

## An expedient multicomponent assembling of 1-azaxanthonones

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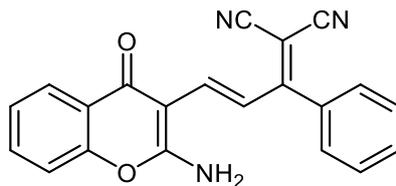
### Experimental

3-Formylchromones, hydroxylammonium chloride, malononitrile, and acetophenone were obtained from Merck (Germany) and Fluka (Switzerland) and were used without further purification. Elemental analyses for C, H, and N were performed using a Heraeus CHN–O–Rapid analyzer. Mass spectra were recorded on a FINNIGAN-MATT 8430 mass spectrometer operating at an ionization potential of 70 eV. <sup>1</sup>H NMR (300 and 500 MHz) and <sup>13</sup>C NMR (75 and 125 MHz) spectra were obtained using Bruker DRX-300 AVANCE and Bruker DRX-400 AVANCE spectrometers. IR spectra were recorded as KBr pellets on a NICOLET FT-IR 100 spectrometer; absorbencies are reported in cm<sup>-1</sup>.

#### General procedure for preparation of compounds **3** (for example **3a**).

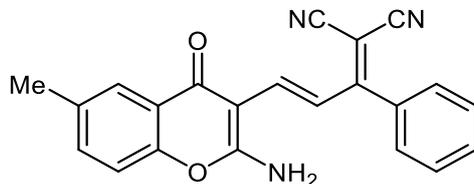
A mixture of 4-oxo-4*H*-chromene-3-carbaldehyde (1 mmol) and hydroxylamine hydrochloride (1 mmol) in EtOH (2 ml) was stirred at reflux for 12 h. Then the carbanion obtained from alkylidene malononitrile **1** with Et<sub>3</sub>N (30 mol%) was added to the mixture. The mixture was stirred at room temperature until completion, monitoring by TLC. The reaction mixture was filtered to give the crude product, which was further washed with EtOH to obtain pure product.

**(E)-2-[3-(2-Amino-4-oxo-4H-chromen-3-yl)-1-phenylallylidene]malononitrile (3a).**



Yellow powder, mp = 256-258 °C, 0.5 g, yield: 85%. IR (KBr) ( $\nu_{\max}$ ,  $\text{cm}^{-1}$ ): 3315 ( $\text{NH}_2$ ), 2214 (CN), 1654 (C=O), 1494 and 1444 (Ar). Anal. Calcd. for  $\text{C}_{21}\text{H}_{13}\text{N}_3\text{O}_2$  (339.35): C, 74.33; H, 3.86; N, 12.38%. Found: C, 74.35; H, 3.89; N, 12.39%. MS (EI, 70 eV):  $m/z$  (%) = 339 (1), 273 (93), 237 (100), 209 (14), 121 (14), 92 (10).  $^1\text{H}$  NMR (300.13 MHz, DMSO):  $\delta_{\text{H}}$  6.96 (1H, d,  $^3J_{\text{HH}} = 14.5$  Hz, CH), 7.36 (1H, d,  $^3J_{\text{HH}} = 8.2$  Hz,  $\text{CH}^8$  of chromone), 7.40 (1H, t,  $^3J_{\text{HH}} = 8.0$  Hz,  $\text{CH}^6$  of chromone), 7.42 (2H, d,  $^3J_{\text{HH}} = 6.6$  Hz,  $2\text{CH}_{\text{ortho}}$  of Ph), 7.53-7.57 (3H, m,  $3\text{CH}$  of Ph), 7.65 (1H, t,  $^3J_{\text{HH}} = 7.9$  Hz,  $\text{CH}^7$  of chromone), 8.02 (1H, d,  $^3J_{\text{HH}} = 7.8$  Hz,  $\text{CH}^5$  of chromone), 8.77 (2H, bs,  $\text{NH}_2$ ), 8.79 (1H, d,  $^3J_{\text{HH}} = 14.5$  Hz, CH).  $^{13}\text{C}$  NMR (75 MHz, DMSO):  $\delta_{\text{C}}$  74.90 ( $\text{C}(\text{CN})_2$ ), 96.97 ( $\text{C}^3$  of chromone), 114.94 (CN), 115.70 (CN), 116.83 ( $\text{CH}^8$  of chromone), 121.74 (CH), 122.36 ( $\text{C}^{4a}$  of chromone), 125.61 ( $\text{CH}^6$  of chromone), 126.03 ( $\text{CH}^6$  of chromone), 129.07 ( $2\text{CH}_{\text{meta}}$  of Ph), 129.80 ( $2\text{CH}_{\text{ortho}}$  of Ph), 131.08 ( $\text{CH}_{\text{para}}$  of Ph), 133.74 ( $\text{CH}^7$  of chromone), 134.00 ( $\text{C}_{\text{ipso}}$  of Ph), 142.99 (CH), 152.29 ( $\text{C}^{8a}$  of chromone), 166.55 ( $\text{C}=\text{C}(\text{CN})_2$ ), 174.27 ( $\text{C}^2\text{-NH}_2$ ), 174.45 (C=O).

**(E)-2-[3-(2-Amino-6-methyl-4-oxo-4H-chromen-3-yl)-1-phenylallylidene]malononitrile (3f).**

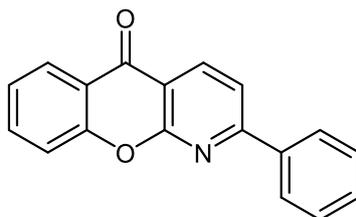


Yellow powder, mp = 265-267 °C, 0.5 g, yield: 84%. IR (KBr) ( $\nu_{\max}$ ,  $\text{cm}^{-1}$ ): 3373 ( $\text{NH}_2$ ), 2220 (CN), 1651 (C=O), 1501 and 1457 (Ar). Anal. Calcd. for  $\text{C}_{22}\text{H}_{15}\text{N}_3\text{O}_2$  (353.38): C, 74.78; H, 4.28; N, 11.89%. Found: C, 74.81; H, 4.29; N, 11.90%. MS (EI, 70 eV):  $m/z$  (%) = 353 (9), 287 (100), 258 (41), 230 (17), 200 (20), 66 (32).  $^1\text{H}$  NMR (300.13 MHz, DMSO):  $\delta_{\text{H}}$  2.38 (3H, s,  $\text{CH}_3$ ), 6.94 (1H, d,  $^3J_{\text{HH}} = 14.4$  Hz, CH), 7.25 (1H, d,  $^3J_{\text{HH}} = 8.4$  Hz,  $\text{CH}^8$  of chromone), 7.41 (2H, d,  $^3J_{\text{HH}} = 7.0$  Hz,  $2\text{CH}_{\text{ortho}}$  of Ph), 7.46 (1H, d,  $^3J_{\text{HH}} = 8.8$  Hz,  $\text{CH}^7$  of chromone), 7.51-7.60 (3H, m,  $3\text{CH}$  of Ph), 7.81 (1H, s,  $\text{CH}^5$  of chromone), 8.68 (2H, bs,  $\text{NH}_2$ ), 8.78 (1H, d,  $^3J_{\text{HH}} = 14.4$  Hz, CH).  $^{13}\text{C}$  NMR (75 MHz, DMSO):  $\delta_{\text{C}}$  20.41 ( $\text{CH}_3$ ), 74.28 ( $\text{C}(\text{CN})_2$ ), 96.48 ( $\text{C}^3$  of chromone), 114.48 (CN), 115.26 (CN), 116.15 ( $\text{CH}^8$  of chromone), 121.16 (CH), 121.53 ( $\text{C}^{4a}$  of chromone), 125.18 ( $\text{CH}^5$  of chromone), 128.59 ( $2\text{CH}_{\text{meta}}$  of Ph), 129.31 ( $2\text{CH}_{\text{ortho}}$  of Ph), 130.59 ( $\text{CH}_{\text{para}}$  of Ph), 133.51 ( $\text{C}_{\text{ipso}}$  of Ph), 134.03 ( $\text{CH}^7$  of chromone), 134.50 ( $\text{C}_{\text{ipso-Me}}$ ), 142.60 (CH), 149.99 ( $\text{C}^{8a}$  of chromone), 166.05 ( $\text{C}=\text{C}(\text{CN})_2$ ), 173.80 ( $\text{C}^2\text{-NH}_2$ ), 174.05 (C=O).

### The procedure for preparation of compound 4a.

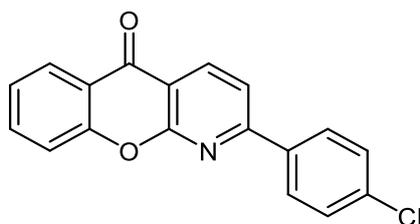
A mixture of 4-oxo-4*H*-chromene-3-carbaldehyde (1 mmol) and hydroxylamine hydrochloride (1 mmol) in EtOH (2 ml) was stirred at reflux for 12 h. Then the carbanion obtained from alkylidenemalononitrile **1** with Et<sub>3</sub>N (50 mol%) was added to the mixture. The mixture was stirred at room temperature until completion, monitoring by TLC. The solvent was removed, and the residue purified by column chromatography (hexane–EtOAc, 1:10) to afford the pure products **4a**.

### 2-Phenyl-5*H*-chromeno[2,3-*b*]pyridin-5-one (4a).



Cream powder, mp = 222-224 °C, 0.5 g, yield: 58%. IR (KBr) ( $\nu_{\max}$ , cm<sup>-1</sup>): 1665 (C=O), 1598 (C=N), 1578 and 1444 (Ar). Anal. Calcd. for C<sub>18</sub>H<sub>11</sub>NO<sub>2</sub> (273.29): C, 79.11; H, 4.06; N, 5.13%. Found: C, 79.13; H, 4.09; N, 5.19%. MS (EI, 70 eV):  $m/z$  (%) = 273 (100), 245 (43), 216 (29), 189 (14), 102 (14), 57 (7). <sup>1</sup>H NMR (300.13 MHz, DMSO-*d*<sub>6</sub>):  $\delta_{\text{H}}$  7.38 (1H, td, <sup>3</sup> $J_{\text{HH}}$  = 8.1 Hz, <sup>4</sup> $J_{\text{HH}}$  = 1.1 Hz, CH<sup>6</sup> of chromone), 7.45-7.48 (3H, m, CH<sub>para</sub> of Ph and 2CH<sub>meta</sub> of Ph), 7.60 (1H, dd, <sup>3</sup> $J_{\text{HH}}$  = 8.4 Hz, <sup>4</sup> $J_{\text{HH}}$  = 1.1 Hz, CH<sup>8</sup> of chromone), 7.73 (1H, td, <sup>3</sup> $J_{\text{HH}}$  = 8.7 Hz, <sup>4</sup> $J_{\text{HH}}$  = 1.8 Hz, CH<sup>7</sup> of chromone), 7.82 (1H, d, <sup>3</sup> $J_{\text{HH}}$  = 8.1 Hz, CH of pyridin), 8.12 (2H, d, <sup>3</sup> $J_{\text{HH}}$  = 7.4 Hz, 2CH<sub>ortho</sub> of Ph), 8.27 (1H, dd, <sup>3</sup> $J_{\text{HH}}$  = 7.9 Hz, <sup>4</sup> $J_{\text{HH}}$  = 1.8 Hz, CH<sup>5</sup> of chromone), 8.68 (1H, d, <sup>3</sup> $J_{\text{HH}}$  = 8.1 Hz, CH of pyridin). <sup>13</sup>C NMR (75 MHz, DMSO-*d*<sub>6</sub>):  $\delta_{\text{C}}$  115.00 (C<sup>3</sup> of chromone), 117.57 (CH of pyridin), 118.40 (CH<sup>8</sup> of chromone), 121.69 (C<sup>4a</sup> of chromone), 124.51 (CH<sup>6</sup> of chromone), 126.57 (CH<sup>5</sup> of chromone), 127.71 (2CH<sub>meta</sub> of Ph), 128.92 (2CH<sub>ortho</sub> of Ph), 130.77 (CH<sub>para</sub> of Ph), 135.36 (CH<sup>7</sup> of chromone), 137.03 (C<sub>ipso</sub> of Ph), 137.89 (CH of pyridin), 155.78 (C<sup>8a</sup> of chromone), 160.15 (C=N), 161.68 (C<sup>2</sup> of chromone), 177.21 (C=O).

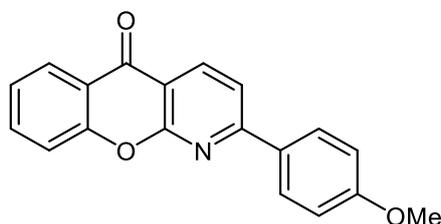
### 2-(4-Chlorophenyl)-5*H*-chromeno[2,3-*b*]pyridin-5-one (4b).



Cream powder, mp = 233-234 °C, 0.5 g, yield: 73%. IR (KBr) ( $\nu_{\max}$ , cm<sup>-1</sup>): 1664 (C=O), 1598 (C=N), 1585 and 1460 (Ar). Anal. Calcd. for C<sub>18</sub>H<sub>10</sub>ClNO<sub>2</sub> (307.73): C, 70.26; H, 3.28; N, 4.55%. Found: C, 70.26; H, 3.29; N, 4.59%. MS (EI, 70 eV):  $m/z$  (%) = 307 (100), 279 (20), 255 (7), 237 (67), 216 (14),

140 (14), 122 (20).  $^1\text{H}$  NMR (300.13 MHz,  $\text{DMSO-}d_6$ ):  $\delta_{\text{H}}$  7.48 (1H, t,  $^3J_{\text{HH}} = 7.6$  Hz,  $\text{CH}^6$  of chromone), 7.58 (2H, d,  $^3J_{\text{HH}} = 8.5$  Hz, 2CH of Ar), 7.71 (1H, d,  $^3J_{\text{HH}} = 8.4$  Hz,  $\text{CH}^8$  of chromone), 7.88 (1H, t,  $^3J_{\text{HH}} = 7.9$  Hz,  $\text{CH}^7$  of chromone), 8.13 (1H, d,  $^3J_{\text{HH}} = 8.1$  Hz, CH of pyridin), 8.13 (1H, d,  $^3J_{\text{HH}} = 8.1$  Hz, CH of pyridin), 8.21 (2H, d,  $^3J_{\text{HH}} = 8.2$  Hz, 2CH of Ar), 8.60 (1H, d,  $^3J_{\text{HH}} = 8.2$  Hz,  $\text{CH}^5$  of chromone).  $^{13}\text{C}$  NMR (75 MHz,  $\text{DMSO-}d_6$ ):  $\delta_{\text{C}}$  115.08 ( $\text{C}^3$  of chromone), 117.86 (CH of pyridin), 118.45 ( $\text{CH}^8$  of chromone), 121.22 ( $\text{C}^{4a}$  of chromone), 124.87 ( $\text{CH}^6$  of chromone), 125.96 ( $\text{CH}^5$  of chromone), 129.15 (2CH of Ar), 129.29 (2CH of Ar), 135.35 ( $\text{CH}^7$  of chromone), 135.91 ( $\text{C}_{\text{ipso}}$  of Ar), 135.91 (CH of pyridin), 138.07 ( $\text{C}_{\text{ipso-Cl}}$ ), 155.30 ( $\text{C}^{8a}$  of chromone), 159.09 (C=N), 159.62 ( $\text{C}^2$  of chromone), 176.43 (C=O).

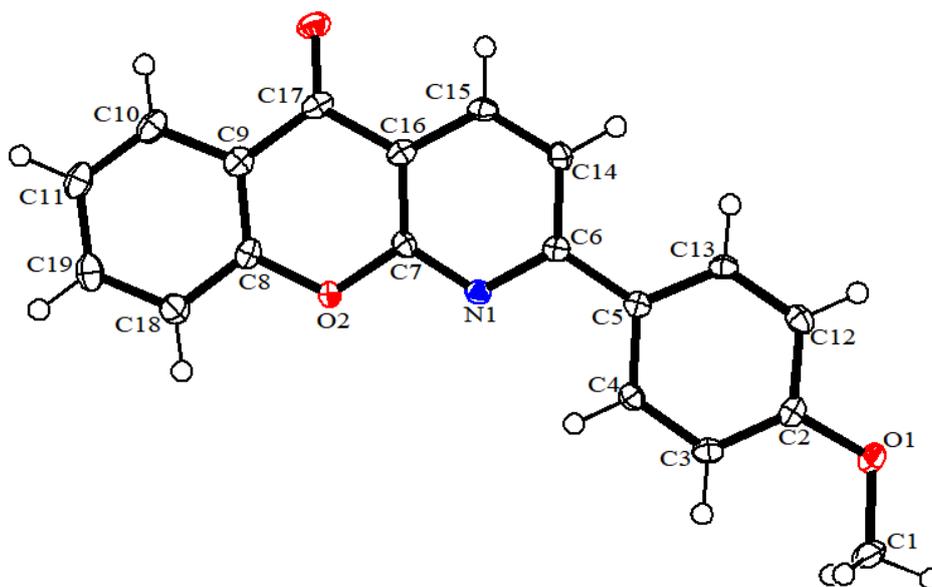
### 2-(4-Methoxyphenyl)-5H-chromeno[2,3-b]pyridin-5-one (**4c**).



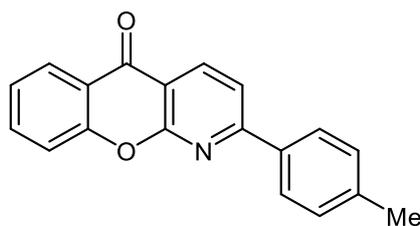
Cream powder, mp = 241-243 °C, 0.5 g, yield: 59%. IR (KBr) ( $\nu_{\text{max}}$ ,  $\text{cm}^{-1}$ ): 1652 (C=O), 1596 (C=N), 1583 and 1456 (Ar). Anal. Calcd. for  $\text{C}_{19}\text{H}_{13}\text{NO}_3$  (303.32): C, 75.24; H, 4.32; N, 4.62%. Found: C, 75.26; H, 4.39; N, 4.69%. MS (EI, 70 eV):  $m/z$  (%) = 303 (100), 288 (27), 260 (73), 237 (22), 203 (14), 138 (13).  $^1\text{H}$  NMR (300.13 MHz,  $\text{DMSO-}d_6$ ):  $\delta_{\text{H}}$  3.84 (3H, s, OMe), 7.09 (2H, d,  $^3J_{\text{HH}} = 8.4$  Hz, 2CH of Ar), 7.49 (1H, t,  $^3J_{\text{HH}} = 7.5$  Hz,  $\text{CH}^6$  of chromone), 7.73 (1H, d,  $^3J_{\text{HH}} = 8.3$  Hz,  $\text{CH}^8$  of chromone), 7.89 (1H, t,  $^3J_{\text{HH}} = 7.9$  Hz,  $\text{CH}^7$  of chromone), 8.09 (1H, d,  $^3J_{\text{HH}} = 8.2$  Hz, CH of pyridin), 8.09 (1H, d,  $^3J_{\text{HH}} = 8.2$  Hz, CH of pyridin), 8.20 (2H, d,  $^3J_{\text{HH}} = 8.3$  Hz, 2CH of Ar), 8.57 (1H, d,  $^3J_{\text{HH}} = 8.7$  Hz,  $\text{CH}^5$  of chromone).  $^{13}\text{C}$  NMR (75 MHz,  $\text{DMSO-}d_6$ ):  $\delta_{\text{C}}$  55.39 (OMe), 114.00 ( $\text{C}^3$  of chromone), 114.49 (2CH of Ar), 117.07 (CH of pyridin), 118.40 ( $\text{CH}^8$  of chromone), 121.24 ( $\text{C}^{4a}$  of chromone), 124.75 ( $\text{CH}^8$  of chromone), 125.89 ( $\text{CH}^5$  of chromone), 129.24 (2CH of Ar), 135.78 ( $\text{CH}^7$  of chromone), 137.51 (CH of pyridin), 144.12 ( $\text{C}_{\text{ipso}}$  of Ar), 155.27 ( $\text{C}^{8a}$  of chromone), 159.70 ( $\text{C}_{\text{ipso-OMe}}$ ), 160.27 (C=N), 161.72 ( $\text{C}^2$  of chromone), 176.31 (C=O).

