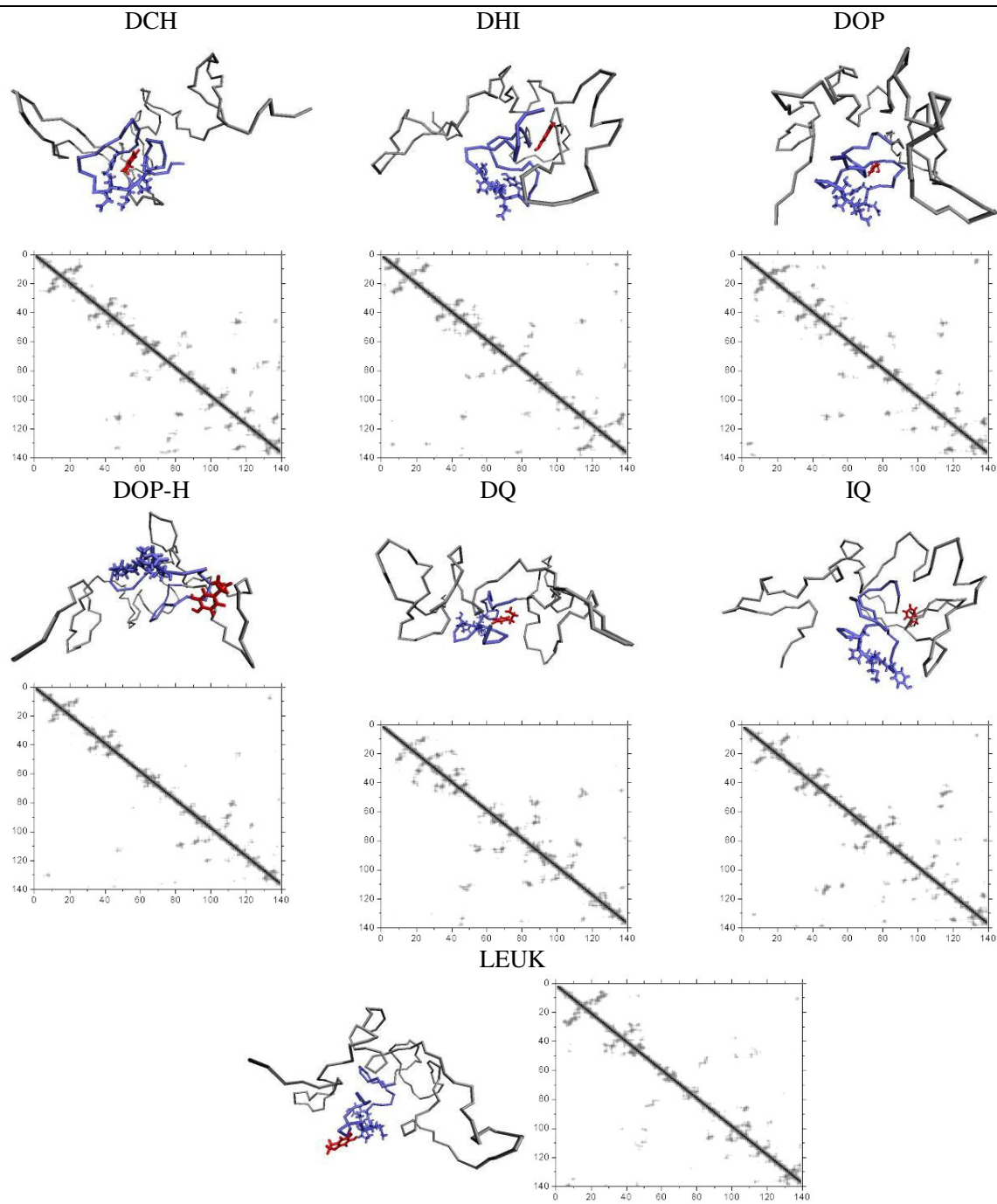
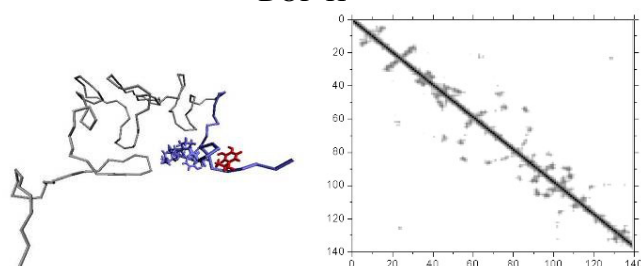


