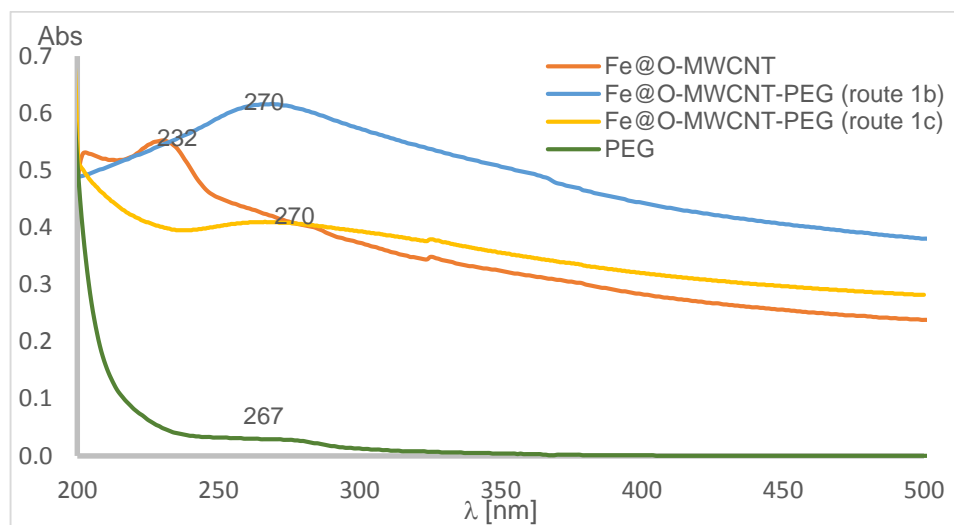


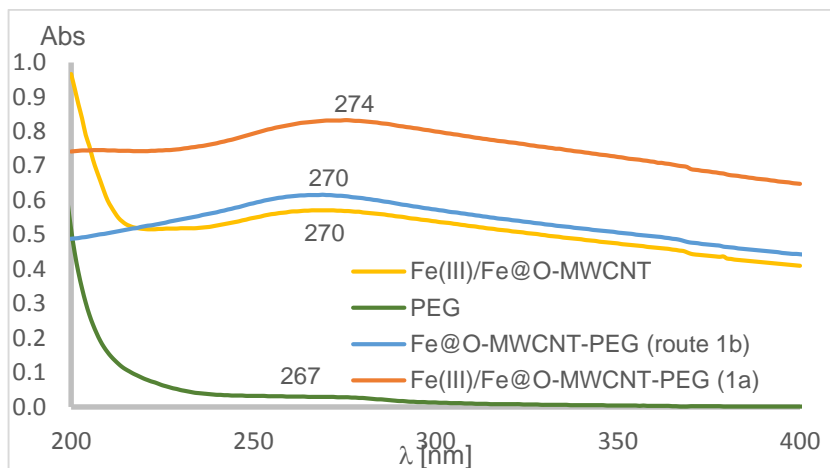
## Supplementary materials

### Transformation of Fe@O-MWCNT to Fe@O-MWCNT-PEG

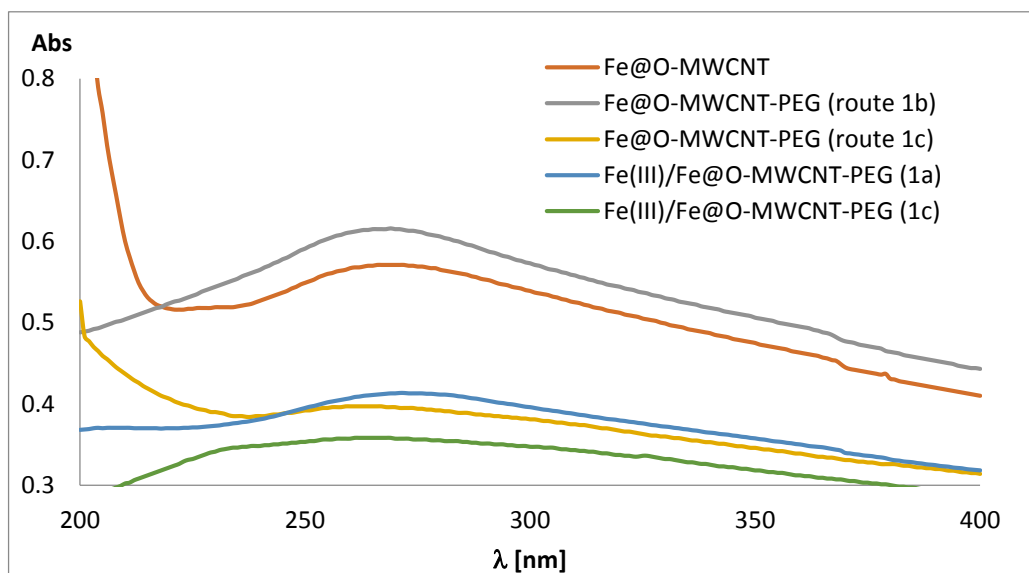


**Figure S1** UV-Vis spectra of PEGylation products formed via routes **1b** and **1c** presented on Scheme 2 in the main manuscript.

