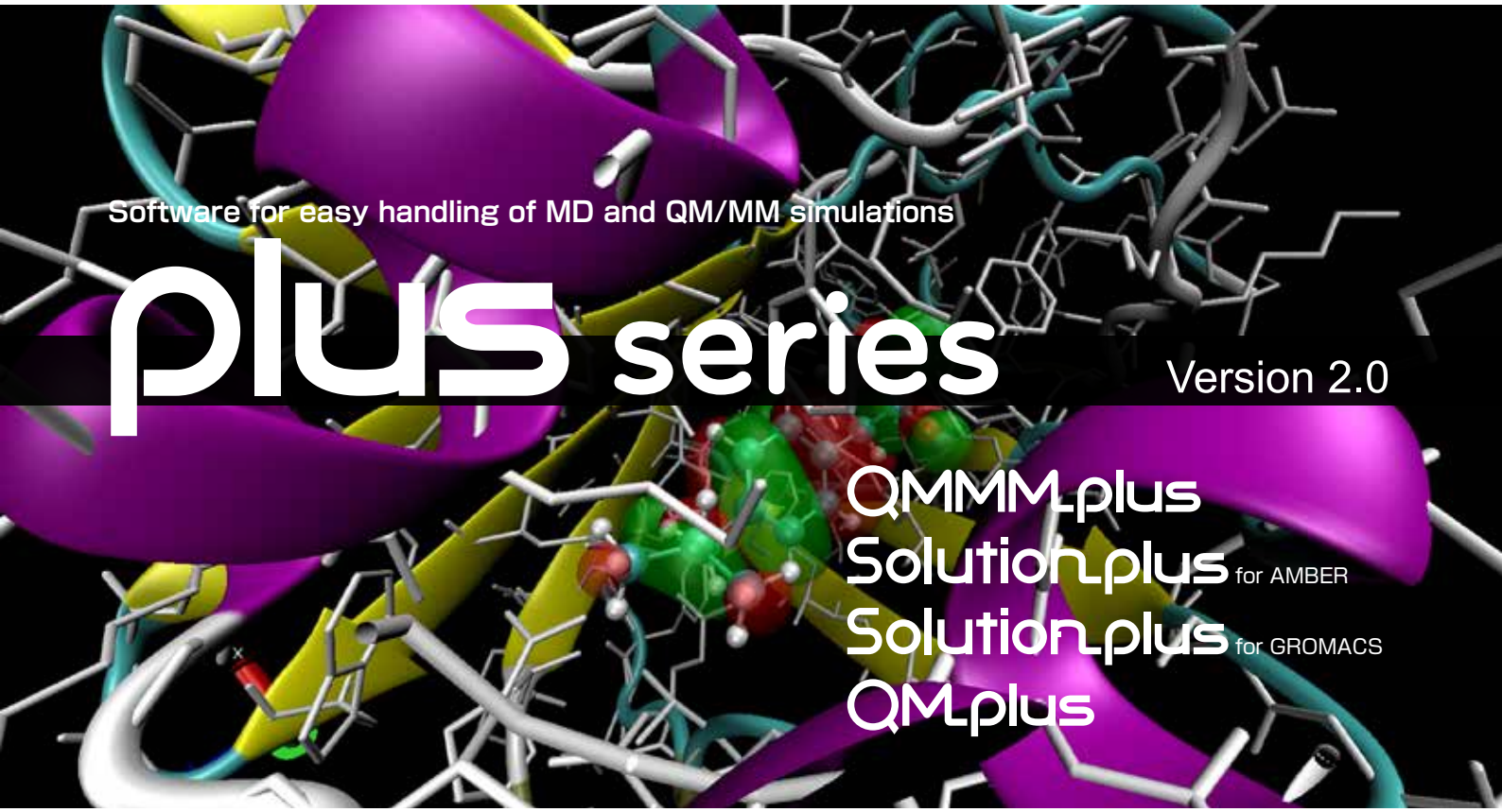
Software

HPC SYSTEMS



Software for easy handling of MD and QM/MM simulations

# plus series

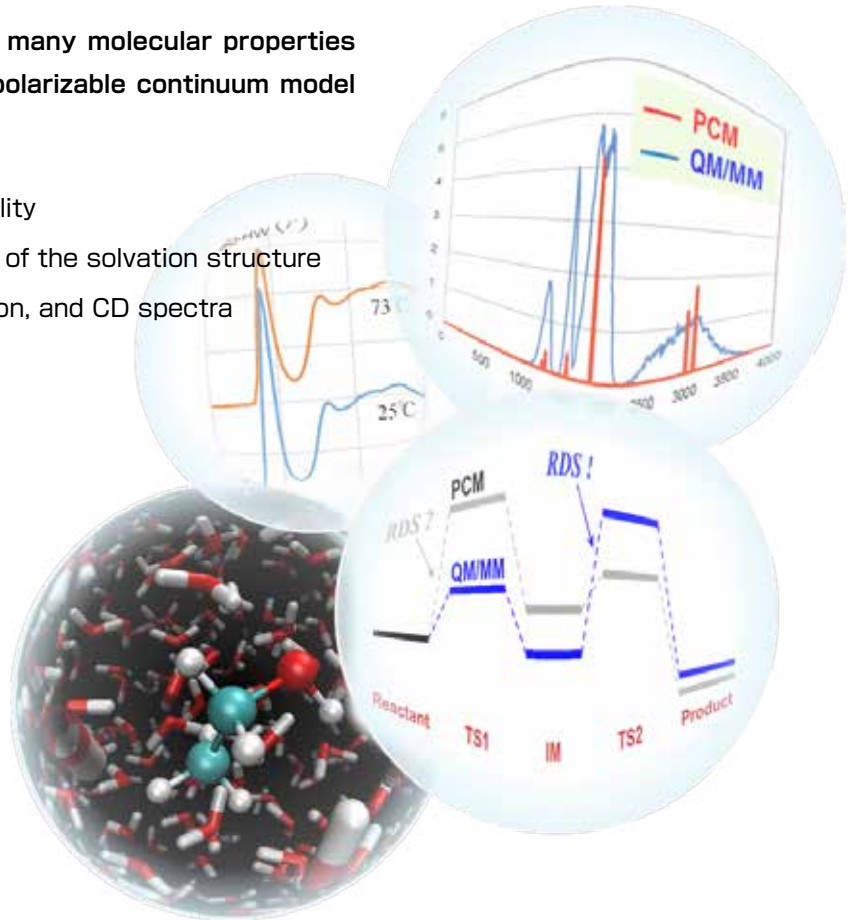
Version 2.0

## QMMM plus
## Solution plus for AMBER
## Solution plus for GROMACS
## QM plus

**You can easily and automatically obtain many molecular properties in mixed solvent beyond the traditional polarizable continuum model (PCM), for example,**

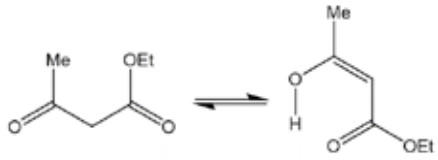
- Solvent dependence of the isomer stability
- Spectral band shape due to fluctuation of the solvation structure
- Solvatochromism for absorption, emission, and CD spectra
- Radial distribution functions
- Temperature effects

