ECD Simulation Prediction

Electronic circular dichroism (CD) spectroscopy is an important tool for the elucidation of biomolecular structure. The calculation method used for prediction comes from the CD spectrum of the structure including ab initio quantum chemistry technology, time-varying density functional theory and exciton theory. ECD can describe the importance of vibration coupling and the influence of protein environmental static electricity on the electronic transition of chromophores for the CD signal in the near ultraviolet. The increase in the accuracy of calculation methods should allow more quantitative research to be applied to various interesting problems by combining experimental data and modeling.

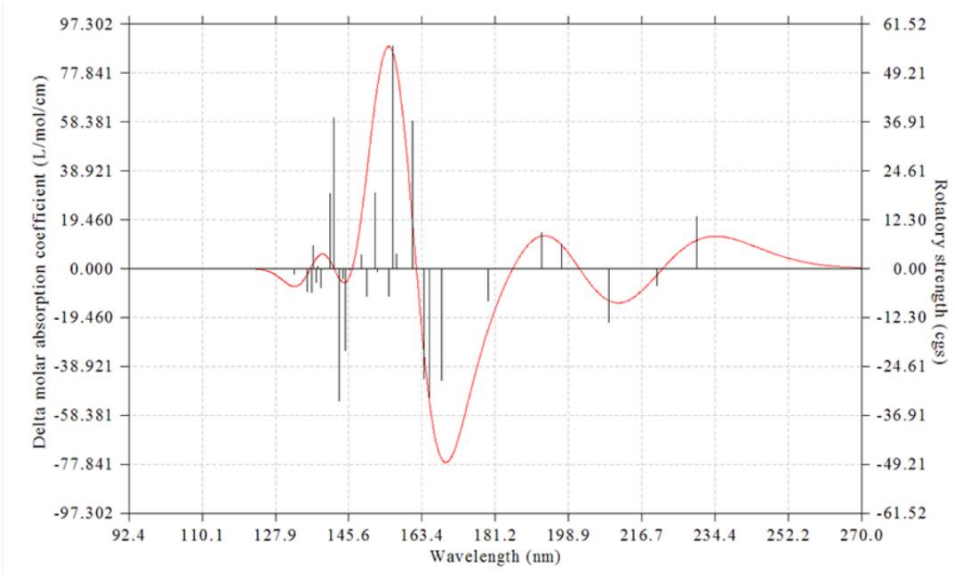

Figure 1.

Electronic circular dichroism.

Influencing factors

- The influence of the solvent, the solution used in the specific calculation is consistent with the experiment.
- The method of conformation search is to obtain as many possible conformations as possible for calculation with limited computing resources.

- The choice of functional and method basis set used in the calculation needs to be adjusted for different substances. If the structure of the initial conformation search is relatively complete, the experimental spectrum will show better, otherwise the result must be adjusted.

Overall solutions

Many organic molecules have optical chirality. Correctly determining the three-dimensional configuration of organic molecules is a task that organic chemists, especially pharmaceutical scientists, must complete. Electrostatic circular dichroism (ECD) is very sensitive to the spatial orientation of molecular groups. MedAI can provide information about the three-dimensional structure of chiral molecules. This has become a powerful tool for exploring the absolute configuration of chiral molecules in nature.

- Currently, MedAI uses theoretical simulations to calculate the electronic circular dichroism (ECD) of chiral molecules.
- MedAI usually uses the method of determining chiral compounds through experimental values to determine the absolute configuration of chiral compounds.
- Time-varying density functional theory (TDDFT) is currently the most popular theoretical method, and the multi-format Boltzmann weighted average method is the most stable and reliable simulation method.
- Combining ECD calculations and experiments can quickly determine the absolute configuration of chiral molecules.

Services items

PROJECT NAME	ECD SIMULATION PREDICTION SERVICE
Requirements	Conformation screening

PROJECT NAME	ECD SIMULATION PREDICTION SERVICE
	Optimization and calculation of excited states; The software fits the CD calculation curve and compares it with the experiment CD.
Cycle	Depends on the time you need to simulate and the time required for the system to reach equilibrium.
Product delivery mode	The simulation results provide you with the raw data and analysis results of molecular dynamics.

MedAI's ECD simulation prediction service can reduce the cost of subsequent experiments. ECD simulation prediction service is a personalized and customized innovative scientific research service. Before determining the corresponding analysis plan and price, each project needs to be evaluated. If you want to know more about service prices or technical details, please feel free to contact us. If you want to know more about service prices or technical details, please feel free to contact us.