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SUPPL. MATERIAL

In silico antimalarial bioprospecting of neem (*Azadirachta indica*) quinine-derivative alkaloids

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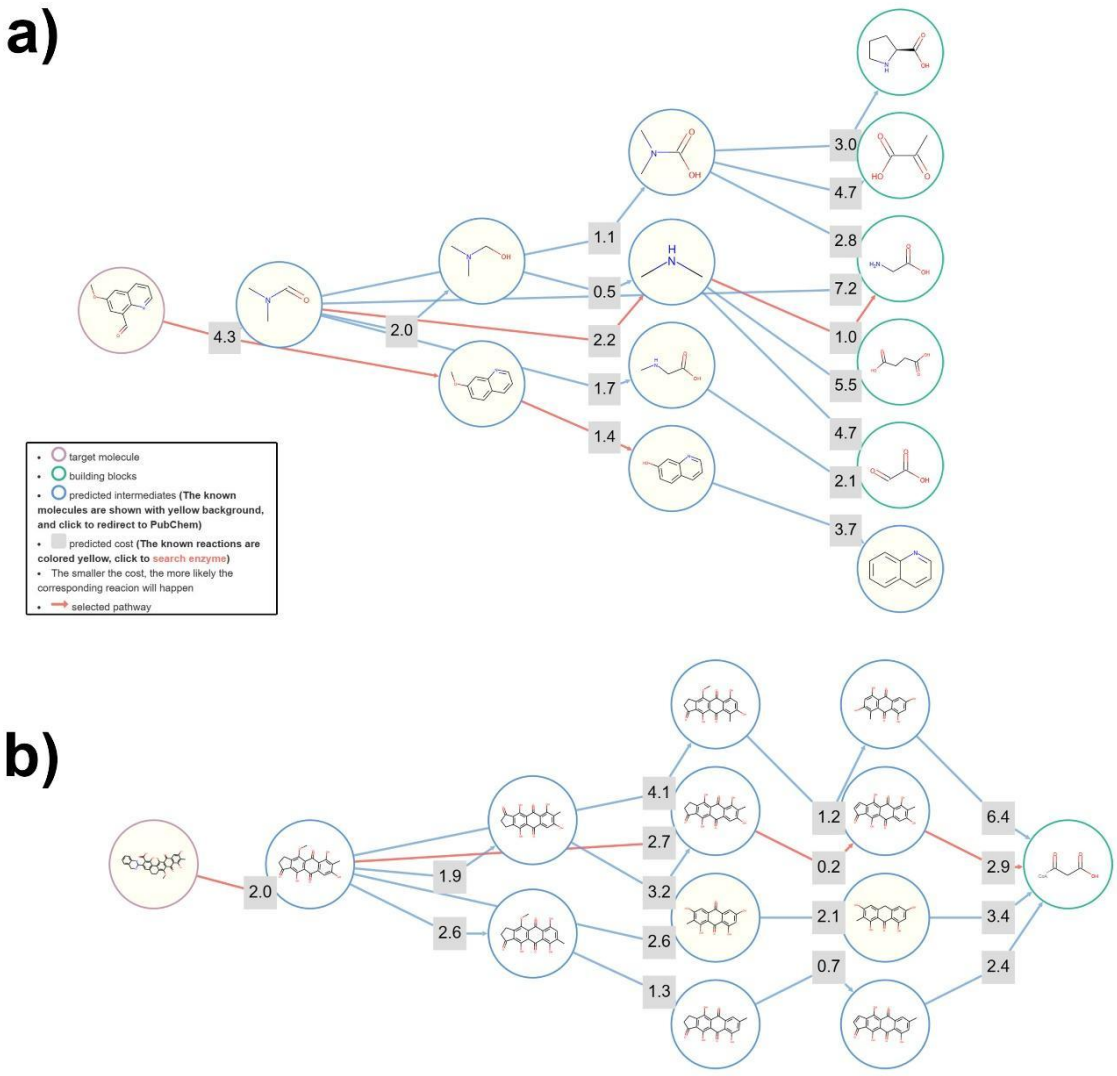

Figure 1. BioNavi-predicted metabolic pathway of compounds a) A and b) B. Further details on BioNavi results in Supplementary Data.

