PAUL SCHERRER INSTITUT PSI

:: :: Paul Scherrer Institute

CMT presentation to LSM

March 8th 2018,

CMT presentation to LSM

Christopher Mudry[1] ($\hbar \neq 0$)
Markus Müller[1] ($\hbar \neq 0$)
Peter Derlet[1] ($\hbar = 0$)
Xavier Deupi[1] ($\hbar = 0$)

[1]Paul Scherrer Institut, Switzerland

PSI, March 8 2018

History of CMT

- Walter Fischer and Hans Rudolf Ott were instrumental in the creation of a condensed matter theory group (CMT) at PSI within the division Festkörperforschung mit Neutronen (FUN) to be modeled on the high-energy theory group at PSI.
- DIRK approved the creation of CMT in 1997 within FUN with four staff positions of which three were already filled by Rudolf Morf, Bernard Delley, and Hans-Benjamin Brown. Christopher Mudry was chosen as a fourth member after an open search in 1999.
- Christopher Mudry replaced Rudolf Morf as group head in 2009.
- Peter Derlet joined CMT in 2009.
- Xavier Deupi joined CMT in 2010.
- Markus Müller joined CMT in 2015.

Mission of CMT

1. To maintain state-of-the-art expertise on the forefront of theoretical research in classical and quantum condensed matter theory.
2. To conduct original, independent, and curiosity-driven research in classical and quantum condensed matter theory.
3. To nurture internal collaboration at PSI, to provide theoretical support to the experimentalists at PSI, and to inspire experiments to test new concepts in classical and quantum condensed matter theory.

Christopher Mudry: Biography

- Born in 1962, raised in Geneva until high-school graduation.
- Physics Diploma from ETHZ with diploma thesis *"Viability of Gluon Annihilation into a Higgs Associated to a Pair of Top Quarks as a Mechanism for detecting the Heavy Higgs in SSC,"* under Prof. C. Schmid and Prof. D. Wyler.
- Obtained in 1994 PhD from UIUC (University of Ilinois at Urbana Champaign) with thesis title *"The Problem of Spin and Charge Separation,"* under Prof. Eduardo Fradkin.
- Postdoctoral position at MIT with Prof. Xiao-Gang Wen: Disorder-induced quantum criticality.
- Postdoctoral position at Harvard with Prof. Bertrand I. Halperin: Quasi-one-dimensional quantum transport.
- As of 1999, staff of CMT at PSI: disordered systems, unconventional superconductivity, frustrated magnetism, graphene, topological insulators, topological order, etc.

Christopher Mudry: Miscellaneous at PSI

- 2000-2016: Initiated and ran the CMT journal club and CMT seminar.
- 2002-2018: Lecture one semester a year, mostly at ETHZ.
- 2003-2018: Supervised 4 PhD students, all co-funded by SNF.
- 2005-2016: Initiated and co-ran the Condensed Matter Colloquium at PSI. Ran the PSI colloquium until 2016.
- 2014-2018 Member of FOKO.

Christopher Mudry: Example I of research interests

PHYSICAL REVIEW X **8**, 011005 (2018)

Multiferroic Magnetic Spirals Induced by Random Magnetic Exchanges

Andrea Scaramucci,[1,2,*] Hiroshi Shinaoka,[3,4,8,†] Maxim V. Mostovoy,[5] Markus Müller,[6,7] Christopher Mudry,[6]
Matthias Troyer,[3,9] and Nicola A. Spaldin[2]

[1]*Laboratory for Scientific Development and Novel Materials, Paul Scherrer Institut, 5235, Villigen PSI, Switzerland*
[2]*Materials Theory, ETH Zurich, CH-8093 Zürich, Switzerland*
[3]*Institute for Theoretical Physics, ETH Zurich, CH-8093 Zürich, Switzerland*
[4]*Department of Physics, University of Fribourg, 1700 Fribourg, Switzerland*
[5]*Zernike Institute for Advanced Materials, University of Groningen, Nijenborgh 4, 9747 AG, Groningen, Netherlands*
[6]*Condensed Matter Theory Group, Paul Scherrer Institute, CH-5232 Villigen PSI, Switzerland*
[7]*The Abdus Salam International Centre for Theoretical Physics, 34151 Trieste, Italy*
[8]*Department of Physics, Saitama University, Saitama 338-8570, Japan*
[9]*Microsoft Research, Redmond, Washington 98052, USA*

Question: What mechanisms can deliver high-temperature multiferroics?

Answer I: Disorder can under certain circumstances!

Answer II: Answer I is relevant to $YBaCuFeO_5$

Christopher Mudry: Example I motivation

PHYSICAL REVIEW B **91**, 064408 (2015)

Incommensurate magnetic structure, Fe/Cu chemical disorder, and magnetic interactions in the high-temperature multiferroic $YBaCuFeO_5$

M. Morin,[1] A. Scaramucci,[1,2] M. Bartkowiak,[1] E. Pomjakushina,[1] G. Deng,[1,3] D. Sheptyakov,[4] L. Keller,[4] J. Rodriguez-Carvajal,[5] N. A. Spaldin,[2] M. Kenzelmann,[1] K. Conder,[1] and M. Medarde[1,*]

[1]*Laboratory for Developments and Methods, Paul Scherrer Institut, 5232 Villigen PSI, Switzerland*
[2]*Materials Theory, ETH Zürich, 8093 Zürich, Switzerland*
[3]*Bragg Institute, ANSTO, New Illawarra Road, Lucas Height, New South Wales 2233, Australia*
[4]*Laboratory for Neutron Scattering and Imaging, Paul Scherrer Institut, 5232 Villigen PSI, Switzerland*
[5]*Institut Laue Langevin, BP 156, 6, rue Jules Horowitz, 38042 Grenoble Cedex 9, France*

(Received 22 December 2014; published 6 February 2015)

nature COMMUNICATIONS

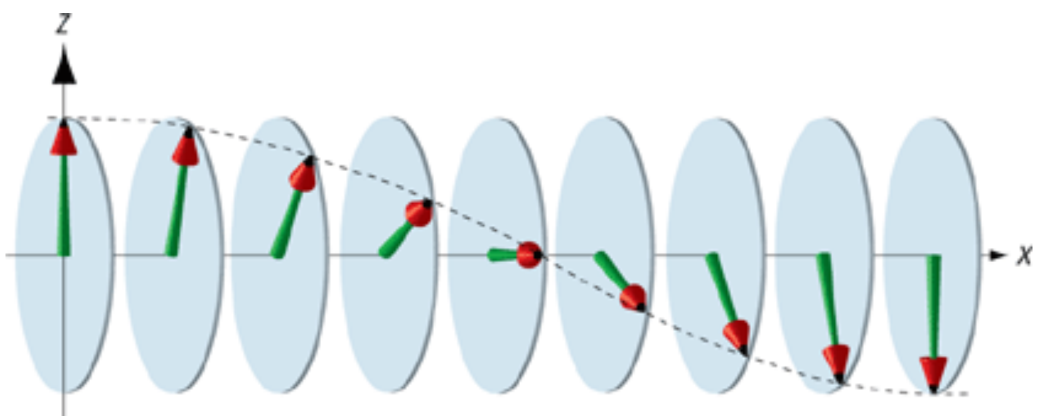
ARTICLE

Received 21 Jul 2016 | Accepted 31 Oct 2016 | Published 16 Dec 2016 DOI: 10.1038/ncomms13758 OPEN

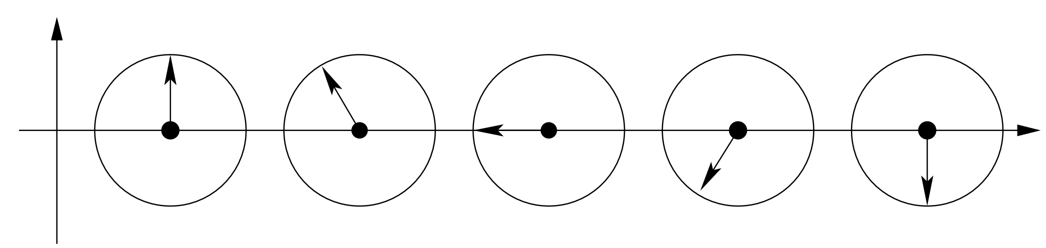
Tuning magnetic spirals beyond room temperature with chemical disorder

Mickaël Morin[1], Emmanuel Canévet[2], Adrien Raynaud[1], Marek Bartkowiak[1], Denis Sheptyakov[2], Voraksmy Ban[3], Michel Kenzelmann[1], Ekaterina Pomjakushina[1], Kazimierz Conder[1] & Marisa Medarde[1]

(a)



(b)



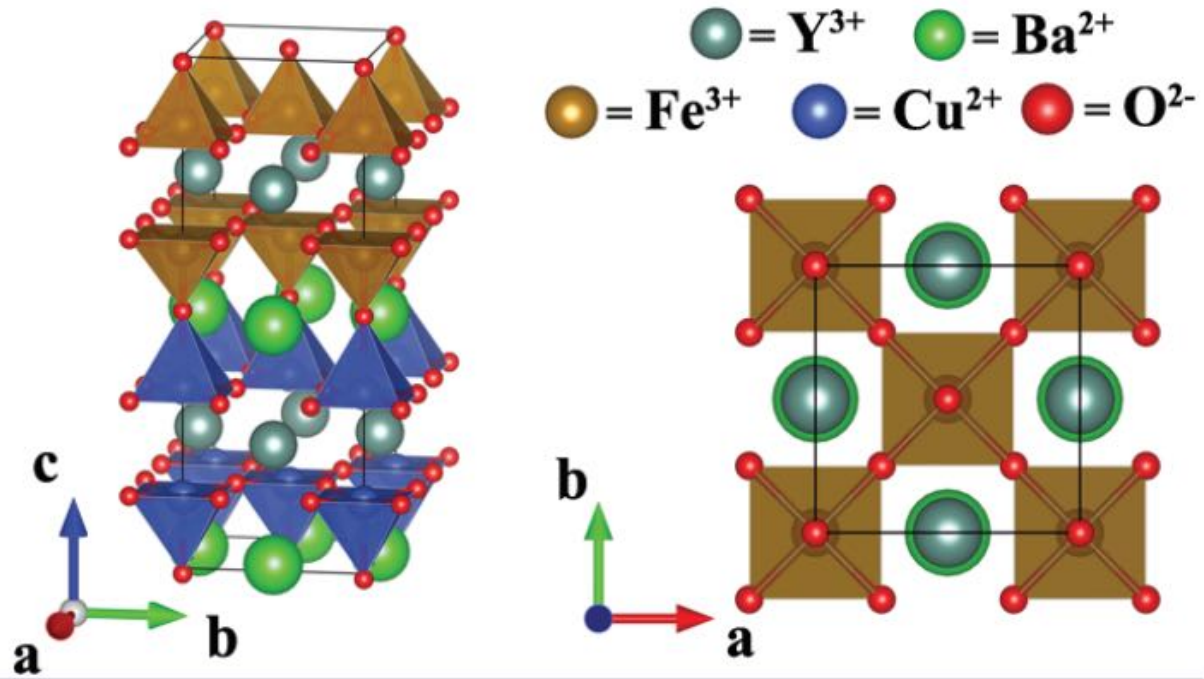
Examples of helical order (a) Spiral order (b) Cycloidal order.
Helical order breaks inversion symmetry, a prerequisite for multiferroelectricity.

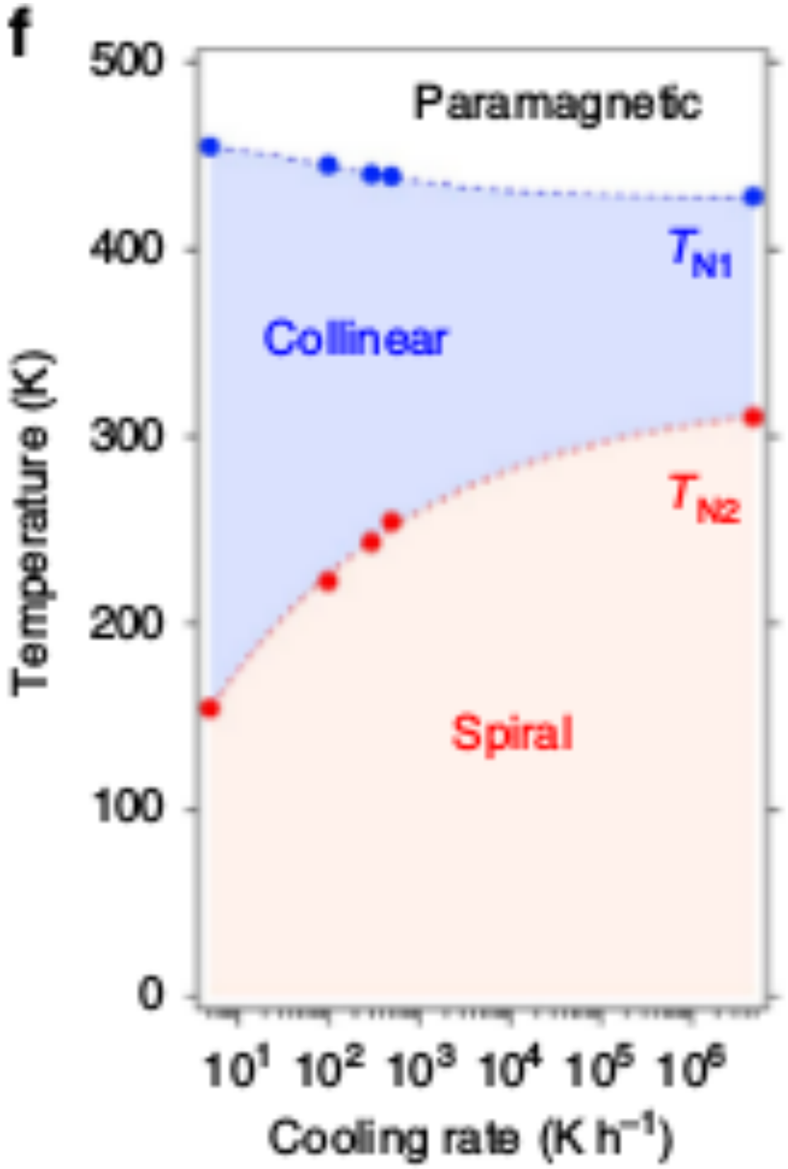
Christopher Mudry: Example I history of $YBaCuFeO_5$

1988 Er-Rakho, Michel, Lacorre, and Riveau discovered $YBaCuFeO_5$.

2015 Morin, Scaramucci, Bartkowiak, Pomjakushina, Deng, Sheptyakov, Keller, Rodriguez-Carvajal, Spaldin, Kenzelmann, Conder, and Medarde resolved a long-standing controversy regarding the crystalline structure of $YBaCuFeO_5$. They also identified the incommensurate magnetic order as being an antiferromagnetic spiral which they characterized in a quantititative way.

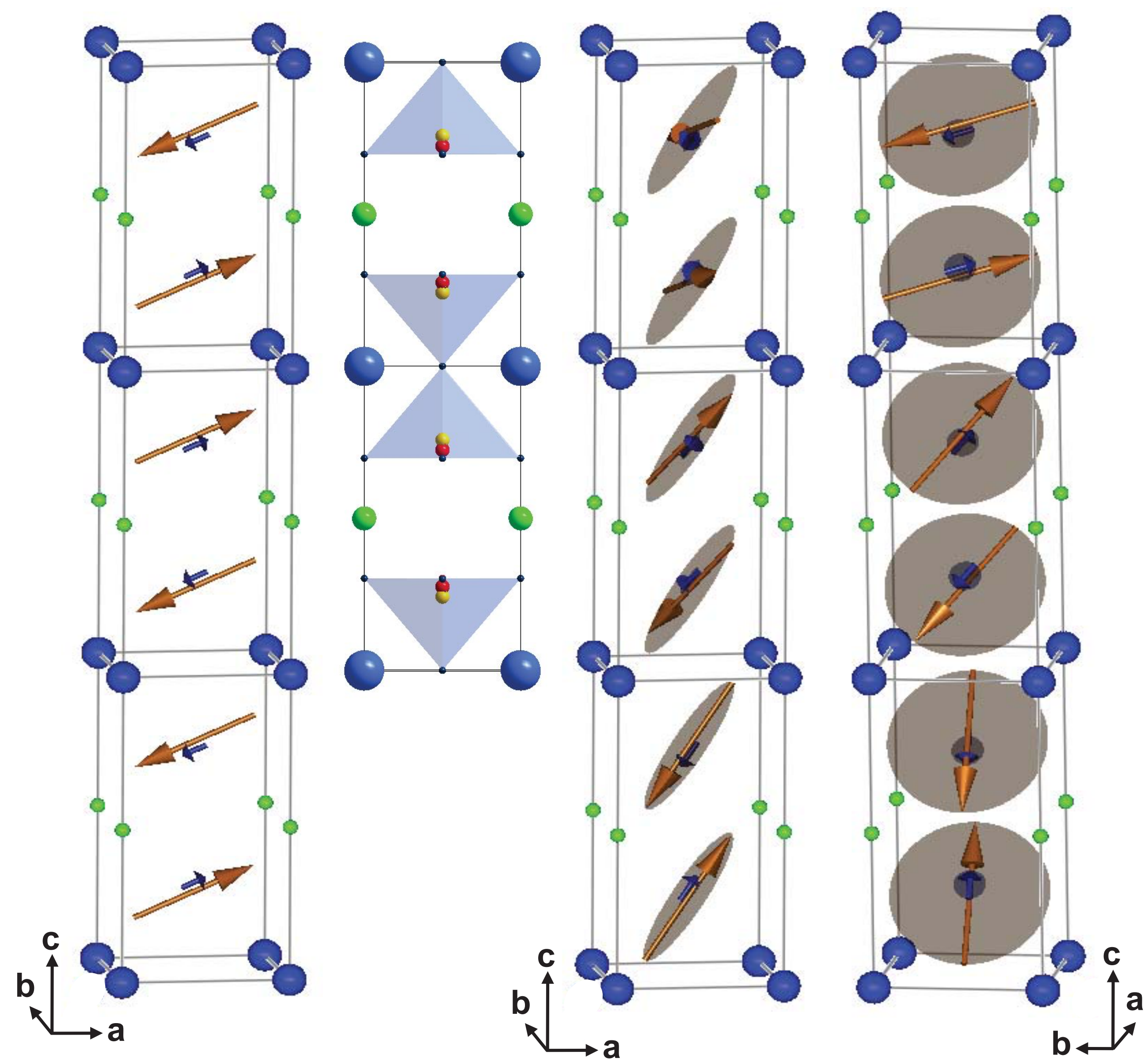
2016 Morin, Canévet, Raynaud, Bartkowiak, Sheptyakov, Ban, Kenzelmann, Pomjakushina, Conder, and Medarde increased the transition temperature to the spiral phase up to 310 K through a controlled manipulation of the Fe/Cu chemical disorder.





a) 230 K

b) 1.5 K



$\mathbf{k}_c = (½ \, ½ \, ½)$

$\mathbf{k}_i = (½ \, ½ \, ½ \pm q)$

Christopher Mudry: Example I who did what

Scaramucci (at ETHZ) used DFT to model (i) the energy cost for defectuous corner sharing square pyramids, i.e., instead of $\mathrm{CuO_5} - \mathrm{FeO_5}$ consider $\mathrm{CuO_5} - \mathrm{CuO_5}$ or $\mathrm{FeO_5} - \mathrm{FeO_5}$:

$$\rightarrow J_{\boldsymbol{r},\boldsymbol{r}'} \in \left\{ J_{||}, J'_{\perp}, J_{\perp}, J_{\mathrm{imp}} \right\} \tag{1a}$$

and (ii) the single-ion anisotropy Δ entering the proposed classical spin Hamiltonian

$$H := H_{O(3)} + H_{\mathrm{DM}} + H_{\mathrm{SIA}}, \tag{1b}$$

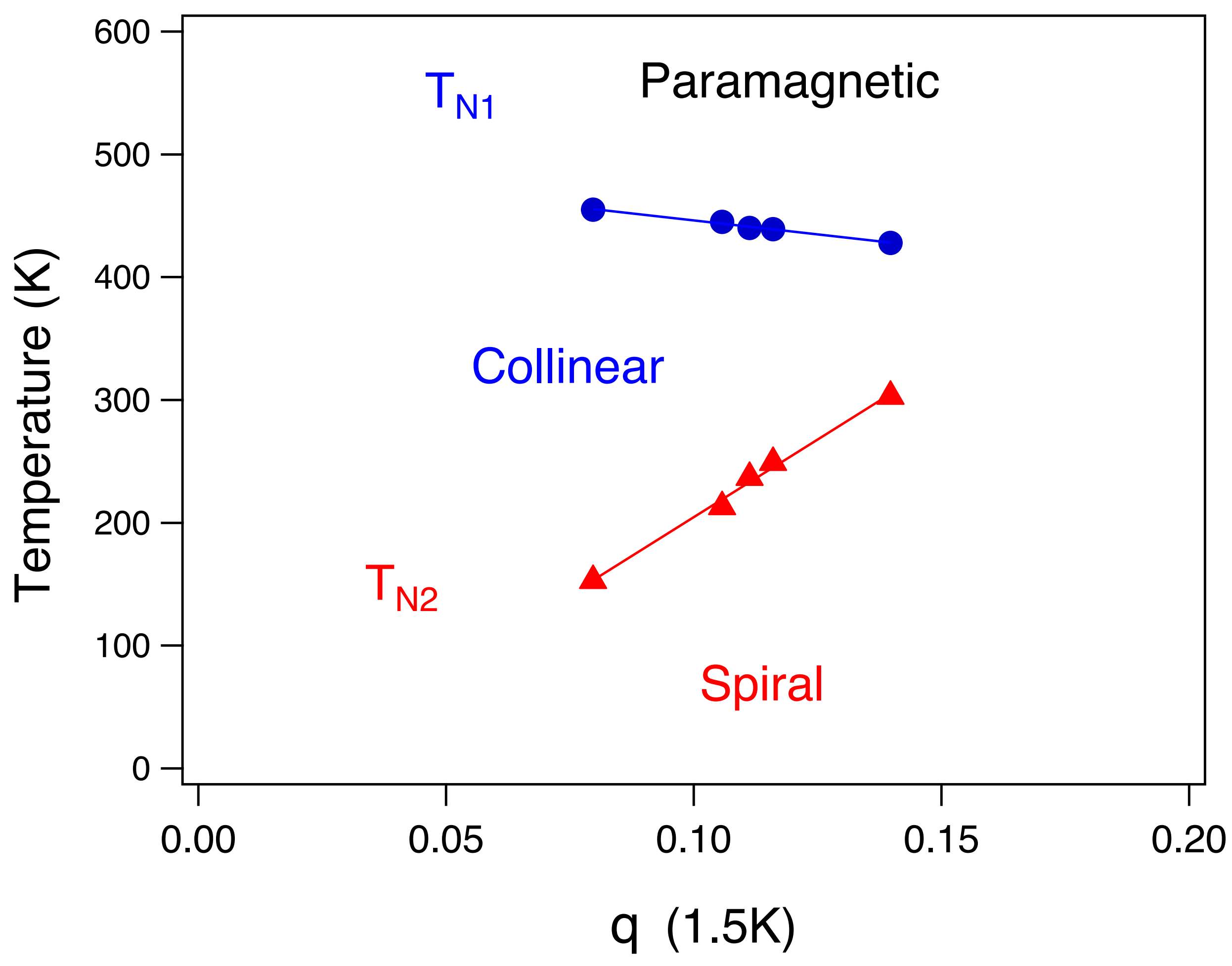
$$H_{O(3)} := -\frac{1}{2} \sum_{\boldsymbol{r},\boldsymbol{r}'} J_{\boldsymbol{r},\boldsymbol{r}'} \, \boldsymbol{S}_{\boldsymbol{r}} \cdot \boldsymbol{S}_{\boldsymbol{r}'}, \tag{1c}$$

$$H_{\mathrm{DM}} := \frac{1}{2} \sum_{\boldsymbol{r},\boldsymbol{r}'} \boldsymbol{D}_{\boldsymbol{r}\boldsymbol{r}'} \cdot \left(\boldsymbol{S}_{\boldsymbol{r}} \wedge \boldsymbol{S}_{\boldsymbol{r}'} \right), \tag{1d}$$

$$H_{\mathrm{SIA}} := \frac{\Delta}{2} \sum_{\boldsymbol{r}} (\boldsymbol{S}_{\boldsymbol{r}} \cdot \hat{\boldsymbol{c}})^2. \tag{1e}$$

Hiroshi Shinaoka performed classical Monte-Carlo simulations of $H_{O(3)} + H_{\mathrm{SIA}}$ and established a transition to antiferromagnetic order followed by a transition to spiral order upon decreasing temperature.

