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Relationship between quality of spectra and peptide-spectrum matches

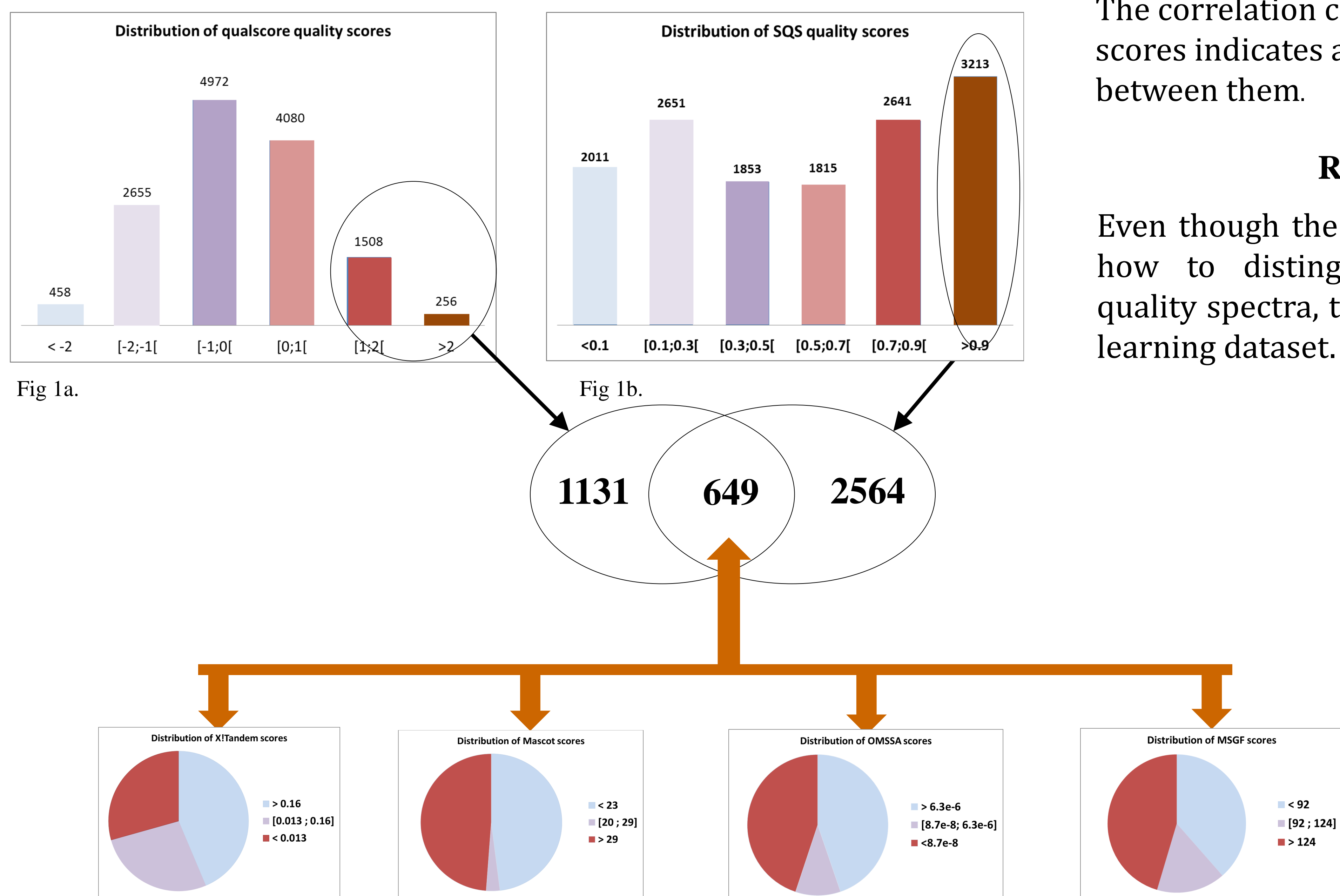
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Context

It is thought intuitively that good quality MS/MS data give rise to confident peptide-spectrum matches if the corresponding peptides are in the database. If it is true, a high quality spectrum that remains unidentified by a search engine will be a good candidate for more intensive search strategies. On the other hand, when only a few observed peptides suggest the presence of a protein, does it need more verification if the quality of spectra is low?

