Supplemental Data

Analysis of Naphthalene Adduct Binding Sites in Model Proteins by Tandem Mass Spectrometry

Nathalie T. Pham[†*], William T. Jewell[‡], Dexter Morin[†], Alan R. Buckpitt[†]

**

Each of the following figures presents the MS/MS spectra of the adducted peptide products from actin and PDI.

For each figure, the *m/z* of the adducted peptide is given along with the corresponding MS/MS fragmentation.

Adducted fragment ions (modified by a metabolite) are ***italicized bold*.** Nonadducted fragment ions are not.

$[M+H]^+$ = the nonadducted parent peptide ion; $\boldsymbol{[M+H]^+}$ = the monoadducted parent peptide ion.

H_2O = water to the mass of the ion.

= modification by naphthalene epoxide (NPO).

Ψ = modification by naphthalene diol epoxide (NDO).

† = modification of 1,2-naphthoqinone (1,2NPQ).

° = modification by 1,4-naphthoquinone (1,4NPQ).

Figure S1: MS/MS of adducted actin peptide **[MEEEIAALVIDNGSGMCK + NPO]** at *m/z* 1026.9643 (doubly charged).

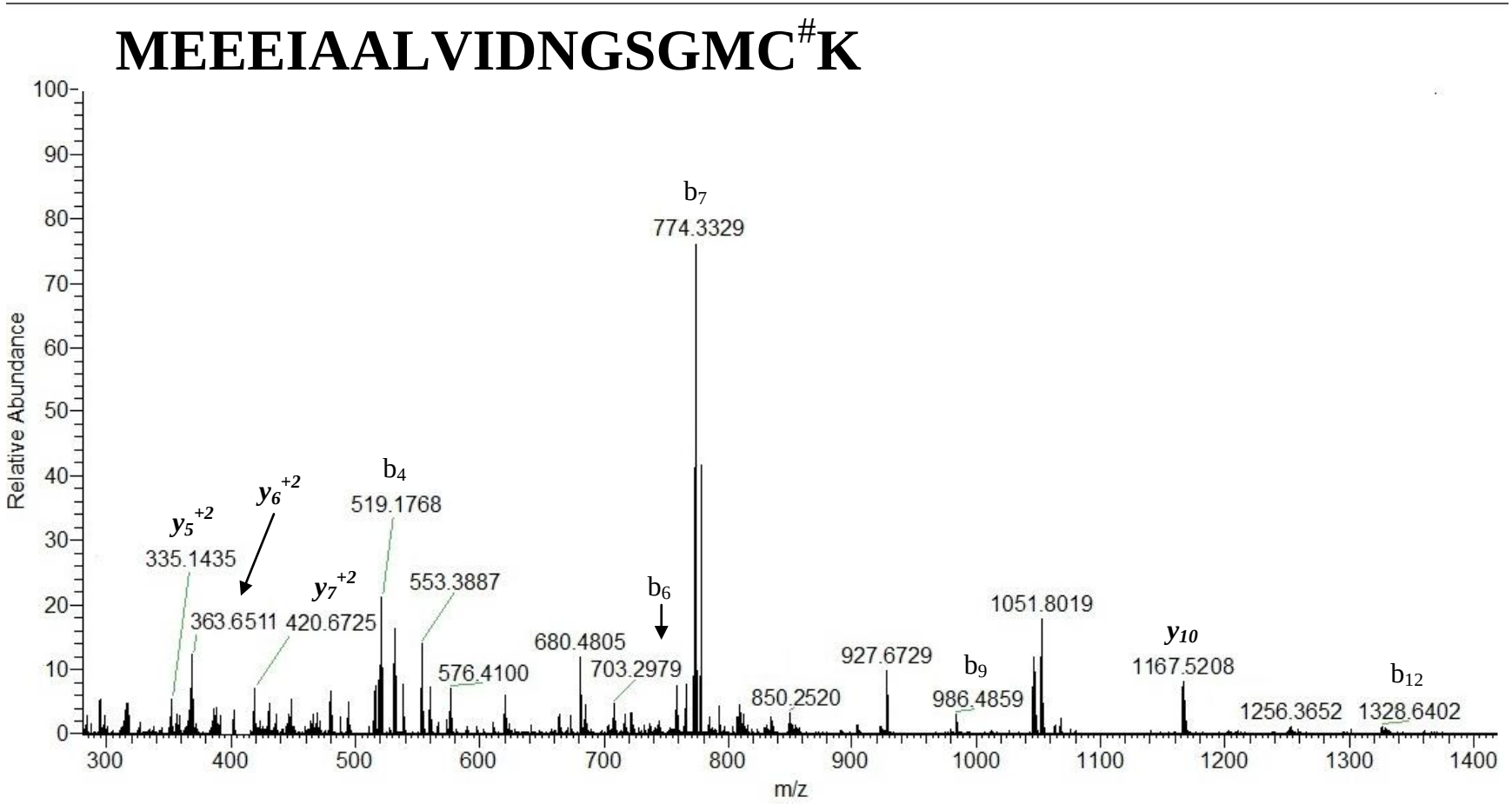


Figure S2: MS/MS of adducted actin peptide **[MEEEIAALVIDNGSGMCK + NDO]** at *m/z* 1043.9679 (doubly charged).

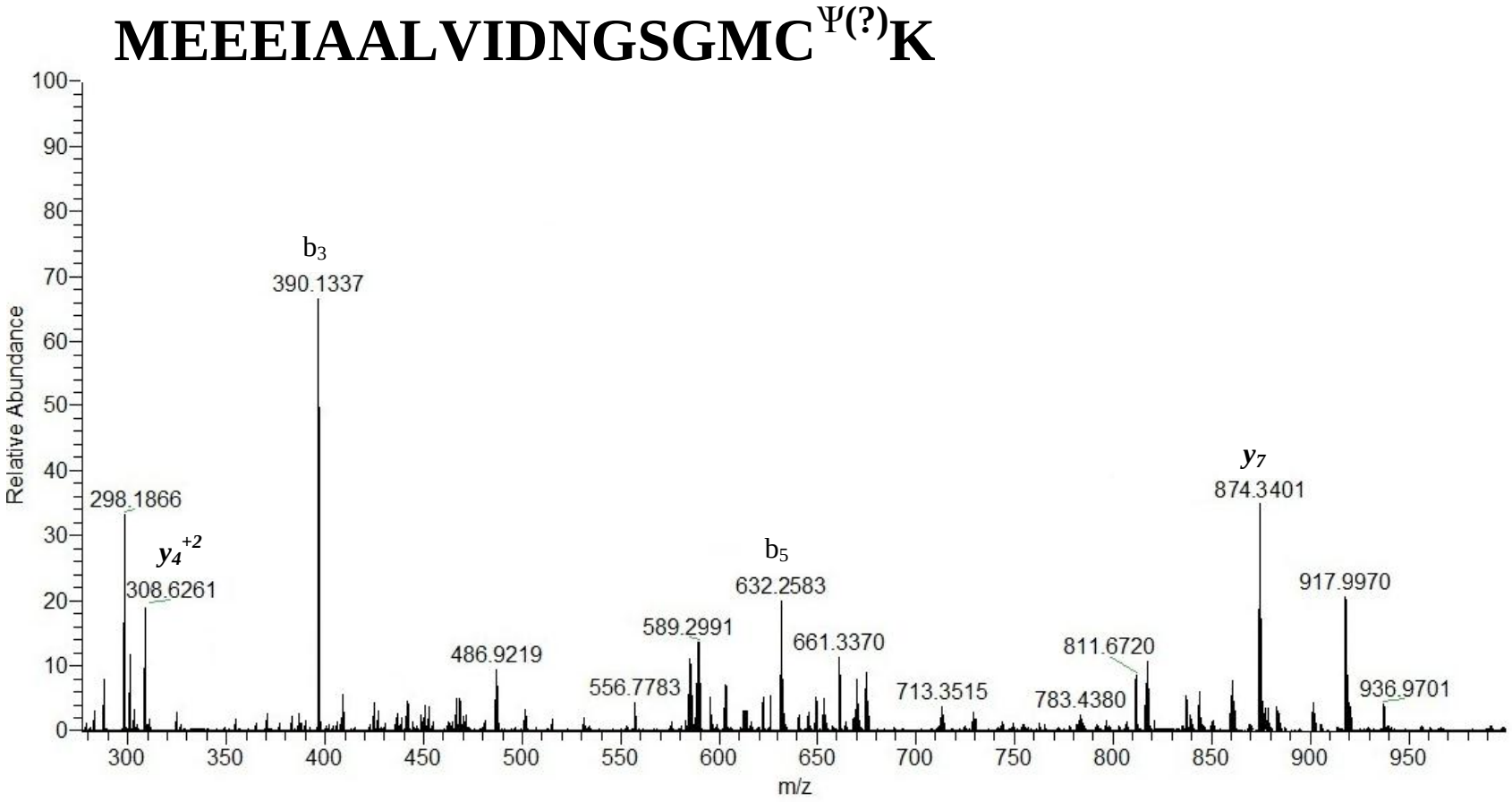


Figure S3: MS/MS of adducted actin peptide **[MEEEIAALVIDNGSGMCK + 1.2NPQ]** at *m/z* 1033.9498 (doubly charged).

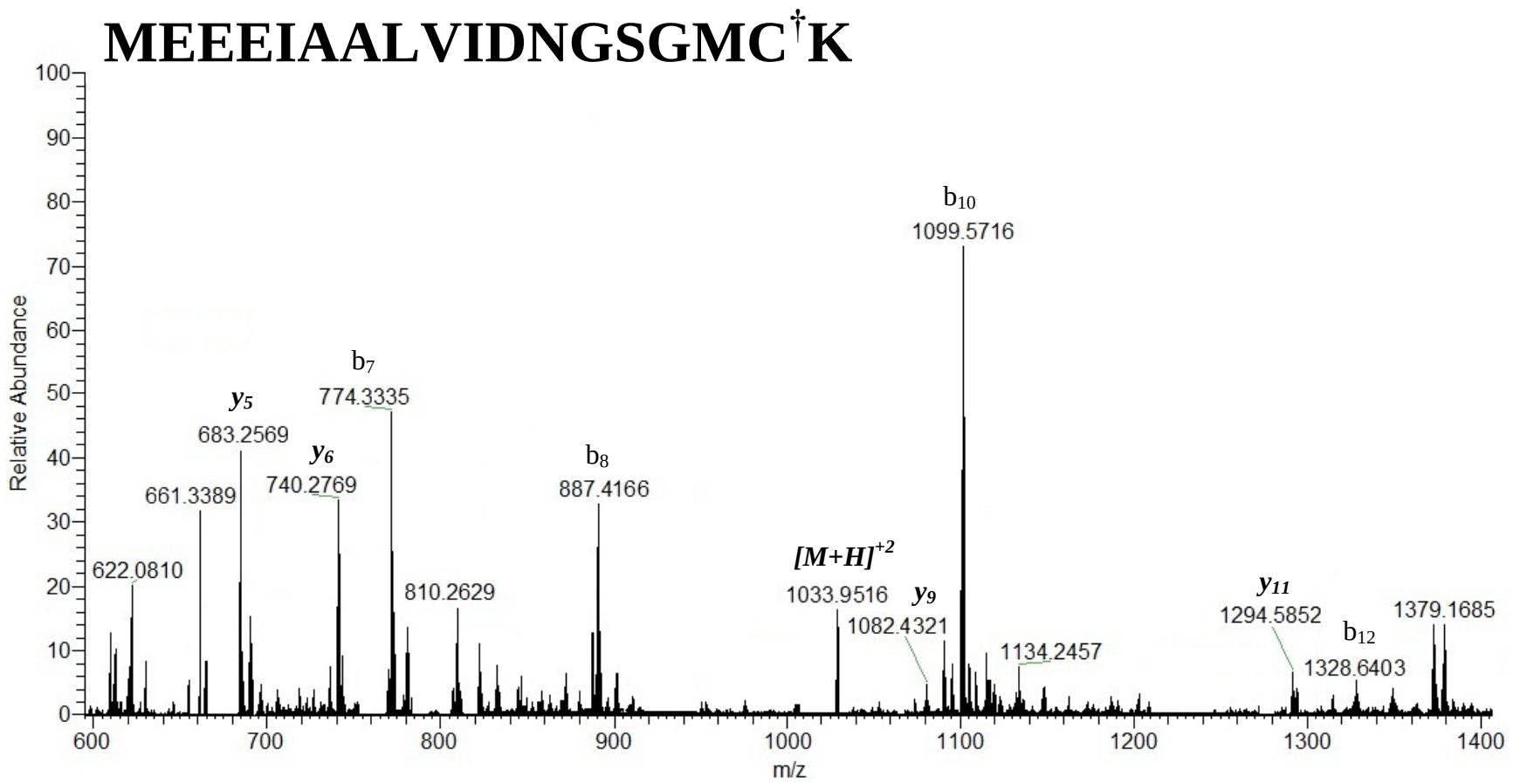


Figure S4: MS/MS of adducted actin peptide **[HQGVMVGMGQK + NDO]** at *m/z* 674.8164 (doubly charged).

