



ROMÂNIA  
UNIVERSITATEA BABEŞ-BOLYAI CLUJ-NAPOCA

Str. Mihail Kogălniceanu, nr. 1, 400084 Cluj-Napoca  
Tel. (00) 40 - 264 - 40.53.00\*; 40.53.01; 40.53.02; 40.53.22  
Fax: 40 - 264 - 59.19.06  
E-mail: [staff@staff.ubbcluj.ro](mailto:staff@staff.ubbcluj.ro)

RECTORATUL

## Universitatea Babeş-Bolyai Competiția Excelenței 2010

### Dosar individual

**Notă: Toate datele se referă la perioada 2005-2009**

Nume, prenume, grad did.	CONF. DR. ING. MONICA IOANA TOSA
Facultatea, Catedra	Chimie si inginerie chimica, Catedra de biochimie si inginerie biochimica
Domeniul științific	Biotehnologii, Ingineria si securitatea alimentelor
Adresa paginii web personale	<a href="http://www.chem.ubbcluj.ro/catedre/biochimie-inginerie.html">http://www.chem.ubbcluj.ro/catedre/biochimie-inginerie.html</a>
Adresa e-mail	<a href="mailto:mtosa@chem.ubbcluj.ro">mtosa@chem.ubbcluj.ro</a>

### Criteriaul I – Output

**1. Articole științifice publicate în reviste indexate ISI (cu menționare factorului de impact în cazul celor cotate)**

Titlu	Autori	Revista	Factor impact
NIR surface enhanced Raman spectroscopy and bands assignment by DFT calculations of non-natural $\beta$ -amino acids	Iliescu, T., Maniu, D., Chiș, V., Irimie, F. D., Paizs, Cs., Toșa, M.	Chemical Physics <b>2005</b> , 310, 189-199.	1.961
Experimental and quantum chemical study on the vibrational spectroscopy of N-methylphenothiazines: Part 1	Endredi, Henrietta; Billes, Ferenc; Tosa, Monica; Majdik, Cornelia; Irimie, Florin Dan.	Spectrochimica Acta, Part A: Molecular and Biomolecular Spectroscopy <b>2006</b> , 63A(2), 349-360.	1.510
Inhibition of Histidine Ammonia-Lyase by Heteroaryl-alanines and Acrylates.	Katona, A., Toșa, M. I., Paizs, Cs., Rétey, J	Chemistry and Biodiversity <b>2006</b> , 3, 502-508.	1.659
Chemoenzymatic preparation of enantiopure L-benzofuranyl- and L-benzo[b]thiophenyl alanines	Podea, P., Toșa, M. I., Paizs, Cs., Irimie, F. D.	Tetrahedron: Asymmetry <b>2008</b> , 19, 500-511.	2.796
Lipase-catalyzed kinetic resolution of racemic 1-heteroarylethanol—experimental and QM/MM study	Toșa, M. I., Pilbák, S., Moldovan, P., Paizs, Cs., Szatzker, G., Szakács, Gy., Novák, L., Irimie, F. D., Poppe, L.	Tetrahedron: Asymmetry <b>2008</b> , 19, 1844-1852.	2.796
Chemoenzymatic synthesis of (R)- and (S)-1-heteroarylethanol.	Toșa, M. I., Podea, P., Paizs, Cs., Irimie, F. D	Tetrahedron: Asymmetry <b>2008</b> , 19, 2068-2071.	2.796
Baker's yeast-mediated synthesis of (R)- and (S)-heteroaryl-ethane-1,2-diols	Podea, P., Paizs, Cs., Toșa, M. I., Irimie, F.	Tetrahedron: Asymmetry <b>2008</b> , 19, 1959-1964.	2.796
Enzyme-catalyzed synthesis of (R)- and (S)-3-heteroaryl-3-hydroxypropanoic acids and their	Brem J., Paizs Cs., Toșa M. I., Vass E., Irimie F. D	Tetrahedron: Asymmetry <b>2009</b> , 20, 489-496.	2.796

derivatives.

Formyl- and acetylandols: Billes, F., Podea, P.V., Spectrochimica acta. Part 1.51  
vibrational spectroscopy of an Mohammed-Ziegler, I., A, Molecular and  
expectably pharmacologically active Toşa, M., Mikosch, H., biomolecular spectroscopy  
compound family. Irimie, D.F. **2009**, 74 (5), 1031-1045  
New ways for old structures Irimie, F.D., Paizs, C., *Studia Universitatis* 0  
Tosa, M., Podea, P. *Babes-Bolyai Chemia*  
**2009**, 4 (1), 7-16

## 6. Cărți științifice publicate în edituri naționale acreditate

1. Toşa Monica-Ioana, Paizs Csaba, Irimie Florin-Dan, *Bioprocese pentru obținerea medicamentelor și intermediarilor*. Editura Napoca Star, Cluj-Napoca 2007, ISBN 978-973-647-531-5, 215 pag
2. Irimie Florin Dan, Paizs Csaba, Toşa Monica *Biotransformări în sinteza organică. Aspecte Fundamentale*. Editura Napoca Star, Cluj-Napoca 2006, ISBN 978-973-647-467-5, 180 pag
3. Moldovan Paula, Toşa Monica Ioana, Leţ Daniela, Majdik Cornelia, Paizs Csaba, Irimie Florin Dan *Aplicații pentru laboratorul de biochimie* Editura Napoca Star, Cluj Napoca 2006, ISBN 978-973-647-464-4, 153 pag.

