

**A novel one-Pot Three Component Reaction for the Synthesis of [2-(alkylsulfanyl)imidazo[1,2-a]pyridin-3-yl](aryl)methanone**

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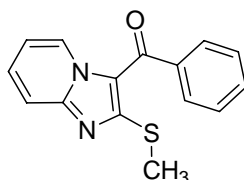
**SUPPORTING INFORMATION**

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## Experimental Section:

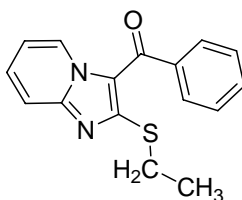
**General Methods:** Chemicals were purchased from Merck and were used as received. Column chromatography was performed on silica gel (0.063-0.200 mm; Merck). IR Spectra: Shimadzu FTIR-4300 spectrometer; in  $\text{cm}^{-1}$ .  $^1\text{H}$ - and  $^{13}\text{C}$ -NMR Spectra: Bruker DRX -500-Avance instrument; in  $\text{CDCl}_3$  at 500.1 and 125.7 MHz, resp;  $\delta$  in ppm, J in Hz. EI-MS (70 eV): HP 5973 GC-MS instrument; in m/z. Melting points: Electrothermal 9200 apparatus.

### Typical procedure for preparation of [2-(methylsulfanyl)imidazo[1,2-a]pyridin-3-yl](phenyl)methanone 4{1,1,1}



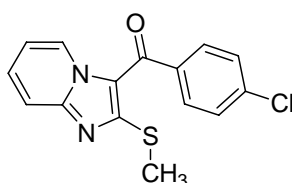
Pyridine (0.097 ml, 1.2 mmol) and phenacyl bromide (0.239 g, 1.2 mmol) were taken up in toluene (10 ml) and the mixture was stirred at rt for 1 h. To this mixture methyl thiocyanate (0.074 g, 1.0 mmol) and potassium carbonate (0.28 g, 2.0 mmol) were added and it was allowed to stir at reflux for 12 h. Upon completion, the toluene was removed under reduced pressure, then water was added and the reaction mixture was extracted with dichloromethane ( $3 \times 15$  ml). The organic layer was dried over  $\text{Na}_2\text{SO}_4$ . Evaporation of the solvent followed by purification on silica gel (*n*-hexane-ethyl acetate, 90-10) afforded the pure 4{1,1,1} as yellow solid (yield 78%); mp 140-141 °C, lit.<sup>1,2</sup> mp 140 °C dec. IR (KBr) ( $\nu_{\text{max}}/\text{cm}^{-1}$ ): 1490, 1571, 1597, 3060.  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta_{\text{H}}$  (ppm): 2.58 (3H, s, S-CH<sub>3</sub>), 7.08-7.10 (1H, m), 7.52-7.57 (3H, m), 7.61-7.63 (1H, m), 7.68-7.72 (3H, m), 9.60 (1H, d,  $^3J_{\text{HH}} = 6.9$  Hz).  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )  $\delta_{\text{C}}$  (ppm): 15.32, 114.70, 116.24, 128.63, 129.07, 130.02, 132.05, 140.33, 148.55, 156.49, 186.05 (C=O). MS, *m/z* (%): 268 ( $\text{M}^+$ , 100), 235 (67), 207 (33), 163 (26), 77 (44), 51 (23).

### [2-(ethylsulfanyl)imidazo[1,2-a]pyridin-3-yl](phenyl)methanone 4{1,1,2}



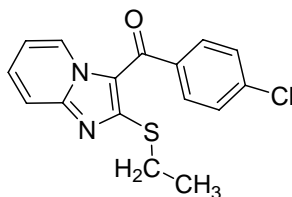
Brown solid (yield 76%); mp 136 °C dec. IR (KBr) ( $\nu_{\max}/\text{cm}^{-1}$ ): 649, 702, 1220, 1332, 1442, 1596, 3037.  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta_{\text{H}}$  (ppm): 1.33 (3H, t,  $^3J_{\text{HH}}=7.3$  Hz,  $\text{CH}_3$ ), 3.21 (2H, q,  $^3J_{\text{HH}}=7.3$  Hz), 7.07 (1H, t,  $^3J_{\text{HH}}=6.8$  Hz), 7.50-7.56 (3H, m), 7.61-7.68 (2H, m), 7.71-7.73 (2H, m), 9.57 (1H, d,  $^3J_{\text{HH}}=6.8$  Hz).  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )  $\delta_{\text{C}}$  (ppm): 15.08, 26.71, 114.55, 116.26, 128.79, 129.01, 129.89, 132.10, 140.31, 148.55, 155.72, 186.21 (C=O). MS,  $m/z$  (%): 282 ( $\text{M}^+$ ,100), 249 (88), 234 (35), 221 (35), 177 (77), 105 (44), 77 (55).

**(4-chlorophenyl)[2-(methylsulfanyl)imidazo[1,2-*a*]pyridin-3-yl]methanone**  
**4{1,2,1}**



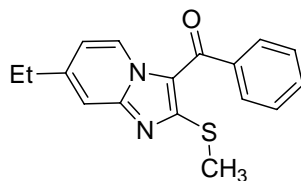
Brown solid (yield 81%); mp 152 °C, lit.<sup>1</sup> mp 168 °C dec. IR (KBr) ( $\nu_{\max}/\text{cm}^{-1}$ ): 1220, 1355, 1444, 1606, 2906, 3055.  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta_{\text{H}}$  (ppm): 2.58 (3H, s,  $\text{S-CH}_3$ ), 7.08 (1H, t,  $^3J_{\text{HH}}=6.9$  Hz), 7.45-7.54 (3H, m), 7.63-7.70 (3H, m), 9.5 (1H, d,  $^3J_{\text{HH}}=6.8$  Hz).  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )  $\delta_{\text{C}}$  (ppm): 15.28, 114.93, 116.26, 120.38, 129.06, 129.39, 130.19, 131.92, 138.40, 138.49, 148.65, 156.52, 184.69 (C=O). MS,  $m/z$  (%): 302 ( $\text{M}^+$ ,100), 269 (60), 177 (45), 111 (45), 78 (60).

**(4-chlorophenyl)[2-(ethylsulfanyl)imidazo[1,2-*a*]pyridin-3-yl]methanone** 4{1,2,2}



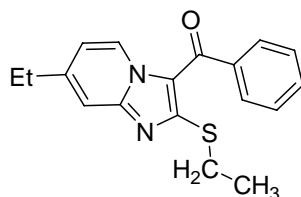
Brown solid (yield 74%); mp 146 °C dec. IR (KBr) ( $\nu_{\max}/\text{cm}^{-1}$ ): 1220, 1334, 1440, 1608, 2827, 3130.  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta_{\text{H}}$  (ppm): 1.33 (3H, t,  $^3J_{\text{HH}}=7.3$  Hz,  $\text{CH}_3$ ), 3.21 (2H, q,  $^3J_{\text{HH}}=7.3$  Hz,  $\text{CH}_2$ ), 7.06 (1H, t,  $^3J_{\text{HH}}=6.8$  Hz), 7.49-7.53 (3H, m), 7.64-7.66 (3H, m), 9.53 (1H, d,  $^3J_{\text{HH}}=6.8$  Hz).  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )  $\delta_{\text{C}}$  (ppm): 15.09, 26.78, 114.76, 116.29, 120.54, 129.02, 129.33, 130.22, 130.33, 138.42, 138.53, 148.60, 184.78 (C=O). MS,  $m/z$  (%): 316 ( $\text{M}^+$ ,80), 283 (70), 177 (100), 139 (50), 111 (50), 78 (40).

**[7-ethyl-2-(methylsulfanyl)imidazo[1,2-*a*]pyridin-3-yl](phenyl)methanone  
4{2,1,1}**



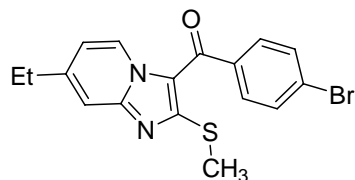
Brown solid (yield 82%); mp 138 °C dec. IR (KBr) ( $\nu_{\max}/\text{cm}^{-1}$ ): 1218, 1336, 1444, 1568, 1602, 1645, 2931, 3147.  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta_{\text{H}}$  (ppm): 1.34 (3H, t,  $^3J_{\text{HH}}=7.5$  Hz), 2.54 (3H, s, S- $\text{CH}_3$ ), 2.79 (2H, q,  $^3J_{\text{HH}}=7.5$  Hz), 6.91 (1H, dd,  $^3J_{\text{HH}}=7$  Hz,  $^4J_{\text{HH}}=1$  Hz), 7.46 (1H, d,  $^4J_{\text{HH}}=1$  Hz), 7.50-7.52 (2H, m), 7.57-7.58 (1H, m), 7.66-7.68 (2H, m), 9.46 (1H, d,  $^3J_{\text{HH}}=7$  Hz).  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )  $\delta_{\text{C}}$  (ppm): 14.60, 15.29, 28.97, 113.65, 116.06, 120.38, 128.46, 128.58, 129.02, 131.86, 140.49, 147.81, 149.11, 156.67, 185.65 (C=O). MS,  $m/z$  (%): 296 ( $\text{M}^+$ ,100), 279 (30), 263 (70), 191 (50), 105 (90), 77 (90).

**[7-ethyl-2-(ethylsulfanyl)imidazo[1,2-*a*]pyridin-3-yl](phenyl)methanone 4{2,1,2}**



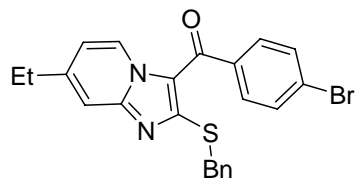
Brown solid (yield 79%); mp 139 °C dec. IR (KBr) ( $\nu_{\max}/\text{cm}^{-1}$ ): 1342, 1602, 1637, 2960.  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta_{\text{H}}$  (ppm): 1.28 (3H, t,  $^3J_{\text{HH}}=7.5$  Hz), 1.32 (3H, t,  $^3J_{\text{HH}}=7.5$  Hz), 2.77 (2H, q,  $^3J_{\text{HH}}=7.5$  Hz), 3.15 (2H, q,  $^3J_{\text{HH}}=7.5$  Hz), 6.89 (1H, dd,  $^3J_{\text{HH}}=7$  Hz,  $^4J_{\text{HH}}=2$  Hz), 7.26 (1H, d,  $^4J_{\text{HH}}=2$  Hz), 7.43-7.51 (2H, m), 7.55-7.59 (1H, m), 7.65-7.67 (2H, m), 9.42 (1H, d,  $^3J_{\text{HH}}=7$  Hz).  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )  $\delta_{\text{C}}$  (ppm): 14.16, 14.64, 26.20, 28.51, 113.20, 115.49, 127.95, 128.29, 128.51, 128.61, 131.48, 140.00, 147.24, 148.66, 155.47, 185.37 (C=O). MS,  $m/z$  (%): 310 ( $\text{M}^+$ ,90), 293 (30), 277 (90), 205 (100), 105 (45), 77 (60).

**(4-bromophenyl)[7-ethyl-2-(methylsulfanyl)imidazo[1,2-*a*]pyridin-3-yl]methanone 4{2,3,1}**



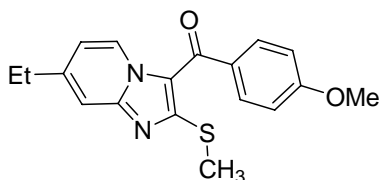
Brown solid (yield 83%); mp 137 °C dec. IR (KBr) ( $\nu_{\max}/\text{cm}^{-1}$ ): 1222, 1342, 1436, 1598, 1641, 2962.  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta_{\text{H}}$  (ppm): 1.34 (3H, t,  $^3J_{\text{HH}}=7.5$  Hz), 2.56 (3H, s, S- $\text{CH}_3$ ), 2.80 (2H, q,  $^3J_{\text{HH}}=7.5$  Hz), 6.93 (1H, dd,  $^3J_{\text{HH}}=7$  Hz,  $^4J_{\text{HH}}=1$  Hz), 7.46 (1H, d,  $^4J_{\text{HH}}=1$  Hz), 7.55 (2H, d,  $^3J_{\text{HH}}=8.4$  Hz), 7.65 (2H, d,  $^3J_{\text{HH}}=8.4$  Hz), 9.44 (1H, d,  $^3J_{\text{HH}}=7$  Hz).  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )  $\delta_{\text{C}}$  (ppm): 14.54, 15.20, 28.00, 113.72, 116.21, 120.12, 126.60, 128.47, 130.27, 132.28, 139.17, 148.15, 149.24, 156.84, 184.27 (C=O). MS,  $m/z$  (%): 376 ( $\text{M}^+$ , 30), 341 (15), 262 (20), 205 (20), 105 (60), 77 (60), 57 (100).

**[2-(benzylsulfanyl)-7-ethylimidazo[1,2-*a*]pyridin-3-yl](4-bromophenyl)methanone 4{2,3,3}**



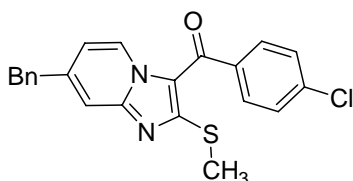
Brown solid (yield 79%); mp 139 °C dec. IR (KBr) ( $\nu_{\max}/\text{cm}^{-1}$ ): 1217, 1334, 1440, 1598, 1639, 2929, 3057.  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta_{\text{H}}$  (ppm): 1.35 (3H, t,  $^3J_{\text{HH}}=7.5$  Hz,  $\text{CH}_3$ ), 2.78 (2H, q,  $^3J_{\text{HH}}=7.5$  Hz), 4.45 (2H, s), 6.91 (1H, dd,  $^3J_{\text{HH}}=7$  Hz,  $^4J_{\text{HH}}=2$  Hz), 7.21-7.27 (2H, m), 7.32-7.33 (2H, m), 7.44-7.47 (3H, m), 7.53 (1H, m), 7.63-7.65 (2H, m), 9.41 (1H, d,  $^3J_{\text{HH}}=7$  Hz).  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )  $\delta_{\text{C}}$  (ppm): 14.18, 28.53, 36.27, 113.30, 115.61, 119.94, 127.07, 127.94, 128.34, 128.51, 128.73, 129.10, 131.62, 130.54, 139.77, 147.27, 148.45, 154.73, 185.34 (C=O). MS,  $m/z$  (%): 452 ( $\text{M}^+$ , 4), 372 (28), 339 (20), 267 (24), 105 (100), 91 (50), 77 (52).

**[7-ethyl-2-(methylsulfanyl)imidazo[1,2-*a*]pyridin-3-yl](4-methoxyphenyl)methanone 4{2,4,1}**



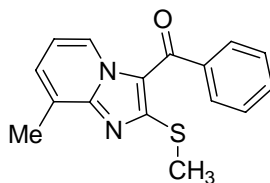
Yellow solid (yield 86%); mp 139 °C dec. IR (KBr) ( $\nu_{\max}/\text{cm}^{-1}$ ): 1258, 1336, 1427, 1595, 1641, 2908, 3024.  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta_{\text{H}}$  (ppm): 1.34 (3H, t,  $^3J_{\text{HH}}=7.5$  Hz,  $\text{CH}_3$ ), 2.58 (3H, s, S- $\text{CH}_3$ ), 2.79 (2H, q,  $^3J_{\text{HH}}=7.5$  Hz,  $\text{CH}_2$ ), 3.92 (3H, s, O- $\text{CH}_3$ ), 6.89 (1H, d,  $^3J_{\text{HH}}=7$  Hz), 7.02 (2H, d,  $^3J_{\text{HH}}=8.4$  Hz), 7.46 (1H, s), 7.71 (2H, d,  $^3J_{\text{HH}}=8.4$  Hz), 9.34 (1H, d,  $^3J_{\text{HH}}=7$  Hz).  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )  $\delta_{\text{C}}$  (ppm): 14.61, 15.40, 28.95, 55.83, 113.63, 114.23, 115.85, 120.63, 128.22, 130.81, 131.16, 132.80, 147.30, 148.92, 163.19, 184.94 (C=O). MS,  $m/z$  (%): 326 ( $\text{M}^+$ , 90), 293 (55), 217 (100), 184 (50), 135 (75), 77 (40), 57 (60).

**[7-benzyl-2-(methylsulfanyl)imidazo[1,2-*a*]pyridin-3-yl](4-chlorophenyl)methanone 4{3,2,1}**



Yellow solid (yield 78%); mp 136 °C dec. IR (KBr) ( $\nu_{\max}/\text{cm}^{-1}$ ): 1222, 1353, 1438, 1595, 1639, 2845, 3028.  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta_{\text{H}}$  (ppm): 2.55 (3H, s,  $\text{CH}_3$ ), 4.10 (2H, s,  $\text{CH}_2$ ), 6.91-6.93 (1H, m), 7.24-7.26 (2H, m), 7.27-7.30 (1H, m), 7.35-7.38 (2H, m), 7.43 (1H, s), 7.48-7.50 (2H, m), 7.61-7.63 (2H, m), 9.43 (1H, d,  $^3J_{\text{HH}}=7.0$  Hz).  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )  $\delta_{\text{C}}$  (ppm): 15.21, 42.00, 115.09, 116.56, 120.17, 127.36, 128.60, 129.32, 129.35, 129.55, 130.14, 138.26, 138.59, 138.79, 145.24, 148.96, 156.70, 184.34 (C=O). MS,  $m/z$  (%): 392 ( $\text{M}^+$ , 85), 359 (40), 267 (45), 181 (50), 139 (70), 111 (50), 57 (100).

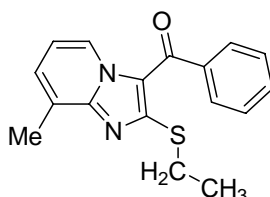
**[8-methyl-2-(methylsulfanyl)imidazo[1,2-*a*]pyridin-3-yl](phenyl)methanone 4{4,1,1}**



Brown solid (yield 75%); mp 122 °C, lit.<sup>2</sup> mp 136 °C dec. IR (KBr) ( $\nu_{\max}/\text{cm}^{-1}$ ): 1342, 1427, 1600, 2910, 3058.  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta_{\text{H}}$  (ppm): 2.55 (3H, s, S- $\text{CH}_3$ ), 2.62 (3H, s,  $\text{CH}_3$ ), 6.93 (1H, t,  $^3J_{\text{HH}}=7$  Hz), 7.27 (1H, d,  $^3J_{\text{HH}}=7$  Hz), 7.48-7.51 (2H, m), 7.55-7.59 (1H, m), 7.65-7.67 (2H, m), 9.40 (1H, d,  $^3J_{\text{HH}}=7$  Hz).  $^{13}\text{C}$  NMR (125

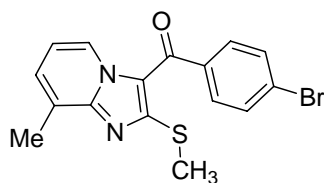
MHz, CDCl<sub>3</sub>)  $\delta_C$  (ppm): 14.88, 16.63, 114.21, 120.58, 125.94, 126.32, 128.57, 128.59, 128.74, 140.04, 148.14, 155.17, 185.59 (C=O). MS,  $m/z$  (%): 282 (M<sup>+</sup>,100), 249 (80), 221 (40), 177 (35), 92 (37), 77 (48).

**[2-(ethylsulfanyl)-8-methylimidazo[1,2-*a*]pyridin-3-yl](phenyl)methanone 4{4,1,2}**



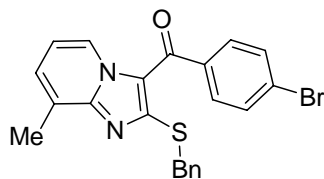
Brown solid (yield 74%); mp 135 °C dec. IR (KBr) ( $\nu_{\max}/\text{cm}^{-1}$ ): 1336, 1450, 1573, 1602, 2958. <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>)  $\delta_H$  (ppm): 1.29 (3H, t, <sup>3</sup> $J_{\text{HH}}=7.5$  Hz), 2.62 (3H, s, CH<sub>3</sub>), 3.18 (2H, q, <sup>3</sup> $J_{\text{HH}}=7.5$  Hz, CH<sub>2</sub>), 6.92 (1H, dd, <sup>3</sup> $J_{\text{HH}}=7$  Hz, <sup>3</sup> $J_{\text{HH}}=6.5$  Hz), 7.26 (1H, d, <sup>3</sup> $J_{\text{HH}}=7$  Hz), 7.48-7.51 (2H, m), 7.57 (1H, m), 7.66-7.68 (2H, m), 9.37 (1H, d, <sup>3</sup> $J_{\text{HH}}=6.5$  Hz). <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>)  $\delta_C$  (ppm): 14.74, 16.63, 26.37, 114.06, 120.76, 125.92, 126.26, 128.35, 128.44, 128.51, 131.53, 140.00, 148.15, 154.41, 185.74 (C=O). MS,  $m/z$  (%): 296 (M<sup>+</sup>,100), 263 (95), 248 (50), 235 (50), 191 (80), 105 (40), 77 (70).

**(4-bromophenyl)[8-methyl-2-(methylsulfanyl)imidazo[1,2-*a*]pyridin-3-yl]methanone 4{4,3,1}**



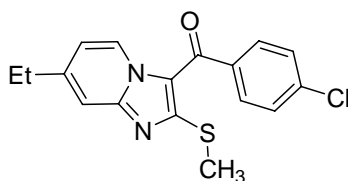
Brown solid (yield 77%); mp 139 °C dec. IR (KBr) ( $\nu_{\max}/\text{cm}^{-1}$ ): 1255, 1342, 1485, 1598, 1641, 2956, 3382. <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>)  $\delta_H$  (ppm): 2.60 (3H, s, S-CH<sub>3</sub>), 2.65 (3H, s, CH<sub>3</sub>), 6.95-6.98 (1H, m), 7.29-7.32 (1H, m), 7.56-7.57 (2H, m), 7.65-7.67 (2H, m), 9.40 (1H, d, <sup>3</sup> $J_{\text{HH}}=6.8$  Hz). <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>)  $\delta_C$  (ppm): 15.23, 17.05, 114.82, 116.56, 120.78, 126.50, 129.32, 130.76, 132.29, 132.56, 139.21, 148.73, 155.77, 184.67 (C=O). MS,  $m/z$  (%): 362 (M<sup>+</sup>,20), 360 (18), 177 (100), 135 (20), 77 (35).

**[2-(benzylsulfanyl)-8-methylimidazo[1,2-*a*]pyridin-3-yl](4-bromophenyl)  
methanone 4{4,3,3}**



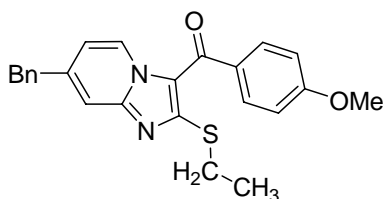
Brown solid (yield 72%); mp 139 °C dec. IR (KBr) ( $\nu_{\max}/\text{cm}^{-1}$ ): 1342, 1430, 1596, 1672, 2945.  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta_{\text{H}}$  (ppm): 2.69 (3H, s,  $\text{CH}_3$ ), 4.49 (2H, s,  $\text{CH}_2$ ), 6.95 (1H, dd,  $^3J_{\text{HH}} = 7$  Hz,  $^3J_{\text{HH}} = 6.9$  Hz), 7.24 (1H, d,  $^3J_{\text{HH}} = 7$  Hz), 7.27-7.31 (3H, m), 7.39-7.40 (2H, m), 7.53 (2H, d,  $^3J_{\text{HH}} = 8.4$  Hz), 7.61 (2H, d,  $^3J_{\text{HH}} = 8.4$  Hz), 9.35 (1H, d,  $^3J_{\text{HH}} = 6.9$  Hz).  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )  $\delta_{\text{C}}$  (ppm): 17.16, 36.67, 114.80, 120.78, 126.56, 126.72, 126.87, 127.53, 128.73, 129.20, 129.70, 130.54, 132.23, 138.60, 138.98, 148.54, 154.14, 184.73 (C=O). MS,  $m/z$  (%): 438 ( $\text{M}^+$ , 10), 382 (10), 253 (15), 181 (15), 105 (100), 91 (20), 77 (50).

**(4-chlorophenyl)[7-ethyl-2-(methylsulfanyl)imidazo[1,2-*a*]pyridin-3-yl]methanone 4{2,2,1}**



Brown solid (yield 77%); mp 137 °C dec. IR (KBr) ( $\nu_{\max}/\text{cm}^{-1}$ ): 1210, 1338, 1434, 1587, 1637, 2968, 3453.  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta_{\text{H}}$  (ppm): 1.35 (3H, t,  $^3J_{\text{HH}} = 7.5$  Hz), 2.57 (3H, s,  $\text{CH}_3$ ), 2.80 (2H, q,  $^3J_{\text{HH}} = 7.5$  Hz,  $\text{CH}_2$ ), 6.94 (1H, d,  $^3J_{\text{HH}} = 6.9$  Hz), 7.47-7.50 (3H, m), 7.61-7.63 (2H, m), 9.45 (1H, d,  $^3J_{\text{HH}} = 6.9$  Hz).  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )  $\delta_{\text{C}}$  (ppm): 14.56, 15.23, 28.99, 113.70, 116.25, 120.16, 128.47, 129.34, 130.13, 138.16, 138.17, 148.20, 149.19, 156.73, 184.26 (C=O). MS,  $m/z$  (%): 330 ( $\text{M}^+$ , 100), 297 (60), 205 (50), 139 (70), 111 (50), 57 (30).

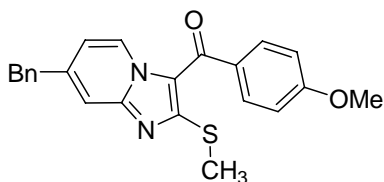
**[7-benzyl-2-(ethylsulfanyl)imidazo[1,2-*a*]pyridin-3-yl](4-methoxyphenyl)  
methanone 4{3,4,2}**





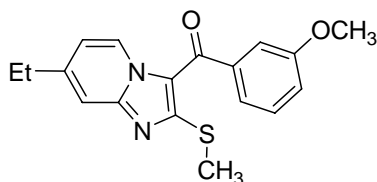
Yellow solid (yield 81%); mp 113 °C dec. IR (KBr) ( $\nu_{\max}/\text{cm}^{-1}$ ): 1222, 1336, 1434, 1604, 1637, 2871, 3020.  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta_{\text{H}}$  (ppm): 1.31 (3H, t,  $^3J_{\text{HH}}=7.3$  Hz), 3.18 (2H, q,  $^3J_{\text{HH}}=7.3$  Hz), 3.92 (3H, s,  $\text{OCH}_3$ ), 4.08 (2H, s,  $\text{CH}_2$ ), 6.85-6.87 (1H, m), 7.01 (2H, d,  $^3J_{\text{HH}}=8.6$  Hz), 7.24-7.30 (3H, m), 7.34-7.40 (3H, m), 7.73 (2H, d,  $^3J_{\text{HH}}=8.6$  Hz), 9.29 (1H, d,  $^3J_{\text{HH}}=7.05$  Hz).  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )  $\delta_{\text{C}}$  (ppm): 15.15, 26.80, 41.98, 55.85, 114.20, 115.06, 116.03, 127.28, 128.30, 129.28, 129.55, 131.39, 132.67, 138.99, 144.19, 163.31, 185.10 (C=O). MS,  $m/z$  (%): 402 ( $\text{M}^+$ , 70), 369 (65), 267 (80), 167 (45), 149 (100), 135 (70), 72 (35).

