Development of Total System for Molecular Design

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Research on method for molecular design and structure-activity relationship, and development of the corresponding computer softwares have been carried out in our laboratory. Some of these softwares are original ones developed by us. Mutual use of them will be powerful for molecular design research work. Recently, these softwares were integrated by giving common user-interface. Molecular alignment, construction of 3D-QSAR model and automated generation of candidate structure of drugs are possible under this total system.