

## Supporting Information for

# Copper(I)-Catalyzed Synthesis of Azoles. DFT Study Predicts Unprecedented Reactivity and Intermediates.

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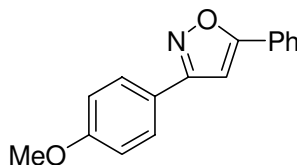
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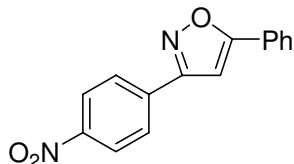
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### 3-(4-Methoxyphenyl)-5-phenyl-isoxazole



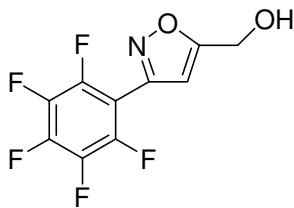
<sup>1</sup>H-NMR (CDCl<sub>3</sub>): δ 3.89 (s, 3H), 6.78 (s, 1H), 7.00 (m, 2H), 7.47 (m, 3H), 7.82 (m, 4H);  
<sup>13</sup>C-NMR (CDCl<sub>3</sub>): δ 55.4, 97.3, 114.5, 120.7, 125.8, 127.3, 128.2, 129.0, 130.2, 157.3,  
159.2, 160.6; m.p. 122 °C.

### 3-(4-Nitrophenyl)-5-phenyl-isoxazole



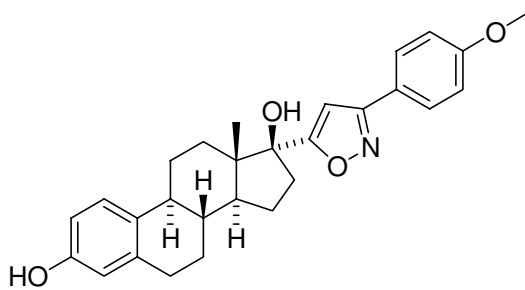
<sup>1</sup>H-NMR (CDCl<sub>3</sub>): δ 6.99 (s, 1H), 7.47 (m, 4H), 7.82 (m, 2H), 8.11 (m, 2H); <sup>13</sup>C-NMR  
(CDCl<sub>3</sub>): δ 97.4, 124.2, 125.9, 126.9, 127.7, 129.1, 130.7, 135.2, 148.7, 161.2, 171.5;  
m.p. 222 °C.

### 3-Pentafluorophenyl-5-isoxylyl-methanol



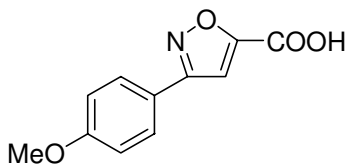
$^1\text{H-NMR}$  ( $\text{CDCl}_3$ ):  $\delta$  4.87 (s, 2H), 6.60 (s, 1H);  $^{13}\text{C-NMR}$  ( $\text{CDCl}_3$ ):  $\delta$  56.3, 103.7, 104.9, 136.9, 141.0, 143.2, 151.5, 172.4; m.p. 63 °C.

### 3-(4-Methoxyphenyl)-5-(17 $\alpha$ -estradiol)-isoxazole



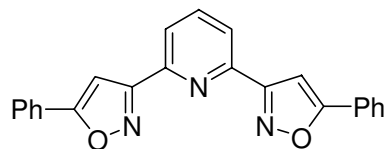
$^1\text{H-NMR}$  ( $\text{CDCl}_3$ ):  $\delta$  0.74 (m, 1H), 0.95 (s, 3H), 1.16-1.91 (m, 10H), 1.95 (m, 1H), 2.13 (m, 1H), 2.30 (m, 1H), 2.71 (m, 2H), 3.81 (s, 3H), 6.43 (m, 2H), 6.82 (s, 1H), 6.95 (d, 1H), 7.04 (d, 2H), 7.81 (d, 2H);  $^{13}\text{C-NMR}$  ( $\text{CDCl}_3$ ):  $\delta$  14.1, 23.3, 26.0, 27.2, 29.2, 30.7, 33.1, 36.9, 43.1, 47.8, 48.4, 55.3, 82.2, 100.3, 112.7, 114.4, 114.9, 121.3, 126.0, 128.1, 130.2, 137.1, 155.0, 160.6, 178.9; m.p. 192 °C.

### 3-(4-Methoxyphenyl)-5-carboxy-isoxazole



$^1\text{H-NMR}$  ( $d^6$ -DMSO):  $\delta$  3.82 (s, 3H), 7.07 (d, 2H), 7.72 (s, 1H), 7.89 (d, 2H);  $^{13}\text{C-NMR}$  ( $d^6$ -DMSO):  $\delta$  55.3, 107.3, 115.0, 120.1, 128.3, 157.8, 161.1, 162.4, 174.9; m.p. 138 °C.

**3,3'-(2,6-Pyridinediyl)-bis(5-phenyl)isoxazole**



$^1\text{H-NMR}$  ( $\text{d}^6\text{-DMSO}$ ):  $\delta$  7.39-8.18 (m, 15H);  $^{13}\text{C-NMR}$  ( $\text{d}^6\text{-DMSO}$ ):  $\delta$  99.4, 122.3, 125.7, 126.7, 129.4, 131.7, 139.1, 147.8, 163.3, 170.1; m.p. 145 °C.