**Electronic Supplementary Information (ESI)**

# Efficient Method for Selective Oxidation of 1,2-Diols in Water Catalyzed by $Me_2SnCl_2$

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***General***

All melting points are not corrected. $^1$H NMR spectra were taken at 400 MHz and $^{13}$C NMR spectra were taken at 100 MHz. Chemical shift values are expressed in ppm relative to internal or external TMS. Abbreviations are as follows: s, singlet; d, doublet; t, triplet; q, quartet; m, multiplet; br, broad. Mass spectra (MS) and high-resolution mass spectra (HRMS) were recorded using electron ionization (EI) or fast atom bombardment (FAB) mass spectrometry. The products were isolated by silica gel column chromatography. All reagents and solvents were of high purity and used as supplied.

All reagents and solvents were of high purity and used as supplied. Diols **1c**–**i**, **1k-o,** triol **1p**, and mono-ol **1q**, are commercially available. Diols **1a** and **1b** were prepared by osmium oxidation of their corresponding alkenes, through Sharpless dihydroxylation procedure. α-Hydroxyketones **2a**,[1] **2b**,[1] **2c**,[2] **2d**,[2] **2h**,[3] **2j**,[4] **2k**,[5] **2l**,[6] **2n**,[7] **2o**,[8] **2p**,[9] and ketone **2q**[10] are known compounds.

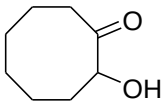
***2. General Procedure for selective oxidation of 1,2-diols in water using $Br_2$ as an oxidant***

Bromine (1.5 mmol) was added dropwise at 0 $^o$C under dark conditions to a solution of 1,2-diol **1a** (1.0 mmol), $Me_2SnCl_2$ (0.1 mmol), and $K_2CO_3$ (1.2 mmol) in water (5 mL). After the reaction mixture had been stirred for 30 min, aqueous sat. $Na_2S_2O_3$ (10 mL) was added. The organic portion was extracted with AcOEt (3 x 40 mL) and then dried over anhydrous $MgSO_4$. The solvent was removed in vacuo and the residue was subjected to silica-gel column chromatography (n-hexane/AcOEt 5:1) to afford
(129.3 mg, 91% yield) of product **2a**.

***3. General Procedure for selective oxidation of 1,2-diols in water using DBI as an oxidant***

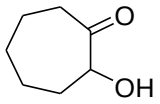
DBI (1.0 mmol) was added at 0 $^o$C under dark conditions to a solution of 1,2-diol **1a** (1.0 mmol) and $Me_2SnCl_2$ (0.1 mmol), and $K_2CO_3$ (1.2 mmol) in water (5 mL). After the reaction mixture had been stirred for 1 h, aqueous sat. $Na_2S_2O_3$ (10 mL) was added. The organic portion was extracted with AcOEt (3 x 40 mL) and then dried over MgSO4. The solvent was removed in vacuo and the residue was subjected to silica-gel column chromatography (n-hexane/AcOEt 5:1) to afford (127mg, 90% yield) of product **2a**.

***4. Characterization of 2***



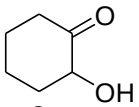

**2a**

**2-Hydroxycyclooctanone (2a)** (Table 1)**:** Waxy solid; mp 114−118 °C. $^{1}$H-NMR (400 MHz, $CDCl_3$) δ 0.78−1.04 (m, 1 H), 1.30−1.48 (m, 2 H), 1.57−1.89 (m, 4 H), 1.89−2.13 (m, 2 H), 2.23−2.48 (m, 2 H), 2.72 (td, *J*=12.21, 3.91 Hz, 1 H), 3.76 (br. s, 1 H), 4.19 (dd, *J*=6.35, 2.69 Hz, 1 H). $^{13}$C-NMR (100 MHz, $CDCl_3$) δ 22.00, 24.36, 25.37, 28.53, 29.17, 37.16, 76.08, 217.4.



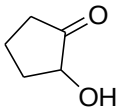

**2b**

**2-Hydroxycycloheptanone (2b)** (Table 4, entry 1): Yellow oil. $^{1}$H-NMR (400 MHz, $CDCl_3$) δ 1.27−1.43 (m, 1 H), 1.52−2.13 (m, 7 H), 2.47 (ddd, *J*=17.33, 11.11, 3.54 Hz, 1 H), 2.61−2.79 (m, 1 H), 3.86 (d, *J*=3.66 Hz, 1 H), 4.21−4.40 (m, 1 H). $^{13}$C-NMR (100 MHz, $CDCl_3$) δ 23.43, 26.61, 29.51, 33.76, 40.06, 77.03, 213.81.



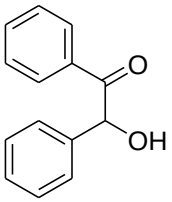

**2c**

**2-Hydroxycyclohexanone (2c)** (Table 4, entry 2)**:** Colorless oil. $^{1}$H-NMR (400 MHz, $CDCl_3$) δ 1.40−2.00 (m, 4 H), 2.04−2.21 (m, 1 H), 2.28−2.67 (m, 3 H), 3.68 (br. s, 1 H), 4.13 (dd, *J*=11.84, 6.71 Hz, 1 H). $^{13}$C-NMR (100 MHz, $CDCl_3$) δ 23.33, 27.52, 36.67, 39.44, 75.30, 211.35.



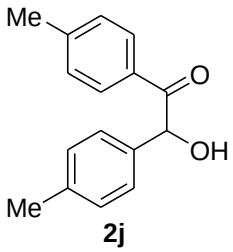

**2d**

**2-Hydroxycyclopentanone (2d)** (Table 4, entry 3)**:** Colorless oil. $^{1}$H-NMR (400 MHz, $CDCl_3$) δ 1.45−2.74 (m, 6 H), 3.16 (br. s, 1 H), 3.84−4.26 (m, 1 H). $^{13}$C-NMR (100 MHz, $CDCl_3$) δ 16.26, 30.58, 33.91, 75.82, 218.43.



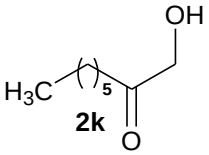

**2h**

**Benzoin (2h)** (Table 4, entry 7): White solid; mp 136−137 °C. $^{1}$H-NMR (400 MHz, $CDCl_3$) δ 4.56 (d, *J*=6.10 Hz, 1 H), 5.96 (d, *J*=6.10 Hz, 1 H), 7.22−7.36 (m, 5 H), 7.37−7.44 (m, 2 H), 7.48−7.58 (m, 1 H), 7.88−7.96 (m, 2 H)**.** $^{13}$C-NMR (100 MHz, $CDCl_3$) δ 76.18, 127.74 (2C), 128.54, 128.65 (2C), 129.09, 129.11(2C), 133.44, 133.87 (2C), 138.97, 198.91.



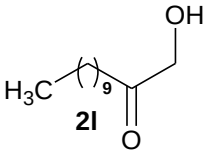

**2j**

**4,4-Dimethylbenzoin (2j)** (Table 4, entry 9): White solid; mp 89−90 °C. $^{1}$H-NMR (400 MHz, $CDCl_3$) δ 2.22−2.38 (m, 6 H), 4.57 (d, *J*=6.10 Hz, 1 H), 5.89 (d, *J*=6.10 Hz, 1 H), 7.10 (d, *J*=8.06 Hz, 2 H), 7.13−7.24 (m, 4 H), 7.66−7.97 (m, 2 H). $^{13}$C-NMR (100 MHz, $CDCl_3$) δ 21.05, 2161, 75.72, 127.57 (2C), 129.19 (2C), 129.27 (2C), 129.68, 130.88, 136.32, 138.21, 144.79, 198.47.



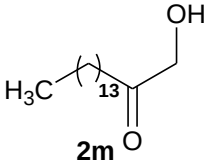

**2k**

**1-Hydroxyoctan-2-one (2k)** (Table 4, entry 10): Colorless oil. $^{1}$H-NMR (400 MHz, $CDCl_3$) δ 0.79−0.95 (m, 3 H), 1.20−1.38 (m, 6 H), 1.52−1.70 (m, 2 H), 2.41 (t, *J*=7.45 Hz, 2 H), 3.24 (br. s, 1 H), 4.24 (s, 2 H). $^{13}$C-NMR (100 MHz, $CDCl_3$) δ 13.76, 22.24, 23.46, 28.67, 31.28, 38.19, 67.89, 209.91.