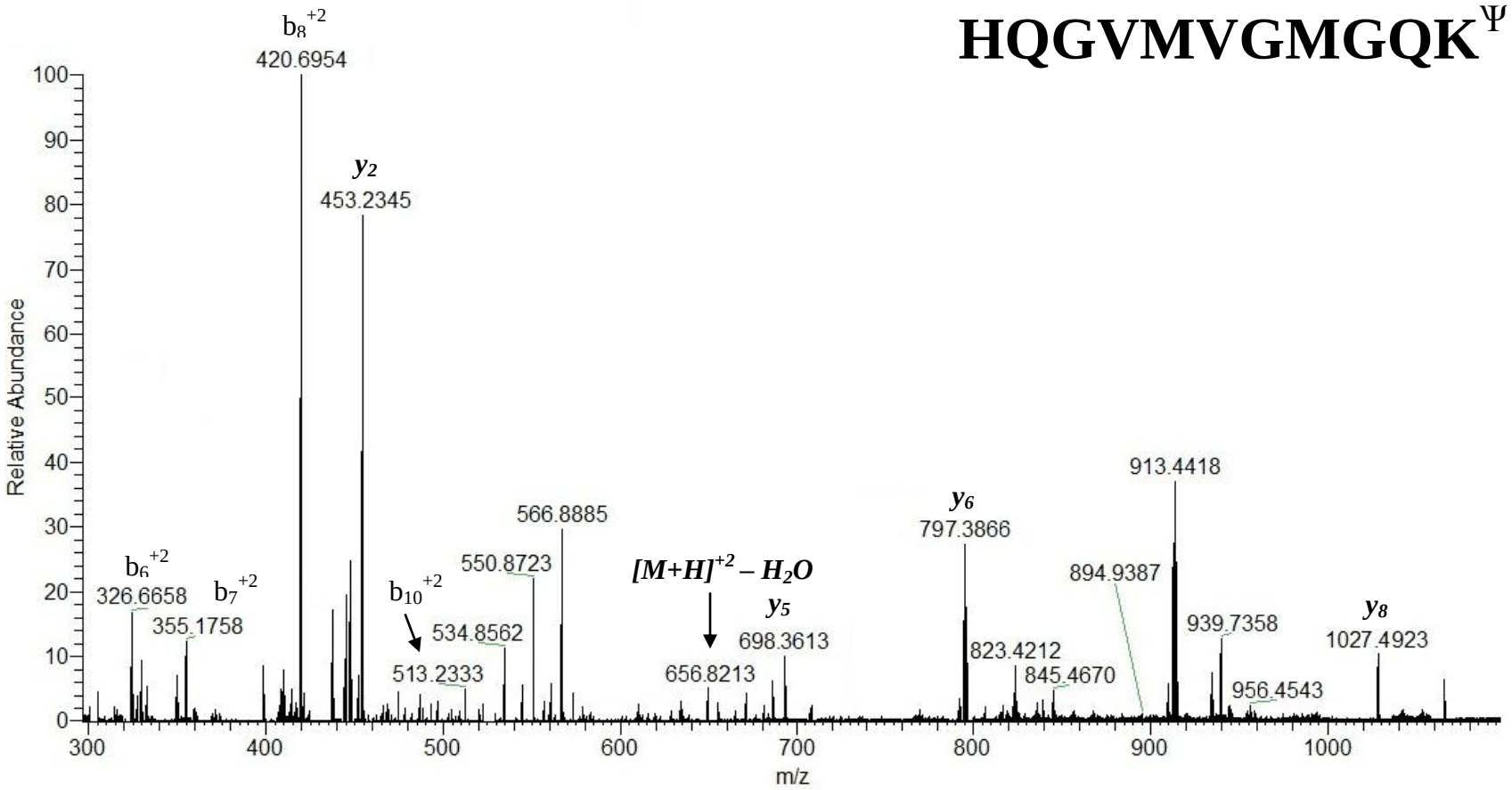
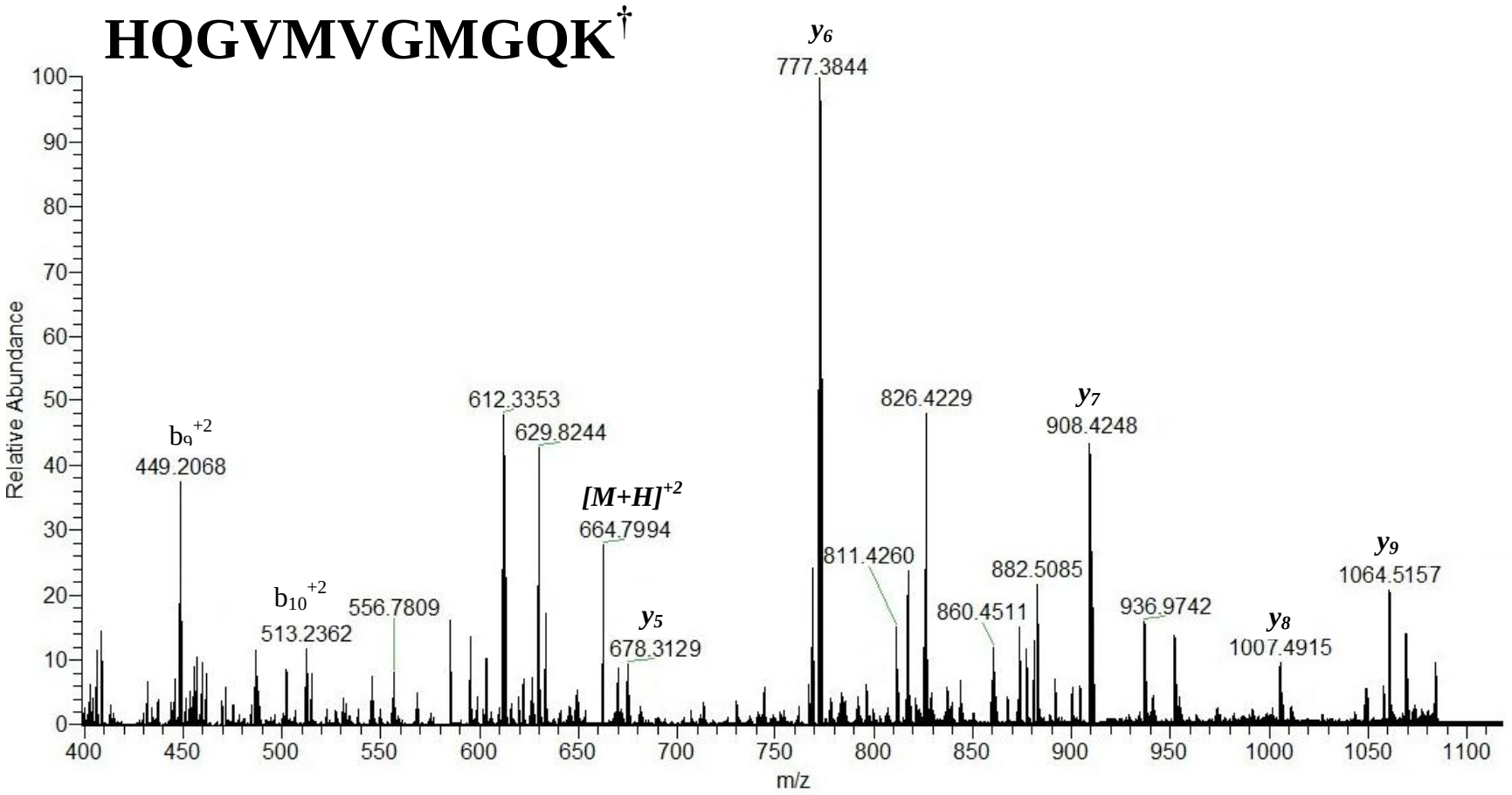


Figure S5: MS/MS of adducted actin peptide **[HQGVMVGMGQK + 1,2NPQ]** at *m/z* 664.7988 (doubly charged).



.

Figure S6: MS/MS of adducted actin peptide **[HQGVMVGMGQK + 1,4NPQ]** at *m/z* 664.7988 (doubly charged).

