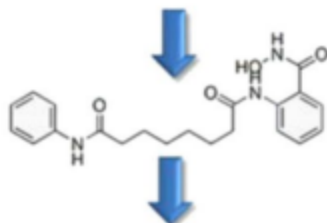


Drug Molecule



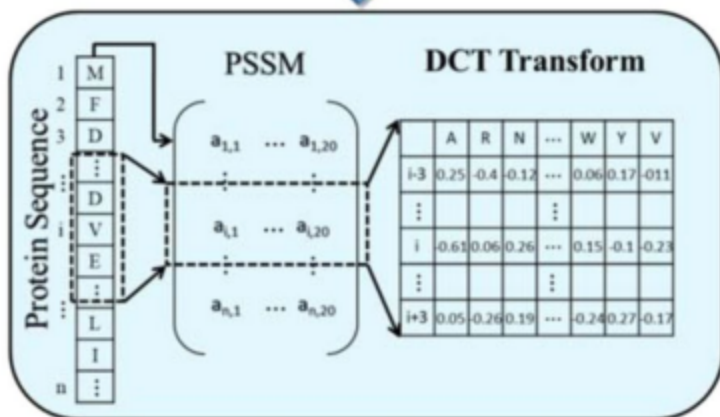
1	1	0	0	...	0	1	0
...				...			
0	0	0	1	...	1	0	1
...				...			
0	1	1	0	...	0	0	1

Molecular Fingerprint Descriptor

Fusion of Multi-Source Features

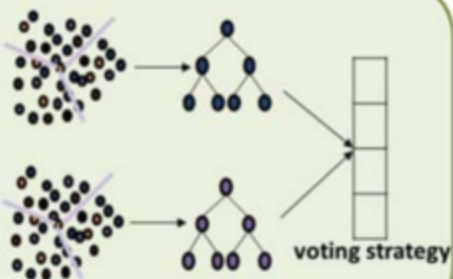


Protein

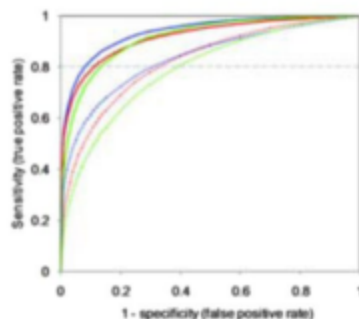


$$DCT(i, j) = d_i d_j \sum_{x=0}^{M-1} \sum_{y=0}^{N-1} f(x, y) \cos \frac{\pi(2x+1)i}{2M} \cos \frac{\pi(2y+1)j}{2N}$$

$$d_i = \begin{cases} \sqrt{\frac{1}{M}}, & i = 0 \\ \sqrt{\frac{2}{M}}, & 1 \leq i \leq M-1 \end{cases} \quad d_j = \begin{cases} \sqrt{\frac{1}{N}}, & j = 0 \\ \sqrt{\frac{2}{N}}, & 1 \leq j \leq N-1 \end{cases}$$



Rotation Forest Classifier



Prediction Results