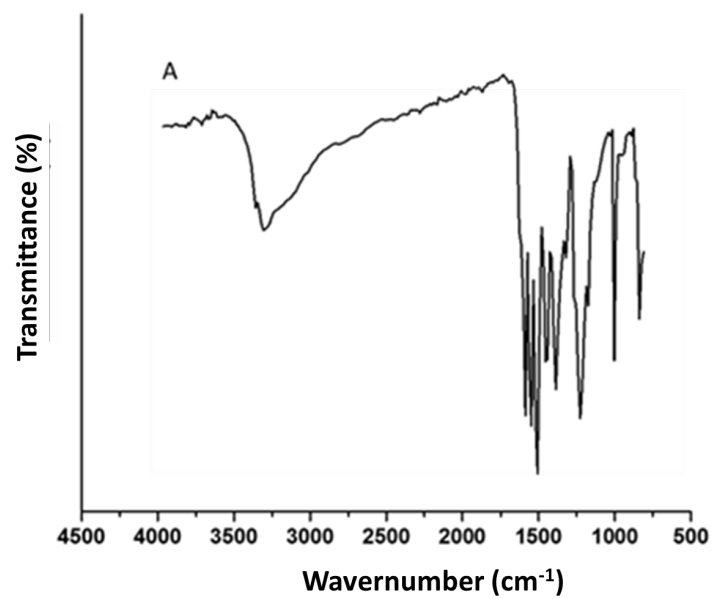


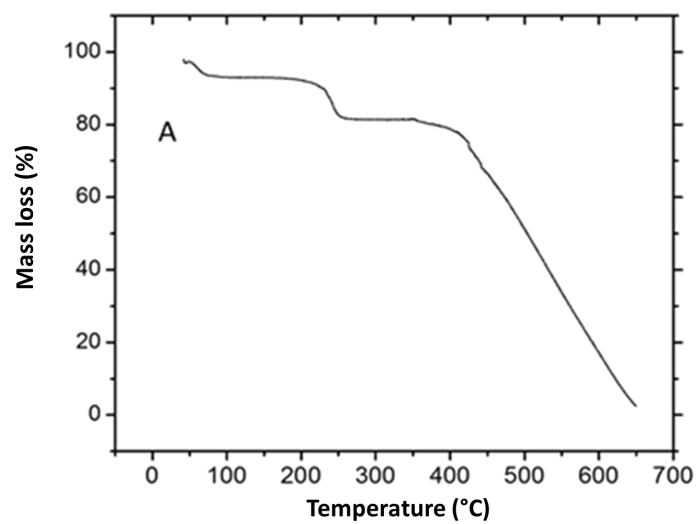
Supplementary Information

***In-silico* and *in vitro* analysis of the 4,4',4''-((1,3,5-triazine-2,4,6-triyl)tris(azanediyl))triphenol, an antioxidant agent with a possible anti-inflammatory function**