Cluster 1



## Cluster 2

DOP-H

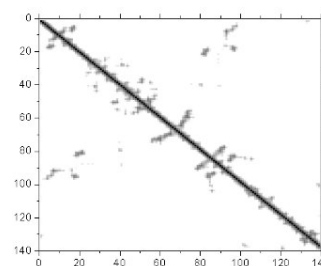
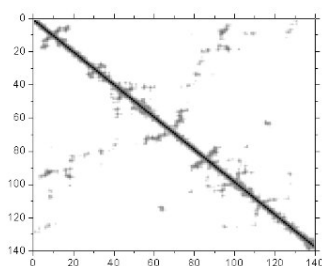
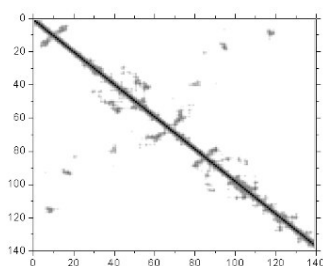
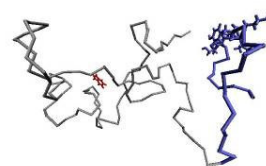
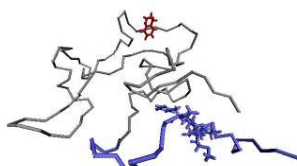
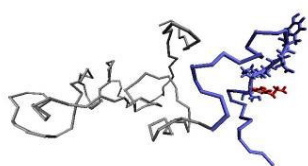


## Cluster 3

DOP

DQ

IQ

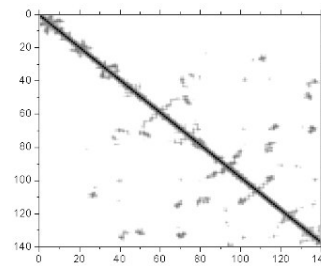
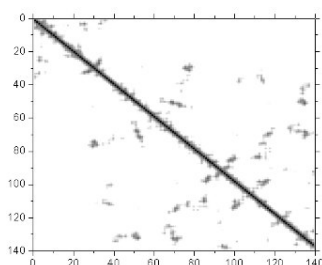
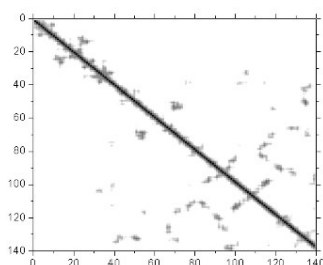
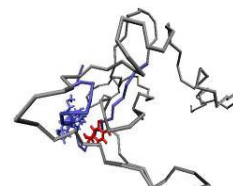
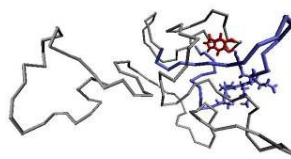
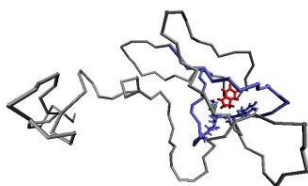


