
Algorithm S1. (H-bond based) Exchange State Identification Algorithm

Input: WW domain trajectory frames in set \mathcal{T} .

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while  $|\rho_{best} - \rho_{old}| > \epsilon$  do ▷  $\epsilon = 0.0001$ 
  for All  $i$  H-bonds in loop with probability of occurrence  $> 0$  do
     $\mathcal{N} \leftarrow \mathcal{N} \cup f(i)$  ▷  $f(i)$ : set of frames with H-bond  $i$ 
    if  $\rho(\mathbf{R}_{ex}, \Phi_{ex}(\mathcal{N}, \mathcal{T} \setminus \mathcal{N})) > \rho_{best}$  then
       $\rho_{old} \leftarrow \rho_{best}$ 
       $\rho_{best} \leftarrow \rho(\mathbf{R}_{ex}, \Phi_{ex}(\mathcal{N}, \mathcal{T} \setminus \mathcal{N}))$ 
       $\mathcal{N}_{best} \leftarrow \mathcal{N}_{best} \cup i$ 
       $\mathcal{N} \leftarrow \mathcal{N}_{best}$ 
    end if
  end for
end while
Output:  $\mathcal{A} \leftarrow \mathcal{N}_{best}$  and  $\mathcal{B} \leftarrow \mathcal{T} \setminus \mathcal{N}_{best}$ 

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