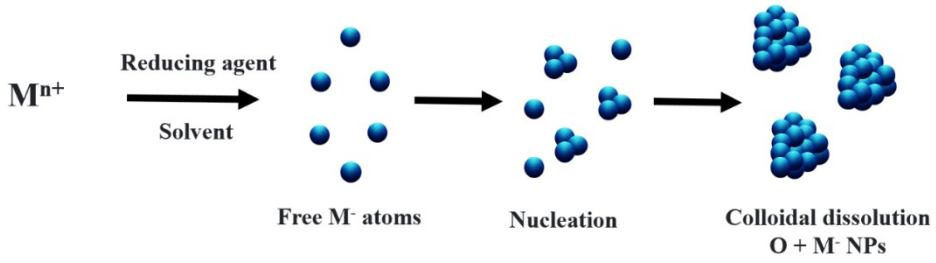
Electronic Supplementary Material (ESI) for Analyst.

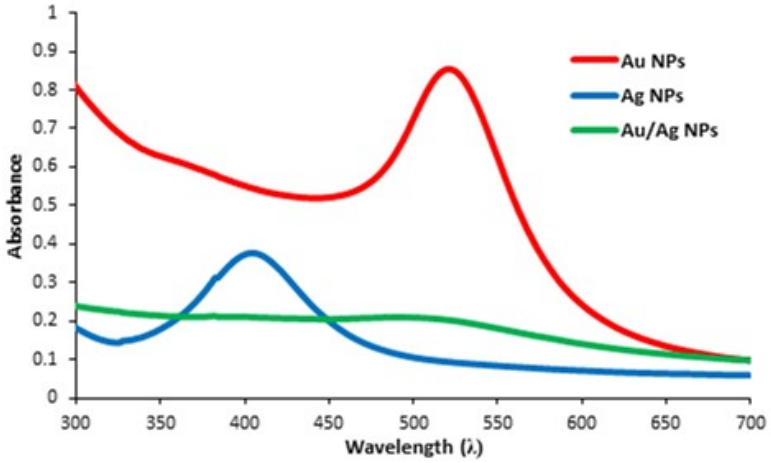
Rapid electrochemical recognition of trimethoprim in urine sample using new modified electrode (CPE/Ag/AuNPs) analyzing tunable electrode properties: Experimental and theoretical studies

Supplementary materials



$M^{n+} = Ag^{+}$ or Au^{3+}

Scheme S1. Synthesize of AgNPs, AuNPs, and Ag/Au NPs.



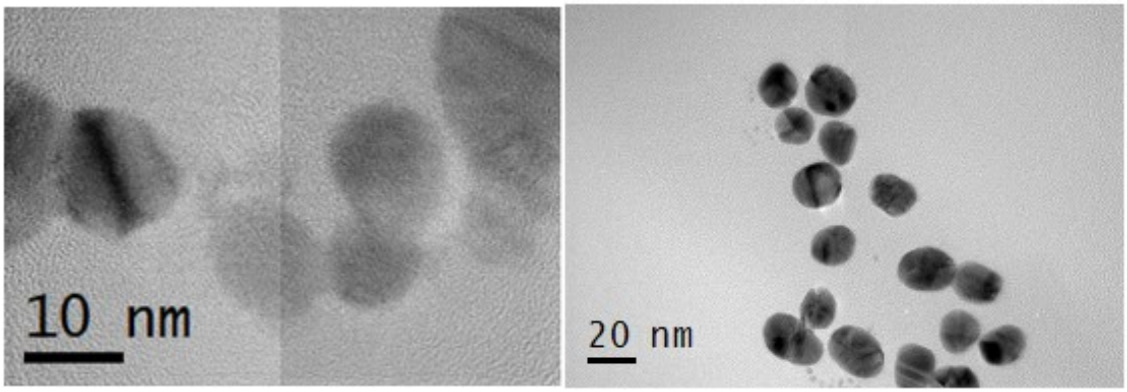


Figure S1. a) UV-Visible spectra: Ag NPs (λ = 400 nm), AuNPs (λ = 520 nm) and Ag/AuNPs (λ = 510 nm); TEM images: **b)** AgNPs, and **c)** AuNPs