## Anchoring Fe<sup>3+</sup> onto PEGylated CNTs

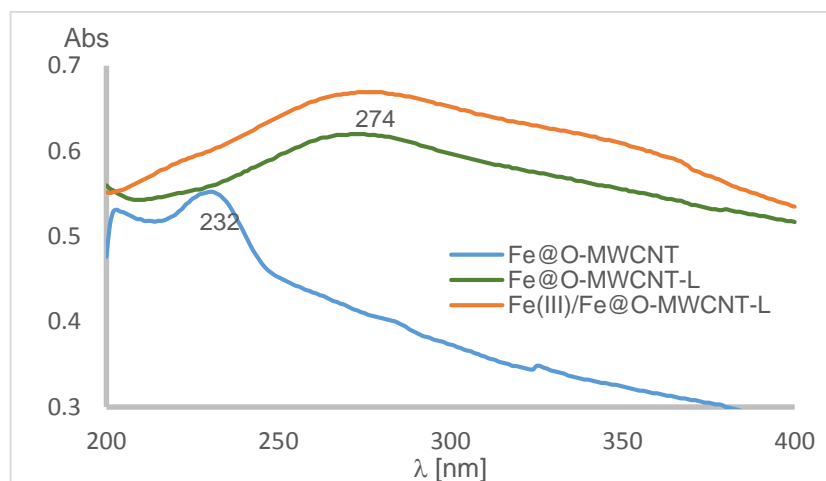


**Figure S2** UV-Vis spectra of PEGylation via route *a* (Scheme 2) of Fe(III)/Fe@O-MWCNT.



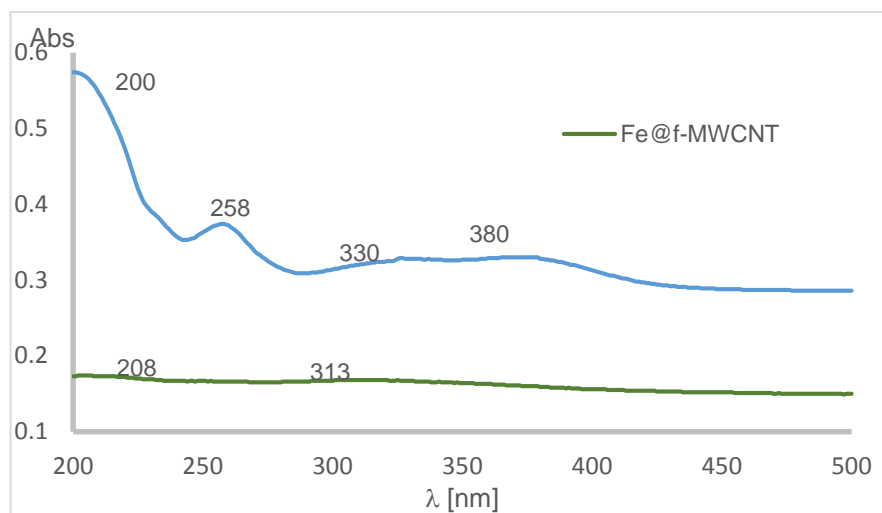
**Figure S3** UV-Vis spectra of iron(III) anchoring on the PEGylated product (Scheme 2).

