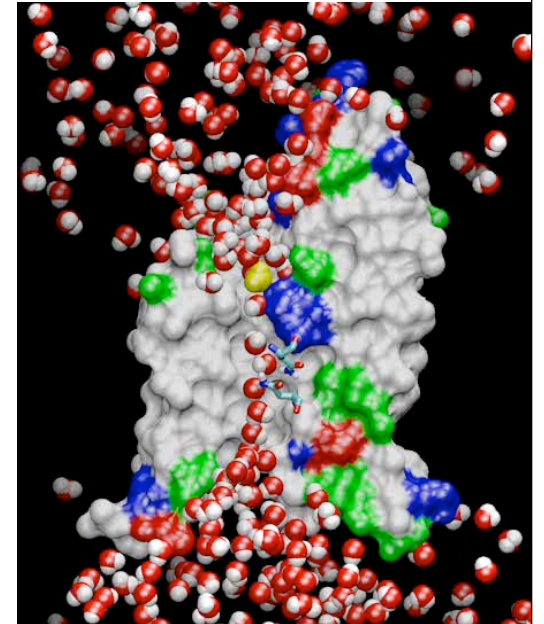
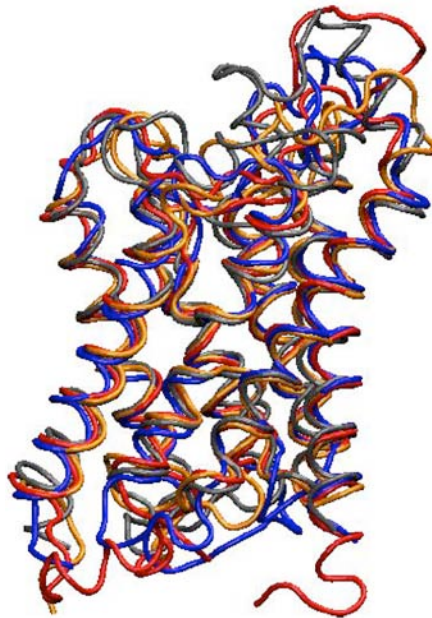


Sequence and Structure Alignment - Illustrated for the Water Channel Aquaporin



Multiple Sequence Alignment

F... To... H...

Align Molecules...
FASTA
Highlight PDB
Pairwise RMSD
Sequence Display

```
1fgy -----KLFWRVVAEFLATTLFVVISIGSAL-GF-KY---PVGNNQTAVDNPKVSLAPGLSIATLAQS-VGHISGAHLNPAVTLGLLLSCQISIF-RAI
1j4n MASEFKKKLFWRAVVAEFLANILFIFVISIGSAL-GF-HYPIKSNQT-TGAVQDNPKVSLAPGLSIATLAQSVGH-ISGAHLNPAVTLGLLLSCQ-ISVLRAI
1lda -----TLKGQCIAEFLGTGLLIFPGVCVA-ALKVA-----G-A-SFGQNEISVIWGLGVAMAIYLTA-GVSGAHLNPAVTIALWLFA-CFDKRRVI
1rc2 -----MFRKLAAEFCGTFWLVPFGCGSAVLA-AG-----PPE-LGIGFAGVALAFGLTVLTMFAVAVG-HISGGHFNPAVTIGLWAGG-RPPAKEV
```

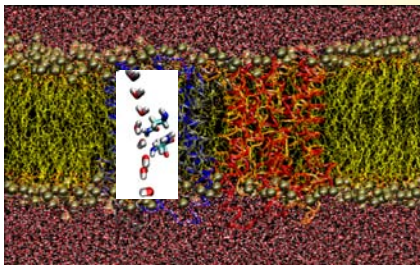
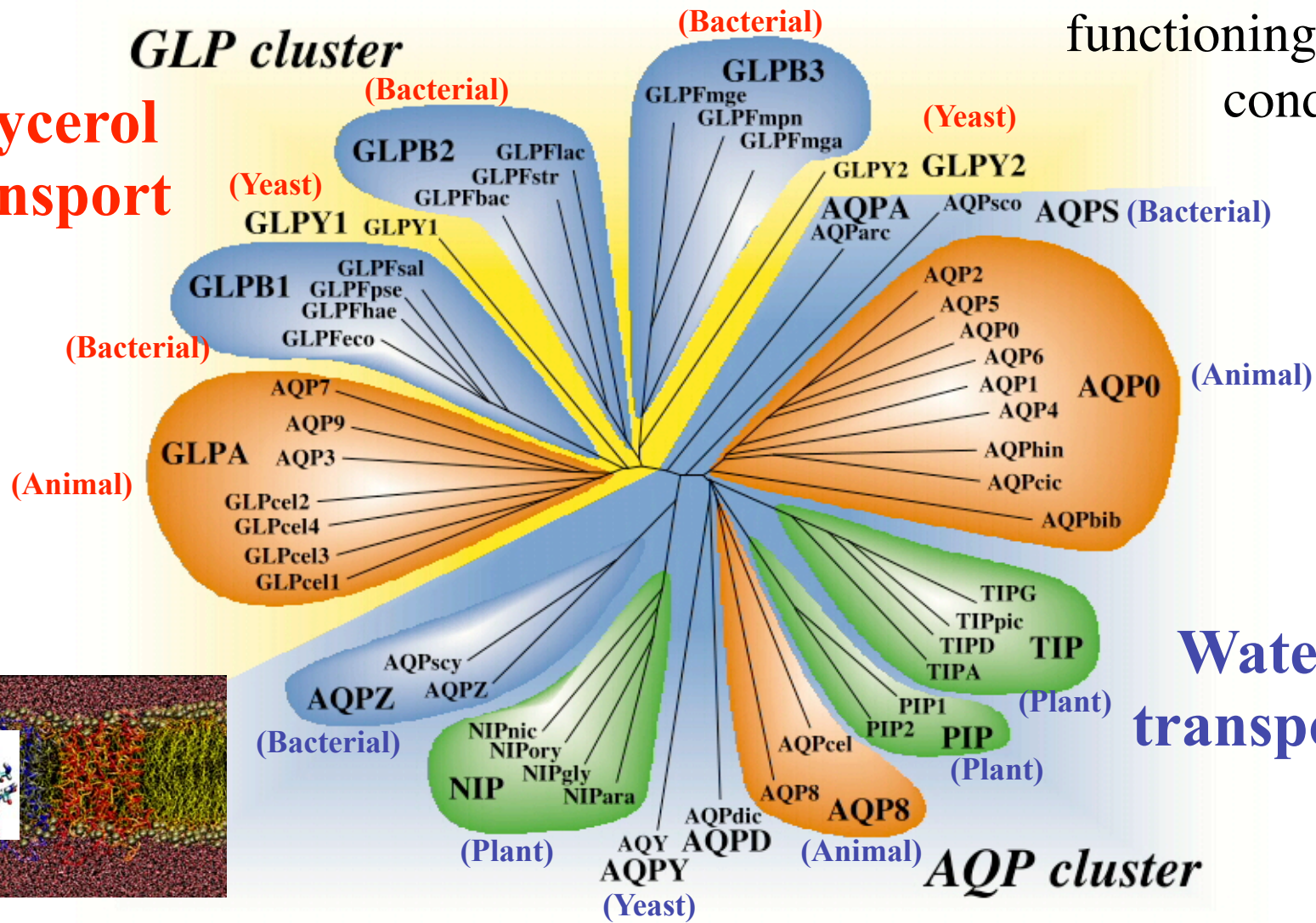
Physical Bioinformatics - A Case Study

Sequence and structure information are the bedrock on which an understanding of cellular functions and the underlying physical mechanisms can be built. This lecture illustrates how the two sources of information are combined to investigate by means of the program VMD function and mechanism of the aquaporin family of membrane channels that transport water and certain small solutes across cell walls. Introducing first the key architectural features of a single aquaporin, structures and sequences of four aquaporins are aligned and common features recognized. The shared and distinct features are examined closely and used as guideposts leading quickly to key questions regarding the mechanism underlying aquaporin's efficient conduction and selection.

The Aquaporin Superfamily

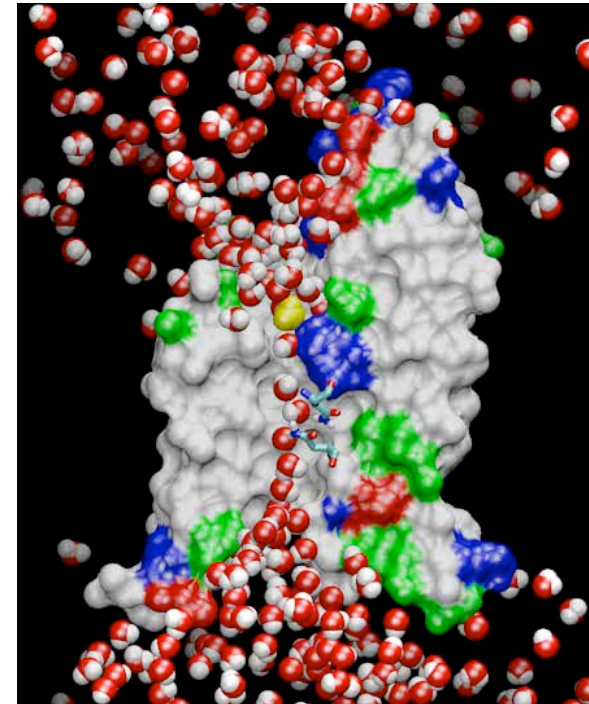
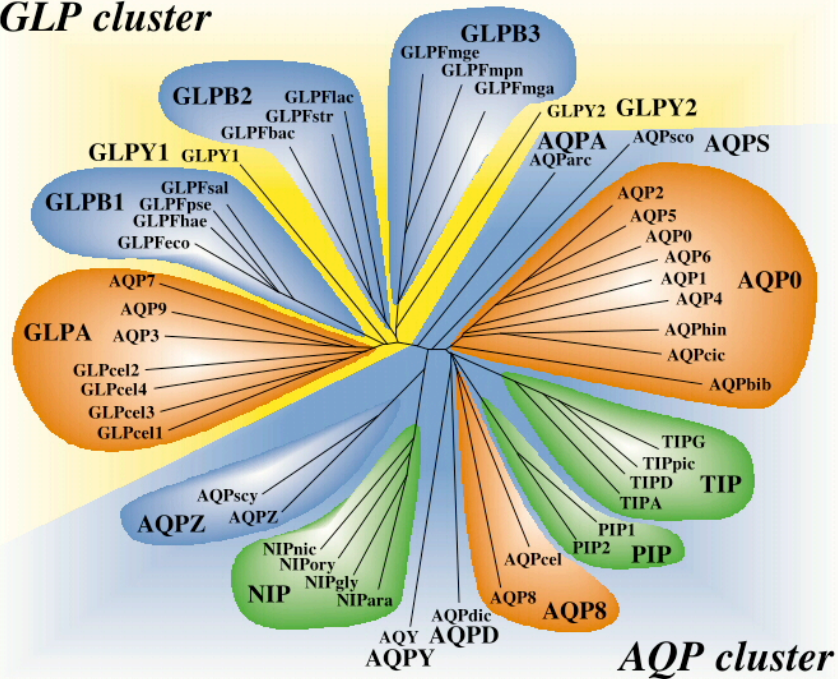
aquaporins are also functioning as gas conductors

