Locality in amino-acid based imidazolium ionic liquids. Supporting information.

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Experimental Methodology

Material and Purification

Unless stated otherwise all materials were used as received without further purification. L-alanine ($\geq$ 99.5%), L-phenylalanine ($\geq$ 99.5%), L-proline ($\geq$ 99.5%), L-histidine ($\geq$ 99.5%), L-tyrosine ($\geq$ 99.5%), L-tryptophan ($\geq$ 99.5%), acetic acid ($\geq$ 99.8%), silver nitrate ($\geq$ 99%), 1-methyl imidazole ($\geq$ 99%), bromoethane ($\geq$ 98%) were purchased from Sigma-Aldrich. Amberlite IRN-78, OH^- form, ion-exchange resin (particle size = 25-30 mesh, 500-600 mm) was purchased from Acros Organics. Starting materials which have been stored over a long time need to purify before use. 1-ethyl imidazole ($\geq$ 99.9%), which was purchased from Fluorochem, and 1-methyl imidazole were stirred over potassium hydroxide overnight, followed by distillation under vacuum. Bromoethane was extracted with concentrated sulfuric acid until the acid layer remained colourless. Then the organic layer was separated and neutralised with saturated sodium bicarbonate aqueous solution, followed by washing with deionised water. The resulting organic layer was dried with anhydrous magnesium sulphate overnight, followed by distillation under vacuum. Upon purification, all reagents were stored in the nitrogen atmosphere prior to reaction.

Equipment

Infrared (IR) spectra were recorded on a Perkin Elmer 1600 series FT-IR spectrometer.

Method

The ILs were synthesized by anion-exchange method.

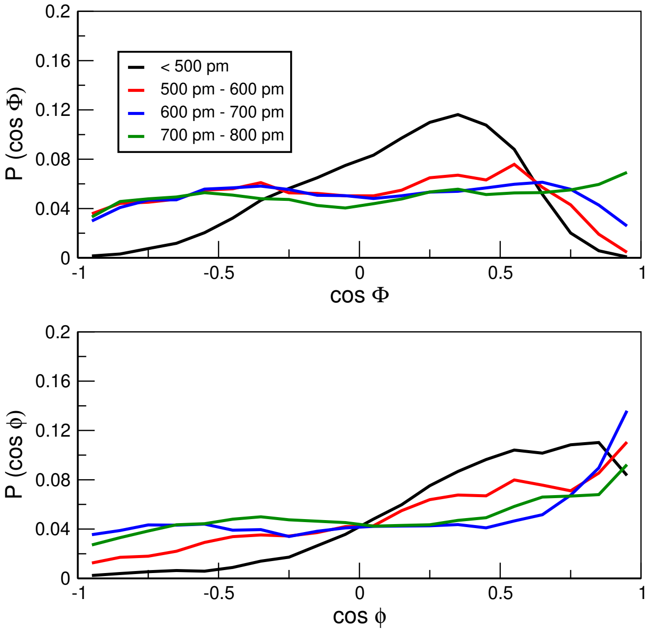

Figure 1: Angular probability distribution of cos Φ (charge-dipole) and cos ϕ (dipole-dipole) separated by distance below 500 pm (black), from 500-600 pm (red), from 600-700 pm (blue) and 700-800 pm (green) for cations in [C_2C_1Im][his].

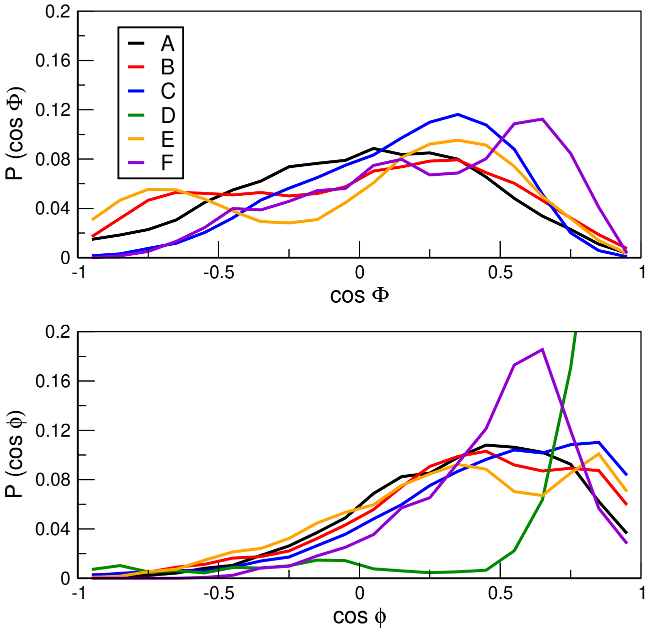

Figure 2: Angular probability distribution of cos Φ (charge-dipole) and cos ϕ (dipole-dipole) of cations separated by distances below 500 pm of all ILs analyzed.

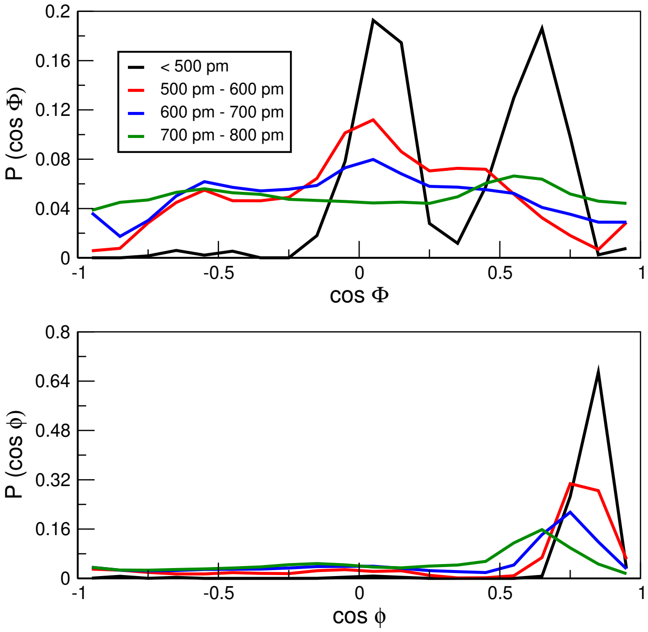

Figure 3: Angular probability distribution of cos Φ (charge-dipole) and cos ϕ (dipole-dipole) separated by distance below 500 pm (black), from 500-600 pm (red), from 600-700 pm (blue) and 700-800 pm (green) for anions in [C_2C_1Im][his].

