
IOCB SERVICE DAYS

Presentation of services by:
Research-Service Groups / Service Groups / Core Facilities

20
23

X-ray and bioNMR Research Core Facility

Pavλίna Maloy Řezáčová



ÚOCHB AV
CR
IOCB PRAGUE





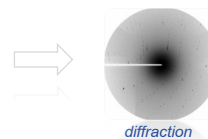
Overview of services

Small-molecular X-ray crystallography

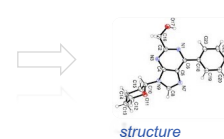
- complete service structure determination



crystallization



diffraction



structure



Dr. Blanka Klepetářová

room A.01.65, ext. 340

klepetarova@uochb.cas.cz

Macromolecular X-ray crystallography

- crystallization and diffraction



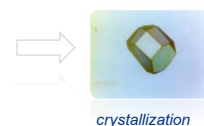
cloning



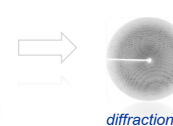
expression



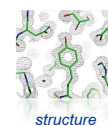
purification



crystallization



diffraction



structure



Dr. Jiří Brynda

room A.01.61, ext. 210

brynda@uochb.cas.cz

Biomolecular NMR

- preparation of labeled proteins
- data collection



cloning



expression



purification



isotope labelling



data acquisition



analysis

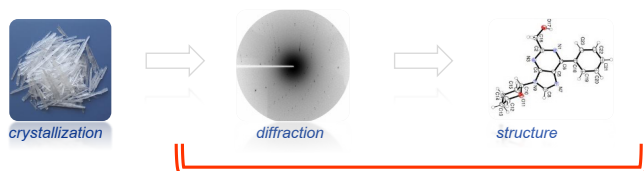


Dr. Pavel Srb

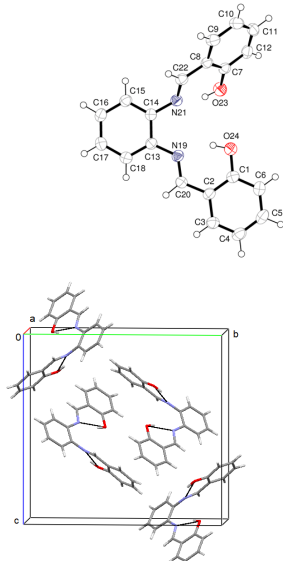
room A.01.53, ext. 498

srb@uochb.cas.cz

Small-molecular crystallography



- diffraction data are collected at UCT
- result is 3D structure, including stereochemistry, bond lengths, angles and hydrogen bonds
- final structures are deposited in the Cambridge Structural Database (CCDC number)
- all material (incl. figures) is prepared for publication



Dr. Blanka Klepetářová

room A.01.65, ext. 340

klepetarova@uochb.cas.cz

Bring me your crystals.

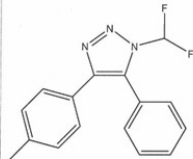
Email me Crystal submission form.



Skupina struktur biologie
Ústav organické chemie a biochemie AV ČR, v.v.i.
Flemingovo nám. 2., 166 10 Praha 6
Tel.: 220183135

X-ray structure analysis of small molecules

Crystal submission form

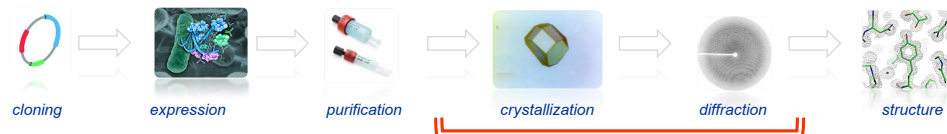
Name	Svatava Votravá
Telephone	446
E-mail	votrava@uochb.cas.cz
Department	Organic synthesis
Supervisor	Petr Beier
Sample label	SVB1365
Chemical formula	C ₁₈ H ₁₃ F ₃ N ₃
Solvents used during crystallization	ethanol, ether, hexane
Stability problems (specify if any)	-
Toxicity problems (specify if any)	unknown
Expected structure (please, indicate the atom labelling scheme)	
Notes	
Date	

Submit form to:
Blanka Klepetářová (building A, NE wing, door A 01.65, phone: 340, klepetarova@uochb.cas.cz)

- crystals should be transparent
- no visible imperfections (cracks, twinning)
- optimal size 0.1-0.5 mm
- keep the crystals in solution in sealed flask to avoid evaporation

Crystal submission form available at Intraweb → [Forms](#)

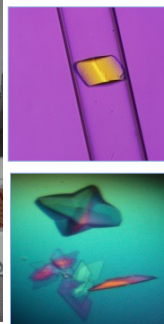
Macromolecular crystallography



- we maintain equipped crystallization laboratory



- we provide
training
crystallization plates (3 types)
crystallization screens (2 types)
good advises (100+ types:)



Dr. Klára Pospíšilová
room A.01.58, ext. 512
pospisilova@uochb.cas.cz

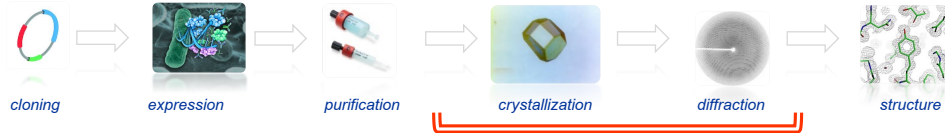
Email me if you want
become crystallization
room user.

