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THE USSR ACADEMY OF SCIENCES
SIBERIAN BRANCH
INSTITUTE
OF CYTOLOGY AND GENETICS

MODELLING AND COMPUTER METHODS
IN MOLECULAR BIOLOGY AND
GENETICS

ABSTRACTS OF THE INTERNATIONAL CONFERENCE



NOVOSIBIRSK. 1990

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EDITED BY N.A. KOLCHANOV AND V.A. RATNER

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INTRODUCTION

The present book contains reports of the International Conference "Modelling and Computer Methods in Molecular Biology and Genetics" which took place from August 27 to September 1, 1990 in Novosibirsk (USSR) on the initiative of the Institute of Cytology and Genetics, Siberian Branch of Academy of Sciences of the USSR.

The Conference was held under the organizational support of Siberian Branch of Academy of Sciences of the USSR, General Biology Department of the USSR Academy of Sciences, the Complex Program of Scientifical and Technical Progress (The 5.5.5.3 Project) with the countries members of the Council of Mutual Economic Assistance, All-Union scientific-technical program "Geninform" and the National "Human Genome" Project.

The materials presented correspond to the following fields:

- Computer analysis of nucleotide sequences;
- Computer analysis and modelling of proteins structure;
- Molecular Evolution Theory;
- Molecular-genetic systems' modelling;
- Molecular-genetical and molecular-biological data banks;
- Program packages for molecular-genetical and molecular-biological data analysis;
- New computer-informational techniques in molecular biology and genetics, including expert systems, artificial intelligence systems and knowledge bases.

This book gives a profound outlook on the elaborations and scientific investigations in the mentioned above fields of bioinformatics in 1990.

We hope it will be interesting for specialists, engaged in bioinformatics; mathematical simulation and theoretical examining of macromolecules' (DNA, RNA and proteins) structure, functioning and evolution.

The book can also attract attention of the scientists, interested in applying mathematical and computer analysis to molecular biology, molecular genetics and biophysics.

Dr. N.A. Kolchanov
Prof. V.A. Ratner

A COMPUTER PROGRAM FOR AUTOMATED DNA SEQUENCERS

DATA HANDLING.

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Using the fluorescent automated sequencer is particularly important to analyze the final sequence obtained from the instrument because of the presence of ambiguity and errors related to the raw data software processing . We have developed a computer program written in Fortran 77 using GKS standard graphic library, running on VaxStations based on VMS operative system. This program allows an easy handling of the sequences and related raw data produced by a fluorescent automated sequencer. It is based on menus and mouse driven choice. It allows to review the sequences linked with the raw data , in order of making the final corrections. It is also possible to compare the results obtained from two different runs of the same sequence, in presence of both the sequences and the related raw data, in order to obtain the best final sequence. The software is able to compare two sequences with partial overlap by means of Bestfit program, contained in GCG package from University of Wisconsin based on the "local homology" algoritm of Smith and Waterman, in order to get the contig. This feature is really relevant when building sequence blocks in large DNA fragment assembly projects .

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