s1.m8.p34 **Determination of the structure of the serine-type protease acylaminoacyl peptidase (AAP).** Helena Wright,[a] Zoltan Szeltner,[b] Andras Kiss,[b] Lasllo Polgar[b] and Vilmos Fulop[b], [a]*University of Warwick, UK, and* [b]*Hungarian Academy of Sciences, Budapest, Hungary. E-mail: helena.wright@warwick.ac.uk*

Keywords: Acylaminoacyl peptidase; Prolyl peptidase family; Cognitive disorders

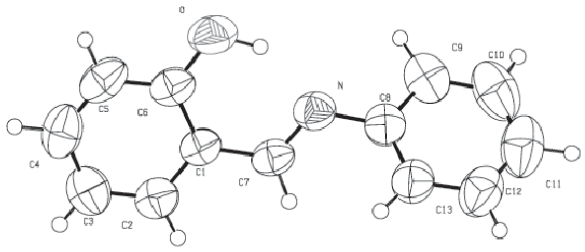
Serine peptidases are fundamentally important enzymes that participate in the regulation of a variety of biological processes. Prolyl oligopeptidases are a serine protease subfamily and members of the family are involved in several diseases including depression, type 2 diabetes and trypanosomiasis. Notably, these oligopeptidases select oligopeptide substrates that comprise of not more than about 30 amino acid residues. Acylaminoacyl peptidase (AAP) is unique in the prolyl peptidase family due to its substrate preference. It is a cytoplasmic exopeptidase catalysing the removal of an N-acylated amino acid from blocked peptides [1]. Little is known about the biological role of AAP, however recent evidence suggests that it is a more sensitive target of organophosphorus compounds than acetylcholinesterase. It is hypothesised that AAP may be involved in the regulation of neuropeptide turnover. Human AAP function has also been correlated with cell proliferation in small cell lung carcinomas and renal carcinomas [2], however the potential role of the enzyme in the malignant state of these cell lines has not been established. Although human AAP crystals were reported ten years ago, no structure has been solved [3]. We have produced highly diffracting crystals of AAP purified from porcine liver using different crystallisation conditions to those previously reported. Chemical cross-linking using glutaraldehyde was necessary to allow crystal diffraction after freezing. A preliminary full data set has been collected to a 3 Å resolution using a synchrotron radiation source. We are currently looking for suitable heavy atom derivatives to solve the crystallographic phase problem by multiple isomorphous replacement.

[1] Jones, W. M., Scaloni A. and Manning, J. M. (1994) *Methods Enzymol*., **244**, 227-231
[2] Scaloni, A., Jones, W. M., Pospischil, M., Schneewind, O., Popowicz, A., Bossa, F., Graziano, F. and Manning, J. M. (1992) *J. Lab. Clin. Med* **120**, 546-552.
[3] Feese, M., Scaloni, A., Jones, W. M., Manning, J. M. and Remington, S. J. (1993) **22**3, 546-549.

s2.m9.p1 **Polymorphism and Photochromism of Salicylideneaniline.** Frédéric Arod,[a] Manuel Gardon,[a] Philip Pattison[b] and Gervais Chapuis[a], [a]*LCr1, BSP, EPFL, 1015-Lausanne, Switzerland, and* [b]*SNBL, ESRF, Grenoble, France, Metropolitan. E-mail: frederic.arod@epfl.ch*

Keywords: Photochromism; Salicylideneaniline; Polymorphism

Organic compounds exhibiting photo- or thermochromicity have been of considerable interests owing to their properties and possible applications. The photochromism of salicylideneaniline (SA) was discovered by Senier *et al*. at the beginning of last century. In 1964, Cohen *et al*. observed polymorphism [1] and indicated that the colour change was not accompanied by any observable changes in X-ray diffraction pattern and infrared spectrum. Destro *et al*. [2] gave a possible solution of the structure of the a1-polymorph, but could not go further due to the lability of the irradiated product. It is generally accepted that the stable form of SA in the ground state is the enol form, with an intramolecular hydrogen bond between the hydroxyl group and the nitrogen atom. Upon photoexcitation of this enol form with UV light, it undergoes an ultrafast proton transfer from the hydroxyl group to the nitrogen, due to the electronic redistribution in the excited state. The proton transfer generates a keto tautomer in the excited singlet state. However, the details of the structure configuration give rise to controversy between a cis and a trans form in which the oxygen and the imine hydrogen atom will be in cis or trans configuration with regard to the C1-C7 bond [3]. Here, we report for the first time, on the α2-polymorph structure of SA in the ground state, already mentioned by Cohen. Then, we revisit the α1-polymorph structure of SA described by Destro, but reconsidering his hypothesis. We suggest a lowering of the symmetry from orthorhombic to triclinic with the aim to remove the ambiguity of the two-fold axis and improve the structure solution. Spectroscopic measurements on both modifications reveal characteristic changes in absorption spectrum during irradiation.



[1] Cohen, M. D.; Schmidt, G. M. J.; Flavian, S. *J. Chem. Soc*. **1964**, 2041-2051.
[2] Destro, R.; Gavezzotti, A.; Simonetta, M. *Acta Cryst.* 1978, B**34**, 2867-2869.
[3] Shen, M. Y.; Zhao, L. Z. ; Goto, T.; Mordzinski, A. *J. Chem. Phys.* 2000, **112**(5), 2490-2497.