We evaluated the quality of a set of 13952 MS/MS spectra obtained from *Brachypodium distachion* with 2 scores: one was calculated by Qualscore (Nesvizhskii et al, 2006) and the other was the Sequence Quality Score (SQS) given by PepNovo+ (Frank, 2009). In a second step, the 13952 spectra were tentatively interpreted with X!Tandem, MSGF, Mascot, OMSSA and PepNovo.



The correlation coefficient of the 2 quality scores indicates a very weak relationship between them.

$$R = 0.18$$

Even though the 2 methods try to learn how to distinguish high from poor quality spectra, they do not agree on the learning dataset.

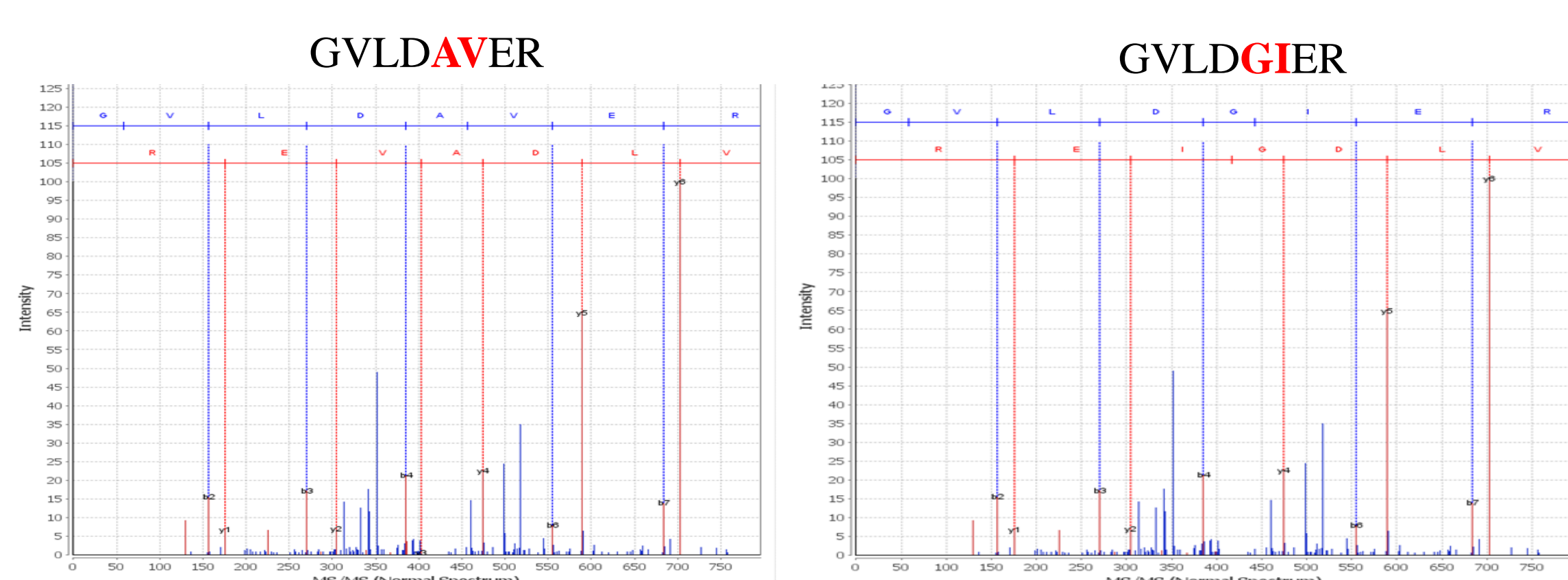


Fig 3. A good quality spectrum - Qualscore=3.4; SQS=0.936 - interpreted as 2 confident peptides by Mascot (35.09) and non-confident peptides by OMSSA (7.5E-5 and 1.1E-4), MSGF (89) and X!Tandem (4.1). PepNovo suggests these 2 interpretations with high confidence.

