Electronic Supplementary Information

S1. HPLC quantitative profiles

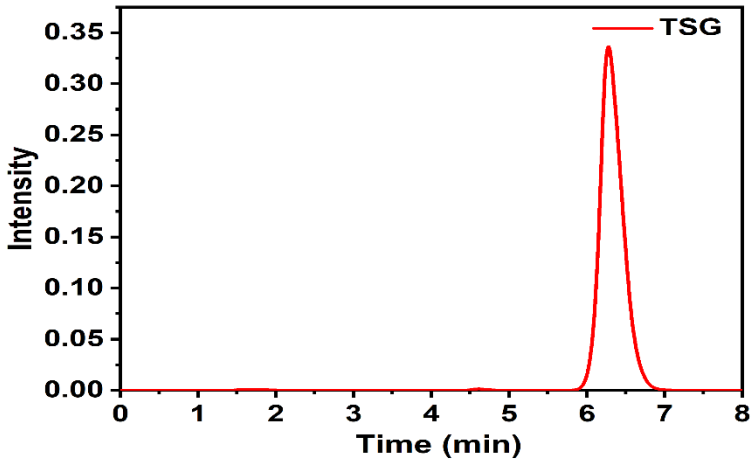

Figure S1. HPLC profile of TSG.

S2. The AFM characterization

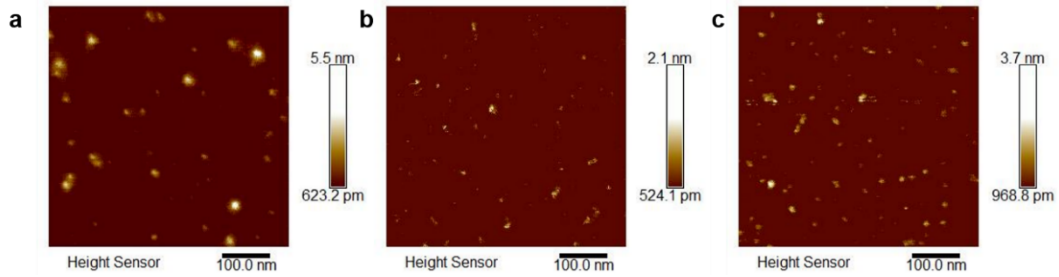

Figure S2. 2D view of AFM images: a) TSG; b) C3G; c) TSG/C3G.

Table S1 The roughness parameters from AFM

	R_g (nm)	R_a (nm)
TSG	0.210	0.158
TSG/C3G	0.394	0.286
C3G	0.459	0.317

S3. The SAXS profiles

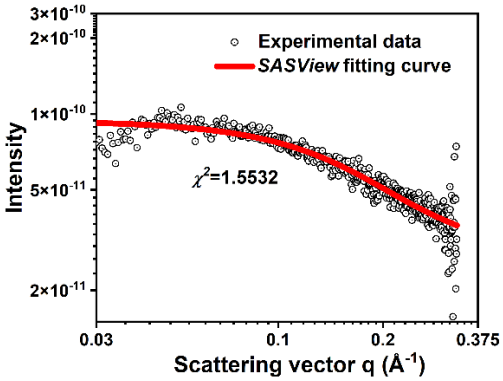

Figure S3. The SAXS profiles of C3G solution (6 mg mL^{-1}). Black circle: experimental scattering data; Red line: Cylinder model fitting from SASView.

Table S2 Fitting parameters obtained from SASView cylinder model

	Scale	Background (cm^{-1})	sld (estimated) (10^{-6} Å)	sld_solvent (10^{-6} Å)	radius (Å)	length (Å)	χ^2
C3G	1.63e-11	2.91e-11	16	9.53	4.0313	30.705	1.3915
TSG/C3G	4.92e-12	3.01e-11	15.2	9.53	6.5828	29.669	1.5532

