winmostar tutorial

Modeling Molecule
Organic Molecule

V11.5.6

18 December 2023 X-Ability Co., Ltd.

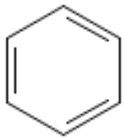
About This Document

- This manual is a tutorial demonstrating use cases for Winmostar V11.
- For those using Winmostar V11 for the first time, please consult Beginner's Guide.
- For those who wish to explore the details of each feature, please refer to Winmostar User Manual.
- If you are unable to proceed with the operations as outlined in this manual, please first consult Frequently asked questions.
- If your issue is not resolved through the Frequently Asked Questions, for the purpose of information accumulation and management, please contact us from Contact. Attach files generated at the time of the issue and provide steps to reproduce the problem.
-

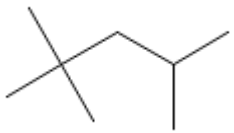
Overview

- Winmostar provides four methods for creating organic molecules:
  A. Inputting structural formulas
  B. Import SMILES
  C. Importing files created by other software or obtained from various databases
     - Supports formats like pdb, mol, mol2, cif, xyz, sdf
  D. Directly modeling 3D molecular structures

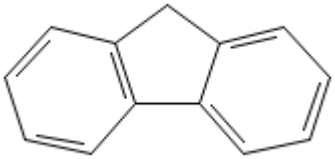
- In this tutorial, we will introduce each method using the following molecules as examples.



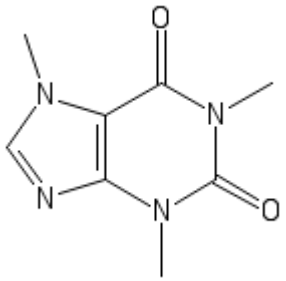
Benzene
C_6H_6



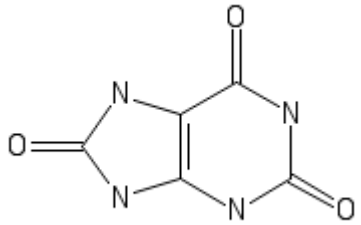
Isooctane
C_8H_{18}



Fluorene
$C_{13}H_{10}$



Caffeine
$C_8H_{10}N_4O_2$

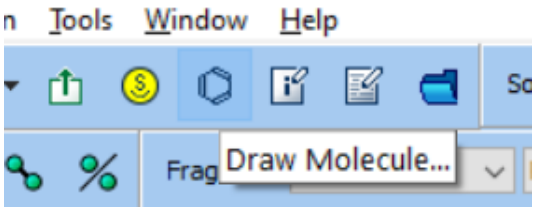


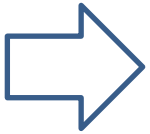
Uric acid
$C_5H_4N_4O_3$

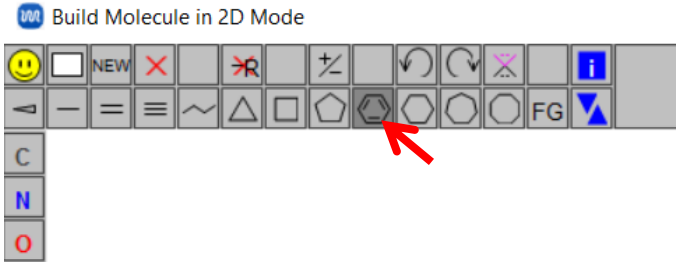
A. Inputting structural formulas (Benzene)

A. Click **File | New File**, **New Project**, or **Edit | Reset Structure**.

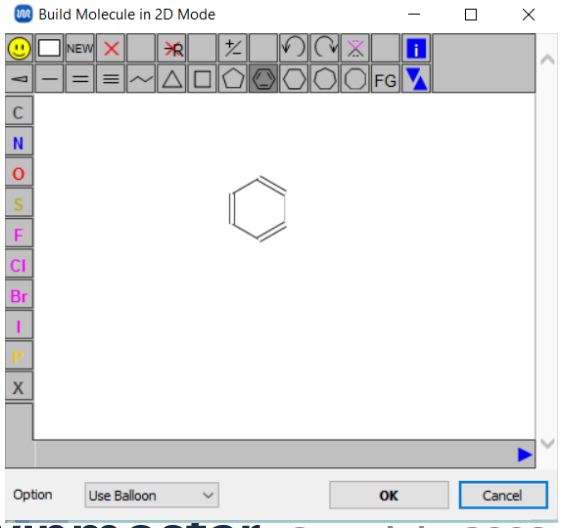
B.  Click **Draw Molecule**, then click on the phenyl group button.



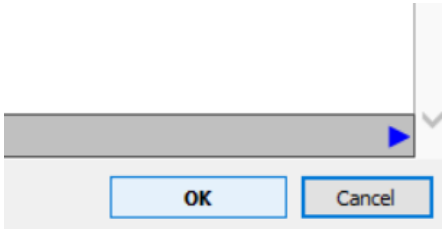


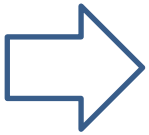


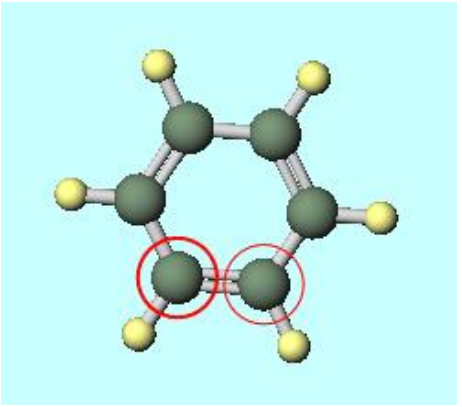
C. Click near the center of the window to generate a benzene ring.



D. Click **OK** at the bottom right of the window to display the 3D structure of benzene.

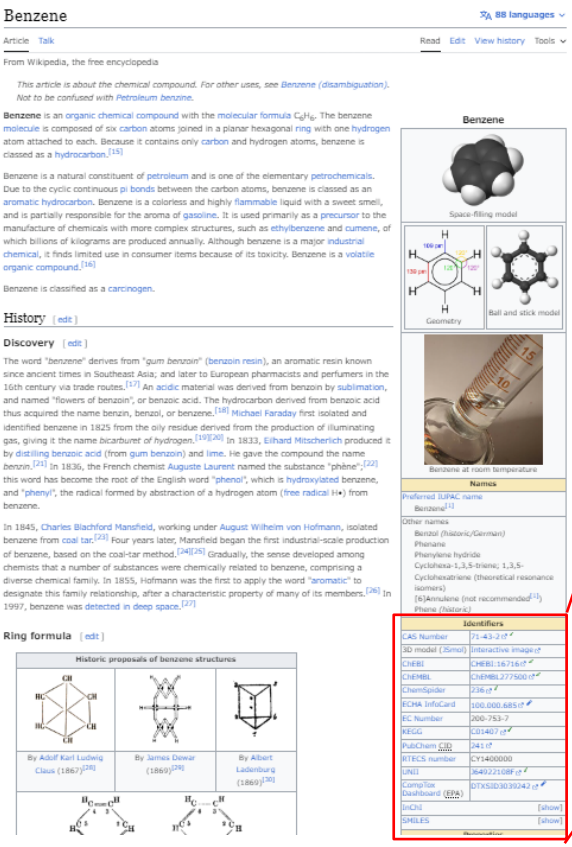






B. Import SMILES（Benzene)

A. Copy the SMILES string for Benzene (c1ccccc1) from Wikipedia. (Be mindful of uppercase and lowercase letters.)


Benzene

From Wikipedia, the free encyclopedia

This article is about the chemical compound. For other uses, see Benzene (disambiguation). Not to be confused with Petroleum benzine.

Benzene is an organic chemical compound with the molecular formula C_6H_6. The benzene molecule is composed of six carbon atoms joined in a planar hexagonal ring with one hydrogen atom attached to each. Because it contains only carbon and hydrogen atoms, benzene is classed as a hydrocarbon.[15]

Benzene is a natural constituent of petroleum and is one of the elementary petrochemicals. Due to the cyclic continuous pi bonds between the carbon atoms, benzene is classed as an aromatic hydrocarbon. Benzene is a colorless and highly flammable liquid with a sweet smell, and is partially responsible for the aroma of gasoline. It is used primarily as a precursor to the manufacture of chemicals with more complex structures, such as ethylbenzene and cumene, of which billions of kilograms are produced annually. Although benzene is a major industrial chemical, it finds limited use in consumer items because of its toxicity. Benzene is a volatile organic compound.[16]

Benzene is classified as a carcinogen.