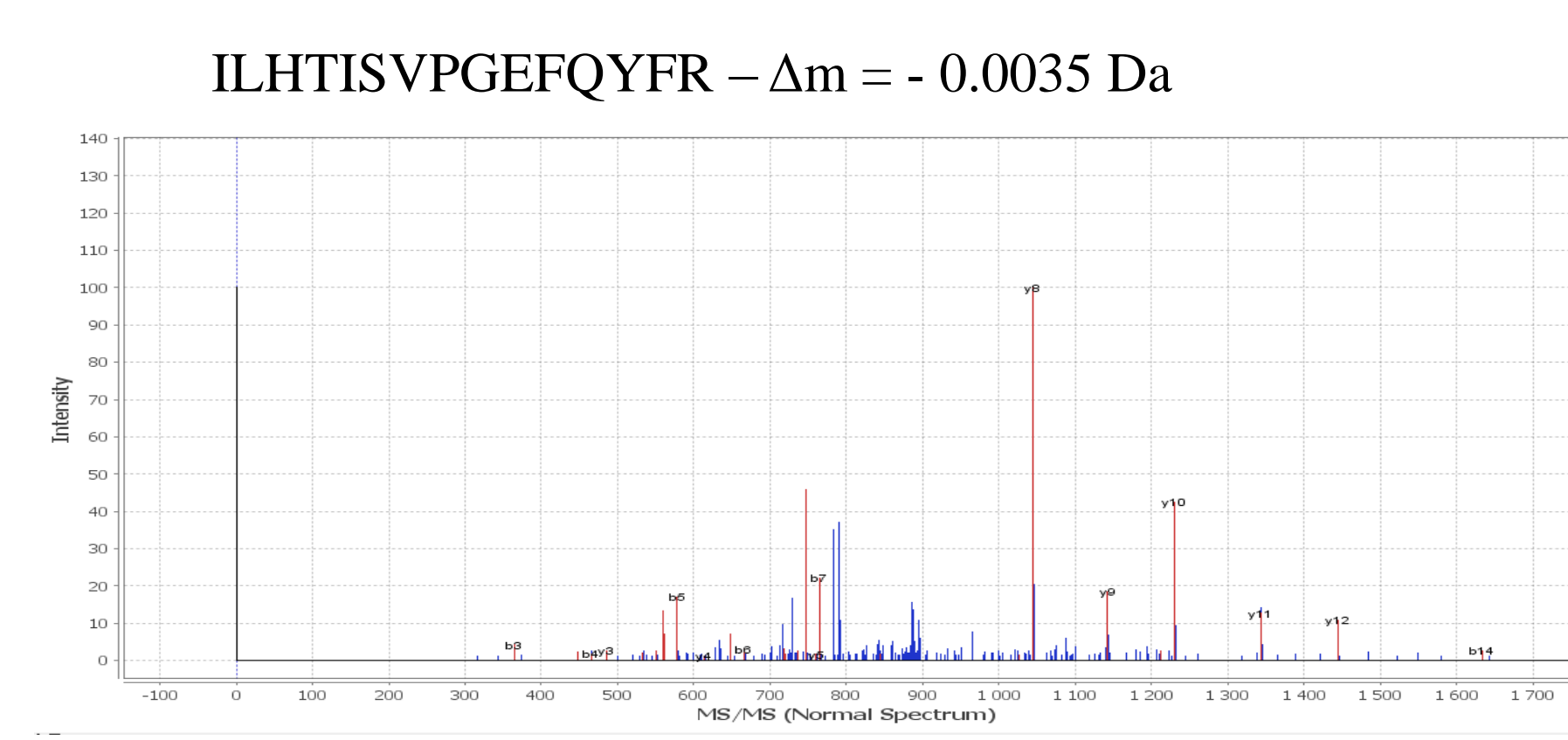


Fig 4. A good quality spectra according to qualscore (1.07) and a very poor quality spectrum according to SQS (0.03). This spectrum is interpreted confidently by X!Tandem (0.0068) whereas Mascot (22.6); OMSSA (2.2E-5); and MSGF (87) suggest the same interpretation with a low score.

