

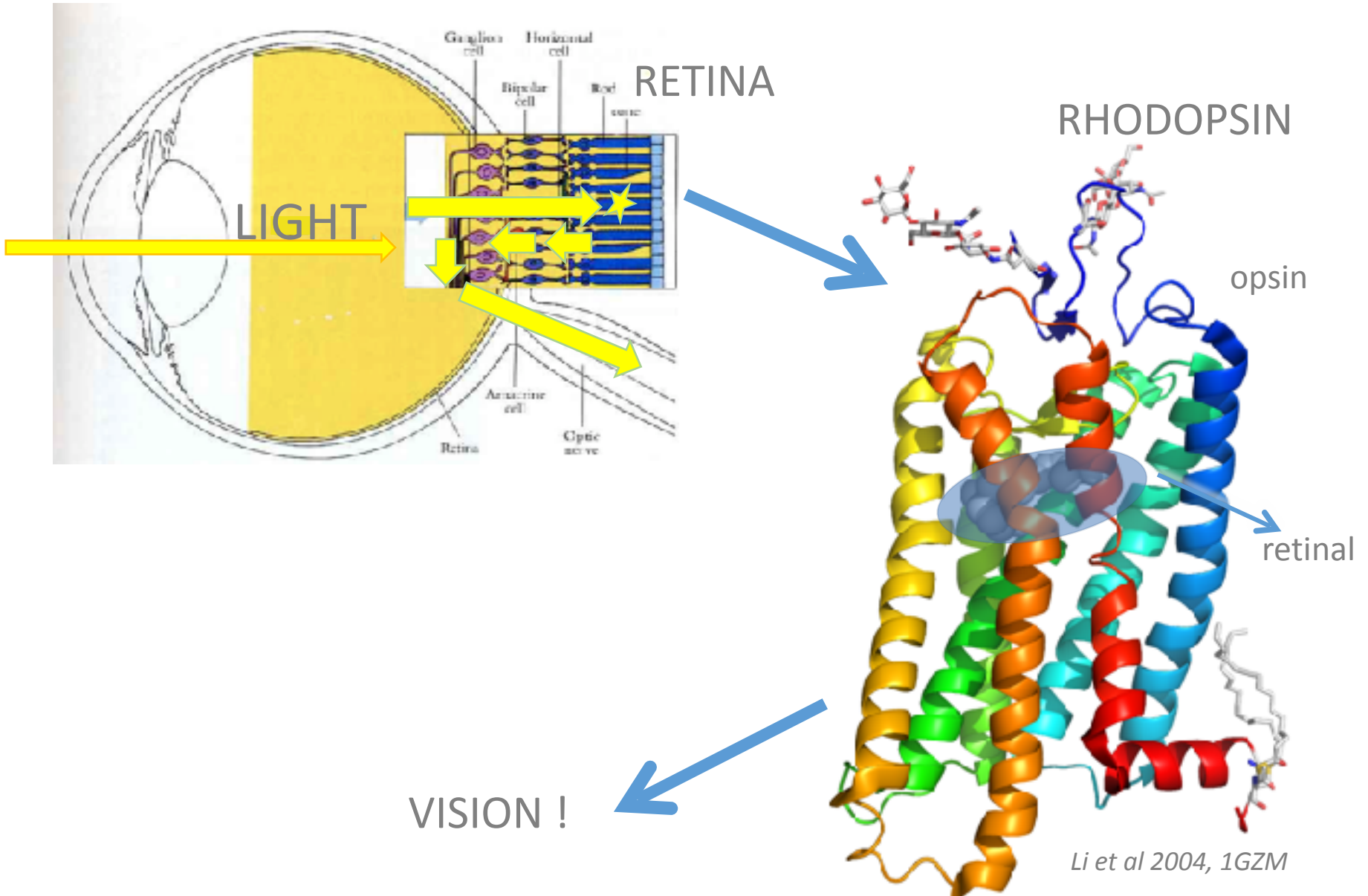


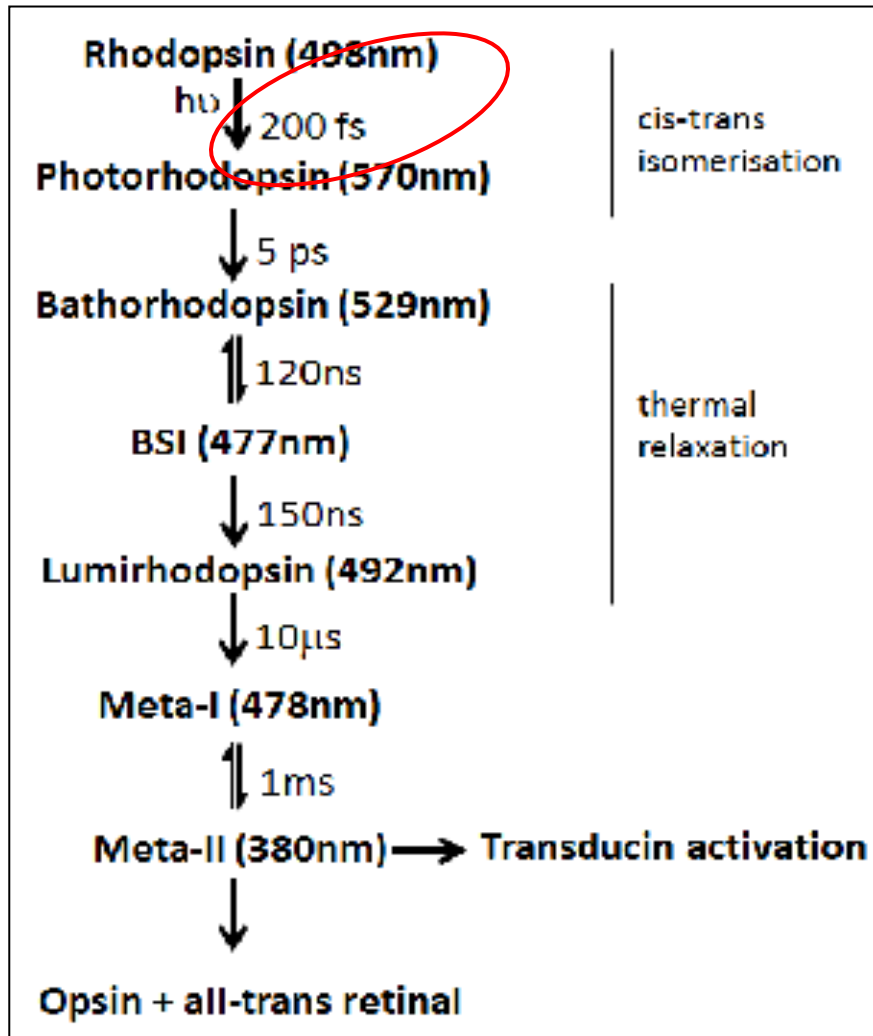
## SwissFEL Exchange Meeting

