Electronic Supplementary Information

A direct approach toward investigating DNA–ligand interactions via surface-enhanced Raman spectroscopy combined with molecular dynamics simulations

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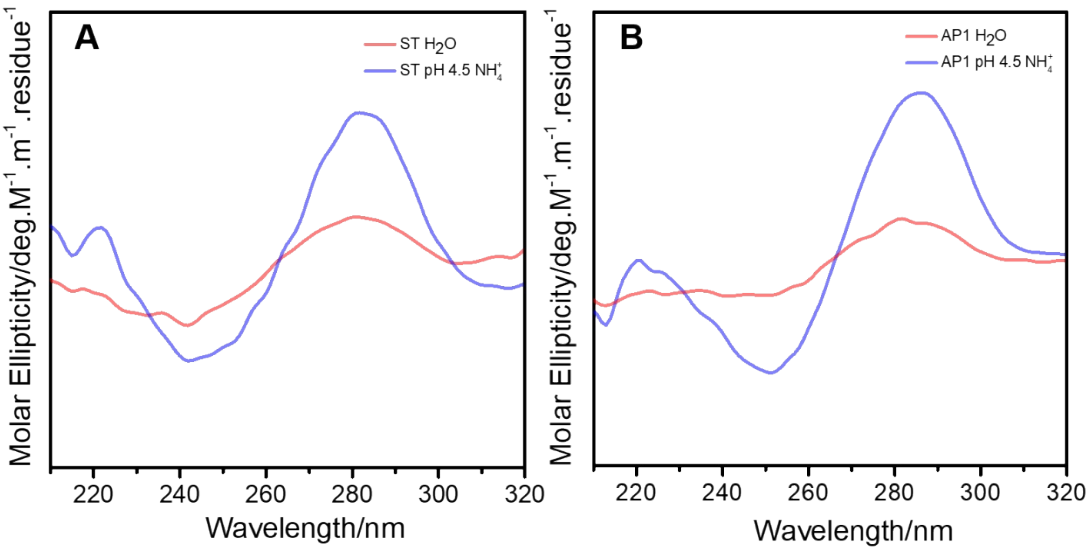

Figure S1. (A) CD spectra of ST in aqueous (red line) and ammonium acetate buffer solutions (pH=4.5; 500 mM) (blue line); (B) CD spectra of AP1 in aqueous (red line) and ammonium acetate buffer solutions (pH=4.5; 500 mM) (blue line)

