

## **Effect of model peptide on struvite mineralization and implication for pathological biomineralization**

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Pathological stones have been plaguing human beings since the beginning of civilization. To conquer these diseases, researchers have made many efforts to understand the mechanisms in stone formation and found that certain urinary proteins can efficiently inhibit stone formation. These discoveries are significant for developing effective stone disease therapies. However, the crystallization inhibition mechanism remains elusive. Herein, synthetic polyaspartic acid (PASP) was employed as a model biomacromolecule to understand the effect of urinary proteins on crystal growth and morphology evolution of struvite in ammonia diffusion system. The results demonstrate that stereoselective recognition and binding of PASP onto (010) faces and (101) faces of struvite crystals result in arrowhead-shaped morphology, which further evolves into X-shaped and unusual tabular structures with time. Noticeably, these morphologies are reminiscent of biogenic struvite morphology. In addition, concentration-dependent experiments show that PASP can inhibit struvite growth and the inhibitory capacity increases with PASP concentration increasing, while aspartic acid monomers show no detectable effect. Considering that PASP is structural and functional analogues of subdomains of aspartic acid-rich proteins, our results reveal that aspartic acid-rich proteins play a key role in regulation of biogenic struvite morphogenesis, and aspartic acid residues conduce to the inhibitory capacity of urinary proteins. Therefore, our work provides a new insight into the mechanism of pathological biomineralization. Moreover, we believe that PASP can potentially be developed as a therapeutic agent for urinary stone disease based on its excellent properties.