Supporting Information (SI)

Molecular Docking of Intercalators and Groove-binders to Nucleic Acids Using Autodock and Surflex

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Test Ligand	Grid Point Characteristics				Grid Center Characteristics		
	X Dimension	Y Dimension	Z Dimension	Total Number of Points	X Dimension	Y Dimension	Z Dimension
Daunorubicin	52	42	28	66091	14.332	13.212	-5.489
Distamycin	34	50	64	98175	9.776	21.55	76.162
Ellipticine	58	32	40	79827	0.992	19.28	46.762
Pentamidine	34	54	52	102025	10.298	20.854	8.457

Table SI1. Autodock Grid Map Coordinate Dimensions and Grid Center Information

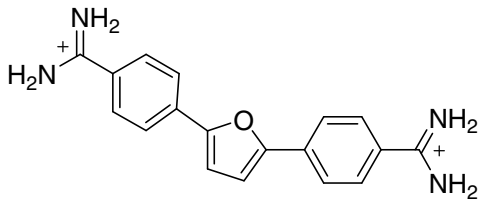

Figure SI1. Chemical structure of Furamidine, the ligand used to generate Surflex 2.11 protomols

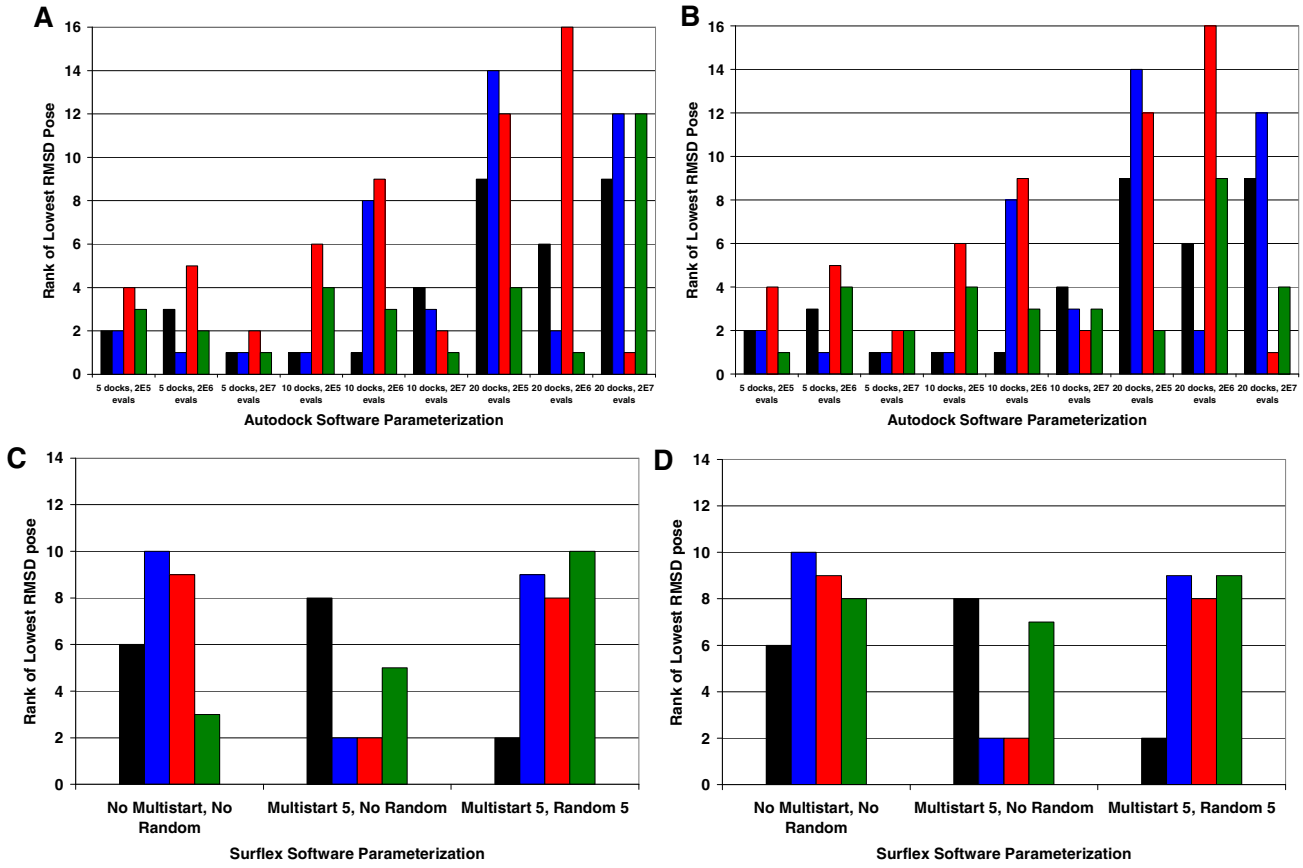

Figure SI2: The rank of the lowest RMSD pose out of all dockings. Figures A and C present the rank without taking into account ligand or nucleic acid symmetry, for Autodock and Surflex, respectively. Figures B and D includes ligand and nucleic acid symmetry, for Autodock and Surflex, respectively. Black = Daunorubicin, Blue = Distamycin, Red = Ellipticine, Green = Pentamidine.

