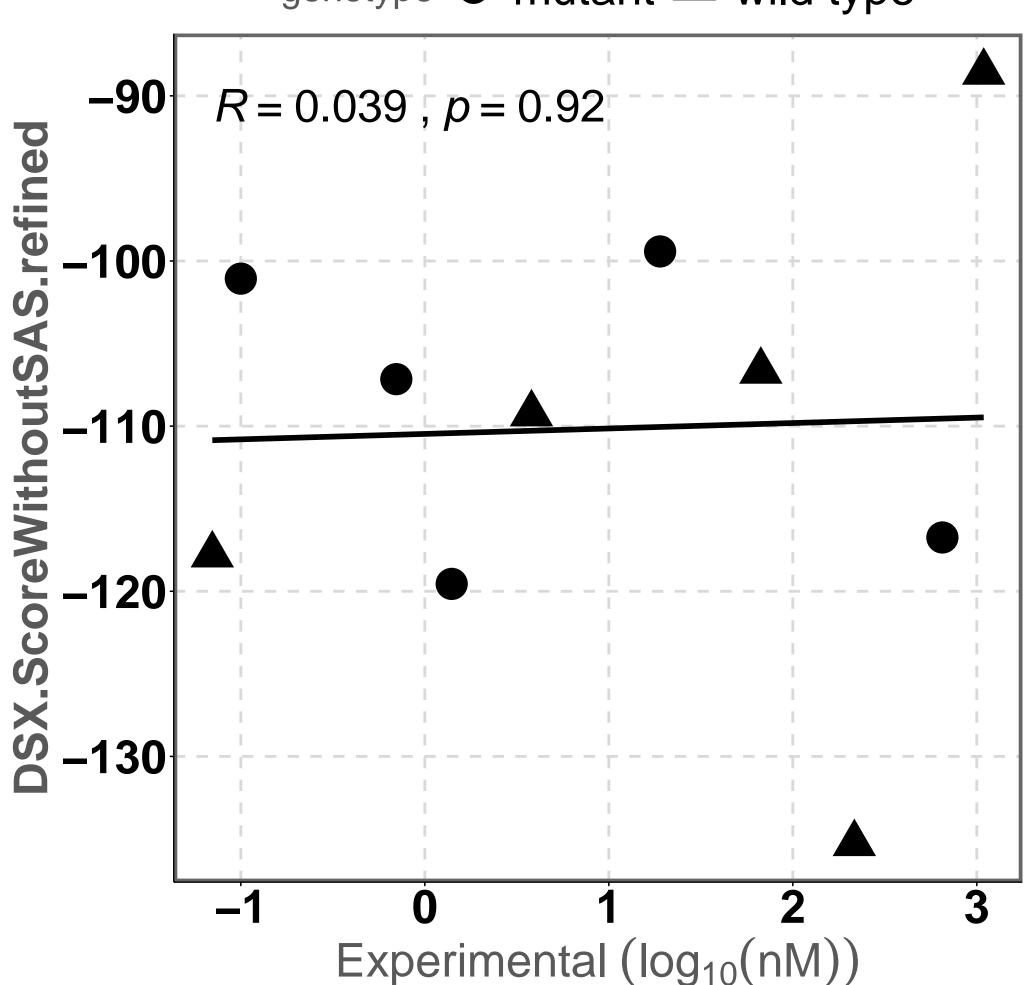
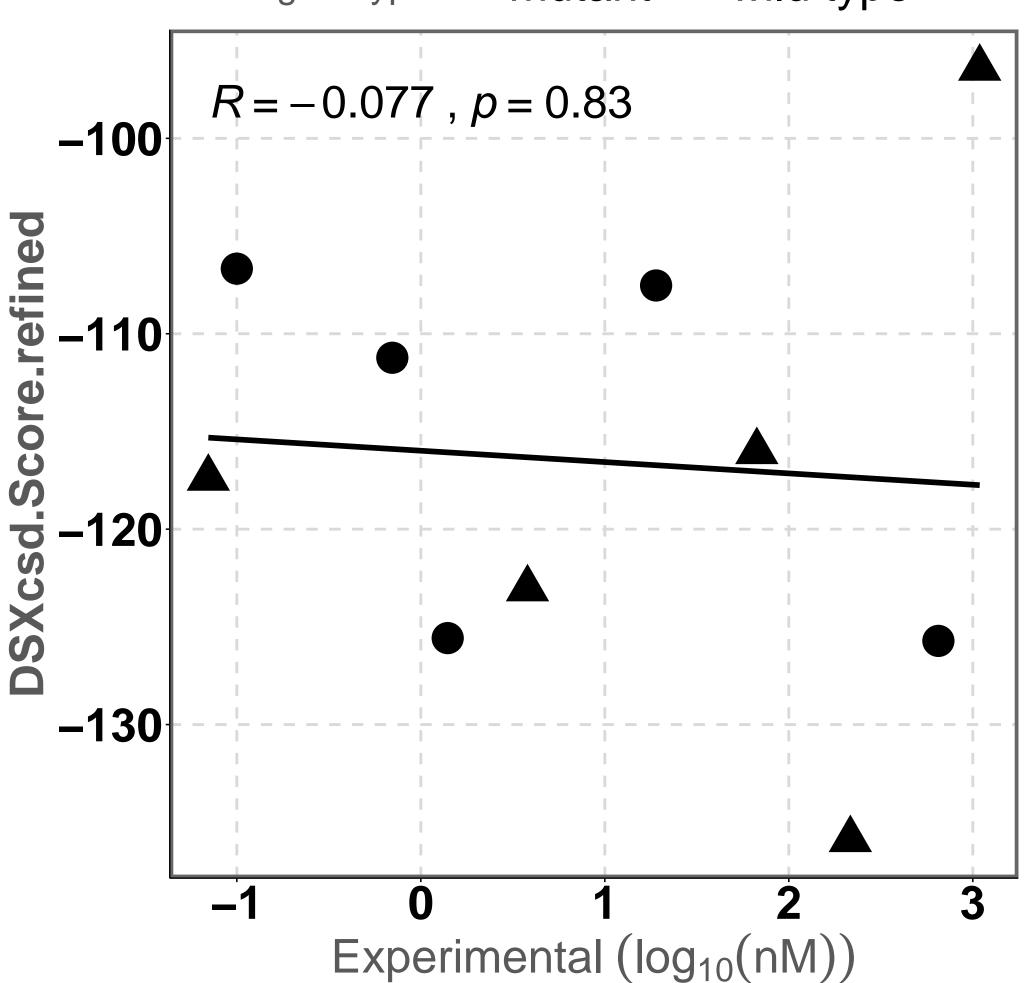
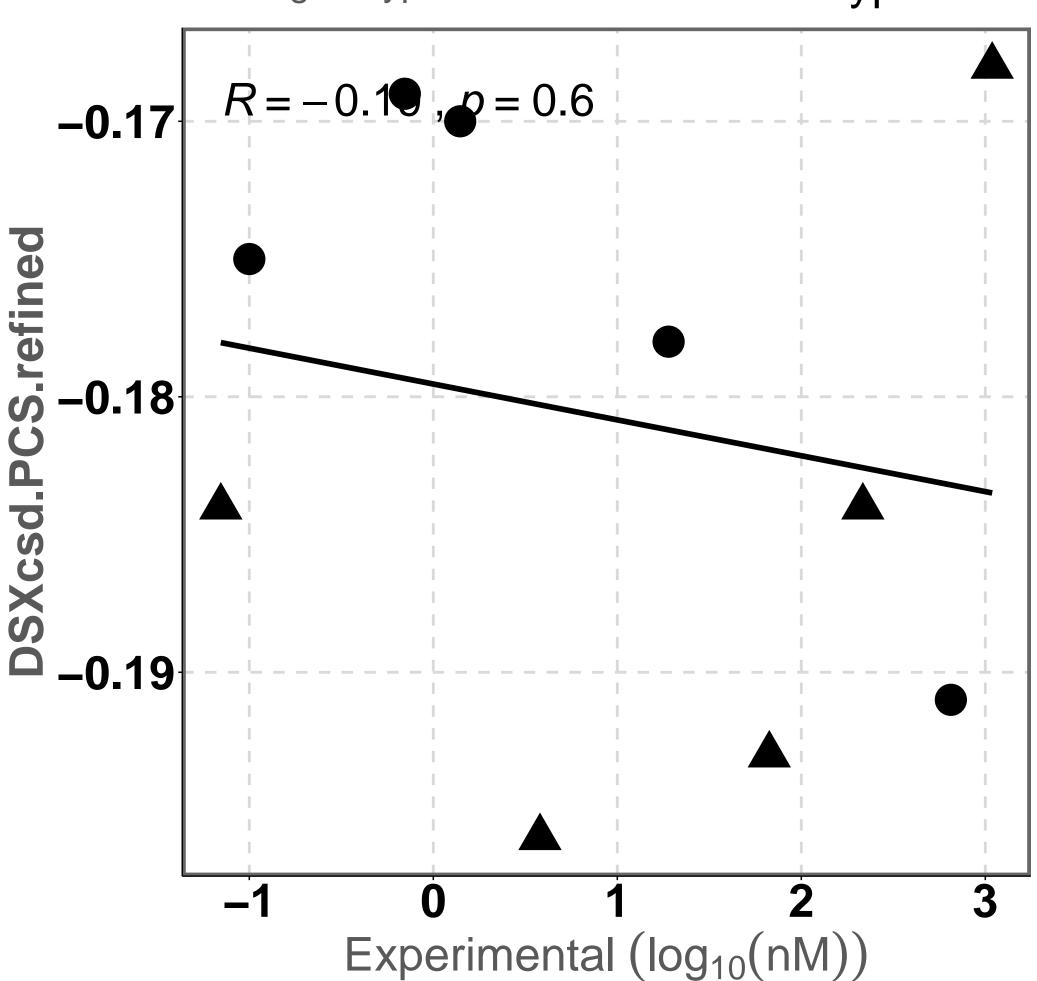


