chemosensors

MDPI

Supplementary Materials

Analyzing the electrochemical interaction of the angiogenesis inhibitor batimastat by surface-enhanced Raman spectroscopy

Ewa Pięta,[1] CzesławaPaluszkiewicz,[1] W. M. Kwiatek, [1] Maria Rosa Lopez-Ramirez[2]*

[1] Institute of Nuclear Physics Polish Academy of Sciences, PL-31342 Krakow, Poland
[2] Department of Physical Chemistry, Faculty of Science, University of Málaga, E-29071 Málaga, Spain
* Correspondence: María Rosa López-Ramírez, mrlopez@uma.es

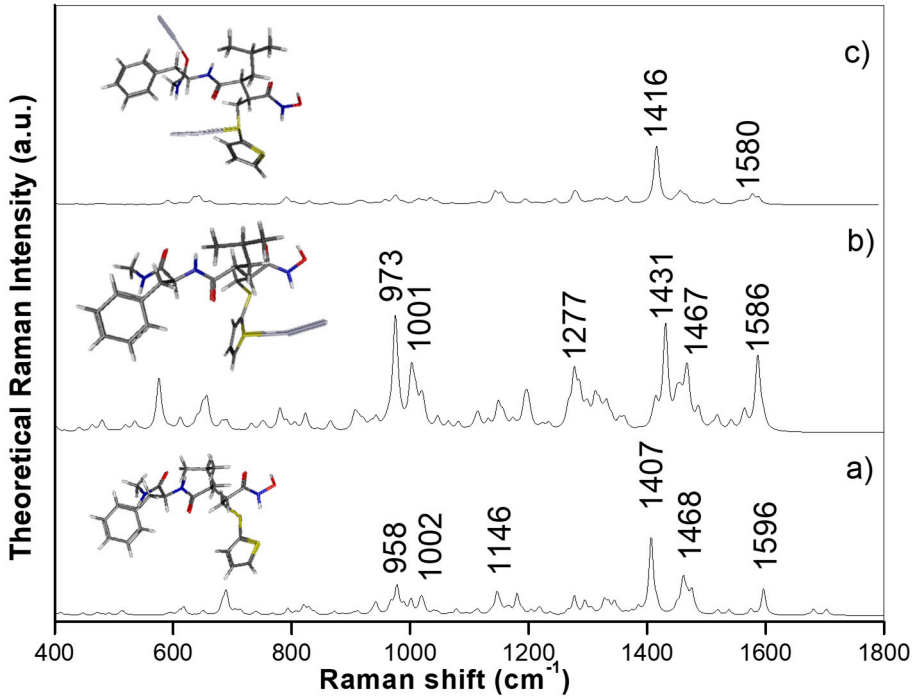
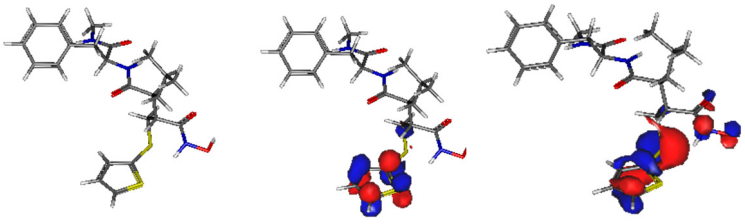
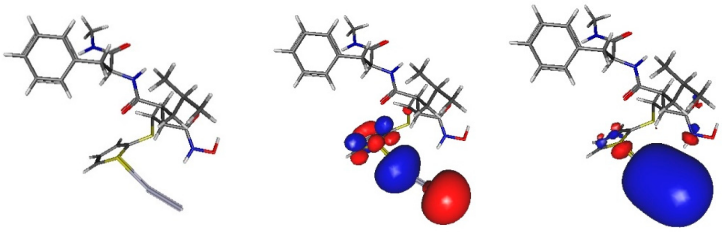
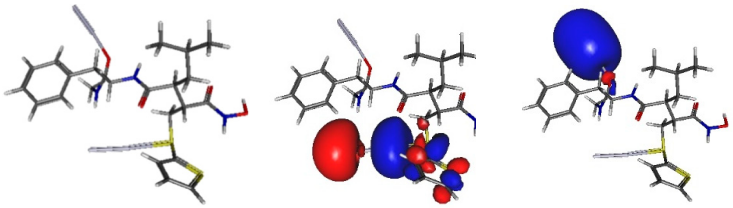


Figure S1. Theoretical Raman spectra (inset: molecular optimized structure of each species) calculated at B3LYP/6-31G(d,p) level of theory of: a) BB-94 and at B3LYP/LanL2DZ level of theory of b) BB-94-SAg and c) BB-94-SAg-OAg.

