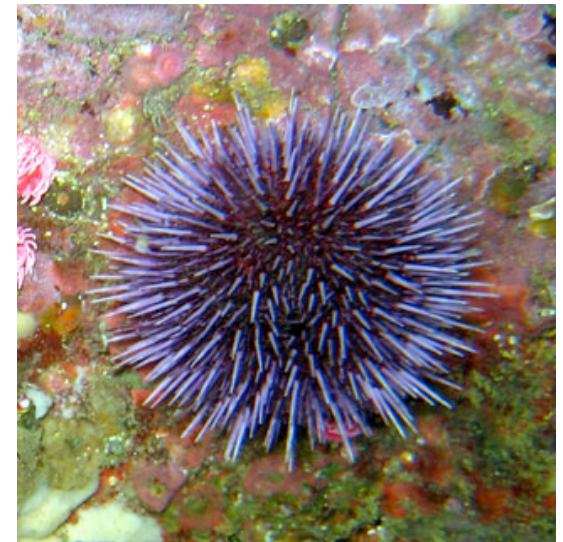
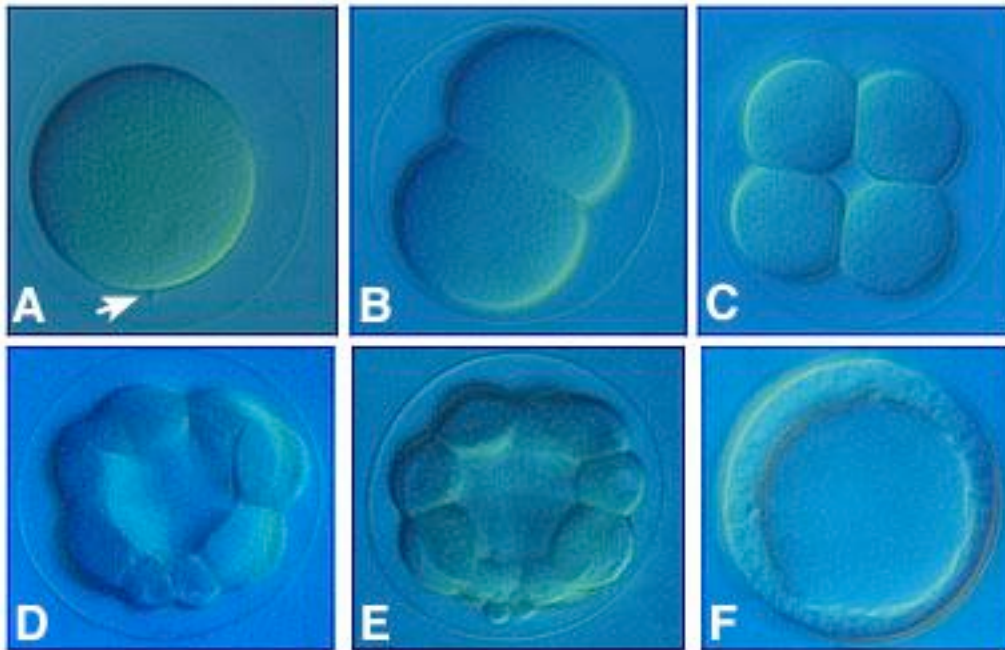




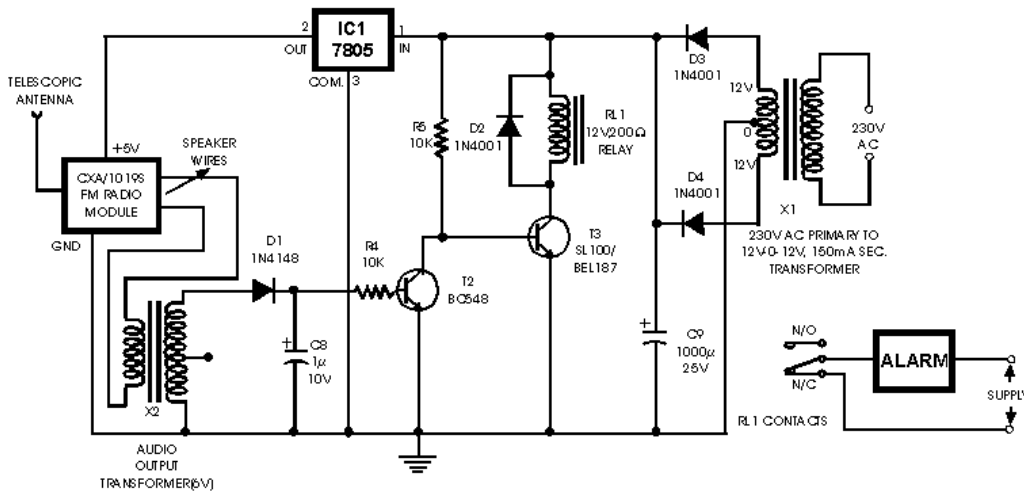
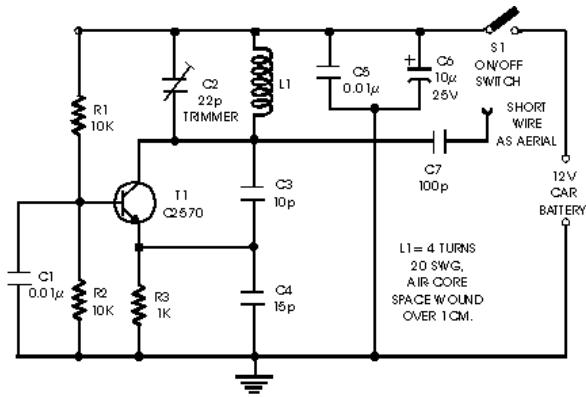
# Die Evolution Molekularer Netzwerke

Sarah A. Teichmann

# Embryonale Entwicklung des Seeigels (*Strongylocentrotus purpuratus*)



# Systembiologie: Biologen als molekulare Ingenieure





# “Schaltkreise” der embryonalen Entwicklung

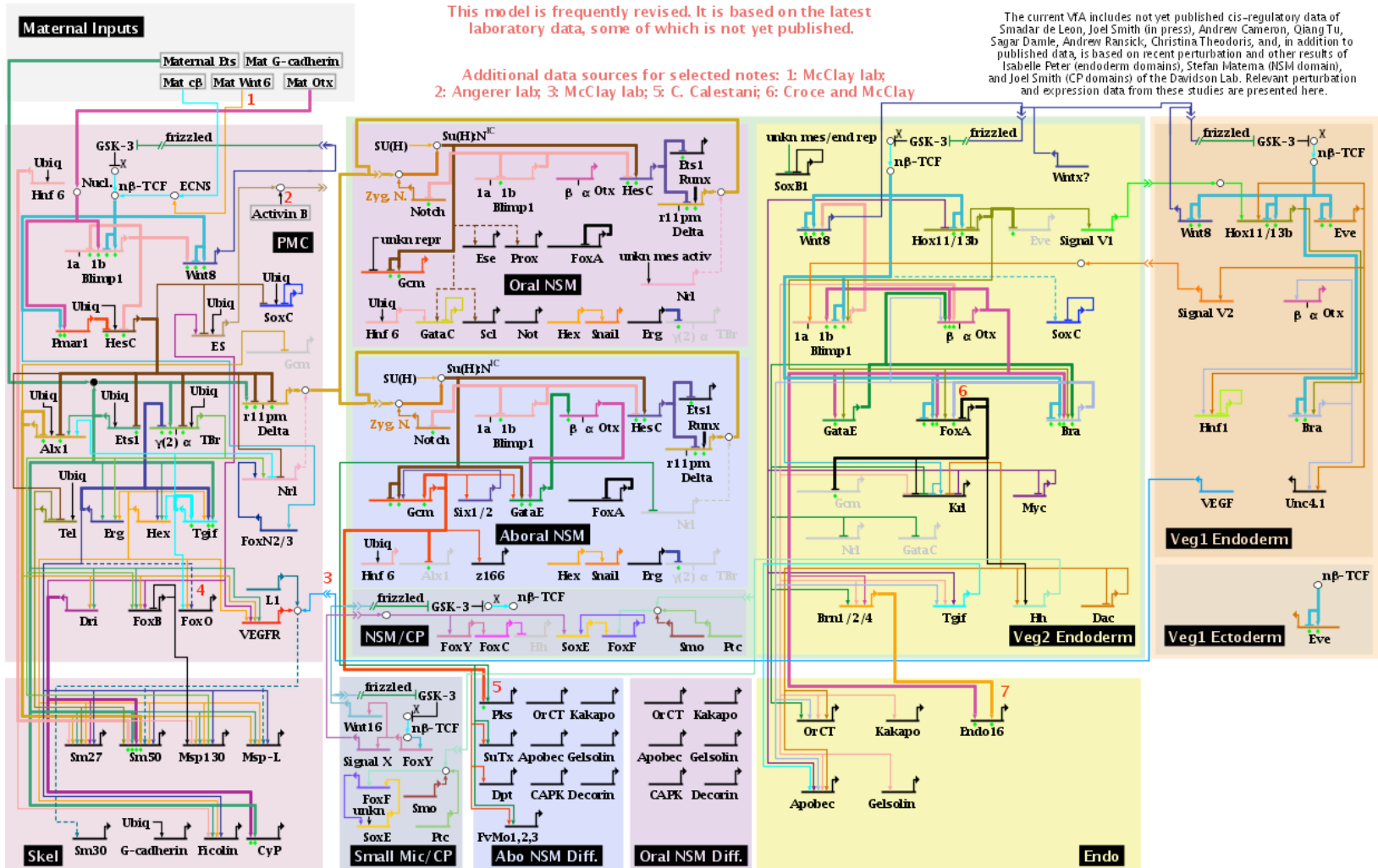
Endomesoderm Specification up to 30 Hours

February 10, 2010

This model is frequently revised. It is based on the latest laboratory data, some of which is not yet published.

Additional data sources for selected notes: 1: McClay lab; 2: Angerer lab; 3: McClay lab; 5: C. Calestani; 6: Croce and McClay

The current MFA includes not yet published cis-regulatory data of Smadar de Leon, Joel Smith (in press), Andrew Cameron, Qiang Tu, Sagar Dangle, Andrew Ransick, Christina Theodoris, and, in addition to published data, is based on recent perturbation and other results of Isabelle Peter (endoderm domains), Stefan Matema (NSM domain), and Joel Smith (CP domains) of the Davidson Lab. Relevant perturbation and expression data from these studies are presented here.



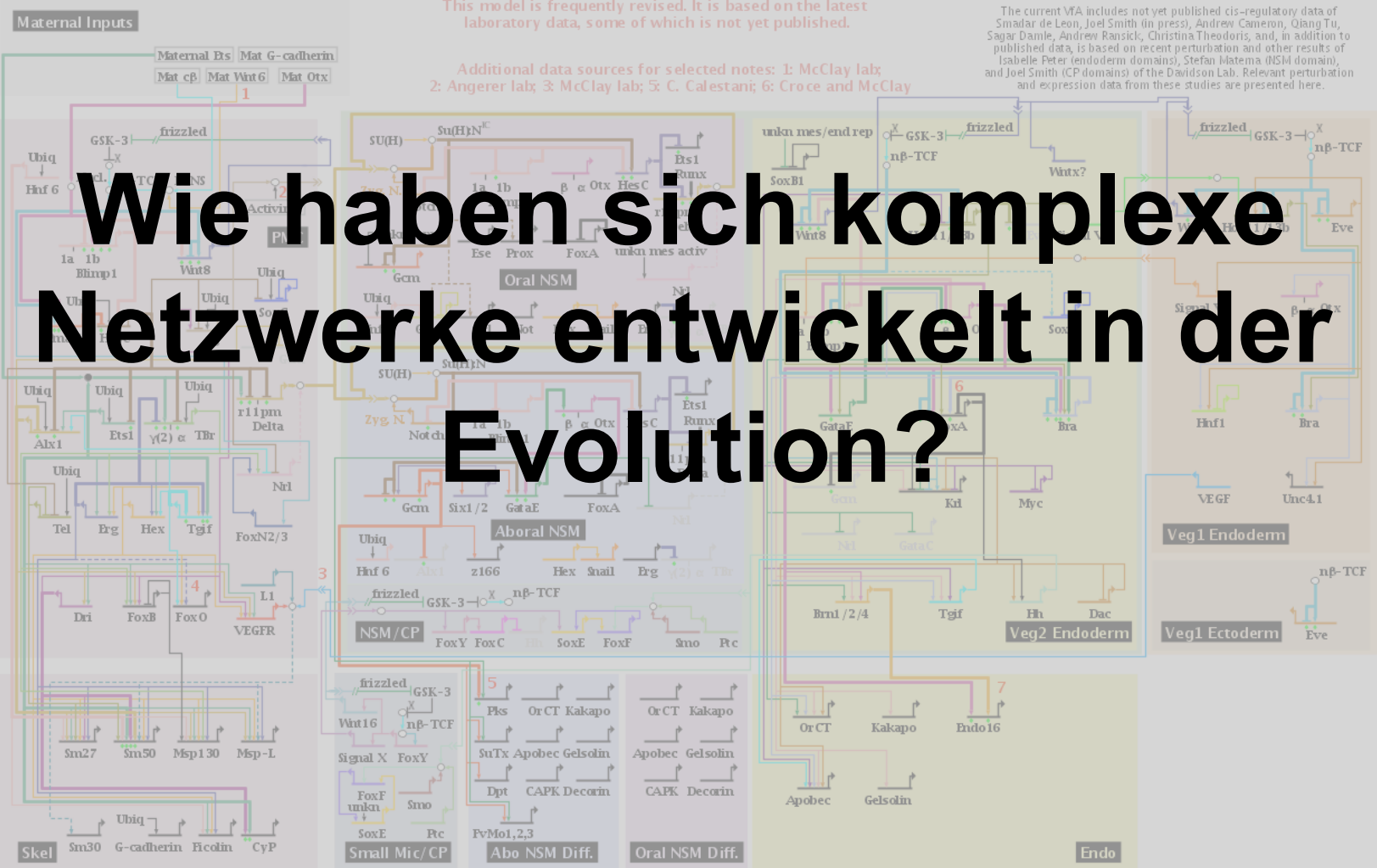
Ubiq=ubiquitous; Mat = maternal; activ = activator; rep = repressor; unkn = unknown; Nucl = nuclearization;  $\beta$  =  $\beta$ -catenin source; n $\beta$ -TCF = nuclearized b- $\beta$ -catenin-Tcf1; ES = early signal; ECNS = early cytoplasmic nuclearization system; Zyg. N. = zygotic Notch



This model is frequently revised. It is based on the latest laboratory data, some of which is not yet published.

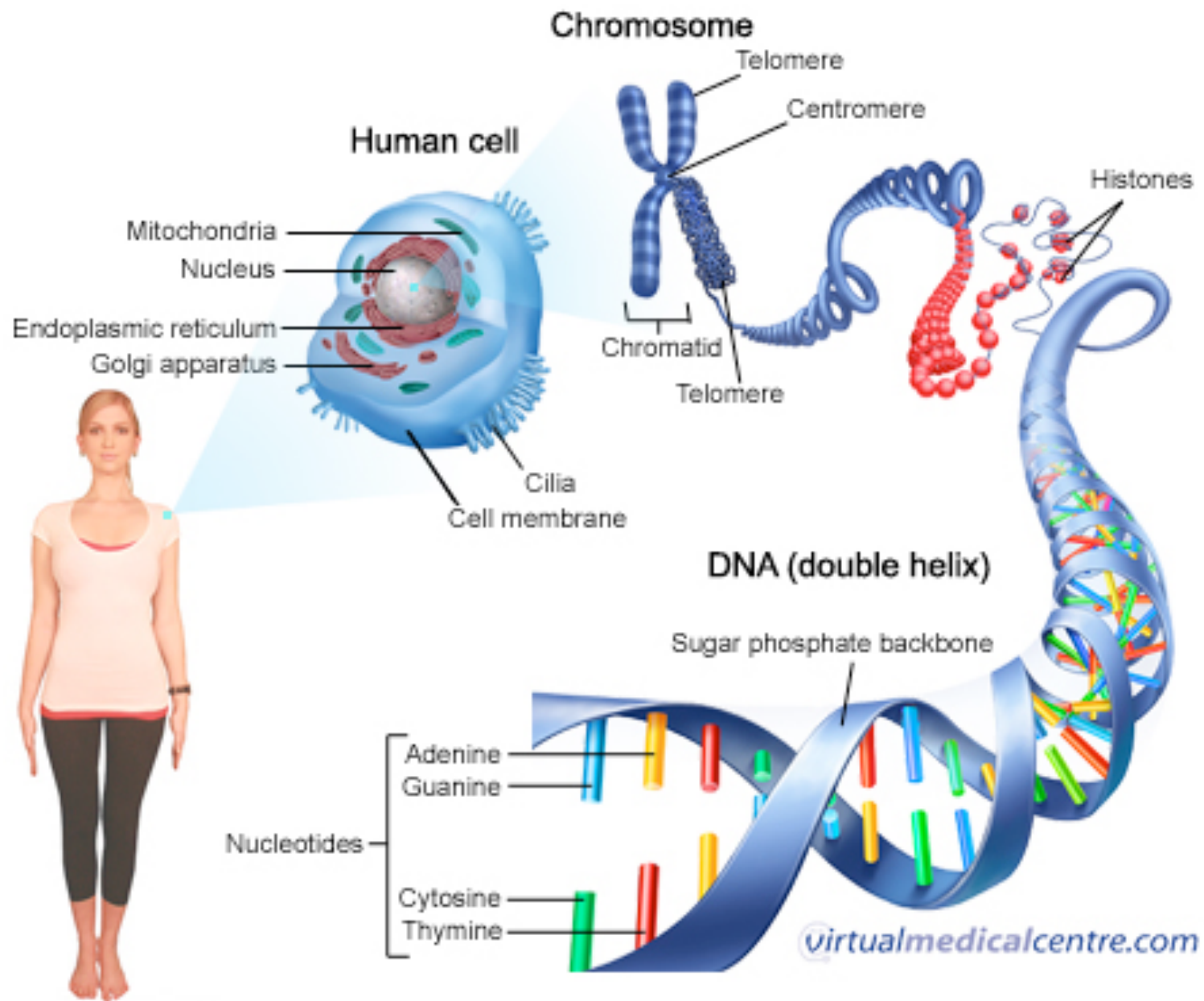
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The current MTA includes not yet published cis-regulatory data of Smadar de Leon, Joel Smith (in press), Andrew Cameron, Qiang Tu, Sagar Dangle, Andrew Ransick, Christina Theodoris, and, in addition to published data, is based on recent perturbation and other results of Isabelle Peter (endoderm domains), Stefan Matema (NSM domain), and Joel Smith (CP domains) of the Davidson Lab. Relevant perturbation and expression data from these studies are presented here.

