Supplementary Information

Sonochemical synthesis of polyoxometalate-stabilized gold nanoparticles for point-of-care determination of acetaminophen levels: preclinical study in animal model

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Table 4

Figure 4

Table S1: Physicochemical properties of acetaminophen.

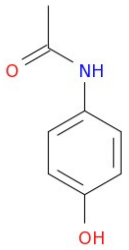
Drug	Chemical name and formula	Structure	So H2O (25°C mg.mL^{-1})	pKa
Acetaminophen (AP)	4-hydroxyacetanilide $C_8H_9NO_2$		14	9.5

Table S2. The most important IR vibrations for PMo_{12} and AuNPs@PMo_{12} nano-hybrid.

Band assignment	Observed band (cm^{-1}) AuNPs@PMo_{12}	Observed band (cm^{-1}) PMo_{12}
ν_{as} (P-O)	1080	1060
ν_{as} (Mo-Od)	1033	966
ν (Mo–Ob–Mo)	---	876
ν (Mo–Oc–Mo)	619	796
δ H2O	1660	1600
ν OH	3430	3400

Table S3. Effect of temperature on maximum absorbance of AuNPs@ PMo_{12} nano-hybrid upon addition of AP (synthesis condition: intensity= 26 Wcm^{-2}, Au: POM ratio (1:2)).

Sample	Maximum Absorbance, nm		
	27±1°C	**37±1°C**	**47±1°C**
AuNPs@ PMo_{12}	533	538	550
AuNPs + 30 mg/L	559	572	612
AuNPs + 70 mg/L	565	588	650

Table S4: Effect of acoustic intensity on maximum absorbance of AuNPs@ PMo_{12} nano-hybrid upon addition of AP (synthesis condition; T=37±1°C, Au: POM ratio (1:2)).

Sample	Maximum Absorbance, nm		
	21 Wcm^{-2}	**26 Wcm^{-2}**	**30.5 Wcm^{-2}**
AuNPs@ PMo_{12}	537	541	550
AuNPs + 30 mg/L	558	556	570
AuNPs + 70 mg/L	568	607	593

Table S5: Effect of Au: POM ratio on maximum absorbance of AuNPs@ PMo_{12} nanohybrid upon addition of AP (synthesis condition; intensity= 26 Wcm^{-2}, T=37±1°C).

Material	Maximum Absorbance, nm		
	Au1:POM2	**Au1:POM1**	**Au2:POM1**
AuNPs@ PMo_{12}	543	541	552
AuNPs + 30 mg/L	554	545	552
AuNPs + 70 mg/L	602	566	559

