Electronic Supplementary Material (ESI) for RSC Advances.

Electronic Supplementary Information

Cyclodextrin-Based Ordered Rotaxane-Monolayers at Gold Surface

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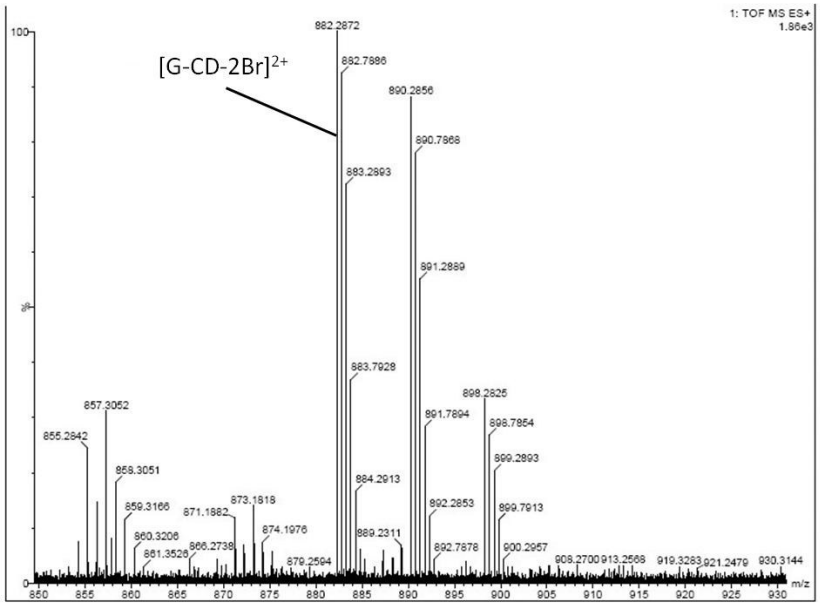

Figure S1. ESI-MS spectra of **G-CD** in aqueous solution.

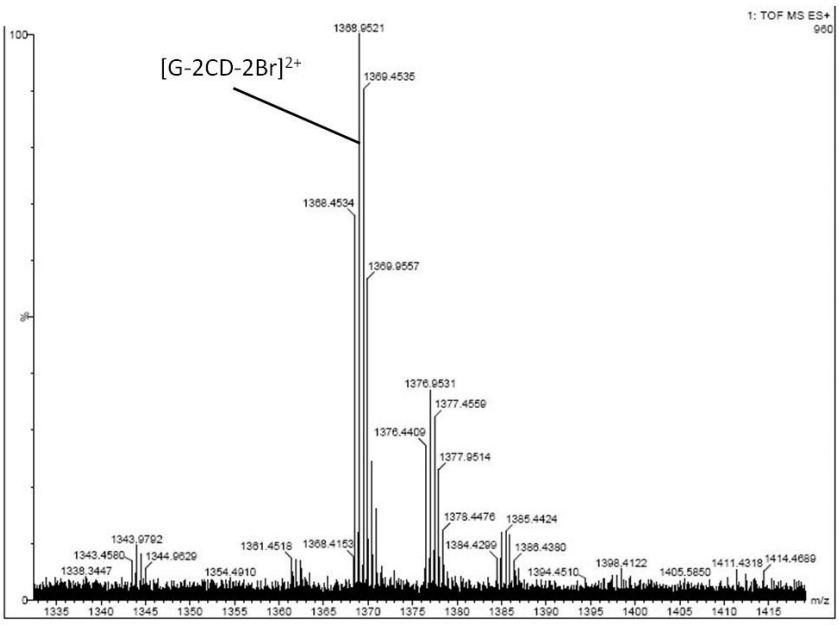

Figure S2. ESI-MS spectra of **G-2CD** in aqueous solution.

