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MDPI

Supporting Information for

Complexation of Gold(III) with Pyridoxal 5′-Phosphate-Derived Hydrazones in Aqueous Solution

Natalia N. Kuranova, Daniil N. Yarullin, Maksim N. Zavalishin, George A. Gamov *

Department of General Chemical Technology, Ivanovo State University of Chemistry and Technology, 153000 Ivanovo, Russia

* Correspondence: ggamov@isuct.ru; Tel.: +7-(915)-821-85-62

Table S1. Preliminary virtual screening results using PASS Online software [1].

Compound	Strain	Disease	Confidence
PLP-INH	*RESISTANT Mycobacterium tuberculosis H37Rv*	Tuberculosis	0.1909
	Enterococcus faecalis ATCC 29212	Bacterial infection	0.1762
Complex Au^{3+}-**PLP-INH**	*RESISTANT Mycobacterium tuberculosis H37Rv*	Tuberculosis	0.2552
	Enterococcus faecalis ATCC 29212	Bacterial infection	0.1930
Complex Au^{3+}-**PLP-F2H**	*RESISTANT Mycobacterium tuberculosis H37Rv*	Tuberculosis	0.1781
PLP-T2H	*Dialister micraerophilus*	Periodontitis	0.3580
	Dialister pneumosintes		0.3580
	Dialister propionicifaciens		0.2577
	Dialister invisus		0.2190
	Mycobacterium mageritense	Tuberculosis	0.1647
Complex Au^{3+}-**PLP-T2H**	*Dialister pneumosintes*	Periodontitis	0.3812
	Dialister micraerophilus		0.3812
	Dialister propionicifaciens		0.2850
	Dialister invisus		0.2349
	Mycobacterium mageritense	Tuberculosis	0.1582
PLP-T3H	*Dialister invisus*	Periodontitis	0.5628
Complex Au^{3+}-**PLP-T3H**	*Dialister invisus*	Periodontitis	0.5836

"AntiBac-Pred functional of PASS Online software allows user to predict the fact that chemical compound can inhibit the growth of one or more of 353 bacteria in concentration below the 10000 nM. The score for each compound is expressed as confidence in its activity, which is a difference between probabilities for chemical compound to inhibit and to do not inhibit the growth of the particular bacteria. The higher confidence means the higher chance of the positive prediction to be true.

Only activities with $P_a > P_i$ (confidence > 0) are considered as possible for a particular compound". The description is taken from [2].

