Covalent links in ACEDRG

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Covalent Links in Acedrg

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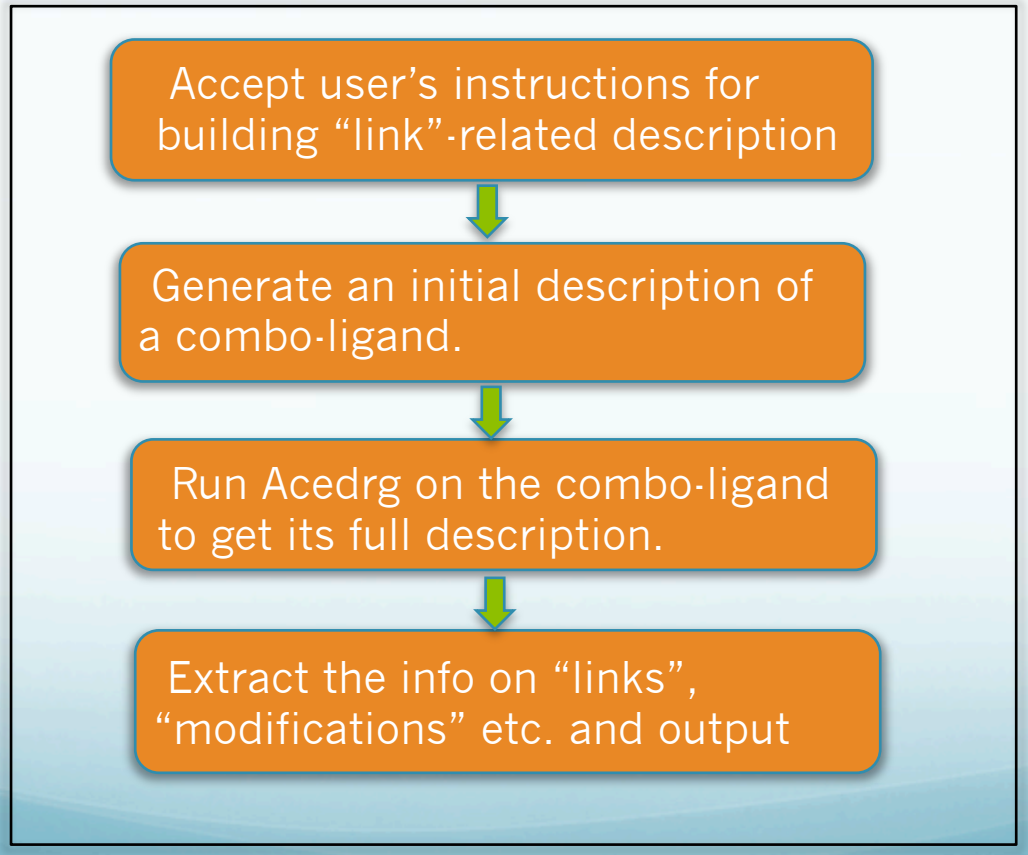
Covalent Links in Acedrg