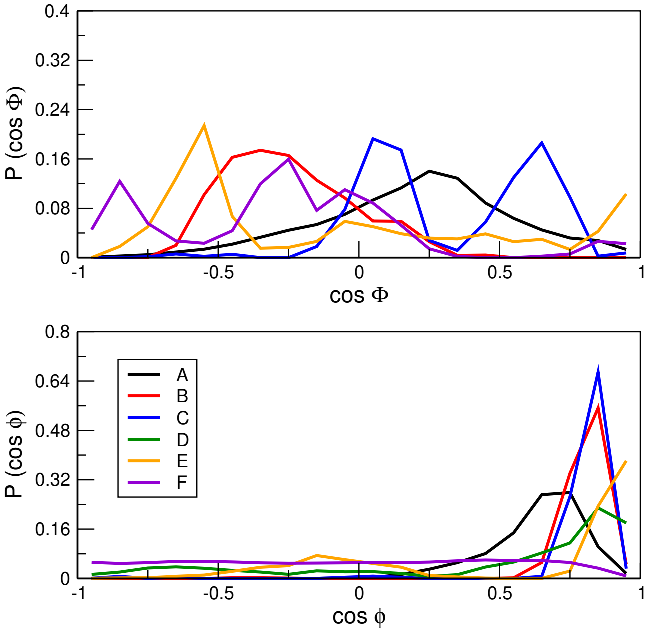

Figure 4: Angular probability distribution of cos Φ (charge-dipole) and cos ϕ (dipole-dipole) of anions separated by distances below 500 pm of all ILs analyzed.

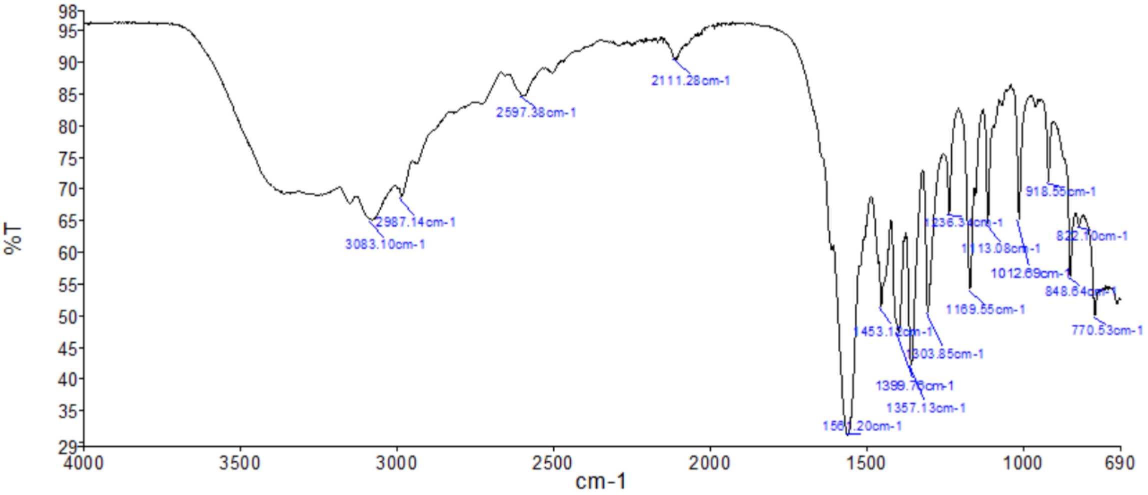

Figure 5: The experimental IR spectrum of $[C_2C_1Im][ala]$.

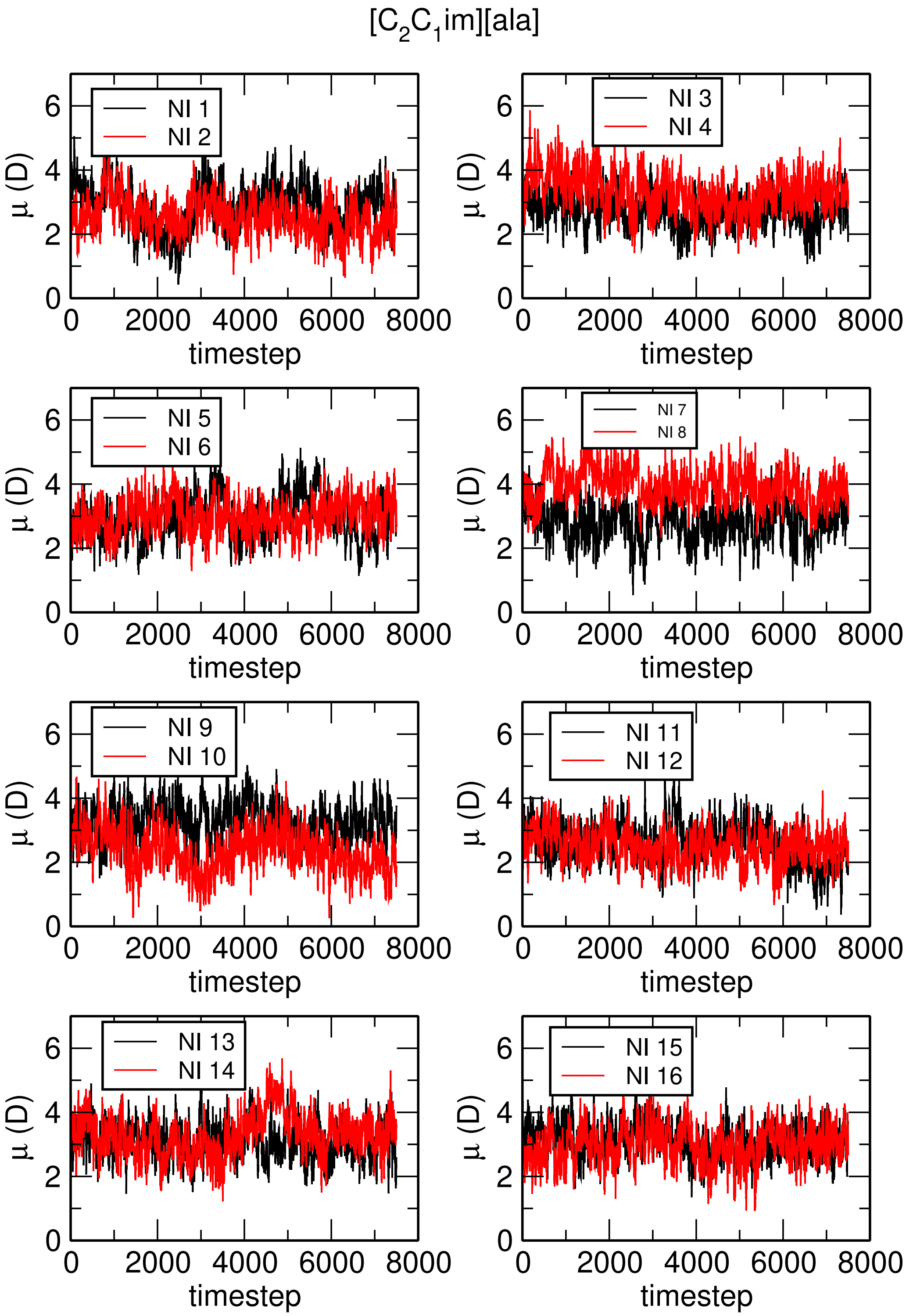

Figure 6: The every time development of the dipole moment (μ) of one randomly selected ion of anion in $[C_2C_1Im][ala]$.