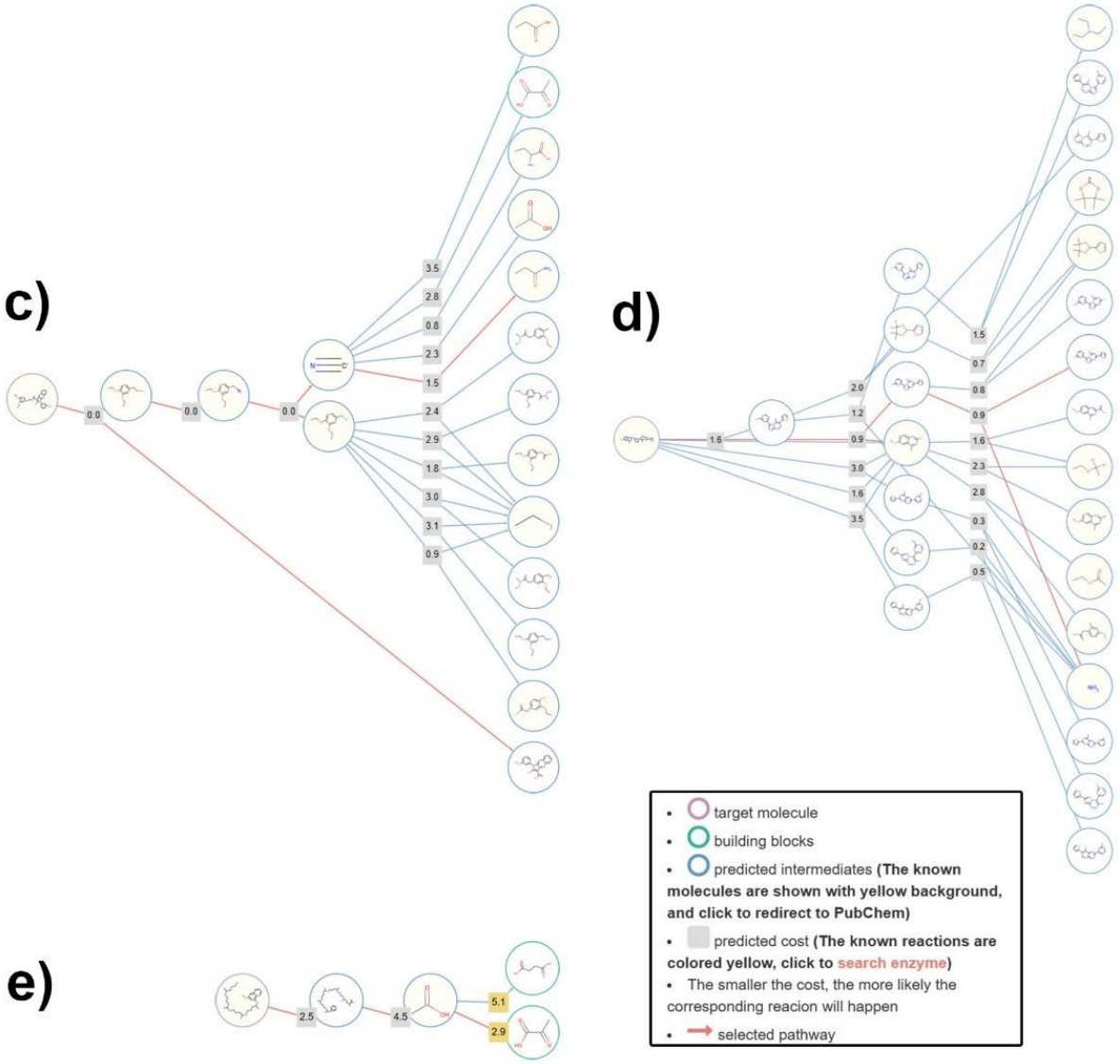

Figure 2. BioNavi-predicted metabolic pathway of compounds c) C, d) D, and e) E. Further details on BioNavi results in Supplementary Data upon request..