Scaramucci, Mudry, and Müller (at PSI) proposed an approximation to the classical Hamiltonian (1) from which it was possible to deduce analytically that the ordering temperature for the spiral phase is proportional to the impurity concentration n_{imp} of the frustrated Heisenberg bonds. This theoretical prediction has been verified by Medarde et al. at PSI (manuscript in preparation).

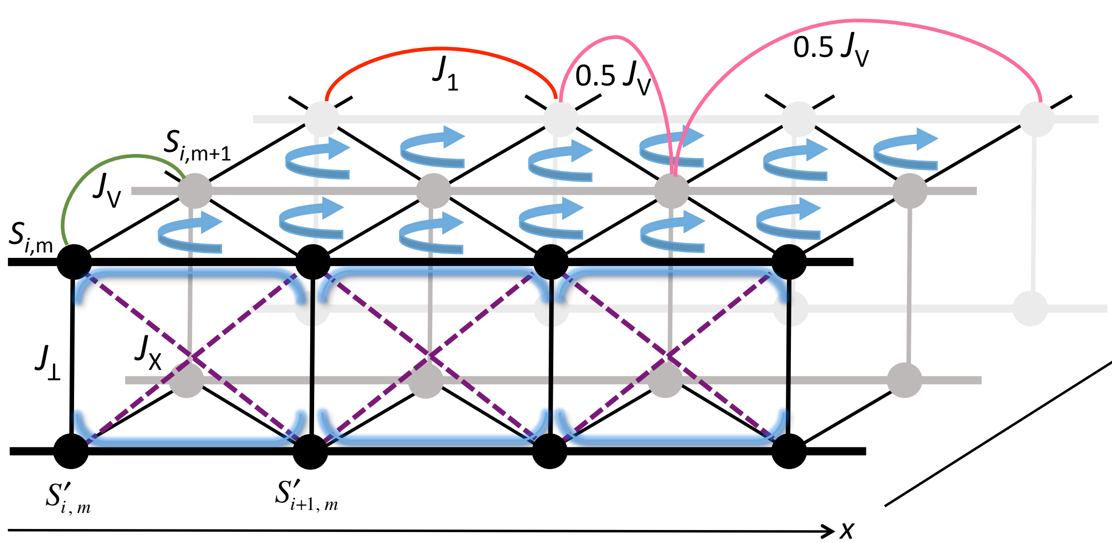


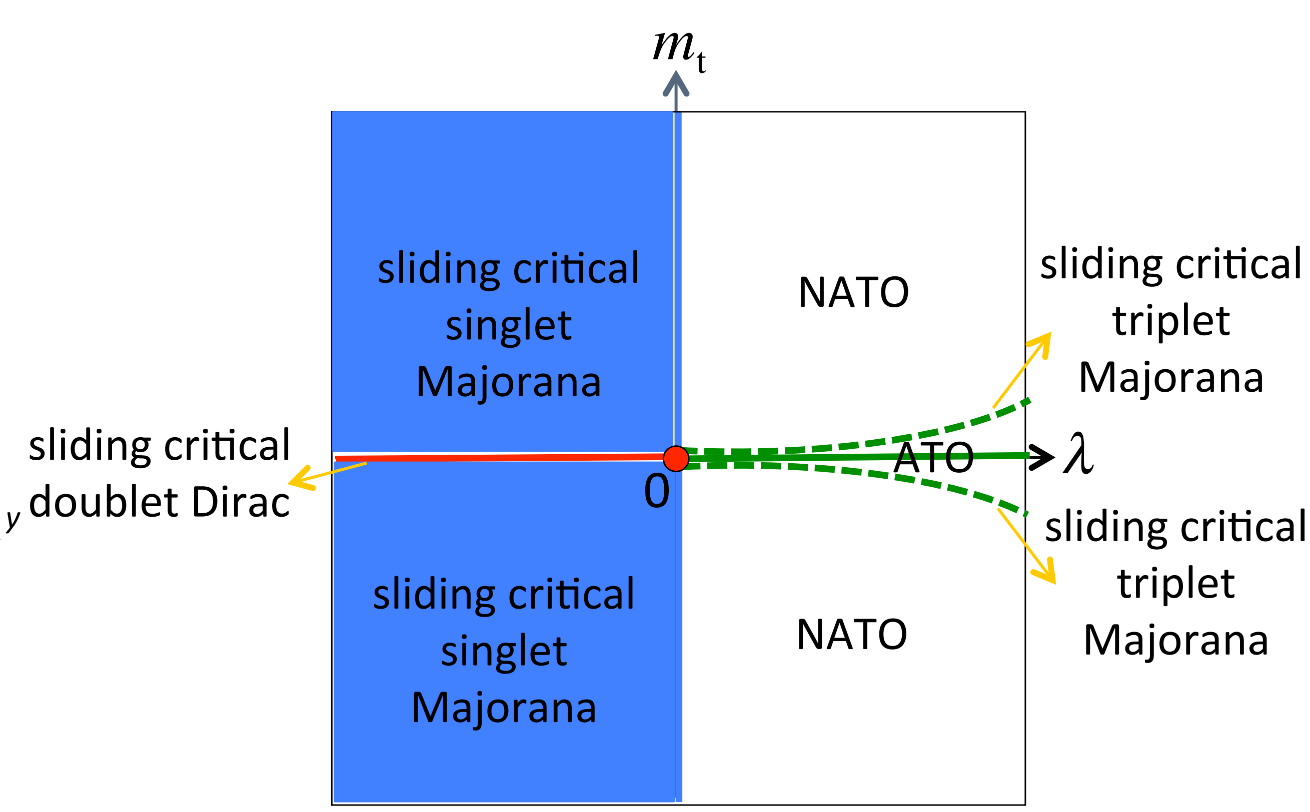
Christopher Mudry: Example II of research interests

PHYSICAL REVIEW B 96, 224420 (2017)

Model of chiral spin liquids with Abelian and non-Abelian topological phases

Jyong-Hao Chen,[1] Christopher Mudry,[1] Claudio Chamon,[2] and A. M. Tsvelik[3]
[1]*Condensed Matter Theory Group, Paul Scherrer Institute, CH-5232 Villigen PSI, Switzerland*
[2]*Department of Physics, Boston University, Boston, Massachusetts 02215, USA*
[3]*Condensed Matter Physics and Materials Science Division, Brookhaven National Laboratory, Upton, New York 11973-5000, USA*
(Received 5 September 2017; revised manuscript received 3 November 2017; published 15 December 2017)





Markus Müller - Brief Biography

- Born 1976, grown up in Münchenstein BL
- Diploma in Physics, **ETH Zürich**, 2000
  "Pinning of disordered elastic manifolds"
- PhD: **LPTMS, Paris-Sud, Orsay**, 2003
  "Folding of heteropolymers" (classical stat mech, glasses)
- Postdoc: **Rutgers**, 2003-2006 (quantum glasses/localization)
  Harvard, 2006-2008 (quantum criticality, quantum transport, hydrodynamics of electrons)
- SNF Junior Professorship, **Geneva** 2008-2009
- Staff Scientist at **ICTP Trieste** 2009-2016
- @ **CMT/PSI** since 2015:
  - Organization of PSI, CM Colloquia, CMT seminar
  - Board member of Quantum Technology Collaboration
  - Effort toward non-equilibrium, driven systems, quantum control (NCCR?)

Exploit SwissFEL
Use it in new ways

Research activity and interests

Fields of research :

- Complexity and non-ergodicity in disordered & interacting systems:
  - Glasses, amorphous systems
  - (Many-body) localization:

    Non-thermalization despite interactions
  - Disordered bosons/fermions

- Quantum and classical magnetism;

  frustrated magnets

- Quantum transport

Research activity and interests

Fields of research :

- Complexity and non-ergodicity in disordered & interacting systems:
  - Glasses, amorphous systems
  - (Many-body) localization:
    Non-thermalization despite interactions
  - Disordered bosons/fermions

- Quantum and classical magnetism;
  frustrated magnets

- Quantum transport

Example I

Example II

PAUL SCHERRER INSTITUT PSI

Example I: Quantum coherence and quantum computation in random magnets

Hole burning and magnetic q-bits in rare earth magnets:

Current SNF project:

Joint experiment (Adrian Beckert) + theory (Manuel Grimm)

Based on long-standing, mysterious experiments

(G. Aeppli & T. Rosenbaum et al., 2002++)

1) Explaining mysterious quantum coherence in $LiYHoF_4$

Further goals:

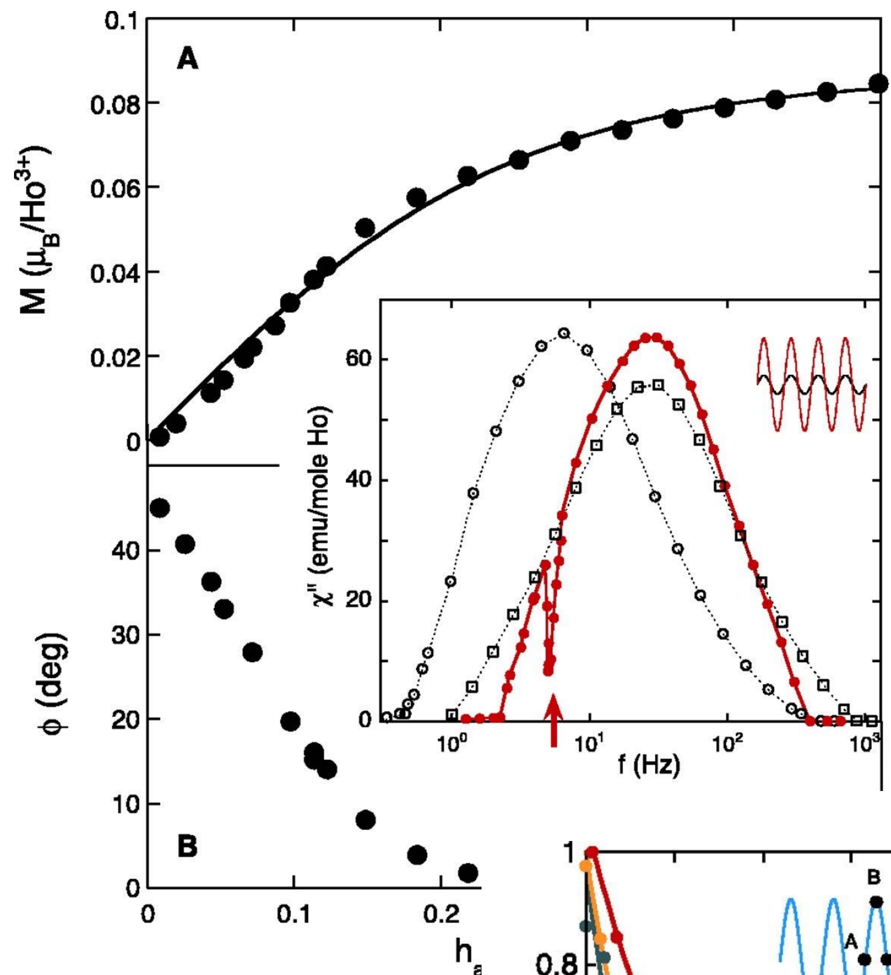
2) Quantum computing scheme based on
- nuclear spins as memory qubits
- rare earth electronic spins as working qubits

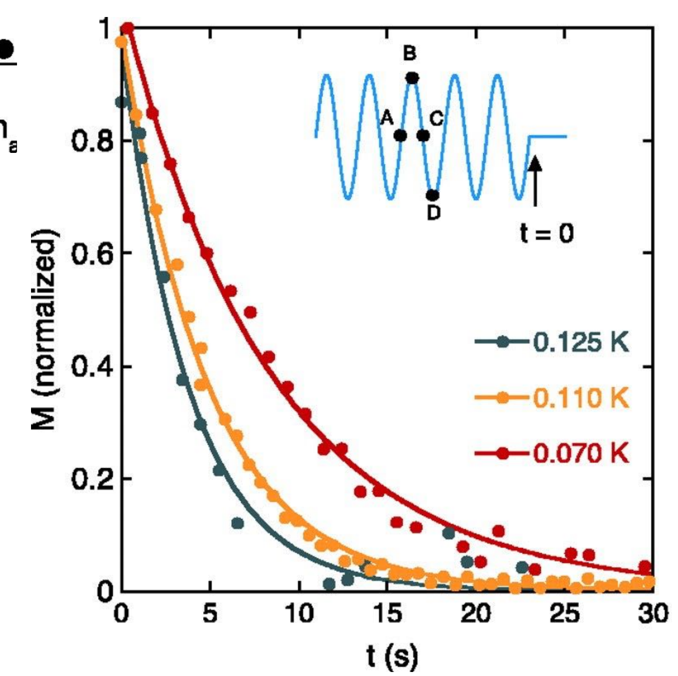
3) Induce magnetic order by driving

Hole burning at low ω in AC susceptibility

Non-linear pumping at low ω saturates absorption ("a sharp hole is burnt")!

Afterwards: Persistent ringing!





→ Coherent oscillators at
ultra-low frequencies O(10Hz) << T ???

S. Ghosh et al. "Coherent spin oscillations in a disordered magnet.," *Science*, vol. 296, no. 5576, pp. 2195–2198, 2002.

Hole burning at low ω in AC susceptibility

Lots of theoretical reasoning and conclusion by elimination:

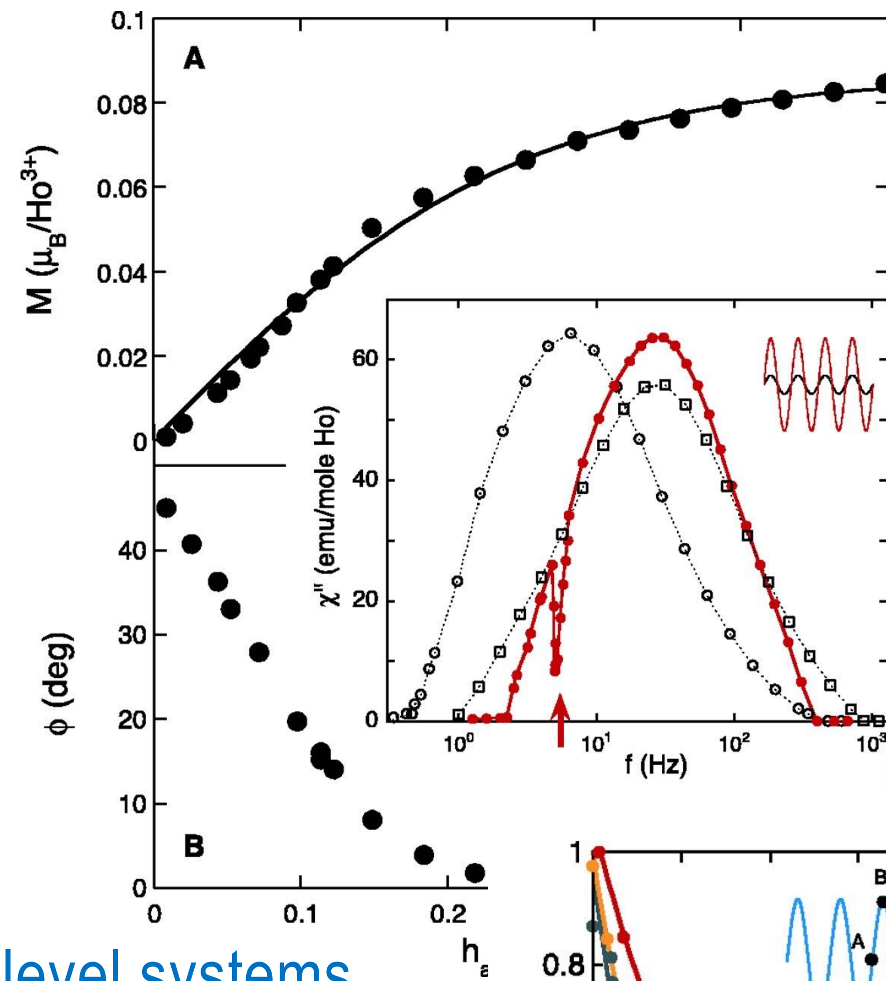
Coherence **cannot** be due to usual suspects: Ho!

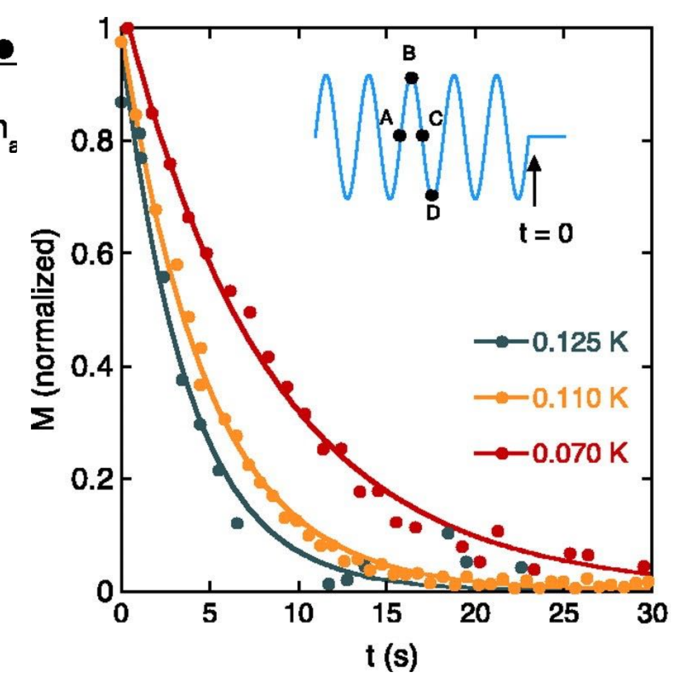
But: Nuclear spins, polarizing paramagnetic electronic spins:

→ Very low frequency el-nuclear two-level systems

→ Frozen moments stabilize themselves by weak polarization of environment.

→ Plan: build on electro-nuclear coupling to make and entangle qubits





S. Ghosh et al. "Coherent spin oscillations in a disordered magnet.," *Science*, vol. 296, no. 5576, pp. 2195–2198, 2002.

PAUL SCHERRER INSTITUT PSI

Example II: Off-equilibrium electrons

Electronic hydrodynamics: driven quantum fluids

Collision-dominated transport in electronic systems

(MM, L. Fritz, J. Schmalian, S. Sachdev 2008/9)

→ **Flow of quantum fluids? Electron hydrodynamics?**

Yes, if:

1) Electron-electron interactions are marginal:

→ Fermi liquid, with strong coupling down to low T!

2) Momentum is well conserved (not lost to lattice!)

Theoretical predictions confirmed in graphene, and in other Dirac/Weyl matter!

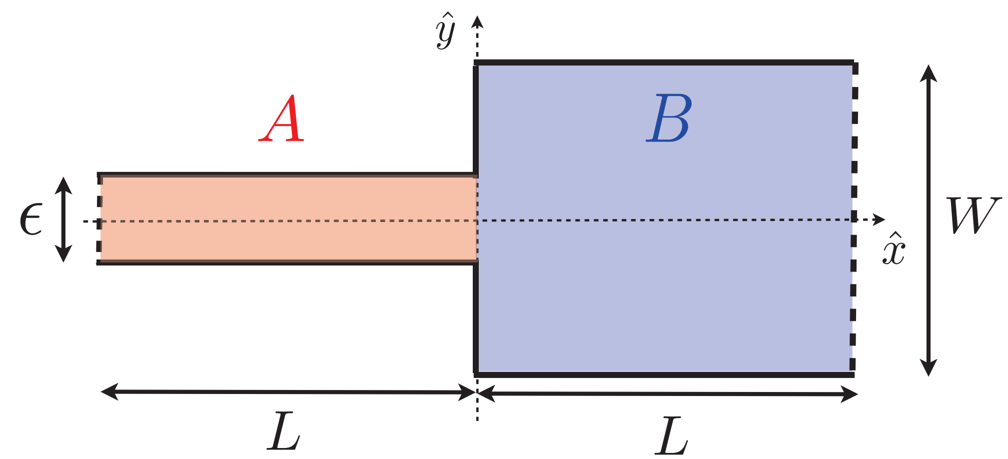
→ Hydrodynamics of a relativistic plasma

Example II: Off-equilibrium electrons

M. Beria, Y. Iqbal, M. DiVentra, MM PRA ***88****, 043611 (2013)*

Steady state of flows in **non-interacting** driven fermions?

Let free fermions stream out from suddenly opened a constriction, $\epsilon \sim \lambda_F$

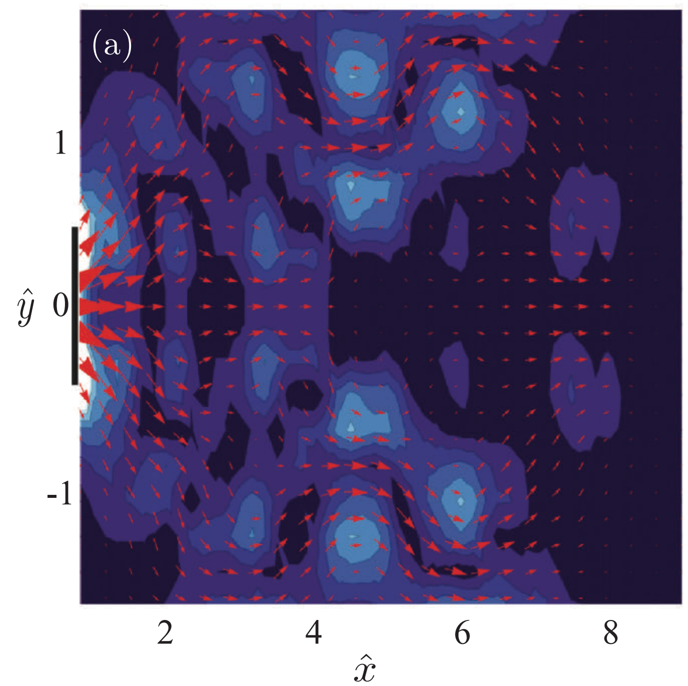


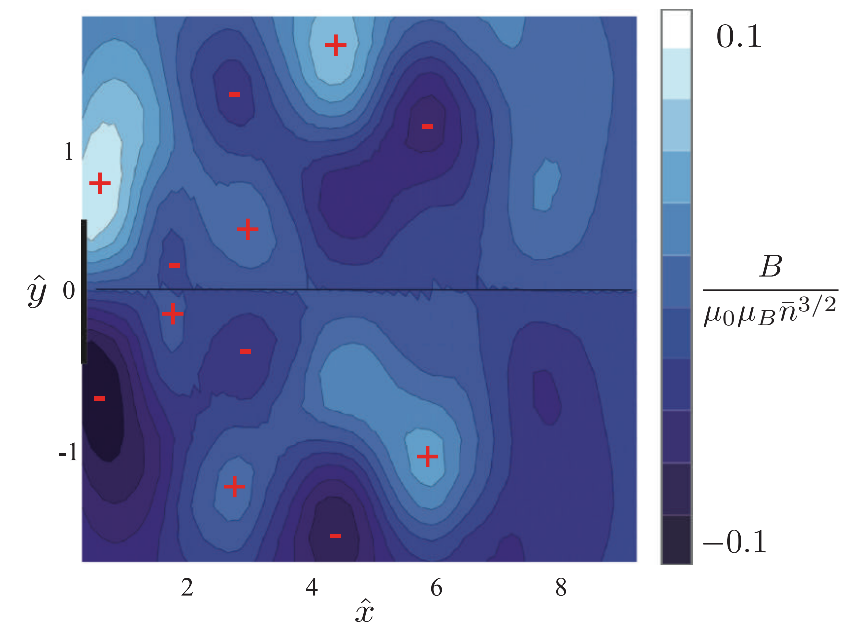
Steady state establishes over intermediate times!

Non-interacting fermions: Interference patterns in driven fermions

*M. Beria, Y. Iqbal, M. DiVentra, MM PRA **88**, 043611 (2013)*

Magnetic field in the steady state?





Low density: $n = 1.1/\epsilon^2$ non-trivial flow!

