

Abstract Submitted  
for the MAR17 Meeting of  
The American Physical Society

**The stability of DOTA-chelated radiopharmaceuticals within  $^{225}\text{Ac}$  decay pathway studied with density functional theory.**<sup>1</sup> ALEXANDRA KAROLAK, H. Lee Moffitt Cancer Center and Research Institute, ARTEM KHABIBULLIN, University of South Florida, MIKALAI BUDZEVICH, M. MARTINEZ, MICHAEL DOLIGANSKI, MARK MCLAUGHLIN, LILIA WOODS, DAVID MORSE, H. Lee Moffitt Cancer Center and Research Institute — Ligand structures encapsulating metal ions play a central role as contrast agents in Magnetic Resonance Imaging (MRI) or as agents delivering toxic cargo directly to tumor cells in targeted cancer therapy. The structural stability and interaction with solutions of such complexes are the key elements in understanding the foundation of delivery process. We present a comparative study for the 1,4,7,10-tetraazacyclododecane-1,4,7,10-tetraacetic acid (DOTA) chelated to radioactive isotopes of  $^{225}\text{Ac}$ ,  $^{221}\text{Fr}$ ,  $^{217}\text{At}$ ,  $^{213}\text{Bi}$  and a control  $^{68}\text{Gd}$ . Using density functional theory methods we investigate the structural stability of complexes for cancer therapy including binding energies, charge transfer, electron densities. The van der Waals interactions are included in the simulations to take into account weak dispersion forces present in such structures. Our results reveal that Ac-DOTA, Bi-DOTA and Gd-DOTA are the most stable complexes in the group. We also show that the water environment is a key ingredient for the structural coordination of the DOTA structures.

<sup>1</sup>Support from the US Department of Energy under Grant No. DE-FG02-06ER46297 is acknowledged.

Artem Khabibullin  
University of South Florida