Aiding the Design of High-Potential Dendritic Molecules for *Life*- and *Nano*-Science Applications With Molecular Modeling

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Dendrimers and dendrons are hyperbranched polymers with an extremely regular architecture. These molecules are very interesting for a many diverse *life*- and *nano*-science applications due to their multivalent character. Their structure can be controlled with high precision and their highly branched surface constitutes a scaffold which can be functionalized with multiple active surface groups. Owing to the so-called multivalent effect, such molecules are able of strong binding with a large variety of organic and inorganic molecules.

The dendritic multivalent behavior can be controlled in principle by tuning different structural parameters (i.e., surface chemistry, architecture, size, shape and rigidity/flexibility).[1] The design and engineering of dendritic constructs with precise functionalities is however not trivial due to the fact that both dendrimers and dendrons are extremely sensitive to the external environment.[2] In this framework, molecular modeling can create a "virtual bridge" between theory (molecular design) and application (experiments), providing a unique insight into the characteristic behavior of these molecules and useful assisting eventual structural modifications to enhance properties.[3]

In this presentation different applications of dendrimers and dendrons will be shown and different examples will be discussed. Molecular dynamics simulation represents an exceptional tool to support the design of new dendritic candidates which can serve as drug and gene nano-carriers,[4,2-3] sensors[5] and catalytic switches.[6] Moreover, due to the possibility to control their multivalent recognition with diverse bio- and ionorganic molecules, dendrimers and dendrons can be used as a real tunable "molecular glue" for the creation of well-defined self-assembled bio-hybrid materials.[7]

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