

## Supporting Information

### Comparison Between Different Mesoporous Carbons in the Removal of Doxycycline Antibiotic: Experimental Assays and Description of Adsorbate Features by Density Functional Theory (DFT)

Tauany de Figueiredo Neves<sup>a,b</sup>, Thayna Reis<sup>a</sup>, Natália Gabriele Camparotto<sup>a</sup>, Maria Vitória Rapôso<sup>a</sup>, Valmor Roberto Mastelaro<sup>c</sup>, Rafael L. Oliveira<sup>d,\*</sup> and Patrícia Prediger<sup>a,\*</sup>

<sup>a</sup> School of Technology, University of Campinas, 13484-332, Limeira, São Paulo, Brazil.

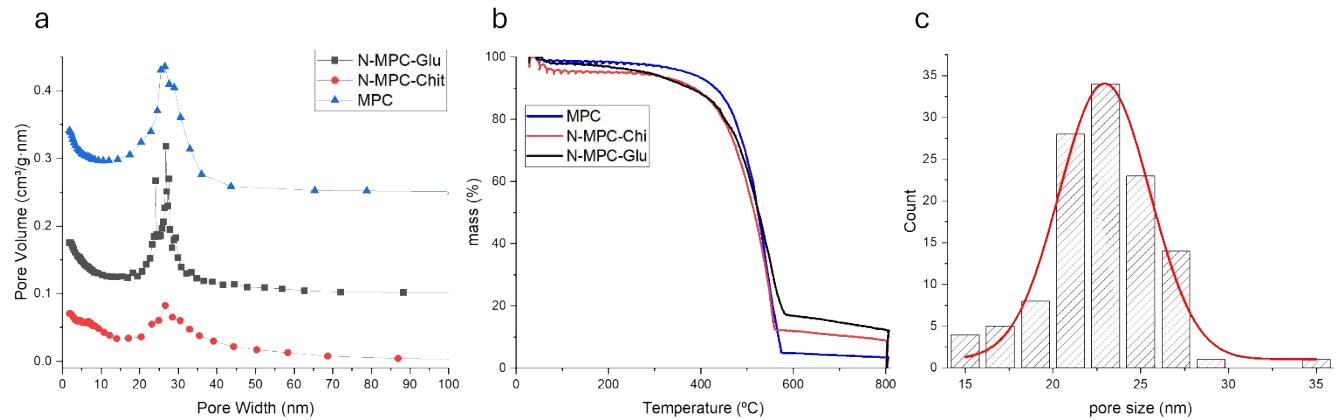
<sup>b</sup> Faculty of Philosophy, Sciences and Letters of Ribeirão Preto, University of São Paulo, 14040-901, Ribeirão Preto, São Paulo, Brazil.

<sup>c</sup> Institute of Physics, University of São Paulo, 13566-590, São Carlos, São Paulo, Brazil.

<sup>d</sup> Institute of Low Temperature and Structure Research of the Polish Academy of Sciences, 50-422, Wrocław, Poland.

\*Corresponding author e-mail address: [prediger@unicamp.br](mailto:prediger@unicamp.br); [r.oliveira@intibs.pl](mailto:r.oliveira@intibs.pl); Telephone number: +55 192113-3406; +48713954152

## 1. Characterization of prepared MPC

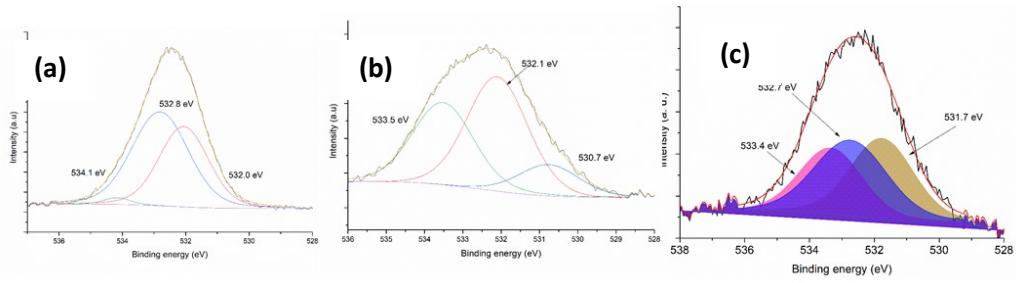


**Figure S1** – (a) Pore size distribution of the carbonaceous materials, the distributions of N-MPC-Glu and MPC were offset by 0.1 and 0.25, respectively: (b)–TG analysis of carbonaceous materials, (c) pore size distribution of N-MPC-Chit derived from TEM analyses.

