Supporting information

Investigation of neutral losses and the citrulline effect for modified H4 *N*-terminal pentapeptides

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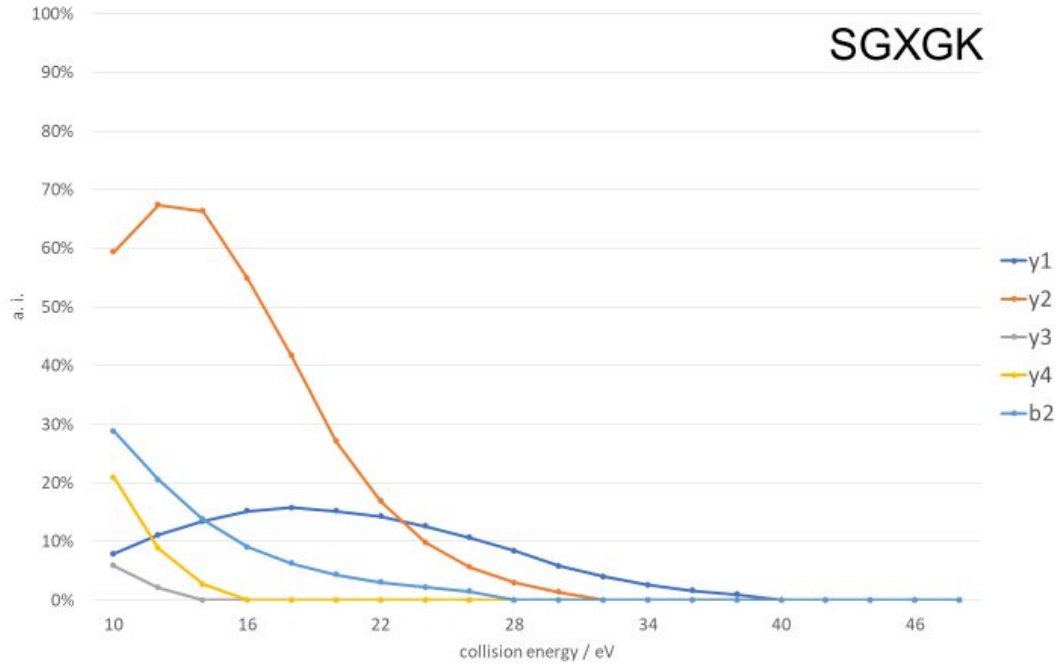


Figure S1a Fragment distribution of the peptide SGXGK upon higher-energy collision-induced dissociation (HCD) as a function of collision energy

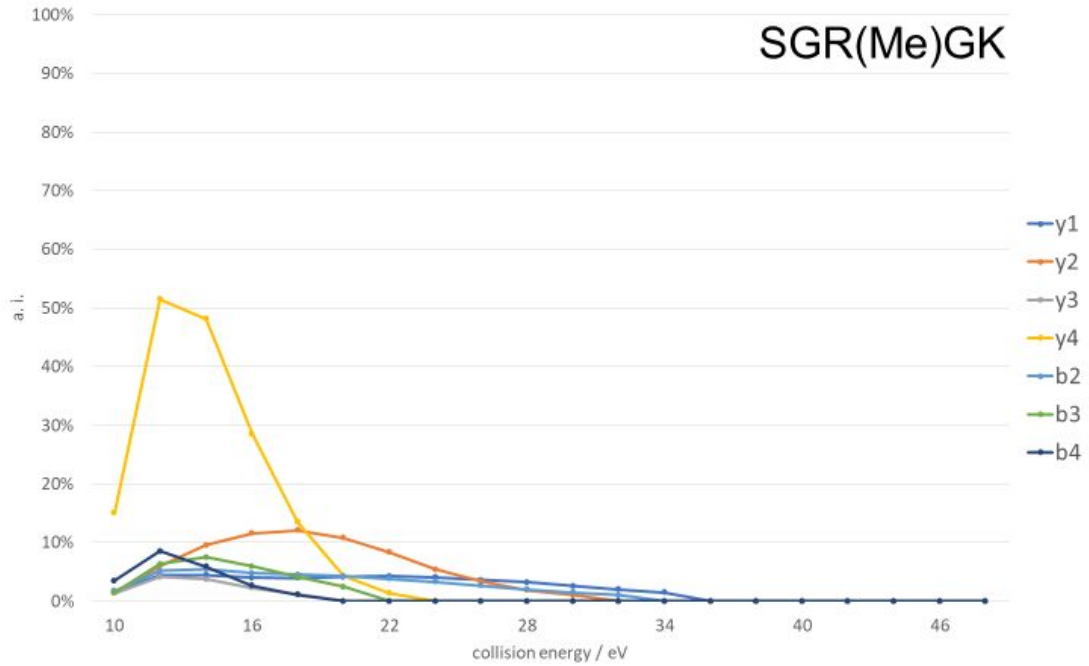


Figure S1b Fragment distribution of the peptide SGR(Me)GK upon higher-energy collision-induced dissociation (HCD) as a function of collision energy

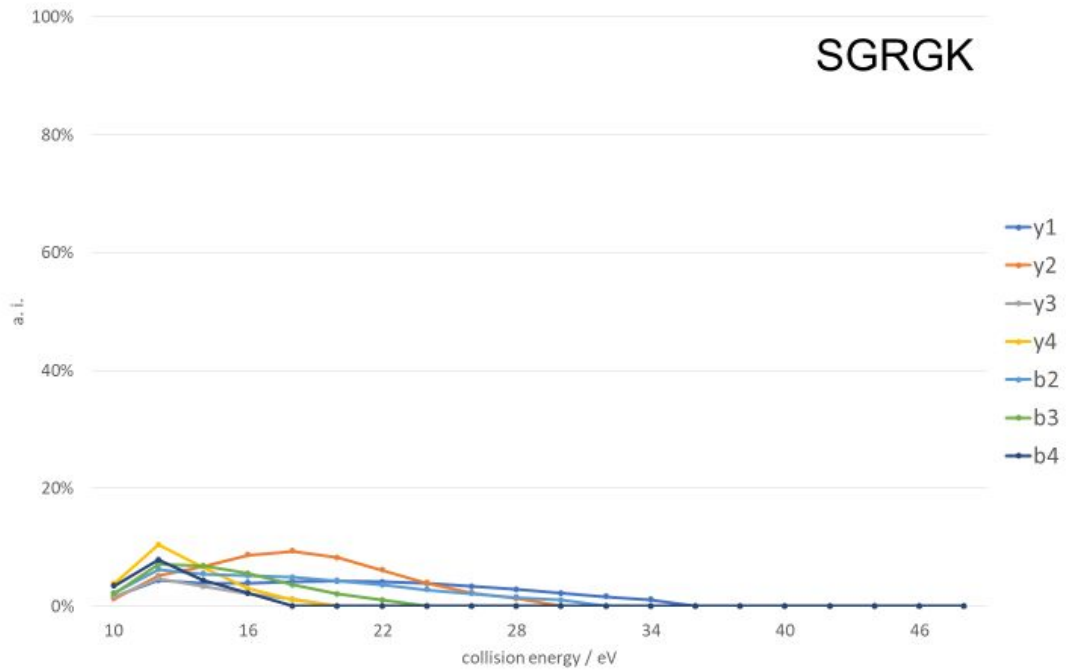


Figure S1c Fragment distribution of the peptide SGRGK upon higher-energy collision-induced dissociation (HCD) as a function of collision energy

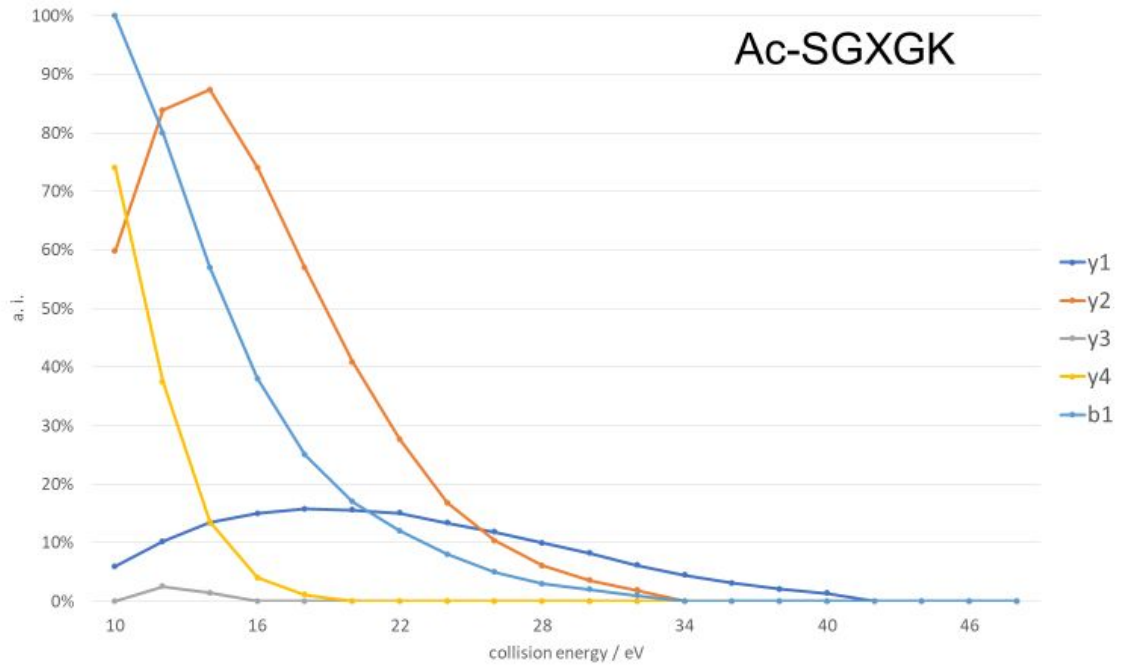


Figure S1d Fragment distribution of the peptide Ac-SGXGK upon higher-energy collision-induced dissociation (HCD) as a function of collision energy