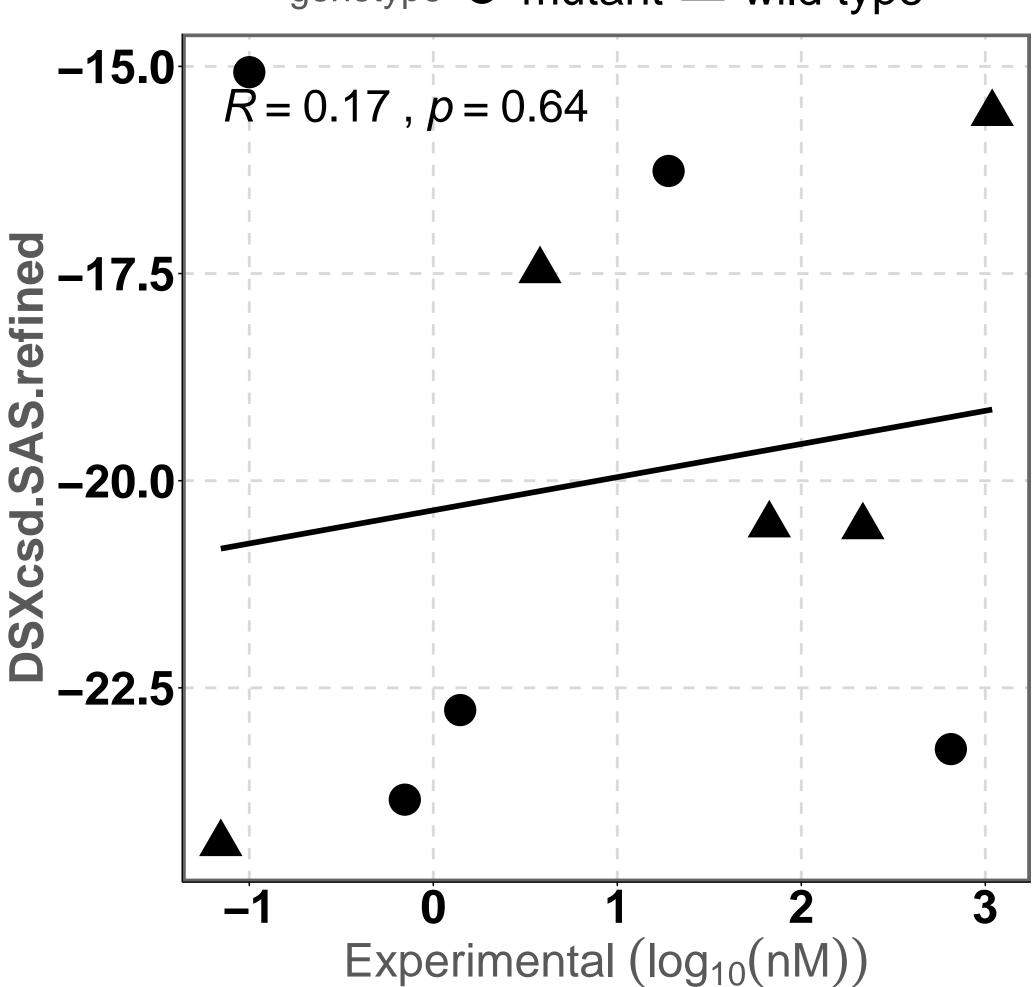
genotype • mutant • wild type



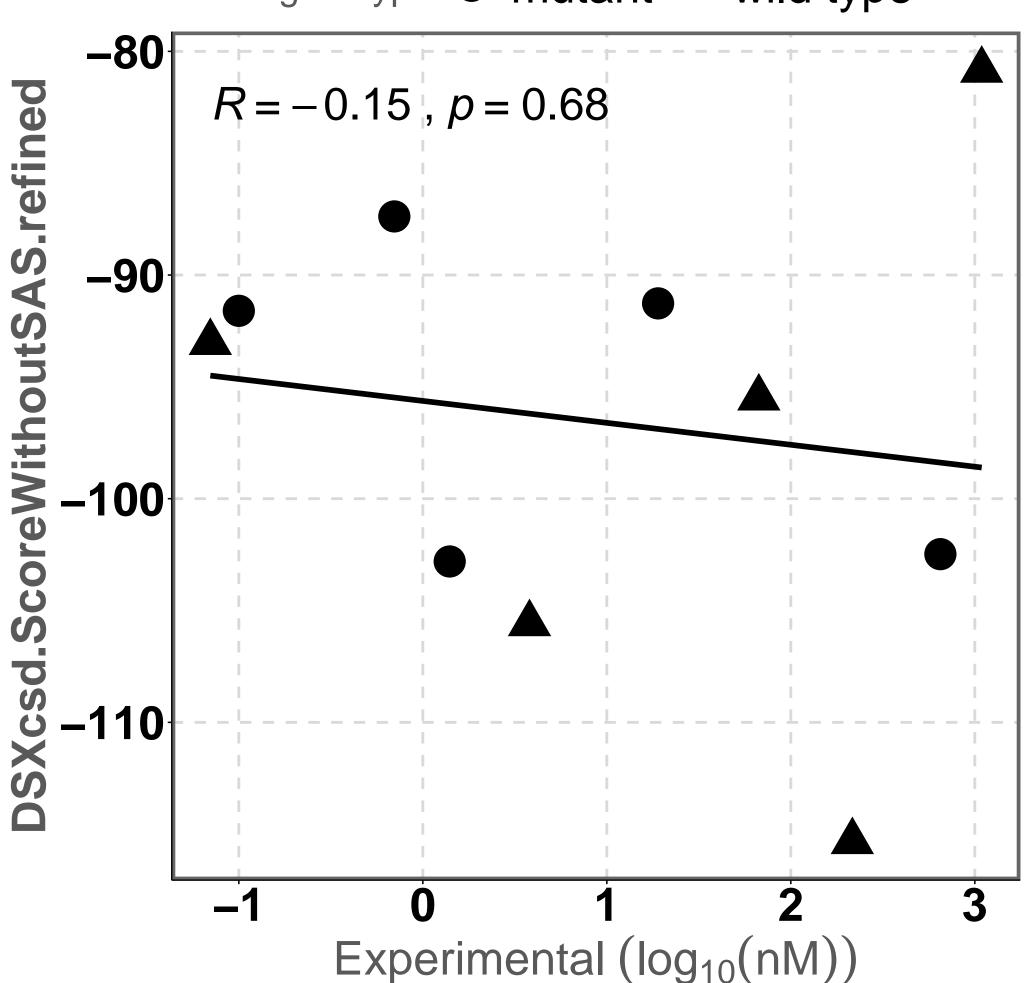
genotype • mutant • wild type



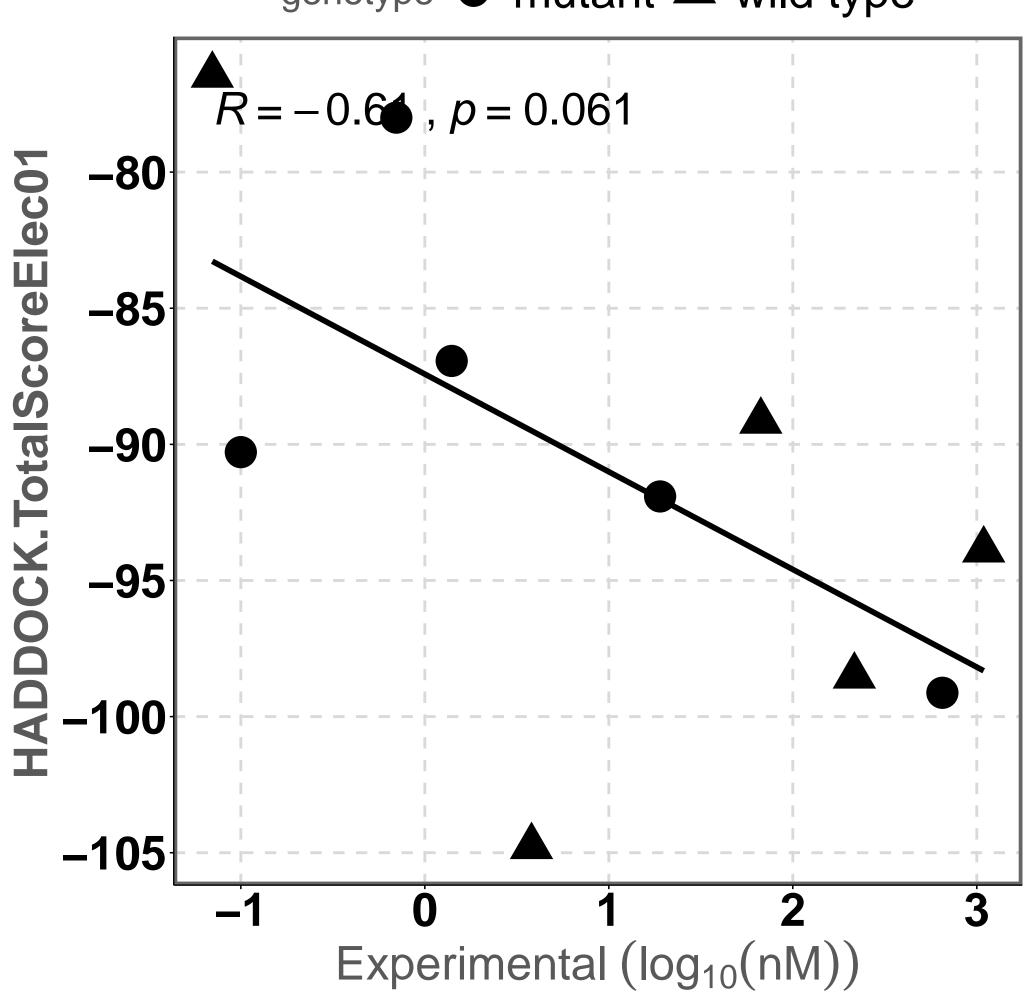




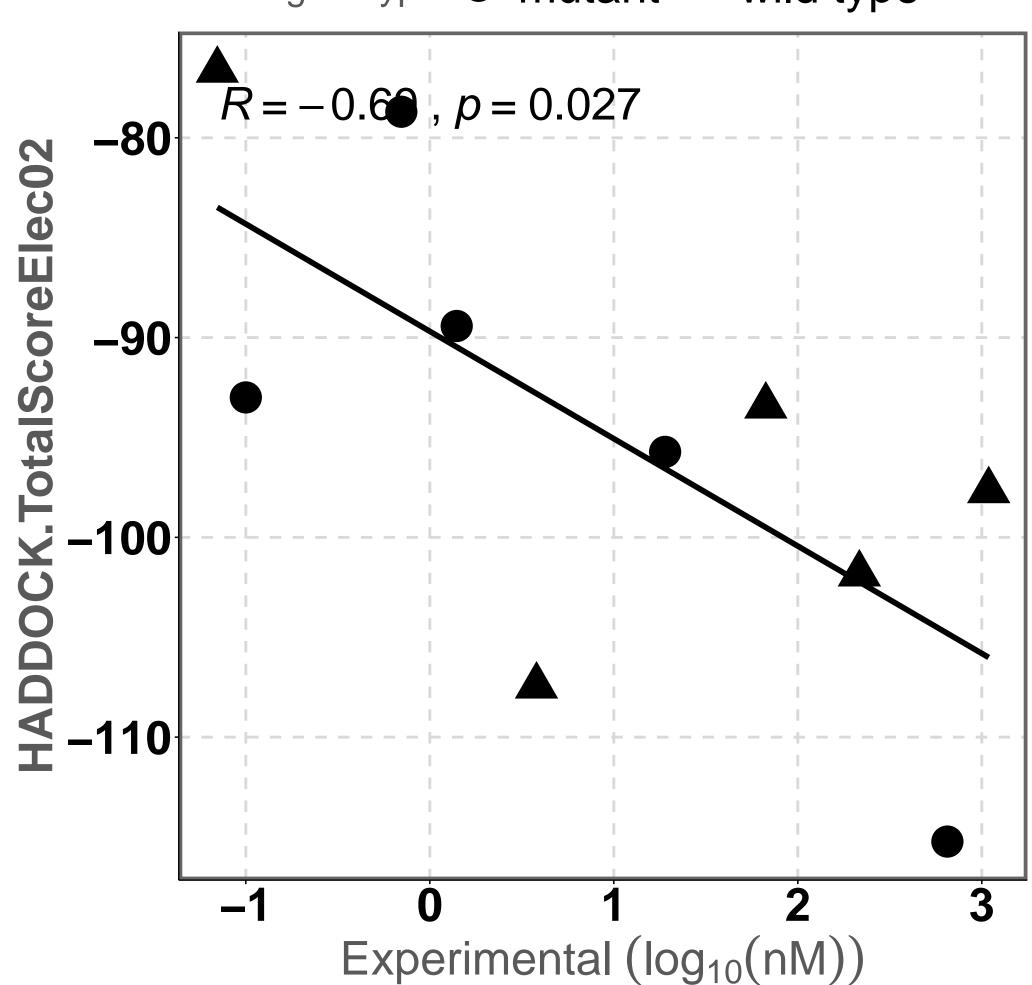
genotype • mutant • wild type



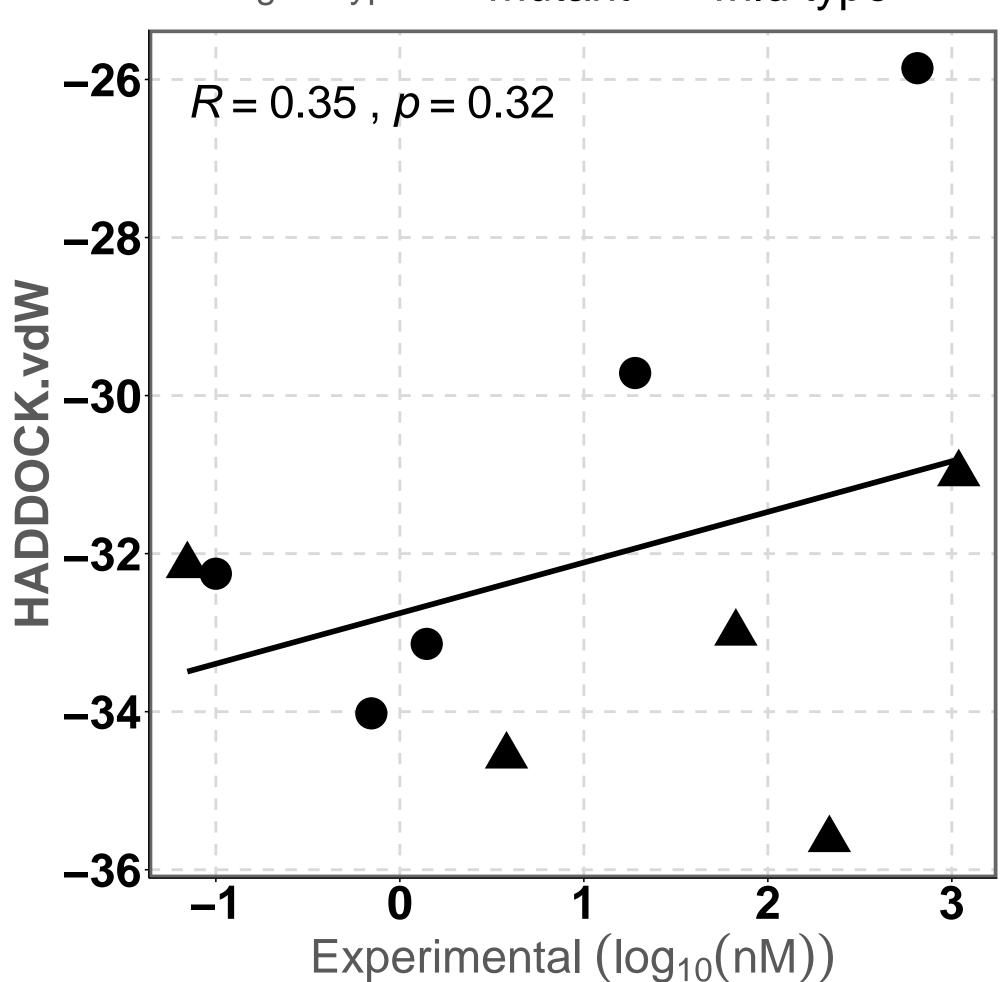
genotype • mutant • wild type



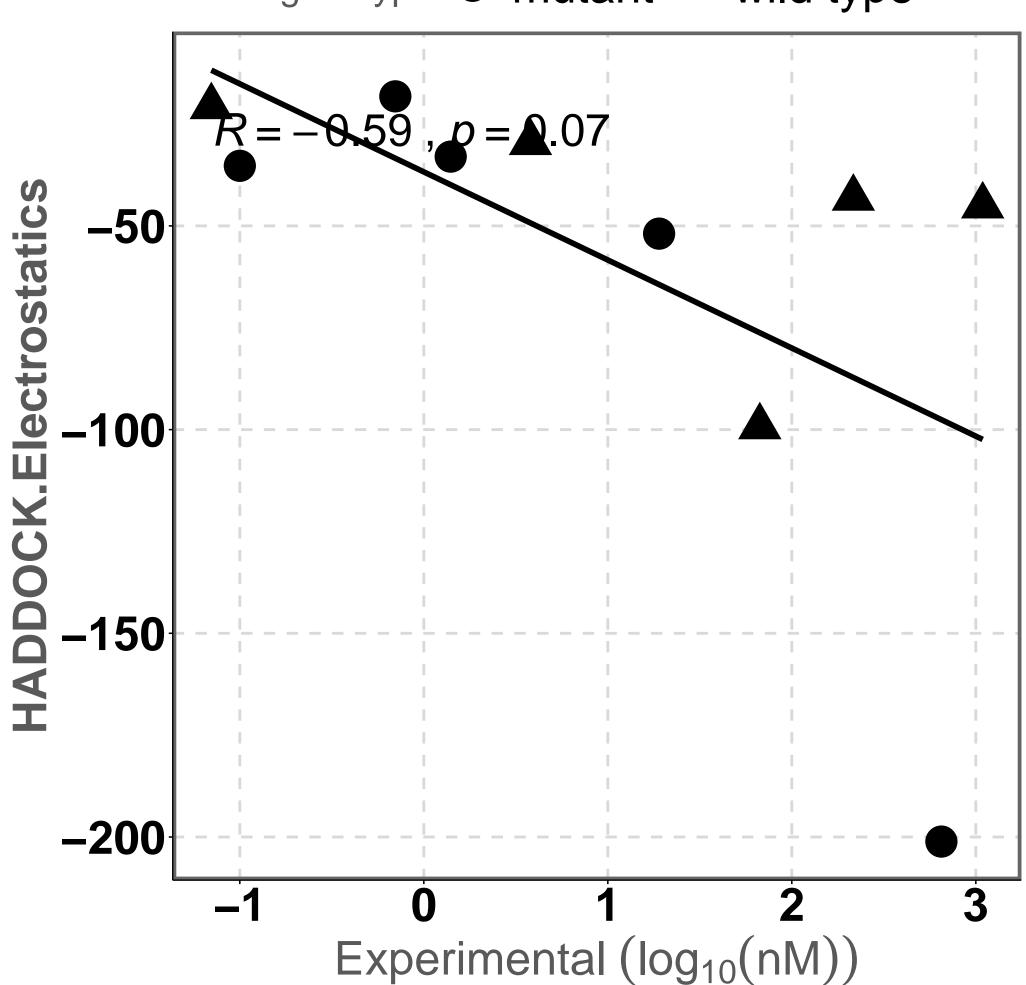
genotype • mutant • wild type

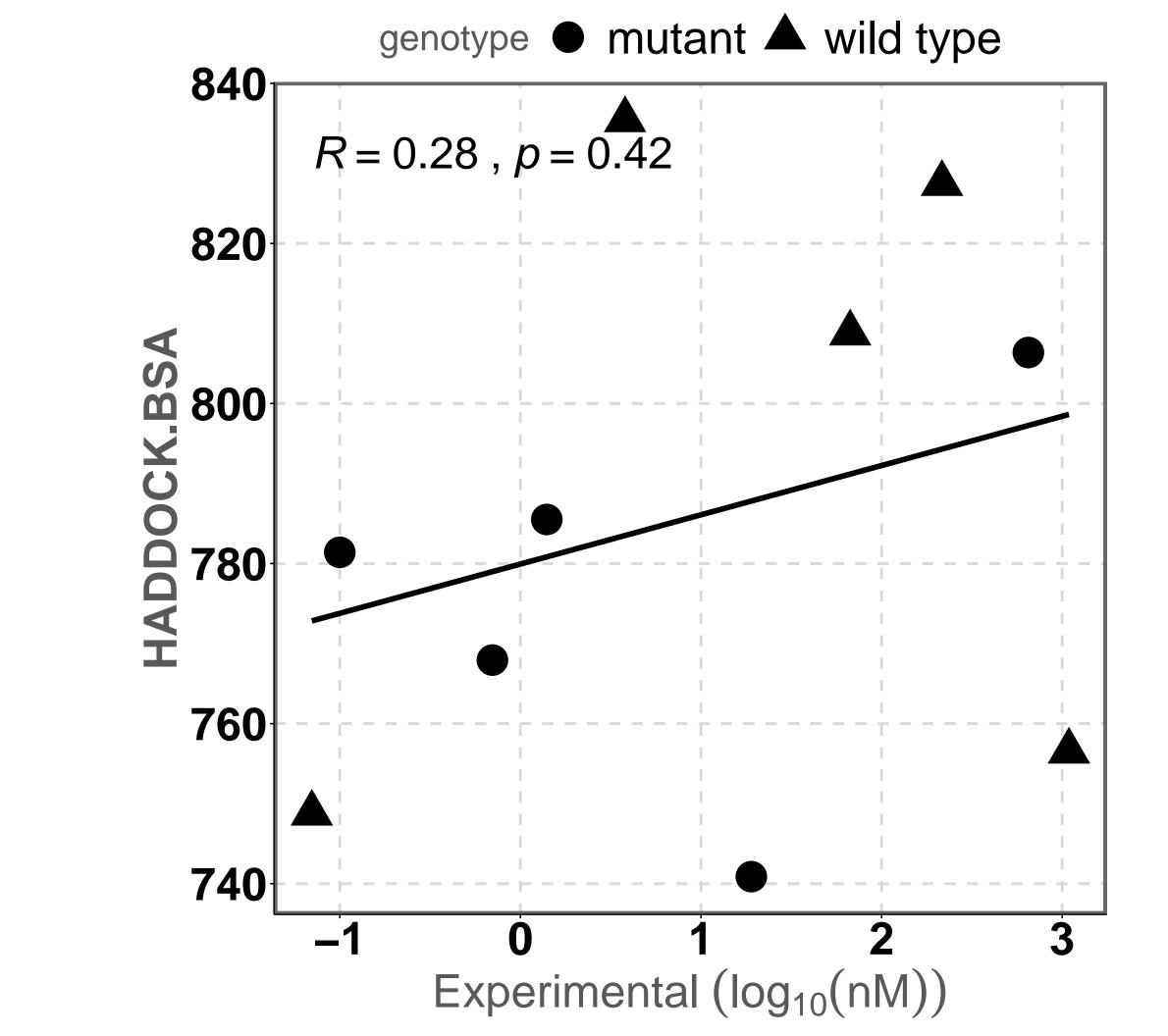


genotype • mutant • wild type