History [edit]

Discovery [edit]

The word "benzene" derives from "gum benzoin" (benzoin resin), an aromatic resin known since ancient times in Southeast Asia; and later to European pharmacists and perfumers in the 16th century via trade routes.[17] An acidic material was derived from benzoin by sublimation, and named "flowers of benzoin", or benzoic acid. The hydrocarbon derived from benzoic acid thus acquired the name benzin, benzol, or benzene.[18] Michael Faraday first isolated and identified benzene in 1825 from the oily residue derived from the production of illuminating gas, giving it the name *bicarburet of hydrogen*.[19][20] In 1833, Eilhard Mitscherlich produced it by distilling benzoic acid (from gum benzoin) and lime. He gave the compound the name *benzin*.[21] In 1836, the French chemist Auguste Laurent named the substance "phène";[22] this word has become the root of the English word "phenol", which is hydroxylated benzene, and "phenyl", the radical formed by abstraction of a hydrogen atom (free radical H•) from benzene.

In 1845, Charles Blachford Mansfield, working under August Wilhelm von Hofmann, isolated benzene from coal tar.[23] Four years later, Mansfield began the first industrial-scale production of benzene, based on the coal-tar method.[24][25] Gradually, the sense developed among chemists that a number of substances were chemically related to benzene, comprising a diverse chemical family. In 1855, Hofmann was the first to apply the word "aromatic" to designate this family relationship, after a characteristic property of many of its members.[26] In 1997, benzene was detected in deep space.[27]

Ring formula [edit]

Historic proposals of benzene structures

By Adolf Karl Ludwig Claus (1867)[28] | By James Dewar (1869)[29] | By Albert Ladenburg (1869)[30]

Benzene

Space-filling model

Geometry | Ball and stick model

Benzene at room temperature

Names

Preferred IUPAC name

Benzene[1]

Other names

Benzol (historic/German)
Phenene
Phenylene hydride
Cyclohexa-1,3,5-triene; 1,3,5-Cyclohexatriene (theoretical resonance isomers)
[6]Annulene (not recommended[1])
Phene (historic)

Identifiers

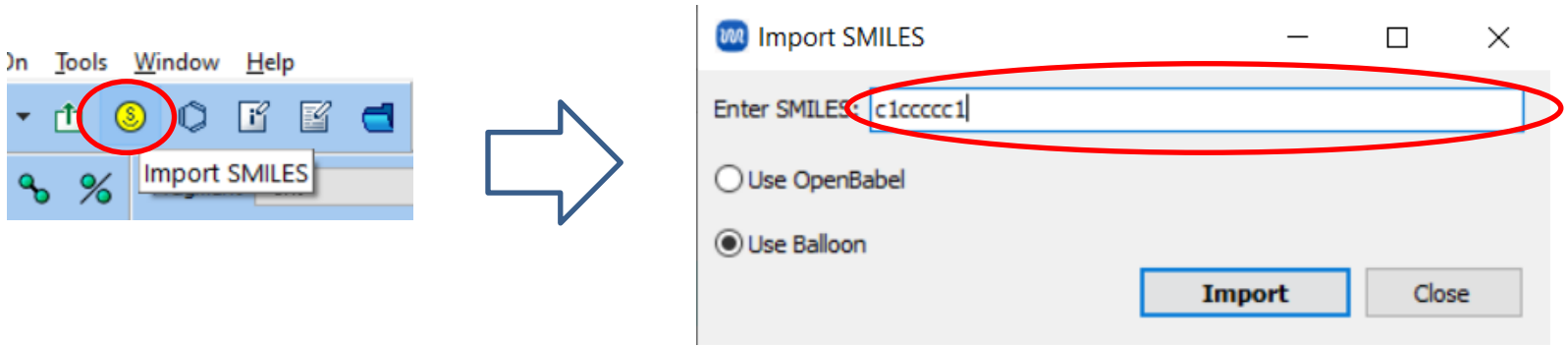
CAS Number	71-43-2
3D model (JSmol)	Interactive image
ChEBI	CHEBI:16716
ChEMBL	ChEMBL277500
ChemSpider	236
ECHA InfoCard	100.000.685
EC Number	200-753-7
KEGG	C01407
PubChem CID	241
RTECS number	CY1400000
UNII	J64922108F
CompTox Dashboard (EPA)	DTXSID3039242
InChI	[show]
SMILES	[show]

Identifiers	
CAS Number	71-43-2
3D model (JSmol)	Interactive image
ChEBI	CHEBI:16716
ChEMBL	ChEMBL277500
ChemSpider	236
ECHA InfoCard	100.000.685
EC Number	200-753-7
KEGG	C01407
PubChem CID	241
RTECS number	CY1400000
UNII	J64922108F
CompTox Dashboard (EPA)	DTXSID3039242
InChI	[show]
SMILES	[hide]
c1ccccc1	

B. Import SMILES（Benzene）

B. Click **File | New File**, **New Project**, or **Edit | Reset Structure**.

C. Click **Import SMILES** and paste the SMILES string into **Enter SMILES** field.

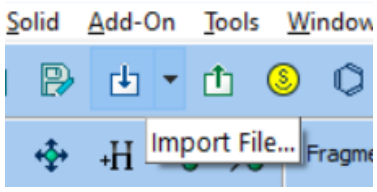


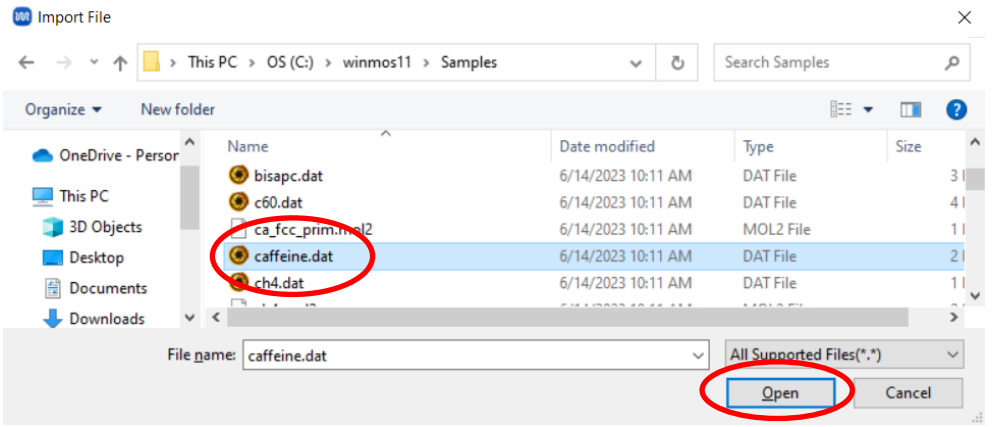
D. Click **Import**, then click **OK**, and the 3D structure of Benzene will appear.

C. Import File（Caffeine）

A. Click **File | New File**, **New Project**, or **Edit | Reset Structure**.

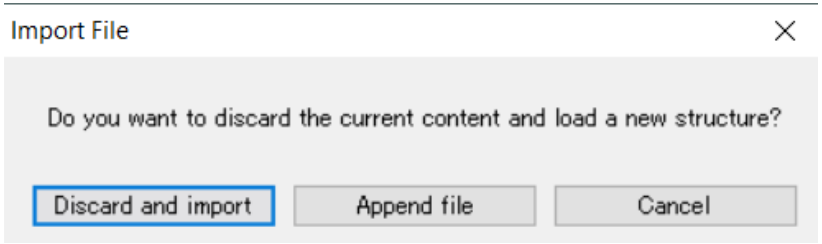
B.  Click **File | Import File**, select **caffeine.dat** from the Samples folder one level above, then click **Open**.

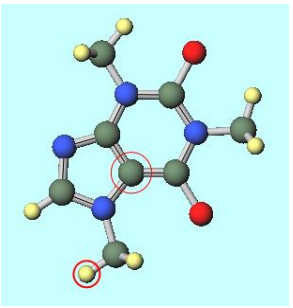




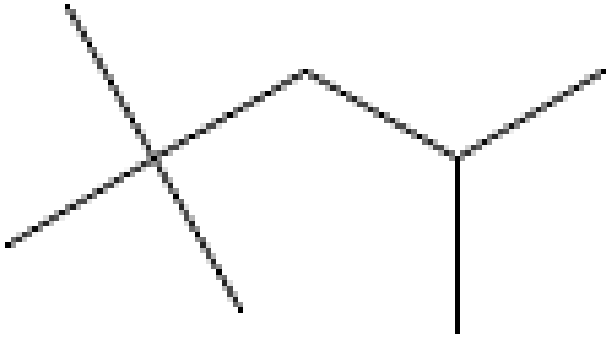
Note: You can perform the same operation by dragging and dropping a file from Explorer into Winmostar.