# Rhodopsin ultrafast dynamics at the SwissFEL.

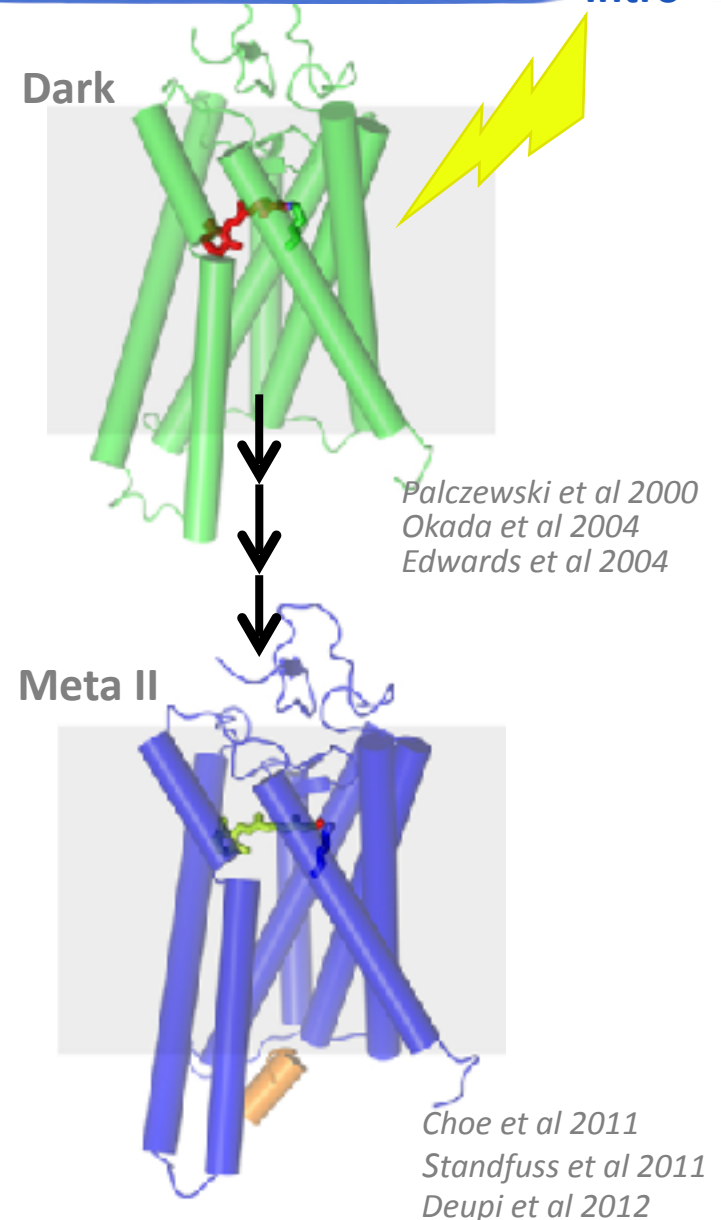
Proposal Panneels-Schertler # 20200597

