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 1H, 13C and 31P chemical shift

7. Databases of 4,000 13C and 4,000 31P 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