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## PROGRAM & ABSTRACTS

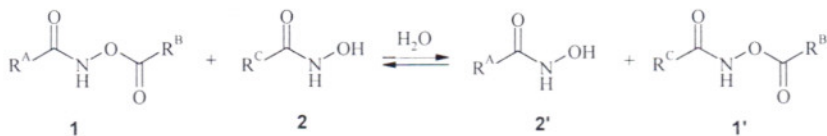
# Development of Dynamic Combinatorial *N,O*-Diacylhydroxylamine Libraries in Aqueous Media PO125

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Dynamic Combinatorial Chemistry (DCC) is a new tool for drug discovery that is based on the library members of which are in equilibrium through reversible chemical processes<sup>1</sup>. Addition of a template (enzyme, receptor) to such a library leads to an amplification of the component which is the best ligand of the bio-macromolecule. One of the main directions in DCC is development of new reversible reactions between building blocks that can be done in aqueous media around neutral pH.

We have investigated acyl group transfer from *N,O*-diacylhydroxylamines **1** (**1'**) to hydroxamic acids **2** (**2'**) as a potential reversible reaction useful for DCC.



Using two component systems, trans-acylation rate, hydrolysis rate, influence of temperature and pH were studied by using both <sup>1</sup>H-NMR and HPLC. It was found that: a) transacylation is faster than hydrolysis of *N,O*-diacylhydroxylamines **1** around neutral pH; b) both transacylation and hydrolysis depend on pH and are practically stopped at pH 2 that serves as an equilibrium switch-off. A simple multi-component library of *N,O*-diacylhydroxylamines **1** was made and rate for reaching equilibrium was determined at room temperature at pH 7.2 and pH 6.2, using HPLC. Our studies have revealed that the *N,O*-diacylhydroxylamine library is suitable for Dynamic Combinatorial Chemistry.

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**References:** 1) Sanders J. K. M., Otto S., Corbett P. T., *Chem. Rev.* **2006**, 106, 3652