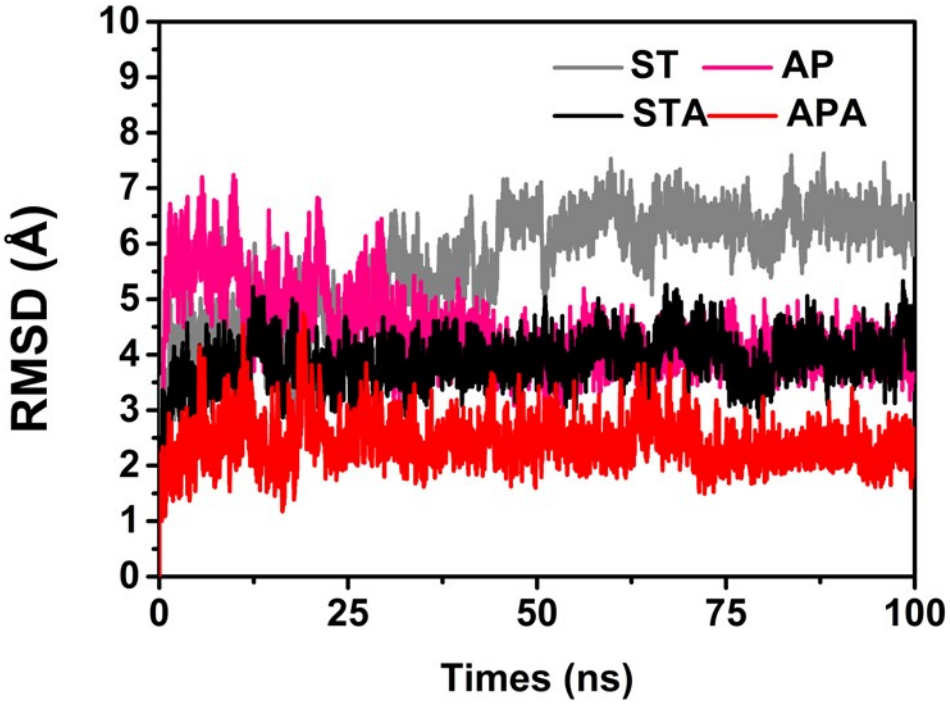

Figure S2. The root-mean-square-deviation (RMSD) values of backbone atoms of DNA during the molecular dynamics simulations

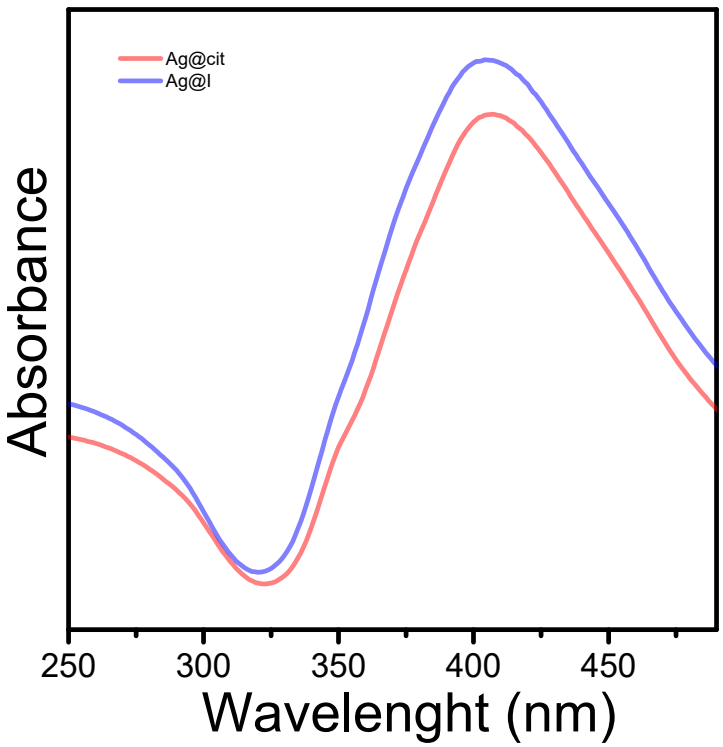

Figure S3. UV-vis absorption spectrum of Ag@cit and Ag@I.

