Electronic Supplementary Material (ESI) for Soft Matter


# A molecular dynamics investigation of structure and dynamics of SDS and SDBS micelle.

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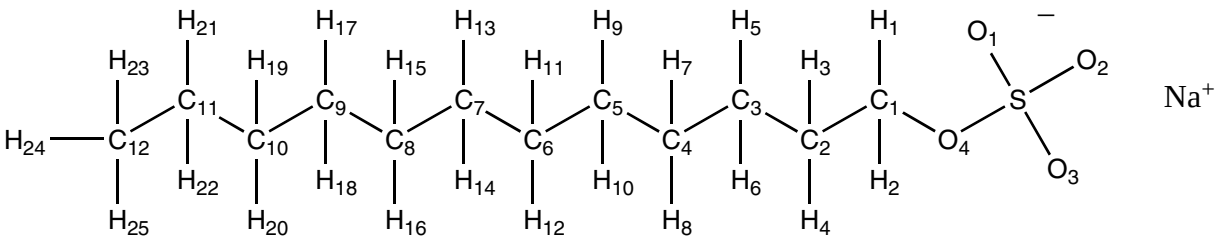


**Scheme S1.** SDS molecule. The reference number of each atom is showed.

**Table S1.** SDS RESP charges as obtained with a Gaussian 03 geometry optimisation, at the DFT B3LYP[46]/6-31G* level.

| Atom | Charghe (e) | Atom | Charge (e) |
|---|---|---|---|
| $C_{12}$ | -0.23130 | $H_{1\text{-}2}$ | 0.01417 |
| $C_{11}$ | 0.13319 | $H_{3\text{-}4}$ | 0.00772 |
| $C_{10}$ | -0.00138 | $H_{5\text{-}6}$ | 0.04199 |
| $C_9$ | -0.02646 | $H_{7\text{-}8}$ | -0.00112 |
| $C_8$ | 0.08235 | $H_{9\text{-}10}$ | 0.01105 |
| $C_7$ | 0.01430 | $H_{11\text{-}12}$ | 0.01171 |
| $C_6$ | -0.08212 | $H_{13\text{-}14}$ | -0.00837 |
| $C_5$ | 0.06455 | $H_{15\text{-}16}$ | -0.02543 |
| $C_4$ | -0.05631 | $H_{17\text{-}18}$ | -0.00344 |
| $C_3$ | -0.06812 | $H_{19\text{-}20}$ | -0.00363 |
| $C_2$ | -0.02807 | $H_{21\text{-}22}$ | -0.02112 |
| $C_1$ | 0.11865 | $H_{23\text{-}24\text{-}25}$ | 0.04916 |
| $O_4$ | -0.37265 | S | 0.92329 |
| $O_{1\text{-}2\text{-}3}$ | -0.55482 | $Na^+$ | +1 |

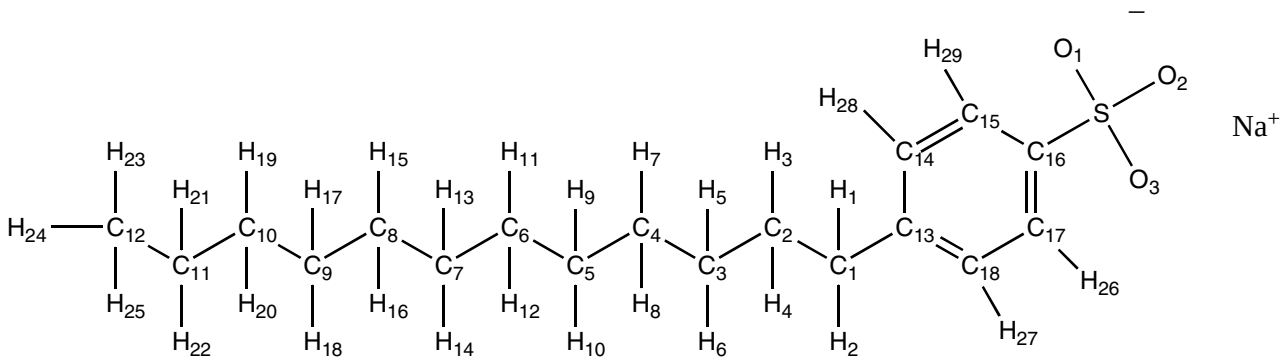


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**Table S1.** SDS RESP charges as obtained with a Gaussian 03 geometry optimisation, at the DFT B3LYP[46]/6-31G* level.

