

D_k : Measure to describe how compact cluster k is

$$D_k = \sum_{x_i \in C_k} \sum_{x_j \in C_k} \|x_i - x_j\|^2$$

W_k : Normalized sum of these measures for a given 'partition'

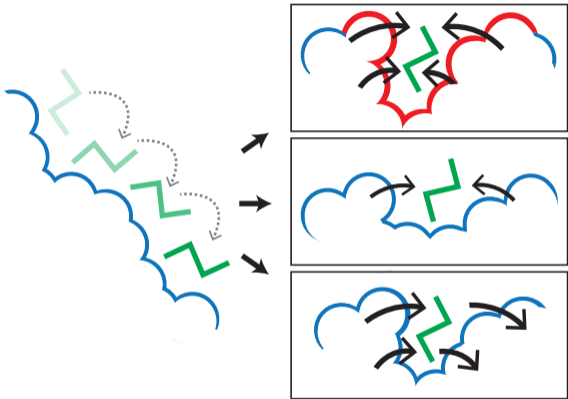
$$W_k = \sum_{k=1}^K \frac{1}{2n_k} D_k$$

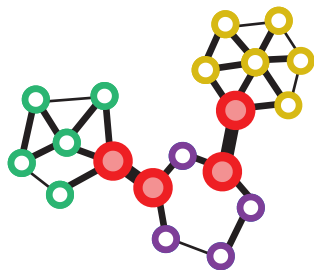
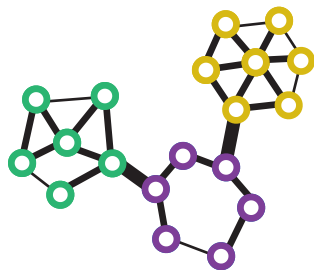
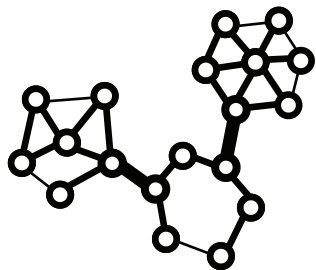
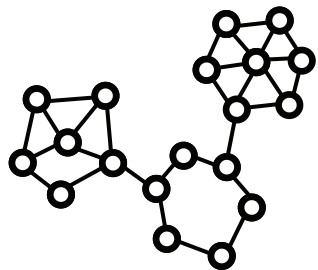
How much does this score differ from that in a randomized null?

$$\text{Gap}_n(k) = E_n^* \{ \log W_k \} - \log W_k$$

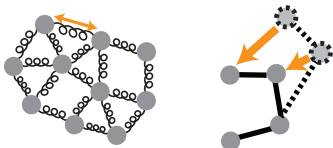
Best K : value for which the gap value is higher than the next K