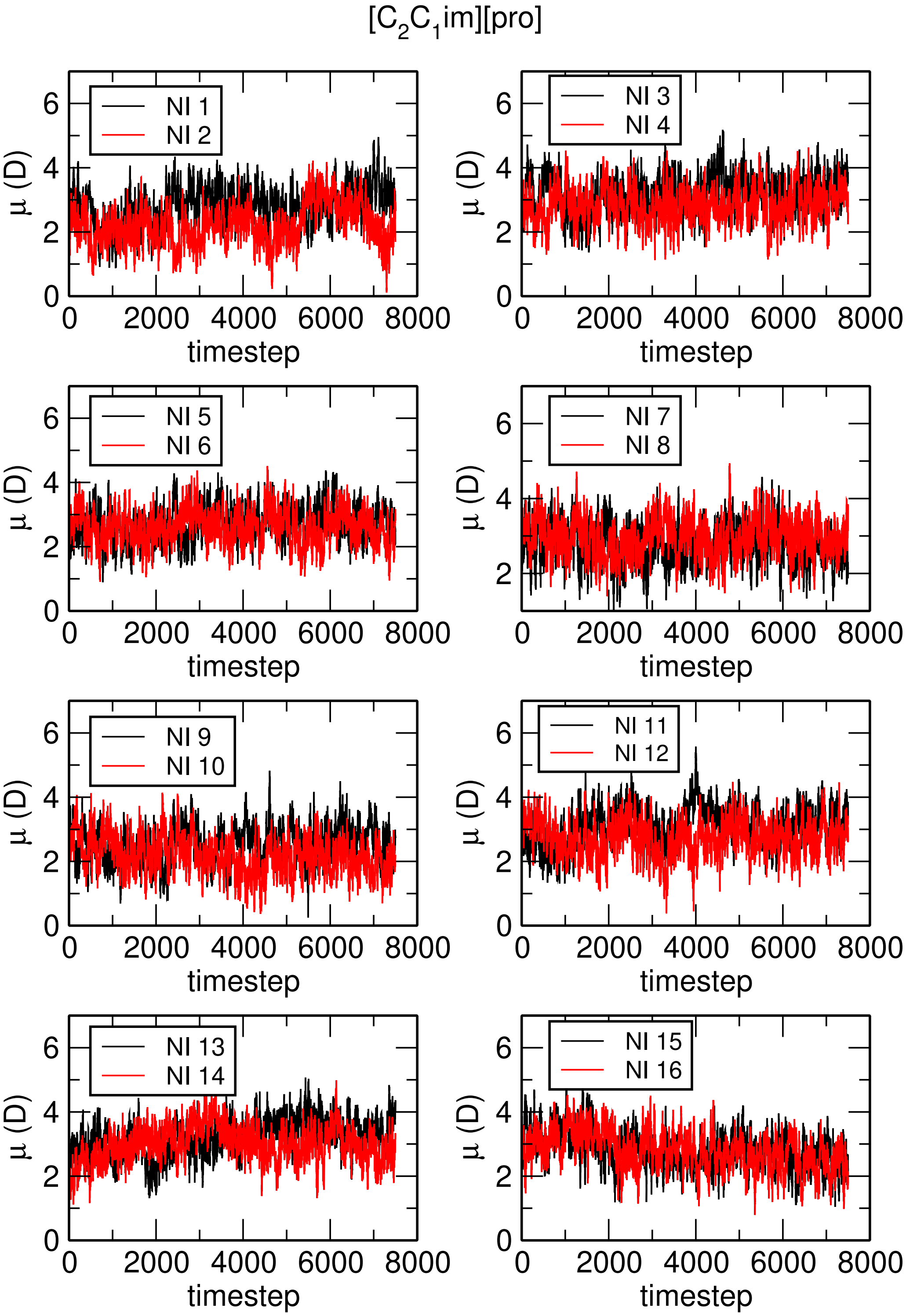

Figure 7: The every time development of the dipole moment (μ) of one randomly selected ion of cation in [C$_2$C$_1$Im][pro].

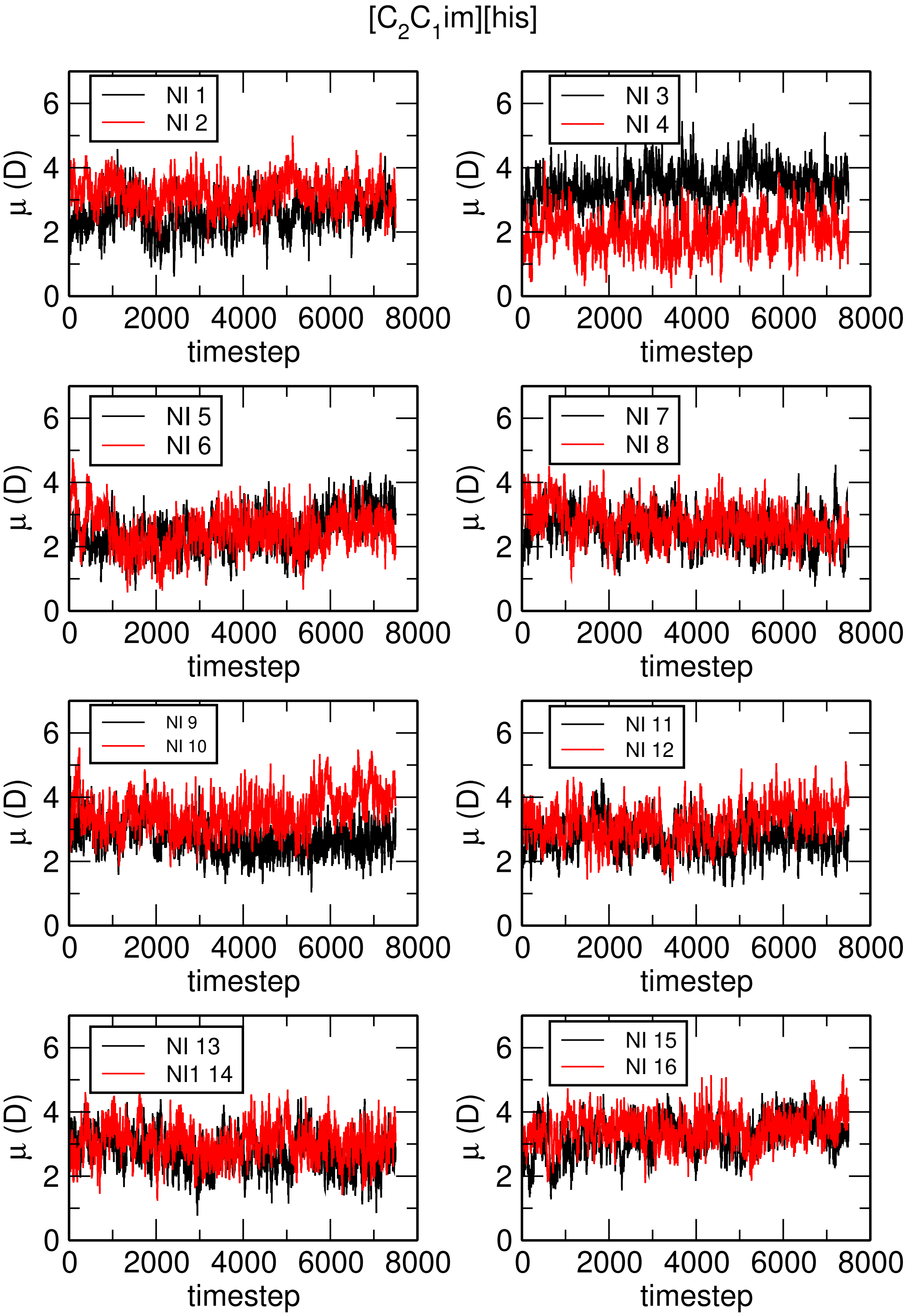

Figure 8: The every time development of the dipole moment (μ) of one randomly selected ion of cation in [C$_2$C$_1$Im][his].