Crystal data for **4c**  $\text{C}_{19}\text{H}_{13}\text{NO}_3$  (CCDC 1955484):  $M_{\text{w}} = 303.30$ , orthorhombic, P b c a,  $a = 10.6856(11)$  Å,  $b = 9.4219(6)$  Å,  $c = 27.671(3)$  Å,  $\alpha = 90$ ,  $\beta = 90$ ,  $\gamma = 90$ ,  $V = 2785.9(4)$  Å<sup>3</sup>,  $Z = 8$ ,  $D_{\text{c}} = 1.446$  mg/m<sup>3</sup>,  $F(000) = 1264$ , crystal dimension 0.20 × 0.10 × 0.10 mm, radiation, Mo K $\alpha$  ( $\lambda = 0.71073$  Å),  $2.94 \leq 2\theta \leq 27.41$ , intensity data were collected at 100(2) K with a Bruker APEX area-detector diffractometer, and employing  $\omega/2\theta$  scanning technique, in the range of  $-12 \leq h \leq 12$ ,  $-11 \leq k \leq 11$ ,  $-32 \leq l \leq 32$ ; the structure was solved by a direct method, all non-hydrogen atoms were positioned and anisotropic thermal parameters refined from 2457 observed reflections with R (into)

= 0.0908 by a full-matrix least-squares technique converged to R1 = 0.0510, and wR2 = 0.1354 [I>2sigma(I)].

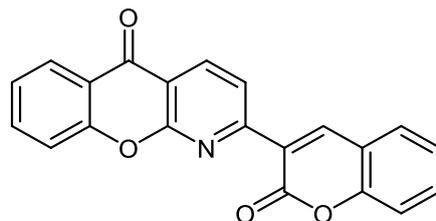


**2-(*p*-Tolyl)-5*H*-chromeno[2,3-*b*]pyridin-5-one (4d).**



Cream powder, mp = 227-229 °C, 0.5 g, yield: 63%. IR (KBr) ( $\nu_{\max}$ ,  $\text{cm}^{-1}$ ): 1658 (C=O), 1612 (C=N), 1596 and 1459 (Ar). Anal. Calcd. for  $\text{C}_{19}\text{H}_{13}\text{NO}_2$  (287.09): C, 79.43; H, 4.56; N, 4.88%. Found: C, 79.49; H, 4.54; N, 4.85%. MS (EI, 70 eV):  $m/z$  (%) = 287 (100), 258 (11), 233 (61), 115 (24), 91 (22).  $^1\text{H}$  NMR (300.13 MHz,  $\text{DMSO-}d_6$ ):  $\delta_{\text{H}}$  2.36 (3H, s, Me), 7.34 (2H, d,  $^3J_{\text{HH}} = 8.1$  Hz, 2CH of Ar), 7.49 (1H, t,  $^3J_{\text{HH}} = 7.8$  Hz,  $\text{CH}^6$  of chromone), 7.73 (1H, d,  $^3J_{\text{HH}} = 8.4$  Hz,  $\text{CH}^8$  of chromone), 7.89 (1H, t,  $^3J_{\text{HH}} = 7.4$  Hz,  $\text{CH}^7$  of chromone), 8.10 (1H, d,  $^3J_{\text{HH}} = 8.2$  Hz, CH of pyridin), 8.10 (1H, d,  $^3J_{\text{HH}} = 8.2$  Hz, CH of pyridin), 8.11 (2H, d,  $^3J_{\text{HH}} = 8.1$  Hz, 2CH of Ar), 8.59 (1H, d,  $^3J_{\text{HH}} = 8.1$  Hz,  $\text{CH}^5$  of chromone).  $^{13}\text{C}$  NMR (75 MHz,  $\text{DMSO-}d_6$ ):  $\delta_{\text{C}}$  20.69 (Me), 114.51 ( $\text{C}^3$  of chromone), 117.51 (CH of pyridin), 118.45 ( $\text{CH}^8$  of chromone), 121.22 ( $\text{C}^{4a}$  of chromone), 124.79 ( $\text{CH}^6$  of chromone), 125.92 ( $\text{CH}^5$  of chromone), 127.45 (2CH of Ar), 129.70 (2CH of Ar), 133.75 (CH of pyridin), 135.87 ( $\text{CH}^7$  of chromone), 137.68 ( $\text{C}_{\text{ipso}}$  of Ar), 141.03 ( $\text{C}_{\text{ipso}}\text{-CH}_3$ ), 155.29 ( $\text{C}^{8a}$  of chromone), 159.65 (C=N), 160.42 ( $\text{C}^2$  of chromone), 176.40 (C=O).

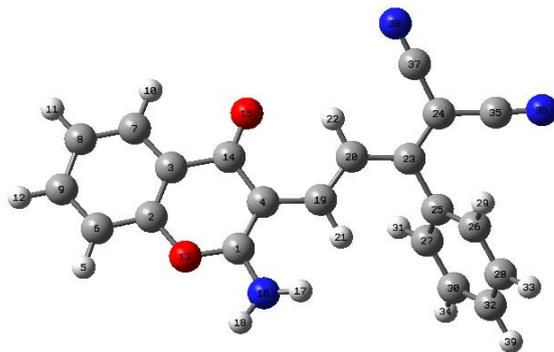
**2-(2-Oxo-2H-chromen-3-yl)-5H-chromeno[2,3-b]pyridin-5-one (4e).**



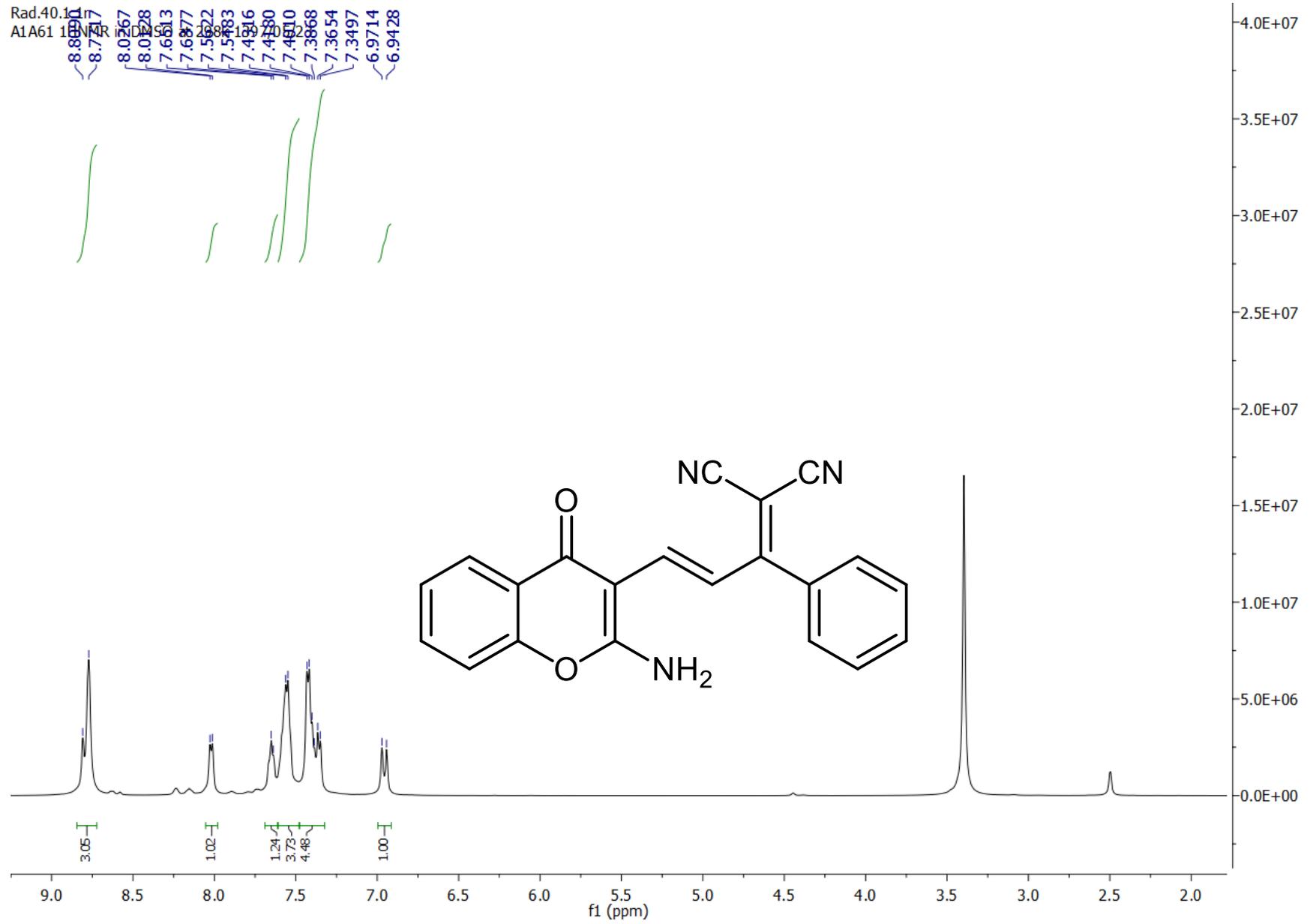
Cream powder, mp = 283-284 °C, 0.5 g, yield: 70%. IR (KBr) ( $\nu_{\max}$ ,  $\text{cm}^{-1}$ ): 1724 ( $\text{CO}_2\text{R}$ ), 1656 ( $\text{C}=\text{O}$ ), 1598 ( $\text{C}=\text{N}$ ), 1540 and 1434 (Ar). Anal. Calcd. for  $\text{C}_{21}\text{H}_{11}\text{NO}_4$  (341.07): C, 73.90; H, 3.25; N, 4.10%. Found: C, 73.96; H, 3.22; N, 4.08%. MS (EI, 70 eV):  $m/z$  (%) = 341 (76), 313 (99), 256 (27), 228 (100), 202 (25), 153 (22), 92 (18).  $^1\text{H}$  NMR (300.13 MHz,  $\text{DMSO}-d_6$ ):  $\delta_{\text{H}}$  7.45 (1H, t,  $^3J_{\text{HH}} = 7.9$  Hz, CH of Ar), 7.47 (1H, t,  $^3J_{\text{HH}} = 7.9$  Hz,  $\text{CH}^6$  of chromone), 7.57 (1H, d,  $^3J_{\text{HH}} = 8.4$  Hz,  $\text{CH}^8$  of chromone), 7.72 (1H, d,  $^3J_{\text{HH}} = 7.6$  Hz, CH of Ar), 7.81 (1H, t,  $^3J_{\text{HH}} = 7.8$  Hz, CH of Ar), 7.91 (1H, t,  $^3J_{\text{HH}} = 8.0$  Hz,  $\text{CH}^7$  of chromone), 8.06 (1H, d,  $^3J_{\text{HH}} = 7.7$  Hz, CH of Ar), 8.16 (1H, d,  $^3J_{\text{HH}} = 7.9$  Hz,  $\text{CH}^5$  of chromone), 8.48 (1H, d,  $^3J_{\text{HH}} = 8.1$  Hz, CH of pyridin) 8.60 (1H, s, CH of Ar), 8.69 (1H, d,  $^3J_{\text{HH}} = 8.2$  Hz, CH of pyridin).  $^{13}\text{C}$  NMR (75 MHz,  $\text{DMSO}-d_6$ ):  $\delta_{\text{C}}$  115.48 ( $\text{C}_{\text{ipso}}$  of Ar), 115.90 ( $\text{C}^3$  of chromone), 118.05 (CH of pyridin), 118.30 (CH of Ar), 120.74 ( $\text{CH}^8$  of chromone), 121.12 ( $\text{C}^{4a}$  of chromone), 124.87 (CH of Ar), 124.91 ( $\text{CH}^6$  of chromone), 125.79 ( $\text{CH}^5$  of chromone), 130.12 (CH of Ar), 133.58 (CH of Ar), 135.28 ( $\text{CH}^7$  of chromone), 136.02 ( $\text{C}_{\text{ipso}}$  of Ar), 137.84 (CH of pyridin), 144.10 (CH of Ar), 145.15 ( $\text{C}_{\text{ipso}}$  of Ar), 153.69 ( $\text{C}^{8a}$  of chromone), 154.48 ( $\text{C}=\text{N}$ ), 155.19 ( $\text{C}^2$  of chromone), 161.26 ( $\text{CO}_2\text{R}$ ), 173.96 ( $\text{C}=\text{O}$ ).

<b>Table 1</b> Quantum descriptors of <b>3a-f</b>						
Compound	$E_{\text{LUMO}}$ (eV)	$E_{\text{HOMO}}$ (eV)	$\Delta E$ (eV)	( $m$ )	( $z$ )	( $\mathcal{K}$ )
<b>3a</b>	-2.5026	-5.9016	3.3990	4.202	1.699	0.294
<b>3b</b>	-2.6528	-6.0109	3.3581	4.332	1.679	0.297
<b>3c</b>	-2.4137	-5.8186	3.4050	4.116	1.703	0.293
<b>3d</b>	-2.4713	-5.8649	3.3935	4.168	1.697	0.294
<b>3e</b>	-2.7356	-5.8309	3.0953	4.283	1.548	0.323
<b>3f</b>	-2.4825	-5.8627	3.3802	4.172	1.690	0.295

**Table 2:** Second-order perturbation theory analysis in the NBO basis of compound **3a**

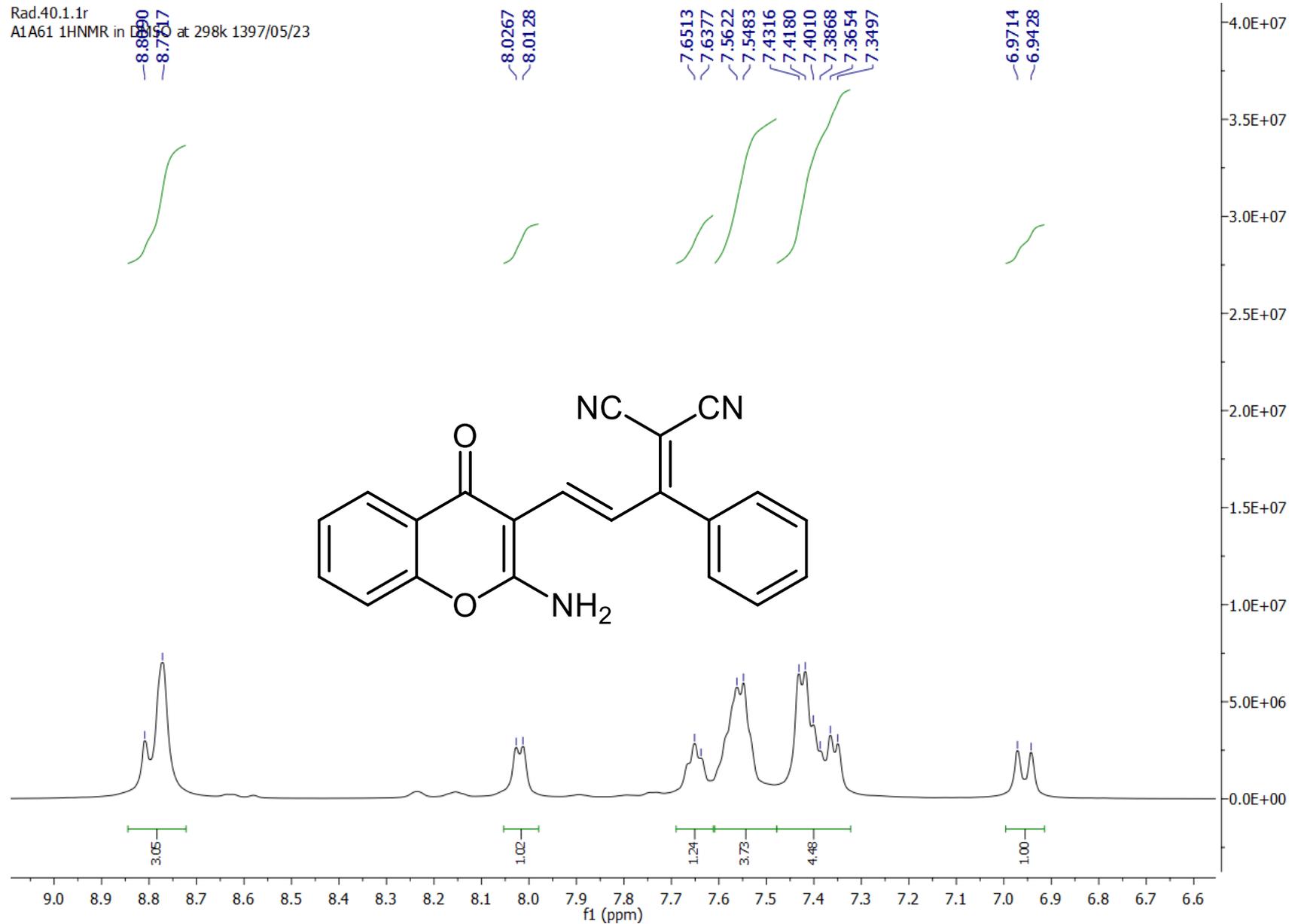


Donor NBO	Acceptor NBO	$E^{(2)}$ (kJ/mol)	Donor NBO	Acceptor NBO	$E^{(2)}$ (kJ/mol)
p (C1-C4)	p* (C14-O15)	109.12	p (C23-C24)	p* (C35-N36)	84.68
	p* (C19-C20)	77.57		p* (C37-N38)	82.89
p (C2-C3)	p* (C6-C9)	71.80	LP(2) O13	p* (C1-C4)	148.74
	p* (C7-C8)	76.11		p* (C2-C3)	99.99
	p* (C14-O15)	81.96		y* (C1-N16)	10.38
p (C6-C9)	p* (C2-C3)	93.26	LP(2) O15	$\sigma^*$ (C3-C14)	83.39
	p* (C7-C8)	68.28		$\sigma^*$ (C4-C14)	80.29
p (C19-C20)	p* (C23-C24)	88.78	LP(1) N16	p* (C1-C4)	175.94
p (C7-C8)	p* (C2-C3)	79.04			
	p* (C6-C9)	93.68			