**[7-benzyl-2-(methylsulfanyl)imidazo[1,2-*a*]pyridin-3-yl](4-methoxyphenyl)  
methanone 4{3,4,1}**



Yellow solid (yield 84%); mp 144 °C dec. IR (KBr) ( $\nu_{\max}/\text{cm}^{-1}$ ): 1255, 1340, 1431, 1598, 1637, 2923, 3062.  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta_{\text{H}}$  (ppm): 2.56 (3H, s, S- $\text{CH}_3$ ), 3.91 (3H, s,  $\text{OCH}_3$ ), 4.08 (2H, s,  $\text{CH}_2$ ), 6.86-6.88 (1H, m), 7.01 (2H, d,  $^3J_{\text{HH}}=8.2$  Hz), 7.24-7.29 (3H, m), 7.33-7.40 (3H, m), 7.71 (2H, d,  $^3J_{\text{HH}}=8.2$  Hz), 9.32 (1H, d,  $^3J_{\text{HH}}=7.1$  Hz).  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )  $\delta_{\text{C}}$  (ppm): 15.36, 41.97, 55.89, 114.25, 115.17, 116.12, 120.65, 127.28, 128.36, 129.28, 129.55, 131.20, 132.68, 138.96, 144.31, 148.71, 155.26, 163.25, 184.98 (C=O). MS,  $m/z$  (%): 388 ( $\text{M}^+$ , 100), 255 (65), 267 (40), 135 (75), 77 (25).

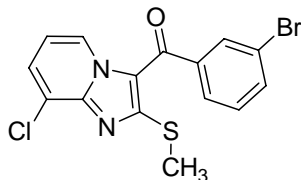
**[7-ethyl-2-(methylsulfanyl)imidazo[1,2-*a*]pyridin-3-yl](3-methoxyphenyl)  
methanone 4{2,6,1}**



Brown solid (yield 90%); mp 75 °C dec. IR (KBr) ( $\nu_{\max}/\text{cm}^{-1}$ ): 1237, 1330, 1468, 1577, 2964.  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta_{\text{H}}$  (ppm): 1.33 (3H, t,  $^3J_{\text{HH}}=7.6$  Hz), 2.55 (3H, s, S- $\text{CH}_3$ ), 2.79 (2H, q,  $^3J_{\text{HH}}=7.6$  Hz), 3.88 (3H, s,  $\text{OCH}_3$ ), 6.91 (1H, dd,  $^3J_{\text{HH}}=7$  Hz,  $^4J_{\text{HH}}=1.5$  Hz), 7.11-7.13 (1H, m), 7.19 (1H, d,  $^4J_{\text{HH}}=1.5$  Hz), 7.25-7.28 (1H, m),

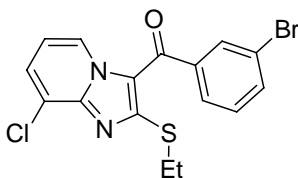
7.40-7.46 (2H, m), 9.45 (1H, d,  $^3J_{\text{HH}} = 7$  Hz).  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )  $\delta_{\text{C}}$  (ppm): 14.71, 15.38, 28.96, 55.86, 113.21, 113.64, 114.65, 116.08, 118.31, 120.98, 128.49, 130.19, 141.62, 147.87, 149.07, 156.77, 160.11, 185.25 (C=O). MS,  $m/z$  (%): 326 ( $\text{M}^+$ , 100), 293 (70), 217 (75), 191 (30), 77 (35).

**(3-bromophenyl)[8-chloro-2-(methylsulfonyl)imidazo[1,2-*a*]pyridin-3-yl]  
methanone 4{5,5,1}**



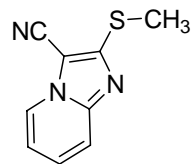
White solid (yield 78%); mp 151 °C dec. IR (KBr) ( $\nu_{\text{max}}/\text{cm}^{-1}$ ): 1196, 1340, 1425, 1597, 2917, 3053.  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta_{\text{H}}$  (ppm): 2.64 (3H, s, S- $\text{CH}_3$ ), 7.00 (1H, t,  $^3J_{\text{HH}} = 7.1$  Hz), 7.39-7.42 (1H, m), 7.57 (1H, dd,  $^3J_{\text{HH}} = 7.1$  Hz,  $^4J_{\text{HH}} = 1$  Hz), 7.60-7.62 (1H, m), 7.72-7.74 (1H, m), 7.81-7.82 (1H, m), 9.45 (1H, dd,  $^3J_{\text{HH}} = 7.1$  Hz,  $^4J_{\text{HH}} = 1$  Hz).  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )  $\delta_{\text{C}}$  (ppm): 15.42, 114.50, 121.33, 122.39, 123.18, 127.19, 127.54, 129.19, 130.74, 131.73, 135.13, 141.55, 145.93, 157.20, 184.34 (C=O). MS,  $m/z$  (%): 382 ( $\text{M}^+$ , 100), 349 (60), 326 (40), 197 (45), 76 (50).

**(3-bromophenyl)[8-chloro-2-(ethylsulfonyl)imidazo[1,2-*a*]pyridin-3-yl]  
methanone 4{5,5,2}**



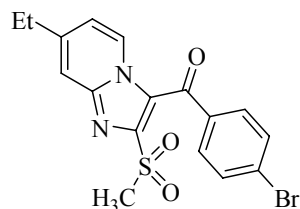
White solid (yield 81%); mp 114 °C dec. IR (KBr) ( $\nu_{\text{max}}/\text{cm}^{-1}$ ): 1193, 1333, 1421, 1596, 2958, 3100.  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta_{\text{H}}$  (ppm): 1.35 (3H, t,  $^3J_{\text{HH}} = 7.2$  Hz,  $\text{CH}_3$ ), 3.28 (2H, q,  $^3J_{\text{HH}} = 7.2$  Hz,  $\text{CH}_2$ ), 6.99 (1H, t,  $^3J_{\text{HH}} = 7.0$  Hz), 7.40-7.42 (1H, m), 7.57 (1H, d,  $^3J_{\text{HH}} = 7.0$  Hz), 7.61-7.63 (1H, m), 7.72-7.74 (1H, m), 7.81-7.82 (1H, m), 9.47 (1H, d,  $^3J_{\text{HH}} = 7.0$  Hz).  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )  $\delta_{\text{C}}$  (ppm): 14.62, 26.59, 113.91, 122.00, 122.69, 126.92, 128.64, 130.24, 131.48, 134.74, 141.09, 145.54, 156.10, 184.52 (C=O). MS,  $m/z$  (%): 396 ( $\text{M}^+$ , 30), 326 (60), 211 (70), 149 (100), 43 (75).

**Procedure for preparation of 2-(methylsulfanyl)imidazo[1,2-*a*]pyridine-3-yl cyanide **6****



Pyridine (0.097 ml, 1.2 mmol) and chloroacetonitrile (0.076 ml, 1.2 mmol) were taken up in toluene (10 ml) and the mixture was stirred at reflux for 72 h. To this mixture methyl thiocyanate (0.074 g, 1.0 mmol) and potassium carbonate (0.28 g, 2.0 mmol) were added and it was allowed to stir at reflux for 24 h. Upon completion, the toluene was removed under reduced pressure, then water was added and the reaction mixture was extracted with dichloromethane (3×15 ml). The organic layer was dried over Na<sub>2</sub>SO<sub>4</sub>. Evaporation of the solvent followed by purification on silica gel (*n*-hexane-ethyl acetate, 90-10) afforded the pure **6** as Brown solid (yield 66%); mp 134 °C, lit.<sup>2</sup> mp 132 °C dec. IR (KBr) ( $\nu_{\max}/\text{cm}^{-1}$ ): 1336, 1461, 1627, 2202, 2959, 3305. <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>)  $\delta_{\text{H}}$  (ppm): 2.77 (3H, s, S-CH<sub>3</sub>), 7.05-7.08 (1H, m), 7.42-7.45 (1H, m), 7.65-7.66 (1H, m), 8.25-8.26 (1H, m). <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>)  $\delta_{\text{C}}$  (ppm): 14.72, 111.64, 114.95, 117.29, 125.66, 129.07, 147.21, 154.80. MS, *m/z* (%): 189 (M<sup>+</sup>, 100), 156 (50), 144 (20), 78 (40).

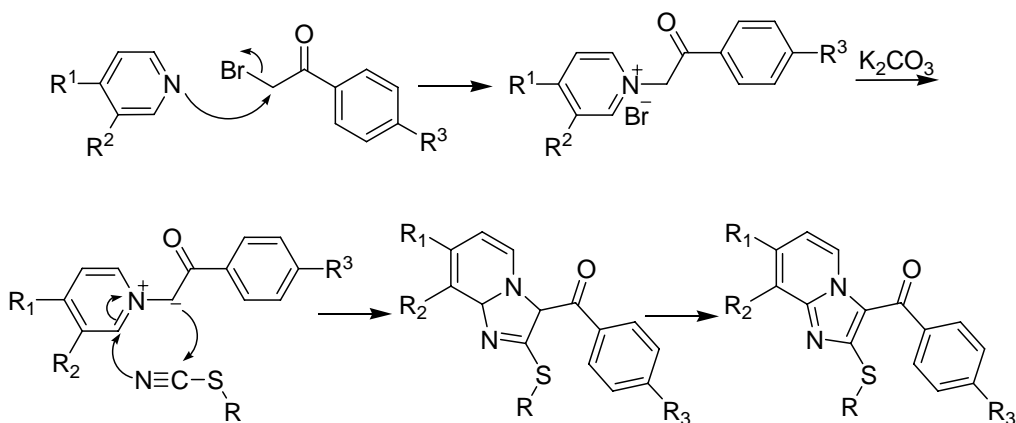
**Procedure for preparation of (4-bromophenyl)[7-ethyl-2-(methylsulfonyl)imidazo[1,2-*a*]pyridin-3-yl]methanone **7****



A solution of (4-bromophenyl)[7-ethyl-2-(methylsulfanyl)imidazo[1,2-*a*]pyridin-3-yl]methanone **4**{2,3,1} (0.37 g, 1.0 mmol) in 10 ml CH<sub>2</sub>Cl<sub>2</sub> was cooled to 0 °C. Then, *m*-CPBA (0.26 g, 1.5 mmol), dissolved in 15 ml CH<sub>2</sub>Cl<sub>2</sub>, was added dropwise to the stirred solution of **4**{2,3,1}. The reaction progress was monitored by TLC. After stirring for 3 h, water was added and the reaction mixture was extracted with CH<sub>2</sub>Cl<sub>2</sub> (3 × 15 ml). The organic layer was dried over Na<sub>2</sub>SO<sub>4</sub>. Evaporation of the solvent

followed by purification on silica gel (*n*-hexane-ethyl acetate, 90-10) afforded the pure title compound as white solid (yield 96%); mp 201 °C dec. IR (KBr) ( $\nu_{\max}/\text{cm}^{-1}$ ): 823, 1228, 1321, 1477, 1631, 2877, 3006.  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta_{\text{H}}$  (ppm): 1.37 (3H, t,  $^3J_{\text{HH}}=7.5$  Hz), 2.83 (2H, q,  $^3J_{\text{HH}}=7.5$  Hz), 3.30 (3H, s,  $\text{SO}_2\text{CH}_3$ ), 7.03 (1H, dd,  $^3J_{\text{HH}}=7.2$  Hz,  $^4J_{\text{HH}}=1.57$  Hz), 7.59 (1H, s), 7.68 (2H, d,  $^3J_{\text{HH}}=10.5$  Hz), 7.80 (2H, d,  $^3J_{\text{HH}}=10.5$  Hz), 8.76 (1H, d,  $^3J_{\text{HH}}=7.2$  Hz).  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )  $\delta_{\text{C}}$  (ppm): 14.44, 28.98, 43.34, 116.04, 118.38, 120.82, 127.29, 129.51, 131.48, 132.29, 138.54, 146.67, 147.87, 148.69, 185.67 (C=O). MS,  $m/z$  (%): 408 ( $\text{M}^+$ , 23), 167 (44), 149 (100), 71 (53), 57 (68), 43 (46).

### Proposed Mechanism



### References

1. Barun, O.; Ila, H.; Junjappa, H. *J. Org. Chem.* **2000**, *65*, 1583-1587.
2. Tominaga, Y.; Hosomi, A. *J. Heterocycl. Chem.* **1988**, *25*, 1449-1454.

B7 <sup>1</sup>H NMR in CDCl<sub>3</sub> at 298 K 86/10/26

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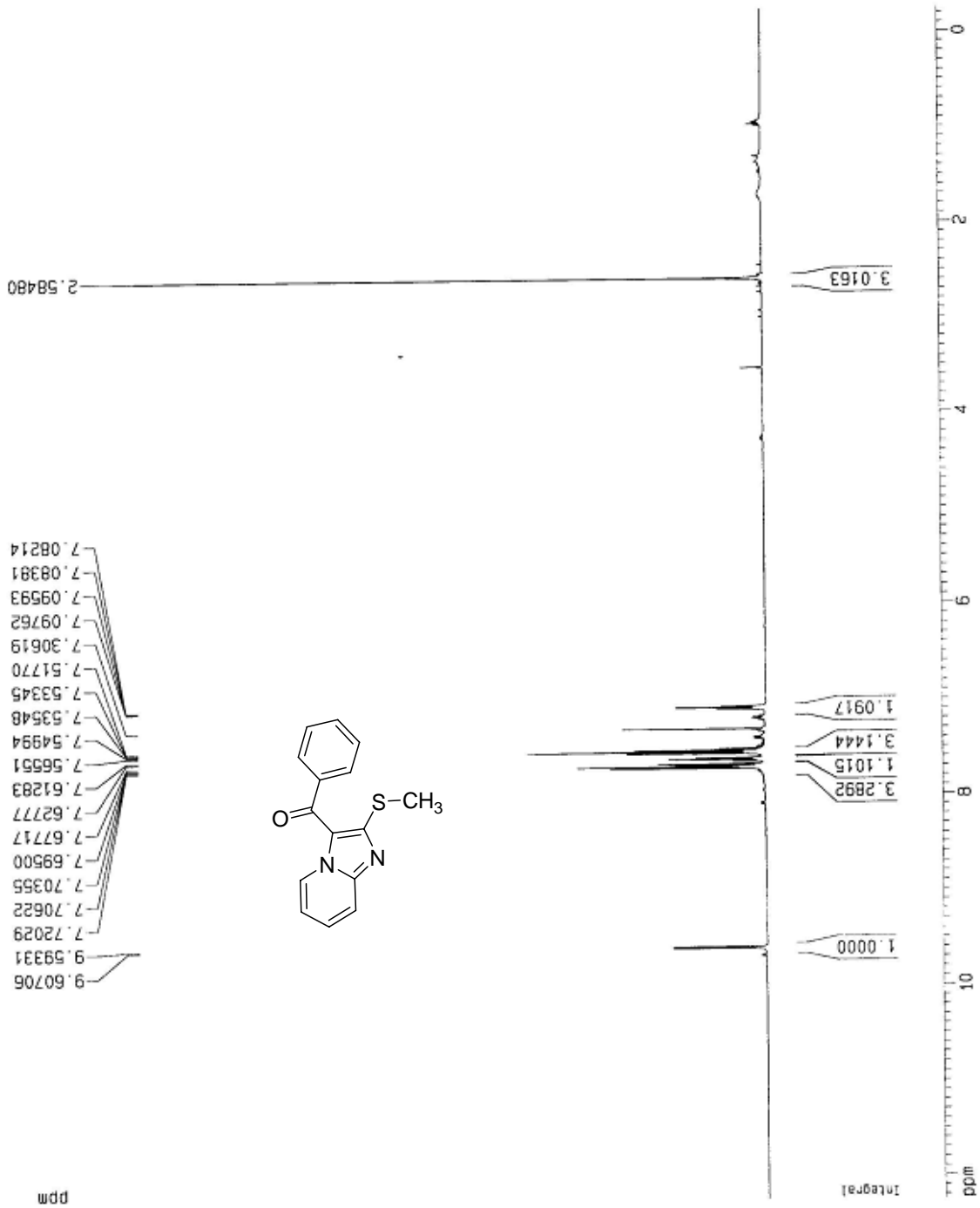
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PL1       2.00 dB
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87 13CNMR in CDCl3 at 298 K 05/10/25

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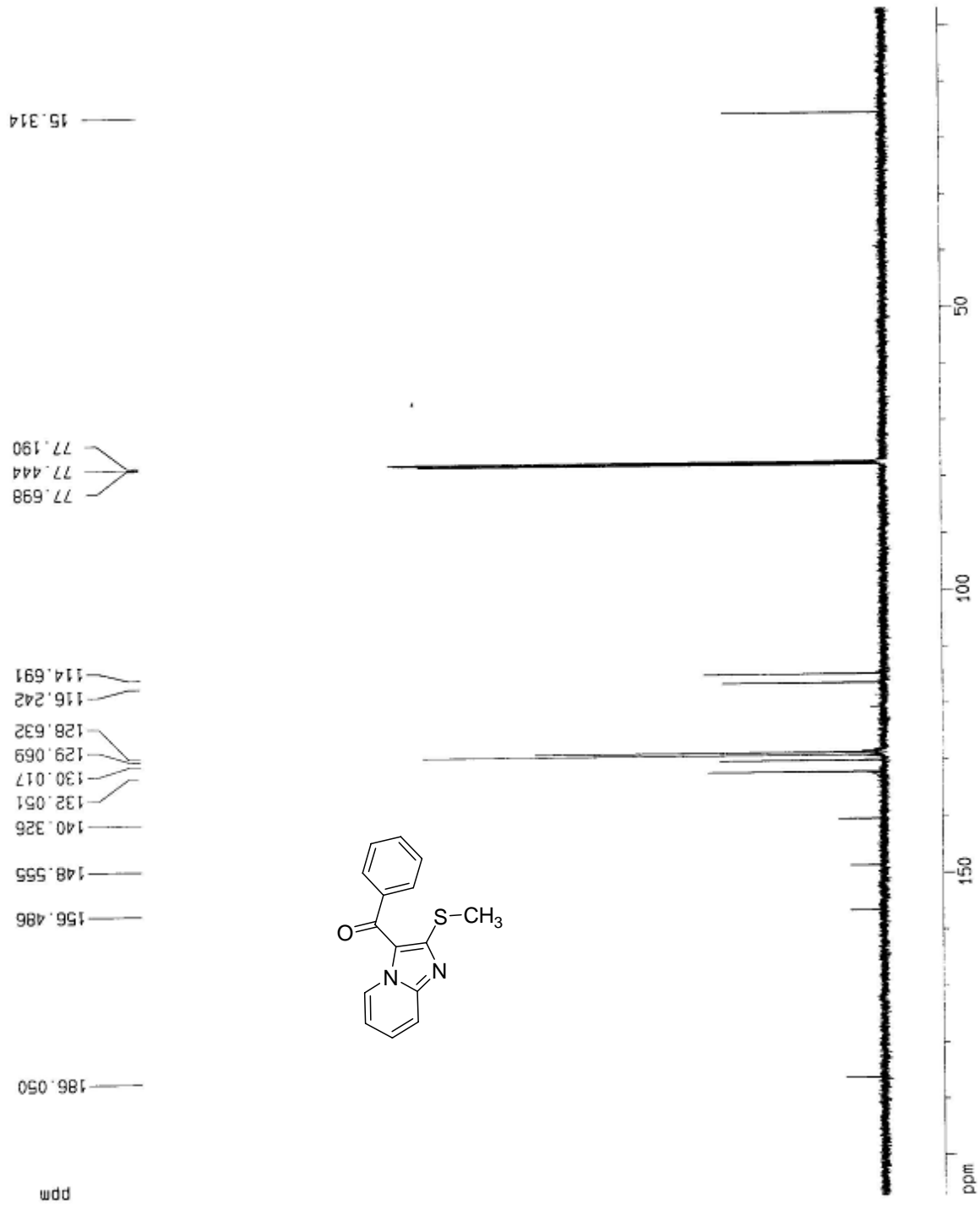
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86 13CNMR in CDCl3 at 298 K 85/10/3

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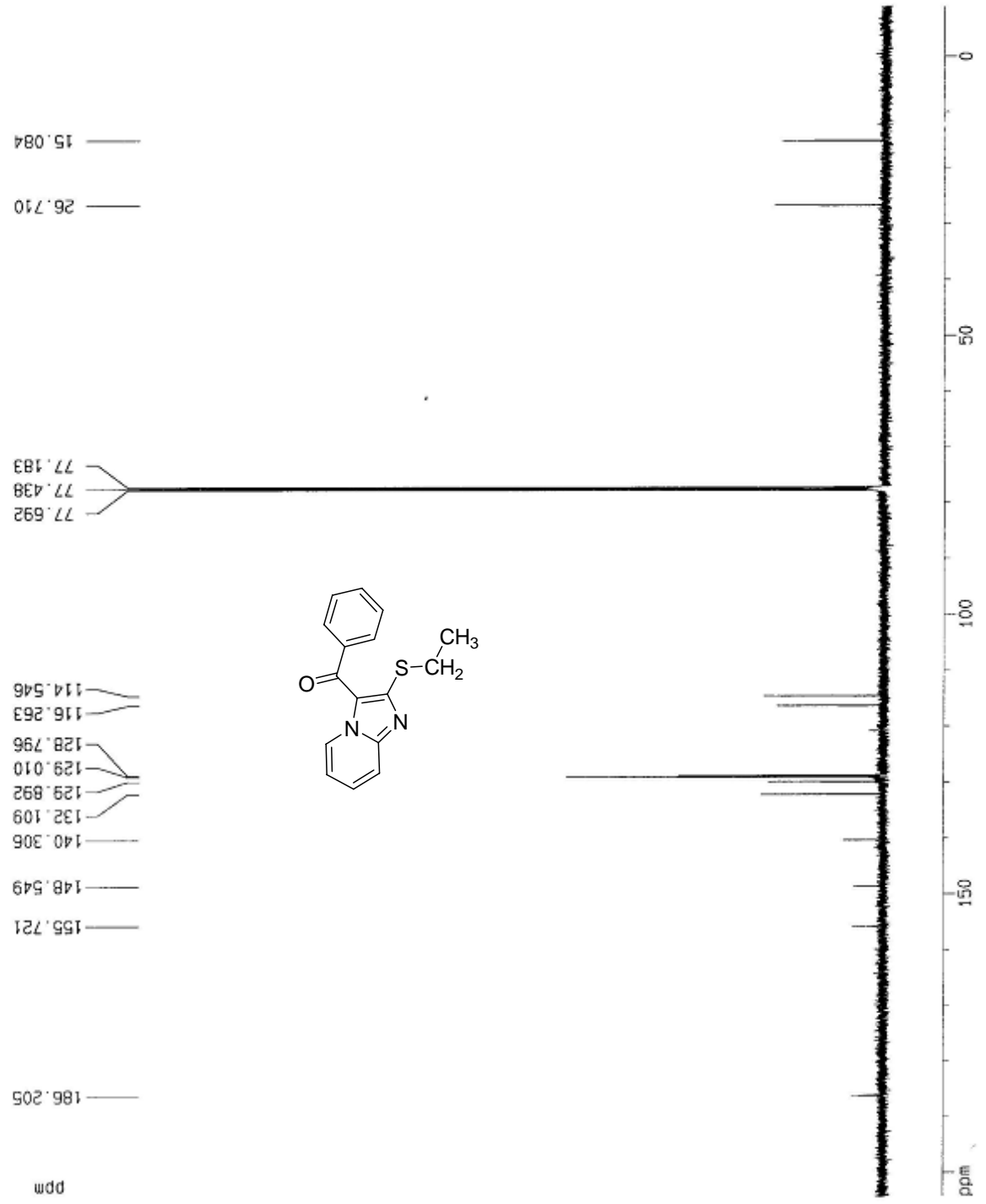
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B40 1H NMR in CDCl3 at 298 K 08/2/16

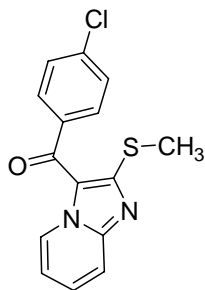
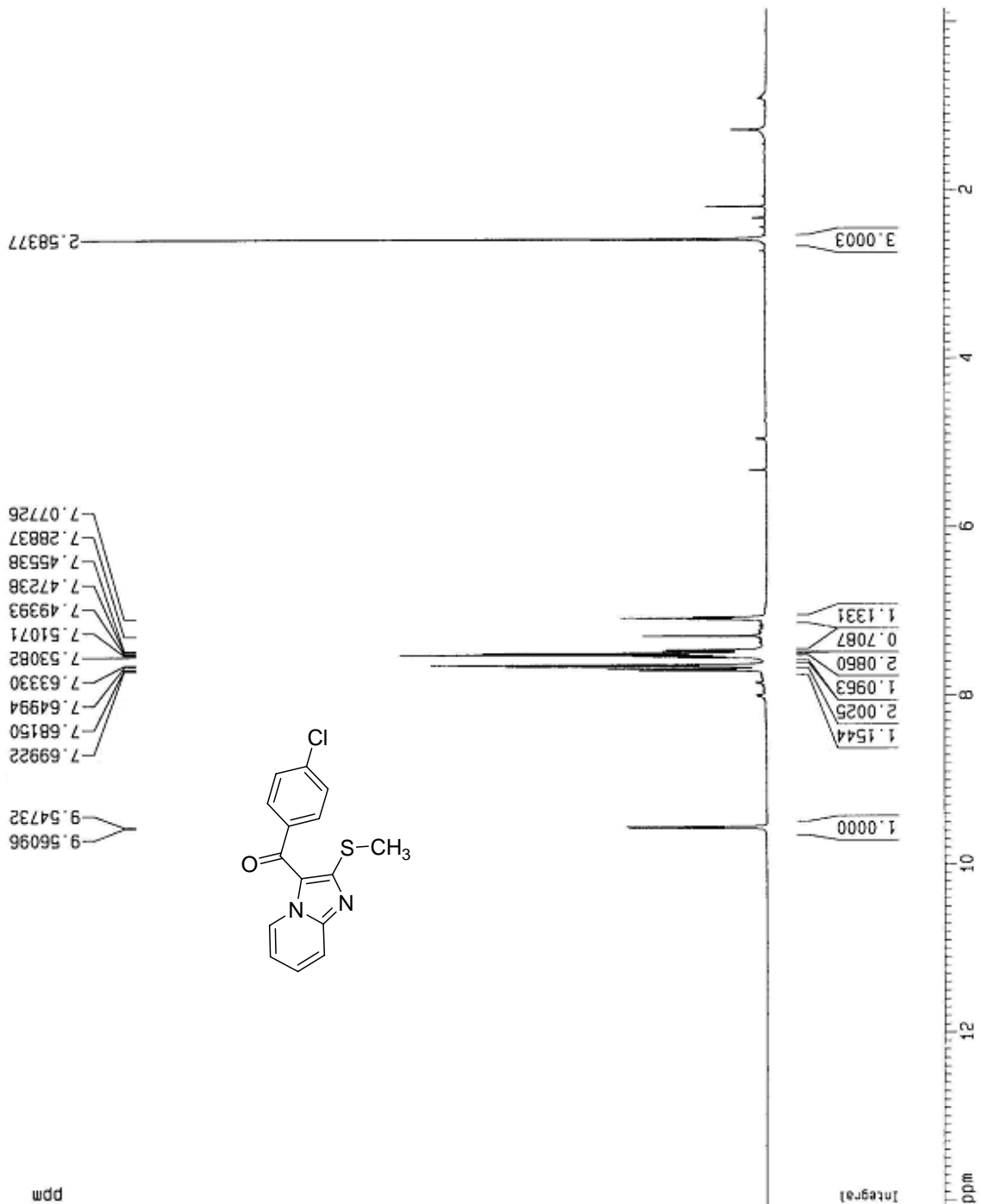
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 Date\_ 20090506  
 Time 12.20  
 INSTRUM spect  
 PROBHD 5 mm QNP 1H/13  
 PULPROG zg30  
 TD 65536  
 SOLVENT MeOH  
 NS 14  
 DS 1  
 SWH 10330.578 Hz  
 FIDRES 0.157632 Hz  
 AQ 3.1720407 sec  
 RG 322.5  
 DW 48.400 usec  
 DE 6.50 usec  
 TE 298.0 K  
 D1 6.00000000 sec  
 MCREST 0.00000000 sec  
 MCPRK 0.01500000 sec