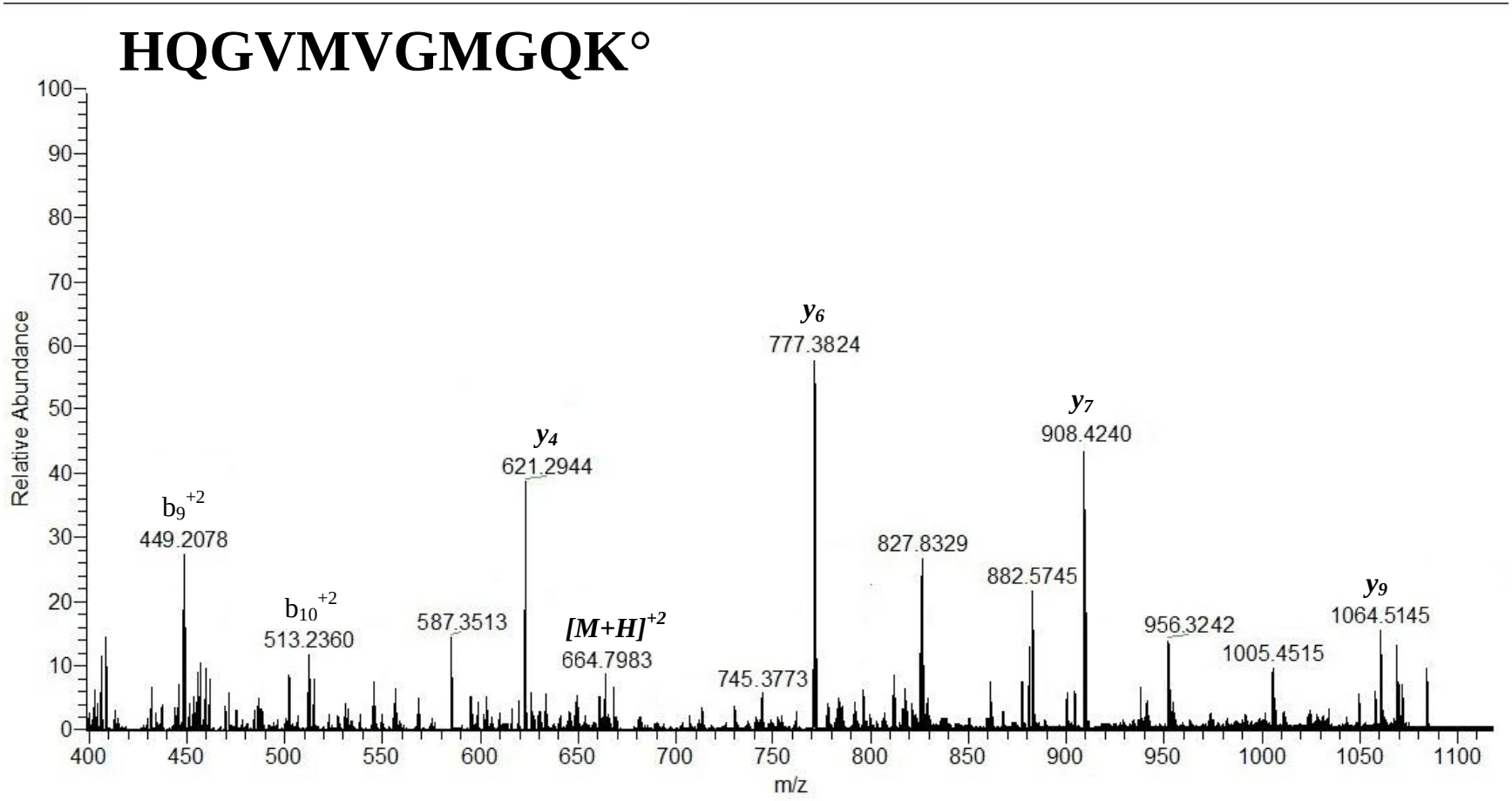
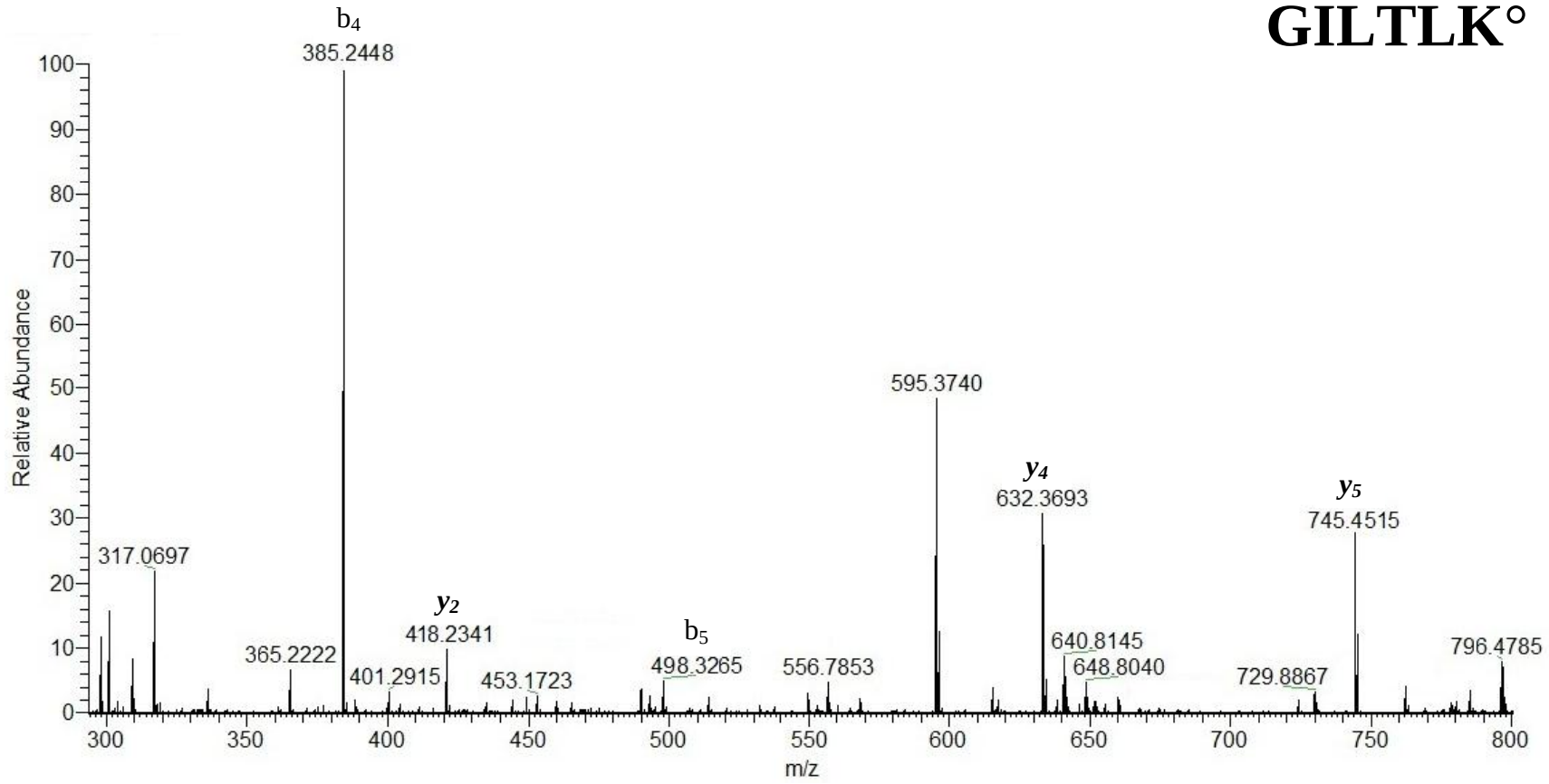


Figure S7: MS/MS of adducted actin peptide **[GILTLK + 1,4NPQ]** at *m/z* 802.4601.



.

Figure S8: MS/MS of adducted actin peptide **[IWHHTFYNELR + 1,2NPQ]** at *m/z* 836.8874 (doubly charged).

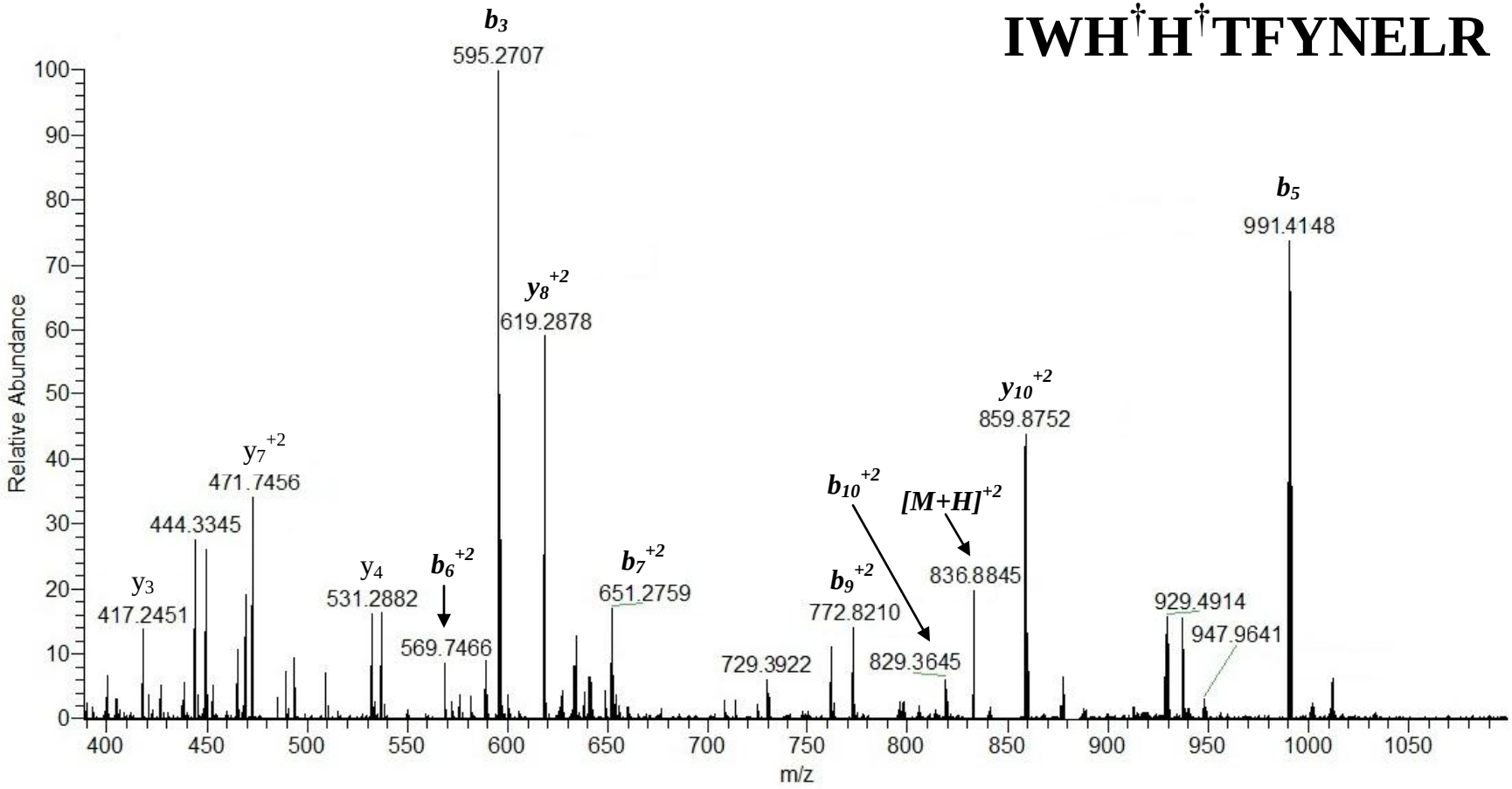


Figure S9: MS/MS of adducted actin peptide **[VAPEEHPVLLTEAPLNPK + NDO]** at *m/z* 1066.0590 (doubly charged).