## Criteriaul II – Prestigiu profesional

### 1. Citări ale articolelor ISI listate la Criteriaul I

Enzyme-catalyzed synthesis of (R)- and (S)-3-heteroaryl-3-hydroxy-propanoic acids and their derivatives, *Tetrahedron Asymmetry* 2009, 20 (4), pp. 489-496

1. Synthesis of a core carbon framework of cyanosporasides A and B, Aburano, D., Inagaki, F., Tomonaga, S., Mukai, C., *Journal of Organic Chemistry* 2009, 74 (15), pp. 5590-5594

Chemoenzymatic synthesis of (R)- and (S)-1-heteroarylethanol, *Tetrahedron Asymmetry* 2008, 19 (17), pp. 2068-2071

1. Chiral spiroaminoborate ester as a highly enantioselective and efficient catalyst for the borane reduction of furyl, thiophene, chroman, and thiochroman-containing ketones, Stepanenko, V., De Jesús, M., Correa, W., Bermúdez, L., Vázquez, C., Guzmán, I., Ortiz-Marciales, M. *Tetrahedron Asymmetry* 2009, 20 (23), pp. 2659-2665
2. Stereoselective chemoenzymatic synthesis of enantiopure 1-(Heteroaryl)ethanamines by lipase-Catalysed kinetic resolutions, Alatorre-Santamaria, S., Gotor-Fernandez, V., Gotor, V. *European Journal of Organic Chemistry* 2009, (15), pp. 2533-2538

Baker's yeast-mediated synthesis of (R)- and (S)-heteroaryl-ethane-1,2-diols, *Tetrahedron Asymmetry* 2008, 19 (16), pp. 1959-1964

1. New ways for old structures, Irimie, F.D., Paizs, C., Tosa, M., Podea, P. *Studia Universitatis Babes-Bolyai Chemia* 2009, 4 (1), pp. 7-16
2. Enantioselective Rh-catalyzed transfer hydrogenation of  $\alpha$ -sulfonyloxy heteroaryl ketones; asymmetric synthesis of (S)-bufuralol, Kwak, S.H., Lee, D.-M., Lee, K.-I. *Tetrahedron Asymmetry* 2009, 20 (22), pp. 2639-2645

Lipase-catalyzed kinetic resolution of racemic 1-heteroarylethanol-experimental and QM/MM study, *Tetrahedron Asymmetry* 2008, 19 (15), pp. 1844-1852

1. Chiral spiroaminoborate ester as a highly enantioselective and efficient catalyst for the borane reduction of furyl, thiophene, chroman, and thiochroman-containing ketones, Stepanenko, V., De Jesús, M., Correa, W., Bermúdez, L., Vázquez, C., Guzmán, I., Ortiz-Marciales, M. *Tetrahedron Asymmetry* 2009, 20 (23), pp. 2659-2665
2. Enantioselective acylation of (RS)-phenylethylamine catalysed by lipases, Pilissão, C., Carvalho, P.d.O., Nascimento, M.d.G. *Process Biochemistry* 2009, 44 (12), pp. 1352-1357
3. New ways for old structures, Irimie, F.D., Paizs, C., Tosa, M., Podea, P. *Studia Universitatis Babes-Bolyai Chemia* 2009, 4 (1), pp. 7-16
4. Enantioselective acetylation of racemic alcohols by *Manihot esculenta* and *Passiflora edulis* preparations, Machado, L.L., de Gonzalo, G., Lemos, T.L.G., de Mattos, M.C., de Oliveira, M.d.C.F., Gotor-Fernández, V., Gotor, V. *Journal of Molecular Catalysis B: Enzymatic* 2009, 60 (3-4), pp. 157-162
5. Chemoenzymatic synthesis of (R)- and (S)-1-heteroarylethanol, Toşa, M.I., Podea, P.V., Paizs, C., Irimie, F.D. *Tetrahedron Asymmetry* 2008, 19 (17), pp. 2068-2071

Chemoenzymatic preparation of enantiopure 1-benzofuranyl- and 1-benzo[b]thiophenyl alanines *Tetrahedron Asymmetry* 2008, 19 (4), pp. 500-511

1. New ways for old structures, Irimie, F.D., Paizs, C., Tosa, M., Podea, P. *Studia Universitatis Babes-Bolyai Chemia* 2009, 4 (1), pp. 7-16

2. Biocatalytic routes to chiral amines and amino acids , Gotor-Fernández, V., Gotor, V. *Current Opinion in Drug Discovery and Development* 2009, 12 (6), pp. 784-797
3. A new and general route to 2-pyrrolylglycine, 2-pyrrolylalanine and homo-2-pyrrolylalanine derivatives, Sarkar, K., Singha, S.K., Chattopadhyay, S.K. *Tetrahedron Asymmetry* 2009, 20 (15), pp. 1719-1721
4. Highly diastereoselective approach to novel phenylindolizidinols via benzothieno analogues of tylophorine based on reductive desulfurization of benzo[b]thiophene, Šafář, P., Žůžiová, J., Marchalín, S., Tóthová, E., Prónayová, N., Švorc, L., Vrábek, V., Dařch, A. *Tetrahedron Asymmetry* 2009, 20 (5), pp. 626-634
5. Enzyme-catalyzed synthesis of (R)- and (S)-3-heteroaryl-3-hydroxy-propanoic acids and their derivatives, Brem, J., Paizs, C., Toşa, M.I., Vass, E., Irimie, F.D. *Tetrahedron Asymmetry* 2009, 20 (4), pp. 489-496

