

## QUESTIONNAIRE

(\* ) – mandatory fields

	<b>Details about organisation</b>
<b>* Organisation name</b>	Molecule Structure Research Center
Organisation acronym	MSRC
<b>* Organisation Activity Type</b> ( <b>RES</b> - Research, <b>HE</b> - University, <b>SME</b> - Small and Medium Enterprise, <b>IND</b> - Industry, <b>OTH</b> - Other)	RES
<b>* Keywords of main research areas</b>	Molecular structure determination
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<b>* Description of organisation and its research achievements for the last five years (~ 5000 signs)</b>
<p>Molecule Structure Research Centre (MSRC) was founded in 1994 as a collective using centre.</p> <p>Staff: 34 workers, from which 20 are scientific researchers.</p> <p>Specialization: Research of molecular structure by X-Ray diffractometry, NMR-, IR-, UV-, mass-spectroscopy, etc.</p> <p>Achievements:</p> <p>The unique method for investigation of processes proceeding in heme-containing proteins has been developed. New metal-containing porphyrine complexes with oxygen and carbon/nitrogen oxides have been obtained. For the first time the complex of NO<sub>2</sub> with the gem-modeling porphyrins has been produced. Coordinated oligomers with the microporous structures containing unsaturated metal-ions have been created. They exhibit many useful properties, particularly, selective sorption and allowing the solid-phase filling and storage of gases, for instance, of nitric oxide. On the base of this research, the sensitive sensors of the various gases can be developed.</p> <p>Together with chemists the target-oriented search of anti- HIV-1 compounds has been done by revealing the structure-biological activity relationship using X-ray crystallography and theoretical calculations. In particular, by this approach a few compounds of classes 2-aryl- and 2-heteryl- prolynes with antiviral properties had been found. A set of new nonlinear optical monocrystals with unique properties had been produced on the basis of the studied interactions of aminoacids and their derivatives with the various inorganic and organic acids. The dependence of the magnetic</p>

properties on structures of new inorganic and semiorganic compounds with giant magnetic resistance has been investigated. These compounds are very attractive for the developers of the memory devices of new generation.

The method of the spatial structure determination of organic molecules and biomolecules in liquid phase on base of NMR spectroscopy in aligning media has been successfully extended. Specific solute-solvent interactions leading to artifacts and decreasing accuracy and precision of determined structure have been revealed. Methods for taking into account these effects and criteria for right choice of orienting media have been developed.

A new method for experimental determination of electric fields in biomolecules using NMR spectroscopy has been proposed.

More than 200 publications in peer reviewed journals in last 10 years.

15 Grants from ISTC, CRDF, INTAS, NFSAT, ANSEF (Total 998 000 U.S.D.).

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<b>International co-operation / Participation in EU RTD programmes or other bilateral / multilateral actions</b>
INTAS, TACIS, TEMPUS, COST, EUREKA, other RTD programmes (please specify programme/s, project title/s and year/s)
CRDF / RESC 17-5 / Purchase NMR spectrometer for regional NMR center / 1997-2006
INTAS / Award # 911 / Reactions of metal atoms, nanoclusters and complexes in matrices / 2001-2004
US CRDF / CGP / AC1-2304-Ye-02 / Structure determination of biological molecules oriented in liquid crystalline solvents / 2002-2004
NFSAT US CRDF / CH 053-02/12001 / Oxo transfer reactions of metalloporphyrins nitrocomplexes / 2002-2004
NFSAT ISIA 04-02 / Foundation of cryogenic research development center / 2003-2006
US CRDF AR2-1027-YE-03 / Strenghtening and modernization of the RESC 17-5 / 2004-2006
NFSAT / ISIMA 03-04 / X-Ray structural investigation in MSRC / 2004-2005
US CRDF / CGP / AE2-2533-YE-03 / Growth and investigation of nonlinear optical crystals of L-arginine, its new derivative and L-histidine salts / 2004-2006
ISTC / A-484 / Gas sensing, catalytica and heme-modeling properties of

metalloporphyrins syblimed layers / 2004-2007  
 US CRDF / ARB2-2701-YE-05 / New 2-heterylprolines as anti-HIV-1, antibacterial, and antitumor agents synthesis and structure-activity relationship investigations / 2005-2007  
 US Fulbright Visiting Scholar award / Georgetown University / 2007-2008  
 US ANSEF / 05-PS-chemorg-0823-306 / Solvent effects on molecular structures determined by NMR spectroscopy in weakly aligning media / 2006-2007  
 NFSAT Graduate Research Support Program / Structural investigations of  $\text{La}_{1-x}\text{Ca}_x\text{MnO}_3$  ( $x=0.18, 0.20, 0.22, 0.25, 0.30$ ) by single crystal X-ray diffraction / 2006-2007  
 US CRDF / ARB2-2834-YE-06 / Design of weakly aligning systems suitable for 3D biomolecular structure determination by NMR spectroscopy / 2006-2008  
 NFSAT / ARC2-3231-YE-04 / Identifying reactive intermediates in the mechanism of catalytic oxo-transfer reactions performed by metalloporphyrins / 2006-2008

	<b>* Please, use "X" to indicate the scientific area/s of your potential project</b>
CHEMISTRY	X
SOCIAL AND HUMAN SCIENCES	
ECONOMIC SCIENCES	
ENGINEERING SCIENCE	
ENVIRONMENT	
AGRICULTURE AND FOOD	
HEALTH	X
MATHEMATICS	
INFORMATION SCIENCE	
PHYSICS	X
NANOTECHNOLOGIES	
ENERGY	
TRANSPORT	
SPACE	

<b>* Summary of potential research project envisaged hosting of European researcher for the period of between 1 and 2 years</b>
<p>Molecular structure determination by NMR spectroscopy of oriented molecules.</p> <p>Search for new nonlinear optical crystals among optically active amino acids salts, their crystal growth and characterization (structural, spectroscopic and nonlinear optical).</p> <p>Structural investigation of modulated structures (commensurate and incommensurate).</p> <p>Structural investigation of twinned crystals.</p> <p>FTIR and UV-Vis spectroscopy of the biologically important intermediats at the very low temperatures.</p> <p><math>\text{NO}_x</math> transformations in the coordination sphere of the heme-modelling metalloporphyrines.</p>

	<b>Please, confirm your agreement on data publication and dissemination</b>
<b>I agree with the publication of the data</b> on the web-site <a href="http://www.inco-ecca.net">http://www.inco-ecca.net</a> , and <b>dissemination</b> among Mobility National Contact Points of the EU MS and AC <b>(YES / NO)</b>	<b>YES</b>
<b>Date</b>	23.10.2008