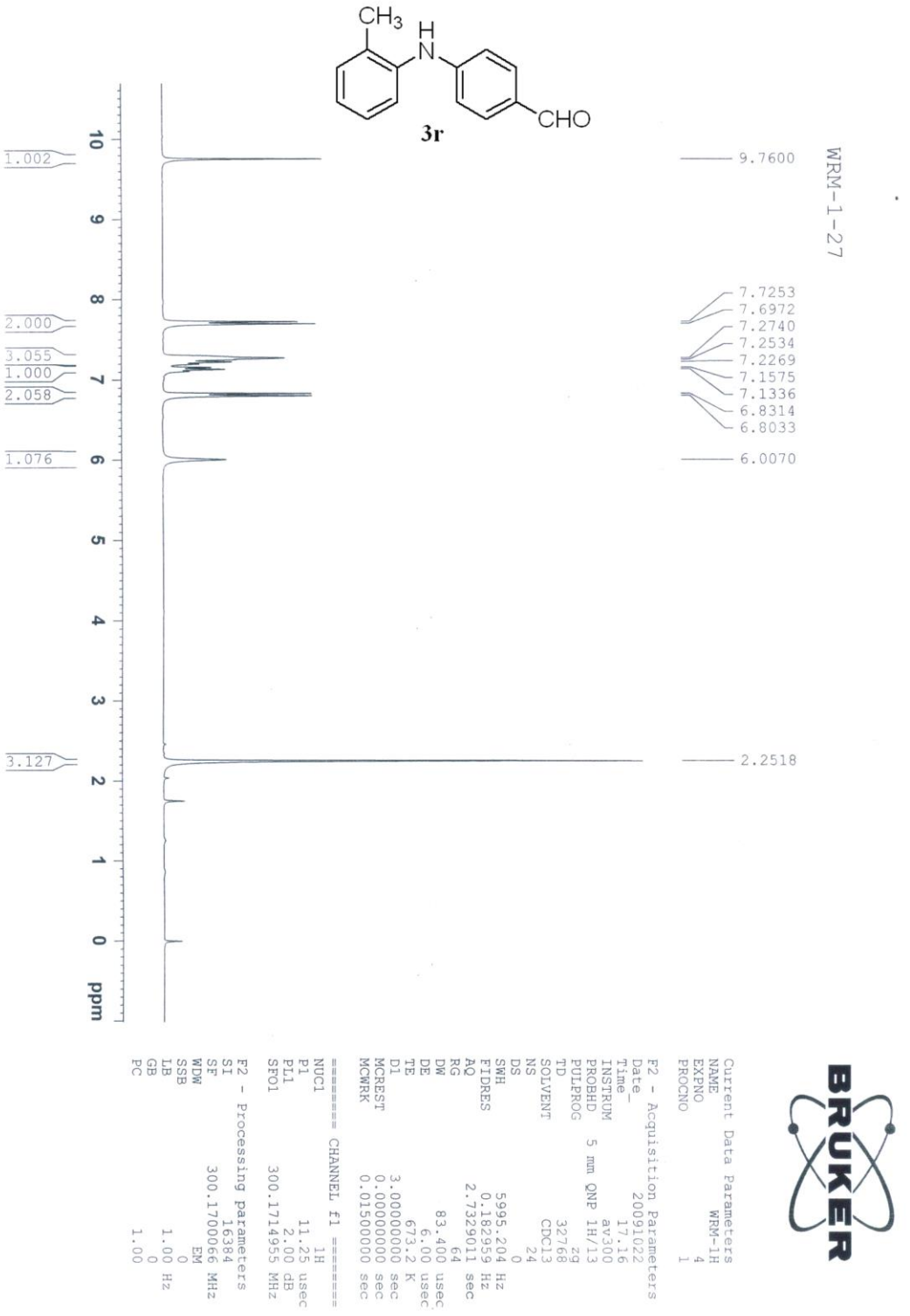

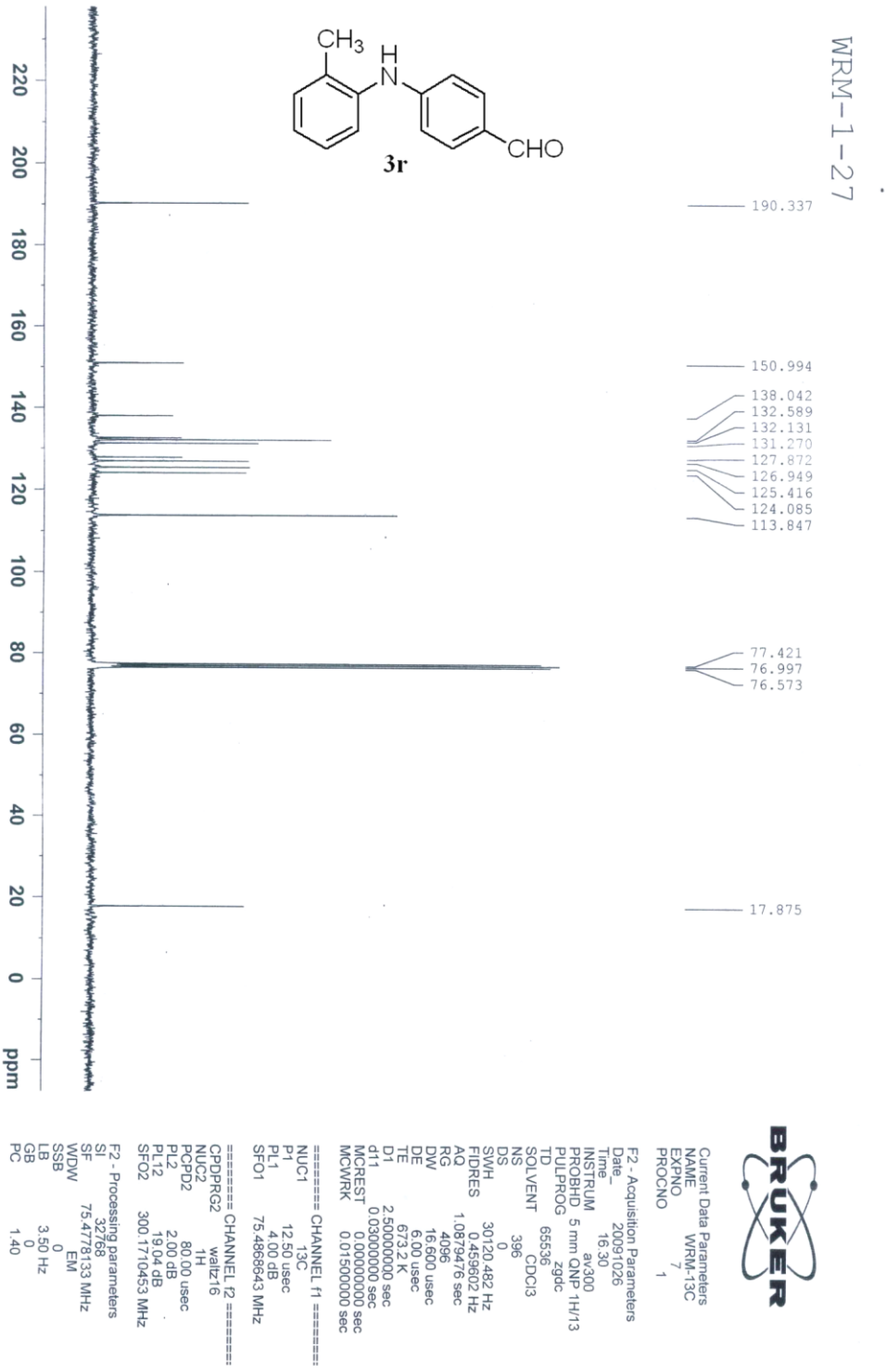

