Novel Method for Syntheses of Furo[3,4-*c*]coumarins and Related Furyl Coumarin Derivatives via Intramolecular Wittig Reactions

Yeong-Jiunn Jang, Siang-en Syu, Yu-Jhang Chen, Mei-Chun Yang and Wenwei Lin*

Department of Chemistry, National Taiwan Normal University
No. 88, Section 4, Tingchow Road, Taipei 11677, Taiwan, ROC
Fax: (+886) 02 29354249
e-mail: wenweilin@ntnu.edu.tw

Supplementary Data

Table of contents:

Ⅰ. Extra Figures and Tables:

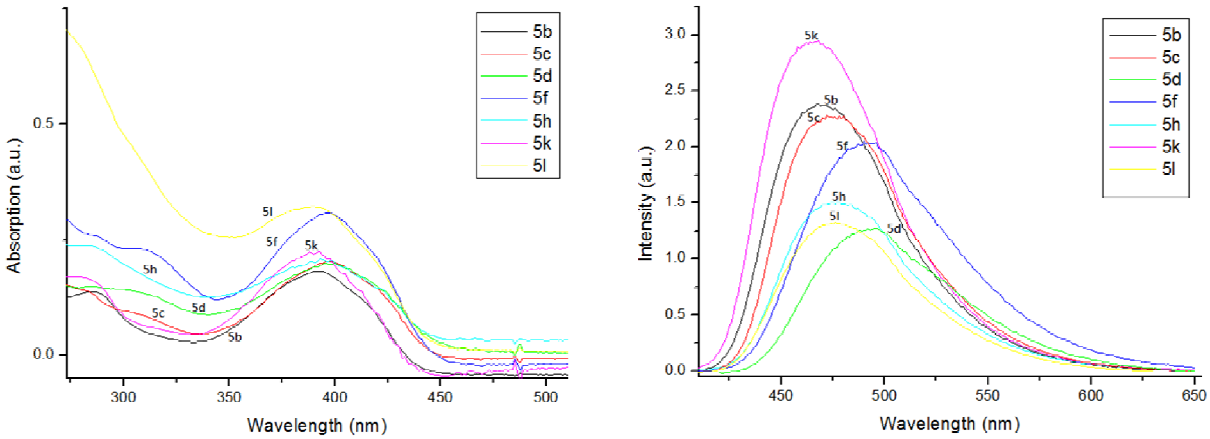
Figure SI-1

Physical data for selected compounds.

Entry	Compound	λ_{max} (nm)[a]	λ_{em} (nm)[a]	ϕ_f[b]
1	**5b**	390	467	44
2	**5c**	398	462	42
3	**5d**	400	495	24
4	**5f**	398	490	38
5	**5h**	393	477	28
6	**5k**	393	468	55
7	**5l**	390	476	25

[a]In ethyl acetate solution. [b]ϕ_f: fluorescence quantum yield, relative to coumarin 1 (99% in ethyl acetate).

Figure SI-2

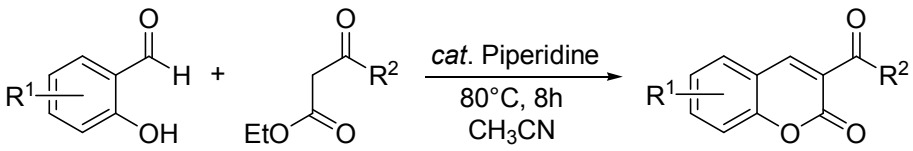


Ⅱ. General Considerations:

All reactions were carried out under a nitrogen atmosphere in dried glassware. The starting materials purchased from commercial sources were used without further purification. THF was continuously refluxed and freshly distilled from sodium benzophenone ketyl under nitrogen. Yields refer to isolated yields of compounds estimated to be > 95 % pure as determined by ^{1}H-NMR. ^{1}H and ^{13}C spectra were generally recorded in a AV-400 or AV-500 Bruker using $CDCl_3$ as solvent at 400 or 500 and 100 or 125 MHz, respectively. Chemical shifts are reported in ppm relative to $CDCl_3$ (δ 7.26 ppm) in indicated cases. Analytical thin layer chromatography (TLC) was performed using Merck 60 F254 precoated silica gel plate (0.2 mm thickness). Flash chromatography was performed using Merck silica gel 60.

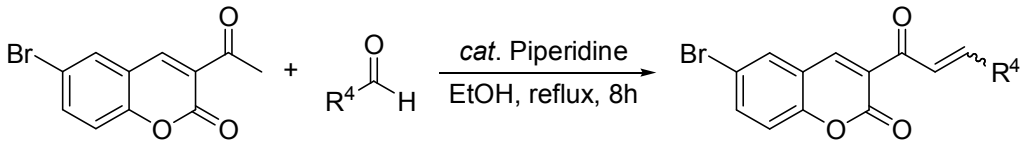
Ⅲ. Representative Experimental procedures:

[1] Typical procedure for syntheses of substrates 1 from substituted salicylaldehydes and ethyl benzoylacetate or ethyl acetoacetate in the presence of piperidine. (TP for Tables 1-4 and Schemes 1)



Piperidine (5 mol %) was added to a stirred solution of substituted salicylaldehyde (10 mmol), ethyl benzoylacetate (1.25 equiv) or ethyl acetoacetate (1.5 equiv) in CH_3CN (10 mL) at room temperature. After 5 min of stirring, the contents were stirred and kept at 80°C for 8h. After returning to the room temperature, the solvent was removed under reduced pressure and the crude product was subjected for column chromatography purification using silica gel with hexane/EtOAc (10:1) as eluent to give 3-benzoylcoumarin or 3-acetylcoumarin **1**.

[2] Typical procedure for syntheses of substrates 4 from 6-bromo-3-acetylcoumarin (1ce) and aromatic aldehyde in the presence of piperidine. (TP for Table 4 and Scheme 1)



Piperidine (20 mol %) was added to a stirred solution of 6-bromo-3-acetylcoumarin (10 mmol) and corresponding aromatic aldehyde (1.25 equiv) in EtOH (20 mL) at room temperature. After 5 min of stirring, the contents were stirred under reflux for 8h. After returning to the room temperature, the solvent was removed under reduced pressure. The crude product was filtered, dried, and recrystallized from ethanol to give pure coumarin-chalcone hybrids **4**.

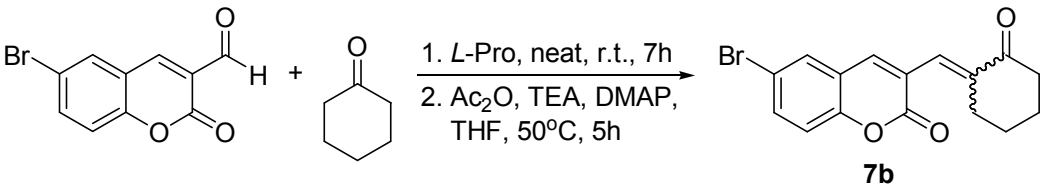
[3] Typical preparation of 3-(3-coumarinyl)propen-1-ones 7a-c. (TP for Scheme 2)

7a and 7c:

7a / 7c

Commercial available triphenyl phosphonium ylide (1.1 equiv) was added to a stirred solution of 6-bromo-3-formylcoumarin (10 mmol) in dichloromethane (20 mL) at room temperature. After 12h of stirring, the solvent was removed under reduced pressure and the crude product was subjected for column chromatography purification using silica gel with hexane/EtOAc (20:1) as eluent to give **7a** or **7c**.

7b:



7b

6-Bromo-3-formylcoumarin (5.0 mmol) was added to a mixture of cyclohexaneone (2 equiv) and *L*-proline (10 mol %) at room temperature. The reaction mixture was stirred and the progress of the reaction monitored by TLC. After the completion of the reaction (7h), the reaction mixture was diluted with EtOAc and extracted three times with EtOAc. The organic layer was washed with brine, dried over anhydrous $MgSO_4$, and concentrated to give the crude aldol product. Without further purification, this crude product was added to a mixture of Ac_2O (1.2 equiv), Et_3N (2 equiv), and DMAP (10 mol %) in THF (10 mL) at room temperature, and the solution was heated at 50°C for 6h. After returning to the room temperature, the solvent was removed under reduced pressure and the crude product was subjected for column chromatography purification using silica gel with hexane/EtOAc (10:1) as eluent to give **7b**.

[4] Typical preparation of furo[3,4-*c*]coumarins 3. (TP for Tables 1-3)

3caa: In a dry, nitrogen-flushed Schlenk flask equipped with a septum and a magnetic stirring bar, compound **1ca** (164.6 mg, 0.50 mmol) was dissolved in dry THF (2.5 mL) and stirred. After 5 min of stirring, tributylphosphine (187.3 μL, 0.75 mmol), benzoyl chloride (**2a**) (116.1 μL, 1.0 mmol), and Et_3N (152.9 μL, 1.1 mmol) were successively added. The resulting solution was stirred at 27°C until completion (monitoring by NMR). After full completion (2.5 h), the solvent was removed in vacuo, and the crude product was purified by flash chromatography (silica gel; hexane/EtOAc, 13:1) to yield the desired product **3caa** (147.5 mg, 71%) as a white solid.

[5] Typical preparation of 3-(2-furyl)coumarins 5. (TP for Table 4 and Scheme 1)

5a: In a dry, nitrogen-flushed Schlenk flask equipped with a septum and a magnetic stirring bar, compound **4a** (71.0 mg, 0.20 mmol) was dissolved in dry THF (1.0 mL) and stirred. After 5 min of stirring, tributylphosphine (55.0 μL, 0.22 mmol), benzoyl chloride (**2a**) (30.2 μL, 0.26 mmol), and Et_3N (41.7 μL, 0.30 mmol) were successively added. The resulting solution was stirred at 27°C until completion (monitoring by NMR). After full completion (1.5 h), the solvent was removed in vacuo, and the crude product was purified by flash chromatography (silica gel; hexane/ethyl acetate, 13:1) to yield the desired product **5a** (71.9 mg, 81%) as a orange solid.

[6] Typical preparation of 3-(3-furyl)coumarins 8. (TP for Scheme 2)

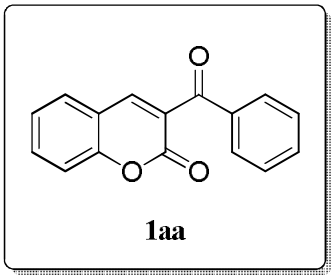
8a: In a dry, nitrogen-flushed Schlenk flask equipped with a septum and a magnetic stirring bar, compound **7a** (71.1 mg, 0.20 mmol) was dissolved in dry THF (1.0 mL) and stirred. After 5 min of stirring, tributylphosphine (55.0 μL, 0.22 mmol), benzoyl chloride (**2a**) (30.2 μL, 0.26 mmol), and Et_3N (41.7 μL, 0.30 mmol) were successively added. The resulting solution

was stirred at 27°C until completion (monitoring by NMR). After full completion (1.0 h), the solvent was removed in vacuo, and the crude product was purified by flash chromatography (silica gel; hexane/ethyl acetate, 13:1) to yield the desired product **8a** (58.1 mg, 52%) as a pale yellow solid.

Ⅳ. Spectra data of the substrates and products:

[1] Spectra data of the substrates 1 in Tables 1-2.

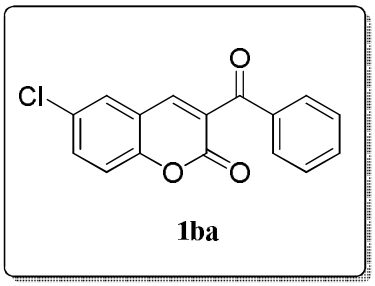
3-benzoyl-2*H*-chromen-2-one (1aa):



1aa

pale yellow solid; mp: 137.8-138.4 °C; ^{1}H NMR (400 MHz, $CDCl_3$, 25 °C) δ 8.08 (s, 1H), 7.89 (d, 2H, J = 7.4 Hz), 7.70-7.57 (m, 3H), 7.49 (t, 2H, J = 7.7 Hz), 7.41 (d, 1H, J = 8.4 Hz), 7.36 (t, 1H, J = 7.7 Hz); ^{13}C NMR (100 MHz, $CDCl_3$, 25 °C) δ 191.5, 158.3, 154.6, 145.2, 136.1, 133.7, 133.5, 129.5, 129.1, 128.5, 126.8, 124.9, 118.0, 116,7; IR (KBr) 3055 (w), 1721 (s), 1240 (m) cm^{-1}; MS (20eV, EI) *m/z* (%) 250 (M^+, 100), 105 (39); HRMS (MALDI) for $(C_{16}H_{10}O_3 + H)^+$: 251.0708, found: 251.0714.

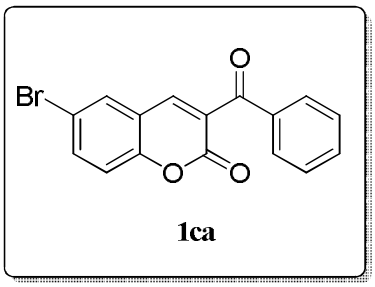
3-benzoyl-6-chloro-2*H*-chromen-2-one (1ba):



1ba

white solid; mp: 169.4-170.1 °C; ^{1}H NMR (400 MHz, $CDCl_3$, 25 °C) δ 7.96 (s, 1H), 7.84 (d, 2H, J = 7.6 Hz), 7.67-7.51 (m, 3H), 7.46 (t, 2H, J = 7.7 Hz), 7.36-7.29 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$, 25 °C) δ 191.0, 157.7, 152.9, 143.7, 135.8, 133.9, 133.3, 130.1, 129.5, 128.6, 128.1, 128.0, 119.1, 118.2; IR (KBr) 3078 (w), 1724 (s), 1657 (s), 1241 (m), 684 (m) cm^{-1}; MS (20eV, EI) *m/z* (%) 286 (M+2, 45), 284 (M^+, 100), 210 (5); HRMS (MALDI) for $(C_{16}H_9{}^{35}ClO_3 + H)^+$: 285.0318, found: 285.0324.

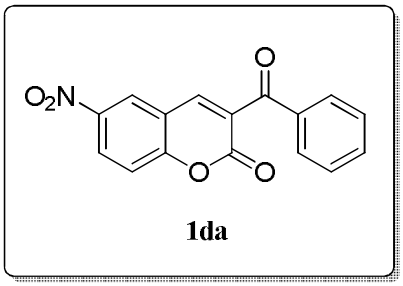
3-benzoyl-6-bromo-2*H*-chromen-2-one (1ca):



1ca

white solid; mp: 177.8-178.7 °C; ^{1}H NMR (400 MHz, $CDCl_3$, 25 °C) δ 7.97 (s, 1H), 7.91-7.84 (m, 2H), 7.76-7.69 (m, 2H), 7.63 (t, 1H, J = 7.4 Hz), 7.49 (t, 2H, J = 7.7 Hz), 7.34-7.27 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$, 25 °C) δ 191.0, 157.6, 153.5, 143.6, 136.1, 135.9, 133.9, 131.2, 129.5, 128.6, 128.1, 119.6, 118.6, 117.4; IR (KBr) 3070 (w), 1716 (s), 1657 (s), 1237 (m), 570 (m) cm^{-1}; MS (20eV, EI) *m/z* (%) 330 (M+2, 53), 329 (M+1, 100), 328 (M^+, 51), 221 (67), 105 (91); HRMS (MALDI) for $(C_{16}H_9{}^{79}BrO_3 + H)^+$: 328.9813, found: 328.9822.

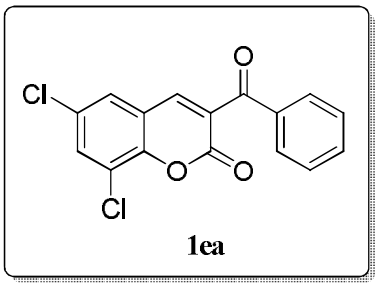
3-benzoyl-6-nitro-2*H*-chromen-2-one (1da):



1da

orange solid; mp: 179.7-180.6 °C; ^{1}H NMR (400 MHz, $CDCl_3$, 25 °C) δ 8.54-8.48 (m, 2H), 8.11 (s, 1H), 7.88 (d, 2H, J = 7.6 Hz), 7.66 (t, 1H, J = 7.4 Hz), 7.56-7.49 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$, 25 °C) δ 190.3, 157.9, 156.8, 144.3, 143.4, 135.5, 134.4, 129.6, 129.2, 128.8, 127.9, 124.8, 118.2; IR (KBr) 3070 (w), 1745 (s), 1660 (s), 1520 (s), 1340 (s), 1244 (s) cm^{-1}; MS (20eV, EI) *m/z* (%) 295 (M^+, 100), 105 (24); HRMS (MALDI) for $(C_{16}H_9NO_5 + Na)^+$: 318.0378, found: 318.0385.

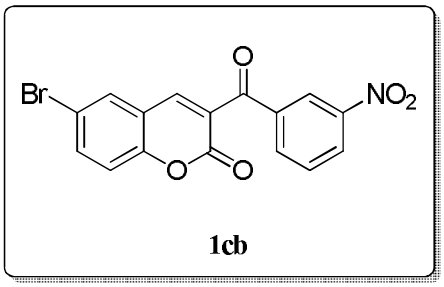
3-benzoyl-6,8-dichloro-2*H*-chromen-2-one (1ea):



1ea

orange solid; mp: 193.7-194.5 °C; ^{1}H NMR (400 MHz, $CDCl_3$, 25 °C) δ 7.96 (s, 1H), 7.87 (d, 2H, J = 7.8 Hz), 7.69 (d, 1H, J = 2.1 Hz), 7.66 (t, 1H, J = 7.4 Hz), 7.50 (t, 3H, J = 7.7 Hz); ^{13}C NMR (100 MHz, $CDCl_3$, 25 °C) δ 190.6, 156.7, 149.0, 143.3, 135.6, 134.2, 133.3, 130.1, 129.6, 129.0, 128.7, 126.7, 122.9, 120.0; IR (KBr) 3063 (w), 1731 (s), 1661 (s), 1244 (m), 684 (m), 669 (m) cm^{-1}; MS (20eV, EI) *m/z* (%) 322 (M+4, 11), 320 (M+2, 67), 318 (M^+, 100), 105 (38); HRMS (MALDI) for $(C_{16}H_8{}^{35}Cl_2O_3 + H)^+$: 318.9929, found: 318.9941.

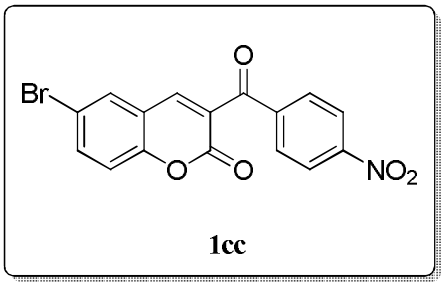
6-bromo-3-(3-nitrobenzoyl)-2*H*-chromen-2-one (1cb):



1cb

orange solid; mp: 237.7-238.5 °C; ^{1}H NMR (400 MHz, $CDCl_3$, 25 °C) δ 8.66-8.62 (m, 1H), 8.51-8.44 (m, 1H), 8.21-8.14 (m, 2H), 7.83-7.76 (m, 2H), 7.71 (t, 1H, J = 8.0 Hz), 7.34 (d, 1H, J = 8.5 Hz); ^{13}C NMR (125 MHz, $CDCl_3$, 25 °C) δ 189.4, 157.8, 153.9, 148.3, 145.9, 137.7, 137.1, 134.7, 131.7, 129.8, 127.9, 126.7, 124.2, 119.5, 118.8, 117.9; IR (KBr) 3085 (m), 1720 (s), 1661 (s), 1521 (s), 1351 (s), 1237 (m), 577 (m) cm^{-1}; MS (20eV, EI) *m/z* (%) 375 (M+2, 100), 373 (M^+, 10), 372 (M-1, 94), 328 (12); HRMS (MALDI) for $(C_{16}H_8{}^{79}BrO_5 + Na)^+$: 395.9484, found: 395.9492.

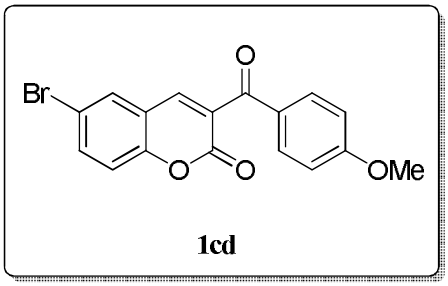
6-bromo-3-(4-nitrobenzoyl)-2*H*-chromen-2-one (1cc):



1cc

brown solid; mp: 280.4-281.3 °C; ^{1}H NMR (400 MHz, $CDCl_3$, 25 °C) δ 8.34 (d, 2H, J = 8.7 Hz), 8.19 (s, 1H), 7.98 (d, 2H, J = 8.5 Hz), 7.83-7.76 (m, 2H), 7.33 (d, 1H, J = 8.4 Hz); ^{13}C NMR (125 MHz, $CDCl_3$, 25 °C) δ 157.7, 153.9, 146.0, 141.1, 137.2, 131.7, 130.2, 123.8, 119.5, 118.8, 117.9, 114.6, 114.1; IR (KBr) 3078 (m), 1712 (s), 1668 (s), 1524 (s), 1351 (s), 1237 (s), 573 (m) cm^{-1}; MS (20eV, EI) *m/z* (%) 375 (M+2, 14), 373 (M^+, 11), 372 (M-1, 100), 328 (17); HRMS (EI) for $(C_{16}H_8{}^{79}BrO_5)^+$: 372.9586, found: 372.9579.

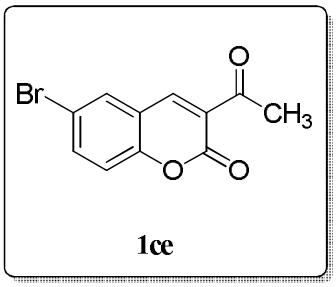
6-bromo-3-(4-methoxybenzoyl)-2*H*-chromen-2-one (1cd):



1cd

yellow solid; mp: 227.6-228.4 °C; ^{1}H NMR (400 MHz, $CDCl_3$, 25 °C) δ 7.91 (s, 1H), 7.87 (d, 2H, J = 8.8 Hz), 7.74-7.69 (m, 2H), 7.33-7.27 (m, 1H), 6.96 (d, 2H, J = 8.8 Hz), 3.89 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$, 25 °C) δ 189.4, 164.5, 157.9, 153.4, 142.8, 136.0, 132.2, 131.1, 128.8, 119.8, 118.6, 117.5, 114.0, 55.6; IR (KBr) 3092 (w), 2841 (w), 1720 (s), 1650 (m), 1255 (s), 1240 (s), 570 (m) cm^{-1}; MS (20eV, EI) *m/z* (%) 360 (M+2, 12), 359 (M+1, 100), 358 (M^+, 13), 357 (M-1, 95), 135 (58); HRMS (MALDI) for $(C_{17}H_{11}{}^{79}BrO_4 + H)^+$: 358.9919, found: 358.9927.

3-acetyl-6-bromo-2*H*-chromen-2-one (1ce):



1ce

yellow solid; mp: 227.4-228.2 °C; ^{1}H NMR (400 MHz, $CDCl_3$, 25 °C) δ 8.40 (s, 1H), 7.78 (d, 1H, J = 2.1 Hz), 7.76-7.69 (m, 1H), 7.27 (d, 1H, J = 8.8 Hz), 2.72 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$, 25 °C) δ 195.0, 158.5, 154.1, 145.9, 137.0, 132.2, 125.5, 119.8, 118.4, 117.5, 30.5; IR (KBr) 3041 (m), 2923 (w), 1735 (s), 1676 (s), 1233 (s), 559 (s) cm^{-1}; MS (20eV, EI) *m/z* (%) 268 (M+2, 98), 266 (M^+, 100), 253 (28); HRMS (MALDI) for $(C_{11}H_7{}^{79}BrO_3 + H)^+$: 266.9657, found: 266.9663.

[2] Spectra data of the substrates in Figure 3.

3-benzoyl-2*H*-thiochromen-2-one (Figure 3A):

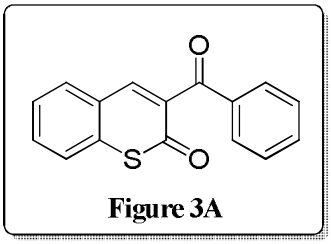


Figure 3A

mp: 123.9-124.4 °C; ^{1}H NMR (400 MHz, $CDCl_3$, 25 °C) δ 7.95 (s, 1H), 7.92-7.86 (m, 2H), 7.71 (d, 1H, J = 7.5 Hz), 7.64-7.56 (m, 2H), 7.54 (d, 1H, J = 7.3 Hz), 7.50-7.42 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$, 25 °C) δ 193.3, 182.9, 144.9, 139.2, 136.4, 134.3, 133.7, 132.9, 131.1, 129.6, 128.6, 126.9, 125.8, 125.4; IR (KBr) 3028 (w), 1665 (s), 1617 (s) cm^{-1}; MS (20eV, EI) *m/z* (%) 266 (M^+, 100), 238 (54), 161 (19), 105 (11); HRMS (MALDI) for $(C_{16}H_{10}O_2S + H)^+$: 267.0480, found: 267.0484.

3-acetyl-6-bromo-2*H*-chromene-2-thione (Figure 3B):

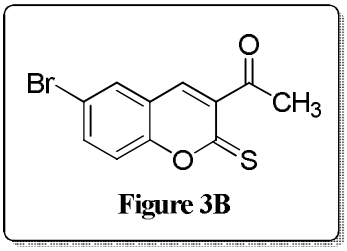


Figure 3B

mp: 211.8-212.3 °C; ^{1}H NMR (400 MHz, $CDCl_3$, 25 °C) δ 7.80-7.67 (m, 2H), 7.61 (s, 1H), 7.35 (d, 1H, J = 9.4 Hz), 2.70 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$, 25 °C) δ 198.6, 192.6, 155.9, 141.0, 136.3, 133.1, 131.1, 121.4, 118.5, 118.1, 29.9; IR (KBr) 3097 (w), 3039 (w), 1695 (s), 1189 (s), 569 (m) cm^{-1}; MS (20eV, EI) *m/z* (%) 284 (M+2, 100), 282 (M^+, 85), 265 (45), 241 (11); HRMS (MALDI) for $(C_{11}H_7{}^{79}BrO_2S + H)^+$: 282.9428, found: 282.9434.

6-bromo-2-oxo-2*H*-chromene-3-carbaldehyde (Figure 3C):

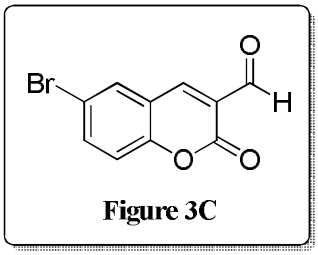


Figure 3C

orange solid; mp: 173.7-174.2 °C; ^{1}H NMR (400 MHz, $CDCl_3$, 25 °C) δ 10.22 (s, 1H), 8.32 (s, 1H), 7.81 (d, 1H, J = 2.1 Hz), 7.75 (dd, 1H, J = 8.4, 2.1 Hz), 7.28 (d, 1H, J = 8.4 Hz); ^{13}C NMR (100 MHz, $CDCl_3$, 25 °C) δ 187.3, 159.3, 154.2, 144.1, 137.6, 132.7, 122.4, 119.6, 118.8, 117.8; MS (20eV, EI) *m/z* (%) 254 (M+2, 34), 252 (M^+, 45), 226 (100).

ethyl 6-bromo-2-oxo-2*H*-chromene-3-carboxylate (Figure 3D):

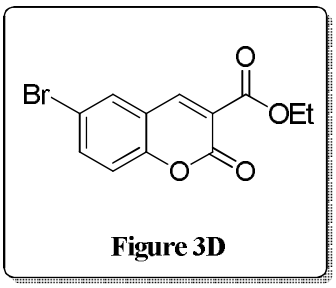


Figure 3D

white solid; mp: 174.2-174.8 °C; ^{1}H NMR (400 MHz, $CDCl_3$, 25 °C) δ 8.42 (s, 1H), 7.75-7.69 (m, 2H), 7.24 (d, 1H, J = 8.8 Hz), 4.40 (q, 2H, J = 7.1 Hz), 1.39 (t, 3H, J = 7.1 Hz) ; ^{13}C NMR (100 MHz, $CDCl_3$, 25 °C) δ 162.6, 155.9, 153.9, 147.0, 136.9, 131.5, 119.4, 119.3, 118.5, 117.3, 62.2, 14.1; IR (KBr) 3092 (w), 3070 (m), 2974 (m), 2900 (w), 1753 (s), 1705 (s), 1288 (s), 1241 (s), 599 (m) cm^{-1}; MS (20eV, EI) *m/z* (%) 298 (M+2, 75), 296 (M^+, 95), 253 (30), 224 (100), 84 (13); HRMS (MALDI) for $(C_{12}H_9{}^{79}BrO_4 + H)^+$: 296.9762, found: 296.9969.

6-bromo-3-(piperidine-1-carbonyl)-2*H*-chromen-2-one (Figure 3E):

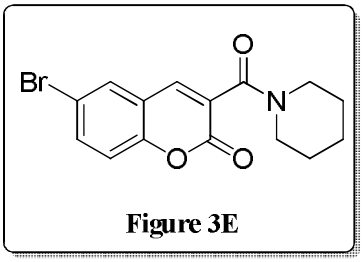
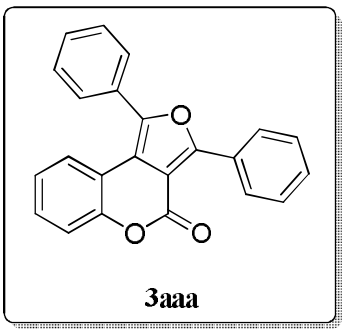


Figure 3E

white solid; mp: 219.2-220.0 °C; ^{1}H NMR (400 MHz, $CDCl_3$, 25 °C) δ 7.75 (s, 1H), 7.65-7.62 (m, 2H), 7.24-7.21 (m, 1H), 3.69 (brs, 2H), 3.30 (t, 2H, J = 5.2 Hz), 1.75-1.52 (m, 6H); ^{13}C NMR (100 MHz, $CDCl_3$, 25 °C) δ 162.7, 157.3, 152.8, 140.5, 135.2, 130.5, 127.1, 119.9, 118.4, 117.4, 48.3, 43.0, 26.2, 25.3, 24.3; IR (KBr) 3055 (m), 2989 (w), 2967 (w), 2937 (m), 2907 (m), 2893 (w), 2849 (m), 1731 (s), 1639 (s), 1613 (s), 1248 (s), 588 (m) cm^{-1}; MS (20eV, EI) *m/z* (%) 337 (M+2, 11), 335 (M^+, 9), 84 (100); HRMS (MALDI) for $(C_{15}H_{14}{}^{79}BrNO_3 + H)^+$: 336.0235, found: 336.0240.

[3] Spectra data of the products 3 in Tables 1-3.

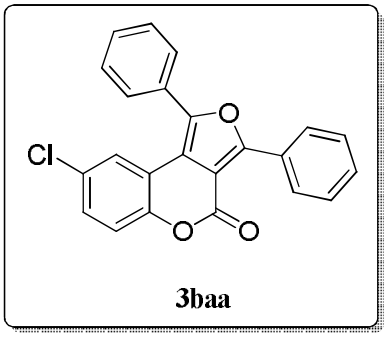
1,3-diphenyl-4*H*-furo[3,4-*c*]chromen-4-one (3aaa):



3aaa

white solid; mp: 238.6-239.4 °C; ^{1}H NMR (400 MHz, $CDCl_3$, 25 °C) δ 8.41 (d, 2H, J = 7.4 Hz), 7.88 (d, 1H, J = 7.8 Hz), 7.80 (d, 2H, J = 7.0 Hz), 7.63-7.42 (m, 6H), 7.40-7.28 (m, 2H), 7.10 (t, 1H, J = 7.0 Hz); ^{13}C NMR (100 MHz, $CDCl_3$, 25 °C) δ 157.9, 157.7, 151.4, 146.9, 130.3, 129.7, 129.4, 129.0, 128.8, 128.6, 128.5, 128.2, 124.1, 123.2, 117.6, 117.3, 114.9, 108.0; IR (KBr) 1735 (s), 1274 (m), 1185 (m) cm^{-1}; MS (20eV, EI) *m/z* (%) 339 (M+1, 100); HRMS (EI) for $(C_{23}H_{14}O_3)^+$: 338.0943, found: 338.0943.

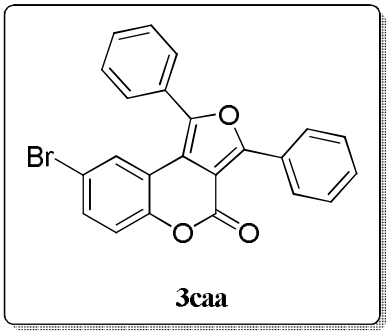
8-chloro-1,3-diphenyl-4*H*-furo[3,4-*c*]chromen-4-one (3baa):



3baa

white solid; mp: 259.7-260.3 °C; ^{1}H NMR (400 MHz, $CDCl_3$, 25 °C) δ 8.39 (d, 2H, J = 7.2 Hz), 7.84 (d, 1H, J = 2.0 Hz), 7.78 (d, 2H, J = 6.8 Hz), 7.65-7.43 (m, 6H), 7.34-7.28 (m, 1H), 7.26-7.19 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$, 25 °C) δ 158.0, 157.3, 149.8, 147.5, 130.5, 130.1, 129.7, 129.4, 129.3, 129.2, 128.6, 128.5, 128.3, 128.2, 122.8, 119.0, 116.4, 116.3, 107.5; IR (KBr) 1742 (s), 1263 (m), 1174 (s), 688 (s) cm^{-1}; MS (20eV, EI) *m/z* (%) 374 (M+2, 68), 372 (M^+, 100), 105 (18); HRMS (MALDI) for $(C_{23}H_{13}{}^{35}ClO_3 + H)^+$: 373.0631, found: 373.0641.

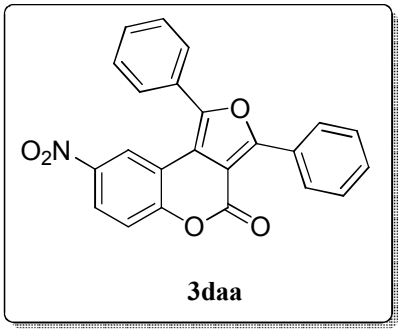
8-bromo-1,3-diphenyl-4*H*-furo[3,4-*c*]chromen-4-one (3caa):



3caa

white solid; mp: 259.5-259.9 °C; ^{1}H NMR (400 MHz, $CDCl_3$, 25 °C) δ 8.39 (d, 2H, J = 7.3 Hz), 8.00 (d, 1H, J = 2.0 Hz), 7.78 (d, 2H, J = 7.0 Hz), 7.65-7.41 (m, 7H), 7.19 (d, 1H, J = 8.8 Hz); ^{13}C NMR (100 MHz, $CDCl_3$, 25 °C) δ 158.0, 157.2, 150.3, 147.5, 132.2, 130.5, 130.1, 129.7, 129.1, 128.6, 128.2, 128.1, 125.7, 119.3, 116.9, 116.8, 116.2, 107.5; IR (KBr) 1742 (s), 1266 (s), 1178 (s), 570 (w) cm^{-1} ; MS (20eV, EI) *m/z* (%) 418 (M+2, 100), 416 (M^+, 87); HRMS (MALDI) for $(C_{23}H_{13}{}^{79}BrO_3 + H)^+$: 417.0126, found: 417.0137.

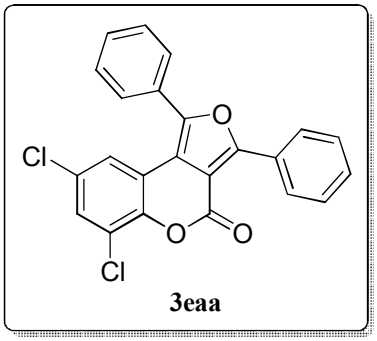
8-nitro-1,3-diphenyl-4*H*-furo[3,4-*c*]chromen-4-one (3daa):



3daa

light yellow solid; mp: 294.2-294.8 °C; ^{1}H NMR (400 MHz, $CDCl_3$, 25 °C) δ 8.84 (d, 1H, J = 2.2 Hz), 8.39 (d, 2H, J = 7.8 Hz), 8.21 (dd, 1H, J = 9.0, 2.2 Hz), 7.81 (d, 2H, J = 7.6 Hz), 7.70-7.59 (m, 3H), 7.58-7.46 (m, 3H), 7.42 (d, 1H, J = 9.0 Hz); ^{13}C NMR (100 MHz, $CDCl_3$, 25 °C) δ 158.6, 156.4, 155.1, 148.4, 144.0, 130.9, 130.7, 129.4, 129.1, 128.7, 128.5, 128.2, 128.0, 124.4, 119.1, 118.5, 115.9, 115.6, 106.9; IR (KBr) 1753 (s), 1524 (s), 1348 (s), 1255 (s), 1189 (s) cm^{-1}; MS (20eV, EI) *m/z* (%) 383 (M^+, 100); HRMS (MALDI) for $(C_{23}H_{13}NO_5 + H)^+$: 384.0872, found: 384.0881.

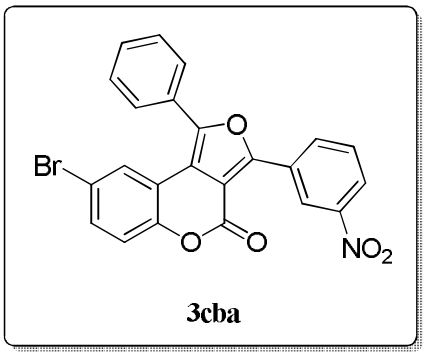
6,8-dichloro-1,3-diphenyl-4*H*-furo[3,4-*c*]chromen-4-one (3eaa):



3eaa

pale yellow solid; mp: 263.7-264.2 °C; ^{1}H NMR (400 MHz, $CDCl_3$, 25 °C) δ 8.37 (d, 2H, J = 7.6 Hz), 7.82-7.69 (m, 3H), 7.66-7.43 (m, 6H), 7.39 (d, 1H, J = 1.5 Hz); ^{13}C NMR (100 MHz, $CDCl_3$, 25 °C) δ 158.2, 156.0, 148.0, 145.9, 130.7, 130.3, 129.4, 129.3, 129.2, 129.1, 128.7, 128.6, 128.1, 128.0, 123.3, 121.1, 117.5, 115.9, 107.1; IR (KBr) 1742 (s), 1292 (w), 1174 (s), 688 (m), 669 (w) cm^{-1}; MS (20eV, EI) *m/z* (%) 410 (M+4, 48), 408 (M+2, 84), 406 (M^+, 100), 105 (21); HRMS (EI) for $(C_{23}H_{12}{}^{35}Cl_2O_3)^+$: 406.0163, found: 406.0154.

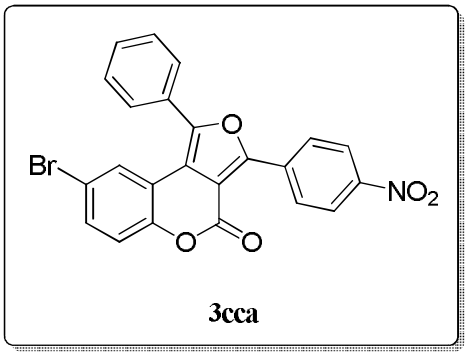
8-bromo-3-(3-nitrophenyl)-1-phenyl-4*H*-furo[3,4-*c*]chromen-4-one (3cba):



3cba

pale yellow solid; mp: 305.0-305.7 °C; ^{1}H NMR (400 MHz, $CDCl_3$, 25 °C) δ 9.19 (s, 1H), 8.90 (d, 1H, J = 7.3 Hz), 8.32 (d, 1H, J = 8.7 Hz), 8.00 (d, 1H, J = 2.0 Hz), 7.80 (d, 2H, J = 6.4 Hz), 7.72 (t, 1H, J = 8.3 Hz), 7.68-7.57 (m, 3H), 7.49 (dd, 1H, J = 8.3, 1.8 Hz), 7.22 (d, 1H, J = 8.7 Hz); ^{13}C NMR (100 MHz, $CDCl_3$, 25 °C) δ 133.8, 132.6, 130.7, 129.9, 129.3, 128.7, 125.9; IR (KBr) 1735 (s), 1524 (s), 1349 (s), 1204 (m), 1175 (m), 569 (w) cm^{-1}; MS (20eV, EI) *m/z* (%) 463 (M+2, 100), 461 (M^+, 88); HRMS (EI) for $(C_{16}H_8{}^{79}BrNO_5)^+$: 460.9895, found: 460.9899.

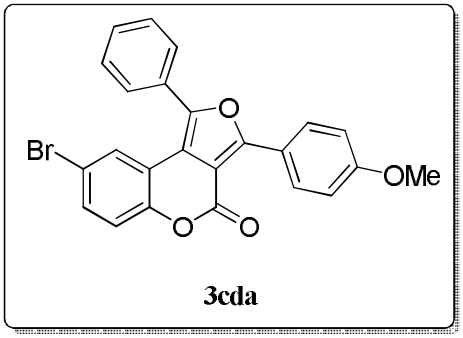
8-bromo-3-(4-nitrophenyl)-1-phenyl-4*H*-furo[3,4-*c*]chromen-4-one (3cca):



3cca

light yellow solid; mp: 264.9-265.5 °C; ^{1}H NMR (400 MHz, $CDCl_3$, 25 °C) δ 8.69-8.60 (m, 2H), 8.40-8.32 (m, 2H), 8.00 (d, 1H, J = 2.3 Hz), 7.85-7.75 (m, 2H), 7.69-7.57 (m, 3H), 7.79 (dd, 1H, J = 7.9, 2.0 Hz), 7.22 (d, 1H, J = 8.8 Hz); ^{13}C NMR (100 MHz, $CDCl_3$, 25 °C) δ 156.9, 154.6, 150.2, 149.3, 148.3, 133.8, 132.7, 130.8, 129.3, 129.1, 128.8, 128.7, 125.8, 123.9, 123.8, 119.4, 117.3, 117.0, 116.3; IR (KBr) 1739 (s), 1516 (s), 1341 (s), 1205 (m), 1173 (m), 570 (w) cm^{-1}; MS (20eV, EI) *m/z* (%) 463 (M+2, 100), 461 (M^+, 80); HRMS (MALDI) for $(C_{16}H_8{}^{79}BrNO_5 + H)^+$: 461.9977, found: 461.9989.

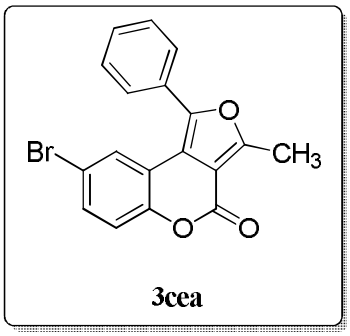
8-bromo-3-(4-methoxyphenyl)-1-phenyl-4*H*-furo[3,4-*c*]chromen-4-one (3cda):



3cda

gray solid; mp: 230.8-231.6 °C; ^{1}H NMR (400 MHz, $CDCl_3$, 25 °C) δ 8.38 (d, 2H, J = 8.6 Hz), 7.99 (brs, 1H), 7.77 (d, 2H, J = 7.2 Hz), 7.67-7.50 (m, 3H), 7.42 (d, 1H, J = 8.0 Hz), 7.17 (d, 1H, J = 8.7 Hz), 7.02 (d, 2H, J = 8.7 Hz), 3.89 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$, 25 °C) δ 161.4, 158.4, 157.5, 150.3, 146.6, 132.0, 130.0, 129.8, 129.1, 128.6, 125.7, 121.0, 119.2, 117.0, 116.8, 115.9, 114.1, 106.1, 55.4; IR (KBr) 2843 (w), 1735 (s), 1224 (m), 1181 (m), 575 (w) cm^{-1}; MS (20eV, EI) *m/z* (%) 448 (M+2, 100), 446 (M^+, 93); HRMS (MALDI) for $(C_{24}H_{15}{}^{79}BrO_4 + H)^+$: 447.0232, found: 447.0239.

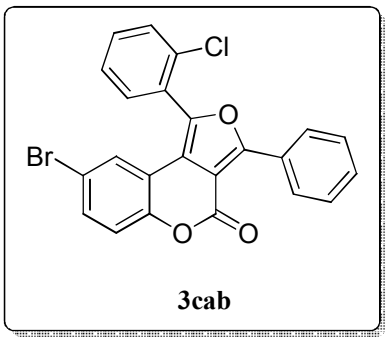
8-bromo-3-methyl-1-phenyl-4*H*-furo[3,4-*c*]chromen-4-one (3cea):



3cea

yellow solid; mp: 242.2-242.8 °C; ^{1}H NMR (400 MHz, $CDCl_3$, 25 °C) δ 7.98 (d, 1H, J = 2.2 Hz), 7.70 (d, 2H, J = 7.1 Hz), 7.60-7.47 (m, 3H), 7.41 (dd, 1H, J = 8.8, 2.2 Hz), 7.15 (d, 1H, J = 8.8 Hz); ^{13}C NMR (100 MHz, $CDCl_3$, 25 °C) δ 159.8, 157.9, 150.6, 147.1, 132.0, 129.9, 129.8, 129.1, 128.2, 125.9, 119.5, 117.3, 116.9, 114.1, 108.5, 13.7; IR (KBr) 3048 (w), 1760 (s), 1266 (m), 1163 (w), 577 (w) cm^{-1}; MS (20eV, EI) *m/z* (%) 356 (M+2, 20), 355 (M+1, 82), 354 (M^+, 36), 353 (M-1, 100); HRMS (MALDI) for ($C_{18}H_{11}{}^{79}BrO_3$ + H)$^+$: 354.9970, found: 354.9982.

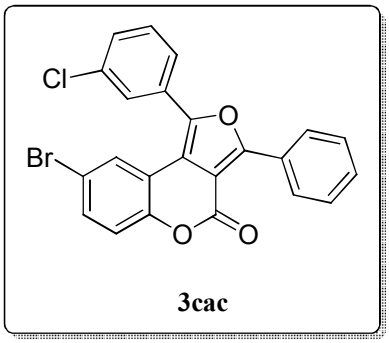
8-bromo-1-(2-chlorophenyl)-3-phenyl-4*H*-furo[3,4-*c*]chromen-4-one (3cab):



3cab

white solid; mp: 229.3-229.8 °C; ^{1}H NMR (400 MHz, $CDCl_3$, 25 °C) δ 8.46-8.37 (m, 2H), 7.70-7.63 (m, 2H), 7.60-7.36 (m, 7H), 7.18 (d, 1H, J = 8.8 Hz); ^{13}C NMR (100 MHz, $CDCl_3$, 25 °C) δ 158.6, 157.1, 150.5, 143.8, 135.0, 132.3, 132.2, 131.9, 130.7, 128.7, 128.6, 128.2, 127.3, 126.4, 119.0, 118.4, 116.9, 116.4, 107.0; IR (KBr) 1735 (s), 1259 (s), 1178 (m), 691 (m), 570 (w) cm^{-1}; MS (20eV, EI) *m/z* (%) 454 (M+4, 23), 452 (M+2, 100), 450 (M^+, 66); HRMS (MALDI) for ($C_{23}H_{12}{}^{79}Br^{35}ClO_3$ + Na)$^+$: 472.9556, found: 472.9567.

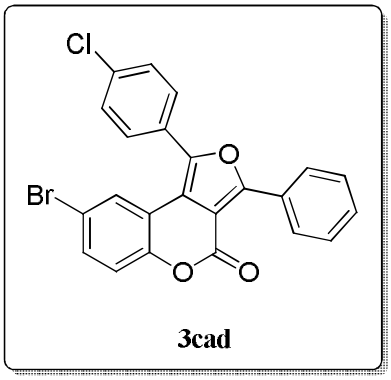
8-bromo-1-(3-chlorophenyl)-3-phenyl-4*H*-furo[3,4-*c*]chromen-4-one (3cac):



3cac

white solid; mp: 265.6-265.9 °C; ^{1}H NMR (400 MHz, $CDCl_3$, 25 °C) δ 8.38 (d, 2H, J = 7.0 Hz), 7.98 (d, 1H, J = 2.2 Hz), 7.78 (s, 1H), 7.72-7.65 (m, 1H), 7.59-7.44 (m, 6H), 7.21 (d, 1H, J = 8.8 Hz); ^{13}C NMR (100 MHz, $CDCl_3$, 25 °C) δ 158.5, 157.0, 150.4, 145.7, 135.3, 132.5, 131.4, 130.8, 130.4, 130.2, 128.7, 128.6, 128.3, 128.0, 126.5, 125.8, 119.4, 117.0, 116.5, 107.6; IR (KBr) 1746 (s), 1193 (s), 1174 (s), 573 (w) cm^{-1}; MS (20eV, EI) *m/z* (%) 454 (M+4, 25), 452 (M+2, 100), 450 (M^+, 65); HRMS (MALDI) for ($C_{23}H_{12}{}^{79}Br^{35}ClO_3$ + H)$^+$: 450.9736, found: 450.9747; Anal. calcd. for $C_{23}H_{12}BrClO_3$: C: 61.16, H: 2.68, found: C: 61.08, H: 2.62.

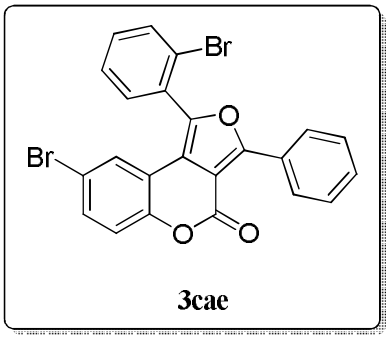
8-bromo-1-(4-chlorophenyl)-3-phenyl-4*H*-furo[3,4-*c*]chromen-4-one (3cad):



3cad

white solid; mp: 262.2-262.6 °C; ^{1}H NMR (400 MHz, $CDCl_3$, 25 °C) δ 8.36 (dd, 2H, J = 8.4, 1.8 Hz), 7.94 (d, 1H, J = 2.4 Hz), 7.72 (d, 2H, J = 8.5 Hz), 7.60-7.43 (m, 6H), 7.19 (d, 1H, J = 8.8 Hz); ^{13}C NMR (100 MHz, $CDCl_3$, 25 °C) δ 158.3, 157.1, 150.4, 146.1, 136.2, 132.4, 130.7, 129.8, 129.5, 129.4, 128.7, 128.2, 128.1, 128.0, 125.6, 119.4, 116.9, 116.6, 107.6; IR (KBr) 1746 (s), 1196 (m), 1178 (m), 507 (w) cm^{-1}; MS (20eV, EI) *m/z* (%) 454 (M+4, 23), 452 (M+2, 100), 450 (M^+, 61); HRMS (MALDI) for $(C_{23}H_{12}{}^{79}Br^{35}ClO_3 + H)^+$: 450.9736, found: 450.9749.

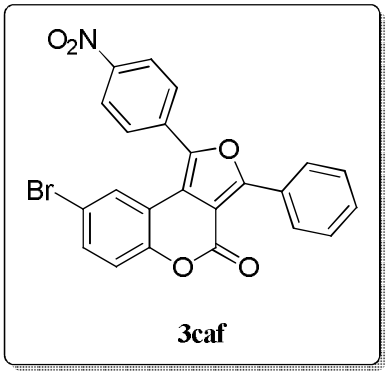
8-bromo-1-(2-bromophenyl)-3-phenyl-4*H*-furo[3,4-*c*]chromen-4-one (3cae):



3cae

yellow solid; mp: 234.7-235.1 °C; ^{1}H NMR (400 MHz, $CDCl_3$, 25 °C) δ 8.43-8.40 (m, 2H), 7.85 (d, 1H, J = 8.0 Hz), 7.63 (dd, 1H, J = 7.6, 1.6 Hz), 7.58-7.42 (m, 6H), 7.35 (d, 1H, J = 2.2 Hz), 7.18 (d, 1H, J = 8.8 Hz); ^{13}C NMR (100 MHz, $CDCl_3$, 25 °C) δ 158.4, 157.1, 150.4, 145.2, 133.8, 132.5, 132.2, 132.1, 130.7, 130.6, 128.6, 128.2, 127.9, 126.4, 124.7, 119.0, 118.1, 116.9, 116.4, 106.8; IR (KBr) 1738 (s), 1218 (m), 1174 (m), 647 (m), 570 (w) cm^{-1}; MS (20eV, EI) *m/z* (%) 498 (M+4, 61), 496 (M+2, 100), 494 (M^+, 52); HRMS (EI) for $(C_{23}H_{12}{}^{79}Br_2O_3)^+$: 493.9153, found: 493.9160.

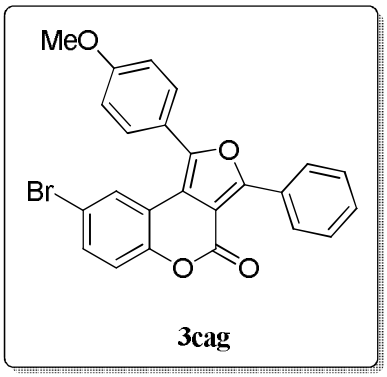
8-bromo-1-(4-nitrophenyl)-3-phenyl-4*H*-furo[3,4-*c*]chromen-4-one (3caf):



3caf

light yellow solid; mp: 234.1-234.6 °C; ^{1}H NMR (400 MHz, $CDCl_3$, 25 °C) δ 8.46 (d, 2H, J = 8.7 Hz) 8.43-8.33 (m, 2H), 8.06-7.94 (m, 3H), 7.61-7.47 (m, 4H), 7.31-7.20 (m, 1H); ^{13}C NMR (125 MHz, $CDCl_3$, 25 °C) δ 159.5, 156.7, 150.6, 148.2, 144.5, 135.8, 133.2, 131.1, 129.0, 128.8, 128.4, 127.7, 125.7, 124.5, 119.7, 118.6, 117.1, 116.0, 108.0; IR (KBr) 1738 (s), 1521 (s), 1344 (s), 1266 (w), 1178 (m), 566 (w) cm^{-1}; MS (20eV, EI) *m/z* (%) 463 (M+2, 100), 461 (M^+, 85); HRMS (EI) for $(C_{23}H_{12}{}^{79}BrNO_5)^+$: 460.9899, found: 460.9890.

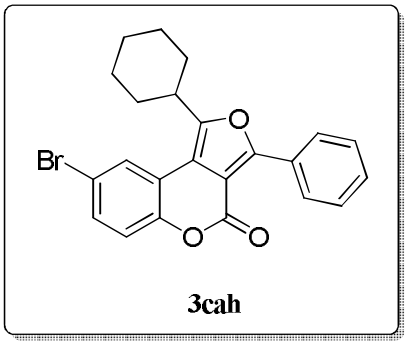
8-bromo-1-(4-methoxyphenyl)-3-phenyl-4*H*-furo[3,4-*c*]chromen-4-one (3cag):



3cag

pale yellow solid; mp: 206.8-207.2 °C; ^{1}H NMR (400 MHz, $CDCl_3$, 25 °C) δ 8.45-8.33 (m, 2H), 7.97 (d, 1H, J = 2.2 Hz), 7.69 (d, 2H, J = 8.6 Hz), 7.58-7.37 (m, 4H), 7.17 (d, 1H, J = 8.7 Hz), 7.11 (d, 2H, J = 8.7 Hz), 3.94 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$, 25 °C) δ 161.0, 157.5, 157.3, 150.2, 147.7, 131.9, 130.4, 130.1, 128.6, 128.3, 128.1, 125.6, 121.9, 119.2, 117.1, 116.8, 115.4, 114.6, 107.4, 55.5; IR (KBr) 2967 (w), 1738 (s), 1259 (s), 1171 (m), 562 (w) cm^{-1}; MS (20eV, EI) *m/z* (%) 448 (M+2, 99), 446 (M^+, 100); HRMS (MALDI) for $(C_{24}H_{15}{}^{79}BrO_4 + H)^+$: 447.0232, found: 447.0244.

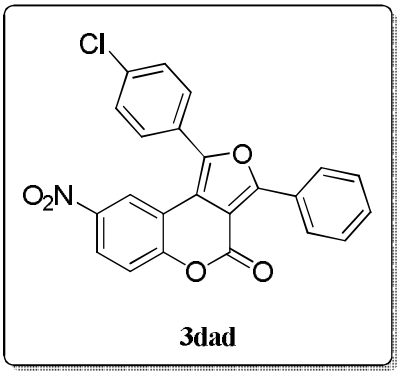
8-bromo-1-cyclohexyl-3-phenyl-4*H*-furo[3,4-*c*]chromen-4-one (3cah):



3cah

white solid; mp: 239.5-240.0 °C; ^{1}H NMR (400 MHz, $CDCl_3$, 25 °C) δ 8.37-8.28 (m, 2H), 7.77 (d, 1H, J = 2.2 Hz), 7.55-7.37 (m, 4H), 7.17 (d, 1H, J = 8.7 Hz), 3.23-3.10 (m, 1H), 2.12-2.02 (m, 2H), 2.02-1.92 (m, 2H), 1.90-1.73 (m, 3H), 1.60-1.32 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$, 25 °C) δ 157.4, 156.2, 153.9, 150.1, 131.1, 130.0, 128.6, 128.5, 127.8, 126.3, 119.2, 117.6, 117.1, 113.9, 106.6, 38.1, 30.9, 26.2, 25.7; IR (KBr) 2930 (m), 2849 (m), 1746 (s), 1252 (s), 1174 (s), 570 (w) cm^{-1}; MS (20eV, EI) *m/z* (%) 424 (M+2, 100), 422 (M^+, 91), 105 (11); HRMS (MALDI) for $(C_{23}H_{19}{}^{79}BrO_3 + Na)^+$: 445.0416, found: 445.0427.

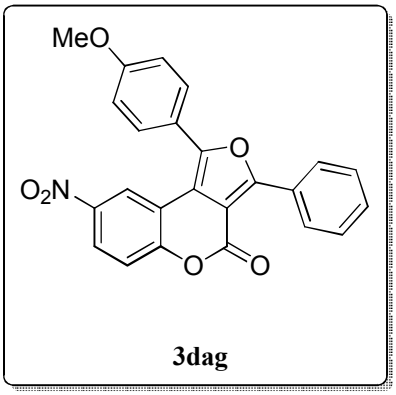
1-(4-chlorophenyl)-8-nitro-3-phenyl-4*H*-furo[3,4-*c*]chromen-4-one (3dad):



3dad

yellow mp: 281.2-281.7 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.80 (d, 1H, J = 3.4 Hz), 8.38 (d, 2H, J = 8.0 Hz), 8.24 (dd, 1H, J = 9.1, 2.4 Hz), 7.76 (d, 2H, J = 8.3 Hz), 7.62 (d, 2H, J = 8.4 Hz), 7.59-7.49 (m, 3H), 7.44 (d, 1H, J = 9.0 Hz); ^{13}C NMR (125 MHz, $CDCl_3$) δ 158.9, 156.2, 155.2, 147.0, 144.0, 136.8, 131.1, 129.8, 129.7, 128.8, 127.7, 127.6, 124.6, 119.0, 118.6, 116.0, 115.6, 106.9; IR (KBr) 1757 (s), 1528 (s), 1344 (s), 1252 (m), 1185 (m), 680 (m) cm^{-1}; MS (20eV, EI) *m/z* (%) 419 (M+2, 35), 417 (M^+, 100); HRMS (MALDI) for $(C_{23}H_{12}{}^{35}ClNO_5 + H)^+$: 418.0482, found: 418.0493.

1-(4-methoxyphenyl)-8-nitro-3-phenyl-4*H*-furo[3,4-*c*]chromen-4-one (3dag):

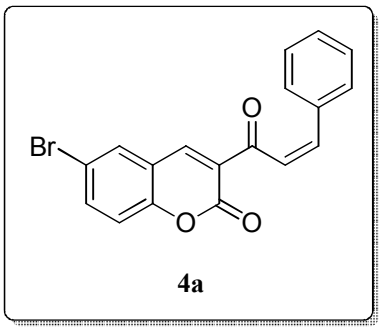


3dag

yellow solid; mp: 232.4-232.7 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.83 (d, 1H, J = 2.6 Hz), 8.42-8.35 (m, 2H), 8.20 (dd, 1H, J = 9.0, 2.7 Hz), 7.73 (d, 2H, J = 8.8 Hz), 7.58-7.47 (m, 3H), 7.41 (d, 1H, J = 9.1 Hz), 7.14 (d, 2H, J = 8.7 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ 161.3, 158.0, 156.4, 155.0, 148.5, 144.0, 130.7, 130.0, 128.7, 128.1, 128.0, 124.1, 121.3, 118.9, 118.3, 116.2, 114.9, 114.7, 106.7, 55.5; IR (KBr) 2937 (w), 1742 (s), 1532 (s), 1351 (s), 1252 (s), 1178 (s) cm^{-1}; MS (20eV, EI) *m/z* (%) 412 (M-1, 100); HRMS (MALDI) for $(C_{24}H_{15}NO_6 + H)^+$: 414.0977, found: 414.0987.

[4] Spectra data of the substrates 4 in Table 4 and Scheme 1.

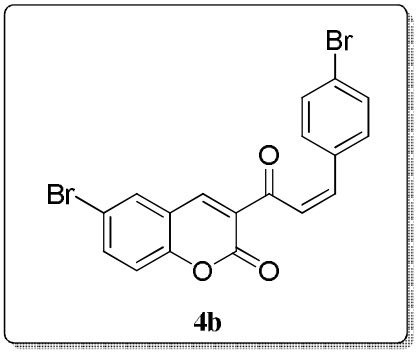
(*Z*)-6-bromo-3-(3-phenylacryloyl)-2*H*-chromen-2-one (4a):



4a

light yellow solid; mp: 209.0-209.6 °C; ^{1}H NMR (400 MHz, $CDCl_3$, 25 °C) δ 8.48 (s, 1H), 7.95-7.83 (m, 2H), 7.41 (d, 1H, J = 1.9 Hz), 7.73 (dd, 1H, J = 8.8, 2.1 Hz), 7.70-7.63 (m, 2H), 7.48-7.37 (m, 3H), 7.29 (d, 1H, J = 8.8 Hz); ^{13}C NMR (100 MHz, $CDCl_3$, 25 °C) δ 186.0, 158.6, 154.0, 146.5, 145.6, 136.8, 134.7, 132.0, 131.0, 129.0, 126.3, 123.6, 120.0, 118.4, 117.5; IR (KBr) 3092 (w), 3055 (w), 1735 (s), 1661 (m), 1252 (m), 559 (m) cm^{-1}; MS (20eV, EI) *m/z* (%) 356 (M+2, 100), 354 (M^+, 86); HRMS (MALDI) for $(C_{18}H_{11}{}^{79}BrO_3 + H)^+$: 354.9970, found: 354.9983.

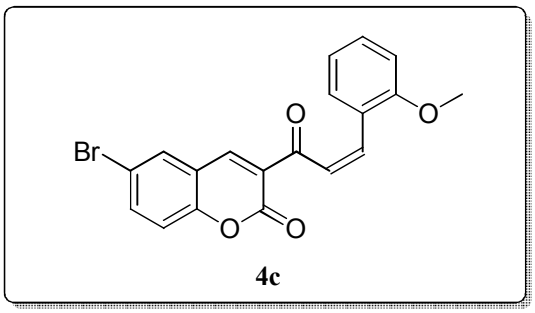
(*Z*)-6-bromo-3-[3-(4-bromophenyl)acryloyl]-2*H*-chromen-2-one (4b):



4b

yellow solid; mp: 269.5-269.8 °C; ^{1}H NMR (400 MHz, $CDCl_3$, 25 °C) δ 8.49 (s, 1H), 7.93-7.73 (m, 4H), 7.54 (m, 4H), 7.30 (d, 1H, J = 8.9 Hz); ^{13}C NMR (125 MHz, $CDCl_3$, 25 °C) δ 185.8, 158.7, 154.1, 146.8, 144.0, 137.0, 133.6, 132.2, 132.1, 130.3, 126.0, 125.4, 124.2, 120.0, 118.5, 117.6; IR (KBr) 3044 (w), 1724 (s), 1609 (s), 1474 (m), 1400 (m), 1185 (m), 581 (m); MS (20eV, EI) m/z (%) (relative intensity) 435 (M+3, 42), 433 (M+1, 100), 431 (M-1, 48), 353 (29); HRMS (MALDI) for $(C_{18}H_{10}{}^{79}Br_2O_3 + Na)^+$: 454.8894, found: 454.8911.

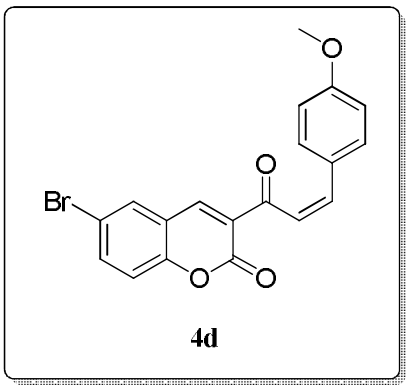
(*Z*)-6-bromo-3-[3-(2-methoxyphenyl)acryloyl]-2*H*-chromen-2-one (4c):



4c

yellow solid; mp: 204.7-205.6 °C; ^{1}H NMR (400 MHz, $CDCl_3$, 25 °C) δ 8.44 (s, 1H), 8.21 (d, 1H, J =15.9 Hz), 7.92 (d, 1H, J = 15.8 Hz), 7.78 (d, 1H, J = 2.0 Hz), 7.72-7.67 (m, 2H), 7.40-7.36 (m, 1H), 7.27 (d, 1H, J = 8.8 Hz), 7.00-6.97 (m, 1H), 6.93 (d, 1H, J = 8.3 Hz), 3.91 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$, 25 °C) δ 186.4, 159.1, 158.6, 153.9, 146.0, 141.0, 136.6, 132.3, 131.9, 129.5, 126.7, 124.1, 123.7, 120.8, 120.1, 118.4, 117.4, 111.2, 55.6; IR (KBr) 3035 (w), 1735 (s), 1570 (m), 1335 (m), 1250 (m), 1182 (m), 577 (m); MS (20eV, EI) m/z (%) (relative intensity) 386 (M+2, 15), 384 (M^+, 16), 354 (81), 352 (100); HRMS (MALDI) for $(C_{19}H_{13}{}^{79}BrO_4 + H)^+$: 385.0075, found: 385.0083.

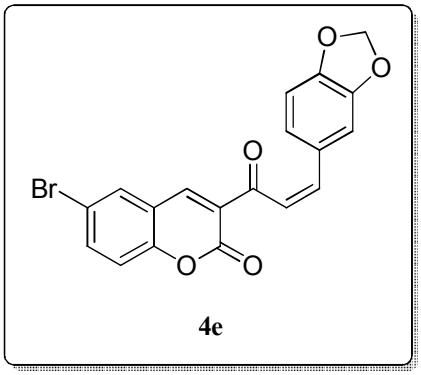
(*Z*)-6-bromo-3-[3-(4-methoxyphenyl)acryloyl]-2*H*-chromen-2-one (4d):



4d

yellow solid; mp:223.3-223.5; ^{1}H NMR (400 MHz, $CDCl_3$, 25 °C) δ 8.47 (s, 1H), 7.89-7.71 (m, 4H),7.64 (d, 2H, J = 8.7 Hz), 7.29(d, 1H, J = 8.8 Hz); 6.93 (d, 2H, J = 8.7 Hz), 3.86 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$, 25 °C) δ 185.8, 162.1, 158.7, 154.0, 146.2, 145.6, 136.7, 131.9, 130.9, 127.5, 126.6, 121.4, 120.2, 118.4, 117.5, 114.5, 55.4; IR (KBr) 3096 (w), 1737 (s), 1567 (s), 1513 (m), 1168 (s), 533 (m); MS (20eV, EI) m/z (%) (relative intensity) 386 (M+2, 87), 384 (M^+, 100); HRMS (MALDI) for $(C_{19}H_{13}{}^{79}BrO_4 + Na)^+$: 406.9895, found: 406.9903.

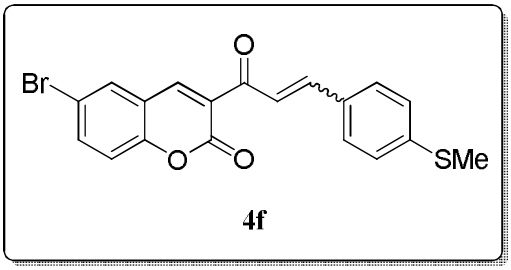
(*Z*)-6-bromo-3-[3-(3,4-methylenedioxyphenyl)acryloyl]-2*H*-chromen-2-one (4e):



4e

orange solid; mp: 277.5-280.3 °C; ^{1}H NMR (500 MHz, $CDCl_3$, 25 °C) δ 8.47 (s, 1H), 7.84-7.69 (m, 4H), 7.29 (d, 2H, J = 7.7 Hz), 7.20 (s, 1H), 7.16 (d, 1H, J = 8.2 Hz), 6.84 (d, 1H, J = 8.2 Hz), 6.03 (s, 2H); ^{13}C NMR (100 MHz, $CDCl_3$, 25 °C) δ 186.4, 158.1, 154.0, 146.1, 141.1, 136.6, 132.9, 132.2, 131.9, 129.6, 126.7, 124.2, 124.0, 121.0, 118.4, 117.9, 117.4, 112.5, 69.4; IR (KBr) 3085 (w), 3048 (w), 2923 (w), 1731 (s), 1654 (m), 1248 (m), 1185 (m), 577 (w) cm^{-1}; MS (20eV, EI) *m/z* (%) 400 (M+2, 96), 398 (M^+, 52), 397 (M-1, 100), 122 (30); HRMS (MALDI) for $(C_{19}H_{11}{}^{79}BrO_5 + H)^+$: 398.9868, found: 398.9882.

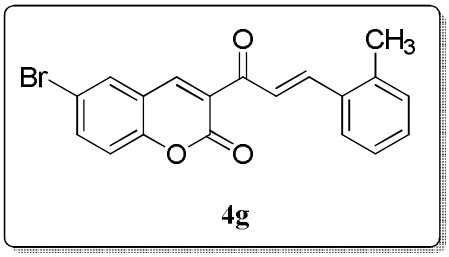
6-bromo-3-[3-(4-methylthiophenyl)acryloyl]-2*H*-chromen-2-one (4f):



4f

yellow solid; mp: 205.4-205.9 °C; ^{1}H NMR (400 MHz, $CDCl_3$, 25 °C) δ 8.48 (s, 1H), 7.93-7.78 (m, 3H), 7.77-7.69 (m, 1H), 7.59 (d, 2H, J = 7.3 Hz), 7.37-7.17 (m, 3H), 2.52 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$, 25 °C) δ 185.8, 158.6, 154.0, 146.4, 145.1, 143.2, 136.8, 132.0, 131.2, 129.3, 126.4, 125.9, 122.6, 120.1, 118.4, 117.5, 15.1; IR (KBr) 3092 (w), 3041 (w), 2915 (w), 1735 (s), 1654 (m), 1185 (m), 584 (w) cm^{-1}; MS (20eV, EI) *m/z* (%) 402 (M+2, 100), 400 (M^+, 92), 353 (17), 177 (11), 124 (19); HRMS (MALDI) for $(C_{19}H_{13}{}^{79}BrO_3S + H)^+$: 400.9847, found: 400.9855.

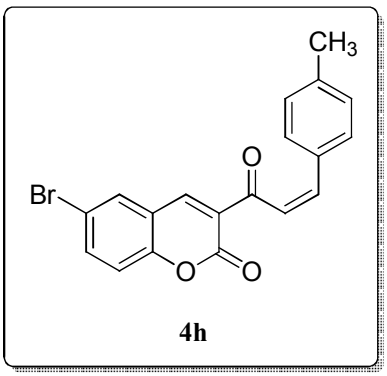
(*E*)-6-bromo-3-[3-(2-methylphenyl)acryloyl]-2*H*-chromen-2-one (4g):



4g

orange solid; mp: 143.8-144.6 °C; ^{1}H NMR (400 MHz, $CDCl_3$, 25 °C) δ 8.47 (s, 1H), 8.18 (d, 1H, J = 15.6 Hz), 7.85-7.78 (m, 2H), 7.77-7.69 (m, 2H), 7.36-7.18 (m, 4H), 2.49 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$, 25 °C) δ 186.1, 158.6, 154.0, 146.5, 143.0, 138.8, 136.8, 133.6, 132.0, 131.0, 130.7, 127.1, 126.4, 124.6, 120.0, 118.4, 117.5, 19.9; IR (KBr) 3100 (w), 3041 (w), 2974 (w), 1724 (s), 1657 (m), 1174 (s), 581 (s) cm^{-1}; MS (20eV, EI) *m/z* (%) 370 (M+2, 23), 368 (M^+, 25), 354 (50), 352 (100); HRMS (MALDI) for $(C_{19}H_{13}{}^{79}BrO_3 + H)^+$: 390.9946, found: 390.9951.

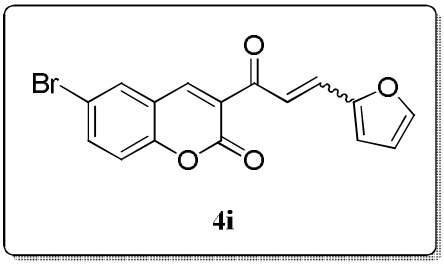
(*Z*)-6-bromo-3-[3-(4-methylphenyl)acryloyl]-2*H*-chromen-2-one (4h):



4h

light yellow solid; mp: 234.0-234.8 °C; ^{1}H NMR (400 MHz, $CDCl_3$, 25 °C) δ 8.47 (s, 1H), 7.93-7.77 (m, 3H), 7.73 (d, 1H, J = 8.8 Hz), 7.57 (d, 2H, J = 7.8 Hz), 7.35-7.16 (m, 3H), 2.39 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$, 25 °C) δ 186.0, 158.6, 154.0, 146.3, 145.7, 141.7, 136.7, 131.9, 129.7, 129.0, 126.4, 122.7, 120.1, 118.4, 117.5, 21.6; IR (KBr) 3092 (w), 3041 (w), 1731 (s), 1657 (s), 1178 (s), 592 (m) cm^{-1}; MS (20eV, EI) *m/z* (%) 370 (M+2, 98), 368 (M^+, 86), 354 (100), 352 (34); HRMS (MALDI) for $(C_{19}H_{13}{}^{79}BrO_3 + H)^+$: 369.0126, found: 369.0137.

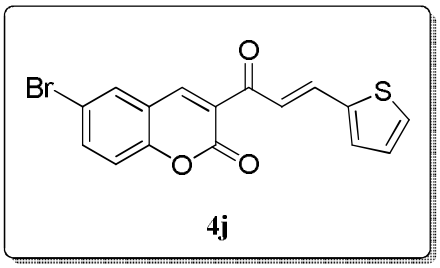
6-bromo-3-[3-(furan-2-yl)acryloyl]-2*H*-chromen-2-one (4i):



4i

dark solid; mp: 238.6-239.3 °C; ^{1}H NMR (400 MHz, $CDCl_3$, 25 °C) δ 8.45 (s, 1H), 7.87-7.69 (m, 3H), 7.68-7.48 (m, 2H), 7.38-7.16 (m, 1H), 6.83-6.75 (m, 1H), 6.55-6.48 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$, 25 °C) δ 185.6, 158.5, 154.0, 146.2, 145.7, 136.7, 132.2, 132.0, 131.2, 126.3, 121.2, 120.1, 118.4, 117.5, 117.2, 112.8; IR (KBr) 3092 (w), 3048 (w), 1735 (s), 1654 (s), 1200 (m), 1175 (m), 584 (w) cm^{-1}; MS (20eV, EI) *m/z* (%) 346 (M+2, 64), 344 (M^+, 100); HRMS (MALDI) for $(C_{16}H_9{}^{79}BrO_4 + H)^+$: 344.9762, found: 344.9765.

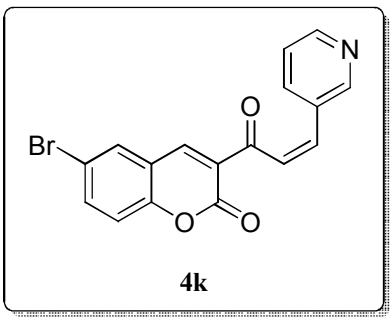
(*E*)-6-bromo-3-[3-(thien-2-yl)acryloyl]-2*H*-chromen-2-one (4j):



4j

reddish brown solid; mp: 211.6-212.2 °C; ^{1}H NMR (400 MHz, $CDCl_3$, 25 °C) δ 8.46 (s, 1H), 8.00 (d, 1H, J = 15.5 Hz), 7.80 (d, 1H, J = 1.8 Hz), 7.76-7.63 (m, 2H), 7.50-7.38 (m, 2H), 7.33-7.21 (m, 1H), 7.13-7.07 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$, 25 °C) δ 185.4, 158.5, 154.0, 146.3, 140.4, 137.8, 136.8, 132.6, 132.0, 130.0, 128.4, 126.2, 122.4, 120.0, 118.4, 117.5; IR (KBr) 3100 (w), 3041 (w), 1735 (s), 1720 (m), 1178 (m), 570 (m) cm^{-1}; MS (20eV, EI) *m/z* (%) 362 (M+2, 55), 361 (M+1, 100), 360 (M^+, 50), 334 (44), 253 (33), 137 (59); HRMS (MALDI) for $(C_{16}H_9{}^{79}BrO_3S + H)^+$: 360.9534, found: 360.9551.

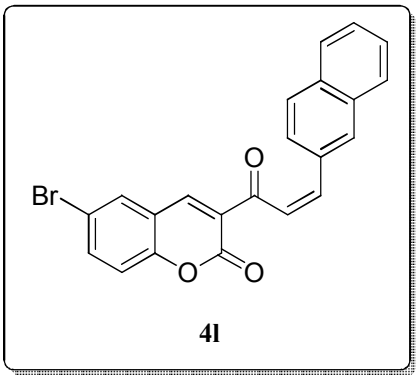
(*Z*)-6-bromo-3-[3-(pyridin-3-yl)acryloyl]-2*H*-chromen-2-one (4k):



4k

orange solid; mp: 227.6-228.2 °C; ^{1}H NMR (400 MHz, $CDCl_3$, 25 °C) δ 8.85 (s, 1H), 8.64 (d, 1H, J = 3.8 Hz), 8.52 (s, 1H), 8.07-7.94 (m, 2H), 7.91-7.79 (m, 2H), 7.76 (d, 1H, J = 8.9 Hz), 7.42-7.34 (m, 1H), 7.31 (d, 1H, J = 8.9 Hz); ^{13}C NMR (100 MHz, $CDCl_3$, 25 °C) δ 185.6, 158.7, 154.1, 151.4, 150.7, 147.1, 141.4, 137.1, 134.7, 132.1, 130.5, 125.7, 125.5, 123.8, 120.0, 118.5, 117.7; IR (KBr) 3091 (w), 3041 (w), 1720 (s), 1667 (s), 1181 (s), 578 (m) cm^{-1}; MS (20eV, EI) *m/z* (%) 357 (M+2, 71), 355 (M^+, 100), 328 (47); HRMS (MALDI) for $(C_{17}H_{10}{}^{79}BrNO_3 + Na)^+$: 377.9742, found: 377.9753.

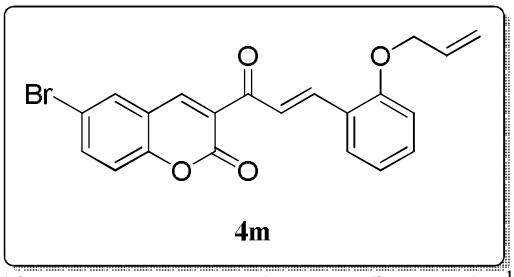
(*Z*)-6-bromo-3-[3-(naphthalene-2-yl)acryloyl]-2*H*-chromen-2-one (4l):



4l

yellow solid; mp: 227.2-228.0 °C; ^{1}H NMR (400 MHz, $CDCl_3$, 25 °C) δ 8.51 (s, 1H), 8.13-7.97 (m, 3H), 7.94-7.78 (m, 5H), 7.74 (d, 1H, J = 8.9 Hz), 7.59-7.48 (m, 2H), 7.30 (d, 1H, J = 8.9 Hz); ^{13}C NMR (100 MHz, $CDCl_3$, 25 °C) δ 185.9, 158.7, 154.0, 146.5, 145.7, 136.8, 134.7, 133.3, 132.3, 132.0, 131.3, 128.8, 127.8, 127.6, 126.8, 126.3, 124.1, 123.8, 120.1, 118.4, 117.5; IR (KBr) 3055 (w), 1735 (s), 1657 (s), 1189 (s), 577 (m) cm^{-1}; MS (20eV, EI) *m/z* (%) 406 (M+2, 13), 405 (M+1, 100), 404 (M^+, 46), 153 (29); HRMS (MALDI) for ($C_{22}H_{13}{}^{79}BrO_3$ + H)$^+$: 405.0126, found: 405.0139.

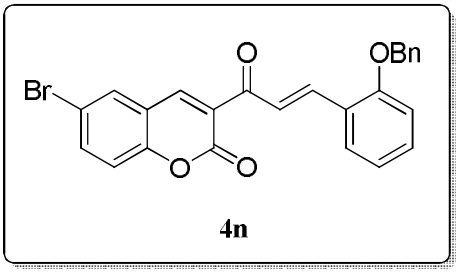
(*E*)-3-[3-(2-allyloxyphenyl)acryloyl]-6-bromo-2*H*-chromen-2-one (4m):



4m

goose yellow solid; mp: 165.0-165.9 °C; ^{1}H NMR (500 MHz, $CDCl_3$, 25 °C) δ 8.45 (s, 1H), 8.25 (d, 1H, J = 16.7 Hz), 7.95 (d, 1H, J = 16.4 Hz), 7.87-7.62 (m, 3H), 7.44-7.20 (m, 2H), 7.08-6.87 (m, 2H), 6.24-6.03 (m, 1H), 5.44 (d, 1H, J = 16.1 Hz), 5.32 (d, 1H, J = 10.9 Hz), 4.65 (brs, 2H); ^{13}C NMR (100 MHz, $CDCl_3$, 25 °C) δ 186.4, 158.5, 158.1, 154.0, 146.1, 141.1, 136.6, 132.9, 132.2, 131.9, 129.6, 126.7, 124.2, 124.0, 121.0, 120.1, 118.4, 117.9, 117.4, 112.6, 69.4; IR (KBr) 3097 (w), 2044 (w), 2908 (w), 2864 (w), 1726 (s), 1606 (s), 1174 (s), 583 (m) cm^{-1}; MS (20eV, EI) *m/z* (%) 412 (M+2, 22), 410 (M^+, 22), 353 (100), 253 (27), 251 (41), 159 (21), 144 (69); HRMS (MALDI) for ($C_{21}H_{21}{}^{79}BrO_4$ + H)$^+$: 411.0232, found: 411.0243.