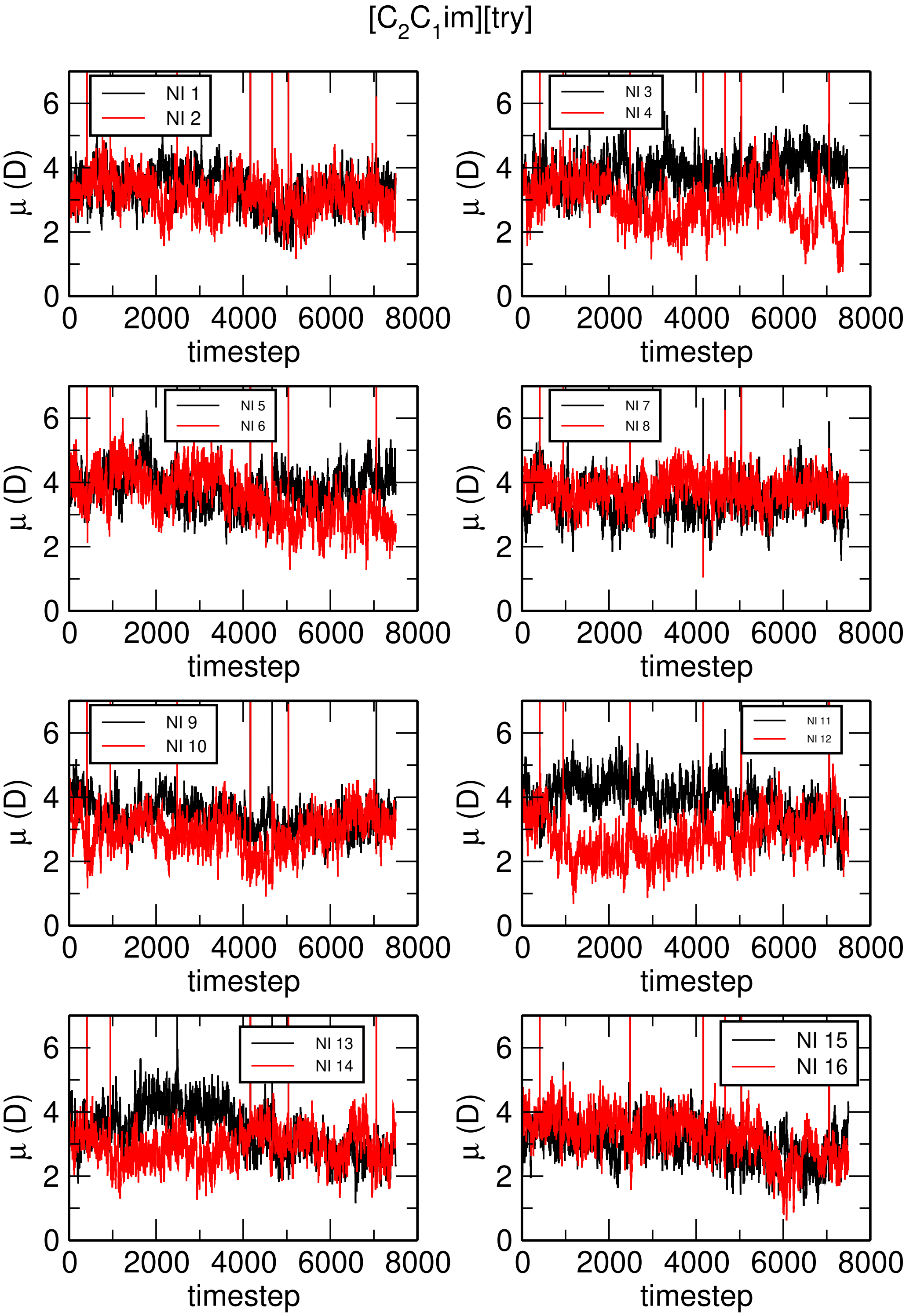

Figure 9: The every time development of the dipole moment (μ) of one randomly selected ion of cation in [C_2C_1Im][trp].

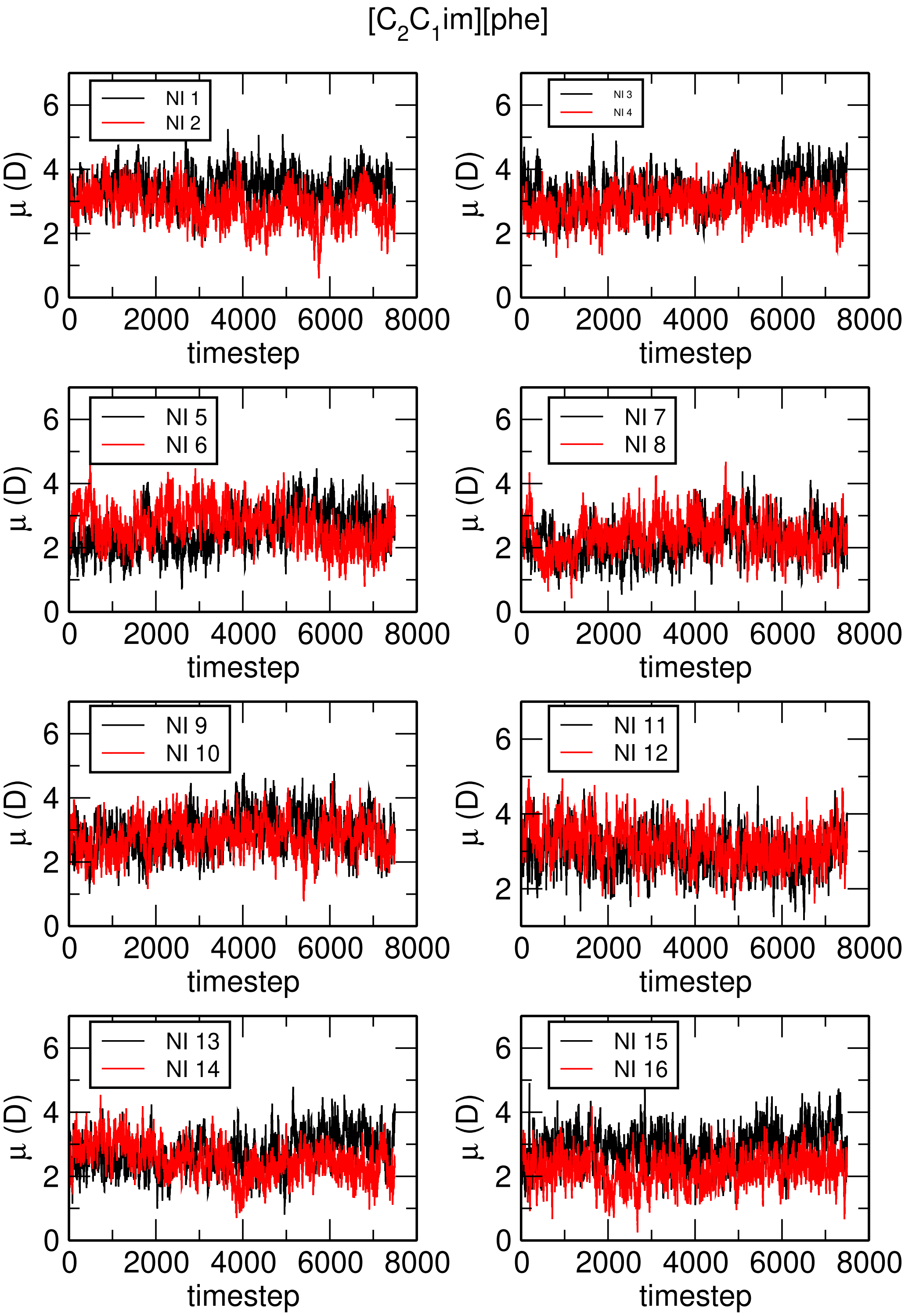

Figure 10: The every time development of the dipole moment (μ) of one randomly selected ion of cation in [C_2C_1Im][phe].

