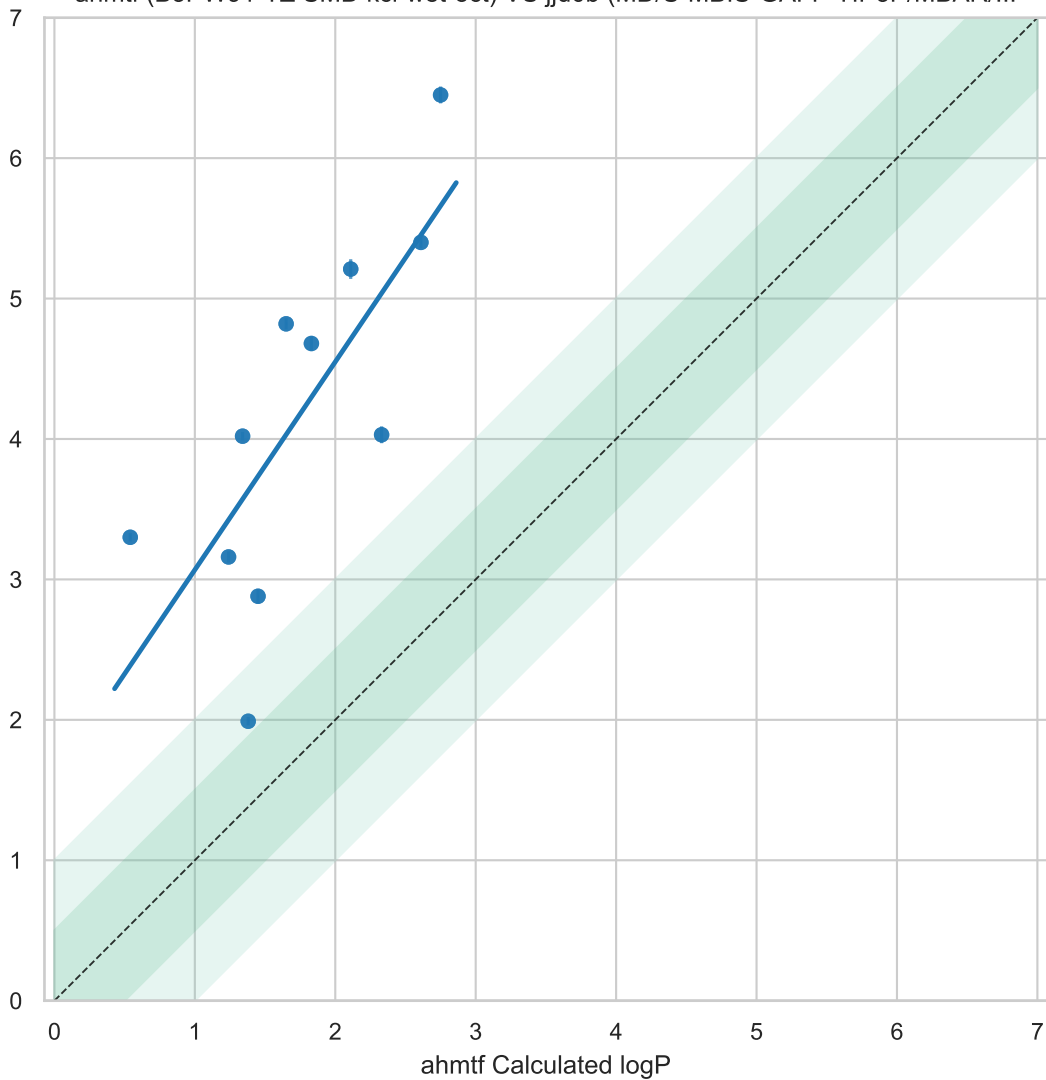


ahmtf (B3PW91-TZ SMD kcl-wet-oct) VS jjd0b (MD/S-MBIS-GAFF-TIP3P/MBAR/...

jjd0b Calculated logP



ahmtf Calculated logP