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Supporting Information

Intrinsic acetamide brush-off by polyurea biodendrimers

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Fig. S1 Acetamide crystals that crystalized out of a PURE_{G4} biodendrimer crude mixture.



Fig. S2 Root mean square deviation of simulated $PURE_{G4}$ biodendrimers at different pH values. Equilibration was achieved after approximately 10 ns.



Fig. S3 Interactions of ibuprofen with the $PURE_{G4}$ biodendrimer in the last snapshot. Several interactions are observed: terminal amines from multiple dendrimer branches with the carboxylic acid of ibuprofen, as well as bidentate bridges between the urea motif of $PURE_{G4}$ and the carboxylic acid of ibuprofen.



Fig. S4 Radial distribution of dendrimer branches, ibuprofen, and water molecules from the core of a $PURE_{G4}$ biodendrimer. Ibuprofen is majorly distributed at the terminal branches while water has a high penetration into the interior.