Electronic Supplementary Material (ESI) for Soft Matter.

Supporting Information

Hydrophobic domains of amphiphilic polymeric nanoparticles: Probing self-assembly dynamics and interior structure by fluorescence spectroscopy and molecular dynamics simulations

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1. ^{1}H NMR spectra of HA amphiphiles

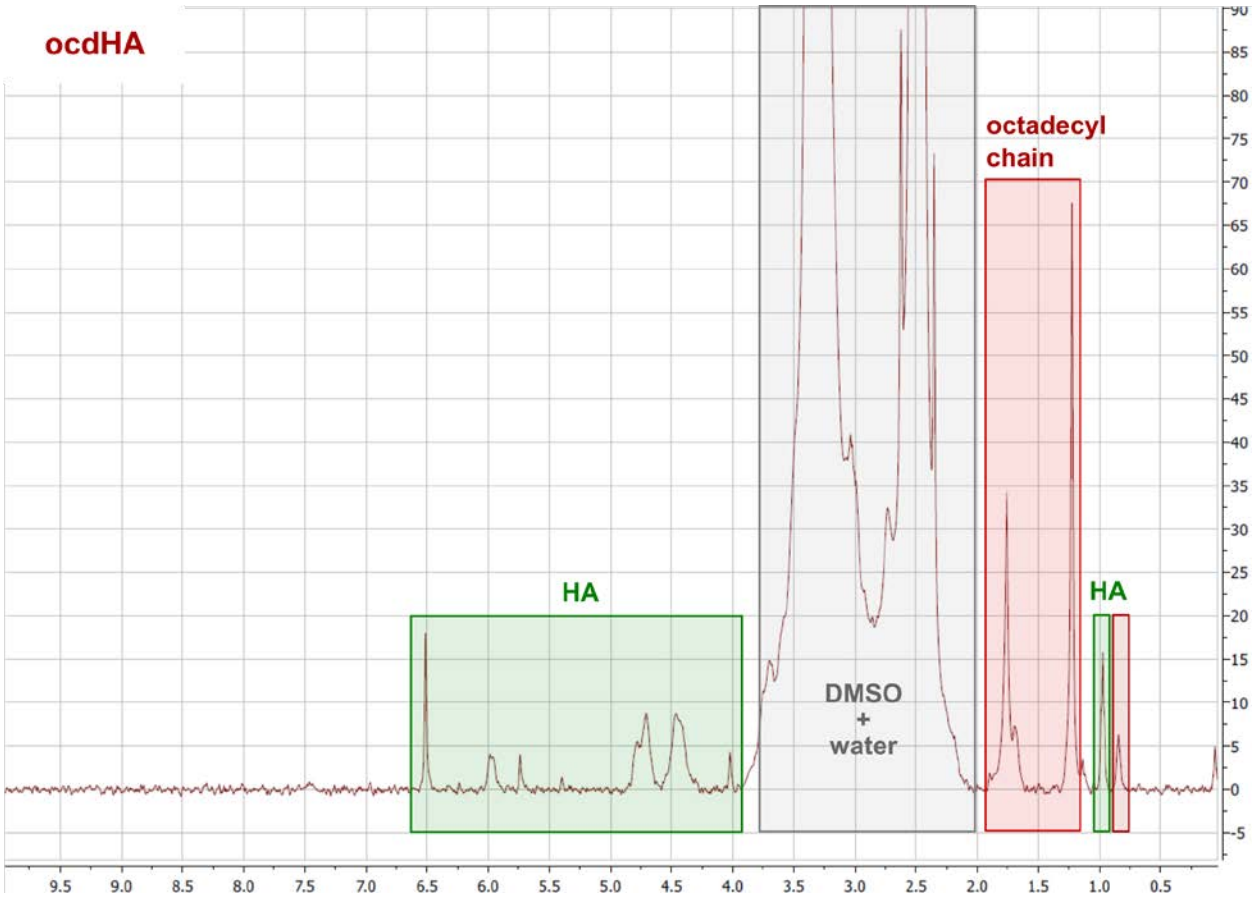

Figure S1. ^{1}H NMR spectrum of ocdHA.

