

# **SUPPORTING INFORMATION**

**for**

## **Substituent Effects on the Ultraviolet Absorption Properties of 2,4-Dihydroxy Dibenzophenone**

**Feng Wu, Shengqiong Tan, Zhengjun Fang \*, Jiyu Deng, Zhengjie He, Chaoyi Huang, Chaktong Au and  
Bing Yi \***

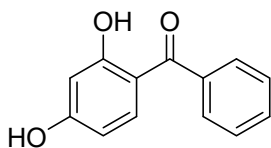
(Hunan Provincial Key Laboratory of Environmental Catalysis & Waste Recycling, College of Materials and  
Chemical Engineering, Hunan Institute of Engineering, Xiangtan 411104, China)

### **Contents**

<b>1. Data for <math>^1\text{H}</math> NMR and <math>^{13}\text{C}</math> NMR of compounds 1-9.....</b>	<b>2</b>
<b>2. Spectrum of <math>^1\text{H}</math> NMR and <math>^{13}\text{C}</math> NMR of compounds 1-9.....</b>	<b>4</b>
<b>3. The standard curve of absorbance versus concentration of compounds 1-9.....</b>	<b>13</b>

## 1、Data for $^1\text{H}$ NMR and $^{13}\text{C}$ NMR of compounds 1-9.

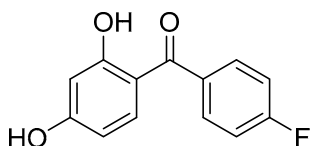
(1)  $\text{C}_{13}\text{H}_{10}\text{O}_3$



**Yield: 69.8%.**  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  12.61 (s, 1H), 7.64 – 7.62 (m, 2H), 7.57 (t,  $J = 7.5$  Hz, 1H), 7.49 (t,  $J = 7.5$  Hz, 3H), 6.47 – 6.47 (m, 1H), 6.35 (dd,  $J_1 = 10.0$ ,  $J_2 = 5.0$  Hz, 1H), 5.85 (s, 1H).

$^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )  $\delta$  200.22, 166.05, 138.14, 136.07, 131.52, 130.13, 128.81, 128.31, 113.32, 107.74, 103.60.

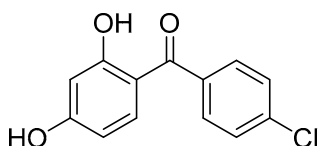
(2)  $\text{C}_{13}\text{H}_9\text{FO}_3$



**Yield: 42%.**  $^1\text{H}$  NMR (400 MHz, DMSO)  $\delta$  11.97 (s, 1H), 10.69 (s, 1H), 7.71 (q,  $J = 4.0$ , 2H), 7.37 – 7.33 (m, 3H), 6.40 – 6.37 (m, 2H).

$^{13}\text{C}$  NMR (100 MHz, DMSO)  $\delta$  197.05, 164.69, 163.98, 163.96 (d,  $J = 248.0$  Hz), 135.00, 134.59 (d,  $J = 2.0$  Hz), 131.49 (d,  $J = 9.0$  Hz), 115.38 (d,  $J = 22.0$  Hz), 112.79, 108.19, 102.75.

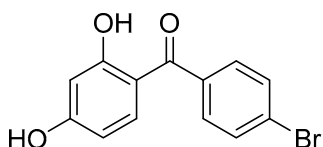
(3)  $\text{C}_{13}\text{H}_9\text{ClO}_3$



**Yield: 51%.**  $^1\text{H}$  NMR (400 MHz, DMSO)  $\delta$  11.93 (s, 1H), 10.72 (s, 1H), 7.65 – 7.63 (m, 2H), 7.60 – 7.58 (m, 2H), 7.35 (d,  $J = 8.0$  Hz, 1H), 6.40 – 6.37 (m, 2H).

$^{13}\text{C}$  NMR (100 MHz, DMSO)  $\delta$  197.11, 164.84, 164.00, 136.79, 136.39, 135.00, 130.54, 128.44, 112.73, 108.27, 102.75.

(4)  $\text{C}_{13}\text{H}_9\text{BrO}_3$

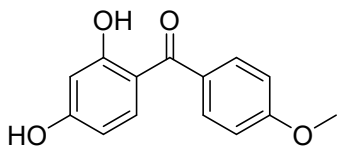


**Yield: 50%.**  $^1\text{H}$  NMR (400 MHz, DMSO)  $\delta$  11.92 (s, 1H), 10.71 (s, 1H), 7.74 – 7.72 (m, 2H), 7.57 –

7.55 (m, 2H), 7.35 (d,  $J = 8.0$  Hz, 1H), 6.40 – 6.36 (m, 2H).

$^{13}\text{C}$  NMR (100 MHz, DMSO)  $\delta$  197.23, 164.84, 163.99, 137.14, 135.01, 131.37, 130.67, 125.32, 112.70, 108.27, 102.74.

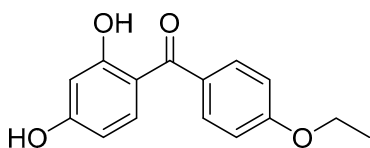
(5)  $\text{C}_{14}\text{H}_{12}\text{O}_4$



**Yield: 55%.**  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  12.61 (s, 1H), 7.66 (d,  $J = 10.0$  Hz, 2H), 7.54 (d,  $J = 10.0$  Hz, 1H), 6.99 (d,  $J = 5.0$  Hz, 2H), 6.46 – 6.46 (m, 1H), 6.36 (dd,  $J_1 = 10.0$ ,  $J_2 = 5.0$  Hz, 1H), 6.03 (s, 1H), 3.89 (s, 3H).

$^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )  $\delta$  198.85, 165.86, 162.55, 162.38, 135.73, 131.39, 130.65, 113.64, 108.89, 107.30, 103.67, 55.49.

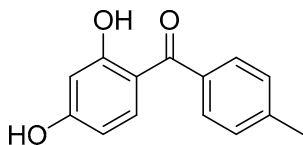
(6)  $\text{C}_{15}\text{H}_{14}\text{O}_4$



**Yield: 48%.**  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  12.63 (s, 1H), 7.64 (d,  $J = 8.0$  Hz, 2H), 7.53 (d,  $J = 8.0$  Hz, 1H), 6.96 (d,  $J = 8.0$  Hz, 2H), 6.46 (d,  $J = 4.0$  Hz, 1H), 6.36 (dd,  $J_1 = 12.0$ ,  $J_2 = 4.0$  Hz, 1H), 4.12 (q,  $J = 6.6$  Hz, 2H), 1.45 (t,  $J = 6.0$  Hz, 3H).

$^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  199.06, 165.78, 162.74, 162.02, 135.84, 131.41, 130.35, 114.13, 113.50, 107.52, 103.65, 63.79, 14.66.

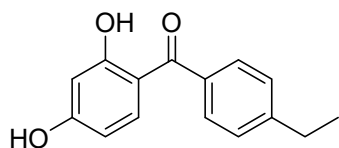
(7)  $\text{C}_{14}\text{H}_{12}\text{O}_3$



**Yield: 41%.**  $^1\text{H}$  NMR (400 MHz, DMSO)  $\delta$  12.23 (s, 1H), 10.68 (s, 1H), 7.53 (d,  $J = 8.0$  Hz, 2H), 7.39 (d,  $J = 8.0$  Hz, 1H), 7.34 – 7.32 (m, 2H), 6.39 – 6.37 (m, 2H), 2.39 (s, 3H).

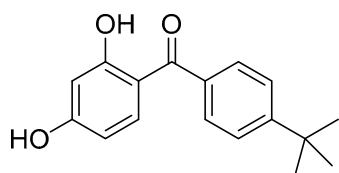
$^{13}\text{C}$  NMR (100 MHz, DMSO)  $\delta$  198.45, 164.65, 164.39, 141.79, 135.26, 135.17, 128.87, 128.85, 112.59, 108.06, 102.73, 21.04.

