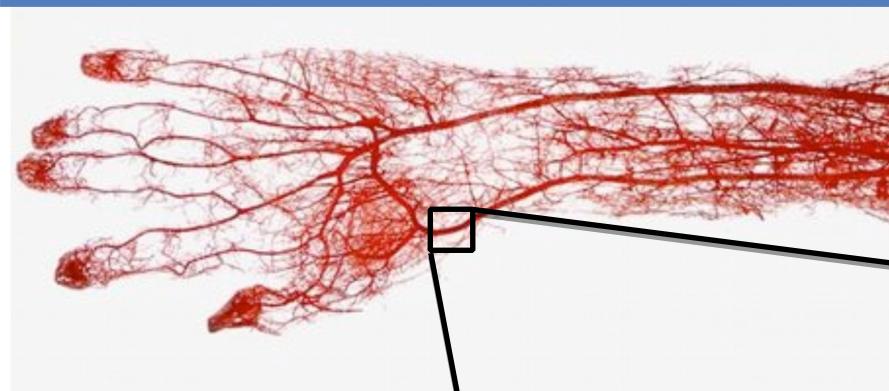
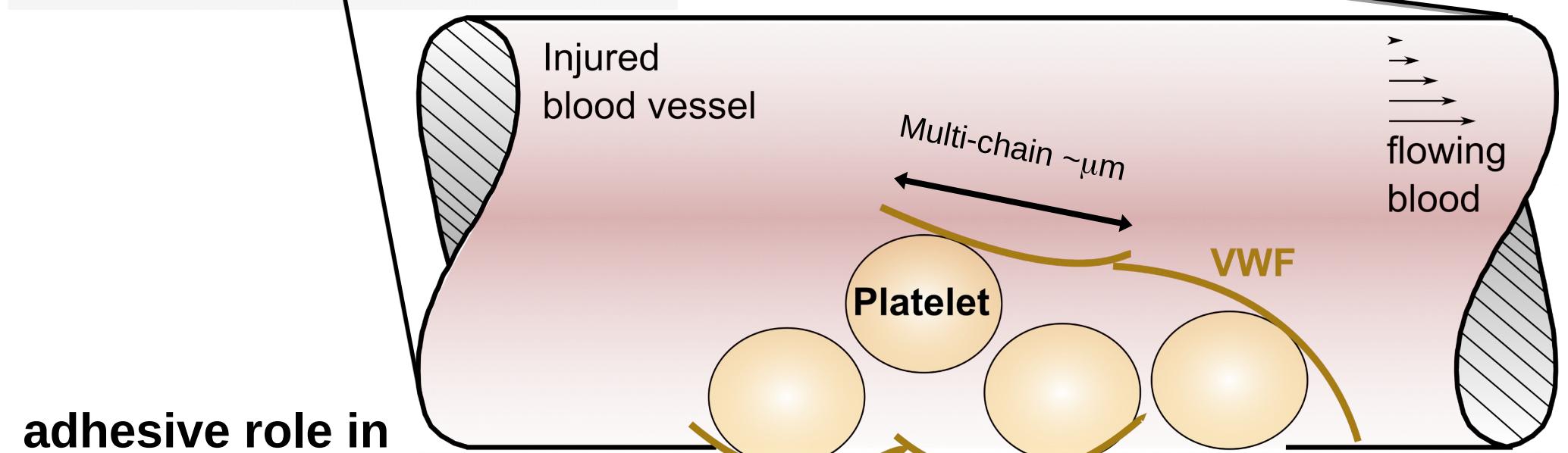


von Willebrand factor (VWF)



