Electronic Supplementary Information

The Miscibility and Solubility of Uric Acid and Vitamin C in the Solution Phase and Their Structural Alignment in the Solid-Liquid Interface

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(Dated: May 28, 2021)

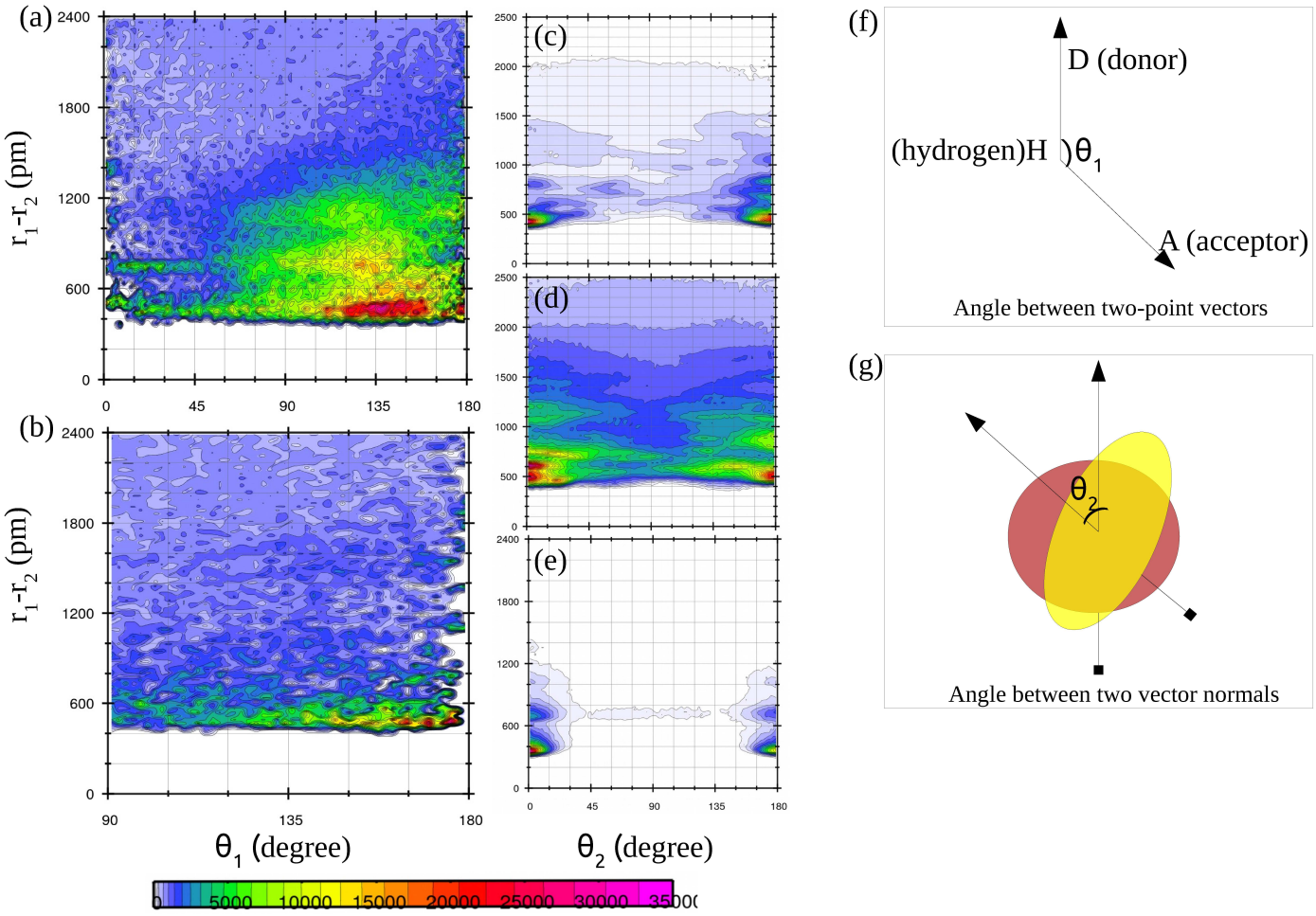


FIG. S1: The distribution of orientational angle between (a) UA and Vit-C molecules and (b) Vit-C and Vit-C molecules considering two-point vectors of these two molecules. The angle between two vector normals is shown for (c) UA–Vit-C, (d) Vit-C–Vit-C, and (e) UA–UA interactions. (f) represents an angle between two-point vectors and (g) represents the approach of an angle between two vector normals. Here, both angles θ_1 and θ_2 are plotted against the COM-COM (center-of-mass) distance between any two molecules.