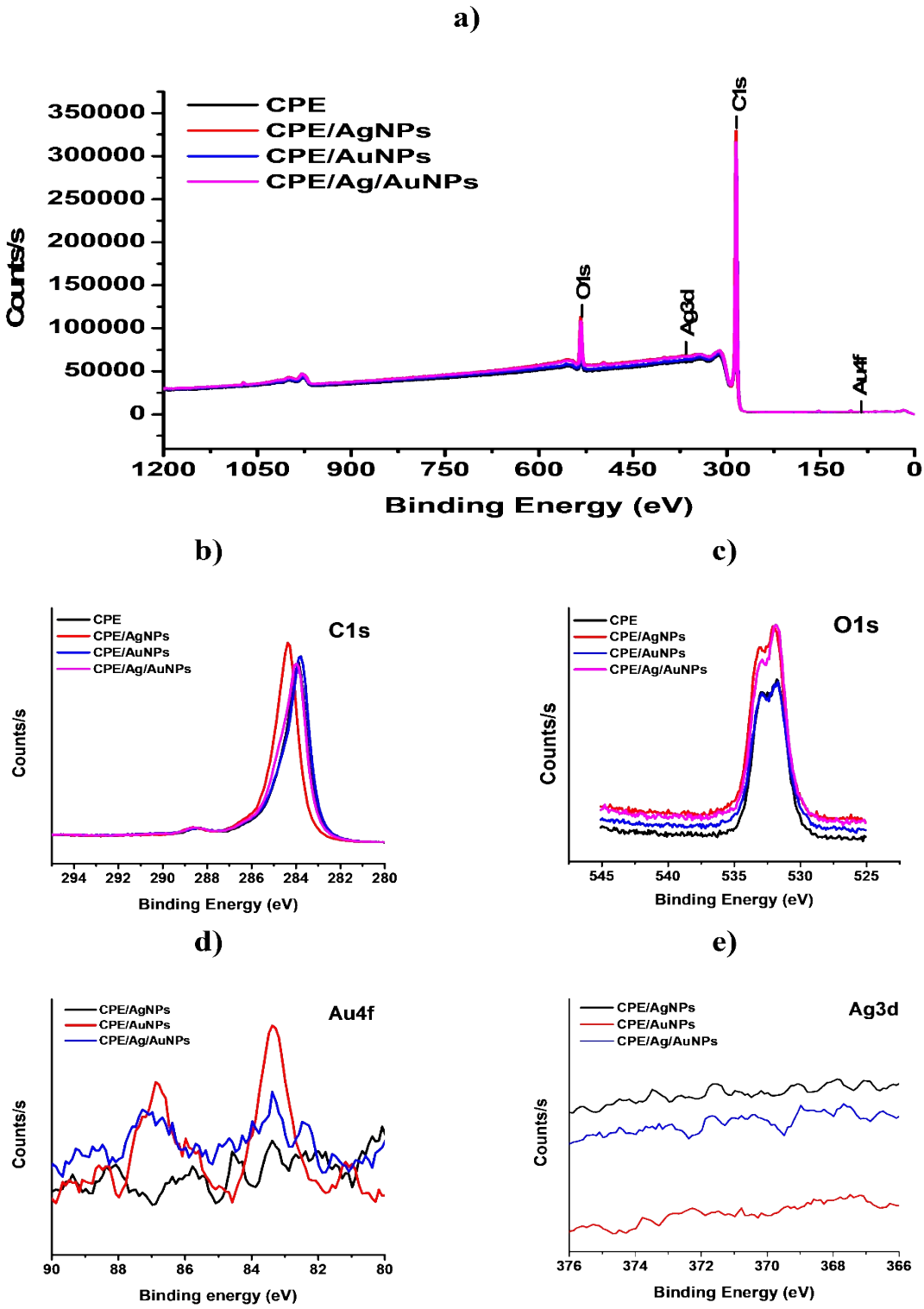


Figure S2. XPS studies for the different modified carbon pastes.

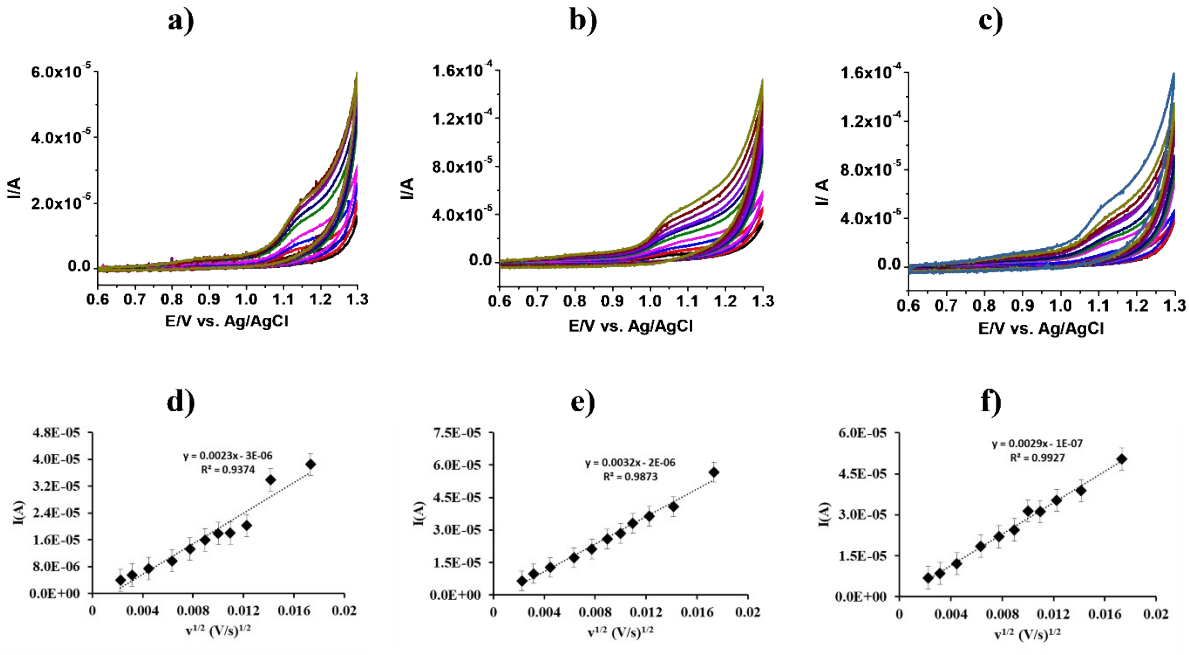


Figure S3. Dependence of the cyclic voltammetric response at **a and d)** CPE; **b and e)** CPE/AgNPs; **c and f)** CPE/AuNPs on sweep rate in 100 µmol/L TMP in B-R buffer solution (pH 7.0, 0.2 mol/L). Scan rates from bottom to top: 5, 10, 20, 40, 60, 80, 100, 150, 200, 300 mV/s.

