SUPPLEMENTARY INFORMATION for:

Looking at human cytosolic sialidase NEU2 structural features with an interdisciplinary approach

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Figure SI1 Calculated CD spectra of NEU2 on the basis of MD trajectories for representative structures at 300 K through program PROTPOL.

Table SI1 Percent fractions of secondary structures calculated from MD structures.

Figure SI2 Time evolution of poly-Pro-II percent fraction of NEU2 at 300 K and 500 K, as of MD simulations.

Figure SI3 Comparison of calculated CD spectra of NEU2 in presence of divalent ions with corresponding calculations in *ss* condition.

Figure SI4 Calculated CD spectra of NEU2 on the basis of MD trajectories for representative structures at 500 K through program PROTPOL.

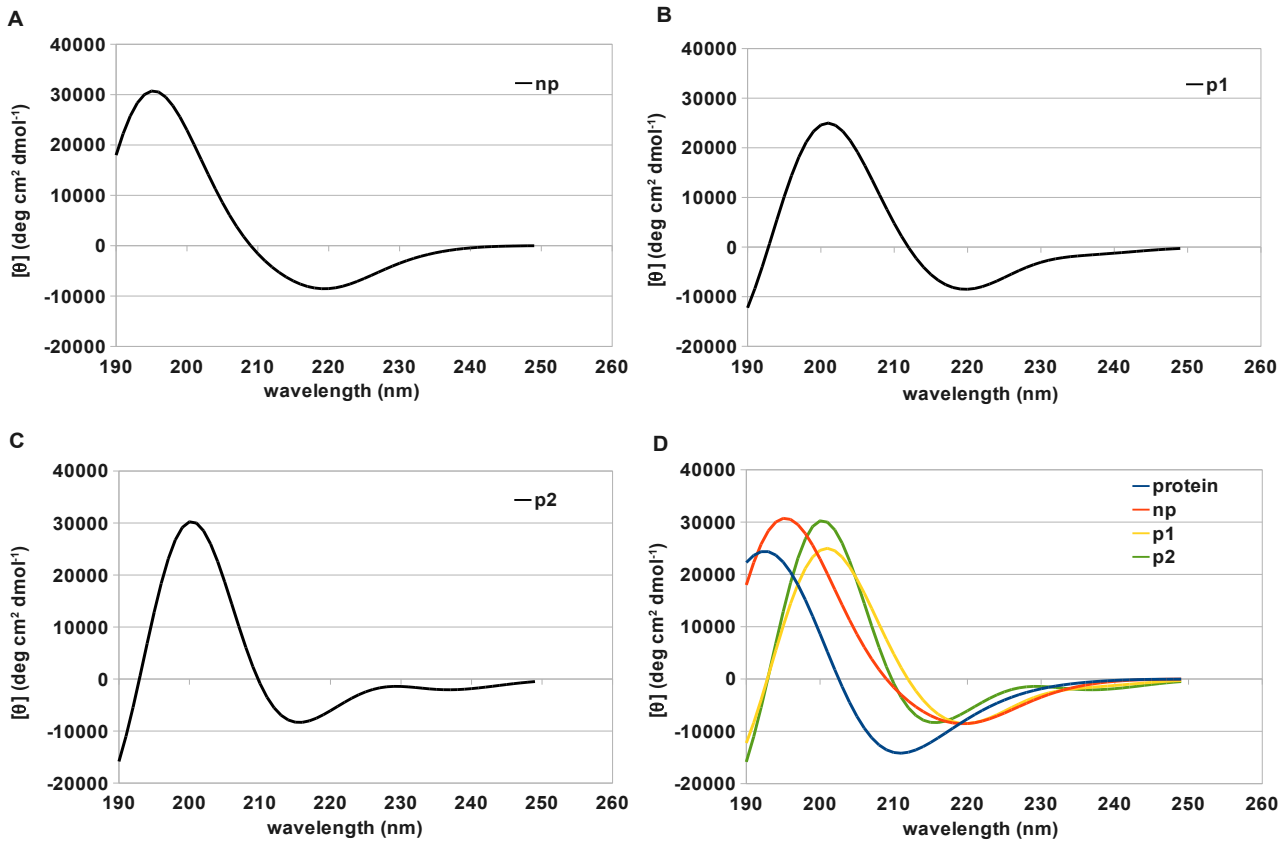

Figure SI1. CD spectra calculated using representative structures from 10 clusters from a trajectory in ss at 300 K. (A) Results from program PROTPOL with no polarizability contribution (np). **(B)** Results from program PROTPOL with polarizability contributions on wavelengths (p1). **(C)** Results from program PROTPOL with polarizability contributions on both wavelengths and rotational strengths (p2). **(D)** Comparison of results from PROTPOL in the three previously defined conditions (np, p1, and p2) and results from protein.

