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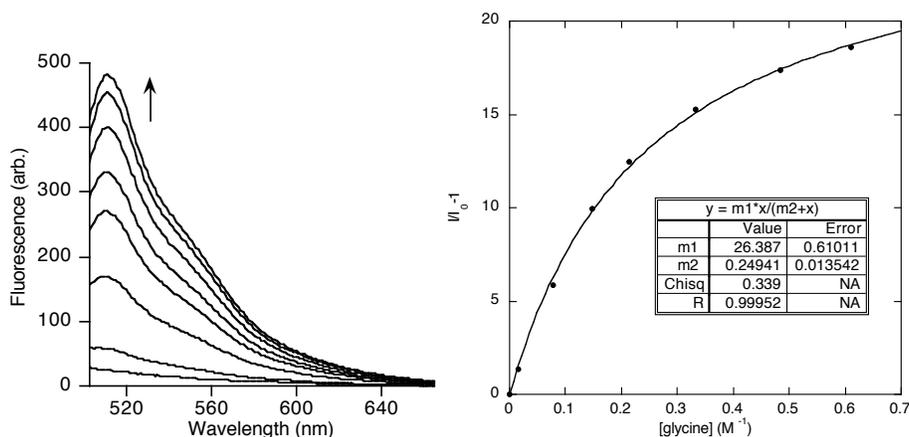
## Detection of Amines and Unprotected Amino Acids in Aqueous Conditions by Formation of Highly Fluorescent Iminium Ions

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### Titration methods

For UV/Vis and fluorescence assays, a  $10^{-5}$  M solution of the sensor was prepared in buffer solution (100 mM NaCl, 50 mM HEPES, adjusted to pH=7.4). This solution was placed in a cuvette (1 ml for UV/Vis and 2.5 ml for fluorescence) and the temperature adjusted to 37°C. The sample was then titrated with a solution of amino acid (1 M in 100 mM NaCl, 50 mM HEPES, adjusted to pH=7.4 with  $10^{-5}$  M sensor to prevent dilution). The change in absorbance or fluorescence was fit to a typical equilibrium model (see below)<sup>1</sup> to derive an equilibrium constant ( $K_{eq}=1/m2$ ). The maximum change in fluorescence was calculated from the theoretical fit at complete saturation ( $I_{max}/I_0=m1+1$ ).



NMR titrations were performed in  $D_2O$  with no buffer or NaCl. For compound **3**, 10 mg of aldehyde was dissolved in  $D_2O$  (1 ml) with a small amount of  $NaHCO_3$ . To this sample was added 100 mg of  $d_5$ -glycine. The subsequent NMR consisted of the aldehyde and imine only. The ratio of aldehyde and imine signals along with the known concentration of glycine were used to calculate a  $K_{eq} = 0.47 M^{-1}$ . For compound **4**, 4 mg of aldehyde was dissolved in  $D_2O$  (1 ml) with a small amount of DCl such that the pD = 7.0. To this sample was added 100 mg of  $d_5$ -glycine. The subsequent NMR consisted of the aldehyde and imine only. The ratio of aldehyde and imine signals along with the known concentration of glycine were used to calculate a  $K_{eq} = 0.29 M^{-1}$ .

## Synthetic Procedures

### Compound 1b:

A suspension of CuI (0.3 g, 1.8 mmol) and Et<sub>2</sub>O (15 mL) was cooled to 0°C and n-BuLi (1.7 mL, 3.4 mmol, 2 M in pentane) was slowly added. After 20 min, the resultant blue solution was cooled to -78°C and THF (15 mL) was added. 4-Chloro-7-diethylamino-3-formylcoumarin<sup>2</sup> (0.5 g, 1.8 mmol) in THF (8 mL) was added dropwise over 10 min. The reaction was stirred at -78°C for 10 min and then quenched with saturated NH<sub>4</sub>Cl. The aqueous layer was extracted with CH<sub>2</sub>Cl<sub>2</sub> (3 x 50 mL). The organic layer was then dried over MgSO<sub>4</sub> and the solvent was removed *in vacuo*. Flash chromatography (EtOAc/Hex, 20:80) gave compound **1b** as an orange solid (0.4 g, 78% yield), M.P. 69-72°C.

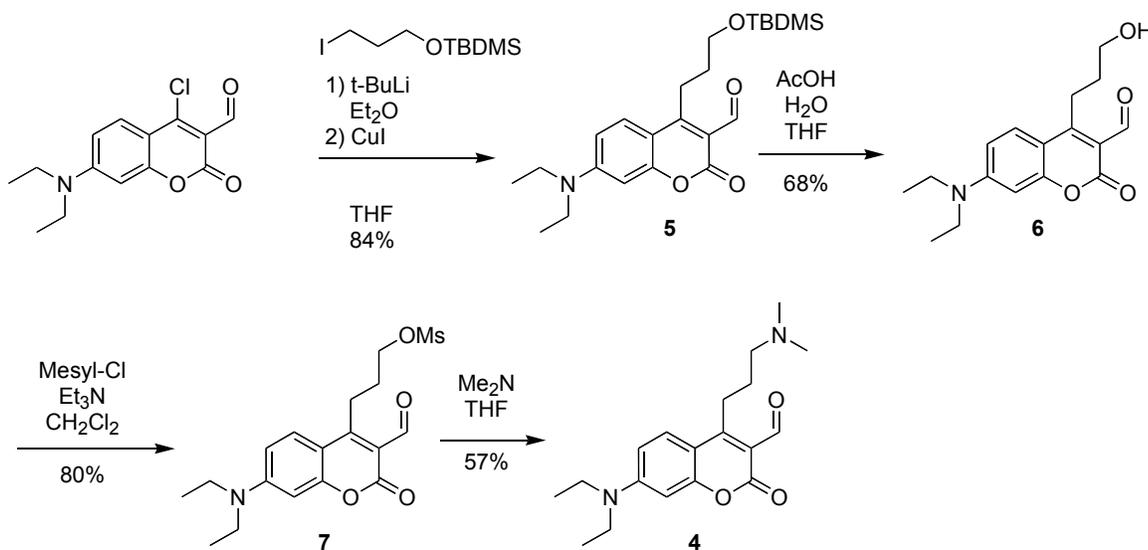
<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>);  $\delta$  0.99 (t, *J* = 7.0 Hz, 3H), 1.24 (t, *J* = 7.1 Hz, 6H), 1.49-1.60 (m, 4H), 3.26 (t, *J* = 7.9 Hz, 2H), 3.46 (q, *J* = 7.1 Hz, 4H), 6.48 (d, *J* = 2.6 Hz, 1H), 6.65 (dd, *J* = 2.6, 9.3 Hz, 1H), 7.62 (d, *J* = 9.3 Hz, 1H), 10.37 (s, 1H).

<sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>);  $\delta$  12.5, 13.8, 23.3, 27.5, 32.6, 45.0, 97.3, 108.5, 109.8, 111.7, 128.5, 152.5, 157.5, 163.2, 164.1, 164.2, 190.8.

FTIR (neat) 1708, 1672, 1608, 1555, 1502, 1443, 1349, 1267, 1202, 1149, 1114 cm<sup>-1</sup>.

HRMS Calculated for C<sub>18</sub>H<sub>24</sub>NO<sub>3</sub> (M + H<sup>+</sup>): 302.1756. Found: 302.1751.

### Compound 4:



(*tert*-Butyl-dimethylsilyl)-3-iodo-propanol<sup>3</sup> (0.4 g, 1.4 mmol) and Et<sub>2</sub>O (15 mL) were cooled to  $-78^{\circ}\text{C}$  and *tert*-BuLi (1.8 mL, 3.0 mmol, 1.6 M in pentane) was slowly added. The mixture was stirred at  $-78^{\circ}\text{C}$  for 5 min then warmed to ambient temperature and stirred 1 h. After cooling to  $0^{\circ}\text{C}$ , CuI (0.14 g, 0.7 mmol) was added and stirred 10 min. The reaction was cooled to  $-78^{\circ}\text{C}$  and THF was added (8 mL). 4-Chloro-7-diethylamino-3-formylcoumarin (0.2 g, 1.4 mmol) in THF (6 mL) was added dropwise over 10 mins. The reaction was stirred 0.5 h at  $-78^{\circ}\text{C}$  and then quenched with saturated NH<sub>4</sub>Cl. The aqueous layer was extracted with CH<sub>2</sub>Cl<sub>2</sub> (3 x 50 mL). The organic layer was then dried over MgSO<sub>4</sub> and the solvent was removed *in vacuo*. Flash chromatography (EtOAc/Hex, 20:80) gave compound **5** as an orange solid (0.2 g, 73% yield), M.P.  $98-100^{\circ}\text{C}$ .

<sup>1</sup>H NMR (360 MHz, CDCl<sub>3</sub>)  $\delta$  0.10 (s, 6H), 0.95 (s, 9H), 1.25 (t,  $J = 6.9$  Hz, 6H), 1.79-1.84 (m, 2H), 3.31-3.36 (m, 2H), 3.46 (q,  $J = 7.1$  Hz, 4H), 3.77 (t,  $J = 5.9$  Hz, 2H), 6.45 (d,  $J = 2.6$  Hz, 1H), 6.61 (dd,  $J = 2.6, 9.3$  Hz, 1H), 7.75 (d,  $J = 9.3$  Hz, 1H), 10.34 (s, 1H).

<sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>)  $\delta$  -5.3, 12.5, 18.3, 24.5, 25.9, 33.2, 45.0, 62.7, 97.2, 108.6, 109.8, 111.8, 129.0, 152.6, 157.5, 163.1, 164.0, 190.8.

FTIR (neat) 2928, 1788, 1678, 1615, 1561, 1510, 1458, 1355, 1269, 1204, 1148, 1098 cm<sup>-1</sup>.

HRMS Calculated for C<sub>23</sub>H<sub>36</sub>NO<sub>4</sub>Si (M + H<sup>+</sup>): 418.2414. Found: 418.2408.

Compound **5** (0.2 g, 0.5 mmol) was dissolved in a solution of AcOH: H<sub>2</sub>O: THF (3:1:1) and stirred at ambient temperature for 4 h. The reaction was carefully poured over saturated NaHCO<sub>3</sub> and the aqueous layer was extracted with CH<sub>2</sub>Cl<sub>2</sub> (3 x 15 mL). The organic layer was dried over MgSO<sub>4</sub> and the solvent was removed *in vacuo*. The resulting residue was purified via flash chromatography (EtOAc/Hex, 50:50) and compound **6** was isolated as an orange solid (0.9 g, 62% yield), M.P.  $122-125^{\circ}\text{C}$ .

<sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>)  $\delta$  1.25 (t,  $J = 7.1$  Hz, 6H), 1.85-1.94 (m, 2H), 3.37 (t,  $J = 7.6$  Hz, 2H), 3.46 (q,  $J = 7.1$  Hz, 4H), 3.74 (t,  $J = 5.6$  Hz, 2H), 6.45 (d,  $J = 2.4$  Hz, 1H), 6.66 (dd,  $J = 2.4, 9.3$  Hz, 1H), 7.69 (d,  $J = 9.3$  Hz, 1H), 10.34 (s, 1H).

<sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>)  $\delta$  12.4, 24.0, 33.1, 45.1, 61.6, 97.2, 108.4, 110.0, 111.9, 128.8, 152.8, 157.6, 163.0, 163.4, 191.6.

FTIR (neat) 3396, 2913, 1706, 1670, 1610, 1552, 1503, 1453, 1347, 1267, 1150, 1069 cm<sup>-1</sup>.

HRMS Calculated for C<sub>17</sub>H<sub>22</sub>NO<sub>4</sub> (M + H<sup>+</sup>): 304.1549. Found: 304.1543.

A solution of compound **6** (70 mg, 0.2 mmol), Et<sub>3</sub>N (40  $\mu$ L, 0.3 mmol), and CH<sub>2</sub>Cl<sub>2</sub> (3 mL) was stirred at 0°C. Methanesulfonyl chloride (20  $\mu$ L, 0.3 mmol) was added and the reaction was stirred at 0°C for 10 mins. The solvent was removed *in vacuo* and the resulting residue was purified using flash chromatography (EtOAc/Hex, 30:70) and compound **7** was isolated as a yellow solid (73 mg, 83% yield), M.P. 126-128°C.

**<sup>1</sup>H NMR** (300 MHz, CDCl<sub>3</sub>)  $\delta$  1.23 (t, *J* = 7.1 Hz, 6H), 2.01-2.10 (m, 2H), 3.08 (s, 3H), 3.30-3.39 (m, 2H), 3.46 (q, *J* = 7.1 Hz, 4H), 4.42 (t, *J* = 5.9 Hz, 2H), 6.50 (sd, *J* = 2.6 Hz, 1H), 6.68 (dd, *J* = 2.6, 9.3 Hz, 1H), 7.65 (d, *J* = 9.4 Hz, 1H), 10.34 (s, 1H).

**<sup>13</sup>C NMR** (75 MHz, CDCl<sub>3</sub>)  $\delta$  12.9, 24.6, 30.1, 37.9, 45.6, 70.5, 97.8, 108.7, 110.7, 112.1, 129.0, 153.4, 158.1, 162.0, 163.4, 191.4.

FTIR (neat) 2975, 1712, 1673, 1613, 1556, 1506, 1454, 1352, 1172 cm<sup>-1</sup>.

**HRMS** Calculated for C<sub>18</sub>H<sub>24</sub>NO<sub>6</sub>S (M + H<sup>+</sup>): 382.1324. Found: 382.1319.

In a 15 mL sealed tube, compound **7** (61 mg, 0.2 mmol) and Me<sub>2</sub>NH (5 mL, 2 M in THF) were capped and stirred at ambient temperature for 20 h. The solvent was removed *in vacuo*. The resulting residue was purified using flash chromatography (EtOAc/Et<sub>3</sub>N, 90:10) and compound **4** was isolated as an orange solid (32 mg, 57% yield), M.P. 119-121°C.

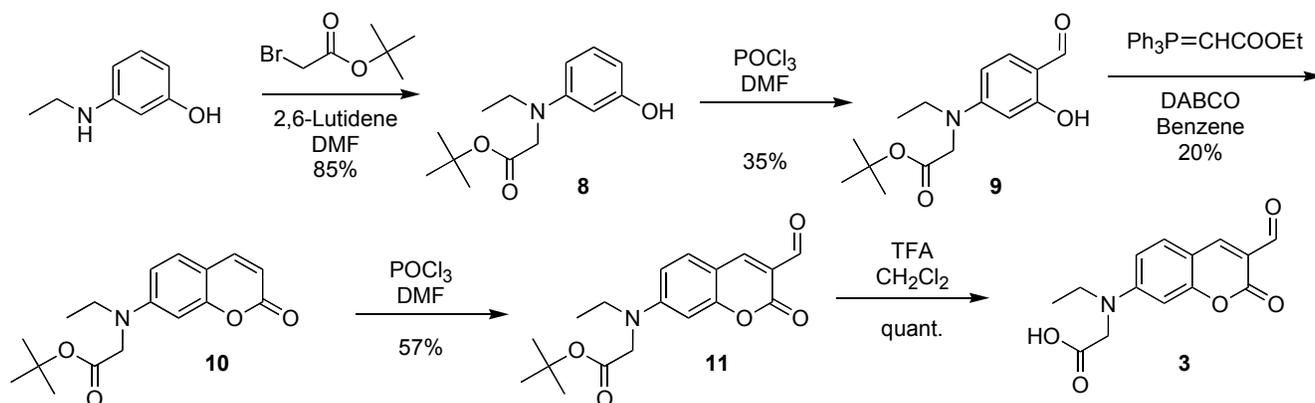
**<sup>1</sup>H NMR** (300 MHz, CDCl<sub>3</sub>)  $\delta$  1.25 (t, *J* = 7.1 Hz, 6H), 1.73 (m, 2H), 2.27 (s, 6H), 2.46 (t, *J* = 7.1 Hz, 2H), 3.29 (m, 2H), 3.46 (q, *J* = 7.1 Hz, 4H), 6.45 (d, *J* = 2.6 Hz, 1H), 6.64 (dd, *J* = 2.6, 9.3 Hz, 1H), 7.70 (d, *J* = 9.3 Hz, 1H), 10.36 (s, 1H).

**<sup>13</sup>C NMR** (75 MHz, CDCl<sub>3</sub>)  $\delta$  12.5, 25.7, 28.2, 45.0, 45.4, 59.4, 97.2, 108.6, 109.8, 111.7, 128.7, 152.6, 157.5, 163.1, 163.8, 190.8.

FTIR (neat) 2972, 1716, 1674, 1615, 1558, 1506, 1456, 1354, 1142, 1075 cm<sup>-1</sup>.

**HRMS** Calculated for C<sub>19</sub>H<sub>27</sub>N<sub>2</sub>O<sub>3</sub> (M + H<sup>+</sup>): 331.2022. Found: 331.2016.

### Compound 3:



A solution of 3-(ethylamino)phenol (1.0 g, 5.6 mmol), 2,6-lutidine (5 mL), *tert*-butyl bromoacetate (1.0 mL, 6.4 mmol), and DMF (40 mL) was stirred at ambient temperature for 20 h. The solvent was removed *in vacuo* and the resulting residue was purified using flash chromatography ( $\text{CH}_2\text{Cl}_2/\text{Et}_2\text{O}$ , 95:5). Compound **8** was isolated as a brown oil (0.7 g, 50% yield).

$^1\text{H NMR}$  (300 MHz,  $\text{CDCl}_3$ )  $\delta$  1.15 (t,  $J = 7.1$  Hz, 3H), 1.43 (s, 9H), 3.39 (q,  $J = 7.1$  Hz, 2H), 3.87 (s, 2H), 6.04 (s, 1H), 6.12–6.18 (m, 3H), 7.00 (t,  $J = 8.0$  Hz, 1H).

$^{13}\text{C NMR}$  (75 MHz,  $\text{CDCl}_3$ )  $\delta$  12.4, 28.0, 46.1, 53.2, 81.8, 99.2, 103.9, 104.4, 129.9, 149.3, 156.8, 171.2.

