



OXMAN, H.

DEPARTMENT OF HEALTH, EDUCATION, AND WELFARE
PUBLIC HEALTH SERVICE
NATIONAL INSTITUTES OF HEALTH
BETHESDA, MARYLAND 20014

December 14, 1973

Dr. Thomas C. Rindfleisch
Stanford University School
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Stanford, California 94305

Dear Dr. ^{*Tom*} Rindfleisch:

The following are my comments on the DENDRAL draft renewal application sent to me on November 30, 1973.

1. I find it difficult to see a strong connection between the Djerassi mass spectrometry laboratory (GC-HRMS) and the AI effort. Looking at the pros and cons, it is much easier to separate your proposal as it now stands into the two components allowing each to sink or swim on its own merit. The bridge between the two, DENDRAL's need for MS data and the MS resource's need for DENDRAL, is insufficient justification, in my opinion to combine both into one project. If we consider AI as the primary focus, then a case for on-line MS data acquisition must be strengthened considerably. A question that comes to mind immediately is this - why must DENDRAL have its own MS capability? Can't other laboratories (such as Burlingame's) and the literature satisfy your needs?
2. If we turn things around and use MS as the driving force behind DENDRAL, we are confronted with another set of problems. Now it is necessary to justify DENDRAL in terms of the research community's need for much improved methods of interpreting MS data and showing how DENDRAL can meet this need. Also, we must face the possibility that by the time DENDRAL reaches the point of being generally useful, technology might be developed to the point that MS is no longer a useful analytical tool or other methods of dealing with MS could be far superior to DENDRAL. The doubts raised by these considerations are important when a priority

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must be placed upon investing substantial sums of money into a long-term project.

3. In order to support the need for direct involvement with a MS laboratory, you should cite cases in which it was necessary to go to the lab for additional data obtained under controlled conditions and requiring quick turn around.
4. Upgrading the Djerassi MS resources in the present proposal must be justified on the basis of DENDRAL's needs. If the resulting capability exceeds that required by DENDRAL, then it is logical to make full utilization by offering specialized services to the biomedical research community.

I hope you find these comments useful. Call on me if you desire further explanation.

Sincerely yours,



Michael A. Oxman, Ph.D.
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