ESR 2

3D Electron Diffraction on Organic Nanocrystals

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DIRECTION

- 3D Electron diffraction on organic samples synthesized

- Sample preparation of beam sensitive organic crystals

- Structure solution of unknown organic crystals and polymorphs

- Identification of phases of polymorphs of organic crystals

- Synthesis of new organic crystals and cocrystals

CURRENT ACTIVITIES

Cryoplunging & Cooling of beam sensitive materials

Structure Solution & Refinement Shelxt and Shelxle
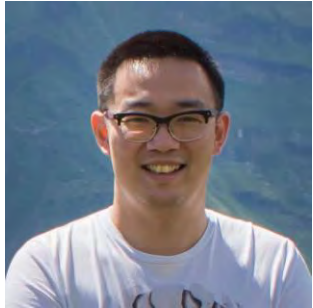
Secondment in Stockholm University (October – December 2022)
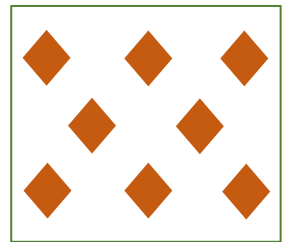
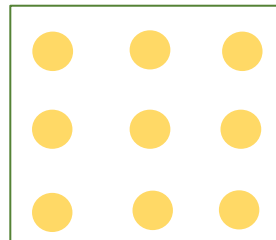**Data collection using the instamatic software**

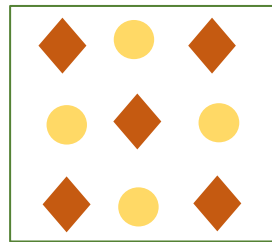**Data Processing and Structure Using XDS ,XPrep, Redp**

CURRENT ACTIVITIES

Active Pharmaceutical Ingredients (APIs)

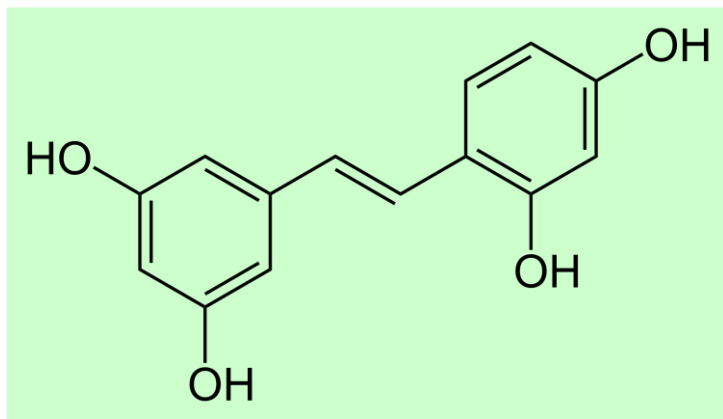Generally Recognised as Safe (GRAS) drugs

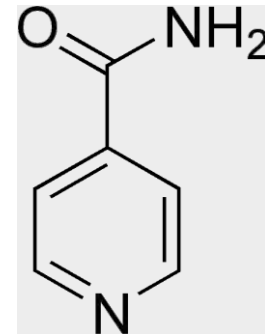Cocrystal using mechanosynthesis

Applications
- Solubility
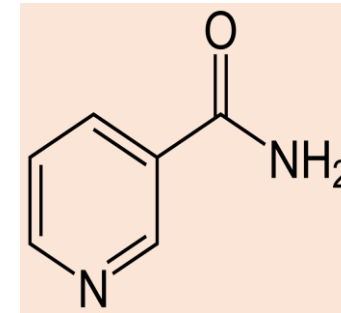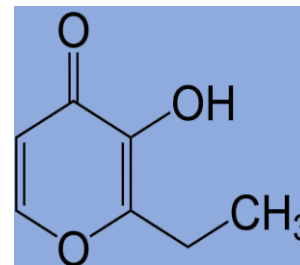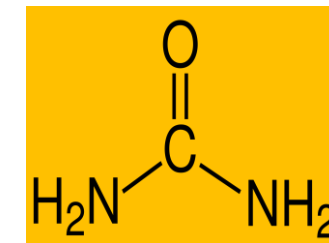- Patentability
- Bioactivity
- Stability