Current (**j**) and vorticity curl(**j**) in the steady state

Magnetic fields from current distribution:

Staggered field pattern, with measurable magnitude:

$$B_z \sim \left(\frac{V}{E_F}\right) \mu_0 \mu_B k_F^3 \sim 0.1\text{T} \left(\frac{V}{E_F}\right) (k_F \text{nm})^3$$

Non-interacting fermions: Interference patterns in driven fermions

PSI Fellow M. Schütt, MM in progress

Steady state patterns

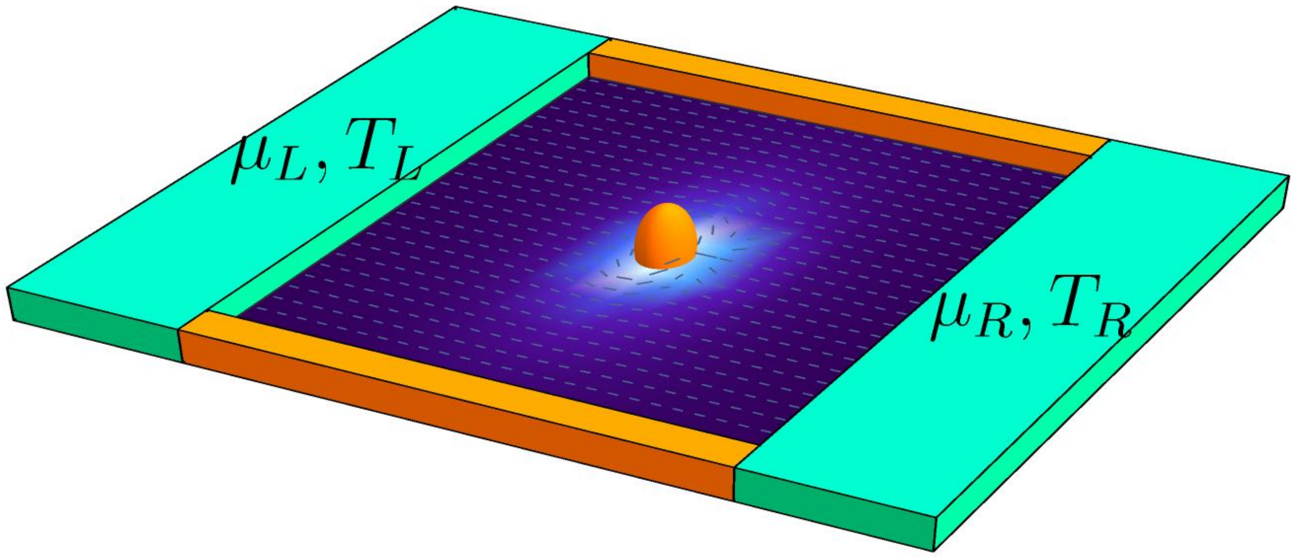
More analytical insight?

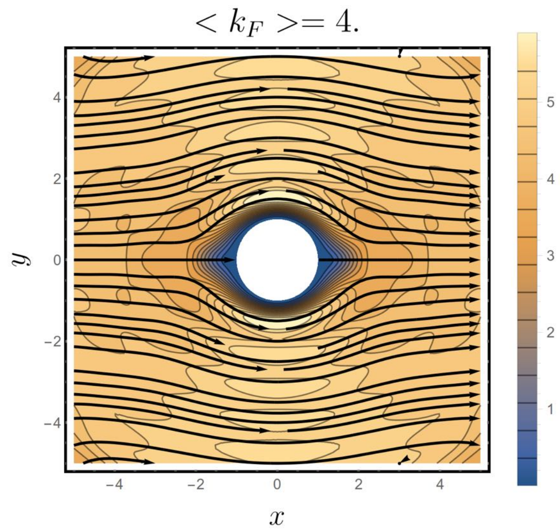
Non-interacting fermions: Interference patterns in driven fermions

PSI Fellow M. Schütt, MM in progress

Steady state patterns

I. Construct steady state by filling left- and right inflowing scattering states up to $V_{L/R}$





Flow of Fermi gas around the obstacle

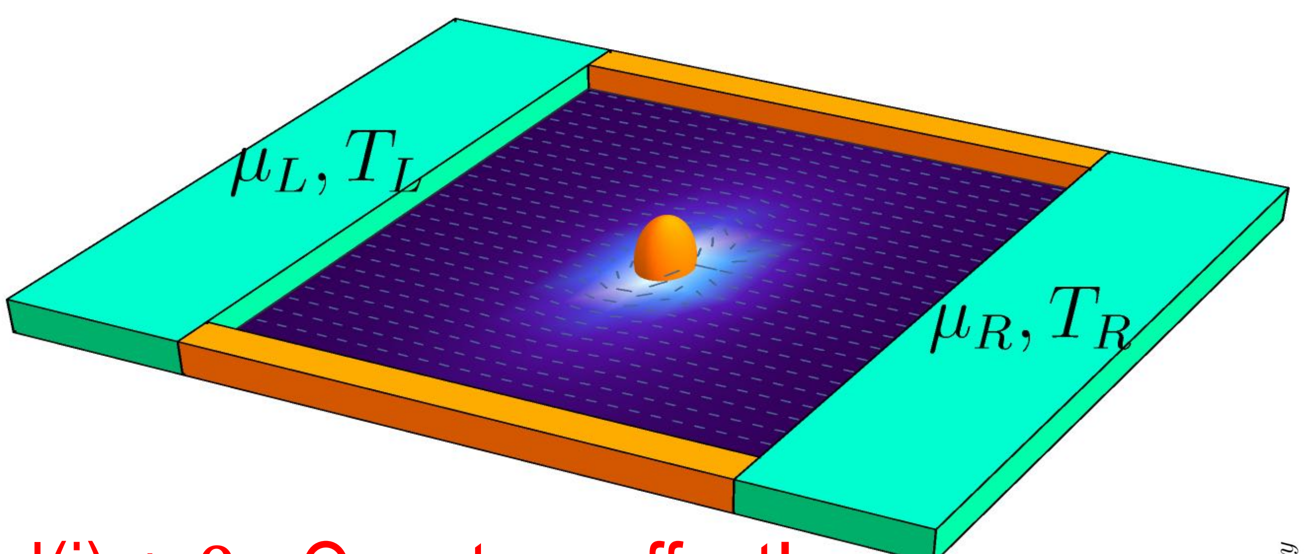
PAUL SCHERRER INSTITUT

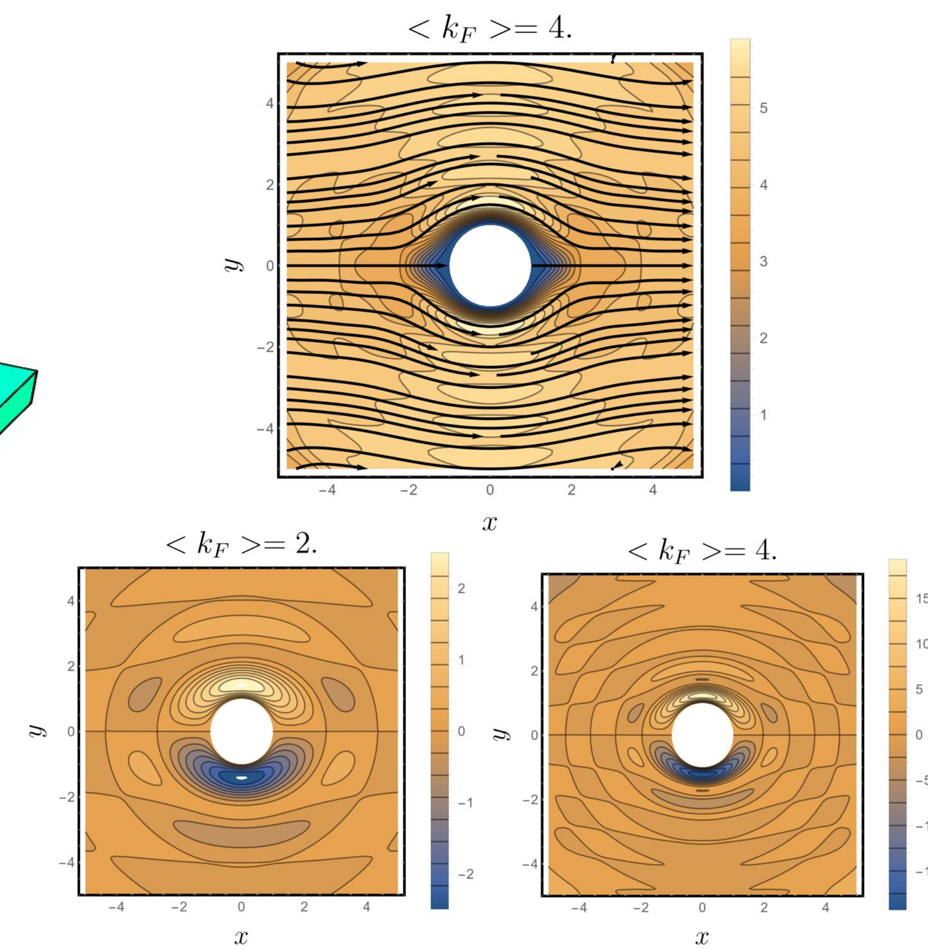
Non-interacting fermions: Interference patterns in driven fermions

PSI Fellow M. Schütt, MM in progress

Steady state patterns

I. Construct steady state by filling left- and right inflowing scattering states up to $V_{L/R}$





curl(j)$\neq$ 0: Quantum effect!

Non-eq Friedel oscillations

Analyt. description of non-eq steady state!

Non-interacting fermions: Interference patterns in driven fermions

PSI Fellow M. Schütt, MM in progress

Steady state patterns

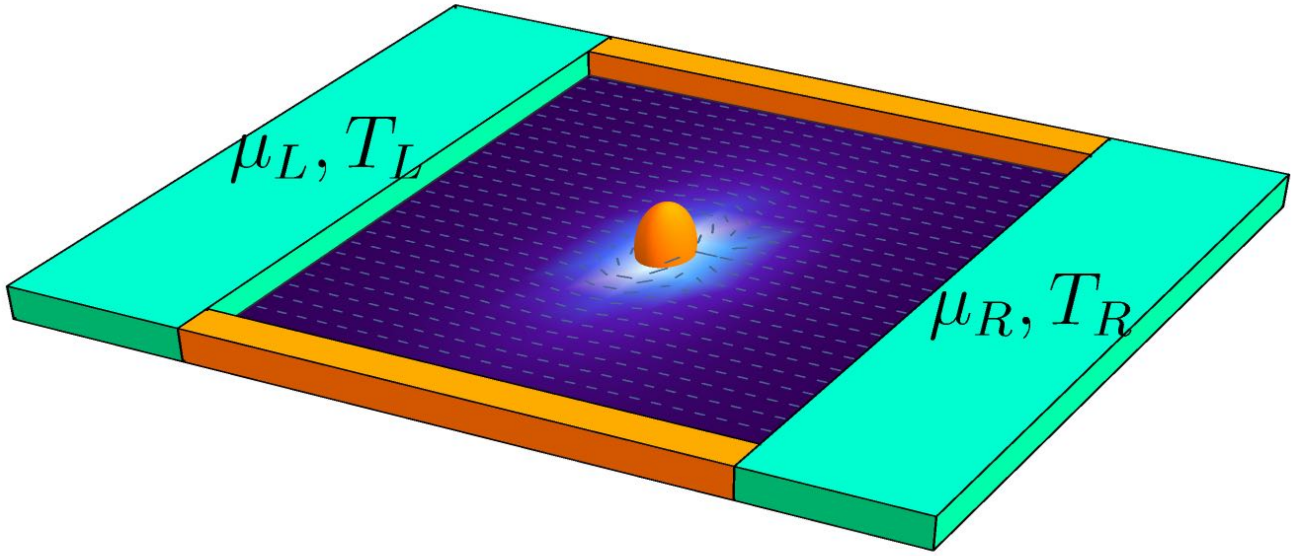
Next steps:

II. Add interactions (Hartree-Fock + beyond)

III. Analyze instabilities → Reynolds criterion?

IV. Relate to hydrodynamics:

Quantum traces, quantum turbulence?



Peter Derlet, born in 1968, Melbourne, Australia

Academic history

1990 – Honours degree in theoretical physics
1994 – PhD. in physics
1996 – Diploma in education

} Monash University Australia

Professional history

1995-97 – Post-doc, Monash university, Australia
1997-00 – Post-doc, NTNU, Norway
2000-09 – PSI, Materials science and simulation group
2009- – PSI, Condensed matter theory group

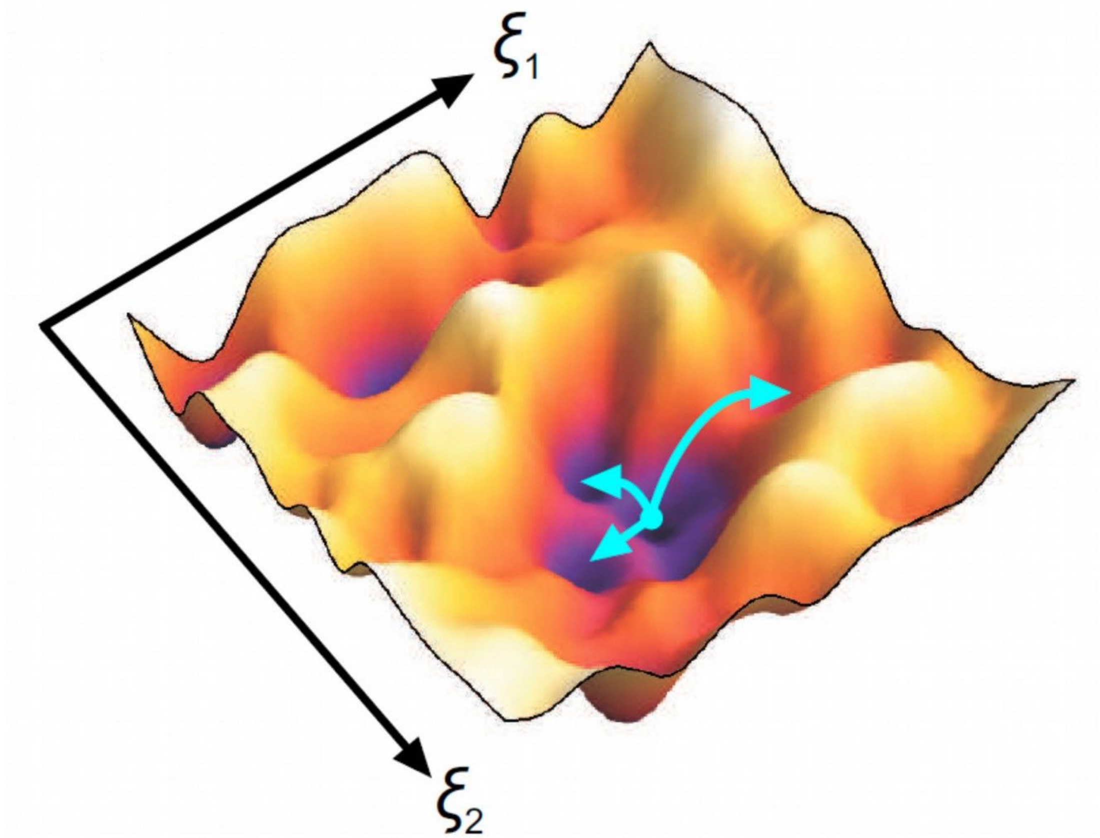
Teaching activities

2015- – lecturer @ ETHZ (undergraduate course)
2014- – lecturer @ EPFL (masters course)

My activities & approach

Interests

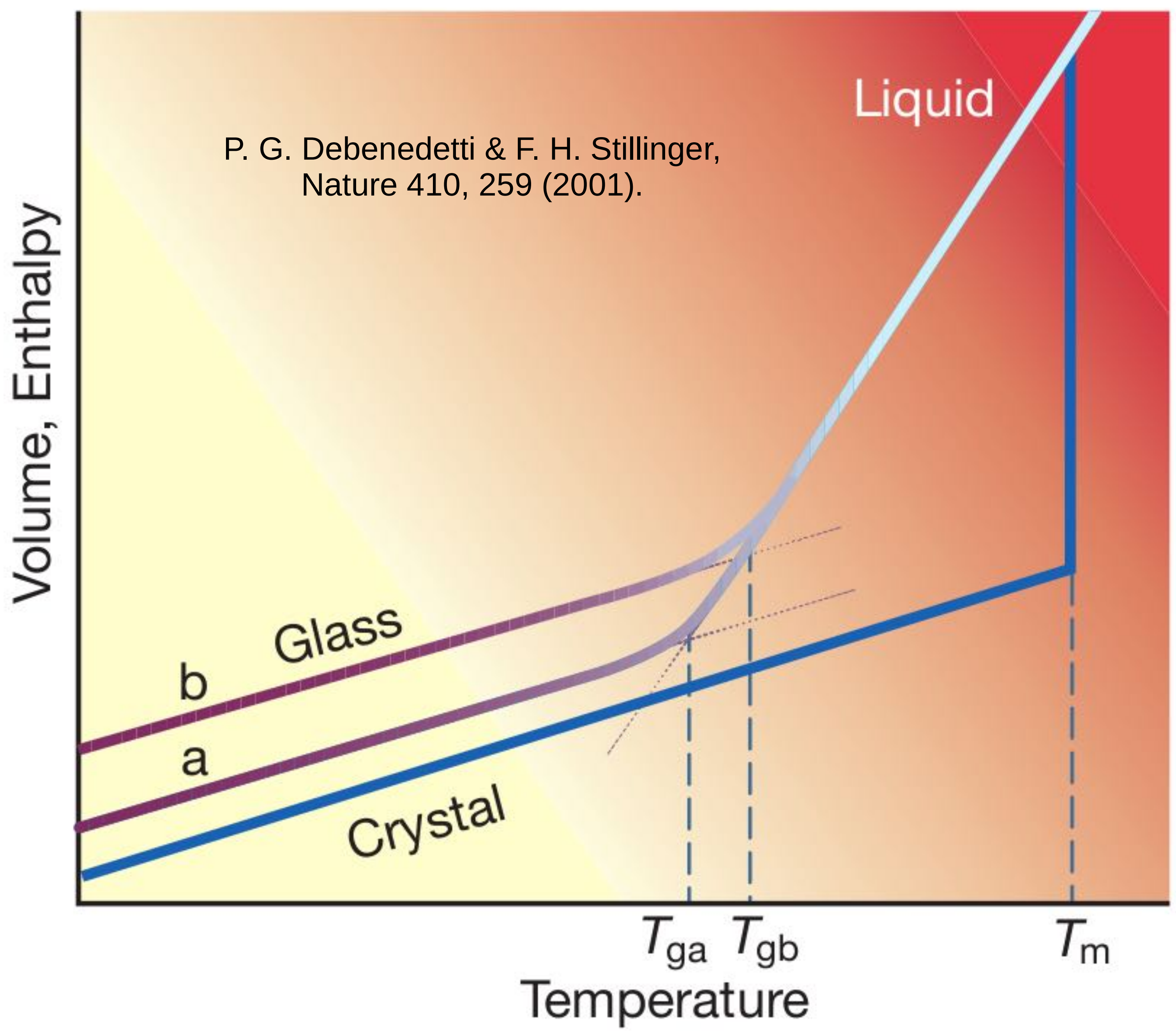
- Micro-plasticity in strongly disordered systems
  - Bulk metallic glasses – local structural frustration
  - Work hardened crystalline metals – dislocation networks
- Classical frustrated magnetism – spin ice physics
  - 2D – artificial spin systems
  - 3D – rare earth pyrochlores



Methodology

- Molecular dynamics
- Dislocation dynamics
- PEL exploration algorithms
- Kinetic and ensemble monte carlo
- Classical magnetization statistics & dynamics
- Statistical models of thermally activated plasticity

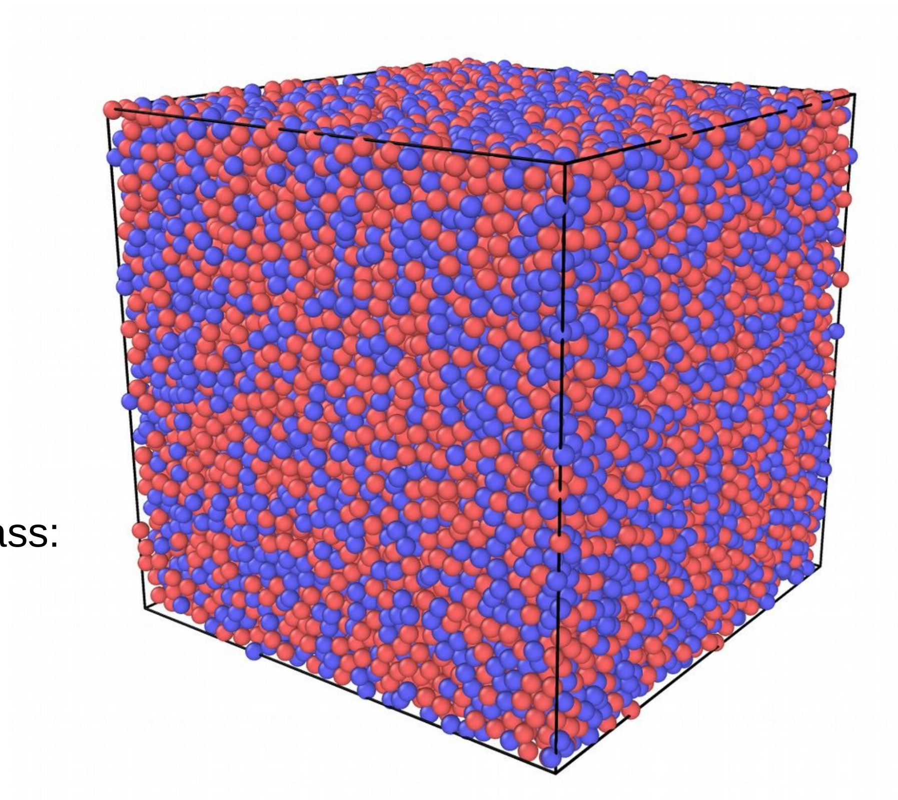
Structural glasses – the amorphous solid



P. G. Debenedetti & F. H. Stillinger,
Nature 410, 259 (2001).

Bulk metallic glasses – Alloys with atoms of different sizes – CuZr, CuNb, TiCuNi

Strucutral glass – the potential energy landscape

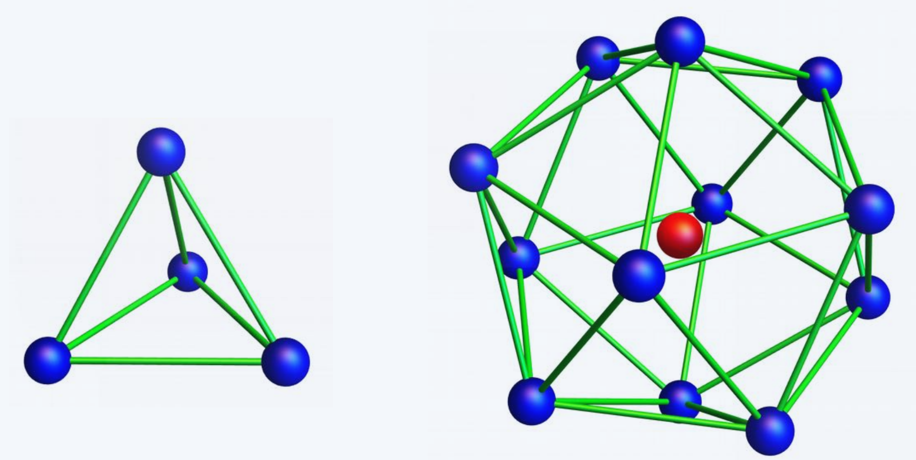


Model Binary Glass:
32000 atoms

Central questions to answer

- low energy structural excitations?
- local structural state variables?
- their connectivity?

