

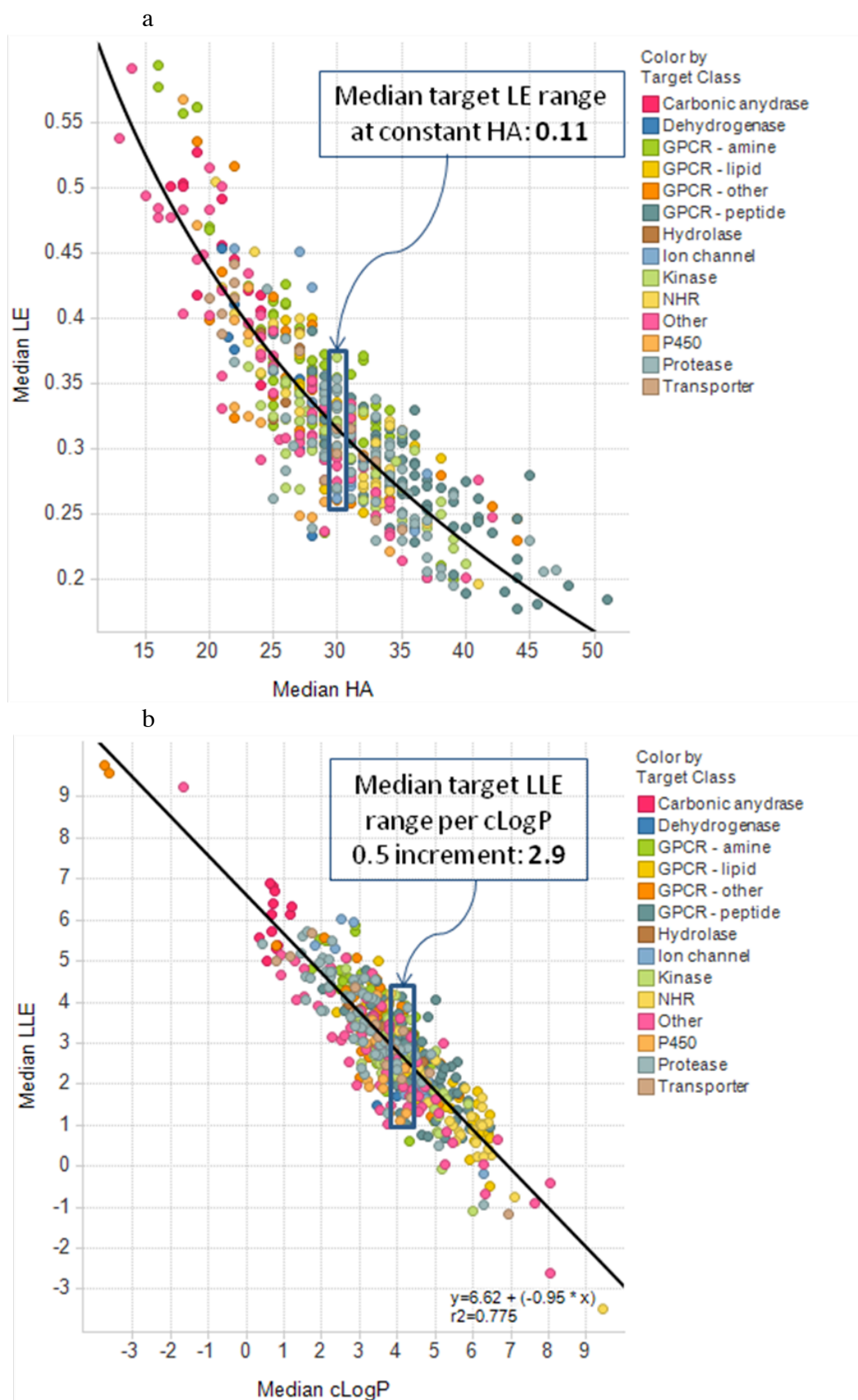


Figure S1 | Ligand efficiencies versus corresponding physical properties.

Relationships between a) LE and HA (non linear, see Box 2) and b) LLE and cLogP, (linear), exemplified by the median values of 480 assay-target pairs (see Box 4). The approximate ranges of LE and LLE values across targets at fixed values of HA and cLogP is shown. $LE = \text{median target potency} / HA \times 1.37$. $LLE = \text{median target potency} - cLogP$