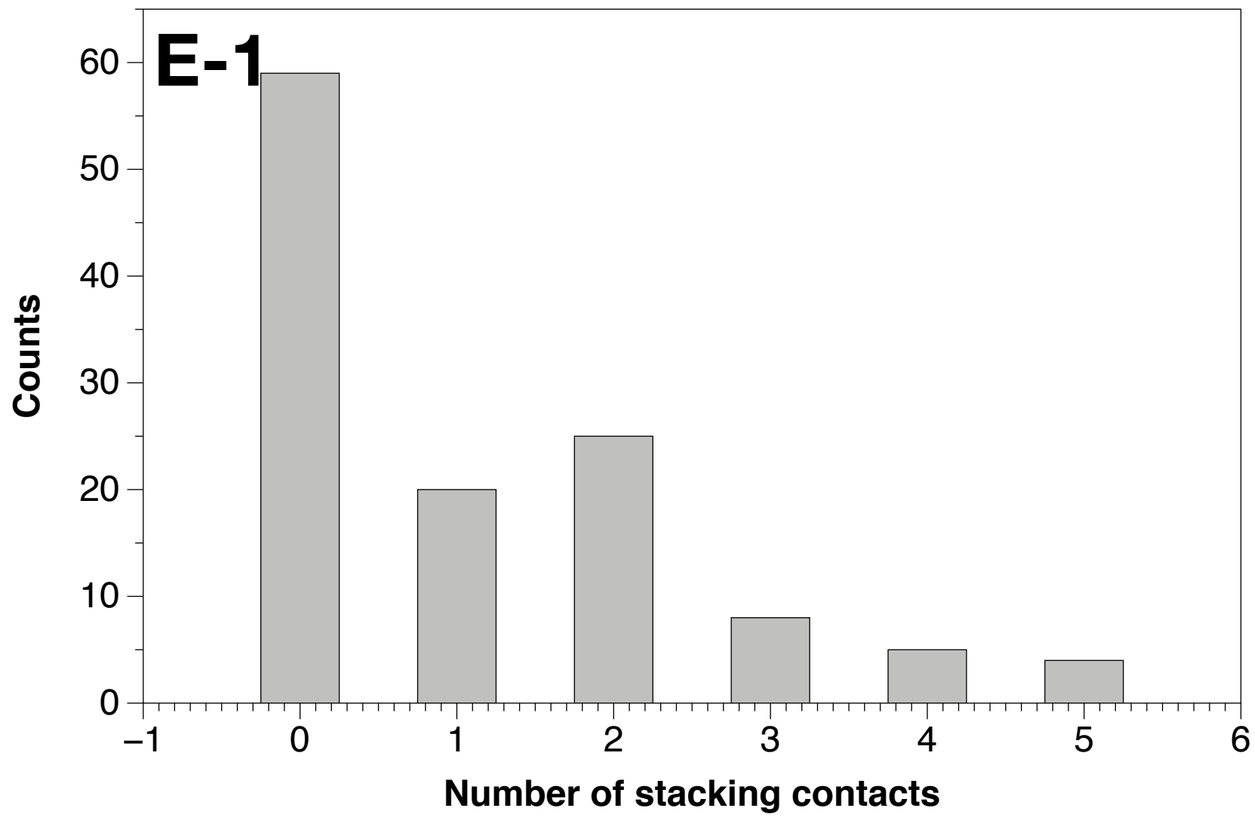
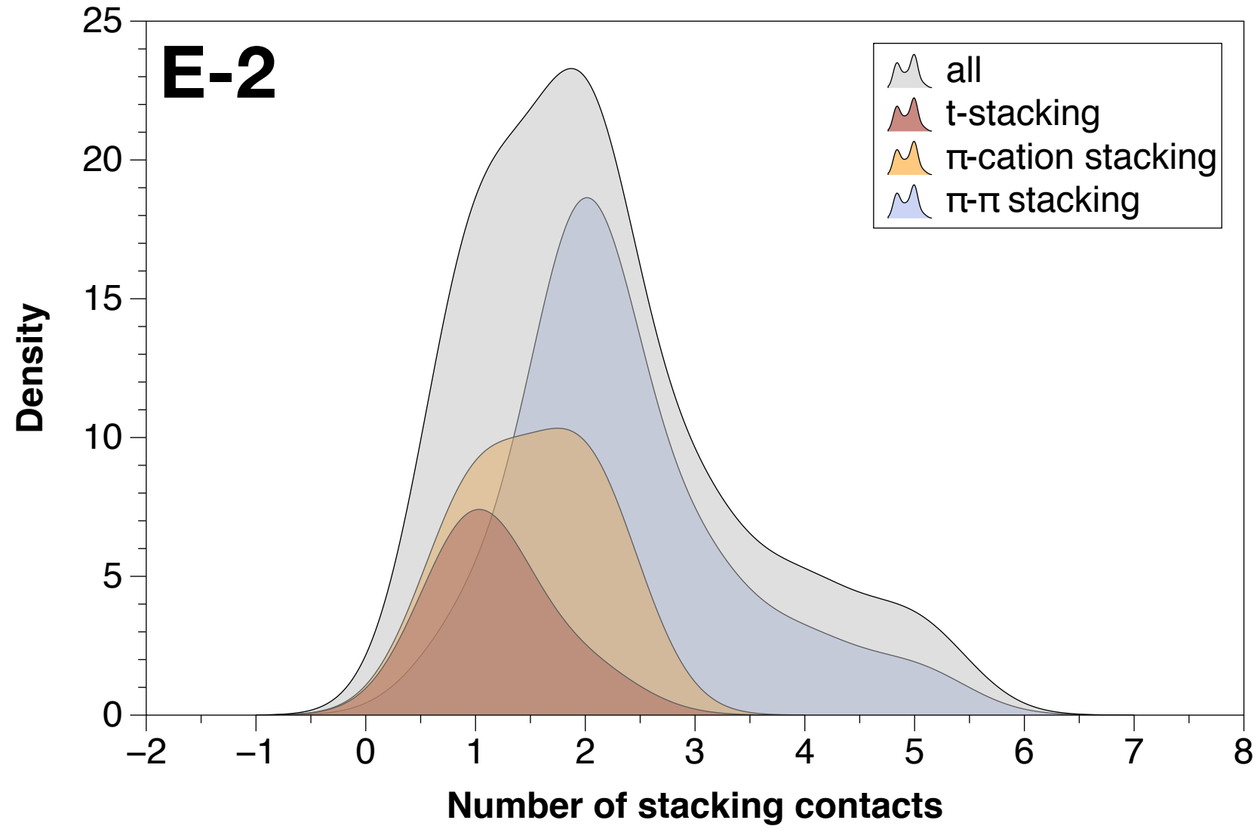
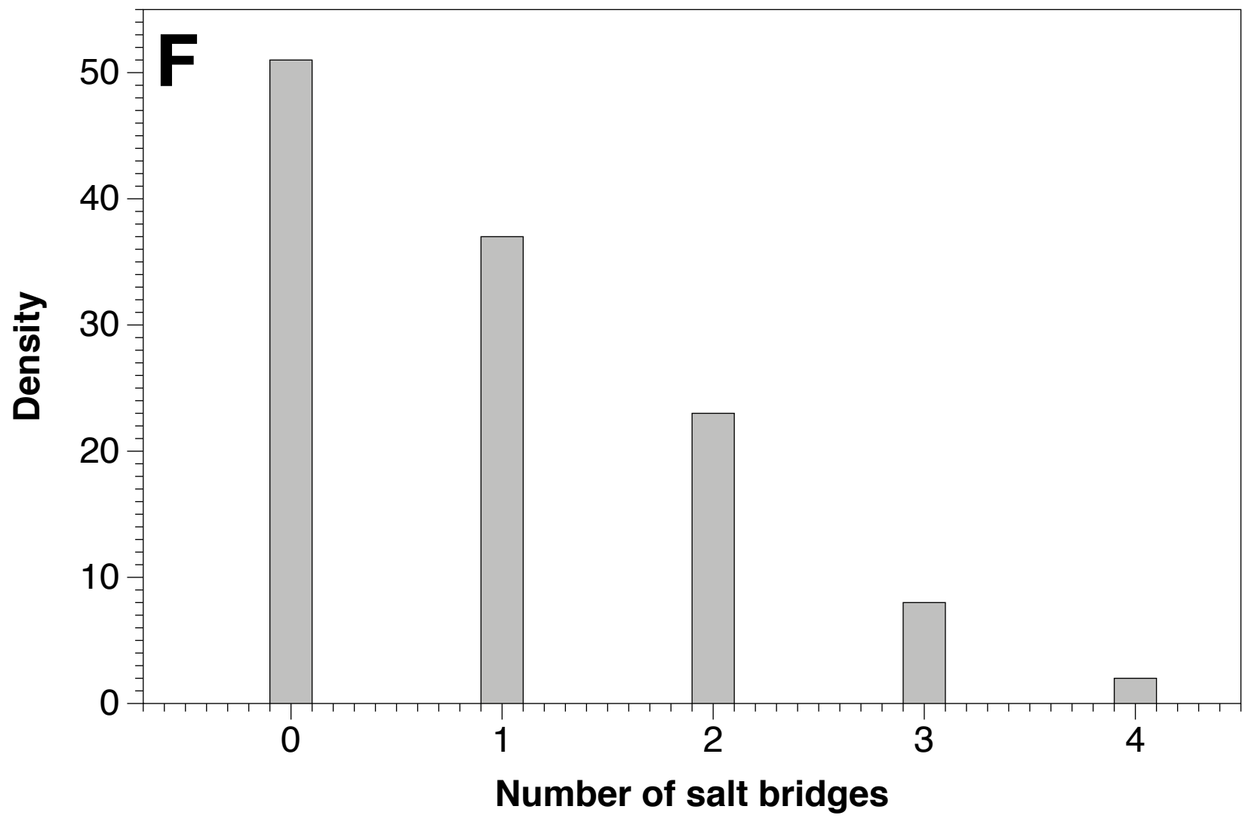
