

## Molecular Organization of Hydrophobic Molecules and co-Adsorbed Water in SBA-15 Ordered Mesoporous Silica Material

Randy Mellaerts,<sup>a</sup> Maarten B.J. Roeffaers,<sup>b</sup> Kristof Houthoofd,<sup>a</sup> Michiel Van Speybroeck,<sup>c</sup> Gert De Cremer,<sup>a</sup> Jasper A.G. Jammaer,<sup>a</sup> Guy Van den Mooter,<sup>c</sup> Patrick Augustijns,<sup>c</sup> Johan Hofkens<sup>b</sup> and Johan Martens<sup>a\*</sup>

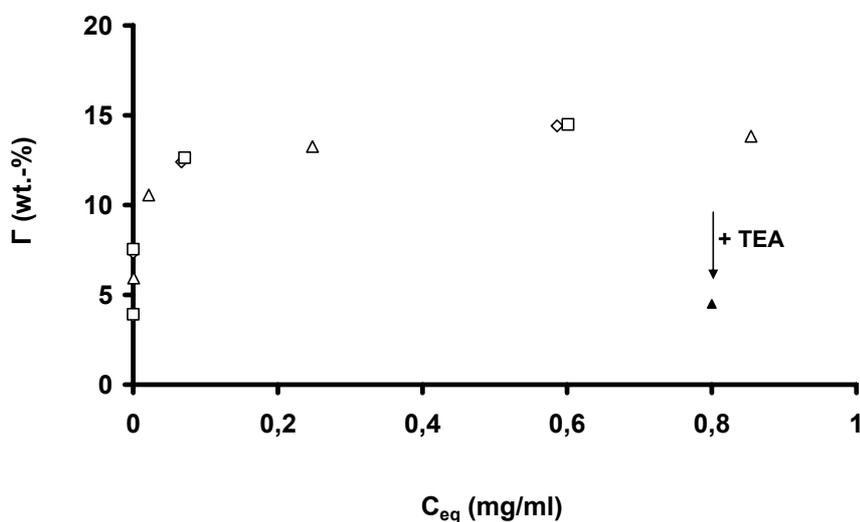
<sup>a</sup> Centre for Surface Chemistry and Catalysis, Kasteelpark Arenberg 23, Katholieke Universiteit Leuven, BE-3001 Heverlee, Belgium.

E-mail: johan.martens@biw.kuleuven.be; Fax: +32 16 321998;

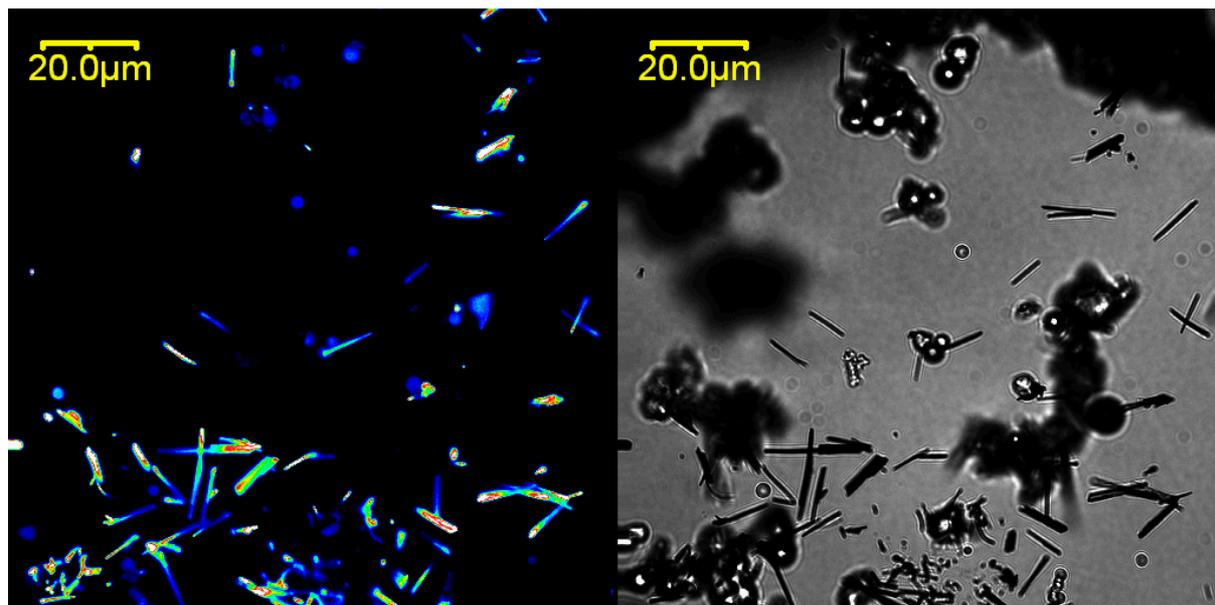
Tel: +32 16 321637.

