

# Fe-Doped Carbon Dots as Dual-Mode T1/T2 Nano-Contrast Agents for Ultra-High Field MRI

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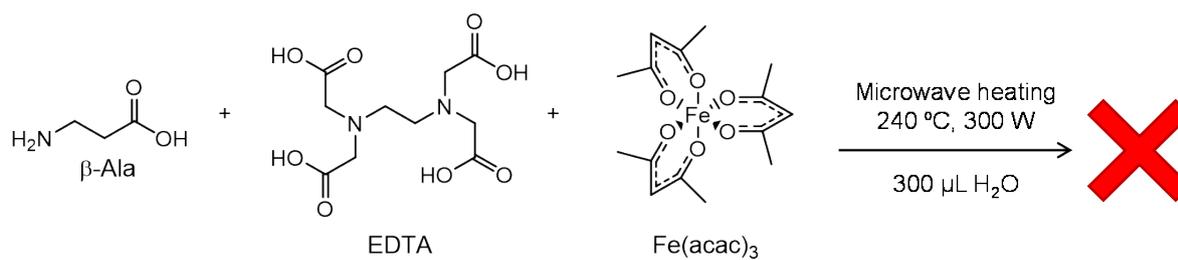
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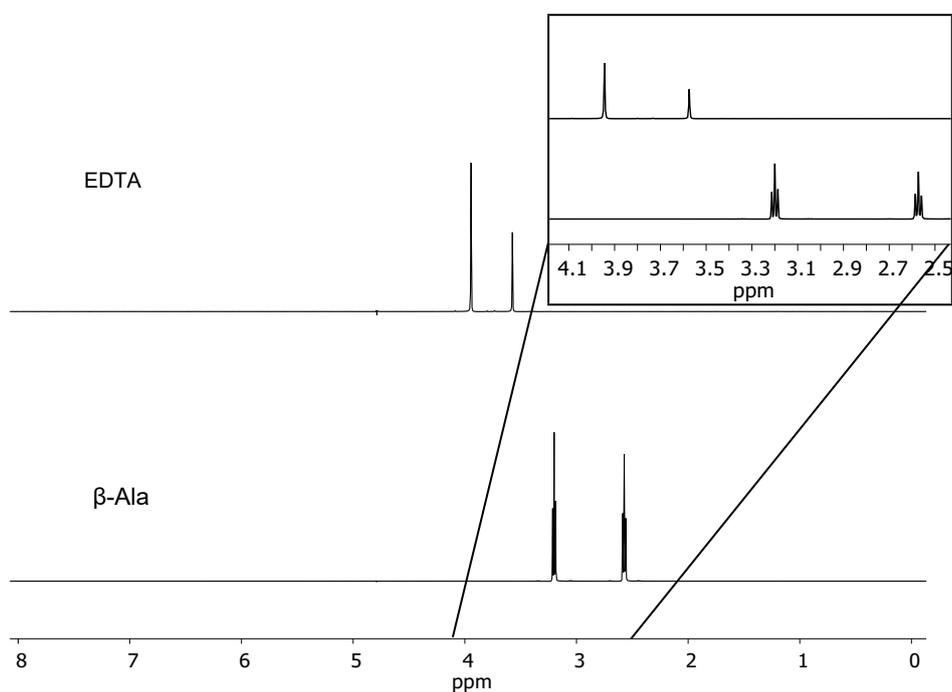
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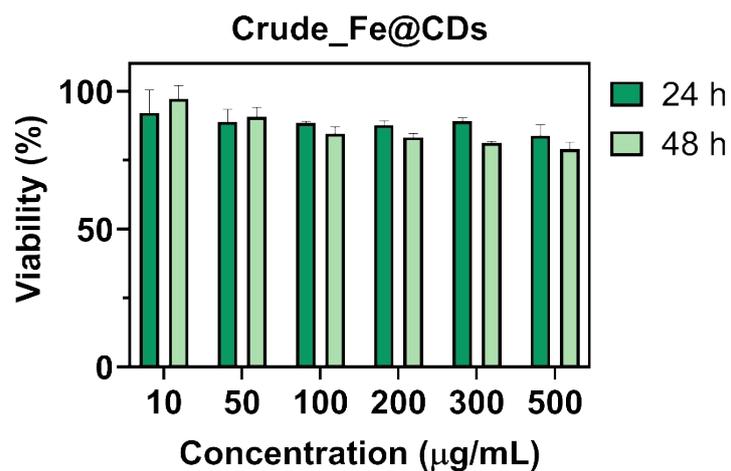
## 1. Synthesis of Fe-doped Carbon Dots



