Supporting Information

Elucidating the Mechanism of Nucleation Inhibition of Pathology Crystallization of Gout based on the evidence from Amorphous Form and in Solution

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Experimental

Materials. Uric acid (>99%), xanthine (>99%) were obtained from Sigma Aldrich and used without purification. Aqueous solutions were prepared using deionized water (18.2 MΩ) purified with a Nanjing Yipuyida purification system.

![Graph showing the solubility of urate in different concentrations of xanthine.]

Fig S1 Influence of xanthine in different added concentration on solubilities of MSUM at 15 °C (pH = 7.4) in the presence of 8mM MSUM and 150mM NaCl, with a typical standard deviation of 0.015 mg/100g of H₂O.
**Fig. S2.** Dynamic light scattering experiments were measured at 37 °C (pH = 7.4) in 10 mM MSUM solution in the presence of 150 mM NaCl and used as control samples. And the measurements were performed at a solution in the presence of 150 mM NaCl, 10mM MSUM and 0.5 or 1mM xanthine (at 37 °C; pH = 7.4). Data are the average of more than three measurements using separately prepared samples. Error bars equal 2 standard deviation.

![Diagram of urate− and xanthine ion](image)

**Fig. S3** The urate− and xanthine ion of Natural Bond Orbital partial atomic charges. 

**Figure S4.** Optimized conformations and their binding energies (kcal mol⁻¹) of different structures of dimers in solute-solute system in presence of Na ion.
Figure S5. Optimized conformations and their binding energies (kcal mol$^{-1}$) of different structures of dimers in solute-xanthine system in presence of Na ion.

References