Table S1. Plot showing the optimized structures and HOMO and LUMO energy levels for BB-94 and corresponding metal complexes. The orbital energies are in atomic units (a. u.) and the GAP is in electron volts (eV).

Name	Optimized structure	HOMO (a.u.)	LUMO (a.u.)	GAP (eV)
BB-94				
		-0.23169	**-0.03563**	**5.34**

BB-94-SAg				
		-0.19489	**-0.07838**	**3.17**
BB-94-SAg-OAg				
		-0.17118	**-0.08388**	**2.38**

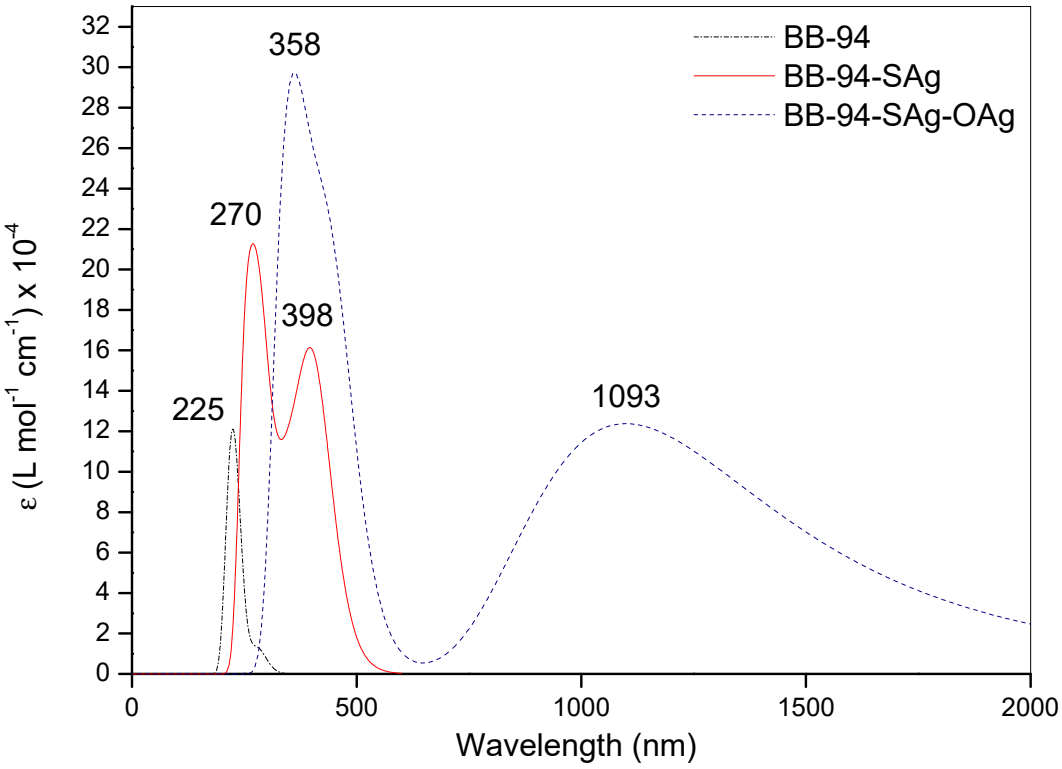


Figure S2. Computed UV-Vis absorptionspectra calculated by using DFT-TD at B3LYP/6-31G(d,p) level of theory for BB-94 and B3LYP/LanL2DZ level of theory for BB-94-SAg and BB-94-SAg-OAg.