### Fe@O-MWCNT-L and Fe(III)/Fe@O-MWCNT-L



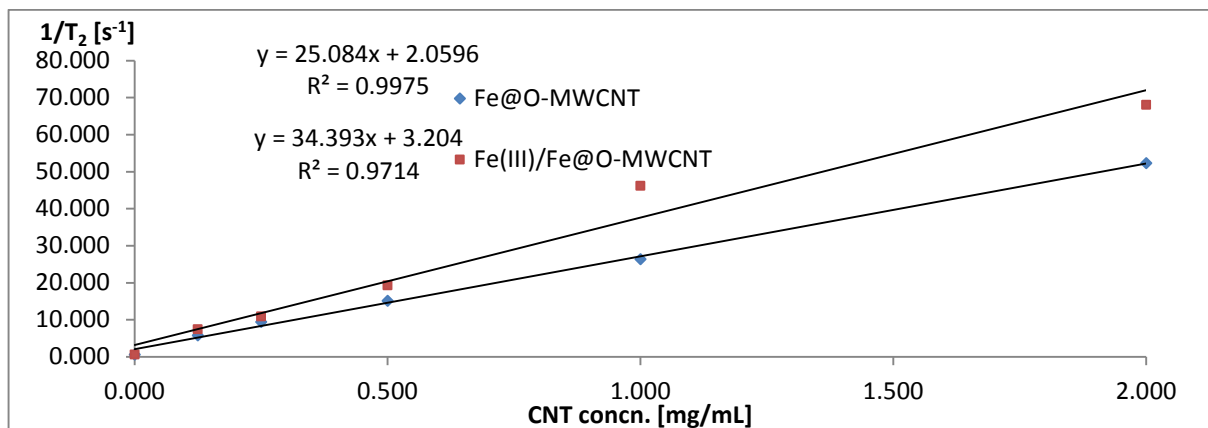
**Figure S4** UV-Vis spectra of Fe@O-MWCNT-L and its iron(III) anchoring product