| Atom | Charge (e) | Atom | Charghe (e) |
|---|---|---|---|
| $C_{16}$ | -0.028178 | $H_{1\text{-}2}$ | 0.027325 |
| $C_{15}$ - $C_{17}$ | -0.072424 | $H_{3\text{-}4}$ | -0.005745 |
| $C_{14}$ - $C_{18}$ | -0.228125 | $H_{5\text{-}6}$ | -0.009135 |
| $C_{13}$ | 0.091262 | $H_{7\text{-}8}$ | -0.008927 |
| $C_{12}$ | -0.224551 | $H_{9\text{-}10}$ | -0.016216 |
| $C_{11}$ | 0.116532 | $H_{11\text{-}12}$ | -0.007669 |
| $C_{10}$ | -0.004258 | $H_{13\text{-}14}$ | -0.009308 |
| $C_9$ | -0.026108 | $H_{15\text{-}16}$ | -0.015929 |
| $C_8$ | 0.050513 | $H_{17\text{-}18}$ | -0.004334 |
| $C_7$ | 0.016189 | $H_{19\text{-}20}$ | -0.000540 |
| $C_6$ | -0.009316 | $H_{21\text{-}22}$ | -0.017102 |
| $C_5$ | 0.034392 | $H_{23\text{-}24\text{-}25}$ | 0.049422 |
| $C_4$ | -0.011194 | $H_{27\text{-}28}$ | 0.109710 |
| $C_3$ | -0.003231 | $H_{29\text{-}26}$ | 0.113213 |
| $C_2$ | -0.073608 | $O_{1\text{-}3}$ | -0.582119 |
| $C_1$ | -0.113071 | $Na^+$ | +1 |
| S | 0.869915 | | |

