

Ed Lederberg

DATE: March 28, 1974

TO : J. Lederberg

FROM : E. Levinthal *ELV*

SUBJECT: SUMEX - DENDRAL Resources

This memo is mainly to get my own thoughts organized on this subject and to set forth some possible actions for further discussion. I have tried to classify the communities with whom we might interact into four main, but not necessarily orthogonal groups.

I. Organic Chemists. This is the most complex group to characterize. It involves a possible use of both SUMEX and DENDRAL resources. Our attention could be focussed only on mass spectrometry or even more sharply on those aspects of GC/MS most closely matching the currently completed DENDRAL developments. Specialists in GC/MS are likely to be somewhat experienced in the use of computers and to be both sources and sinks of software. Their interests would be in DENDRAL per se rather than AI per se.

Burlingame's review article (Anal. Chem. 44, No. 5, April 1972), gives over 50 references that might identify members of this community. Similar review articles covering instrumentation other than MS such as NMR could serve to even further broaden the net.

Hamming's committee of the ASMS could serve both as a source and a sink of programs as well as to identify chemists who might be interested in using such programs.

The Division of Research Resources is currently funding nine mass spectrometry centers for the further development of mass spectrometric techniques for biomedical analysis. (See attached announcement from pages 7 and 8 of NIH Guide for Grants and Contracts, Vol. 3, No. 3, Feb. 21, 1974.)

There are, of course, in addition, organic chemists and biochemists who have no particular expertise in mass spectrometry or computers. Their input would be problems or samples that could take advantage of the analytical capabilities of the mass spectrometry resource. Professor Raymond Clayton might be an example of such a user.

Based on the assumption that the earliest date on which we are likely to have networking capability is Bastille Day. I suggest the following:

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1. We try by June 14 to describe, document and debug a limited set of DENDRAL programs that we would be in a position to offer over the network as soon as we have established operating network connections.
2. By that date we can have contacted Hamming, have acquired some knowledge of what he might have to offer, and be in a position to offer something to him in return if it seems desirable.
3. We should contact each of the NIH resources, recognizing Carl Djerassi's concern for the feeling of competitiveness that might exist. We do not now have knowledge about what is going on in each of these resources. I presume the state of ignorance is to some extent mutual. It might be useful to host a conference, perhaps sometime this summer, of representatives of each of these resources so that we could each describe our plans and what we are doing and discover how we might reinforce each others efforts.
4. From those identified in one through three above, we should try to pick two or three who are very knowledgeable in mass spectrometry and use of computers with whom we might have a very early and successful interaction.
5. With regard to the general community of organic ^{or biochemists}, I think relationships should remain for sometime ad hoc. I don't think we should broadcast any generally available DENDRAL/Mass Spectrometry interaction or service. Interaction should be pursued when particular individual activities are identified such as, for example, Clayton's, which overlap the intellectual interests of the principal investigators on our grants and where a high degree of personal rapport could be established between the scientists involved. Certainly individuals like Naganishi (Sp?) at Columbia should be among those contacted.

II. This group includes established centers of applications of computers to medicine. The best of such centers would have a high degree of competence in computers but may have no present interests that are convergent with our SUMEX/AI goals. There is a great deal of reference material available which would allow one to make a listing of such centers. By centers I don't wish to limit the definition to computer service centers at medical schools, it should include activities such as Cyrus Levinthal's at Columbia, particularly since his interests have broadened beyond the question of enzyme structure. There are resources we could draw on which could help us judge the quality of members of this group. After we have defined the AI character of our resource such centers could play a very useful role. In effect they could serve as retailers of our resource to the medical establishments with which they are associated. Thus through them we could gain a significant leverage

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factor for our resources. I suggest that we make up such a list and be prepared by the middle of the summer to send to places on the list a description of our resources and our interest in artificial intelligence. Sometime in the future we might wish to consider international establishments of the same kind and satellite communication.

III. This group are the present centers of excellence in AI. They may have no presently developed interests in applications of AI to medicine. They are likely to be both sources and sinks of software with or without network connections. The list of such places is well-known to Amarel and Feigenbaum and are contained probably with a great deal of completeness in the bibliographies of Feigenbaum's reviews of the field. In addition to exchanges of software we might to some extent serve as "marriage" brokers between this group and the previous group.

IV. The fourth general class is the medical community which have no well-developed skills in computers or artificial intelligence. Here, vis a vis SUMEX, I believe this group should be treated in a similar manner to the general group of organic chemists, vis a vis DENDRAL. Namely, strong overlapping intellectual interests and personal rapport are the essential ingredients. In some cases we might be able to serve as "marriage" brokers between this group and the preceding group III. I recommend that at least for the first year of our grant, our contact with this group at large be somewhat pro forma. An announcement in Science early this fall might be an adequate first step.

ECL/mla