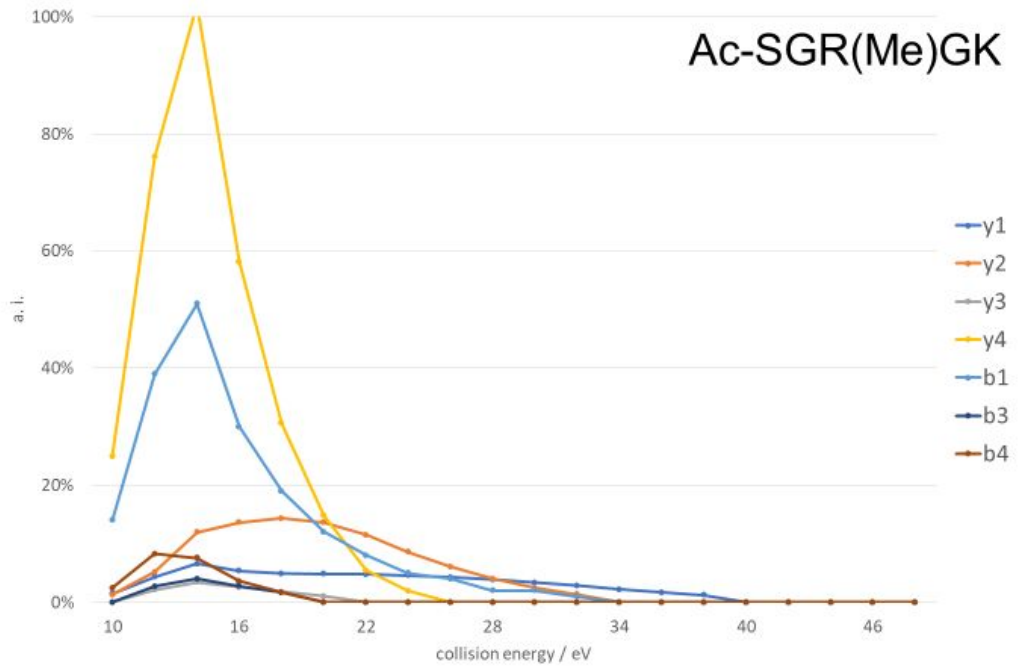


Figure S1e Fragment distribution of the peptide Ac-SGR(Me)GK upon higher-energy collision-induced dissociation (HCD) as a function of collision energy

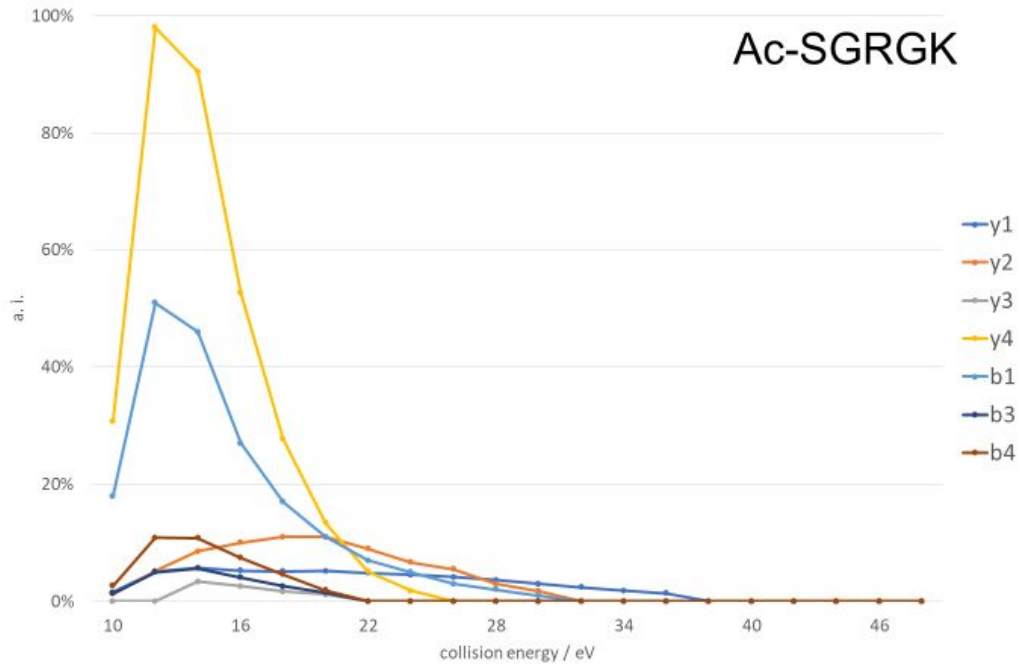


Figure S1f Fragment distribution of the peptide Ac-SGRGK upon higher-energy collision-induced dissociation (HCD) as a function of collision energy

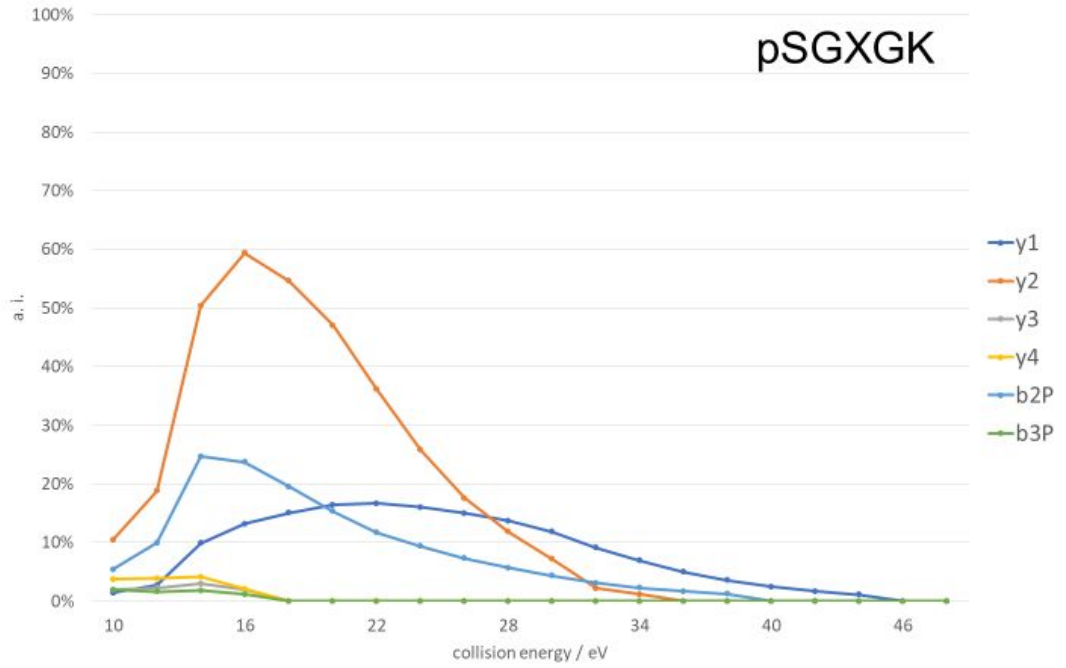


Figure S1g Fragment distribution of the peptide pSGXGK upon higher-energy collision-induced dissociation (HCD) as a function of collision energy

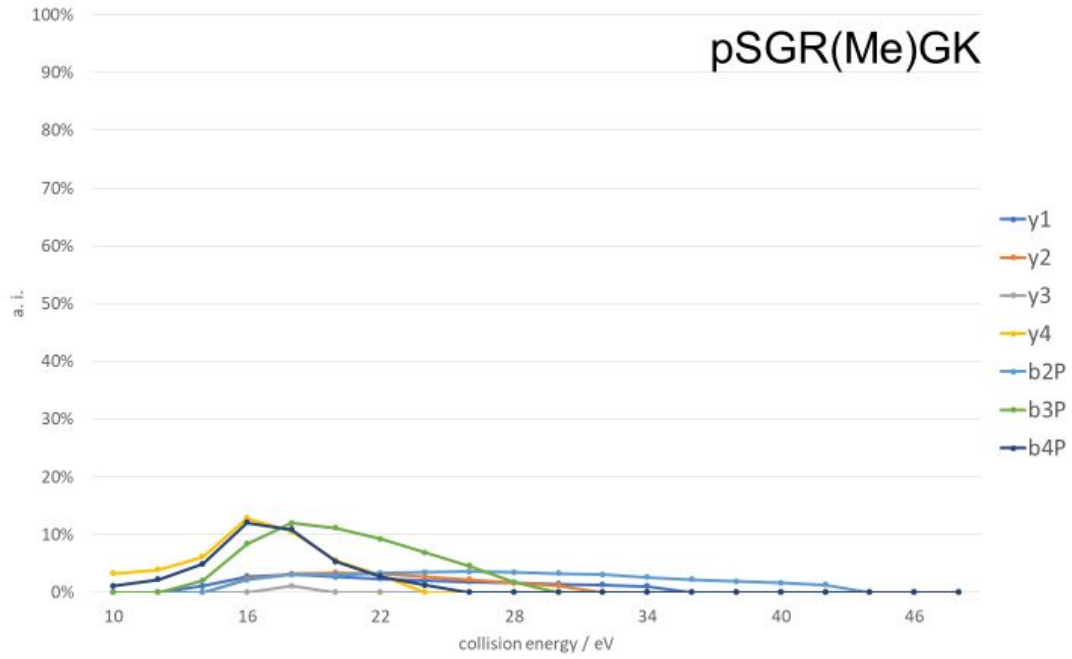


Figure S1h Fragment distribution of the peptide pSGR(Me)GK upon higher-energy collision-induced dissociation (HCD) as a function of collision energy

