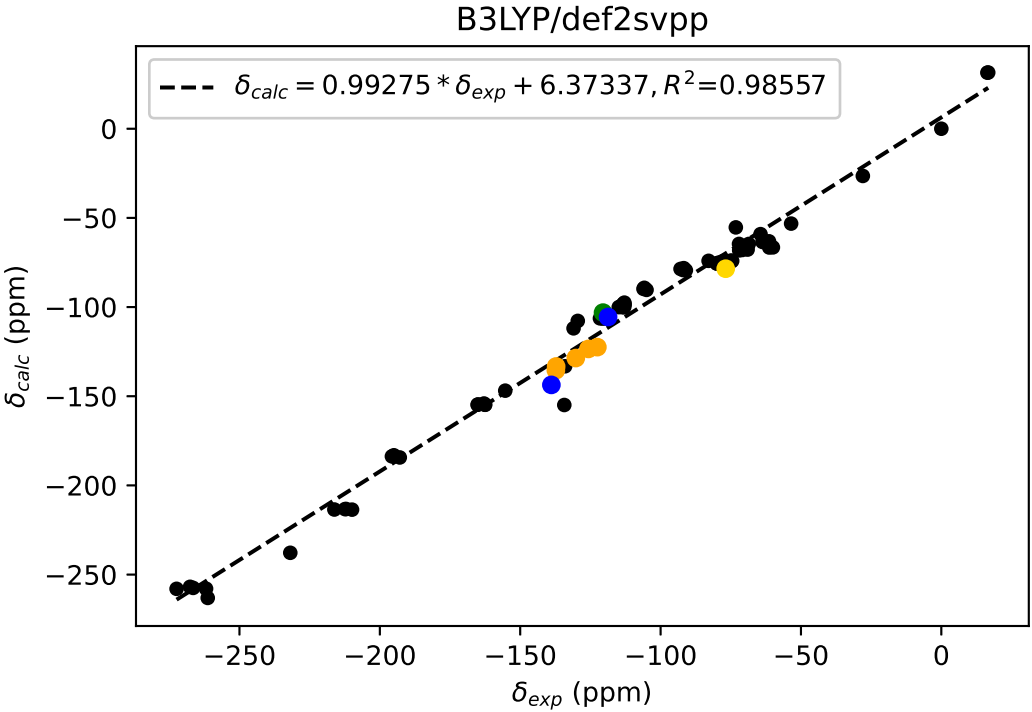
B3LYP/def2svpp
$\delta_{calc} = 0.99275 * \delta_{exp} + 6.37337, R^2$=0.98557
0
−50
−100
−150
−200
−250
δ_{calc} (ppm)
−250
−200
−150
−100
−50
0
δ_{exp} (ppm)