

## **Supplemental Information**

### **Effects of the surface polarity of nanomaterials on their interaction with complement protein gC1q**

Shuai Wang,<sup>a,b</sup> Xinwen Ou,<sup>b</sup> Yanee Wutthinitikornkit,<sup>b</sup> Ming Yi,<sup>\*a,c</sup> Jingyuan Li<sup>\*b</sup>

Table S1. Partial charges,  $\sigma$  and  $\epsilon$  for atoms in epoxy and hydroxyl groups of GO.

Functional group	Atom	Charge (e)	$\sigma$ (nm)	$\epsilon$ (kJ·mol <sup>-1</sup> )
Hydroxyl	C	0.150	0.355	0.293
	O	-0.585	0.307	0.711
	H	0.435	0.000	0.000
Epoxy	C	0.200	0.350	0.276
	O	-0.400	0.290	0.586

Table S2. Number of residues on the surface of the ghB and ghC modules.

Binding module	Positively charged	Negatively charged	Polar	Non-polar
ghB module	14	8	21	18
ghC module	9	7	24	27

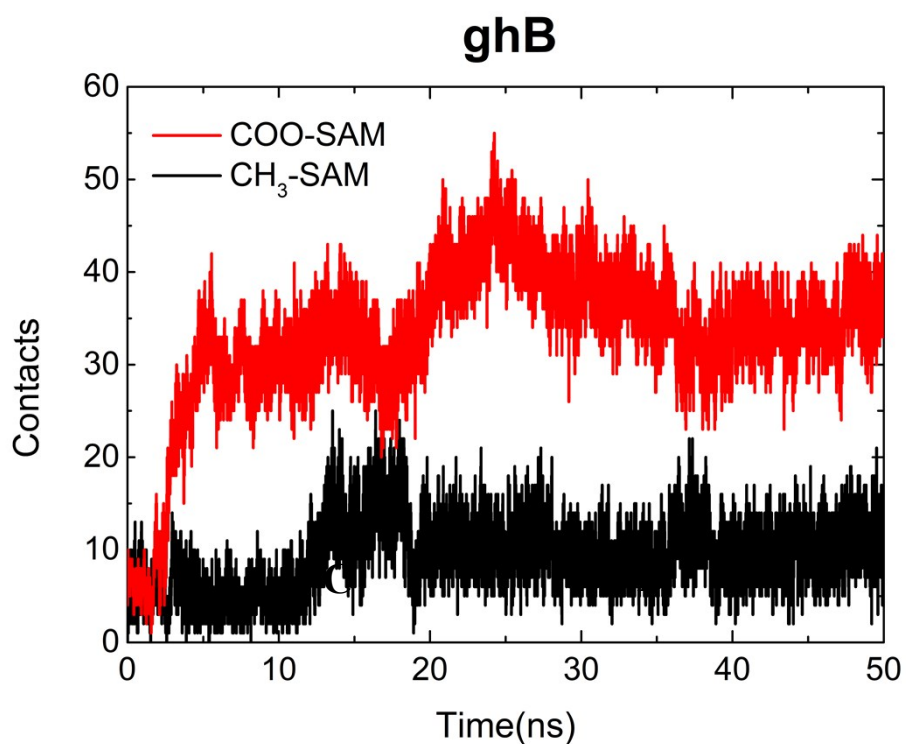


Fig. S1. The number of contact heavy atoms of gC1q (ghB) with SAMs with two different surfaces (i.e., CH<sub>3</sub>-SAM, COO-SAM).

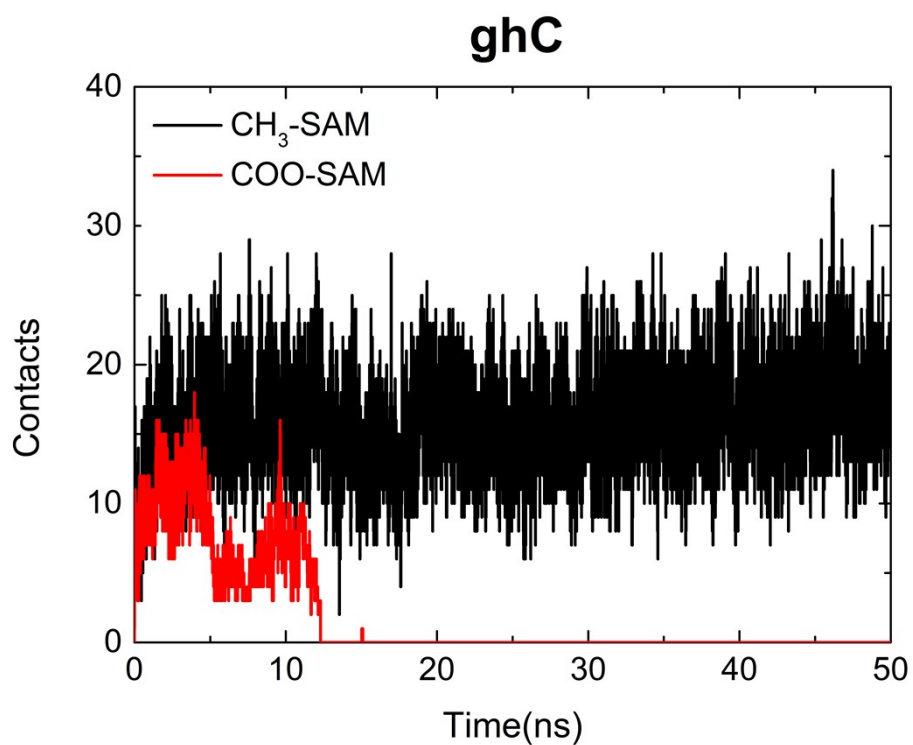


Fig. S2. The number of contact heavy atoms of gC1q (ghC) with SAMs with two different surfaces (i.e., CH<sub>3</sub>-SAM, COO-SAM).