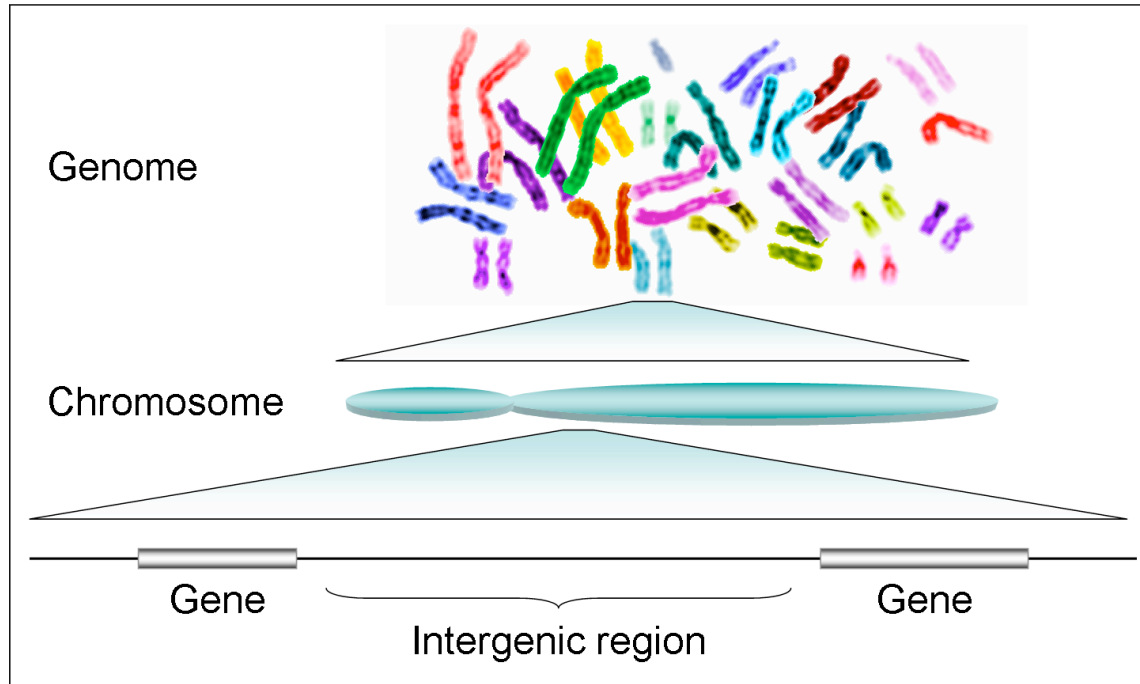


# Wie haben sich komplexe Netzwerke entwickelt in der Evolution?

Ubiq=ubiquitous; Mat = maternal; activ = activator; rep = repressor; unkn = unknown; Nucl = nuclearization;  $\chi$  =  $\beta$ -catenin source; n $\beta$ -TCF = nuclearized b- $\beta$ -catenin-Tcf1; E $\delta$  = early signal; ECNS = early cytoplasmic nuclearization system; Zyg. N. = zygotic Notch



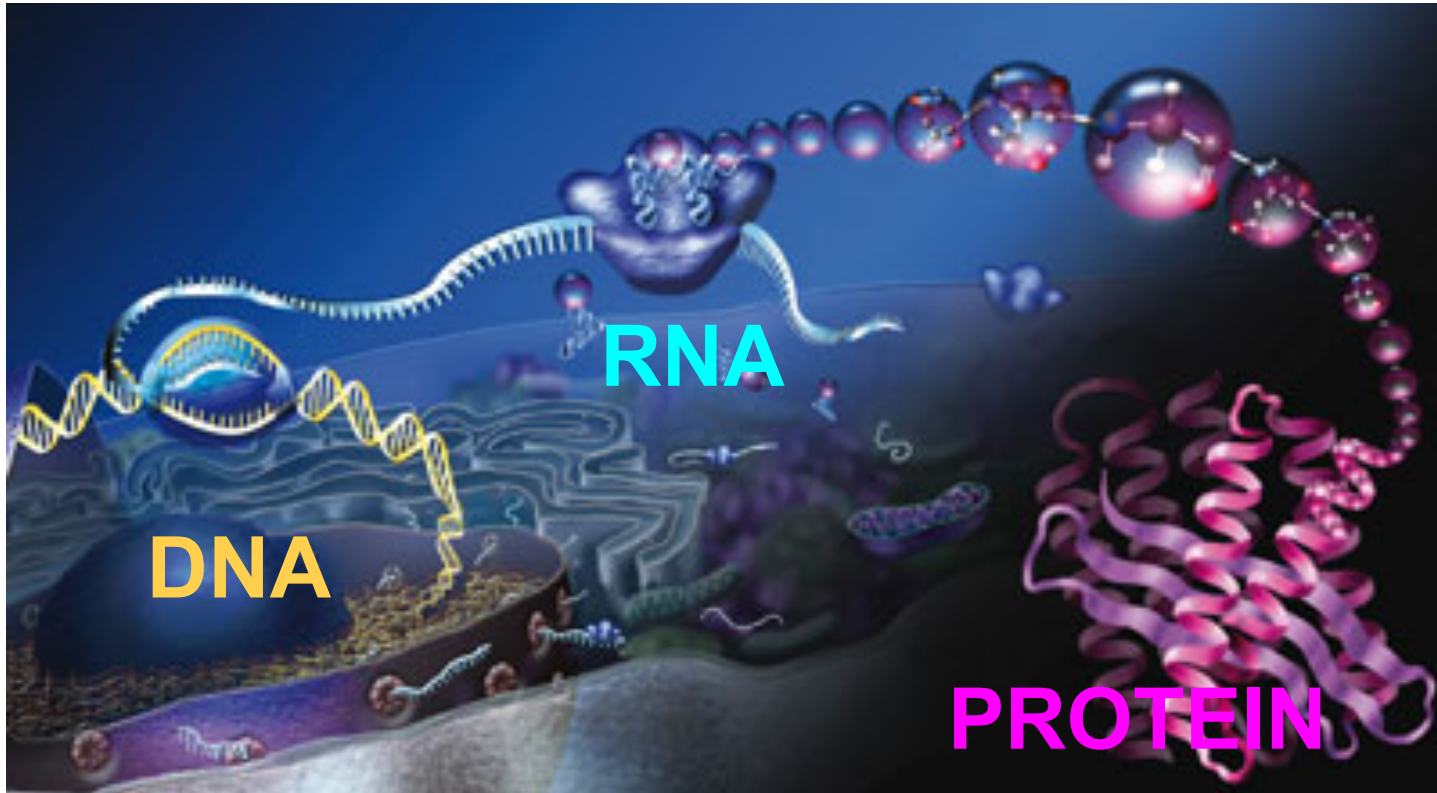
# Evolutionsvorgaenge in der DNA



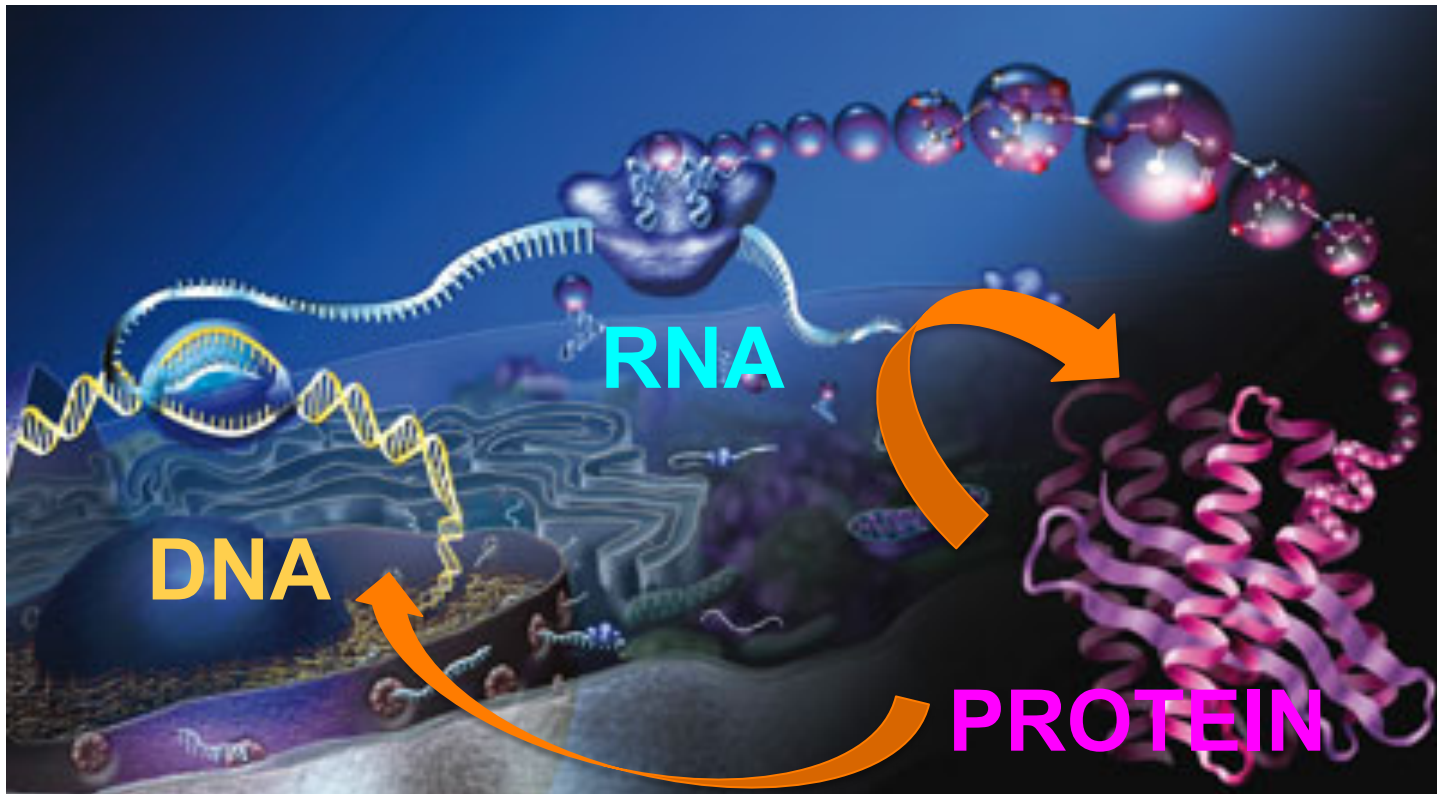
1. Mutation: Divergenz oder Konservierung der Sequenz
2. Duplikation: Kopieren der Gene
3. Genfusion: Zusammenfuegen von 2 Genen



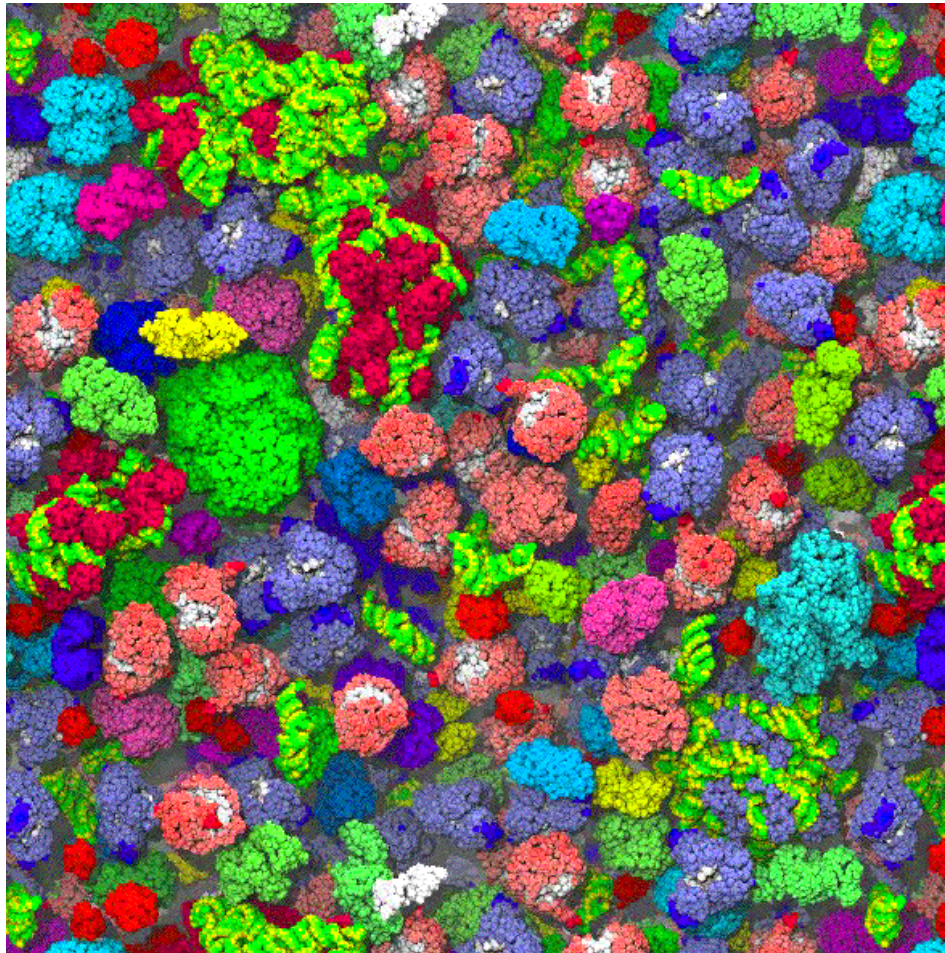
# Das zentrale Dogma der Molekularbiologie



# Das zentrale Dogma der Molekularbiologie



# Das Innenleben einer Zelle





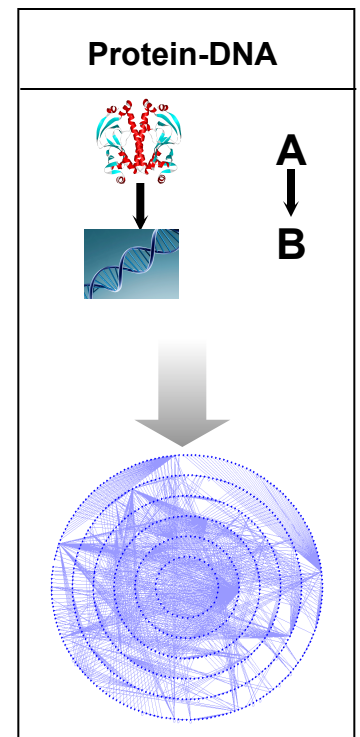
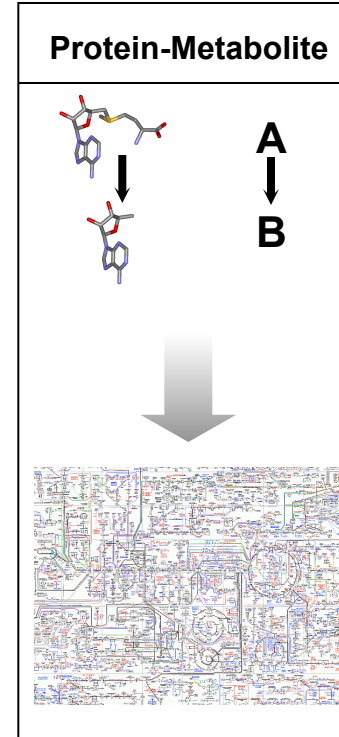
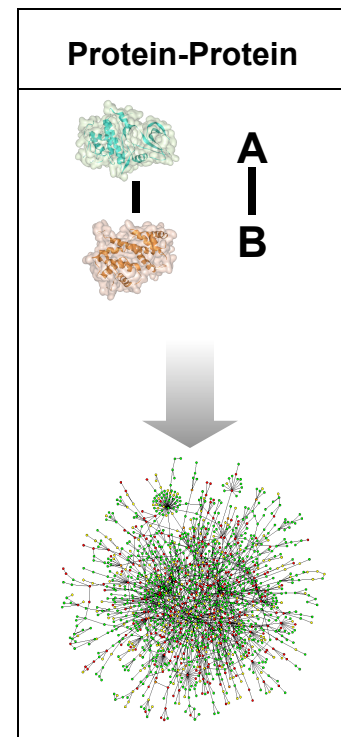
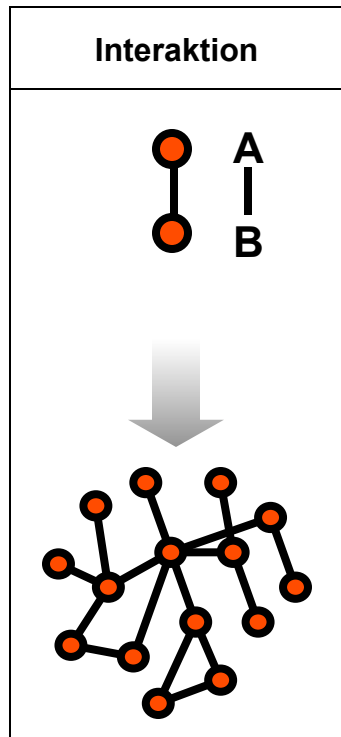
# Netzwerke in der Biologie

