Fluoride-specific fluorescence/MRI bimodal probe based on a 
Gadolinium(III)-flavone complex: Synthesis, mechanism and bioimaging application in vivo

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**Fig. S1.** ESI-MS spectrum of [EDTA-Gd]−

**Fig. S2.** Fluorescence spectra of EDTA-Gd-HF (10 μM) in the presence of increasing amount of fluoride ions (0–10 μM) in aqueous (C2H5OH: H2O = 3:7). Insert: plot of the fluorescence intensity changes of EDTA-Gd-HF (10 μM) observed at 476 nm versus fluoride ions concentration. Excitation was performed at 400 nm.
**Fig. S3.** Fluorescence spectra of HF (10 μM) in the presence of increasing amount of fluoride ions in aqueous (C₂H₅OH: H₂O = 3:7). Excitation was performed at 400 nm.

**Fig. S4.** ESI-MS spectrum of EDTA-Gd-HF in presence of fluoride ions in aqueous
Fig. S5. Linear relationship between fluorescence intensity of EDTA-Gd-HF (3 μM) at 476 nm versus the concentration of fluoride ion (10–30 μM) in aqueous (CH₃OH: H₂O = 3:7). Excitation was performed at 400 nm.

Fig. S6. Fluorescence responses of EDTA-Gd-HF (10 μM) in the presence of various biological cations (0.5 mM) in aqueous (C₂H₅OH: H₂O = 3:7). The intensities were recorded at 476 nm. Excitation was performed at 400 nm.
Fig. S7. Influence of pH on the fluorescence intensities of HF, EDTA-Gd-HF and EDTA-Gd-HF in the presence of fluoride ion. The intensities were recorded at 476 nm. Excitation was performed at 400 nm.

Fig. S8. T₁-weighted MR transection images of living white mice after injection of: (a) EDTA-Gd-HF (0.2 mL, 0.2 mM), (b) 3.5 mM fluoride ions only, (c) 3.5 mM fluoride ions followed by injection of 0.2 mL EDTA-Gd-3HF (0.2 mM), and (d) further injection of 3.5 mM mixed anions into (c).