**even if you know only Gaussian usage.**



# Overview

## Tautomerism in Different Solvents

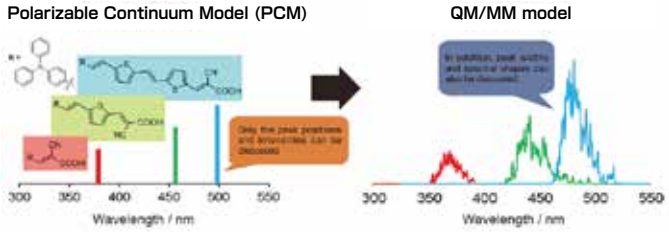



Keto form　　Enol form

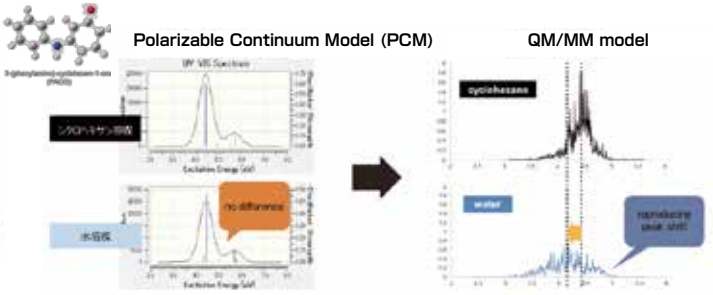
**Prediction of stable isomer in solution**

| Solvents | Experiment<br>population (keto:enol) | Calculation (PCM)<br>relative energy (keto-enol) | Calculation (QM/MM)<br>relative energy (keto-enol) |
|---|---|---|---|
| Cyclohexane | enol<br>(38% : 62%) | ○ enol<br>(+4.3kcal/mol) | ○ enol<br>(+3.8kcal/mol) |
| Acetone | keto<br>(99.9% : 0.13%) | × enol<br>(+2.4kcal/mol) | ○ keto<br>(-3.2kcal/mol) |
| Water | keto<br>(93.5% : 6.5%) | × enol<br>(+0.9kcal/mol) | ○ keto<br>(-10.4kcal/mol) |

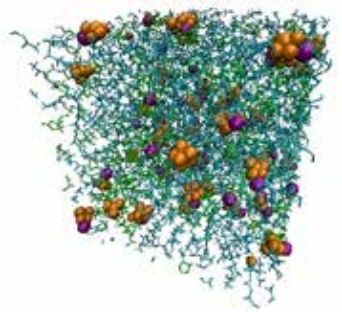
## Spectrum Width and Shift in Different Solvents



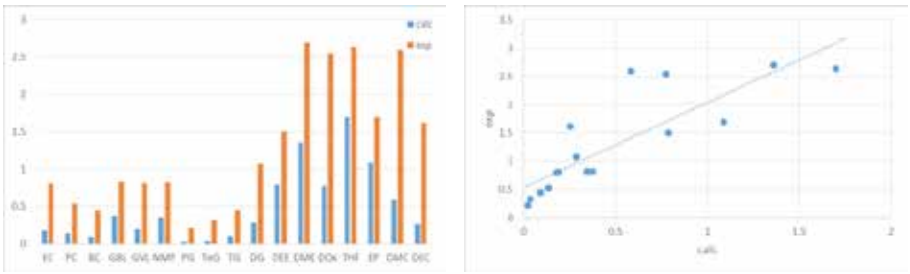

Only the peak positions and intensities can be discussed.




## Efficient Evaluation of Many Materials



**Electrolyte consisting of four molecular (ionic) species.**
Concentration can be set easily.



**Diffusion coefficients for many electrolytes.**
One material can be evaluated in only 30 minutes, hence 480 materials per a day using ten computers (16 core).

# How to Use

## ① Create the input file

Set only molecule files, number of molecules, temperature and pressure conditions, and so on.
User also can modify details of MD calculation processes.

