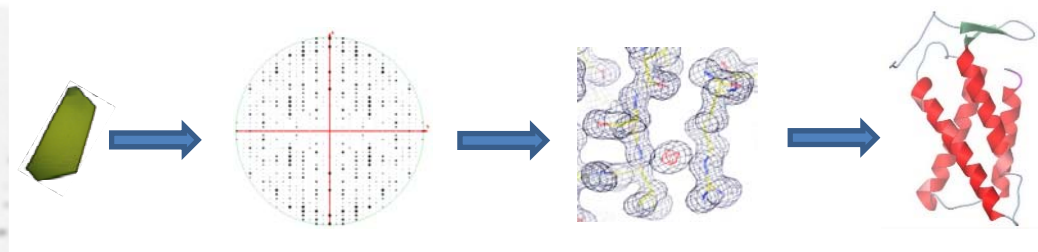


# X-Ray Crystallography Platform

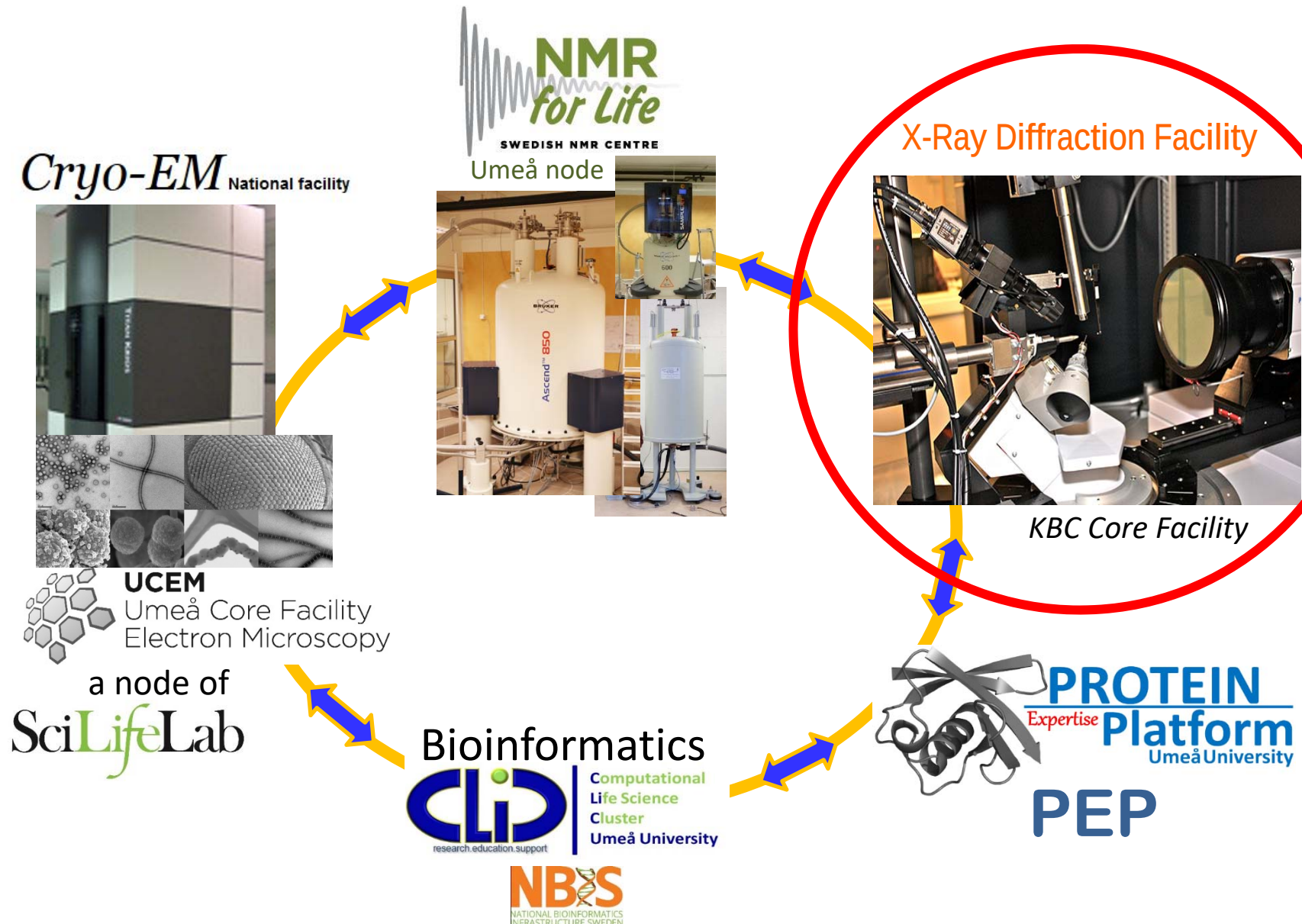
Expertise in Single Crystal X-Ray Diffraction (XRD)  
and  
Access to Crystallographic Equipment



