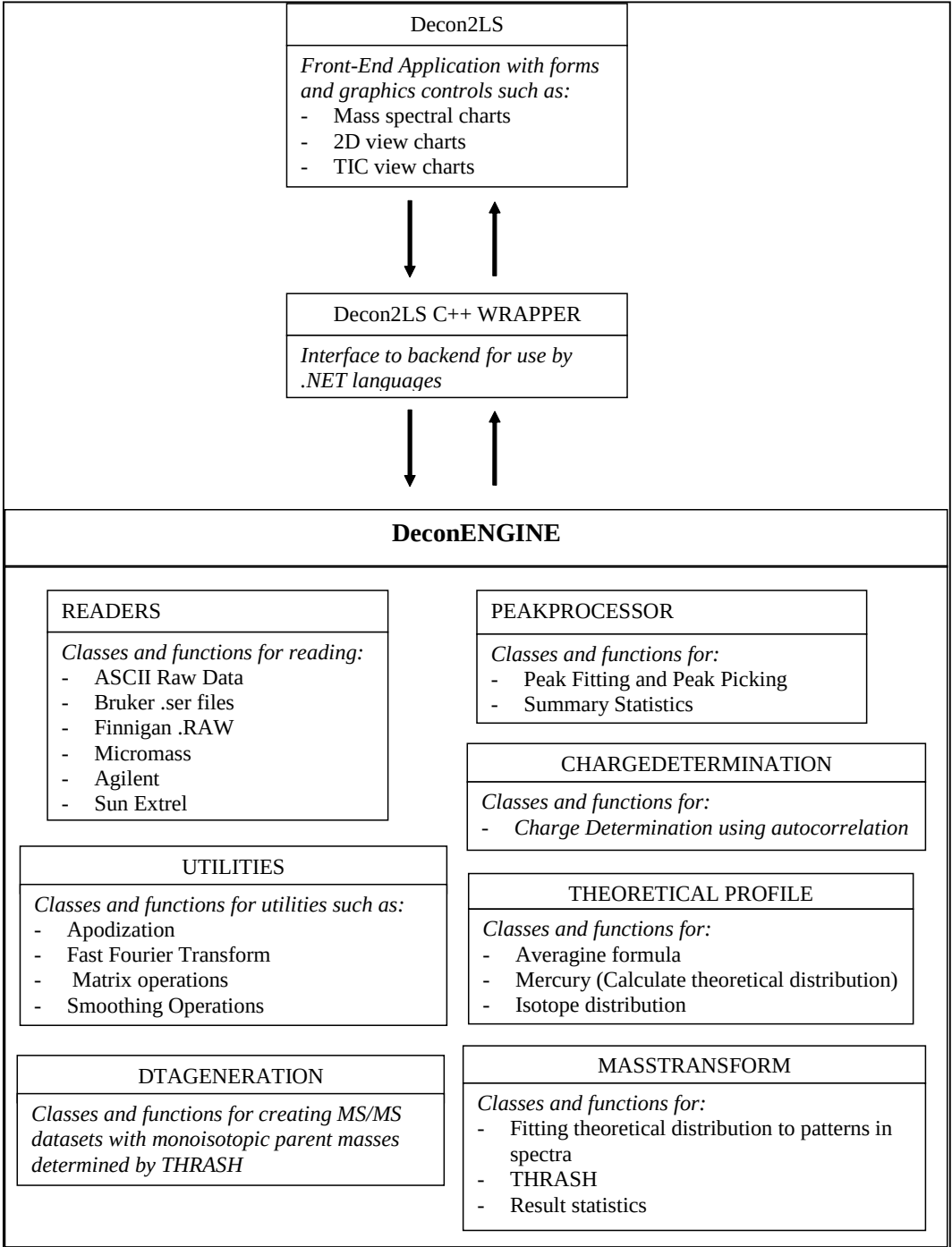
Decon2LS
Front-End Application with forms and graphics controls such as:
- Mass spectral charts
- 2D view charts
- TIC view charts
Decon2LS C++ WRAPPER
Interface to backend for use by .NET languages
DeconENGINE
READERS
Classes and functions for reading:
- ASCII Raw Data
- Bruker .ser files
- Finnigan .RAW
- Micromass
- Agilent
- Sun Extrel
PEAKPROCESSOR
Classes and functions for:
- Peak Fitting and Peak Picking
- Summary Statistics
CHARGEDETERMINATION
Classes and functions for:
- Charge Determination using autocorrelation
UTILITIES
Classes and functions for utilities such as:
- Apodization
- Fast Fourier Transform
- Matrix operations
- Smoothing Operations
THEORETICAL PROFILE
Classes and functions for:
- Averagine formula
- Mercury (Calculate theoretical distribution)
- Isotope distribution
DTAGENERATION
Classes and functions for creating MS/MS datasets with monoisotopic parent masses determined by THRASH
MASSTRANSFORM
Classes and functions for:
- Fitting theoretical distribution to patterns in spectra
- THRASH
- Result statistics