(8)  $\text{C}_{15}\text{H}_{14}\text{O}_3$



**Yield: 40%.**  $^1\text{H}$  NMR (400 MHz, DMSO)  $\delta$  12.25 (s, 1H), 10.68 (s, 1H), 7.55 (d,  $J = 8.0$  Hz, 2H), 7.40 – 7.35 (m, 3H), 6.40 – 6.37 (m, 2H), 2.69 (q,  $J = 6.6$  Hz, 2H), 1.21 (t,  $J = 8.0$  Hz, 3H).  
 $^{13}\text{C}$  NMR (100 MHz, DMSO)  $\delta$  198.48, 164.69, 164.45, 147.88, 135.51, 135.21, 128.95, 127.71, 112.56, 108.08, 102.74, 28.11, 15.21.

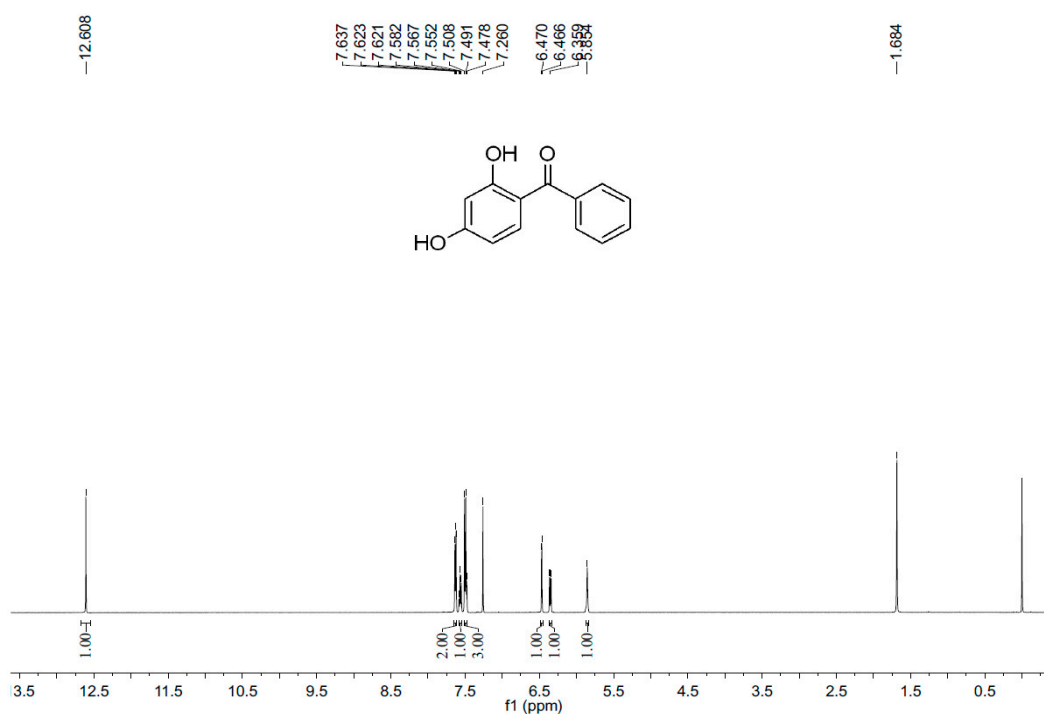
(9)  $\text{C}_{17}\text{H}_{18}\text{O}_3$



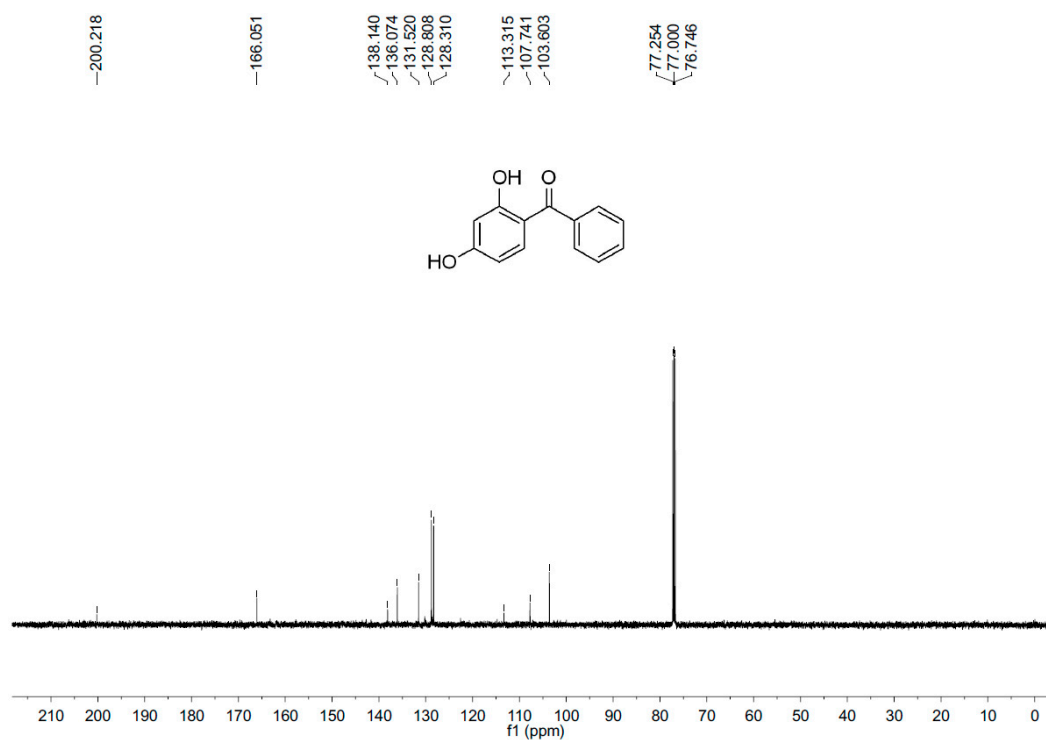
**Yield: 36%.**  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  12.72 (s, 1H), 7.58 (d,  $J = 8.0$  Hz, 2H), 7.51 (t,  $J = 10.0$  Hz, 3H), 6.46 (d,  $J = 4.0$  Hz, 1H), 6.37 – 6.34 (m, 1H), 1.36 (s, 9H).  
 $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  200.37, 165.84, 163.60, 155.33, 136.21, 135.13, 128.88, 125.27, 113.17, 107.95, 103.55, 34.97, 31.07.

## 2. Spectrum of $^1\text{H}$ NMR and $^{13}\text{C}$ NMR of compounds 1-9.

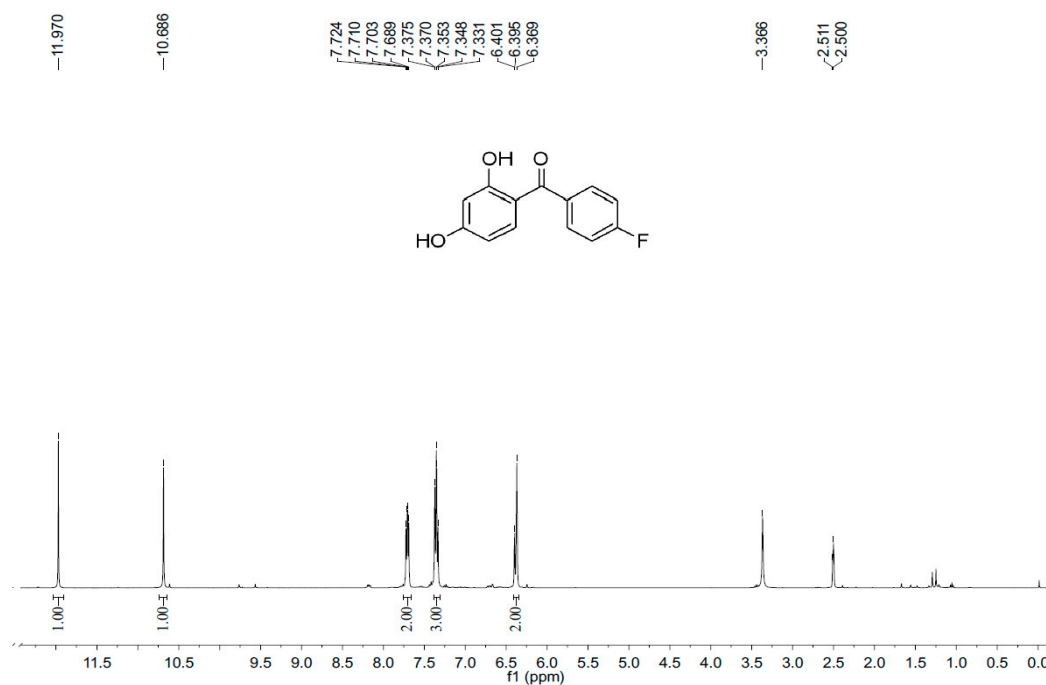
### 2.1 The $^1\text{H}$ NMR spectrum of 2,4-dihydroxybenzophenone



