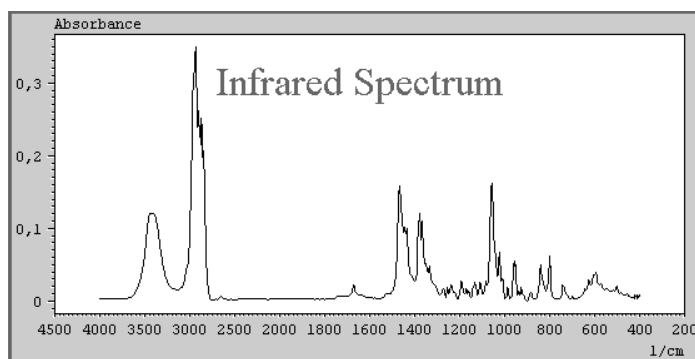
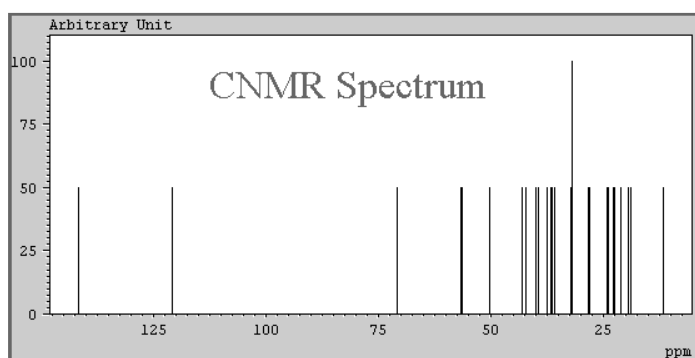
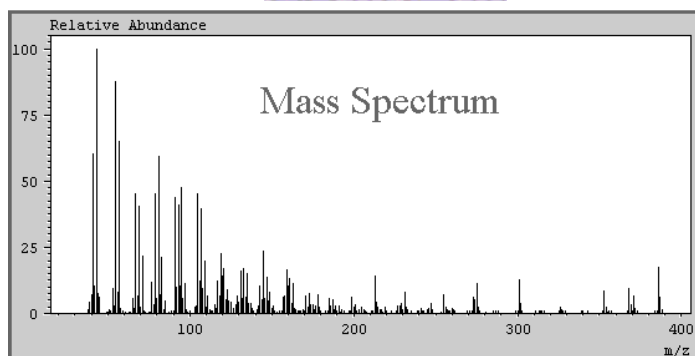
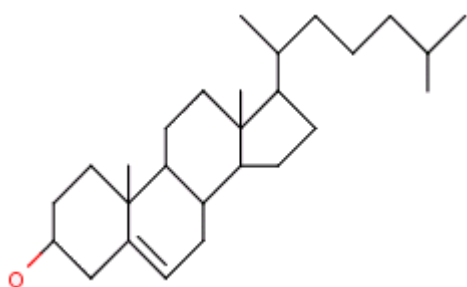


SpecInfo comprises one of the largest spectral data collections on the Internet worldwide



### SpecInfo Data Collections

The following NMR, IR and MS data collections are included in SpecInfo Online:

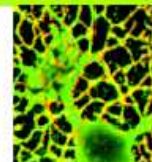
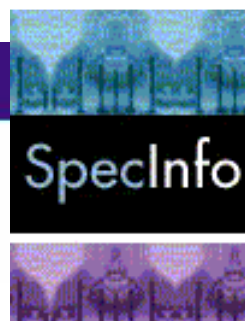
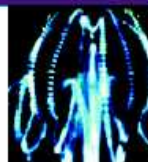
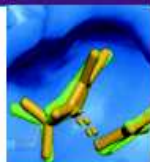
- <sup>13</sup>CNMR 332,000
- <sup>1</sup>HNMR 91,500
- <sup>31</sup>P, <sup>19</sup>F, <sup>29</sup>Si, <sup>15</sup>N 42,000
- MS: 95,000
- IR: 30,000