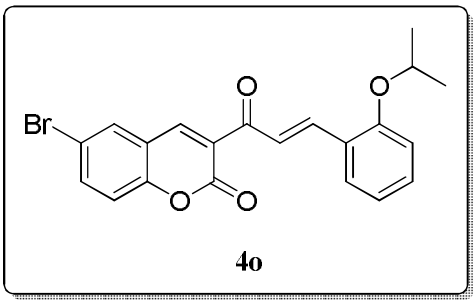
(*E*)-3-[3-(2-benzyloxyphenyl)acryloyl]-6-bromo-2*H*-chromen-2-one (4n):



4n

pale yellow solid; mp: 163.8-164.4 °C; ^{1}H NMR (400 MHz, $CDCl_3$, 25 °C) δ 8.37 (s, 1H), 8.28 (d, 1H, J = 15.9 Hz), 7.88 (d, 1H, J = 15.9 Hz), 7.79-7.68 (m, 3H), 7.45 (d, 2H, J = 7.3 Hz), 7.42-7.28 (m, 5H), 7.04-6.94 (m, 2H), 5.19 (s, 2H); ^{13}C NMR (100 MHz, $CDCl_3$, 25 °C) δ 186.6, 158.4, 158.1, 153.9, 145.7, 141.0, 136.6, 136.5, 132.3, 131.9, 129.5, 128.7, 128.0, 127.3, 126.9, 124.3, 124.1, 121.1, 120.1, 118.4, 117.4, 112.8, 70.5; IR (KBr) 3092 (w), 2915 (w), 2863 (w), 1735 (s), 1728 (s), 1183 (m), 574 (m) cm^{-1}; MS (20eV, EI) *m/z* (%) 369 (44), 355 (23), 208 (23), 91 (M-369, 100); HRMS (MALDI) for ($C_{25}H_{17}{}^{79}BrO_4$ + Na)$^+$: 483.0208, found: 483.0216.

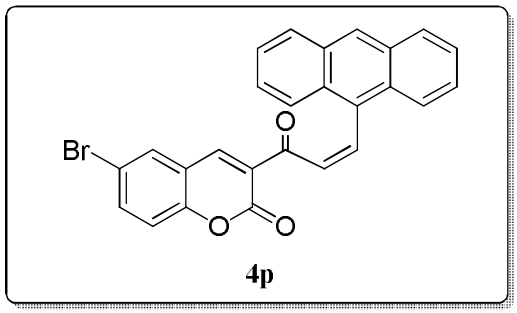
(*E*)-6-bromo-3-[3-(2-isopropoxyphenyl)acryloyl]-2*H*-chromen-2-one (4o):



4o

light yellow solid; mp: 164.0-164.8 °C; ^{1}H NMR (400 MHz, $CDCl_3$, 25 °C) δ 8.46 (s, 1H), 8.19 (d, 1H, J = 15.8 Hz), 8.02 (d, 1H, J = 15.8 Hz), 7.80 (d, 1H, J = 1.9 Hz), 7.75-7.69 (m, 1H), 7.66 (d, 1H, J = 7.8 Hz), 7.40-7.31 (m, 1H), 7.28 (d, 1H, J = 9.3 Hz), 7.00-6.90 (m, 2H), 4.74-4.61 (m, 1H), 1.43 (d, 6H, J = 6.1 Hz); ^{13}C NMR (100 MHz, $CDCl_3$, 25 °C) δ 186.4, 158.5, 157.8, 153.9, 146.1, 141.7, 136.6, 132.1, 131.9, 130.4, 126.7, 124.6, 124.0, 120.5, 120.1, 118.3, 117.4, 113.6, 70.9, 22.1; IR (KBr) 3139 (w), 3045 (m), 2978 (w), 2931 (w), 1738 (s), 1654 (s), 1170 (s), 581 (m) cm^{-1}; MS (20eV, EI) *m/z* (%) 414 (M+2, 8), 412 (M^+, 11), 369 (33), 252 (16), 224 (34), 119 (100); HRMS (MALDI) for $(C_{21}H_{17}{}^{79}BrO_4 + H)^+$: 413.0388, found: 413.0397.

(*Z*)-3-[3-(anthracen-9-yl)acryloyl]-6-bromo-2*H*-chromen-2-one (4p):

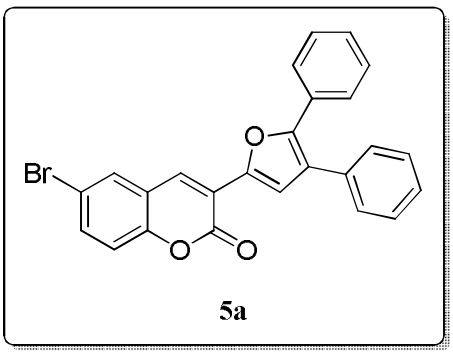


4p

red solid; mp: 218.9-219.5 °C; ^{1}H NMR (400 MHz, $CDCl_3$, 25 °C) δ 8.88 (d, 1H, J = 15.9 Hz), 8.55 (s, 1H), 8.49 (s, 1H), 8.40 (d, 2H, J = 8.7 Hz), 8.03 (d, 2H, J = 8.3 Hz), 7.85-7.79 (m, 2H), 7.74 (dd, 1H, J = 8.9, 2.2 Hz), 7.58-7.49 (m, 4H), 7.29 (d, 1H, J = 8.8 Hz); ^{13}C NMR (100 MHz, $CDCl_3$, 25 °C) δ 186.1, 158.5, 154.0, 146.5, 142.1, 136.9, 132.4, 132.0, 131.3, 129.9, 129.4, 129.1, 128.9, 126.7, 126.5, 125.5, 125.3, 120.0, 118.4, 117.5; IR (KBr) 3045 (w), 1748 (s), 1554 (s), 1355 (m), 1175 (s), 543 (m); MS (EI) m/z (relative intensity) 456 (M+2, 22), 455 (M+1, 29), 203 (100); HRMS (EI) for $(C_{26}H_{15}{}^{79}BrO_3)^+$: 454.0205, found: 454.0203.

[5] Spectra data of the products 5 and 6 in Table 4 and Scheme 1.

6-bromo-3-(4,5-diphenylfuran-2-yl)-2*H*-chromen-2-one (5a):

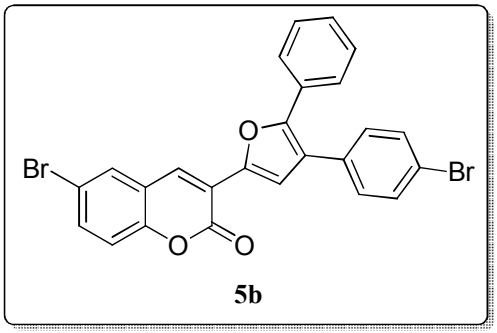


5a

orange solid; mp: 210.0-211.7 °C; ^{1}H NMR (400 MHz, $CDCl_3$, 25 °C) δ 8.11 (s, 1H), 7.76 (d, 1H, J = 2.0 Hz), 7.67-7.55 (m, 4H), 7.47 (d, 2H, J = 7.0 Hz), 7.42-7.30 (m, 6H), 7.28-7.23 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$, 25 °C) δ 157.5, 151.4, 149.7, 145.9, 133.6, 133.5, 131.7, 130.4, 130.0, 128.7, 128.6, 128.5, 128.3, 127.6, 126.5, 125.3, 121.1, 118.7, 118.2, 118.0, 117.3; IR (KBr) 2930 (w), 1729 (s), 1241 (m), 1115 (m), 691 (w) cm^{-1}; MS (20eV, EI) *m/z* (%) 444 (M+2, 100),

442 (M^+, 81), 105 (10); HRMS (MALDI) for ($C_{25}H_{15}{}^{79}BrO_3$ + H)$^+$: 443.0283, found: 443.0299.

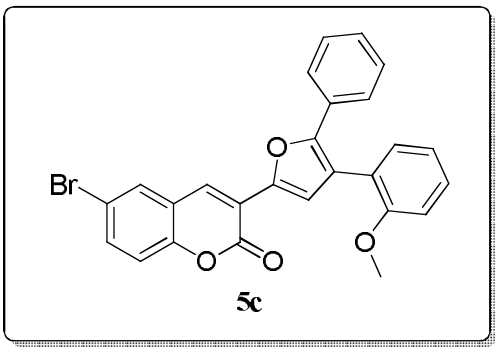
6-bromo-3-[4-(4-bromophenyl)-5-phenylfuran-2-yl]-2*H*-chromen-2-one (5b):



5b

yellow solid; mp: 259.5-260.0 ^oC; ^1H NMR (400 MHz, $CDCl_3$, 25 ^oC) δ 8.10 (s, 1H), 7.75 (d, 1H, J = 1.4 Hz), 7.60-7.50 (m, 6H), 7.37-7.32 (m, 5H), 7.25 (d, 1H, J = 8.6 Hz); ^{13}C NMR (100 MHz, $CDCl_3$, 25 ^oC) δ 157.5, 151.4. 149.9, 146.1, 133.8, 132.4, 131.9, 131.9, 130.2, 130.1, 130.1, 128.7, 128.6, 126.6, 124.1, 121.6, 121.0, 118.5, 118.2, 117.5, 117.4; IR (KBr) 3086 (w), 1733 (s), 1474 (m), 1243 (m), 1114 (m), 610 (m); MS (20eV, EI) m/z (%) (relative intensity) 522, (M+2, 55), 521 (M+1, 100), 520 (M^+, 85), 519 (M-1,41), (M+3, 38); HRMS (MALDI) for ($C_{25}H_{14}{}^{79}Br_2O_3$ + H)$^+$: 520.9388, found: 520.9396.

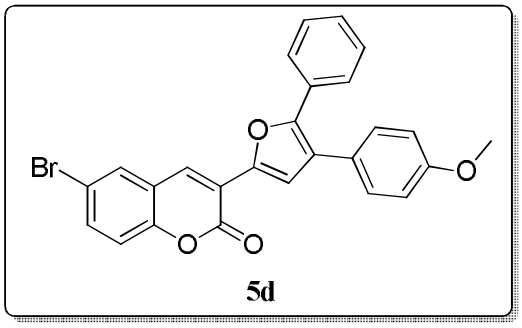
6-bromo-3-[4-(2-methoxyphenyl)-5-phenylfuran-2-yl]-2*H*-chromen-2-one (5c):



5c

yellow solid; mp: 206.3-207.0 ^oC; ^1H NMR (400 MHz, $CDCl_3$, 25 ^oC) δ 8.35 (s, 1H), 8.01 (s, 1H), 7.91-7.82 (m, 4H), 7.63-7.49 (m, 6H), 7.31 (d, 1H, J = 7.4 Hz), 7.15 (d, 1H, J =8.0 Hz), 4.04 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$, 25 ^oC) δ 159.8, 157.5, 151.4, 149.8, 145.8, 134.8, 133.6, 131.7, 130.4, 130.0, 129.7, 128.5, 128.4, 126.6, 125.2, 121.1, 121.0, 118.6, 118.2, 117.9, 117.3, 113.9, 113.5, 55.3; IR (KBr) 3076 (m), 1731 (s), 1601 (m), 1476 (m), 1238 (m), 1114 (m), 612 (w); MS (20eV, EI) m/z (%) (relative intensity) 474 (M+2, 92), 472 (M^+, 79), 471 (M-1, 100); HRMS (MALDI) for ($C_{26}H_{17}{}^{79}BrO_4$+ H)$^+$: 473.0388, found: 473.0399.

6-bromo-3-[4-(4-methoxyphenyl)-5-phenylfuran-2-yl]-2*H*-chromen-2-one (5d):

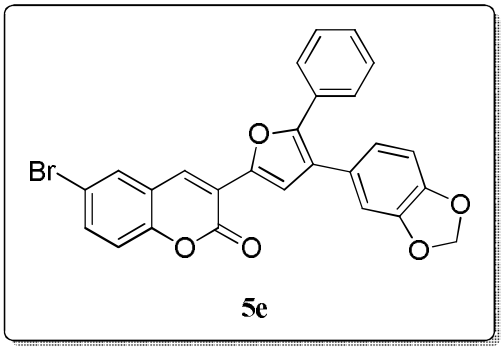


5d

yellow solid; mp: 207.8-208.2 ^oC; ^1H NMR (400 MHz, $CDCl_3$, 25 ^oC) δ 8.09 (s, 1H), 7.75 (d, 1H, J = 2.0 Hz), 7.63 (d, 2H, J = 7.0 Hz), 7.58 (dd, 1H, J = 8.8, 2.1 Hz), 7.53 (s, 1H), 7.39-7.28 (m, 5H), 7.24(d, 1H, J = 8.8 Hz), 6.92 (d, 2H, J = 8.6 Hz), 3.85 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$, 25 ^oC) δ 159.1, 157.6, 151.4, 149.4, 145.8, 133.6, 131.6, 130.6, 130.0, 129.8, 128.5, 128.2, 126.4, 125.7, 125.0, 121.1, 118.7, 118.2, 118.1, 117.3, 114.2, 55.3; IR (KBr) 2952 (w), 1727 (s), 1509 (m),

1241 (s), 1174 (m), 624 (m); MS (20eV, EI) m/z (%) (relative intensity) 473 (M+1, 26), 472 (M^+, 22), 105 (100); HRMS (MALDI) for $(C_{26}H_{17}{}^{79}BrO_4 + H)^+$: 473.0388, found: 473.0395.

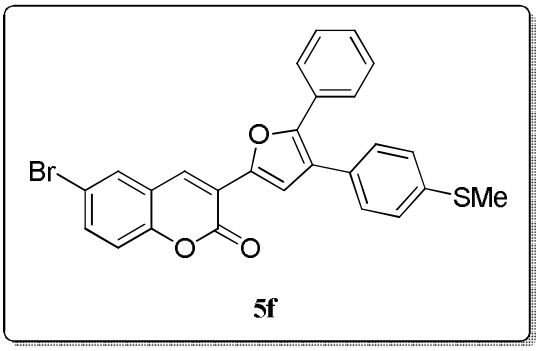
6-bromo-3-[4-(3,4-methylenedioxyphenyl)-5-phenylfuran-2-yl]-2*H*-chromen-2-one (5e):



5e

orange solid; mp: 200.0-200.9 °C; ^{1}H NMR (500 MHz, $CDCl_3$, 25 °C) δ 8.09 (s, 1H), 7.76 (d, 1H, J = 2.2 Hz), 7.66-7.61 (m, 2H), 7.59 (dd, 1H, J = 7.8, 1.9 Hz), 7.51 (s, 1H), 7.39-7.30 (m, 3H), 7.27-7.23 (m, 1H), 6.94 (dd, 1H, J = 7.8, 1.9 Hz), 6.91 (d, 1H, J = 1.4 Hz), 6.84 (d, 1H, J = 7.8 Hz), 6.00 (s, 2H); ^{13}C NMR (125 MHz, $CDCl_3$, 25 °C) δ 157.6, 151.4, 149.6, 147.9, 147.2, 145.8, 133.6, 131.7, 130.4, 130.0, 128.6, 128.5, 128.3, 127.2, 126.5, 125.1, 122.3, 121.1, 118.2, 118.1, 117.3, 109.2, 108.7, 101.2; IR (KBr) 3063 (w), 2924 (w), 1728 (s), 1237 (s), 1108 (m), 695 (w) cm^{-1}; MS (20eV, EI) *m/z* (%) 488 (M+2, 100), 486 (M^+, 79), 105 (27); HRMS (FAB) for $(C_{26}H_{15}{}^{79}BrO_5)^+$: 486.0103, found: 486.0107.

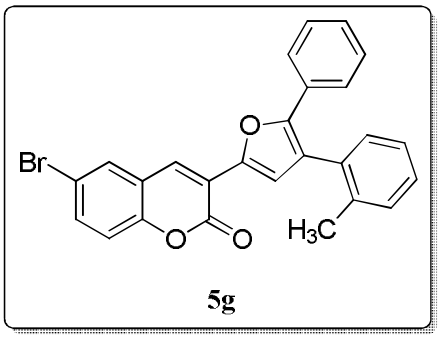
6-bromo-3-[4-(4-methylthiophenyl)-5-phenylfuran-2-yl]-2*H*-chromen-2-one (5f):



5f

orange solid; mp: 199.6-200.0 °C; ^{1}H NMR (400 MHz, $CDCl_3$, 25 °C) δ 8.10 (s, 1H), 7.76 (d, 1H, J = 2.0 Hz), 7.67-7.52 (m, 5H), 7.42-7.30 (m, 5H), 7.29-7.22 (m, 2H), 2.53 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$, 25 °C) δ 157.5, 151.4, 149.7, 146.0, 137.9, 133.6, 131.7, 130.4, 130.0, 129.0, 128.6, 128.4, 126.6, 126.5, 124.7, 121.0, 118.6, 118.2, 117.8, 117.3, 15.7; IR (KBr) 2959 (w), 2925 (w), 2854 (w), 1731 (s), 1241 (m), 1182 (w), 555 (w) cm^{-1}; MS (20eV, EI) *m/z* (%) 490 (M+2, 70), 489 (M+1, 85), 488 (M^+, 77), 487 (M-1, 100), 105 (12); HRMS (MALDI) for $(C_{26}H_{17}{}^{79}BrO_3S + H)^+$: 489.0160, found: 489.0172.

6-bromo-3-[4-(2-methylphenyl)-5-phenylfuran-2-yl]-2*H*-chromen-2-one (5g):

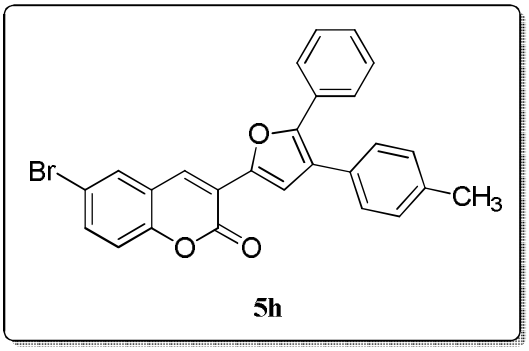


5g

orange solid; mp: 199.2-199.9 °C; ^{1}H NMR (400 MHz, $CDCl_3$, 25 °C) δ 7.99 (d, 1H), 7.86-7.73 (m, 4H), 7.65-7.53 (m, 4H), 7.43 (dd, 1H, J = 8.1, 2.4 Hz), 7.28-7.14 (m, 4H), 2.48 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$, 25 °C) δ 162.3, 157.4, 157.1, 150.6, 147.5, 137.0, 134.5, 132.2, 130.7, 130.6, 130.1, 129.2, 129.1, 128.9, 128.5, 126.4, 125.9, 125.8, 119.5, 116.9, 114.8, 108.0, 20.0; IR (KBr) 3067 (w), 2953 (w), 2922 (w), 2851 (w), 1735 (s), 1213 (m), 1180 (m), 557 (w) cm^{-1}; MS

(20eV, EI) *m/z* (%) 458 (M+2, 100), 456 (M^+, 64), 455 (M-1, 92); HRMS (FAB) for $(C_{26}H_{17}{}^{79}BrO_3)^+$: 456.0361, found: 456.0364.

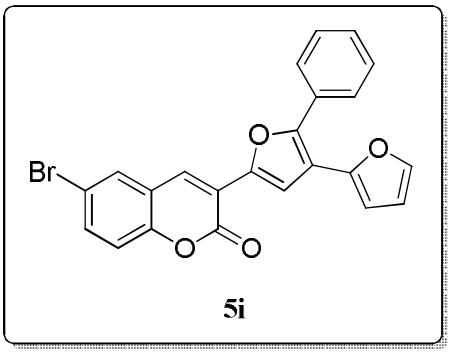
6-bromo-3-[4-(4-methylphenyl)-5-phenylfuran-2-yl]-2*H*-chromen-2-one (5h):



5h

light yellow solid; mp: 242.1-242.8 °C; ^{1}H NMR (500 MHz, $CDCl_3$, 25 °C) δ 8.08 (s, 1H), 7.74 (s, 1H), 7.63 (d, 2H, J = 7.4 Hz), 7.60-7.55 (m, 1H), 7.54 (s, 1H), 7.39-7.28 (m, 5H), 7.27-7.15 (m, 3H), 2.40 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$, 25 °C) δ 157.5, 151.4, 149.5, 145.8, 137.3, 133.6, 131.6, 130.6, 130.4, 130.0, 129.4, 128.5, 128.4, 128.2, 126.5, 125.3, 121.1, 118.7, 118.2, 118.1, 117.3, 21.3; IR (KBr) 2924 (w), 2855 (w), 1727 (s), 1180 (m), 555 (w) cm^{-1}; MS (20eV, EI) *m/z* (%) 458 (M+2, 100), 456 (M^+, 95), 105 (9); HRMS (MALDI) for $(C_{26}H_{17}{}^{79}BrO_3 + H)^+$: 457.0439, found: 457.0449.

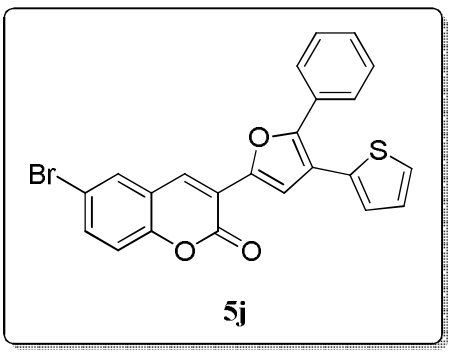
6-bromo-3-[4-(furan-2-yl)-5-phenylfuran-2-yl]-2*H*-chromen-2-one (5i):



5i

orange solid; mp: 188.7-189.5 °C; ^{1}H NMR (400 MHz, $CDCl_3$, 25 °C) δ 8.03 (s, 1H), 7.79 (d, 2H, J = 7.5 Hz), 7.70 (d, 1H, J = 2.0 Hz), 7.60 (s, 1H), 7.55 (dd, 1H, J = 8.0, 2.2 Hz), 7.49-7.34 (m, 4H), 7.21 (d, 1H, J = 7.4 Hz), 6.57-6.51 (m, 1H), 6.49-6.42 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$, 25 °C) δ 157.4, 151.4, 149.8, 147.1, 146.0, 141.8, 133.7, 132.1, 130.3, 130.1, 128.7, 128.5, 127.0, 120.9, 118.3, 118.1, 117.3, 115.6, 111.3, 107.8; IR (KBr) 3143 (w), 2960 (w), 2925 (w), 2851 (w), 1727 (s), 1243 (m), 1117 (m), 564 (w) cm^{-1}; MS (20eV, EI) *m/z* (%) 434 (M+2, 94), 432 (M^+, 100), 105 (20); HRMS (MALDI) for $(C_{23}H_{13}{}^{79}BrO_4 + H)^+$: 433.0075, found 433.0086.

6-bromo-3-[4-(thien-2-yl)-5-phenylfuran-2-yl]-2*H*-chromen-2-one (5j):

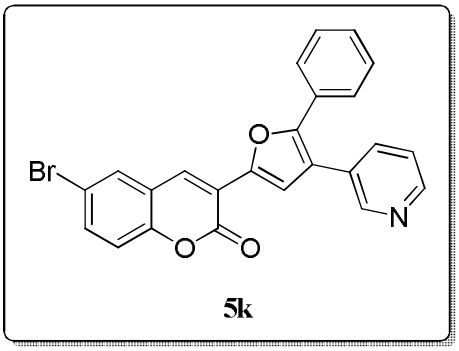


5j

orange solid; mp: 196.2-196.8 °C; ^{1}H NMR (500 MHz, $CDCl_3$, 25 °C) δ 8.08 (s, 1H), 7.77-7.68 (m, 3H), 7.62-7.54 (m, 2H), 7.43-7.33 (m, 3H), 7.31 (d, 1H, J = 5.1 Hz), 7.28-7.22 (m, 1H), 7.15 (d, 1H, J = 3.1 Hz), 7.07-7.04 (m, 1H); ^{13}C NMR (125 MHz, $CDCl_3$, 25 °C) δ 157.4, 151.4, 150.2, 145.9, 134.5, 133.8, 132.0, 130.1, 130.0, 128.7, 128.6, 127.4, 126.9, 126.3, 125.5, 121.0, 118.5, 118.4, 118.2, 117.9, 117.3; IR (KBr) 2962 (w), 2926 (w), 2867 (w), 1726 (s), 1113 (m), 564 (w) cm^{-1}; MS (20eV, EI) *m/z* (%) 450 (M+2, 63), 449 (M+1, 88), 448 (M^+, 78), 447 (M-1,

100), 105 (16); HRMS (MALDI) for $(C_{23}H_{13}{}^{79}BrO_3S + H)^+$: 448.9847, found: 448.9860.

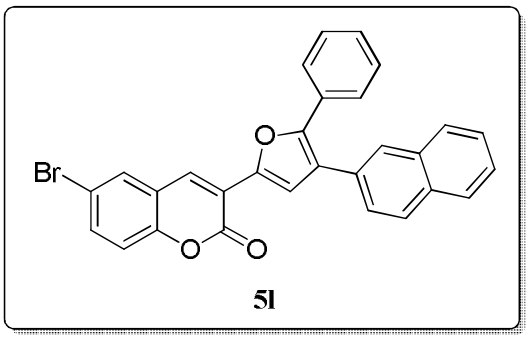
6-bromo-3-[4-(pyridin-3-yl)-5-phenylfuran-2-yl]-2*H*-chromen-2-one (5k):



5k

light yellow solid; mp: 216.6-217.2 °C; ^{1}H NMR (500 MHz, $CDCl_3$, 25 °C) δ 8.73 (brs, 1H), 8.61 (brs, 1H), 8.13 (s, 1H), 7.81-7.75 (m, 2H), 7.63-7.55 (m, 4H), 7.41-7.31 (m, 4H), 7.29-7.24 (m, 2H); ^{13}C NMR (125 MHz, $CDCl_3$, 25 °C) δ 157.5, 151.5, 150.6, 149.4, 148.6, 146.5, 136.0, 133.9, 132.2, 130.2, 130.0, 129.9, 128.8, 128.4, 126.6, 121.6, 120.9, 118.4, 118.3, 117.4, 117.3; IR (KBr) 3078 (w), 3033 (w), 2923 (w), 2856 (w), 1727 (s), 1206 (w), 1178 (m), 559 (w) cm^{-1}; MS (20eV, EI) *m/z* (%) 445 (M+2, 100), 443 (M^+, 86), 105 (14); HRMS (MALDI) for $(C_{24}H_{14}{}^{79}BrNO_3 + H)^+$: 444.0235, found: 444.0241.

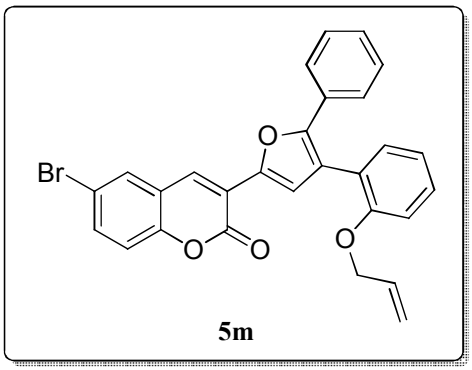
6-bromo-3-[4-(naphthalene-2-yl)-5-phenylfuran-2-yl]-2*H*-chromen-2-one (5l):



5l

yellow solid; mp: 168.6-169.4 °C; ^{1}H NMR δ 8.13 (s, 1H), 7.98 (s, 1H), 7.89-7.80 (m, 3H), 7.77 (d, 1H, J = 2.1 Hz), 7.70-7.62 (m, 3H), 7.59 (dd, 1H, J = 8.0, 2.1 Hz), 7.56-7.47 (m, 3H), 7.37-7.30 (m, 3H), 7.28-7.23 (m, 1H); ^{13}C NMR δ 157.5, 151.4, 150.0, 146.0, 134.9, 133.6, 132.7, 131.7, 130.9, 130.4, 130.0, 129.1, 128.3, 128.0, 127.7, 127.4, 126.8, 126.3, 126.1, 125.3, 123.6, 121.0, 119.5, 118.6, 118.2, 118.1, 117.3; IR (KBr) 3055 (w), 2959 (m), 2923 (m), 2856 (w), 1738 (s), 1240 (m), 1112 (m), 698 (w) cm^{-1}; MS (20eV, EI) *m/z* (%) 494 (M+2, 30), 493 (M+1, 100), 492 (M^+, 58), 491 (M-1, 76), 105 (34); HRMS (MALDI) for $(C_{29}H_{17}{}^{79}BrO_3 + H)^+$: 493.0439, found: 493.0450.

3-[4-(2-allyloxyphenyl)-5-phenylfuran-2-yl]-6-bromo-2*H*-chromen-2-one (5m):

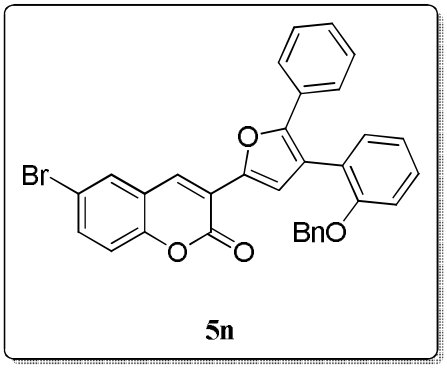


5m

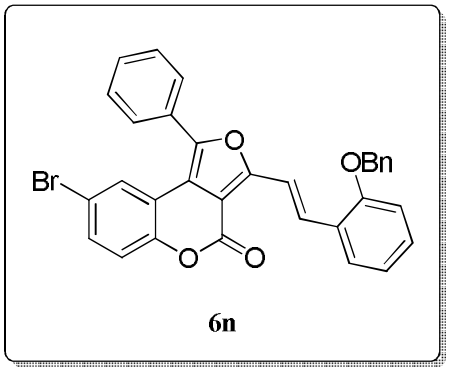
orange solid; mp: 181.7-182.6 °C; ^{1}H NMR (400 MHz, $CDCl_3$, 25 °C) δ 8.10 (s, 1H), 7.76 (d, 1H, J = 2.3 Hz), 7.60-7.54 (m, 4H), 7.39-7.27 (m, 5H), 7.26-7.23 (m, 1H), 7.03-6.94 (m, 2H), 5.74-5.62 (m, 1H), 5.22-5.14 (m, 1H), 5.11-5.05 (m,1H), 4.45-4.39 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$, 25 °C) δ 157.5, 155.9, 151.3, 150.5, 145.4, 133.4, 133.0, 131.3, 131.2, 131.1, 130.0, 129.2, 128.3, 127.9, 125.8, 122.9, 121.4, 121.2, 121.0, 119.4, 118.9, 118.2, 117.3, 117.2, 112.6, 69.1; IR (KBr) 3063 (w), 2923 (w), 2856 (w), 1737 (s), 1243 (m), 1112 (m), 695 (w) cm^{-1};

MS (20eV, EI) *m/z* (%) 500 (M+2, 100), 498 (M^+, 52), 497 (M-1, 63), 105 (22); HRMS (MALDI) for $(C_{28}H_{19}{}^{79}BrO_4 + H)^+$: 499.0545, found: 499.0553.

Mixture of **5n** & **6n** (the ratio between them is 1:0.06)



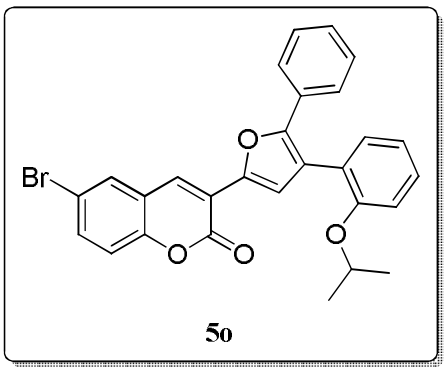
5n



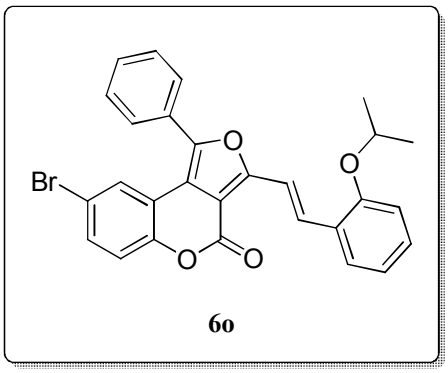
6n

3-[4-(2-benzyloxyphenyl)-5-phenylfuran-2-yl]-6-bromo-2*H*-chromen-2-one (5n): ^{1}H NMR (400 MHz, $CDCl_3$, 25 °C) δ 8.20-8.14 (m, 1H), 8.09 (s, 1H), 7.76 (d, 1H, J = 2.2 Hz), 7.72-7.62 (m, 1H), 7.61-7.50 (m, 5H), 7.41-7.18 (m, 10H), 7.11-7.06 (m, 2H), 7.05-6.98 (m, 2H), 4.97 (s, 2H); IR (KBr) 3063 (w), 3034 (w), 2926 (w), 2868 (w), 1733 (s), 1238 (m), 1179 (w), 554 (w) cm^{-1}; HRMS (MALDI) for $(C_{32}H_{21}{}^{79}BrO_4 + Na)^+$: 571.0521, found: 571.0534.

Mixture of **5o** & **6o** (the ratio between them is 1:1.46)



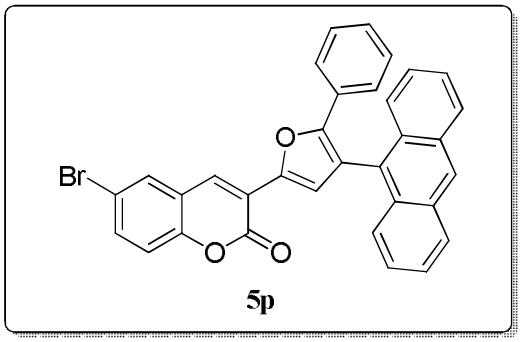
5o



6o

5n & 6o: ^{1}H NMR (400 MHz, $CDCl_3$, 25 °C) δ 8.10 (s, 1H), 8.01 (d, 1H', J = 2.2 Hz), 7.90 (d, 1H', J = 16.4 Hz), 7.85-7.75 (m, 3H+2H'), 7.62-7.52 (m, 4H+4H'), 7.43 (dd, 2H, J = 8.9, 2.2 Hz), 7.37-7.28 (m, 2H+3H'), 7.17 (d, 1H', J = 8.6 Hz), 7.01-6.91 (m, 2H+2H'), 4.72-4.60 (m, 1H'), 4.48-4.38 (m, 1H), 1.45 (d, 6H', J = 6.3 Hz), 1.08 (d, 6H, J = 6.1 Hz); HRMS (FAB) for $(C_{28}H_{20}{}^{79}BrO_4 + H)^+$: 500.0623, found: 500.0620

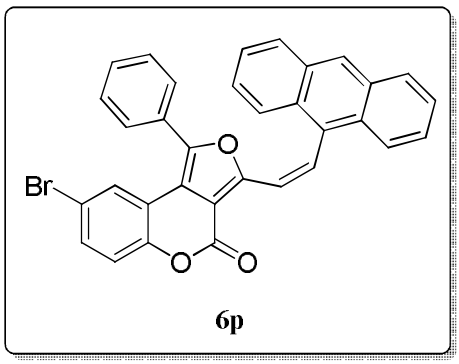
6-bromo-3-[4-(anthracen-9-yl)-5-phenylfuran-2-yl]-2*H*-chromen-2-one (5p)



5p

orange solid; mp: 261.5-262.0 °C; ^{1}H NMR (400 MHz, $CDCl_3$, 25 °C) δ 8.53 (d, 1H, J =16.0 Hz), 8.45 (s, 1H), 8.39 (d, 2H, J = 9.3 Hz), 8.06-8.02 (m, 3H), 7.90-7.86 (m, 2H), 7.67-7.62 (m, 3H), 7.60-7.58 (m, 1H), 7.54-7.49 (m, 4H), 7.46 (dd, 1H, J = 8.8, 2.3 Hz), 7.19 (d, 1H, J =8.8 Hz); ^{13}C NMR (100 MHz, $CDCl_3$, 25 °C) δ 157.3, 156.3, 150.6, 148.0, 132.3, 131.9, 131.4, 130.6, 130.2, 129.8, 129.7, 129.2, 128.9, 128.5, 127.9, 126.2, 125.9, 125.4, 125.3, 122.5, 119.6, 117.0, 116.9, 115.6, 108.5; IR (KBr) 3051 (w), 1743 (s), 1467 (m), 1371 (m), 1174 (s), 1008 (s), 600 (w); MS (20eV, EI) m/z (%) (relative intensity) 544 (M+2, 100), 542 (M^+, 85), 436 (29); HRMS (MALDI) for ($C_{33}H_{19}{}^{79}BrO_3$+ H)$^+$: 543.0596, found: 543.0607.

(*Z*)-3-[2-(anthracen-9-yl)vinyl]-8-bromo-1-phenyl-4*H*-furo[3,4-*c*]chromen-4-one (6p):

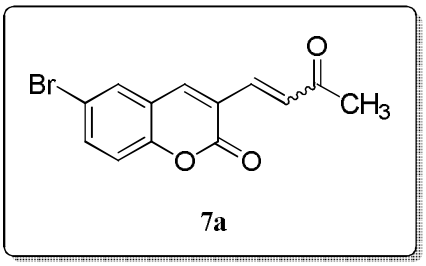


6p

orange solid; mp: 241.0-241.6 °C; ^{1}H NMR (400 MHz, $CDCl_3$, 25 °C) δ 8.45 (s, 1H), 8.17 (d, 2H, J = 6.9 Hz), 8.05 (d, 2H, J = 6.9 Hz), 7.92-7.89 (m, 2H), 7.67 (d, 1H, J = 9.8 Hz), 7.49-7.38 (m, 5H), 7.21-7.14 (m, 2H), 7.10-7.07 (m, 2H), 6.34 (d, 2H, J = 6.0 Hz); ^{13}C NMR (100 MHz, $CDCl_3$, 25 °C) δ 157.5, 155.0, 150.4, 148.4, 132.1, 131.9, 131.7, 131.4, 129.3, 129.3, 128.9, 128.7, 128.3, 127.4, 127.0, 125.9, 125.8, 125.7, 125.2, 119.9, 119.5, 116.9, 116.9, 114.3, 109.8; IR (KBr) 3051 (w), 1737 (s), 1625 (w), 1443 (m), 1264 (m), 1183 (s), 1014 (s), 694 (m); MS (20eV, EI) m/z (%) (relative intensity) 544 (M+2, 88), 542 (M^+, 100), 439 (31); HRMS (MALDI) for ($C_{33}H_{19}{}^{79}BrO_3$ + H)$^+$: 543.0596, found: 543.0608.

[6] Spectra data of the compounds 7 and 8 in Scheme 2.

6-bromo-3-(3-oxobut-1-enyl)-2*H*-chromen-2-one (7a):

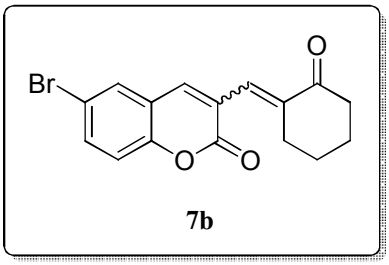


7a

orange solid; mp: 185.7-186.5 °C; ^{1}H NMR (400 MHz, $CDCl_3$, 25 °C) δ 8.55 (s, 1H'), 7.84 (s, 1H), 7.74-7.65 (m, 2H), 7.63 (d, 1H', J = 8.8 Hz), 7.44 (d, 1H, J = 16.1), 7.35-7.23 (m, 2H+1H'), 7.21 (d, 1H', J = 8.8 Hz), 6.85 (d, 1H', J = 12.8 Hz), 6.52 (d, 1H', J = 12.7 Hz), 2.40 (s, 3H), 2.33 (s, 3H'); ^{13}C NMR (100 MHz, $CDCl_3$, 25 °C) δ 198.7, 198.2, 158.6, 152.3, 141.8, 135.6,

135.3, 134.9, 132.5, 131.4, 131.0, 130.6, 123.5, 123.1, 120.4, 118.3, 118.2, 117.4, 117.2, 31.3, 28.6; IR (KBr) 3097 (w), 3050 (w), 2922 (w), 1734 (s), 1718 (s), 1177 (m), 564 (m) cm^{-1}; MS (20eV, EI) *m/z* (%) 293 (M+2, 9), 292 (M^+, 11), 249 (100); HRMS (MALDI) for $(C_{13}H_9{}^{79}BrO_3 + H)^+$: 292.9813, found: 292.9825.

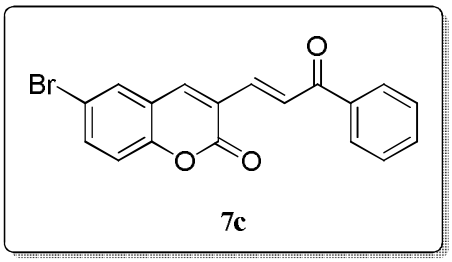
6-bromo-3-[(2-oxocyclohexylidene)methyl]-2*H*-chromen-2-one (7b):



7b

orange solid; mp: 190.2-191.2 °C; ^{1}H NMR (400 MHz, $CDCl_3$, 25 °C) δ 7.71-7.50 (m, 3H), 7.34 (brs, 1H), 7.23-7.16 (m, 1H), 2.84-2.71 (m, 2H), 2.54 (t, 2H, J = 6.6 Hz), 2.00-1.88 (m, 2H), 1.85-1.73 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$, 25 °C) δ 200.5, 159.6, 152.2, 141.4, 140.1, 134.7, 130.4, 127.0, 124.9, 120.3, 118.4, 117.2, 40.4, 29.8, 23.7, 23.5; IR (KBr) 3096 (w), 3069 (w), 3052 (w), 2924 (w), 2899 (w), 2866 (w), 1721 (s), 1670 (m), 1188 (m), 565 (m) cm^{-1}; MS (20eV, EI) *m/z* (%) 334 (M+2, 68), 332 (M^+, 39), 67 (100); HRMS (MALDI) for $(C_{16}H_{13}{}^{79}BrO_3 + H)^+$: 333.0126, found: 333.0134.

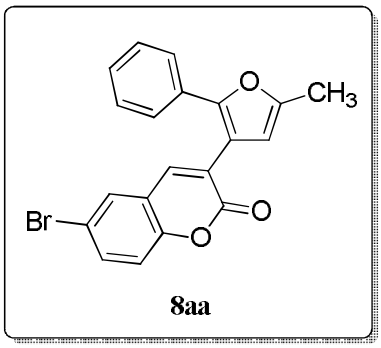
(*E*)-6-bromo-3-(3-oxo-3-phenylprop-1-enyl)-2*H*-chromen-2-one (7c):



7c

light yellow solid; mp: 209.3-209.9 °C; ^{1}H NMR (400 MHz, $CDCl_3$, 25 °C) δ 8.36 (d, 1H, J = 15.5 Hz), 8.08 (d, 2H, J = 7.4 Hz), 7.76-7.56 (m, 5H), 7.56-7.47 (m, 2H), 7.31-7.22 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$, 25 °C) δ 190.2, 158.5, 152.3, 143.4, 137.6, 137.2, 135.6, 133.3, 130.6, 128.8, 128.7, 127.8, 123.9, 120.6, 118.4, 117.4; IR (KBr) 3064 (w), 3050 (w), 1740 (s), 1736 (s), 1199 (m), 587 (m) cm^{-1}; MS (20eV, EI) *m/z* (%) 355 (M+1, 6), 249 (100); HRMS (EI) for $(C_{18}H_{11}{}^{79}BrO_3)^+$: 353.9892, found: 353.9886.

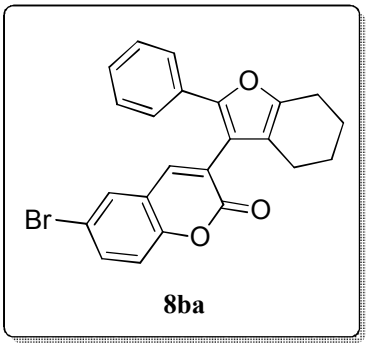
6-bromo-3-(5-methyl-2-phenylfuran-3-yl)-2*H*-chromen-2-one (8aa):



8aa

pale yellow solid; mp: 145.8-146.4 °C; ^{1}H NMR (400 MHz, $CDCl_3$, 25 °C) δ 7.62-7.51 (m, 4H), 7.47 (d, 1H, J = 2.2 Hz), 7.37-7.31 (m, 2H), 7.30-7.23 (m, 5H), 6.38 (s, 1H), 2.39 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$, 25 °C) δ 159.7, 152.3, 151.8, 149.6, 139.2, 133.9, 130.6, 129.8, 128.7, 127.9, 126.3, 123.6, 120.9, 118.2, 117.0, 115.8, 109.8, 13.5; IR (KBr) 2918 (w), 2850 (w), 1733 (s), 1185 (w) cm^{-1}; MS (20eV, EI) *m/z* (%) 382 (M+2, 45), 380 (M^+, 48), 379 (M-1, 100), 105 (10); HRMS (MALDI) for $(C_{20}H_{13}{}^{79}BrO_3 + H)^+$: 381.0126, 381.0144.

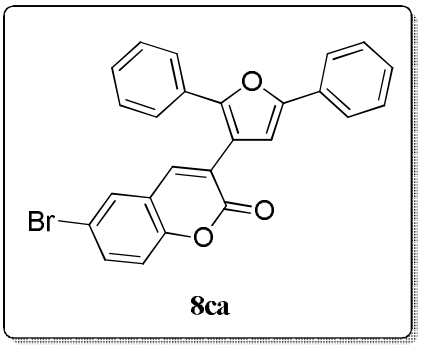
6-bromo-3-(2-phenyl-4,5,6,7-tetrahydrobenzofuran-3-yl)-2*H*-chromen-2-one (8ba):



8ba

pale yellow solid; mp: 178.7-179.5 °C; ^{1}H NMR (400 MHz, $CDCl_3$, 25 °C) δ 7.61 (dd, 1H, J = 8.0, 2.2 Hz), 7.58-7.46 (m, 4H), 7.34-7.27 (m, 3H), 7.25-7.18 (m, 1H), 2.70 (t, 2H, J = 6.0 Hz), 2.39 (t, 2H, J = 6.0 Hz), 1.99-1.85 (m, 2H), 1.83-1.71 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$, 25 °C) δ 159.5, 152.5, 150.9, 149.1, 140.9, 134.1, 130.8, 129.9, 128.6, 127.4, 125.8, 123.9, 120.9, 119.9, 118.4, 117.0, 115.3, 23.2, 22.8, 22.7, 21.3; IR (KBr) 2937 (w), 2919 (w), 2851 (w), 1723 (s), 1182 (m), 559 (w) cm^{-1}; MS (20eV, EI) *m/z* (%) 422 (M+2, 86), 420 (M^+, 87), 419 (M-1, 100), 105 (17); HRMS (MALDI) for ($C_{25}H_{17}{}^{79}BrO_3$ + H)$^+$: 421.0439, found: 421.0458.

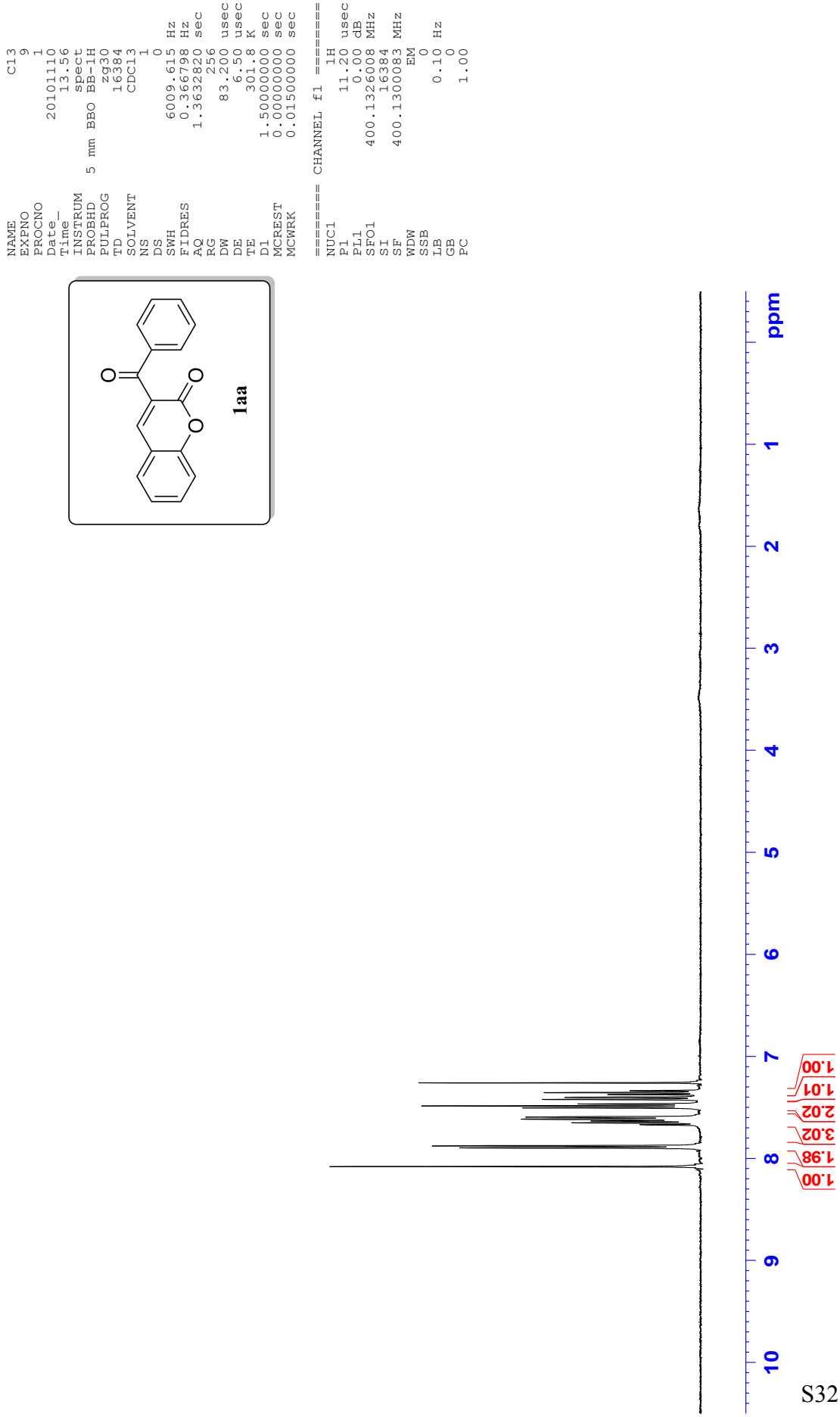
6-bromo-3-(2,5-diphenylfuran-3-yl)-2*H*-chromen-2-one (8ca):

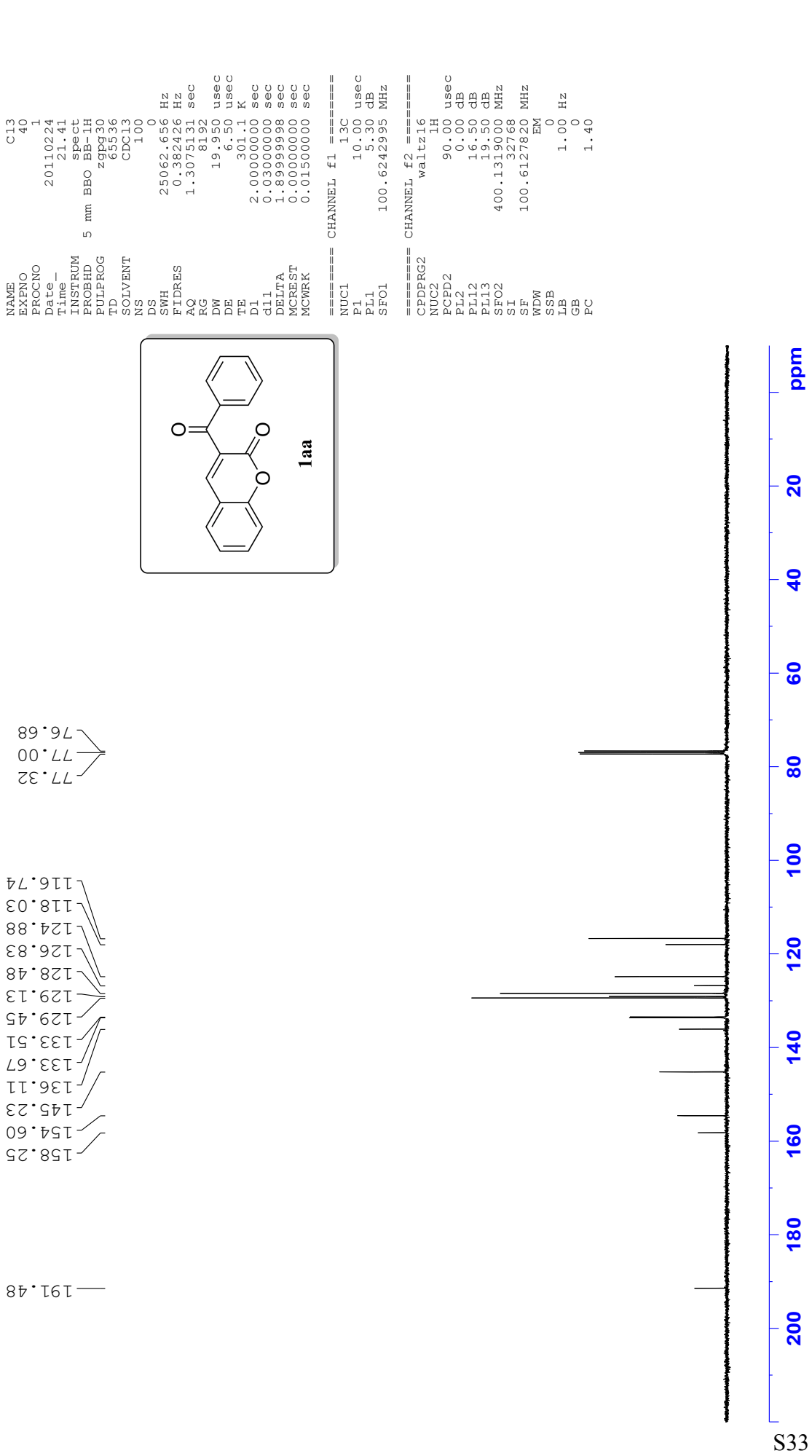


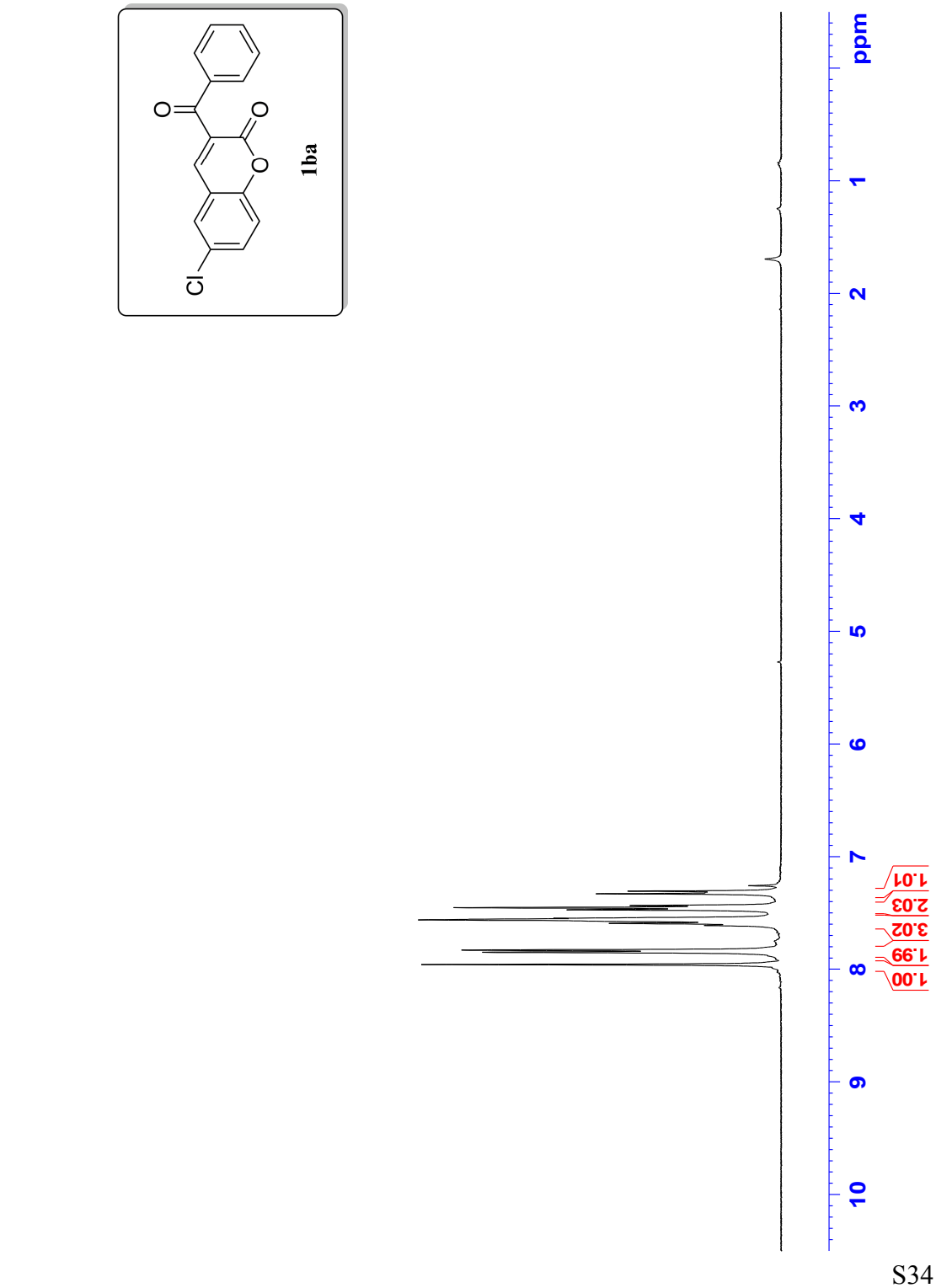
8ca

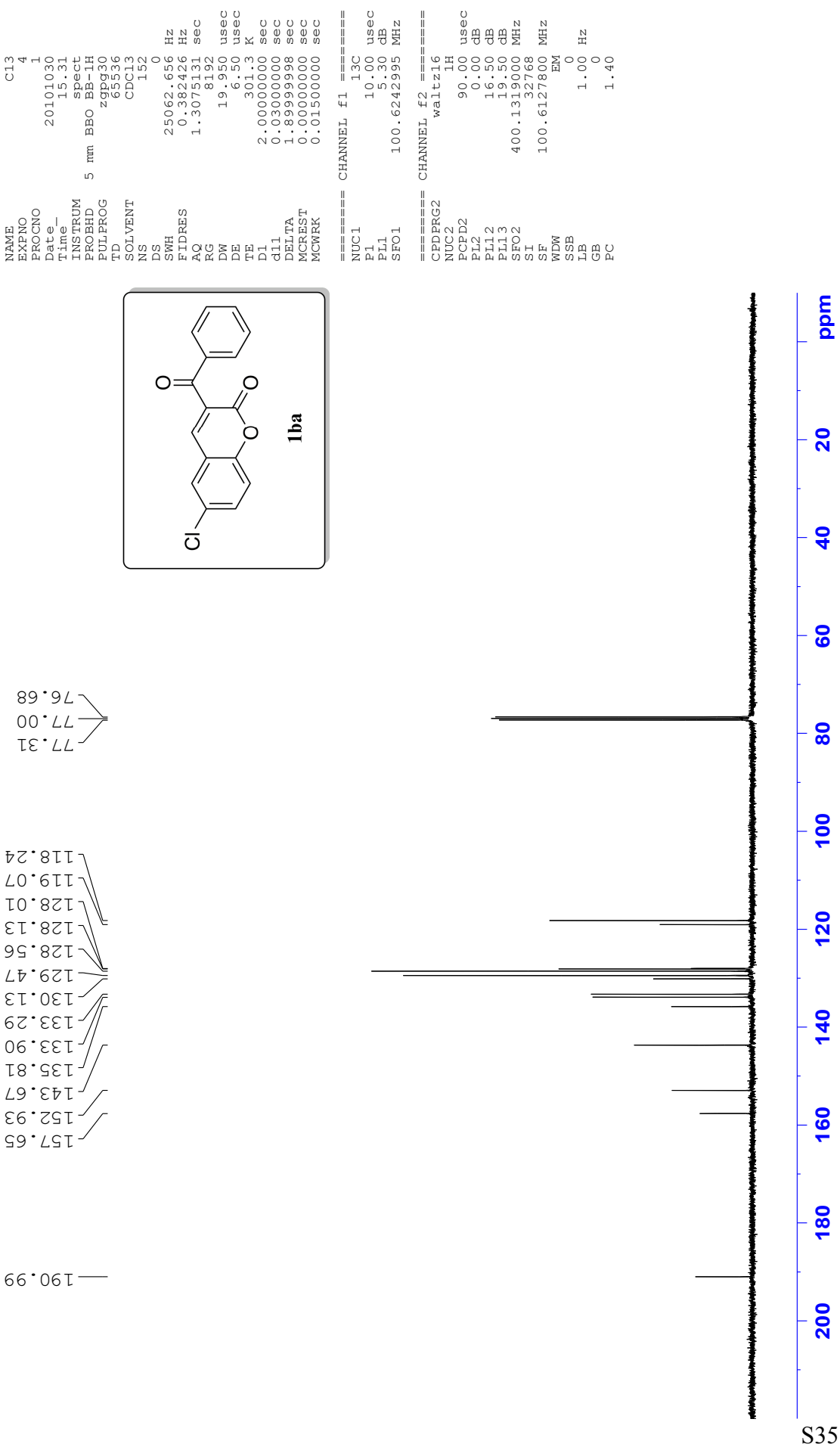
yellow solid; mp: 160.9-161.6 °C; ^{1}H NMR (400 MHz, $CDCl_3$, 25 °C) δ 7.80-7.73 (m, 2H), 7.70-7.59 (m, 4H), 7.51 (d, 2H, J = 2.2 Hz), 7.45-7.36 (m, 4H), 7.35-7.24 (m, 2H), 7.04 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$, 25 °C) δ 159.6, 153.1, 152.4, 150.6, 139.6, 134.2, 130.4, 130.1, 129.9, 128.8, 128.7, 128.4, 127.9, 126.6, 124.0, 123.2, 120.8, 118.3, 117.2, 117.0, 109.0; IR (KBr) 3063 (w), 1733 (s), 1240 (w), 695 (w) cm^{-1}; MS (20eV, EI) *m/z* (%) 444 (M+2, 100), 442 (M^+, 80), 105 (71); HRMS (MALDI) for ($C_{25}H_{15}{}^{79}BrO_3$ + H)$^+$: 443.0283, found: 443.0294.

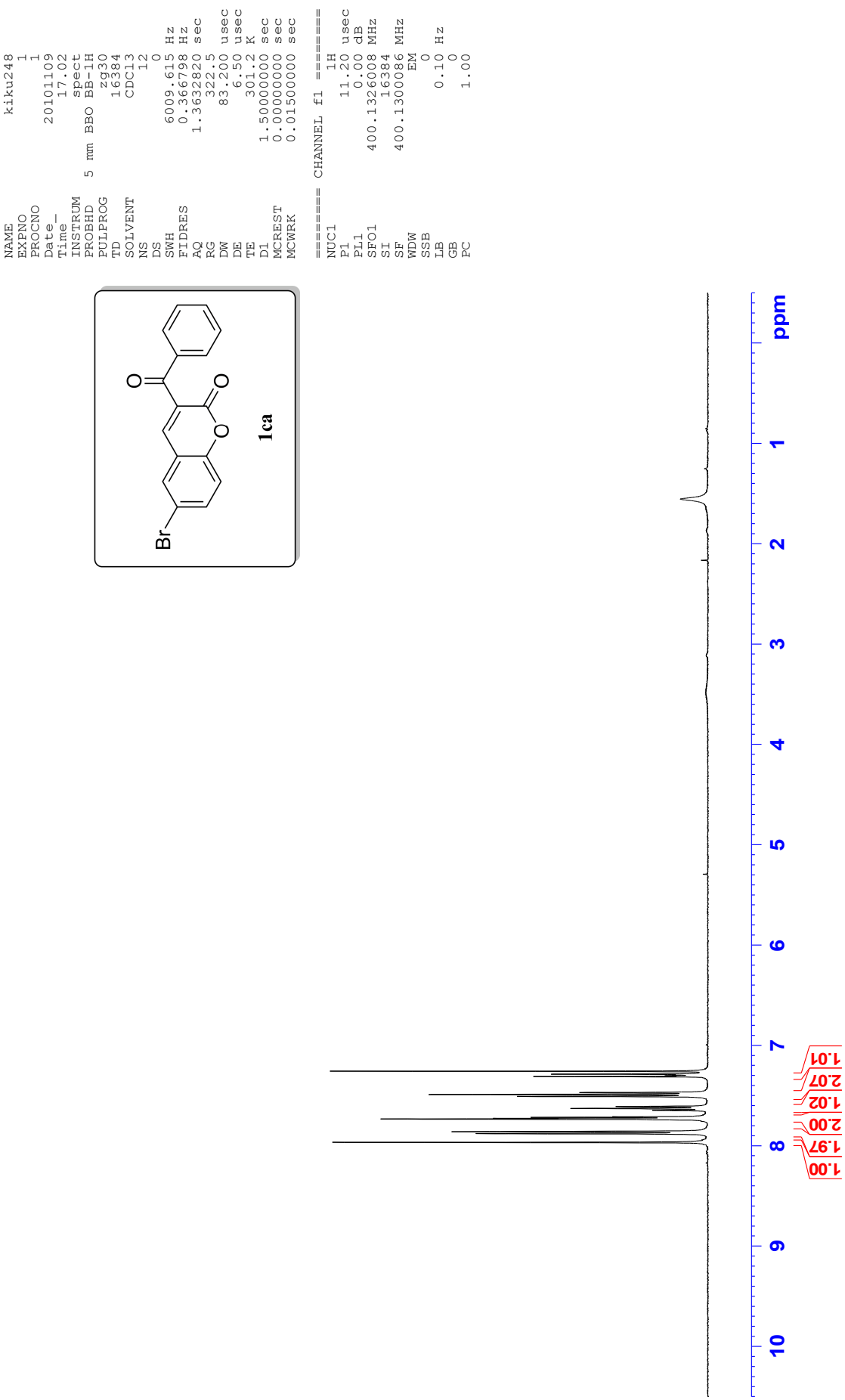
V. ^{1}H NMR and ^{13}C NMR spectra of the substrates and products

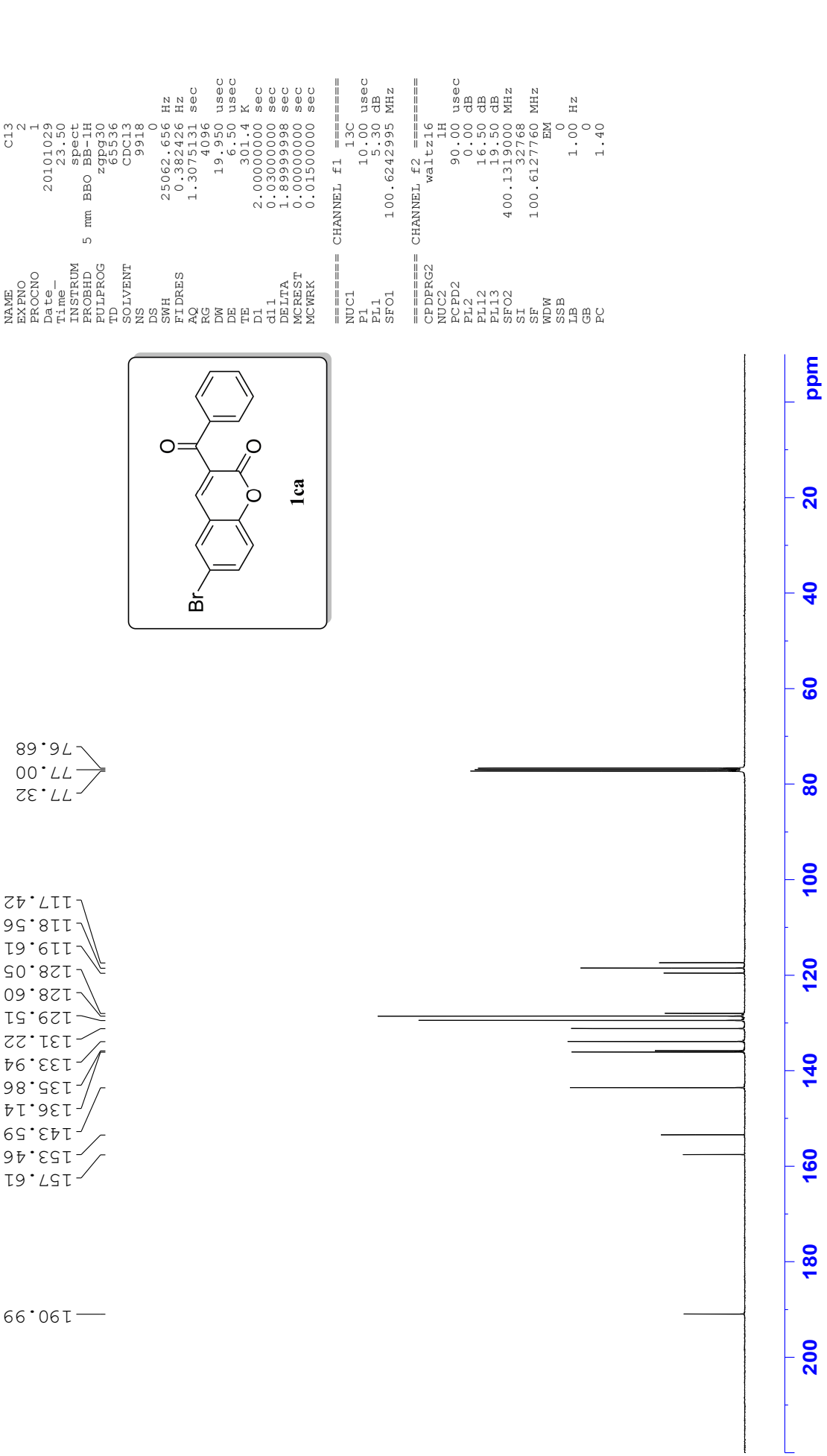


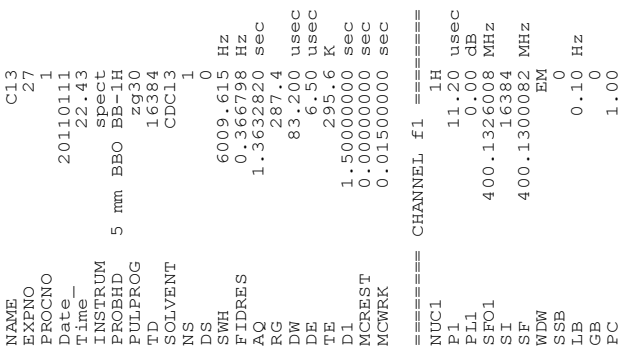


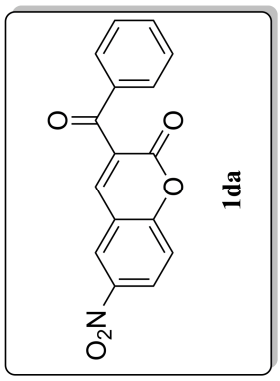

NAME C13
EXPNO 3
PROCNO 1
Date_ 20101030
Time_ 15.28
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 16384
SOLVENT CDCl3
NS 1
DS 0
SWH 6009.615 Hz
FIDRES 0.366798 Hz
AQ 1.3632820 sec
RG 128
DW 83.200 usec
DE 6.50 usec
TE 301.0 K
D1 1.50000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
========== CHANNEL f1 ==========
NUC1 1H
P1 11.20 usec
PL1 0.00 dB
SFO1 400.1326008 MHz
SI 16384
SF 400.1300079 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00
O
O
O
Cl
1ba
ppm
1
2
3
4
5
6
7
8
9
10
1.00
1.99
3.02
2.03
1.01