Central concept

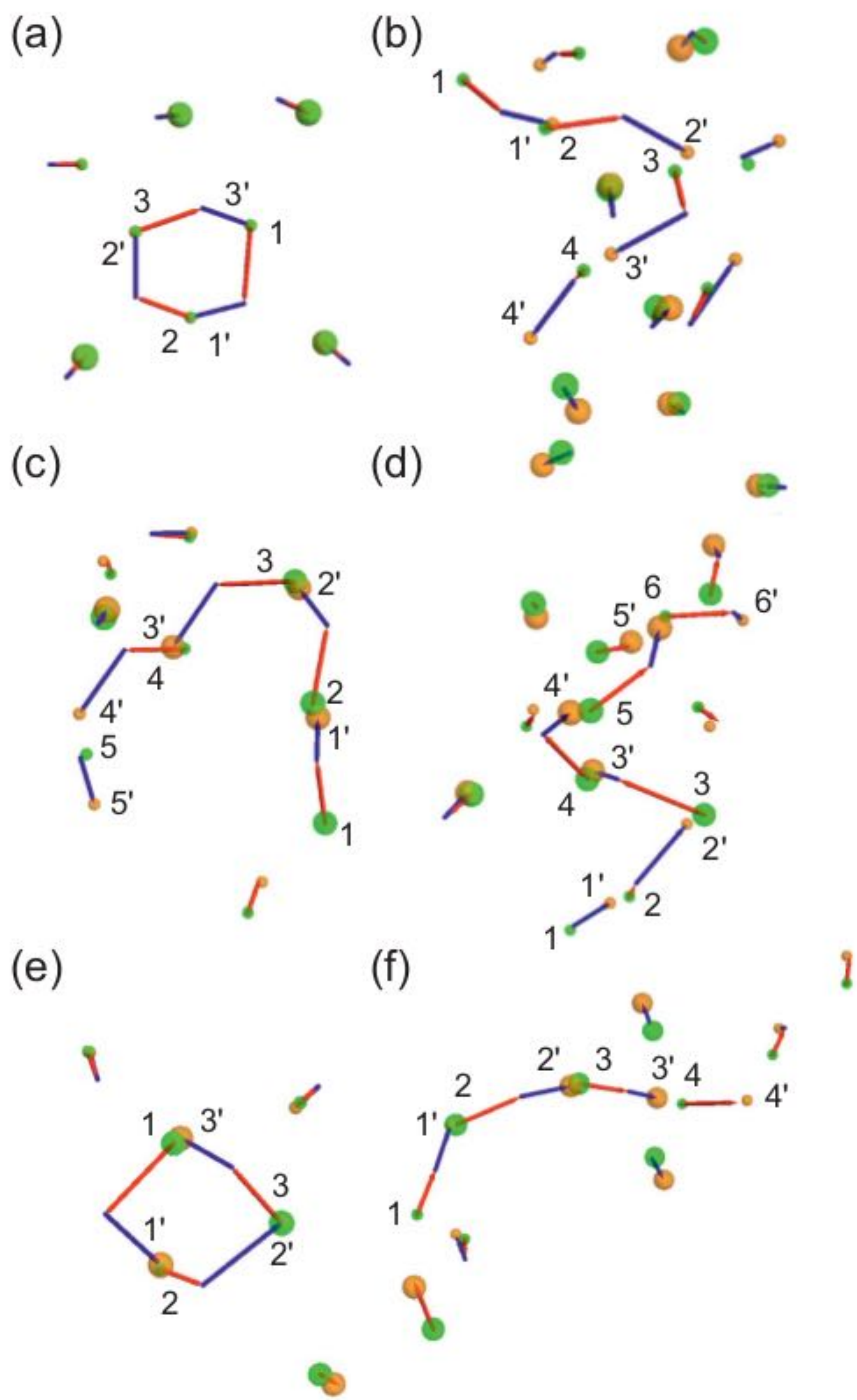


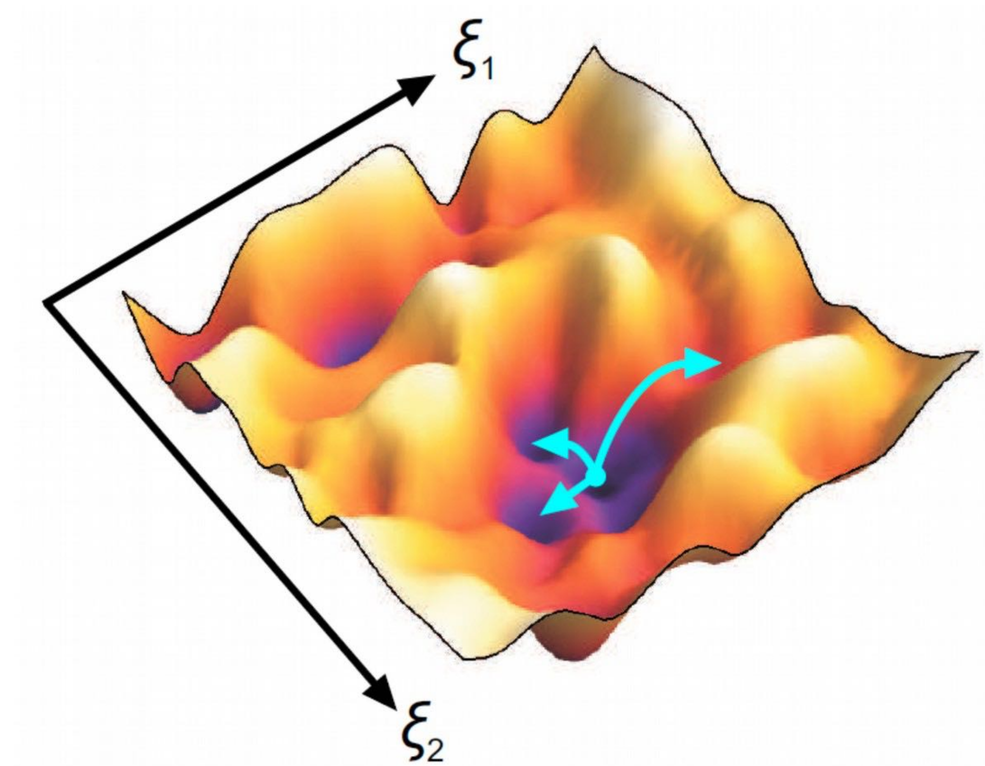
tetrahedron → icosahedron

Locally minimizes bond energy frustration and maximizes atomic packing

Collaborators: R. Maass, UIUC-MSE, USA, J. Loefler, ETHZ-MATL (SNF PhD: S. Jekal)

Strucutral glass – localized structural excitations





PEL exploration algorithm

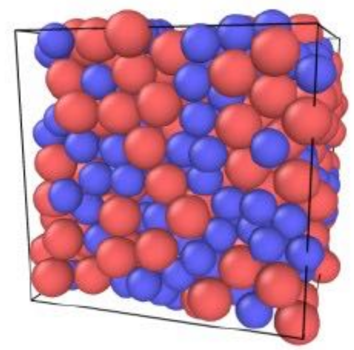
S. Swayamjyoti, J.F. Löffler, and PMD, PRB 89, 224201 (2014); Phys. Rev. B 93, 144202 (2016).

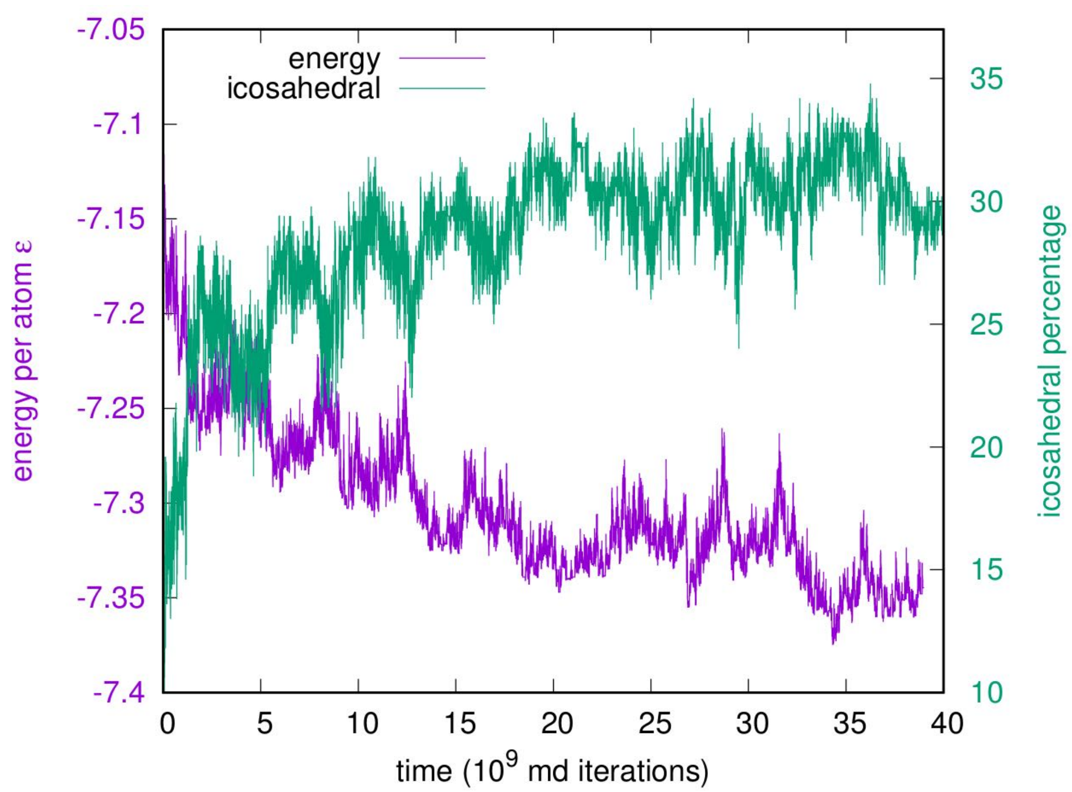
Direct molecular dynamics

PMD & R. Maass, JMR 32 (2017) 2668; Acta Mater 143 (2018) 338; Acta Mater 143 (2018) 205

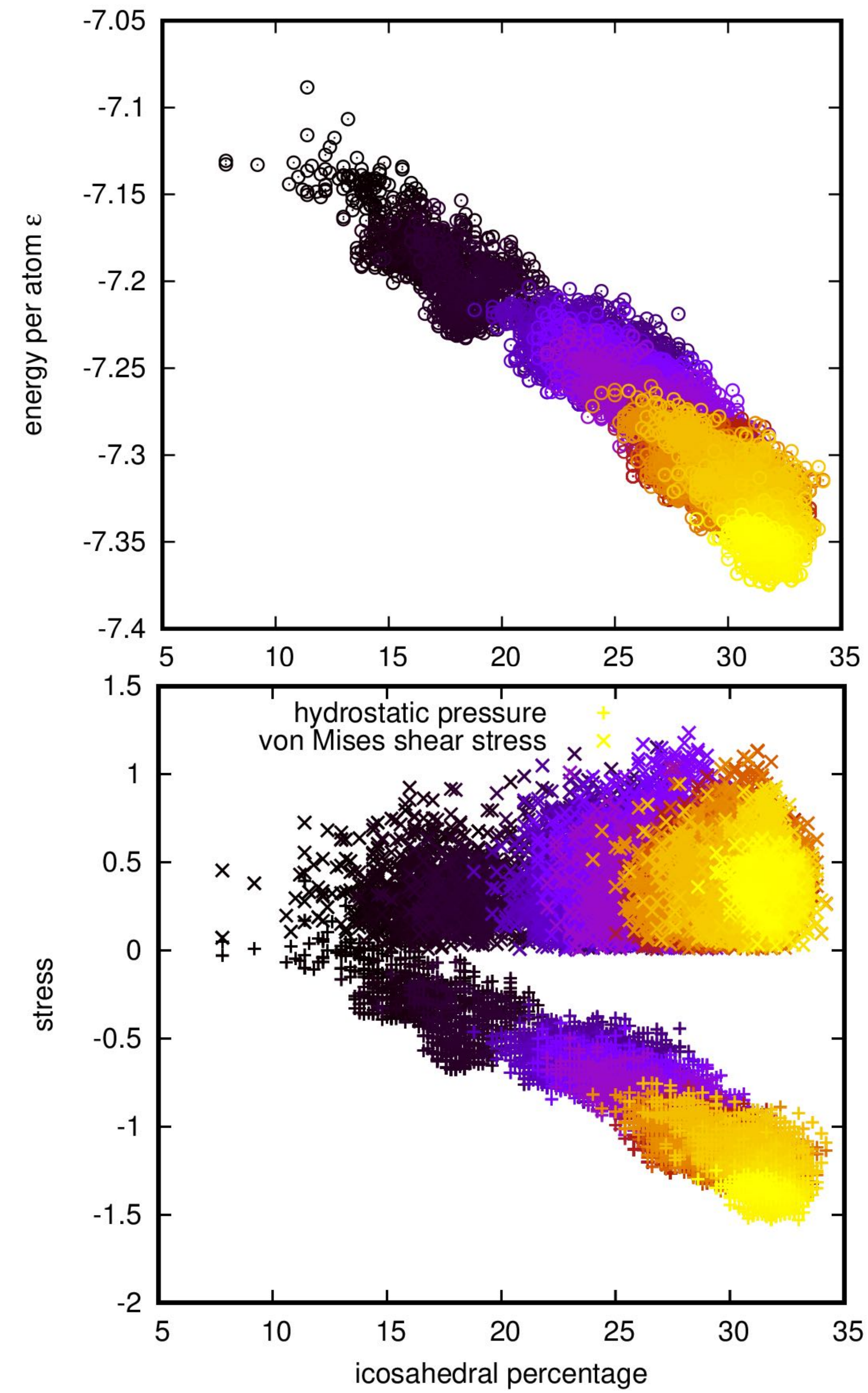
Strucutral glass – icosahedral content

GPU MD
simulation of ~50
micro-seconds



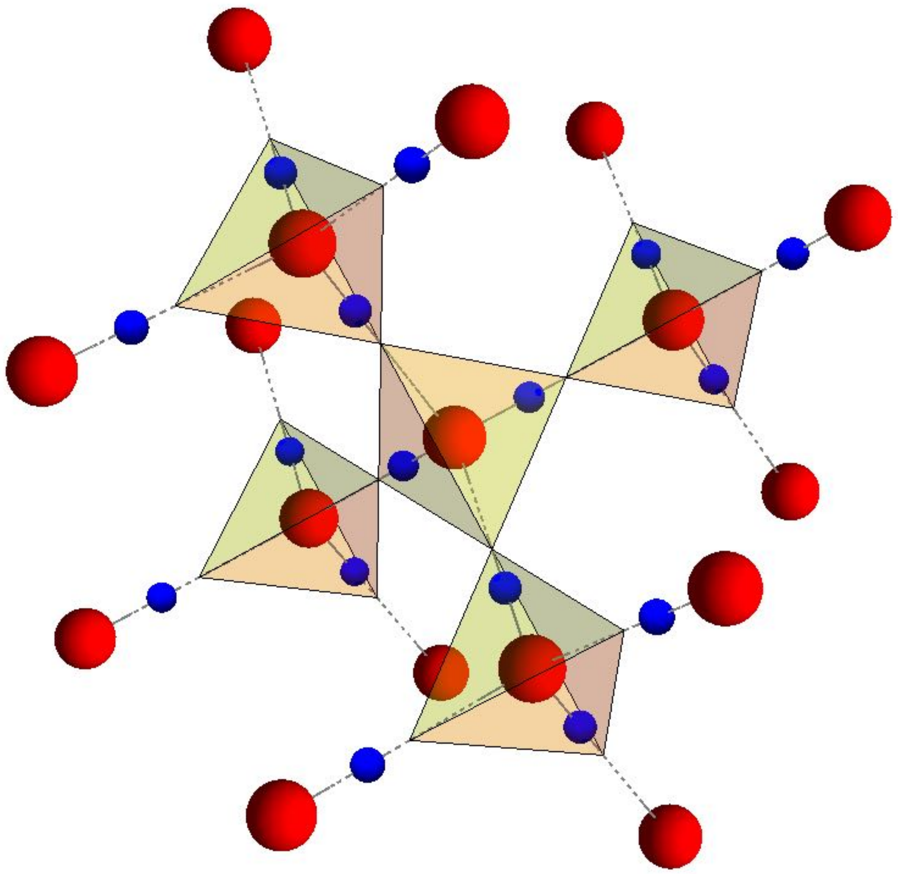


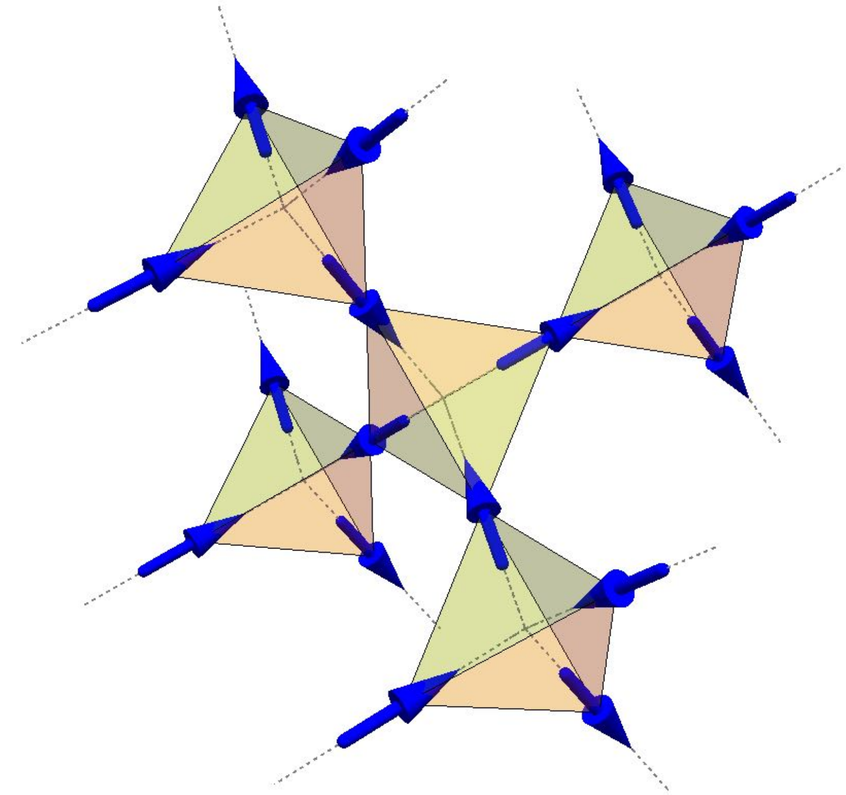
Icosahedral content directly controls energy and pressure (volume) relaxation



PMD & R. Maass, in preparation (2018)

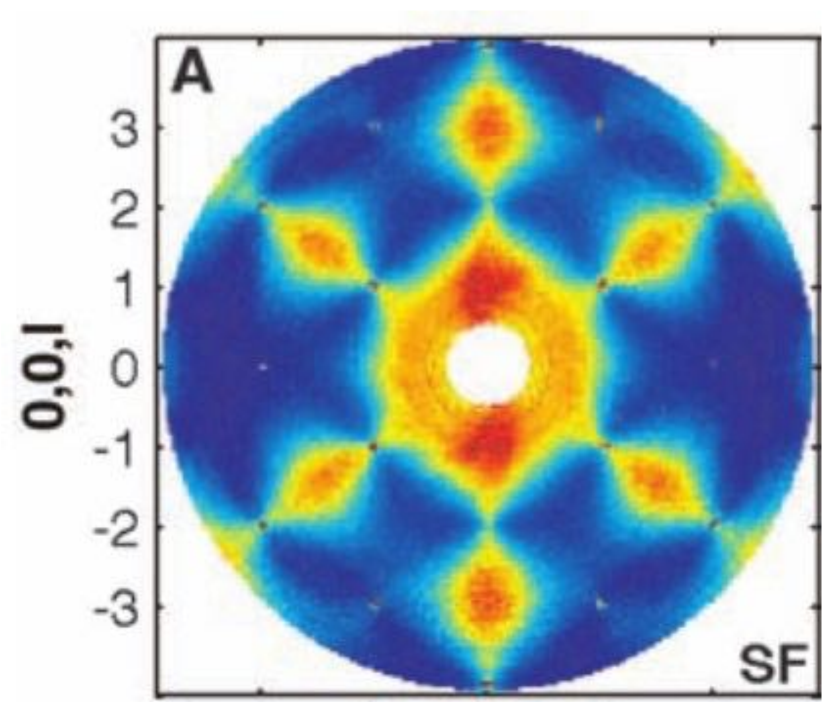
Example of PSI collaborations – ice physics





displacement-ice

spin-ice



- finite configurational entropy
- no long range order, but a local constraint

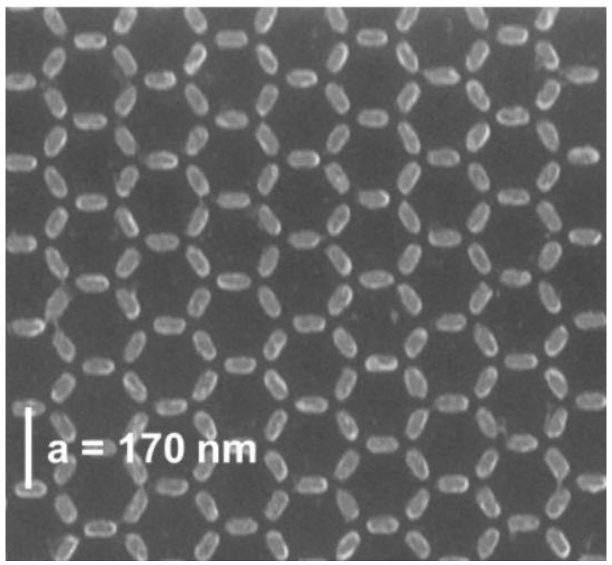
$$\nabla \cdot \mathbf{M}(\mathbf{r}) = 0 \rightarrow \mathbf{q} \cdot \mathbf{M}(\mathbf{q}) = 0$$

→ pinch-points in diffuse scattering

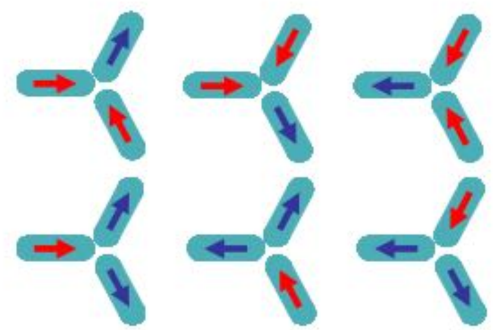
Magnetic Coulomb Phase in the Spin Ice $Ho_2Ti_2O_7$
Fennell et al, Science 326 (5951), 415

Example of PSI collaborations – 2D ice physics

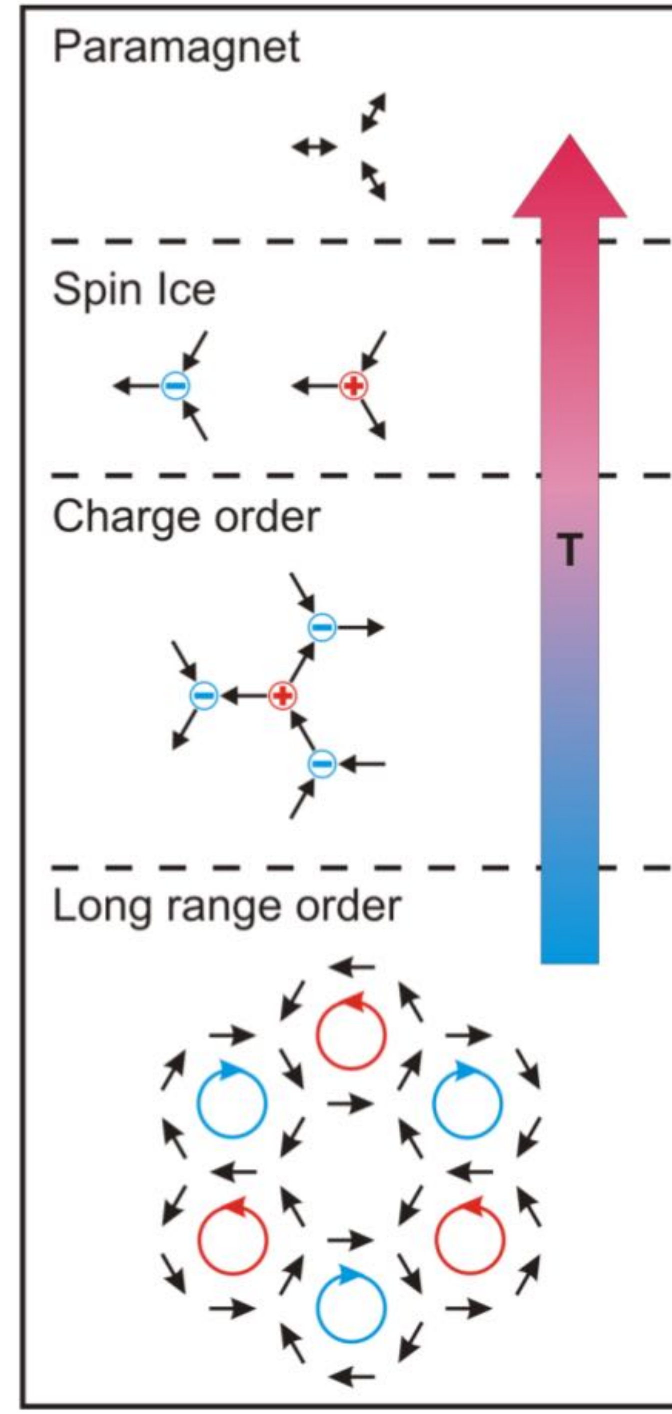
2D kagome system



Spin-ice rule



2 in/1 out – 1 in/2 out



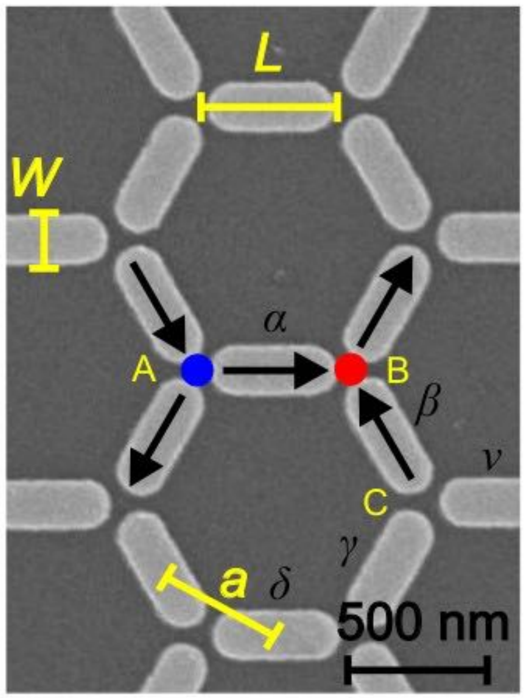
For modelling … treat each island as a point magnetic dipole

$$V_{ij} = -\frac{\mu_0 (M_s \Delta V)^2}{4\pi} \frac{3(\hat{\mathbf{m}}_i \cdot \hat{\mathbf{e}}_{ij})(\hat{\mathbf{m}}_j \cdot \hat{\mathbf{e}}_{ij}) - \hat{\mathbf{m}}_i \cdot \hat{\mathbf{m}}_j}{r_{ij}^3}$$