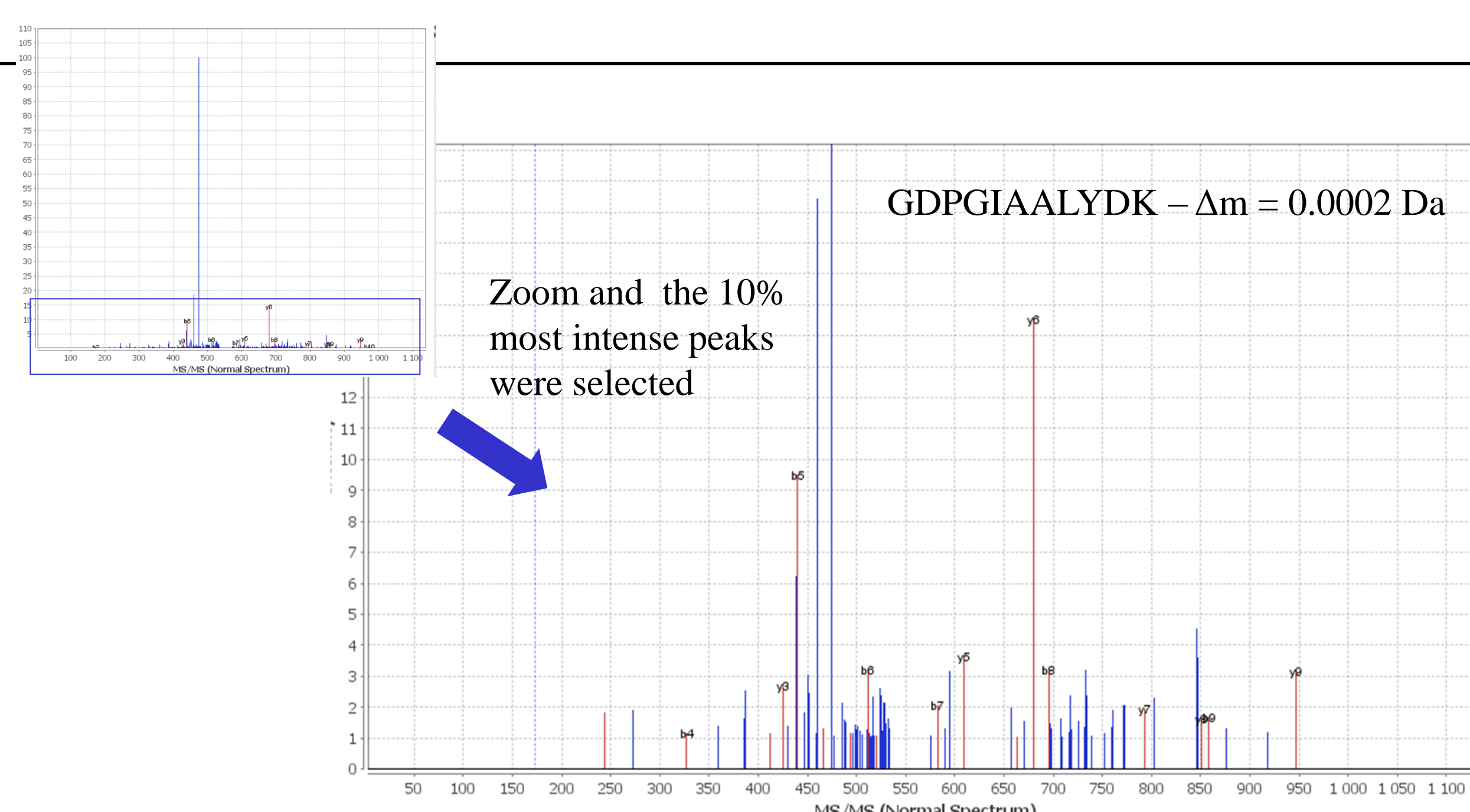


Fig 5. A high quality spectrum according to SQS- (0.991) and a poor quality spectra according to qualscore (-1.13) - interpreted as a confident peptide by Mascot (49.9) and a non-confident peptide by OMSSA (1.7E-6), MSGF (44) and X!Tandem (0.55). PepNovo suggests this interpretation with a low confidence (3.1)

