# Supplementary data

# One pot synthesis of 1,2,4,5-tetrasubstituted-imidazoles

# catalyzed by trityl chloride in neutral media

## Ahmad Reza Moosavi-Zare,<sup>a</sup>\* Zhila Asgari,<sup>b</sup> Abdolkarim Zare,<sup>c</sup>\*

### Mohammad Ali Zolfigol,<sup>b</sup> Mohsen Shekouhy<sup>d</sup>

<sup>a</sup>Department of Chemistry, University of Sayyed Jamaleddin Asadabadi, Asadabad,

#### 6541835583, Iran

<sup>b</sup>Faculty of Chemistry, Bu-Ali Sina University, Hamedan, 6517838683, Iran

<sup>c</sup>Department of Chemistry, Payame Noor University, PO Box 19395-3697, Tehran, Iran

<sup>d</sup>Department of Chemistry, College of Science, Shiraz University, 71454, Shiraz, Iran

### **Table of Contents**

Data of compounds	2
NMR spectra of compounds	10
IR spectra of PhCHO, and the mixture of PhCHO and TrCl	13
Chemical shift of the aldehydic hydrogen in <sup>1</sup> H NMR spectra of PhCHO, a	and the
complexes (I and II) formed from PhCHO and TrCl at room temprature in CDCl3	13
UV spectra of PhCHO, and the mixture of PhCHO and TrCl at room tempratur	e in n-
hexane	14

**Data of Compounds:** 



### 1-Benzyl-4,5-diphenyl-2-*p*-tolyl-1*H*-imidazole (1c).

<sup>1</sup>HNMR (500 MHz, DMSO-*d*<sub>6</sub>) δ: 2.33 (s, 3H), 5.14 (s, 2H), 7.13-7.16 (m, 2H), 7.18-7.21 (m, 2H), 7.24-7.29 (m 4H), 7.32-7.35 (m, 3H), 7.39-7.44 (m, 6H), 7.54 (d, *J* =8.0 Hz, 2H).



#### 1,2-Bis(4-chlorophenyl)-4,5-diphenyl-1*H*-imidazole (1d).

<sup>1</sup>H NMR (500 MHz, DMSO- $d_6$ )  $\delta$ : 7.17-7.19 (m, 1H), 7.23-7.25 (m, 4H), 7.29-7.32 (m, 5H), 7.38-7.42 (m, 6H), 7.50 (d, J = 7.0 Hz, 2H). <sup>13</sup>C NMR (125 MHz, DMSO- $d_6$ )  $\delta$ : 127.2, 127.4, 129.0, 129.2, 129.44, 129.49, 129.9, 130.1, 130.8, 130.9, 131.3, 132.0, 132.3, 134.1, 134.3, 135.0, 136.2, 145.8.



### 2-(3-Nitrophenyl)-4,5-diphenyl-1-*p*-tolyl-1*H*-imidazole (1f).

<sup>1</sup>H NMR (500 MHz, DMSO- $d_6$ )  $\delta$ : 7.32-7.39 (m, 6H), 7.54-7.56 (m, 8H), 7.77 (t, J = 7.7 Hz, 1H), 8.20 (d, J = 8.0 Hz, 1H), 8.52 (d, J = 7.5 Hz, 1H), 8.95 (s, 1H).



#### 2-(4-Nitrophenyl)-4,5-diphenyl-1-*p*-tolyl-1*H*-imidazole (1g).

<sup>1</sup>H NMR (500 MHz, DMSO-*d*<sub>6</sub>) δ: 2.28 (s, 3H), 7.15-7.20 (m, 5H), 7.24-7.27 (m, 4H), 7.31-7.32 (m, 3H), 7.50 (d, *J* = 7.5 Hz, 2H), 7.63 (d, *J* = 8.5 Hz, 2H), 8.14 (d, *J* = 9.0 Hz, 2H). <sup>13</sup>C NMR (125 MHz, DMSO-*d*<sub>6</sub>) δ: 21.5, 124.3, 127.2, 127.6, 129.0, 129.1, 129.3, 129.5, 129.6, 130.7, 130.8, 131.9, 133.7, 134.5, 134.8, 137.3, 138.7, 139.5, 144.7, 147.5.