*review: Jedi Knight of the Bloodstream.
T. Springer. Blood. 2014*

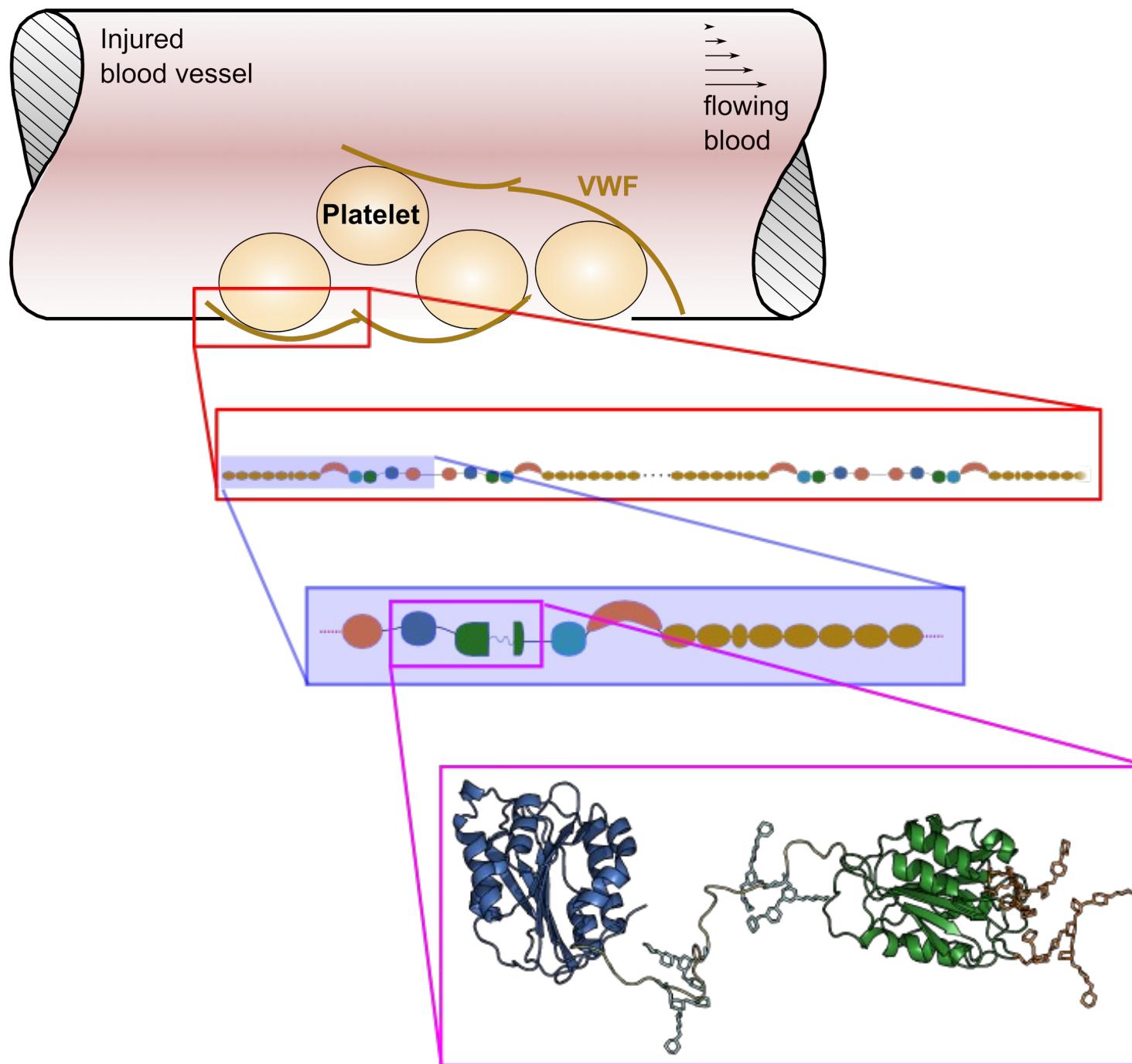


**adhesive role in
primary hemostasis**

**activated by the shear
of flowing blood**

malfunction: bleeding disorders -> **drug targets**
biology - medicine - pharmaceutics
bio-inspired nanotechnology
material science - engineering

von Willebrand factor (VWF)



