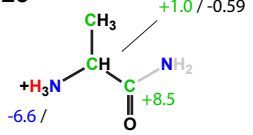
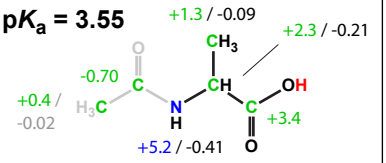
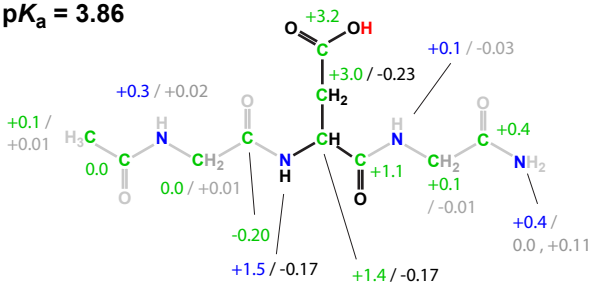
N-term
pK_a = 8.23



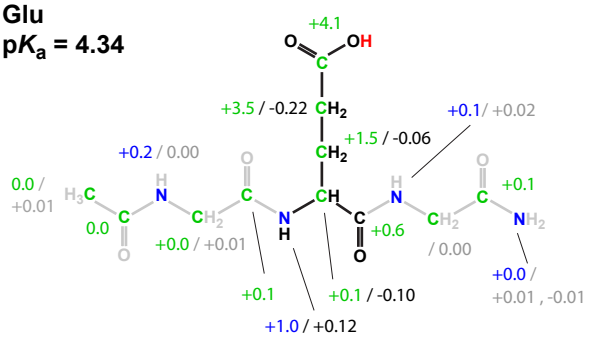
C-term
pK_a = 3.55



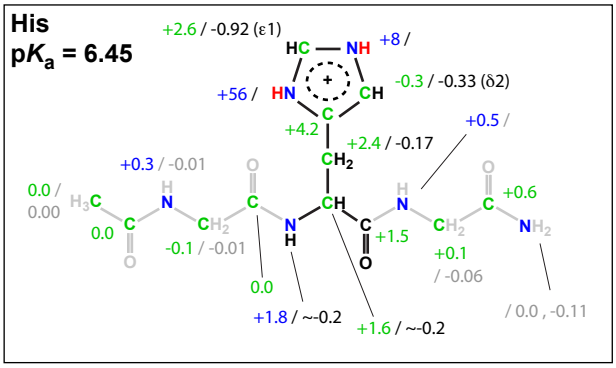
Asp
pK_a = 3.86



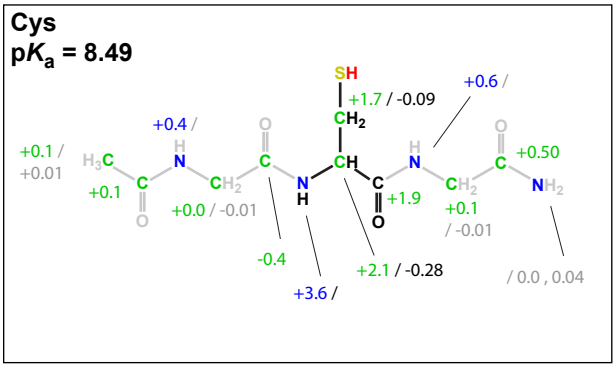
Glu
pK_a = 4.34



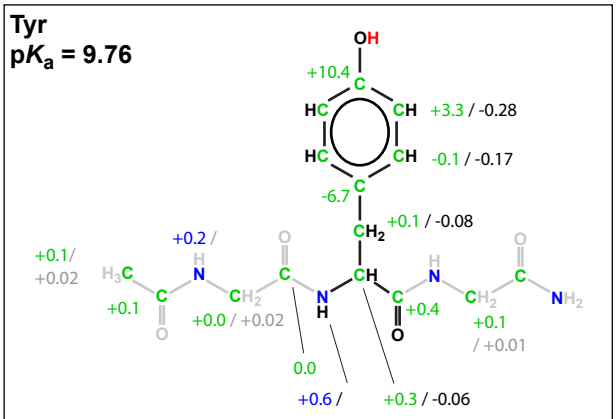
His
pK_a = 6.45



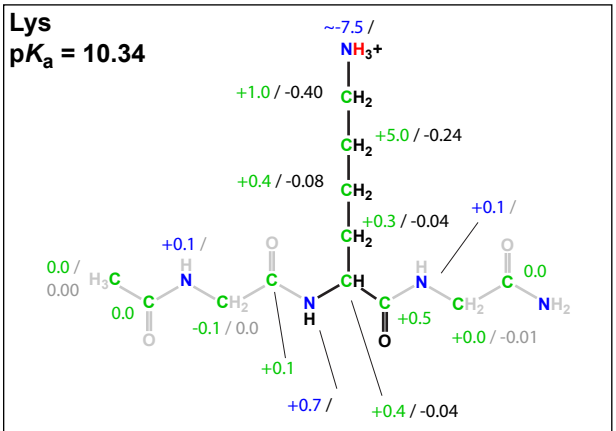
Cys
pK_a = 8.49



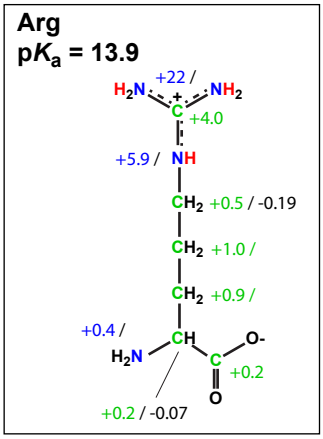
Tyr
pK_a = 9.76



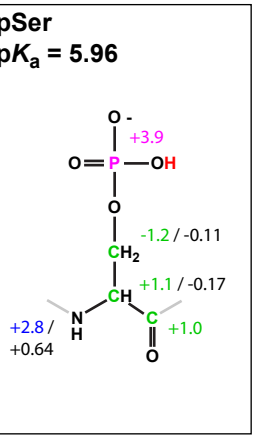
Lys
pK_a = 10.34



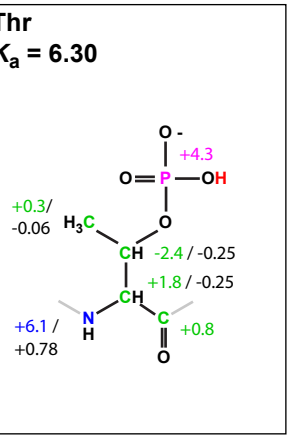
Arg
pK_a = 13.9



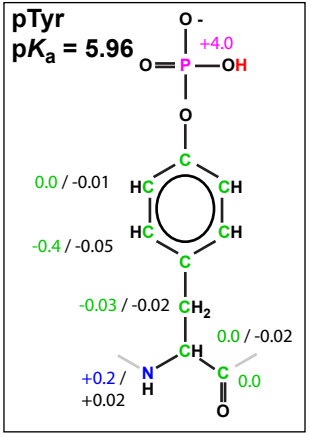
pSer
pK_a = 5.96



pThr
pK_a = 6.30



pTyr
pK_a = 5.96



pH-Dependent random coil ^{1}H, ^{13}C, and ^{15}N chemical shifts of the ionizable amino acids: a guide for protein pK_a measurements

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A summary of the pH-dependent chemical shift changes upon *deprotonation* of the ionizable amino acid functional groups within the context of the blocked acetyl-Gly-X-Gly-amide (X = Asp, Glu, His, Cys, Tyr, or Lys) tripeptides. Alanine amide and N-acetyl alanine are models of the N- and C-termini, respectively. The atoms and Δδ values (ppm; negative is upfield) are colored as: acidic protons, red; oxygens and non-labile protons, black within the named residue and grey in flanking blocked glycines; carbons, green; nitrogens, blue; sulfurs, yellow; and phosphates, magenta. Results for $^{13}C_6/^{15}N_4$-L-arginine are due to deprotonation of the guanidinium moiety in the context of deprontonated α-amino (pK_a 9.15) and α-carboxyl groups. Values for the neutral forms of the Gly-His-Gly tripeptide and arginine are tautomer averaged.

The tripeptides and alanine derivatives were initially in 50 mM NaCl with 5% D_2O (D = ^{2}H). DSS (4,4-dimethyl-4-silapentane-1-sulfonic acid; 1 mM) was included as a pH-independent internal reference. For the cysteine tripeptide, 10 mM TCEP (tris(2-carboxyethyl)phosphine) was also present as a reductant. The $^{13}C_6/^{15}N_4$-L-arginine was initially 10 or 100 mM in 50 mM NaCl with 1 mM DSS and 5% D_2O. Spectra were recorded at 25 ^{o}C.

The data are from Platzer et al. *J Biomol NMR* 60:109-129 (2014), or in the case of the phosphoamino acid peptides (second ionization step for acetyl-Gly-Gly-X-Gly-Gly-amide, X=pSer, pThr, or pTyr), from Bienkiewicz & Lumb, *J Biomol NMR* 15:203-206 (1999).