Center for BioMolecular Modeling

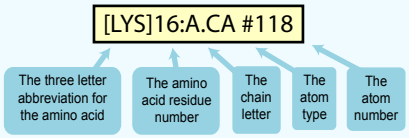
Jmol Quick Reference Sheet

version 2.1 - 6-18-18

For Use with the CBM's Jmol Design Environment: *http://cbm.msoe.edu/newWebsite/learnToModel*

Mouse Movements

Hovering over an atom will display some information about the atom in the Jmol Display Window



Rotate on the X-Y axes:

Zoom in and out: Shift

Translate the Molecule: Ctrl Alt

Rotate on the Z axis: Shift

Display Formats

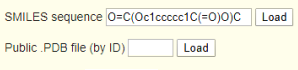
wireframe - *displays bonds as sticks*
- *example:* `wireframe`
- *example:* `wireframe 1.0`

spacefill - *displays atoms as spheres*
- *example:* `spacefill`
- *example:* `spacefill 1.25`
- *example:* `spacefill 40%`

backbone - *displays alpha carbon backbone*
- *example:* `backbone`
- *example:* `backbone 1.5`

Loading Structures and Saving Your Work

To load a new molecular structure, use the red load menu



To save or export your work, use the orange save menu

To load a previous design, simply drag your .spt file from your local computer into the Jmol Display Window on the right side of the screen.

Color Formats

color <color type> - *colors the selected area*
- *example:* `color red`
- *example:* `color [200,140,215]`
- *example:* `color structure`

List of Common Color Types:

`cpk`	`red`	`[R,G,B]`
`structure`	`green`	`chain`
`temperature`	`darkblue`	`group`

For a full list of the predefined colors available in Jmol, visit: http://jmol.sourceforge.net/jscolors/

Selection and Restriction

select <selection type> - *selects part of the file*
- *example:* `select helix`
- *example:* `select :a`
- *example:* `select 1-40`
- *example:* `select atomno=10`

restrict <selection type> - *removes the display of everything except what was restricted*
- *example:* `restrict carbon`
- *example:* `restrict atomno<50`

List of Common Selection Types:

`backbone`	`sidechain`	`hydrophobic`
`polar`	`charged`	`hetero`
`water`	`nucleic`	`protein`
`helix`	`sheet`	

`:<letter>` - *use a colon for selecting by chain letter*

`<number>` - *use numbers for selecting by residue*

`<number>-<number>` - *for selecting by residue range*

`atomno=<number>` - *for selecting by atom number*

`atomno>=<number> and atomno<=<number>` - *for selecting by atom range*

`<element name>` - *for selecting by atom type*

Standard Sizes for 3D Printing

`backbone 1.5`	`hbond 1.0`
`wireframe 1.0`	`strut 1.0`
`spacefill 1.25`	`ssbond 1.0`

Adding a "Clean" Sidechain

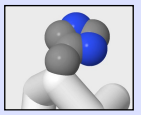
select <residue number> and sidechain - *select only the sidechain atoms of a specific amino acid*

example:
```
select cys30 and sidechain
spacefill 1.25
wireframe 1.0
```

To remove an incorrectly displayed sidechain:

example:
```
select cys30 and sidechain
spacefill off
wireframe off
```

Sidechain with "bumpy" backbone atoms showing



A "clean" sidechain with no backbone atoms poking out

Bonds and Struts

Hydrogen Bonds:

`calculate hbonds` - *algorithmically dads hydrogen bonds to all selected areas*
`hbonds 0.0` - *removes hydrogen bonds in a selected area*
`hbonds <number>` - *adds thickness to hydrogen bonds*
`color hbonds <color>` - *colors hydrogen bonds*
`set hbonds solid` - *displays hydrogen bonds as solid lines*
`set hbonds backbone` - *connects hydrogen bonds to the alpha carbon*
`set hbonds sidechain` - *connects hydrogen bonds to the nitrogen and oxygen atoms*

To add or remove a single hbond, select only the two **amino acids** that that the hbond connects and use the `hbonds 1.0` or `hbonds off` command

example:
```
select 716 or 1341
hbonds 1.0
```

example:
```
select 14 or 342
hbonds off
```

Disulfide Bonds:

