Supplemental Information for

Detection of methylation, acetylation and glycosylation of protein residues by monitoring ^{13}C chemical-shift changes: A quantum-chemical study

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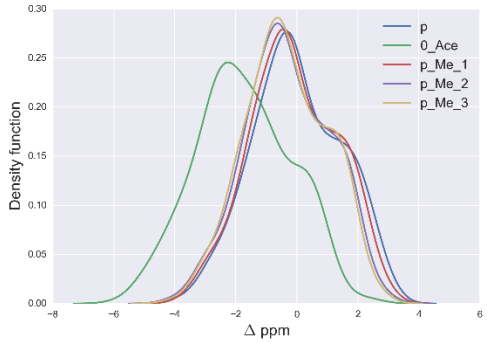
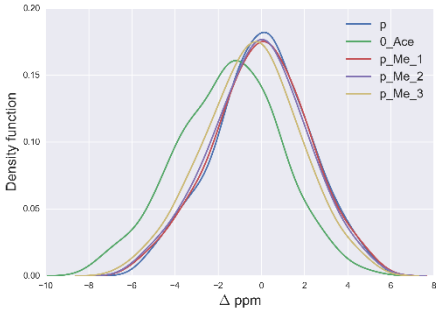


(a)



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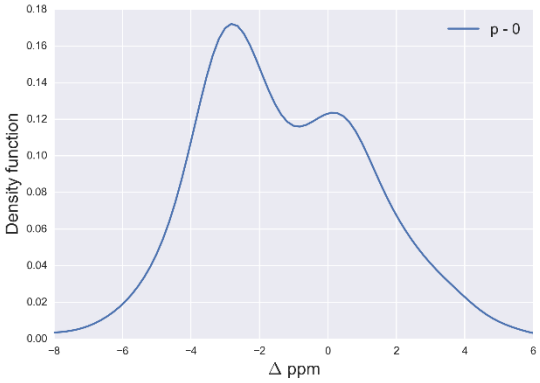
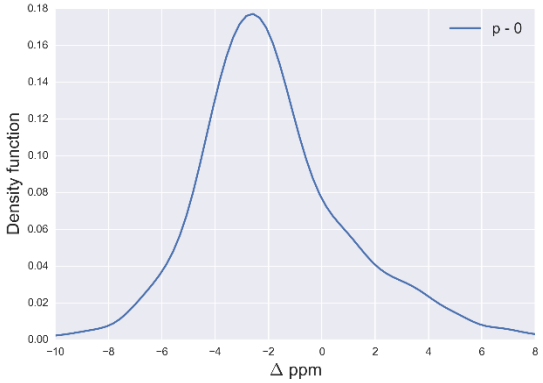
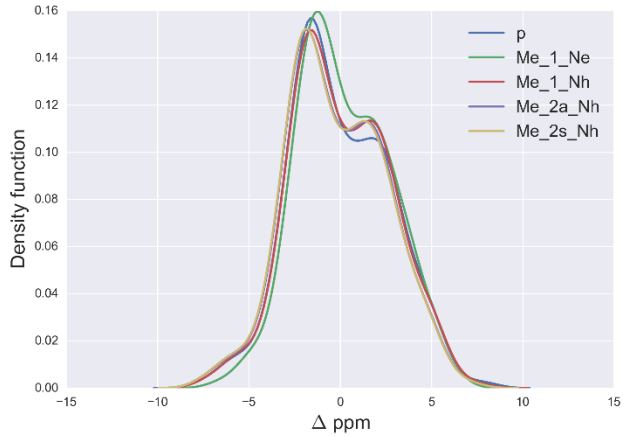


(c)