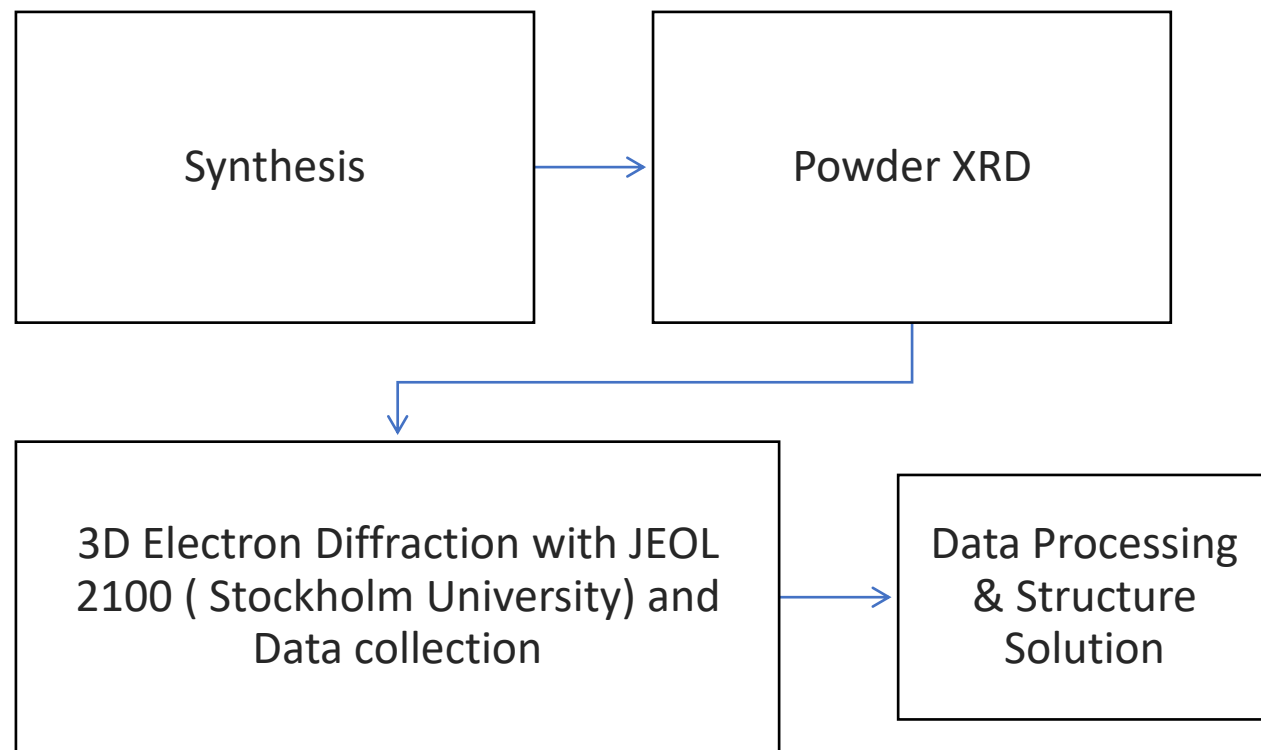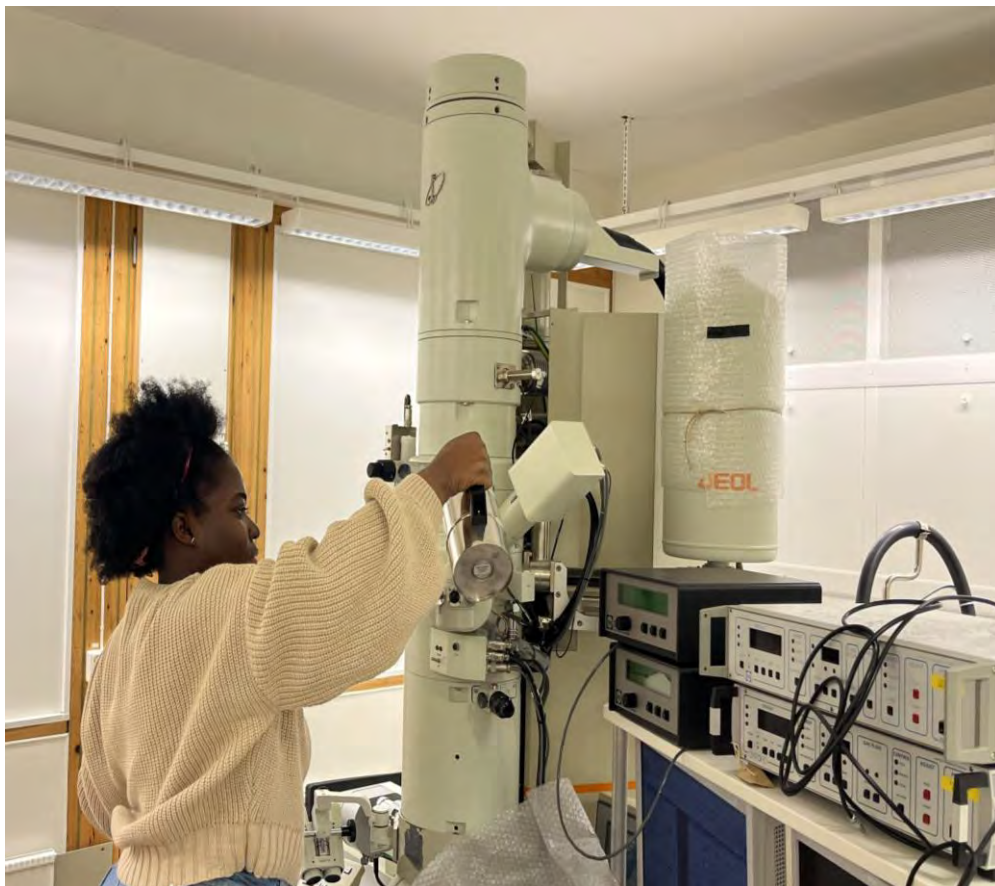Oxyresveratrol (API)
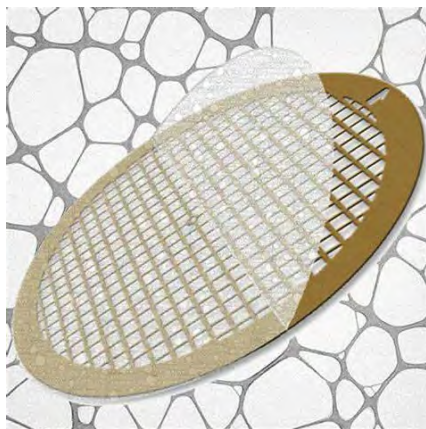
+