<sup>b</sup> Laboratory of Photochemistry and Spectroscopy, Celestijnenlaan 200F, Katholieke Universiteit Leuven, BE-3001 Heverlee, Belgium.

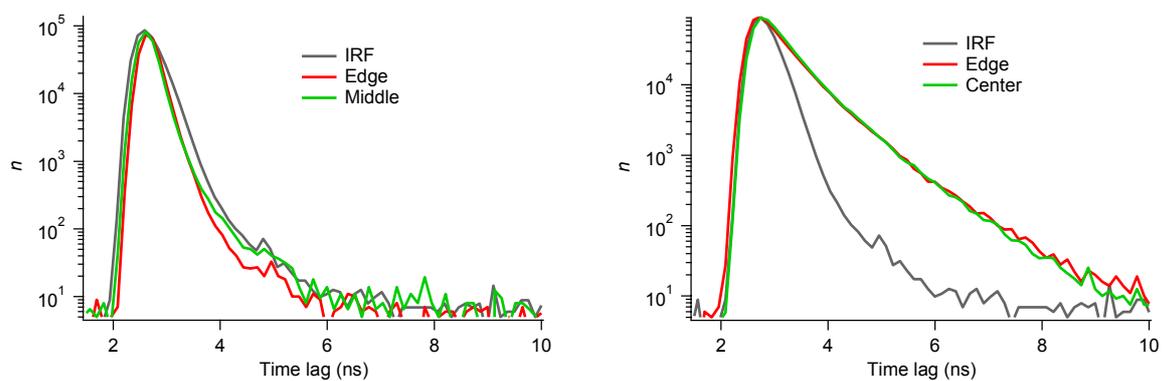
<sup>c</sup> Laboratory for Pharmaceutics and Biopharmacy, O&N2, Herestraat 49-box 921, Katholieke Universiteit Leuven, BE-3000 Leuven, Belgium.



**Figure ESI-1:**  $\Gamma$  (wt.-%) weight fraction itraconazole adsorbed into SBA-15 as a function of  $C_{eq}$  (mg/ml) itraconazole equilibrium concentration in dichloromethane. The material was pretreated for one week at different relative humidities (RH-%) to obtain different water contents (WC-wt.-%):  $\diamond$  RH0 WC1.4 ;  $\square$  RH52 WC4.3 ;  $\triangle$  RH97 WC38.4. Adsorption isotherms were corrected for the physisorbed water. Influence of addition of traces of triethylamine (TEA) on itraconazole adsorption ( $\blacktriangle$ ) with the RH0 WC1.4 SBA-15.



**Figure ESI-2:** Confocal fluorescence (left) and transmission images (right) of SBA-15 spheres loaded with Nile red and containing a pre-adsorbed water content of 1.4 wt.-% after 4 h exposure to SGF.



**Figure ESI-3:** Fluorescence decay curves of Nile red adsorbed into SBA-15 spheres with pre-adsorbed water content of 1.4 wt.-% (left) and 38.5 wt.-% (right) after exposure to SGF. Decay curves originate from the edge and middle of the SBA-15 sphere. IRF represents the instrument response function.