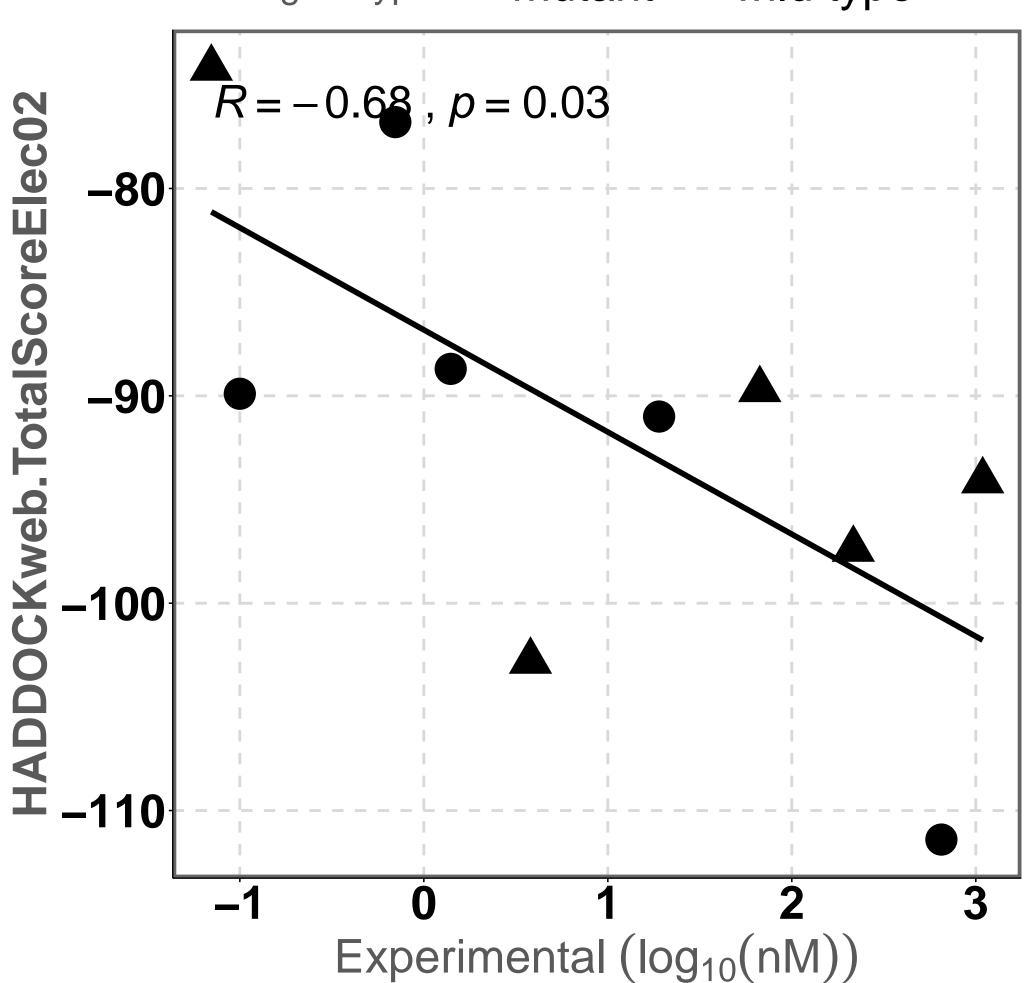


genotype • mutant • wild type

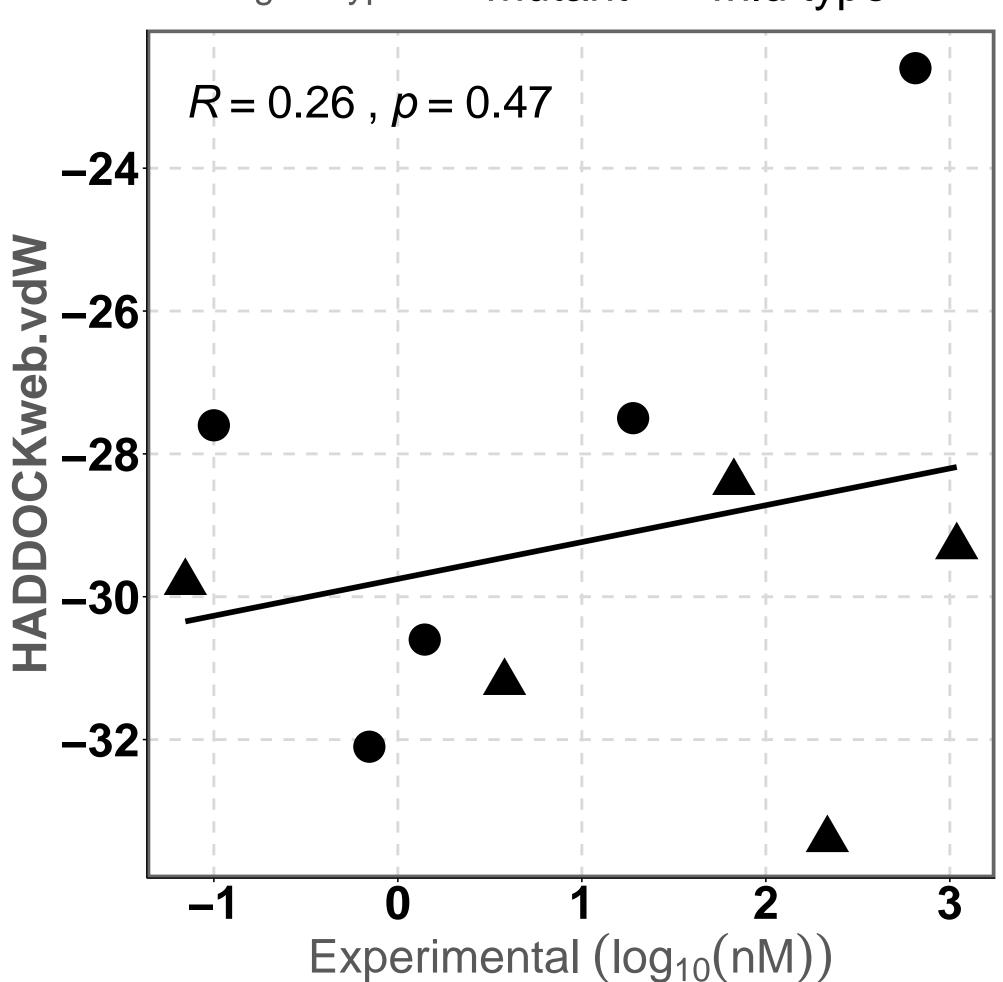




genotype • mutant • wild type



genotype • mutant • wild type



genotype • mutant • wild type 0.58, p = 0.077Experimental $(log_{10}(nM))$

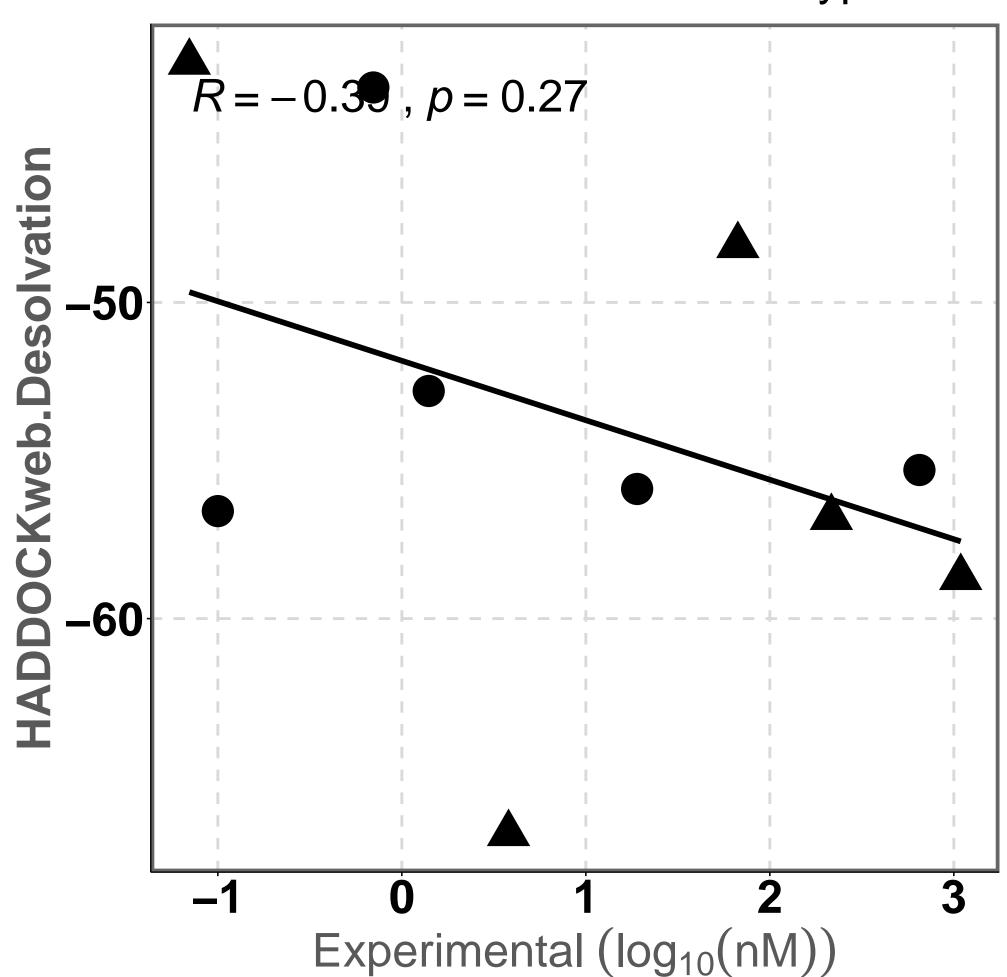
HADDOCKweb. Electrostatics

-50

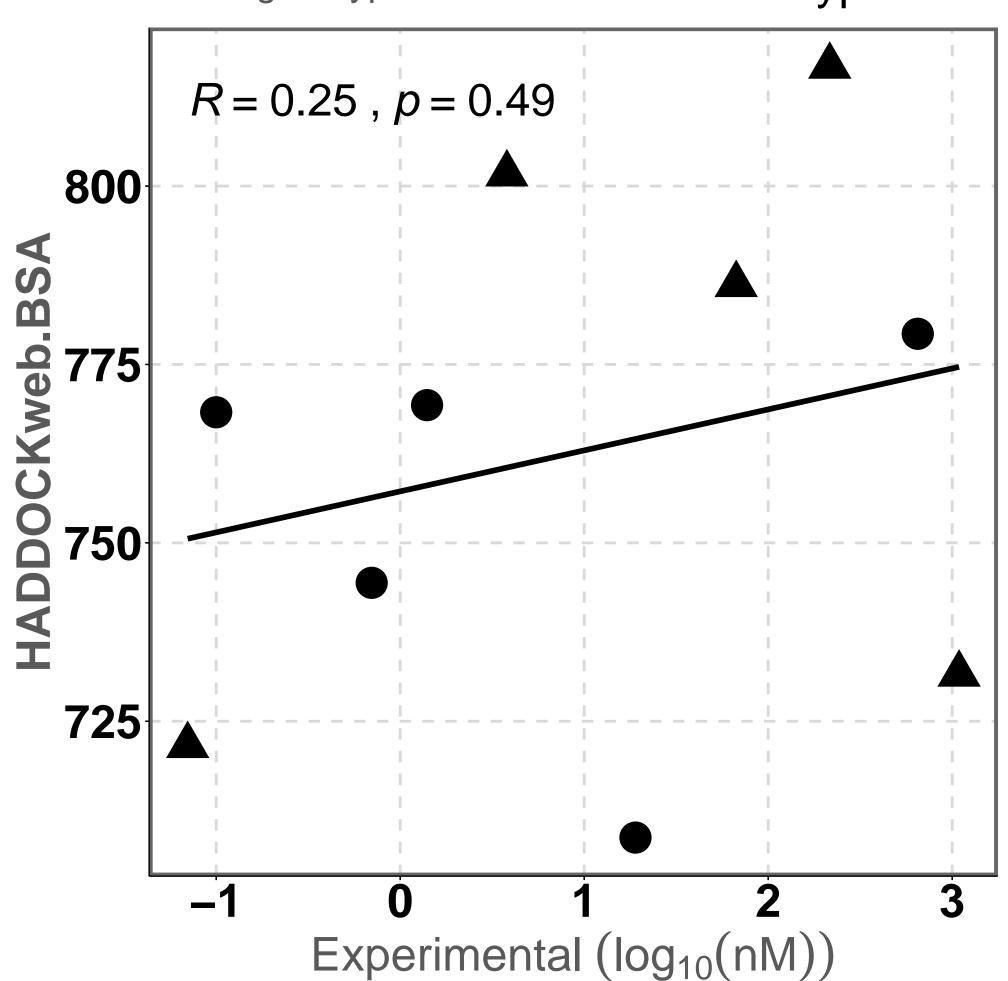
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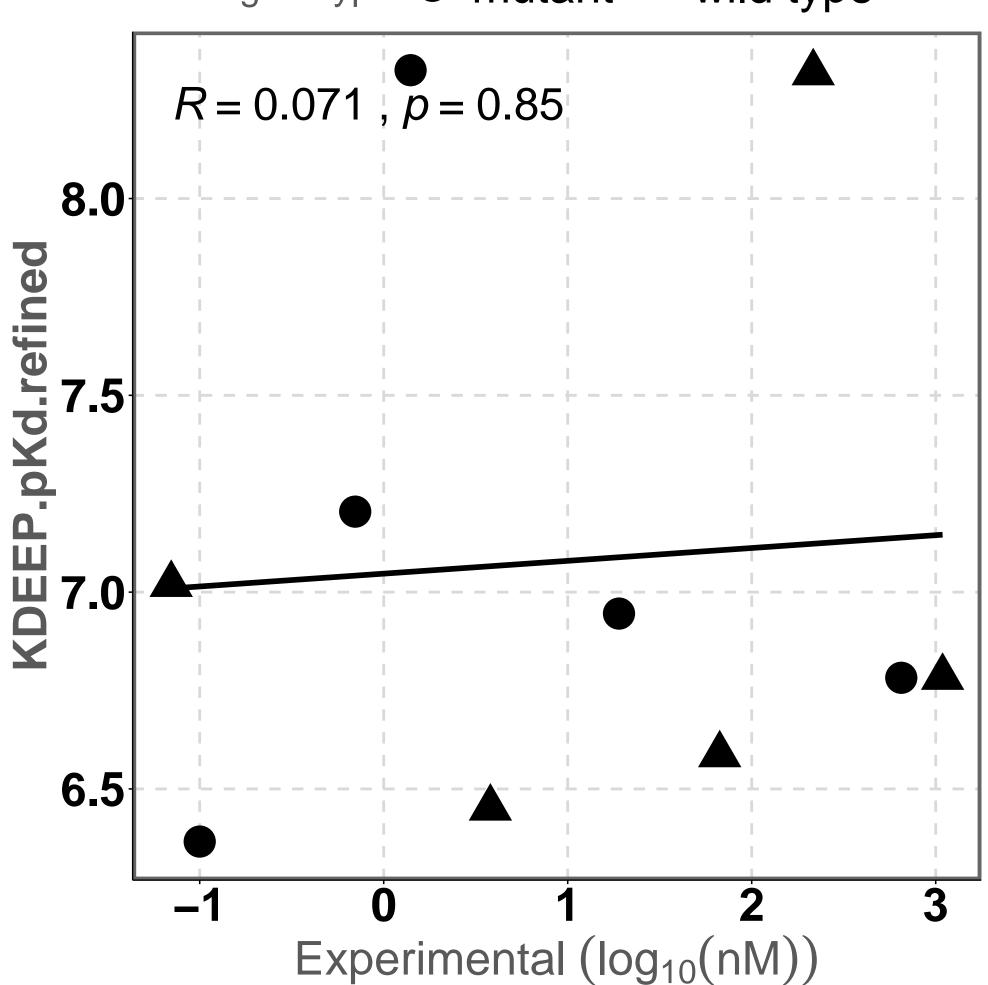
-150

