UNIVERSITY OF RHODE ISLAND Department of Chemistry Ph.D. Seminar

> Room 105 Beaupre 3:00 P.M., Monday, April 18, 2022

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"Exploring supramolecular scaffolds: The synthetic development of rotaxanes for drug delivery and imaging"

HOST

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Exploring supramolecular scaffolds: The synthetic development of resourceful rotaxanes for drug delivery and imaging

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Mechanically interlocked molecules, particularly rotaxanes, have been of significant interest to scientists in the last several decades. This is mainly due to their robust tunability and subsequent inherent ability to be employed in numerous applications in various fields. Rotaxanes are typically synthesized by threading a linear axle-like guest through a wheel-like macrocyclic host, in which threading, or binding, is often directed via non-covalent interactions. The guest is then locked in place by the addition of bulky molecular caps that are coupled to the ends of the guests, generating the kinetically stable interlocked rotaxane. This is a viable synthetic method we have previously employed using a variety of hosts and guests. The work discussed herein involves two different approaches to rotaxane syntheses tuned towards their desired applications. The first rotaxane discussion will explore the efficient and robust synthesis of cyclodextrin-based rotaxanes with the end purpose of forming higher order ternary complexes, to be used for drug delivery. The following rotaxane synthesis will focus on the design of a cucurbit[6]uril-based cleavable rotaxane with the goal of developing an innovative biosensor for the early detection of lung cancer by means of HyperCEST ¹²⁹Xe MRI.