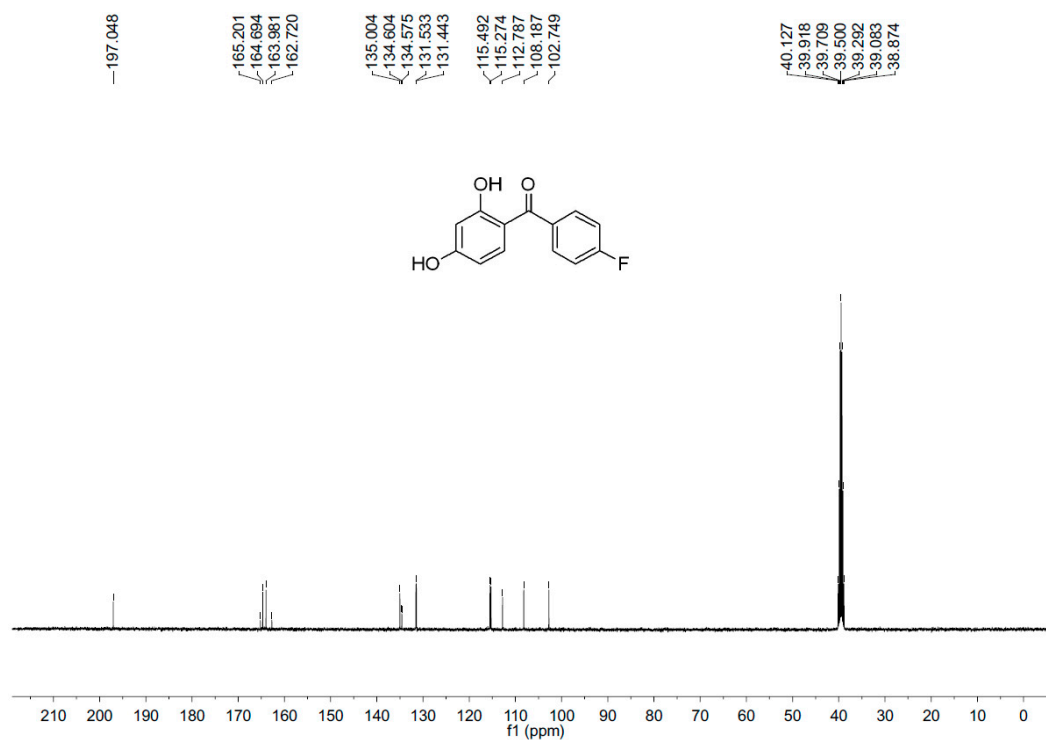
## 2.2 The $^{13}\text{C}$ NMR spectrum of 2,4-dihydroxybenzophenone



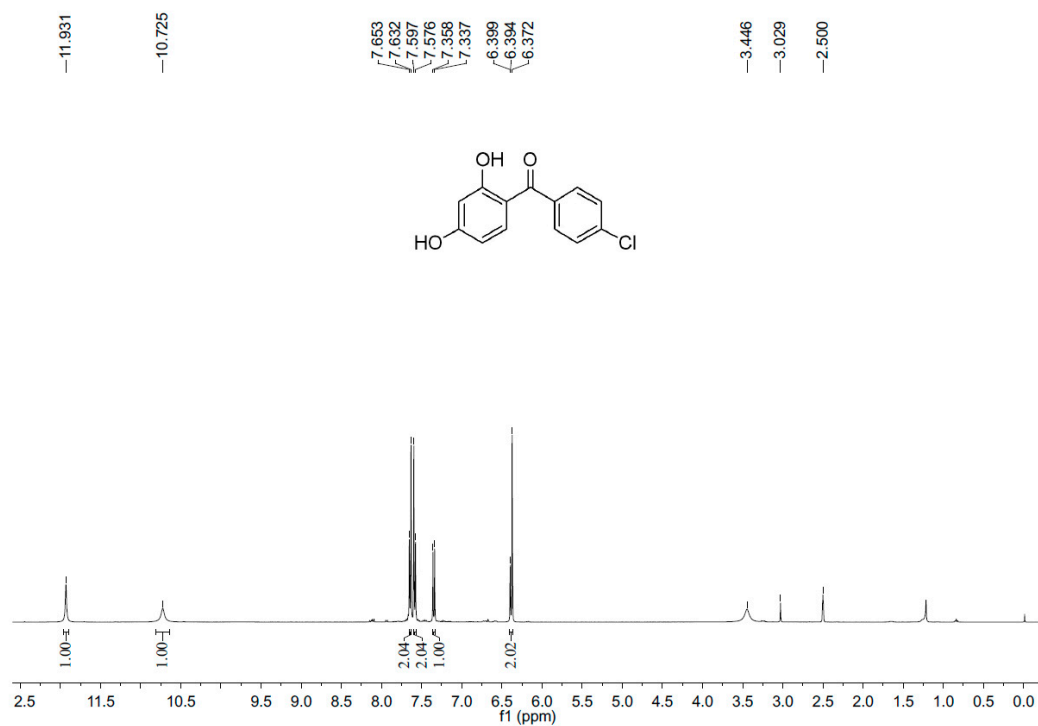
## 2.3 The $^1\text{H}$ NMR spectrum of 2,4-dihydroxy-4'-fluorophenone



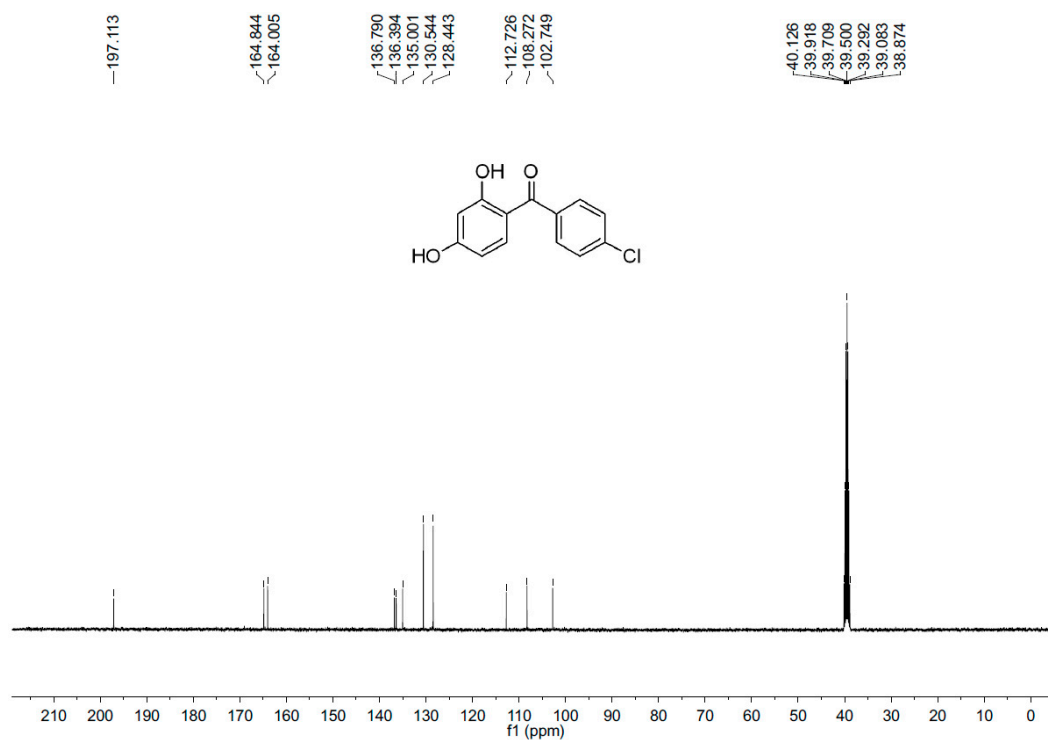
## 2.4 The $^{13}\text{C}$ NMR spectrum of 2,4-dihydroxy-4'-fluorophenone



