

Princeton University

DEPARTMENT OF CHEMISTRY

PRINCETON, NEW JERSEY 08540

April 8, 1972

Professor Joshua Lederberg  
Department of Genetics  
Stanford University  
Stanford, California 94305

Dear Professor Lederberg:

Dr. Ernest Hyde of ICI in England and I are planning for May 1973 a NATO Advanced Study Institute Programme concerning "Computer Representation and Manipulation of Chemical Information" to be held tentatively in Holland. As you probably know, an Advanced Study Institute is primarily a high level teaching activity at which a carefully defined subject is presented in a systematic and coherently structured program. The subject is treated in considerable depth by lecturers imminent in their field and is presented to other scientists who will already have specialized in the field or possess an advanced general background. There will probably be fifteen lecturers and about fifty-five other participants. The conference will last about two weeks and it is particularly desirable that lecturers should be prepared to stay for the duration of the Institute to insure good and stimulating interaction in the group.

The course will deal with a broad range of problems and methodologies encountered in computer representation and manipulation of various types of chemical information. Each lecturer has expertise in one or more unique areas and will present, in the context of these areas, his methodologies and most important the reasoning behind his choice of representation and the features of his manipulative methods.

We plan on-line demonstrations of chemical manipulative and retrieval programs using both local and remote computers. The fifteen lecturers will provide good coverage of the many types of chemical representations and manipulations. This diversity will provide a unique opportunity for the participants to learn the assets and limitations of each methodology and to see how developments in one area can be helpful to another quite different area. Participants will also obtain a representative view of what systems are actually operational today and what problems remain today unsolved. The joint sponsorship by the Chemical Notation Association of the United Kingdom which has a fine reputation for organizing excellent seminars in the area of chemical representation and manipulation by computer should further assure a successful Study Institute Programme.

Because of the prominence of the work done by you and your research group in the area of Mass Spectra Analysis and Chemical Representation, I, as director, would like to invite you to participate in this Advanced Study

Institute as an invited lecturer to present the techniques, methodologies, and problems relating to the Dendral Project and mass spectral analysis. Since the conference is only in its planning stages now, I only ask for an expression of interest at this time. The Advanced Study Institute would pay all travel expenses, room and board in a beautiful castle in Holland, and at least one organized excursion. We also plan to furnish telephone communications to remote computers as well as certain limited local computing facilities. A tentative list of lecturers and their subjects is given below:

W. T. Wipke	U.S.A.	(Chemical synthesis, interactive graphics)
E. Hyde	England	(The Crossbow System)
R. Feldman	U.S.A.	(Substructure search, display, storage/retrieval)
S. Heller	U.S.A.	(NMR and MS analysis/retrieval systems)
M. Lynch	England	(Reaction documentation, indexing)
Schenk	Switzerland	(Substructure Searching)
P. Jurs	U.S.A.	(Learning machines in spectral identification)
J. Valls	France	(Reaction documentation)
J. DuBois	France	(The DARC System)
W. Knord	England	(X-ray file systems)
E. Meyer	Germany	(Structure Search)
R. Ellis	U.S.A.	(Macromolecular modeling)
Lederberg	U.S.A.	(Dendral Mass Spec analysis)
Levinthal	U.S.A.	(Macromolecular modeling)
Vledüts	U.S.S.R.	(Chemical Information System)
F. Tate	U.S.A.	(Chemical Abstracts Service)

I do hope that you can participate in this Study Institute for I feel it will be a unique opportunity to discuss this interdisciplinary problem and your contribution would be of great value.

Very truly yours,



W. Todd Wipke  
Assistant Professor of Chemistry  
Director, NATO Advanced Study Institute

WTW:dc