Electronic Supplementary Material (ESI) for Molecular BioSystems

Supplementary Material

Interactions between CD44 protein and hyaluronan: insights from the computational study

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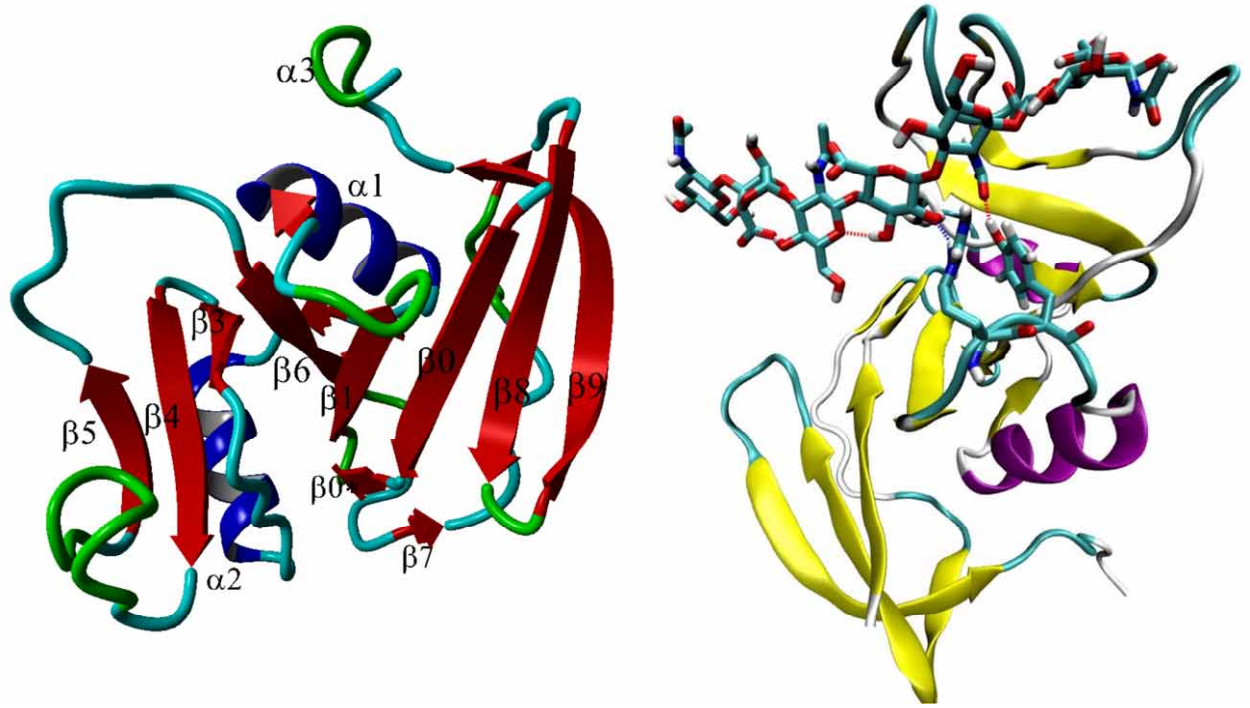

Figure S1. The structures of the CD44 receptor and CD44/HA7 complex according to the XRD data by Banerji et al. [S. Banerji, A. J. Wright, M. Noble, D. J. Mahoney, I. D. Campbell, A. J. Day, D. G. Jackson, *Nat. Struct. Mol. Biol.* 2007, **14**, 234-239]; the two crucial residues (R45 and Y46) interacting with HA are shown.