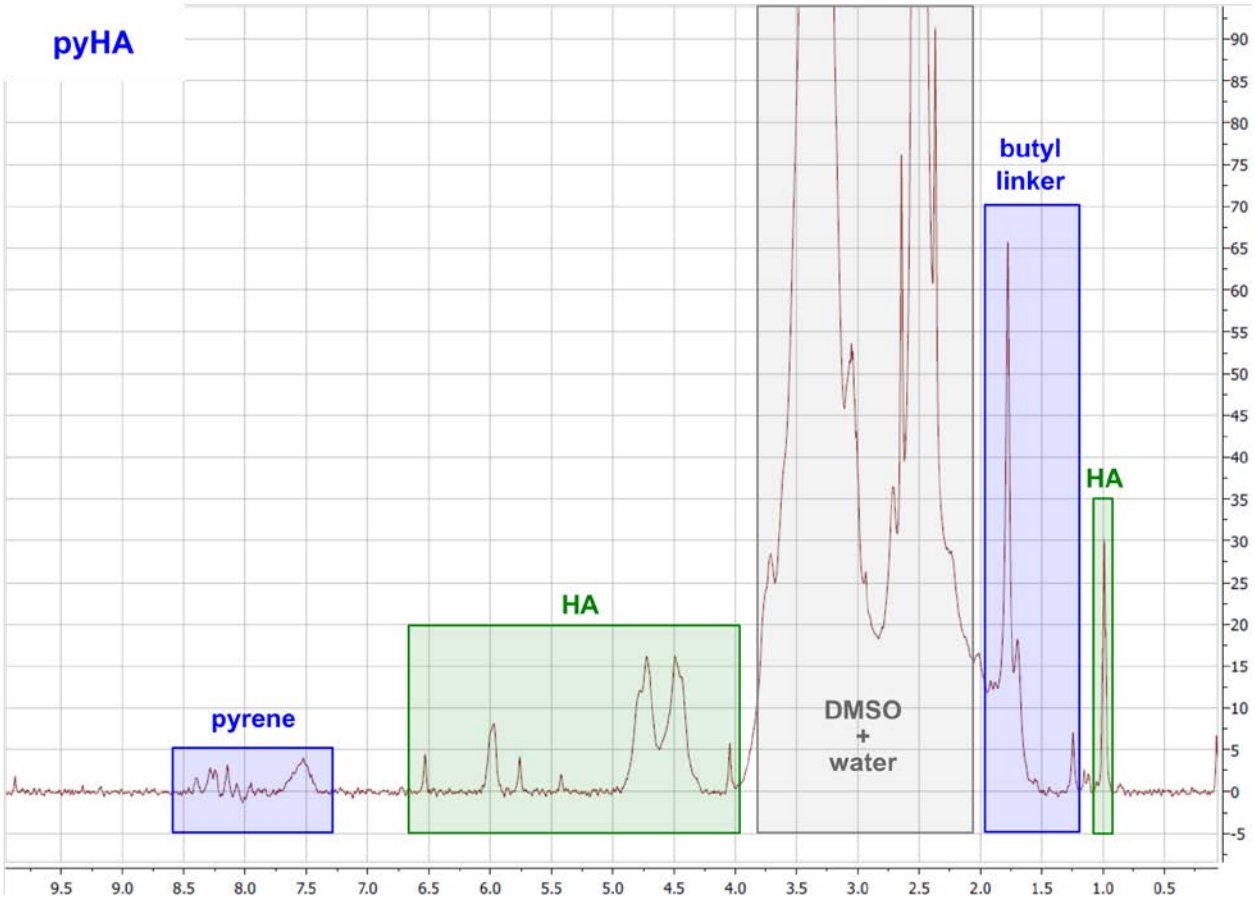

Figure S2. ^{1}H NMR spectrum of pyHA.

