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#### SECTION 1

DEPARTMENT OF HEALTH, EDUCATION, AND WELFARE PUBLIC HEALTH SERVICE

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#### RESEARCH OBJECTIVES

### NAME AND ADDRESS OF APPLICANT ORGANIZATION

Stanford University, Stanford, California 94305



USE THIS SPACE TO ABSTRACT YOUR PROPOSED RESEARCH. OUTLINE OBJECTIVES AND METHODS. UNDERSCORE THE KEY WO (NOT TO EXCEED 10) IN YOUR ABSTRACT.

The objectives of this research program are the development of innovative computer and biochemical analysis techniques for application in medical research and closely related aspects of investigative patient care. We will apply the unique analytical capabilities of gas chromatography/mass spectrometry (GC/MS) and Carbon(13) Nuclear Magnetic Resonance Spectrometry (CMR) with the assistance of data interpreting computer programs utilizing artificial intelligence techniques, to investigate the chemical constituents of human body fluids in a variety of clinical contexts. Specific subtasks of this program include; 1) the application of artificial intelligence techniques to programs capable of interpreting mass spectra from basic principles as well as extending mass spectral theory by analysis of solved spectrumstructure examples, 2) the extension of GC/MS data systems incorporating an increasing level of automation and allowing the directed collection of specialized information, 3) the application of GC/MS techniques to analyze body fluids such as urine and blood, and to relate detected metabolic abnormalities to clinically observable disease states, and 4) the application of CMR techniques to assist in the determinatic of chemical structure.

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The undersigned agrees to accept responsibility for the scientific and technical conduct of this project and for provision of required progress reports if a grant is awarded as the result of this application.

APR 26 1373 ٩, Date

Joshua Lederber Principal Investigator

#### RESOURCE-RELATED RESEARCH: COMPUTERS AND CHEMISTRY

(RR-00612 - Renewal Application)

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