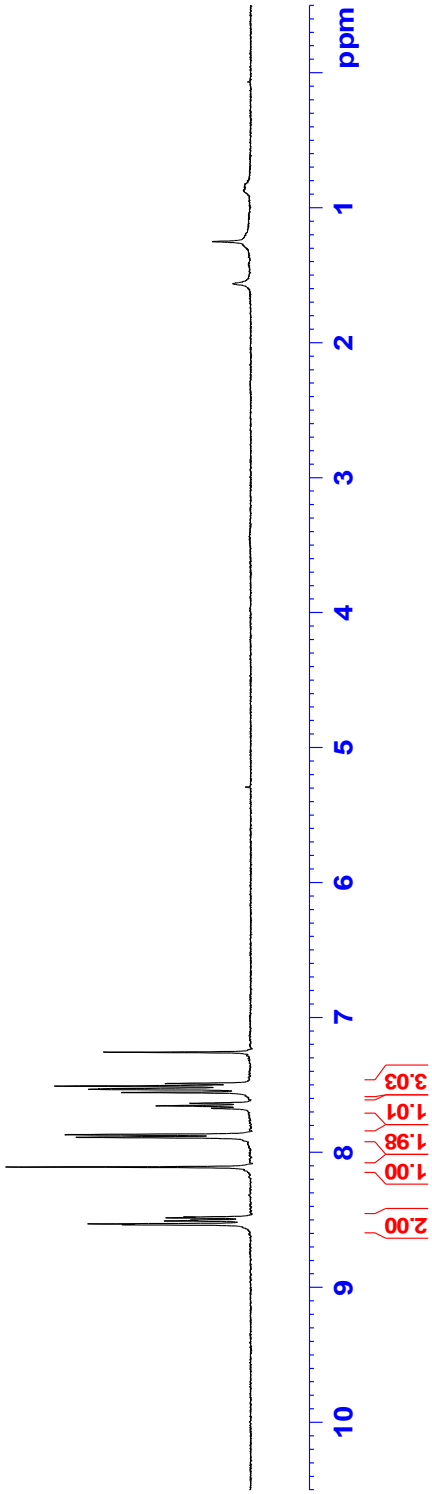


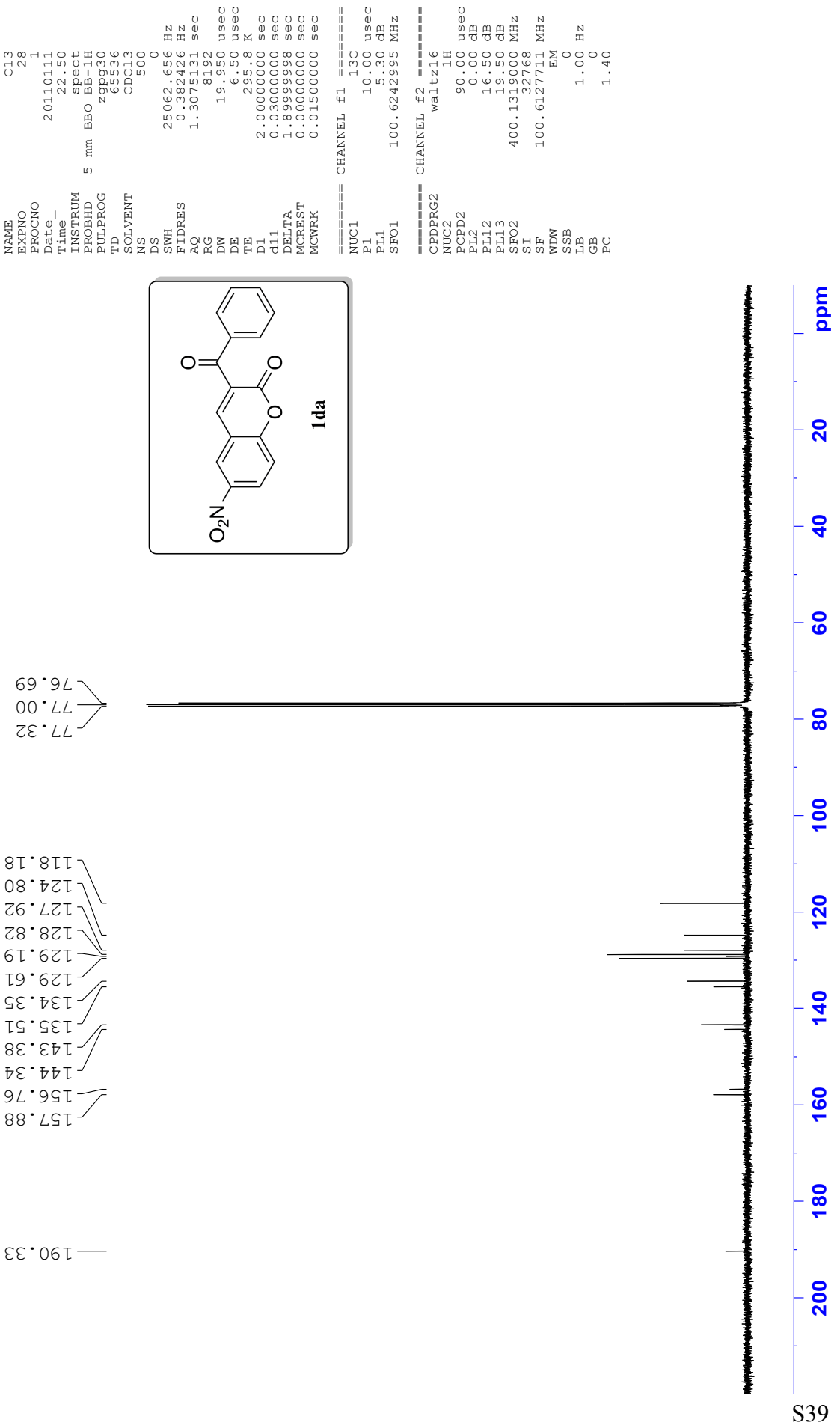


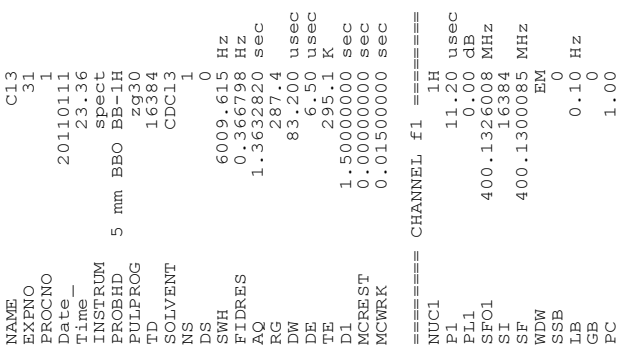


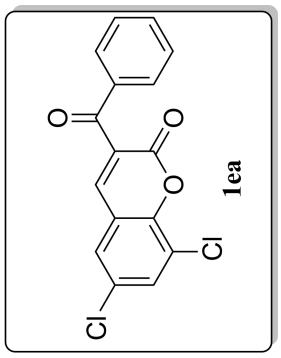


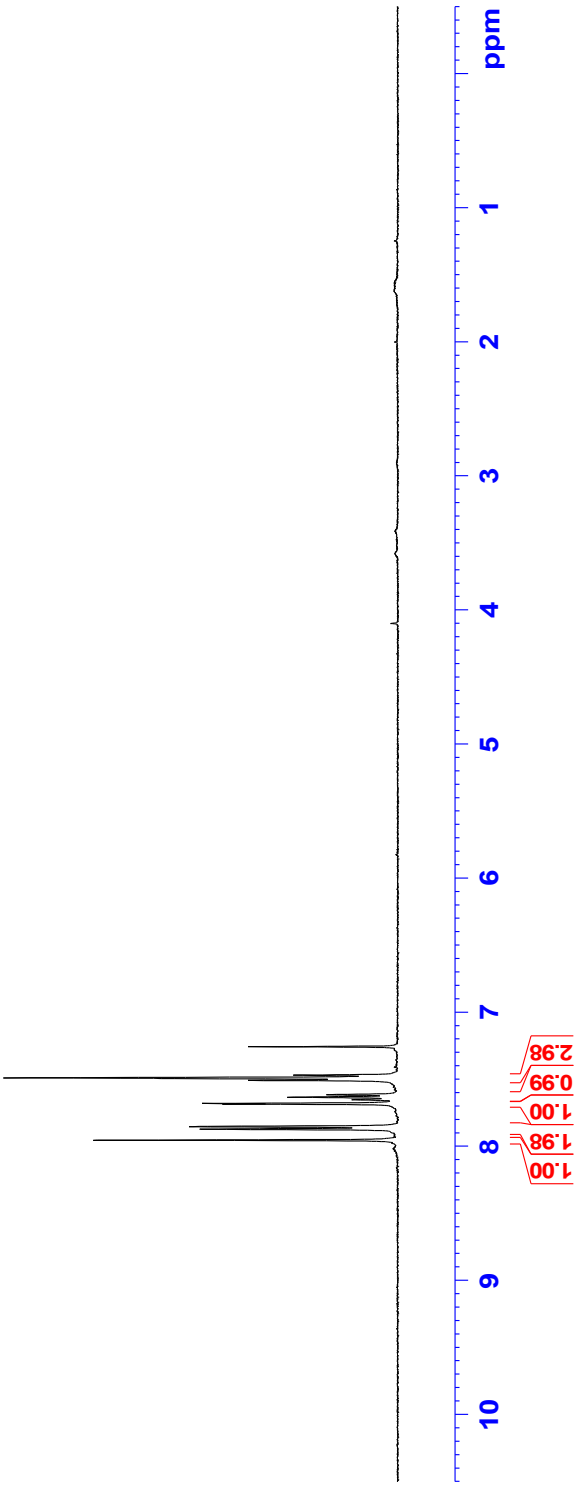


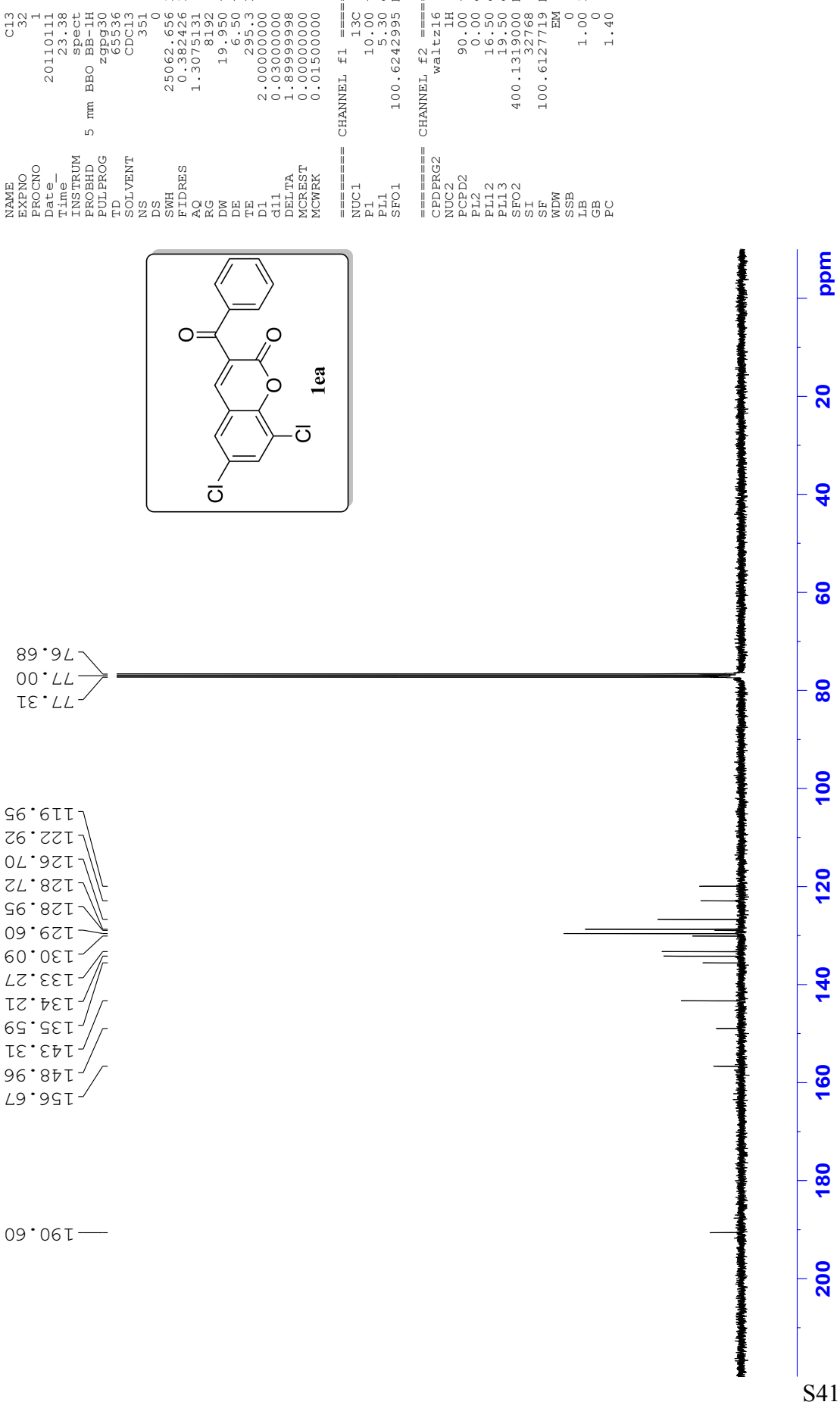


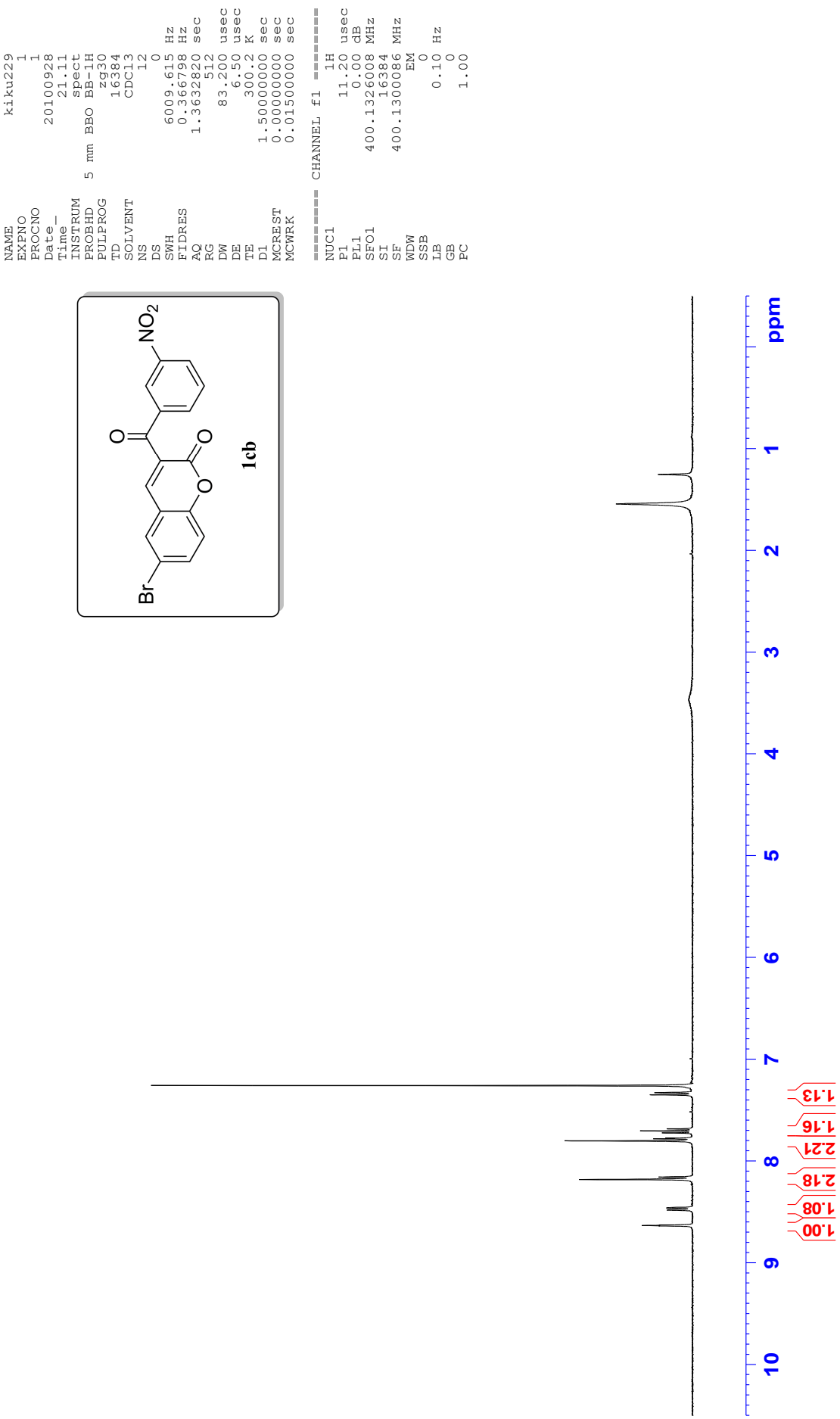


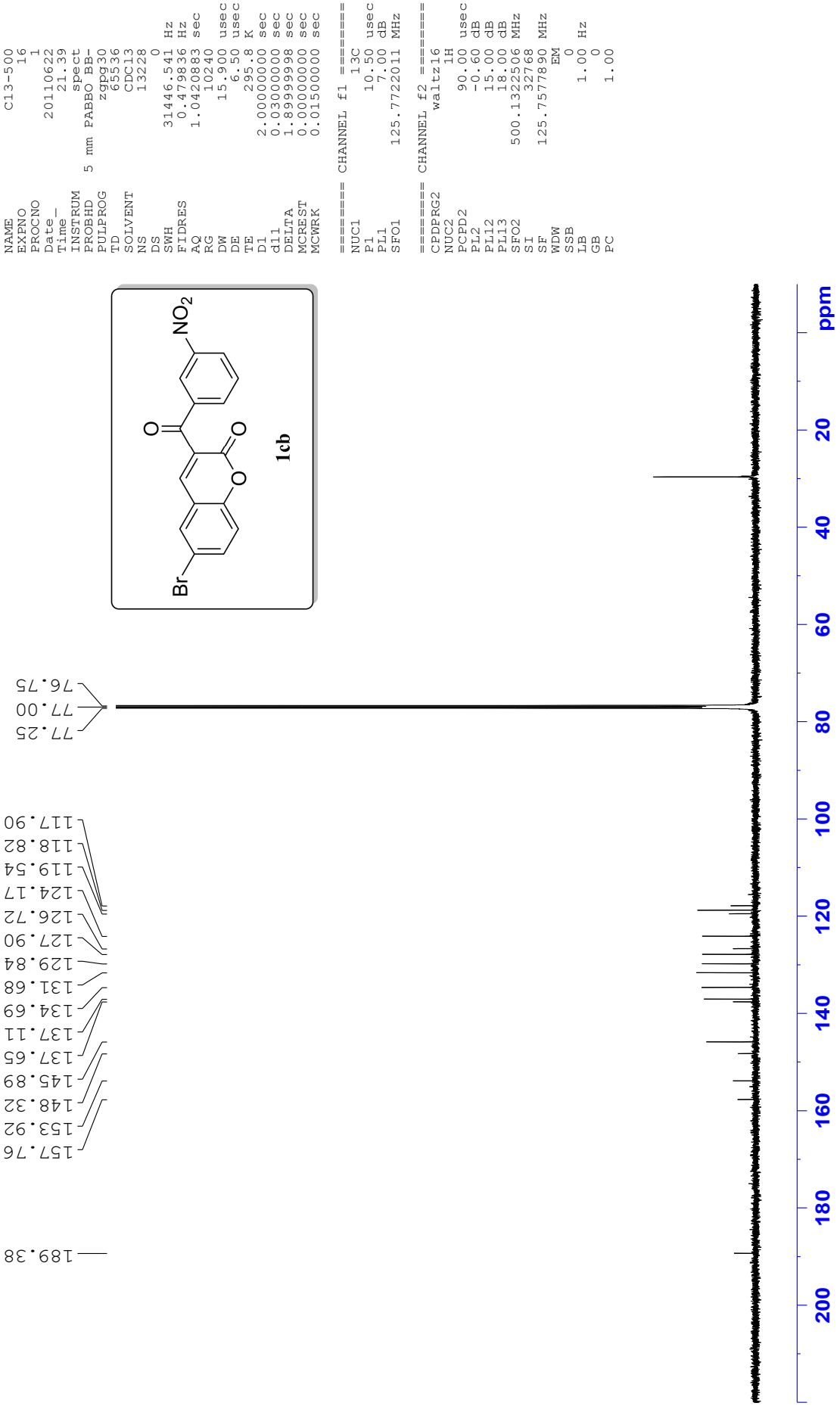


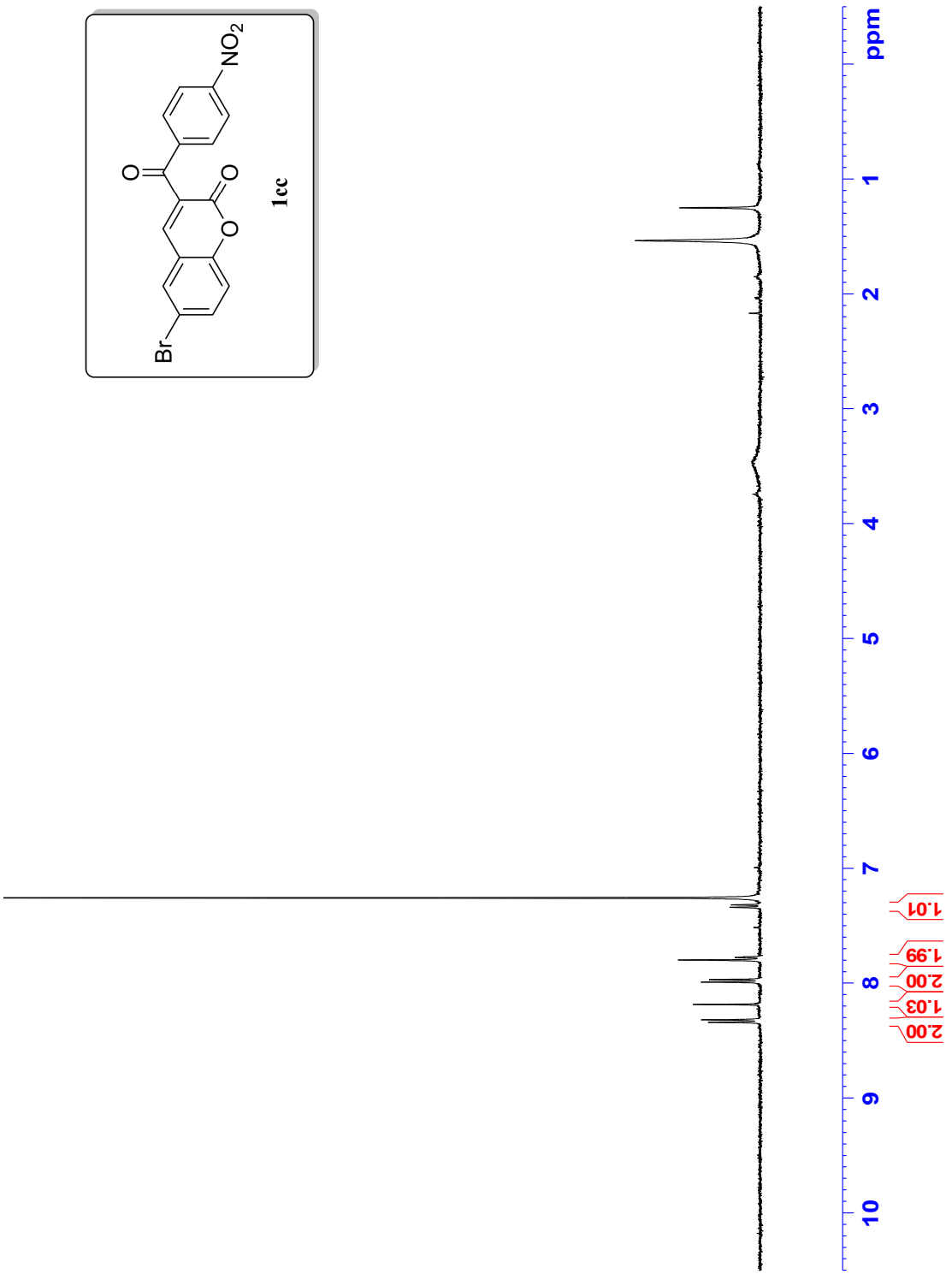


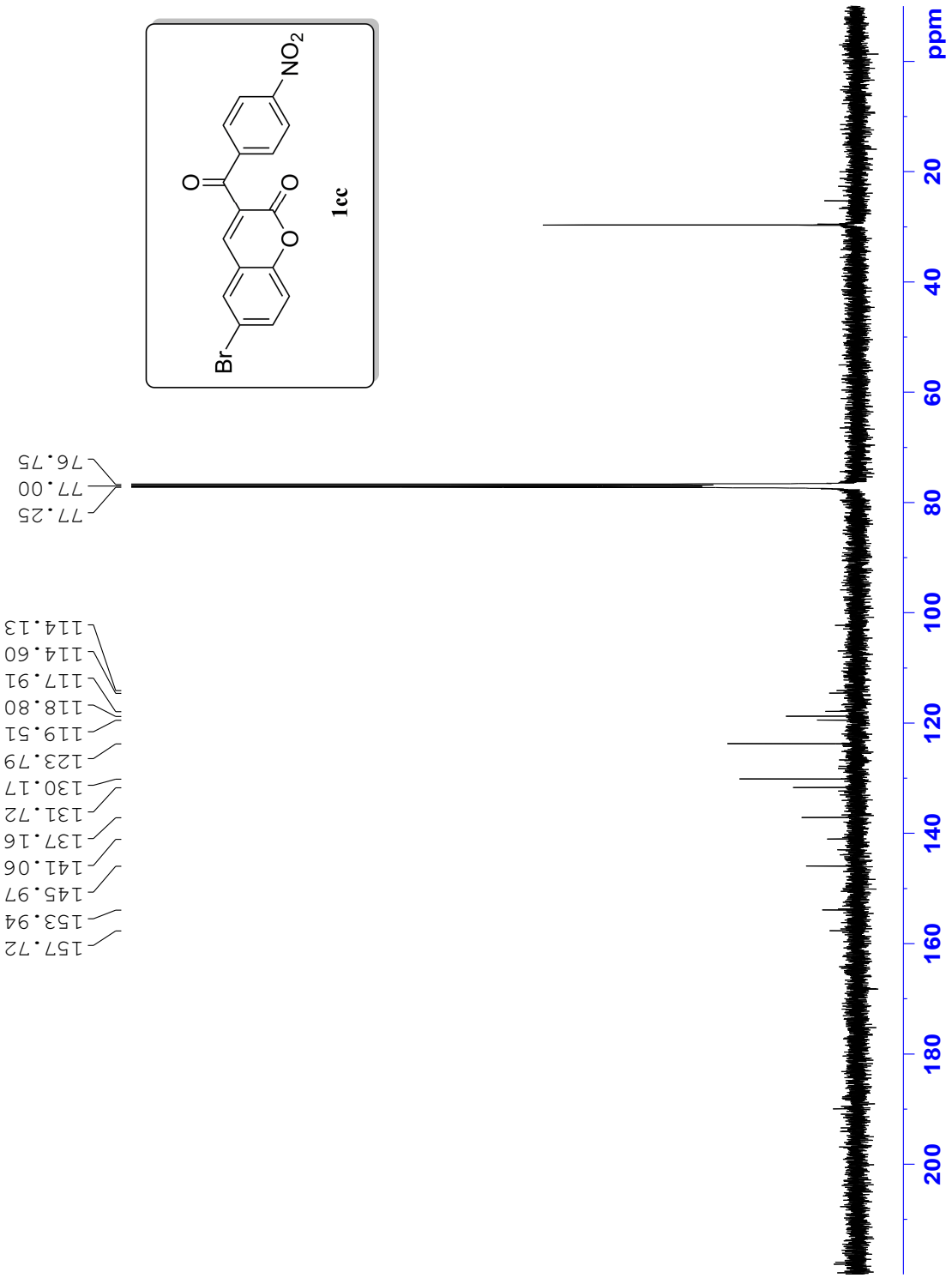


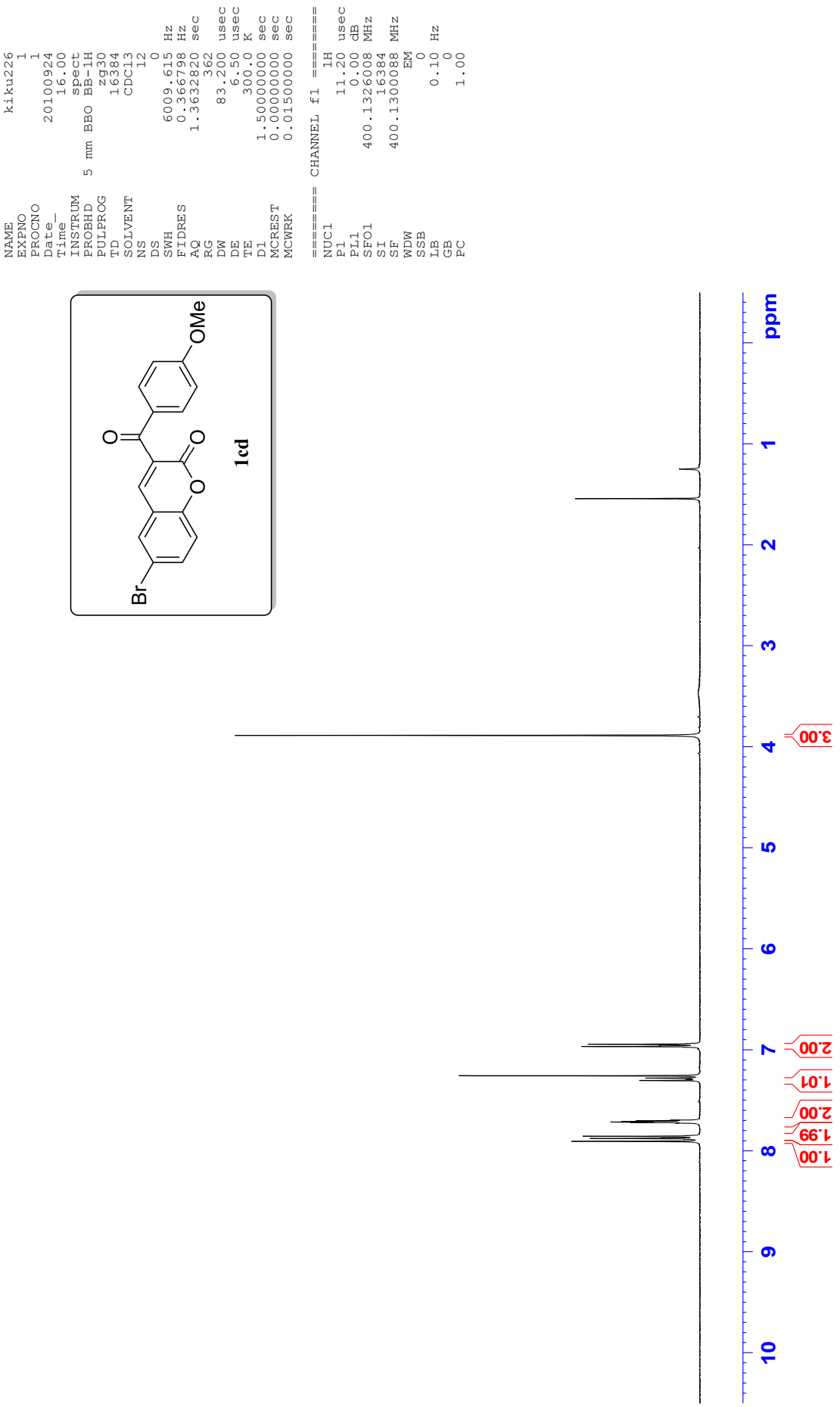


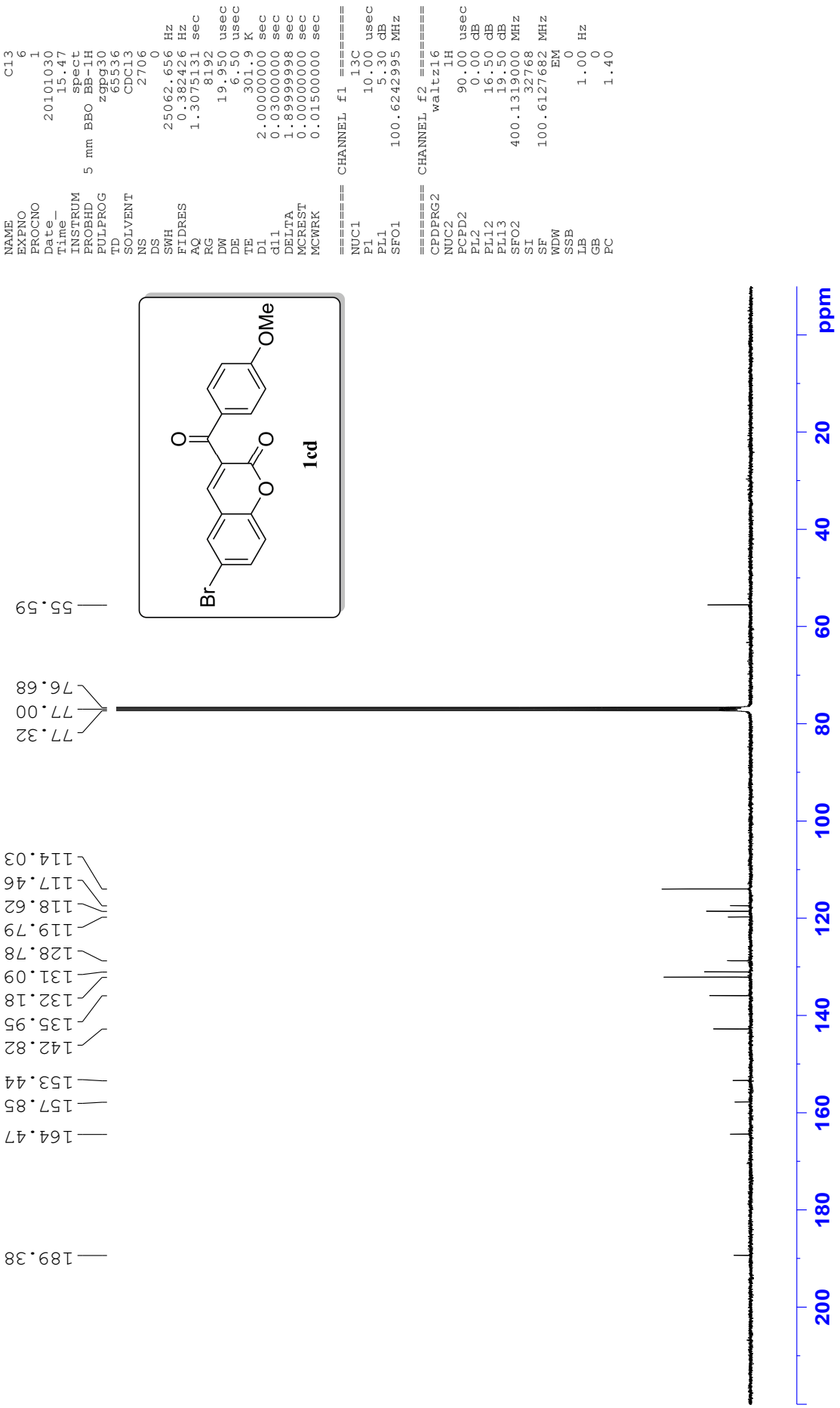


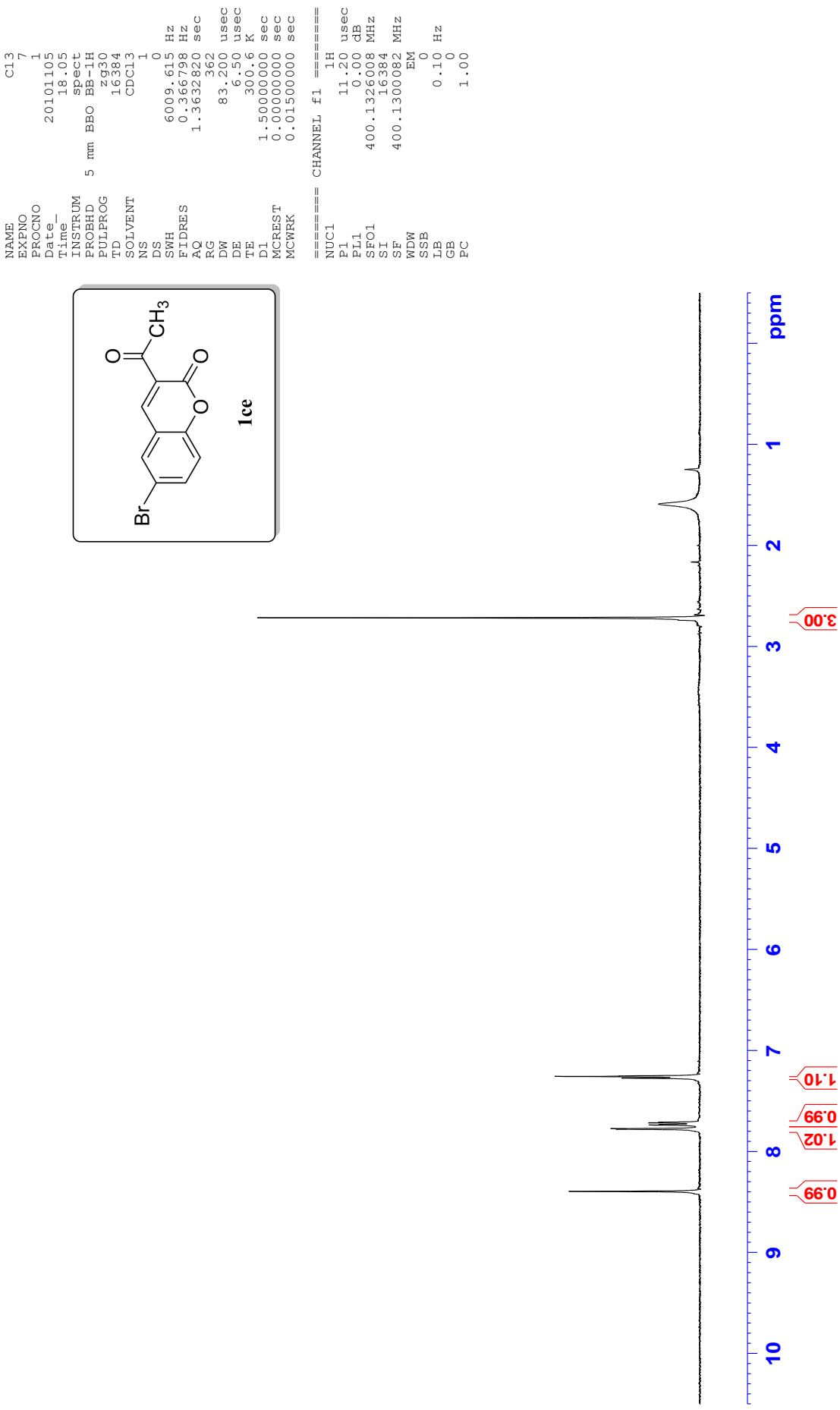


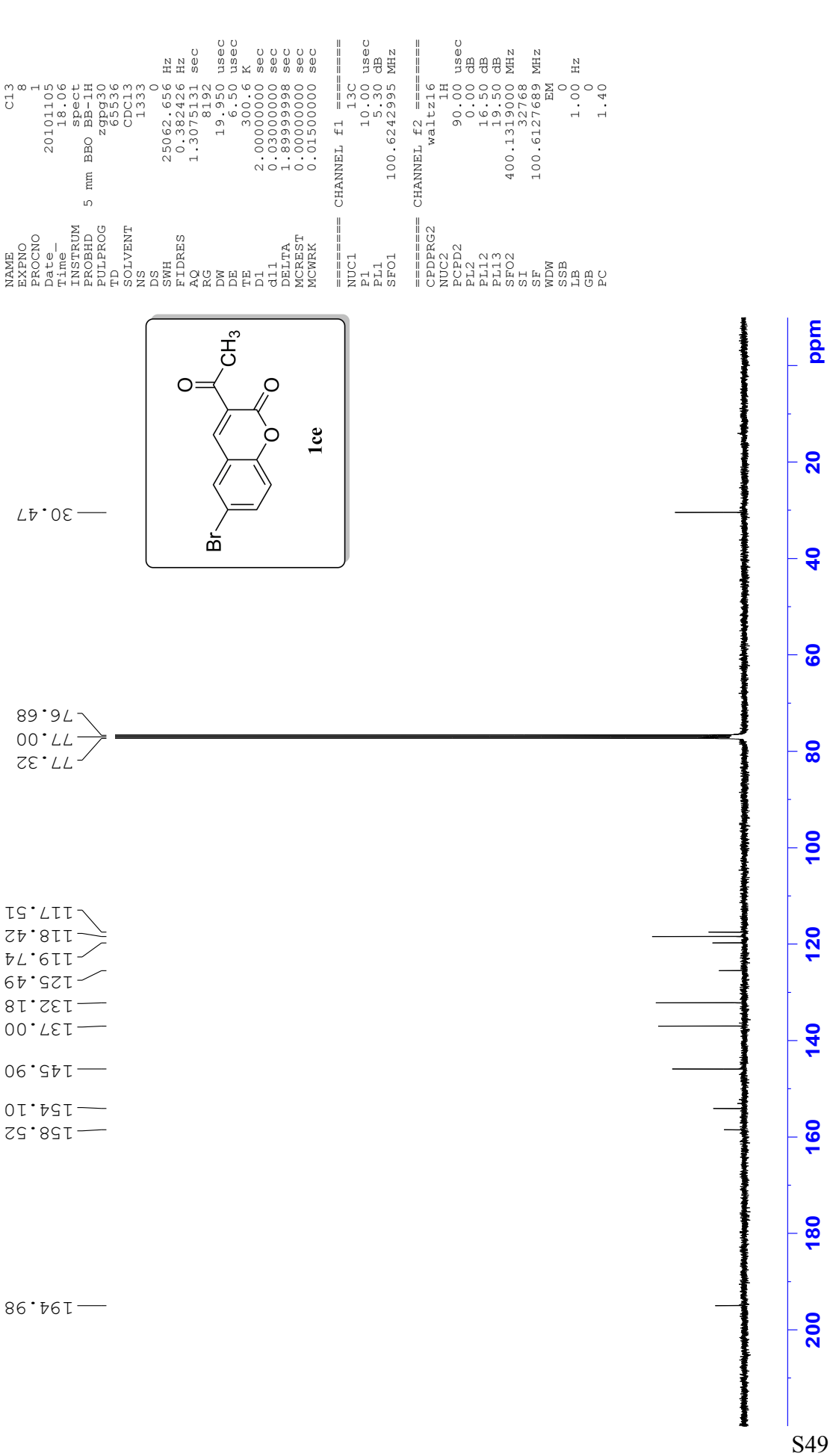


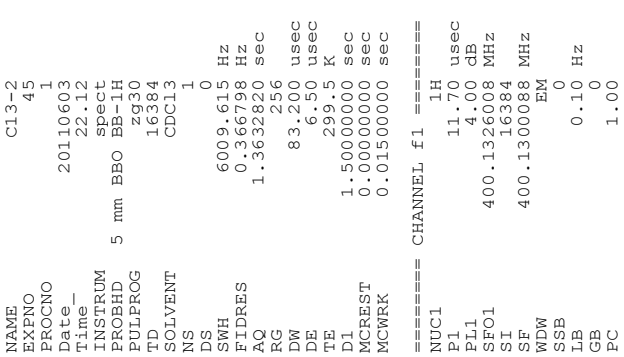












```
NAME                  C13-2
EXPNO                    45
PROCNO                    1
Date_              20110603
Time_                 22.12
INSTRUM                spect
PROBHD     5 mm BBO BB-1H
PULPROG                zg30
TD                    16384
SOLVENT               CDCl3
NS                        1
DS                        0
SWH                6009.615 Hz
FIDRES             0.366798 Hz
AQ                 1.3632820 sec
RG                      256
DW                   83.200 usec
DE                    6.50 usec
TE                   299.5 K
D1                 1.50000000 sec
MCREST             0.00000000 sec
MCWRK              0.01500000 sec

======== CHANNEL f1 ========
NUC1                      1H
P1                     11.70 usec
PL1                     4.00 dB
SFO1               400.1326008 MHz
SI                    16384
SF                 400.1300088 MHz
WDW                       EM
SSB                        0
LB                      0.10 Hz
GB                         0
PC                      1.00
```

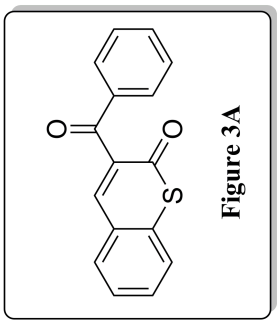
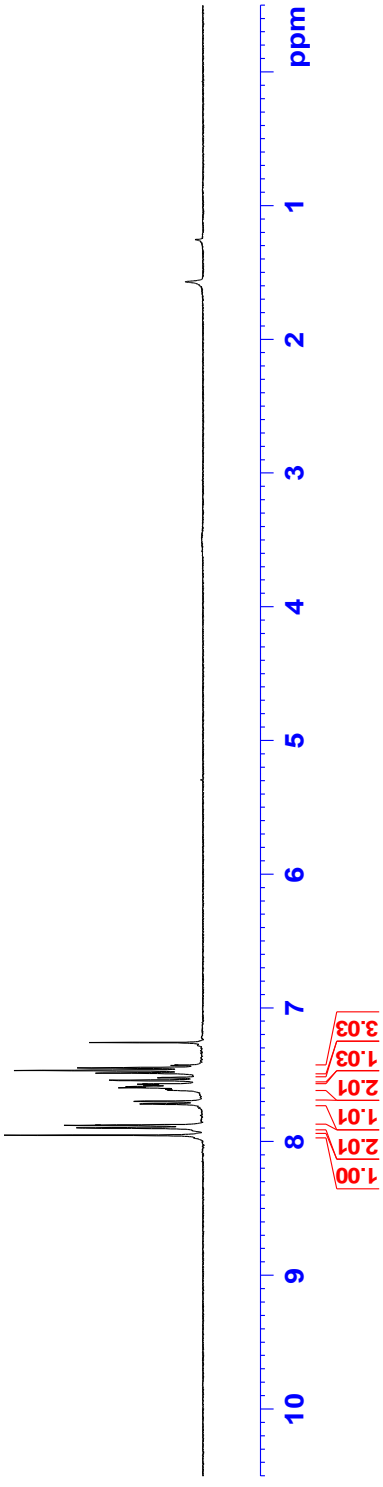
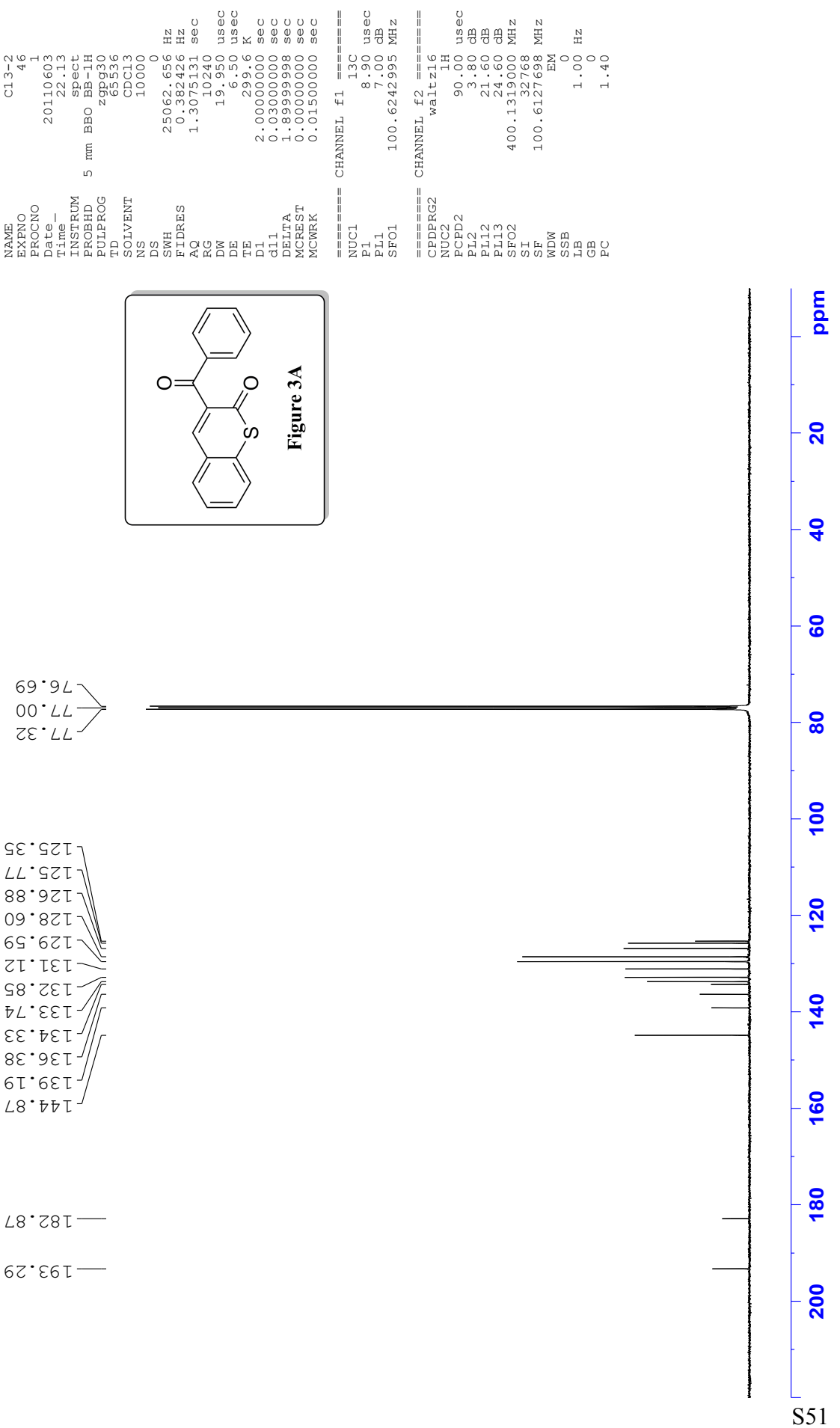
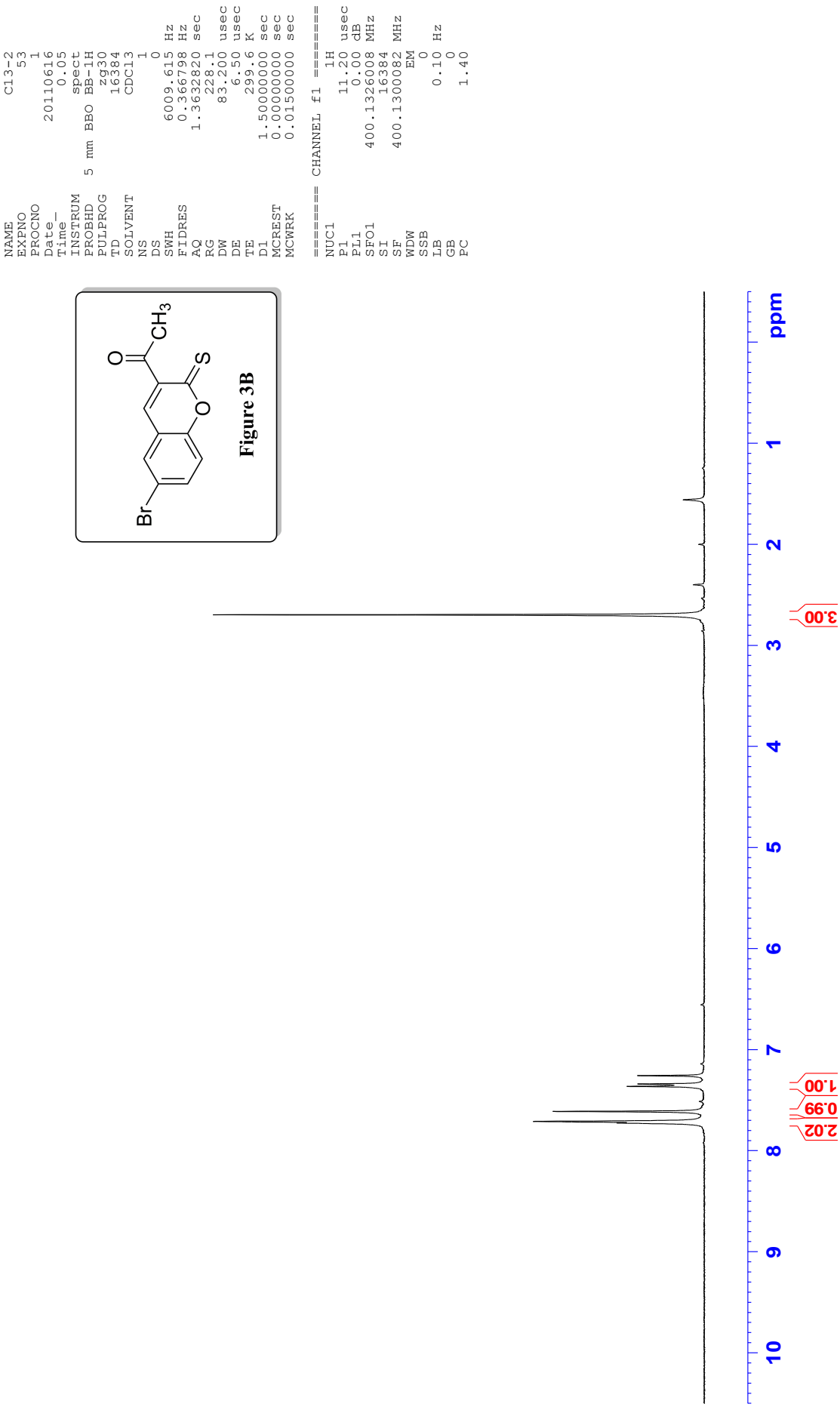
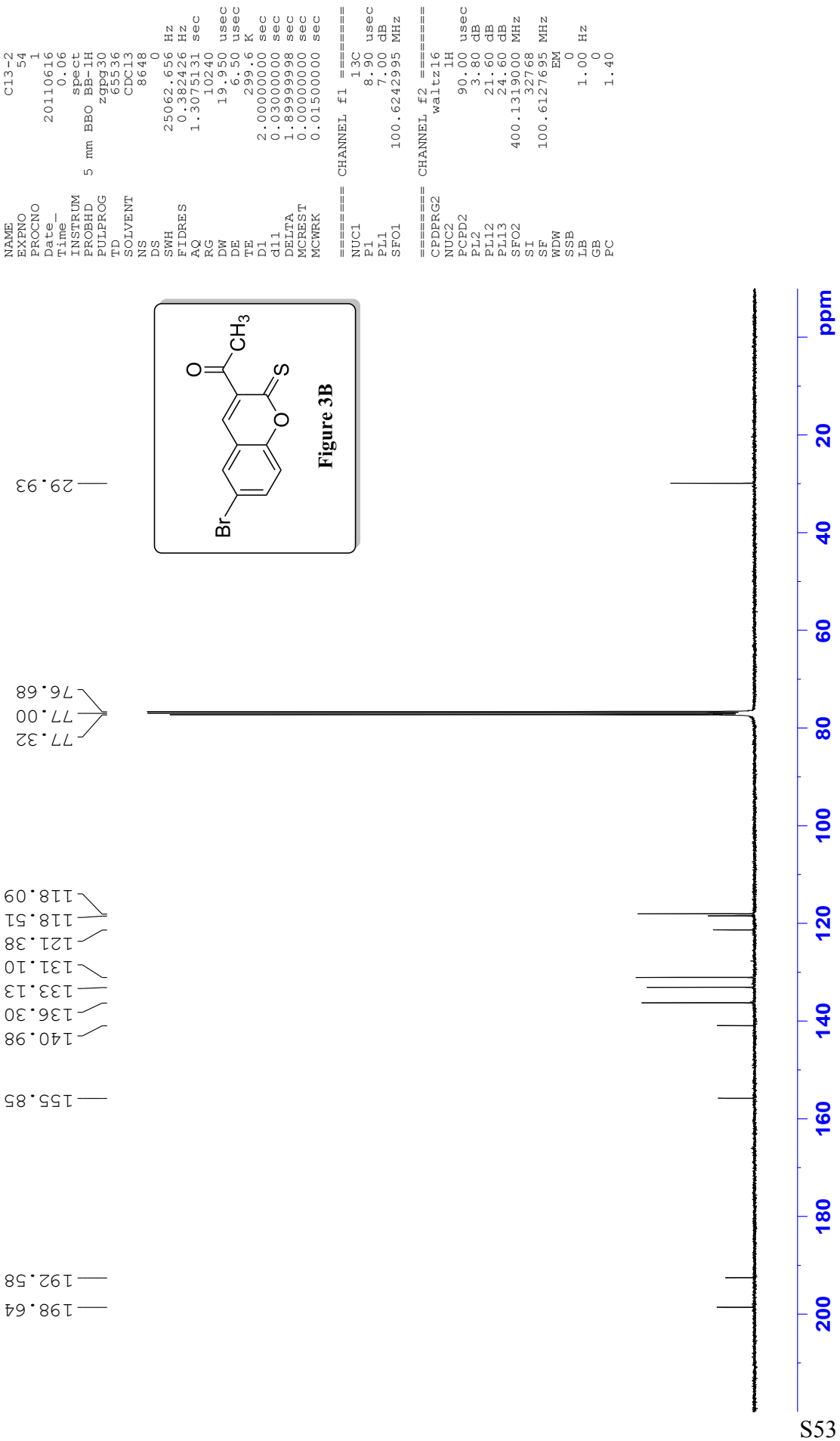


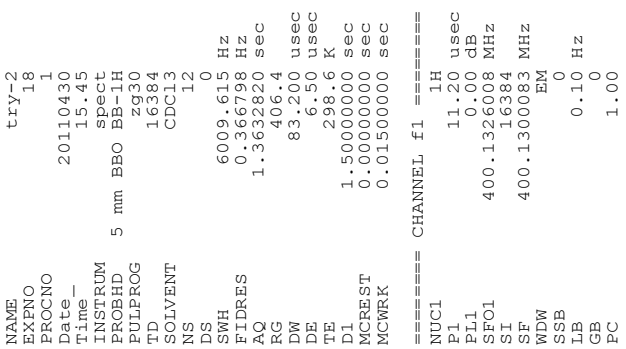
Figure 3A











```
NAME                try-2
EXPNO                  18
PROCNO                  1
Date_            20110430
Time_                15.45
INSTRUM              spect
PROBHD   5 mm BBO BB-1H
PULPROG              zg30
TD                  16384
SOLVENT             CDCl3
NS                     12
DS                      0
SWH              6009.615 Hz
FIDRES           0.366798 Hz
AQ               1.3632820 sec
RG                   406.4
DW                  83.200 usec
DE                   6.50 usec
TE                  298.6 K
D1               1.50000000 sec
MCREST           0.00000000 sec
MCWRK            0.01500000 sec

======== CHANNEL f1 ========
NUC1                    1H
P1                   11.20 usec
PL1                   0.00 dB
SFO1          400.1326008 MHz
SI                  16384
SF            400.1300083 MHz
WDW                    EM
SSB                     0
LB                   0.10 Hz
GB                      0
PC                   1.00
```

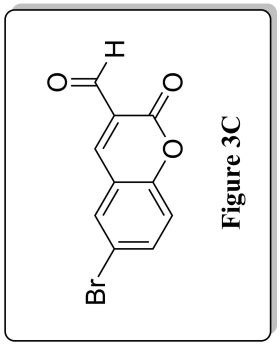
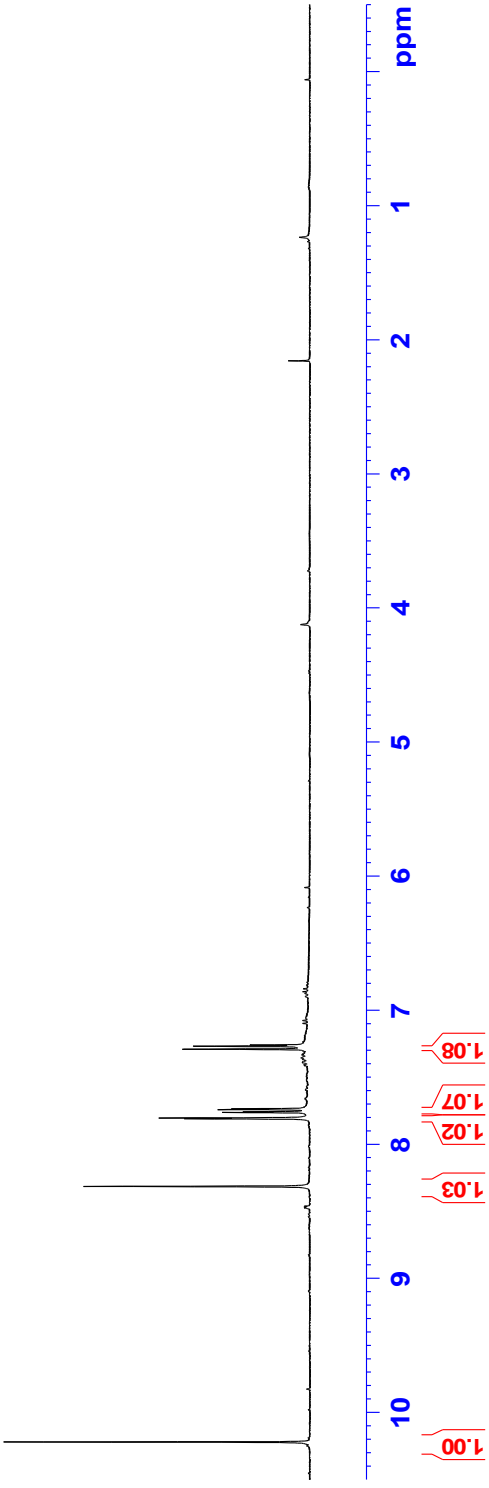


Figure 3C



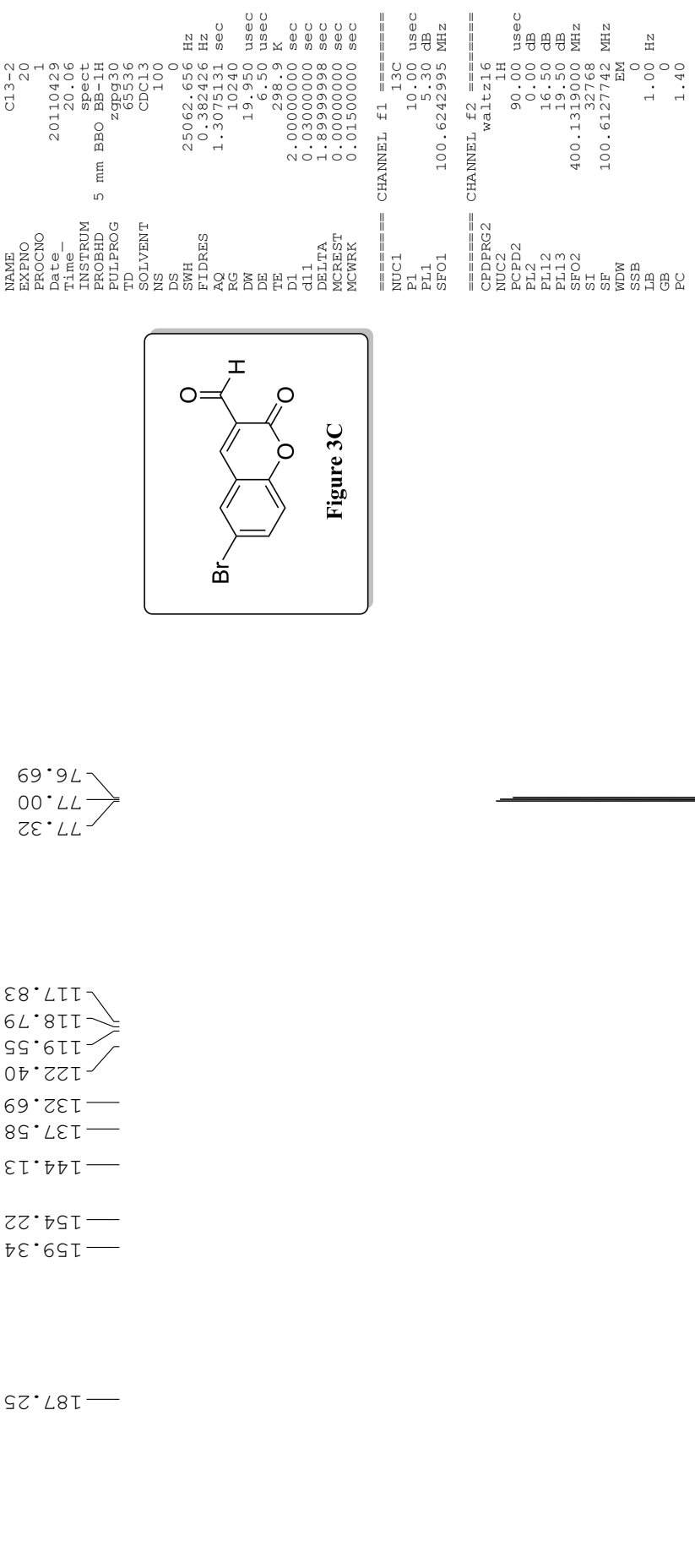
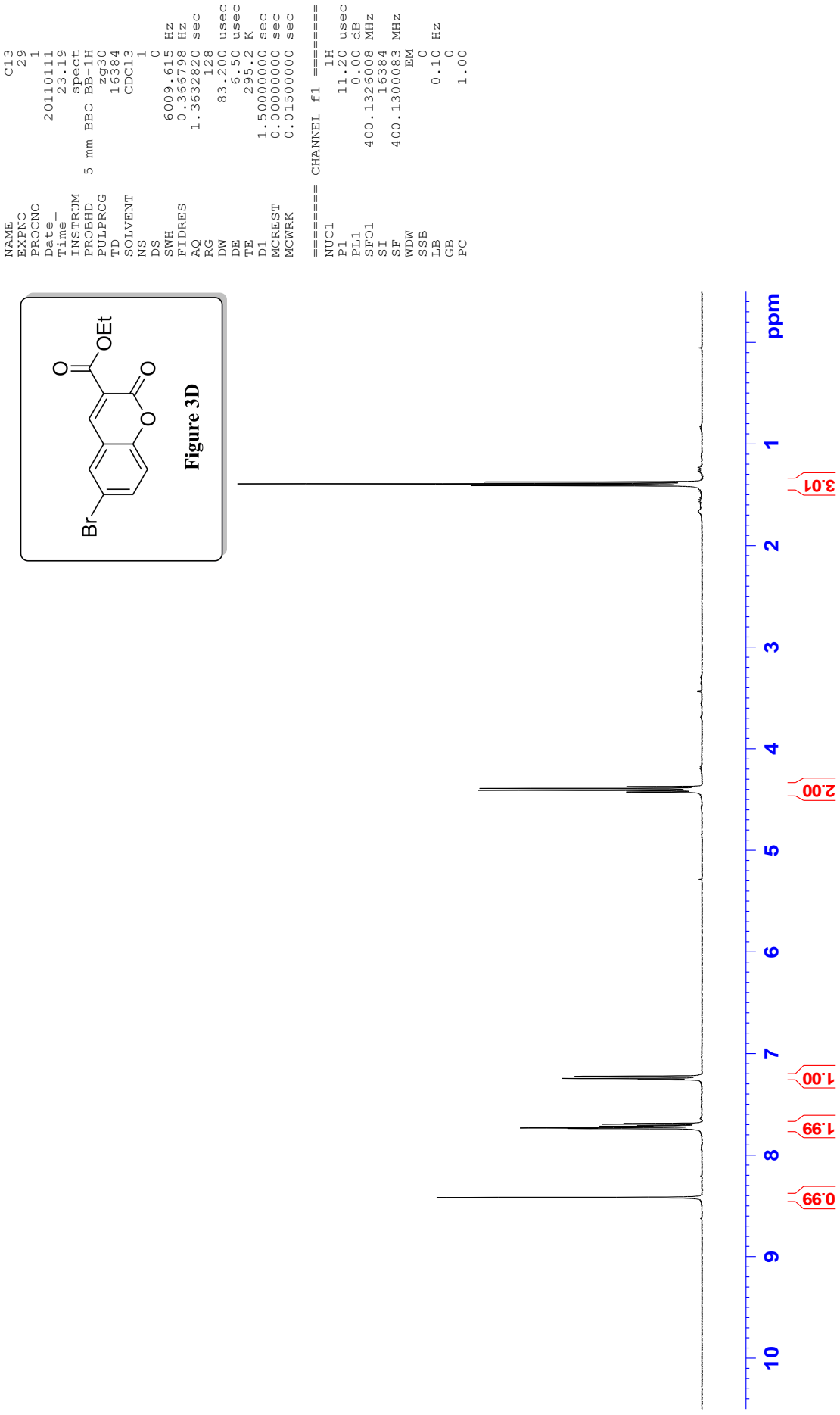
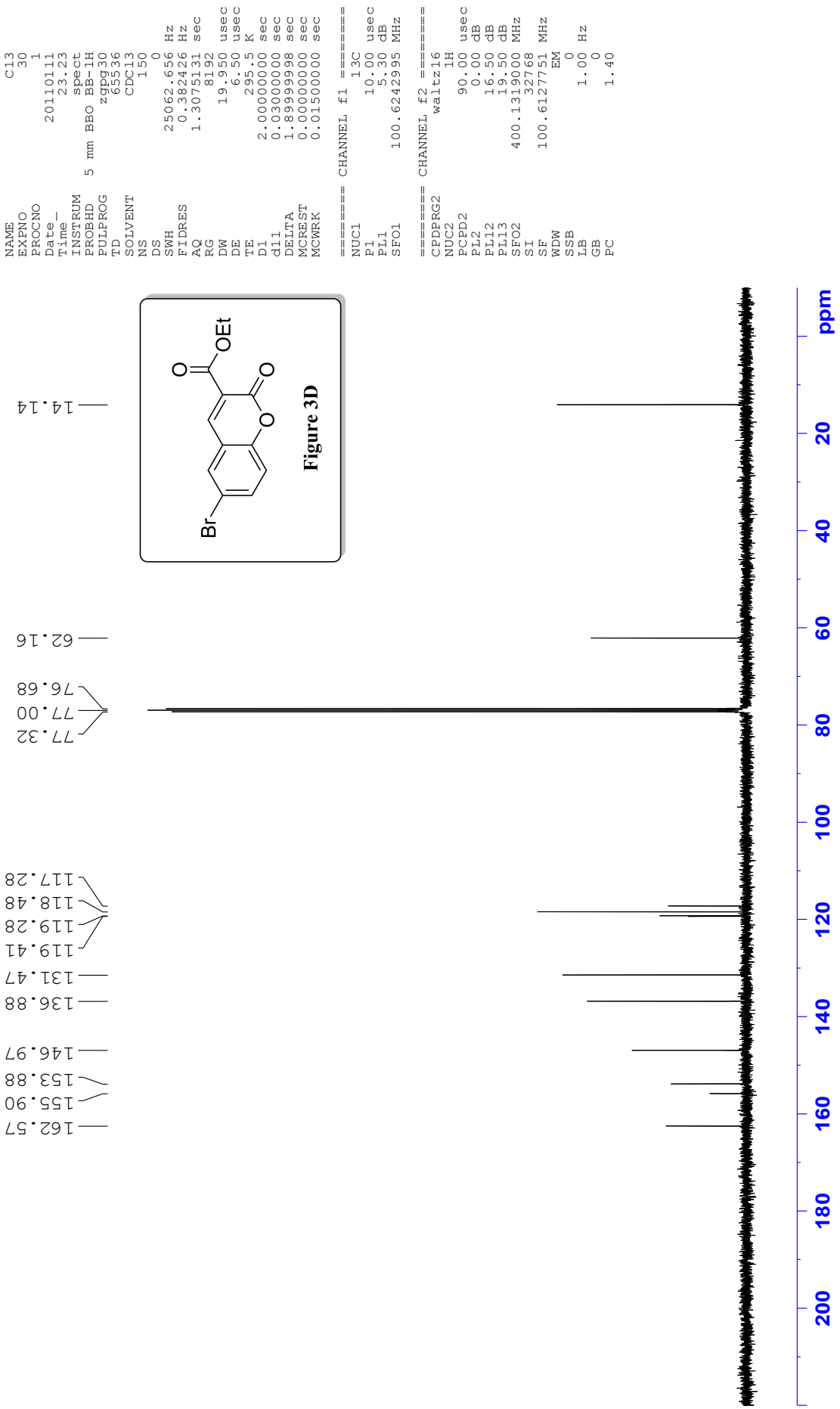
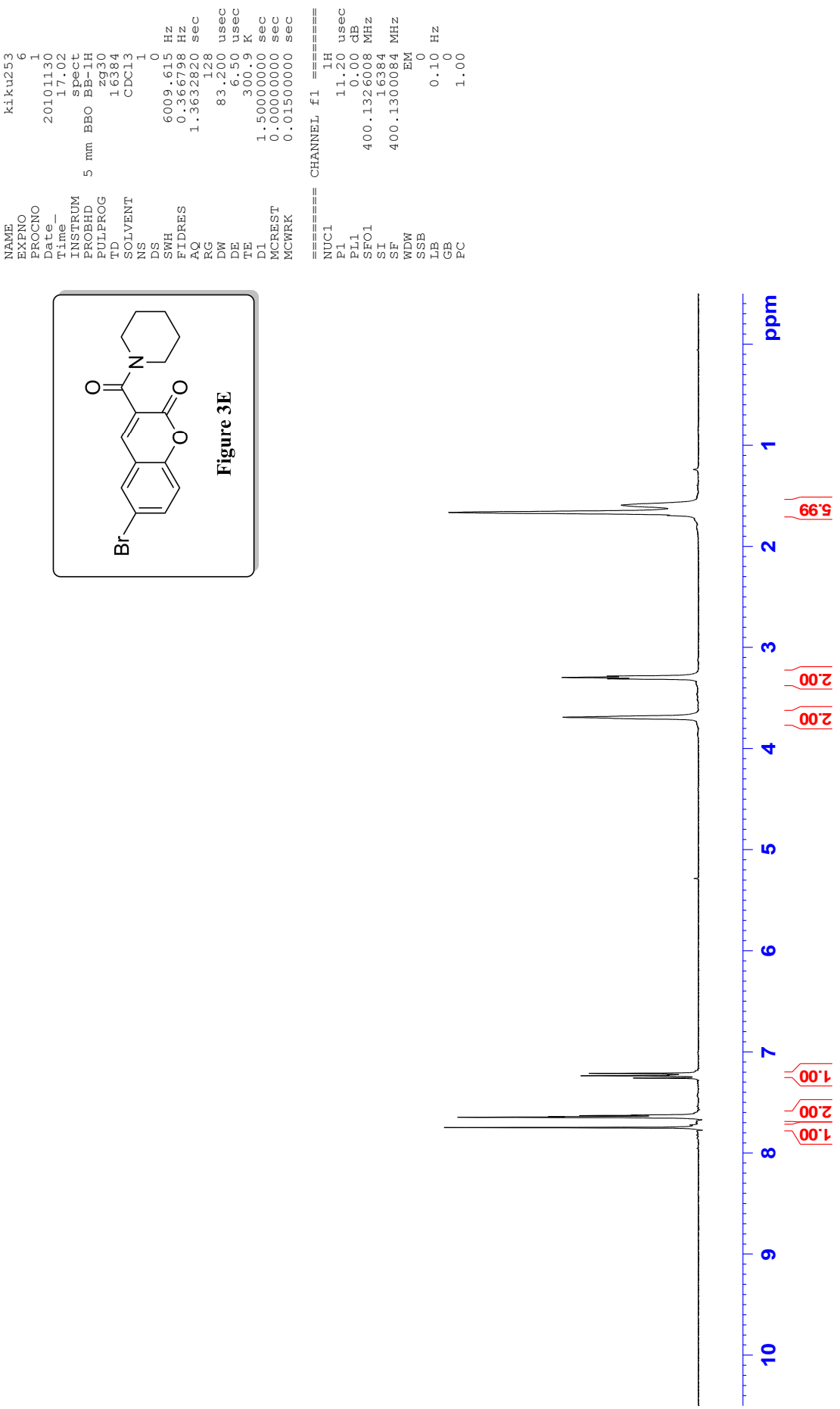
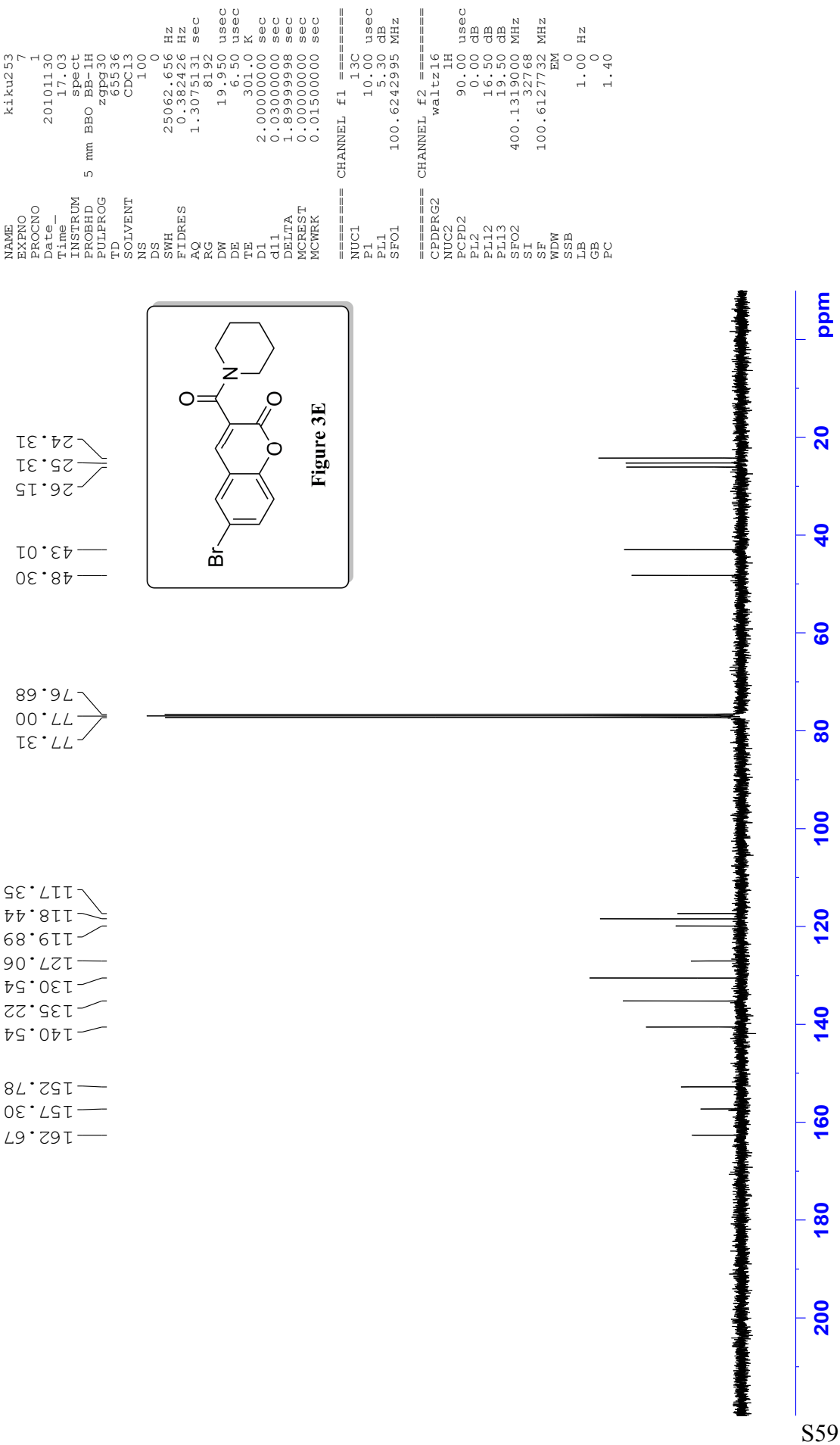


Figure 3C

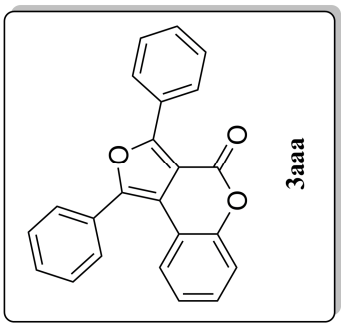


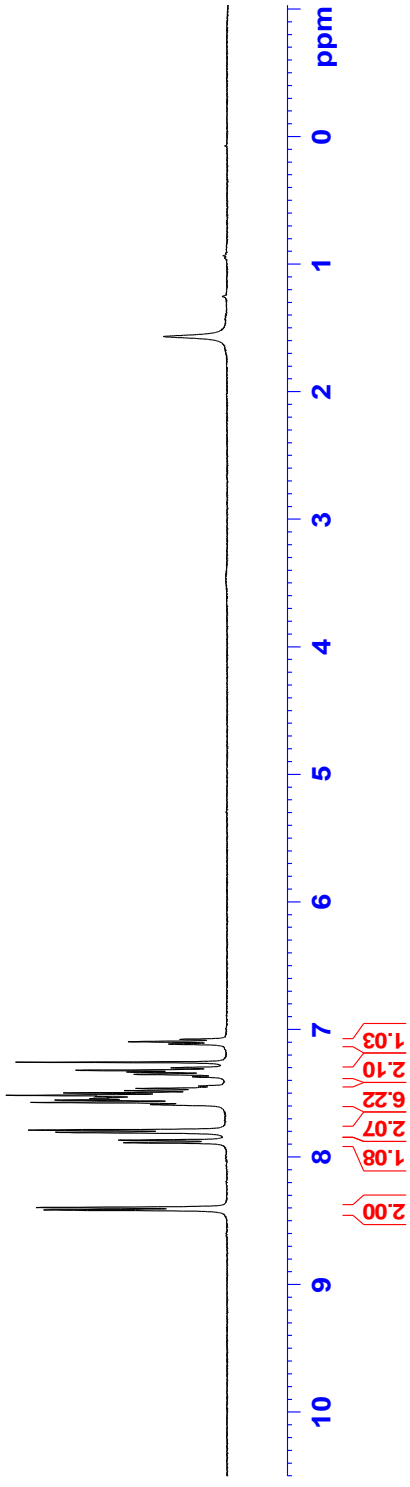

NAME C13
EXPNO 30
PROCNO 1
Date_ 20110111
Time_ 23.23
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 150
DS 0
SWH 25062.656 Hz
FIDRES 0.382426 Hz
AQ 1.3075131 sec
RG 8192
DW 19.950 usec
DE 6.50 usec
TE 295.5 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 10.00 usec
PL1 5.30 dB
SFO1 100.6242995 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 0.00 dB
PL12 16.50 dB
PL13 19.50 dB
SFO2 400.1319000 MHz
SI 32768
SF 100.6127751 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
14.14
62.16
76.68
77.00
77.32
117.28
118.48
119.28
119.41
131.47
136.88
146.97
153.88
155.90
162.57
OEt
O
O
O
Br
Figure 3D
ppm
200
180
160
140
120
100
80
60
40
20

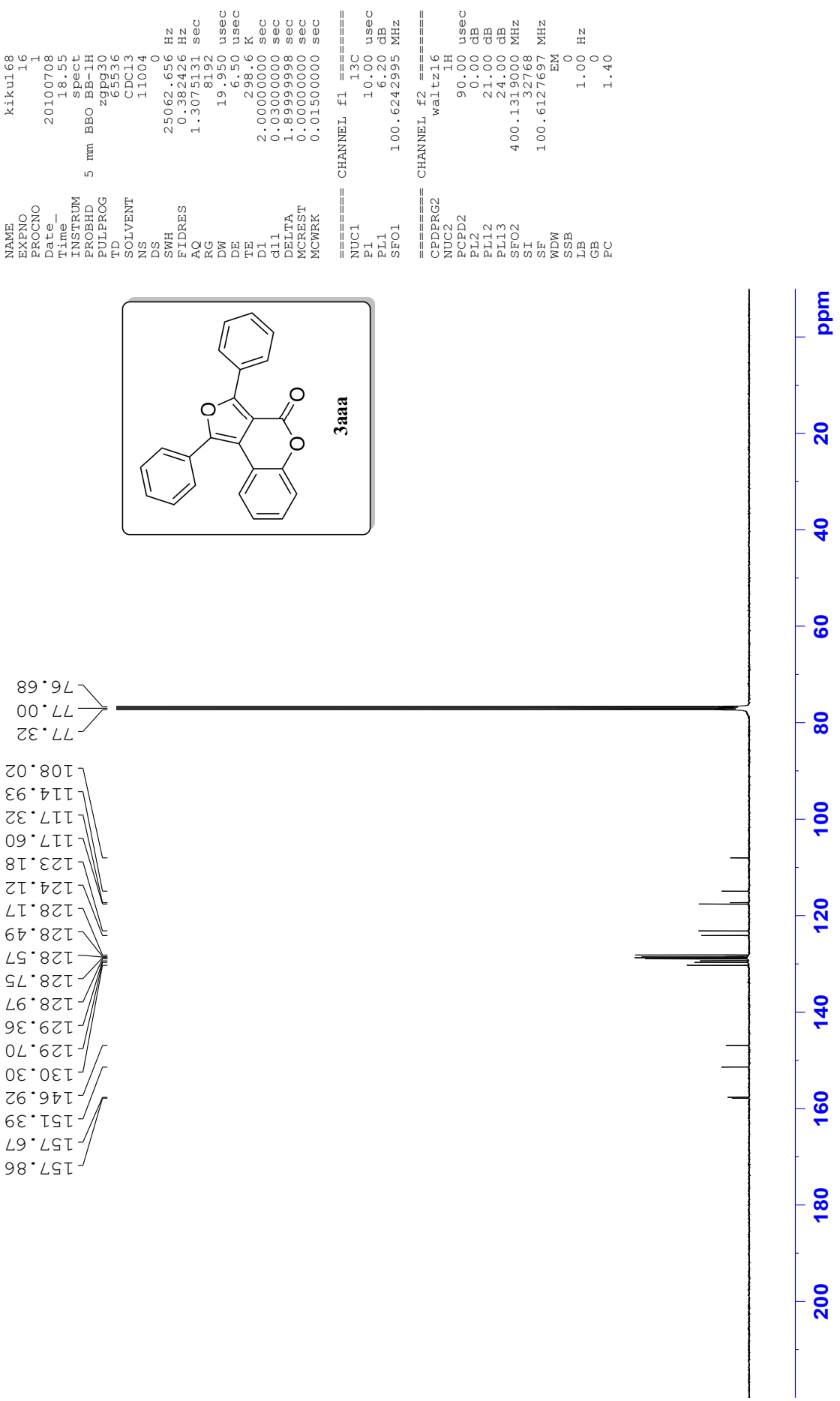


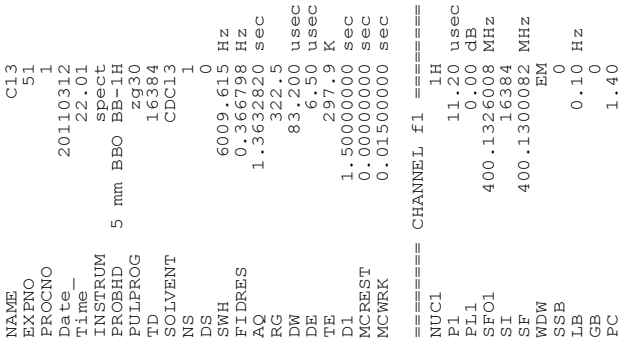


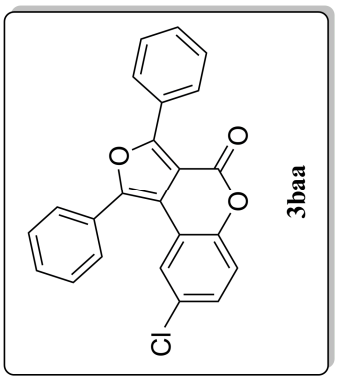
```
NAME                 kiku168
EXPNO                     17
PROCNO                     1
Date_               20100708
Time_                 20.31
INSTRUM                spect
PROBHD     5 mm BBO BB-1H
PULPROG                 zg30
TD                     16384
SOLVENT                CDCl3
NS                         8
DS                         0
SWH                 6009.615 Hz
FIDRES              0.366798 Hz
AQ                  1.3632820 sec
RG                        71.8
DW                       83.200 usec
DE                        6.50 usec
TE                       297.8 K
D1                  1.50000000 sec
MCREST              0.00000000 sec
MCWRK               0.01500000 sec

======== CHANNEL f1 ========
NUC1                       1H
P1                       8.80 usec
PL1                      0.00 dB
SFO1                400.1326008 MHz
SI                     16384
SF                  400.1300086 MHz
WDW                        EM
SSB                         0
LB                       0.10 Hz
GB                          0
PC                       1.40
```