2. Simulations of ocdHA and pyHA self-assembly

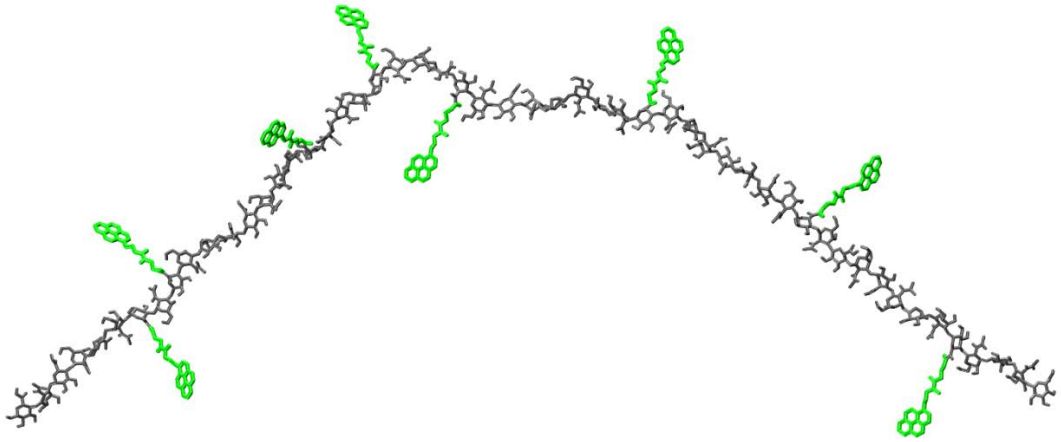

Figure S3. Structure of 10 kDa pyHA. The pyrenyl-butanamide fragments located at the randomly selected positions are shown in *green*.

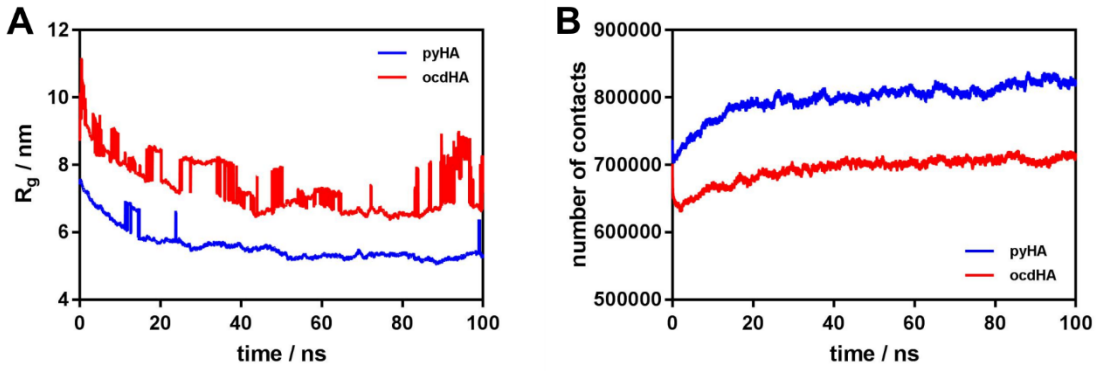

Figure S4. Dynamics of radius of gyration **(A)** and polymer-polymer contacts **(B)** during 100 ns of MD simulations of the system consisting of 22 molecules of modified 10 kDa HA.

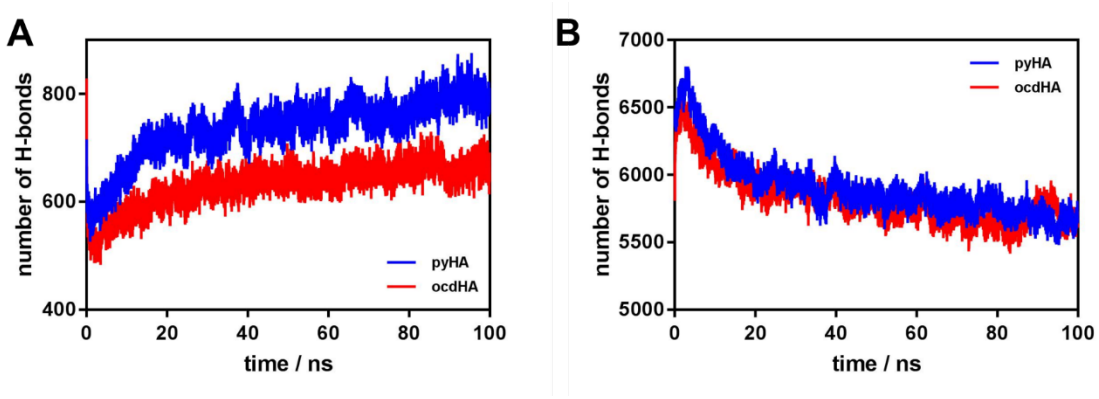

Figure S5. Dynamics of polymer-polymer **(A)** and polymer-water **(B)** hydrogen bonds during 100 ns of MD simulations of the system consisting of 22 molecules of modified 10 kDa HA.