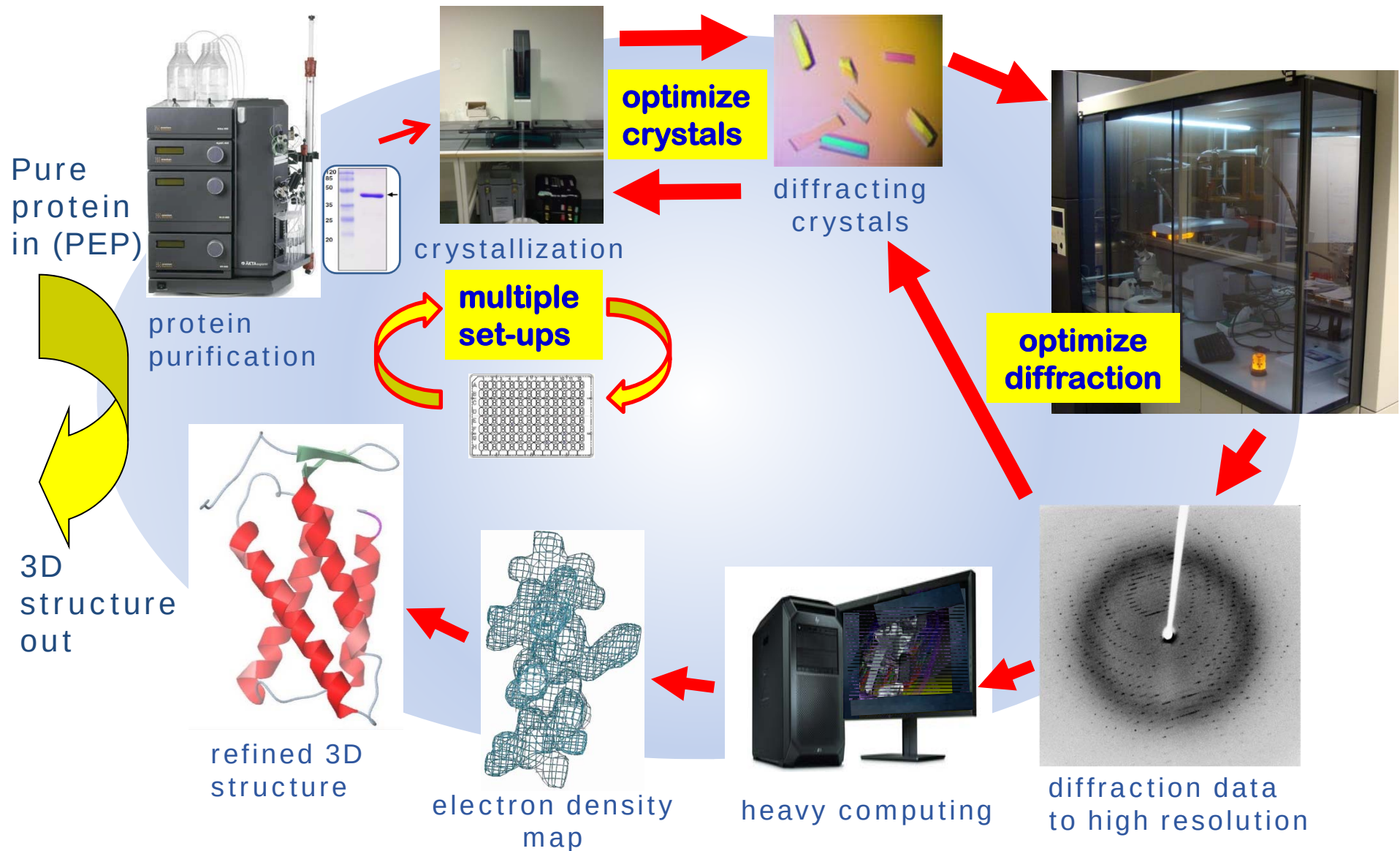
Uwe H. Sauer, Assoc. Prof.  
Structural Biology & Bioinformatics  
Dept. of Chemistry