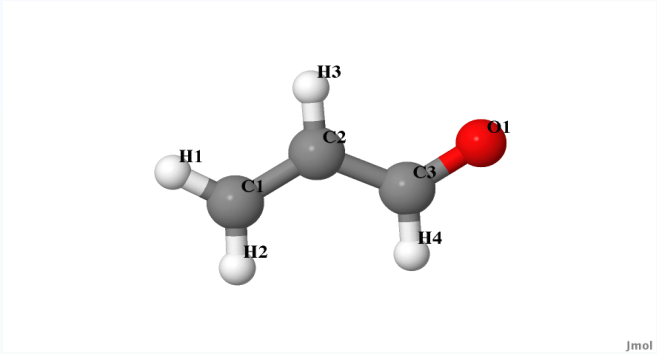
Flowchart for ‘‘link’’ in Acedrg



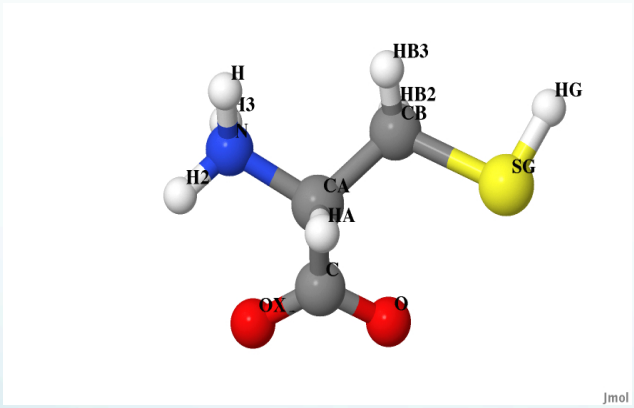
Covalent Links in Acedrg

A Few Cases on Covalent Links in Acedrg

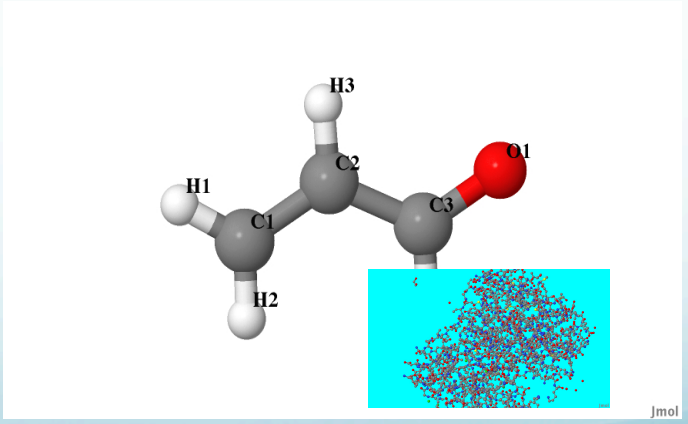
Case 1



Monomer ‘‘TMP’’



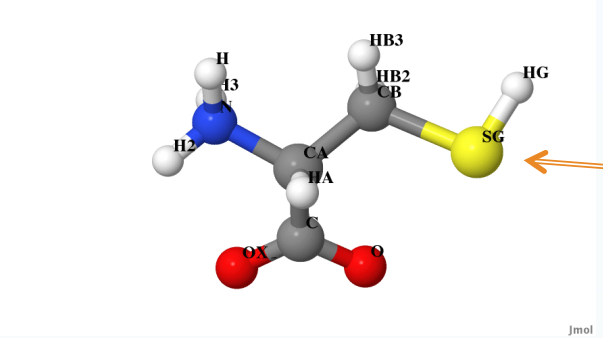
CYS

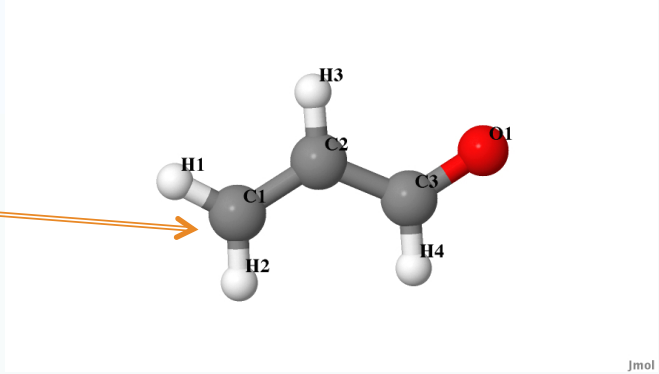


Real Structure

Covalent Links in Acedrg

Case 1: Scenario 1





CYS

Monomer ‘‘TMP’’

No change in the bond between C1 and C2 in ‘‘TMP’’

Covalent Links in Acedrg

Case 1: Scenario 1

Acedrg command-line

acedrg -L inFiles/instruct_case1_sce1.txt -o case1_CYS_TMP_1

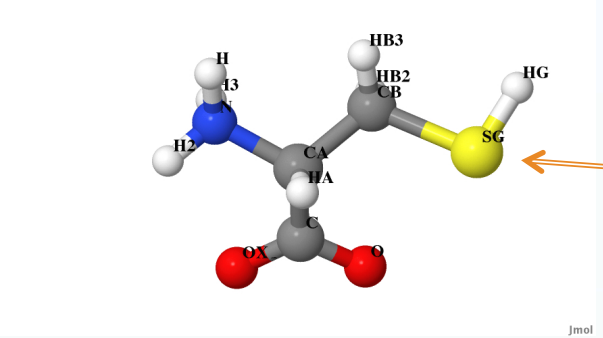
- It uses an instruction file: **instruct_case1_sce1.txt**
- It generates the dictionary file: **case1_CYS_TMP_1_link.cif**