**FTIR** (neat) 3403, 1725, 1620, 1582, 1504, 1369, 1219, 1156, 1127  $\text{cm}^{-1}$ .

**HRMS** Calculated for  $\text{C}_{14}\text{H}_{22}\text{NO}_3$  ( $M + \text{H}^+$ ): 252.1600. Found: 252.1594.

A solution of DMF (0.5 mL, 6.8 mmol) and phosphorous oxychloride (0.3 mL, 2.7 mmol) were stirred at ambient temperature for 2 h. Compound **8** (0.7 g, 2.7 mmol) in DMF (15 mL) was added via cannula. The reaction was stirred at ambient temperature for 20 h. The mixture was slowly poured over ice, and the aqueous layer was extracted with  $\text{CH}_2\text{Cl}_2$  (3 x 50 mL). The organic layer was dried over  $\text{MgSO}_4$  and the solvent was removed *in vacuo*. The resulting residue was purified by flash chromatography ( $\text{EtOAc}/\text{Hex}$ , 20:80) and compound **9** was isolated as a white solid (0.6 g, 73% yield), M.P. 77–79°C.

$^1\text{H NMR}$  (360 MHz,  $\text{CDCl}_3$ )  $\delta$  1.30 (t,  $J = 7.2$  Hz, 3H), 1.46 (s, 9H), 3.49 (q,  $J = 7.2$  Hz, 2H), 3.97 (s, 2H), 6.05 (d,  $J = 2.3$  Hz, 1H), 6.21 (dd,  $J = 2.3, 8.8$  Hz, 1H), 7.28 (d,  $J = 8.8$  Hz, 1H), 9.53 (s, 1H), 11.55 (s, 1H).

$^{13}\text{C NMR}$  (75 MHz,  $\text{CDCl}_3$ )  $\delta$  12.2, 27.8, 46.6, 52.8, 82.1, 97.3, 104.4, 112.0, 135.2, 154.5, 164.0, 168.6, 192.4.

**FTIR** (neat) 2978, 1741, 1635, 1561, 1523, 1340, 1233, 1152  $\text{cm}^{-1}$ .

**HRMS** Calculated for  $\text{C}_{15}\text{H}_{22}\text{NO}_4$  ( $\text{M} + \text{H}^+$ ): 280.1549. Found: 280.1543.

A solution of compound **9** (0.5 g, 1.9 mmol), DABCO (0.4 g, 3.7 mmol), (carbethoxymethylene)-triphenylphosphorane (0.8 g, 2.2 mmol) and benzene (20 mL) was heated to a vigorous reflux for 20 h. The solution was cooled to ambient temperature and poured into 1% HCl (30 mL). The aqueous layer was extracted with  $\text{CH}_2\text{Cl}_2$  (3 x 20 mL). The organic layer was dried over  $\text{MgSO}_4$  and the solvent was removed *in vacuo*. The resulting residue was purified by flash chromatography (EtOAc/Hex, 15:85) and compound **10** was isolated as an amorphous white solid (120 mg, 20% yield).

**$^1\text{H}$  NMR** (300 MHz,  $\text{CD}_2\text{Cl}_2$ )  $\square$  1.22 (t,  $J = 7.2$  Hz, 3H), 1.45 (s, 9H), 3.50 (q,  $J = 7.2$  Hz, 2H), 3.98 (s, 2H), 6.00 (d,  $J = 9.4$  Hz, 1H), 6.44 (d,  $J = 2.4$  Hz, 1H), 6.53 (dd,  $J = 2.5, 8.8$  Hz, 1H), 7.28 (d,  $J = 8.8$  Hz, 1H), 7.55 (d,  $J = 9.4$  Hz, 1H).

**$^{13}\text{C}$  NMR** (75 MHz,  $\text{CD}_2\text{Cl}_2$ )  $\square$  12.4, 28.1, 47.1, 53.3, 82.3, 98.3, 109.1, 109.5, 110.4, 129.1, 143.9, 151.4, 156.8, 161.9, 169.4.

**FTIR** (neat) 1732, 1615, 1520, 1415, 1224, 1154, 1121  $\text{cm}^{-1}$ .

**HRMS** Calculated for  $\text{C}_{17}\text{H}_{22}\text{NO}_4$  ( $\text{M} + \text{H}^+$ ): 304.1549. Found: 304.1543.

A solution of DMF (0.2 mL, 2.6 mmol) and phosphorous oxychloride (0.1 mL, 1.1 mmol) were stirred at ambient temperature for 2 h. Compound **10** (65 mg, 0.2 mmol) in DMF (2 ml) was added via cannula. The reaction was stirred at ambient temperature for 20 h. The mixture was slowly poured over ice, and the aqueous layer was extracted with  $\text{CH}_2\text{Cl}_2$  (3 x 20 mL). The organic layer was dried over  $\text{MgSO}_4$  and the solvent was removed *in vacuo*. The resulting residue was purified via flash chromatography (EtOAc/Hex, 10:90) and compound **11** was isolated as a yellow solid (40 mg, 57% yield), M.P. 124-126°C.

**$^1\text{H}$  NMR** (300 MHz,  $\text{CDCl}_3$ )  $\square$  1.29 (t,  $J = 7.2$  Hz, 3H), 1.48 (s, 9H), 3.56 (q,  $J = 7.2$  Hz, 2H), 4.04 (s, 2H), 6.45 (d,  $J = 2.4$  Hz, 1H), 6.61 (dd,  $J = 2.4, 9.0$  Hz, 1H), 7.45 (d,  $J = 9.0$  Hz, 1H), 8.27 (s, 1H), 10.13 (s, 1H).

**$^{13}\text{C}$  NMR** (75 MHz,  $\text{CDCl}_3$ )  $\square$  12.1, 27.9, 47.2, 53.1, 82.8, 97.7, 108.9, 110.2, 115.2, 132.3, 145.5, 153.8, 158.5, 161.5, 168.1, 187.8.

**FTIR** (neat) 2977, 1720, 1683, 1618, 1576, 1510, 1393, 1349, 1155, 1123  $\text{cm}^{-1}$ .

**HRMS** Calculated for  $\text{C}_{18}\text{H}_{22}\text{NO}_5$  ( $\text{M} + \text{H}^+$ ): 332.1498. Found: 332.1492.

Compound **11** (11.3 mg, 0.03 mmol), trifluoroacetic acid (1 mL), and CH<sub>2</sub>Cl<sub>2</sub> (1 mL) were stirred at ambient temperature for 1.5 h. The solvent was removed *in vacuo* to afford compound **3**, a yellow solid (8.3 mg, 100% yield), M.P. 180°C (decomp.).

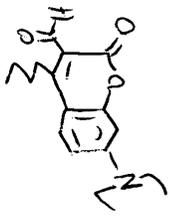
**<sup>1</sup>H NMR** (300 MHz, D<sub>2</sub>O with NaOD)  $\delta$  0.99 (t, *J* = 7.1 Hz, 3H), 3.22 (q, *J* = 7.0 Hz, 2H), 5.66 (d, *J* = 2.5 Hz, 1H), 5.91 (dd, *J* = 2.4, 9.2 Hz, 1H), 7.34 (d, *J* = 9.2 Hz, 1H), 7.51 (s, 1H), 8.78 (s br, 1H).

**<sup>13</sup>C NMR** (75 MHz, d<sub>6</sub>-DMSO)  $\delta$  12.0, 46.3, 51.6, 97.0, 108.2, 110.6, 114.1, 132.8, 146.4, 154.1, 158.0, 160.5, 170.8, 187.3.