Inhibition of histidine ammonia lyase by heteroaryl-alanines and acrylates, *Chemistry and Biodiversity* 2006, 3 (5), pp. 502-508

1. Structure and chemistry of 4-methylideneimidazole-5-one containing enzymes , Cooke, H.A., Christianson, C.V., Bruner, S.D. *Current Opinion in Chemical Biology* 2009, 13 (4), pp. 453-461
2. Palladium-catalyzed sequential oxidative cyclization/coupling of 2-alkynylphenols and alkenes: A direct entry into 3-alkenylbenzofurans , Martínez, C., Álvarez, R., Aurrecoechea, J.M. *Organic Letters* 2009, 11 (5), pp. 1083-1086

Experimental and quantum chemical study on the vibrational spectroscopy of N-methylphenothiazines: Part 1 *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy* 2006, 63 (2), pp. 349-360

1. Azure A chloride: Computational and spectroscopic study , Snehathala, M., Hubert Joe, I., Ravikumar, C., Jayakumar, V.S. *Journal of Raman Spectroscopy* 2009, 40 (2), pp. 176-182

NIR surface enhanced Raman spectroscopy and bands assignment by DFT calculations of non-natural  $\beta$ -amino acids *Chemical Physics* 2005, 310 (1-3), pp. 189-199

1. Identification and characterisation of the E951 artificial food sweetener by vibrational spectroscopy and theoretical modelling , Peica, N. *Journal of Raman Spectroscopy* 2009, 40 (12), pp. 2144-2154
2. Dopamine molecules on Au@Ag shell bimetallic nanocolloids: Fourier transform infrared, raman, and surface-enhanced Raman spectroscopy study aided by density functional theory , Pande, S., Jana, S., Sinha, A.K., Sarkar, S., Basu, M., Pradhan, M., Pal, A., (...), Pal, T. *Journal of Physical Chemistry C* 2009, 113 (17), pp. 6989-7002
3. Mulberry non-engineered silk gland pKundu, J., Dewan, M., Ghoshal, S., Kundu, S.C. rotein vis-à-vis silk cocoon protein engineered by silkworms as biomaterial matrices , *Journal of Materials Science: Materials in Medicine* 2008, 19 (7), pp. 2679-2689
4. Raman and surface enhanced Raman spectroscopy on molecules of pharmaceutical and biological interest , Iliescu, T., Baia, M., Maniu, D. *Romanian Reports on Physics* 2008, 60 (3), pp. 829-855
5. Surface-enhanced Raman scattering and DFT computational studies of a benzotriazole derivative , Li, M.-Y., Liao, Q., Zhang, M., Ai, X.-C., Li, F.-Y. *Journal of Molecular Structure* 2008, 888 (1-3), pp. 2-6
6. N-acetylalanine monolayers at the silver surface investigated by surface enhanced Raman scattering spectroscopy and X-ray photoelectron spectroscopy: Effect of metallic ions , Yang, H., Zhu, X., Song, W., Sun, Y., Duan, G., Zhao, X., Zhang, Z. *Journal of Physical Chemistry C* 2008, 112 (38), pp. 15022-15027
7. Concentration-dependent orientational changes of 2-amino-2-thiazoline molecule adsorbed on silver nanocolloidal surface investigated by SERS and DFT , Chowdhury, J., Sarkar, J., Tanaka, T., Talapatra, G.B. *Journal of Physical Chemistry C* 2008, 112 (1), pp. 227-239
8. Surface-enhanced Raman scattering and DFT computational studies of a cyanuric chloride derivative, Liao, Q., Li, M.-Y., Hao, R., Ai, X.-C., Zhang, J.-P., Wang, Y. *Vibrational Spectroscopy* 2007, 44 (2), pp. 351-356
9. Adsorption of 2-amino-6-methylbenzothiazole on colloidal silver particles: Quantum chemical calculations and surface enhanced Raman scattering study, Chowdhury, J., Sarkar, J., De, R., Ghosh, M., Talapatra, G.B. *Chemical Physics* 2006, 330 (1-2), pp. 172-183
10. Electromagnetic mechanism of SERS, Schatz, G.C., Young, M.A., Van Duyne, R.P. *Topics in Applied Physics* 2006, 103, pp. 19-46
11. Ab initio, DFT vibrational calculations and SERRS study of Rhodamine 123 adsorbed on colloidal silver particles , Sarkar, J., Chowdhury, J., Pal, P., Talapatra, G.B. *Vibrational Spectroscopy* 2006, 41 (1), pp. 90-96
12. Experimental and theoretical surface enhanced raman scattering study of 2-amino-4-methylbenzothiazole adsorbed on colloidal silver particles , Sarkar, J., Chowdhury, J., Ghosh, M., De, R., Talapatra, G.B. *Journal of Physical Chemistry B* 2005, 109 (47), pp. 22536-22544

### 3. Citări în perioada 2005-2009 ale articolelor anterioare anului 2005

Biocatalytic enantioselective preparation of phenothiazine-based cyanohydrin acetates: Kinetic and dynamic kinetic resolution *Tetrahedron* 2004, 60 (46 SPEC. ISS.), pp. 10533-10540