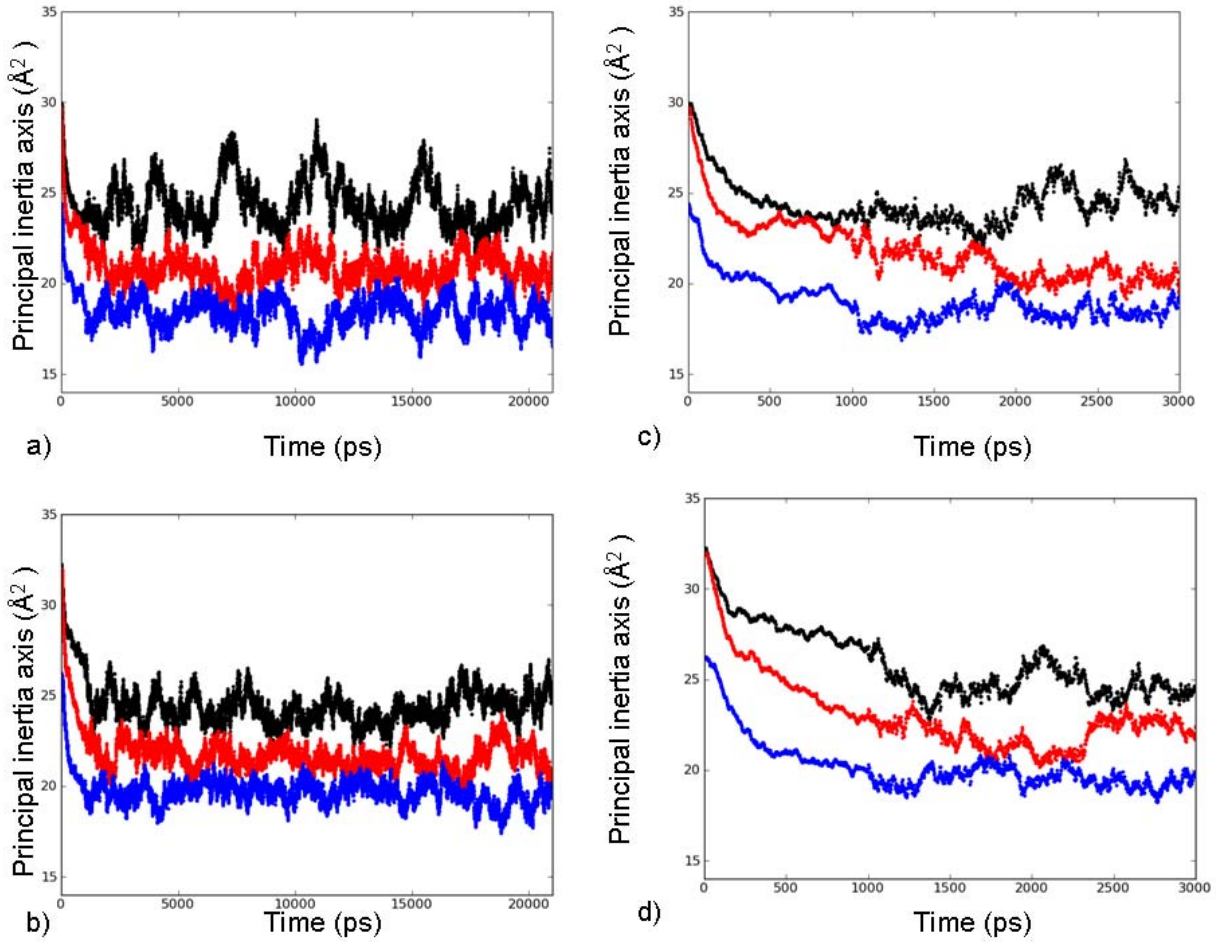


**Fig S1.** Values of the three axes of inertia during the simulation including the first ns of equilibration for (a) SDS and b) SDBS. c) and d) Blow up of the first 3 ns