----- CHANNEL f1 -----  
 NUC1 1H  
 P1 10.50 usec  
 PL1 -3.00 dB  
 SF01 500.1330985 MHz

F2 - Processing parameters  
 SI 32768  
 SF 500.1300090 MHz  
 WDM EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00

1D NMR plot parameters  
 CX 20.00 cm  
 CY 18.40 cm  
 F1P 14.044 ppm  
 F1 7023.93 Hz  
 F2P -0.157 ppm  
 F2 -78.34 Hz  
 PPMCM 0.71004 ppm/cm  
 HZCM 355.11365 Hz/cm



840 13CNMR in CDC13 at 298 K 88/2/16

```

Current Data Parameters
NAME      Nadrin1
EXPNO    39
PROCNO   1

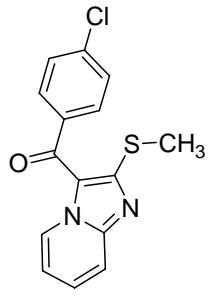
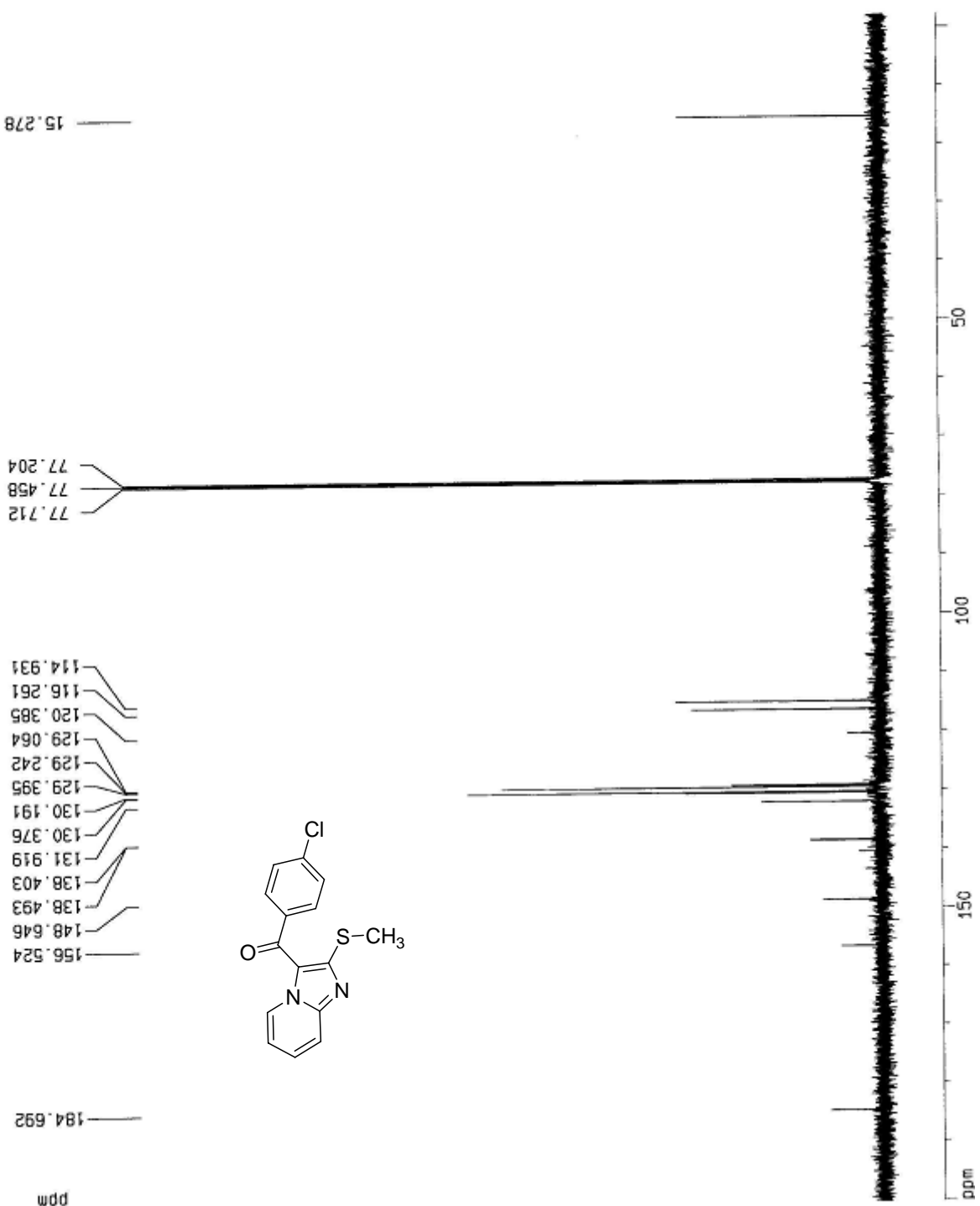
F2 - Acquisition Parameters
Date_    20090506
Time     12.22
INSTRUM  spect
PROBHD   5 mm QNP 1H/13
PULPROG  zgpg30
TD       32768
SOLVENT  CDC13
NS       296
DS       4
SWH      30030.029 Hz
FIDRES   0.915444 Hz
AQ       0.5456539 sec
RG       10321.3
DM       16.650 usec
DE       6.50 usec
TE       298.0 K
D1       1.00000000 sec
d11      0.03000000 sec
DELTA    0.89999998 sec
NCREST   0.00000000 sec
NCPK     0.01500000 sec

***** CHANNEL F1 *****
NUC1     13C
P1       9.10 usec
PL1      3.00 dB
SFO1     125.7703643 MHz

***** CHANNEL F2 *****
COPROG2  waltz16
NUC2     1H
P2       90.00 usec
PL2      0.00 dB
PL12     15.50 dB
PL13     15.50 dB
SFO2     500.1320005 MHz

F2 - Processing parameters
SI       32768
SF       125.7577390 MHz
MVM      EM
SSB      0
LB       1.00 Hz
GB       0
PC       1.40

ID NMR plot parameters
CX       20.00 cm
CY       13.56 cm
FIP      200.253 ppm
F1       25183.32 Hz
F2       -2.178 ppm
PCMK     -273.96 Hz
HZCM     10.12155 ppm/cm
         1272.85377 Hz/cm
    
```



B-41 1H NMR in CDCl3 at 298 K 88/2/16

Current Data Parameters  
 NAME Nad1r1  
 EXPNO 40  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20090506  
 Time 12.34  
 INSTRUM spect  
 PROBHD 5 mm QNP 1H/13  
 PULPROG zg30  
 TD 65536  
 SOLVENT MeOH  
 NS 16  
 DS 1  
 SMH 10330.578 Hz  
 FIDRES 0.157632 Hz  
 AQ 3.1720407 sec  
 RG 812.7  
 DW 48.400 usec  
 DE 6.50 usec  
 TE 298.0 K  
 D1 6.00000000 sec  
 MCREST 0.00000000 sec  
 MCNREK 0.01500000 sec

\*\*\*\*\* CHANNEL f1 \*\*\*\*\*  
 NUC1 1H  
 P1 10.50 usec  
 PL1 -3.00 dB  
 SF01 500.1330885 MHz

F2 - Processing parameters  
 SI 32768  
 SF 500.1300090 MHz  
 MDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00

1D NMR plot parameters  
 CX 20.00 cm  
 CY 5.72 cm  
 FIP 13.387 ppm  
 F1 6695.23 Hz  
 F2P -0.227 ppm  
 F2 -113.56 Hz  
 PPWM 0.68070 ppm/cm  
 HZCM 340.43951 Hz/cm



B41 13C NMR in CDCl3 at 298 K 88/2/16

```

Current Data Parameters
NAME      Nedir1
EXPNO    41
PROCNO   1

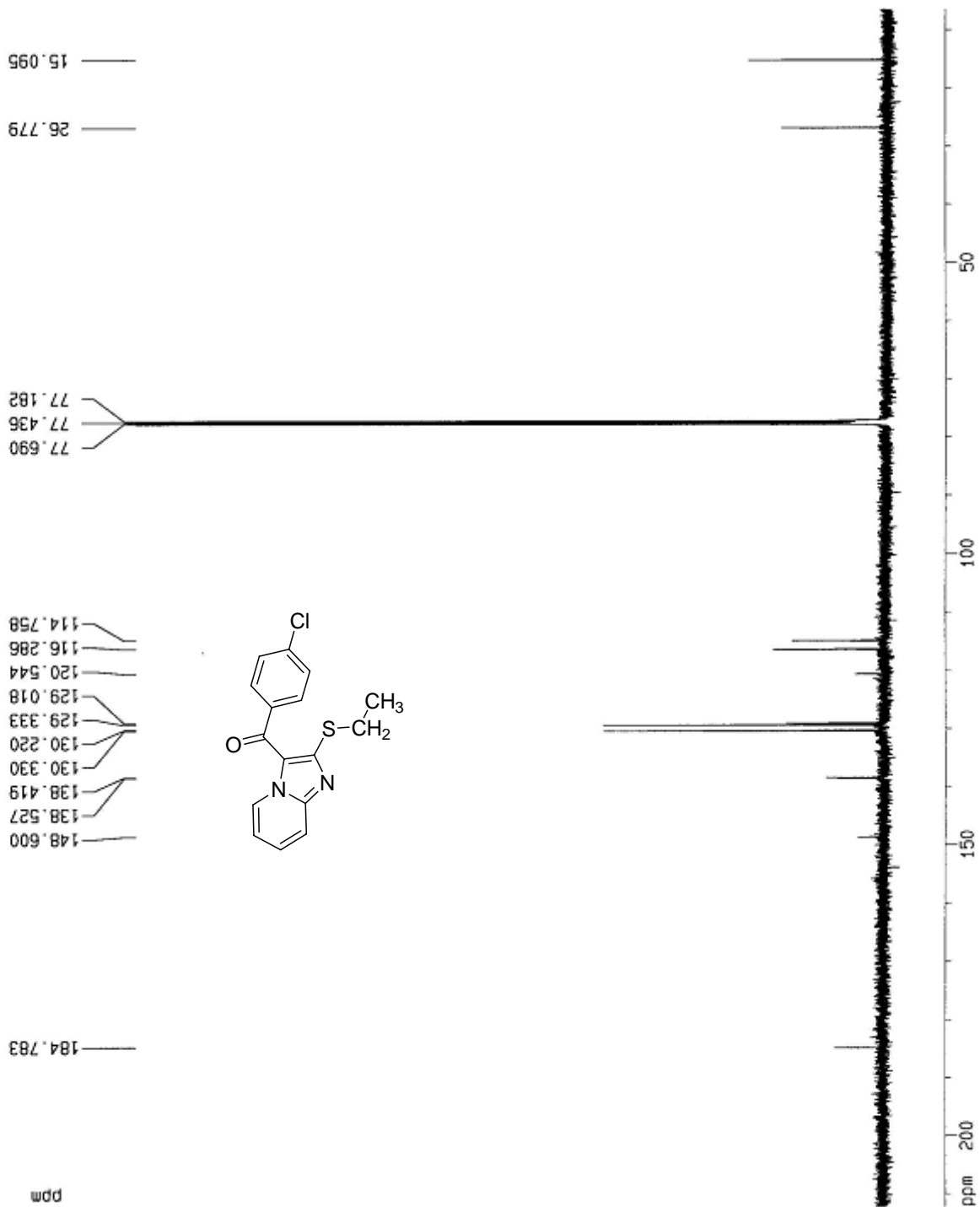
F2 - Acquisition Parameters
Date_    20090506
Time     14.44
INSTRUM  spect
PROBHD   5 mm QNP 1H/13
PULPROG  zgpg30
TD        32768
SOLVENT  DMSO
NS        2158
DS        4
SWH       30030.029 Hz
FIDRES   0.916444 Hz
AQ        0.5466539 sec
RG        3251
DM        18.850 usec
DE        6.50 usec
TE        298.0 K
D1        3.0000000 sec
d11       0.0300000 sec
DELTA    2.9000010 sec
MCREST   0.0000000 sec
MCNMRK   0.01500000 sec

***** CHANNEL f1 *****
NUC1      13C
P1        9.10 usec
PL1       3.00 dB
SFO1     125.7703643 MHz

***** CHANNEL f2 *****
CPDPRG2   waltz16
NUC2       1H
PCPD2     60.00 usec
PL2       0.00 dB
PL12      15.50 dB
PL13      15.50 dB
SFO2     500.1320005 MHz

F2 - Processing parameters
SI        32768
SF        125.7577390 MHz
WDW       EM
SSB       0
LB        1.00 Hz
GB        0
PC        1.40

1D NMR plot parameters
CK        20.00 cm
CY        45.85 cm
FJP       212.192 00H
F1        26684.82 Hz
F2P       6.505 ppm
F2        818.04 Hz
PRNCK     10.28437 ppm/cm
HZCM      1293.33875 Hz/cm
    
```



8.19 1H-NMR in CDCl3 at 298 K 87/8/13

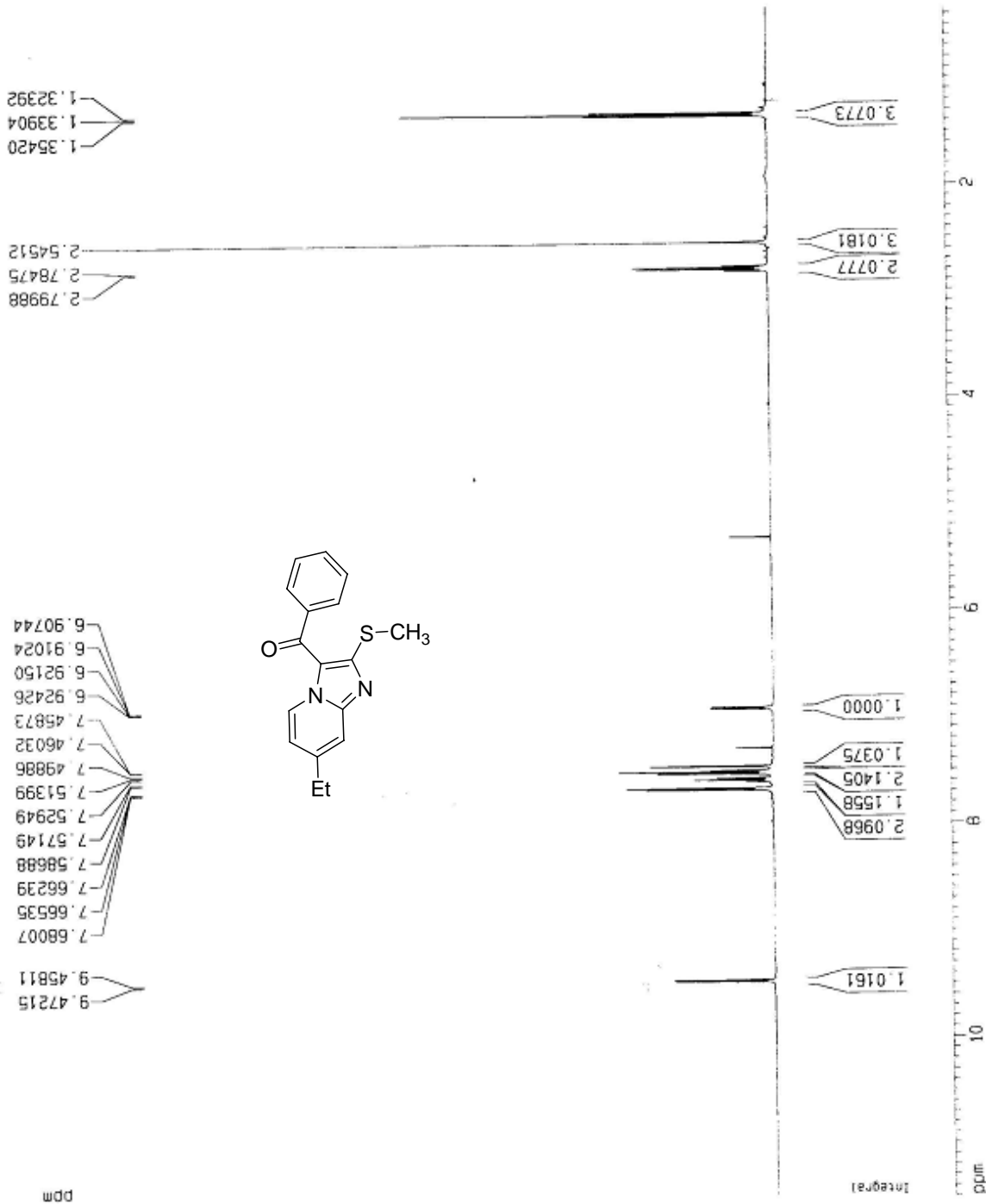
Current Data Parameters  
 Name Nadin1  
 EXPNO 11  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20081103  
 Time 14:32  
 INSTRUM spect  
 PROBHD 5 mm QNP 1H/13  
 PULPROG zg30  
 TO 65536  
 SOLVENT MeOH  
 NS 8  
 DS 1  
 SWH 10330.578 Hz  
 FIDRES 0.157632 Hz  
 AQ 3.1720407 sec  
 RG 181  
 DM 48.400 usec  
 DE 6.50 usec  
 TE 298.4 K  
 O1 5.00000000 sec  
 MCHST 0.00000000 sec  
 MCHRK 0.01500000 sec

\*\*\*\*\* CHANNEL f1 \*\*\*\*\*  
 NUC1 1H  
 P1 10.50 usec  
 PL1 -3.00 dB  
 SFO1 500.1330885 MHz

F2 - Processing parameters  
 SI 32768  
 SF 500.1300090 MHz  
 MDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00

10 NMR plot parameters  
 CX 20.00 cm  
 CY 12.50 cm  
 F1P 11.503 ppm  
 F1 5752.79 Hz  
 F2P 0.337 ppm  
 F2 168.39 Hz  
 PPM0 0.55830 ppm/cm  
 HZ0 279.22015 Hz/cm



B-19 13CNMR in CDCl3 at 298 K 87/8/13

```

Current Data Parameters
NAME      Nadiri
EXPNO    12
PROCNO   1

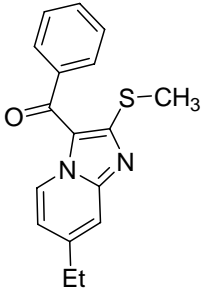
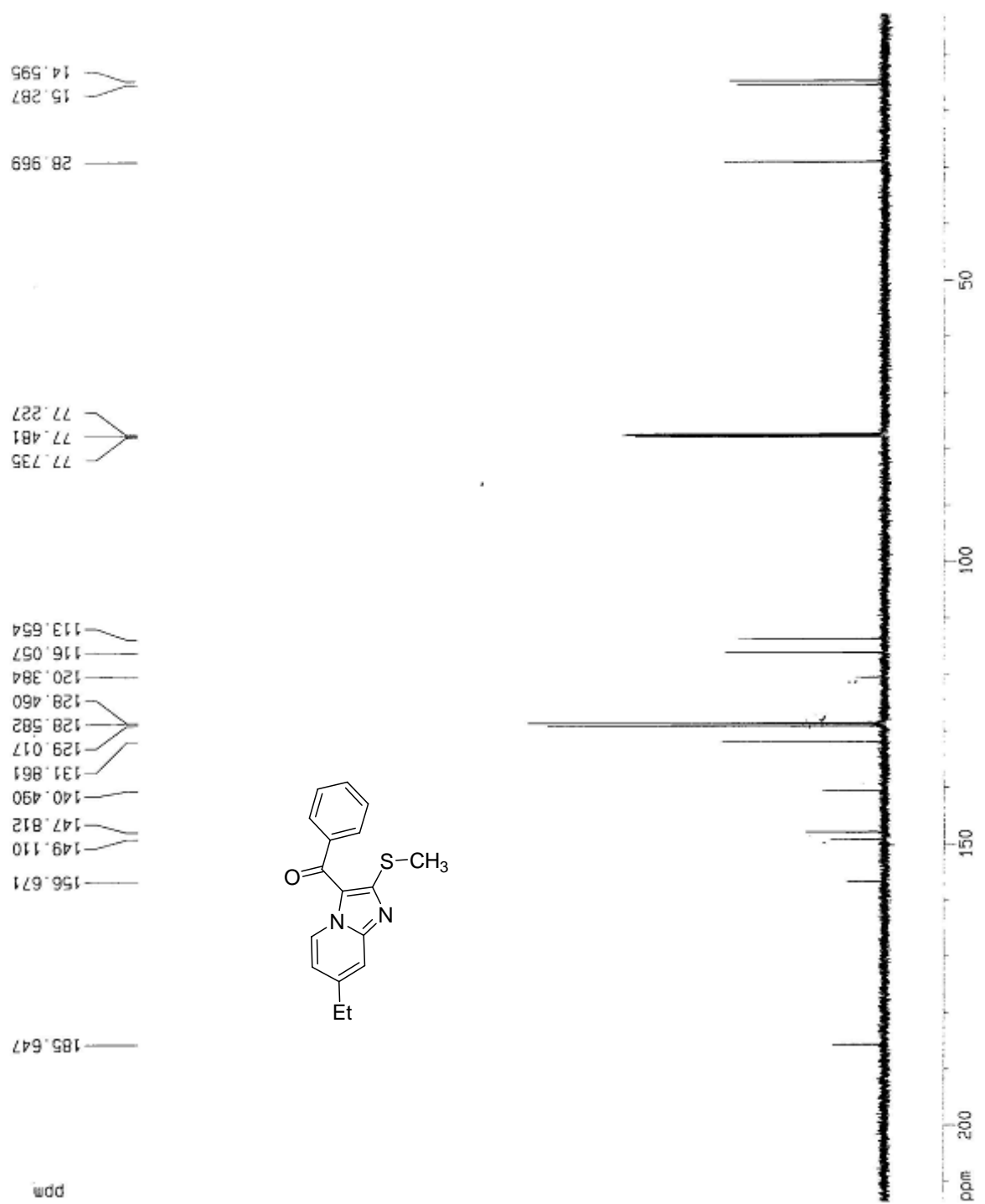
F2 - Acquisition Parameters
Date_    20081103
Time     14 37
INSTRUM  spect
PROBHD   5 mm DNP 1H/13
PULPROG  zgpg30
TO       32768
SOLVENT  MeOH
NS       112
DS       4
SWH      30030.029 Hz
FIDRES   0.916444 Hz
AQ       0.7465539 sec
RG       13004
DM       16.1650 usec
DE       6.50 usec
TE       298.3 K
D1       2.0000000 sec
d11      0.03000000 sec
DELTA    1.8895998 sec
MGREST   0.00000000 sec
MCNPK    0.01500000 sec

***** CHANNEL f1 *****
NUC1     13C
P1       9.10 usec
PL1      3.00 dB
SFO1     125.7703643 MHz

***** CHANNEL f2 *****
CPDPRG2  waltz16
NUC2     1H
PCPD2    80.00 usec
RL2      0.00 dB
PL12     15.50 dB
PL13     15.50 dB
SFO2     500.1320005 MHz

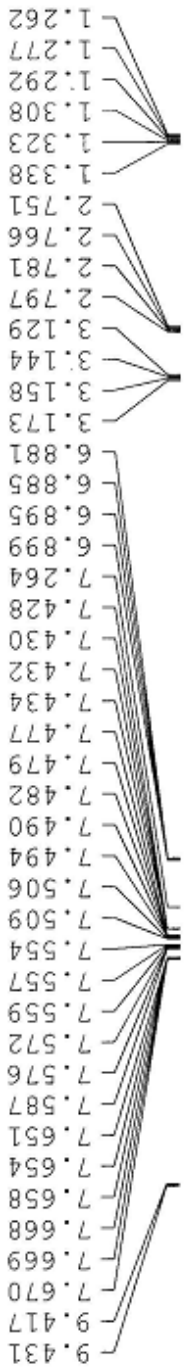
F2 - Processing parameters
SI       32768
SF       125.757190 MHz
WDW      EM
SSB      0
LB       1.00 Hz
GB       0
PC       1.40

1D NMR plot parameters
CX       20.00 cm
CY       5.99 cm
F1p      213.505 ppm
F1       26850.05 Hz
F2p      2.750 ppm
F2       343.29 Hz
PWCNM    10.93862 ppm/cm
HZCM     1325.10850 Hz/cm
    
```





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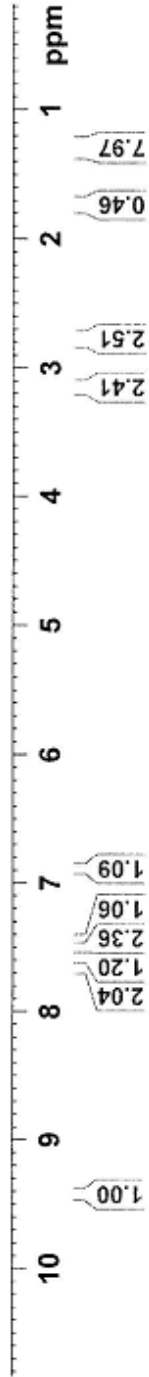
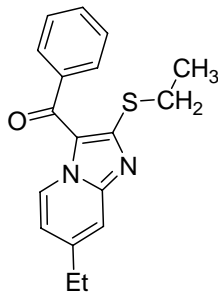


Current Data Parameters  
NAME aaa  
EXPNO 28  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20080715  
Time\_ 12.14  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zg  
TD 32768  
SOLVENT CDCl3  
NS 4  
DS 0  
SWH 8012.820 Hz  
FIDRES 0.244532 Hz  
AQ 2.0447731 sec  
RG 322  
DW 62.400 usec  
DE 6.50 usec  
TE 294.1 K  
D1 1.0000000 sec  
TD0 1

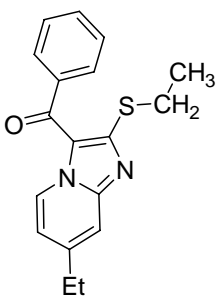
==== CHANNEL f1 =====  
NUC1 1H  
P1 9.50 usec  
PL1 -1.00 dB  
SF01 500.1337510 MHz

F2 - Processing parameters  
SI 32768  
SF 500.1300054 MHz  
WDW no  
SSB 0  
LB 0.00 Hz  
GB 0  
PC 1.00





B17



81.181  
80.181

24.140  
23.140

131.111  
130.111

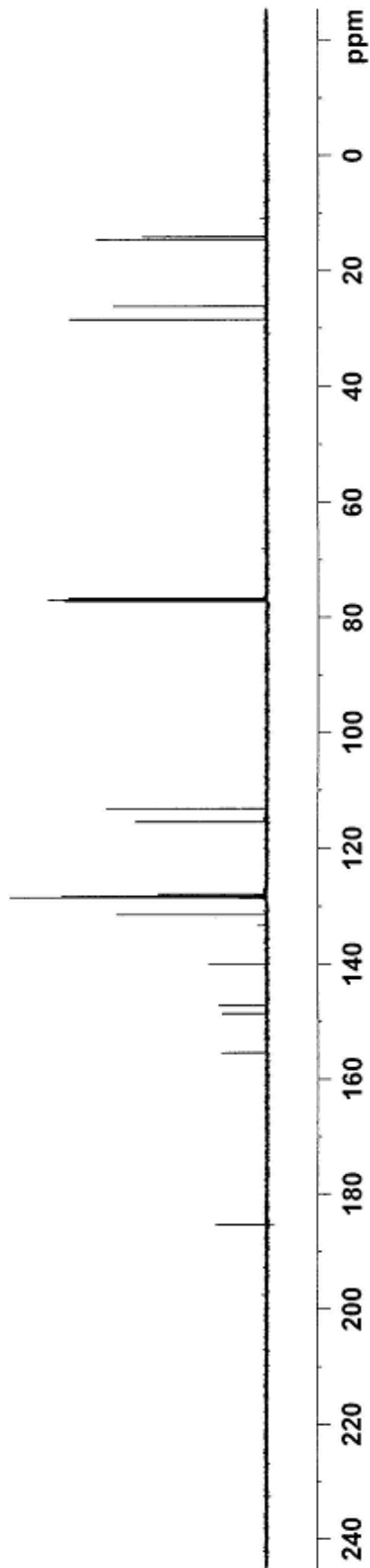
127.111  
126.111  
125.111  
124.111  
123.111