$$\text{Gap}(k) \geq \text{Gap}(k+1) - s_{k+1}$$

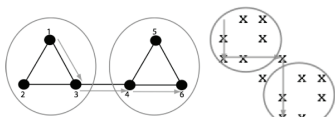




weigh edges using
motion vectors



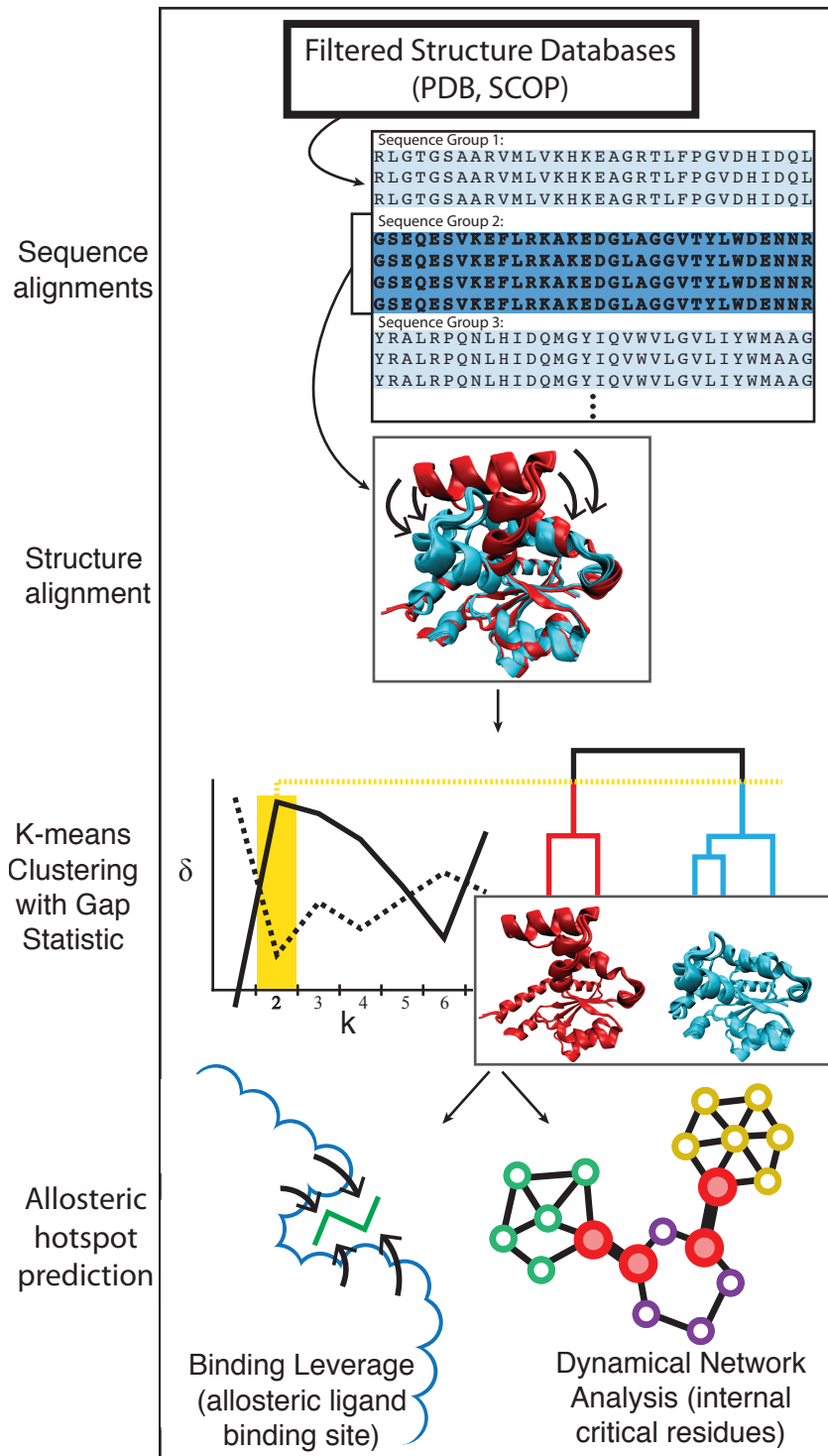
identify
communities (GN*)



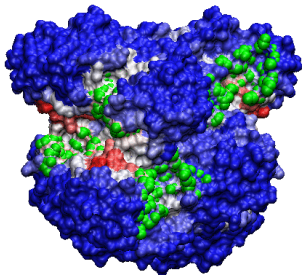
call critical residues

```

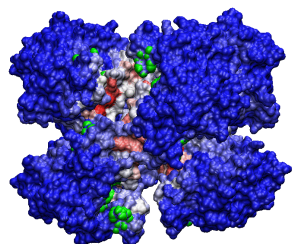
res 1: 11  LYS  A
res 2: 25  GLU  A
res 3: 136 ASP  A
res 4: 204 ASN  A
      .
      .
  
