

RAPORT DE AUTOEVALUARE 2013

ȘTIINȚE EXACTE – CHIMIE

1. Date de identificare institut/centru

1.1. Denumire: **INSTITUTUL DE CHIMIE TIMIȘOARA AL ACADEMIEI ROMÂNE (ICT)**

- 1.2. Statut juridic: institutie publica cu personalitate juridica
1.3. Act de înființare: HG. 1366/2001
1.4. Număr de înregistrare în Registrul Potențialilor Contractori: **I-AR 3216**
1.5. Director general/Director: **Dr. Otilia Costisor**
1.6. Adresă: 300223-Timisoara, Bul. Mihai Viteazul, 24
1.7. Telefon, fax, pagină web, e-mail: **0256 491818; 0256 491824**
<http://acad-icht.tm.edu.ro>
E-mail: ocostisor@acad-icht.tm.edu.ro

2. Domeniu de specialitate

- 2.1. Conform clasificării UNESCO: **2303 - 07**
2.2. Conform clasificării CAEN: 7219

3. Stare institut/centru

3.1. Misiunea institutului/centrului, direcțiile de cercetare, dezvoltare, inovare.
Rezultate de excelență în îndeplinirea misiunii (maximum 2000 de caractere):

ICT - instituție publică cu personalitate juridica, institut al Academiei Române, asigură competența cercetării românești în domeniul chimiei organice, anorganice și computationale prin efectuarea de cercetări fundamentale și aplicative.

Misiunea **ICT** este de a efectua:

A. Activități de cercetare – dezvoltare:

- a. în cadrul Programului de cercetare al Academiei Române;
- b. în afara Programului de cercetare al Academiei Române, prin cercetare competitivă:
 - prin sistemul de Programe fundamentale și Programe prioritare ale A.R.;
 - prin sisteme de granturi ale A.R. și MEC inclusiv PNCD;
 - în cadrul programelor de cercetare – dezvoltare europene;
 - în cadrul programelor europene transfrontaliere ;
 - colaborari internationale în cadrul relațiilor de schimb interacademic sau al colaborărilor bilaterale agreate.

B. Activități conexe în domeniul său de activitate:

- acordă asistență tehnică și consultanță unităților productive din zona de vest a țării;
- efectuează expertize tehnice și analize chimice;
- acorda consultanță la construirea și implementarea sistemelor de asigurare a calității pentru zona de vest.

C. Activități de formare și specializare profesională:

- Unitate de cercetare abilitată (ICA) să organizeze doctorate în cadrul SCOSAR

3.2. Modul de valorificare a rezultatelor de cercetare, dezvoltare, inovare și gradul de recunoaștere a acestora (maximum 1000 de caractere):

Valorificarea rezultatelor cercetărilor prin diseminarea acestora astfel:

- publicarea lor în reviste cu un standard cât mai înalt evidențiată de creșterea calității revistelor în care apar lucrările însă de scaderea numărului de publicații.
- publicarea de cărți și monografii;
- supunerea lor discutiei specialiștilor prin participarea la manifestari naționale și internaționale;
- obținerea de brevete și,
- implementarea lor în unități productive.

Recunoașterea rezultatelor evidențiată prin:

- creșterea numărului de publicații cotate ISI și a prestigiului acestora;
- creșterea numărului de citări și a prestigiului revistelor care citează;
- atragerea de fonduri: număr de granturi și proiecte acordate în urma competiției directe;
- participarea la proiecte europene: fiecare laborator al ICT este implicat într-un proiect european(FP 7 – 3 proiecte).
- colaborarea cu unitatile de invatamant și cercetare din țara și încadrarea într-un sistem interdisciplinar/multidisciplinar(conform capitolului NOTE);
- colaborările internaționale bilaterale cu unități prestigioase (conform capitolului NOTE);
- recunoașterea cercetărilor prin implicarea în acțiuni de evaluare a proiectelor europene și naționale. (conform capitolului NOTE);
- vizita unor personalități la ICT.

3.3. Situația financiară - datorii la bugetul de stat: **Nu sunt**.

3.4. Numărul personalului de cercetare (CS - CS I):

39 personal de cercetă atestat (2 concediu de maternitate)

37 doctori

3.5. Numărul total al personalului:

94.5 posturi din care **14** asistenți de cercetare

ȘTIINȚE EXACTE
(FIZICA, CHIMIE, separat MATEMATICA)

4. Criterii de performanță în cercetarea științifică (toate criteriile analizează numai perioada de evaluare) (40%)

Nr. crt.	Criteriu	n	Punctaj unitar	Punctaj acordat
1.	Participarea la un program fundamental sau prioritar al Academiei Române și realizarea obiectivelor sale.		25	-
2.	Un tratat apărut într-o editură consacrată din străinătate ²		$25 \times (N_{ic}/N_a)$	-
3.	O carte apărută într-o editură consacrată din străinătate ²		$20 \times (N_{ic}/N_a)$	-
4.	O monografie apărută într-o editură consacrată din străinătate ²		$15 \times (N_{ic}/N_a)$	-
5.	O carte editată într-o editură consacrată din străinătate ²		$10 \times (N_{ic}/N_a)$	-
6.	Un tratat editat într-o editură consacrată din străinătate ²		$13 \times (N_{ic}/N_a)$	-
7.	O monografie editată într-o editură consacrată din străinătate ²		$8 \times (N_{ic}/N_a)$	-
8.	Un tratat apărut în Editura Academiei Române		$13 \times (N_{ic}/N_a)$	-
9.	O carte apărută în Editura Academiei Române		$10 \times (N_{ic}/N_a)$	-

10.	O monografie apărută în Editura Academiei Române		$8 \times (N_{ic}/N_a)$	-
11.	Un tratat editat în Editura Academiei Române		$7 \times (N_{ic}/N_a)$	-
12.	O carte editată în Editura Academiei Române		$5 \times (N_{ic}/N_a)$	-
13.	O monografie editată în Editura Academiei Române		$3 \times (N_{ic}/N_a)$	-

² Se vor lua în considerare următoarele edituri străine: Academic Press, Appleton & Lange, Birkhauser, Blackwell, Cambridge University Press, CRC Press, Elsevier, Garland Publishing, Kluwer Academic Publishers, McGraw-Hill, Mosby, Nova Science Publishers, Oxford University Press, QMP, Springer Verlag,

