# STANFORD UNIVERSITY STANFORD, CALIFORNIA 94305

**DEPARTMENT OF CHEMISTRY** 

March 25, 1974

Dr. Michael Oxman, Program Director Biomolecular Characterization Resources Biotechnology Resources Branch National Institutes of Health Bethesda, Maryland 20014

Re: RR-00612

Dear Mike:

This is in response to your telephone call on March 18 and Dr. Raub's letter of the same date conveying the good news in regard to our DENDRAL grant renewal. Since that time, we have been examining our budget estimate along the guidelines you discussed with us, attempting to modify the manpower cost allocation so as to be able to implement a better long term data system solution and to increase the effectiveness of the MS-9 instrument.

In line with our discussions of March 18, we have tried to accommodate the increased hardware costs by reductions in personnel. The attached budget reflects the limit to which we feel this can be done without prejudicing the goals of the project. This formulation of the instrumentation and computer support will maximize our ability to use standard systems and facilitate software interchange between DENDRAL and other research efforts.

To this end we have constructed a plan, detailed in the attached modified first year budget estimate, which provides for the purchase and maintenance of a minimal PDP-11/45 computer data system and an up-grading of our MS-9 spectrometer which we feel would be advantageous to the project by allowing a greater concentration of the MAT-711 capabilities on GC/HRMS. In order to offset these increased hardware costs in the first year, we have modified our manpower cost allocations in a number of small increments throughout the staffing plan. These changes include several painful cuts and take advantage of support from other sources which we were not able to anticipate at the time our proposal was submitted last December. In fact, even at this time some of the allocation changes are proposed based on anticipated rather than in-hand funding. The risks involved are relatively small and we feel are warranted in light of this opportunity for enhancing the overall project capabilities.

I trust the attached budget estimate is self explanatory. If questions arise, please do not hesitate to call. As I mentioned on the telephone, I am going on a five-week trip for the National Academy of Sciences starting Monday, March 25. In

my absence please refer all correspondence and questions relating to these matters to Professor Lederberg in the Department of Genetics.

I am anxiously looking forward to completing these negotiations for a May 1 award so we can once again concentrate on the substantive technical issues of applying GC/MS to medical problems. I recognize that this past year of grant application and reapplication has been painful for you at BRB as well as for us. I am grateful for your patience and cooperation in charting a course through the many obstacles and am very pleased at the successful outcome.

Sincelety yours

Carl Djerassi

Professor of Chemistry, Principal Investigator

CD:ab

Enclosure

Robert D. Simmons
Contracts and Grants Manager
Sponsored Projects Office
Stanford University
Stanford, California 94305