<b>Netzwerk</b>
<b>Knoten</b> ●
<b>Kanten</b> ●—●

<b>Proteinbindung</b>
<i>Proteine</i>
<i>Direkte Bindung</i>

<b>Metabolite</b>
<i>Kleine Molekuele</i>
<i>Enzymatische Katalyse</i>

<b>Genexpression</b>
<i>Transkriptionsfaktor Targetgen</i>
<i>Genregulation</i>

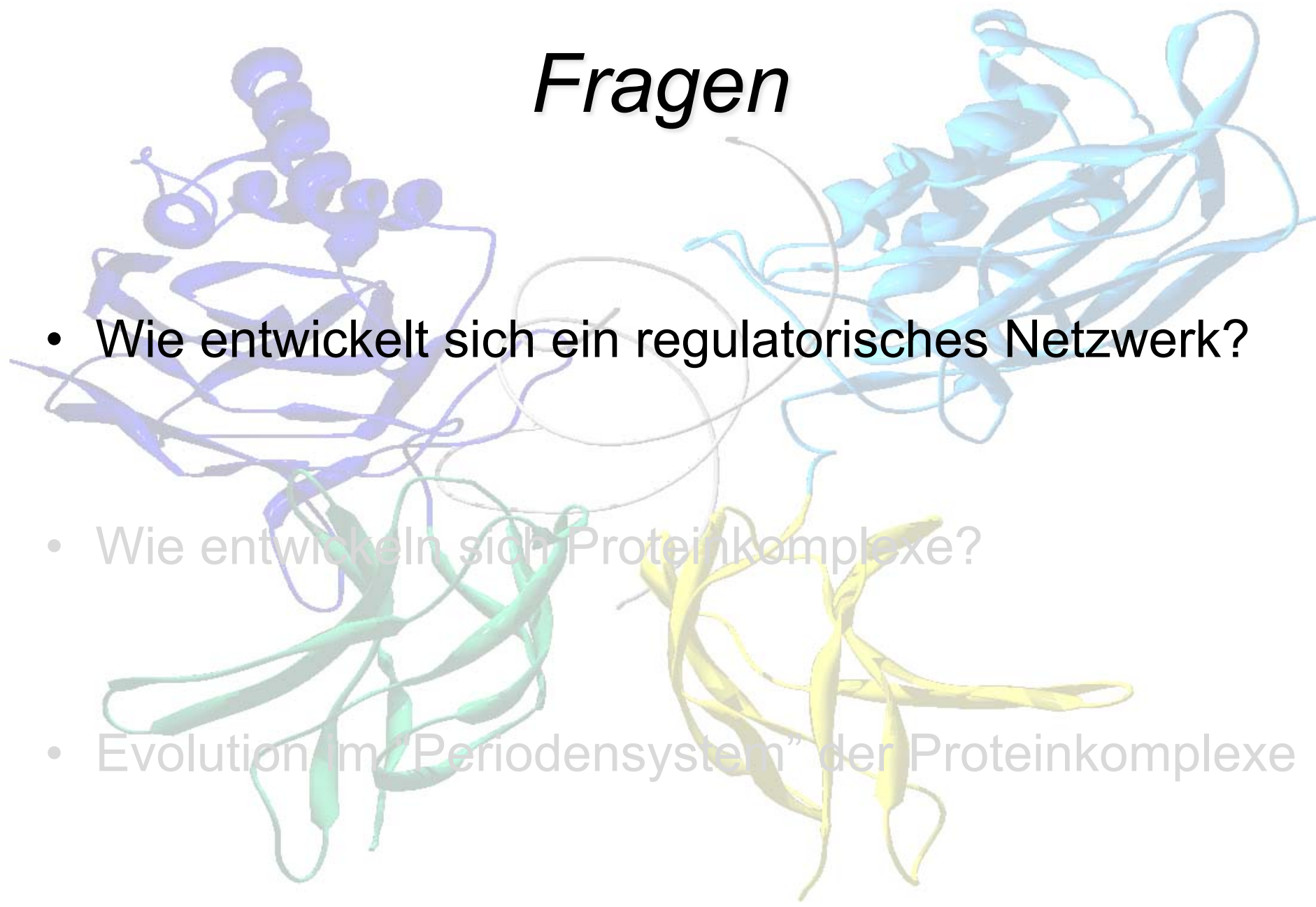


# *Fragen*

- Wie entwickelt sich ein regulatorisches Netzwerk?
- Wie entwickeln sich Proteinkomplexe?
- Evolution im “Periodensystem” der Proteinkomplexe

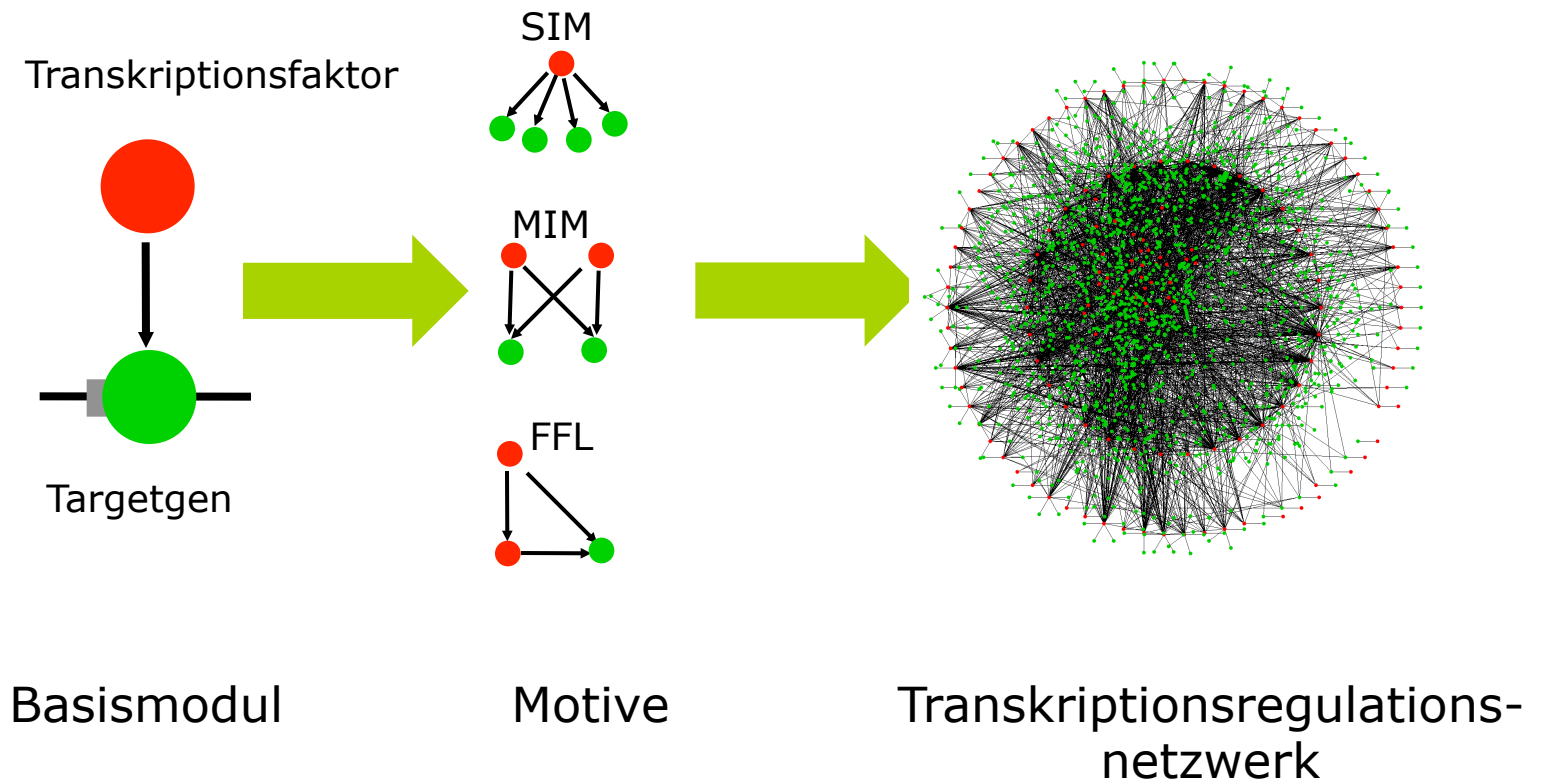
# *Fragen*

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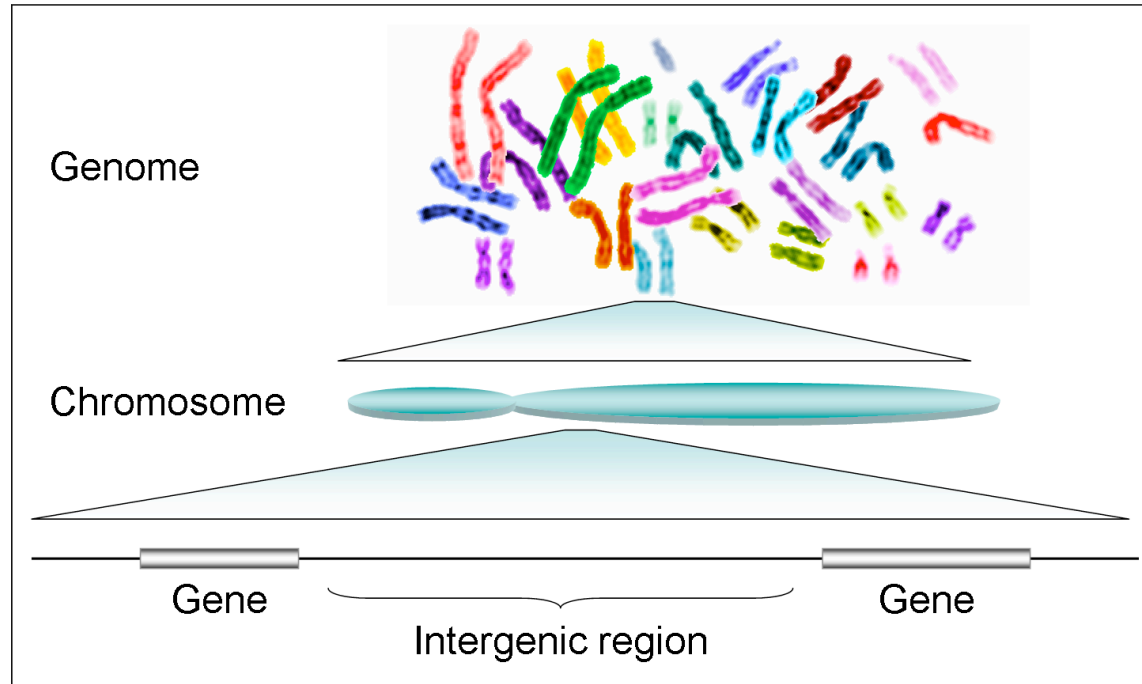




# Organisation des Netzwerks der Genregulation

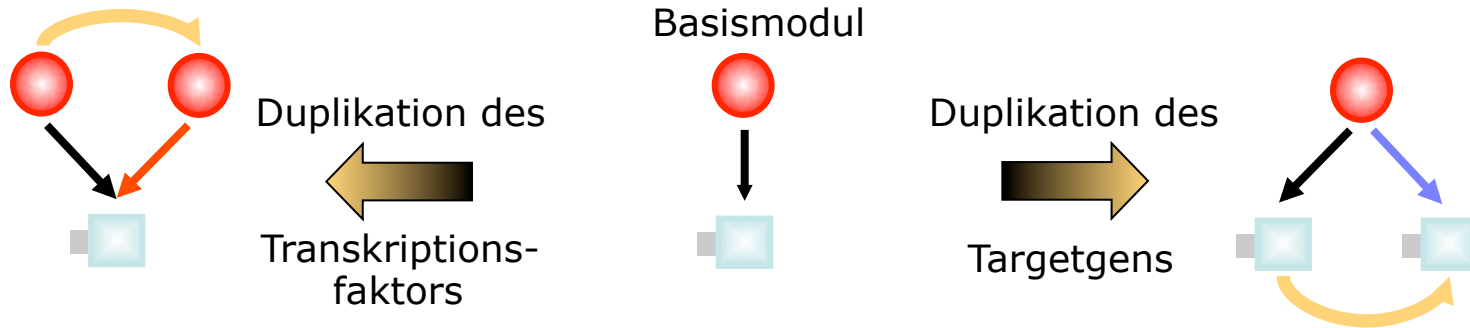


# Evolutionsvorgaenge in der DNA



1. Mutation: Divergenz oder Konservierung der Sequenz
- 2. Duplikation: Kopieren der Gene**
3. Genfusion: Zusammenfuegen von 2 Genen

# Duplikation des Basismoduls und Vererbung der Interaktion

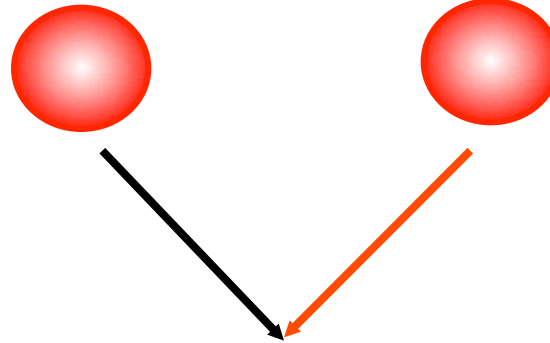




# Beispiel: Transkriptionsfaktorduplikation im Hefegenom

**PDR1**

**PDR3**



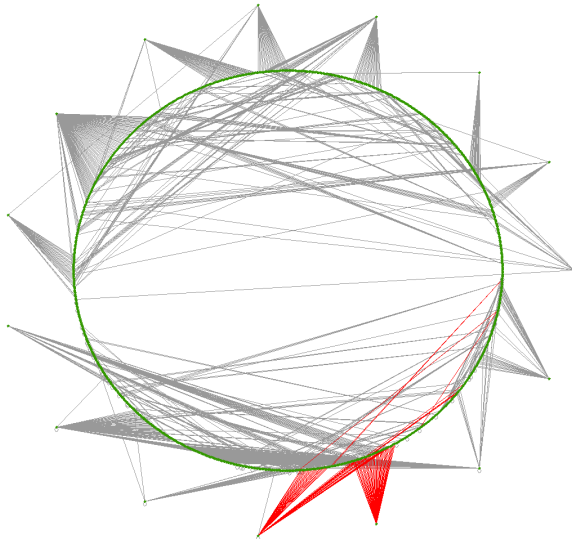
**FLR1**

# Wie häufig treten Transkriptionsfaktorduplikationen auf?

*E. coli*

128 Interaktionen aus 1233 insgesamt

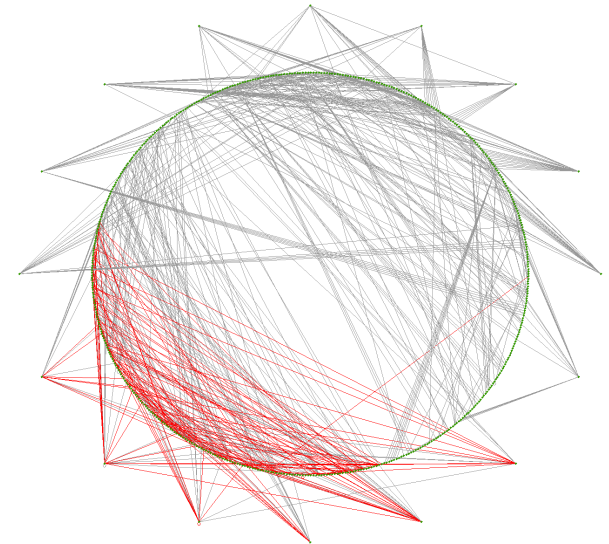
~ 10%



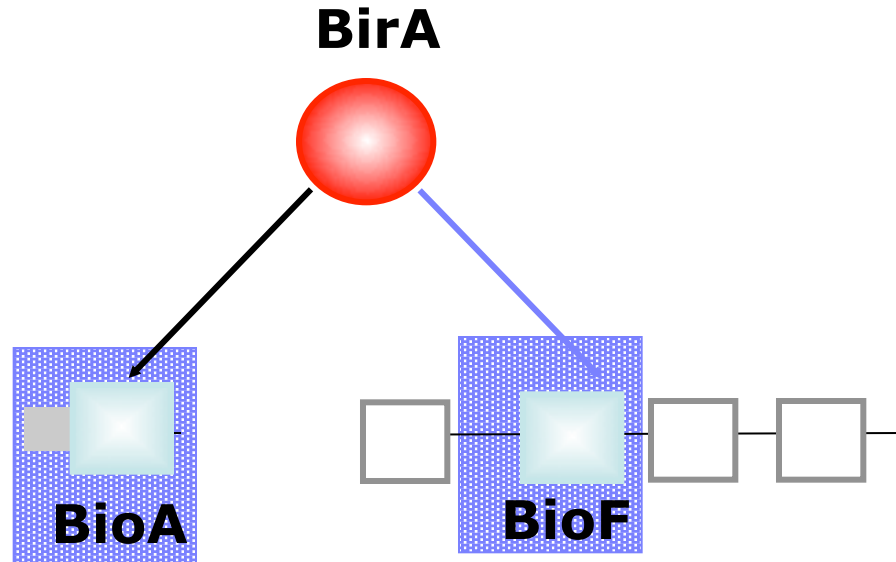
Hefe

188 Interaktionen aus 851 insgesamt

~ 22%



# Beispiel: Targetgenduplikation in *E. coli*



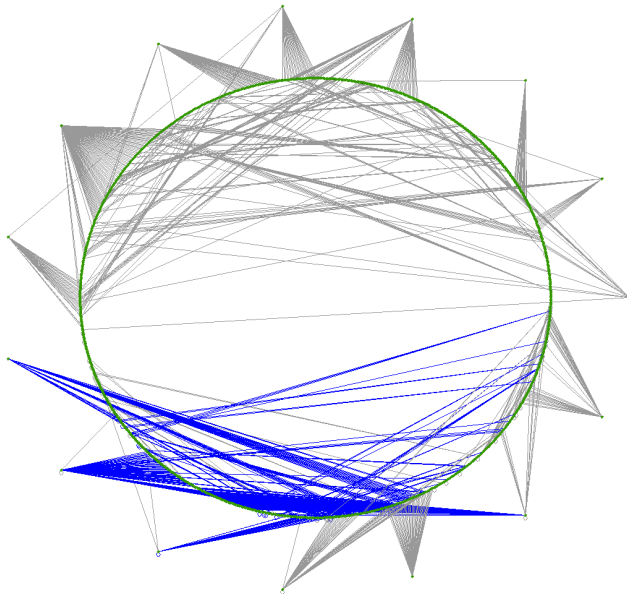
Duplication of target gene

# Wie häufig treten Targetenduplikationen auf?

***E. coli***

272 Interaktionen aus 1233 insges.

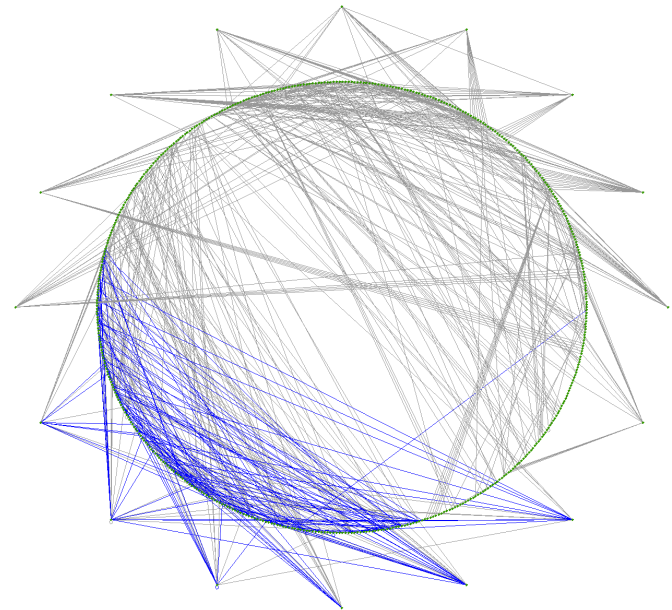
**~ 22%**



**Hefe**

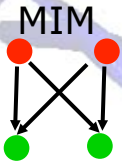
166 Interaktionen aus 851 insges.