Isonicotinamide

Nicotinamide

Ethyl Maltol

Urea

GRAS drugs

The structure of the cocrystals are determined using 3D ED


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┌─────────────────┐        ┌─────────────────┐
│                 │        │                 │
│    Synthesis    │ ────▶  │   Powder XRD    │
│                 │        │                 │
└─────────────────┘        └─────────────────┘
          ┌────────────────────────┘
          ▼
┌─────────────────────────────┐      ┌──────────────────┐
│ 3D Electron Diffraction     │      │ Data Processing  │
│ with JEOL 2100 ( Stockholm  │ ───▶ │ & Structure      │
│ University) and Data        │      │ Solution         │
│ collection                  │      │                  │
└─────────────────────────────┘      └──────────────────┘
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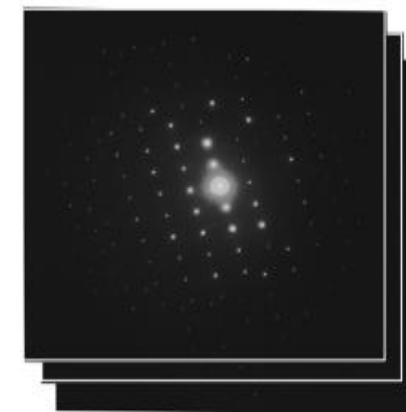
Data Collection Protocols