C. Click **Discard and Load** to display the 3D structure of caffeine.

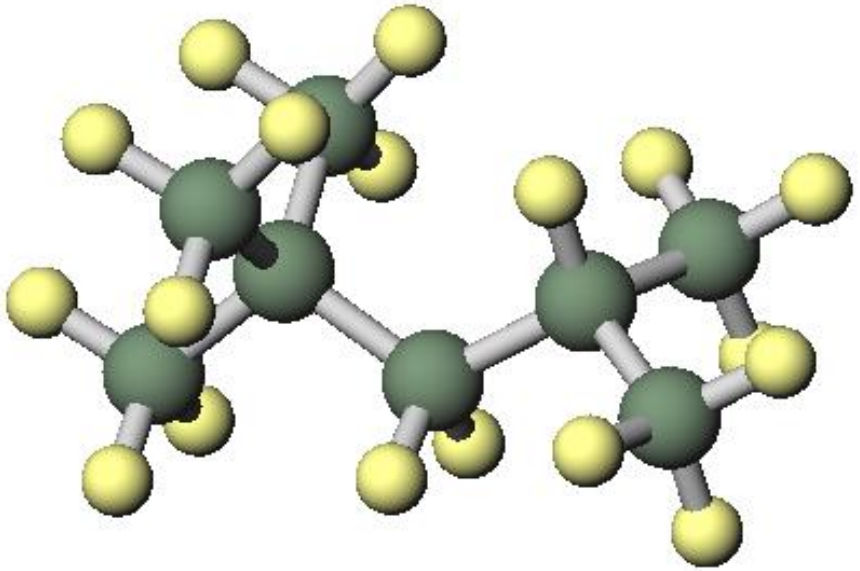




D. Directly modeling （Isooctane)



Structural Formula



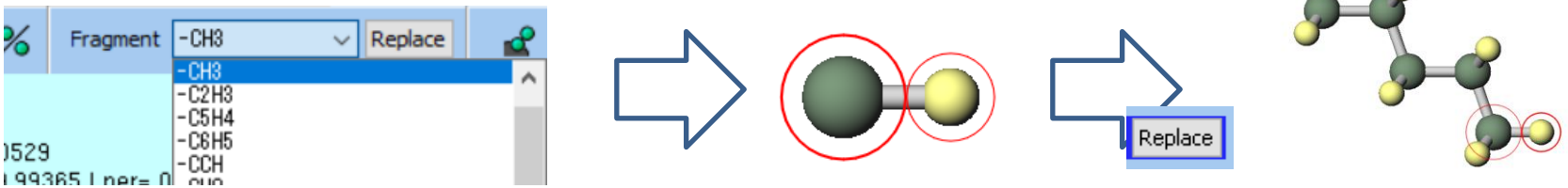
3D Model

D. Directly modeling (Isooctane)

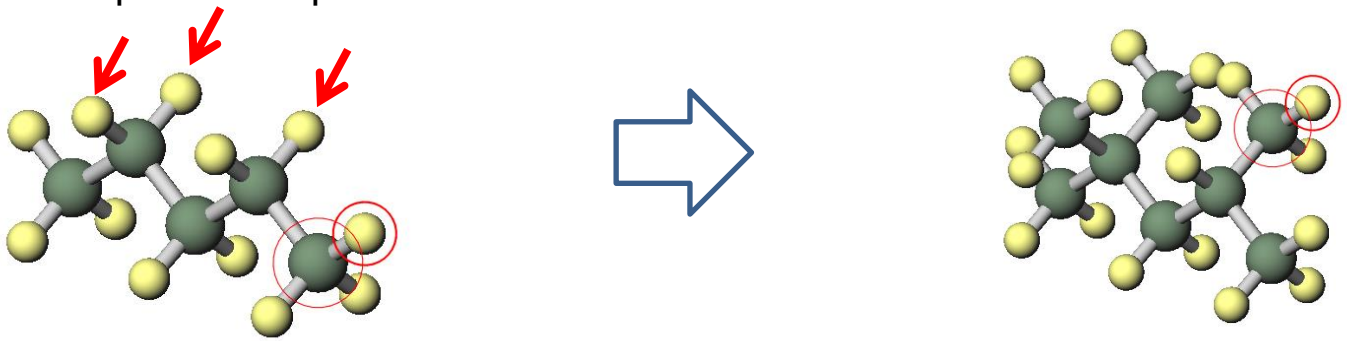
If only 'Click' is mentioned, it refers to left-clicking.

A. Click **File | New File**, **New Project**, or **Edit | Reset Structure**.

B. Select '-CH3' under **Fragment**, and click Replace **Replace marked atom with fragment** five times to create n-pentane.



C. After adjusting the camera angle by dragging, click on each of the three hydrogen atoms indicated by the arrows in the figure, then **click Replace marked atom with fragment**. Repeat this process to create isooctane.

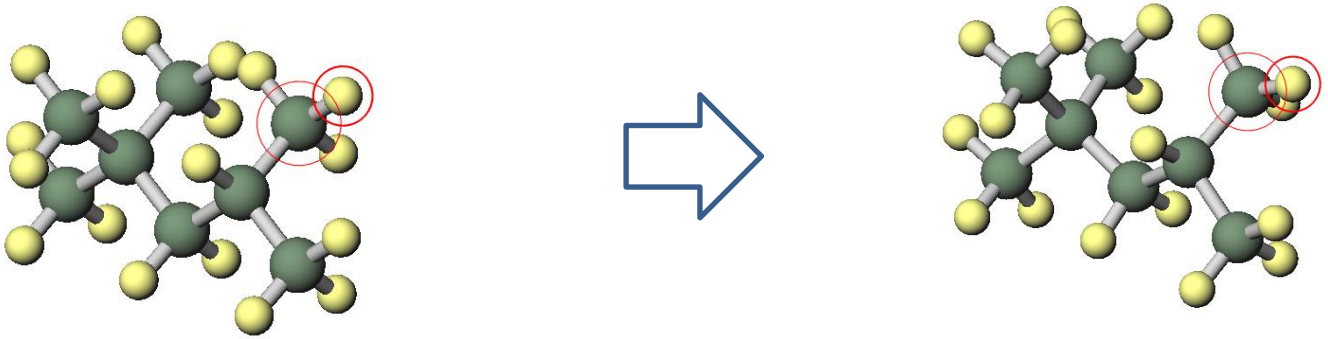


Note: You can perform an equivalent operation to 'Replace with Fragment' more easily by directly Shift+Ctrl+right-clicking on an atom.

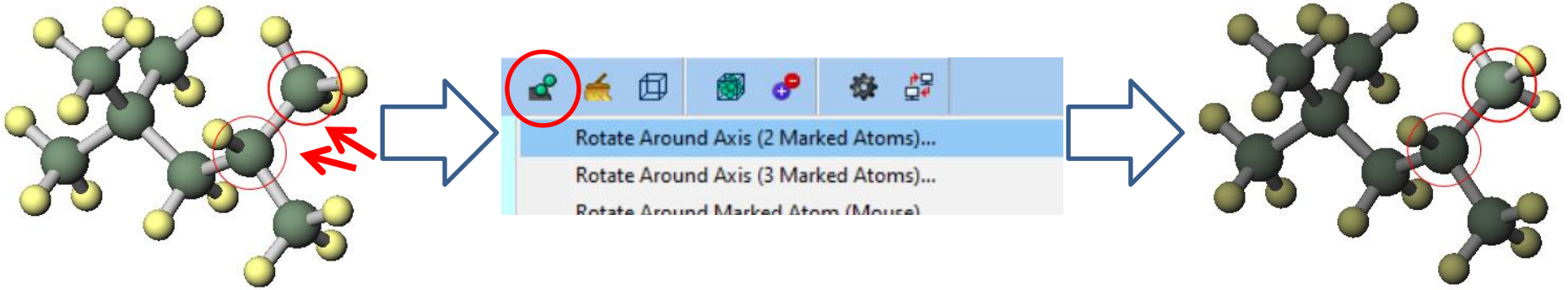
D. Directly modeling (Isooctane)

If only 'Click' is mentioned, it refers to left-clicking.

