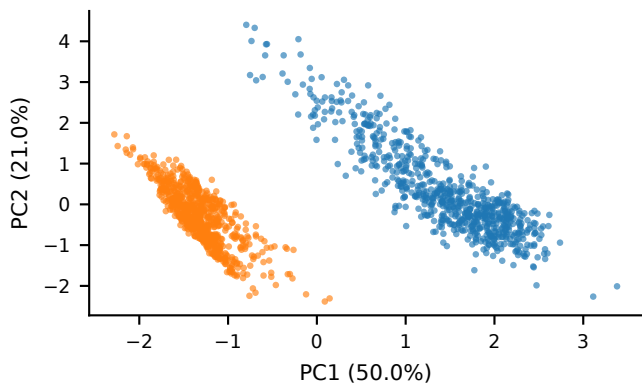


Zatom-2 (IV): without E/F prediction

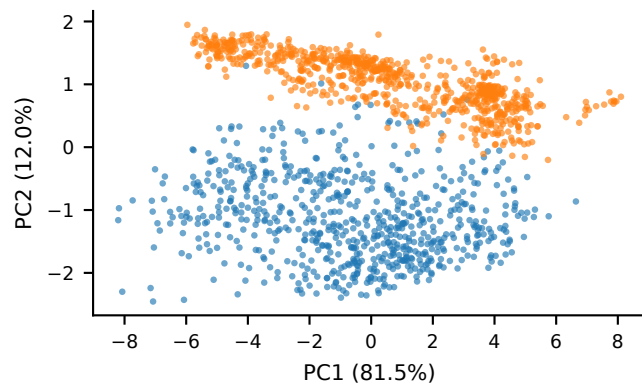
a Joint ($n = 1,472$)



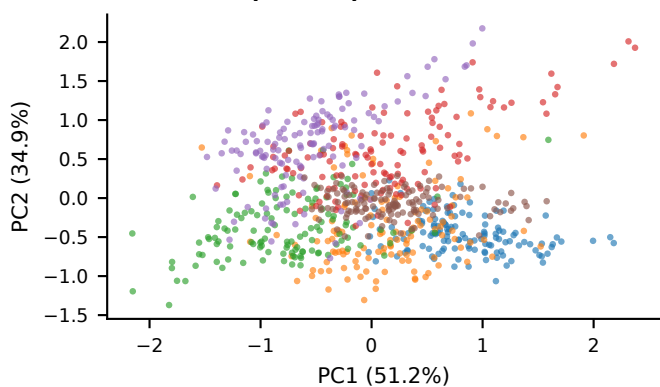
● OMat24 ● OMol25

Zatom-2 (V): with E/F prediction

b Joint ($n = 1,472$)

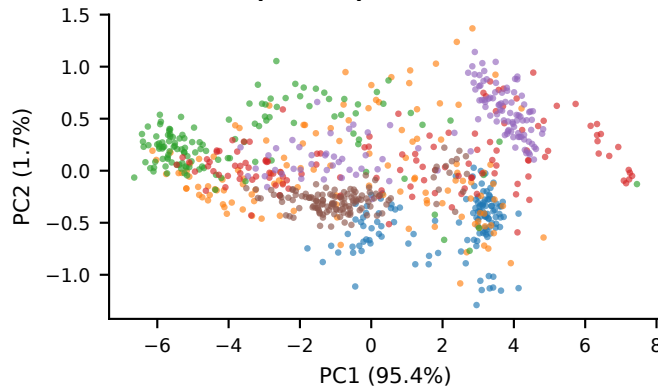


c OMol25 ($n = 768$)

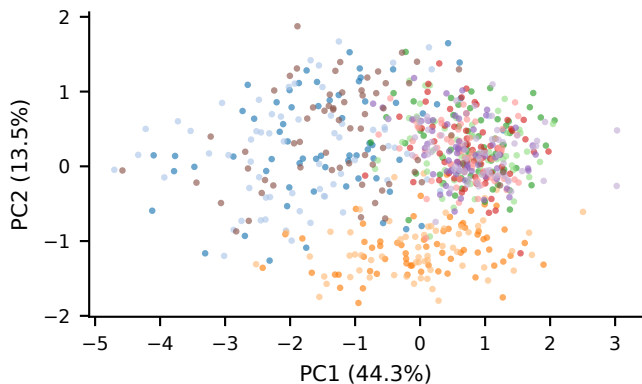


● Biomolecules ● Metal complexes ● Reactivity
● Electrolytes ● Neutral organics ● SPICE

d OMol25 ($n = 768$)



e OMat24 ($n = 704$)



● AIMD 1000-npt ● rattled-1000 ● rattled-500
● AIMD 1000-nvt ● rattled-1000 (sub) ● rattled-500 (sub)
● AIMD 3000-npt ● rattled-300 ● rattled-relax
● AIMD 3000-nvt ● rattled-300 (sub)

f OMat24 ($n = 704$)