#### 1-Benzyl-2-(4-chlorophenyl)-4,5-diphenyl-1*H*-imidazole(1h).

<sup>1</sup>HNMR (500 MHz, DMSO- $d_6$ )  $\delta$ : 5.16 (s, 2H), 6.75 (d, J = 7.0 Hz, 2H), 7.12-7.22 (m, 6H), 7.29-7.30 (m, 2H), 7.40-7.41 (m, 3H), 7.45-7.50 (m, 4H), 7.68 (d, J = 8.0 Hz, 2H). <sup>13</sup>CNMR (125 MHz, DMSO- $d_6$ )  $\delta$ : 48.6, 126.5, 127.0, 127.2, 128.1, 128.9, 129.4, 129.5, 129.8, 130.5, 131.0, 131.3, 131.4, 131.6, 134.4, 135.2, 137.9, 146.7.



#### 4,5-Diphenyl-1,2-dip-tolyl-1*H*-imidazole (1j).

<sup>1</sup>HNMR (500 MHz, DMSO-*d*<sub>6</sub>) δ: 2.25 (s, 3H), 2.26 (s, 3H), 7.08-7.10 (m, 6H), 7.15-7.17 (m, 1H), 7.21-7.24 (m, 5H), 7.47-7.49 (m, 2H). <sup>13</sup>CNMR (125 MHz, DMSO-*d*<sub>6</sub>) δ: 21.4, 21.5, 127.2, 128.6, 128.9, 129.0, 129.1, 129.2, 129.3, 129.5, 130.4, 131.4, 132.0, 135.0, 135.4, 137.5, 138.5, 138.8, 147.0.



#### 1-Benzyl-2-(3-methoxyphenyl)-4,5-diphenyl-1*H*-imidazole (1k).

<sup>1</sup>H NMR (500 MHz, DMSO- $d_6$ )  $\delta$ : 3.68 (s, 3H), 5.16 (s, 2H), 6.79 (d, J = 7.5 Hz, 2H), 6.98-7.00 (m, 1H), 7.13-7.16 (m, 3H), 7.17-7.25 (m, 5H), 7.29-7.35 (m, 3H), 7.40-7.41 (m, 3H), 7.46-7.47 (m, 2H). <sup>13</sup>C NMR (125 MHz, DMSO- $d_6$ )  $\delta$ : 48.6, 55.9, 114.6, 115.6, 121.7, 126.4, 127.0, 127.1, 128.0, 128.9, 129.4, 129.74, 129.78, 130.5, 131.1, 131.4, 131.7, 132.8, 135.4, 137.7, 138.2, 147.7, 160.0.



#### 1-Benzyl-2-(4-methoxyphenyl)-4,5-diphenyl-1*H*-imidazole (1n).

<sup>1</sup>H NMR (500 MHz, DMSO-*d*6)  $\delta$ : 3.77 (s, 3H), 5.13 (s, 2H), 6.76 (d, J = 7.0 Hz, 2H), 6.90 (d, J = 9.0 Hz, 2H), 7.11-7.21 (m, 6H), 7.26-7.28 (m, 2H), 7.38-7.39 (m, 3H), 7.46 (d, J = 7.0 Hz, 2H), 7.58 (d, J = 9.0 Hz, 2H). <sup>13</sup>C NMR (125 MHz, DMSO-*d*<sub>6</sub>)  $\delta$ : 48.5, 56.0, 114.9, 124.0, 126.4, 126.9, 127.0, 128.0, 128.9, 129.3, 129.6, 129.7, 130.6, 130.8, 131.6, 131.7, 135.5, 137.5, 138.3, 147.9, 160.5.