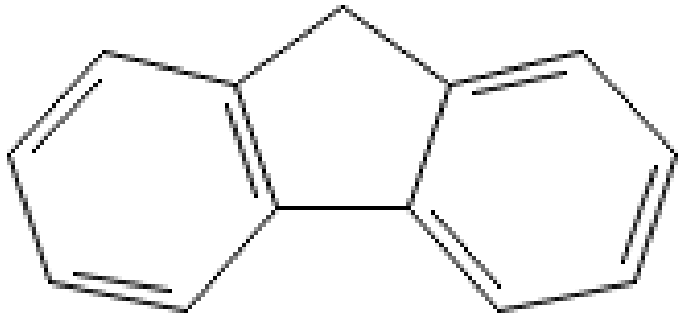
D. Clicking  **Quick Optimization** automatically adjusts bond lengths and angles to reasonable values.



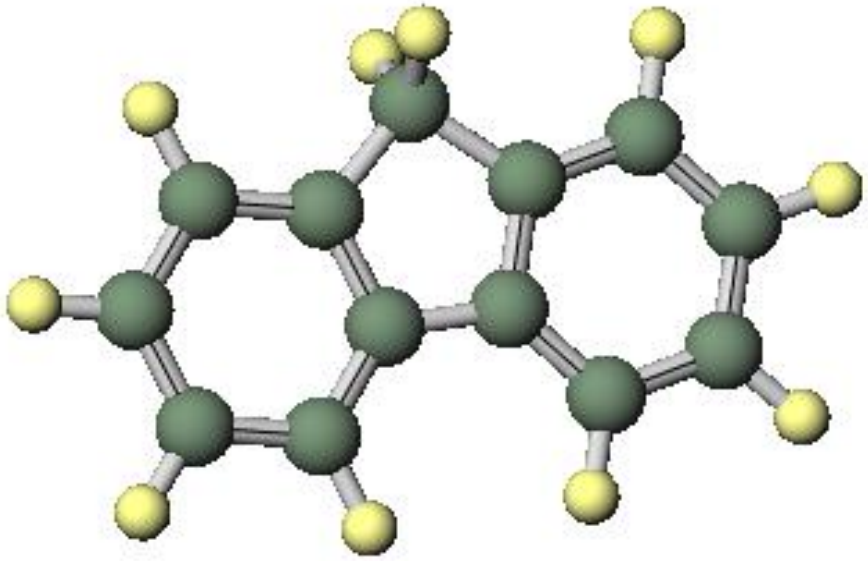
E. To explicitly rotate a dihedral angle, click both atoms at the ends of the bond you want to rotate, then click  **Modify Selected Group | Rotate Around Axis (2 Marked atoms)**. After that, drag over the molecular structure to rotate the dihedral angle.



E. Directly modeling（Fluorene)



Structural Formula



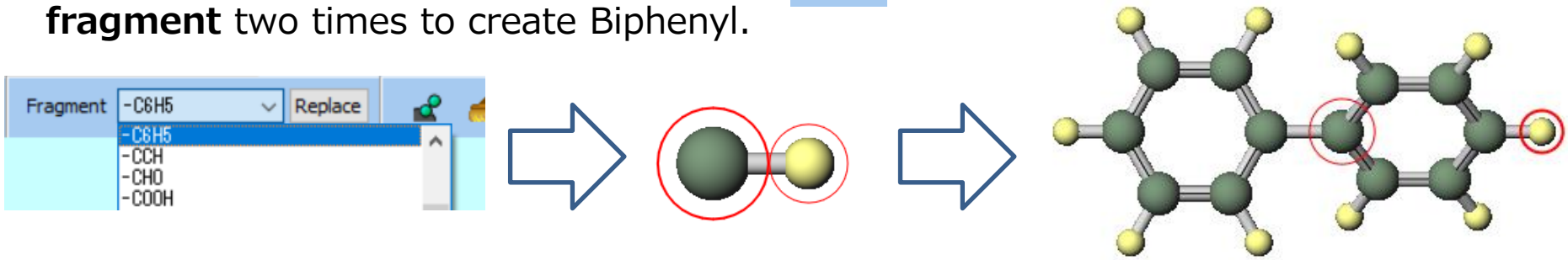
3D Model

E. Directly modeling（Fluorene)

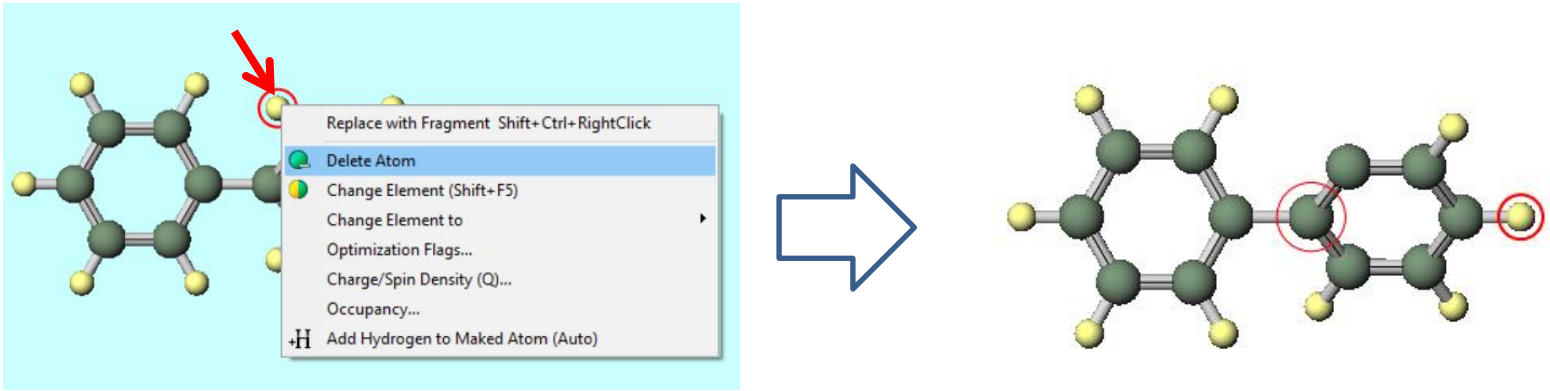
If only 'Click' is mentioned, it refers to left-clicking.

A. Click **File | New File**, **New Project**, or **Edit | Reset Structure**.

B. Select '-C6H5' under **Fragment**, and click Replace **Replace marked atom with fragment** two times to create Biphenyl.



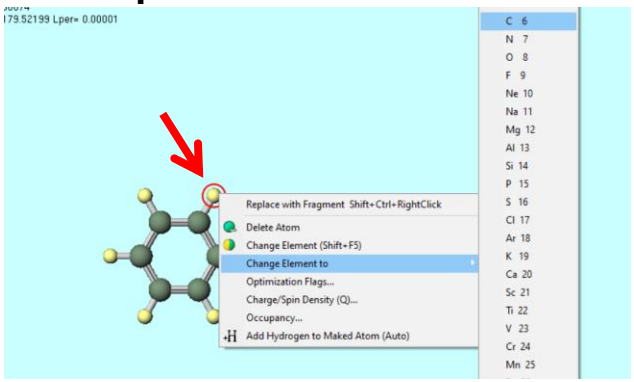
C. Right-click on the hydrogen atom shown in the diagram below and click **Delete Atom**.

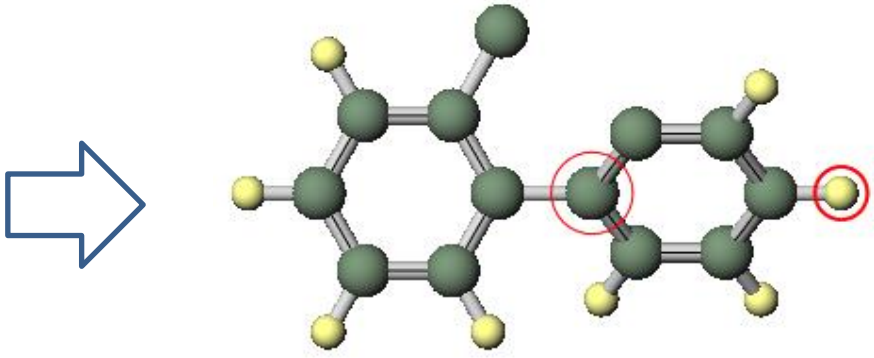


E. Directly modeling （Fluorene)

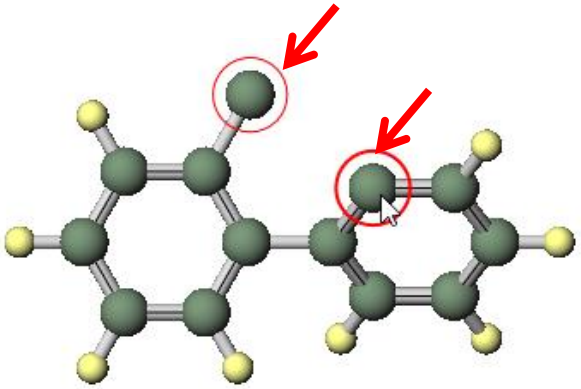
If only 'Click' is mentioned, it refers to left-clicking.