## Fe@f-MWCNT and Fe(III)/Fe@f-MWCNT

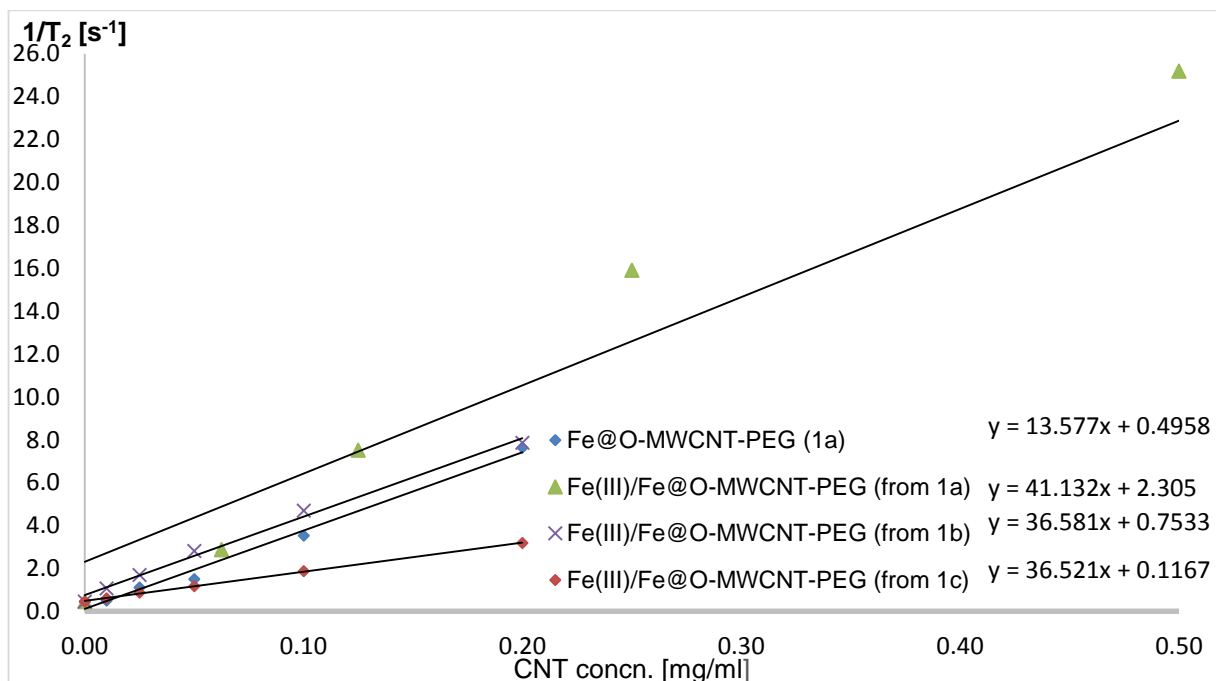


**Figure S5** UV-Vis spectra of Fe@f-MWCNT and its iron(III) anchoring product.

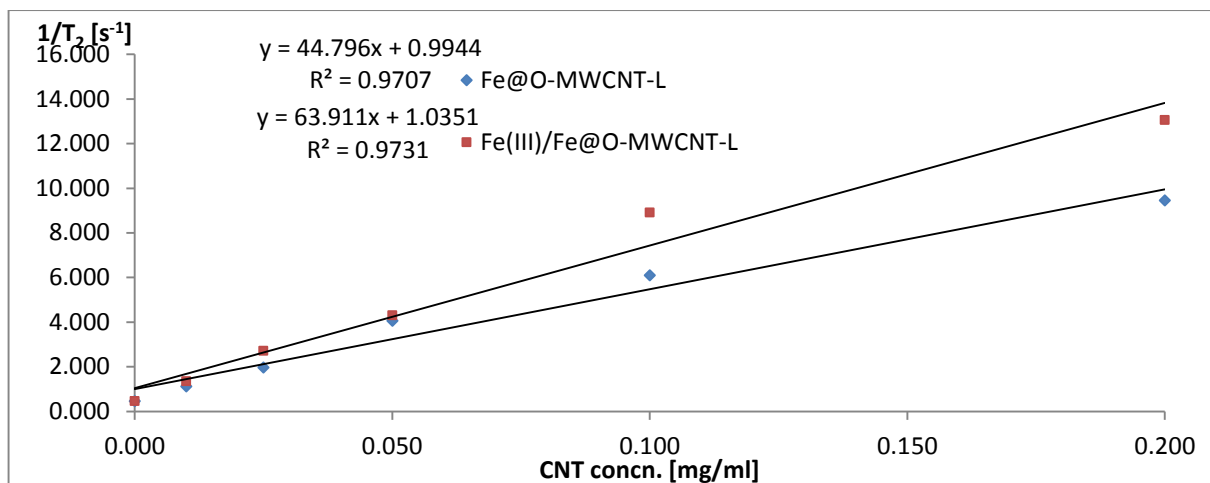
## Relaxivity measurements



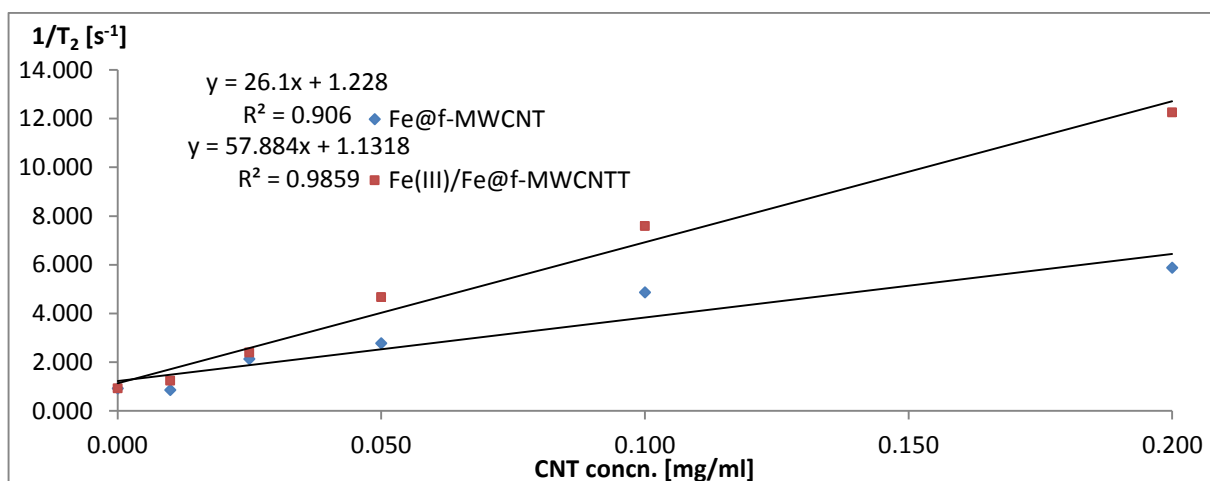
**Figure S6** Relaxivity  $r_2$  at 300 MHz for entries 1 - Fe@O-MWCNT and 2 - Fe(III)/Fe@O-MWCNT presented in Table 4.