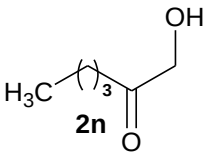

**2l**

**1-Hydroxydodecan-2-one (2l)** (Table 4, entry 11)**:** White solid; mp 52-53 °C. $^{1}$H-NMR (400 MHz, $CDCl_3$) δ 0.88 (t, *J*=6.84 Hz, 3 H), 1.14−1.41 (m, 15 H), 1.55−1.76 (m, 3 H), 2.41 (t, *J*=7.57 Hz, 2 H), 3.13 (br. s, 1 H), 4.24 (d, *J*=2.93 Hz, 2 H). $^{13}$C-NMR (100 MHz, $CDCl_3$) δ 14.07, 22.64, 23.72, 29.18, 29.25, 29.26, 29.38, 29.50, 31.84, 38.42, 68.05, 209.88.



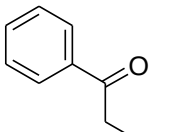

**2m**

**1-Hydroxyhexadecan-2-one** (**2m)** (Table 4, entry 12)**:** White solid; mp 72−73 °C. IR (neat) 3347, 2914, 2847, 1462, 1375, 1070, 993, 717cm$^{-1}$; $^{1}$H-NMR (400 MHz, $CDCl_3$) δ 0.88 (t, *J*=6.84 Hz, 3 H), 1.12−1.37 (m, 22 H), 1.53−1.74 (m, 2 H), 2.41 (t, *J*=7.45 Hz, 2 H), 3.13 (t, *J*=4.64 Hz, 1 H), 4.24 (d, *J*=4.39 Hz, 2 H). $^{13}$C-NMR (100 MHz, $CDCl_3$) δ 14.09, 22.67, 23.72, 29.18, 29.27, 29.33, 29.38, 29.55, 29.60, 29.62, 29.63, 29.65, 31.90, 38.42, 68.06, 209.88. HRMS calcd for $C_{16}H_{32}O_2$ ($M^+$): 256.2402, found, 256.2394.



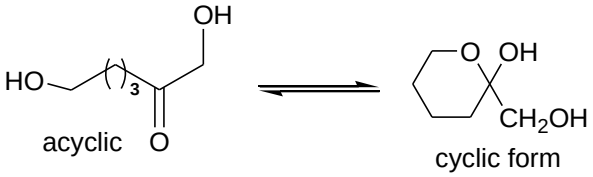

**2n**

**1-Hydroxyhexan-2-one (2n)** (Table 4, entry 13): Colorless oil. $^{1}$H-NMR (400 MHz, $CDCl_3$) δ 0.92 (t, *J*=7.45 Hz, 3 H), 1.34 (dq, *J*=14.95, 7.39 Hz, 2 H), 1.62 (quin, *J*=7.57 Hz, 2 H), 2.42 (t, *J*=7.45 Hz, 2 H), 3.28 (br. s, 1 H), 4.25 (d, *J*=1.95 Hz, 2 H). $^{13}$C-NMR (100 MHz, $CDCl_3$) δ 13.58, 22.16, 25.60, 37.96, 67.94, 209.87.



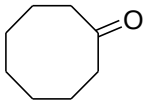

**2o**

**2-Hydroxy-1-phenylethanone (2o)** (Table 4, entry 14): White solid; 86−88°C. $^{1}$H-NMR (400 MHz, $CDCl_3$) δ 3.53 (t, *J*=4.27 Hz, 1 H), 4.89 (d, *J*=4.15 Hz, 2 H), 7.45−7.58 (m, 2 H), 7.58−7.71 (m, 1 H), 7.93 (d, *J*=7.57 Hz, 2 H). $^{13}$C-NMR (100 MHz, $CDCl_3$) δ 65.46, 127.66 (2C), 128.94 (2C), 133.34, 134.27, 198.37.




**2p**

**1,6-Dihydroxyhexan-2-one (2p) exist in (mixture of open-chain and cyclic form)** [9] (Table 4, entry 15): Colorless oil. $^{13}$C-NMR (100 MHz, $CDCl_3$) δ acyclic form 6: 19.76 (C(4)), 31.68 (C(5)), 37.80 (C(3)), 61.85 (C(6)), 67.96 (C(l)), 210.07 (C(2)); cyclic form 6: 18.16 (C(4)), 25.20 (C(5)), 30.34 (C(3)), 61.07 (C(6)), 69.00 (C(l)), 95.05 (C(2)).




**2q**

**Cyclooctanone (2q)** (Scheme 2)**:** Yellow oil. $^{1}$H-NMR (400 MHz, $CDCl_3$) δ 1.33−1.44 (m, 1 H), 1.49−1.62 (m, 3 H), 1.62−1.71 (m, 1 H), 1.76−1.97 (m, 4 H), 2.36−2.49 (m, 3 H), 2.56−2.67 (m, 1 H). $^{13}$C-NMR (100 MHz, $CDCl_3$) δ 21.14, 24.62, 25.57, 26.34, 27.08, 39.92, 41.85, 218.19.