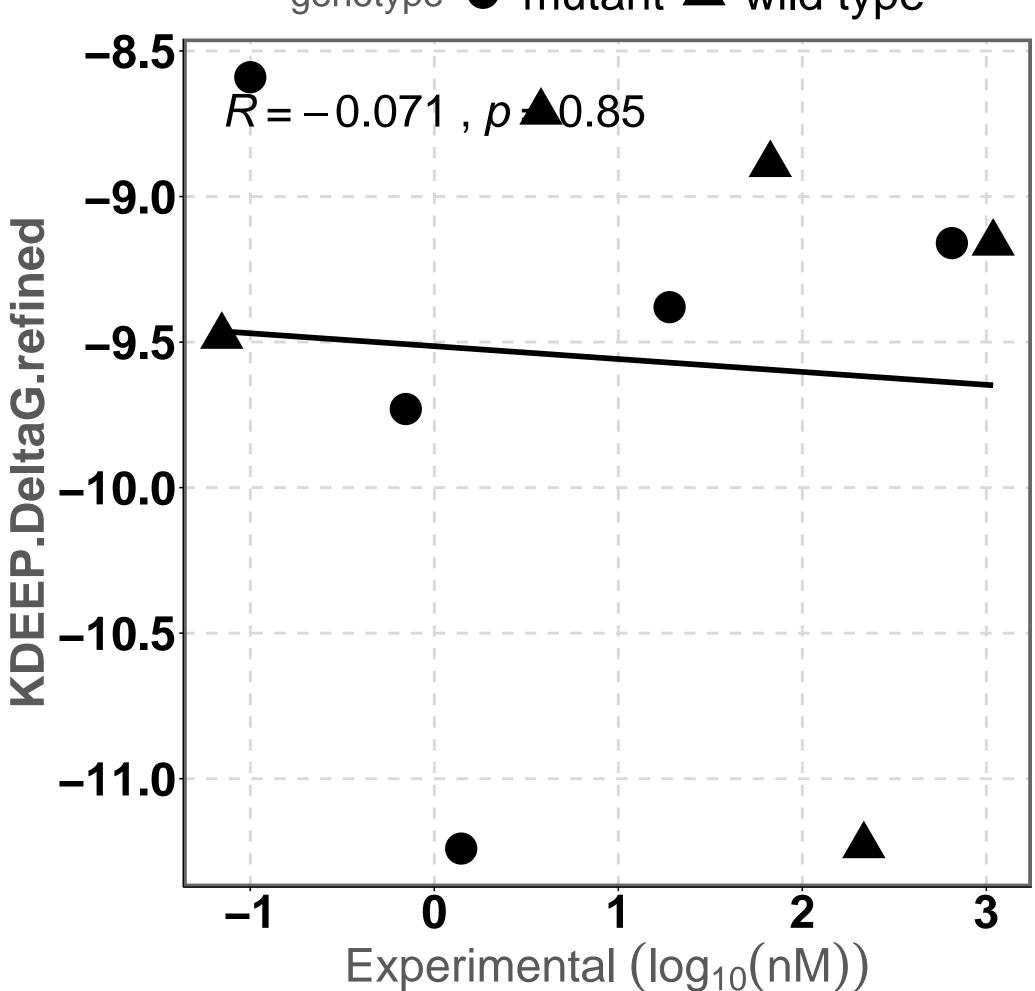
genotype • mutant • wild type

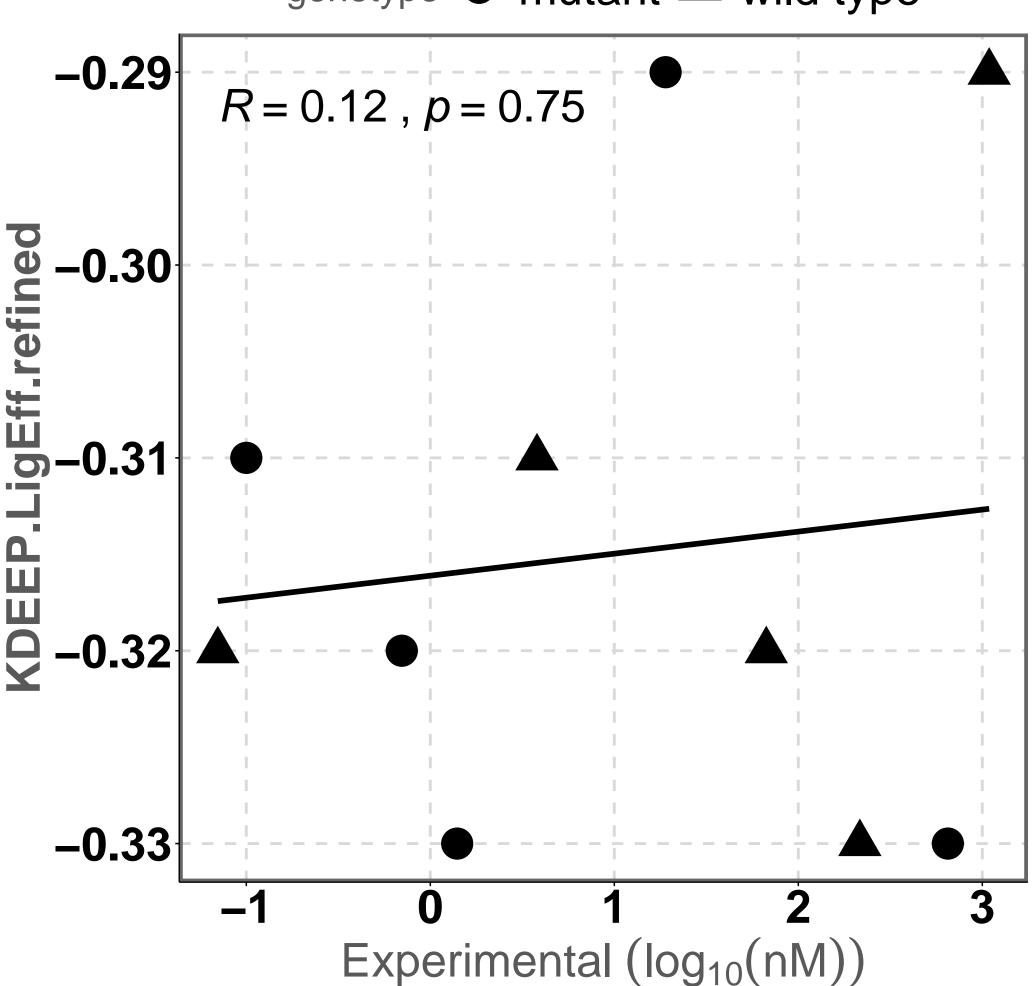


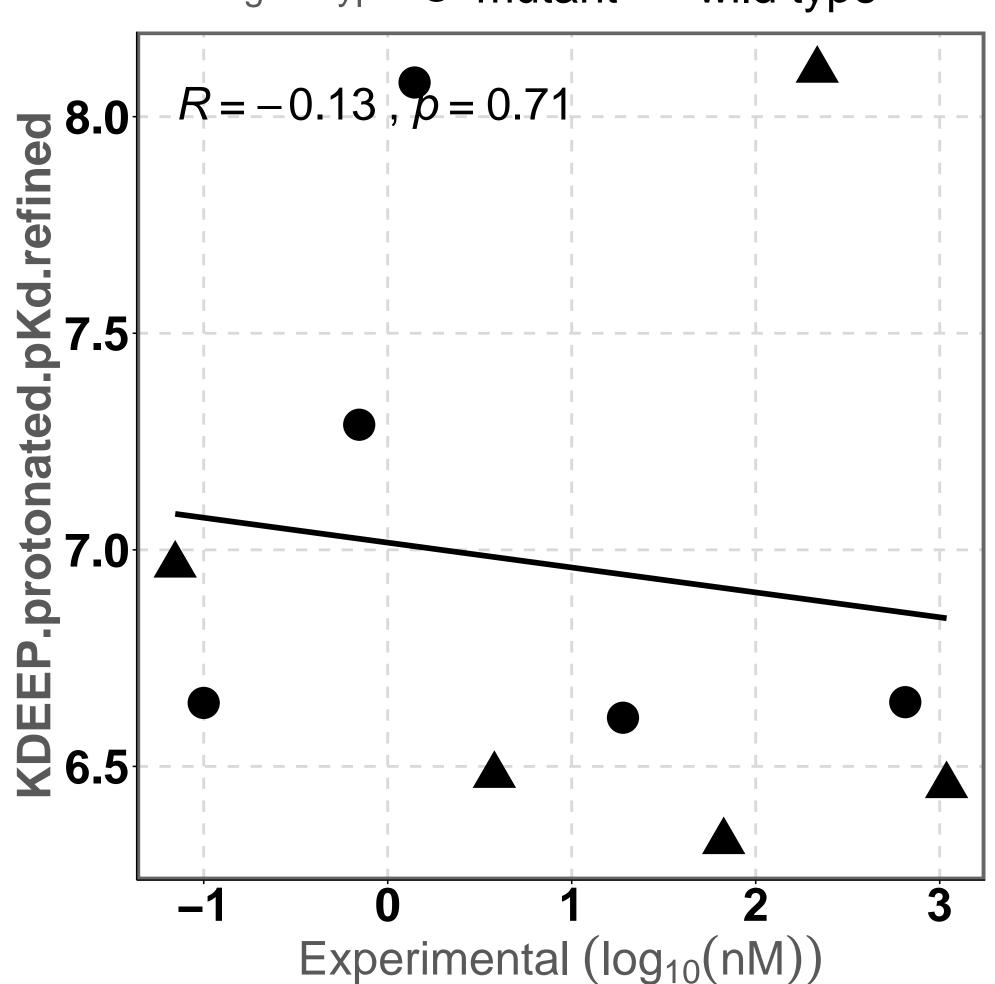
genotype • mutant • wild type

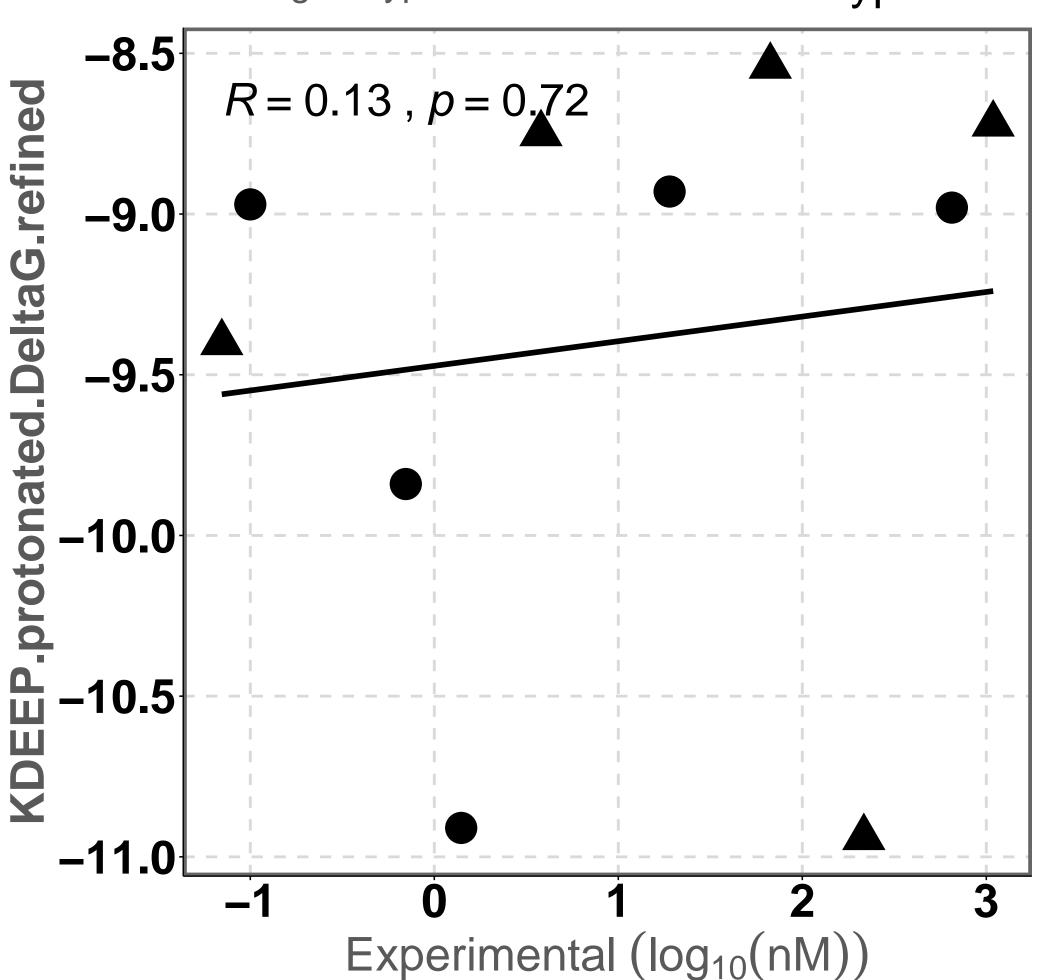


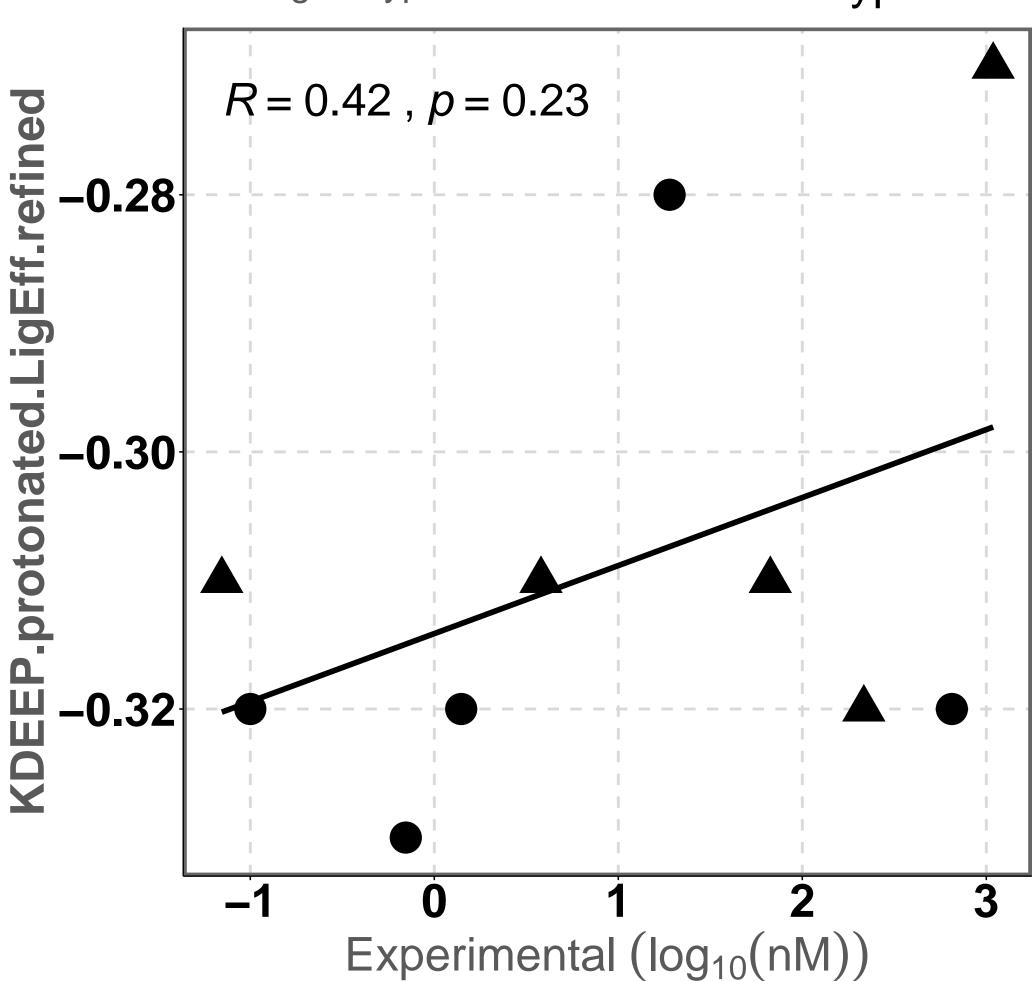




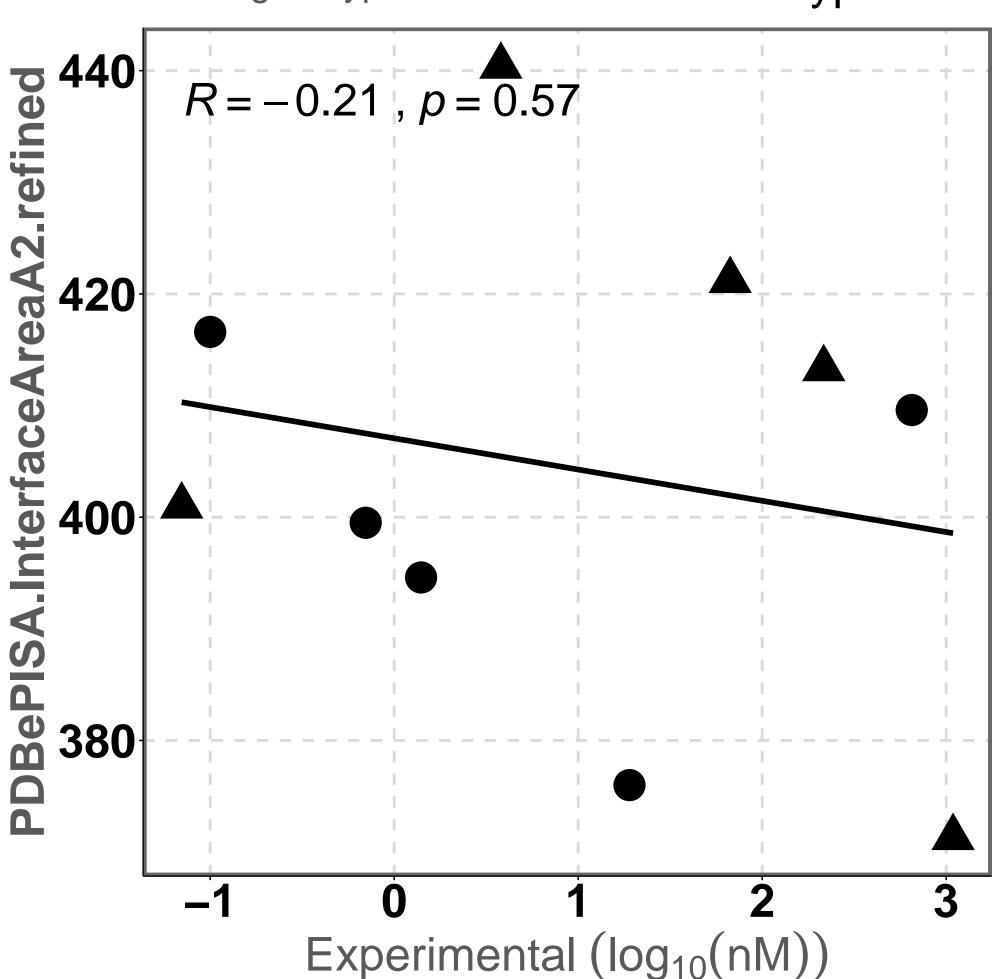