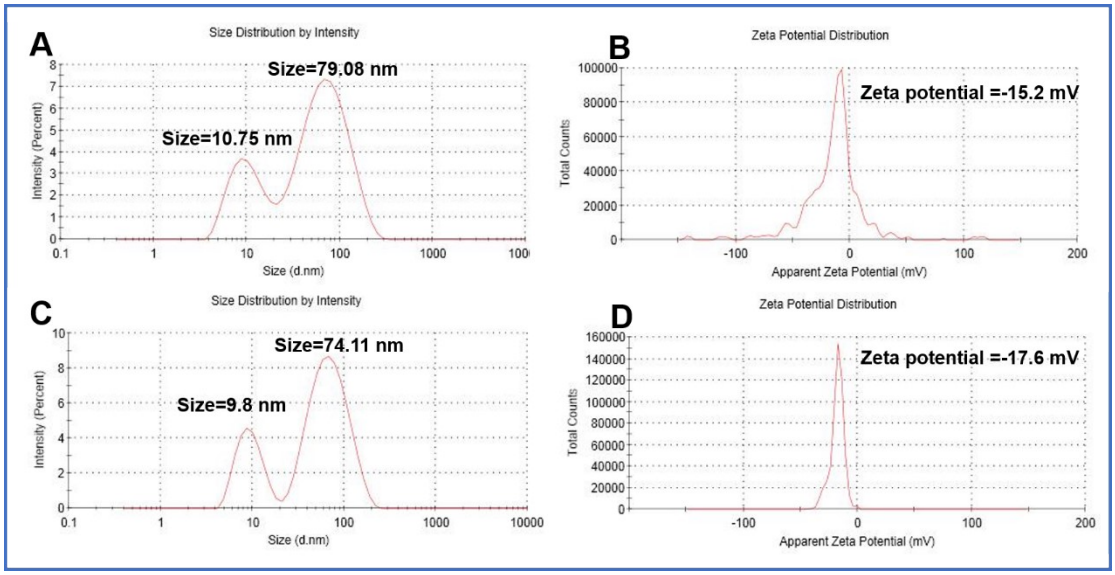

Figure S4. Detection of samples by dynamic light scattering method. Size and Zeta potential distribution of Ag@cit

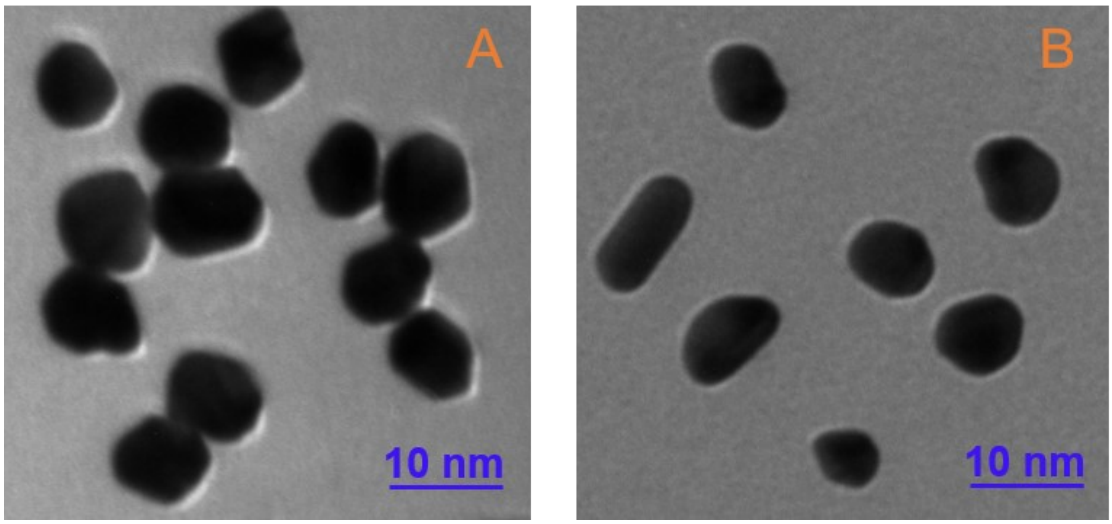

Figure S5. TEM image of Ag@cit(A) and Ag@I(B)

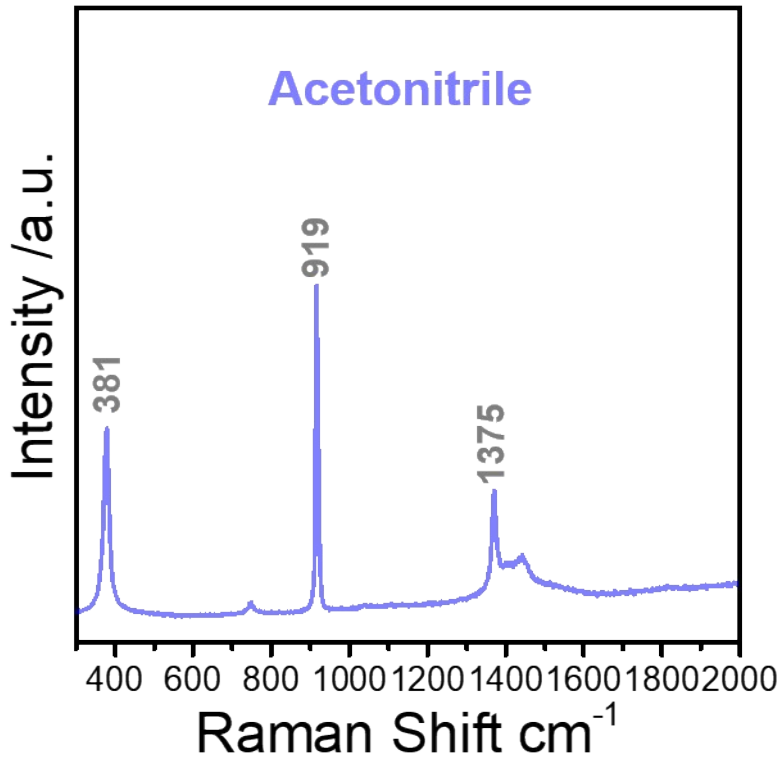

Figure S6. SERS spectrum of the acetonitrile.

