

QMax - stand-alone quantification analysis application based on a Weighted Multi-band CLS Algorithm.

What does QMax do?

- Allows the user to create an SPGAS Quantification set based on pre-collected or generated standard calibrated spectra.
- Quantification analysis based on the information provided by the quantification set.
- On screen display of the quantification analysis, which includes: concentration estimation, standard error of the estimation, and residual spectra, weighted analysis and concentration analysis per band/molecule.
- Fine-tuning of the quantification set based on the quantification analysis provided on screen.
- Offers deviation correction from Beer's law based upon the provided standard calibrated spectra.
- Visual detection of unknown spectral features based on the residual spectrum
- Visual verification of the goodness of the quantification set against a sample absorption spectrum.
- Allows the incorporation of reference spectra (Spectra with spectral features that may improve the quantification analysis, but which concentration is irrelevant) into the quantification analysis.

What doesn't QMax do?

- Generation or collection of standard calibrated spectra.
- Spectral manipulation:
 - Collection
 - Correction
 - Modification
- Read other spectral file format besides Galactic spc file format
- Print reports (forthcoming)
- It does not integrate directly into software packages like Onmic or Grams
- Ideal gas pressure and temperature correction of the concentration estimation
- Support DDE communication

What is an SPGAS Quantification set?

- An SPGAS quantification set is a small spectral database, which contains all the information required by weighted multi-band CLS Algorithm (standard calibrated spectra per molecule to be analyzed, band selection per molecule, reference spectra, deviation from Beer's law parameters, unique serial number, password protection, and CRC file verification).