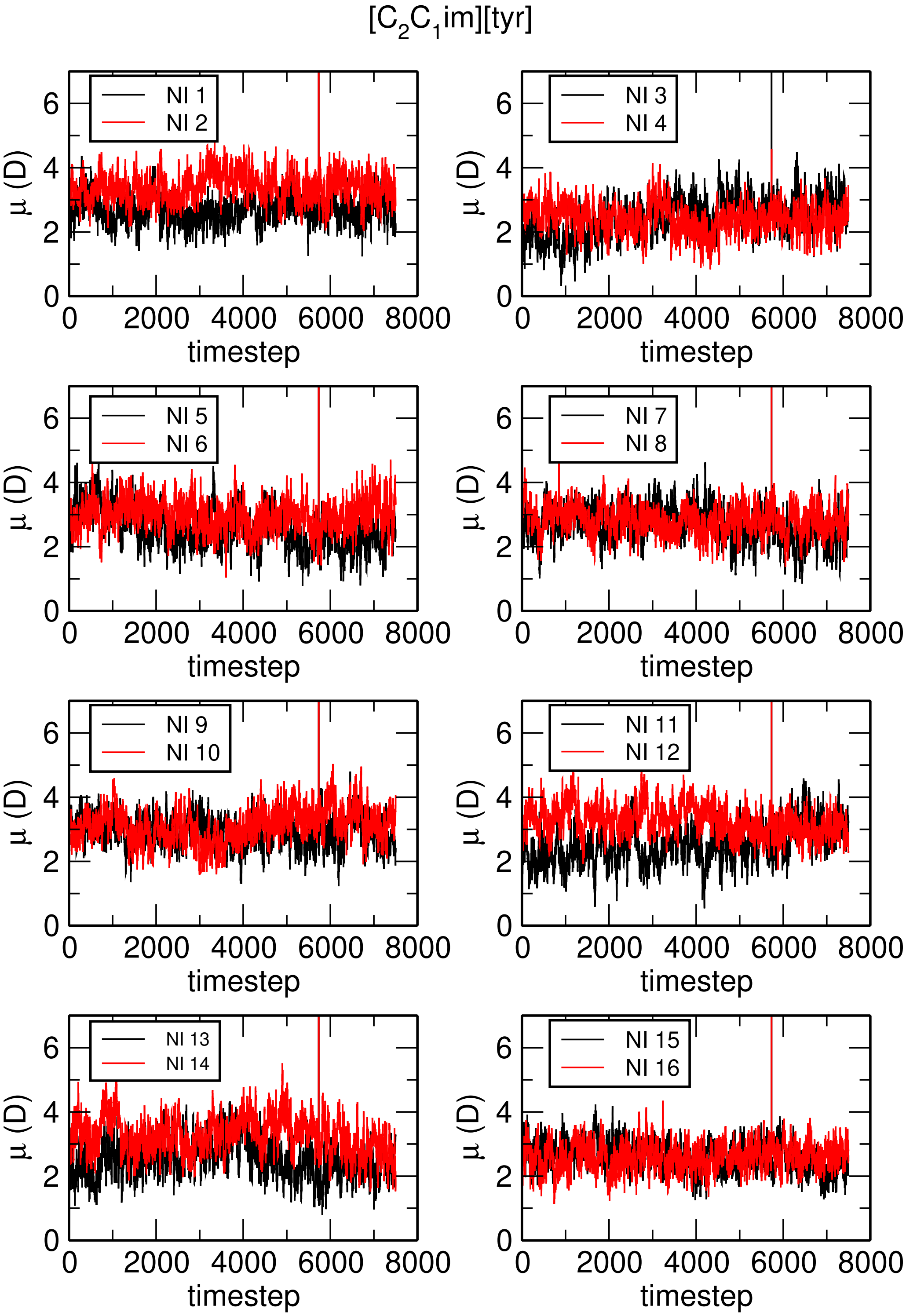

Figure 11: The every time development of the dipole moment (μ) of one randomly selected ion of cation in [C_2C_1Im][tyr].