S4. The NMR titration experiments

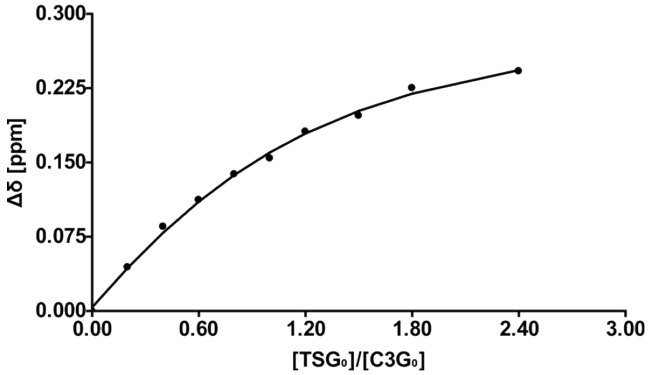

Figure S4. 1:1 model fitting curve of TSG and C3G via SupraFit software.

Table S3 Summary of binding constant and Gibb's free energy

No.	K (M^{-1})	ΔG (KJ mol^{-1})
1	1155.69	-17.474
2	1235.35	-17.639
3	1009.25	-17.138

S5. ^{1}H NMR spectrum of C3G

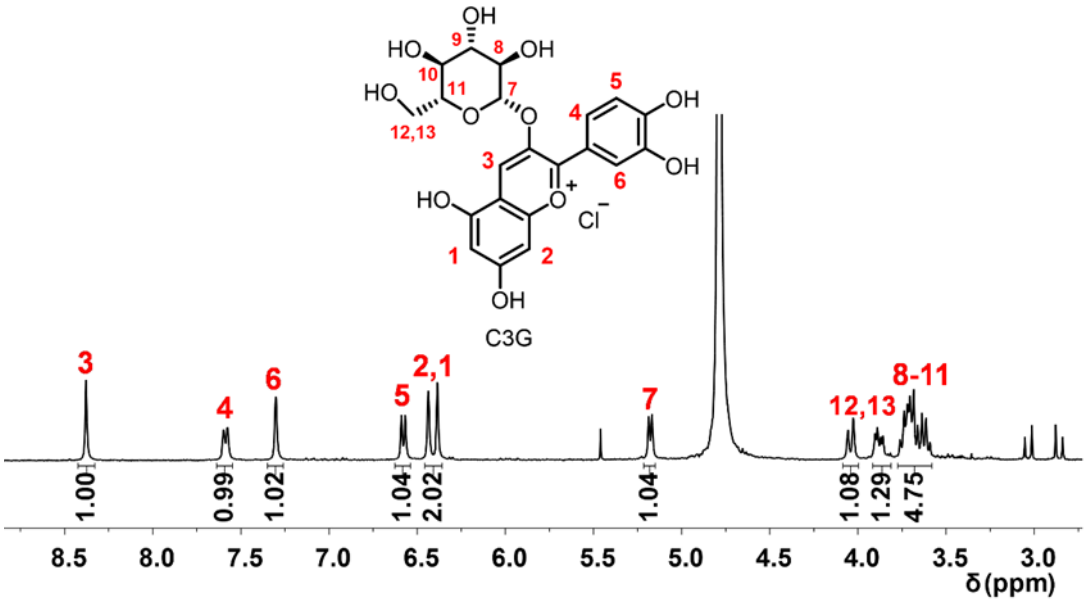

Figure S5. ^{1}H NMR spectrum of C3G (solvent: D_2O)