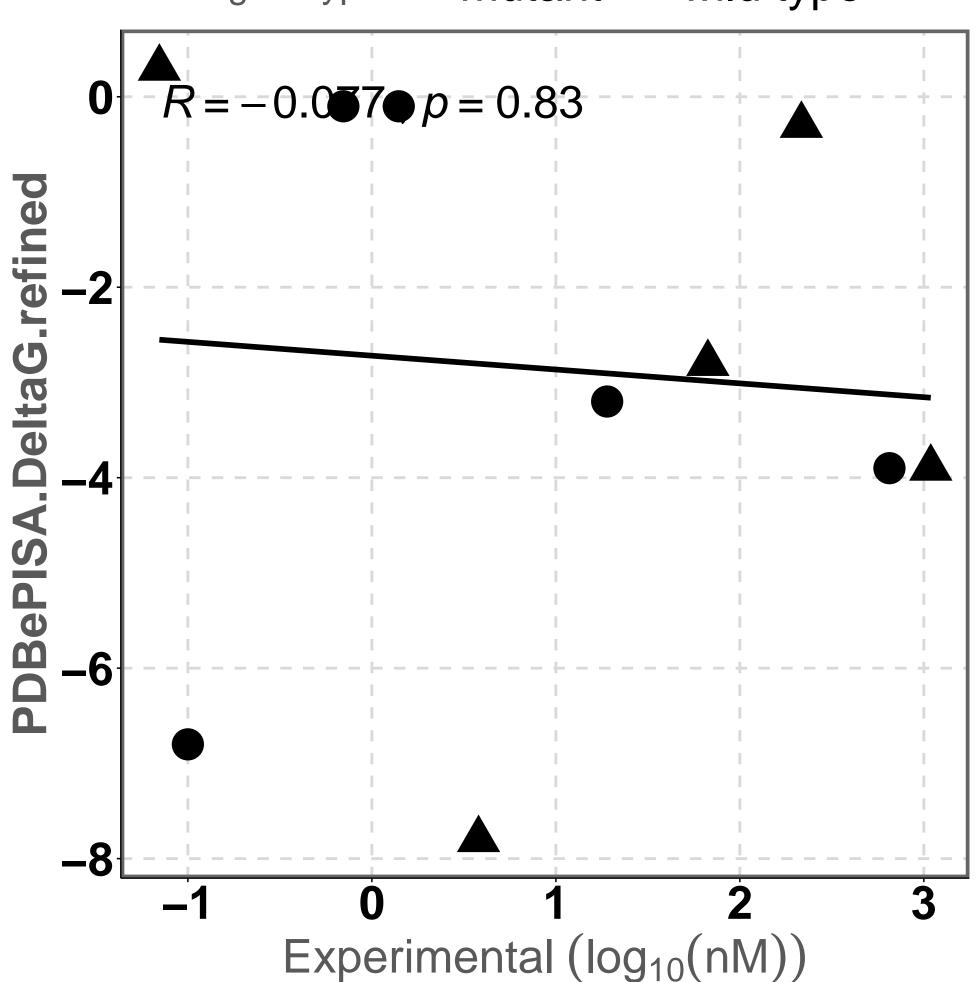




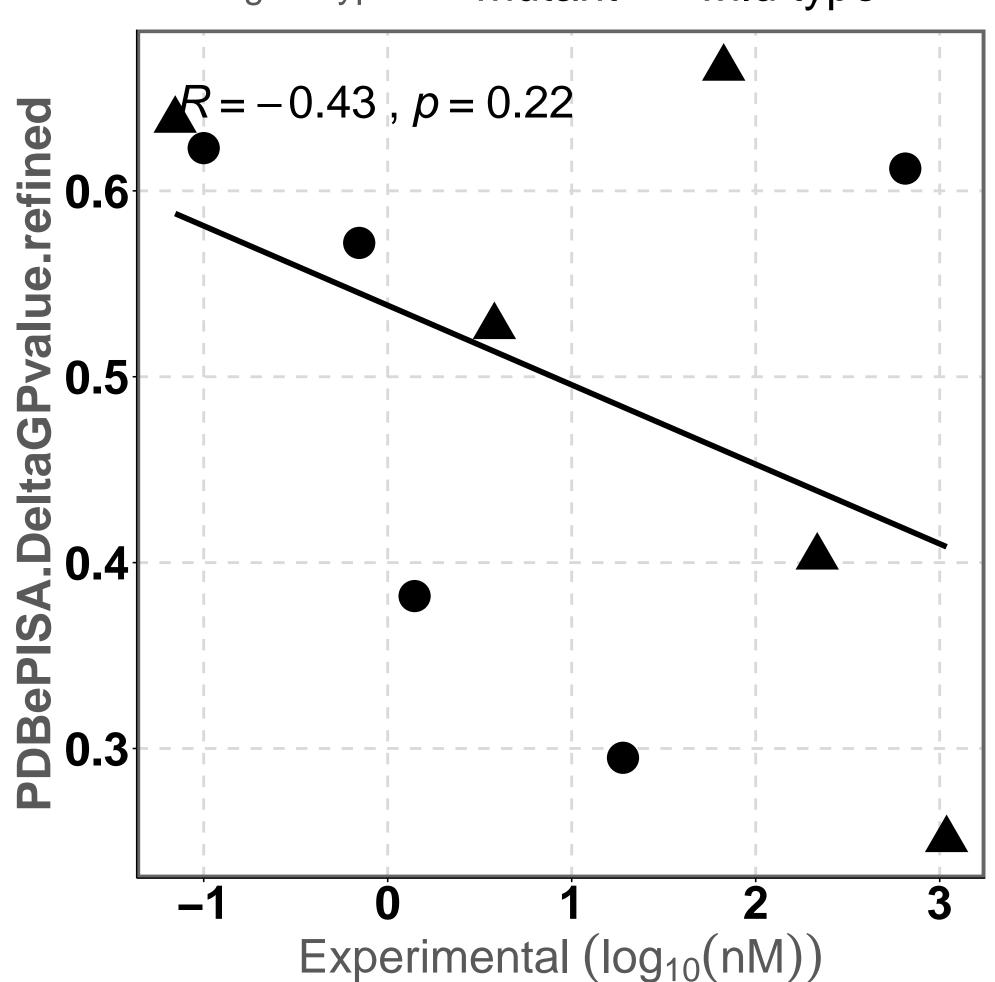


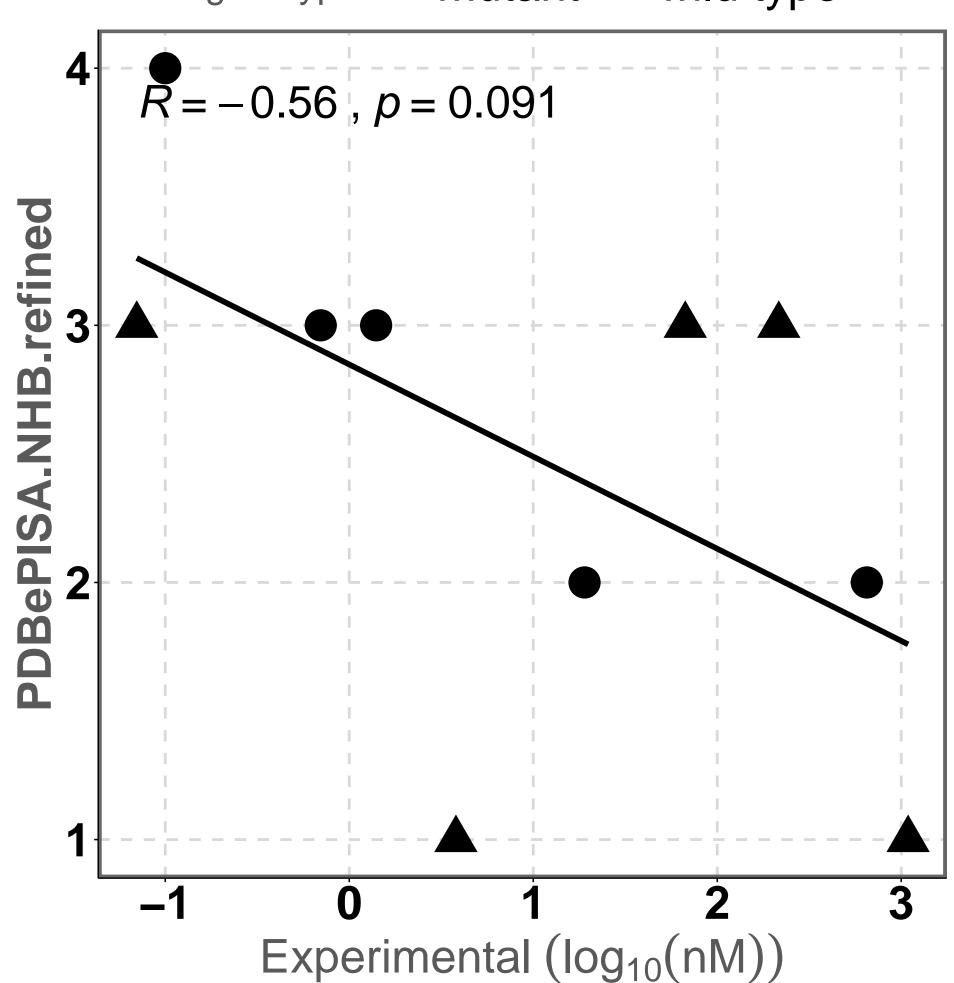
genotype • mutant • wild type



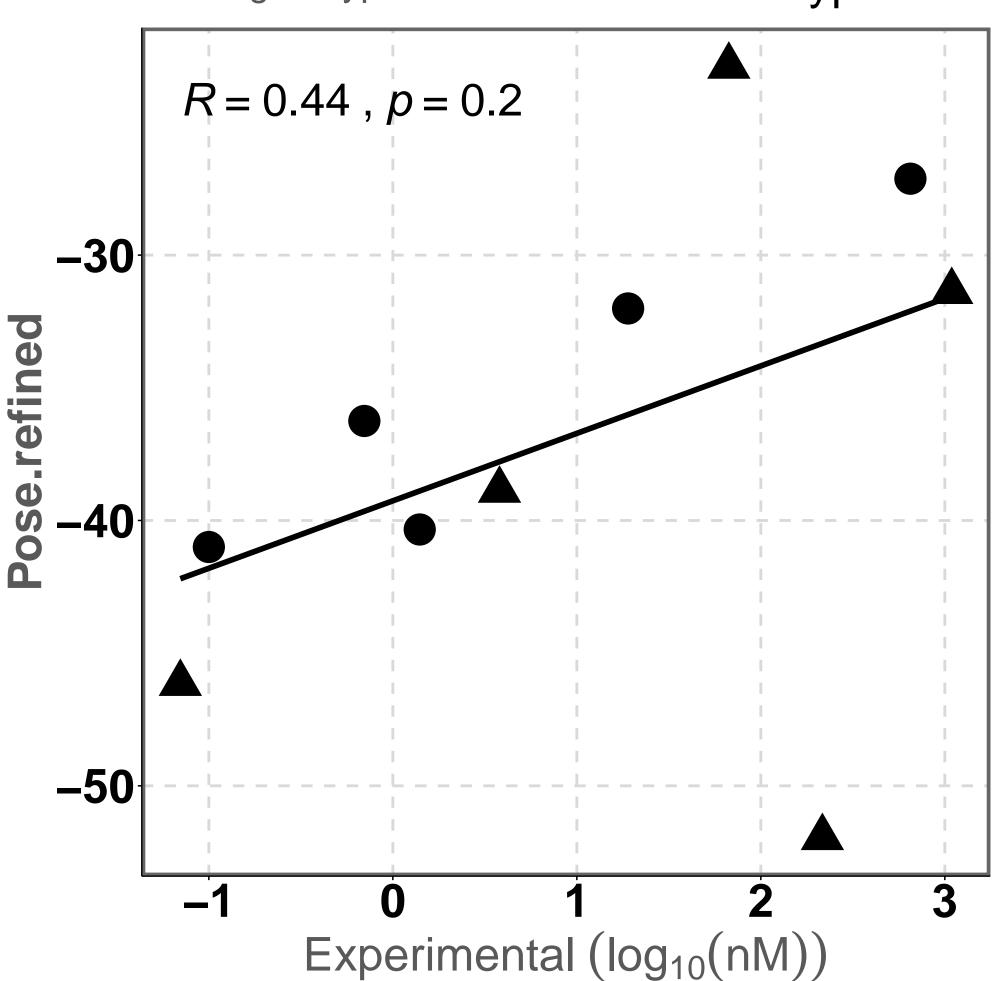


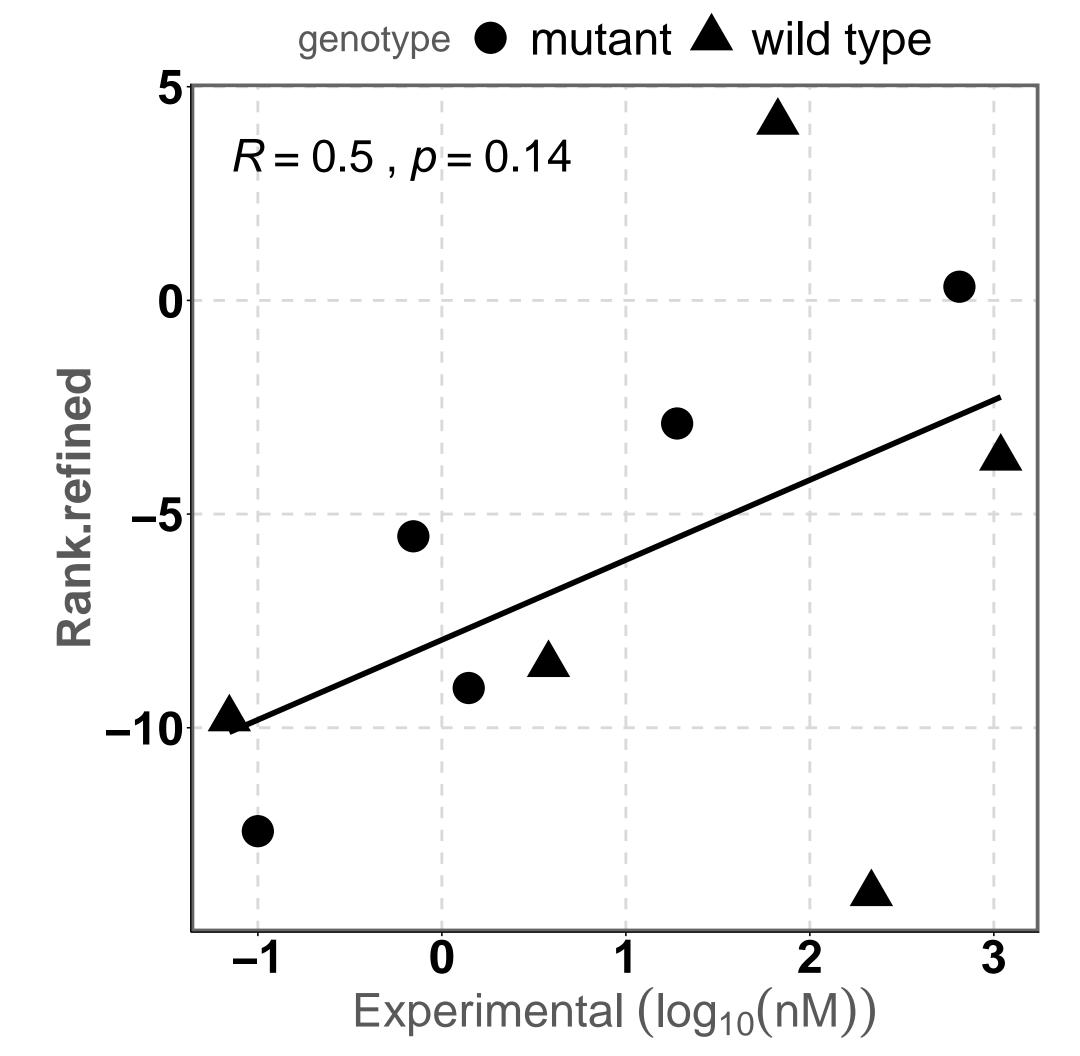
genotype • mutant • wild type