1. Dynamic enzymatic kinetic resolution of methyl 2,3-dihydro-1h-indene-1- carboxylate , Pietruszka, J., Simon, R.C., Kruska, F., Braun, M. *European Journal of Organic Chemistry* 2009, (35), pp. 6217-6224
2. New ways for old structures, Irimie, F.D., Paizs, C., Tosa, M., Podea, P. *Studia Universitatis Babes-Bolyai Chemia* 2009, 4 (1), pp. 7-16
3. Chemoenzymatic method to enantiopure Sulphur heterocyclic  $\beta$ -hydroxy nitriles, Turcu, M.C., Perkiö, P., Kanerva, L.T. *Arkivoc* 2009 (3), pp. 251-263
4. Enantioselective enzyme-catalysed synthesis of cyanohydrins, Holt, J., Hanefeld, U. *Current Organic Synthesis* 2009, 6 (1), pp. 15-37
5. Chemoenzymatic and microbial dynamic kinetic resolutions, Kamaruddin, A.H., Uzir, M.H., Aboul-Enein, H.Y., Halim, H.N.A. *Chirality* 2009, 21 (4), pp. 449-467
6. Lipase-catalyzed dynamic kinetic resolution giving optically active cyanohydrins: use of silica-supported ammonium hydroxide and porous ceramic-immobilized lipase, Sakai, T., Wang, K., Ema, T. *Tetrahedron* 2008, 64 (9), pp. 2178-2183
7. Recent developments in dynamic kinetic resolution, Pellissier, H. *Tetrahedron* 2008, 64 (8), pp. 1563-1601
8. Enantiomers of amino ethanols and their precursors by lipase catalysis in non-aqueous solvents, Lundell, K., Kanerva, L.T. *Chimica Oggi* 2007, 25 (5 SUPPL. 2), pp. 26-30
9. Emulation of racemase activity by employing a pair of stereocomplementary biocatalysts , Gruber, C.C., Nestl, B.M., Gross, J., Hildebrandt, P., Bornscheuer, U.T., Faber, K., Kroutil, W. *Chemistry - A European Journal* 2007, 13 (29), pp. 8271-8276
10. An asymmetric, chemo-enzymatic synthesis of O-acetylcyanohydrins , Belokon, Y.N., Blacker, A.J., Clutterbuck, L.A., Hogg, D., North, M., Reeve, C. *European Journal of Organic Chemistry* 2006, (20), pp. 4609-4617
11. Catalytic hydrogenation of cyanohydrin esters as a novel approach to N-acylated  $\beta$ -amino alcohols - Reaction optimisation by a design of experiment approach, Veum, L., Pereira, S.R.M., Van Der Waal, J.C., Hanefeld, U. *European Journal of Organic Chemistry* 2006, (7), pp. 1664-1671
12. Carrier enabled catalytic reaction cascades, Veum, L., Hanefeld, U. *Chemical Communications* 2006, (8), pp. 825-831
13. Biotechnological applications of *Candida antarctica* lipase A: State-of-the-art , Domínguez De María, P., Carboni-Oerlemans, C., Tuin, B., Bargeman, G. , Van Der Meer, A., Van Gemert, R. *Journal of Molecular Catalysis B: Enzymatic* 2005, 37 (1-6), pp. 36-46
14. Enantioselective synthesis of aliphatic cyanohydrin acetates , Veum, L., Hanefeld, U. *Synlett* 2005, (15), pp. 2382-2384
15. Enantioselective C-C bond synthesis catalysed by enzymes , Sukumaran, J., Hanefeld, U. *Chemical Society Reviews* 2005, 34 (6), pp. 530-542
16. Optimisation of the enantioselective synthesis of cyanohydrin esters , Veum, L., Kanerva, L.T., Halling, P.J., Maschmeyer, T., Hanefeld, U. *Advanced Synthesis and Catalysis* 2005, 347 (7-8), pp. 1015-1021
17. Chemoenzymatic preparation of the enantiomers of  $\beta$ -tryptophan ethyl ester and the  $\beta$ -amino nitrile analogue , Li, X.-G., Kanerva, L.T. *Tetrahedron Asymmetry* 2005, 16 (9), pp. 1709-1714

Kinetic resolution of 1-(benzofuran-2-yl)ethanols by lipase-catalyzed enantiomer selective reactions *Tetrahedron Asymmetry* 2003, 14 (13), pp. 1943-1949