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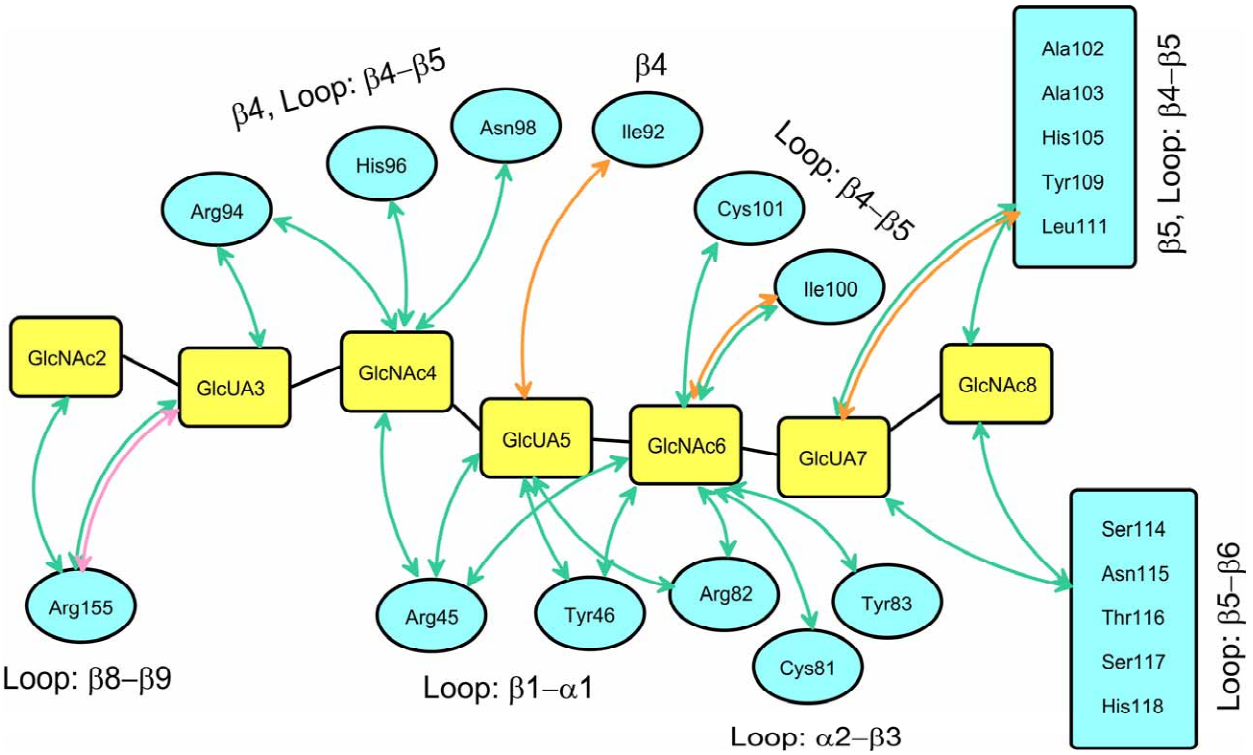

Figure S2. The symbolic illustration of interactions between heptamer of HA and CD44. GREEN: hydrogen bonds; ORANGE: hydrophobic interactions; VIOLET: salt bridge. Other details follow the convention presented in Figure 1. The large degree of flexibility of both HA chain and amino acid sidechains of binding groove was observed. Therefore the same sidechain can interact with several different carbohydrate units (e.g. R45).

