Supplementary Information: Recalibrating the calcium trap in amino acid carboxyl groups via classical molecular dynamics simulations

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Lennard-Jones potentials Ca – Aspartic Acid

The intermolecular Lennard-Jones potentials between Ca and Aspartic Acid according to the different calcium potential parameters, Set_1, Set_2, and Set_3 as mentioned in Table 1 in the main text.

Table S1 Lennard-Jones potential parameters Ca - Aspartic acid Set_1

Atom i	Atom j	ε_{ij} eV	σ_{ij} (Å)
Ca	N	0.01212336177754750	3.33809926201551
Ca	H1	0.00368424682452194	2.24763923086026
Ca	CT	0.00972539310852265	3.41293475422537
Ca	H2	0.00368424682452194	2.69308858950367
Ca	H3	0.00368424682452194	3.03786639363011
Ca	C2	0.00862279272582844	3.41293475397241
Ca	OD	0.01347436327552800	3.19306095082234

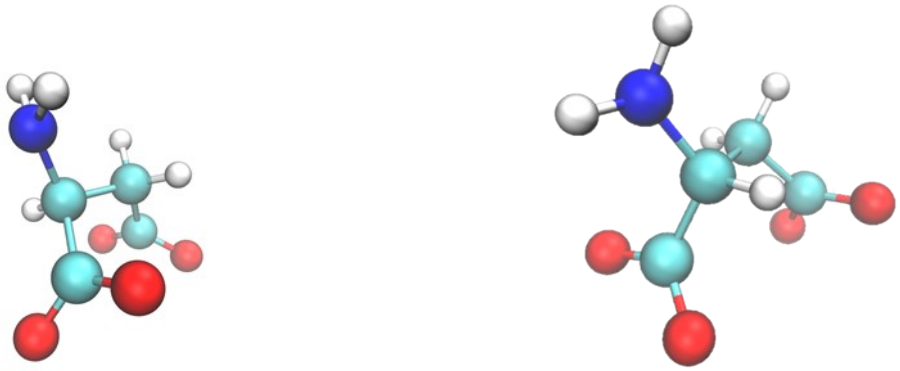
Table S2 Lennard-Jones potential parameters Ca - Aspartic acid Set_2

Atom i	Atom j	ε_{ij} eV	σ_{ij} (Å)
Ca	N	0.000993522376406289	3.39225326201551
Ca	H1	0.000301927941072037	2.30179323086026
Ca	CT	0.000797006296599970	3.46708875422537
Ca	H2	0.000301927941072037	2.74724258950367
Ca	H3	0.000301927941072037	3.09202039363011
Ca	C2	0.000706647023937694	3.46708875397241
Ca	OD	0.001104238384344610	3.24721495082234

Table S3 Lennard-Jones potential parameters Ca - Aspartic acid Set_3

Atom i	Atom j	ε_{ij} eV	σ_{ij} (Å)
Ca	N	0.00285309254151	3.24860426201551
Ca	H1	0.00086704474625	2.15814423086026
Ca	CT	0.00228875843601	3.32343975422537
Ca	H2	0.00086704474625	2.60359358950367
Ca	H3	0.00086704474625	2.94837139363011
Ca	C2	0.00202927422809	3.32343975397241
Ca	OD	0.00317103507000	3.10356595082234

Supplementary Graphs and Figures



D-aspartic acid **L-aspartic acid**

Figure S1 Molecular structure of the studied biomolecules. Nitrogen (blue), Carbon (cyan), Oxygen (red) and Hydrogen (white).

