Supporting figures for

Supramolecular adducts between macrocyclic Gd (III) complexes and polyaromatic systems: a route to enhance the relaxivity through the formation of hydrophobic interactions.

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Supplementary figures

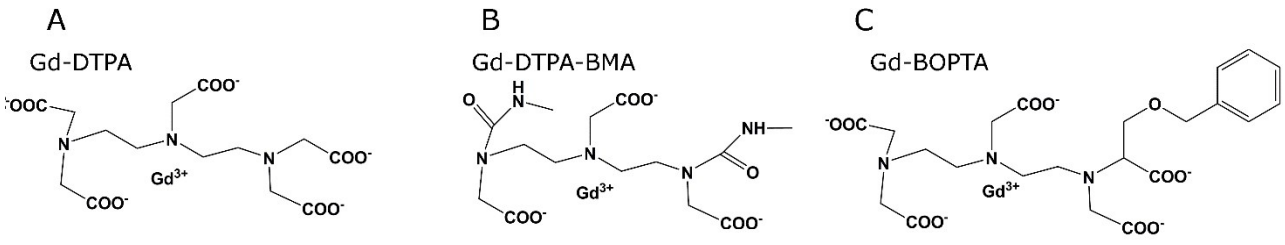

Figure S1. Chemical structure of linear Gd-based contrast agents.

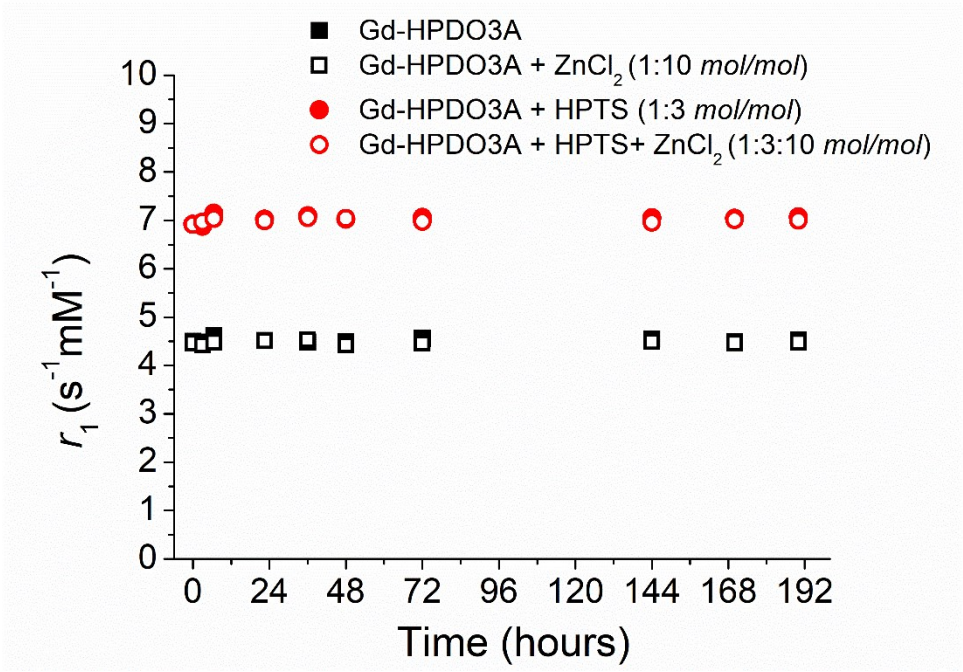

Figure S2. Zinc transmetallation experiment for Gd-HPDO3A and Gd-HPDO3A/HPTS (1:3 *mol/mol*) in the presence of an excess (10 fold) of $ZnCl_2$: assessment by measuring of r_1 over time (up to t=8 days).