***References***

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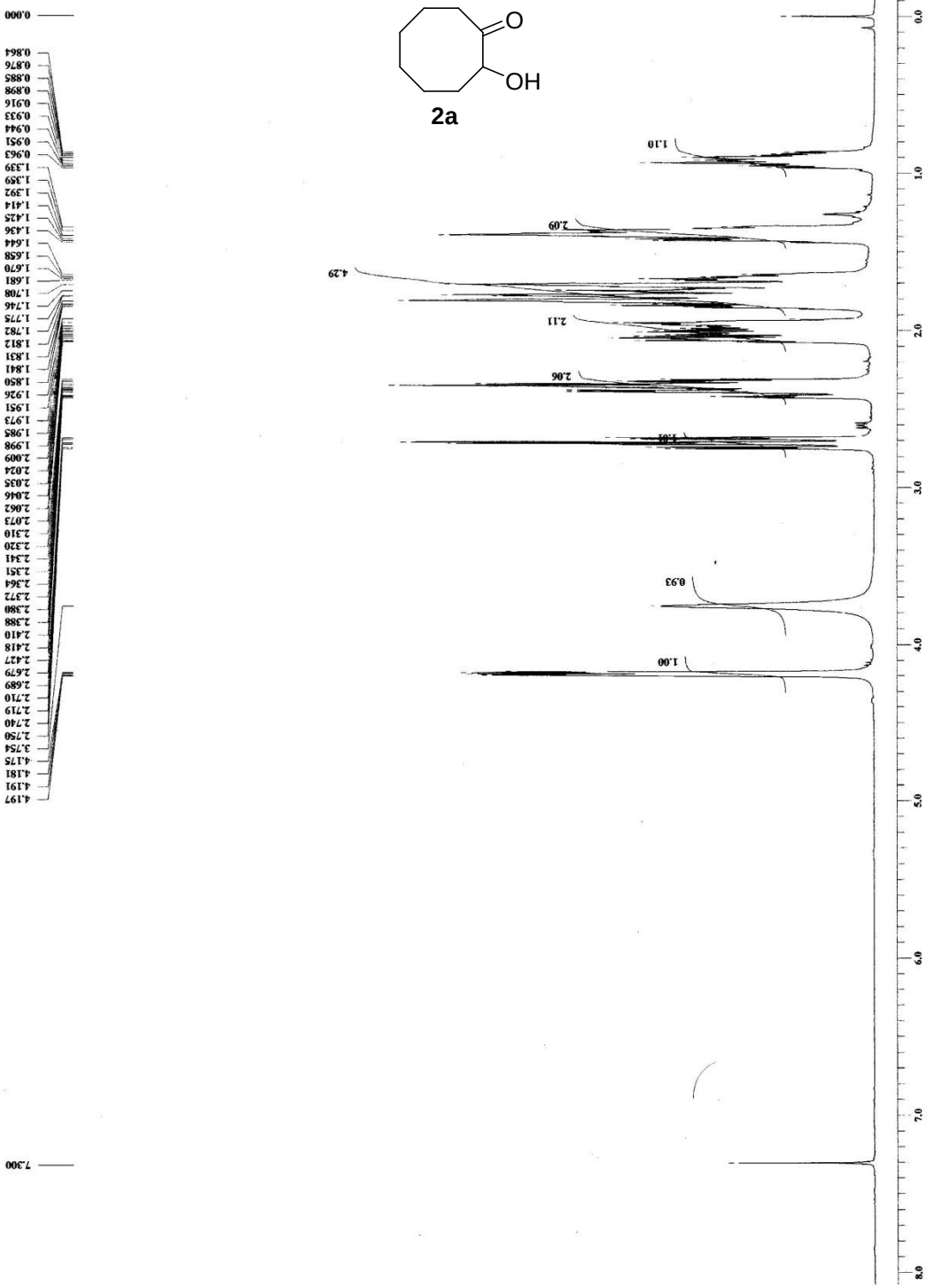
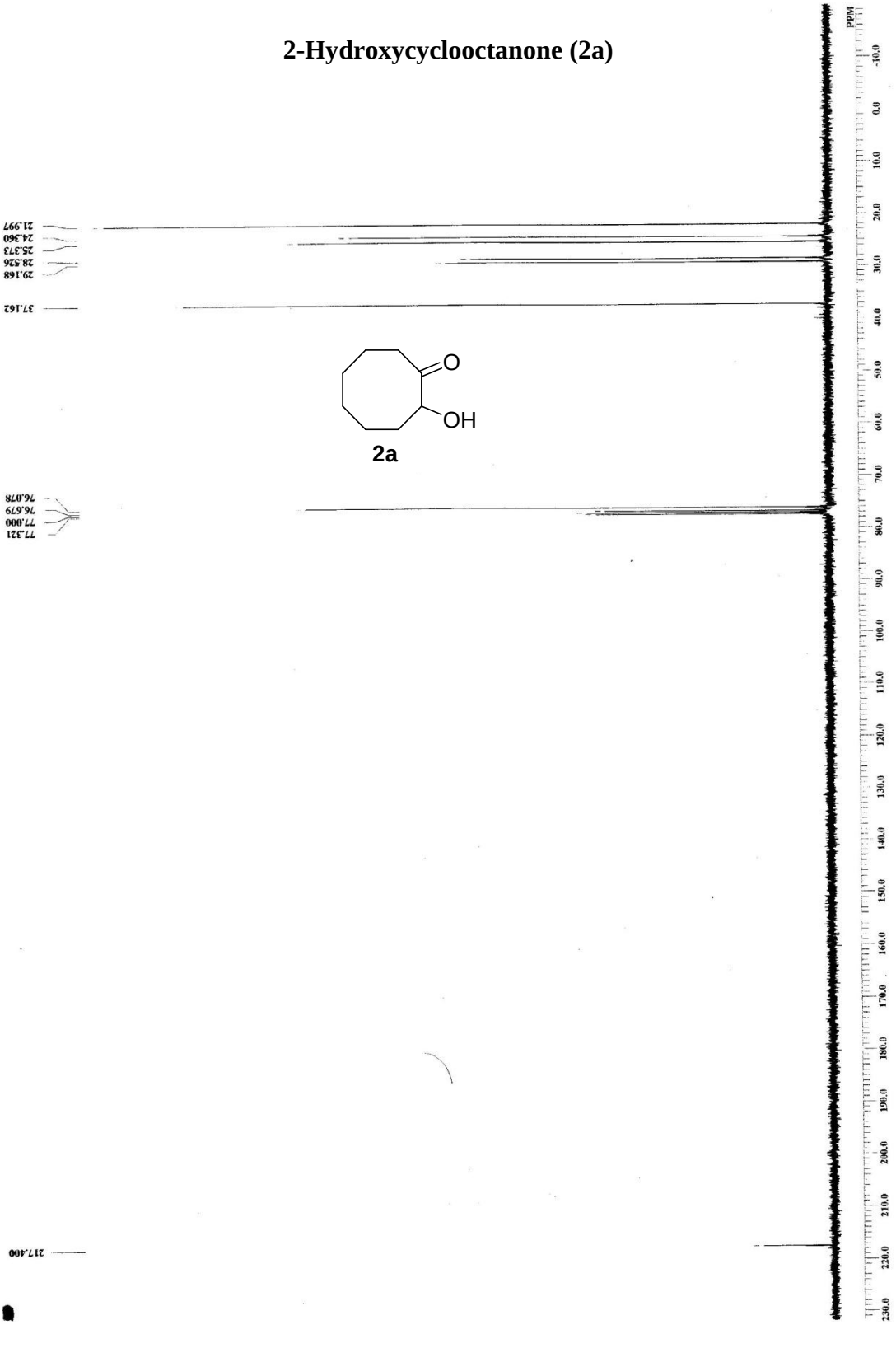
***Proton and Carbon NMR spectra***