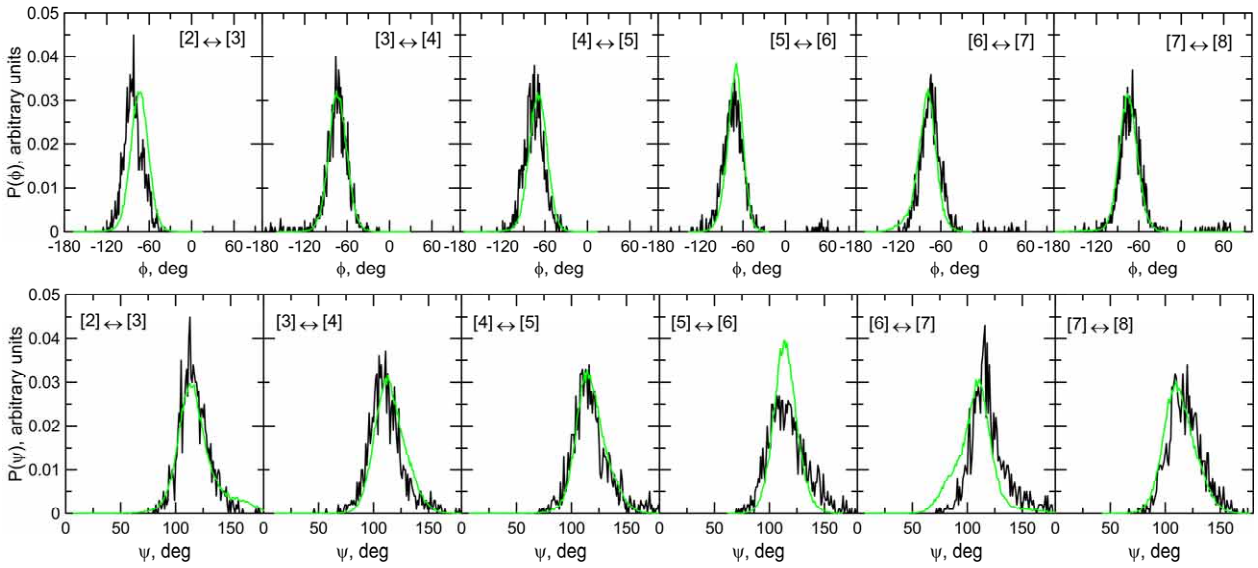

Figure S3. The probability distributions of glycosidic dihedral angles values, which are responsible for the conformation of HA chain; the HA chain in the water solution (unbound): BLACK; the HA chain bound to CD44: GREEN. Units numbering (e.g. [2], [3], ...) follows the convention presented in Fig. S2.

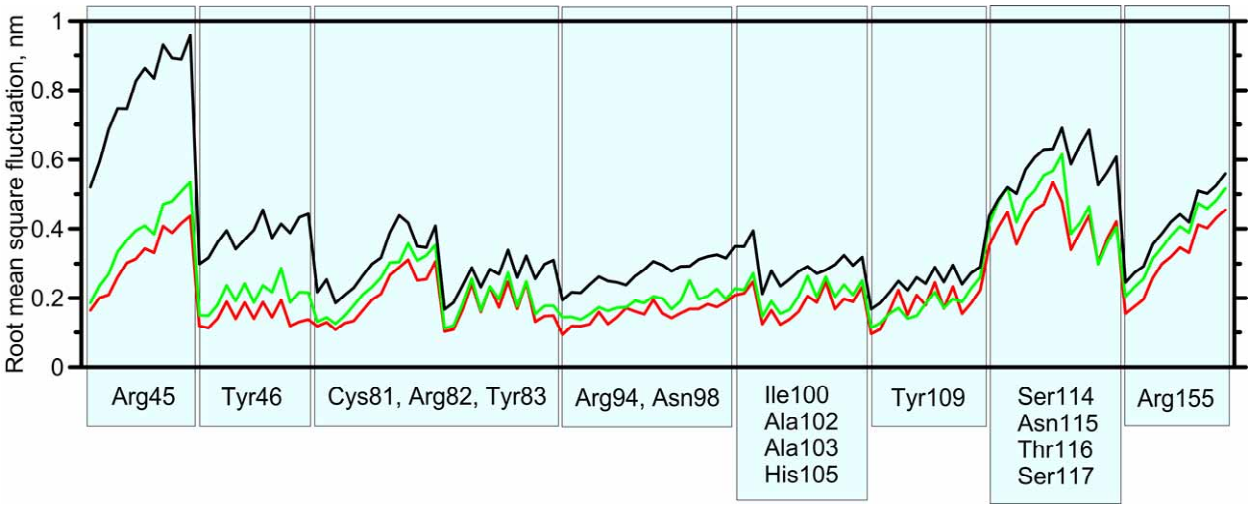

Figure S4. The RMSF (root mean square fluctuation) values for the atoms belonging to the binding groove of CD44. BLACK: unbound states; CD44 interacts only with solvent; GREEN: starting structure: 'A'; RED: starting structure: 'B'.

