

A glimpse of computational methods in biological physics:
Case study on three proteins and a cellular organelle

Klaus Schulten

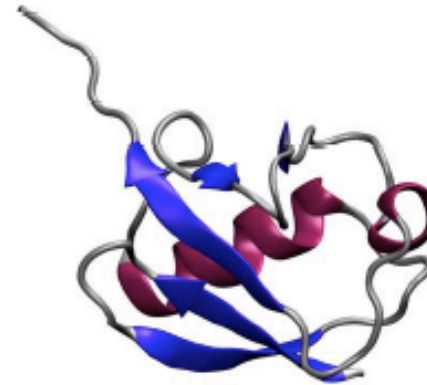
Theoretical and Computational Biophysics Group
September 16, 2014

Administrative issues

- Assignment from this lecture: read the case study on ubiquitin and choose **Three** out of the six exercises to complete: <http://www.ks.uiuc.edu/Training/CaseStudies/index.html#ubqcs>
- You will have to download and install the software VMD: <http://www.ks.uiuc.edu/Research/vmd/>
- For any questions and assistance on the assignment, email Marco Tjioe at tjioe2@gmail.com
- Assignments should be given to Professor Selvin before class on October 1 (next Tuesday).

Case Study: Ubiquitin

Eduardo Cruz-Chu and JC Gumbart



1 Introduction

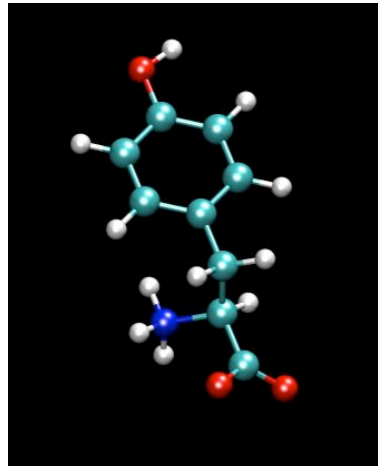
Without a doubt, the most organized and coordinated machine known is the biological cell. Inside its micrometer-scale diameter, a wide variety of macromolecules (DNA, proteins, sugars, lipids, etc.) work together in a cooperative way, balancing energy and matter to keep the cell alive. Within the cell, proteins are the overachievers. They allow the movement of water and ions through the cell membrane, help ATP to store energy, assist DNA during replication, recognize foreign infections, and more. However, all of these functions don't work independently of each other. To maintain harmony and efficiency between various functions, most processes have to be turned on or off according to different cellular stages and changes within the environment.

To this end, together with the mechanisms to assemble functional proteins and to turn on their functions, there should be counterparts to suppress and disassemble proteins when they are no longer needed. The cellular machine depends on assembly and disassembly to regulate the effective concentration of proteins and their corresponding activities [1]. Furthermore, defective

Introduction to Protein Structures and Molecular Graphics Tool

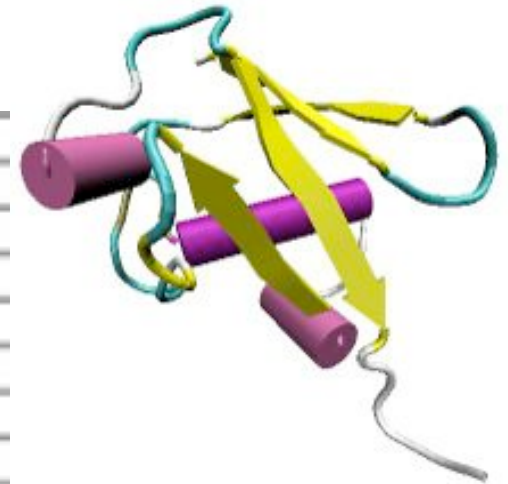
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IQKESTLHLV LRLRGG
  
```



*amino acid
tyrosine, Y*

Amino Acid	SLC	DNA codons
Isoleucine	I	ATT, ATC, ATA
Leucine	L	CTT, CTC, CTA, CTG, TTA, TTG
Valine	V	GTT, GTC, GTA, GTG
Phenylalanine	F	TTT, TTC
Methionine	M	ATG
Cysteine	C	TGT, TGC
Alanine	A	GCT, GCC, GCA, GCG
Glycine	G	GGT, GGC, GGA, GGG
Proline	P	CCT, CCC, CCA, CCG
Threonine	T	ACT, ACC, ACA, ACG
Serine	S	TCT, TCC, TCA, TCG, AGT, AGC
Tyrosine	Y	TAT, TAC
Tryptophan	W	TGG
Glutamine	Q	CAA, CAG
Asparagine	N	AAT, AAC
Histidine	H	CAT, CAC
Glutamic acid	E	GAA, GAG
Aspartic acid	D	GAT, GAC
Lysine	K	AAA, AAG
Arginine	R	CGT, CGC, CGA, CGG, AGA, AGG
Stop codons	Stop	TAA, TAG, TGA

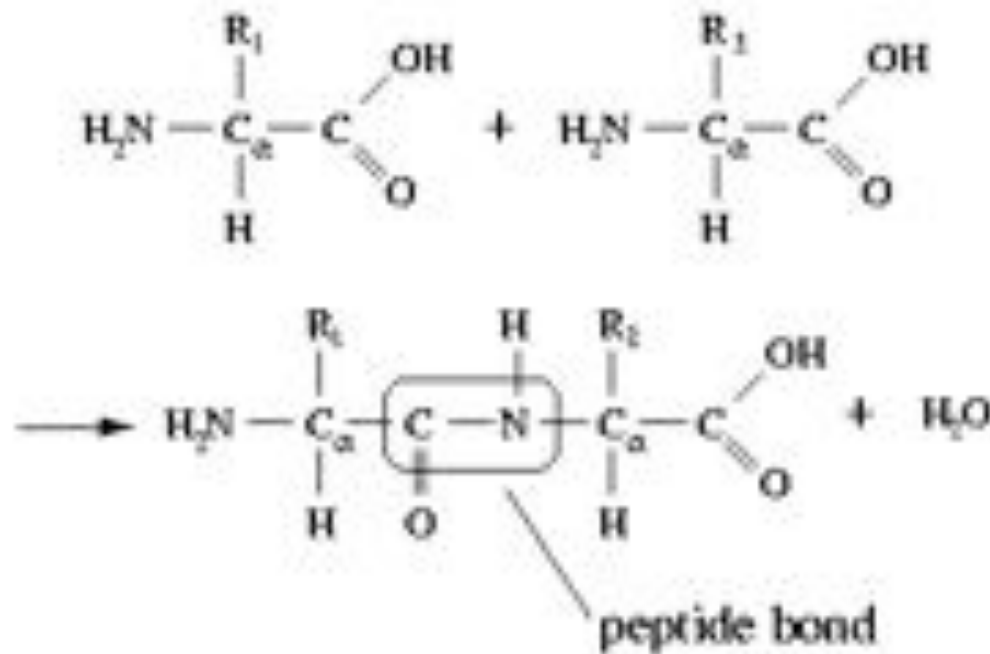


Ubiquitin

Quick Overview of Protein Structure

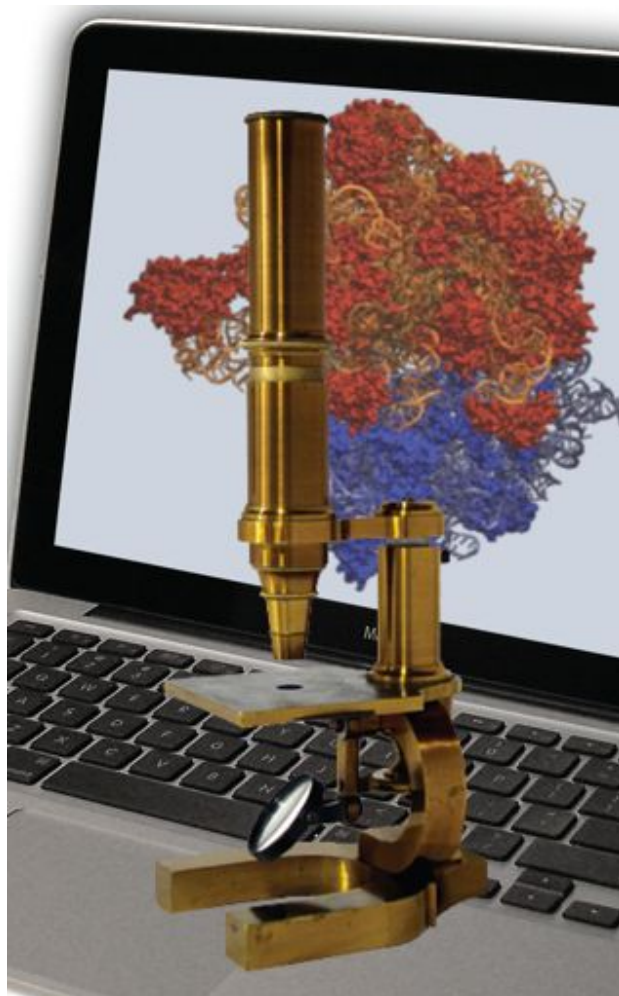
What Proteins are Made of: Primary Structure (Sequence) of Amino Acids

Proteins: polymeric molecules linking amino acids through peptide bonds



Peptide bond linking two amino acids

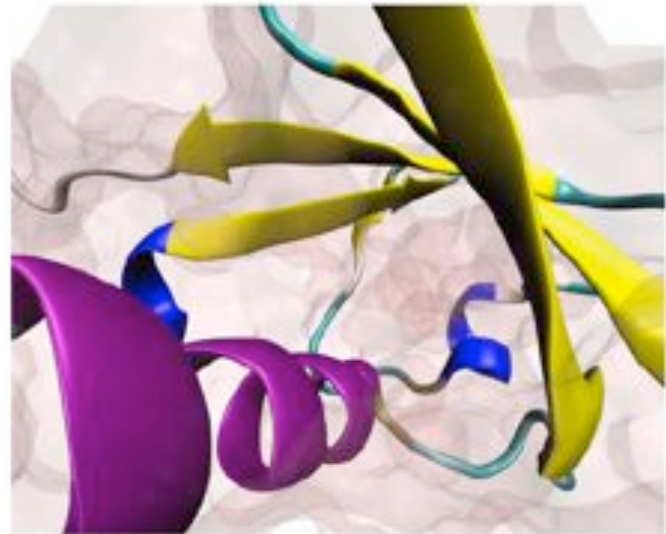
Looking at Proteins Through the Program VMD



Learn to use VMD from the
“Using VMD” tutorial available at
<http://www.ks.uiuc.edu/Training/Tutorials/>

VMD for Mac OS X, Unix, and
Windows is available for download at
<http://www.ks.uiuc.edu/Research/vmd/>

Using VMD



VMD Developer:
John Stone

Tutorial Contributors:

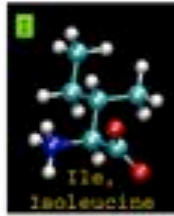
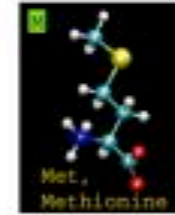
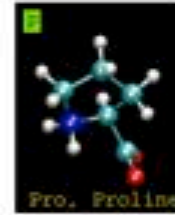
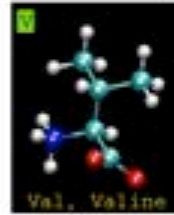
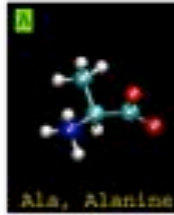
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VMD Demo 0

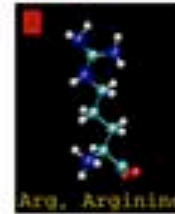
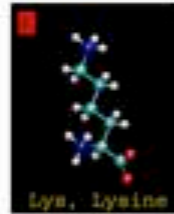
Protein Primary Structure

The twenty amino acids

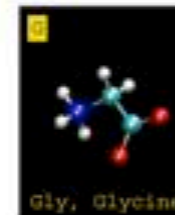
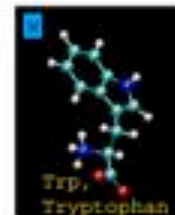
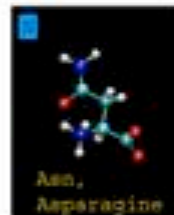
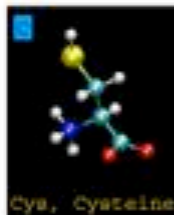
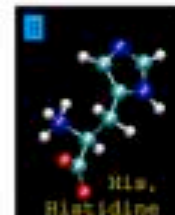
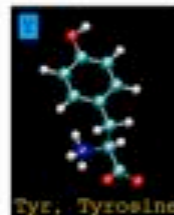
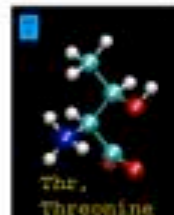
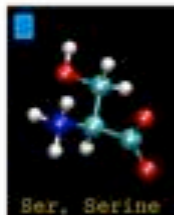
non-polar



charged



polar



Protein Structure and

Function, Gregory Petsko and
Dagmar Ringe, 2004

Molecular Biology of The Cell

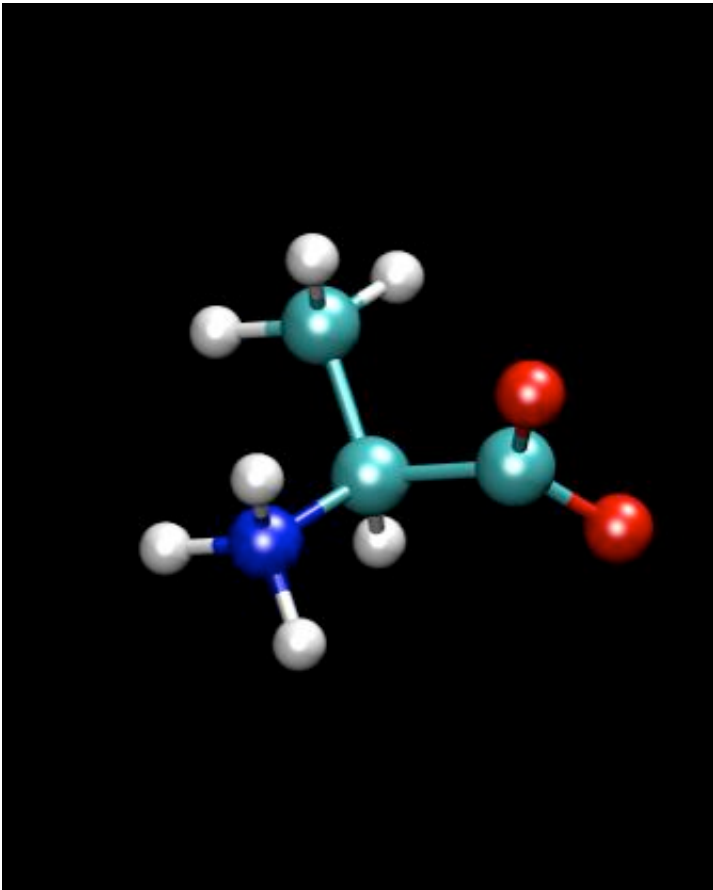
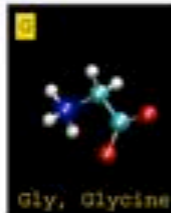
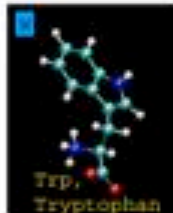
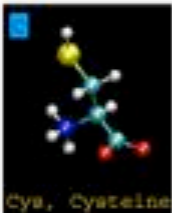
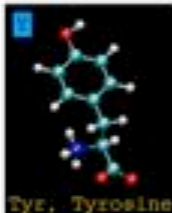
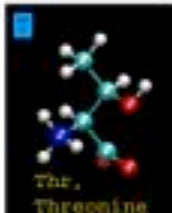
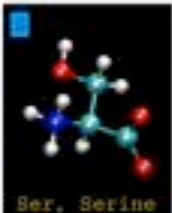
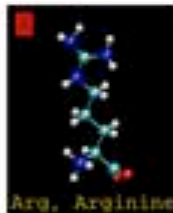
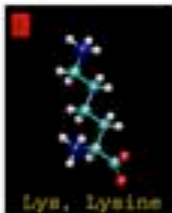
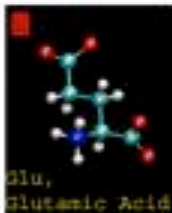
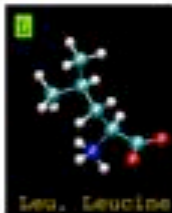
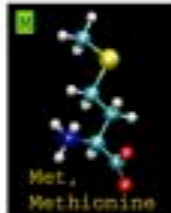
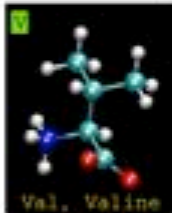
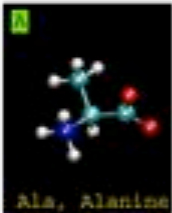
Alberts, Johnson, Lewis, Raff, Roberts,
Walter, 2008, 3rd Ed.

