empirical force field simulation should use the surface of the ribosomal exit region and bulk water.
In eucaryotic organisms the placement of protein synthesis is the rough endoplasmic reticulum. The growing peptide chain is channelled through the membrane into the matrix. The simulation should include the structure of the surface of the matrix sided channel protein. During folding molecular interactions with this region can be expected. After the last domain has been channelled and folded the domains rearrange and leave the synthisis/channelling exit side.

Acknowledgement
I appreciated it very well to get the honor of being a new member of the european peptide society. Thanks to my colleages in Europe.
Greetings to all paticipants of the ecm-24, and to the organizing committee in Marocco.

MS01 P04

Protein conformation families for automatic model building. Frantisek Pavelcik[a,b]. [a]*Department of Inorganic Chemistry, PRIF UK, Bratislava, Slovakia.* [b]*Department of Chemical Drugs, FaF VFU, Brno, Czech Republic.*
E-mail: pavelcikf@vfu.cz

Keywords: conformation, protein, model building

Conformation families were determined for di-peptides, tri-peptides, tetra-peptides and penta-peptides. These are related to model building fragments called AlphaD, AlphaT, AlphaQ, and AlphaP. The conformation family is a region of a conformation space highly populated with experimental conformations. The smoothed conformation density in this region should have a local or global maximum. The conformation space is an infinite periodic torsion angle space. The conformation families were determined by direct multidimensional mapping (2-D, 4-D, and 6-D). A method of Pavelcik & Vanco [1] was used. All PDB structures (Febr. 2007) with resolution better than 1.5 Å, and 90% homology criterion were selected for analysis. The number of calculated torsion angles was almost 500 000. The grid of mapping was 16. The search probe was variable: $R=R_D\sqrt{0.5N}$; R_D is empirically found radius for 2-D search, N is dimension of the conformation space. Penta-peptide conformations (8-D) were generated by a combination of two tri-peptide conformation families. Less populated families were removed. The number of conformation families for di-peptides is 6, for tri-peptides 24-26, and 130-140 for tetra-peptides.
The conformation families are used as search fragments in the model building program NUT [2], and will be used for automatic model building at lower resolutions.

[1] Pavelcik, F.; Vanco, J., *J. Appl. Cryst.*, 2006, 39, 315-319.
[2] Pavelcik, F., *J. Appl. Cryst.*, 2006, 39, 483-486.

MS01 P05

RegX3 – a full-length response regulator that exhibits 3D-Domain swapping. J. King-Scott, E. Nowak, S. Panjikar, E. Mylonas, M. Roessle and P.A. Tucker *European Molecular Biology Laboratory, Hamburg Outstation, EMBL c/o DESY, Notkestr. 85, 22603 Hamburg, Germany.*
E-mail: tucker@embl-hamburg.de

Keywords: Two-component system, response regulator, *Mycobacterium tuberculosis*

RegX3, annotated as Rv0491 in the *Mycobacterium tuberculosis* (MTB) genome, is the response regulator (RR) from the SenX3-RegX3 two-component system (TCS). Two component systems are the predominant signalling systems found in prokaryotes. The SenX3-RegX3 TCS is one of the twelve TCS within the MTB genome [1,2]. These systems monitor environmental stresses and allow the bacteria to respond to the external threat by altering gene expression patterns. The sensor histidine kinase (SK), which is normally membrane anchored detects the external signal and passes it to the cytosolic response regulators (RR) [3]. The two components communicate through phosphotransfer between a histidine residue in the SK and an aspartic acid in the RR.
RRs are usually multi-domain proteins with the first domain being the characteristic receiver domain, which contains the conserved aspartic acid. The second domain can vary but is most commonly a DNA-binding domain. RRs are classified according to the C-terminal (effector) domain. Based on sequence comparisons, the RegX3 contains a winged-helix-turn-helix DNA-binding domain placing it in the OmpR/PhoB subfamily, the largest subfamily of Rrs [4-6]. RRs from this subfamily have been hypothesised to dimerise on a highly conserved interface in the receiver domain [7]. The crystal structure of RegX3 was solved in 2005 and revealed the first structure of a full-length RR exhibiting domain swapping on the proposed dimerisation interface. To support the high-resolution model, small-angle scattering measurements were made on the RR at various concentrations. According to the molecular mass estimate, RegX3 is monomeric in solution at low concentrations and becomes dimeric at higher concentrations. The molecular mass calculated from the scattering curve of RegX3 at the highest concentration agrees well with the molecular mass of the dimer.

[1] Cole, S. T., Brosch, R., Parkhill, J., Garnier, T., Churcher, C., Harris, D., Gordon, S. V., Eiglmeier, K., Gas, S., Barry, C. E., 3rd, Tekaia, F., Badcock, K., Basham, D., Brown, D., Chillingworth, T., Connor, R., Davies, R., Devlin, K., Feltwell, T., Gentles, S., Hamlin, N., Holroyd, S., Hornsby, T., Jagels, K., Krogh, A., McLean, J., Moule, S., Murphy, L., Oliver, K., Osborne, J., Quail, M. A., Rajandream, M. A., Rogers, J., Rutter, S., Seeger, K., Skelton, J., Squares, R., Squares, S., Sulston, J. E., Taylor, K., Whitehead, S., and Barrell, B. G. (1998) *Nature* 393(6685), 537-544
[2] Morth, J. P., Gosmann, S., Nowak, E., and Tucker, P. A. (2005) *FEBS Lett* 579(19), 4145-4148
[3] Stock, A. M., Wylie, D. C., Mottonen, J. M., Lupas, A. N., Ninfa, E. G., Ninfa, A. J., Schutt, C. E., and Stock, J. B. (1988) *Cold Spring Harb Symp Quant Biol* 53 Pt 1, 49-57
[4] Brennan, R. G. (1993) *Cell* 74(5), 773-776
[5] Martinez-Hackert, E., and Stock, A. M. (1997) *J Mol Biol* 269(3), 301-312
[6] Kondo, H., Nakagawa, A., Nishihira, J., Nishimura, Y., Mizuno, T., and Tanaka, I. (1997) *Nat Struct Biol* 4(1), 28-31
[7] Toro-Roman, A., Mack, T. R., and Stock, A. M. (2005) *J Mol Biol* 349(1), 11-26