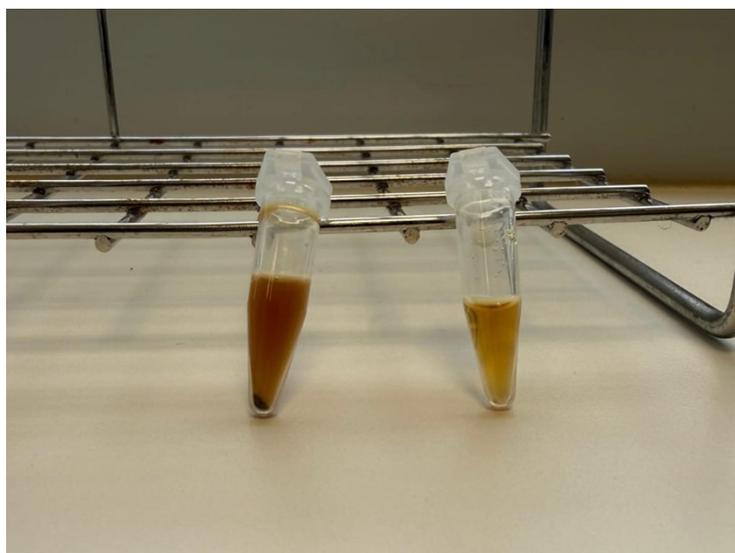
**Scheme S1:** Reaction scheme for CDs from tris(acetylacetonate) iron (III) ( $\text{Fe}(\text{acac})_3$ ),  $\beta$ -Ala and EDTA. Reactions trials did not end up in the formation of iron-doped nanoparticles.



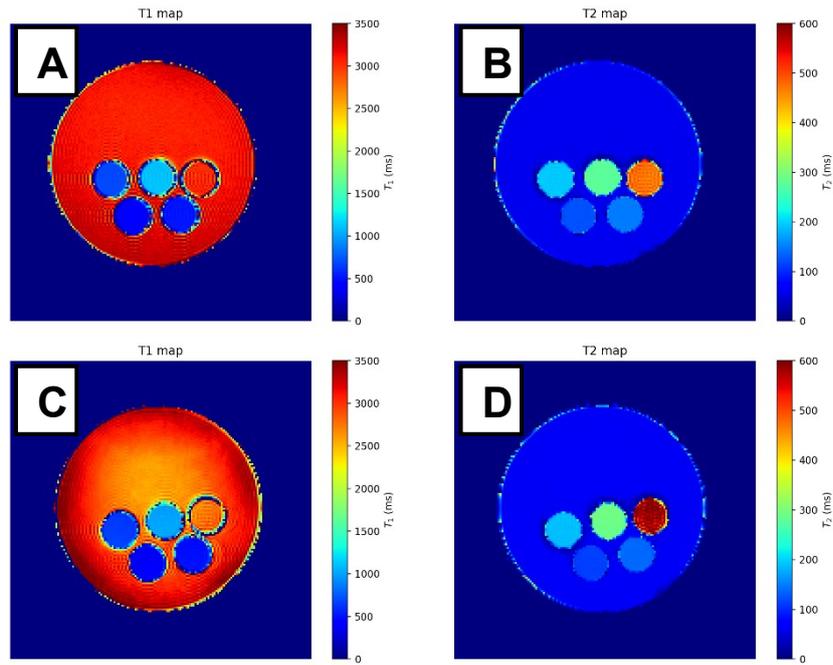
**Figure S1:**  $^1\text{H}$  NMR spectra of precursors in  $\text{D}_2\text{O}$  at 500 MHz.  $\beta$ -Ala: 3.20 (t,  $J = 6.7$  Hz, 2H), 2.57 (t,  $J = 6.7$  Hz, 2H). EDTA: 3.94 (s, 8H), 3.57 (s, 4H).



**Figure S2:** Viability of A549 cell line by MTT assay after incubation with crude\_Fe@CDs at different incubation times (green for 24 hours, light green for 48 hours).



**Figure S3:** Crude\_Fe@CDs (left) and Fe@CDs (right) in water (solution at 10 mg/mL). Differences in water dispersibility are clearly visible comparing the materials. SEC-HPLC chromatography afforded Fe-doped CDs, free from insoluble molecular artifacts and metal doped byproducts.



**Figure S4:** A and B) T<sub>1</sub> and T<sub>2</sub> maps MR images of Fe@CDs phantoms at 7 T. A and B) T<sub>1</sub> and T<sub>2</sub> maps MR images of Fe@CDs phantoms at 11.7 T.

**Table S1:**  $r_2/r_1$  ratios for commercially available Gd-based CAs in water at 37 °C at different magnetic fields. Values are extracted from the work of Rohrer *et al.*, 2005.<sup>[1]</sup>

<b>Gd-based CA</b>	<b>1.5 T</b>	<b>4.7 T</b>
<b>Gadovist</b>	<b>1.1</b>	<b>1.2</b>
<b>Prohance</b>	<b>1.1</b>	<b>1.3</b>
<b>Multihance</b>	<b>1.0</b>	<b>1.3</b>
<b>Dotarem</b>	<b>1.1</b>	<b>1.3</b>
<b>Omniscan</b>	<b>1.0</b>	<b>1.2</b>

## BIBLIOGRAPHY

[1] M. Rohrer, H. Bauer, J. Mintorovitch, M. Requardt, H.-J. Weinmann, Comparison of magnetic properties of MRI contrast media solutions at different magnetic field strengths., *Invest. Radiol.* 40 (2005) 715–24. <https://doi.org/10.1097/01.rli.0000184756.66360.d3>.