Methods: **Precursor Isotopic eNvelope Quality** score

- The PINQ score is computed as the best Chi-squared fit of observed m/z and intensities of isotopic peaks to those predicted by theory.
- Data are extracted from pepXML and mzML files.

![PINQ scores](image)

**Methods: PINQ-1 (isolation) score**

- Computed by adding the peak intensities of all isotopic peaks within the selection window, and dividing by the total signal in the window.
- The intensity used is the lower of:
  - observed signal
  - intensity attributable via PINQ fit

PINQ scores are written back to the source pepXML file.

### Results (examples)

- **PINQ** = 3.52
- **PINQ-1** = 0.61
- **Prob** = 0.15

Very good isotopic pattern fit, but low probability and marginal isolation score suggest co-fragmentation of another ion.

- **PINQ** = 2.44
- **PINQ-1** = 0.92
- **Prob** = 0.00

Excellent isotopic pattern fit and isolation score. Poor probability suggests this is a real peptide that was not in the search database—perhaps a variant, contaminant, or from another organism.

- **PINQ** = 98.0
- **PINQ-1** = 0.83
- **Prob** = 0.00

Very poor isotopic pattern fit and probability, and good isolation score would indicate that the charge state might be incorrect. Quick examination via the interface suggests a charge of +2 instead of +4.

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###References

- [How Well Did You Capture that Ion? Find Out with PeptidePrisoner](https://www.tppms.org)
- [PeptidePrisoner](https://www.tppms.org)
- [Trans-Proteomic Pipeline](https://www.tppms.org)

###Future Work

- Incorporate the PINQ and PINQ-1 scores as extra discriminants for PSM validation in PeptideProphet
- Flag potentially chimeric spectra
- Consider fragment ion isotopes

###Conclusions and Availability

- The TPP is a widely used and well-validated free and open source suite of software tools that facilitates and standardizes proteomics analysis.
- These various updates will allow TPP users to analyze, validate, and visualize precursor isolation quality results from any supported search engine.
- These features will be available as of the next release of TPP, version 6.4.0, planned for Summer 2023, or in preview mode in an upcoming dev build.