- we have 70 registered users from 9 scientific teams
- each team has (at least) one superuser who is fully trained, serves as a communication point and has access to Owncloud shared folder
- we organize seminars and workshops on crystallization methods

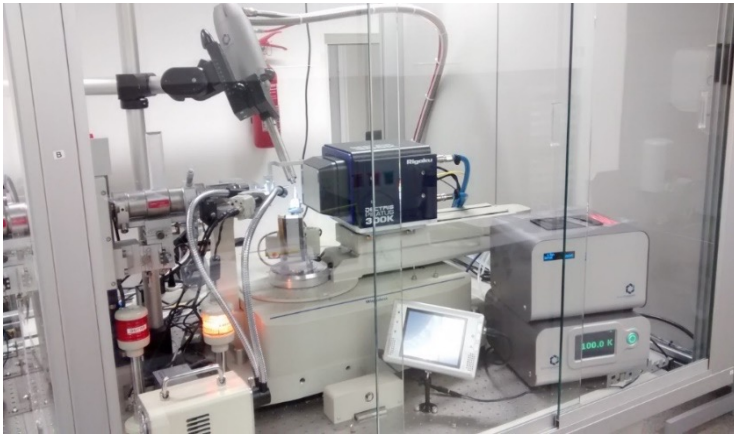


Patrick Steward
Sample preparation
for structural biology
21/2 13h B2.29

Macromolecular crystallography



- we maintain X-ray diffraction laboratory



- we provide
 - testing of diffraction quality
 - diffraction data collection
 - training to become user
 - data collection at synchrotrone
 - data processing
 - data storage/archiving



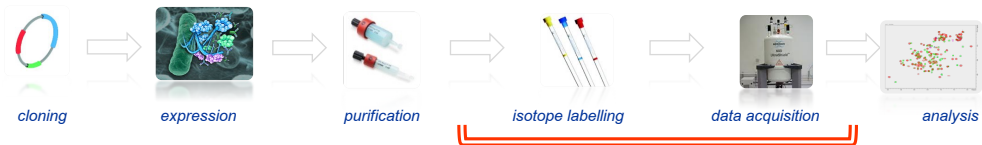
Dr. Jiří Brynda

room A.01.61, ext. 210
brynda@uochb.cas.cz

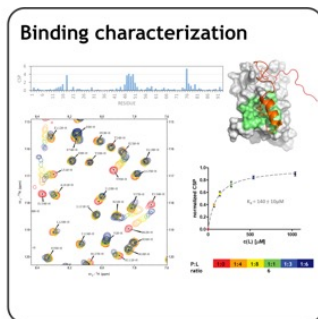
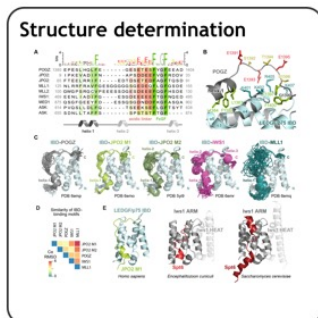
Ask me if you need
diffraction data from
your protein crystal.

- we have 26 trained users from 7 scientific teams
- each team has (at least) one superuser who is trained and can reserve self-measurement time through Intraweb reservation system
- synchrotrone data collection is organized every (other) month
- diffraction data are archived at CESNET

Biomolecular NMR



- we advise on preparation of labeled protein
- we operate 850 MHz NMR instrument
- we train users to collect and analyze data



incl. fragment screening



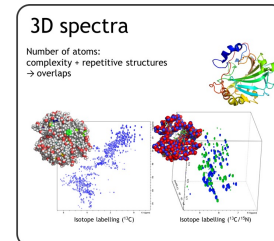
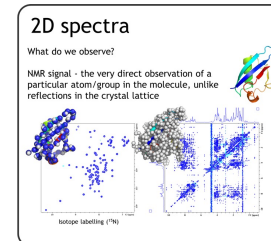
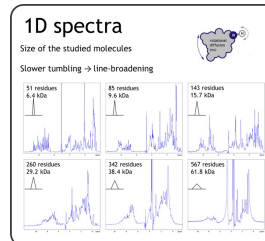
Dr. Pavel Srb

room A.01.53, ext. 498

srb@uochb.cas.cz

Ask me if you plan
NMR experiment
on your protein
or nucleic acid.

- we provide instrument time
- We support for the experimental work
- We provide training (7 users from 4 group)
- We help with experimental design



NMR sample: • 160 - 350 μ L • > 50 μ M • common protein buffers

Teaching and training

Determination of 3D structures of macromolecules

Semestral course, Faculty of Science, Charles University Prague
Biochemistry, winter semester

Structural biology of the cell

Semestral course, Faculty of Science, Charles University Prague
Cell biology, summer semester

Just starting!
February 17 at 9:30.
Still time to join.

Practical course of Structural biology

Faculty of Science, Charles University Prague Cell biology
1-week in summer semester (**organized at IOCB**)

Planned for
May 15-19, 2023.
Still time to join.

Advanced methods in protein crystallization FEBS practical course

Ceska Budejovice, Czech Republic
since 2006 (every 2 years), next one planned for 2024

International School on Biological Crystallization

Granada Spain, www.isbcgranada.org
since 2007 (every 2 years), next one planned for 2023

Planned for
May 21-26, 2023.
Registration
is open now.