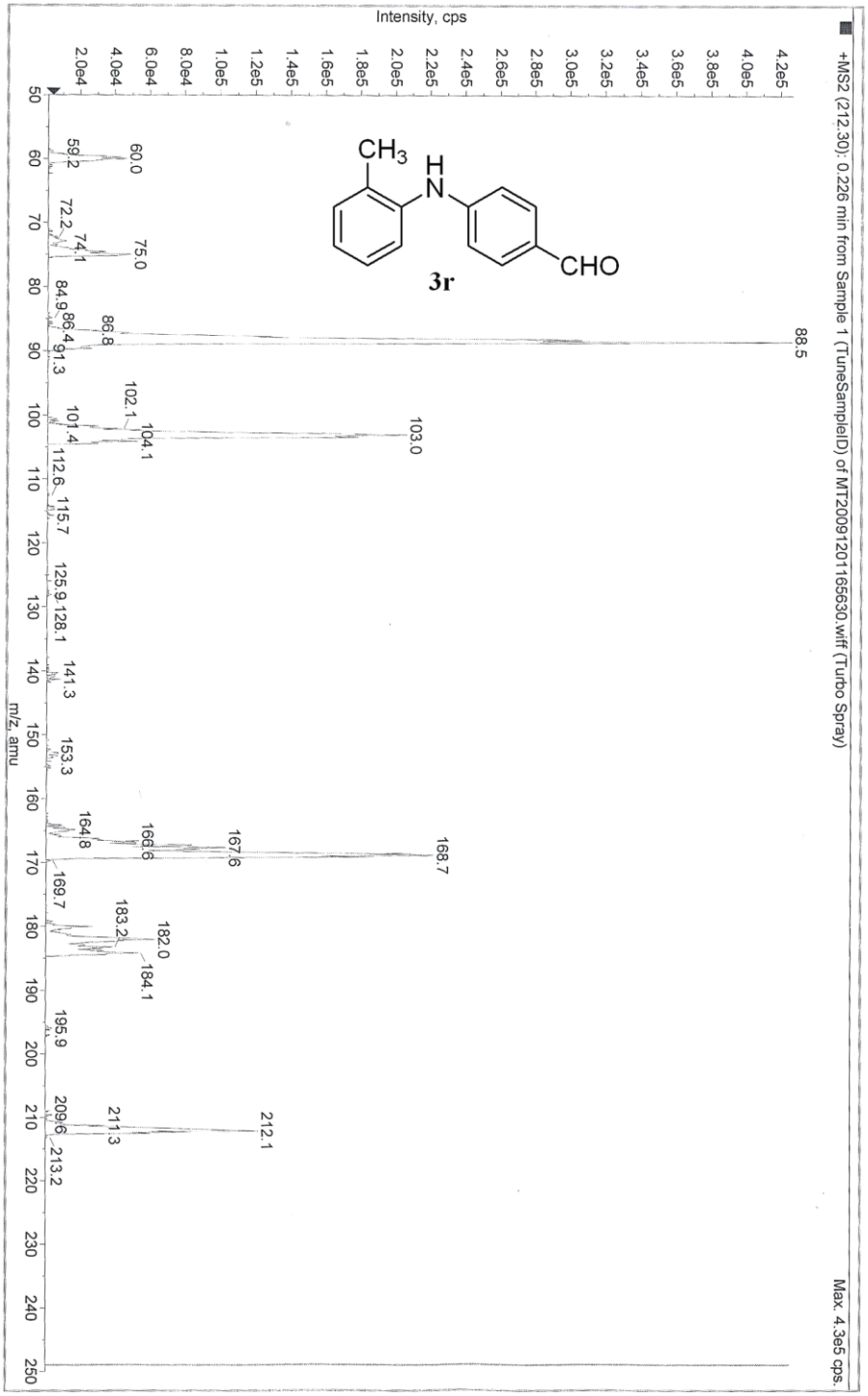