	H	G	E	T	N	P	O
average ss 300 K	4.59	1.55	28.80	6.67	4.65	9.28	44.45
st. dev. ss 300 K	1.0	0.9	2.1	1.2	1.1	1.2	2.2
average ss 500 K	1.93	1.08	27.47	6.83	4.56	8.72	49.41
st. dev. ss 500 K	1.1	0.9	2.7	1.5	1.5	1.7	3.0

Table SI1. Percent fraction of secondary structure calculated by means of the program XTLSSTR [1] and averaged over 20 ns of MD trajectory at 300 K in ss (first two rows) and over 70 ns of MD trajectory at 500 K in ss (third and fourth row). Column headers are defined as follows: H: alpha helix; G: 3-10 helix; E: extended beta strand; T: beta turn; N: beta turn without a hydrogen bond; P: poly-pro-II structure; O: other.

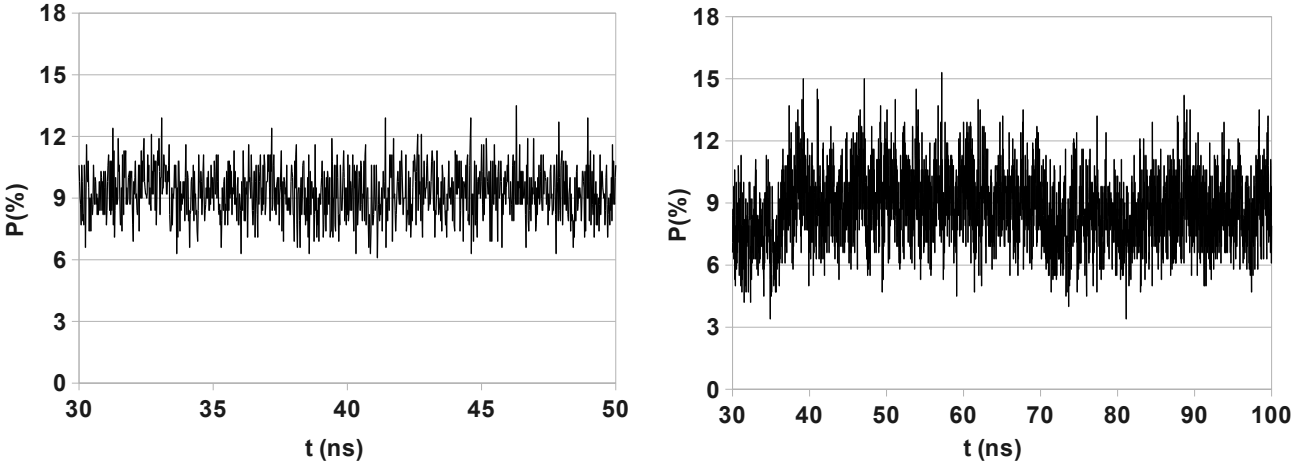

Figure SI2. Time evolution of the poly-pro-II percent fraction, calculated by means of the program XTLSSTR [1], in the structure of NEU2 during a simulation in ss at 300 K (left) and at 500 K (right).

[1] Program XTLSSTR, version 1.3.9, 28 Sep 2001. Written by Sonya M. King and W. Curtis Johnson, Biochem/Biophys, Oregon State University, Corvallis OR 97331. http://biochem.science.oregonstate.edu/people/w-curtis-johnson

