Adaptable water networks for capturing bioactive molecules inside the pores of a coordination network

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Keywords: Coordination networks; Host-guest interactions; Single crystal analysis; Structure determination; Bioactive compounds

X-ray analysis of compounds incorporated into the pores of coordination networks could not only reveal important information about the guest structures[1] and host-guest interactions,[2] but also monitor reaction intermediates[3] and detect metastable species.[4] However, to date, only a handful of host networks have been identified to be compatible for a wide range of substrates since guest capture and stabilization is typically promoted by a series of finely-balanced host-guest interactions, which are difficult to rationally design.

In this study, a coordination network with hexaazaphenalenyl based ligands was used for the encapsulation and structural characterization of several bioactive compounds. The single crystal analysis revealed that guest binding was facilitated by hydrogen-bonded water networks and clusters inside the pores, which adapted depending on the guest molecule, providing clearly defined crystallographic sites (Fig. 1). As a result, the guest structures could be determined with high resolution, and limited number of constraints and restraints.

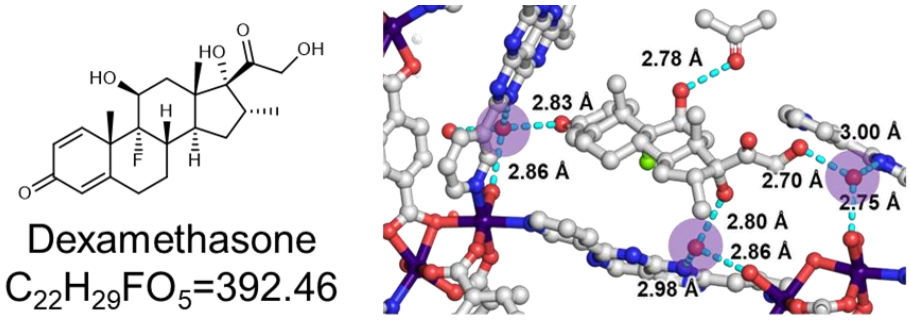

Fig. 1 Dexamethasone structure (left) and a crystal structure of encapsulated dexamethasone showing key hydrogen bonding interactions and their corresponding distances (right). Purple circles highlight water molecules that act as binding sites.

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