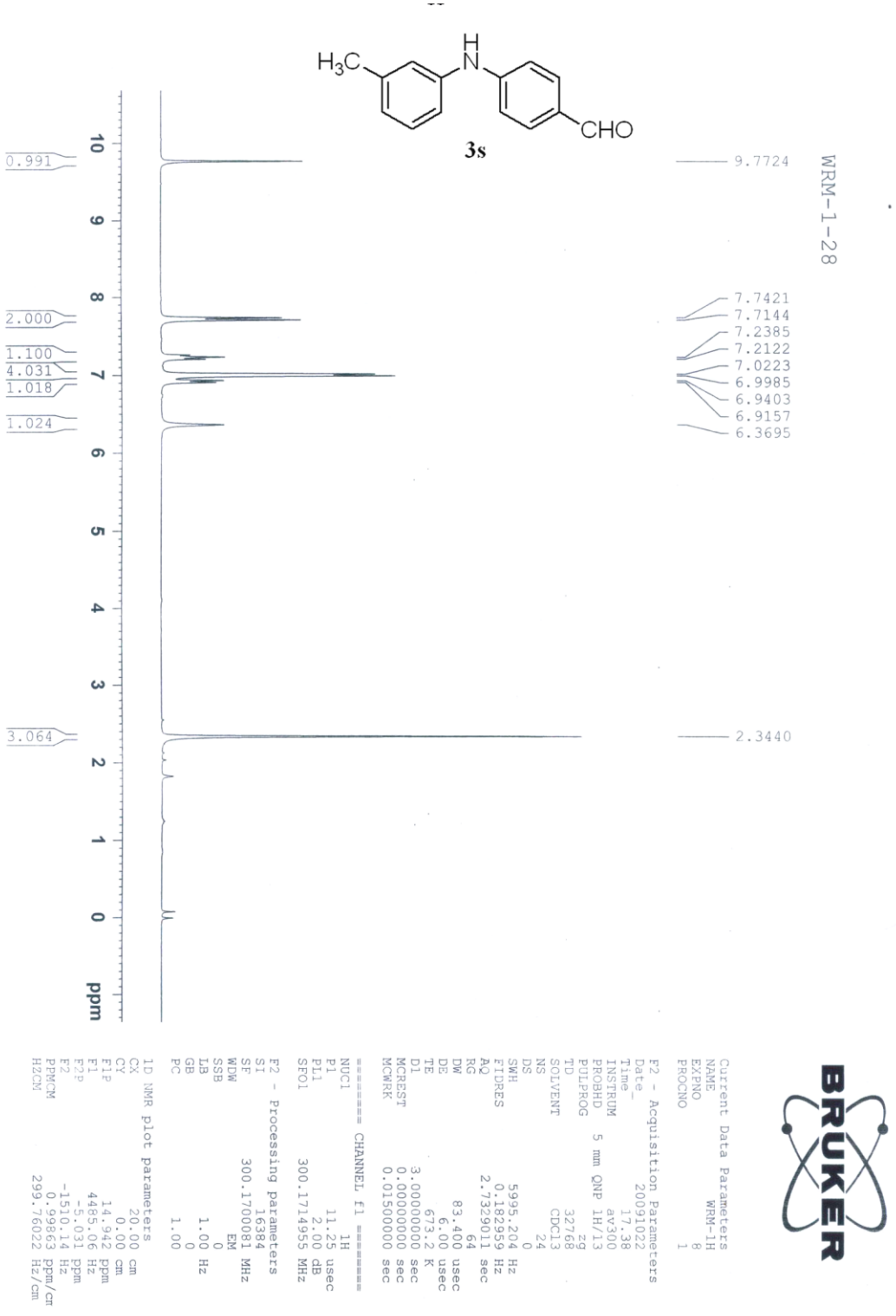

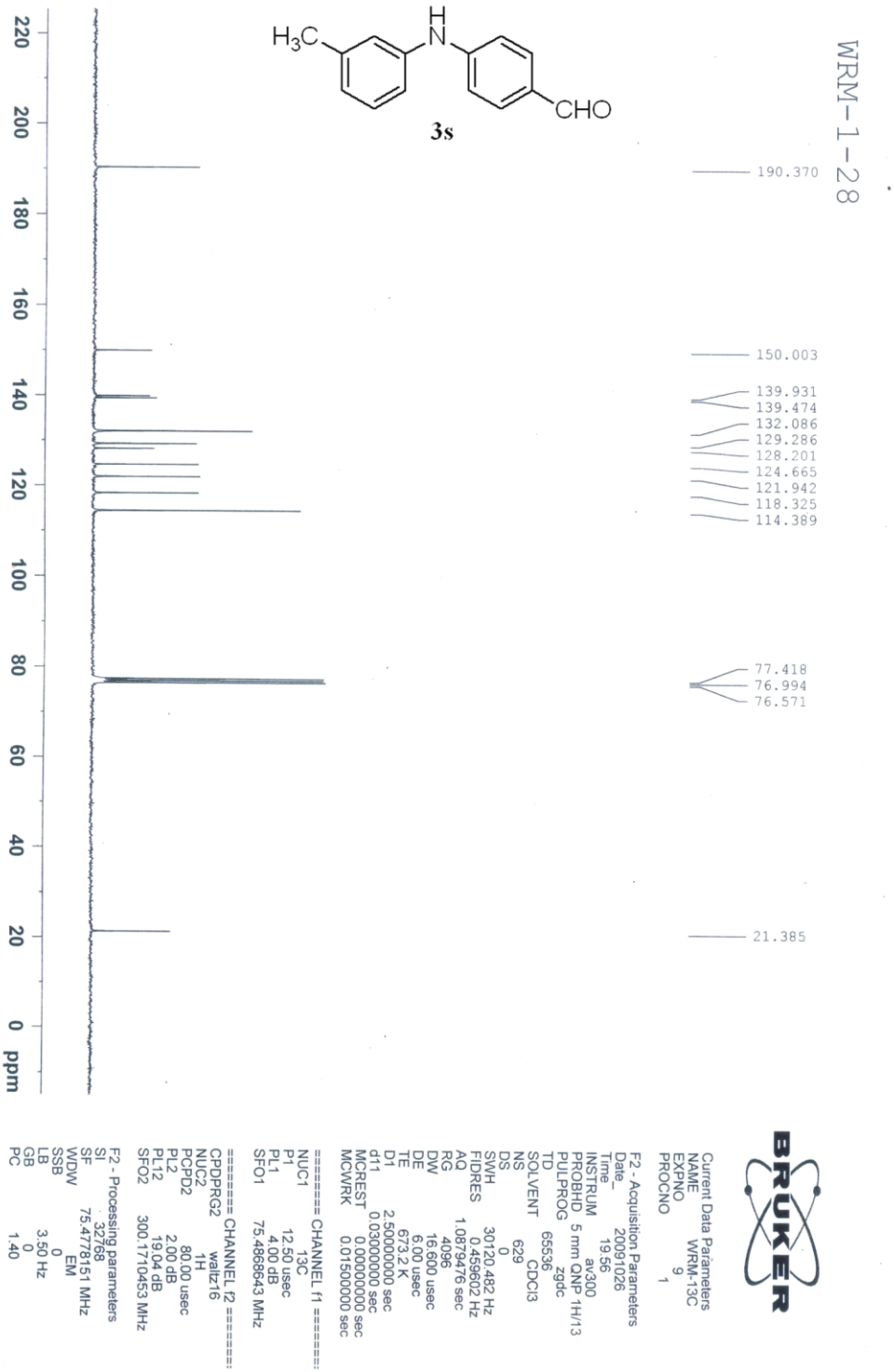