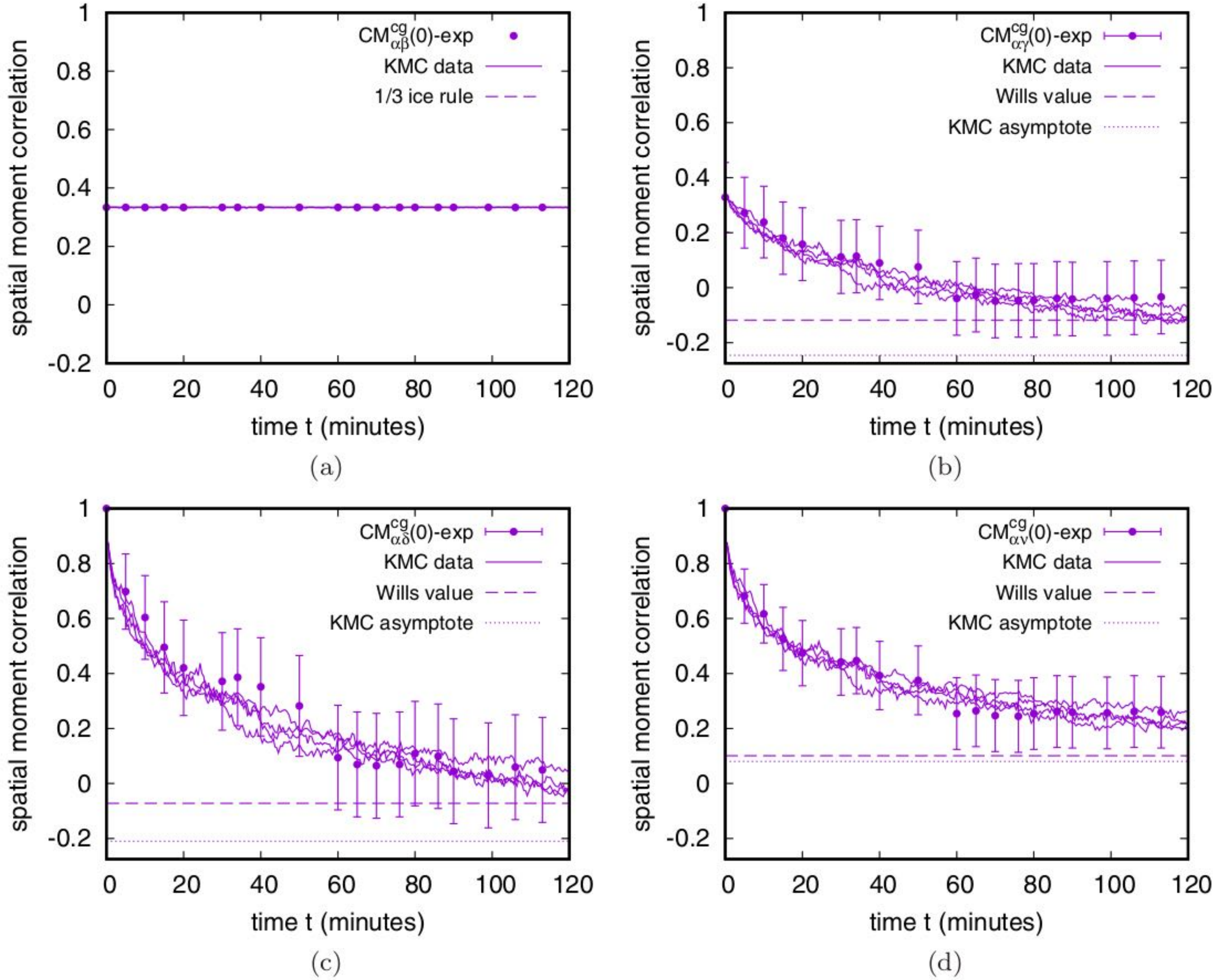
Collaborators: L. J. Heydermann, PSI/ETHZ-MATL (CROSS PhD: D. Schildknecht)
F. Nolting & A. Kleibert, PSI-SYN
M. Fiebig, ETHZ-MATL

Example of PSI collaborations – relaxation in spin ice I

2D kagome system



$$\mathrm{CM}_{ij}^{\mathrm{cg}}(0) = \langle \mathrm{sgn}[\hat{\mathbf{m}}_i(t) \cdot \hat{\mathbf{m}}_{i+j}(t)] \rangle$$



Kinetic monte carlo simulations

A. Farhan, PMD, L. Anghinolfi, A. Kleibert, and L. J. Heyderman, Phys. Rev. B 96, 064409 (2017).

Future PSI collaboration – 3D spin and displacement ice physics

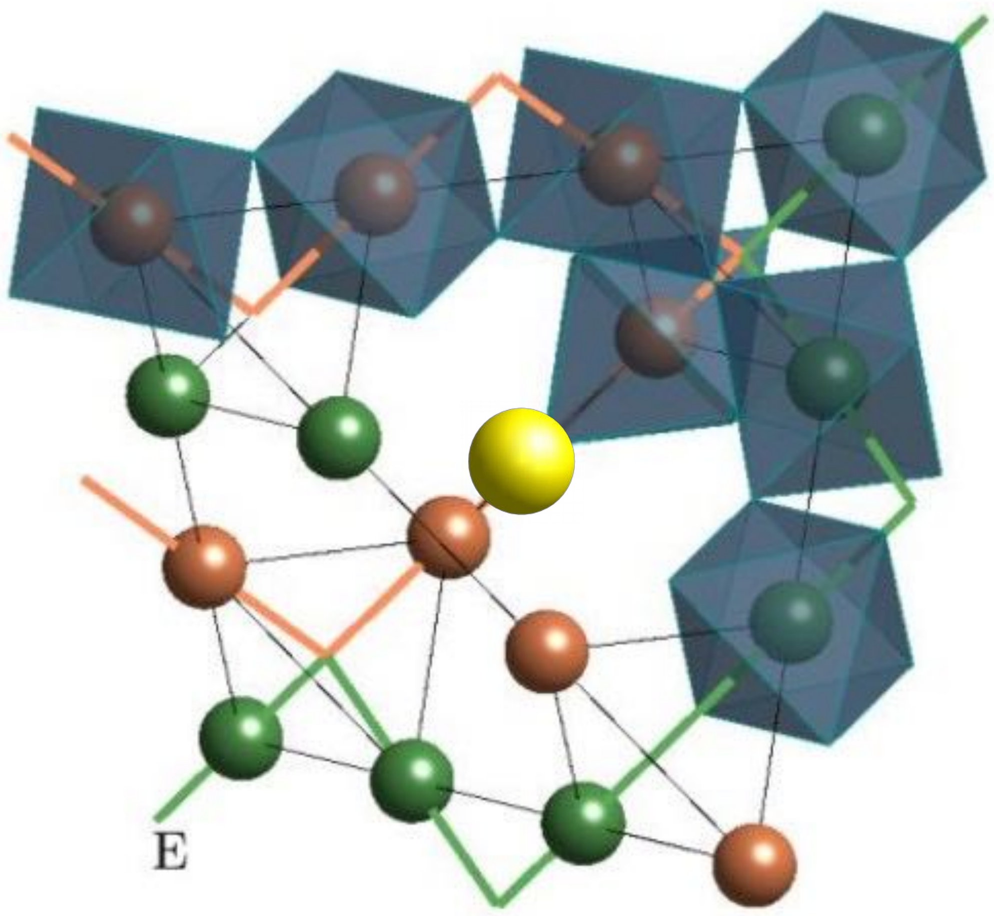
Multiple Coulomb phase in the fluoride pyrochlore $CsNiCrF_6$

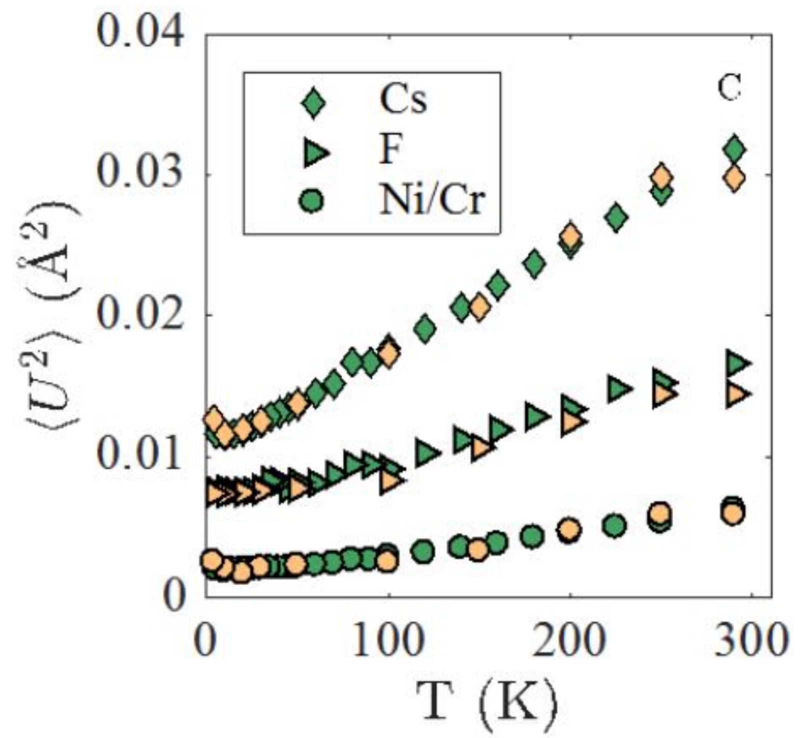
F^-

Cr^{3+}

Ni^{2+}

Cs^+





T. Fennell et al, submitted (2018)

Collaborators: T. Fennell - PSI-NUM

Xavier Deupi: Biography

1973	Born in Barcelona.
1998	BSc in Organic **Chemistry**. Institut Quimic de Sarria (Barcelona)
2003	PhD in Biochemistry and **Molecular Biology**. Universitat Autonoma de Barcelona.
2003	Postdoc Stanford University.
2005	Research Scientist (tenure track). Universitat Autonoma de Barcelona.
2010	Scientific Officer at LBR/CMT.
	BIO/SLS
2015	Senior Scientist at LBR/CMT.

General interests and methodology

Structure of proteins

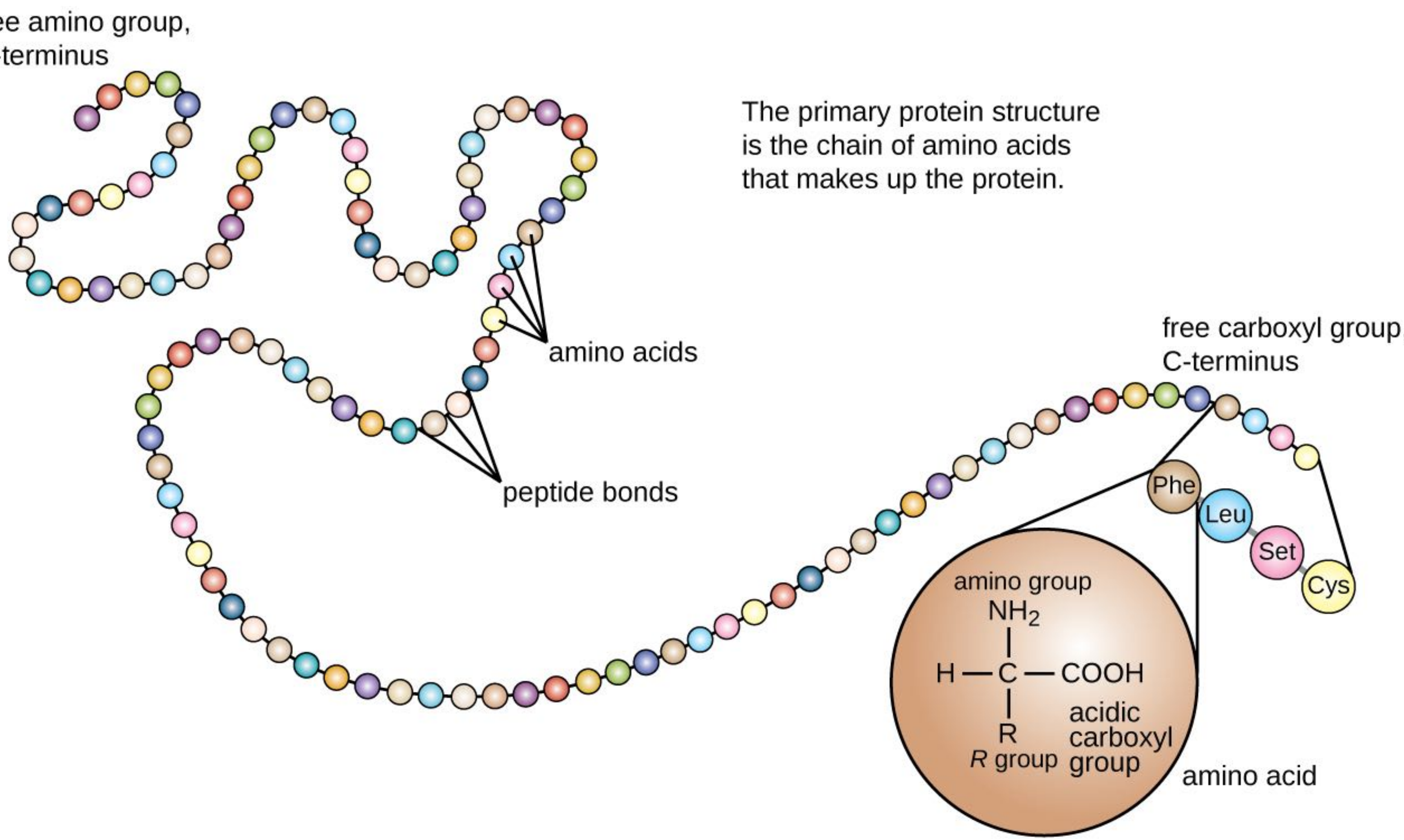
G protein-coupled receptors

Structural modeling

Molecular dynamics simulations

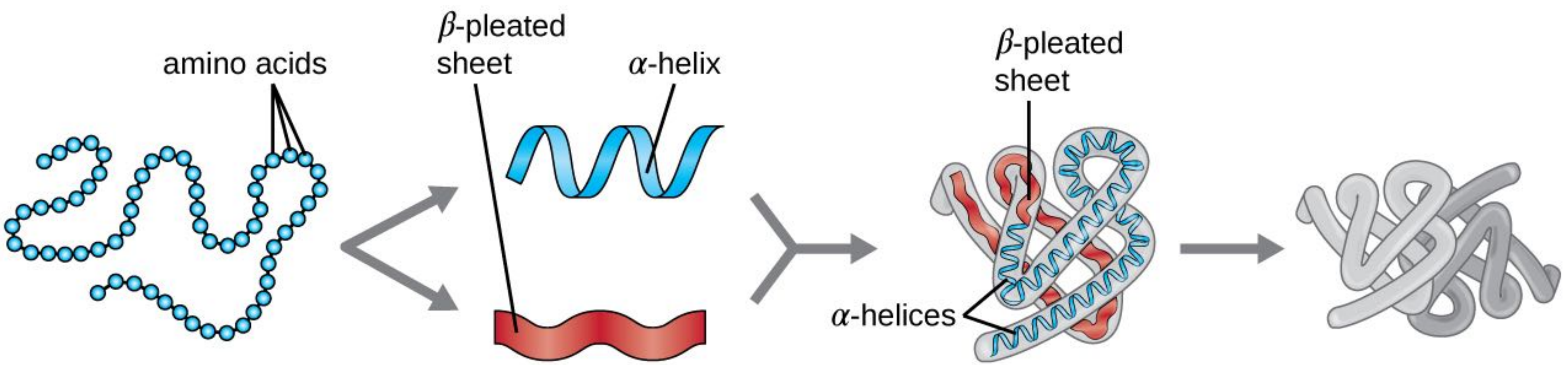
Structure of proteins

The primary protein structure is the chain of amino acids that makes up the protein.



bio.libretexts.org

Structure of proteins



Primary Protein Structure
Sequence of a chain of amino acids

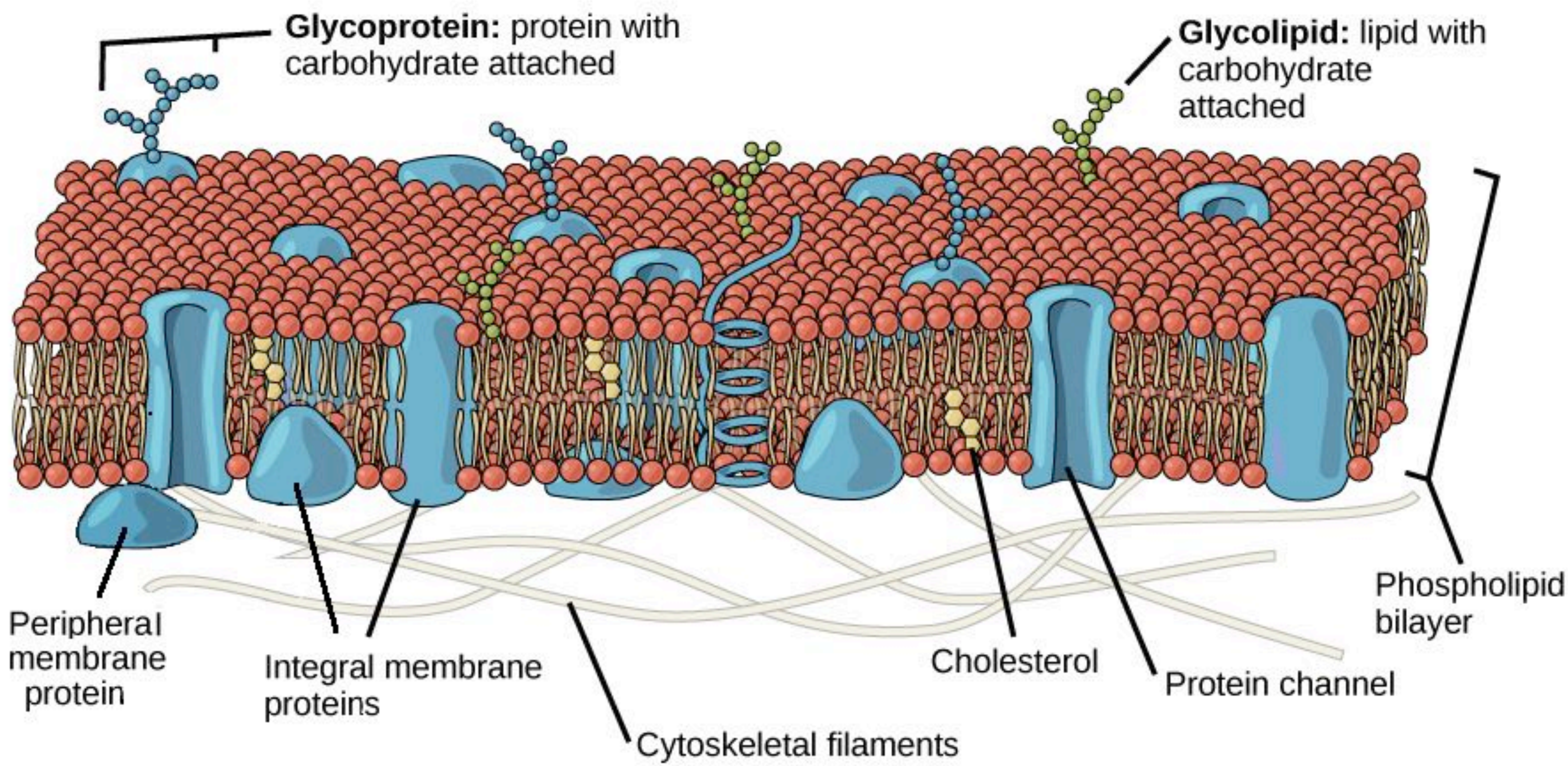
Secondary Protein Structure
Local folding of the polypeptide chain into helices or sheets

Tertiary Protein Structure
three-dimensional folding pattern of a protein due to side chain interactions

Quaternary Protein Structure
protein consisting of more than one amino acid chain

