

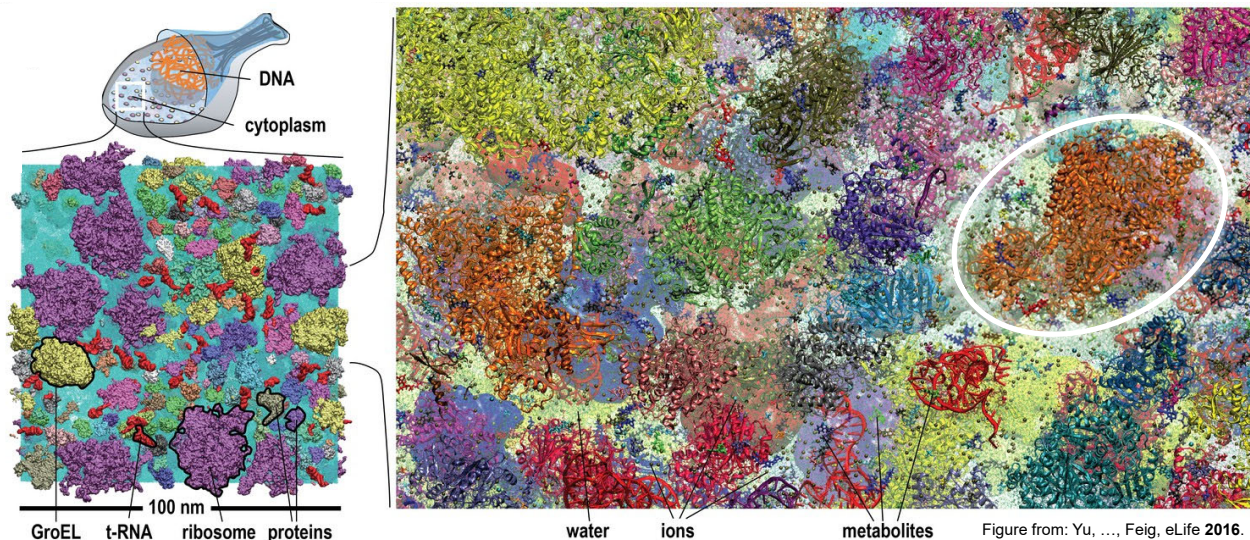
ELUCIDATING AND MODULATING MOLECULAR INTERACTIONS AND FUNCTION 25TH ANNIVERSARY OF NIC

21.4.2023 | HOLGER GOHLKE | IBG-4 [JSC/NIC/IBI-7]

Mitglied der Helmholtz-Gemeinschaft



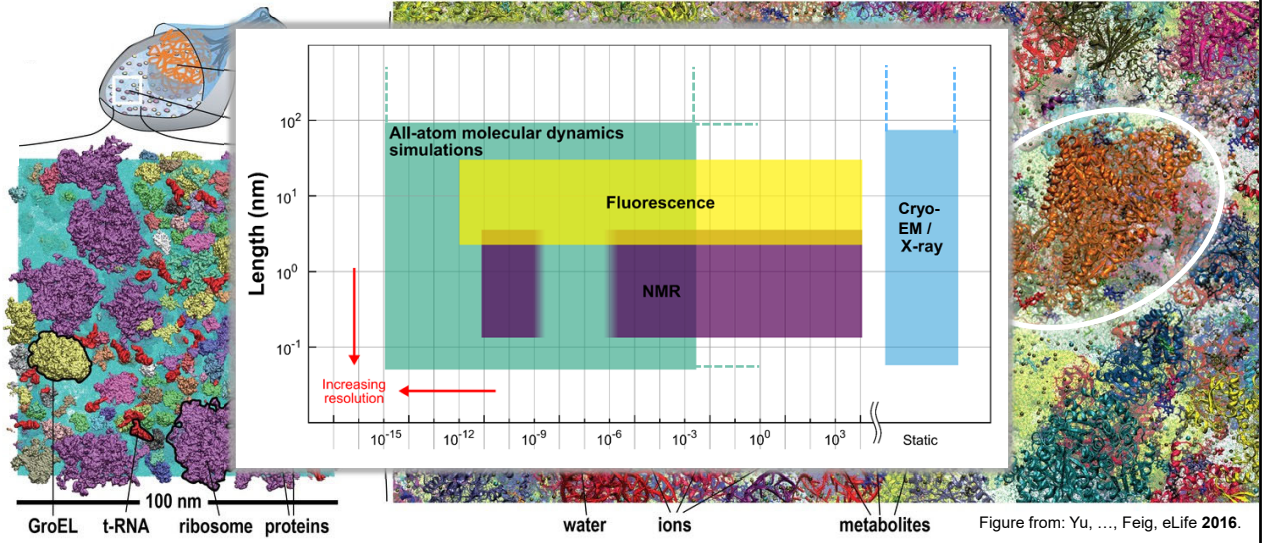
MOLECULAR SIMULATIONS AS COMPUTATIONAL MICROSCOPE