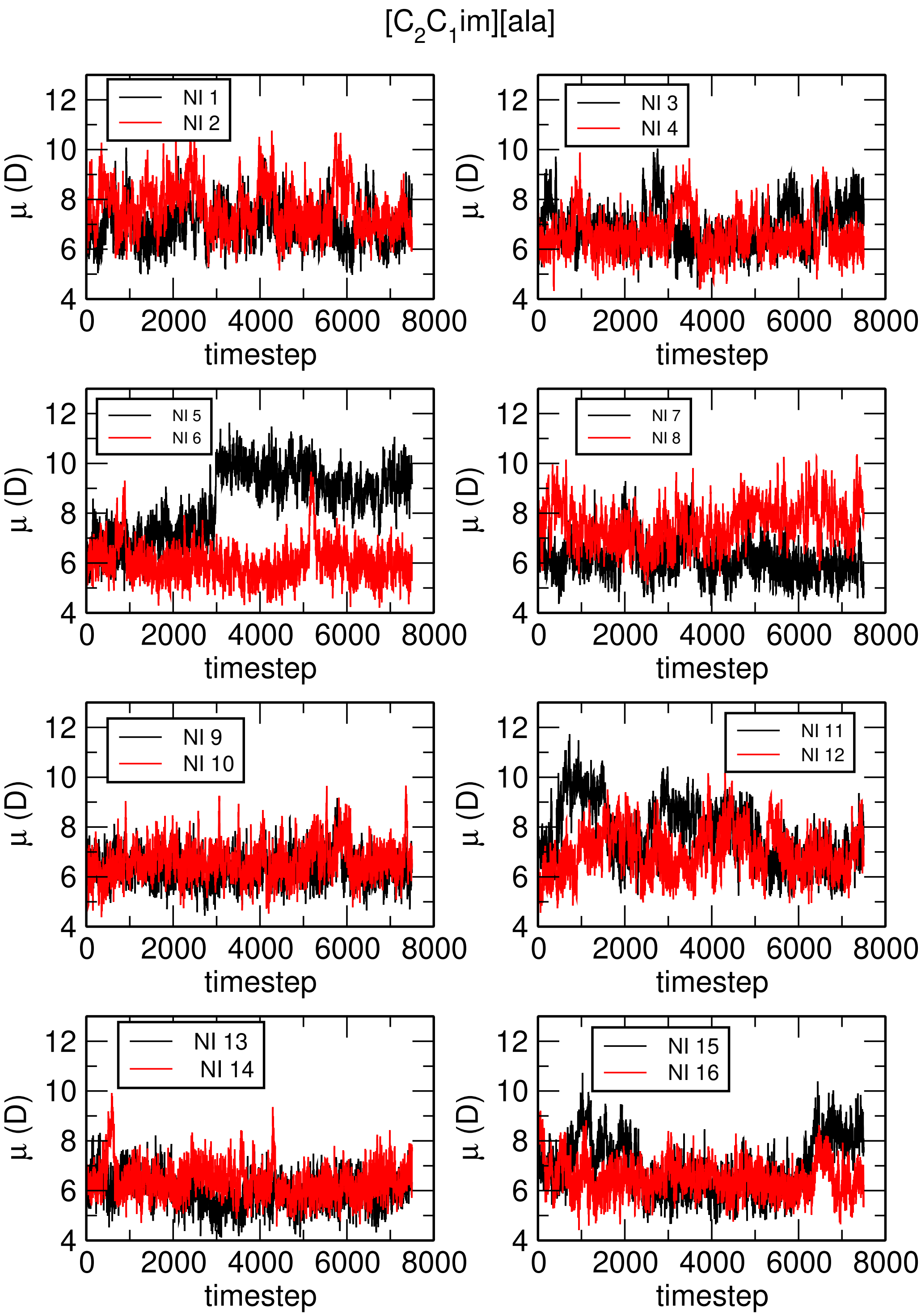

Figure 12: The every time development of the dipole moment (μ) of one randomly selected ion of anion in [C_2C_1Im][ala].

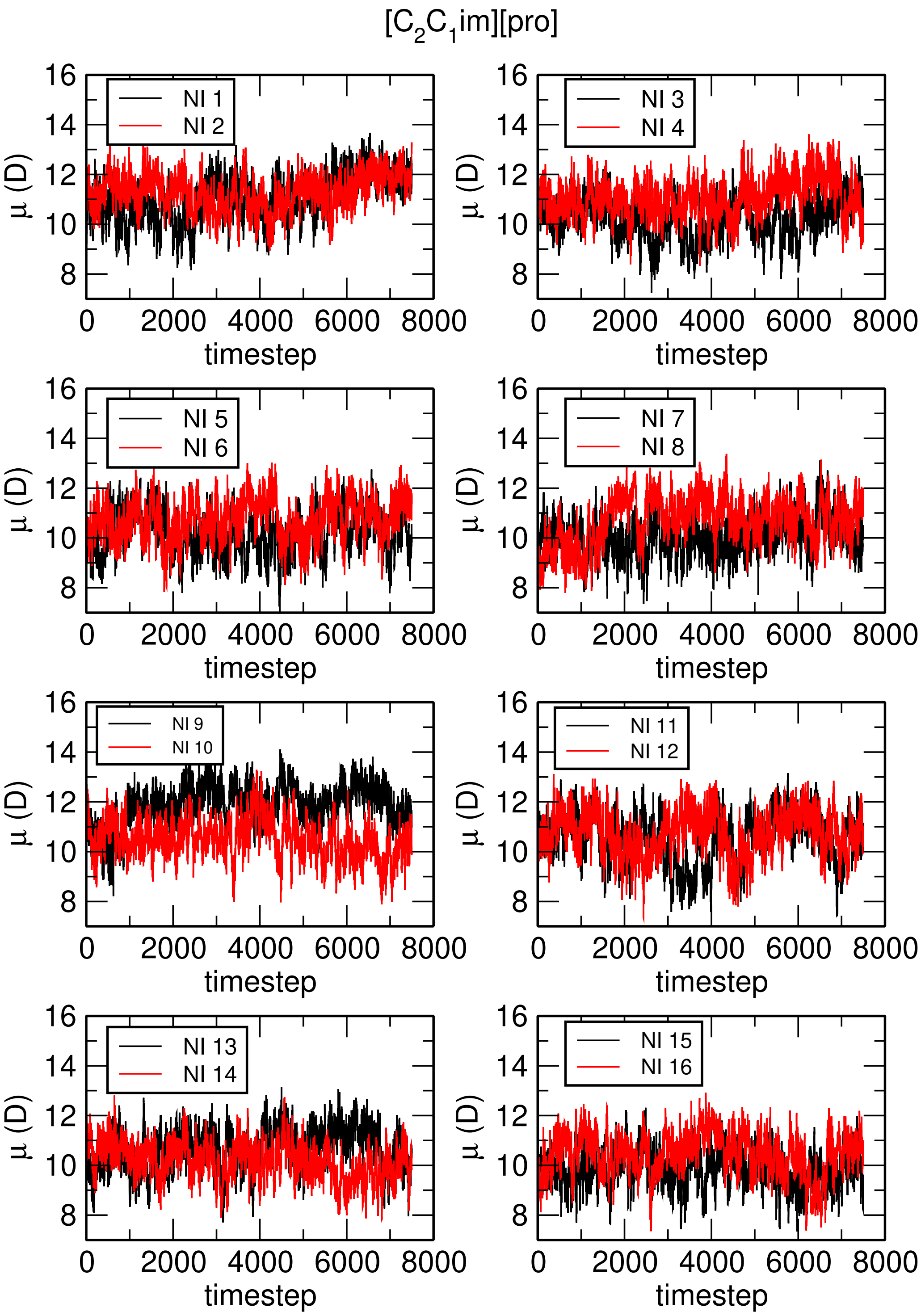

Figure 13: The every time development of the dipole moment (μ) of one randomly selected ion of anion in [C$_2$C$_1$Im][pro].

