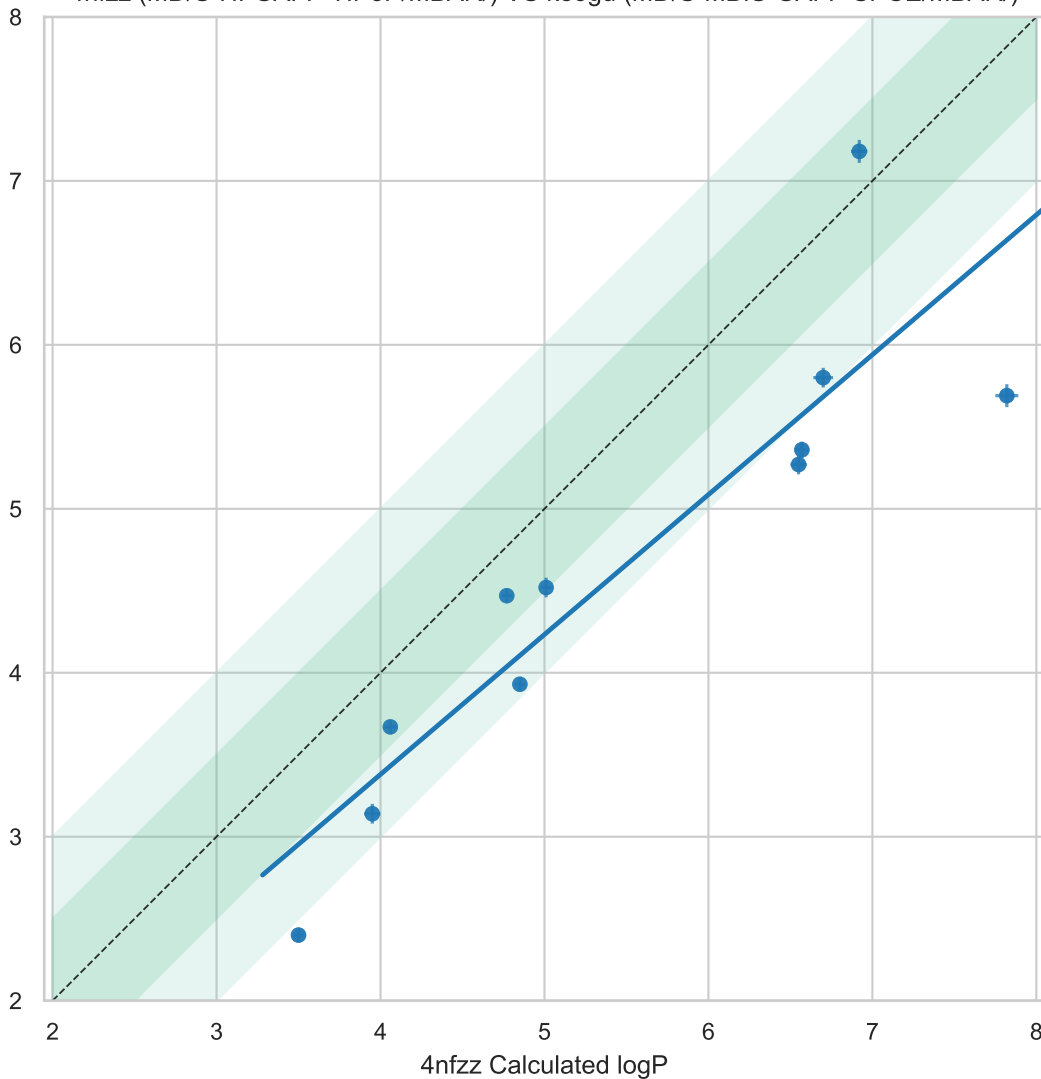


4nfzz (MD/S-HI-GAFF-TIP3P/MBAR/) VS ke5gu (MD/S-MBIS-GAFF-SPCE/MBAR/)

ke5gu Calculated logP



4nfzz Calculated logP