

Electronic Supporting Information

A gadolinium(III) complex with 8-amidequinoline based ligand as copper(II) ion responsive contrast agent

Wei-Sheng Li, Jian Luo, Zhong-Ning Chen*

State Key Laboratory of Structural Chemistry, Fujian Institute of Research on the Structure of Matter, Chinese Academy of Sciences, Fuzhou, Fujian 350002, China.

E-mail: czn@fjirsm.ac.cn

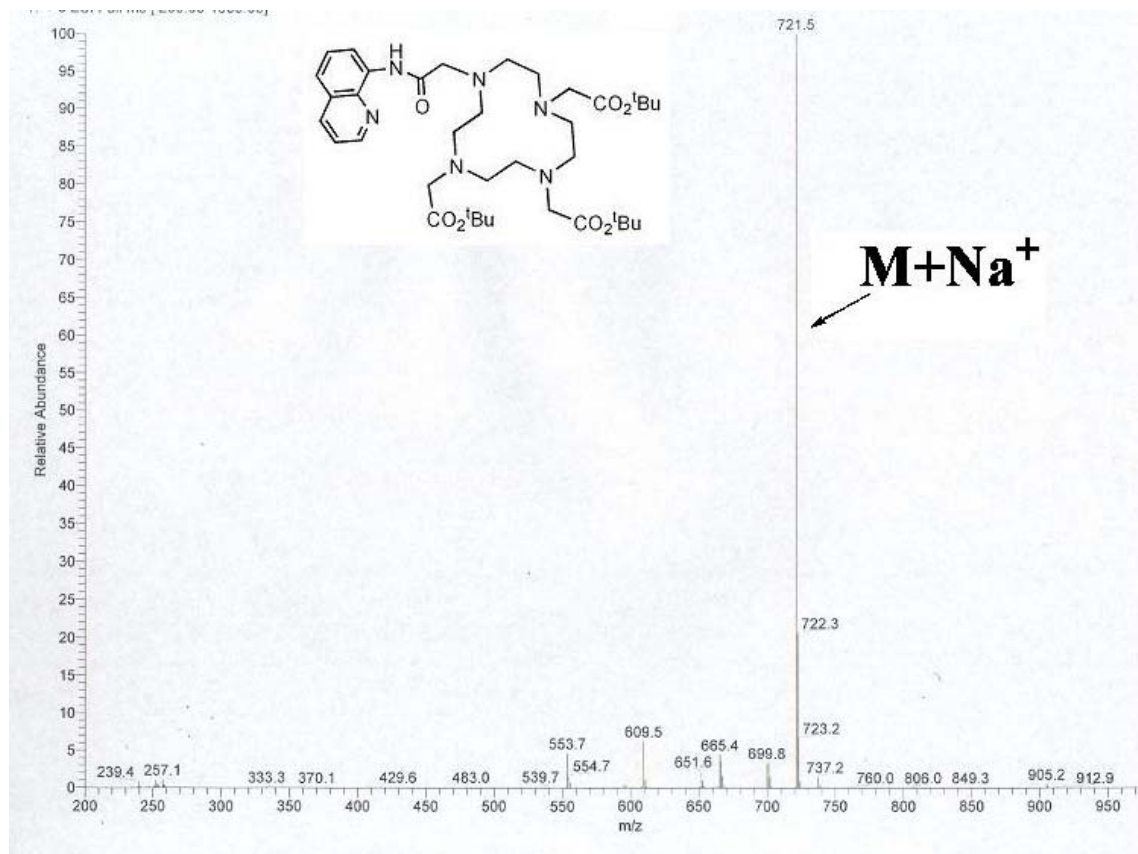


Fig. S1. ESI-MS of 1-(N-quinolin-8-yl-acetamide)-4,7,10-tris(acetic acid)-1,4,7,10-tetraazacyclododecane (3).