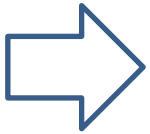
D. Right-click on the hydrogen atom shown in the diagram below and click **Change Element to | C 6.**

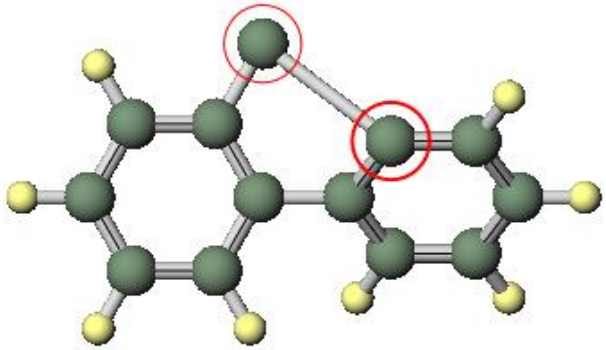




E. Sequentially click  on the two carbon atoms indicated by arrows in the diagram below, then click **Add/Change Bond**.

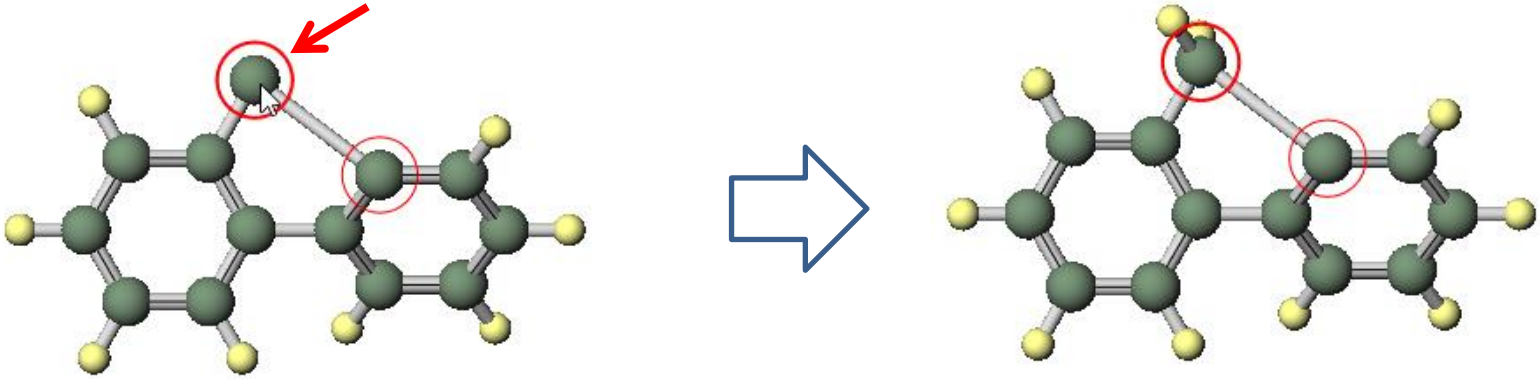




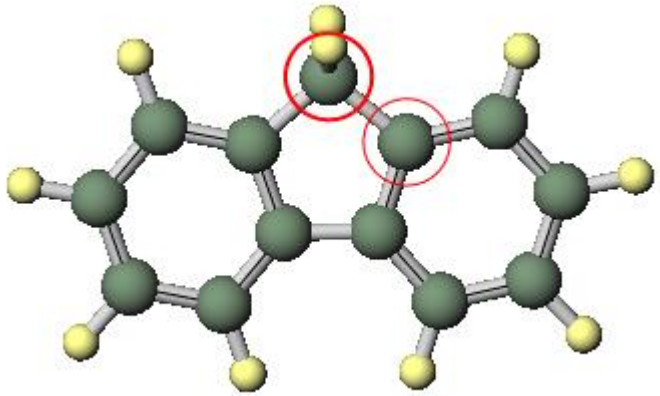


E. Directly modeling（Fluorene)

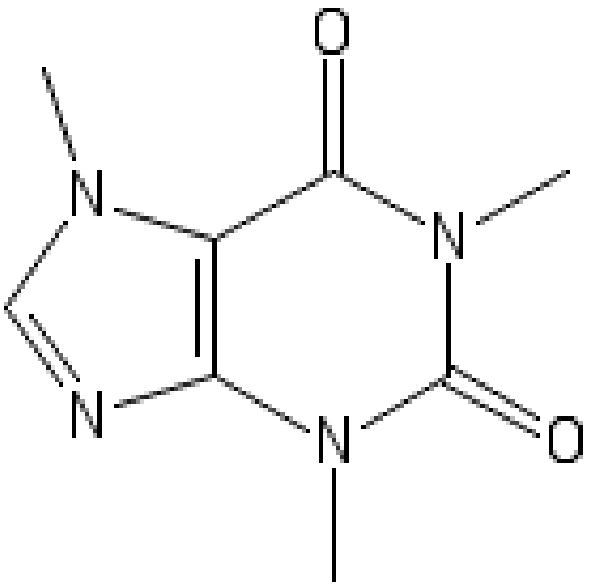
F. Click on the carbon atom shown in the diagram below and then double-click  **Add Hydrogen to Maked Atom**.



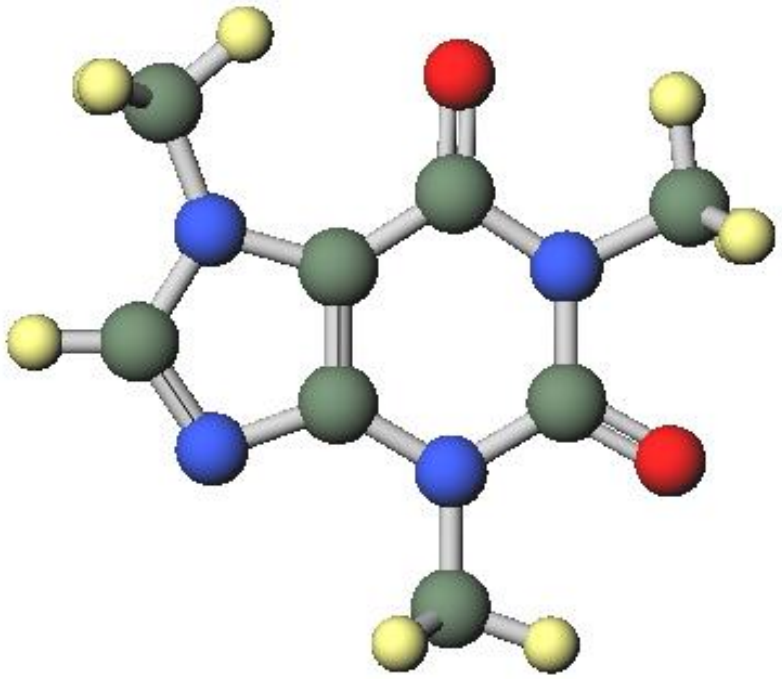
G. Clicking  **Quick Optimization** automatically adjusts bond lengths and angles to reasonable values.