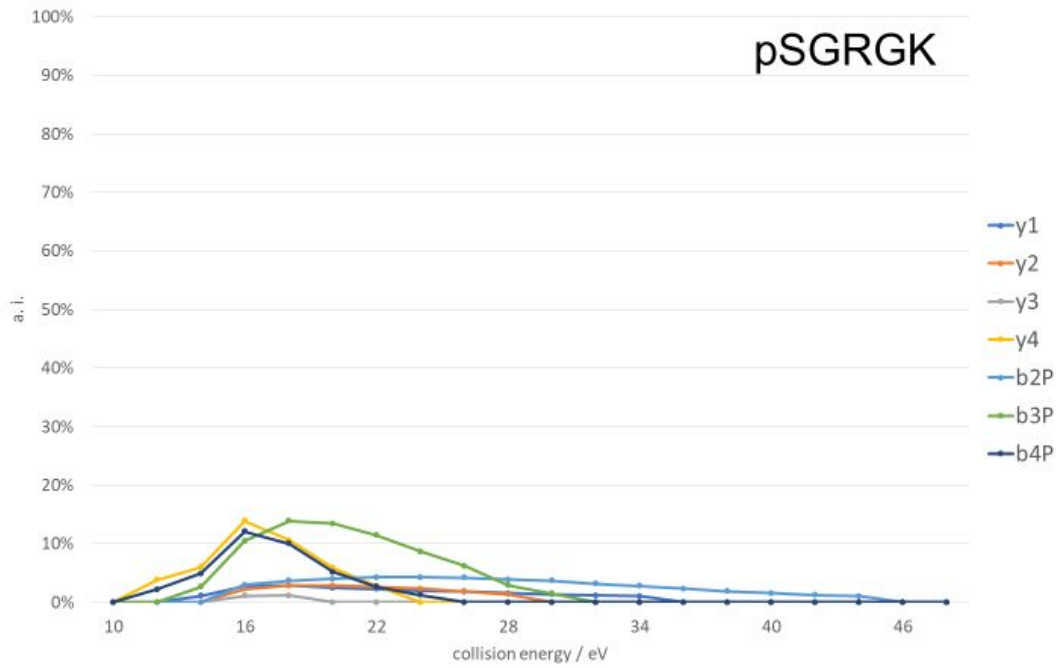


Figure S1i Fragment distribution of the peptide pSGRGK upon higher-energy collision-induced dissociation (HCD) as a function of collision energy

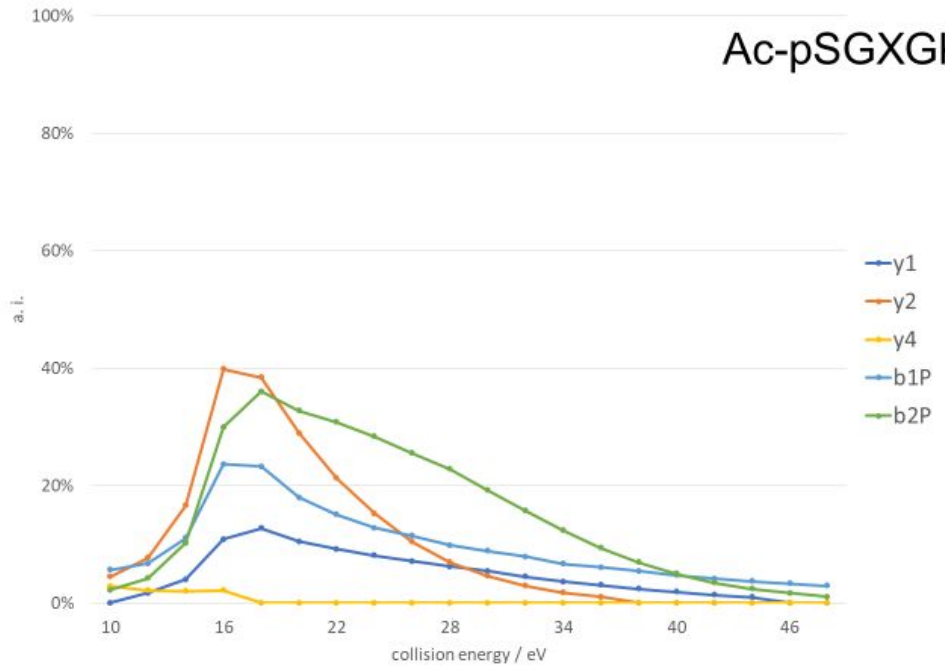


Figure S1j Fragment distribution of the peptide Ac-pSGXGK upon higher-energy collision-induced dissociation (HCD) as a function of collision energy

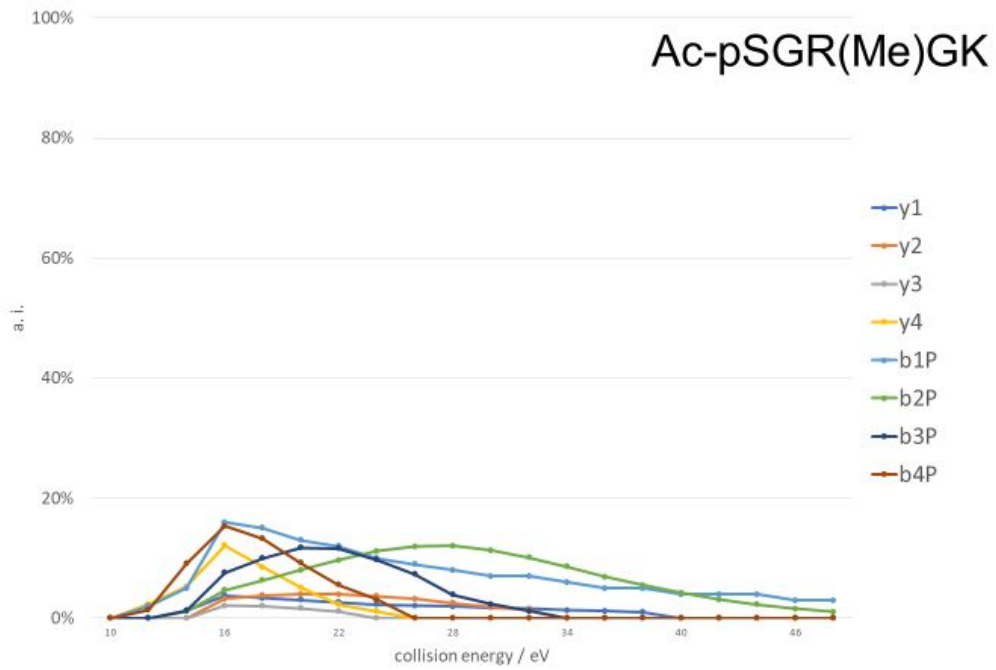


Figure S1k Fragment distribution of the peptide Ac-pSGR(Me)GK upon higher-energy collision-induced dissociation (HCD) as a function of collision energy

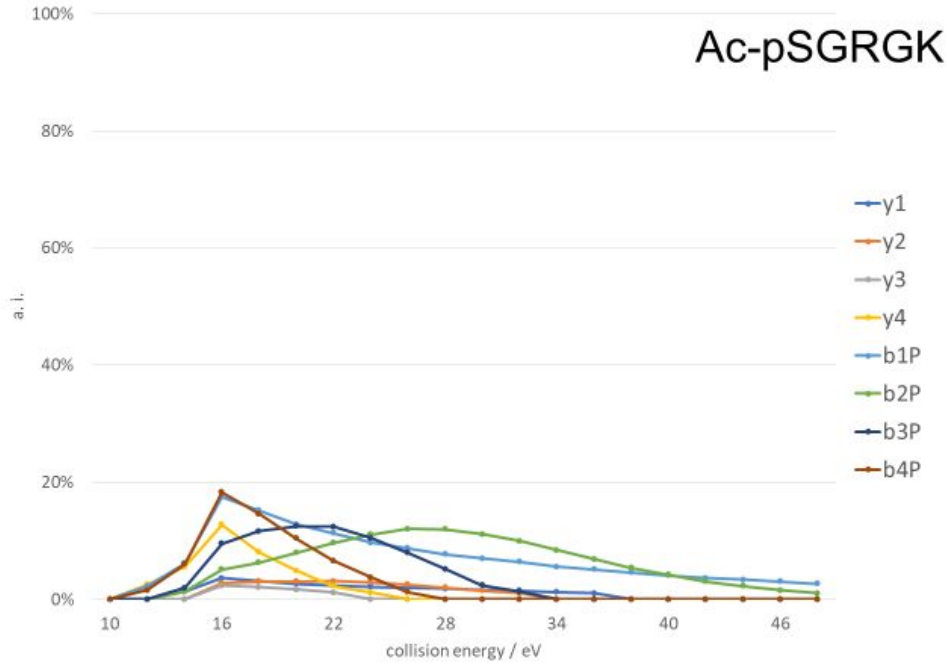


Figure S1l Fragment distribution of the peptide Ac-pSGRGK upon higher-energy collision-induced dissociation (HCD) as a function of collision energy