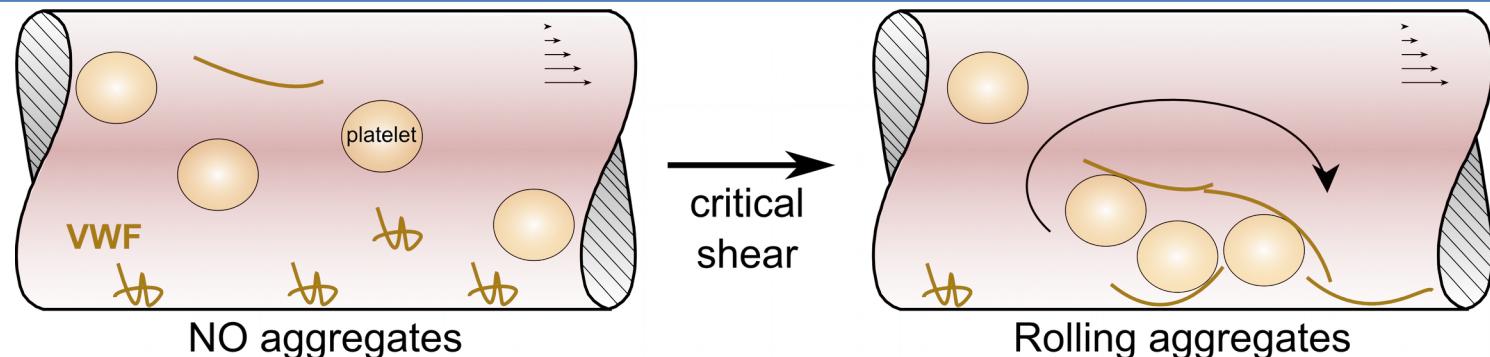
multi-chain (<100 chains)
~ μm

chain (13 domains)
~60-80 nm

protein domain < 8 nm

VWF-platelet rolling-aggregates

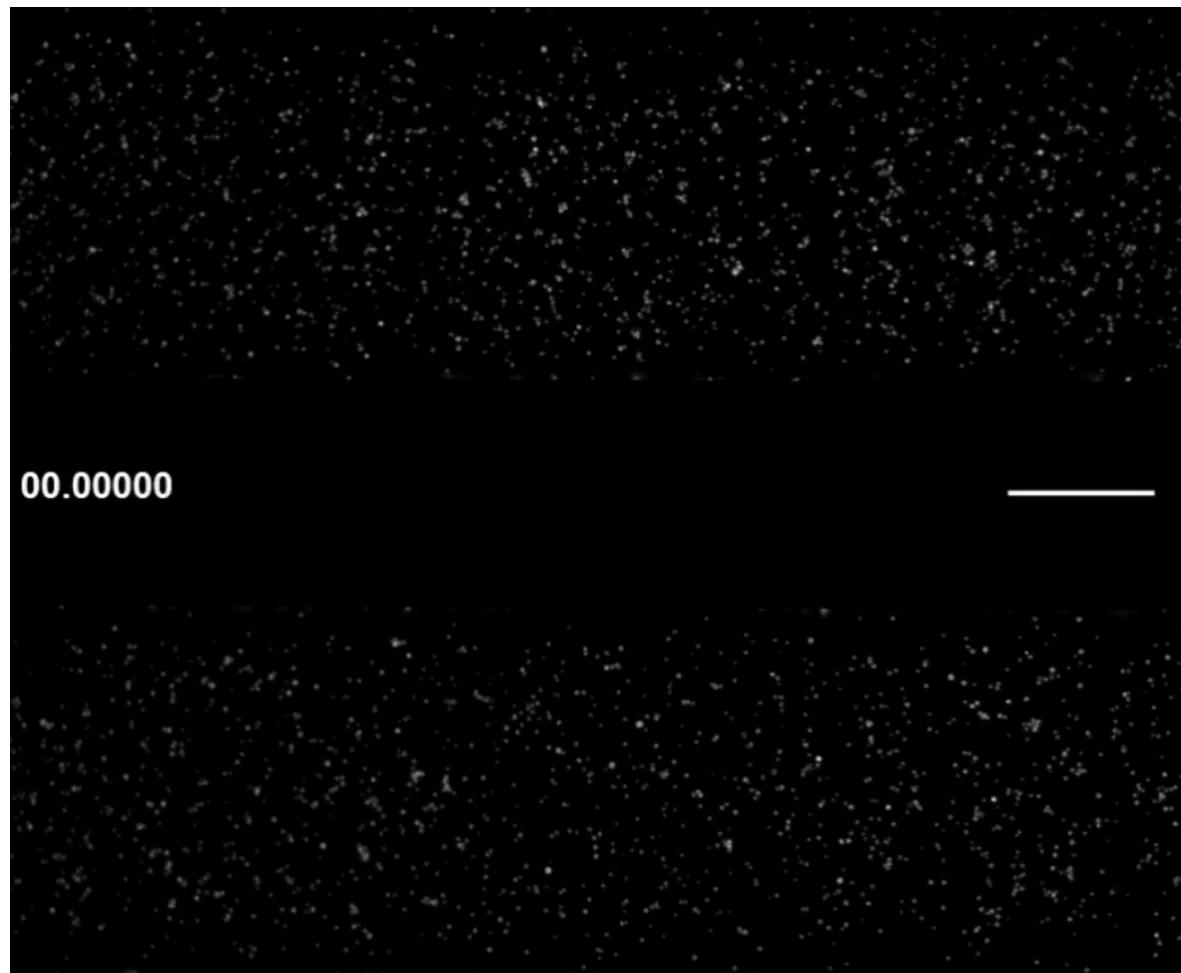
*microfluidic
experiments
Huck, Schneider
Mannheim (Germany)*



