

COMPUTER-AIDED MOLECULAR DESIGN OF NANO BIO SENSORS

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ABSTRACT

Progress in human genome projects continues to unveil the biological processes associated with disease. In conjunction with the advances in nano technology, both therapeutic methods and diagnostic tools have been developed to identify sufferers and to combat the disease. Research dedicated to the development of nano bio sensors aims to render reliable, rapid, and cost-effective diagnostic instruments. Requisite components for effectively functionalized nano sensors are composed of the recognition unit for guest molecules with high selectivity and the signal transducer unit which converts the event of recognition into signals with high sensitivity. In designing the sensors, therefore, the recognition moiety linked to the detection unit can be a key factor to consider since they are responsible for the selectivity and binding efficiency of the whole molecular sensors. For that purpose, computational modeling can offer enormous generality for designing and engineering structures and functions of molecular sensors.

Herein, the recent computer-aided molecular modeling on the structural preference, thermodynamic stability, electronic properties of calixarene-based fluorescent sensors and their molecular recognition mechanisms are provided. The predicted stability orders by computer simulation for host molecules are compared with the experimental results. Relative complexation efficiency for each host is presented and discussed in terms of the conformational characteristics, binding sites, and physical nature of the interactions. In addition, the nature of the fluorescence changes of ion-selective sensors is discussed on the basis of the electron density analyses of the frontier molecular orbital.