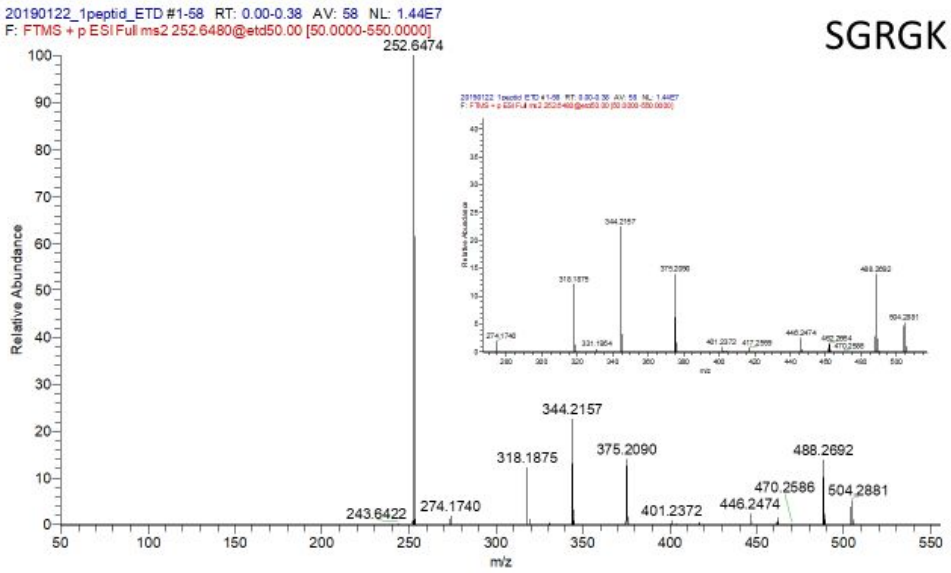


Figure S2a ETD tandem mass spectrum of the peptide SGRGK

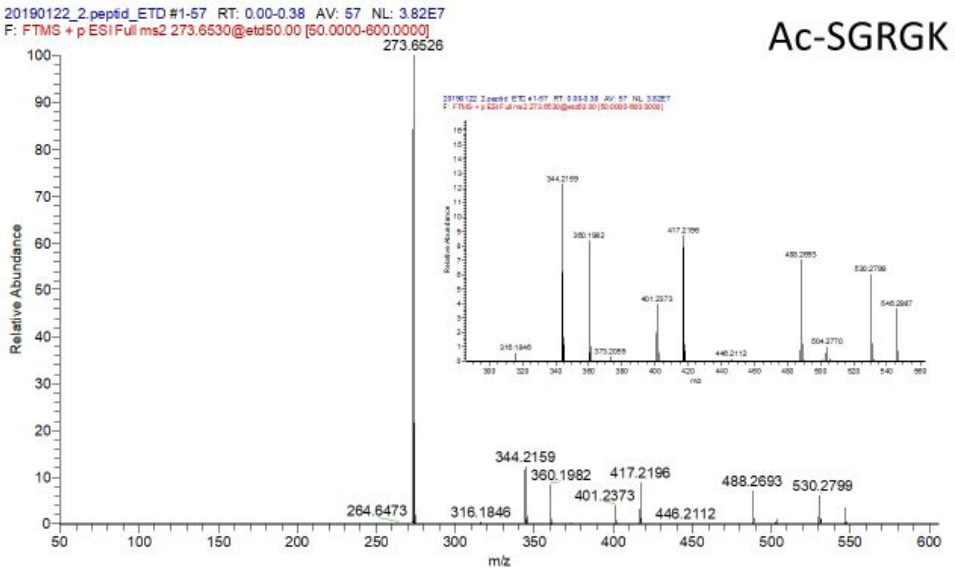
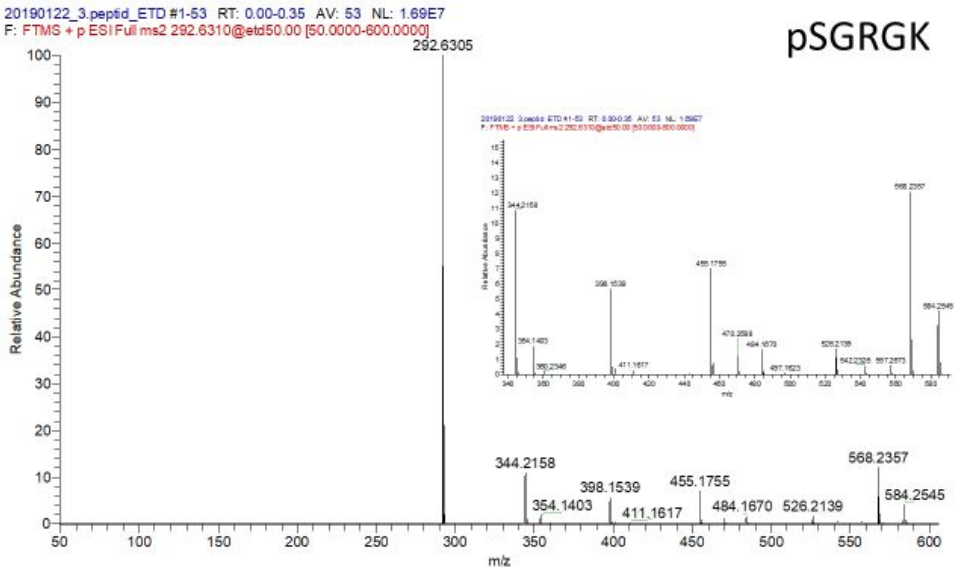


Figure S2b ETD tandem mass spectrum of the peptide Ac-SGRGK



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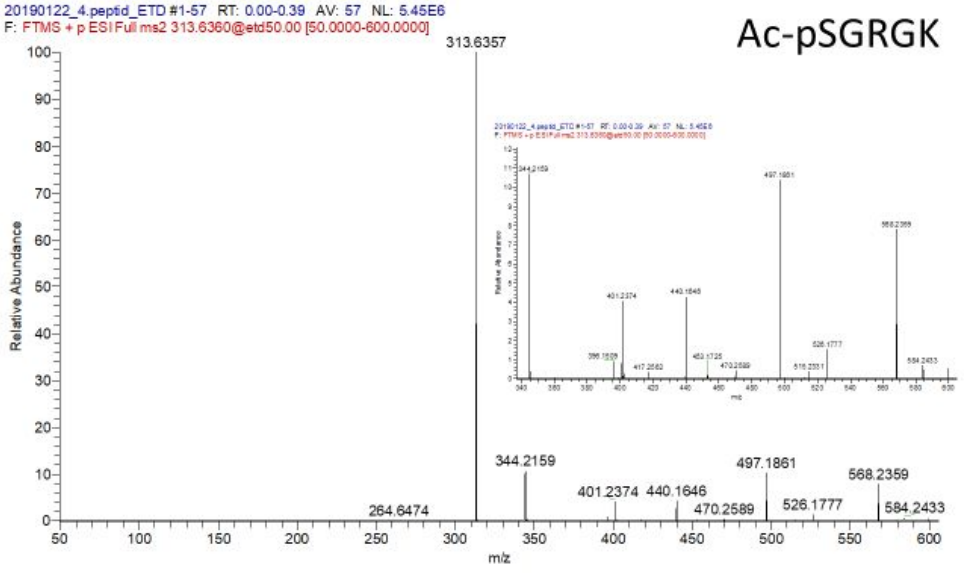


Figure S2d ETD tandem mass spectrum of the peptide Ac-pSGRGK

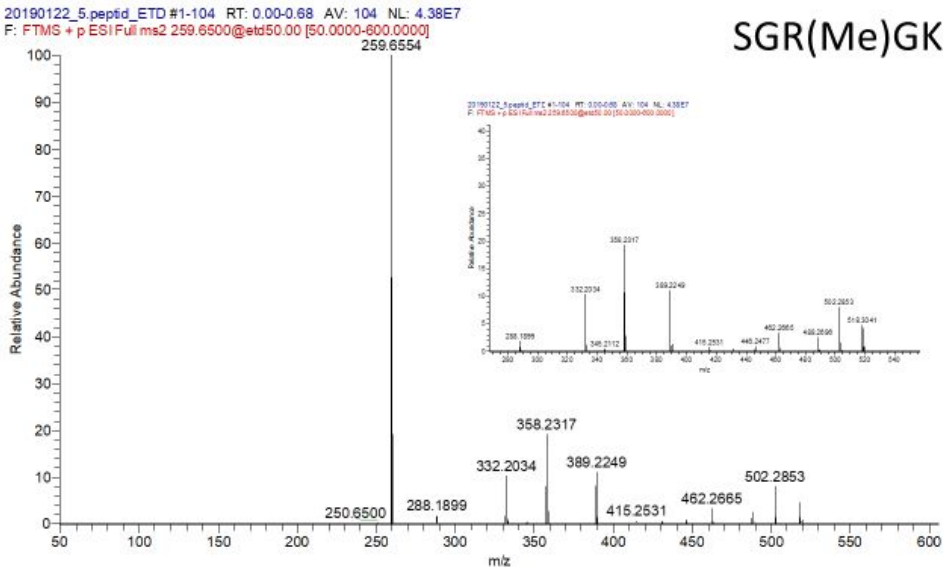


Figure S2e ETD tandem mass spectrum of the peptide SGR(Me)GK

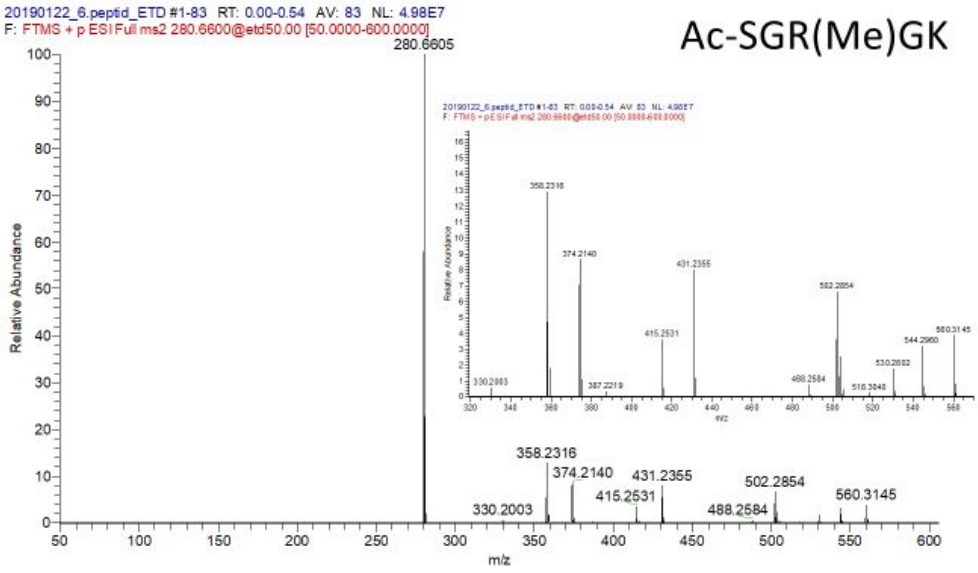
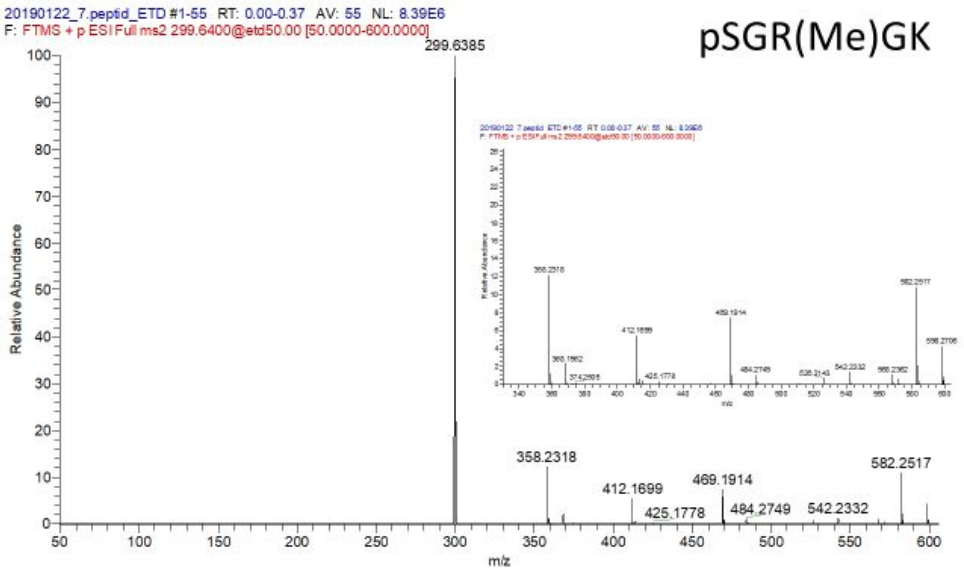