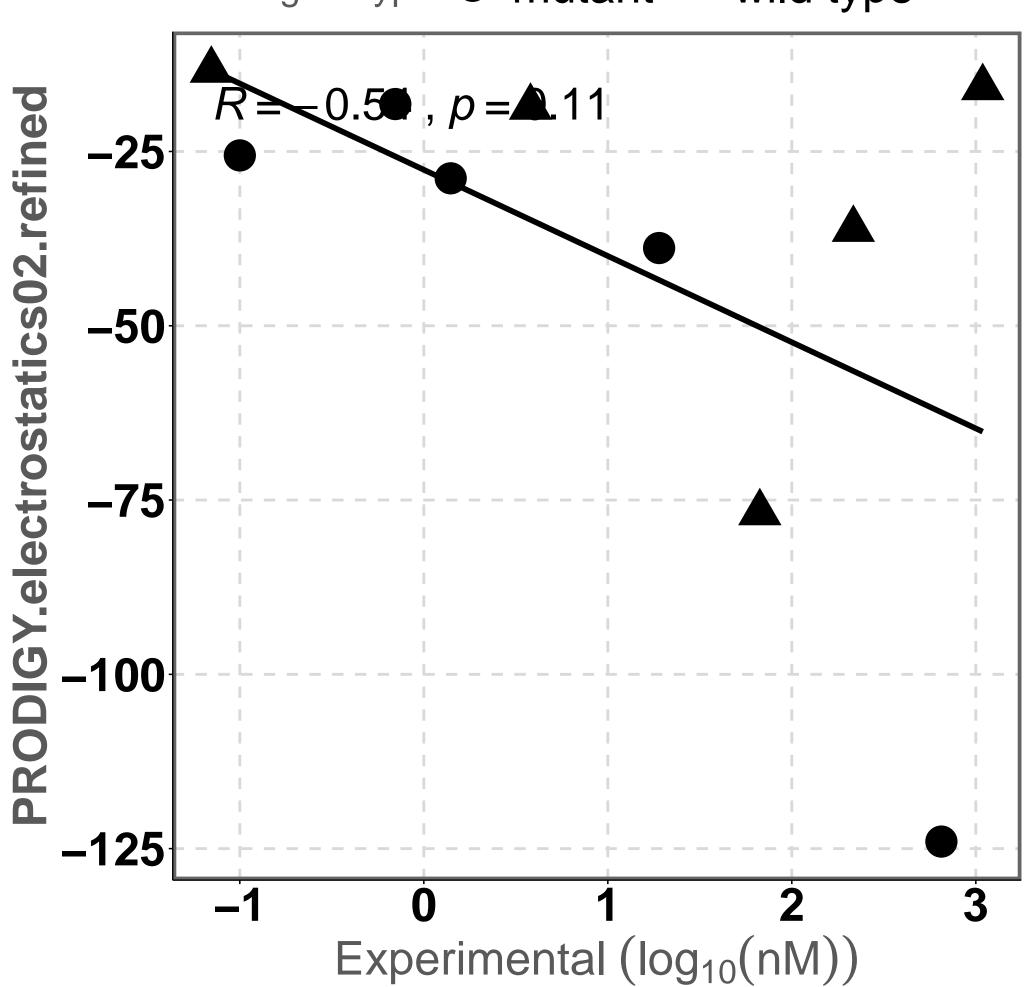


genotype • mutant • wild type

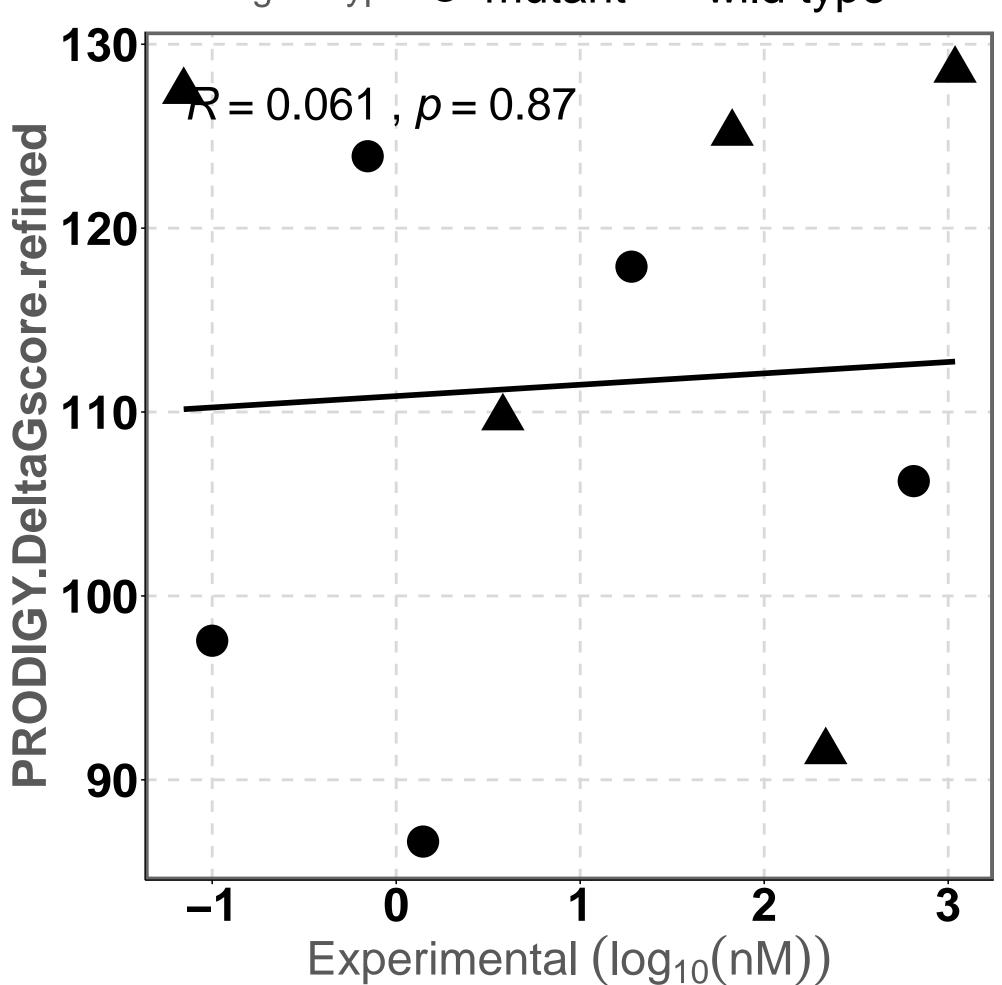


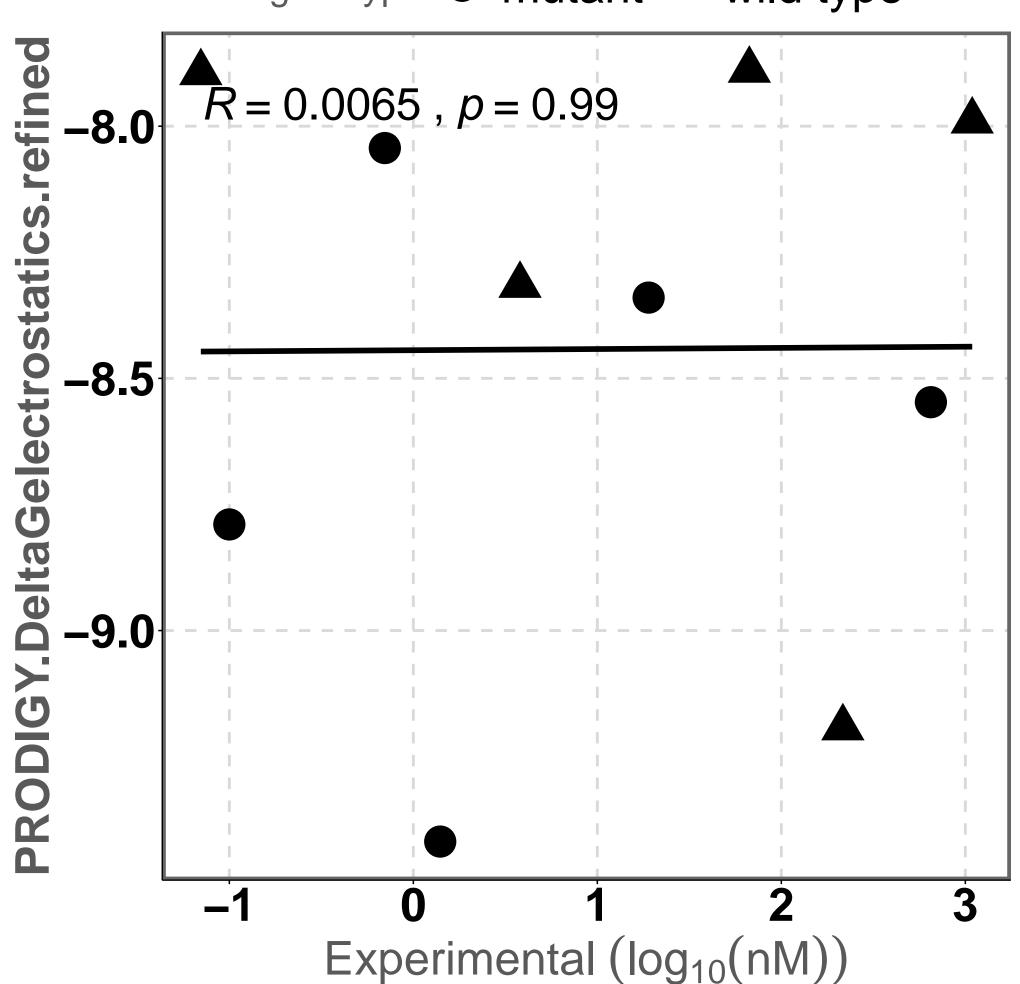


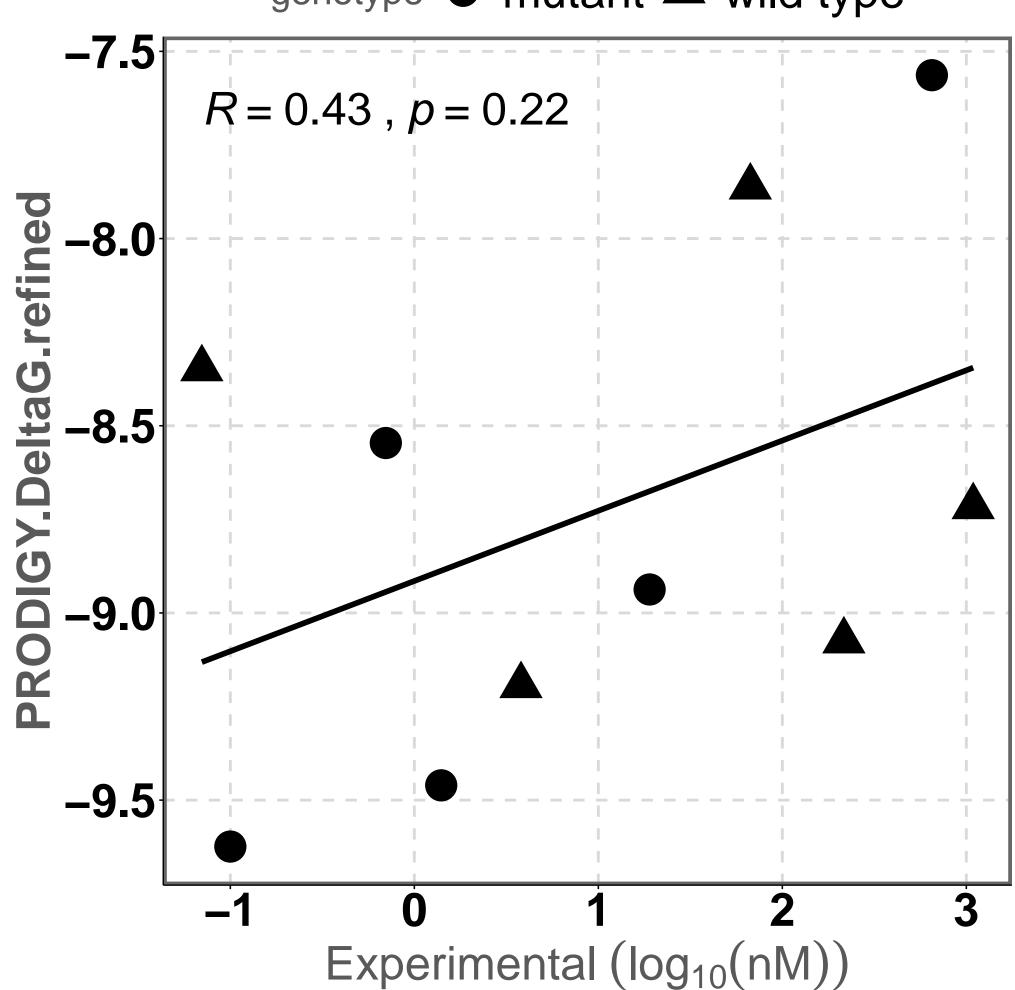
genotype • mutant • wild type



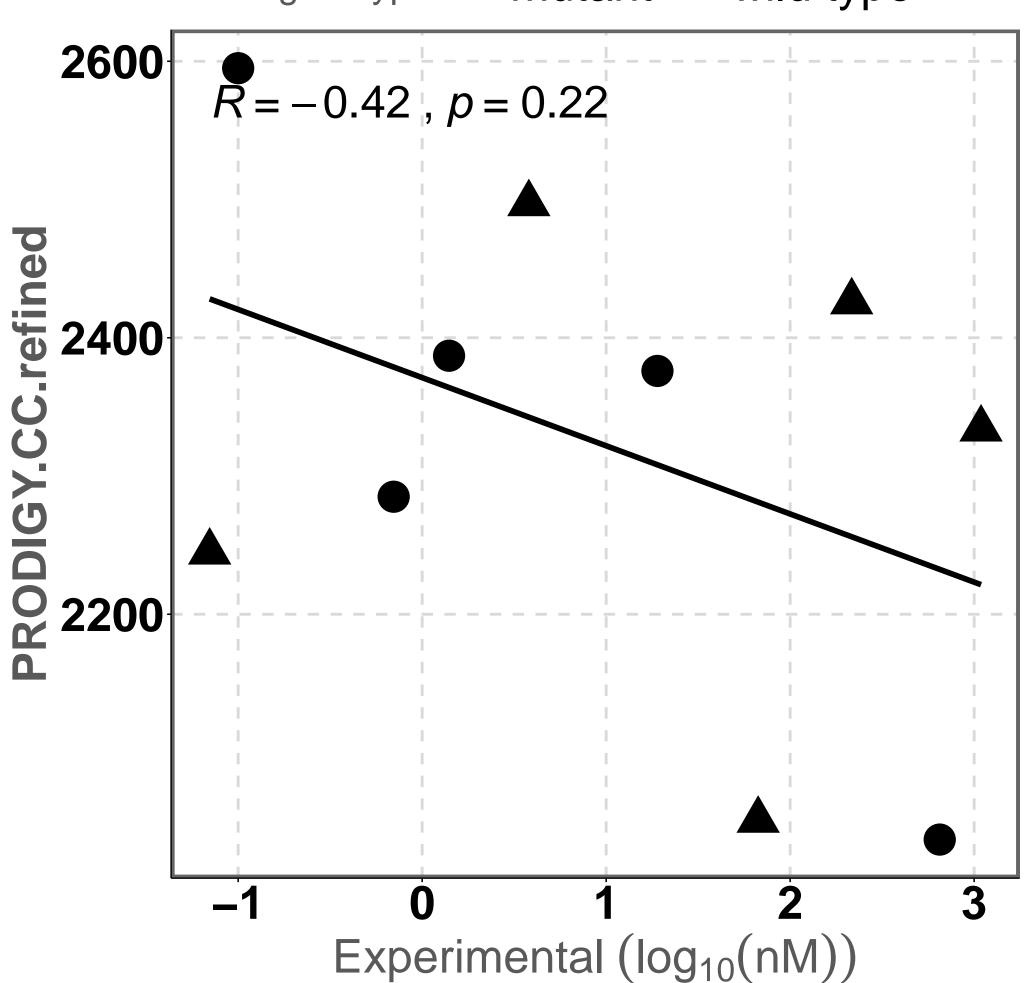
genotype • mutant • wild type