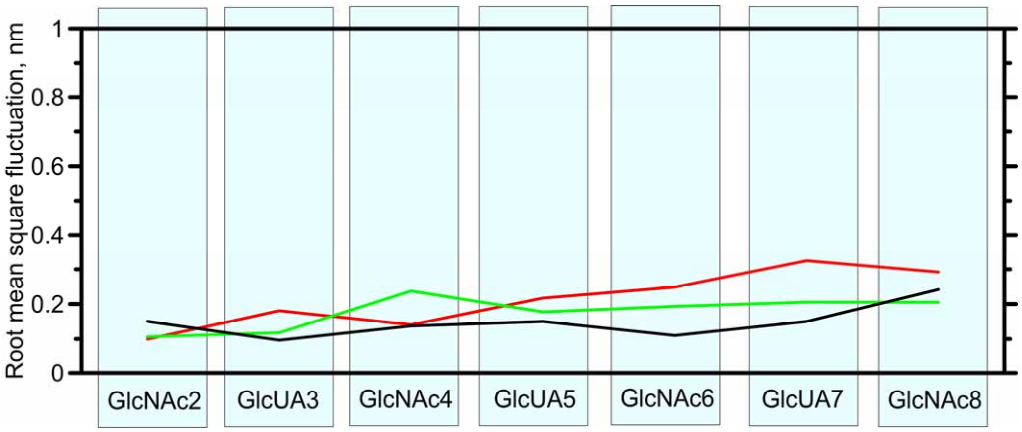

Figure S5. The RMSF (root mean square fluctuation) values for C1 atoms belonging to the HA chain. BLACK: unbound states; HA interacts only with solvent; GREEN: starting structure: 'A'; RED: starting structure: 'B'.

