

Supporting Information

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

*Dan Zhou[#], Shiqi Jiao, Pengfei Zhang[#], Yige Jin, Yonglan Pan, Chunyan Ou, Xingde Zhang, Tingming Fu, and Yonghai Liu**

School of Pharmacy, Nanjing University of Chinese Medicine, Nanjing 210046, China

liuyh@njucm.edu.cn

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 M Ω) purified with a Nanjing Yipuyida purification system.

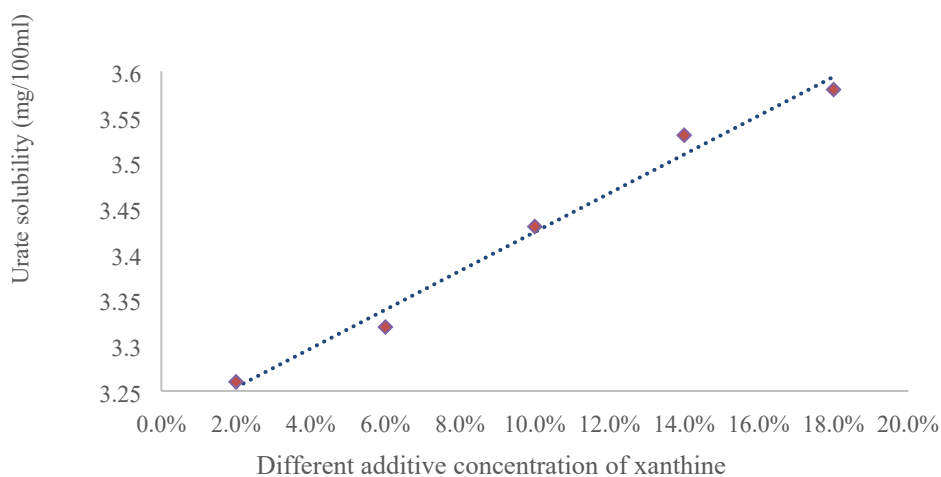


Fig S1 Influence of xanthine in different added concentration on solubilities of MSUM at 15 °C (pH = 7.4) in the presence of 8mM MSUM and 150mM NaCl, with a typical standard deviation of 0.015 mg/100g of H₂O.

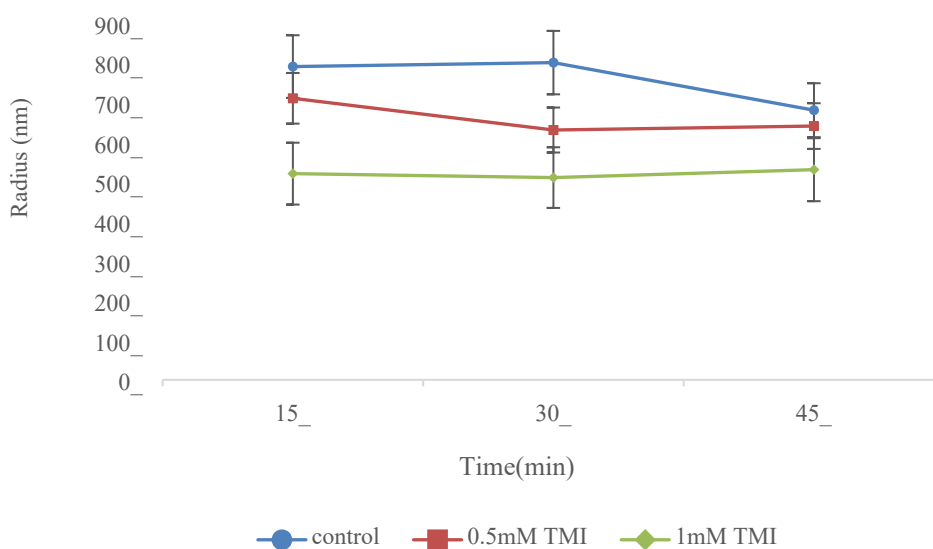


Fig. S2. Dynamic light scattering experiments were measured at 37 °C (pH = 7.4) in 10 mM MSUM solution in the presence of 150 mM NaCl and used as control samples. And the measurements were performed at a solution in the presence of 150 mM NaCl, 10mM MSUM and 0.5 or 1mM xanthine (at 37 °C; pH = 7.4). Data are the average of more than three measurements using separately prepared samples. Error bars equal 2 standard deviation.