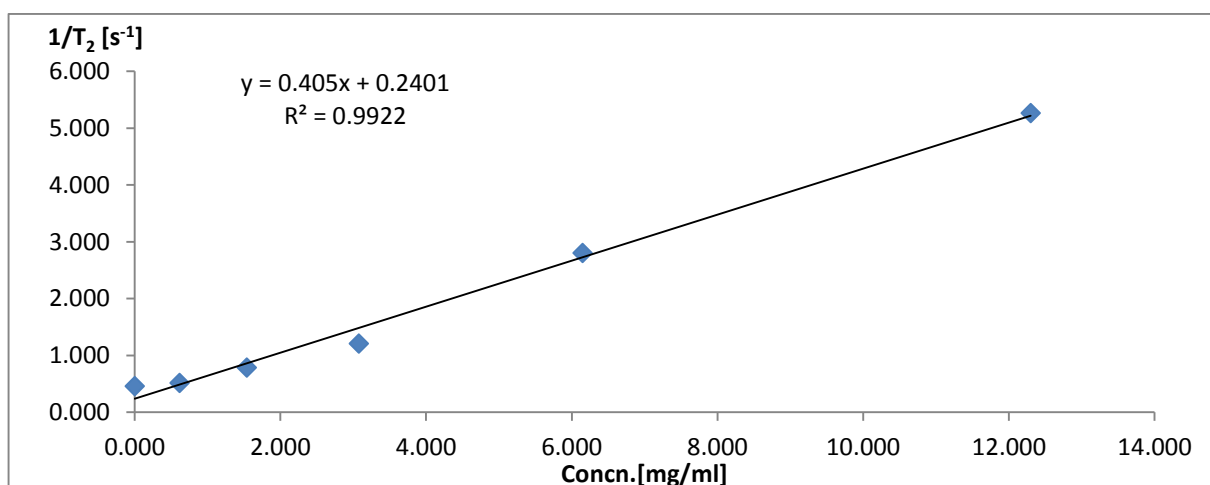
**Figure S7** Relaxivity  $r_2$  at 300 MHz for entries 3 - Fe@O-MWCNT-PEG (**1a**), 4 - Fe(III)/Fe@O-MWCNT (from **1a**), 5 - Fe(III)/Fe@O-MWCNT (from **1b**), 6 - Fe(III)/Fe@O-MWCNT (from **1c**), presented in Table 4.



**Figure S8** Relaxivity  $r_2$  at 300 MHz for entries 7 - Fe@O-MWCNT-L and 8 - Fe(III)/Fe@O-MWCNT-L presented in Table 4.



**Figure S9** Relaxivity  $r_2$  at 300 MHz for entries 9 - Fe@f-MWCNT and 10 - Fe(III)/Fe@f-MWCNT presented in Table 4.



**Figure S10** Relaxivity  $r_2$  at 300 MHz for entry 10 – FeCl<sub>3</sub>, presented in Table 4.

## Thermogravimetric analysis

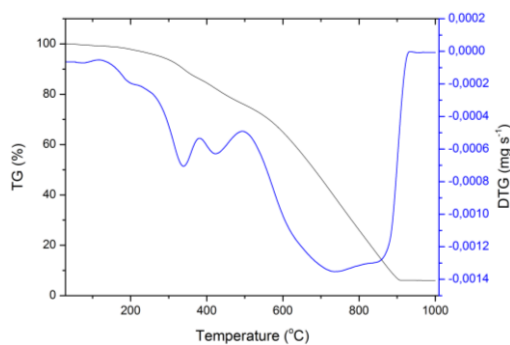


Figure S11 TGA/DTA curves of Fe@O-MWCNT-PEG (1a).