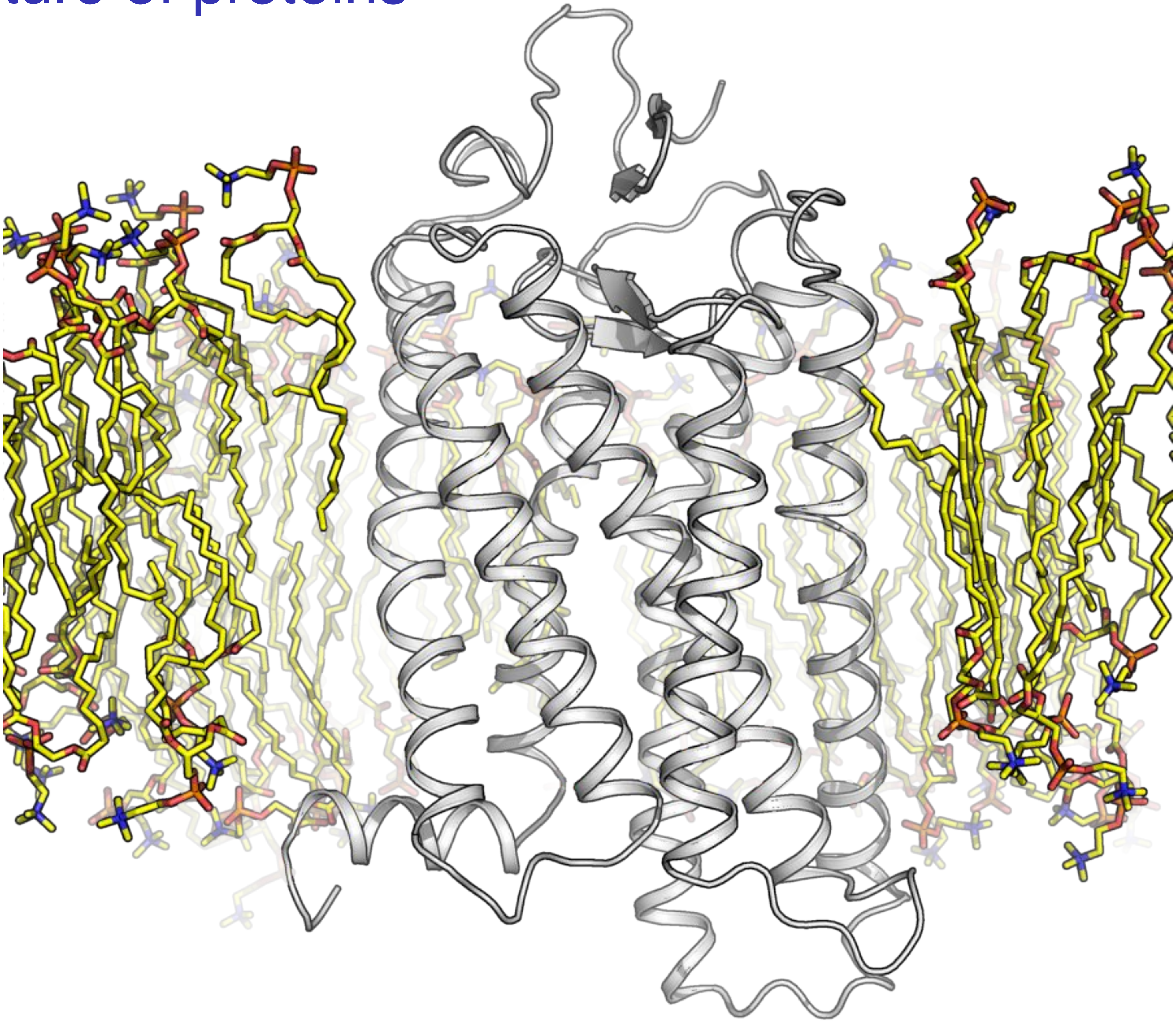
bio.libretexts.org

Structure of proteins

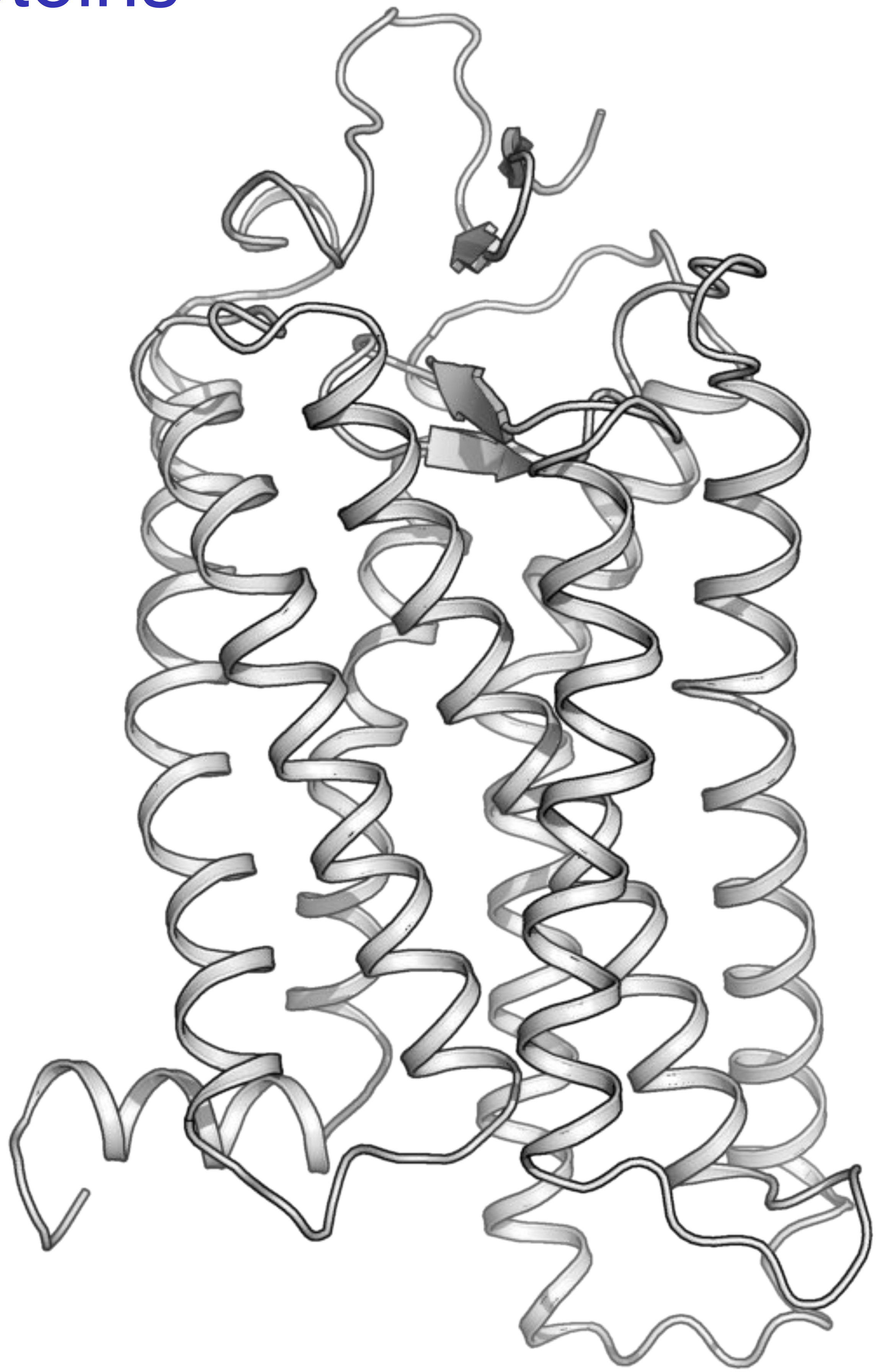


www.khanacademy.org

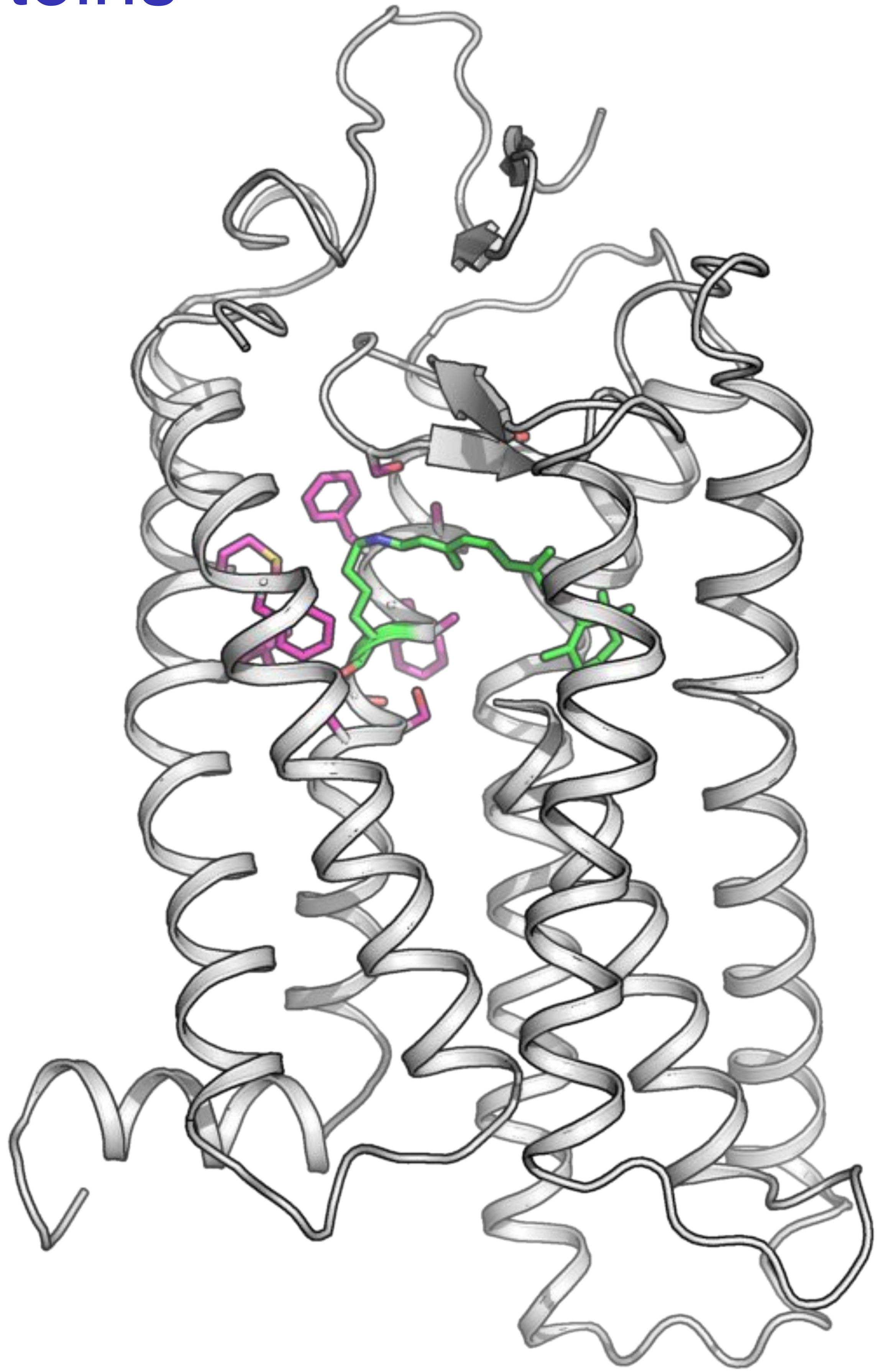
Structure of proteins



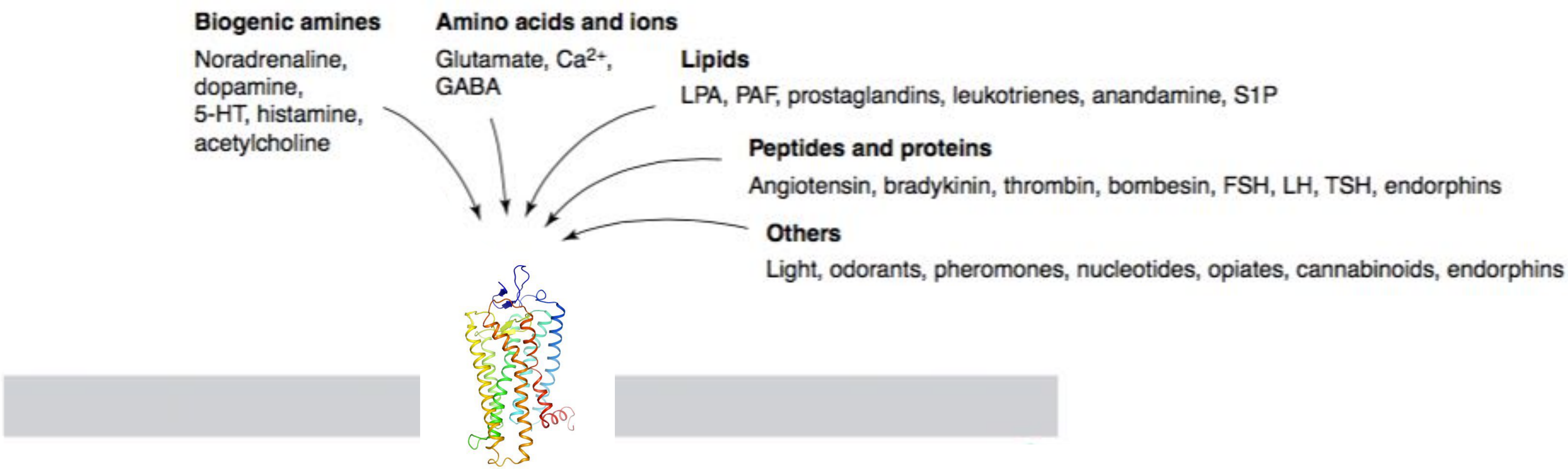
Structure of proteins



Structure of proteins



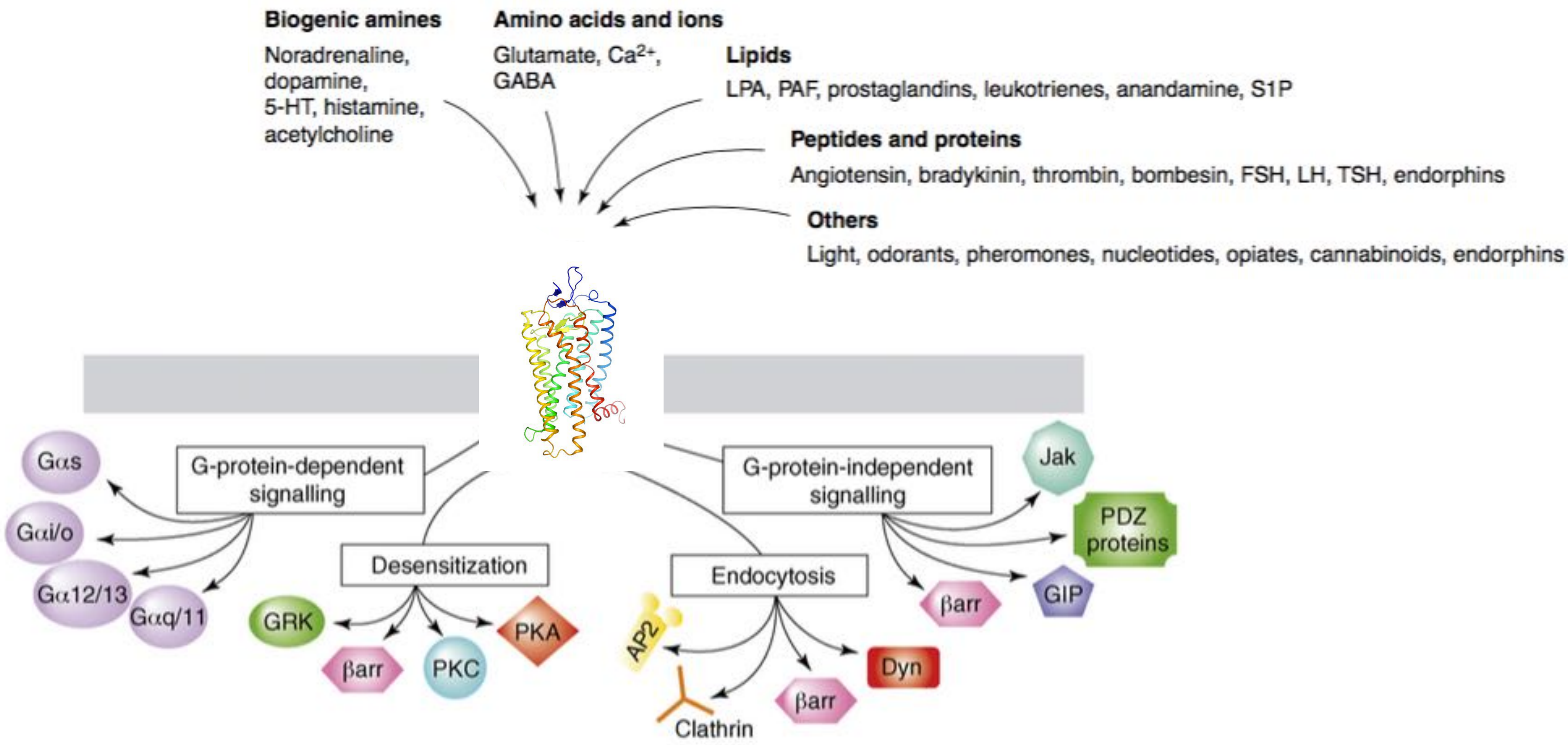
G protein-coupled receptors



Marinissen, M. J. & Gutkind, J. S. Trends Pharmacol. Sci. 22, 368–376 (2001)

Galandrin et al. Trends Pharmacol. Sci. 28, 423–430 (2007)

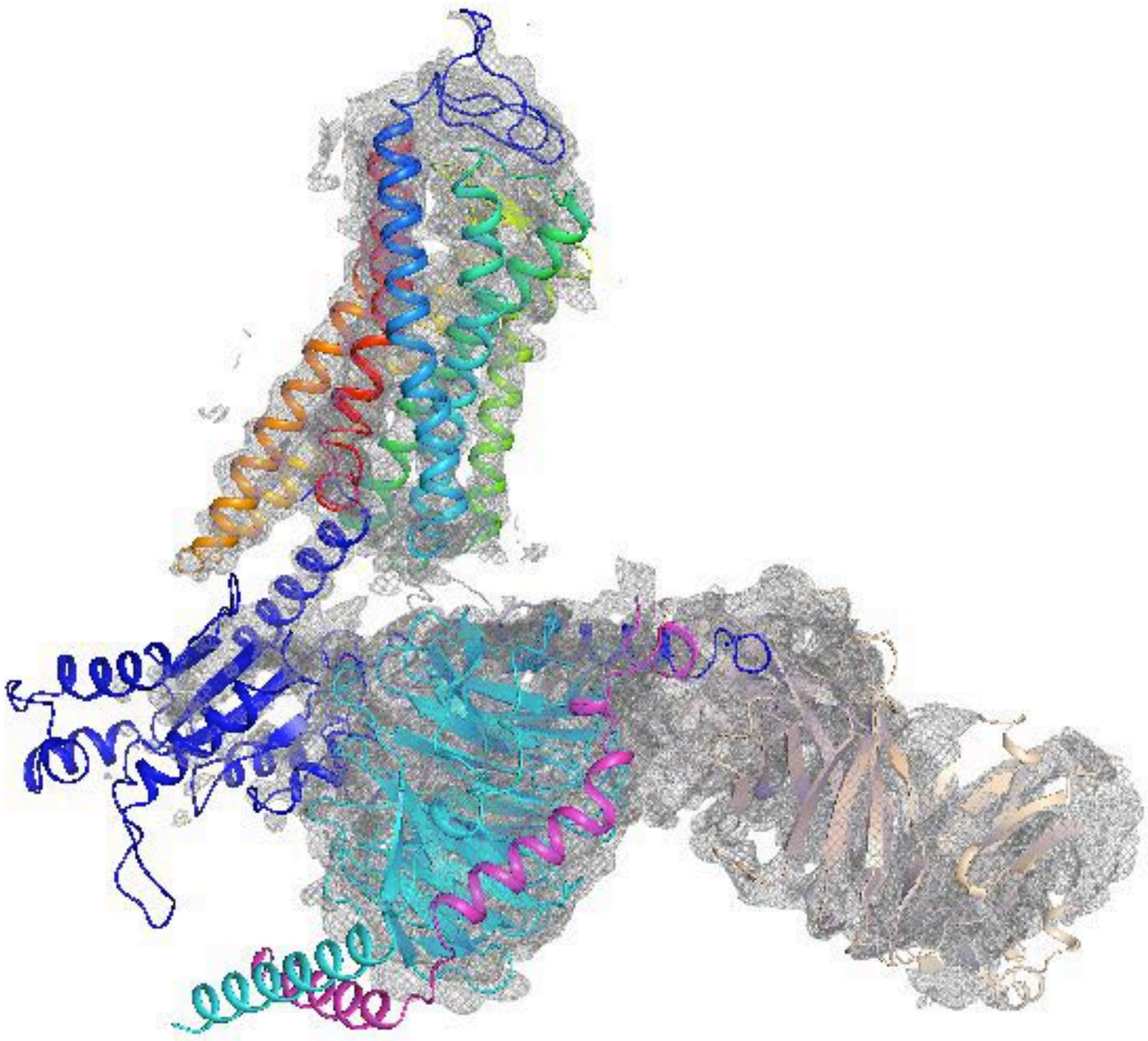
G protein-coupled receptors



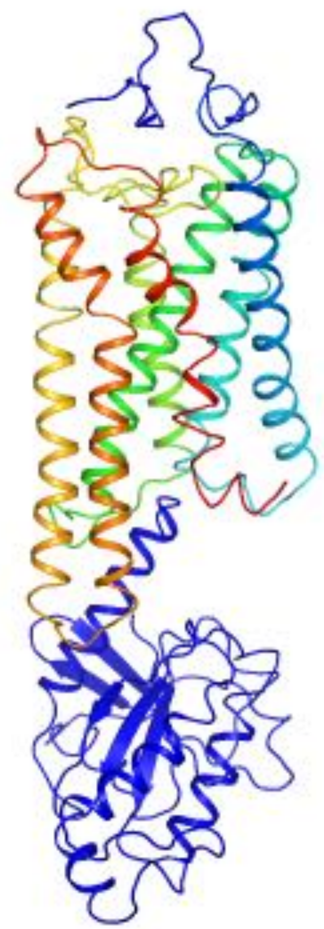
Marinissen, M. J. & Gutkind, J. S. Trends Pharmacol. Sci. 22, 368–376 (2001)

Galandrin et al. Trends Pharmacol. Sci. 28, 423–430 (2007)

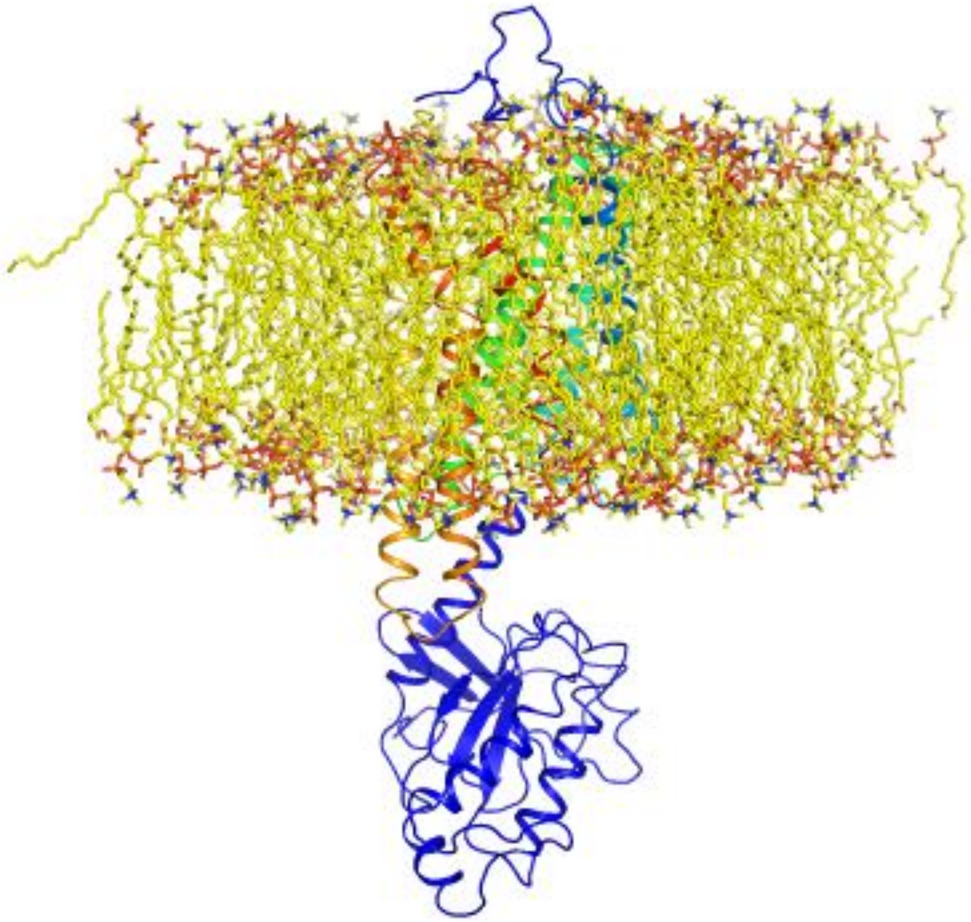
Research interests: structure of protein complexes



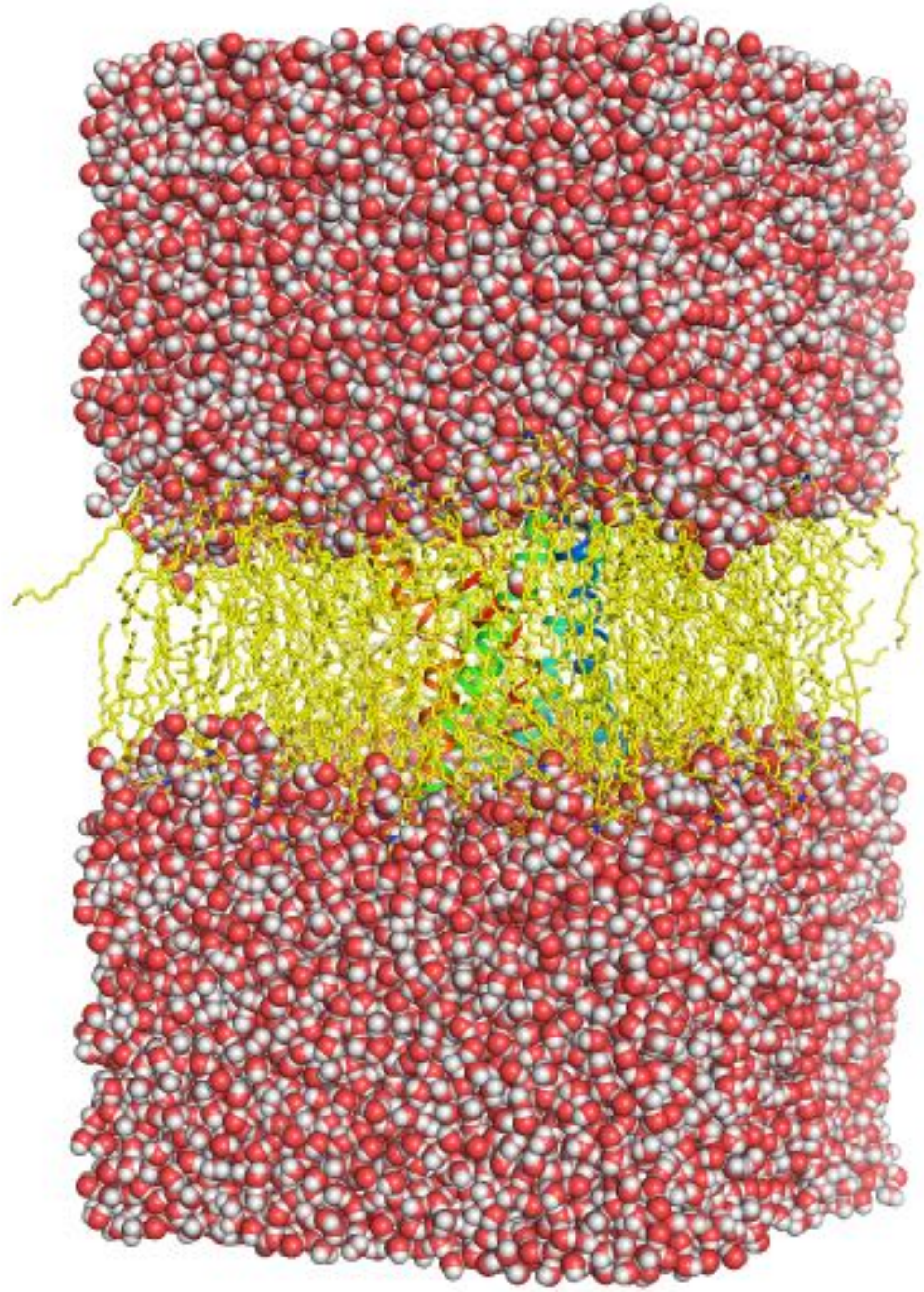
Research interests: structure of protein complexes



