JENS SPANGET-LARSEN:
Computer Chemistry and Optical Spectroscopy

• Theoretical molecular modeling procedures contribute to the solution of complicated problems in current chemistry and biochemistry. To the left is shown a crystal model for quantum chemical calculations on C4-HSL, which is an important signal molecule in the extracellular communication of biofilm-forming bacteria.

• Quantum chemical model calculations and optical spectroscopy (UV-VIS, IR) is a strong combination. With modern theoretical methods it is possible, e.g., to predict the infrared (IR) spectra of interesting compounds, which is applied in the solution of structural problems.

• Molecular Linear Dichroism (LD) spectroscopy is the application of optical spectroscopy with linearly polarized light on ordered molecular assemblies. This yields information on molecular symmetry and other properties which are otherwise difficult to obtain. The photo to the left illustrates the preparation of stretched polymer samples with oriented solute molecules for IR LD spectroscopy.

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