

*Bio-Algorithms  
and  
Med-Systems*

*Irena Rotermań-Konieczna*

***DEPARTMENT OF  
BIOINFORMATICS AND  
TELEMEDICINE***

***JAGIELLONIAN UNIVERSITY  
CRACOW***

***MEDICAL COLLEGE***



# ***MEDICINE***

## ***MEDICINE ORIENTED PROJECTS***

- ***TELEMEDICINE - "PATIENTS" LEVEL***

***MEDICAL DATA MINING***

***TELECONSULTATIONS***

***STREAMING SERVERS***

- ***BIOINFORMATICS - MOLECULAR LEVEL***

# ***BIOINFORMATICS***

***GENOMICS – COMPARATIVE DNA SEQUENCE ANALYSIS***  
***DISEASE RELATED***  
***TANDEMLY REPEATED TRINUCLEOTIDES***

***PROTEOMICS – PROTEIN STRUCTURE PREDICTION***  
***SEQUENCE – STRUCTURE RELATION***  
***CONTINGENCY TABLE 160 000 x 2 401***  
***SIMILARITY SEARCH***

***COMPUTER AIDED DRUG DESIGN***  
***COLLABORATION WITH EXPERIMENTALISTS***

# ***COMPUTER AIDED DRUG DESIGN***

## **POTENTIAL DRUG – LIGAND**

***GAUSSIAN – PARTIAL CHARGES + GEOMETRY***

***SUPRAMOLECULAR FORM***

***GEOMETRY and STABILITY***

***MOLECULAR DYNAMICS SIMULATION***

## **PROTEIN-LIGAND COMPLEX**

***AMBER, CHARMM, GROMAX***

***STRUCTURE and STABILITY***

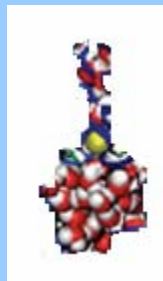
***MOLECULAR DYNAMICS SIMULATION***

## **ENVIRONMENT**

***MEMBRANE***

***WATER***

# *LIGAND*



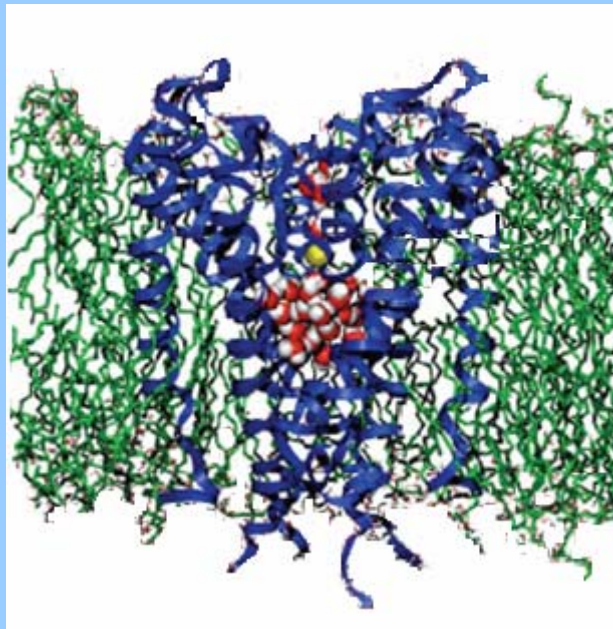