F. Directly modeling （Caffeine）



Structural Formula

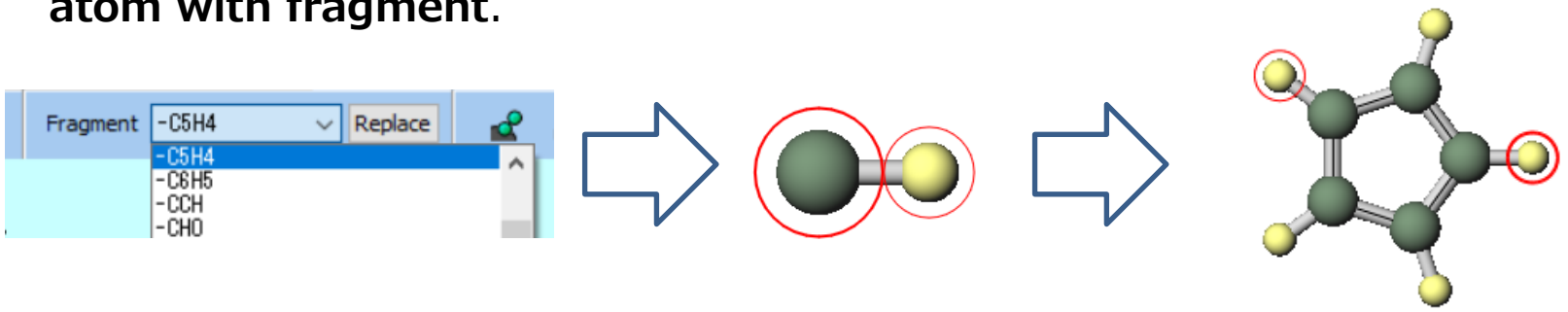


3D Model

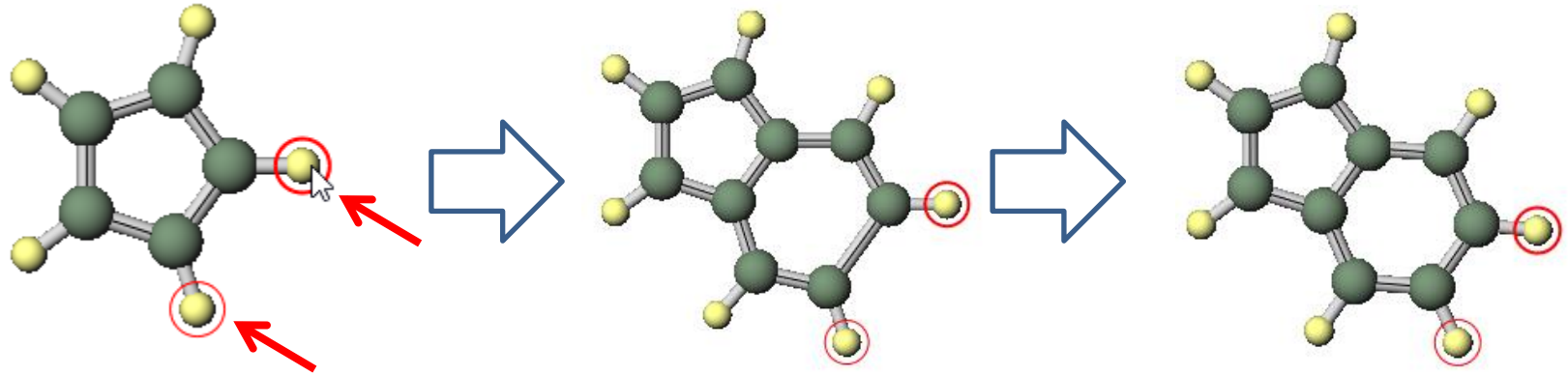
F. Directly modeling （Caffeine）

A. Click **File | New File**, **New Project**, or **Edit | Reset Structure**.

B. Select '-C5H4' under **Fragment**, and double-click Replace **Replace marked atom with fragment**.



C. Sequentially click on the two hydrogen atoms indicated by arrows in the diagram below, then click **Edit | Build Ring** and finally click **Quick Optimization**.

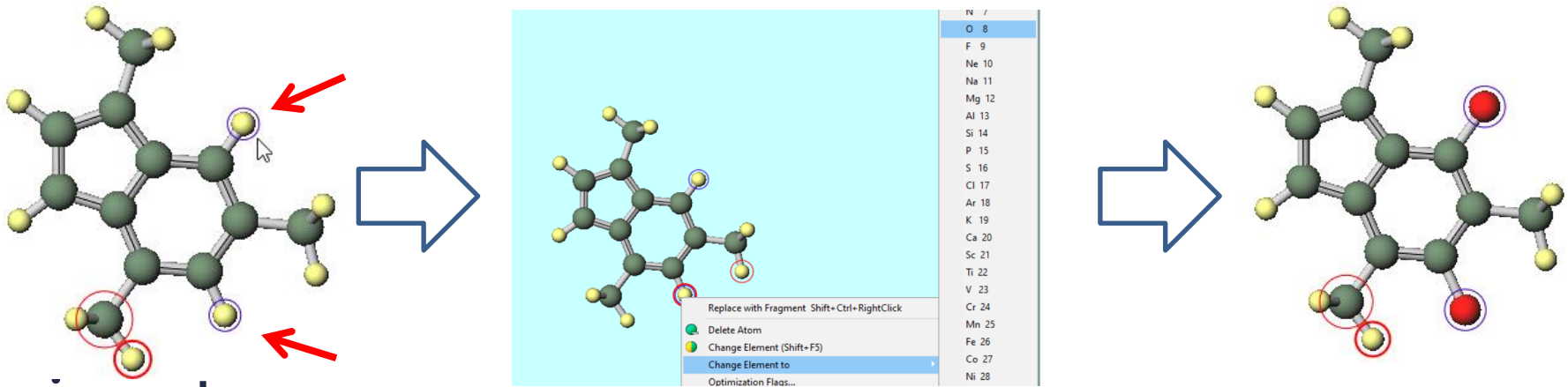


F. Directly modeling （Caffeine）

If only 'Click' is mentioned, it refers to left-clicking.

D. Select '-CH3' from **Fragment**, for the three hydrogen atoms indicated by the arrows in the figure, click each atom followed by clicking Replace **Replace marked atom with fragment**, and repeat this process.

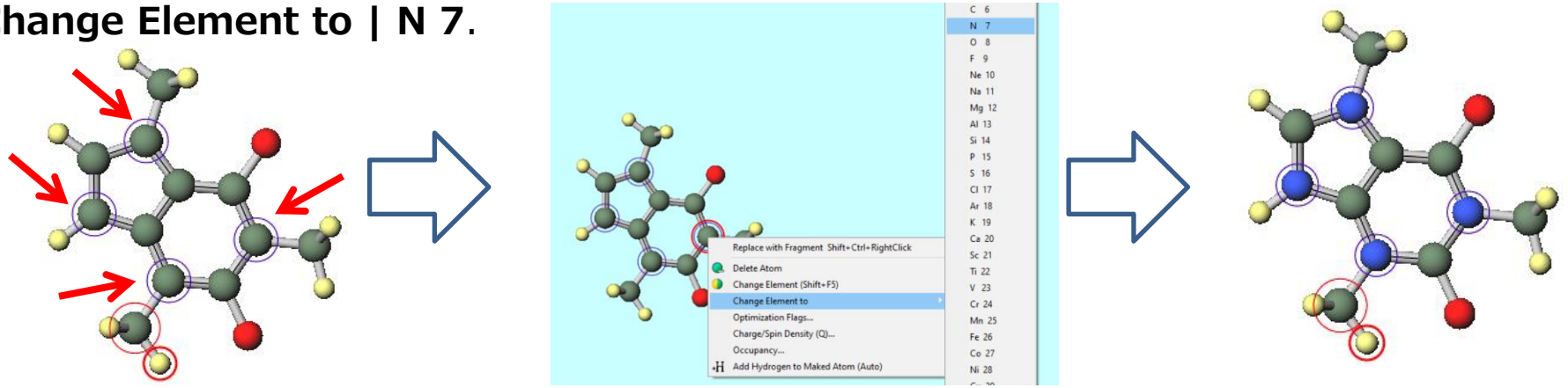
E. Sequentially Ctrl+click on the two hydrogen atoms indicated by arrows in the diagram below, then right-click on one of the atoms and click **Change Element to | O 8**.



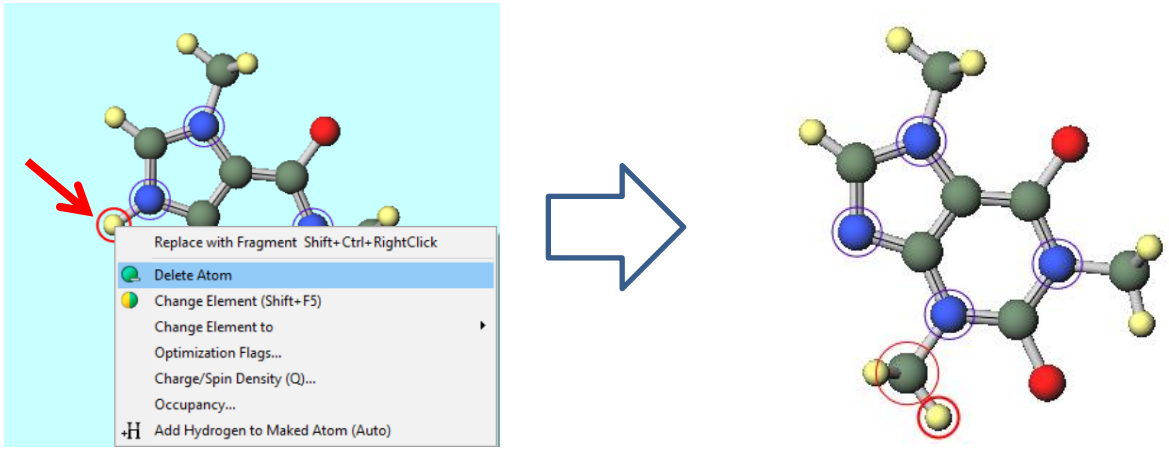
F. Directly modeling (Caffeine)

If only 'Click' is mentioned, it refers to left-clicking.

