

## Operating Policy – Southeast Collaboratory for Biomolecular NMR

June 2006 (Rev. 2.1)

**Purpose.** The Southeast Collaboratory for Biomolecular NMR was established with support of grants from the National Institutes of General Medical Sciences and the Georgia Research Alliance (GRA). Its purpose is to share, among a group of researchers across the Southeast region of the country, both high field NMR equipment (900 MHz NMR) and ideas that facilitate application to molecules of biomedical importance.

**Organization.** Activities are organized around five initial focus groups, and a GRA / new projects group. Each group has a coordinator (and one or more co-coordinators) who will serve to prioritize projects to be served by the facility. The coordinators for the focus groups and GRA / new projects group serve on the collaboratory council, the advisory body for the facility. The five initial groups emphasize areas identified in the establishing grants as being important: methods development, dynamics, nucleic acids, membrane proteins, and large assemblies. The GRA / new projects group will emphasize a broader spectrum of applications of interest to the GRA and the biomolecular NMR community. It will serve as an incubator for the establishment of new focus groups. Training and maintenance will be responsibility of the NMR manager.

**Allocation.** Instrument time will be divided approximately equally among the above groups, with a similar allotment to training and maintenance. Within each group we anticipate an approximate 75/25 division of instrument time between direct user access and use by the coordinators in support of focus group objectives. Priorities will be set within each group taking into account potential contributions to development of unique high field applications, the need for high field in the proposed study, the qualifications of the proposed operator, and the potential impact on the biomedical field. Allocations will be reviewed semi annually and adjustments recommended by the collaboratory council.

**Charges.** As of May 1, 2006 the facility began charging \$7.50/hr of spectrometer time used. Time used in training of new operators is not charged. We continue to be partially subsidized by a grant from NIGMS and expect to keep rates low for the next year.

**Submitting projects.** All potential participants in the collaboratory must submit a request for participant status. This can be done online at [secnmr.org](http://secnmr.org). The required information includes a title for the project, a brief description of the project including scientific factors used in setting priorities (less than 500 words), a proposed instrument operator with an indication of prior high field NMR experience, funding sources for the project, and an example spectrum (HSQC or suitable substitute) relevant to the project collected at 600 MHz or higher (see form for more details). These forms will be forwarded to the appropriate focus group coordinator for approval of participant status, approval of an operator for training and assignment of instrument priority for a six month period.

**Scheduling.** Exploratory experiments on new projects can be scheduled and run with assistance of the facility staff. After appropriate exploration a potential operator must be identified. New operators must schedule with the NMR manager a time for training prior to making any instrument time requests. Once approved, operators may make instrument time requests via an on-line booking tool. Time may be reserved as much as two months in advance. Operators with a priority 1 project will have access to a priority booking period on the first two days of each month. They may reserve up to 48 hrs in single or multiple periods during this

time; those with a priority 1 or 2 may book additional time on the third and subsequent days of each month. No operator may reserve more than 48 hrs during a single booking day. This procedure is intended to allow an equitable distribution of time among participants while allowing booking of longer periods of time by combining 48 hr blocks. The NMR manager will make any adjustments in time needed to combine blocks or optimize use of the spectrometer and will make every effort to notify operators at least three weeks in advance of any changes.

**Training.** To ensure efficient use of spectrometer time and minimize hardware or software problems, operators of the 900 must have a reasonable level of skill. A brief description of the user's experience is required by the Operator form (filled out after submission of the Request for Participant Status form). An evaluation will be made by the facility manager, and depending on experience, may require successful completion of a standard set of experiments and tasks. These would include achievement of suitable line shape in 90% H<sub>2</sub>O, calibration and setup of a multi-dimensional heteronuclear experiment with appropriate settings of pulse widths, decoupler levels, pulse-train power levels, shaped pulses, etc. Demonstration of the spectrometer operation can be done either locally or remotely, using one of the CCRC lower field instruments, or at any conveniently located facility that is running similar spectrometers. In the latter situation, the acquired data and a letter of recommendation would be required. All users, regardless of experience, will go through at least one orientation session to learn the particulars of the 900 MHz instrument in our facility.

**i) STANDARD EXPERIMENTS. SINCE THE SPECTROMETER IS OPERATED BY A VARIAN CONSOLE AND SOFTWARE, AND WE ANTICIPATE A VARIETY OF USER BACKGROUNDS, WE WILL TRY TO ACCOMMODATE RESEARCHERS BY PROVIDING SOME TRAINING AND TUTORIAL MATERIAL. THIS WILL CONSIST OF INSTRUCTIONS AND EXPLANATIONS FOR SETTING UP MOCK EXPERIMENTS THAT CAN BE IMPLEMENTED BY REMOTE OPERATION OF A SUN WORKSTATION RUNNING THE VARIAN SOFTWARE. WHEN ACQUISITION OF TEST DATA OR PRACTICE IN BASIC SETUP IS REQUIRED, ARRANGEMENTS CAN BE MADE TO RUN EXPERIMENTS ON OUR 600 MHZ SPECTROMETER USING A SMALL LABELED PROTEIN SAMPLE.**

**ii) New pulse programs.** An experiment not previously run by the facility manager will have to be first tested on our 600 MHz spectrometer, then on the 900 with a standard sample. The user will have to demonstrate full understanding of the parameters, their values, and the accepted spectrometer limits before executing it on the 900.

**Table 1. Focus Groups**

Development	Dynamics	Nucleic Acids	Memb. Proteins	GRA/New Projects	Large Assemb.
J. Prestegard, UGA coordinator	W. Chazin Vanderbilt coordinator	P. Legault UGA coordinator	Tim Cross Florida St. coordinator	J. Urbauer UGA coordinator	L. Spicer/R. Venters Duke coordinators
M. Rance U. Cincinnati co-coordinator	J.Cavanaugh N.CarolinaSt. co-coordinator	M.Germann Georgia St. co-coordinator	S. Campbell U.N. Carolina co-coordinator	D. Dixon GA State cocoordinator	J. Omichinski UGA co-coordinator