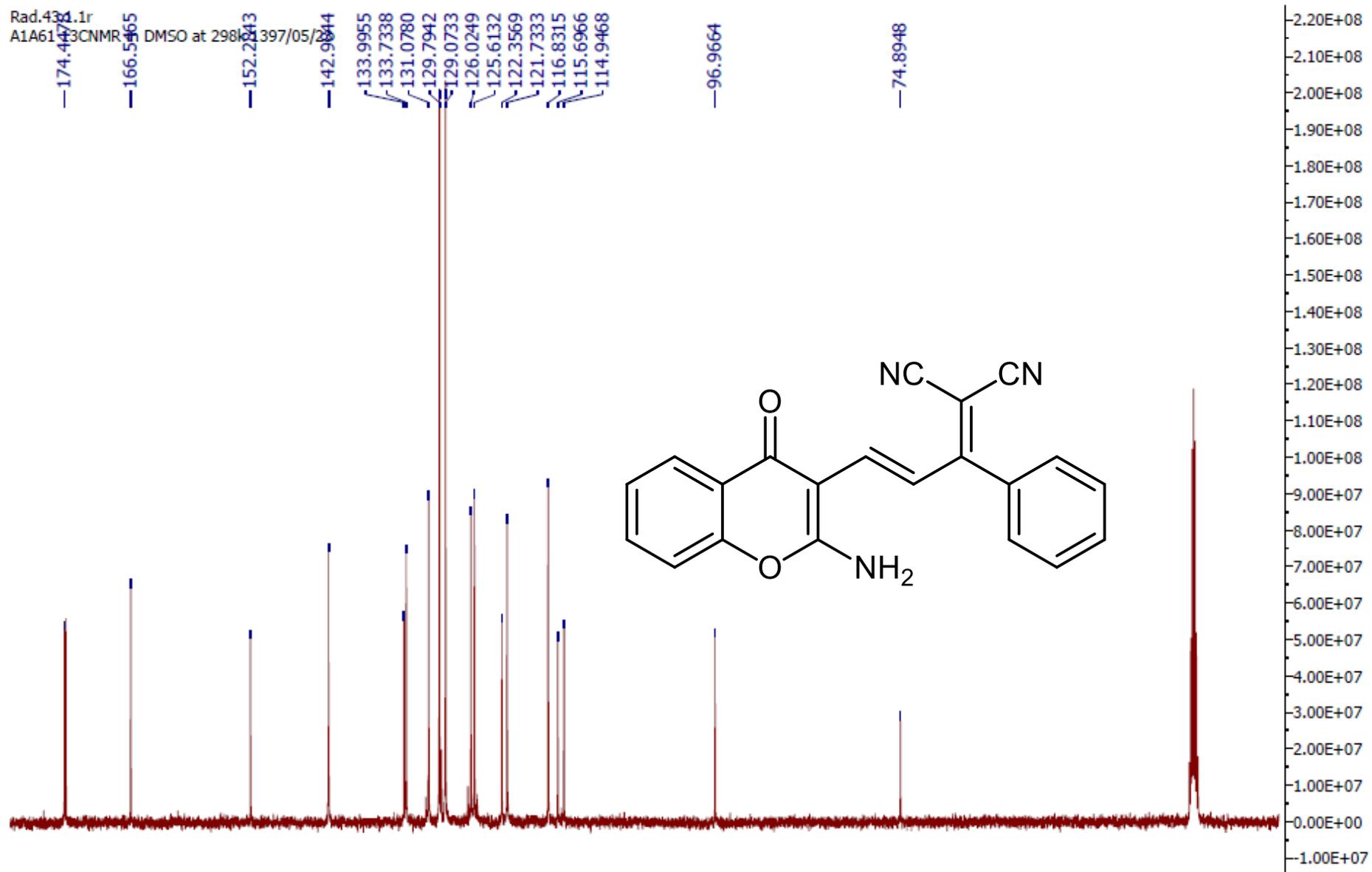


<sup>1</sup>H NMR of 3a

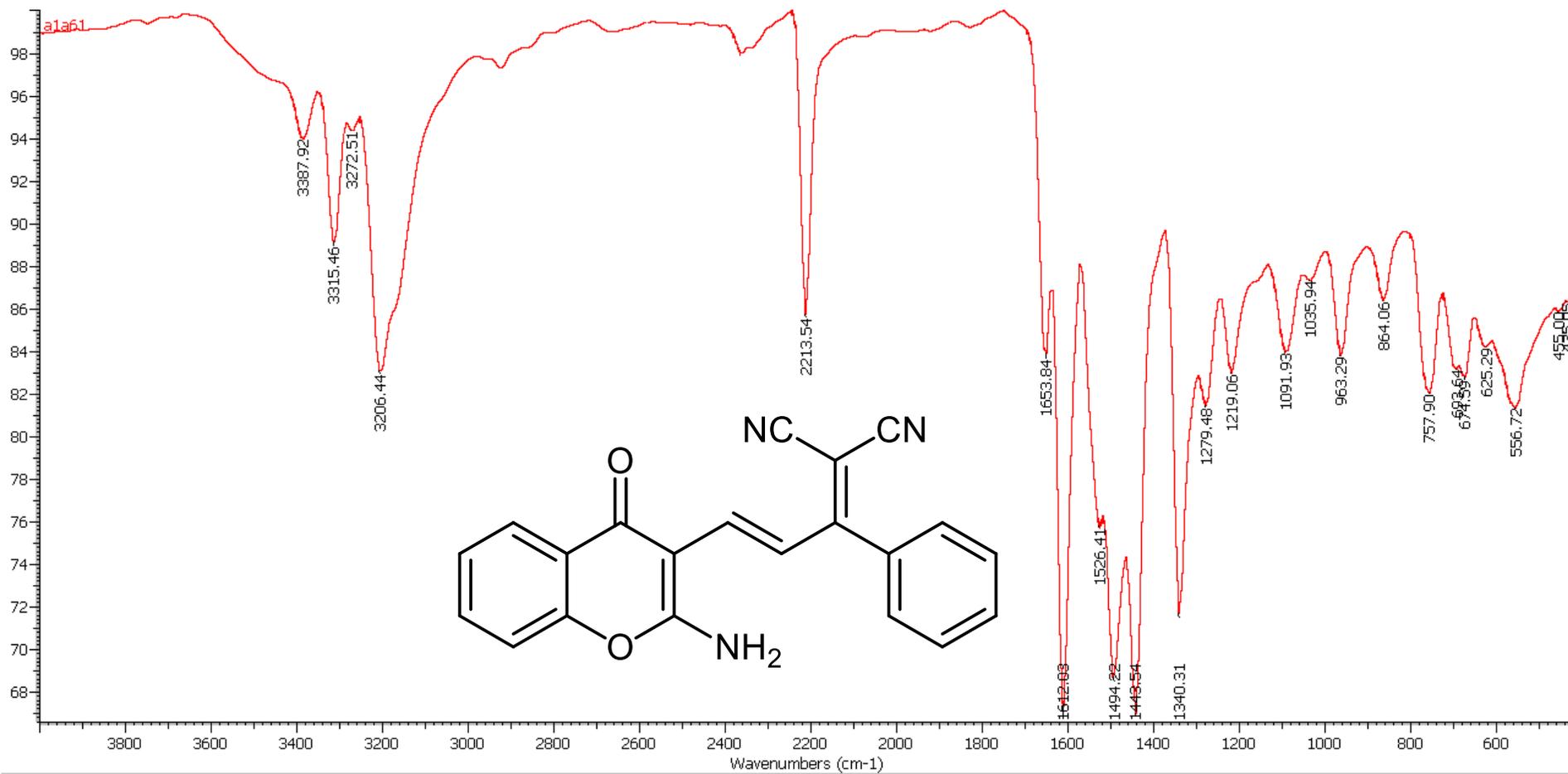
Rad.40.1.1r  
A1A61 1HNMR in DMSO at 298k 1397/05/23



<sup>1</sup>H NMR of 3a



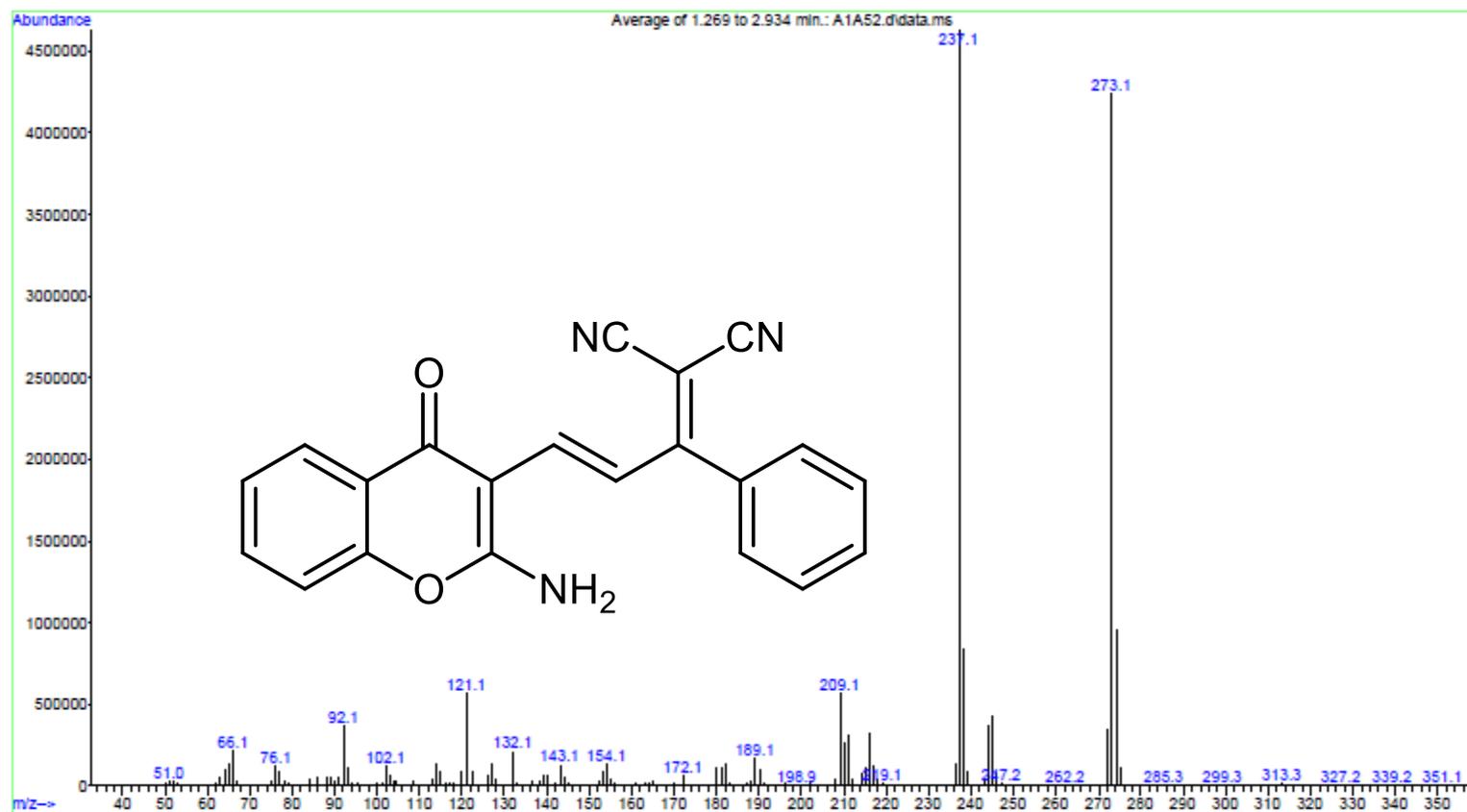
<sup>13</sup>C NMR of 3a



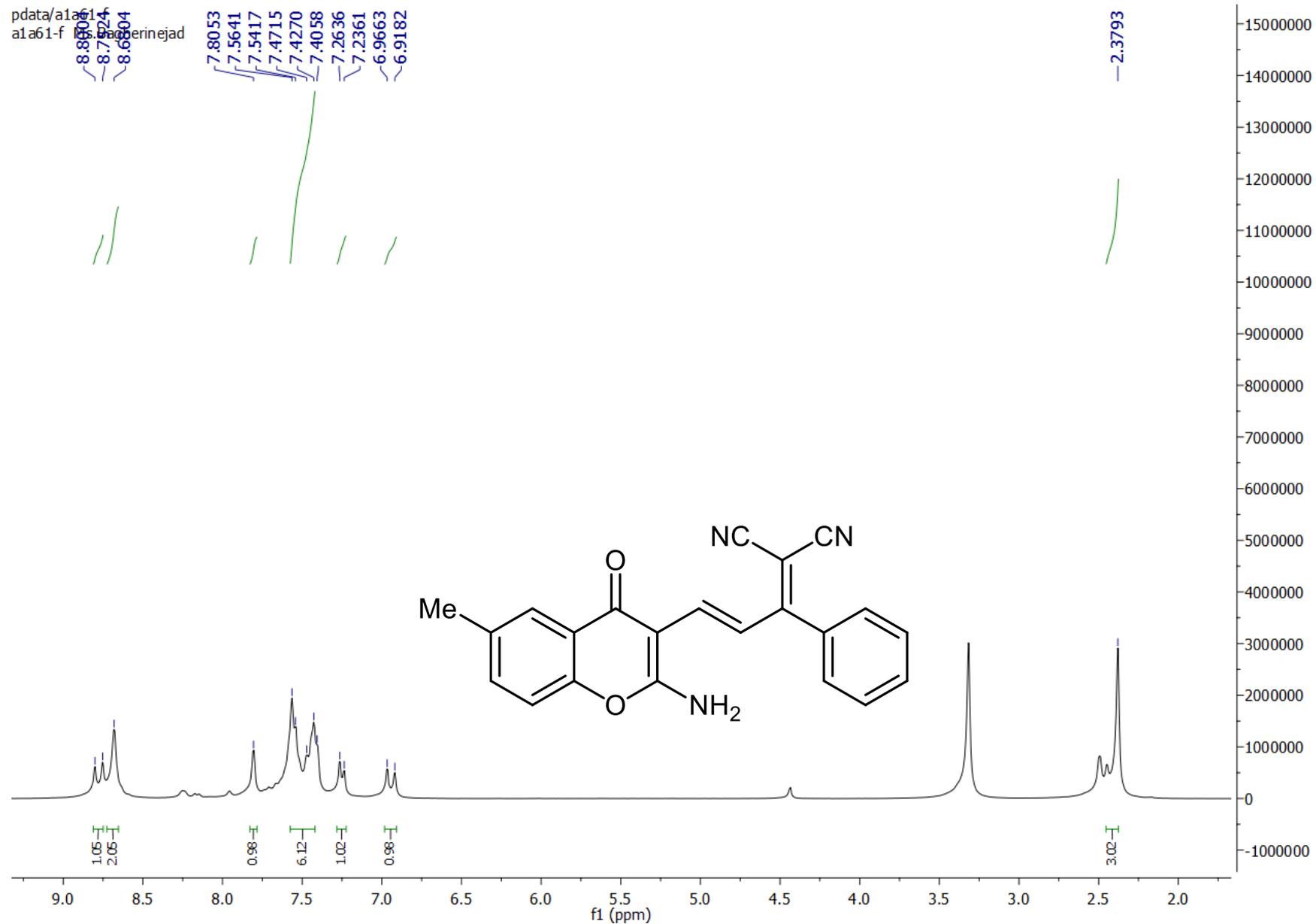
IR of 3a



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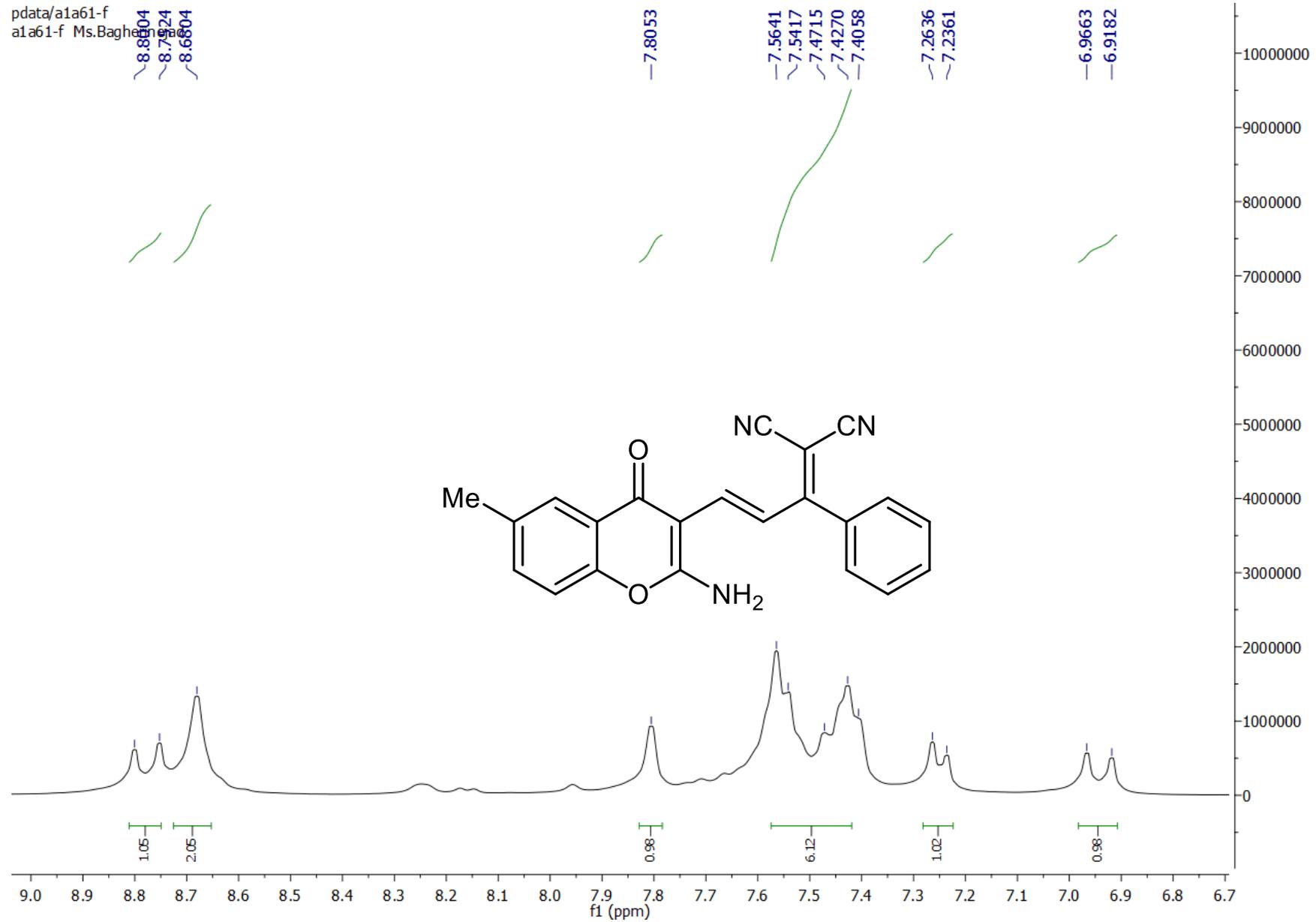