Glycerol transport



Aquaporin Function and Human Aquaporins

GLP cluster

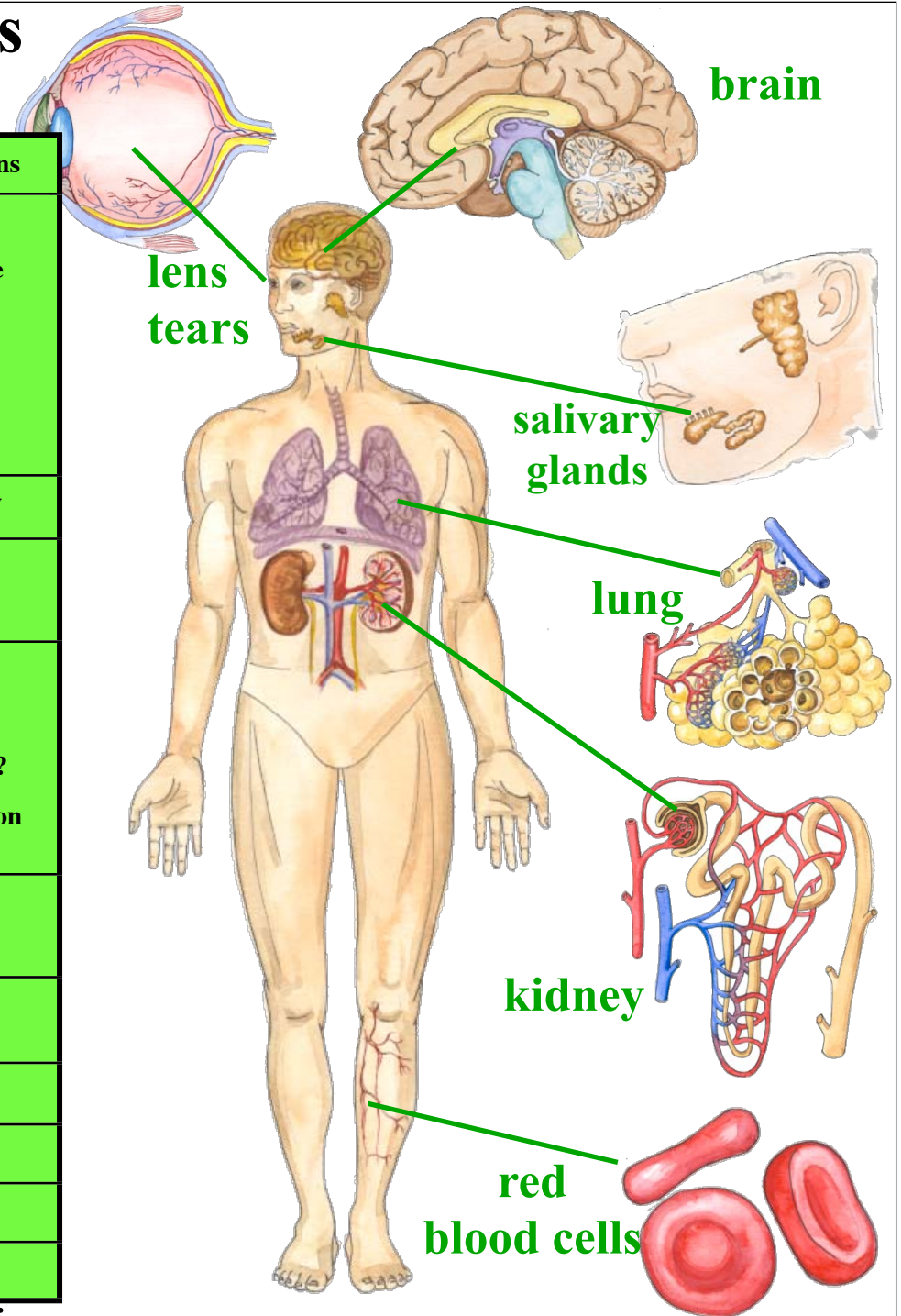


		.	:	*	:	:		.	:*:	:		:*	:									
AQP0_HUMAN	---	LNTLHP	AVSV	GOATT	VEIF	LTLO	QFVLC	IFATY	DE--	RRNG	QLGS	VALAV	GFSL	LALGH	LFGMY	YTGAGM	183					
AQP1_HUMAN	---	RNDLAD	GVNSG	QGLG	IEI	IGTL	QLVLC	VLAT	TDR--	RRRD	LGGSA	PLAIG	LSVAL	GHL	LAI	DYTGCGI	191					
AQP2_HUMAN	---	VNALSN	STTAG	QAVT	VELF	LTLO	QVLC	IFAST	DE--	RRGE	NP	GT	PALS	IGFS	VALGH	LLGIHY	TGCSM	183				
AQP3_HUMAN		GIFATY	PSGH	LD	MING	FFDQ	FIGT	ASLIV	CVLAI	VD	PYNN	NP	VPRG	LEAFT	VGLV	LVVIG	TSMGF	NSGYAV	214			
AQP4_HUMAN	---	VTMVH	GNLT	AGH	LL	VELI	IITF	QLVFT	IFAS	CDS--	KRTD	VTG	SIAL	AIGF	SVAI	GHLF	AINYT	TGASM	212			
AQP5_HUMAN	---	VNALNN	NTTQ	QAMV	VELI	ILTF	QALC	IFAST	DTS--	RRTS	SPV	G	SPAL	SIGL	SVTL	GHLV	GIYFT	TGCSM	184			
AQP6_HUMAN	---	INVRNS	SVST	GQAV	AVEL	LLTL	QLVLC	VFAST	DTS--	RQTS	--	GSPAT	MIGI	SWAL	GHLI	GILFT	TGCSM	195				
AQP7_HUMAN		GIFATY	LPDH	MTLW	RGFL	NEAW	L	TGML	QLCL	FAIT	DQEN	NP	AL	PGTE	ALVIG	ILVVI	IGVSL	GMNTGYAI	225			
AQP8_HUMAN	-	AAFVT	VQEQ	QVAG	ALVA	EI	IL	TLL	LALAV	CMGAIN--	EKTK	G	PLAP	FSIG	FAVT	VDIL	AGPVS	GGCM	209			
AQP9_HUMAN		HIFATY	PAPY	LSLAN	AFAD	QVAT	MILLI	IIVFA	IFDS	RNLG	APRG	LEPI	AIGL	LI	I	VI	ASSL	GLNSGCAM	215			
GLPF_ECOLI		GT	FSTY	PNPH	INFV	QAF	AVEM	VITAIL	MGLIL	LAL	TDDG	NGV	PRG	PLAP	LLI	G	LLI	AVIG	ASMG	PLTG	FAM	202
ruler	...	180	190	200	210	220	230	240							

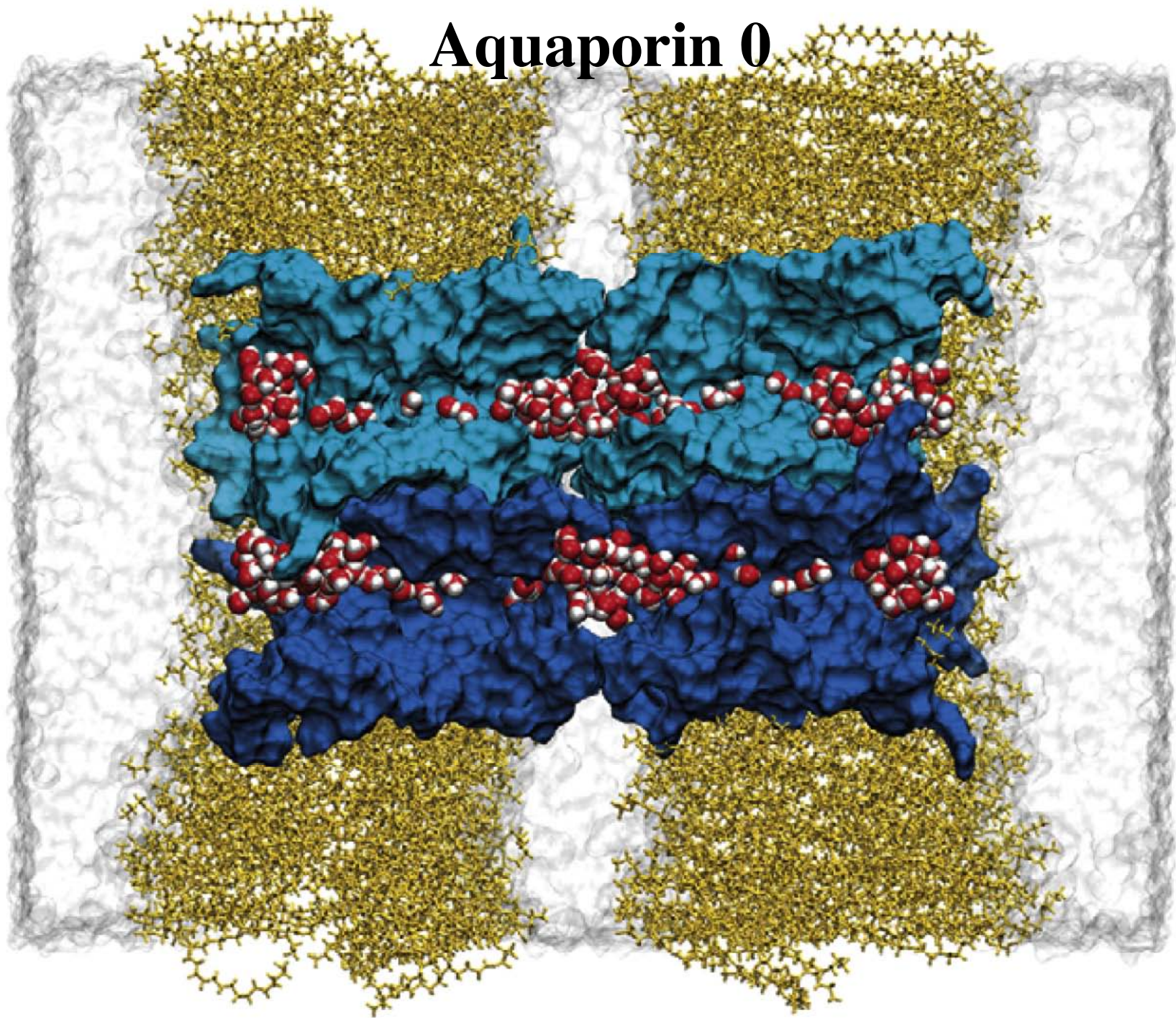
Water and **Glycerol** Channels in the Human Body