#### 4-(1,4,5-Triphenyl-1*H*-imidazol-2-yl)phenol (10).

<sup>1</sup>HNMR (500 MHz, DMSO- $d_6$ )  $\delta$ : 6.64 (d, J= 9.0 Hz, 2H), 7.14-7.24 (m, 9H), 7.27-7.28 (m, 3H), 7.30-7.32 (m, 3H), 7.48 (d, J = 7.0 Hz, 2H), 9.60 (s, 1H). <sup>13</sup>CNMR (125 MHz, DMSO-d6)  $\delta$ : 115.8, 122.1, 127.1, 127.2, 128.9, 129.1, 129.3, 129.6, 129.9, 130.6, 131.4, 131.5, 132.0, 135.5, 137.3, 137.7, 147.3, 158.4.



#### 4-(4,5-Diphenyl-1-*p*-tolyl-1*H*-imidazol-2-yl)benzonitrile (1p).

<sup>1</sup>H NMR (500 MHz, DMSO- $d_6$ )  $\delta$ : 2.24 (s, 3H), 7.08-7.49 (m, 14H), 6.68 (d, J = 7.5 Hz, 2H), 7.95 (d, J = 7.5 Hz, 2H). <sup>13</sup>C NMR (125 MHz, DMSO- $d_6$ )  $\delta$ : 21.4, 111.3, 115.2, 121.0, 127.12, 127.18, 128.7, 129.1, 129.36, 129.39, 130.1, 130.3, 131.1, 131.4, 132.0, 137.2, 138.7, 143.9, 147.5, 153.33, 153.66.



**4,5-Diphenyl-2-(thiophen-2-yl)-1**-*p*-tolyl-1*H*-imidazole (1r). <sup>1</sup>H NMR (500 MHz, DMSO-*d*<sub>6</sub>) δ: 2.31 (s, 3H), 6.51(d, *J* = 3.5 Hz, 1H), 6.62 (t, *J* = 4.5 Hz, 1H), 7.18-7.29 (m, 12H), 7.47-7.50 (m, 3H). <sup>13</sup>C NMR (125 MHz, DMSO-*d*<sub>6</sub>) δ: 21.6, 126.1, 127.1, 127.3, 127.9, 128.3, 129.0, 129.3, 129.6, 130.8, 130.9, 131.9, 132.1, 133.8, 134.4, 134.9, 137.6, 139.9, 142.3.



**4-(4,5-Diphenyl-2-(thiophen-2-yl)-1***H***-imidazol-1-yl)phenol (1s).** <sup>1</sup>H NMR (500 MHz, DMSO-*d*<sub>6</sub>) δ: 6.58 (s, 1H), 6.77 (d, *J* = 8.0 Hz, 2H), 6.95 (m, 1H), 7.18-7.50 (m, 13H), 9.88 (s, 1H). <sup>13</sup>C NMR (125 MHz, DMSO-*d*<sub>6</sub>) δ: 116.7, 126.1, 127.1, 127.3, 127.8, 127.9, 128.3, 129.0, 129.23, 129.29, 131.0, 131.1, 131.9, 132.3, 133.9, 135.0, 137.4, 142.6, 158.9.



1-Benzyl-2-(4-chlorophenyl)-4,5-diphenyl-1*H*-imidazole(1c).

ppm 180 160 140 120 100 80 60 40 20



2-(4-Nitrophenyl)-4,5-diphenyl-1-*p*-tolyl-1*H*-imidazole (1g).

# 4,5-Diphenyl-1,2-dip-tolyl-1H-imidazole (1j).



10



# 1-Benzyl-2-(4-methoxyphenyl)-4,5-diphenyl-1*H*-imidazole (1n).

![](_page_11_Figure_0.jpeg)

4-(1,4,5-Triphenyl-1*H*-imidazol-2-yl)phenol (10).

![](_page_12_Figure_0.jpeg)

Figure S1. IR spectra of PhCHO, and the mixture of PhCHO and TrCl.

![](_page_12_Figure_2.jpeg)

**Figure S2.** Chemical shift of the aldehydic hydrogen in <sup>1</sup>H NMR spectra of PhCHO, and the complexes (I and II) formed from PhCHO and TrCl at room temprature in CDCl<sub>3</sub>.

![](_page_13_Figure_0.jpeg)

Figure S3. UV spectra of PhCHO, and the mixture of PhCHO and TrCl at room temprature in *n*-hexane.