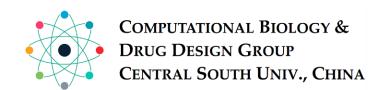


BioTriangle

--BioCPI, BioDPI, BioCDI



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