instruct_case1_sce1.txt

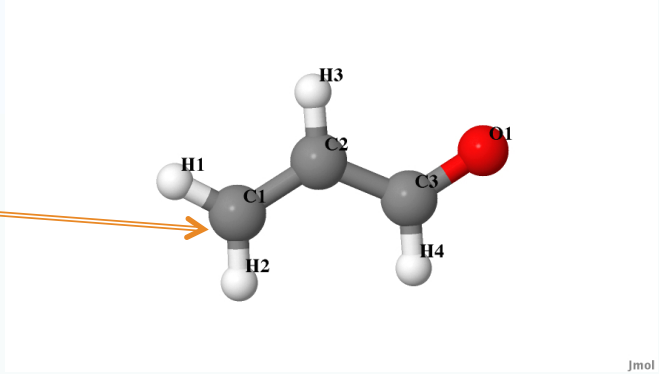
LINK: RES-NAME-1 CYS ATOM-NAME-1 SG RES-NAME-2 TMP FILE-2 inFiles/case2_comp1.cif ATOM-NAME-2 C1

Covalent Links in Acedrg

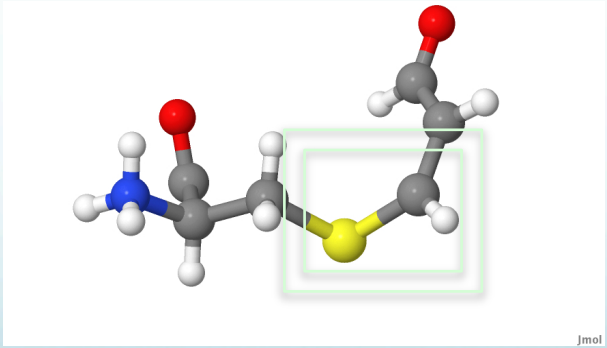
Case 1: Scenario 1



CYS



Monomer ‘‘TMP’’



The Linked molecule

Covalent Links in Acedrg

Case 1: Scenario 1

case1_CYS_TMP_1_link.cif

List Section

```
data_link_list

loop_
_chem_link.id
_chem_link.comp_id_1
_chem_link.mod_id_1
_chem_link.group_comp_1
_chem_link.comp_id_2
_chem_link.mod_id_2
_chem_link.group_comp_2
_chem_link.name
CYS-TMP       CYS      CYSmod1    L-PEPTIDE          TMP      TMPmod1
non-polymer         CYS-TMP
```

Covalent Links in Acedrg

Case 1: Scenario 1

case1_CYS_TMP_1_link.cif

Component Section

```
data_comp_CYS

#
loop_
_chem_comp_atom.comp_id
_chem_comp_atom.atom_id
_chem_comp_atom.type_symbol
_chem_comp_atom.type_energy
_chem_comp_atom.charge
_chem_comp_atom.x
_chem_comp_atom.y
_chem_comp_atom.z
CYS     N       N       NT3     1       1.551       14.790      38.686
CYS     CA      C       CH1     0       0.616       13.682      39.054
CYS     C       C       C       0       1.049       13.053      40.388
```

Covalent Links in Acedrg

Case 1: Scenario 1

case1_CYS_TMP_1_link.cif

Component Section

```
data_comp_CYS

#
loop_
_chem_comp_atom.comp_id
_chem_comp_atom.atom_id
_chem_comp_atom.type_symbol
_chem_comp_atom.type_energy
_chem_comp_atom.charge
_chem_comp_atom.x
_chem_comp_atom.y
_chem_comp_atom.z
CYS     N       N       NT3     1       1.551       14.790      38.686
CYS     CA      C       CH1     0       0.616       13.682      39.054
CYS     C       C       C       0       1.049       13.053      40.388
```

