

# Supporting Information

## Trends for isolated amino acids and dipeptides: Conformation, divalent ion binding, and remarkable similarity of binding to calcium and lead

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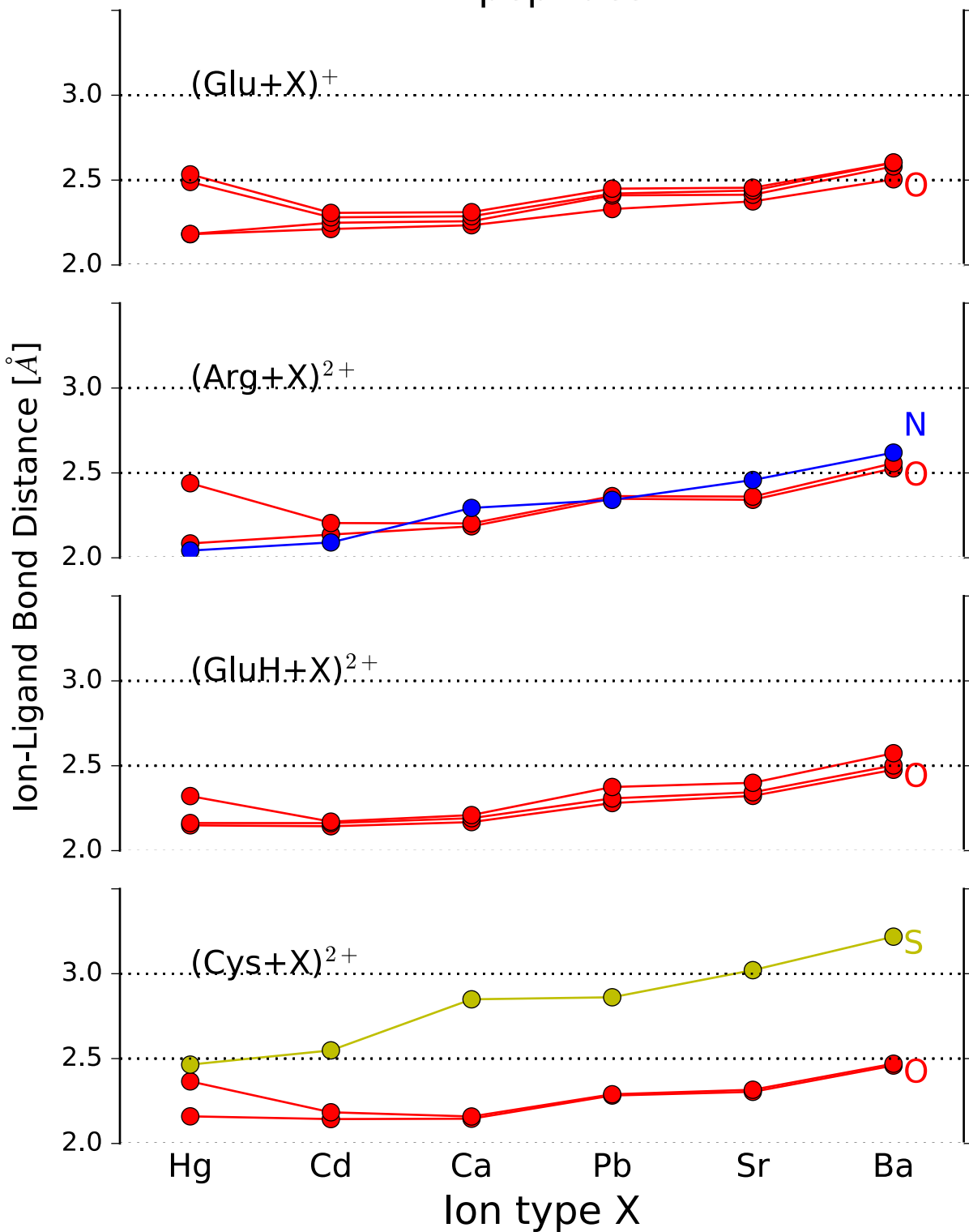
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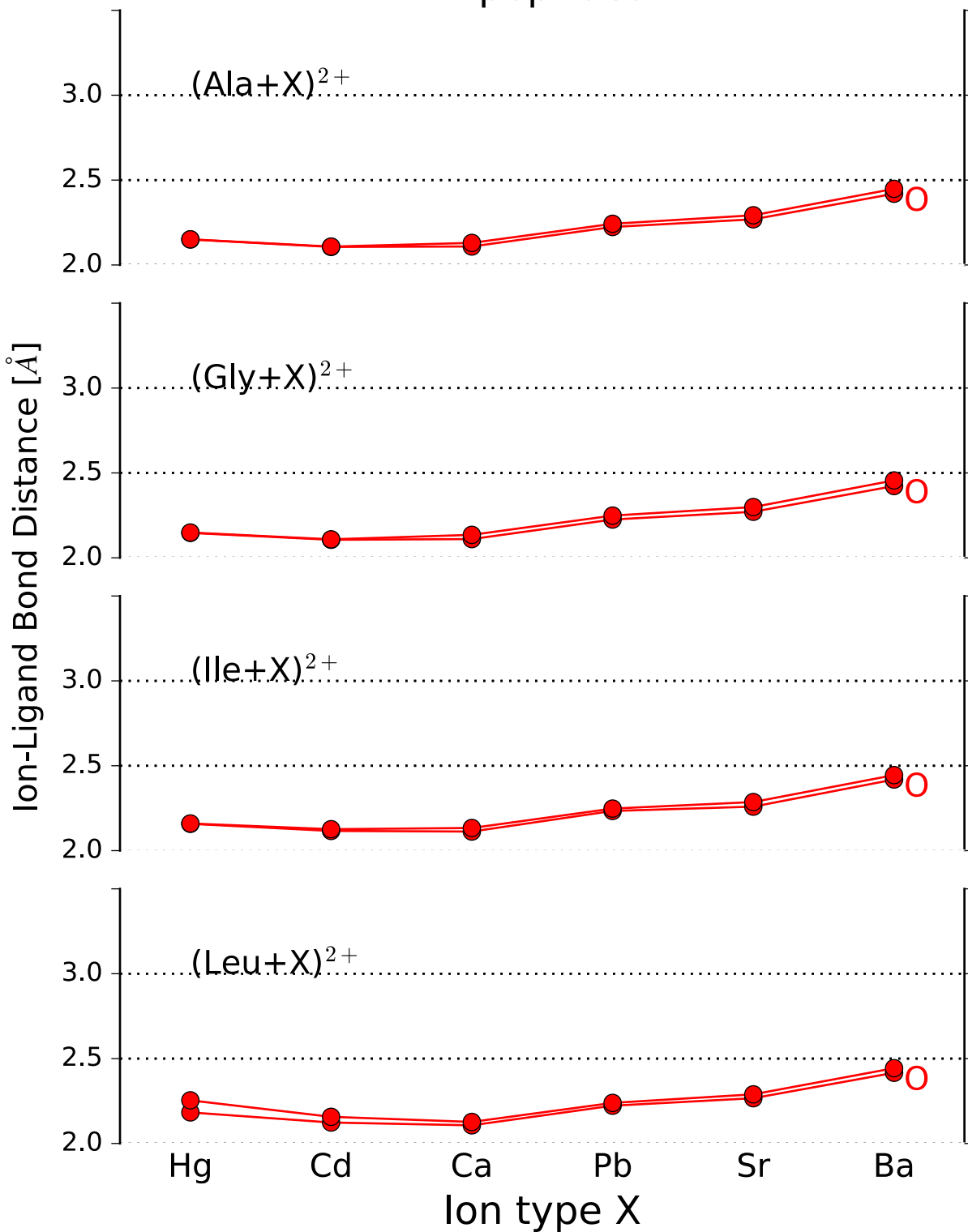
### Cation-ligand distances

Binding distances between the divalent cations and their nearest ligands in the lowest-energy conformations of 20 cation-coordinated proteinogenic dipeptides. Different ligand atoms are distinguished by different-colored curves (red: O, blue: N, orange: S), as noted in the following figures.