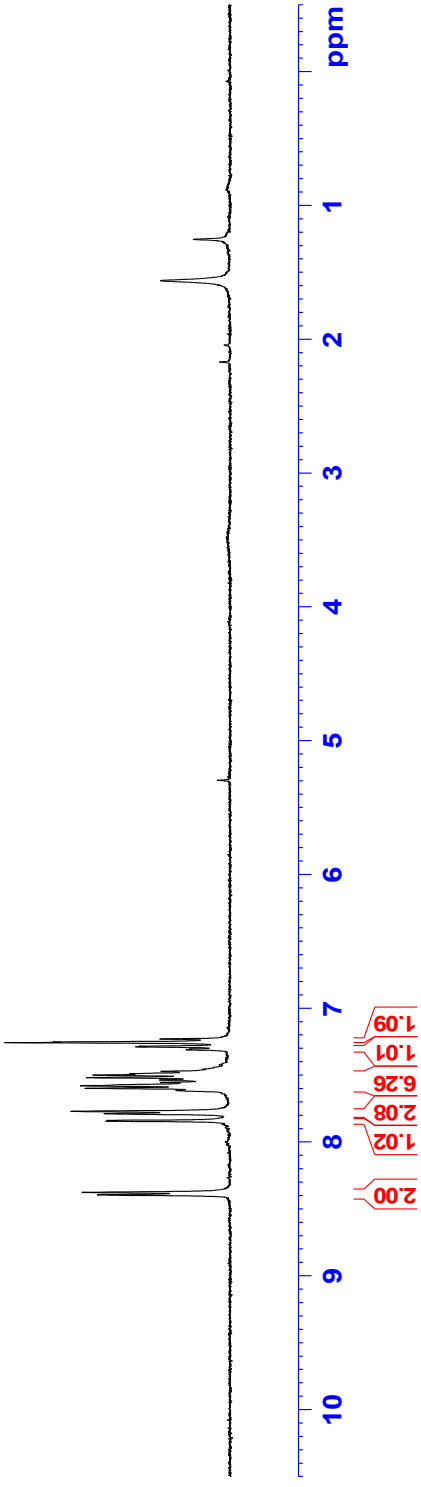


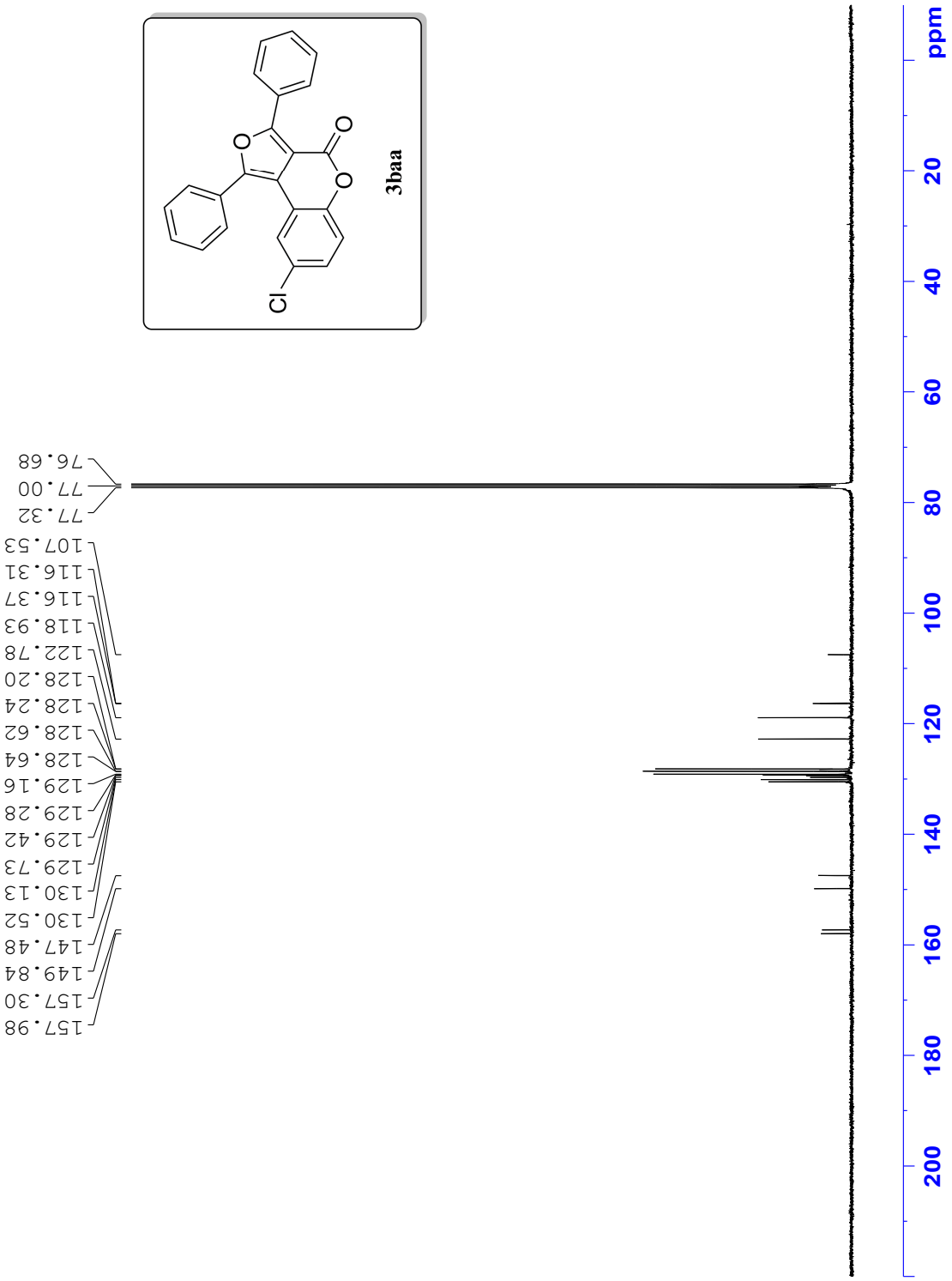


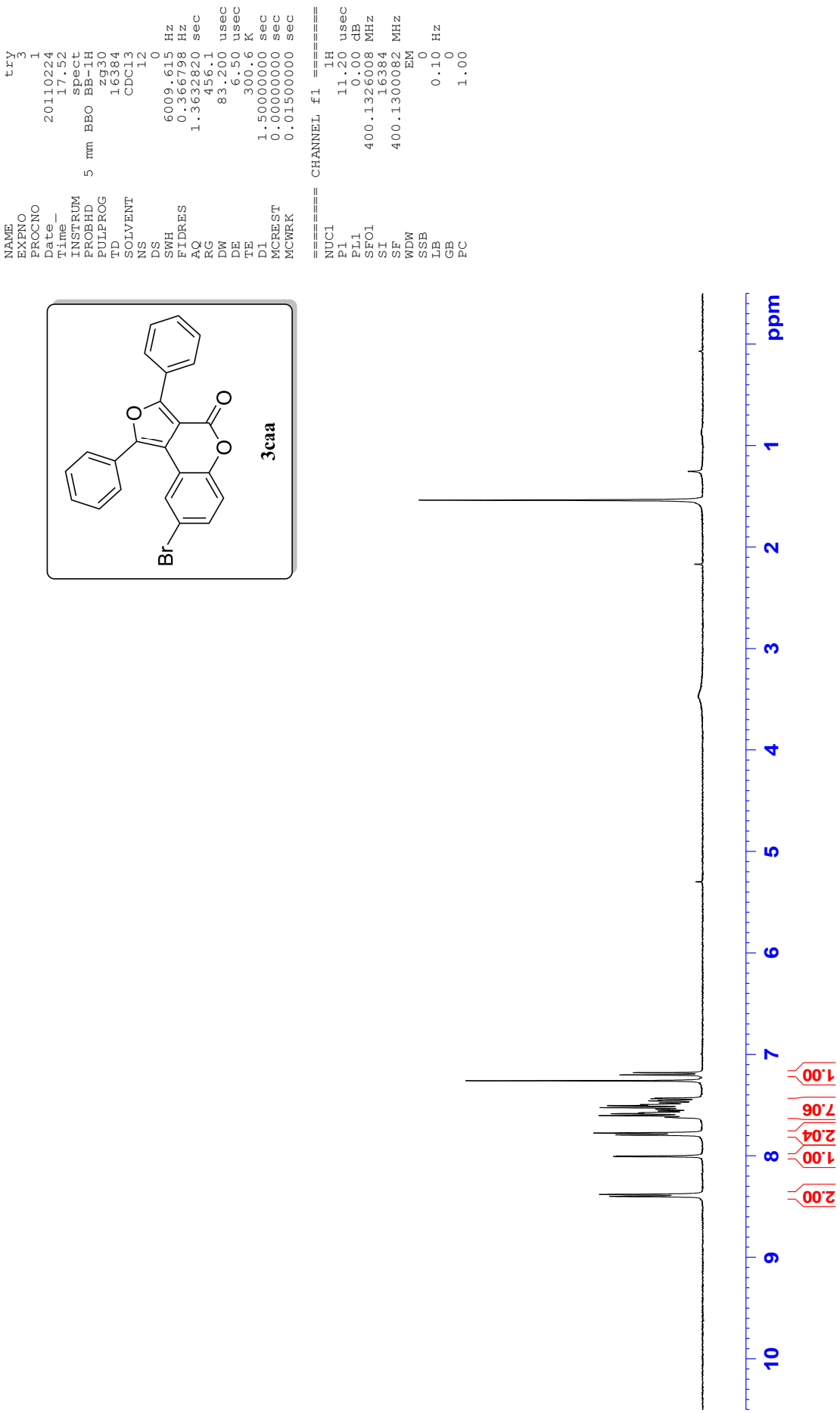


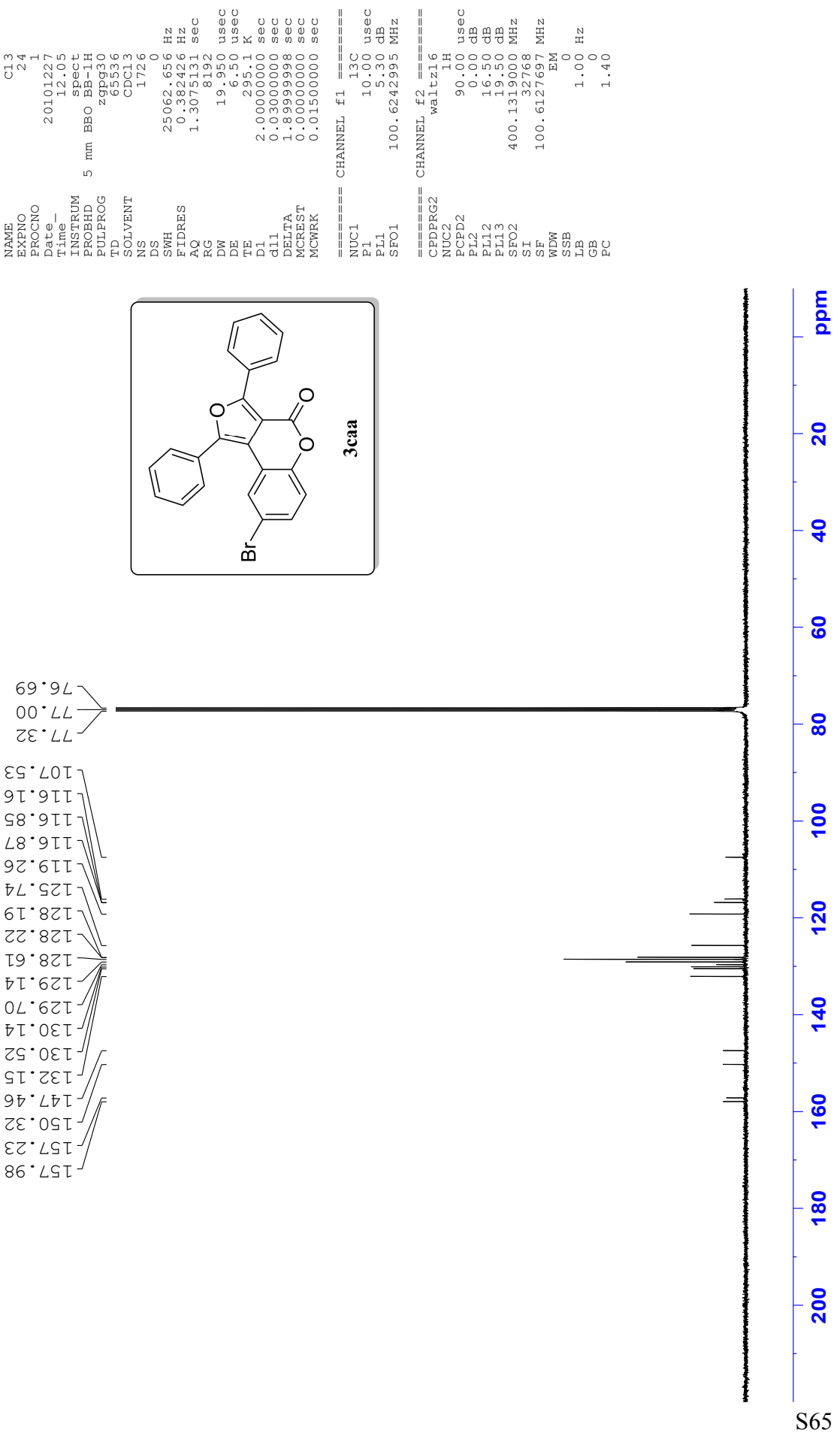


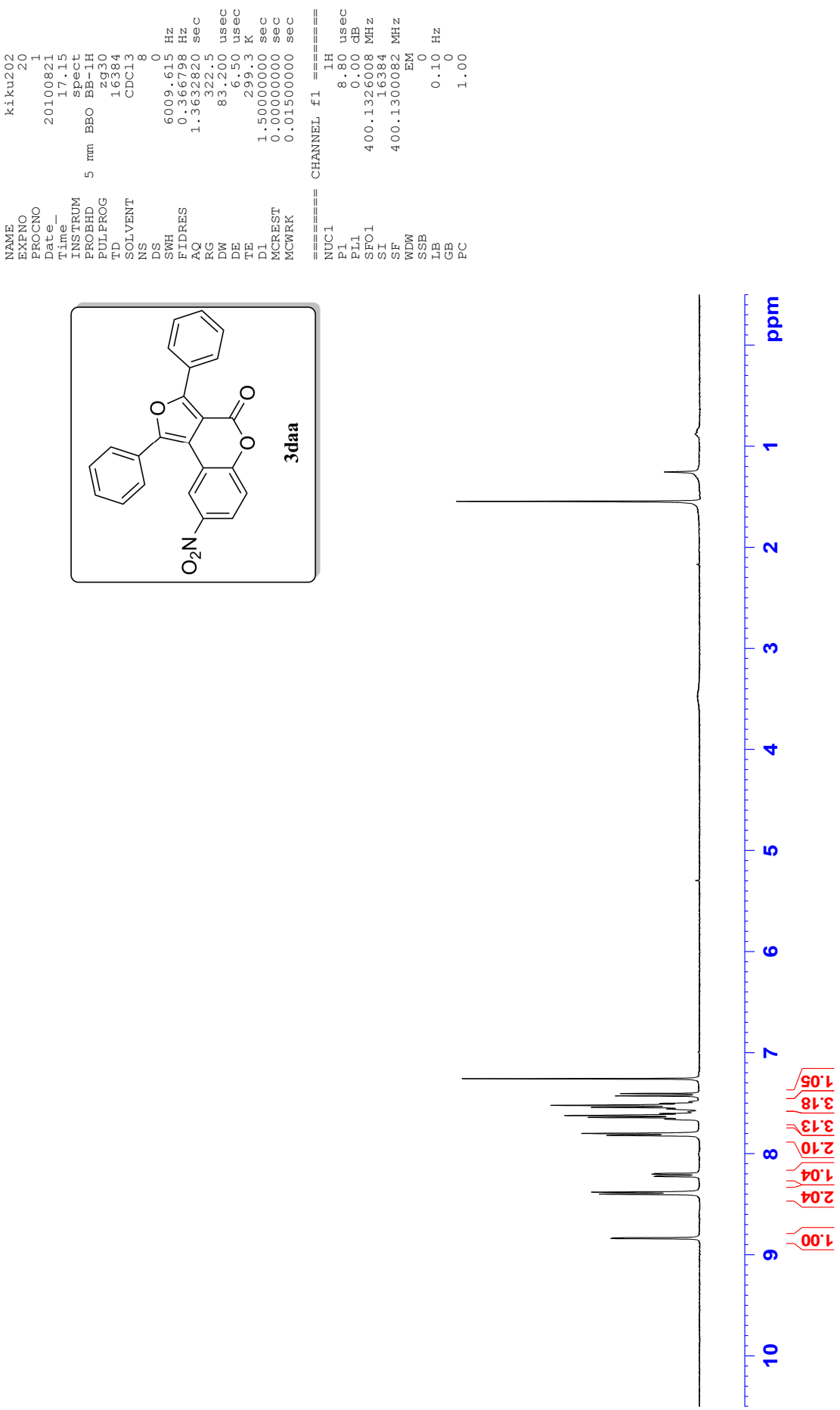


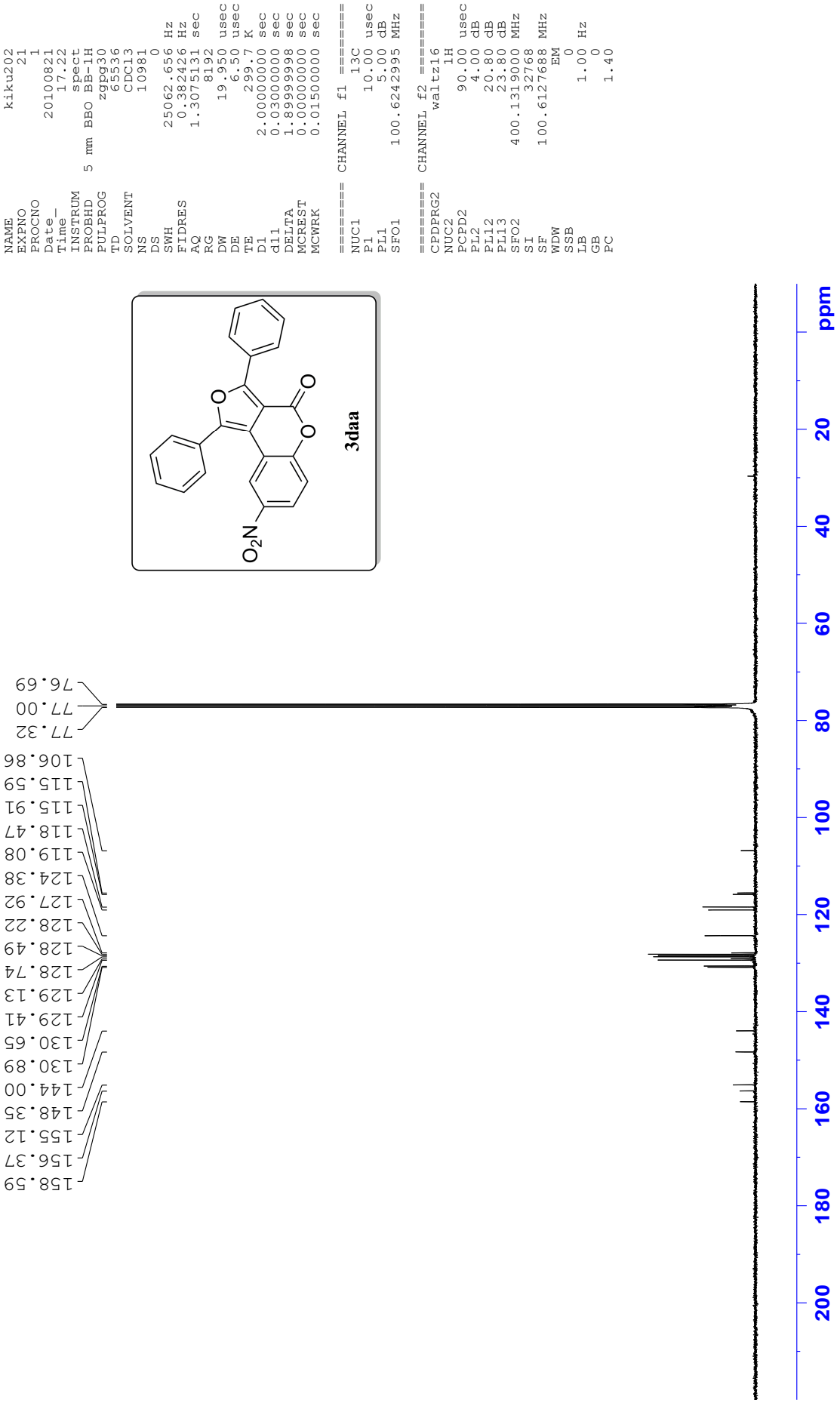


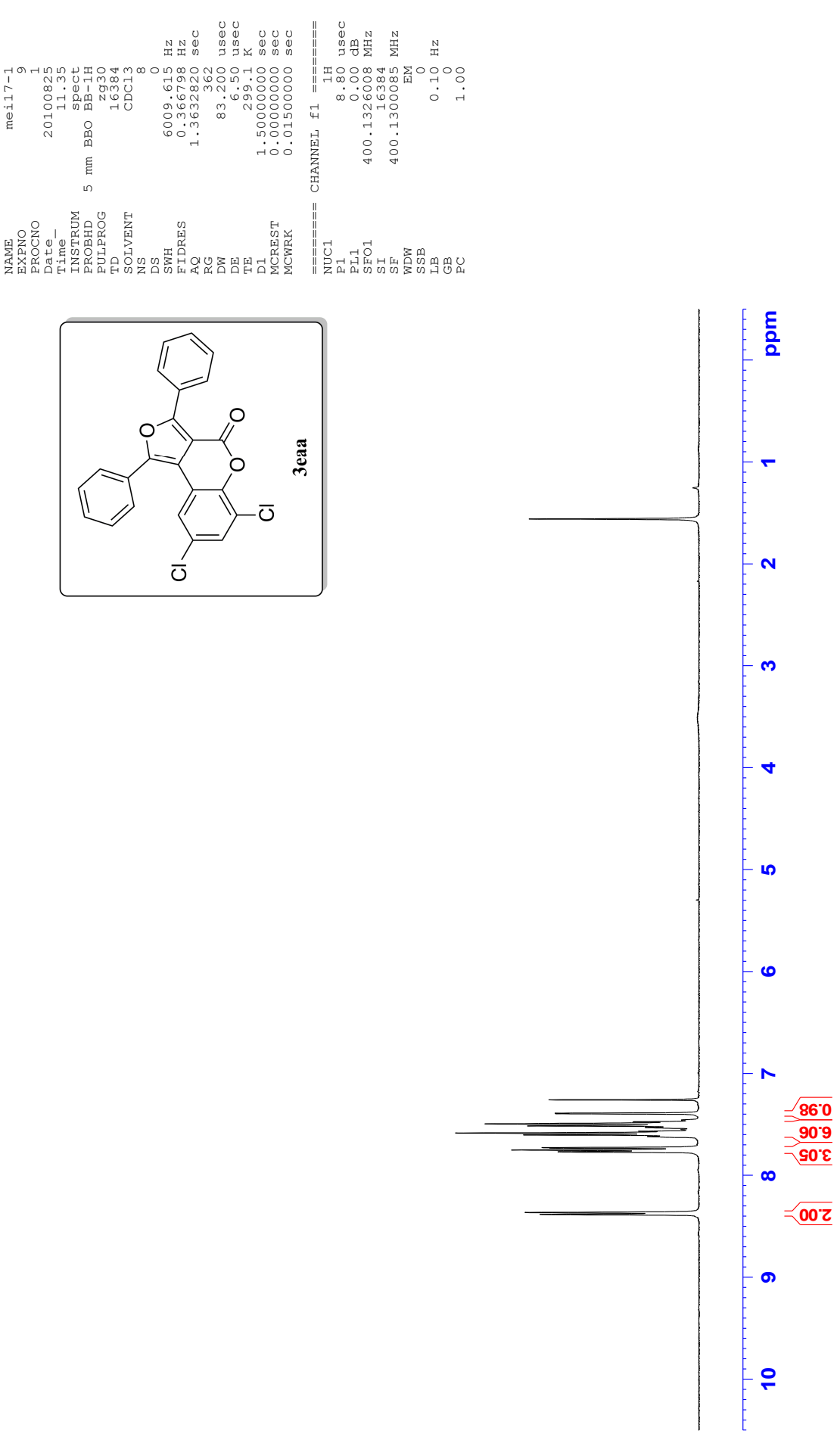

C13
52
1
20110312
22.04
spect
5 mm BBO BB-1H
zgpg30
65536
CDCl3
12909
0
25062.656 Hz
0.382426 Hz
1.3075131 sec
10240
19.950 usec
6.50 usec
298.0 K
2.00000000 sec
0.03000000 sec
1.89999998 sec
0.00000000 sec
0.01500000 sec
CHANNEL f1
13C
10.00 usec
5.30 dB
100.6242995 MHz
CHANNEL f2
waltz16
1H
90.00 usec
0.00 dB
16.50 dB
19.50 dB
400.1319000 MHz
32768
100.6127691 MHz
EM
0
1.00 Hz
0
1.40
3baa
Cl
O
O
O
77.32
77.00
76.68
107.53
116.31
116.37
118.93
122.78
128.20
128.24
128.62
128.64
129.16
129.28
129.42
129.73
130.13
130.52
147.48
149.84
157.30
157.98
ppm
200
180
160
140
120
100
80
60
40
20

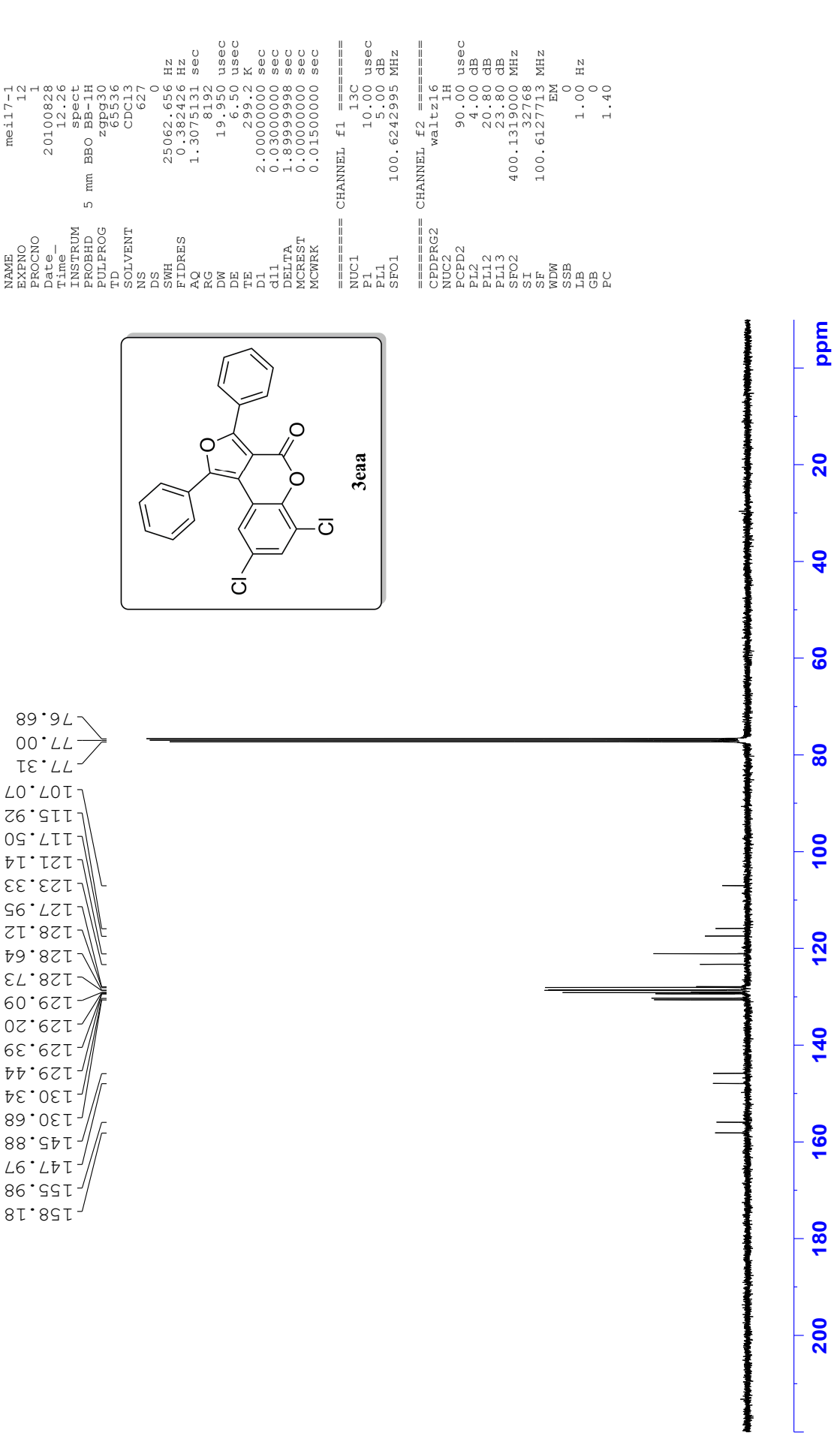


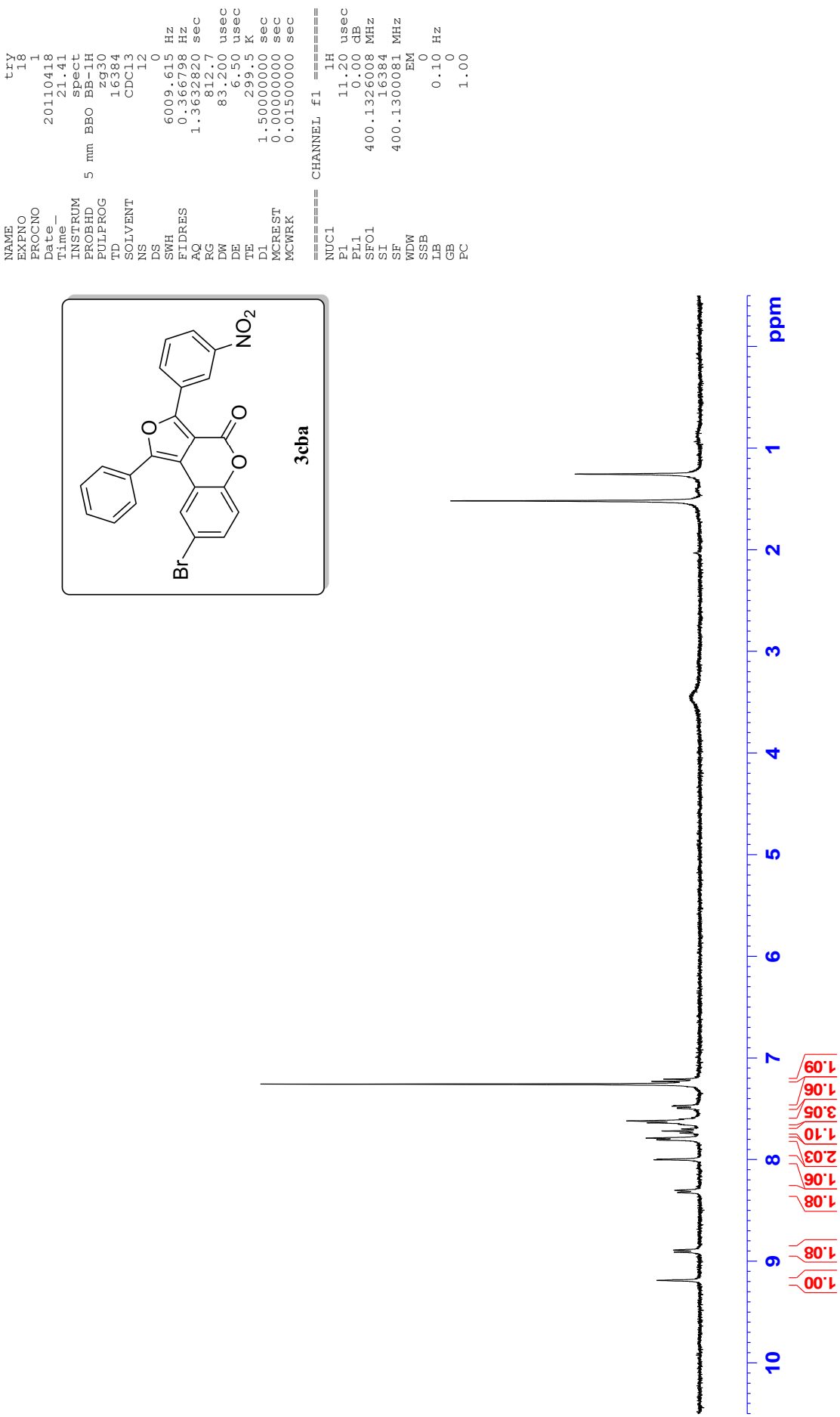


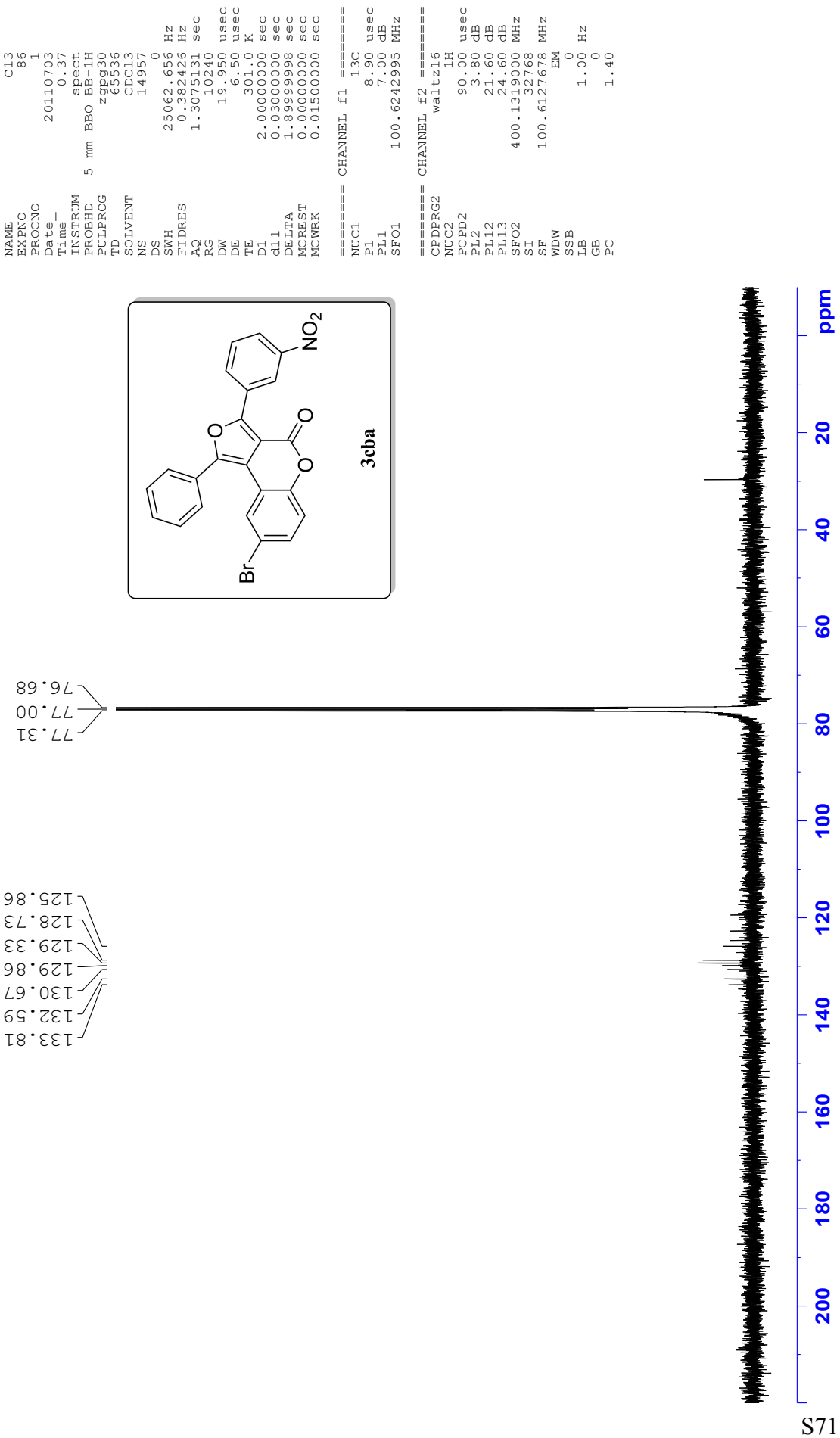


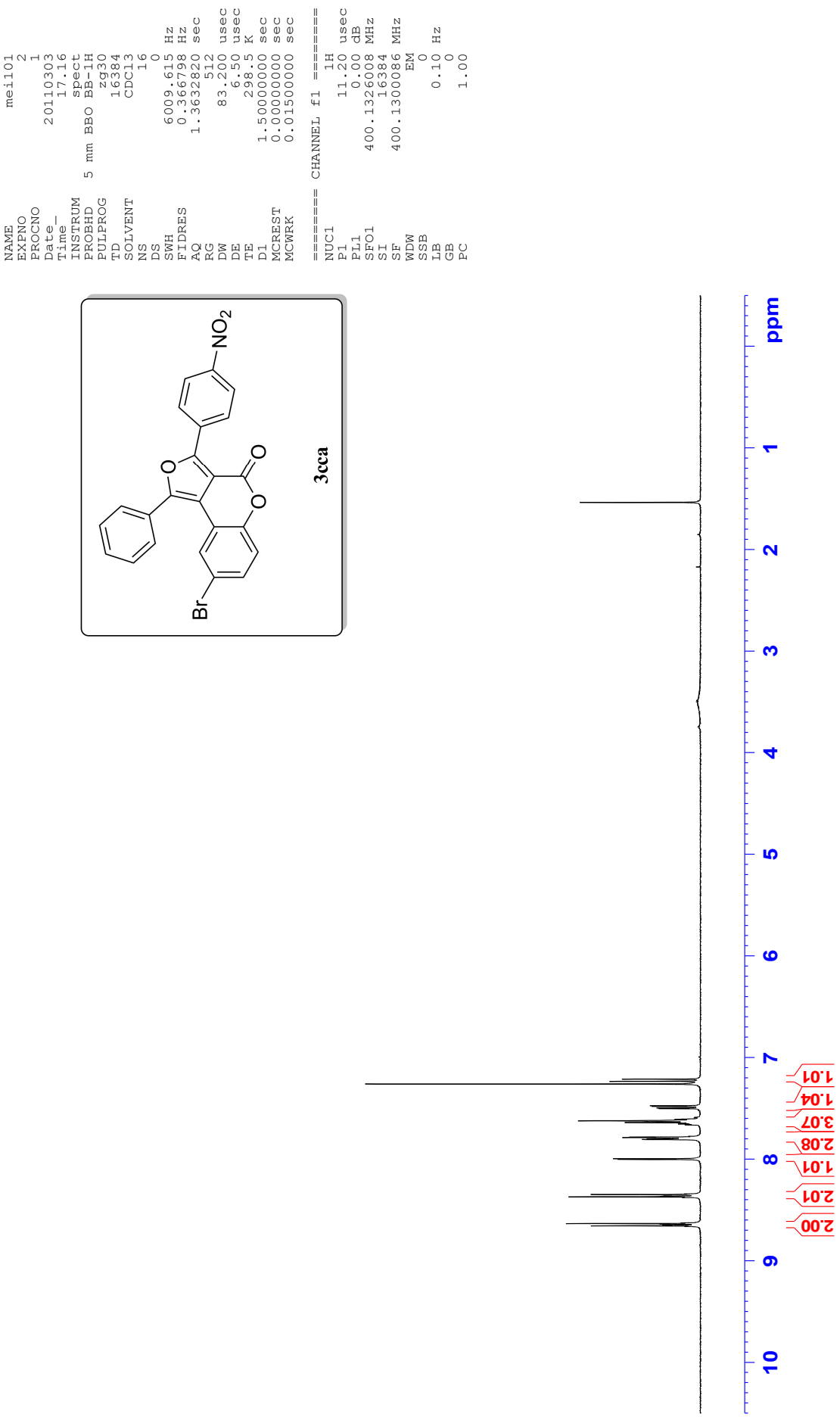


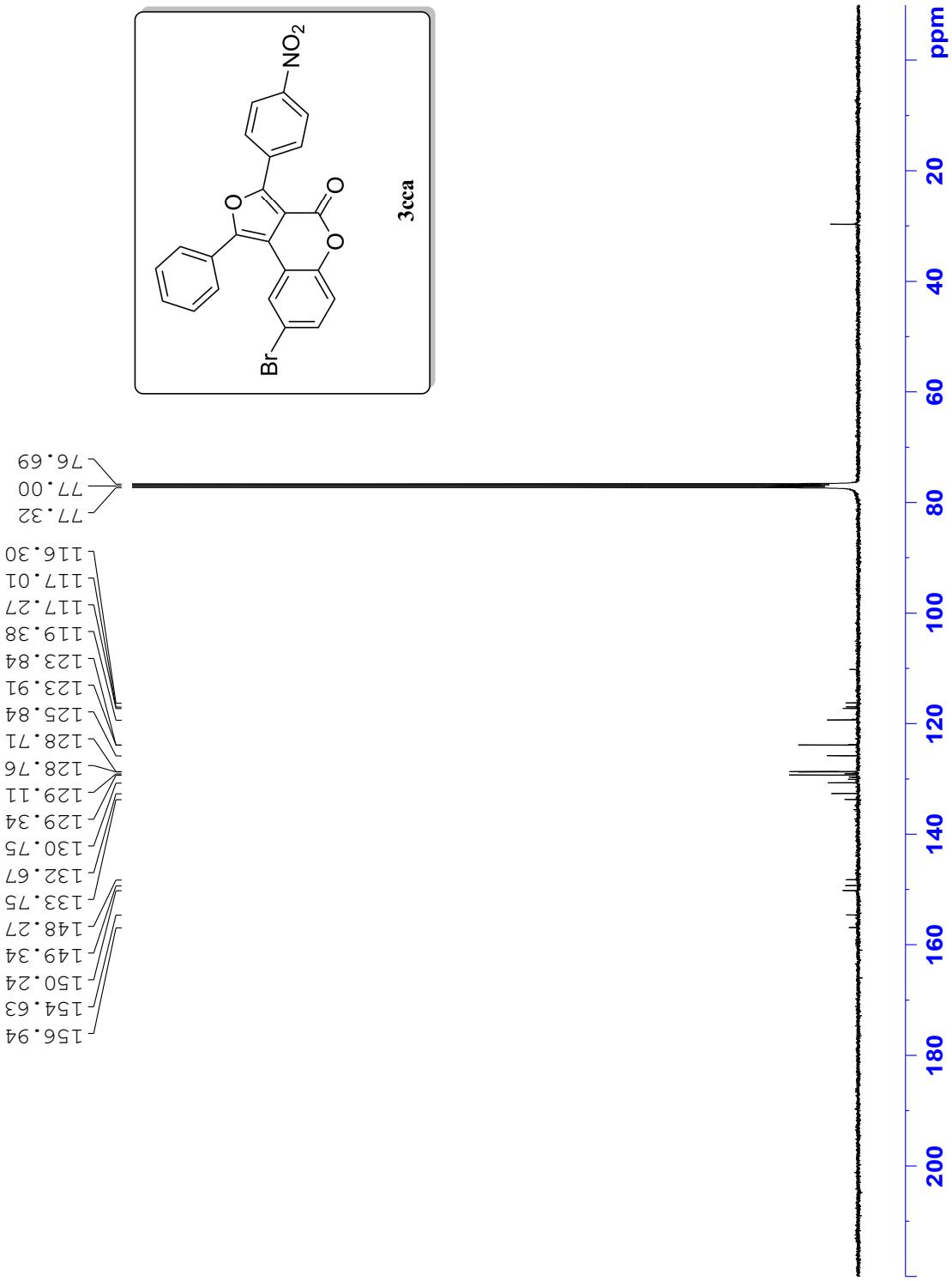


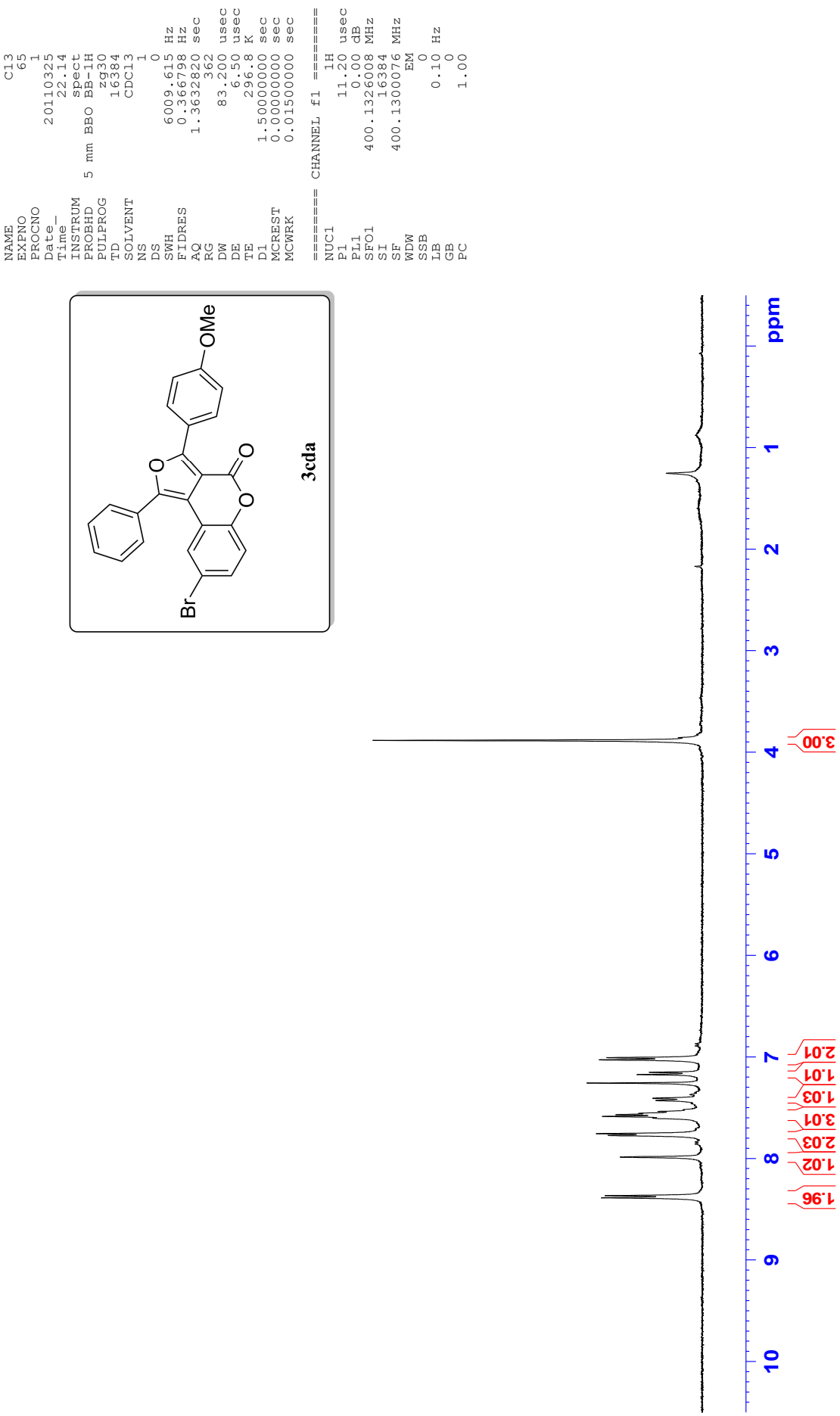


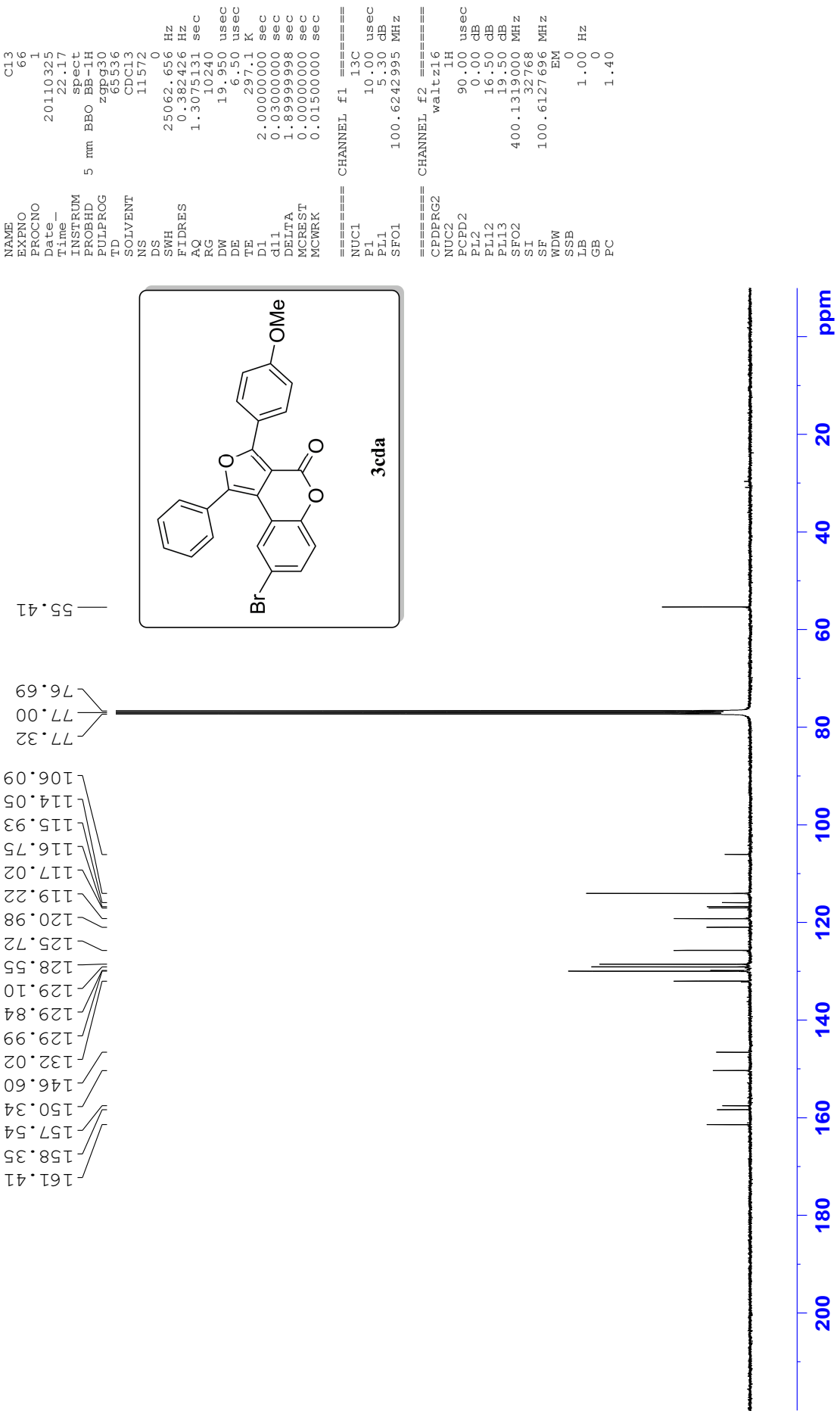


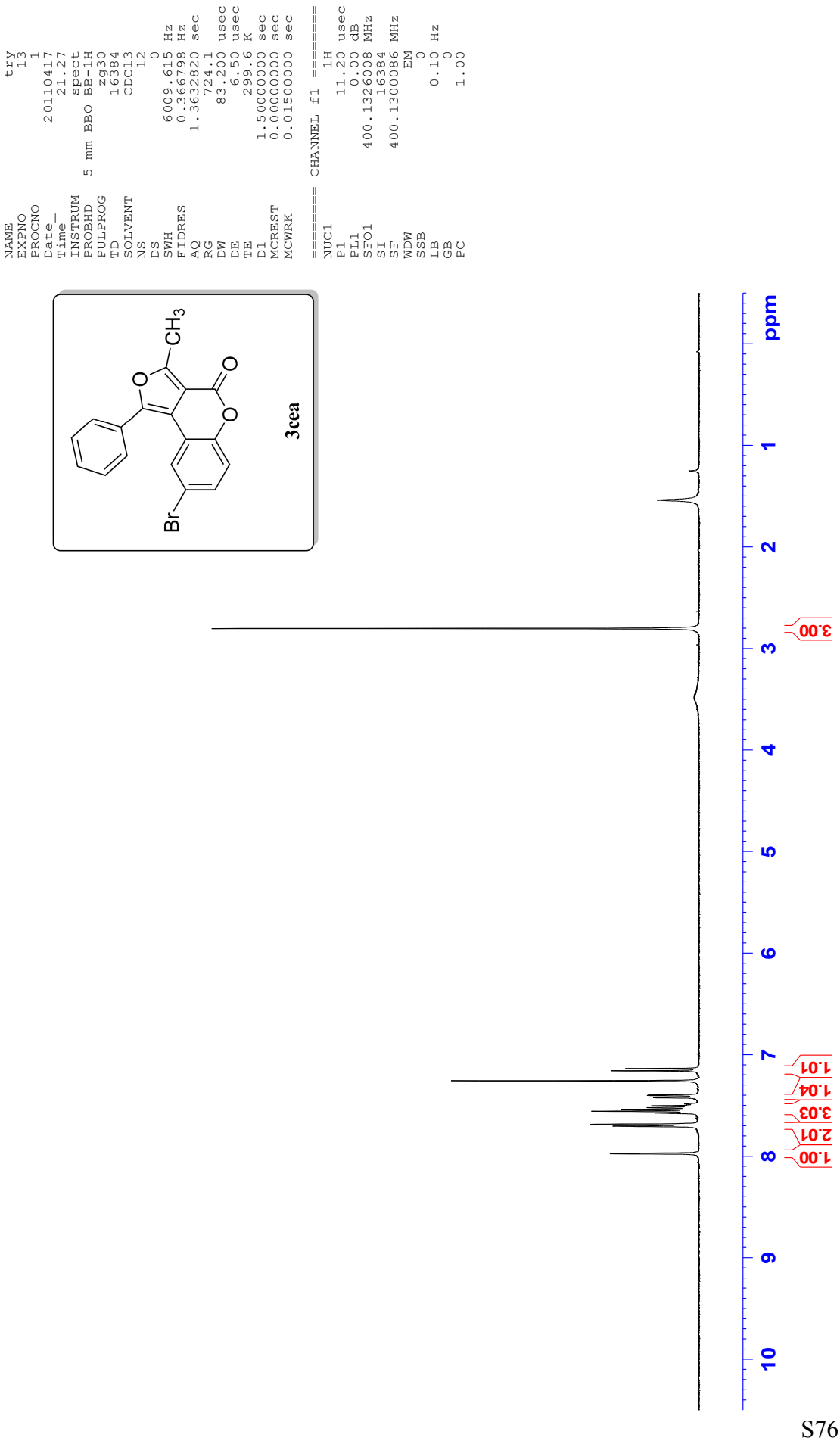


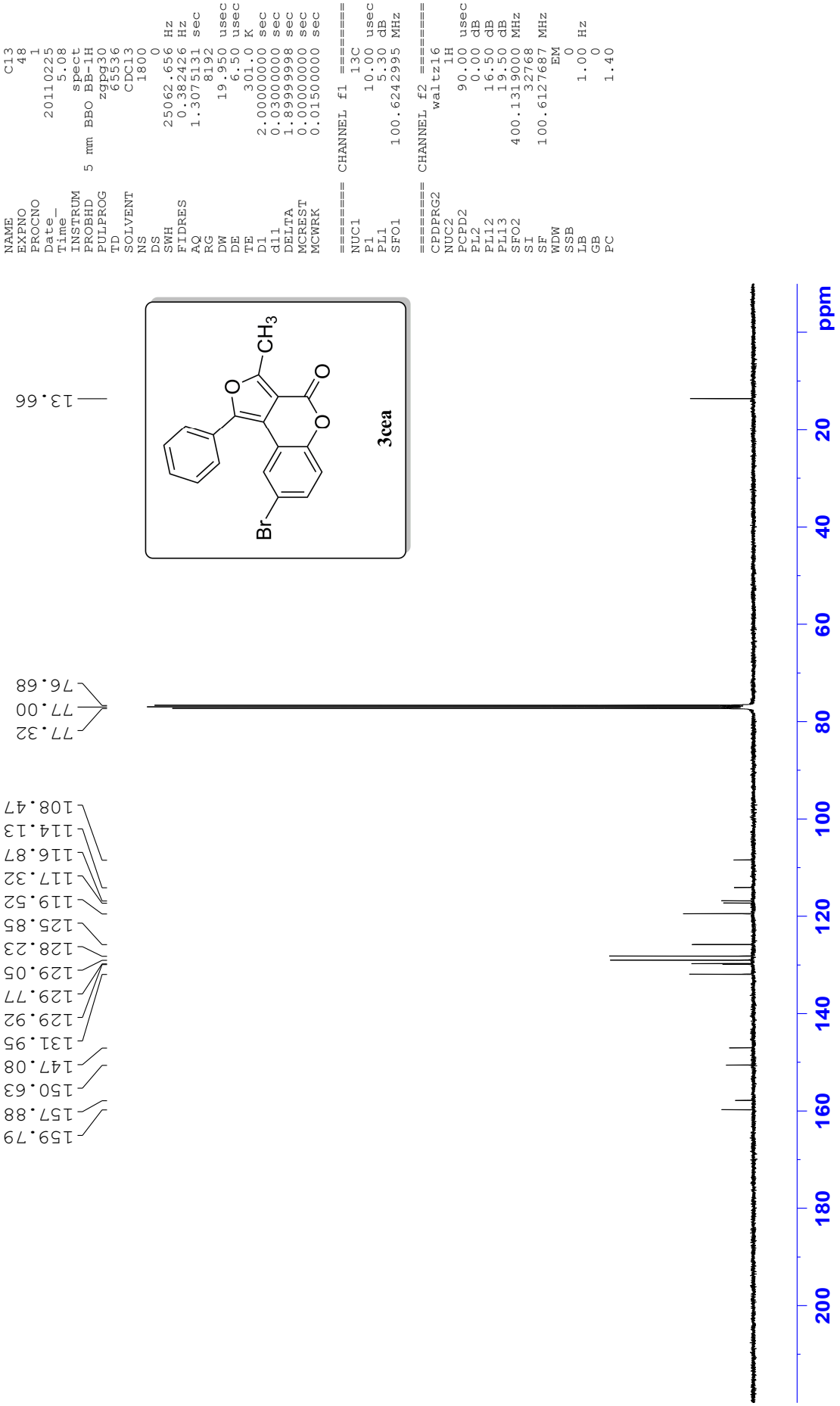




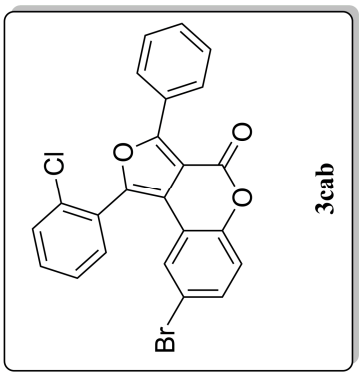

NAME C13
EXPNO 65
PROCNO 1
Date_ 20110325
Time_ 22.14
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 16384
SOLVENT CDC13
NS 1
DS 0
SWH 6009.615 Hz
FIDRES 0.366798 Hz
AQ 1.3632820 sec
RG 362
DW 83.200 usec
DE 6.50 usec
TE 296.8 K
D1 1.50000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 11.20 usec
PL1 0.00 dB
SFO1 400.1326008 MHz
SI 16384
SF 400.1300076 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00
OMe
O
O
O
Br
3cda
ppm
1
2
3
4
5
6
7
8
9
10
3.00
1.96
1.02
2.03
3.01
1.03
1.01
2.01



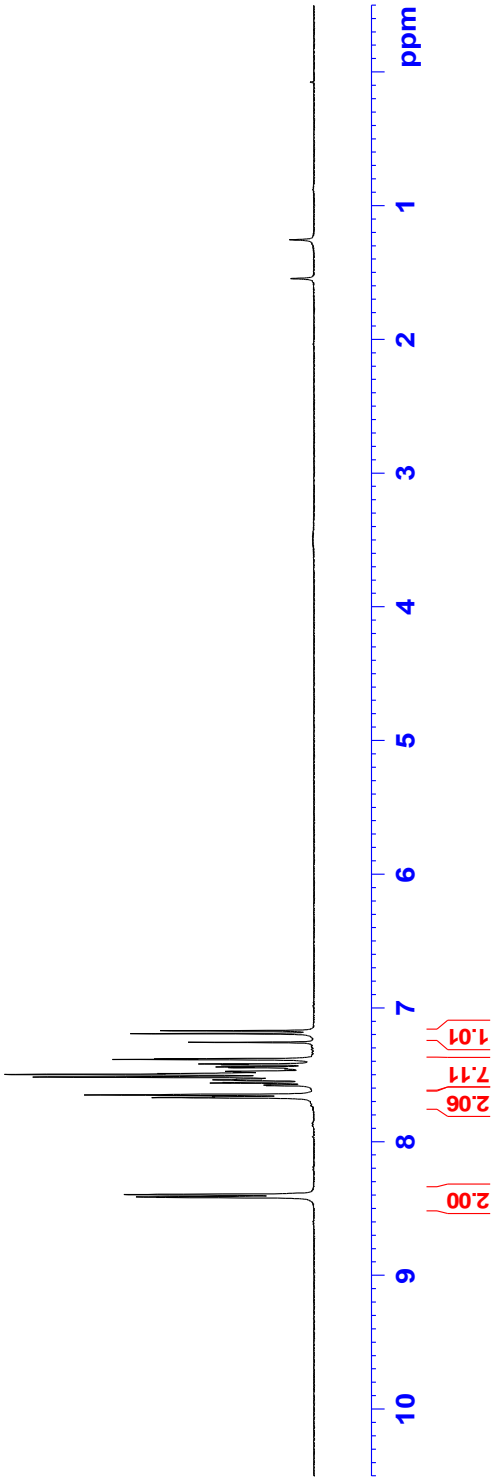

try
13
1
20110417
21.27
spect
5 mm BBO BB-1H
zg30
16384
CDC13
12
0
6009.615 Hz
0.366798 Hz
1.3632820 sec
724.1
83.200 usec
6.50 usec
299.6 K
1.50000000 sec
0.00000000 sec
0.01500000 sec
CHANNEL f1
1H
11.20 usec
0.00 dB
400.1326008 MHz
16384
400.1300086 MHz
EM
0
0.10 Hz
0
1.00
NAME
EXPNO
PROCNO
Date_
Time_
INSTRUM
PROBHD
PULPROG
TD
SOLVENT
NS
DS
SWH
FIDRES
AQ
RG
DW
DE
TE
D1
MCREST
MCWRK
NUC1
P1
PL1
SFO1
SI
SF
WDW
SSB
LB
GB
PC
3cea
Br
CH3
O
O
O
ppm
1
2
3
4
5
6
7
8
9
10
3.00
1.00
2.01
3.03
1.04
1.01

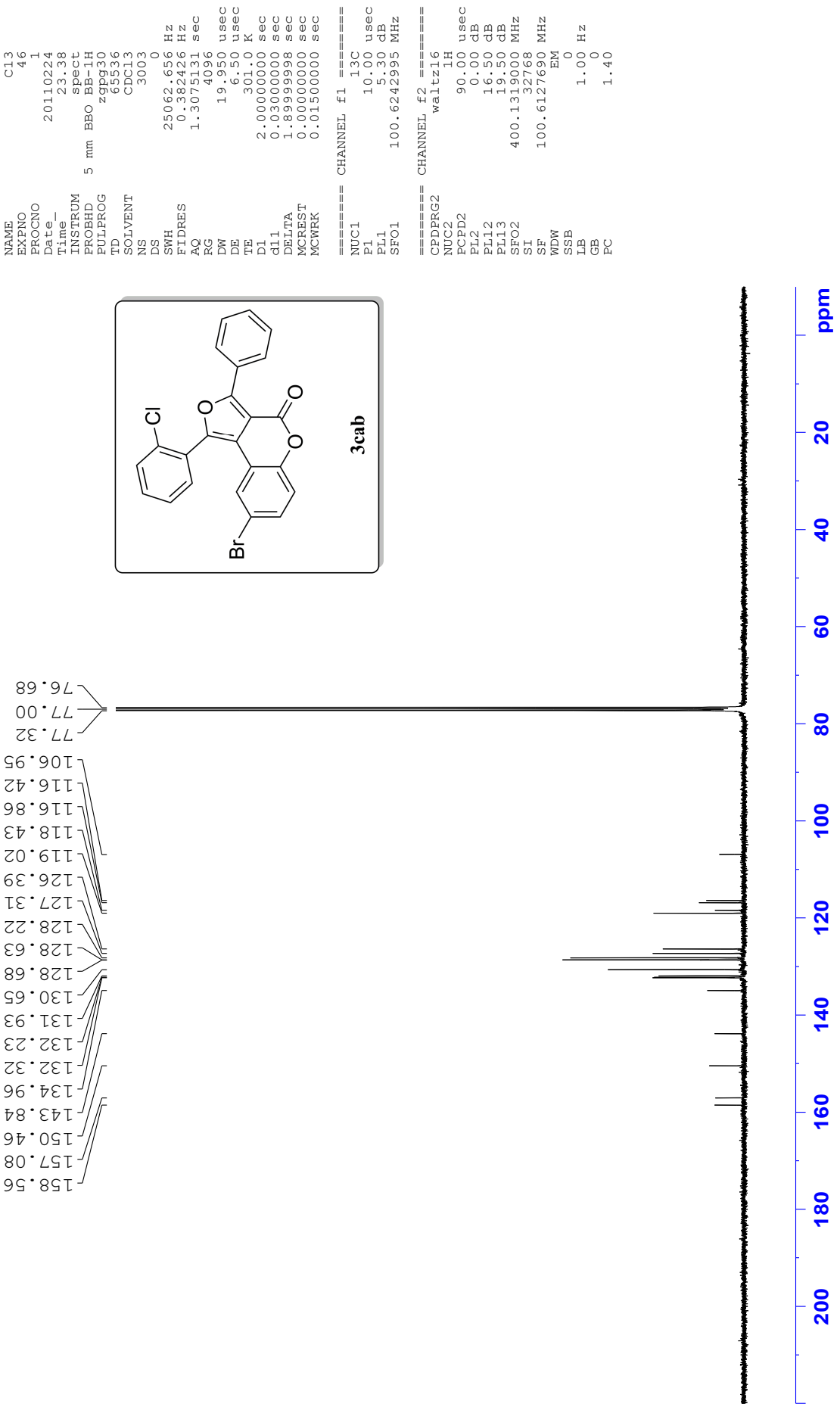

13.66
77.32
77.00
76.68
108.47
114.13
116.87
117.32
119.52
125.85
128.23
129.05
129.77
129.92
131.95
147.08
150.63
157.88
159.79
3cea
Br
CH3
O
O
O
ppm
200
180
160
140
120
100
80
60
40
20

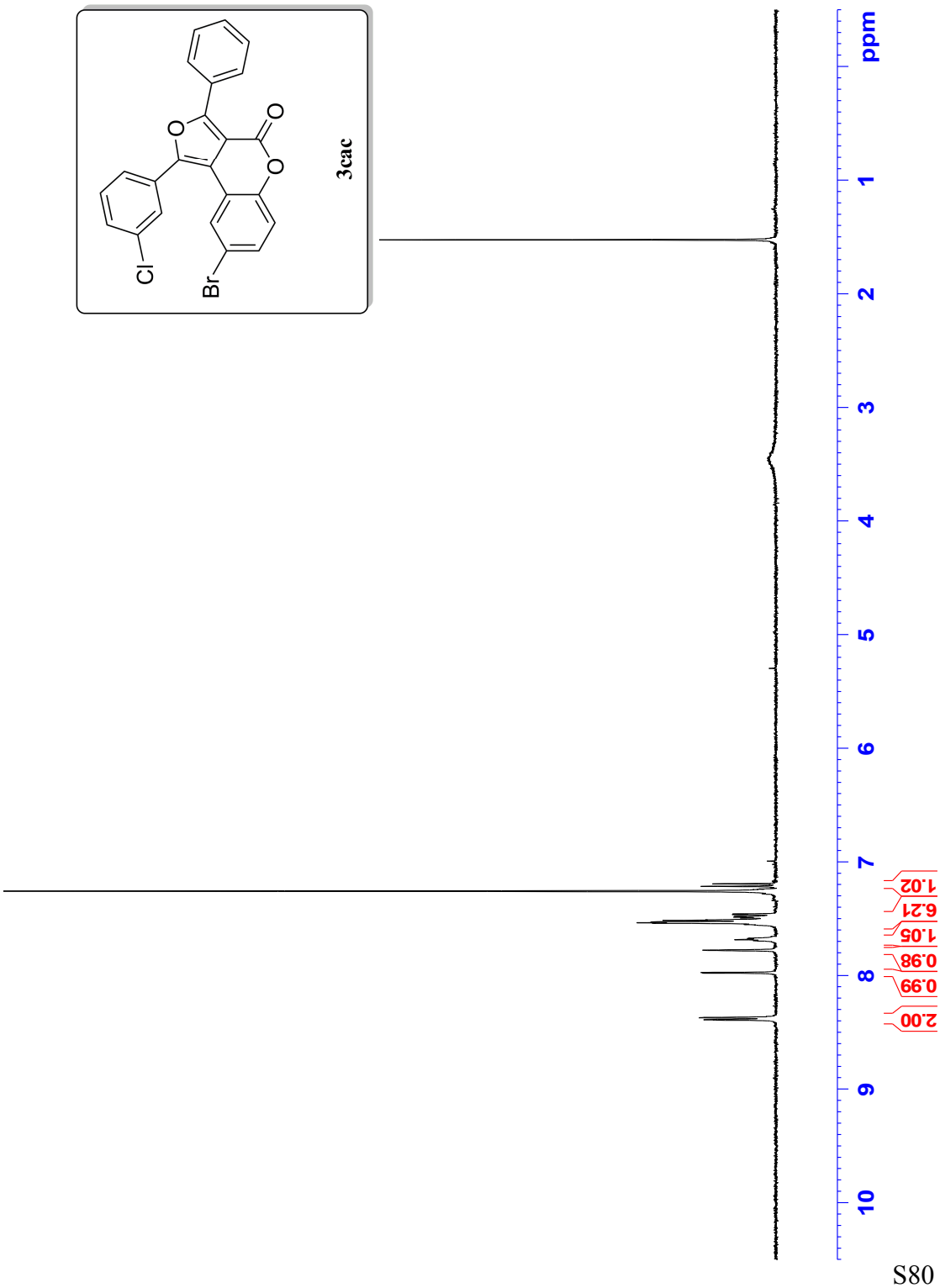
```
NAME                 try
EXPNO                 27
PROCNO                 1
Date_           20110425
Time_               12.12
INSTRUM              spect
PROBHD     5 mm BBO BB-1H
PULPROG              zg30
TD                  16384
SOLVENT             CDCl3
NS                     12
DS                      0
SWH                6009.615 Hz
FIDRES             0.366798 Hz
AQ                 1.3632820 sec
RG                       362
DW                  83.200 usec
DE                   6.50 usec
TE                   299.2 K
D1                 1.50000000 sec
MCREST             0.00000000 sec
MCWRK              0.01500000 sec

======== CHANNEL f1 ========
NUC1                     1H
P1                   11.20 usec
PL1                   0.00 dB
SFO1           400.1326008 MHz
SI                  16384
SF             400.1300086 MHz
WDW                     EM
SSB                      0
LB                    0.10 Hz
GB                       0
PC                    1.00
```

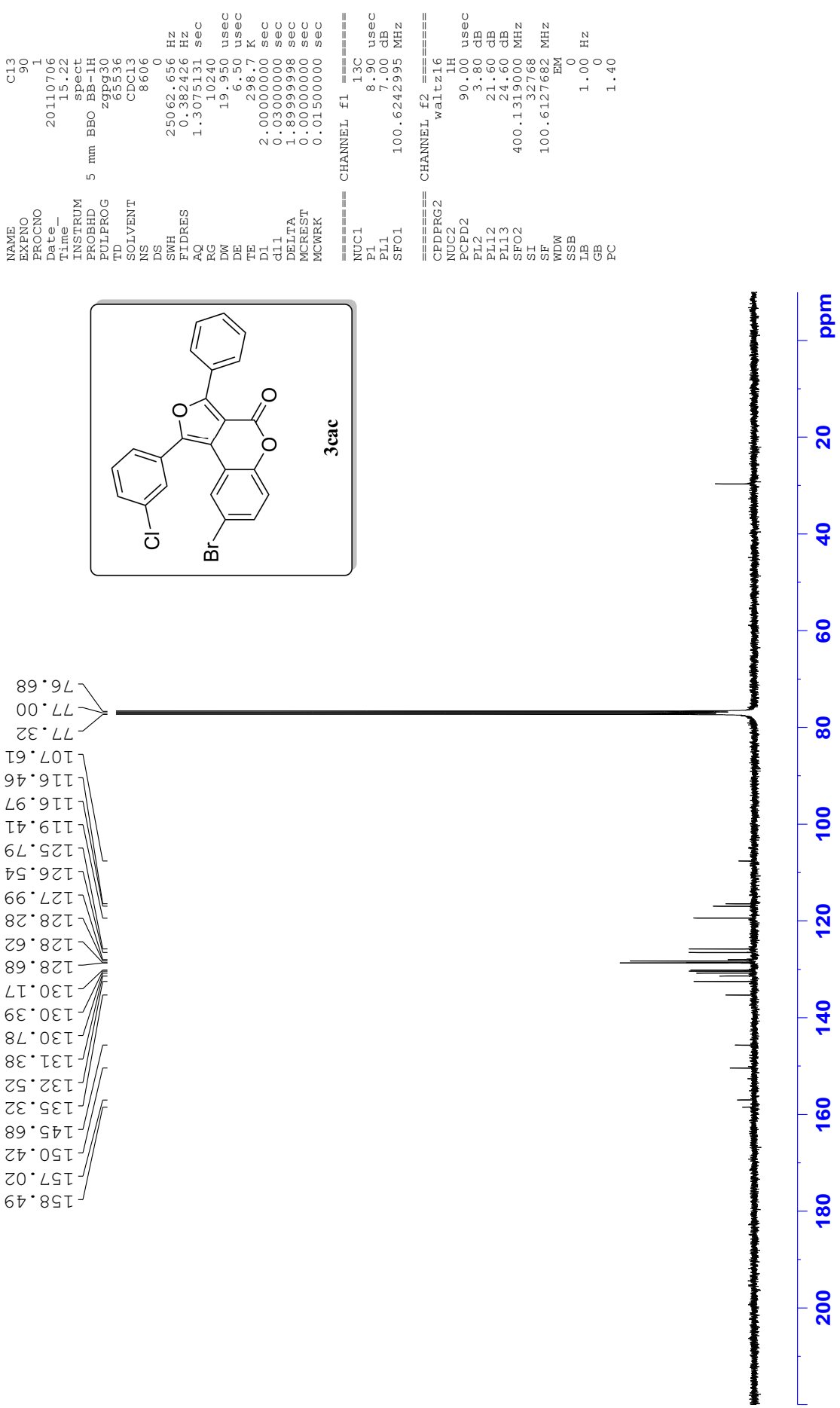


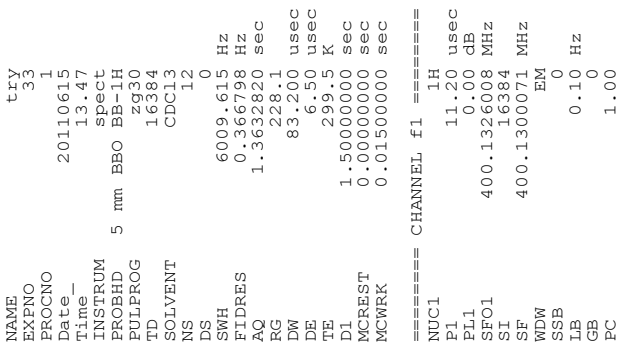
3cab

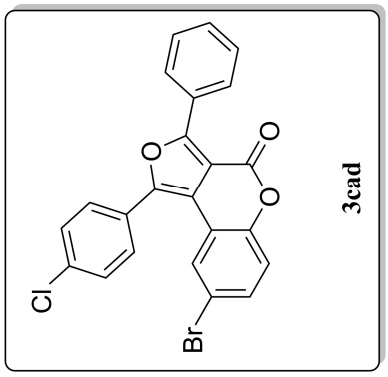


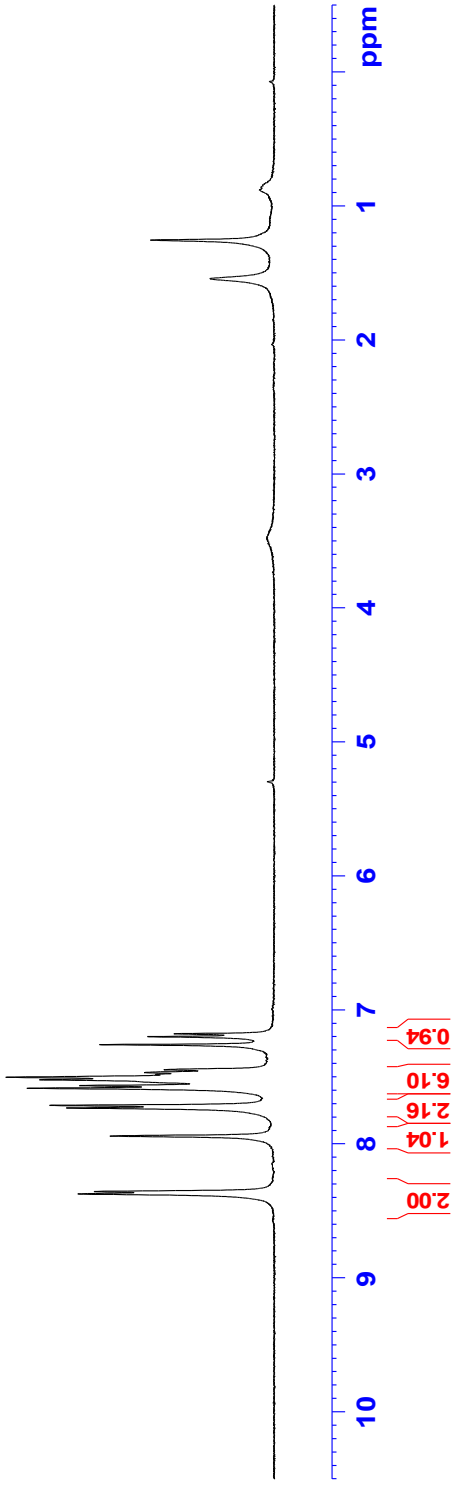


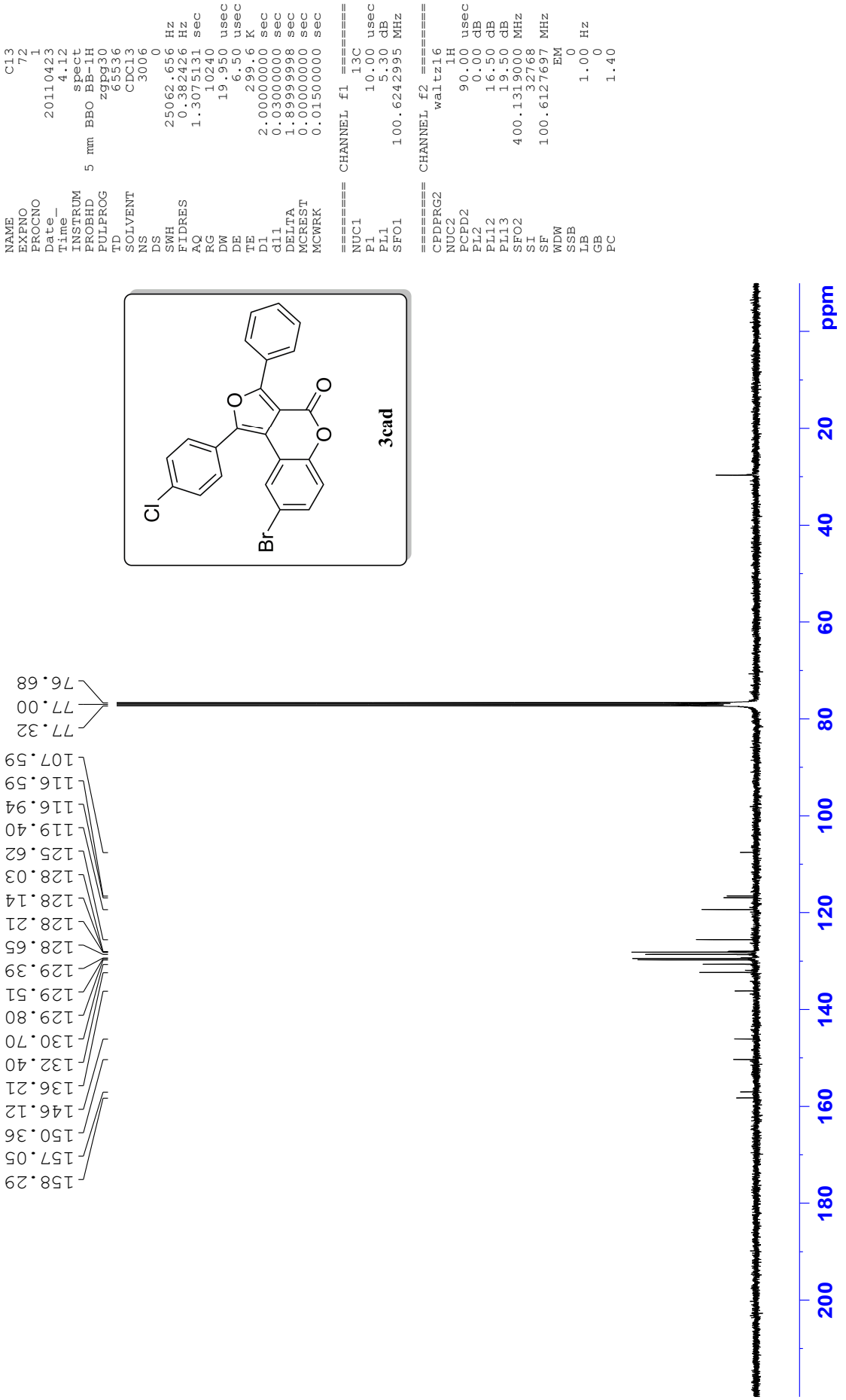






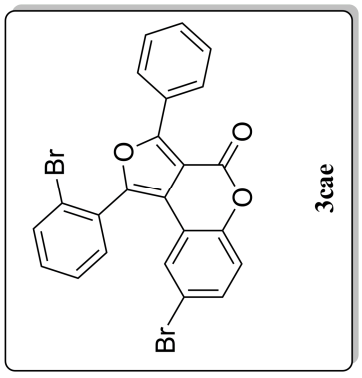


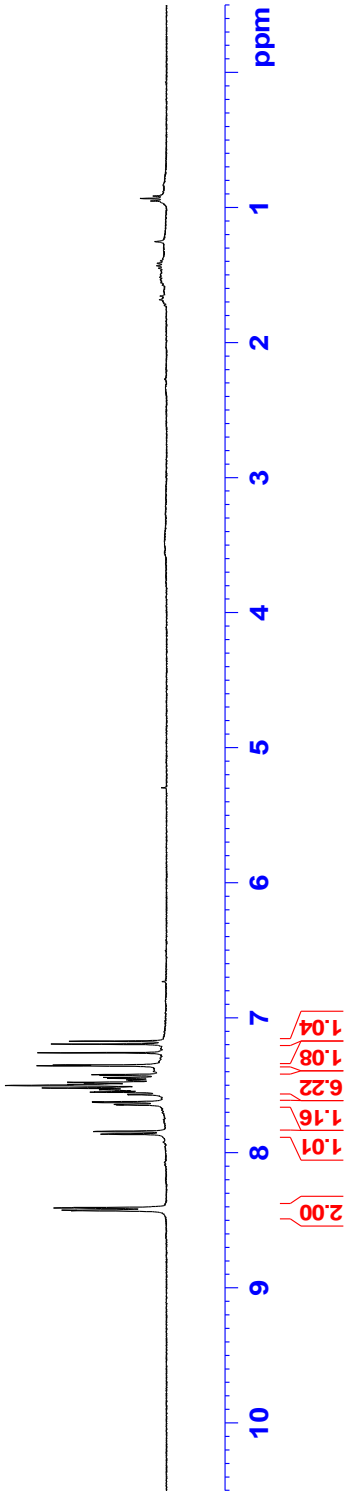


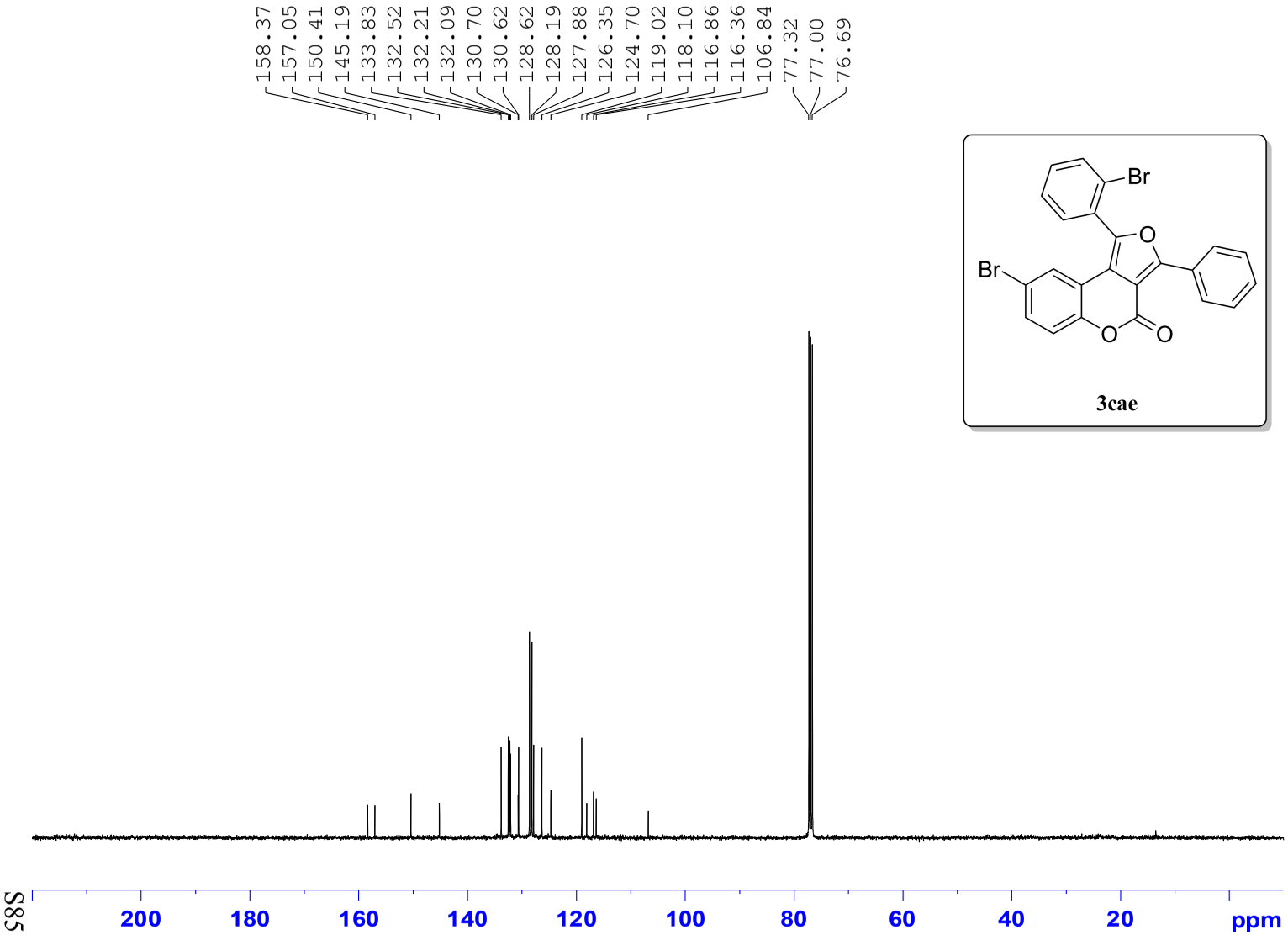



```
NAME                 C13
EXPNO                 72
PROCNO                 1
Date_           20110423
Time_               4.12
INSTRUM             spect
PROBHD   5 mm BBO BB-1H
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                 3006
DS                    0
SWH           25062.656 Hz
FIDRES            0.382426 Hz
AQ                1.3075131 sec
RG                   10240
DW                19.950 usec
DE                 6.50 usec
TE                 299.6 K
D1            2.00000000 sec
d11           0.03000000 sec
DELTA         1.89999998 sec
MCREST        0.00000000 sec
MCWRK         0.01500000 sec

======== CHANNEL f1 ========
NUC1               13C
P1               10.00 usec
PL1               5.30 dB
SFO1        100.6242995 MHz

======== CHANNEL f2 ========
CPDPRG2         waltz16
NUC2                1H
PCPD2            90.00 usec
PL2               0.00 dB
PL12             16.50 dB
PL13             19.50 dB
SFO2        400.1319000 MHz
SI                 32768
SF          100.6127697 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```

