Supplemental Data:

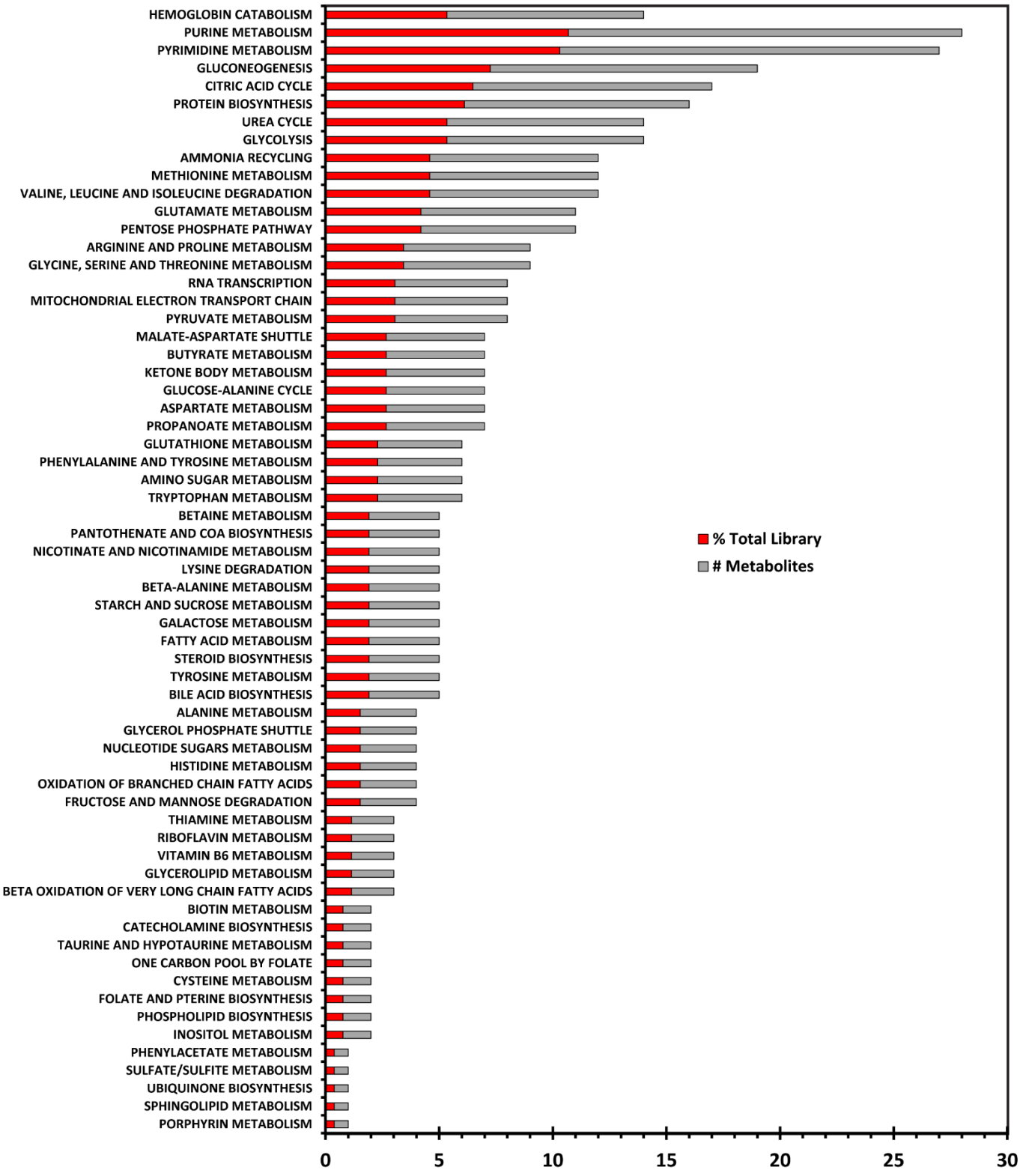

Fig. S1. Targeted metabolite coverage. Coverage analysis demonstrating the distribution of validated compounds from our library of known metabolites across the parasite metabolome, as well as the coverage within a metabolic pathway. The validated library encompasses 242 compounds (Table S1) run as pure standards and contains the m/z and retention time used for peak/compound identification during analysis.

