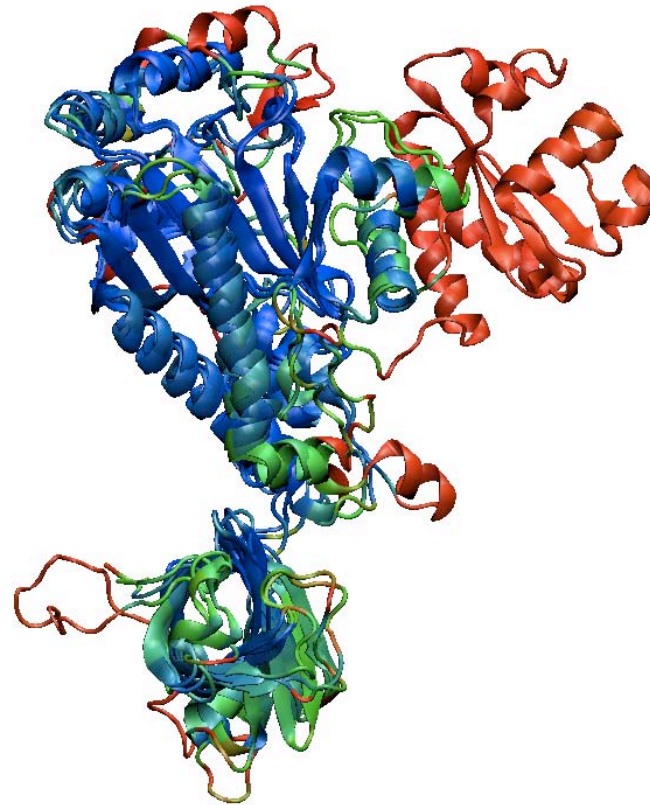


Sequence and Structure Alignment










Z. Luthey-Schulten, UIUC

Pittsburgh, 2006

Part I



VMD 1.8.5

Sequence Name		530		540		550																										
VMD Structures																																
<input checked="" type="checkbox"/> 1c0a_A	   429	W	V	I	D	F	P	M	F	E	D	D	G	E	G	G	L	T	A	M	H	H	P	F	T	S	P	K	D	.	M	T
<input checked="" type="checkbox"/> 1asy_A	   444	I	L	D	K	F	P	L	E	I	R	P	F	Y	T	M	P	D	P	A	N	.
<input checked="" type="checkbox"/> 1b8a_A	   327	F	L	Y	Q	Y	P	S	E	A	K	P	F	Y	I	M	K	Y	D	N	K	.

Why Look at More Than One Sequence?

1. Multiple Sequence Alignment shows patterns of conservation

Sequence Name	800	810	820	830
<input checked="" type="checkbox"/> SYN_THEAC 357	S Q R I W N Y D E L M Q R I R E A N L D			E S . A Y Y W Y V
<input checked="" type="checkbox"/> SYNC_CAEL 473	S M R I W K E D Q L L A A F E K G G L D			S K N . Y Y W Y M
<input checked="" type="checkbox"/> SYNC_MOUSE 475	S M R S W D S E E I L E G Y K R E G I D			P A P . Y Y W Y T
<input checked="" type="checkbox"/> SYNC_DEBHA 480	S M R T Y D N D E L V A A I K R E G L D			L D S . Y Y W F T
<input checked="" type="checkbox"/> SYNC_YEAST 482	S M R I D D M D E L M A G F K R E G I D			. T D A Y Y W F I
<input checked="" type="checkbox"/> SYNC_HUMAN 476	S M R I F D S E E I L A G Y K R E G I D			P T P . Y Y W Y T
<input checked="" type="checkbox"/> SYK2_METMA 433	Y S E L N D P L E Q E K R F E E Q D K K R K L G			D L E A Q T V D Y D F I
<input checked="" type="checkbox"/> SYK_HUMAN 499	Y T E L N D P M R Q R Q L F E E Q A K A K A A G			D D E A M F I D E N F C
<input checked="" type="checkbox"/> SYK2_METAC 433	Y S E L N D P L E Q E K R F E E Q D K K R K L G			D L E A Q T V D Y D F I
<input checked="" type="checkbox"/> SYK_MOUSE 497	Y T E L N D P V R Q R Q L F E E Q A K A K A A G			D D E A M F I D E N F C
<input checked="" type="checkbox"/> SYK_CRIGR 499	Y T E L N D P M R Q R Q L F E E Q A K A K A A G			D D E A M F I D E N F C
<input checked="" type="checkbox"/> SYK_ORYSA 524	Y T E L N D P V V Q R Q R F E E Q L K D R Q S G			D D E A M A L D E T F C