Covalent Links in Acedrg

case1_CYS_TMP_1_link.cif

Modification Section

```
data_mod_TMPmod1
loop_
_chem_mod_atom.mod_id
_chem_mod_atom.function
_chem_mod_atom.atom_id
_chem_mod_atom.new_atom_id
_chem_mod_atom.new_type_symbol
_chem_mod_atom.new_type_energy
_chem_mod_atom.new_charge
TMPmod1       delete       H2       .       H       H       0
TMPmod1       change       C1       .       C       C1       0
loop_
_chem_mod_bond.mod_id
_chem_mod_bond.function
_chem_mod_bond.atom_id_1
_chem_mod_bond.atom_id_2
_chem_mod_bond.new_type
_chem_mod_bond.new_value_dist
_chem_mod_bond.new_value_dist_esd
TMPmod1       delete       C1       H2       single       .            .
```

Covalent Links in Acedrg

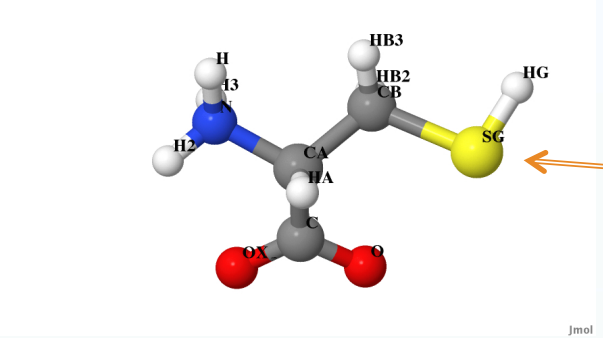
case1_CYS_TMP_1_link.cif

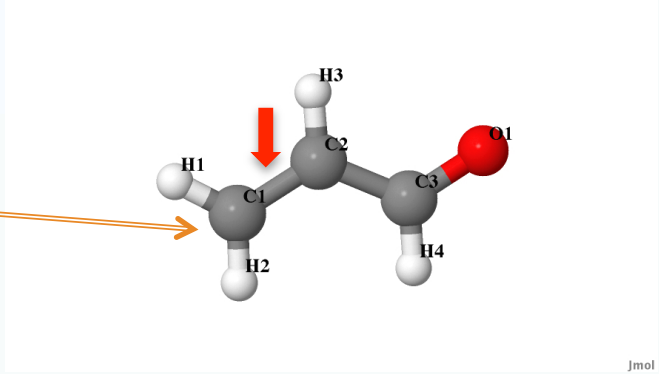
Link Section

```
data_link_CYS-TMP
loop_
_chem_link_bond.link_id
_chem_link_bond.atom_1_comp_id
_chem_link_bond.atom_id_1
_chem_link_bond.atom_2_comp_id
_chem_link_bond.atom_id_2
_chem_link_bond.type
_chem_link_bond.value_dist
_chem_link_bond.value_dist_esd
CYS-TMP   1       SG      2       C1      SINGLE    1.732     0.010
loop_
_chem_link_angle.link_id
_chem_link_angle.atom_1_comp_id
_chem_link_angle.atom_id_1
_chem_link_angle.atom_2_comp_id
_chem_link_angle.atom_id_2
_chem_link_angle.atom_3_comp_id
_chem_link_angle.atom_id_3
_chem_link_angle.value_angle
_chem_link_angle.value_angle_esd
CYS-TMP   1       CB      1       SG      2       C1      100.987     2.18
CYS-TMP   2       C2      2       C1      1       SG      122.125     3.00
CYS-TMP   1       SG      2       C1      2       H1      117.563     1.50
```

Covalent Links in Acedrg

Case 1: Scenario 1





CYS

Monomer ‘‘TMP’’

The bond between C1 and C2 in ‘‘TMP’’ becomes ‘‘single’’