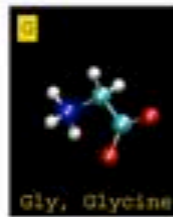
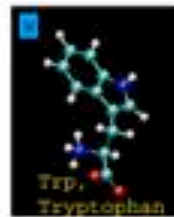
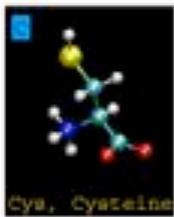
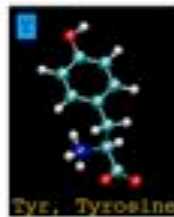
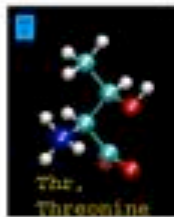
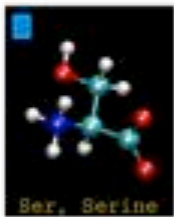
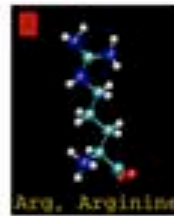
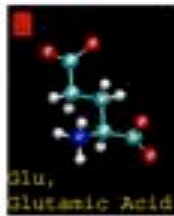
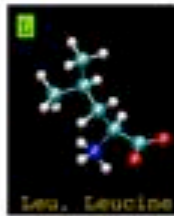
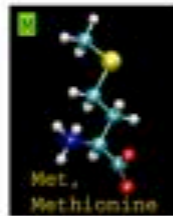
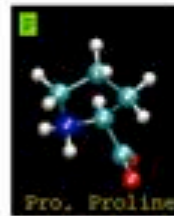
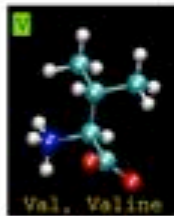
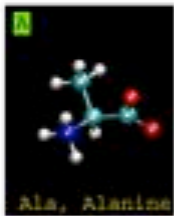
*Introduction to Protein
Structure*, 2nd ed.

Carl Branden & John Tooze, 1999

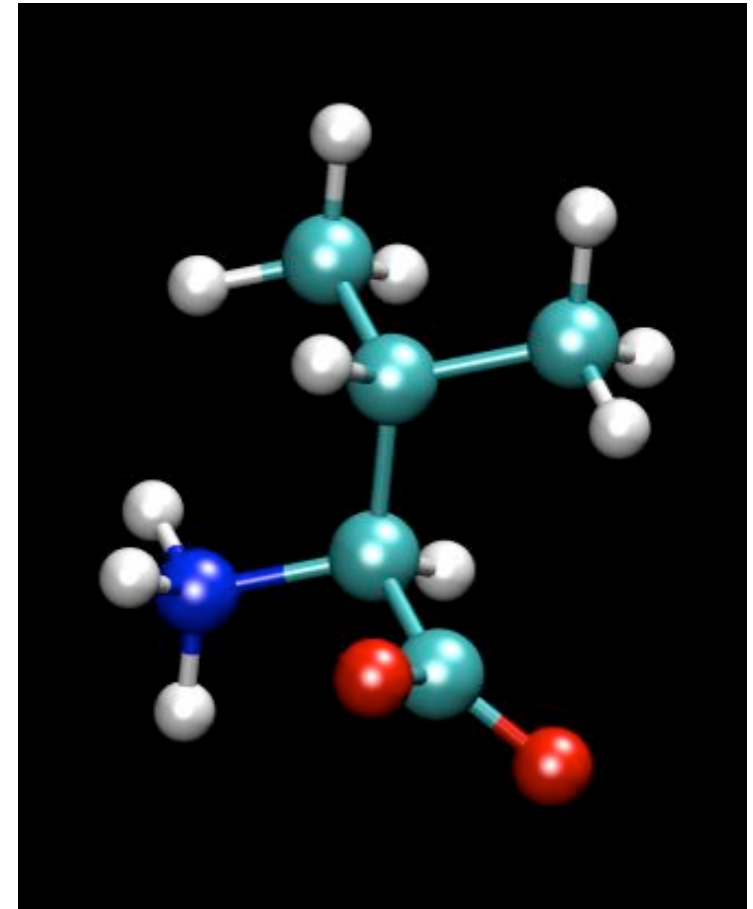
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Alanine

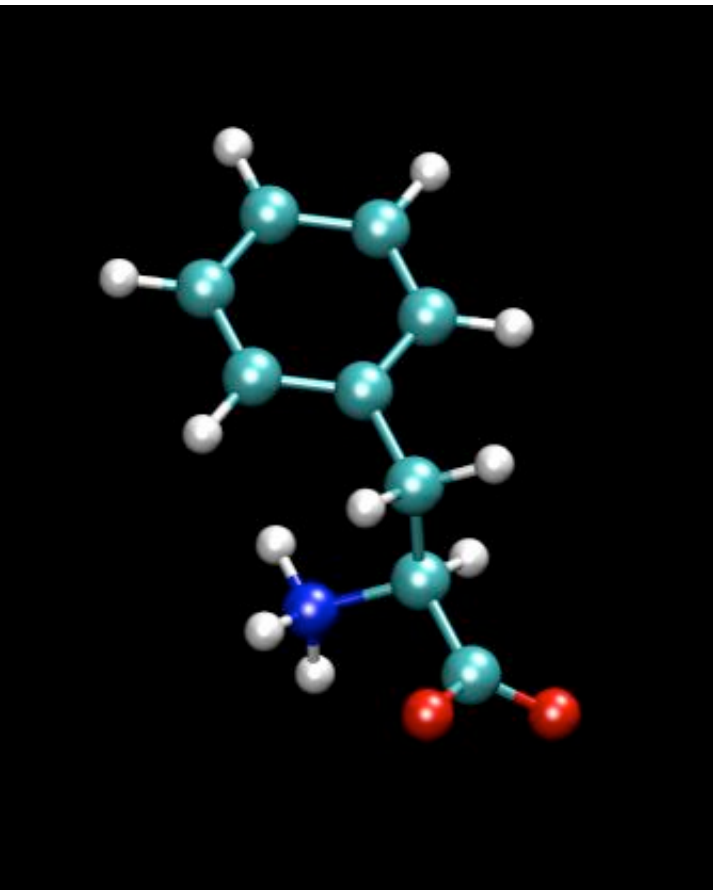
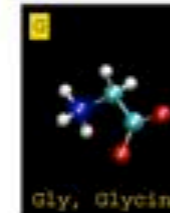
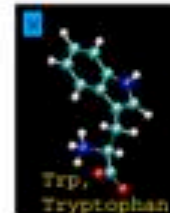
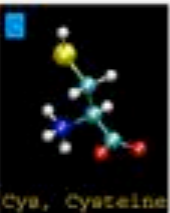
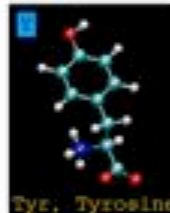
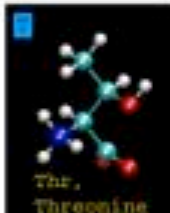
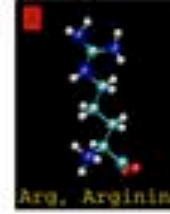
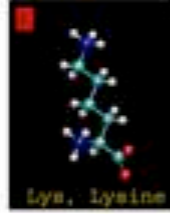
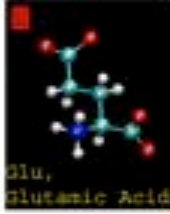
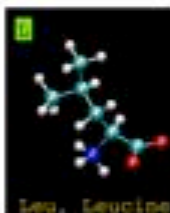
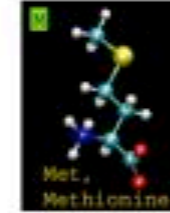
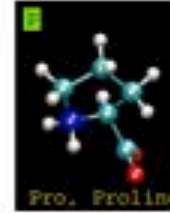
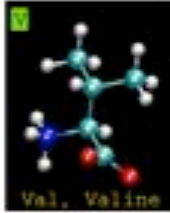
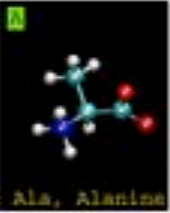


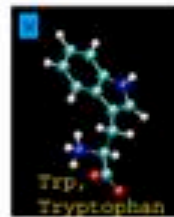
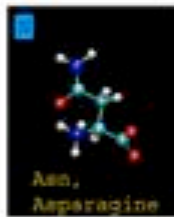
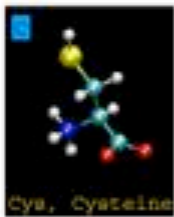
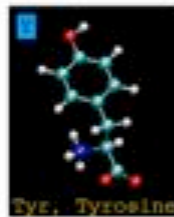
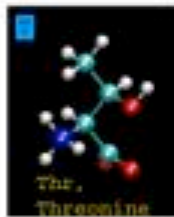
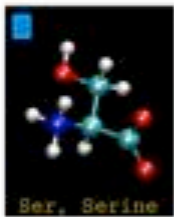
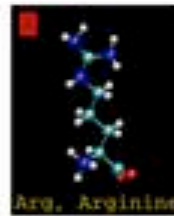
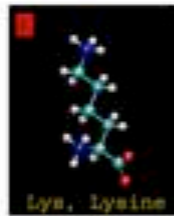
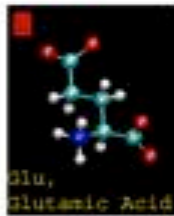
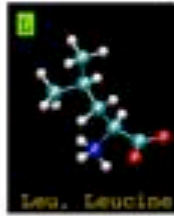
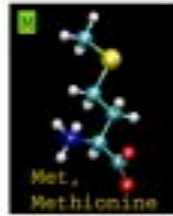
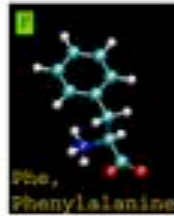
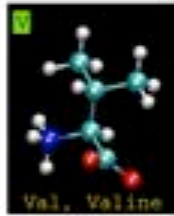
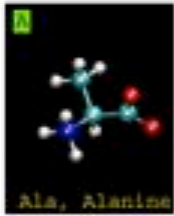


Valine

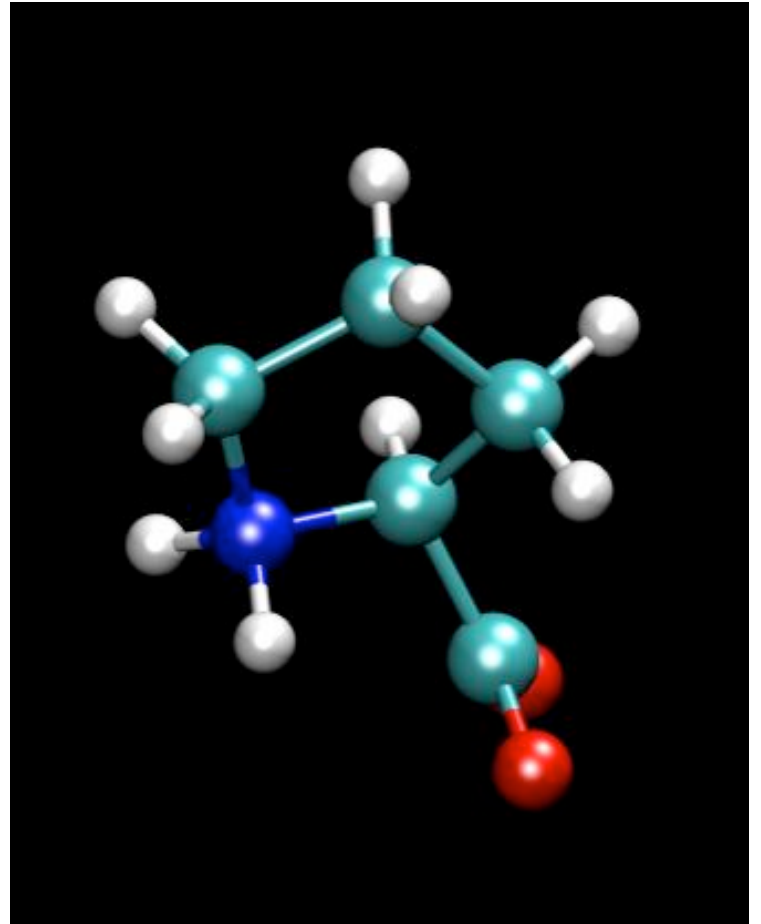


Phenylalanine

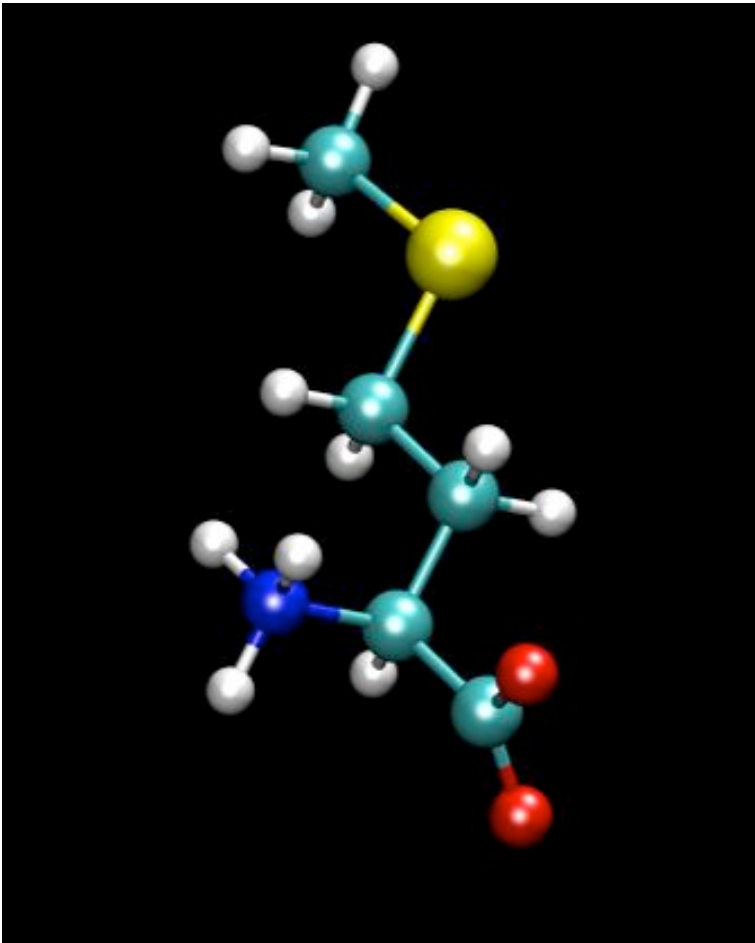
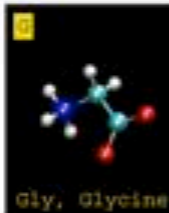
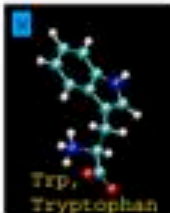
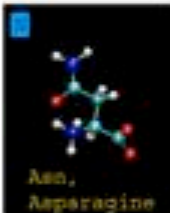
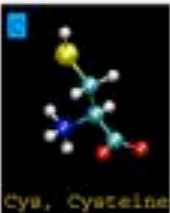
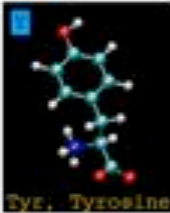
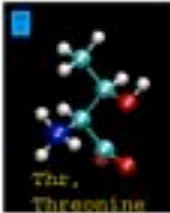
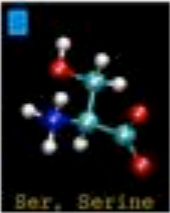
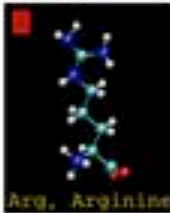
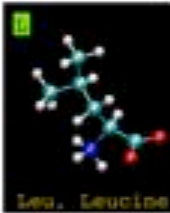
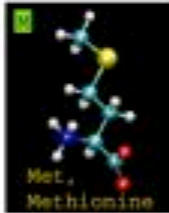
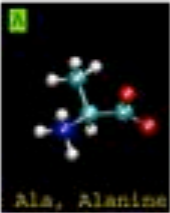


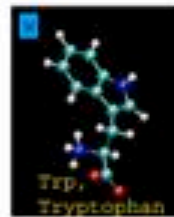
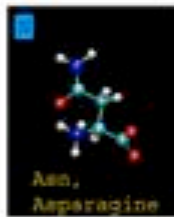
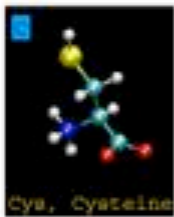
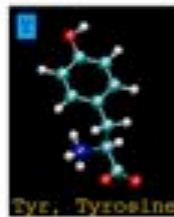
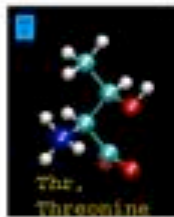
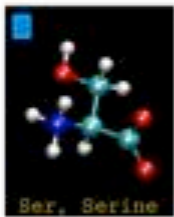