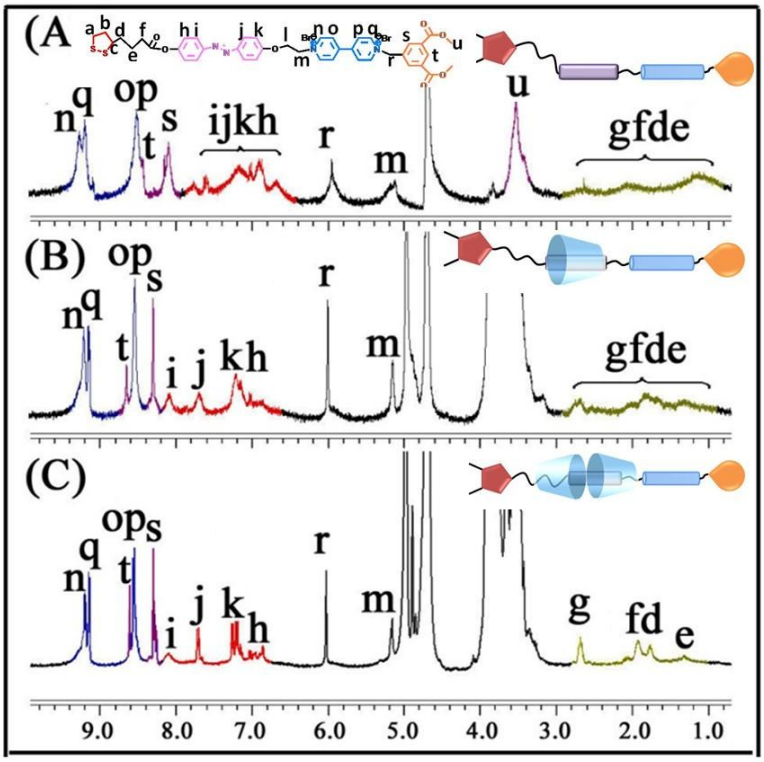

Figure S3. ^{1}H NMR spectra (400 MHz in D_2O at 298 K) of A) **G**, B) **G-CD** (**G** + 1.0 eq. of α-CD), and C) **G-2CD** (**G** + 2.0 eq. of α-CD).

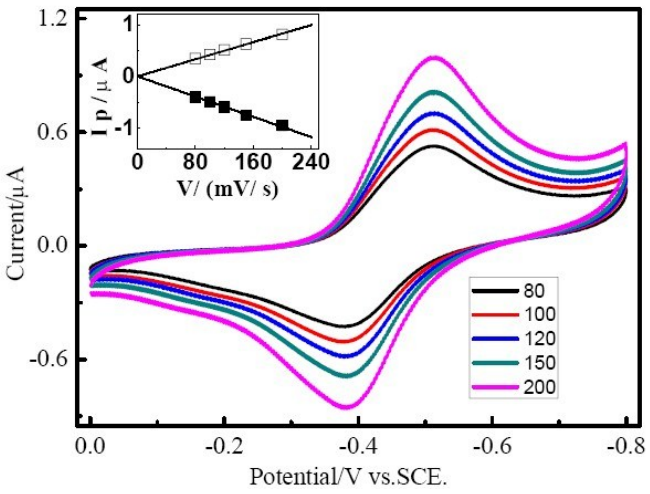

Figure S4. CVs of **G@Au** in DIW containing 0.2M $NaClO_4$, at different scan rates. All measurements are recorded at a Nitrogen atmosphere. The microscopic area was measured at 0.016cm^2. Q=0.812μC, Γ=5.26×10^{-10}mol/ cm^{-2}.

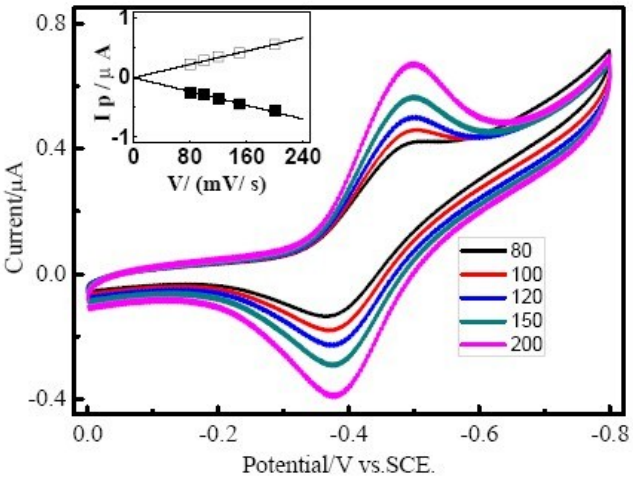

Figure S5. CVs of **G-CD@Au** in DIW containing 0.2M $NaClO_4$, with different scan rates, at a Nitrogen atmosphere. The microscopic area was measured at 0.00806cm^2. Q=0.244μC, Γ=3.14×10^{-10}mol/ cm^{-2}.