**10 atoms**

# ***PROTEIN-LIGAND COMPLEX***



**348aa – 3532 atoms**

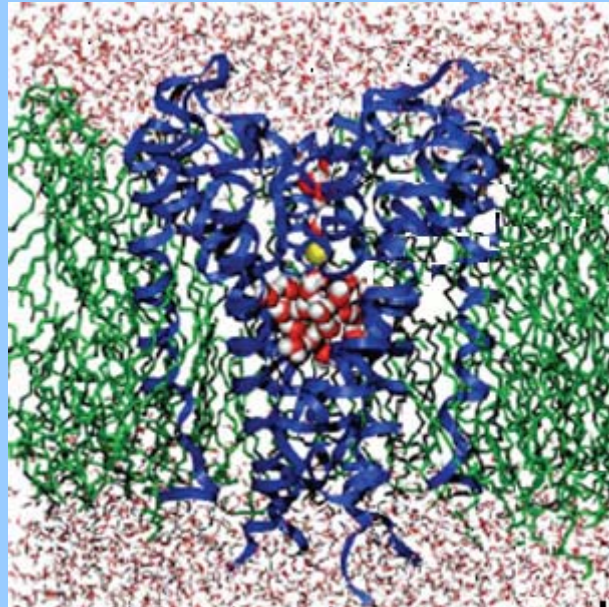
# ***ENVIRONMENT MEMBRANE***



**128 phospholipids – 6656 atoms**

# ***ENVIRONMENT WATER***

**MDS – 2ns**



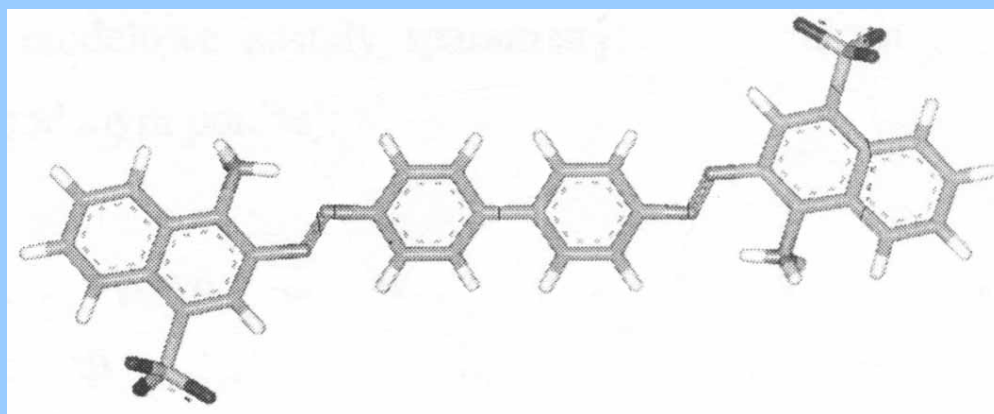
**2460 H<sub>2</sub>O – 7380 atoms**

**TOTAL NUMBER OF ATOMS 15 108**

# ***IMMUNOLOGICAL SIGNAL***

***LIGAND – 70 ATOMS***

***GAUSSIAN***

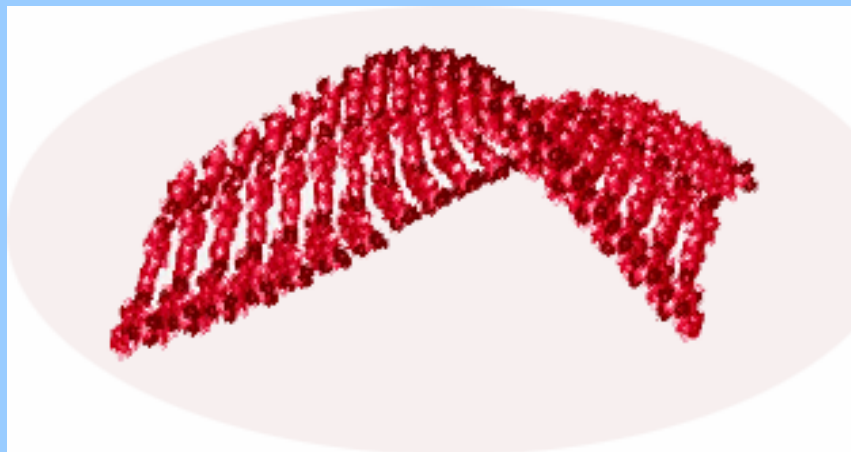


# ***SUPRAMOLECULAR FORM***

***RIBBON-LIKE STRUCTURE***

***n \* 70 ATOMS***

***MDS***



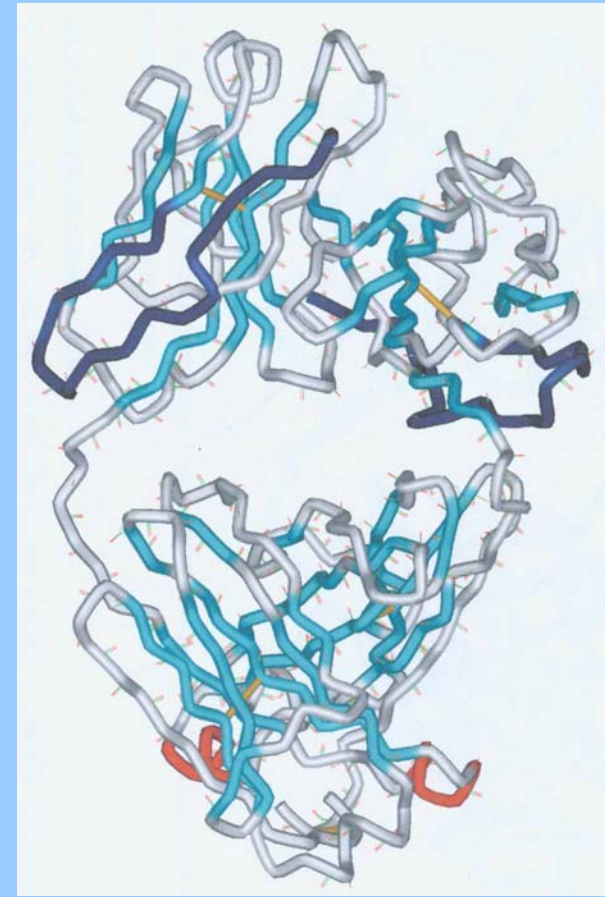
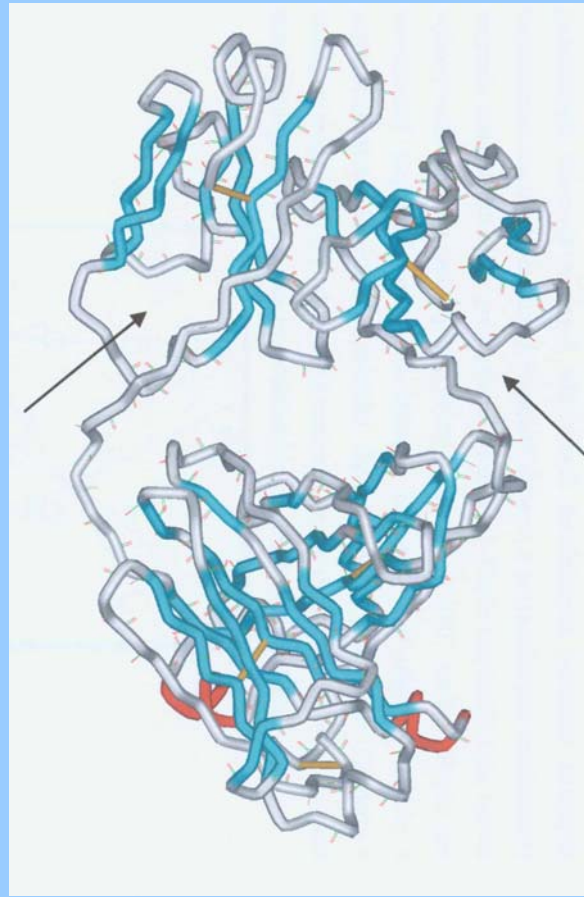
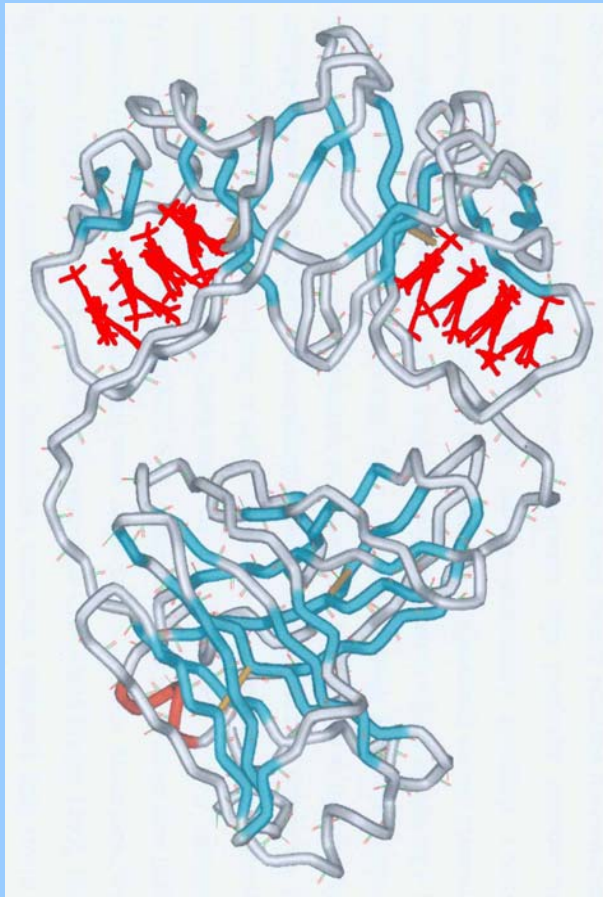
**Immunological Signal**

