

W0168

Radiation-Damage-Induced Phasing with Anomalous Scattering. P.H. Zwart^a, S. Banumathi^b, M. Dauter^a & Z. Dauter^b, ^aSAIC-Frederick Inc, MCL/SRRS, Argonne National Lab, Argonne, IL, ^bNCI, MCL/SRRS, Argonne National Lab, Argonne, IL.

Recent developments in experimental phasing have shown that X-ray-damage induced derivatives can be a potent source of phase information^{1,2} in a phasing scenario called RIP (Radiation-damage Induced Phasing). Although most efforts to develop this method into a standard phasing technique are focused on the use of disulphide breakage, the radiolytic dehalogenation of a brominated uridine has shown to be a powerful RIP derivative³. Another well known halogenated aromatic derivative can be obtained by iodinating tyrosine residues with N-Iodosuccinimide or a tri-iodide containing solution. This classic derivative, developed by Sigler⁴, will be shown to be a potent RIP derivative as well. Furthermore, the fact that iodine has a significant f'' value at wavelengths easily reachable at synchrotron beam lines and home sources, suggests that the combination of anomalous scattering signal with the RIP signal could enhance the capabilities of RIP-like scenarios, both in substructure solution and phasing. The phasing scenario that utilizes both the RIP signal and the anomalous signal, has been called RIPAS, in strict analogy with MIRAS/SIRAS.

¹Banumathi, S., Zwart, P.H., Ramagopal, U.A., Dauter, M. & Dauter, Z. (2004). *Acta Cryst.* D60, 1085-1093.

²Ravelli, R.B.G., Schröder Leiros, H.-K., Pan, B., Caffrey, M. & McSweeney, S. (2003). *Structure*, 11, 217-224.

³Schiltz, M., Dumas, P., Ennifar, E., Flensburg, C., Paciorek, W., Vonrhein, C. & Bricogne, G. (2004). *Acta Cryst.* D60, 1024-1031.

⁴Sigler, P.B. (1970). *Biochemistry*, 9, 3609-3617.