**FTIR** (neat) 2925, 1717, 1682, 1616, 1575, 1510, 1394, 1348, 1186 cm<sup>-1</sup>.

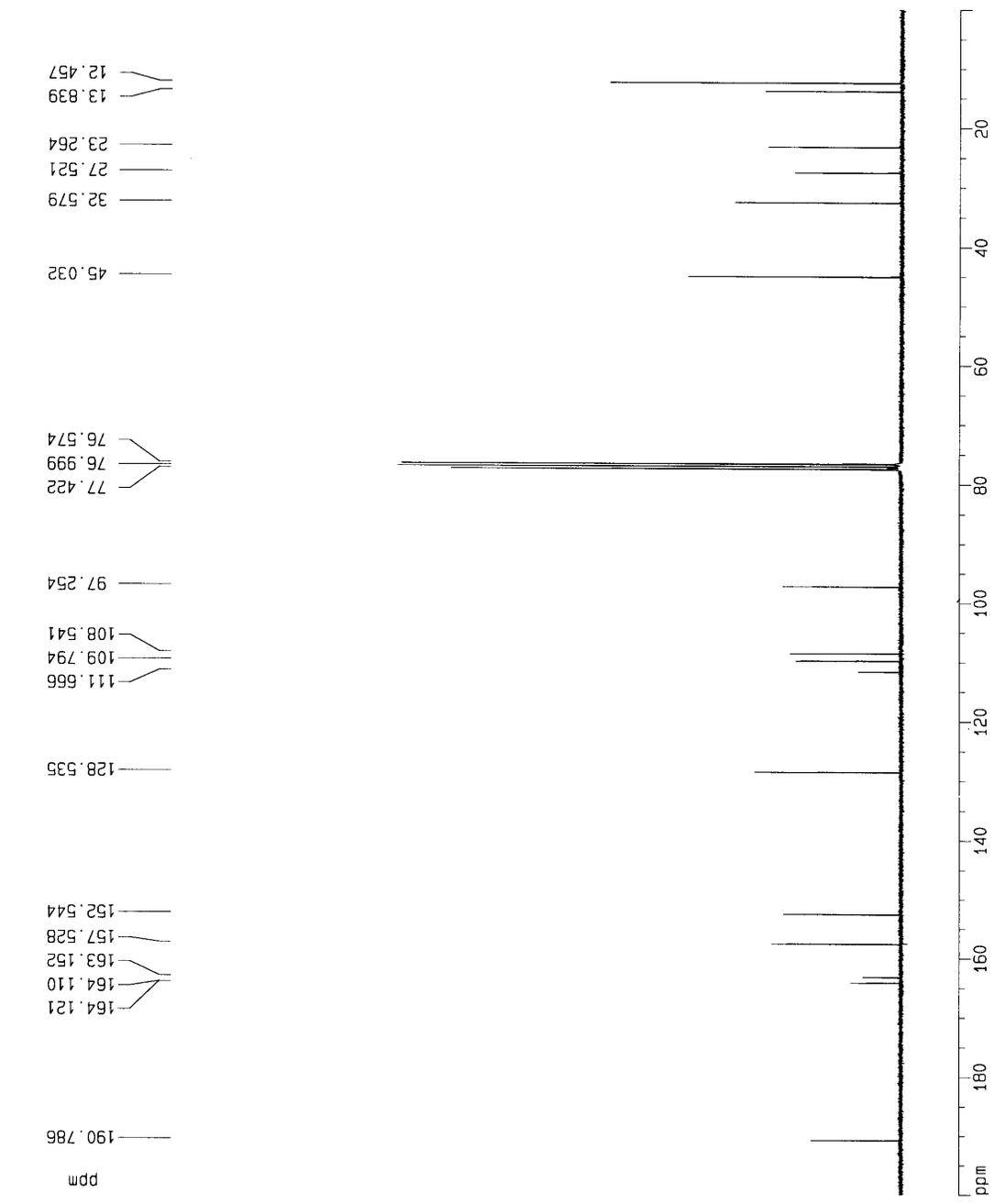
**HRMS** Calculated for C<sub>14</sub>H<sub>13</sub>NO<sub>5</sub> (M + H<sup>+</sup>): 276.0870. Found: 276.0873.

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1. Connors, K. A. *Binding Constants*; John Wiley; New York, 1987.
  2. (a) Kirpichenok, M. A.; Baukulev, V. M.; Karandashova, L. A.; Grandberg, I. I. *Chem. Heterocycl. Compd.* **1991**, *27*, 1193-1199. (b) Knierzinger, A.; Wolfbeis, O. S. *J. Heterocyclic Chem.* **1980**, *17*, 225-229.
  3. Nicolaou, K. C.; Papahatjis, D. P.; Claremon, D. A.; Dolle, R. E., III *J. Am. Chem. Soc.* **1981**, *103*, 6967-6969.



1b

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butyl aldehyde carbon



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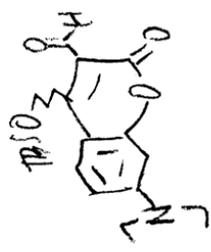
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5



EKF V OTBS  
for characterization

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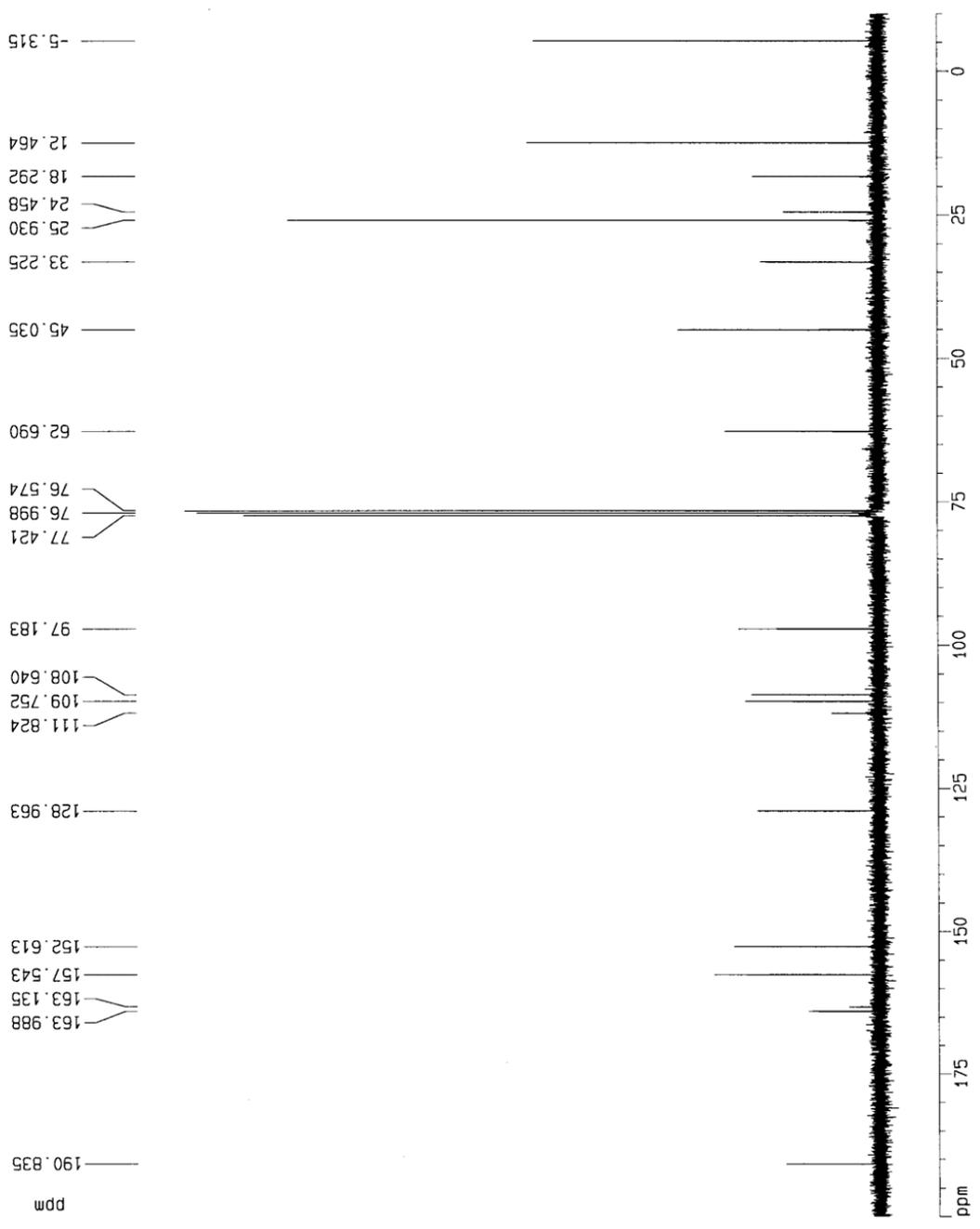
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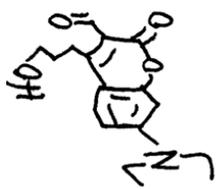
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6



