Scientific Reports, 2017, vol.7, N1

Hydration number: Crucial role in nuclear magnetic relaxivity of Gd(III) chelate-based nanoparticles

Zairov R., Khakimullina G., Podyachev S., Nizameev I., Safiullin G., Amirov R., Vomiero A., Mustafina A.

Kazan Federal University, 420008, Kremlevskaya 18, Kazan, Russia

Abstract

 Today, nanostructure-based contrast agents (CA) are emerging in the field of magnetic resonance imaging (MRI). Their sensitivity is reported as greatly improved in comparison to commercially used chelate-based ones. The present work is aimed at revealing the factors governing the efficiency of longitudinal magnetic relaxivity (r 1) in aqueous colloids of core-shell Gd(III)-based nanoparticles. We report for the first time on hyd ration number (q) of gadolinium(III) as a substantial factor in controlling r 1 values of polyelectrolyte-stabilized nanoparticles built from water insoluble complexes of Gd(III). The use of specific complex structure enables to reveal the impact of the inner-sphere hydration number on both r 1 values for the Gd(III)-based nanoparticles and the photophysical properties of their luminescent Tb(III) and Eu(III) counterparts. The low hydration of TTA-based Gd(III) complexes (q ≈ 1) agrees well with the poor relaxivity values (r 1 = 2.82 mM -1 s -1 and r 2 = 3.95 mM -1 s -1), while these values tend to increase substantially (r 1 = 12.41 mM -1 s -1 , r 2 = 14.36 mM -1 s -1) for aqueous Gd(III)-based colloids, when macrocyclic 1,3-diketonate is applied as the ligand (q ≈ 3). The regularities obtained in this work are fundamental in understanding the efficiency of MRI probes in the fast growing field of nanoparticulate contrast agents.

http://dx.doi.org/10.1038/s41598-017-14409-6

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