Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.


# Novel dehydropeptide-based magnetogels containing manganese ferrite nanoparticles as antitumor drug nanocarriers

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# Supplementary Information

## 1. UV-Visible absorption spectrum of $MnFe_2O_4$ nanoparticles

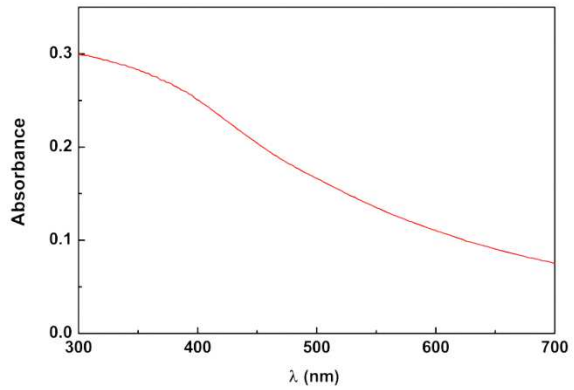


**Figure S1.** UV-visible absorption spectrum of a dilute dispersion of $MnFe_2O_4$ nanoparticles in water.

## 2. Evidence of no aggregation of the nanoparticles during gel formation

From UV-Visible absorption measurements overtime (Figure S2), it can be observed that the nanoparticles/gel dispersion takes about one hour to lose 0.02% of its initial transmittance, with no evidence of aggregation. As the hydrogels/magnetogels take in average 2-3 hours to form a stable gel, most (>90%) of the nanoparticles will remain encapsulated at the used concentration.

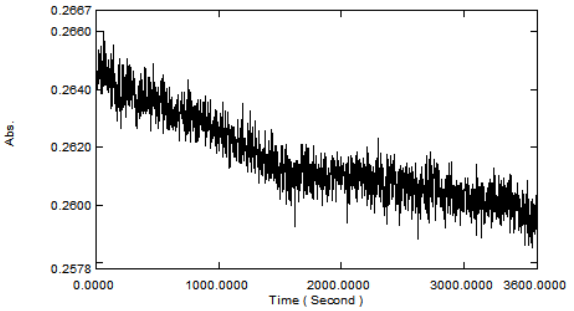


**Figure S2.** UV-visible absorption spectrum of nanoparticles/hydrogel dispersion over time.

## 3. FTIR absorption spectrum assignments of hydrogels and magnetogels

**Table S1.** Vibrational wavenumber (in $cm^{-1}$) assignments according to previously reported values for naproxen and amino acids. The symbols are ν: stretching; δ: bending; $\delta_{o.o.p}$: out-of-plane bending; as: asymmetric; s: symmetric.

| | Vibrational wavenumber ($cm^{-1}$) | | |
|---|---|---|---|
| **Assignments** | **H1** | **H2** | **H3** |
| ν C-N | - | 1076 | - |
| δ C-$H_{ring}$ | - | 1095 | - |
| $\nu_s$ C-O-C | 1030 | 1030 | 1030 |
| ν $C_{ext}$-$C_{ring}$ | - | 1209 | - |
| $\nu_{as}$ C-C-O | 1265 | 1265 | 1265 |
| $\nu_{as}$ C-C-O-H | 1394 | 1394 | 1394 |
| ν C-C | 1494 | 1494 | 1494 |
| δ C-H | 1506 | 1506 | 1506 |
| $\nu_s$ C-$C_{ring}$ | 1604 | 1604 | 1604 |
| δ NH | 1580 | 1580 | ~1577 |
| ν C-H | 2850-3000 | 2850-3000 | - |
| $\delta_{o.o.p}$ C-$H_{ring}$ | 682-750 | - | - |
| $\delta_{o.o.p}$ ring | - | 617 | - |