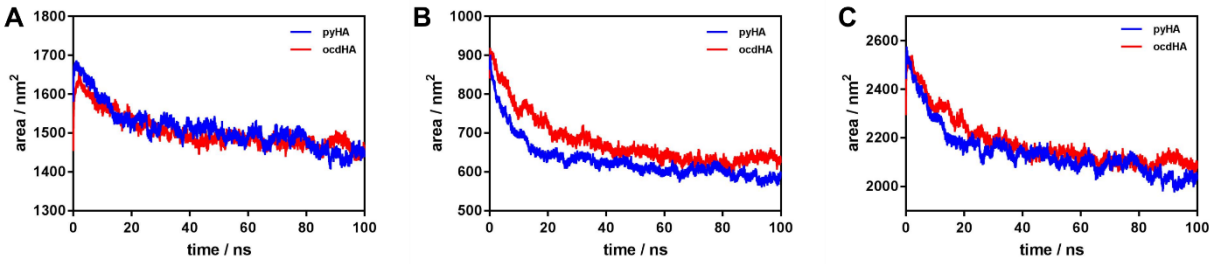

Figure S6. Dynamics of hydrophilic **(A)**, hydrophobic **(B)** and total **(C)** solvent-accessible surface during 100 ns of MD simulations of the system consisting of 22 molecules of modified 10 kDa HA.

3. Spectral properties of the dyes

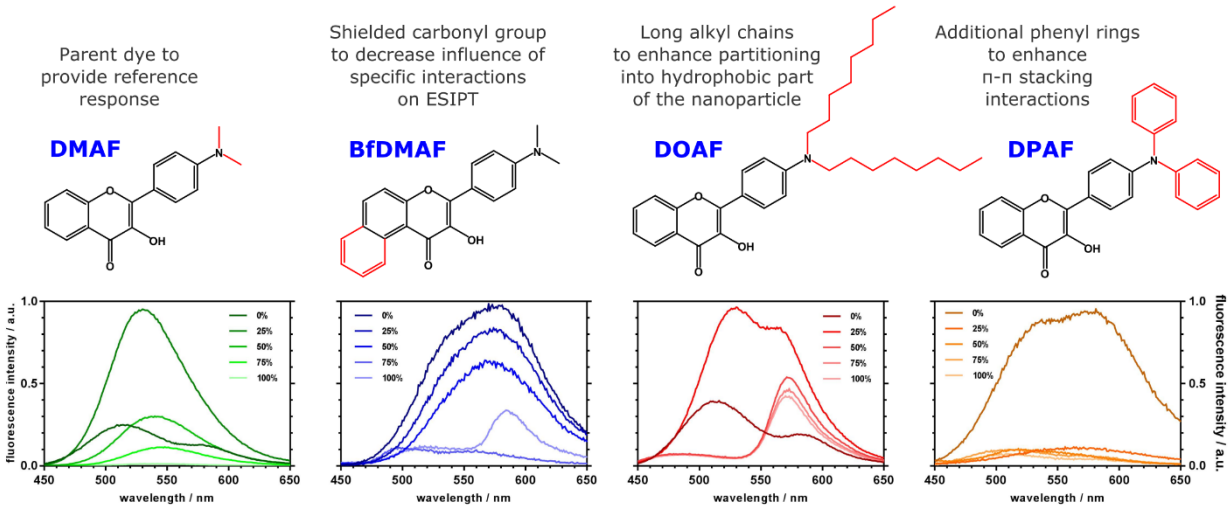

Figure S7. Structures of the dyes used for probing the interior of modified HA nanoparticles (top) and their fluorescence spectra in DMSO-water binary systems (bottom, water content is shown in the legends).