<https://www.umu.se/en/research/infrastructure/x-ray-crystallography-platform/>

## Integrated Structural Biology (ISB) at UmU

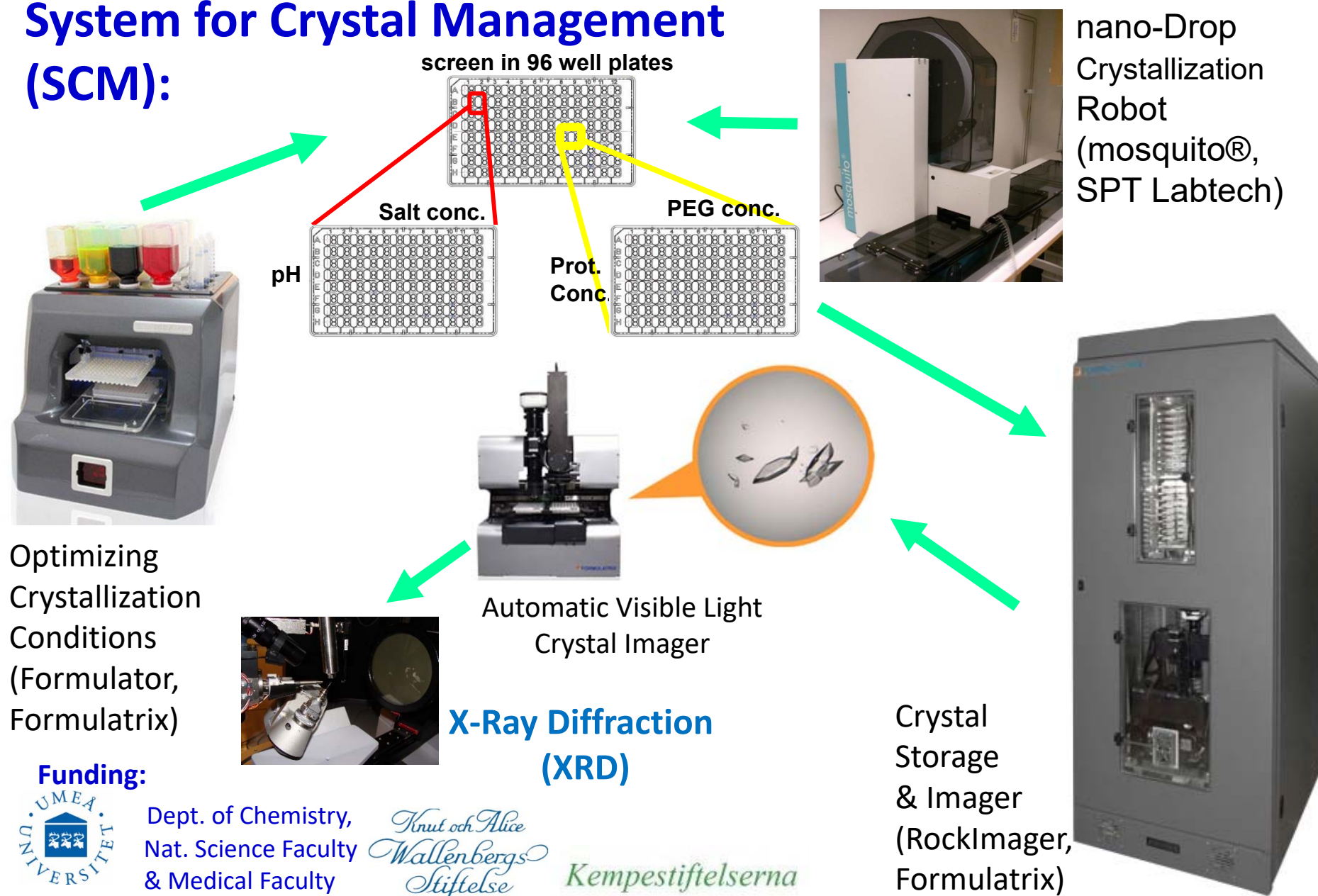


# From protein - to crystal - to structure





### System for Crystal Management (SCM):



### Crystallization Services

- Crystallization Set-ups in 96-Well Plates (up to 288 different conditions per plate) using Commercial and Custom Crystallization Screens (Cost: ~**800 SEK**/plate)
- Crystal Imaging, Evaluation & Storage (Cost: ~**50 SEK**/plate and month)
- **Optimization** of initial hits (cost: see above)