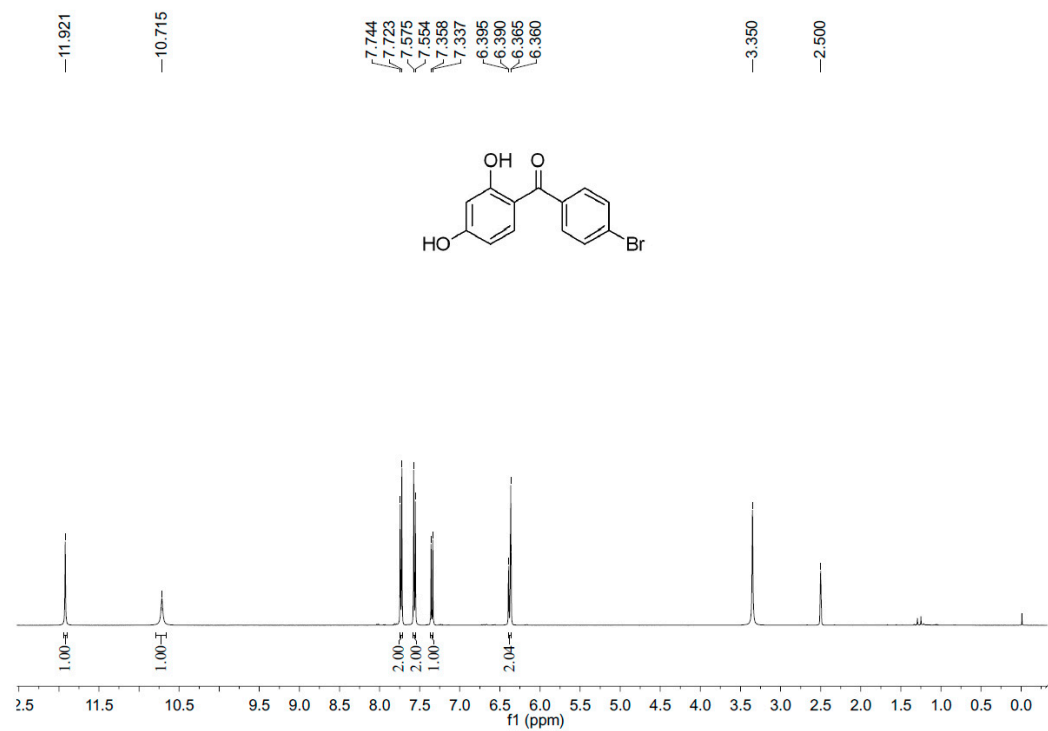
## 2.5 The $^1\text{H}$ NMR spectrum of 2,4-dihydroxy-4'-chlorobenzophenone



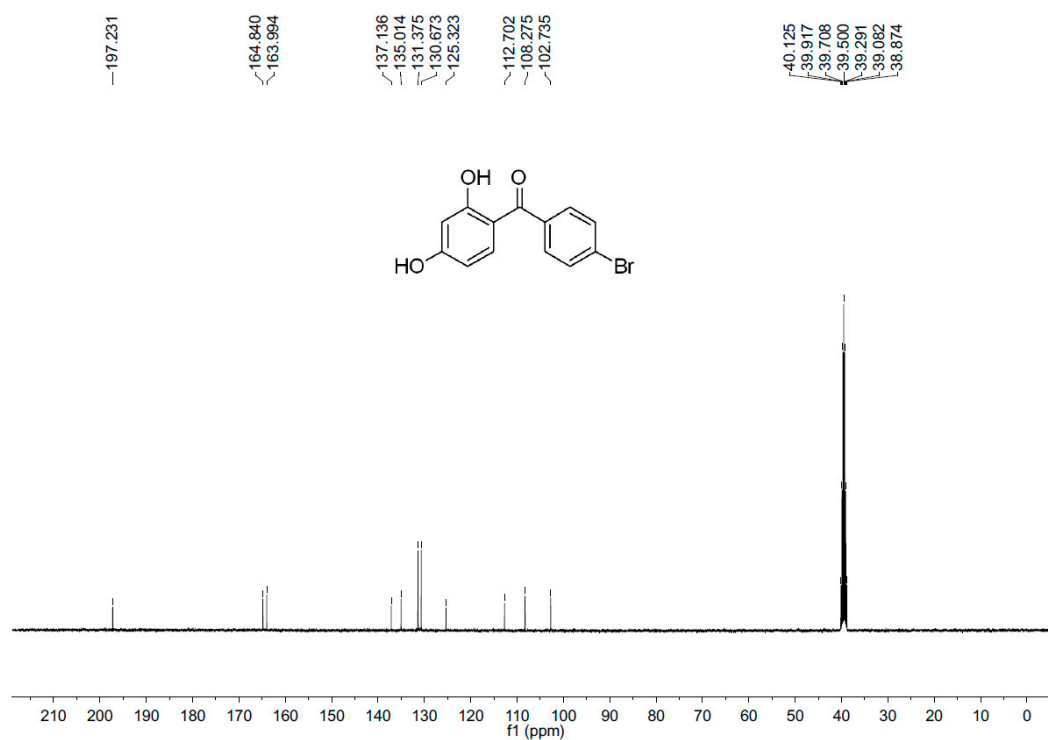
## 2.6 The $^{13}\text{C}$ NMR spectrum of 2,4-dihydroxy-4'-chlorobenzophenone