PRIVILEGE	D COMMUNIC	HOITA		SECTION	<b>111</b> s	UBSTITUTE	THIS PAG	E FOR DET	AILED BUDGET PAGE	
SUBSTITUTE				PERIOD COVERED			GRANT NU	ANT NUMBER		
DETAILED BUDGET FOR FIRST 12-MONTH PERIOD				FROM May 1 107/		April 30, 1975		RR-0	-00612	
PERSONNEL (List all personnel engaged on project)				riay 1, 1	TIME OR	<del> </del>		OUSSES	(0.11)	
NAME (Last, first, initial)  TITLE OF PO			OSITION	EFFORT		AMOUNT RE	QUESTED (	Omit cents)		
See att det	ached pers	sonnel	Principal Invest Program Directo	igator or	%/HRS.					
						TOTA	\L		\$ 156,307	
2. CONSULTANT COSTS (Include Fees and Travel)							s			
3. EQUIPMENT (Itemize) (A) Equipment Maintenance: (B) DEC GT-40 Display Terminal \$13,400 PDP-11 (DEC Contract) \$7,940 PDP 11/45 Mini Computer 59,750 Mat-711 (Parts, etc.) 6,500 MS-9 Spectrometer Upgrade 7,100							A) \$80,250 B) 14,440 s			
GC Supplies (Columns, gasses, etc. 1,000 Data Recording Media 1,000 Chemicals, glassware, stock, etc. 1,500 Minicomputer Supplies 700							\$1,000 1,000 700	s 9,600		
STAFF	STAFF 0. DOMESTIC								s 1,200	
	TRAVEL (See Instructions) b. FOREIGN								s	
6. PATIENT COSTS (Separate Inpatient and Outpatient)						· · · · · · · · · · · · · · · · · · ·	s			
7. ALTERATIONS AND RENOVATIONS										
8. OTHER EXPENSES (Itemize per instructions) Publications, telephone, office supplies, postage \$4,000 Computer Terminal Lease (4) 5,400 Computer Usage - 370/158 (First Year Item Only) 5,000										
9.				Sub	total – Item:	s 1 thru 8			s 276,197	
	10. TRAINEE	EXPENSES (Se	ee Instructions)							
İ		PREDOCTOR		No.	Proposed _		s			
FOR	a. STIPENDS	POSTDOCTO			Proposed _		s			
TRAINING	-	OTHER (Spec		No.	Proposed _		\$			
27		DEPENDENC	Y ALLOWANCE	τ.	TAL STIPE	ND FXPFN	SES		s	
GRANTS	h Turren	NO ECC				- F EACEN				
ONLY					·	\$				
		TRAVEL (Desc	ribe)						S	
	11.	· · ·		Subtotal	- Trainee l	xpenses			s	
12. TOTAL D	RECT COST (	Add Subtotals,	Items 9 and 11, and	enter on Page	e 1)		<del></del>		\$ 276,197	

## Supplementary Information for Personnel Costs Requested

It is the policy of the DHEW to omit specific salary rates or amounts for individuals from those copies of grant applications which are made available to reviewing consultants. Therefore, a substitute budget page is enclosed and must be used in lieu of the present budget page in all competing applications. Note that individual salaries will not be shown on the substitute budget page; however, if a grant is to be awarded as a result of this application, the awarding unit will need information concerning specific salaries. Please use the space below to list all personnel shown on the substitute budget page, and include the salary and fringe benefits requested for each, following the appropriate guidelines in the Information and Instructions.

THIS INFORMATION WILL BE USED ONLY BY PHS ADMINISTRATIVE STAFF.

DESCRIPTION (Itemize)			AMOUN'	T REQUESTED	Omit cents)	
RSONNEL		FFFORT %/HRS.		FRINGE	1	
NAME	TITLE OF POSITION	Alans.	SALARY	BENEFITS	TOTA	
C. Djerassi	PRINCIPAL INVESTIGATOR	10%			\$ _0_	
J. Lederberg	Principal Investigator	10%			-0-	
E. Feigenbaum	Principal Investigator	10%	2,910		3,42	
A. Duffield	Research Associate	15%	3,532		4,15	
). Smith	Research Associate	100%	16,200		19,06	
I. Sridharan	Research Associate		10,690		12,59	
. Brown	Research Associate		16,200		19,06	
• Dromey	Research Associate	100%	7,750		9,11	
. White	Programmer	100%	14,400		16,94	
. Tucker	Programmer		14,100		16,59	
• Wegmann	Senior Research Assistant		15,000		17,65	
. Veizades	Electronics Engineer		10,200		12,00	
. Steed	Glass Blower/Machinist	15%	3,046		3,58	
. Masinter	Research Assistant	100%	5,070		5,07	
. Stefik	Research Assistant	75%	3,781		3,78	
. Friedland	Research Assistant	50%	2,206		2.206	
. Wharton	Secretary	100%	9,400		11.06	
		11				
TOTAL Same as Askal (						
TOTAL - Same as total for Substitute Detail	led Budget Page			>	156,307	
INDIRECT COS (  (See Instruction.)	DATE OF DHEW AGREEMENT:  WAIVED  WAIVED  UNDER NEGOTIATION WITH:  "IF THIS IS A SPECIAL RATE (e.g. off-site), SO INDICATE.					