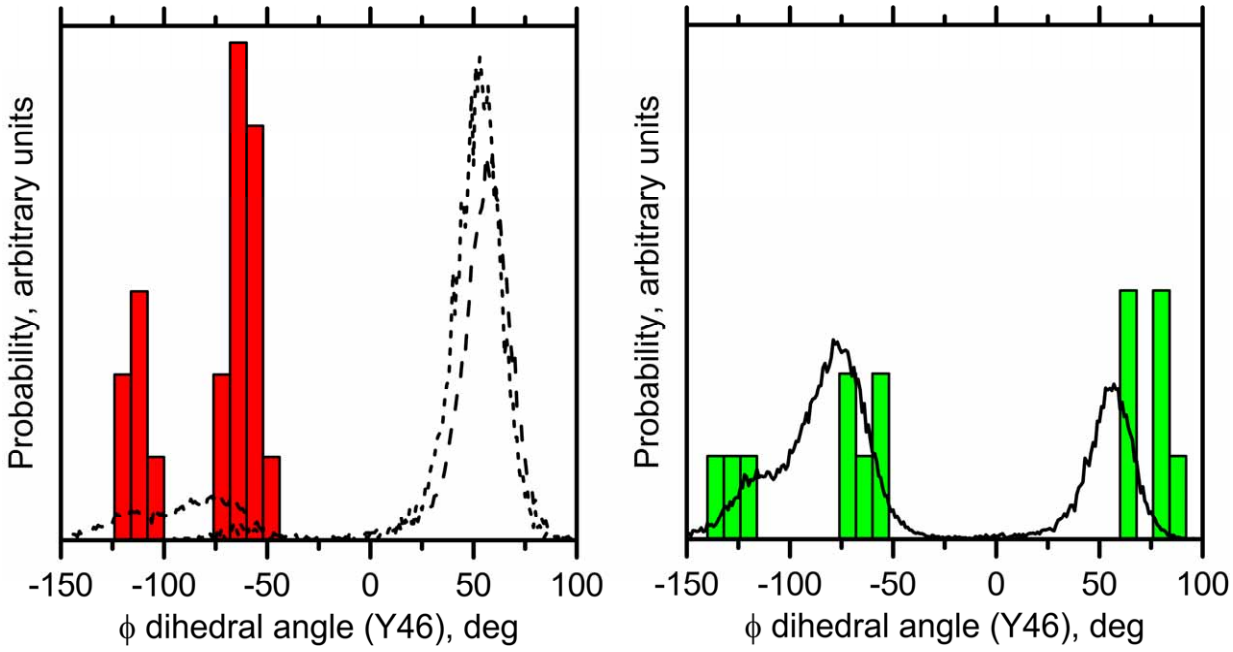

Figure S6. The comparison of the experimental and theoretical values of the ϕ dihedral angle (at Y46) for CD44 in the complex with HA (left) and in the unbound state (right). The data (bars) were taken from the PDB structures repoted in [P. Teriete, S. Banerji, M. Noble, C. D. Blundell, A. J. Wright, A. R. Pickford, E. Lowe, D. J. Mahoney, M. I. Tammi, J. D. Kahmann, I. D. Campbell, A. J. Day, D. G. Jackson, *Mol. Cell* **2004**, *13*, 483-496] and [M. Takeda, S. Ogino, R. Umemoto, M. Sakakura, M. Kajiwara, K. N. Sugahara, H. Hayasaka, M. Miyasaka, H. Terasawa, I. Shimada, *J. Biol. Chem.* 2006, **281**, 40089-40095]. Dashed and dotted lines represent the starting structures 'A' and 'B', respectively.

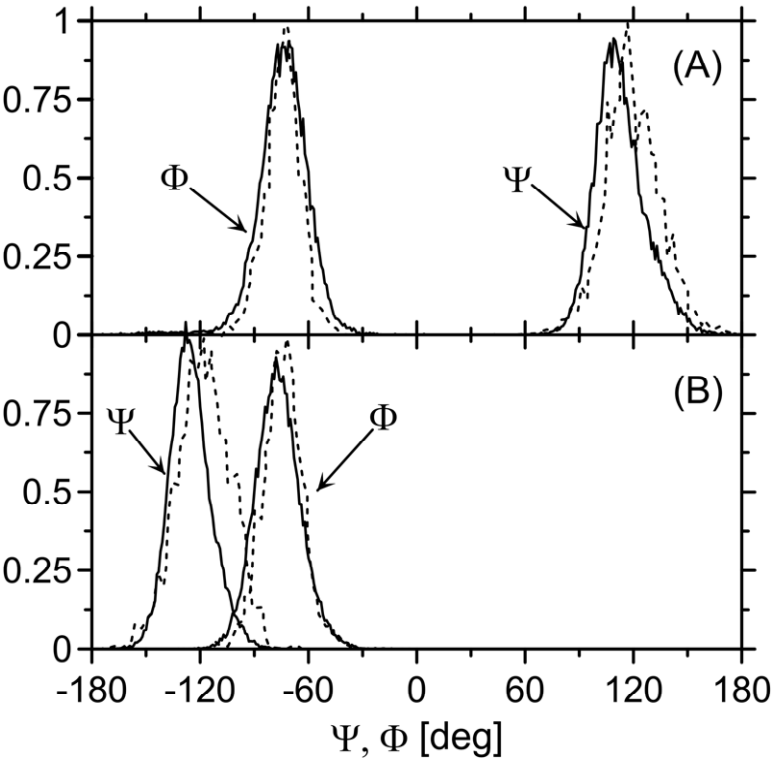

Figure S3. The probability distributions of glycosidic dihedral angles values for the free (unbound) HA_7 chain. Solid lines: our simulations; dotted lines: the data taken from [V. Gargiulo, M. A. Morando, A. Silipo, A. Nurisso, S. Pérez, A. Imberty, F. J. Cañada, M. Parrilli, J. Jiménez-Barbero, C. De Castro, *Glycobiology* 2010, **20**, 1208-1816]. The upper and bottom parts represent 1-3 and 1-4 linkages, respectively.