



BioTriangle

--BioCPI, BioDPI, BioCDI



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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 $\mathbf{F}_t(\mathbf{F}_t(i), i = 1, 2, \dots, p_t)$ and chemical descriptor vector $\mathbf{F}_d(\mathbf{F}_d(i), i = 1, 2, \dots, p_d)$:

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

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