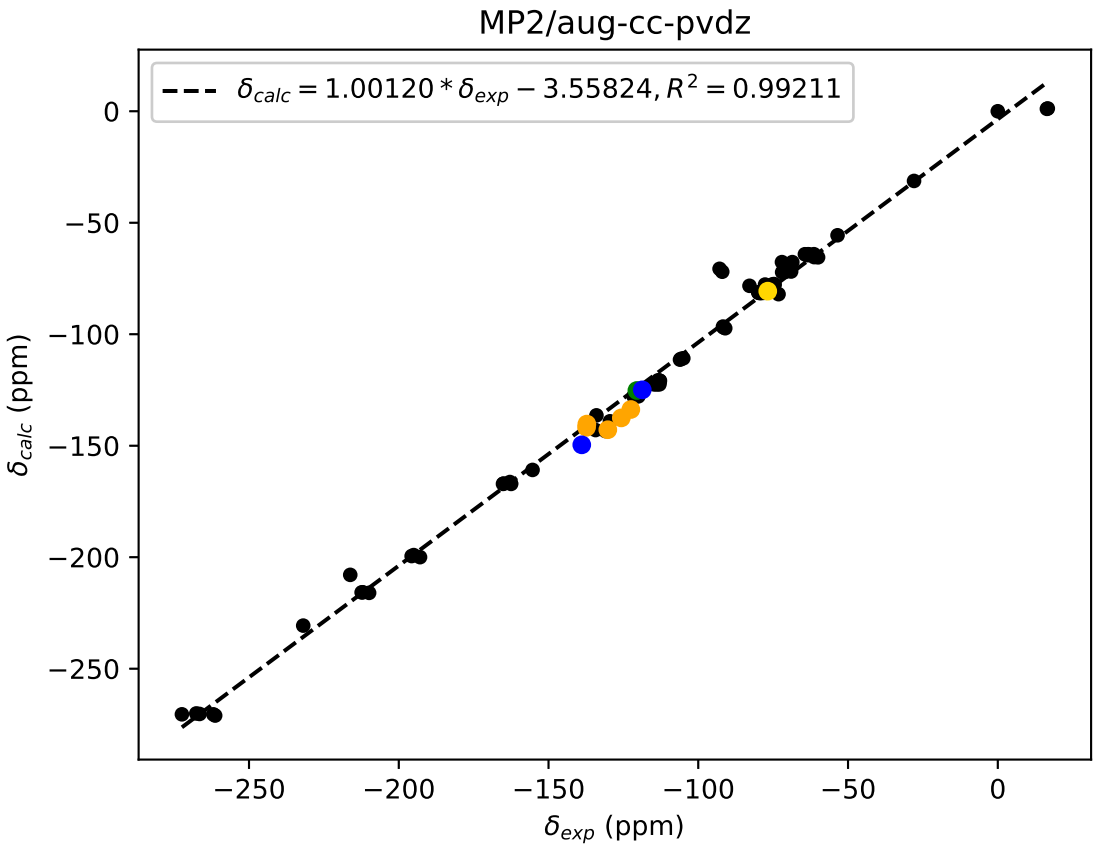
MP2/aug-cc-pvdz
$\delta_{calc} = 1.00120 * \delta_{exp} - 3.55824, R^2 = 0.99211$
0
−50
−100
−150
−200
−250
δ_{calc} (ppm)
−250
−200
−150
−100
−50
0
δ_{exp} (ppm)