## Cluster 4

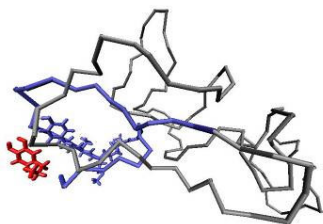
DCH

DHI

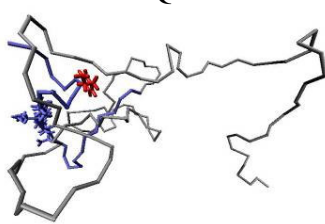
DOP



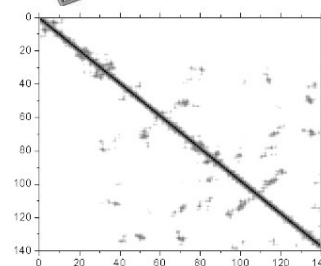
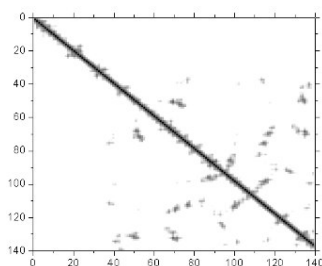
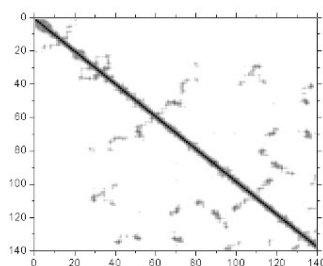
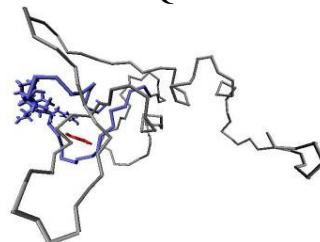
DOP-H



DQ

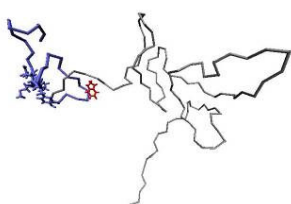


IQ

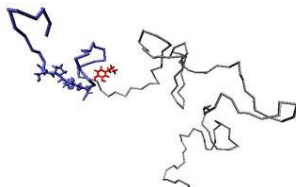


Cluster 5

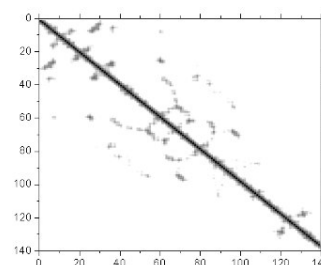
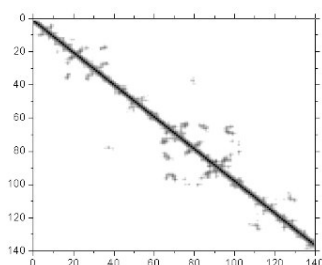
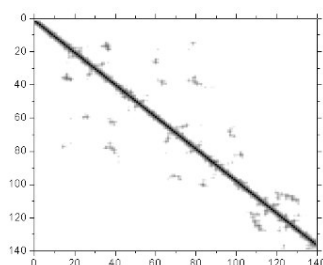
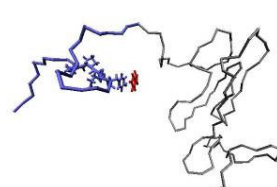
DCH



