Electronic Supplementary Material (ESI) for RSC Advances.

Supplementary Information

Gold nanoclusters as prospective carriers and detectors of pramipexole

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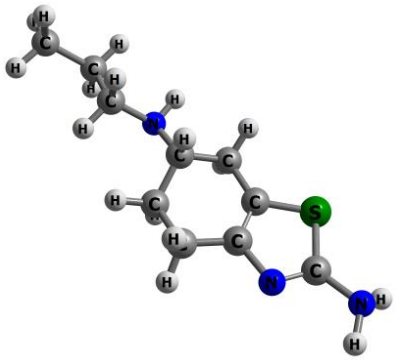
Table S1. Some basic properties of PPX tautomers including energies (eV) of frontier orbitals, HOMO–LUMO gap (E_g) and proton affinities (PA, kcal/mol) (PBE/cc-pVTZ + ZPE).

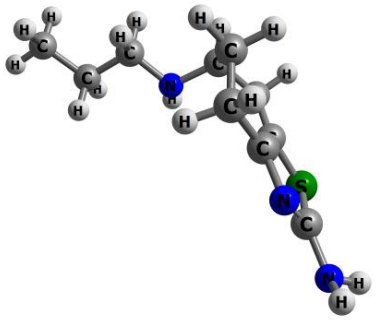
	HOMO	**LUMO**	**E_g**	**PA, kcal/mol**
PPX	-4.66	-0.87	3.79	
N (thiazole)				230.5
N (side chain)				229.3
N (amine)				205.1
S (thiazole)				192.8
***t*-PPX**	-4.55	-0.79	3.76	
N (thiazole)				232.5
N (side chain)				232.9
N (amine)				206.8
S (thiazole)				194.8

Table S2. Binding energy E_b, enthalpy $\Delta H°$, Gibbs energy $\Delta G°$ (in kcal.mol^{-1}) for the ***t*-PPX** binding to Au_N (N = 6, 8, 20) clusters (PBE/cc-pVDZ-PP/cc-pVTZ).

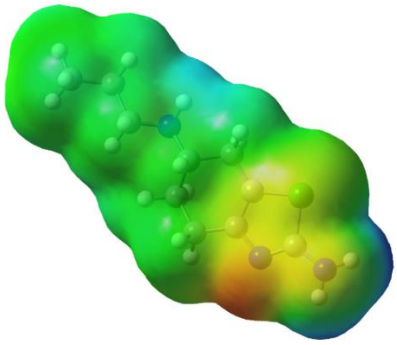
Complex	In gas phase			In water		
	E_b	$\Delta H°$	$\Delta G°$	E_b	$\Delta H°$	$\Delta G°$
Au_6-*t*-PPX_1	-24.94	-23.54	-14.77	-21.86	-20.47	-11.93
Au_6-*t*-PPX_2	-21.94	-20.26	-8.65	-20.02	-18.03	-7.29
Au_6-*t*-PPX_3	-16.91	-15.68	-7.77	-13.72	-12.58	-3.98
Au_6-*t*-PPX_4	-13.79	-12.08	-3.96	-12.06	-10.26	-0.78
Au_8-*t*-PPX_1	-31.30	-29.51	-15.65	-30.42	-27.89	-13.61
Au_8-*t*-PPX_2	-30.63	-29.03	-15.73	-23.40	-21.41	-10.50
Au_8-*t*-PPX_3	-29.19	-27.03	-12.90	-30.43	-27.90	-13.63
Au_8-*t*-PPX_4	-20.59	-19.87	-9.30	-18.42	-17.80	-6.26
Au_{20}-*t*-PPX_1	-23.22	-21.86	-13.96	-18.91	-17.51	-9.45
Au_{20}-*t*-PPX_2	-22.54	-20.78	-9.22	-19.78	-17.91	-8.72
Au_{20}-*t*-PPX_3	-15.29	-14.55	-5.72	-13.58	-12.80	-3.28
Au_{20}-*t*-PPX_4	-13.18	-11.95	-2.39	-11.66	-10.33	-0.08



PPX (0.0)



t-PPX (1.2 kcal/mol)



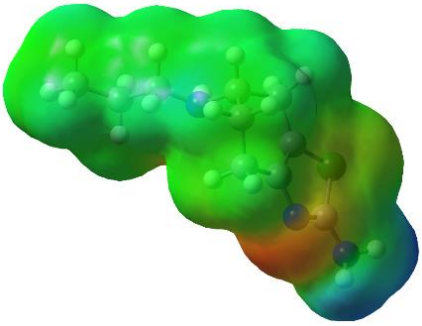


Figure S1. Optimized structures and molecular electrostatic maps of PPX tautomers.