Mitglied der Helmholtz-Gemeinschaft



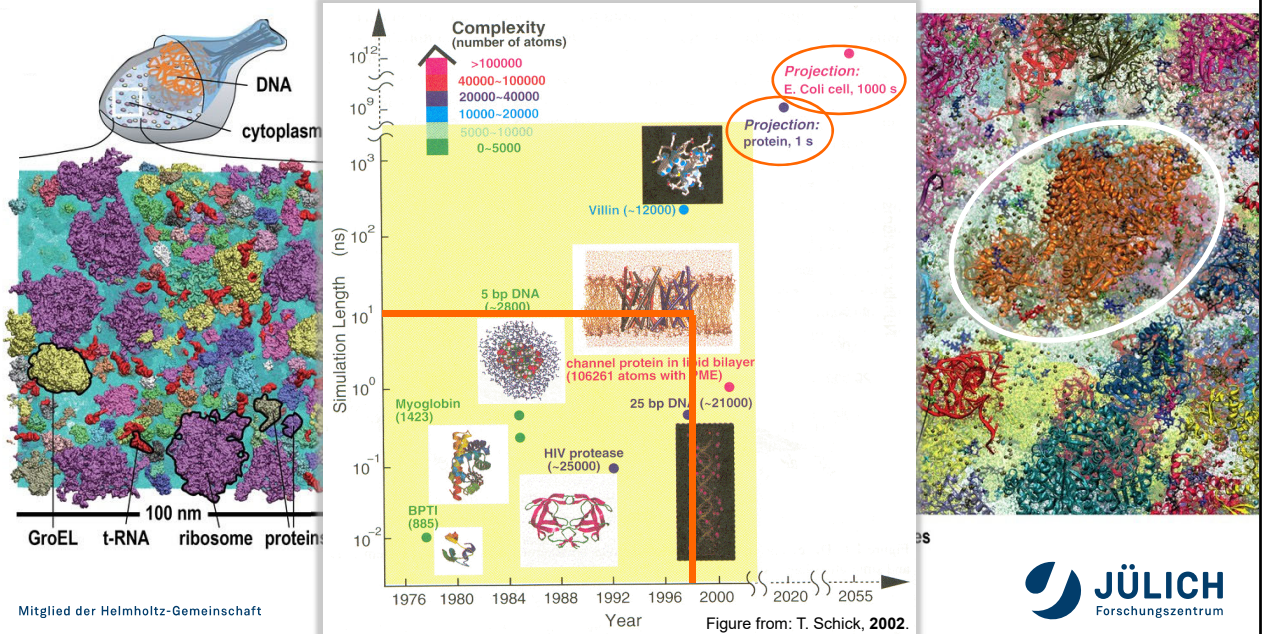
MOLECULAR SIMULATIONS AS COMPUTATIONAL MICROSCOPE