Figure S2f ETD tandem mass spectrum of the peptide Ac-SGR(Me)GK



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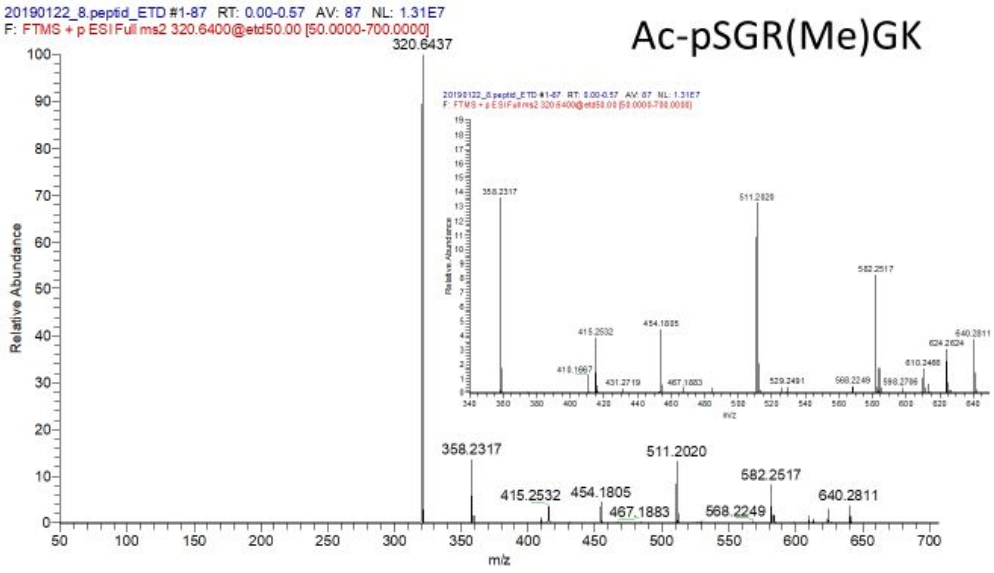