0-1 min: 500 Hz

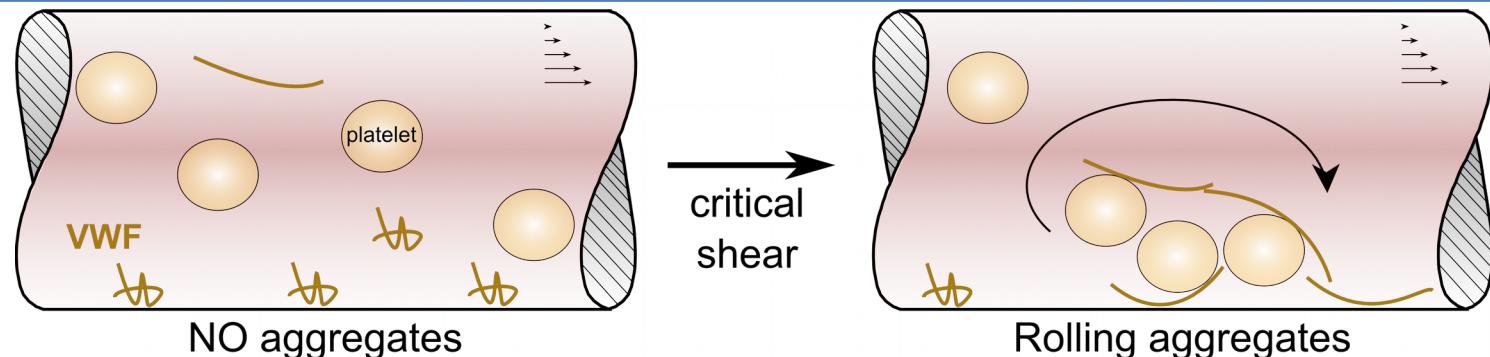
1-5 min: 2500 Hz

>5min: 4000 Hz



VWF-platelet rolling-aggregates

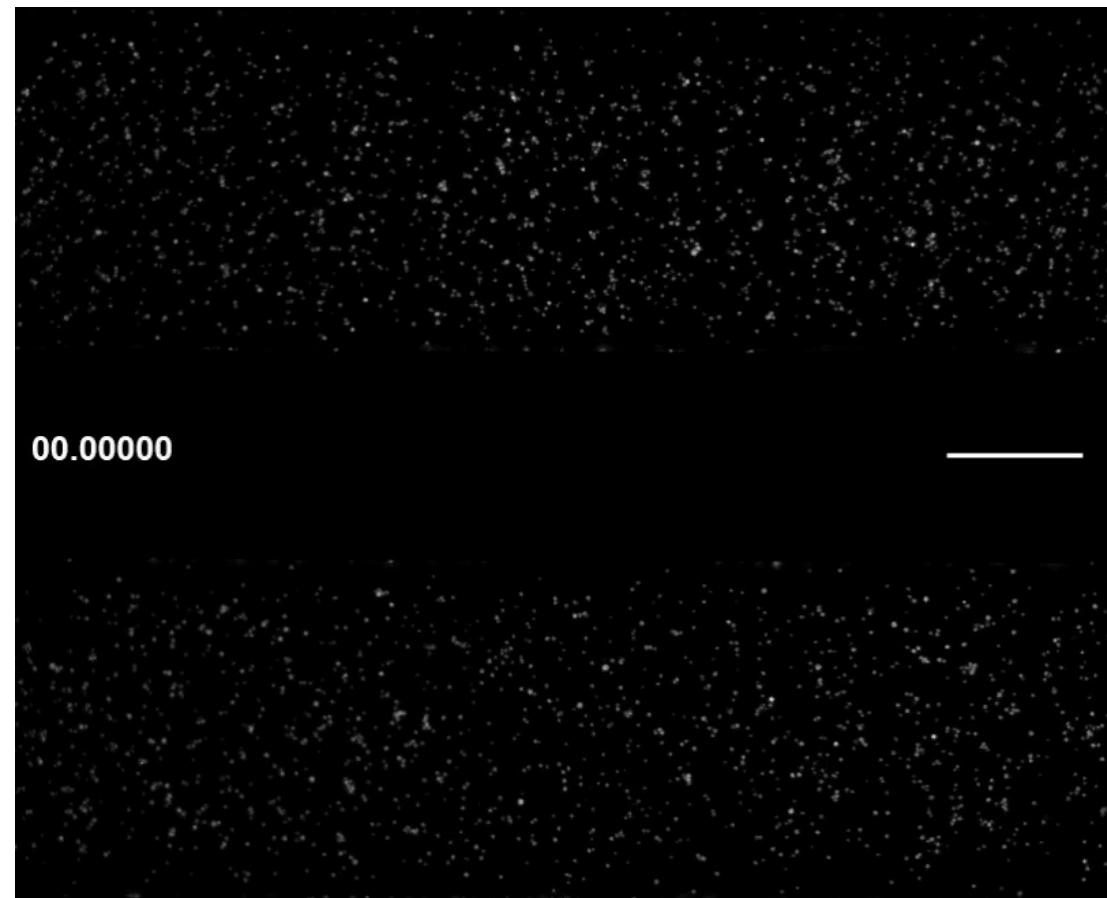
*microfluidic
experiments
Huck, Schneider
Mannheim (Germany)*



0-1 min: 500 Hz

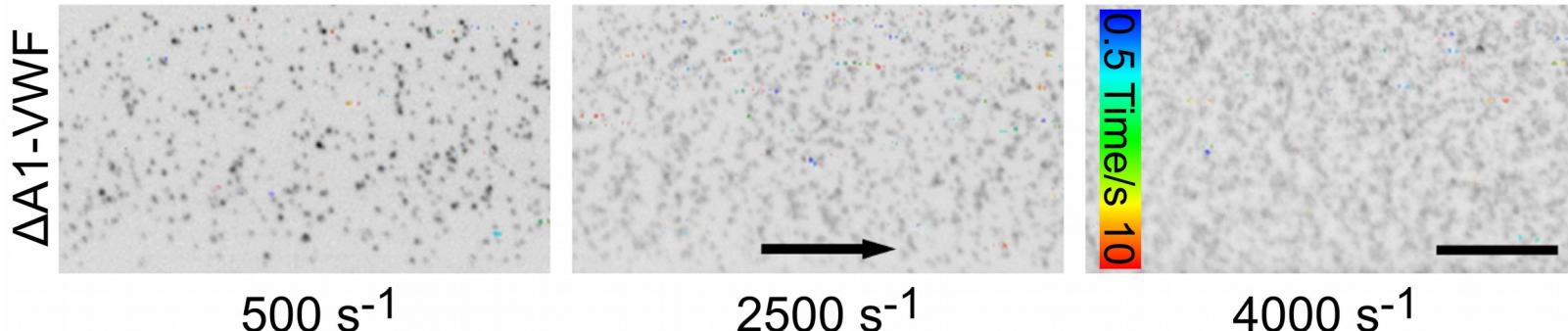
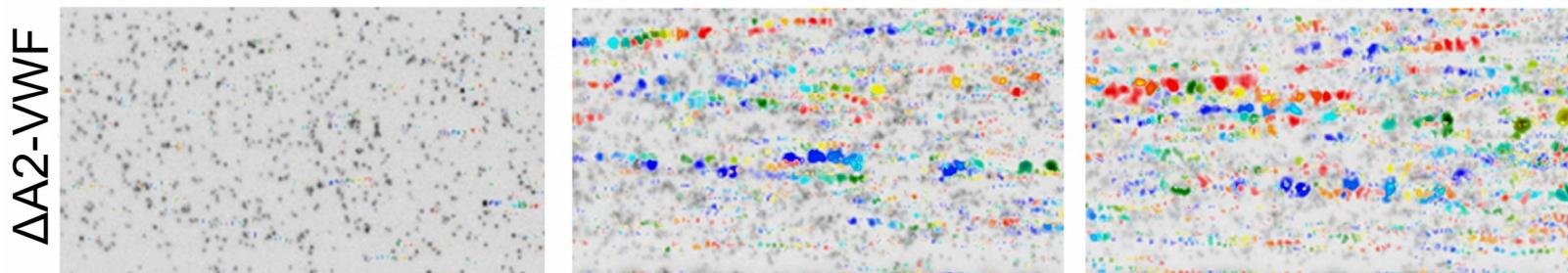
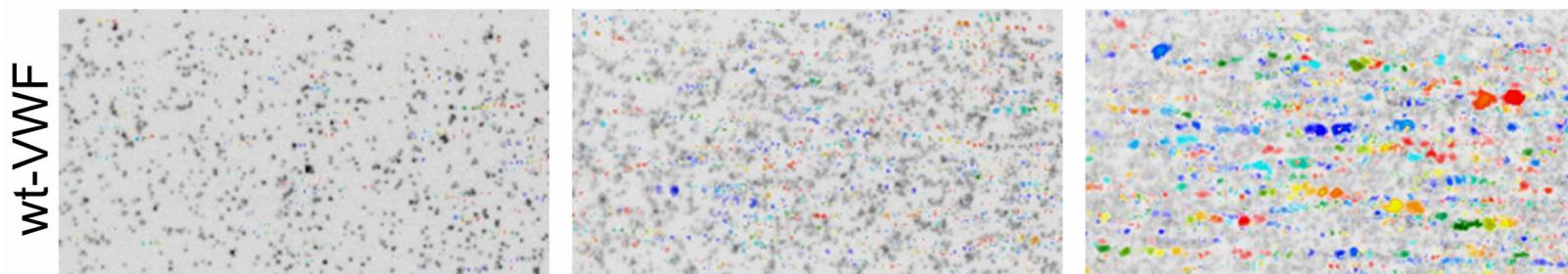
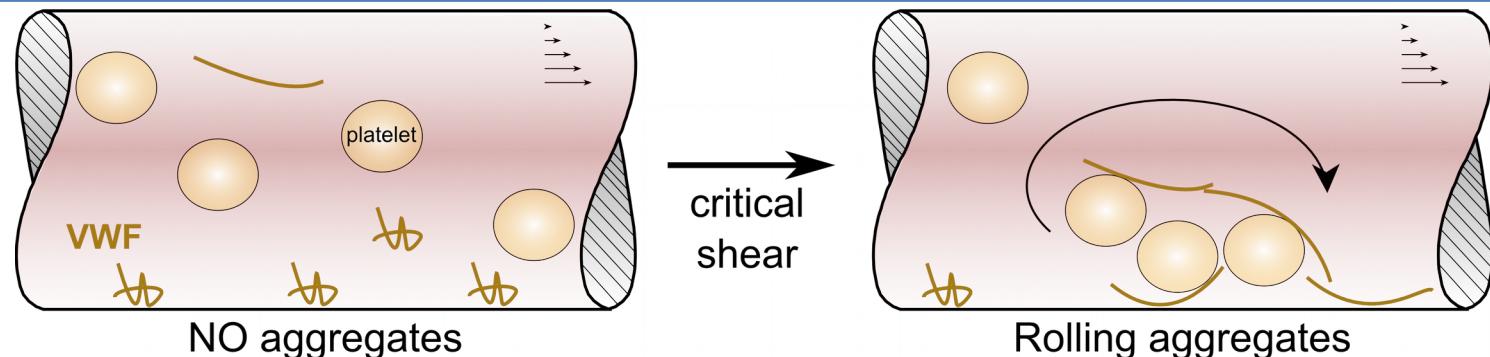
1-5 min: 2500 Hz