EKF V alcohol  
for characterization

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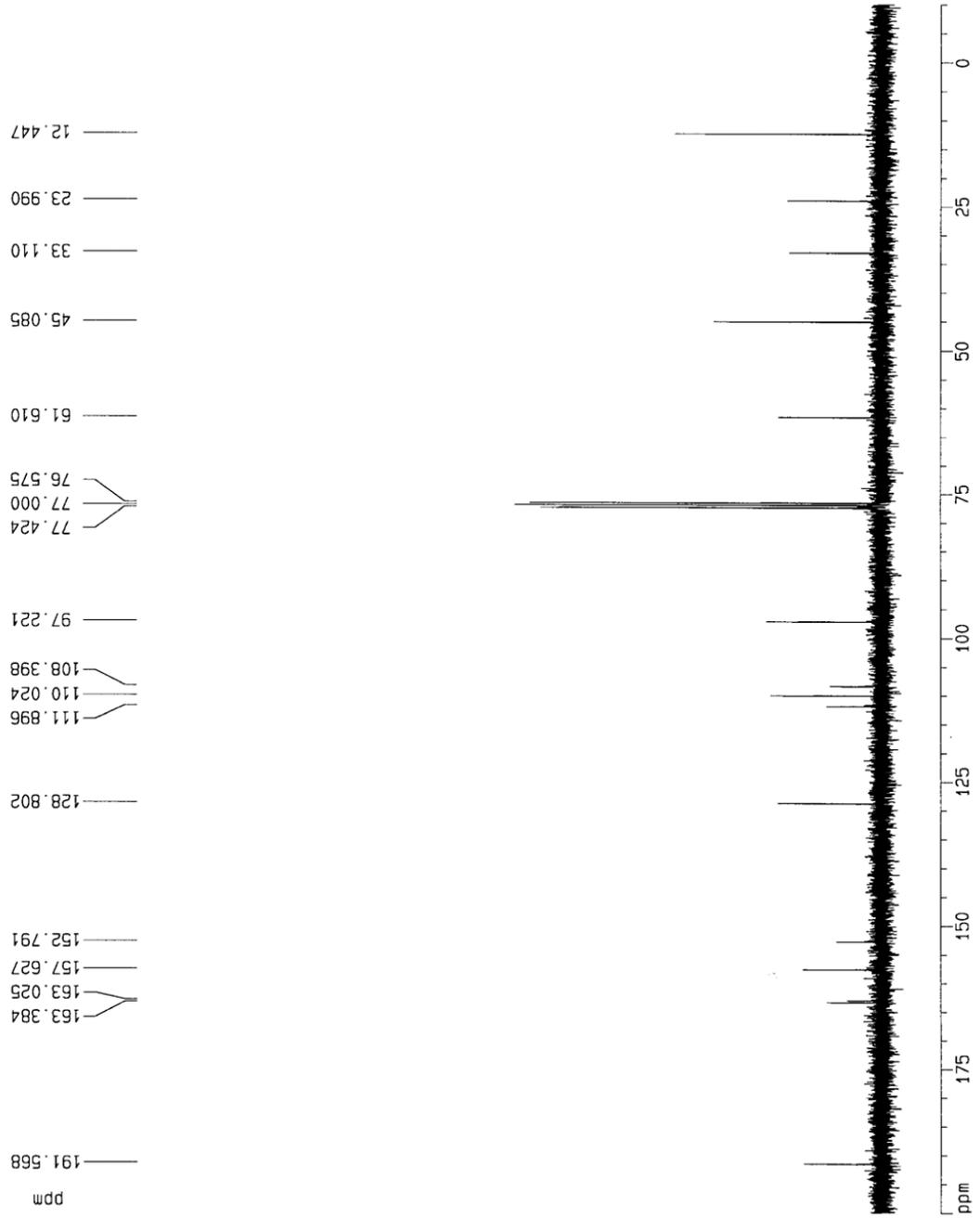
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Time      10.58
INSTRUM   spect
PROBHD    5 mm QNP 1H/1
PULPROG   zgpg30
TD         65536
SOLVENT   CDCl3
NS         313
DS         4
SMH       18795.992 Hz
FIDRES    0.266819 Hz
AQ         1.7433076 sec
RG         1024
DM         26.600 usec
DE         6.00 usec
TE         300.0 K
D1         2.00000000 sec
D11        0.03000000 sec
D12        0.00002000 sec

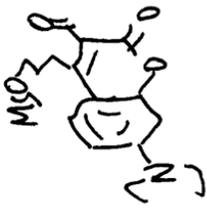
===== CHANNEL f1 =====
NUC1       13C
P1         5.40 usec
PL1        -6.00 dB
SFO1       75.4106357 MHz

===== CHANNEL f2 =====
CPDPRG2    waltz16
NUC2       1H
PCPD2     115.00 usec
PL2        0.00 dB
PL12       20.00 dB
PL13       20.00 dB
SFO2       299.8711995 MHz

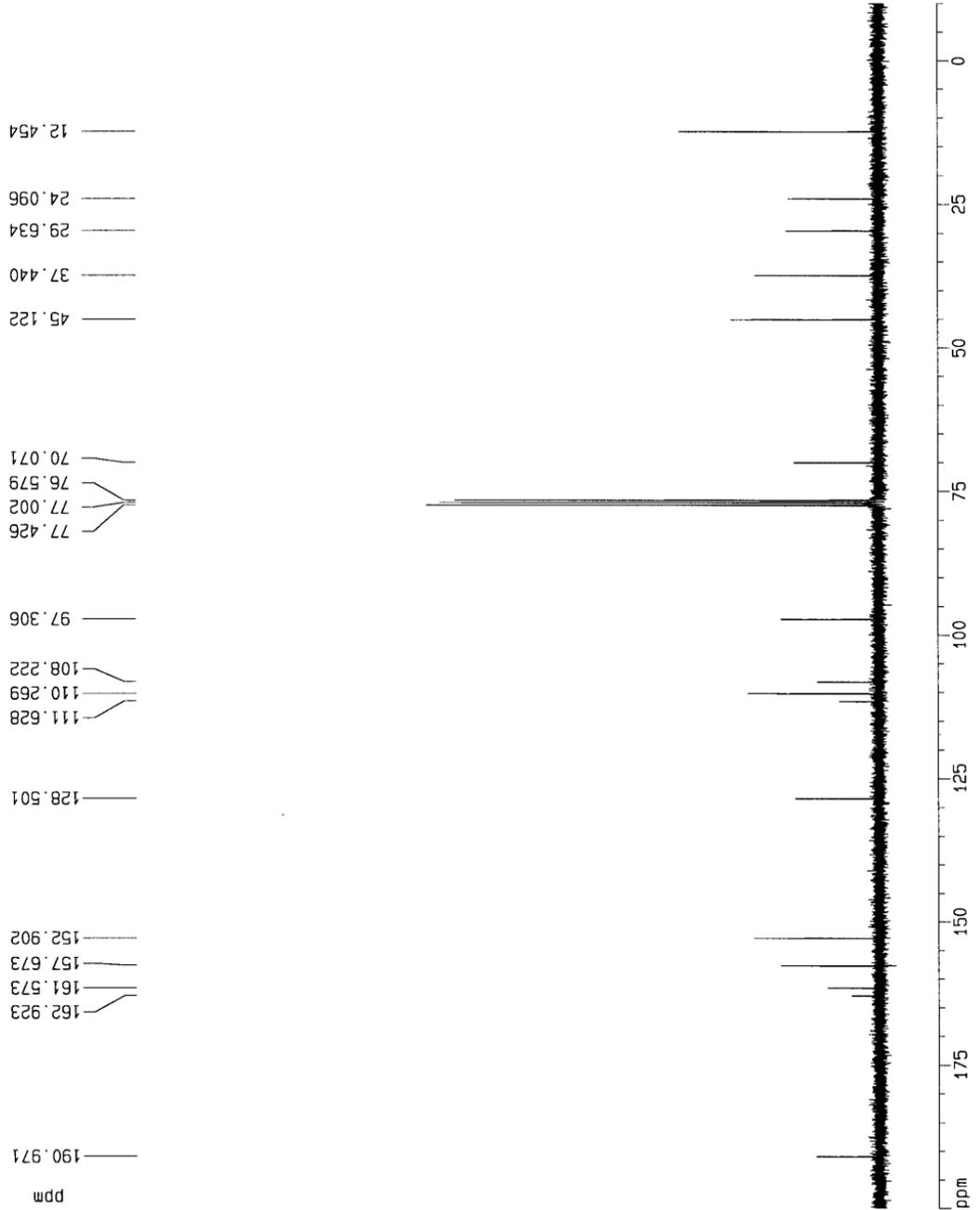
F2 - Processing parameters
SI         32768
SF         75.4023763 MHz
WDW        nc
SSB        0
LB         0.00 Hz
GB         0
PC         1.40

10 NMR plot parameters
CX         20.00 cm
F1P        200.000 ppm
F1         15080.47 Hz
F2P        -10.000 ppm
F2         -754.02 Hz
PPMCM      10.50000 ppm/cm
HZCM       791.72491 Hz/cm
  
```





EKF V mesylate  
for characterization



```

Current Data Parameters
NAME      EKF-04-24-03
EXPNO    6
PROCNO   1

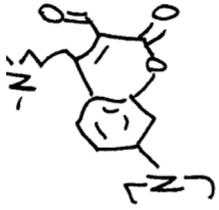
F2 - Acquisition Parameters
Date_    20030424
Time     18.10
INSTRUM spect
PROBHD   5 mm QNP 1H/1
PULPROG zgpg30
TD       65536
SOLVENT  CDCl3
NS       823
DS       4
SWH      18795.992 Hz
FIDRES   0.286819 Hz
AQ       1.7433076 sec
RG       1024
DM       25.600 usec
DE       6.00 usec
TE       300.0 K
D1       2.00000000 sec
D11      0.03000000 sec
D12      0.00002000 sec

===== CHANNEL f1 =====
NUC1     13C
P1       5.40 usec
PL1      -6.00 dB
SFO1     75.4106357 MHz

===== CHANNEL f2 =====
CPDPRG2  waltz16
NUC2     1H
PCPD2    115.00 usec
PL2      0.00 dB
PL12     20.00 dB
PL13     20.00 dB
SF02     289.8711995 MHz

F2 - Processing parameters
SI       32768
SF       75.4023757 MHz
MGM      no
SSB      0
LB       0.00 Hz
GB       0
PC       1.40

1D NMR plot parameters
CX       20.00 cm
FIP      200.000 ppm
F1       15080.47 Hz
F2       -10.000 ppm
F2P      -754.02 Hz
PPMCM    10.50000 ppm/cm
HZCM     791.72491 Hz/cm
  
```



4

EKF VI 21 A  
dimethylamino coumarin for characterization