Covalent Links in Acedrg

Case 1: Scenario 1

Acedrg command-line

acedrg -L inFiles/instruct_case1_sce2.txt -o case1_CYS_TMP_2

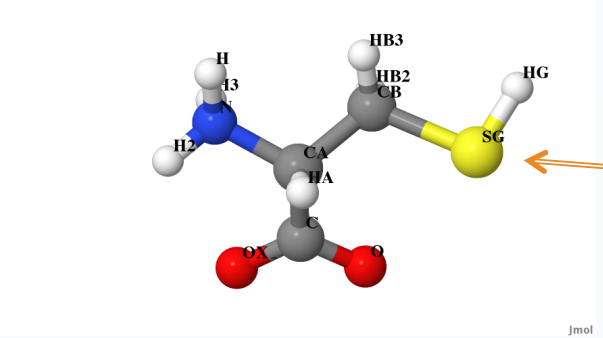
- It uses an instruction file: **instruct_case1_sce2.txt**
- It generates the dictionary file: **case1_CYS_TMP_2_link.cif**

instruct_case1_sce2.txt

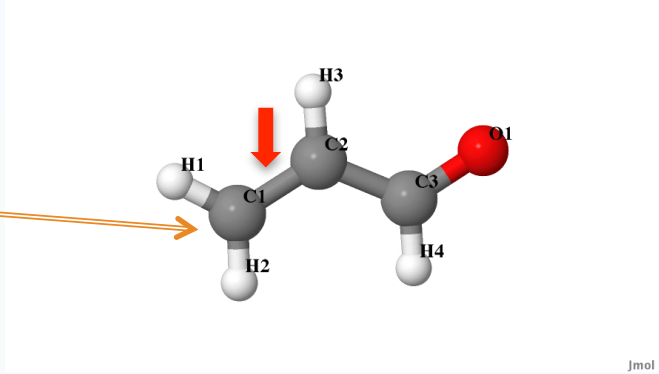
```
LINK: RES-NAME-1 CYS ATOM-NAME-1 SG RES-NAME-2 TMP FILE-2 inFiles/case2_comp1.cif ATOM-NAME-2 C1
CHANGE BOND C1 C2 SINGLE 2
```

Covalent Links in Acedrg

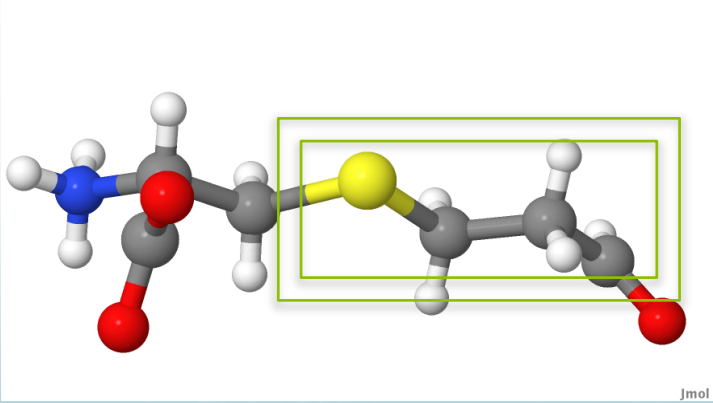
Case 1: Scenario 2



CYS



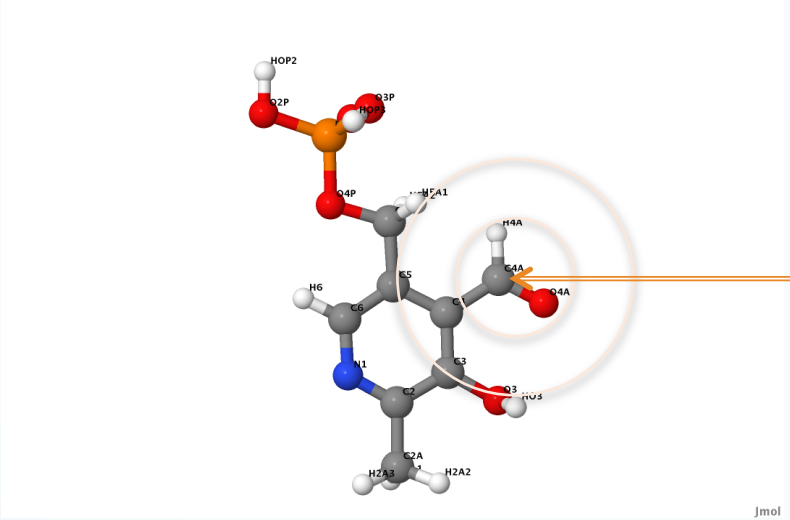
Monomer ‘‘TMP’’