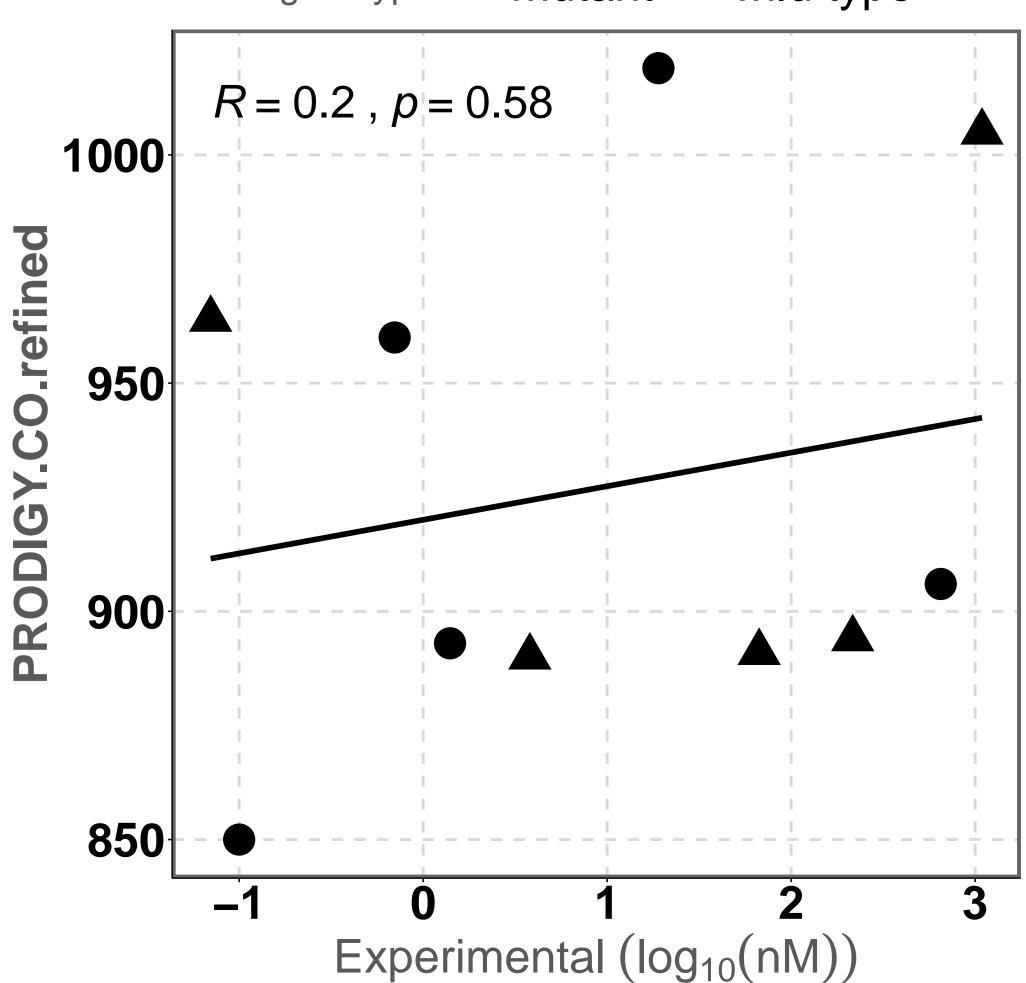




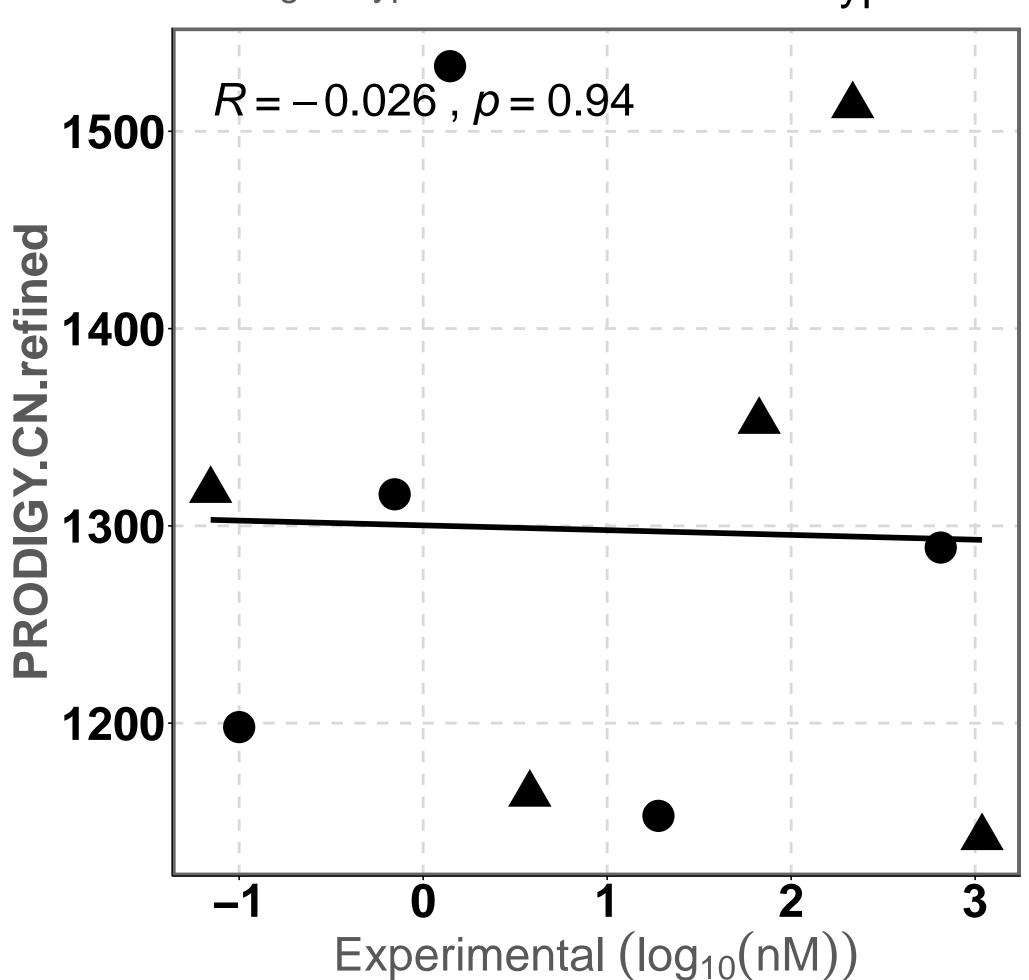
genotype • mutant • wild type



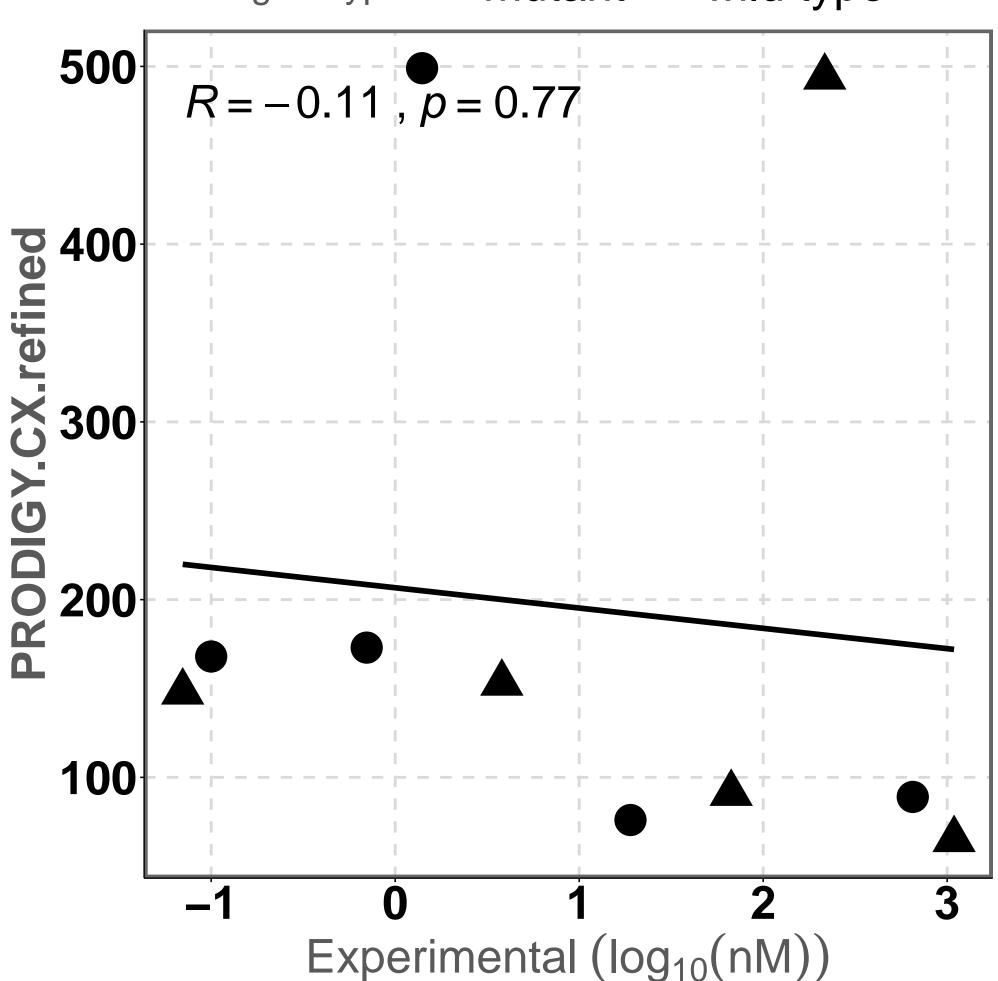
genotype • mutant • wild type



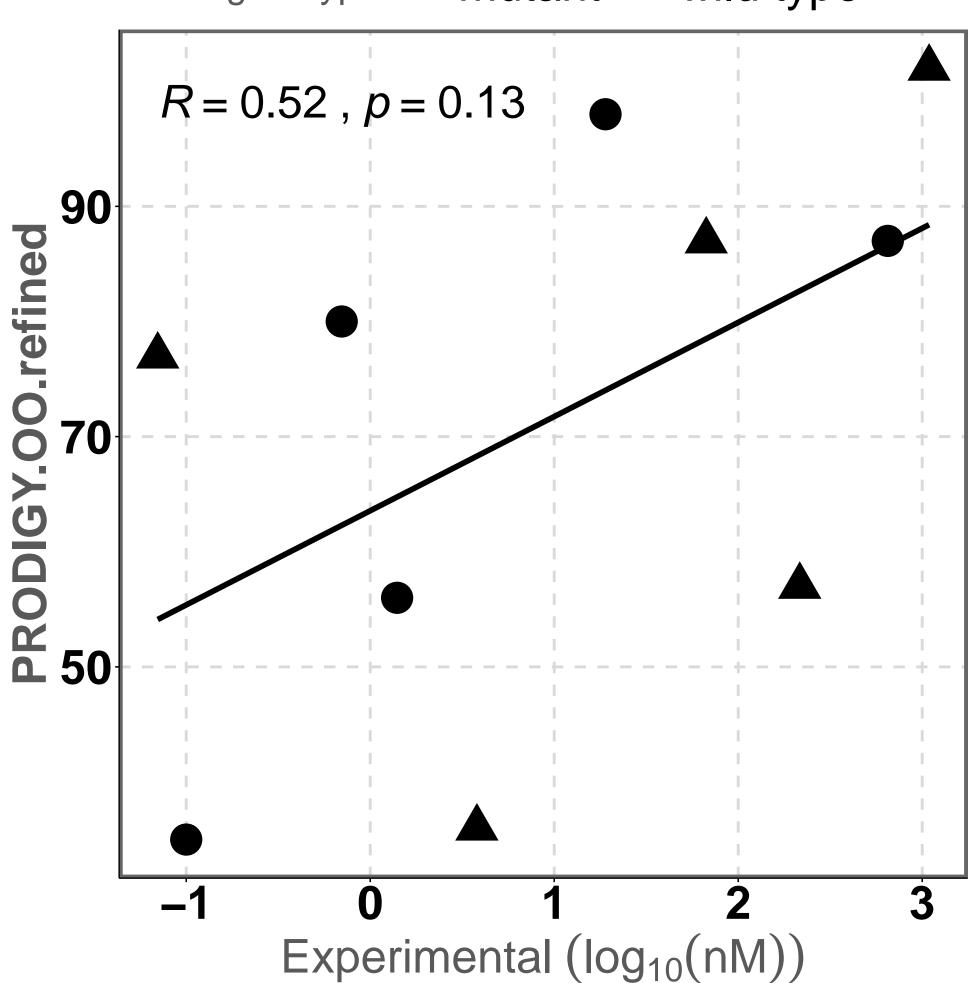
genotype • mutant • wild type

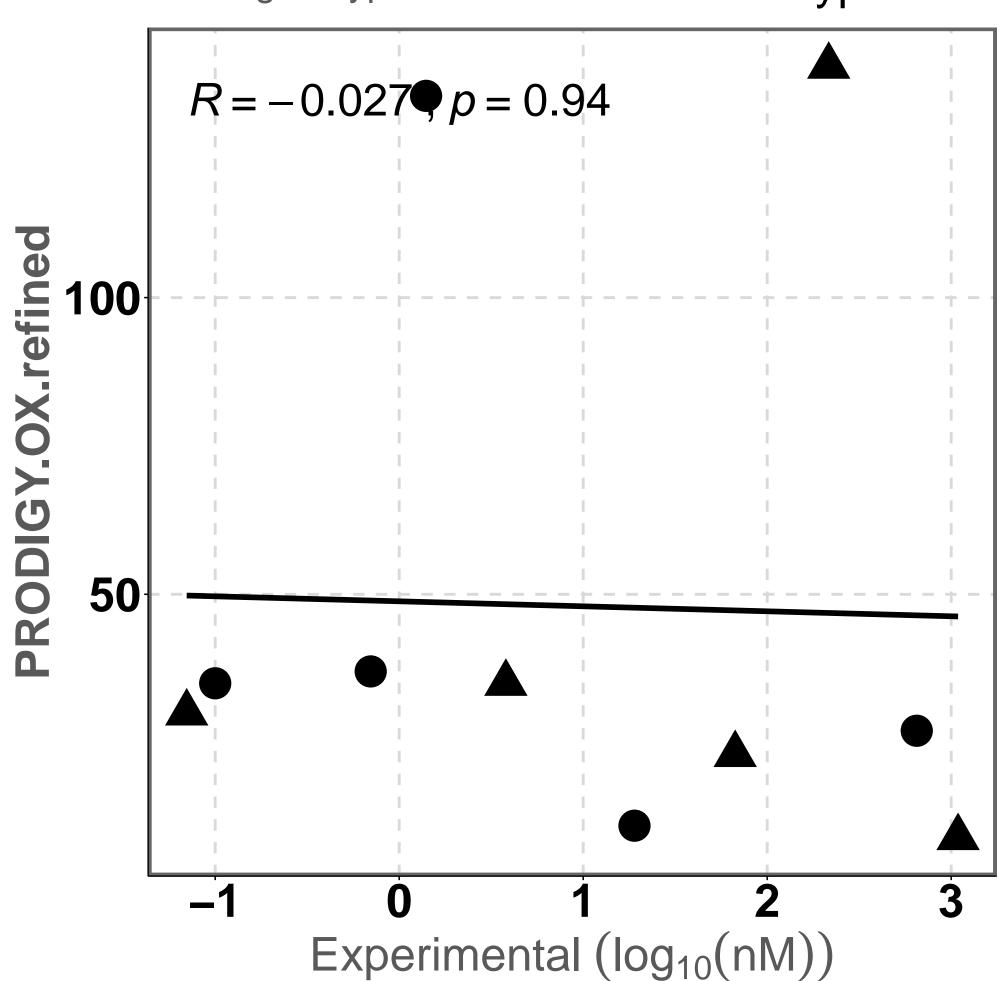