1. Chiral spiroaminoborate ester as a highly enantioselective and efficient catalyst for the borane reduction of furyl, thiophene, chroman, and thiochroman-containing ketones , Stepanenko, V., De Jesús, M., Correa, W., Bermúdez, L., Vázquez, C., Guzmán, I., Ortiz-Marciales, M. *Tetrahedron Asymmetry* 2009, 20 (23), pp. 2659-2665
2. New ways for old structures Irimie, F.D., Paizs, C., Tosa, M., Podea, P. *Studia Universitatis Babes-Bolyai Chemia* 2009, 4 (1), pp. 7-16
3. Combined sol-gel entrapment and adsorption method to obtain solid-phase lipase biocatalyst, Zarcu, C., Claudia, K., Corici, L., Croitoru, R., Csunderlik, C., Peter, F. *Revista de Chimie* 2009, 60 (9), pp. 922-927
4. Stereoselective chemoenzymatic synthesis of enantiopure 1-(Heteroaryl)ethanamines by lipase-Catalysed kinetic resolutions , Alatorre-Santamaria, S., Gotor-Fernandez, V., Gotor, V. *European Journal of Organic Chemistry* 2009, (15), pp. 2533-2538
5. Lipase-catalyzed kinetic resolution of racemic 1-heteroarylethanols-experimental and QM/MM study , Tosa, M., Pilbák, S., Moldovan, P., Paizs, C., Szatzker, G., Szakács, G., Novák, L., (...), Poppe, L. *Tetrahedron Asymmetry* 2008, 19 (15), pp. 1844-1852
6. Effect of chain length on enzymatic hydrolysis of p-nitrophenyl esters in supercritical carbon dioxide , Varma, M.N., Madras, G. *Applied Biochemistry and Biotechnology* 2007, 144 (3), pp. 213-223
7. Biocatalysis in supercritical fluids, in fluorinated solvents, and under solvent-free conditions, Hobbs, H.R., Thomas, N.R. *Chemical Reviews* 2007, 107 (6), pp. 2786-2820
8. Trends in lipase-catalyzed asymmetric access to enantiomerically pure/enriched compounds, Ghanem, A. *Tetrahedron* 2007, 63 (8), pp. 1721-1754

9. Lipase-catalyzed deacylation by alcoholysis: A selective, useful transesterification reaction, Santaniello, E., Casati, S., Ciuffreda, P. *Current Organic Chemistry* 2006, 10 (10), pp. 1095-1123
10. Asymmetric synthesis using hydrolytic enzymes in supercritical carbon dioxide, Matsuda, T., Harada, T., Nakamura, K., Ikariya, T. *Tetrahedron Asymmetry* 2005, 16 (5), pp. 909-91
11. Biocatalysis in supercritical CO<sub>2</sub>, Matsuda, T., Harada, T., Nakamura, K. *Current Organic Chemistry* 2005, 9 (3), pp. 299-315
12. Application of lipases in kinetic resolution of racemates, Ghanem, A., Aboul-Enein, H.Y. *Chirality* 2005, 17 (1), pp. 1-15
13. Lipase-mediated chiral resolution of racemates in organic solvents, Ghanem, A., Aboul-Enein, H.Y. *Tetrahedron Asymmetry* 2004, 15 (21), pp. 3331-3351
14. Investigation of biocatalysts and biocatalytic processes and their synthetic applications, Bóday, V. *Periodica Polytechnica: Chemical Engineering* 2003, 47 (1), pp. 55-56

Optically active 1-(benzofuran-2-yl)ethanols and ethane-1,2-diols by enantiotopic selective bioreductions *Tetrahedron Asymmetry* 2003, 14 (11), pp. 1495-1501

1. The effect of electromagnetic fields on baker's yeast population dynamics, biocatalytic activity and selectivity, Sandu, D., Lingvay, I., Lányi, S., Micu, D.D., Popescu, C.L., Brem, J., Bencze, L.C., Paizs, C. *Studia Universitatis Babes-Bolyai Chemia* 2009, 4 (2), pp. 195-201
2. New ways for old structures Irimie, F.D., Paizs, C., Tosa, M., Podea, P. *Studia Universitatis Babes-Bolyai Chemia* 2009, 4 (1), pp. 7-16
3. Enantioselective Rh-catalyzed transfer hydrogenation of  $\alpha$ -sulfonyloxy heteroaryl ketones; asymmetric synthesis of (S)-bufuralol, Kwak, S.H., Lee, D.-M., Lee, K.-I. *Tetrahedron Asymmetry* 2009, 20 (22), pp. 2639-2645
4. Chemoenzymatic synthesis of (R)- and (S)-1-heteroarylethanol, Toşa, M.I., Podea, P.V., Paizs, C., Irimie, F.D. *Tetrahedron Asymmetry* 2008, 19 (17), pp. 2068-2071
5. Baker's yeast-mediated synthesis of (R)- and (S)-heteroaryl-ethane-1,2-diols, Podea, P.V., Paizs, C., Toşa, M.I., Irimie, F.D. *Tetrahedron Asymmetry* 2008, 19 (16), pp. 1959-1964
6. Lipase-catalyzed kinetic resolution of racemic 1-heteroarylethanol-experimental and QM/MM study, Toşa, M., Pilbák, S., Moldovan, P., Paizs, C., Szatzker, G., Szakács, G., Novák, L., (...), Poppe, L. *Tetrahedron Asymmetry* 2008, 19 (15), pp. 1844-1852
7. RhIII- and IrIII-catalyzed asymmetric transfer hydrogenation of ketones in water, Wu, X., Li, X., Zanotti-Gerosa, A., Pettman, A., Liu, J., Mills, A.J., Xiao, J. *Chemistry - A European Journal* 2008, 14 (7), pp. 2209-2222
8. Biocatalytic reduction of carbonyl groups, Nakamura, K., Matsuda, T. *Current Organic Chemistry* 2006, 10 (11), pp. 1217-1246
9. Microwave-assisted preparation of fused bicyclic heteroaryl boronates: Application in one-pot Suzuki couplings, DiMauro, E.F., Vitullo, J.R. *Journal of Organic Chemistry* 2006, 71 (10), pp. 3959-3962
10. Synthesis and conversion of 3-(2-hydroxythiobenzamido)benzo[b]furans, Briel, D. *Heterocycles* 2005, 65 (6), pp. 1295-1309
11. Synthesis of 2-, 4- and 5-(2-alkylcarbonyl-1-methylvinyl)-7-alkoxybenzo[b]furans and their leukotriene B<sub>4</sub> receptor antagonistic activity, Ando, K. *Yakugaku Zasshi* 2005, 125 (11), pp. 863-874
12. Synthesis of 2-, 4- and 5-(2-alkylcarbonyl-1-methylvinyl)-7-alkoxybenzo[b]furans and their leukotriene B<sub>4</sub> receptor antagonistic activity, Ando, K., Tsuji, E., Ando, Y., Kunitomo, J.-I., Kobayashi, R., Yokomizo, T., Shimizu, T., (...), Ohishi, Y. *Organic and Biomolecular Chemistry* 2005, 3 (11), pp. 2129-2139