# *IgG(Fab) – LIGAND COMPLEX*

Fab+supramolecular  
Ligand  
biological activity  
protected

Pathological form of Fab  
N-terminal fragment  
missing  
no biological activity

Natural form of  
Fab  
Normal  
biological activity



**Immunological Signal**

# Protein Function - Immunological Signal

Marcin Król<sup>1</sup>  
Irena Roterman<sup>1</sup>  
Barbara Piekarska<sup>2</sup>  
Leszek Konieczny<sup>2</sup>  
Janina Rybarska<sup>2</sup>  
Barbara Stopa<sup>2</sup>  
Paweł Spólnik<sup>2</sup>  
Edward Szneler<sup>3</sup>

Biopolymers, Vol. 77, 155–162 (2005)  
© 2005 Wiley Periodicals, Inc.

## An Approach to Understand the Complexation of Supramolecular Dye Congo Red with Immunoglobulin L Chain $\lambda$

Marcin Król<sup>1</sup>  
Irena Roterman<sup>1</sup>  
Barbara Piekarska<sup>2</sup>  
Leszek Konieczny<sup>2</sup>  
Janina Rybarska<sup>2</sup>  
Barbara Stopa<sup>2</sup>

Biopolymers, Vol. 69, 189–200 (2003)  
© 2003 Wiley Periodicals, Inc.

## Local and Long-Range Structural Effects Caused by the Removal of the N-Terminal Polypeptide Fragment from Immunoglobulin L Chain $\lambda$



*Journal of Computer-Aided Molecular Design* **18**: 41–53, 2004.  
© 2004 Kluwer Academic Publishers. Printed in the Netherlands.

## Force-field parametrization and molecular dynamics simulations of Congo red

Marcin Król<sup>a,\*</sup>, Tomasz Borowski<sup>b</sup>, Irena Roterman<sup>a</sup>, Barbara Piekarska<sup>c</sup>, Barbara Stopa<sup>c</sup>, Joanna Rybarska<sup>c</sup> & Leszek Konieczny<sup>c</sup>