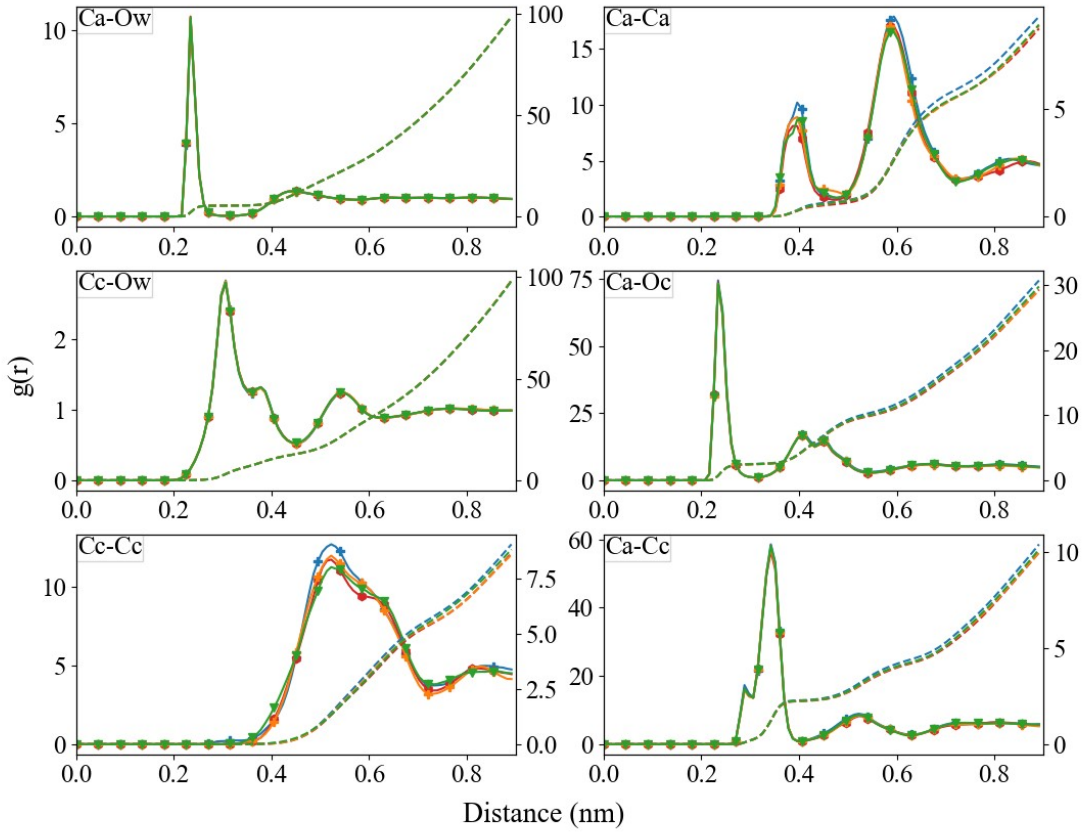


Figure S2 Radial distribution function (left axis) and corresponding integral (N(r)) (right axis) between Ca^{2+}, C_c, O_c, and O_w, after 30 ns of simulation. **D-Asp** using different forcefields; $Set\_3_{unmodified}$ (red; ●), $Set\_3_{\sigma+0.5\%\sigma}$ (blue; ✚), $Set\_3_{\sigma+1.0\%\sigma}$ (orange; ┼), and $Set\_3_{\sigma+2.0\%\sigma}$ (green; ▼)

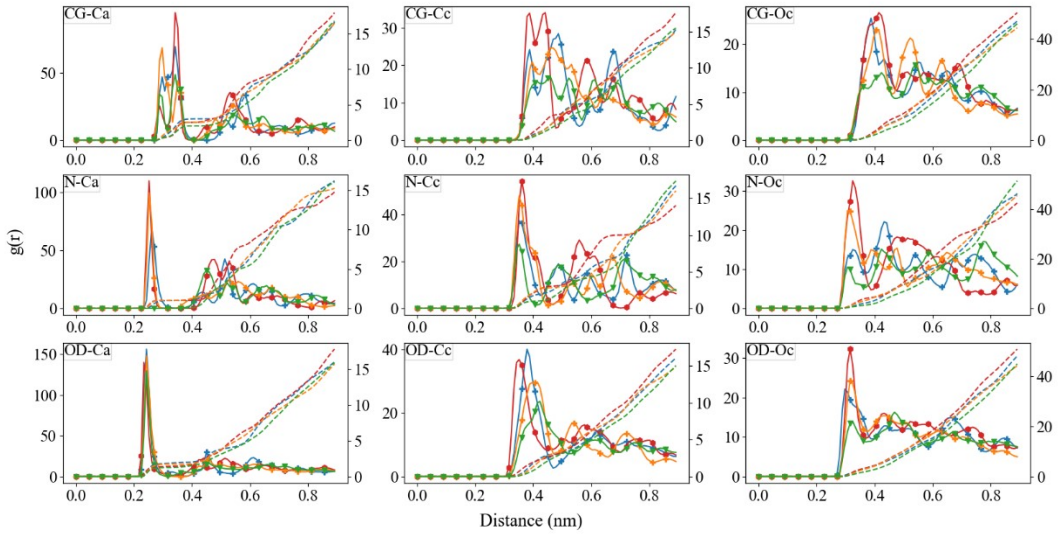


Figure S3 Radial distribution function between Ca^{2+}, C_c, O_c, with the different functional groups in aspartic acid after 30 ns of simulation. **D-Asp** using different forcefields**;** $Set\_3_{unmodified}$ (red; ●), $Set\_3_{\sigma+0.5\%\sigma}$ (blue; ✚), $Set\_3_{\sigma+1.0\%\sigma}$ (orange; ┼), and $Set\_3_{\sigma+2.0\%\sigma}$ (green; ▼)