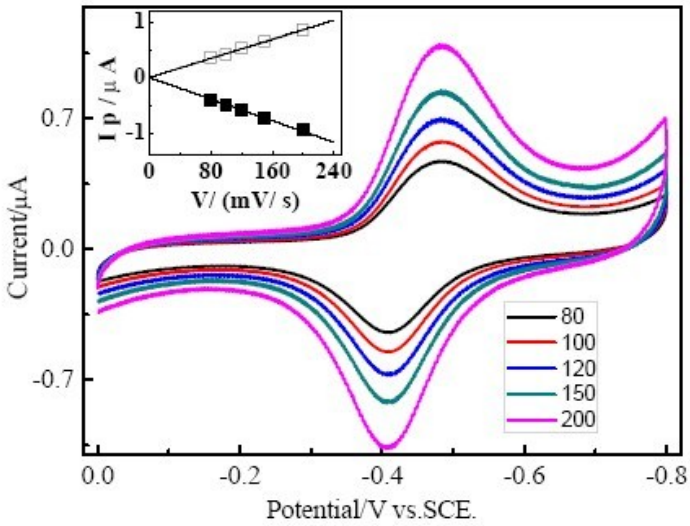

Figure S6. CVs of **G-2CD@Au** in DIW containing 0.2M $NaClO_4$, with different scan rates, at a Nitrogen atmosphere. The microscopic area was measured at 0.0124cm^2. Q=0.683μC, Γ=5.71×10^{-10}mol/ cm^{-2}.

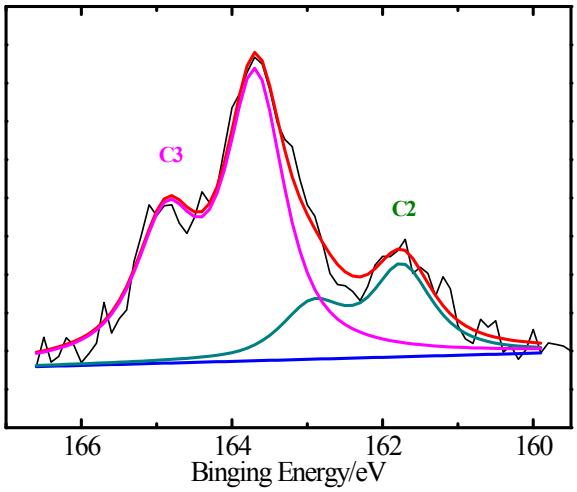

Figure S7. S 2p XPS spectra of **G@Au**. C2 (blue): thiolate; C3 (magenta): free SH-terminal group. Average binding energy, C2 (161.7), C3 (163.7).

Table S1: Frequence (in cm^{-1}) and assignments of the SERS bands of various SAMs on gold surface[a]

G	G-CD	G-2CD	assignments
624 m	624 w	624 sh	
652 w	654 w	652 s	δC-N-C/ δC-C-N/ in plane ring deformation
		690 ms	
717 vw	716 w	724 w	
790 m		751 m	
800 m	792 m	791 ms	Ring vibration Para-desubstuted benzenes
835 m	835 m	839 s	νsC-O-C/ δviologen ring
917 m	919 m	916 m	
1033 vw	1033 vw	1029 vw	Ring breathing Pyridines
998 m	998 m	998 s	δCH ring/ in plane ring deformation
1138 s	1138 s	1131 s	δCH ring/ ν7a/ νφ - N
1181 ms	1181 ms	1187 s	δCH ring/ ν7b / νφ - N / νN^{+}-(CH_2)n
1197 sh/m			
1236 w	1231 w	1213 sh	
1293 m	1297 m	1297 m	νC-$C_{i.\,r.}$/ δH−C−C
1309 sh	1310 sh	1311 sh	νφ - N assymmetric
	1393 sh	1393 s	
1407 m	1407 ms		Fermi resonance of νN=N with γC-H (phenol rings)
	1437 sh	1439 ms	
1454 ms	1455 ms	1455 sh	ωC=C/ δC-H & Fermi resonance of νN=N with γC-H (phenol rings)
1595 m	1593 m	1595 m	Benzene ring mode: ωC=C
1641 m	1643 m	1646 m	νC-C/ νC-$C_{i.\,r.}$
1721 w	1721 w	1720 w	

[a]s, strong; ms, medium strong; sh, shoulder; m, medium; w, weak; vw, very weak; ν, stretching vibration; ω, wagging; δ, in-plane bending; γ, out-of-plane bending; i. r., inter-ring.