The peak close to 1580 $cm^{-1}$ is assigned to NH bending, which is followed by the vibration modes in the amide II region (1480 – 1575 $cm^{-1}$). A sharper peak observed in the magnetogels close to 3272 $cm^{-1}$ is assigned to secondary amide N-H stretching resonance with the first amide II overtone (amide A band), which is superimposed by the broad carboxylic acid O-H dimers in the 3100 – 3400 $cm^{-1}$ region. Considering the amide I region (1610 – 1695 $cm^{-1}$), a high absorption enhancement is observed for the amide C=O stretching at 1641 $cm^{-1}$, accompanied by the 1710 $cm^{-1}$ amide C=O dimers vibration in the hydrogel **H1**. The hydrogel **H2** exhibits the most prominent C=O dimers vibrations at 1733 $cm^{-1}$ and 1703 $cm^{-1}$, while **H3** shows peaks at 1714 $cm^{-1}$ and 1660 $cm^{-1}$.

## 4. Spectral overlaps for FRET measurements (magnetogels/drugs)

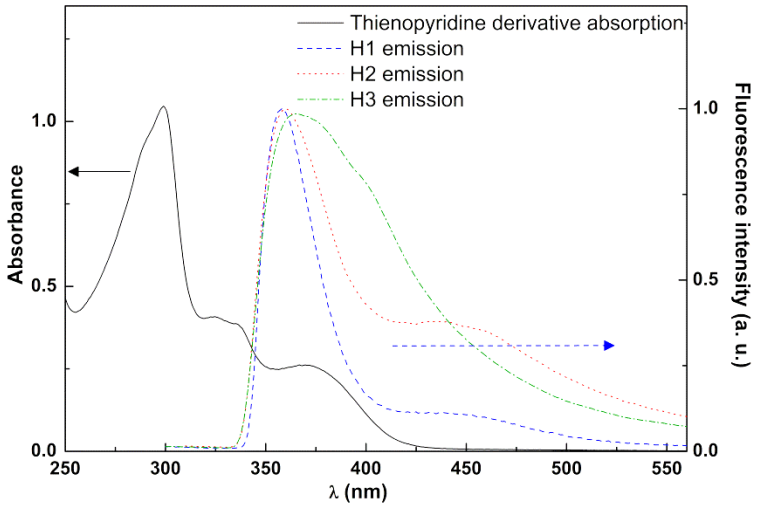


**Figure S3.** Spectral overlap (spectra are normalized) between magnetogels fluorescence emission, **H1**: Npx-*L*-Phe-*Z*-ΔAbu-OH; **H2**: Npx-*L*-Trp-*Z*-ΔPhe-OH; **H3:** Npx-*L*-Ala-*Z*-ΔPhe-Gly-*L*-Arg-Gly-*L*-Asp-Gly-OH, and thienopyridine derivative absorption.

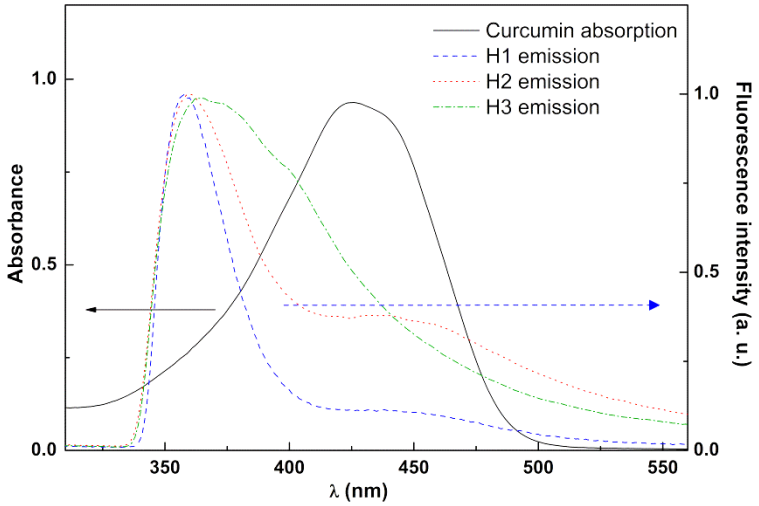


**Figure S4.** Spectral overlap (spectra are normalized) between magnetogels fluorescence emission, **H1**: Npx-*L*-Phe-*Z*-ΔAbu-OH; **H2**: Npx-*L*-Trp-*Z*-ΔPhe-OH; **H3:** Npx-*L*-Ala-*Z*-ΔPhe-Gly-*L*-Arg-Gly-*L*-Asp-Gly-OH, and curcumin absorption.