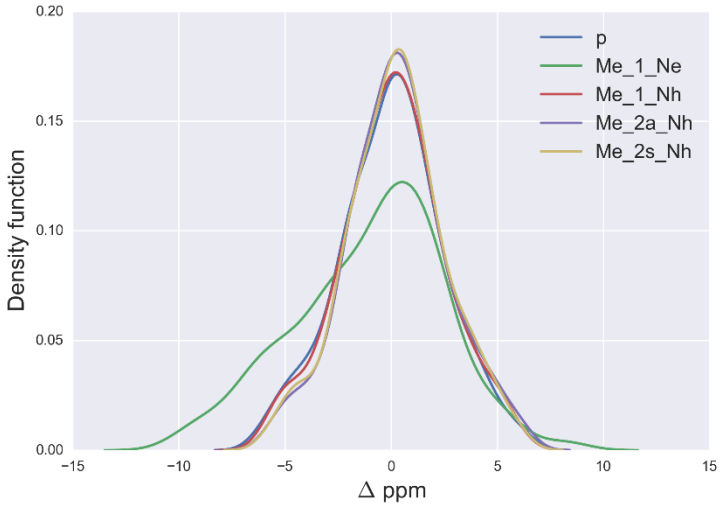


(d)

Figure S1.- (**a**) Kernel Density Estimation of the Δ values of the $^{13}C^{\alpha}$ nucleus of charged non-modified (blue-line), acetylated (green-line), *mono*- (red-line), *di*- (violet-line), and *tri*-methylated (yellow-line) Lys; (**b**) same as (**a**) for the $^{13}C^{\beta}$ nucleus; (**c**) Kernel Density Estimation of the Δ values of the $^{13}C^{\alpha}$ nucleus of non-modified Lys upon protonation/deprotonation; (**d**) same as (**c**) for the $^{13}C^{\beta}$ nucleus.



(a)



(b)

Figure S2.- (**a**) Kernel Density Estimation of the Δ values of the $^{13}C^{\alpha}$ nucleus of *non*-modified (blue-line), N^{ε} (green-line) and N^{η} (red-line) *mono*-methylated, asymmetric (violet-line) and symmetric (yellow-line) *di*-methylated Arg; (**b**) same as (**a**) for the $^{13}C^{\beta}$ nucleus.

