

Project name:

SPAGO Pix: Cancer selective MRI contrast agent

Beamtime Report

dd.mm.yyyy - dd.mm.yyyy (Date of the report to be added)

General information

Name of the rapporteur	Name of the rapporteur's organisation
Rodrigo M. Petoral Jr	SPAGO Imaging
Type of research (nanotechnology/health care/chemistry etc.)	Name of the research facility
Nanotechnology/biotechnology	MAX-lab
Date of the measurement, duration	Location of the event
2013-03-05 (whole day); 2013-09-18 (whole day)	Lund, Sweden
Facility personnel participating in the measurement	
<i>Stefan Carlsson & Kajsa Sigfridsson (BL I811); Tomas Plivelic (BL I911-SAXS)</i>	

Description of the project

Research description (short summary as written in the application)
<p>SPAGO Imaging is a Swedish biotech company focusing on the development of contrast agents for early and accurate visualization of cancer with MRI (fig.1). The nanoparticle-based contrast agent has exceptionally high relaxivity (signal strength) and selectively accumulates in tumor tissue via passive tumor targeting (EPR effect). The nanoparticle is composed of paramagnetic metal ions and polymeric framework. The detailed information on the average size, its distribution (polydispersity), shape and structure (including interatomic distances) is essential in understanding and improving the particles' properties as blood pool contrast agent. Such information can be extracted using synchrotron and neutron based techniques, complemented with lab-based techniques such as DLS, NMR and IR, to name a few. In specific, Small Angle Scattering of X-rays (SAXS) or Neutrons (SANS), and X-ray Absorption Spectroscopy such as EXAFS, would aid visualize/determine the comprehensive and complex (nano)structure at the molecular/atomic level. Facilities at MAX-lab in Lund or HASYLAB in Hamburg (SAXS and EXAFS) and at FRM-II in Munich (SANS), among others, are preferred to execute the above characterization techniques. We will need assistance with the measurements (including sample preparations), data analysis and interpretations.</p>
Summary of activities (experiments performed, beamtime used, preliminary overview of results, next steps and other relevant information)
<p>Experiments in MAX-lab were performed accessing beamlines I811 (XAS) and I911-SAXS. SPAGO has verified size, composition, and manganese coordination geometry for</p>

the SPAGO Pix MRI contrast agent.

SPAGO Pix MRI contrast agent contains Mn-ions in the polymeric matrix. X-ray absorption spectroscopy (XAS) was used to learn more about the Mn oxidation state and ligand coordination in the polymeric scaffold. Results from XANES study (fig.2) revealed that the Mn oxidation state is Mn^{II} and has a very similar edge as to MnCl₂ which suggested a Mn^{II} in Jan-Tellerdistorted octahedral coordination (rhombohedral lattice), rather than the cubic octahedral symmetry found in MnO. EXAFS results (fig.3), extracted from the fitting of the first coordination sphere of Mn^{II}, supported the same Mn-coordination structure suggested by XANES findings. The coordination geometry was predicted by high level *ab-initio*, quantum chemistry calculations and the results were found to be in excellent agreement.

SAXS technique was used to verify the size of the nanoparticles. Preliminary analysis of the results agrees with the size extracted from other techniques. The core size of the particle is estimated to be about 4 nm.

How would you describe cooperation and assistance from industrial liaison officers and national contact points while preparing and carrying out the research at large scale facilities?

The cooperation and assistance of MAX-lab staffs are highly appreciated. They were all very helpful in executing the measurements and assisting in the analysis of the results.

Other personal remarks

Annexes

Annexes

(list of annexes; meeting minutes, graphical illustrations, tables and other supplementary data)

Figure 1. The images show a MRI scan of a rat with breast tumors before and after injection of the contrast agent. The tumors have been color coded in blue as an aid for the eye.

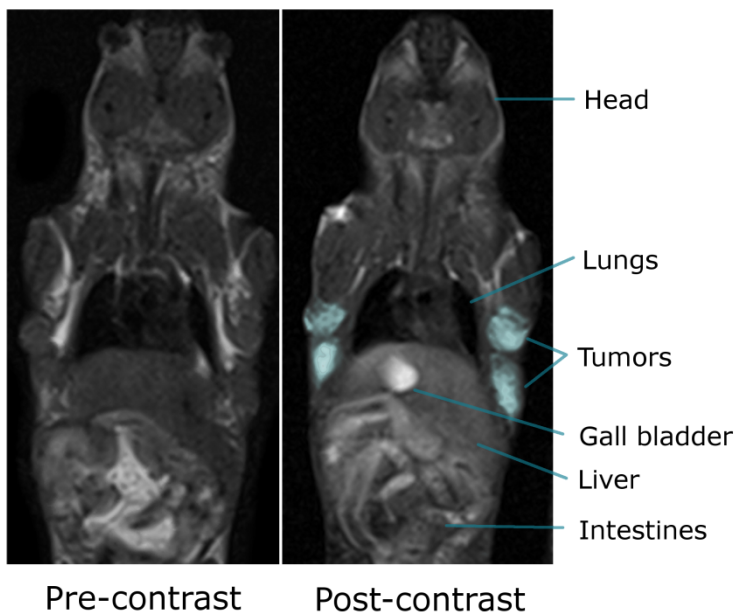


Figure 2. XANES Mn K-edge of SPAGO Pix compared to other Mn-based compounds

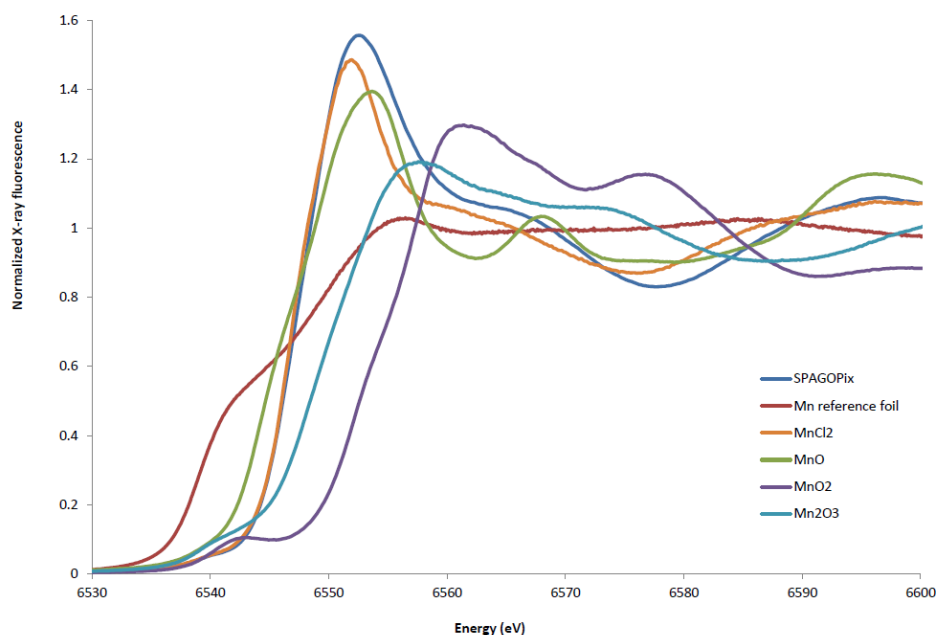


Figure 3. Mn EXAFS spectra of SPAGO Pix