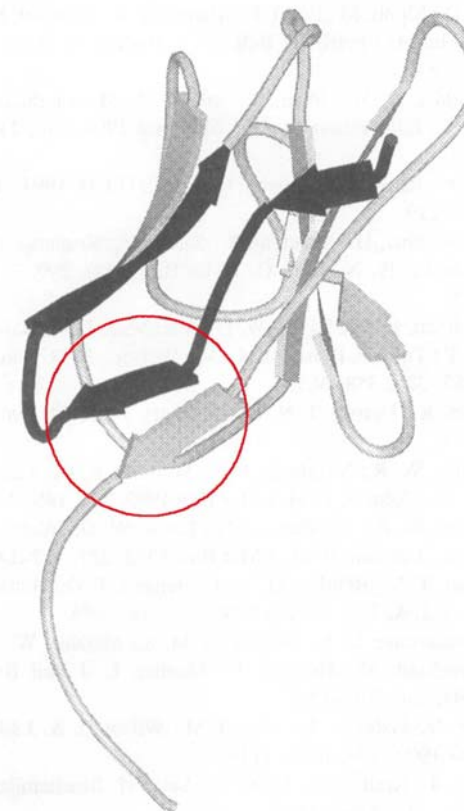
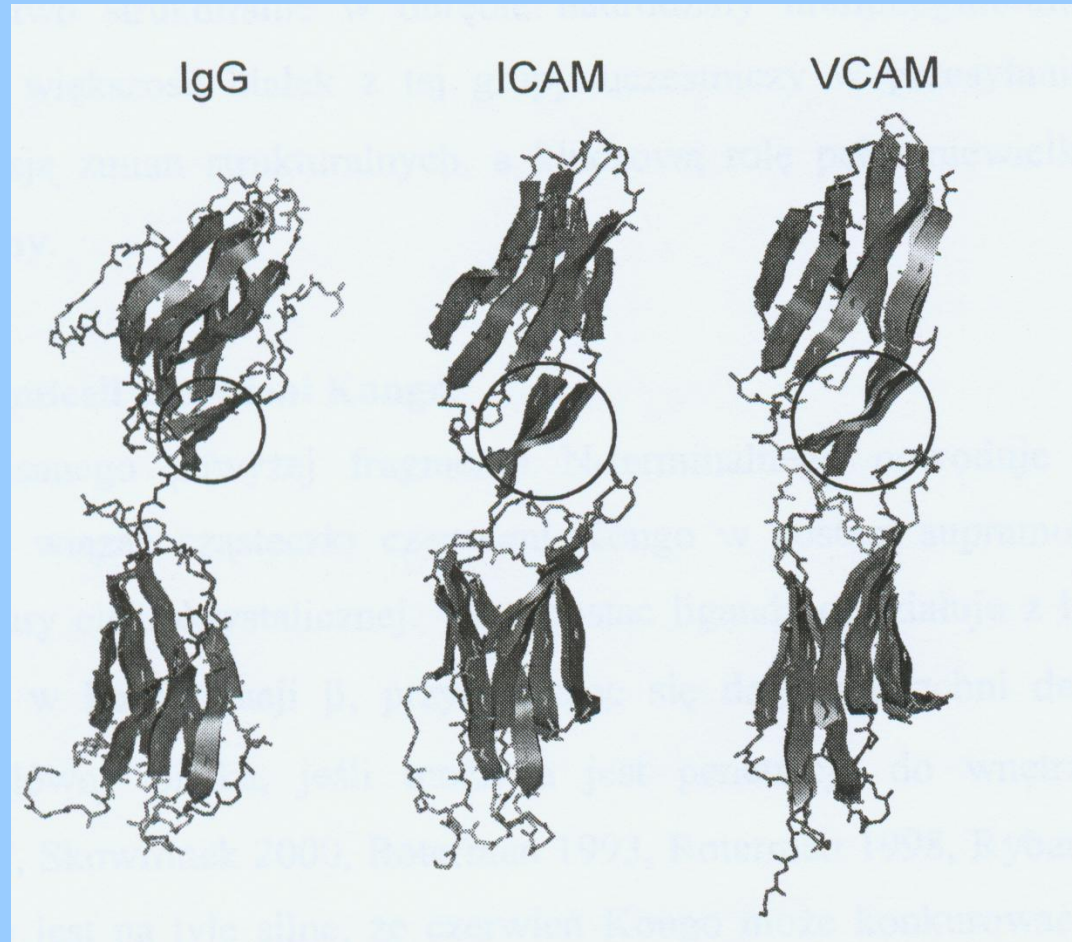
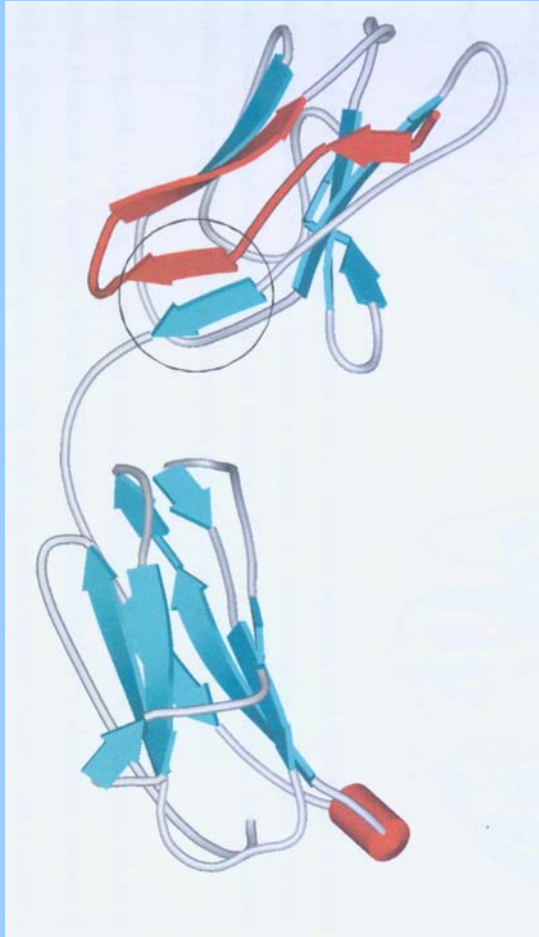


FIGURE 8 The two-parallel-strand  $\beta$ -sheet responsible for the limited elasticity of the hinge region.