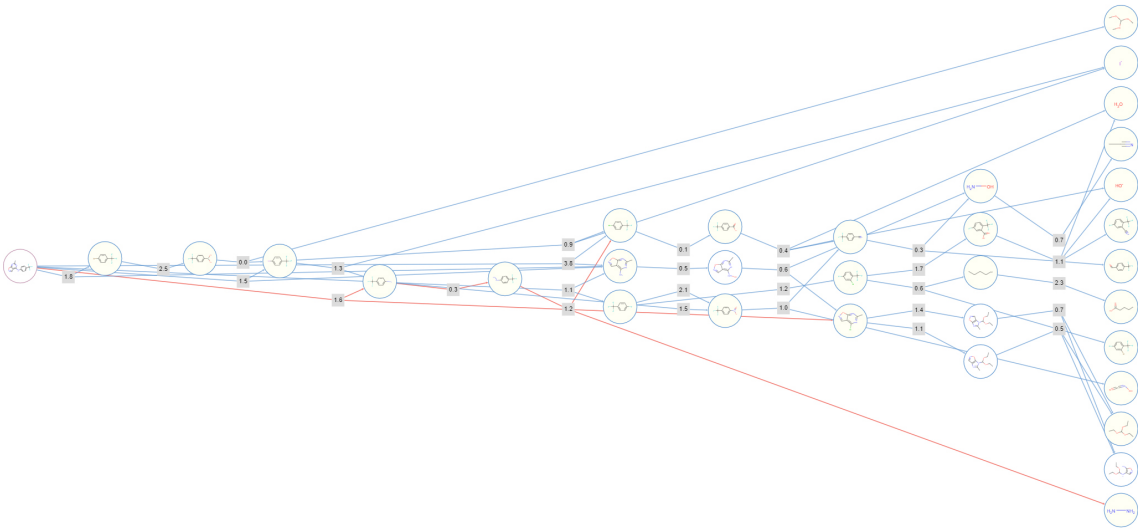

Figure 3. BioNavi-predicted metabolic pathway of control drug isoxazole pyrimidine (IZP). Further details on BioNavi results in Supplementary Data.

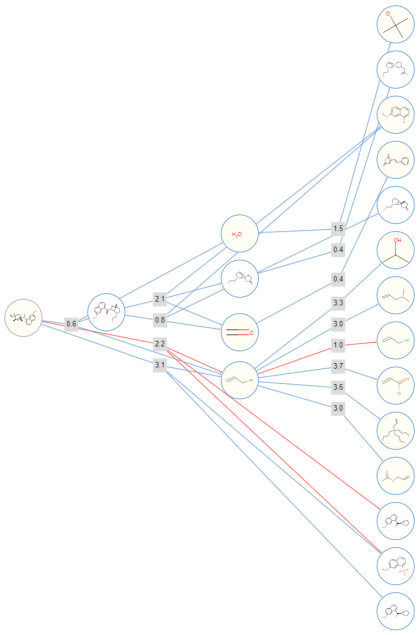

Figure 4. BioNavi-predicted metabolic pathway of control quinine. Further details on BioNavi results in Supplementary Data.

Figure 5. Swiss Target Prediction pie charts of all five metabolites, on which protein predicted to target the compounds. Pie chart a) to e), respectively referred to Compound A to E (corresponding to Table 1), and ct1) is control drug isoxazole pyrimidine (IZP) and ct2) is control drug quinine.

