Supplementary Information: New tricks for old dogs: Improving the accuracy of biomolecular force fields by pair-specific corrections to non-bonded interactions

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Figure S1: Validation and calibration of Rb\(^{+}\)--Cl\(^{-}\) (A) and Cs\(^{+}\)--Cl\(^{-}\) (B) ion pair interactions for the AMBER ff99 force fields using osmotic pressure simulations. Standard ion parameters optimized for the TIP3P water were taken from Joung and Cheatham.\(^1\) The simulation method for computing osmotic pressure was similar to that used in Ref. 2 and 3. NBFIX corrections, if necessary, were applied to the Lennard-Jones \(\sigma\) parameters for cation–anion atom pairs. Experimental data were taken from Ref. 4. See Table 3 for the changes in \(\sigma\) parameters.
Figure S2: Validation and calibration of Li$^+$–Br$^-$ (A), Na$^+$–Br$^-$ (B), K$^+$–Br$^-$ (C), Rb$^+$–Br$^-$ (D), and Cs$^+$–Br$^-$ (E) ion pair interactions for the AMBER ff99 force fields using osmotic pressure simulations. Standard ion parameters optimized for the TIP3P water were taken from Joung and Cheatham.\textsuperscript{1} The simulation method for computing osmotic pressure was similar to that used in Ref. 2 and 3. NBFIX corrections, if necessary, were applied to the Lennard-Jones $\sigma$ parameters for cation–anion atom pairs. Experimental data were taken from Ref. 4. See Table 3 for the changes in $\sigma$ parameters.
Figure S3: Validation and calibration of Li$^{+}$–I$^{-}$ (A), Na$^{+}$–I$^{-}$ (B), K$^{+}$–I$^{-}$ (C), Rb$^{+}$–I$^{-}$ (D), and Cs$^{+}$–I$^{-}$ (E) ion pair interactions for the AMBER ff99 force fields using osmotic pressure simulations. Standard ion parameters optimized for the TIP3P water were taken from Joung and Cheatham. The simulation method for computing osmotic pressure was similar to that used in Ref. 2 and 3. NBFIX corrections, if necessary, were applied to the Lennard-Jones $\sigma$ parameters for cation–anion atom pairs. Experimental data were taken from Ref. 4. See Table 3 for the changes in $\sigma$ parameters.
Figure S4: Validation and calibration of Rb$^+$–Ac$^-$ (A) and Cs$^+$–Ac$^-$ (B) ion pair interactions for the AMBER ff99 force fields using osmotic pressure simulations. Standard ion parameters optimized for the TIP3P water were taken from Joung and Cheatham. Standard parameters for acetate were taken from AMBER ff99. The simulation method for computing osmotic pressure was similar to that used in Ref. 2 and 3. NBFIX corrections, if necessary, were applied to the Lennard-Jones $\sigma$ parameters for cation–acetate oxygen atom pairs. Experimental data were taken from Ref. 4. See Table 3 for the changes in $\sigma$ parameters.
Figure S5: Validation and calibration of Mg$^{2+}$–Br$^-$ (A), Mg$^{2+}$–I$^-$ (B), Ca$^{2+}$–Br$^-$ (C), and Ca$^{2+}$–I$^-$ (D) ion pair interactions for the AMBER ff99 force fields using osmotic pressure simulations. Standard parameters for Mg$^{2+}$ and Ca$^{2+}$ were taken from the CHARMM36 force field. In all calibration simulations that used NBFIX, Mg$^{2+}$ and Ca$^{2+}$ ions were in the hexahydrate and heptahydrate forms, respectively; the dipole moment of the water molecules forming hexa- and heptahydrates was adjusted to account for the polarization effect. Standard parameters for Br$^-$ and I$^-$ were taken from Joung and Cheatham. The simulation method for computing osmotic pressure was similar to that used in Ref. 2 and 3. NBFIX corrections, if necessary, were applied to the Lennard-Jones $R_{\text{min}}$ parameter of the hexa- or heptahydrate water oxygen – anion atom pairs. Experimental data were taken from Ref. 4. See Table 3 for the changes in $\sigma$ parameters.
Figure S6: Validation and calibration of Rb$^+$–Cl$^-$ (A) and Cs$^+$–Cl$^-$ (B) ion pair interactions for the CHARMM36 force field using osmotic pressure simulations. The simulation method for computing osmotic pressure was similar to that used in Ref. 2 and 3. NBFIX corrections, if necessary, were applied to the Lennard-Jones $R_{\text{min}}$ parameters for cation–anion atom pairs. Experimental data were taken from Ref. 4. See Table 4 for the changes in $R_{\text{min}}$ parameters.
Figure S7: Validation and calibration of Rb\(^+\)–Ac\(^-\) (A) and Cs\(^+\)–Ac\(^-\) (B) ion pair interactions for the CHARMM36 force field using osmotic pressure simulations. The simulation method for computing osmotic pressure was similar to that used in Ref. 2 and 3. NBFIX corrections, if necessary, were applied to the Lennard-Jones $R_{\text{min}}$ parameters for cation–acetate oxygen atom pairs. Experimental data were taken from Ref. 4. See Table 4 for the changes in $R_{\text{min}}$ parameters.
References


(2) Yoo, J.; Aksimentiev, A. Improved Parametrization of Li\(^+\), Na\(^+\), K\(^+\), and Mg\(^{2+}\) Ions for All-Atom Molecular Dynamics Simulations of Nucleic Acid Systems. *J. Phys. Chem. Lett.* 2012, 3, 45–50.