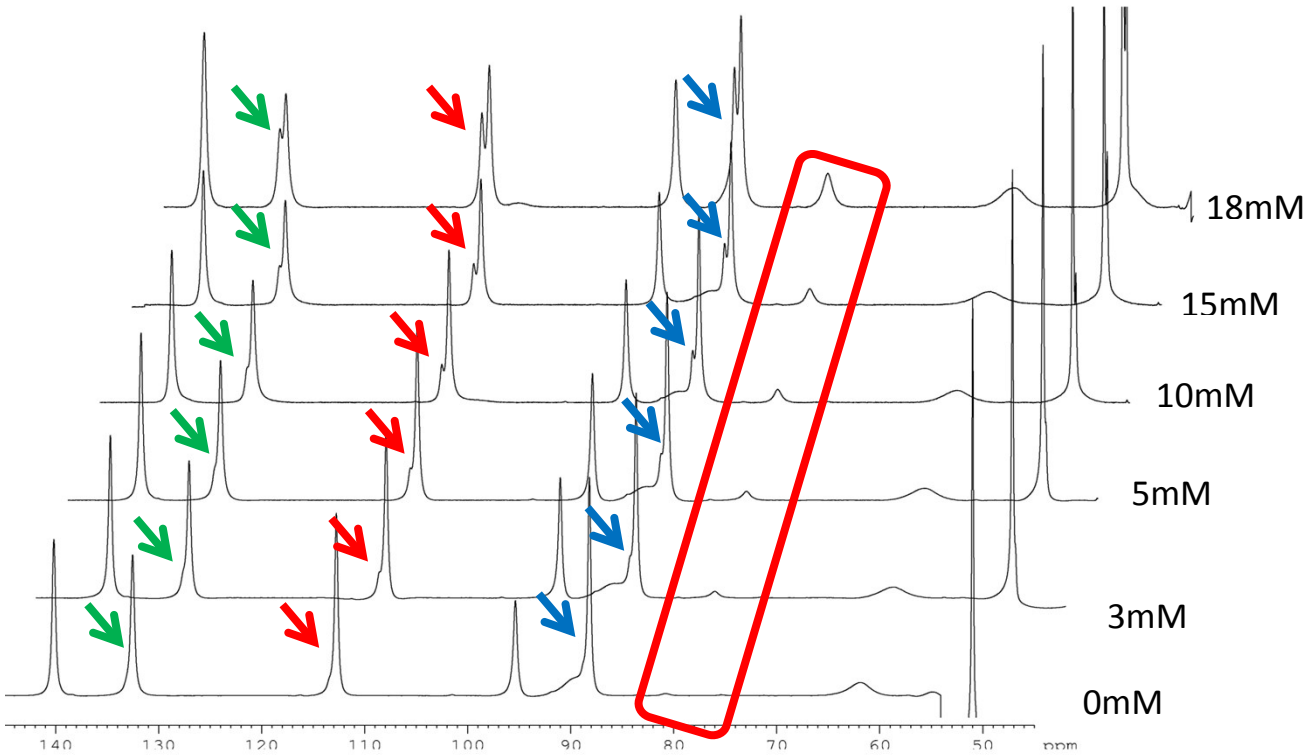

Figure S3. ^{1}H-NMR spectra and shift of HPTS protons resonances at variable concentration of HPTS ([Yb-HPDO3A]=20 mM). Arrows indicate splitting of peaks (T=15°C, B_0=14.1T).

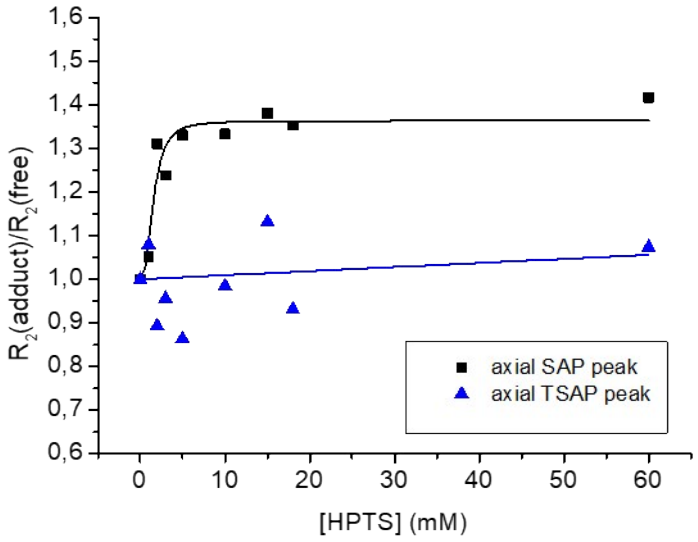

Figure S4. Ratio of transversal relaxation rates (R_2) of selected peaks measured from ^{1}H-NMR spectra of Yb-HPDO3A + HPTS with respect to free Yb-HPDO3A. ([Yb-HPDO3A]=20 mM, T=15°C, B_0=14.1T).