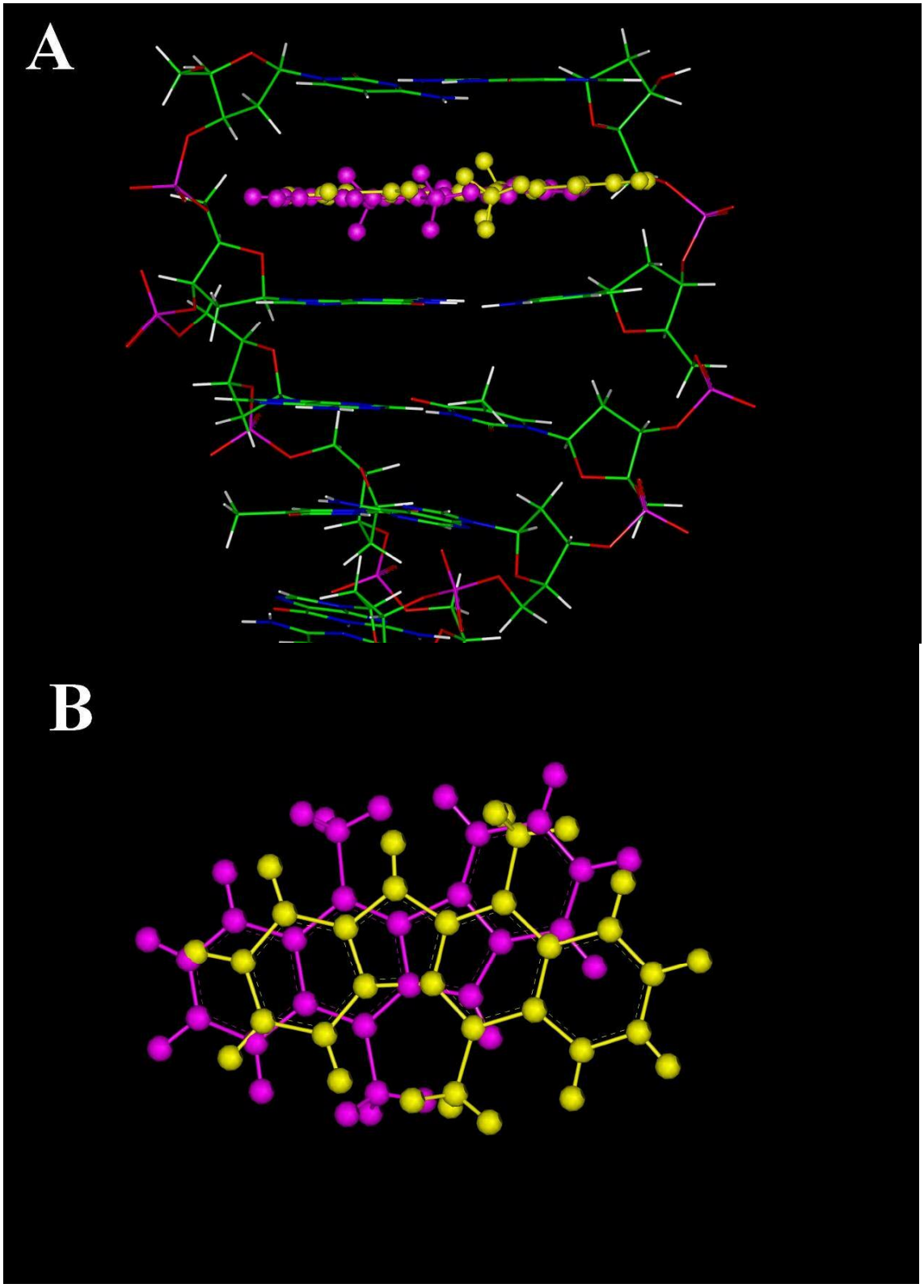

Figure SI3. Ellipticine. Visualization of the lowest RMSD pose (magenta) compared to the PDB crystallographic pose (yellow) with the nucleic acid target (A) and without the nucleic acid target (B) for Autodock with a software parameterization of "5 docks" and "2E7 energy evaluations."

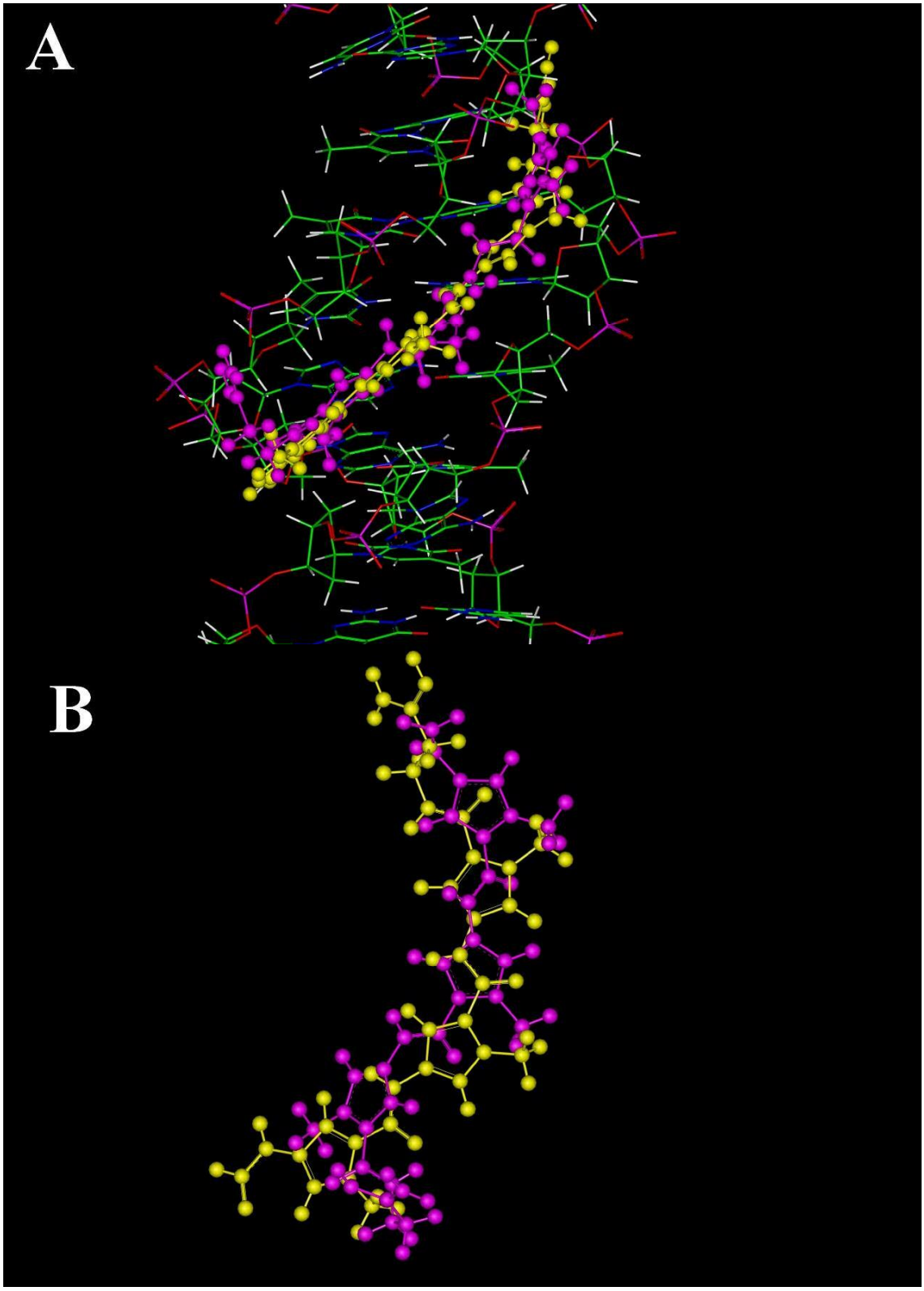

Figure SI4. Distamycin. Visualization of a high RMSD (> 12 Å) pose (magenta) compared to the PDB crystallographic pose (yellow) with the nucleic acid target (A) and without the nucleic acid target (B) for Autodock with a software parameterization of "20 docks" and "2E6 energy evaluations."

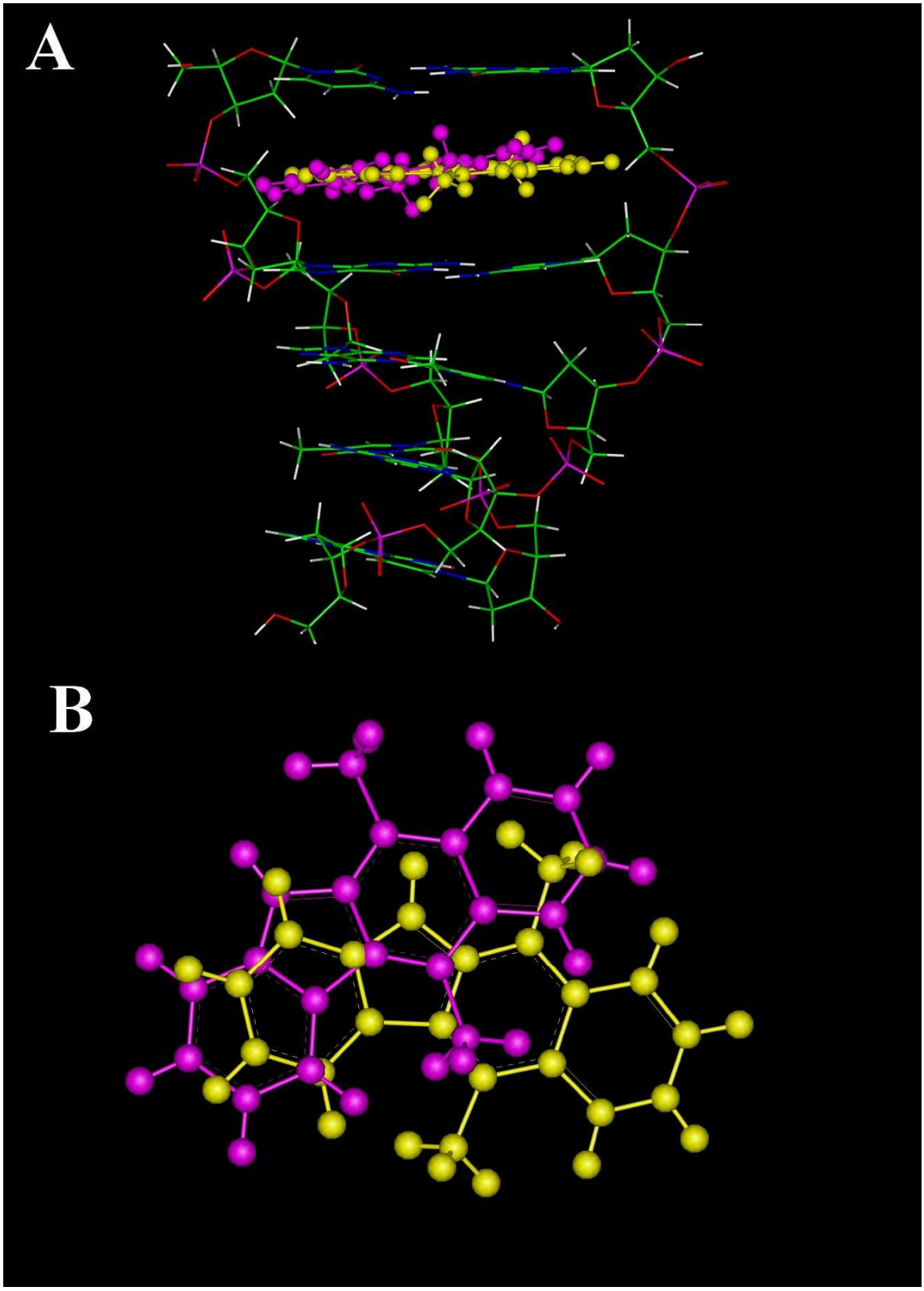

Figure SI5. Ellipticine. Visualization of the lowest RMSD pose (magenta) compared to the PDB crystallographic structure (yellow) with the nucleic acid target (A) and without the nucleic acid target (B) from Surflex with a software parameterization of "Multistart 5" only.

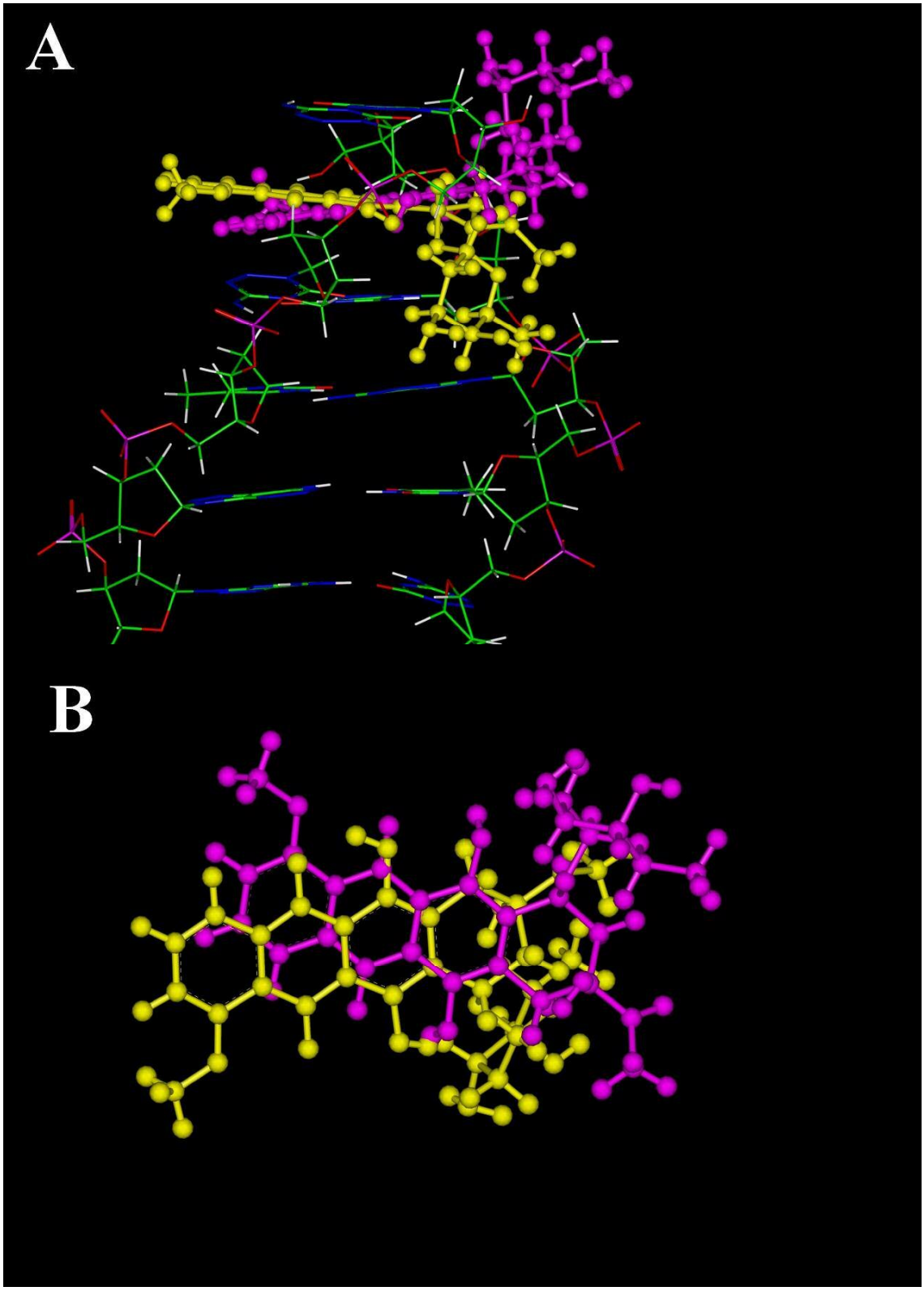

Figure SI6. Daunorubicin. Visualization of the top ranked pose (magenta) and the PDB Crystallographic Structure (yellow) from Surflex with a software parameterization of "No Multistart" and "No Random."

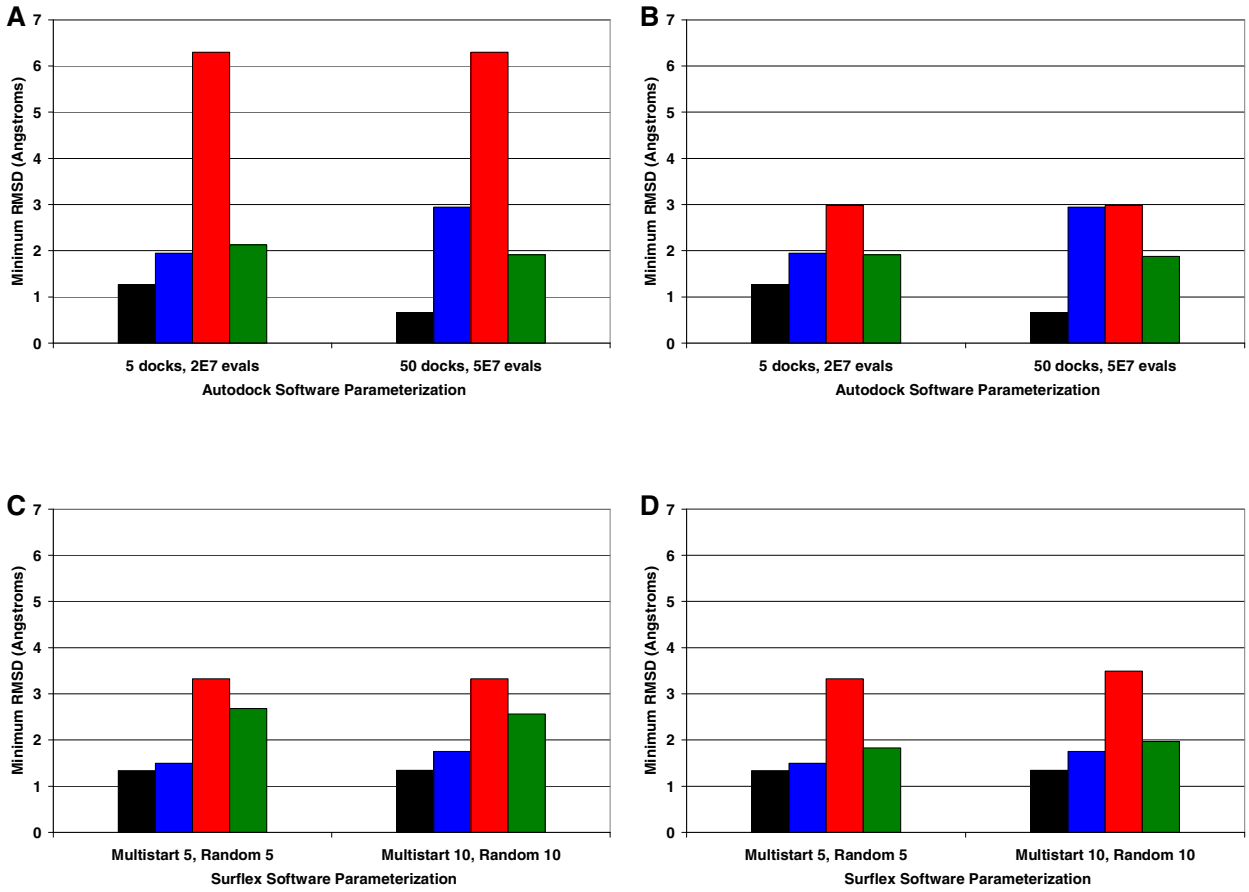

Figure SI7. Autodock and Surflex Parameterization Accuracy. The dock with the lowest RMSD is presented, regardless of ranking. Figures SI7A and SI7C present the RMSD calculated without taking into account ligand or nucleic acid symmetry, for Autodock and Surflex, respectively. Figures SI7B and SI7D includes ligand and nucleic acid symmetry, for Autodock and Surflex, respectively. Black = Daunorubicin, Blue = Distamycin, Red = Ellipticine, Green = Pentamidine.