### Functionality

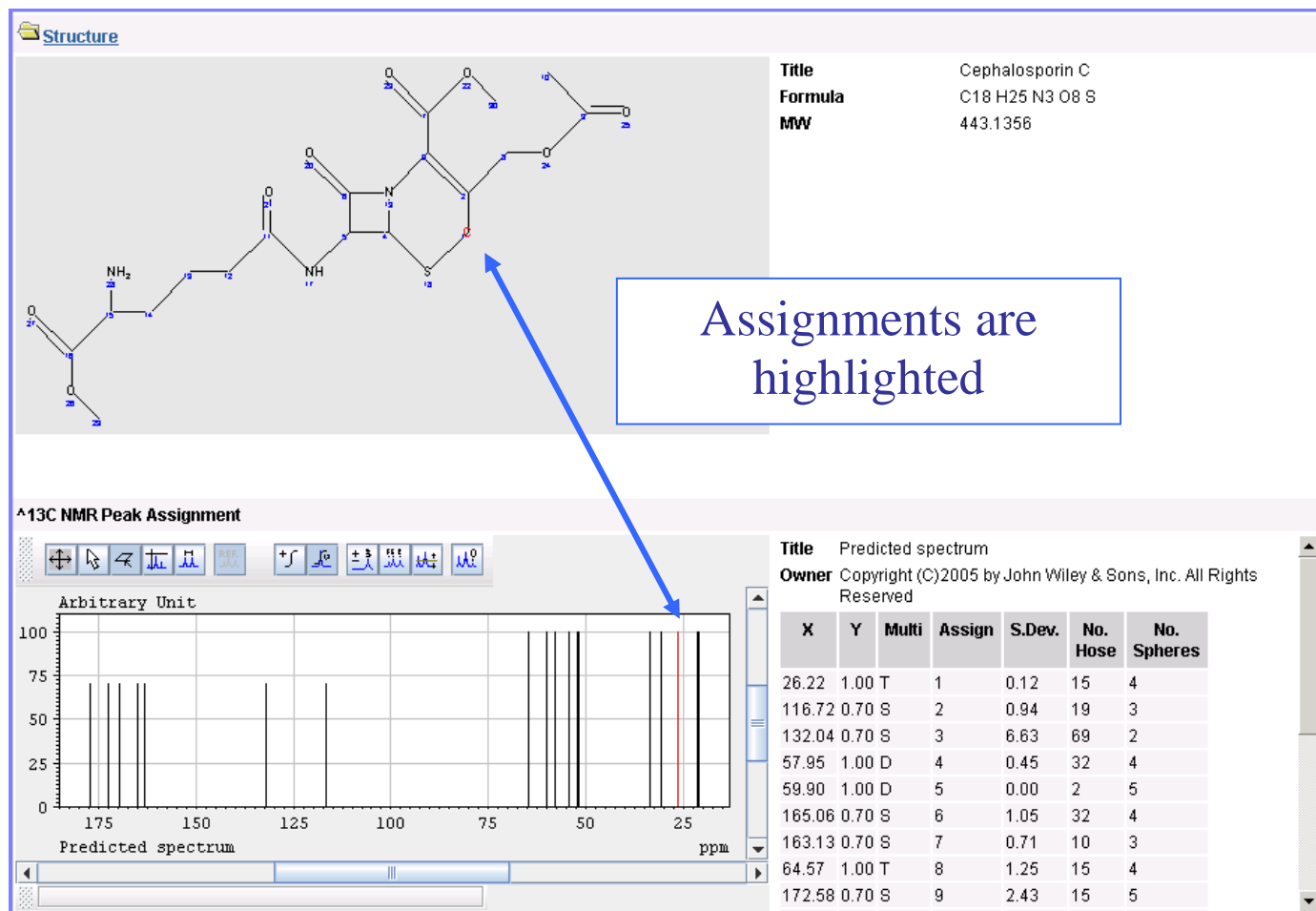
- Structure and substructure search
- Spectrum search
- Keyword search
- Spectrum prediction → see next page

### Ordering Information

- For a price quote: [rneudert@wiley-vch.de](mailto:rneudert@wiley-vch.de)
- More information about databases: [www.stmdata.de](http://www.stmdata.de)
- SpecInfo Online Home page: <http://www.interscience.wiley.com/>



## Spectrum Prediction in SpecInfo is based on 332,000 CNMR and 91,500 HNMR Spectra



- The highlighting feature visualizes the assignment of the Carbon (or Hydrogen) atoms to the chemical shifts in the spectrum
- The standard deviation (S.Dev. in the table above) is a measure of the prediction quality of the individual shifts
- Number of Hose codes is the number of spherical structure codes used for the prediction
- Number of Spheres is the range of the individual spherical structure codes