MOLECULAR INTERACTIONS DRIVING THE COMPLEXATION OF ROSE BENGAL BY TRIAZINE-CARBOSILANE DENDRONS

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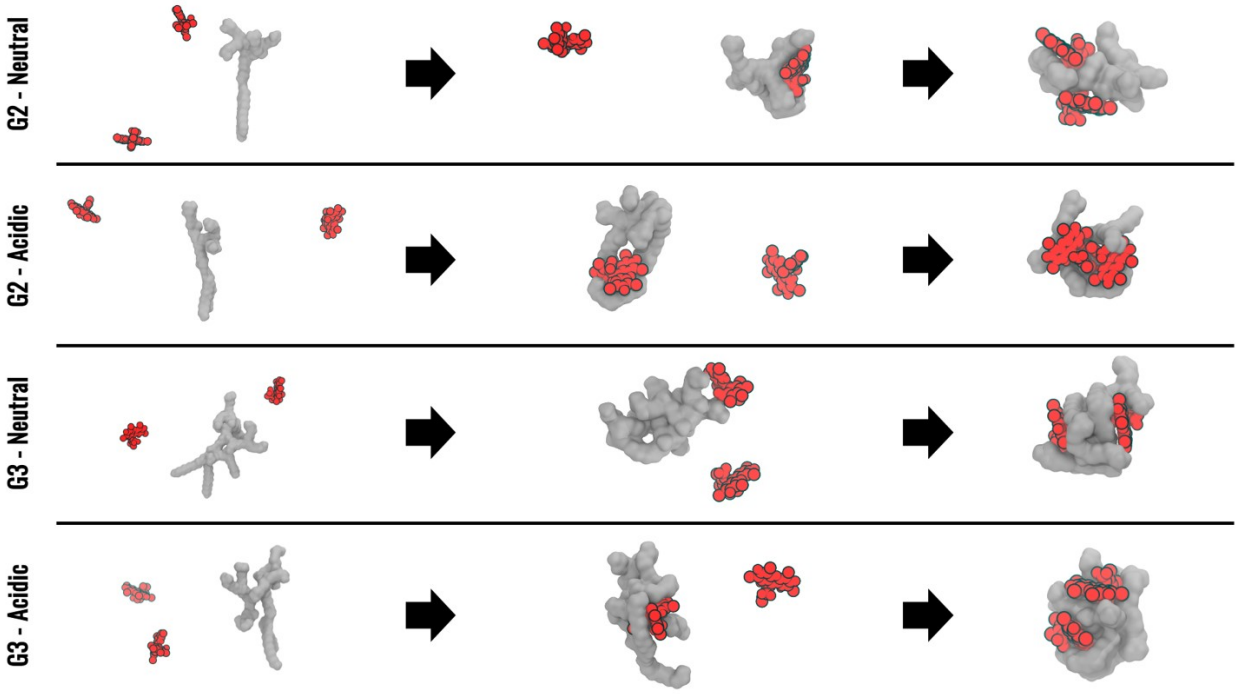
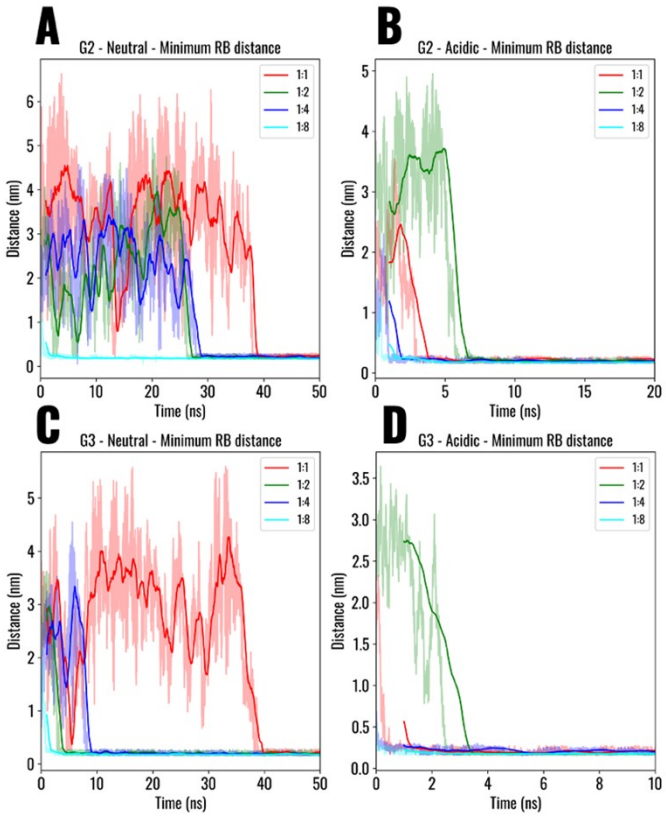
SUPPLEMENTARY INFORMATION



Supplementary Figure 1. Visualization of the process of dendron-RB complex formation at 1:2 stoichiometry, for different dendron generations and pH conditions. Left column represents initial configuration, prior to complex formation. Middle column reports snapshots during complex formation, with one RB molecule bound to the dendron. Rightmost column represents final snapshot of 2 RB molecules in complex with the dendrons. Dendrons shown in grey, RB molecules in red.



Supplementary Figure 2. Minimum distance vs. time between Rose Bengal atoms and dendron atoms. A: G2 – neutral pH; B: G2 – acidic pH; C: G3 – neutral pH; D: G3 – acidic pH. Solid line represents moving average over 1-ns windows. Raw data sampled every 2 ps shown as a faded line.

LIST OF SUPPLEMENTARY VIDEOS

SV1: rendering of MD simulation of system G2c

SV2: rendering of MD simulation of system G2_1:2

SV3: rendering of MD simulation of system G2_1:4

SV4: rendering of MD simulation of system G2ac

SV5: rendering of MD simulation of system G2a_1:2

SV6: rendering of MD simulation of system G2a_1:4

SV7: rendering of MD simulation of system G3c

SV8: rendering of MD simulation of system G3_1:2

SV9: rendering of MD simulation of system G3_1:4

SV10: rendering of MD simulation of system G3ac

SV11: rendering of MD simulation of system G3a_1:2

SV12: rendering of MD simulation of system G3a_1:4