

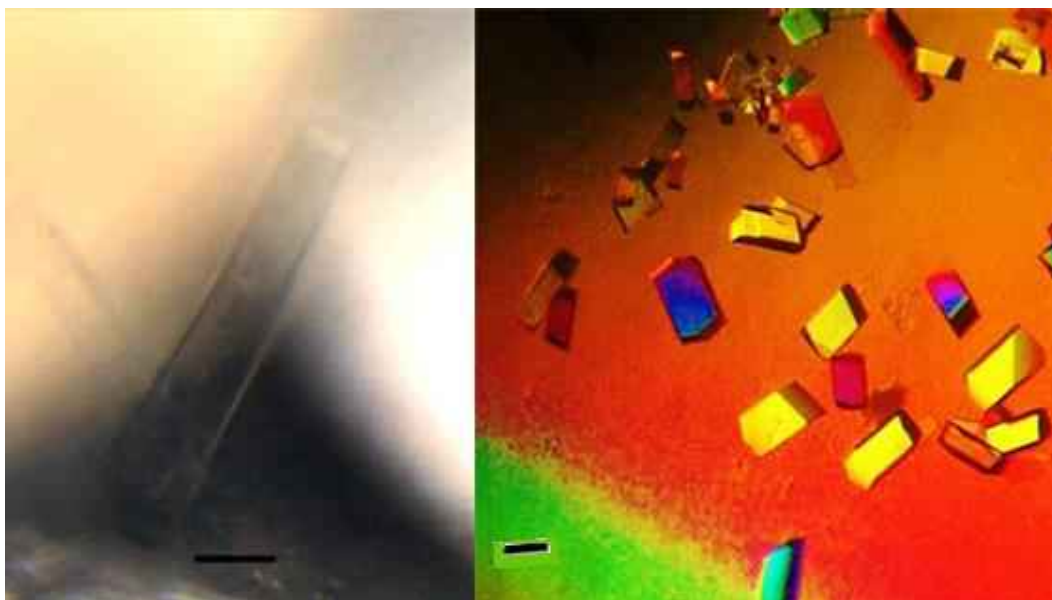
Poster Presentation

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Crystal structure of the novel haloalkane dehalogenases

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Haloalkane dehalogenases (EC 3.8.1.5; HLDs) are microbial enzymes with catalytic activity for the hydrolytic conversion of xenobiotic and highly toxic halogenated aliphatic compounds to the corresponding alcohols. Biodegradation, biosensing, biocatalysis and cellular imaging are potentially practical applications for the HLDs. Two newly isolated and purified psychrophilic haloalkane dehalogenases, exhibiting interesting catalytic properties, DpcA from *Psychrobacter cryohalolentis* K5 and DmxA from *Marinobacter* sp. ELB17, were used for the crystallization experiments and structure determination. Diffracted crystals of DpcA(left) and DmxA(right) (see figure, the scale bar -100 μ m) were refined up to the 1.05 Å and 1.45 Å resolutions, respectively. Diffraction data for DpcA were collected on beamline 14.2 at the BESSY II electron-storage ring (Helmholtz-Zentrum Berlin (HZB), Germany) and equipped with a Rayonics MX-225 CCD detector at the wavelengths of 0.978 Å, and for DmxA were collected using Pilatus 6M-F detector at the wavelengths of 0.972 Å on the beamline ID29, at the European Synchrotron Radiation Facility (ESRF) in Grenoble (France). Crystals of DpcA belonged to P21 space group with unit-cell parameters: a = 41.3, b = 79.4, c = 43.5 Å, $\alpha = \beta = 90.0$, $\gamma = 95.0$ and contained 1 molecule in the asymmetric unit. Crystals of DmxA belonged to P212121 space group, with unit-cell parameters: a = 43.371, b = 78.343, c = 150.51; $\alpha = \gamma = \beta = 90.0$ and contained 2 molecules in the asymmetric unit. The structures were solved by molecular replacement with MOLREP from the CCP4 software suite. The coordinates of *Xanthobacter autotrophicus* (PDB code: 1B6G; 40% sequence identities for 121 residues and 53% sequence similarity) was used as search model for DpcA structure and for DmxA from *Rhodococcus rhodochrous* (PDB entry 4E46; 48% sequence identity for 142 residues and 63% sequence similarity). Belonging to the superfamily of α/β - hydrolases, according to the catalytic pentad, HLDs are subdivided onto the three subfamilies. DpcA belongs to the HLD - I: Asp - His - Asp + Trp - Trp and DmxA to the HLD - II: Asp - His - Glu + Asn - Trp. We thank M. Weiss and S. Pühringer (BESSY). This work is supported by the Grant Agency of the Czech Republic (P207/12/0775). Also by the Ministry of Education of the Czech Republic (CZ.1.05/2.1.00/01.0024 and CZ.1.05/2.1.00/01.0001). The support of the Academy of Sciences of the Czech Republic is acknowledged as well.



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