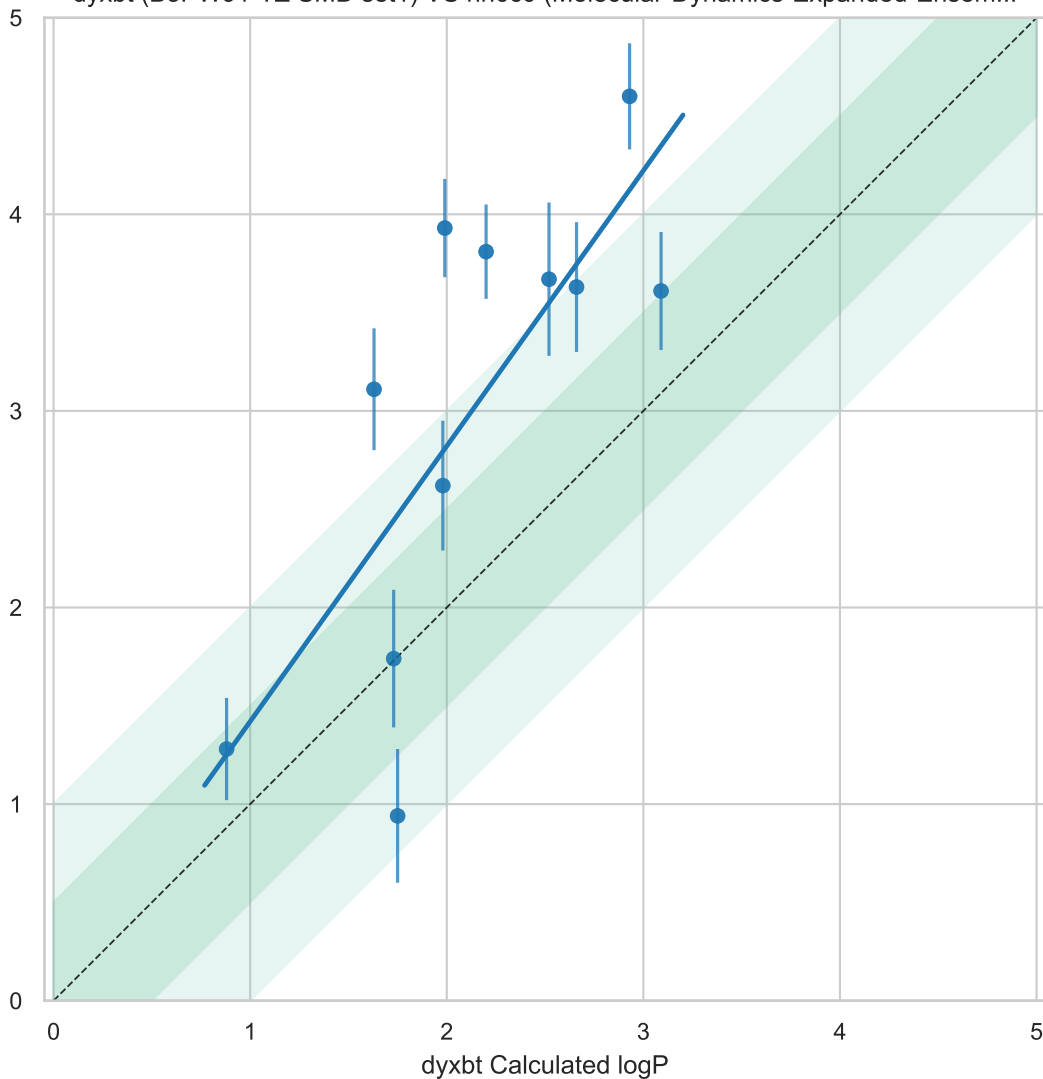


dyxbt (B3PW91-TZ SMD set1) VS nh6c0 (Molecular-Dynamics-Expanded-Ensem...

nh6c0 Calculated logP



dyxbt Calculated logP