**~ 20%**



# Fragen

- Wie entwickelt sich ein regulatorisches Netzwerk?



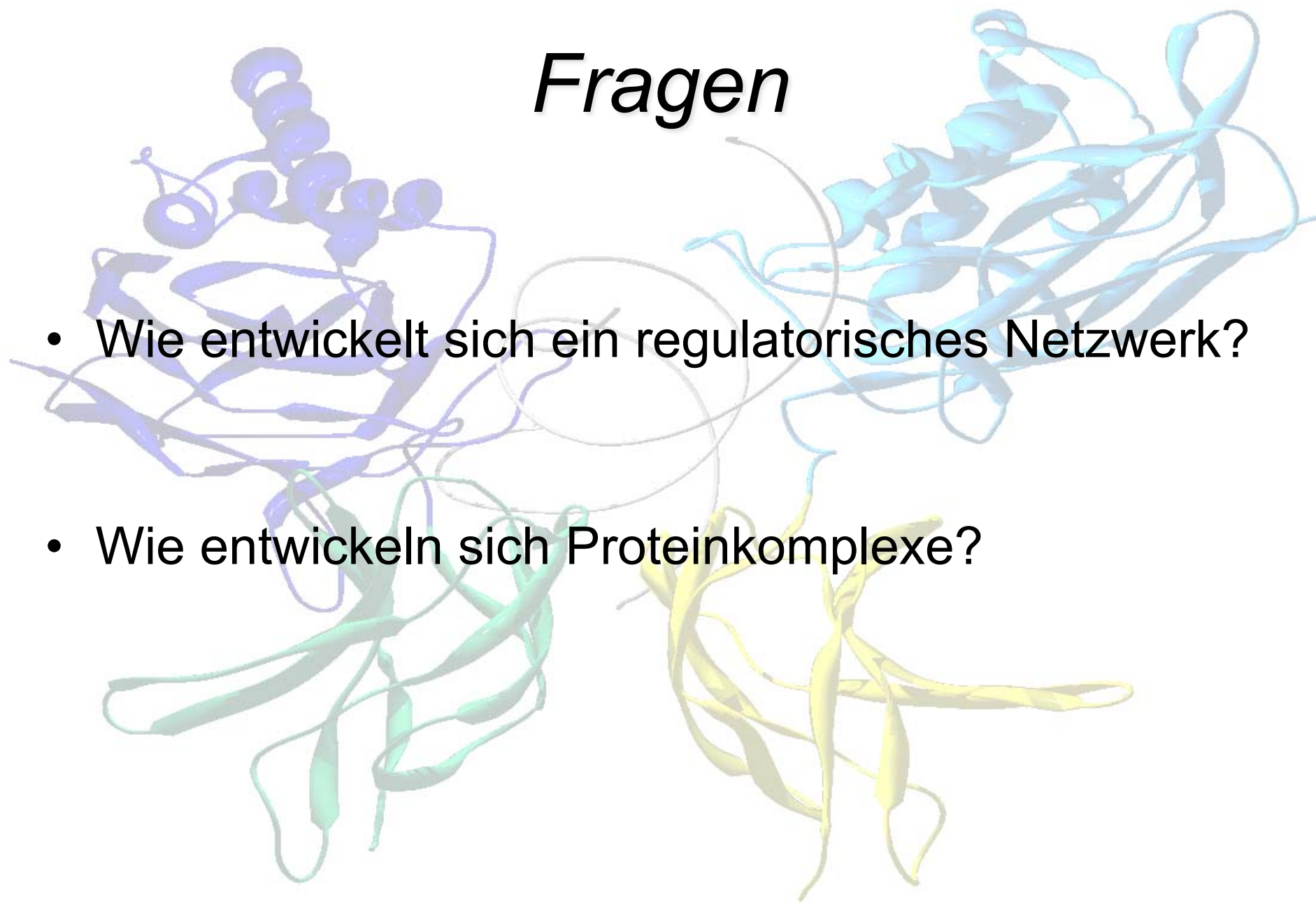
## Genduplikation als Motor der Evolution

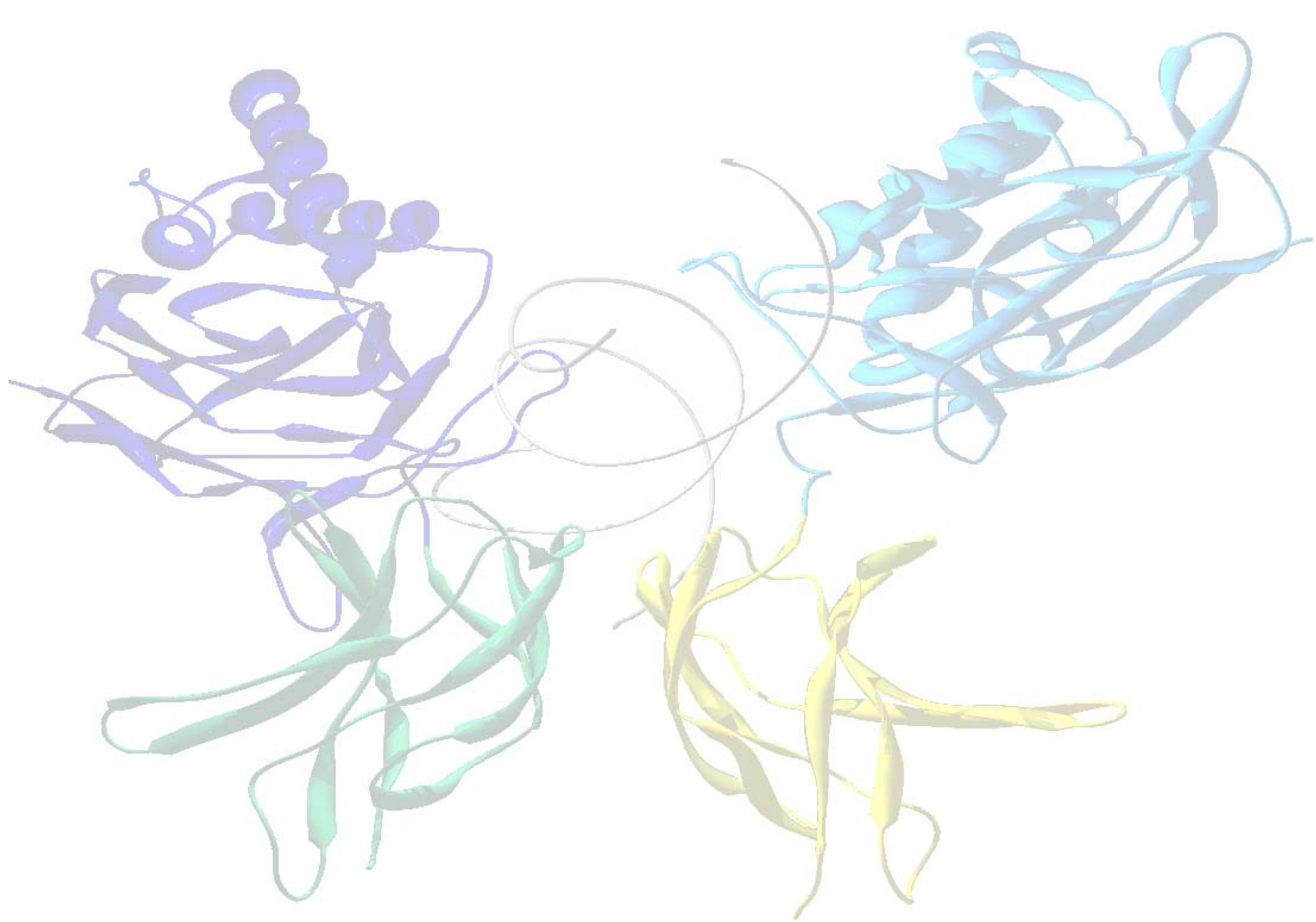
- Wie entwickeln sich Proteinkomplexe?
- Evolution im "Periodensystem" der Proteinkomplexe



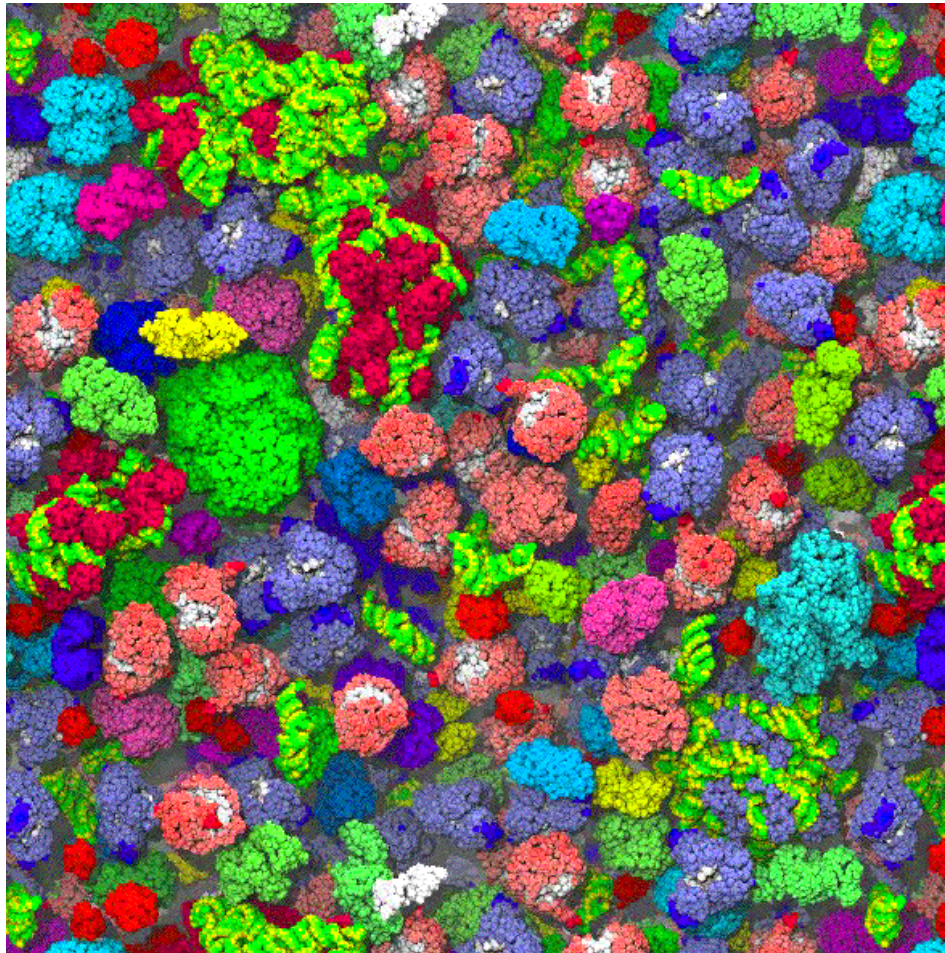
# *Fragen*

- Wie entwickelt sich ein regulatorisches Netzwerk?
- Wie entwickeln sich Proteinkomplexe?



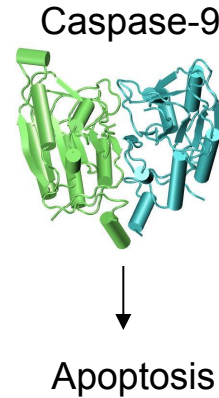


# Das Innenleben einer Zelle

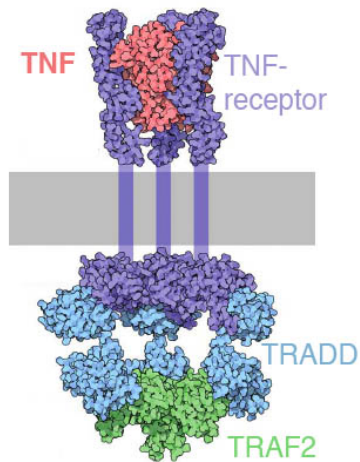


# Two types of protein complexes

- Homomers



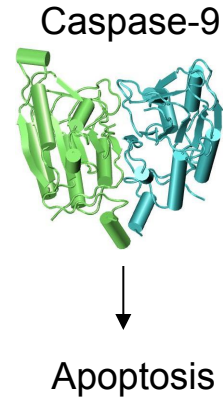
- Heteromers

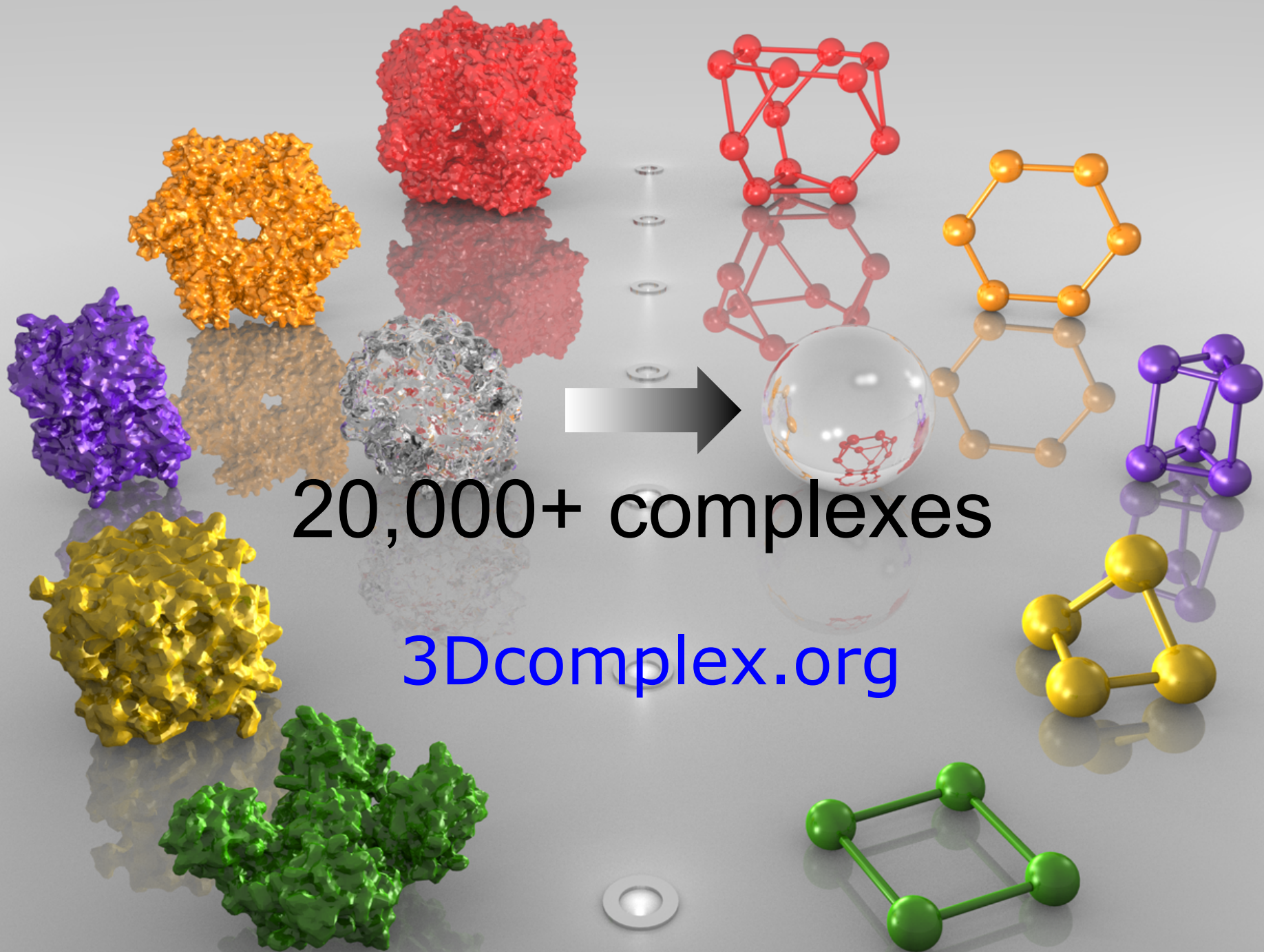




# Two types of protein complexes

- Homomers





20,000+ complexes

[3Dcomplex.org](http://3Dcomplex.org)

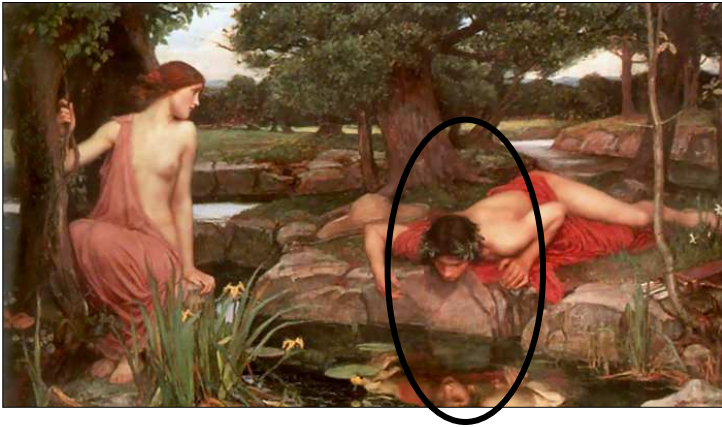
# Molecular Narcissism: 2/3 of proteins form homomers





# Symmetrie

## Reflektion



## Rotation

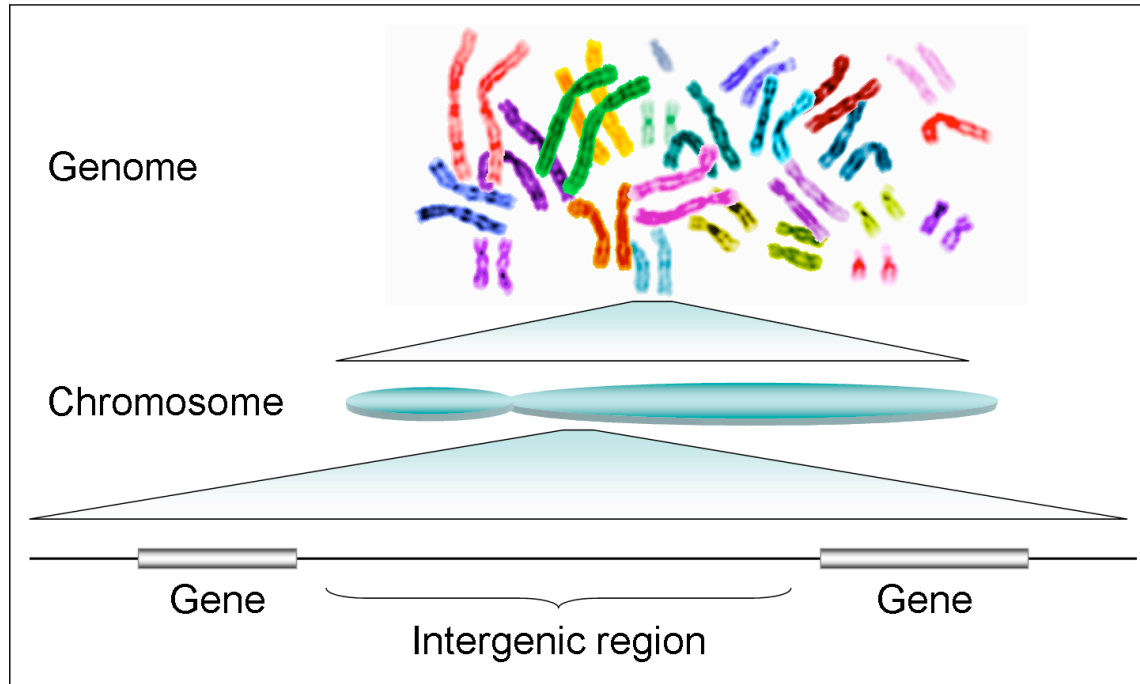




# Evolution der Symmetrie



# Evolutionsvorgaenge in der DNA



**1. Mutation: Divergenz oder Konservierung der Sequenz**

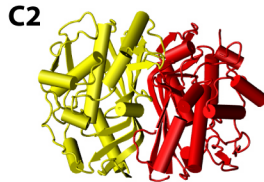
2. Duplikation: Kopieren der Gene

3. Genfusion: Zusammenfuegen von 2 Genen

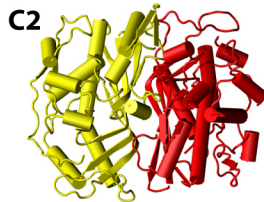
# Konserviertheit oder Divergenz der Strukturen?