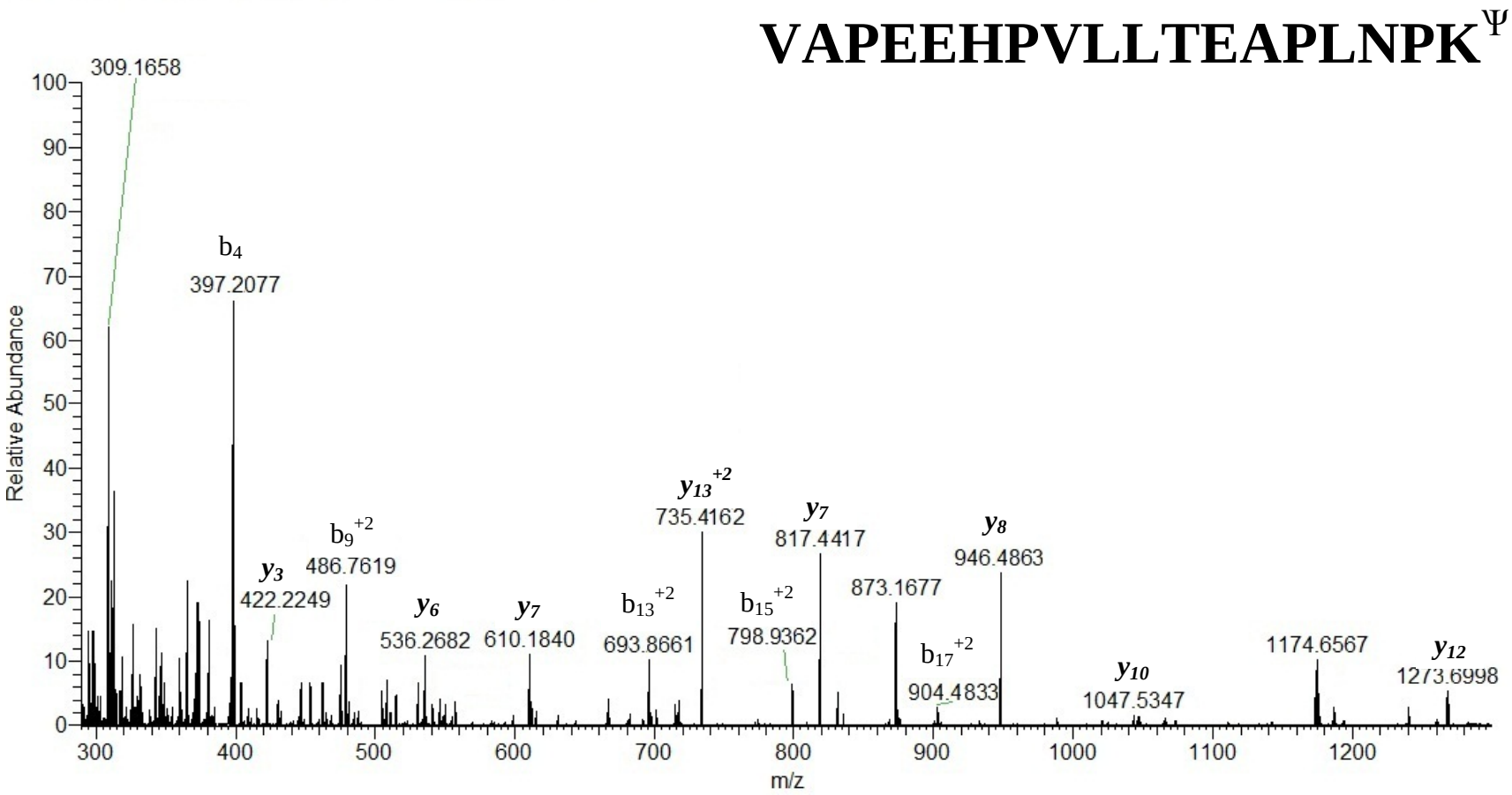


Figure S10: MS/MS of adducted actin peptide **[DLTDYLMKILTER + NPO]** at *m/z* 996.5738 (doubly charged).

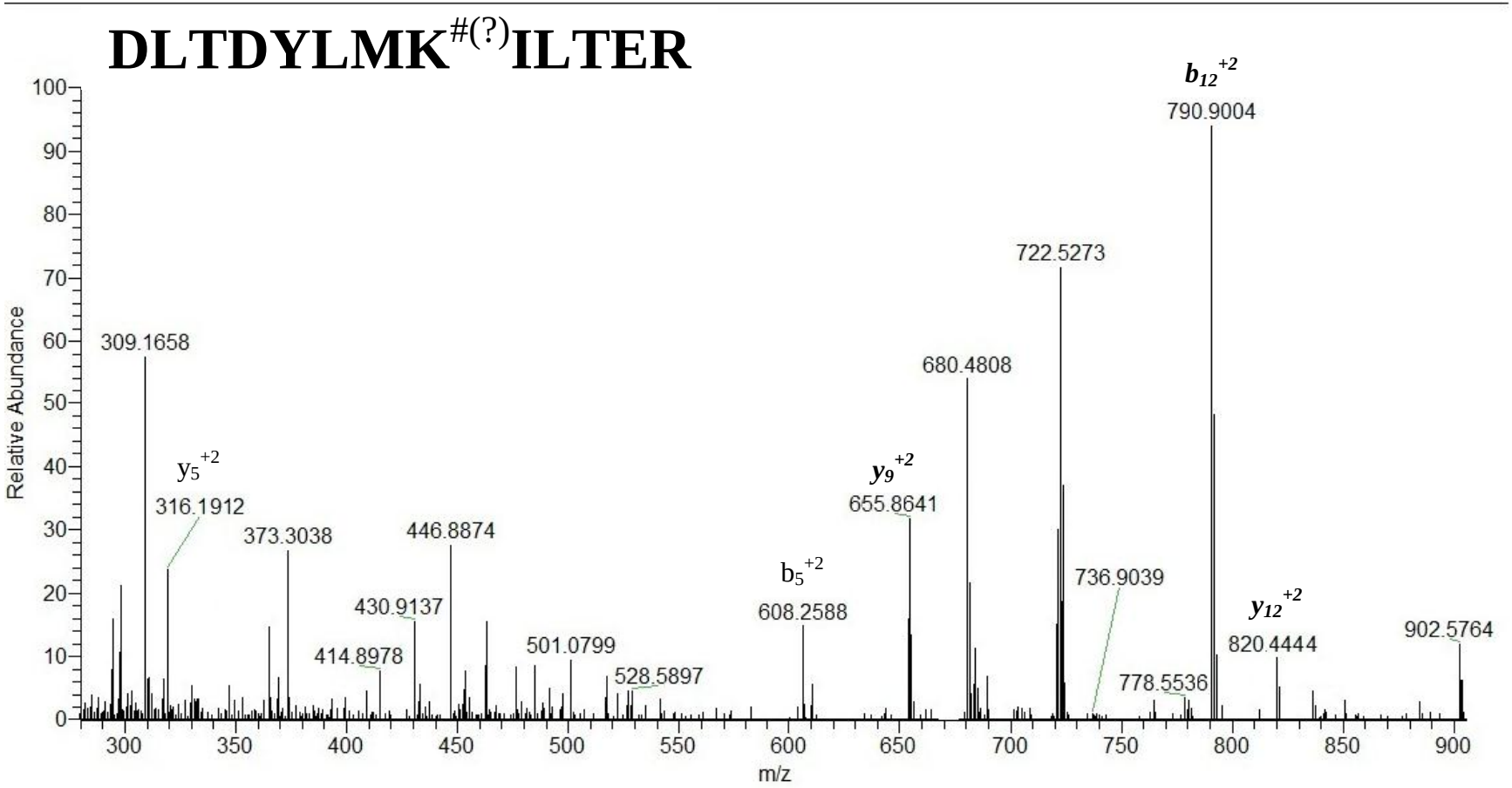


Figure S11: MS/MS of adducted actin peptide **[DIKEK + 1,4NPQ]** at *m/z* 790.3892.

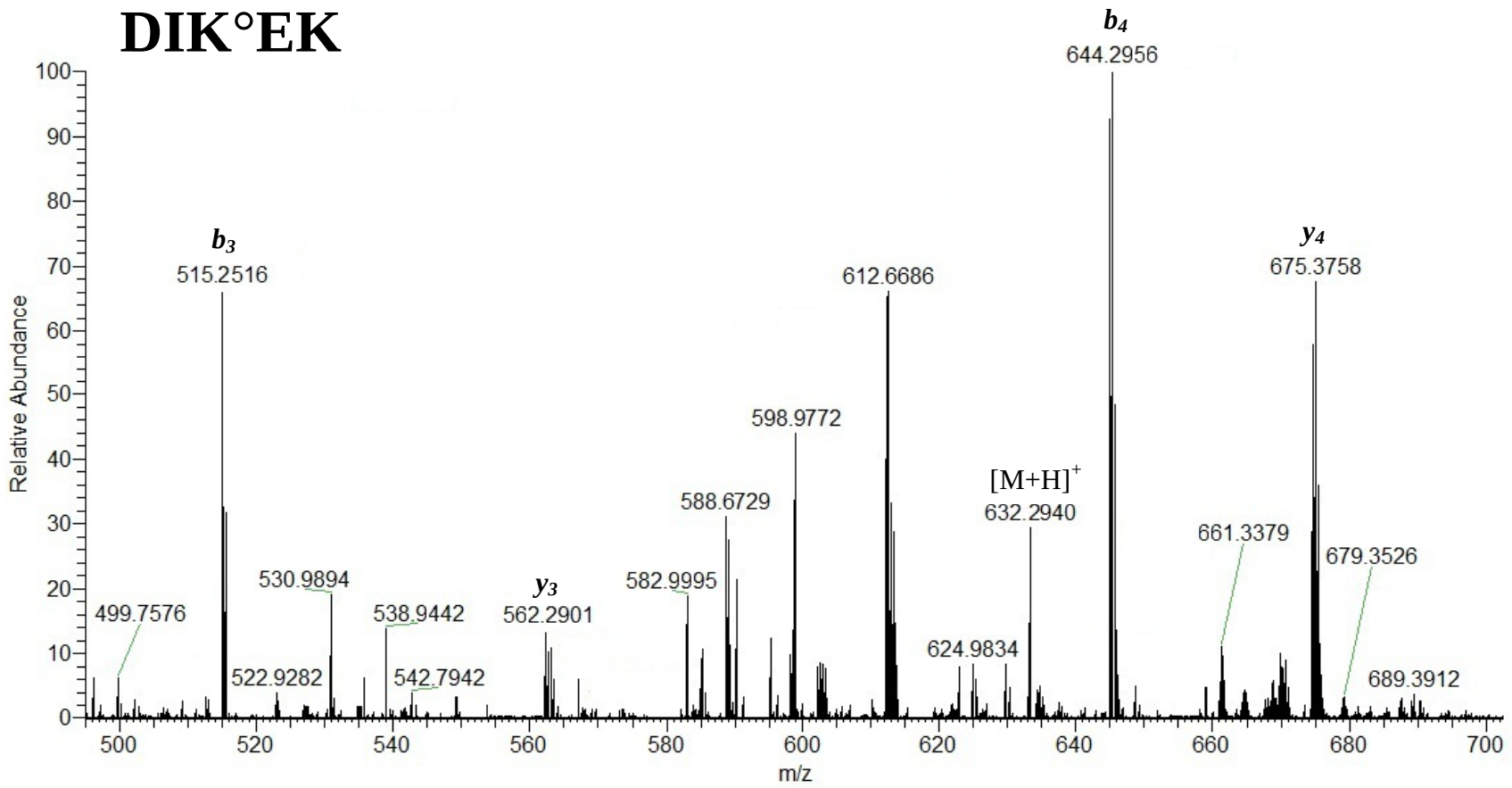


Figure S12: MS/MS of adducted actin peptide **[CPEALFQPSFLGMESCGIHETTFNSIMK + 1,2NPQ]** at *m/z* 1091.8143 (triply charged).

