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RECTORATUL

Universitatea Babeş-Bolyai Competiția Excelenței 2010

Dosar individual

Notă: Toate datele se referă la perioada 2005-2009

| | |
|-------------------------------------|---|
| Nume, prenume, grad did. | PROF. DR. ING. FLORIN DAN IRIMIE |
| Facultatea, Catedra | Chimie și inginerie chimică, Catedra de biochimie și inginerie biochimică |
| Domeniul științific | Inginerie chimică |
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Criteria 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 β -amino acids | Iliescu, T., Maniu, D., Chiș, V., Irimie, F. D., Paizs, Cs., Toșa, M. | Chemical Physics 2005 , 310, 189-199. | 1.961 |
| Role of chemical structure in molecular recognition by transferrin | Takatsy, Aniko; Hodrea, Judit; Majdik, Cornelia; Irimie, Florin Dan; Kilar, Ferenc. | Journal of Molecular Recognition 2006 , 19(4), 270-274. | 3.16 |
| 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 2006 , 63A(2), 349-360. | 1.510 |
| Chemoenzymatic preparation of enantiopure L-benzofuranyl- and L-benzo[b]thiophenyl alanines | Podea, P., Toșa, M. I., Paizs, Cs., Irimie, F. D. | Tetrahedron: Asymmetry 2008 , 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 2008 , 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 2008 , 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 2008 , 19, 1959-1964. | 2.796 |
| Enzyme-catalyzed synthesis of (R)- and (S)-3-heteroaryl-3-hydroxypropanoic acids and their derivatives. | Brem J., Paizs Cs., Toșa M. I., Vass E., Irimie F. D. | Tetrahedron: Asymmetry 2009 , 20, 489-496. | 2.796 |

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| Formyl- and acetyldols: vibrational spectroscopy of an expectably pharmacologically active compound family. New ways for old structures | Billes, F., Podea, P.V., Mohammed-Ziegler, I., Toşa, M., Mikosch, H., Irimie, D.F. Irimie, F.D., Paizs, C., Tosa, M., Podea, P. | Spectrochimica acta. Part A, Molecular and biomolecular spectroscopy 2009 , 74 (5), 1031-1045 <i>Studia Universitatis Babeş-Bolyai Chemia</i> 2009 , 4 (1), 7-16 | 1.51 0 |
| Improvement of sunflower oil extraction by modelling and simulation | Brăţfălean, D., Cristea, V.M., Agachi, P.Ş., Irimie, D.F. | Revue Roumaine de Chimie 2008 , 53 (9), pp. 881-888 | 0.284 |
| ,Evaluation of tumor angiogenesis through VEGF modulation in ovarian cancer in vivo using RNA interference. | Tudoran, O., I.B. Neagoie, O. Balacescu, E. Dronca, C. Burz, L. Balacescu, I. Nedelea, A. Irimie, O. Popescu, F.D. Irimie and V. Cristea | Rom. Biotechnol. Lett., 2009. 14(4): p. 4560-4566. | 0 |

6. Cărţi ştiinţifice publicate în edituri naţionale acreditate

- Toşa Monica-Ioana, Paizs Csaba, Irimie Florin-Dan, *Bioprocese pentru obţinerea medicamentelor şi intermediarilor*. Editura Napoca Star, Cluj-Napoca 2007, ISBN 978-973-647-531-5, 215 pag
- 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
- Moldovan Paula, Toşa Monica Ioana, Leţ Daniela, Majdik Cornelia, Paizs Csaba, Irimie Florin Dan *Aplicaţii pentru laboratorul de biochimie* Editura Napoca Star, Cluj Napoca 2006, ISBN 978-973-647-464-4, 153 pag.
- Florin Dan Irimie, *Elemente de biochimie*, Ed. Erdelyi Hirado, ISBN 973-98374-92, Cluj-Napoca, 1998, 373 pag
- Gavril Neamtu, Florin Irimie, *Fitoregulatori de creştere*, Ed. Ceres ISBN-10: 973-40-0182-5, Bucuresti, ,1991 420 pg.