```

Current Data Parameters
NAME      ekf-05-08-03
EXPNO    2
PROCNO   1

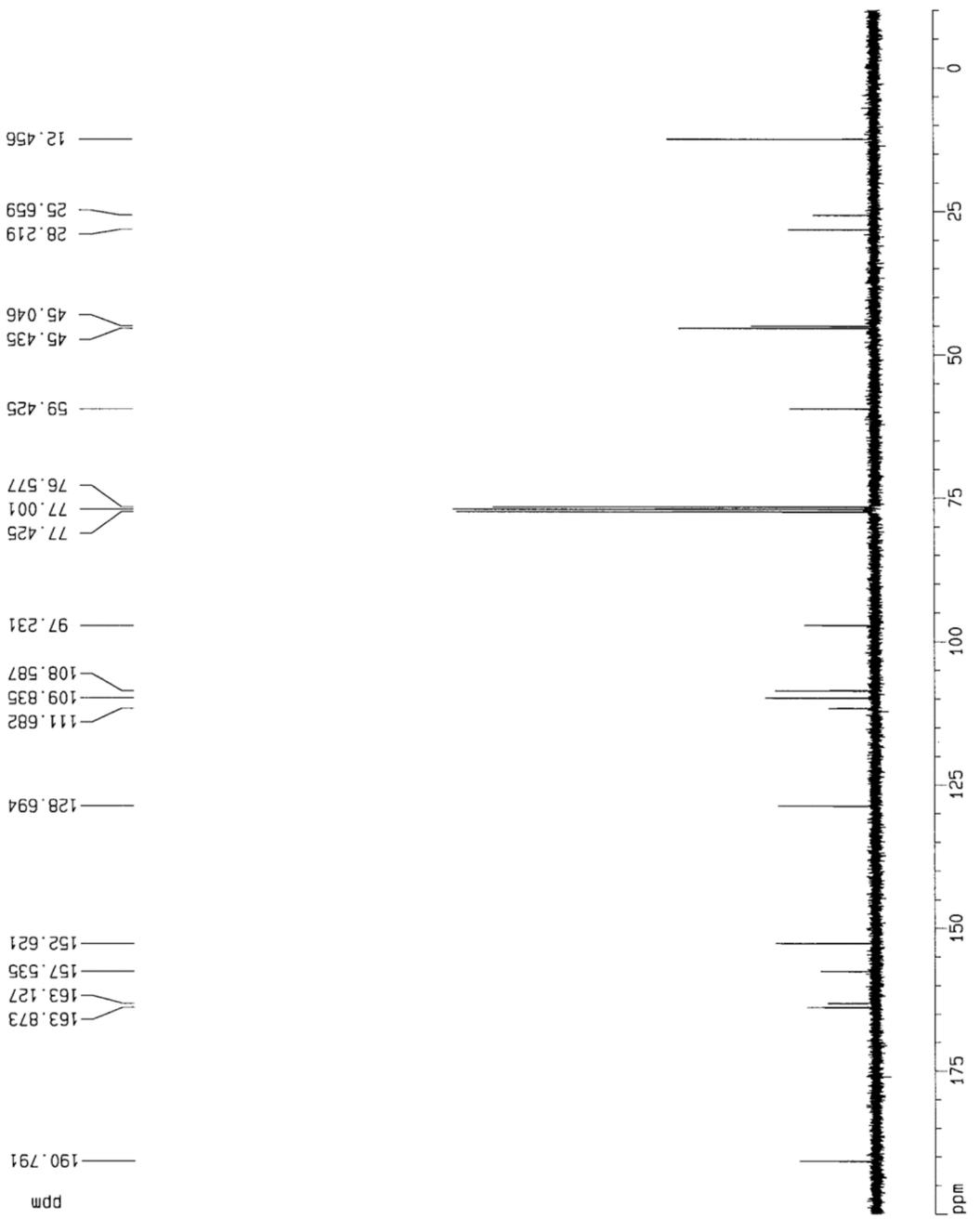
F2 - Acquisition Parameters
Date_    20030508
Time     14:52
INSTRUM  spect
PROBHD   5 mm QNP 1H/1
PULPROG  zgpg30
TD        65536
SOLVENT  CDCl3
NS        785
DS        4
SWH       18796.992 Hz
FIDRES    0.286819 Hz
AQ         1.7433076 sec
RG         16384
DM         26.600 usec
DE         6.00 usec
TE         300.0 K
D1         2.00000000 sec
D11        0.03000000 sec
D12        0.00002000 sec

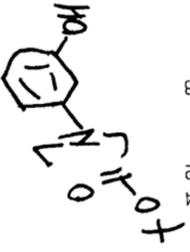
===== CHANNEL f1 =====
NUC1      13C
P1         5.40 usec
PL1        -6.00 dB
SFO1      75.4106357 MHz

===== CHANNEL f2 =====
CPDPRG2   waltz16
NUC2       1H
PCPD02    115.00 usec
PL2        0.00 dB
PL12       20.00 dB
PL13       20.00 dB
SFO2      299.8711995 MHz

F2 - Processing parameters
SI         32768
SF         75.4023757 MHz
WDW        no
SSB         0
LB         0.00 Hz
GB         0
PC         1.40

1D NMR plot parameters
CX         20.00 cm
F1P        200.000 ppm
F1         15080.47 Hz
F2P        -10.000 ppm
F2         -754.02 Hz
PPMCM     10.50000 ppm/cm
HZCM       791.72491 Hz/cm
  
```





8

EKF VI 4 A  
for characterization

```

Current Data Parameters
NAME      ekf-05-01-03
EXPNO    5
PROCNO   1

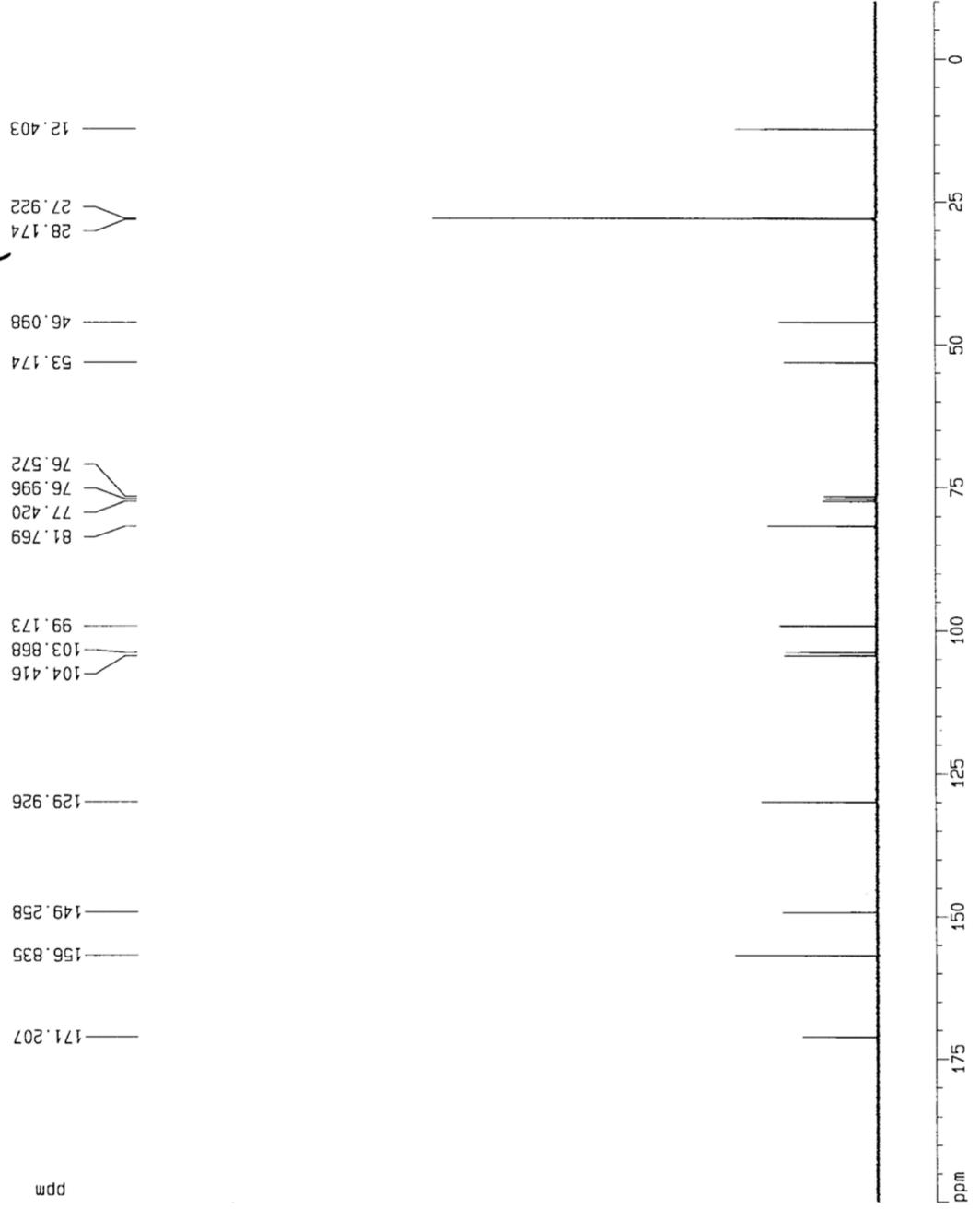
F2 - Acquisition Parameters
Date_    20030501
Time     14.24
INSTRUM  spect
PROBHD   5 mm GNP 1H/1
PULPROG  zgpg30
TD       65536
SOLVENT  CDCl3
NS       408
DS       4
SWH      18796.992 Hz
FIDRES   0.286819 Hz
AQ       1.7433076 sec
RG       1024
DM       26.600 usec
DE       6.00 usec
TE       300.0 K
D1       2.00000000 sec
D11      0.03000000 sec
D12      0.00002000 sec

