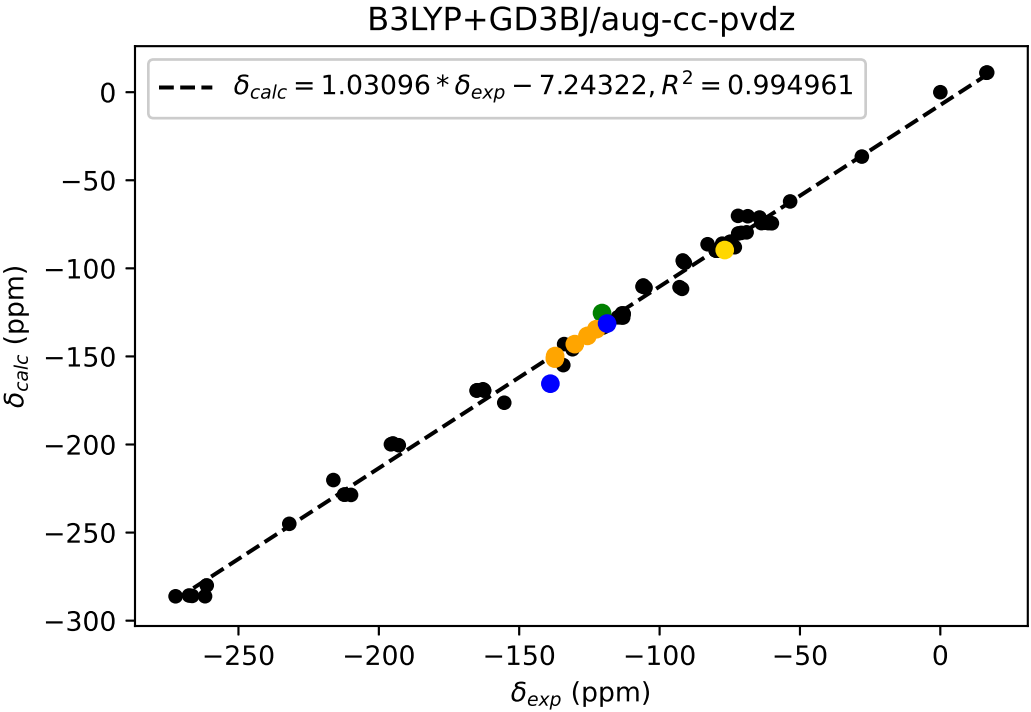
B3LYP+GD3BJ/aug-cc-pvdz
$\delta_{calc} = 1.03096 * \delta_{exp} - 7.24322, R^2 = 0.994961$
0
−50
−100
−150
−200
−250
−300
δ_{calc} (ppm)
−250
−200
−150
−100
−50
0
δ_{exp} (ppm)