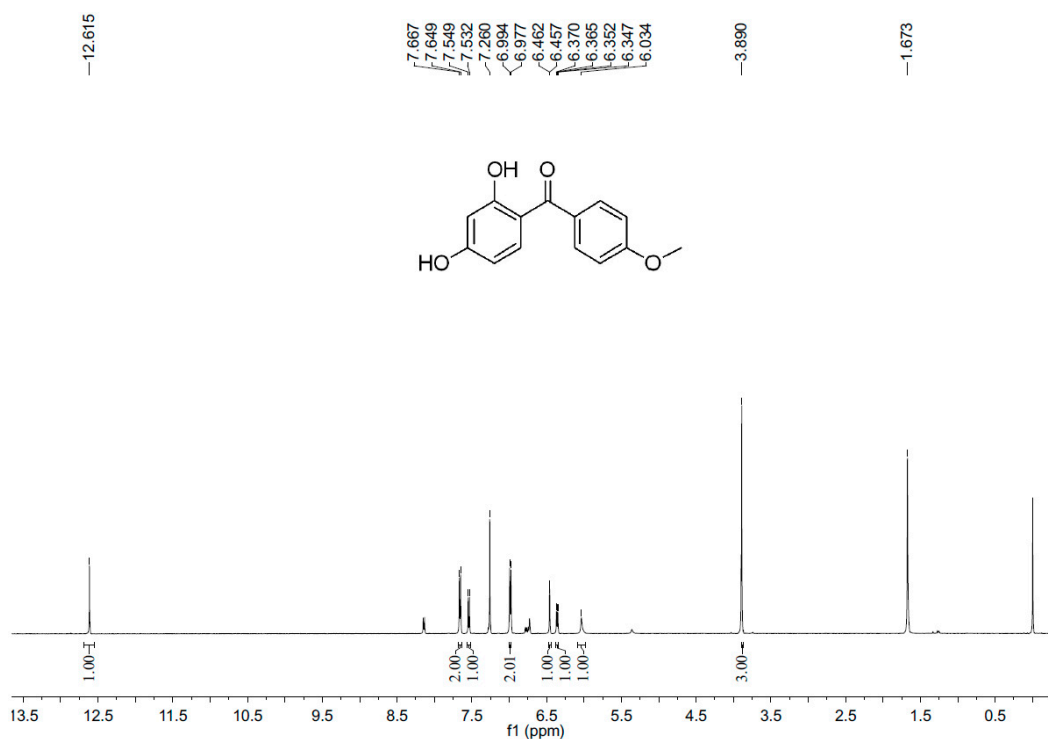
## 2.7 The $^1\text{H}$ NMR spectrum of 2,4-dihydroxy-4'-bromobenzophenone