F. Click **Select | Invert Selection**, then sequentially Ctrl+click on the four hydrogen atoms indicated by arrows in the diagram below. Right-click on one of the atoms and click **Change Element to | N 7**.

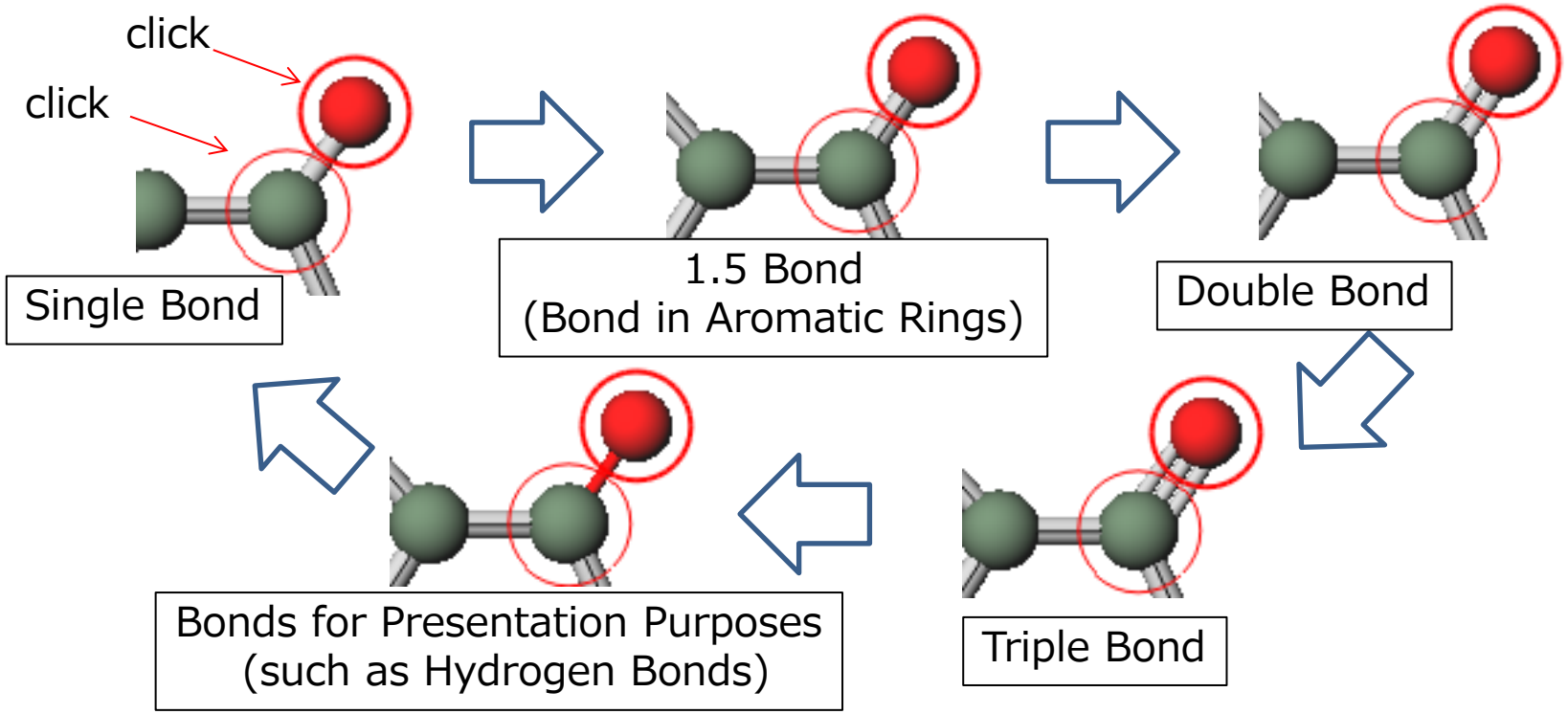


G. Right-click on the hydrogen atom shown in the diagram below and click **Delete Atom**.

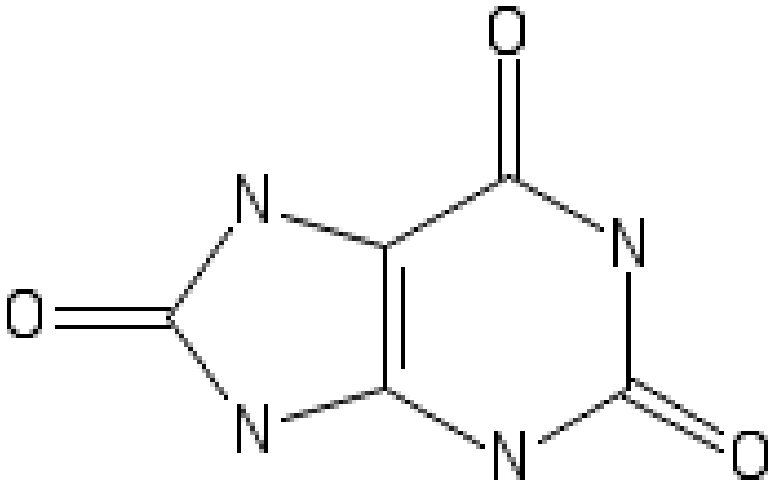


Supplement: Changing Bonds

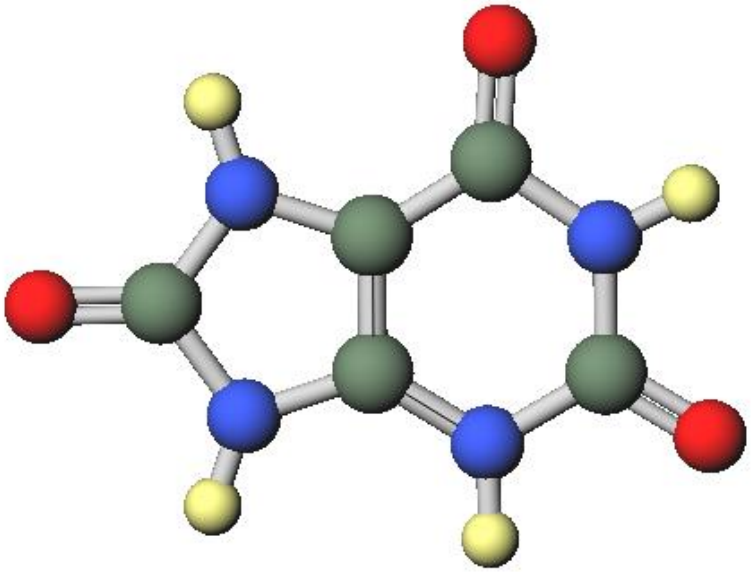
- To change the bond order (such as single or double bonds), sequentially click on the two atoms at either end of the bond and then click **Add/Change Bond**.
- However, keep in mind that the bond order does not affect the results of quantum chemical calculations and first-principles simulations. Therefore, it is not problematic for these calculations if the bond order is not accurately represented.