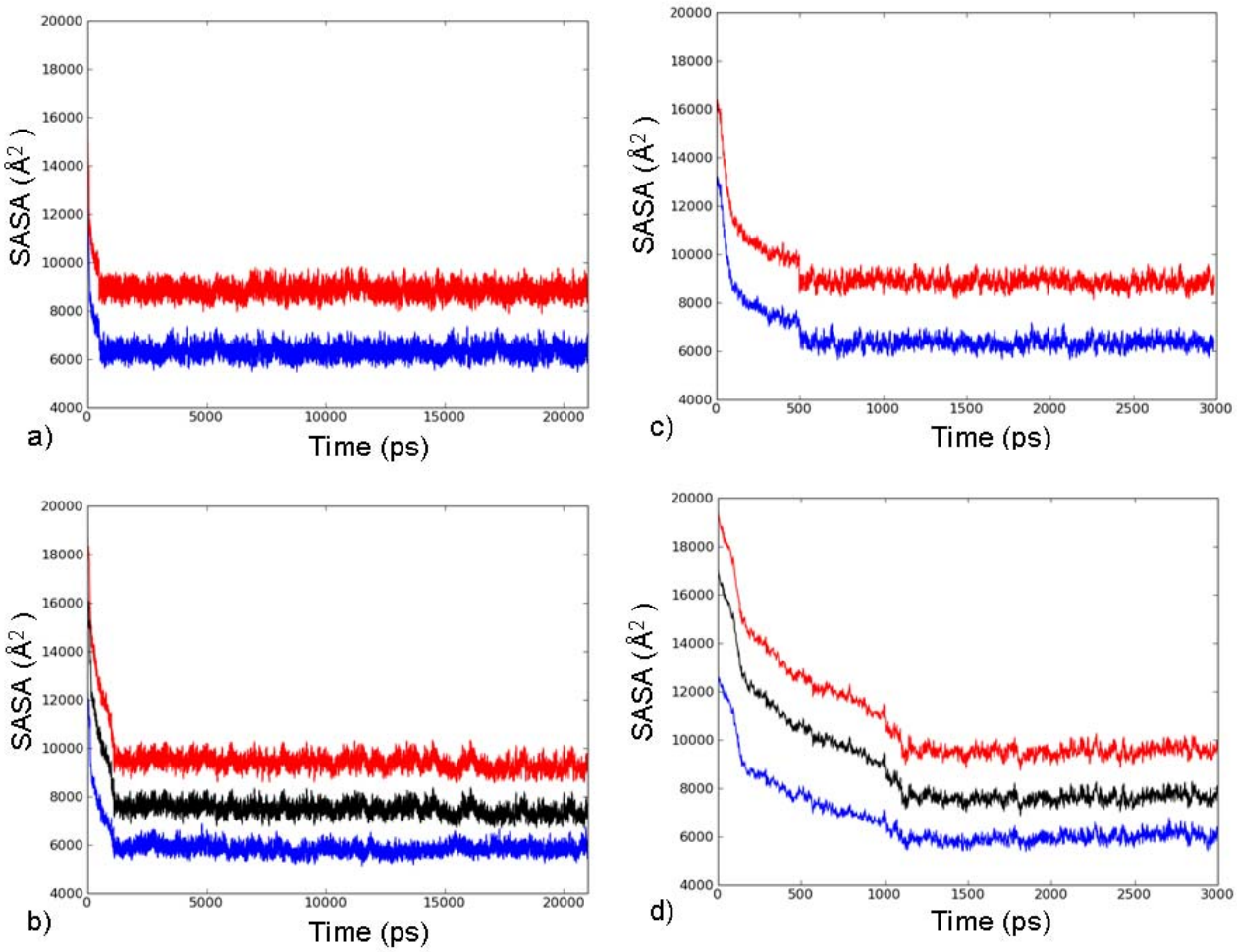


**Fig S2.** a) Accessible surface area for (a) SDS and (b) SDBS micelles including the first ns of equilibration. Hydrocarbon tail surface (blue line), phenyl ring surface (red line) and total micelle surface (green line). c) and d) Blow up of the first 3 ns

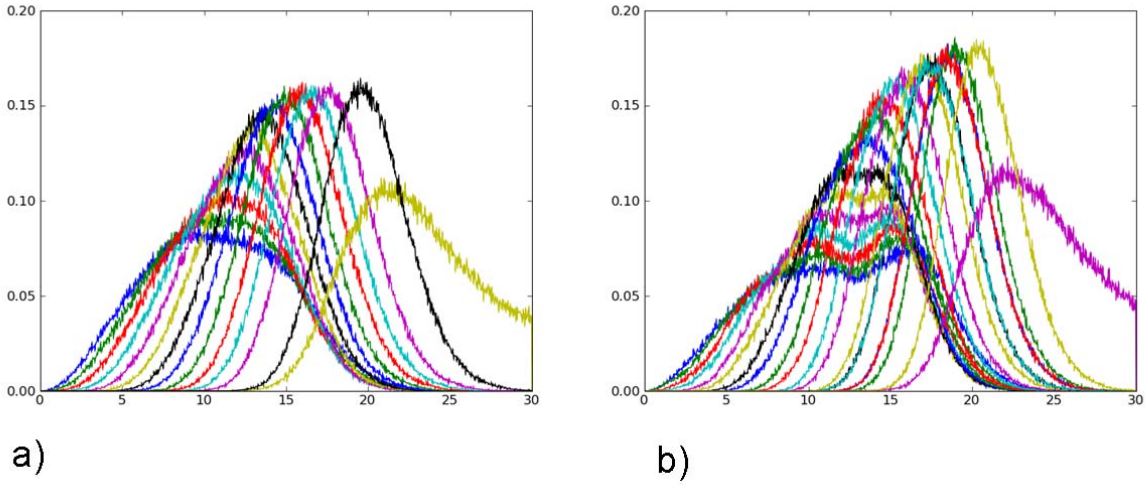


**Fig S3.** Probability distribution for the atom-to-micelle center-of-mass distance for individual carbons, sulphurs, and sodiums, for SDS (a) and SDBS (b).