## ② Run

Just a single command.　All simulation processes are automatically performed.

```
$ solution mer.input
```

```
[control]
n_core          = 16        parallel number and
style           = normal    calculation style

[molecule]
molecule01      = 1, BMC, input/merocyanine.gjf
molecule02      = 1000, AC, input/acetone.mol2
                  number of molecules and molecule files
                  (merocyanine : 1 molecule + acetone: 1000 molecules)

[md_default]
qmcondition     = PM6       conditions for QM/MM calculation
temperature     = 298.15    temperature
t               = 0.1       time
dt_output       = 0.001

[analysis]                  number of snapshots for quantum
n_data          = 64        chemistry analysis
gjf_template    = input/template-td.gjf
```

**Input file**

# Functions

## 1. Molecular Dynamics Automatic Simulator

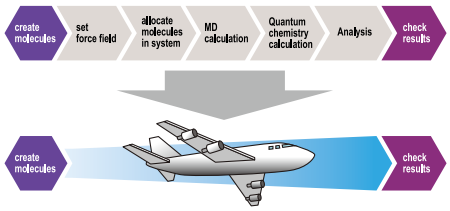
### Automatic Calculation

Simulation for liquid solution have ever required many procedures such as creation of molecule, set of force field, allocation of molecules in system using many programs.

QMMM plus automates all these procedures. Only molecular structure files as well as conditions for temperature and pressure are required. No action required.  Energy and spectra in liquid solution can be automatically calculated.

### Restart

Available for restarting in middle of procedures.




Everyone can easily perform MD calculations even that experts have ever examined after a day.

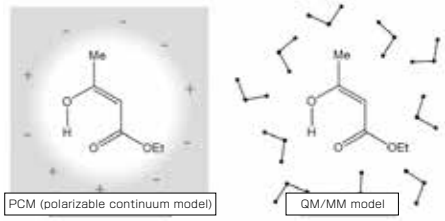
## 2. Molecular Dynamics Analysis

### Time Evolution and Statistics of Energy and Temperature

Time evolution and statistics of energy, temperature, density, and interaction energy between a solute molecule and solvent molecules can be calculated.

### Distribution and Diffusion of Molecules

RDF (radial distribution function) and diffusion behavior can be calculated.




Available also for QM/MM model.

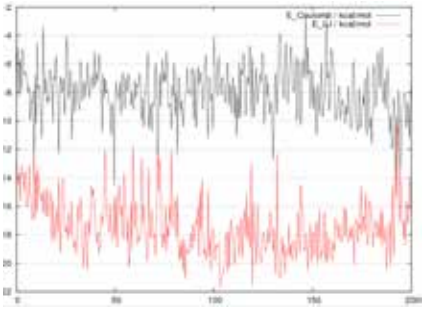
## 3. Quantum Chemistry Tools

### Bulk Editor

Many Gaussian input files can be edited at once.

### Bulk Execution

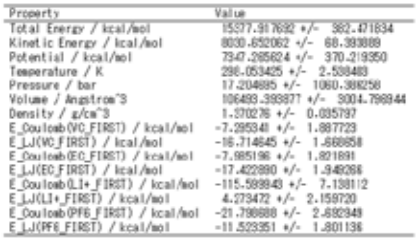
Many Gaussian jobs can be executed under limited number of CPU cores.



## 4. Quantum Chemistry Analysis

### Statistics of Energy, Dipole, Atomic charges

Statistical analysis is available from many Gaussian output files. Energy, dipole moments and atomic charges are represented as values with standard deviations.  Therefore, a new perspective such as softness of molecular structure as is proposed.



| Property | Value |
|---|---|
| Total Energy / kcal/mol | 15377.917692 +/- 382.471834 |
| Kinetic Energy / kcal/mol | 8030.652062 +/- 68.393889 |
| Potential / kcal/mol | 7347.265624 +/- 370.219350 |
| Temperature / K | 296.053425 +/- 2.538483 |
| Pressure / bar | 17.204885 +/- 1060.388258 |
| Volume / Angstrom^3 | 106493.393877 +/- 3004.799844 |
| Density / g/cm^3 | 1.370276 +/- 0.035797 |
| E_Coulomb(VC_FIRST) / kcal/mol | -7.295341 +/- 1.887723 |
| E_LJ(VC_FIRST) / kcal/mol | -16.714645 +/- 1.668658 |
| E_Coulomb(EC_FIRST) / kcal/mol | -7.985196 +/- 1.821891 |
| E_LJ(EC_FIRST) / kcal/mol | -17.422890 +/- 1.949266 |
| E_Coulomb(Li+_FIRST) / kcal/mol | -115.589843 +/- 7.138112 |
| E_LJ(Li+_FIRST) / kcal/mol | 4.273472 +/- 2.159720 |
| E_Coulomb(PF6_FIRST) / kcal/mol | -21.799888 +/- 2.692949 |
| E_LJ(PF6_FIRST) / kcal/mol | -11.523351 +/- 1.801136 |

