Reaction plus function table

Function	Reaction plus Pro 2	Reaction plus Pro	Reaction plus Express 2	Reaction plus Express
Input creating method[*1, *2]	GaussView Text editor ONIOM calculation supporting tool	GaussView Text editor	GaussView Text editor	GaussView Text editor
Specification of intermediate structure	Able to specify as many as you want	Able to specify as many as you want	Able to specify as many as you want	Able to specify as many as you want
Readable file format of initial structure	xyz pdb mol2	xyz	xyz pdb mol2	xyz
Auto-adjustment of initial bead structure	○	○ (Constant)	○	○ (Constant)
Auto-modification of coordinate axis	○	○	○	○
Quantum chemistry calculation	○	○	×	×
PM6 calculation	○	○	○ (High speed)	○ (High speed)
ONIOM calculation	○	×	×	×
Fixing of specific atomic coordinate	○	×	○	×
Calculation of open-shell reaction system	○	○	○	×
Importing initial orbit from chk file	○	×	×	×
Output file format for animation[*3]	Gaussian log xyz pdb	Gaussian log xyz	Gaussian log xyz pdb	Gaussian log xyz

*1 Checked operation with GaussView 5.0.9 for Windows.
*2 ONIOM calculation supporting tool can transform AMBER/GROMACS file into Gaussian (ONIOM) input (attached in Linux version).
*3 log file can be read in animation with GaussView, while xyz and pdb file can be displayed in animation with VMD or Avogadro (checked by GaussView 5.0.9, VMD 1.9.1 for Windows Avogadro 1.2.0 for Windows).