

# Supporting Information

## 1,2,3-Triazole Framework: A Strategic Structure for C-H...X Hydrogen Bonding and Practical Design of an Effective Pd-Catalyst for Carbonylation and Carbon-Carbon Bond Formation

Fatemeh Mohammadsaleh<sup>\*a</sup>, Maryam Dehdashti Jahromi<sup>b</sup>, Abdol Reza Hajipour<sup>c,d</sup>, Seyed Mostafa Hosseini<sup>c</sup> and Khodabakhsh Niknam<sup>\*a</sup>

<sup>a</sup> aDepartment of Chemistry, Faculty of Nano and Bio Science and Technology, Persian Gulf University, Bushehr, Iran. E-mail address: f.mohammadsaleh@gmail.com, niknam@pgu.ac.ir

<sup>b</sup>Faculty of engineering, Jahrom University, Jahrom, Iran

<sup>c</sup>Department of Chemistry, Pharmaceutical and Organic Synthesis Research Laboratory, Isfahan University of Technology, Isfahan 84156, Iran

<sup>d</sup>Department of Pharmacology, University of Wisconsin, Medical School, 1300 University Avenue, Madison, 53706-1532 WI, USA

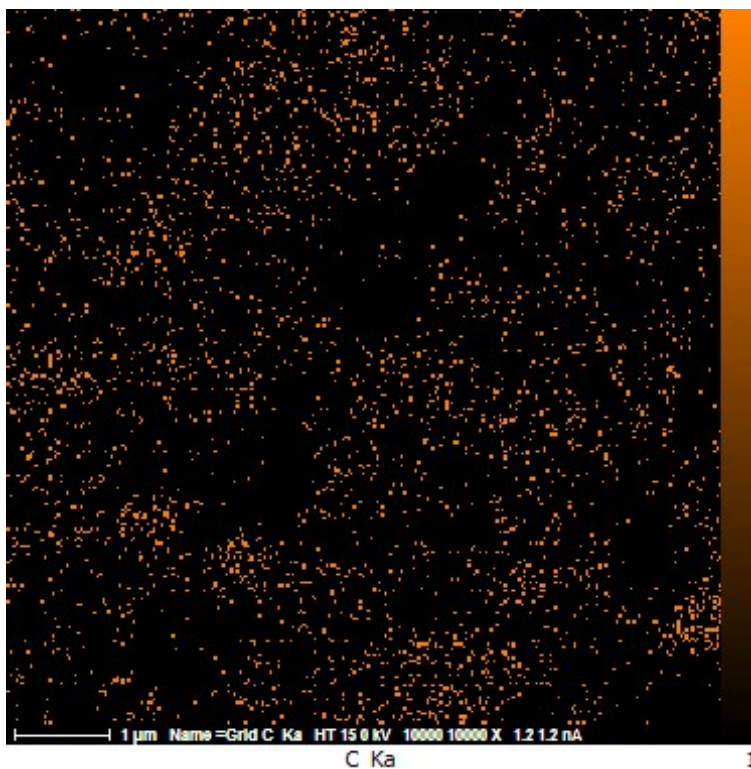
### Table of Contents

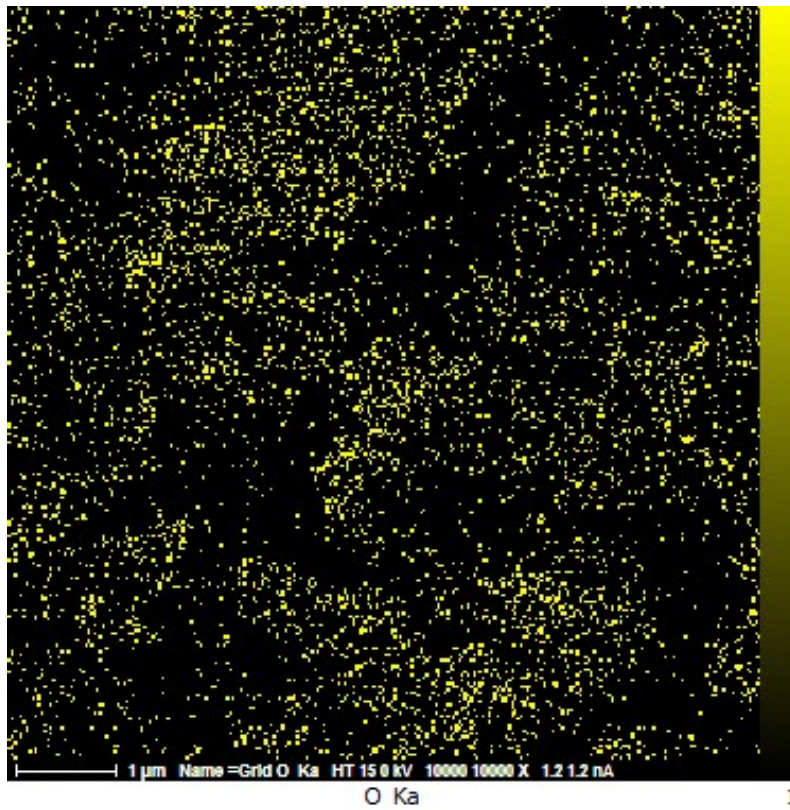
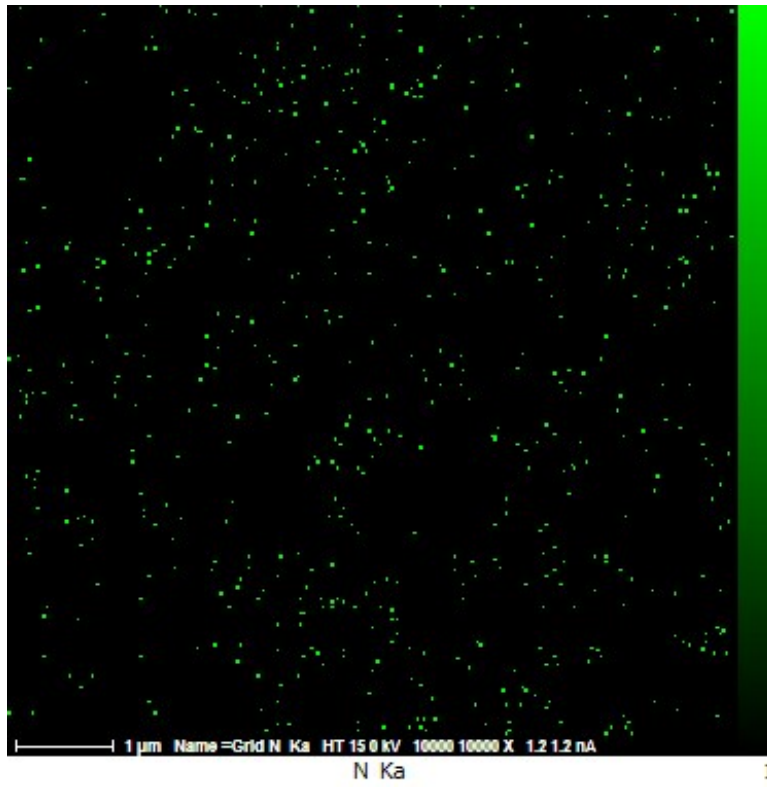
1. General Remarks
2. Elemental EDX mapping of the catalyst Pd@click-MNPs/CS
3. Characteristic data of the products

