MRC Laboratory of Molecular Biology

# ACEDRG: Current Status And Future

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# Functionality and usage

A. ACEDRG used as  a Ligand/Dictionary/ Restraint generator

B. ACEDRG used to derive  molecules, atom types, bond lengths and angles in small molecule structures or ligands (table generator)

# Functionality and usage

## A. ACEDRG used as a Ligand/Dictionary/ Restraint generator:

1) Take input files of SMILES, SYBIL/MOL2, SDF/MDL, mmCIF formats

2) Output Dictionary (restraint) files of mmCIF format, which contain atom types, bond lengths and angles, torsion angles, planes and chirality centers, and are used as restraint files for refinements.

3) Output coordinate files of PDB format, which represent one of lower energy conformations for the ligands under consideration.

# Functionality and usage

## A. ACEDRG used as a Ligand/Dictionary/ Restraint generator:

Some command options:

1) Input: MMCIF Output : MMCIF and PDB

```
acedrg –c your_cif_file –r your_three_letter –o your_out_root
```

2) Input: MMCIF Output: MMCIF and PDB (no intensive geometric optimization, interested in Dictionary only)

```
acedrg –z –c your_cif_file –r your_three_letter –o your_out_root
```

3) Input : MMCIF Output: a file containing atom types only

```
acedrg –n –c your_cif_file –r your_three_letter –o your_out_root
```

# Functionality and usage

## A. ACEDRG used as a Ligand/Dictionary/ Restraint generator:

Some command options:

1) Input: SMILES Output : MMCIF and PDB

acedrg –i your_cif_file –r your_three_letter –o your_out_root

2) Input: Mol2 Output: MMCIF and PDB

acedrg –m your_cif_file –r your_three_letter –o your_out_root

3) Input : Others Output: MMCIF and PDB

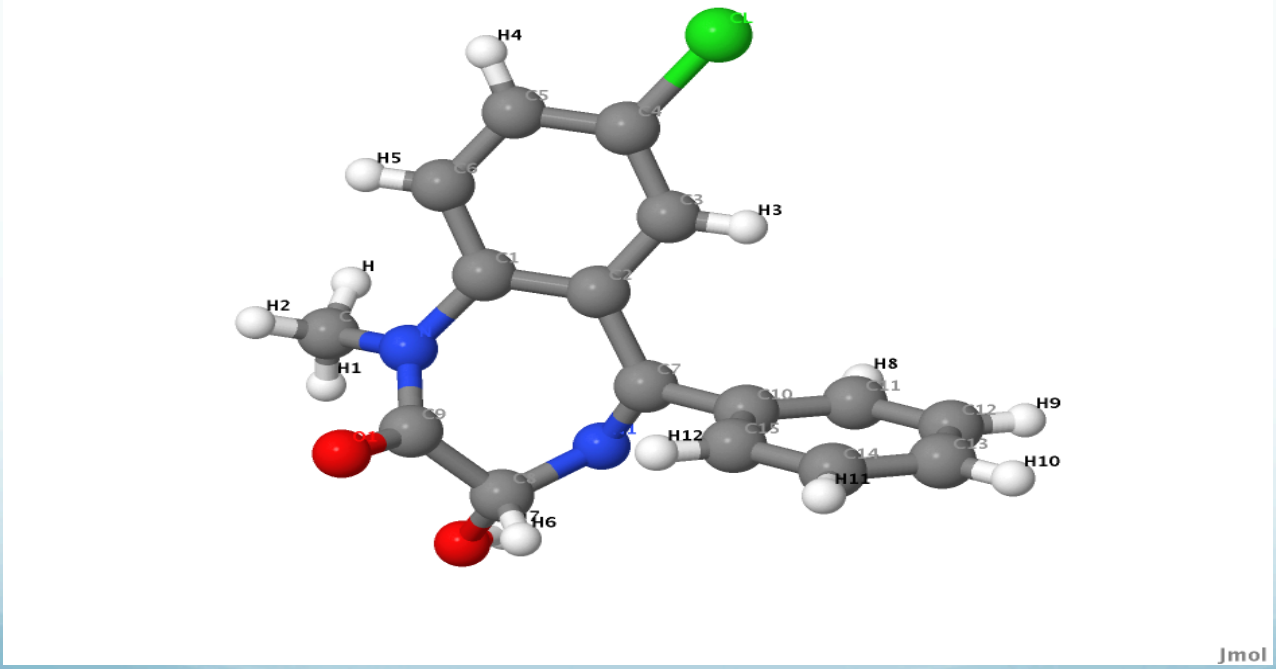
SDF –s. Small molecule files from CSD are CIF format, will be done.

