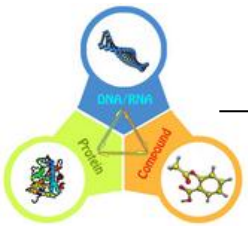

BioTriangle

--BioCPI, BioDPI, BioCDI

COMPUTATIONAL BIOLOGY &
DRUG DESIGN GROUP
CENTRAL SOUTH UNIV., CHINA

The descriptor calculation of chemical-protein interaction, protein-DNA/RNA interaction, and chemical-DNA/RNA interaction is similar to each other in BioCPI, BioDPI and BioCDI. Next, we will show how to construct an interaction feature by the chemical-protein interaction example.

Chemical-protein interaction descriptors

There are two methods for construction of descriptor vector **F** for chemical-protein interaction from the protein descriptor vector $\mathbf{F_t}(\mathbf{F_t}(i), i = 1, 2, ..., p_t)$ and chemical descriptor vector $\mathbf{F_d}$ $(\mathbf{F_d}(i), i = 1, 2, ..., p_d)$**:**

(1) One vector **V** with dimension of $p_t + p_d$ are constructed: $\mathbf{F} = (\mathbf{F_t}, \mathbf{F_d})$ for interaction between protein T and ligand D.

(2) One vector **V** with dimension of $p_t \times p_d$ is constructed by the tensor product: $\mathbf{F} = \{\mathbf{F}(k) = \mathbf{F_t}(i) \times \mathbf{F_d}(j), i = 1, 2, \ldots, p_t, \quad j = 1, 2, \ldots, p_d, k = (i-1) \times p_t + j\}$.