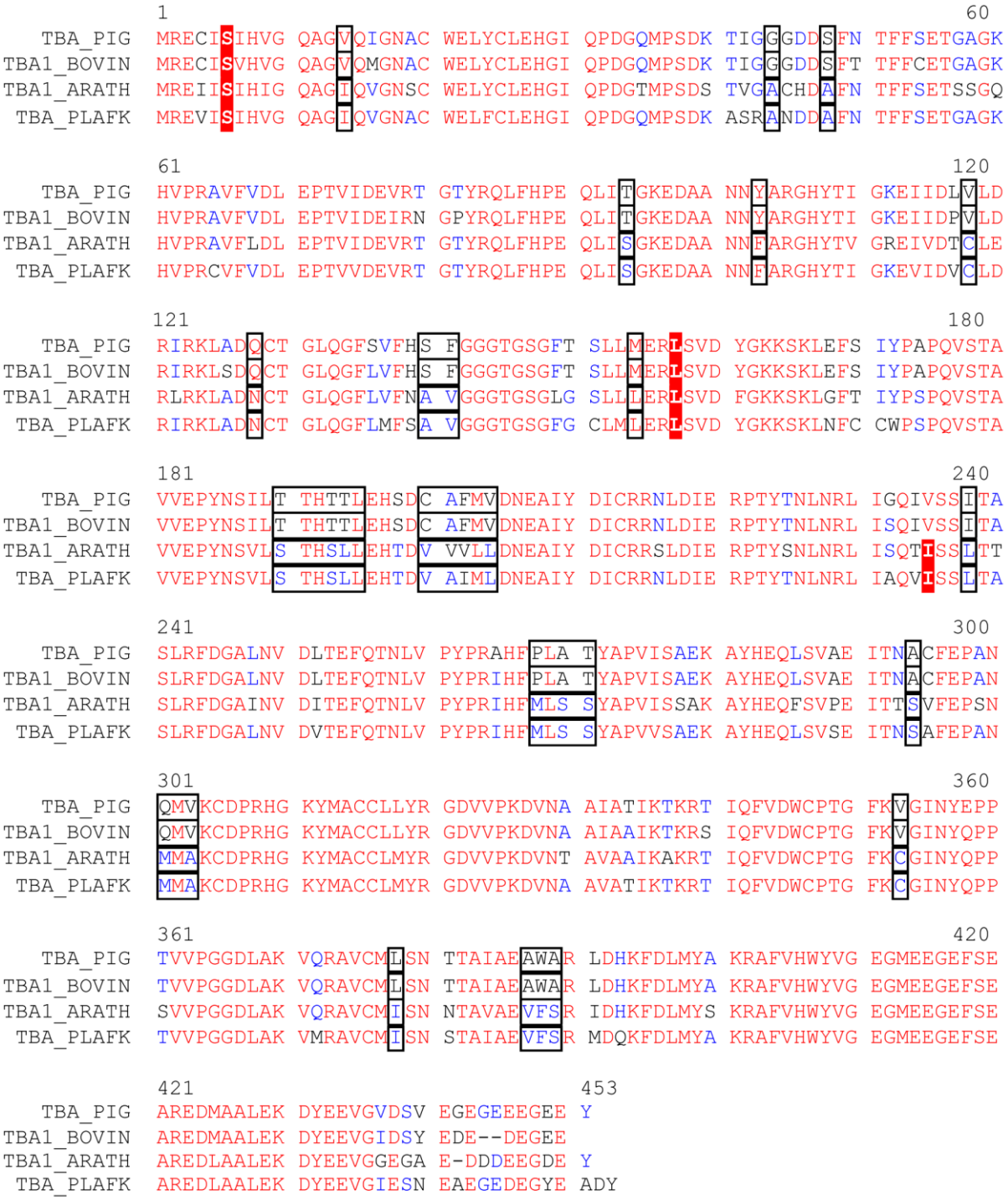
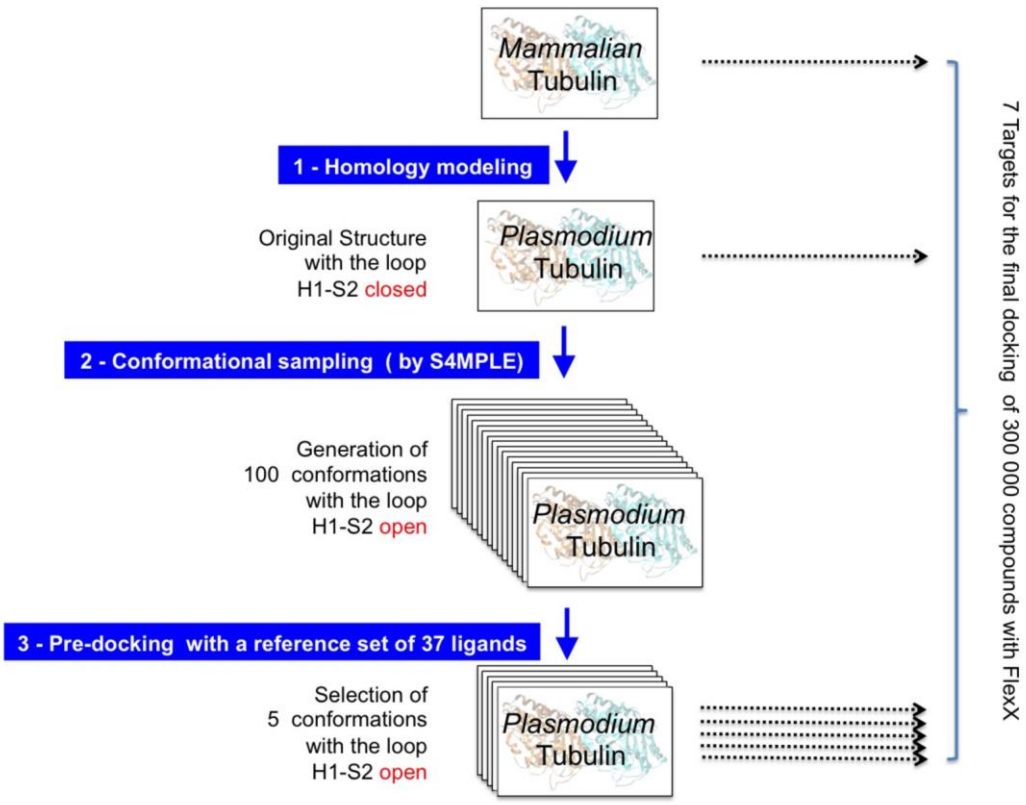
Supplementary