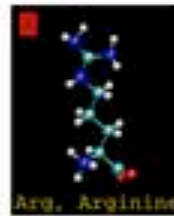
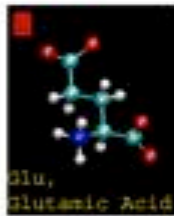
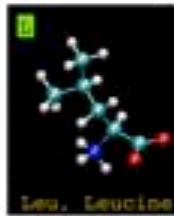
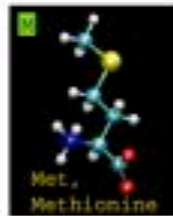
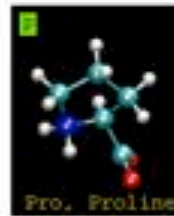
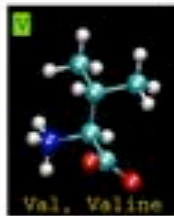
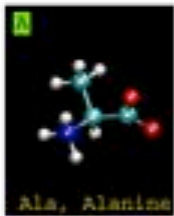


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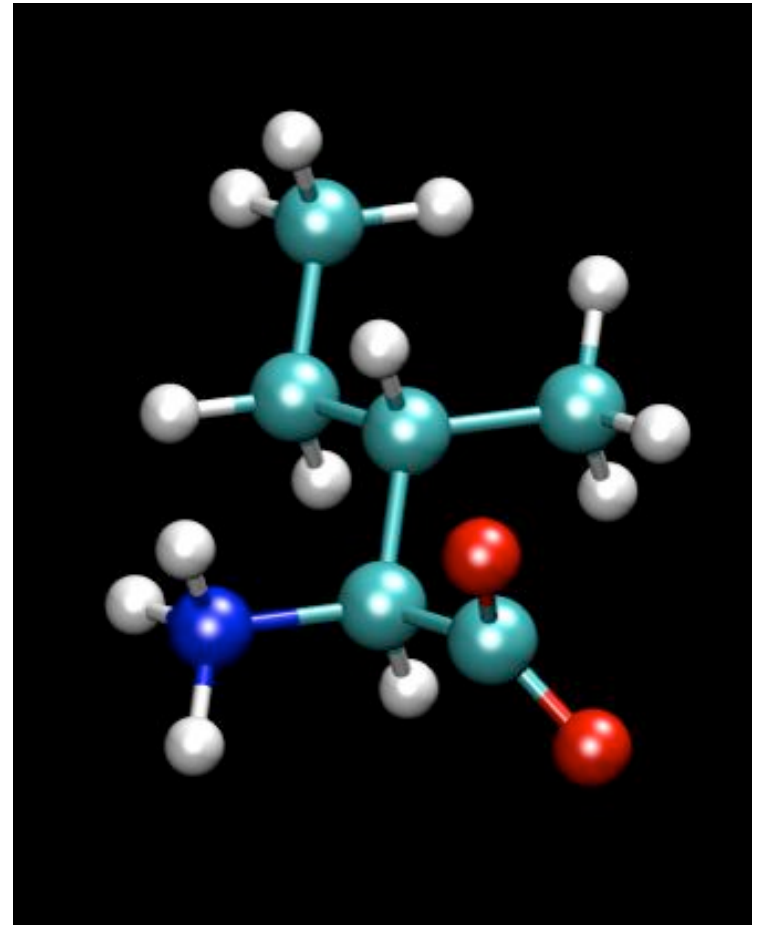


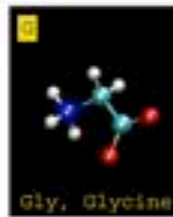
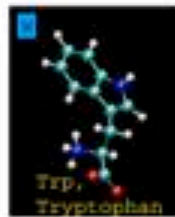
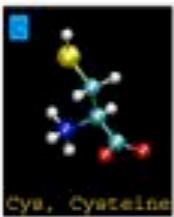
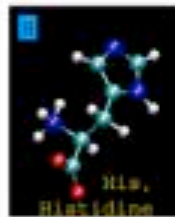
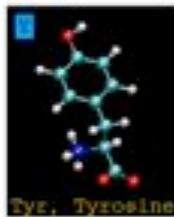
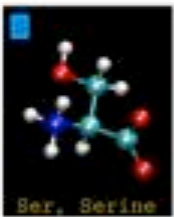
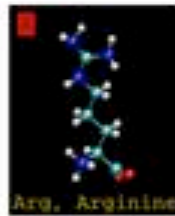
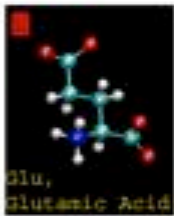
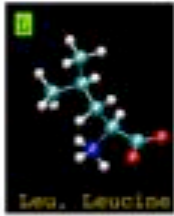
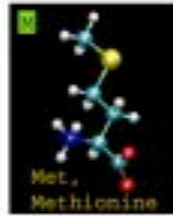
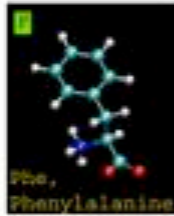
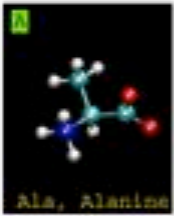
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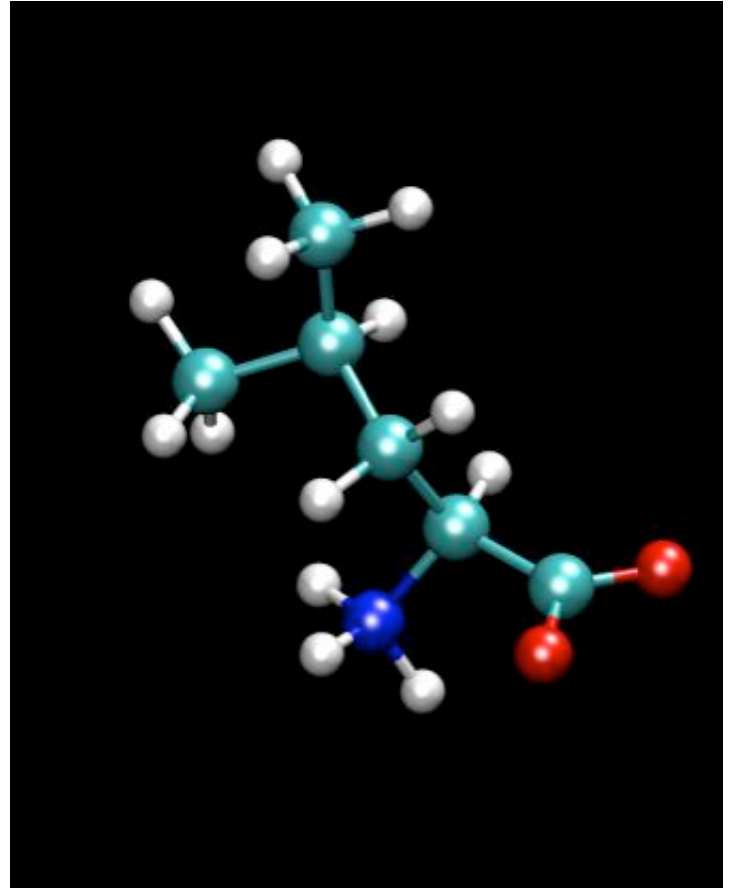


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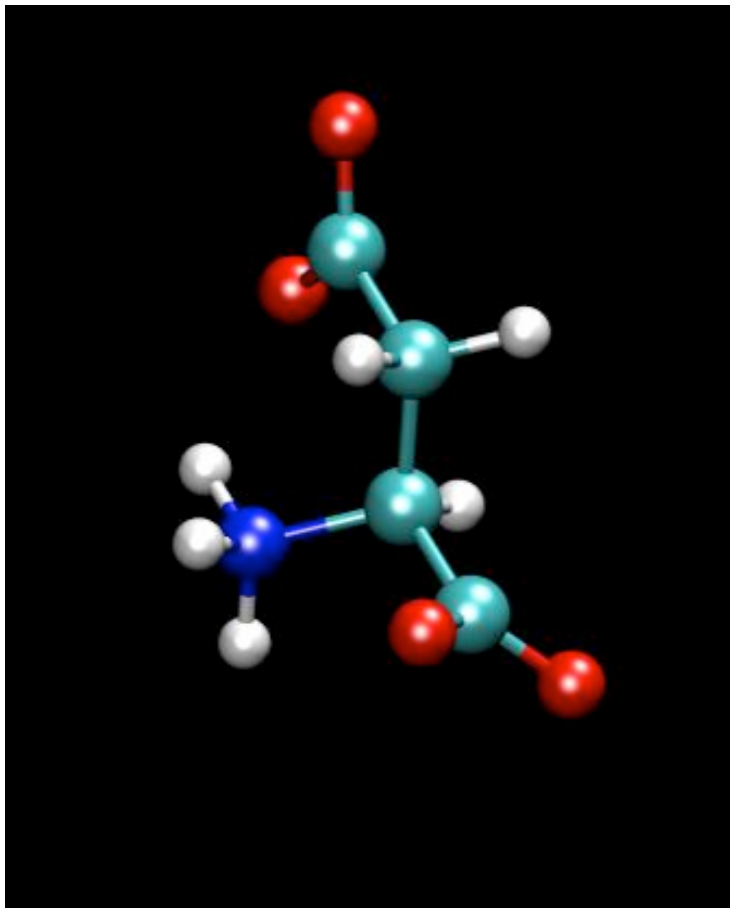
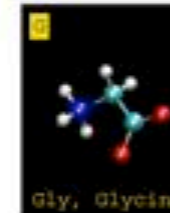
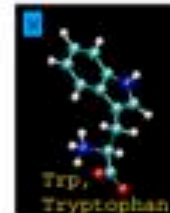
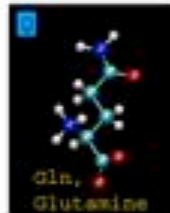
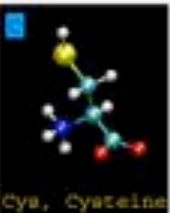
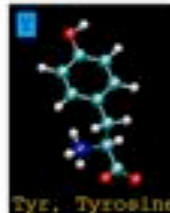
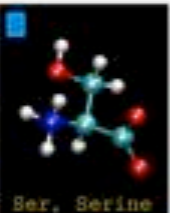
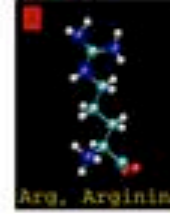
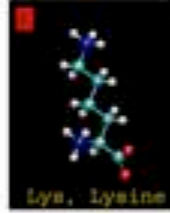
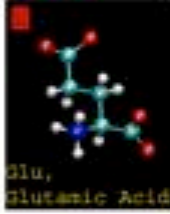
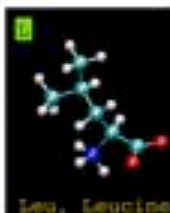
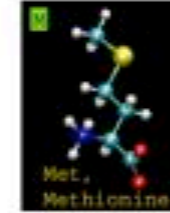
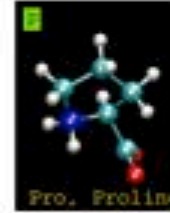
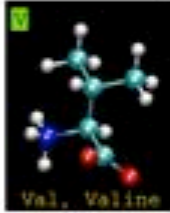
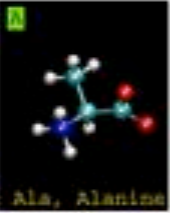


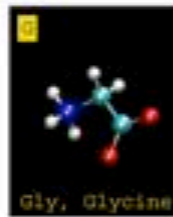
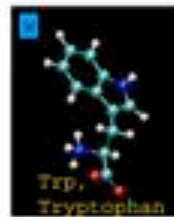
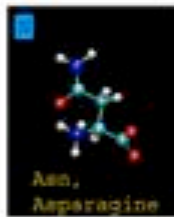
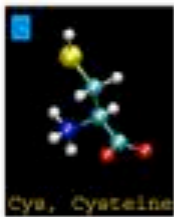
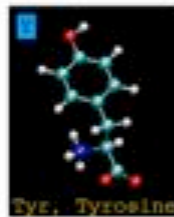
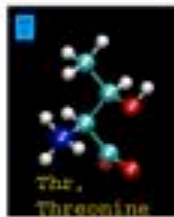
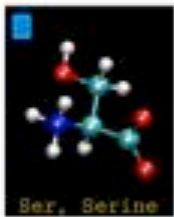
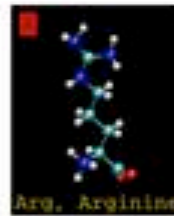
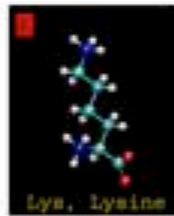
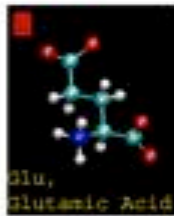
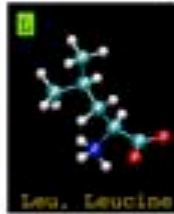
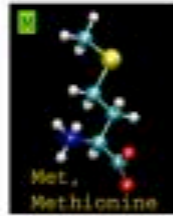
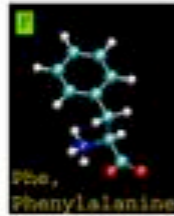
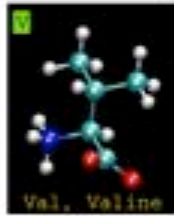
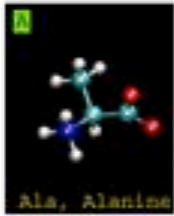


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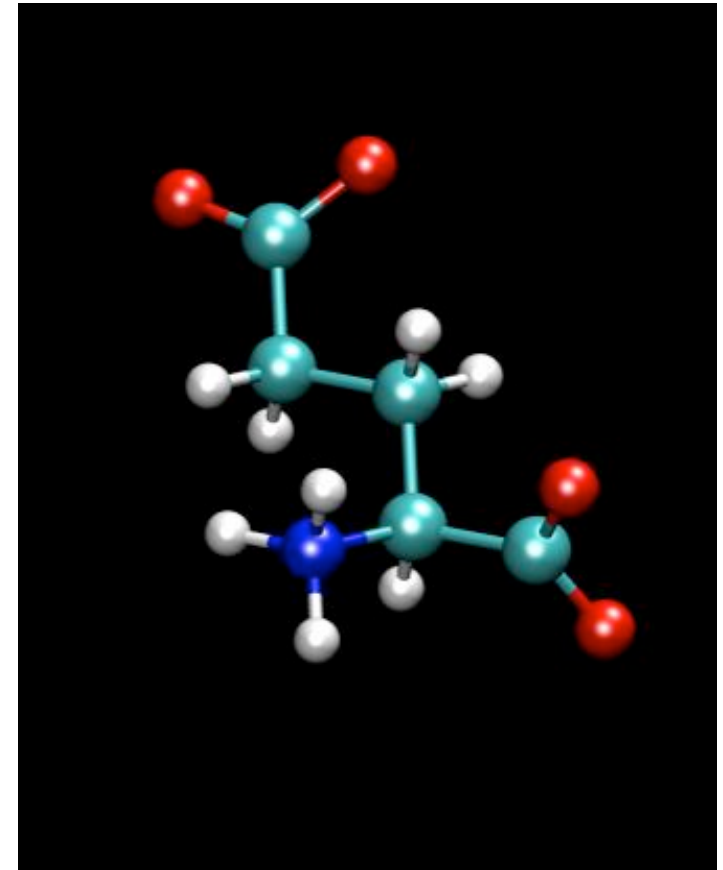


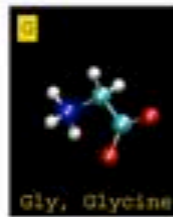
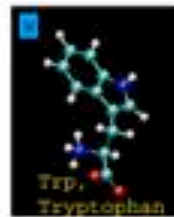
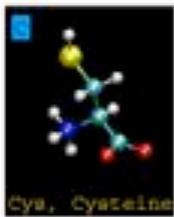
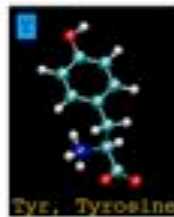
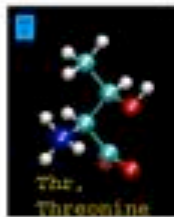
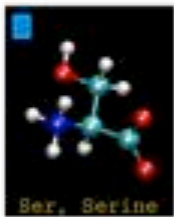
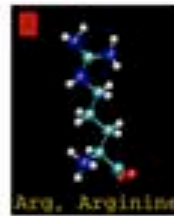