*Candida antarctica* lipase A in the dynamic resolution of novel furylbenzotiazol-based cyanohydrin acetates *Tetrahedron Asymmetry* 2003, 14 (5), pp. 619-627

1. New ways for old structures Irimie, F.D., Paizs, C., Tosa, M., Podea, P. *Studia Universitatis Babes-Bolyai Chemia* 2009, 4 (1), pp. 7-16
2. Chemoenzymatic method to enantiopure Sulphur heterocyclic  $\beta$ -hydroxy nitriles, Turcu, M.C., Perkiö, P., Kanerva, L.T. *Arkivoc* 2009 (3), pp. 251-263
3. Chemoenzymatic synthesis of optically active 1,2-disubstituted ferrocenes with planar chirality, Merabet-Khellasi, M., Aribi-Zouieche, L., Riant, O. *Tetrahedron Asymmetry* 2009, 20 (12), pp. 1371-1377
4. Enantioselective enzyme-catalysed synthesis of cyanohydrins, Holt, J., Hanefeld, U. *Current Organic Synthesis* 2009, 6 (1), pp. 15-37
5. Donor- $\pi$ -acceptor benzothiazole-derived dyes with an extended heteroaryl-containing conjugated system: synthesis, DFT study and antimicrobial activity, Zajac, M., Hrobárik, P., Magdolen, P., Foltínová, P., Zahradník, P. *Tetrahedron* 2008, 64 (46), pp. 10605-10618
6. Recent developments in dynamic kinetic resolution, Pellissier, H. *Tetrahedron* 2008, 64 (8), pp. 1563-1601
7. Enantiomers of amino ethanols and their precursors by lipase catalysis in non-aqueous solvents, Lundell, K., Kanerva, L.T. *Chimica Oggi* 2007, 25 (5 SUPPL. 2), pp. 26-30
8. An asymmetric, chemo-enzymatic synthesis of O-acetylcyanohydrins, Belokon, Y.N., Blacker, A.J., Clutterbuck, L.A., Hogg, D., North, M., Reeve, C. *European Journal of Organic Chemistry* 2006, (20), pp. 4609-4617

9. A chemoenzymatic scalable route to optically active (R)-1-(pyridin-3-yl)-2-aminoethanol, valuable moiety of  $\beta$ 3-adrenergic receptor agonists, Perrone, M.G., Santandrea, E., Giorgio, E., Bleve, L., Scilimati, A., Tortorella, P. *Bioorganic and Medicinal Chemistry* 2006, 14 (4), pp. 1207-1214
10. Biotechnological applications of *Candida antarctica* lipase A: State-of-the-art, Domínguez De María, P., Carboni-Oerlemans, C., Tuin, B., Bargeman, G., Van Der Meer, A., Van Gemert, R. *Journal of Molecular Catalysis B: Enzymatic* 37 (1-6), pp. 36-46
11. Enantioselective synthesis of aliphatic cyanohydrin acetates, Veum, L., Hanefeld, U. *Synlett* 2005, (15), pp. 2382-2384
12. Optimisation of the enantioselective synthesis of cyanohydrin esters, Veum, L., Kanerva, L.T., Halling, P.J., Maschmeyer, T., Hanefeld, U. *Advanced Synthesis and Catalysis* 2008, 347 (7-8), pp. 1015-1021
13. Chemoenzymatic preparation of the enantiomers of  $\beta$ -tryptophan ethyl ester and the  $\beta$ -amino nitrile analogue, Li, X.-G., Kanerva, L.T. *Tetrahedron Asymmetry* 2005, 16 (9), pp. 1709-1714

Chemo-enzymatic preparation of hydroxymethyl ketones *Journal of the Chemical Society. Perkin Transactions 1* 2002, (21), pp. 2400-2402

