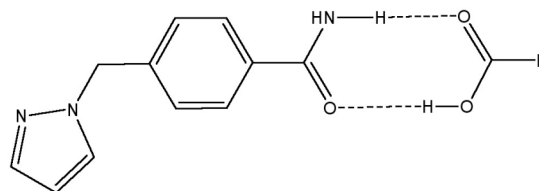


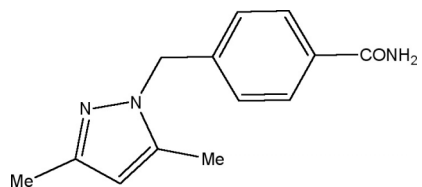
W0215

Giving Pyrazole a Helping Hand in the Competition Against the Amide. Benjamin Scott, Christer Aakeroy, John Desper, Chemistry, Kansas State Univ., 111 Willard Hall, Manhattan, KS 66506 USA.

Previous work has shown predictable co-crystal formation between a pyrazole-benzamide ligand and carboxylic acids. In these cases, the pyrazole nitrogen is not able to compete with the amide due to its poor binding ability (based on electrostatic potential) resulting in co-crystals consisting of an acid:amide dimer via O-H...O and N-H...O hydrogen bonds (Scheme 1).



In order to synthesise ternary co-crystals, it is essential to have two different 'active' binding sites available for hydrogen bonding, making it necessary for the pyrazole nitrogen to have the ability to compete with the amide functionality for the carboxylic acid. To improve the acceptor ability (based on electrostatic potential) of the pyrazole nitrogen, methyl substituents have been added to the heterocycle (Scheme 2).



The design and synthesis of the new supramolecular reagent and the subsequent formation of co-crystals with carboxylic acids will be presented.

C. B. Aakerøy, J. Desper, B. M. T. Scott, *Chem. Commun.* 2006, ASAP, DOI:10.1039/b517118k