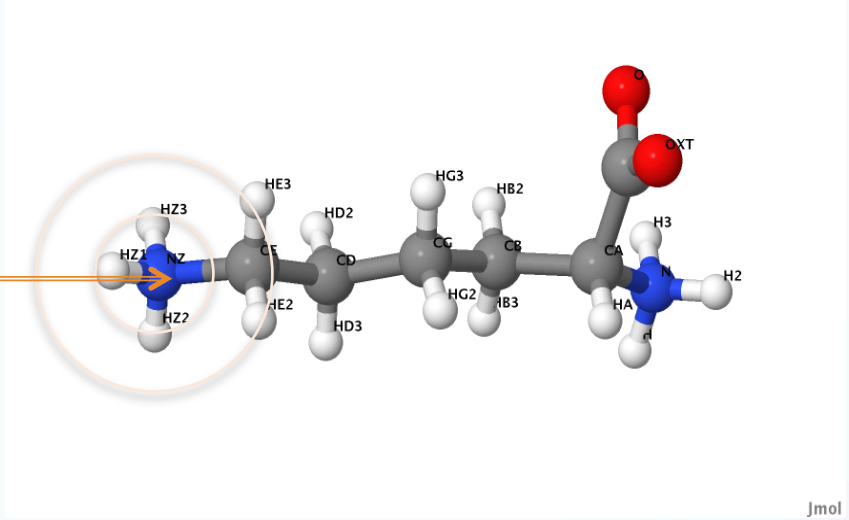


The Linked molecule

Covalent Links in Acedrg

Case 2





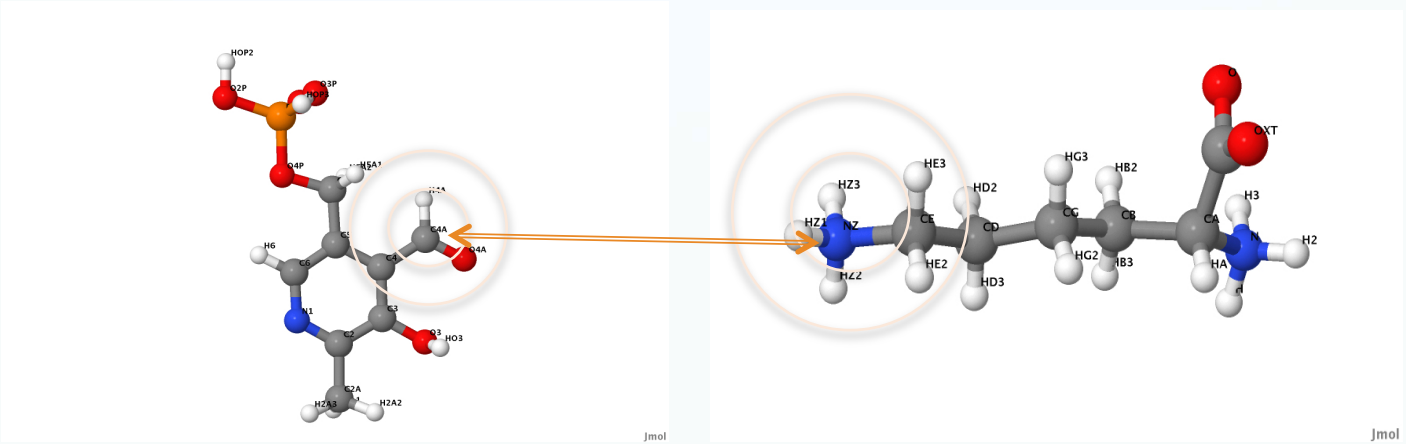
PLP **LYS**

instruct_LYS_PLP.txt

LINK: RES-NAME-1 LYS ATOM-NAME-1 NZ RES-NAME-2 PLP ATOM-NAME-2 C4A
DELETE ATOM O4A 2

Covalent Links in Acedrg

Case 2



PLP **LYS**