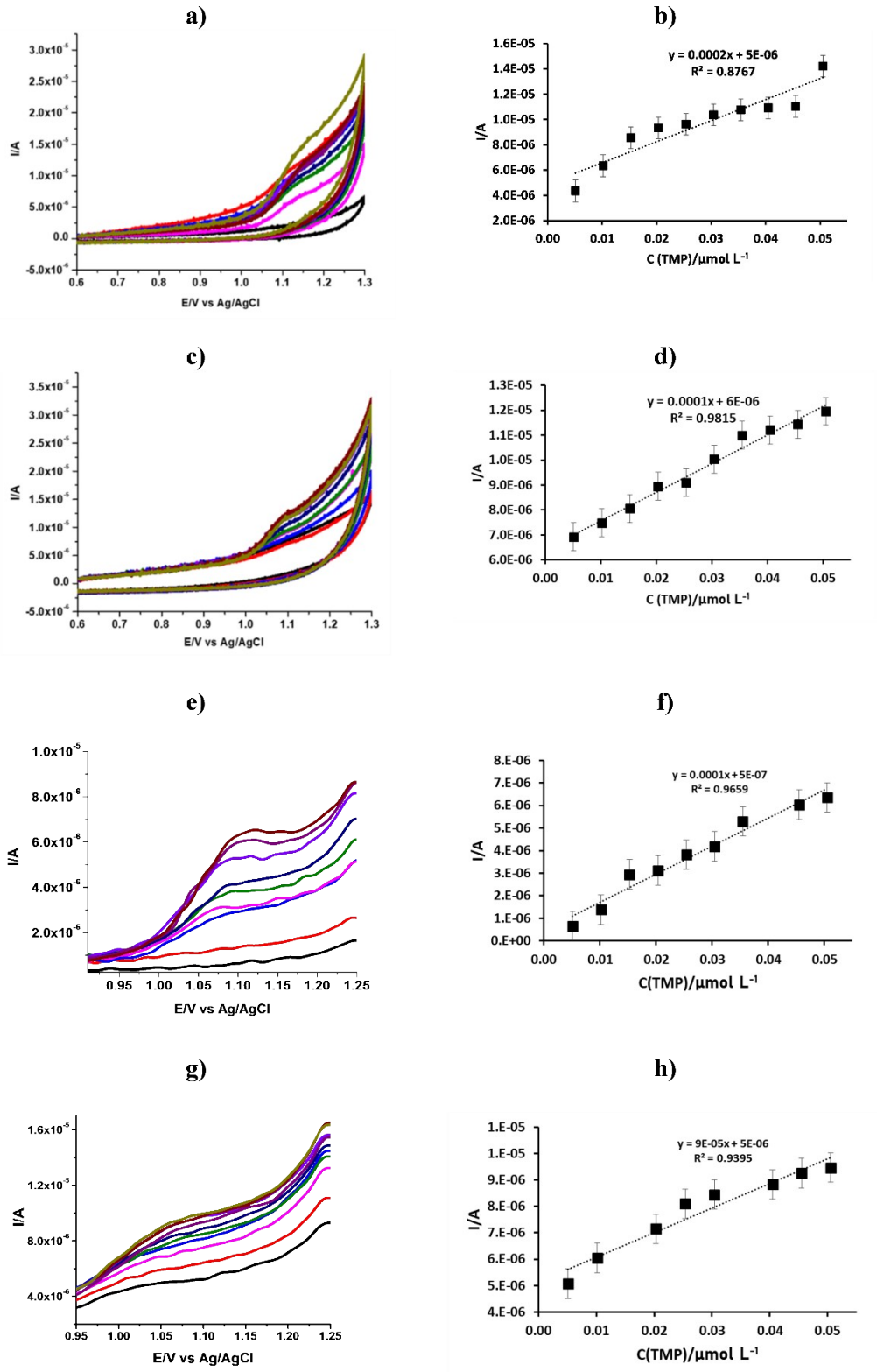


Figure S4. a and b) The CV detection of TMP at CPE/AgNPs, and measured anodic currents at different concentrations (0.005 to 0.05 µmol/L) in B-R buffer solution (pH 7.0, 0.2 mol/L) at scan rate of 50 mV/s; **c and d)** The CV detection of TMP at CPE/AuNPs, and measured anodic currents

at different concentrations (0.005 to 0.05 µmol/L) in B-R buffer solution at scan rate of 50 mV/s; **e and f**) the DPV detection of TMP at CPE/AgNPs with the different concentration (0.005–0.05 µmol/L); **e and f**) the DPV detection of TMP at CPE/AuNPs with the different concentration (0.005–0.05 µmol/L).

The regression equations applied for TMP is as described below: CV at different scan rates

CPE: I_{ap} (A) = 0.0023 v (V/s) + 3.0 x10^{-6}

CPE/Ag NPs: I_{ap} (A) = 0.0032 v (V/s) + 2.0 x10^{-6}

CPE/Au NPs: I_{ap} (A) = 0.0029 v (V/s) + 1.0 x10^{-7}

CPE/Ag/Au NPs: I_{ap} (A) = 0.0031 v (V/s) + 8.0 x10^{-7}

CV at different concentration of TMP:

CPE/AgNPs: I_{pa} (A) = (2x10^{-4} C_{TMP} (µmol/L) + 5x10^{-6}); correlation coefficient: 0.951

CPE/AuNPs: I_{pa} (A) = (1x10^{-4} C_{TMP} (µmol/L) + 6x10^{-6}); correlation coefficient: 0.991

CPE/Ag/AuNPs: I_{pa} (A) = (3X10^{-4} C_{TMP} (µmol/L) + 8x10^{-7}); correlation coefficient: 0.963

DPV at different concentration of TMP:

CPE/AgNPs: I_{pa} (A) = (1x10^{-3} C_{TMP} (µmol/L) + 5x10^{-7}); correlation coefficient: 0.971

CPE/Au NPs: I_{pa} (A) = (9x10^{-5} C_{TMP} (µmol/L) + 5x10^{-6}); correlation coefficient: 0.945

CPE/Ag/AuNPs: I_{pa} (A) = (5.0 x10^{-5} C_{TMP} (µmol/L) + 1.0 x10^{-6}); correlation coefficient: 0.960

