*Supporting Information Available*

# Cellulose nanofibers - titania nanocomposites as potential drug delivery systems for dermal applications

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**Table TS1** Characteristic IR-absorption bands for the samples

| Description | Wavenumber of samples ($cm^{-1}$) | |
|---|---|---|
| | **PCNF** | **CNF_$TiO_2$** |
| ν (C-H) stretching | 2980 | 2980 |
| ν (C-H) stretching | 2896 | 2896 |
| ν (C=O) stretching | - | 1710 |
| δ (OH) of water absorbed from cellulose | 1644 | 1645 |
| ν ($COO^-$) stretching | - | 1565 |
| δ ($CH_2$) symmetric bending | 1418 | 1415 |
| δ (OH) in plane bending | 1337 | 1340 |
| ν ($CH_2$) rocking vibration at $C_6$ | 1314 | 1313 |
| δ (CH) bending, | 1278 | 1279 |
| ν (C-O-C) stretching | 1227 | 1225 |
| ν(C-O-C) symmetric stretching,<br>-OH plane deformation | 1198 | 1197 |
| ν (C-O-C) asymmetric stretching at β-glucosidic linkage | 1157 | 1158 |
| ν (C-O-C), ν(CCO) and ν(CCH) deformation and stretching | 894 | 893 |
| ν (Ti-O-Ti) stretching | - | 815,835 |

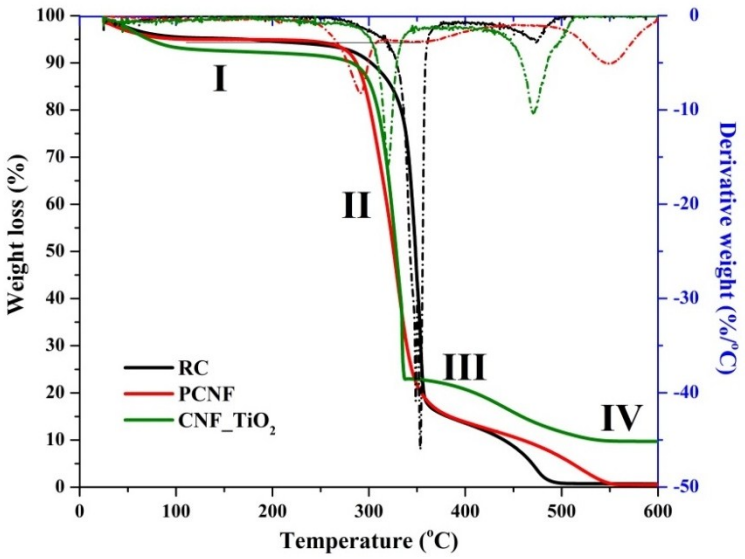


**Figure. FS1** TGA and DTG curves for raw cotton, pure cellulose nanofibers and the nanocomposite based on cellulose nanofibers and $TiO_2$

The visual optical images of the nanocomposite based on cellulose nanofibers and $TiO_2$ with different type of drugs such as Diclofenac Sodium, Penicillamine D and Phoshomycin are presented in Fig.FS2

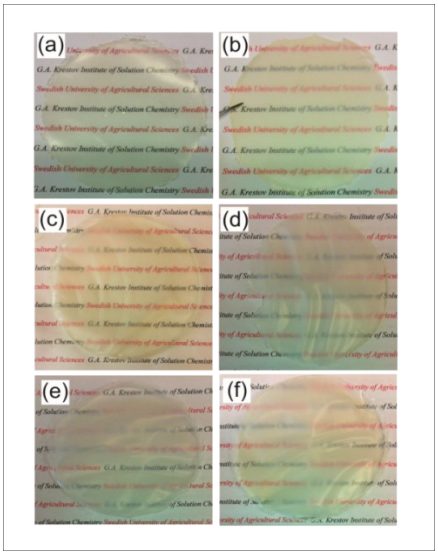


**Figure**. **FS2** Visual images of the samples: (a) CNF_ $TiO_2$_DS_M1, (b) CNF_$TiO_2$_DS_M2, (c) CNF_$TiO_2$_PCA-_M1, (d) CNF_$TiO_2$_PCA-D_M2, (e) CNF_$TiO_2$_Phos_M2, (f) CNF_$TiO_2$_Phos_M3.

Fig.FS3 showed SEM image together with EDS analysis of $TiO_2$-modified nanocomposites with Diclofenac sodium prepared by method #3.