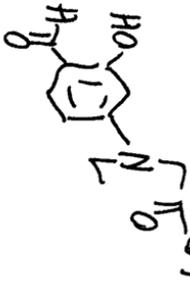
===== CHANNEL f1 =====
NUC1     13C
P1       5.40 usec
PL1      -6.00 dB
SF01     75.4106357 MHz

===== CHANNEL f2 =====
CPDPRG2  waltz16
NUC2     1H
PCPD02   115.00 usec
PL2      0.00 dB
PL12     20.00 dB
PL13     20.00 dB
SF02     299.8711995 MHz

F2 - Processing parameters
SI       32768
SF       75.4023826 MHz
WDW      no
SSB      0
LB       0.00 Hz
GB       0
PC       1.40

1D NMR plot parameters
CX       20.00 cm
F1P      200.000 ppm
F1       15080.48 Hz
F2P      -10.000 ppm
F2       -754.02 Hz
PPMCH   10.50000 ppm/cm
HZCM     791.72504 Hz/cm
  
```





EKF VI 23  
Vilsmeyer for characterization

Current Data Parameters  
 NAME ekf-05-09-03  
 EXPNO 3  
 PROCNO 1

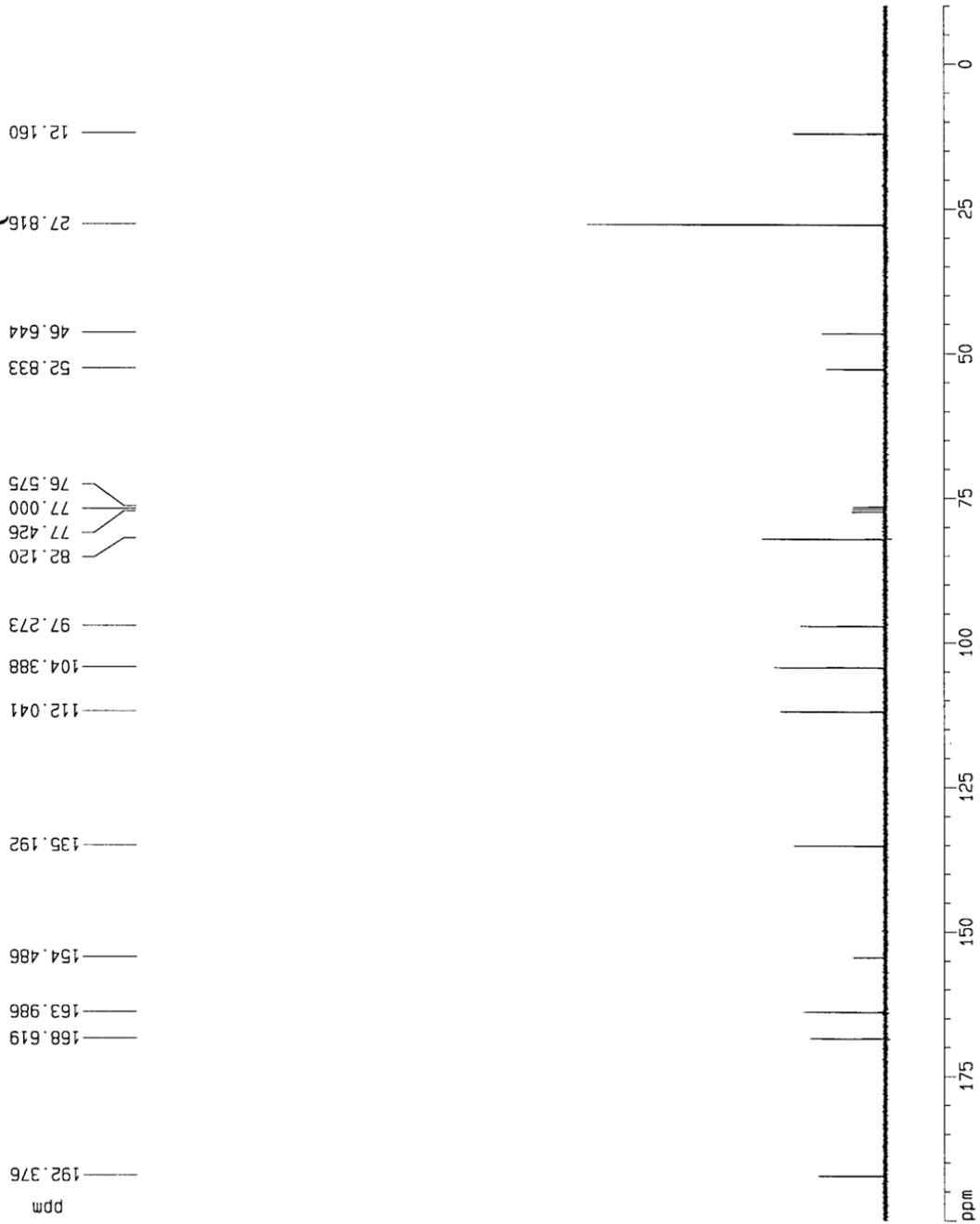
F2 - Acquisition Parameters  
 Date\_ 20030509  
 Time 11.00  
 INSTRUM spect  
 PROBHD 5 mm QNP 1H/1  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDC13  
 NS 49  
 DS 4  
 SWH 18796.992 Hz  
 FIDRES 0.286819 Hz  
 AQ 1.7433076 sec  
 RG 1024  
 DM 26.600 usec  
 DE 6.00 usec  
 TE 300.0 K  
 D1 2.0000000 sec  
 D11 0.0300000 sec  
 D12 0.0002000 sec

===== CHANNEL f1 =====  
 NUC1 13C  
 P1 5.40 usec  
 PL1 -6.00 dB  
 SF01 75.4106357 MHz

===== CHANNEL f2 =====  
 CPDPRG2 waltz16  
 NUC2 1H  
 PCPD2 115.00 usec  
 PL2 0.00 dB  
 PL12 20.00 dB  
 PL13 20.00 dB  
 SF02 299.8711995 MHz

F2 - Processing parameters  
 SI 32768  
 SF 75.4023849 MHz  
 WDW no  
 SSB 0  
 LB 0.00 Hz  
 GB 0  
 PC 1.40

1D NMR plot parameters  
 CX 20.00 cm  
 F1P 200.000 ppm  
 F1 15080.48 Hz  
 F2P -10.000 ppm  
 F2 -754.02 Hz  
 PPMCM 10 50000 ppm/cm  
 HZCM 791.72504 Hz/cm





EKF  
water soluble bare coumarin

Current Data Parameters  
 NAME ekf-05-01-03  
 EXPNO 2  
 PROCNO 1

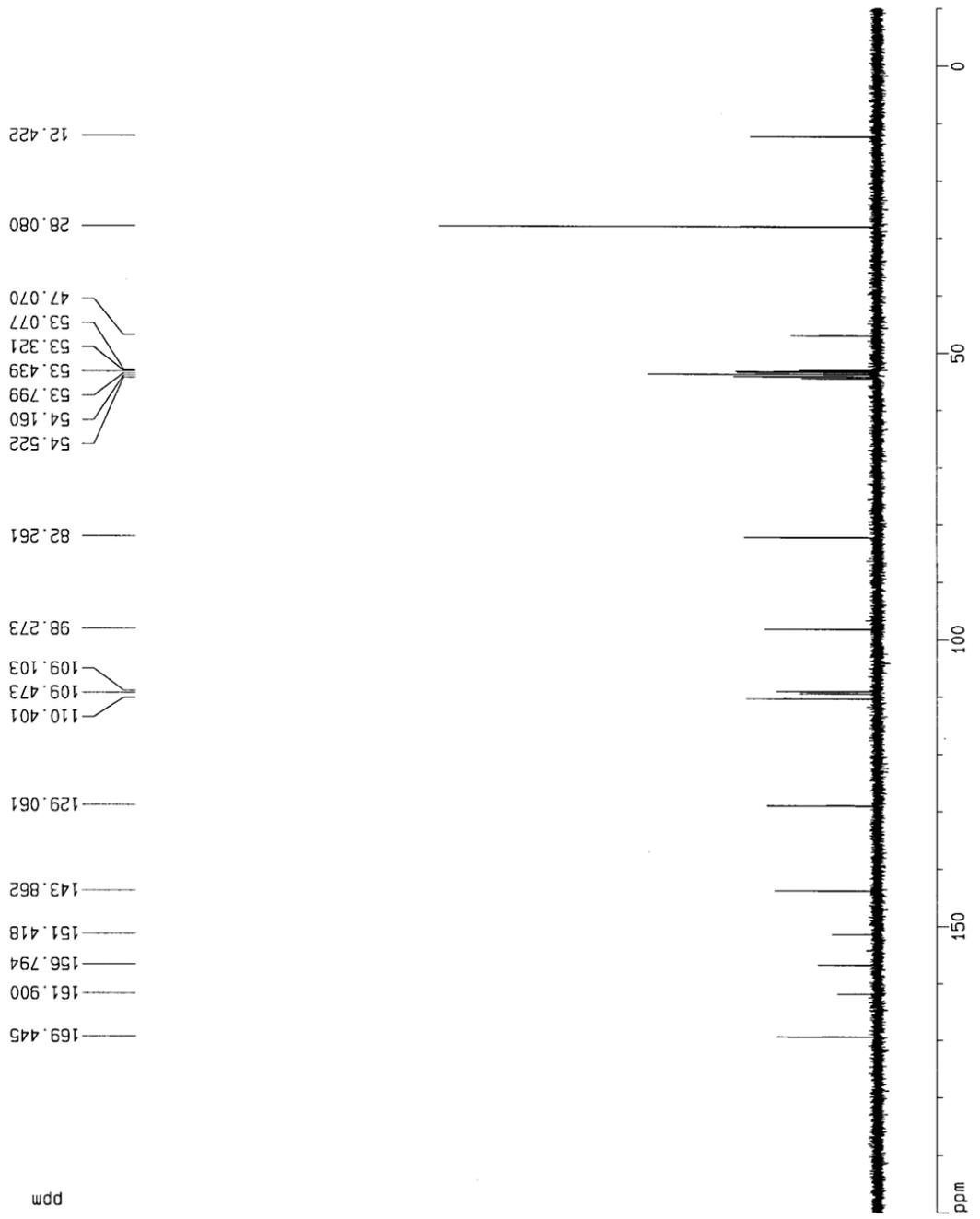
F2 - Acquisition Parameters  
 Date\_ 20030501  
 Time 12.34  
 INSTRUM spect  
 PROBHD 5 mm GNP 1H/1  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 207  
 DS 4  
 SWH 18796.992 Hz  
 FIDRES 0.286819 Hz  
 AQ 1.7433076 sec  
 RG 512  
 DW 26.600 usec  
 DE 6.00 usec  
 TE 300.0 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 D12 0.00002000 sec

===== CHANNEL f1 =====  
 NUC1 13C  
 P1 5.40 usec  
 PL1 -6.00 dB  
 SF01 75.4106357 MHz

===== CHANNEL f2 =====  
 CPDPRG2 waltz16  
 NUC2 1H  
 PCPD2 115.00 usec  
 PL2 0.00 dB  
 PL12 20.00 dB  
 PL13 20.00 dB  
 SF02 299.871995 MHz

F2 - Processing parameters  
 SI 32768  
 SF 75.4023468 MHz  
 MDW no  
 SSB 0  
 LB 0.00 Hz  
 GB 0  
 PC 1.40

1D NMR plot parameters  
 CX 20.00 cm  
 F1P 200.000 ppm  
 F1 15080.47 Hz  
 F2P -10.000 ppm  
 F2 -754.02 Hz  
 PPMCM 10.50000 ppm/cm  
 HZCM 791.72461 Hz/cm





EKF VI 26 A  
Vilsmeier of t-butyl ester coumarin  
for characterization