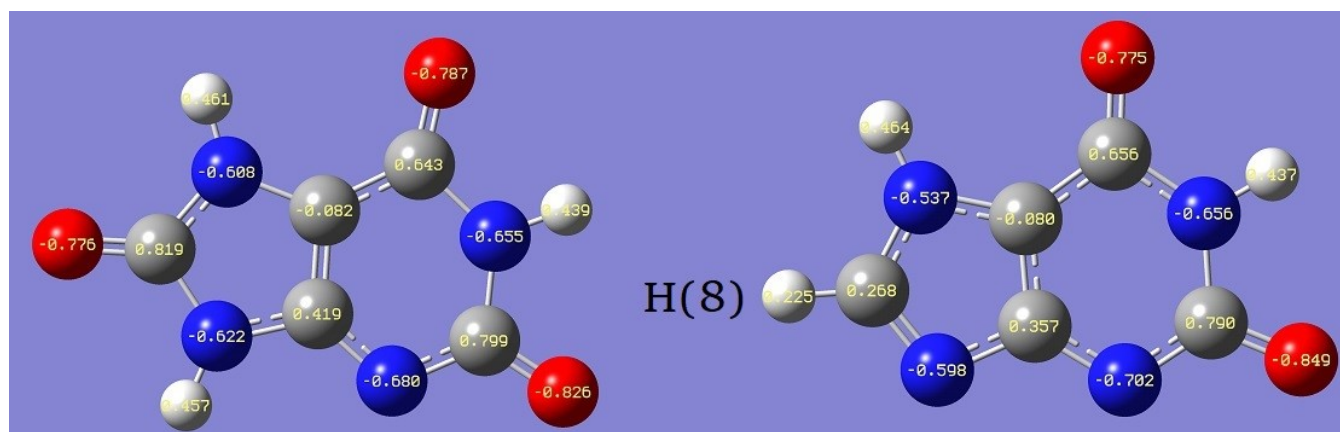


Fig. S3 The urate⁻ and xanthine ion of Natural Bond Orbital partial atomic charges. ^[1]