### X-ray diffraction data collection (in-house & synchrotron)

- From Single Crystals and Crystalline Powders (~**500 SEK/d** plus cost for LN<sub>2</sub>)
- X-Ray Crystal Structure Determination
- Refinement, Quality Validation & PDB data deposition (~**20 kSEK**)

### User Training Courses (driver's licences)

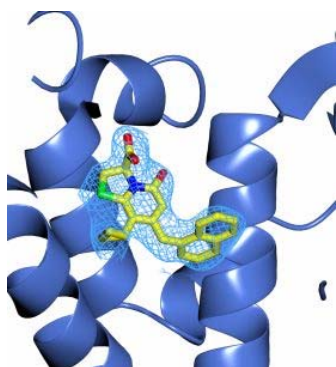
### Course in Crystallography & Crystallization

### Collaborations with KBC platforms (added value):

PEP, UCEM, NMR, LCBU, Imaging facility, ..

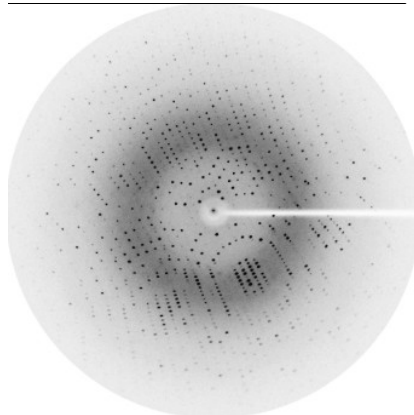
## A Versatile In-House Platform for a wide variety of applications

### Drug screening

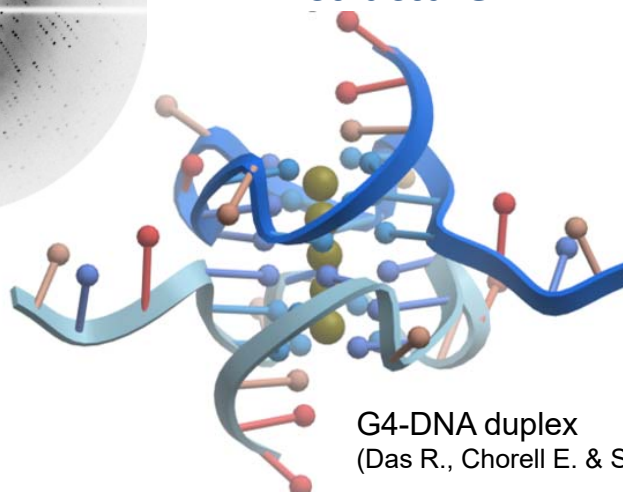


Compound C10 bound to PrfA  
J.A.D. Good et al. (2016) Cell Chem Biol

### Crystal Diffraction Optimization

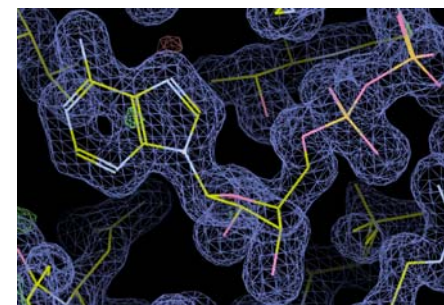


### DNA structure



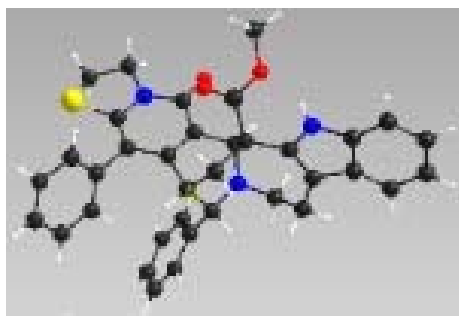
G4-DNA duplex  
(Das R., Chorell E. & Sauer U.H.)

