



Subcontract Executive Summary

Centralized Information Technology (IT) System for Data Collection and Storage¹

CambridgeSoft Corporation

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CambridgeSoft Corporation is providing the SMA Project with a web-based centralized informatics system for chemical compound registration and tracking, biological data collection and storage, and structure-activity-relationship analysis. CambridgeSoft will provide secure web hosting services, the underlying Oracle data base, and ChemOffice Enterprise Ultra software suite. Features of the system include:

- Inventory Manager, Registration System, BioAssay, and BioSAR browser applications.
- Viewing access for at least 100 researchers and investigators. Access roles are set up within the system to determine which data each individual is permitted to view.
- Capacity for uploading and storing chemical structures and other identity information for more than 250,000 compounds.
- Structure-based querying using built-in ChemDraw control or ISIS/Draw, as well as substructure searching.
- Similarity searching capability through the ChemDraw control based on the Tanimoto similarity index.
- Integrated Inventory module that can manage inventory and track assay requests/compound distribution among various sites, as well as request/disbursement workflow support.
- BioAssay, an integrated assay management system that allows the entry, storage, and output of in vitro bioactivity screening data and in vivo efficacy, pharmacokinetic, and toxicity data that are linked to identification number, chemical structure, lot number, and (where applicable) plate number. All of the data are linked through the integrated product suite.
- Ability to enter, store, and output textual assay protocols that are linked to assay data through the integrated BioAssay module.
- User-friendly forms-based interface for uploading biological information. The system can accept imports from Microsoft Excel spreadsheets and automatically load machine data files.
- Simple, easy-to-use graphing capability.
- Ability to generate tabular formatted reports that include all data stored within the system.

¹ A proposal to support this subcontract was submitted to the SMA Project's JL-030805-01, "A Centralized IT System for the SMA Project." SAIC provides management support for The SMA Project to the NINDS through contract N01-NS-3-2356.

- Comprehensive database of approximately 400 chemical catalogs (including all major reagent vendors) that provides structure, text, CA number, synonym and cross reference search capability, and pricing information. This database is integrated into the Inventory Manager module.
- Ability to track compound synthesis, as well as purchase and delivery of chemicals and reagents.
- Ability to enter, store, and output large-file objectives, including Microsoft Word and PDF documents, PowerPoint presentations, Excel spreadsheets, photographs, other graphics, and short videos.
- Provide Informatics support for data analysis and statistics from in vitro and in vivo assays. Work collaboratively with SMA Project team to define metrics for compound performance.