S6. The theoretical investigations

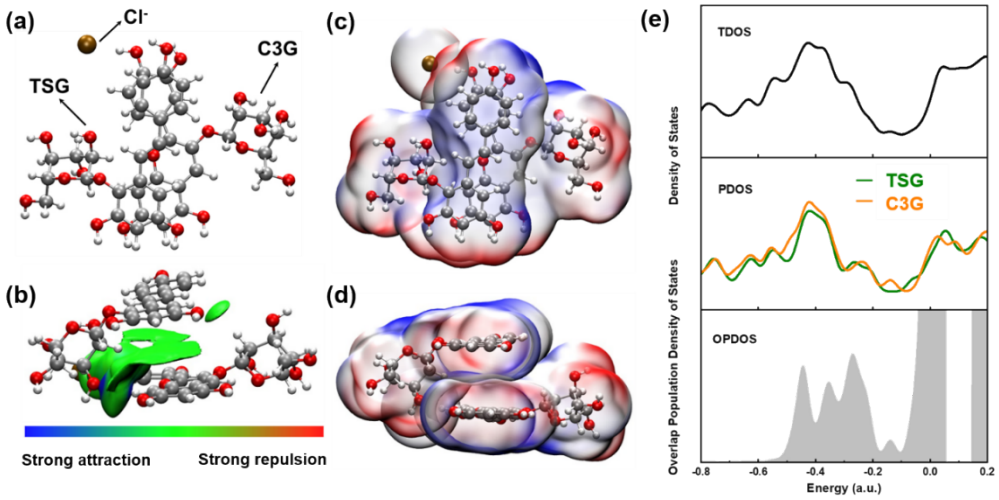

Figure S6. (a) The labeled three fragments of conformation-1; (b) The non-covalent interactions (NCI) between TSG and C3G; (c) the vertical view and (d) side view of the electrostatic potential (ESP); (e) The total density of state (TDOS), the partial density of state (PDOS), and overlap population density of state (OPDOS) of TSG and C3G.

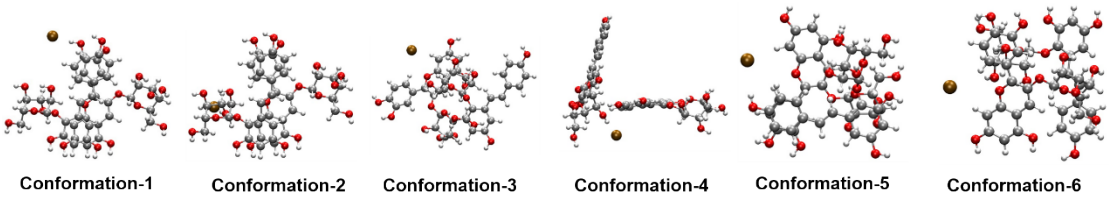

Figure S7. The structures of six candidate conformations.

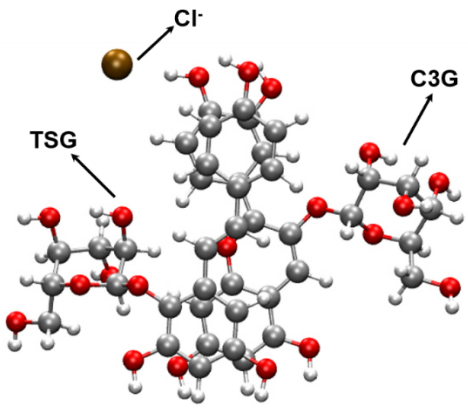

Figure S8. The labeled three fragments of conformation-1.

Table S4 The interaction energies of six conformations

Conformations	Total Energy (Hartree)	Fragment-TSG Energy (Hartree)	Fragment-C3G Energy (Hartree)	Fragment-Cl Energy (Hartree)	Interaction Energy (kcal·mol^{-1})
1	-3553.845683	-1452.78614	-1640.766059	-460.16802	-78.7
2	-3553.841284	-1452.785592	-1640.767728	-460.16802	-75.3
3	-3553.840147	-1452.785691	-1640.767618	-460.16802	-74.6
4	-3553.835317	-1452.786127	-1640.767669	-460.16802	-71.2
5	-3553.834138	-1452.786128	-1640.767517	-460.16802	-70.6
6	-3553.833413	-1452.786176	-1640.767704	-460.16802	-70.0

S7. Improved stability of TSG by co-assembling with C3G

Table S5 Summary of TSG degradation under different conditions

Condition	Form	$t_{\frac{1}{2}}$(h)	Degradation type
Vis	TSG	0.40	First order degradation
	TSG/C3G	1.72	
UV	TSG	0.83	First order degradation
	TSG/C3G	3.21	
pH=6.8	TSG	9.79	Zero order degradation
	TSG/C3G	23.36	
pH=10	TSG	7.06	Zero order degradation
	TSG/C3G	7.94	