### Enzyme substrate/ product interactions

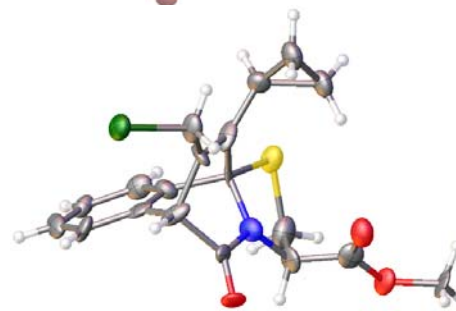


ADP bound to Adenylate Kinase  
P. Ojeda-May et al. Nature Catal. (subm.)

### Small Molecule Structures

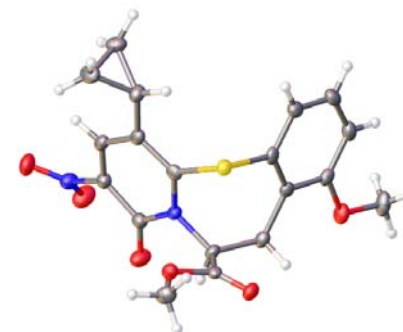


1R,2S,15S,16S)/(1S,2R,15R,16R)-2,24-Diphenyl-3,13,19-triaza-22-thiaheptacyclo [13.10.1.0<sup>3,16</sup>.0<sup>6,14</sup>.0<sup>7,12</sup>.0<sup>17,25</sup>.0<sup>19,23</sup>]hexacosane-6(14),7,9,11,17(25),23-hexaene-18-one-15-carboxylic acid methyl ester  
Sellsted M., et al., (2013) Eur. J. Org. Chem., 7476–7479



Compound **4h** (C<sub>19</sub>H<sub>18</sub>NO<sub>3</sub>SCl)

Singh P., et al. (2019) Org.Lett., 21, 6946–6950



Compound **V** (C<sub>19</sub>H<sub>18</sub>N<sub>2</sub>O<sub>6</sub>S)

## X-Ray Crystallography Platform at KBC

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### ***Users: 44 PIs***

#### ***Single Crystal X-ray Diffraction (XRD)***

**Dept. of Chemistry (12 PIs):** E. Sauer-Eriksson, K. Persson, U.H. Sauer, F. Almqvist, L. Sandblad, M. Elofsson, M. Wolf-Watz, L. Backman, W. Schröder, C. Funk, J-P. Mikkola and E. Chorell,

**Dept. of Molecular Biology, UCMR and MIMS (12 PIs):** B.E. Uhlin, S.N. Wai, J. Johansson, H. Wolf-Watz, S. Bergström, M. Francis, V. Shingler, D. Cisneros, G. Atkinson, Vasili Hauryliuk, Anna Överby Wernstedt and F. Cava

**Dept. of Plant Physiology, UPSC (6 PIs):** G. Samuelsson, Å. Strand, S. Jansson, L. Kleczkowski, M. Eriksson, R. Garcia Gil,

**Dept. of Med. Chem. and Biophysics (6 PIs):** E. Johansson, R. Berntsson, I. Mir-Sanchis, A. Olofsson and L.-A. Carlsson  
and Sjoerd Wanrooij

**Dept. of Pharmacology and Clinical Neuroscience (1 PI):** A. Öhman

**Dept. of Odontology/Cardiology (1 PI):** N. Strömberg

**Luleå Technical University (1 PI):** Dept. of Health Sciences: S. Velaga

#### ***Powder diffraction***

**Dept. of Chemistry (3 PI):** P. Persson, F. Broily, K. Irgum

**Dept. of Physics (1 PI):** T. Wågberg

#### ***Commercial XRD users:***

**FOI:** F. Ekström (PI), N. Forsgren, A. Allgardsson



## Scientific Publications:

2020 – 6 publications

2019 – 7 publications

2018 – 6 publications

2017 – 4 publications

2016 – 9 publications

2015 – 6 publications

**total:** 38 publications  
since 2015.

5712–5722 *Nucleic Acids Res*  
doi: 10.1093/nar/gkz248

**Structural basis for the catalytic activity of the catalytic subunit of the RNA polymerase  $\sigma^{54}$**

Josy ter Beek<sup>1,†</sup>, V. Elisabeth Sauer-Eriksson<sup>1,†</sup>

**Organic Letters**

Cite This: *Org. Lett.* 2019, 21, 6946–6950

Letter  
pubs.acs.org/OrgLett

**Synthesis of Densely Functionalized *N*-Alkenyl 2-Pyridones via Benzyne-Induced Ring Opening of Thiazolino-Fused 2-Pyridones**