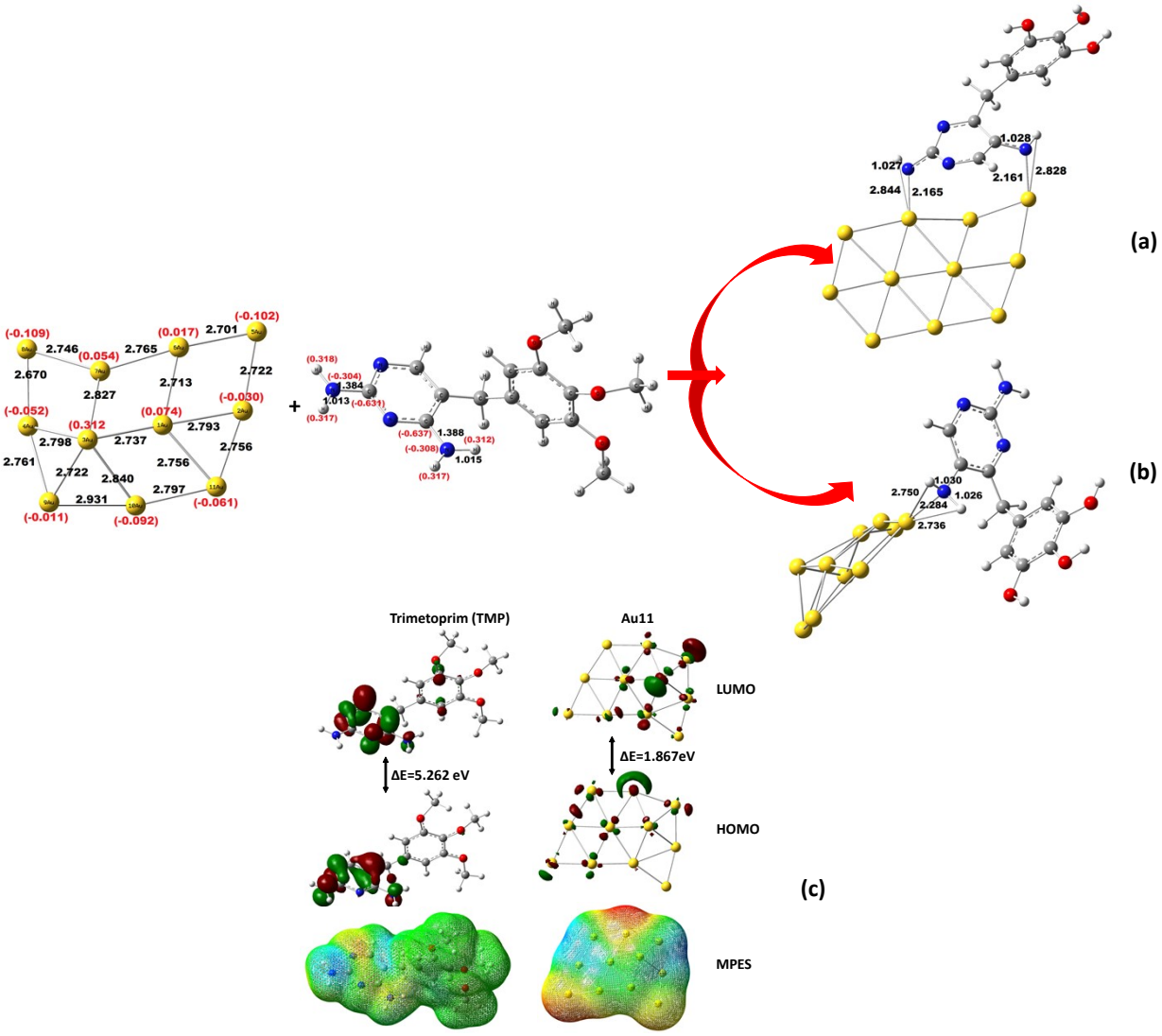


Figure S5. The optimization of TMP with Au11 cluster surface in the different positions at B3LYP/CEP-31G: (a) at the parallel plane surface to Au11; (b) in the corner of Au11 plane; c) electrostatic map potential of TMP and Au11.

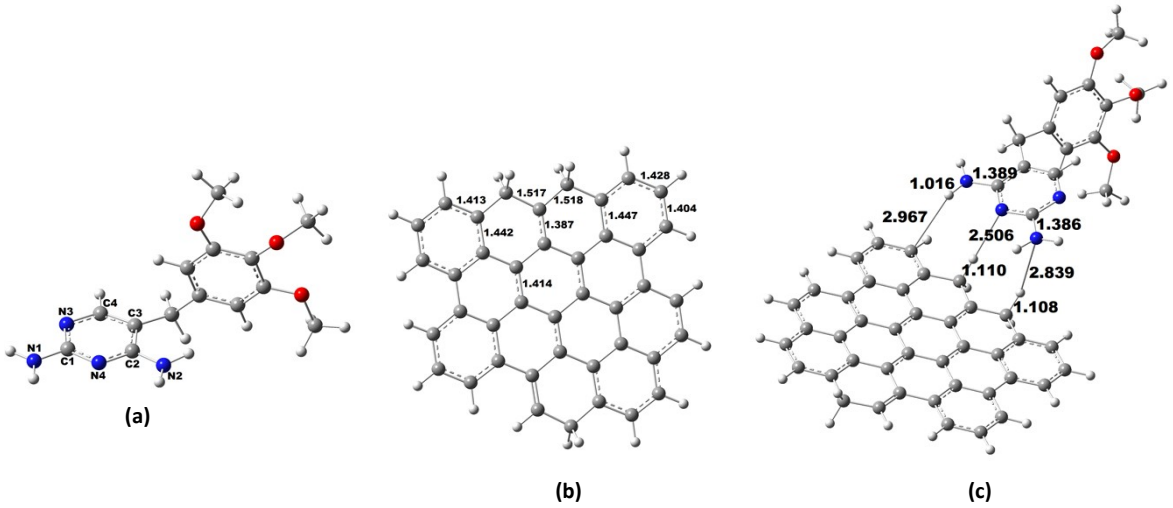


Figure S6. Molecular structure: a) Trimethoprim; b) Graphite and c) Trimethoprim plus Graphite

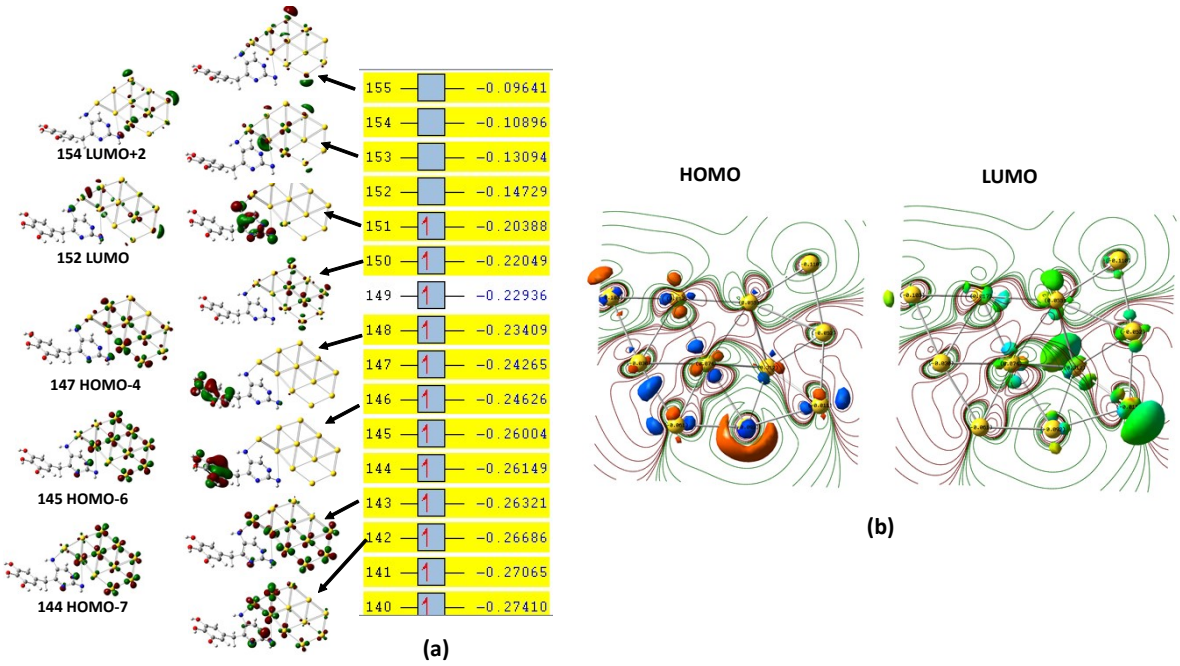


Figure S7. a) Natural Transition Orbitals determined with B3LYP/CEP-31G basis set at S=0, orbital 105 (*particle*), and orbital 106 (*hole*); **a)** for canonical basis, excited state number 26 at S=0 and **b**) The electron density isosurface at [Au11] at gaseous state: Color code use for the structure of molecule C(grey), H(white), N(blue), O(red) and Ru (turquoise/green), and (contour 0.05 e/Å^3), HOMO and LUMO determined by B3LYP/CEP-31G: HOMO and LUMO contour plots (isosurface value = 0.05 au).