1. Microwave-assisted one-carbon chain extension in the preparation of terminal -hydroxy ketones, Vaismaa, M.J.P., Leskinen, M.V., Lajunen, M.K. *Synthetic Communications* 2009, 39 (11), pp. 2042-2052
2. Convenient synthesis and evaluation of biological activity of benzyl (2S)-2-[(R)-1-hydroxy-2-oxo-(1-phenethyl)prop-3-ylcarbamoyl]-4-oxopiperidine- (or -4-oxopyrrolidine)-1-carboxylate as novel histone deacetylase inhibitor, Oh, S., Moon, H.-I., Jung, J.-C. *Zeitschrift für Naturforschung - Section B Journal of Chemical Sciences* 2008, 63 (11), pp. 1300-1304
3. Baker's yeast-mediated synthesis of (R)- and (S)-heteroaryl-ethane-1,2-diols, Podea, P.V., Paizs, C., Toşa, M.I., Irimie, F.D. *Tetrahedron Asymmetry* 2009, 19 (16), pp. 1959-1964
4. A simple synthesis of 4-substituted 2-(3-hydroxy-2-oxo-1-phenethyl-propylcarbamoyl)pyrrolidine-1-carboxylic acid benzyl esters as novel cysteine protease inhibitors, *Zeitschrift für Naturforschung - Section B Journal of Chemical Sciences* 2008, 63 (2), pp. 210-216
5. Application of bioreduction by microorganisms in the enantioselective synthesis of alpha-substituted-1-phenylethanol, Andrade, L.H., Polak, R., Porto, A.L.M., Schoenlein-Crusius, I.H., Comasseto, J.V. *Letters in Organic Chemistry* 2006, 3 (8), pp. 613-618

Baker's yeast mediated preparation of (10-alkyl-10H-phenothiazin-3-yl)methanols *Journal of Molecular Catalysis - B Enzymatic* 2002, 17 (6), pp. 241-248

1. Experimental and quantum chemical study on the vibrational spectroscopy of N-methylphenothiazines: Part 1, Endrédi, H., Billes, F., Toşa, M., Majdik, C., Irimie, F.D. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy* 2006, 63 (2), pp. 349-360
2. Synthesis and photophysical properties of phenothiazine-labeled conjugated dendrimers, Zhang, X.-H., Choi, S.-H., Dong, H.C., Ahn, K.-H. *Tetrahedron Letters* 2005, 46 (32), pp. 5273-5276

Separation of N-alkyl phenothiazine sulfones by HPTLC using an optimum mobile phase *Journal of Pharmaceutical and Biomedical Analysis* 2002, 28 (2), pp. 385-389

1. The behavior of some phenothiazines and their demethylated derivatives in reversed-phase liquid chromatography, Le, D.C., Beljean, M., Siouffi, A.-M. *Journal of Chromatographic Science* 2006, 44 (1), pp. 49-54

Synthesis of optically active 3-substituted-10-alkyl-10H-phenothiazine-5-oxides by enantioselective biotransformations *Tetrahedron Asymmetry* 2002, 13 (2), pp. 211-221

1. Synthesis and structure of new 3,7,10-substituted-phenothiazine derivatives, Turdean, R., Bogdan, E., Terec, A., Petran, A., Vlase, L., Turcu, I., Grosu, I. *Central European Journal of Chemistry* 2009, 7 (1), pp. 111-117
2. (E)-3-(2-Alkyl-10H-phenothiazin-3-yl)-1-arylprop-2-en-1-ones: Preparative, IR, NMR and DFT study on their substituent-dependent reactivity in hydrazinolysis and sonication-assisted oxidation with copper(II)nitrate, Găină, L., Csámpai, A., Túrós, G., Lovász, T., Zsoldos-Mády, V., Silberg, I.A., Sohár, P. *Organic and Biomolecular Chemistry* 2006, 4 (23), pp. 4375-4386
3. Lipase-catalyzed deacylation by alcoholysis: A selective, useful transesterification reaction, Santaniello, E., Casati, S., Ciuffreda, P. *Current Organic Chemistry* 2006, 10 (10), pp. 1095-1123
4. Experimental and quantum chemical study on the vibrational spectroscopy of N-methylphenothiazines: Part 1, Endrédi, H., Billes, F., Toşa, M., Majdik, C., Irimie, F.D. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy* 2006, 63 (2), pp. 349-360

Selective oxidation methods for preparation of N-alkylphenothiazine sulfoxides and sulfones *Heterocyclic Communications* 2001, 7 (3), pp. 277-282

1. Microwave-assisted synthesis of Phenothiazine sulfoxide derivatives, Găină, L., Surducian, M., Cristea, C., Silaghi-Dumitrescu, L. *Studia Universitatis Babeş-Bolyai Chemia* 2002, 2, pp. 65-71

2. (E)-3-(2-Alkyl-10H-phenothiazin-3-yl)-1-arylprop-2-en-1-ones: Preparative, IR, NMR and DFT study on their substituent-dependent reactivity in hydrazinolysis and sonication-assisted oxidation with copper(II)nitrate, Găină, L., Csámpai, A., Túrós, G., Lovász, T., Zsoldos-Mády, V., Silberg, I.A., Sohár, P. *Organic and Biomolecular Chemistry* 2006, 4 (23), pp. 4375-4386

Bakers' yeast-mediated reductions of some nitro-dibenzofurans *Heterocyclic Communications* 1997, 3 (6), pp. 549-553

1. New ways for old structures Irimie, F.D., Paizs, C., Tosa, M., Podea, P. *Studia Universitatis Babeş-Bolyai Chemia* 2009, 4 (1), pp. 7-16