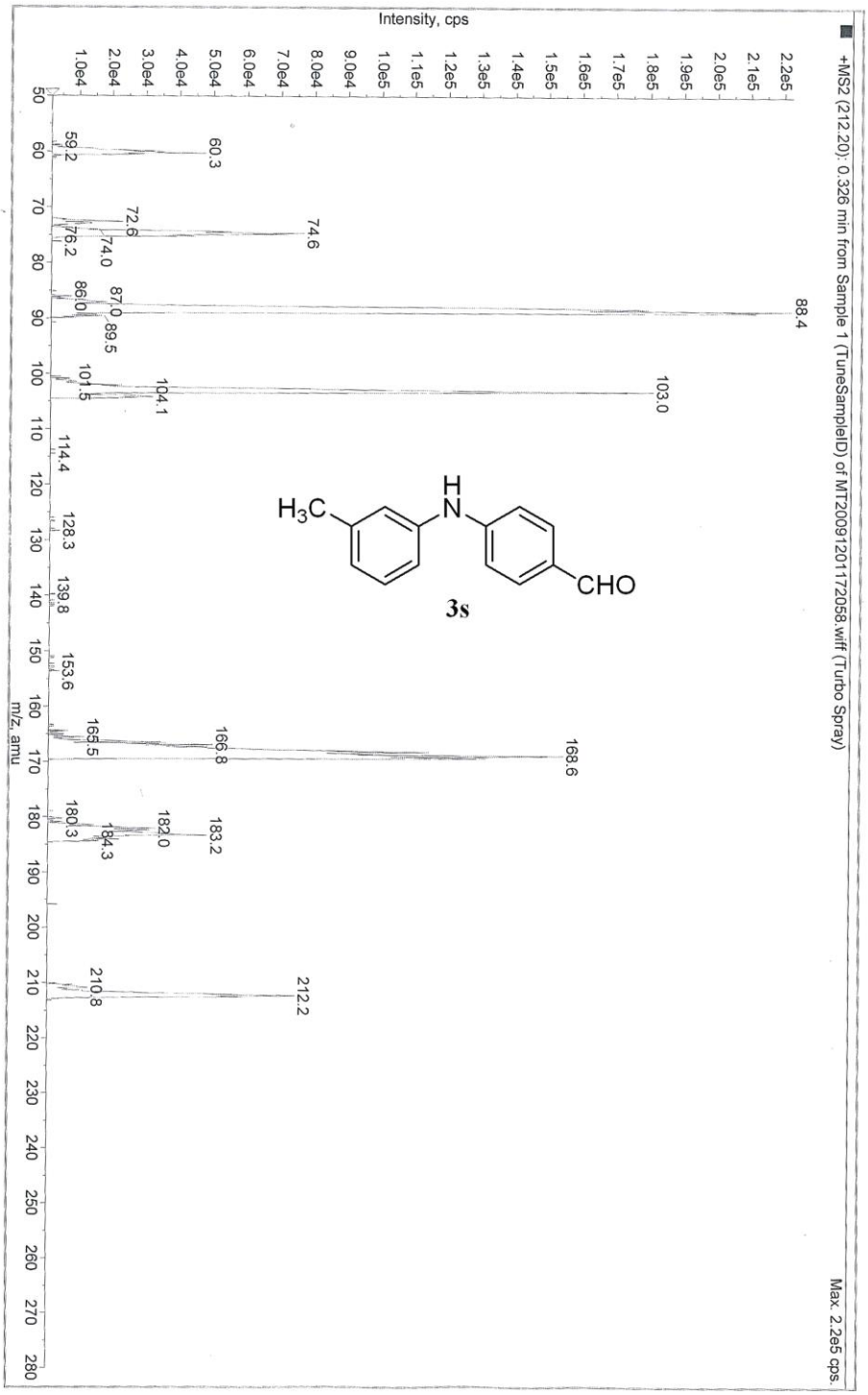