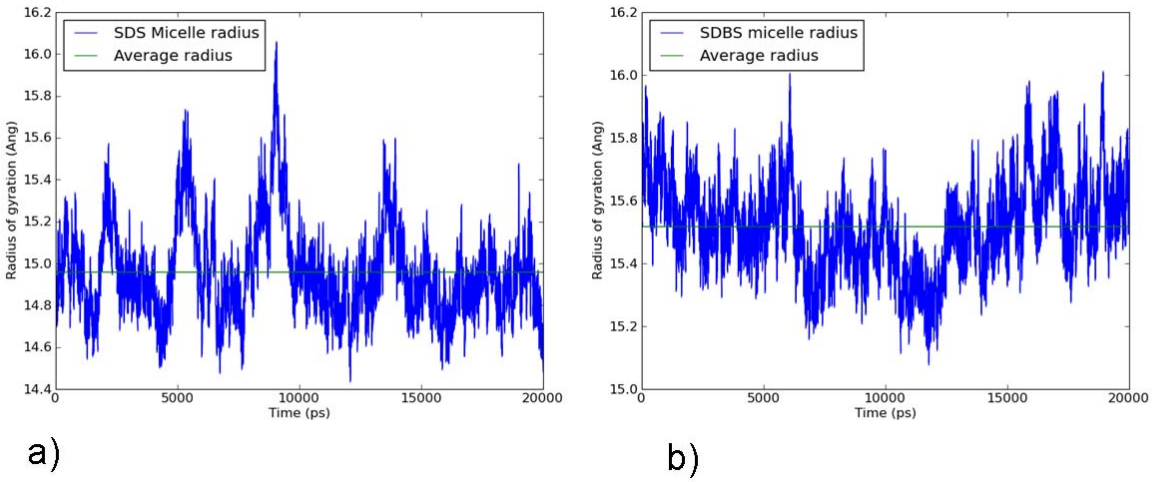


**Fig S4.** Values of the radius of gyration during the simulation fir SDS (a) and SDBS (b).

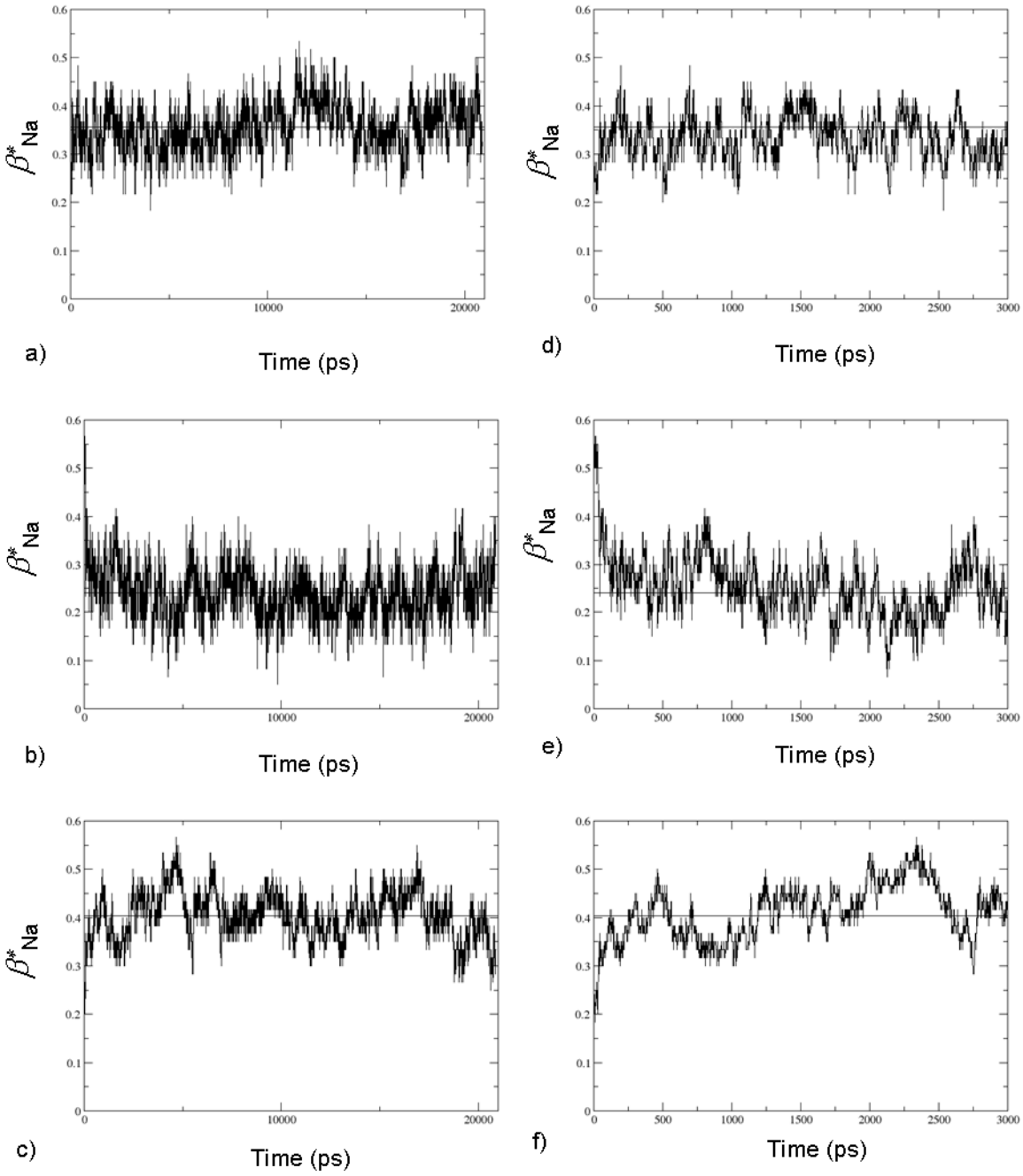


**Fig S5** Counterion binding for SDS during the simulation for the a) first shell, b) second shell and c) bulk. d), e) and f) Blow up of the first 3 ns