Aquaporin-0	Eye: lens fiber cells	Fluid balance of the lens
Aquaporin-1	Red blood cells Kidney: proximal tubules Eye: ciliary epithelium Brain: choroid plexus Lung: alveolar epithelial cells	Osmotic protection Concentration of urine Aqueous humor Production of CSF Alveolar hydration cells
Aquaporin-2	Kidney: collecting ducts	ADH hormone activity
Aquaporin-3	Kidney: collecting ducts Trachea: epithelial cells	Reabsorption of water Secretion of water
Aquaporin-4	Kidney: collecting ducts Brain: ependymal cells Brain: hypothalamus Lung: bronchial epithelium	Reabsorption of water CSF fluid balance Osmosensing function? Bronchial fluid secretion
Aquaporin-5	Salivary glands Lacrimal glands	Production of saliva Production of tears
Aquaporin-6	Kidney	Very low water permeability!
Aquaporin-7	Testis and sperm	
Aquaporin-8	Testis, pancreas, liver	
Aquaporin-9	Leukocytes	
Aquaporin-10	Intestines	

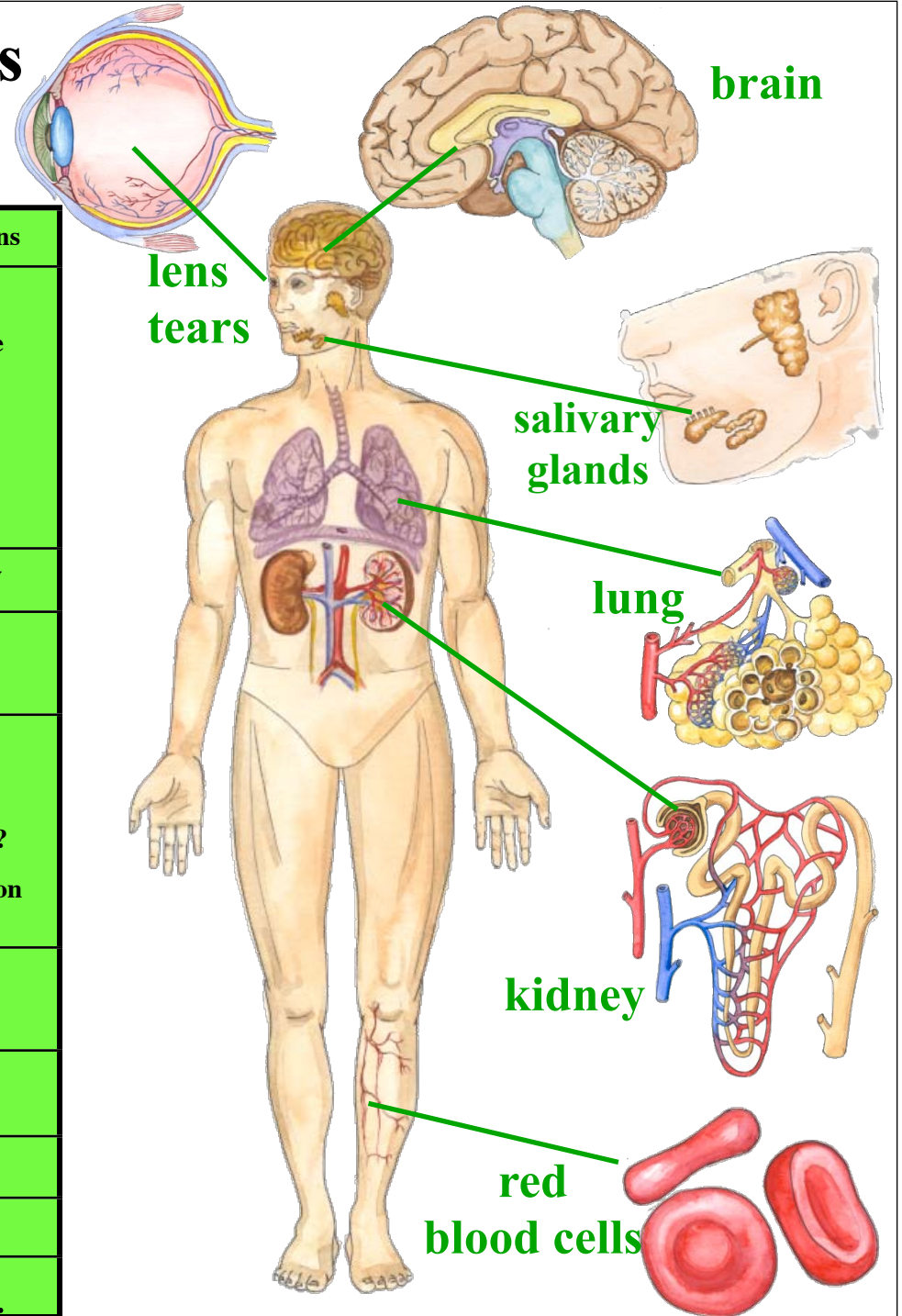
Additional members are suspected to exist.



Aquaporin 0



Water and **Glycerol** Channels in the Human Body



Aquaporin-0	Eye: lens fiber cells	Fluid balance of the lens
Aquaporin-1	Red blood cells Kidney: proximal tubules Eye: ciliary epithelium Brain: choroid plexus Lung: alveolar epithelial cells	Osmotic protection Concentration of urine Aqueous humor Production of CSF Alveolar hydration
Aquaporin-2	Kidney: collecting ducts	ADH hormone activity
Aquaporin-3	Kidney: collecting ducts Trachea: epithelial cells	Reabsorption of water Secretion of water
Aquaporin-4	Kidney: collecting ducts Brain: ependymal cells Brain: hypothalamus Lung: bronchial epithelium	Reabsorption of water CSF fluid balance Osmosensing function? Bronchial fluid secretion
Aquaporin-5	Salivary glands Lacrimal glands	Production of saliva Production of tears
Aquaporin-6	Kidney	Very low water permeability!
Aquaporin-7	Testis and sperm	
Aquaporin-8	Testis, pancreas, liver	
Aquaporin-9	Leukocytes	

Additional members are suspected to exist.

Functionally Important Features of Aquaporins

- Water, gas, and glycerol transport
- Exclusion of ions and protons
- Tetrameric arrangement in membrane

Aquaporins of known structure:

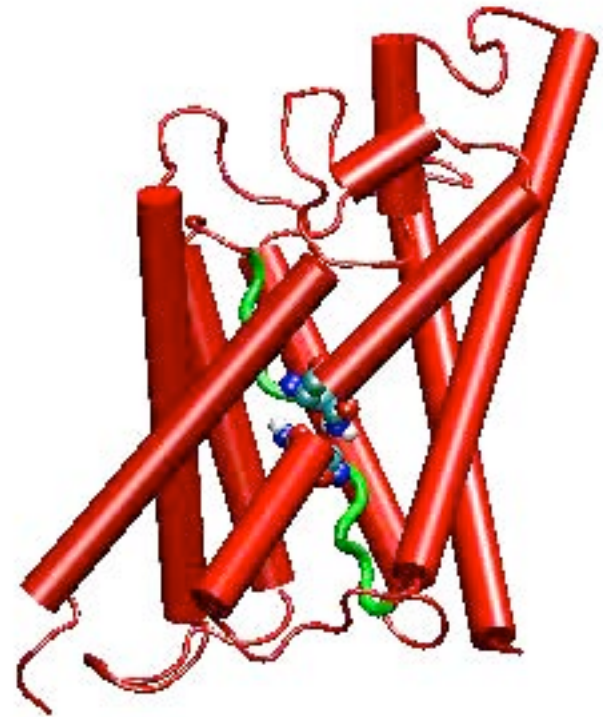
GlpF – E. coli glycerol channel (aquaglyceroporin)

– Fu, et al., Science (2000)

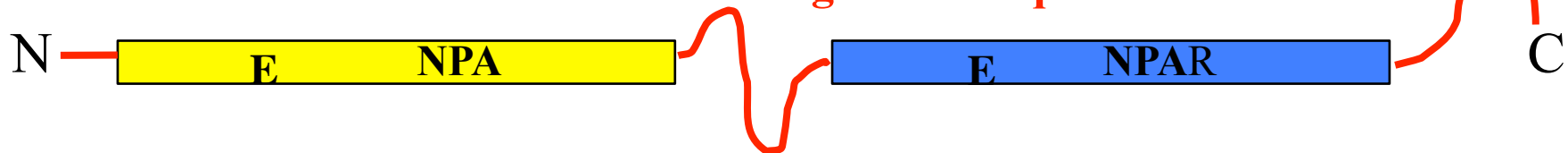
AQP1 – Mammalian aquaporin-1 (pure water channel) -Sui et al, Nature (2001)

AQP1 - Bovine - Murata et al, Nature (2000)

AQPZ - E. coli water channel - Savage et al, PLOS Biol (2003)



~100% conserved -NPA- signature sequence



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- Exclusion of ions and protons
- Tetrameric arrangement in membrane

Aquaporins of known structure:

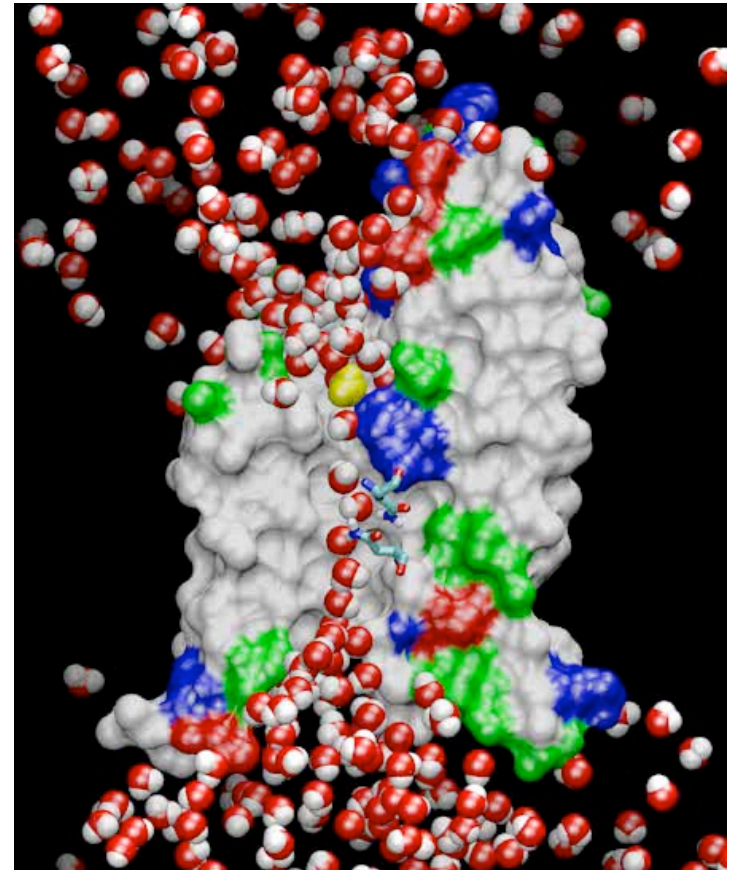
GlpF – E. coli glycerol channel (aquaglyceroporin)