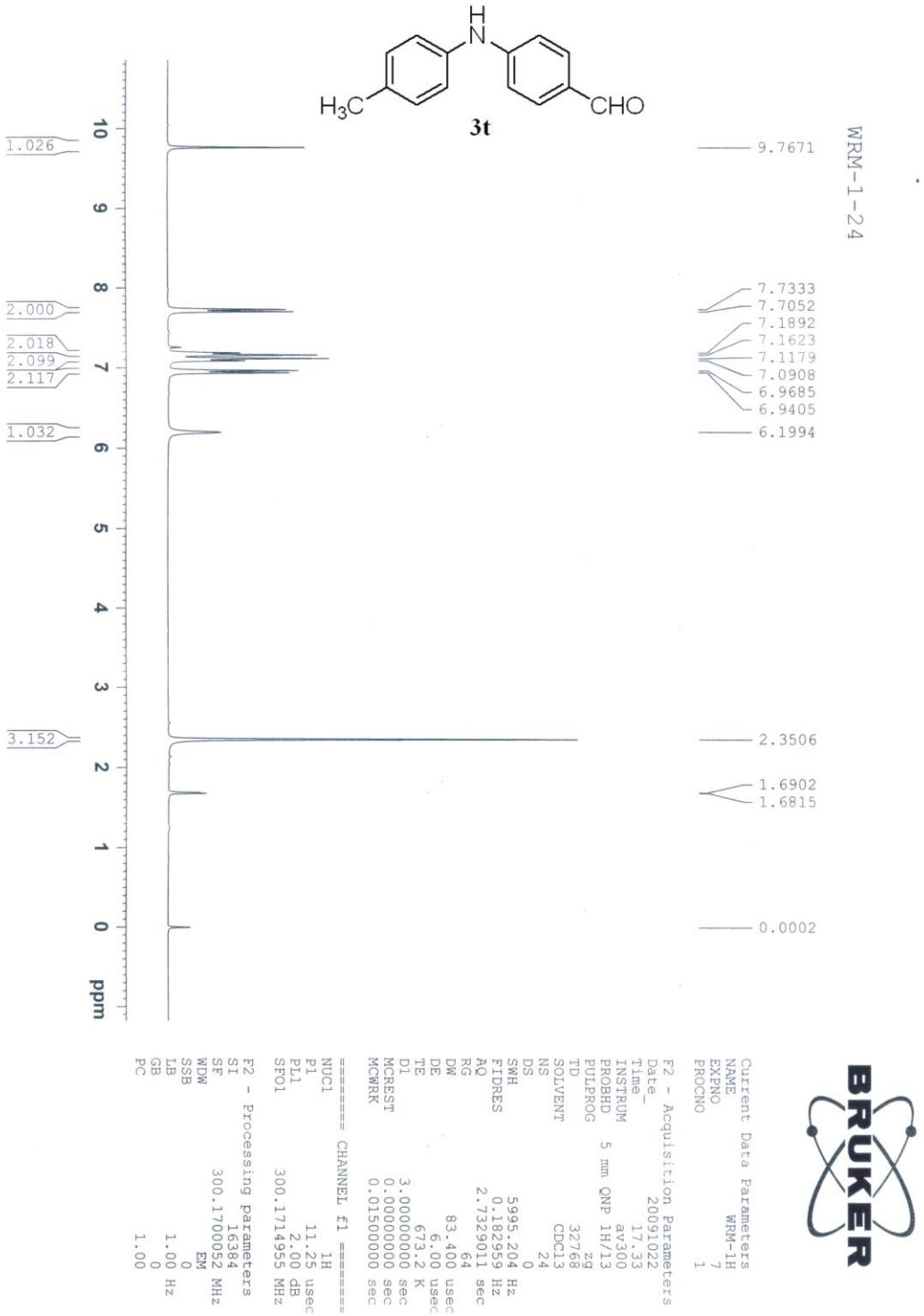

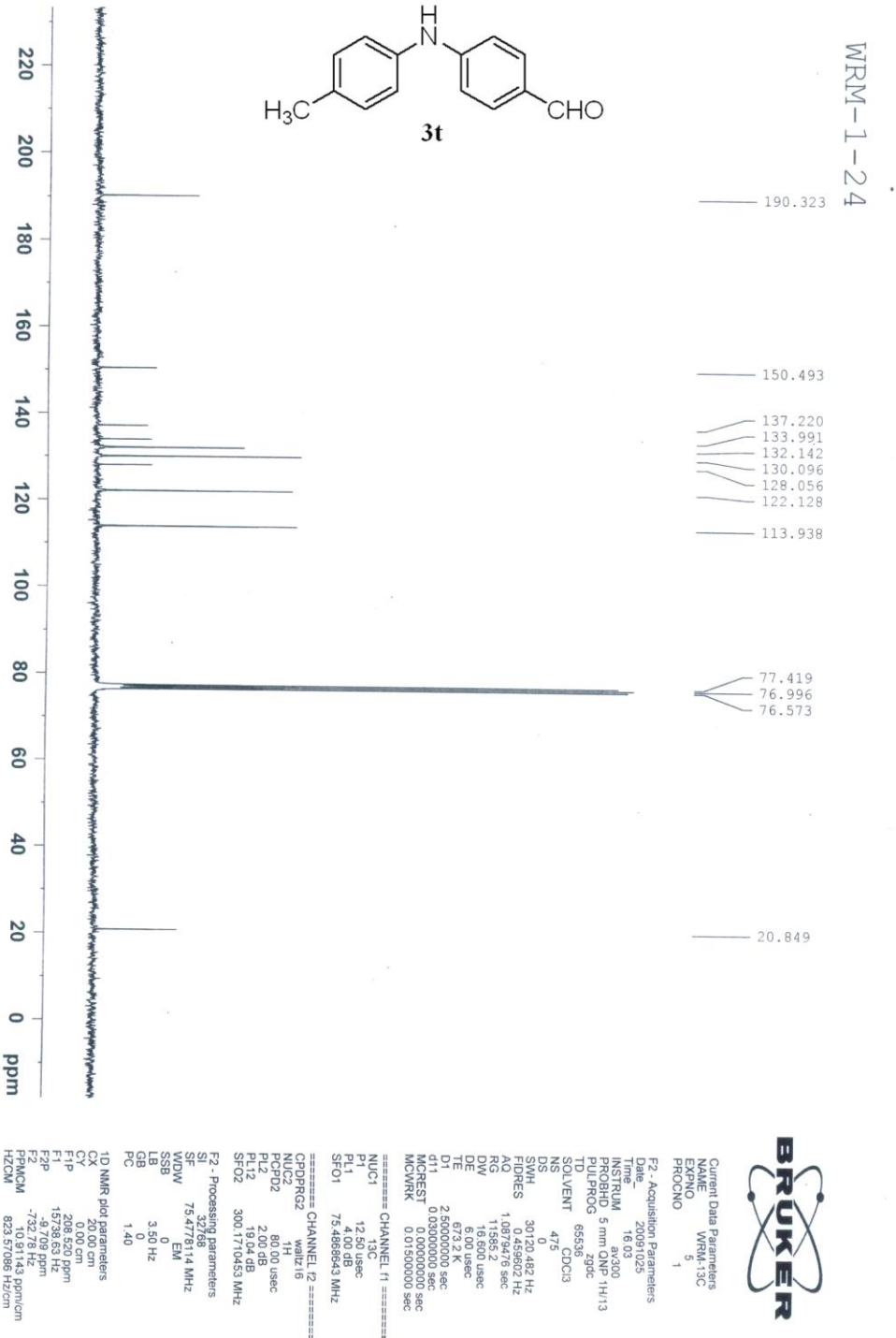