## Thymidylate Synthase

*E. coli*



*B. subtilis*



C2 *H. sapiens*

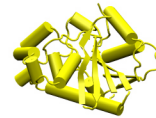


High

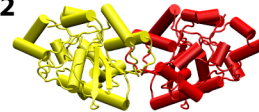
# Konserviertheit oder Divergenz der Strukturen?

## Phosphoglycerate Mutase

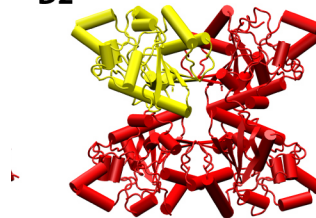
*B. stearrowthermophilus*  
C1



*H. sapiens*  
C2



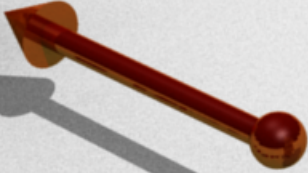
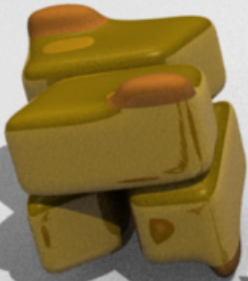
*S. cerevisiae*  
D2



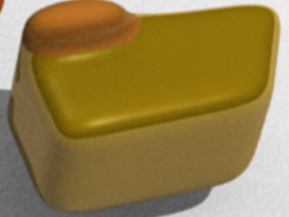
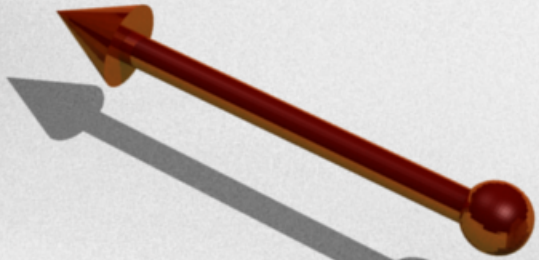
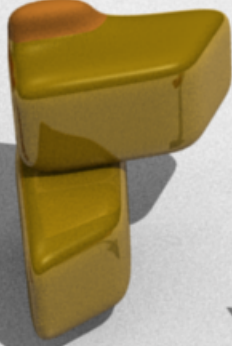


# Evolutionary path: Monomer-Dimer-Tetramer

**D2**

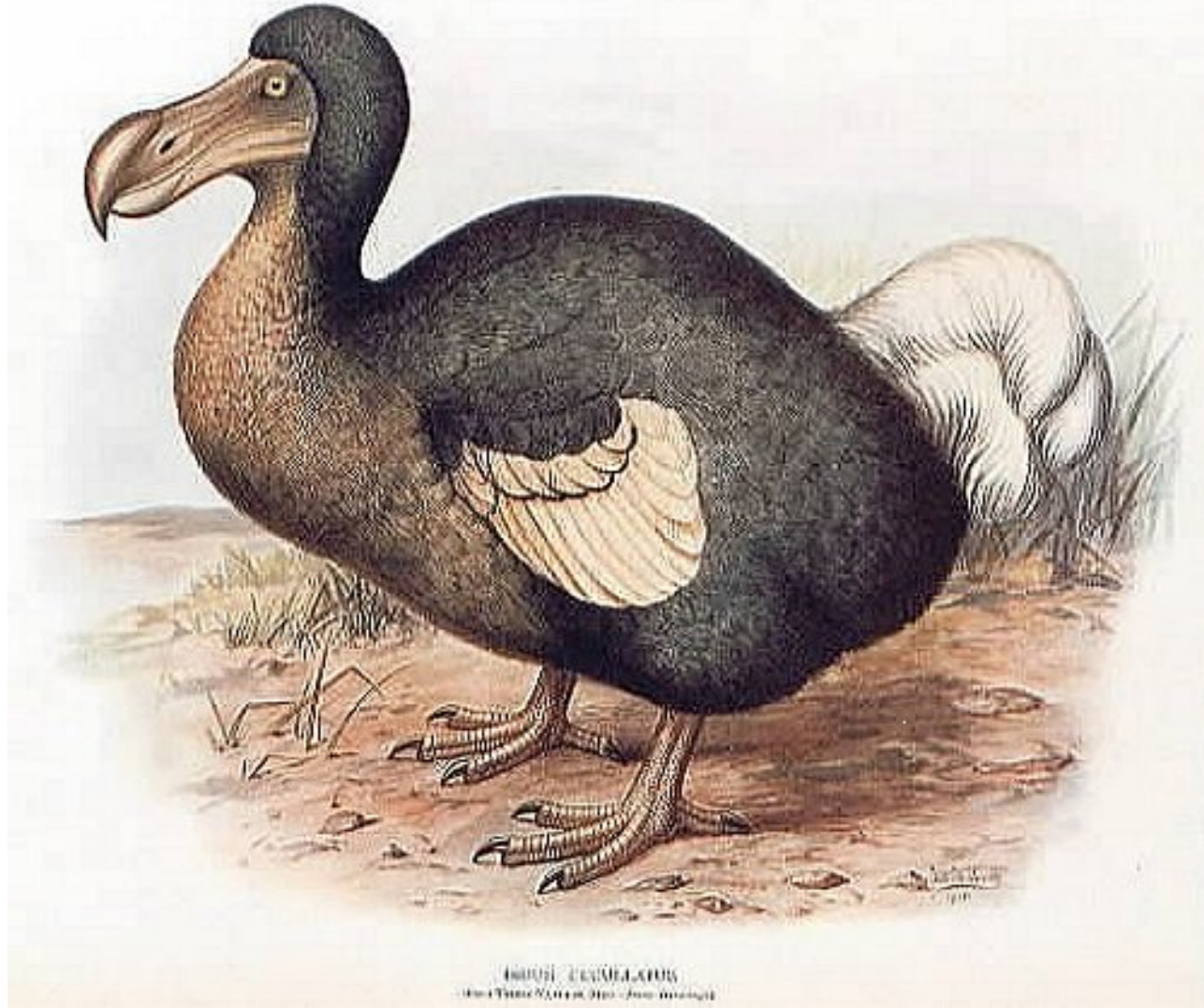


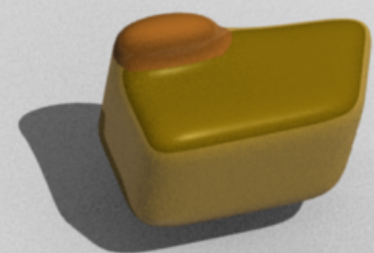
**C2**



*Dimerization*

Warum diese Wege? Unnuetzes Evolutionsrelikt?

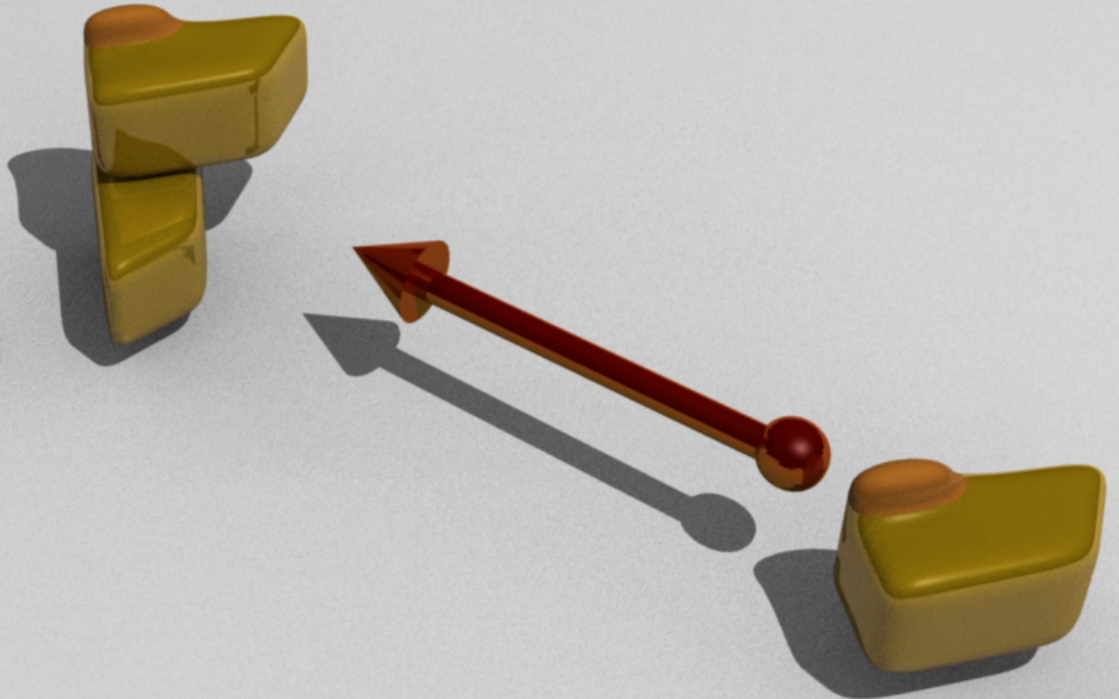




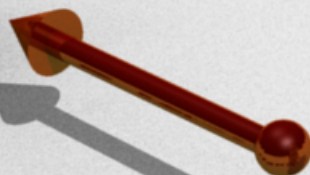
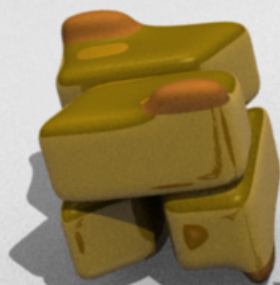


**C2**

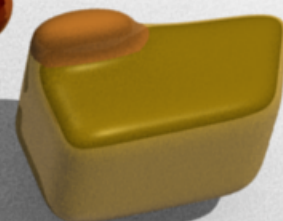
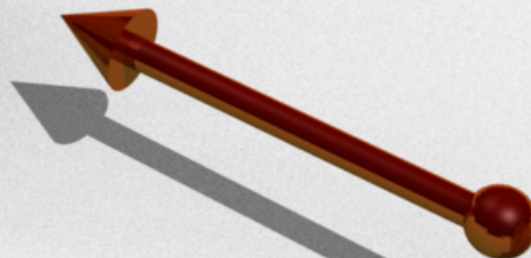
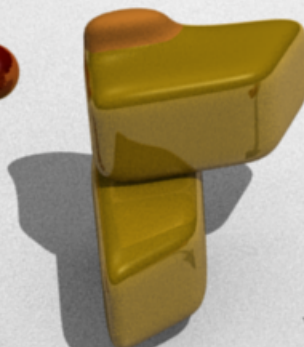
● *Dimerization*



**D2**



**C2**



**Dimerization**



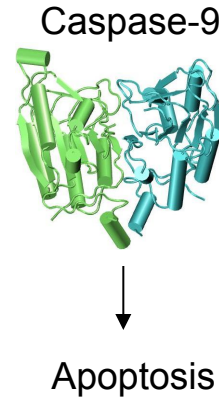
# Proteinkomplexe:

Assemblierungsweg  
spiegelt die Evolution wider

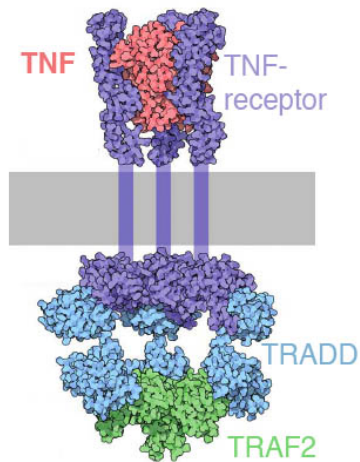


# Two types of protein complexes

- Homomers

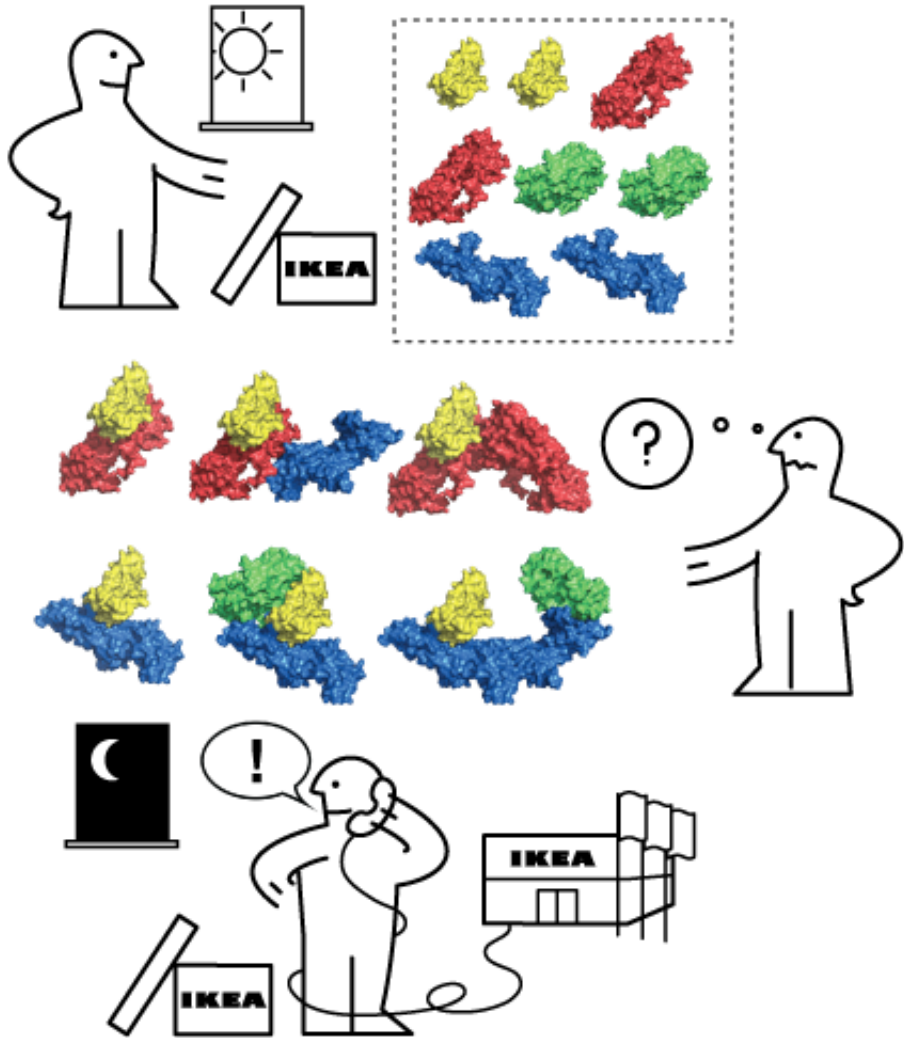


- Heteromers



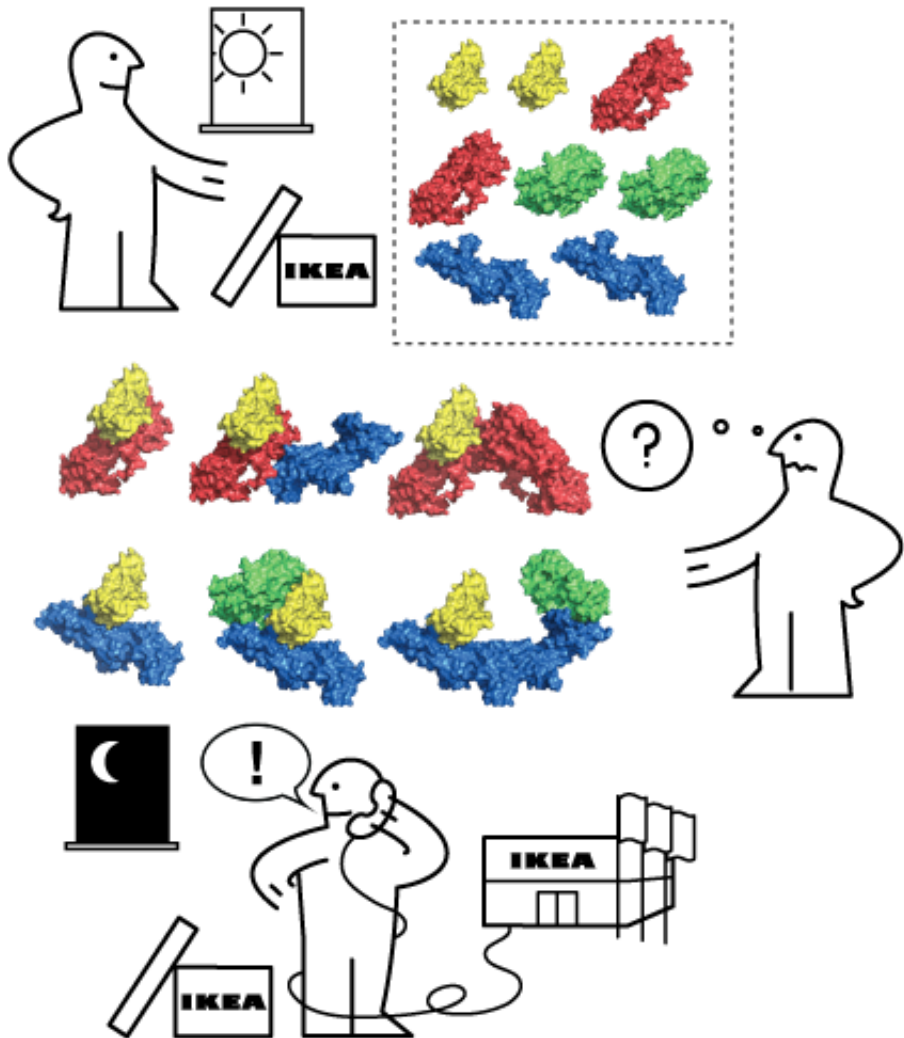
# The order of assembly is important

Random assembly

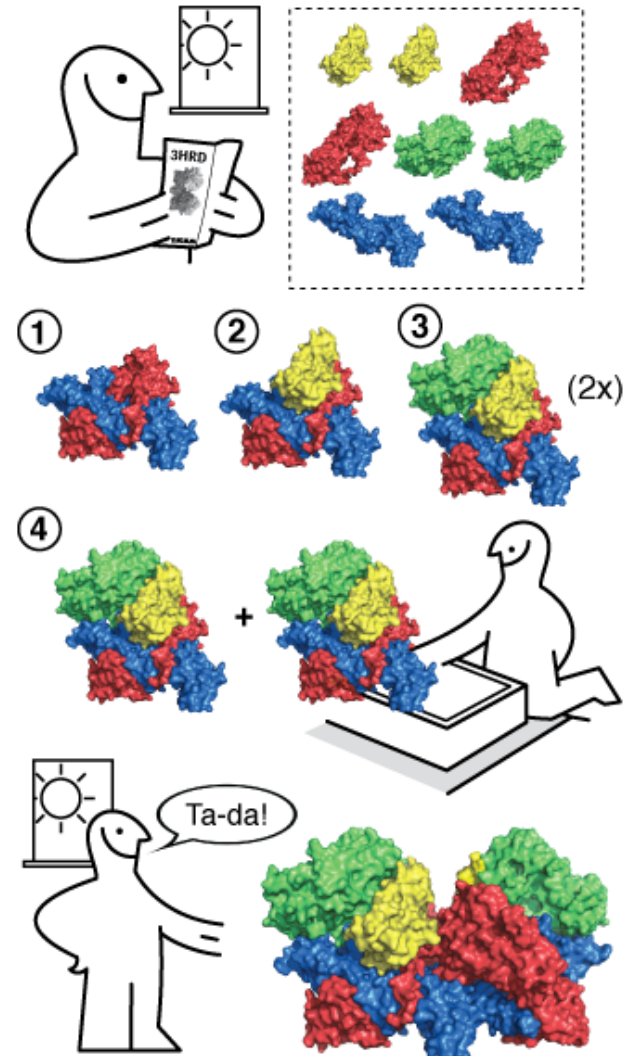


# The order of assembly is important

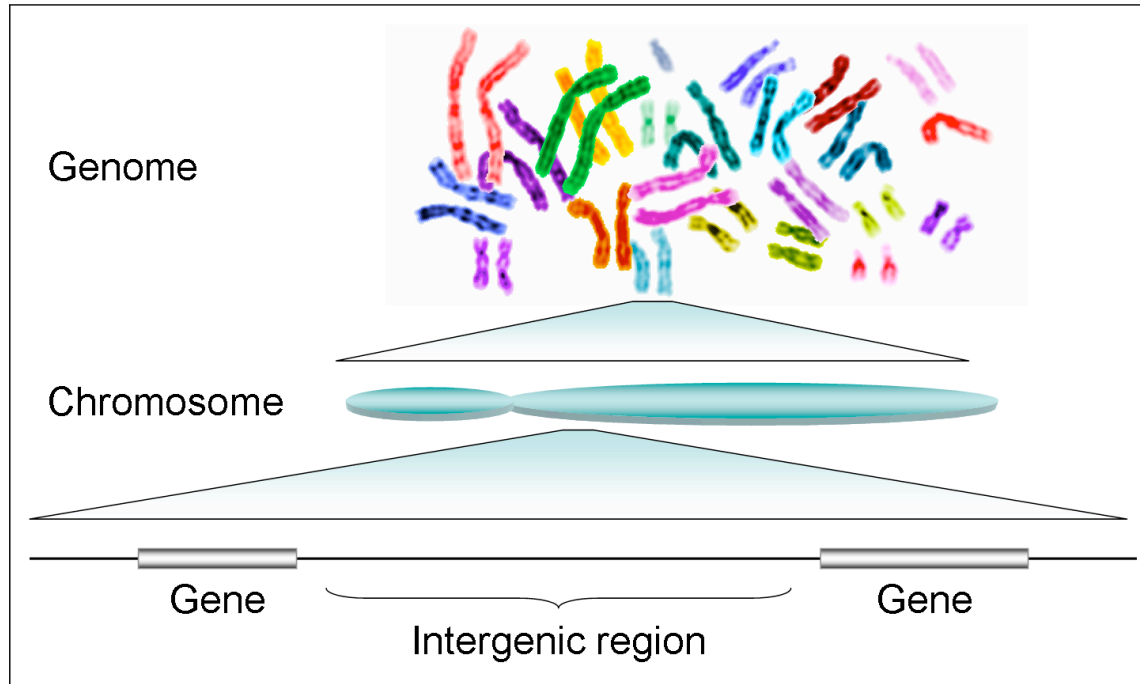
Random assembly



Ordered assembly



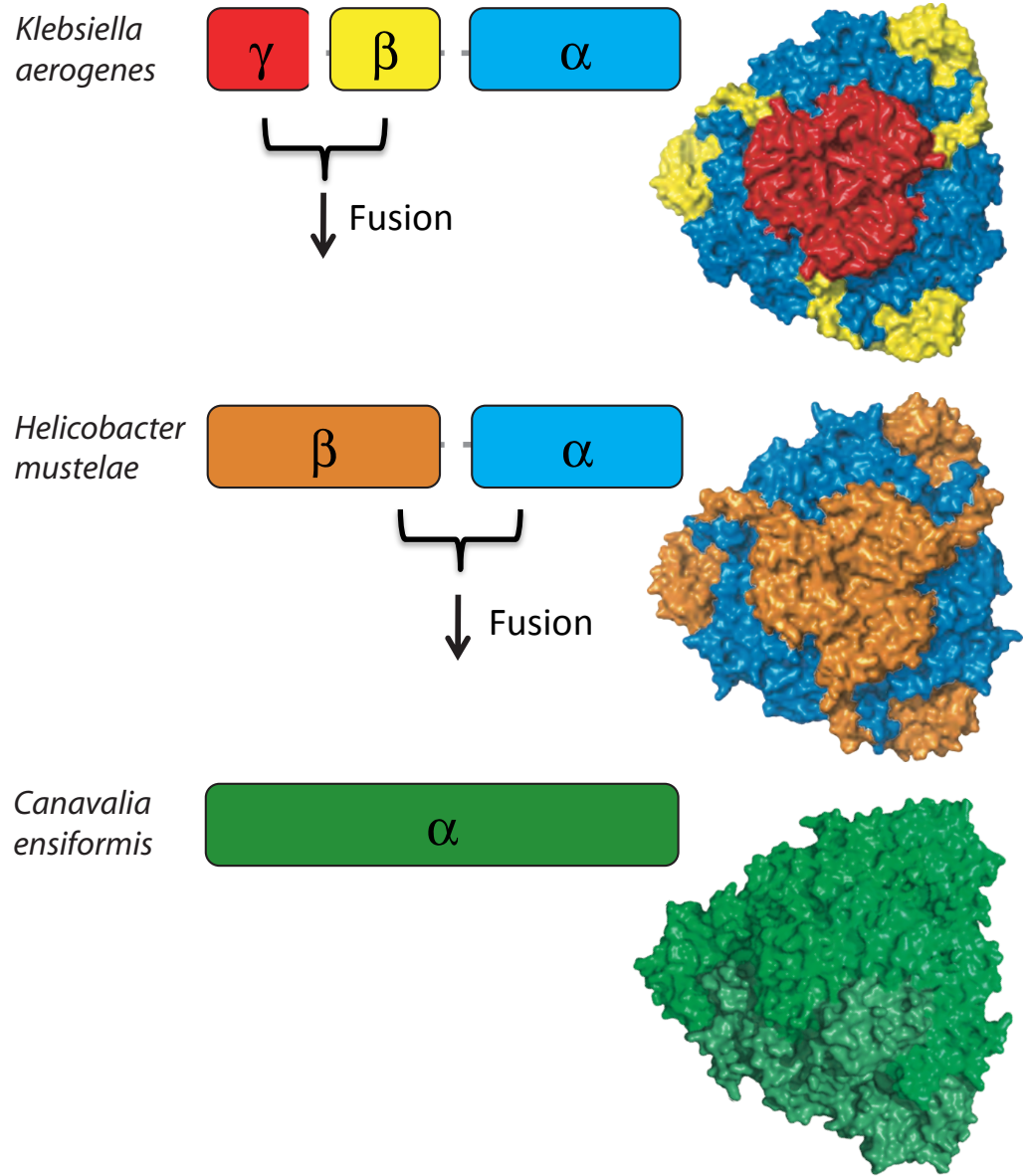
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1. Mutation: Divergenz oder Konservierung der Sequenz
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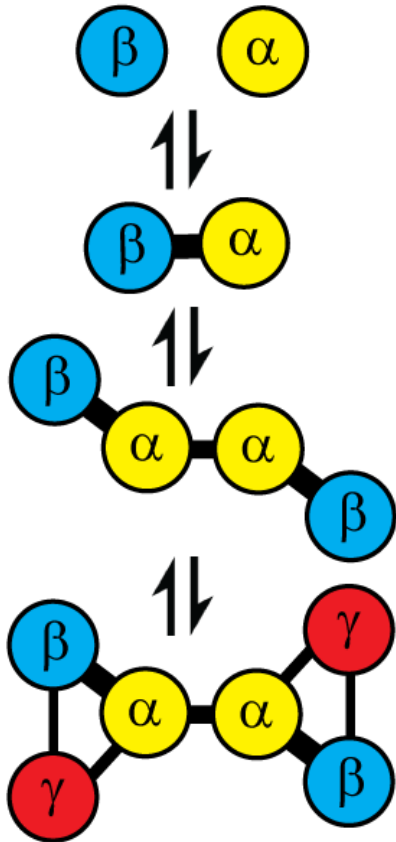


