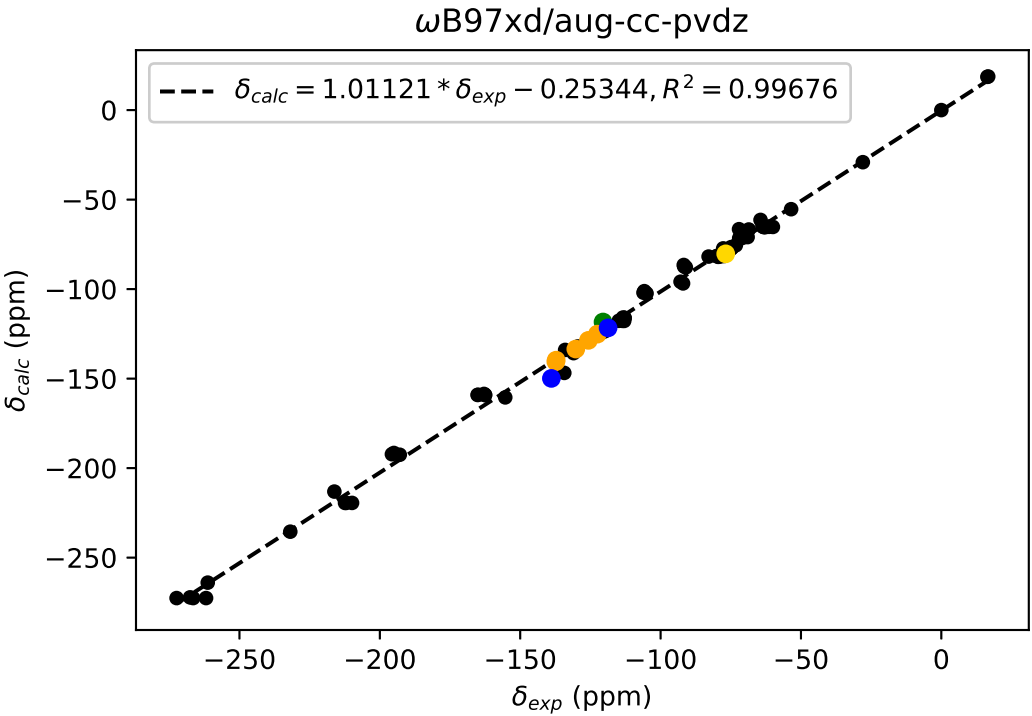
ωB97xd/aug-cc-pvdz
$\delta_{calc} = 1.01121 * \delta_{exp} - 0.25344, R^2 = 0.99676$
0
−50
−100
−150
−200
−250
δ_{calc} (ppm)
−250
−200
−150
−100
−50
0
δ_{exp} (ppm)