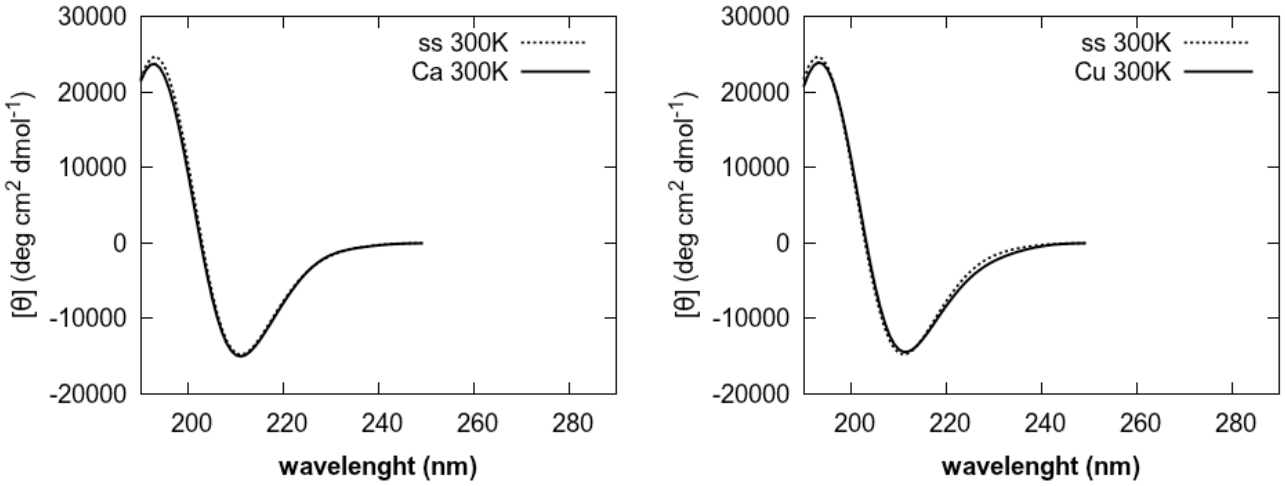

Figure SI3. Left: CD spectrum calculated in a simulation at 300K in Ca compared with the spectrum calculated in a simulation at 300K in ss. Right: CD spectrum calculated in a simulation at 300K in Cu compared with the spectrum calculated in a simulation at 300K in ss.

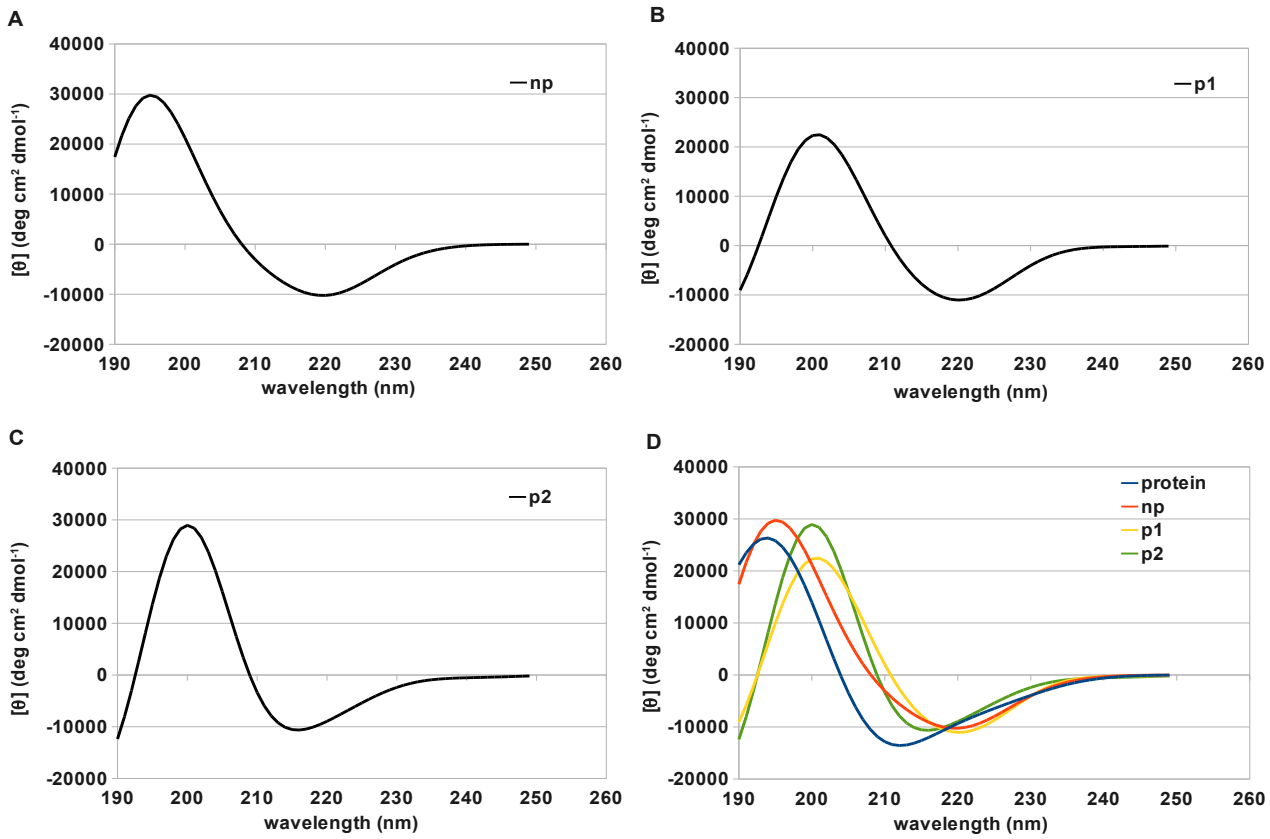

Figure SI4. CD spectra calculated using representative structures from eight clusters from a trajectory in ss at 500 K. (A) Results from program PROTPOL with no polarizability contribution (np). (B) Results from program PROTPOL with polarizability contributions on wavelengths (p1). (C) Results from program PROTPOL with polarizability contributions on both wavelengths and rotational strengths (p2). (D) Comparison of results from PROTPOL in the three previously defined conditions (np, p1, and p2) and results from protein.