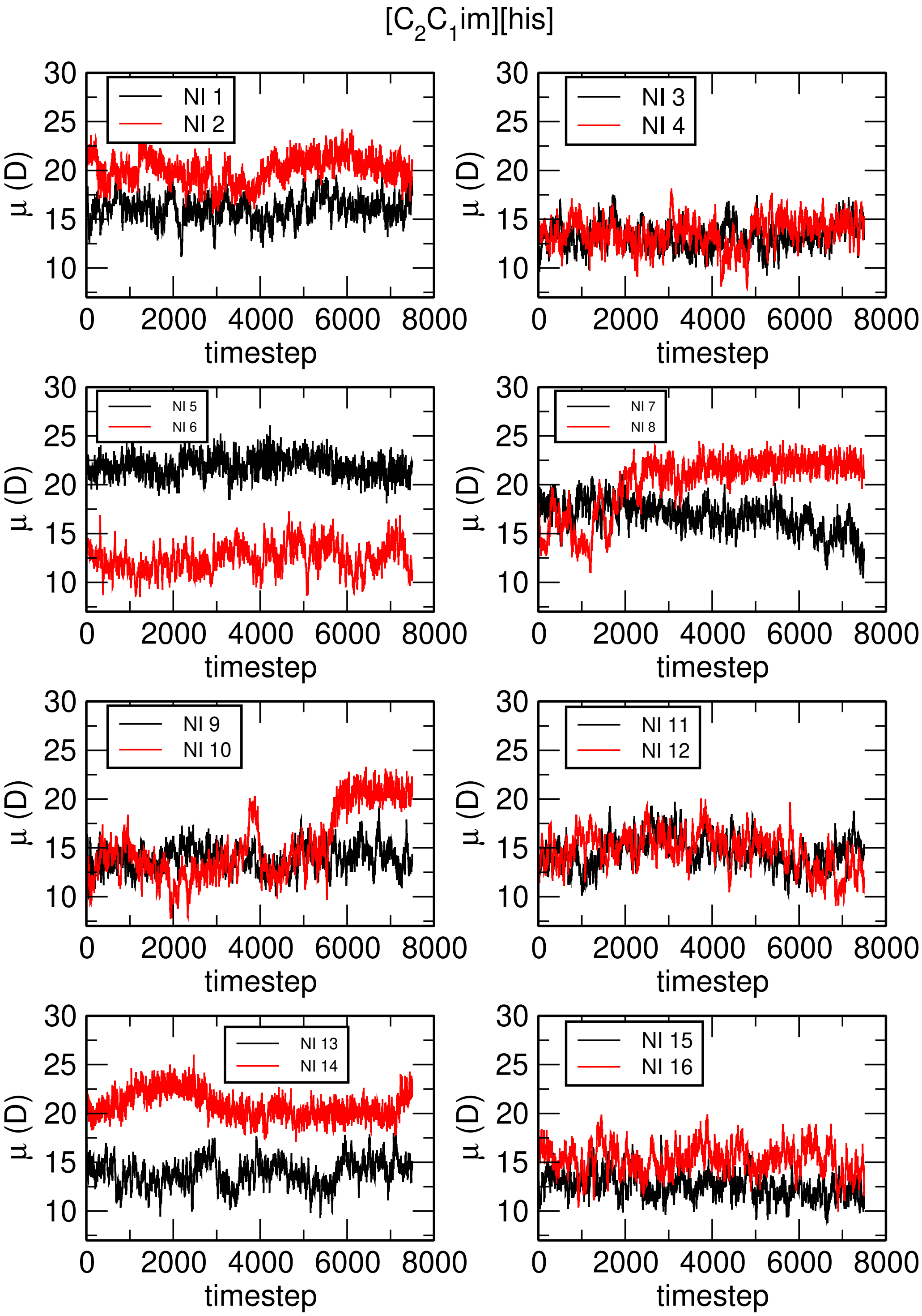

Figure 14: The every time development of the dipole moment (μ) of one randomly selected ion of anion in [C_2C_1Im][his].

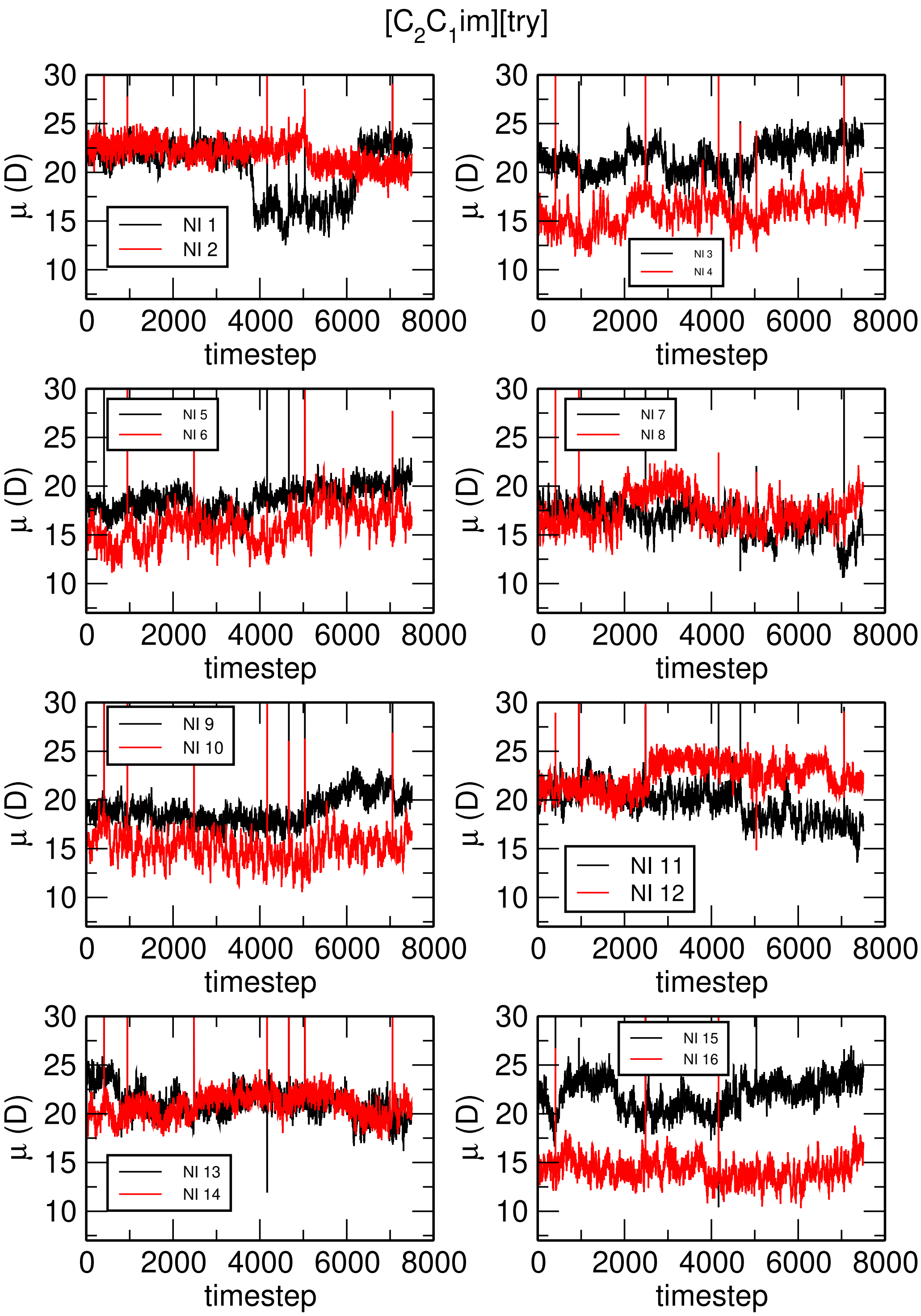

Figure 15: The every time development of the dipole moment (μ) of one randomly selected ion of anion in [C$_2$C$_1$Im][trp].