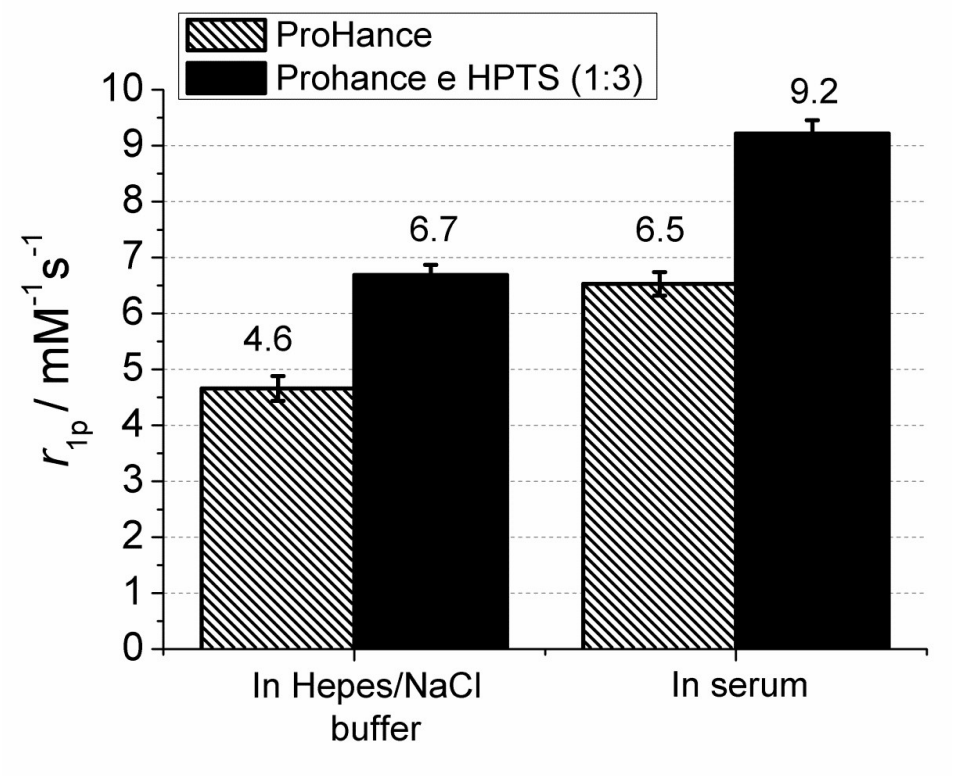

Figure S5. r_{1p} of Gd-HPDO3A and Gd-HPDO3A/HPTS in hepes/NaCl or in human serum (T=25°C, B_0=0.5T).

