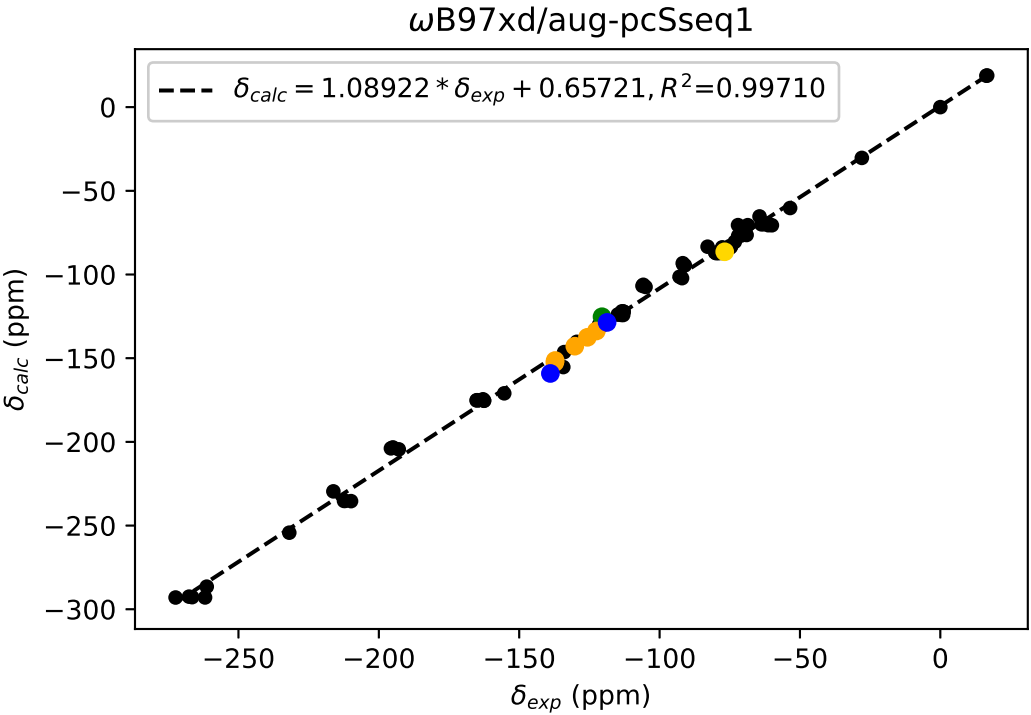
ωB97xd/aug-pcSseq1
$\delta_{calc} = 1.08922 * \delta_{exp} + 0.65721, R^2$=0.99710
0
−50
−100
−150
−200
−250
−300
δ_{calc} (ppm)
−250
−200
−150
−100
−50
0
δ_{exp} (ppm)