Mitglied der Helmholtz-Gemeinschaft



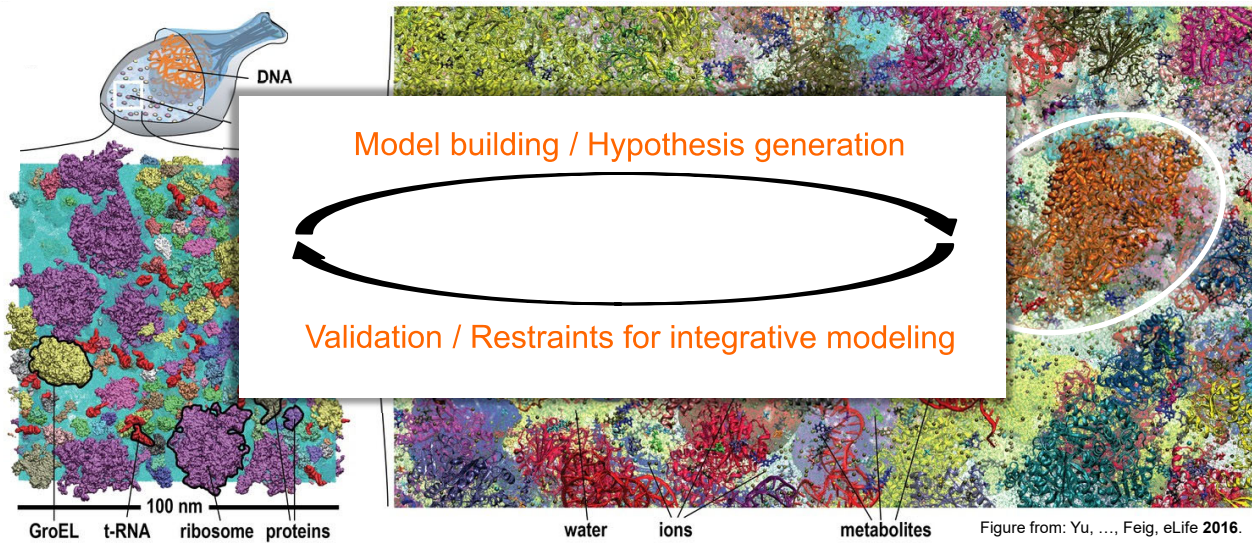
MOLECULAR SIMULATIONS AS COMPUTATIONAL MICROSCOPE



Mitglied der Helmholtz-Gemeinschaft



MOLECULAR SIMULATIONS AS COMPUTATIONAL MICROSCOPE

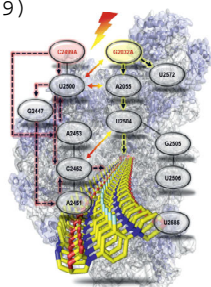


Mitglied der Helmholtz-Gemeinschaft



FROM DAWN TO LIGHT

Binding, selectivity, and specificity of oxazolidinone antibiotics to ribosomes
(05/09)



Ribosomal subunit
($8 \cdot 10^5$ atoms)
Nucl Acids Res 2015.

JUROPA, 150000 core-h / month,
8 nodes, 1 GB / node

Mitglied der Helmholtz-Gemeinschaft



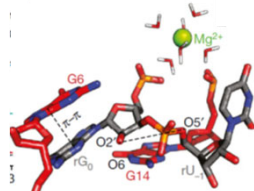
FROM DAWN TO LIGHT

57 applications
later ...

