**Poster Presentation**

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# *$Pd_8L_4$ Barrel: an aqueous carrier for hydrophobic curcumin*

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Metal–ligand coordination driven self-assembly has emerged as a convincing tool to design and construct numerous coordination assemblies ranging from discrete two-dimensional (2D) to three-dimensional (3D) architectures. The unique interior environment of these 3D architectures has been exploited for myriad applications such as host–guest chemistry, stabilization of reactive species, drug delivery,1 supramolecular catalysis and as sensors. Cylindrical and barrel shaped architectures are very promising as they have windows similar to their cavity size. Barrel-shaped molecules have immense importance in biological systems such as β-barrel proteins allow the diffusion of small molecules and ions through cell membranes.2 Despite the fact that there has been a mounting interest in barrel shaped molecules with large cavities due to various applications, the synthesis of discrete water soluble barrel-shaped architectures by metal–ligand self-assembly remains very challenging. On the other hand, curcumin, which is widely known for its pharmacological activities including anti-inflammatory, antitumor, antioxidant and anti-amyloid properties.3 Despite of its efficacy and safety, the major limitations deterring the approval of curcumin as a therapeutic agent are: i) low bioavailability due to poor aqueous solubility, ii) lack of stability under physiological pH, and iii) photodegradation.

Here in we report a tetrafacial water-soluble molecular barrel (1) synthesized by coordination driven self-assembly of a symmetrical tetrapyridyl donor (L) with a cis-blocked 90° acceptor [cis-(en)Pd(NO3)2] (en = ethane-1,2-diamine). The open barrel structure of (1) was confirmed by single crystal X-ray diffraction. Presence of hydrophobic cavity with large windows makes it an ideal candidate for encapsulation and carrying hydrophobic drug like curcumin in aqueous medium. The barrel (1) encapsulates curcumin inside its molecular cavity and protects highly photosensitive curcumin from photo degradation by acting as a shield even against sunlight/UV radiations. As compared to free curcumin in water, we noticed a significant increase in solubility as well as cellular uptake of curcumin upon encapsulation inside the water-soluble molecular barrel (1) in aqueous medium. Fluorescence imaging confirmed that curcumin was delivered into HeLa cancer cells by the aqueous barrel (1) with the retention of its potential anticancer activity. While free curcumin is inactive towards cancer cells in aqueous medium at room temperature due to negligible solubility, the determined IC50 value of ~14 μM for curcumin in aqueous medium in presence of the barrel (1) reflects the efficiency of the barrel as a potential curcumin carrier in aqueous medium without any other additives. Thus, two major challenges of increasing the bioavailability and stability of curcumin in aqueous medium even in presence of UV light have been addressed by using a new supramolecular water soluble barrel (1) as a drug carrier.

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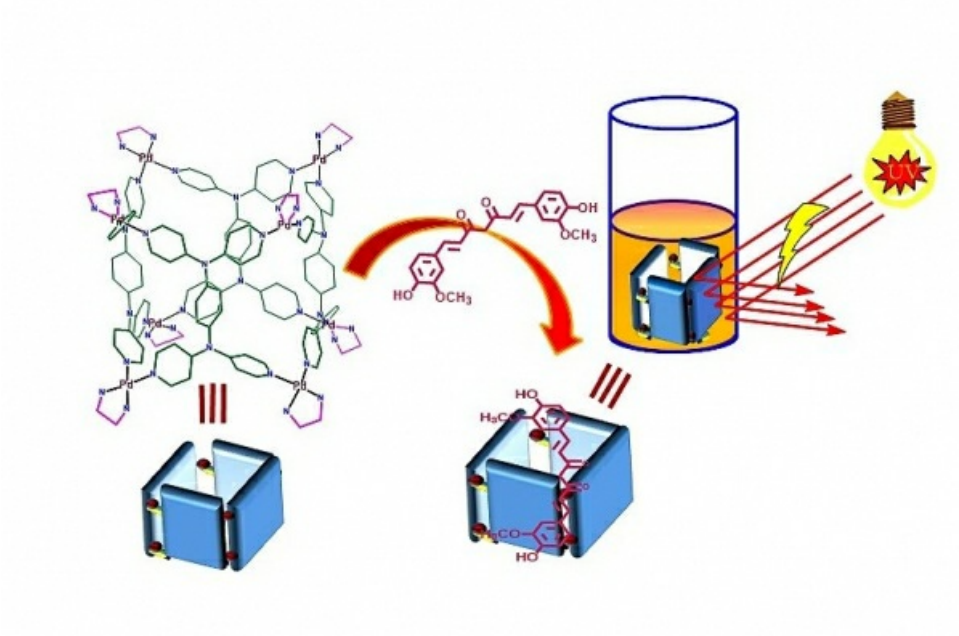


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