Numerical simulations as virtual microscope at the nanoscale: some examples with dendritic molecules

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Dendritic molecules like dendrimers and dendrons have an extremely regular structure and a multivalent surface, which can be functionalized in many different ways and this gives them a particular ability to bind and compact several molecules of interest like siRNA or DNA to aid gene transfection, or viruses. Understanding the factors that influence their interactions with such molecules is an important prerequisite for their controlled manipulation. A key role in this phenomenon is played by the multivalency principle, which implies that the strength of a multivalent binding interaction can be much stronger than the sum of a corresponding number of monovalent interactions. While the number of binding sites and size of the molecules increase, also the binding event between ligand and receptor becomes more complex to understand and tune. Moreover, the multivalent behavior of dendrimers and dendrons is strongly influenced by the interactions with the external solution which modify the folded configuration assumed by the nano-carrier in determined conditions. Due to complex nature of multivalent binding that often occurs in biological environment, experiments alone are not able to find clear indication to support the scientists in the design of improved dendritic molecules.

In this talk, we illustrate some examples where Molecular Dynamics has shown to be a very useful tool to gain a deeper insight into the binding mechanism. Simulations were able to provide important information about the multivalent behavior of the dendritic scaffold and about the efficiency of different dendritic architectures, giving therefore a real support to the scientists in the design and the creation of improved dendritic binding agents.