Abstract

The topic of my Master degree thesis is the development of a conceptually new class of contrast agents for the ^{31}P magnetic resonance imaging (^{31}P MRI). These agents are based on nanoparticles of calcium(II) phytate. Phytate (*myo*-inositol-1,2,3,4,5,6-hexakisphosphate) is largely present in plants, seeds and grains. It is non-biodegradable but nontoxic for animals and human beings and most importantly around 22% of its mass is phosphorus, so it is easily detectable by ^{31}P NMR/MRI.

These nanoparticles of Ca(II) phytate were doped with paramagnetic Fe^{3+} ions which broaden the ^{31}P signal, making the nanoparticles invisible in healthy tissues. In the presence of bacteria producing siderophores (for example in *Helicobacter pylori* in gastric ulcers), Fe^{3+} is released from the gel and ^{31}P MRI signal becomes detectable. In vitro simulation of this release was performed with deferroxamine, a compound possessing high affinity to Fe^{3+} ions forming coloured complex with it exploitable for the UV-VIS evaluation.

The Ca(II) phytate can be synthesized in two possible ways. The first way is by direct precipitation of the Ca^{2+} salt with sodium phytate. The second way is ion exchange of phosphate in the nanoparticles of hydroxyapatite which creates electrostatically stabilized calcium phytate nanoparticles. Both these ways were tested and compared.

Preparation of the nanoparticles from hydroxyapatite was successful, size of these particles is around 100nm. However, synthesis of Ca(II) phytate nanoparticles doped with Fe^{3+} was partly problematic and needs further optimization.

The best method for preparing doped particles has been the synthesis by agregation of sodium fytate by calcium salt. These samples, referred to as $CaIP_6$ 2, had a sufficient ^{31}P broadening of signal with concentration of Fe^{3+} 2,1 mol%. Two samples with different concentration (2,1 mol% Fe^{3+} a 8,1 mol% Fe^{3+}) were complexated with deferoxamine, where in both cases all of Fe^{3+} ions were released from the phytate after two hours. Siganl restoration was also observed on ^{31}P NMR, where there was a significan difference in signal intenzity before and after addition of deferoxamine.