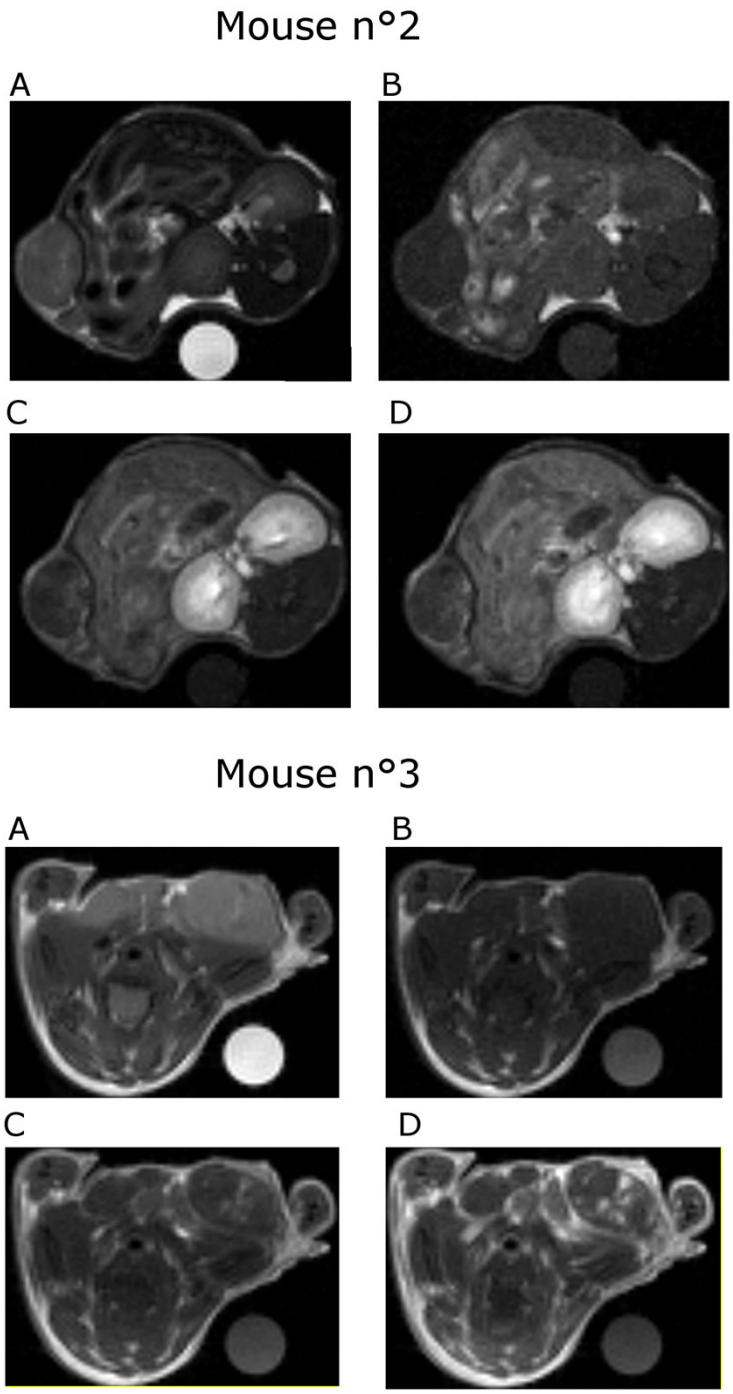

Figure S6. Representative *in vivo* axial MR images of tumor region in two additional Balb/c mouse bearing subcutaneous TS/A tumor. (A) T_{2w} MR image, (B) uncontrasted (*pre*) T_{1w} MR image without Gd-CA, (C) T_{1w} MR image after 2 min from injection of Gd-HPDO3A (0.15 mmol/kg) (D) T_{1w} MR image after 2 min from the injection of Gd-HPDO3A (0.15 mmol/kg) and HPTS (0.45 mmol/Kg). B_0=7.1T, room temperature.

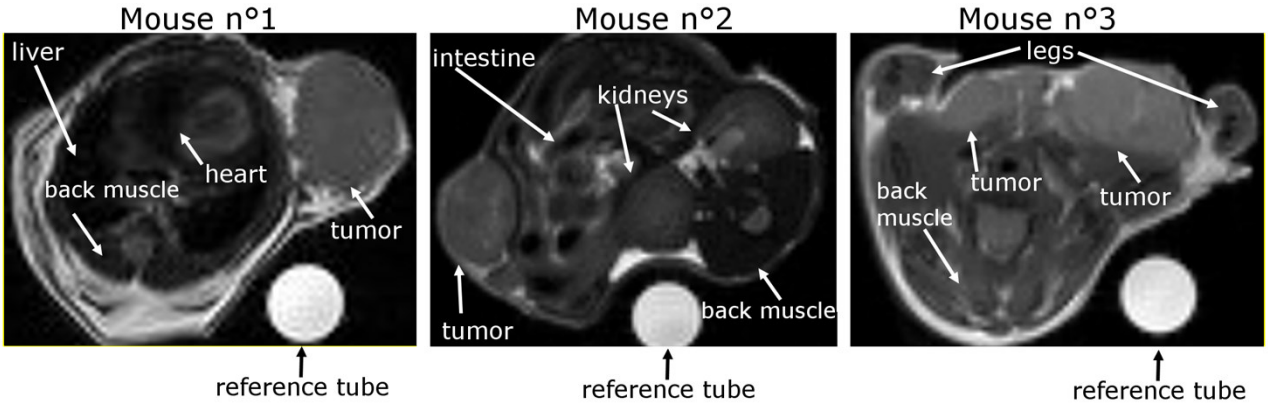

Figure S7. Morphological T_{2w} MR images of the three analyzed mice showing the label of the most important organs.

