Bisphosphonate Inhibition of Phosphoglycerate Kinase: A Quantitative Structure Activity Relationship and Pharmacophore Modeling Investigation

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Supporting Information

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Figure S1. Docked poses of: **A**, **1**; **B**, **13** and **C**, **38** bound to a homology model of *H. sapiens* PGK.

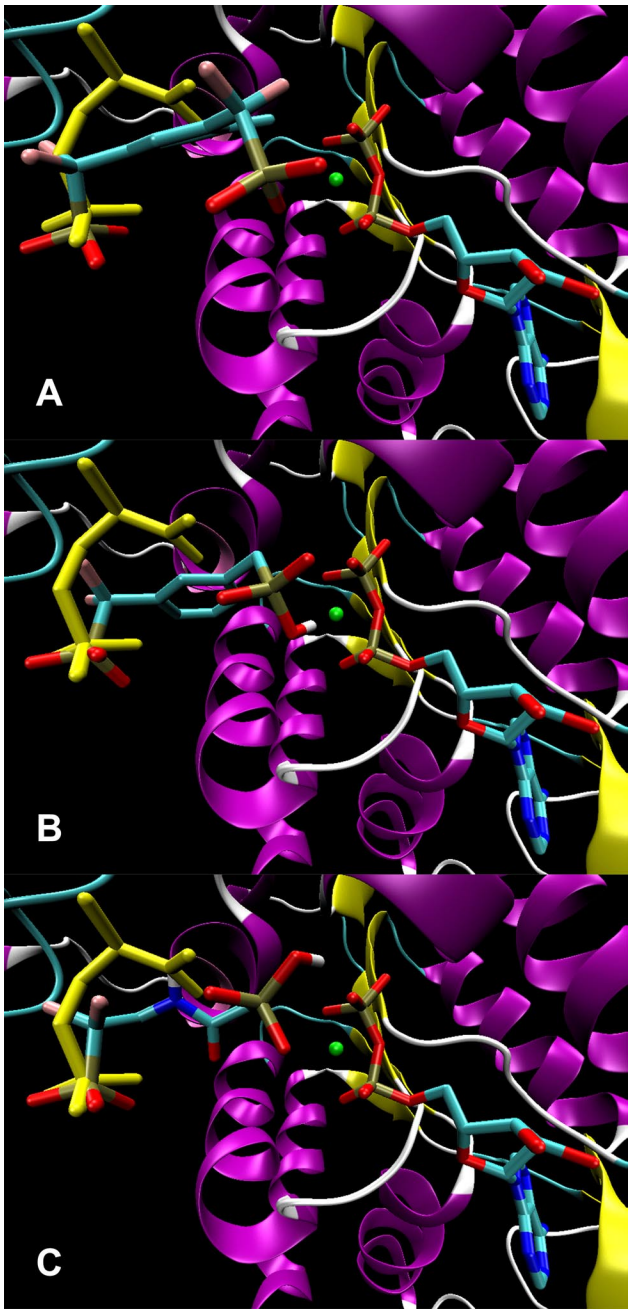

Figure S2. Docked poses of: **A**, **1**; **B**, **13** and **C**, **38** bound to a homology model of *S. cerevisae* PGK.

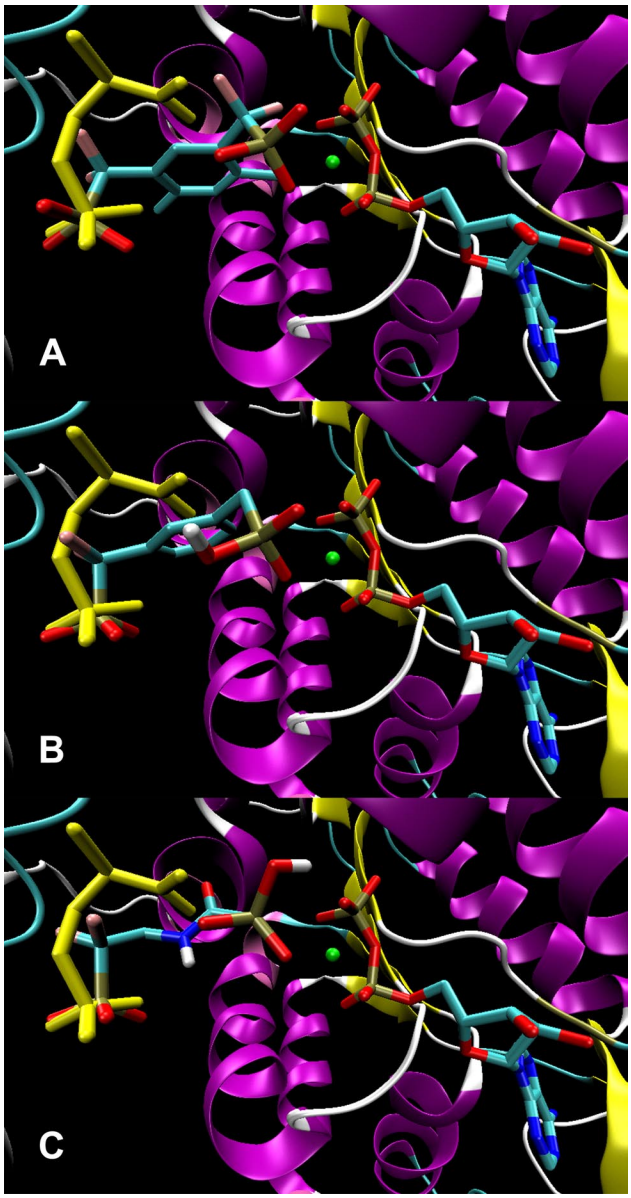

Figure S3. A, **B**, CoMSIA fields (Alignment I) and **C**, **D**, Pharmacophore models (Alignment I) superimposed on *T. brucei* PGK