>5min: 4000 Hz

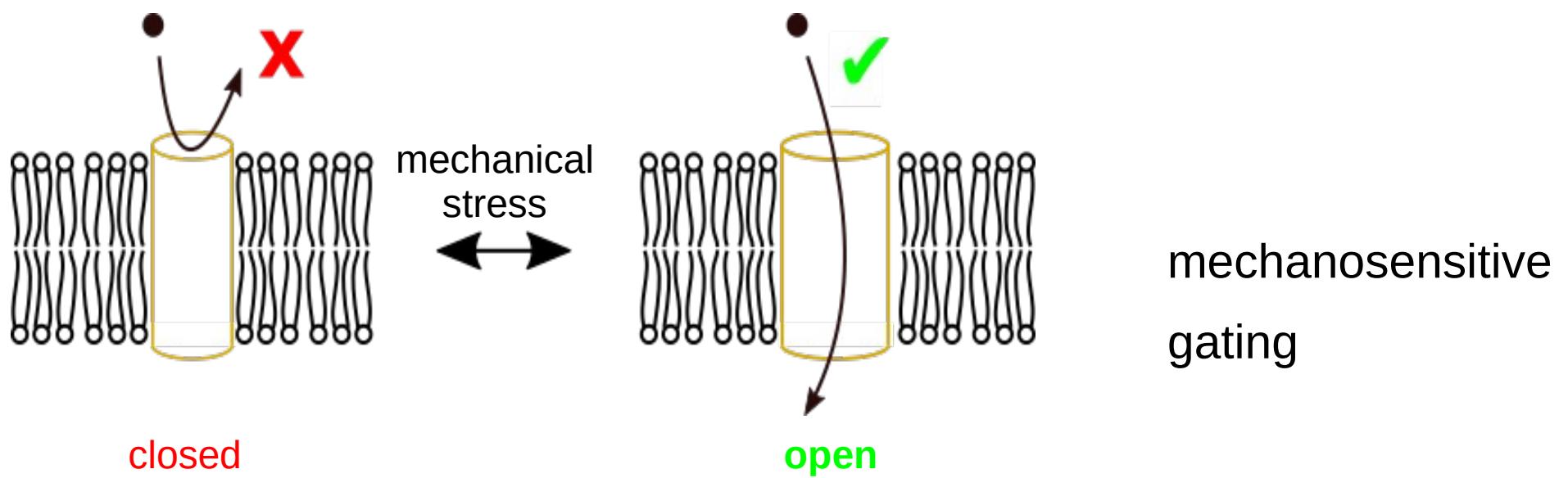
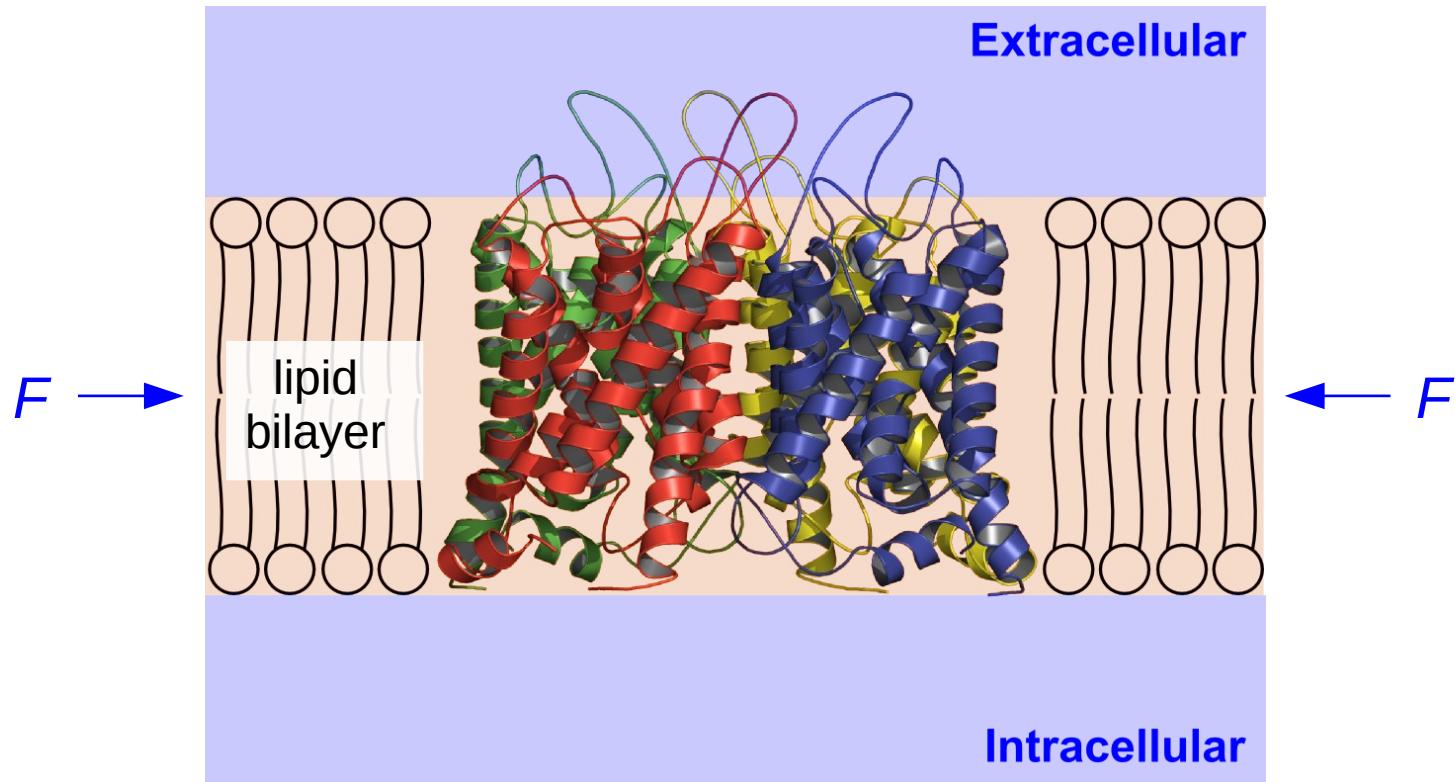