Mass of compound 3a

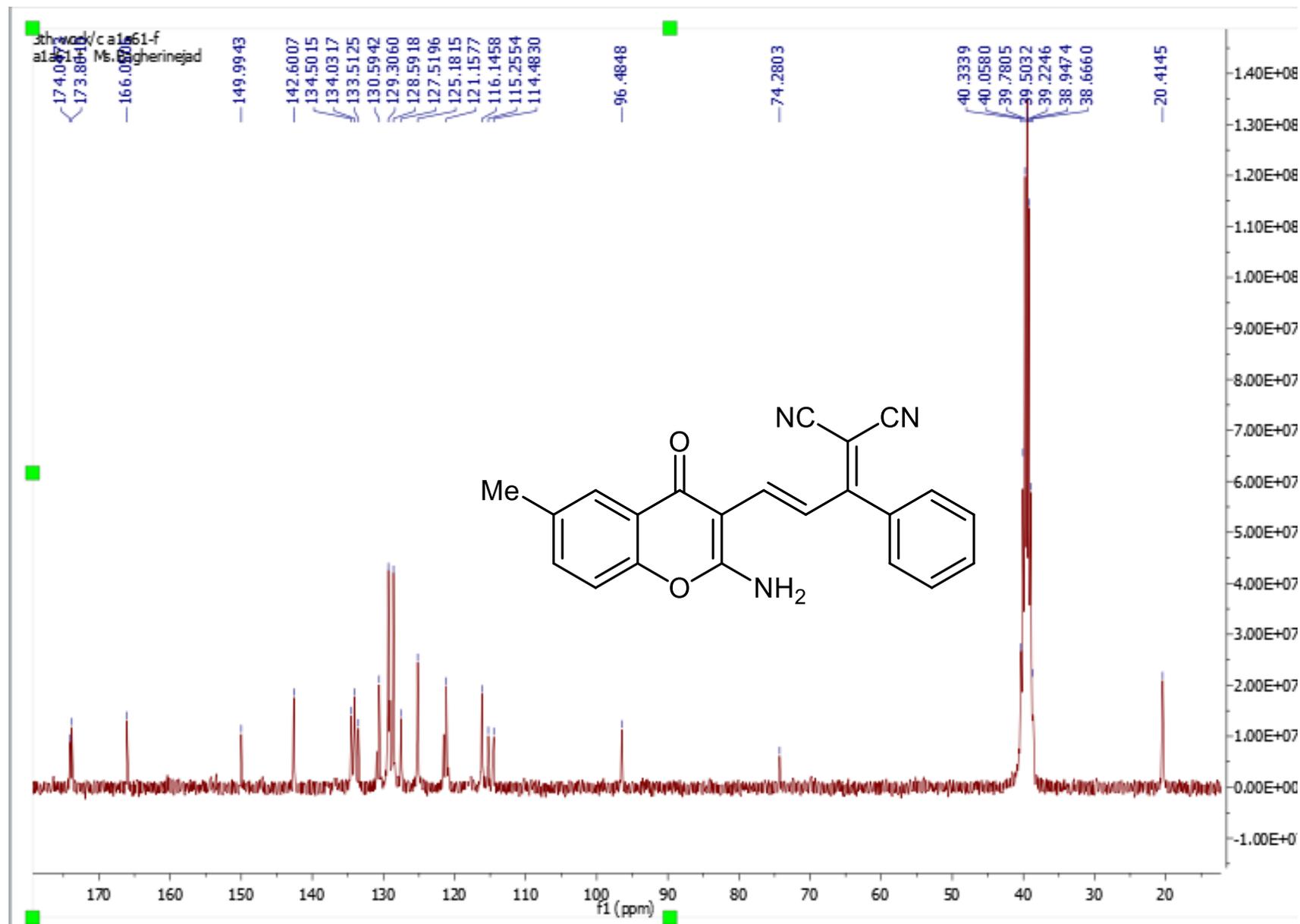


<sup>1</sup>H NMR of **3f**

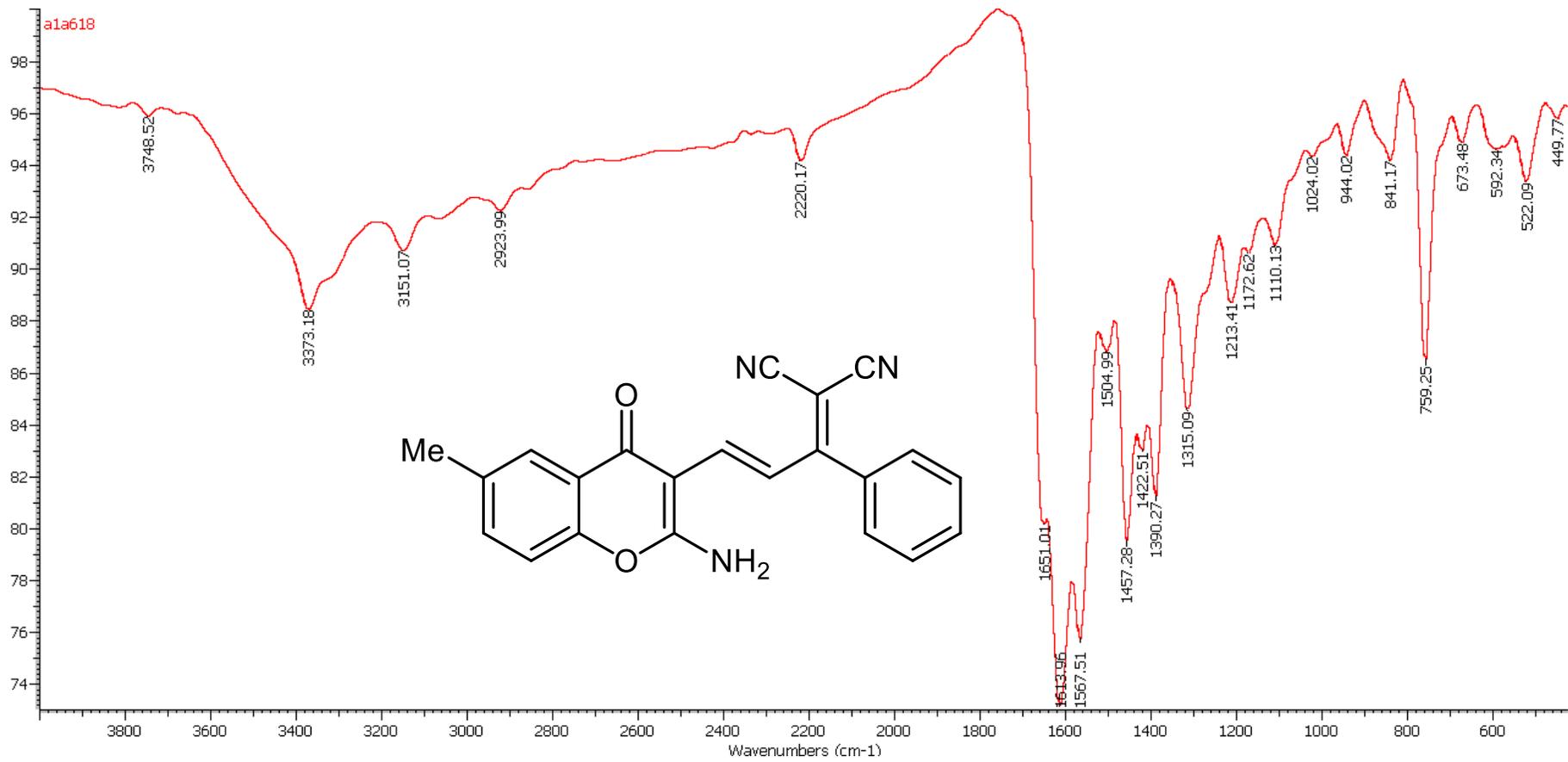
pdata/a1a61-f  
a1a61-f Ms.Baghe



<sup>1</sup>H NMR of 3f



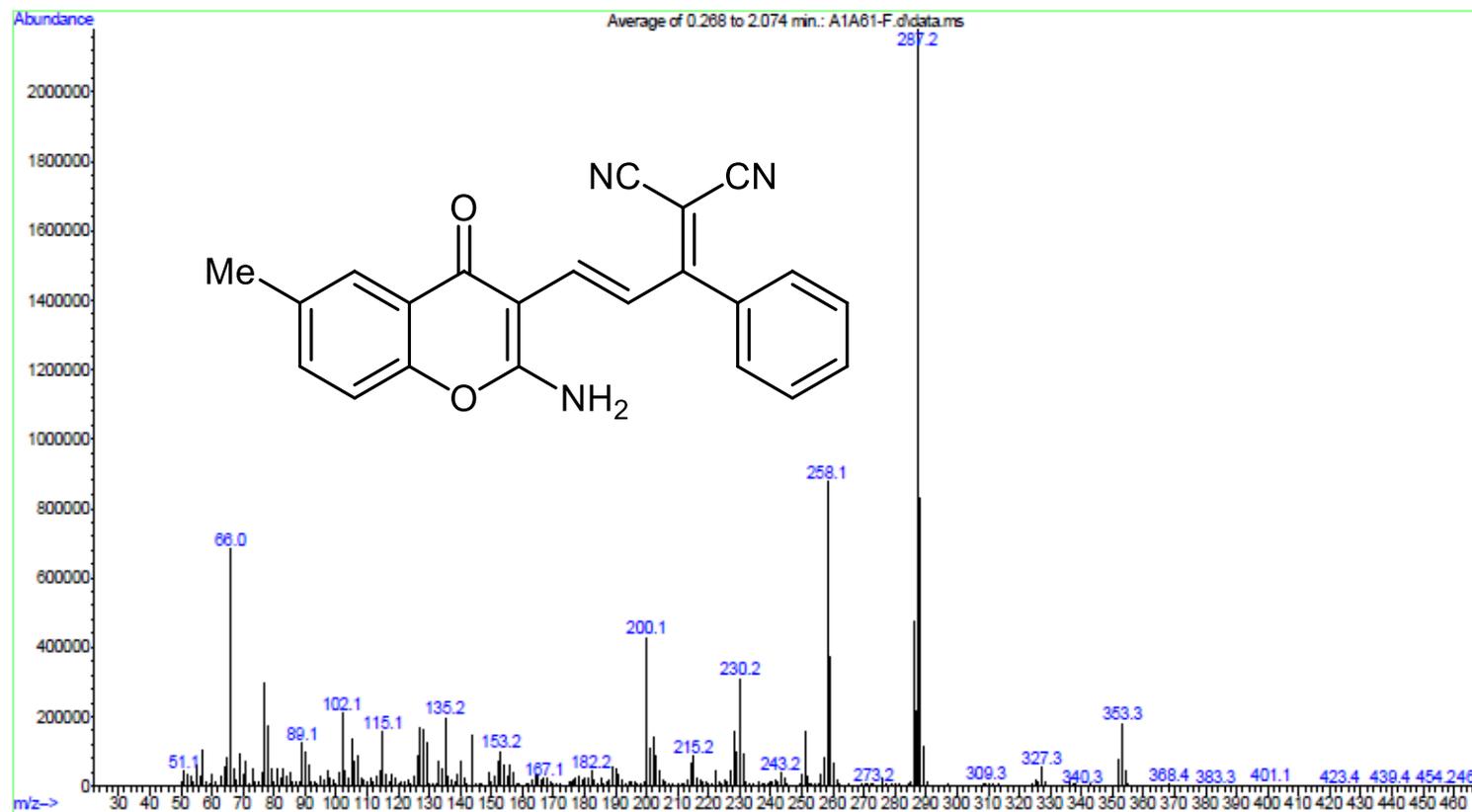
<sup>13</sup>C NMR of **3f**



IR of 3f

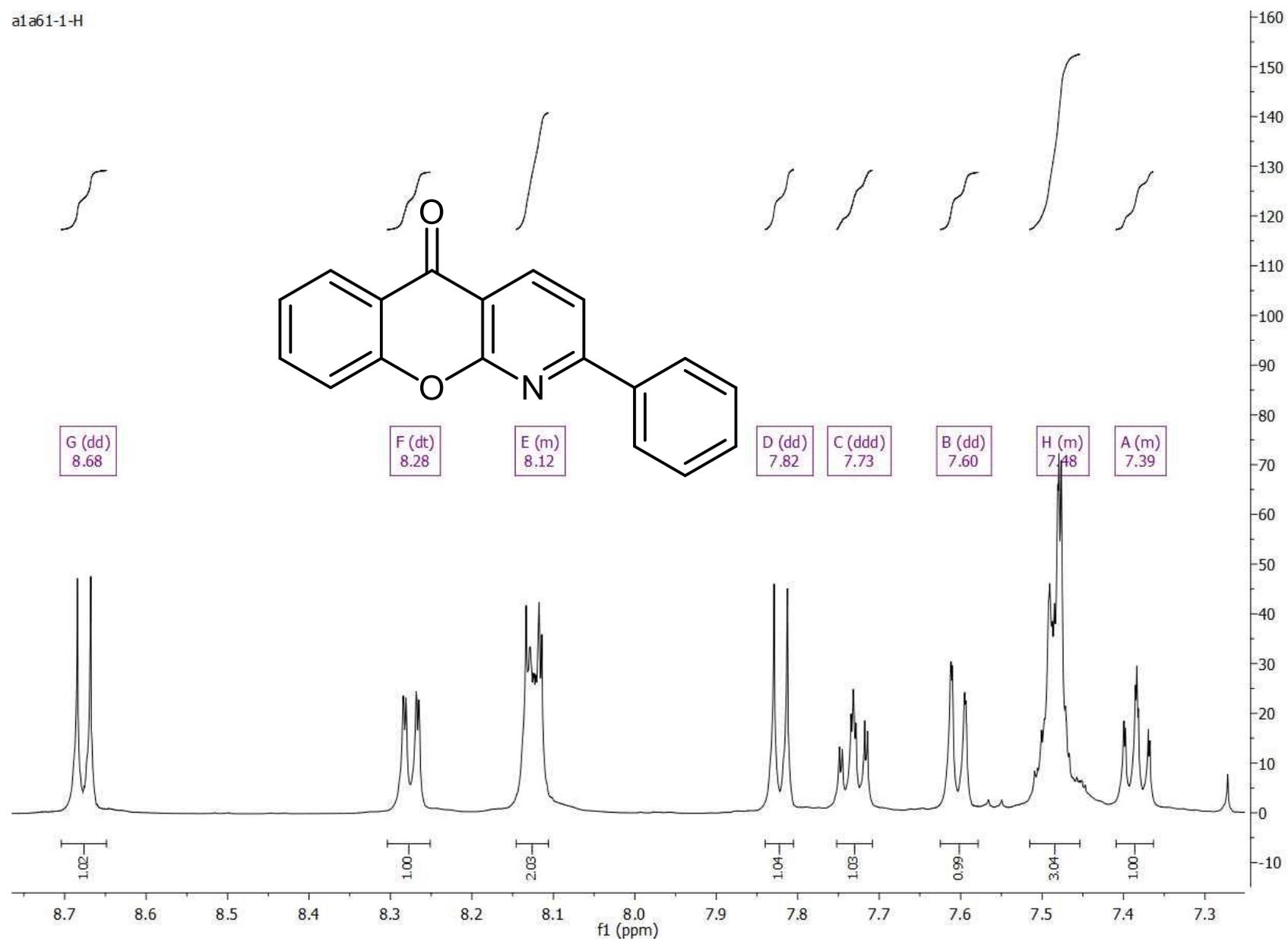


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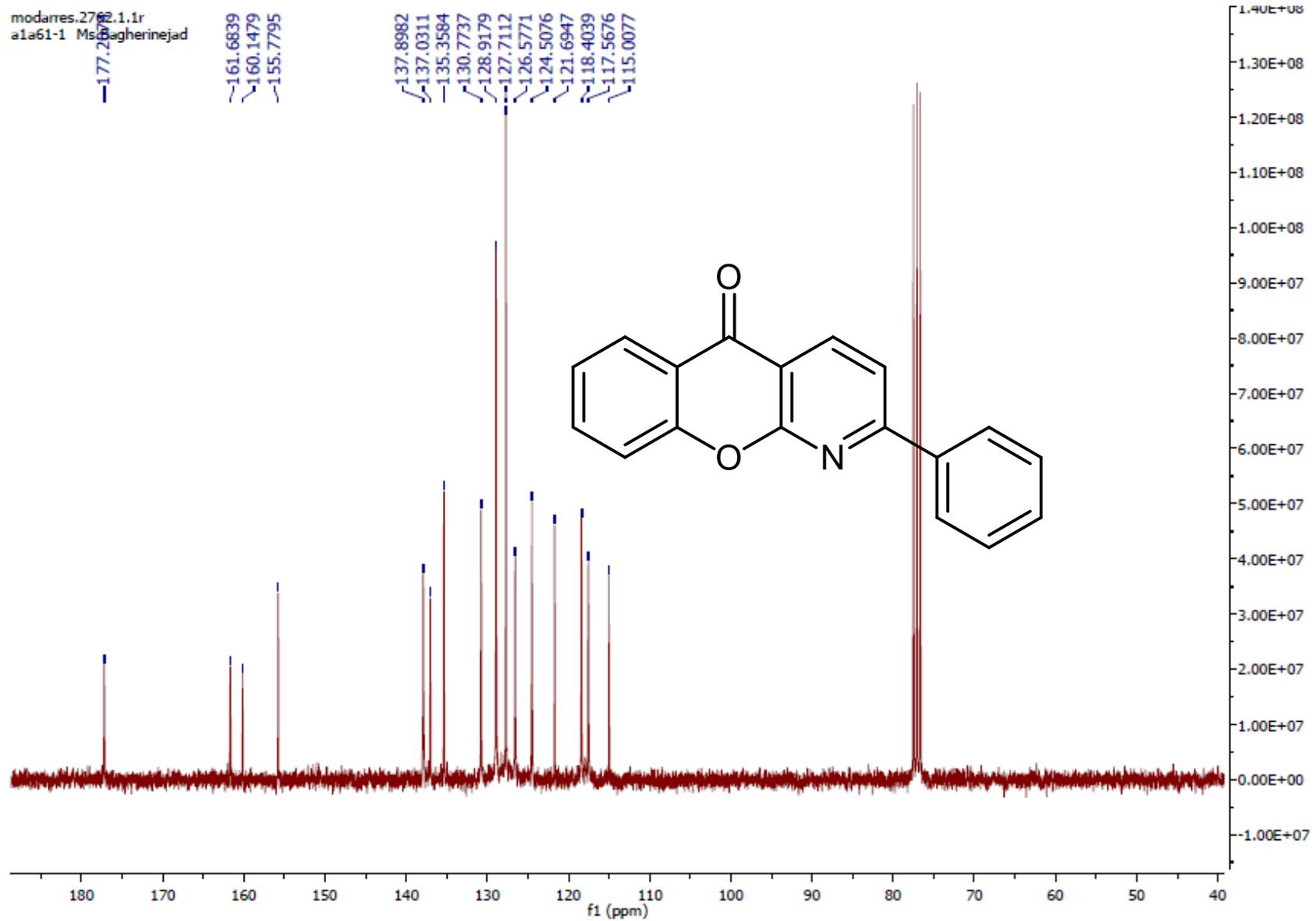
Mass of compound **3f**

