



Solve charge conflict

present

↓

explore

↓

identify

encode

+

navigate

+

select

+

annotate

+

record

input: fragment

→

output: fragment

input: unparameter. atom

→

output: molecule

Solve charge conflict

produce

derive

+

record

input: fragment

→

output: fragment

input: unparameter. atom

→

output: molecule

Fine-tune charges

present

↓

explore

↓

identify

navigate

+

select

+

annotate

+

record

input: molecule

→

output: molecule

Legend

Why

How

What