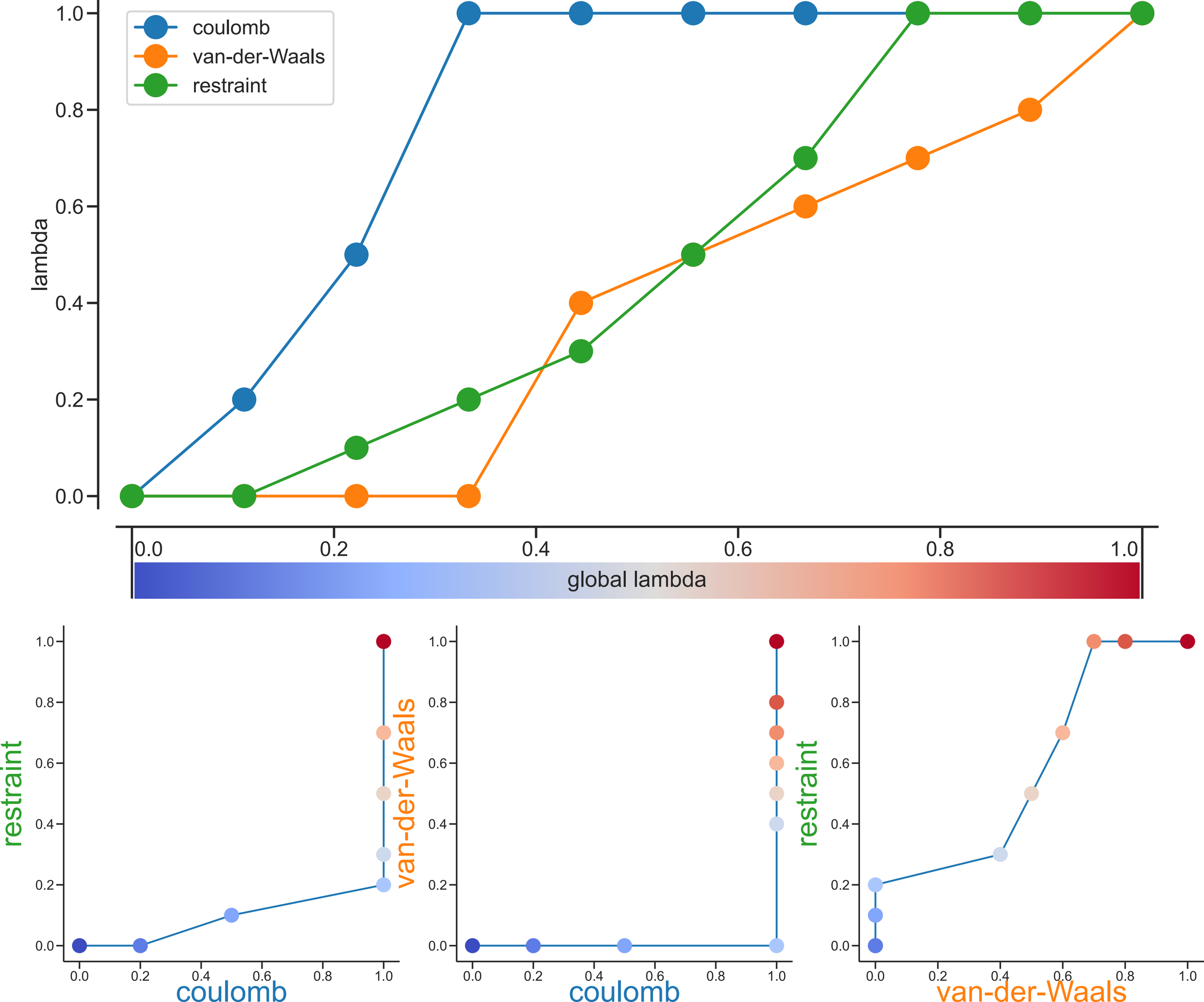
coulomb
van-der-Waals
restraint
lambda
1.0
0.8
0.6
0.4
0.2
0.0
global lambda
restraint
van-der-Waals
coulomb
van-der-Waals