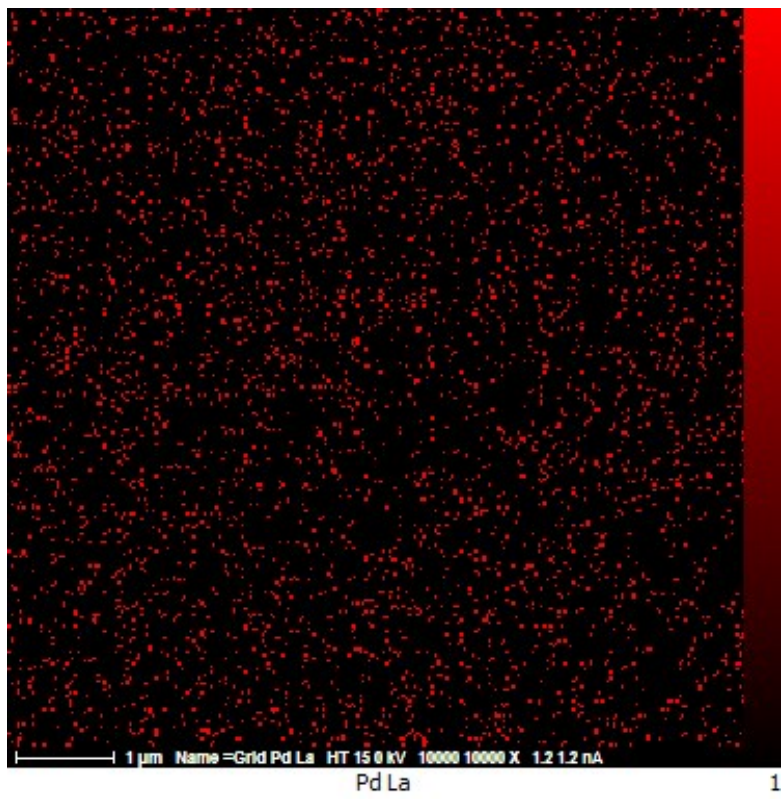
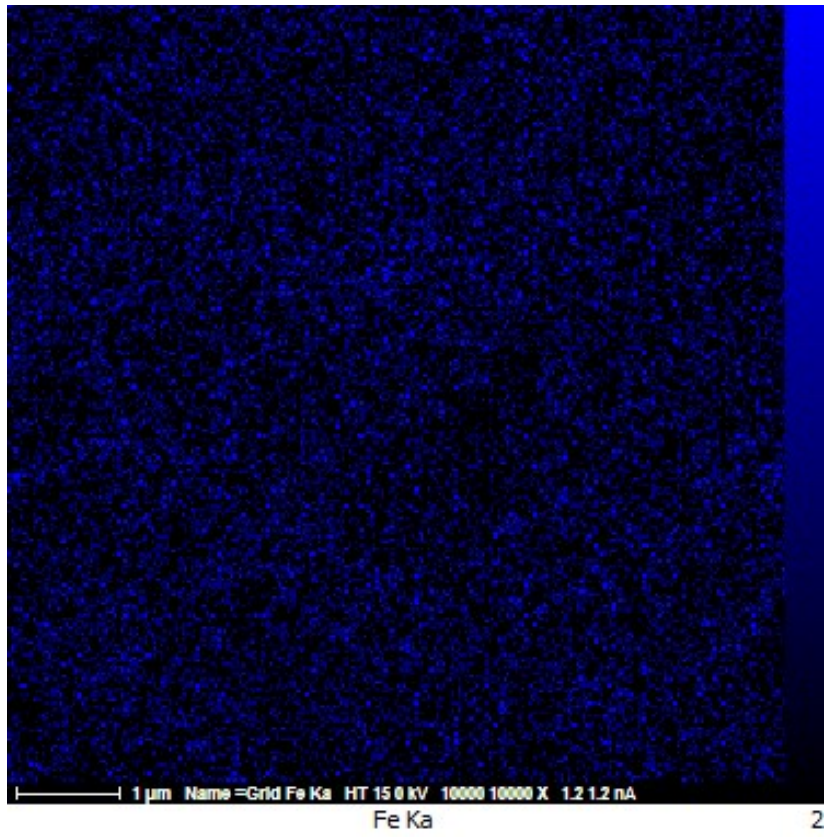
## 1) General Remarks

All reagents were purchased from commercial suppliers (Merck and Aldrich) and used without further purification. The FT-IR spectra of products were measured as KBr disc by Jasco-680 FTIR spectrophotometer. The X-ray diffraction (XRD) patterns were recorded by using a Philips Xpert MPD diffractometer with Cu K $\alpha$  radiation ( $\lambda = 0.15418$  nm). Transmission Electron Microscopy (TEM) was carried out on Philips CM120 microscope 100 KV. Scanning electron microscopy (FE-SEM) images were obtained using a Hitachi S-4160 instrument. Analysis of Pd content was measured by inductively coupled plasma spectroscopy (ICP) using Perkin Elmer Optima 7300 DV. Melting points were determined by a Gallenkamp melting apparatus. Gas chromatography (GC) analyses were performed on a BEIFIN 3420 gas chromatograph equipped with a Varian CP SIL 5CB column: 30 m, 0.32 mm, 0.25 mm for consideration of reactions conversions and yields. The  $^1\text{H}$  and  $^{13}\text{C}$  NMR spectra were recorded on a Bruker AVANCE spectrometer at 400, 300 and 100 MHz using TMS as an internal standard in  $\text{CDCl}_3$  and DMSO at RT.