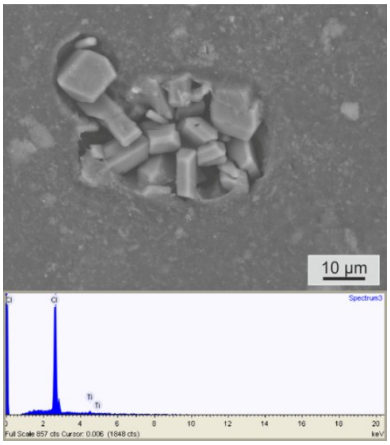


**Figure. FS3** SEM micrographs and EDX analysis of the nanocomposites based on cellulose nanofibers and TiO2 and modified with DS by M3

**Surface modification**

Cellulose nanofibers surface were modified by Diclofenac Sodium, Penicillamine D and Phoshomycin in amounts calculated to achieve uniform, single layer coverage. The surface of titania was estimated using simple mathematical model where the particles are spherical, uniform and homogenous. According to our assumption that drug bonded with the biopolymer through interaction with $TiO_2$, we firstly calculated the total number of titania nanoparticles, which was added to the cellulose nanofibers, by following formula:

$$N_{total} = m_{total}/m_p$$

where $m_{total}$ – total mass of $TiO_2$ particles (g), $m_p$ – mass of the single $TiO_2$ particle (g).

The total surface area of titania nanoparticles grafted onto cellulose nanofibers can be estimated as follows:

$$S_{total} = N_{total} \cdot S_p$$

where $N_{total}$ – total number of titania nanoparticles, $S_p$ - surface of the single $TiO_2$ particle ($nm^2$). Then, the amount of drug $n$ (mol) can be found as follows:

$$n = S_{total} \cdot N_A / S$$

where $S$ – area of functional group ($nm^2$) and $N_A$ is Avogadro number. The approximate area of 0.24 $nm^2$ per phoshponate group is commonly proposed in literature[1] and utilized by us in our previous papers[2,3].

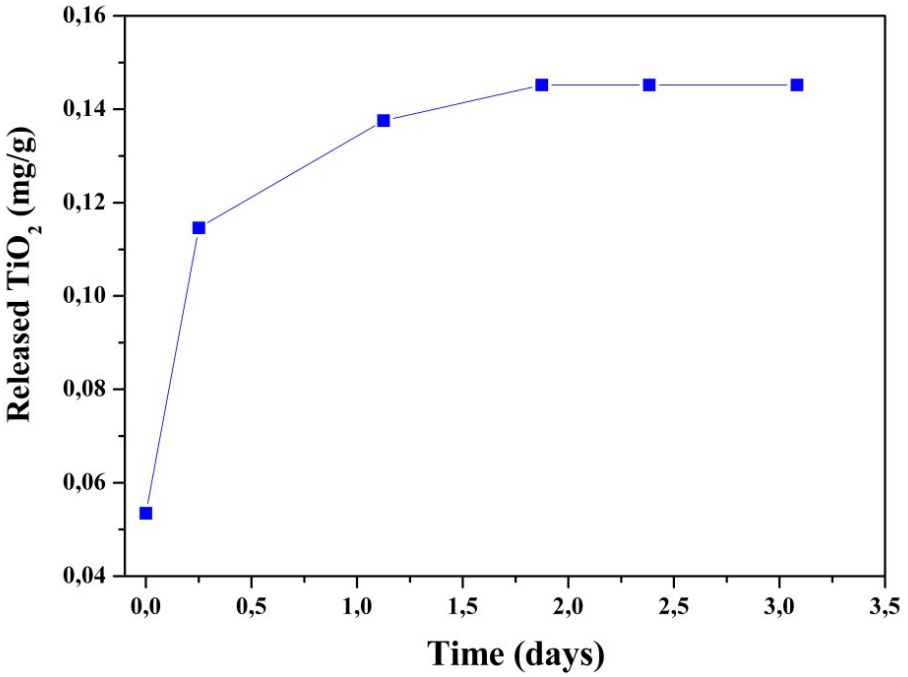


**Figure. FS4** In vitro drug release profile of TiO2 from the nanocomposites based on cellulose nanofibers and titania nanocomposites

The release of $TiO_2$ from the nanocomposite samples was followed spectrophotometrically. The absorbance was calibrated using serial dilution of the CaptiGel colloid solution, which initial $TiO_2$ concentration was determined gravimetrically. The release stabilized after 2 days at the value below 0.15 mg/g, i.e. ca 1.5% of the total titania content (please, compare Fig. FS1).

## References

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