Pardeep Singh,<sup>†</sup> Andrew G. Cairns,<sup>†</sup> Dan E. Adolfsson,<sup>†</sup> Jörgen Ådén, Uwe H. Sauer, and Fredrik Almqvist<sup>\*☉</sup>

Department of Chemistry, Umeå University, 90187 Umeå, Sweden

**Molecular mechanism of ATP versus GTP selectivity of adenylate kinase**

Per Rogne<sup>\*,</sup> Marie Rosselin<sup>\*,1</sup>, Christin Grundström

<sup>\*</sup>Department of Chemistry, Umeå University, Umeå SE-901 87, Sw



**Enterococcal Prg Cell and Provides Protect against U**

Andreas Schmitt<sup>1,†</sup>, Helmut Hirt<sup>2,†</sup>, Michae

**SCIENTIFIC REPORTS** The regulatory protein PrtA in *Listeria*

Vimal Parkash<sup>☉1</sup>, Yashraj Kulkarni<sup>☉2</sup>, Josy ter Beek<sup>☉1</sup>, Polina V. Shcherbakova<sup>3</sup>, Caroline Lynn Kamerlin<sup>☉2</sup> & Erik Johansson<sup>☉1</sup>

**Active-site plasticity revealed in the asymmetric dimer of AnPrx6 1-Cys peroxiredoxin and molecular chaperone from *Anabaena* sp 7120**

Yogesh Mishra<sup>1,2,3</sup>, Michael Hall<sup>1</sup>, Roland Loomis<sup>1</sup>, Kwangho Nam<sup>1,2,3</sup>, Chris Söderberg<sup>1</sup>, Patrik Storm<sup>1</sup>, Neha Chaurasia<sup>1</sup>, Lal Chand Rai<sup>1</sup>, Stefan Jansson Wolfgang P. Schröder<sup>1,2</sup> & Uwe H. Sauer<sup>1,3</sup>

**environmental microbiology**

Environmental Microbiology (2019) 21(4), 1321–1330

doi:10.1111/1462-2920.14567

**The Y233 gatekeeper of DmpR modulates effector-responsive transcriptional control of  $\sigma^{54}$ -RNA polymerase**

Henrik Seibt,<sup>1</sup> Uwe H. Sauer<sup>2</sup> and Victoria Shingler<sup>☉1\*</sup>

<sup>1</sup>Department of Molecular Biology, Umeå University, SE-901 87, Umeå, Sweden.

<sup>2</sup>Department of Chemistry, Umeå University, SE-901 87, Umeå, Sweden.

### Introduction

Members of the XylR/DmpR subfamily of  $\sigma^{54}$ -dependent mechano-transcriptional activators play pivotal roles in controlling bacterial degradation of aromatic compound (Shingler, 2003; Tropel and van der Meer, 2004). DmpR is the master regulator required for production of a suite

**Structural basis for ligand binding to an enzyme by a conformational selection pathway**

Michael Kovermann<sup>a,b,1</sup>, Christin Grundström<sup>a</sup>, A. Elisabeth Sauer-Eriksson<sup>a</sup>, Uwe H. Sauer<sup>a</sup>, and Magnus Wolf-Watz<sup>a,1</sup>

<sup>a</sup>Department of Chemistry, Umeå University, SE-901 87 Umeå, Sweden; and <sup>b</sup>Department of Chemistry, University of Konstanz, 78457 Konstanz, Germany  
Edited by Michael F. Summers, Howard Hughes Medical Institute, University of Maryland, Baltimore County, Baltimore, MD, and approved May 8, 2017 (received for review January 19, 2017)

Proteins can bind target molecules through either induced fit or structural ensembles. The catalytically active state of adenylate

PNAS

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Accepted: 16 November 2017  
Published online: 07 December 2017



### X-Ray Crystallography Platform Steering Board:

Prof. Elisabeth Sauer-Eriksson (Chem.)

Prof. Erik Johansson (Med. Biochem. & Biophys.)

Assoc. Prof. Karina Persson (Chem.)

Assist. Prof. Ronnie Berntson (Med. Biochem. & Biophys.)

Assoc. Prof. Uwe H. Sauer (Chem.)

# X-ray Structures determined at Umeå University