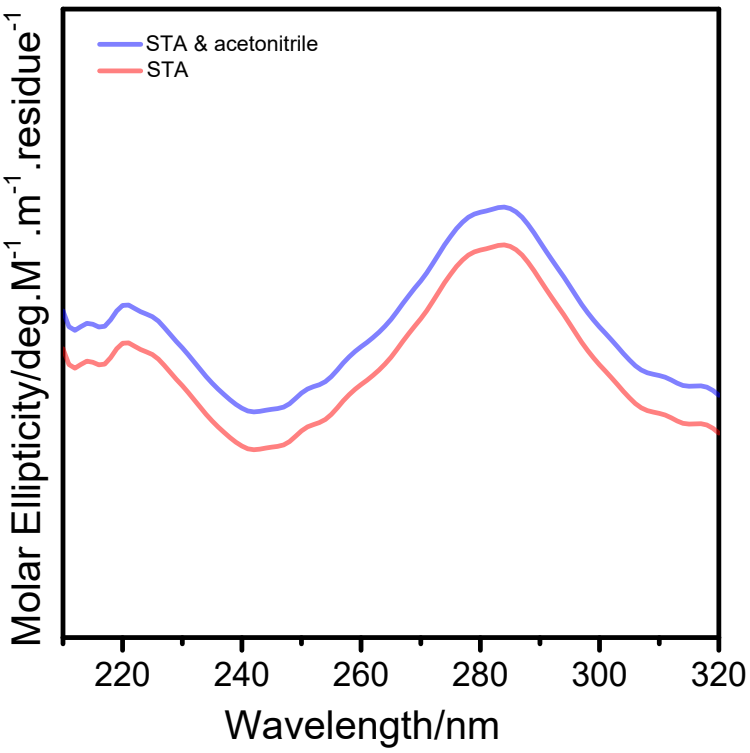

Figure S7. CD spectra of STA before (red line) and after (blue line) acetonitrile addition