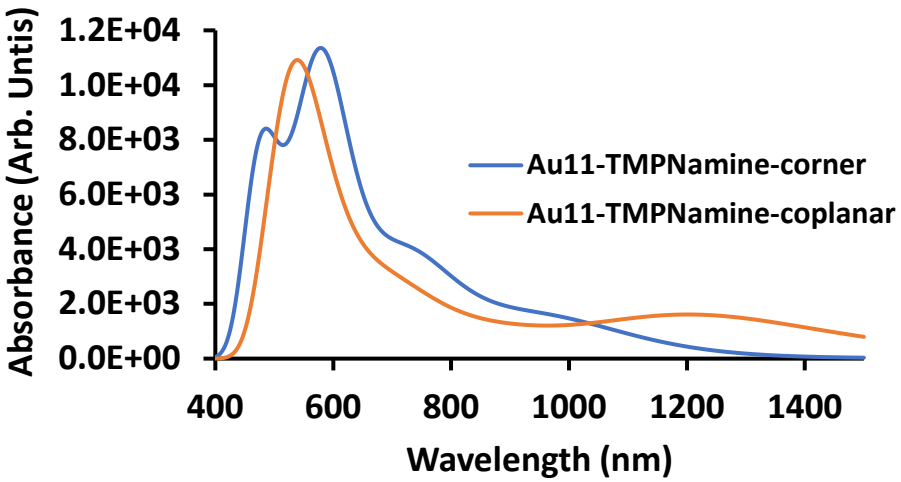


Figure S8. TD-DFT spectra of Au11 cluster with trimethoprim: **a)** Au11-TMP N_{amine} corner and b) Au11-TMP Namine coplanar/corner at b3lyp/dgdzvp basis set at gaseous state.

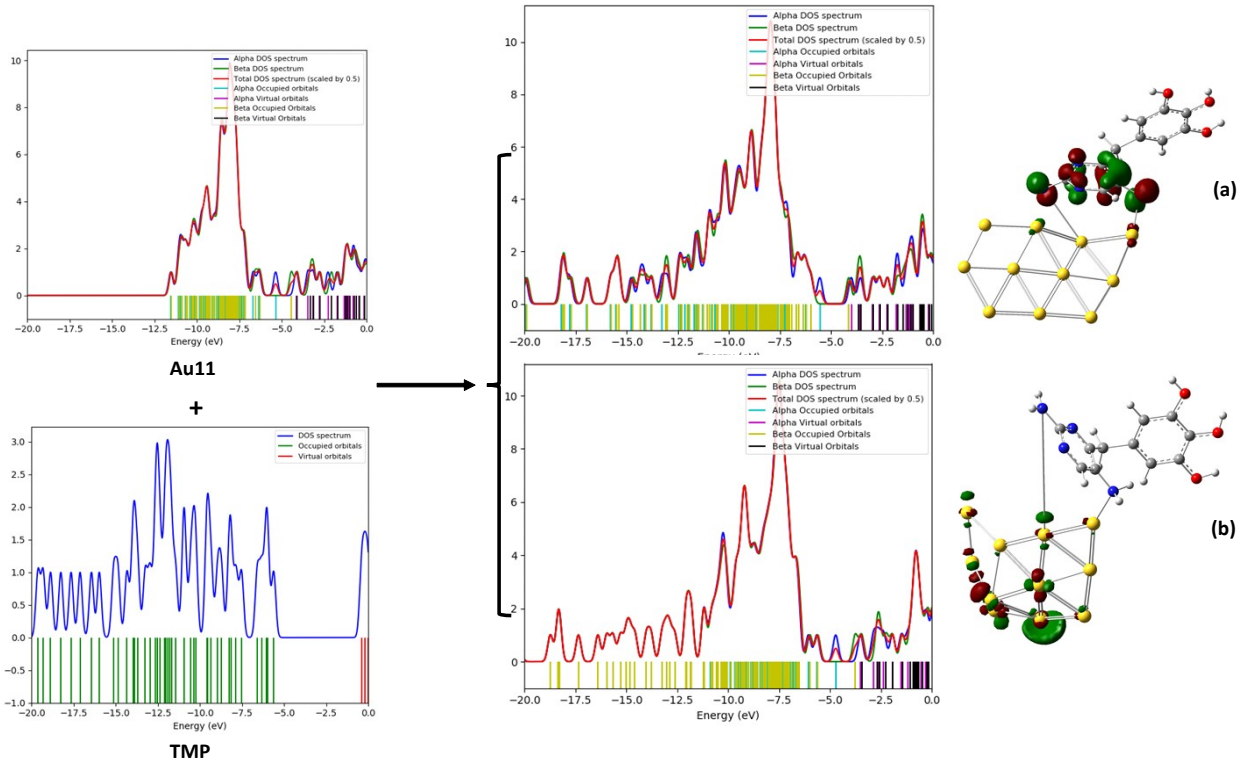


Figure S9. Density of state (DOS) and HOMOs of [TMP- Au11]: (a) parallel; (b) corner of Au11 plane.

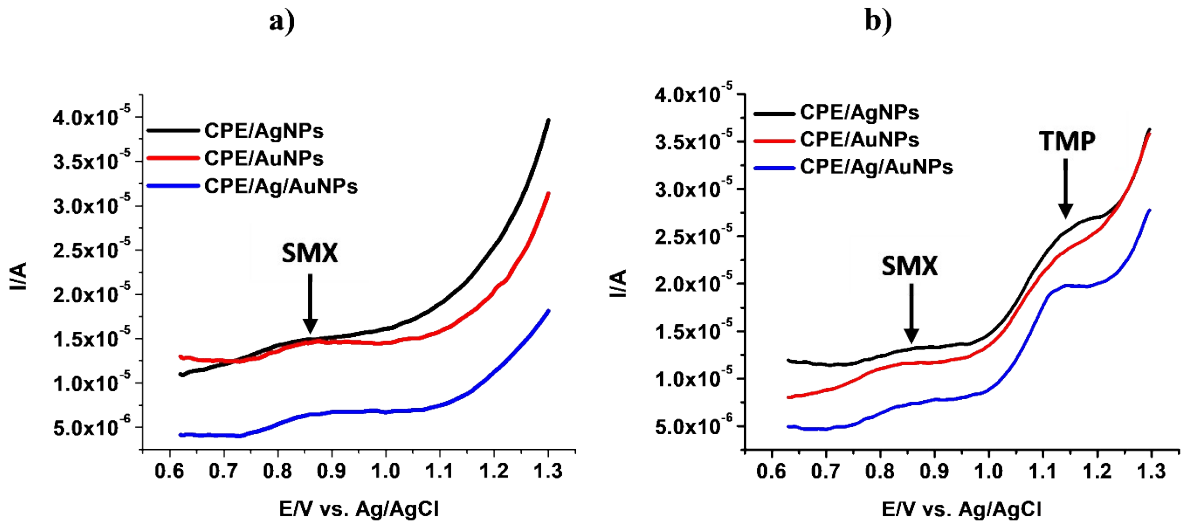


Figure S10. DPV profiles obtained from 0.6 to 1.3 V in urine samples a) SMX 100 µM b) SMX and TMP 100 µM.