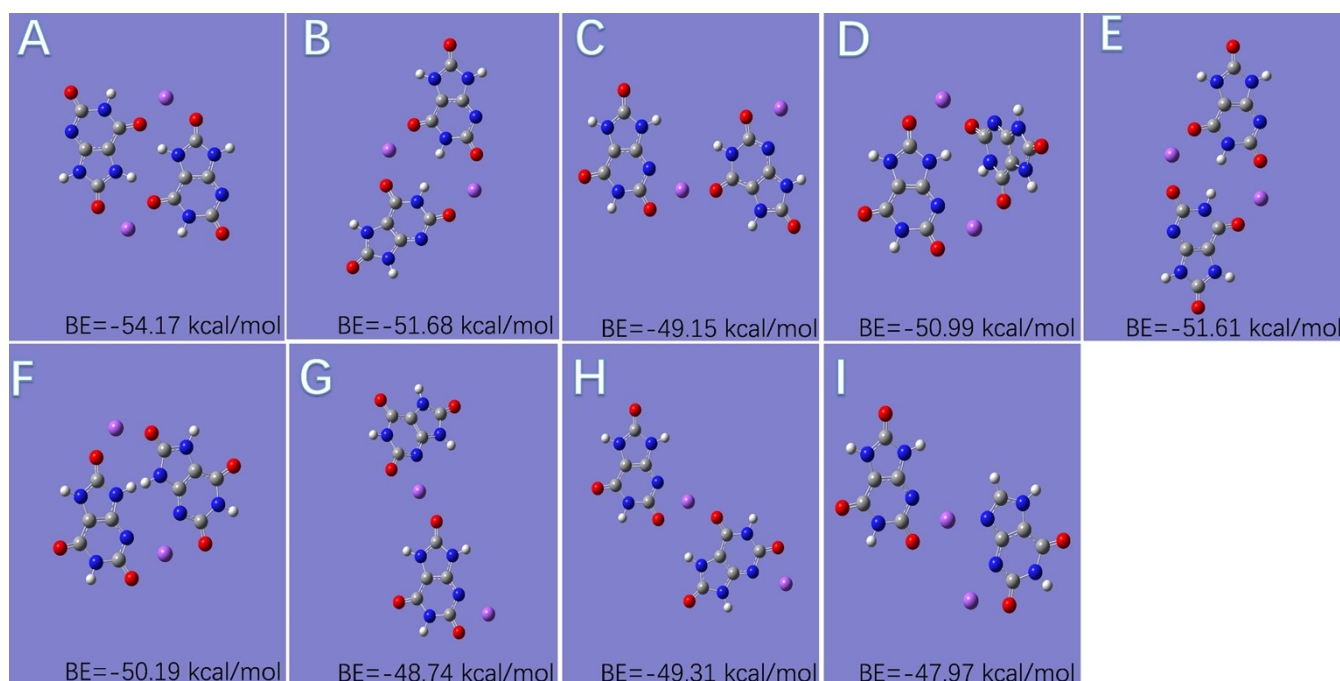


Figure S4. Optimized conformations and their binding energies (kcal mol⁻¹) of different structures of dimers in solute-solute system in presence of Na ion.

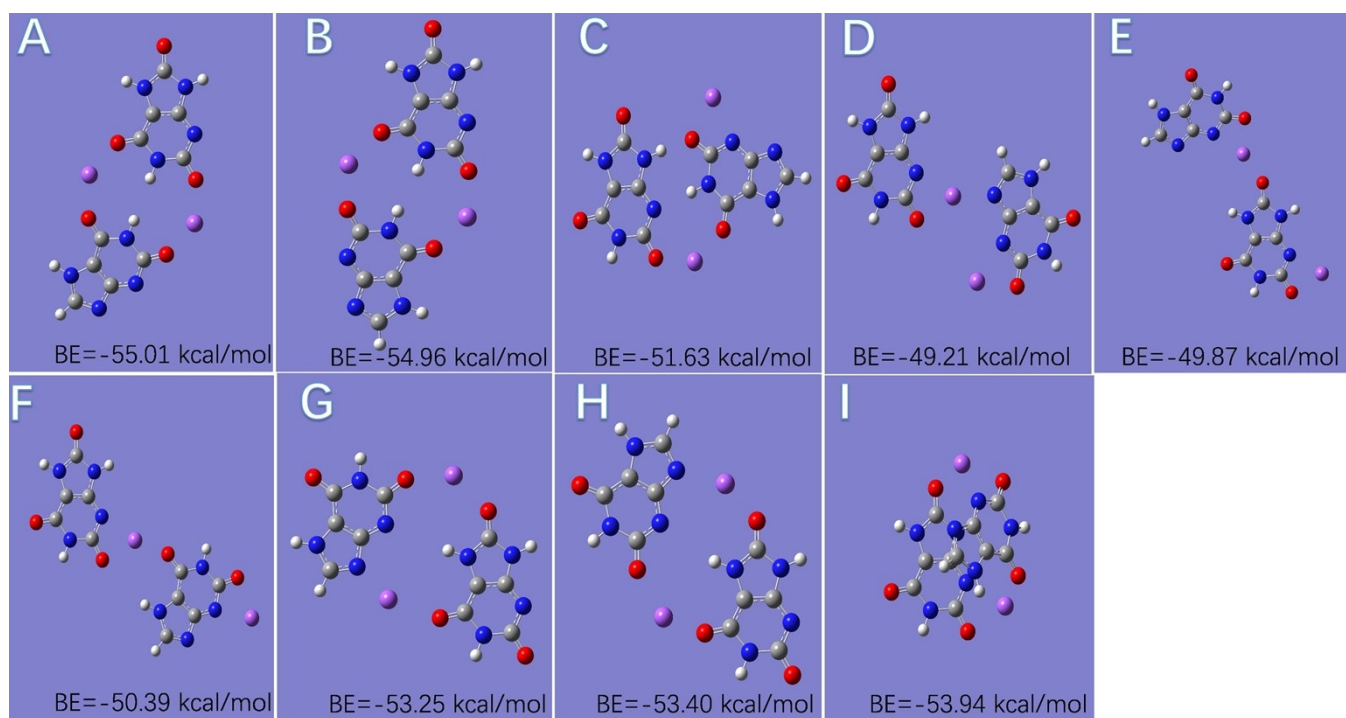


Figure S5. Optimized conformations and their binding energies (kcal mol^{-1}) of different structures of dimers in solute-xanthine system in presence of Na ion.

References

- [1] M. J. Frisch, et al. Gaussian 09, Gaussian Inc., Wallingford, CT, 2009.