Figure S2h ETD tandem mass spectrum of the peptide Ac-pSGR(Me)GK

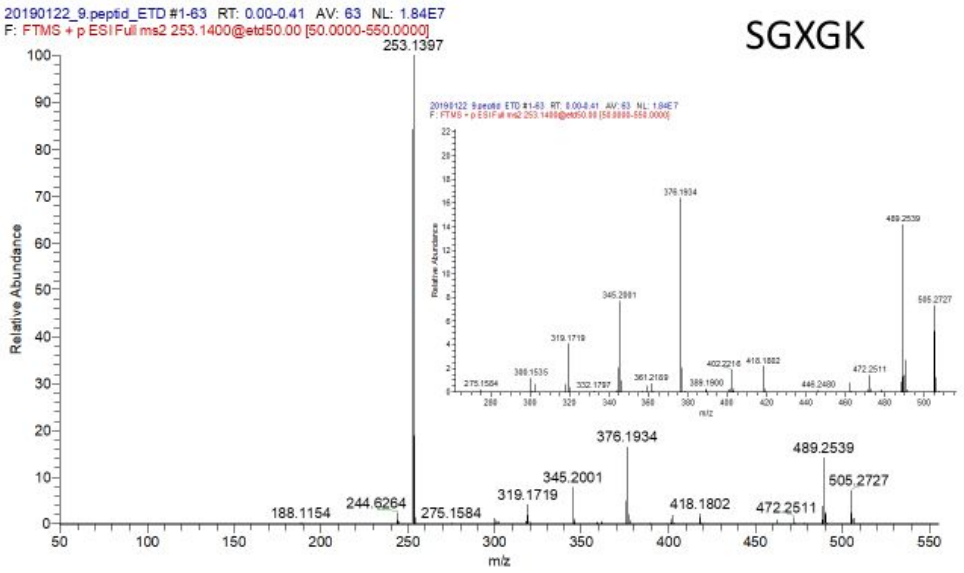

Figure S2i ETD tandem mass spectrum of the peptide SGXGK

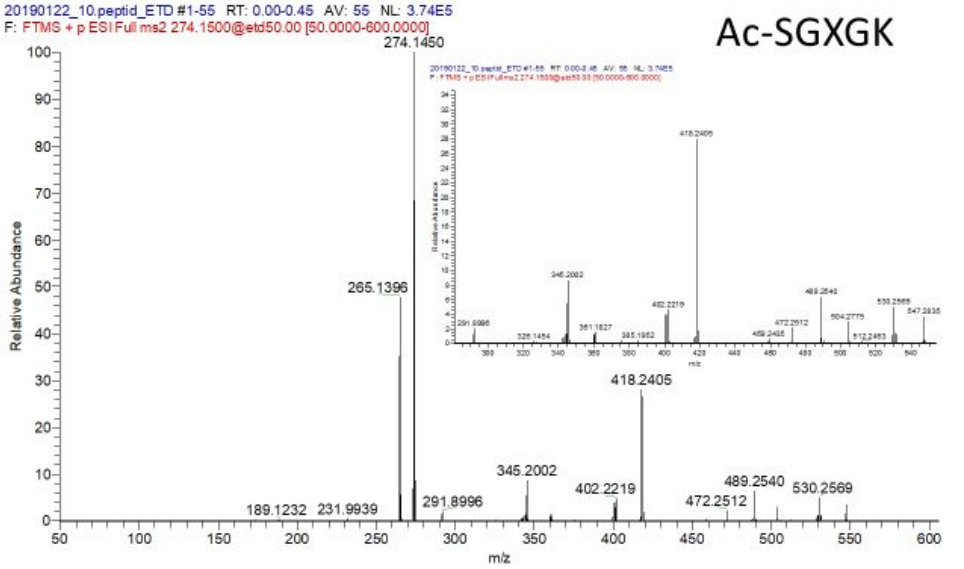

Figure S2j ETD tandem mass spectrum of the peptide Ac-SGXGK

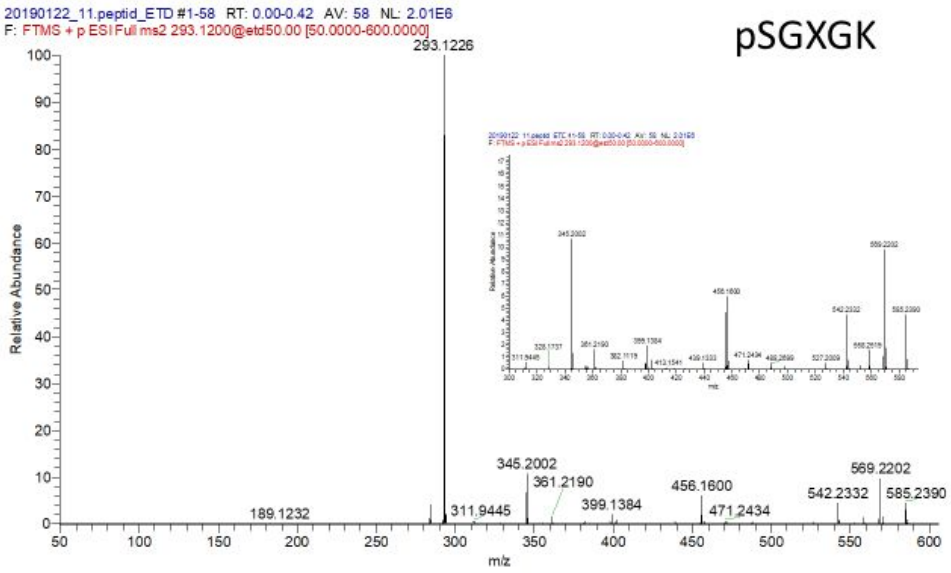

Figure S2k ETD tandem mass spectrum of the peptide pSGXGK

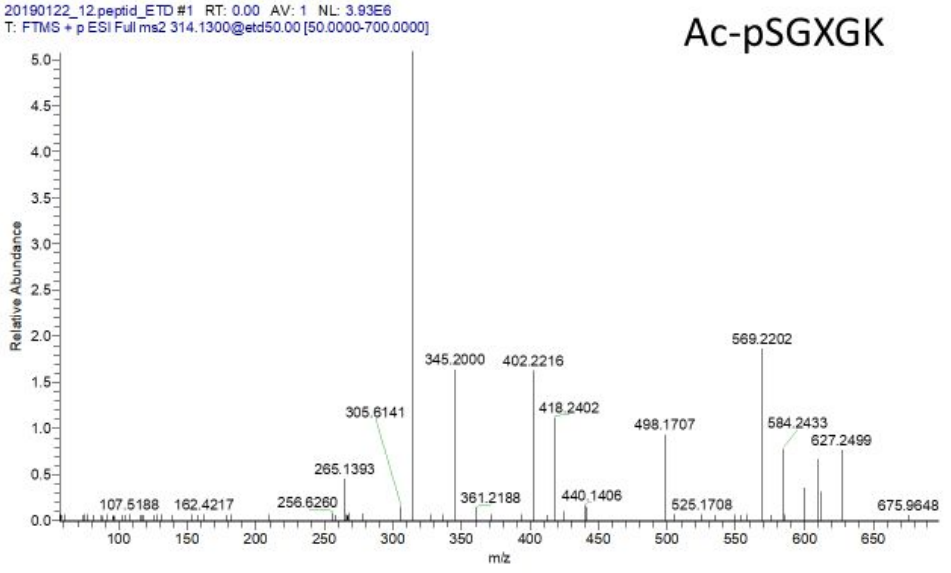

Figure S2l ETD tandem mass spectrum of the peptide Ac-pSGXGK

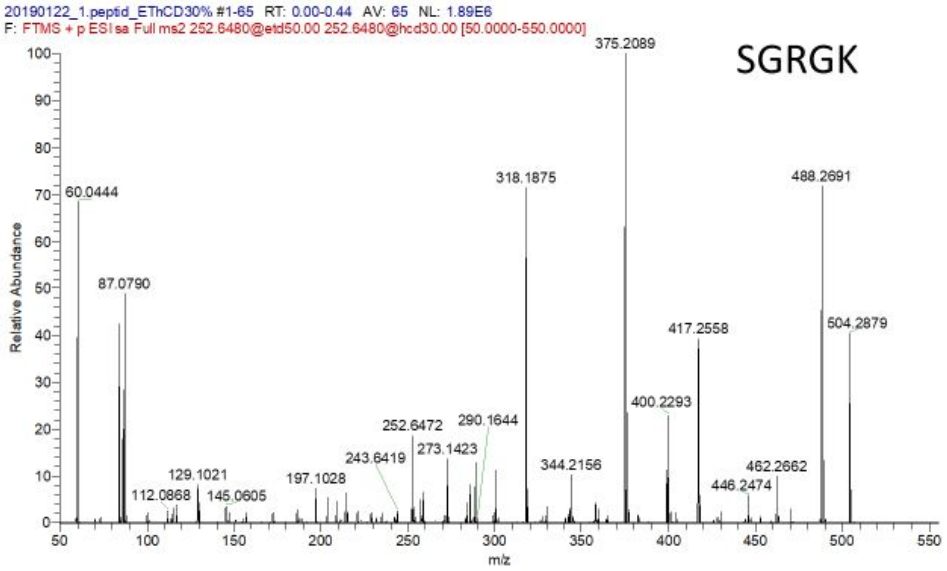

Figure S3a EThcD tandem mass spectrum of the peptide SGRGK

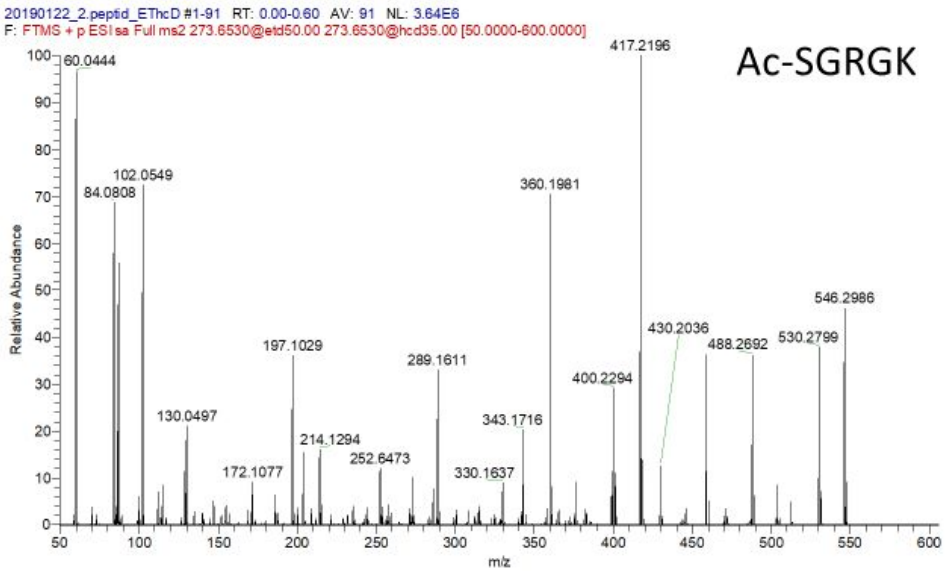

Figure S3b EThcD tandem mass spectrum of the peptide Ac-SGRGK

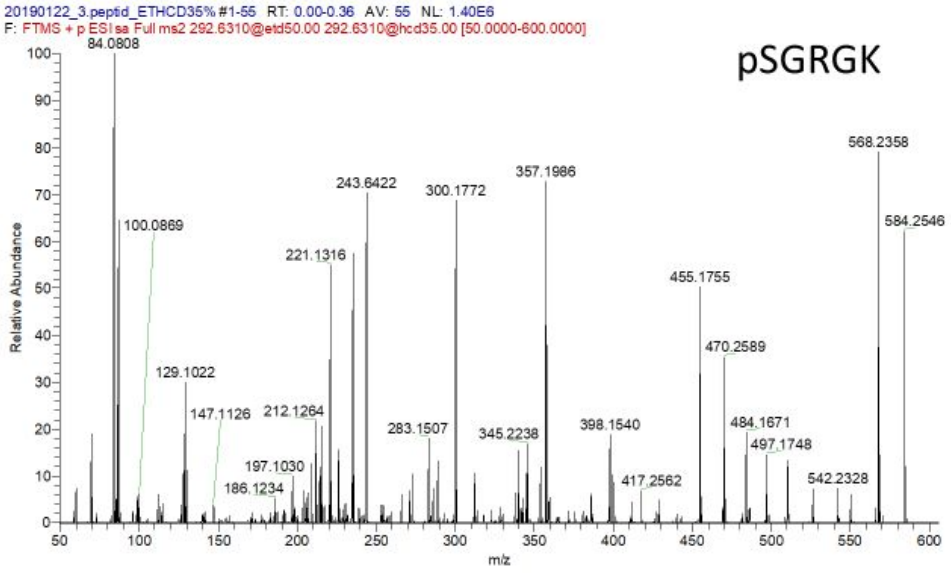