# Probing assembly conservation: Gene fusion and fission

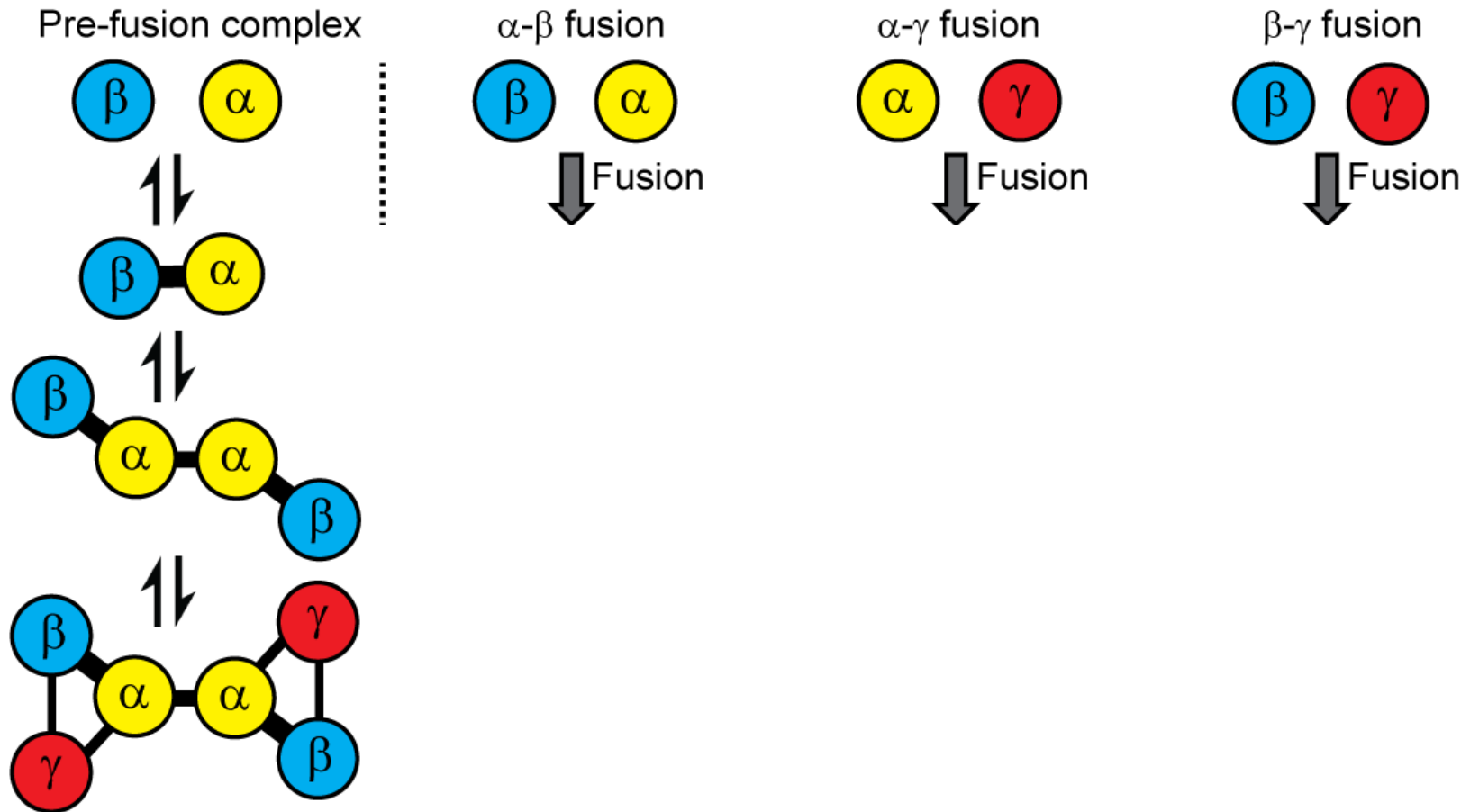


# Probing assembly conservation with gene fusion events

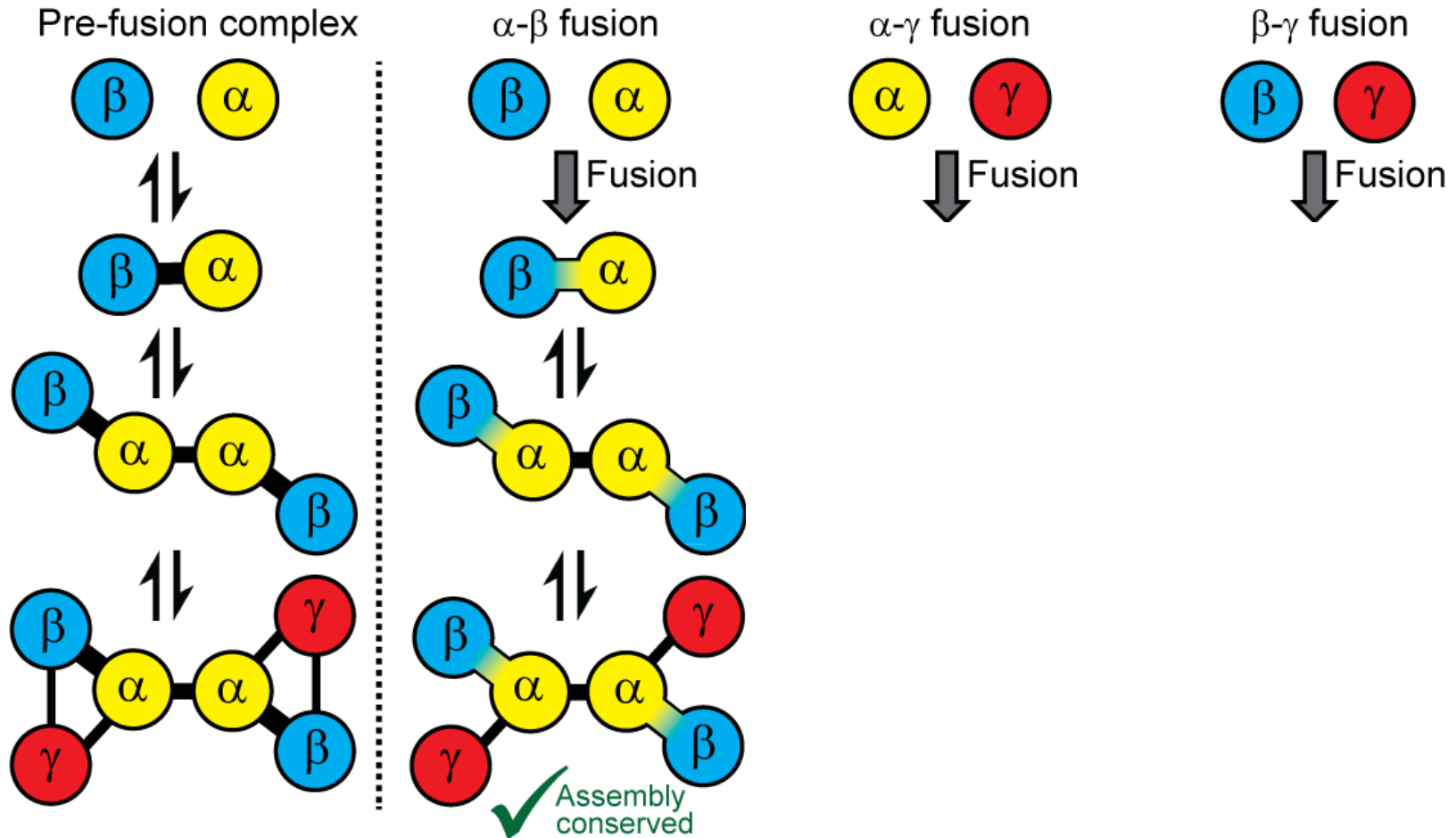
Pre-fusion complex



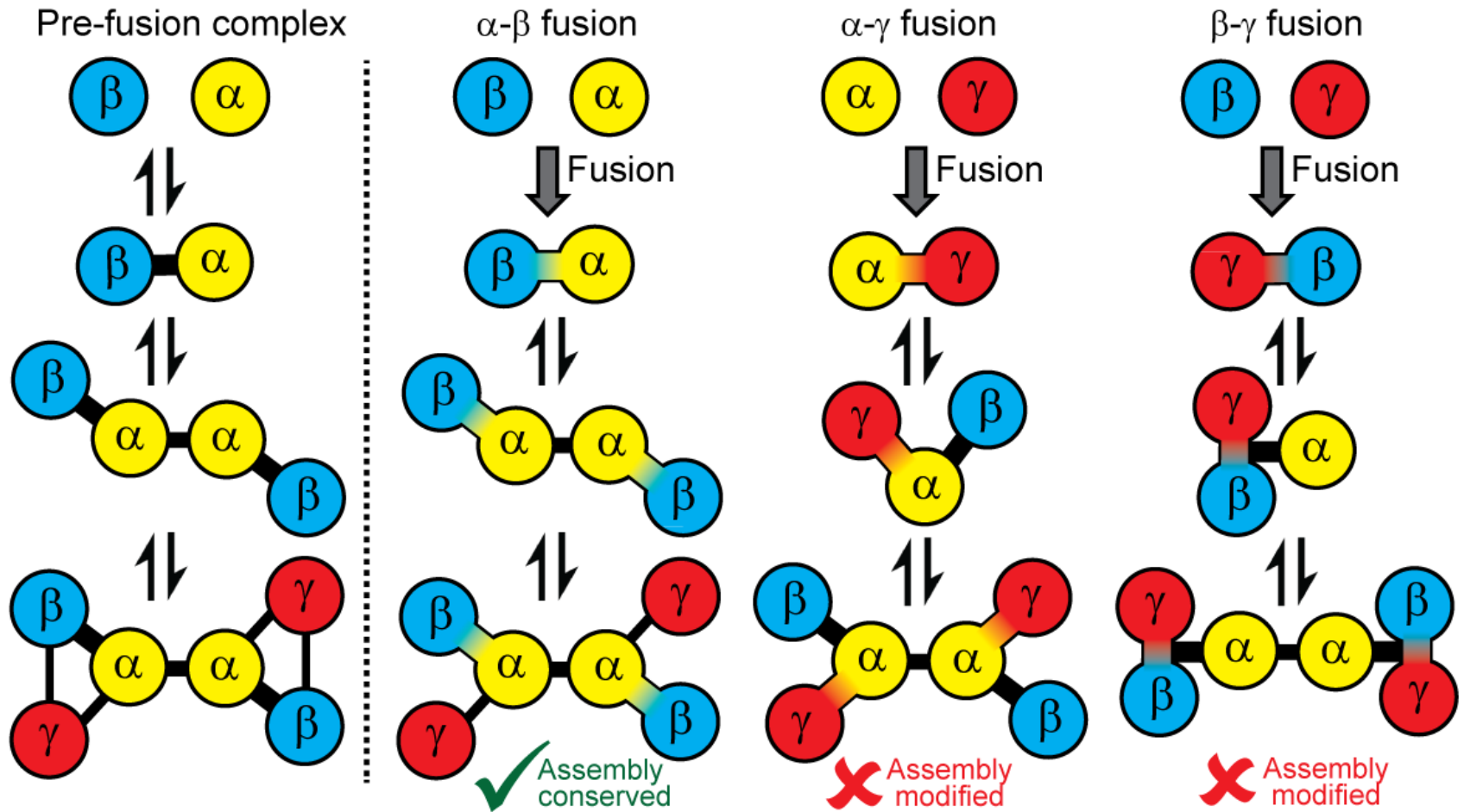
# Probing assembly conservation with gene fusion events



# Probing assembly conservation with gene fusion events



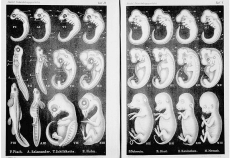
# Probing assembly conservation with gene fusion events





# *Fragen*

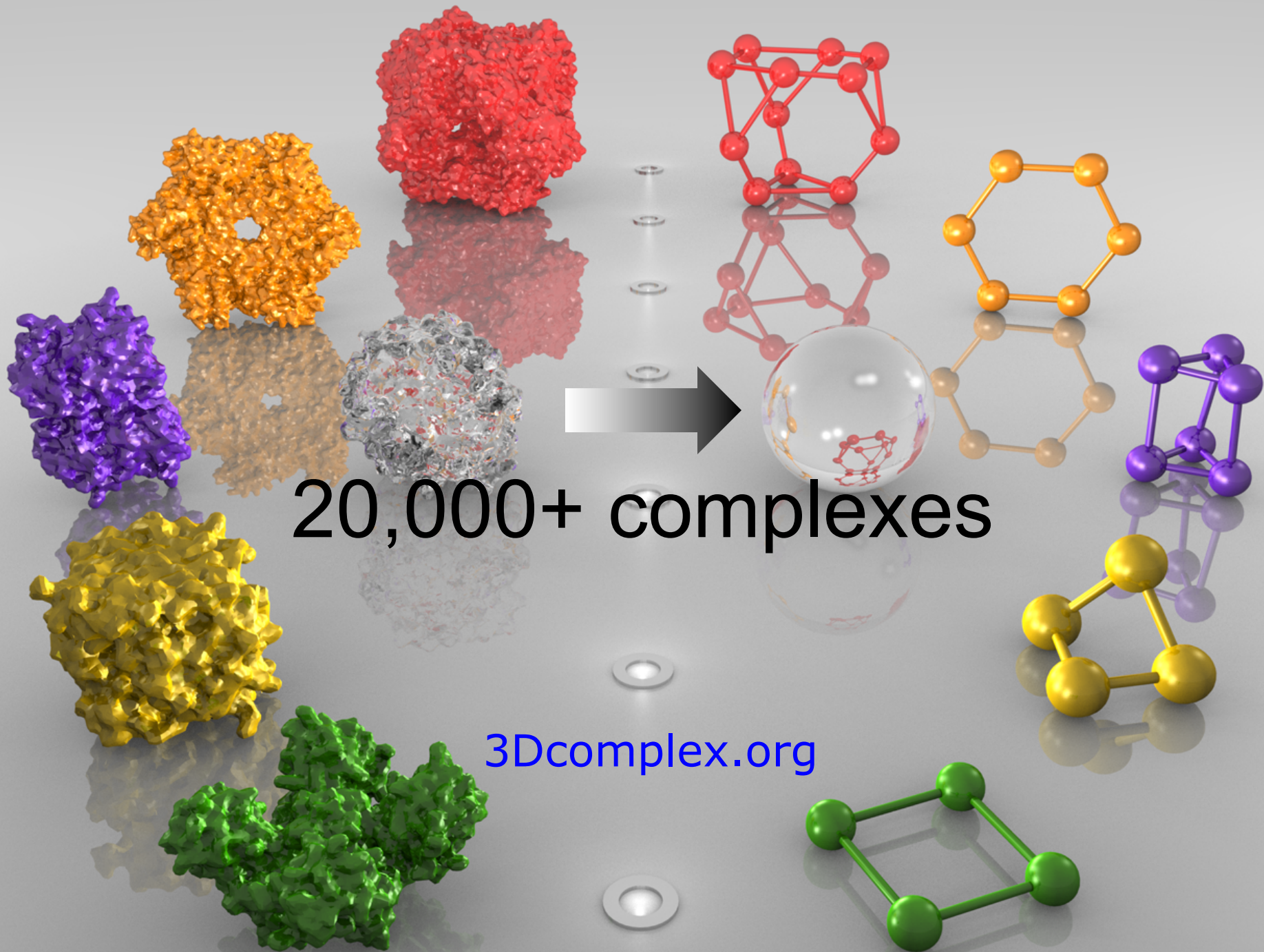
- Wie entwickelt sich ein regulatorisches Netzwerk?
- Wie entwickeln sich Proteinkomplexe?



**Evolution widerspiegelt Assemblierungsweg**

# *Fragen*

- Wie entwickelt sich ein regulatorisches Netzwerk?
- Wie entwickeln sich Proteinkomplexe?
- Evolution im “Periodensystem” der Proteinkomplexe



20,000+ complexes

[3Dcomplex.org](http://3Dcomplex.org)



# Klassifizierung der Proteinkomplexe

## 20,000+ Komplexe



hydrogen 1 H 1.008																helium 2 He 4.0026																			
lithium 3 Li 6.941		beryllium 4 Be 9.0122												boron 5 B 10.81		carbon 6 C 12.011		nitrogen 7 N 14.007		oxygen 8 O 15.999		fluorine 9 F 18.998		neon 10 Ne 20.180											
sodium 11 Na 22.990		magnesium 12 Mg 24.305												aluminum 13 Al 26.982		silicon 14 Si 28.086		phosphorus 15 P 30.974		sulfur 16 S 32.065		chlorine 17 Cl 35.453		argon 18 Ar 39.948											
potassium 19 K 39.098		calcium 20 Ca 40.078		scandium 21 Sc 44.956		titanium 22 Ti 47.867		vanadium 23 V 50.942		chromium 24 Cr 51.996		manganese 25 Mn 54.938		iron 26 Fe 55.845		cobalt 27 Co 58.933		nickel 28 Ni 58.693		copper 29 Cu 63.546		zinc 30 Zn 65.39		gallium 31 Ga 69.723		germanium 32 Ge 72.61		arsenic 33 As 74.922		selenium 34 Se 78.96		bromine 35 Br 79.904		krypton 36 Kr 83.80	
rubidium 37 Rb 85.468		strontium 38 Sr 87.62		yttrium 39 Y 88.906		zirconium 40 Zr 91.224		niobium 41 Nb 92.906		molybdenum 42 Mo 95.94		technetium 43 Tc [98]		ruthenium 44 Ru 101.07		rhodium 45 Rh 101.07		palladium 46 Pd 106.42		silver 47 Ag 107.87		cadmium 48 Cd 112.41		indium 49 In 114.82		tin 50 Sn 118.71		antimony 51 Sb 121.76		tellurium 52 Te 127.60		iodine 53 I 126.905		xenon 54 Xe 131.29	
cesium 55 Cs 132.91		barium 56 Ba 137.33		lanthanum 57 La 138.905		cerium 58 Ce 140.12		praseodymium 59 Pr 140.908		neodymium 60 Nd 144.24		promethium 61 Pm [145]		samarium 62 Sm 150.36		europium 63 Eu 151.96		gadolinium 64 Gd 157.25		terbium 65 Tb 158.93		dysprosium 66 Dy 162.50		holmium 67 Ho 164.93		erbium 68 Er 167.26		thulium 69 Tm 168.93		ytterbium 70 Yb 173.04					
francium 87 Fr [223]		radium 88 Ra [226]		actinium 89-102 Ac-Lr [227]		rutherfordium 103 Rf [261]		bohrium 104 Bh [264]		hassium 105 Hs [277]		meitnerium 106 Mt [268]		darmstadtium 107 Ds [271]		roentgenium 108 Rg [272]		copernicium 109 Cn [285]		nihonium 110 Nh [286]		flerovium 111 Fl [289]		tennessine 112 Ts [289]		oganesson 114 Og [284]									

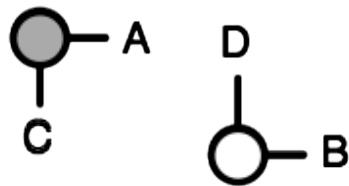
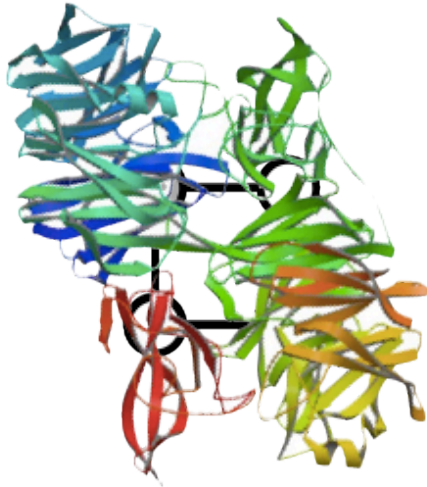
\* Lanthanide series

lanthanum 57 La 138.91	cerium 58 Ce 140.12	praseodymium 59 Pr 140.91	neodymium 60 Nd 144.24	promethium 61 Pm [145]	samarium 62 Sm 150.36	europium 63 Eu 151.96	gadolinium 64 Gd 157.25	terbium 65 Tb 158.93	dysprosium 66 Dy 162.50	holmium 67 Ho 164.93	erbium 68 Er 167.26	thulium 69 Tm 168.93	ytterbium 70 Yb 173.04
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\*\* Actinide series

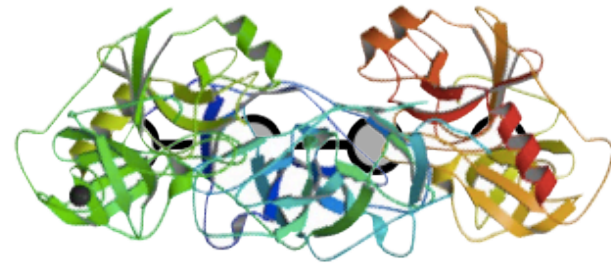
actinium 89 Ac [227]	thorium 90 Th 232.04	protactinium 91 Pa 231.04	uranium 92 U 238.03	neptunium 93 Np [237]	plutonium 94 Pu [244]	americium 95 Am [243]	curium 96 Cm [247]	berkelium 97 Bk [247]	californium 98 Cf [251]	esboium 99 Es [252]	fermium 100 Fm [257]	mendelevium 101 Md [258]	nobelium 102 No [259]
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# KODIERUNG DES ASSEMBLIERUNGSWEGS



A-B C-D

$$(2,2) \begin{pmatrix} 0 & 2 \\ 2 & 0 \end{pmatrix}$$

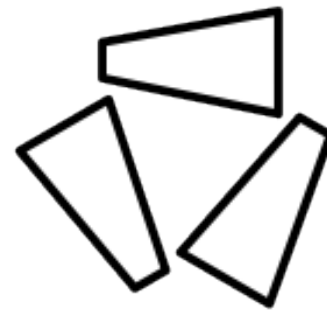
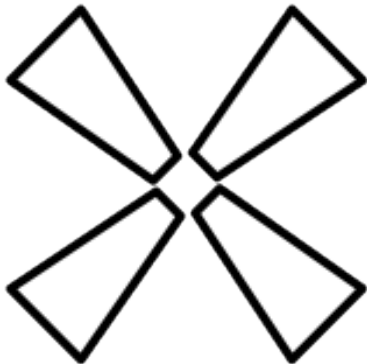
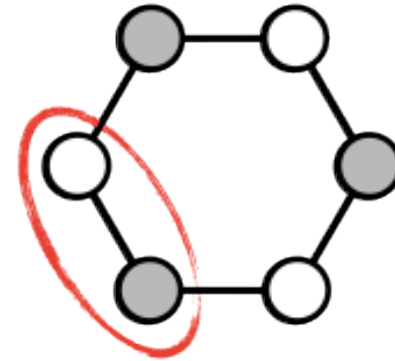
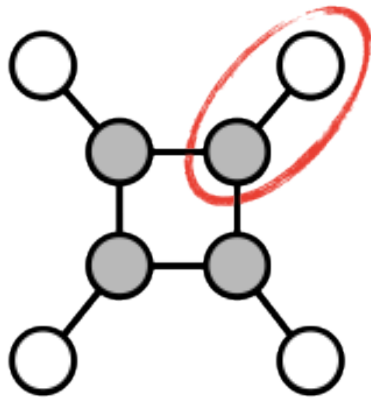