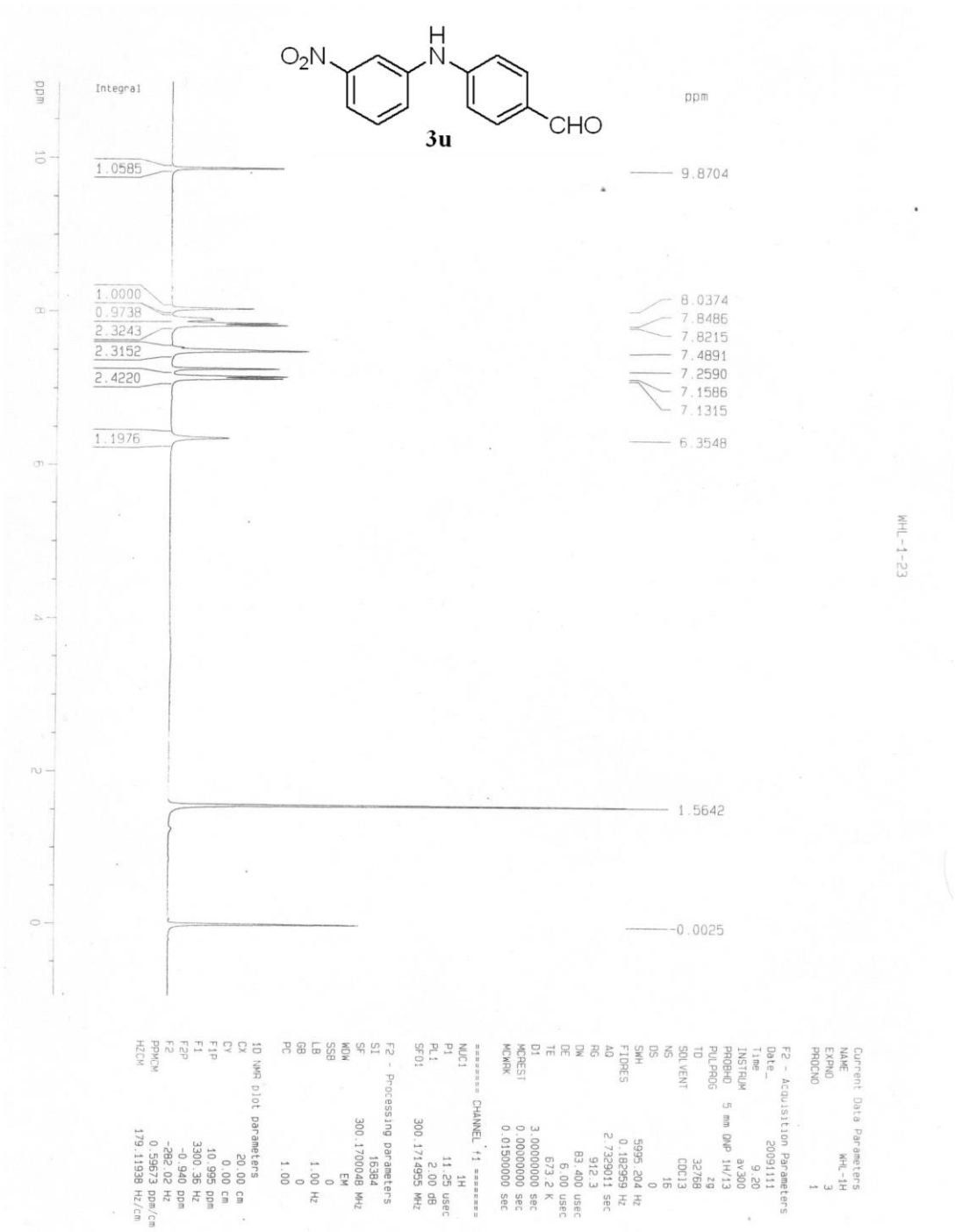