## 2.8 The $^{13}\text{C}$ NMR spectrum of 2,4-dihydroxy-4'-bromodibenzophenone

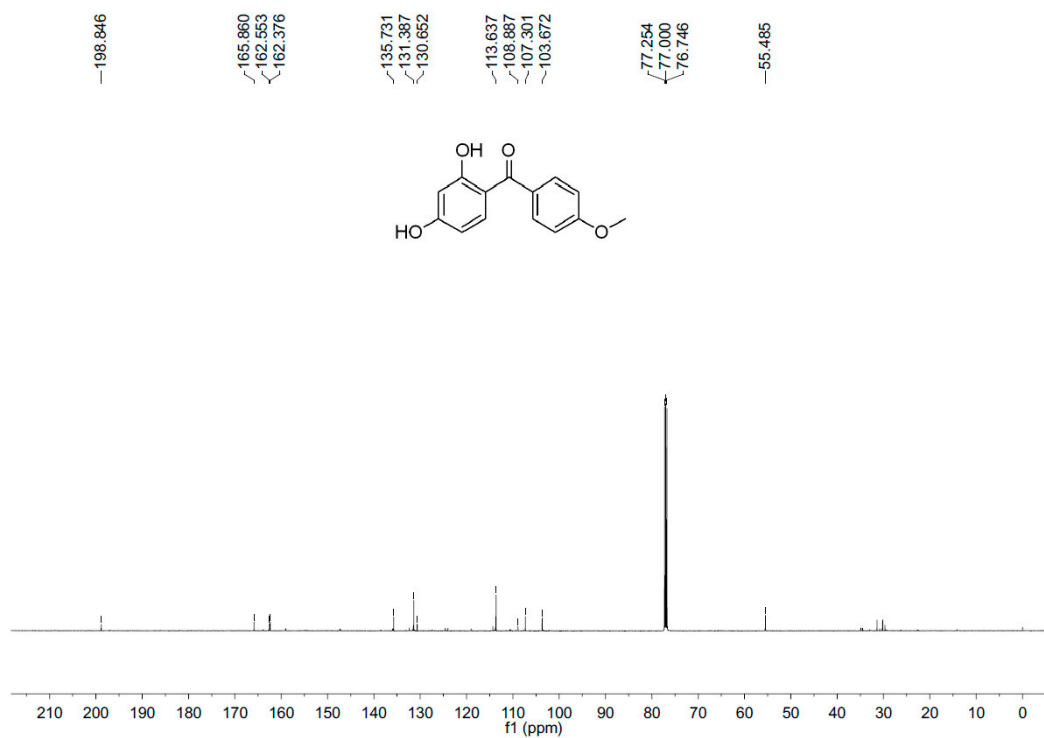


## 2.9 The $^1\text{H}$ NMR spectrum of 2,4-dihydroxy-4'-methoxydibenzophenone

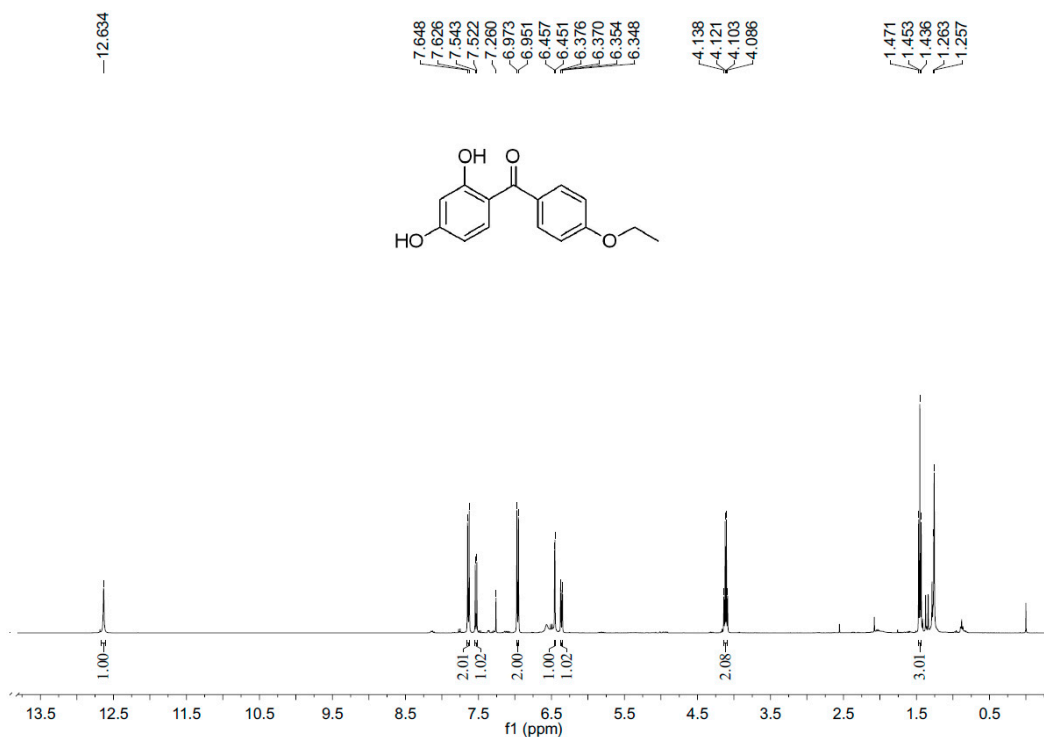




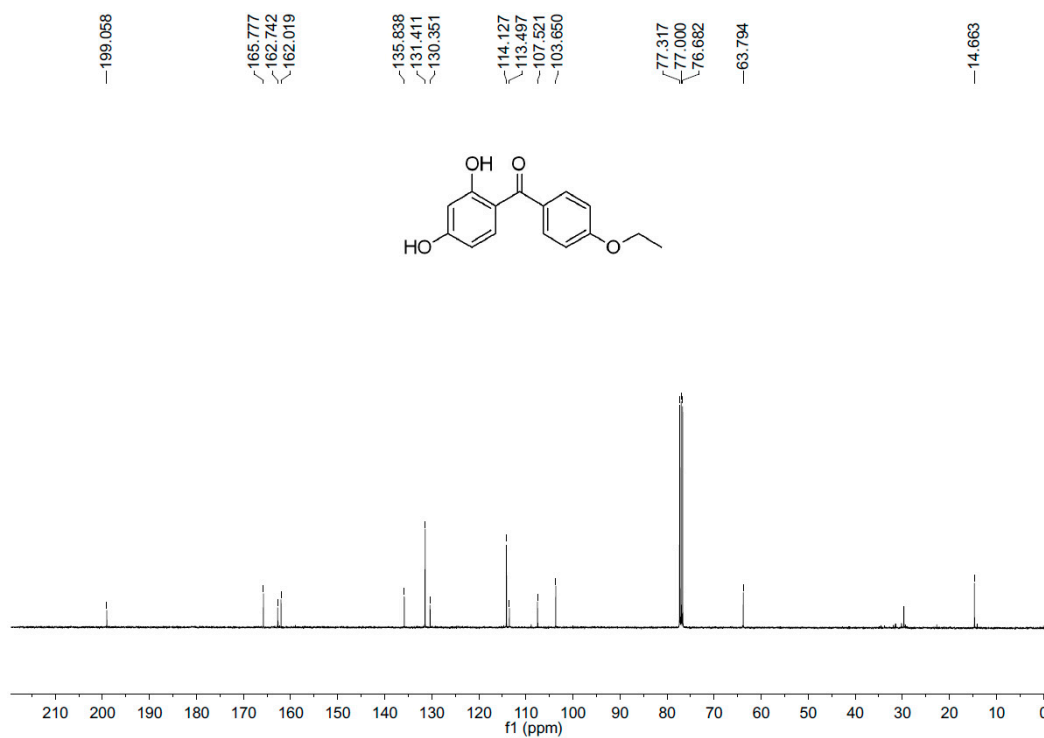
## 2.10 The $^{13}\text{C}$ NMR spectrum of 2,4-dihydroxy-4'-methoxydibenzophenone



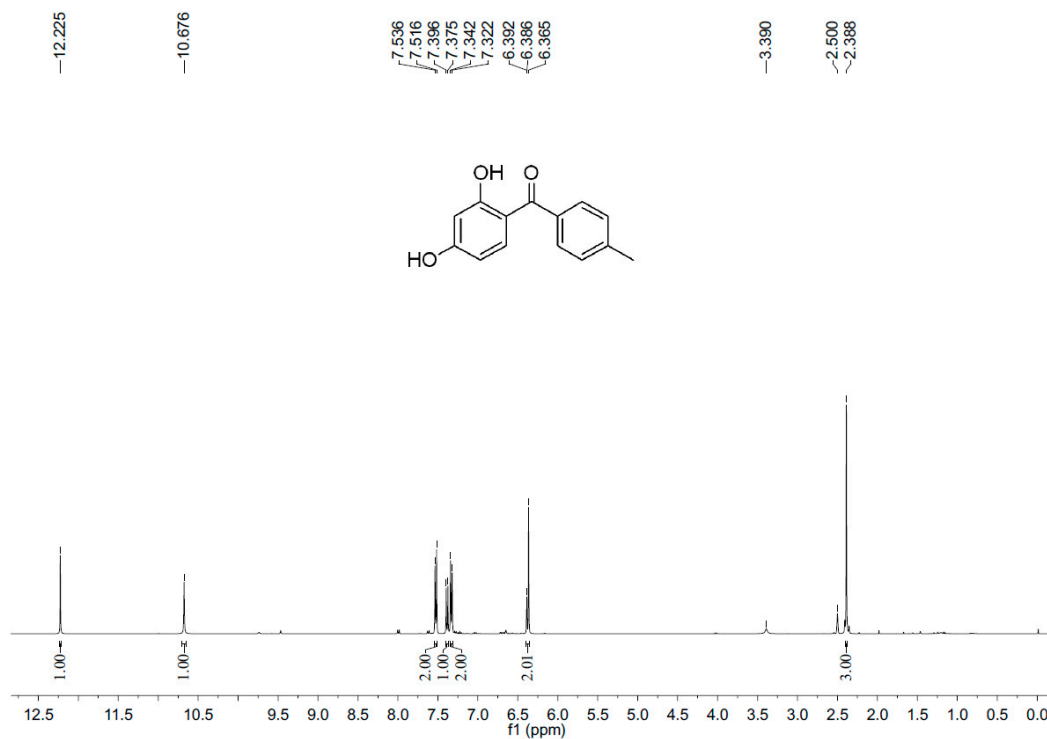
## 2.11 The $^1\text{H}$ NMR spectrum of 2,4-dihydroxy-4'-ethoxydibenzophenone



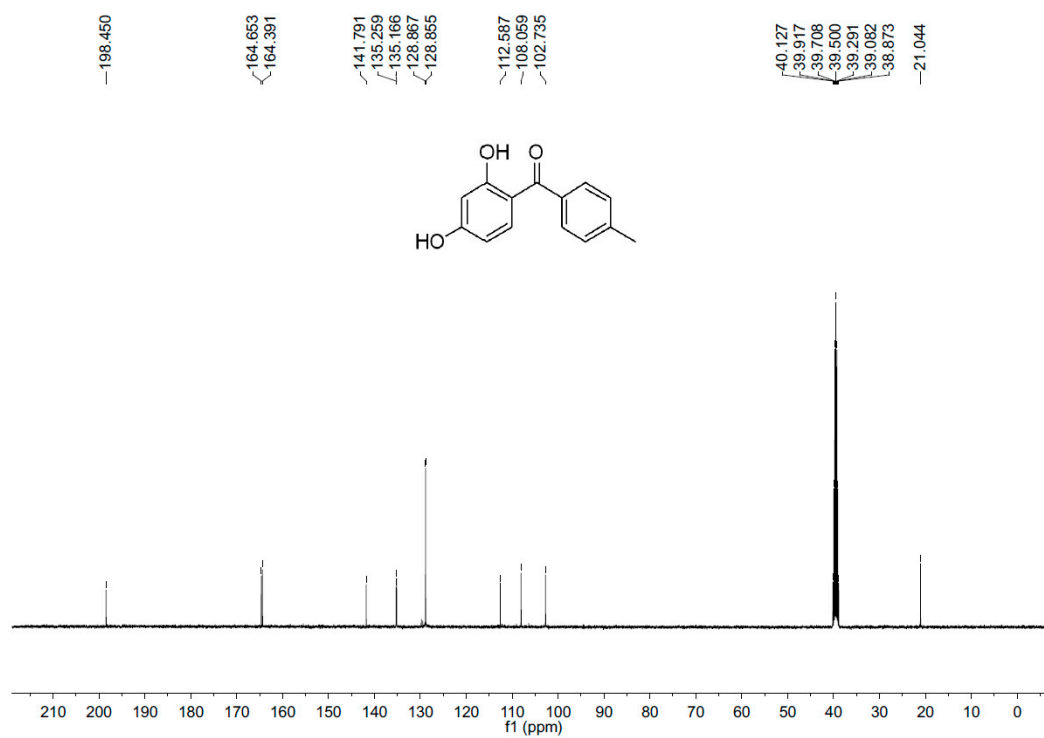
## 2.12 The $^{13}\text{C}$ NMR spectrum of 2,4-dihydroxy-4'-ethoxydibenzophenone



