SUPPORTING INFORMATION

Conformational Preferences of Heparan Sulfate to Recognize CXCL8 Dimer in Aqueous Medium: Degree of Sulfation and Hydrogen Bonds

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1.1 Molecular docking

Molecular docking studies were performed to estimate the probable binding affinities of the HS molecules with the active sites of the CXCL8. The AutoDock Vina application[1] was used to perform the docking trials. The initial coordinates of the CXCL8 were obtained from the corresponding crystal structure[2], whereas the coordinates of the HS molecules were generated from the GAG builder webserver of GLYCAM.[3] The Lamarckian genetic algorithm (LGA)[4] was implemented in AutoDock Vina to determine the binding conformations. The CXCL8 was kept rigid while all the torsions of the GAGs were allowed to rotate during the docking experiment. The grid box dimension of 100×100×100 along X, Y, and Z direction was created during the docking. From each docking experiment, nine docked conformations were generated. Finally, the lowest energy conformer of the CXCL8-HS complexes, obtained from each docking experiment was isolated and considered to perform MD simulation.

Reference:

1. O. Trott, A. J. Olson, *J. Comp. Chem.* 2010, **31**, 455-461.

2. G. M. Clore, E. Appella, M. Yamada, K. Matsushima, A. M. Gronenborn, *Biochem.* 1990, **29**, 1689–1696.

3. R. J. Woods Group. GLYCAM Web. Complex Carbohydrate Research Center, University of Georgia, Athens, GA. USA. 2005-XXXX.

4. J. Fuhrmann, A. Rurainski, H.-P, Lenhof, D. Neumann, *J. Comput. Chem.* 2010, 31, 1911–1918.