Table S1. Bond lengths (Å) and bond angles (°) resulted in different spin states for [Au11-TMP], using Functional B3LYP/CEP-31G level of theory.

Bond length ligand **(L^1)**	CEP-31G	Bond length complexes (Å)	**[Au11-tmp]** at the parallel plane surface to Au11 (Secondary N_{amine})	**[Au11-tmp] in the corner of Au11 surface** (Primary N_{amine})
$N1_{amine}$-C1	1.384	6Au-N1	2.165	-
$N2_{amine}$-C2	1.388	6Au-HN1	2.844	-
C1-$N3_{amine}$	1.376	5Au-N2	2.161	2.284
C1-$N4_{amine}$	1.372	5Au-H_1N2	2.828	2.736
$N3_{amine}$-C4	1.369	5Au-H_2N2	-	2.750
$N4_{amine}$-C2	1.369	N1-H1	1.027	1.026
C2-C3	1.446	N1-H2	-	1.030
C3-C4	1.415	N2-H	1.028	
N1-H	1.013	N1-C1	1.346	
N2-H	1.015	N2-C2	1.375	-
		Bond Angle (º)		
		6Au-N1-H	121.8	
		6Nu-N1-C1	117.2	
		5Au-N2-H_1	120.8	105.1
		5Au-N2-H_2	-	105.9
		5Au-N2-C2	107.8	112.7

Table S2. Mulliken charges of L^1 and its complexes with: [Au11-TMP]. Functional B3LYP/CEP-31G basis set

L^1		**Atoms**	Au11-cluster	[Au11-tmp] at the parallel plane surface to Au11 (Secondary N_{amine})	[Au11-tmp] in the corner of Au11 surface (Primary

					N_{amine})
N1	-0.330	1-Au	0.074	0.180	0.074
N2	-0.320	2-Au	-0.030	-0.028	-0.102
N3	0.258	3-Au	0.312	0.199	0.274
N4	0.221	4-Au	-0.052	-0.108	-0.080
C1	-0.689	5-Au	-0.103	0.008	-0.051
C2	-0.740	6-Au	0.017	0.151	-0.049
C3	0.598	7-Au	0.055	-0.078	-0.124
C4	-0.820	8-Au	0.110	-0.118	-0.026
		9-Au	-0.011	-0.002	-0.138
		10-Au	-0.092	-0.111	-0.046
		11-Au		0.135	0.055
H1	0.276	H1		0.305	0.328
H2	0.275	H4		0.283	0.326
H3	0.271	N1		-0.208	-0.287
H4	0.292	N2		-0.209	-0.486
		N3		0.316	0.328
		N4		0.420	0.396
		C1		-0.597	-0.563
		C2		-0.031	0.386
		C3		-0.534	-0.643
		C4		-0.489	-0.711

Table S3. Electronic properties of the ligands (TMP and C graphite) and Au cluster.

	Functional: B3LYP/CEP-31g					
Compounds	E_{HF}	HOMO (eV)	LUMO (eV)	ΔE (eV)	Hardness (η, eV)	Softness (σ, eV)
L^1	-1310.624	-6.284	-1.136	5.148	2.574	0.388
TMP	-177.149	-5.659	-0.397	5.262	2.631	0.380
Graphite	-243.328	-4.481	-2.191	2.290	1.145	0.873
Au11	-1497.563	-6.333	-4.466	1.867	0.933	0.1.071
[Au11-tmp] at the parallel plane surface to Au11 (Secondary N_{amine})	-1652.982	-6.015	-4.159	1.855	0.928	1.078
[Au11-tmp] in the corner	-1654.238	-5.640	-3.784	1.856	0.928	1.077

of Au11 surface (Primary N_{amine})						

Table S4. TD-DFT spectral data of electronic transitions of Au cluster with TMP at the plane with oscillator strength f > 0.0001.

Wavelength (nm)	Osc. Strength (f)	[Au11-tmp] in the corner of Au11 surface (Primary N_{amine})	Character	Theory (nm)
2357.1	0.0006	HOMO->LUMO (99%)	CT	
1108.7	0.0001	HOMO->LUMO (96%) HOMO->LUMO+1 (2%)	CT	
977.7	0.012	HOMO->LUMO+1 (56%) HOMO->LUMO+1 (26%) HOMO-1->LUMO (8%) HOMO->LUMO (3%) HOMO-1->LUMO (2%)	CT	
976.0	0.0057	HOMO-1->LUMO (43%) HOMO->LUMO+1 (30%) HOMO->LUMO+1 (23%) HOMO-1->LUMO (2%)	CT	
870.6	0.0012	HOMO->LUMO+2 (97%)	CT	271
815.6	0.0052	HOMO-1->LUMO (90%) HOMO-1->LUMO (2%) HOMO->LUMO+1 (2%)	CT	
761.3	0.0179	HOMO-1->LUMO (23%) HOMO->LUMO+3 (33%) HOMO-1->LUMO+1 (11%) HOMO->LUMO+1 (25%) HOMO-1->LUMO (2%)	CT	
721.8	0.0085	HOMO-2->LUMO (54%) HOMO-1->LUMO+1 (29%) HOMO-1->LUMO (8%) HOMO->LUMO+1 (3%)	CT	
709.0	0.0237	HOMO->LUMO+3 (55%) HOMO-1->LUMO+1 (13%) HOMO->LUMO+1 (11%) HOMO-2->LUMO (7%) HOMO-1->LUMO (5%) HOMO-6->LUMO (2%) HOMO-4->LUMO (2%)	CT	
636.9	0.0072	HOMO-2->LUMO (50%) HOMO-3->LUMO (17%) HOMO-1->LUMO+1 (12%) HOMO-2->LUMO (11%)	CT	
609.8	0.0005	HOMO-1->LUMO+1 (63%) HOMO->LUMO+2 (17%) HOMO-6->LUMO (6%) HOMO->LUMO+3 (3%)	CT	
598.1	0.0131	HOMO-4->LUMO (25%) HOMO-5->LUMO (24%)	CT	251

		HOMO-3->LUMO (17%) HOMO-1->LUMO+1 (8%) HOMO-2->LUMO (6%) HOMO-2->LUMO+1 (4%)
584.7	0.0729	HOMO-5->LUMO (32%) HOMO-1->LUMO+1 (15%) HOMO-2->LUMO (12%) HOMO-2->LUMO (6%) HOMO-1->LUMO+1 (5%) HOMO-6->LUMO (4%) HOMO-4->LUMO (3%) HOMO-1->LUMO (2%) HOMO-3->LUMO (2%) HOMO->LUMO+1 (2%) HOMO->LUMO+2 (2%) HOMO->LUMO+3 (2%)
577.4	0.0324	HOMO-6->LUMO (17%) HOMO->LUMO+3 (17%) HOMO-1->LUMO+2 (9%) HOMO-7->LUMO (9%) HOMO-5->LUMO (7%) HOMO-4->LUMO (6%) HOMO-2->LUMO (5%) HOMO-2->LUMO+1 (4%) HOMO-2->LUMO (3%) HOMO-3->LUMO (3%) HOMO->LUMO+3 (2%) HOMO-1->LUMO+1 (2%) HOMO-1->LUMO+2 (2%)
572.6	0.0133	HOMO-1->LUMO+2 (27%) HOMO-4->LUMO (16%) HOMO->LUMO+3 (14%) HOMO-2->LUMO+1 (9%) HOMO-1->LUMO+1 (6%) HOMO-5->LUMO (5%) HOMO-3->LUMO+1 (4%) HOMO-2->LUMO (3%) HOMO-6->LUMO (3%) HOMO-7->LUMO (2%)
557.8	0.0087	HOMO-2->LUMO+1 (31%) HOMO-4->LUMO (20%) HOMO-1->LUMO+2 (10%) HOMO->LUMO+3 (10%) HOMO-2->LUMO (5%) HOMO-3->LUMO+1 (3%) HOMO->LUMO+2 (3%) HOMO-3->LUMO (2%) HOMO-4->LUMO (2%)
548.8	0.008	HOMO-7->LUMO (62%) HOMO-5->LUMO (7%) HOMO-2->LUMO+1 (4%) HOMO-9->LUMO (3%) HOMO-2->LUMO+1 (2%)

		HOMO->LUMO+3 (2%)
544.7	0.0039	HOMO->LUMO+2 (52%) HOMO-1->LUMO+1 (19%) HOMO-2->LUMO+1 (3%) HOMO-1->LUMO+2 (3%) HOMO-10->LUMO (3%) HOMO-5->LUMO (3%) HOMO-9->LUMO (2%) HOMO-7->LUMO (2%) HOMO-6->LUMO (2%) HOMO->LUMO+3 (2%)
534.2	0.0007	HOMO-4->LUMO+1 (16%) HOMO-4->LUMO (12%) HOOM-7->LUMO (11%) HOMO-5->LUMO (9%) HOMO-5->LUMO+1 (7%) HOMO-3->LUMO+1 (6%) HOMO-2->LUMO+1 (6%) HOMO-9->LUMO (6%) HOMO-6->LUMO (3%) HOMO-6->LUMO+1 (3%) HOMO-6->LUMO (2%) HOMO-2->LUMO+1 (2%) HOMO-1->LUMO+2 (2%)
527.6	0.0014	HOMO-4->LUMO (34%) HOMO-2->LUMO+1 (16%) HOMO-3->LUMO+1 (11%) HOMO-6->LUMO (10%) HOMO-5->LUMO+1 (5%) HOMO-1->LUMO+2 (4%) HOMO-7->LUMO (4%) HOMO-4->LUMO+1 (4%) HOMO->LUMO+3 (3%) HOMO-3->LUMO (2%)
526.1	0.0004	HOMO-6->LUMO (23%) HOMO-5->LUMO+1 (15%) HOMO-10->LUMO (9%) HOMO-6->LUMO (9%) HOMO-3->LUMO (6%) HOMO-6->LUMO+1 (4%) HOMO-2->LUMO+1 (4%) HOMO-4->LUMO (3%) HOMO->LUMO+2 (3%) HOMO->LUMO+3 (3%) HOMO-11->LUMO (3%) HOMO-9->LUMO (3%) HOMO-5->LUMO (3%) HOMO-3->LUMO+1 (2%)
519.5	0.0013	HOMO-6->LUMO (14%) HOMO-11->LUMO (11%) HOMO-6->LUMO (10%) HOMO-5->LUMO+1 (8%)

		HOMO-3->LUMO (8%) HOMO-6->LUMO+1 (6%) HOMO->LUMO+2 (6%) HOMO-2->LUMO (5%) HOMO-7->LUMO (3%) HOMO-10->LUMO (3%) HOMO-2->LUMO+1 (2%) HOMO-3->LUMO+1 (2%) HOMO-1->LUMO+2 (2%)
513.4	0.0006	HOMO-9->LUMO (25%) HOMO-11->LUMO (16%) HOMO-6->LUMO (6%) HOMO-1->LUMO+3 (8%) HOMO-2->LUMO+1 (5%) HOMO-7->LUMO (4%) HOMO-1->LUMO+2 (4%) HOMO-14->LUMO (3%) HOMO->LUMO+4 (3%) HOMO-13->LUMO (2%) HOMO-10->LUMO (2%) HOMO->LUMO+2 (2%)
510.9	0.0027	HOMO-9->LUMO (36%) HOMO-2->LUMO+1 (11%) HOMO-11->LUMO (7%) HOMO-10->LUMO (5%) HOMO-1->LUMO+2 (5%) HOMO-7->LUMO (2%) HOMO-6->LUMO+1 (4%) HOMO-4->LUMO+1 (3%) HOMO-5->LUMO (2% HOMO-13->LUMO (2%) HOMO-7->LUMO+1 (2%) HOMO-3->LUMO+1 (2%)
506.9	0.0005	HOMO(A)->LUMO+4 (97%)
503.0	0.0058	HOMO-11->LUMO (31%) HOMO-2->LUMO+1 (11%) HOMO-3->LUMO (8%) HOMO-7->LUMO+1 (6%) HOMO-1->LUMO+2 (6%) HOMO-2->LUMO (5%) HOMO-12->LUMO (3%) HOMO-1->LUMO+3 (3%) HOMO-2->LUMO+2 (2%) HOMO-15->LUMO (2%) HOMO-13->LUMO (2%) HOMO-9->LUMO (2%)
1236.9	0.0199	[Au11-tmp] at the parallel plane surface to Au11 (Secondary N_{amine}) HOMO->LUMO (95%)
1097.7	0.0015	HOMO->LUMO (74%) HOMO-1->LUMO (23%)