9. Brevete naţionale

| r. | Titlu | Autori | Revista |
|----|--|--|--|
| | <i>Sunburn alleviating lotion</i> | Timbus, Ioan Victor; Turdean, Ioana Virginia; Schenker, Mariana Nicoleta; Irimie, Florin Dan | CODEN: RUXXA3 RO 121364 B1 20070430; RO 2002-200201195 20020910/2007 |
| | <i>Sun protective emulsion with SPF 15</i> | Timbus, Ioan Victor; Turdean, Ioana Virginia; Schenker, Mariana Nicoleta; Irimie, Florin Dan | CODEN: RUXXA3 RO 121367 B1 20070430 RO 2002-200201196 20020910/2007 |
| | <i>Remineralizing tonic lotion</i> | Timbus, Ioan Victor; Botar, Alexandru; Turdean, Liviu; Schenker, Mariana; Irimie, Florin Dan | CODEN: RUXXA3 RO 121081 B1 20061229 RO 2000-200001160 20001127/2006 |
| | <i>Day moisturizing cream</i> | Timbus, Ioan Victor; Botar, Alexandru; Turdean, Liviu; Schenker, Mariana; Irimie, Florian Dan. | CODEN: RUXXA3 RO 120885 B1 20060929 Patent written in Romanian. Application: RO 2000-200001159 20001127/2006 |

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

- 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

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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

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2. Enantioselective Rh-catalyzed transfer hydrogenation of α -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
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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
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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

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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
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4. Highly diastereoselective approach to novel phenylindolizidinols via benzothieno analogues of tylophorine based on reductive desulfurization of benzo[b]thiophene, Šafář, P., Žúžiová, J., Marchalín, S., Tóthová, E., Prónayová, N., Švorc, L., Vrabel, 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

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

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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
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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
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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
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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

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2. 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
3. Chemoenzymatic method to enantiopure Sulphur heterocyclic β -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
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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
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15. Enantioselective C-C bond synthesis catalysed by enzymes, Sukumaran, J., Hanefeld, U. *Chemical Society Reviews* 2005, 34 (6), pp. 530-542
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1. Electromagnetic mechanism of SERS, Schatz, G.C., Young, M.A., Van Duyne, R.P. *Topics in Applied Physics* 2006, 103, pp. 19-46

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5. Synthesis, biological evaluation and molecular modeling of arylfurans as potential trypanothione reductase inhibitors | [Síntese, avaliação biológica e modelagem molecular de arilfuranos como inibidores da enzima, tripanotiona redutase] De Oliveira, R.B., Zani, C.L., Ferreira, R.S., Leite, R.S., Alves, T.M.A., Da Silva, T.H.A., Romanha, A.J. *Química Nova* 2008, 31 (2), pp. 261-267
6. Recent developments in dynamic kinetic resolution, Pellissier, H. *Tetrahedron* 2008, 64 (8), pp. 1563-1601
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4. Distincții, premii și alte recunoașteri naționale și internaționale

5. Studenți naționali atrași (activități de coordonare științifică și didactică)

Doctoranzi înmatriculați:

1. Bencze Laszlo Csaba
2. Brem Jurgen
3. Isprava Laura
4. Mot Augustin
5. Chis Laura
6. Marcovici Adriana
7. Muncean Anca
8. Trif Maria
9. Vulcu Adriana Elena
10. Tudoran Oana Mihaela

Doctoranzi cu teza finalizată

1. Podea Paula Veronica (2008)

7. Membru în comitetul de redacție la reviste ISI

Studia Universitatis Babes-Bolyai, Chemia
Croatia Chimica Acta

8. Membru în comitetul de redacție la reviste BDI

Progress in Catalysis

9. Participări la programe/granturi de cercetare finanțate din sursă internațională (se menționează și valoarea)

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

| Nr. | Titlu | Funcție |
|-----|--|----------------------------------|
| 1 | <i>Metoda noua de separare a compusilor enantiopuri utilizand anticorpi selectivi (2004-2006), Contract CERES 532/2004</i> | Responsabil UBB Irimie 2003-2005 |
| 2 | <i>Metodologie biocatalitica de obtinere selectiva a unor sintoni chirali pentru sinteza de compusi cu activitate biologica (2003-2005), Contract Ceres 189/2003</i> | Director ICIA Irimie 2003-2005 |
| 3 | <i>Model experimental bioreactor-extractor pentru obtinerea enzimatica a unor compusi anti-sida (2003-2005), Contract Ceres 1990/2003</i> | Director ICIA Irimie 2003-2005 |
| 4 | <i>Tehnologie de transesterificare enzimatica destinata obtinerii de biocarburanti de generatia a 2-a PNCD II</i> | Responsabil UBB Irimie 2008-2010 |
| 5 | <i>Sinteza enzimatică a unor amino- și hidroxiacizi heterociclici nenaturali.</i> | membru 2006-2008 |
| 6 | <i>Investigarea mecanismului de actiune al histidin- si fenilalanin-amoniac liazelor, CNCSIS Idei H</i> | membru 2009-2011 |

11. Coordonări de programe/granturi finanțate din sursă internațională (se menționează și valoarea)

Coordonatorul Programului CEEPUS HU-0010, Teaching and Learning Bio-Analysis. Mobilitati al vadrelor didactice si studentilor, cel puțin 4 cadre si 2 studenti annual. Valoarea burselor depinde de tara.