Time evolution and statistics of many properties.

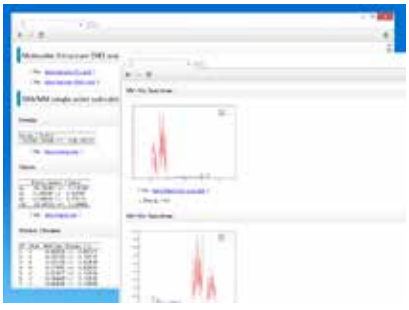
### Spectrum in Liquid Solution (IR, Raman, UV-Vis, CD, NMR)

Since QMMM plus collects statistics from quantum chemistry calculations of many molecular structures in liquid solution, it provides continuous spectra with width and shape, whereas traditional quantum chemistry have ever provided line spectra.

## 5. Report

### HTML-formatted Report

Calculation results are available in HTML format which can be viewed in a Internet browser.  Tab-delimited output files are stored in “data” directory.



Calculation results are available from a browser.

## ■ Software Components

| Functions | plus series | | | |
|---|---|---|---|---|
| | QMMM plus | Solution plus for Amber | Solution plus for GROMACS | QM plus |
| MD Automatic Simulator | SOLUTION | SOLUTION | SOLUTION | – |
| MD Analysis | AMBINFO<br>GMXINFO<br>TRJ2GJF | AMBINFO | GMXINFO | – |
| QC Tools | GAUEDIT<br>GAURUN<br>GJOB | – | – | GAUEDIT<br>GAURUN<br>GJOB |
| QC Analysis | GAUINFO<br>GAUCUBE | – | – | GAUINFO<br>GAUCUBE |

| | |
|---|---|
| SOLUTION | Automatic simulator of MD and QC for liquid solution |
| AMBINFO | Analyzer for MD outputs of AMBER |
| GMXINFO | Analyzer for MD outputs of GROMACS |
| GAUINFO | Analyzer for QC outputs of Gaussian |
| GAUCUBE | Analyzer for Gaussian Cube files |
| GAUEDIT | Editing tool for Gaussian input files |
| GAURUN/GJOB | Job controller for multiple Gaussian calculations |
| TRJ2GJF | AMBER trajectory to Gaussian input converter |

*MD : Molecular Dynamics,　QC : Quantum Chemistry

## ■ System Requirements

| Requirements<br>◎ : necessary<br>○ : recommended | plus series | | | |
|---|---|---|---|---|
| | QMMM plus | Solution plus for Amber | Solution plus for GROMACS | QM plus |
| Python 2.6 | ◎ | ◎ | ◎ | ◎ |
| LSF, LAVA or Grid Engine | ○ | ○ | ○ | ○ |
| Gaussian09 | ○ | ○ | ○ | ◎ |
| AMBER14 | ○ | ○ | ○ | – |
| AmberTools14 | ◎ | ◎ | ◎ | – |
| GROMACS 4.6 or 5.0 | ◎ | ◎ | ◎ | – |
| acpype.py | ◎ | ◎ | ◎ | – |
| Open Babel 2.x | ◎ | ◎ | ◎ | – |
| Gnuplot | ○ | ○ | ○ | ○ |
| Image Magick | ○ | ○ | ○ | ○ |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