Nr. crt.	Criteriu	n	Punctaj unitar	Punctaj acordat
14.	Un articol publicat într-o revistă cotată de <i>Web of Science</i> (Thomson Reuters)	40	$(1 + FI) \times (N_{ic}/N_a)^4$	56.181
15.	O lucrare prezentată la o manifestare științifică internațională, publicată integral într-o revistă cotată de <i>Web of Science</i> (Thomson Reuters)	-	$(1 + FI) \times (N_{ic}/N_a)^4$	-
16.	O lucrare prezentată la o manifestare științifică internațională, publicată integral într-un volum editat într-o editură consacrată din străinătate, inclusiv electronic (<i>Conference Proceedings Citation Index- Science, Web of Science</i> , Thomson Reuters) ²	14	$2 \times (N_{ic}/N_a)$	17.665
17.	Un capitol într-un tratat, carte sau monografie editată într-o editură consacrată din străinătate ²	5	$13 \times (N_{ic}/N_a) \times (N_p/N_{tp})$	1.897
18.	Un capitol într-un tratat, carte sau monografie editată în Editura Academiei Române	-	$7 \times (N_{ic}/N_a) \times (N_p/N_{tp})$	-
19.	Număr de citări conform <i>Web of Science</i> (Thomson Reuters)	352	0,5	176
20.	Factor de impact cumulat conform <i>Web of Science</i> (Thomson Reuters) ³	- 40	$FI \times (N_{ic}/N_a)$	35.139
21.	O carte apărută într-o editură consacrată din țară ⁷	1	$7 \times (N_{ic}/N_a)$	6
22.	O carte editată într-o editură consacrată din țară ⁷	-	$3 \times (N_{ic}/N_a)$	-
23.	Un articol apărut într-o revistă recunoscută de CNCS (B+) sau indexată într-o bază internațională de date (BDI)	-	$1 \times (N_{ic}/N_a)$	-
24.	O conferință invitată/plenară/keynote prezentată la o manifestare științifică internațională	3	10	30
25.	O conferință invitată/plenară/keynote prezentată la o manifestare științifică națională	-	5	-
26.	O comunicare orală prezentată la o manifestare științifică internațională	14	$5 \times (N_{ic}/N_a)$	52.143
27.	O comunicare orală prezentată la o manifestare științifică națională	-	$2 \times (N_{ic}/N_a)$	-
Punctaj total criterii de performanță în cercetarea științifică				375.025

Thieme, Willey-Liss, Williams and

Pondere 40% x 375.025 = 150.01

Wilkins, World Scientific Publishing, alte edituri străine de aceeași anvergura.

³ Pentru fiecare articol se va lua în calcul factorul de impact (FI) al revistei împărțit la numărul total de autori (N_a) și înmulțit cu numărul de autori din institutul/centrul evaluat (N_{ic}). Factorul de impact este publicat anual de *Web of Knowledge, Journal Citation Report* (Thomson Reuters), iar pentru calcul se va utiliza valoarea corespunzătoare anului apariției articolului.

⁴ Pentru revistele din domeniile: Botanică, Zoologie, Ecologie, Agronomie etc., al căror FI este $\leq 2,0$ punctajul total se înmulțește cu 1,5.

⁵ Punctajul total va fi suma punctajelor unitare rezultate prin calcul.

⁶ Pentru domeniul Științe Agricole produsele sunt soiuri noi de plante, hibrizi etc., iar punctajul unitar va fi 30.

n = număr programe, tratate, cărți, monografii, lucrări, citări etc.; FI = factor de impact; N_{ic} = număr autori din institut/centru; N_a = număr total de autori; N_p = număr pagini capitol; N_{tp} = număr total de pagini volum.

⁷ Se vor lua în considerare cărțile științifice de autor ce apar în evidența Bibliotecii Naționale.

n = număr programe, tratate, cărți, monografii, lucrări, citări etc.; FI = factor de impact; N_{ic} = număr autori din institut/centru; N_a = număr total de autori; N_p = număr pagini capitol; N_{tp} = număr total de pagini volum.

5. Capacitatea de a atrage fonduri de cercetare (20%)

Nr. crt.	Criteriu	n	Punctaj unitar	Punctaj acordat
1.	Un grant câștigat de către institut/centru de la organizații internaționale	5000 - 10000 EUR	1	2
		10001 - 50000 EUR	1	4
		50001 - 200000 EUR	1	6
		200001 - 1000000 EUR		8
		peste 1000000 EUR		10
2.	Un grant câștigat de către institut/centru de la organisme naționale	sub 10000 RON		1
		10001 - 100000 RON	3	2
		100001 - 500000 RON	2	3
		peste 500000 RON		4
3.	Un contract extrabugetar obținut de către institut/centru de la organizații internaționale sau naționale	sub 5000 RON	3	0,5
		5001 - 10000 RON	2	1
		10001 - 100000 RON	2	2
		peste 100000 RON	1	3
4.	O manifestare științifică (congres, conferință, simpozion) sau școală de vară internațională organizată de institut	2	10	20
5.	O manifestare științifică (congres, conferință, simpozion) sau școală de vară națională organizată de institut		5	-
Punctaj total atragere fonduri de cercetare				54.50

Pondere de 20% x 54.50 = 10.90

6. Capacitatea de a dezvoltă servicii, tehnologii, produse (10%)

Nr. crt.	Criteriu	n	Punctaj unitar	Punctaj acordat
1.	Un brevet acordat	la nivel internațional	-	10
		la nivel național	-	5
2.	Un brevet aplicat	la nivel internațional	-	20
		la nivel național	-	10
3.	Un brevet citat în <i>Web of Science</i> (Thomson Reuters)	-	5	-
4.	Produse și tehnologii rezultate din activități de cercetare bazate pe omologări sau inovații proprii (produs vândut, sume încasate) ⁶	-	20	-
5.	Un laborator de cercetare-dezvoltare acreditat	-	20	-
6.	Studii de impact și servicii comandate de un beneficiar	18	5	90
Punctaj total dezvoltare servicii s.a.				90

Pondere de 10% x 90 = 9

7. Capacitatea de a pregăti superior tineri cercetatori (doctorat, post-doctorat) (10%)

Nr. crt.	Criteriu	n	Punctaj unitar	Punctaj acordat
1.	Institutul/centrul are dreptul de a conduce doctorate	1	20	20
2.	Un conducător de doctorat care activează în institut/centru	5	20	100

3.	Un doctorand	16	10	160
4.	Un post-doctorand	3	10	30
5.	Un cercetator angajat în institut/centru care a obținut titlul de doctor în perioada de evaluare	3	10	30
Punctaj total prezentare tineri cercetatori				340

Pondere de 10% x 340 = 34

8. Prestigiul științific (toată perioada de activitate) (20%)

Nr. crt.	Criteriu	n	Punctaj unitar	Punctaj acordat
1.	Un membru în colectivul de redacție al unei reviste naționale/internăționale (cotate de <i>Web of Science</i> , Thomson Reuters sau indexată într-o BDI) sau în colectivul editorial al unor edituri internaționale consacrate ²	14	20	280
2.	Un membru în conducerea unei organizații internaționale de specialitate	1	20	20
3.	Un membru al Academiei Române	1	50	50
4.	Un cercetător cu un indice Hirsch peste 8	6	20	120
5.	Un membru de onoare (<i>fellow, senior</i>) al unei societăți științifice naționale/internăționale	1	20	20
6.	Un premiu al Academiei Române	-	20	-
7.	Un premiu (distincție) al unei societăți științifice naționale obținut printr-un proces de selecție	1	10	10
8.	Un premiu (distincție) al unei societăți științifice internaționale obținut printr-un proces de selecție	3	40	120
Punctaj total prestigiul științific				620