The disulfide bond commands are similar to the hydrogen bond commands, except the term **ssbonds** is used in place of **hbonds,** and the command **calculate hbonds** is replaced by **ssbonds on**

example: `ssbonds on`
example: `color ssbond yellow`

example:
```
select 14 or 342
ssbonds 1.0
```

Struts

The strut commands are identical to the hydrogen bond commands, except the term **strut** is used in place of **hbonds**

example: `calculate struts`
example: `color strut green`

example:
```
select 14 or 342
strut 1.0
```

To add or remove struts, select the atoms that the struts connect to and use the `connect strut` or `connect strut delete` command

example:
```
select atomno=716 or atomno=1341
connect strut
```

example:
```
select :a
connect strut delete
```

`set picking strut` - *allows you to add struts manually by clicking with the mouse on two atoms*
`set picking ident` - *turns off "set picking struts" and returns you to normal mouse clicking*

3-D Molecular Designs
...where molecules become real™

Amino Acid Side Chain Chart©

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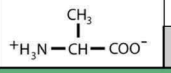
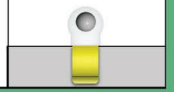
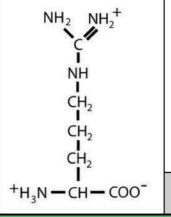
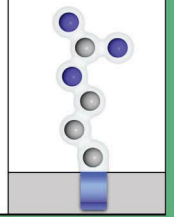
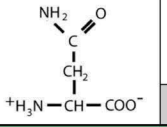
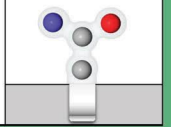
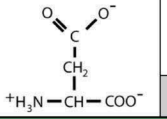
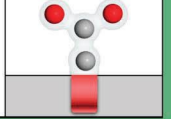
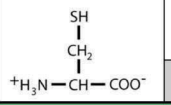
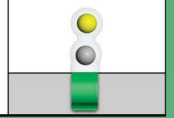
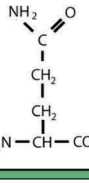
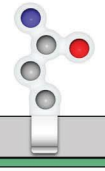
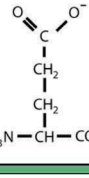
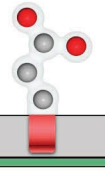
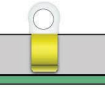
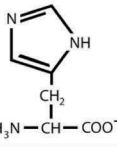
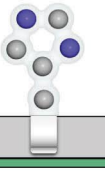
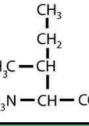
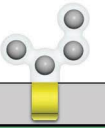
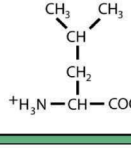
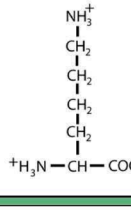
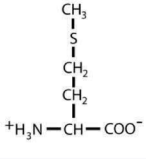
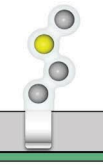
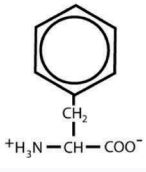
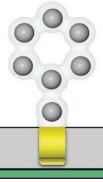
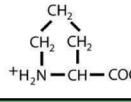
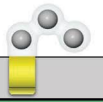
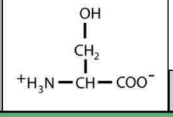
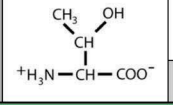
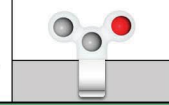
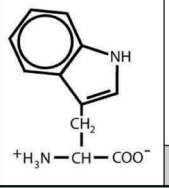
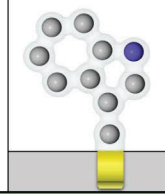
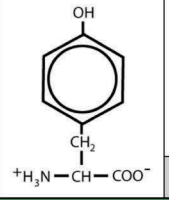
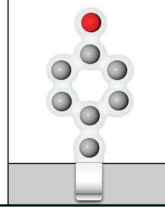
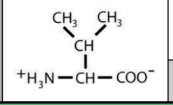
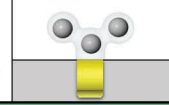
Name	Amino Acid	Side Chain
Alanine Ala A		
Arginine Arg R		
Asparagine Asn N		
Aspartic Acid Asp D		
Cysteine Cys C		

Name	Amino Acid	Side Chain
Glutamine Gln Q		
Glutamic Acid Glu E		
Glycine Gly G		
Histidine His H		
Isoleucine Ile I		

Name	Amino Acid	Side Chain
Leucine Leu L		
Lysine Lys K		
Methionine Met M		
Phenylalanine Phe F		
Proline Pro P		

Name	Amino Acid	Side Chain
Serine Ser S		
Threonine Thr T		
Tryptophan Trp W		
Tyrosine Tyr Y		
Valine Val V		

Atom Color Key

Carbon · Oxygen · Nitrogen · Sulfur · Hydrogen

Amino Acid Property Key

Amino acid clip color and name color indicate property

Negative Charge · Positive Charge · Hydrophilic · Cysteine · Hydrophobic