VWF-platelet rolling-aggregates

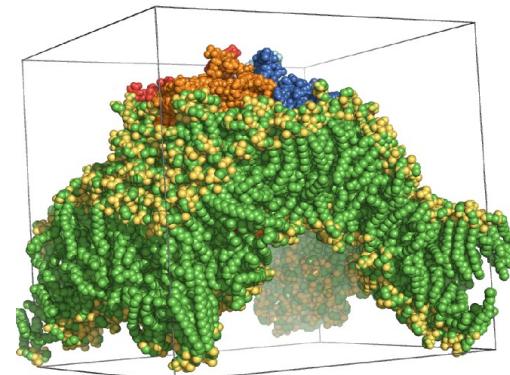
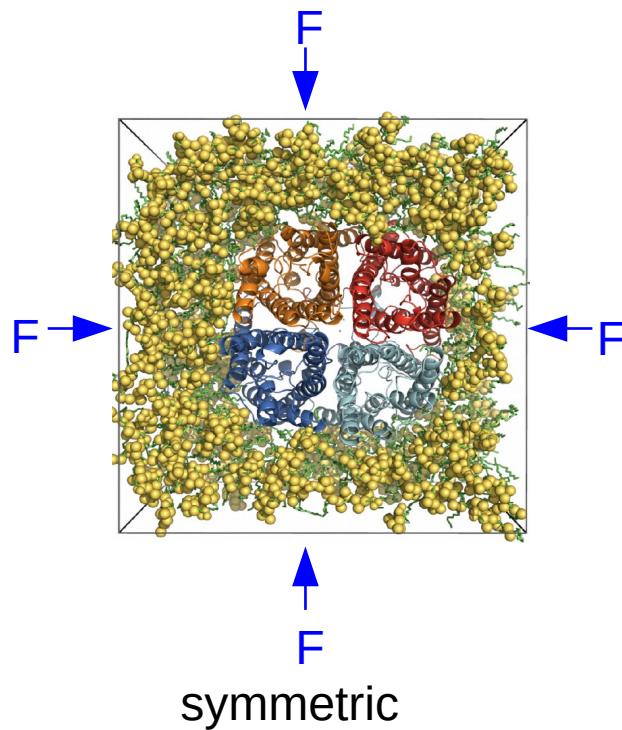
*microfluidic
experiments
Huck, Schneider
Mannheim (Germany)*