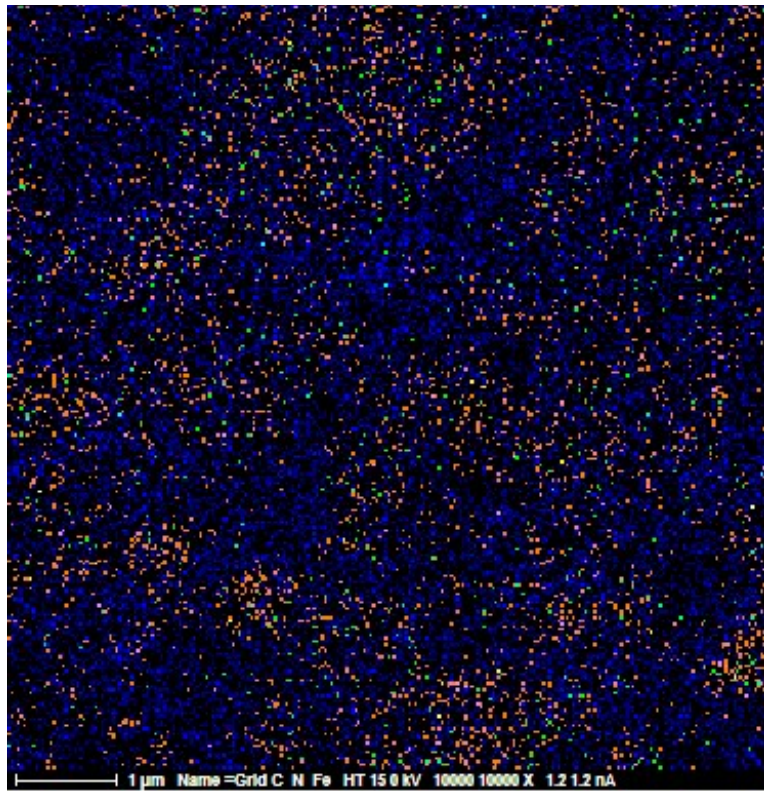
## 2) Elemental EDX mapping of the catalyst Pd@click-MNPs/CS (Figure 1S.)



