Supplementary Materials

Molecular Dynamics Approaches Dissect Molecular Mechanisms Underlying Methylene Blue–Glycosaminoglycan Interactions

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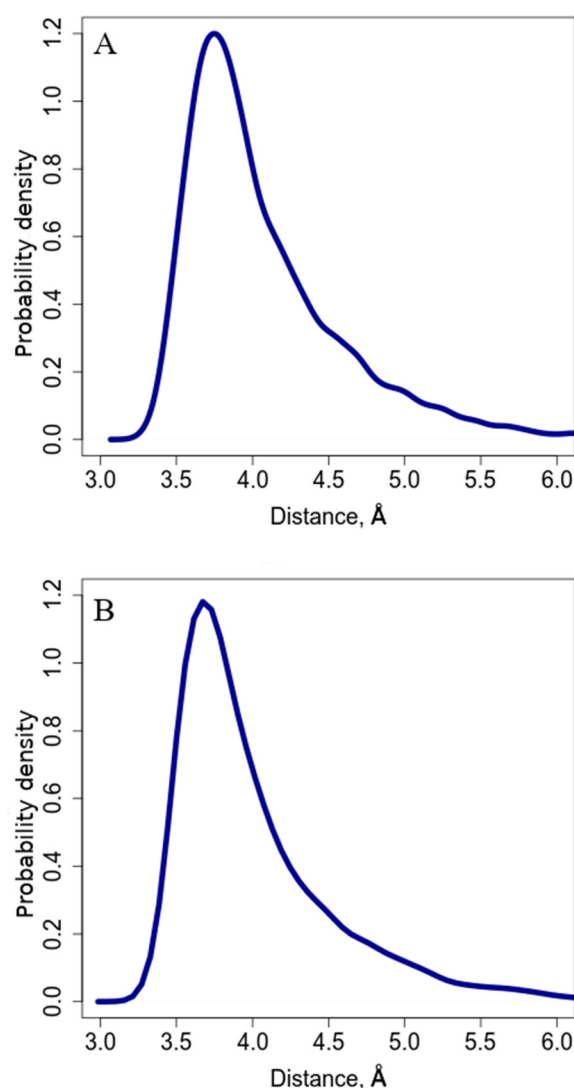* Correspondence: sergey.samsonov@ug.edu.pl; Tel.: +48-58-523-5166

Figure S1. Density of probability for the distance between the planes defined by the aromatic carbons of two MB molecules in a stack for the: A) two unbound MB and B) MB-HP dp10.

Table S1. Comparison of the binding free energies in MB-GAG dp10 complexes analyzed in the present study to the previously obtained binding ratios by Jia et al. [35].

GAG dp10	ΔG/drugs number[*]	Binding ratio [35][**]
deHP	+	-
HP	+++	+
HS1	+	+++
HS2	+++	++
HS3	+	+++
CS4	++	-
CS6	+++	-

[*] +: $\Delta G < 0$ kcal/mol; ++: -5 kcal/mol $< \Delta G < -3$ kcal/mol; +++: $\Delta G < -5$ kcal/mol;. [**] + binding ratio>0; ++ 3<binding ratio<4; +++ binding ratio>4 (higher binding ratio corresponds to stronger binding).