

Supplementary Materials: Triose Phosphate Isomerase Structure-Based Virtual Screening and In Vitro Biological Activity of Natural Products as *Leishmania mexicana* Inhibitors

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The supplementary material corresponds to the additional docking studies of the compounds B-3 and S-3 as well as the prediction of pKa values.

Docking results

The next figures (Fig. 1S and 2S) describe the interactions of B-3 and S-3 at *Lm*TIM and *Hs*TIM interface, respectively.

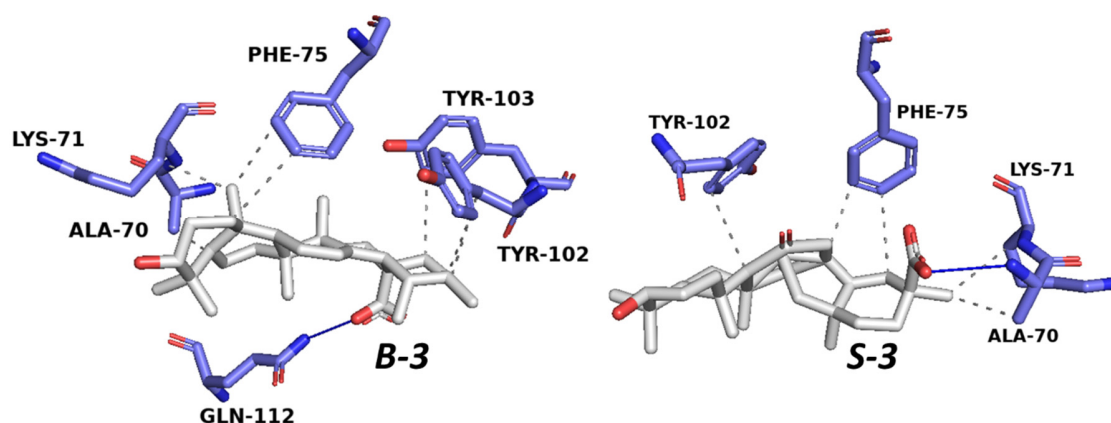


Figure S1. 3D interactions of compounds B-3 and S-3 in their ionized form at *Lm*TIM interface.

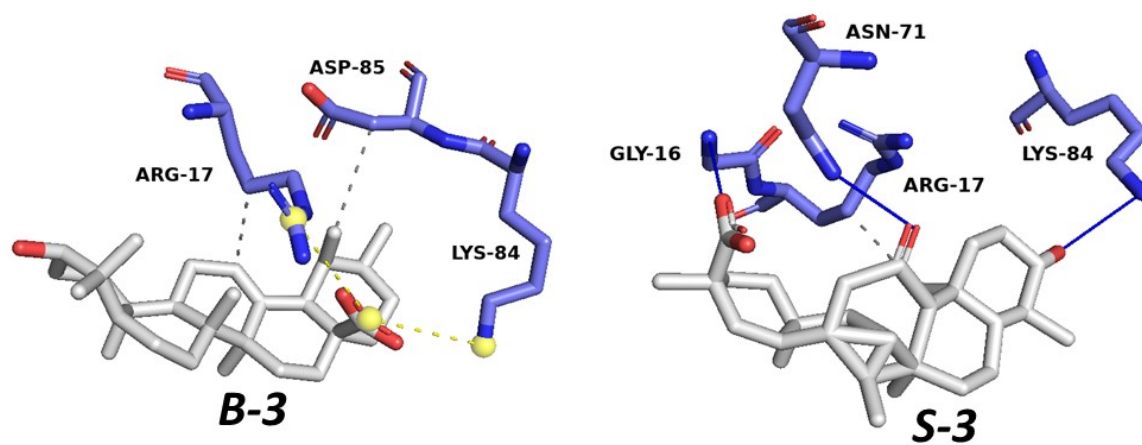
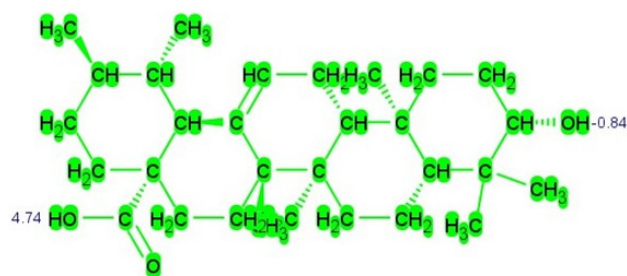


Figure S2. 3D interactions of compounds **B-3** and **S-3** in their ionized form.

