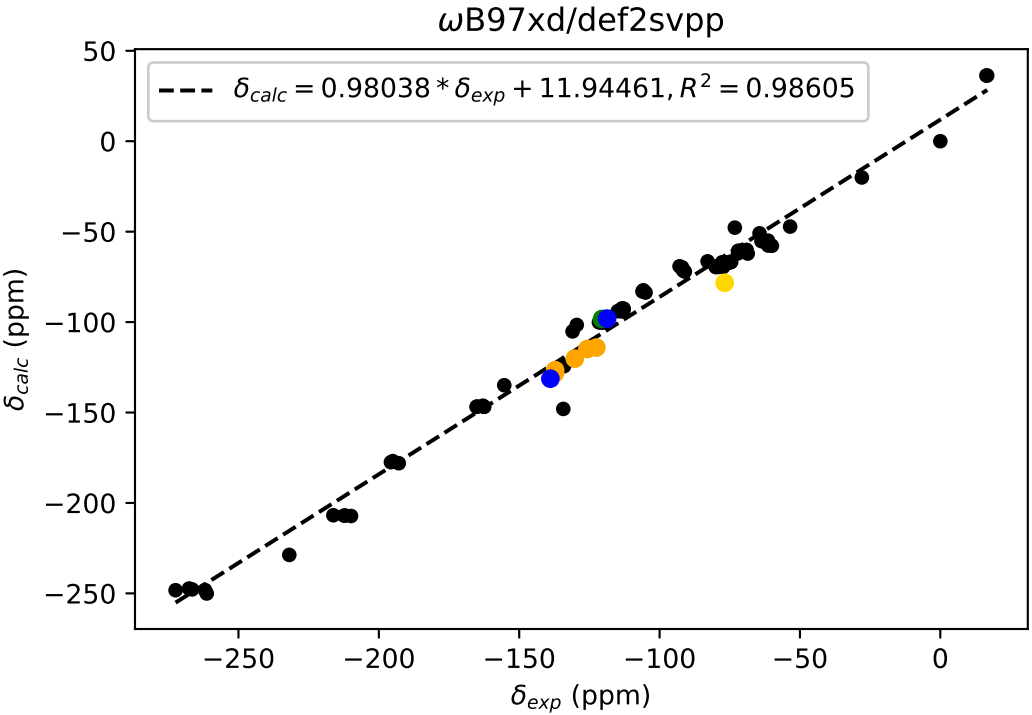
ωB97xd/def2svpp
$\delta_{calc} = 0.98038 * \delta_{exp} + 11.94461, R^2 = 0.98605$
δ_{calc} (ppm)
δ_{exp} (ppm)
50
0
−50
−100
−150
−200
−250
−250
−200
−150
−100
−50
0