```
NAME                try
EXPNO                14
PROCNO                1
Date_          20110417
Time_              21.30
INSTRUM            spect
PROBHD   5 mm BBO BB-1H
PULPROG             zg30
TD                 16384
SOLVENT            CDCl3
NS                    12
DS                     0
SWH             6009.615 Hz
FIDRES          0.366798 Hz
AQ              1.363820 sec
RG                 456.1
DW                83.200 usec
DE                 6.50 usec
TE                299.6 K
D1              1.50000000 sec
MCREST          0.00000000 sec
MCWRK           0.01500000 sec

========== CHANNEL f1 ==========
NUC1                1H
P1                 11.20 usec
PL1                 0.00 dB
SFO1        400.1326008 MHz
SI                 16384
SF          400.1300086 MHz
WDW                   EM
SSB                    0
LB                  0.10 Hz
GB                     0
PC                  1.00
```

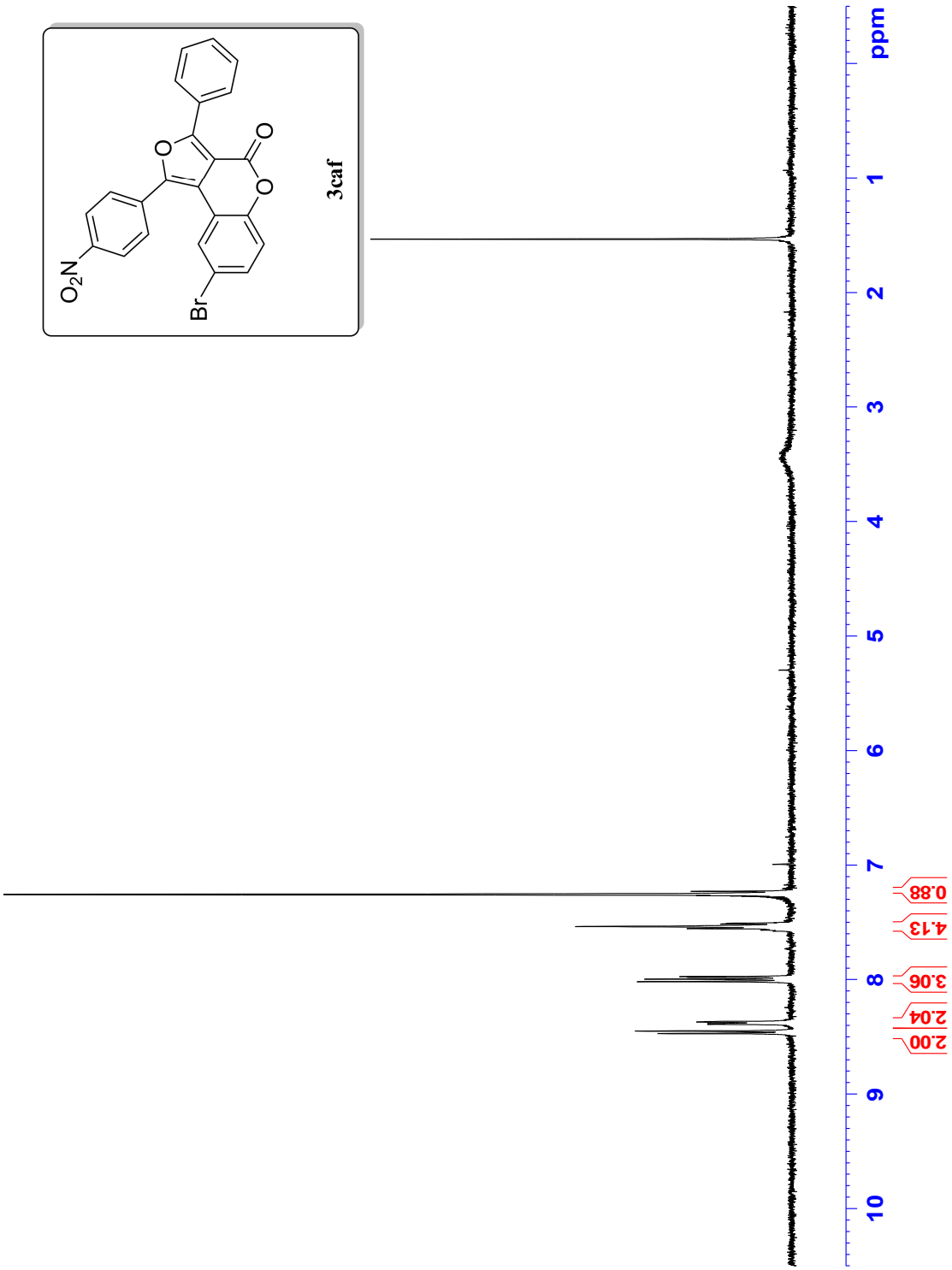


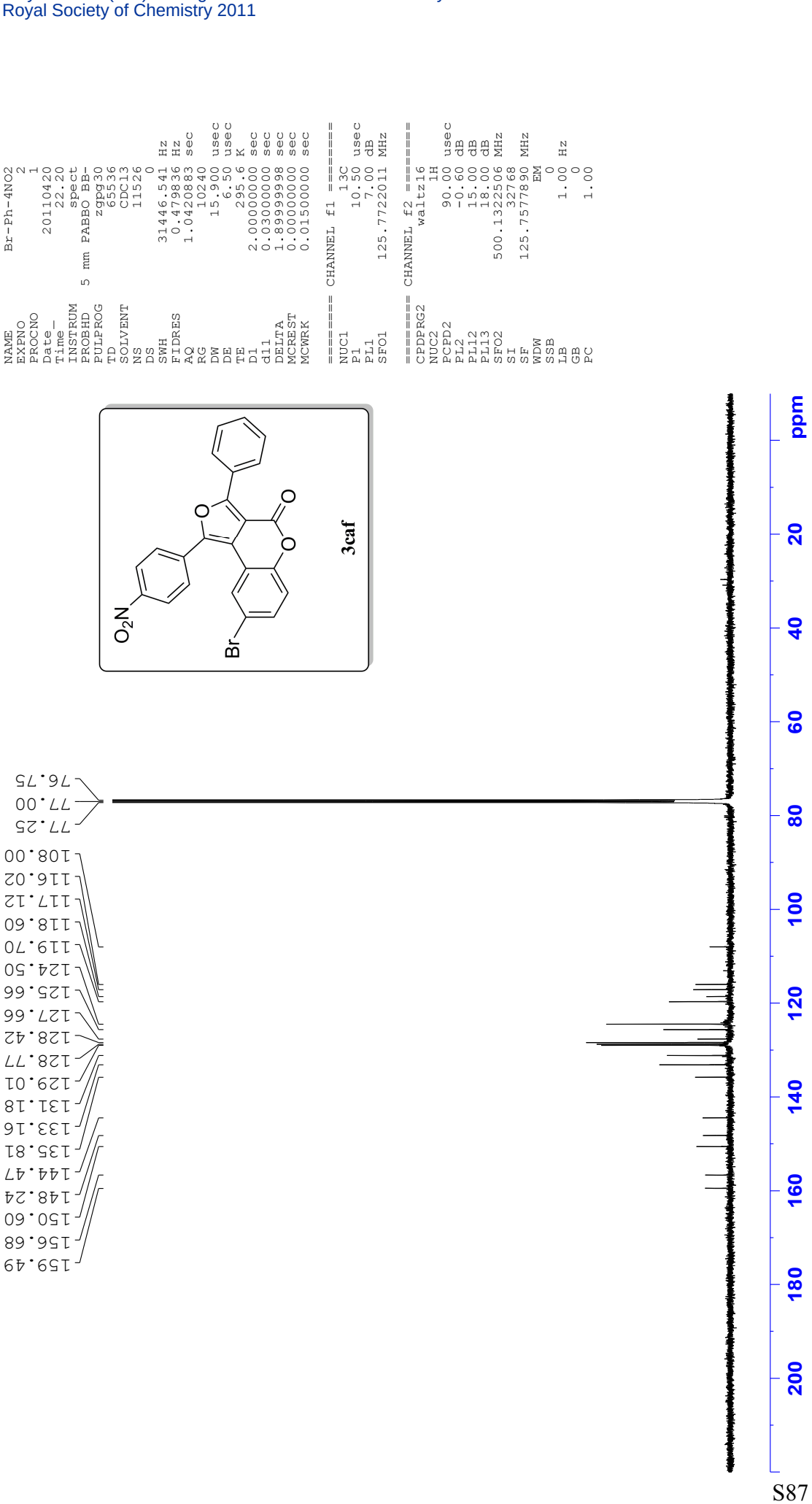


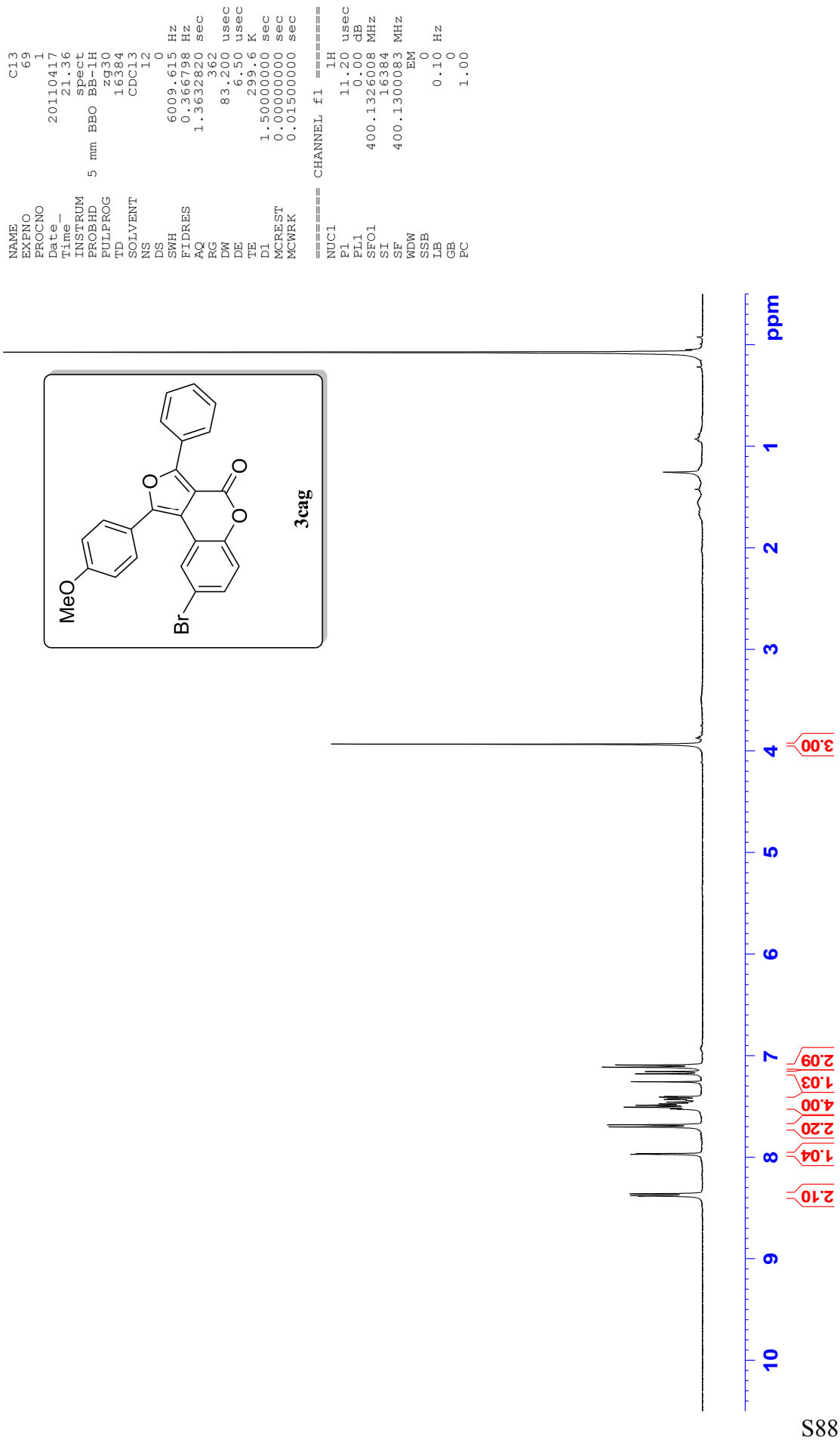


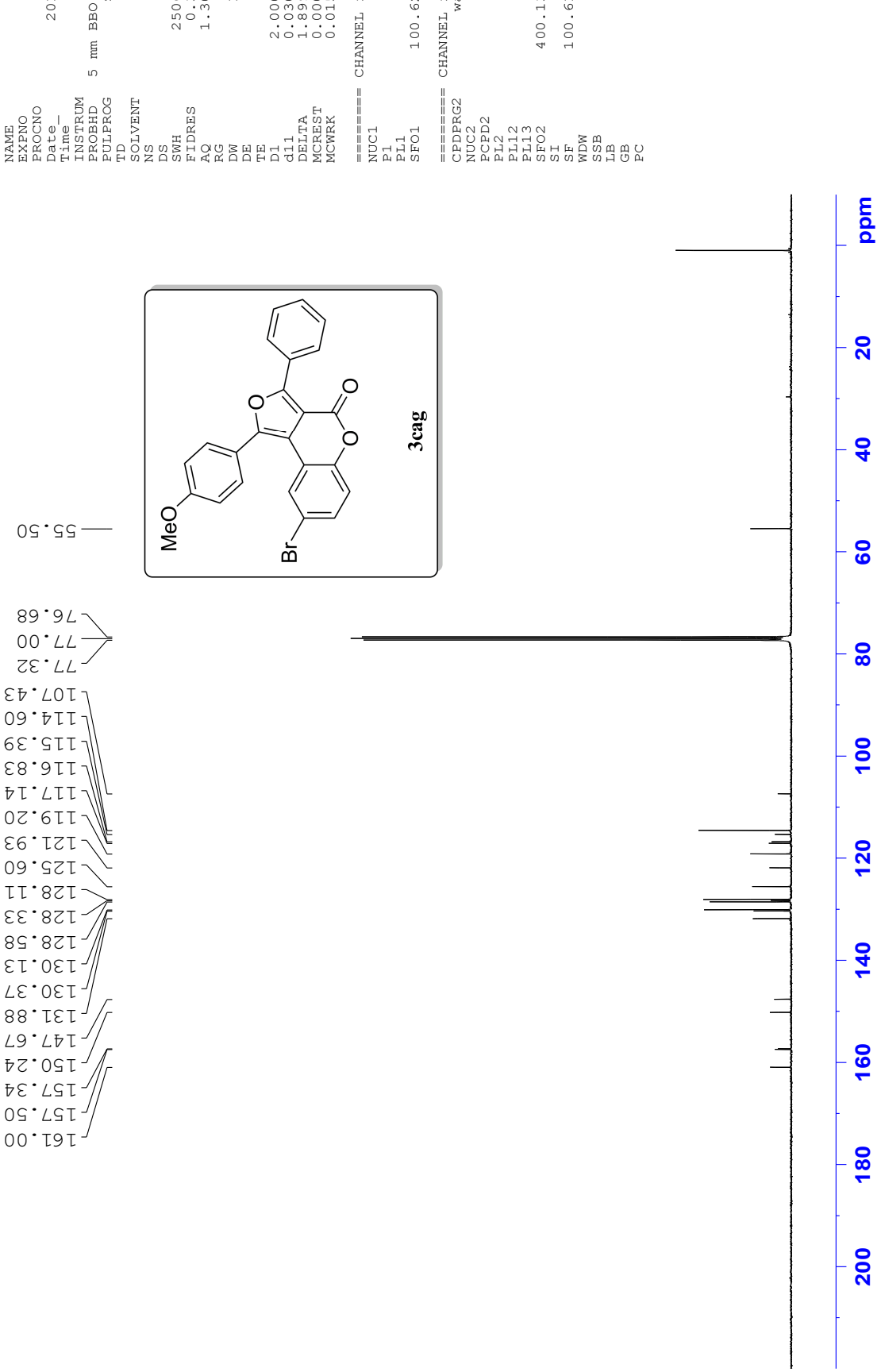
3cae

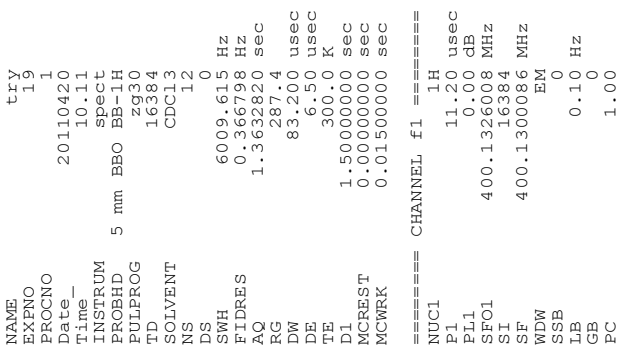
NAME	C13	
EXPNO	58	
PROCNO	1	
Date_	20110318	
Time	18.42	
INSTRUM	spect	
PROBHD	5 mm BBO BB-1H	
PULPROG	zgpg30	
TD	65536	
SOLVENT	CDCl3	
NS	1268	
DS	0	
SWH	25062.656	Hz
FIDRES	0.382426	Hz
AQ	1.3075131	sec
RG	10240	
DW	19.950	usec
DE	6.50	usec
TE	300.5	K
D1	2.00000000	sec
d11	0.03000000	sec
DELTA	1.89999998	sec
MCREST	0.00000000	sec
MCWRK	0.01500000	sec
======== CHANNEL f1 ========		
NUC1	13C	
P1	10.00	usec
PL1	5.30	dB
SFO1	100.6242995	MHz
======== CHANNEL f2 ========		
CPDPRG2	waltz16	
NUC2	1H	
PCPD2	90.00	usec
PL2	0.00	dB
PL12	16.50	dB
PL13	19.50	dB
SFO2	400.1319000	MHz
SI	32768	
SF	100.6127713	MHz
WDW	EM	
SSB	0	
LB	1.00	Hz
GB	0	
PC	1.40	

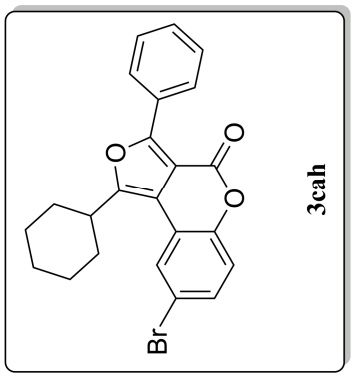


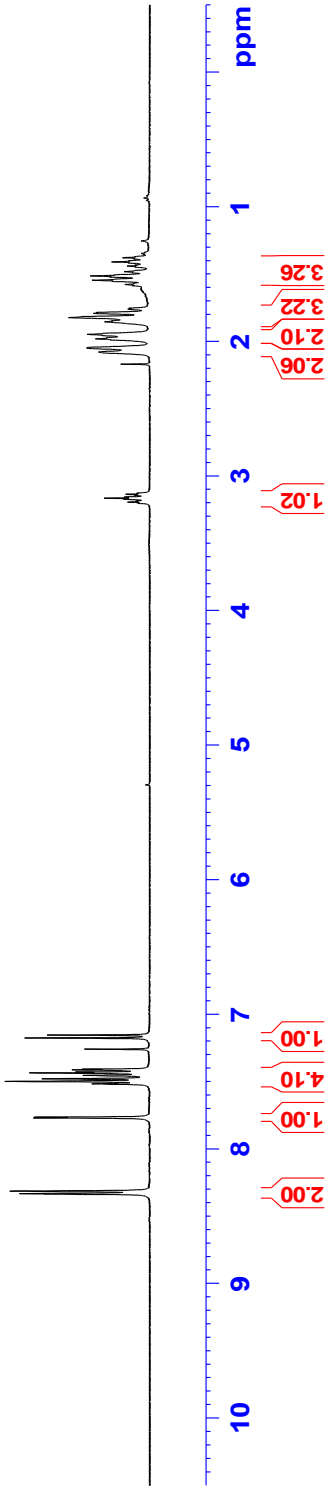


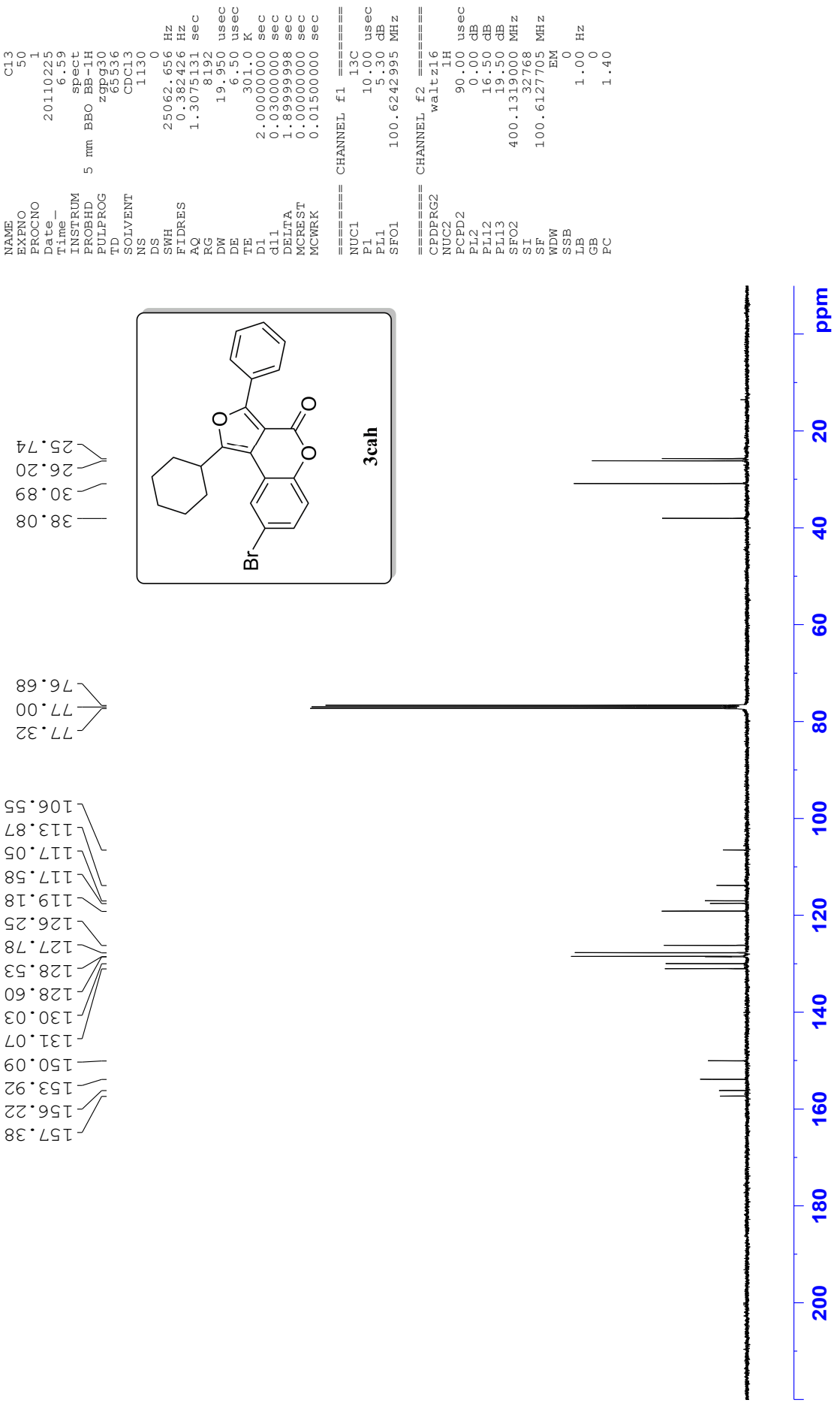


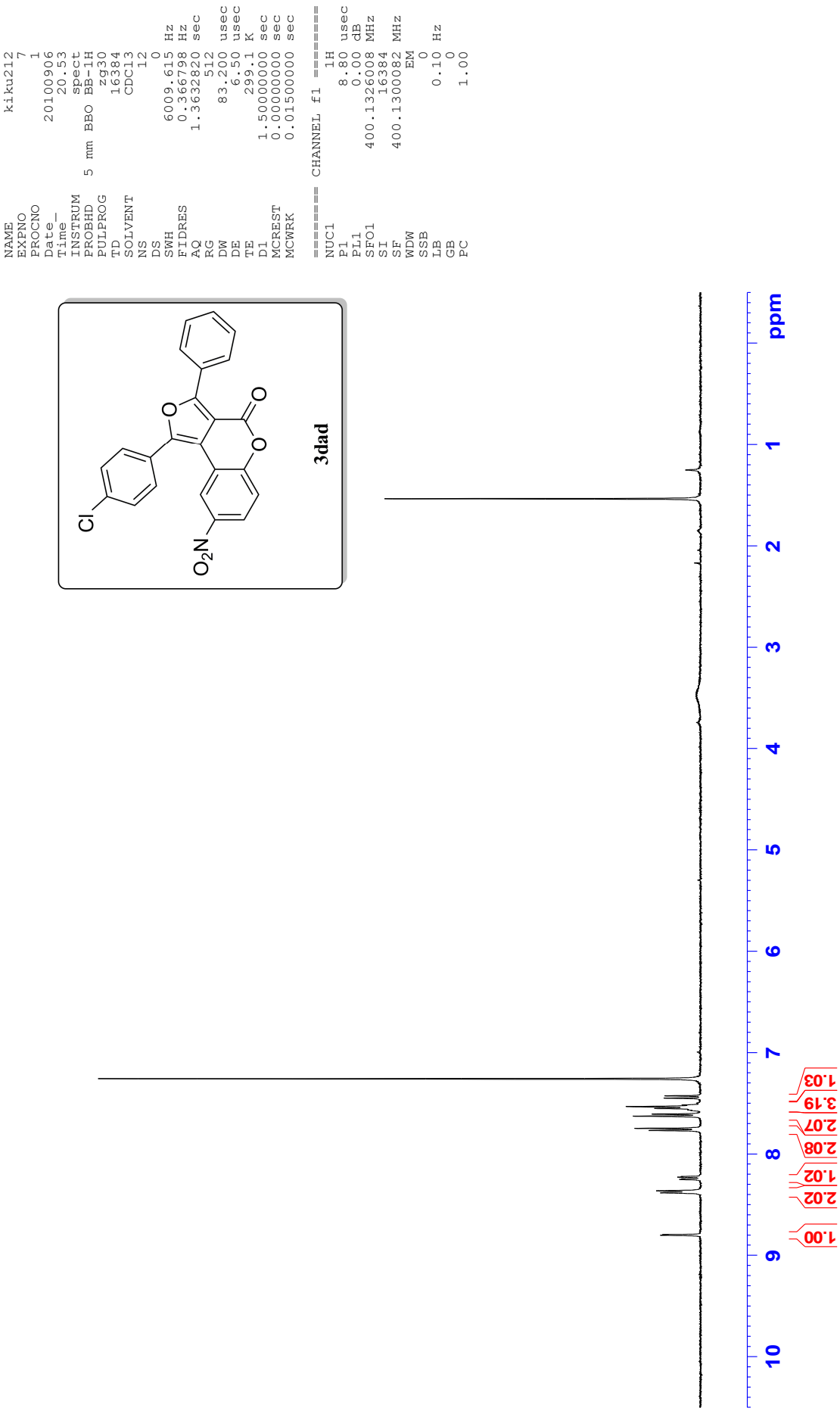

C13
70
1
20110417
21.39
spect
5 mm BBO BB-1H
zgpg30
65536
CDCl3
10000
0
25062.656 Hz
0.382426 Hz
1.3075131 sec
10240
19.950 usec
6.50 usec
299.6 K
2.00000000 sec
0.03000000 sec
1.89999998 sec
0.00000000 sec
0.01500000 sec
CHANNEL f1
13C
10.00 usec
5.30 dB
100.6242995 MHz
CHANNEL f2
waltz16
1H
90.00 usec
0.00 dB
16.50 dB
19.50 dB
400.1319000 MHz
32768
100.6127697 MHz
EM
0
1.00 Hz
0
1.40
MeO
Br
O
O
O
3cag
55.50
76.68
77.00
77.32
107.43
114.60
115.39
116.83
117.14
119.20
121.93
125.60
128.11
128.33
128.58
130.13
130.37
131.88
147.67
150.24
157.34
157.50
161.00
ppm
200
180
160
140
120
100
80
60
40
20

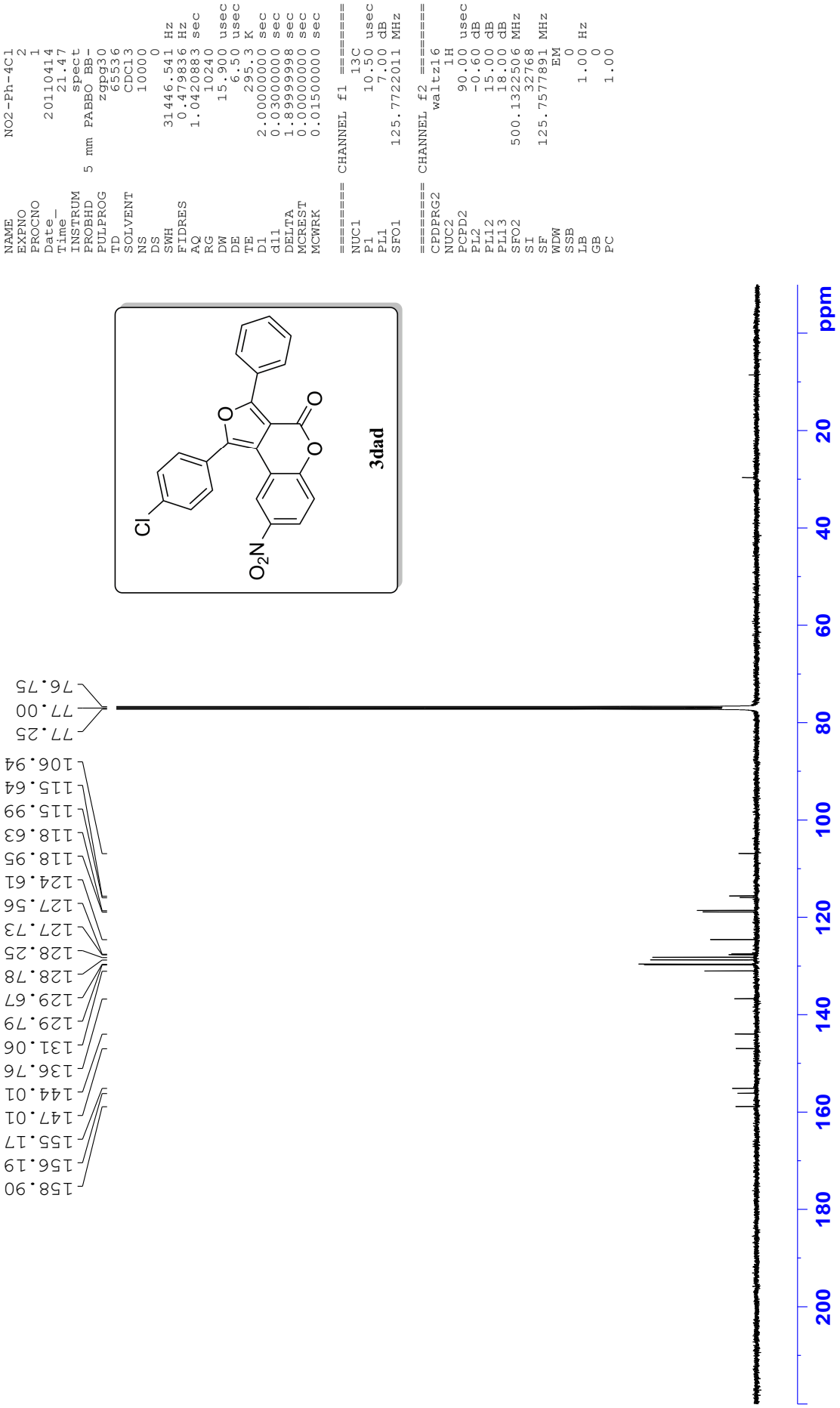


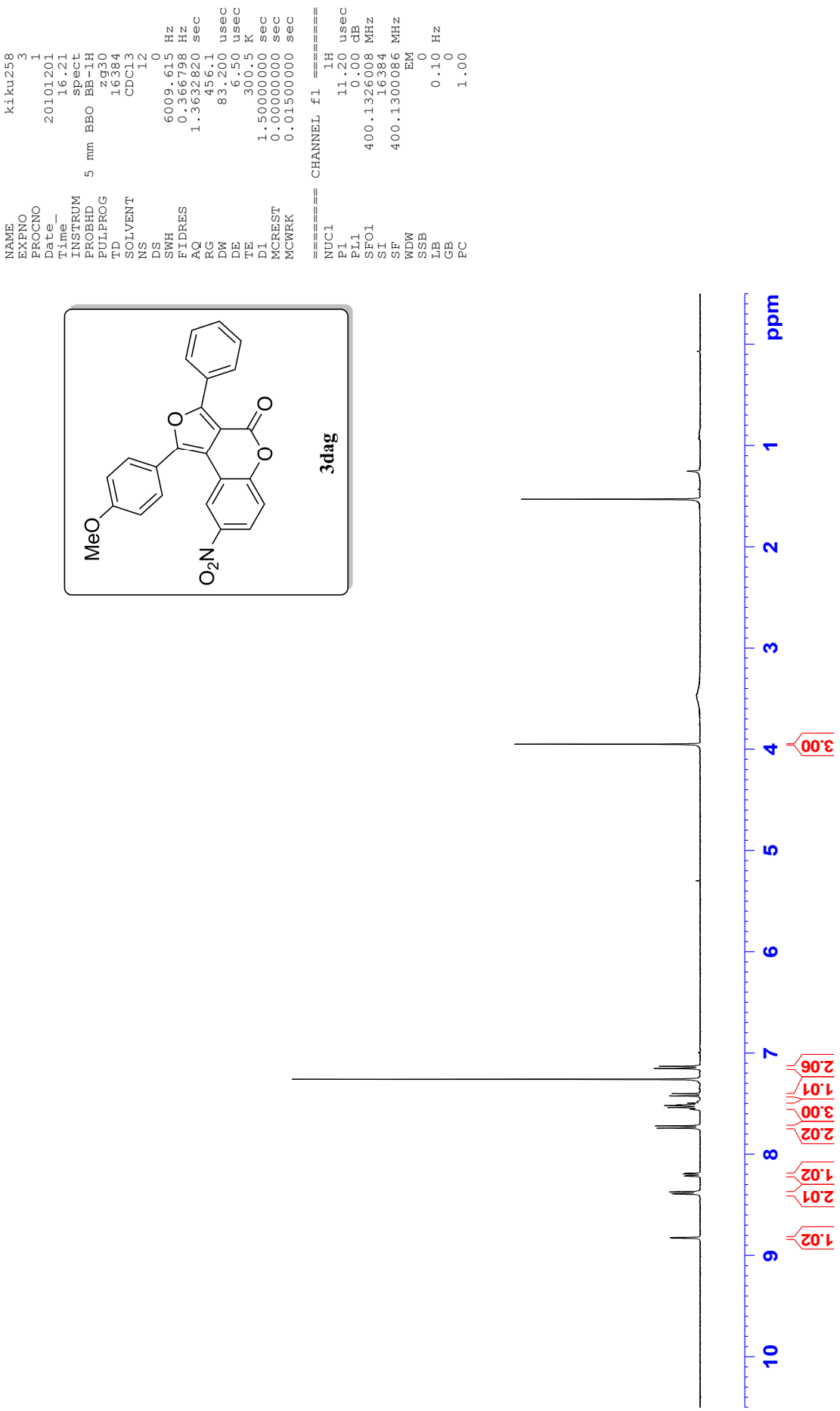


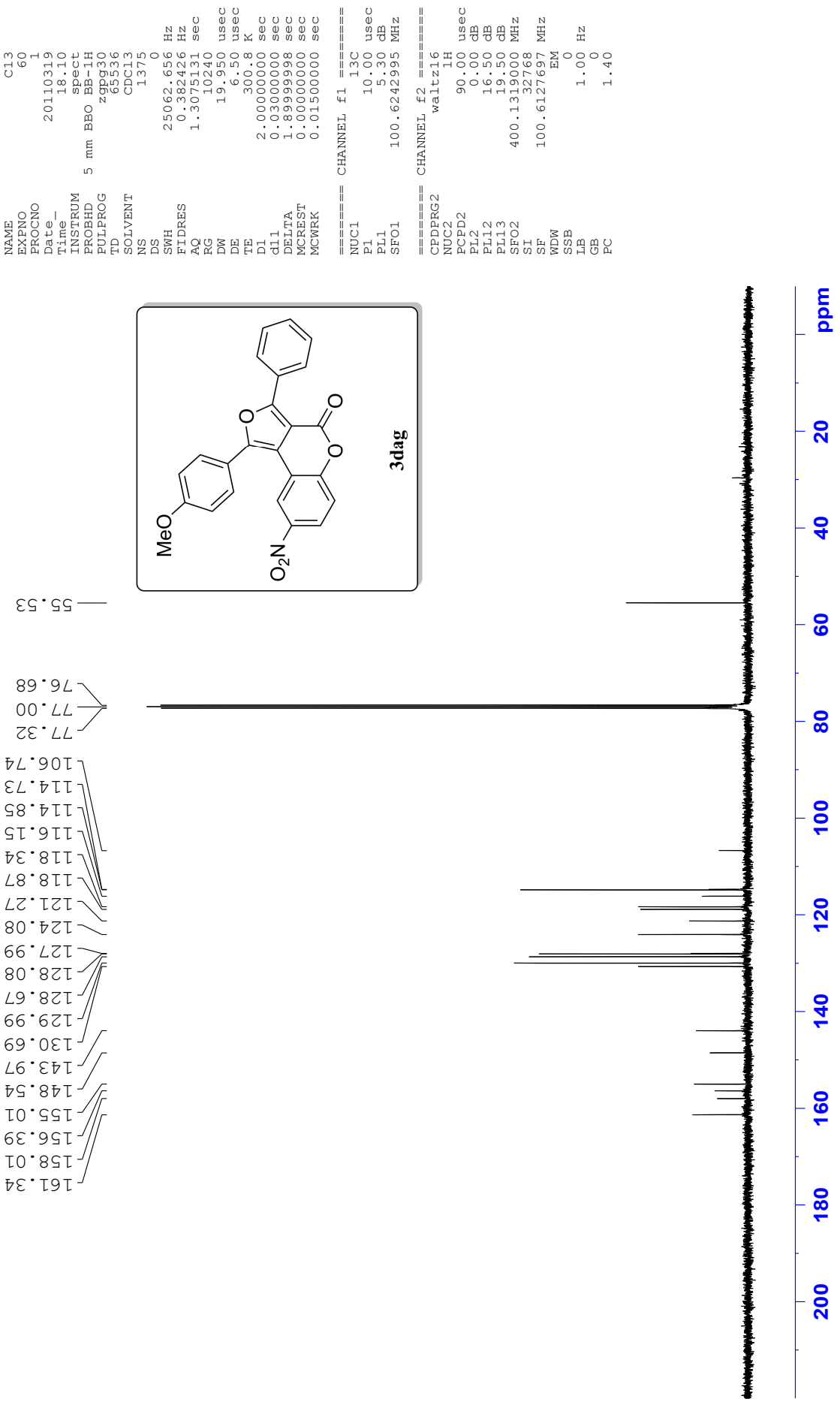



C13
50
1
20110225
6.59
spect
5 mm BBO BB-1H
zgpg30
65536
CDC13
1130
0
25062.656 Hz
0.382426 Hz
1.30751131 sec
8192
19.950 usec
6.50 usec
301.0 K
2.00000000 sec
0.03000000 sec
1.89999998 sec
0.00000000 sec
0.01500000 sec
CHANNEL f1
13C
10.00 usec
5.30 dB
100.6242995 MHz
CHANNEL f2
waltz16
1H
90.00 usec
0.00 dB
16.50 dB
19.50 dB
400.1319000 MHz
32768
100.6127705 MHz
EM
0
1.00 Hz
0
1.40
3cah
Br
O
O
O
25.74
26.20
30.89
38.08
77.32
77.00
76.68
106.55
113.87
117.05
117.58
119.18
126.25
127.78
128.53
128.60
130.03
131.07
150.09
153.92
156.22
157.38
ppm
200
180
160
140
120
100
80
60
40
20

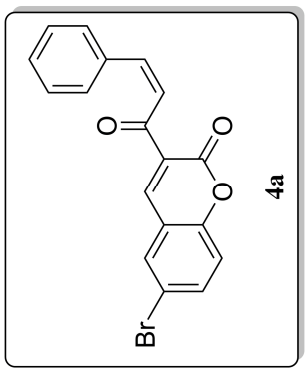


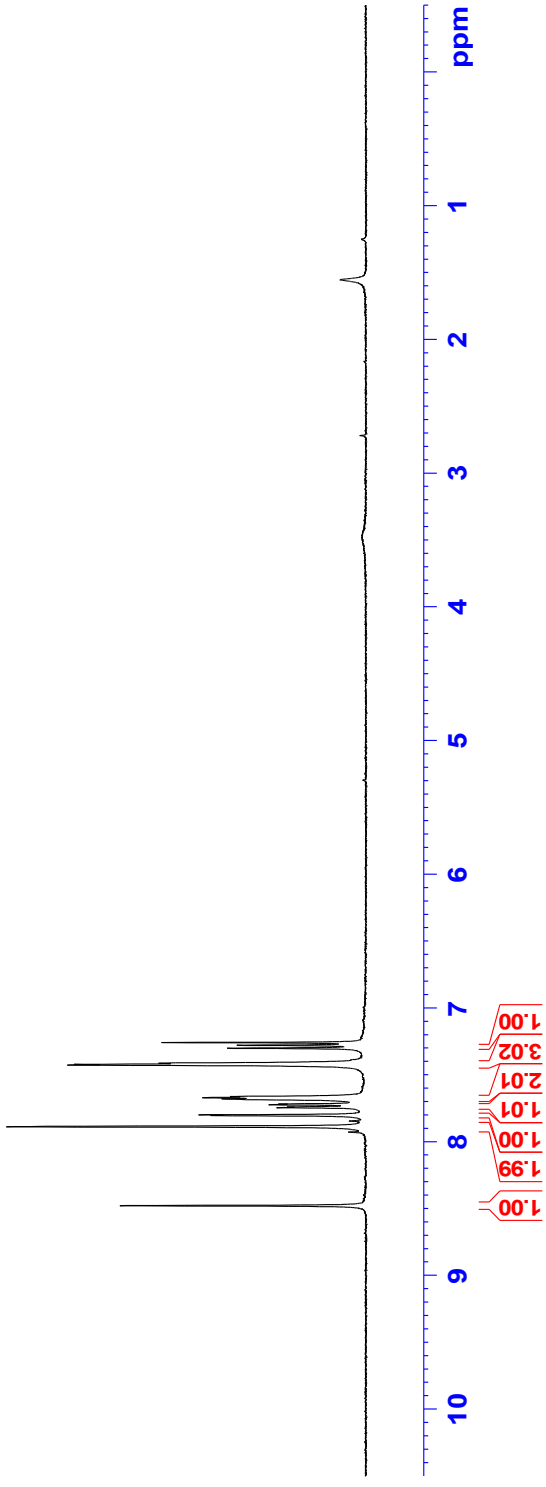


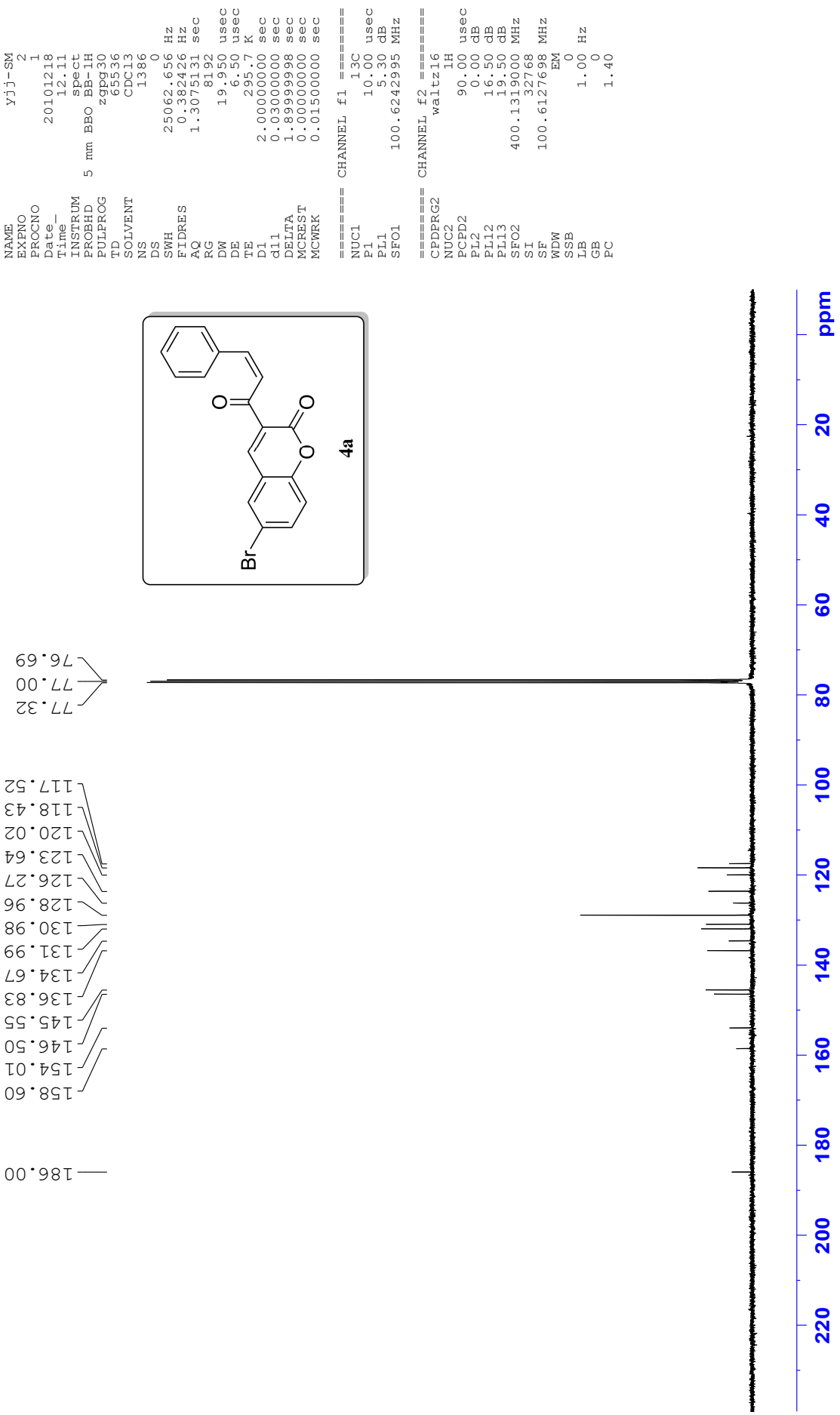


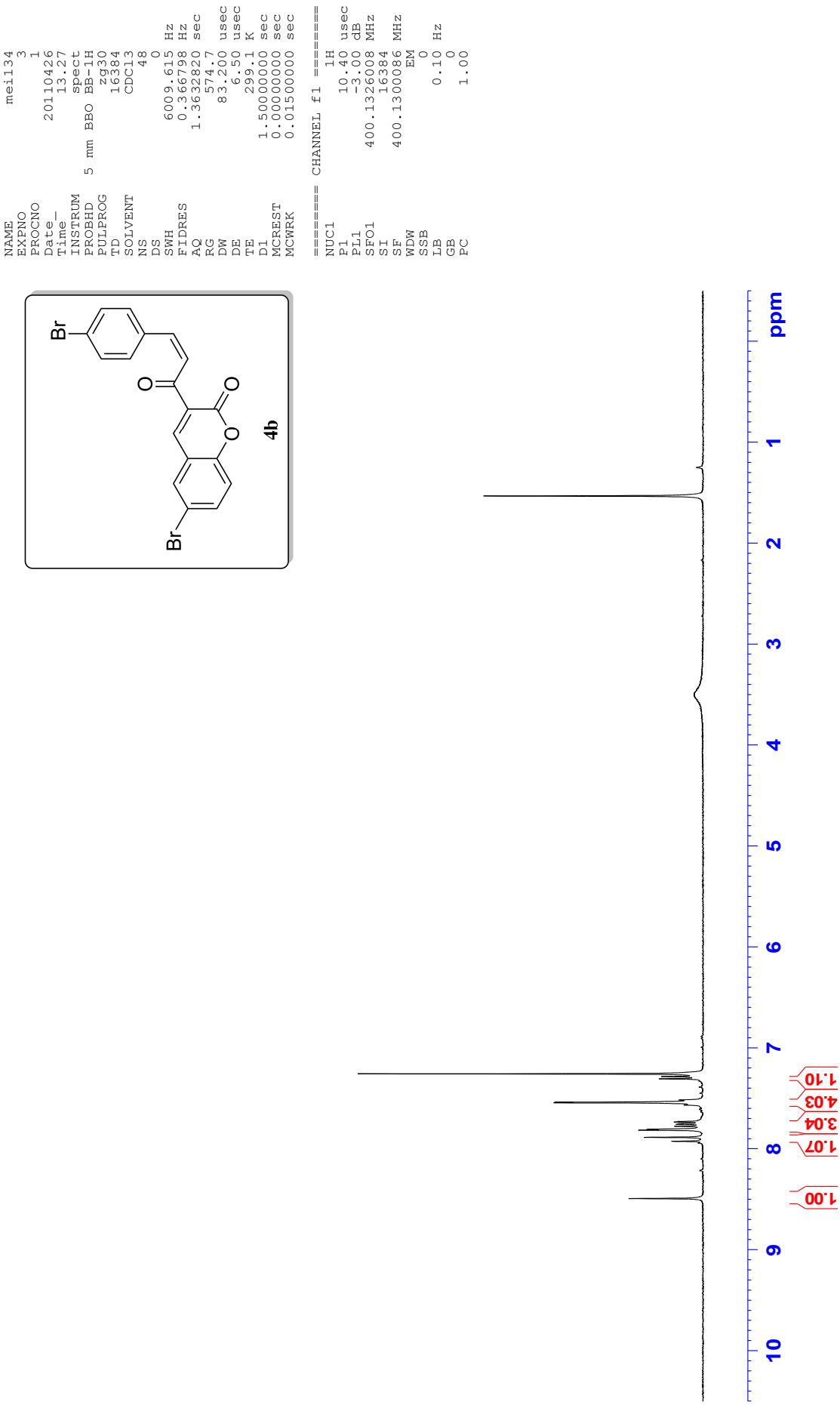


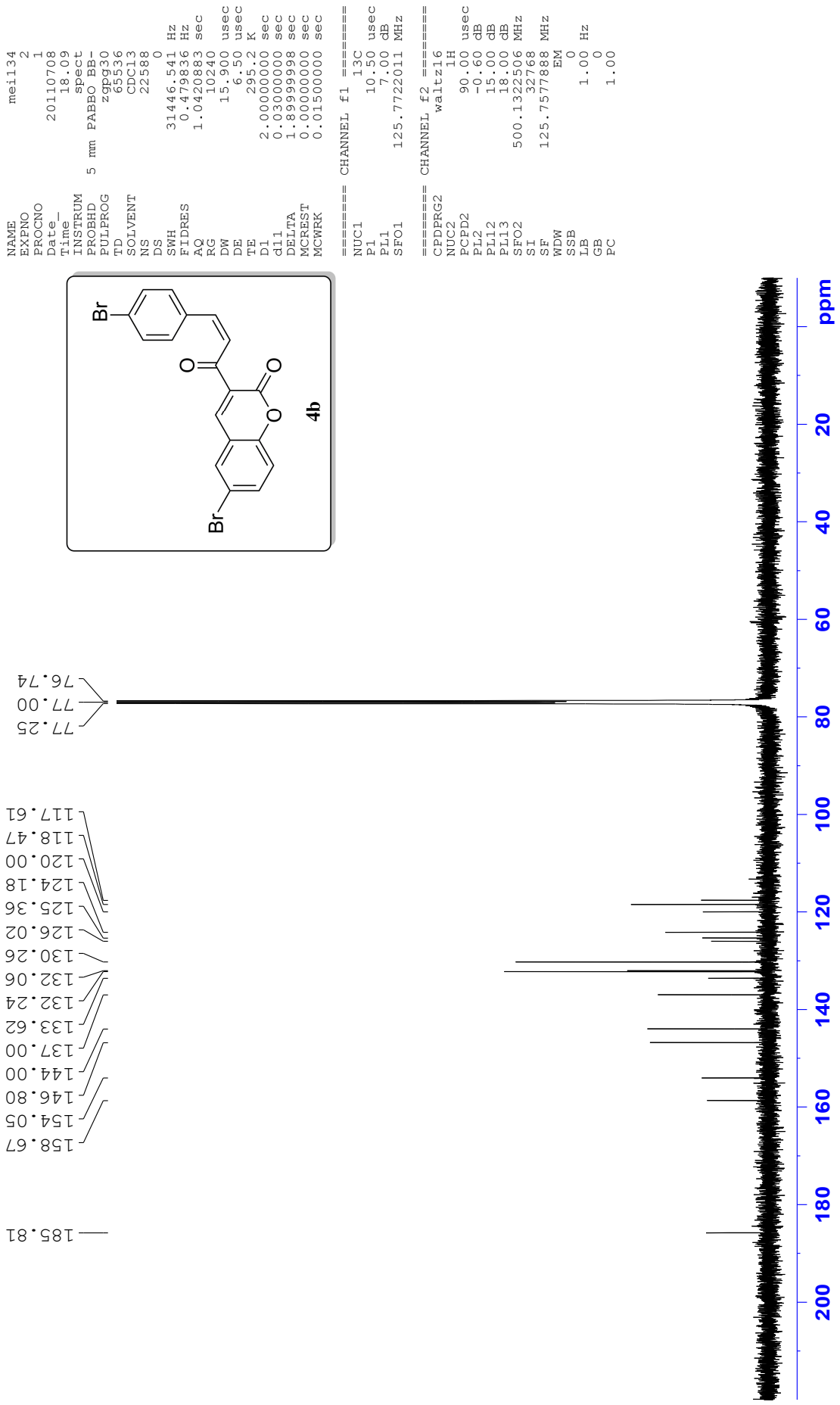
```
NAME                 try-2
EXPNO                   10
PROCNO                   1
Date_             20110427
Time_                15.27
INSTRUM                spect
PROBHD     5 mm BBO BB-1H
PULPROG              zg30
TD                  16384
SOLVENT             CDCl3
NS                     12
DS                      0
SWH                6009.615 Hz
FIDRES             0.366798 Hz
AQ                 1.3632820 sec
RG                     645.1
DW                    83.200 usec
DE                     6.50 usec
TE                    298.8 K
D1                 1.50000000 sec
MCREST             0.00000000 sec
MCWRK              0.01500000 sec

======== CHANNEL f1 ========
NUC1                      1H
P1                     11.20 usec
PL1                     0.00 dB
SFO1           400.1326008 MHz
SI                     16384
SF             400.1300087 MHz
WDW                       EM
SSB                        0
LB                      0.10 Hz
GB                         0
PC                      1.00
```

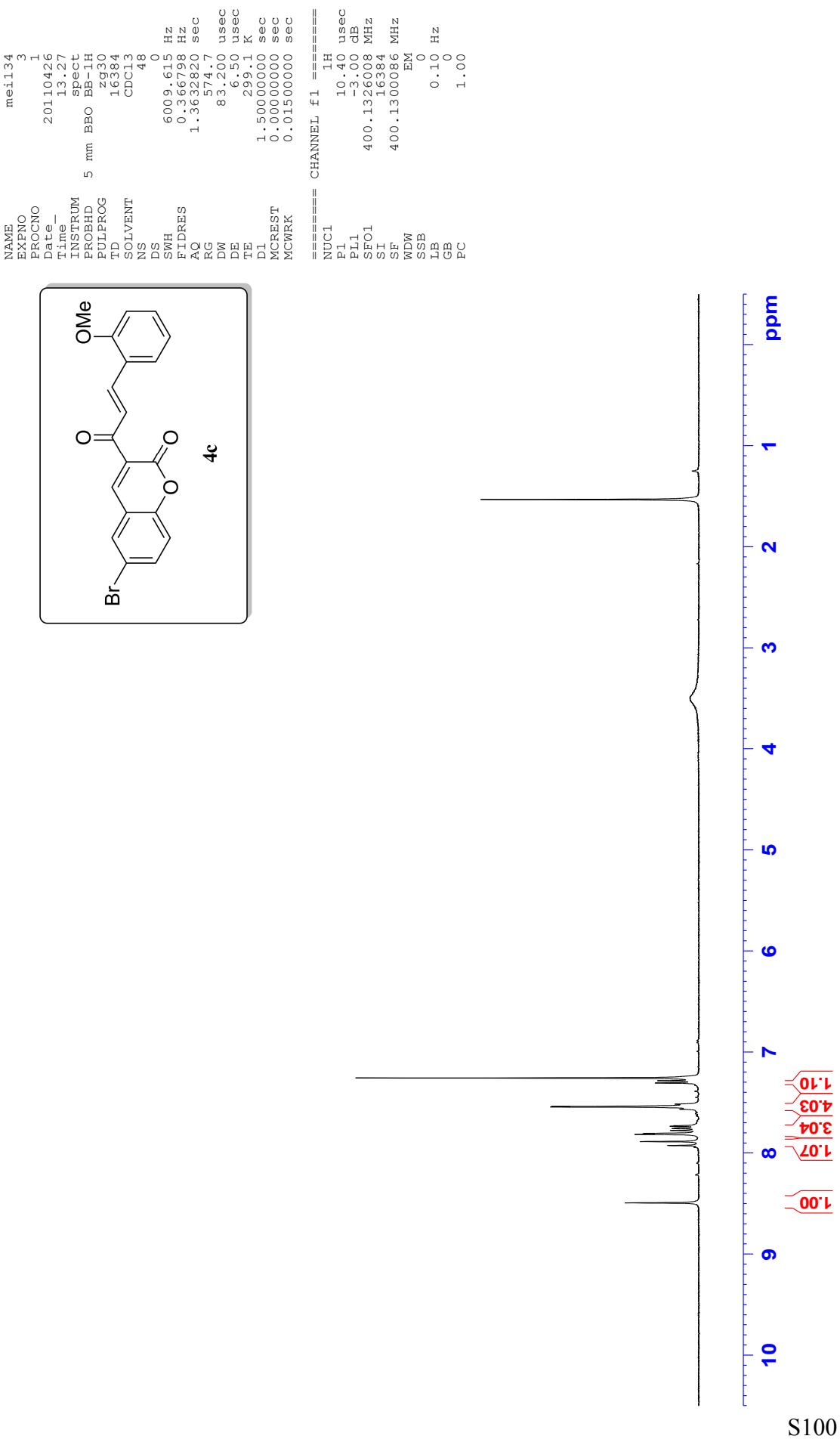


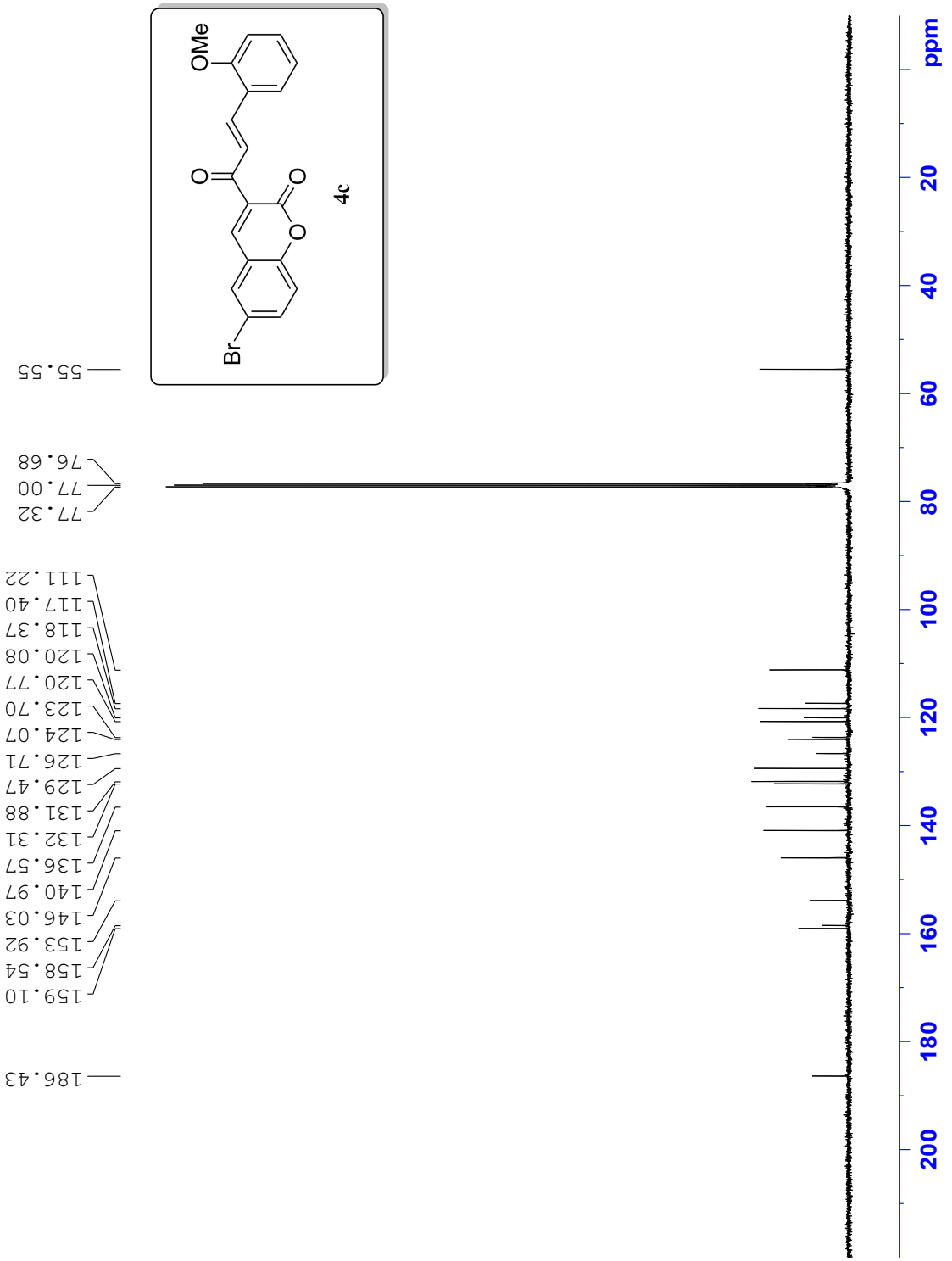


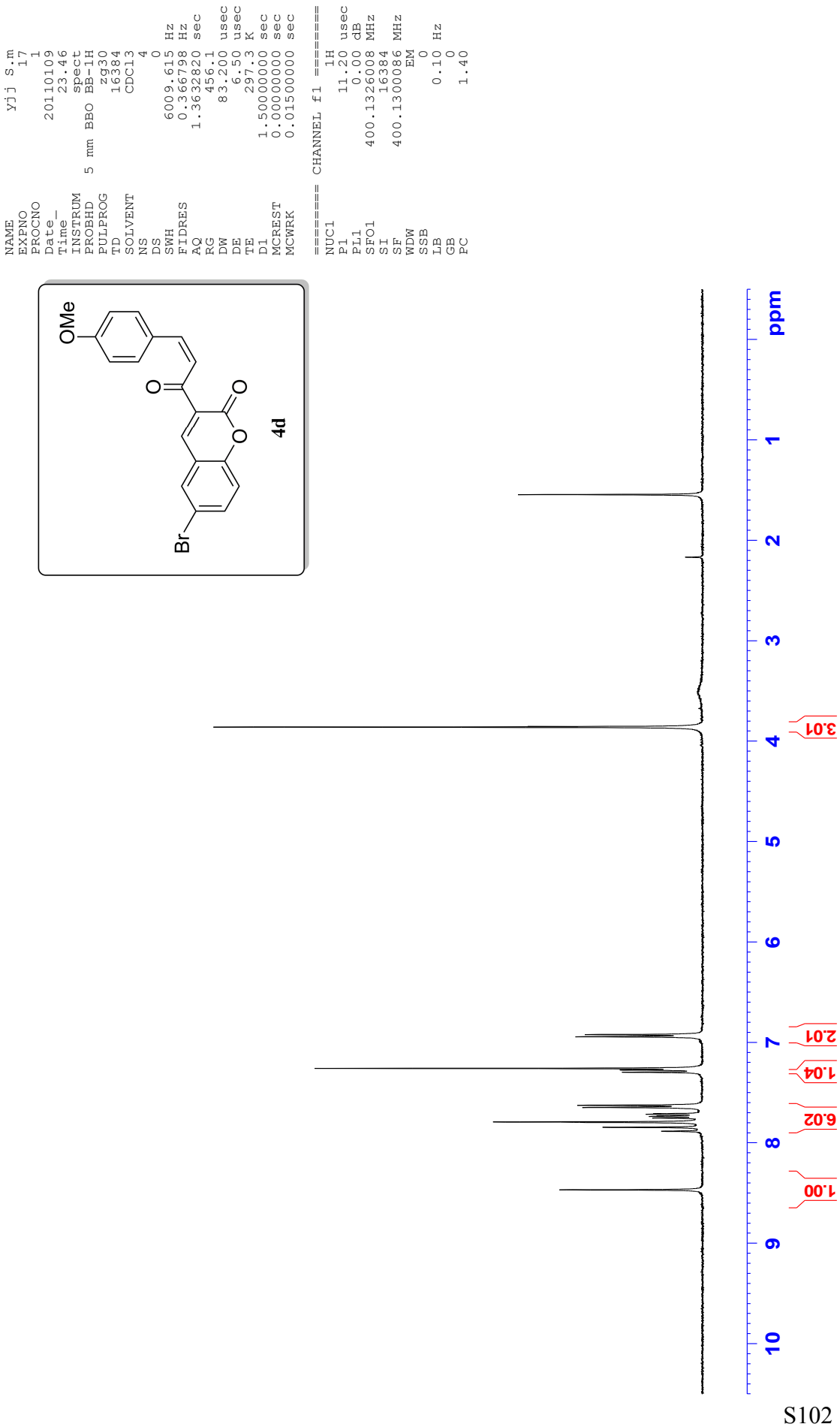


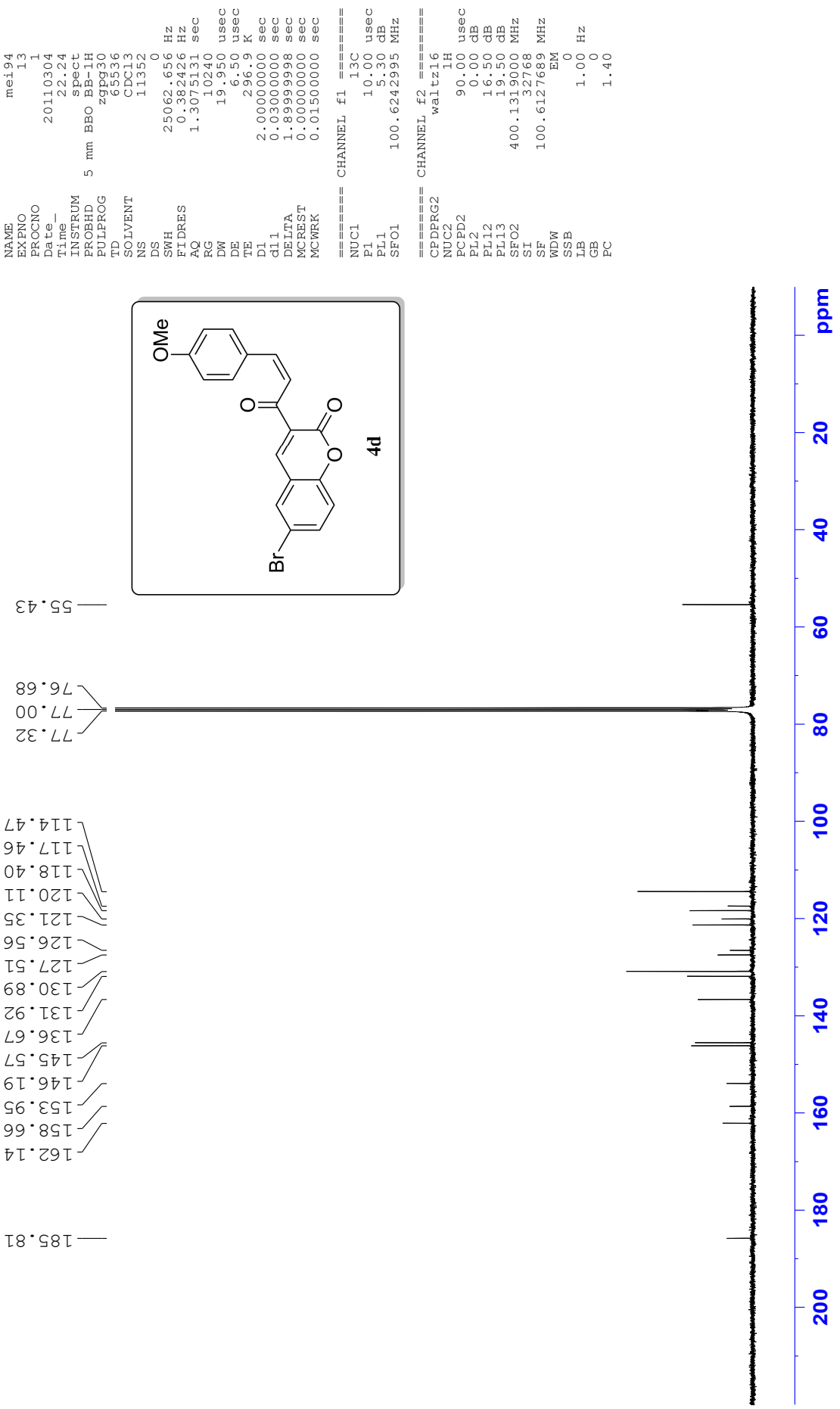


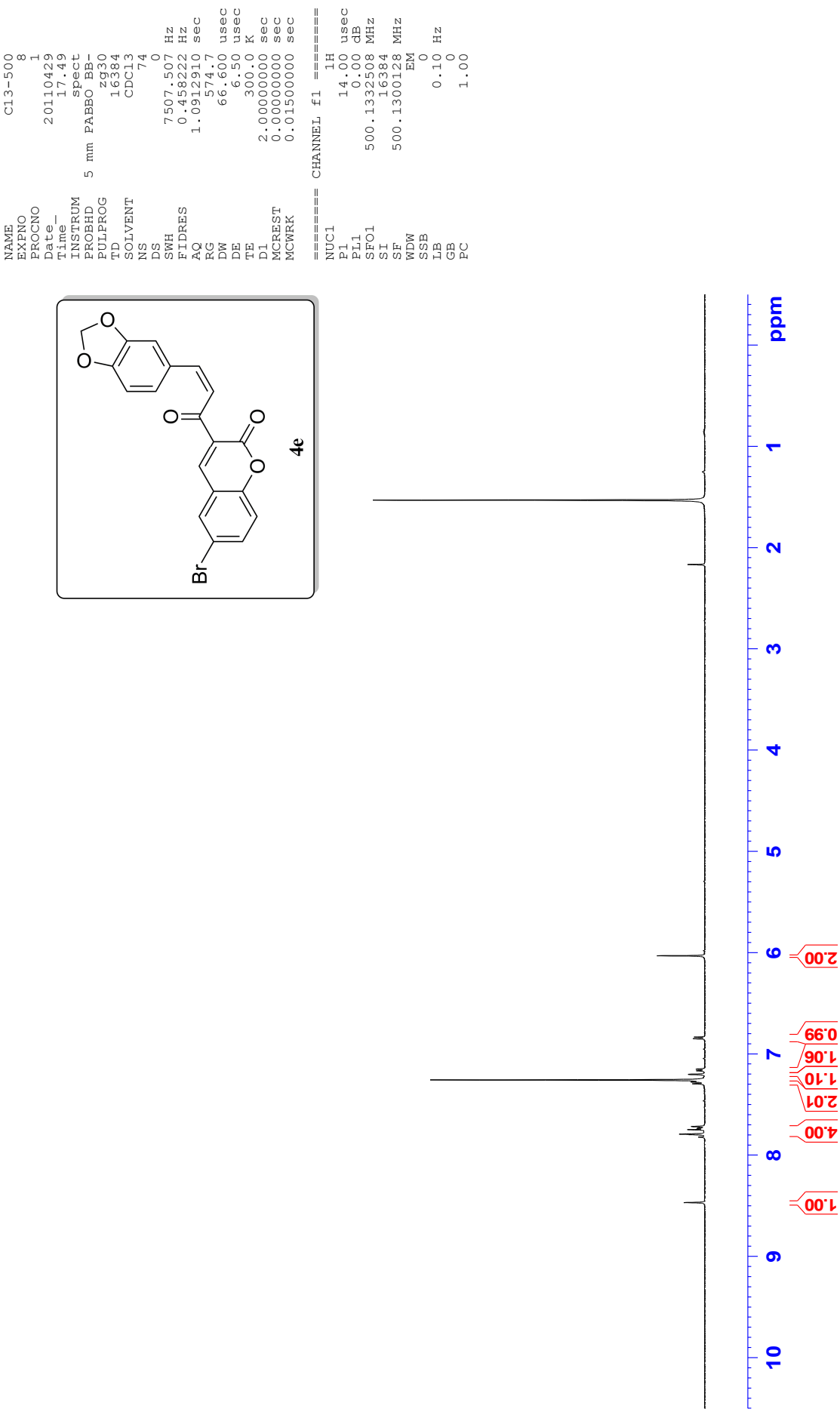


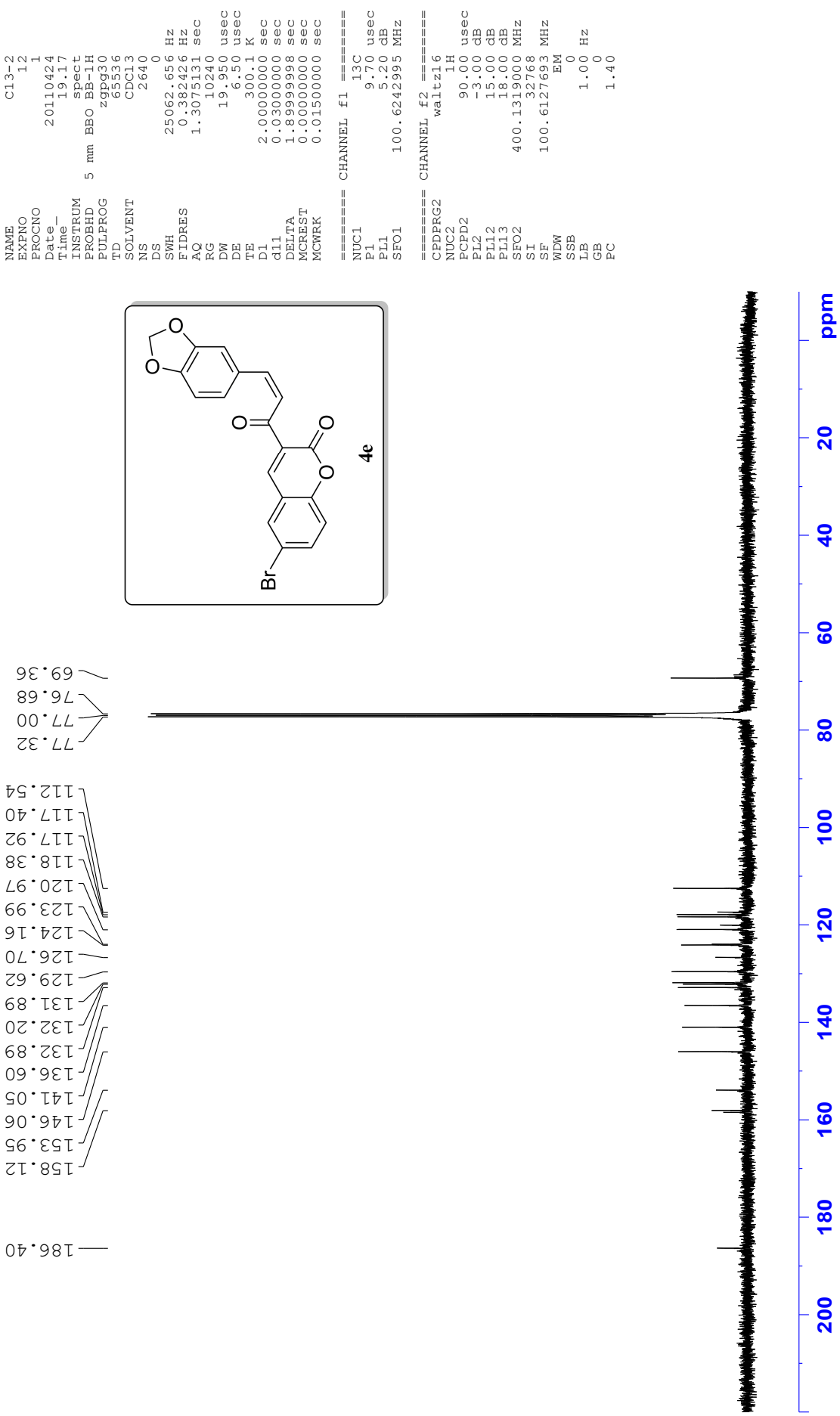


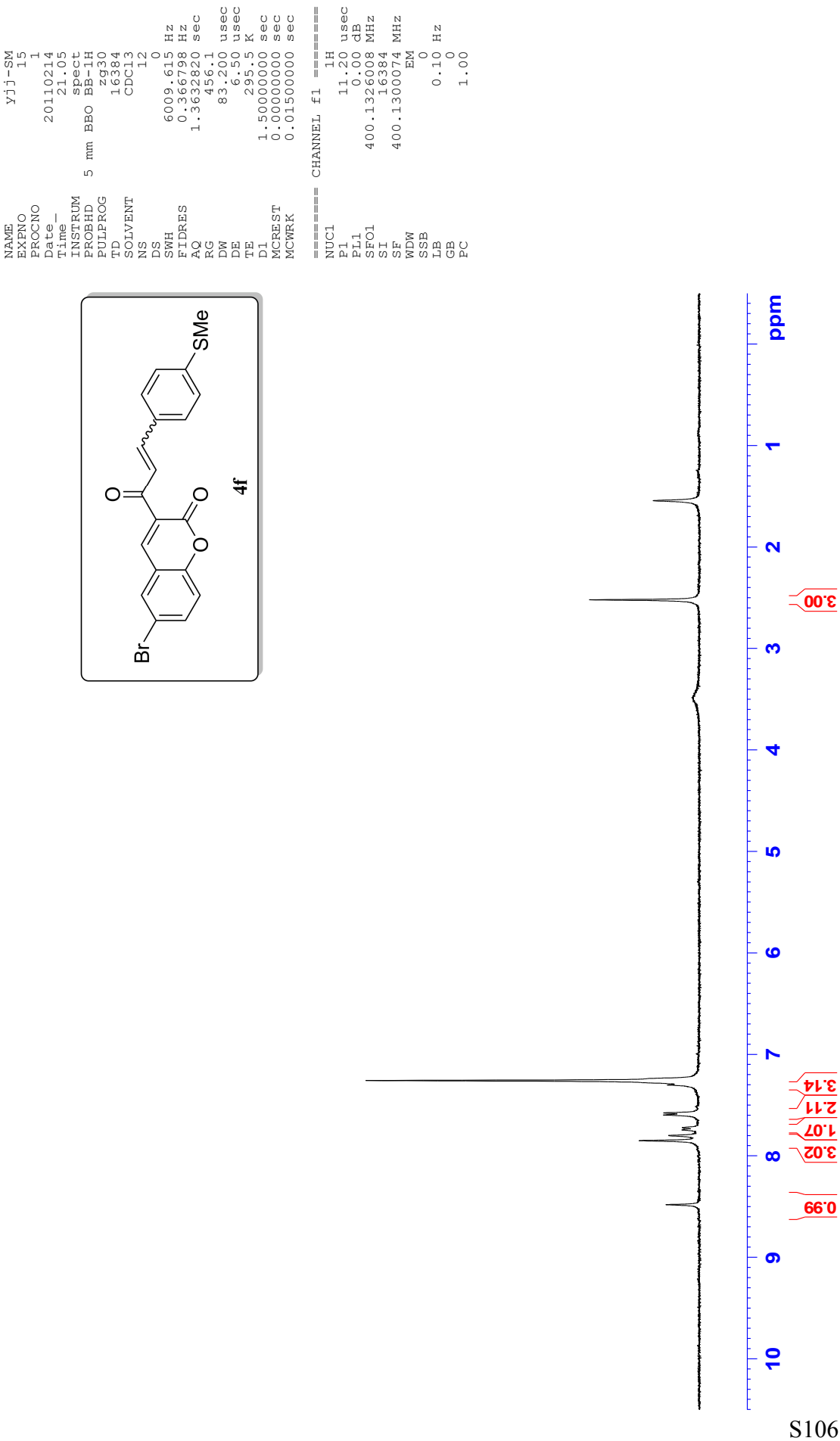

NAME mei93
EXPNO 9
PROCNO 1
Date_ 20110318
Time_ 13.08
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1935
DS 0
SWH 25062.656 Hz
FIDRES 0.382426 Hz
AQ 1.3075131 sec
RG 10240
DW 19.950 usec
DE 6.50 usec
TE 299.2 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
CHANNEL f1 13C
NUC1 13C
P1 10.00 usec
PL1 5.30 dB
SFO1 100.6242995 MHz
CHANNEL f2 1H
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 0.00 dB
PL12 16.50 dB
PL13 19.50 dB
SFO2 400.1319000 MHz
SI 32768
SF 100.6127705 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
OMe
O
O
O
Br
4c
55.55
76.68
77.00
77.32
111.22
117.40
118.37
120.08
120.77
123.70
124.07
126.71
129.47
131.88
132.31
136.57
140.97
146.03
153.92
158.54
159.10
186.43
ppm
200
180
160
140
120
100
80
60
40
20

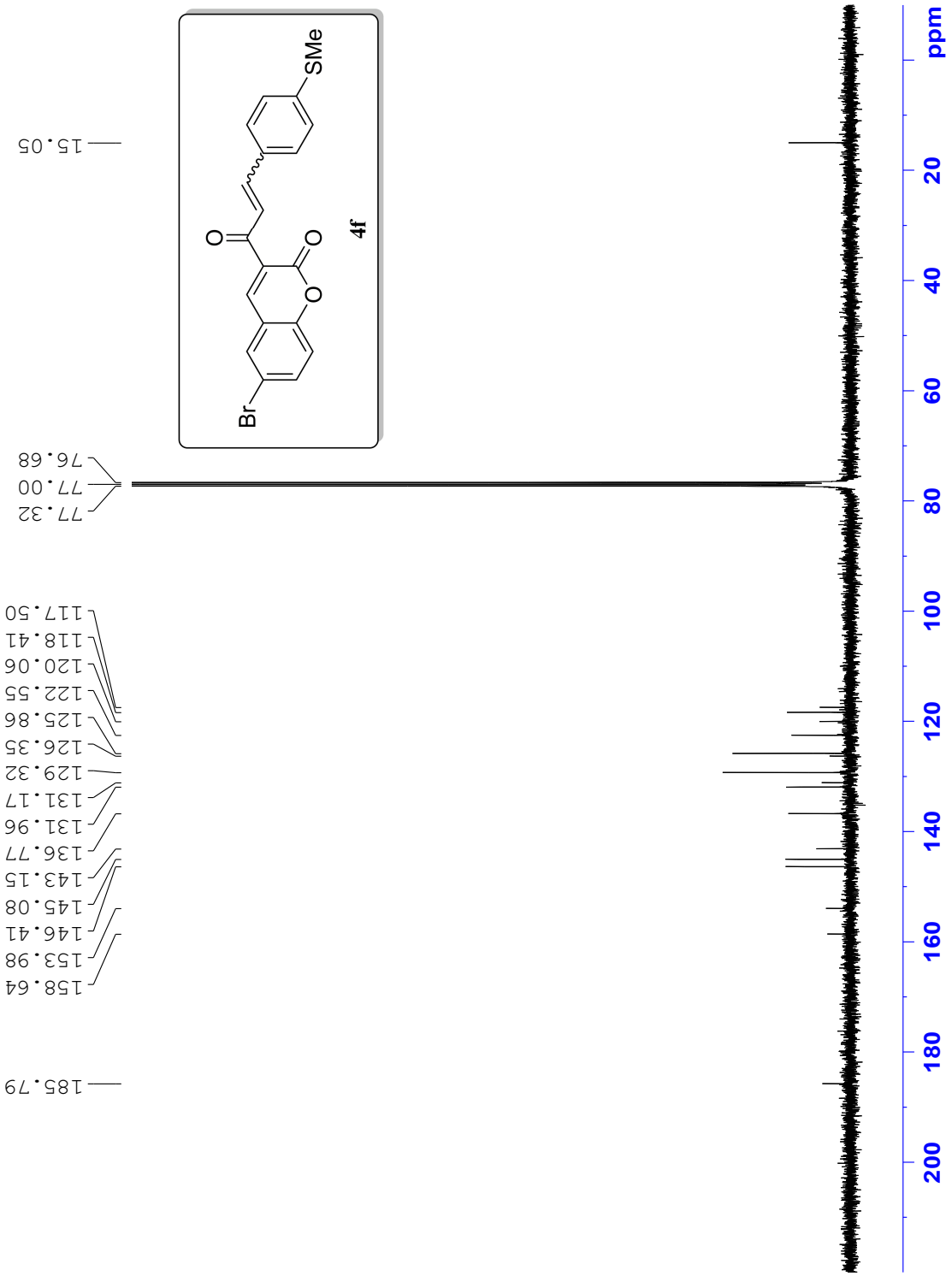


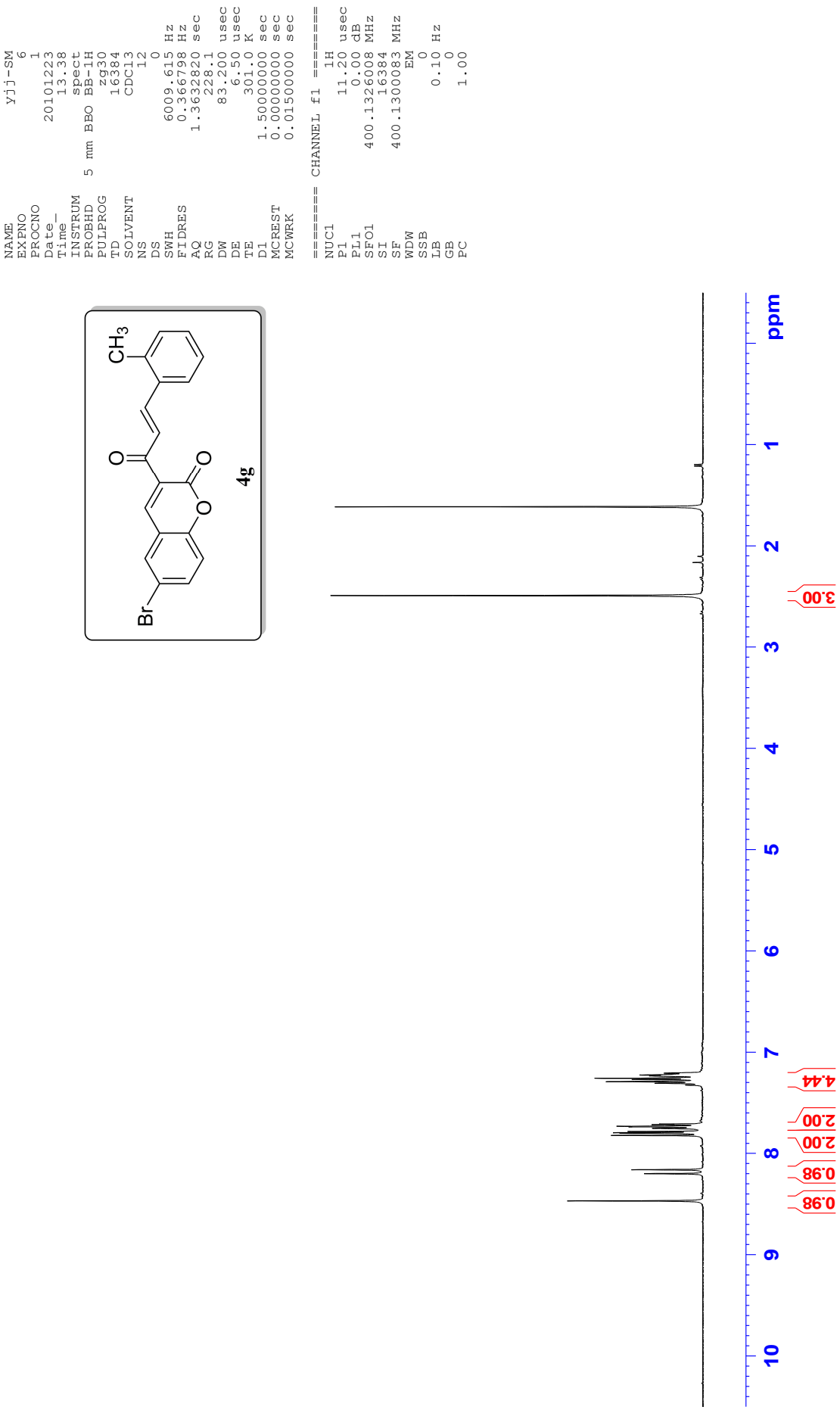


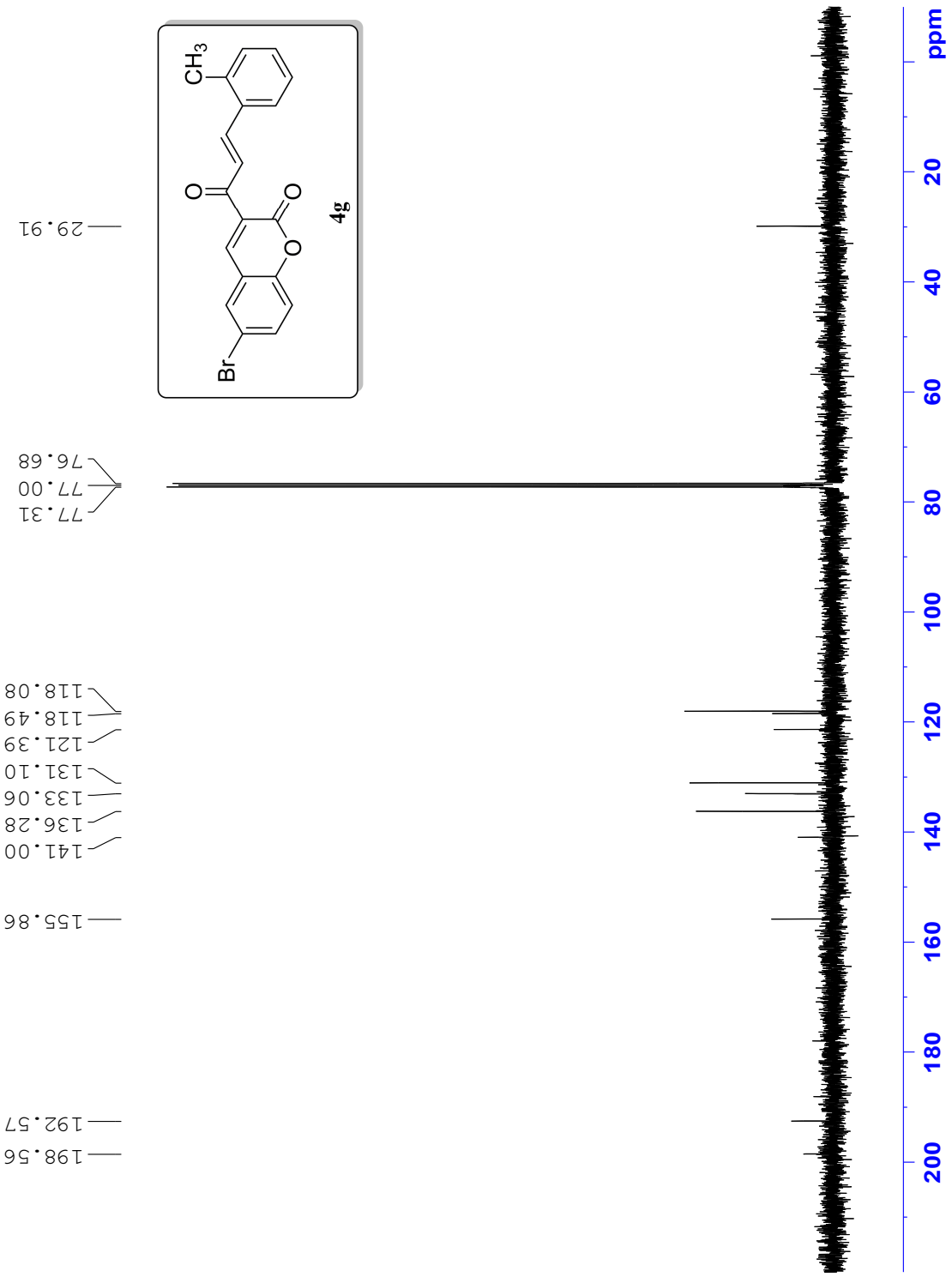




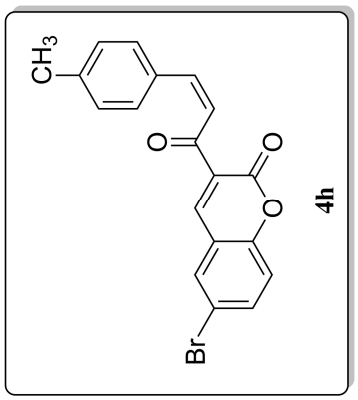


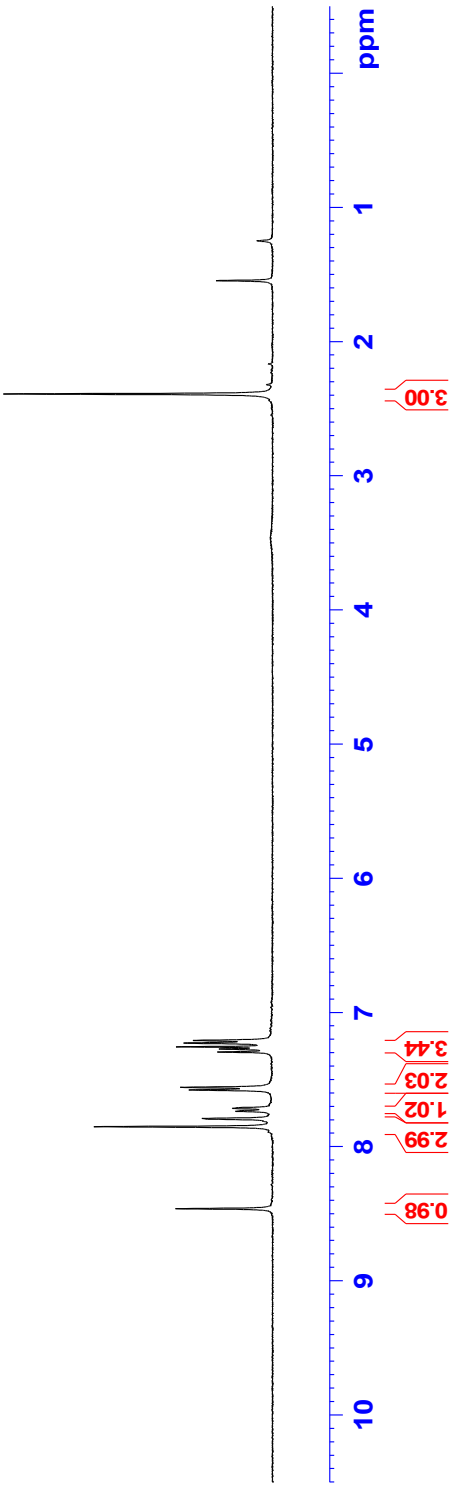


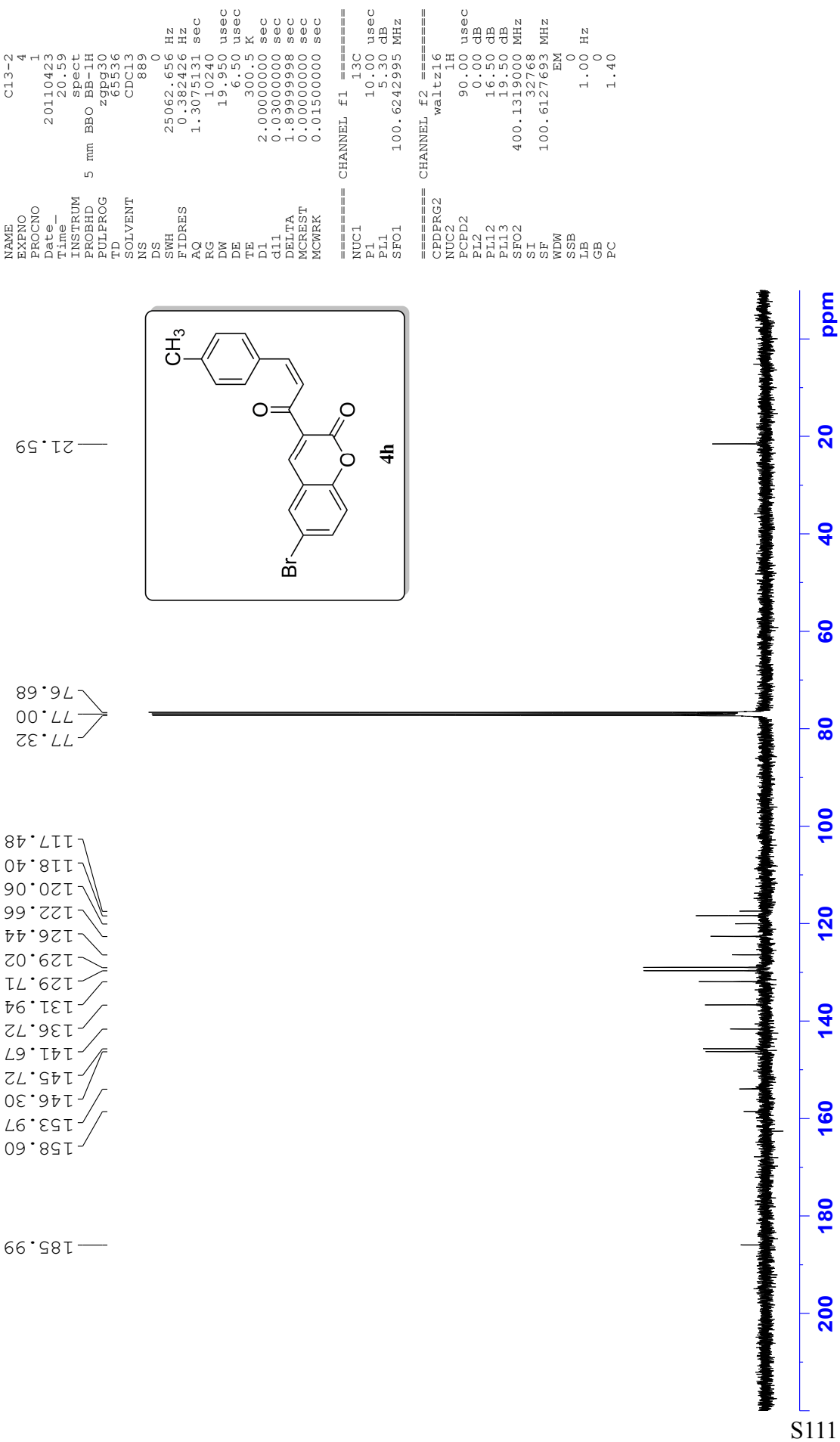


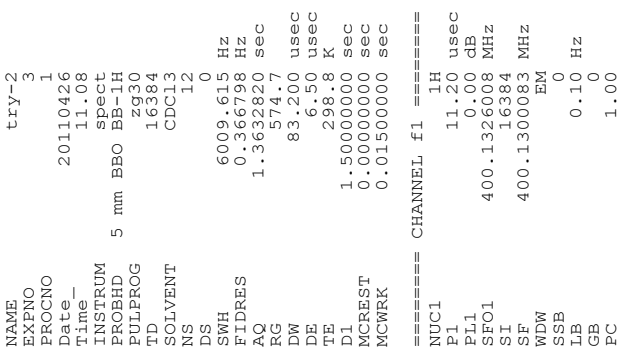

NAME C13-2
EXPNO 36
PROCNO 1
Date_ 20110520
Time_ 15.06
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 150
DS 0
SWH 25062.656 Hz
FIDRES 0.382426 Hz
AQ 1.3075131 sec
RG 10240
DW 19.950 usec
DE 6.50 usec
TE 299.9 K
D1 2.00000000 sec
D11 0.03000000 sec
DELTA 1.89999998 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 10.00 usec
PL1 5.30 dB
SFO1 100.6242995 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 0.00 dB
PL12 16.50 dB
PL13 19.50 dB
SFO2 400.1319000 MHz
SI 32768
SF 100.6127689 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
CH3
O
O
O
Br
4g
29.91
76.68
77.00
77.31
118.08
118.49
121.39
131.10
133.06
136.28
141.00
155.86
192.57
198.56
ppm
200
180
160
140
120
100
80
60
40
20

