SITE-SELECTIVE CARBONYLATIVE ROUTES TO FUSED POLYHETEROCYCLIC STRUCTURES

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The regioselective formation of strikingly elaborated polyheterocyclic structures in a straightforward manner is an outstanding challenge in organic chemistry. Step-economical domino reactions are wonderful tools to rapidly build up molecular complexity from simple starting materials [1]. In this contribution, novel palladium-catalyzed sequential carbonylative cascades to highly functionalized polyheterocyclic structures are reported. The regioselective one-pot synthesis of oxazino[5,6-c]quinolin-5-ones and quinolin-2(1H)-one-fused pyrimido[2,1-b][1,3]oxazines from amide/amine-tethered ortho-alkynylanilines, respectively, have been described (Scheme). In the latter case, the Pd-catalyzed carbonylative process involves the insertion of three CO molecules and the sequential formation of 8 new bonds (one C–O, two C-C, five C-N). In both situations, the exclusive formation of six-membered heterocycles was observed. Control experiments and DFT studies provided key insights on these site-selective transformations.