#### 10. Participări la programe/granturi finanțate din sursă națională (se menționează și valoarea)

Nr.	Titlu	Funcție
1	<i>Sinteza enzimatică a unor amino- și hidroxiacizi heterociclici nenaturali.</i>	membru 2006-2008
	<i>Metoda noua de separare a compusilor enantiopuri utilizand anticorpi selectivi (2004-2006), Contract CERES 532/2004</i>	membru 2003-2005
	<i>Metodologie biocatalitica de obtinere selectiva a unor sintoni chirali pentru sinteza de compusi cu activitate biologica (2003-2005), Contract Ceres 189/2003</i>	membru 2003-2005
	<i>Metodologie biocatalitica de obtinere selectiva a unor sintoni chirali pentru sinteza de compusi cu activitate biologica (2003-2005), Contract Ceres 189/2003</i>	membru 2003-2005
	<i>Model experimental bioreactor-extractor pentru obtinerea enzimatica a unor compusi anti-sida (2003-2005), Contract Ceres 1990/2003</i>	membru 2003-2005
	<i>Model experimental bioreactor-extractor pentru obtinerea enzimatica a unor compusi anti-sida (2003-2005), Contract Ceres 1990/2003</i>	membru 2003-2005
	<i>Investigarea mecanismului de actiune al histidin- si fenilalanin-amoniac liazelor, CNCSIS Idei II</i>	membru 2009-2011
	<i>Tehnologie de transesterificare enzimatica destinata obtinerii de biocarburanti de generatia a 2-a PNCD II</i>	membru 2008-2010
	<i>Tehnologie de transesterificare enzimatica destinata obtinerii de biocarburanti de generatia a 2-a PNCD II</i>	membru 2008-2010
	<i>Substitute de sange pe baza de metaloproteine: strategii pentru combaterea stresului oxidativ si a celui nitroziv Idei</i>	Membru, 2007-2010

#### 15. Conferințe invitate internaționale

1. Moldovan, P., Paizs, Cs., Tosa M., Majdik, C., Daniela Let, D., Florin Dan Irimie, F. D. (2006): *Dynamic enzymatic resolution of some non-proteinogenic amino acids*, 1<sup>st</sup> European Chemistry Congress, 27-31 August, Budapest, Hungary 546.

2. Moldovan, P., Paizs, Cs., Tosa M., Majdik, C., Daniela Let, D., Florin Dan Irimie, F. D. (2006): *Optically active 1-(indole-3'-yl)ethane-1,2-diols by enantiotopic selective bioreductions*, 33<sup>rd</sup> International Conference of Slovak Society of Chemical Engineering, Tatranske Matliare, Slovakia, 22-26 May, 2006, 228.

3. Majdik, C., Toşa, M., Moldovan, P., Pénczes, A., Let, D., Paizs, Cs., Irimie, F. D. (2006): *Application of immobilization techniques for heavy metals biosorption with Saccharomyces cerevisiae cells*, 33<sup>rd</sup> International Conference of Slovak Society of Chemical Engineering, Tatranske Matliare, Slovakia, 22-26 May, 2006, 230.

4. Moldovan, P., Paizs, Cs., Tosa M., Majdik, C., Daniela Let, D., Florin Dan Irimie, F. D. (2006): *Dynamic enzymatic resolution of some non-proteinogenic amino acids*, 33<sup>rd</sup> International Conference of Slovak Society of Chemical Engineering, Tatranske Matliare, Slovakia, 22-26 May, 2006, 229.

5. Irimie, F.D., Paizs, Cs., Tosa, M.I., Majdik, C. (2006): *Selectivity of biocatalysts. Applications in organic synthesis*. 33<sup>rd</sup> International Conference of Slovak Society of Chemical Engineering, Tatranske Matliare, Slovakia, 22- 26 May, 2006, 231.

### III. Realizare remarcabilă

(Descrieți într-o manieră cât mai accesibilă (în maximum 1 pagină) cea mai importantă realizare științifică/tehnică/artistică din ultimii 5 ani și impactul acesteia.)

Industria medicamentelor este un domeniu fierbinte al activității umane, prin faptul că oferă mijloace de menținere a stării de sănătate prin prevenirea sau vindecarea unor boli, respectiv prin atenuarea simptomelor anumitor maladii. Utilizarea biocatalizei în industria farmaceutică este deja un fapt obișnuit, explicabil prin avantajele pe care aceasta le oferă variantelor clasice chimice.

Obiectivul major al activității de cercetare desfășurate de mine în ultimii 5 ani l-a reprezentat utilizarea metodelor biocatalitice în obținerea medicamentelor chirale în stare înaltă de puritate optică (a eutomerilor) sau a unor intermediari chirali necesari sintezei acestora.

Disponibilitatea comercială a unui număr mare de enzime a permis efectuarea unor biotransformări înalt selective atât prin utilizarea catalizei celulare, cât și a enzimelor liofilizate sau imobilizate în clasa unor derivați heterociclici cu structura fenotiazinică (alcooli, esteri, hidroxiacizi, derivați S-oxidici).

Dotarea laboratoarelor catedrei cu aparatură performantă de analiză a purității (UV-VIS, cromatografie), inclusiv a purității optice (polarimetrie, HPLC și GC chiral), a permis efectuarea unor studii complexe de optimizare a proceselor studiate (la scară analitică) și elaborarea unor metodologii sintetice la nivel preparativ.

Impactul științific al rezultatelor obținute este reflectat de publicarea lor în reviste științifice cotate ISI.

Data:

18 martie 2010

**Certific validitatea datelor prezentate**

Sef de catedră,

Semnătura: