Supporting Information

The Conformational Free Energy Surface of α-*N*-Acetylneuraminic Acid: An Interplay Between Hydrogen Bonding and Solvation

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Figure S1: GLYCAM 06 force field parameters were converted from the AMBER format to GROMACS using the *amb2gmx.pl* script (http://chemistry.csulb.edu/ffamber/tools.html). It was necessary to modify the script to allow conversion of torsional parameters with negative force constants. This conversion was evaluated by comparing energies calculated using AMBER and GROMACS for structures representing free energy minima in vacuum (Figure 3). Results for individual force field terms are presented.

Figure S2: Projection of Neu5Ac residues in experimental (PDB) structures to ring-puckering coordinates. Neu5Ac residues in the active site of influenza neuraminidases are in red, others in yellow. Also structures of neuraminidase transition-state-mimicking inhibitors are shown as blue spheres. Structures of 207 residues in 78 experimental structures (**A**), structures of 72 residues in 28 experimental structures with resolution better than 2.0 Å (**B**, identical to Figure 6B) and structures of 48 residues in 16 experimental structures of sialidases (**C**). Note that sialidases can bind Neu5Ac residues not only in their catalytic sites, but also in their noncatalytic binding sites.

Figure S1

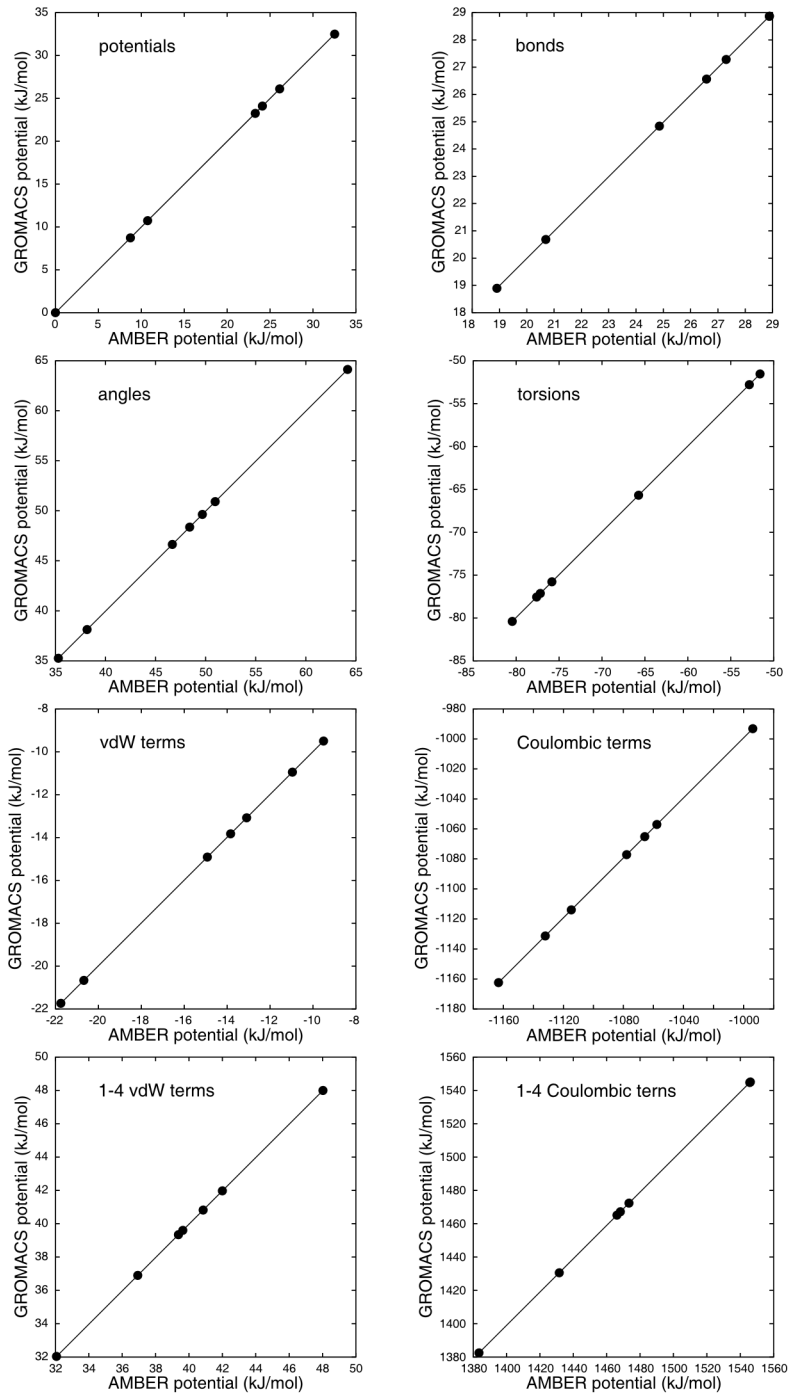
potentials
GROMACS potential (kJ/mol)
AMBER potential (kJ/mol)
bonds
GROMACS potential (kJ/mol)
AMBER potential (kJ/mol)
angles
GROMACS potential (kJ/mol)
AMBER potential (kJ/mol)
torsions
GROMACS potential (kJ/mol)
AMBER potential (kJ/mol)
vdW terms
GROMACS potential (kJ/mol)
AMBER potential (kJ/mol)
Coulombic terms
GROMACS potential (kJ/mol)
AMBER potential (kJ/mol)
1-4 vdW terms
GROMACS potential (kJ/mol)
AMBER potential (kJ/mol)
1-4 Coulombic terns
GROMACS potential (kJ/mol)
AMBER potential (kJ/mol)

Figure S2