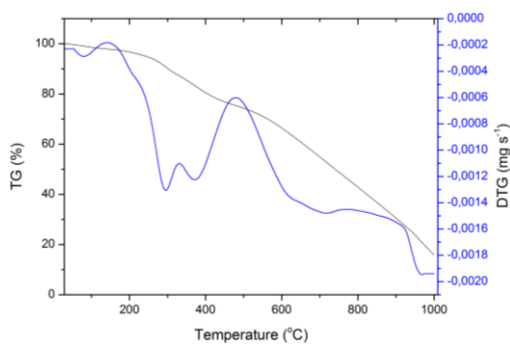


Figure S12 TGA/DTA of Fe(III)/Fe@O-MWCNT-PEG (from 1a).

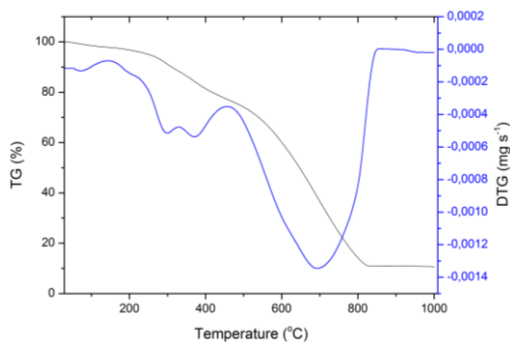


Figure S13 TGA/DTA curves of Fe(III)/Fe@O-MWCNT-PEG (from 1b).

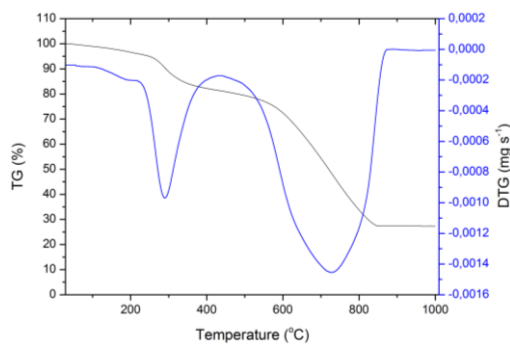
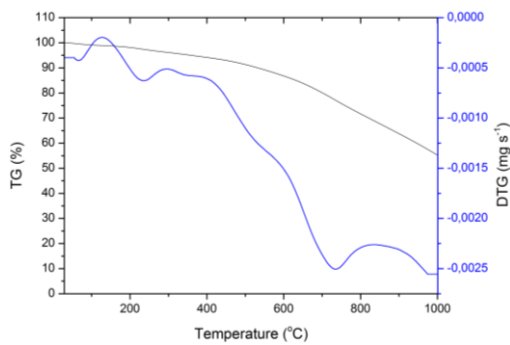
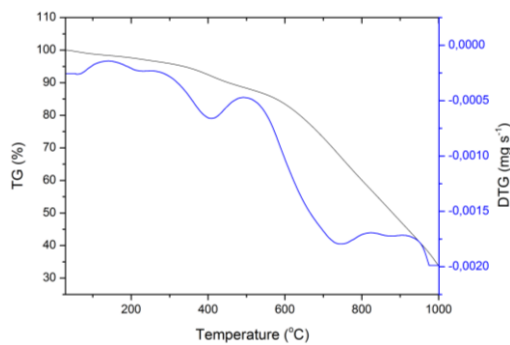


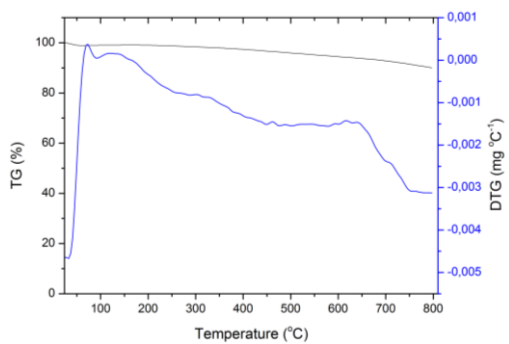
Figure S14 TGA/DTA curves of Fe(III)/Fe@O-MWCNT-PEG (from 1c).



**Figure S15** TGA/DTA curves of Fe@O-MWCNT-L.



**Figure S16** TGA/DTA curves of Fe(III)/Fe@O-MWCNT-L.



**Figure S17** TGA/DTA curves of Fe@f-MWCNT.