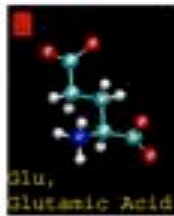
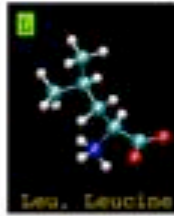
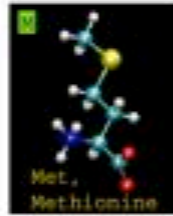
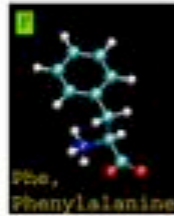
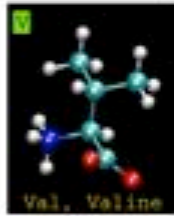
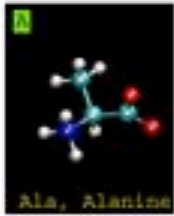
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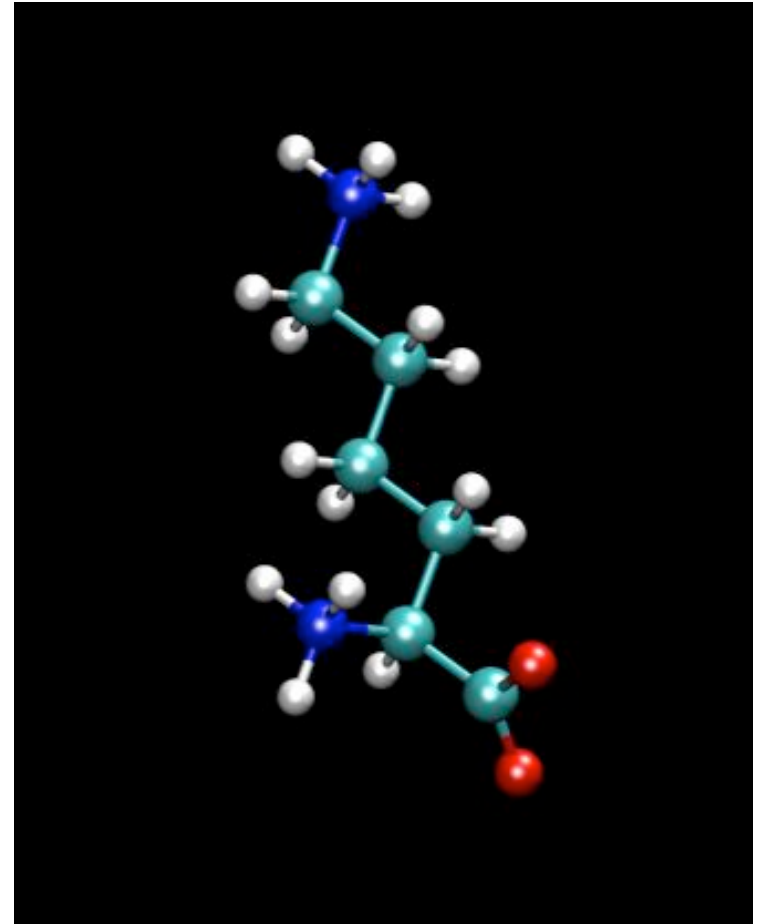


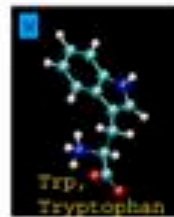
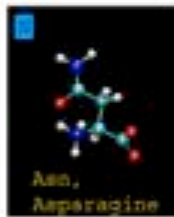
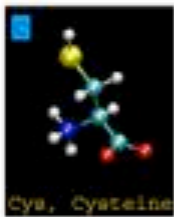
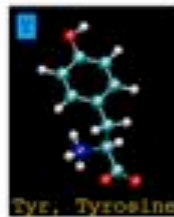
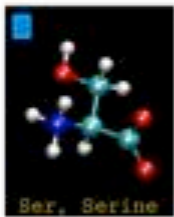
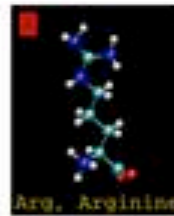
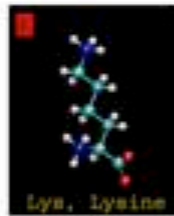
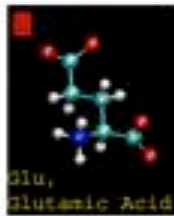
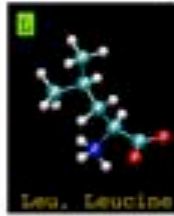
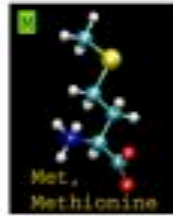
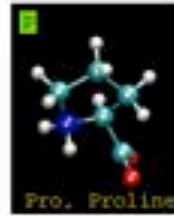
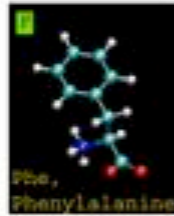
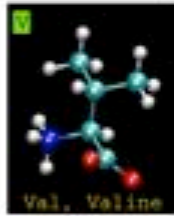
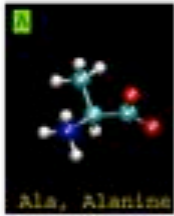
Glutamate



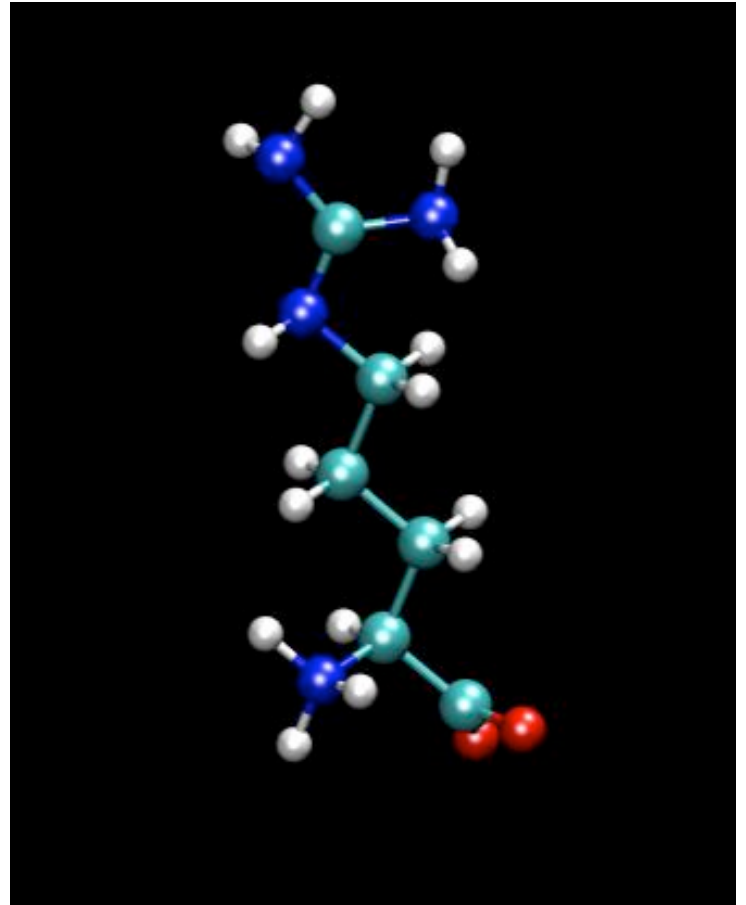


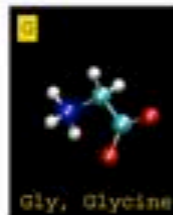
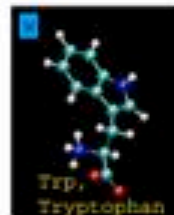
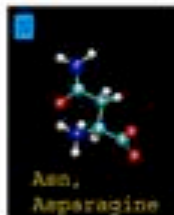
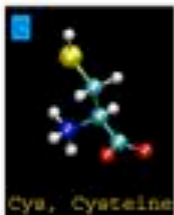
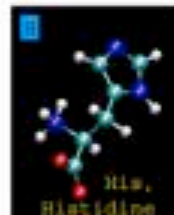
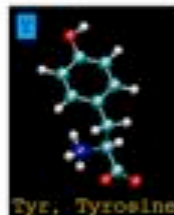
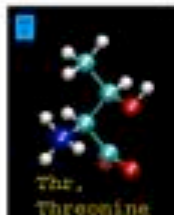
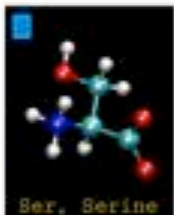
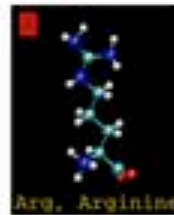
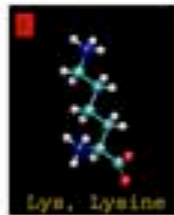
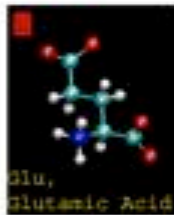
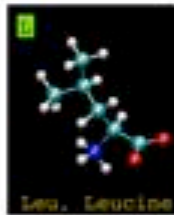
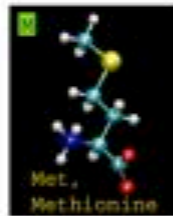
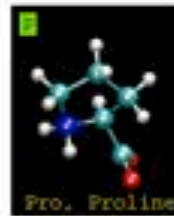
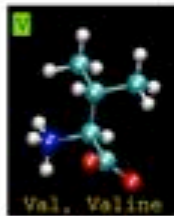
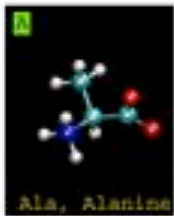
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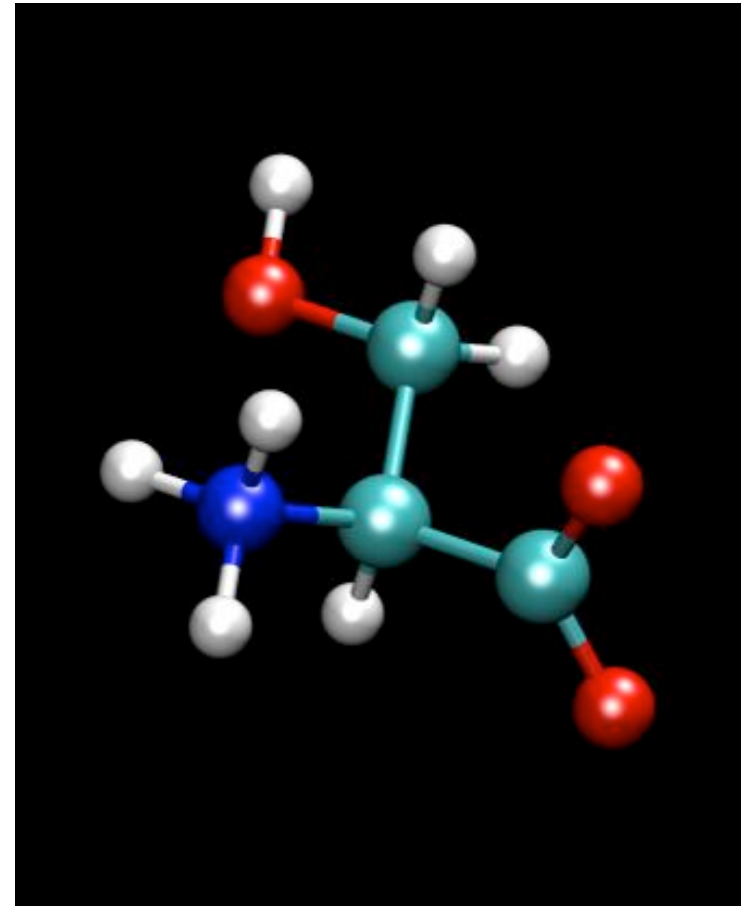


Arginine

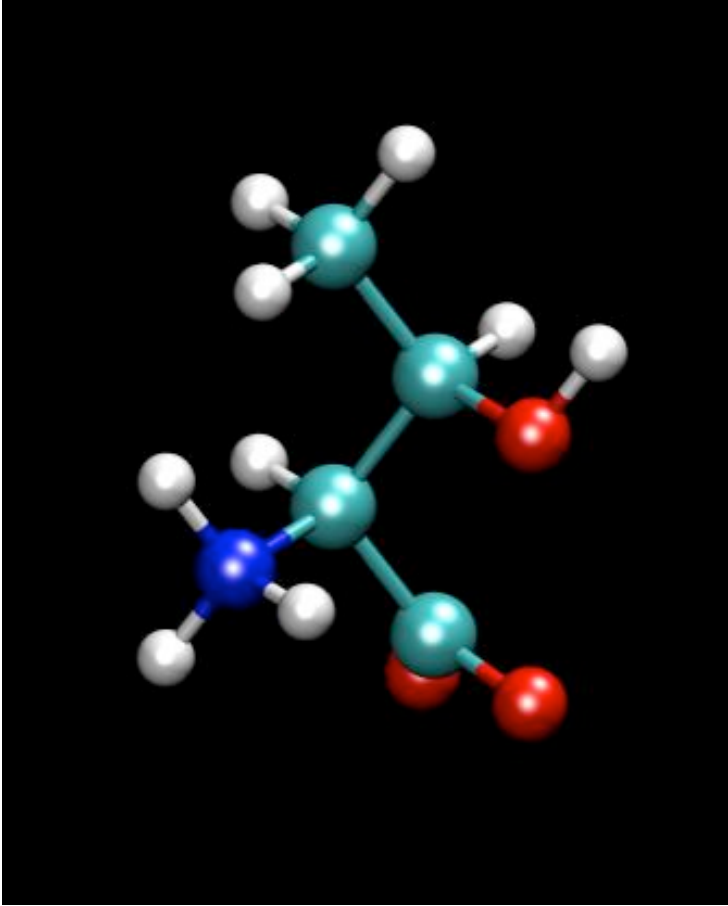
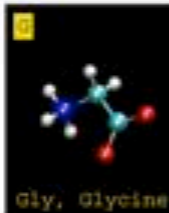
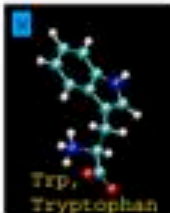
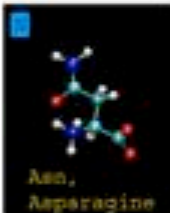
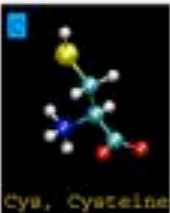
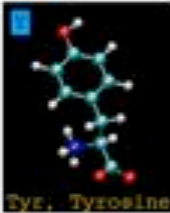
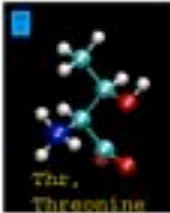
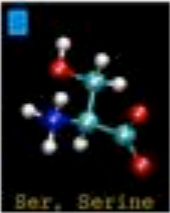
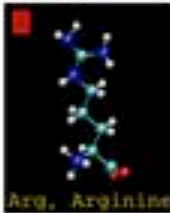
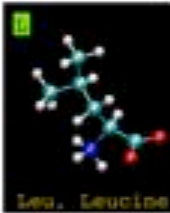
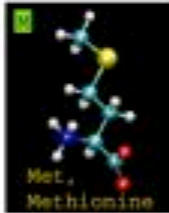
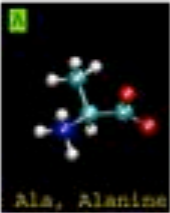


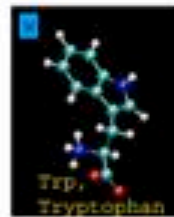
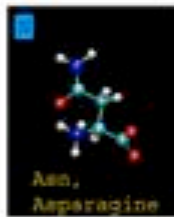
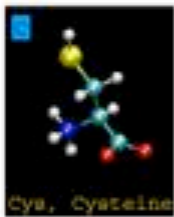
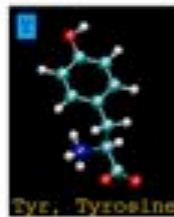
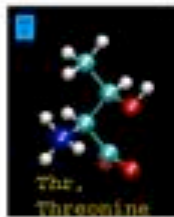
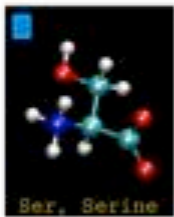
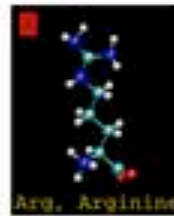
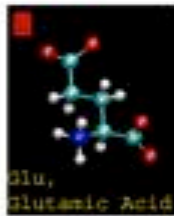
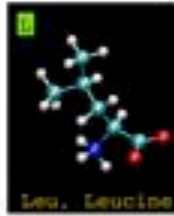
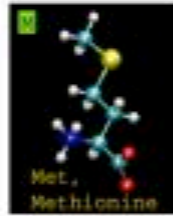
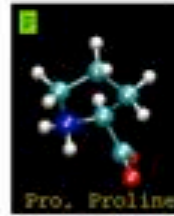