Ricardo I. Castro, Felipe Valenzuela-Riffo, Luis Morales-Quintana



**Figure S1. FTIR spectrum of synthetic TP derivate**



**Figure S2. TGA thermogram of triazine phenol derivative.**

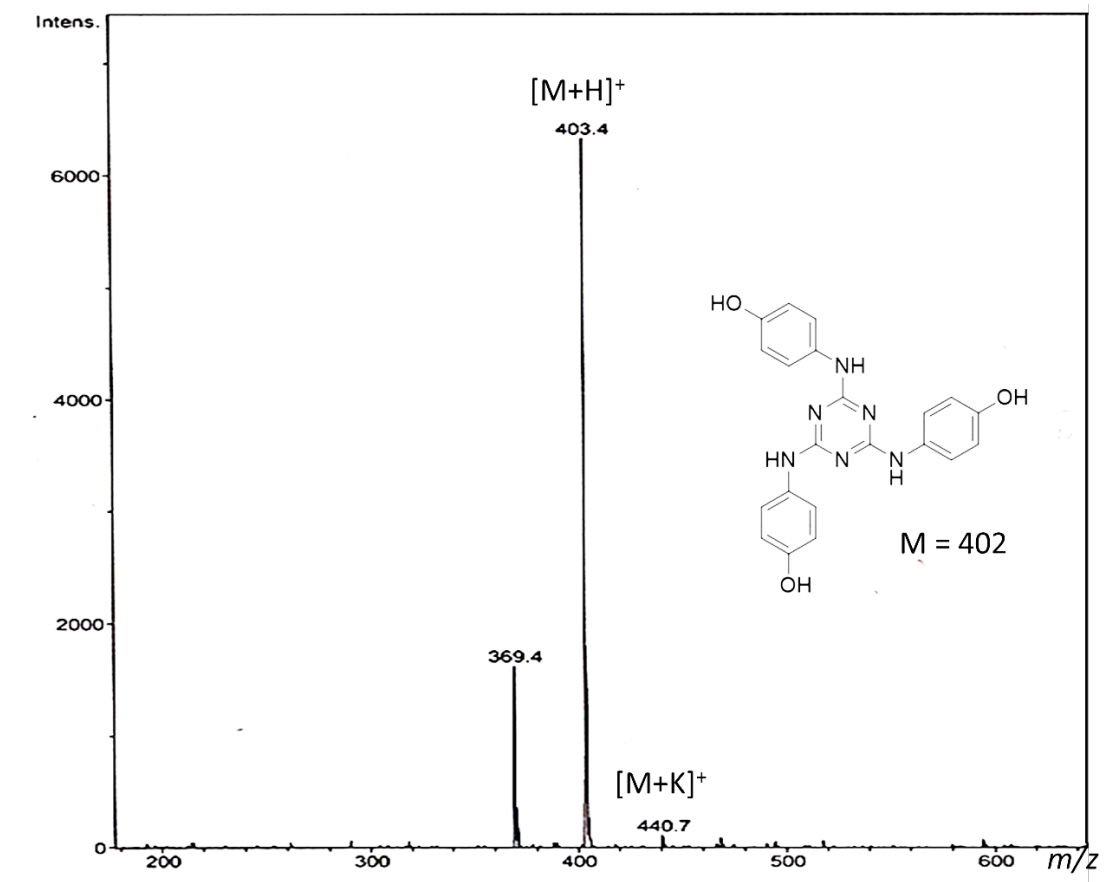
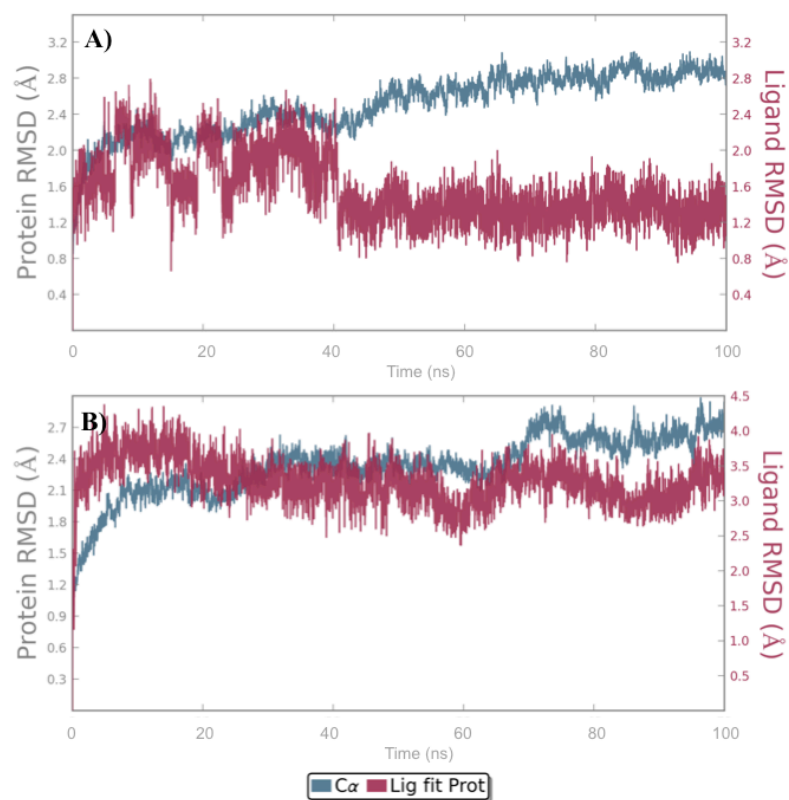
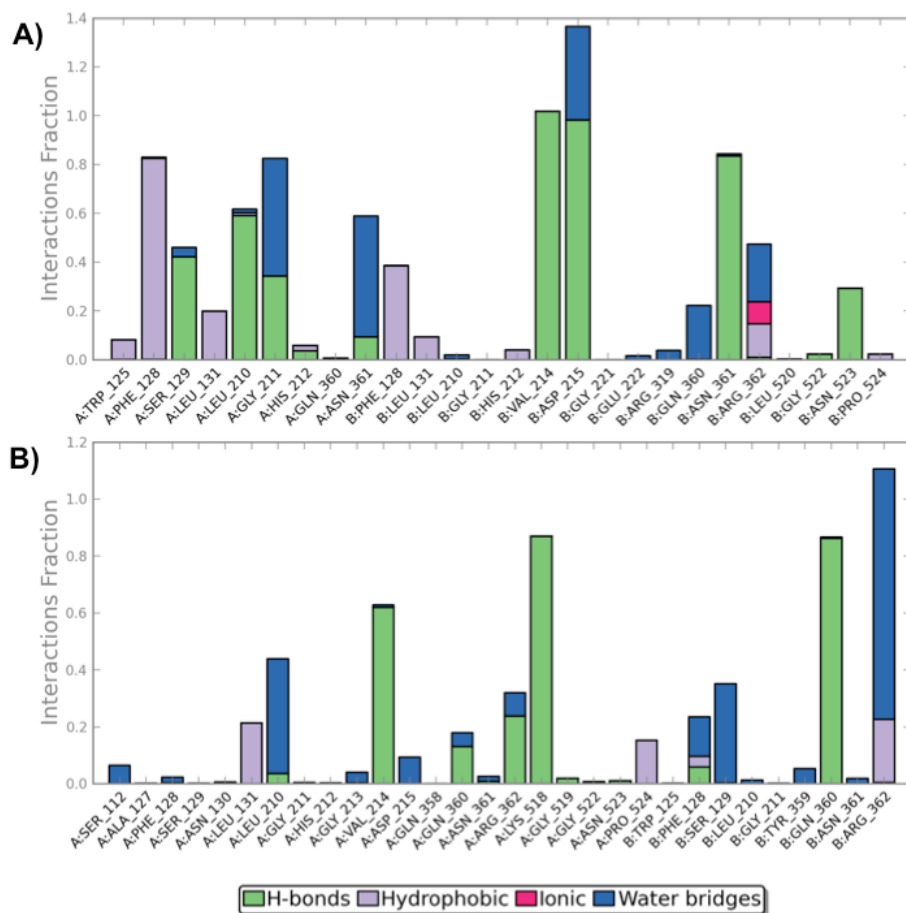


Figure S3. MASS spectrometry spectrum.



**Figure S4. RMSD of the protein ligand complex.** A) COX-2\_TP derivative complex. B) COX-2\_Quercetin complex. In dark blue showed the RMSD value of the  $C\alpha$  of the COX-2 protein, in red showed the RMSD value of the each ligand in the respective graph.



**Figure S5. Protein-ligand interactions (or 'contacts') in each protein-ligand complex.**

A) COX-2\_TP derivative complex. B) COX-2\_Quercetin complex. Four types of interaction were described; the hydrogen bonds are showed in green, the hydrophobic interactions are showed in purple, the ionic interactions are showed in red and water bridges is showed in blue.