a1a61-1-H

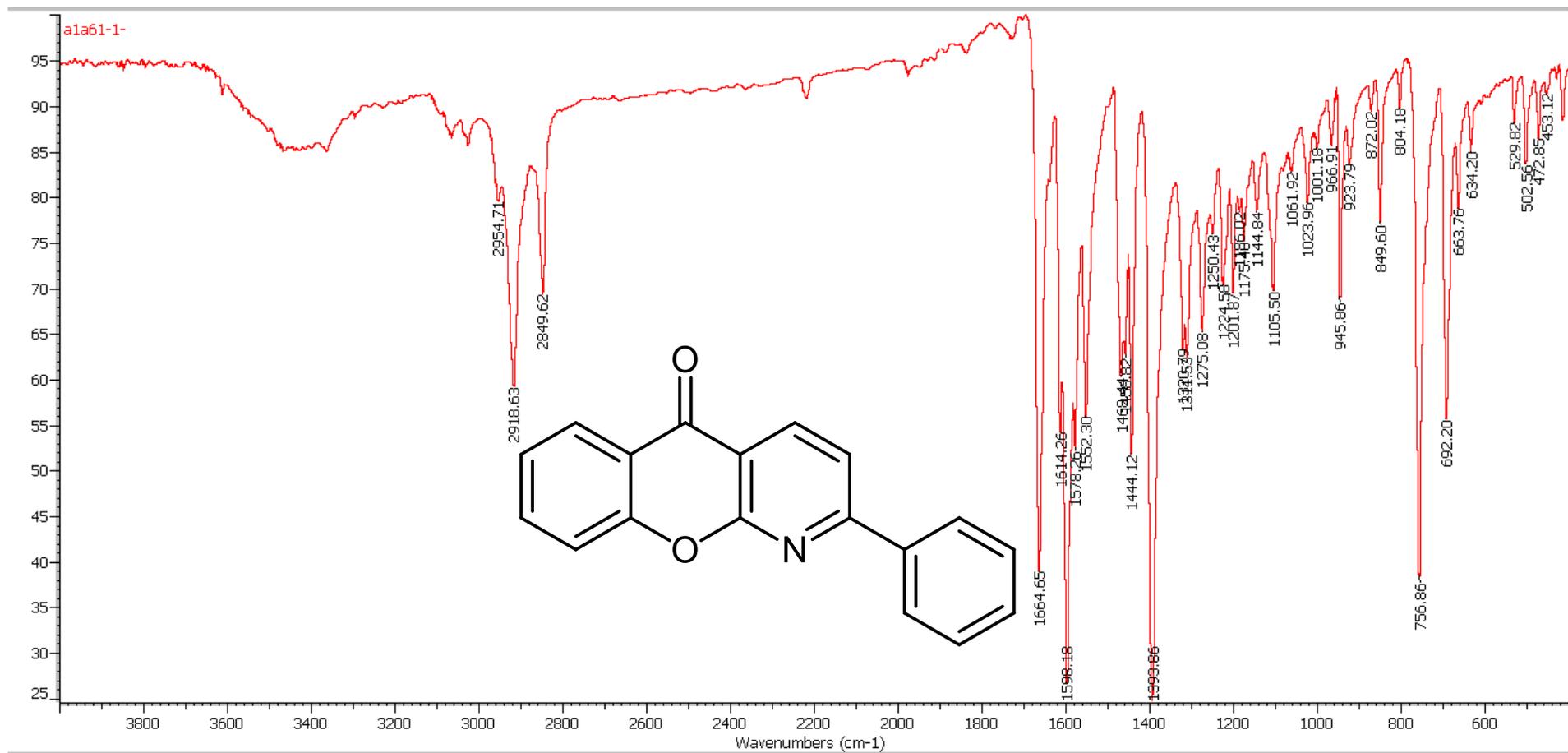


<sup>1</sup>H NMR of 4a

modarres.2762.1.1r  
a1a61-1 Ms Bagherinejad



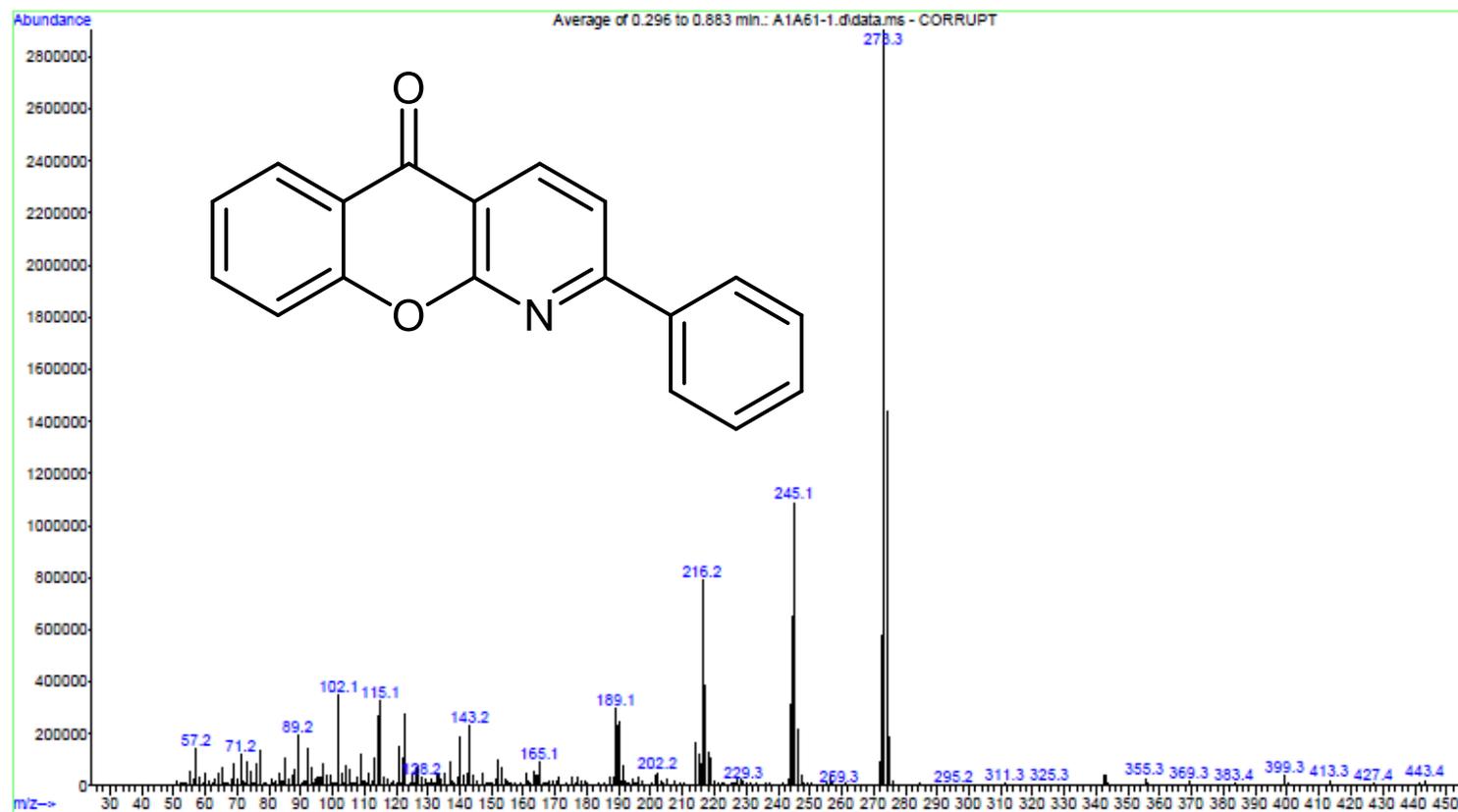
$^{13}\text{C}$  NMR of **4a**



IR of 4a



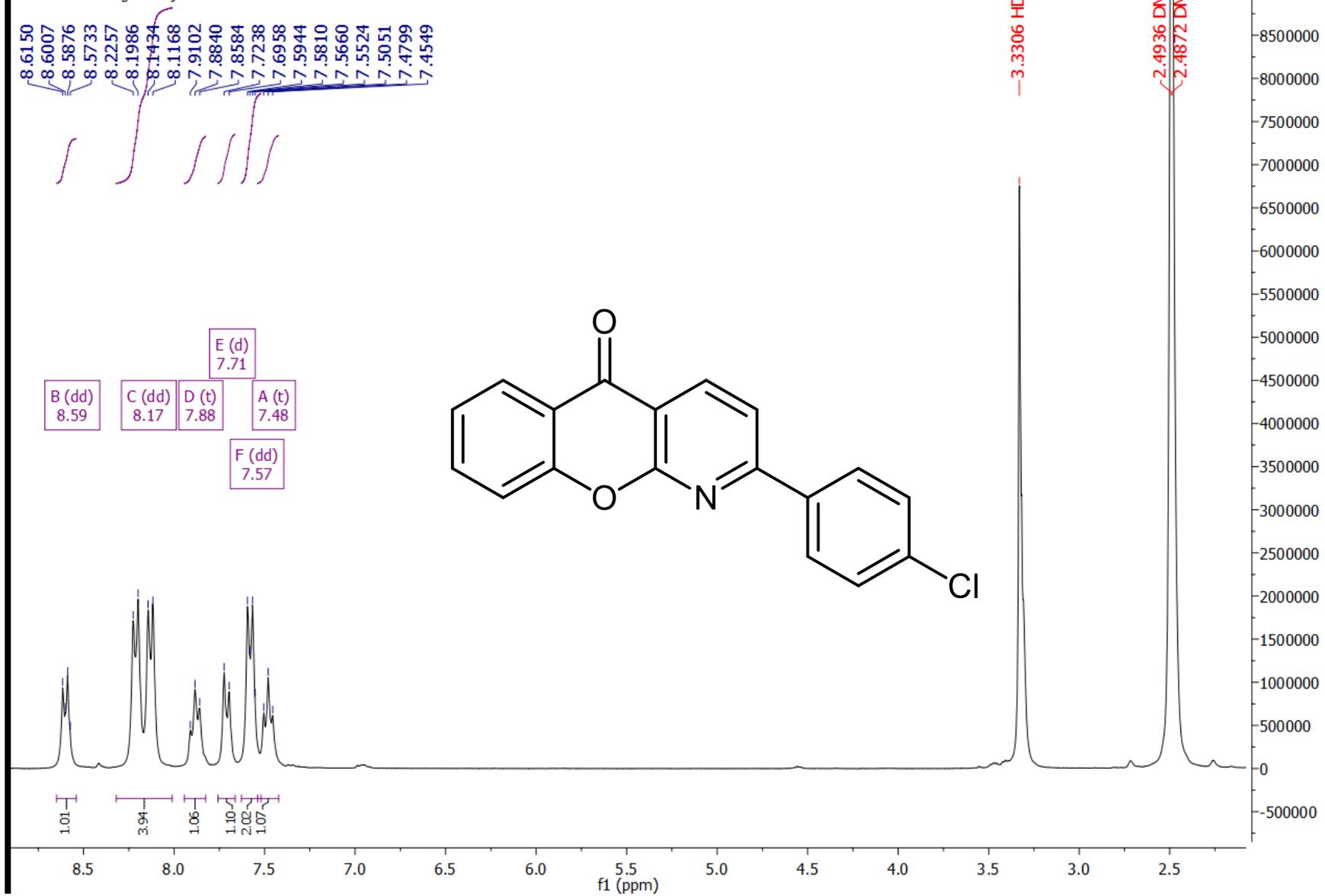
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Mass of compound **4a**