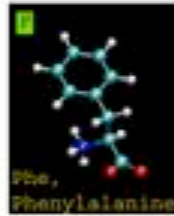
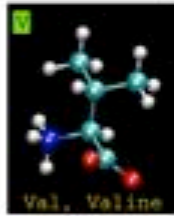
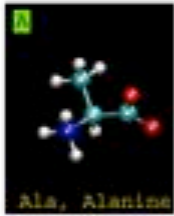


Serine

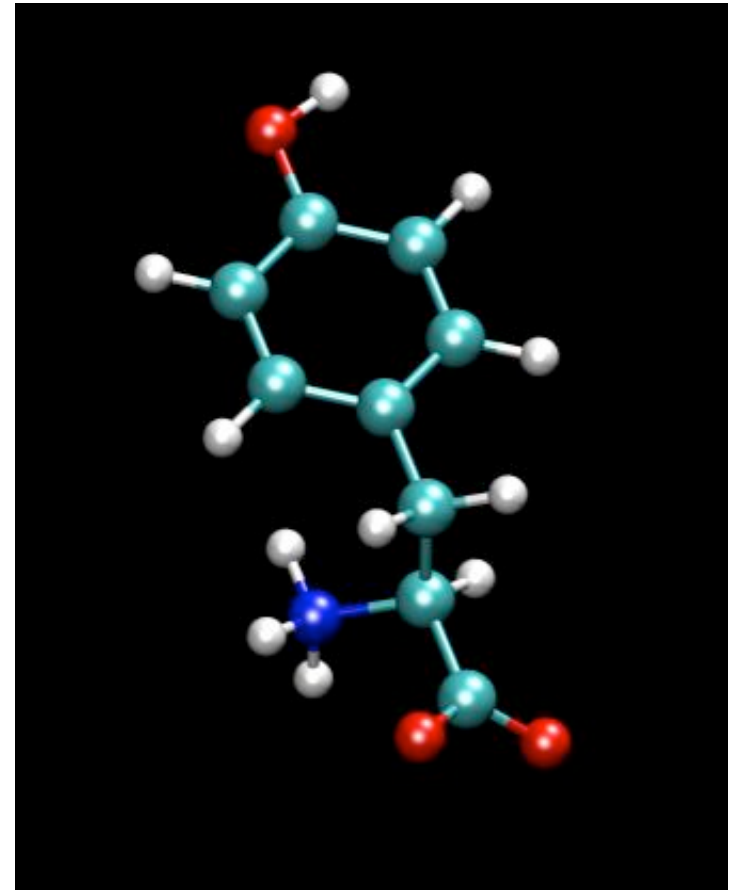


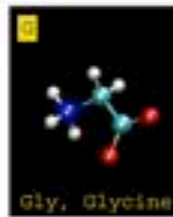
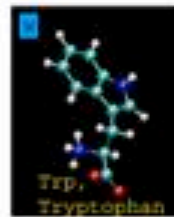
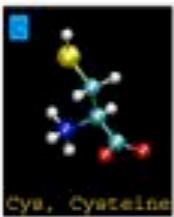
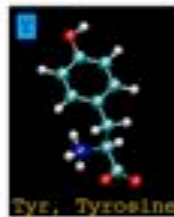
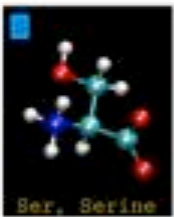
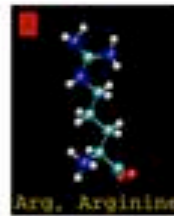
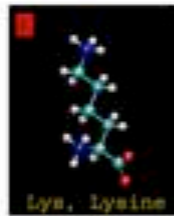
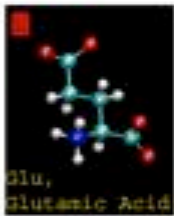
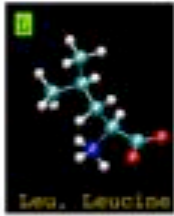
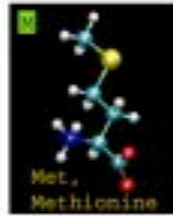
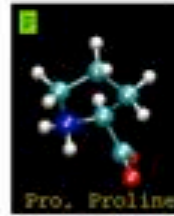
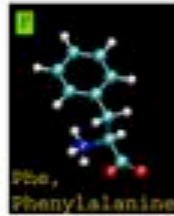
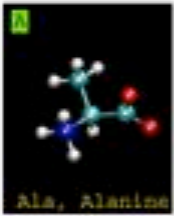
Threonine



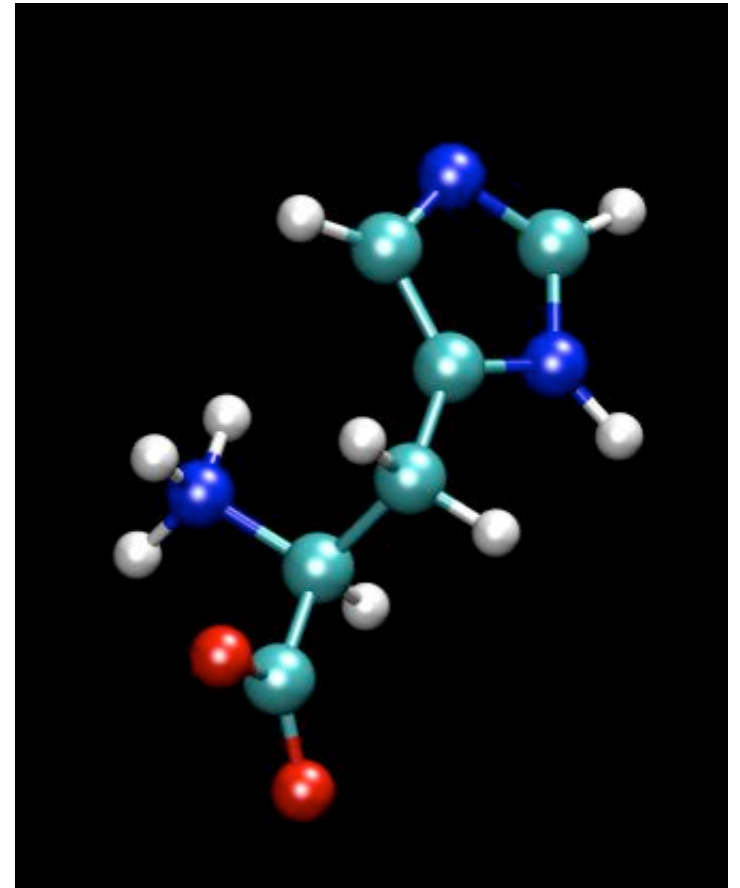


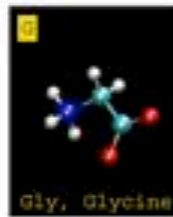
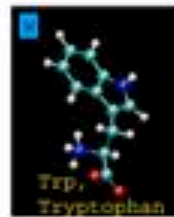
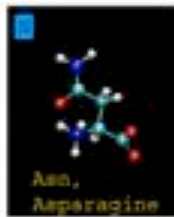
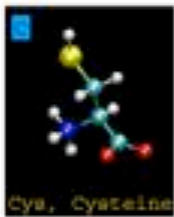
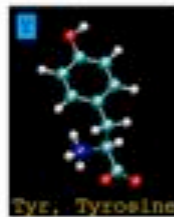
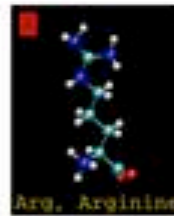
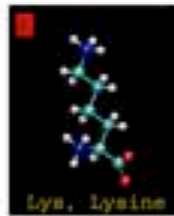
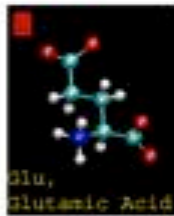
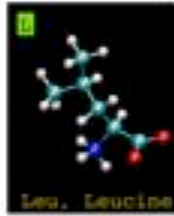
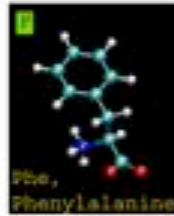
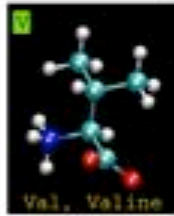
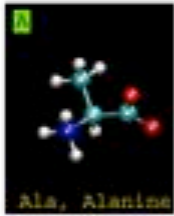
Tyrosine



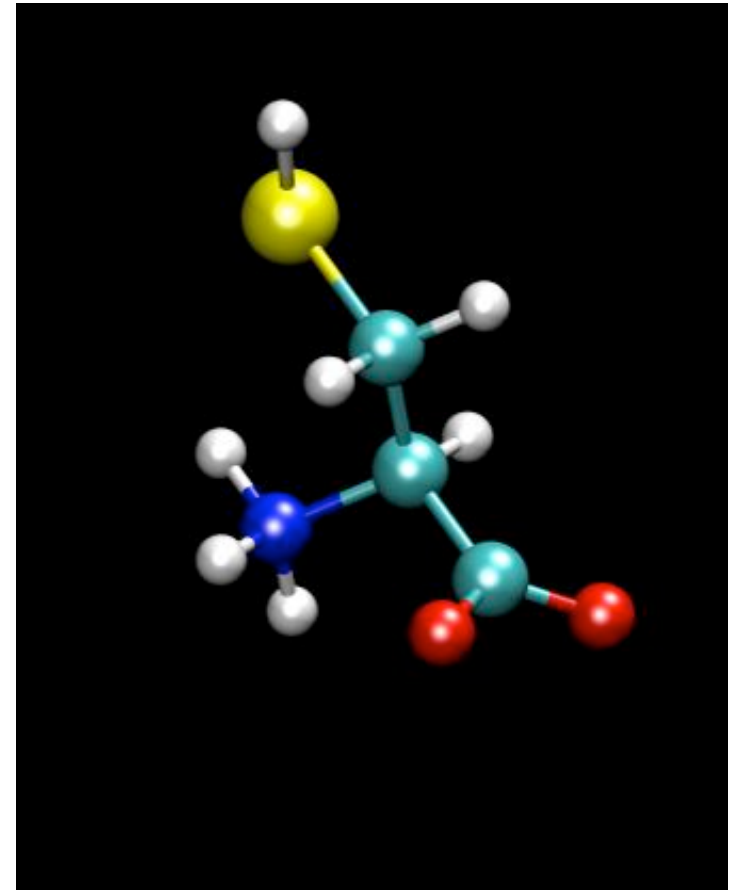


Histidine

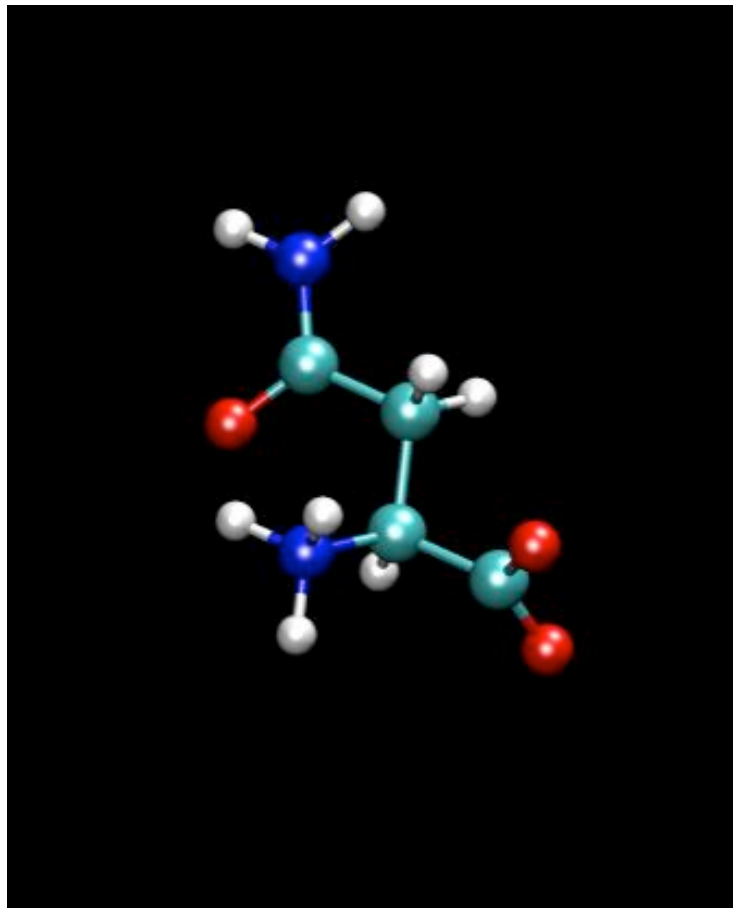
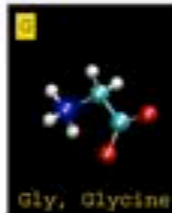
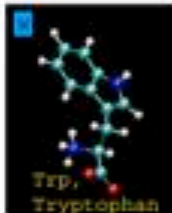
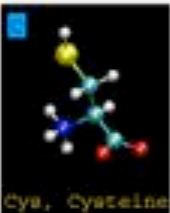
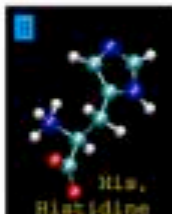
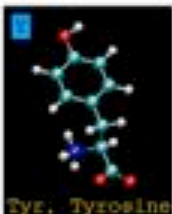
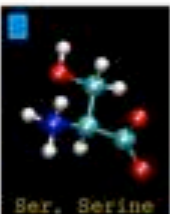
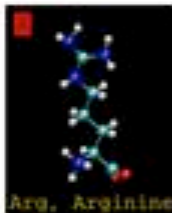
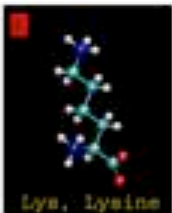
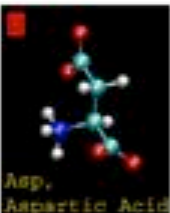
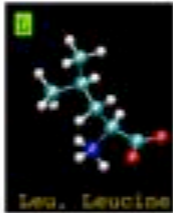
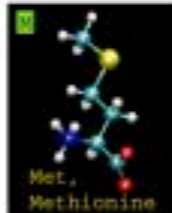
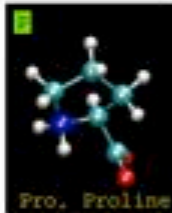
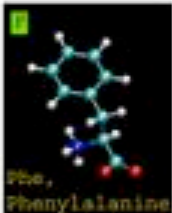
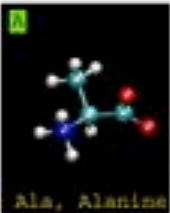


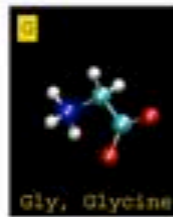
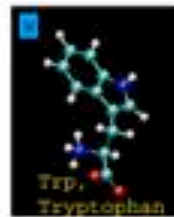
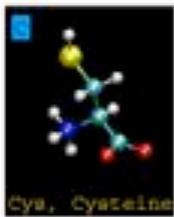
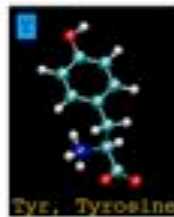
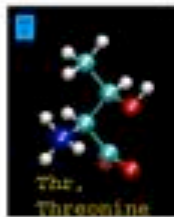
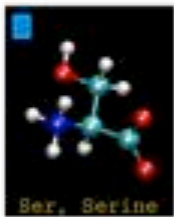
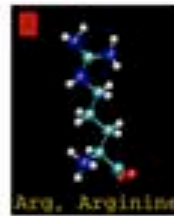
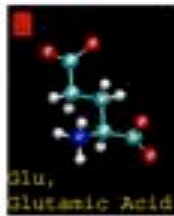
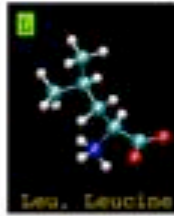
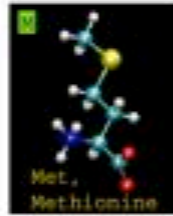
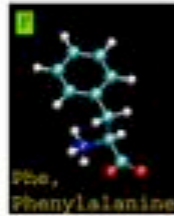
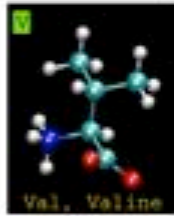
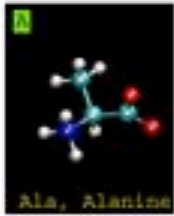


Cysteine

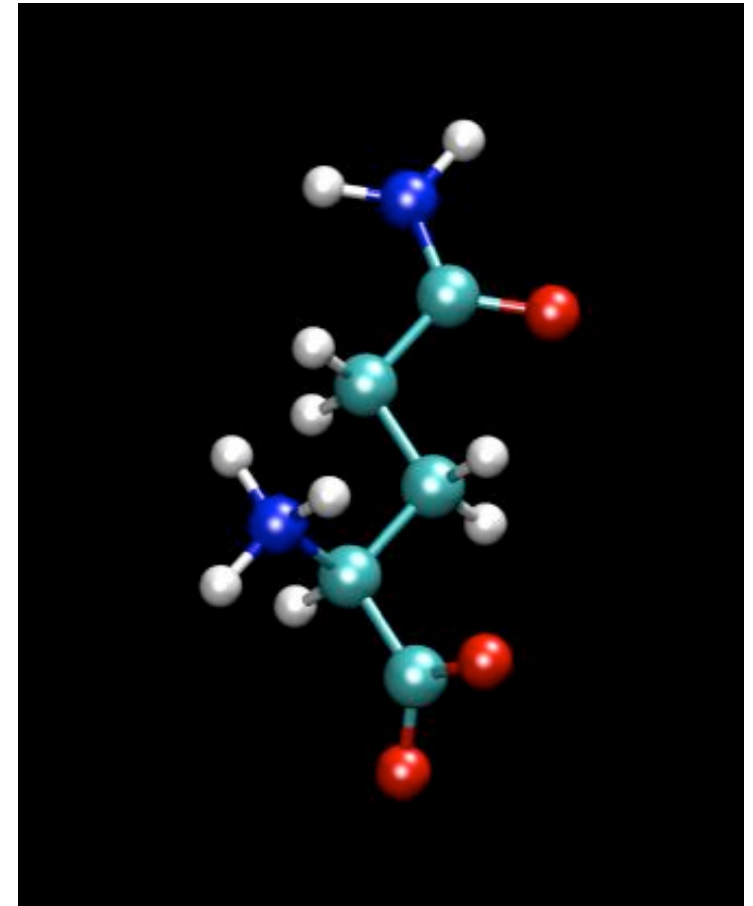


Asparagine

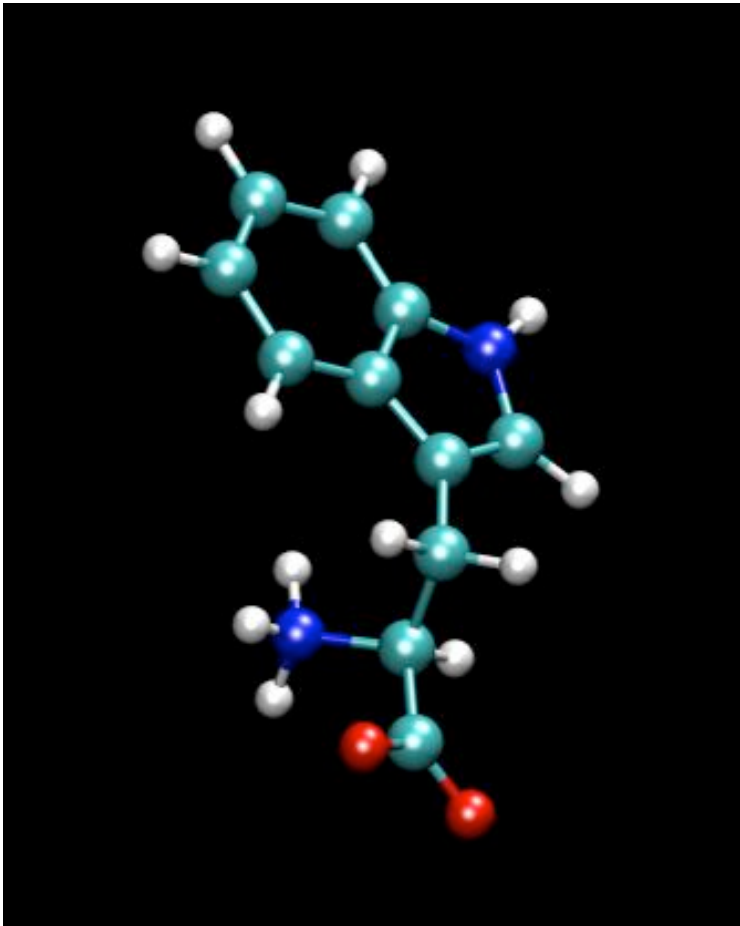
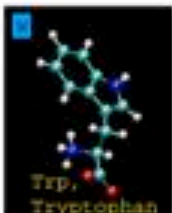
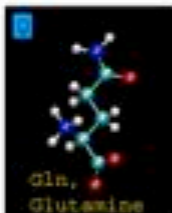