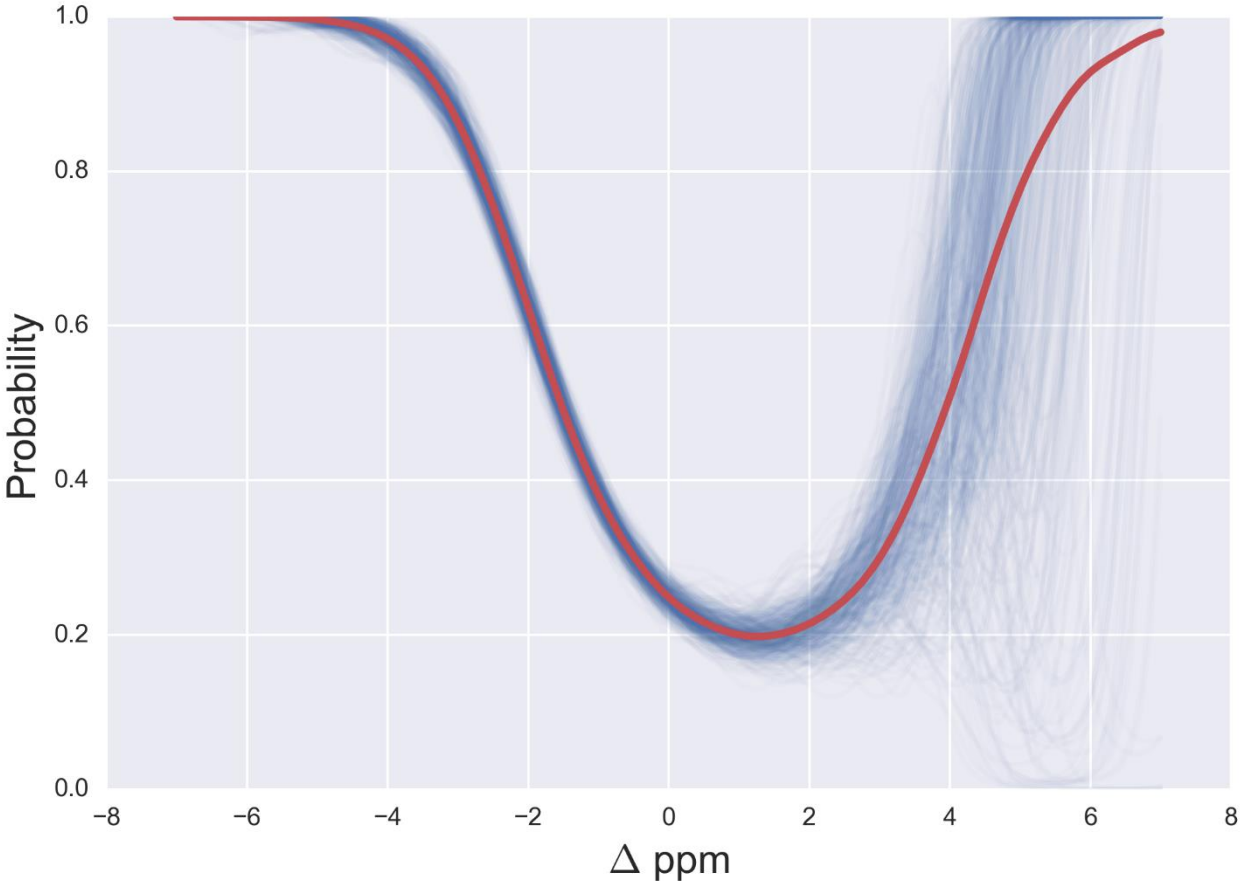


Figure S3. Probability to detect glycosylation of Ser, i.e., either α-D-GalpNAc-(1-O)-Ser or β-D-GlcpNAc-(1-O)-Ser, as a function of the Δ values of the $^{13}C^{\beta}$ nucleus of Ser (shown in Figure 4 in the main text). The red line represents the expected probability-profile and the blue lines the uncertainty in the data according to the Bayesian model.

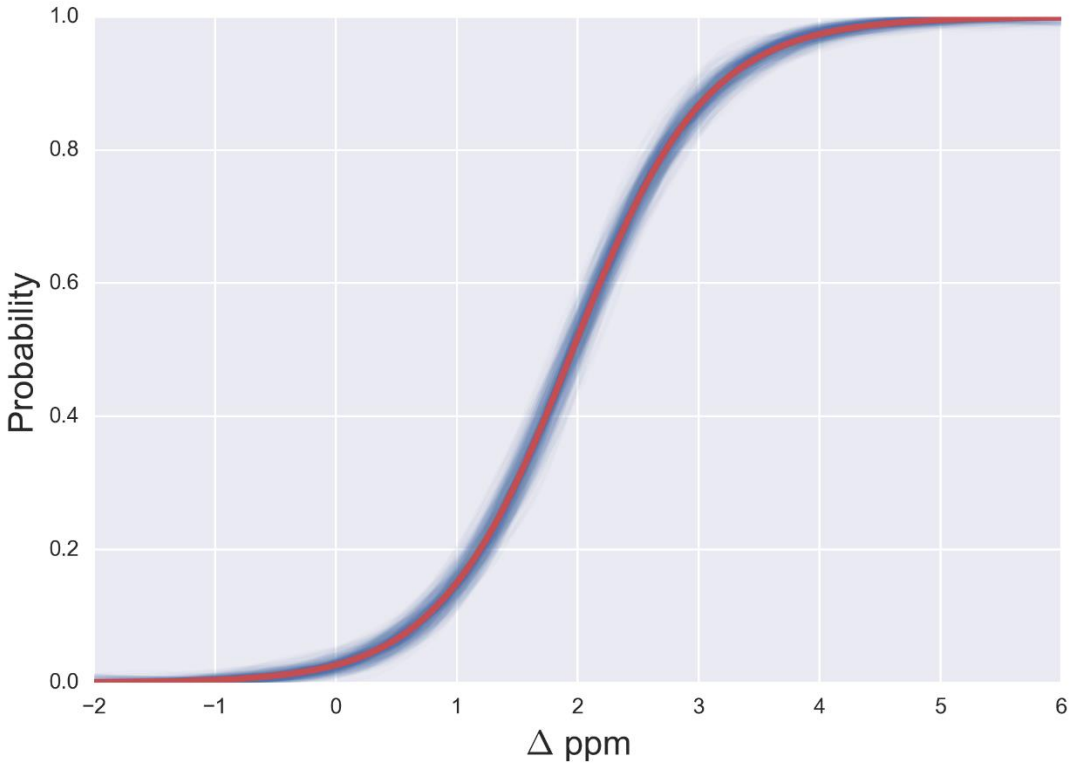


Figure S4. Probability to detect glycosylation of Thr [α-D-GalpNAc-(1-O)-Thr], as a function of the chemical-shift differences (Δ) for the $^{13}C^{\beta}$ nucleus of Thr (shown in Figure 6 in the main text). The red line represents the expected probability-profile and the blue lines the uncertainty in the data according to the Bayesian model.