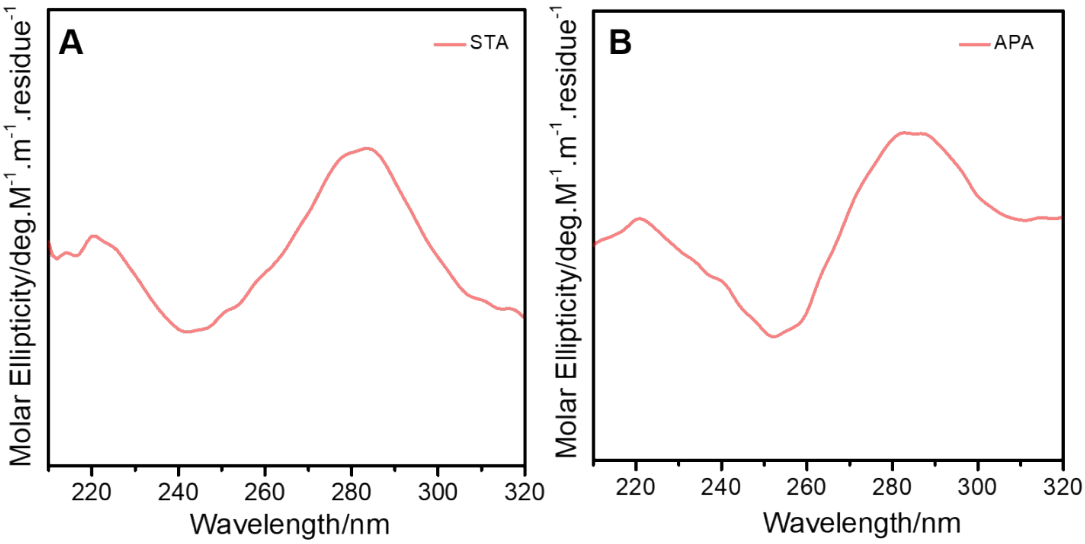

Figure S8. CD spectra of STA and APA

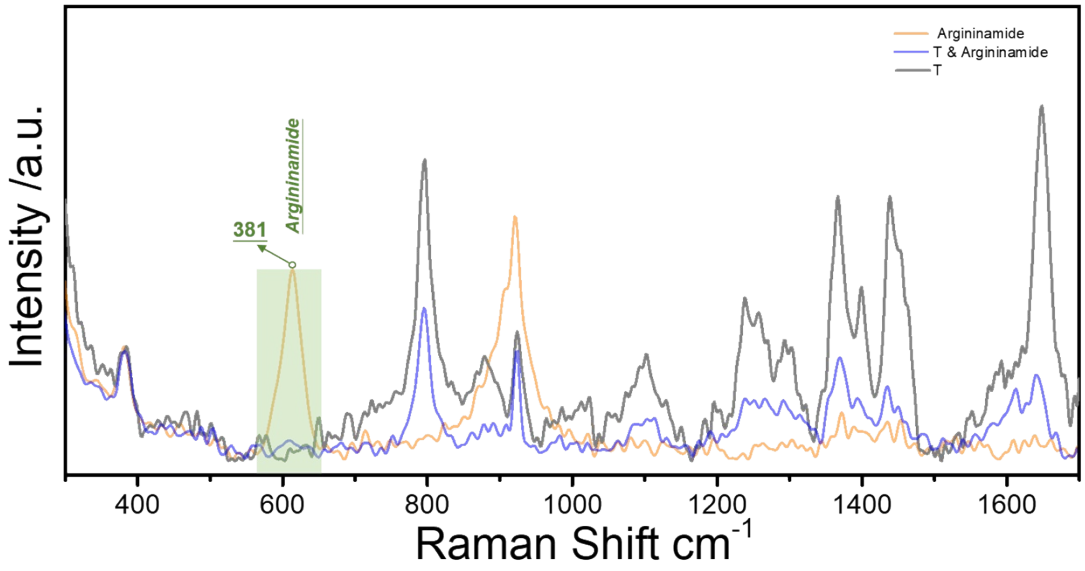

Figure S9. SERS spectra of T12 sequence, pure argininamide and mixture after incubation

Table S1. The SERS peak assign to DNA

Raman Shift/cm^{-1}	Assignment		Ref.
NH4+	DNA	DNA/Ligand	
654	dG	dG ring br, dG C2′-endo/anti	[1]
731	dA	dA ring br	[1]
791	dT ring br	νs OPO, dT ring br	[1]
949-960	d	d, dG δ R5	[2]
1089	ν_S, PO_2	$\nu_s PO_2^-$, bk	[2, 3]
1095	νs PO2-	bk[PO2-]	[1, 2, 4]
1188-1205	dT	C, C^+, C•C^+, T	[5]
1218-1227	dT	C, C^+, C•C^+, T, dT C2′-endo/anti	[5, 6]
1240-1245	dT	dT, dG δNH(N2)	[2, 3]
1258	dT	dT, dG δNH(N2)	[2, 3]
1268-1271	dC	C, C^+, C•C^+	5
1317-1319	-	C^+, C•C^+	9
1321-1323	dG	dG C2′-endo/anti, C^+, C•C^+	[4, 5]
1349	dG	dG ν(C-N) δ(C8-H) C2'-endo/anti	[2, 3]
1358-1365	-	dG C2'-endo/syn	[2]
1407-1411	d	C, C^+, C•C^+	[1, 3, 5]
1573-1580	-	dG δ NH (N2H interbase H-bone), C	[2]
1635-1640	dT	T[C=O], C, C^+, C•C^+	[5]

Note: d = deoxyribose, ν = stretch, δ = deformation, br = breathing, s = symmetric, bk = backbone

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