Pondere de 20% x 620 = 124

Punctaj total criteriul performanța științifică, atragere de fonduri, performanța dezvoltare, prezentare tineri și prestigiul științific	327.91
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Director

Dr. Otilia Costisor

Anexa 4.14

Un articol publicat într-o revistă cotată de *Web of Science* (Thomson Reuters)

1.	Goodarzi M., Funar-Timofei S., Vander Heyden Y. Towards better understanding of feature selection/reduction techniques for QSAR models <i>TrAC-Trend. Anal. Chem.</i> . 42: 49-63, 2013	(1+6.273)x(1/3)	2.424
2.	Margan D., Ilia G., Borota A., Mracec M. Conformational analysis of prostaglandin E2. II <i>Rev.Roum.Chim.</i> . 57: 449-456, 2012	(1 + 0.418)x(2/4)	0.709
3.	Halip L., Gruia A.T., Borota A., Mracec M., Curpan R.F., Mracec M. 3D homology model of the alpha(2C)-adrenergic receptor subtype <i>Rev.Roum.Chim.</i> , 57, 763-768, 2012	(1 + 0.418)x(4/6)	0.945
4.	Ostopovici-Halip L., Rad-Curpan R., Modeling of ligand binding to dopamine D2 receptor, <i>J.Serb. Chem. Soc.</i> (2013) doi: 10.2298/JSC130208046O	(1+0.912)x(2/2)	1.912
5.	Crisan L., Pacureanu L., Bora A., Avram S., Kurunczi L., Implementation of PLS discriminant analysis to rank indirubin derivatives against decoys, <i>Cent. Eur. J. Chem.</i> . 11(10): 1644-1656, 2013	(1 + 1.167)x(4/5)	1.734
6.	Crisan L., Pacureanu L., Avram S., Bora A., Avram S., Kurunczi L., Shape-based similarity and PLS analysis of maleimide derivatives, <i>J. Enz. Inhib. Med. Chem.</i> , DOI:10.3109/14756366.2013.833196, 2013	(1 + 1.495)x(4/6)	1.664
7.	Avram S.I., Crisan L., Bora A., Pacureanu L.M., Avram S., Kurunczi L. Retrospective group fusion similarity search based on eROCE evaluation metric, <i>Bioorg. Med. Chem.</i> . 21(5): 1268-1278, 2013	(1+2.903)x(4/6)	2.602
8.	Ivan D., Funar-Timofei S., Medeleanu M., Mracec M., Mracec M. Formation Enthalpy for conformers of (3s,5s,6s)-6-Acetylaminopenicillanic Acid calculated by the PM6 and PM7 semiempirical MO Methods, <i>Rev. Roum. Chim.</i> . 58(4-5): 463-472, 2013	(1+0.331)x(3/5)	0.799
9.	Tarabukina E., Fagadar-Cosma E., Enache C., Zakharova N., Birdeanu M. Molecular Properties and Aggregation of Porphyrin Modified Polysiloxane in Solutions <i>J. Macromol. Sci. Phys.</i> . 52(8): 1077-1091, 2013	(1+0.807)x(2/5)	0.723
10.	Vlascici D., Popa I., Chiriac V.A., Fagadar-Cosma G., Popovici H., Fagadar-Cosma E. Potentiometric detection and removal of copper using porphyrins <i>Chem. Centr. J.</i> . 7(1): 111, 2013	(1+1.31)x(1/6)	0.385

11.	Iordache S., Cristescu R., Popescu A.C., Popescu C.E., Dorcioman G., Mihailescu I.N, Ciucu A.A., Balan A., Stamatin I., Fagadar-Cosma E., Chrisey D.B. Functionalized porphyrin conjugate thin films deposited BZ matrix assisted pulsed laser evaporation <i>Appl. Surf. Sci.</i> 278: 207-210, 2013	(1+2.112)x(1/11)	0.283
12.	Bîrdeanu M., Bîrdeanu A.-V., Gruia A.S., Fagadar-Cosma E., Avram C.N. Synthesis and characterization of Zn ₃ Ta ₂ O ₈ nanomaterials by hydrothermal method <i>J. Alloy. Compd.</i> 573: 53-57, 2013	(1+2.390)x(1/5)	0.678
13.	Fagadar-Cosma E., Gil-Agusti M. Press release FP7-Project SOMABAT- Development of novel solid materials for high power Li polymer batteries (SOMABAT) recyclability of components-press release <i>Rev. Chim. Buc.</i> 63(10): 2 pag. 2012	(1+ 0.538)x(1/2)	0.769
14.	Creangă I., Făgădar-Cosma G., Palade A., Lascu A., Enache C., Birdeanu M., Făgădar-Cosma E. New hybrid silver colloid-A ₃ B porphyrin complex exhibiting wide band absorption <i>Digest J. Nanomater. Bios.</i> 8(2): 561-572, 2013	(1+ 1.092)x(5/7)	1.494
15.	Palade A., Fagadar-Cosma G., Lascu A. Creanga I., Birdeanu M., Făgădar-Cosma E. New porphyrin-based spectrometric sensor for Ag ⁰ detection <i>Digest J. Nanomater. Bios.</i> 8(3): 1013-1022, 2013	(1+1.092)x(3/3)	2.092
16.	Birdeanu M, Birdeanu A.V., Fagadar-Cosma E., Enache C., Miron I., Grozescu I. Structural, morphological, optical and thermal properties of the ZnTa ₂ O ₆ nanomaterials obtained by solid state method <i>Digest J. Nanomater. Bios.</i> 8(1): 263-272, 2013	(1+1.092)x(2/6)	0.697
17.	Ilia G., Crasmareanu E., Pascut D., Darabant L., Simulescu V. The use of mass spectrometry in obstetric and gynecology <i>Cent. Eur. J. Chem.</i> 11(5): 645-654, 2013	(1+1.167)x(3/5)	1.300
18.	Balint E., Tajti A., Drahos L., Ilia G., Keglevich G. Alcoholysis of dialkyl phosphites under microwave conditions <i>Curr. Org. Chem.</i> 17(5): 555-562, 2013	(1+3.434)x(1/5)	0.887
19.	Petric M., Crisan L., Crisan M., Micle A., Maranescu B., Ilia G. Synthesis and QSRR Study for a Series of Phosphoramidic Acid Derivatives <i>Heteroatom Chem.</i> 24(2): 138 -145, 2013.	(1+1.577)x(4/6)	1.718
20.	Margan D. Borota A., Ilia G., Mracec M. Conformational Analysis for prostglandin E2II <i>Rev. Roum. Chim.</i> 57(4-5): 449-456, 2012	(1+0.331)x(3/4)	0.998
21.	Crasmareanu E., Simulescu V., Ilia G. Synthesis by Reversed Phase Transfer Catalysis and Characterization of Naphthol AS-D pigment <i>J. Chem.</i> Article ID 545374, 2013.	(1+0.484)x(3/3)	1.484
22.	Crisan M., Bouros P., Chumakov Y., Petric M., Ilia G. Supramolecular assembly and ab initio quantum chemical calculations of 2-hydroxyethylammonium salts of para-	(1+4.689)x(3/5)	3.413