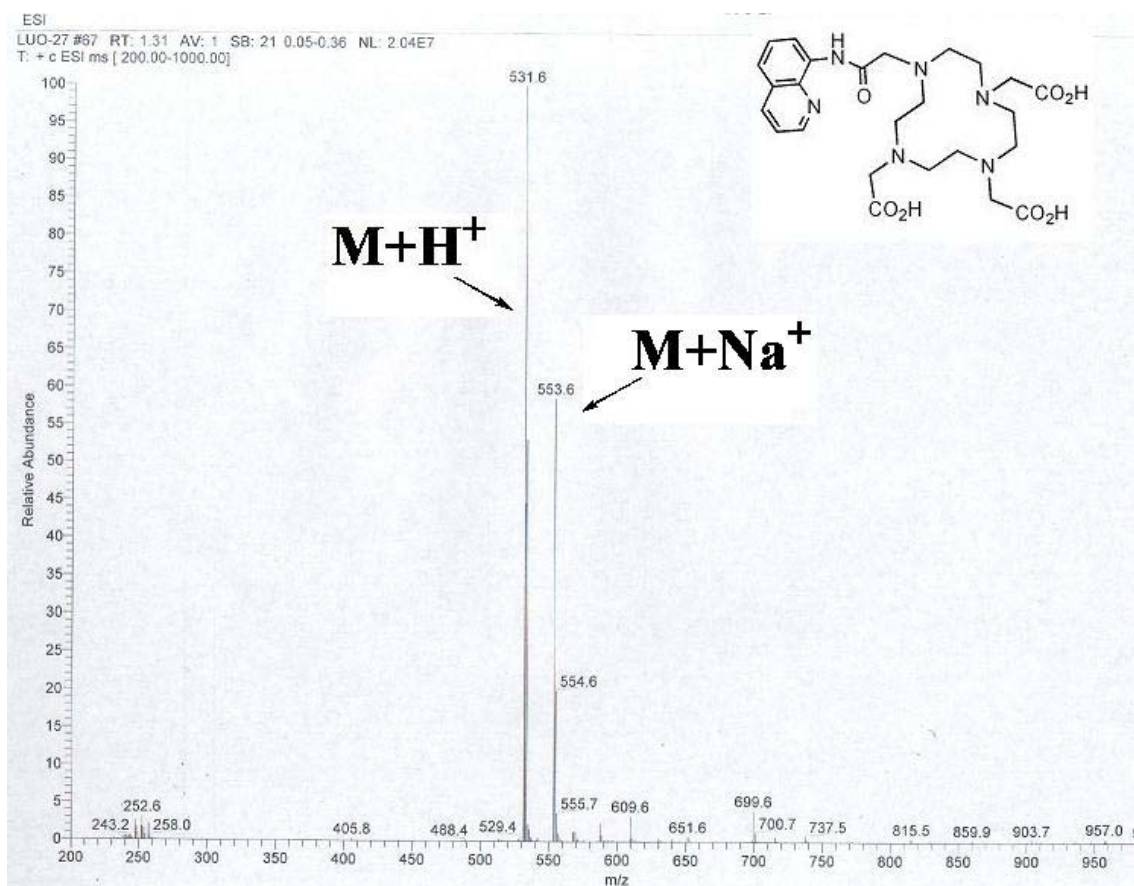


Fig. S2. ESI-MS of ligand H₃QDOTAMA.