– Fu, et al., Science (2000)

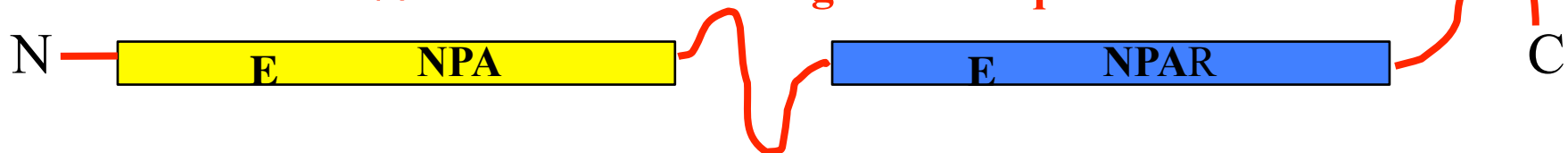
AQP1 – Mammalian aquaporin-1 (pure water channel) -Sui et al, Nature (2001)

AQP1 - Bovine - Murata et al, Nature (2000)

AQPZ - E. coli water channel - Savage et al, PLOS Biol (2003)



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Functionally Important Features of Aquaporins

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- Exclusion of ions and protons
- Tetrameric arrangement in membrane

Aquaporins of known structure:

GlpF – E. coli glycerol channel (aquaglyceroporin)

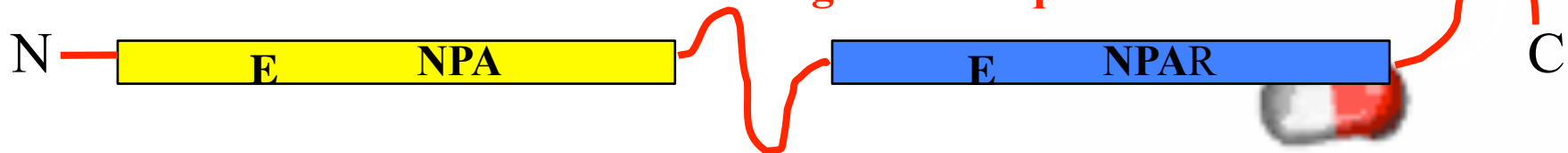
– Fu, et al., Science (2000)

AQP1 – Mammalian aquaporin-1 (pure water channel) -Sui et al, Nature (2001)

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Aquaporins of known structure:

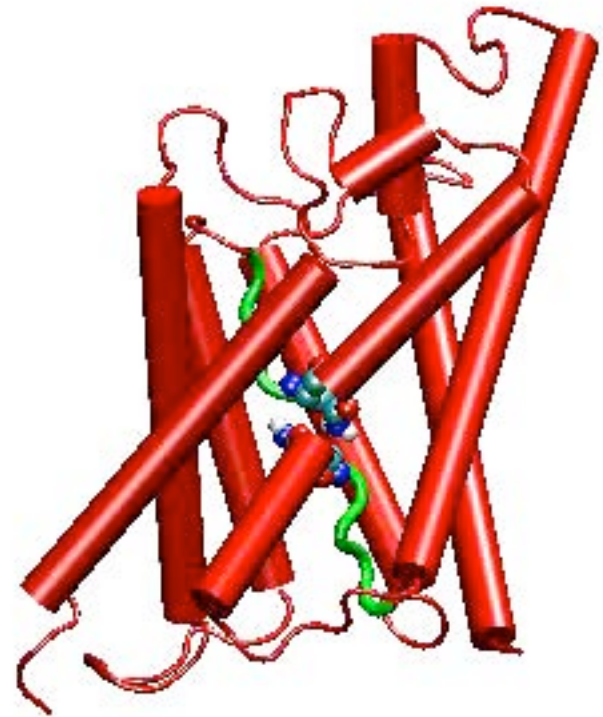
GlpF – E. coli glycerol channel (aquaglyceroporin)

– Fu, et al., Science (2000)

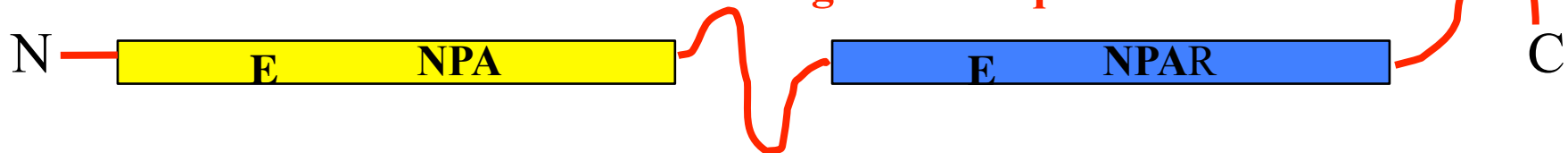
AQP1 – Mammalian aquaporin-1 (pure water channel) -Sui et al, Nature (2001)

AQP1 - Bovine - Murata et al, Nature (2000)

AQPZ - E. coli water channel - Savage et al, PLOS Biol (2003)



~100% conserved -NPA- signature sequence



Load Aquaporin 1J4N into VMD

The image shows the VMD (Visual Molecular Dynamics) interface. The main window, titled "VMD Main", contains a menu bar (File, Molecule, Graphics, Display, Mouse, Extensions, Help) and a table of loaded molecules:

ID	T	A	D	F	Molecule	Atoms	Frames	Vol
1	T	A	D	F	1J4N	2029	1	0

Below the table is a playback control bar with a time slider at 0, a "zoom" checkbox, a "Loop" dropdown, a "step" slider at 1, and a "speed" slider.

The "Graphical Representations" window is open, showing the configuration for the selected molecule "1: 1J4N". It includes buttons for "Create Rep" and "Delete Rep", and a table for defining graphical representations:

Style	Color	Selection
Tube	Name	all

Below this table is a "Selected Atoms" field containing "all". The "Draw style" tab is active, showing settings for "Coloring Method" (Name), "Material" (Opaque), and "Drawing Method" (Tube). At the bottom, there are sliders for "Radius" (0.5) and "Resolution" (11), and an "Apply Changes Automatically" checkbox with an "Apply" button.

The "VMD 1.8.2b7 OpenGL Display" window shows a 3D ribbon representation of the Aquaporin 1J4N protein structure, rendered in a teal color. The structure is a complex, multi-domain protein with several alpha-helices and beta-strands. The bottom right corner of the VMD window shows standard OS navigation icons.

Load Aquaporins 1j4n, 1fqy, 1lda, 1rc2 into VMD

The screenshot displays the VMD (Visual Molecular Dynamics) software interface. The main window, titled "VMD Main", shows a list of loaded molecules:

ID	T	A	D	F	Molecule	Atoms	Frames	Vol
1		A	D	F	1J4N	2029	1	0
2		A	D	F	1FQY	1661	1	0
3		A	D	F	1lda	1997	1	0
5	T	A	D	F	1rc2	3530	1	0

The "Graphical Representations" window shows the selected molecule "5: 1rc2" with the following settings:

- Style: Tube
- Color: ColorID 3
- Selection: chain A
- Coloring Method: ColorID
- Material: Opaque
- Drawing Method: Tube
- Radius: 0.5
- Resolution: 11

The "Multiple Sequence Alignment" window displays the following sequence alignment:

PDB code	Description
1j4n	Bovine AQP1
1fqy	Human AQP1
1lda	E. coli Glycerol Facilitator (GlpF)
1r2c	E. coli AqpZ

The alignment window shows the following sequence alignment:

```
d1fqya_.ent KLPWRVAVAEFLATTLFVFIISIGSALGFKYPVGRNQTAVDNPKVSLAFGLSIATLA
d1j4na_.ent MASEFKKKLFWRAVVAEFLAMILFIPISIGSALGFHYPIKSNQTTGAVODNPKVSLA
d1lda_.ent TLFGQCTAEFLGTGLLFFGVGCVAAALKVAGASFGQWEISVINGLGVAMAIYLTAGV
d1rc2a_.ent MFRKLAAEFCFTFWLVPGGCGSAVLAAGFPPELGI GFAGVALAFGLTVLTMFAVGH
```

Aligning Structures and Sequences

VMD Main

File Molecule Graphics Display Mouse Extensions Help

ID	T	A	D	F	Molecule	Atoms	Frames	Vol
1	A	D	F		1J4N	2029	1	0
2	A	D	F		1FQY	1661	1	0
3	A	D	F		1lda	1997	1	0
5	T	A	D	F	1rc2	3530	1	0

0

zoom Loop step 1 speed

Graphical Representations

Selected Molecule

5: 1rc2

Create Rep Delete Rep

Style	Color	Selection
Tube	ColorID 3	chain A

Selected Atoms

chain A

Draw style Selections Trajectory Periodic

Coloring Method Material

ColorID 3 Opaque

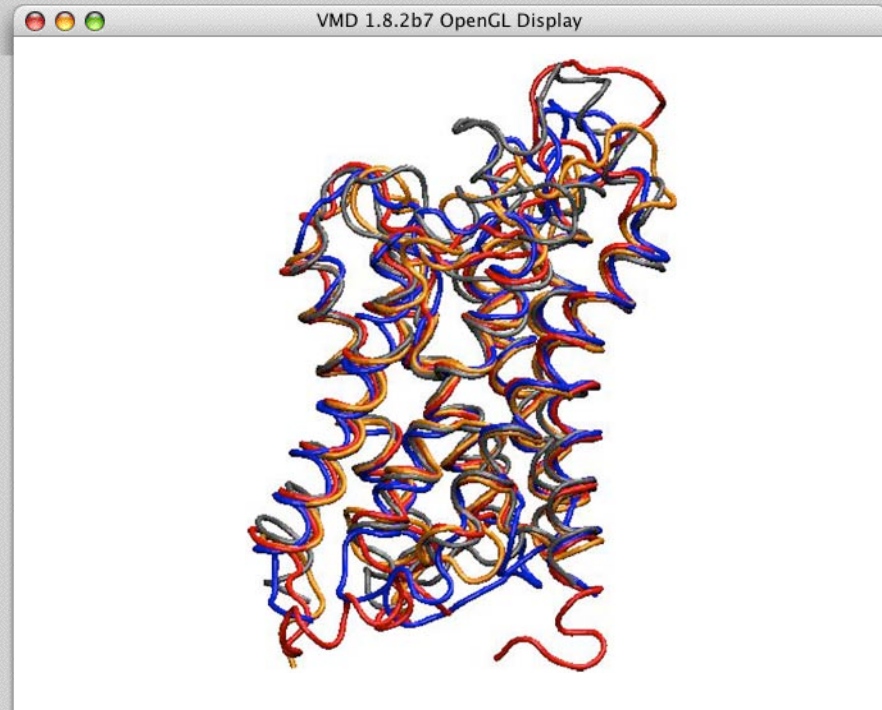
Drawing Method

Tube Default

Radius 0.5

Resolution 11

Apply Changes Automatically Apply



Multiple Sequence Alignment

F... To... H...