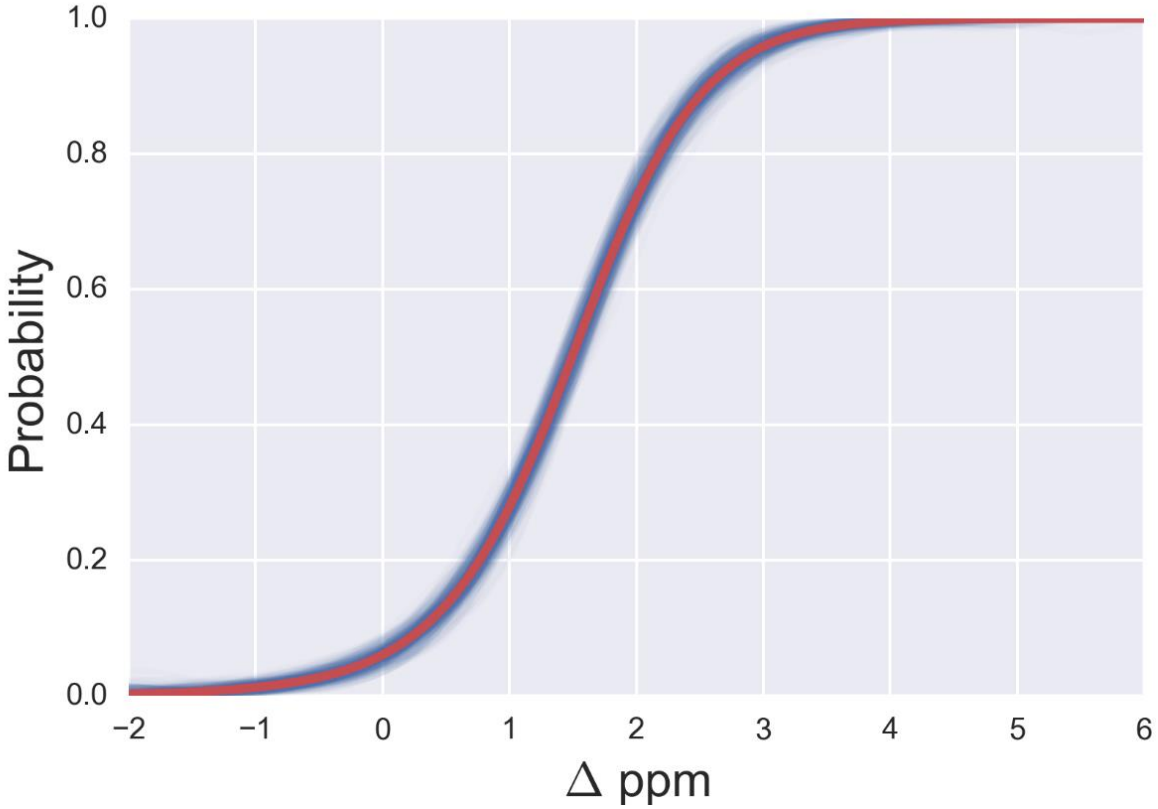


Figure S5.- Probability to detect glycosylation of Asn [β-D-GlcpNAc-(1-N)-Asn], as a function of the chemical-shift differences (Δ) for the $^{13}C^{\gamma}$ nucleus of Asn (shown in Figure 7 in the main text). The red line represents the expected probability-profile and the blue lines the uncertainty in the data according to the Bayesian model.