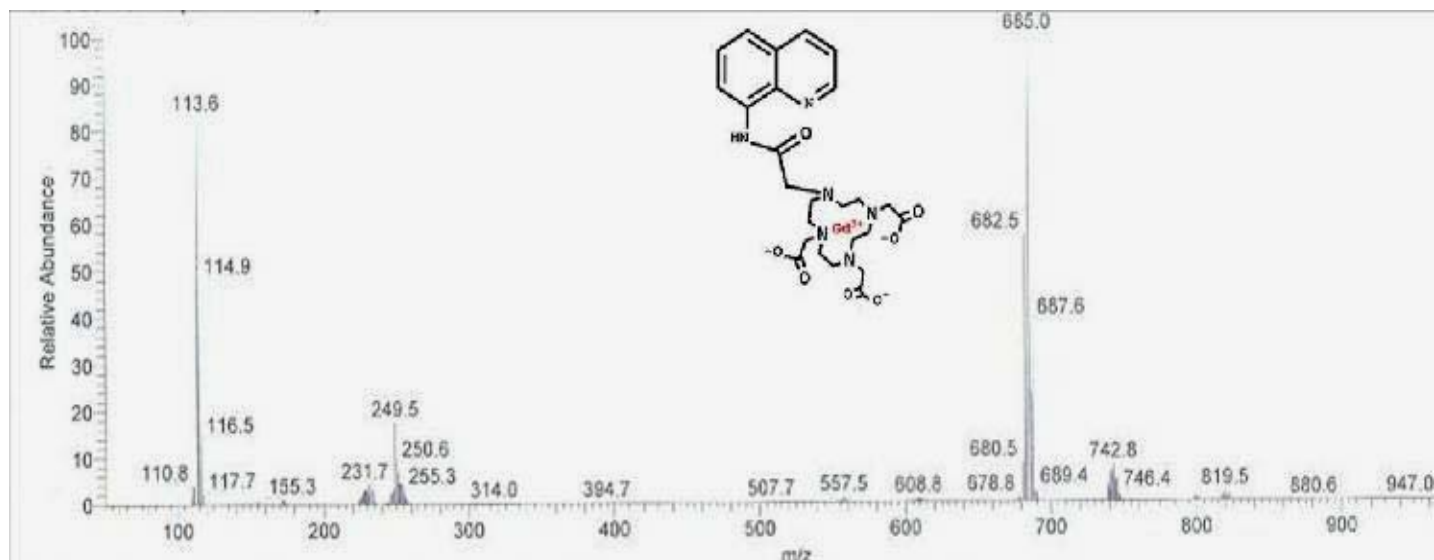


Fig. S3. ESI-MS of Gd-QDOTAMA.

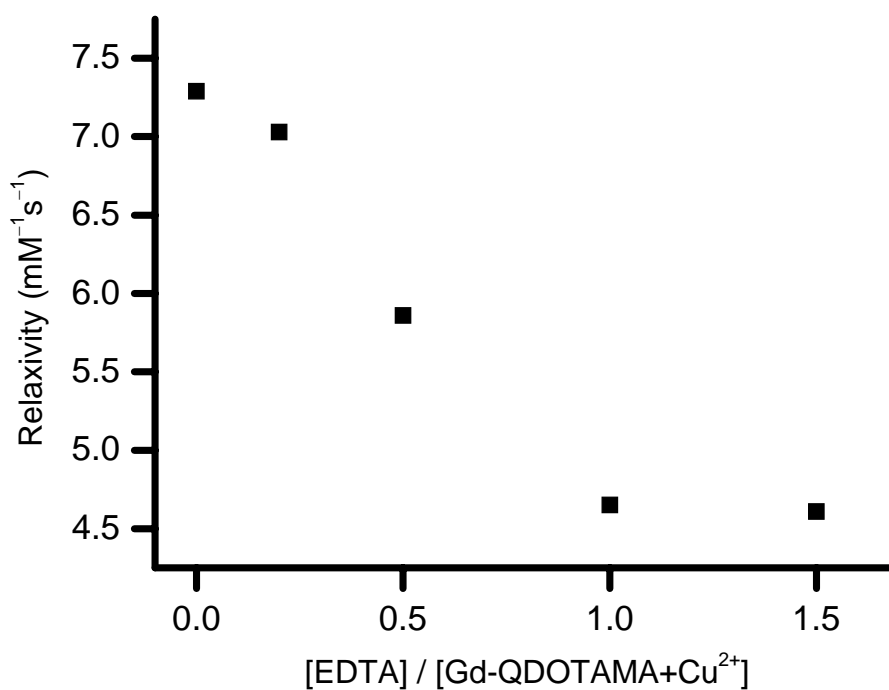


Fig. S4. Relaxivity changes of Gd-QDOTAMA+Cu²⁺ by addition of 0–1.5 equiv. of EDTA in 100 mM hepes buffer at pH 7.2. T_1 measurements were acquired at 400 MHz and 25 °C.