100.111

132.111  
131.111

133.111

181.111





14 <sup>1</sup>H NMR in CDCl<sub>3</sub> at 298 K 87/8/13

```

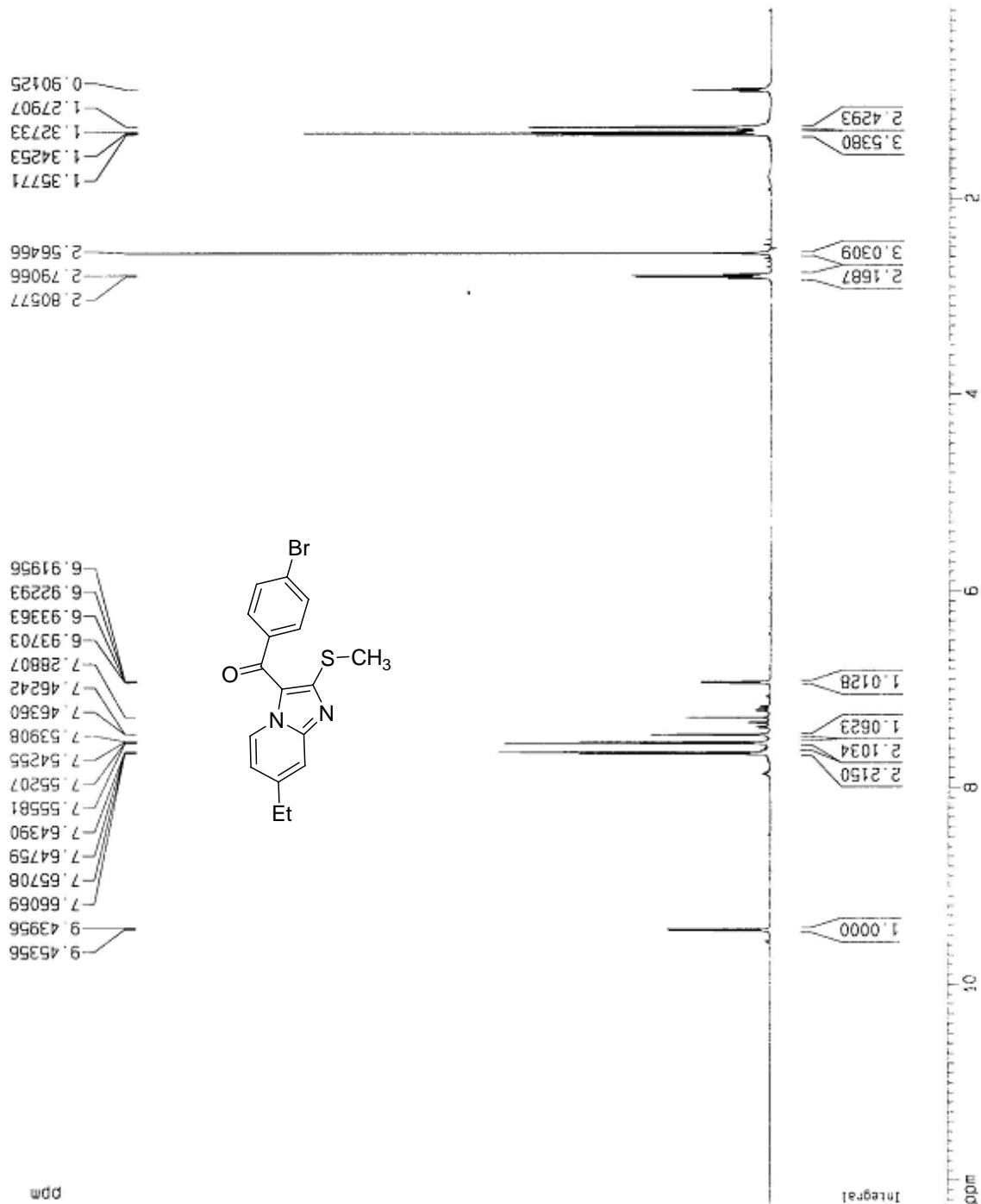
Current Data Parameters
NAME      Ncdp1
EXPNO    9
PROCNO   1

F2 - Acquisition Parameters
Date_    20081103
Time     14.20
INSTRUM spect
PROBHD   5 mm QNP 1H/13
PULPROG zg30
TD       65536
SOLVENT  MeOH
NS       8
DS       1
SWH      10330.578 Hz
FIDRES   0.157632 Hz
AQ       3.1720407 sec
RG       203.2
DN       48.400 USEC
DE       6.50 USEC
TE       298.3 K
D1       5.00000000 sec
MCREST   0.10000000 sec
MCWRRK   0.01500000 sec

----- CHANNEL f1 -----
NUC1     1H
P1       10.50 USEC
PL1      -3.00 dB
SFO1     500.1330885 MHz

F2 - Processing parameters
SI       32768
SF       500.1330090 MHz
WDW      EM
SSB      0
LB       0.30 Hz
GB       0
PC       1.00

1D NMR plot parameters
CX       20.00 cm
CY       16.01 cm
F1P      12.250 ppm
F1       6126.60 Hz
F2P      0.065 ppm
F2       32.46 Hz
PPMCM    0.60926 ppm/cm
HZCM     304.70676 Hz/cm
  
```



14 <sup>13</sup>CNMR in CDCl<sub>3</sub> at 298 K 87/8/13

Current Data Parameters  
 NAME Nadi11  
 EXPNO 10  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20081103  
 Time 14.22  
 INSTRUM spect  
 PROBHD 5 mm QNP 1H/13  
 PULPROG zgpg30  
 TD 32768  
 SOLVENT MeOH  
 NS 176  
 DS 4

SWH 30030.029 Hz  
 FIDRES 0.918444 Hz  
 AQ 0.5456539 sec  
 RG 13004  
 DM 16.850 uSec  
 DE 6.50 uSec  
 TE 298.3 K  
 D1 1.00000000 sec  
 d11 0.30000000 sec  
 DELTA 0.89999998 sec  
 MCREST 0.00000000 sec  
 MCNRK 0.01500000 sec

\*\*\*\*\* CHANNEL f1 \*\*\*\*\*  
 NU1C1 13C  
 P1 9.10 uSec  
 PL1 3.00 dB  
 SF01 125.7703643 MHz

\*\*\*\*\* CHANNEL f2 \*\*\*\*\*  
 CPDPRG2 waltz16  
 NU1C2 1H  
 PCPR2 80.00 uSec  
 PL2 0.00 dB  
 PL12 15.50 dB  
 PL13 15.50 dB  
 SF02 500.1320005 MHz

F2 - Processing parameters  
 SI 32768  
 SF 125.7577390 MHz  
 WDM EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

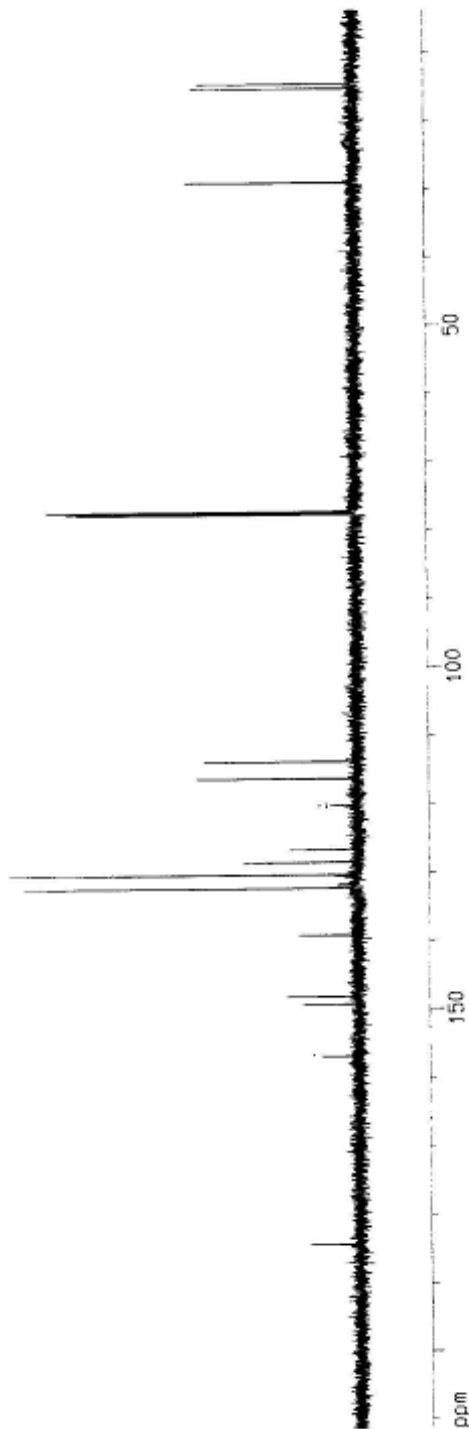
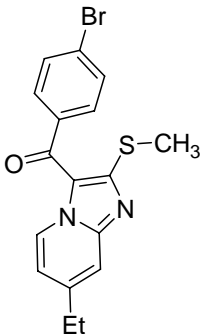
10 NMR plot parameters  
 CX 20.00 cm  
 CY 4.92 cm  
 FJP 211.412 ppm  
 F1 26586.63 Hz  
 F2 3.777 ppm  
 F2 475.00 Hz  
 PPMCM 10.38172 ppm/cm  
 HZCM 1305.58191 Hz/cm

28.986  
 15.196  
 14.536

77.204  
 77.458  
 77.712

156.844  
 149.241  
 148.149  
 139.171  
 132.281  
 130.272  
 128.469  
 126.585  
 120.122  
 116.213  
 113.716

184.271





Current Data Parameters  
 NAME aaa  
 EXPNO 641  
 PROCNO 1

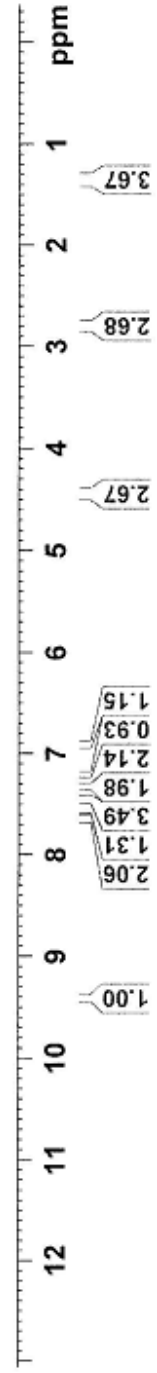
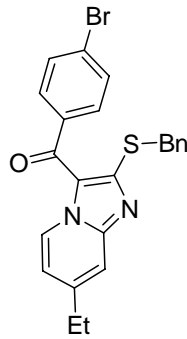
F2 - Acquisition Parameters

Date\_ 20080811  
 Time 16.13  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB-  
 PULPROG zg  
 TD 32768  
 SOLVENT CDCl3  
 NS 9  
 DS 0  
 SWH 8012.820 Hz  
 FIDRES 0.244532 Hz  
 AQ 2.0447731 sec  
 RG 144  
 DW 62.400 usec  
 DE 6.50 usec  
 TE 294.2 K  
 D1 1.0000000 sec  
 TDO 1

----- CHANNEL f1 -----  
 NUC1 1H  
 P1 9.50 usec  
 PL1 -1.00 dB  
 SFO1 500.1332610 MHz

F2 - Processing parameters  
 SI 32768  
 SF 500.1300000 MHz  
 WDW no  
 SSB 0  
 LB 0  
 GB 0  
 PC 1.00

9.424  
9.409  
7.651  
7.641  
7.637  
7.634  
7.553  
7.538  
7.534  
7.526  
7.523  
7.521  
7.472  
7.469  
7.457  
7.445  
7.442  
7.333  
7.330  
7.316  
7.275  
7.271  
7.268  
7.258  
7.254  
7.242  
7.228  
7.225  
7.222  
7.211  
6.920  
6.916  
6.906  
6.902  
4.444  
2.820  
2.805  
2.789  
2.774  
1.363  
1.348  
1.333



Mr Faramarzi B18



B34 1H NMR in CDCl3 at 298 K 87/10/30

```

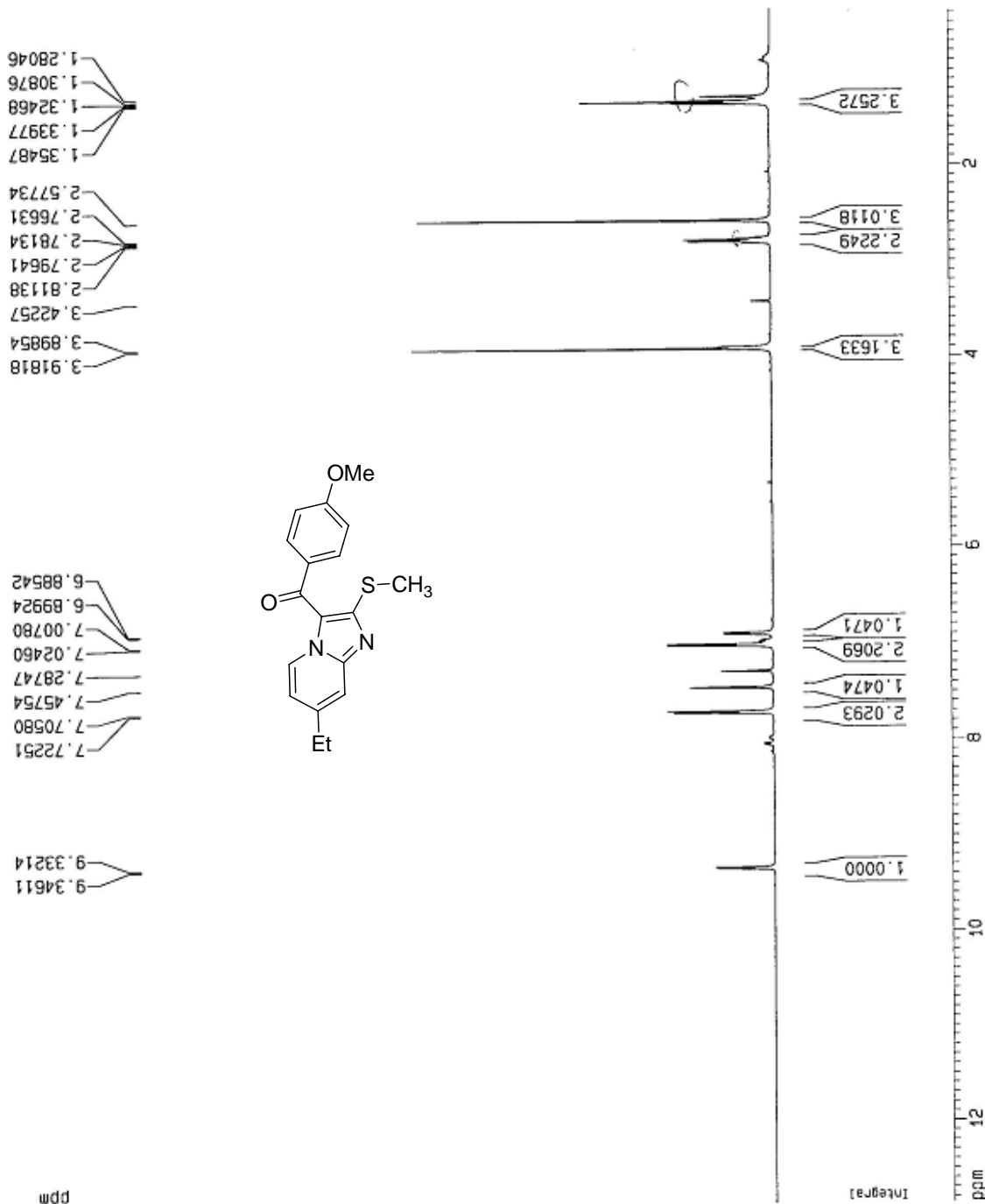
Current Data Parameters
NAME      Ndir1
EXPNO    24
PROCNO   1

F2 - Acquisition Parameters
Date_    20090119
Time     10.02
INSTRUM  spect
PROBHD   5 mm QNP 1H/13
PULPROG  zg30
TD       65536
SOLVENT  MeOH
NS       16
DS       0
SFR      10330.578 Hz
FIDRES   0.157632 Hz
AQ       3.1720407 sec
RG       362
DM       48.400 usec
DE       6.50 usec
TE       298.3 K
D1       5.00000000 sec
MCREST   0.00000000 sec
MCWRK    0.01500000 sec

***** CHANNEL f1 *****
NUC1     1H
P1       10.50 usec
PL1      -3.00 dB
SFO1     500.1330885 MHz

F2 - Processing parameters
SI       32768
SF       500.1300090 MHz
WDW      EM
SSB      0
LB       0.30 Hz
GB       0
PC       1.00

1D NMR plot parameters
CX       20.00 cm
CY       5.98 cm
FIP      12.862 ppm
F1       6432.44 Hz
F2P      0.359 ppm
F2       179.72 Hz
PPMCM    0.62511 ppm/cm
HZCM     312.63593 Hz/cm
  
```



B-34 <sup>13</sup>C NMR in CDCl<sub>3</sub> at 298 K 8/7/10/30

```

Current Data Parameters
NAME      Nadrin
EXPNO    25
PROCNO   1

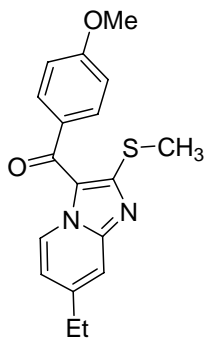
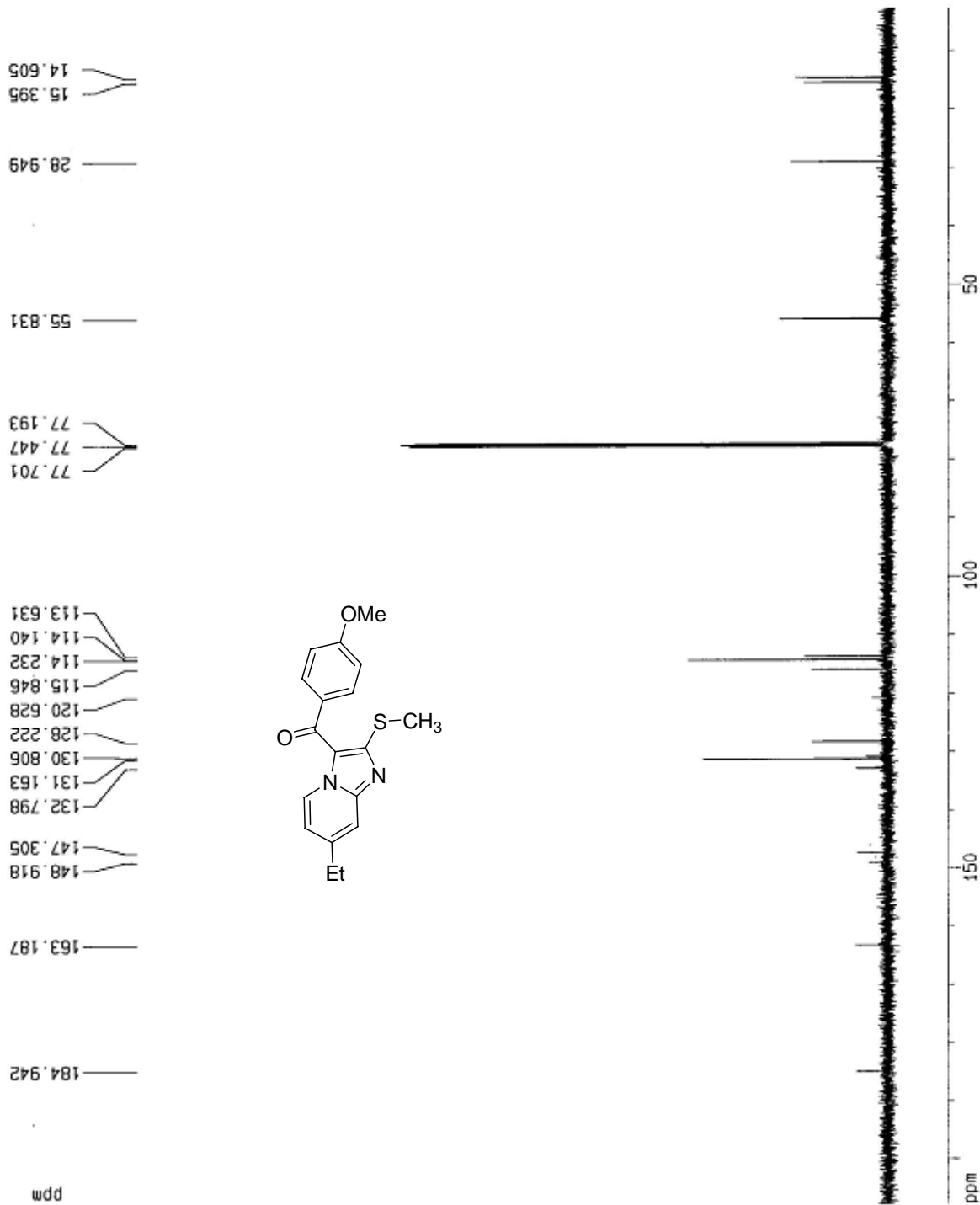
F2 - Acquisition Parameters
Date_    20090119
Time     10.08
INSTRUM  spect
PROBHD   5 mm QNP 1H/13
PULPROG  zgpg30
TD        32768
SOLVENT  CDCl3
NS        281
DS        4
SWH      30030.029 Hz
FIDRES   0.916444 Hz
AQ        0.5456539 sec
RG        5160.6
DM        16.650 usec
DE        6.50 usec
TE        298.3 K
D1        1.0000000 sec
d11       0.0300000 sec
DELTA    0.8898998 sec
MGREST   0.0000000 sec
MCNPRK   0.0150000 sec

***** CHANNEL f1 *****
NUC1      13C
P1        9.10 usec
PL1       3.00 dB
SFO1     125.7703643 MHz

***** CHANNEL f2 *****
CPDPRG2  waltz16
NUC2      1H
PCPD2    80.00 usec
PL2       0.00 dB
PL12     15.50 dB
PL13     15.50 dB
SFO2     500.1330005 MHz

F2 - Processing parameters
SI        32768
SF        125.7577350 MHz
MOM       EM
SSB       0
LB        1.00 Hz
GB        0
PC        1.40

10 NMR plot parameters
CX        20.00 cm
CY        8.16 cm
FIP       207.748 ppm
F1        28125.65 Hz
F2        2.730 ppm
F2C       343.28 Hz
PPMCM     10.25081 ppm/cm
HZCM      1289.11816 Hz/cm
    
```





B42 13CNMR in CDCl3 at 298 K 88/2/16

```

Current Data Parameters
NAME      Nadsr1
EXPNO    37
PROCNO   1

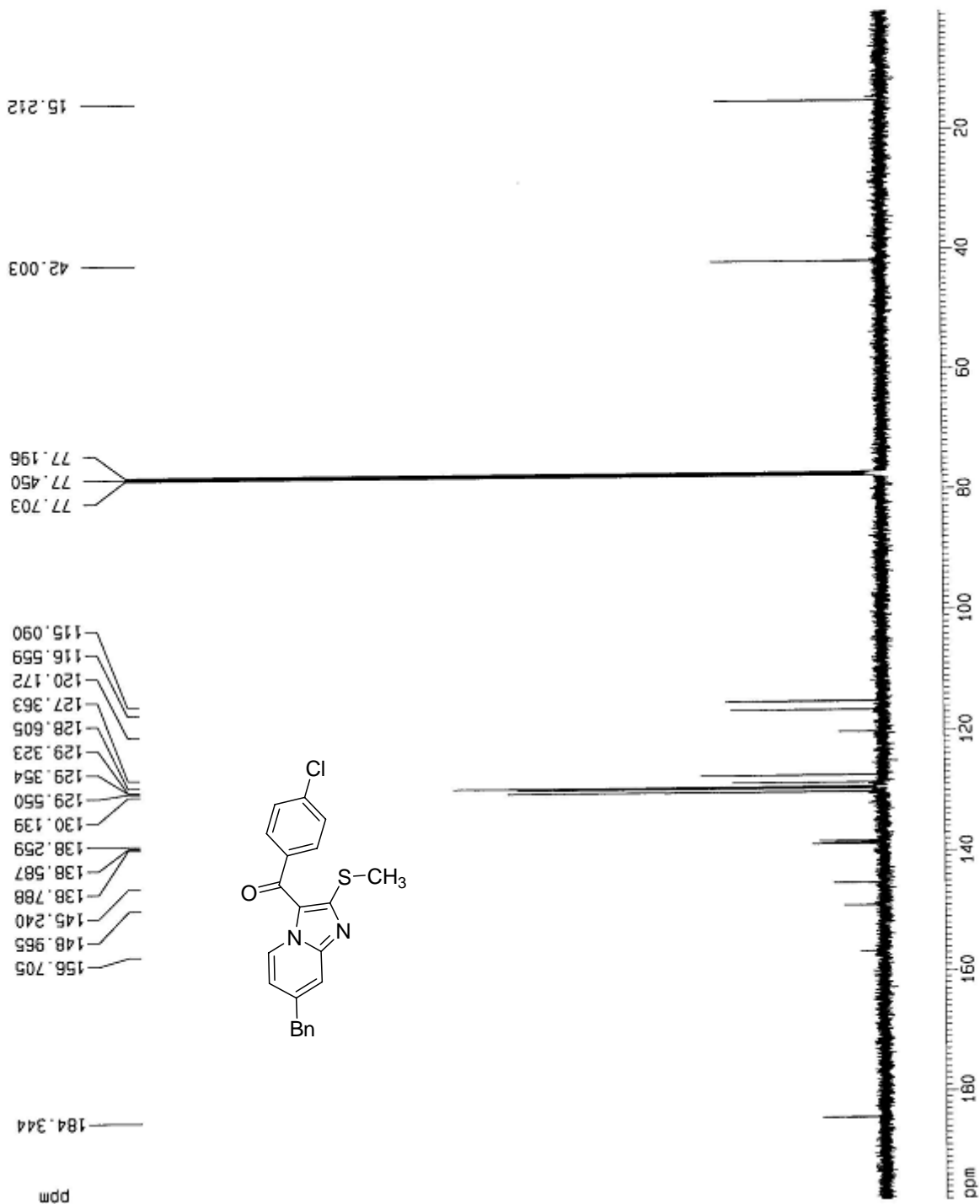
F2 - Acquisition Parameters
Date_    20090506
Time     11.46
INSTRUM  spect
PROBHD   5 mm GNP 1H/13
PULPROG  zgpg30
TD        32768
SOLVENT  CDCl3
NS        1198
DS        4
SWH       30030.029 Hz
FIDRES    0.91644 Hz
AQ         0.5406539 sec
RG         4597.6
DM         16.650 usec
DE         6.50 usec
TE         298.0 K
D1         1.00000000 sec
d11        0.03000000 sec
DELTA     0.89999999 sec
MCREST    0.00000000 sec
MCHWK     0.01500000 sec

***** CHANNEL f1 *****
NUC1      13C
P1         9.10 usec
PL1        3.00 dB
SFO1      125.7703643 MHz

***** CHANNEL f2 *****
CPOPRG2   waltz16
NUC2       1H
P2         90.00 usec
PL2        0.00 dB
PL12       15.50 dB
PL13       15.50 dB
SFO2      500.1320005 MHz

F2 - Processing parameters
SI         32768
SF        125.7577390 MHz
MGM        EM
SSB        0
LB         1.00 Hz
GB         0
PC         1.40

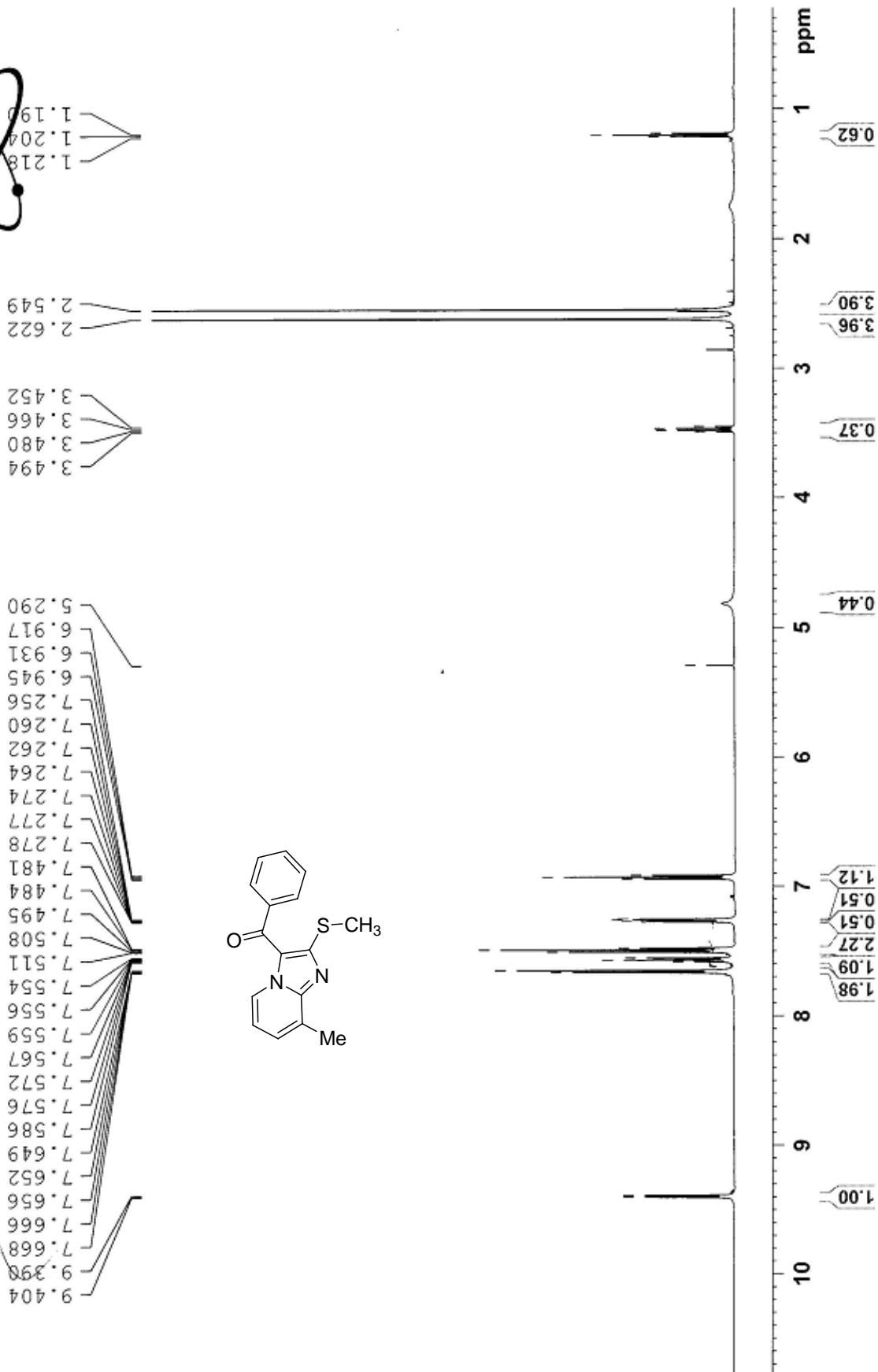
1D NMR plot parameters
CX         20.00 cm
CY         21.20 cm
F1P        198.082 ppm
F1         24910.31 Hz
F2P        0.264 ppm
F2         33.17 Hz
PPMOM      9.89090 ppm/cm
HZCM       1243.85730 Hz/cm
    
```