Align Molecules...

FASTA

Highlight PDB

Pairwise RMSD

Sequence Display

```

1fgy -----KLFWRVAVVAEFLATTLFVFIISIGSAL-GF-KY---PVGNNQTAVDQDNVKSLSLAPGLSIATLAQS-VGHISGABLNPAVTLGLLLSQCISIF-RAI
1j4n MASEFKKKLFWRAVVAEFLAMILFIFISIGSAL-GF-HYPIKSNQT-TGAVQDNVKSLSLAPGLSIATLAQSVGH-ISGABLNPAVTLGLLLSQC-I SVLRAI
1lda -----TLKGQCIAEFLGTGLLIFPGVGCVA-ALKVA-----G-A-SFGQWEISVINGLGVAMAYLTA-GVSGAHLNPAVTIALNLFA-CFDKRRVI
1rc2 -----MFRKLAAECPGTFWLVPFGCGSAVLA-AG-----FPE-LGIGFAGVALAPGLTVLTMFAVAVG-HISGGHFNPAVTIGLWAGG-RFPAKEVV
    
```

Comparing Structures by Similarity - Q Value

The screenshot displays the VMD (Visual Molecular Dynamics) software interface, which is used for visualizing and analyzing molecular structures. The interface is divided into several windows:

- VMD Main:** Contains a menu bar (File, Molecule, Graphics, Display, Mouse, Extensions, Help) and a table listing loaded molecules. Below the table is a playback control bar with a slider and buttons for zoom, loop, step, and speed.
- Graphical Representations:** A configuration panel for the selected molecule (5: 1rc2). It includes buttons for 'Create Rep' and 'Delete Rep', and a table for defining representations. The current representation is 'Tube' with 'ColorID 3' and 'chain A' selected. Below this, there are tabs for 'Draw style', 'Selections', 'Trajectory', and 'Periodic'. The 'Coloring Method' is set to 'ColorID' with a value of 3 and 'Material' set to 'Opaque'. The 'Drawing Method' is set to 'Tube'. At the bottom, there are sliders for 'Radius' (0.5) and 'Resolution' (11), and an 'Apply' button.
- VMD 1.8.2b7 OpenGL Display:** A 3D window showing a protein structure rendered as a multi-colored tube (red, blue, orange, yellow, green, cyan). The structure is a complex, multi-domain protein.
- Multiple Sequence Alignment:** A window showing a sequence alignment of four proteins: 1fqy, 1j4n, 1lda, and 1rc2. A context menu is open over the alignment, with 'Molecule Coloring' selected, and 'Q per residue' checked. Other options in the menu include 'RMSD Per Residue', 'Tree', 'STAMP Parameters', 'Bulk Residue Selection', and 'Highlight Style'. The alignment text is as follows:


```

1fqy  -----LQFWRVAVVAVFLAFLVLSIGSAL*GF*RY---FVGRQTAVDQNVKVSLEAFGLS*ATLAQS-VGHISGAHLNFAVTLGLLLSCOISIF-RAI
1j4n  MASEFKKLFWRVAVVAVFLAMILFIFISIGSAL-GF-HYPIKSNQT--TCAVQDNVKVSLAFGLS*ATLAQSVGH-I SGAHLNPAVTLGLLLSQV--ISVLRV
1lda  -----TLRGQCIAEFLGTGLLIFFGVGVCA-ALKVA-----G-A-SFGQWEISVIWGLGVAMAITYLA-GVSGAHLNPAVTIALWLFV-CFDKRRV
1rc2  -----MFRKLAAECPGTFWLVFVGCGSAVLA-AG-----FPE-LGIGFAGVALAPGLTVLTMFAVAVG-HISGGHPNPAVTIGLWAGG-RFPAKEV
      
```

Comparing Structures by Similarity - Q Value

The image displays the VMD (Visual Molecular Dynamics) software interface, illustrating the process of comparing protein structures by similarity using a Q Value.

VMD Main Window: Shows a table of loaded molecules and playback controls.

ID	T	A	D	F	Molecule	Atoms	Frames	Vol	
1		A	D	F	1J4N	2029	1	0	
2		A	D	F	1FQY	1661	1	0	
3		A	D	F	1lda	1997	1	0	
5		T	A	D	F	1rc2	3530	1	0

Graphical Representations Window: Shows settings for the selected molecule (5: 1rc2). The drawing method is set to Tube, and the coloring method is ColorID 3. The selected atoms are chain A.

VMD 1.8.2b7 OpenGL Display Window: Displays a 3D ribbon representation of the protein structure, colored by residue using the ColorID 3 method.

Multiple Sequence Alignment Window: Shows a sequence alignment of four proteins: 1fqy, 1j4n, 1lda, and 1rc2. The alignment is displayed in a text-based format with gaps represented by dashes. A context menu is open over the alignment, with "Molecule Coloring" selected, and "Q per residue" checked.

```
1fqy  -----LPLFWRVAVAEFLALFLVLSIGSAL*GF*RY---FVDRNQTAVDQNVKVSLEAFGLS*ATLAQS-VGHISGAHLNFAVTLGLLLSCOISIF-RAI
1j4n  MASEFKKLFWRVAVAEFLAMILFIFISIGSAL-GF-HYPIKSNQT-TCAVDQNVKVSLEAFGLS*ATLAQSVGH-I SGAHLNPAVTLGLLLSQV--ISVLRAR
1lda  -----TLRGQCIAEFLGTGLLIFFGVGVCA-ALKVA-----G-A-SFGQWEISVIWGLGVAMAITYLA-GVSGAHLNPAVTIALWLFV-CFDKRRV
1rc2  -----MFRKLAAECPGTFWLVFEGGCGSAVLA-AG-----FPE-LGIGFAGVALAPGLTVLTMFAVAVG-HISGGHPNPAVTIGLWAGG-RFPAKEV
```


Exhibiting Sequence Identity - Side View

The image displays the VMD (Visual Molecular Dynamics) software interface. The main window, titled "VMD 1.8.2b7 OpenGL Display", shows a protein structure rendered as a multi-colored tube, representing sequence identity. The structure is viewed from a side perspective, showing a complex fold with several alpha-helices and beta-strands. The colors range from red to blue, indicating different levels of sequence identity.

The "VMD Main" window in the top left contains a table of loaded molecules:

ID	T	A	D	F	Molecule	Atoms	Frames	Vol
1	A	D	F		1J4N	2029	1	0
2	A	D	F		1FQY	1661	1	0
3	A	D	F		1lda	1997	1	0
5	T	A	D	F	1rc2	3530	1	0

The "Graphical Representations" window in the middle left shows the configuration for the selected molecule "5: 1rc2". The "Style" is set to "Tube", the "Color" is "ColorID 3", and the "Selection" is "chain A". The "Drawing Method" is also set to "Tube". The "Radius" is 0.5 and the "Resolution" is 11. The "Apply Changes Automatically" checkbox is checked.

The "Multiple Sequence Alignment" window in the bottom right shows a sequence alignment of four proteins: 1fgy, 1j4n, 1lda, and 1rc2. The alignment is displayed in a cyan background with yellow highlights indicating conserved residues. The alignment is as follows:

```

1fgy  -----KLFWRVAVAEFLATTILFVETISIGSAL-GF-KY---FVGNQTAVQDNVKVSLAPGLSIATLAQS-VGHISGAEINPAVTLGLLSQCISIF-RV
1j4n  MASEFKKLLFWRVAVAEFLAMILFIFISIGSAL-GF-HYPIKSNQT-TGAVQDNVKVSLAPGLSIATLAQSVGH-I SGAEINPAVTLGLLSCO-I SVLRV
1lda  -----TLKGQCI AEF LGTGLL IFFGVGVVA-ALKVA-----G-A-SFGQWEISVINGLVAMAIYLA-GVSGAEINPAVTIALNLFA-CFDRKV
1rc2  -----MPRKLAECEFGTFWLVFGCCSAVLA-AG-----FPE-LGIGFAGVALAPGLTLVLTMAFAVG-HISGGEINPAVTIGLWAGG-RFPARV
  
```

Exhibiting Sequence Identity - Top View

The screenshot displays the VMD (Visual Molecular Dynamics) software interface. The main window, titled "VMD 1.8.2b7 OpenGL Display", shows a top-down view of a protein structure represented as a multi-colored tube. The structure is composed of several chains, with colors corresponding to different sequence identities. The interface includes several control panels:

- VMD Main:** A menu bar (File, Molecule, Graphics, Display, Mouse, Extensions, Help) and a table listing loaded molecules.
- Graphical Representations:** A panel for configuring the selected molecule (5: 1rc2). It includes buttons for "Create Rep" and "Delete Rep", and a table for defining representations.
- Multiple Sequence Alignment:** A window showing a sequence alignment of four proteins (1fqy, 1j4n, 1lda, 1rc2) with highlighted regions of identity.