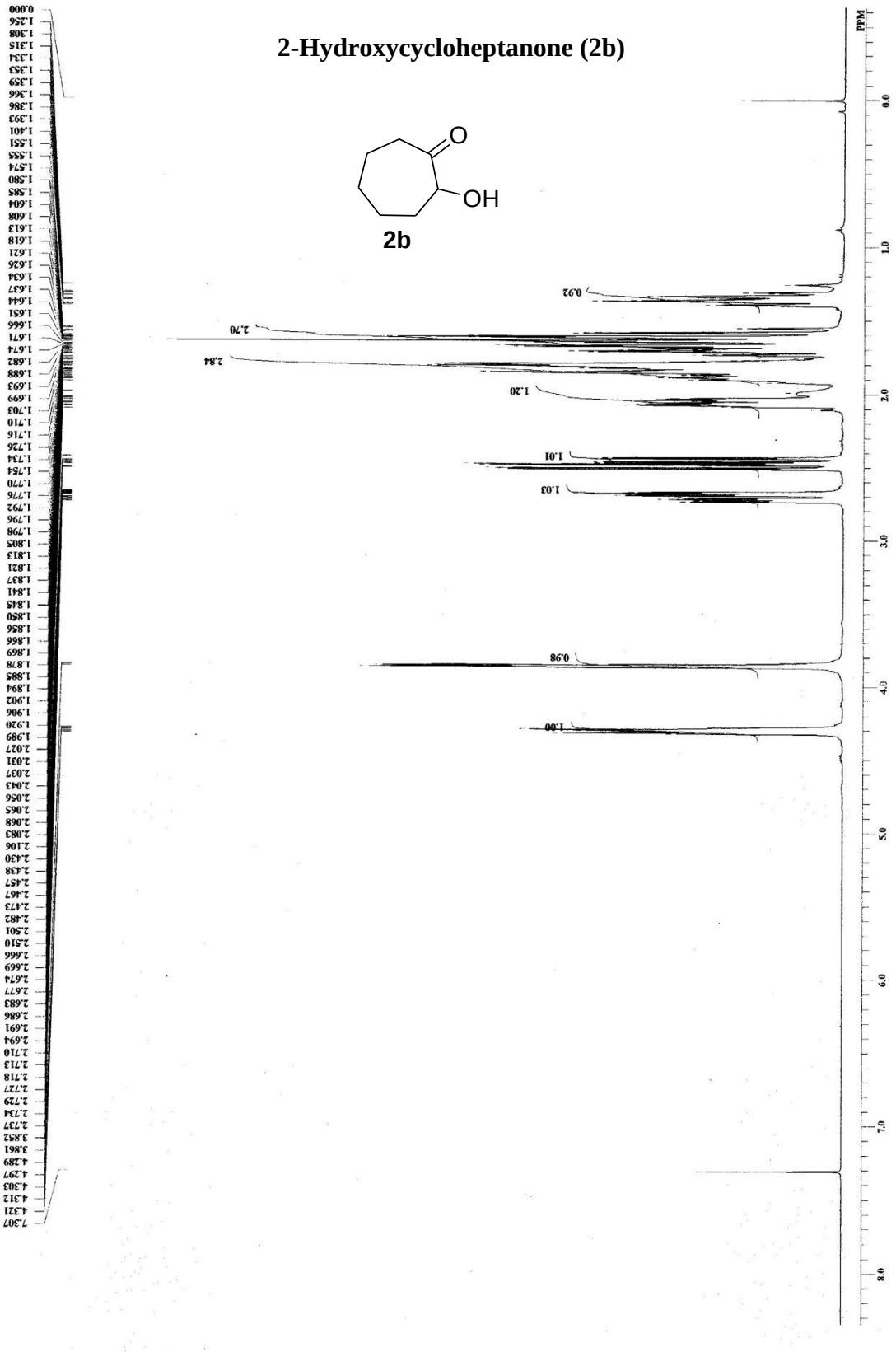
**2-Hydroxycyclooctanone (2a)**



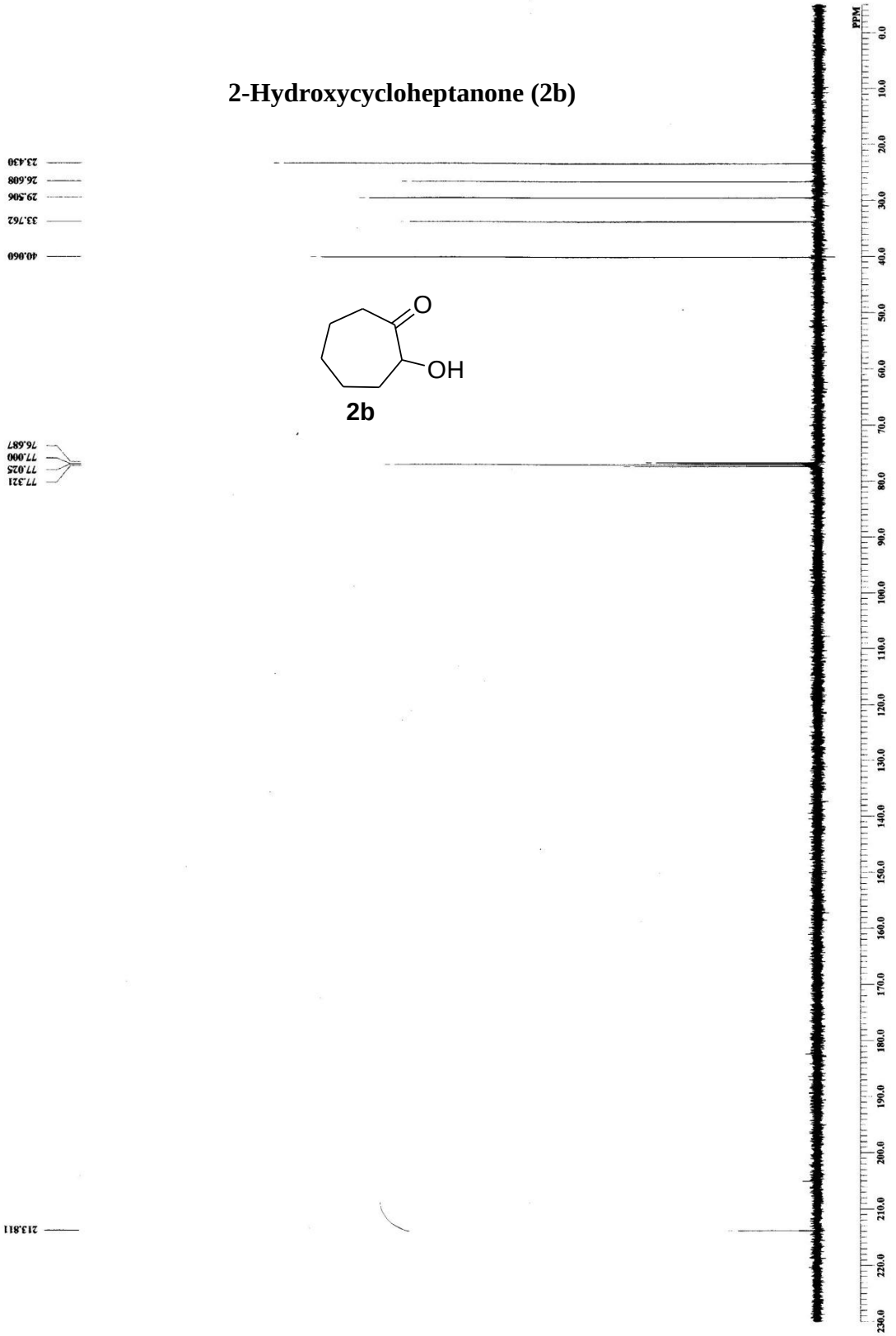
## 2-Hydroxycyclooctanone (2a)