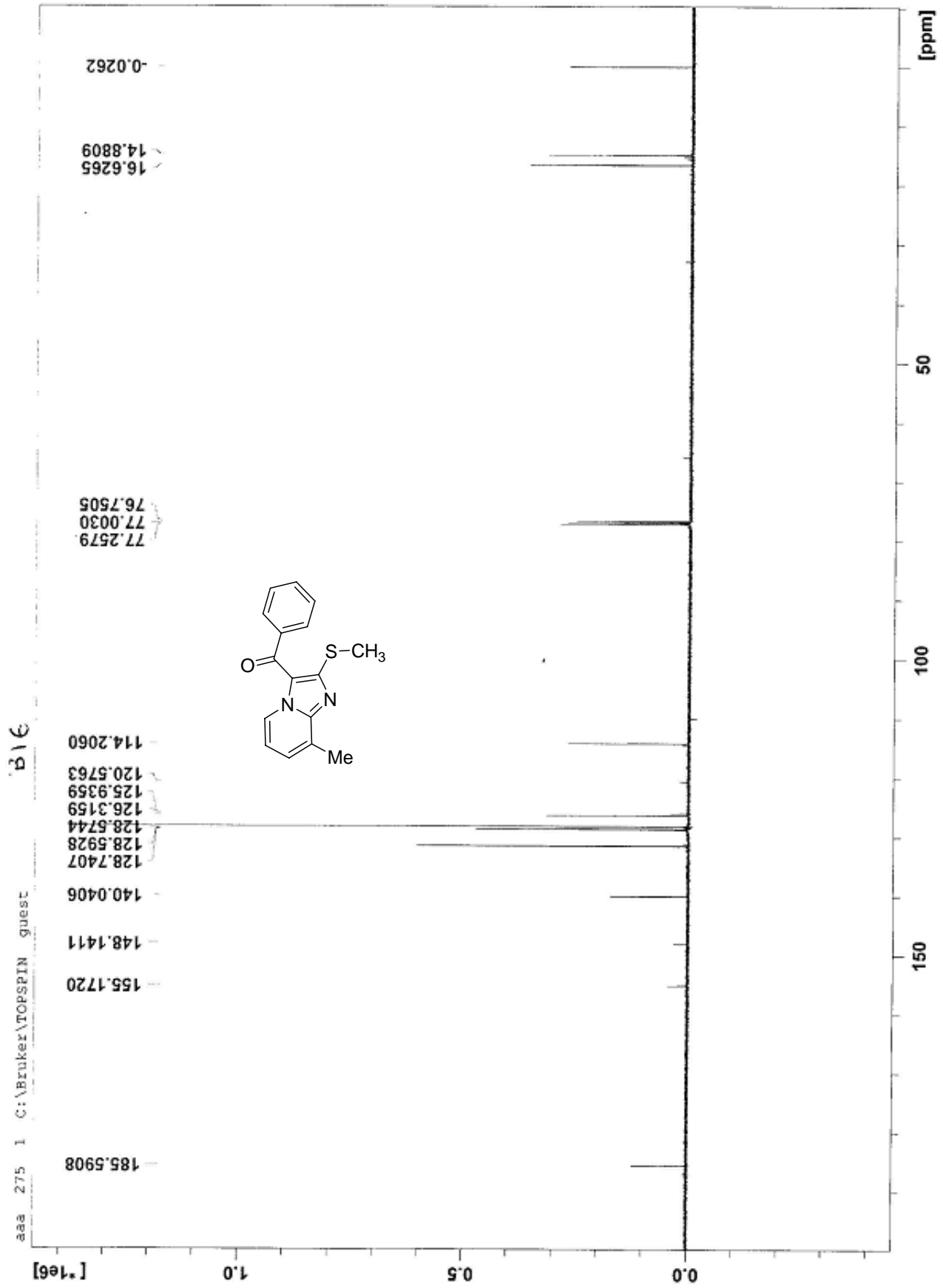






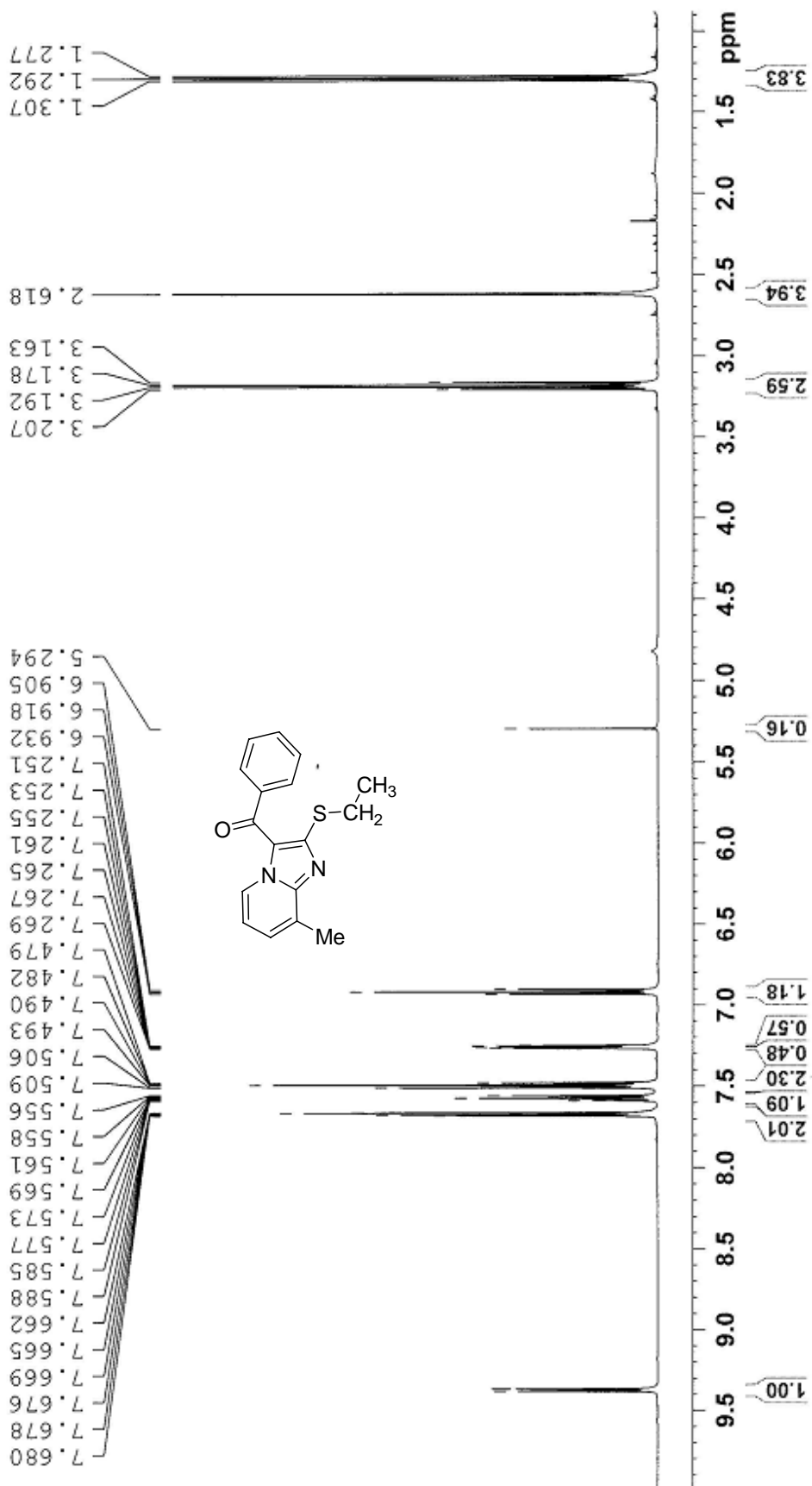
Mr Kianmehr B16

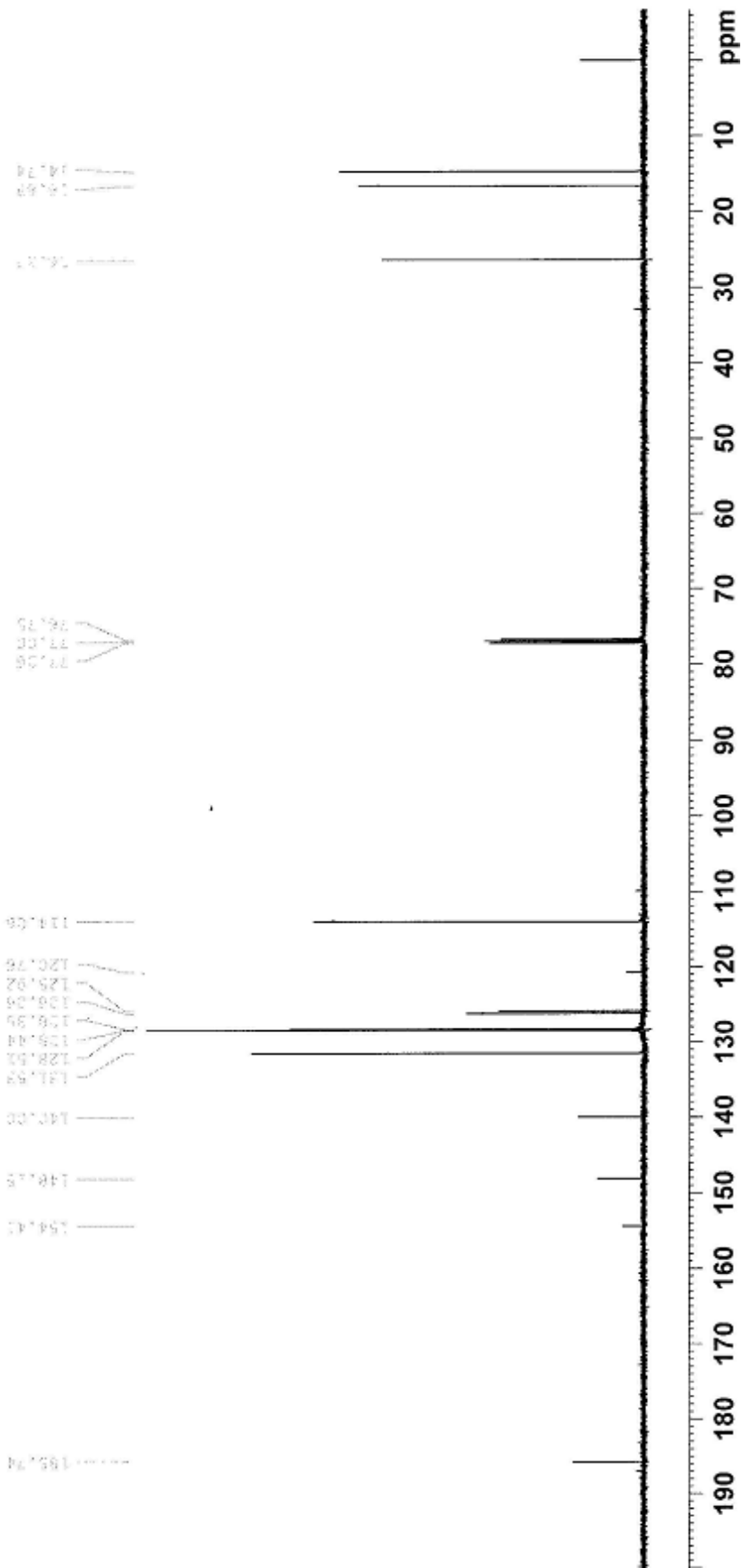
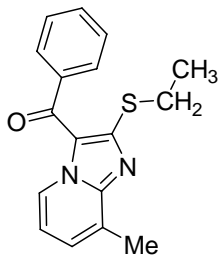






Mr Kianmehr B15





B-27 <sup>1</sup>H NMR in CDCl<sub>3</sub> at 298 K 87/9/10

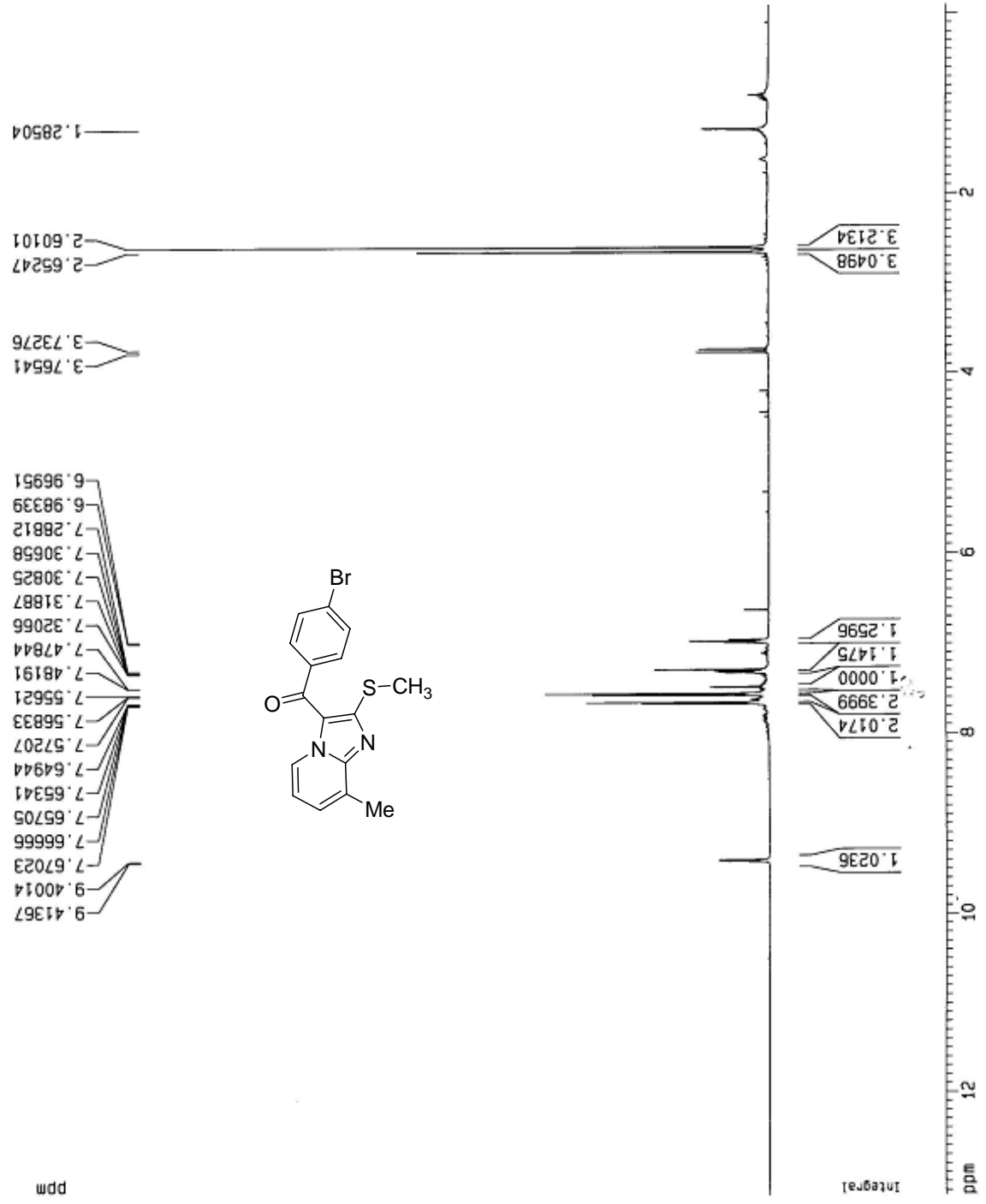
Current Data Parameters  
 NAME Nadiri  
 EXPNO 18  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20081130  
 Time 10.58  
 INSTRUM spect  
 PROBHD 5 mm QNP 1H/13  
 PULPROG zg30  
 TO 65536  
 SOLVENT MeOH  
 NS 16  
 DS 1  
 SWH 10330.578 Hz  
 FIDRES 0.157632 Hz  
 AQ 3.1720407 sec  
 RG 362  
 DM 48.400 usec  
 DE 6.50 usec  
 TE 298.2 K  
 D1 6.0000000 sec  
 MCREST 0.0000000 sec  
 NCMRK 0.01500000 sec

\*\*\*\*\* CHANNEL f1 \*\*\*\*\*  
 NUC1 1H  
 P1 10.50 usec  
 PL1 -3.00 dB  
 SFO1 500.1330885 MHz

F2 - Processing parameters  
 SI 32768  
 SF 500.1300090 MHz  
 NCM EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00

1D NMR plot parameters  
 CX 20.00 cm  
 CY 10.61 cm  
 F1P 13.156 ppm  
 F1 6579.69 Hz  
 F2P -0.094 ppm  
 F2 -46.83 Hz  
 PRNDM 0.66246 ppm/cm  
 HZCM 331.32617 Hz/cm



B-27 <sup>13</sup>CNMR in CDCl<sub>3</sub> at 298 K 87/9/10

Current Data Parameters  
 NAME: Ncd1r1  
 EXPNO: 17  
 PROCNO: 1

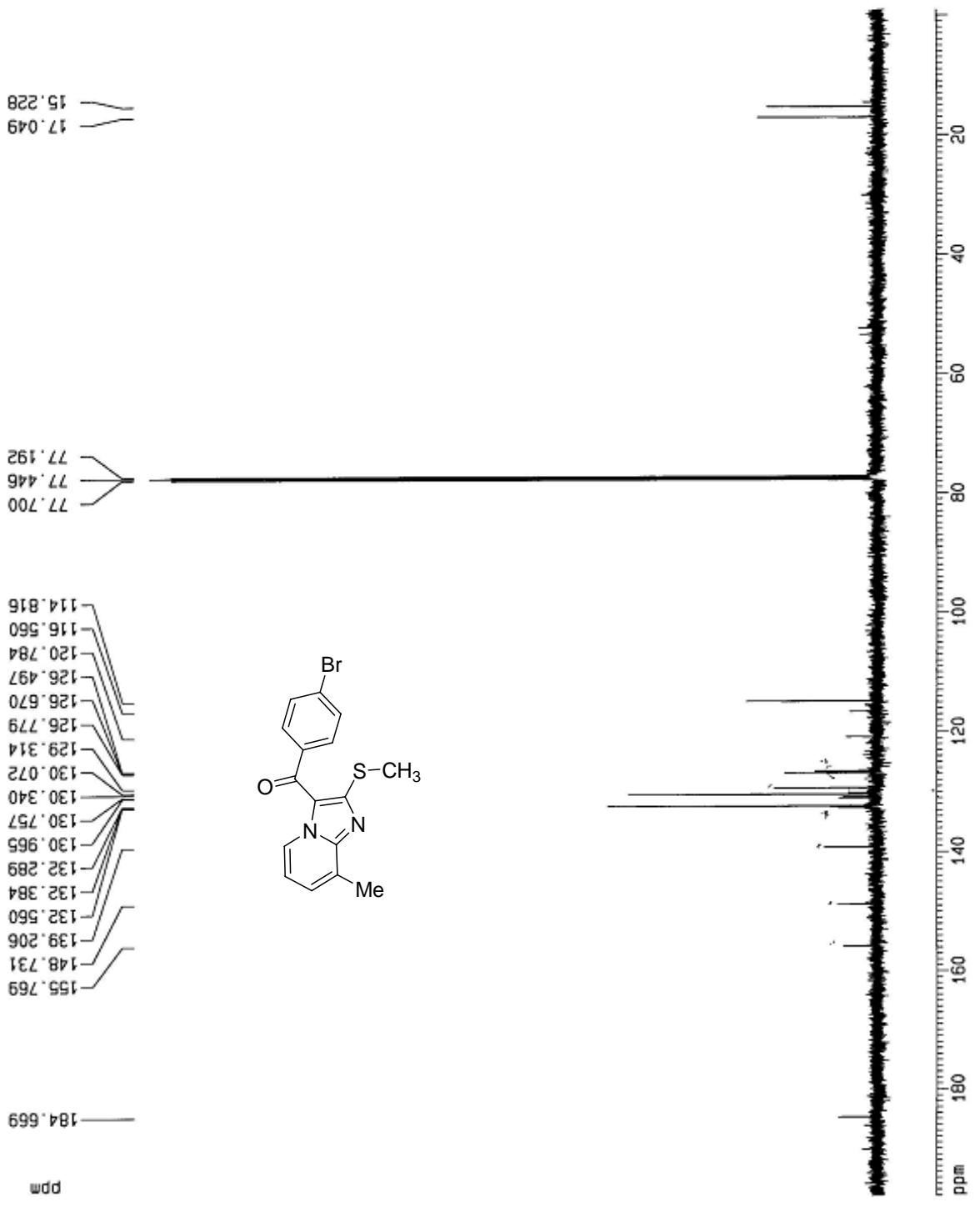
F2 - Acquisition Parameters  
 Date\_: 20081130  
 Time: 11.02  
 INSTRUM: spect  
 PROBHD: 5 mm QNP 1H/13  
 PULPROG: zgpg30  
 TO: 32768  
 SOLVENT: MeOH  
 NS: 512  
 DS: 4  
 SWH: 30030.029 Hz  
 FIDRES: 0.916444 Hz  
 AQ: 0.5456539 sec  
 RG: 5160.6  
 DE: 6.50 usec  
 TE: 299.2 K  
 D1: 2.0000000 sec  
 DELTA: 0.0300000 sec  
 ACQRES: 1.8959998 sec  
 MCREST: 0.0000000 sec  
 PCMRK: 0.0150000 sec

----- CHANNEL f1 -----  
 NUC1: <sup>13</sup>C  
 P1: 9.10 usec  
 PL1: 3.00 dB  
 SF01: 125.7703643 MHz

----- CHANNEL f2 -----  
 CPDPRG2: waltz16  
 NUC2: <sup>1</sup>H  
 PCDP2: 80.00 usec  
 PL2: 0.00 dB  
 PL12: 15.50 dB  
 PL13: 15.50 dB  
 SF02: 500.1320005 MHz

F2 - Processing parameters  
 SI: 32768  
 SF: 125.7677390 MHz  
 NDM: EN  
 SSB: 0  
 LB: 1.00 Hz  
 GB: 0  
 PC: 1.40

1D NMR plot parameters  
 CX: 20.00 cm  
 CY: 12.25 cm  
 F1P: 186.086 ppm  
 F1: 24907.32 Hz  
 F2: -117.70 Hz  
 PPMCM: 9.94970 ppm/cm  
 HZCM: 1251.25134 Hz/cm