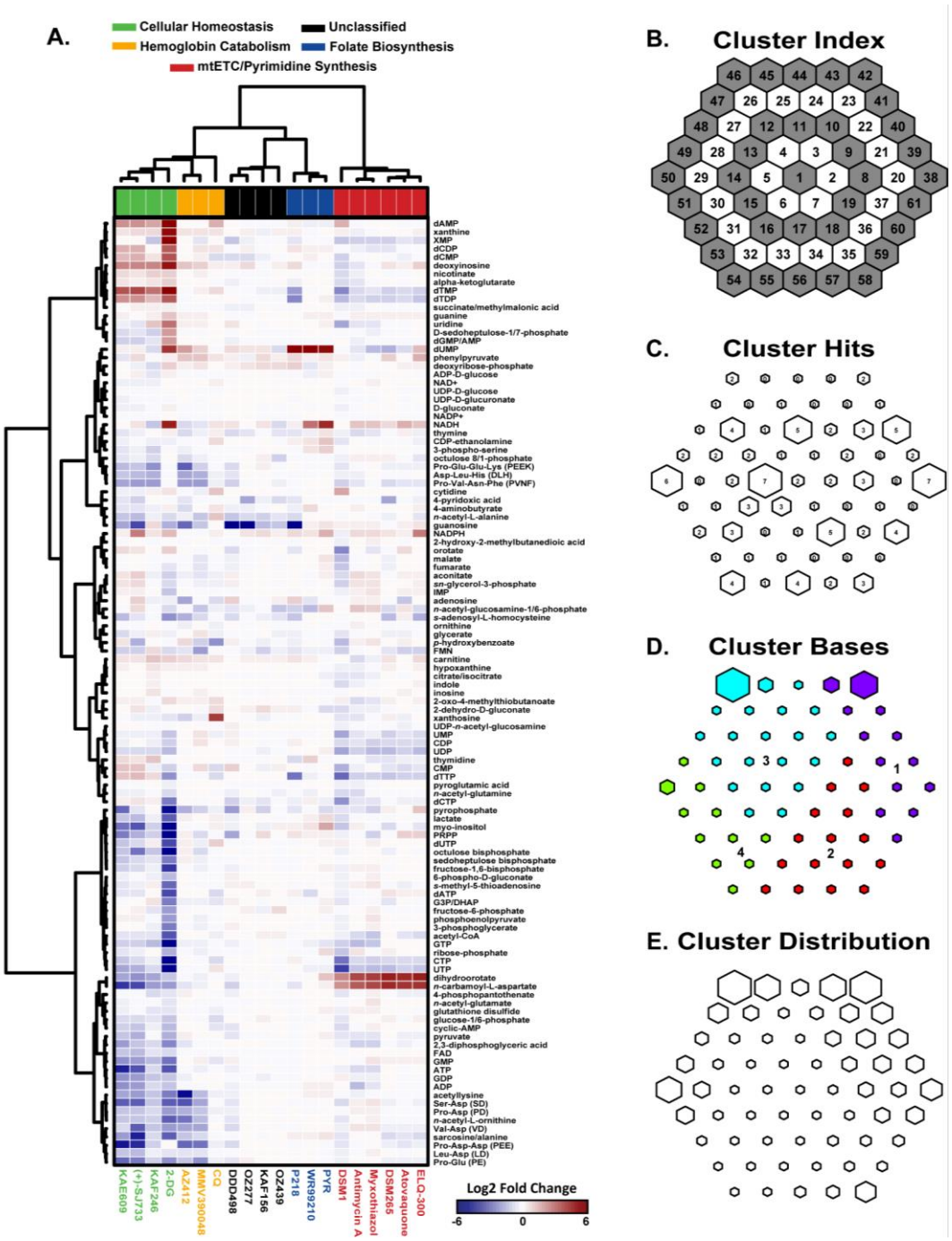

Fig. S2. Clustering of validation set data and supraHex MetaPrint depiction of data. A. Heatmap of $\log_2$ fold change values, relative to an untreated parasite control, for all validated antimalarial drugs tested (Fig 2C, Table 1 and S2) using Pearson-Ward distance-clustering. Compound names are displayed on the x-axis and measured metabolites are displayed on the y-axis. Compound groupings are color-coded and based on MoA classifications. All treatments were carried out in triplicate and each sample was generated as a triplicate technical replicate within a given trial. Values displayed are experimental averages. B. Map index demonstrating the MetaPrint node layout, consisting of 61 hexagons arranged radially outward within a larger hexagon. 113 targeted metabolites, having high quality and reproducibility (>90% of all experiments), were input to automatically generate a suprahexagon of optimal size, in this case 61 (Table S3). C. Hit count map corresponding to the number of metabolites mapping to each node. The size of the hexagon also denotes the relative number of contributing input metabolites. Due to clustering and the requirements for a symmetrical hexagon, several nodes are empty and the resulting displayed data are simply the influences from the weight of its neighbors. D. Map displaying the five major bases or metabolic clusters within the input data. Nodes with the most weight are denoted by an increase in hexagon size. E. Hexagonal map demonstrating the Euclidean distance between the given metabolite nodes. Nodes that are most closely related are larger in size and thus closer in proximity to adjacent nodes. The MetaPrint also functions to place the most influential nodes on the outer portion of the larger hexagon, as demonstrated in this map.