**2a**



## 2-Hydroxycycloheptanone (2b)

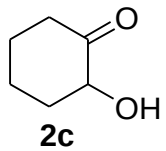






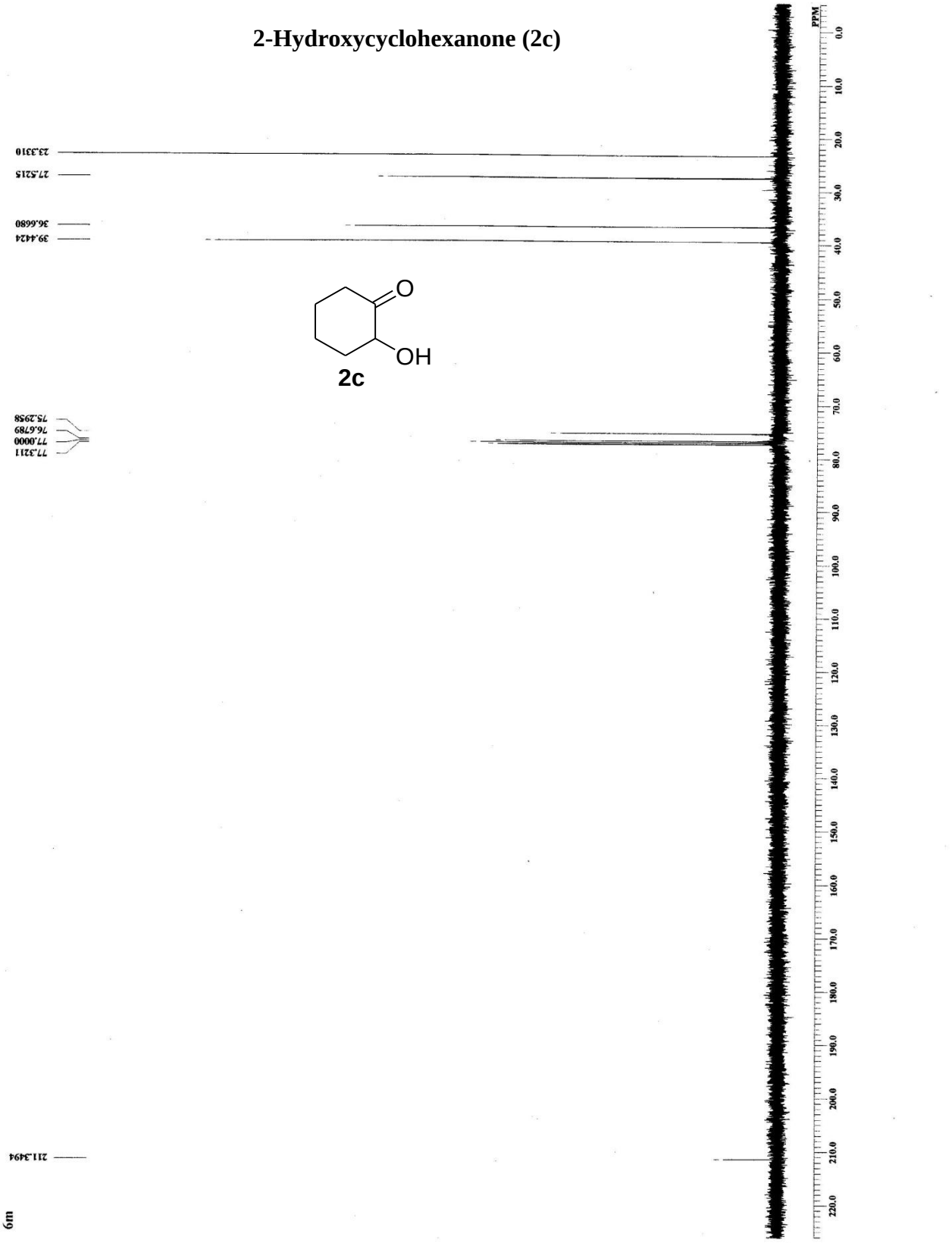
**2b**

**2-Hydroxycyclohexanone (2c)**

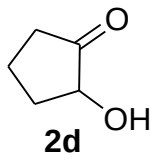



**2c**

**2-Hydroxycyclohexanone (2c)**

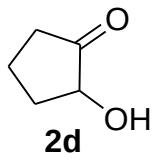


## 2-Hydroxycyclopentanone (2d)



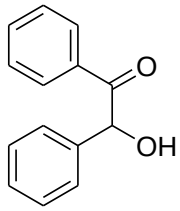

**2d**

## 2-Hydroxycyclopentanone (2d)



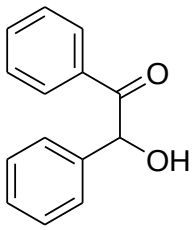