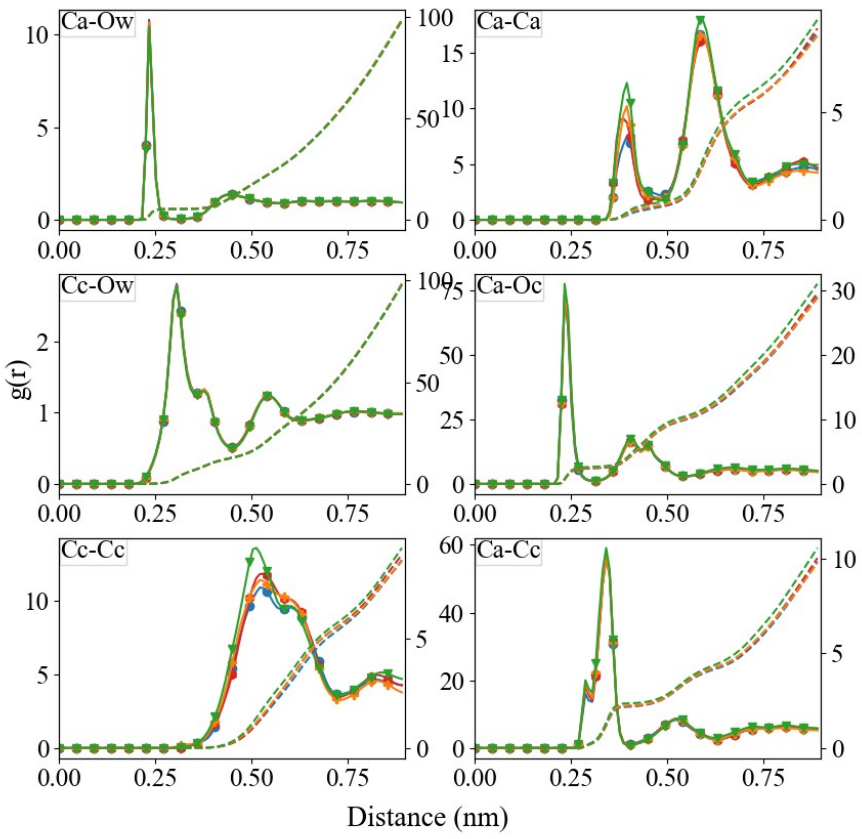


Figure S 4 Radial distribution function (left axis) and corresponding integral (N(r)) (right axis) between Ca^{2+}, C_c, O_c, and O_w, after 30 ns of simulation. **L-Asp** using different forcefields**;** $Set\_3_{unmodified}$ (red; ⬢), $Set\_3_{\sigma+0.5\%\sigma\sigma+0.5\%}$ (blue; ✚), $Set\_3_{\sigma+1.0\%\sigma}$ (orange; ┼), and $Set\_3_{\sigma+2.0\%\sigma}$ (green; ▼)

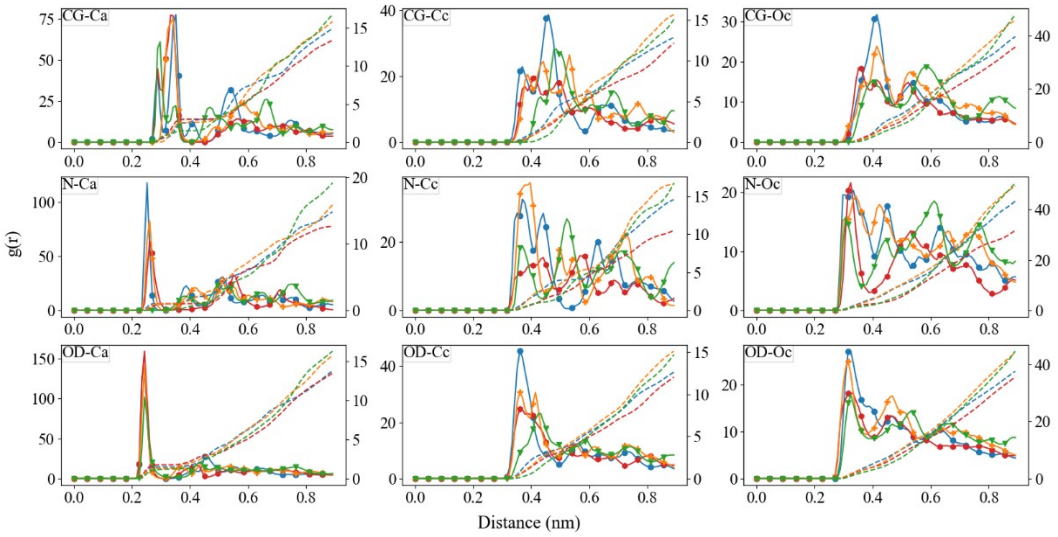


Figure S 5 Radial distribution function between Ca^{2+}, C_c, O_c, with the different functional groups in aspartic acid after 30 ns of simulation. **L-Asp** using different forcefields**;** $Set\_3_{unmodified}$ (red; ●), $Set\_3_{\sigma+0.5\%\sigma}$ (blue; ✚), $Set\_3_{\sigma+1.0\%\sigma}$ (orange; ┼), and $Set\_3_{\sigma+2.0\%\sigma}$ (green; ▼)