	substituted benzoic acids <i>Cryst. Growth Des.</i> 13(1): 143-154, 2013		
23.	Grad M.E., Simu G.M., Muntean S.G., Ilia G. Synthesis, characterization and colour determination using CIELAB colour space of stilbene dyes, <i>J. Iran. Chem. Soc.</i> 10(4): 807-816, 2013	(1+2.072)x(3/4)	2.304
24.	Muntean S.G., Paska O.M., Coseri S., Simu G.M., Grad M.E., Ilia G. Evaluation of a functionalized copolymer as adsorbent on direct dyes removal process: kinetics and equilibrium studies <i>J. Appl. Polym. Sci.</i> 127(6): 4409-4421, 2013	(1+1.395)x(4/6)	1.597
25.	Pacurariu C., Mihoc G., Popa A., Muntean S.G., Ianos R. Adsorption of phenol and p-chlorophenol from aqueous solutions on poly (styrene-co-divinylbenzene) functionalized materials, <i>Chem. Eng. J.</i> 222: 218–227, 2013	(1+3.461)x(2/5)	1.784
26.	Plesu N., Kellenberger A., Taranu I., Taranu B.O., Popa I. Impedimetric detection of dopamine on poly(3-aminophenylboronic acid) modified skeleton nickel electrodes <i>React. Functional Polym.</i> 73(5): 772-778, 2013	(1+2.505)x(1/5)	0.701
27.	Kellenberger A., Plesu N., Tara-Lunga Mihali M., Vaszilcsin N. Synthesis of polyaniline nanostructures by electrochemical deposition on niobium, <i>Polymer</i> 54(13): 3166-3174, 2013	(1+3.379)x(2/4)	2.190
28.	Iliescu S., Zubizarreta L., Plesu N., Macarie L., Popa,A., Ilia G. Polymers containing phosphorus groups and polyethers: from synthesis to application <i>Chem. Cent. J.</i> 6: 132, 2012 (neraportata in 2012)	(1+1.312)x(5/6)	1.927
29.	Buruiana L.-I., Avram E., Popa A., Stoica I., Ioan S. Influence of triphenylphosphonium pendant groups on the rheological and morphological properties of new quaternized polysulfone <i>J. Appl. Polym. Sci.</i> 129(4): 1752-1762, 2013	(1+1.395)x(1/5)	0.479
30.	Ciopec M., Davidescu C.- M., Negrea A., Lupa L., Popa A., Muntean C., R. Ardelean, G. Ilia Synthesis, characterization, and adsorption behavior of aminophosphinic grafted on poly(styrene-Co-divinylbenzene) for divalent metal ions in aqueous solutions <i>Polym. Eng. Sci.</i> 53(5): 1117-1124, 2013	(1+1.243)x(2/8)	0.561
31.	Parvulescu V., Niculescu V., Ene R., Popa A., Mureseanu M., Ene C. D., Andruh M. Supported monocationic copper(II) complexes obtained by coordination with dialkylphosphonate groups on styrene-divinylbenzene copolymer as catalysts for oxidation of organic compounds <i>J. of Molec. Catalysis A-Chemical</i> , 366: 275-281, 2013	(1+3.187)x(1/7)	0.598
32.	Davidescu C.-M., Ciopec M., Negrea A., Popa A., Lupa L., Dragan E.-S., Ardelean R., Ilia G., Iliescu S. Synthesis, characterization, and Ni(II) ion sorption properties of poly(styrene-co-divinylbenzene) functionalized with	(1+1.332)x(3/9)	0.777

	aminophosphonic acid groups, <i>Polym. Bull.</i> 70(1): 277-291, 2013		
33.	Visa A., Maranescu B., Bucur A., Iliescu S., Demadis K. Synthesis and Characterization of a Novel Phosphonate Metal Organic Framework Starting from Copper Salts <i>Phosphorus Sulfur DOI:</i> 10.1080/10426507.2013.843004, 2013	(1+0.601)x(3/5)	0.961
34.	Holclajtner-Antunovic I.D., Popa A., Bajuk-Bogdanovic D.V., Mentus S., Nedic Vasiljevic B.M., Uskokovic-Markovic S.M , Synthesis and characterization of acid silver salts of 12-tungstophosphoric acid, <i>Inorg. Chim. Acta</i> , 407, 197–203, 2013	(1 + 1.899)×(1/6)	0.483
35.	Popa A., Sasca V., Verdes O., Barvinschi P., Holclajtner-Antunović I. Acidic and neutral cesium salts of 12-molybdophosphoric acid supported on SBA-15 mesoporous silica. The influence of Cs concentration and surface coverage on textural and structural properties, <i>Mater. Res. Bull.</i> , 50, 312-322, 2014	(1 + 1.913)×(3/5)	1.748
36.	Vlad-Oros B., Dascalu D., Dudas Z., Popovici H., Preda G., Ostafe V. Equilibrium and Kinetics Studies Regarding the Adsorption of Copper (II) Ions by various types of Chitosan Beads <i>Dig. J. Nanomater. Bios.</i> , 8(3), 917 – 927, 2013	(1+1.092)×(1/6)	0.349
37.	Sasca V., Verdes O., Avram L., Popa A., Erdohelyi A., Oszko A., The $Cs_xH_{3-x}PW_{12}O_{40}$ catalysts microstructure model, <i>Appl Catal A: Gen</i> 451 50–57 2013	(1 + 3,410)×(4/6)	2.940
38.	Sasca V., Popa A., Band-gap energy of heteropoly compounds containing Keggin polyanion- $[PV_xMo_{12-x}O_{40}]^{(3+x)}$ relates to counter-cations and temperature studied by UV-VIS diffuse reflectance spectroscopy <i>J Appl Phys</i> , 114, 133503(1-7) 2013	(1 + 2,210)×(2/2)	3.210
39.	Sasca V., Verdes O., Avram L., Popa A., Thermal decomposition of Pd doped 12-tungstophosphoric acid and some of its cesium salts <i>Rev Roum Chim</i> 58(4-5) 451-461 2013	(1 + 0,331)×(4/4)	1.331
40.	Putz M.V., Putz A.M. DFT Chemical Reactivity Driven by Biological Activity: Applications for the Toxicological Fate of Chlorinated PAHs. <i>Structure and Bonding</i> 150 (2013) 181–232; DOI: 10.1007/978-3-642-32750-6_6;	(1 + 4.068)×(1/2)	2.531
		TOTAL	56.181

