

Table S8. PROPKA Calculations.

Residue/Atom	Theoretical pK_a	1S1P (minus acetate) pK_a	1S2A (minus UNK atom) pK_a	Indomethacin pH 7.5 pK_a
H117 NE2	6.5	1.6	1.5	1.7
Y55 OH	10.0	16.1	16.8	20.4
NADP 01N/O2N	6.0	6.9	11.8	6.7
IMN CO ₂ ⁻ /CO ₂ H	4.5	n/a	6.6	9.3