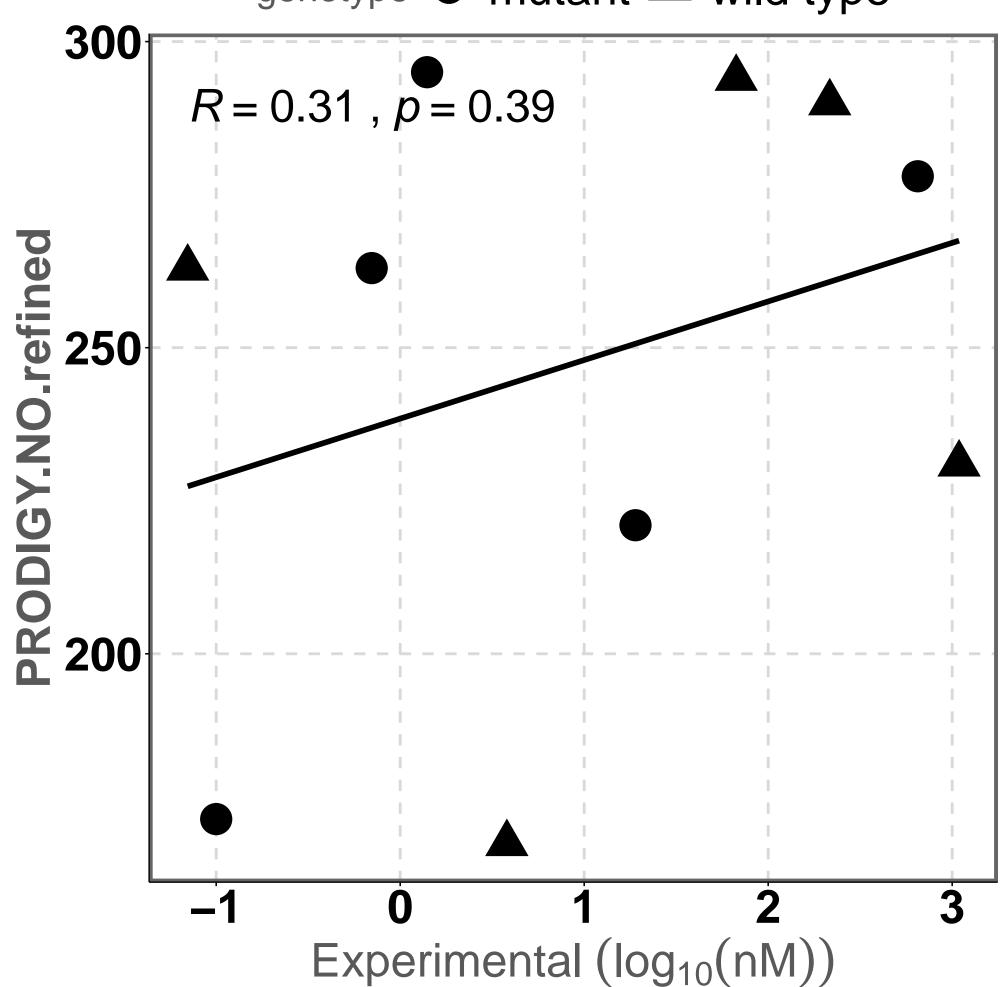
genotype • mutant • wild type



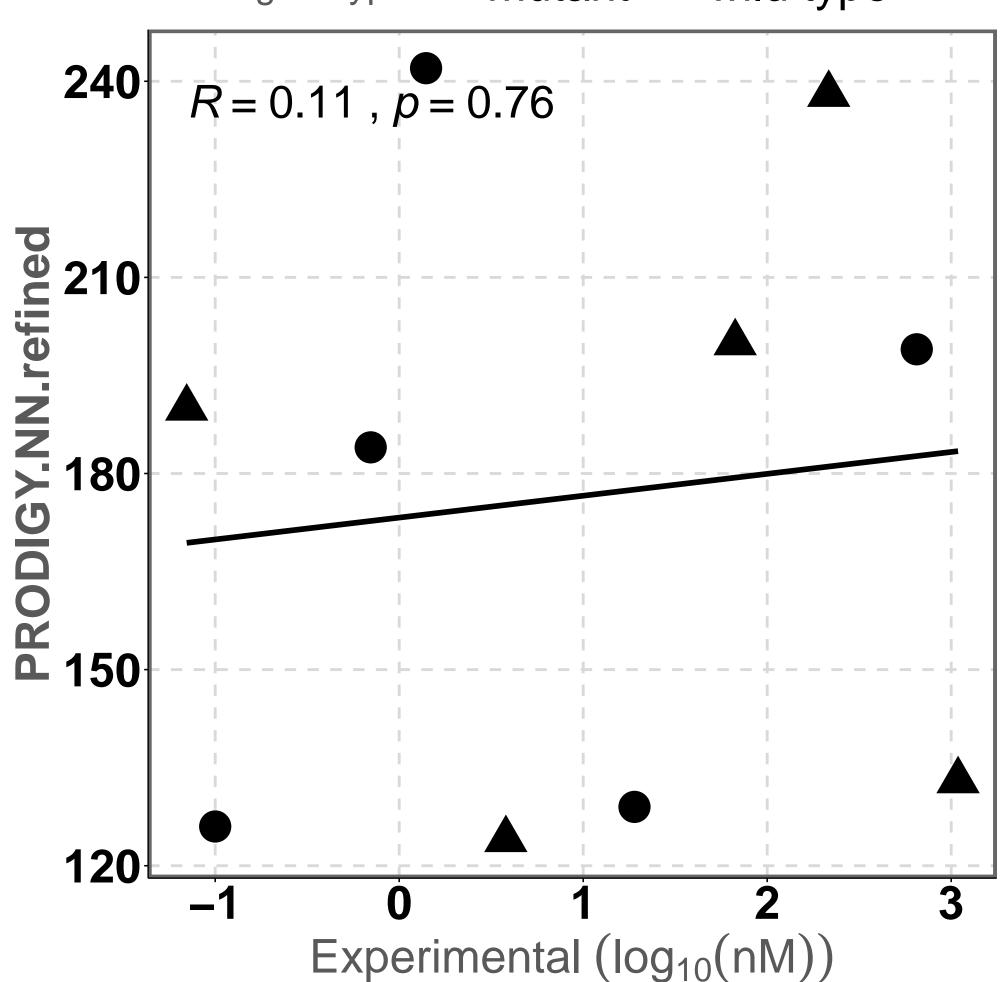
genotype • mutant • wild type







genotype • mutant • wild type



genotype • mutant • wild type 160 R = -0.088, p = 0.81PRODIGY.NX.refined 80 40 Experimental $(log_{10}(nM))$

