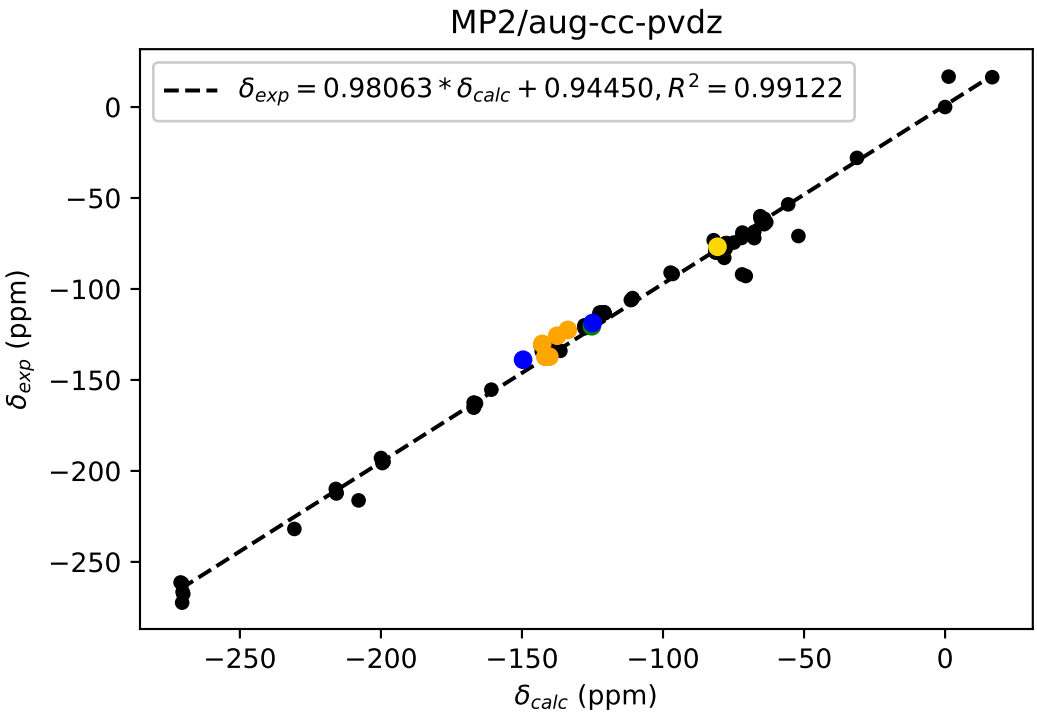
MP2/aug-cc-pvdz
$\delta_{exp} = 0.98063 * \delta_{calc} + 0.94450, R^2 = 0.99122$
0
−50
−100
−150
−200
−250
δ_{exp} (ppm)
−250
−200
−150
−100
−50
0
δ_{calc} (ppm)