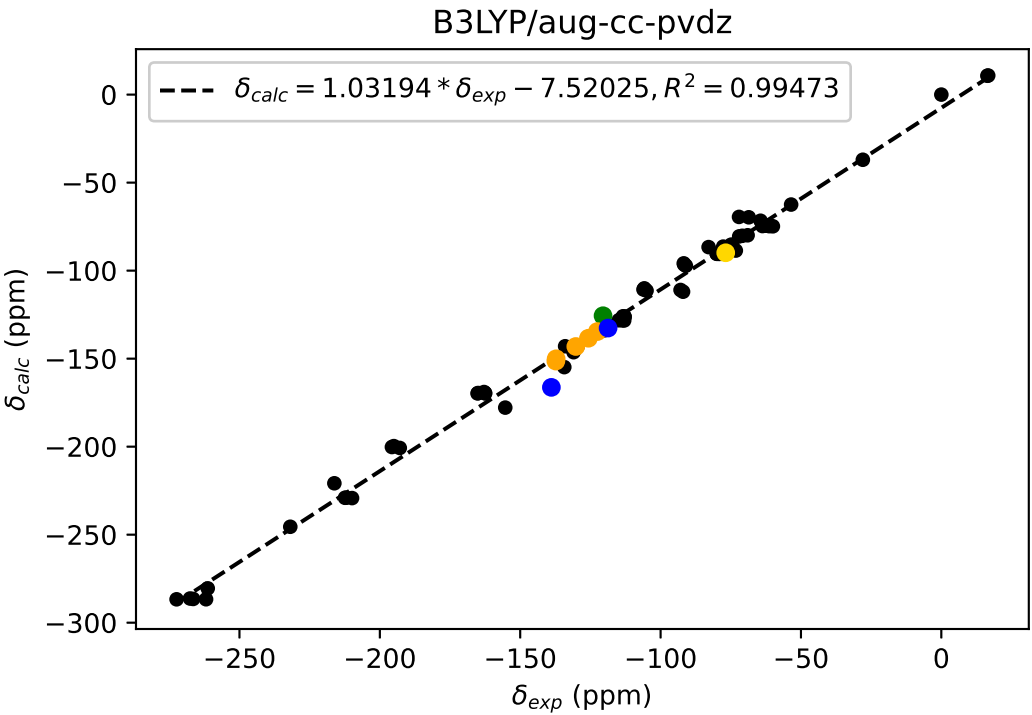
B3LYP/aug-cc-pvdz
$\delta_{calc} = 1.03194 * \delta_{exp} - 7.52025, R^2 = 0.99473$
0
−50
−100
−150
−200
−250
−300
δ_{calc} (ppm)
−250
−200
−150
−100
−50
0
δ_{exp} (ppm)