Glow Discharging of lacey carbon grid

→

Gentle crashing and Deposition of sample unto grid

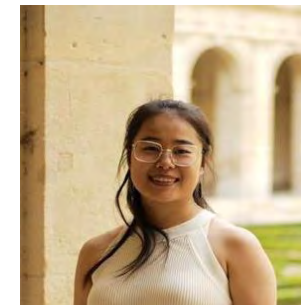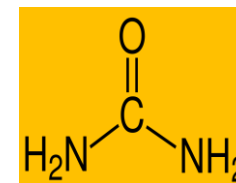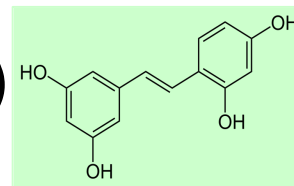
Microscope setup and alignment

Data collection using SAED Aperture (5μ beam size) with Instamatic software

Oxyresveratrol Urea cocrystal (C14H12O4 + CH4N2O)

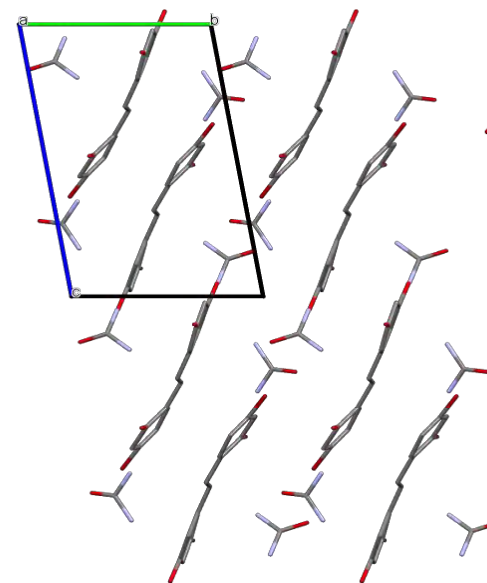Continuous Data Collection at room temperature