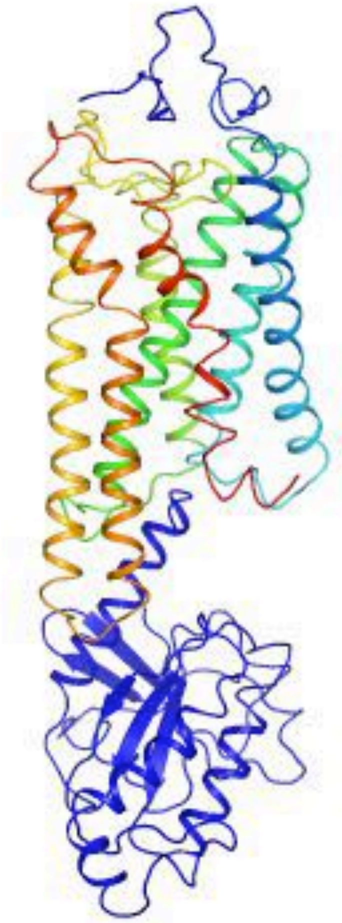
Research interests: structure of protein complexes



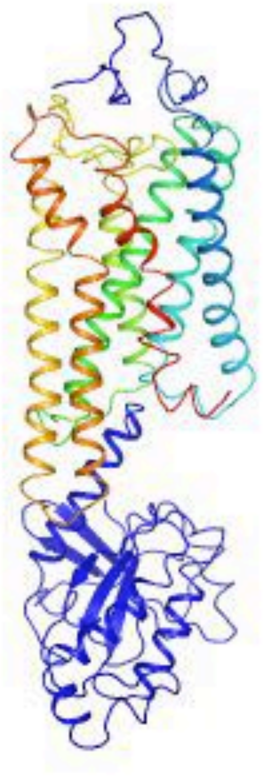
Research interests: structure of protein complexes



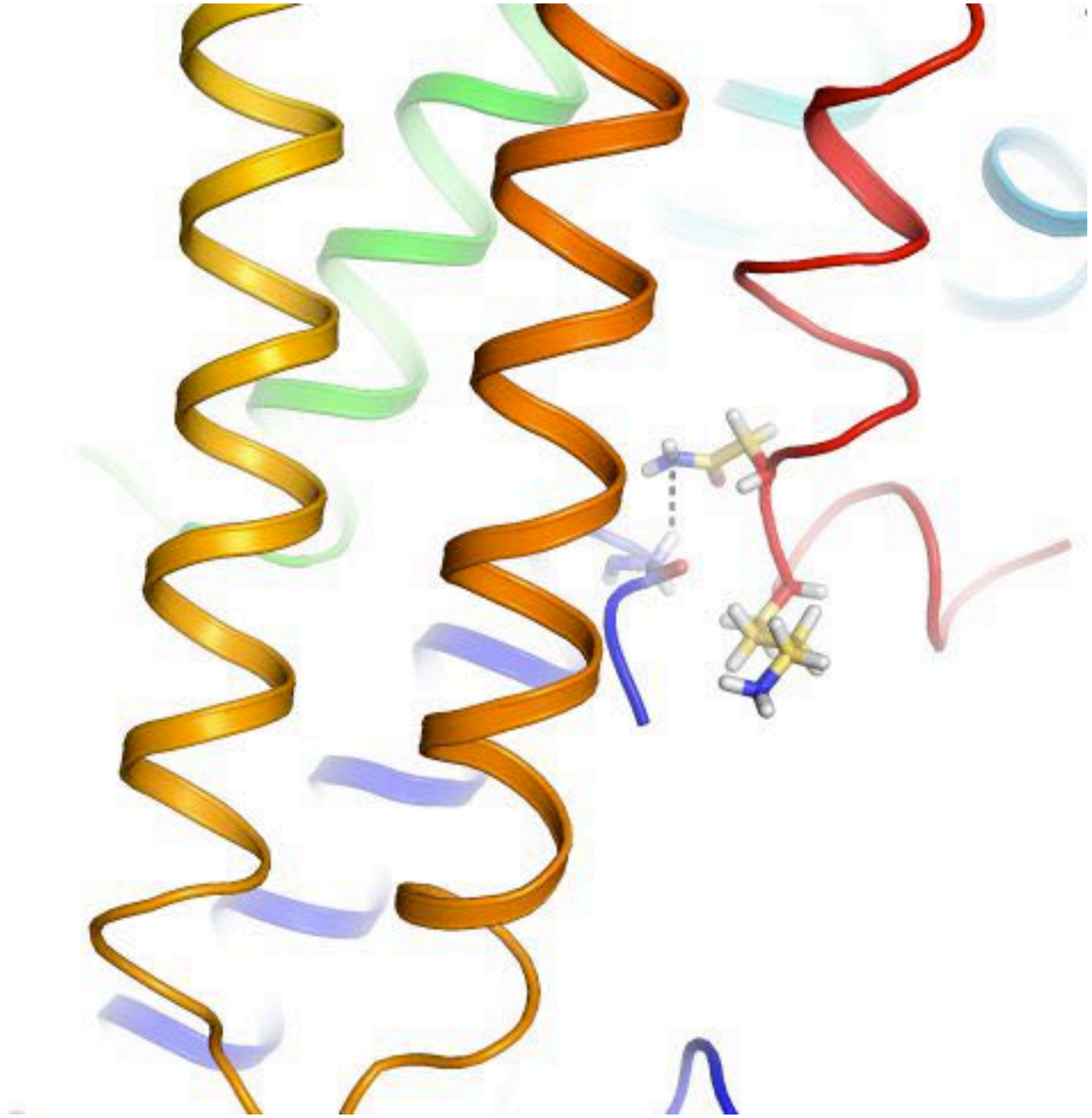
Research interests: structure of protein complexes



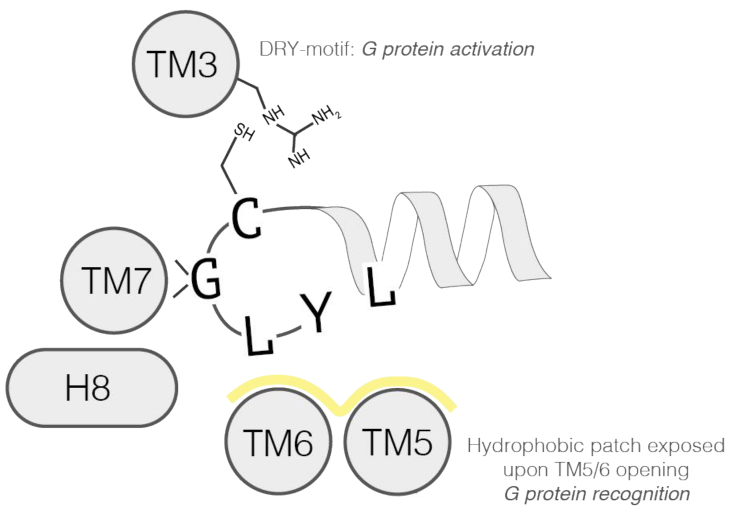
Research interests: structure of protein complexes

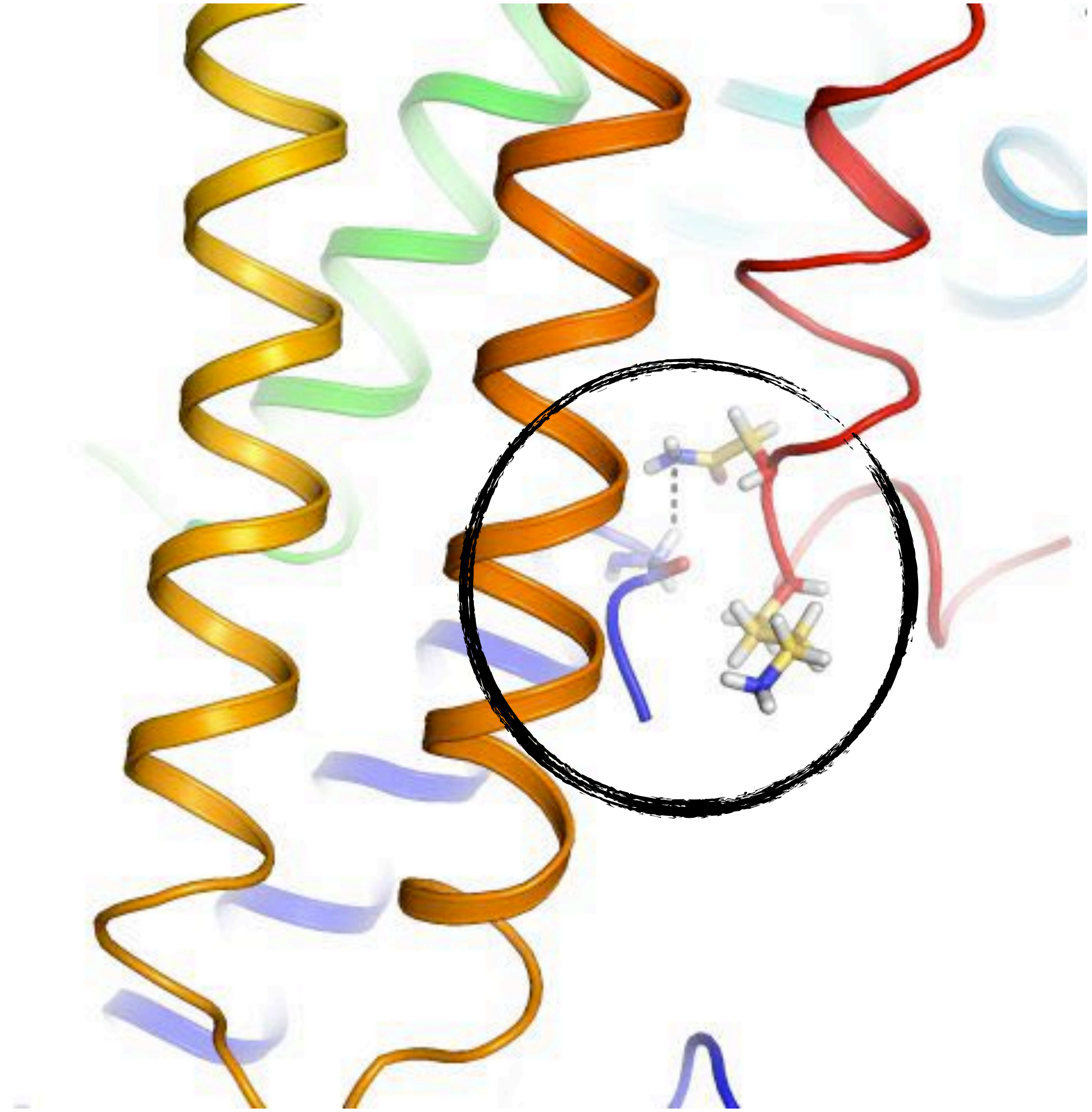


Research interests: structure of protein complexes

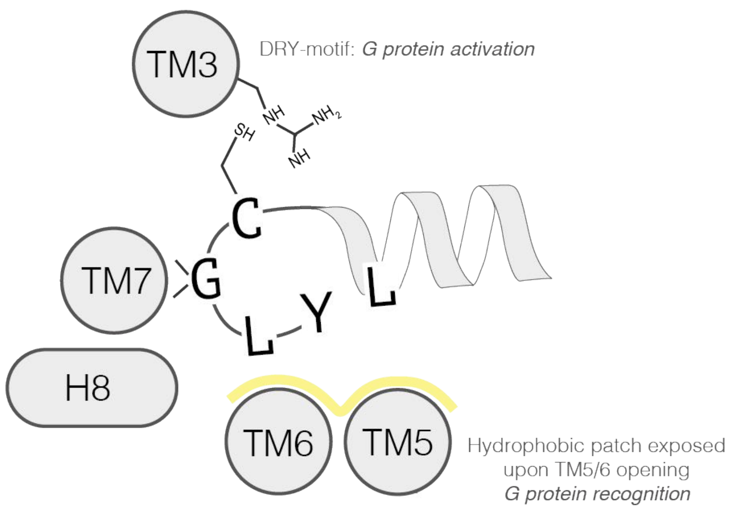


Research interests: structure of protein complexes



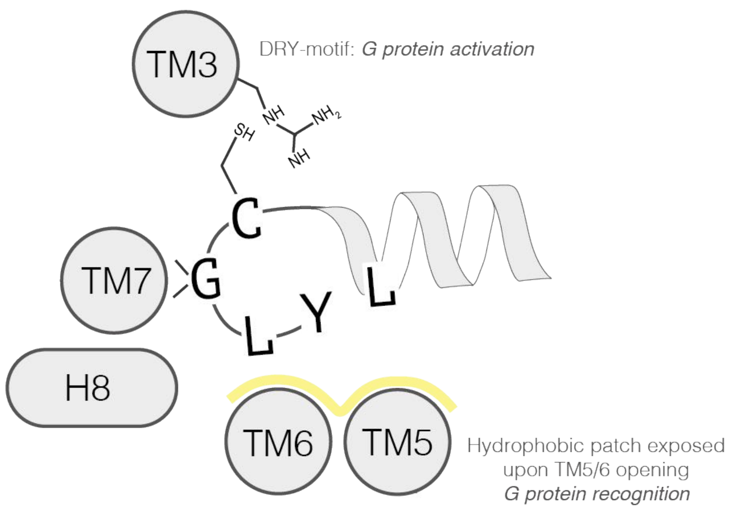


Research interests: structure of protein complexes

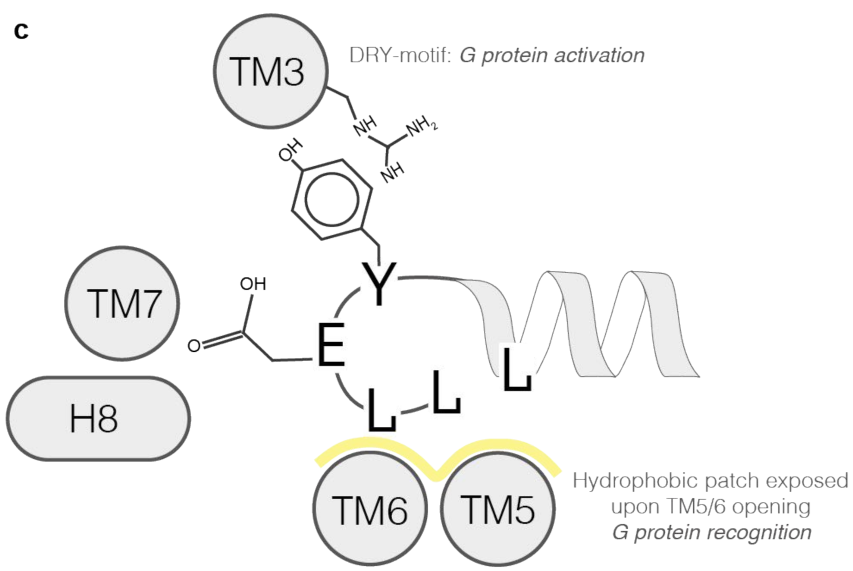


Common G-alpha numbering scheme	H5.23	H5.24	H5.25	H5.26
[Human] G(olf) subunit alpha	Y	E	L	L
[Human] G(s) subunit alpha isoforms short	Y	E	L	L
[Human] G(i) subunit alpha-1	C	G	L	F
[Human] G(i) subunit alpha-2	C	G	L	F
[Human] G(k) subunit alpha	C	G	L	Y
[Human] G(o) subunit alpha	C	G	L	Y
[Human] G(t) subunit alpha-1	C	G	L	F
[Human] G(t) subunit alpha-2	C	G	L	F
[Human] G(t) subunit alpha-3	C	G	L	F

Research interests: structure of protein complexes

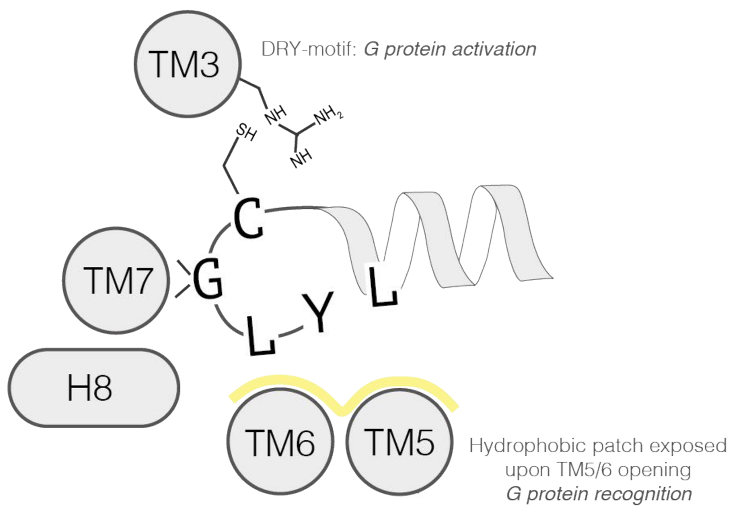


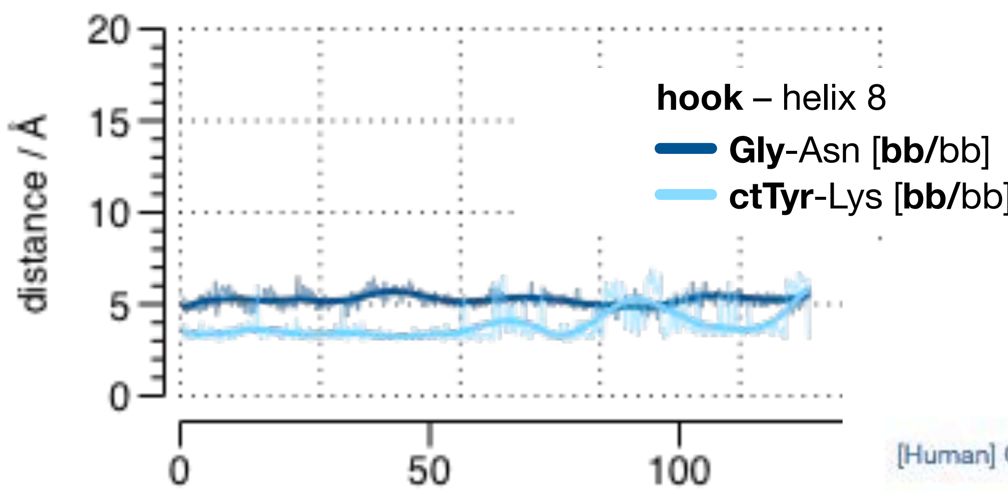
c



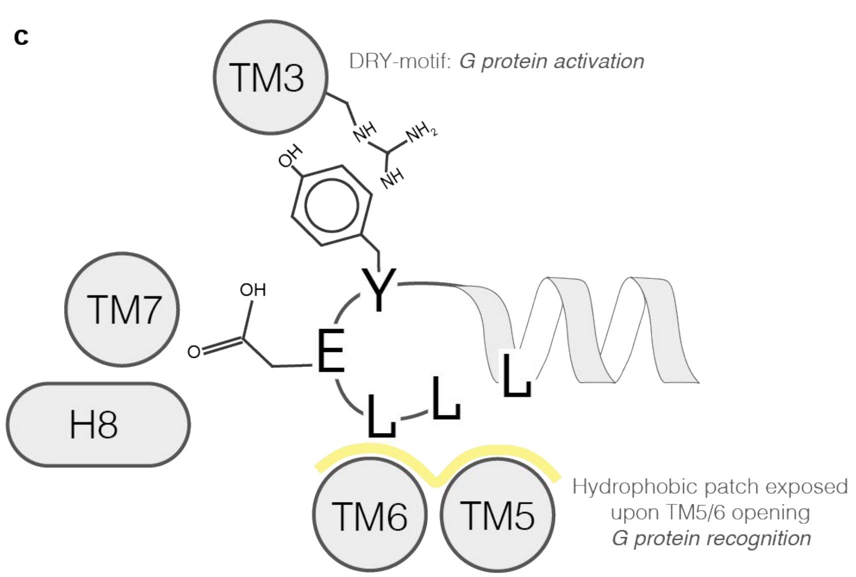
Common G-alpha numbering scheme	H5.23	H5.24	H5.25	H5.26
[Human] G(olf) subunit alpha	Y	E	L	L
[Human] G(s) subunit alpha isoforms short	Y	E	L	L
[Human] G(i) subunit alpha-1	C	G	L	F
[Human] G(i) subunit alpha-2	C	G	L	F
[Human] G(k) subunit alpha	C	G	L	Y
[Human] G(o) subunit alpha	C	G	L	Y
[Human] G(t) subunit alpha-1	C	G	L	F
[Human] G(t) subunit alpha-2	C	G	L	F
[Human] G(t) subunit alpha-3	C	G	L	F

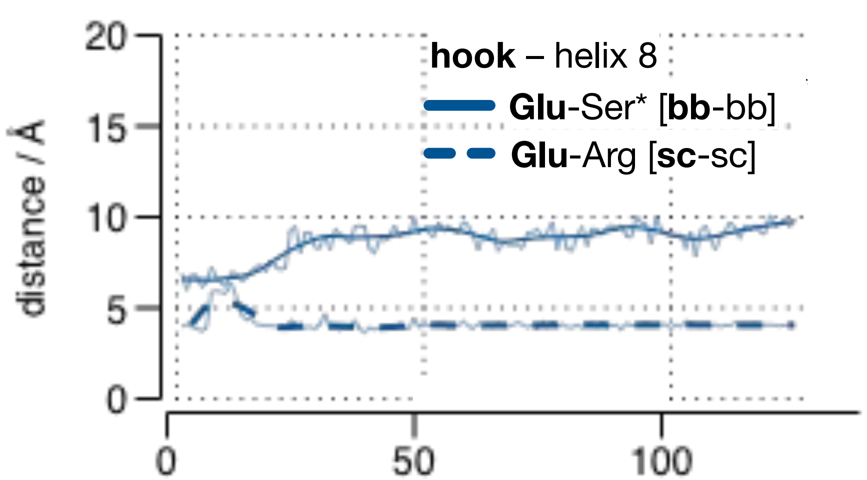
Research interests: structure of protein complexes





c



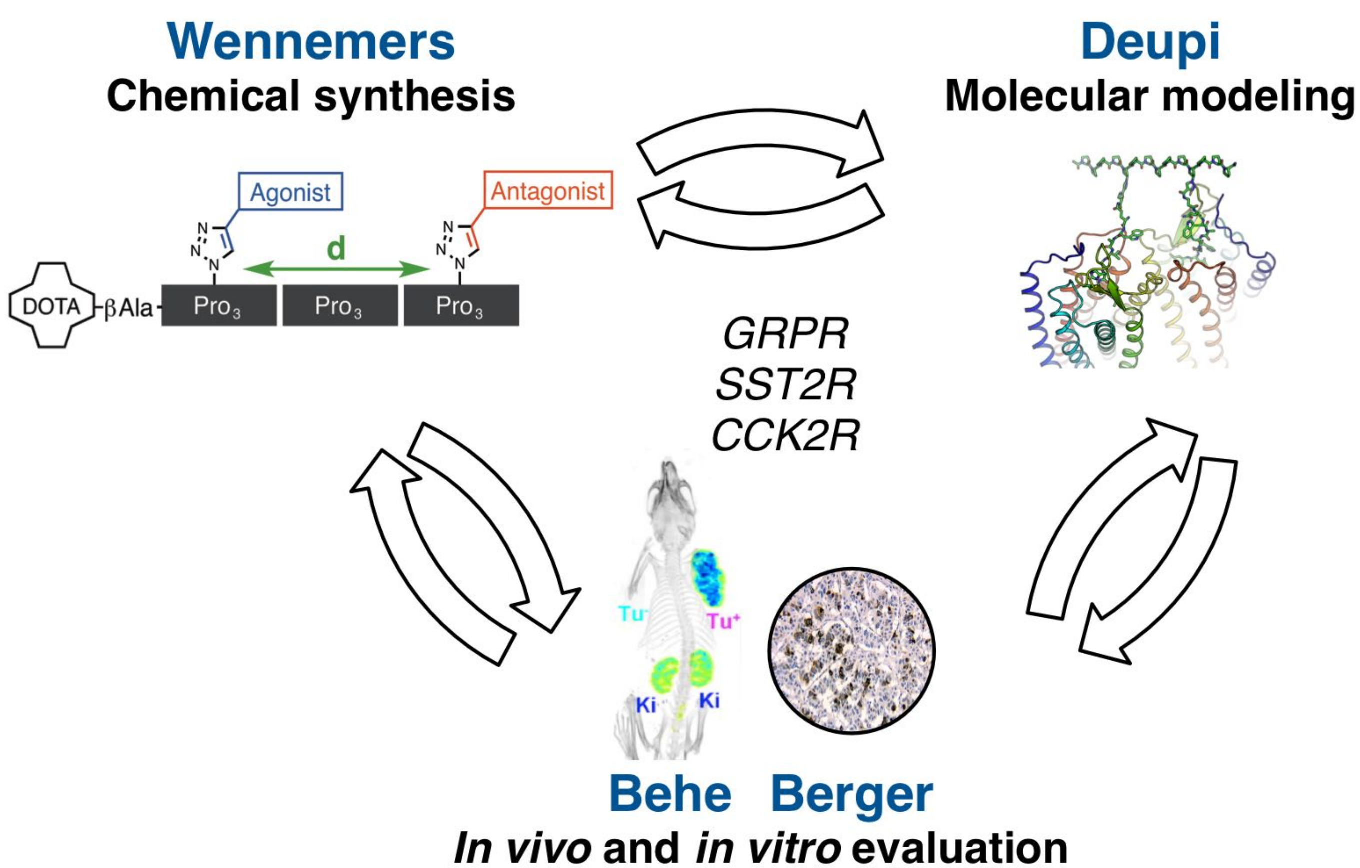


Common G-alpha numbering scheme	H5.23	H5.24	H5.25	H5.26
[Human] G(olf) subunit alpha	Y	E	L	L
[Human] G(s) subunit alpha isoforms short	Y	E	L	L
[Human] G(i) subunit alpha-1	C	G	L	F
[Human] G(i) subunit alpha-2	C	G	L	F
[Human] G(k) subunit alpha	C	G	L	Y
[Human] G(o) subunit alpha	C	G	L	Y
[Human] G(t) subunit alpha-1	C	G	L	F
[Human] G(t) subunit alpha-2	C	G	L	F
[Human] G(t) subunit alpha-3	C	G	L	F