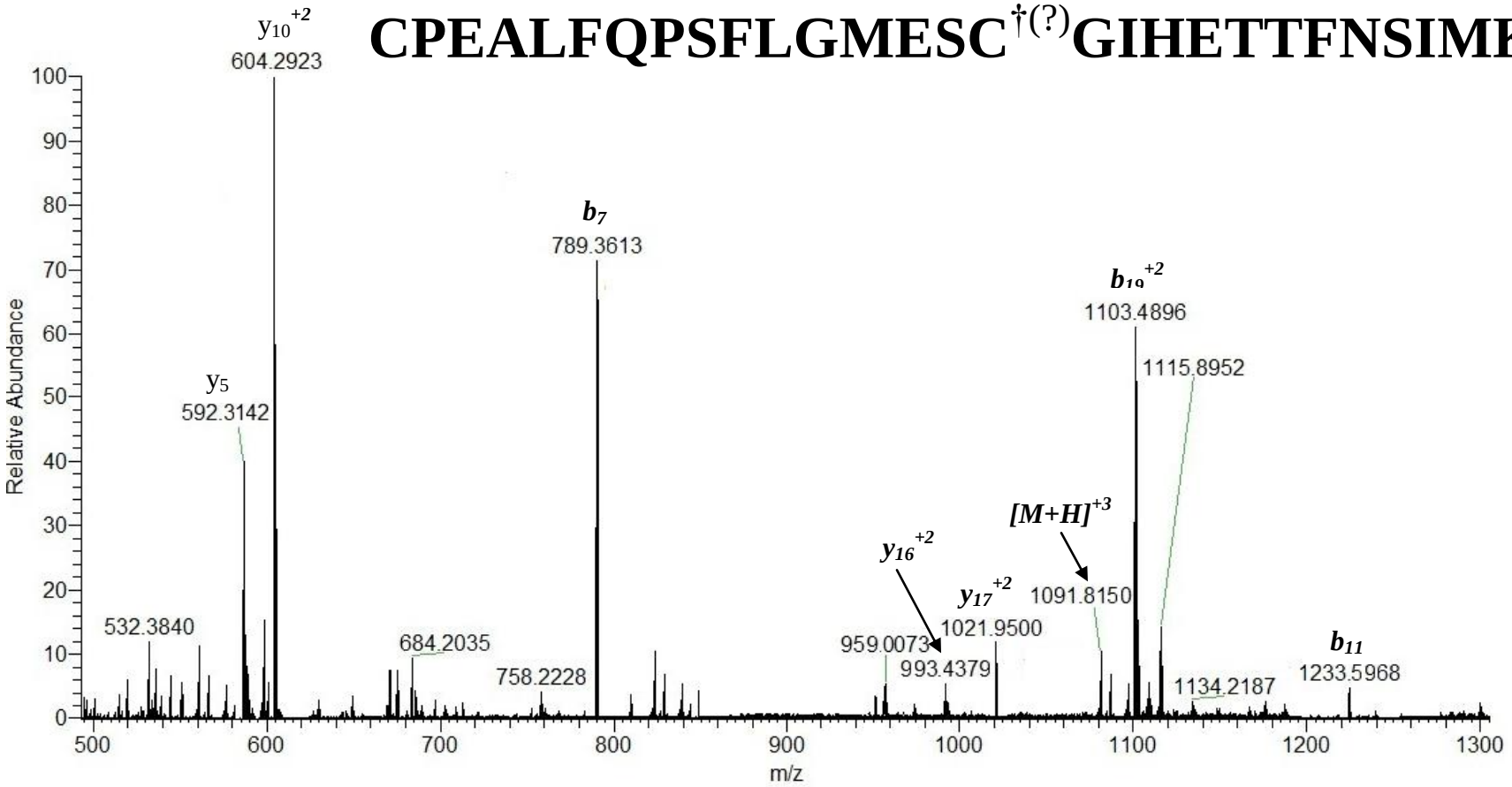


Figure S13: MS/MS of adducted actin peptide **[IKIIAPPER + NPO]** at *m/z* 590.3488 (doubly charged).

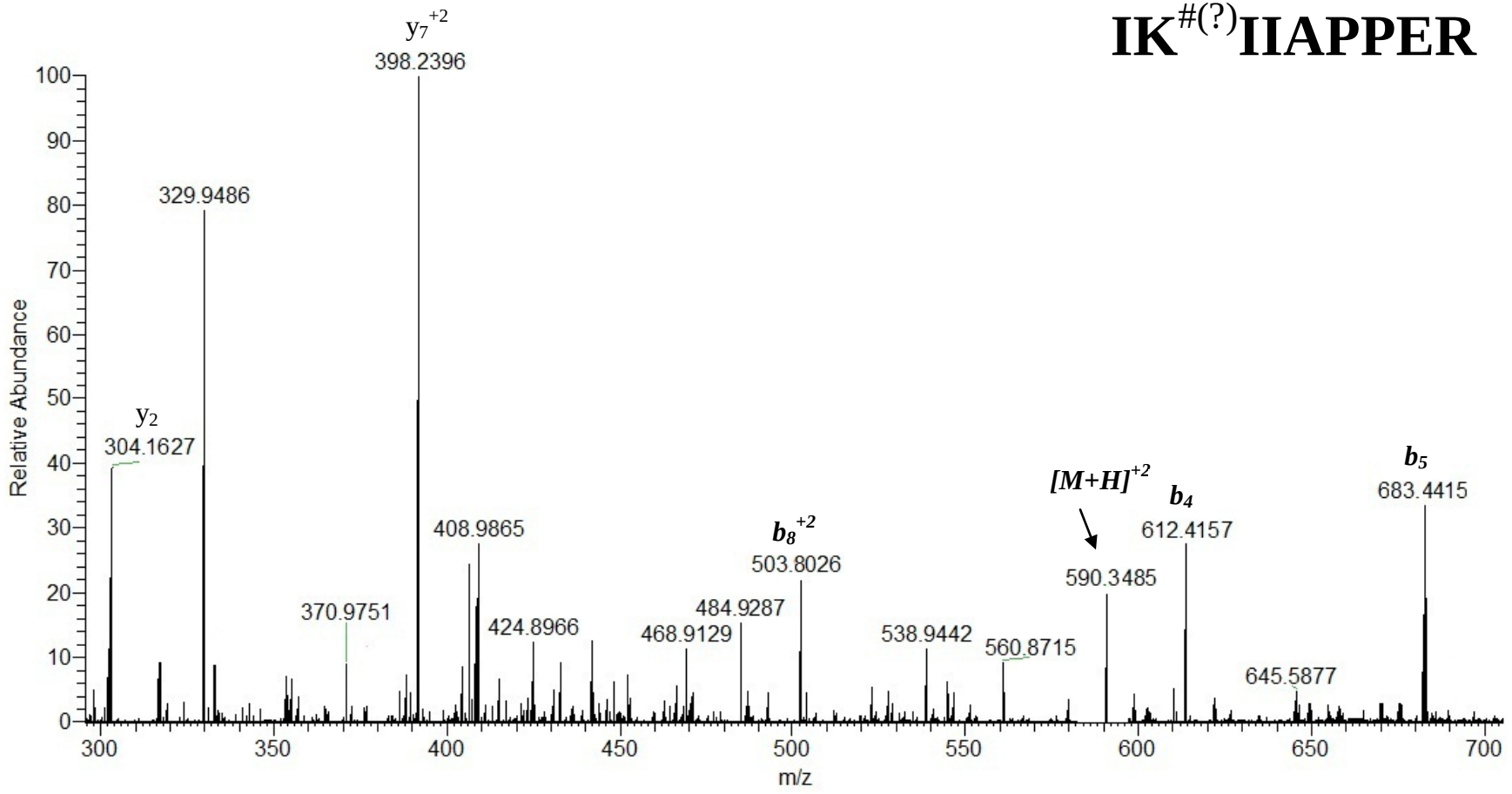


Figure S14: MS/MS of adducted PDI peptide **[MLSRALLCLALAWAAR + NPO]** at *m/z* 951.5223 (doubly charged).

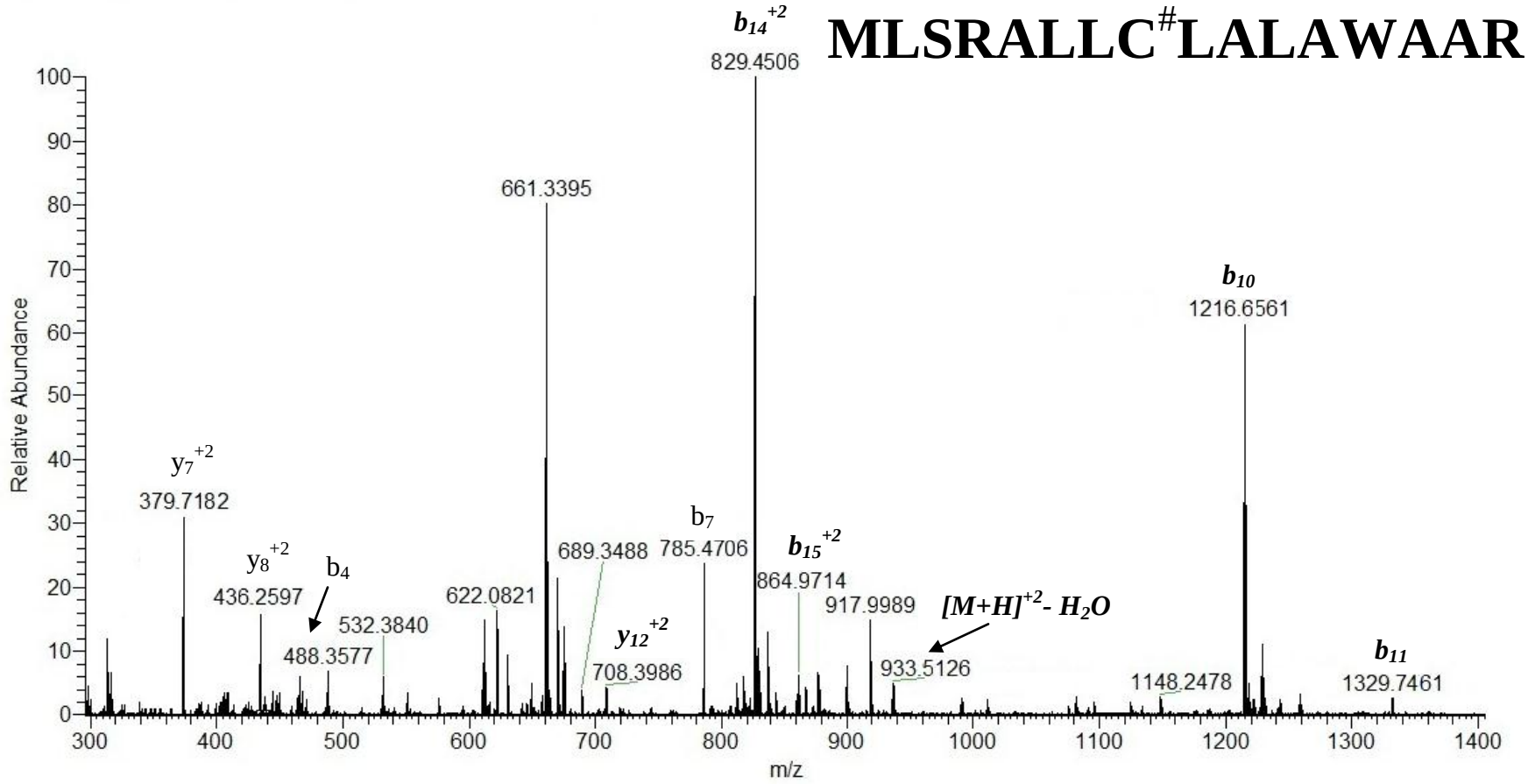


Figure S15: MS/MS of adducted PDI peptide **[YLLVEFYAPWCGHCK + NDO]** at *m/z* 1003.9616 (doubly charged).