Reference

1. Biomed. Chem.: Res. Methods, 2018, 1(1), e00004, doi: 10.18097/bmcrm00004
2. http://www.way2drug.com/antibac/

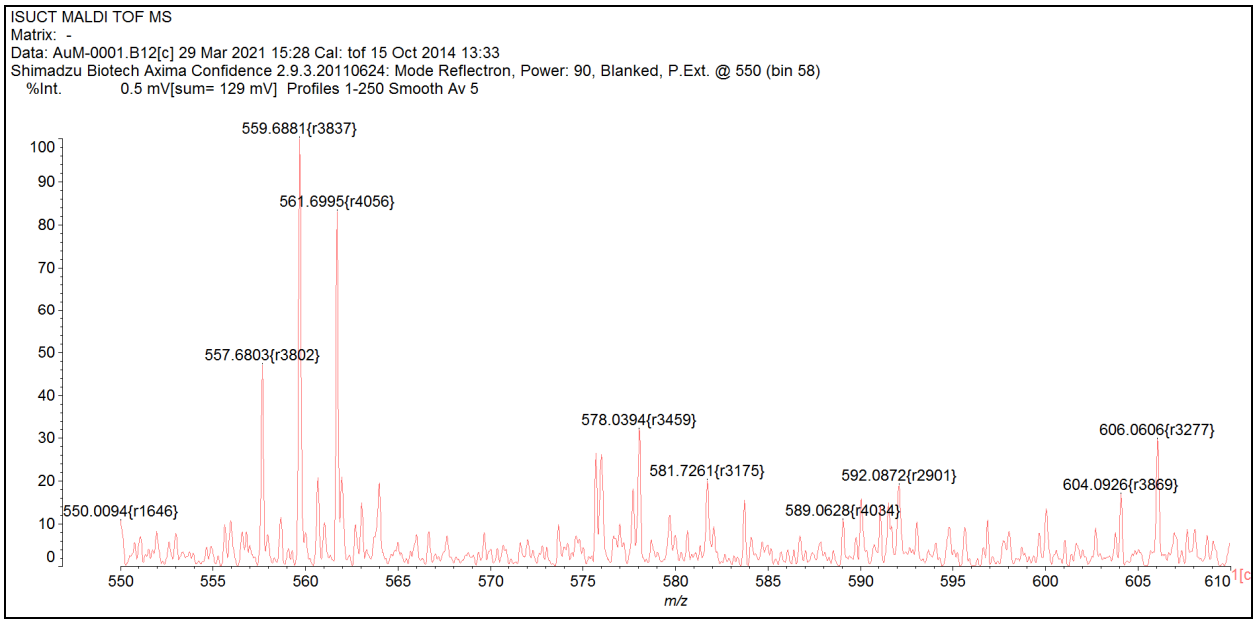

Figure S1. Mass-spectrum of Au-**PLP-INH** complex precipitated from an aqueous solution.

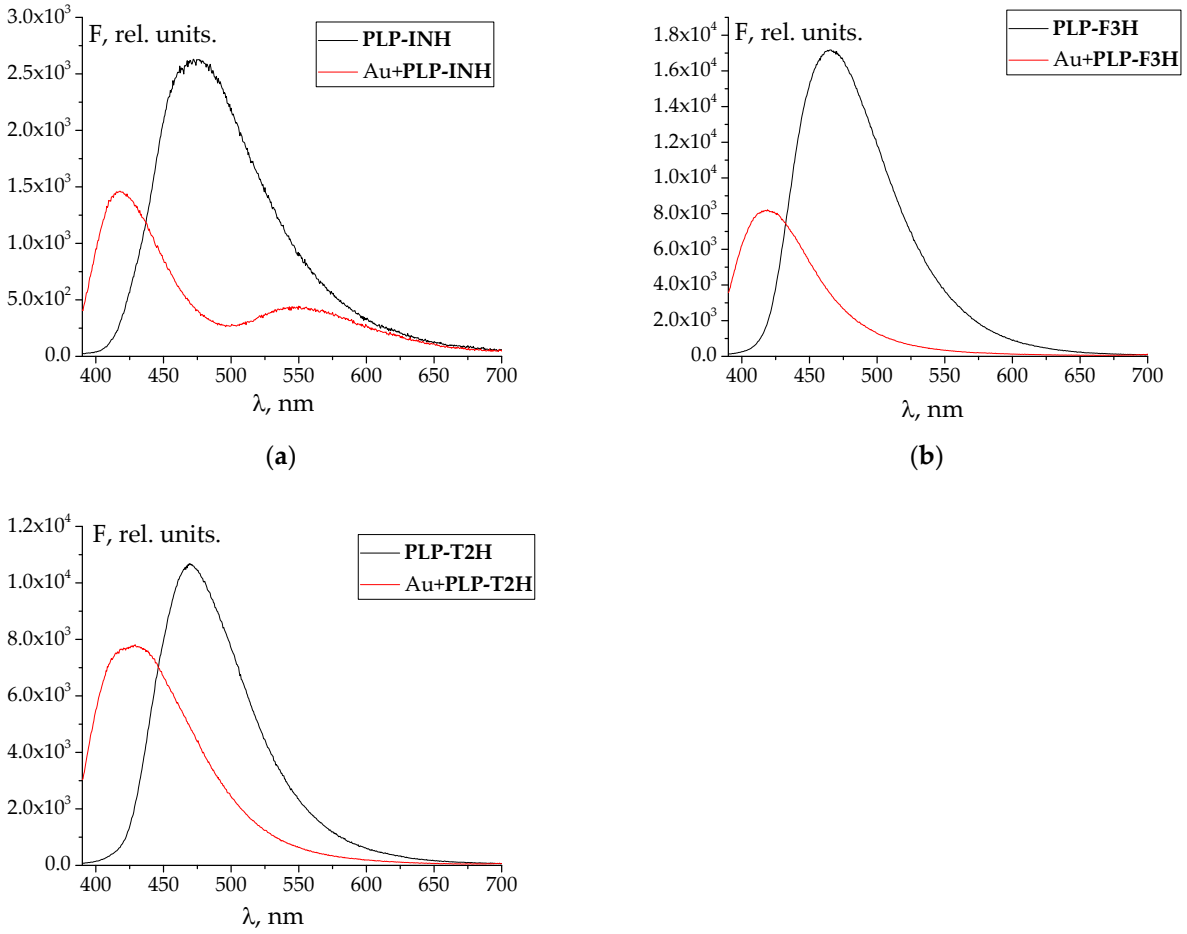

Figure S2. Emission spectra of free hydrazones and their mixtures with Au^{3+}: (**a**) **PLP-INH**; (**b**) **PLP-F3H**; (**c**) **PLP-T2H**. λ_{ex} = 365 nm.