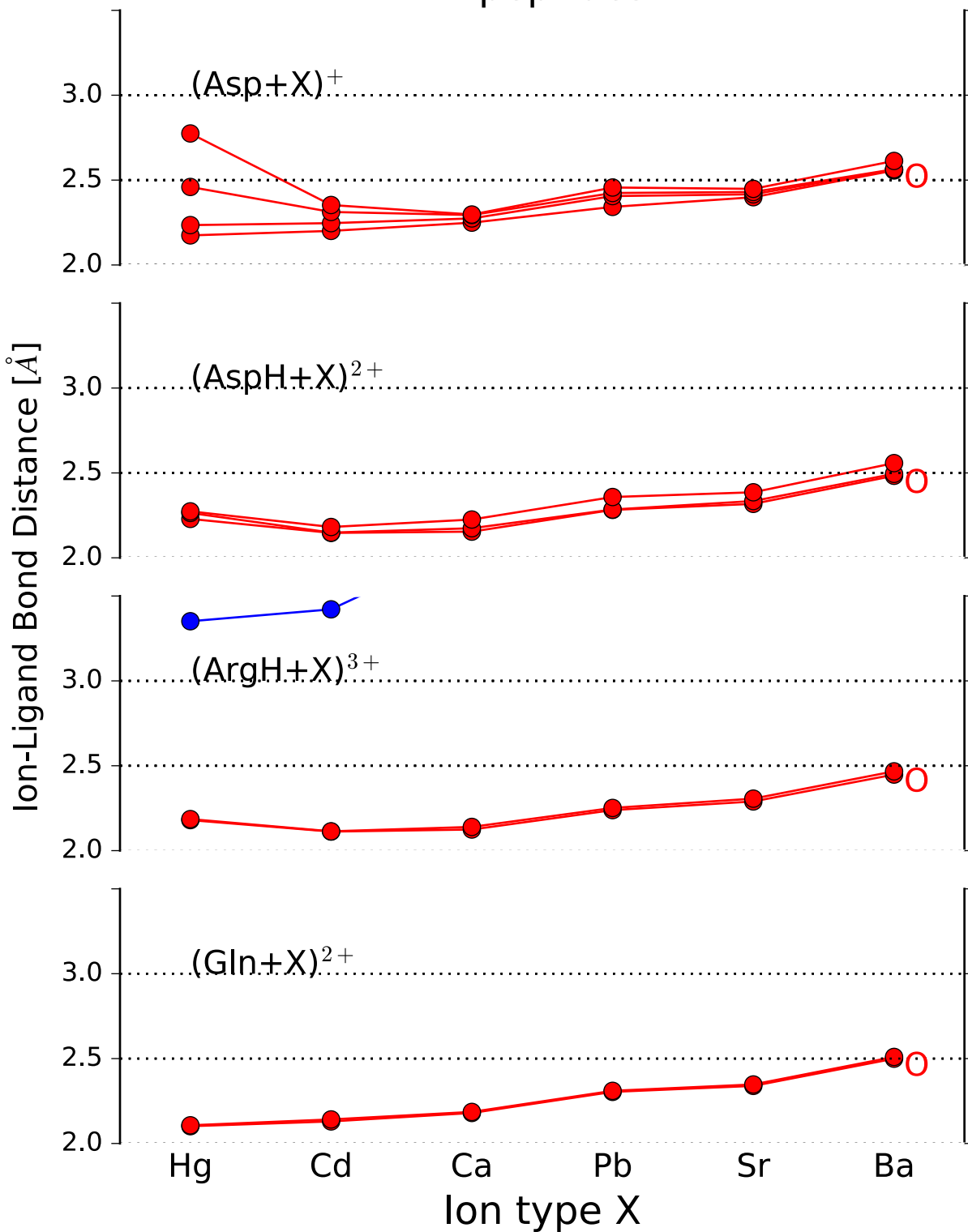
# Dipeptides