Mechanical stress plays key roles in biological membranes



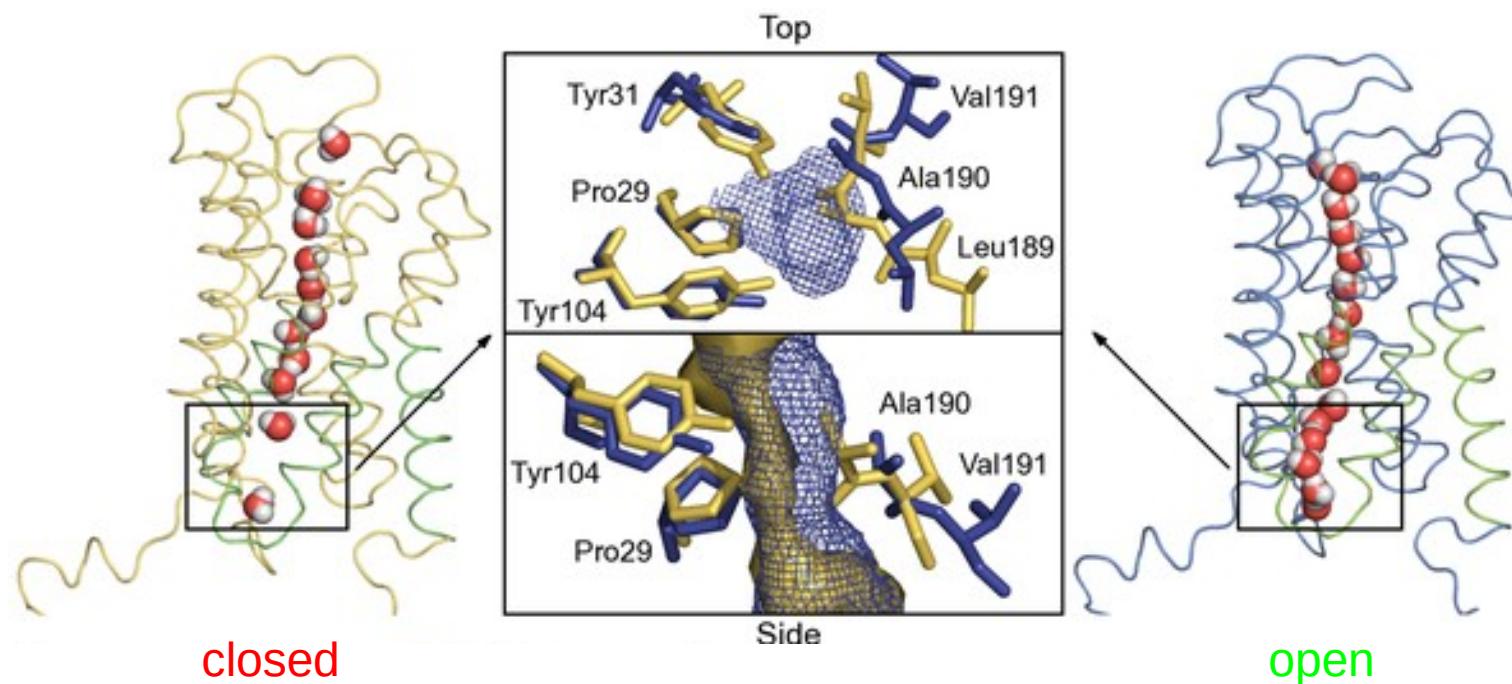
Mechanical stress plays key roles in biological membranes



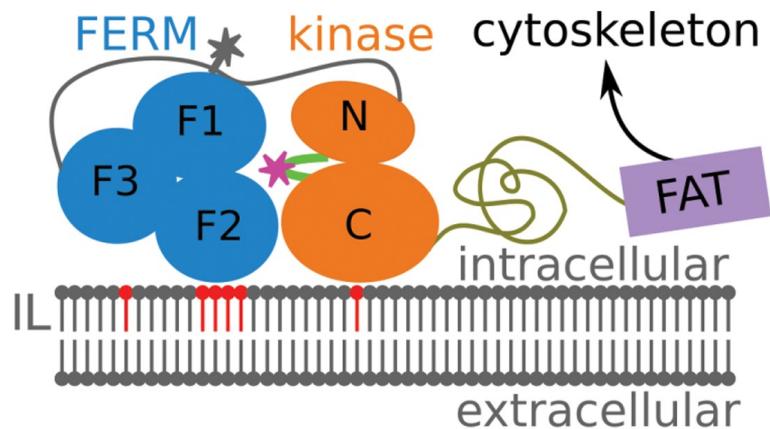
asymmetric

membrane-mediated
mechanosensitive
gating of
yeast aquaporin

*Fischer, Kosinska, CA-S, ...,
de Groot, Neutze, Lindkvist-Petersson
PloS Biol. 2009*