		HOMO-1->LUMO (38%)
		H-OMO2->LUMO (19%)
931.2	0.0065	HOMO-1->LUMO (15%)
		HOMO->LUMO+1 (14%)
		HOMO->LUMO (5%)
		HOMO-1->LUMO (46%)
		HOMO-1->LUMO (22%)
918.1	0008	HOMO->LUMO (13%)
		HOMO-2->LUMO (8%)
		HOMO->LUMO+1 (4%)
		HOMO-1->LUMO (10%)
880.9	0.0045	HOMO->LUMO+1 (78%)
		HOMO-1->LUMO (3%)
		HOMO->LUMO (5%)
		HOMO-1->LUMO+1 (35%)
		HOMO->LUMO+1 (10%)
773.3	0.0006	HOMO->LUMO+2 (42%)
		HOMO-2->LUMO (5%)
		HOMO-3->LUMO (2%)
		HOMO-1->LUMO (3%)
		HOMO-2->LUMO (47%)
		HOMO-1->LUMO+1 (13%)
763.8	0.0099	HOMO-1->LUMO (22%)
		HOMO-3->LUMO (3%)
		HOMO-3->LUMO (9%)
		HOMO-3->LUMO (51%)
		HOMO-4->LUMO (22%)
		HOMO-2->LUMO (5%)
		HOMO->LUMO+1 (4%)
738.2	0.0058	HOMO->LUMO+2 (4%)
		HOMO-2->LUMO (3%)
		HOMO-3->LUMO (2%)
		HOMO-1->LUMO (2%)
		HOMO->LUMO+1 (67%)
		HOMO-5->LUMO (5%)
		HOMO->LUMO+2 (4%)
		HOMO-3->LUMO (4%)
713.3	0.0016	HOMO-5->LUMO+1 (4%)
		HOMO-1->LUMO (3%)
		HOMO-4->LUMO (2%)
		HOMO-1->LUMO+1 (2%)
		HOMO-2->LUMO (2%)
		HOMO-2->LUMO (51%)
		HOMO-4->LUMO (12%)
		HOMO-1->L+1 (10%)
		HOMO-2->LUMO+1 (4%)
681.8	0.0192	HOMO-6->LUMO (3%)
		HOMO-5->LUMO (2%)
		HOMO-4->LUMO (2%)
		HOMO-3->LUMO+1 (2%)
		HOMO-1->LUMO (2%)
		HOMO-1->LUMO+2 (35%)
667.7	0.0019	HOMO-2->LUMO+1 (24%)
		HOMO-3->LUMO (8%)

656.9	0.002	HOMO-1->LUMO+1 (7%) HOMO-2->LUMO (5%) HOMO-1->LUMO+1 (5%) HOMO-4->LUMO (4%) HOMO-3->LUMO+1 (2%) HOMO->LUMO+2 (2%)
645.4	0.0002	HOMO-4->LUMO (28%) HOMO-1->LUMO+1 (15%) HOMO->LUMO+2 (15%) HOMO-2->LUMO+1 (12%) HOMO-3->LUMO (7%) HOMO-1->LUMO+2 (6%) HOMO-1->LUMO+1 (5%)
620.5	0.0037	HOMO-2->LUMO (27%) HOMO-1->LUMO+1 (22%) HOMO-4->LUMO (7%) HOMO-5->LUMO (7%) HOMO-5->LUMO+1 (4%) HOMO-6->LUMO (4%) HOMO-7->LUMO (3%) HOMO-6->LUMO+1 (3%) HOMO-1->LUMO+2 (3%) HOMO-2->LUMO+1 (2%) HOMO-4->LUMO+1 (2%) HOMO-3->LUMO (2%) HOMO-3->LUMO+1 (2%) HOMO->LUMO+1 (2%)
610.8	0.0115	HOMO-1->LUMO+1 (29%) HOMO-5->LUMO (19%) HOMO-2->LUMO+1 (11%) HOMO-4->LUMO (8%) HOMO->LUMO+2 (5%) HOMO-5->LUMO+1 (5%) HOMO-1->LUMO+1 (2%) HOMO-3->LUMO+1 (2%) HOMO-2->LUMO+1 (2%) HOMO->LUMO+1 (2%)
605.8	0.006	HOMO-6->LUMO (14%) HOMO->LUMO+2 (12%) HOMO-3->LUMO+1 (10%) HOMO-1->LUMO+1 (8%) HOMO-1->LUMO+1 (8%) HOMO->LUMO+3 (5%) HOMO-5->LUMO (5%) HOMO-2->LUMO (5%) HOMO-3->LUMO (4%) HOMO-1->LUMO+2 (4%) HOMO->LUMO+2 (4%) HOMO-3->LUMO (4%) HOMO-6->LUMO (3%) HOMO-1->LUMO+2 (3%) HOMO-3->LUMO (55%) HOMO->LUMO+2 (26%)

		HOMO-2->LUMO (5%)
601.8	0.0019	HOMO->LUMO+2 (51%) HOMO-3->LUMO (25%) HOMO-6->LUMO (6%) HOMO-6->LUMO (3%) HOMO-7->LUMO (2%)
593.9	0.0016	HOMO-1->LUMO+3 (2%) HOMO-1->LUMO+2 (40%) HOMO-2->LUMO+1 (34%) HOMO-5->LUMO (8%) HOMO-6->LUMO (4%) HOMO-3->LUMO+1 (2%)
572.2	0.0037	HOMO-4->LUMO+1 (22%) HOMO-3->LUMO+2 (22%) HOMO-8->LUMO (10%) HOMO-4->LUMO (9%) HOMO-3->LUMO+1) (8%) HOMO-7->LUMO (5%) HOMO-7->LUMO (3%) HOMO-9->LUMO (2%) HOMO-2->LUMO+1 (2%)
566.1	0.012	HOMO-4->LUMO (40%) HOMO-4->LUMO+1 (14%) HOMO-3->LUMO+2 (9%) HOMO-1->LUMO+2 (6%) HOMO-2->LUMO+1 (3%) HOMO->LUMO+3 (3%) HOMO-5->LUMO (3%) HOMO-4->LUMO (2%) HOMO->LUMO+2 (2%) HOMO-5->LUMO+1 (2%)
558.9	0.0148	HOMO-4->LUMO (19%) HOMO-7->LUMO (18%) HOMO-6->LUMO (10%) HOMO-1->LUMO+2 (7%) HOMO-8->LUMO (4%) HOMO-8->LUMO (4%) HOMO-9->LUMO (3%) HOMO-4->LUMO (3%) HOMO-4->LUMO+1 (3%) HOMO-5->LUMO+1 (3%) HOMO-3->LUMO (3%) HOMO->LUMO+2 (2%) HOMO->LUMO+2 (2%) HOMO->LUMO+3 (2%)
552.7	0.0011	HOMO-2->LUMO+1 (19%) HOMO-8->LUMO (13%) HOMO-1->LUMO+2 (12%) HOMO-6->LUMO (9%) HOMO->LUMO+3 (8%) HOMO-7->LUMO (4%) HOMO-8->LUMO (3%) HOMO-4->LUMO+1 (3%)

	HOMO-5->LUMO (3%) HOMO-3->LUMO+2 (3%) HOMO-6->LUMO (2%)

Table S5. TD-DFT spectra of metal complexes in different spin states calculated at B3LYP functional with three different basis set: CEP-31G, CEP-121G and def2TZV at gaseous state.

	λ1	λ2	λ3	λ4
Au-TMPN$_{amine}$-corner	502	589	740	989
Au-TMPN$_{amine}$-center	552	726	1190	