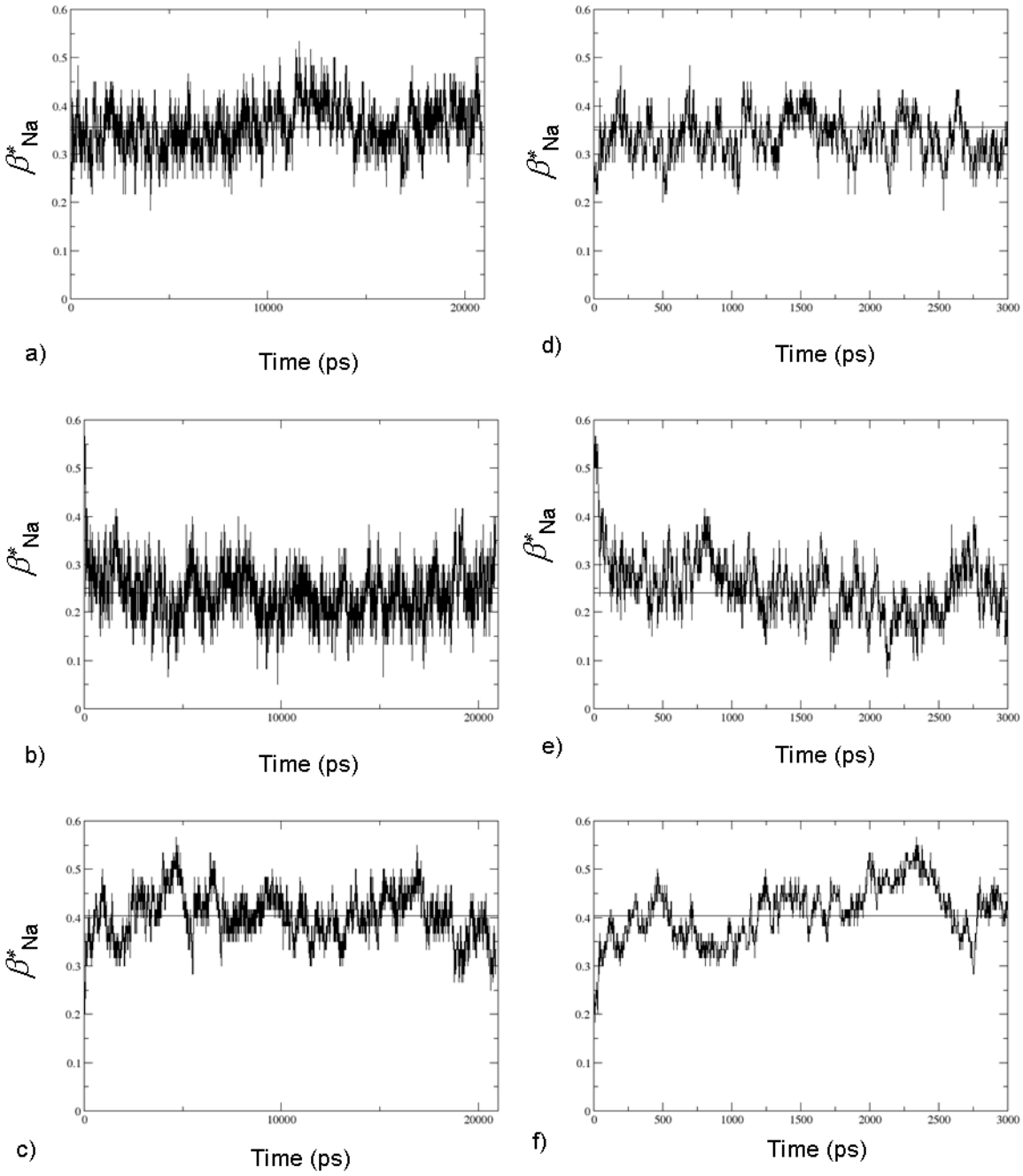


**Fig S6** Counterion binding for SDBS during the simulation for the a) first shell, b) second shell and c) bulk. d), e) and f) Blow up of the first 3 ns