pKa prediction

Compound B-3 (ursolic acid)



pKa = 4.74

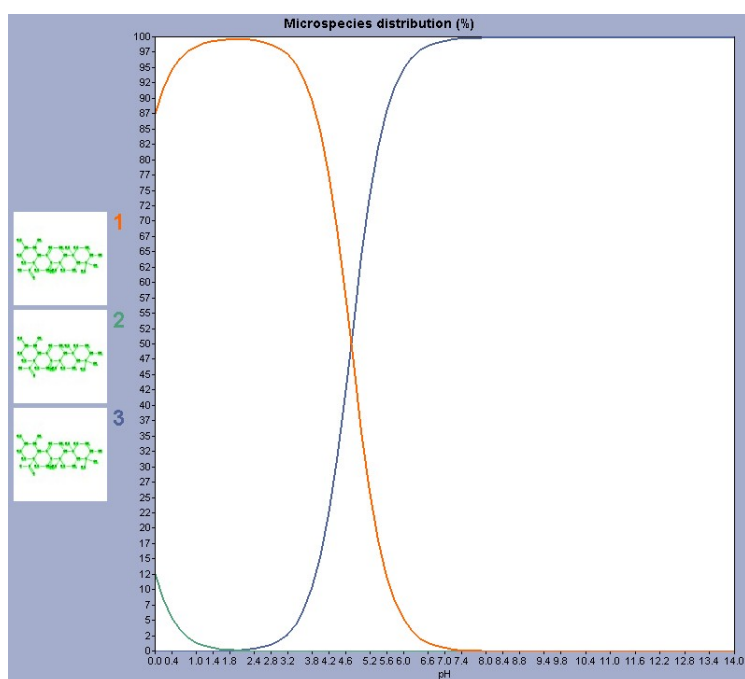
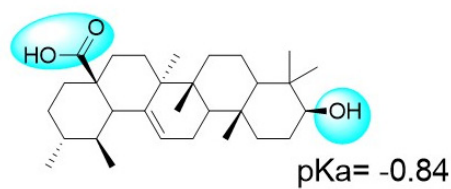


Figure S3. Determination of pKa B-3 using in silico prediction.

Compound S-3

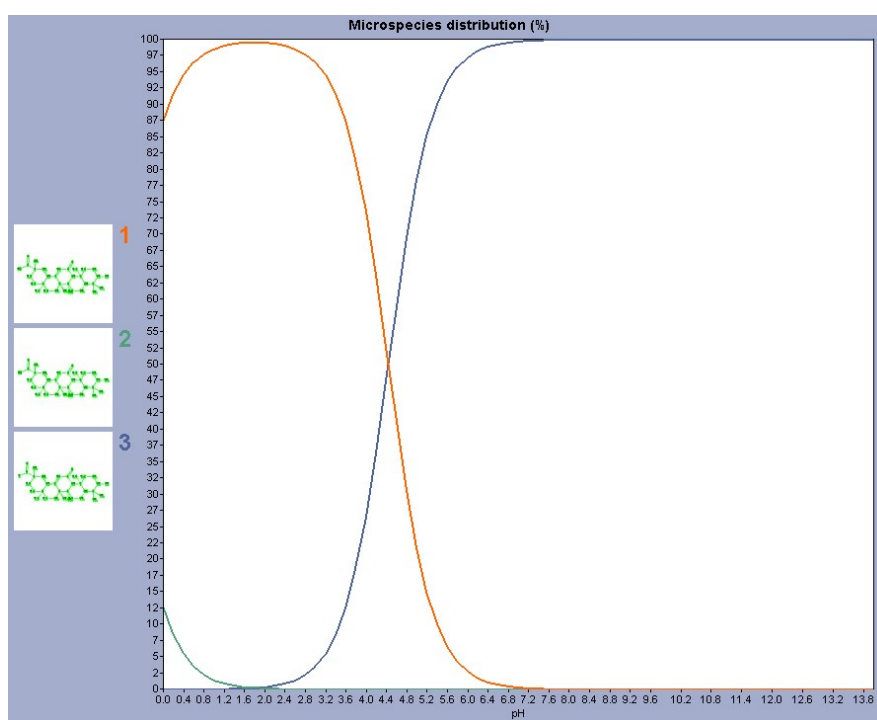
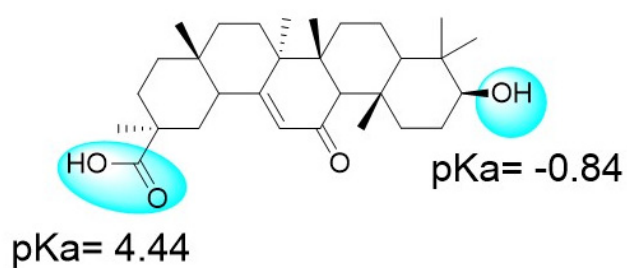
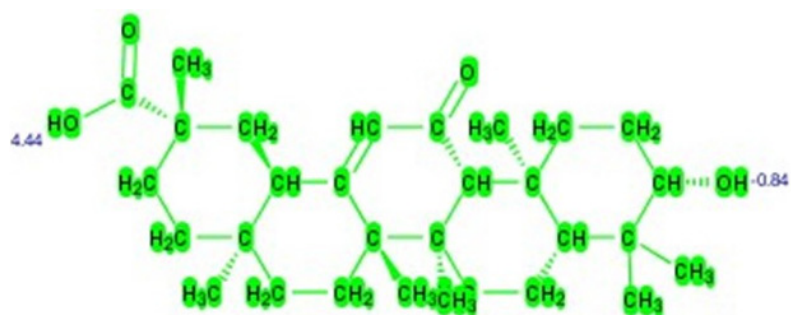


Figure S4. Determination of pKa S-3 using in silico prediction.