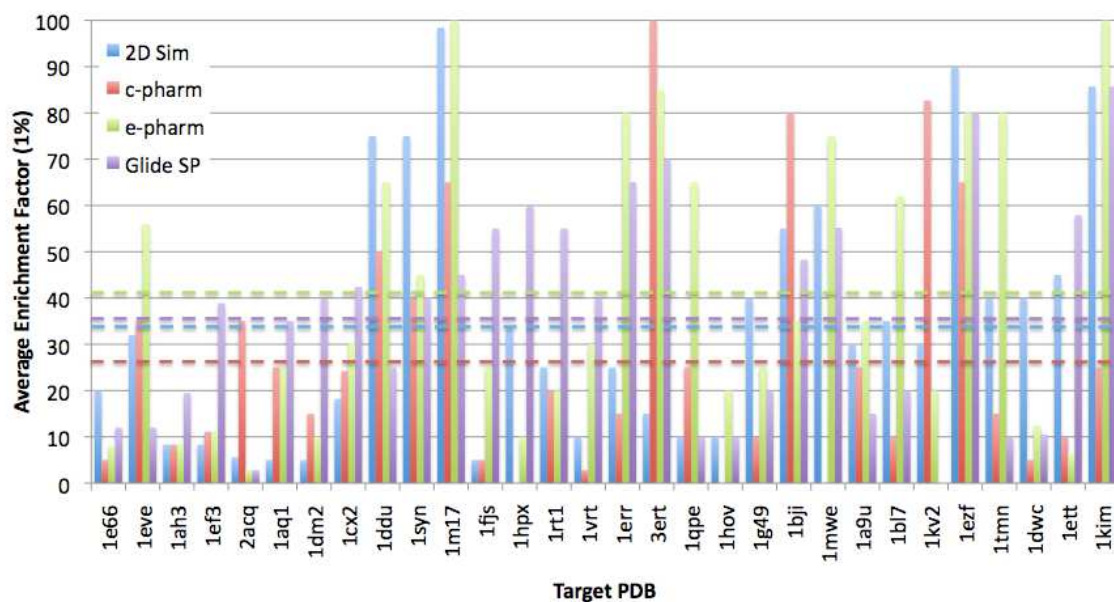
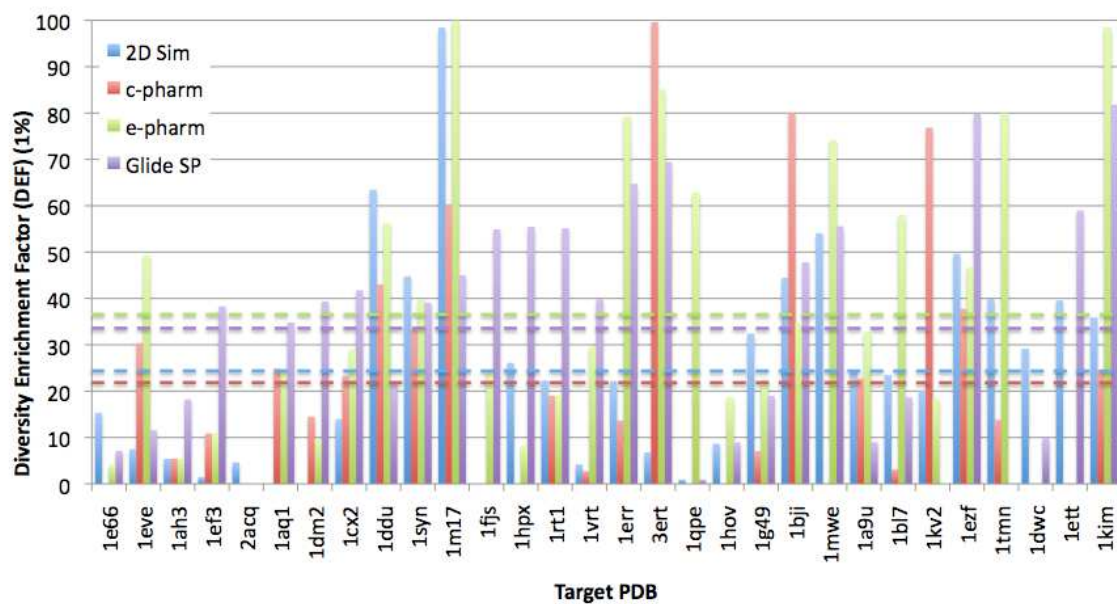