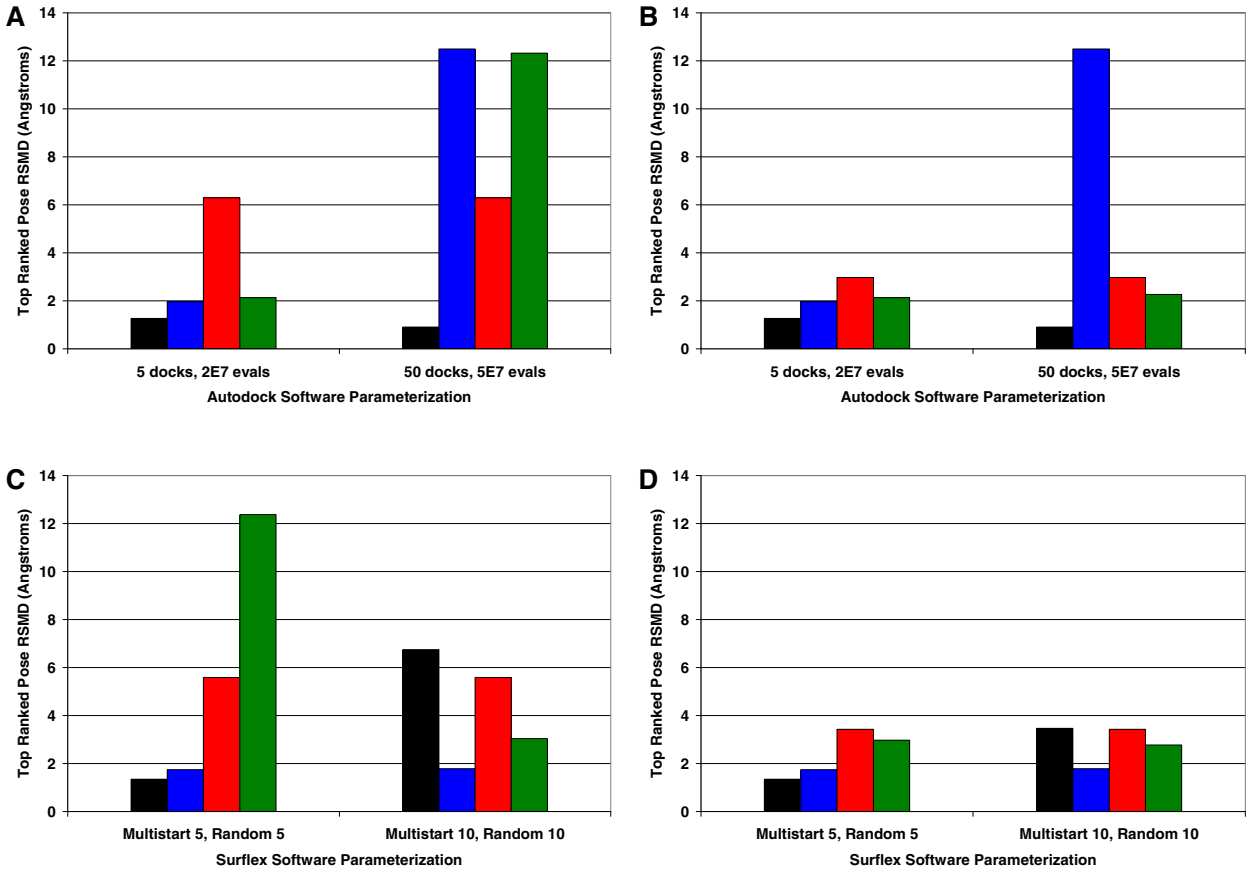

Figure SI8. Autodock and Surflex Parameterization Ranking. Figures SI8A and SI8C present the RMSD calculated without taking into account ligand or nucleic acid symmetry, for Autodock and Surflex, respectively. Figures SI8B and SI8D include ligand and nucleic acid symmetry, for Autodock and Surflex, respectively. Black = Daunorubicin, Blue = Distamycin, Red = Ellipticine, Green = Pentamidine.