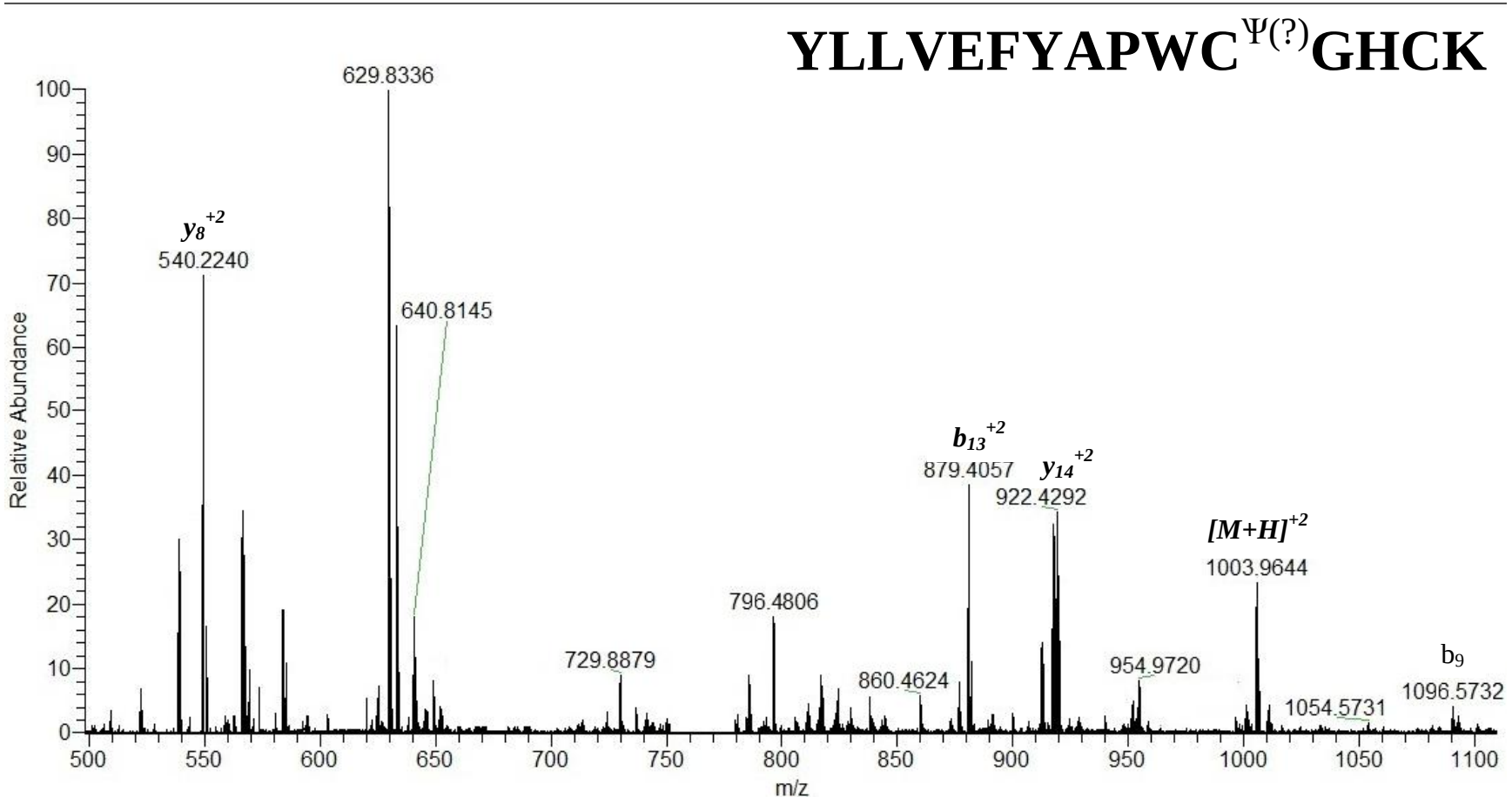


Figure S16: MS/MS of adducted PDI peptide **[EADDIVNWLK + 1,2NPQ]** at *m/z* 1360.6425.

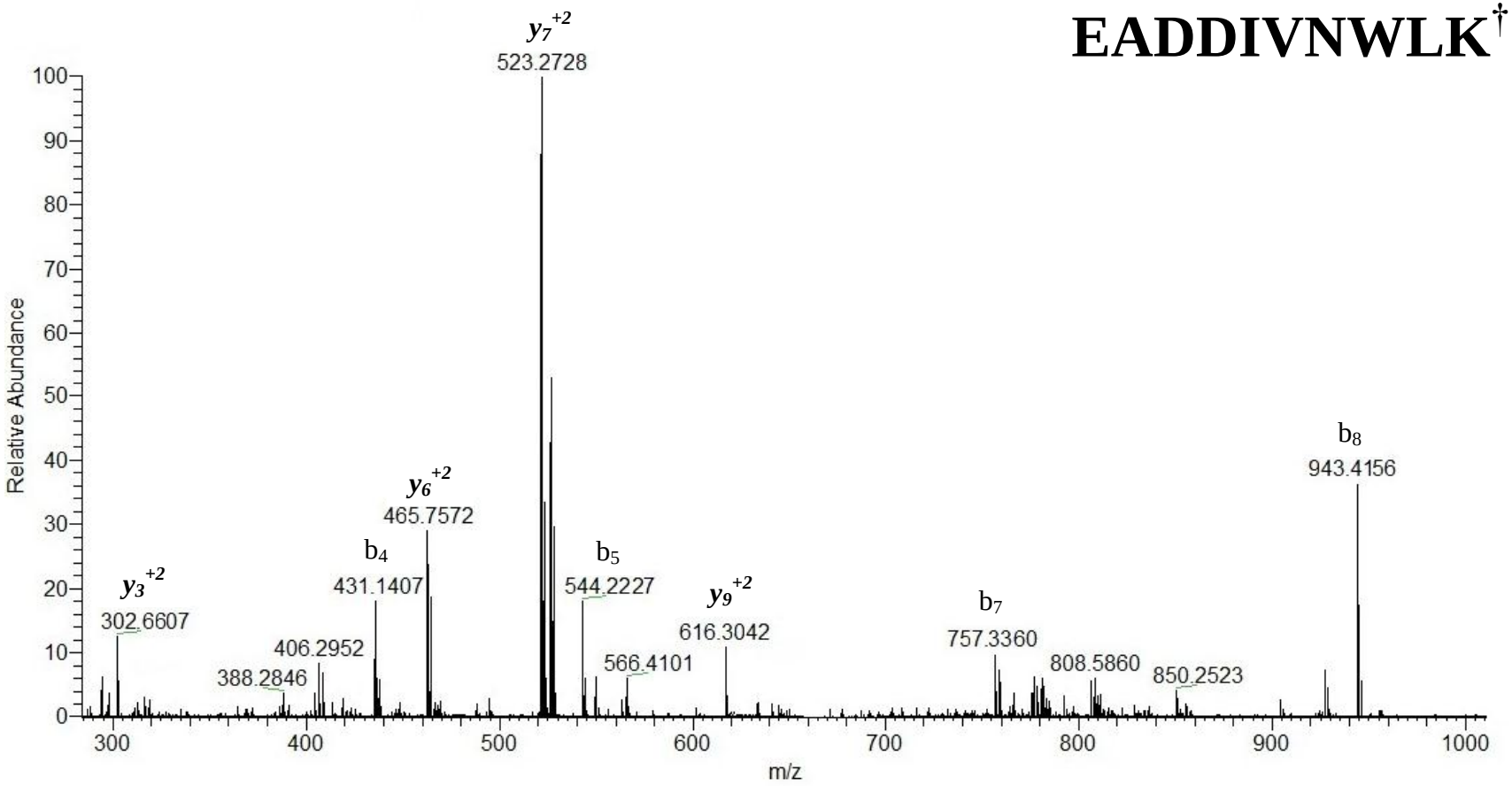


Figure S17: MS/MS of adducted PDI peptide **[TGPAATTLSDTAAAESLVDSSEVTVIGFFK + NDO]** at *m/z* 1581.7780 (doubly charged).

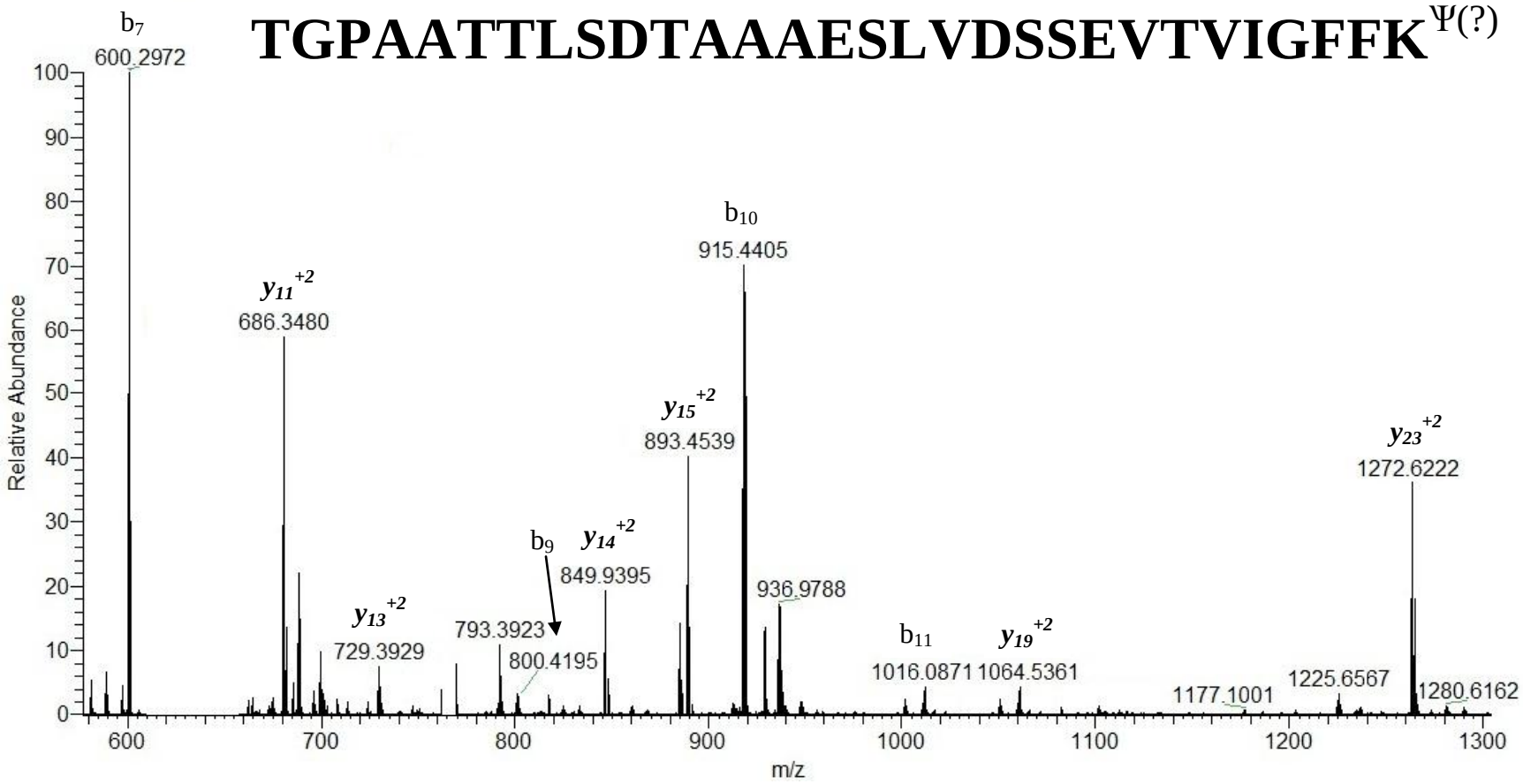


Figure S18: MS/MS of adducted PDI peptide **[TGPAATTLSDTAAAESLVDSSEVTVIGFFK + 1,2NPQ]** at *m/z* 1571.7659 (doubly charged).