The attached budget is derived from that submitted with our proposal in December 1973. We have adjusted our manpower costs so as to be able to budget the purchase in the first year of a PDP-11/45 minicomputer data system in place of augmenting the PDP-11/20 and to upgrade the performance of our MS-9 spectrometer. The manpower cost reallocation needed to offset these costs in the first year could not be fully absorbed in the areas recommended by the Study Section (MS laboratory support) without jeopardizing the entire operation of the laboratory. The proposal budget as submitted had been vigorously pruned to minimize costs, particularly with respect to manpower and GC/MS laboratory support. Our experience has been that Ms. Wegmann is heavily occupied full time in operating the GC/MS system to optimize performance and manage the sample handling. This will be all the more true as our sample load increases for the larger scope sample processing we proposed. We allocated in total less than one full time equivalent to maintain the electronic, mechanical, vacuum, and glass work systems of the instruments as well as to develop the necessary new electronics and controls for metastable and GC/HRMS work. We have been unable (even considering possibly higher costs) to obtain the required maintenance support from other sources (e.g. vendors).

We have implemented a number of small but painful cuts in the laboratory support area as well as elsewhere in the budget and have taken advantage of first year support from other sources for particular individuals connected with the project which could not be anticipated in our earlier submission. These relatively small incremental adjustments distributed over the first year staffing plan allow us to offset the increased hardware costs.

#### PERSONNEL

Dr. Duffield - A small error has been corrected in the previous computation of Dr. Duffield's salary and his salary allocation has been reduced to 15% of his time. This is consistent with the expected but as yet unawarded Genetics Research Center grant which will support part of his body fluid analysis research efforts relevant fo the DENDRAL project.

Dr. Sridharan- Dr. Sridharan has taken a leave of absence through August 1974. We have reduced his salary allocation in proportion.

Dr. Dromey - Dr. Dromey has received fellowship support from the Australian government through October 1974 so that his salary allocation is reduced in proportion.

Mr. Veizades - We have reduced the allocated support for Mr. Veizades to 50%. H is services in the proposed development efforts and for instrument maintenance are indispensable. We feel his support commitment cannot be reduced further without severely degrading performance on the project.

Mr Steed - We have reduced Mr. Steed's allocation to 15%. Again, his services are essential for laboratory maintenance.

Research Assistants - Mr. Stefik's plans for this summer have changed so that he will only spend half time on the project and Mr. Friedland (previously listed as "to be appointed") will not start until September. These changes are reflected in appropriate salary reductions.

#### **EQUIPMENT**

We have budgeted the purchase and maintenance of a PDP-11/45 minicomputer for the mass spectrometer data system rather than augmenting our existing PDP-11/20 machine. This system is minimally configured to do the necessary work, taking advantage of DEC discounts to Stanford and purchasing equipment from other vendors where appropriate. These costs are detailed below including sales tax.

1)	PDP-11/45, TTY, Clock, and 16K memory	\$25,530		
2)	12k additional fast memory (Intel)	6,360		
3)	Floating point processor	5,050		
4)	Industry magnetic tape drive	10,250		
5)	Disk storage drive (System Industries)	11,130		
6)	RT-11 Software	1,430		
		\$59,750		

The maintenance cost for this system will be \$7,940 per year for one shift coverage.

Our MS-9 mass spectrometer has, over a period of years, been kept up to date commensurate with availability of funds. Modifications have included upgrading some of the electronics for increased reliability and to provide the capability for fast scanning at high resolving powers. Other upgrades have included ion source modifications for higher sensitivity and interfacing to the present computer system. As the instrument stands now, together with the \$7,100 budgeted for replacement of certain critical items which hamper achievable sensitivity, and upgrading of the computer interface, the MS-9 can off-load more routine high resolution mass spectrometry experiments, thus freeing the MAT-711 for more concentrated effort on GC/HRMS.

### The planned improvements include:

Ion multiplier replacement	\$2,500
Ion source plate replacement	2,500
Ion source slip replacement	1,600
Computer interface up-grade	500
	\$7,100