A-A B-C

$$(2,2) \begin{pmatrix} 1 & 1 \\ 1 & 0 \end{pmatrix}$$



# Equal numbers of self-assembly building blocks...



# “Periodensystem” der Proteinkomplexe

Wiederholung 

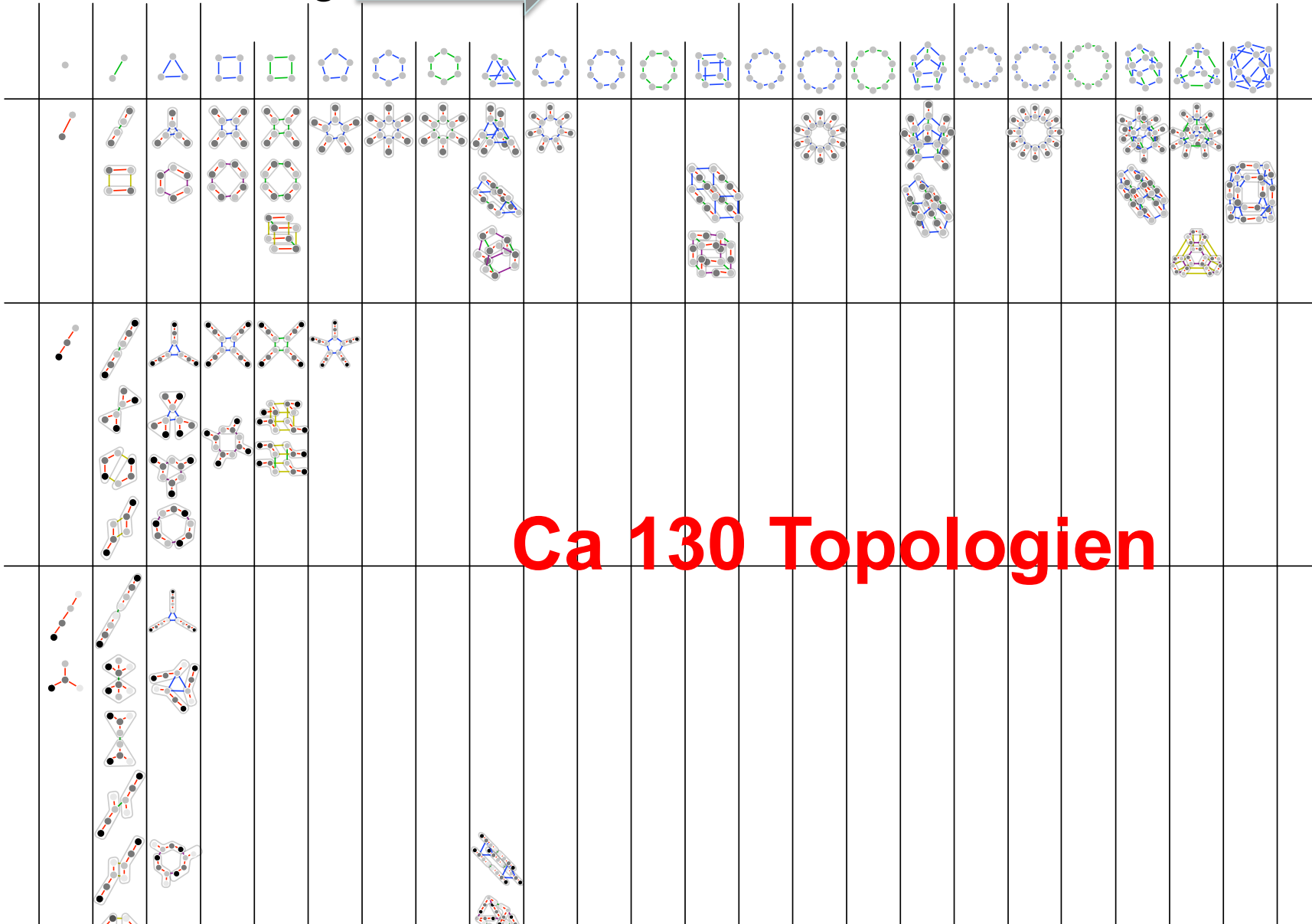
Proteinspezies 



# “Periodensystem” der Proteinkomplexe

Wiederholung 

Proteinspezies 



# Periodensystem der Elemente

hydrogen 1 <b>H</b> 1.0079																	helium 2 <b>He</b> 4.0026		
lithium 3 <b>Li</b> 6.941	beryllium 4 <b>Be</b> 9.0122											boron 5 <b>B</b> 10.811	carbon 6 <b>C</b> 12.011	nitrogen 7 <b>N</b> 14.007	oxygen 8 <b>O</b> 15.999	fluorine 9 <b>F</b> 18.998	neon 10 <b>Ne</b> 20.180		
sodium 11 <b>Na</b> 22.990	magnesium 12 <b>Mg</b> 24.305											aluminium 13 <b>Al</b> 26.982	silicon 14 <b>Si</b> 28.086	phosphorus 15 <b>P</b> 30.974	sulfur 16 <b>S</b> 32.065	chlorine 17 <b>Cl</b> 35.453	argon 18 <b>Ar</b> 39.948		
potassium 19 <b>K</b> 39.098	calcium 20 <b>Ca</b> 40.078	scandium 21 <b>Sc</b> 44.956	titanium 22 <b>Ti</b> 47.867	vanadium 23 <b>V</b> 50.942	chromium 24 <b>Cr</b> 51.996	manganese 25 <b>Mn</b> 54.938	iron 26 <b>Fe</b> 55.845	cobalt 27 <b>Co</b> 58.933	nickel 28 <b>Ni</b> 58.693	copper 29 <b>Cu</b> 63.546	zinc 30 <b>Zn</b> 65.39	gallium 31 <b>Ga</b> 69.723	germanium 32 <b>Ge</b> 72.61	arsenic 33 <b>As</b> 74.922	selenium 34 <b>Se</b> 78.96	bromine 35 <b>Br</b> 79.904	krypton 36 <b>Kr</b> 83.80		
rubidium 37 <b>Rb</b> 85.468	strontium 38 <b>Sr</b> 87.62	yttrium 39 <b>Y</b> 88.906	zirconium 40 <b>Zr</b> 91.224	niobium 41 <b>Nb</b> 92.906	molybdenum 42 <b>Mo</b> 95.94	technetium 43 <b>Tc</b> [98]	ruthenium 44 <b>Ru</b> 101.07	rhodium 45 <b>Rh</b> 102.91	palladium 46 <b>Pd</b> 106.42	silver 47 <b>Ag</b> 107.87	cadmium 48 <b>Cd</b> 112.41	indium 49 <b>In</b> 114.82	tin 50 <b>Sn</b> 118.71	antimony 51 <b>Sb</b> 121.76	tellurium 52 <b>Te</b> 127.60	iodine 53 <b>I</b> 126.90	xenon 54 <b>Xe</b> 131.29		
caesium 55 <b>Cs</b> 132.91	barium 56 <b>Ba</b> 137.33	57-70 *	lutetium 71 <b>Lu</b> 174.97	hafnium 72 <b>Hf</b> 178.49	tantalum 73 <b>Ta</b> 180.95	tungsten 74 <b>W</b> 183.84	rhenium 75 <b>Re</b> 186.21	osmium 76 <b>Os</b> 190.23	iridium 77 <b>Ir</b> 192.22	platinum 78 <b>Pt</b> 195.08	gold 79 <b>Au</b> 196.97	mercury 80 <b>Hg</b> 200.59	thallium 81 <b>Tl</b> 204.38	lead 82 <b>Pb</b> 207.2	bismuth 83 <b>Bi</b> 208.98	polonium 84 <b>Po</b> [209]	astatine 85 <b>At</b> [210]	radon 86 <b>Rn</b> [222]	
francium 87 <b>Fr</b> [223]	radium 88 <b>Ra</b> [226]	89-102 * *	lawrencium 103 <b>Lr</b> [262]	rutherfordium 104 <b>Rf</b> [261]	dubnium 105 <b>Db</b> [262]	seaborgium 106 <b>Sg</b> [266]	bohrium 107 <b>Bh</b> [264]	hassium 108 <b>Hs</b> [269]	meitnerium 109 <b>Mt</b> [268]	ununilium 110 <b>Uun</b> [271]	unununium 111 <b>Uuu</b> [272]	ununbium 112 <b>Uub</b> [277]		ununquadium 114 <b>Uuq</b> [289]					

\* Lanthanide series




































































lanthanum 57 <b>La</b> 138.91	cerium 58 <b>Ce</b> 140.12	praseodymium 59 <b>Pr</b> 140.91	neodymium 60 <b>Nd</b> 144.24	promethium 61 <b>Pm</b> [145]	samarium 62 <b>Sm</b> 150.36	europium 63 <b>Eu</b> 151.96	gadolinium 64 <b>Gd</b> 157.25	terbium 65 <b>Tb</b> 158.93	dysprosium 66 <b>Dy</b> 162.50	holmium 67 <b>Ho</b> 164.93	erbium 68 <b>Er</b> 167.26	thulium 69 <b>Tm</b> 168.93	ytterbium 70 <b>Yb</b> 173.04
actinium 89 <b>Ac</b> [227]	thorium 90 <b>Th</b> 232.04	protactinium 91 <b>Pa</b> 231.04	uranium 92 <b>U</b> 238.03	neptunium 93 <b>Np</b> [237]	plutonium 94 <b>Pu</b> [244]	americium 95 <b>Am</b> [243]	curium 96 <b>Cm</b> [247]	berkelium 97 <b>Bk</b> [247]	californium 98 <b>Cf</b> [251]	einsteinium 99 <b>Es</b> [252]	fermium 100 <b>Fm</b> [257]	mendelevium 101 <b>Md</b> [258]	nobelium 102 <b>No</b> [259]

\*\* Actinide series

# “Periodensystem” der Proteinkomplexe

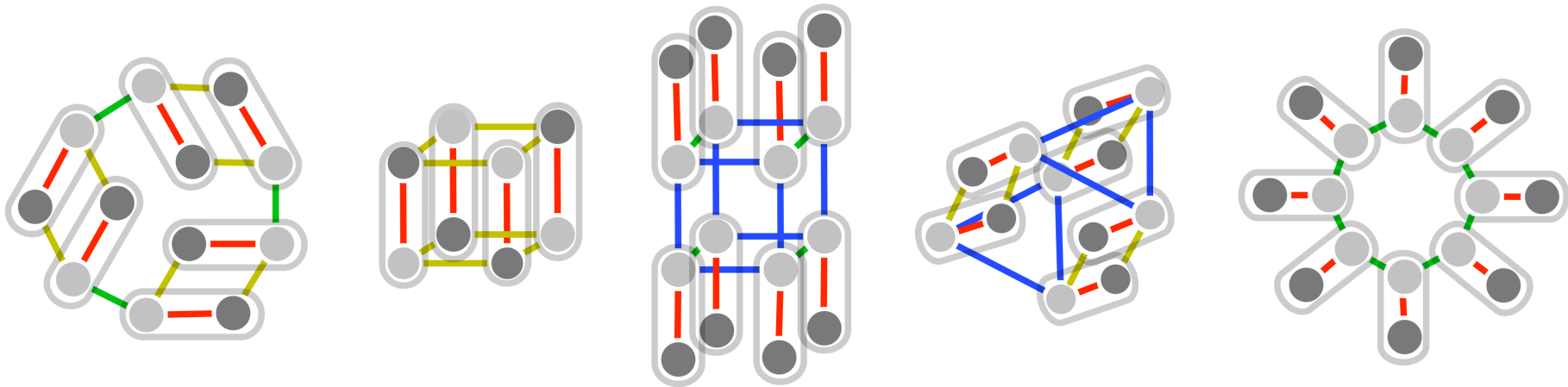
Wiederholung 

Proteinspezies 



# Top 5 noch nicht bekannte Topologien

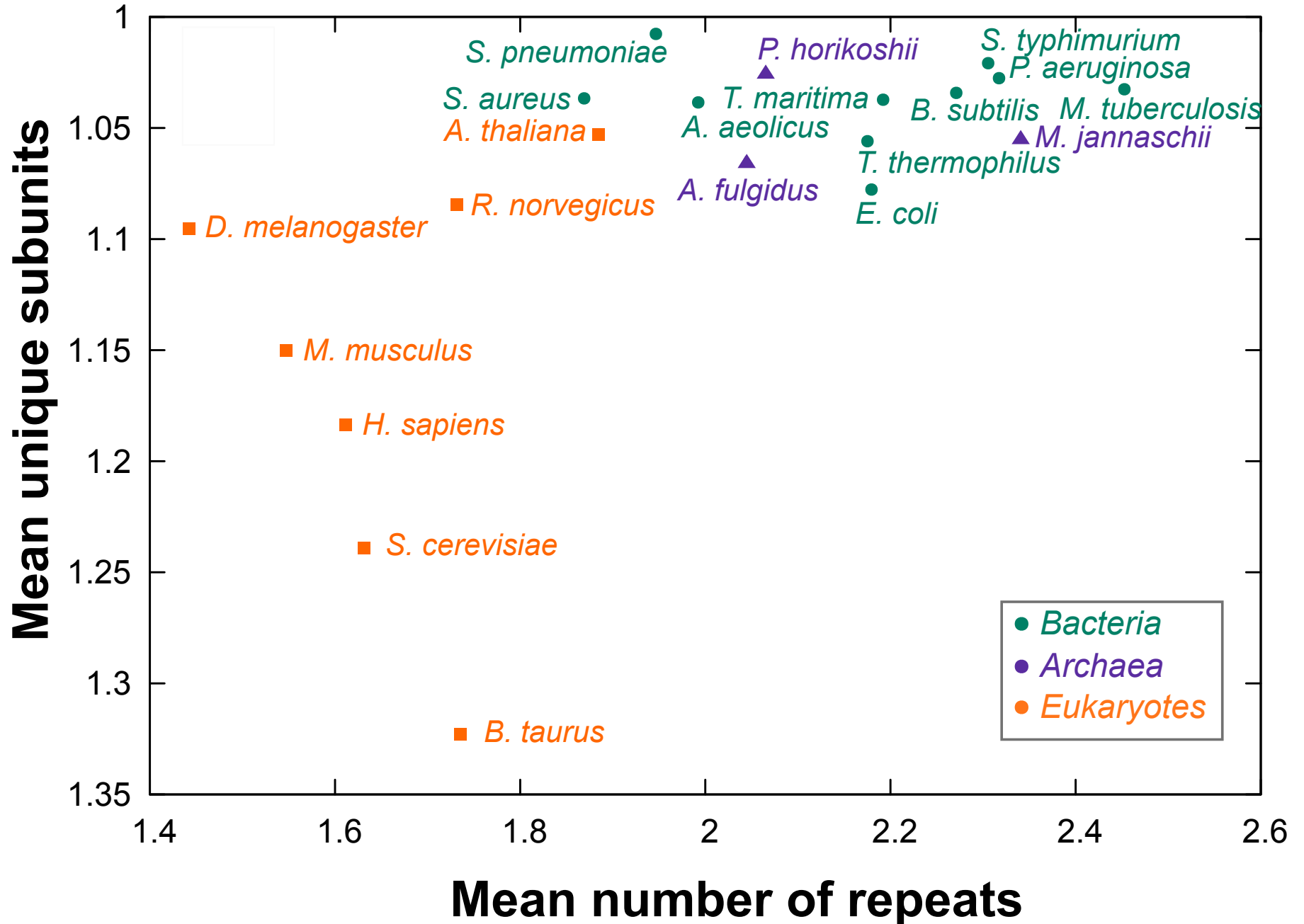


2 Proteinspezies, 8-16 Einheiten insgesamt





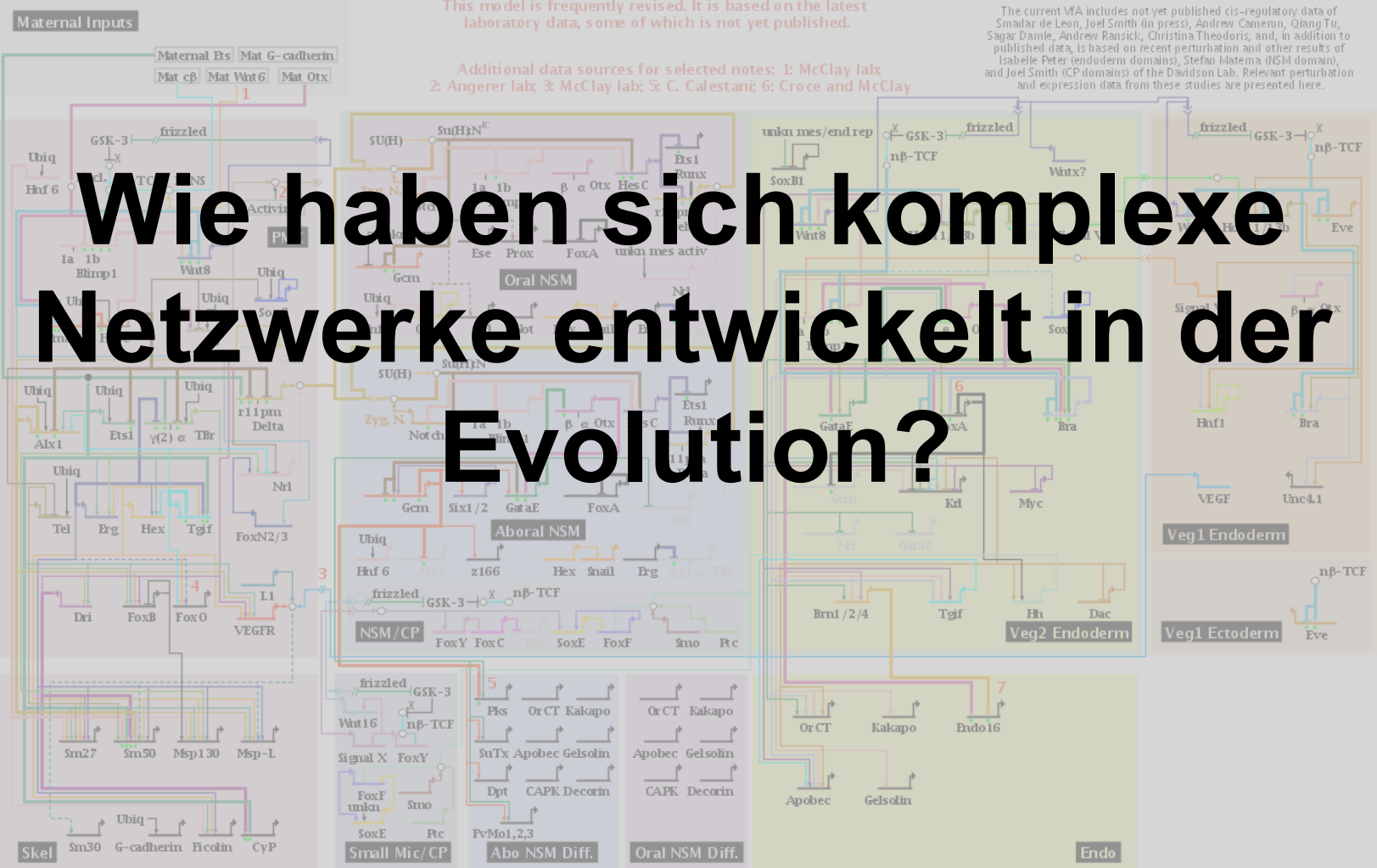
# Unterschiedliche Topologien je nach Genom



This model is frequently revised. It is based on the latest laboratory data, some of which is not yet published.

Additional data sources for selected notes: 1: McClay lab; 2: Angerer lab; 3: McClay lab; 5: C. Caletani; 6: Croce and McClay

The current MTA includes not yet published cis-regulatory data of Smadar de Leon, Joel Smith (in press), Andrew Cameron, Qiang Tu, Sagar Dangle, Andrew Ransick, Christina Theodoris, and, in addition to published data, is based on recent perturbation and other results of Isabelle Peter (endoderm domains), Stefan Matema (NSM domain), and Joel Smith (CP domains) of the Davidson Lab. Relevant perturbation and expression data from these studies are presented here.



# Wie haben sich komplexe Netzwerke entwickelt in der Evolution?

Ubiq=ubiquitous; Mat = maternal; activ = activator; rep = repressor; unkn = unknown; Nucl = nuclearization; x = β-catenin source; nβ-TCF = nuclearized b-β-catenin-Tcf1; E = early signal; ECNS = early cytoplasmic nuclearization system; Zyg. N. = zygotic Notch



# Fragen

- Wie entwickelt sich ein regulatorisches Netzwerk?
- Wie entwickeln sich Proteinkomplexe?
- Evolution im “Periodensystem” der Proteinkomplexe

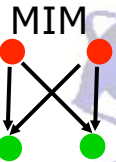
**Repetition bei Prokaryoten vs Eukaryoten**

Periodensystem der Elemente

1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30	31	32	33	34	35	36	37	38	39	40	41	42	43	44	45	46	47	48	49	50	51	52	53	54	55	56	57	58	59	60	61	62	63	64	65	66	67	68	69	70	71	72	73	74	75	76	77	78	79	80	81	82	83	84	85	86	87	88	89	90	91	92	93	94	95	96	97	98	99	100
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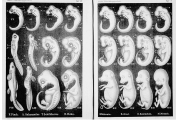
# Fragen

- Wie entwickelt sich ein regulatorisches Netzwerk?



## Genduplikation als Motor

- Wie entwickeln sich Proteinkomplexe?



## Evolution = Assemblierungsweg

- Evolution im “Periodensystem” der Proteinkomplexe

A periodic table of elements, with some elements highlighted in different colors. The table is organized into groups and periods, with elements color-coded by their chemical properties.

## Repetition bei Prokaryoten

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