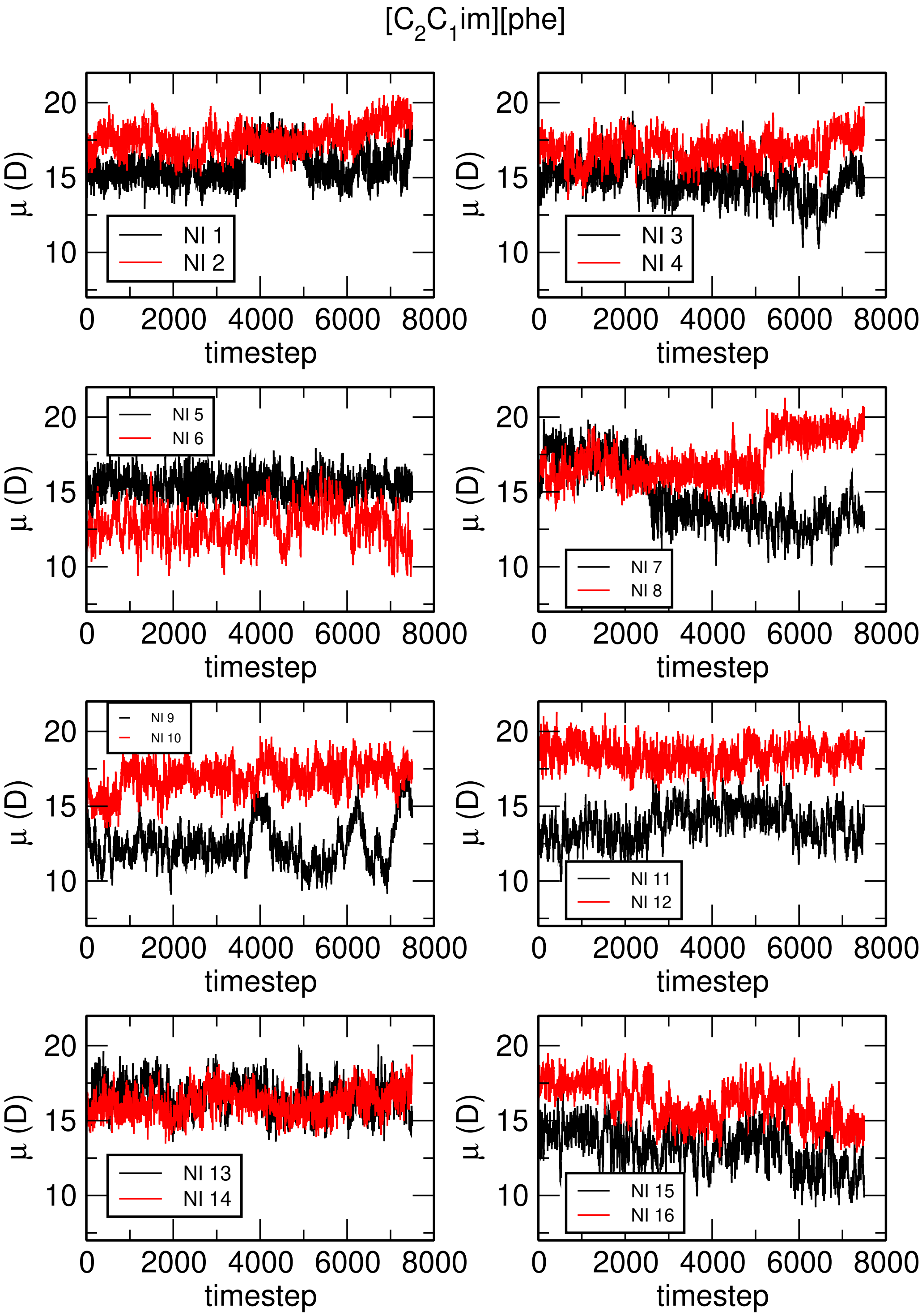

Figure 16: The every time development of the dipole moment (μ) of one randomly selected ion of anion in [C$_2$C$_1$Im][phe].

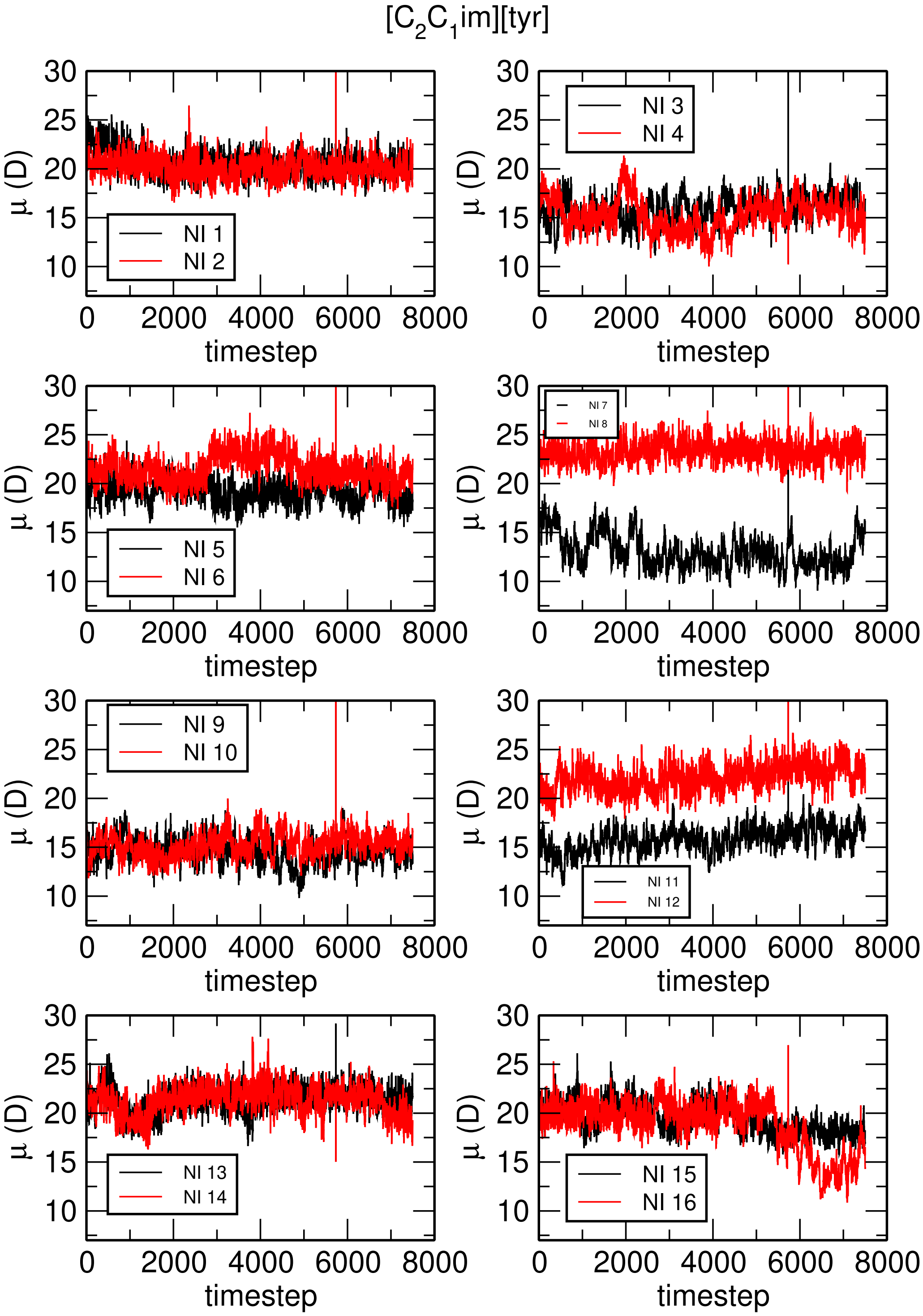

Figure 17: The every time development of the dipole moment (μ) of one randomly selected ion of anion in [C$_2$C$_1$Im][tyr].