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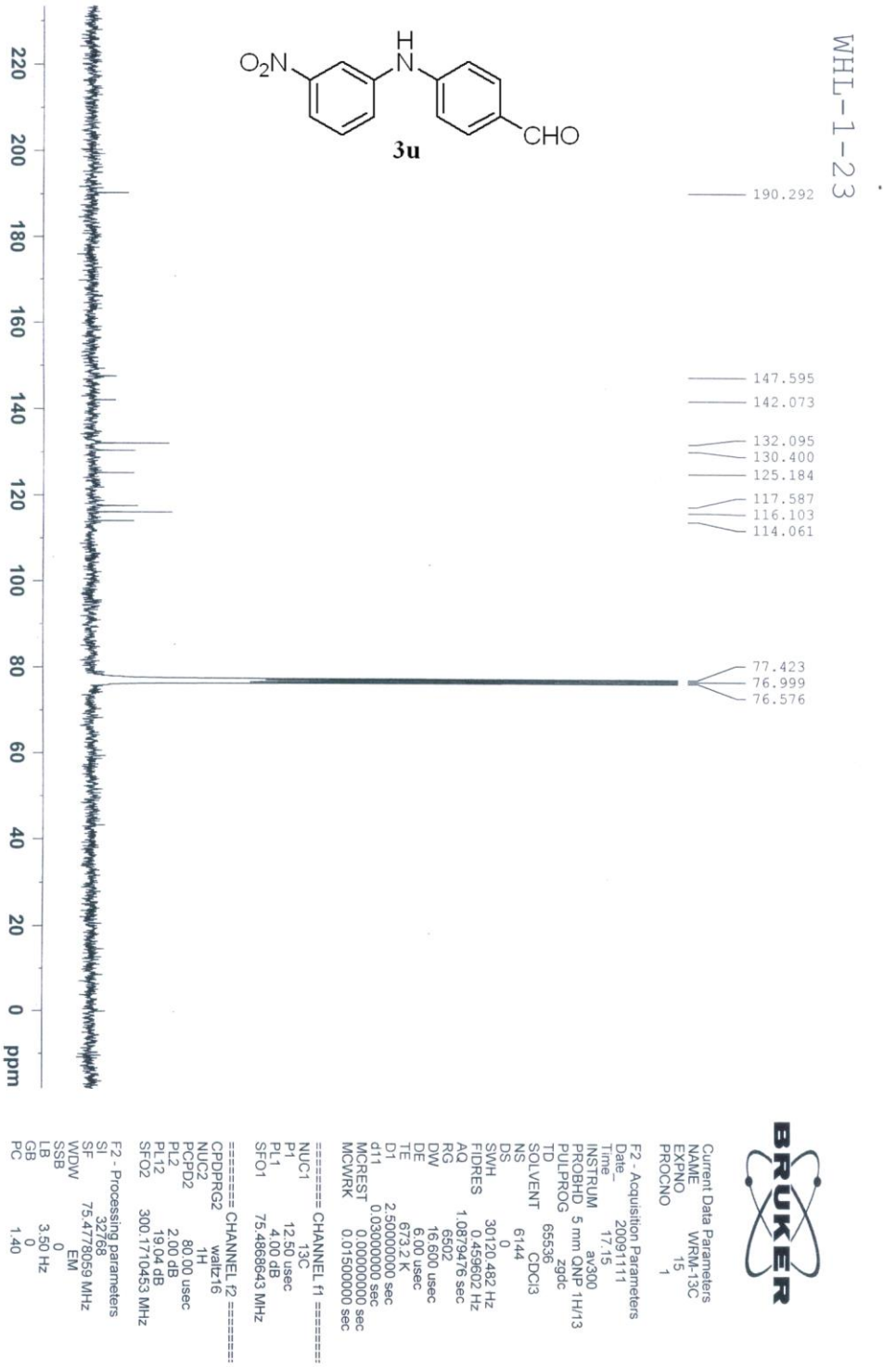

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