Supplemental Information for

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

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Figure S1.- (a) Kernel Density Estimation of the $\Delta$ values of the $^{13}\text{C}^\alpha$ 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 $^{13}\text{C}^\beta$ nucleus; (c) Kernel Density Estimation of the $\Delta$ values of the $^{13}\text{C}^\alpha$ nucleus of non-modified Lys upon protonation/deprotonation; (d) same as (c) for the $^{13}\text{C}^\beta$ nucleus.
Figure S2.- (a) Kernel Density Estimation of the Δ values of the $^{13}$C$^\alpha$ nucleus of non-modified (blue-line), $N^e$ (green-line) and $N^\eta$ (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 $\alpha$-D-GalpNAc-(1-O)-Ser or $\beta$-D-GlcpNAc-(1-O)-Ser, as a function of the $\Delta$ 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 [$\beta$-D-GlcpNAc-(1-N)-Asn], as a function of the chemical-shift differences ($\Delta$) 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 \( \chi_3 \) and \( \chi_4 \) 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 \( \phi, \psi \), and purple, for \( \chi_1 \) and \( \chi_2 \).