ID	T	A	D	F	Molecule	Atoms	Frames	Vol
1	A	D	F		1J4N	2029	1	0
2	A	D	F		1FQY	1661	1	0
3	A	D	F		1lda	1997	1	0
5	T	A	D	F	1rc2	3530	1	0

Style	Color	Selection
Tube	ColorID 3	chain A

```
1fqy  -----KLFWRVVAEFLATTLFVETISIGSAL-GF-KY---FVGNQTAVDNPKVSLAPGLSIATLAQS-VGHISGAEINPAVTLGLLSQCISIF-RV
1j4n  MASEFKKLLFWRVVAEFLAMILFVETISIGSAL-GF-HYPIKSNQT-TGAVQDNPKVSLAPGLSIATLAQSVGH-I-SGAEINPAVTLGLLSCO-I-SVLRV
1lda  -----TLKGQCIAEPLGTGLLFFPGVGVA-ALKVA-----G-A-SFGQWEISVINGLVAMAIYLA-GVSGAEINPAVTIALNLFA-CFDRKV
1rc2  -----MPRKLAECPGTFWLVFGGCSAVLA-AG-----FPE-LGIGFAGVALAPGLTVLTMFAVVG-HISGGEINPAVTIGLWAGG-RFPKRV
```

Showing Conserved Residues - Monomer

The screenshot displays the VMD (Visual Molecular Dynamics) software interface. The main window shows a protein structure rendered as a tube, with residues highlighted in yellow to indicate conservation. The interface includes several panels:

- VMD Main:** A menu bar (File, Molecule, Graphics, Display, Mouse, Extensions, Help) and a table listing loaded molecules.
- Graphical Representations:** A panel for configuring the selected molecule (5: 1rc2), including options for style (Tube), color (ColorID 3), and selection (chain A).
- Multiple Sequence Alignment:** A window showing a sequence alignment of four proteins (1fqy, 1j4n, 1lda, 1rc2) with conserved residues highlighted in yellow.

ID	T	A	D	F	Molecule	Atoms	Frames	Vol
1	A	D	F		1J4N	2029	1	0
2	A	D	F		1FQY	1661	1	0
3	A	D	F		1lda	1997	1	0
5	T	A	D	F	1rc2	3530	1	0

```

1fqy  -----KLFWRVAVAEFLATTILFVVISIGSAL-GF-KY---FVGNQTAVQDNVKVSLAPGLSIATLAQS-VGHISGABLNPAVTLGLLSQCISIF-RV
1j4n  MASEFKKLLFWRVAVAEFLAMILFIFISIGSAL-GF-HYPIKSNQT-TGAVQDNVKVSLAPGLSIATLAQSVGH-I-SGABLNPAVTLGLLSCO-I-SVLRV
1lda  -----TLKGQCIAEPLGTGLLIFPGVGVVA-ALKVA-----G-A-SFGQWEISVINGLVAMAIYLTA-GVSGABLNPAVTIALNLFA-CFDRKRV
1rc2  -----MPRKLAECPGTFWLVFGCCSAVLA-AG-----FPE-LGIGFAGVALAPGLTVLTMFAVVG-HISGGRNPAVTIGLWAGG-RFPARVV
  
```

Showing Conserved Residues - Tetramer

VMD Main

File Molecule Graphics Display Mouse Extensions Help

ID	T	A	D	F	Molecule	Atoms	Frames	Vol
1		A	D	F	1J4N	2029	1	0
2		A	D	F	1FQY	1661	1	0
3		A	D	F	1lda	1997	1	0
5	T	A	D	F	1rc2	3530	1	0