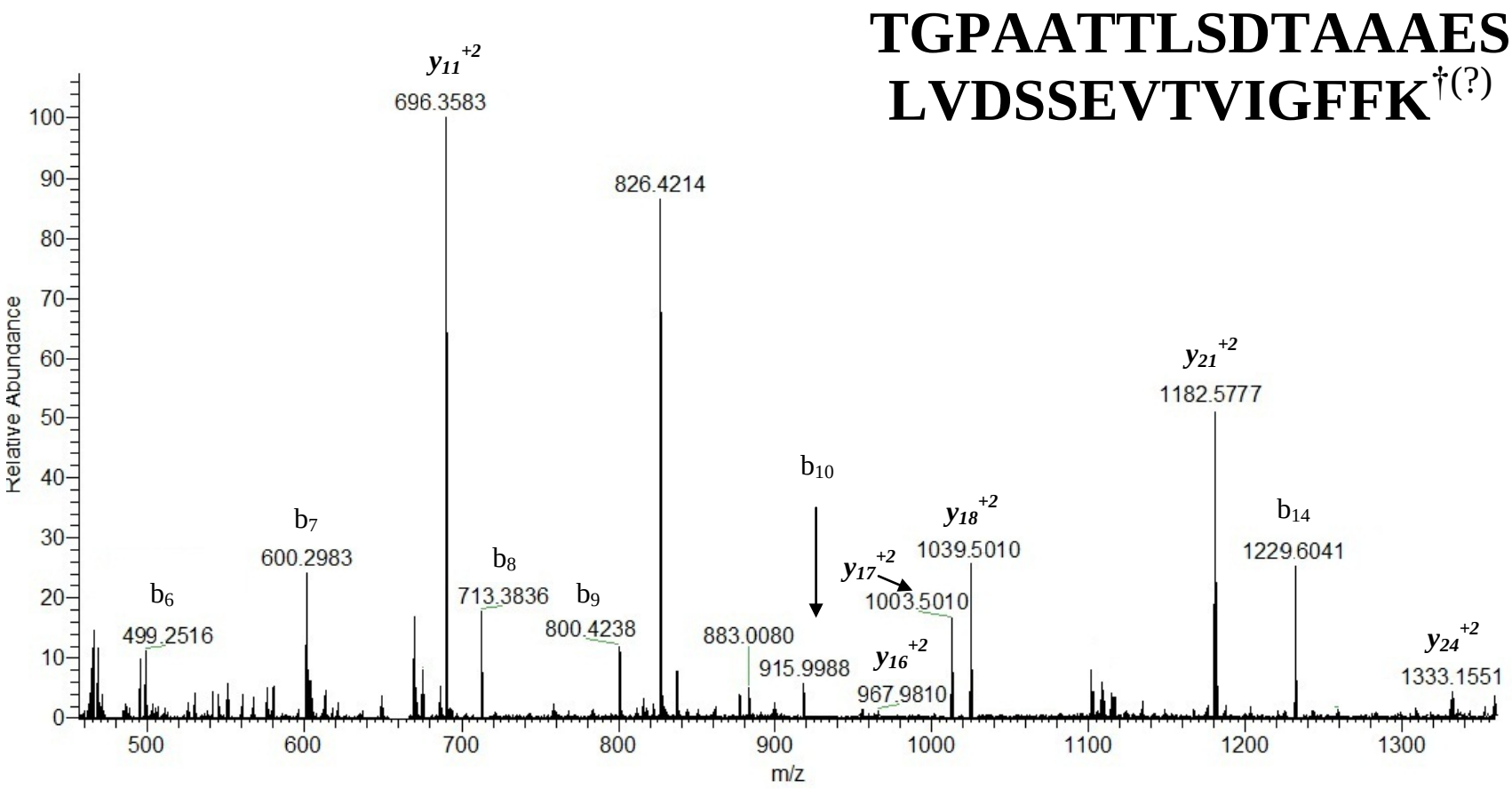


Figure S19: MS/MS of adducted PDI peptide **[DVESDSAK + NPO]** at *m/z* 994.4379.

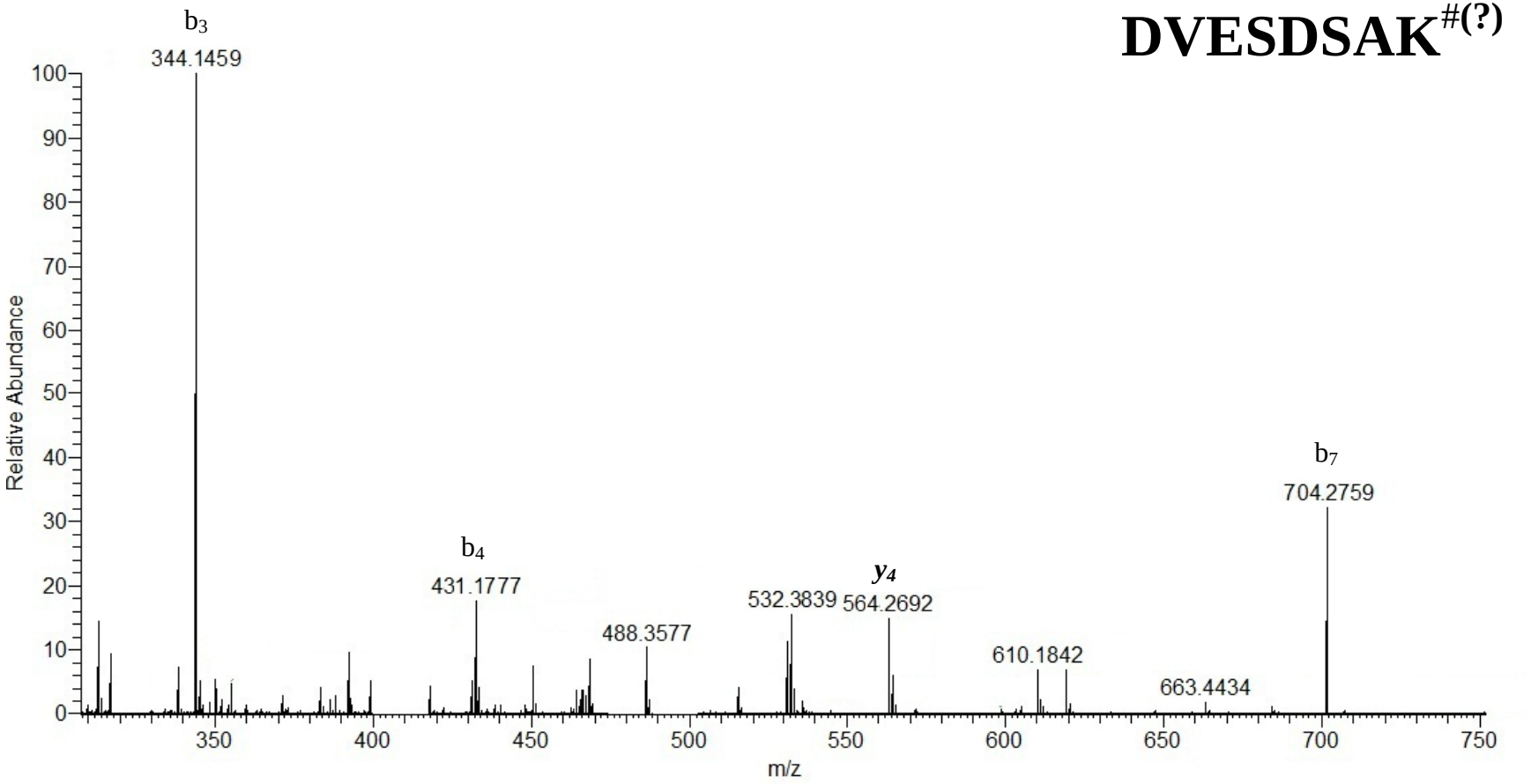


Figure S20: MS/MS of adducted PDI peptide **[THILLFLPK + NDO]** at *m/z* 1259.7401.

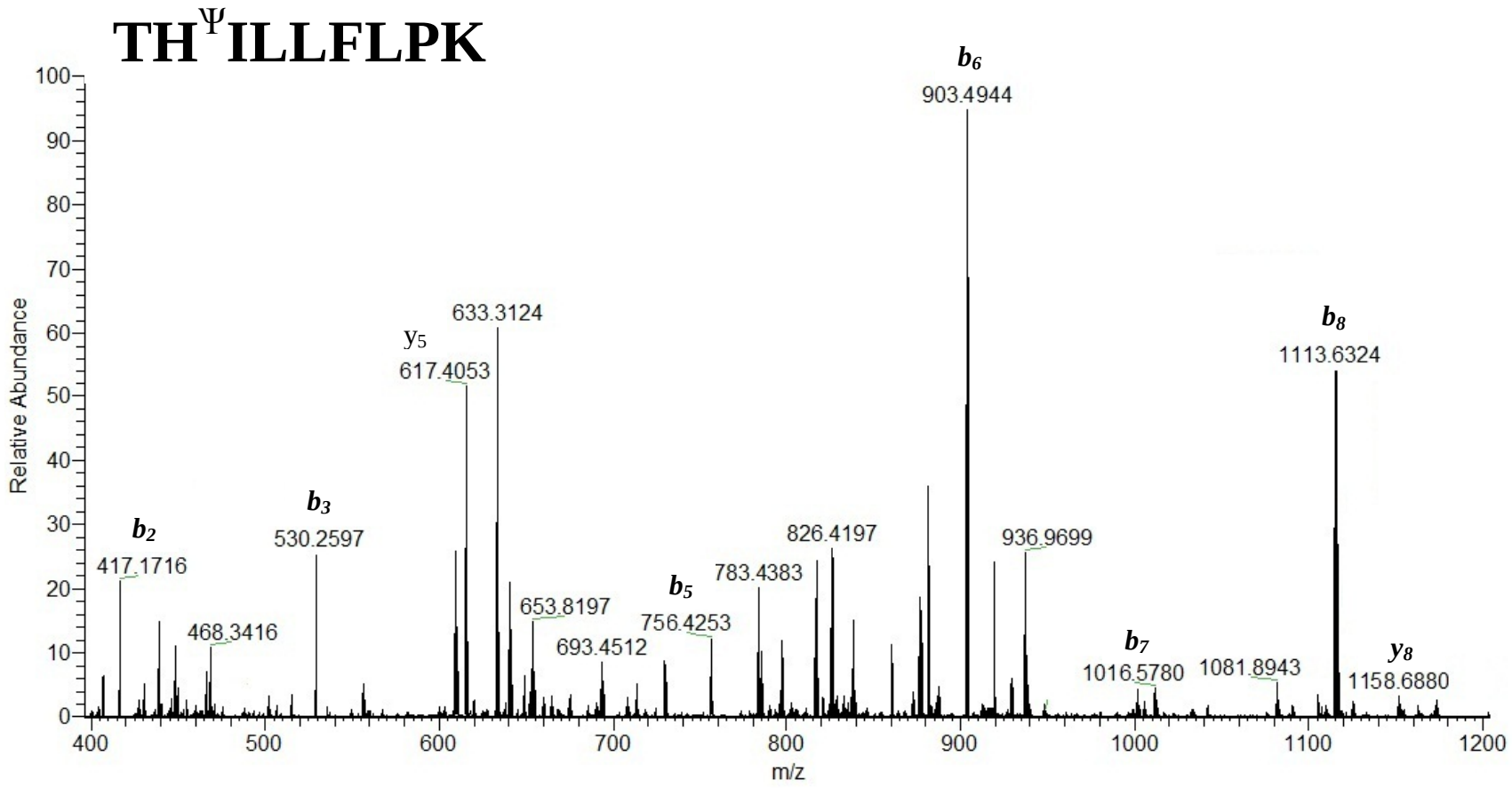


Figure S21: MS/MS of adducted PDI peptide **[THILLFLPK + 1,2NPQ]** at *m/z* 1397.7574.