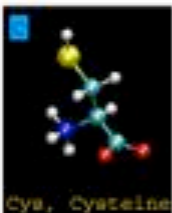
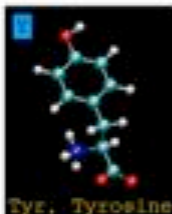
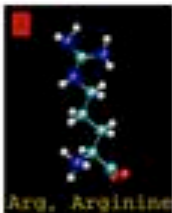
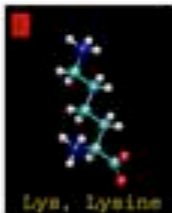
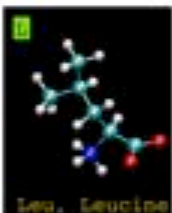
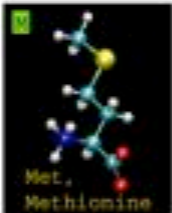
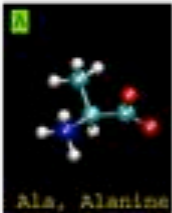


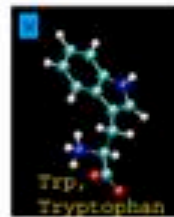
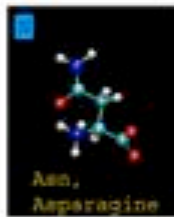
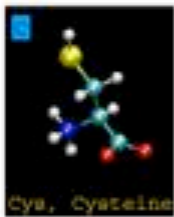
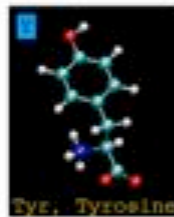
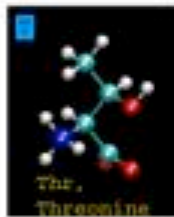
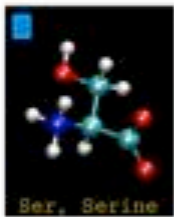
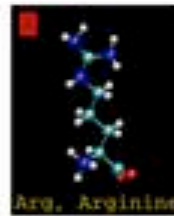
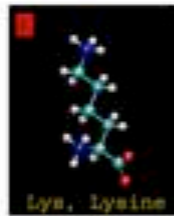
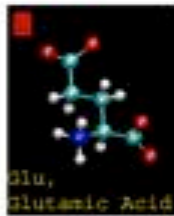
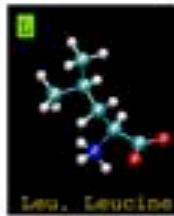
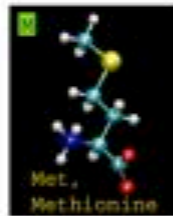
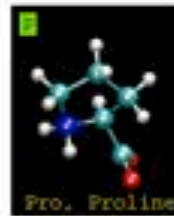
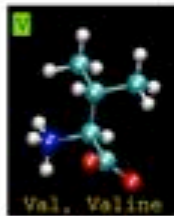
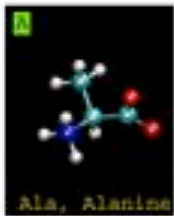


Glutamine

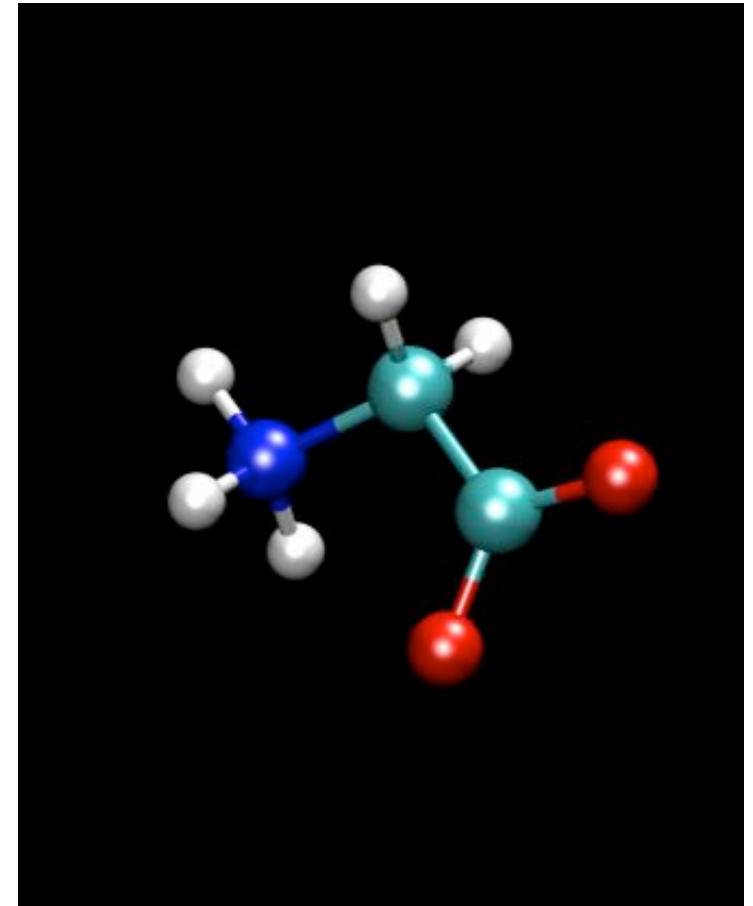


Tryptophane

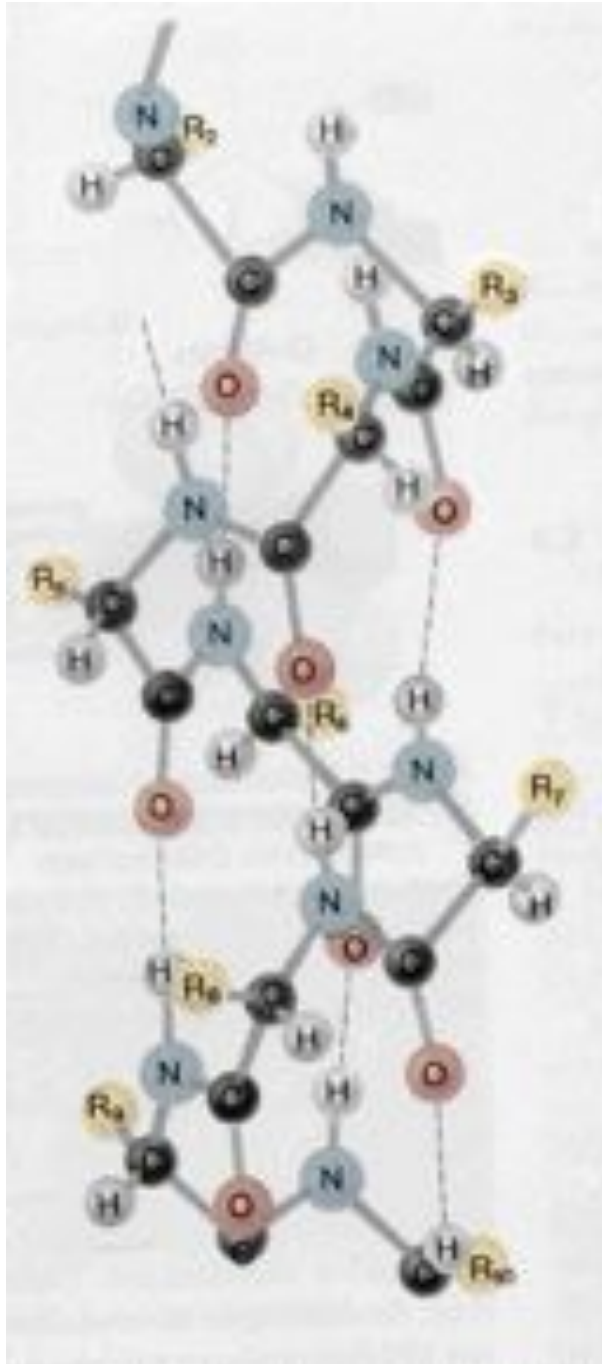




Glycine

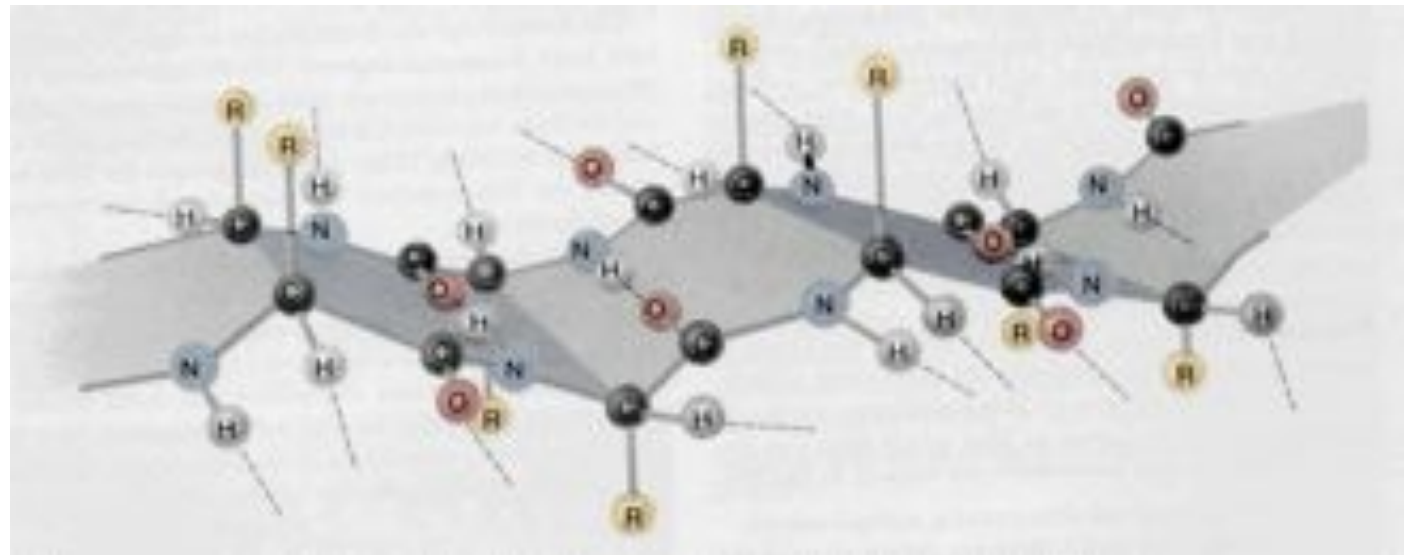


Protein Secondary Structure



An antiparallel beta sheet

Beta sheets are created, when atoms of beta strands are hydrogen bound. Beta-sheets may consist of parallel strands, antiparallel strands or out of a mixture of parallel and antiparallel strands.



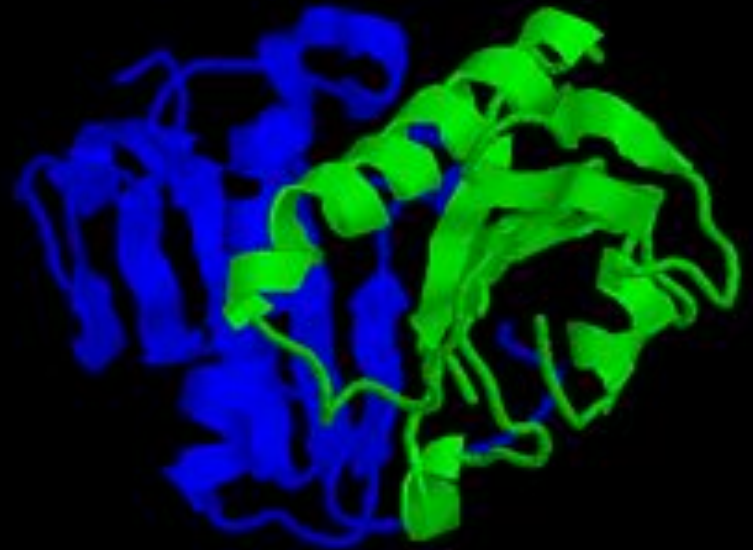
An alpha helix

The backbone is formed as a helix. An ideal alpha helix consists of 3.6 residues per complete turn. The side chains stick out. There are hydrogen bonds between the carboxy group of amino acid and the amino group of another amino acid $n+4$. The mean phi angle is -62 degrees and the mean psi angle is -41 degrees

Tertiary and Quarternary Structures of Proteins

Tertiary structure describes the packing of alpha-helices, beta-sheets and random coils with respect to each other on the level of one whole polypeptide chain.

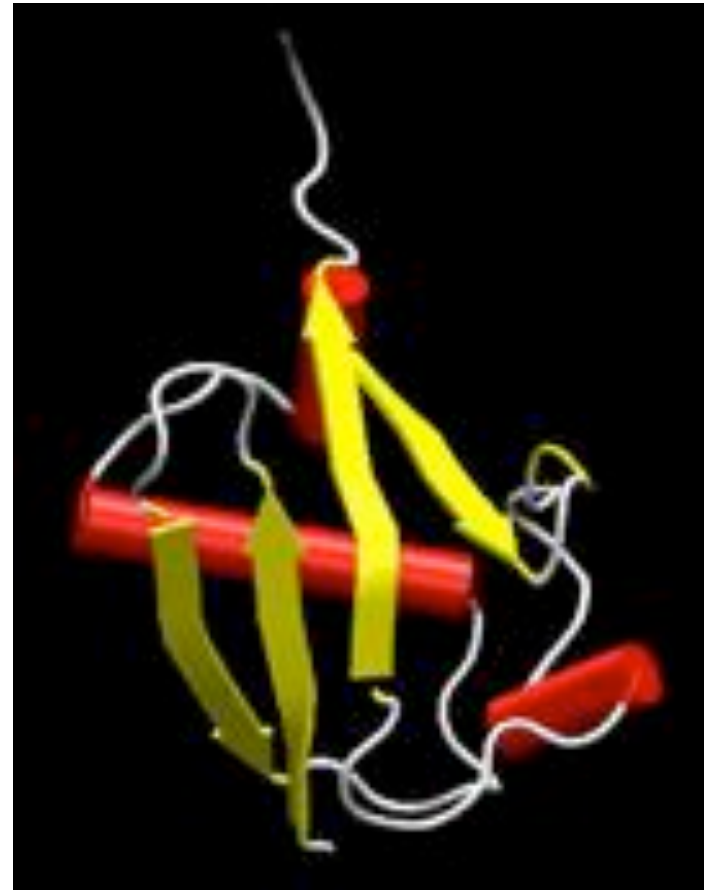
Quaternary structure only exists, if there is more than one polypeptide chain present in a complex protein. Then quaternary structure describes the spatial organization of the chains



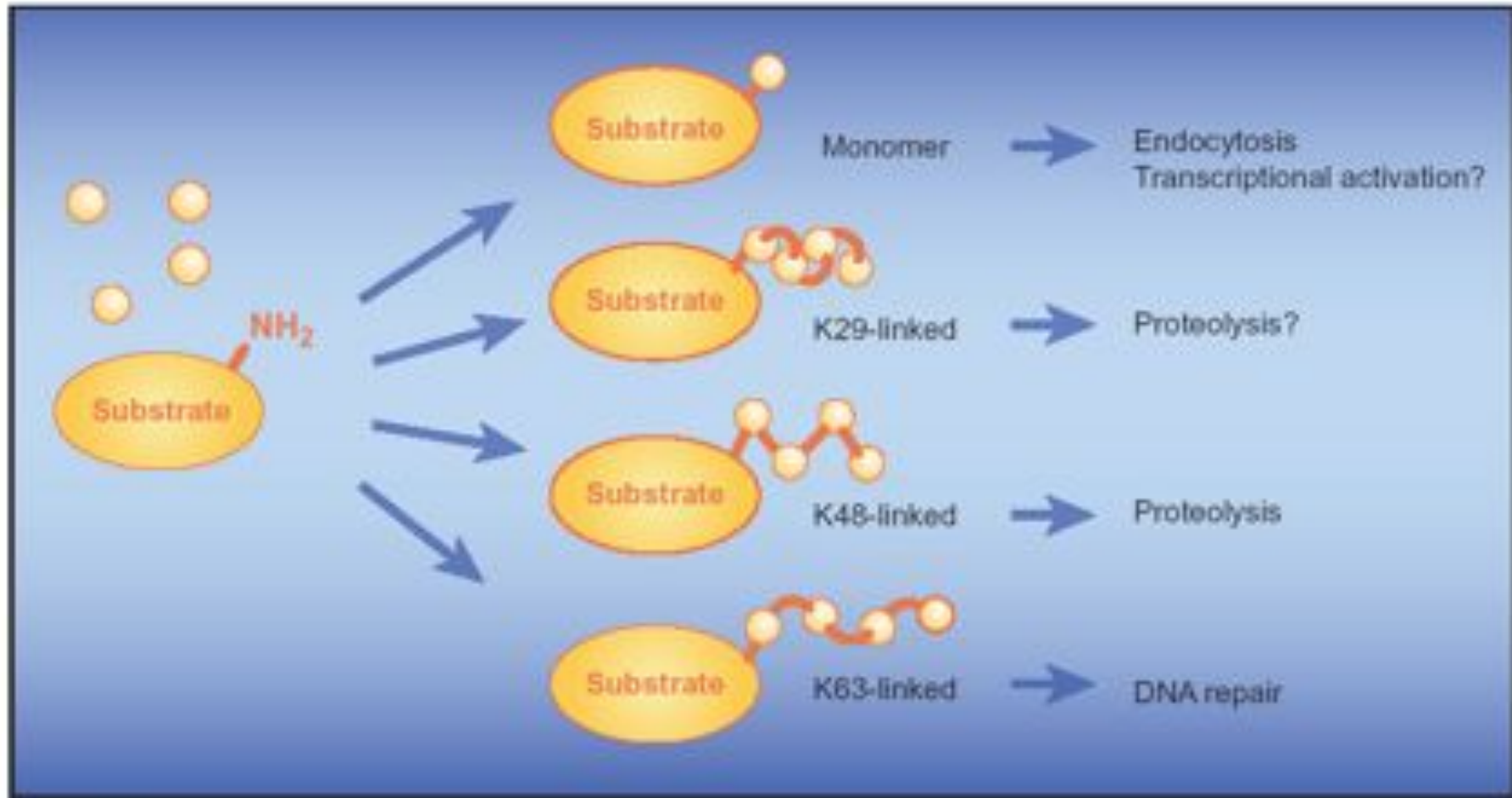
Focus on one protein

Ubiquitin

- 76 amino acids
- highly conserved
- covalently attaches to proteins and tags them for degradation
- other cell trafficking



Mono-ubiquitylation versus multi-ubiquitylation



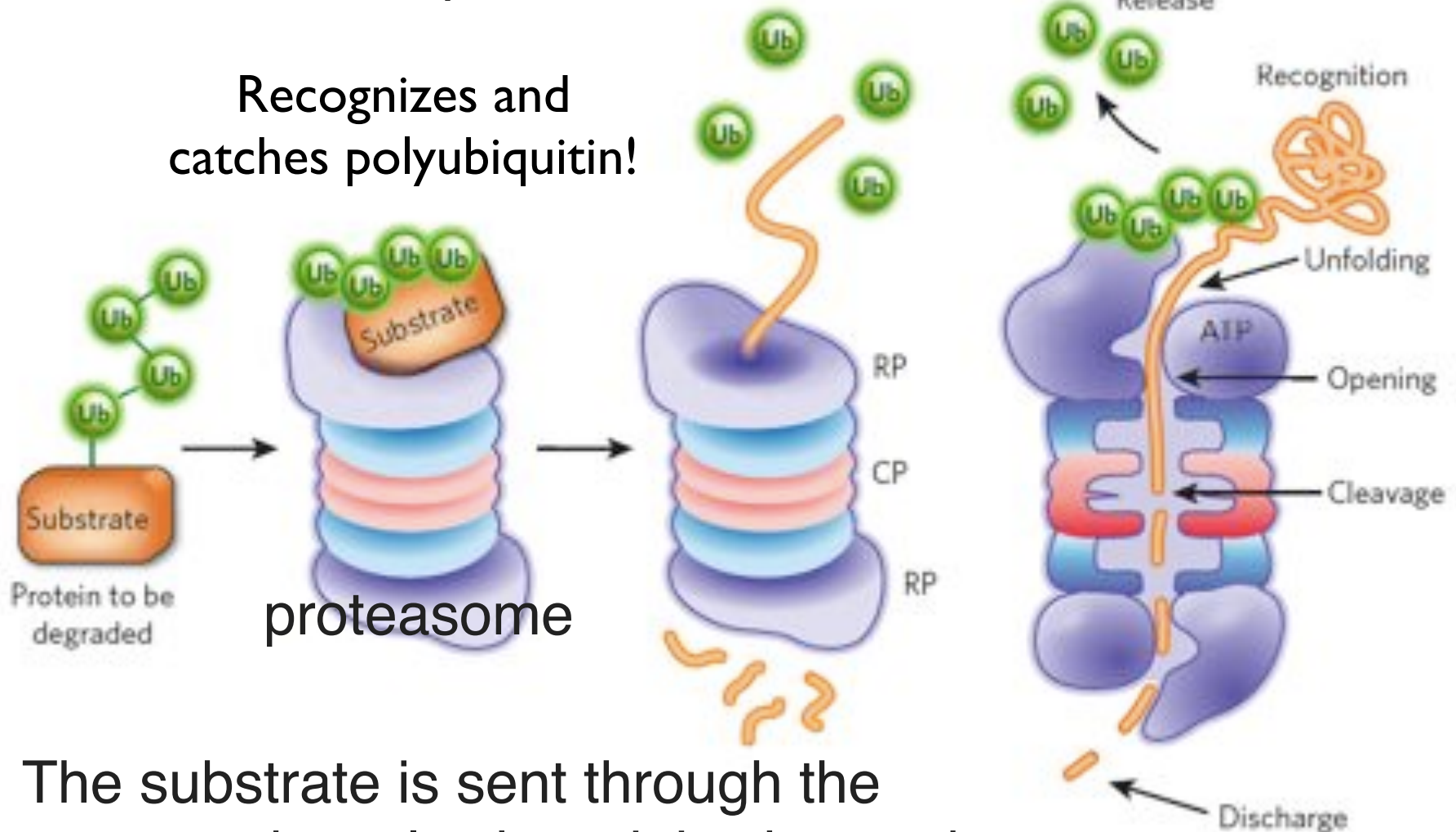
Multifaceted. Ubiquitin can attach to its various substrate proteins, either singly or in chains, and that in turn might determine what effect the ubiquitination has. (K29, K48, and K63 refer to the particular lysine amino acid used to link the ubiquitins to each other.)

