

NMR-spectra processing includes:

1. Element properties - list of nuclei magnetic properties
2. Spectrum calculation - predict NMR peak table spectrum using learning database
3. Check DB content - compare database spectra with predicted ones
4. Standard recalculation - recalculate spectrum to another standard
5. HNMR processing and assignment - loads instrumental FID, processes FT, Phase correction, Integral calculation
6. Prediction  $^1\text{H}$ ,  $^{13}\text{C}$  and  $^{31}\text{P}$  chemical shift
7. Databases of 4,000  $^{13}\text{C}$  and 4,000  $^{31}\text{P}$  assigned spectra

IR-spectra processing includes:

1. Spectrum processing- loads instrumental spectrum, performs base line correction, spectrum normalization, spectra subtraction
2. Peak table generation - calculates peak table from spectral curve

3. Spectrum edit - edits spectrum by points
4. Contour decomposition - decomposes spectral curve into Lorentz/Gauss contours

MASS-spectra processing includes:

1. JCAMP(Wiley)->JCAMP-Link - execute files transformation
2. Import Instrumental files - loads instrumental Finnegan \*.pic and Vector \*.txt files
3. Intensities correction - correct spectrum intensities using calibration table
4. Export in text exchange format - saves spectrum in simple text file
5. Peak's isotopic structure - calculates intensities of isotopic components of mass peak
6. Exact mass - calculate exact mass for given isotopic composition
7. Element properties - isotopes exact mass table
8. Composition of peak - proposes molecular formulas for given mass
9. Expert - analyses mass spectrum using possible fragmentation

10. Calculator - calculates in real time masses and isotopic distribution of selected fragment in structure. Saves assigned fragments in spectrum into learning database.

11. Look assignment database - browser of learning database

12. Spectrum analyzing - analyzes spectrum using learning database