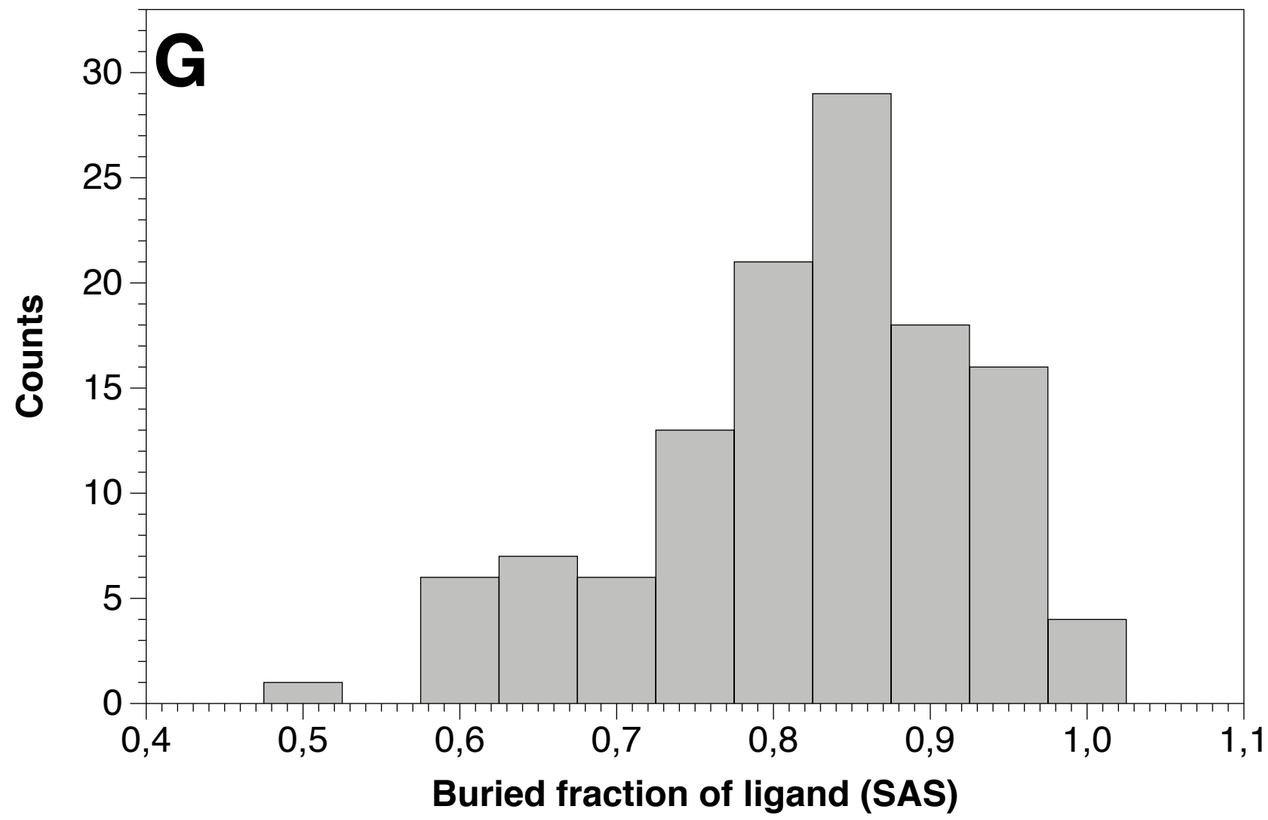
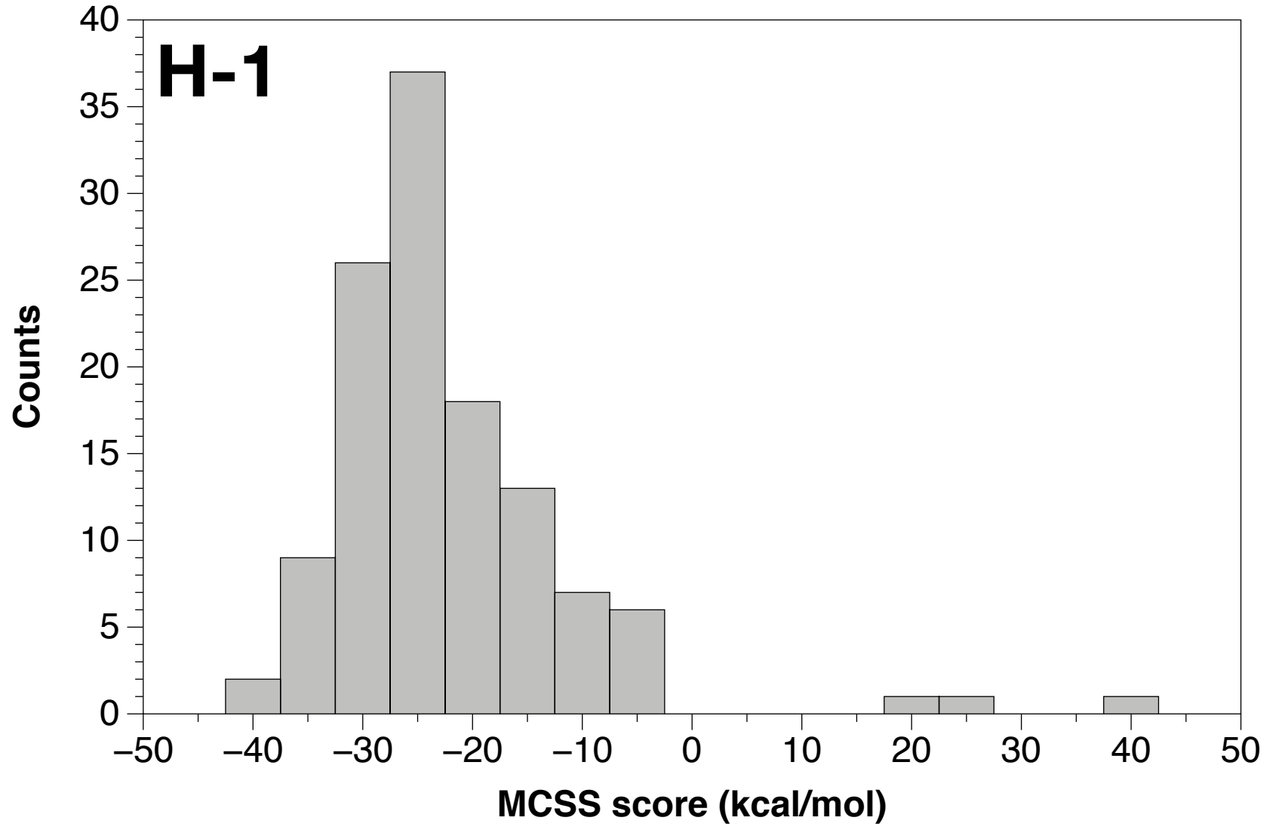