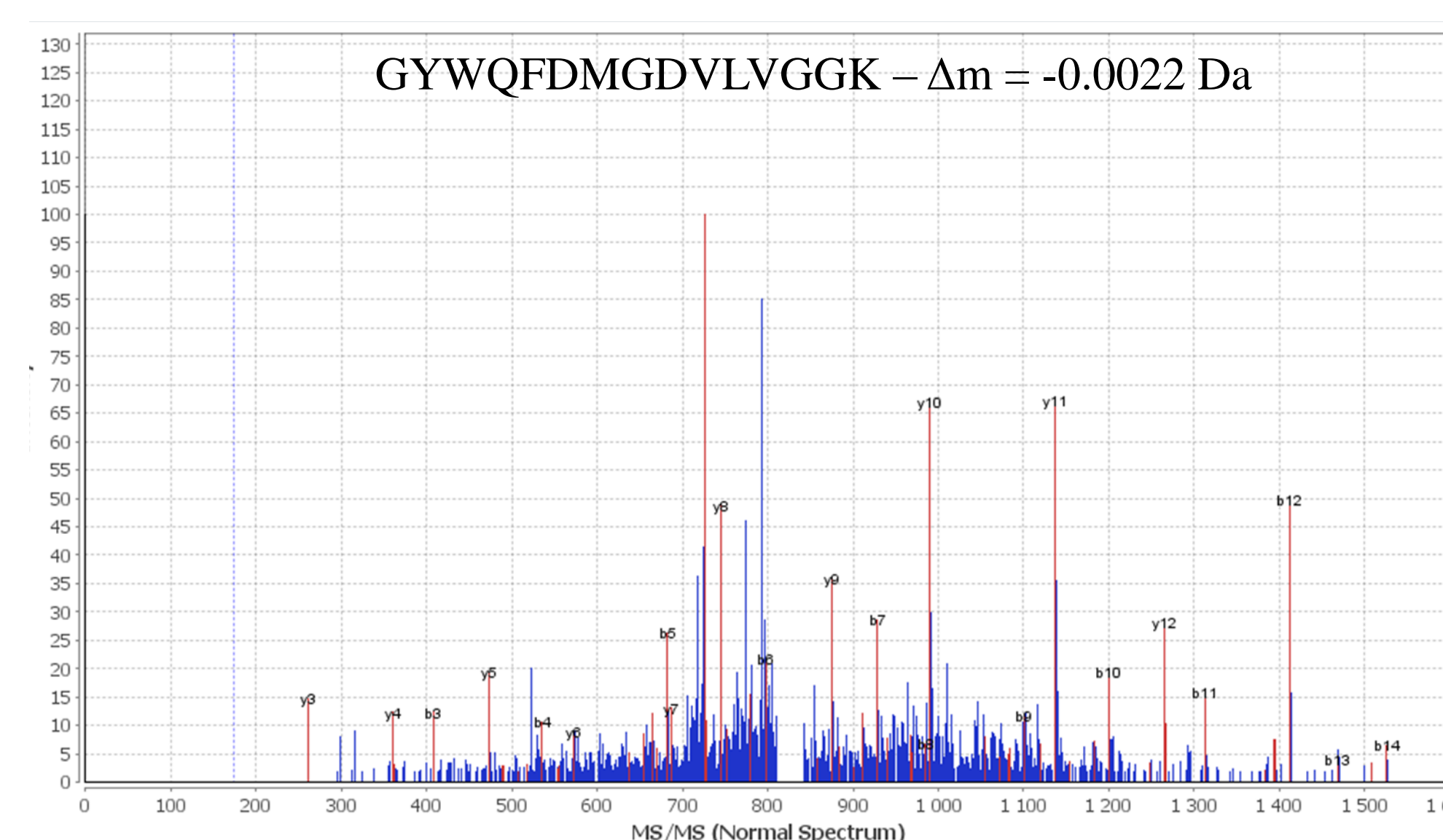


Fig 6. A poor quality spectrum according to SQS - 0.09- and qualscore (-1.13) - and interpreted as a confident peptide by all the software : Mascot (40.7), OMSSA (9.6E-12), MSGF (115) and X!Tandem (0.0017). PepNovo is not able to interpret this spectrum.

Conclusion : The spectral quality score could become an additional score in the process of peptide assignment validation. Nevertheless, it is not easy to define what a spectrum of high quality is.