B30 <sup>1</sup>HNMR in CDCl<sub>3</sub> at 298 K 07/8/26

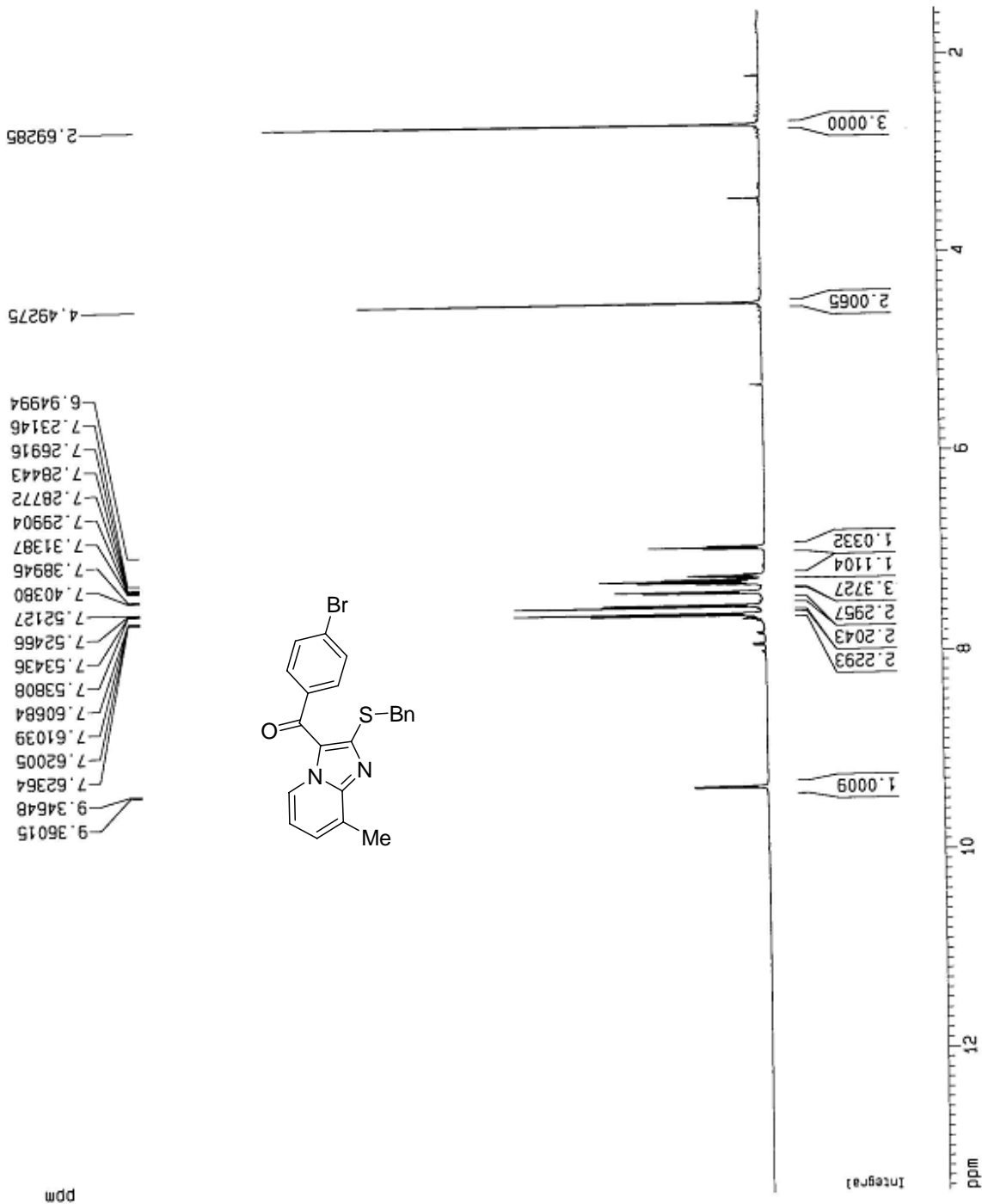
Current Data Parameters  
 NAME Nadin1  
 EXPNO 15  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20081116  
 Time 11.08  
 INSTRUM spect  
 PROBHD 5 mm QNP 1H/13  
 PULPROG zg30  
 TD 65536  
 SOLVENT CDCl<sub>3</sub>  
 NS 16  
 DS 1  
 SWH 10330.578 Hz  
 FIDRES 0.157632 Hz  
 AQ 3.1720407 sec  
 RG 128  
 DM 48.400 usec  
 DE 6.50 usec  
 TE 298.4 K  
 D1 6.00000000 sec  
 MCPRST 0.00000000 sec  
 MCPRK 0.01500000 sec

\*\*\*\*\* CHANNEL f1 \*\*\*\*\*  
 NUC1 <sup>1</sup>H  
 P1 10.50 usec  
 PL1 -3.00 dB  
 SF01 500.130885 MHz

F2 - Processing parameters  
 SI 32768  
 SF 500.130090 MHz  
 NDM EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00

10 NMR plot parameters  
 CX 20.00 cm  
 CY 8.36 cm  
 FIP 13.450 ppm  
 F1 6726.95 Hz  
 F2P 1.537 ppm  
 F2 788.74 Hz  
 PPMCN 0.59567 ppm/cm  
 HZCN 297.91034 Hz/cm



830 <sup>13</sup>CNMR in CDCl<sub>3</sub> at 298 K 8/7/8/26

```

Current Data Parameters
NAME      Nodir1
EXPNO    16
PROCNO   1

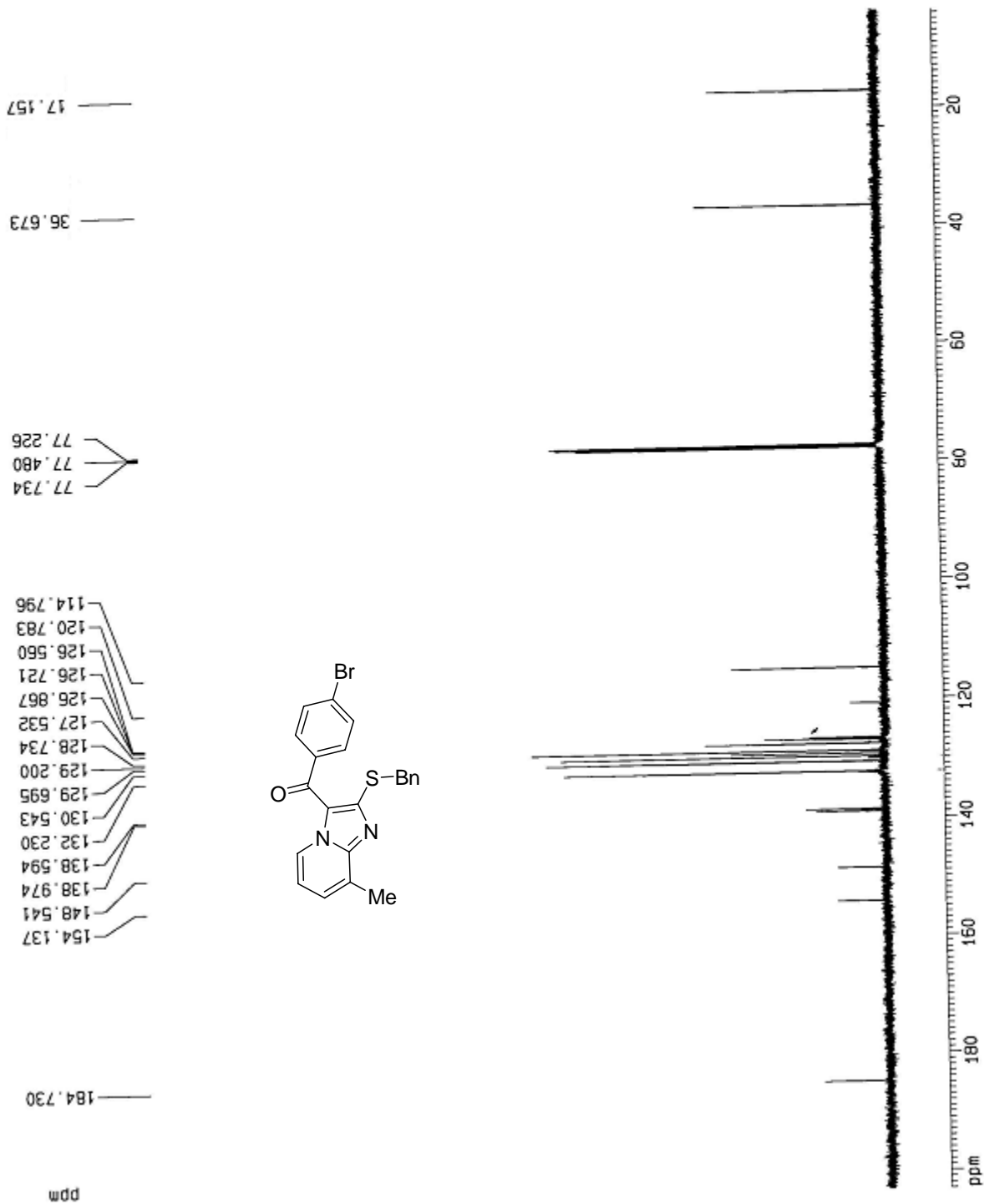
F2 - Acquisition Parameters
Date_    20081116
Time     11.13
INSTRUM spect
PROBHD   5 mm QNP 1H/13
PULPROG zgpg30
TD       32768
SOLVENT  MeOH
NS       230
DS       4
SMH      30030.029 Hz
FIDRES   0.916444 Hz
AQ        0.5456539 sec
RG        6502
DM        16.650 usec
DE        6.50 usec
TE        298.4 K
D1        2.0000000 sec
d11       0.0300000 sec
DELTA    1.8959998 sec
MCREST   0.0000000 sec
MCMARK   0.015000000 sec

***** CHANNEL f1 *****
NUC1      13C
P1        9.10 usec
PL1       3.00 dB
SFO1     125.7703643 MHz

***** CHANNEL f2 *****
CPDPRG2  waltz16
NUC2      1H
PCPD2     90.00 usec
PL2       0.00 dB
PL12      15.50 dB
PL13      15.50 dB
SF02     500.1320000 MHz

F2 - Processing parameters
SI        32768
SF        125.7577390 MHz
WDW       EM
SSB       0
LB        1.00 Hz
GB        0
PC        1.40

10 NMR plot parameters
CX        20.00 cm
CY        5.99 cm
F1P       203.033 ppm
F1        25532.95 Hz
F2P       3.515 ppm
F2        442.07 Hz
PPMCM    9.97488 ppm/cm
HZCM     1254.34407 Hz/cm
    
```





B35 <sup>1</sup>H NMR in CDCl<sub>3</sub> at 298 K 07/11/21

```

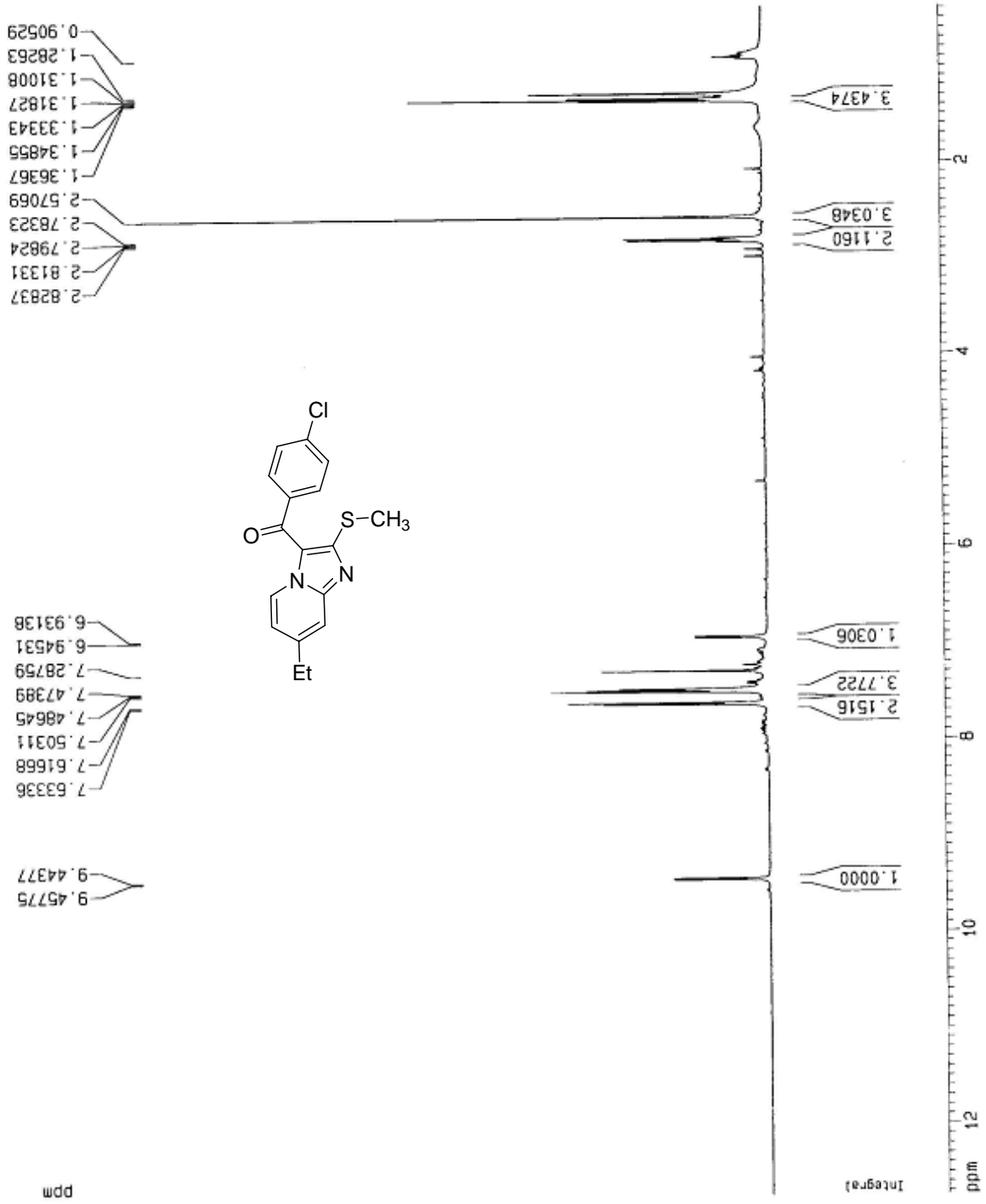
Current Data Parameters
NAME      Nadin1
EXPNO    27
PROCNO   1

F2 - Acquisition Parameters
Date_    20090209
Time     9.57
INSTRUM  spect
PROBHD   5 mm QNP 1H/13
PULPROG  zg30
TD       65536
SOLVENT  MeOH
NS       16
DS       0
SWH      10330.578 Hz
FIDRES   0.157632 Hz
AQ       3.1720407 sec
RG       912.3
DM       48.400 usec
DE       6.50 usec
TE       298.0 K
O1       5.00000000 sec
MCREST   0.00000000 sec
MCMRK    0.01500000 sec

***** CHANNEL f1 *****
NUC1     1H
P1       10.50 usec
PL1      -3.00 dB
SFO1     500.1330885 MHz

F2 - Processing parameters
SI       32768
SF       500.1300090 MHz
WDW      EM
SSB      0
LB       0.30 Hz
GB       0
PC       1.00

1D NMR plot parameters
CX       20.00 cm
CY       11.08 cm
F1P      12.738 ppm
F1       6370.69 Hz
F2P      0.377 ppm
F2       188.34 Hz
PPMCM    0.61807 ppm/cm
HZCM     309.11743 Hz/cm
  
```



835 13CNMR in CDCl3 at 298 K 87/12/14

```

Current Data Parameters
NAME      Nadiri
EXPNO    34
PROCNO   1

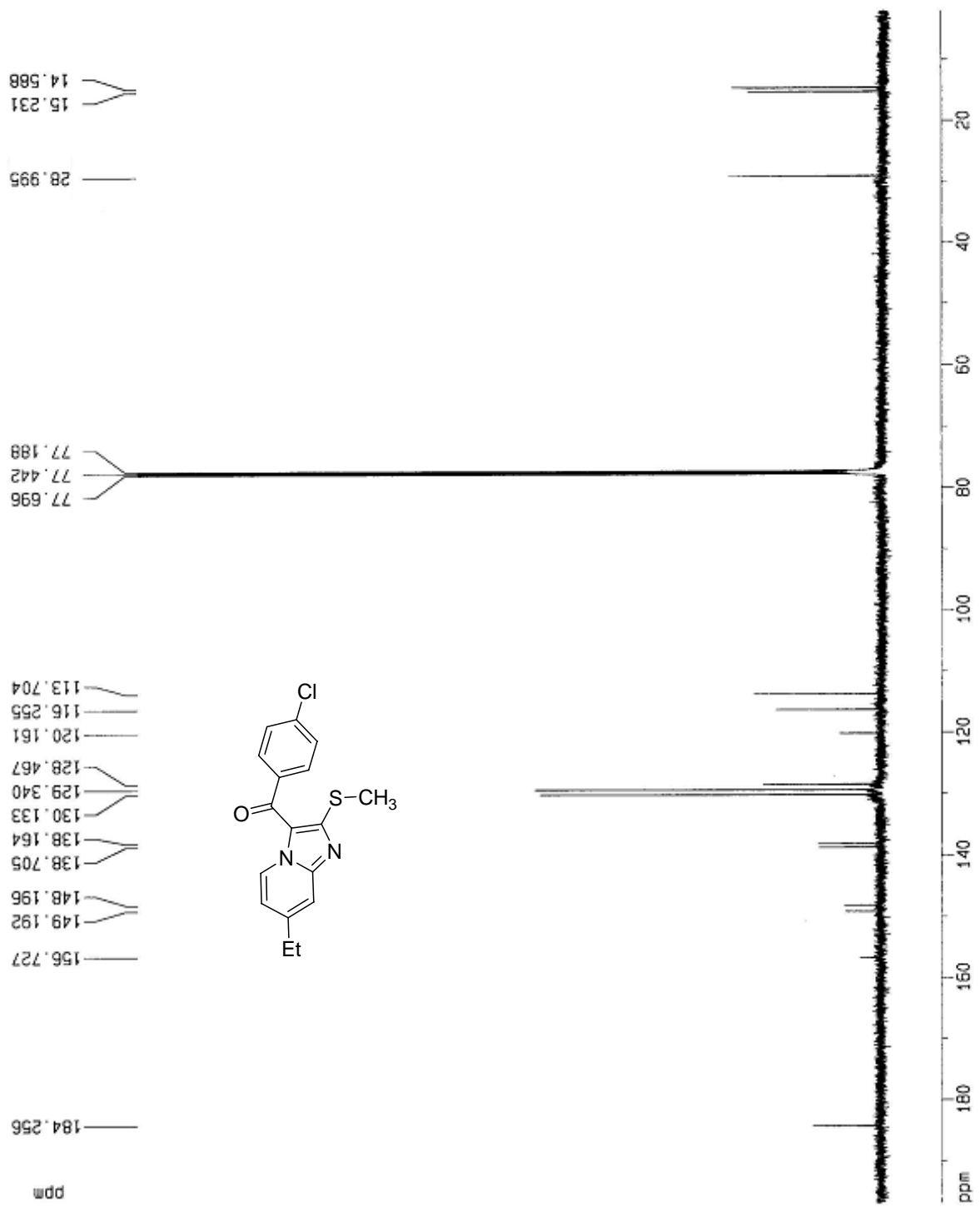
F2 - Acquisition Parameters
Date_    20090304
Time     15.59
INSTRUM  spect
PROBHD   5 mm QNP 1H/13
PULPROG  zgpg30
TO       32768
SOLVENT  CDCl3
NS       2011
DS       4
SMH      30030.029 Hz
FIDRES   0.916444 Hz
AQ        0.5456539 sec
RG        4597.6
DK        16.650 usec
DE        6.50 usec
TE        298.0 K
D1        5.00000000 sec
D11       0.03000000 sec
DELTA    4.90000010 sec
MCREST   0.00000000 sec
MCMARK   0.01500000 sec

***** CHANNEL f1 *****
NUC1      13C
P1        9.10 usec
PL1       3.00 dB
SFO1     125.7703643 MHz

***** CHANNEL f2 *****
CPDPRG2  waltz16
NUC2      1H
PCPD2    60.00 usec
PL2      0.00 dB
PL12     15.50 dB
PL13     15.50 dB
SFO2     500.1320005 MHz

F2 - Processing parameters
SI        32768
SF        125.7577390 MHz
RG        655
WDW       EM
SSB       0
LB        1.00 Hz
GB        0
PC        1.40

ID NMR plot parameters
CX        20.00 cm
CY        44.01 cm
FJP       196.870 din
F1        24757.97 Hz
F2        2.052 ppm
F2        258.02 Hz
PRNCM     9.74033 ppm/cm
HZCM      1224.99744 Hz/cm
    
```



B37 <sup>1</sup>HMR in CDCl<sub>3</sub> at 298 K 87/11/21

```

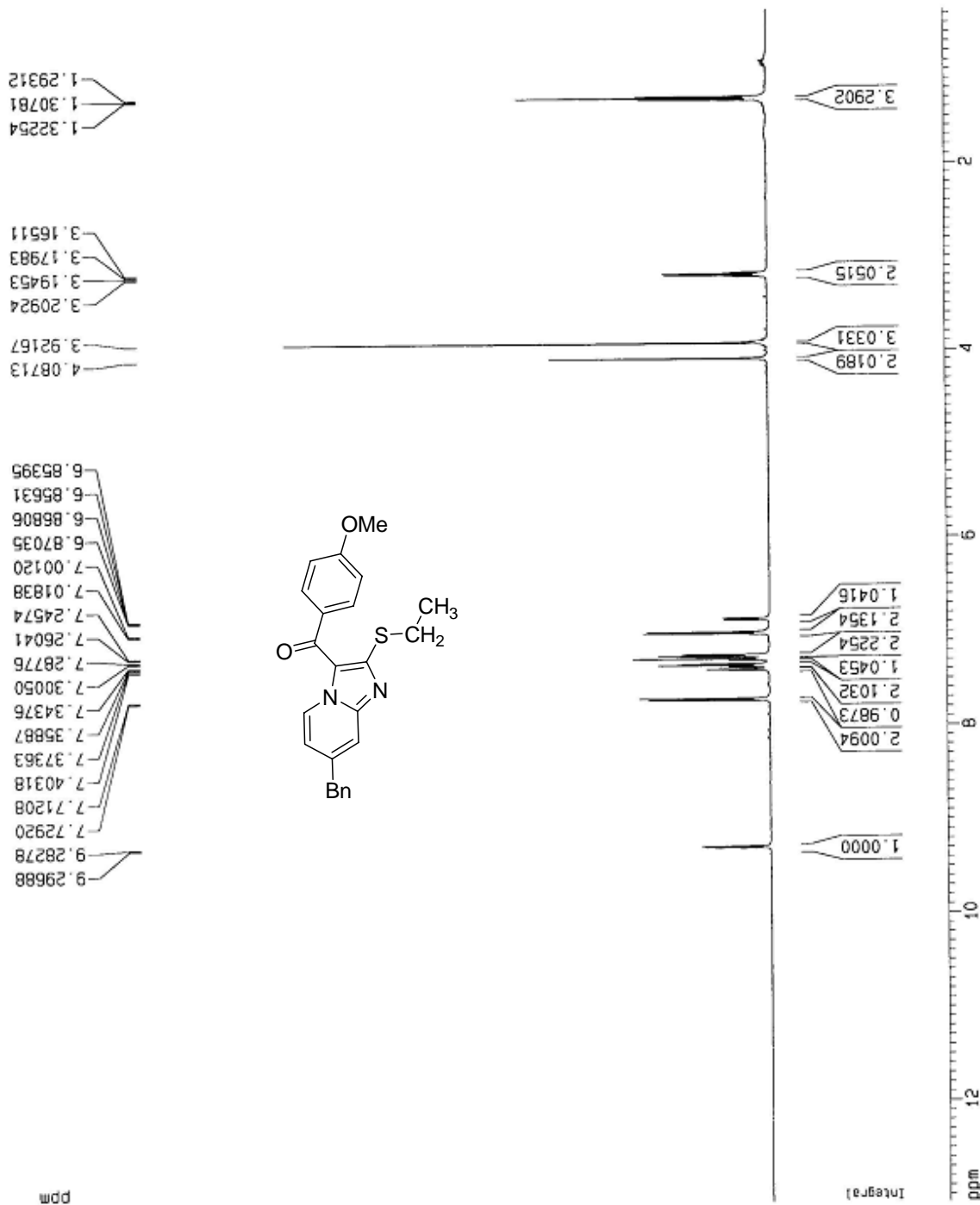
Current Data Parameters
NAME      Nedr1
EXPNO    30
PROCNO   1

F2 - Acquisition Parameters
Date_    20090209
Time     10.19
INSTRUM  spect
PROBHD   5 mm QNP 1H/13
PULPROG  zg30
TD        65536
SOLVENT  MeOH
NS        16
DS        0
SWH       10330.578 Hz
FIDRES    0.157632 Hz
AQ        3.1720407 sec
RG         812.7
DM        48.400 usec
DE         6.50 usec
TE        298.0 K
D1        5.00000000 sec
MCREST    0.00000000 sec
MCWRK     0.01500000 sec

***** CHANNEL f1 *****
NUC1      1H
P1        10.50 usec
PL1       -3.00 dB
SFO1      500.1330885 MHz

F2 - Processing parameters
SI        32768
SF        500.1300090 MHz
WDW       EM
SSB       0
LB        0.30 Hz
GB        0
PC        1.00

1D NMR plot parameters
CX        20.00 cm
CY        8.09 cm
FIP       13.081 ppm
F1        6542.10 Hz
F2P       0.354 ppm
F2        176.91 Hz
PPMCH     0.63635 ppm/cm
HZCN      318.25952 Hz/cm
    
```



B-37 <sup>13</sup>CNMR in CDCl<sub>3</sub> at 298 K 87/11/21

```

Current Data Parameters
NAME      Nadir1
EXPNO    29
PROCNO   1

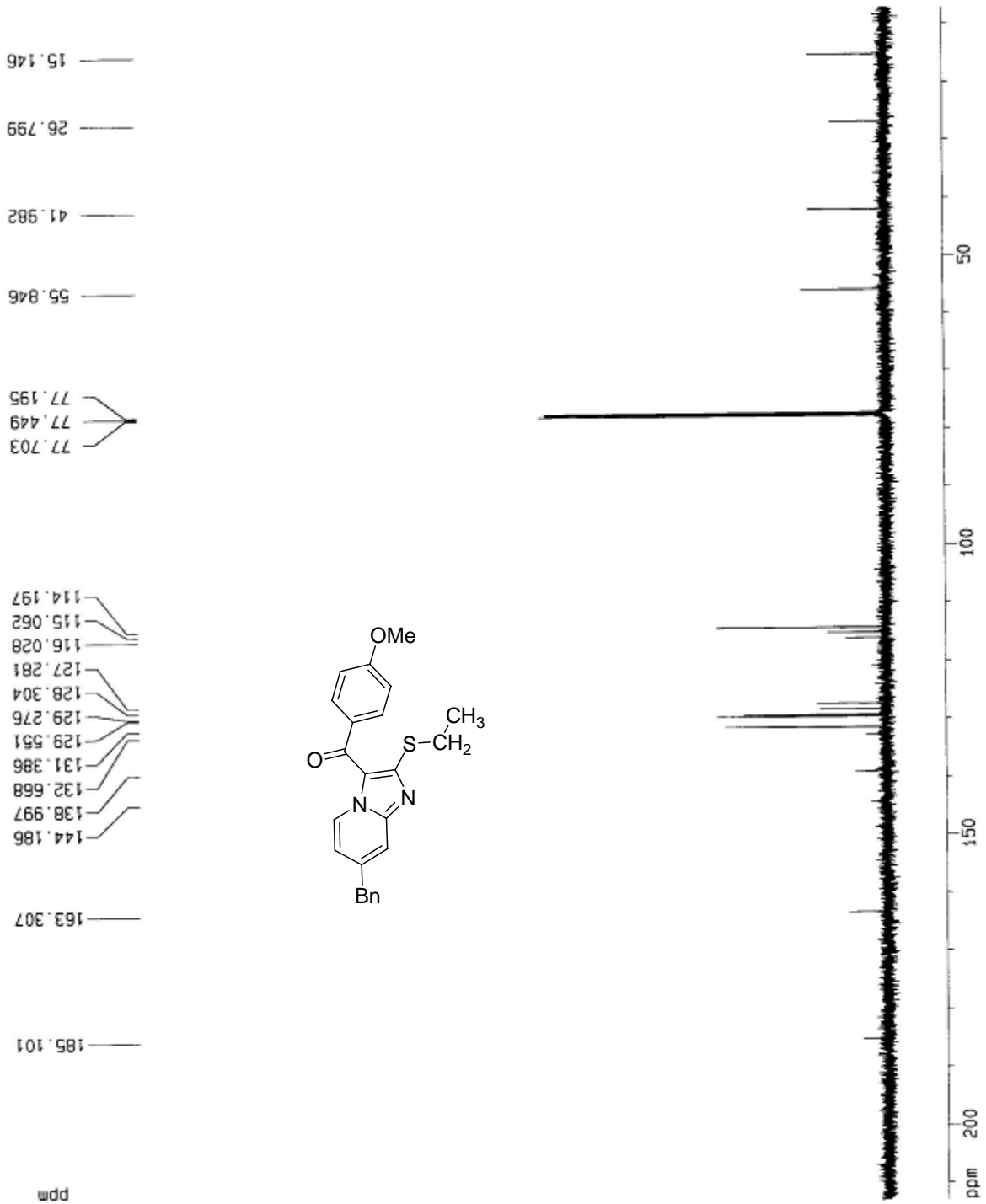
F2 - Acquisition Parameters
Date_    20090209
Time     10.23
INSTRUM spect
PROBHD   5 mm QNP 1H/13
PULPROG zgpg30
TD       32768
SOLVENT  CDCl3
NS       255
DS       4
SMH      30030.079 Hz
FIDRES   0.916444 Hz
AQ       0.9406539 sec
RG       2560.3
DM       16.650 usec
DE       6.50 usec
TE       298.1 K
D1       1.0000000 sec
d11      0.0300000 sec
DELTA    0.6999999 sec
INCREST  0.0000000 sec
MCWRRK   0.0150000 sec

***** CHANNEL f1 *****
NUC1     13C
P1       9.10 usec
PL1      3.00 dB
SFO1    125.7703643 MHz

***** CHANNEL f2 *****
CPDPRG2 waltz16
NUC2     1H
PCPD2    80.00 usec
PL2      0.00 dB
PL12     15.50 dB
PL13     15.50 dB
SFO2    500.1320005 MHz

F2 - Processing parameters
SI       32768
SF       125.7577390 MHz
RG       0
WDW      EM
SSB      0
LB       1.00 Hz
GB       0
PC       1.40

1D NMR plot parameters
CX       20.00 cm
CY       5.94 cm
FJP      212.922 ppm
F1       26776.62 Hz
F2       7.148 ppm
PQMW     10.28869 ppm/cm
HZCM     1293.88232 Hz/cm
    
```