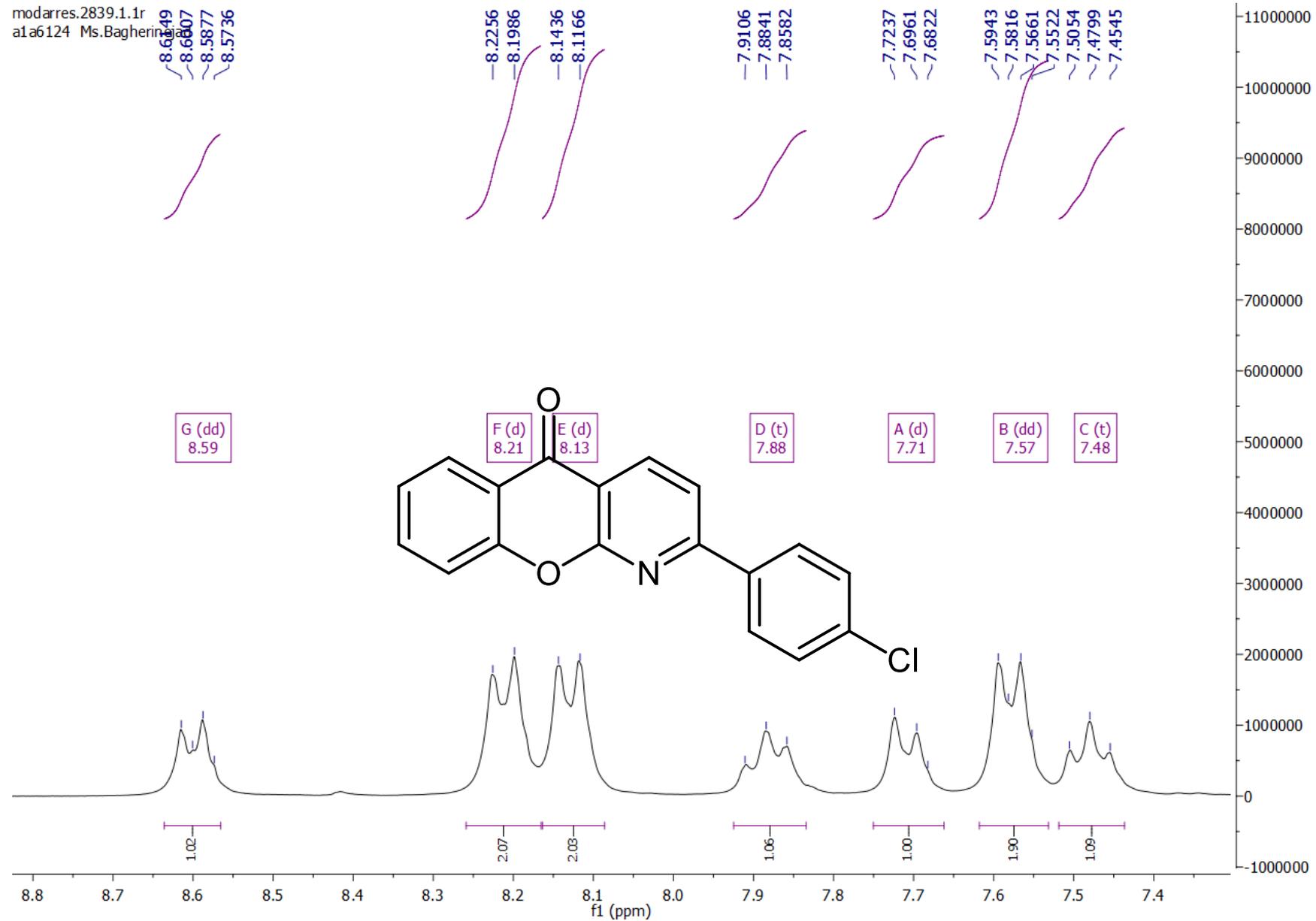
modarres.2839.1.1r

ala6124 Ms.Bagherinejad

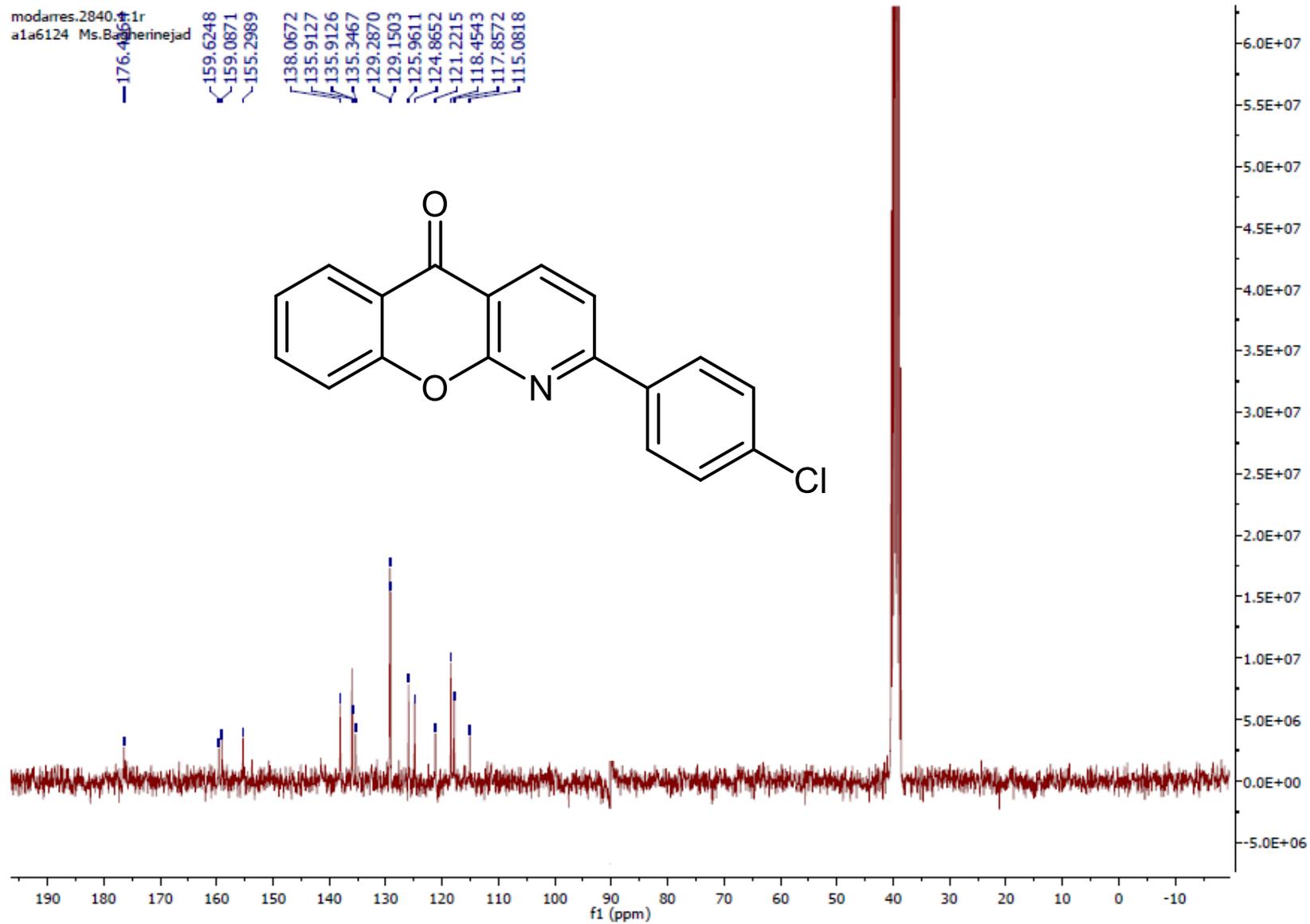


<sup>1</sup>H NMR of 4b

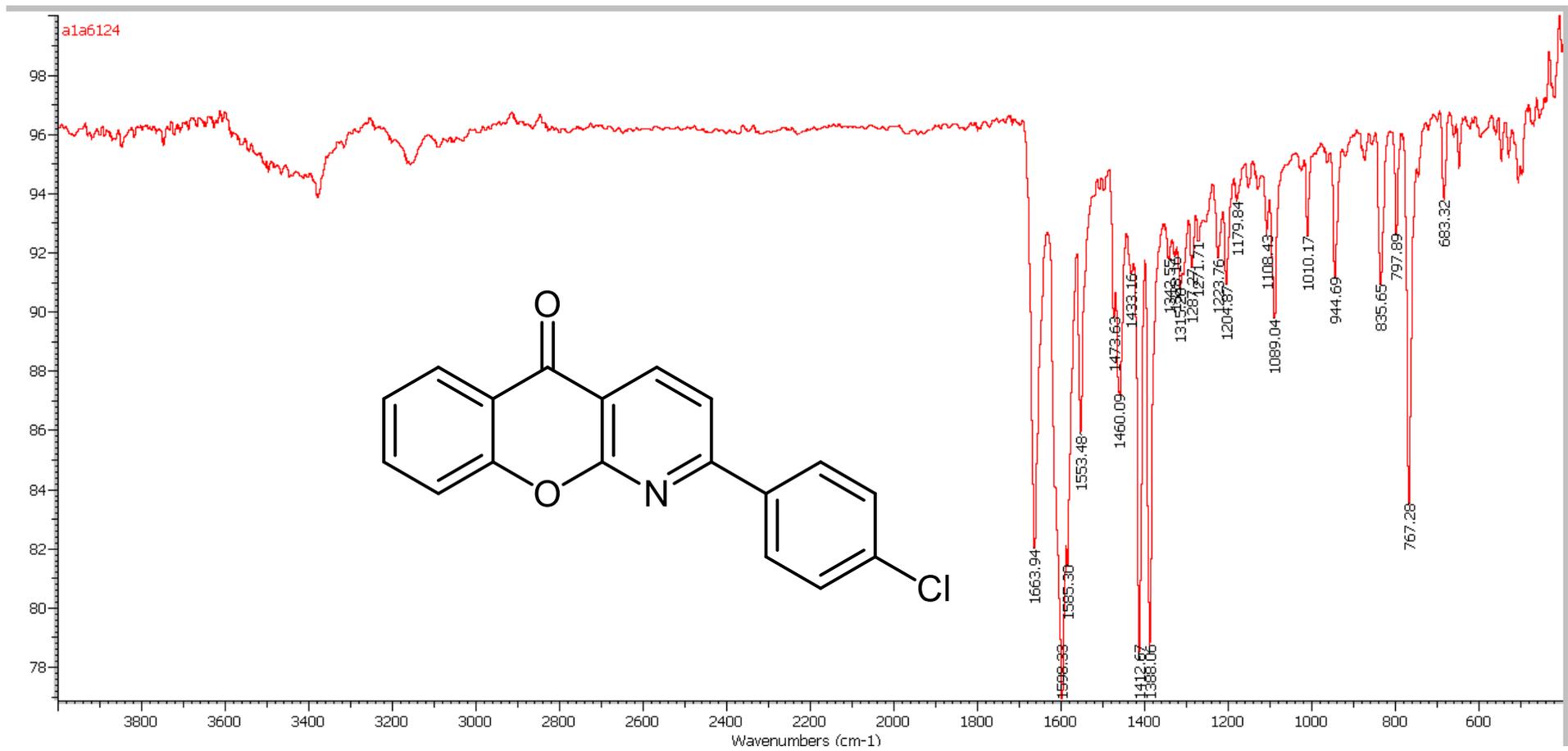
modarres.2839.1.1r  
a1a6124 Ms.Bagheri



<sup>1</sup>H NMR of 4b



$^{13}\text{C}$  NMR of **4b**



IR of **4b**



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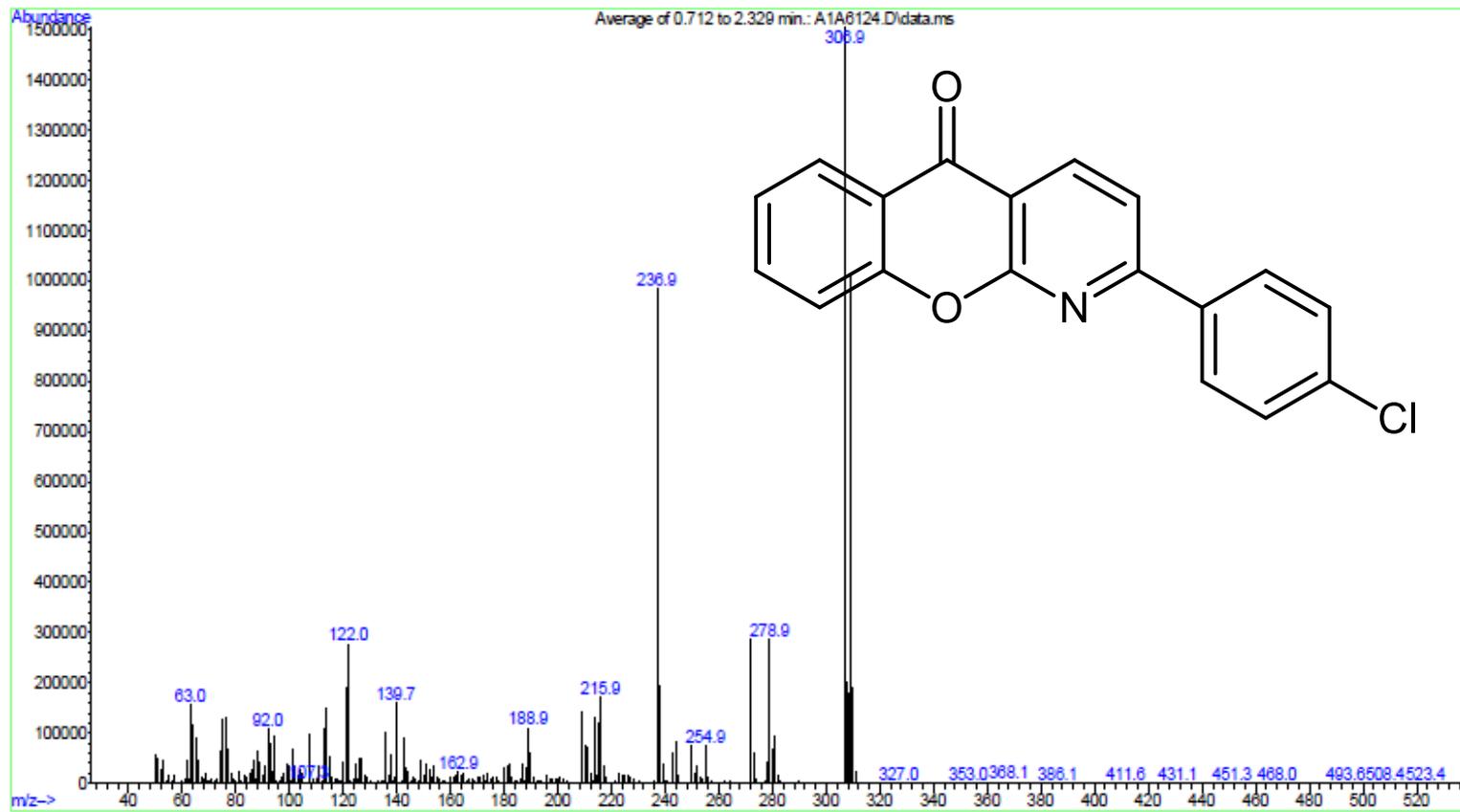
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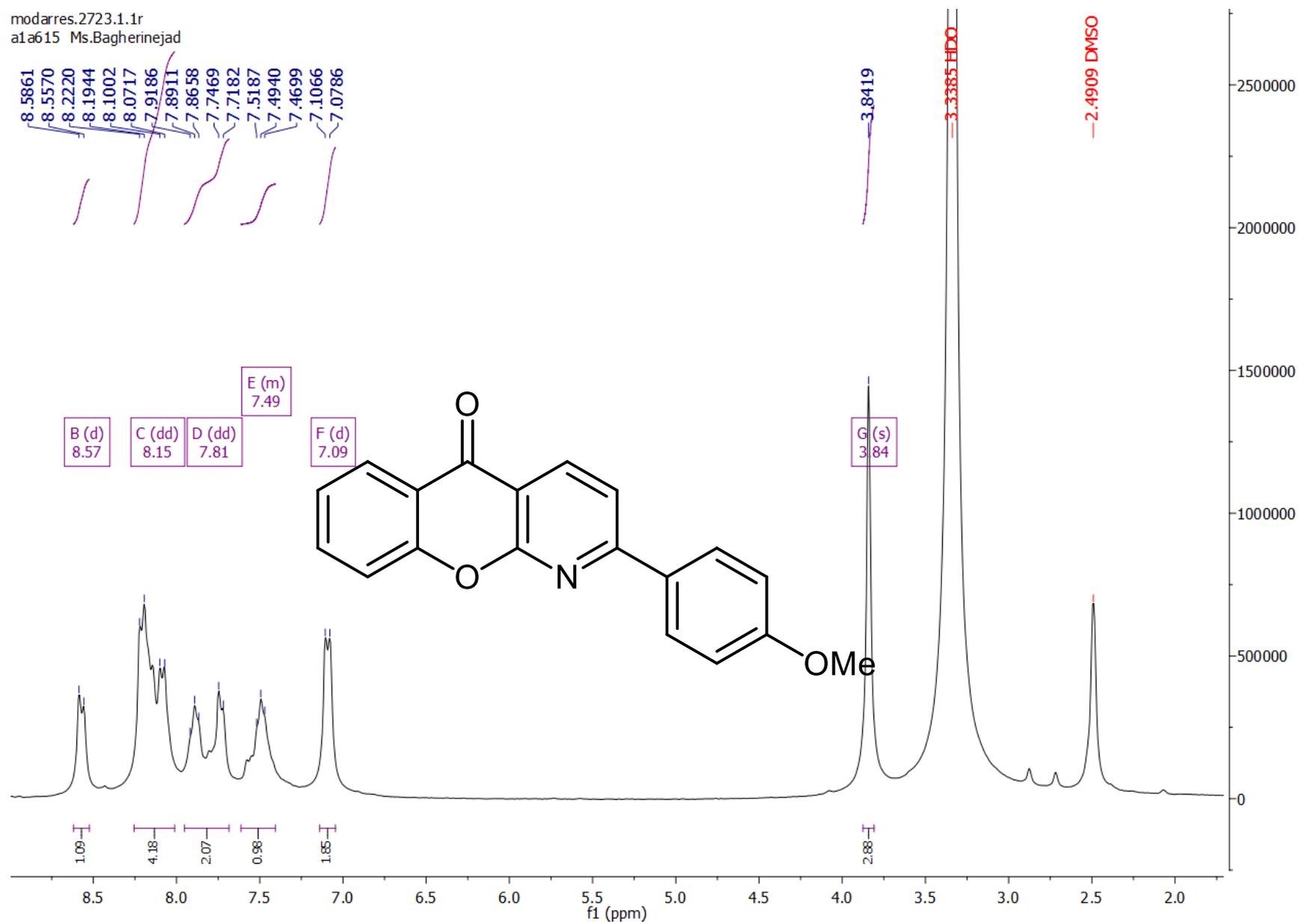
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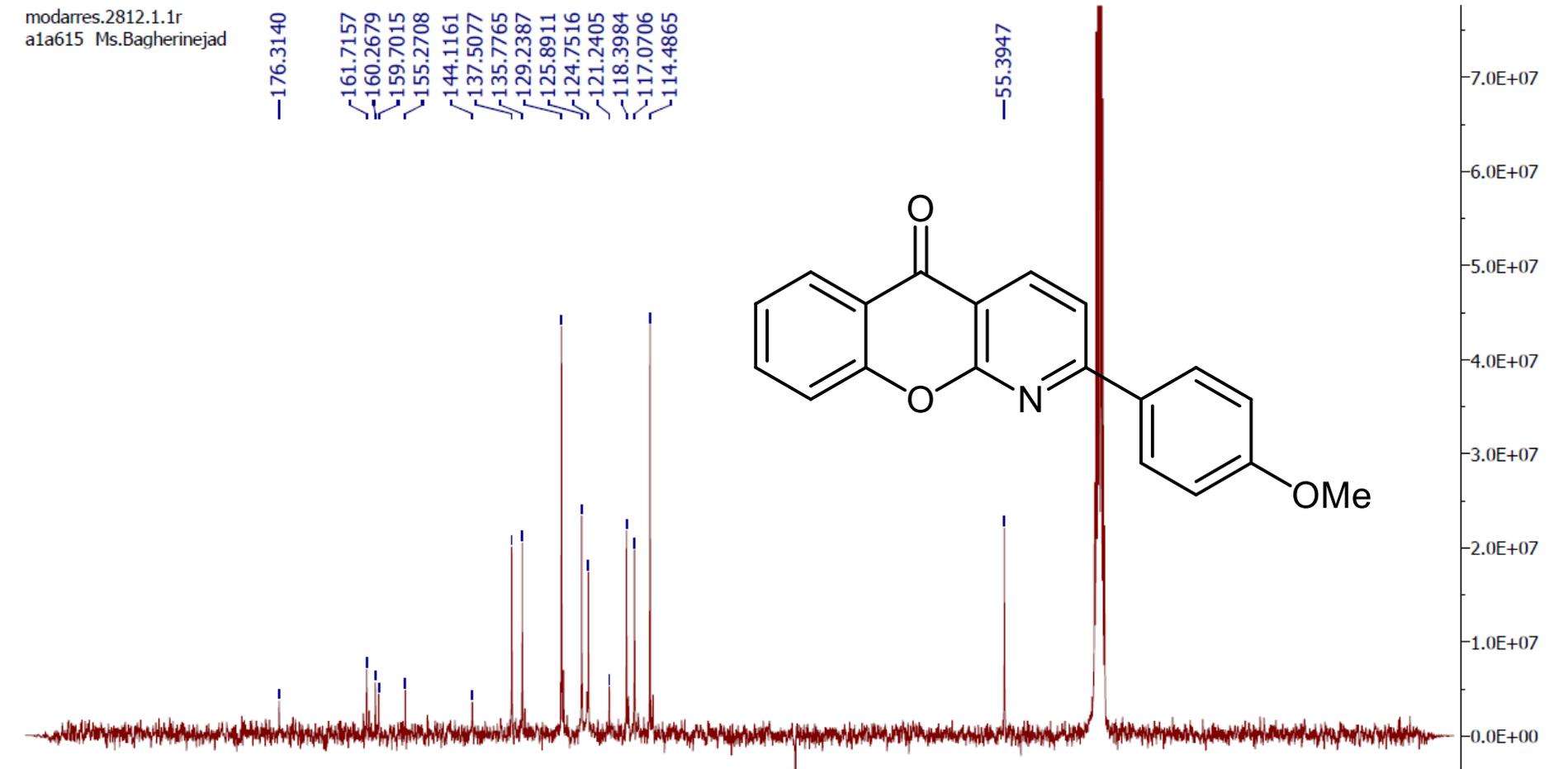
Mass of compound **4b**