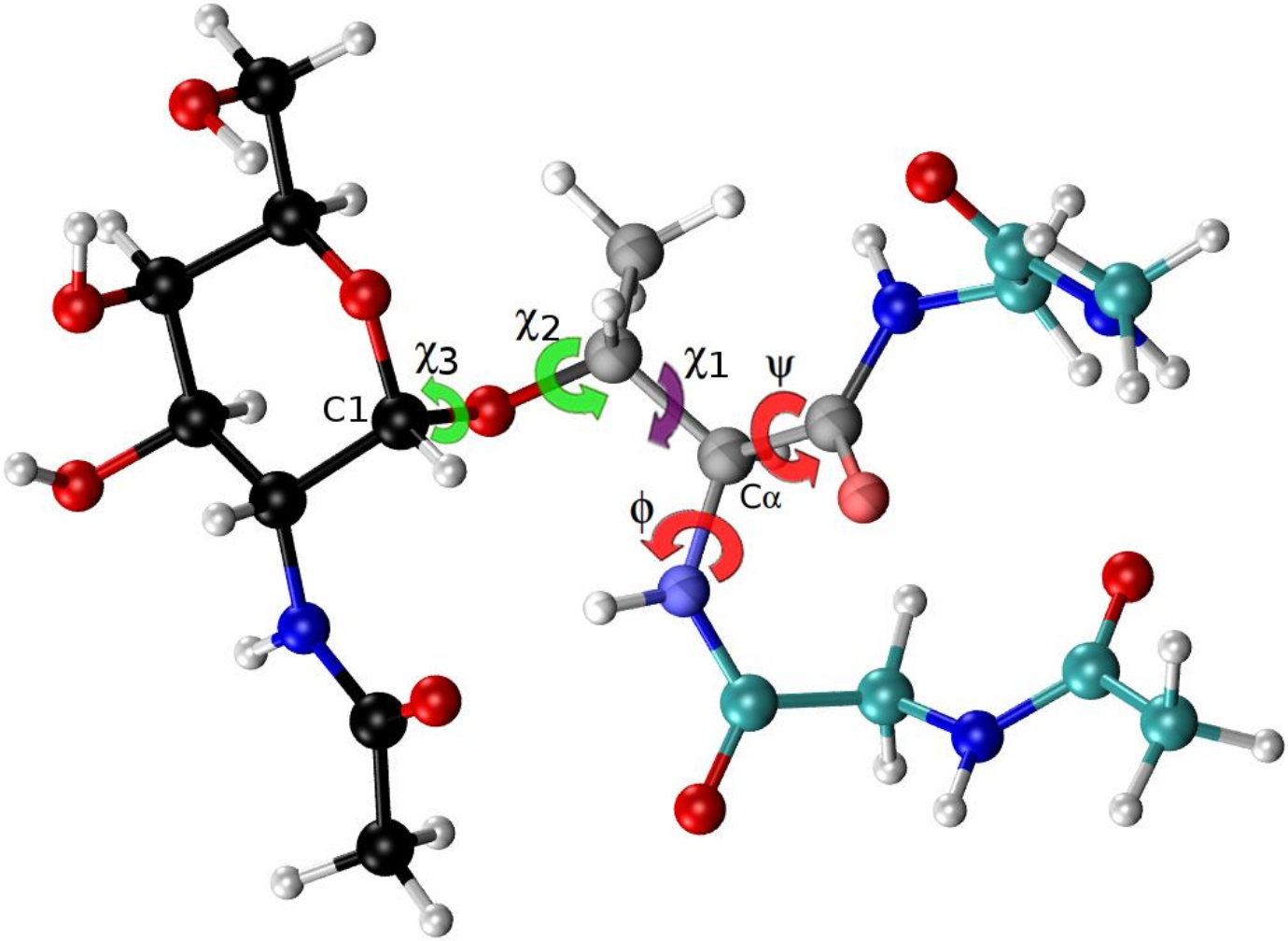


Figure S6.- Ball and stick representation of a glycan-amino acidic residue, namely for α-D-GalpNAc-(1-O)-Thr with "1" representing **C1** of the glycan and "O" representing the oxygen of the side-chain of Thr in an Ac-Gly-Thr-Gly-Nme tripeptide, in an arbitrary conformation. The χ2 and χ3 torsional angle, for the carbohydrate group (α-D-GalpNAc), are highlighted in green, while the one corresponding to the amino-acidic residue (Thr) are in red, for ϕ,ψ, and purple, for χ1.

