

### MS36-P3 Inter- and intramolecular interactions of a series of oligoamide foldamers

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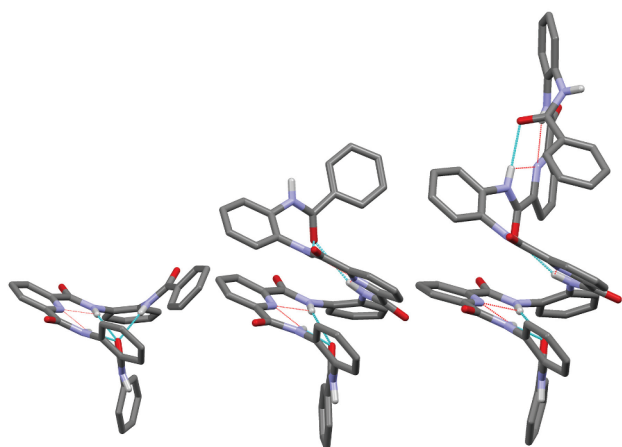
Foldamers are synthetic biomimetic molecules composed of simple repeating units. They have been widely studied because of their vast potential as efficient and even stereoselective organocatalysts and as bioreceptor mimics.<sup>1</sup>

We have prepared and crystallized three aromatic oligoamide foldamers of varying sizes, and analyzed their conformational and crystal packing properties.<sup>2</sup> As expected, hydrogen bonding is the most important non-covalent interaction affecting the molecular conformation and the crystal packing preferences. In addition, aromatic interactions play a stabilizing role.

The oligoamide foldamers adopt two distinct conformations, a helical @-conformation (Fig. 1) stabilized by intramolecular hydrogen bonds, and in the case of the longer molecules also by aromatic interactions, and a more open S-conformation. The choice between these two conformations seems to depend on the crystallization solvent; polar solvents facilitate the folding to an @-conformation whereas the S-conformation is obtained in non-polar solvents. As the molecules have several hydrogen bond donor and acceptor moieties they also display a wide array of crystal packing motifs, including molecular pairs, chains and solvent molecule assisted networks.

#### References

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**Figure 1.** A series of three oligoamide foldamers with one, two and three pyridine core units.

**Keywords:** Foldamers, hydrogen bonding

### MS36-P4 Different compounds from the same reactants: serendipity, misfortune or different reaction conditions?

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The synthesis of chemical entities (pharmaceuticals, ligands, complexes, assemblies, etc.) is classically performed in solution (solvothermal). For example, in the case of Schiff base systems, Lin *et. al* [1] reported that in the solvothermal method of the synthesis of a carboxamide (**opda2pica**) derived from *o*-phenylenediamine (**opda**) and 2-picolinic acid (**2pica**), 70 mL of different solvents (pyridine, methanol, triphenylphosphate) was used. The reactants were dissolved, mixed and heated for more than 24 hours. The carboxamide was subsequently also coordinated to gallium(III) by means of the same solvothermal method using 40 mL of solvents. The total time required for this procedure was 24 hours yielding only 29% of the [**Ga(opda(2pica)<sub>2</sub>**)] coordination compound.

In order to investigate these systems for biological and possible radiopharmaceutical evaluation but to use as little solvents as possible, we have applied a simple solution based method. Only 7 mL of methanol was used and the solutions were mixed and incubated at room temperature. After few hours serendipity played its role in chemistry and only a 1:2 co-crystal of **opda** and **2pica** was obtained. As (almost) solvent-free methods of synthesis (neat, liquid-, seeding-, ion-assisted grinding) have been recognised as potentially faster, environmentally friendly and economically acceptable ways to prepare new but also already known compounds, we re-evaluated the synthesis of the carboxamide and/or co-crystals of **opda** and **2pica** in few stoichiometric ratios.[2]

The success of the methods used was evaluated by means of FT-IR, PXRD, DSC and TG thermal analysis and NMR. Molecular and crystal structures were studied using SCXRD. This presentation will discuss the data obtained from this study to elucidate the reasons that lead to formation of co-crystals and/or carboxamide derived from **opda** and **2pica**.

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