# Functionality and usage

## Ligand/Dictionary generator

SMILES STRING:

CN1C2=C(C=C(Cl)C=C2)C(=NC(O)C1=O)C1=CC=CC=C1



# Functionality and usage

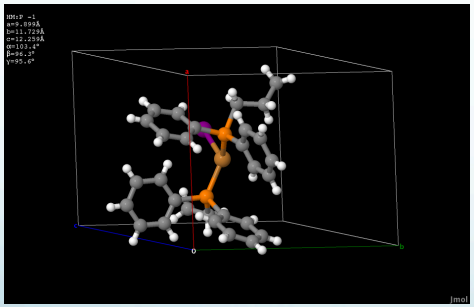
A. ACEDRG used as  a Ligand/Dictionary/ Restraint generator:

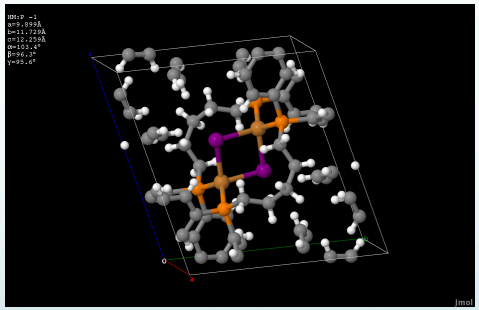
Demonstrations

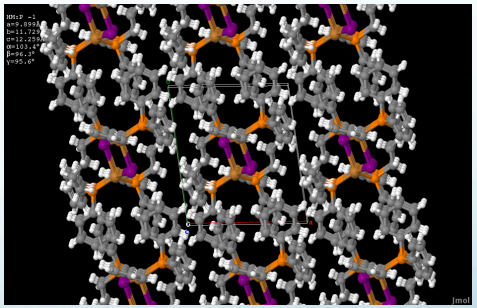
# Functionality and usage

A. ACEDRG used to derive molecules, atom types, bond lengths and angles from small molecule files of CIF format:

From small molecule structures to atom types, bond lengths and molecules







# Functionality and usage

## A. ACEDRG used to derive molecules, atom types, bond lengths and angles from small molecule files of CIF format:

Some command options:

1) Input: CIF  Output : text files for molecules, atom types, bond lengths and angles

```
acedrg –e –b your_cif_file  –o your_out_root
```

2) Input:  a directory containing small molecule CIF files  Output: a table contain molecules, atom types, bond lengths and angles, and some statistics

```
acedrg  –e   –d your directory  –o your_out_root
```

# Functionality and usage

## A. ACEDRG used to derive molecules, atom types, bond lengths and angles from small molecule files of CIF format:

Further improvements:

1) Atom type improvements:
   i. Show explicitly ring planarity

   From: C[6,6](C[5,6]C3)(C[6,6]CC)(C[6]CH)

   To: C[6p,6](C[5,6p]C3)(C[6,6]CC)(C[6]CH)

   ii. Consider the third neighbor atom implicitly

# Functionality and usage

## A. ACEDRG used to derive molecules, atom types, bond lengths and angles from small molecule files of CIF format:

Further improvements:

2) Include small molecule data from sources other than COD.
   i. CSD data have CIF format. They can be input just like we deal with COD data
   ii. Other formats ?

# Future work

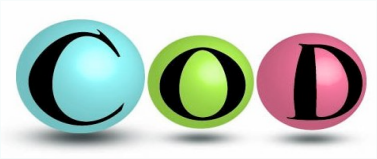
- Paul (?)
- Further improvement in terms of aromatic perception is under way.
- Statistical validations.
- Multiple conformations, modeling for tautomer and protonation.
- Metals. Initial statistical analysis and tabulation on coordination have been done. Substantial further work needed.
- Replace libcheck.

# Acknowledgement


contributors:

MRC Laboratory of Molecular Biology

Garib Murshudov, Paul Emsley, Rob Nicholls




Saulius Grazulis, and Andrius Merky


CCP4 core team