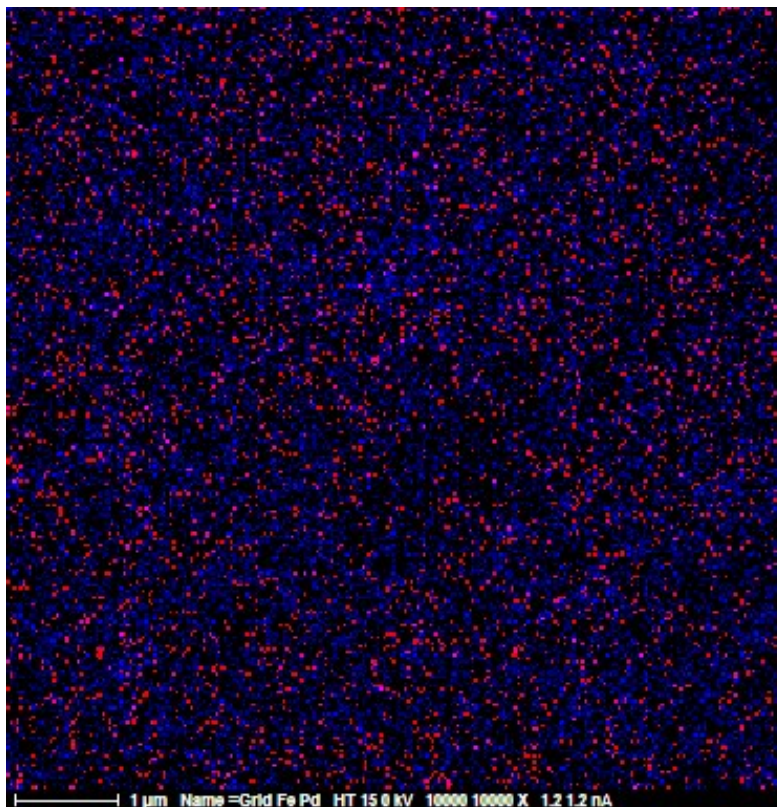








C N Fe



Fe Pd

### 3) Characteristic spectra of the products

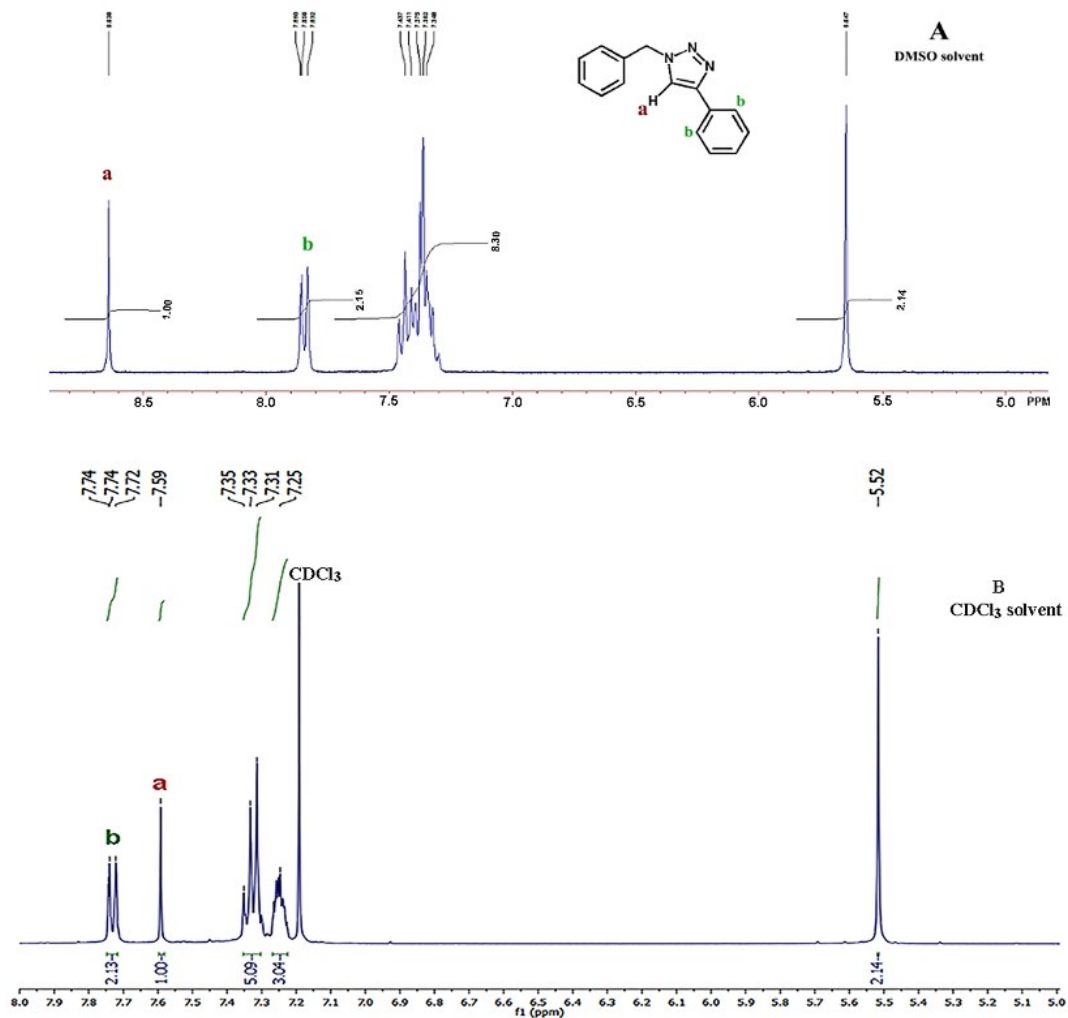


Figure 2S. <sup>1</sup>H NMR spectra of 1-benzyl-4-phenyl-1-*H*-1,2,3-triazole in DMSO and CDCl<sub>3</sub> solvent

