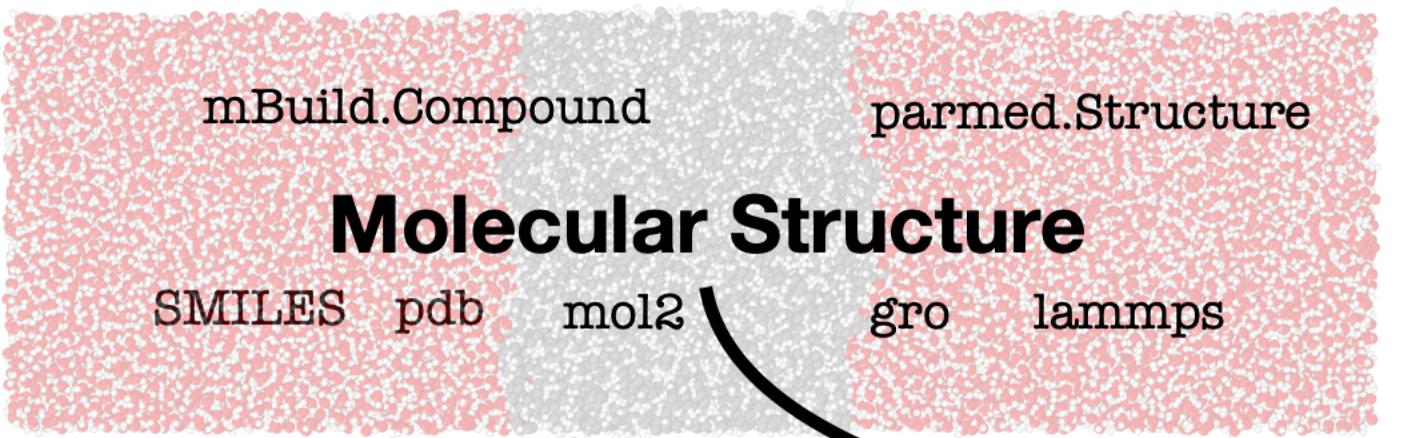


# GMSO

the General Molecular  
Simulation Object



```
<?xml version='1.0' encoding='UTF-8'?>
<ForceField name="TIP3P" version="0.0.1">
  <FFMetaData>
    <Units energy="kJ/mol" mass="amu" charge="elementary_charge" distance="nm"/>
  </FFMetaData>
  <AtomTypes expression="4*epsilon * ((sigma/r)**12 - (sigma/r)**6)">
    <ParametersUnitDef parameter="epsilon" unit="kJ/mol"/>
    <ParametersUnitDef parameter="sigma" unit="nm"/>
    <AtomType name="opls_111" element="O" charge="-0.834" mass="16" definition="0" description="water O">
      <Parameters>
        <Parameter name="epsilon" value="0.636586"/>
        <Parameter name="sigma" value="0.315061"/>
      </Parameters>
    </AtomType>
    <AtomType name="opls_112" element="H" charge="0.417" mass="1.011" definition="H">
      <Parameters>
        <Parameter name="epsilon" value="0.0"/>
        <Parameter name="sigma" value="1.0"/>
      </Parameters>
    </AtomType>
  </AtomTypes>
</ForceField>
```

**Force Field  
Parameters**

A snippet of XML code representing force field parameters for the TIP3P model, showing atom types, parameters like epsilon and sigma, and their units.

Systematic and  
Flexible Unit

Extensible  
Workflow

## Topology

Symbolic Potential  
Expression



## Molecular Topology File



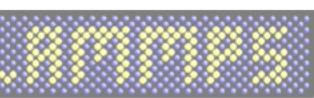
Cassandra

Monte Carlo

SOFTWARE



FAST.  
FLEXIBLE.  
FREE.



**GROMACS**

# MoSDef

Molecular Simulation Design Framework