

Additional file 1: Figure S1. Histograms of interaction energies partitioned with respect to the amino acids of 14 α -demethylase complexed with compounds: a) **7** and b) **8**. The x-axis denotes the residue number of 14 α -demethylase, and the y-axis denotes the interaction energy between the compounds and specific residue. Negative values and positive values are favorable or unfavorable to binding, respectively.