**2d**

**Benzoin (2h)**



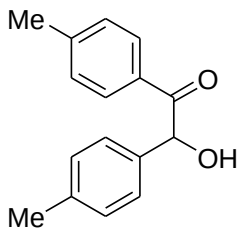

**2h**

**Benzoin (2h)**



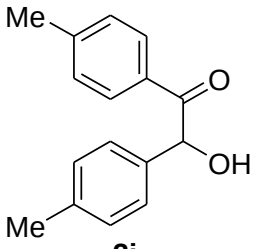

**2h**

**4,4-Dimethylbenzoin (2j)**



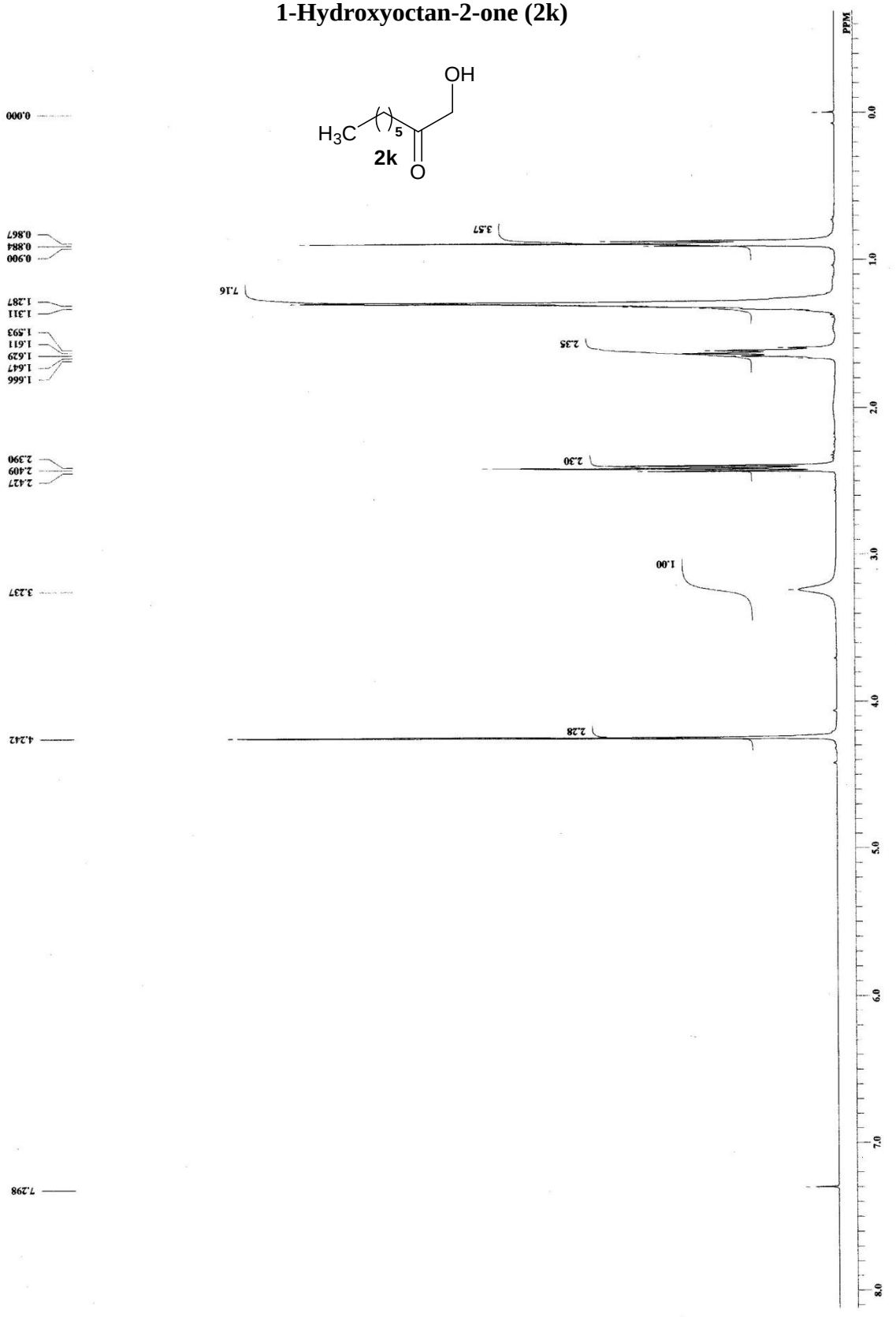

**2j**

**4,4-Dimethylbenzoin (2j)**

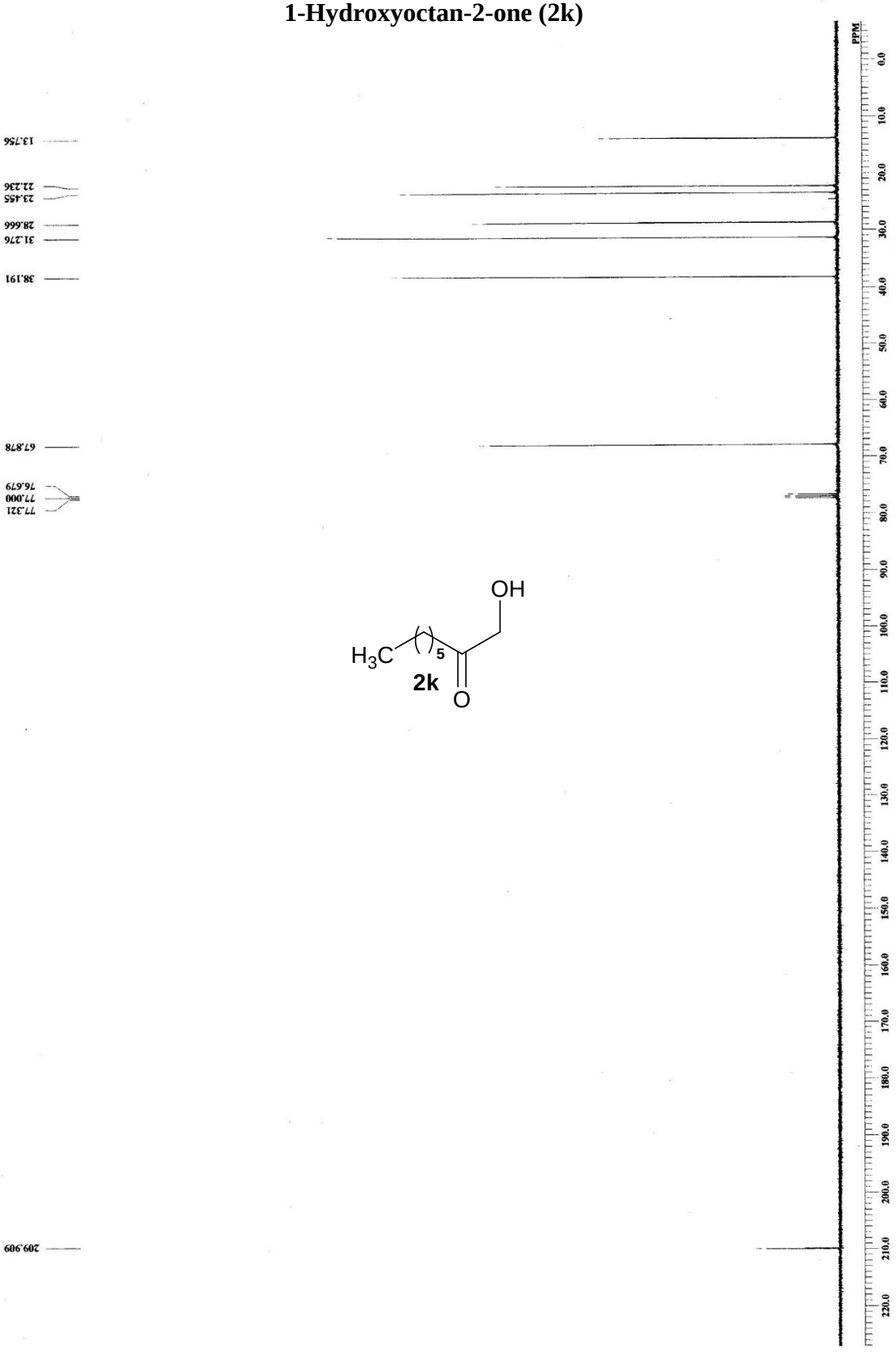



**2j**

**1-Hydroxyoctan-2-one (2k)**



**1-Hydroxyoctan-2-one (2k)**

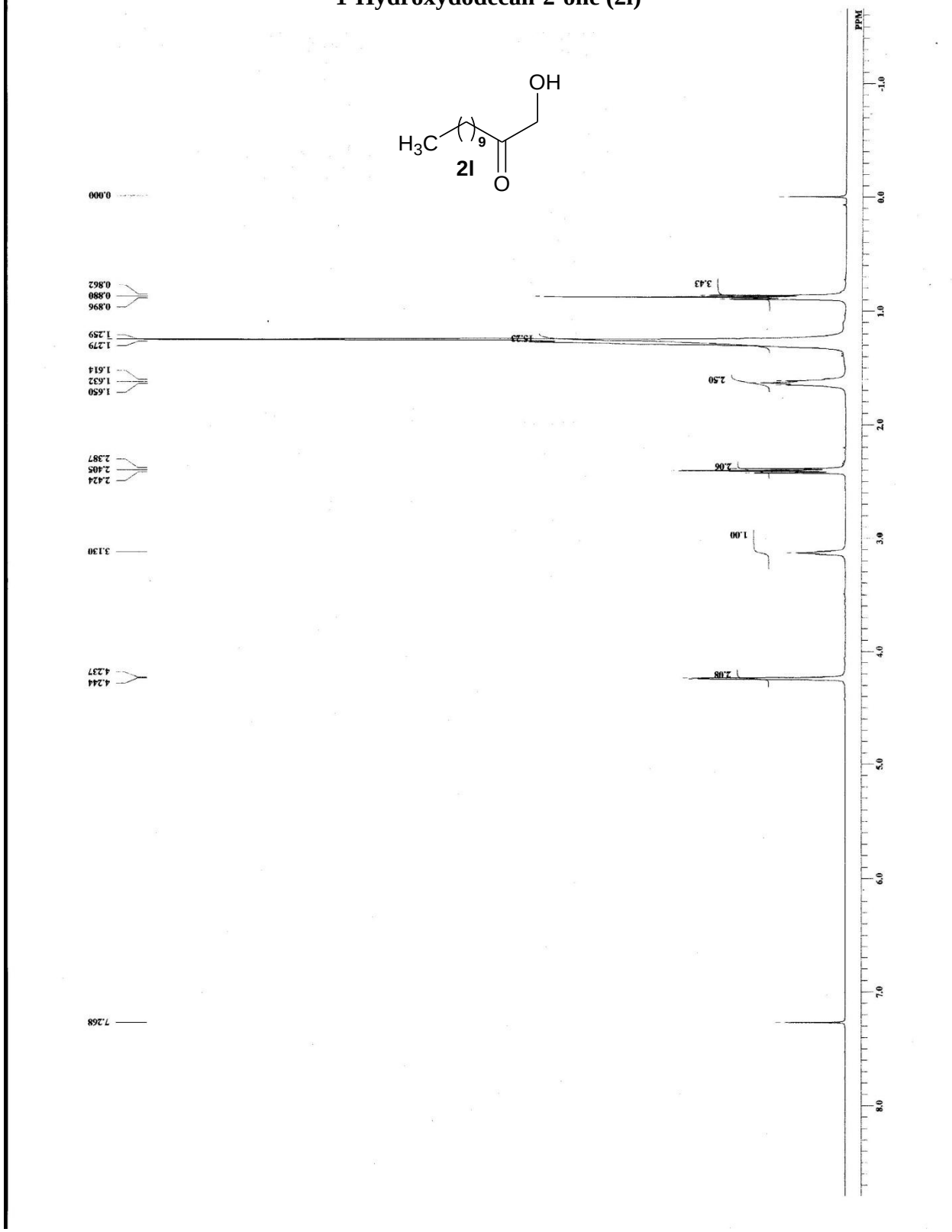




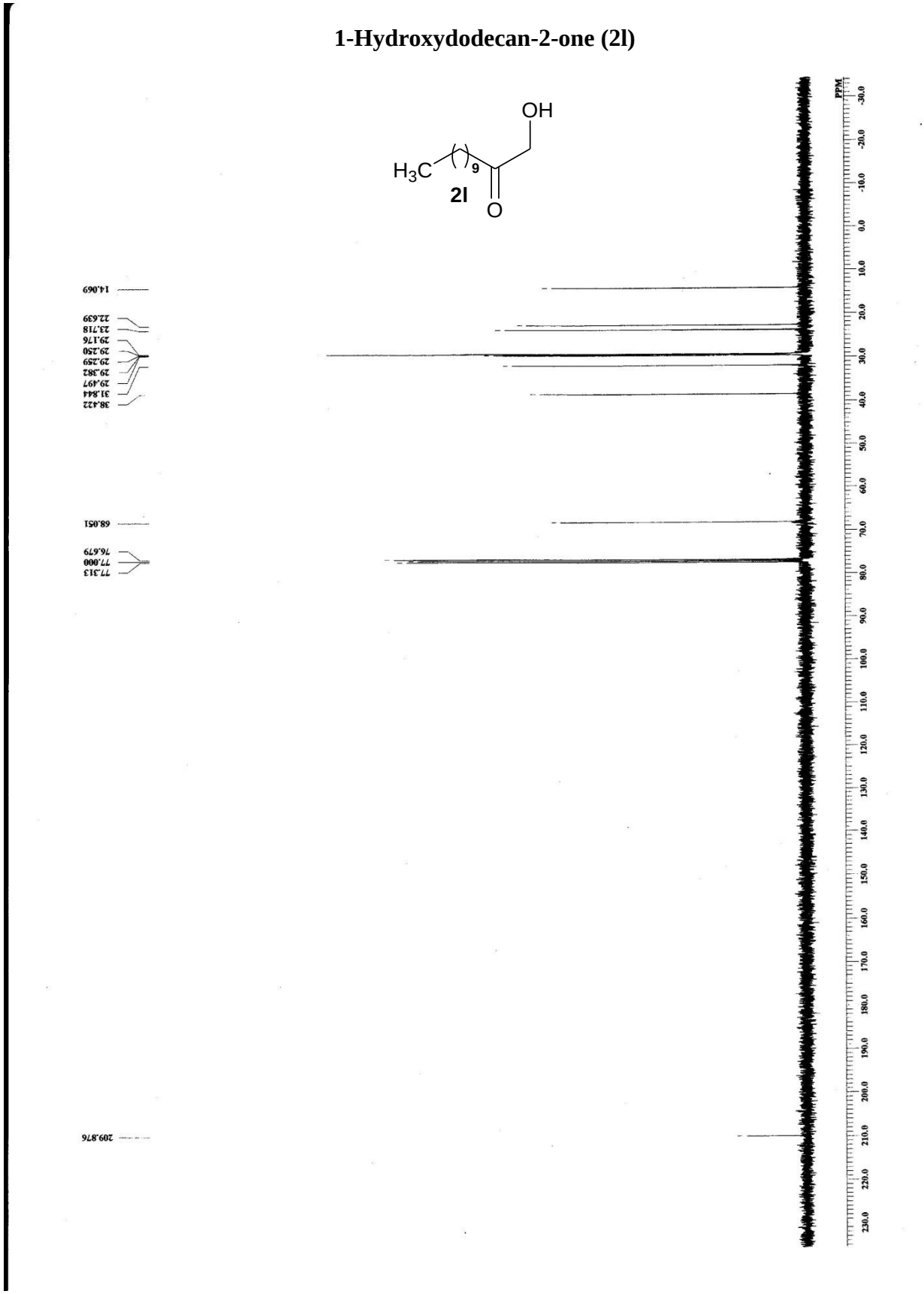