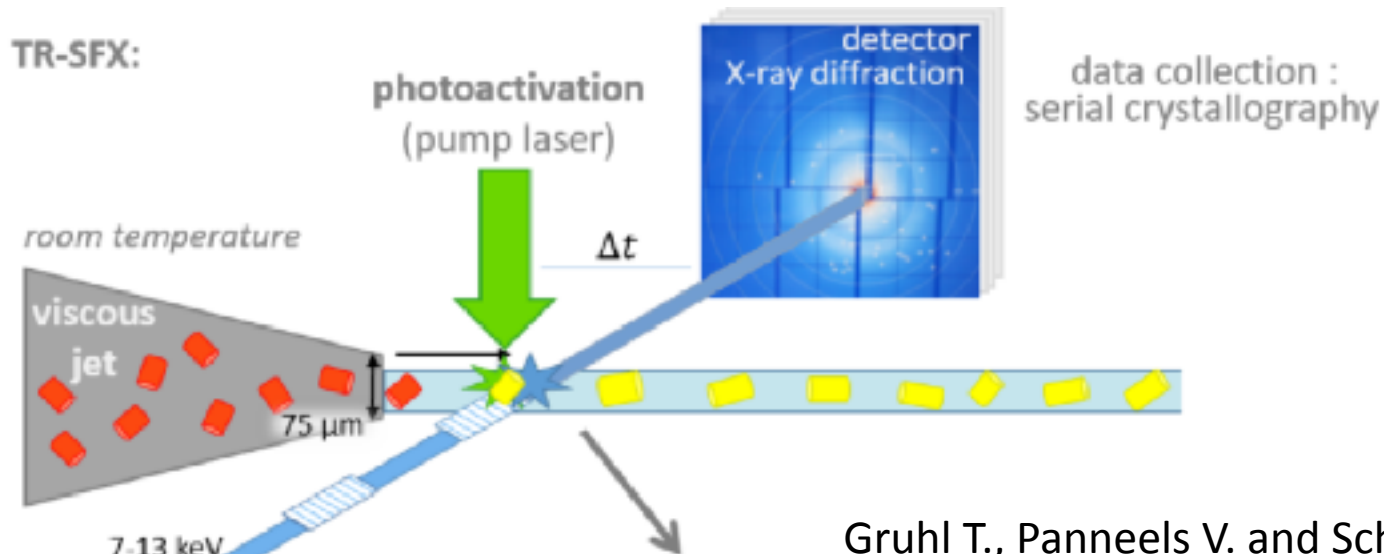
July 21 (Tuesday) 07:00:00 to July 25 (Saturday) 15:00:00 (12 shifts)