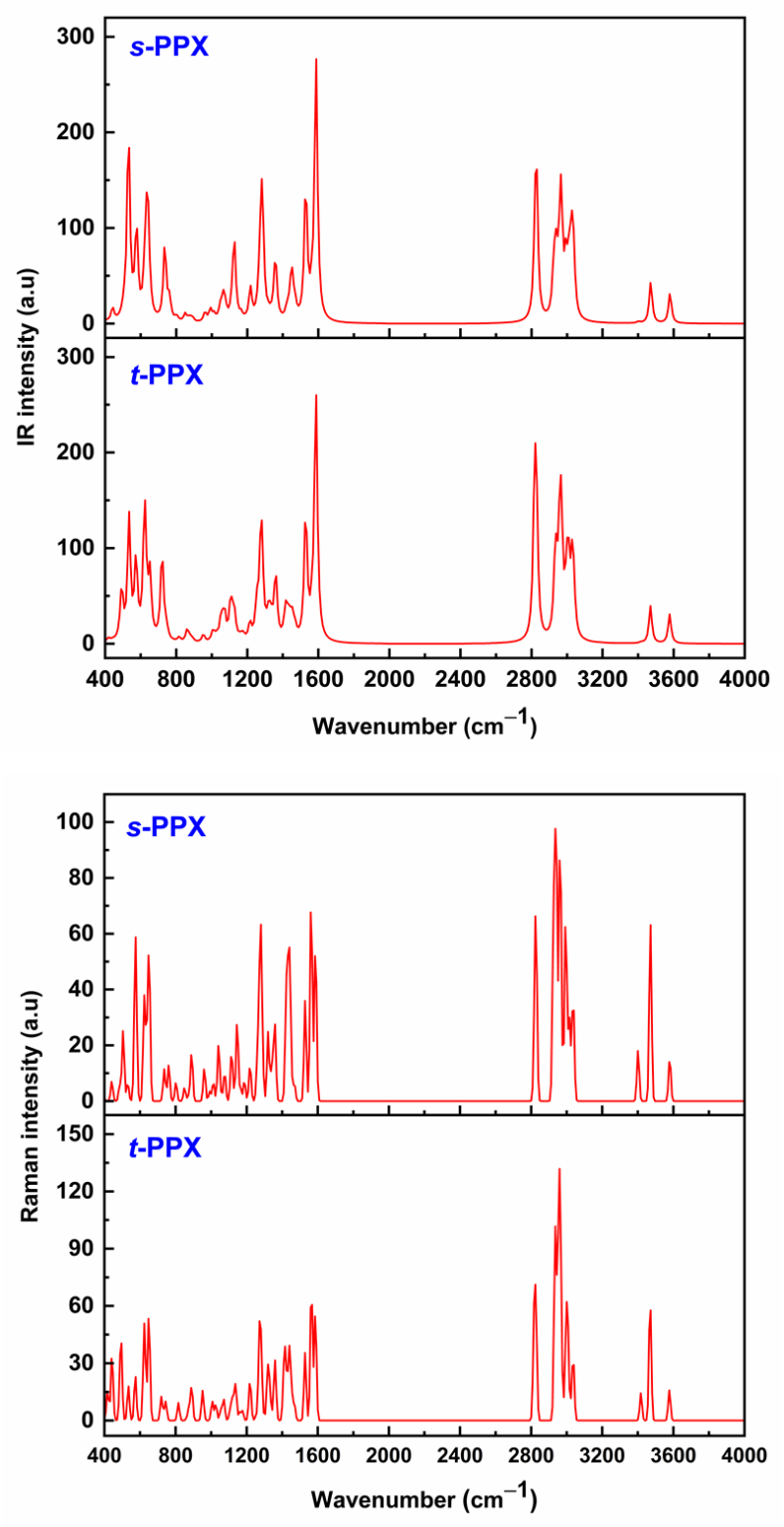


Figure S2. IR and Raman spectra of **PPX** and ***t*-PPX** tautomers in gas-phase