```



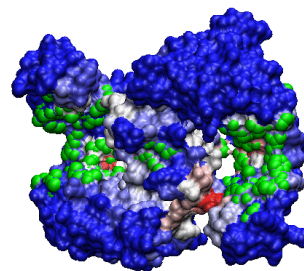
Phosphofructokinase (3pfk)



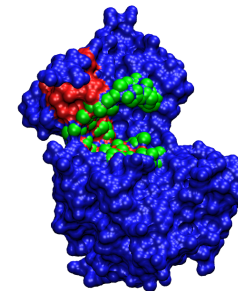
G6P-Deaminase (1cd5)



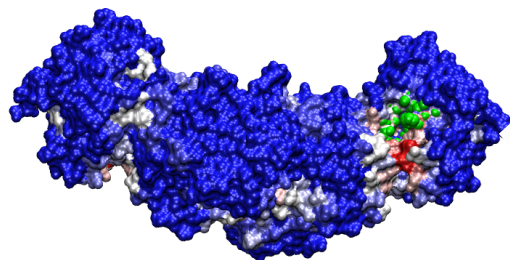
Adenylate Kinase (4ake)



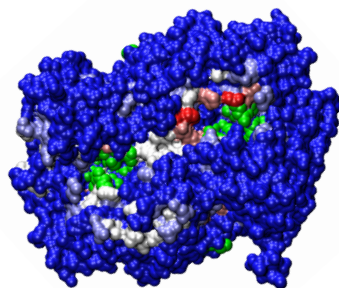
cAMP-Dependent Kinase (1j3h)



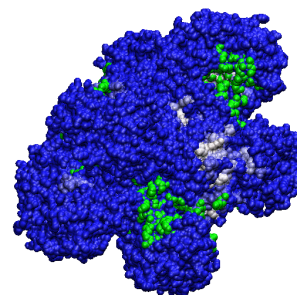
Trp Synthase (1bks)



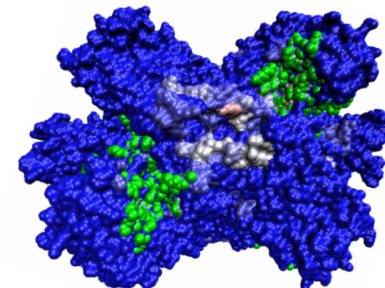
Thr Synthase (1e5x)



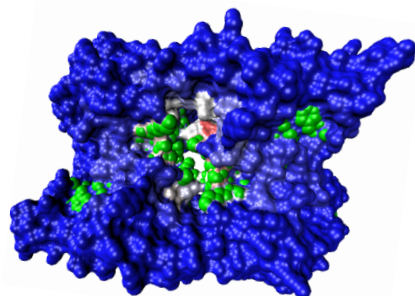
Malic Enzyme (1efk)



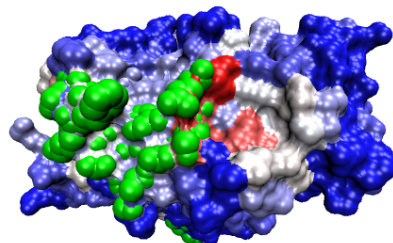
Glu Dehydrogenase (1nr7)



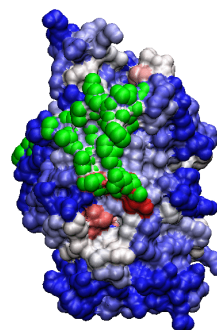
Phosphoribosyl Transferase (1xtt)



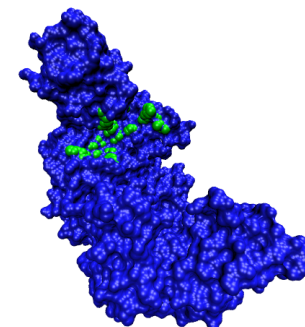
Tyr Phosphatase (2hnp)



Asp Transcarba-Moylase (3d7s)



Arg Kinase (3ju5)



Binding Leverage



Known biological ligand binding sites



GN



Infomap