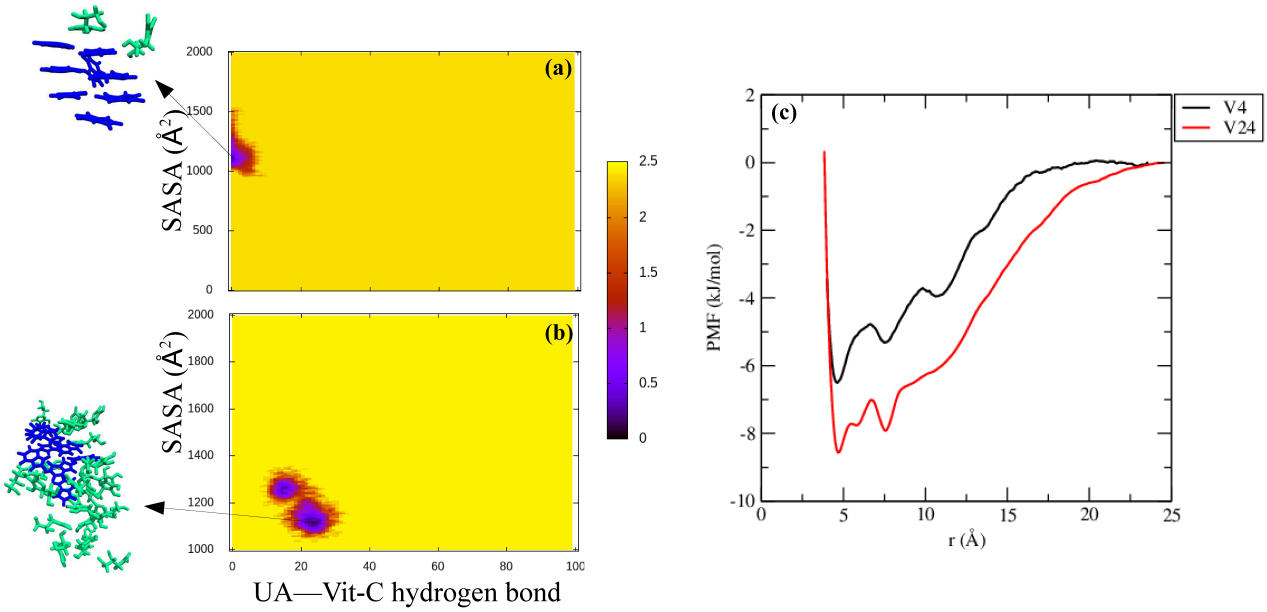


FIG. S2: Free energy landscapes for the solvent-accessible surface area (SASA ($\mathring{A}^2$)) for UA-UA aggregation versus UA–Vit-C hydrogen bonding for systems (a) V4 and (b) V24. The free energy in the color bar on the right side is manifested in kcal/mol unit. The analogous snaps are also conferred for UA (blue)—Vit-C (green) conjugate assemblages for these two systems. (c) presents the potentials of mean forces for UA–Vit-C interaction for systems V4 and V24.

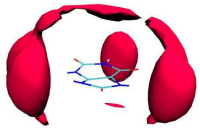
(a)

System	UA-UA	UA—Vit-C	Vit-C--Vit-C	UA-water	Vit-C--water
V0	1.60	--------	--------	9.55	--------
V4	1.59	0.17	0.02	9.25	32.59
V24	1.55	0.30	0.22	4.86	28.24

(b)

System	UA-water	Vit-C--water	water-water
V0	65.99	----------	3.75
V4	63.04	40.65	3.74
V24	37.13	201.50	3.71

(c)



(d)

(e)

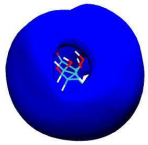


FIG. S3: (a) The first shell coordination number (CN) of various pairs, (b) the total number of hydrogen bonds for numerous couples, (c) the spatial density function of water around UA in system V0, (d) the spatial density function of water around UA in system V24, and (e) the spatial density function of the water around Vit-C in system V24.

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