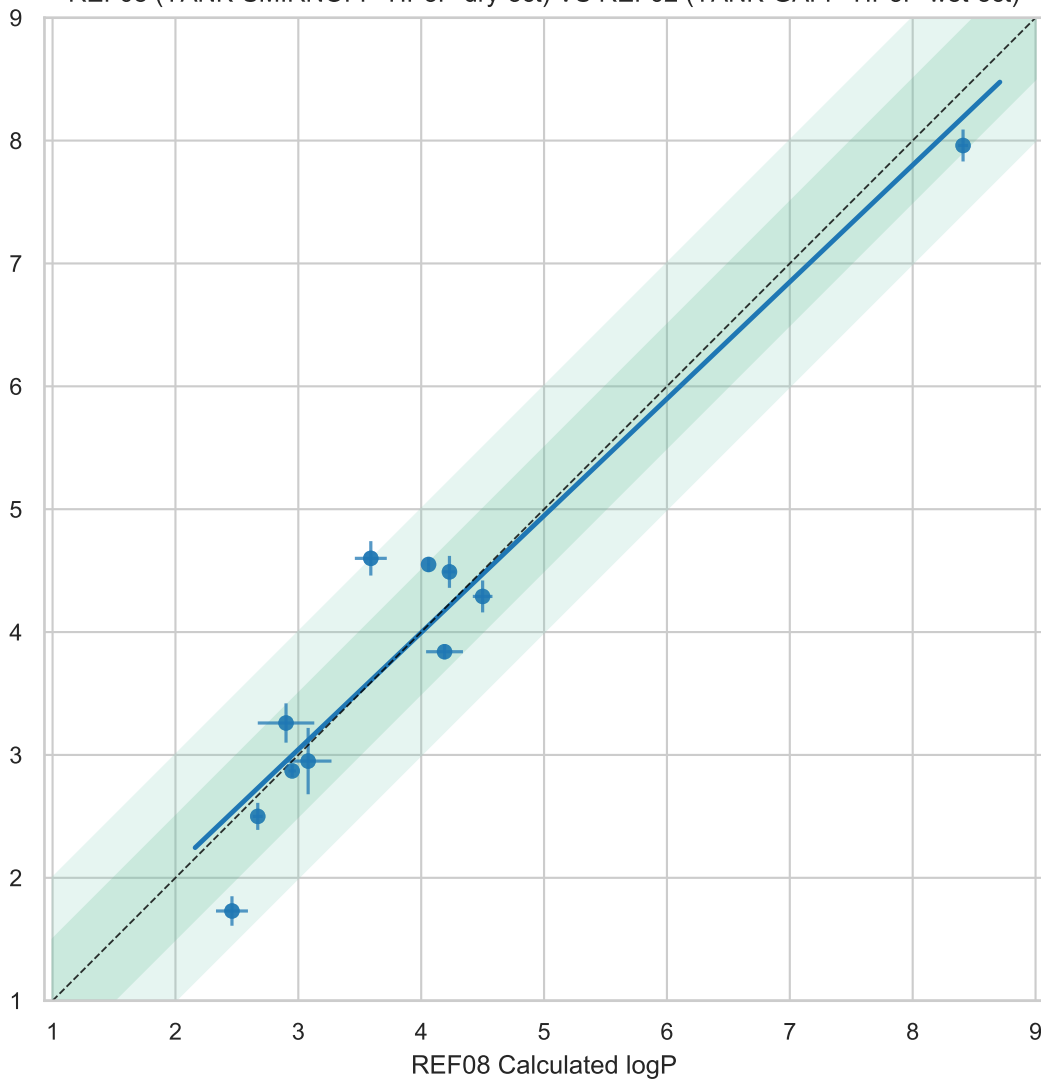


REF08 (YANK-SMIRNOFF-TIP3P-dry-oct) VS REF02 (YANK-GAFF-TIP3P-wet-oct)

REF02 Calculated logP



REF08 Calculated logP