0

zoom Loop step 1 speed

Graphical Representations

Selected Molecule

5: 1rc2

Create Rep Delete Rep

Style	Color	Selection
Tube	ColorID 3	chain A

Selected Atoms

chain A

Draw style Selections Trajectory Periodic

Coloring Method Material

ColorID 3 Opaque

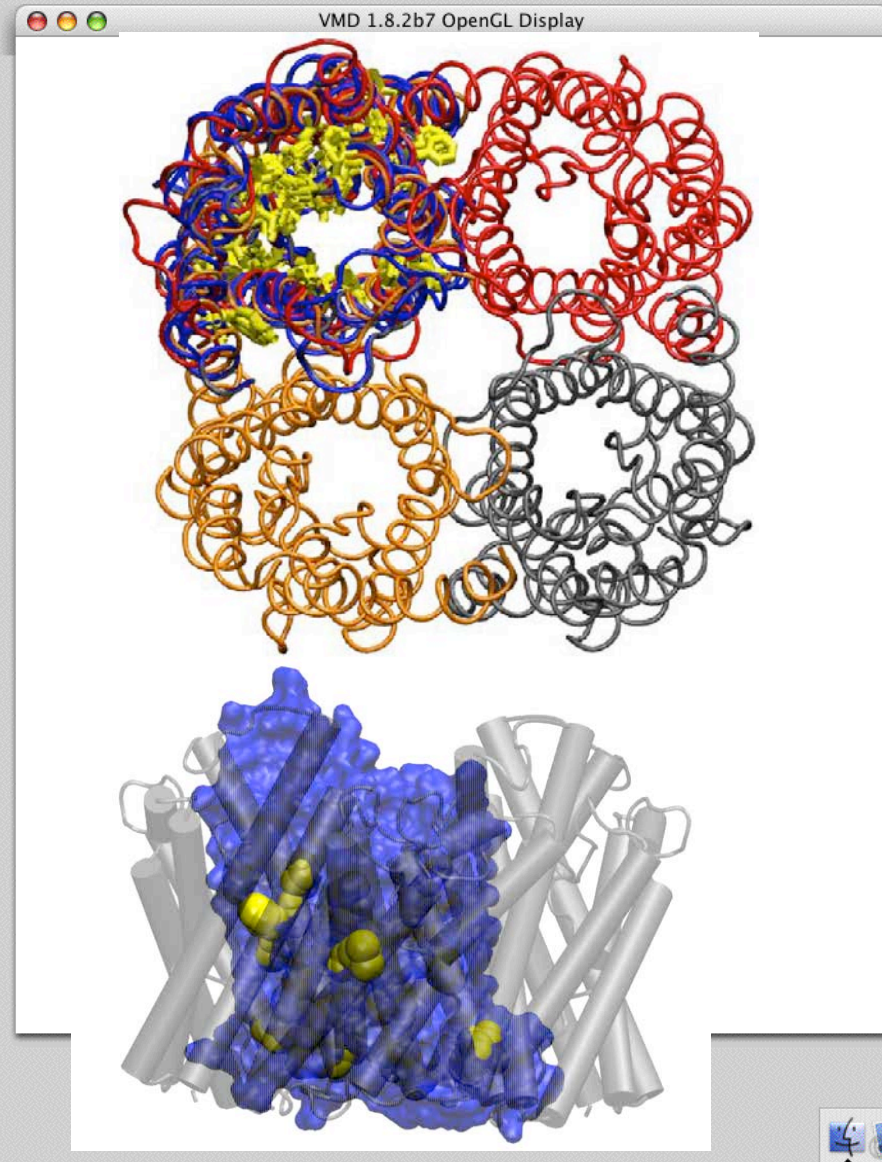
Drawing Method

Tube Default

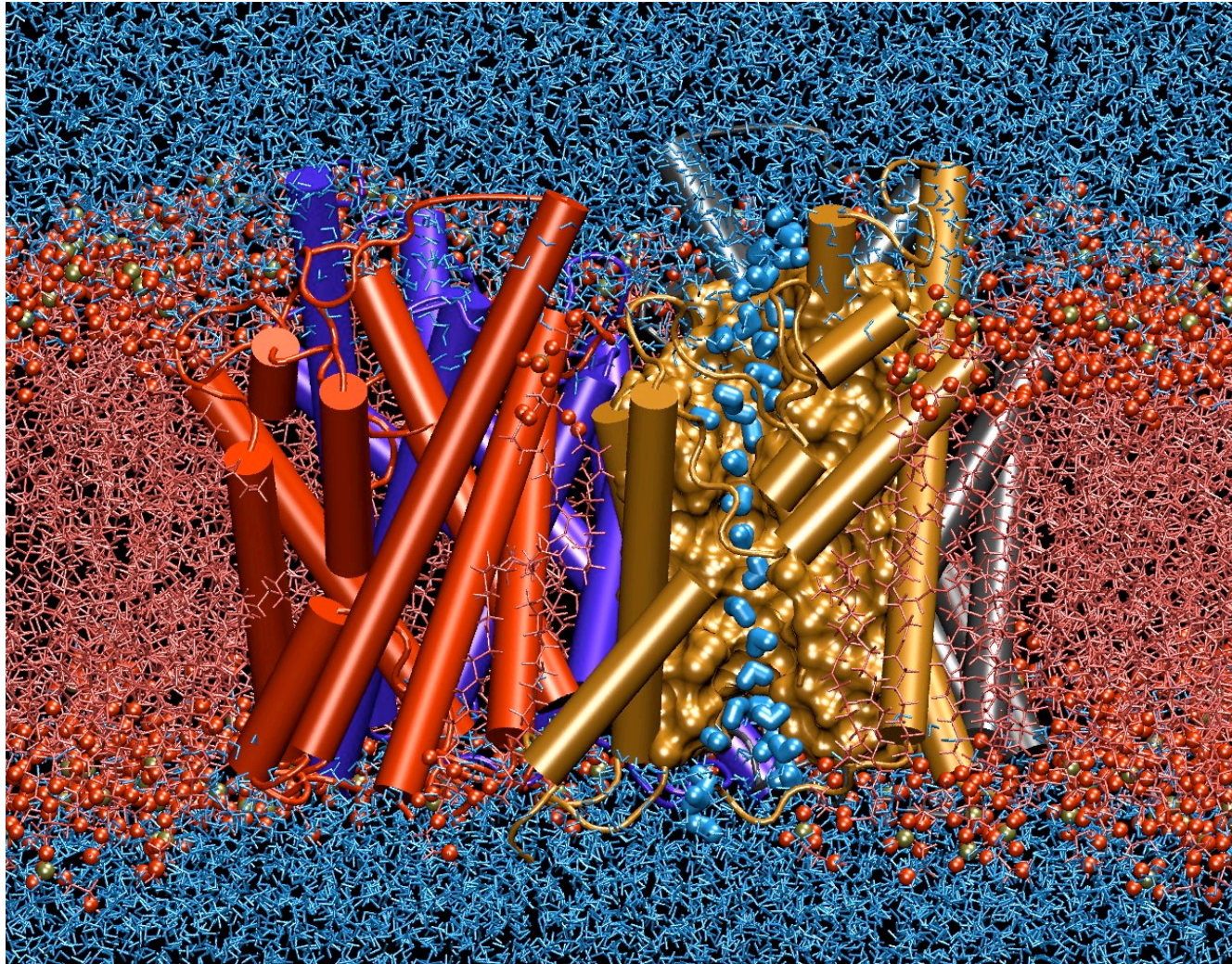
Radius 0.5

Resolution 11

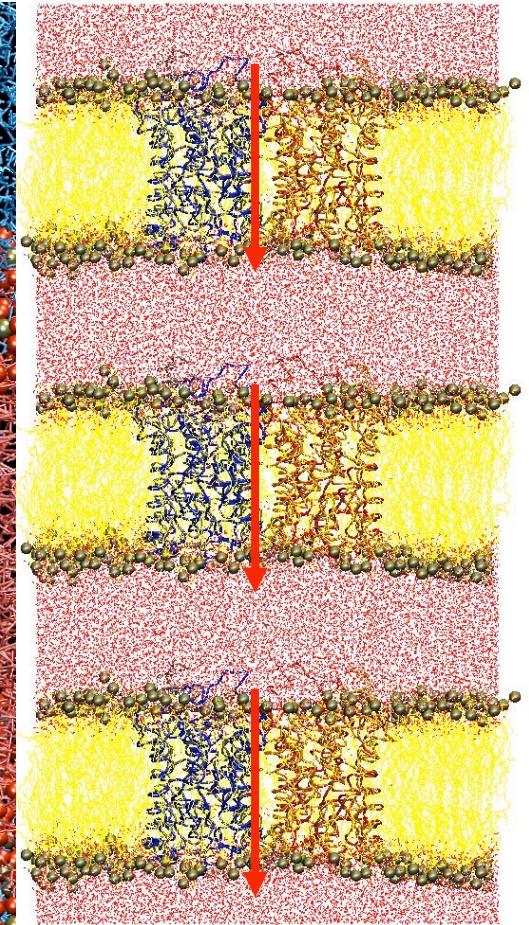
Apply Changes Automatically Apply



Water Transport in Aquaporins



100,000 atoms

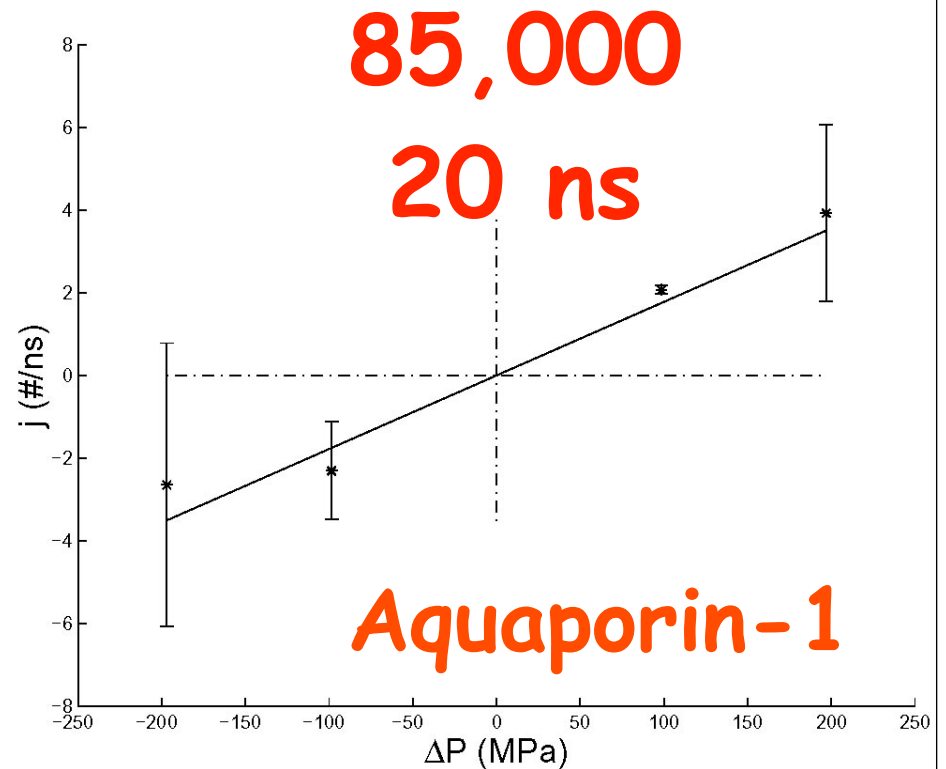
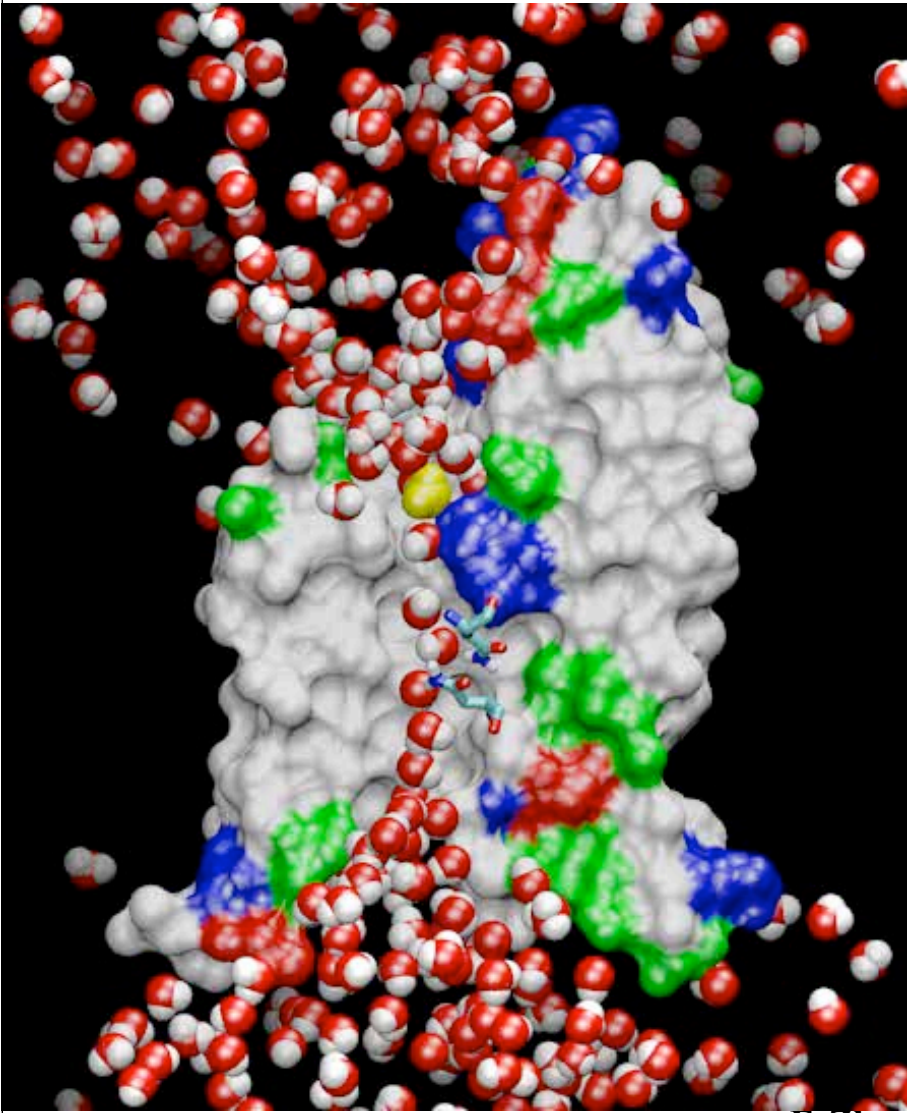


Simulation:

*Apply constant force
on bulk water
molecules*



Osmotic permeability of water channels



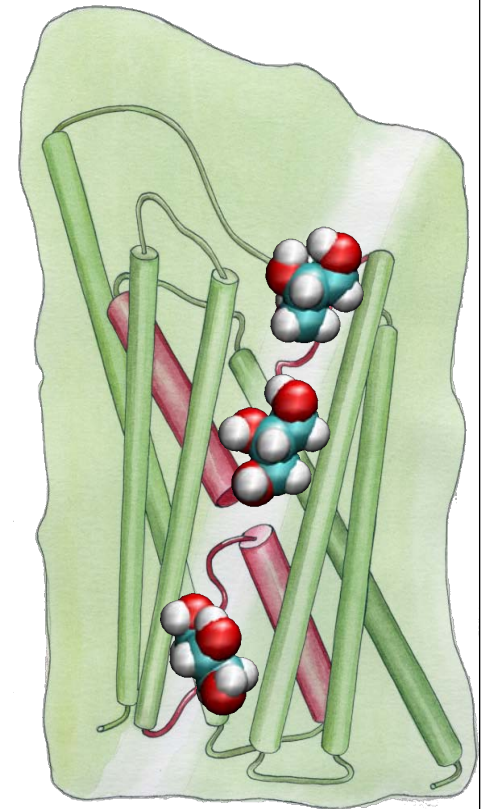
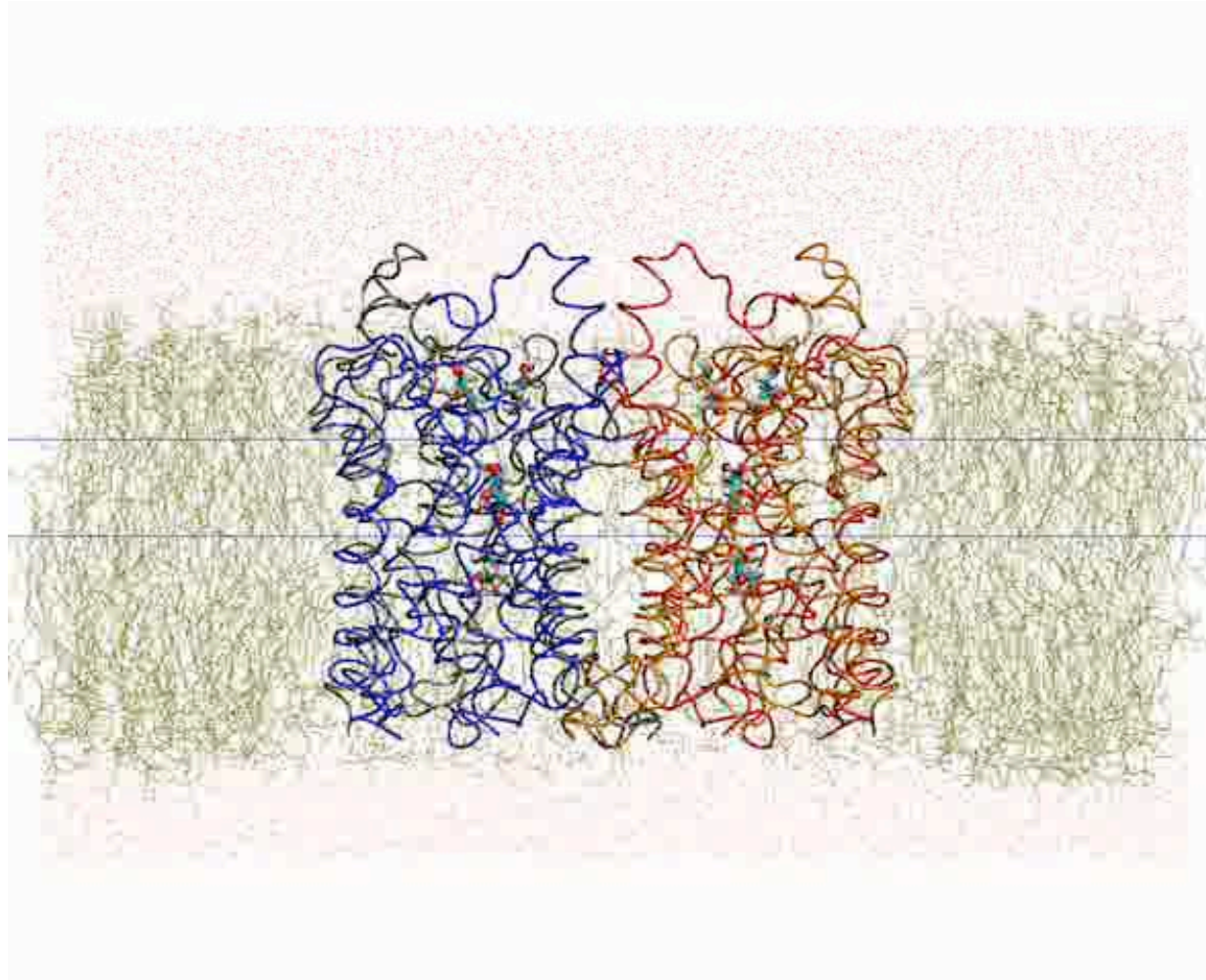
$$p_f: 7.0 \pm 0.9 \times 10^{-14} \text{ cm}^3/\text{s}$$