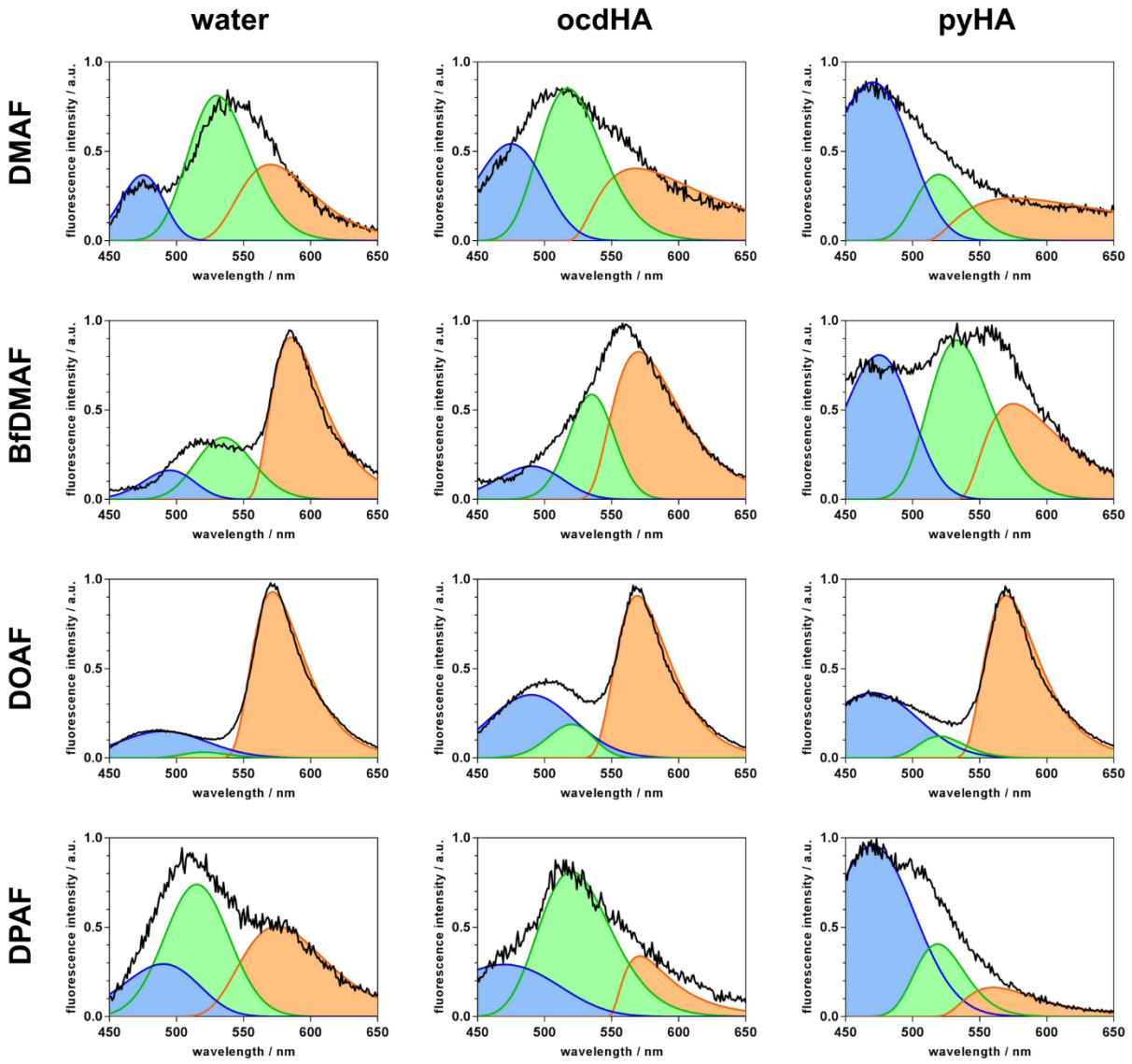

Figure S8. Spectral deconvolution of the emission spectra represented in the Figure 6. Calculated emissions for individual spectral components are colored in blue (normal form, N*), green (anionic form, A*), and orange (phototautomeric form, T*).