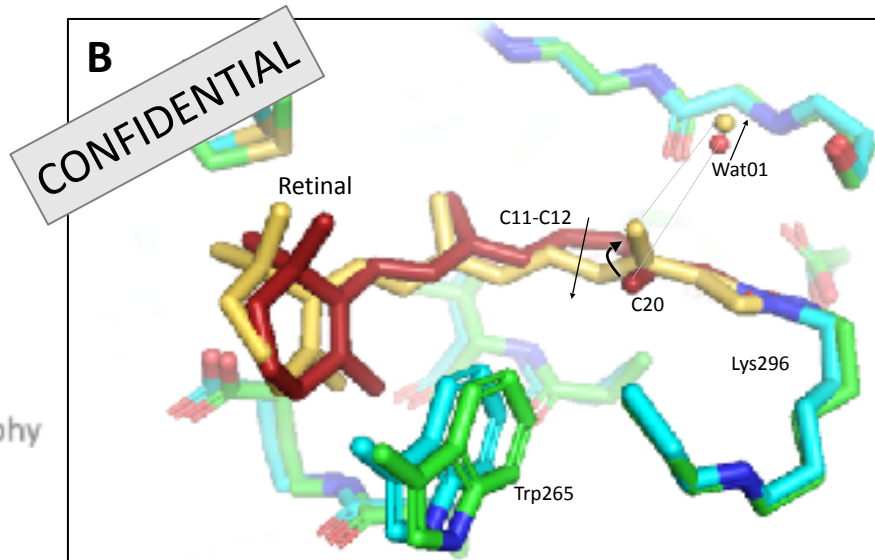


*Mathies et al, Intl Symp. Biophysics  
on Rhodopsins (Y.Shichida) 2017*



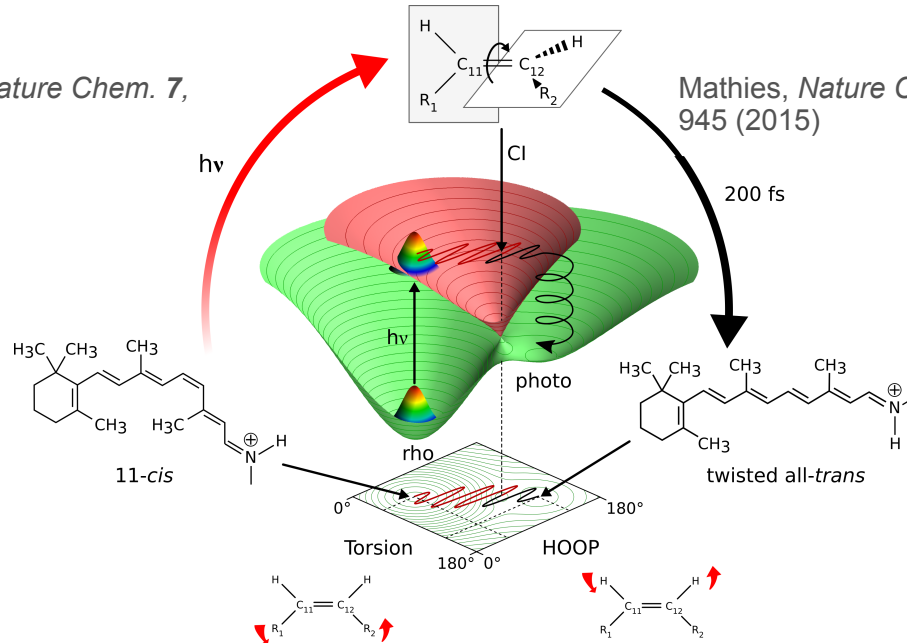
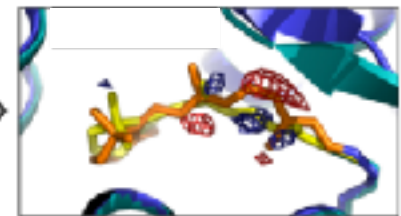
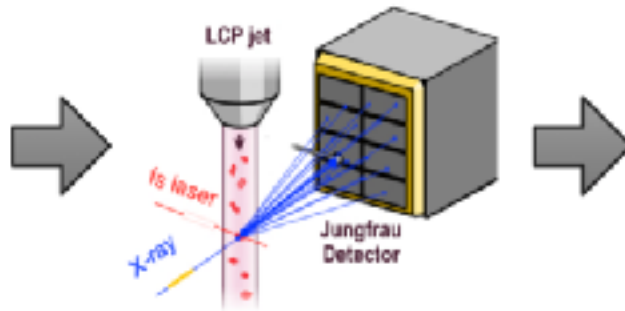
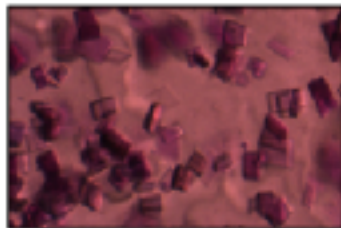