Unit Cell Parameters

a	b	c	α	β	γ	Volume
8	8.8	14	78	80	73	985

Space Group: P-1
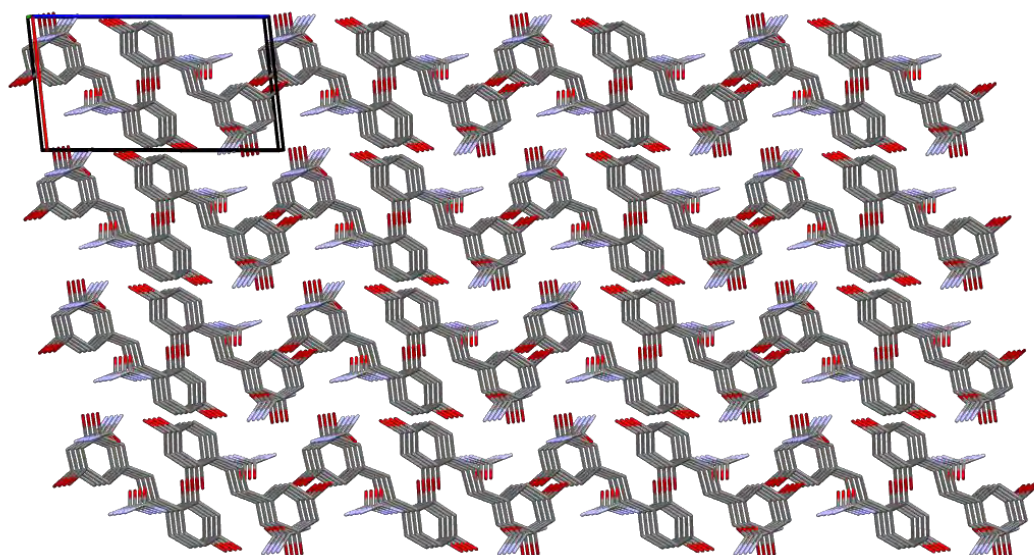
a

b
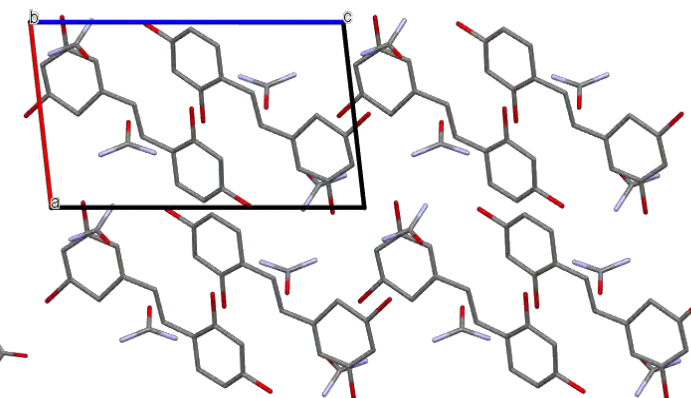
c
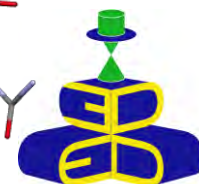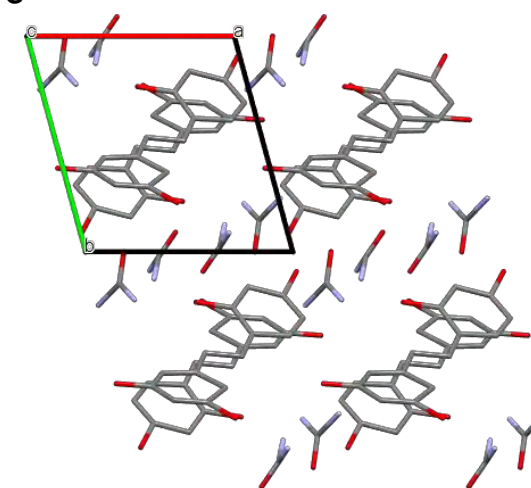
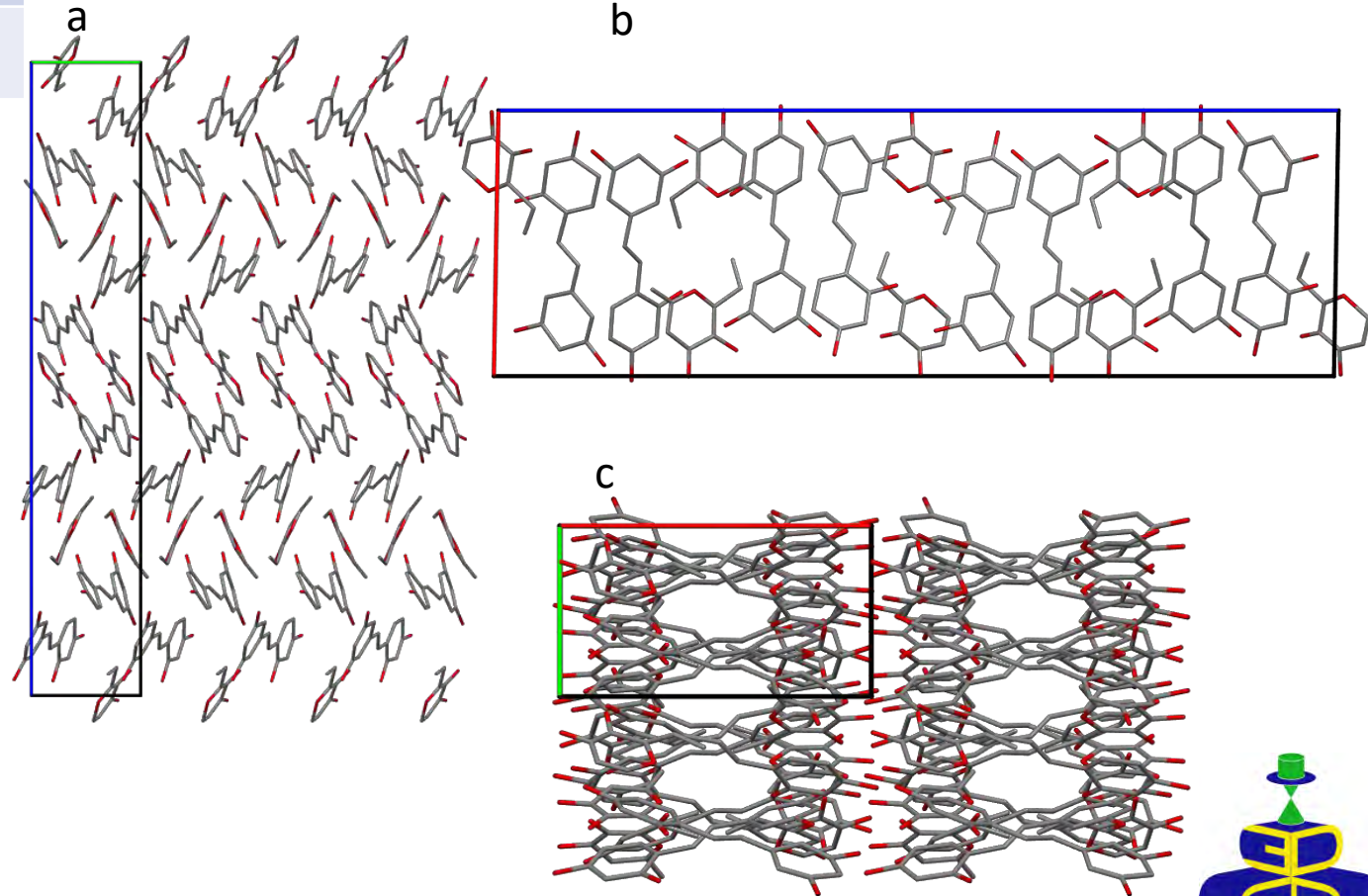