

METAL-FREE C⁵ BOND FUNCTIONALIZATION OF 1,2,3-TRIAZOLES VIA A DIELS-ALDER-LIKE CYCLOADDITION OF 4-ALKENYL-SUBSTITUTED 1,2,3-TRIAZOLES Heather A. Michaels, Lei Zhu, Ronald J. Clark. Department of Chemistry & Biochemistry, Florida State University, 95 Chieftan Way Tallahassee, FL 32306-4390.

The post synthesis functionalization of 1,2,3-triazoles typically employs the use of palladium-catalysts. We sought to circumvent the need for catalysts by employing a Diels-Alder cycloaddition of 4-phenyl-1,2,4-triazoline-3,5-dione (PTAD) with 4-alkenyl substituted 1,2,3-triazoles. We found that although we achieved the desired C⁵ functionalization, we did not isolate the expected products from a Diels-Alder cycloaddition. Interestingly, the major product was found to be the result of a tautomerization of the D.A. product. Side products as well as NMR experiments gave us insight into the reaction mechanism and allowed us to conclude that the reaction proceeds in a step-wise fashion starting from a Michael-type addition. The resulting products are thermally stable and offer a unique fused heterocyclic scaffold that may be useful in pharmaceutical screening.