Figure S3c EThcD tandem mass spectrum of the peptide pSGRGK

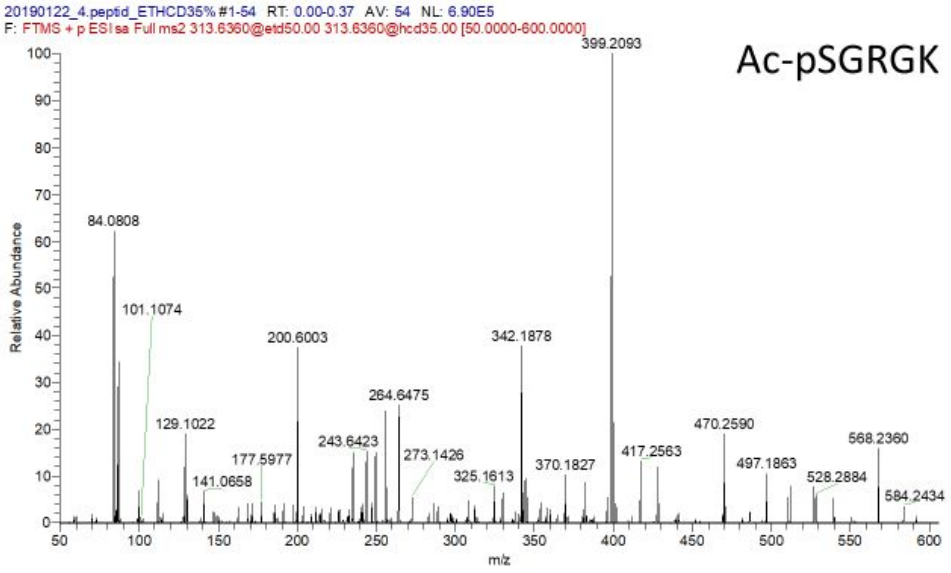

Figure S3d EThcD tandem mass spectrum of the peptide Ac-pSGRGK

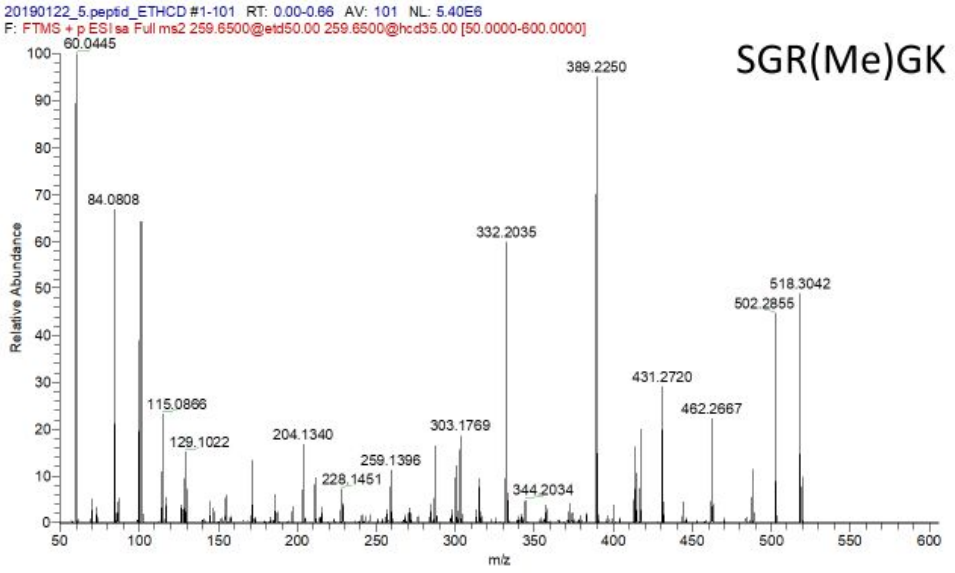

Figure S3e EThcD tandem mass spectrum of the peptide SGR(Me)GK

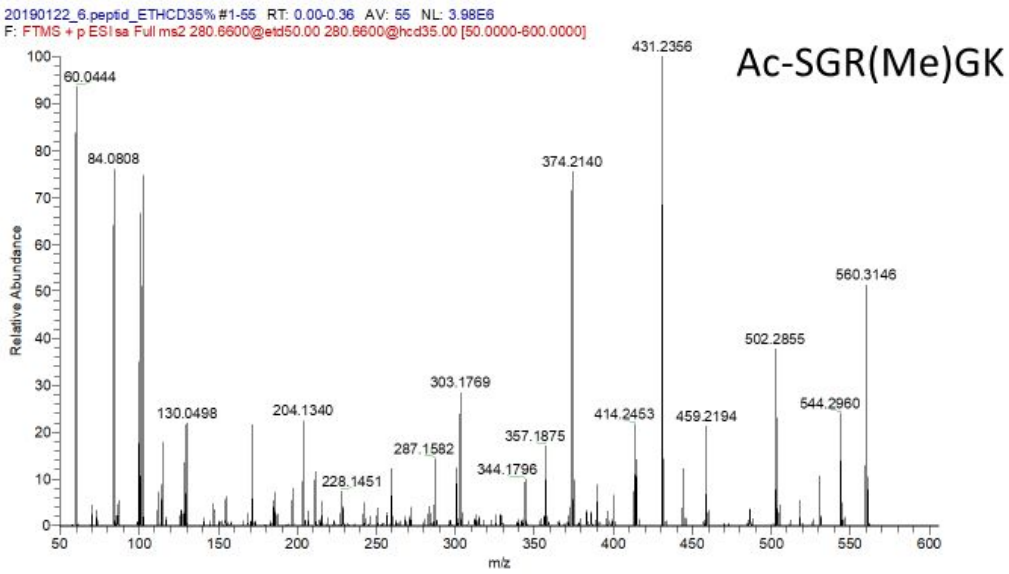

Figure S3f EThcD tandem mass spectrum of the peptide Ac-SGR(Me)GK

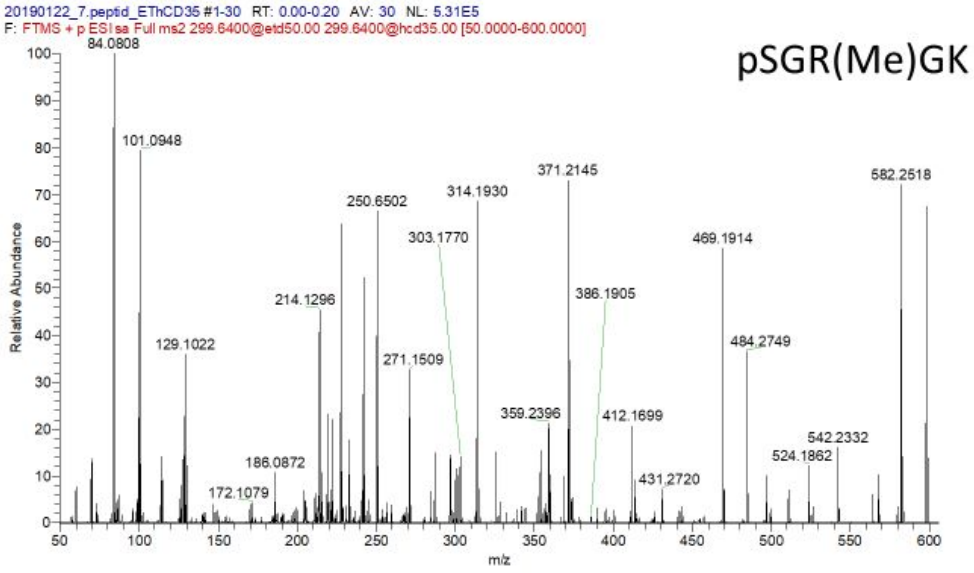

Figure S3g EThcD tandem mass spectrum of the peptide pSGR(Me)GK

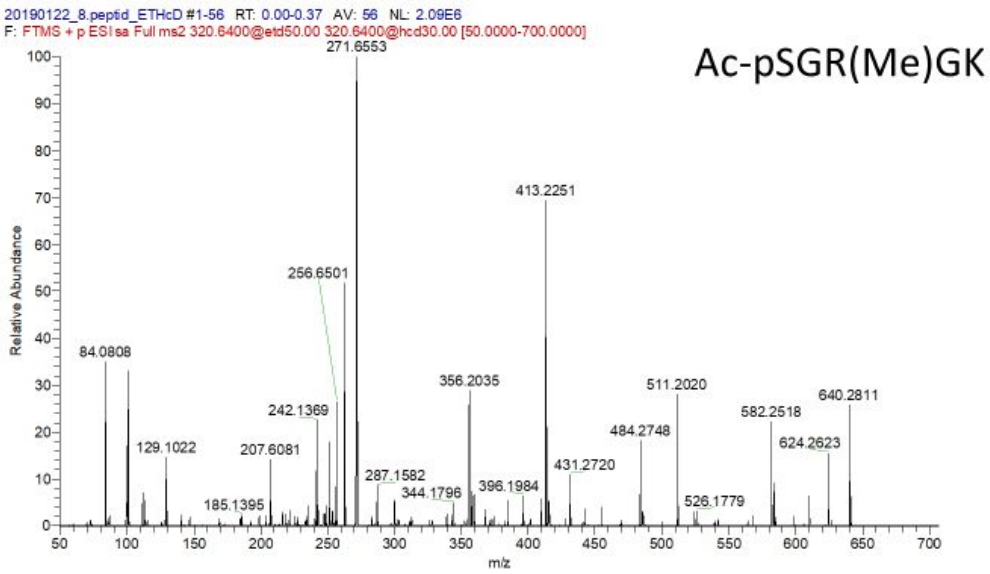

Figure S3h EThcD tandem mass spectrum of the peptide Ac-pSGR(Me)GK

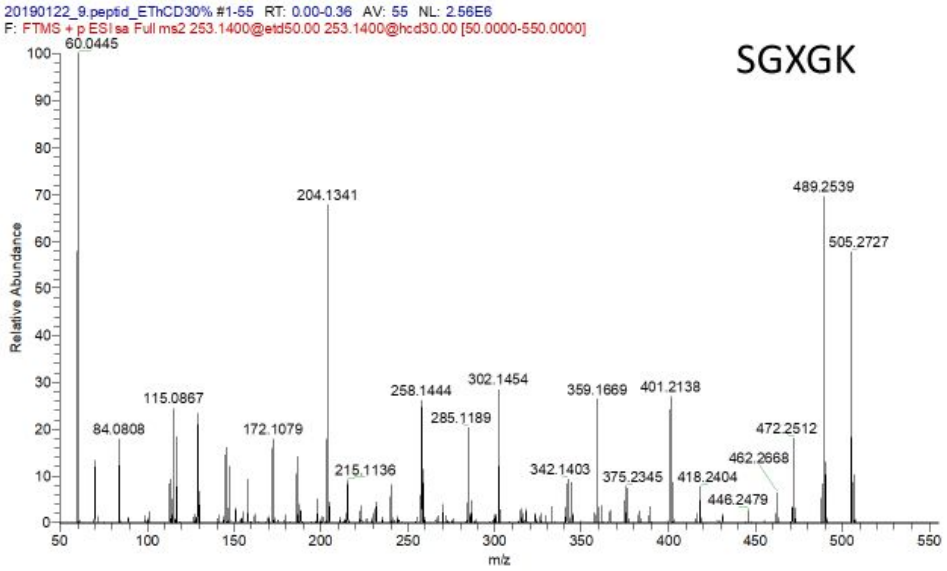

Figure S3i EThcD tandem mass spectrum of the peptide SGXGK

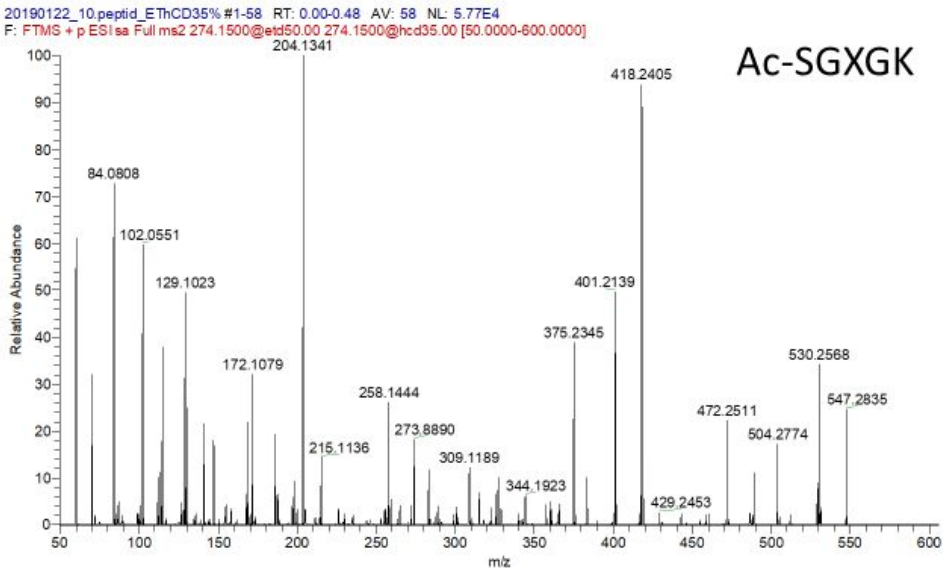