## 2. XPS analysis of prepared MPC

**Table S1** – C-bond distributions from C1s XPS spectrum

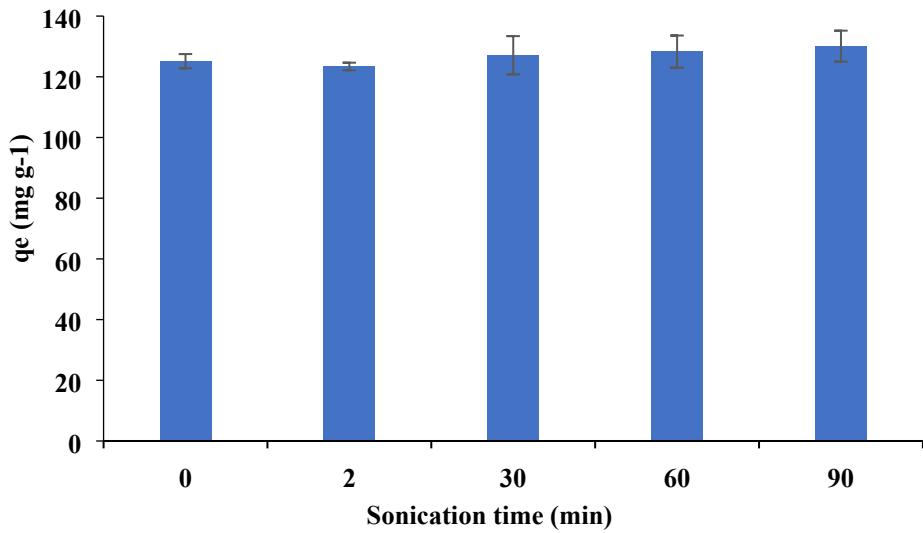
Material	Csp <sup>2</sup> (%)	Csp <sup>3</sup> (%)	C=O (%)	O-C=O (%)	O-C-O (%)	Carbonates (%)
<b>MPC</b>	53.2	30	9.5	4.6	2.7	-
<b>N-MPC-Chi</b>	58.5	22.1	8.7	5.0	3.7	2.0
<b>N-MPC-Glu</b>	68.7	19.7	6.3	5.3	-	-



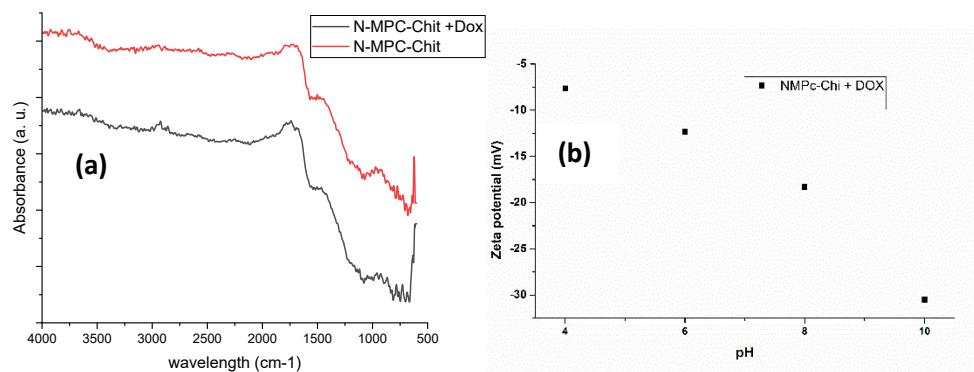
**Figure S2** – O1s XPS spectrum of MPC (a); N-MPC-Chi (b); N-MPC-Glu (c).

**Table S2** O-bond distributions from the O1s XPS spectrum

Material	Energy binding, percentage, functional group		
<b>MPC</b>	532.0 eV; 41.9%, COOH	532.8 eV, 56.2%, C-OH	534.1 eV, 1.9%, C–O in anhydrides
<b>N-MPC-Chi</b>	531.7 eV, 28.2%, COOH	532.7 eV, 37.2%, C-OH	533.4 eV 34.6%, C=O
<b>N-MPC-Glu</b>	530.7 eV, 13.4%, adsorbed H <sub>2</sub> O	532.1 eV, 49.2%, COOH	533.5 eV, 37.4%, C=O



**Figure S3**– Influence of sonication assistance in the removal of DOX by N-MPC-Chi



**Figure S4** – (a) ATR-FTIR spectra of N-MPC-Chi and N-MPC-Chi/DOX loaded. (b) Zeta potential measurements of N-MPC-Chi + DOX.