4. Simulations of dye-polymer systems

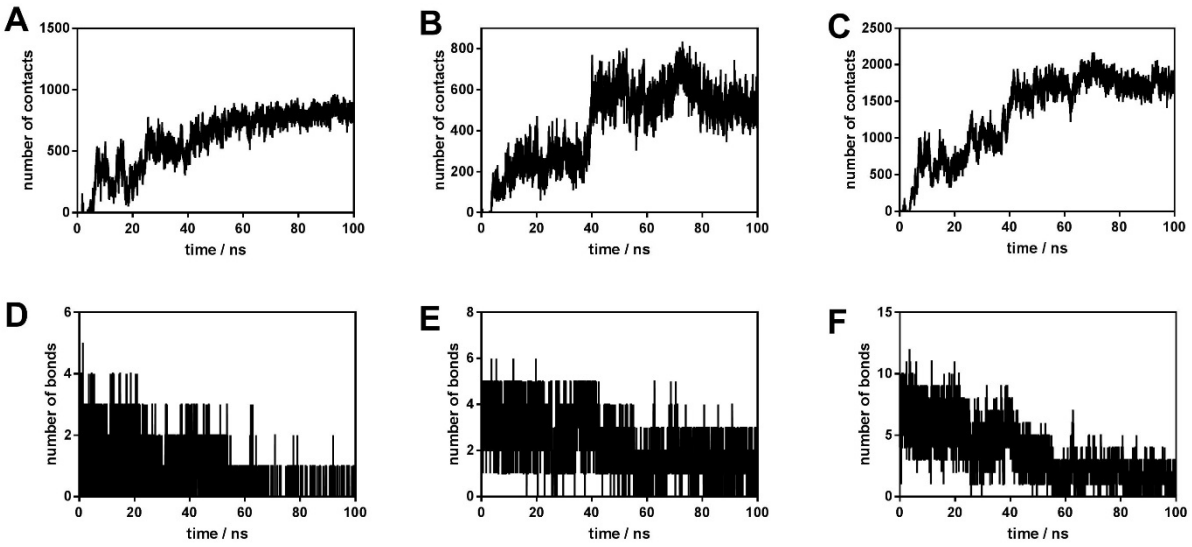

Figure S9. Dynamics of hydrophilic **(A)**, hydrophobic **(B)**, and total **(C)** dye-polymer contacts, hydroxyl-water **(D)**, carbonyl-water **(E)**, and total **(F)** dye-water hydrogen bonds during 100 ns of MD simulations of the system consisting of 2 molecules of DOAF and 4 molecules of ocdHA.

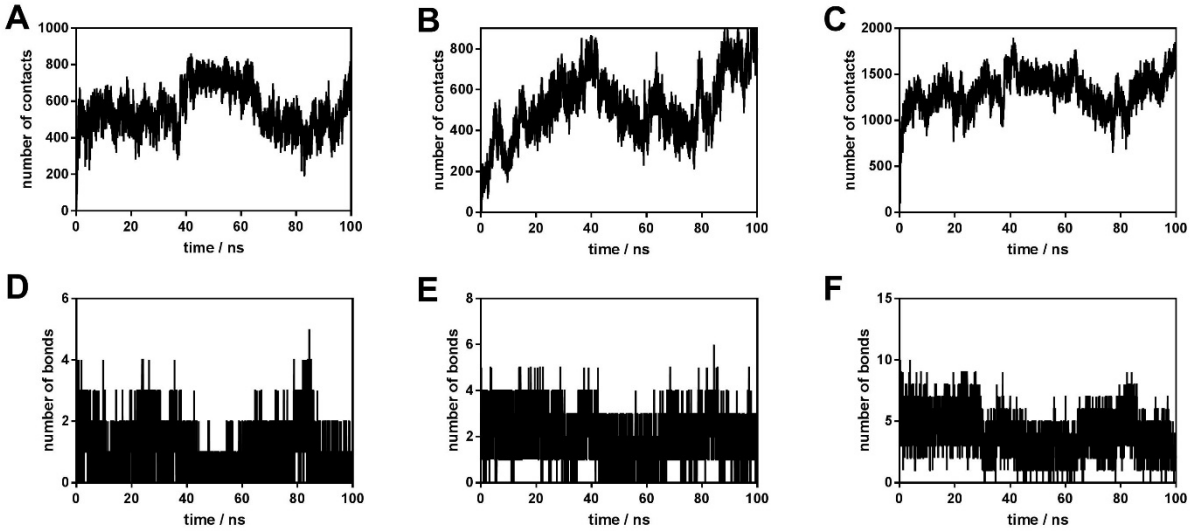

Figure S10. Dynamics of hydrophilic **(A)**, hydrophobic **(B)**, and total **(C)** dye-polymer contacts, hydroxyl-water **(D)**, carbonyl-water **(E)**, and total **(F)** dye-water hydrogen bonds during 100 ns of MD simulations of the system consisting of 2 molecules of DPAF and 4 molecules of ocdHA.