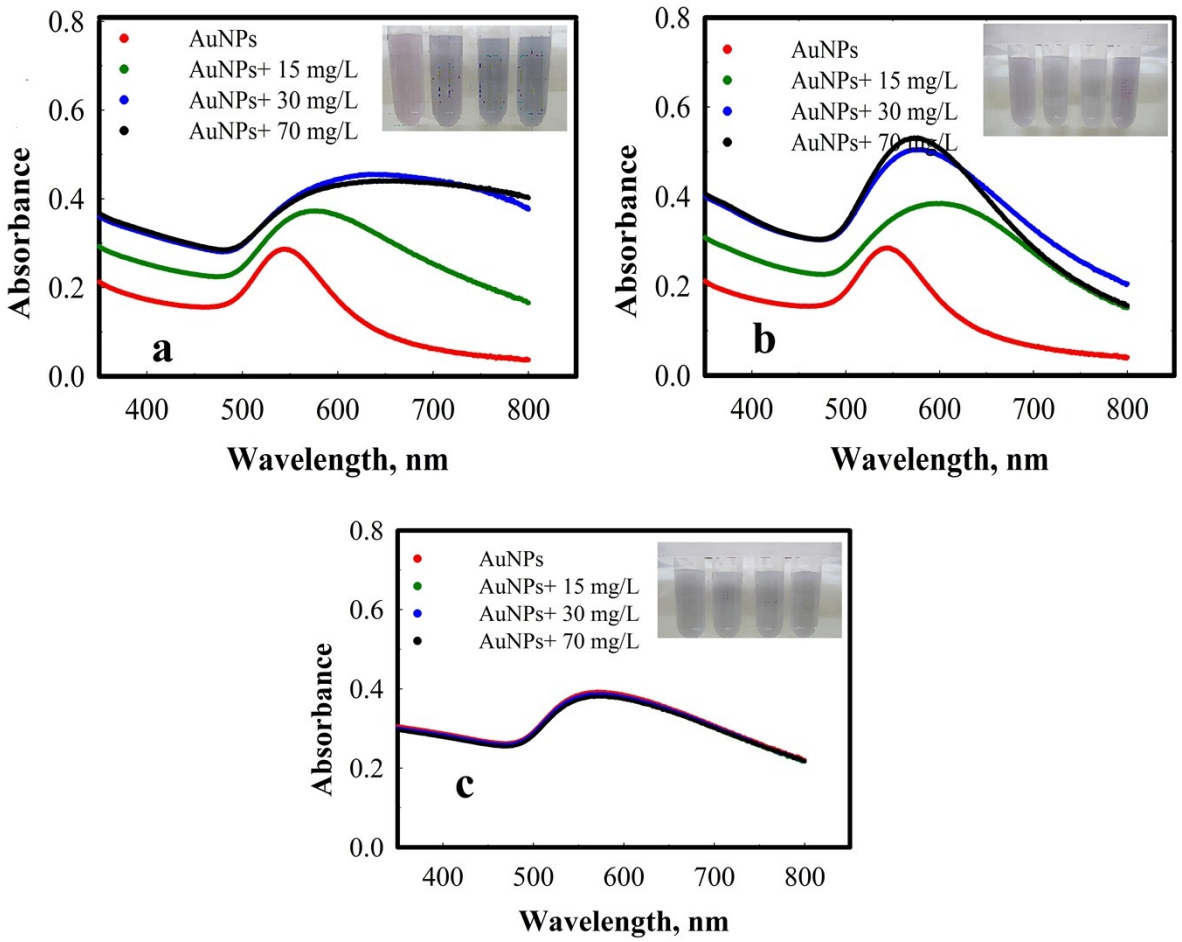


Fig.S1. a) UV-visible absorption spectra of AuNPs@ PMo_{12} upon addition of AP solution at a) pH 6.0±0.5, b) pH 9.0±0.5, c) pH 12.0±0.5. Photographic images from left to right (AuNPs@ PMo_{12} +0 mg/L, AuNPs@ PMo_{12} +15 mg/L, AuNPs@ PMo_{12} +30 mg/L, and AuNPs@ PMo_{12} +70mg/L) (synthesis condition; intensity: 26 Wcm^{-2}, T=37±1°C, Au:POM ratio (1:2)).

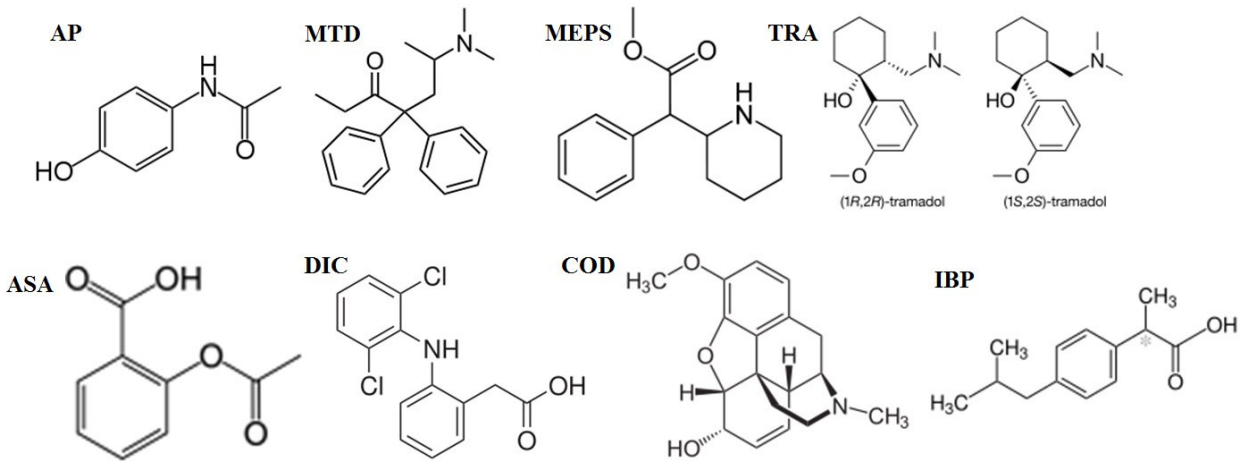


Fig.S2. Chemical structures of drugs

Diagnostic accuracy of the nanosensor

Regarding checking the accuracy of the nanosensor after making 300 standard samples, 100 of which were prepared with concentrations more than 100 µg/mL, 100 with concentrations of 25-100 µg/mL, and 100 with concentrations less than 25 µg/mL and using the area under the ROC curve, it was found that in detection of toxic cases, this nanosensor had 0.972 area under the ROC curve , 99% sensitivity, 97% specificity, 94.28% positive predictive value and 99.48% negative predictive value (Fig. S2). In detection of non-toxic cases, this nanosensor had also 0.969 area under the ROC curve, 92% sensitivity, 98.5% specificity, 96.84% positive predictive value and 96.09% negative predictive value (Figure S3). All these findings confirm the very high diagnostic accuracy of the nanosensor.