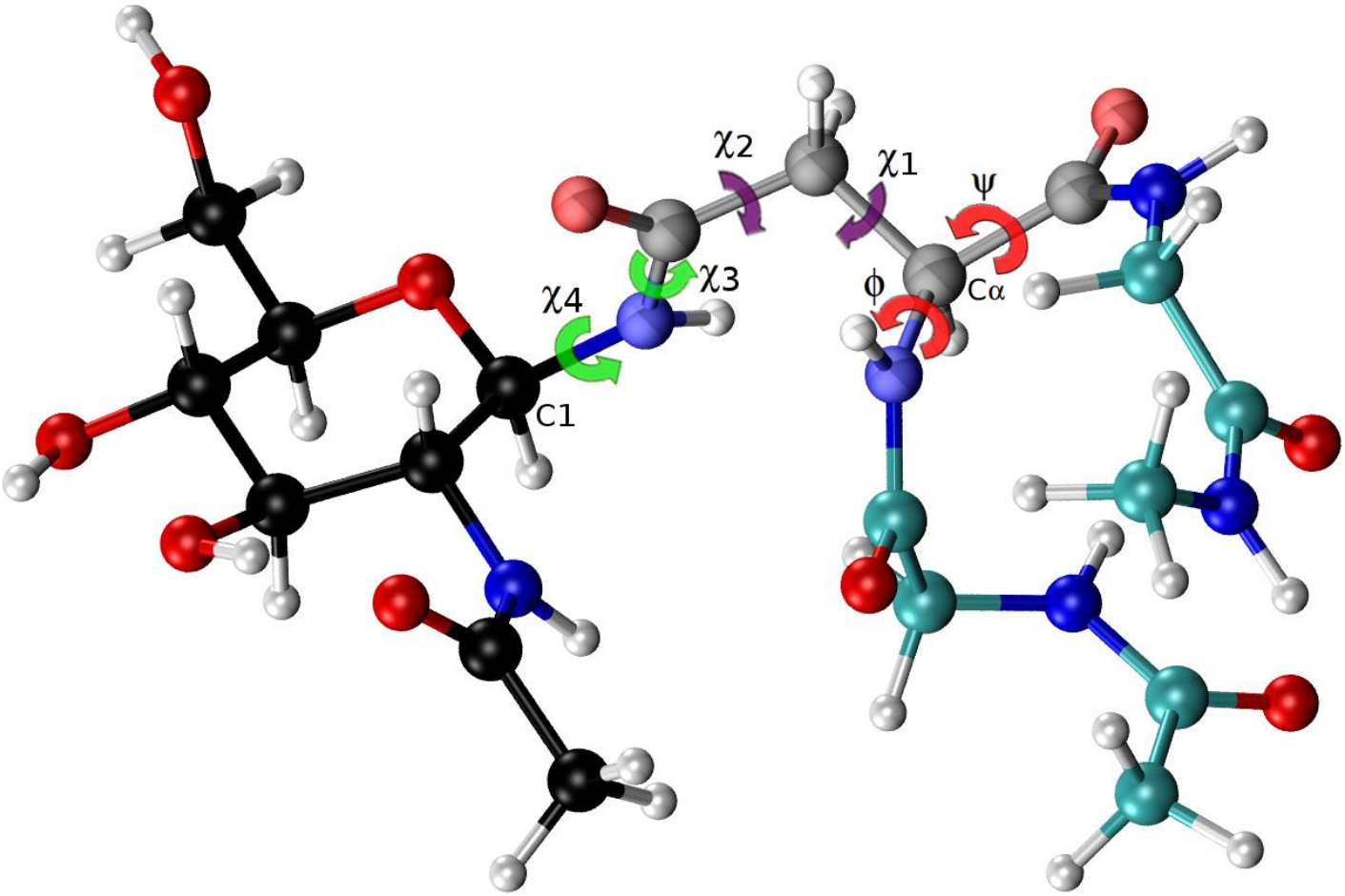


Figure S7.- Ball and stick representation of a glycan-amino acidic residue, namely for β-D-GlcpNAc-(1-N)-Asn with "1" representing **C1** of the glycan and "N" representing the nitrogen of the side-chain of Asn in an Ac-Gly-Asn-Gly-Nme tripeptide, in an arbitrary conformation. The χ3 and χ4 torsional angles, for the carbohydrate group (β-D-GalpNAc), are highlighted in green, while the corresponding one for the amino-acidic residue (Asn) are highlighted in red, for ϕ,ψ, and purple, for χ1 and χ2.

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