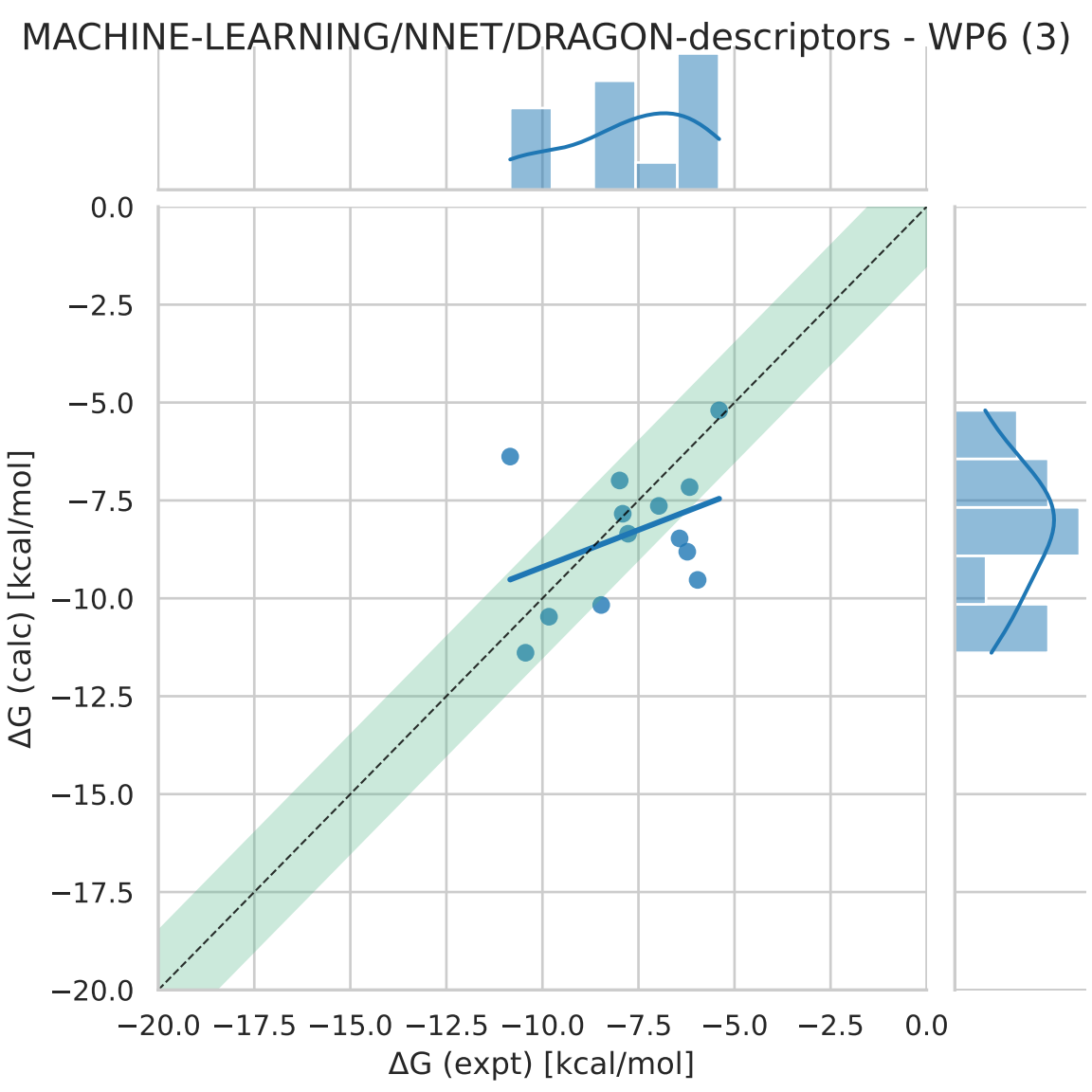
MACHINE-LEARNING/NNET/DRAGON-descriptors - WP6 (3)
0.0
−2.5
−5.0
−7.5
−10.0
−12.5
−15.0
−17.5
−20.0
ΔG (calc) [kcal/mol]
−20.0 −17.5 −15.0 −12.5 −10.0 −7.5 −5.0 −2.5 0.0
ΔG (expt) [kcal/mol]