**2k**

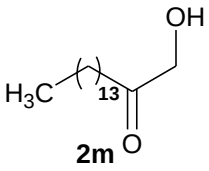
**1-Hydroxydodecan-2-one (2l)**



## 1-Hydroxydodecan-2-one (2l)

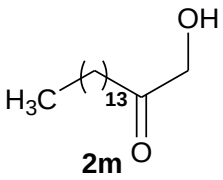


**1-Hydroxyhexadecan-2-one (2m)**



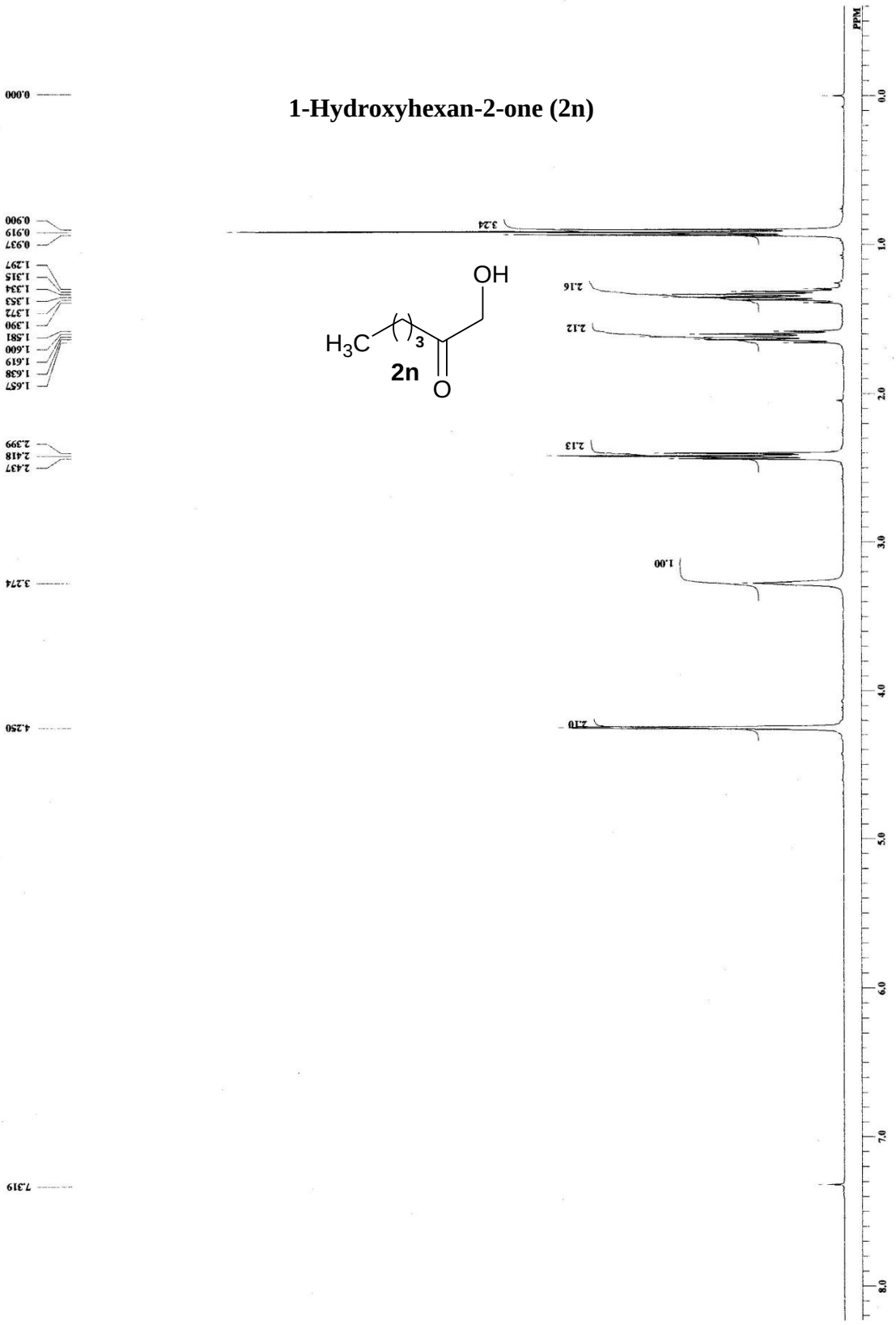

**2m**

**1-Hydroxyhexadecan-2-one (2m)**

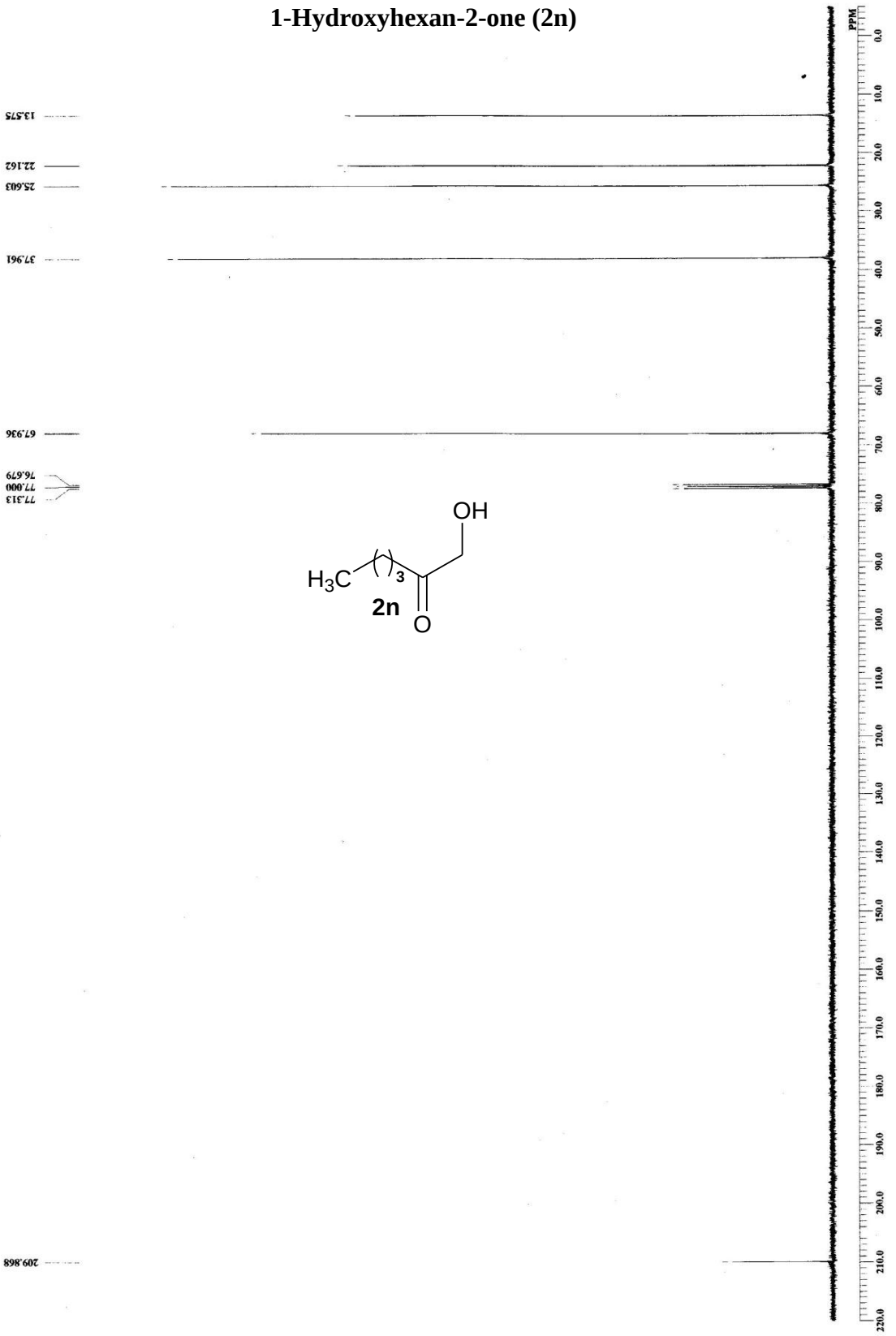



**2m**

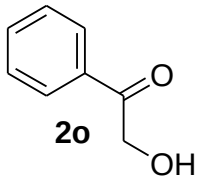
**1-Hydroxyhexan-2-one (2n)**



**1-Hydroxyhexan-2-one (2n)**

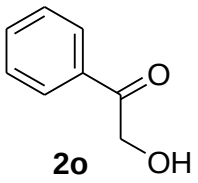