modarres.2723.1.1r  
a1a615 Ms.Bagherinejad

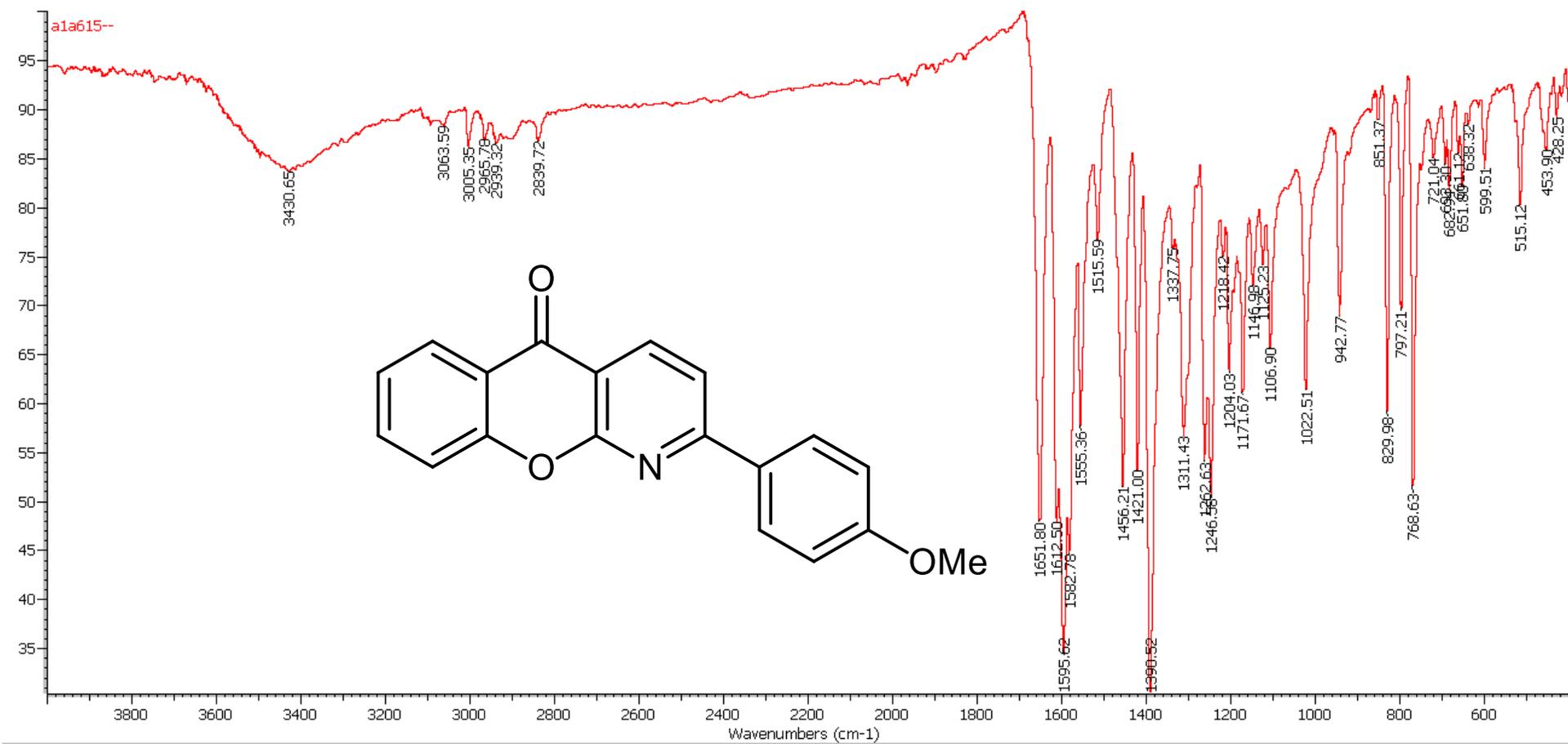


<sup>1</sup>H NMR of 4c

modarres.2812.1.1r  
a1a615 Ms.Bagherinejad



$^{13}\text{C}$  NMR of **4c**



IR of 4c



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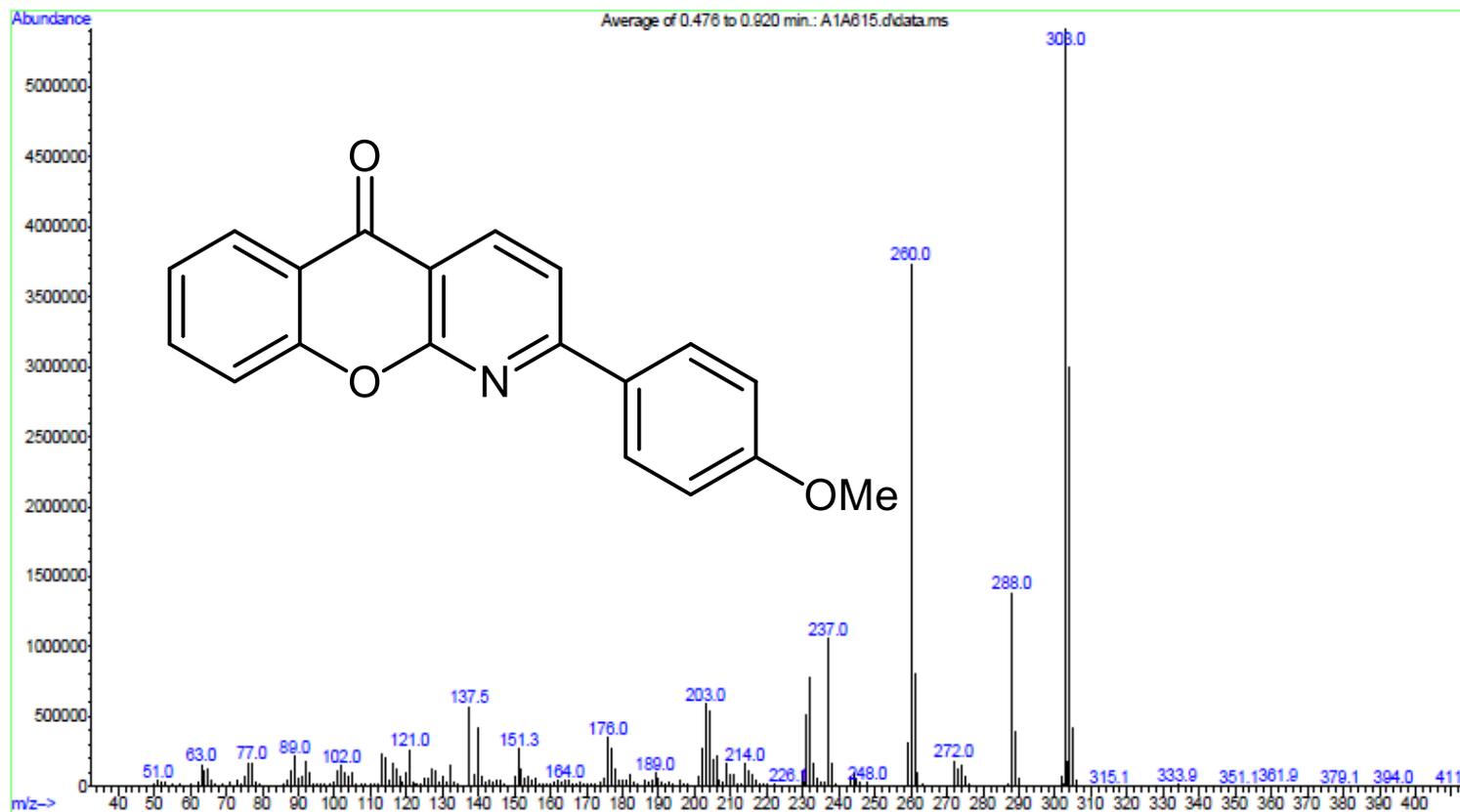
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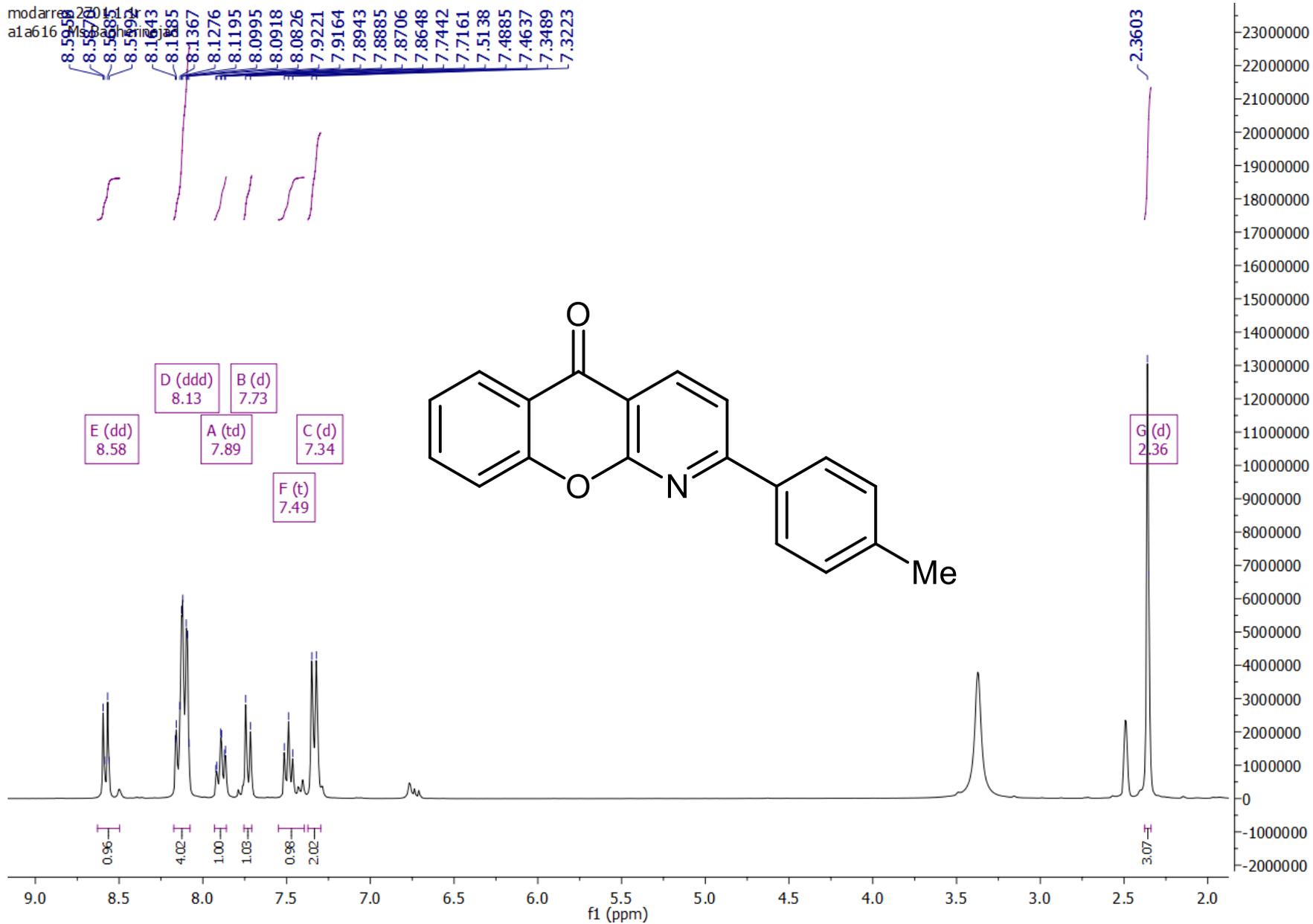
Sample Name:

Misc Info:

Vial Number: 1

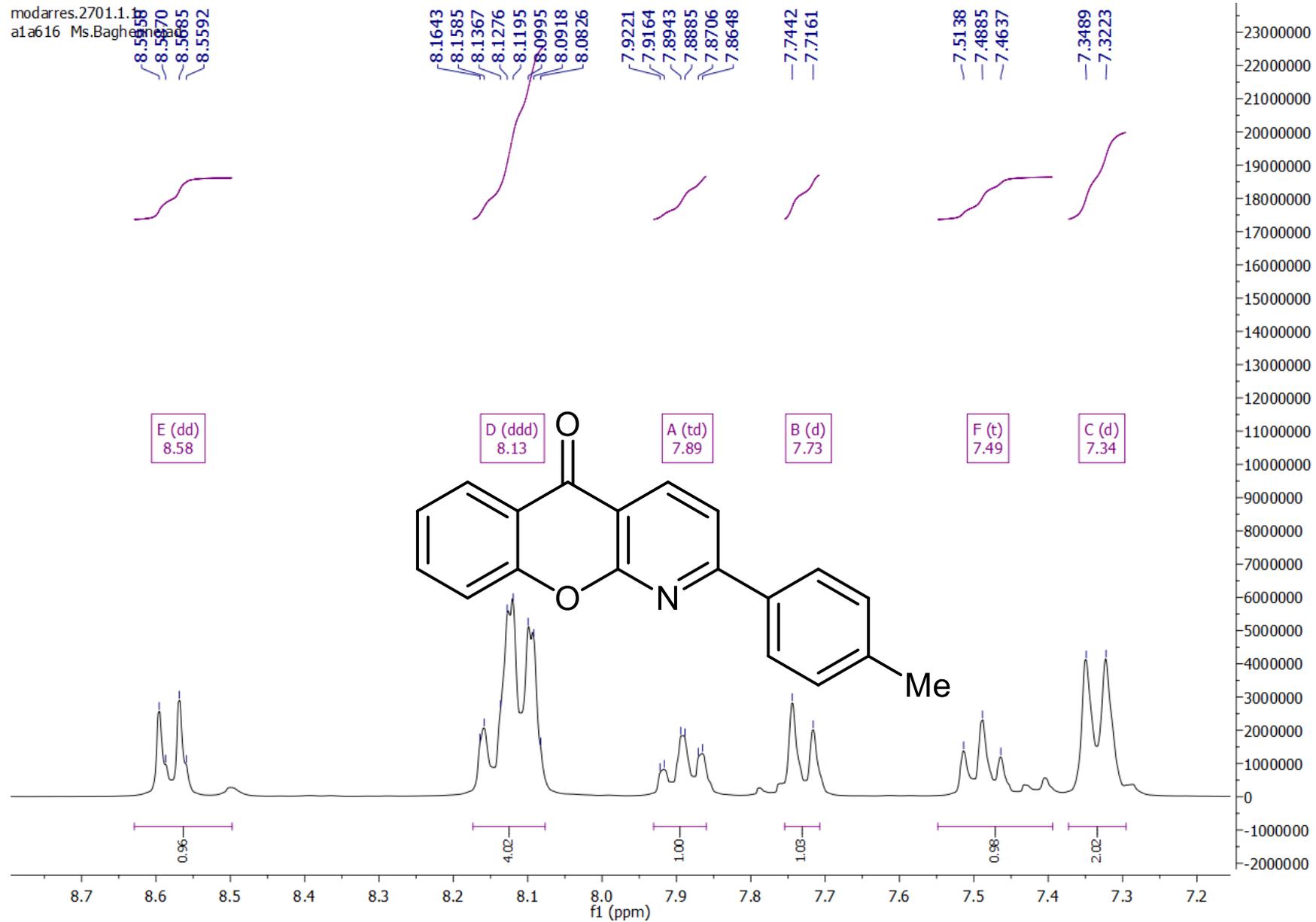


Mass of compound 4c



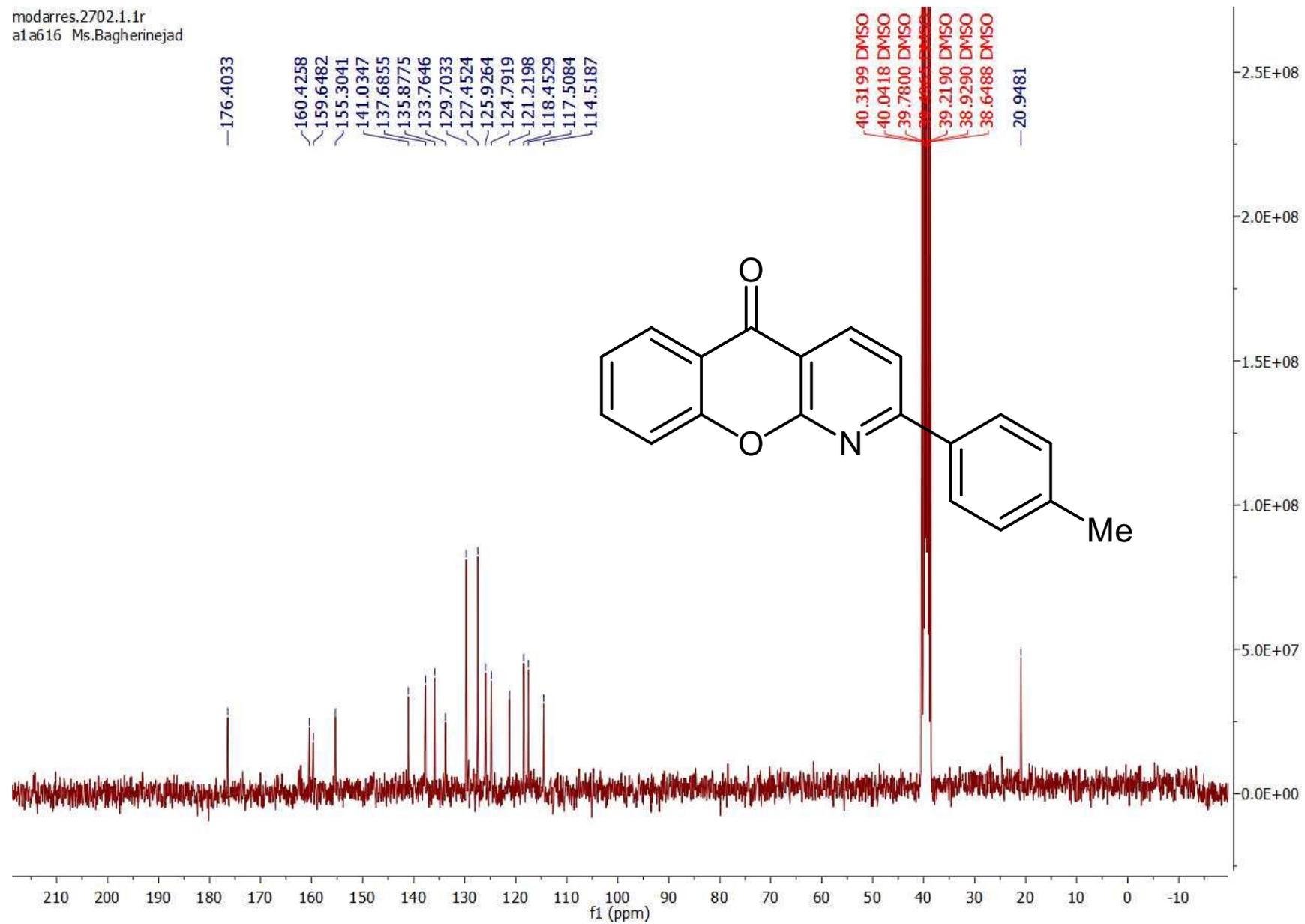
<sup>1</sup>H NMR of 4d

modarres.2701.1.  
a1a616 Ms.Baghe

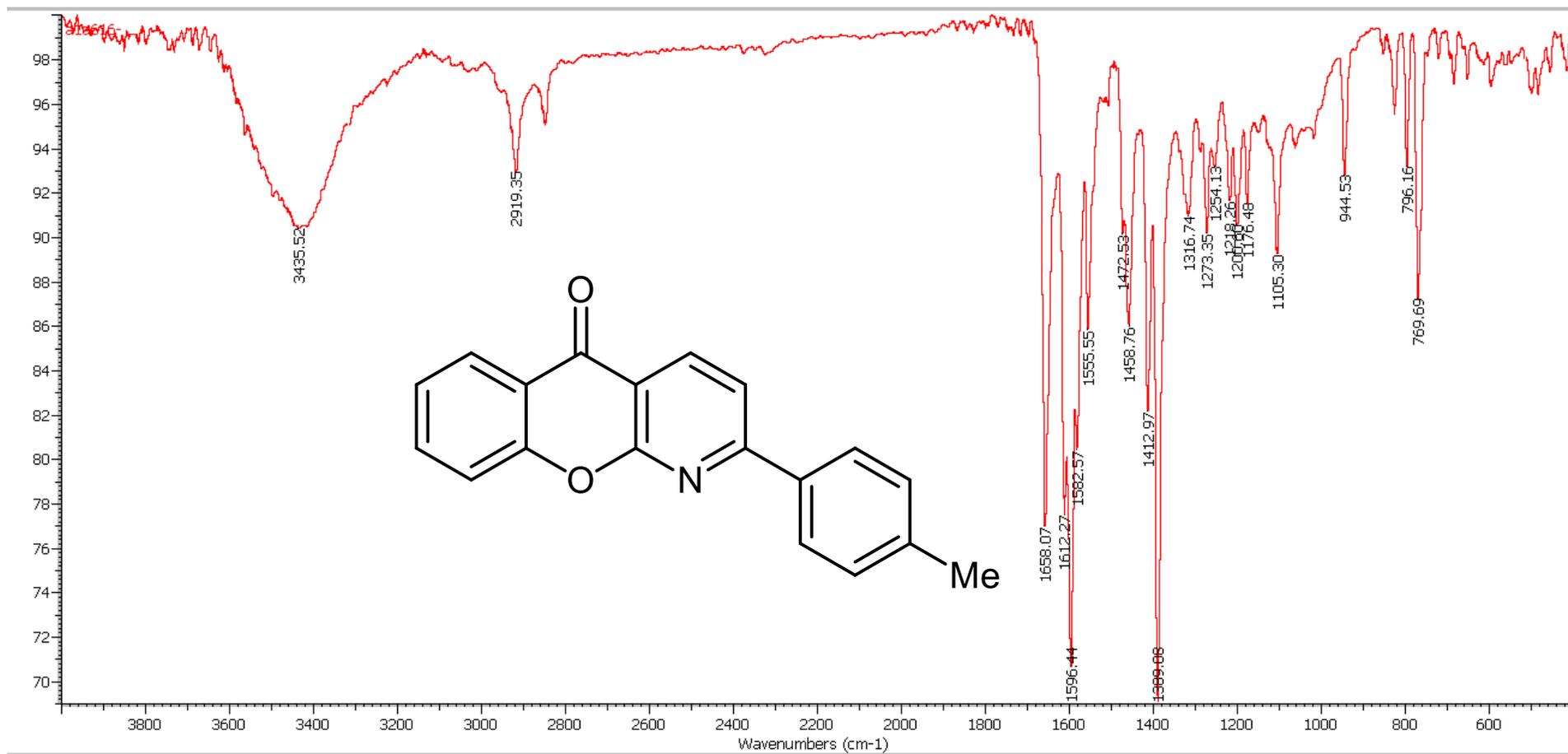


<sup>1</sup>H NMR of 4d

modarres.2702.1.1r  
a1a616 Ms.Bagherinejad



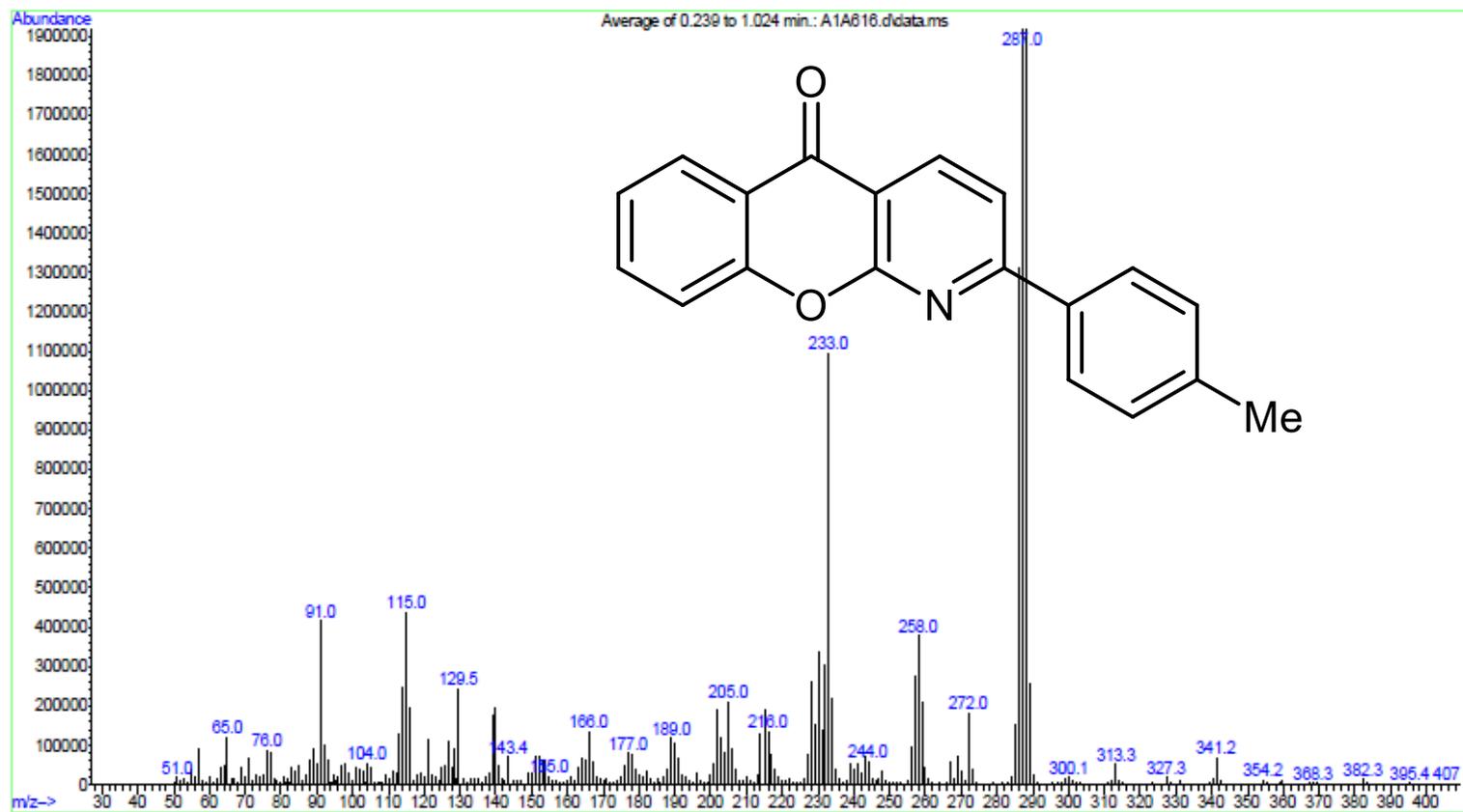
$^{13}\text{C}$  NMR of **4d**



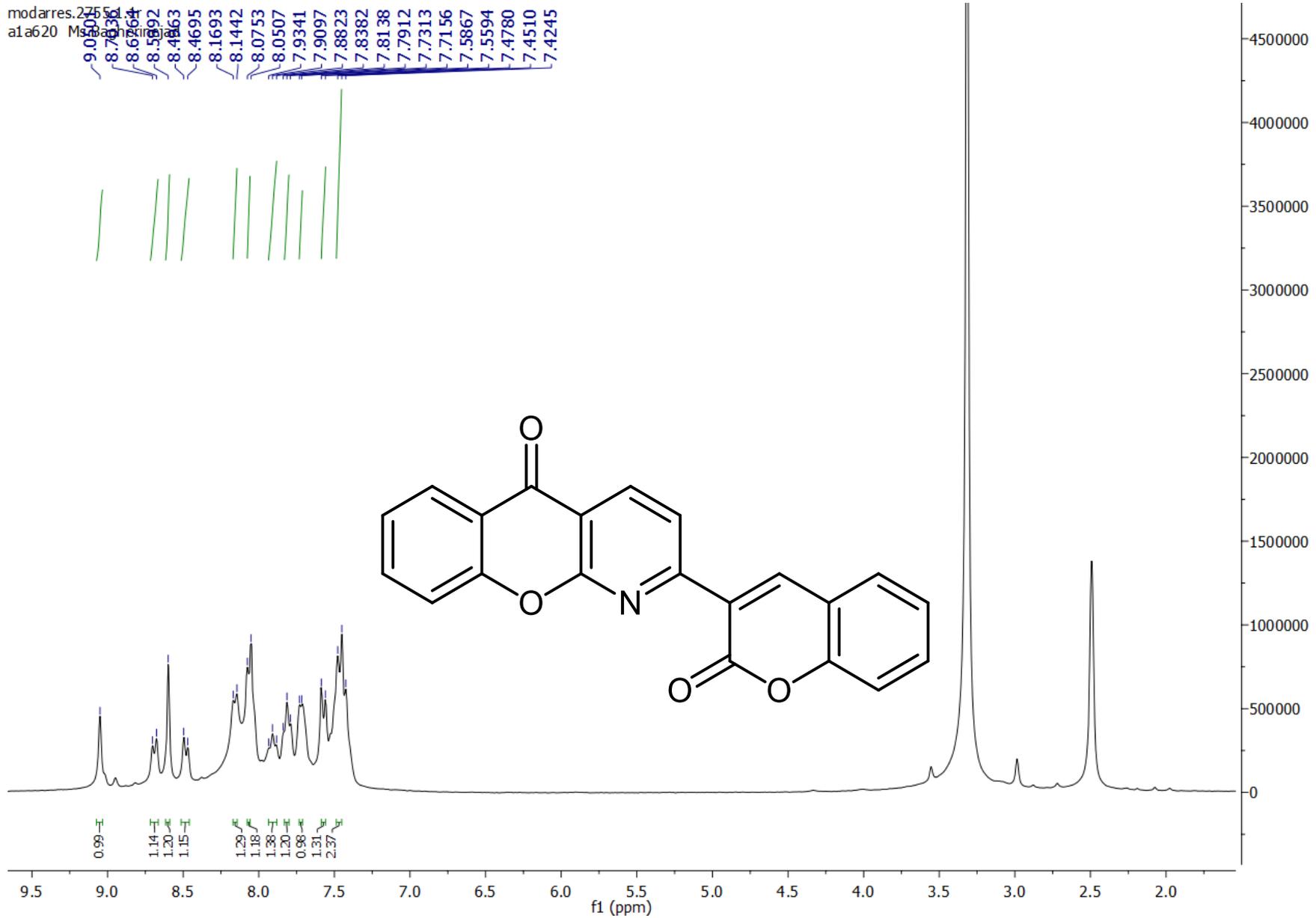
IR of **4d**



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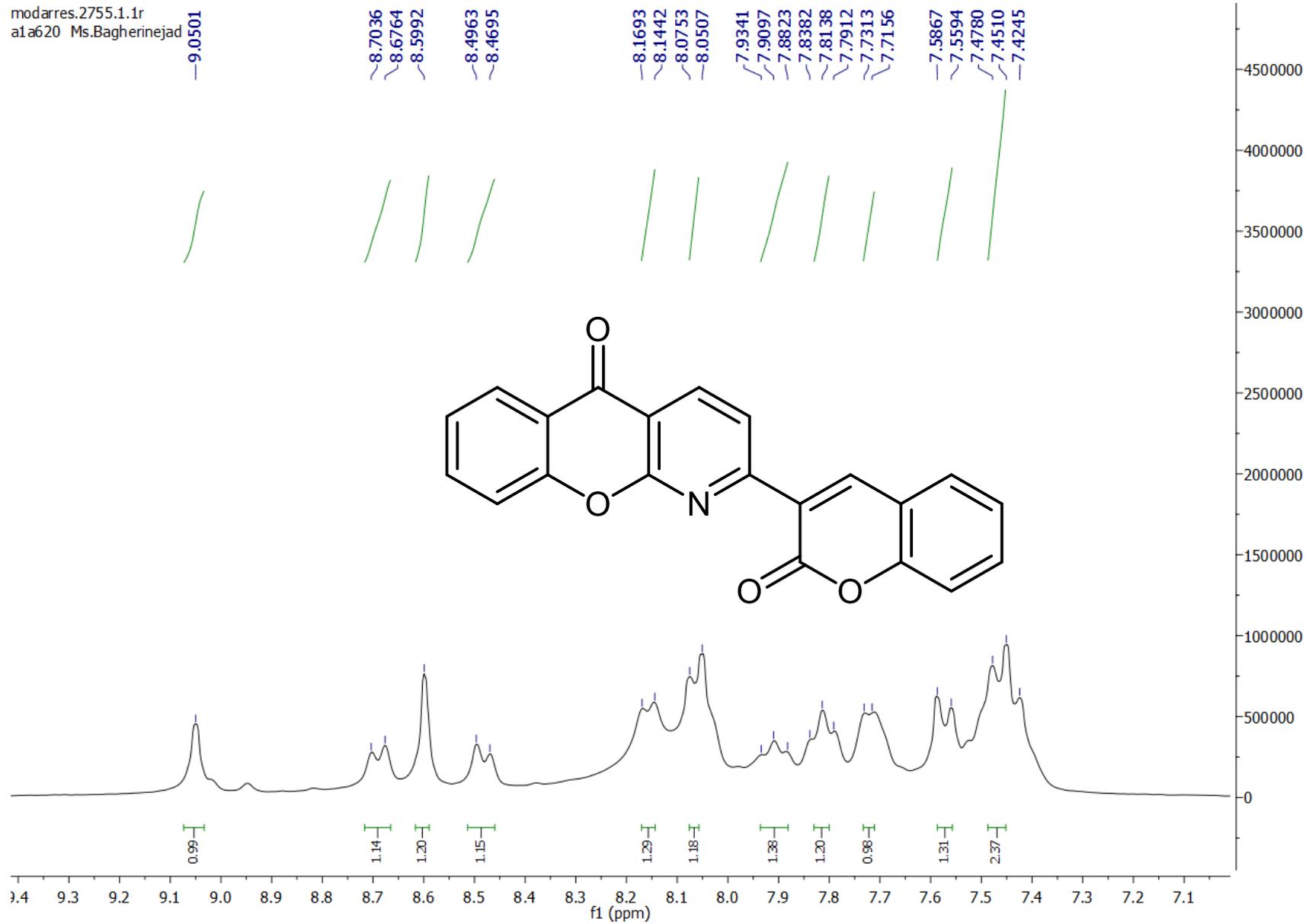


Mass of compound **4d**

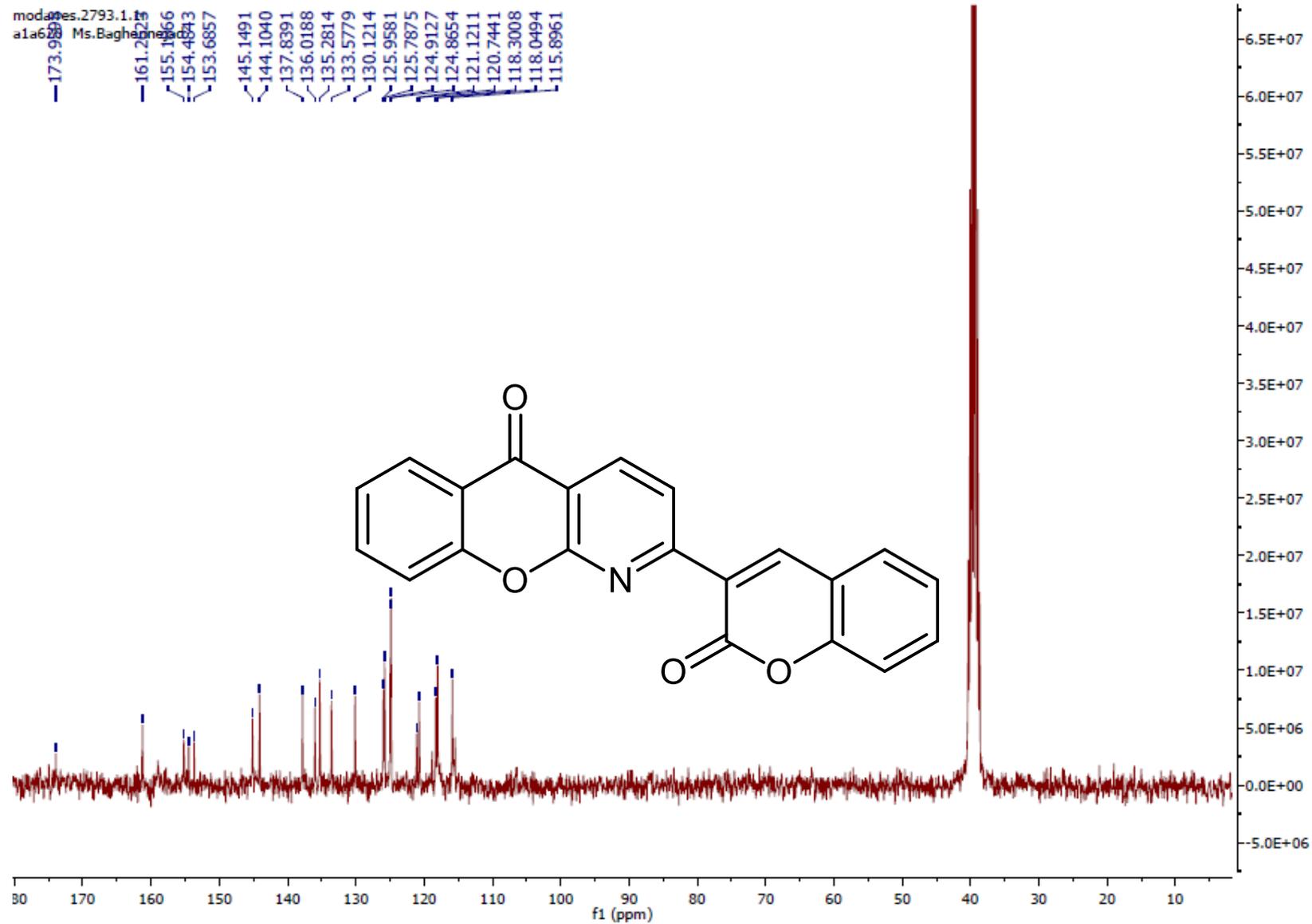


<sup>1</sup>H NMR of 4e

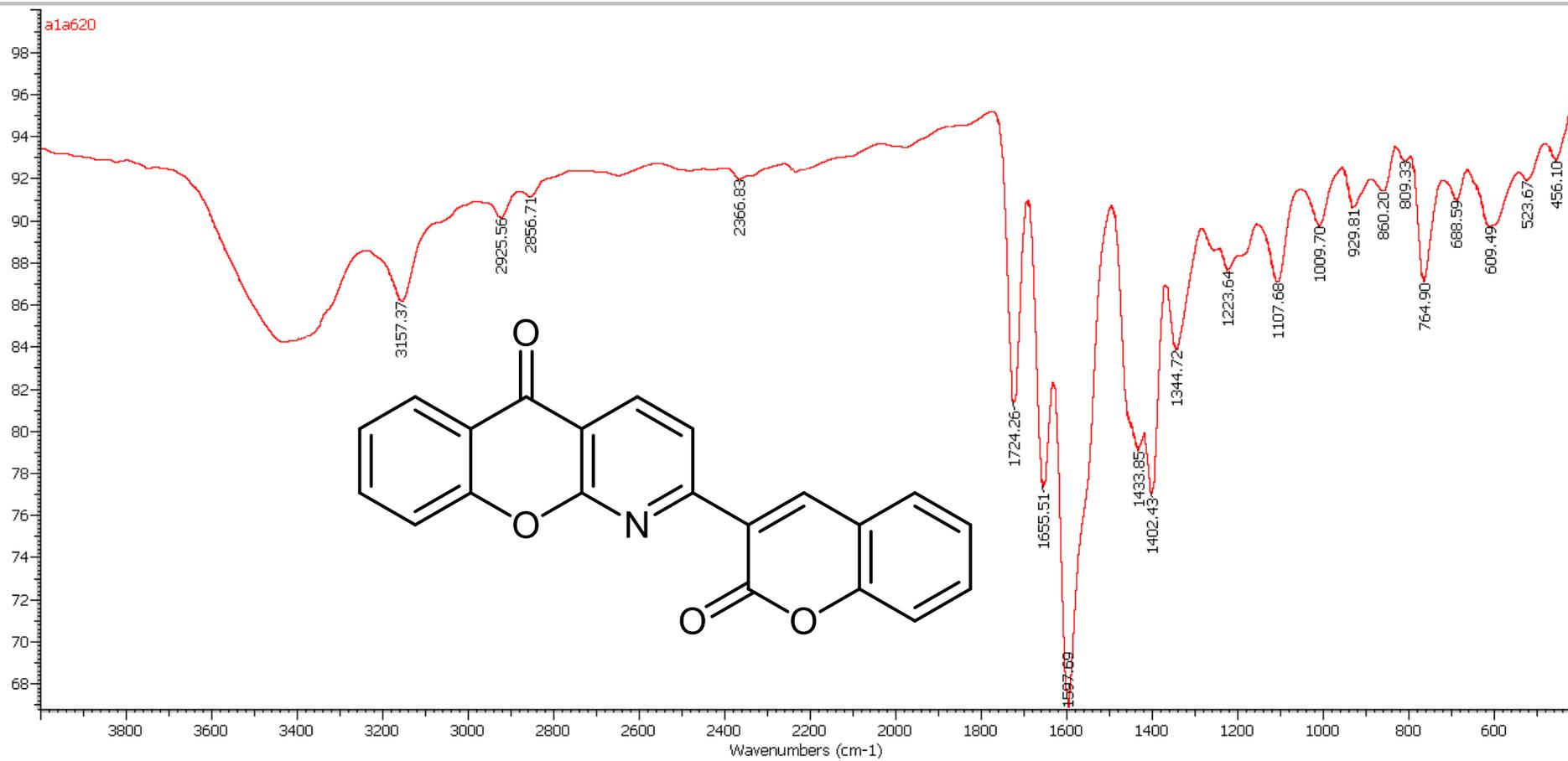
modarres.2755.1.1r  
a1a620 Ms.Bagherinejad



<sup>1</sup>H NMR of 4e



$^{13}\text{C}$  NMR of **4e**



IR of 4e



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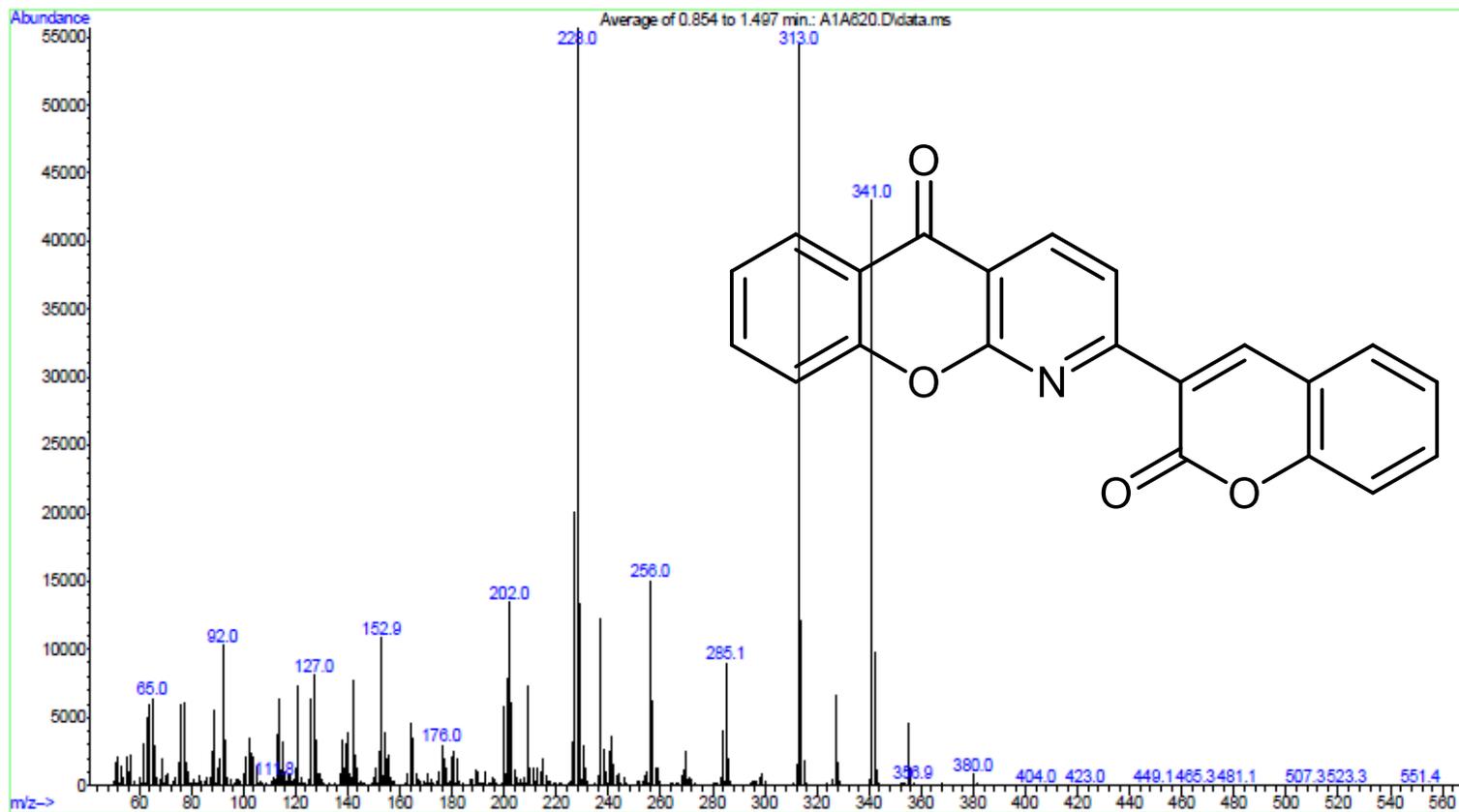
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Instrument: Direct Probe

Sample Name:

Misc Info:

Vial Number: 1



Mass of compound 4e