836 <sup>1</sup>H NMR in CDCl<sub>3</sub> at 298 K 87/12/12

```

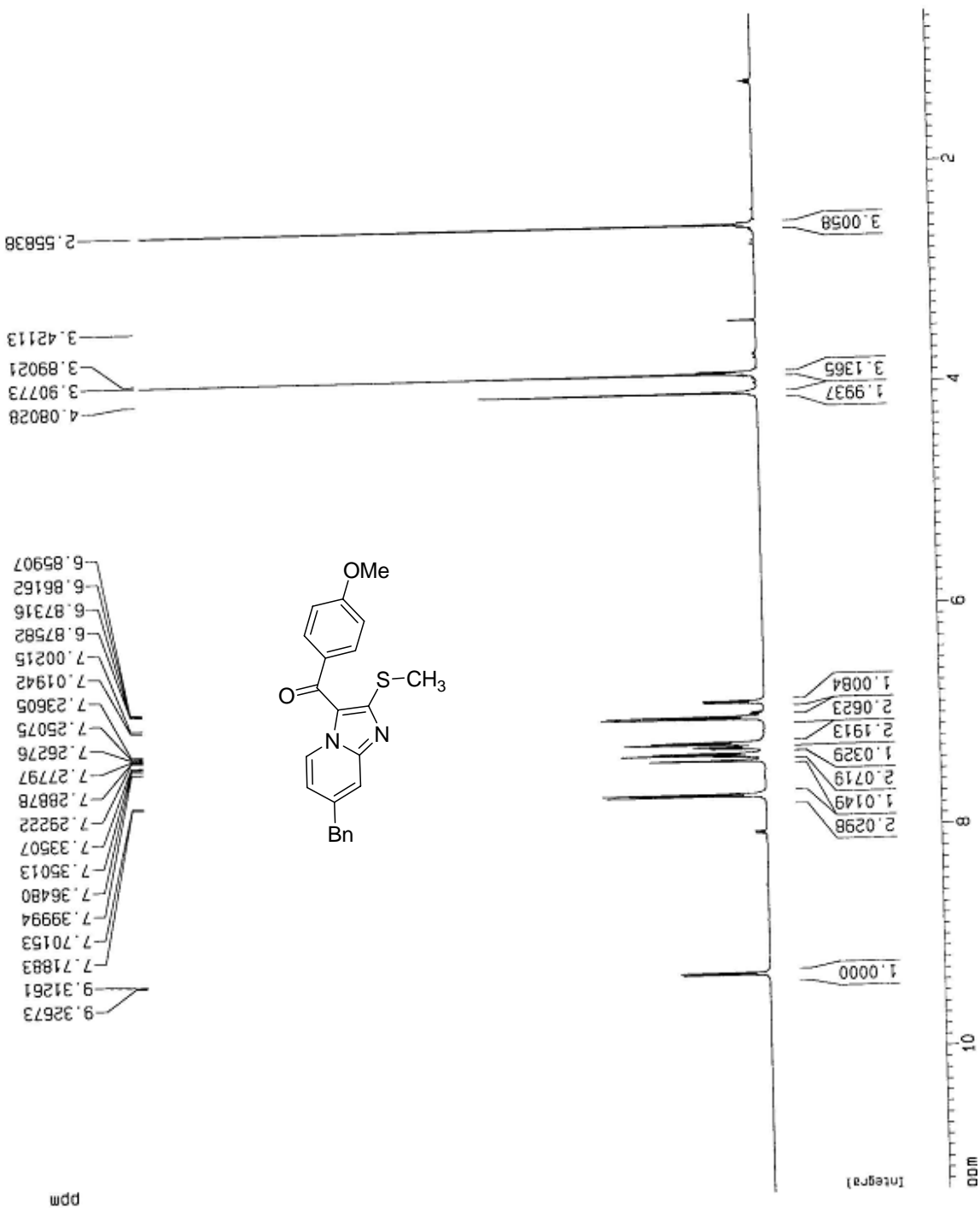
Current Data Parameters
NAME      Nadi11
EXPNO    32
PROCNO   1

F2 - Acquisition Parameters
Date_    20090302
Time     13.16
INSTRUM spect
PROBHD   5 mm QNP 1H/13
PULPROG zg30
TD       65536
SOLVENT  MeOH
NS       8
DS       0
SWH      10330.575 Hz
FIDRES   0.157632 Hz
AQ       3.1720407 sec
RG       322.5
DM       48.400 usec
DE       6.50 usec
TE       298.4 K
D1       5.00000000 sec
MCREST   0.00000000 sec
MCWRRK   0.01500000 sec

***** CHANNEL f1 *****
NUC1     1H
P1       10.50 usec
PL1      -3.00 dB
SFO1     500.1330685 MHz

F2 - Processing parameters
SI       32768
SF       500.1300090 MHz
WDW      EM
SSB      0
LB       0.30 Hz
GB       0
PC       1.00

1D NMR plot parameters
CX       20.00 cm
CY       10.63 cm
F1P      11.298 ppm
F1       5650.54 Hz
F2P      0.645 ppm
F2       322.36 Hz
PPMCKM   0.53268 ppm/cm
HZCM     266.40793 Hz/cm
  
```



B-38 <sup>13</sup>CNMR in CDCl<sub>3</sub> at 298 K 87/12/12

```

Current Data Parameters
NAME      Nadr1
EXPNO    33
PROCNO   1

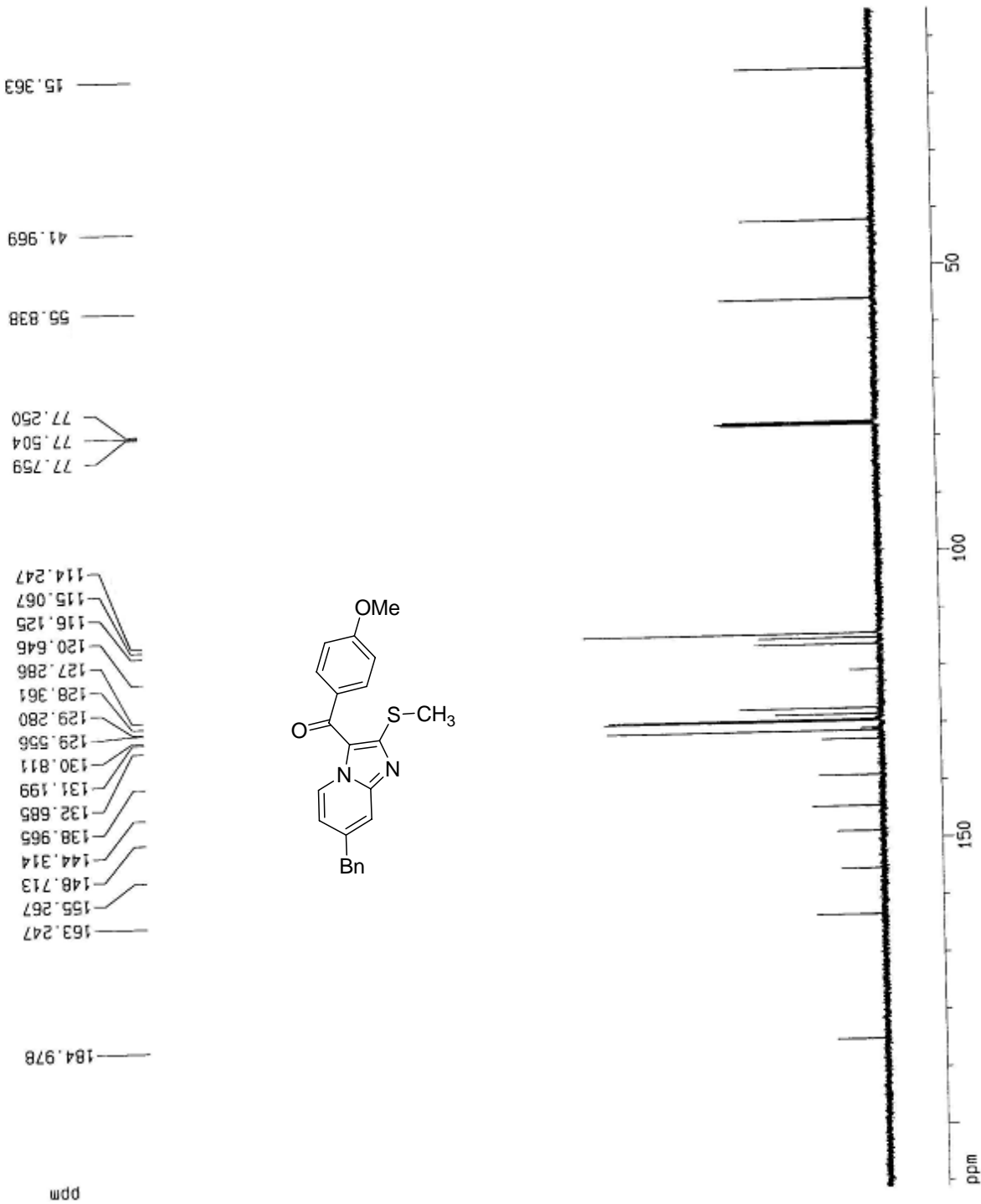
F2 - Acquisition Parameters
Date_    20080302
Time     13.21
INSTRUM  spect
PROBHD   5 mm QNP 1H/13
PULPROG  zgpg30
TD       32768
SOLVENT  CDCl3
NS       201
DS       4
SM1      30030.029 Hz
FIDRES   0.916444 Hz
AQ        0.5456319 sec
RG        2560.3
DM        16.650 usec
DE        6.50 usec
TE        298.3 K
O1        1.0000000 sec
d11       0.0300000 sec
DELTA    0.6999999 sec
INVEST   0.0000000 sec
NCMRK    0.0150000 sec

***** CHANNEL f1 *****
NUC1      13C
P1        9.10 usec
PL1       3.00 dB
SFO1      125.7703643 MHz

***** CHANNEL f2 *****
CPROG2    waltz16
NUC2      1H
PCPD2     80.00 usec
PL2       0.00 dB
PL12     15.50 dB
PL13     15.50 dB
SFO2      500.1320005 MHz

F2 - Processing parameters
SI        32768
SF        125.757590 MHz
WDW       EM
SSB       0
LB        1.00 Hz
GB        0
PC        1.40

ID NMR plot parameters
CX        20.00 cm
CY        5.07 cm
F1P       210.916 ppm
F1        26524.34 Hz
F2P       4.933 ppm
F2        620.06 Hz
PPMCH     10.25928 ppm/cm
HZCM      1295.21411 Hz/cm
    
```



850 1H NMR in CDCl3 at 298 K 88/6/1

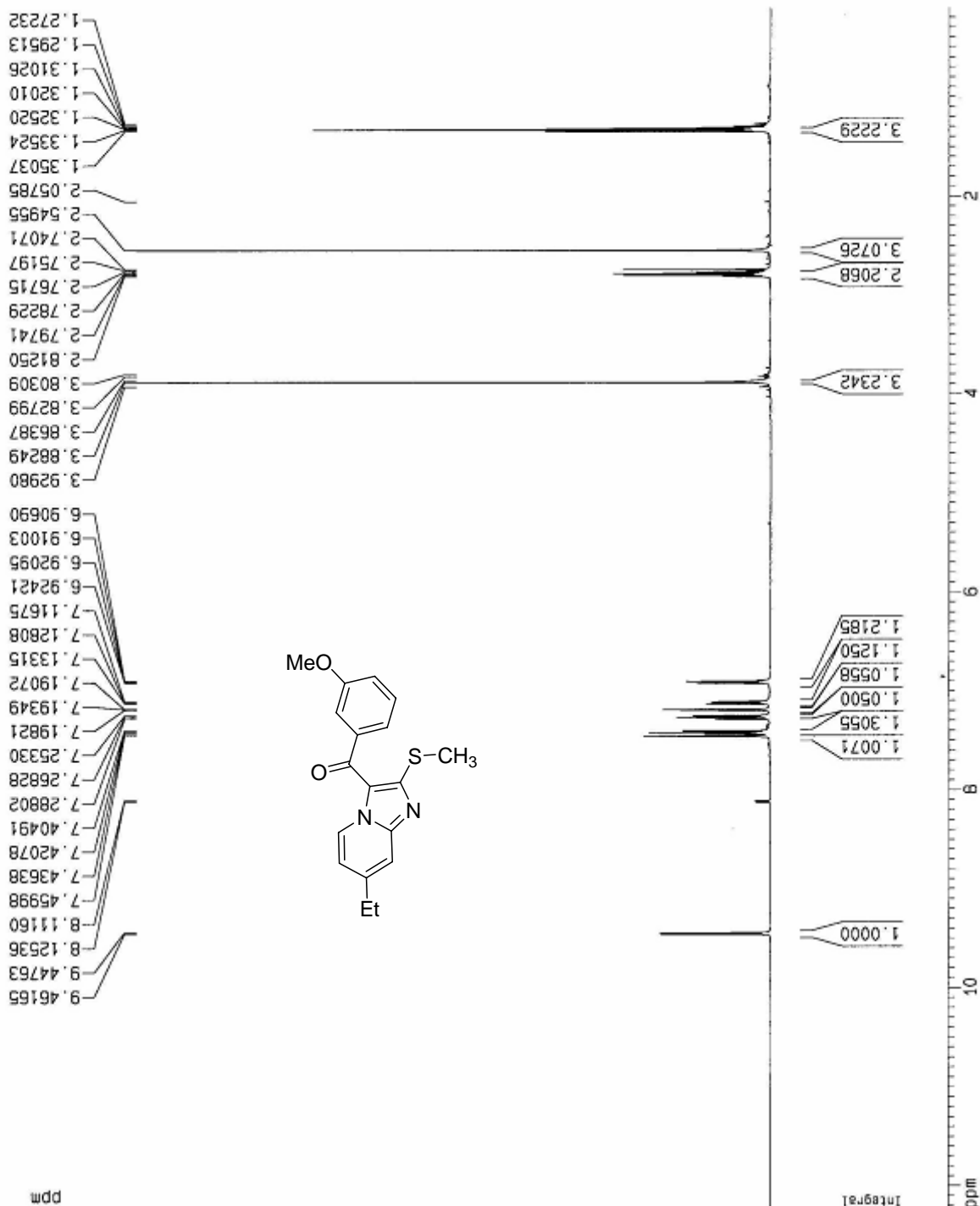
Current Data Parameters  
 NAME NMR01  
 EXPNO 46  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20090823  
 Time 8.27  
 INSTRUM spect  
 PROBHD 5 mm GNP 1H/13  
 PULPROG zg30  
 TD 65536  
 SOLVENT MeOH  
 NS 16  
 DS 0  
 SMH 10330.578 Hz  
 FIDRES 0.157632 Hz  
 AQ 3.1720407 sec  
 RG 143.7  
 DM 48.400 usec  
 DE 6.50 usec  
 TE 298.0 K  
 D1 5.0000000 sec  
 MCREST 0.0000000 sec  
 MCWRR 0.0150000 sec

----- CHANNEL f1 -----  
 NUC1 1H  
 P1 10.50 usec  
 PL1 -3.00 dB  
 SF01 500.1330885 MHz

F2 - Processing parameters  
 SI 32768  
 SF 500.1300090 MHz  
 MDM EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00

10 NMR plot parameters  
 CX 20.00 cm  
 CY 15.08 cm  
 FIP 12.235 ppm  
 F1 6119.28 Hz  
 F2P 0.102 ppm  
 F2 51.21 Hz  
 PPMCM 0.60665 ppm/cm  
 HZCM 303.40359 Hz/cm



B50 13CNMR in CDC13 at 298 K 88/6/1

```

Current Data Parameters
NAME      Nadin1
EXPNO    47
PROCNO   1

F2 - Acquisition Parameters
Date_    20090823
Time     8.32
INSTRUM spect
PROBHD   5 mm DNP 1H/13
PULPROG zgpg30
TO       32768
SOLVENT CDC13
NS       200
DS       4
SWH      30030.029 Hz
FIDRES   0.916444 Hz
AQ       0.5450539 sec
RG       6502
DM       16.650 usec
DE       6.50 usec
TE       298.0 K
d1       1.0000000 sec
d11      0.0300000 sec
DELTA    0.8999998 sec
ACREST   0.0000000 sec
MCWRK    0.01500000 sec

===== CHANNEL f1 =====
NUC1     13C
P1       9.10 usec
PL1      3.00 dB
SFO1     125.7703643 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2     1H
PCPD2    80.00 usec
PL2      0.00 dB
PL12     15.50 dB
PL13     15.50 dB
SFO2     500.1320005 MHz

F2 - Processing parameters
SI       32768
SF       125.7577390 MHz
WDW      EM
SSB      0
LB       1.00 Hz
GB       0
BB       0
PC       1.40

10 NMR plot parameters
CX       20.00 cm
CY       4.45 cm
F1P     215.300 ppm
F1       27075.59 Hz
F2P     4.771 ppm
F2       600.00 Hz
PPMCM   10.52643 ppm/cm
HZCM    1323.77954 Hz/cm
    
```





B52 1HNMR in CDCl3 at 298 K 88/6/2

```

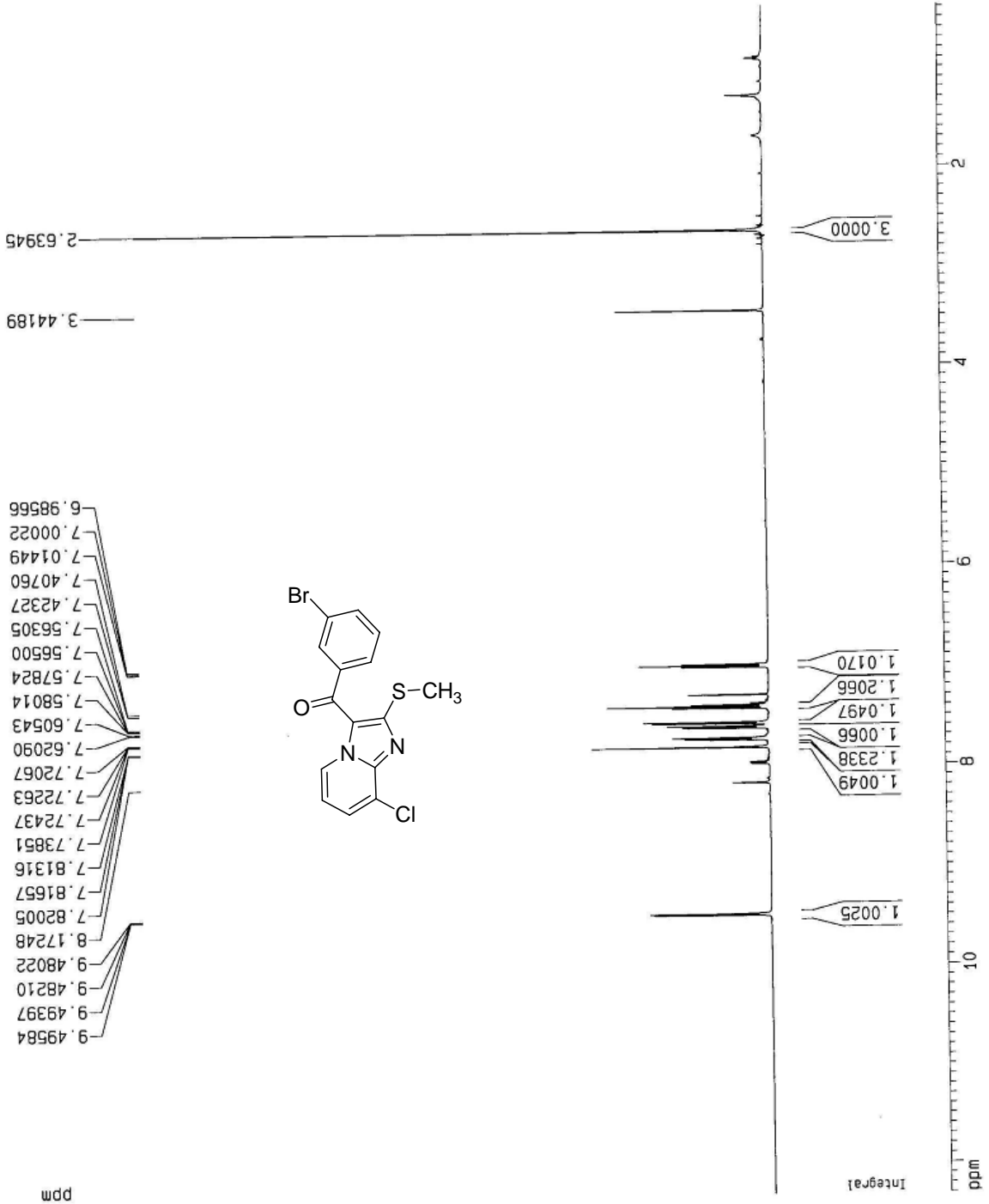
Current Data Parameters
NAME      Nadr1
EXPNO    54
PROCNO   1

F2 - Acquisition Parameters
Date_    20090824
Time     8.39
INSTRUM  spect
PROBHD   5 mm QNP 1H/13
PULPROG  zg30
TD        65536
SOLVENT  MeOH
NS        8
DS        0
SWH       10330.578 Hz
FIDRES    0.157632 Hz
AQ        3.1720407 sec
RG         256
DM         48.400 usec
DE         6.50 usec
TE         298.0 K
D1         5.00000000 sec
MCREST    0.00000000 sec
MCMARK    0.01500000 sec

===== CHANNEL f1 =====
NUC1      1H
P1         10.50 usec
PL1        -3.00 dB
SFO1       500.1330885 MHz

F2 - Processing parameters
SI         32768
SF         500.1300090 MHz
WDW         EM
SSB         0
LB         0.30 Hz
GB         0
PC         1.00

1D NMR plot parameters
CX         20.00 cm
CY         19.63 cm
F1P        12.304 ppm
F1         6153.56 Hz
F2P        0.377 ppm
F2         188.34 Hz
PPMCM      0.59637 ppm/cm
HZCM       298.26117 Hz/cm
    
```



852 13CNMR in CDC13 at 298 K 88/6/2

```

Current Data Parameters
NAME      Nadr1r
EXPNO    95
PROCNO   1

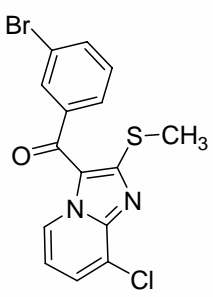
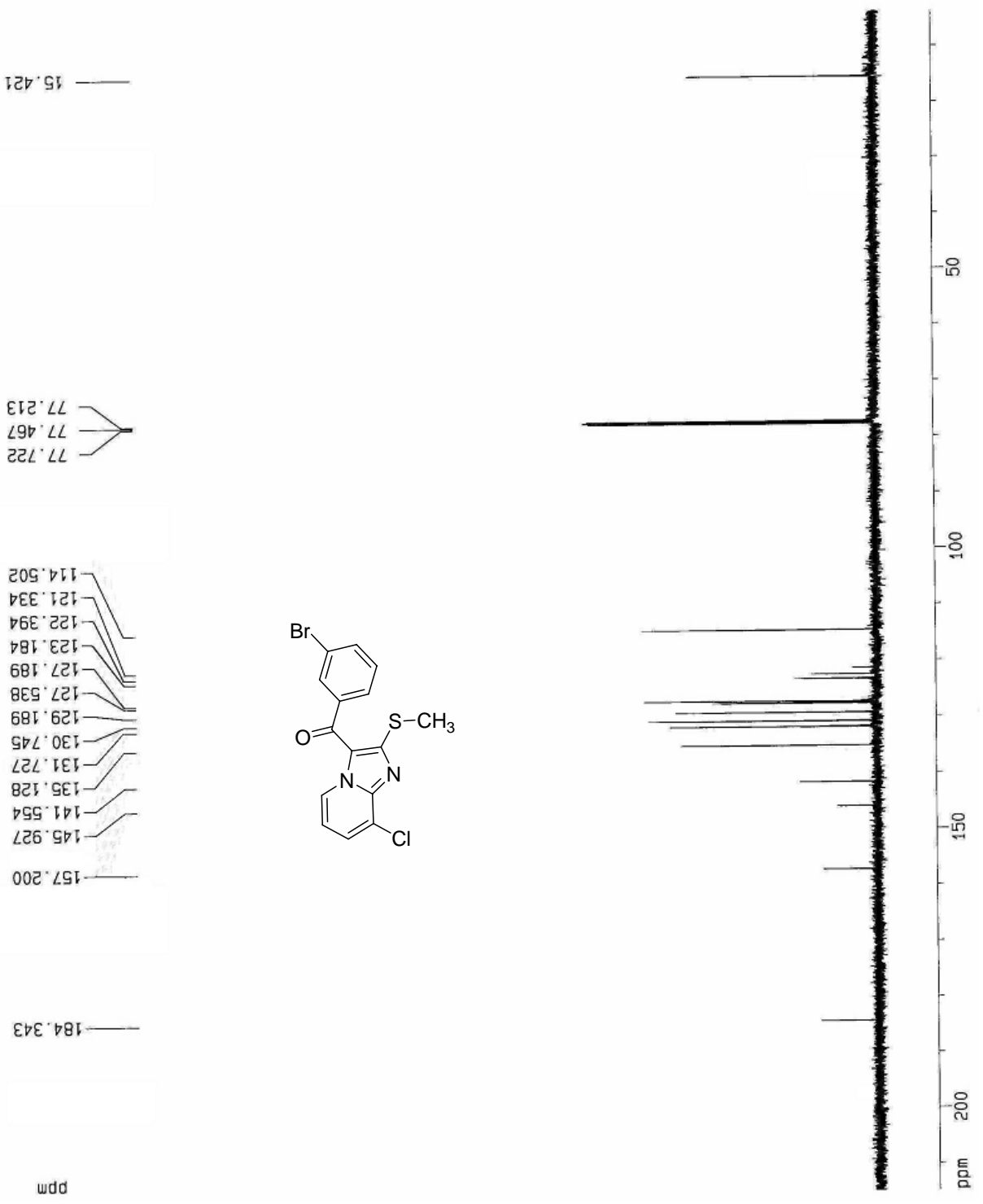
F2 - Acquisition Parameters
Date_    20090824
Time     8.47
INSTRUM spect
PROBHD   5 mm GNP 1H/13
PULPROG zgpg30
TO       32768
SOLVENT  CDC13
NS       283
DS       4
SWH      30030.029 Hz
FIDRES   0.916444 Hz
AQ       0.5456539 sec
RG       6502
DM       16.650 usec
DE       6.50 usec
TE       298.1 K
D1       1.0000000 sec
d11      0.0300000 sec
DELTA    0.88999998 sec
MCHREST  0.0000000 sec
MCHRK    0.0150000 sec

===== CHANNEL f1 =====
NUC1     13C
P1       9.10 usec
PL1      3.00 dB
SF01     125.7703643 MHz

===== CHANNEL f2 =====
CPOPRG2  waltz16
NUC2     1H
PCPD2    80.00 usec
PL2      0.00 dB
PL12     15.50 dB
PL13     15.50 dB
SF02     500.1320005 MHz

F2 - Processing parameters
SI       32768
SF       125.7577390 MHz
WDW      EM
SSB      0
LB       1.00 Hz
GB       0
PC       1.40

1D NMR plot parameters
CX       20.00 cm
CY       4.95 cm
F1P      214.771 ppm
F1       27009.16 Hz
F2P      3.715 ppm
F2       467.13 Hz
PPMCM    10.55284 ppm/cm
HZCM     1327.10144 Hz/cm
    
```