Marx, J., Ubiquitin lives up its name, *Science* 297, 1792-1794 (2002)

Ubiquitin's role in protein degradation

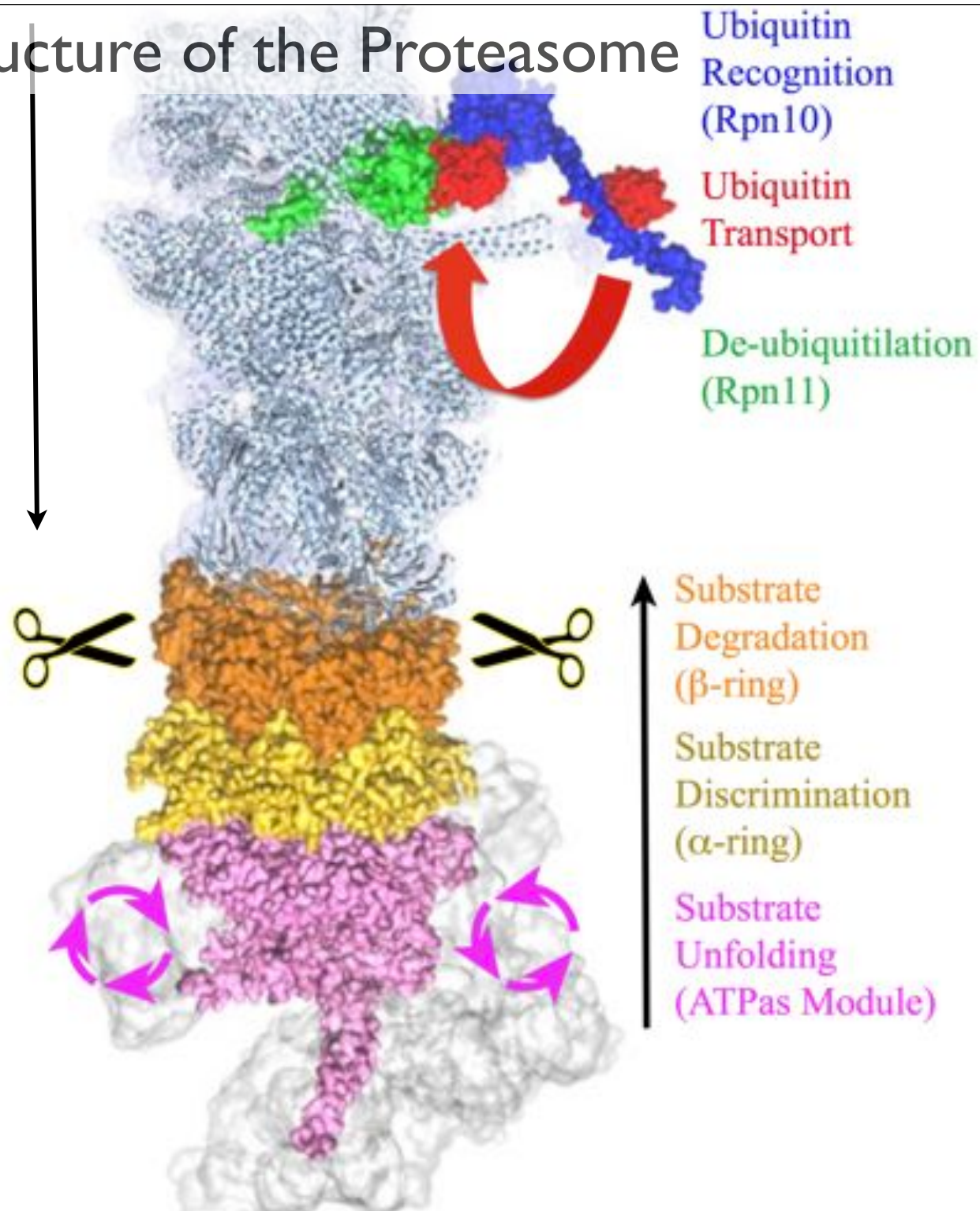
The substrate-polyubiquitin complex is then sent to proteasome

Recognizes and catches polyubiquitin!



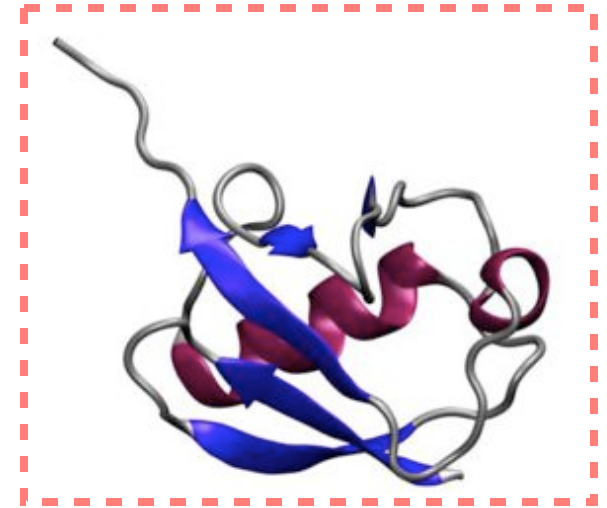
The substrate is sent through the proteasome barrel, where it is chopped up and recycled

Structure of the Proteasome



Highly conserved ubiquitin chain

- The sequence of ubiquitin is highly conserved, in particular the seven lysine residues
- A lysine residue in a ubiquitin can be linked to the C-terminus of another ubiquitin
- By using different lysine for such linkage, ubiquitin is used for different cellular purposes



Organism	Sequence Alignment							Swiss-P																																																														
Amoeba	M	Q	I	F	Y	K	L	T	G	K	T	I	L	E	V	E	S	S	D	T	I	E	N	K	K	Q	E	K	I	G	I	P	P	D	Q	Q	R	L	I	F	A	K	G	L	E	D	G	R	T	L	A	D	Y	N	I	K	E	S	T	L	H	L	V	L	R	L	R	G	G	P40634
Green alga	M	Q	I	F	Y	K	L	T	G	K	T	I	L	E	V	E	S	S	D	T	V	E	N	K	K	Q	E	K	I	G	I	P	P	D	Q	Q	R	L	I	F	A	K	G	L	E	D	G	R	T	L	A	D	Y	N	I	K	E	S	T	L	H	L	V	L	R	L	R	G	G	P42739
Chlamyd. reinhardtii	M	Q	I	F	Y	K	L	T	G	K	T	I	L	E	V	E	S	S	D	T	I	E	N	K	K	Q	E	K	I	G	I	P	P	D	Q	Q	R	L	I	F	A	K	G	L	E	D	G	R	T	L	A	D	Y	N	I	K	E	S	T	L	H	L	V	L	R	L	R	G	G	P14624
Mouse	M	Q	I	F	Y	K	L	T	G	K	T	I	L	E	V	E	P	S	D	T	I	E	N	K	K	Q	E	K	I	G	I	P	P	D	Q	Q	R	L	I	F	A	K	G	L	E	D	G	R	T	L	S	D	Y	N	I	K	E	S	T	L	H	L	V	L	R	L	R	G	G	P62991
Human (**)	M	Q	I	F	Y	K	L	T	G	K	T	I	L	E	V	E	P	S	D	T	I	E	N	K	K	Q	E	K	I	G	I	P	P	D	Q	Q	R	L	I	F	A	K	G	L	E	D	G	R	T	L	S	D	Y	N	I	K	E	S	T	L	H	L	V	L	R	L	R	G	G	P62988
Slime mold	M	Q	I	F	Y	K	L	T	G	K	T	I	L	E	V	E	G	S	D	N	I	E	N	K	K	Q	E	K	I	G	I	P	P	D	Q	Q	R	L	I	F	A	K	G	L	E	D	G	R	T	L	S	D	Y	N	I	K	E	S	T	L	H	L	V	L	R	L	R	G	G	P08818
Purple sea urchin	M	Q	I	F	Y	K	L	T	G	K	T	I	L	E	V	E	P	S	D	S	I	E	N	K	K	Q	E	K	I	G	I	P	P	D	Q	Q	R	L	I	F	A	K	G	L	E	D	G	R	T	L	S	D	Y	N	I	K	E	S	T	L	H	L	V	L	R	L	R	G	G	P23398
Eimeria bovis	M	Q	I	F	Y	K	L	T	G	K	T	I	L	D	V	E	P	S	D	T	I	E	N	K	K	Q	E	K	I	G	I	P	P	D	Q	Q	R	L	I	F	A	K	G	L	E	D	G	R	T	L	S	D	Y	N	I	K	E	S	T	L	H	L	V	L	R	L	R	G	G	P46574
T. pyriformis	M	Q	I	F	Y	K	L	T	G	K	T	I	L	D	V	E	A	S	D	T	I	E	N	K	K	Q	E	K	I	G	I	P	P	D	Q	Q	R	L	I	F	A	K	G	L	E	D	G	R	T	L	S	D	Y	N	I	K	E	S	T	L	H	L	V	L	R	L	R	G	G	P20685
C. elegans	M	Q	I	F	Y	K	L	T	G	K	T	I	L	E	V	E	A	S	D	T	I	E	N	K	K	Q	E	K	I	G	I	P	P	D	Q	Q	R	L	I	F	A	K	G	L	E	D	G	R	T	L	S	D	Y	N	I	K	E	S	T	L	H	L	V	L	R	L	R	G	G	P14792
Red alga	M	Q	I	F	Y	K	L	T	G	K	T	I	L	E	V	E	S	S	D	T	I	E	N	K	K	Q	E	K	I	G	I	P	P	D	Q	Q	R	L	I	F	A	K	G	L	E	D	G	R	T	L	S	D	Y	N	I	K	E	S	T	L	H	L	V	L	R	L	R	G	G	P42740
Neurospora crassa	M	Q	I	F	Y	K	L	T	G	K	T	I	L	E	V	E	S	S	D	T	I	D	N	K	K	Q	E	K	I	G	I	P	P	D	Q	Q	R	L	I	F	A	K	G	L	E	D	G	R	T	L	S	D	Y	N	I	K	E	S	T	L	H	L	V	L	R	L	R	G	G	P13117
Baker's yeast	M	Q	I	F	Y	K	L	T	G	K	T	I	L	E	V	E	S	S	D	T	I	D	N	K	K	Q	E	K	I	G	I	P	P	D	Q	Q	R	L	I	F	A	K	G	L	E	D	G	R	T	L	S	D	Y	N	I	K	E	S	T	L	H	L	V	L	R	L	R	G	G	P61864