Gruhl T., Panneels V. and Schertler G. and collaborators:



■ 1 ps time-delay  
 ■ dark state

TR-SFX:  
 time-resolved serial femtosecond crystallography

**A**Johnson *et al.* *Nature Chem.* **7**, 980 (2015)Mathies, *Nature Chem.* **7**, 945 (2015)Schneidermann *et al.*, *Nature Chemistry* **10**, 449 (2018)**B**Retinal protein  
crystals grown in LCPTime resolved X-FEL  
crystallography at SwissFELRhodopsin difference  
density map

experiment 20200597

SwissFEL : Alvra station ! Darkness !

- . XFEL, focused **5 x 5  $\mu\text{m}$** , energy **12 keV**, pulse length **25 fs**, max rep. rate **50 Hz**.
- . hutch in red DIM light
- . Detector Jungfrau in 4M mode.

fs-Laser : . **480 nm** pulses.

- . energy pulse 1.5  $\mu\text{J/pulse}$ , **100fs pulses**, **50 $\mu\text{m}$  FWHM**, x mJ/mm<sup>2</sup> at sample position, 0.5-2 photons / rhodopsin.
- . repetition rate **50 Hz** mode 4 light/1 blocked.
- . Time Delay: static : **600 fs**, **300 fs**, **150 fs...** - **10 ps** -  
incremental: **from picoseconds to minus numbers through the 0 fs.**

- Jet :
- . Viscous injector under helium and 200 mbar vacuum.
  - . Reservoir opaque, stainless (60  $\mu\text{l}$ ) - Nozzle **75  $\mu\text{m}$**
  - . Flow 3.3 $\mu\text{l/min}$ .

Samples : . bovine rhodopsin crystals in LCP. **DIM light**. Plates (10 - 10 x 1.5  $\mu\text{m}$  or less!) of space group P 2<sub>1</sub> 2<sub>1</sub> 2<sub>1</sub>.

Data : . SwissFEL pipeline: automatic processing and feedback & data storage.

**SwissFEL beamtime (21.07, 7AM to 25.07, 7AM) - Covid19 PSI regulations:**

**4 people maximum in the Alvra Control Room, one person in the lab**, and we can probably have **one other person on-site but located in EH.060 (tech room) or the meeting room.**

**Distribution of people for rhodopsin:** 4 people maximum in the Alvra Control Room, 2 person in the chemical lab, 1 person in the small dark room, 1 "transit-person commuting" in the corridor (attributed "meeting room") and we can probably have one other person on-site but located in EH.060 or the meeting room.

