James Rennie Bequest

The Secretary
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Krystyna Bromek - Burnside

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The report from summer school: Supramolecular Structure and Function.

28th September 2000

Dear Mrs Shand,

I would like to submit this report from the summer school I participated at with James Rennie Bequest's help towards travel. My full transportation cost was £325. I am very grateful that the Bequest has covered most of the expense.

The school lasted for twelve days during which most of modern biophysical techniques were presented. The lectures were generally of two kinds: presentation of the particular technique and presentation of recent results obtained using that method. Most of the techniques were covered with theoretical background, pointing out their typical use, newest developments in the fields and the most commonly made mistakes when utilising the techniques.

During the school also a poster session was held at which I presented a poster titled: "Backbone dynamics and long-range interactions in CP-modules". I have also been voted the most active participant of the lecture sessions.

I was particularly interested in techniques complementary to the NMR studies of protein structure and dynamics, to investigate the properties of proteins which are difficult to ascertain using NMR. For example the nanosecond time-scale internal motions in proteins are much better monitored using fluorescence depolarisation as it is at the most sensitive range there; rather then NMR in which the fast (picosecond) and slow (μs-ms) motion can be measured better. I am continuing the discussion about fluorescence measurements on the type of the protein we are investigating here in Edinburgh with the lecturer from the school.

Particularly good lecture was on: "*Motional averaging and its consequences for interpretation of NMR and CD- derived studies." (W.F. von Gunsteren, Switzerland)*. This lecture has very clearly pointed out the type of structural information that is obtained from NMR and the amount of the time averaging of the dynamical structure of observed bio-molecules. It has shown that the modern Molecular Dynamics can well represent behaviour of small biological compounds in solution (at the moment the computation limits the size of molecules). The lecture gave a good indication about the amount of the flexibility of the

peptides which are supposed to adapt a well defined secondary structure in the solution. The structural parameters as measured be NMR and CD were retained for a peptide which spent 75% of the time unfolded. It will be very interesting to follow this work to the point when proteins large enough to exhibit a full tertiary structure will be possible to model and to see if the more global interactions present in proteins will point towards more permanently folded structures or will we be presented with the picture of biochemistry performed by proteins at least temporarily largely unfolded. I might consider this type of theoretical modelling in my further studies.

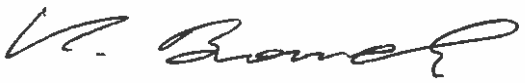
The molecular biology as a tool to ascertain the function of proteins especially when observed together with the structure of the protein or complex was also discussed. An interesting example of this type of work was protein-RNA: Rev-RRE interaction in HIV virus. Engineered differences in stem-loop structure of RRE have shown that naturally occurring bulges have an effect on strength of binding of Rev and produce a "molecular rheostat" effect for transcription dependant on the concentration of Rev in the solution.

Several lectures covered in some detail the techniques used today for study of non-covalently bound proteins (Mass Spectroscopy, Sedimentation, Fluorescence). Pointing out to different processes that can be observed if binding is taking place. While the sedimentation and fluorescence are the well established techniques allowing for observation of binding constants in favourable situations, the Mass-Spectroscopy for non-covalently bound modular proteins is a very new technique in which the sample preparation is optimised so that the bounds are progressively broken from the weaker to stronger allowing for monitoring of tightness of binding.

The summer school was a very good experience, also because of meeting a lot of scientists/students working in biology, biochemistry and biophysics on virtually all kinds of the biologically active molecules. I have learned a lot about different possible approaches to the structural and interaction problems.

I hope this report cover all of the Bequest's requirements, should you also need copies of my tickets receipts please do not hesitate to contact me.

Yours sincerely



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