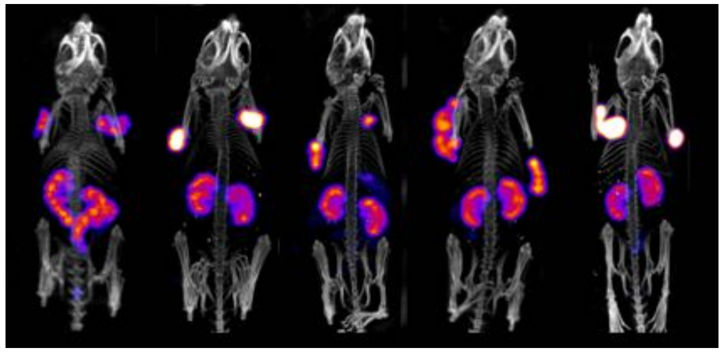
Research interests: tumor targetting drugs

Targeting Cancer Cells with Hybrid and Heterovalent Ligands at Controlled Distances

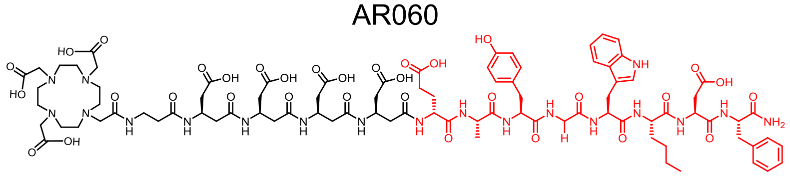
SNF Sinergia: ETH, BIO@PSI



Research interests: tumor targetting drugs

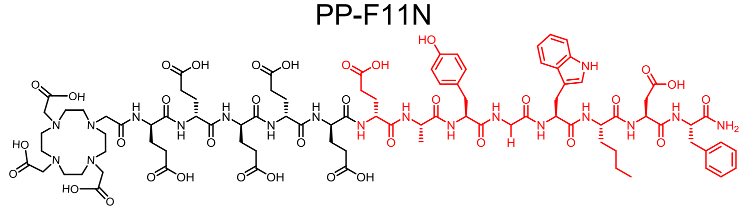


AR060



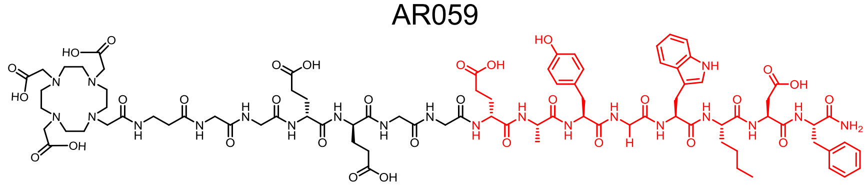
(Beta-glutamic acid sequence)

PP-F11N



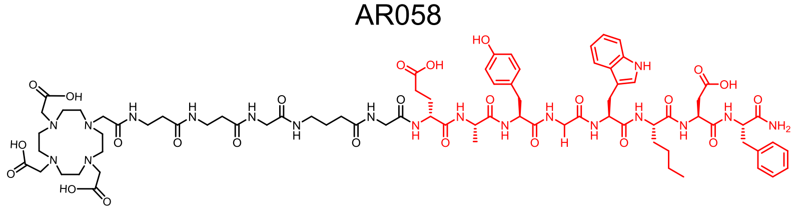
(attention: D-Glu stereochemistry)

AR059



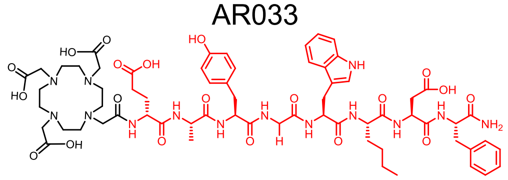
(attention: D-Glu stereochemistry)

AR058



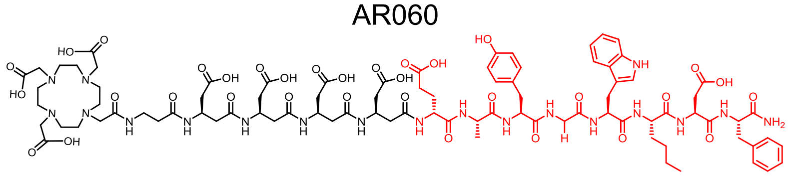
(attention: D-Glu stereochemistry)

AR033



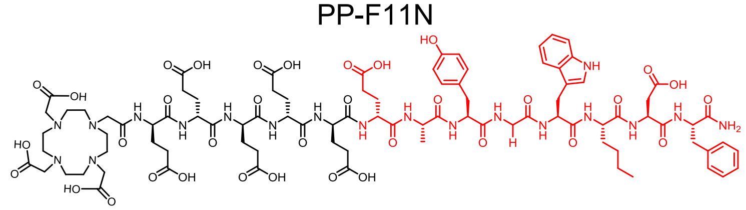
Research interests: tumor targetting drugs

AR060



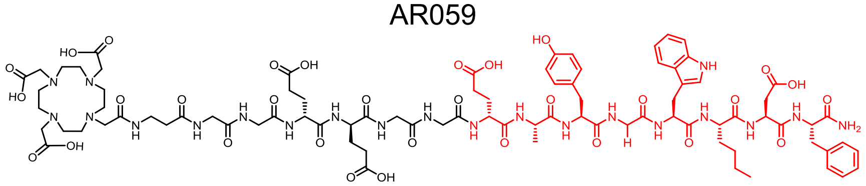
(Beta-glutamic acid sequence)

PP-F11N



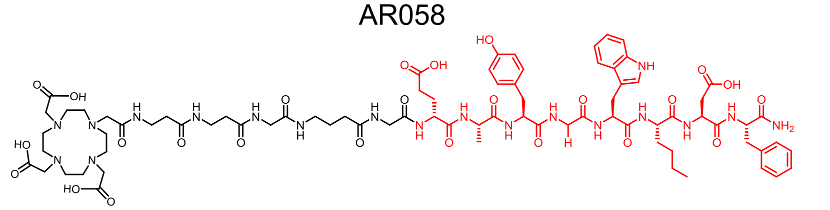
(attention: D-Glu stereochemistry)

AR059



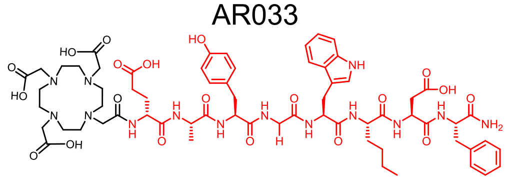
(attention: D-Glu stereochemistry)

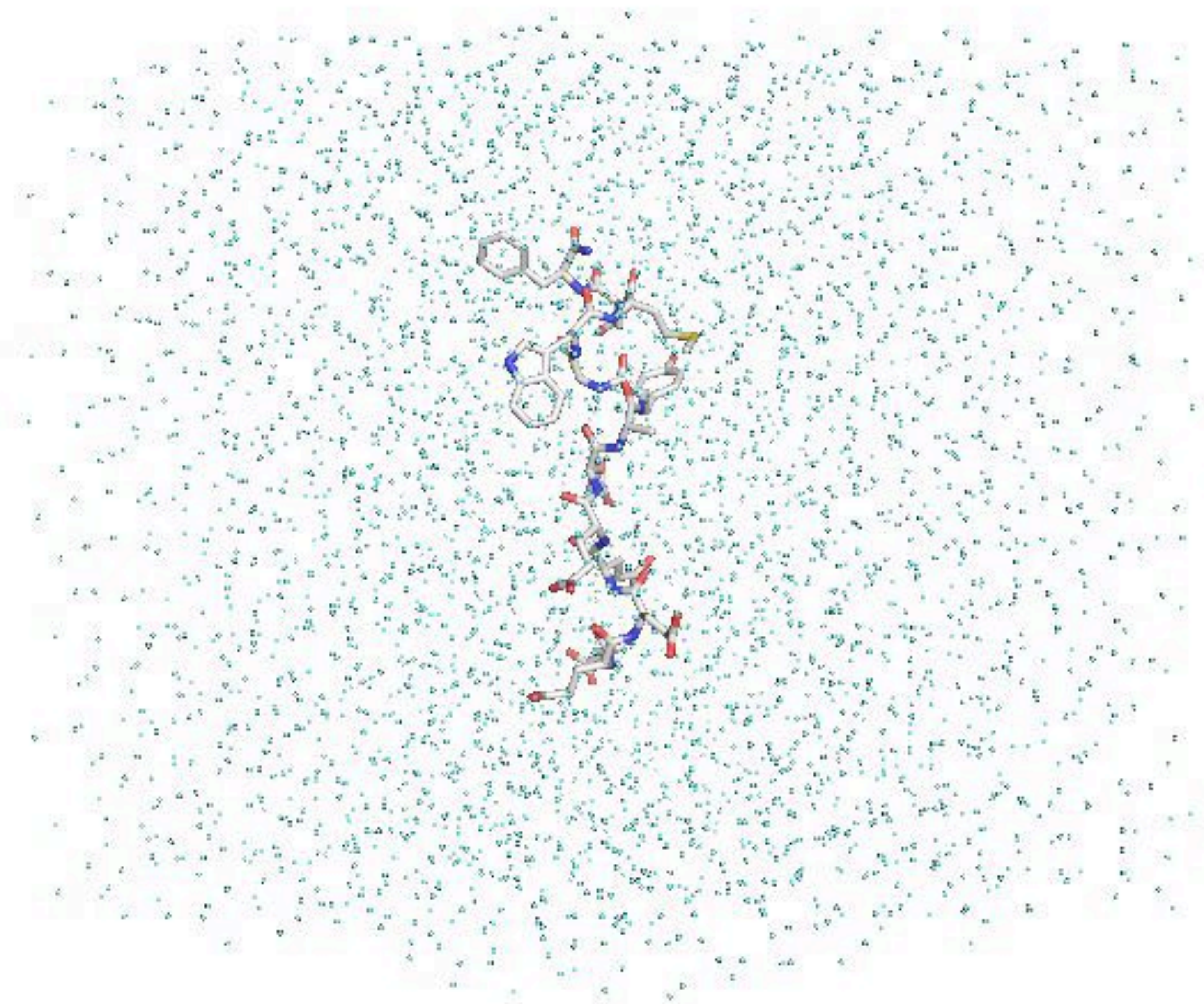
AR058



(attention: D-Glu stereochemistry)

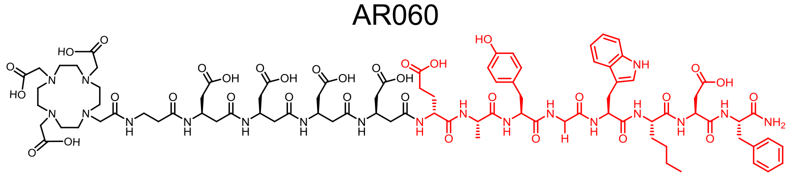
AR033





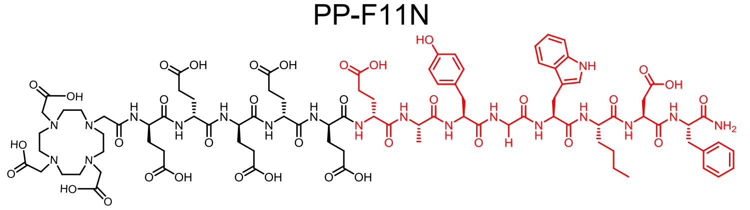
Research interests: tumor targetting drugs

AR060



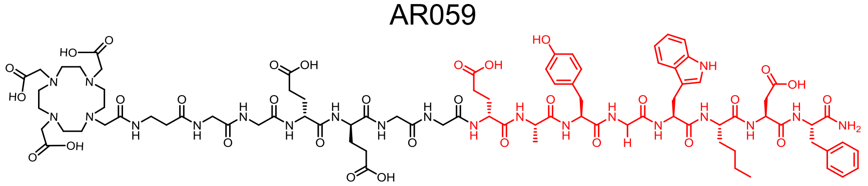
(Beta-glutamic acid sequence)

PP-F11N



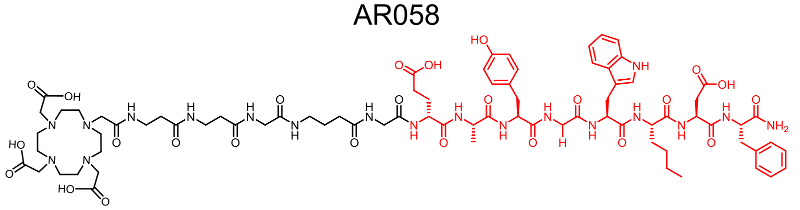
(attention: D-Glu stereochemistry)

AR059



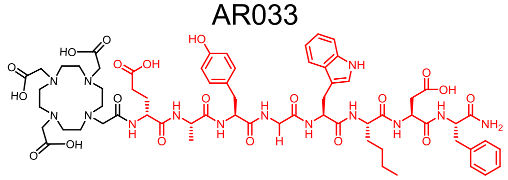
(attention: D-Glu stereochemistry)

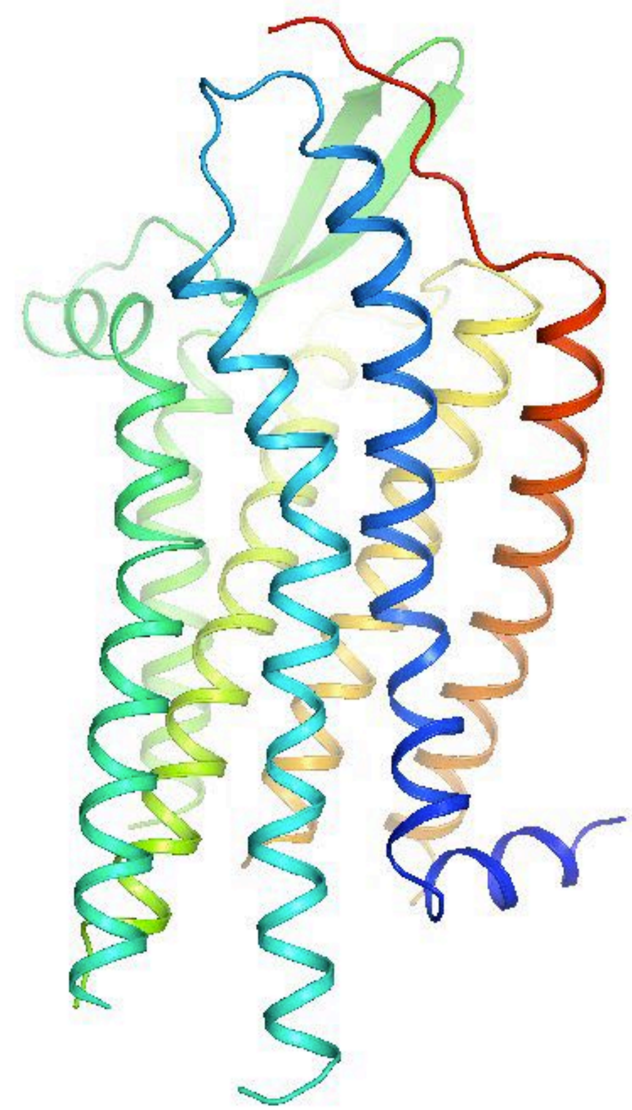
AR058



(attention: D-Glu stereochemistry)

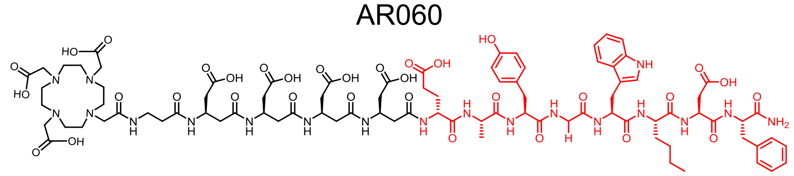
AR033





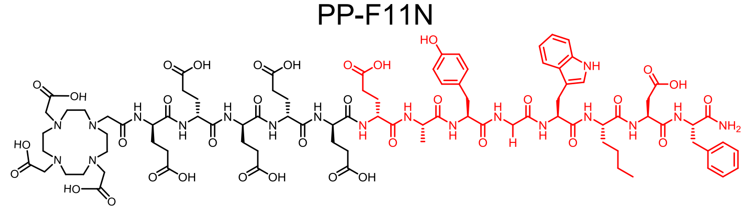
Research interests: tumor targetting drugs

AR060



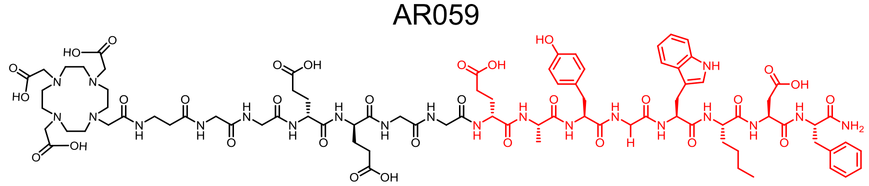
(Beta-glutamic acid sequence)

PP-F11N



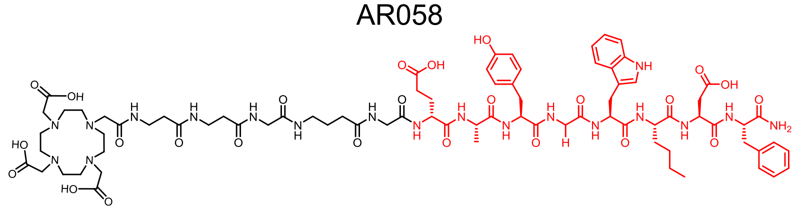
(attention: D-Glu stereochemistry)

AR059



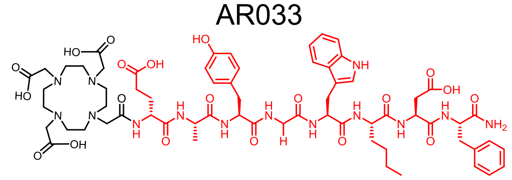
(attention: D-Glu stereochemistry)

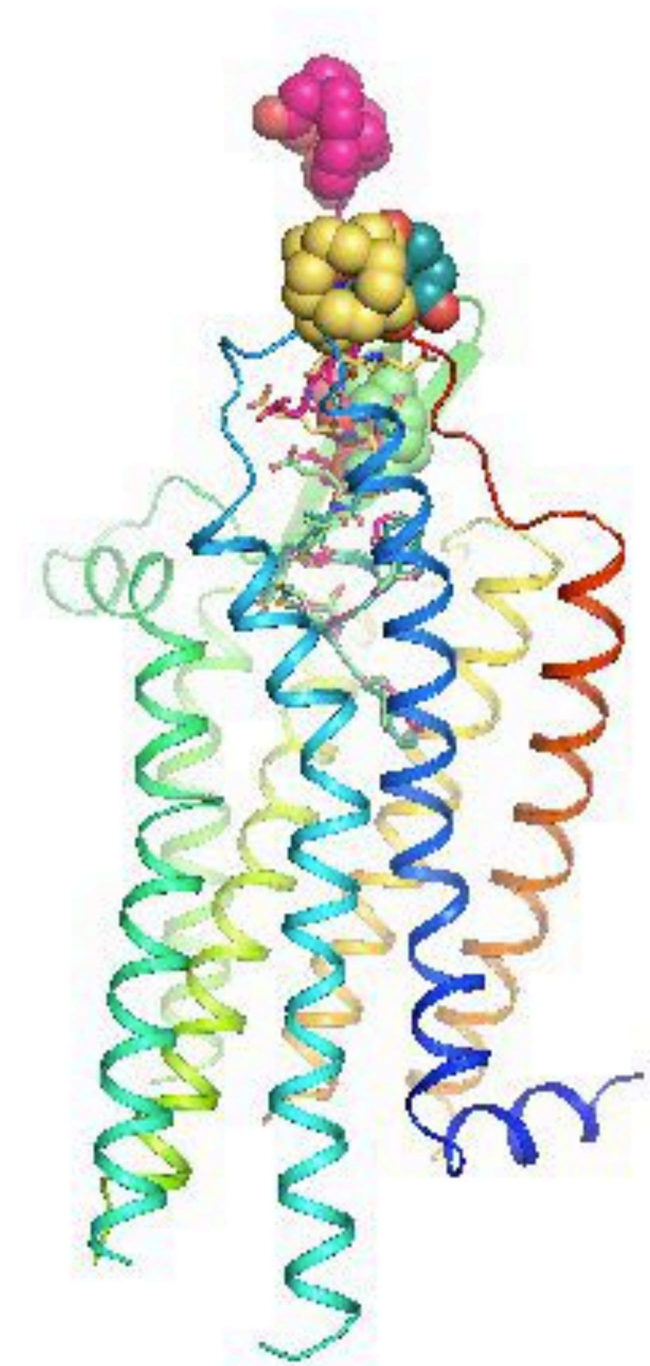
AR058



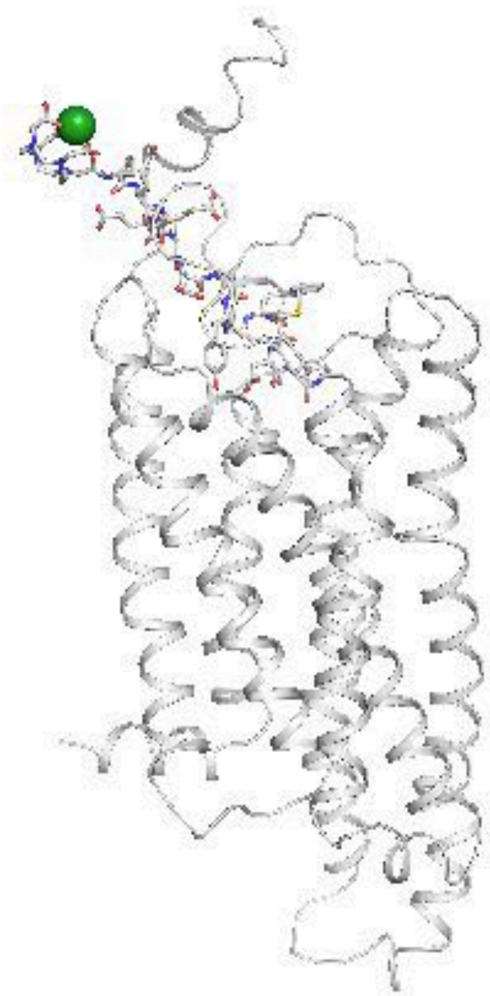
(attention: D-Glu stereochemistry)

AR033





Research interests: tumor targetting drugs



General interests and methodology

Structure of proteins

G protein-coupled receptors

Structural modeling

Molecular dynamics simulations

Future new directions

- The most important challenge facing CMT is to provide theoretical expertise in the field of photonics in- and out- of thermodynamic equilibrium:
  - Quantum optics in the context of many-body physics (no in-house expertise).
  - Driven phases of quantum matter out of equilibrium (complementary to Markus Müller).
  - Ultrafast quantum dynamics (time-dependent DFT and DMFT are two possible computational methods with no in-house expertise).

  In the short term, this expertise cannot be found in house. It can be found in Fribourg (P. Werner) and in IBM Zurich (I. Tavernelli). It could be harnessed through the NCCR QUBE if selected by SNF.
- The expertise of Bernard Delley (DFT) was not replaced within CMT. Many requests for theoretical support at PSI require DFT. Can we find this expertise at LSM\CMT (say with Matthias Krack)?