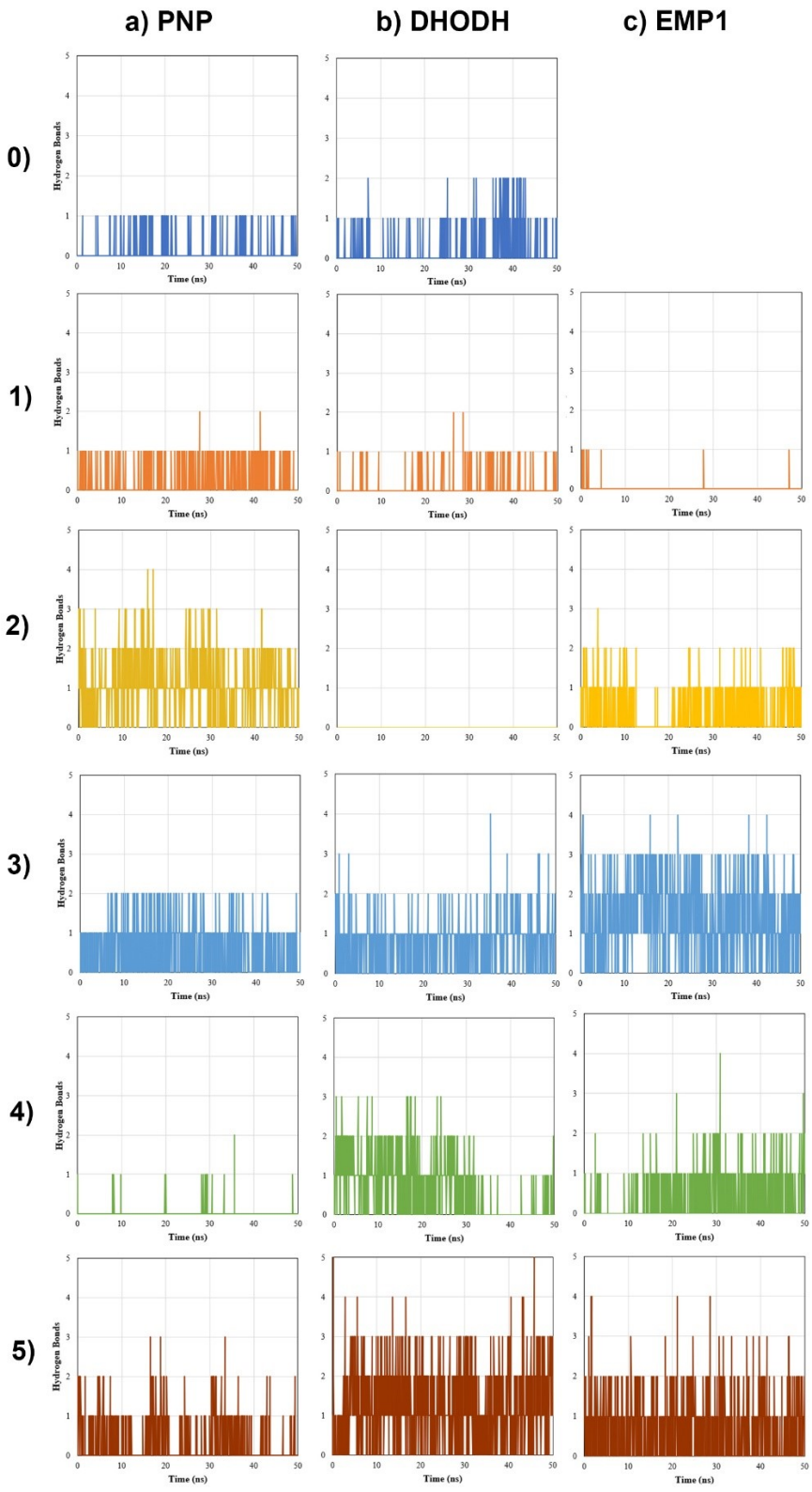

Figure 6. Hydrogen bonds values of the compound-protein pairwise interactions between five tested compounds, two control compounds, and three protein receptors of *Plasmodium falciparum*. Proteins: **a)** PNP, **b)** DHODH, and **c)** EMP1. Ligand-proteins interaction for control compounds: a0) quinine-PNP and b0) isoxazole pyrimidine-DHODH. Tested compound A to E-protein interactions (shown on grid columns 1 to 5, respectively).