**2-Hydroxy-1-phenylethanone (2o)**



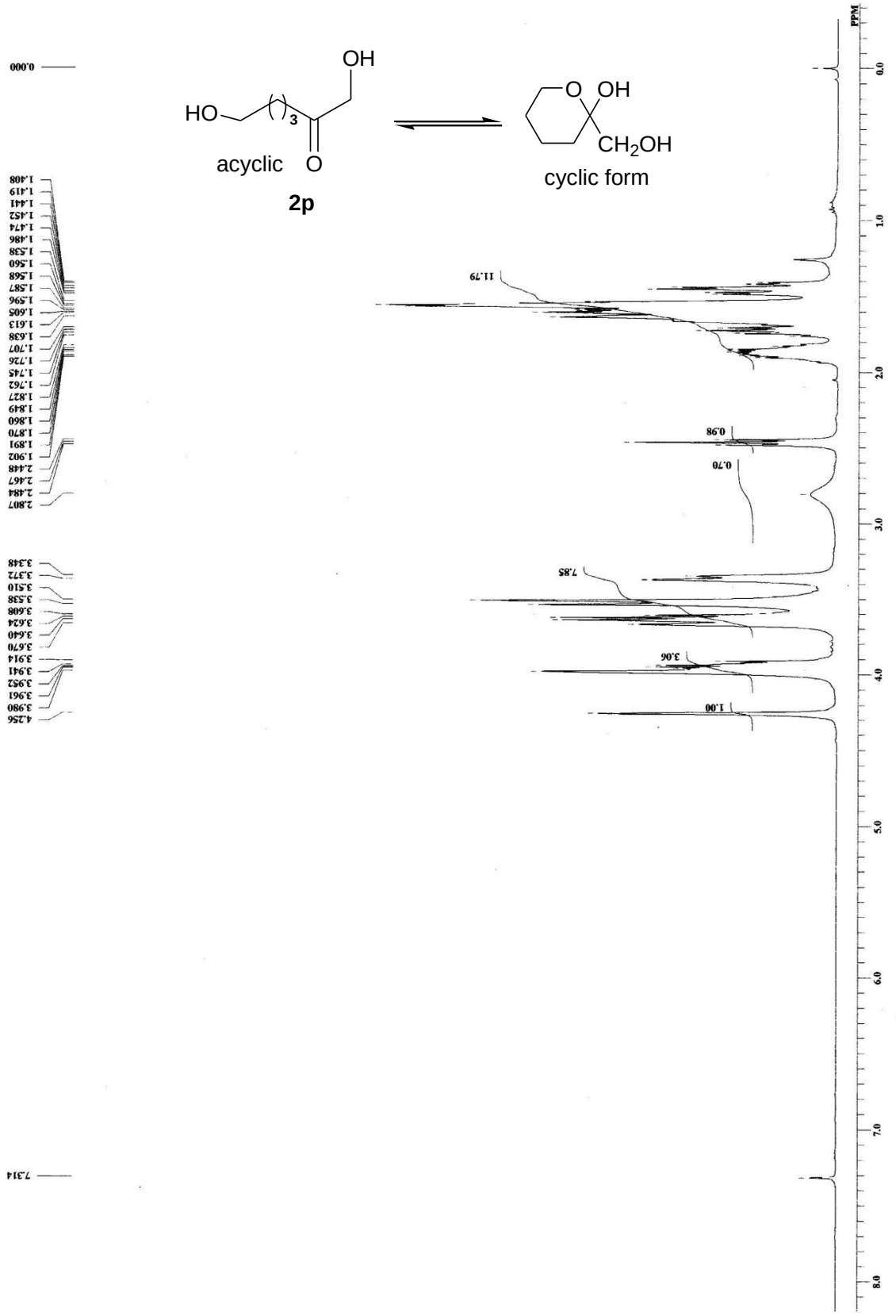

**2o**

## 2-Hydroxy-1-phenylethanone (2o)

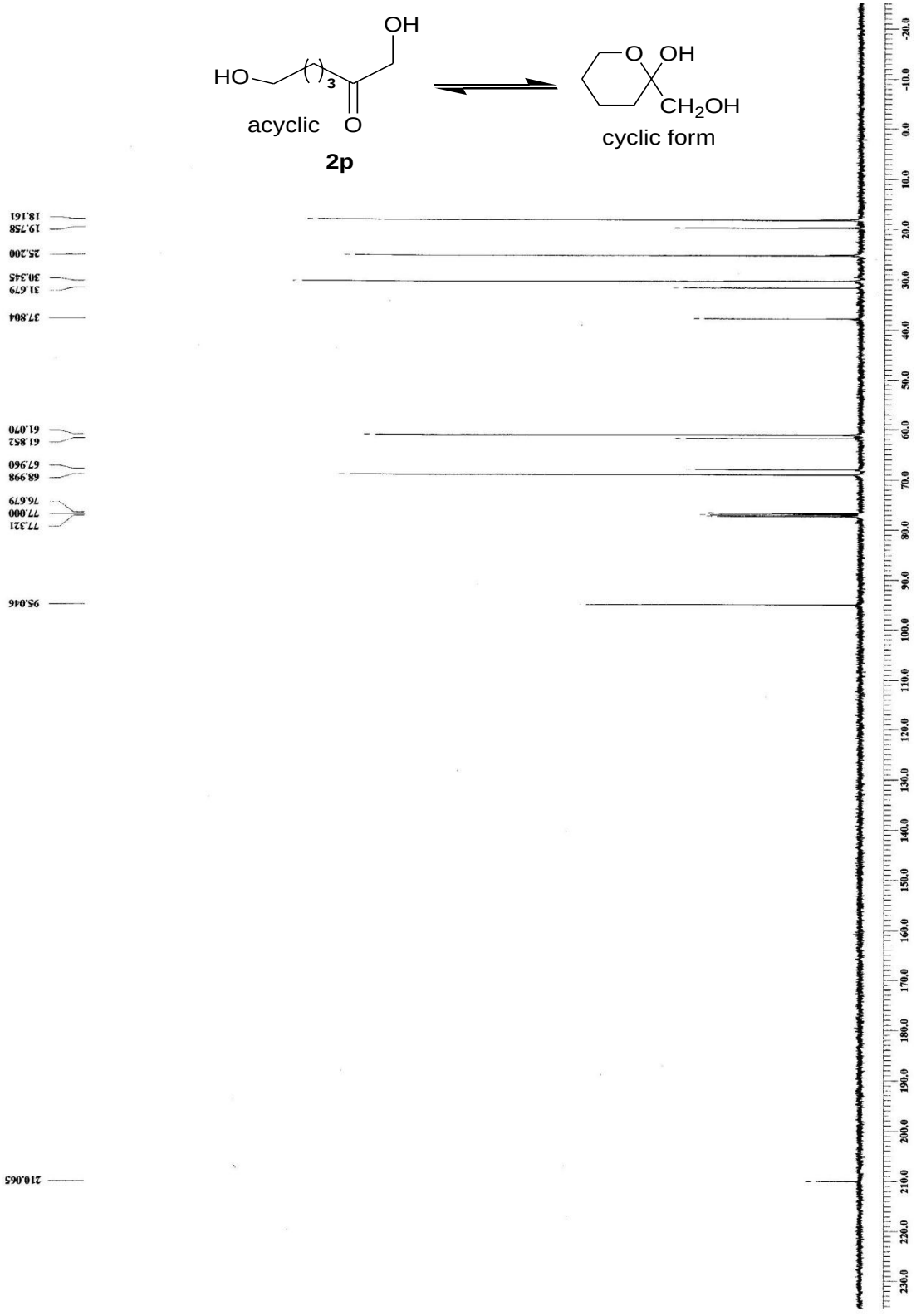



**2o**

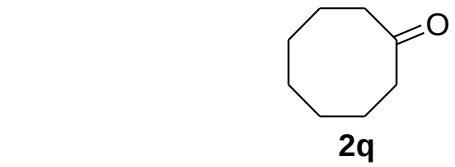
**1,6-Dihydroxyhexan-2-one (2p) (mixture of open-chain and cyclic form)**



**1,6-Dihydroxyhexan-2-one (2p) (mixture of open-chain and cyclic form)**

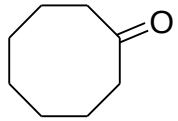


**Cyclooctanone (2q)**



**2q**

**Cyclooctanone (2q)**




**2q**