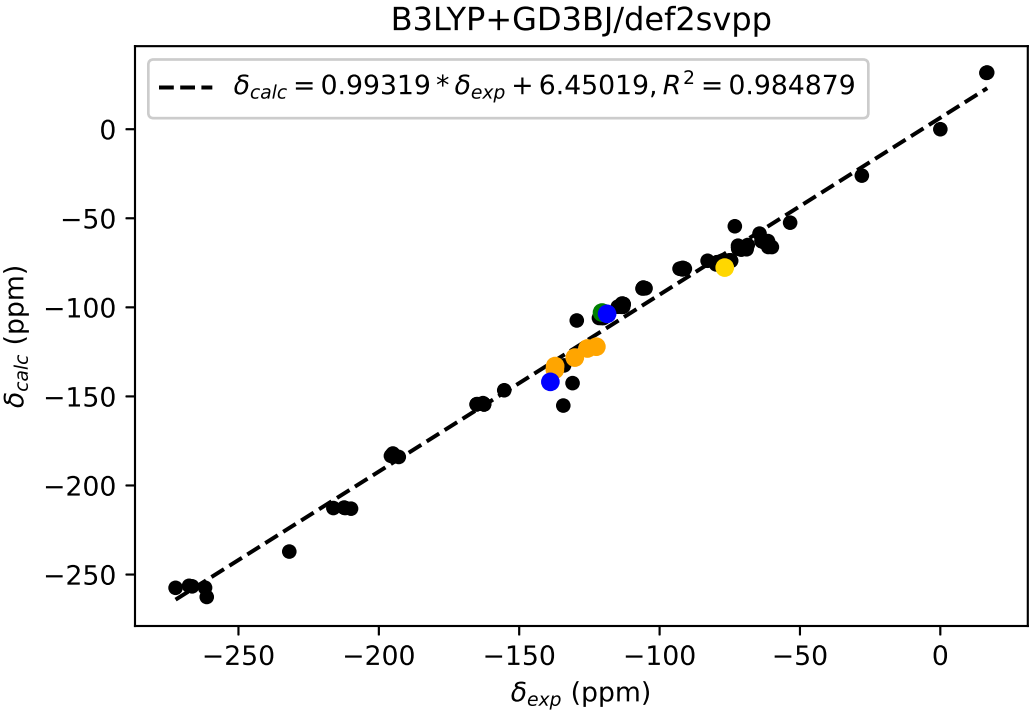
B3LYP+GD3BJ/def2svpp
$\delta_{calc} = 0.99319 * \delta_{exp} + 6.45019, R^2 = 0.984879$
0
−50
−100
−150
−200
−250
δ_{calc} (ppm)
−250
−200
−150
−100
−50
0
δ_{exp} (ppm)