Anexa 4.15

**O lucrare prezentată la o manifestare științifică internațională, publicată integral
într-o revistă cotată de *Web of Science* (Thomson Reuters)**

Anexa 4.16

O lucrare prezentată la o manifestare științifică internațională, publicată integral într-un volum editat într-o editură consacrată din străinătate, inclusiv electronic (*Conference Proceedings Citation Index- Science, Web of Science, Thomson Reuters*)²

1.	Beteringhe A., Soloi A., Balan C., Iosif D., Costea M., Fagadar-Cosma E. HYDROBET – a novel method for calculation of hydrophobic/hydrophilic balance of New Asymmetric Porphyrins as Potential Photosensitizers in Photodynamic Therapy. The usefulness of the new APORBET index in the QSPR studies <i>Proceedings of the 6th WSEAS International Conference on Computational Chemistry (COMPUCHEM '12): Advances in Environment, Computational Chemistry and Bioscience</i> , Montreux, Switzerland, 2012, 308-313	2×(1/6)	0.333
2.	Lascu A., Birdeanu M., Creanga I., Palade A. About the aggregation behaviour of hydroxy-porphyrin Fe(III) complex <i>Proceedings of the 19th International Symposium on Analytical and Environmental Problems</i> , Szeged, 2013, 193-196	2×(3/4)	1.5
3.	Muntean S.G., Rădulescu-Grad M.E. Decontamination of colored wastewaters Using a synthetic sorbent <i>Timisoara's Academic Days, 13th Edition, New trends and strategies in the chemistry of advanced materials with relevance in biological systems, technique and environmental protection</i> , 2013, 96-99.	2×(2/2)	2
4.	Rădulescu-Grad M.E., Muntean S.G. Colour determination using CIELAB colour space of stilbene dye <i>Timisoara's Academic Days, 13th Edition, New trends and strategies in the chemistry of advanced materials with relevance in biological systems, technique and environmental protection</i> , 2013, 113-116	2×(2/2)	2
5.	Plesu N., Kellenberger A., Taranu B.O., Taranu I., Popa I., Dragos A. Poly(3-aminophenylboronic acid) modified nickel Raney Nickel electrode <i>Timisoara's Academic Days, 13th Edition, New trends and strategies in the chemistry of advanced materials with relevance in biological systems, technique and environmental protection</i> , Timișoara, România, 2013, 92-95	2×(1/6)	0.333
6.	Buruiana L.I., Avram E., Popa A., Ioan S. Microarhitecture of quaternized polysulfone/poly(vinylidene fluoride) blend for scaffolds in tissue engineering <i>Research People and Actual Tasks on Multidisciplinary</i>	2×(1/4)	0.5

	<i>Science</i> , 12 - Lozenec, Bulgaria, 2013 , 67-71		
7.	Buruiana L. I., Avram E., Popa A., Ioan S. Origin of shear thinning behaviour of poly(vinylidene fluoride)/quaternized polysulfone solutions with implication in biomedical applications <i>10th HSTAM International Congress on Mechanics Chania, Crete, Greece, 2013</i> , 1-8	2x(1/4)	0.5
8.	Taranu B.-O., Fagadar-Cosma E., Popa I., Fagadar-Cosma G., Vlascici D., Birdeanu M. I., Taranu I. Preliminary studies on glassy carbon electrode modified with a novel functionalized A ₃ B porphyrin. Application as potentiometric cation sensor <i>Proceedings of the 19th International Symposium on Analytical and Environmental Problems</i> , 23 September 2013 , Szeged, Ungaria, 80-83, ISBN 978-963-315-141-9.	2x(1/7)	0.285
9.	Bora A., Crisan L., Avram S., Neanu C., Pacureanu L. Preliminary molecular docking study of 2-phenyl-chroman-4-one derivatives against cyclin dependent kinases <i>13th Edition of Timisoara's Academic Days, New Trends and Strategies in the Chemistry of Advanced materials with relevance in Biological Systems, technique and Environmental Protection, Chemistry</i> , 13-14 June 2013 , 100-105, Timisoara, Romania	2x(5/5)	2
10.	Crisan L., Pacureanu L., Bora A., Avram S., Ivan D., Neanu C., Kurunczi L., Preliminary PLS study of 38 benzofuran-3-yl-(indol-3-yl) maleimide and 18 4-azaindolyl-indolyl-maleimide derivatives using DRAGON and MOPAC descriptors <i>13th Edition of Timisoara's Academic Days, New Trends and Strategies in the Chemistry of Advanced materials with relevance in Biological Systems, technique and Environmental Protection, Chemistry</i> , 3-14 June 2013 , 117-121, Timisoara, Romania, (Electronic vol. ISSN:2065-0760)	2x(6/7)	1.714
11.	Ivan D., Crisan L., Pacureanu L., 3D-similarity analysis of HIV1- reverse transcriptase inhibitors <i>13th Edition of Timisoara's Academic Days, New Trends and Strategies in the Chemistry of Advanced materials with relevance in Biological Systems, technique and Environmental Protection, Chemistry</i> , 3-14 June 2013 , 126-129, Timisoara, Romania, (Electronic vol. ISSN:2065-0760)	2x(3/3)	2
12.	Funar-Timofei, S.; Rad-Curpan, R.; Ostopovici-Halip, L.; Bora A. Conformational Analysis of a Thiosemicarbazone Derivative Having in Vitro Antimicrobial Activity by Molecular Mechanics and Ab Initio Methods. <i>Proceedings of the 16th Int. Electron. Conf. Synth. Org. Chem.</i> , 1-30 November 2012; Sciforum Electronic Conference Series, Vol. 16, 2012 , http://sciforum.net/conference/ecsoc-16/paper/1040 (neraportată în 2012).	2x(4/4)	2
13.	Funar-Timofei, S.; Avram, S.; Borota, A. Structure-Toxicity Study of Some Pyrethroidal Esters		2

	Insecticides. <i>Proceedings of the 17th Int. Electron. Conf. Synth. Org. Chem.</i> , 1-30 November 2013; Sciforum Electronic Conference Series, Vol. 17, 2013 , e012; doi:10.3390/ecsoc-17-e012, http://www.sciforum.net/conference/ecsoc-17/paper/2250	2x(3/3)	
14.	Funar-Timofei, S.; Simu G.; Ionescu D.; Chicu S. A. Sudan I Structure Study By <i>Ab Initio</i> Methods <i>Proceedings of the 19th International Symposium ON Analytical and Environmental Problems</i> , SZAB, 23 September 2013, Szeged, Hungary, Zoltán Galbács (Ed.), ISBN 978-963-315-141-9, pag. 197-200.	2x(1/4)	0.500
		TOTAL	17.665

Anexa 4.17

Un capitol într-un tratat, carte sau monografie editate într-o editură consacrată din străinătate

Punctaj: $13 \times (N_{ic}/N_a) \times (N_p/N_{tp})$

1. Putz, M. V.; Putz, A.-M.

DFT Chemical Reactivity Driven by Biological Activity: Applications for the Toxicological Fate of Chlorinated PAHs