$$\text{Exp: } 5.4 - 11.7 \times 10^{-14} \text{ cm}^3/\text{s}$$

F. Zhu, E. Tajkhorshid, K. Schulten, *Biophys. J.* 86: 50-57 (2004)

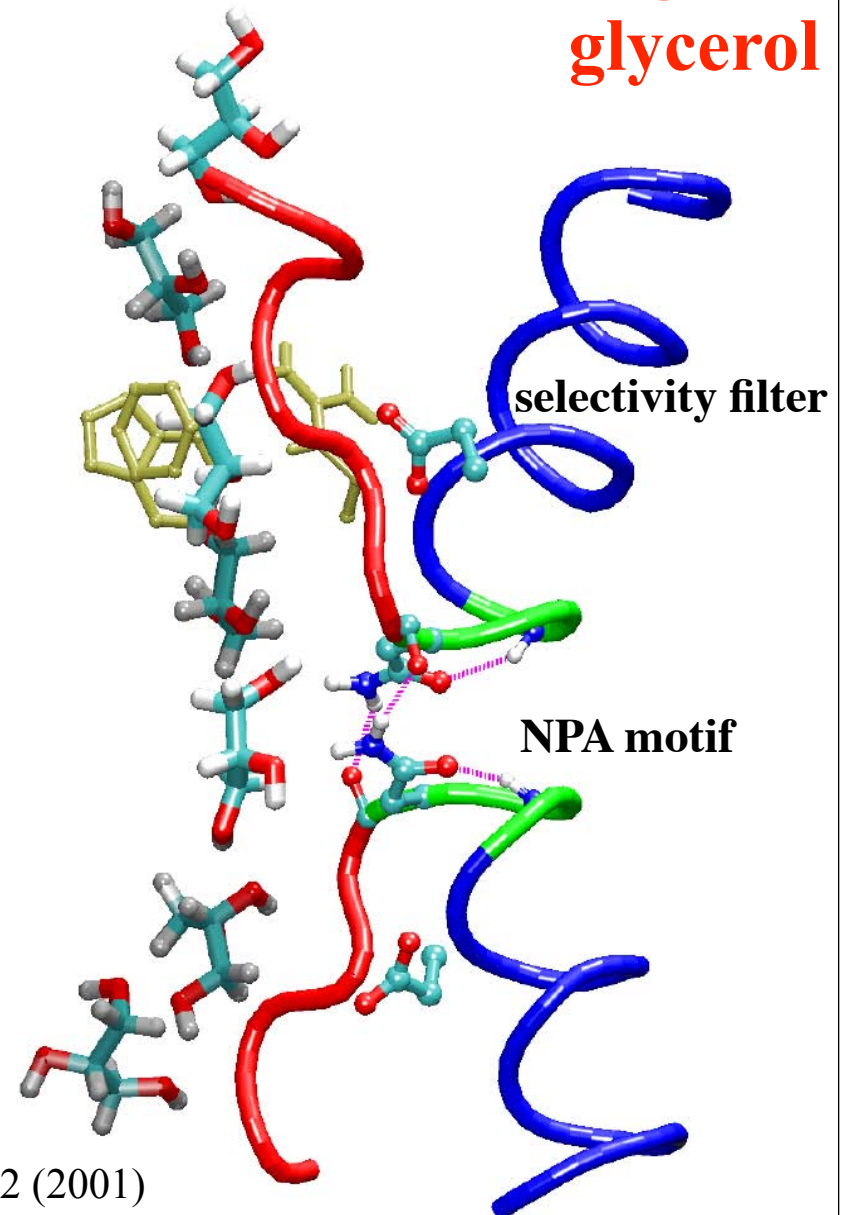
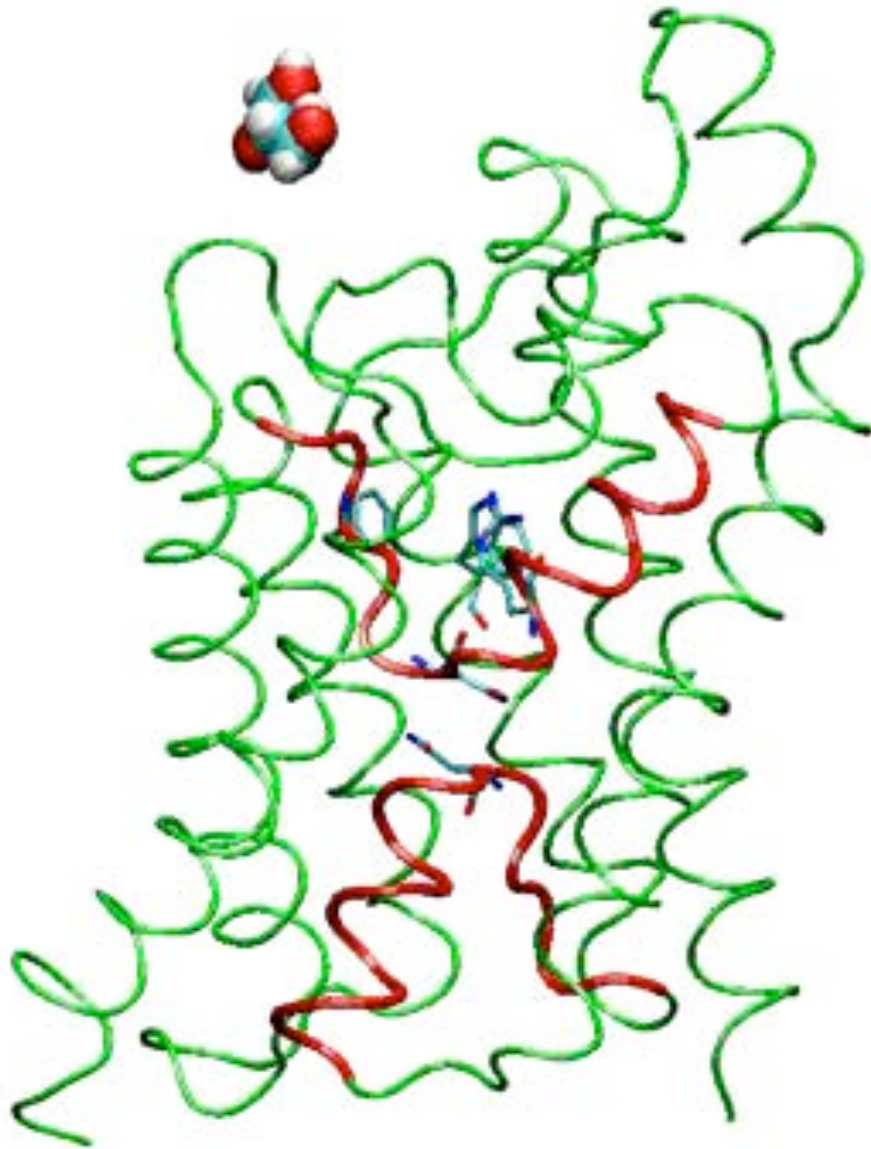
F. Zhu, E. Tajkhorshid, K. Schulten, *Phys. Rev. Lett.* 93: 224501 (2004)

Dynamics of Protein, Lipid, Water System



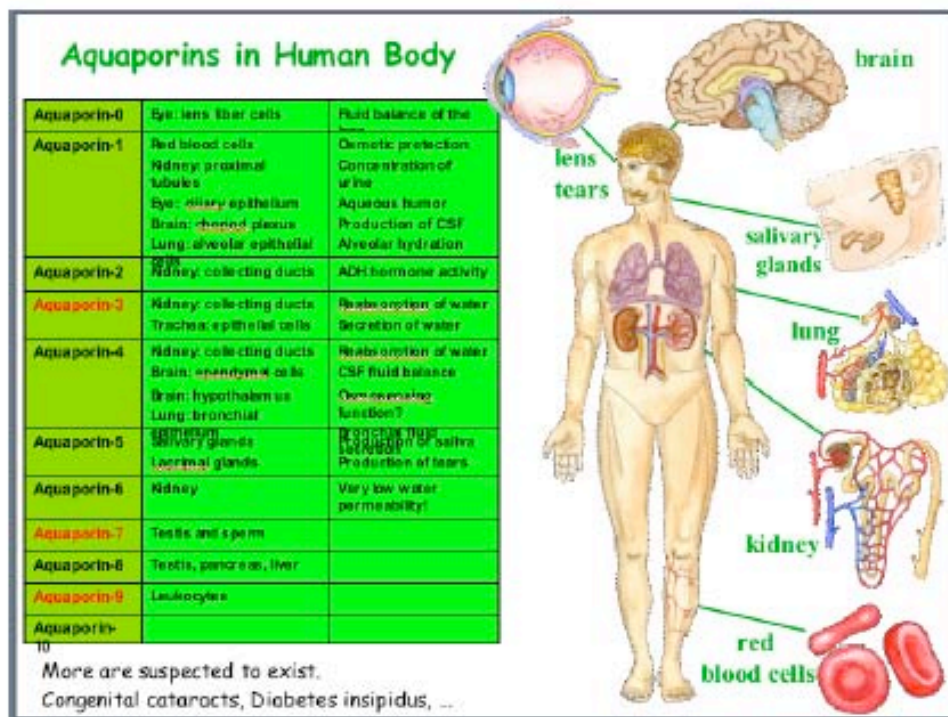
Glycerol Conduction

**Inverted helices guide
glycerol**



Aquaporins

Case study, see at
<http://www.ks.uiuc.edu/Training/CaseStudies/>



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John Eargle

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Brijeet Dhaliwal

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