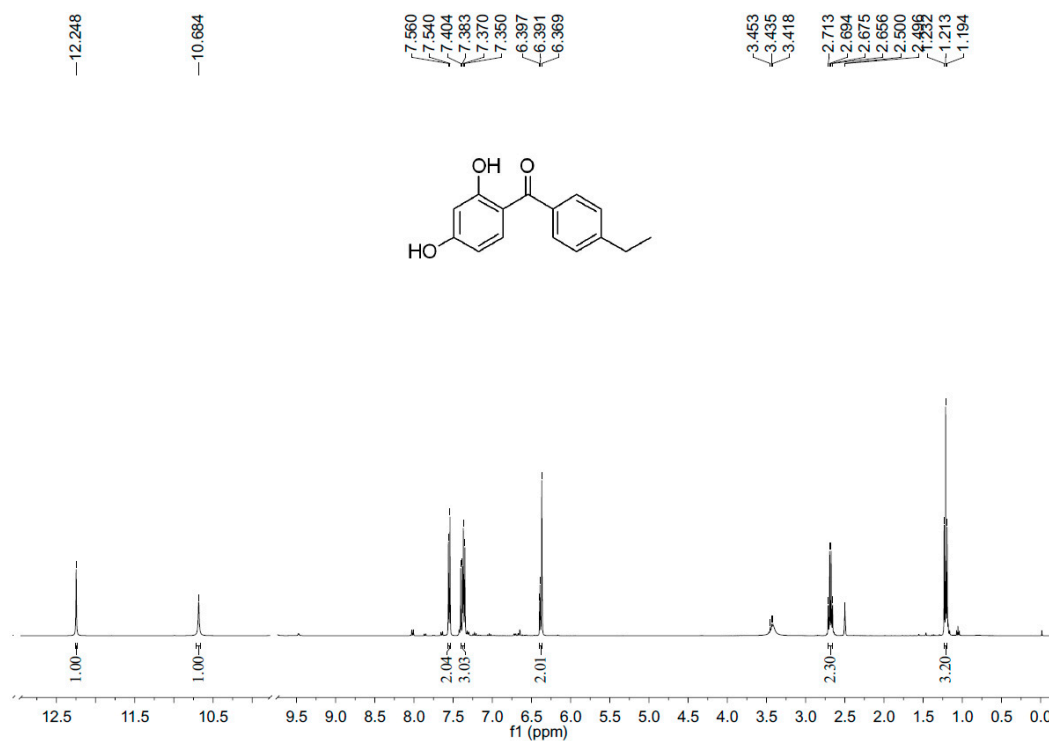
## 2.13 The $^1\text{H}$ NMR spectrum of 2,4-dihydroxy-4'-methyldibenzophenone



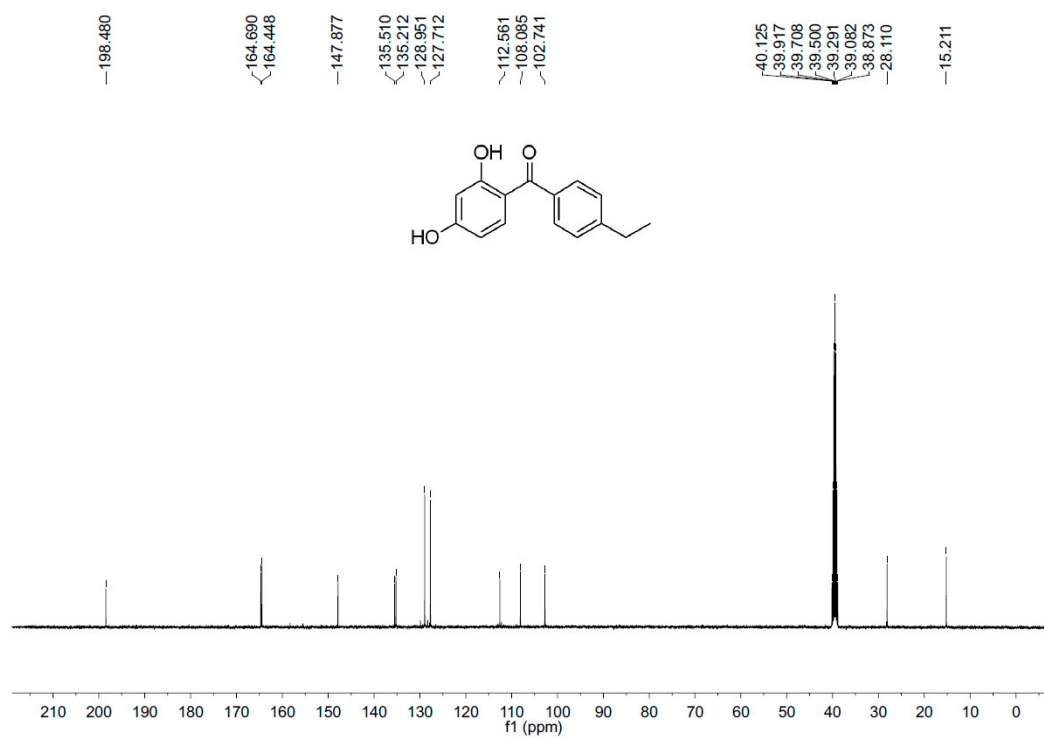
## 2.14 The $^{13}\text{C}$ NMR spectrum of 2,4-dihydroxy-4'-methylbenzophenone



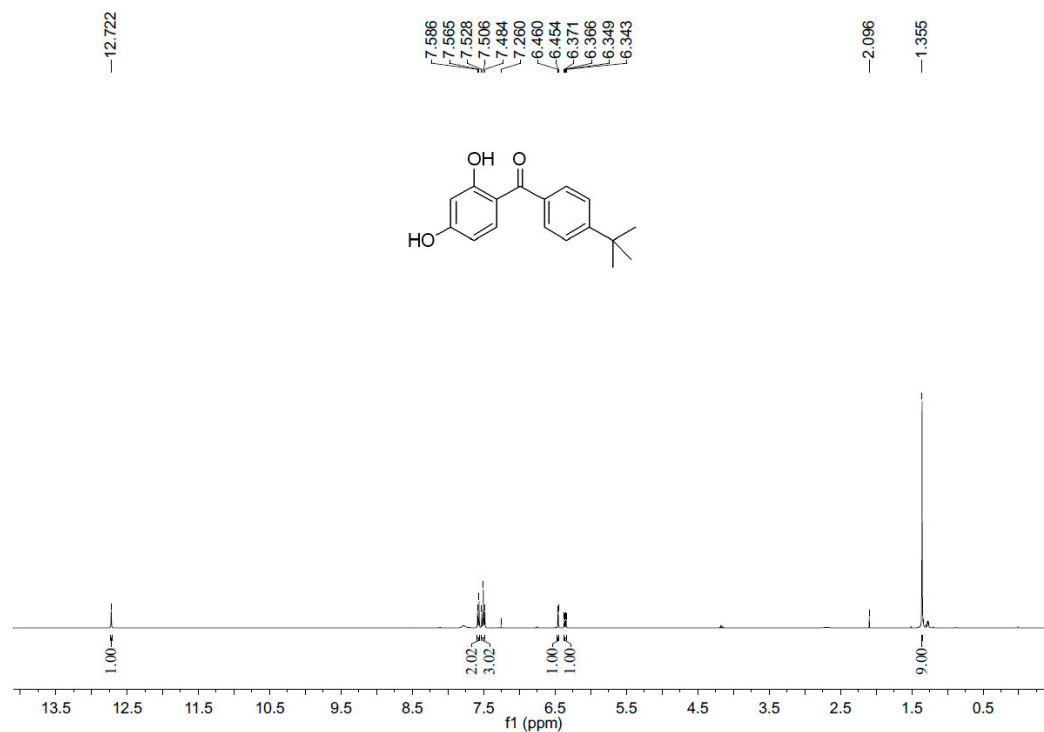
## 2.15 The $^1\text{H}$ NMR spectrum of 2,4-dihydroxy-4'-ethylbenzophenone



