WP18 JRA (Deuteration) Management Meeting, 9th October 2009
Department Chemie, TU Munchen, Garching

Present: V.T. Forsyth (ILL/Keele, JRA Coordinator), C. Ebel (CEA), T. Gutberlet (TUM/FRM-II), M. Haertlein (ILL), H. Heumann (MPI), S. Holt (STFC), M. Sattler (TUM), A. Ostermann (TUM/FRM-II), G. Gemmecker (TUM), T. Madl (TUM), P. Zou (TUM

Apologies: M. Blackledge (CEA), F. Gabel (CEA), C. Neylon (STFC), A. Watts (Oxford), M. Weik (CEA)

1. Welcome

MS welcomed the participants to TUM and summarised arrangement for the meeting.

2. News from the NMI3 coordinators meeting

VTF reported news from the NMI3 coordinators/business meeting, which he had attended on the previous day at TUM/FRM-II. In particular he emphasized the importance of complying with the EU contractual obligations. Specific issues are:

(i) Timesheets: each institute involved is obliged to complete timesheets that demonstrate the hours committed and charged to the project. The mechanism of doing this is for the individual institutions to decide and implement. Time committed to the projects may be audited by the EU, who may apply a wide range of consistency checks. Problems in this area may result in the EU withholding payment;

(ii) Effort implementation: particular care must be taken in allocating effort to the project- specifically there must be no possibility of double-funding or of duplicating effort carried out through another or a previously funded project. If work committed to project activity is found to be funded/supported through some other stream, the EU will not pay for it.

(iii) planning/changes of plan: the current JRA project plan has just been circulated to all of the JRA PIs as a GANTT chart summary. Any proposed changes to this plan (or any part therein) should be sent to VTF, who will consider them and if appropriate make corresponding requests to NMI3 GA. The only request so far has been for a change in STFC's plan. VTF flagged this at the NMI3 business meeting and the matter will be discussed between H. Schober (ILL, NMI3 coordinator) and R. McGreevy (STFC)

(iv) the next I3: discussions have now commenced. If areas of interest relating to this JRA are to be represented in any future I3, significantly new ideas need to be brought forward and a discussion started.

3. Review of progress with contracted work

MH/VTF (ILL) reported on progress with the task on the production of deuterated biomass (task 18.2) and that for protein expression for protein expression in *Pichia Pastoris* (18.3). Both tasks are on running on time, with no delays. Model systems have

been closen for the production of algal biomass – *Chorella sorokinana* and ????. For work on *Pichia Pastoris*, the model proteins chosen are human serum albumin and lysozyme. Preliminary work in these areas is starting and no problems are forseen in complying with deliverables 18.1.1 and 18.2.1.

MS (TUM) reported on task 18.4 on segmental labelling. He discussed the use of SF1 U2AF65/RNA as a complex for structural work, and more generally the combination of NMR RDCs with SAXS/SANS, and combined SANS and solution NMR refinement where the possibility existed to use a potential term for small-angle scattering data that contained a restraint of inter-domain distances. As one model system two domains of U2AF65 have been chosen, where efficient overexpression is established and numerous NMR and SAS data are available already. Vectors for segmental labeling have been established. The work is on time and there are no problems foreseen at the moment.

HH (MPI Martinsried) reported on task 18.5 (deuterated glycerol). Here attention is focusing on *Dunaliella tertiolecta* and on *Chlamydomonas reinhardtii*. Glycerol production in *Chlamodymonas reinhardtii* is presently too low (0,6gr/ltr) to be exploited. Chlamydomonas shows an exhaustion effect which means that cell growth and glycerol production after salt shift is inhibited after about 100h.

CE (CEA) reported on task 18.6 (Deuterated membrane proteins). Her presentation focused on OmpX, AcrB. For this, CEA is focusing on methods to optimise the production of deuterated membrane production.

SH (STFC) reported on task 18.7 (Deuterated lipids). The work is focused on the Oxford Isotopic Facility (OIF) - a facility that is aimed at deuteration for soft matter applications. Project work on time. Changes in implementation under discussion between NMI3 and STFC. SH said that a review of the provision of deuterated lipids by the OIC to the UK user community was planned.

4. Perspectives from FRM-II. TG summarized progress at FRM-II and gave an overview of the facilities and activity at FRM-II. He also focused on the developing capabilities for biology.

5. Closed session.

VTF asked each task leader to report on the administrative status of their projects, and to flag any problems that might hinder compliance with their contractual obligations:

ILL: on time overall, one technician in place. Deliverables 18.2.1.1 and 18.3.1.1 on time

TUM: on time overall, model system design under way. Deliverable 18.4.1.1 on time

MPI: on time overall, growth conditions for *Dunaliella* under way. Deliverable 18.5.1.1 on time

CEA: on time overall, Deliverable 18.6.1.1 on time.

STFC: on time overall. Deliverable 18.7.1.1 (due 28.06.10) on time. Negotiations between NMI3 and STFC re subcontracting under way. SH agreed to report to VTF on progress with these.

VTF noted that all of the tasks were running on time and confirmed this with all of the task leader representatives. He also noted that negotiations were under way between NMI3 and STFC about altering their *modus operandi*, and requested that he was informed as developments occurred with this. He reminded task leaders to make sure that a mechanism for recording costed and contributed effort on their projects was in place and that it could withstand consistency checks. He also

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Future European support. TG suggested that a useful prelude to future EU support under FP8 could be a discussion workshop along the lines of 'Deuteration for biology". Here the aim would be to discuss the next decisive steps for the application of labeling for the study of biological systems, and would involve a relatively small number of neutron scattering and NMR scientists. The group discussed possible topics that could form the basis of discussion at such a meeting. VTF committed to discuss the possibility of NMI3 support for such a meeting,and also to investigate the possibility of ILL support. TG said he would approach TUM/FRM-II.