DOP-H

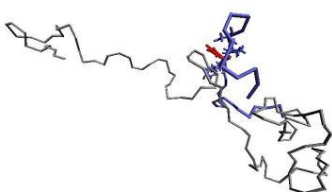


IQ

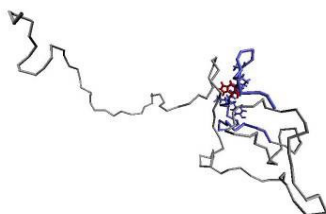


Cluster 6

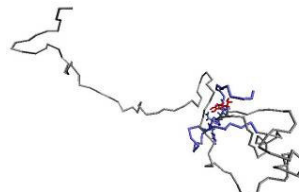
DCH

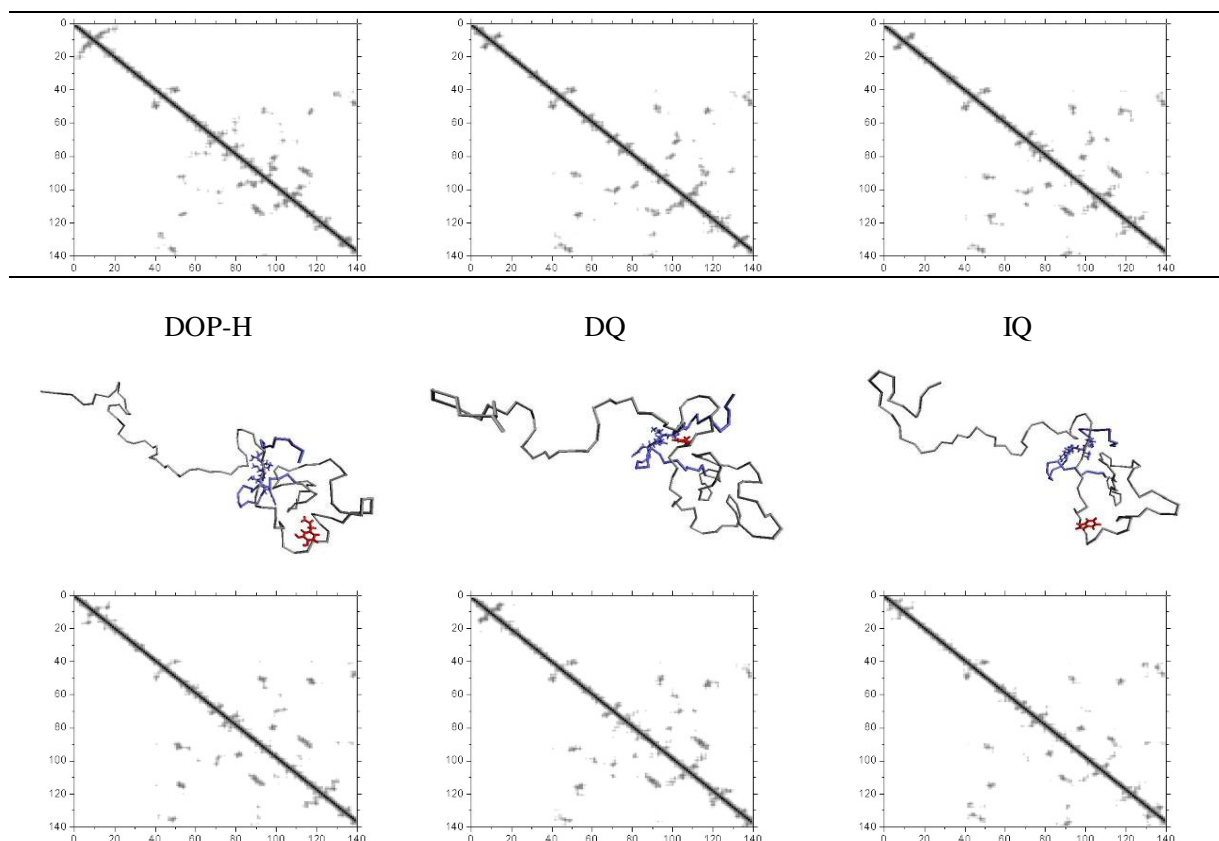


DHI



DOP





**Figure S3. MD simulations of the “stable” DOP/AS complexes.** Structures and C $\alpha$  contacts maps for the last MD snapshots. In the structures, residues 125-129 and E83 are colored in red and blue, respectively. In the contact maps, the x and y axis indicate the residues number in the AS sequence. The contact maps were calculated based on the C $\alpha$ -C $\alpha$  distance (a graph square is colored black at 0.0 Å distance, to a linear gray scale between 0.0 and 10.0 Å, and white when equal to or greater than 10.0 Å).