**Alvra control room:**

Chris Milne,, Karoll Nass, Philip Johnson, Gregor Knopp,  
Camila Bacellar Cases da Silveira

**Coordination:**

team A: Gebhard Schertler  
team B: Elena Lesca (21-22 July only)  
team C: Valérie Panneels

**Data Processing, all remote !**

Cecilia Casadei  
Przemek Nogly, ETHZ  
Tobias Weinert, PSI  
(Matthew Rodrigues)

Dmitry Oserov (Photonics)

**High Viscosity Injector, 1 in lab and 1 in transit, corridor:**

team A: Florian Dworkowski (control room/hutch - 21-23),  
Matthew Rodrigues (meeting room)  
team B: Guillaume Gotthard (lab/hutch), Oliver Tejero  
(meeting room)  
team C: Dardan Gashi (lab/hutch), room), Valerie Panneels  
(meeting room)

**Sample Preparation:**

team A: Antonia Furrer (first shift)  
team B: Sandra Mous  
team C: Demet Kekilli

**8 hours-Shifts for jet and sample teams: overlapping:** 8-16 / 16-24 / 24-8 (overlapping changes at 7.30/15.30 and 23.00)

Thank you for adding  
time on Saturday till 15:00

**Logbook / remote:**  
each of us  
Xavi Deupi

## 10 ps and dark data sets

|                      |         |
|----------------------|---------|
| Total indexed 10 ps: | ~71'000 |
| Total indexed dark:  | ~93'000 |
| Resolution:          | ~2.0 Å  |
| Avg. indexing rate:  | 6%      |
| Injectors used:      | 35      |

### All-dark (no laser)

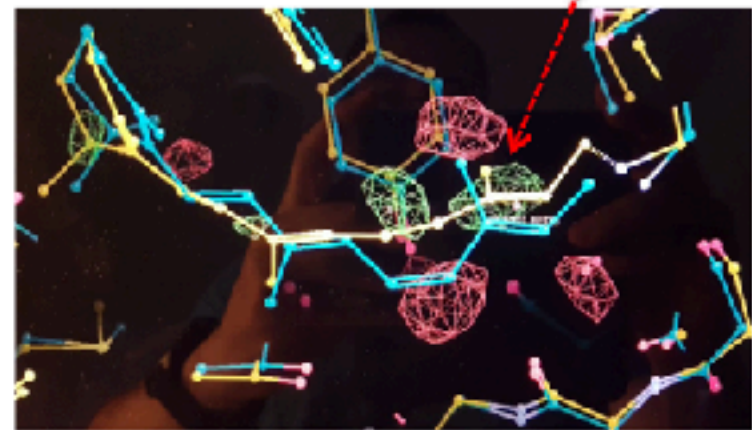
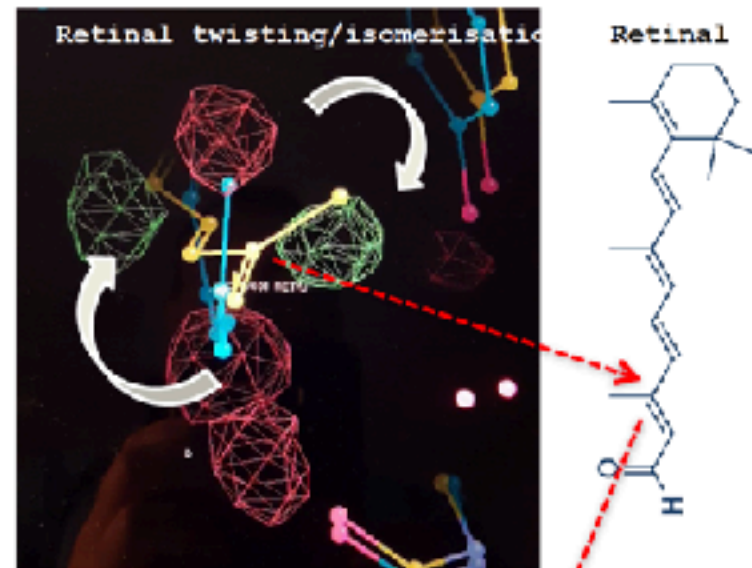
- ~41'000 indexed patterns