12. Coordonări de programe/granturi finanțate din sursă națională (se menționează și valoarea)

13. Profesor invitat la universitati de prestigiu, cu titlu oficial

1. Universitatea din Rouen, Franța 2009
2. Universitatea din Zagreb, Croatia 2007
3. Universitatea de medicină Karl Franzens Graz, Austria, 2006
- 3 Universitatea din Budapesta, Ungaria, 2007, 2008, 2009

15. Conferințe invitate internaționale

1. Moldovan, P., Paizs, Cs., Tosa M., Majdik, C., Daniela Let, D., **Florin Dan Irimie**,. (2006): *Dynamic enzymatic resolution of some non-proteinogenic amino acids*, 1st 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*, 33rd International Conference of Slovak Society of Chemical Engineering, Tatranske Matliare, Slovakia, 22-26 May, 2006, 228.
3. Majdik, C., Toșa, 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*, 33rd 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*, 33rd 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*. 33rd International Conference of Slovak Society of Chemical Engineering, Tatranske Matliare, Slovakia, 22- 26 May, 2006, 231.
6. **Florin Dan Irimie**, Csaba Paizs, Monica Toșa, Paula Podea, Enzyme dynamic kinetic resolution, as a valuable tool for enantiopure compounds synthesis. process and monitoring, International Symposium and Summer School: „Development of Bioanalytical Methods and Actual Applications”, Nitra 2008, Slovacia

16. Membru în comitete de organizare sau științifice ale unor conferințe internaționale
Nitra, Slovacia, 2008; Sofia, 2006

III. Realizare remarcabilă

Direcția de dezvoltare asumată de grupul nostru în domeniul sintezei organice selective asistate biocatalitic, aceea de a crea tehnologii alternative noi, de principiu, care să poată fi utilizate într-o gamă cât mai mare de aplicații concrete. Consecvent acestei direcții, **am demarat, la inițiativa personală un proiect în colaborare cu IRCOF (Institut de Recherche en Chimie Organique Fine) Rouen, Franța.**

Proiectul, considerat de subsemnatul ca realizarea cea mai relevantă din ultimii cinci ani, are ca obiectiv construirea unor componente de schelet de tip 2-hidroximetil și 2-aminometilazol, de înaltă enantiopuritate. Aceste elemente moleculare de construcție au capacitatea dovedită de a avea acțiuni biologice interesante precum citotoxicitate selectivă, inhibiție selectivă de proteosinteză bacteriană, inhibiție pentru formele de rezistență medicamentoasă multiplă.

Proiectul constă în sinteza în compun, în laboratoarele partenere a motivelor heterociclice, și în realizarea etapei înalt stereoselective (enantiomer sau enantiotop-) în laboratoarele grupului coordonat se subsemnatul.

Valoarea proiectului constă, pe lângă rezultatele substanțiale previzionate la limita certitudinii, în implicarea a doi doctoranzi ai subsemnatului dintre care unul este îndrumat în cotutelă, cu șeful grupului omolog din Franța. De asemenea în realizarea proiectului sunt implicați și doi masteranzi.

Anticipăm elaborarea, inițială a unor brevete în comun și ulterior a unor publicații relevante privind aceste structuri natural-mimetice. Ulterior vom trece la o etapă superioară, aceea de asamblare a acestor elemente în construcția bioactiv selectivă și testarea acesteia în vederea elaborării propunerii de validare.

Această realizare, a fost posibilă în condițiile existenței grupului de cercetare „Biotransformări ale substraturilor organice” acreditat CNCSIS din 2005 și a nucleului de cercetare validat prin rezultatele anexate, compus din Conf. Dr. PAIZS Csaba, Monica-Ioana TOSA și Paula PODEA, alături de subsemnatul.

Pe lângă cele de mai sus consider tot ca realizare remarcabilă monografia ”**Biotransformări în sinteza organică – aspecte fundamentale**” elaborată împreună cu cei doi colaboratori PAIZS Csaba și Monica Ioana TOSA în 2006, la Editura Napoca-Star, o sinteză unică, în țară dar și pe plan internațional, a experienței grupului de autori, și a celor mai relevante jaloane ale domeniului.

Data:

Semnătura:

Certific validitatea datelor prezentate
Sef de catedră,