The NMR signature of gluconoylation - a frequent N-terminal modification of recombinant proteins

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N-terminal gluconoylation is a moderately frequent modification in recombinant proteins expressed in *E. coli*, in particular in proteins bearing an N-terminal histidine-tag. N-terminal sequences prone to gluconoylation are rich in histidines, for example (Met)-Gly-Ser-Ser-His_6 – a typical N-terminal sequence found in many commercial vectors. This post-translational modification has been investigated mainly by mass spectrometry. Although its NMR signals must have been observed earlier in spectra of $^{13}C/^{15}N$ labeled proteins, an NMR characterization was lacking so far.

Here we present the complete ^{1}H and ^{13}C chemical shift assignment of the N-terminal gluconoyl modification [1], based on a selection of histidine-tagged protein constructs starting with Met-Gly-...-$(His)_6$. The chemical shifts presented here can now be used as a reference for the identification of gluconoylation in recombinant proteins, in particular when isotopically labeled.

[1] Schweida, D., Barraud, B., Regl, C., Loughlin, F.E., Huber, C.G., Cabrele, C., Schubert, M. (2019). *J. Biomol. NMR* 73, 71-79.