

Title: **Analysis of hydroxylated polychlorinated biphenyls using nESI-TIMS-MS**

Natalie F. Smith<sup>1</sup>; Kendra J. Adams<sup>1</sup>; Francisco Fernandez-Lima<sup>1,2</sup>

<sup>1</sup> *Department of Chemistry and Biochemistry, Florida International University, Miami, USA*

<sup>2</sup> *Biomolecular Science Institute, Florida International University, Miami, USA*

Polychlorinated biphenyls (PCBs) are industrial pollutants classified as endocrine disruptors and can cause antagonistic effects in the reproductive, neurological, and immunity systems in humans and animals. The biological toxicity of PCBs depends on the position and number of chlorine atoms within the molecule, and they work to mimic or block essential hormones, causing significant health damages. In the present work, nine different congeners of hydroxylated PCBs (OH-PCBs), with varying number of chlorine atoms, were studied using trapped ion mobility coupled to mass spectrometry (TIMS-MS). In particular, isomers of OH-hepta-chlorinated biphenyls (e.g., 4-OH-PCB 187, 4-OH-PCB 172 and 3-OH-PCB 180) were analyzed individually and as a mixture, to evaluate the analytical power and capabilities of TIMS-MS. Ion-neutral collisional cross sections were determined experimentally and compared to candidate structures. Different strategies to separate molecular isomers are discussed.