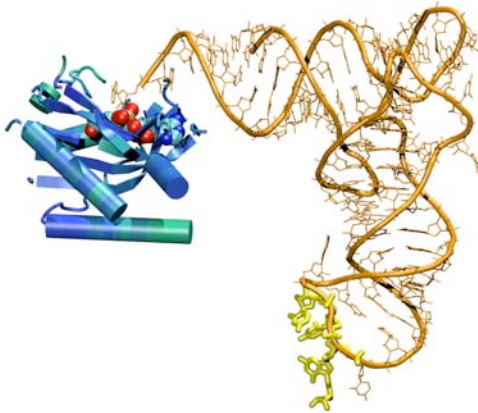
2. What and how many sequences should be included?

3. Where do I find the sequences and structures for MS alignment?

4. How to generate pairwise and multiple sequence alignments?

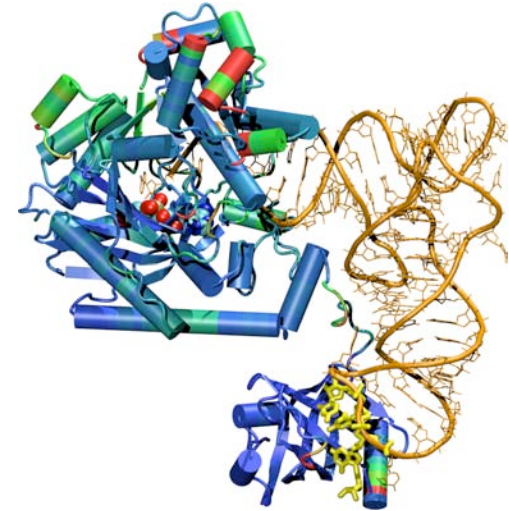
Evolution of Protein Structure

Part II



		Second position					
		U	C	A	G		
U	UUU	Phe	Ser	UAU	Tyr	UGU	Cys
	UUC			UAC		UGC	
	UUA	UCA		UAA	Stop	UGA	Stop
	UUG	UCG		UAG	Stop	UGG	Trp
C	CUU	Leu	Pro	CAU	His	CGU	Arg
	CUC			CCC		CAC	
	CUA	CCA		CAA	Gln	CGA	
	CUG	CCG		CAG	CGG		
A	AUU	Ile	Thr	AAU	Asn	AGU	Ser
	AUC			ACC		AAC	
	AUA	ACA		AAA	Lys	AGA	Arg
	AUG	Met/start		ACG	AAG	AGG	
G	GUU	Val	Ala	GAU	Asp	GGU	Gly
	GUC			GCC		GAC	
	GUA	GCA		GAA	Glu	GGA	
	GUG	GCG		GAG	GGG		

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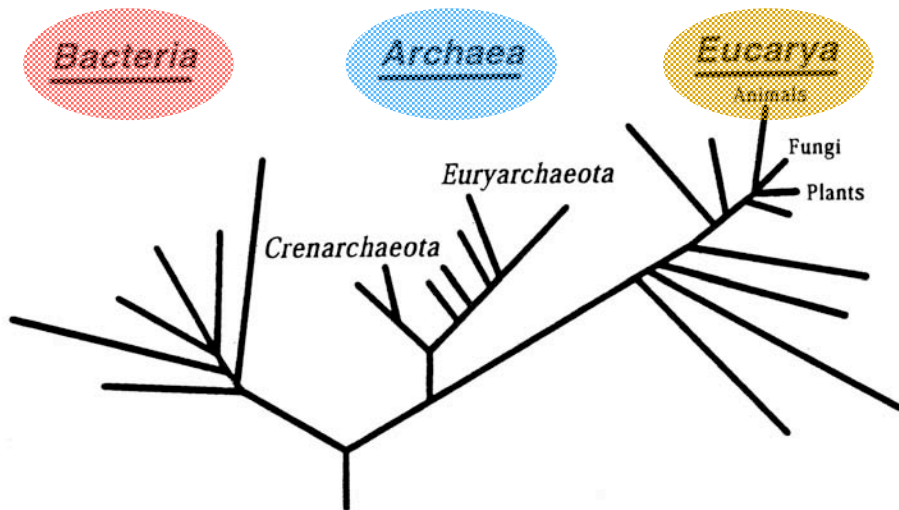


Luthey-Schulten Group

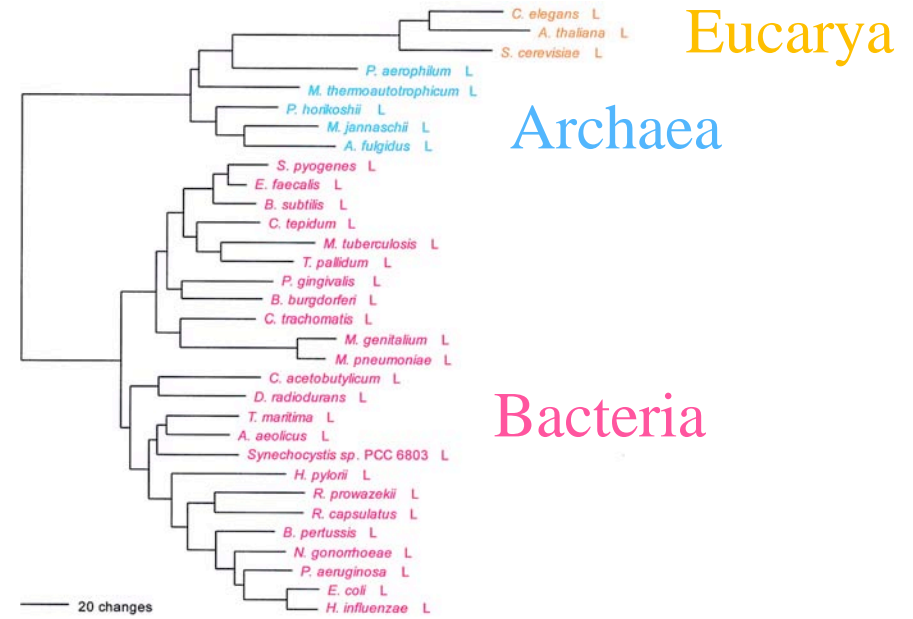
Department of Chemistry, Biophysics, and Beckman Institute
University of Illinois at Urbana-Champaign

Universal Phylogenetic Tree

three domains of life



Based on 16S rRNA



Leucyl-tRNA synthetase displays the full canonical phylogenetic distribution.

Part III - Evolutionary Studies

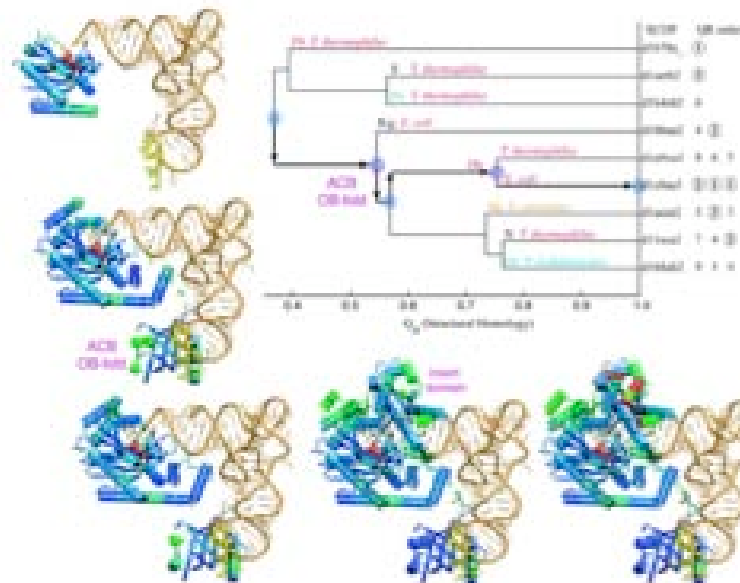
Using Multiseq in VMD

- Aminoacyl tRNA Synthetases
- tRNA
- Aquaporins

Pittsburgh, 2006, Computational Biology Workshop

Evolution of Biomolecular Structure

Class II tRNA-Synthetases and tRNA



MultiSeq Developers:

Elijah Roberts

John Eargle

Dan Wright

Prof. Zan Luthey-Schulten

Patrick O'Donoghue

Anurag Sethi

Brijeet Dhaliwal

March 2006.