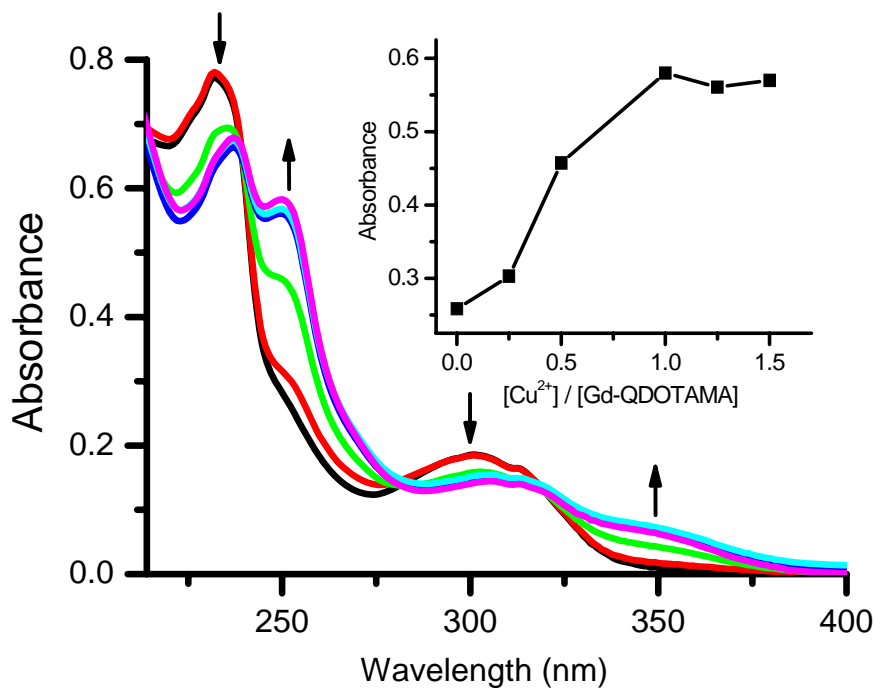


Fig. S5. UV-vis spectral changes for complex Gd-QDOTAMA (0.4 mM) upon titration with CuCl₂ (0–1.5 equiv) in H₂O. Inset: dependence of the absorbance at $\lambda = 250$ nm on the concentration ratio [Cu²⁺]/[Gd-QDOTAMA], showing a 1:1 binding ratio between Gd-QDOTAMA and Cu²⁺.

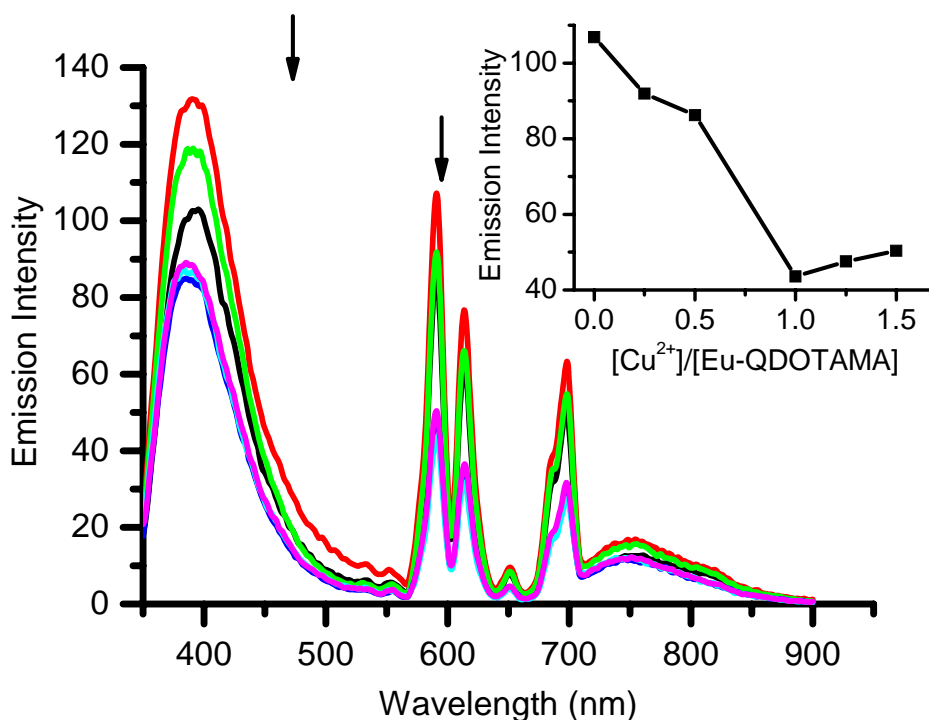


Fig. S6. Emission spectral changes ($\lambda_{\text{ex}} = 300$ nm) for Eu-QDOTAMA (0.4 mM) upon titration with CuCl₂ (0–1.5 equiv) in H₂O. Inset: dependence of Eu^{III}-based emission intensity at $\lambda_{\text{em}} = 591$ nm on the concentration ratio [Cu²⁺]/[Eu-QDOTAMA], showing a 1:1 binding ratio between Eu-QDOTAMA and Cu²⁺.