Electronic Supplementary Material (ESI) for Molecular BioSystems

Supporting Information

Supplementary File S1: Annotation of molecular function, biological process and cellular component of the predicted target proteins of the GSK compounds. The sequences are filtered with a cut-off at 5.0.

Supplementary File S2: A detailed matrix of the predicted interactions between the GSK compounds and the proteome of P. *falciparum*. The matrix has compounds as rows and proteins as columns. '1' denotes an interaction between a compound and a protein in the corresponding cell. In case of no interaction the cell has a value of '0'. The compounds are listed with their PubChem ID. The matrix is stored in open document format and can be opened using the free program Open Office Calc.

Supplementary File S3: Interaction matrix between GSK compounds and the proteome of P. *falciparum*, used for the construction of the heatmap in Figure 2. (0): no interaction, (1): protein target with no human homologue, (2): rest of predicted interactions within the subset of the 130 prioritized proteins. (3): known experimental activity with a non-human protein homologue of *P. falciparum*.

Supplementary File S4: List of 176 small molecule-protein pairs, for which experimental binding activity exists in ChemProt. The list includes 59 unique compounds described with SMILES strings and CID codes and 30 human proteins described with their UniProt identifiers.

Supplementary File S5: Association of human proteins to protein-protein interaction complexes and diseases. Diseases are described with OMIM IDs and proteins with Ensembl identifiers.