NIC ...
... was supportive
of the modular
concept
... open to GPU
computing

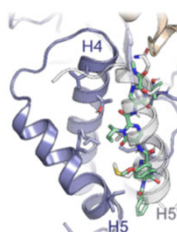
Mitglied der Helmholtz-Gemeinschaft

Enzyme mechanism



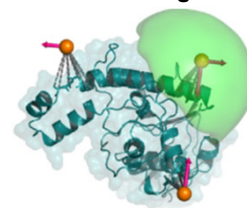
Nature 2022

PPI modulator



ACS Cent Sci 2022

Integrative modeling



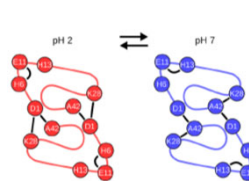
Nature Comm 2020

Thermodynamic profile



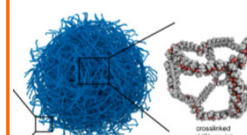
Proc Natl Acad Sci 2021

Amyloid fibril



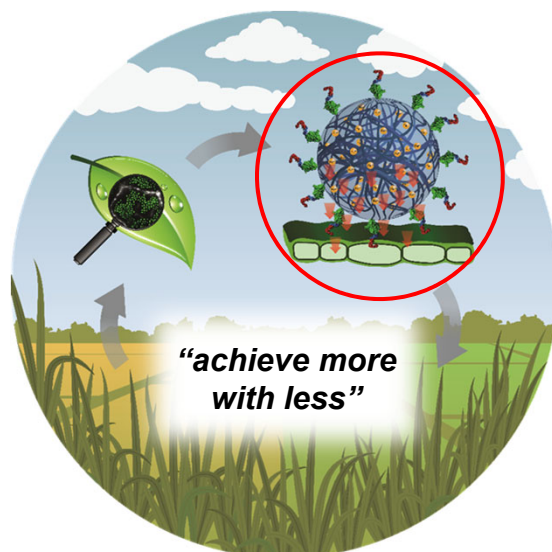
J Am Chem Soc 2023

Microgels as carriers



Chem Eng J 2023

GREENRELEASE – SMART DELIVERY



MAIN GOALS

- increased retention/
rainfastness
- specific binding
- controlled/triggered
release

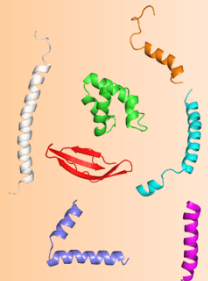
Mitglied der Helmholtz-Gemeinschaft

Meurer, R. A.; [...]; Schwaneberg, U.; Pich, A., *Angew. Chem. Int. Ed.* 2017, 56 (26), 7380-7386

JÜLICH
Forschungszentrum

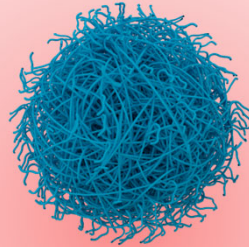
GREENRELEASE – BUILDING BLOCKS

Anchor Peptides



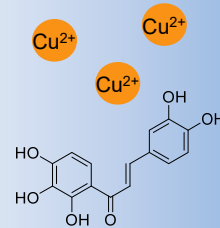
- adhesion promoters for microgels
- increased binding
- selective binding

Microgels



- container/carrier for active agents
- long-term release
- controlled release (T, pH, solvents, light)

Active Agents



- herbicides
- fungicides
- insecticides
- nutrients

Mitglied der Helmholtz-Gemeinschaft
Slides courtesy J. Dittrich

9

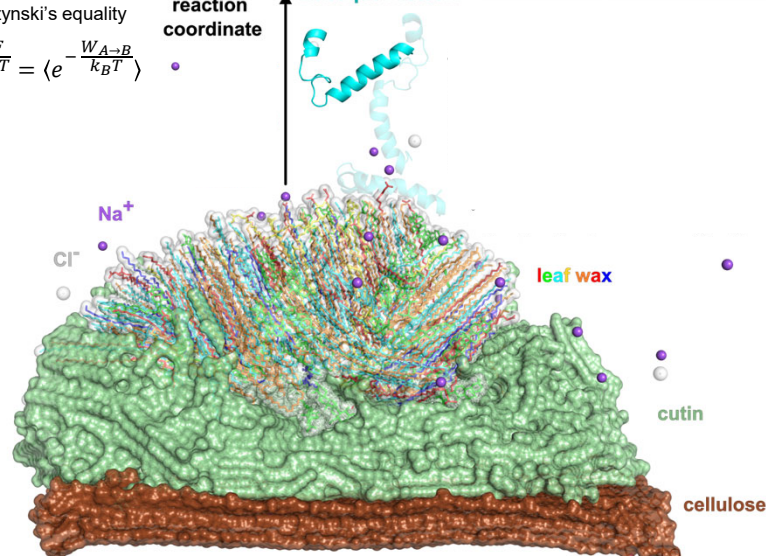
ANCHOR PEPTIDE DESORPTION

Jarzynski's equality

$$e^{-\frac{\Delta F}{k_B T}} = \langle e^{-\frac{W_{A \rightarrow B}}{k_B T}} \rangle$$