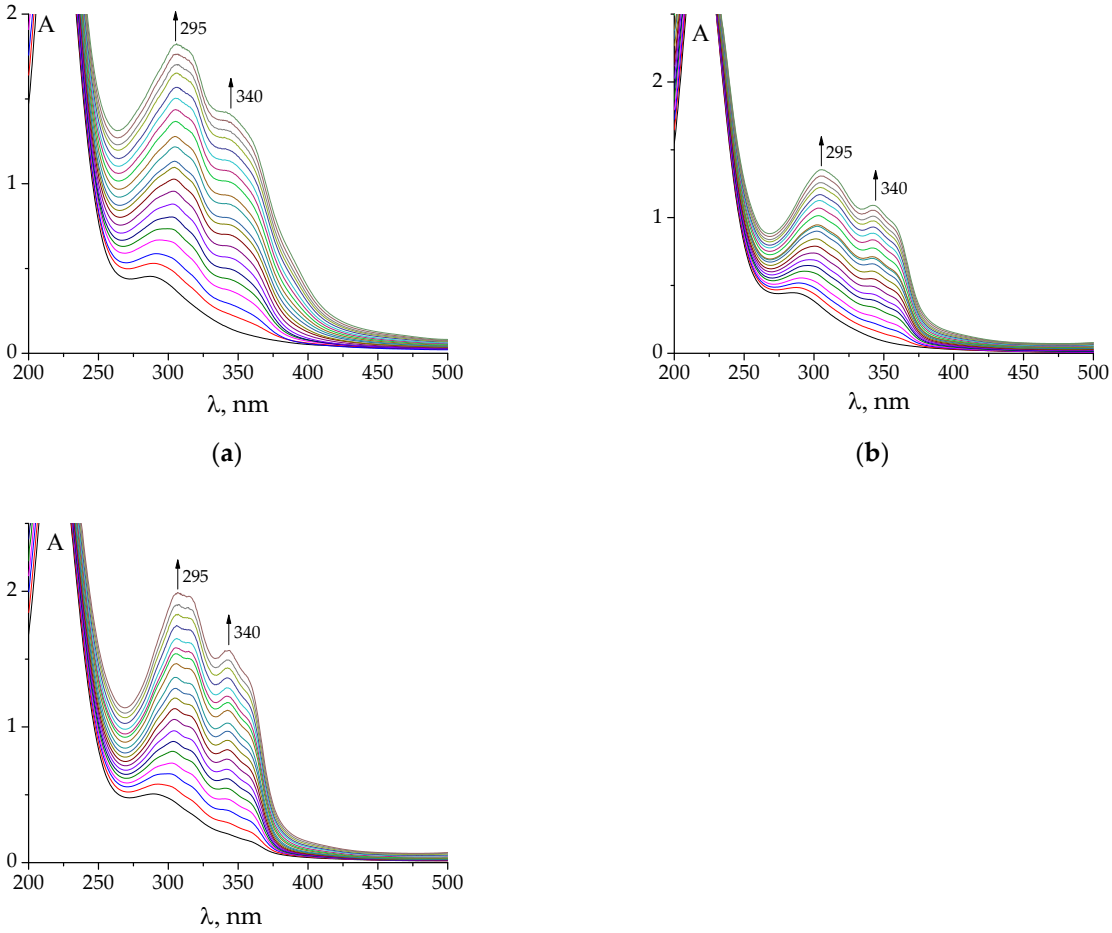

Figure S3. Examples of changes in UV-Vis spectra of $HAuCl_4$ upon addition of **PLP-INH** (**a**), **PLP-F3H** (**b**), **PLP-T3H** (**c**). Titrand: $C(AuCl_4^-) = 2 \cdot 10^{-4}$ mol L^{-1}; $C(H^+) = 5 \cdot 10^{-4}$ mol L^{-1}. Titrant: C(**PLP-INH**) = $1.5 \cdot 10^{-3}$ mol L^{-1}; $C(OH^-) = 0.01074$ mol L^{-1} (**a**); Titrant: C(**PLP-F3H**) = $1.5 \cdot 10^{-3}$ mol L^{-1}; $C(OH^-) = 0.01074$ mol L^{-1} (**b**); Titrant: C(**PLP-T3H**) = $1.5 \cdot 10^{-3}$ mol L^{-1}; $C(OH^-) = 0.01074$ mol L^{-1} (**b**). Twenty additions of 10 μL volume.