G. Directly modeling （Uric acid）



Structural Formula



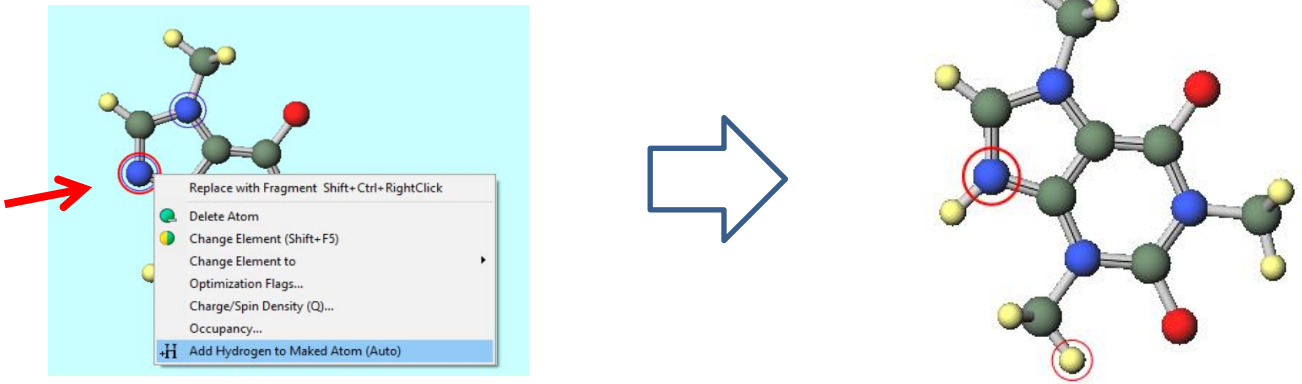
3D Model

G. Directly modeling (Uric acid)

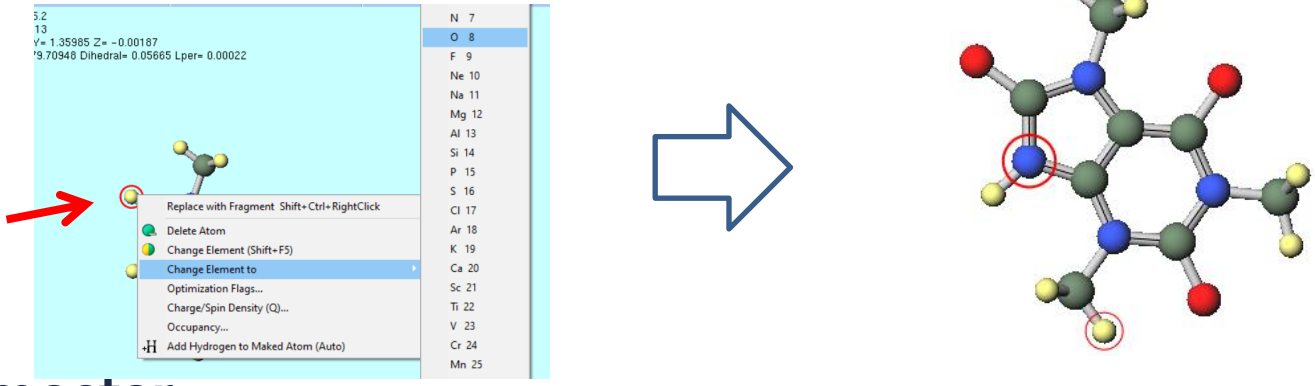
If only 'Click' is mentioned, it refers to left-clicking.

A. Start with the structure from **F. Directly modeling (Caffeine)** .

B. Right-click on the hydrogen atom shown in the diagram below and click **Add Hydrogen to Marked Atom**.

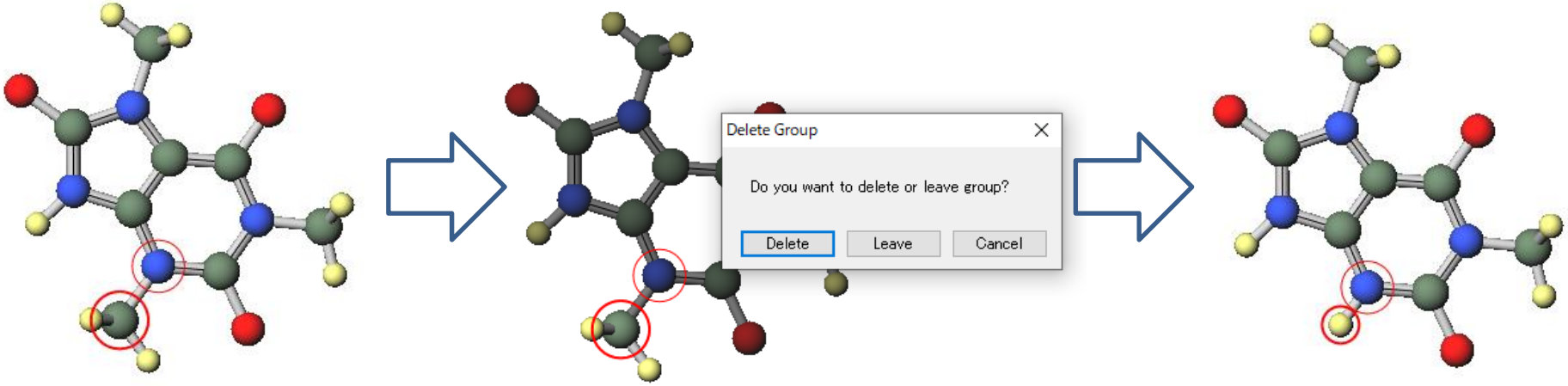


C. Right-click on the hydrogen atom shown in the diagram below and click **Change Element to | O 8**.

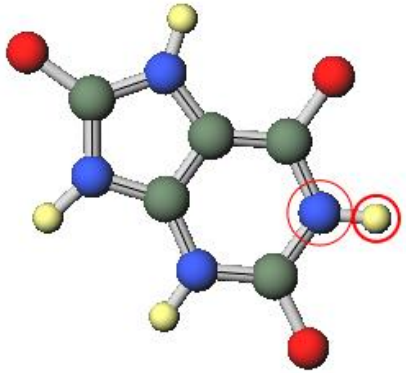


G. Directly modeling (Uric acid)

D. Sequentially click on the atoms indicated by arrows in the diagram below in the order of the numbers, then click **Modify Selected Group | Delete**, and finally click **Delete**.



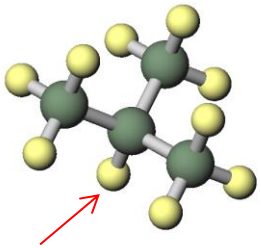
E. Repeat the procedure in step D to remove the remaining two methyl groups.



Supplement: Registration of Fragments

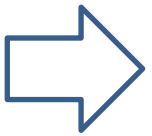
The molecules modeled can be registered as user-defined fragments (substituents).
As an example, the registration procedure for a tert-butyl group is shown below.

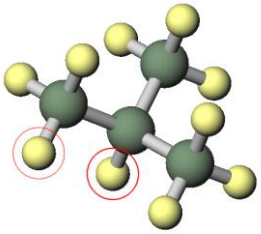
A. Model isobutane and click on the hydrogen atom indicated by the arrow.



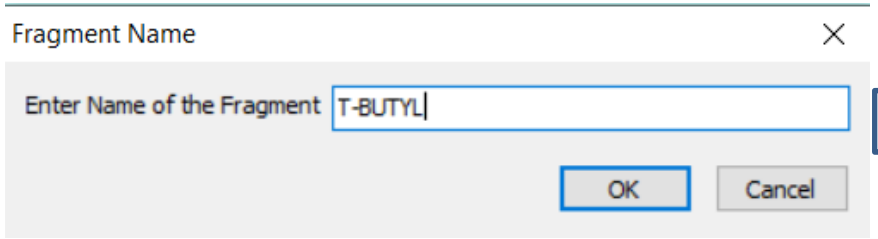
The position of the hydrogen atom selected here will be set as the starting point of the substituent.

B. Click **Edit | Select Fragment | Save Fragment**

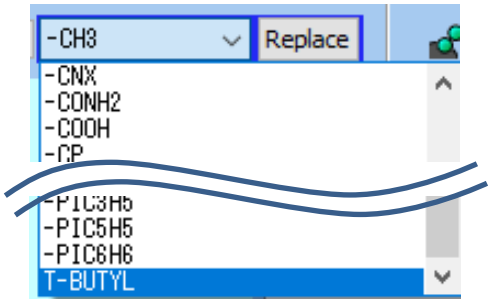




C. Enter 'T-BUTYL' in **Enter Name of the Fragment** and click **OK**.

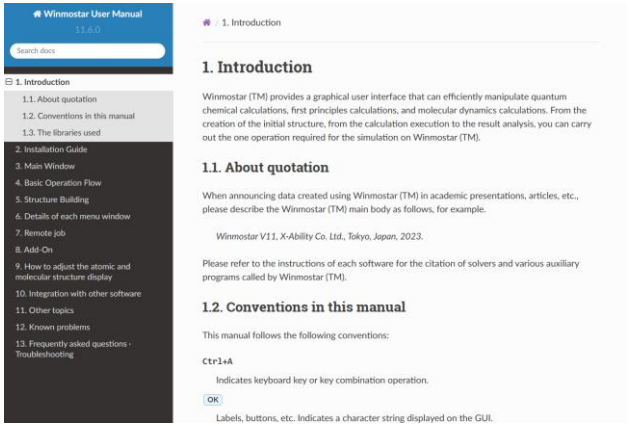


D. T-BUTYL' will now appear in **Fragment**.



Troubleshooting and Additional Resources

- For detailed information on each feature, please refer to Winmostar User Manual.



Winmostar User Manual

- If you are unable to proceed as instructed in this guide, please first refer Frequently asked questions.
- If FAQs do not resolve your issue, for the purposes of information accumulation and management, please contact us through Contact, detailing the steps to reproduce the issue and attaching any generated files at that time.