Inky cap fungus	M	Q	I	F	Y	K	L	T	G	K	T	I	L	E	V	E	S	S	D	T	I	D	N	K	K	Q	E	K	I	G	I	P	P	D	Q	Q	R	L	I	F	A	K	G	L	E	D	G	R	T	L	S	D	Y	N	I	K	E	S	T	L	H	L	V	L	R	L	R	G	G	P19848
Garden pea (**)	M	Q	I	F	Y	K	L	T	G	K	T	I	L	E	V	E	S	S	D	T	I	D	N	K	K	Q	E	K	I	G	I	P	P	D	Q	Q	R	L	I	F	A	K	G	L	E	D	G	R	T	L	A	D	Y	N	I	K	E	S	T	L	H	L	V	L	R	L	R	G	G	P03993
Euplotes eurystomus	M	Q	I	F	Y	K	L	T	G	K	T	I	L	D	V	E	G	S	D	T	I	D	N	K	K	Q	E	K	I	G	I	P	P	D	Q	Q	R	L	I	F	A	K	G	L	E	D	G	R	T	L	A	D	Y	N	I	K	E	S	T	L	H	L	V	L	R	L	R	G	G	P23324
Potato late blight fungus	M	Q	I	F	Y	K	L	T	G	K	T	I	L	D	V	E	P	S	D	S	I	D	N	K	K	Q	E	K	I	G	I	P	P	D	Q	Q	R	L	I	F	A	K	G	L	E	D	G	R	T	L	S	D	Y	N	I	K	E	S	T	L	H	L	V	L	R	L	R	G	G	P22589
Leishmania major	M	Q	I	F	Y	K	L	T	G	K	T	I	A	L	E	V	E	P	S	D	T	I	E	N	K	K	Q	E	K	I	G	I	P	P	D	Q	Q	R	L	I	F	A	K	L	E	E	G	R	T	L	S	D	Y	N	I	K	E	S	T	L	H	L	V	L	R	L	R	G	G	Q05550
Sauroleish. tarentolae	M	Q	I	F	Y	K	L	T	G	T	I	A	L	E	V	E	P	S	D	T	I	E	N	K	K	Q	E	K	I	G	I	P	P	D	Q	Q	R	L	I	F	A	K	L	E	E	G	R	T	L	S	D	Y	N	I	K	E	S	T	L	H	L	V	L	R	L	R	G	G	P49635	
T. brucei brucei	M	Q	I	F	Y	K	L	T	G	K	T	I	A	L	E	V	E	A	S	D	T	I	E	N	K	K	Q	E	K	I	G	I	P	P	D	Q	Q	R	L	I	F	A	K	L	E	E	G	R	T	L	A	D	Y	N	I	K	E	S	T	L	H	L	V	L	R	L	R	G	G	P15174
Trypanosoma cruzi	M	Q	I	F	Y	K	L	T	G	K	T	I	A	L	E	V	E	S	S	D	T	I	E	N	K	K	Q	E	K	I	G	I	P	P	D	Q	Q	R	L	I	F	A	K	L	E	D	G	R	T	L	A	D	Y	N	I	K	E	S	T	L	H	L	V	L	R	L	R	G	G	P08585

VMD Demo 1

Some readings

<http://en.wikipedia.org/wiki/Ubiquitin>

J. Marx, “Ubiquitin lives up to its name.” *Science*, 297. (2002)

M. Hochstrasser, “Origin and function of ubiquitin-like proteins.” *Nature*, 458. (2009)

A. Varshavsky, “The early history of the ubiquitin field.” *Protein Science*, 15. (2006)

C. M. Pickart, “Back to the future with ubiquitin.” *Cell*, 116. (2004)

M. Carrion-Vazquez et al., “The mechanical stability of ubiquitin is linkage dependent.” *Nature Structure Biology*, 10. (2003)

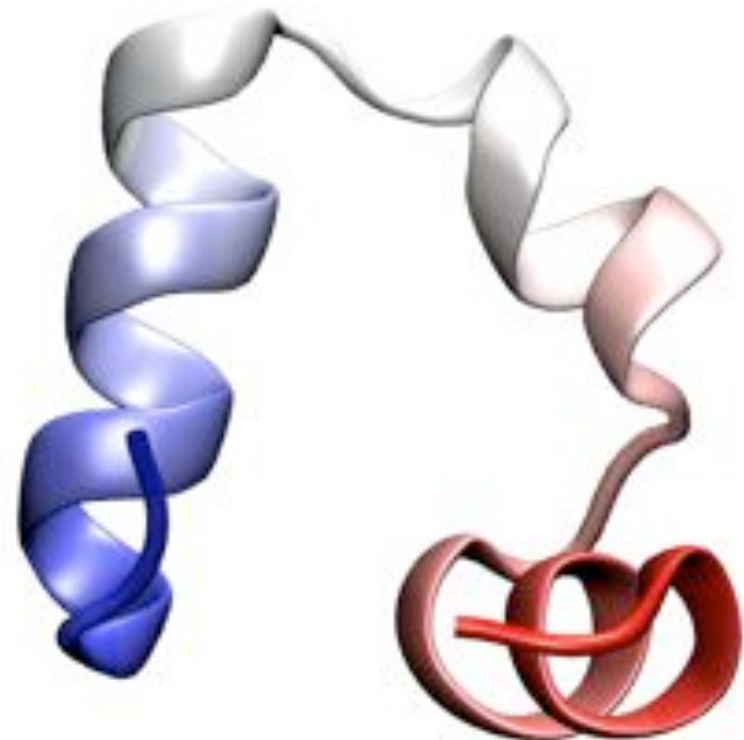
http://nobelprize.org/nobel_prizes/chemistry/laureates/2004/

If you need to get a quick lesson on VMD, here is a short tutorial:

<http://www.ks.uiuc.edu/~jhsin/papers/HSIN2008.pdf>

Protein Folding

- Folding of the Protein called Villin Headpiece
- First protein folded in computer simulation
- Visualization of the “trajectory” of the folding protein reveals how this protein finds its native conformation from an initially stretched-out conformation

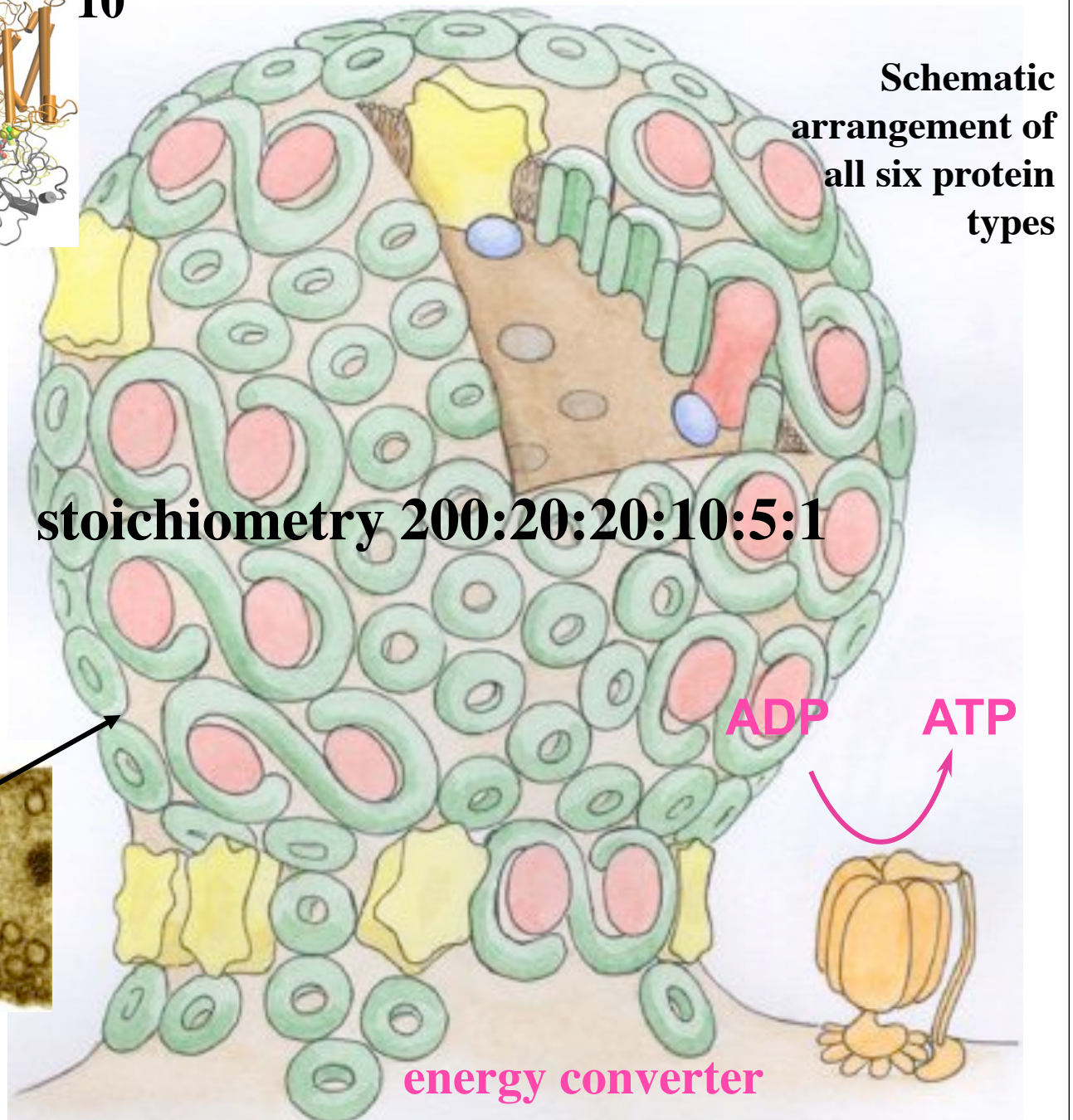
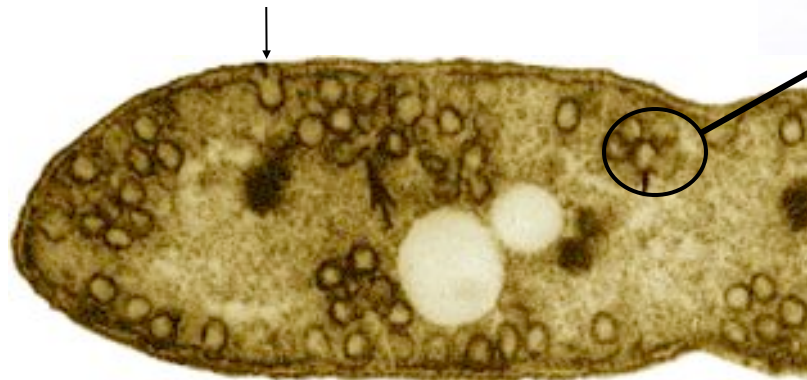
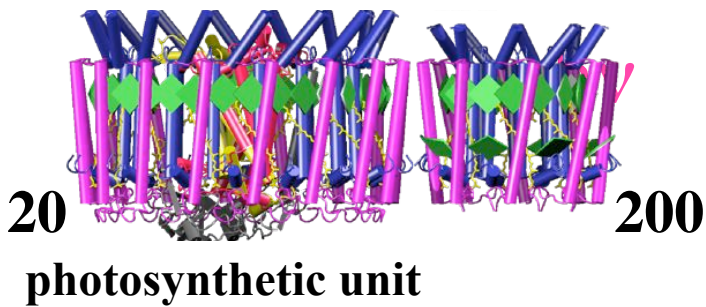
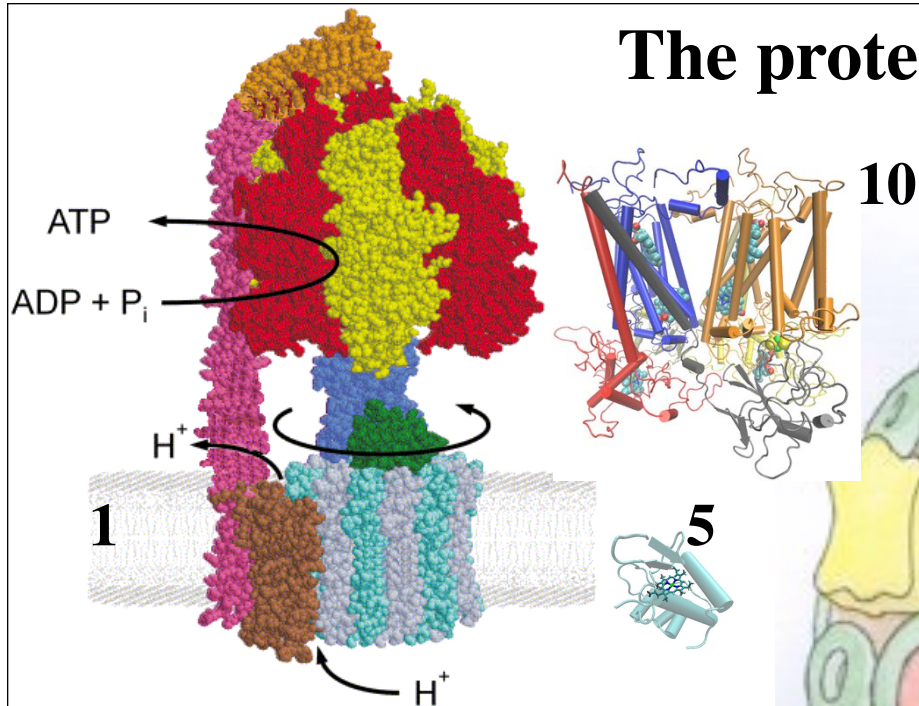


villin headpiece

Observe folding process in unprecedented detail

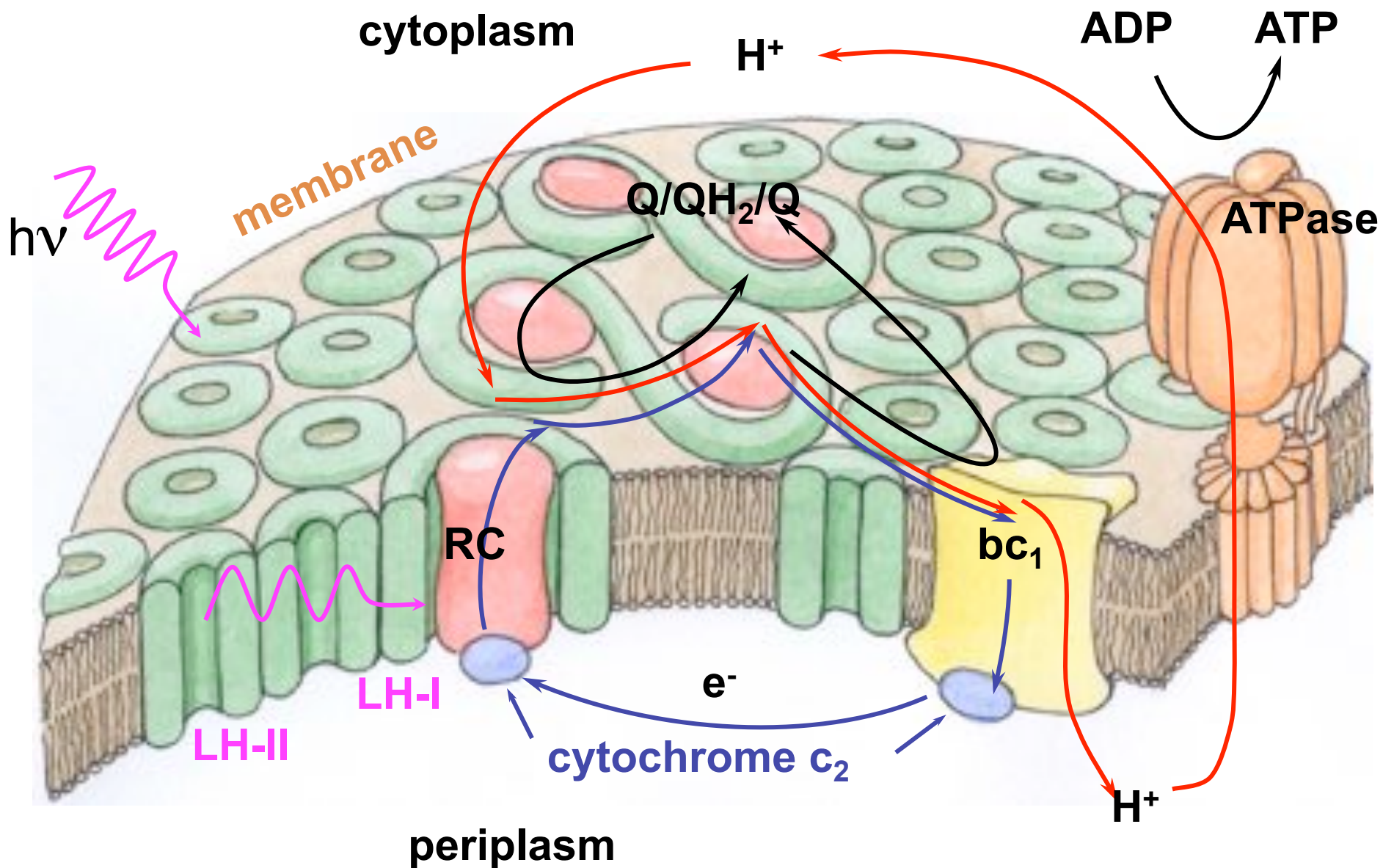
VMD Demo 2

The proteins that make up the chromatophore of photosynthetic bacteria

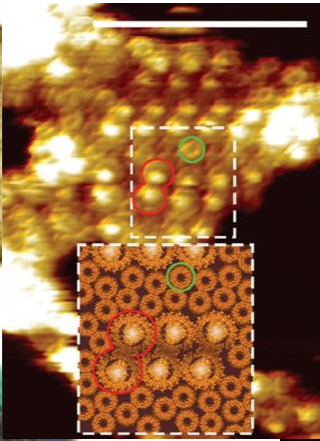


Chromatophore of Purple Bacteria

(section of the chromatophore membrane)



Knowing the Atomic Level Structure of the chromatophore, one can systematically describe its physical mechanism



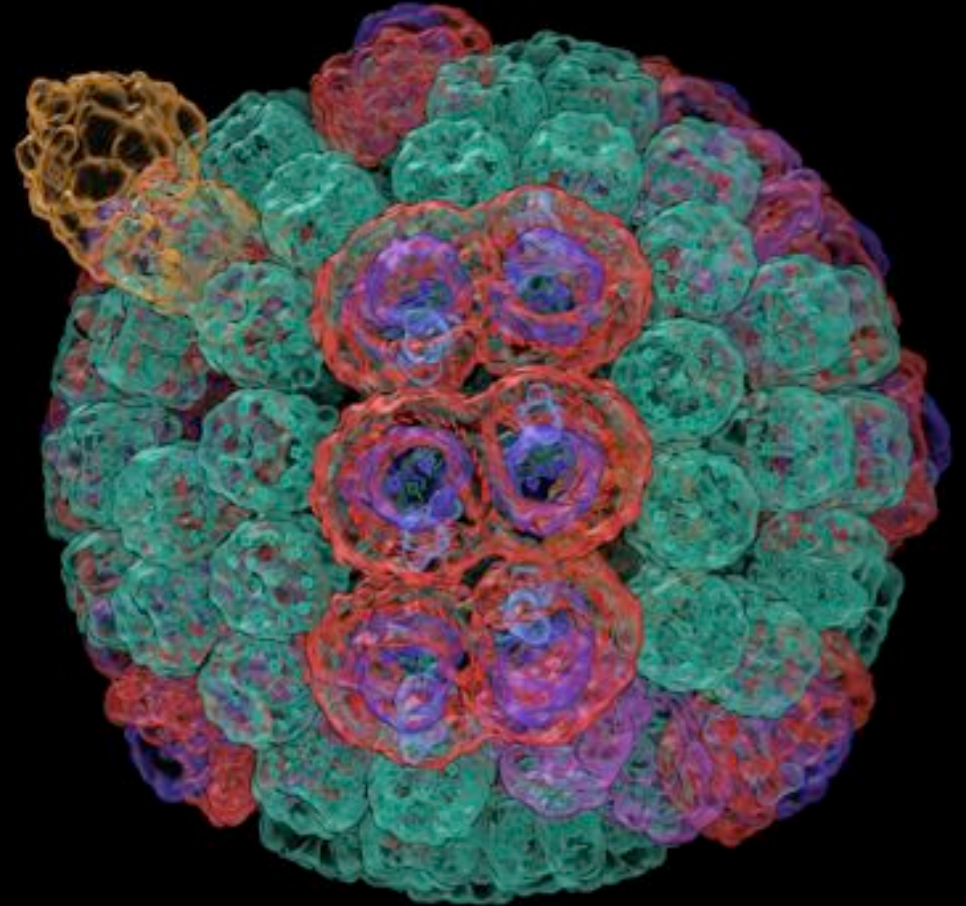
light



ADP

ATP

Melih Sener



A Habitat of Purple Bacteria