```

Current Data Parameters
NAME      ekf-05-13-03
EXPNO    3
PROCNO   1

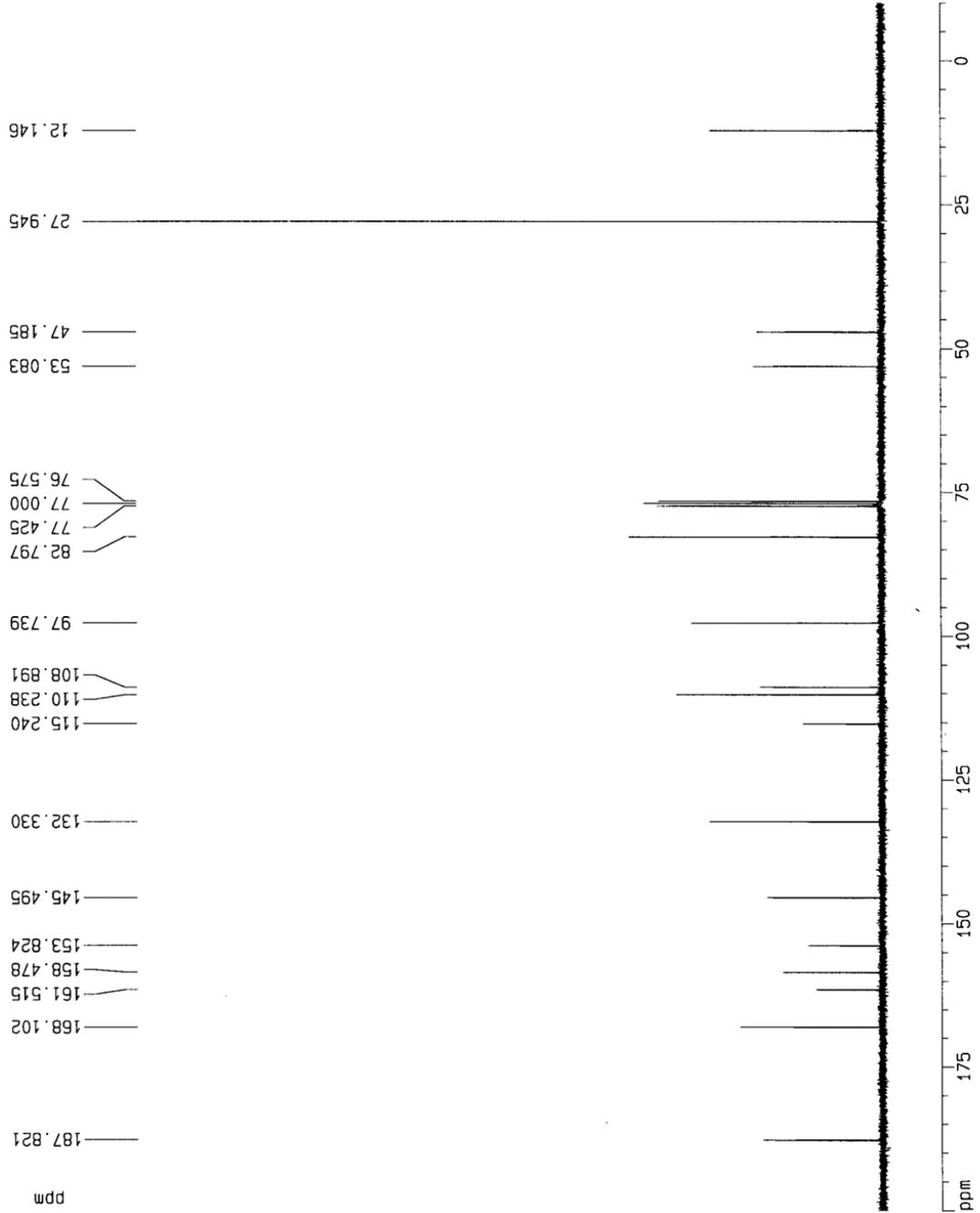
F2 - Acquisition Parameters
Date_    20030513
Time     16.43
INSTRUM  spect
PROBHD   5 mm QNP 1H/1
PULPROG  zgpg30
TD       65536
SOLVENT  CDCl3
NS       723
DS       4
SWH      18796.992 Hz
FIDRES   0.288819 Hz
AQ       1.7433076 sec
RG       1024
DM       26.600 usec
DE       5.00 usec
TE       300.0 K
D1       2.0000000 sec
D11      0.0300000 sec
D12      0.0002000 sec

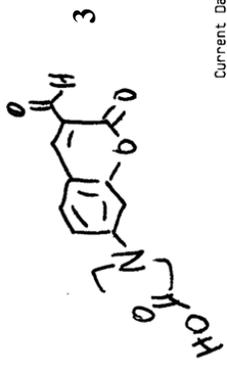
===== CHANNEL f1 =====
NUC1     13C
P1       5.40 usec
PL1      -6.00 dB
SF01     75.4106357 MHz

===== CHANNEL f2 =====
CPOPRG2  waltz16
NUC2     1H
PCPD02   115.00 usec
PL2      0.00 dB
PL12     20.00 dB
PL13     20.00 dB
SF02     299.8711995 MHz

F2 - Processing parameters
SI       32768
SF       75.4023786 MHz
WDW      no
SSB      0
LB       0.00 Hz
GB       0
PC       1.40

1D NMR plot parameters
CX       20.00 cm
F1P     200.000 ppm
F1       15080.48 Hz
F2P     -10.000 ppm
F2       -754.02 Hz
PPMCM   10.50000 ppm/cm
HZCM    791.72504 Hz/cm
    
```





EKF VI water soluble coumarin  
d-DMSO