B53 <sup>1</sup>HNMR in CDCl<sub>3</sub> at 298 K 08/6/2

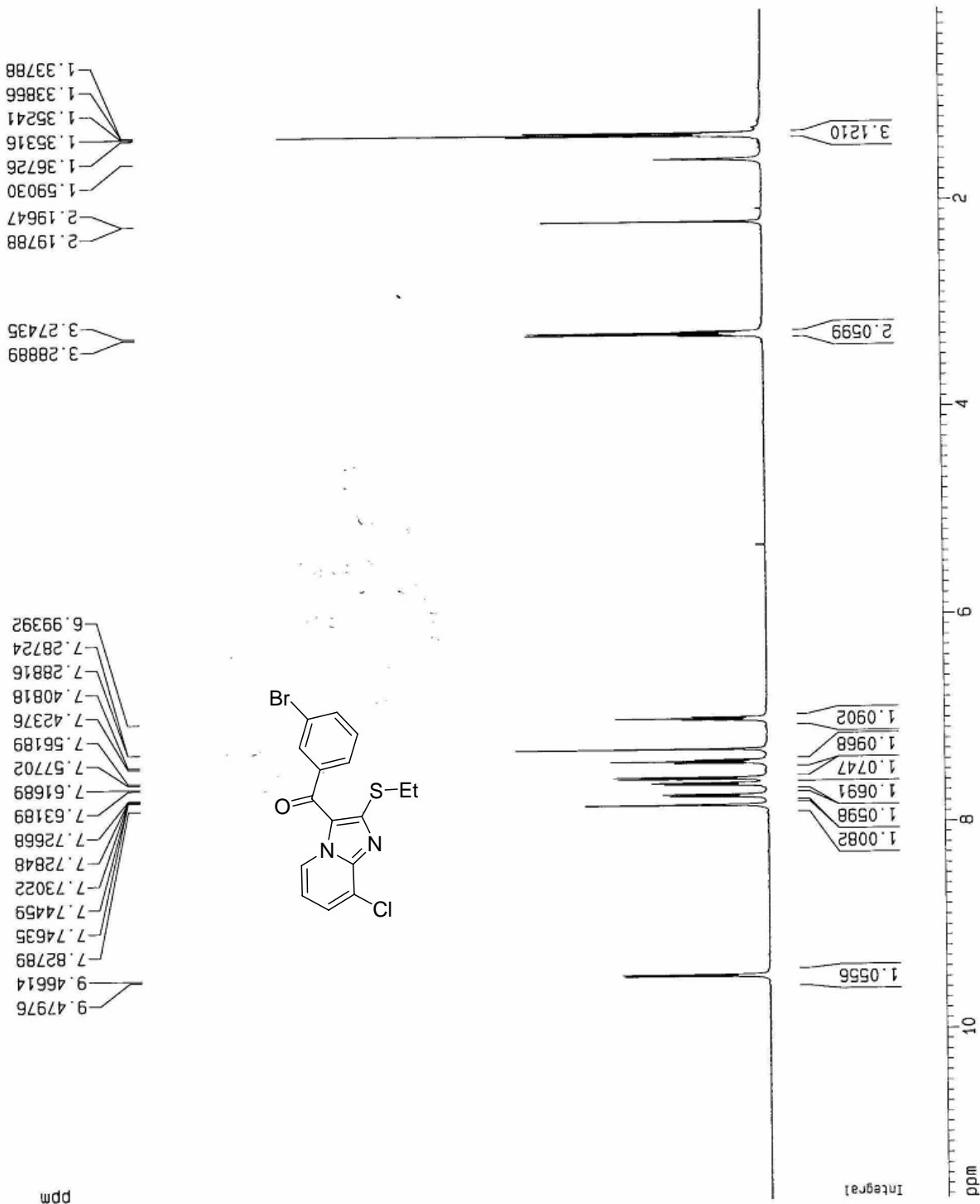
Current Data Parameters  
 NAME Nad1r1  
 EXPNO 53  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20090824  
 Time\_ 8.35  
 INSTRUM spect  
 PROBHD 5 mm GNP 1H/13  
 PULPROG zg30  
 TO 65536  
 SOLVENT MeOH  
 NS 16  
 DS 0  
 SWH 10330.578 Hz  
 FIDRES 0.157632 Hz  
 AQ 3.1720407 sec  
 RG 812.7  
 DM 48.400 usec  
 DE 6.50 usec  
 TE 298.0 K  
 D1 5.0000000 sec  
 MCREST 0.0000000 sec  
 MCPRK 0.01500000 sec

===== CHANNEL f1 =====  
 NUC1 1H  
 P1 10.50 usec  
 PL1 -3.00 dB  
 SF01 500.1330885 MHz

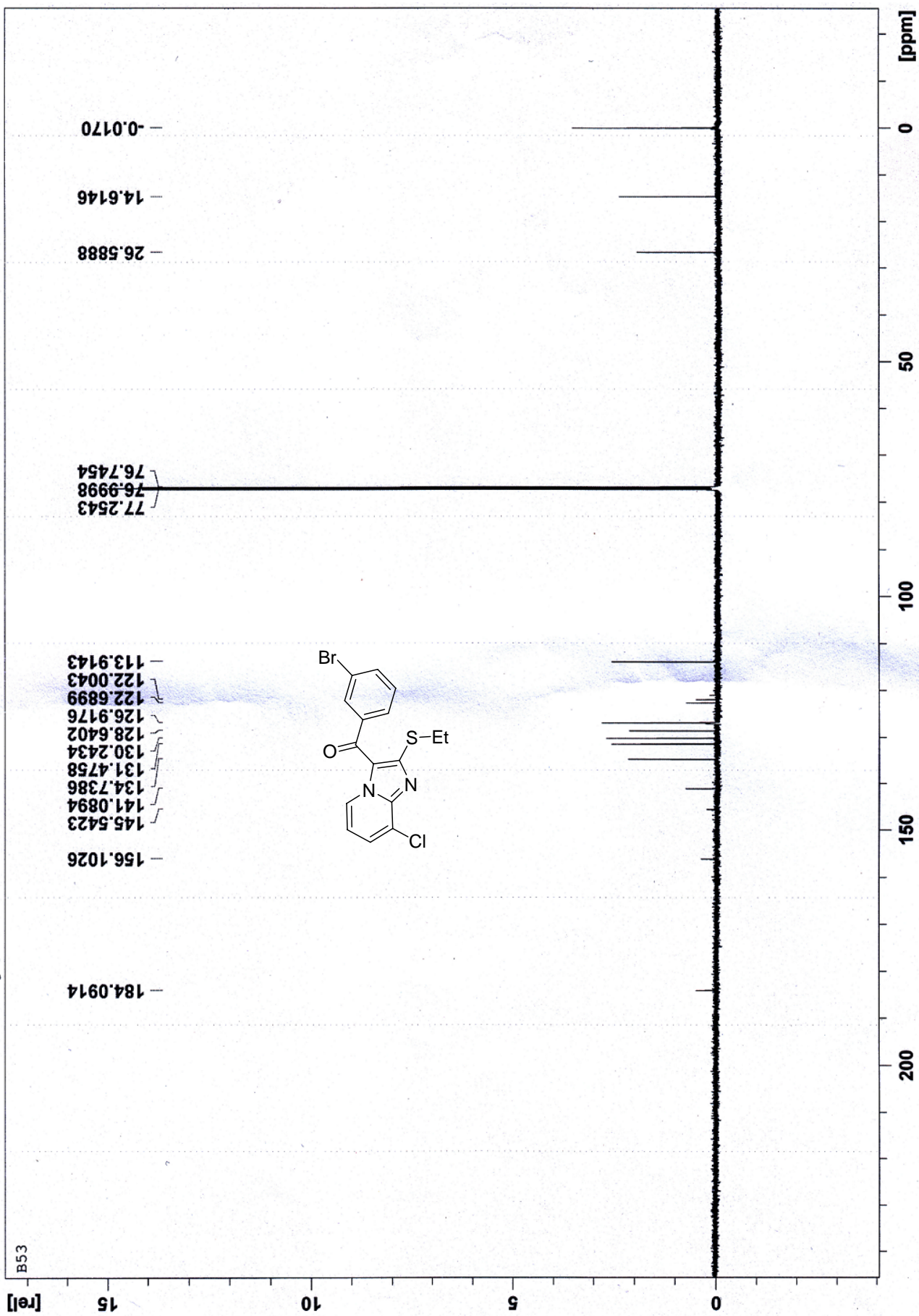
F2 - Processing parameters  
 SI 32768  
 SF 500.1300090 MHz  
 MDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00

1D NMR plot parameters  
 CX 20.00 cm  
 CY 8.21 cm  
 F1P 11.641 ppm  
 F1 5822.16 Hz  
 F2P 0.148 ppm  
 F2 74.06 Hz  
 PPMCM 0.57466 ppm/cm  
 HZCM 287.40494 Hz/cm



J4 21 1 C:\Bruker\TOPSPIN guest

B53



B36 1HMR in CDCl3 at 298 K 87/10/30

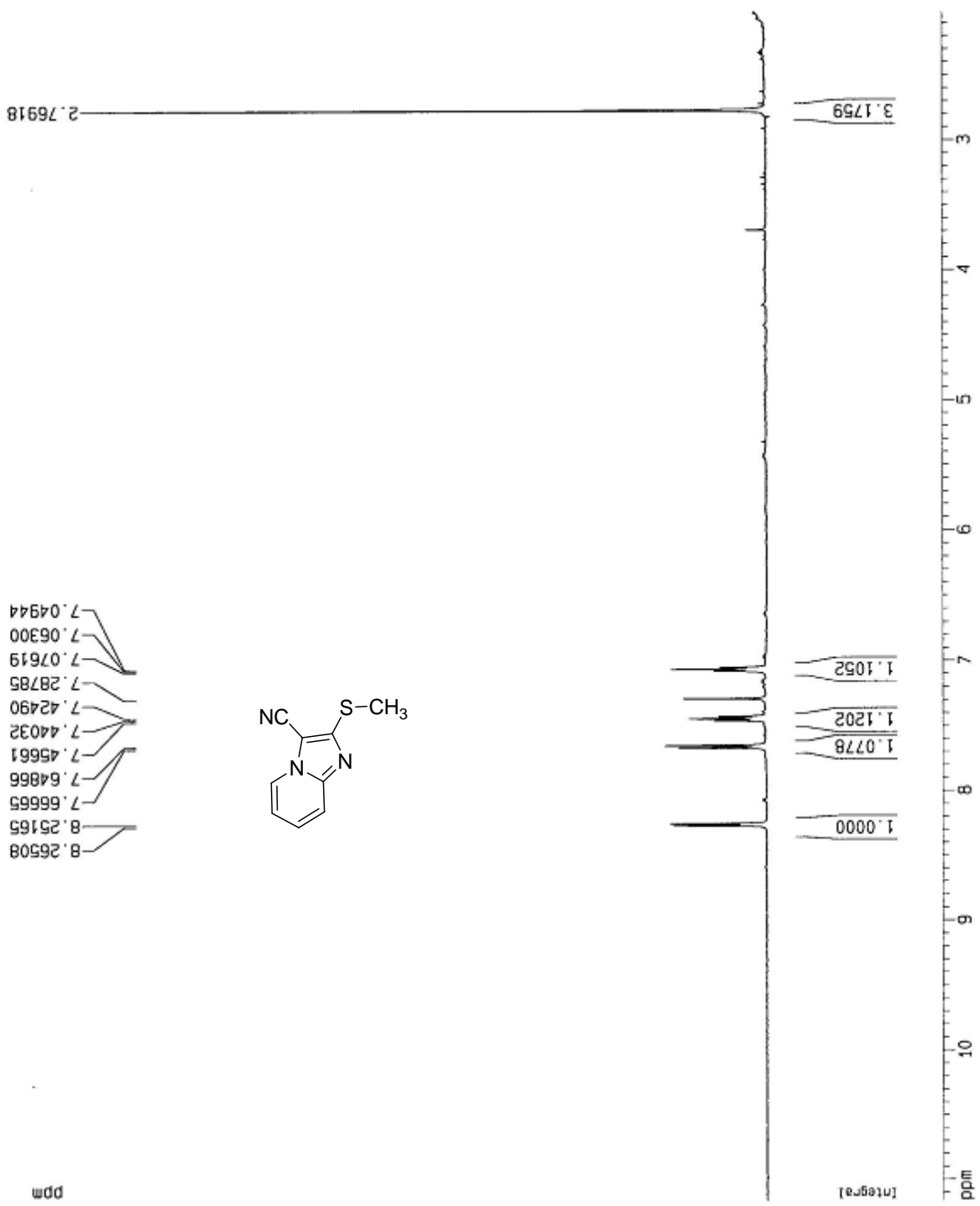
Current Date Parameters  
 NAME Nadjic  
 EXPNO 26  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20090119  
 Time 10.17  
 INSTRUM spect  
 PROBHD 5 mm DNP 1H/13  
 PULPROG zg30  
 TO 65536  
 SOLVENT MeOH  
 NS 16  
 DS 1  
 SNH 10330.578 Hz  
 FIDRES 0.157632 Hz  
 AQ 3.1720407 sec  
 RG 32  
 DM 48.400 usec  
 DE 6.50 usec  
 TE 298.3 K  
 D1 6.00000000 sec  
 MCREST 0.00000000 sec  
 MCMRK 0.01500000 sec

\*\*\*\*\* CHANNEL f1 \*\*\*\*\*  
 NUC1 1H  
 P1 10.50 usec  
 PL1 -3.00 dB  
 SFO1 500.1330885 MHz

F2 - Processing parameters  
 SI 32768  
 SF 500.1330090 MHz  
 MDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00

10 NMR plot parameters  
 CX 20.00 cm  
 CY 146.73 cm  
 FIP 11.163 ppm  
 F1 5582.88 Hz  
 F2 2.013 ppm  
 F2 1006.62 Hz  
 PPMCM 0.45751 ppm/cm  
 HZCM 228.81326 Hz/cm



B-36 <sup>13</sup>CNMR in CDCl<sub>3</sub> at 298 K 8/7/11/21

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Current Data Parameters
NAME      Nadir1
EXPNO    31
PROCNO   1

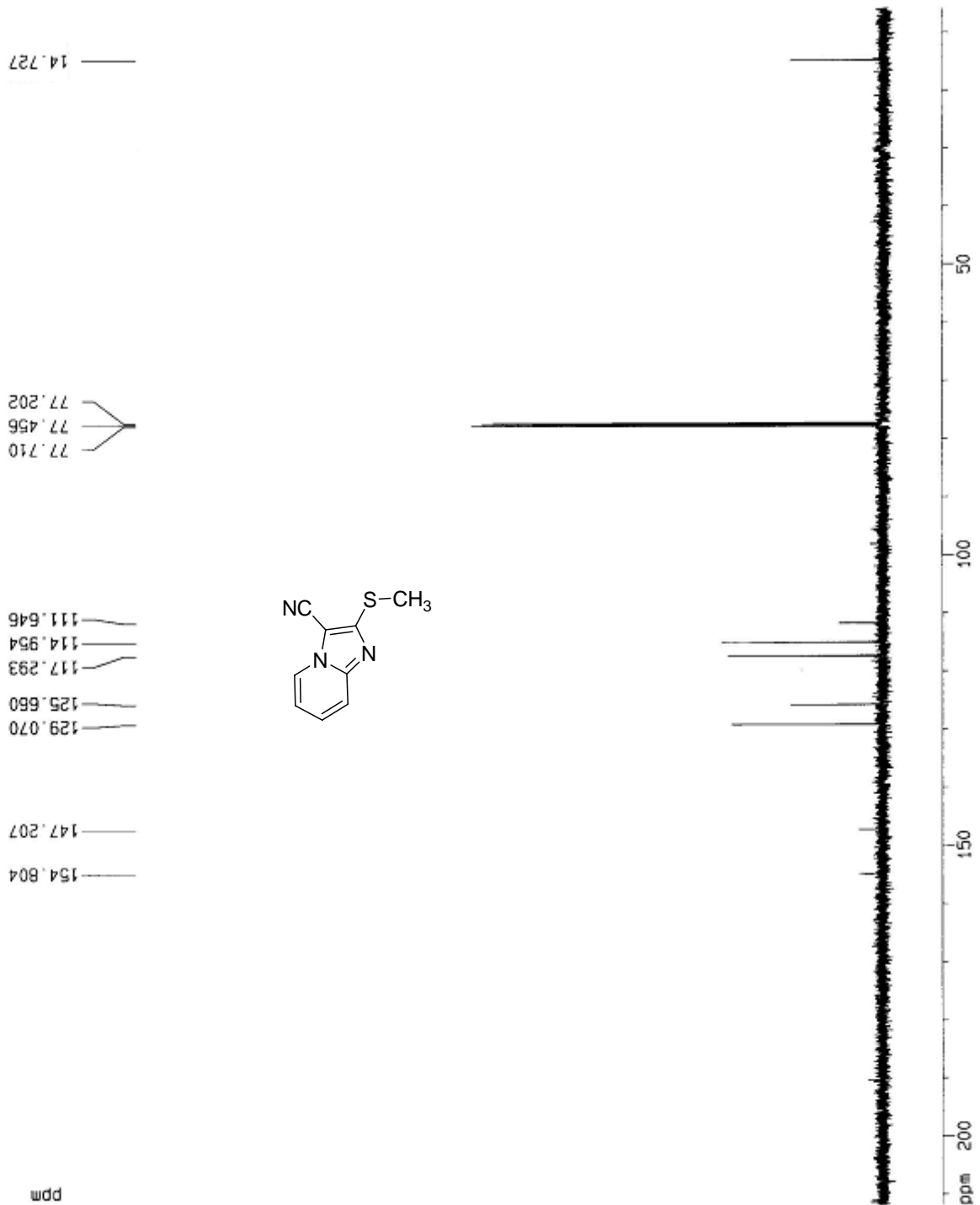
F2 - Acquisition Parameters
Date_    20090209
Time     10.31
INSTRUM  spect
PROBHD   5 mm QNP 1H/13
PULPROG  zgpg30
TD        32768
SOLVENT  CDCl3
NS        409
DS        4
SWH       30030.029 Hz
FIDRES   0.916444 Hz
AQ        0.5456539 sec
RG         2590.3
DM        56.650 usec
DE        6.50 usec
TE        298.0 K
TE        298.0 K
O1        1.00000000 sec
d11       0.03000000 sec
DELTA    0.89599998 sec
MCREST   0.00000000 sec
MCNMRK   0.01500000 sec

***** CHANNEL f1 *****
NUC1      13C
P1        9.10 usec
PL1       3.00 dB
SFO1     125.7703643 MHz

***** CHANNEL f2 *****
CPDPRG2   waltz16
NUC2       1H
PCPD2     80.00 usec
PL2       0.00 dB
PL12      15.50 dB
PL13      15.50 dB
SFO2     500.1320005 MHz

F2 - Processing parameters
SI        32768
SF        125.7577390 MHz
WDW       EM
SSB       0
LB        1.00 Hz
GB        0
PC        1.40

10 NMR plot parameters
CX        20.00 cm
CY        7.02 cm
FLP       211.866 ppm
F1        26643.75 Hz
F2P       5.828 ppm
F2        732.88 Hz
PPHM      10.30150 ppm/cm
HZCN      1295.54333 Hz/cm
    
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B48 <sup>1</sup>H NMR in CDCl<sub>3</sub> at 298 K 88/4/7

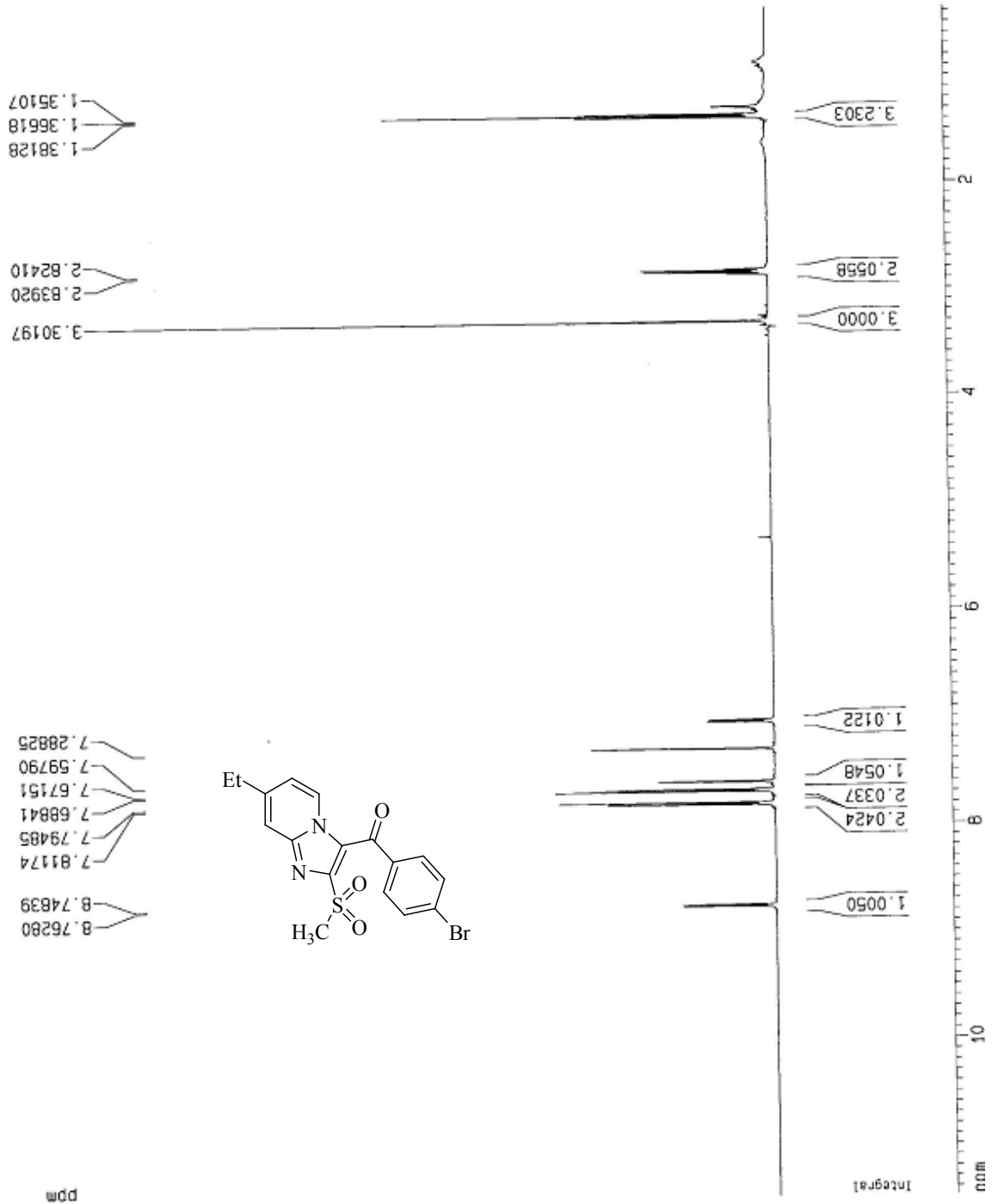
Current Data Parameters  
 NAME Nadir1  
 EXPNO 43  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20090628  
 Time 10.02  
 INSTRUM spect  
 PROBHD 5 mm QNP 1H/13  
 PULPROG zg30  
 TO 65536  
 SOLVENT MeOH  
 NS B  
 DS 0  
 SMH 10330.578 Hz  
 FIDRES 0.157632 Hz  
 AQ 3.1720407 sec  
 RG 512  
 DW 48.400 usec  
 DE 6.50 usec  
 TE 298.0 K  
 D1 5.00000000 sec  
 MCREST 0.00000000 sec  
 MCMRK 0.01500000 sec

----- CHANNEL f1 -----  
 NUC1 1H  
 P1 10.50 usec  
 PL1 -3.00 dB  
 SF01 500.1330885 MHz

F2 - Processing parameters  
 SI 32768  
 SF 500.1300090 MHz  
 WDM EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00

1D NMR plot parameters  
 CX 20.00 cm  
 CY 12.50 cm  
 FIP 11.480 ppm  
 F1 5741.46 Hz  
 F2P 0.359 ppm  
 F2 179.72 Hz  
 PPMCM 0.55603 ppm/cm  
 HZCM 278.08740 Hz/cm



B41 13CNMR in CDCl3 at 298 K 88/2/16

Current Data Parameters  
 NAME Nadi1  
 EXPNO 45  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20090628  
 Time 10:07  
 INSTRUM spect  
 PROBNM 5 mm QNP 1H/13  
 PULPROG zgpg30  
 TD 32768  
 SOLVENT CDCl3  
 NS 520  
 DS 4  
 SWH 30030.029 Hz  
 FIDRES 0.316444 Hz  
 AQ 0.5456539 sec  
 RG 7200.2  
 DM 16.860 usec  
 DE 6.50 usec  
 TE 298.0 K  
 D1 1.0000000 sec  
 D11 0.0300000 sec  
 DELTA 0.8959398 sec  
 MCREST 0.0000000 sec  
 MCORR 0.0150000 sec

\*\*\*\*\* CHANNEL f1 \*\*\*\*\*  
 NUC1 13C  
 P1 9.10 usec  
 PL1 3.00 dB  
 SFO1 125.7703643 MHz

\*\*\*\*\* CHANNEL f2 \*\*\*\*\*  
 CPDPRG2 waltz16  
 NUC2 1H  
 PCPD2 80.00 usec  
 PL2 0.00 dB  
 PL12 15.00 dB  
 PL13 15.00 dB  
 SFO2 500.1320005 MHz

F2 - Processing parameters  
 SI 32768  
 SF 125.7577390 MHz  
 WM EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

10 NMR plot parameters  
 CX 20.00 cm  
 CY 10.31 cm  
 FJP 212.983 ppm  
 F1 26784.20 Hz  
 F2P 6.395 ppm  
 F2 804.27 Hz  
 PPMCK 10.32936 ppm/cm  
 HZCM 1298.95646 Hz/cm

