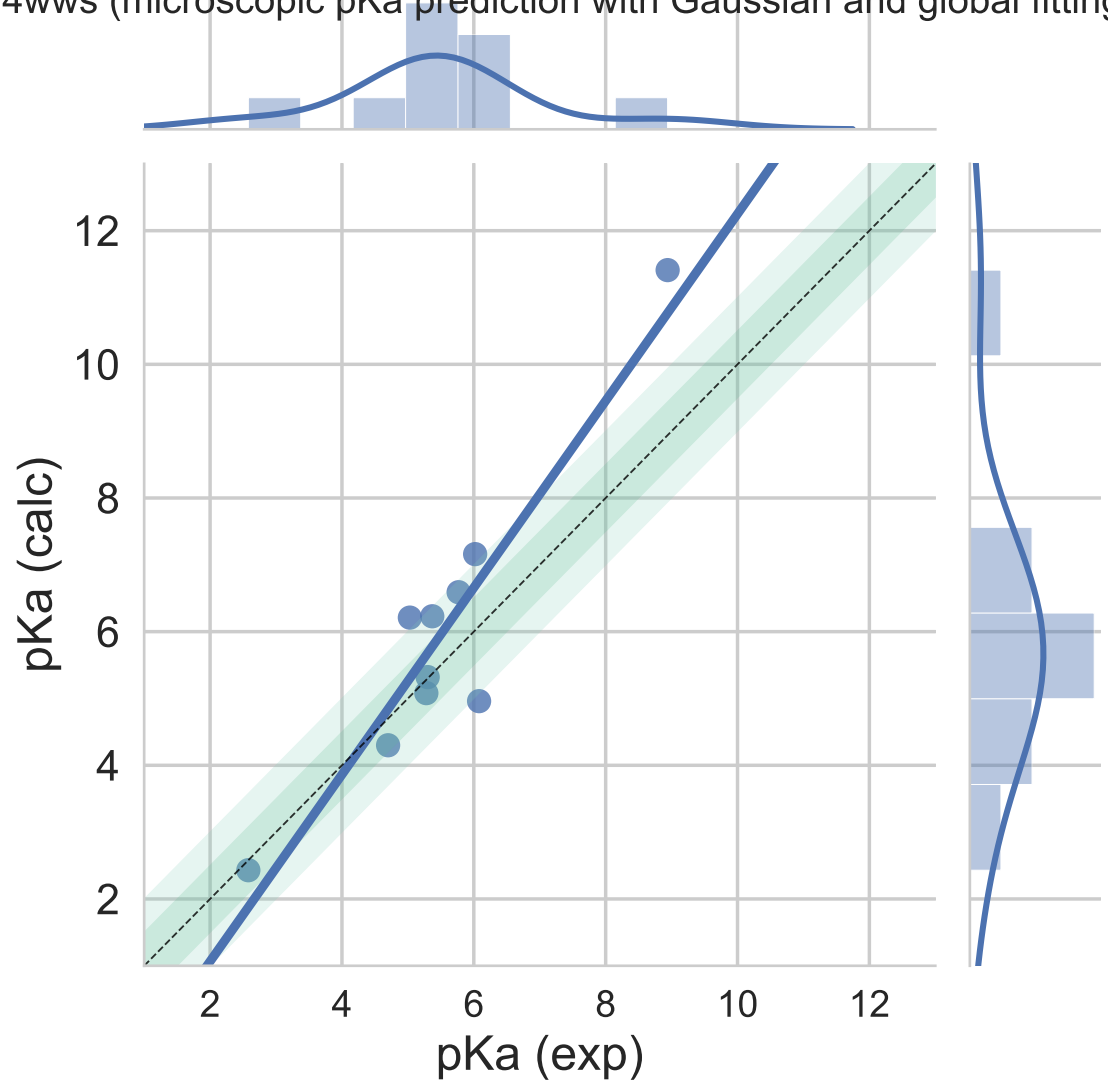y4wws (microscopic pKa prediction with Gaussian and global fitting)