```
NAME                 try-2
EXPNO                    6
PROCNO                   1
Date_             20110426
Time_                14.35
INSTRUM                spect
PROBHD   5 mm BBO BB-1H
PULPROG                zg30
TD                    16384
SOLVENT               CDCl3
NS                       12
DS                        0
SWH                6009.615 Hz
FIDRES             0.366798 Hz
AQ                 1.3632820 sec
RG                      512
DW                   83.200 usec
DE                    6.50 usec
TE                   298.9 K
D1                 1.50000000 sec
MCREST             0.00000000 sec
MCWRK              0.01500000 sec
======== CHANNEL f1 ========
NUC1                      1H
P1                     11.20 usec
PL1                     0.00 dB
SFO1           400.1326008 MHz
SI                    16384
SF             400.1300088 MHz
WDW                      EM
SSB                       0
LB                     0.10 Hz
GB                        0
PC                     1.00
```

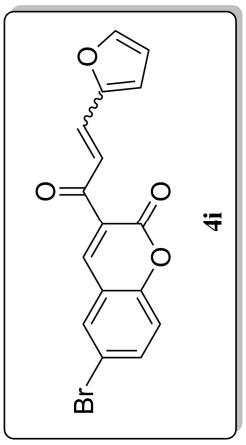


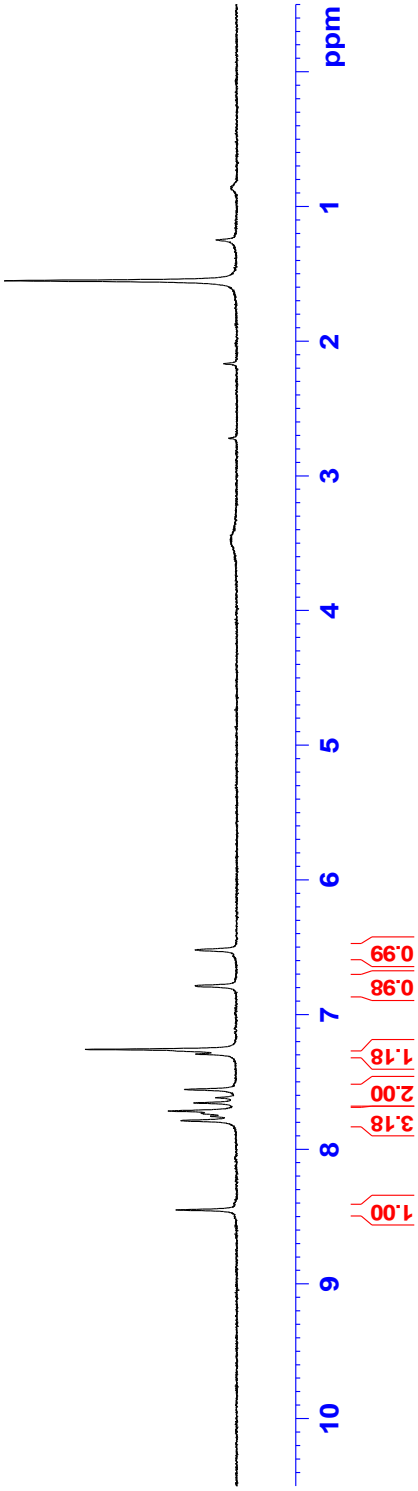


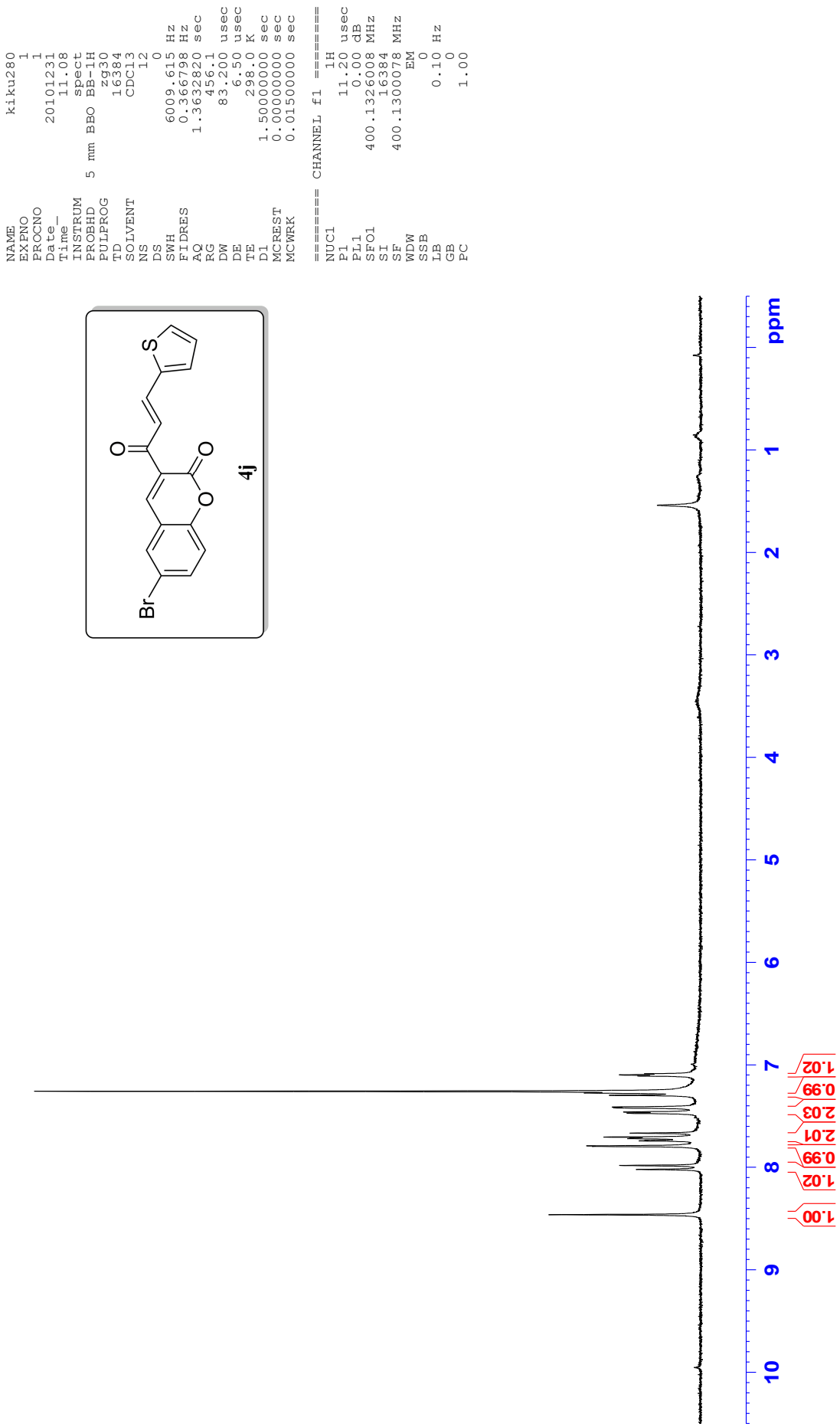


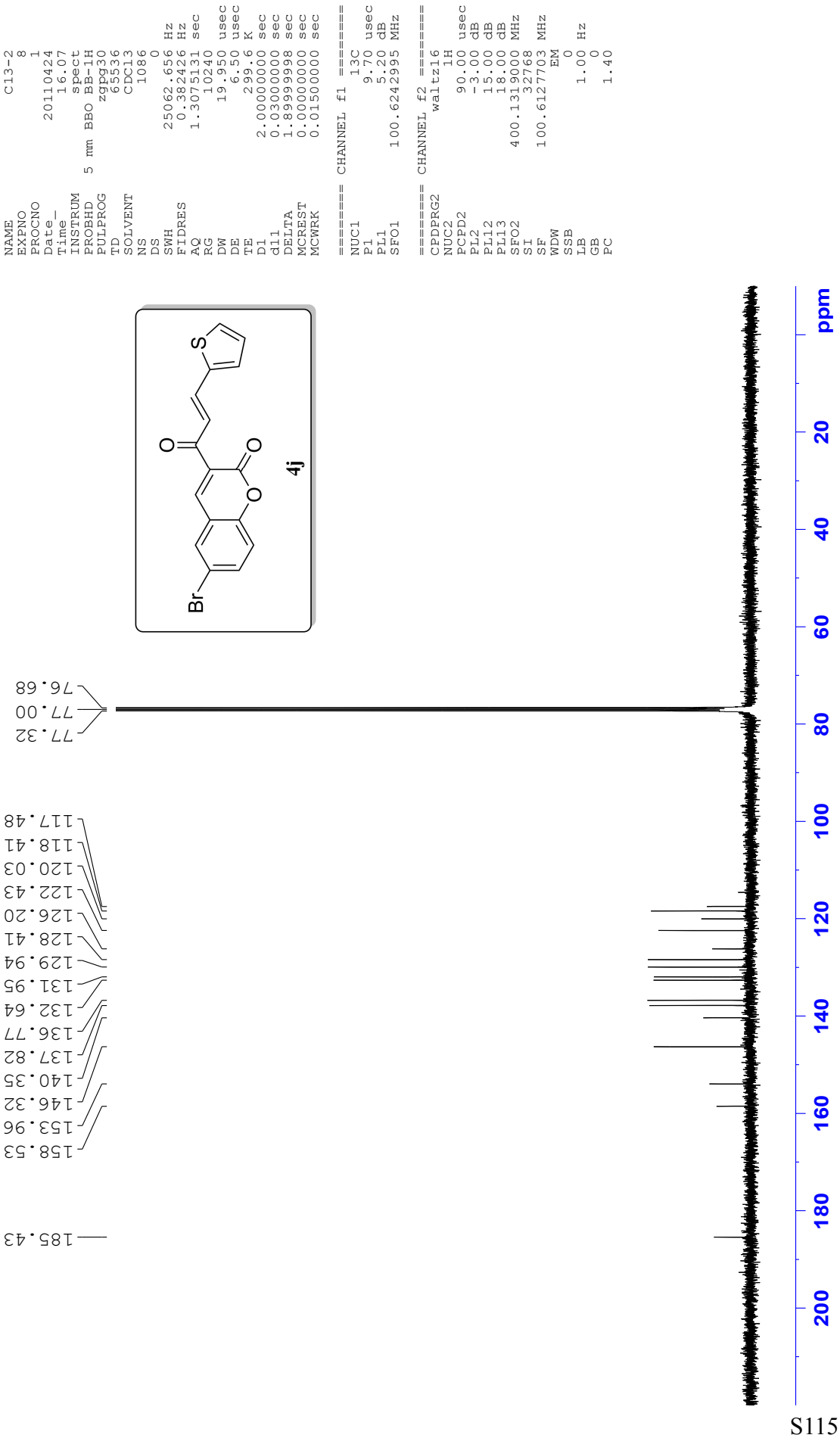


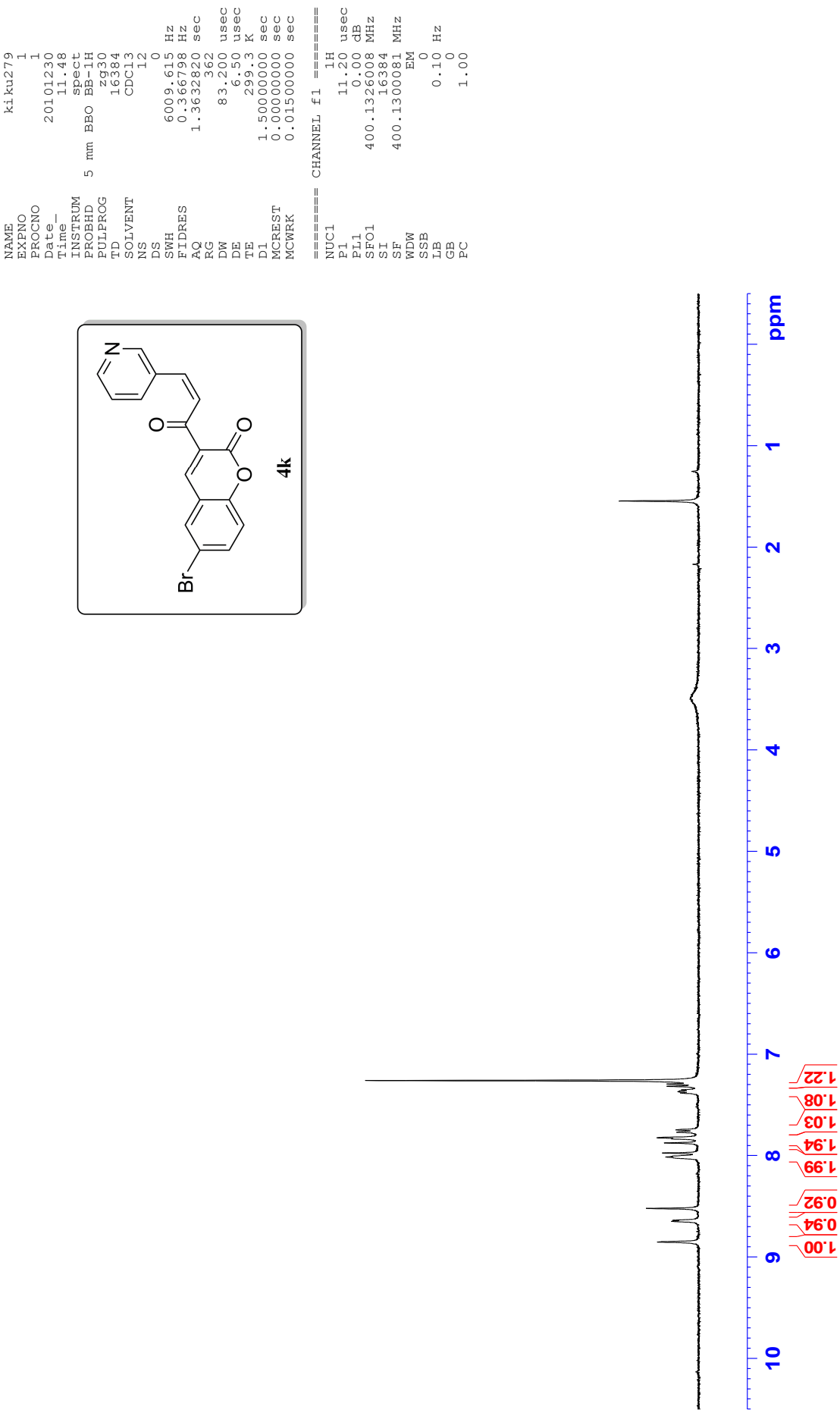
```
NAME                try-2
EXPNO                   3
PROCNO                  1
Date_            20110426
Time_               11.08
INSTRUM              spect
PROBHD   5 mm BBO BB-1H
PULPROG               zg30
TD                   16384
SOLVENT              CDC13
NS                      12
DS                       0
SWH                6009.615 Hz
FIDRES             0.366798 Hz
AQ                 1.3632820 sec
RG                     574.7
DW                    83.200 usec
DE                     6.50 usec
TE                    298.8 K
D1                 1.50000000 sec
MCREST             0.00000000 sec
MCWRK              0.01500000 sec

======== CHANNEL f1 ========
NUC1                      1H
P1                     11.20 usec
PL1                     0.00 dB
SFO1           400.1326008 MHz
SI                   16384
SF             400.1300083 MHz
WDW                      EM
SSB                       0
LB                     0.10 Hz
GB                        0
PC                     1.00
```

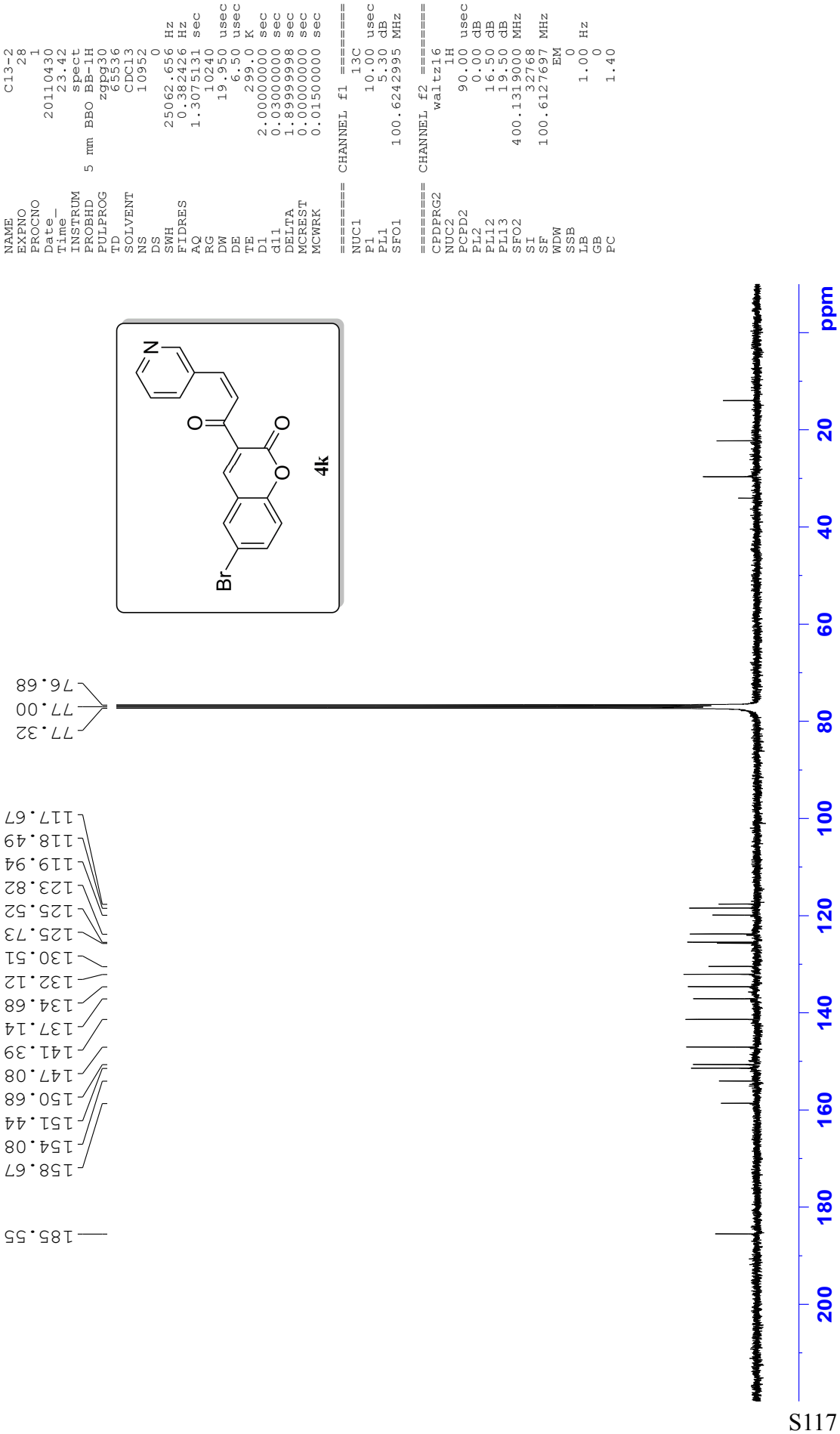


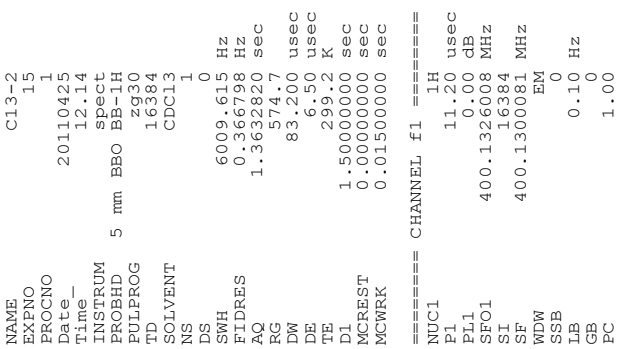


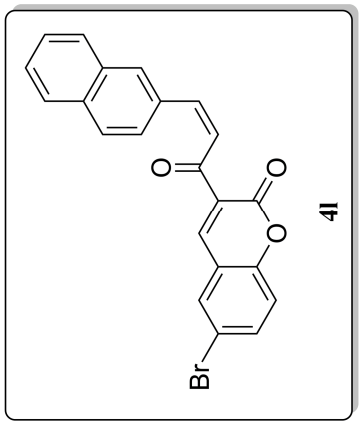


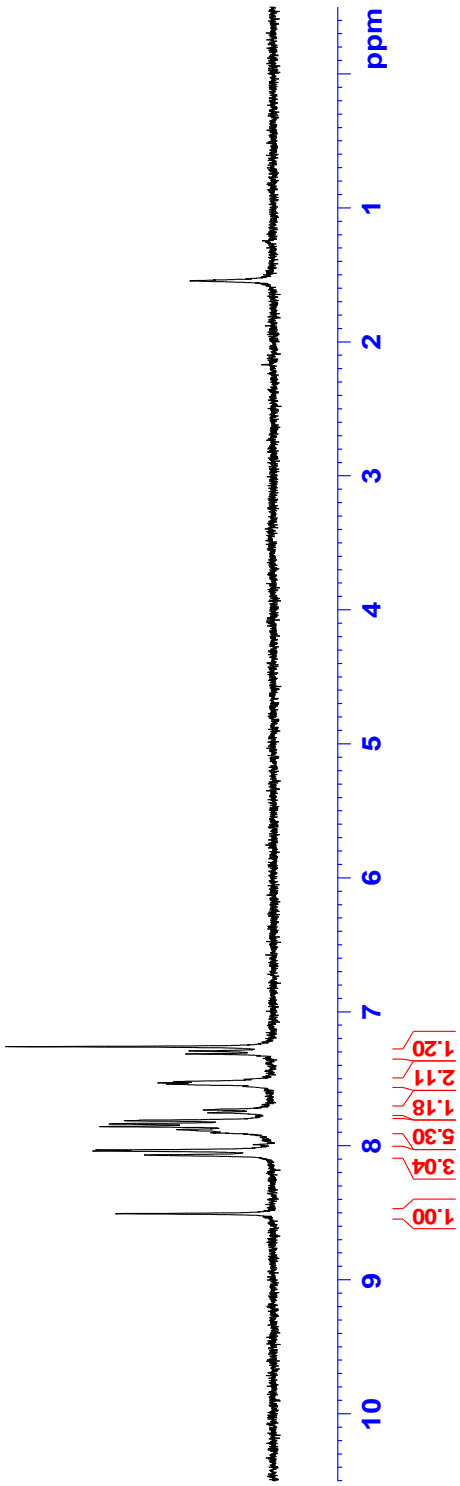


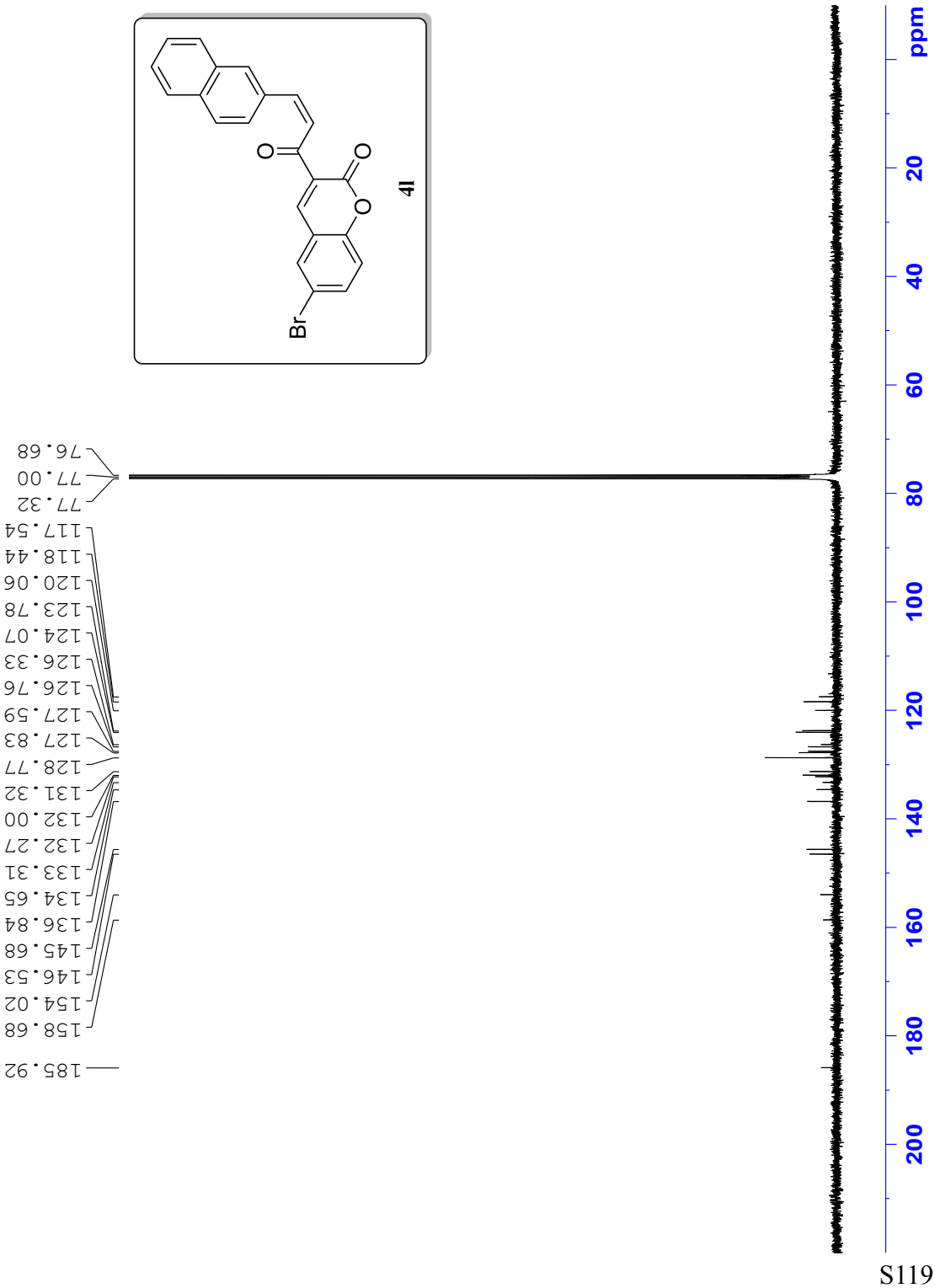

NAME kiku279
EXPNO 1
PROCNO 1
Date_ 20101230
Time_ 11.48
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 16384
SOLVENT CDCl3
NS 12
DS 0
SWH 6009.615 Hz
FIDRES 0.366798 Hz
AQ 1.3632820 sec
RG 362
DW 83.200 usec
DE 6.50 usec
TE 299.3 K
D1 1.50000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 11.20 usec
PL1 0.00 dB
SFO1 400.1326008 MHz
SI 16384
SF 400.1300081 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00
N
O
O
O
Br
4k
ppm
1
2
3
4
5
6
7
8
9
10
1.22
1.08
1.03
1.94
1.99
0.92
0.94
1.00



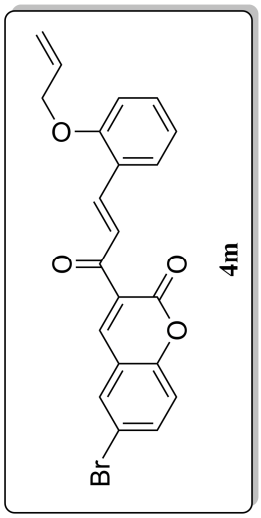


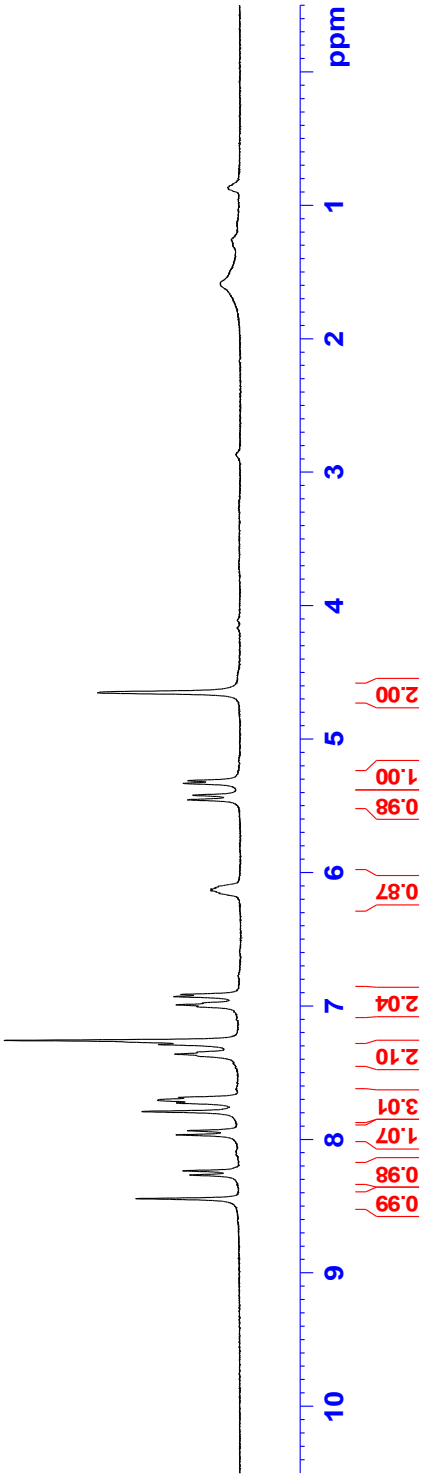


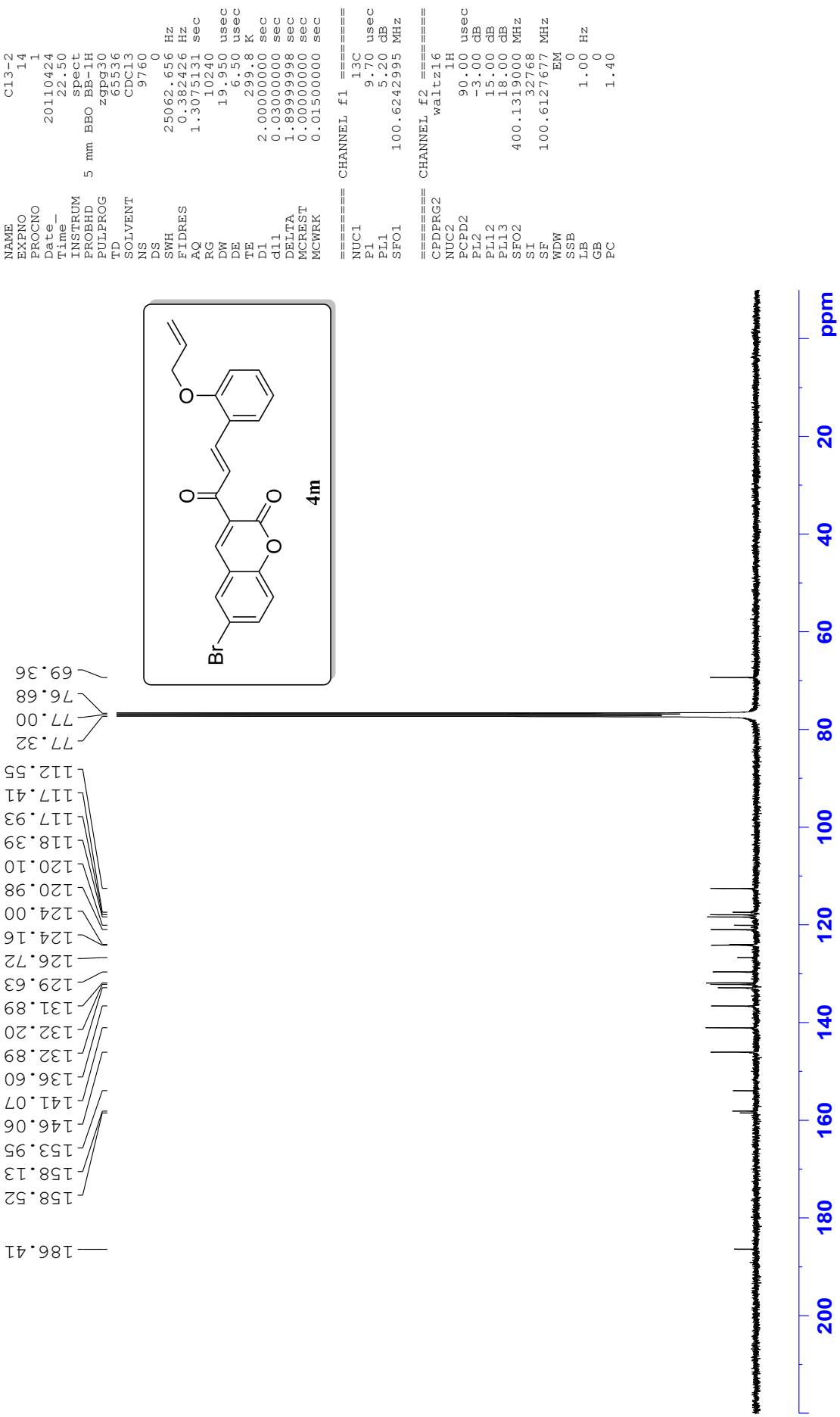


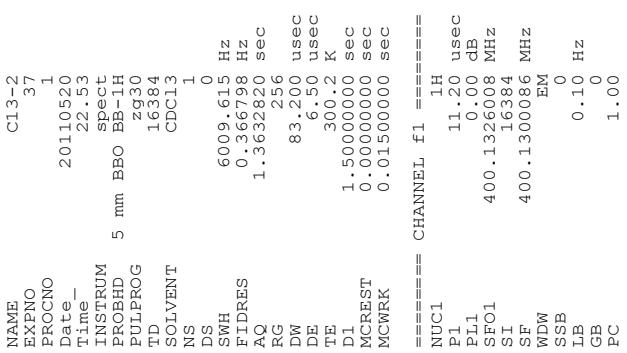


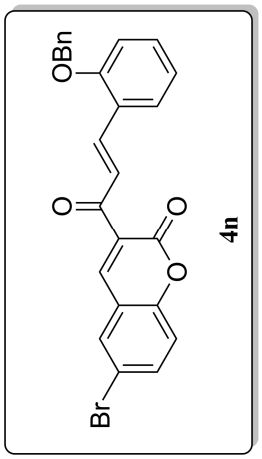
```
NAME                  C13-500
EXPNO                       7
PROCNO                      1
Date_                20110429
Time_                   17.41
INSTRUM                  spect
PROBHD     5 mm PABBO BB-
PULPROG                 zg30
TD                     16384
SOLVENT                CDCl3
NS                        48
DS                         0
SWH                7507.507 Hz
FIDRES             0.458222 Hz
AQ                 1.0912910 sec
RG                       456.1
DW                      66.600 usec
DE                       6.50 usec
TE                      300.0 K
D1                 2.00000000 sec
MCREST             0.00000000 sec
MCWRK              0.01500000 sec

========== CHANNEL f1 ==========
NUC1                        1H
P1                       14.00 usec
PL1                       0.00 dB
SFO1               500.1332508 MHz
SI                     16384
SF                 500.1300120 MHz
WDW                        EM
SSB                         0
LB                       0.10 Hz
GB                          0
PC                       1.00
```

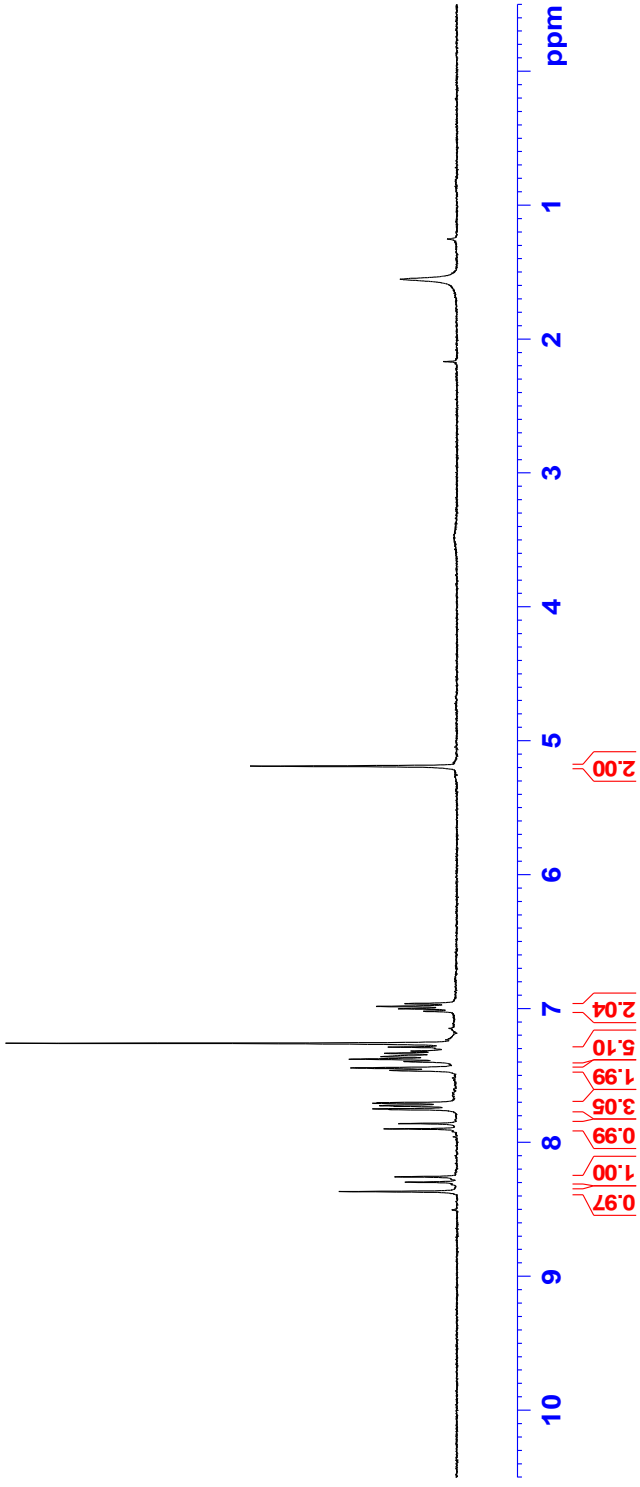


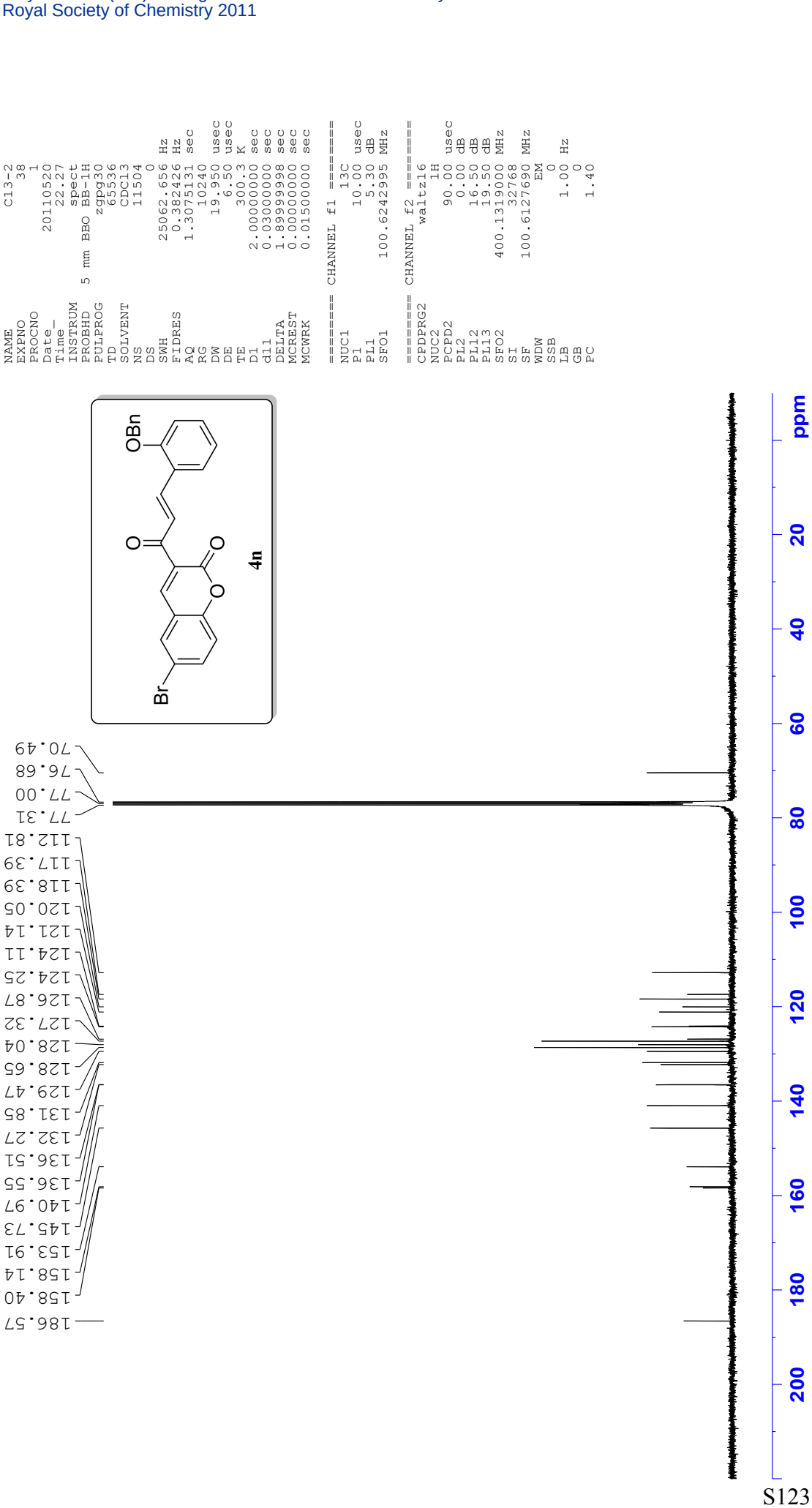


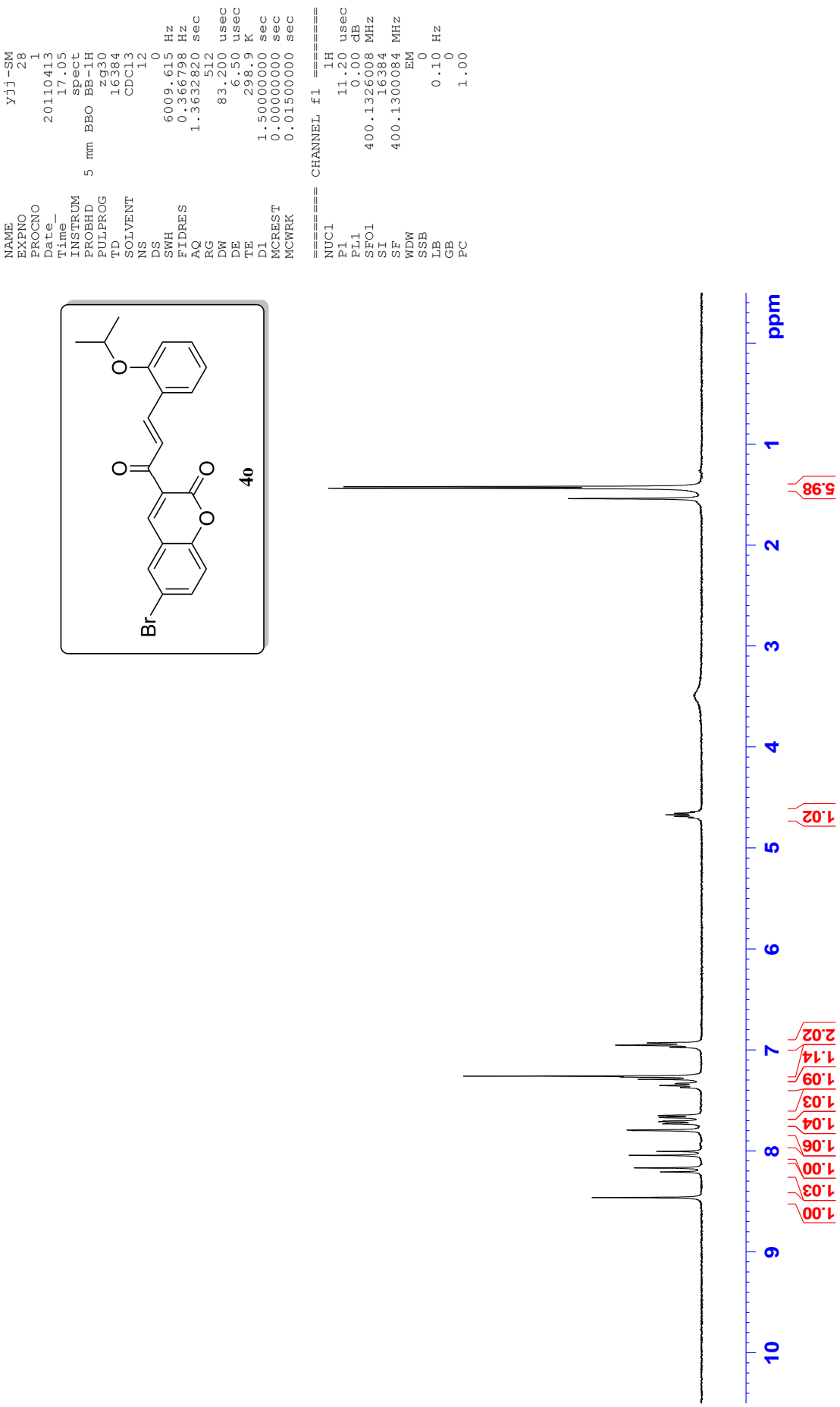


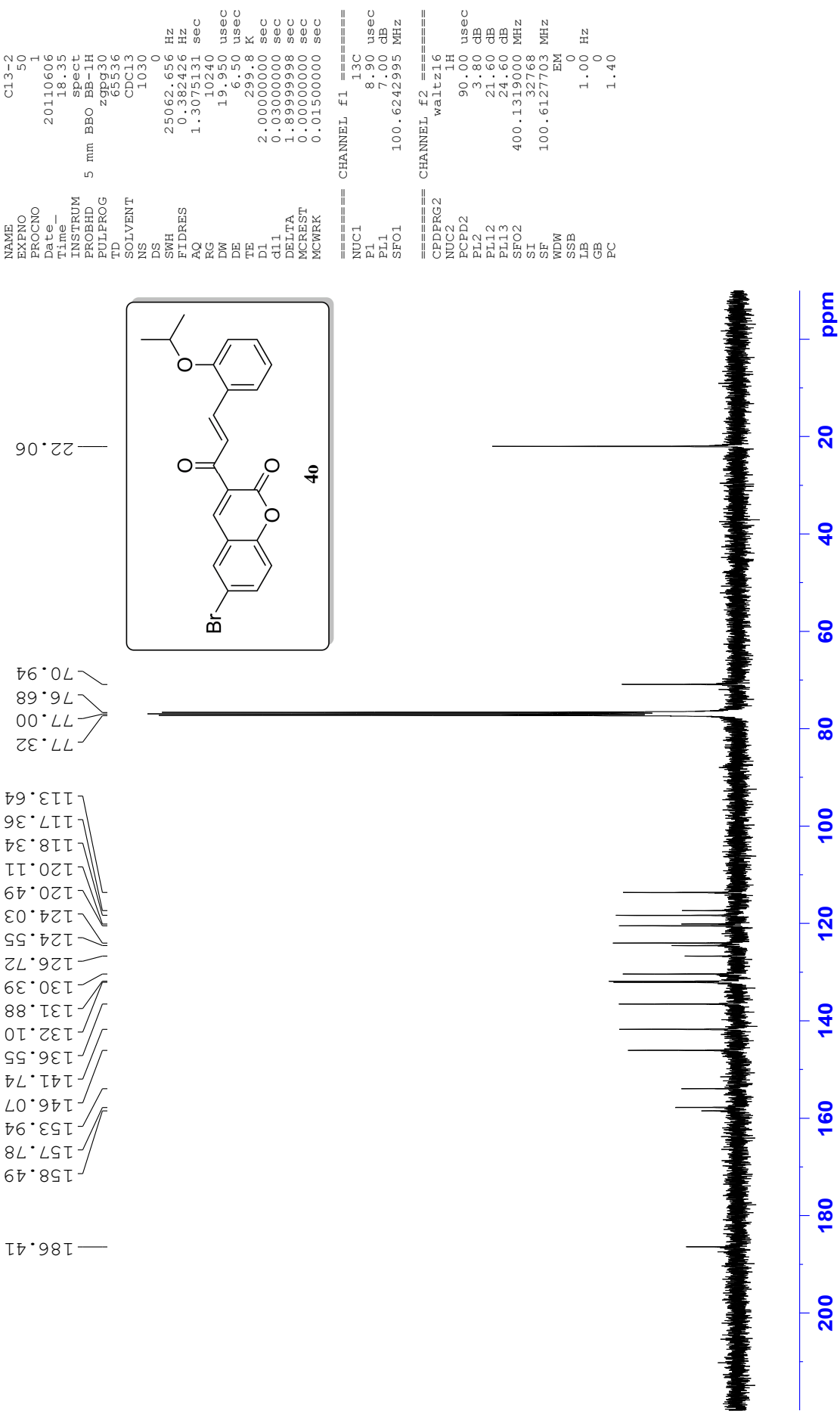


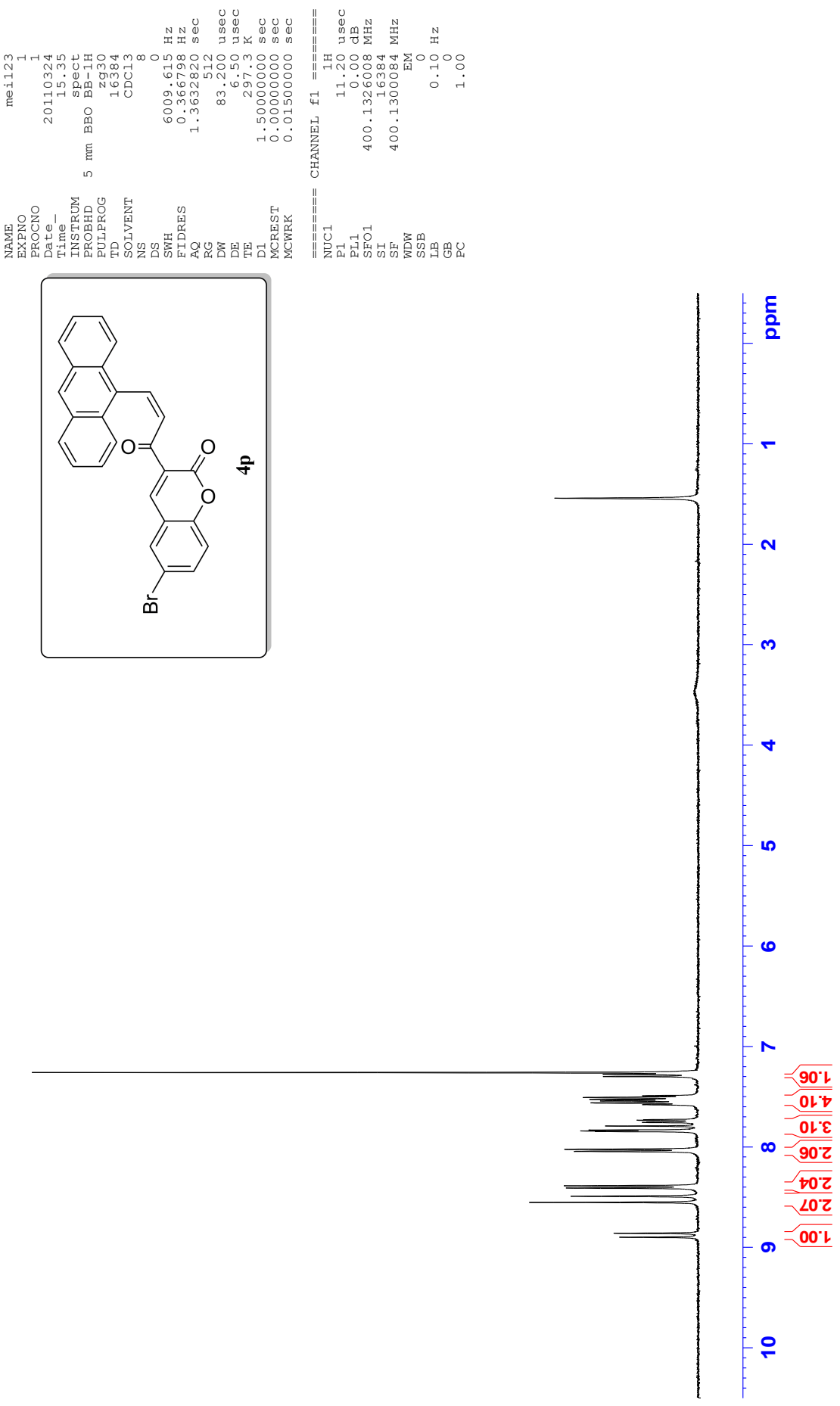


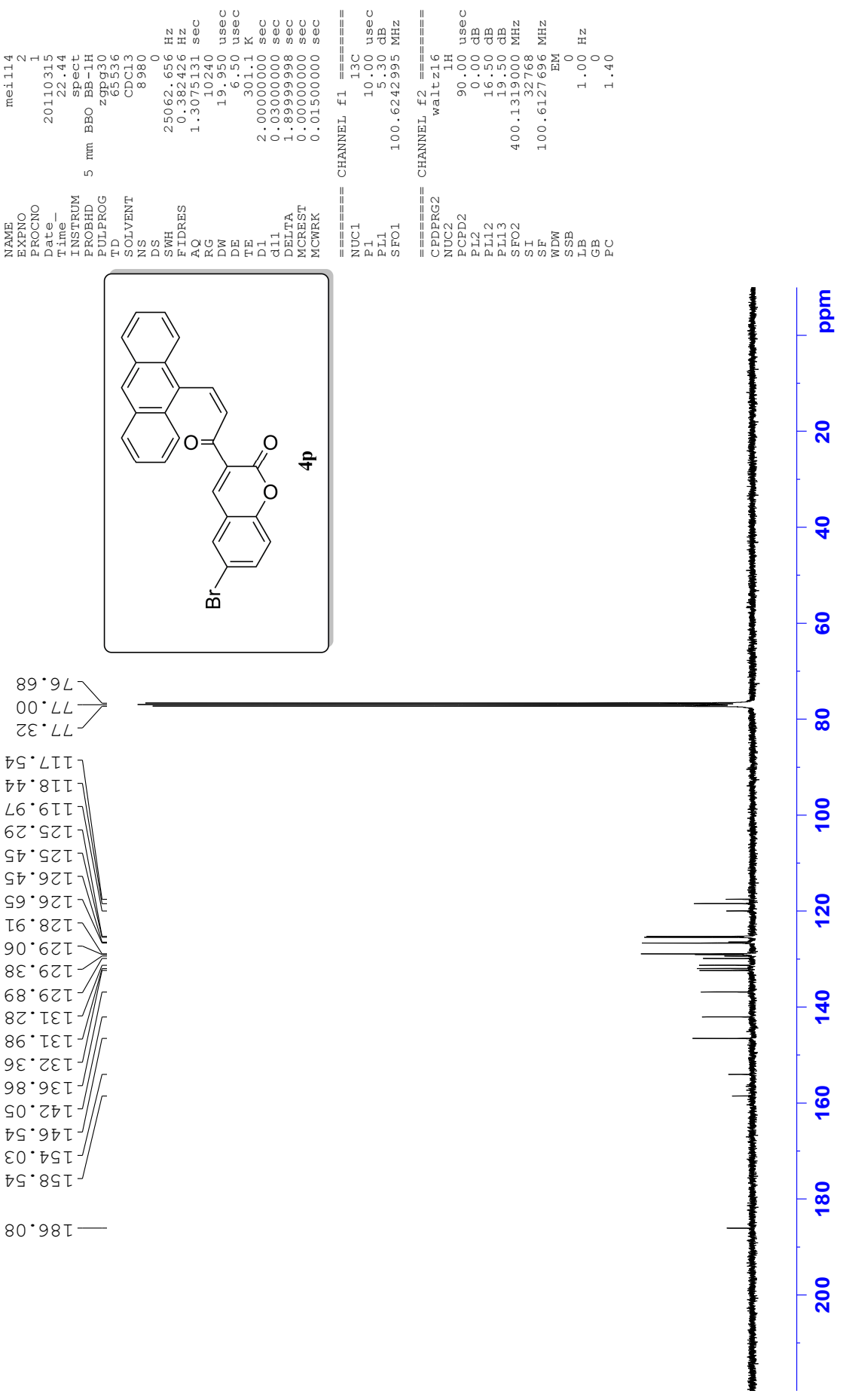




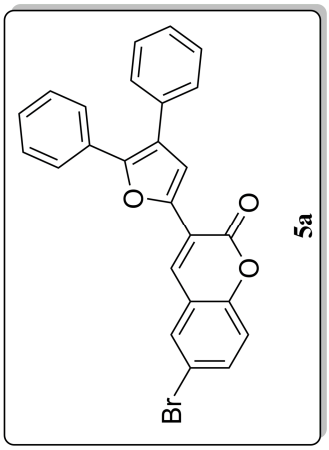


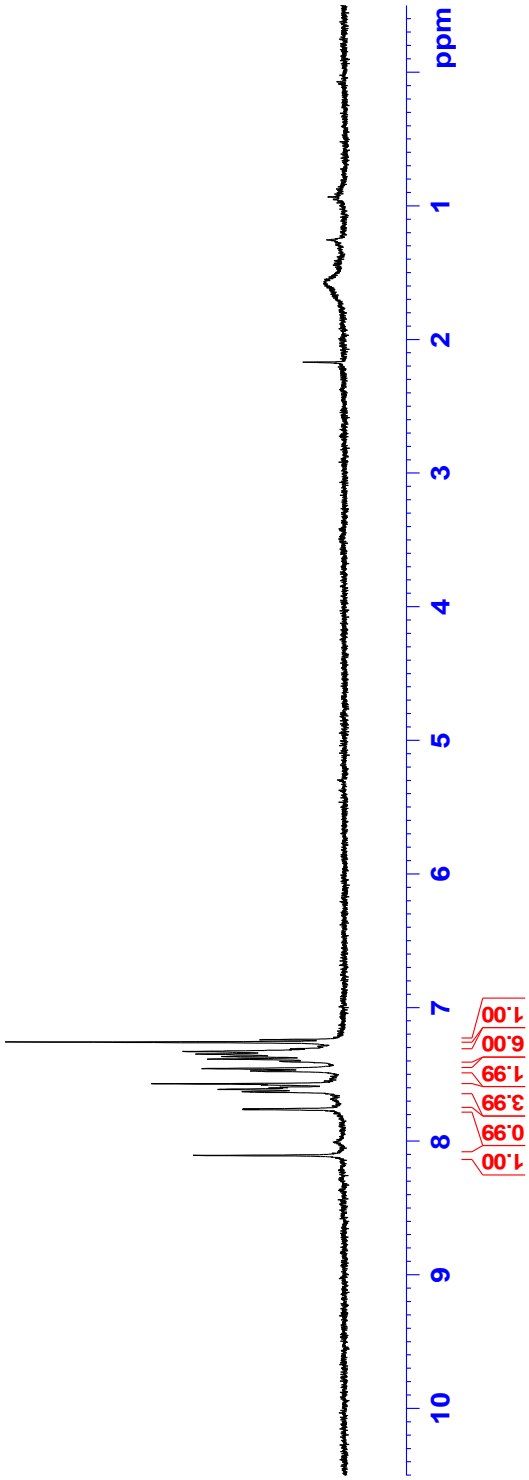


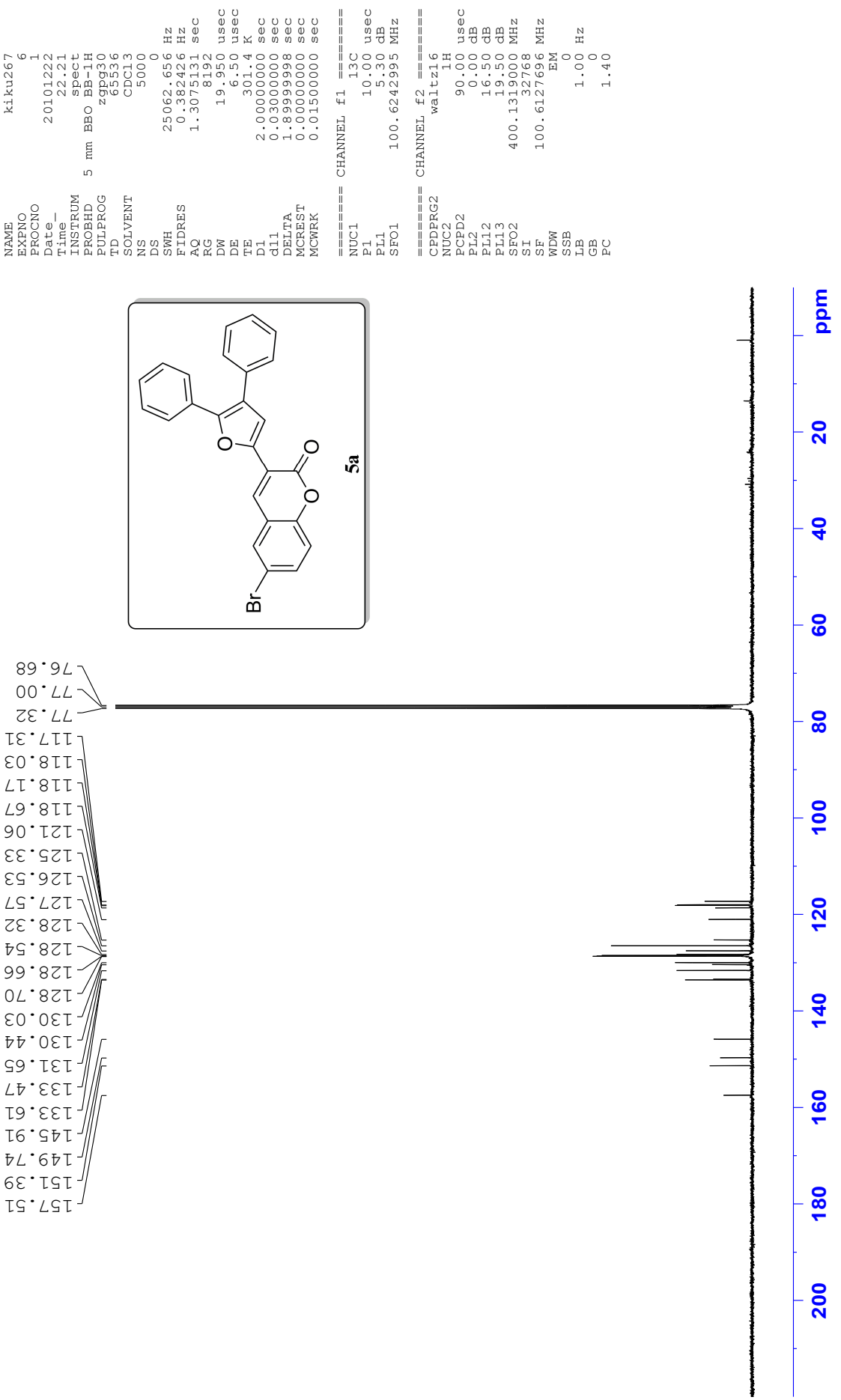


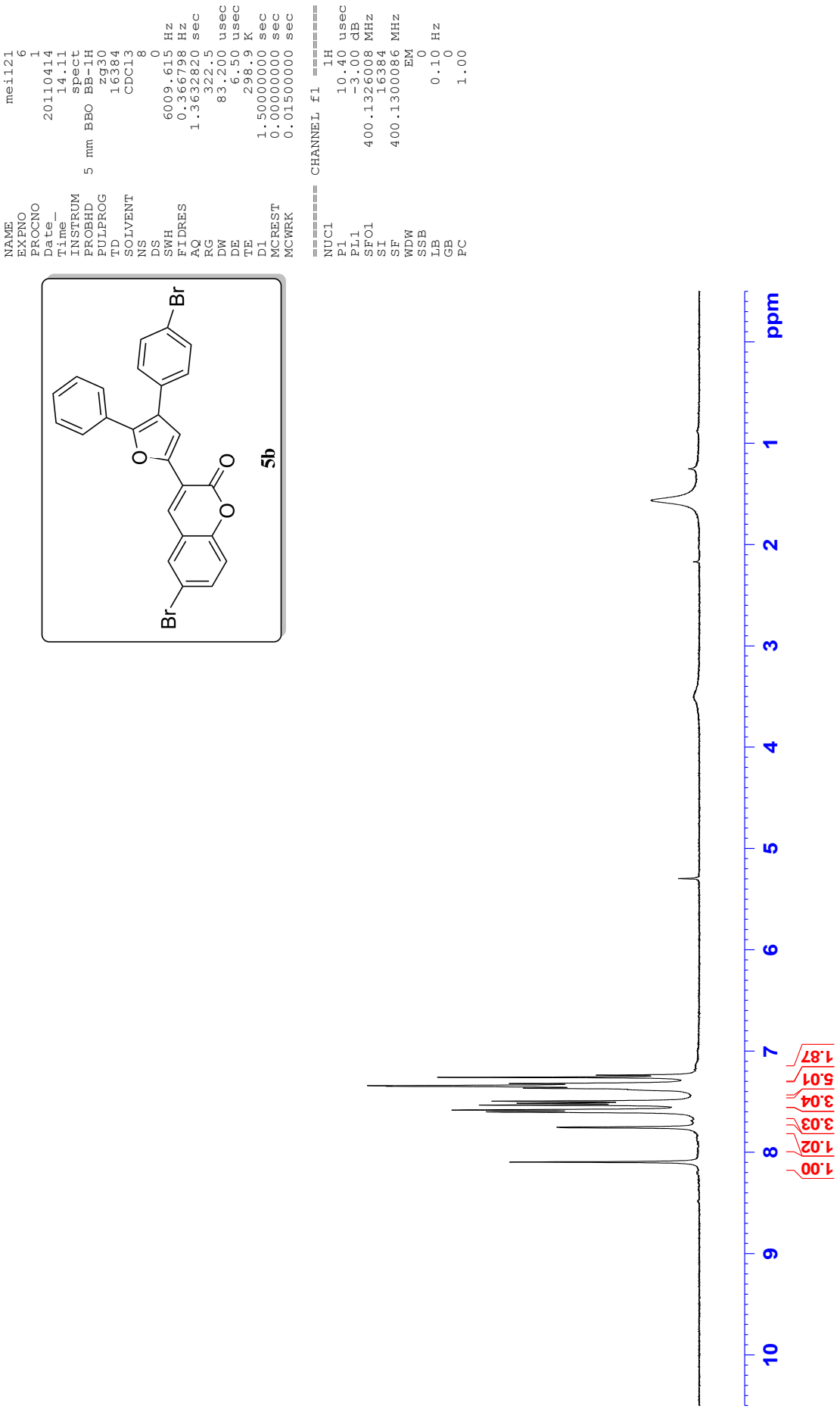


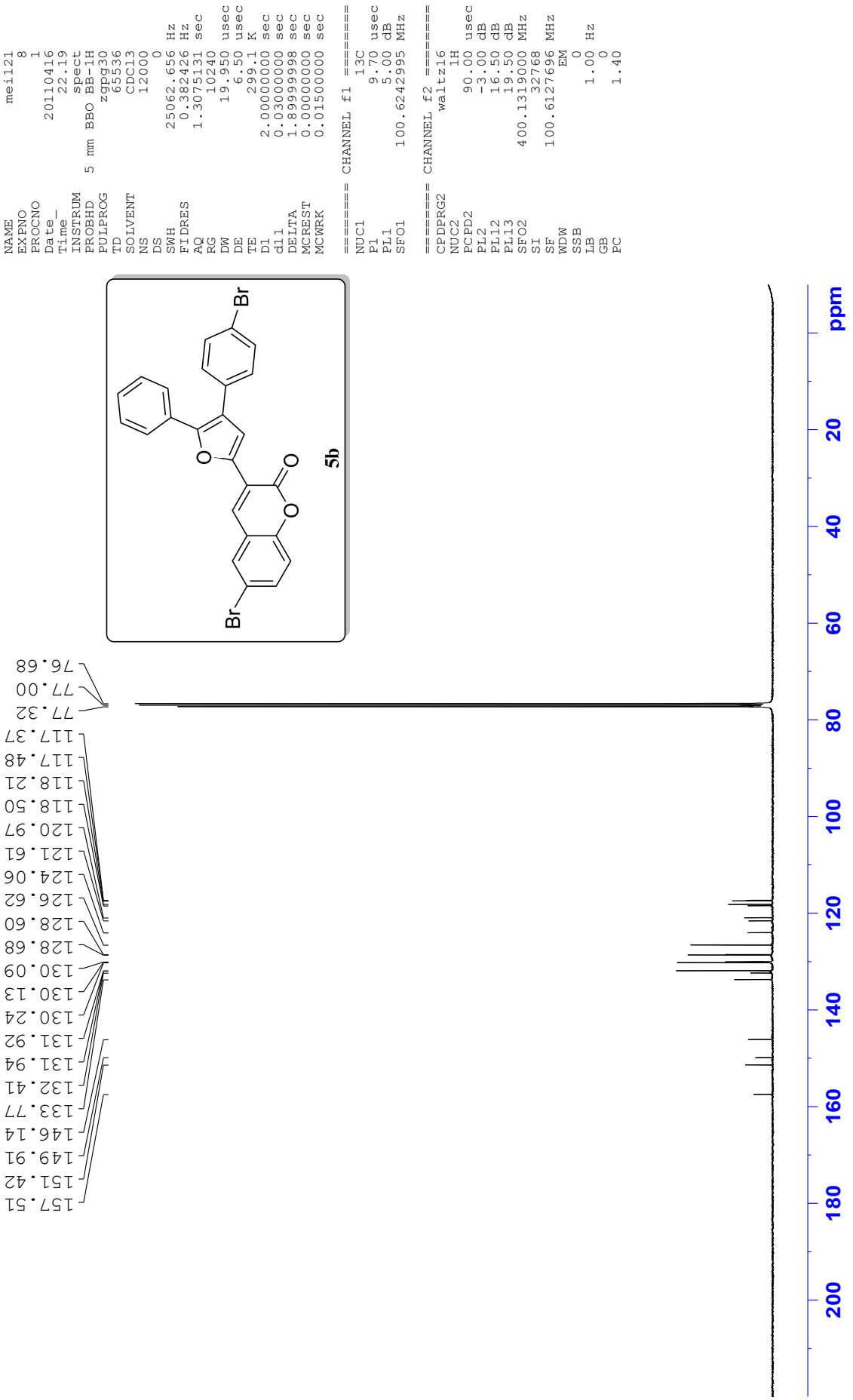
```
NAME          Br-Ph chalcone
EXPNO                      2
PROCNO                     1
Date_           20110424
Time_              15.52
INSTRUM             spect
PROBHD   5 mm BBO BB-1H
PULPROG             zg30
TD                 16384
SOLVENT            CDCl3
NS                    12
DS                     0
SWH              6009.615 Hz
FIDRES           0.366798 Hz
AQ               1.3632820 sec
RG                   512
DW                  83.200 usec
DE                   6.50 usec
TE                  299.5 K
D1               1.50000000 sec
MCREST           0.00000000 sec
MCWRK            0.01500000 sec