Book Editor(s): Putz, MV; Mingos, DMP

Source: APPLICATIONS OF DENSITY FUNCTIONAL THEORY TO BIOLOGICAL AND BIOINORGANIC CHEMISTRY Book Series: Structure and Bonding Volume: 150

Pages: 181-231 DOI: 10.1007/978-3-642-32750-6_6

Ed. Springer Verlag, Berlin-Heidelberg, Germany (2013), 288 pp.; ISBN (Hardcover): 978-3-642-32749-0

$13 \times (1/2) \times (52/288) = 1.174$

2. Putz M.V., Putz A.M., Barou R.

"Spectral-SAR Realization of OECD-QSAR Principles", In: "ADVANCES IN CHEMICAL MODELING. VOLUME 3", M.V. Putz (Ed.) NOVA Science Publishers, Inc., New York, USA (2013), Chapter 32, pp. 449-464, numar de pagini 494

$13 \times (1/3) \times (17/494) = 0.149$

3. Putz A.M., Putz M.V.

" Spectral-Structure Activity Relationship (Spectral-SAR) Assessment of Ionic Liquids' in Silico Ecotoxicity", in "IONIC LIQUIDS - NEW ASPECTS FOR THE FUTURE", Jun-ichi Kadokawa (Ed.), InTech, Inc., Rijeka-New York-Shanghai, Croatia-USA-China (2013), ISBN: 978-953-51-0937-2, Chapter 4 (DOI:10.5772/51657), pp. 85-126, numar de pagini 695

$13 \times (1/2) \times (43/695) = 0.402$

4. Putz M.V., Ori O., De Corato M., Putz A.M., Benedek G., Cataldo F., Graovac A. Introducing „Colored“ Molecular Topology by Reactivity Indices of Electronegativity and Chemical Hardness, in "TOPOLOGICAL MODELING OF NANOSTRUCTURES AND EXTENDED SYSTEMS", 575 p. ;Ali Reza Ashrafi, Franco Cataldo, Ali Iranmanesh, Ottorino Ori (Eds.), Springer Verlag, Dordrecht, NL (2013) Chapter 9, pp. 265-286;

$13 \times (1/7) \times (23/575) = 0.074$

5. Putz M.V., Tudoran M.A., Putz A.M.

Modeling Chlorinated Polycyclic Aromatic Hydrocarbons (Cl-PAH) Eco- and Toxicology by QSAR-OECD ToolBox Facility, 427-438 In: "ADVANCES IN CHEMICAL MODELING. VOLUME 4", M.V. Putz (Ed.) NOVA Science Publishers, Inc., New York, USA (2013), Chapter 30, numar de pagini 572

$13 \times (1/3) \times (13/572) = 0.098$

TOTAL: 1.897

Anexa 4.18

Un capitol într-un tratat, carte sau monografie editate în Editura Academiei Române

Anexa 4.19

Citări conform Web of Science (Thomson Reuters)

T 1. Goodarzi M., Bora A., Borota A., Funar-Timofei S., Avram S., Heyden Y.V. Modeling of 2-Pyridin-3-yl-Benzo[d][1,3]Oxazin-4-one Derivatives by Several Conformational Searching Tools and Molecular Docking

Curr. Pharm. Design 19(12): 2194-2203, 2013

C 1. Correa-Basurto, J.

Molecular Modeling and QSAR Studies for Drug Design

Curr. Pharm. Design 19(12): 2137-2137, APR 2013

T 2. Funar-Timofei S., Kurunczi L., Vlaia V., Olariu T., Ciubotariu D.

Quantitative Dye Structure-Toxicity Relationships Study by PLS

Book Editor(s): Cepisca C., Kouzaev G.A., Mastorakis N.E.

Conference: 2nd European Computing Conference 2008 Location: MALTA Date: SEP 11-13, 2008 *Proceedings of the 2nd European Computing Conference: New Aspects on Computers Research* Book Series: Recent Advances in Computer Engineering, Pages:

108-113, 2008

C 2. Luan F., Xu X., Liu H., Cordeiro M. N. D. S.

Review of quantitative structure-activity/property relationship studies of dyes: recent advances and perspectives

Color. Technol. 129(3): 173-186, JUN 2013

T 3. Funar-Timofei S., Ilia G.

Theoretical study of organic-inorganic hybrids obtained by grafting reaction of vinyl phosphonic acid on titanium oxide

J. Optoelectron. Adv. M. 9(12): 3933-3938, 2007

C 3. Siddabattuni S., Schuman T. P., Petrovsky V., Dogan F.

Impedance Analysis of Dielectric Nanoparticles Enabled via a Self-Assembled Monolayer

J. Am. Ceram. Soc. 96(5): 1490-1496, MAY 2013

T 4. Kurunczi L., Funar-Timofei S., Bora A., Seclaman E.

Application of the MTD-PLS method to Heterocyclic dye-cellulose interactions

Int. J. Quantum Chem. 107(11): 2057-2065, 2007

C 4. Luan F., Xu X., Liu H., Cordeiro M. N. D. S.

Review of quantitative structure-activity/property relationship studies of dyes: recent advances and perspectives

Color. Technol. 129(3): 173-186, JUN 2013

T 5. Funar-Timofei S., Kurunczi L., Iliescu S.

Structure-property study of some phosphorus-containing polymers by computational methods

Polym. Bull. 54(6): 443-449, 2005

C 5. Mallakpour S., Hatami. M., Golmohammadi H.

QSPR prediction of thermal decomposition property of non-vinyl polymers having alpha-amino acids moieties

Polym. Bull. 70(2): 715-732, FEB 2013

T 6. Schuurmann G., Funar-Timofei S.

Multilinear regression and comparative molecular field analysis (CoMFA) of azo dye-fiber affinities. 2. Inclusion of solution-phase molecular orbital descriptors

J. Chem. Inf. Comp. Sci. 43(5): 1502-1512, 2003

C 6. Luan F., Xu X., Liu H., Cordeiro M. N. D. S.

Review of quantitative structure-activity/property relationship studies of dyes: recent advances and perspectives

Color. Technol. 129(3): 173-186, JUN 2013

T 7. Funar-Timofei S., Suzuki T., Paier J.A., Steinreiber A., Faber K., Fabian Walter M.

F. Quantitative structure - Activity relationships for the enantioselectivity of oxirane ring-opening catalyzed by epoxide hydrolases

J. Chem. Inf. Comput. Sci. 43(3): 934-940, 2003

C 7. Hartman Jessica H., Cothren Steven D., Park, S.-H., Yun C.H., Darsey J.A., Miller G.P.

Predicting CYP2C19 catalytic parameters for enantioselective oxidations using artificial neural networks and a chirality code

Bioorgan. Med. Chem. 21(13): 3749-3759, 2013

C 8. Cunha, D.; Gaudin, C.; Colinet, I.; Horcajada P., Maurin G., Serre C.