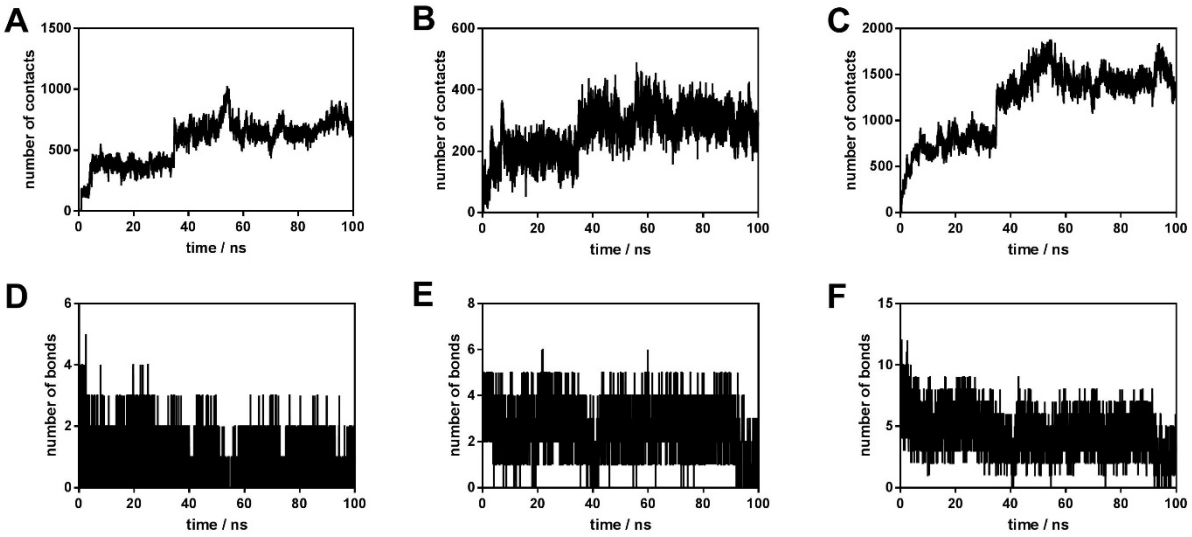

Figure S11. Dynamics of hydrophilic **(A)**, hydrophobic **(B)**, and total **(C)** dye-polymer contacts, hydroxyl-water **(D)**, carbonyl-water **(E)**, and total **(F)** dye-water hydrogen bonds during 100 ns of MD simulations of the system consisting of 2 molecules of DOAF and 4 molecules of pyHA.

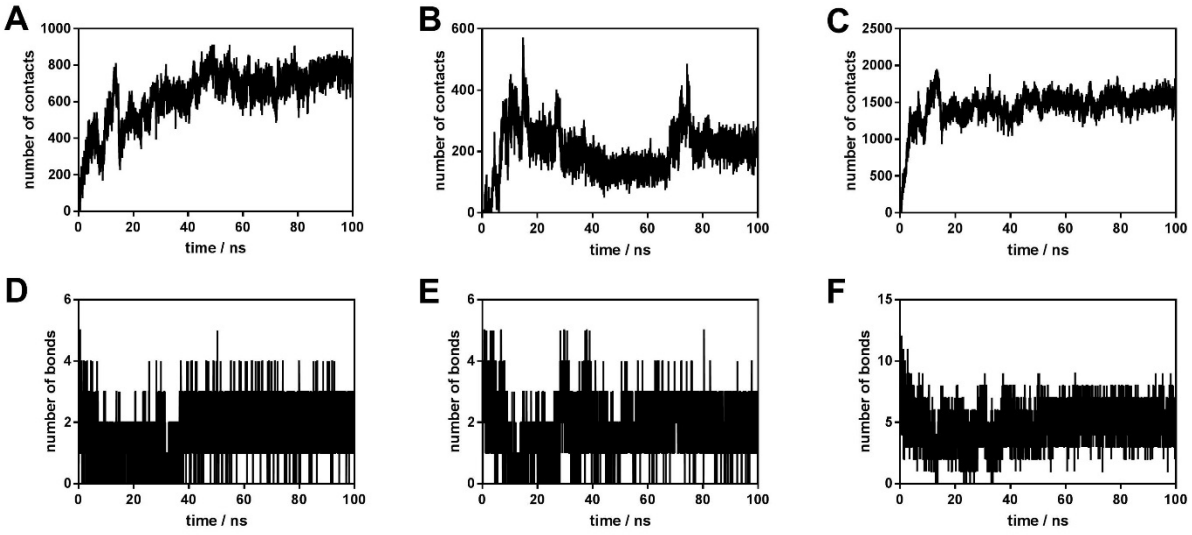

Figure S12. Dynamics of hydrophilic **(A)**, hydrophobic **(B)**, and total **(C)** dye-polymer contacts, hydroxyl-water **(D)**, carbonyl-water **(E)**, and total **(F)** dye-water hydrogen bonds during 100 ns of MD simulations of the system consisting of 2 molecules of DPAF and 4 molecules of pyHA.