========== CHANNEL f1 ==========
NUC1                   1H
P1                  11.20 usec
PL1                  0.00 dB
SFO1          400.1326008 MHz
SI                 16384
SF            400.1300085 MHz
WDW                   EM
SSB                    0
LB                  0.10 Hz
GB                     0
PC                  1.00
```

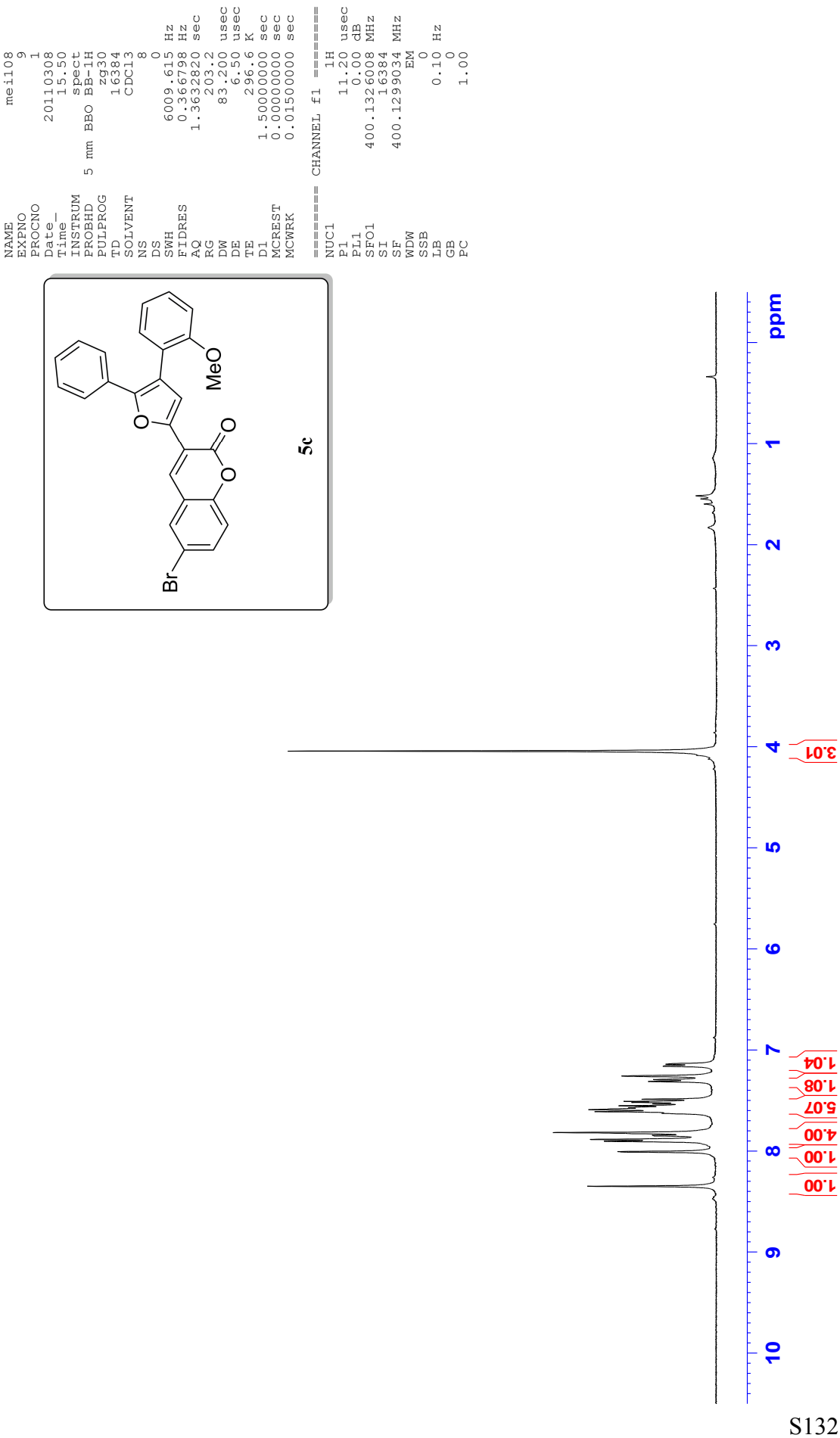


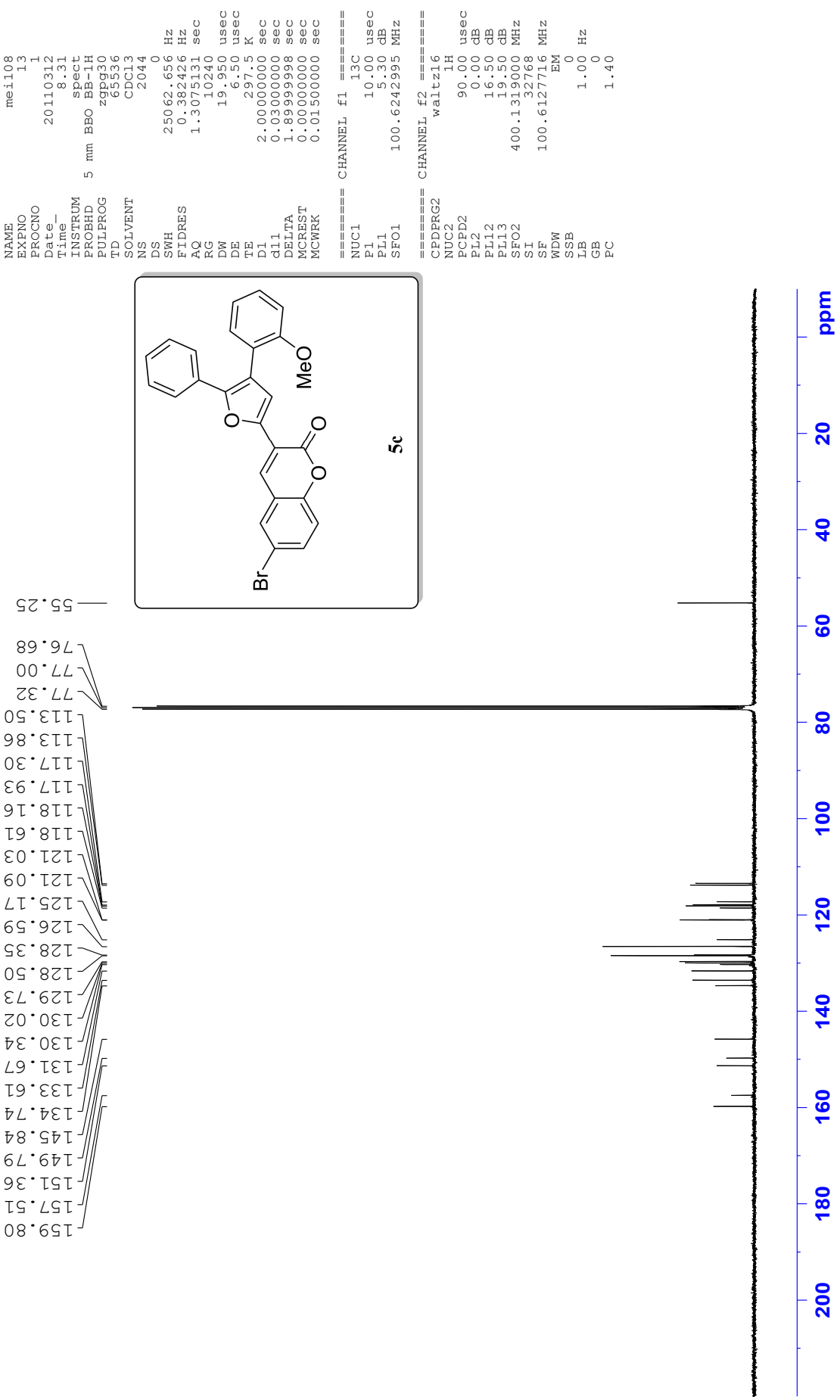


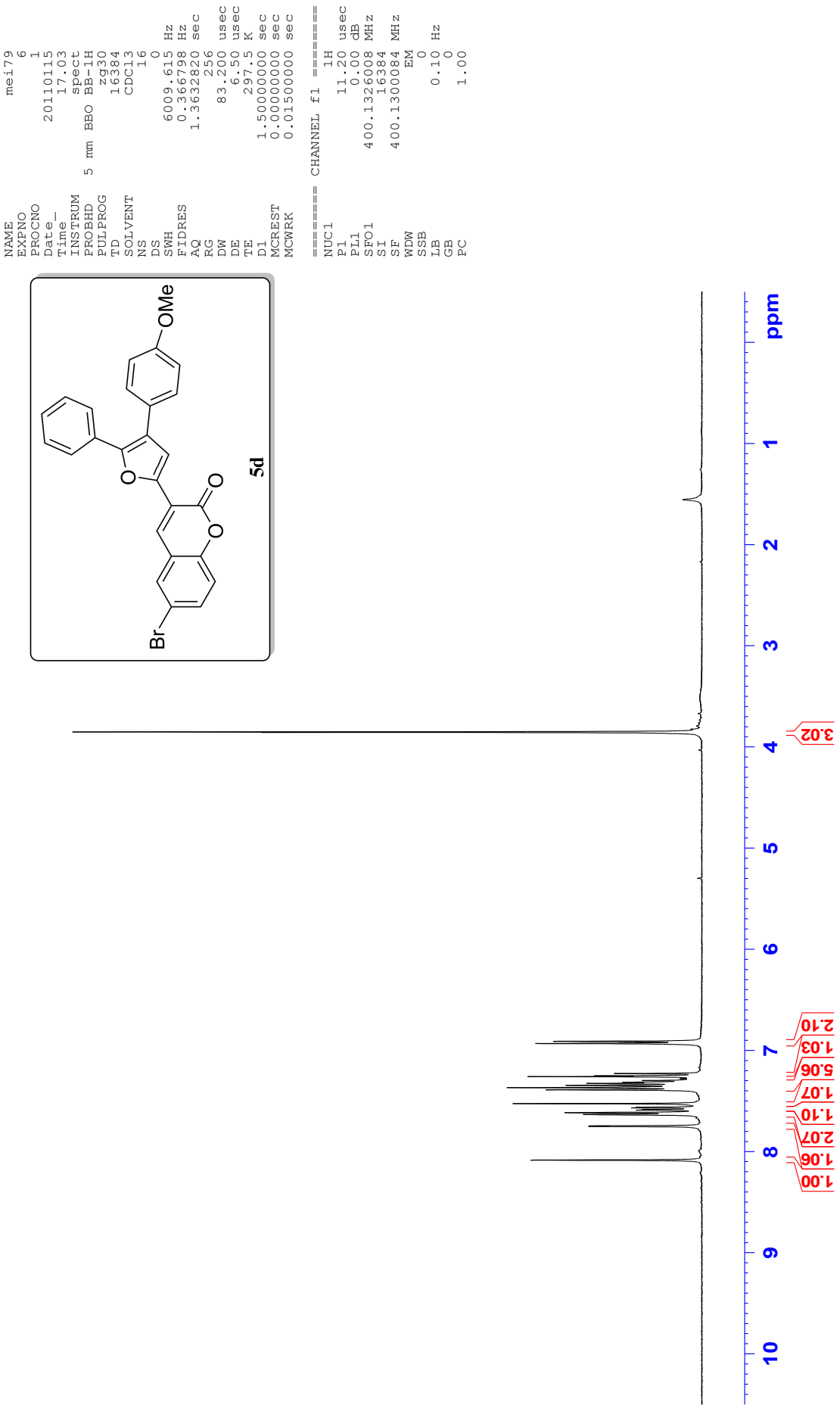


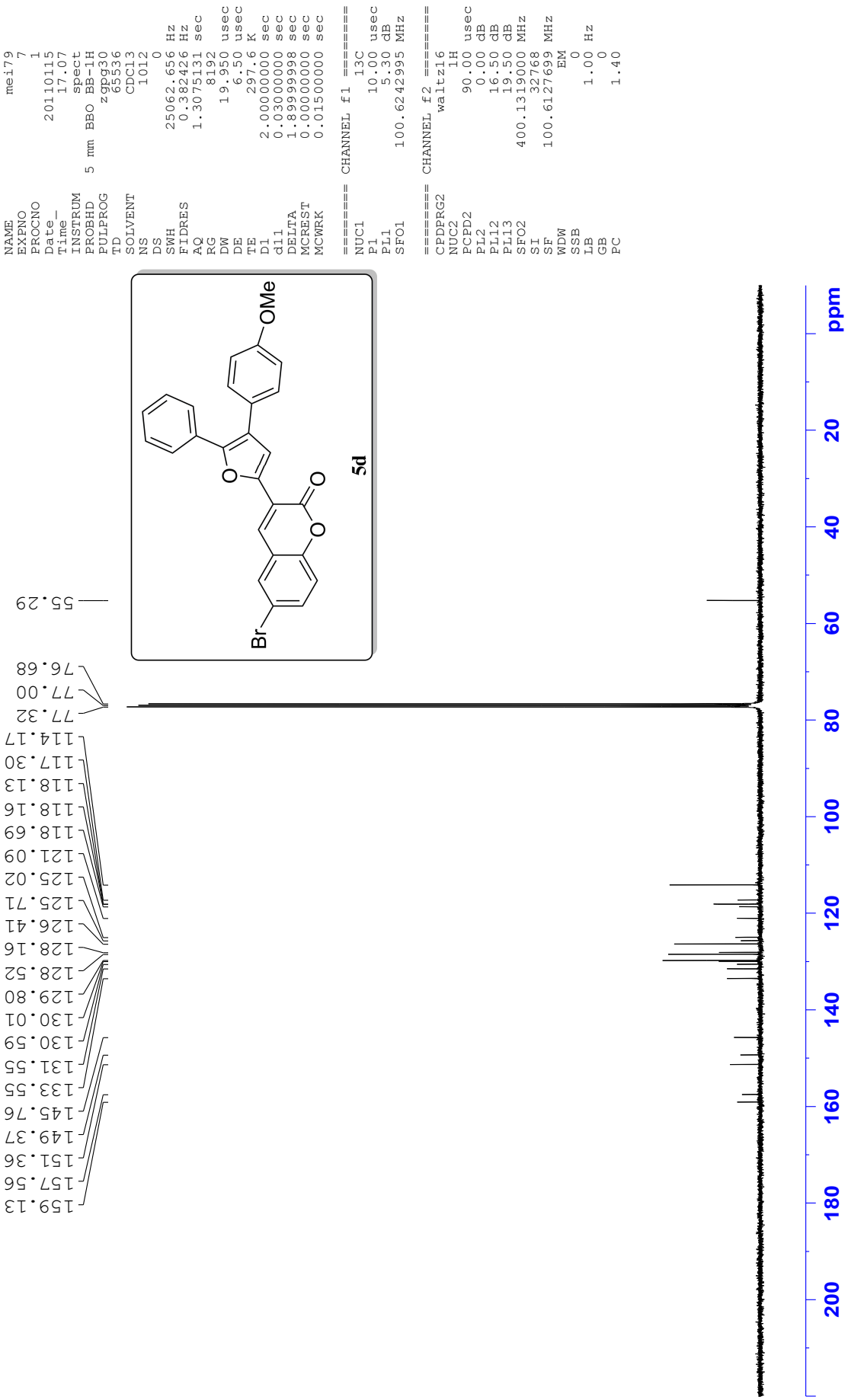


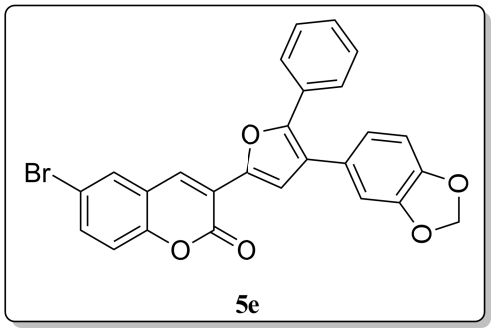






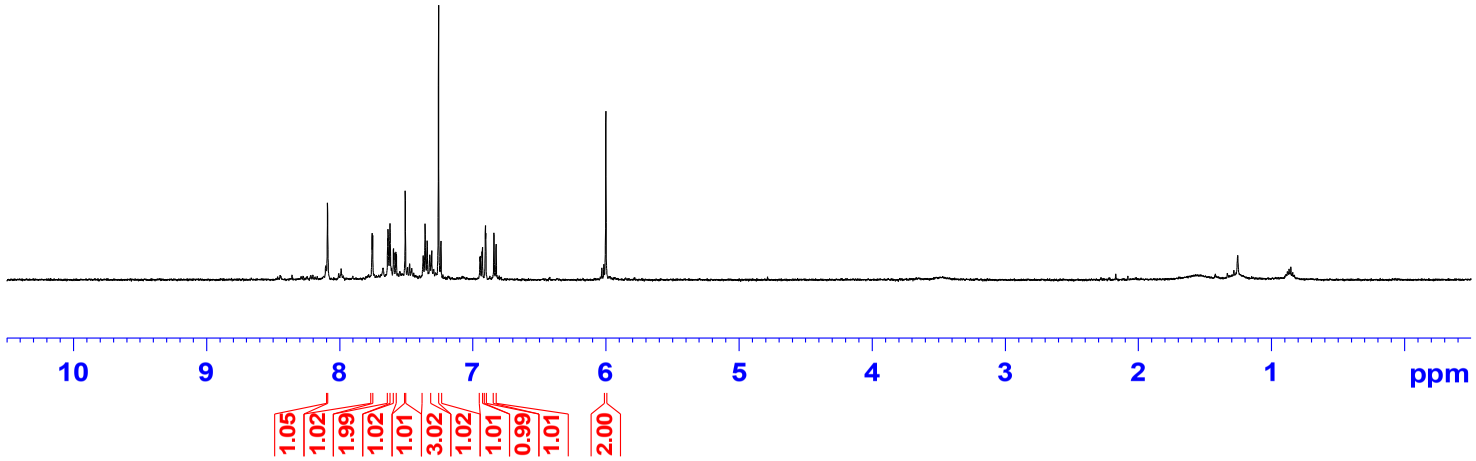


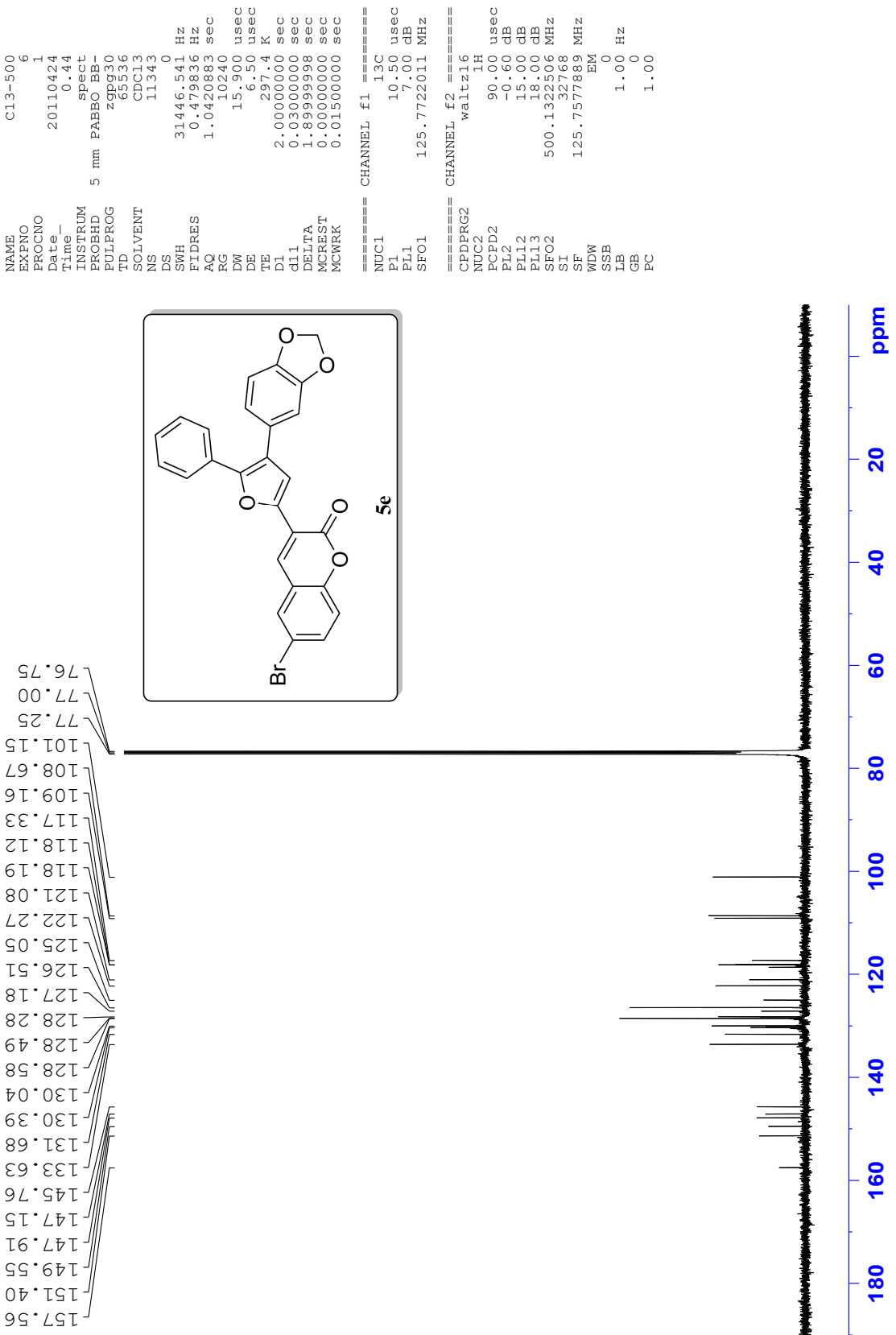


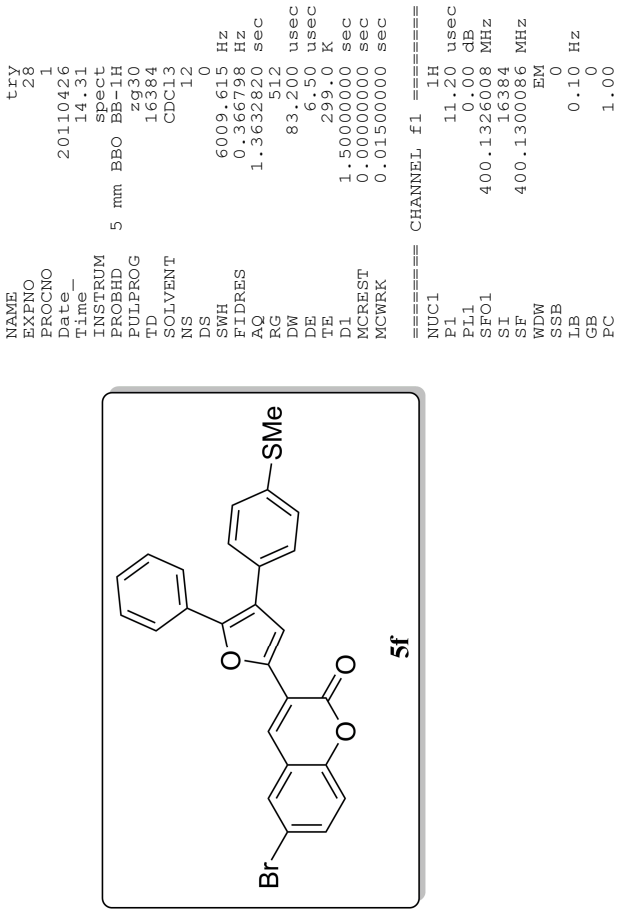


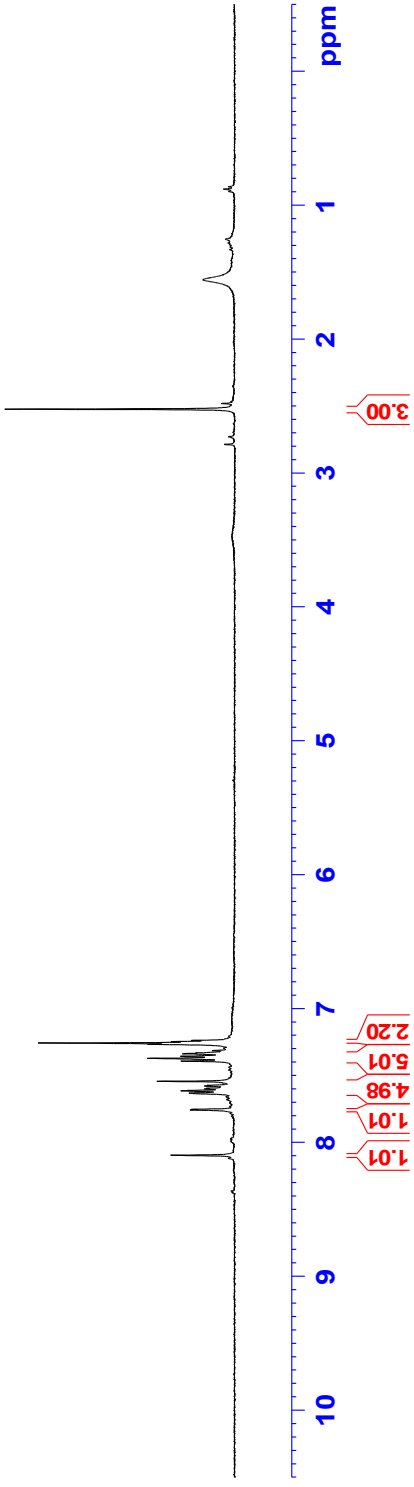
5e

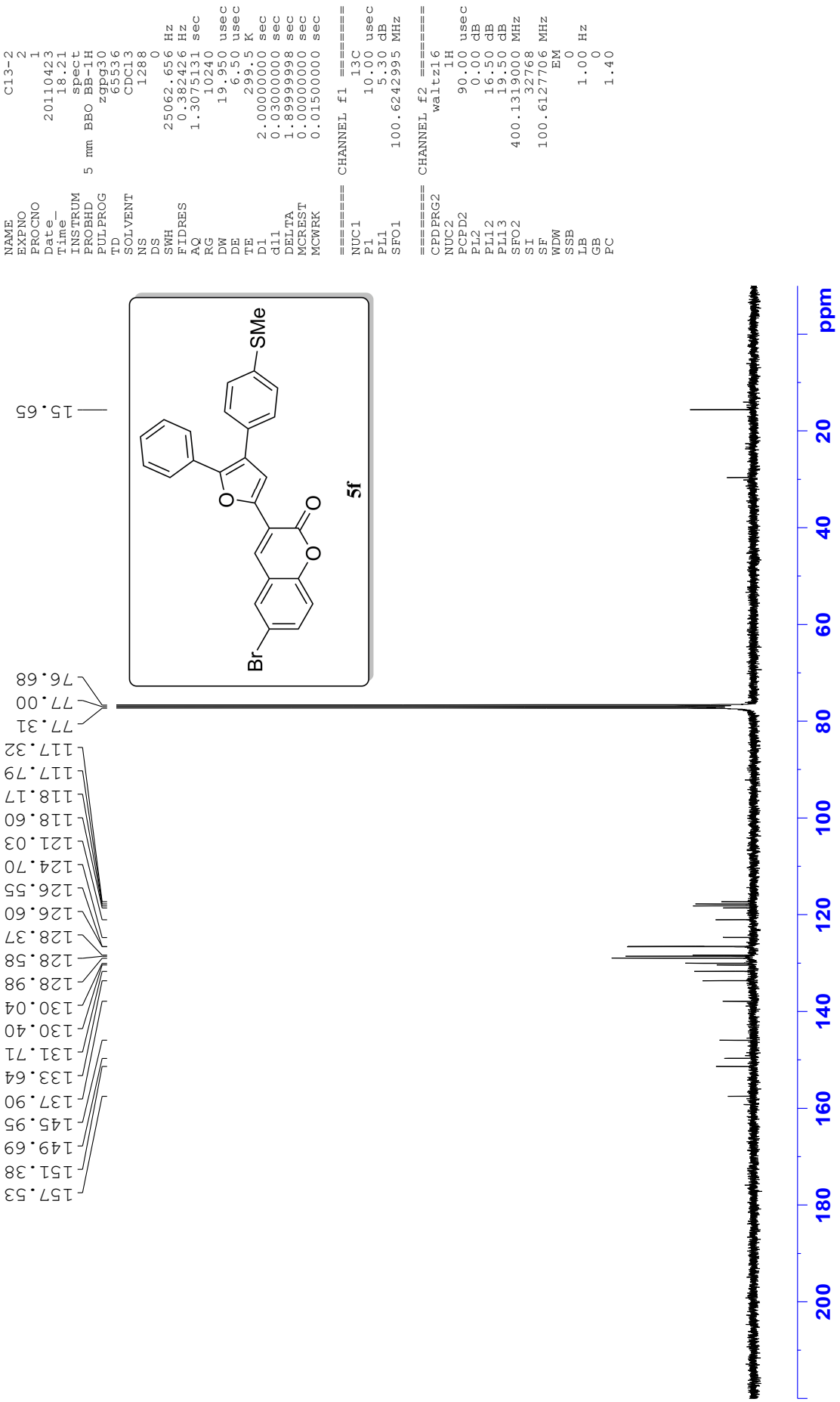
NAME	C13-500
EXPNO	5
PROCNO	1
Date_	20110424
Time	0.43
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	16384
SOLVENT	CDCl3
NS	1
DS	0
SWH	7507.507 Hz
FIDRES	0.458222 Hz
AQ	1.0912910 sec
RG	456.1
DW	66.600 usec
DE	6.50 usec
TE	297.4 K
D1	2.00000000 sec
MCREST	0.00000000 sec
MCWRK	0.01500000 sec
======== CHANNEL f1 ========	
NUC1	1H
P1	14.00 usec
PL1	0.00 dB
SFO1	500.1332508 MHz
SI	16384
SF	500.1300128 MHz
WDW	EM
SSB	0
LB	0.10 Hz
GB	0
PC	1.00

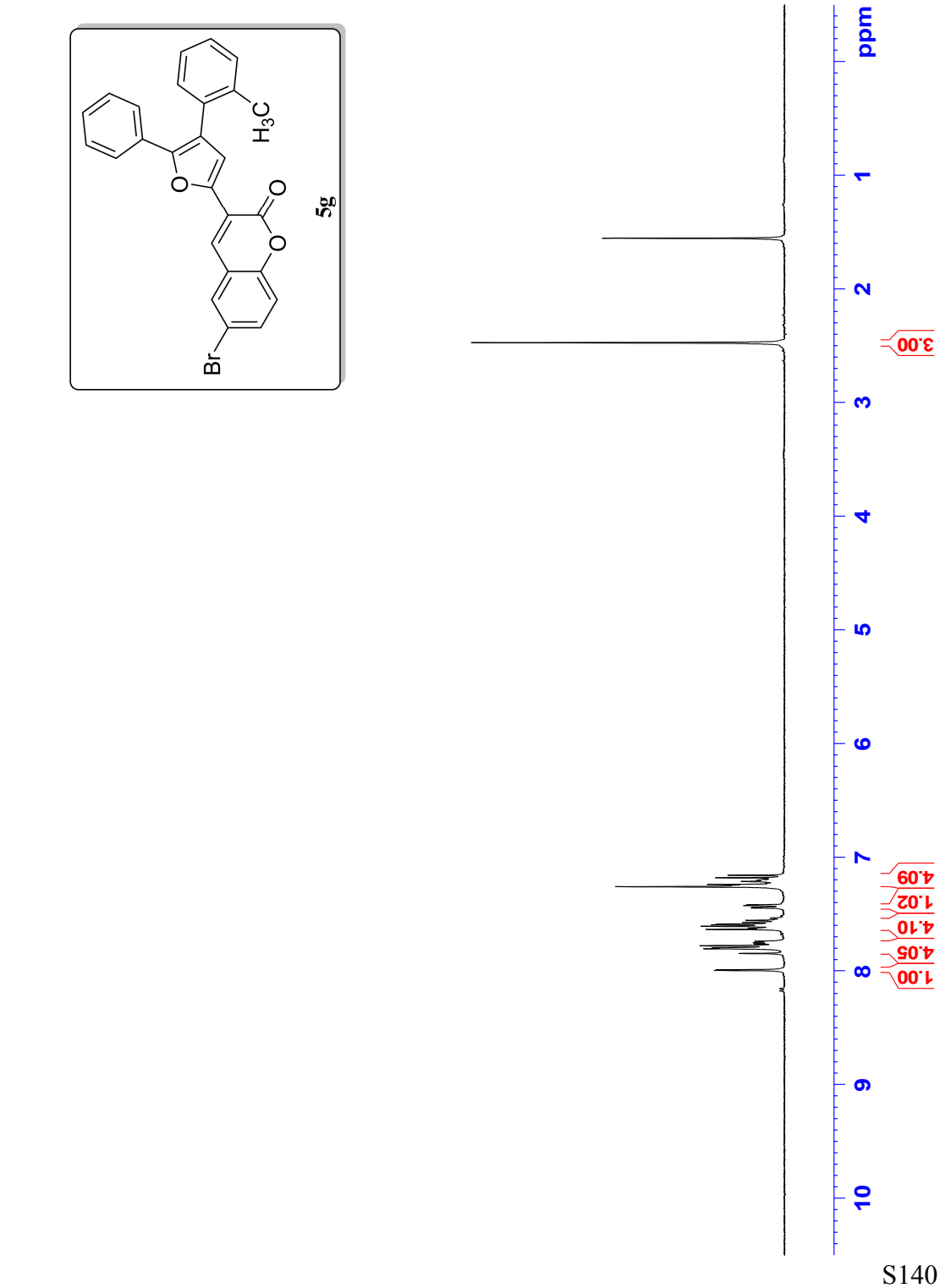


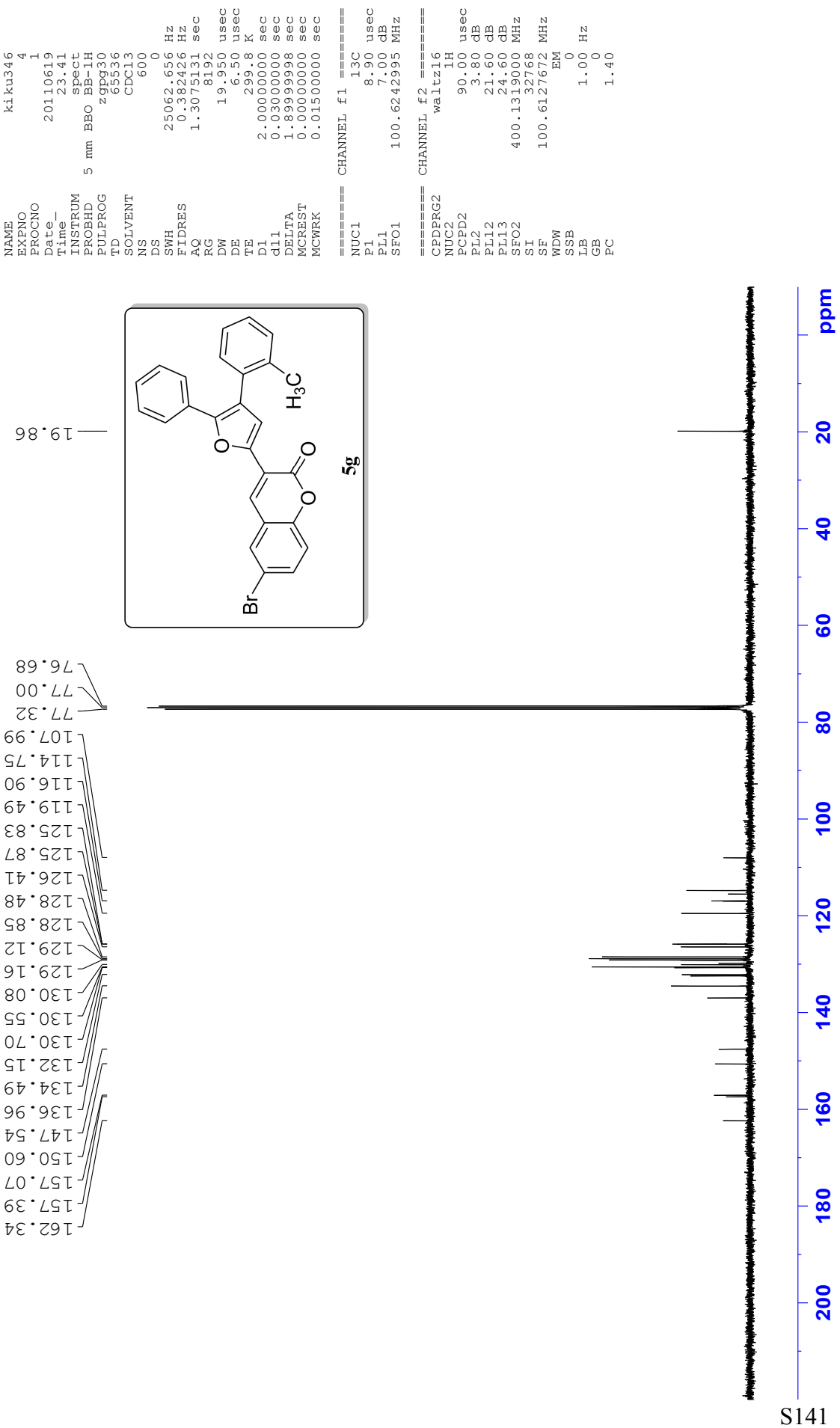








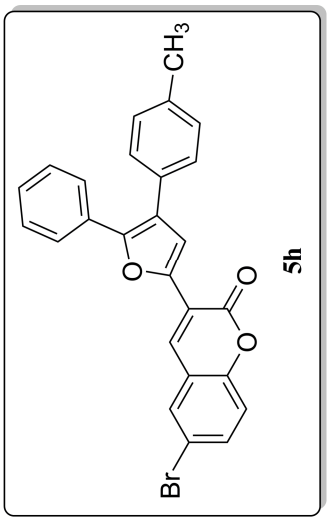


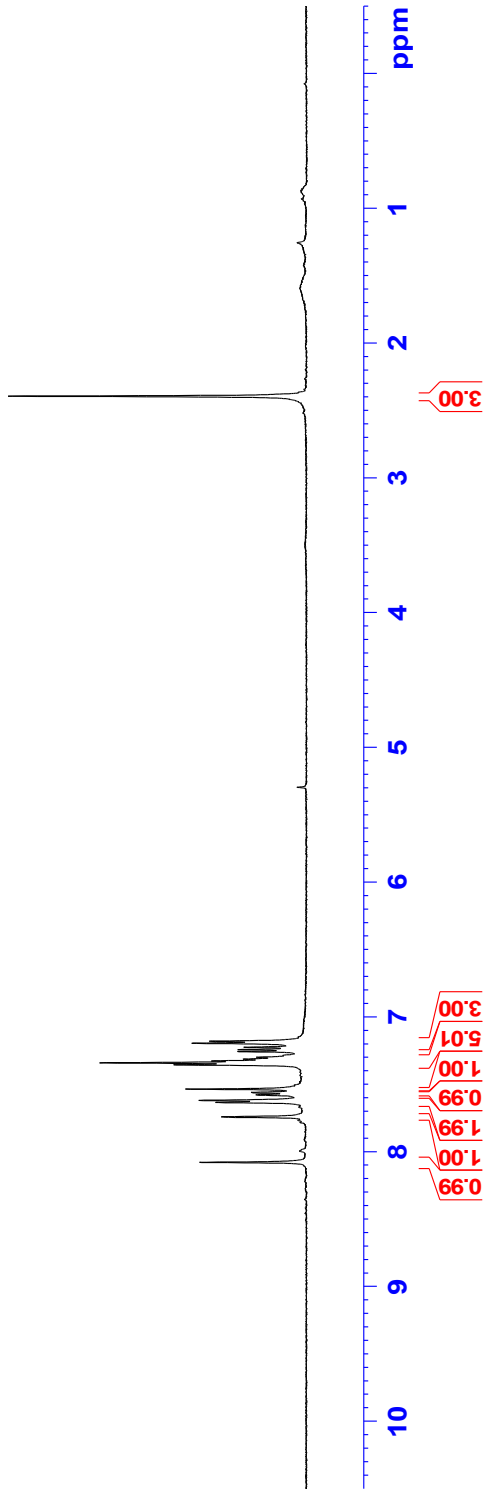

NAME kiku346
EXPNO 4
PROCNO 1
Date_ 20110619
Time_ 23.41
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 600
DS 0
SWH 25062.656 Hz
FIDRES 0.382426 Hz
AQ 1.3075131 sec
RG 8192
DW 19.950 usec
DE 6.50 usec
TE 299.8 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 8.90 usec
PL1 7.00 dB
SFO1 100.6242995 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 3.80 dB
PL12 21.60 dB
PL13 24.60 dB
SFO2 400.1319000 MHz
SI 32768
SF 100.6127672 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
5g
Br
O
O
O
H3C
19.86
77.32
77.00
76.68
107.99
114.75
116.90
119.49
125.83
125.87
126.41
128.48
128.85
129.12
129.16
130.08
130.55
130.70
132.15
134.49
136.96
147.54
150.60
157.07
157.39
162.34
ppm
200
180
160
140
120
100
80
60
40
20

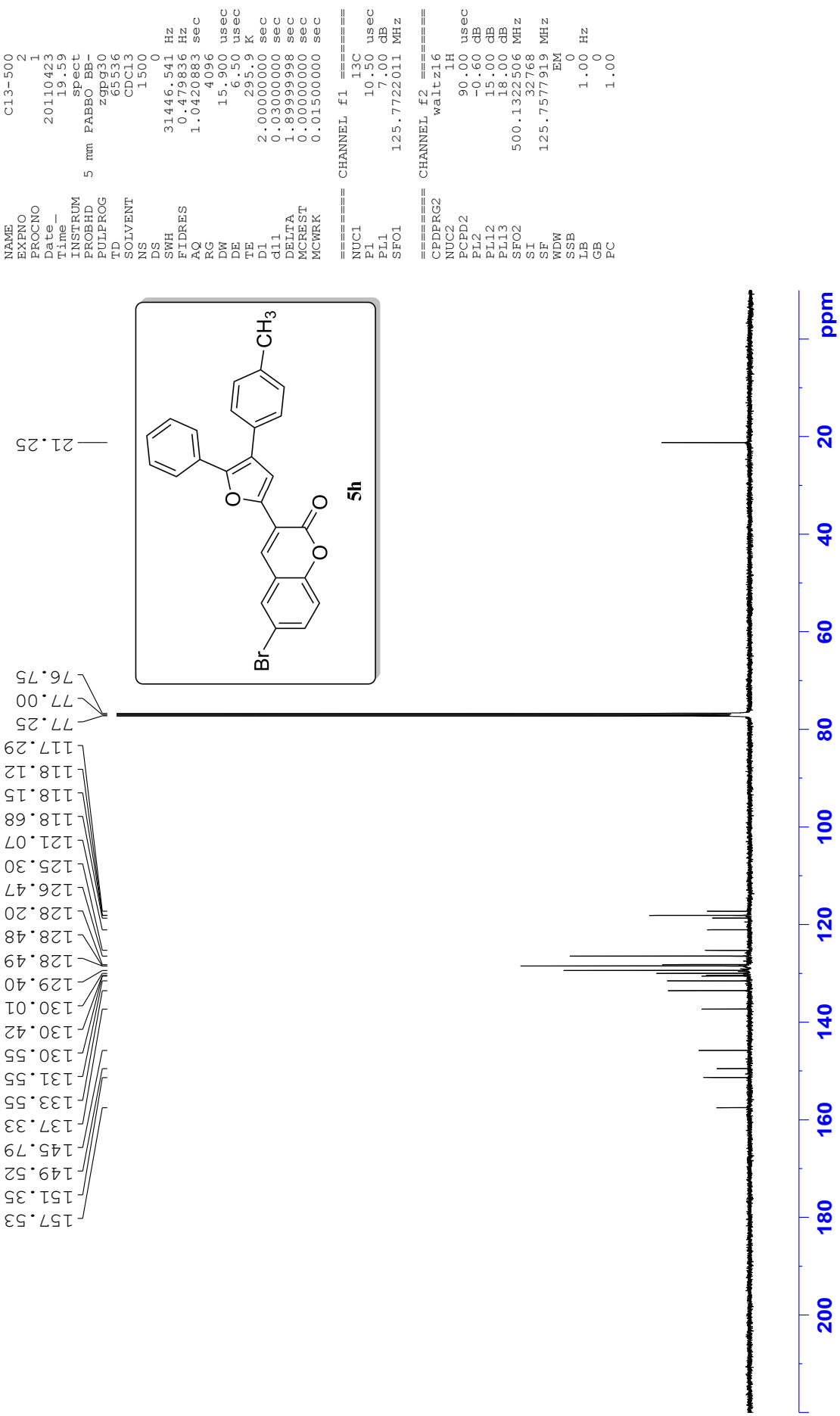
```
C13-500
      1
      1
20110423
   19.58
   spect
5 mm PABBO BB-
   zg30
  16384
  CDC13
      1
      0
 7507.507 Hz
 0.458222 Hz
1.0912910 sec
  228.1
  66.600 usec
   6.50 usec
  295.8 K
2.00000000 sec
0.00000000 sec
0.01500000 sec

======== CHANNEL f1 ========
   1H
  14.00 usec
   0.00 dB
500.1332508 MHz
  16384
500.1300126 MHz
     EM
      0
   0.10 Hz
      0
   1.00
```

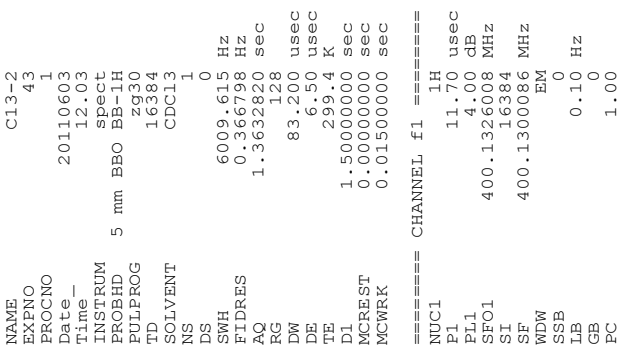
NAME
EXPNO
PROCNO
Date_
Time_
INSTRUM
PROBHD
PULPROG
TD
SOLVENT
NS
DS
SWH
FIDRES
AQ
RG
DW
DE
TE
D1
MCREST
MCWRK

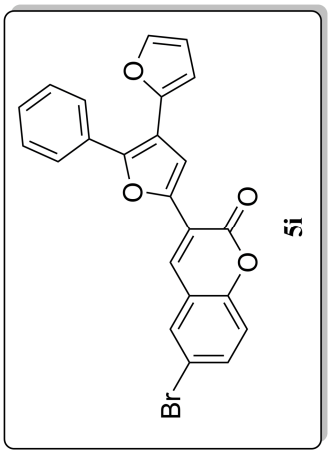
NUC1
P1
PL1
SFO1
SI
SF
WDW
SSB
LB
GB
PC

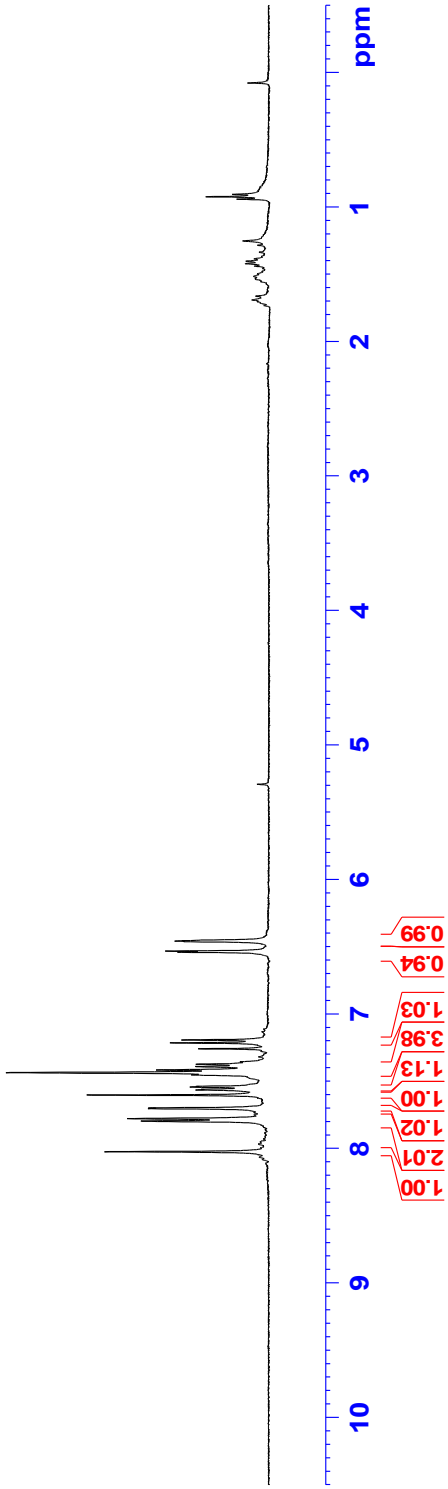


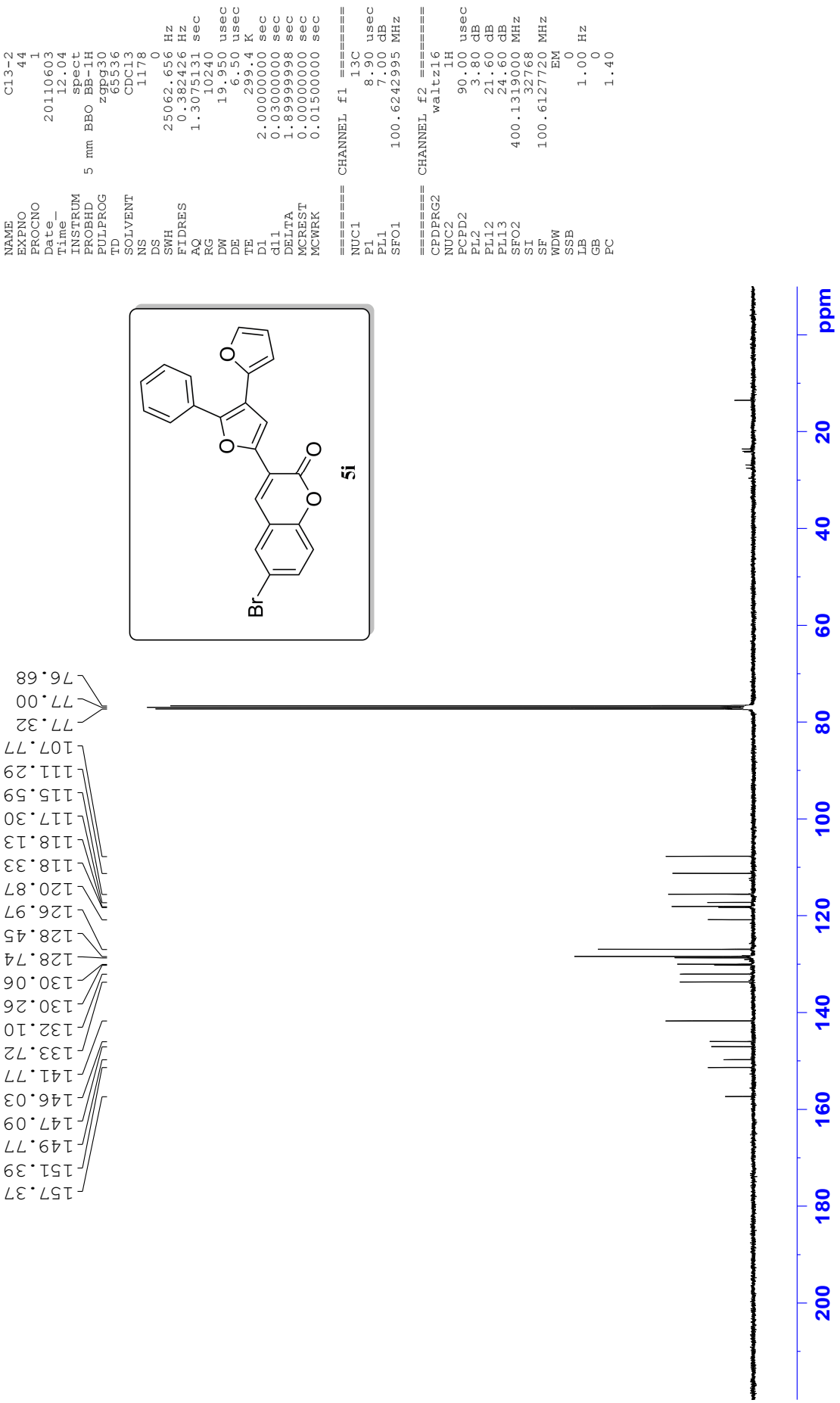


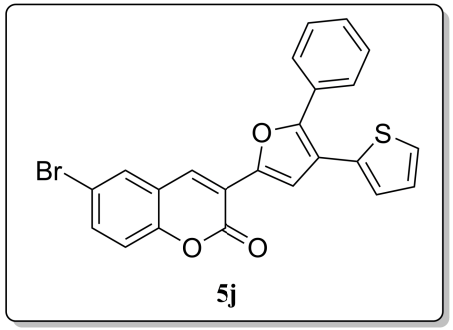






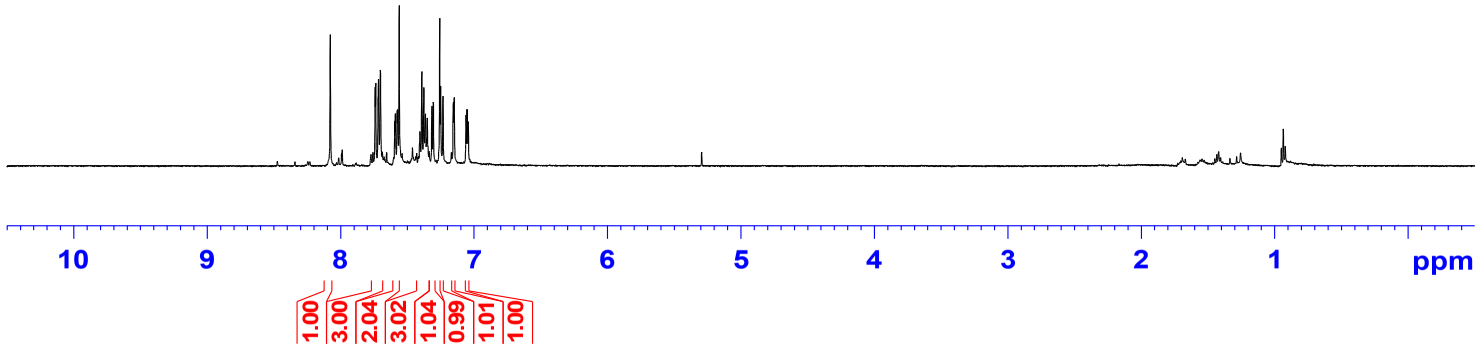


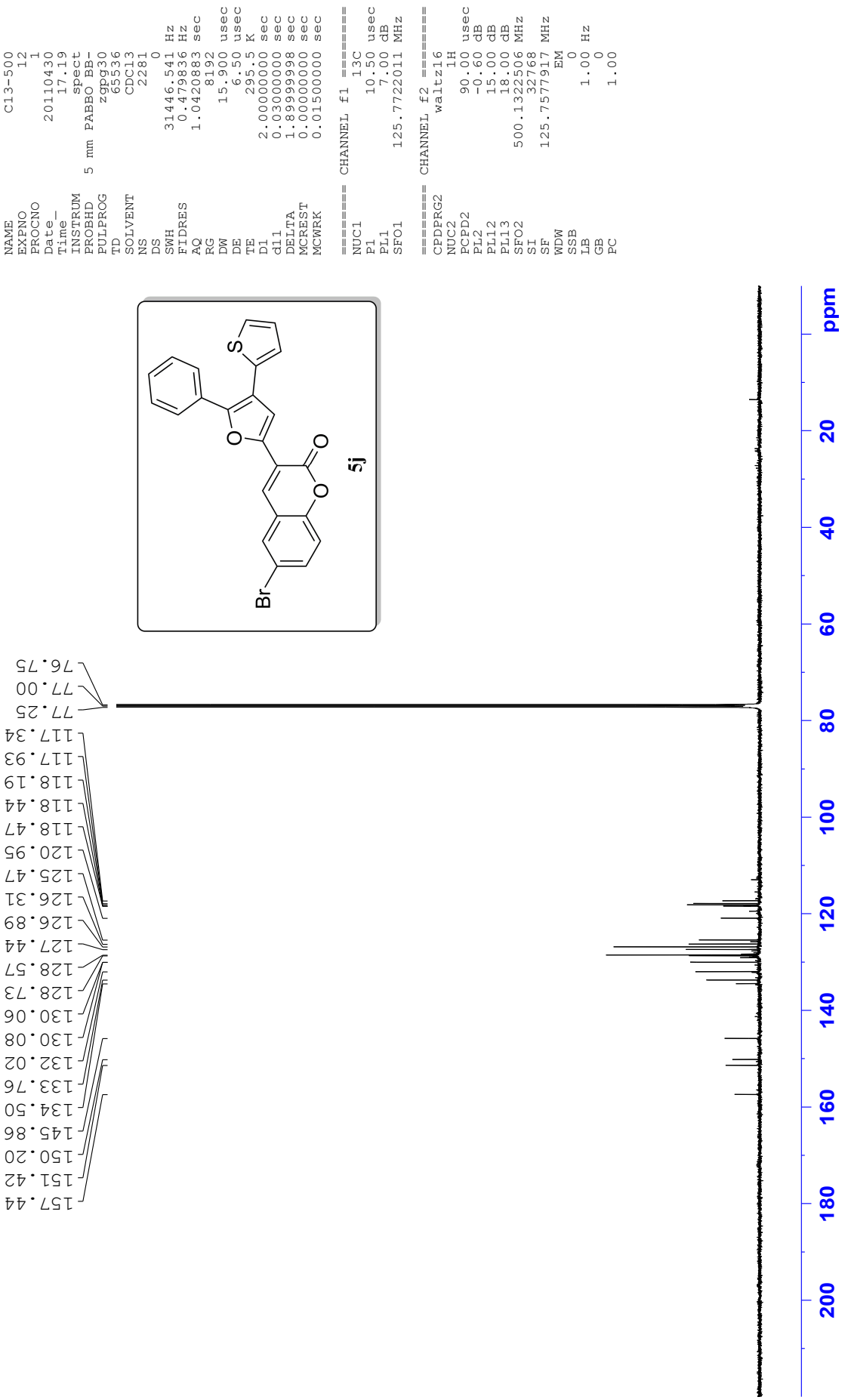




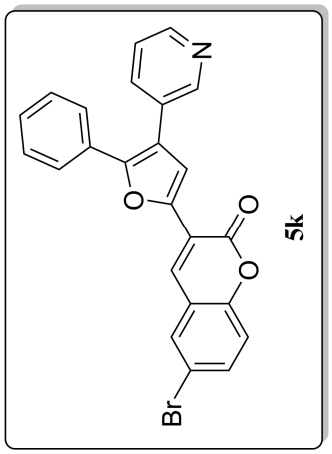
5j

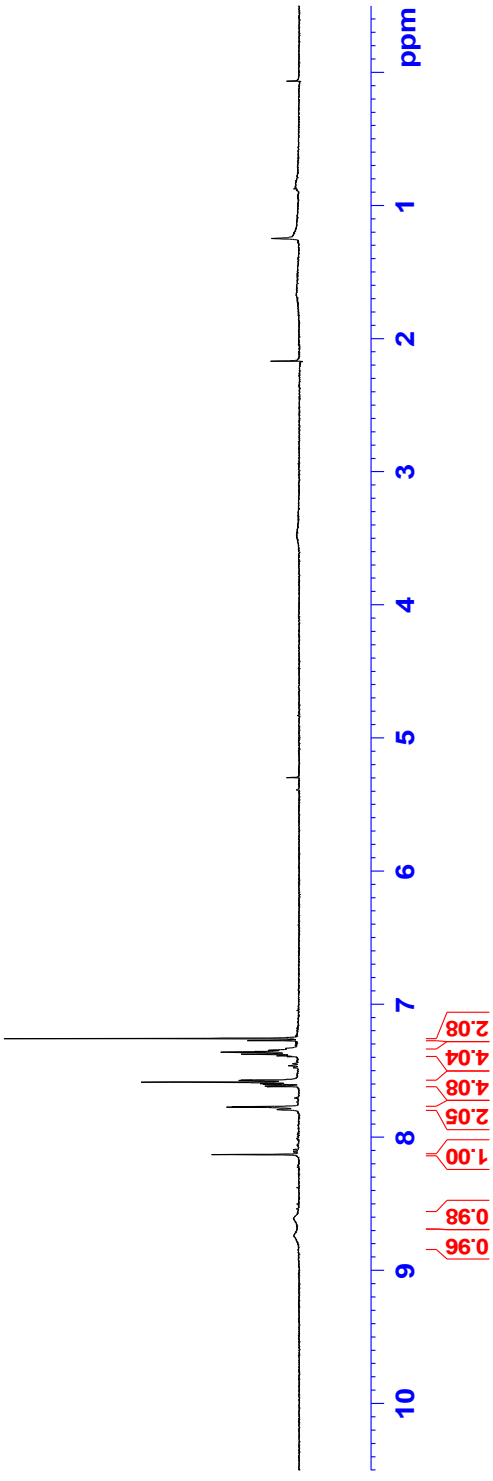
NAME	C13-500
EXPNO	11
PROCNO	1
Date_	20110504
Time	21.48
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	16384
SOLVENT	CDCl3
NS	1
DS	0
SWH	7507.507 Hz
FIDRES	0.458222 Hz
AQ	1.0912910 sec
RG	256
DW	66.600 usec
DE	6.50 usec
TE	300.0 K
D1	2.00000000 sec
MCREST	0.00000000 sec
MCWRK	0.01500000 sec
======== CHANNEL f1 ========	
NUC1	1H
P1	14.00 usec
PL1	0.00 dB
SFO1	500.1332508 MHz
SI	16384
SF	500.1300127 MHz
WDW	EM
SSB	0
LB	0.10 Hz
GB	0
PC	1.00

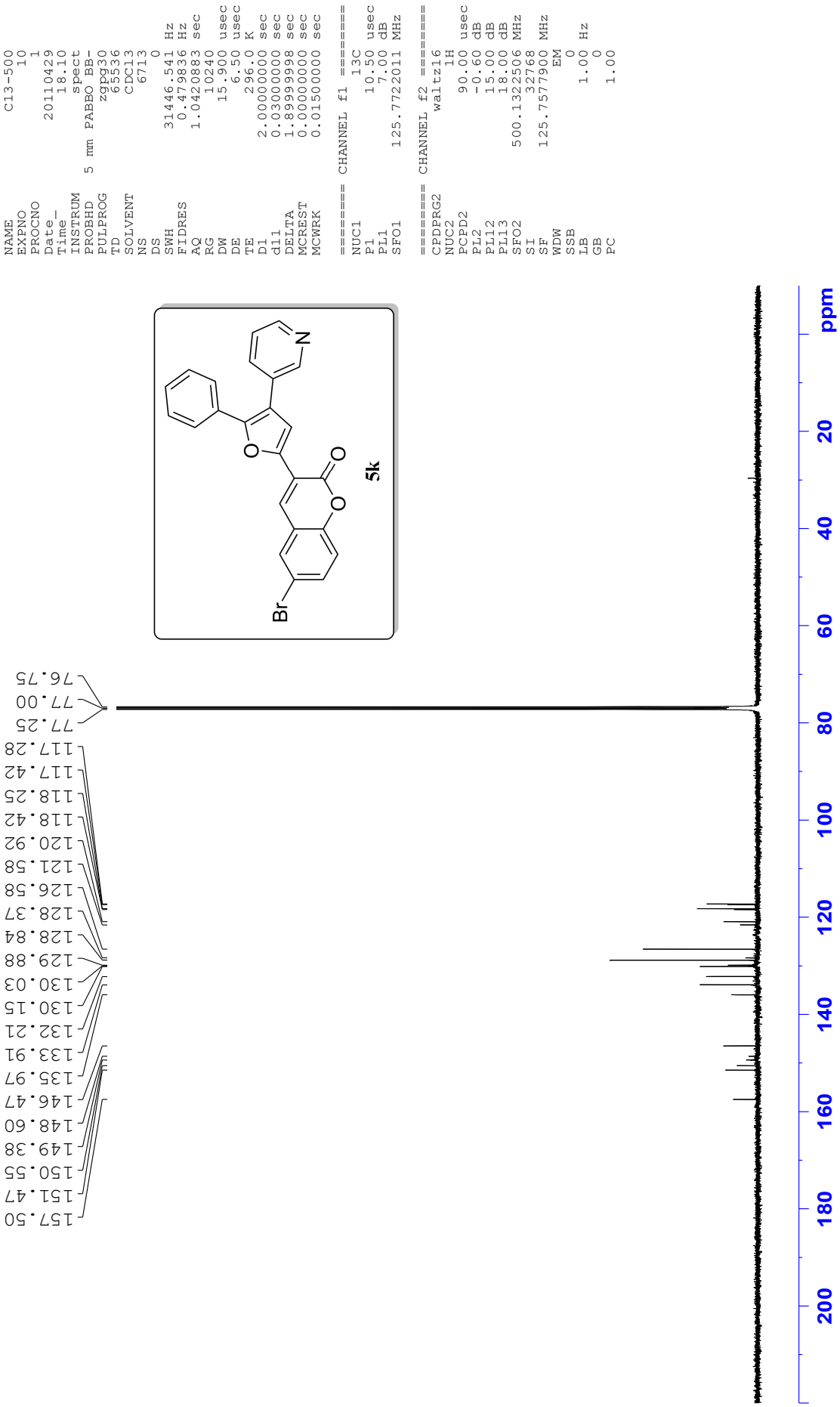


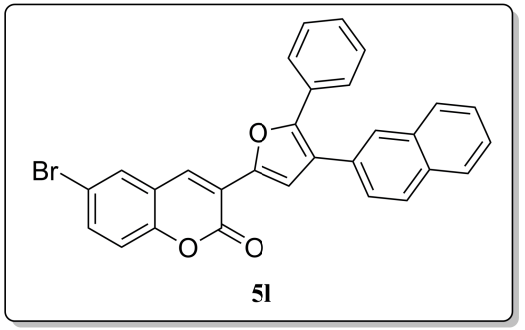


```
NAME                  C13-500
EXPNO                       9
PROCNO                      1
Date_                20110430
Time_                   13.10
INSTRUM                  spect
PROBHD     5 mm PABBO BB-
PULPROG                  zg30
TD                      16384
SOLVENT                 CDCl3
NS                          1
DS                          0
SWH                  7507.507 Hz
FIDRES               0.458222 Hz
AQ                   1.0912910 sec
RG                         362
DW                      66.600 usec
DE                       6.50 usec
TE                      294.7 K
D1                   2.00000000 sec
MCREST               0.00000000 sec
MCWRK                0.01500000 sec