Rationalization of the entrapping of bioactive molecules into a series of functionalized porous zirconium terephthalate MOFs

J. Mater. Chem. B 1(8): 1101-1108, 2013

T 8. Funar-Timofei S., Schuurrnann G.

Comparative molecular field analysis (CoMFA) of anionic azo dye-fiber affinities I: Gas-phase molecular orbital descriptors

J. Chem. Inf. Comp. Sci. 42(4): 788-795 2002

C 9. Luan F., Xu X., Liu H., Cordeiro M. N. D. S.

Review of quantitative structure-activity/property relationship studies of dyes: recent advances and perspectives

Color. Technol. 129(3): 173-186, JUN 2013

T 9. Timofei S., Kurunczi L., Schmidt W., Simon Z.

Steric and electrostatic effects in dye-cellulose interactions by the MTD and CoMFA approaches

SAR QSAR Environ. Res. 13(2): 219-226, 2002

C 10. Luan F., Xu X., Liu H., Cordeiro M. N. D. S.

Review of quantitative structure-activity/property relationship studies of dyes: recent advances and perspectives

Color. Technol. 129(3): 173-186, JUN 2013

T 10. Suzuki T., Timofei S., Kurunczi L., Dietze U., Schueuermann G.

Correlation of aerobic biodegradability of sulfonated azo dyes with the chemical structure

Chemosphere 45(1): 1-9, 2001

C 11. Luan F., Xu X., Liu H., Cordeiro M. N. D. S.

Review of quantitative structure-activity/property relationship studies of dyes: recent advances and perspectives

Color. Technol. 129(3): 173-186, JUN 2013

C 12. Oturkar C. C., Patole, M. S., Gawai, K. R., Madamwar D.

Enzyme based cleavage strategy of *Bacillus latus* BI377 in response to metabolism of azoic recalcitrant
Bioresource Technol. 130: 360-365, FEB 2013

C 13. Singh M. P., Vishwakarma S. K., Srivastava A. K.
Bioremediation of Direct Blue 14 and Extracellular Ligninolytic Enzyme Production by White Rot Fungi: *Pleurotus* spp.

BioMed Research International Article Number: 180156, 2013,
<http://dx.doi.org/10.1155/2013/180156>

C 14. Barka N., Ouzaouit K., Abdennouri M., Makhfouk M. El
Dried prickly pear cactus (*Opuntia ficus indica*) cladodes as a low-cost and eco-friendly biosorbent for dyes removal from aqueous solutions

J Taiwan Inst Chem E 44(1): 52-60, JAN 2013

C 15. Yang M.-M., Zhou S.-Q., Liu D., Zheng K.
Degradation kinetics of activated carbon catalyzed persulfate oxidation orange G
Huanjing Kexue/Environmental Science 34 (3): 962-967, 2013

T 11. Suzuki T., Timofei S., Iuoras B.E., Uray G., Verdino P., Fabian W. M. F.
Quantitative structure-enantioselective retention relationships for chromatographic separation of arylalkylcarbinols on Pirkle type chiral stationary phases

Journal Chromatogr. A 922(1-2): 13-23, 2001

C 16. Giaginis C., Tsantili-Kakoulidou A.
Quantitative Structure-Retention Relationships as Useful Tool to Characterize Chromatographic Systems and Their Potential to Simulate Biological Processes
Chromatographia 76(5-6): 211-226, MAR 2013

T 12. Timofei S., Schmidt W., Kurunczi L., Simon Z.
A review of QSAR for dye affinity for cellulose fibres

Dyes Pigments 47(1-2): 5-16, 2000

C 17. Zanjanchi F., Hadipour N. L., Sabzyan H., Beheshtian J.
Theoretical investigation of azo dyes adsorbed on cellulose fibers: 1. Electronic and bonding structures

J. Iran. Chem. Soc. 10(5): 985-999, OCT 2013

C 18. Luan F., Xu X., Liu H., Cordeiro M. N. D. S.
Review of quantitative structure-activity/property relationship studies of dyes: recent advances and perspectives

Color. Technol. 129(3): 173-186, JUN 2013

C19. Telegin, F, Shushina, I, Ran, J.H., Biba, Y., Mikhaylov, A., Priazhnikova, V.
Structure - Property relationships for dyes of different nature
Adv. Mat. Res. 821-822: 488-492, 2013

T 13. Timofei S., Fabian W.M.F.
Comparative molecular field analysis of heterocyclic monoazo dye-fiber affinities

J. Chem. Inf. Comp. Sci. 38(6): 1218-1222, 1998

C 20. Luan F., Xu X., Liu H., Cordeiro M. N. D. S.
Review of quantitative structure-activity/property relationship studies of dyes: recent advances and perspectives

Color. Technol. 129(3): 173-186, JUN 2013

T 14. Timofei S., Kurunczi L., Suzuki T., Fabian W. M. F., Mureşan S.
Multiple Linear Regression (MLR) and Neural Network (NN) calculations of some disazo dye adsorption on cellulose

Dyes Pigments 34(3): 181-193, 1997

C 21. Luan F., Xu X., Liu H., Cordeiro M. N. D. S.

Review of quantitative structure-activity/property relationship studies of dyes: recent advances and perspectives

Color. Technol. 129(3): 173-186, JUN 2013

T 15. Oprea T.I., Kurunczi L., Timofei S.

QSAR studies of disperse azo dyes. Towards the negation of the pharmacophore theory of dye-fiber interaction?

Dyes Pigments 33(1): 41-64, 1997

C 22. Luan F., Xu X., Liu H., Cordeiro M. N. D. S.

Review of quantitative structure-activity/property relationship studies of dyes: recent advances and perspectives

Color. Technol. 129(3): 173-186, JUN 2013

T 16. Timofei S., Kurunczi L., Schmidt W., Simon Z.

Lipophilicity in dye-cellulose fibre binding

Dyes Pigments 32(1): 25-42, 1996

C 23. Luan F., Xu X., Liu H., Cordeiro M. N. D. S.

Review of quantitative structure-activity/property relationship studies of dyes: recent advances and perspectives

Color. Technol. 129(3): 173-186, JUN 2013

T 17. Funar-Timofei, S., Ionescu, D., Suzuki, T.

A tentative quantitative structure-toxicity relationship study of benzodiazepine drugs

Toxicol. in Vitro 24 (1): 184-200, 2010

C 24. Okuma, K. , Tanabe, Y., Itoyama, R., Nagahora, N., Shioji, K.

One-pot synthesis of 2,3-benzodiazepines from arynes and β -diketones

Chem. Lett. 42(10): 1260-1262, 2013

T 18. Fabian, W.M.F., Timofei, S., Kurunczi, L.

