Supplementary Material

Intermolecular Interaction Energies Between Glycopeptide Antibiotics And Substrates In Complexes Determined by X-ray Crystallography: Application of A Theoretical Databank Of Aspherical Atoms And A Symmetry-Adapted Perturbation Theory Based Set Of Interatomic Potentials

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Table S1. Geometry of hydrogen bonds in the complexes of vancomycin and small ligands used in the current study (van-Ac: Loll *et al*. (1997), PDB 1aa5; van-DLac, van-AcG: Loll *et al*. (1999); van-Ac-D-Ala1-4: Loll *et al*. (1998)).

Complexes	D	H	A	H…A(Å)	D-H…A(°)
Van:Ac	N(2)	H(9)	O(12)	1.83	164
	N(3)	H(13)	O(13)	1.95	152
	N(5)	H(19)	O(13)	1.92	167
Van:DLac	N(2)	H(9)	O(12)	1.78	159
	N(3)	H(13)	O(13)	1.91	146
	N(5)	H(19)	O(13)	1.79	169
	O(14)	H(38)	O(6)	1.70	158
Van:AcG	N(2)	H(9)	O(12)	1.81	163
	N(3)	H(13)	O(13)	2.07	154
	N(5)	H(19)	O(13)	1.98	168
	N(9)	H(40)	O(6)	2.52	104
Van1:AcDA1	N(2)	H(9)	O(12)	1.93	157
	N(3)	H(13)	O(13)	2.11	145
	N(5)	H(19)	O(13)	1.89	170
	N(9)	H(40)	O(6)	2.01	145

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Van2:AcDA2	N(2)	H(9)	O(12)	1.85	160
	N(3)	H(13)	O(13)	2.04	142
	N(5)	H(19)	O(13)	1.82	176
	N(9)	H(40)	O(6)	2.04	157
Van3:AcDA3	N(2)	H(9)	O(12)	1.84	163
	N(3)	H(13)	O(13)	1.99	150
	N(5)	H(19)	O(13)	1.99	169
	N(9)	H(40)	O(6)	1.86	150
Van4:AcDA4	N(2)	H(9)	O(12)	1.86	160
	N(3)	H(13)	O(13)	1.96	151
	N(5)	H(19)	O(13)	1.93	171
	N(9)	H(40)	O(6)	1.91	151