Figure S3j EThcD tandem mass spectrum of the peptide Ac-SGXGK

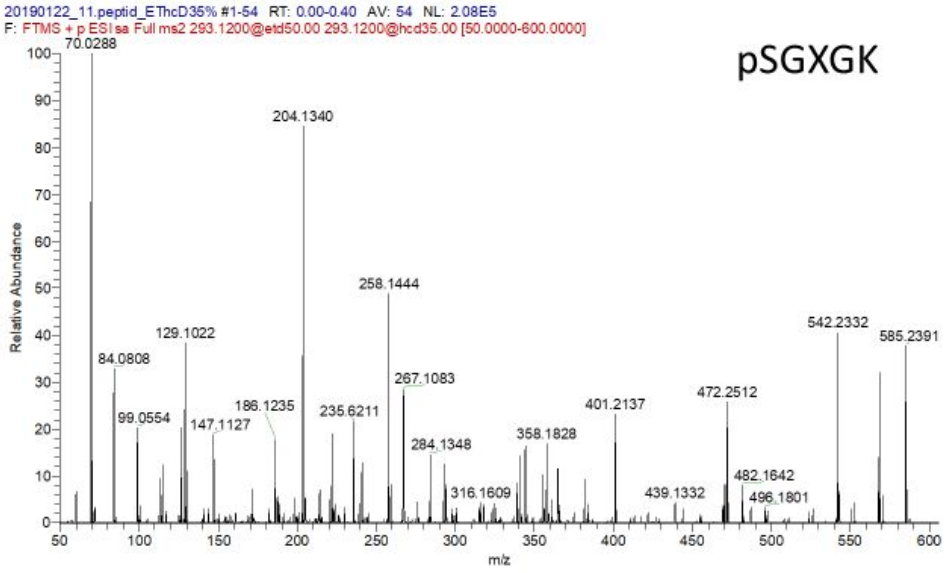

Figure S3k EThcD tandem mass spectrum of the peptide pSGXGK

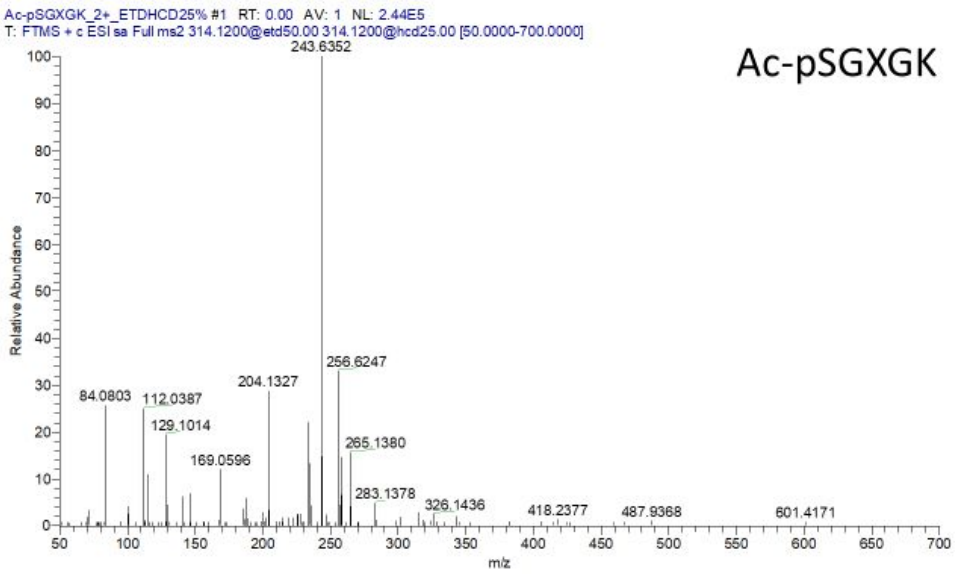

Figure S3l EThcD tandem mass spectrum of the peptide Ac-pSGXGK

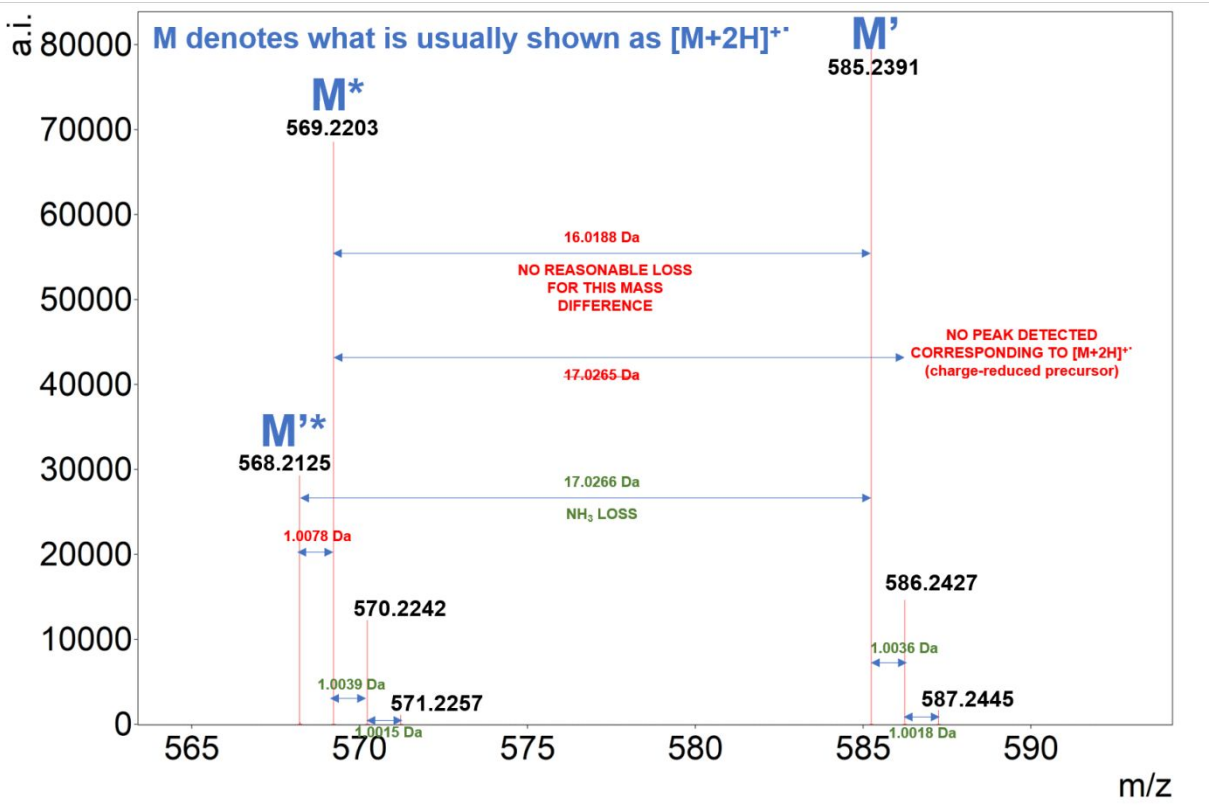

Figure S4 Representation of 'unusual isotope distributions' in the EThcD spectrum of the peptide pSGXGK

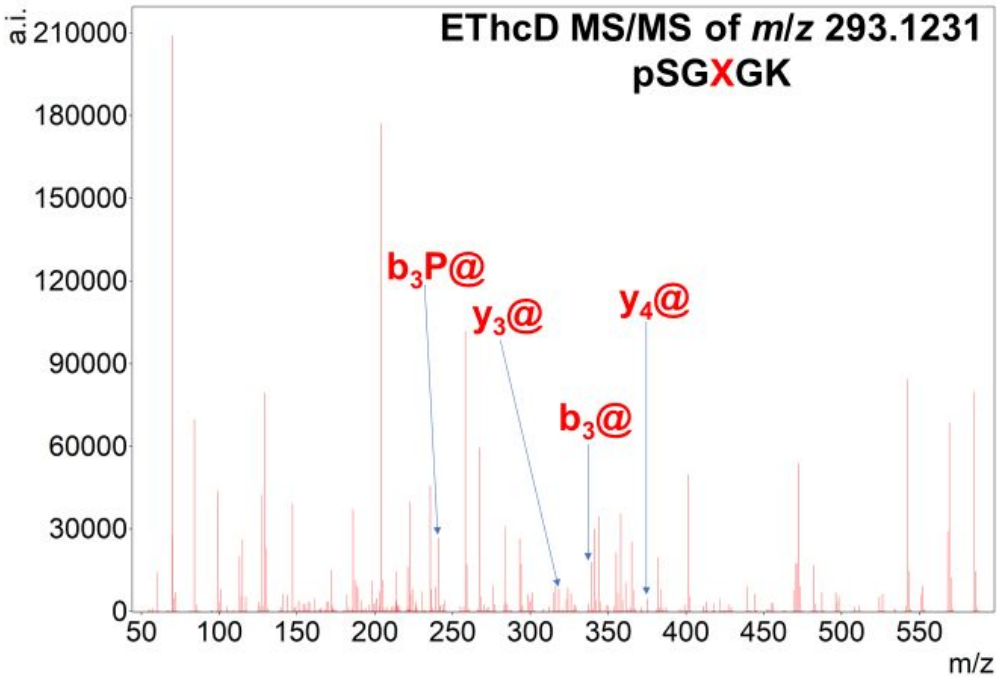

Figure S5 Representation of isocyanic acid loss (@) from all fragments that contain the citrulline residue in an EThcD tandem mass spectrum

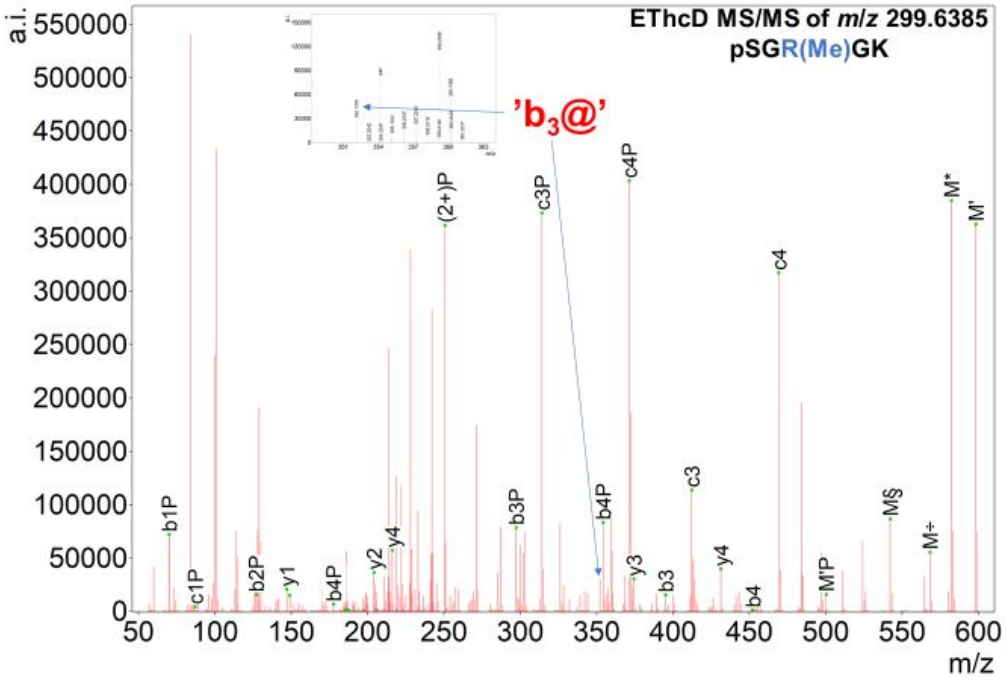

Figure S6 Representation of a false neutral loss of isocyanic acid (@) for the peptide pSGR(Me)GK which lacks a citrulline residue