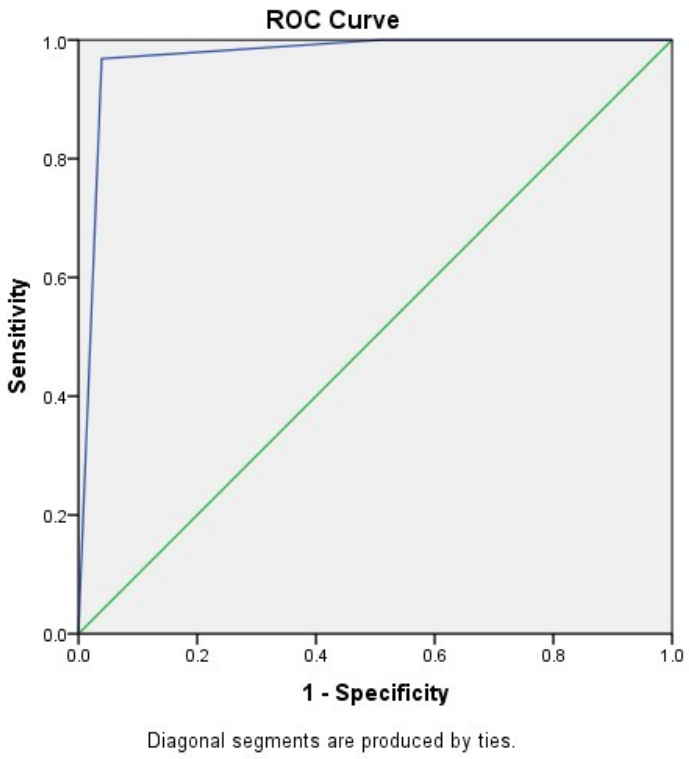


Fig. S3. Evaluation of the diagnostic accuracy of the nanosensor in detection of samples with toxic concentration (AP concentration more than 100 µg/mL).

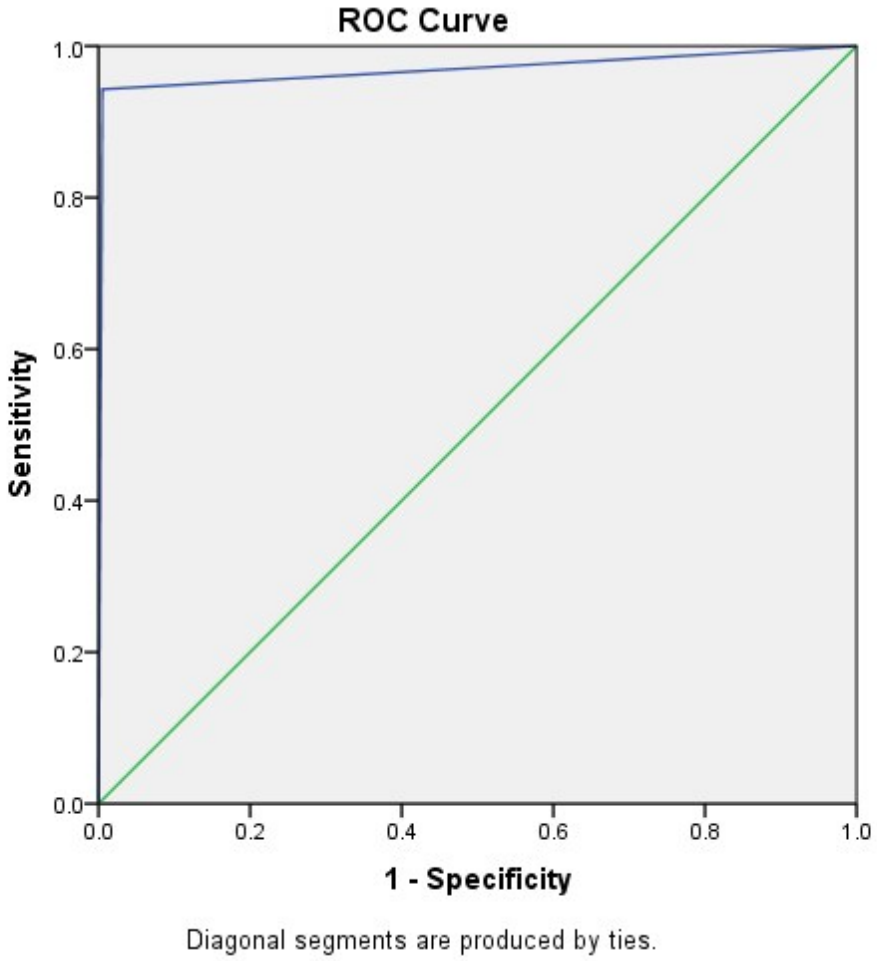


Fig. S4. Evaluation of the diagnostic accuracy of the nanosensor in detection of samples with toxic concentration (AP concentration less than 25 µg/mL).