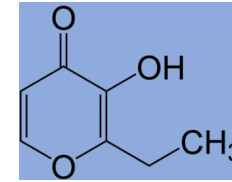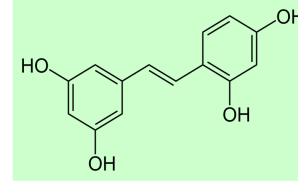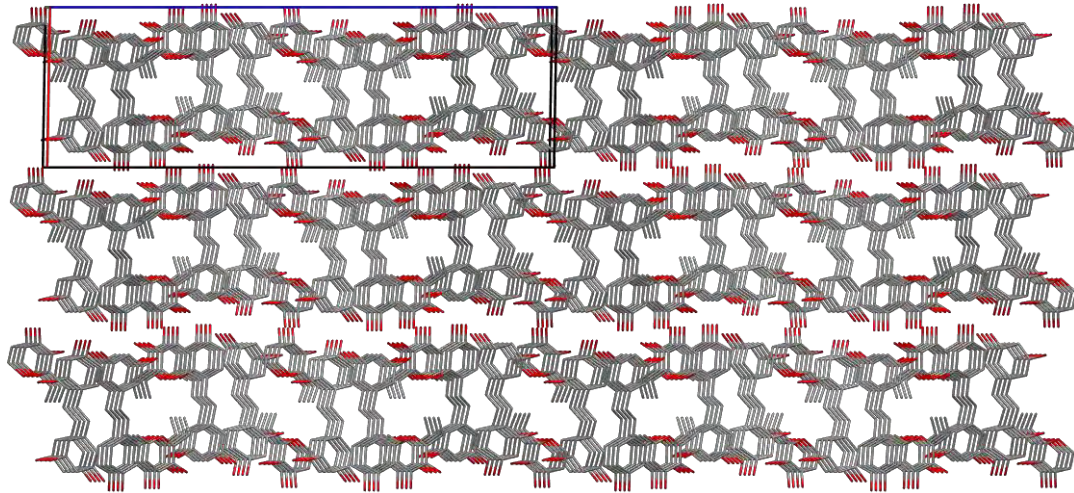# Oxyresveratrol Ethyl Maltol (C14H12O4 + C7H8O3)

Continuous Data Collection at room temperature

Unit Cell Parameters						
a	b	c	α	β	γ	Volume
12.8	7	40.6	90	91	90	3633.3

Space Group : P21/c

THANK YOU