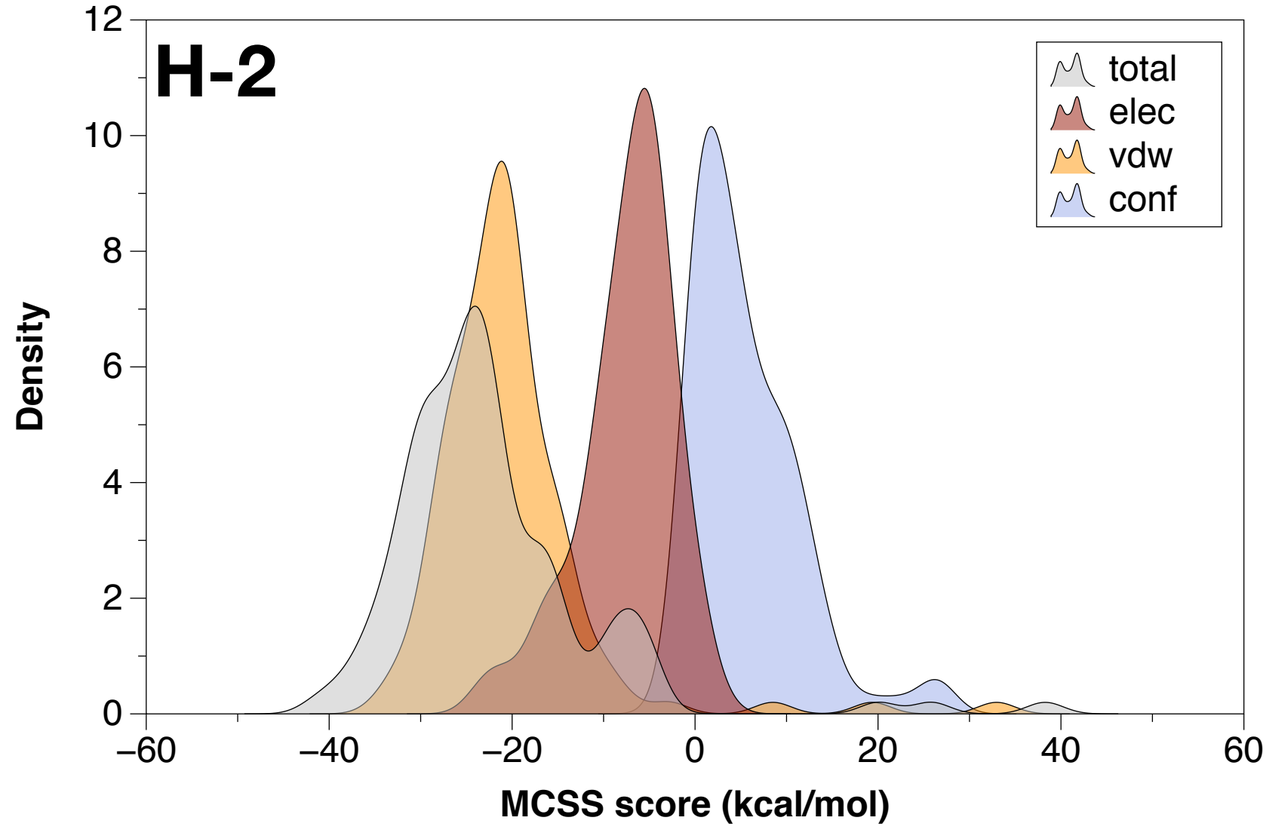

E-1
Counts
Number of stacking contacts


E-2
all
t-stacking
π-cation stacking
π-π stacking
Density
Number of stacking contacts


F
Density
Number of salt bridges


G
Counts
Buried fraction of ligand (SAS)


H-1
Counts
MCSS score (kcal/mol)


H-2
total
elec
vdw
conf
Density
MCSS score (kcal/mol)