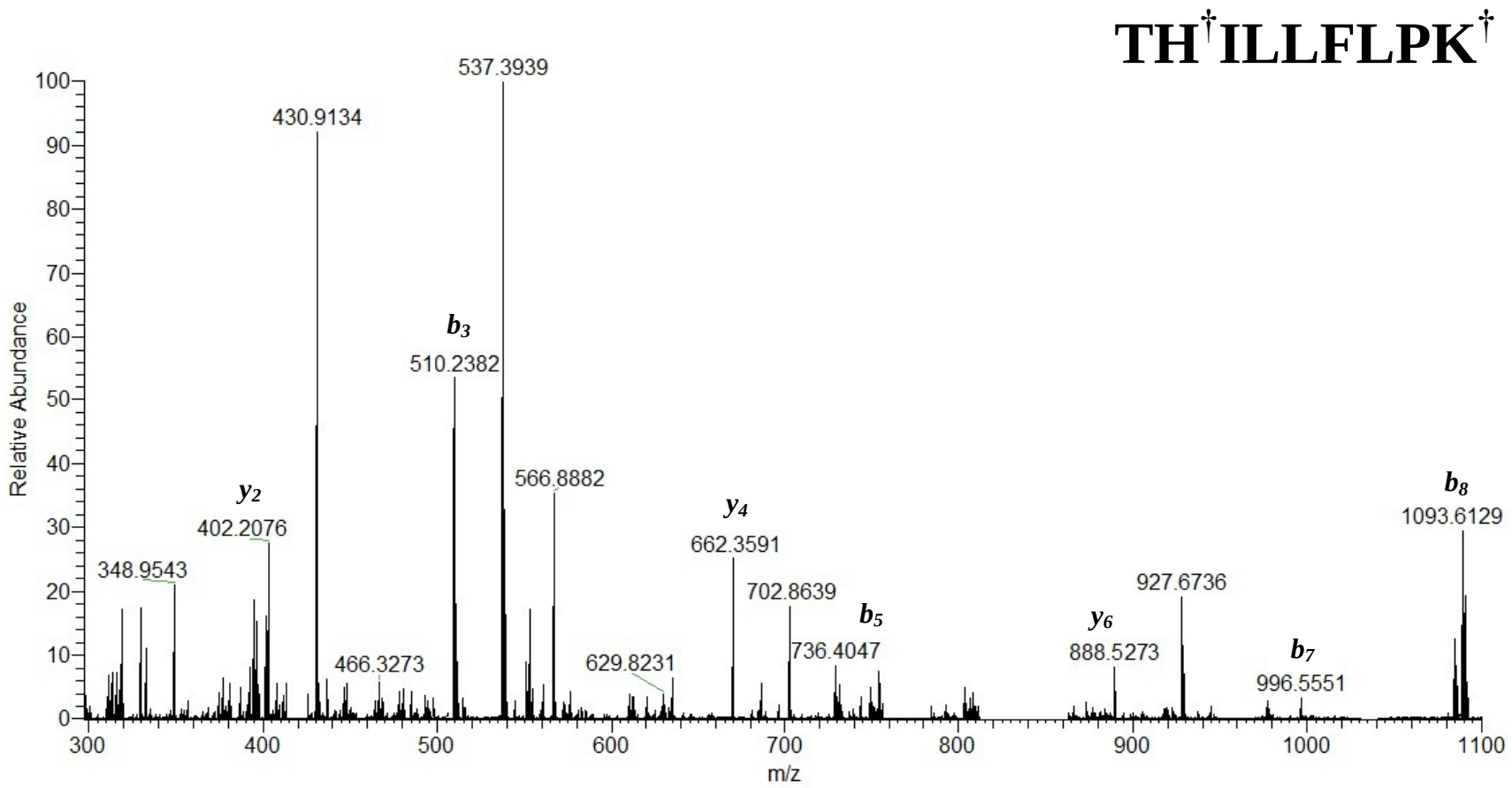


Figure S22: MS/MS of adducted PDI peptide **[AAEGFK + 1,4NPQ]** at *m/z* 780.3569.

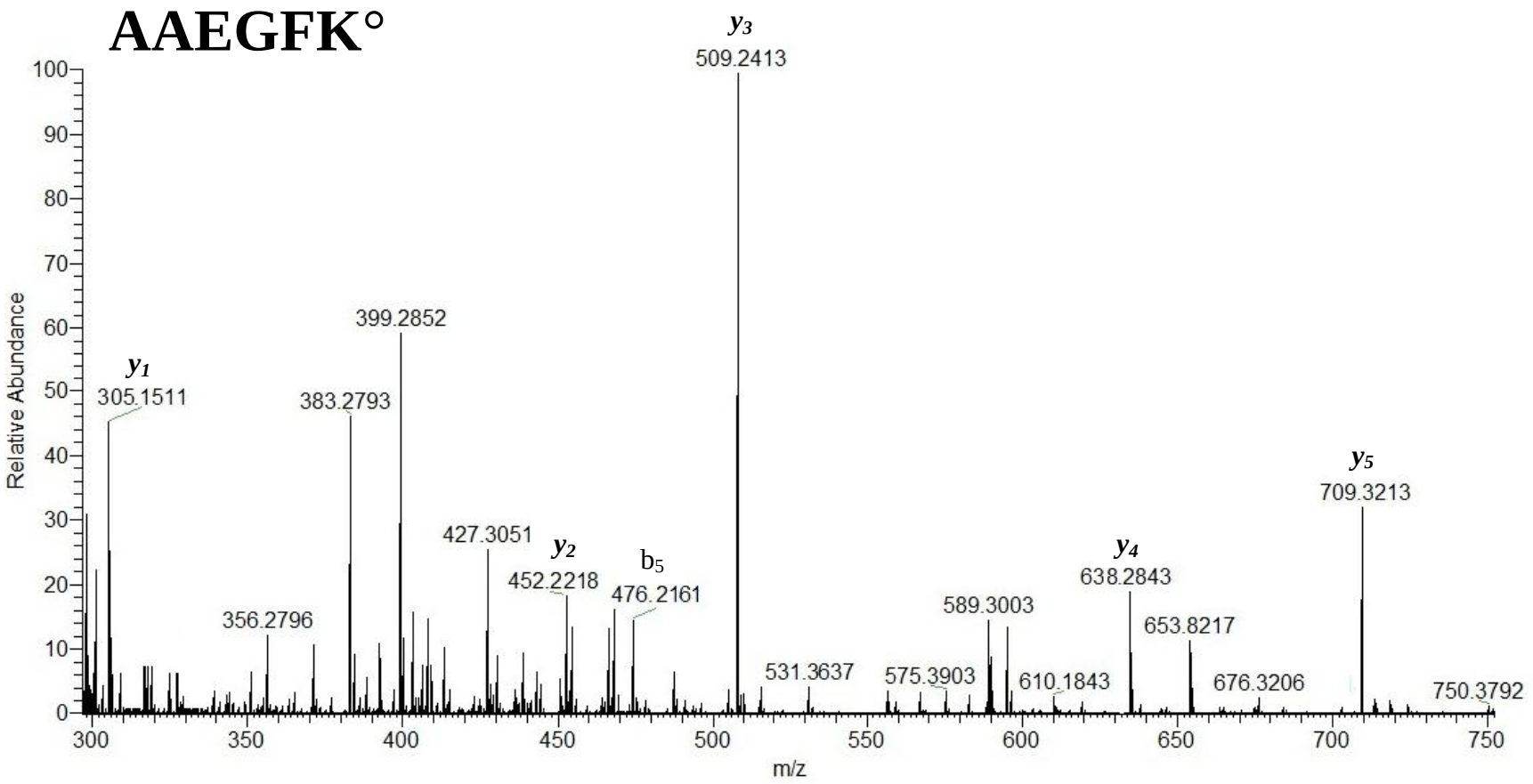


Figure S23: MS/MS of adducted PDI peptide **[ITEFCHR + 1,2NPQ]** at *m/z* 1063.4670.

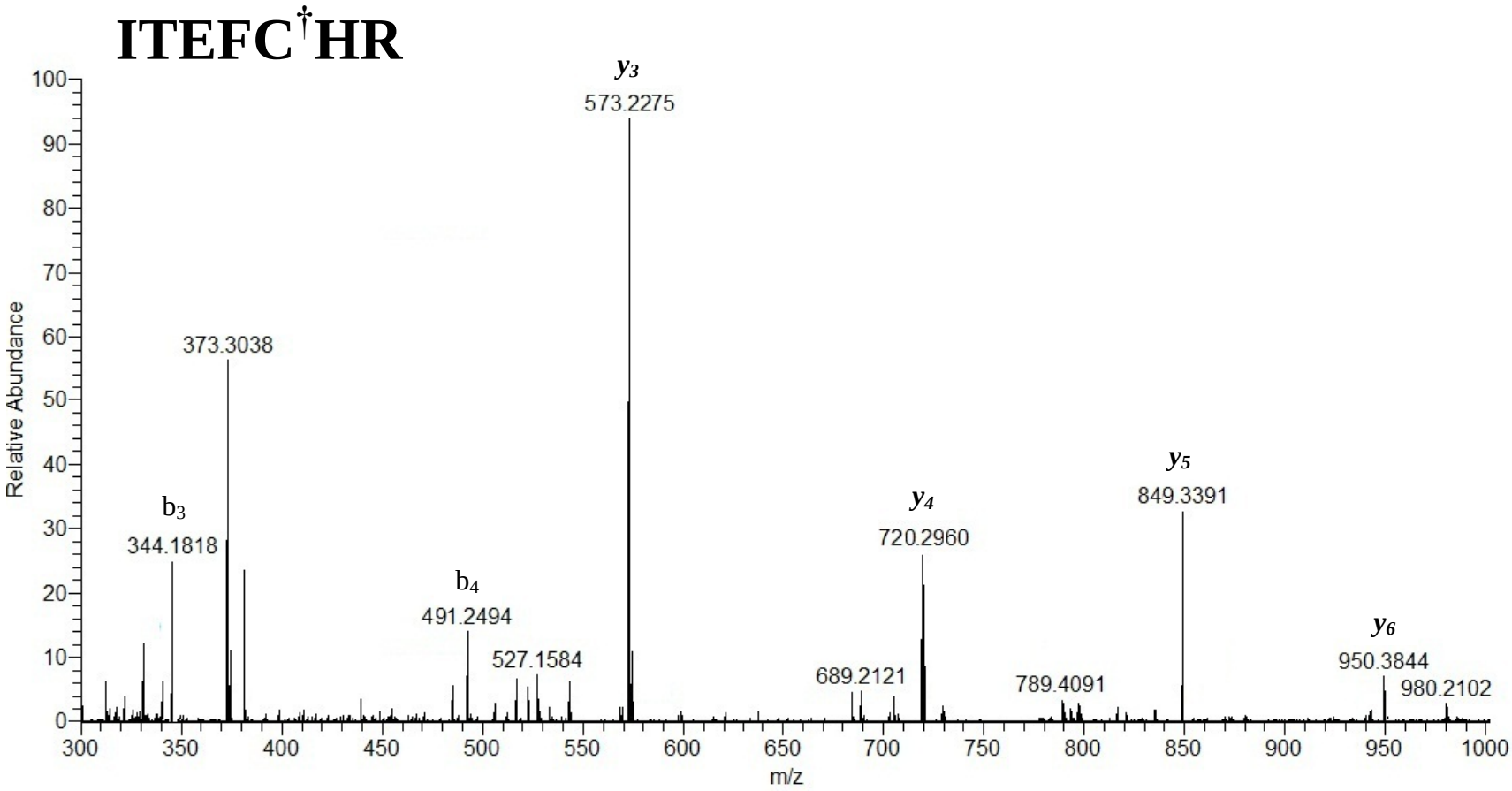


Figure S24: MS/MS of adducted PDI peptide **[ITEFCHR + 1,4NPQ]** at *m/z* 1063.4661.