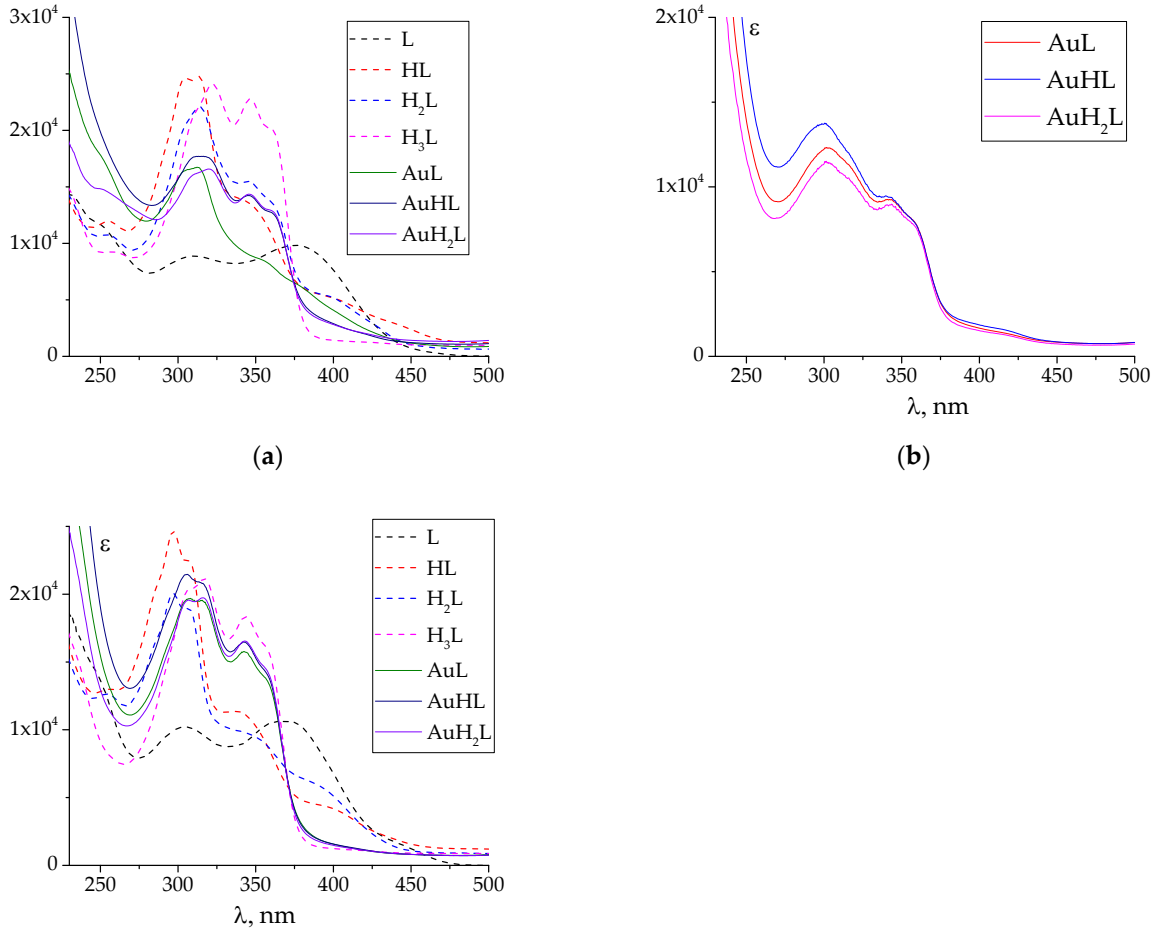

Figure S4. Calculated UV-Vis spectra of individual protonated and complex species of **PLP-T2H** (**a**), **PLP-F3H** (**b**), **PLP-T3H** (**c**). Spectra of protonated species are adopted from paper 10.1016/j.molliq.2020.112822.