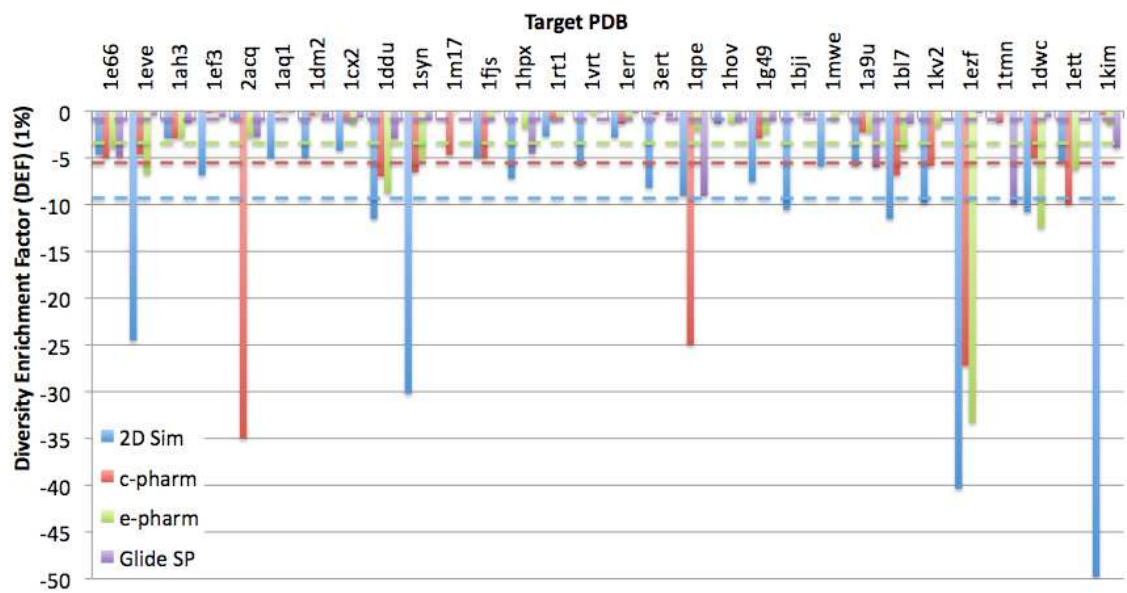
Supplementary Information



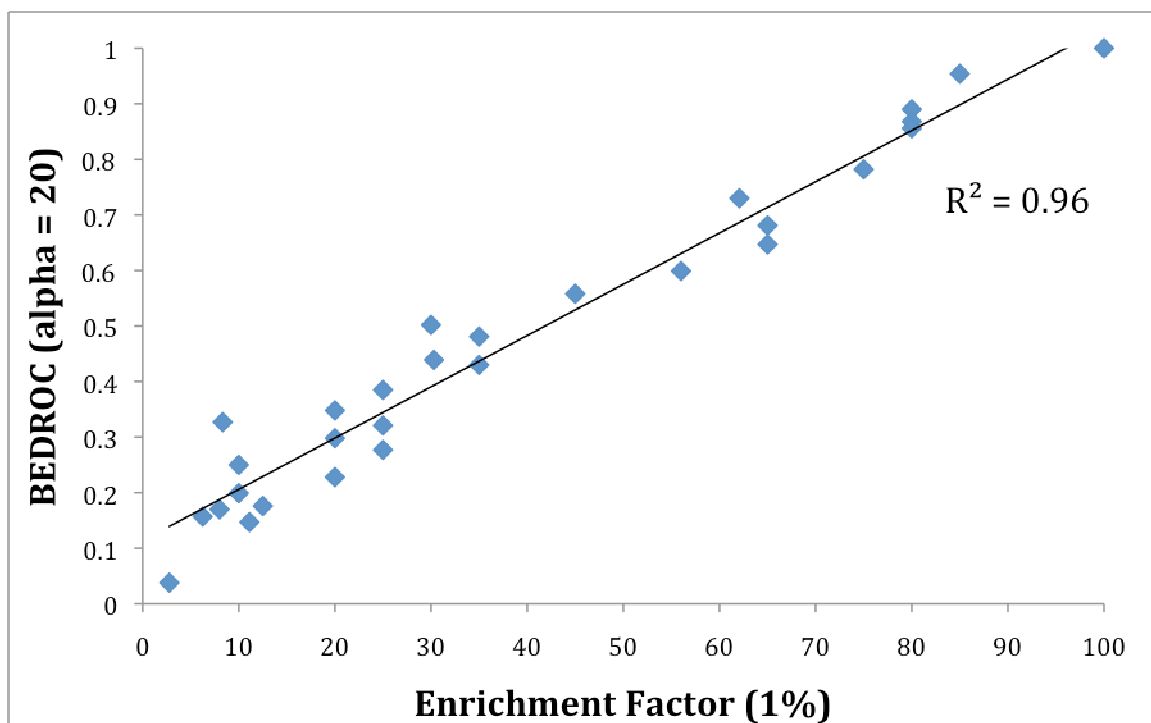
S1. Enrichment factor for top 1% of database. 2D linear fingerprint searching (blue), c-pharmacophores (red), e-pharmacophores (green) and Glide SP docking (purple). Average EF(1%) are shown as dashed lines.



S2. Diversity-base enrichment factor (DEF) of the top 1% of database. 2D linear fingerprint searching (blue), c-pharmacophores (red), e-pharmacophores (green) and Glide SP docking (purple). Average DEF(1%) are shown as dashed line.



S3. Difference between the EF(1%) and the DEF(1%). 2D linear fingerprint searching (blue), c-pharmacophores (red), e-pharmacophores (green) and Glide SP docking (purple). Average differences are shown as dashed lines.



S4. Correlations between EF(1%) vs BEDROC (alpha = 20) for e-pharmacophores.