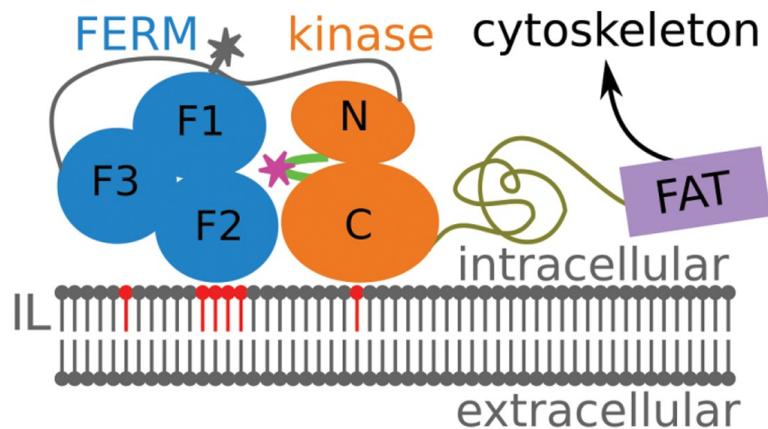


Focal Adhesion Kinase (FAK) mechanoactivation



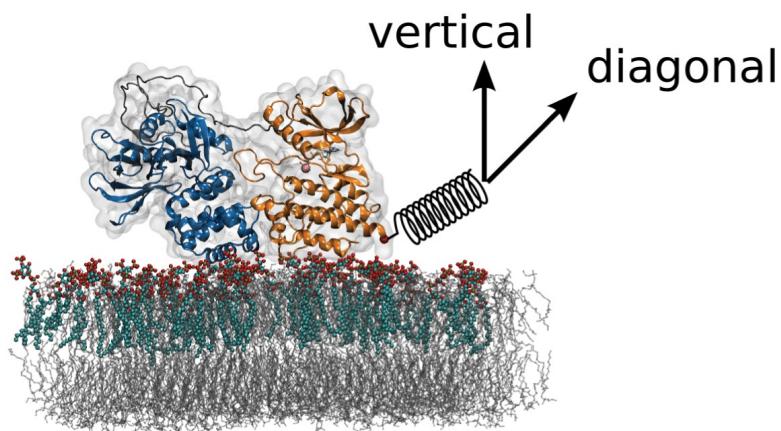
key
signal transductor
at focal adhesions

Focal Adhesion Kinase (FAK) mechanoactivation

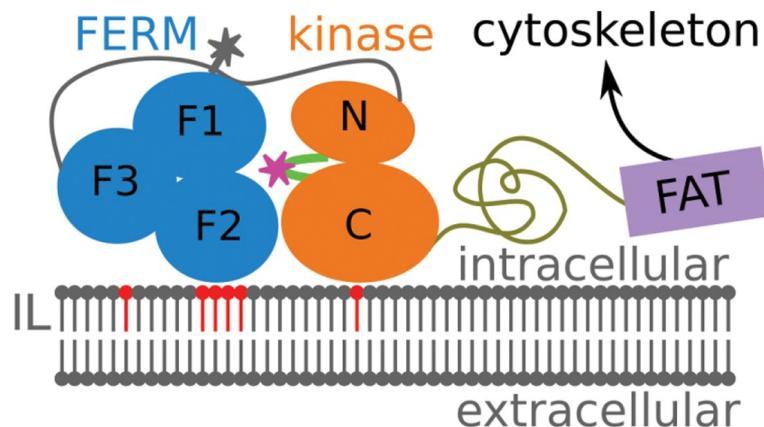


key
signal transductor
at focal adhesions

chemically activated
also
force-activated?

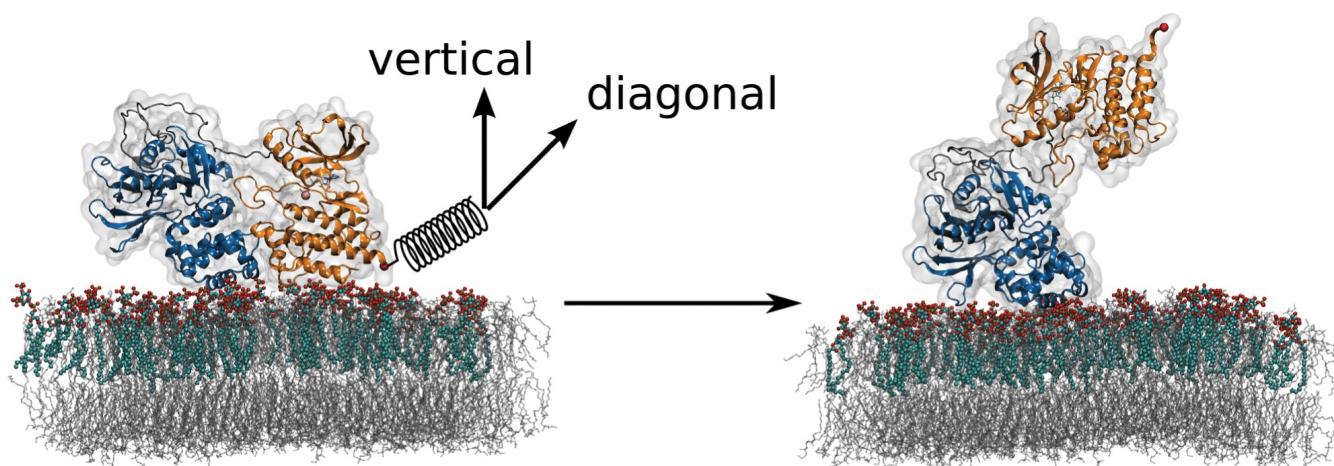


Focal Adhesion Kinase (FAK) mechanoactivation



key
signal transductor
at focal adhesions

chemically activated
also
force-activated?



Force-induced
exposure
of active sites
previous to
domain unfolding



Possible projects

- Collision of two argon droplets
- Equilibrium MD simulation of ubiquitin (or other small protein)
- MD simulation of a membrane protein (with MARTINI)
- MD simulation of a lipid bilayer with two lipid components (with MARTINI)
- 2-dimensional BD simulations of interacting particles
- Free energy changes associated to amino-acid mutation
- Unfolding of a protein using Go-MARTINI
- or your idea?

Workshop

Mechanical Forces in Biology: Theory and Simulation

September 30–October 2, 2019
Universidad de los Andes
Bogotá, Colombia

SPEAKERS:



Alfredo Alexander-Katz
MIT
Cambridge, USA



Pilar Cossio
UdeA
Medellín, Colombia



Frauke Gräter
HITS
Heidelberg, Germany



Helmut Grubmüller
MPI-BPC
Göttingen, Germany



José Daniel Muñoz
UNAL
Bogotá, Colombia



Ulrich Schwarz
Heidelberg U.
Heidelberg, Germany

mptg-cbp.github.io/teaching/for-biol-2019