reaction coordinate

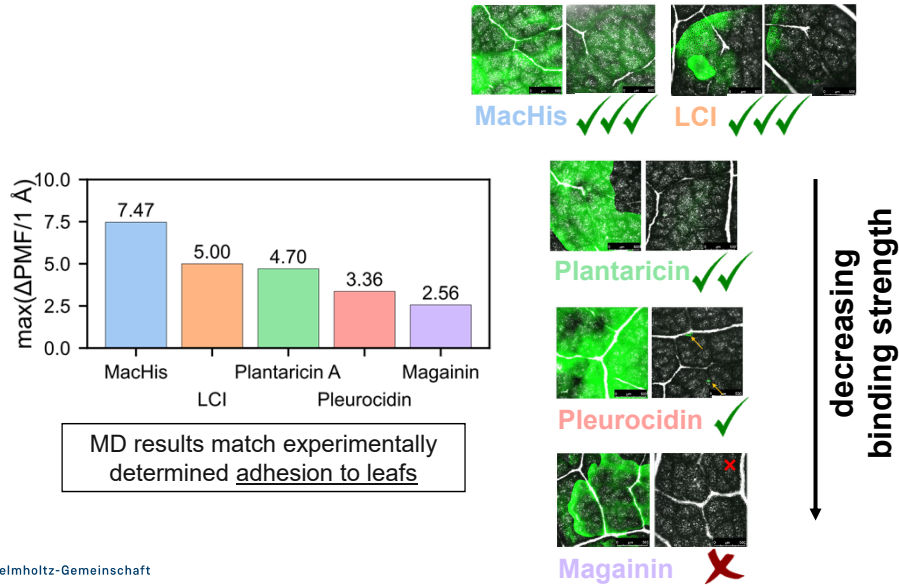
Macaque Histatin



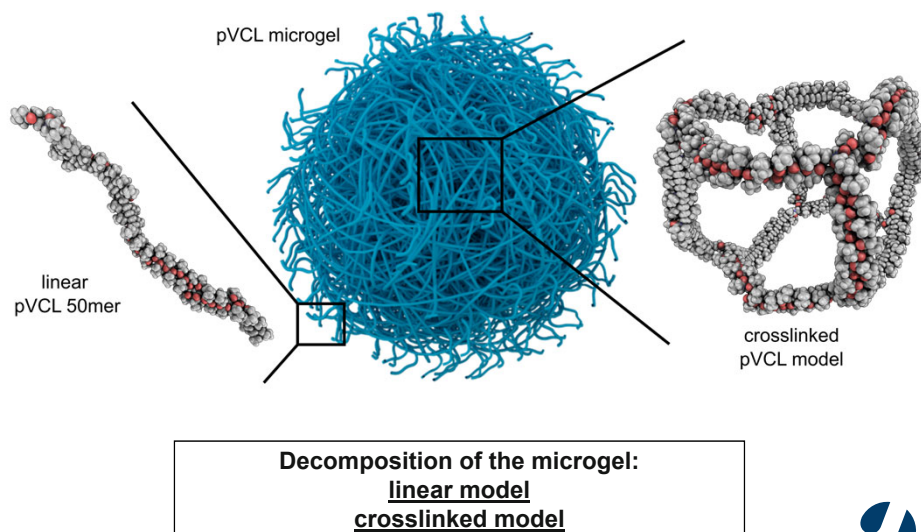
Mitglied der Helmholtz-Gemeinschaft

10

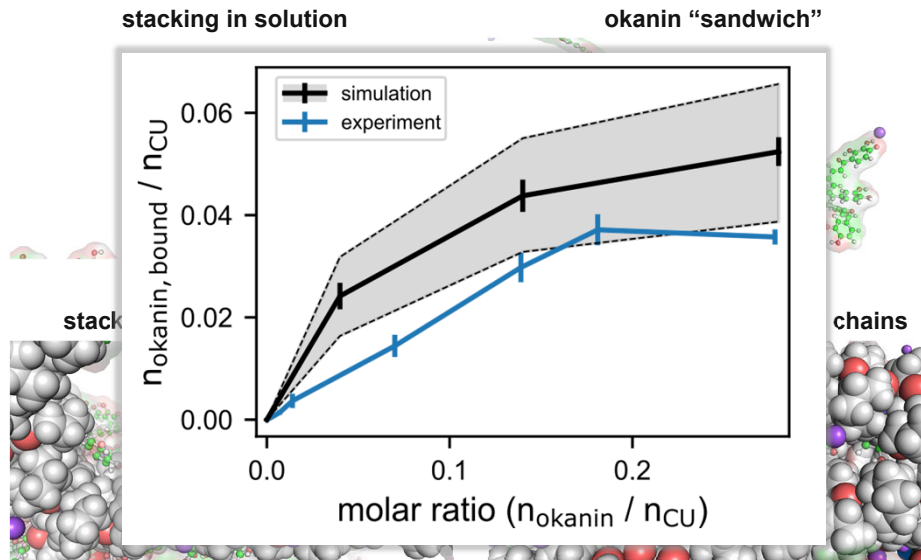
CORRELATION TO EXPERIMENT



MODELING SECTIONS OF PVCL MICROGELS



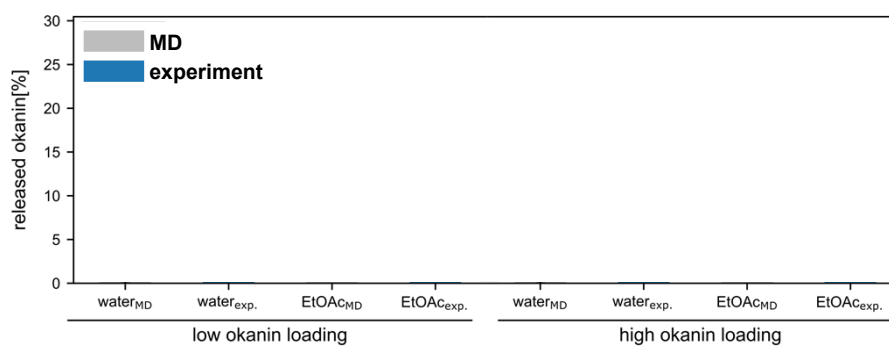
STACKING OF (LOADED) OKANIN



Mitglied der Helmholtz-Gemeinschaft

13

COSOLVENT-TRIGGERED RELEASE



co-solvent triggered release is more effective