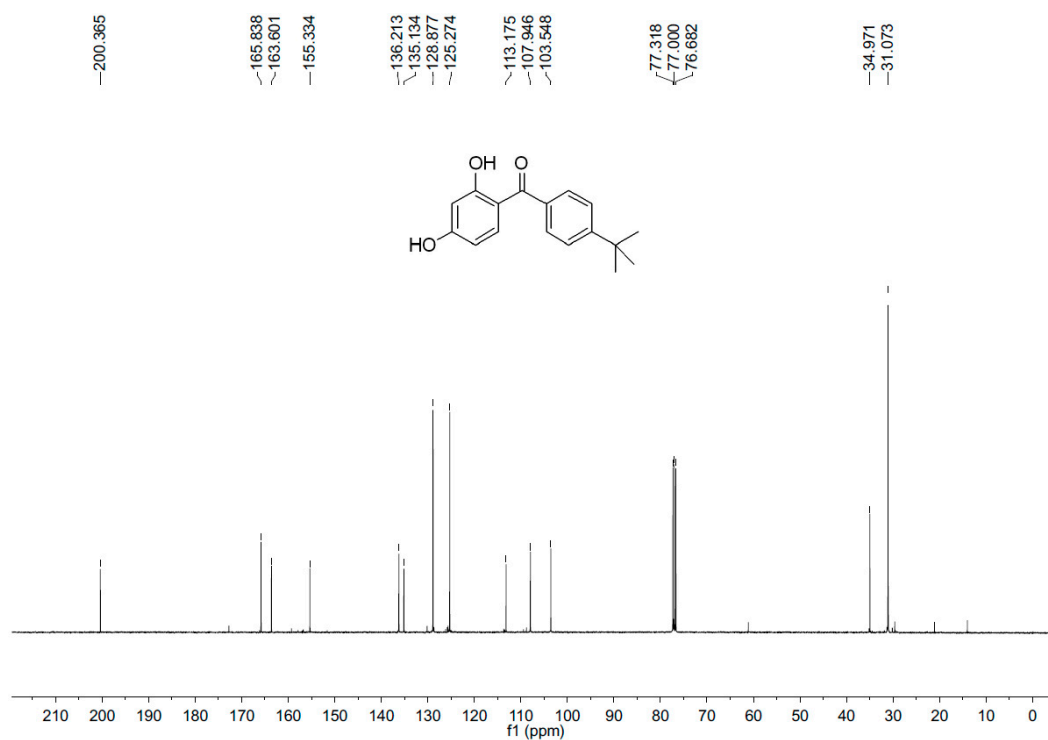
## 2.16 The $^{13}\text{C}$ NMR spectrum of 2,4-dihydroxy-4'-ethyldibenzophenone



## 2.17 The $^1\text{H}$ NMR spectrum of 2,4-dihydroxy-4'-tert-butyldibenzophenone



## 2.18 The $^{13}\text{C}$ NMR spectrum of 2,4-dihydroxy-4'-tert-butylbiphenyl-3-one



## 3. The standard curve of absorbance versus concentration of compounds 1-9

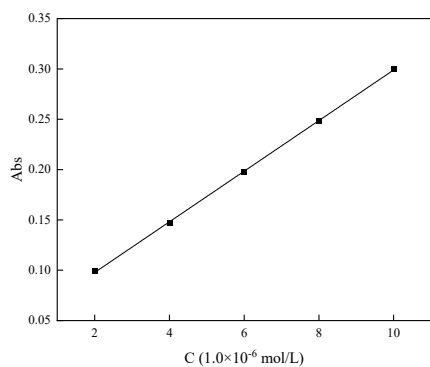


Figure S1. Standard curve of 2,4-dihydroxybenzophenone

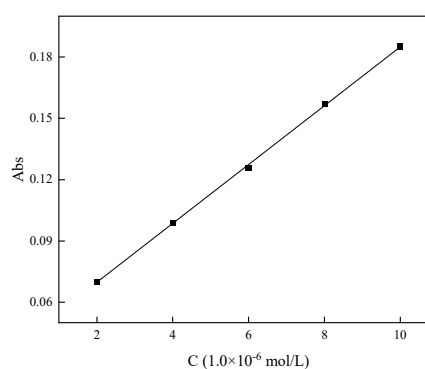


Figure S2. Standard curve of 2,4-dihydroxy-4'-fluorophenone

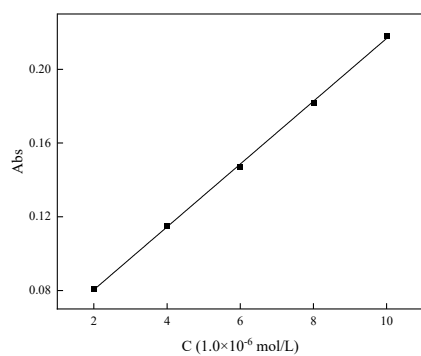


Figure S3. Standard curve of 2,4-dihydroxy-4'-chlorodibenzophenone

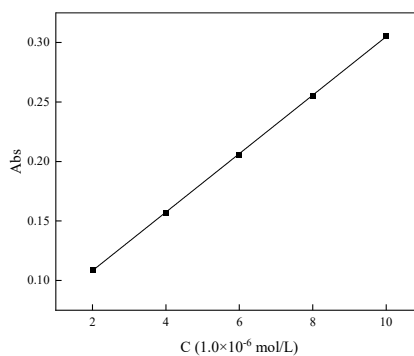


Figure S4. Standard curve of 2,4-dihydroxy-4'-bromodibenzophenone

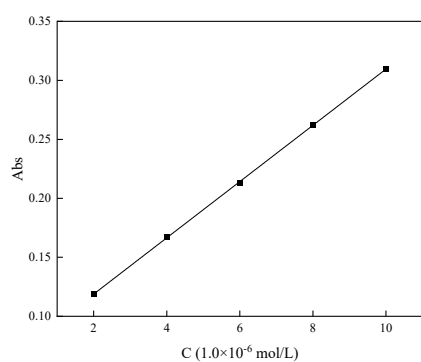


Figure S5. Standard curve of 2,4-dihydroxy-4'-methoxydibenzophenone

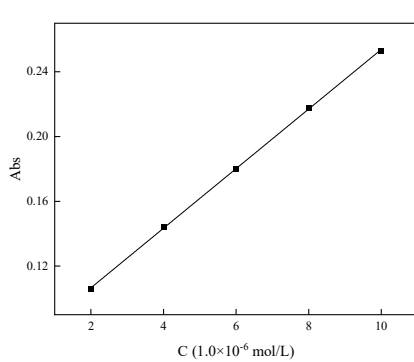


Figure S6. Standard curve of 2,4-dihydroxy-4'-ethoxydibenzophenone

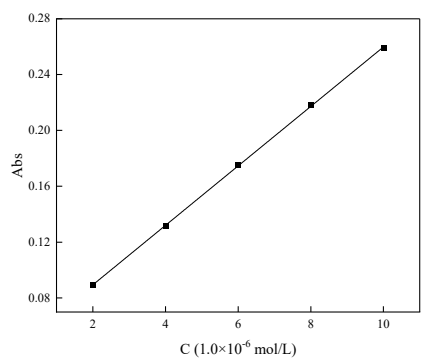


Figure S7. Standard curve of 2,4-dihydroxy-4'-methylidibenzophenone

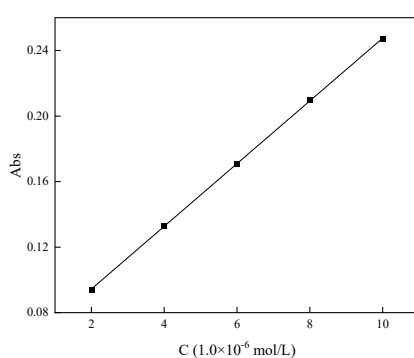


Figure S8. Standard curve of 2,4-dihydroxy-4'-ethyl dibenzophenone

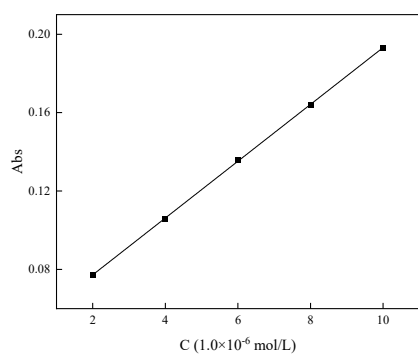


Figure S9. Standard curve of 2,4-dihydroxy-4'-tert-butylbenzophenone