======== CHANNEL f1 ========
NUC1                       1H
P1                      14.00 usec
PL1                      0.00 dB
SFO1             500.1332508 MHz
SI                      16384
SF               500.1300128 MHz
WDW                        EM
SSB                         0
LB                       0.10 Hz
GB                          0
PC                       1.00
```



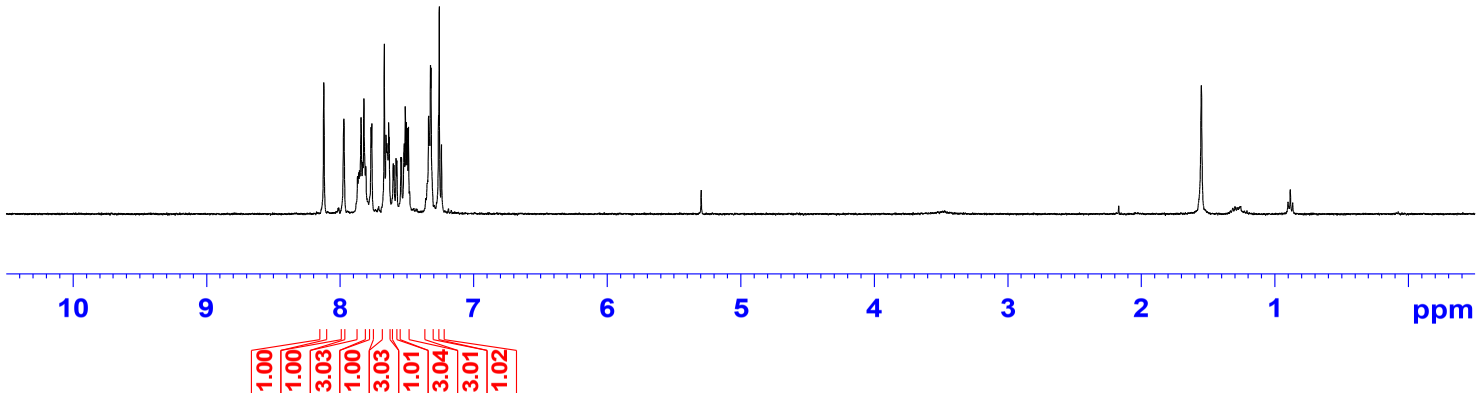


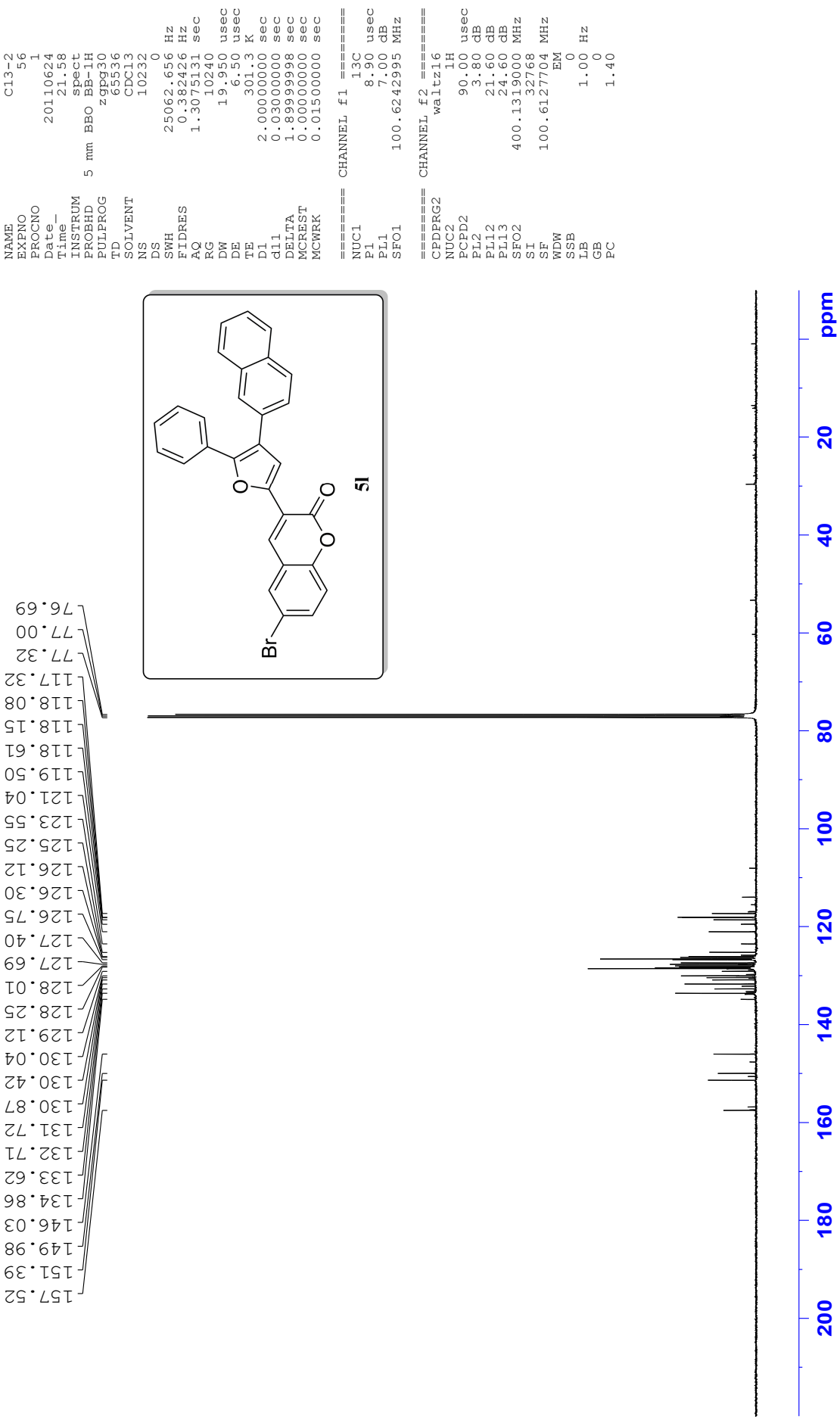


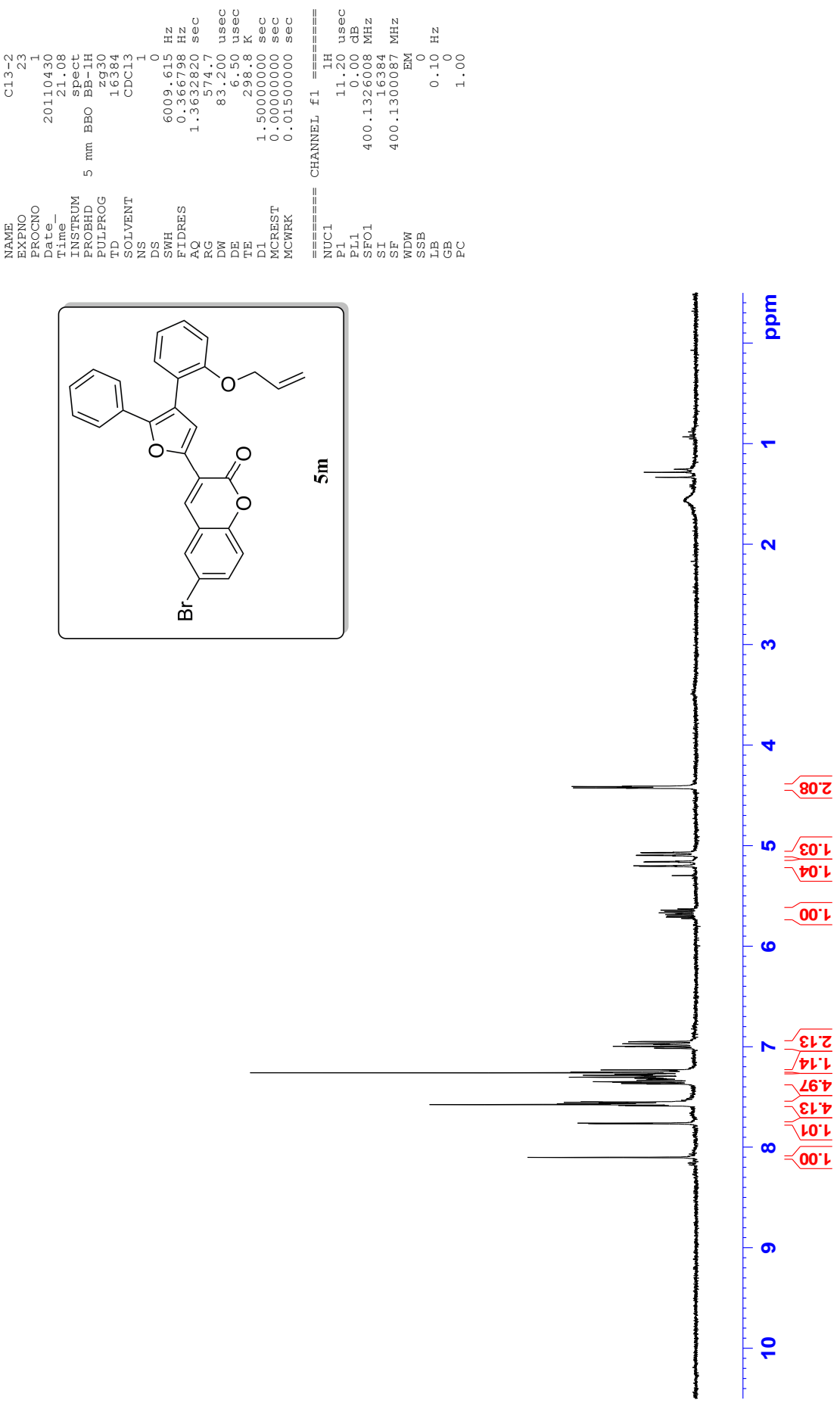


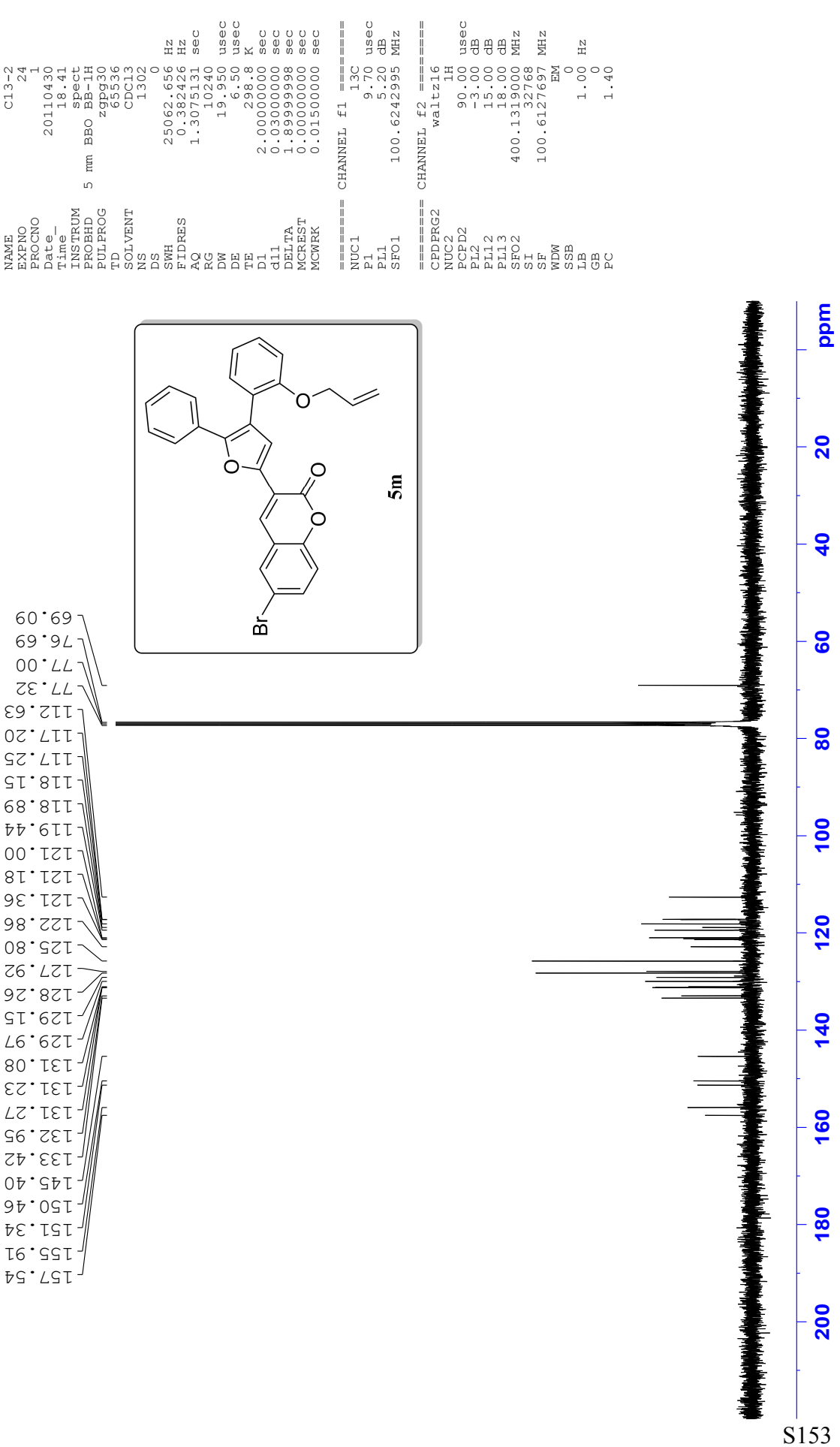
5l

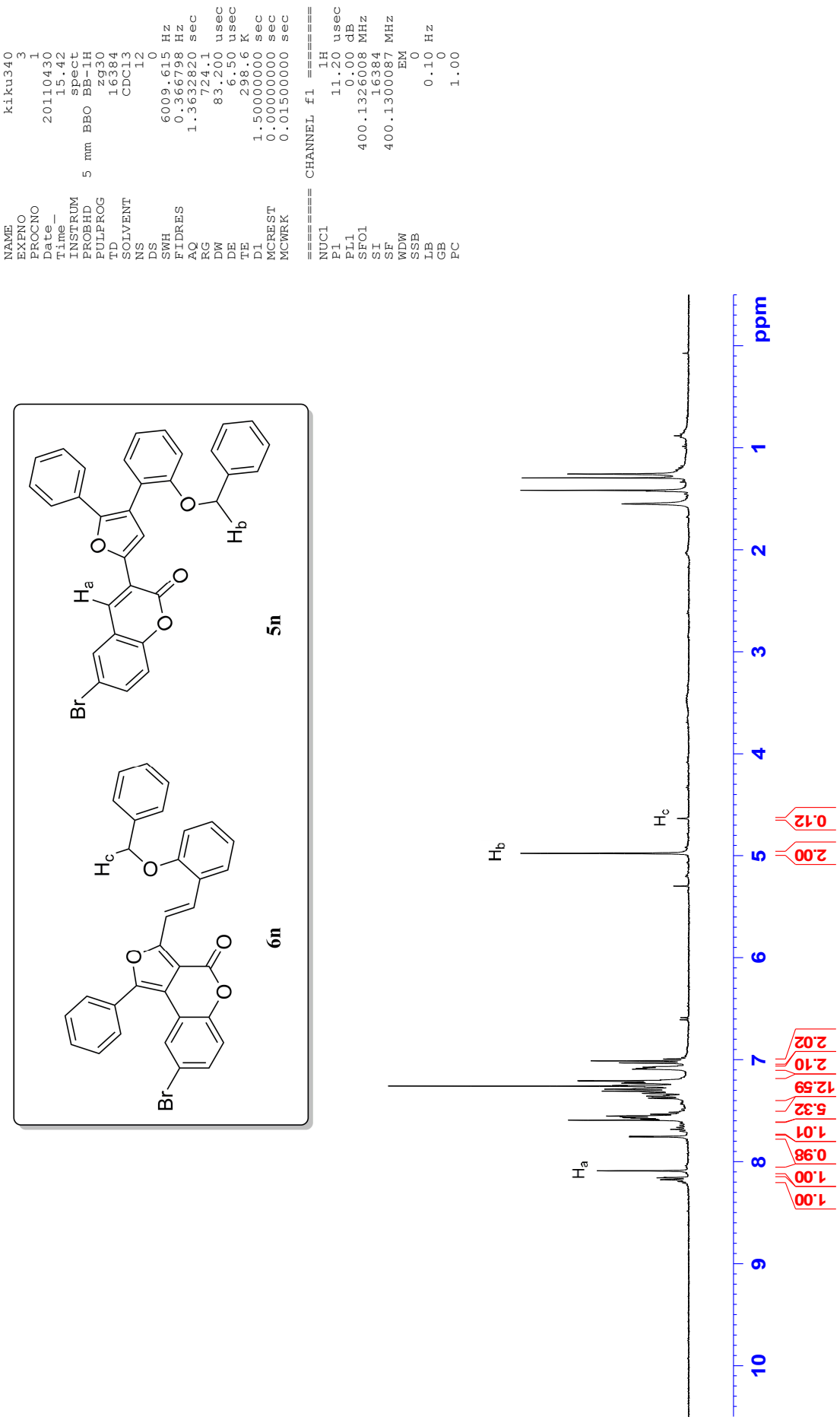
NAME	kiku348	
EXPNO	1	
PROCNO	1	
Date_	20110625	
Time	13.53	
INSTRUM	spect	
PROBHD	5 mm BBO BB-1H	
PULPROG	zg30	
TD	16384	
SOLVENT	CDCl3	
NS	1	
DS	0	
SWH	6009.615	Hz
FIDRES	0.366798	Hz
AQ	1.3632820	sec
RG	287.4	
DW	83.200	usec
DE	6.50	usec
TE	301.0	K
D1	1.50000000	sec
MCREST	0.00000000	sec
MCWRK	0.01500000	sec
======== CHANNEL f1 ========		
NUC1	1H	
P1	11.70	usec
PL1	4.00	dB
SFO1	400.1326008	MHz
SI	16384	
SF	400.1300088	MHz
WDW	EM	
SSB	0	
LB	0.10	Hz
GB	0	
PC	1.00	

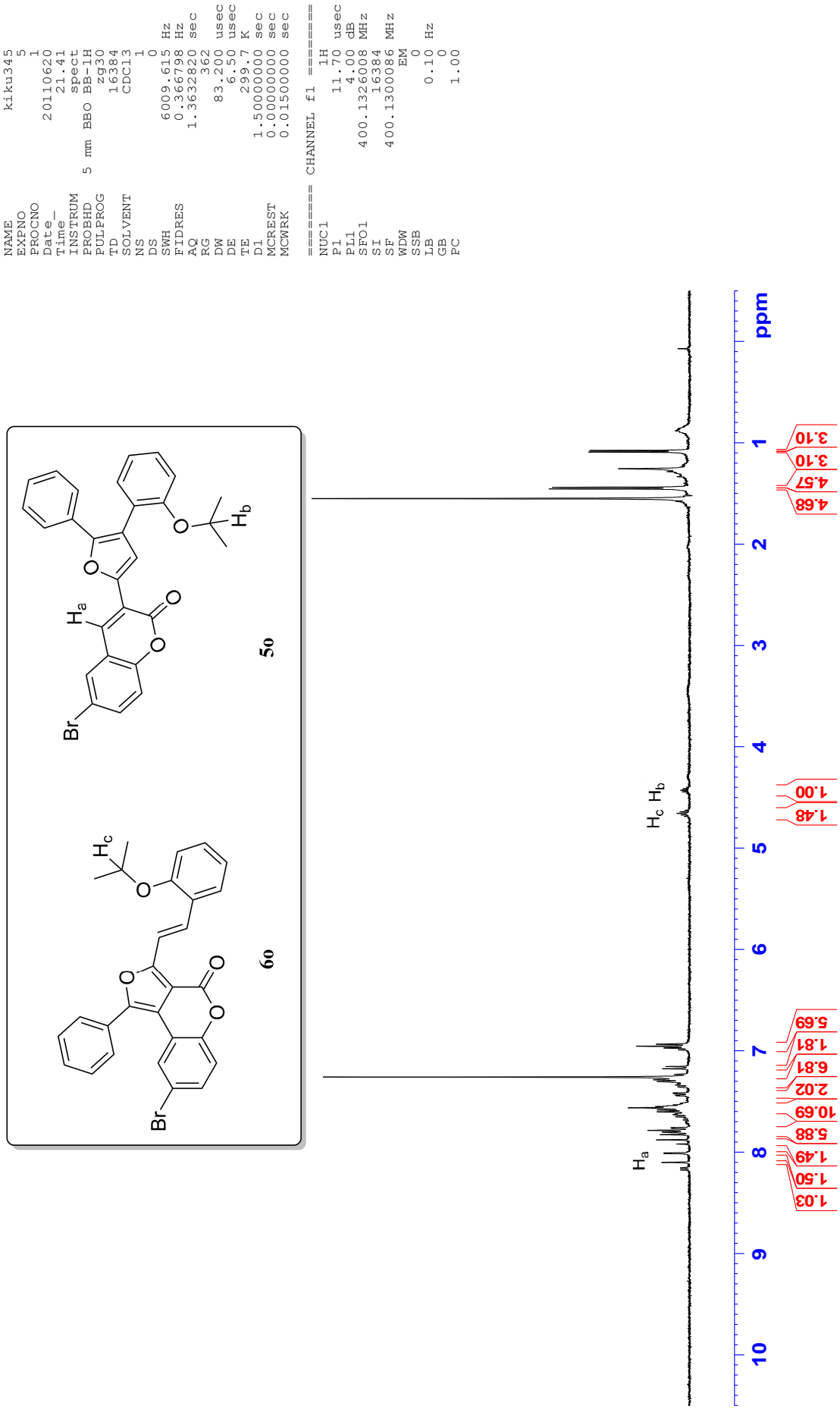


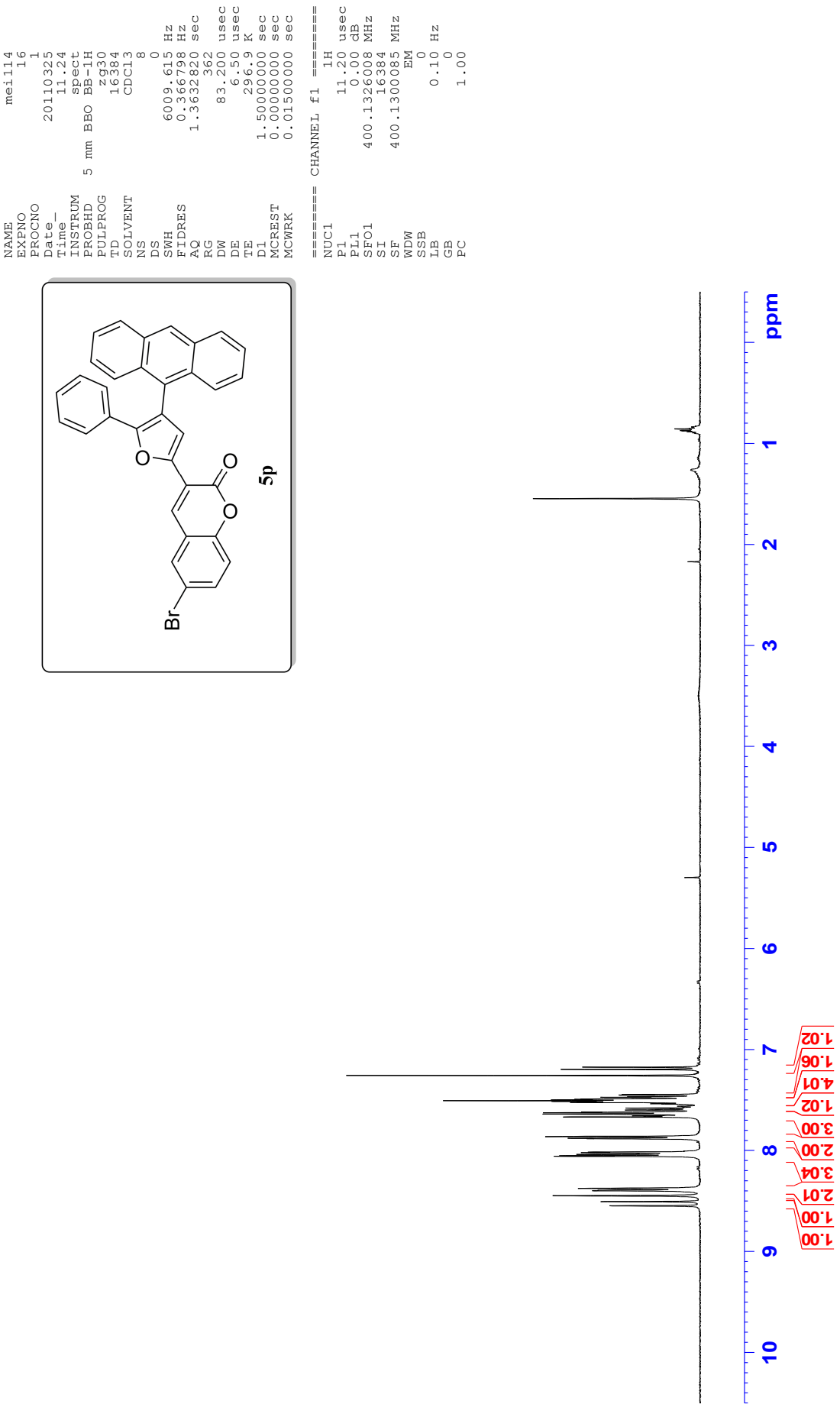


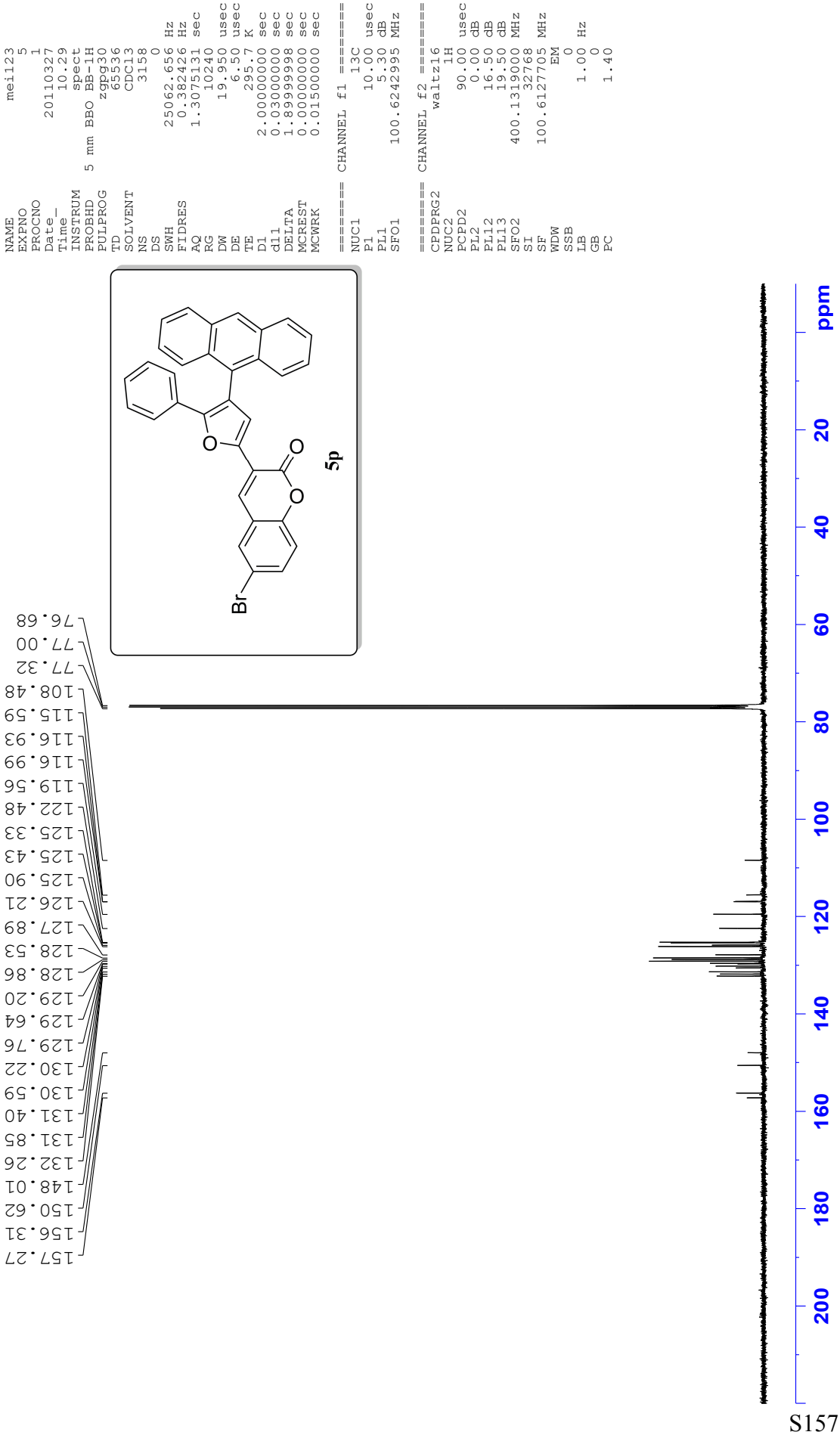


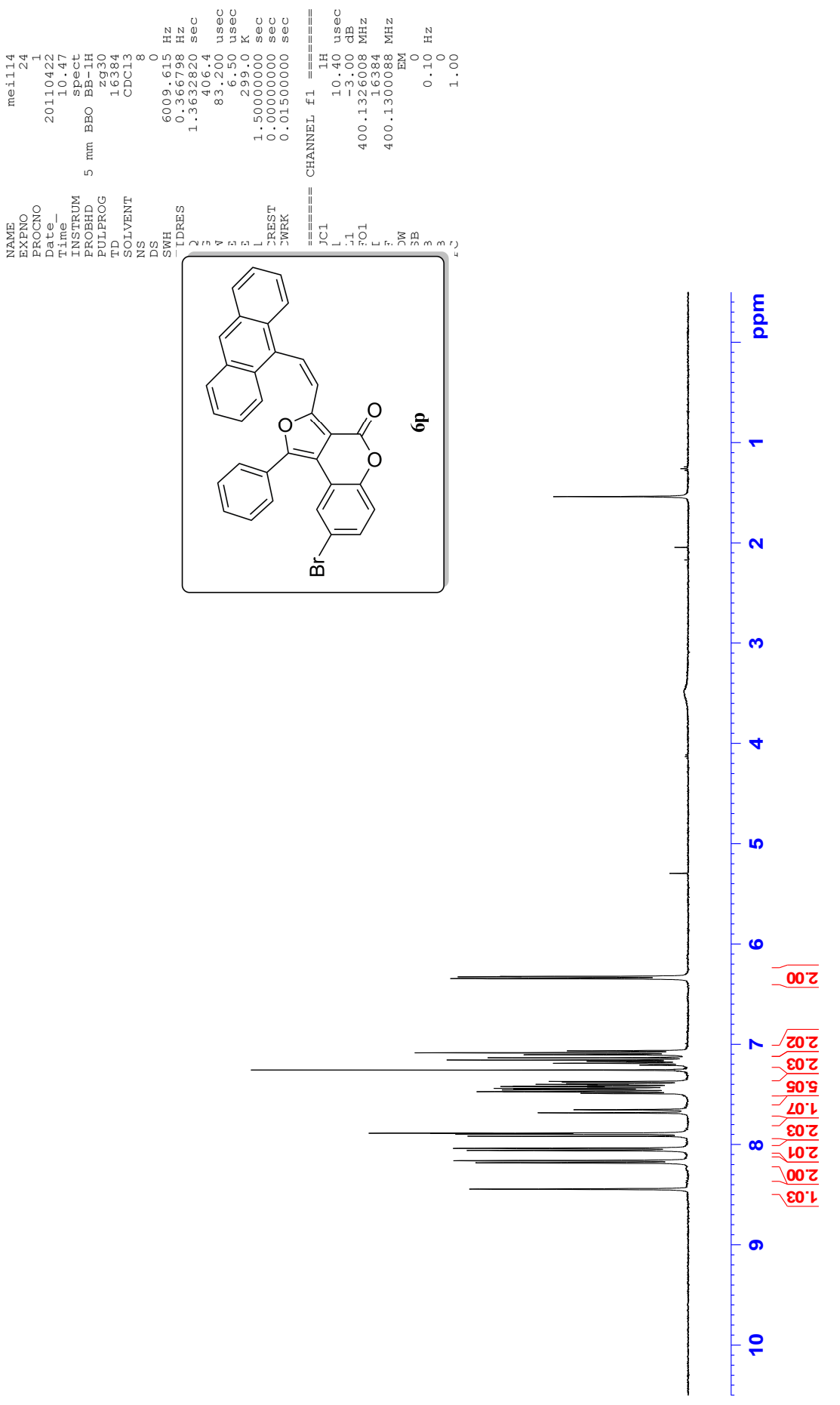


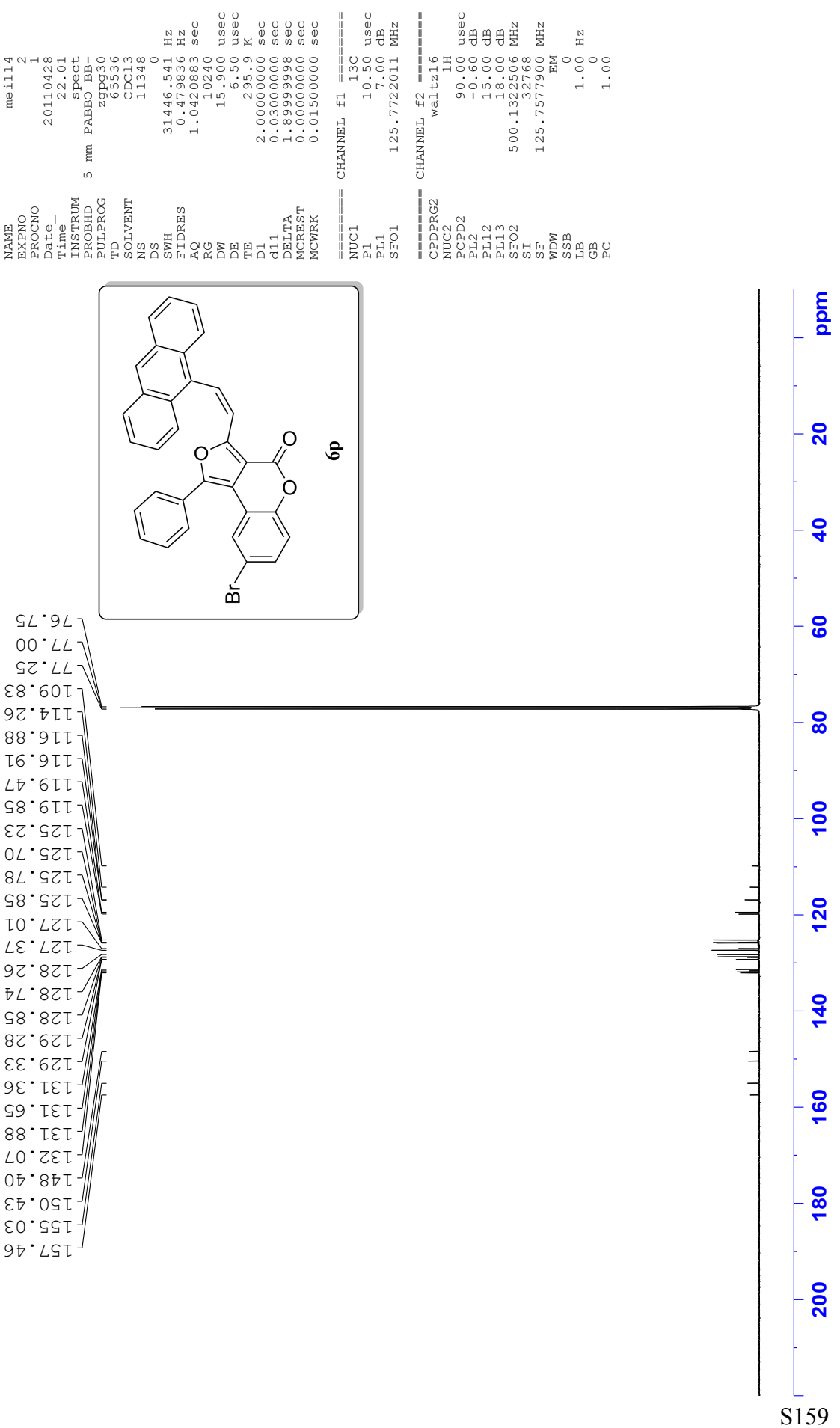


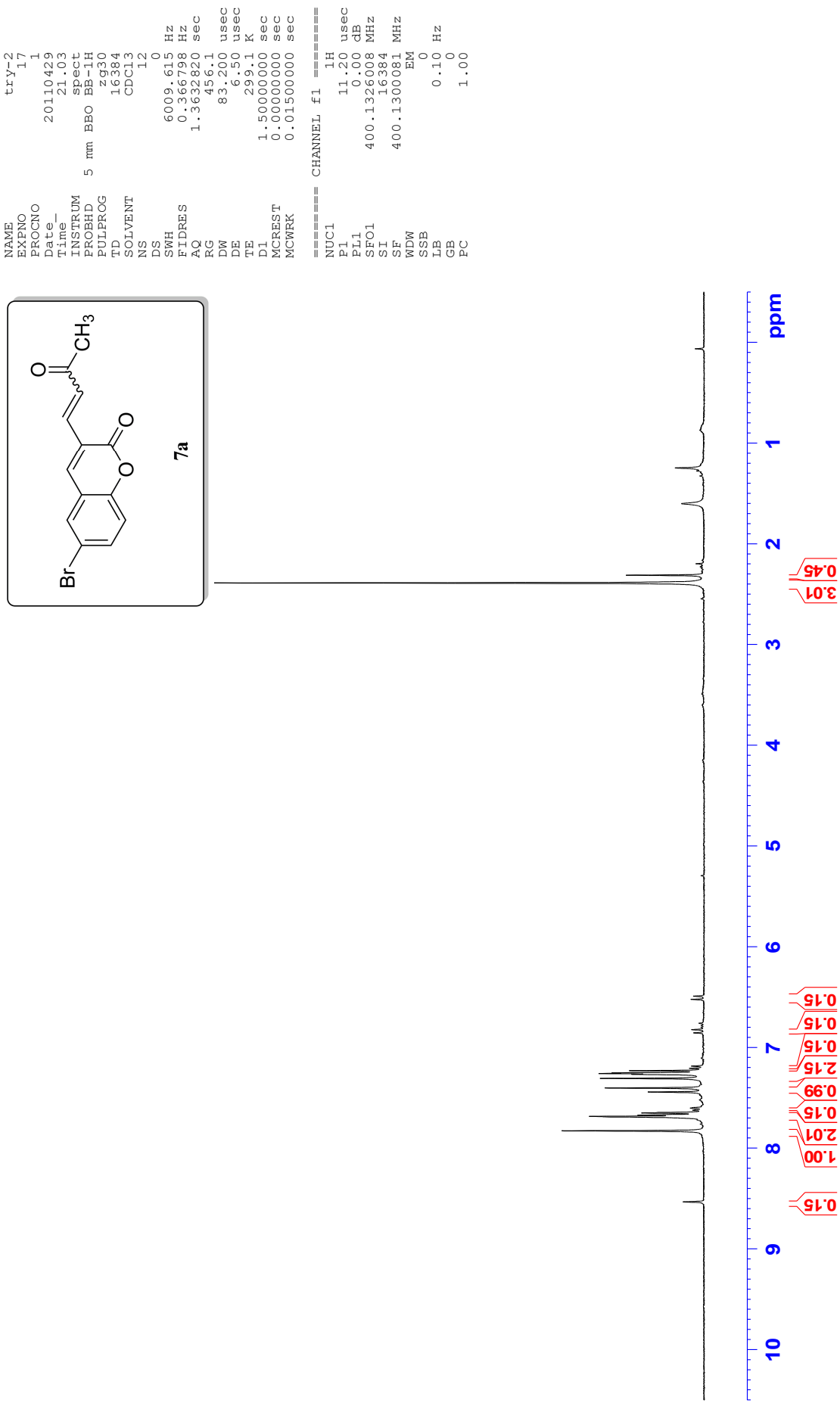

NAME kiku345
EXPNO 5
PROCNO 1
Date_ 20110620
Time_ 21.41
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 16384
SOLVENT CDCl3
NS 1
DS 0
SWH 6009.615 Hz
FIDRES 0.366798 Hz
AQ 1.3632820 sec
RG 362
DW 83.200 usec
DE 6.50 usec
TE 299.7 K
D1 1.50000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
CHANNEL f1
NUC1 1H
P1 11.70 usec
PL1 4.00 dB
SFO1 400.1326008 MHz
SI 16384
SF 400.1300086 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00
5o
6o
Ha
Hb
Hc
Br
O
ppm
1
2
3
4
5
6
7
8
9
10
3.10
3.10
4.57
4.68
1.48
1.00
1.03
1.50
1.49
5.88
10.69
2.02
6.81
1.81
5.69

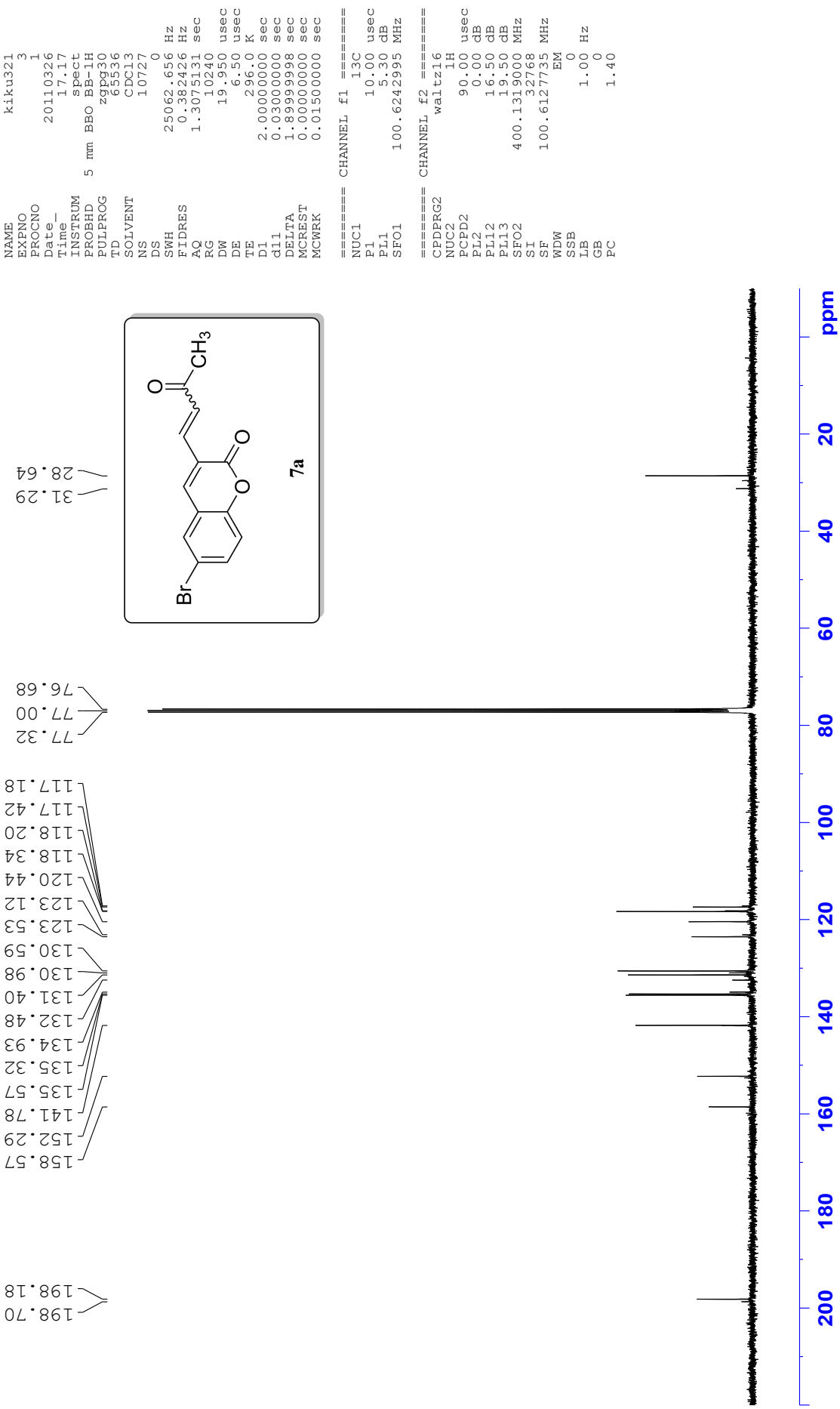


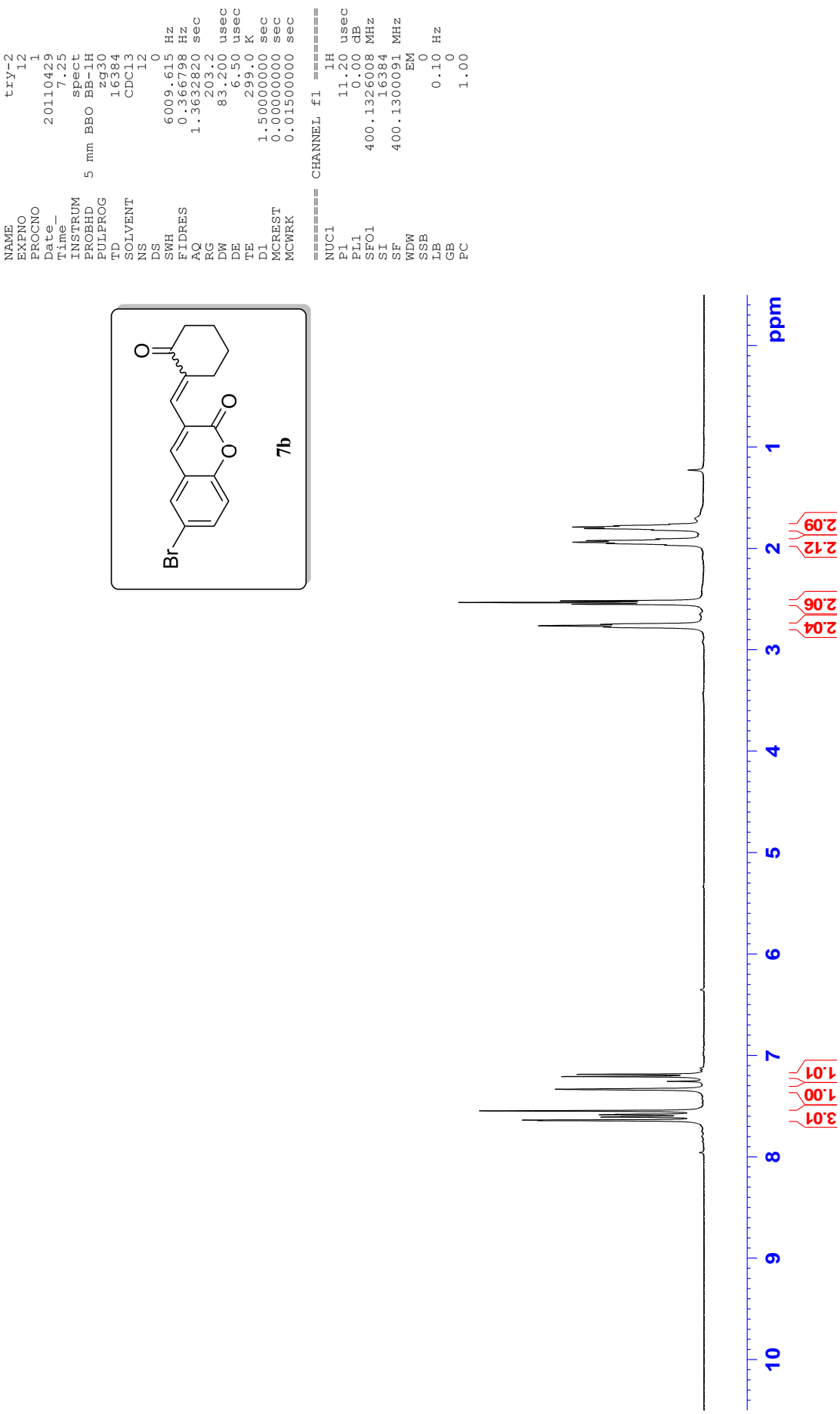


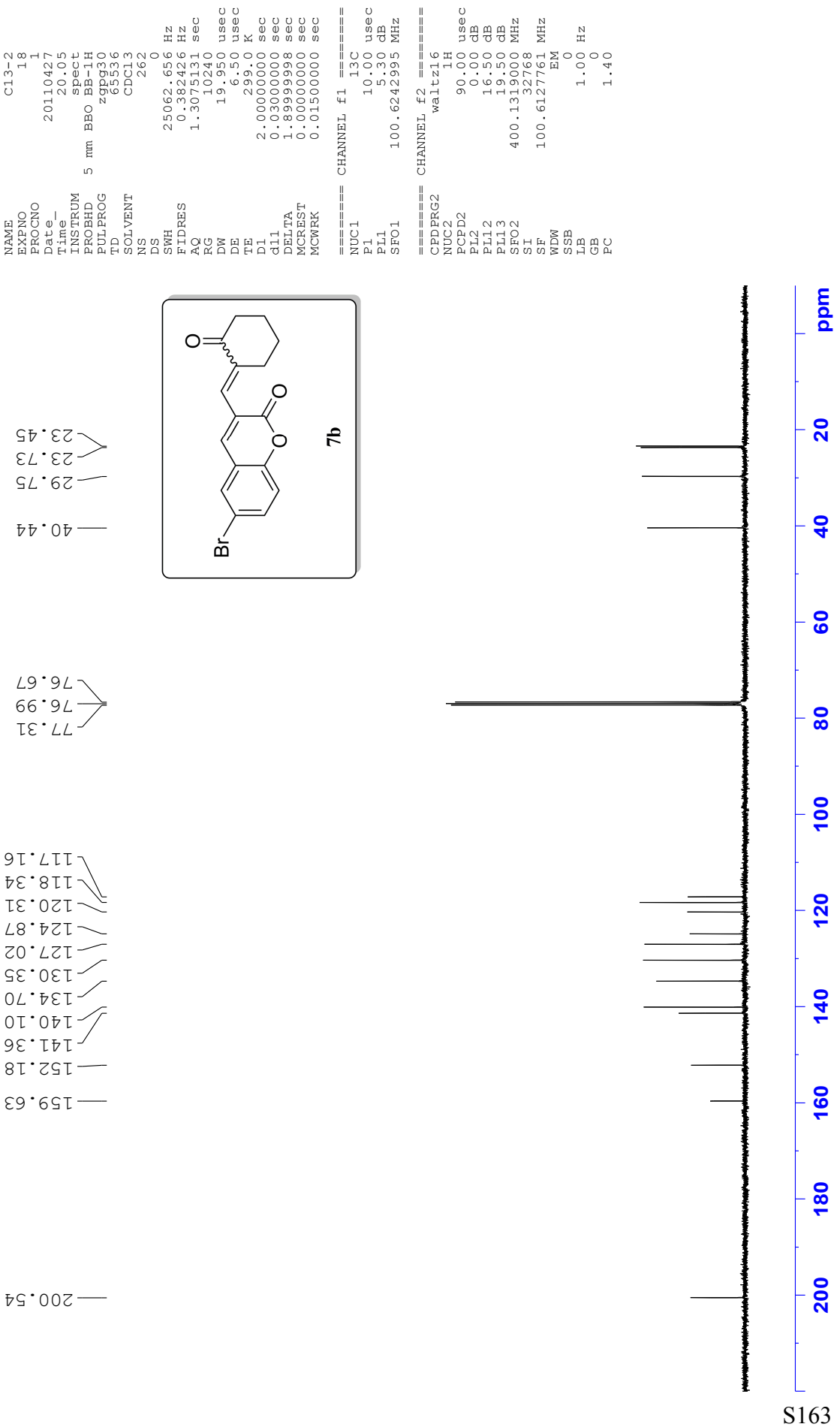


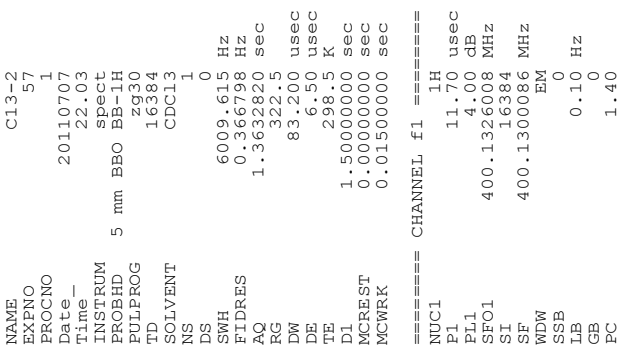


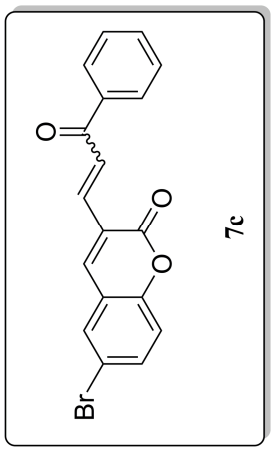


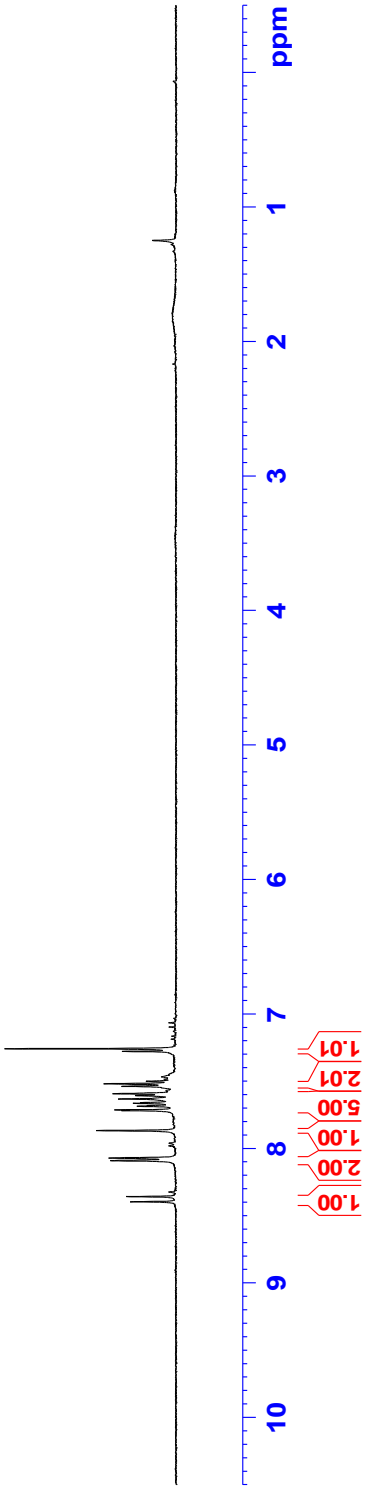


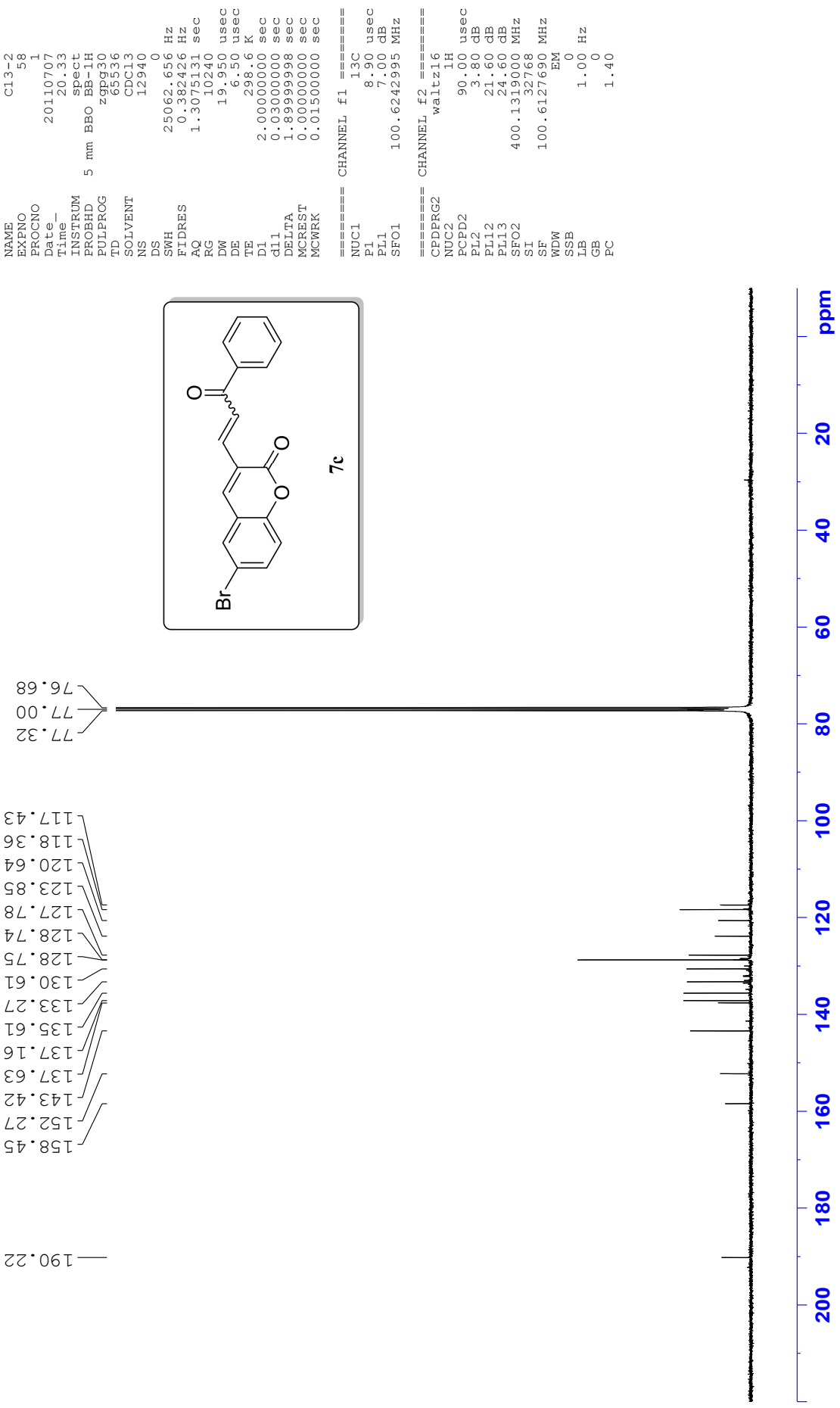


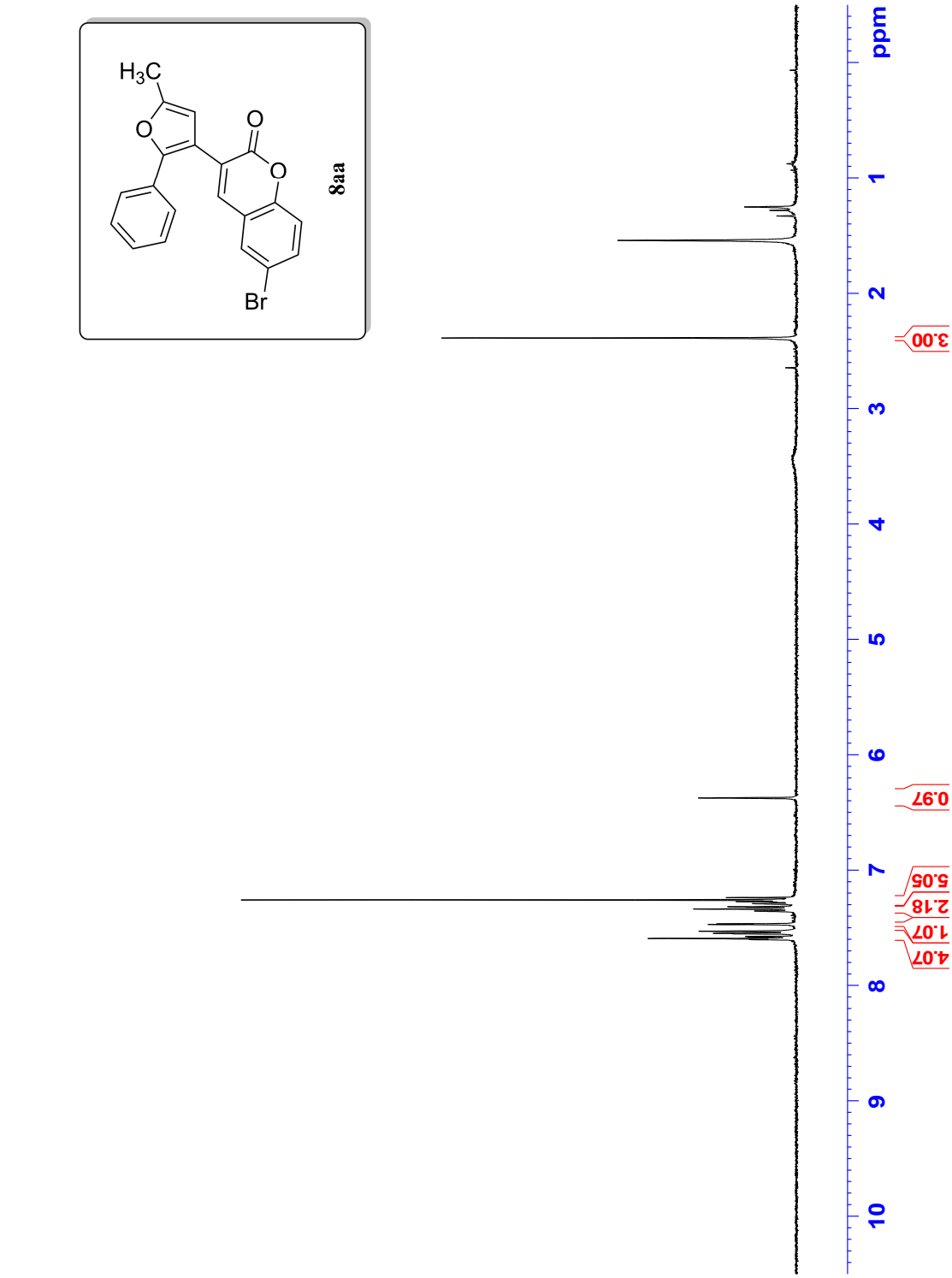

C13-2
18
1
20110427
20.05
spect
5 mm BBO BB-1H
zgpg30
65536
CDCl3
262
0
25062.656 Hz
0.382426 Hz
1.3075131 sec
10240
19.950 usec
6.50 usec
299.0 K
2.00000000 sec
0.03000000 sec
1.89999998 sec
0.00000000 sec
0.01500000 sec
CHANNEL f1
13C
10.00 usec
5.30 dB
100.6242995 MHz
CHANNEL f2
waltz16
1H
90.00 usec
0.00 dB
16.50 dB
19.50 dB
400.1319000 MHz
32768
100.6127761 MHz
EM
0
1.00 Hz
0
1.40
7b
Br
O
O
O
23.45
23.73
29.75
40.44
76.67
76.99
77.31
117.16
118.34
120.31
124.87
127.02
130.35
134.70
140.10
141.36
152.18
159.63
200.54
ppm
20
40
60
80
100
120
140
160
180
200

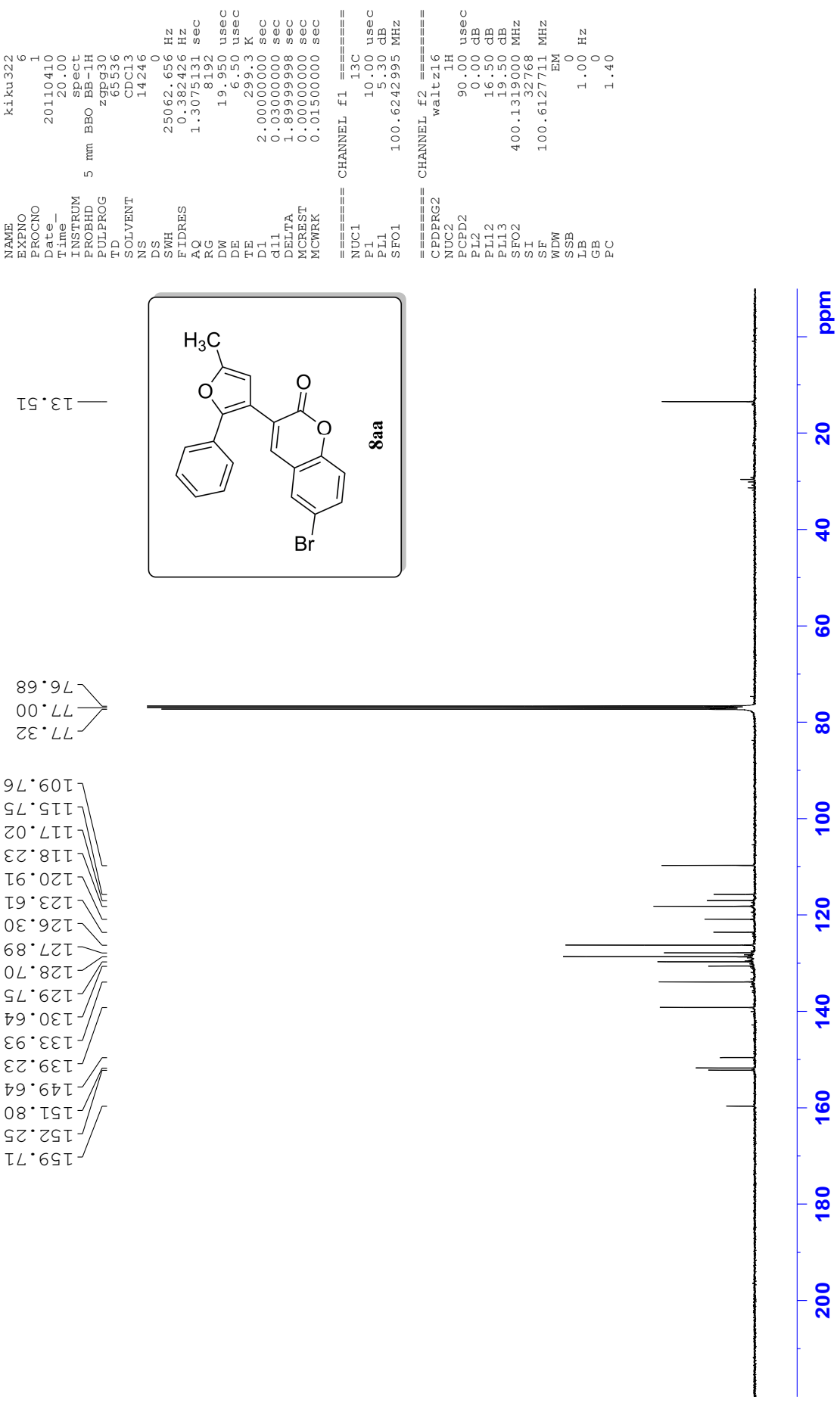


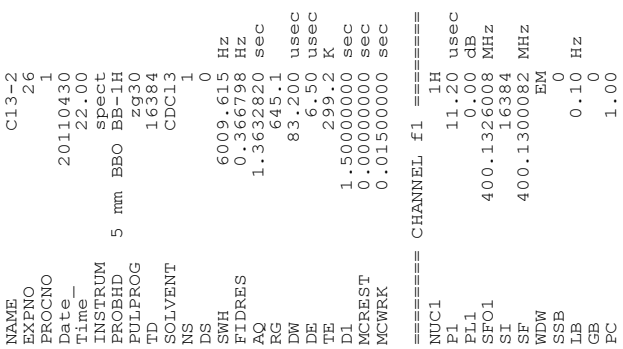


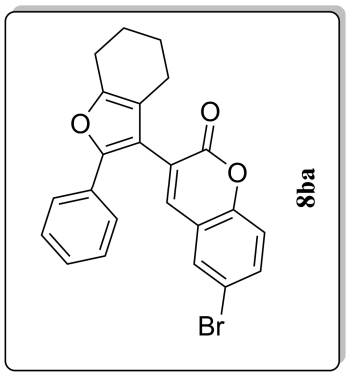


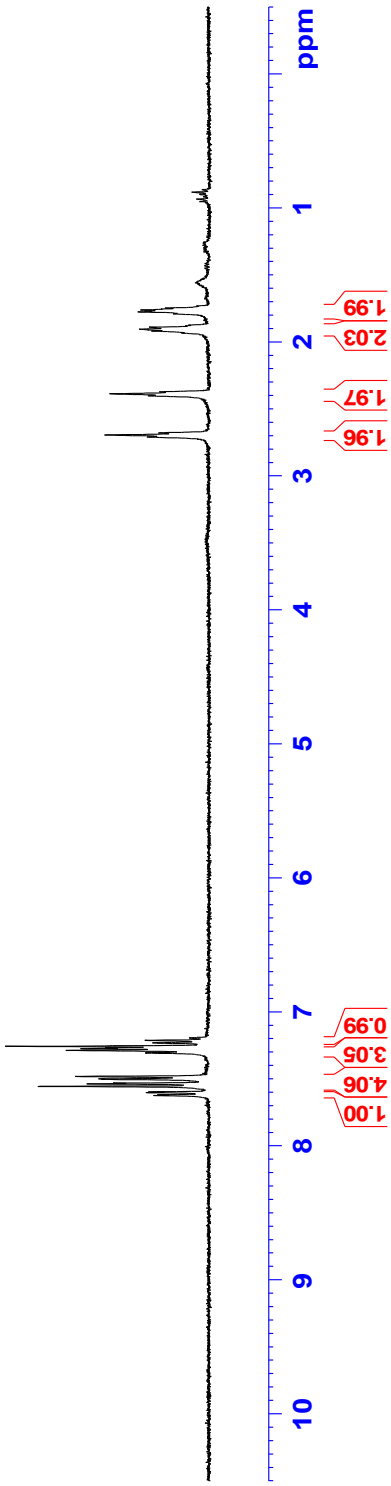


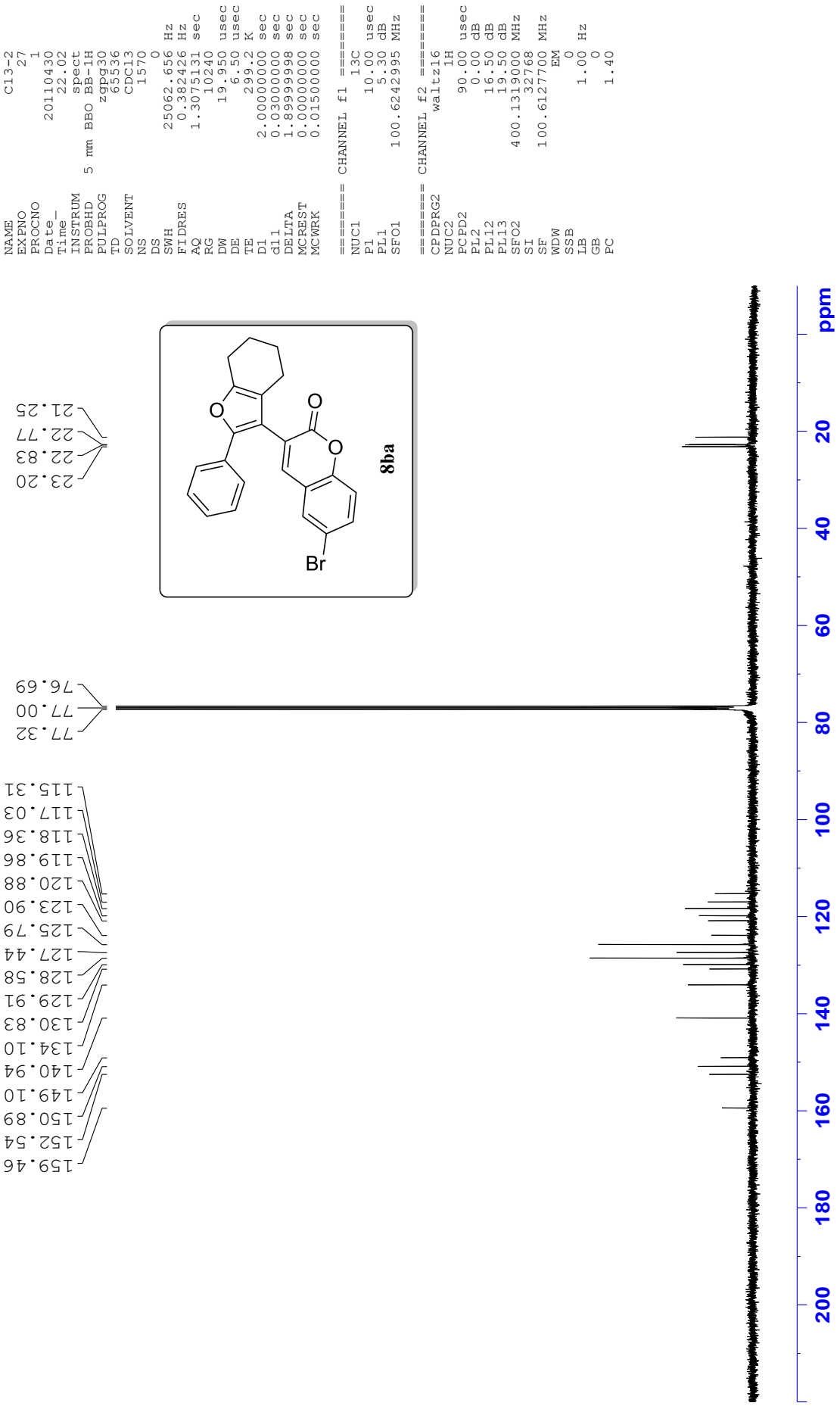


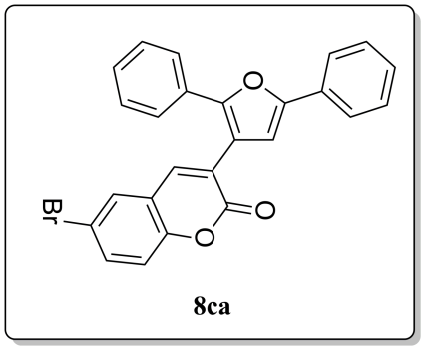

NAME kiku322
EXPNO 6
PROCNO 1
Date_ 20110410
Time_ 20.00
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 14246
DS 0
SWH 25062.656 Hz
FIDRES 0.382426 Hz
AQ 1.3075131 sec
RG 8192
DW 19.950 usec
DE 6.50 usec
TE 299.3 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
CHANNEL f1
NUC1 13C
P1 10.00 usec
PL1 5.30 dB
SFO1 100.6242995 MHz
CHANNEL f2
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 0.00 dB
PL12 16.50 dB
PL13 19.50 dB
SFO2 400.1319000 MHz
SI 32768
SF 100.6127711 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
H3C
O
O
O
Br
8aa
13.51
77.32
77.00
76.68
109.76
115.75
117.02
118.23
120.91
123.61
126.30
127.89
128.70
129.75
130.64
133.93
139.23
149.64
151.80
152.25
159.71
ppm
200
180
160
140
120
100
80
60
40
20





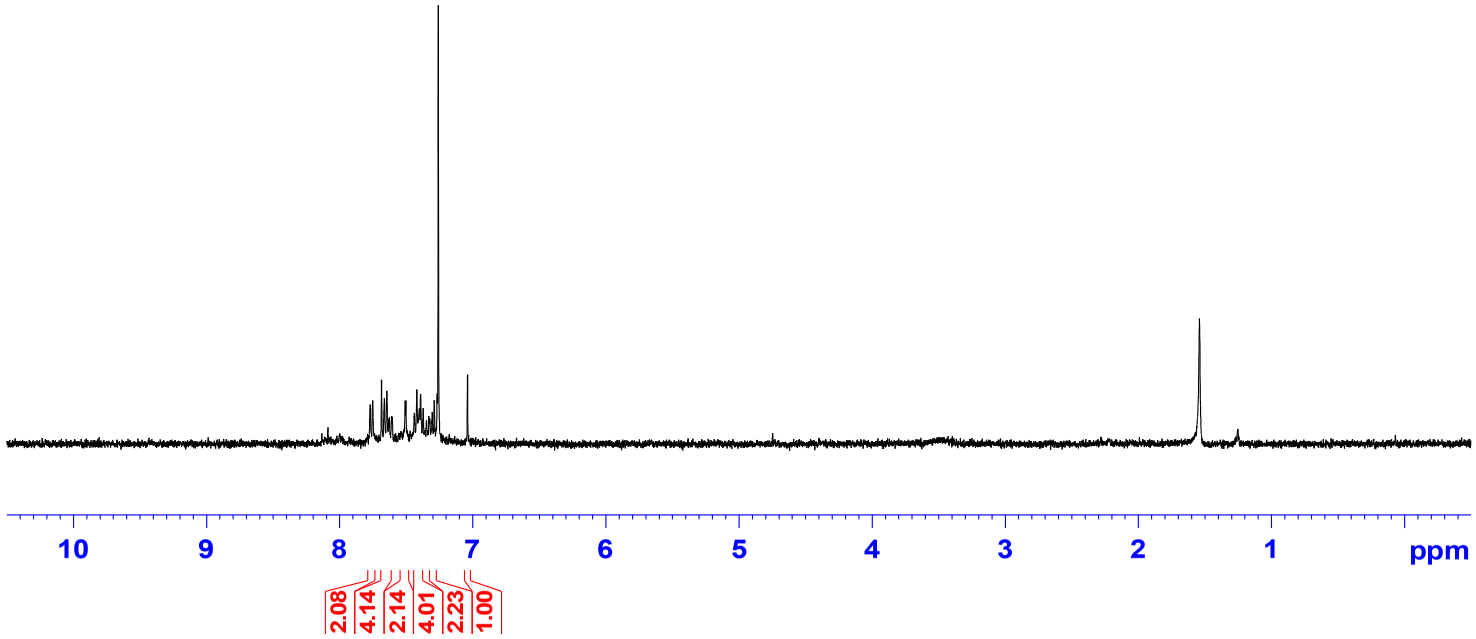


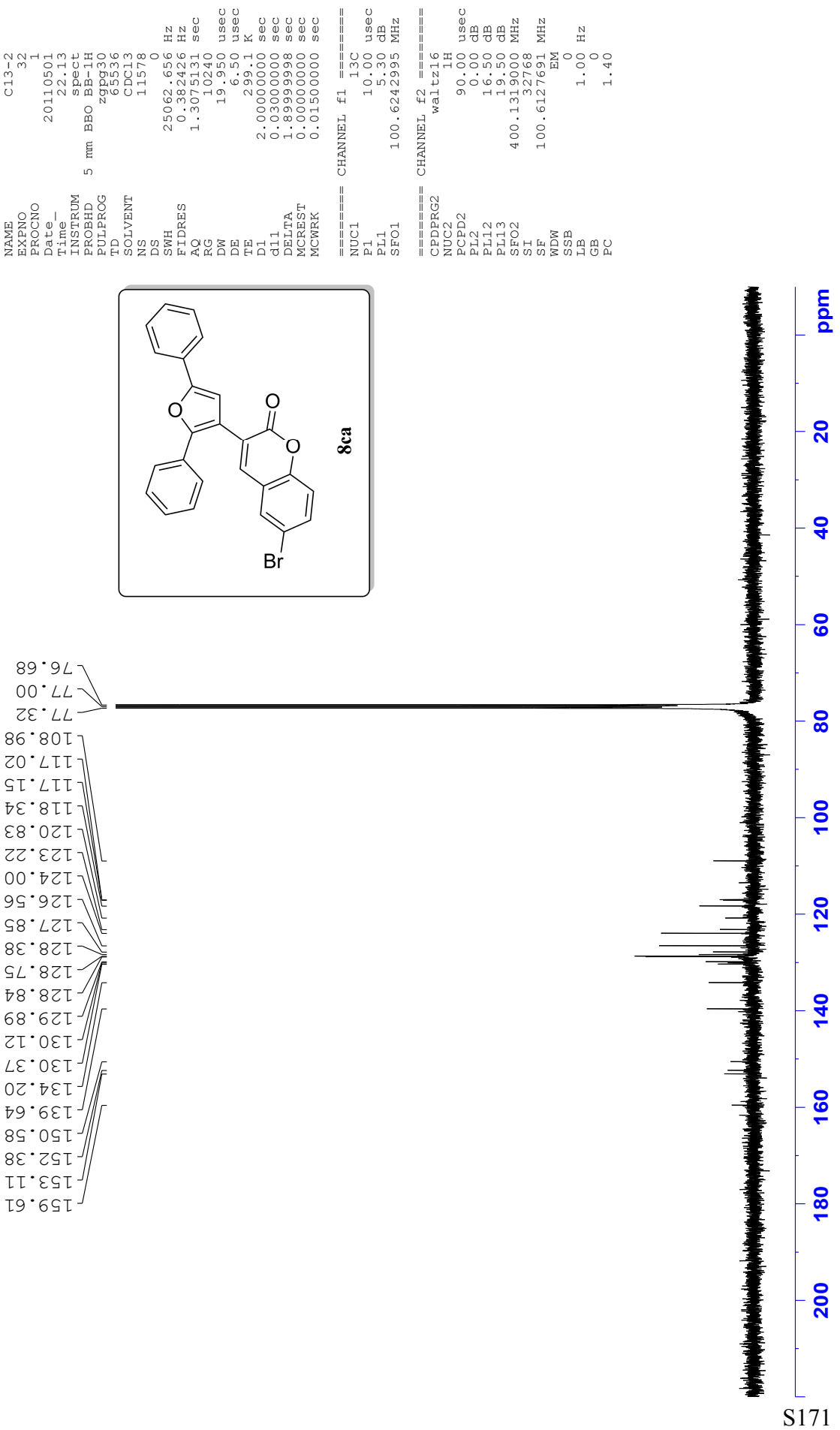




8ca

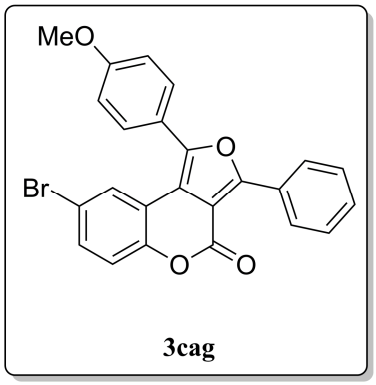
NAME	C13-2
EXPNO	31
PROCNO	1
Date_	20110501
Time	22.12
INSTRUM	spect
PROBHD	5 mm BBO BB-1H
PULPROG	zg30
TD	16384
SOLVENT	CDCl3
NS	1
DS	0
SWH	6009.615 Hz
FIDRES	0.366798 Hz
AQ	1.3632820 sec
RG	812.7
DW	83.200 usec
DE	6.50 usec
TE	299.1 K
D1	1.50000000 sec
MCREST	0.00000000 sec
MCWRK	0.01500000 sec
======== CHANNEL f1 ========	
NUC1	1H
P1	11.20 usec
PL1	0.00 dB
SFO1	400.1326008 MHz
SI	16384
SF	400.1300088 MHz
WDW	EM
SSB	0
LB	0.10 Hz
GB	0
PC	1.40



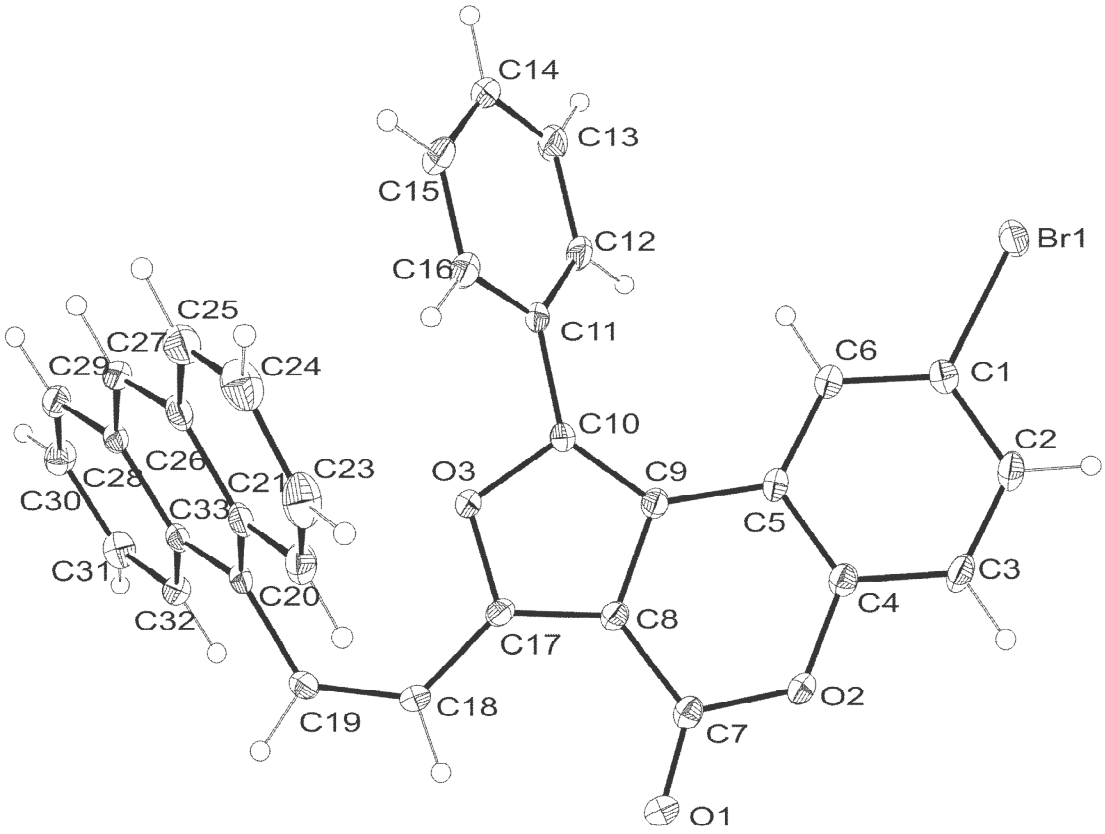


Ⅵ. Spectra of X-ray crystallography

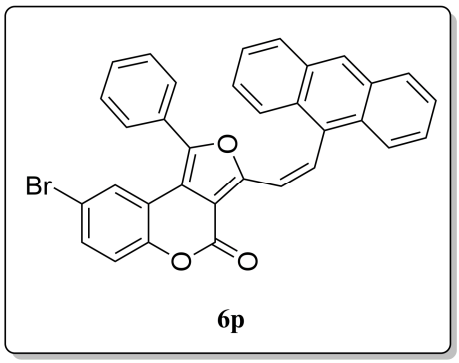
CCDC 805741



3cag



CCDC 833192



6p