Immunological Signal

# ***IgG - SUPERFAMILY***

## ***COMMON MECHANISM***



**Immunological Signal**

# ***COMPUTATIONS***

- ***MOLECULAR DYNAMICS SIMULATION***

**15108 atoms      MDS – 1ns – 56 hours**

**8 procesors 3 GHz 8 \* 500 RAM**

- ***VERY LARGE OUTPUT FILES    8GB***

- ***GRAPHICS***

# Protein Folding – Early Stage

PROTEINS: Structure, Function, and Bioinformatics 55:115–127 (2004)

## Conformational Subspace in Simulation of Early-Stage Protein Folding

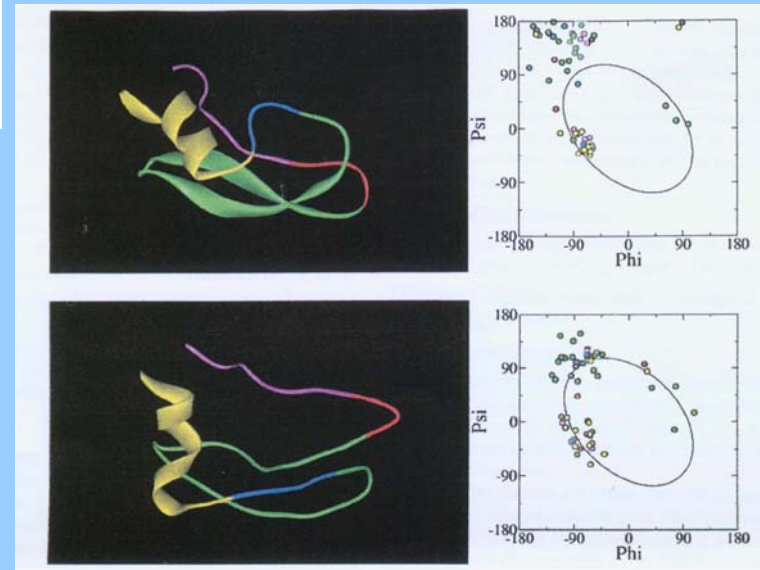
Wiktor Jurkowski,<sup>1,3</sup> Michał Bryliński,<sup>1,3</sup> Leszek Konieczny,<sup>2</sup> Zdzisław Wiśniowski,<sup>3</sup> and Irena Roterman<sup>3\*</sup>

Journal of Biomolecular Structure & Dynamics, ISSN 0739-1102  
Volume 22, Issue Number 2, (2004)  
©Adenine Press (2004)

Lysozyme Folded *In Silico* According to the Limited Conformational Sub-space

<http://www.jbsdonline.com>

W. Jurkowski<sup>1,3</sup>  
M. Bryliński<sup>1,3</sup>  
L. Konieczny<sup>2</sup>  
I. Roterman<sup>3\*</sup>



Vol. 20 no. 2 2004, pages 199–205  
DOI: 10.1093/bioinformatics/btg391



## Limited conformational space for early-stage protein folding simulation

M. Bryliński<sup>1,3</sup>, W. Jurkowski<sup>1,3</sup>, L. Konieczny<sup>2</sup> and I. Roterman<sup>3,\*</sup>

# PERSPECIVES

**1. LONG LIST OF MEDICINE-RELATED PROJECTS**

**2. COLLABORATION WITH PHYSICS FACULTY –  
APPLIED INFORMATICS**

**3. JOURNAL *Bio-Algrithms and Med-Systems*  
for topics of prospective application in medicine**

**[www.bit.cm-uj.krakow.pl](http://www.bit.cm-uj.krakow.pl)**

# ***COLLABORATION***

## ***Department of Bioinformatics and Telemedicine***

**Irena Roterman-Konieczna**

**Marcin Król**

**Weronika Zobnina**

## ***Institute of Biochemistry***

**Leszek Konieczny**

**Paweł Spólnik**

**Barbara Stopa**

**Barbara Piekarska**

**Janina Rybarska**