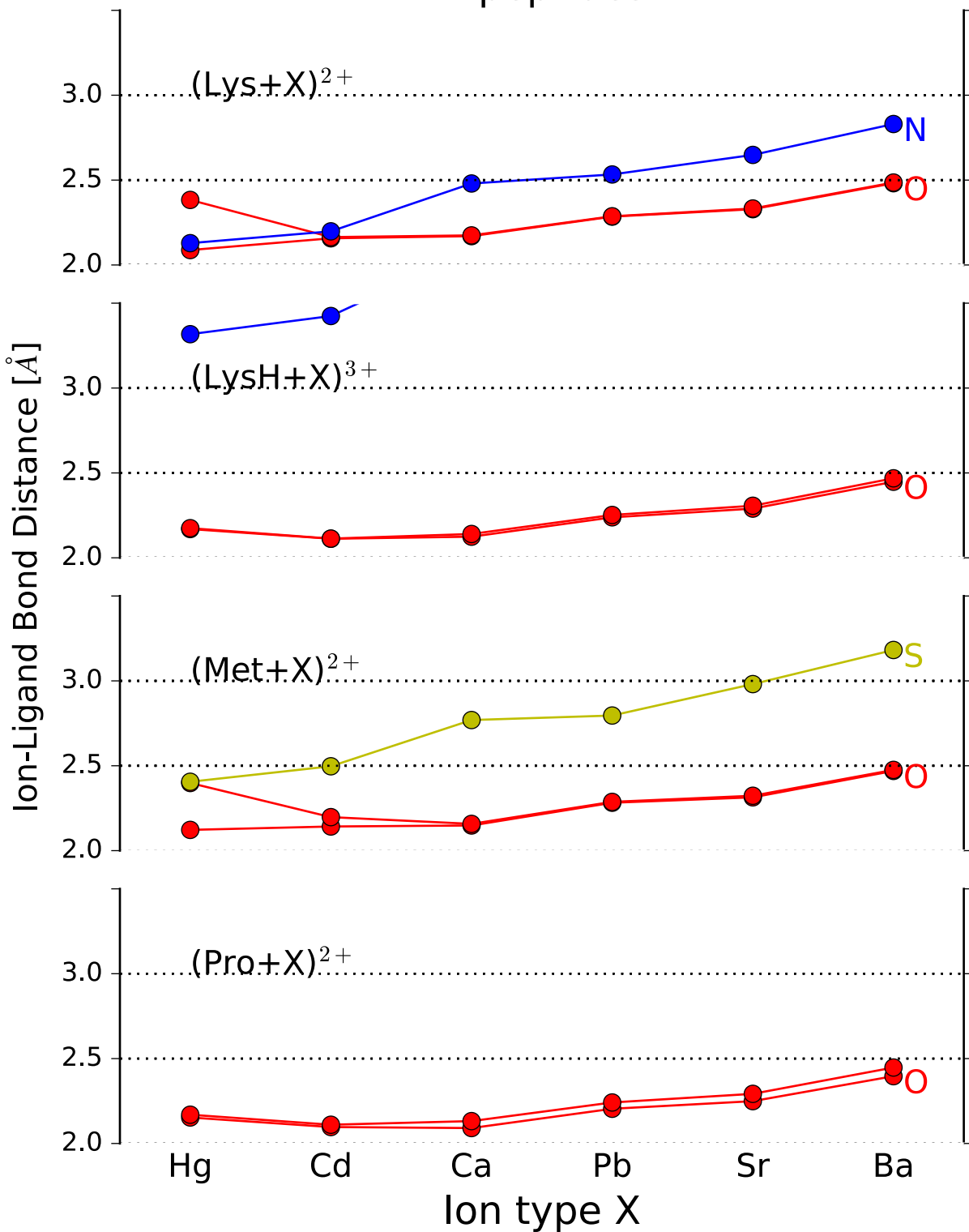
# Dipeptides



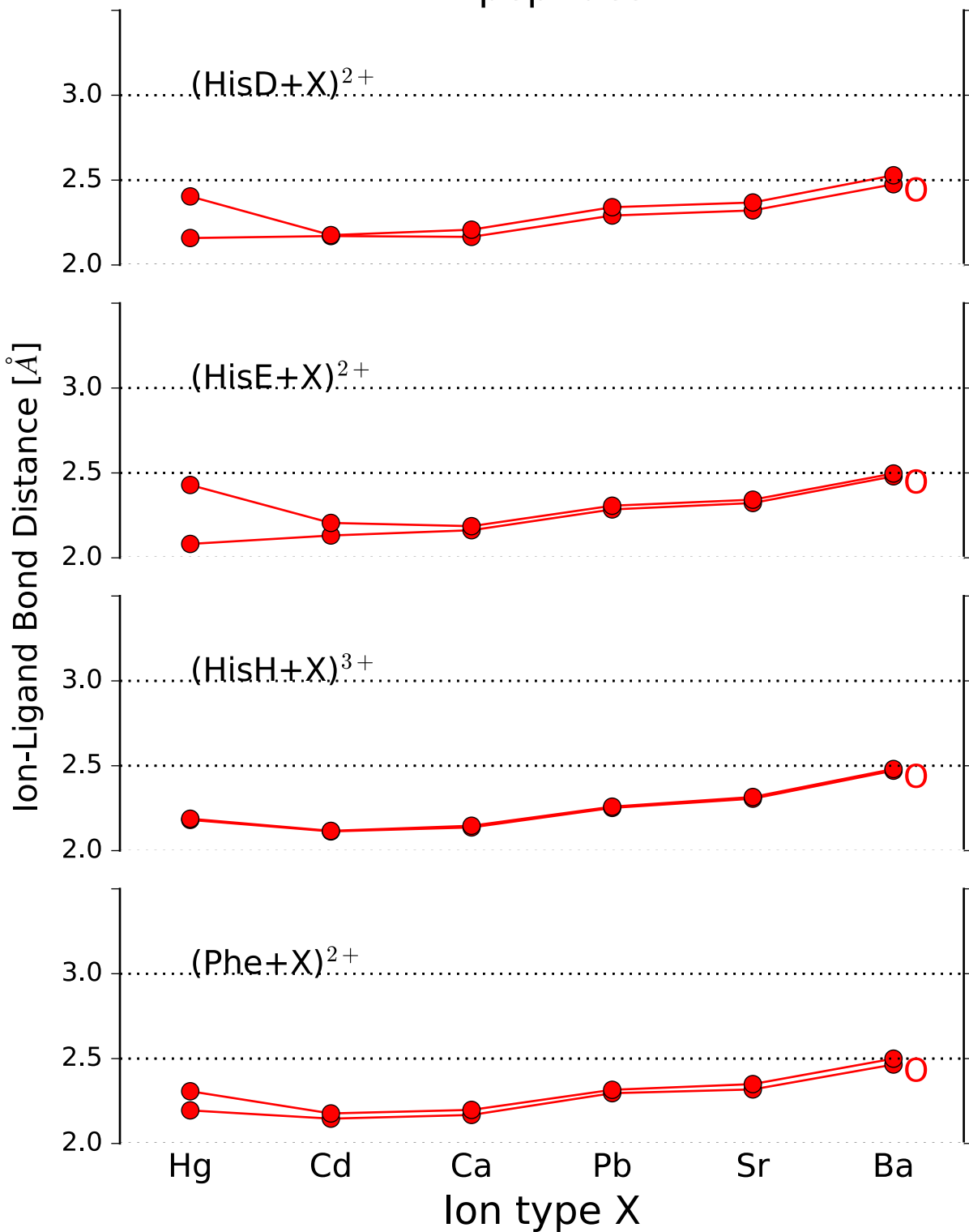
# Dipeptides



# Dipeptides



# Dipeptides



# Dipeptides