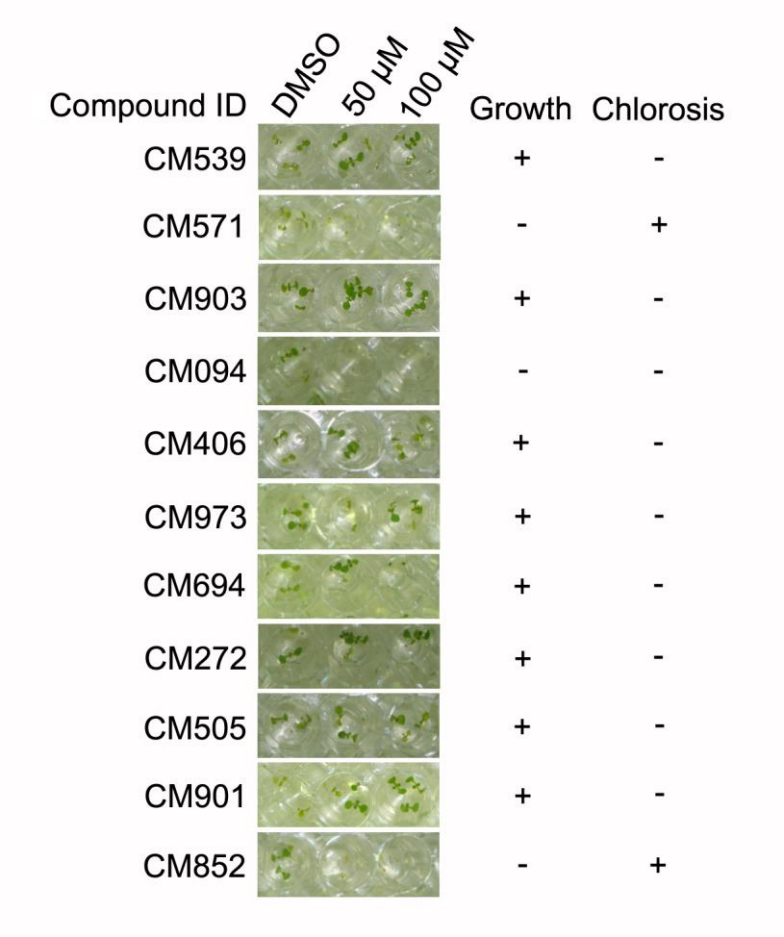
Supplementary Figure 1

Supplementary Figure 1: Alignment of the sequences of *Bos taurus*, *Sus scrofa*, *Arabidopsis thaliana* and *Plasmodium falciparum* α-tubulin. Alignments have been performed using Multalin software with default options [1]. Highly conserved residues appear in red, weakly conserved in blue and divergent residues in black. High consensus regions predominate low ones indicating that α-tubulin is a highly conserved protein. Some plant/mammal differences (framed residues) are also detected in *P. falciparum* α-tubulin. The residues Ser6, Ile235 or Leu167 used in docking as criteria for the selection of ligands are highlighted in white on red background.



Supplementary Figure 2

Supplementary Figure 2 Strategy for the selection of potential 3D structures of plasmodium tubulin to be used as targets for a virtual screen of compounds with FlexX. First, the *Plasmodium* tubulin 3D structure has been predicted by homology with the *Mammalian* tubulin. This original structure has a loop (H1-S2 loop) that locks the dinitroanaline binding site. Using S4MPLE [2], a conformational sampler software, 100 **open** conformations of this loop were generated. A set of 37 molecules (10 known to bind to the dinitroaniline binding site and 27 not having been described to bind tubulin) was docked against the dinitroaniline binding site of these 100 conformations. The 5 conformations which best discriminated the active molecules from the inactive ones were selected. These 5 conformations, the mammalian tubulin and the original *Plasmodium* tubulin conformations were the final targets for the docking of 300 000 compounds with FlexX in the dinitroaniline binding site.



Supplementary Figure 3

Supplementary Figure 3: Effect of the selected compounds on *Arabidopsis thaliana* growth
Arabidopsis seedlings were sawn on 24-well microplates containing an agar-based solid medium containing compounds, as indicated. After 7 days of incubation in a growth chamber, growth was monitored.

Supplementary references

1. Corpet F: Multiple sequence alignment with hierarchical clustering. *Nucleic Acids Res.* 1988, 16:10881–90.
2. Hoffer L, Chira C, Marcou G, Varnek A, Horvath D: S4MPLE--Sampler for Multiple Protein-Ligand Entities: Methodology and Rigid-Site Docking Benchmarking.. *Molecules* 2015, 20:8997–9028.