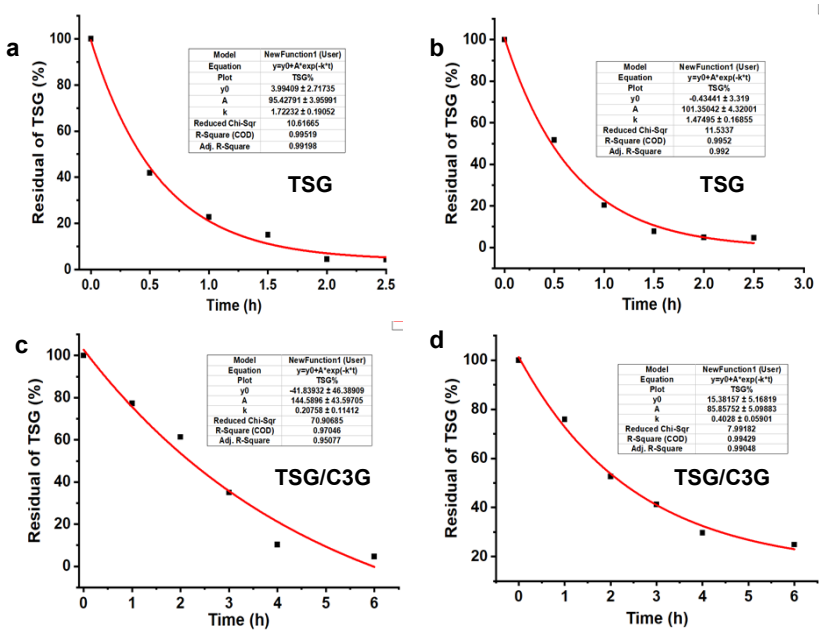

Figure S9. Kinetic profile for TSG degradation under different conditions: a) TSG solution under ultraviolet light (365 nm); b) TSG solution under visible light; c) TSG/C3G solution under ultraviolet light (365 nm); d) TSG/C3G solution under visible light.

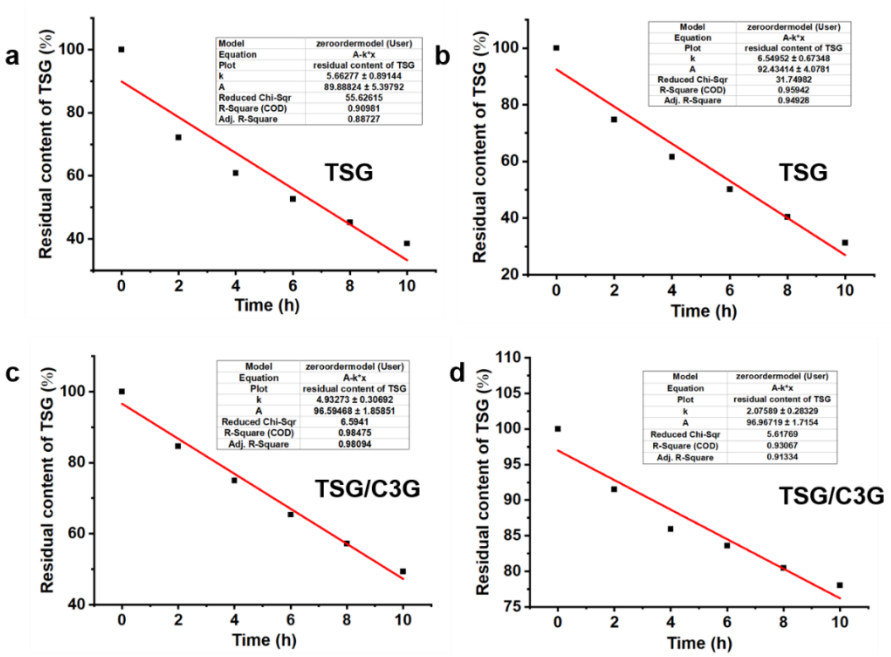

Figure S10. Kinetic profile for TSG degradation under different conditions: a) TSG solution at pH=10; b) TSG solution at pH=6.8; c) TSG/C3G solution at pH=10; d) TSG/C3G solution at pH=6.8.