CLS Protein Crystallography Project: Executive Summary

(10-Feb-00, CMFCsum.doc)

We propose to design, build, commission, and operate an X-ray beamline at the Canadian Light Source (CLS) in Saskatoon. The beamline, together with associated staff, laboratory and office space, would be called the Canadian Macromolecular Crystallography Facility (CMCF). As the CMCF develops we anticipate it will grow, such that at some future time at least one other CLS beamline will be developed for macromolecular crystallography and added to the CMCF infrastructure. However, such growth will be funded through additional proposals and is not covered under this present proposal.

This document is a Conceptual Design Report (CDR) for the CMCF, and is therefore not intended to be a detailed exposition of the CMCF. The budget estimates and schedule contained here only approximate their final values. Technical detail will be developed to higher levels of accuracy, culminating in a Detailed Design Report (DDR) which will take 6-9 months to complete. This subsequent design study cannot begin until the present CDR be approved and funding commitment be made. Budgets and schedules will become progressively better defined as the technical design develops. The DDR will be the basis for funding *obligation* and will have sufficient technical detail to be the basis of the actual construction project. However, the CDR is the basis for funding *authorization*. Therefore, to account for the possibility that the budget will increase as it is more completely fleshed out, this budget follows the accepted business convention of including explicit “contingency” funds, which represent the uncertainty of these budget estimates. This practice allows the funding agency to authorize a realistic budget for the project despite the uncertainty of the budget estimating process. In this CDR, contingency funds represent 25% of the estimates of all capital items and 15% of all other items.

The CMCF requires a long undulator beamline at the CLS to fully develop its scientific potential, preferably one longer than 40 meters. This length will allow sufficient demagnification of the source to match the size of demanding samples, as will be fully explained in this document. The product of the beam crossfire and beam size (the phase space) is conserved by optical elements. To obtain a small beam size and a low divergence at the focal point, it is therefore necessary to select a source that matches the required phase space at the focus. For this reason an undulator insertion device has been selected; it provides a small and highly collimated X-ray source. The properties of the undulator source, combined with the appropriate optical elements to focus, collimate, and

monochromate the X-ray beam will be suited for highly demanding data collection tasks. This includes data collection on very small crystals or crystals with very large unit cells, obtaining ultra-high resolution data, and obtaining highly accurate data for MAD/SAD phasing techniques. The extremely high intensity of the X-ray beam will allow the use of very short exposure times while still obtaining strong diffraction signals. This will make it a highly productive beamline capable of high throughput data collection. To be successful, the CMCF beamline requires that all components are matched in performance, so as not to create bottlenecks. This includes the source, optics, detector, computing hardware, software, and the user interface. The Facility will further need to fully integrate its disparate components into a single well-functioning system. It will need excellent staff, and it will need the committed and supportive participation of the entire Canadian crystallographic community. Building the beamline will be a significant technical and logistic challenge, but one that can build on existing experiences at other facilities, and one that will bring new technical knowledge into Canada.

Canada needs this Facility if it is to maintain growth of its already strong community of macromolecular crystallographers. This growth must occur for Canada to stay at the cutting edge of biotechnology in the 21st century. Construction of the CLS presents a unique opportunity for the crystallographic community in Canada. If this opportunity is successfully developed, the CMCF will become a meeting place for molecular biologists and other scientists from across the continent and a catalyst for new and creative ideas and discoveries. It will be good for science, and it will be good for the country.