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Resonac Dramatically Reduces Materials Development Time Using AI Based on Deep Learning Technology

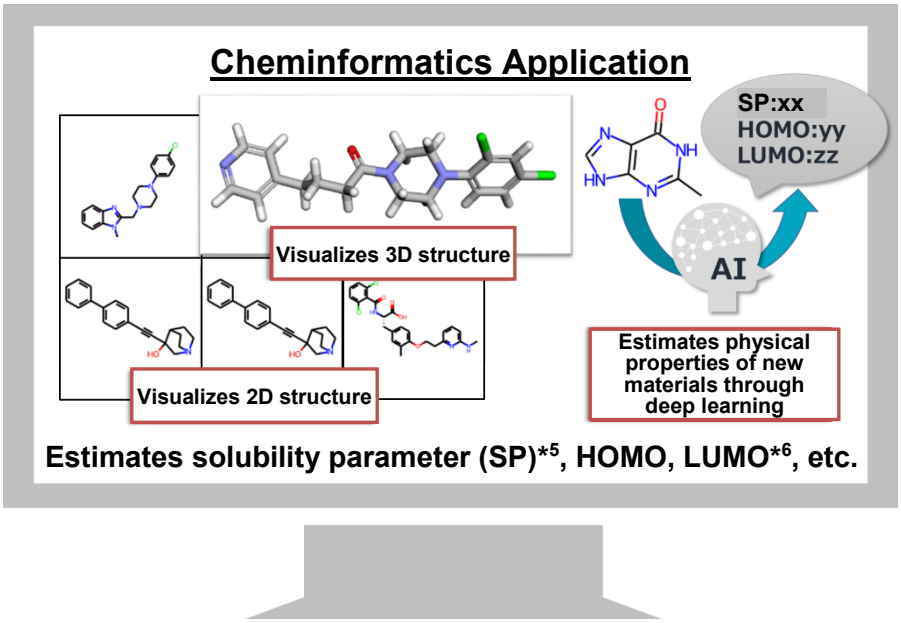
–Resonac has developed a cheminformatics application that increases the speed of physical property calculations thousands of times faster than before–

Resonac Corporation (President: Hidehito Takahashi) has developed in-house a cheminformatics[*1] application program that utilizes artificial intelligence (AI) based on deep learning technology. It has begun using the application to maximize its vast store of physical property data. This application significantly reduces the time required to calculate physical properties in developing new chemicals through prediction technology based on information science[*2], and its simple user interface allows even engineers without expertise in cheminformatics to use it. Thus, the cheminformatics application enables the development of new materials in a shorter time than before, especially in fields such as semiconductor material development, where rapid development is required.

In the conventional development of new materials, engineers often estimate the physical properties of new materials in the early stages of experimentation based on literature and experience. Then, the experiments and physical property measurements are repeated. In addition, estimating the physical properties of new materials by quantum chemical calculations[*3] or chem-informatics-based simulations usually requires descriptors[*4], which are physical property calculations and data input rules. These tasks require expertise and experience in quantum chemical calculations and cheminformatics.

The newly developed cheminformatics application developed by the Research Center for Computational Science and Informatics, Resonac Corporation, utilizes deep learning of calculation results and experimental data accumulated in past materials development. Thus, it is possible to estimate the physical properties of new materials several thousand times faster than quantum chemical calculations. The cheminformatics application is a web application with a simple and intuitive user interface. Therefore, even experimenters unfamiliar with cheminformatics can input data using their usual molecular drawing methods. Thus, by using this cheminformatics application, the experimenter can estimate the physical properties of new materials in advance and design new materials.

Resonac will continue to utilize information science and technology to shorten the development time of new materials, especially in fields requiring speedy development, such as semiconductor materials.



*1. Cheminformatics is one of the research fields in chemistry. It estimates unknown compounds' structure and physical properties by constructing predictive models from accumulated past data. It is used to propose experimental conditions and to search for molecules that can be used as drugs or raw materials. Cheminformatics has some points in common with materials informatics. However, cheminformatics mainly deals with information on molecules and compounds, while materials informatics deals with information on substances and materials.
*2. Comparison between the newly developed cheminformatics application and quantum chemical calculations using conventional computers.
*3 Quantum chemical calculation is a type of molecular simulation technology. It theoretically analyzes molecules' structure and physical properties by calculating their electronic states.
*4. The descriptor is a numerical value that expresses the characteristics of a compound's substructure and physicochemical properties.
*5. The solubility parameter is a numerical value that indicates the solubility behavior of a solvent. It is defined as the square root of the cohesive energy density.
*6. HOMO=Highest Occupied Molecular Orbital. LUMO=Lowest Unoccupied Molecular Orbital. The molecular orbital with the highest energy of electrons is called HOMO, and the molecular orbital with the lowest energy not occupied by electrons is called LUMO.

[About the Resonac Group]
The Resonac Group is a new company established as a result of the integration of the Showa Denko Group and the Showa Denko Materials Group (former Hitachi Chemical Group) in January 2023. The Group's annual sales of semiconductor and electronic materials amount to about 400 billion yen, accounting for about 30% of the Group's annual net sales. The Group especially has global top share of semiconductor materials for packaging process. The integration of the two companies has enabled the Resonac Group to design functions of materials as well as to develop them in-house, going all the way back to raw materials. The new trade name "RESONAC" was created as a combination of two English words, namely, the word of "RESONATE" and "C" as the first letter of CHEMISTRY. The Resonac Group will make the most of its co-creative platform, and accelerate technological innovation with semiconductor manufacturers, material manufacturers, and equipment manufacturers inside and outside Japan.

For detail, please refer to our Website.
Resonac Holdings Corporation: https:// www.resonac.com/

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