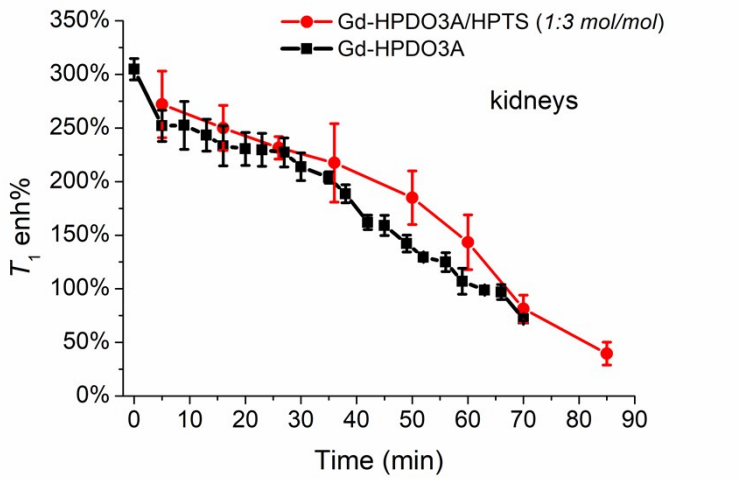

Figure S8. Enh%, of MRI Signal Intensity in the kidneys after injection of ProHance (0.15mmol/Kg) or injection of ProHance/HPTS (0.15mmol/kg ProHance+ 0.45mmol/Kg HPTS) (N=3).

Calculation of Enh%

$$Enh\% = \frac{SI_{post} - SI_{pre}}{SI_{pre}} \times 100$$

Where SI_{post} is the signal intensity in the T_{1w} MR image sfter injection of the GBCA, normalized for signal intensity in the reference tube and SI_{pre} is the signal intensity in the T_{1w} MR image before injection of the GBCA, normalized for signal intensity in the reference tube.

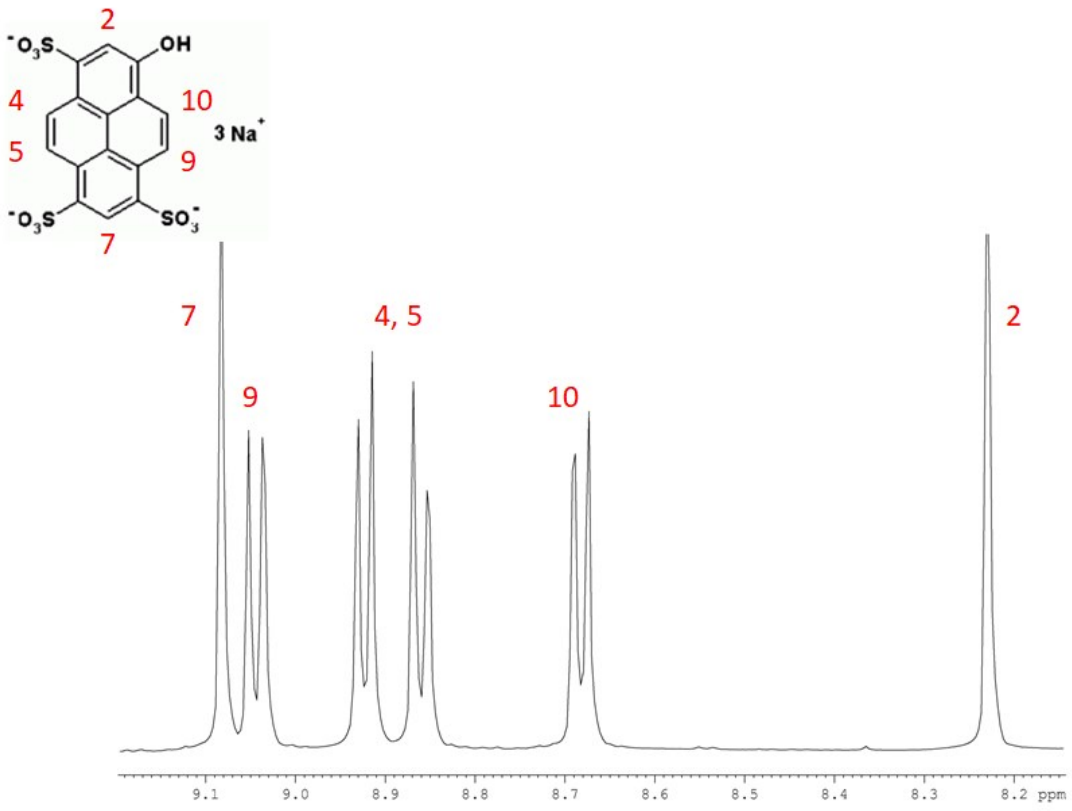

Figure S9. ^{1}H-NMR spectrum of HPTS in D_2O, pH 6.0, T=15°C, B_0=14.1 T.