### Dark1 from 10 ps time delay

- ~29'000 indexed patterns

### Dark1 from NLSA scan

- ~23'000 indexed patterns



Bildschirmfoto

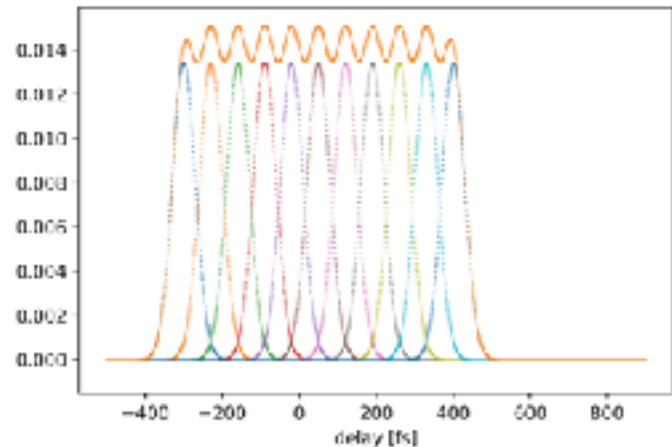
x 190,5 mm

33-23

Difference map: light (10 ps) - dark @ 3σ



**Rhodopsin NLSA scan (start 23 July 2020 18:10)**



- 11 nominal delays
- 70 fs step
- 300 fs
- 230 fs
- 160 fs
- 90 fs
- 20 fs
- +50 fs
- +120 fs
- +190 fs
- +260 fs
- +330 fs
- +400 fs

1'000 shots/delay point @ 50 Hz: 20 s/delay point  
11'000 shots/cycle @ 50 Hz: 220 s/cycle  
1 cycle takes ~4 minutes

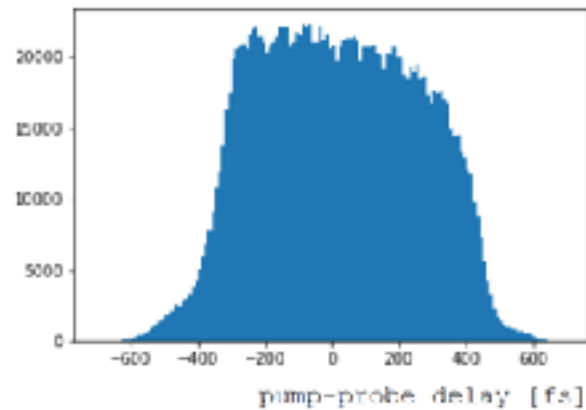
**11 light : 1 dark**

Pump laser: 480 nm, **3 uJ/pulse**, 50 um FWHM, 100 fs FWHM  
X-ray laser: 12 keV, 25 fs (sigma?)

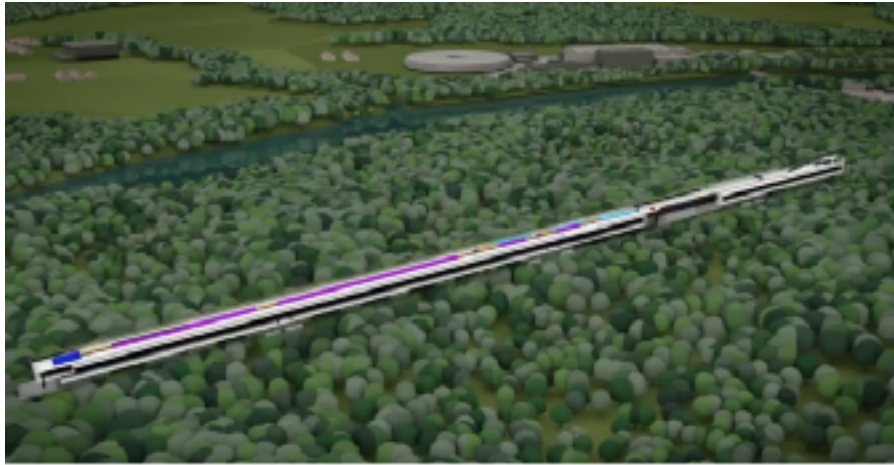
Jet: Bildschirmfoto -> 152 um between shots, ~50 min/reservoir

## NLSA scan timestamps

~ 1.6M collected, light



NLSA scans automatic indexing results:  
251'230 indexed light  
22'995 indexed dark



A team of 22 people contributed

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