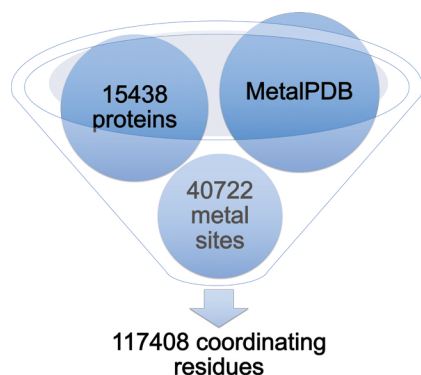


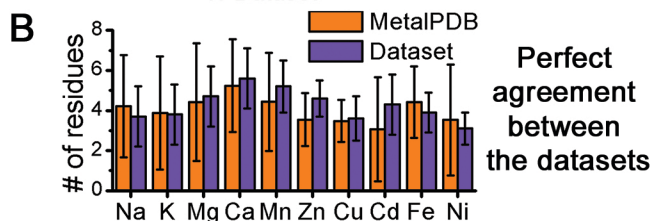
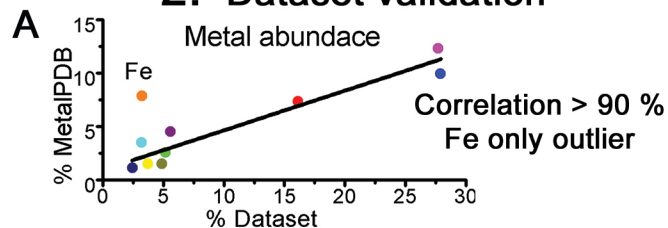
Metal-oriented tertiary structural motifs: a minimal set of bricks for metal coordination in proteins

1. Initial Dataset definition

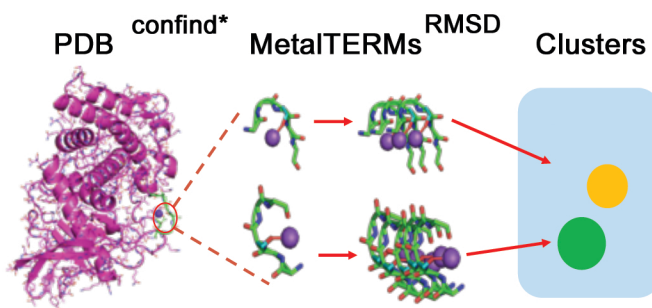


- Filters**
1. Mononuclear metal sites
 2. No exogenous ligands.
 3. X-ray resolution up to 2.6 Å
 4. Rfree factor under 30%

2. Dataset validation

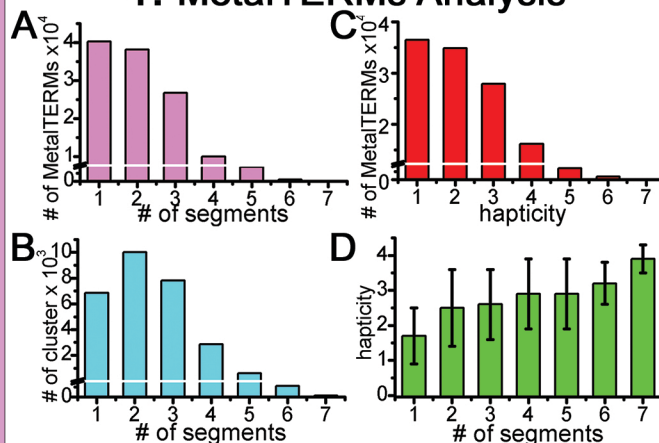


3. Determination and Clusterization of MetaTERMs

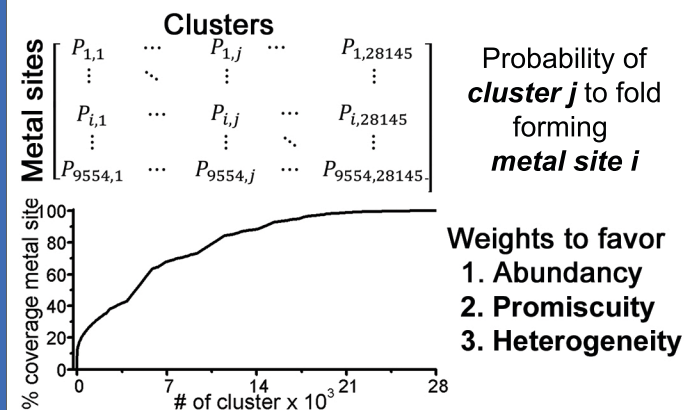


*Mackenzie *et al*, PNAS, 2016, 113 (47), E7438-E7447

4. MetaTERMs Analysis



5. Minimum Set Cover Problem



6. Metal site reconstitution