## 5. Excitation spectra of hydrogel H1

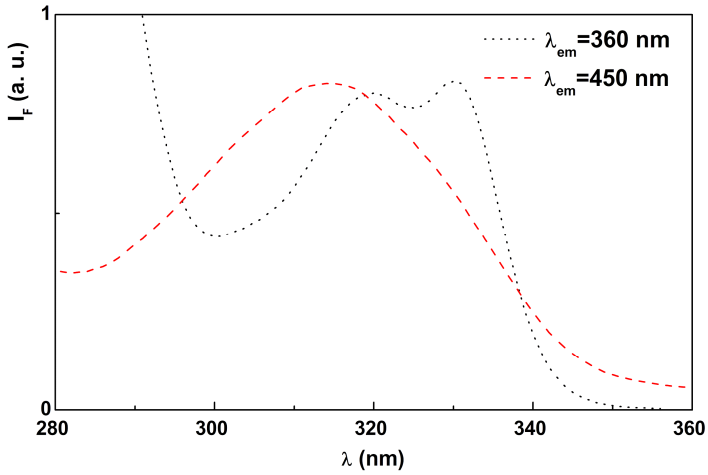


**Figure S5.** Excitation spectra of hydrogel **H1**, at two emission wavelengths: 360 nm (Npx monomer) and 450 nm (aggregate).

## 6. Spectral overlaps for FRET measurements (drugs/Nile Red)

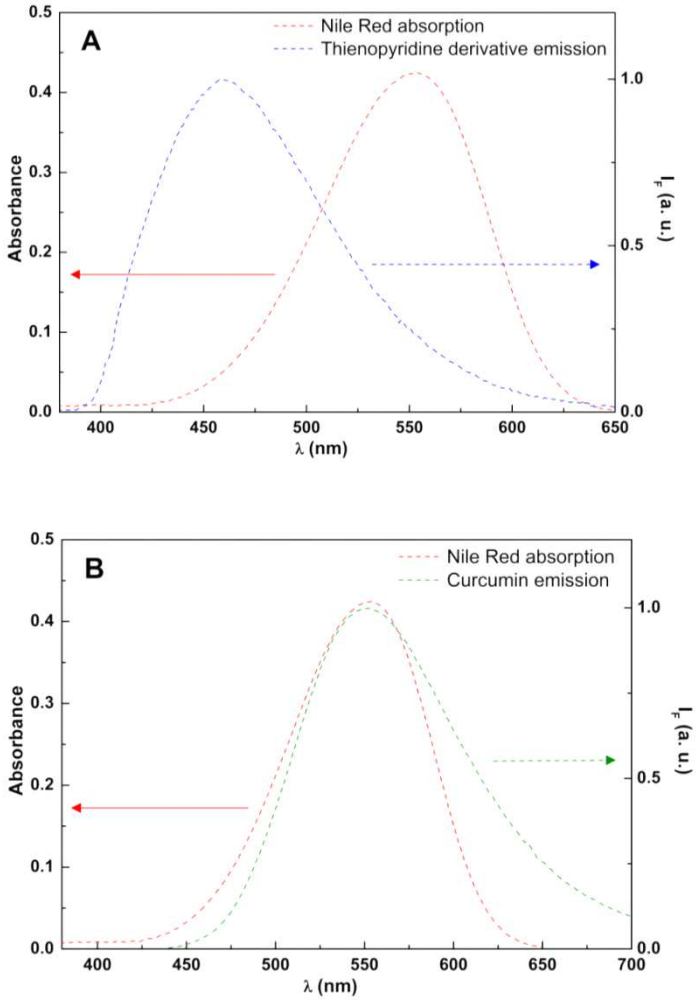


**Figure S6.** Spectral overlap (spectra are normalized) between antitumor drug emission and Nile Red absorption. **A**: Thienopyridine derivative; **B**: Curcumin.