Bile Acids – Natural Building Blocks for Porous Coordination Self-Assemblies

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Self-assembly, metal coordination and chiral cavities are essential features of natural organization. In the past three decades, various supramolecular assemblies were synthesized *via* **coordination-driven self-assembly** using di- or tritopic pyridyl ligands and square planar palladium(II).[1] However, majority of these assemblies are made of achiral ligands and do not contain **chiral cavity**. Therefore, to mimic the natural chiral enzyme-like cavities, our group has introduced the "next-generation" metallo-supramolecular assemblies, *e.g.*, Pd_3L_6 (Fig. 1) using chiral **bile acid**-based (ursodeoxycholic acid, UDCA) ditopic ligands.[2]

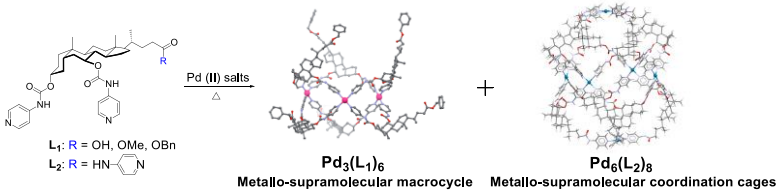

Figure 1. Bile acid-based metallo-macrocycles and coordination cages.

Further study showed that similar Pd_3L_6 can form hexagonal microparticles *via* Hierarchical **Self-Organization**.[3] To investigate the effect of ligand's **bend angle** on coordination self-assembly, chenodeoxycholic acid-based (CDCA, an epimer of UDCA) ditopic ligand was used which results in a mixture of Pd_nL_{2n} species ranging from Pd_2L_4 to a large Pd_6L_{12}.[4] Finally, UDCA-based tritopic ligand was also synthesized and its self-assembly resulted in $Pd_6\mathbf{L}_8$ (Fig. 1) and **the first-ever** $Pd_{12}\mathbf{L}_{16}$ supramolecular cage.[5]

1) Stang P. J. et. al. *Chem.Rev.* **2011**, *111*, 6810. 2) Jurček O. et al. *Angew. Chem. Int. Ed.* **2015**, *54*, 15462. 3) Jurček O. et al. *Cell Rep. Phys. Sci.* **2021**, *2*, 100303. 4-5) Chattopadhyay S. and Jurček O. et al. *manuscripts before submission*.