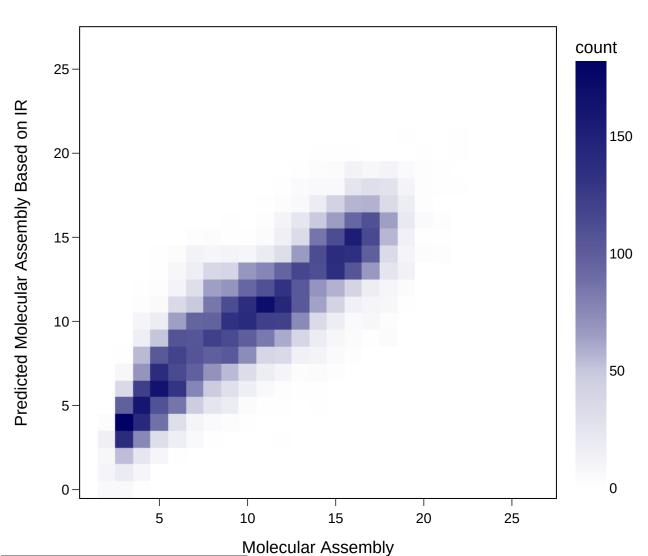# Theoretical IR data (XTB based)