experiments are well described by MD simulations
 ➤ **prediction of co-solvent triggered release of other polyphenolic compounds**

Mitglied der Helmholtz-Gemeinschaft

Dittrich, J.; Kolodzy, F.; [...]; Groth, G.; Pich, A.; Gohlke, H., *Chem. Eng. J.* **2023**, *460*, 141631.

ACKNOWLEDGMENT

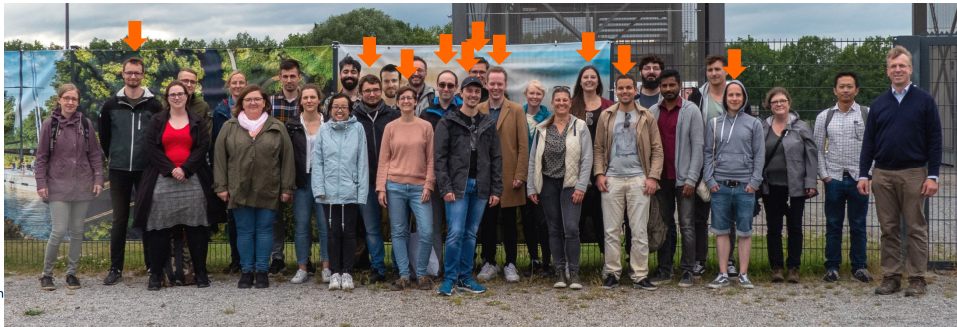
- Computing time



- Funding



Jonas Dittrich
 Ulrich Schwaneberg
 Andrij Pich
 Lukas Schreiber
 Georg Groth



Mitglied der Helm

JÜLICH
 Forschungszentrum