Comparative molecular field analysis (CoMFA), semiempirical (AM1) molecular orbital and multiconformational minimal steric difference (MTD) calculations of anthraquinone dye-fibre affinities

J. Mol. Struc.-THEOCHEM, 340 (1-3): 73-81, 1995

C 25. Telegin, F., Shushina, I., Ran, J.H., Biba, Y., Mikhaylov, A., Priazhnikova, V.

Structure - Property relationships for dyes of different nature

Adv. Mat. Res. 821-822: 488-492, 2013

T 19. Oprea T.I., Allu T.K., Fara, D.C., Rad R.F., Ostropovici L., Bologa C.G.

Lead-like, drug-like or "pub-like": how different are they?

J. Comput. Aid. Mol. Des., 21(1-3): 113-119, 2007

C 26. Bak A., Magdziarz T., Kurczyk A., Serafin K., Polanski J.

Probing a chemical space for fragmental topology-activity landscapes (FRAGTAL): application for diketo acid and catechol HIV integrase inhibitor offspring fragments.

Comb. Chem. High Throughput Screen., 16(4): 274-87, 2013

C 27. Valli M., dos Santos R.N., Figueira L.D., Nakajima C.H., Castro-Gamboa I., Andricopulo A.D., Bolzani V.S.

Development of a natural products database from the biodiversity of Brazil.

J. Nat. Prod., 76(3): 439-444, 2013

C 28. Newby D., Freitas A.A., Ghaforian T.

Coping with unbalanced class data sets in oral absorption models.

J. Chem. Inf. Model., 53(2): 461-474, 2013

C 29. Valerio L.G. Jr, Choudhuri S.

Chemoinformatics and chemical genomics: potential utility of in silico methods.

J. Appl. Toxicol., 32(11): 880-889, 2012

T 20. Ostopovici-Halip L., Curpăn R., Mracec M., Bologa C.G.

Structural determinants of the alpha2 adrenoceptor subtype selectivity.

J. Mol. Graph. Model., 29(8): 1030-1038, 2011

C 30. Yang H., He L., Yan M., He J.G., Yu T.

High throughput screening and structure-activity relationship study of potential α 2A-adrenoceptor agonists by LANCETM cAMP assay.

Comb. Chem. High. Throughput Screen., 16(7): 522-530, 2013

C 31. Hai-Bo L., Yong P., Lu-qı H., Jun X., Pei-Gen X.

Mechanism of Selective Inhibition of Yohimbine and Its Derivatives in Adrenoceptor alpha 2 Subtypes

J. Chem., DOI: 10.1155/2013/ Article ID 783058, 2013

T 21. Oprea T.I., Bologa C.G., Boyer S., Curpan R.F., Glen R.C., Hopkins A.L., Lipinski C.A., Marshall G.R., Martin Y.C., Ostopovici-Halip L., Rishton G., Ursu O., Vaz R.J., Waller C., Waldmann H., Sklar L.A.

A crowdsourcing evaluation of the NIH chemical probes.

Nat. Chem. Biol., 5(7): 441-447, 2009

C 32. Weber G.M., Kohane I.S.

Extracting physician group intelligence from electronic health records to support evidence based medicine.

PLoS One., 8(5): e64933, 2013

C 33. Peng Z., Gillespie P., Weisel M., et al.

A Crowd-Based Process and Tool for HTS Hit Triage

Mol. Inf., 32(4): 337-345, 2013

C 34. Donover P.S., Yohn M., Sim M., Wright A., Gowda S., Allee C., Schabdach A.R., Reichman M.

New informatics and automated infrastructure to accelerate new leads discovery by high throughput screening (HTS).

Comb. Chem. High. Throughput Screen., 16(3): 180-188, 2013

C 35. Ekins S., Waller C.L., Bradley M.P., Clark A.M., Williams A.J.

Four disruptive strategies for removing drug discovery bottlenecks.

Drug Discov. Today., 18(5-6): 265-271, 2013

C 36. Qin C., Tan K.L., Zhang C.L., Tan C.Y., Chen Y.Z., Jiang Y.Y.

What does it take to synergistically combine sub-potent natural products into drug-level potent combinations?

PLoS One., 7(11): e49969, 2012

C 37. Williams A.J., Harland L., Groth P., Pettifer S., Chichester C., Willighagen E.L., Evelo C.T., Blomberg N., Ecker G., Goble C., Mons B.

Open PHACTS: semantic interoperability for drug discovery.

Drug Discov. Today. 17(21-22): 1188-1198, 2012

T 22. Halip Ostopovici L., Borota A., Mracec M., Curpan R., Gruia A., Mracec M.

3D Homology model of the alpha2a adrenergic receptor subtype

Rev. Roum. Chim., 54(2): 157-161, 2009

C 38. Kasetti Y., Bharatam P.V.

Pharmacophoric features of drugs with guanylurea moiety: an electronic structure analysis.

J. Mol. Model., 19(4): 1865-1874, 2013

- T 23.** Chigaev A, Waller A, Amit O, Halip L, Bologa CG, Sklar LA.
 Real-time analysis of conformation-sensitive antibody binding provides new insights into integrin conformational regulation.
J. Biol. Chem., 284(21): 14337-14346, 2009
- C 39.** Rom S, Zuluaga-Ramirez V, Dykstra H, Reichenbach NL, Pacher P, Persidsky Y.
 Selective activation of cannabinoid receptor 2 in leukocytes suppresses their engagement of the brain endothelium and protects the blood-brain barrier.
Am. J. Pathol., 183(5): 1548-1558, 2013
- C 40.** Montuori N, Cosimato V, Rinaldi L, Rea VE, Alfano D, Ragno
 P.uPAR regulates pericellular proteolysis through a mechanism involving integrins and fMLF-receptors.
Thromb Haemost., 109(2): 309-318, 2013
- C 41.** Rom S., Fan S., Reichenbach N., Dykstra H., Ramirez S.H., Persidsky Y.
 Glycogen synthase kinase 3 β inhibition prevents monocyte migration across brain endothelial cells via Rac1-GTPase suppression and down-regulation of active integrin conformation
Am. J. Pathol., 181(4): 1414-1425, 2012
- C 42.** Martinez-Vinambres E., Garcia-Trujillo J.A., Rodriguez-Martin E., Villar L.M., Coll J., Roldan E.
 CD29 expressed on plasma cells is activated by divalent cations and soluble CD106 contained in the bone marrow plasma: refractory activation is associated with enhanced proliferation and exit of clonal plasma cells to circulation in multiple myeloma patients.
Leukemia, 26(5): 1098-1105, 2012
- C 43.** Mateus A.M., Martinez Arias A.
 Patterned cell adhesion associated with tissue deformations during dorsal closure in *Drosophila*
PLoS One, 6(11): e27159, 2011
- T 24.** Slack J.P., Brockhoff A., Batram C., Menzel S., Sonnabend C., Born S., Galindo M.M., Kohl S., Thalmann S., Ostopovici-Halip L., Simons C.T., Ungureanu I., Duineveld K., Bologa C.G., Behrens M., Furrer S., Oprea TI., Meyerhof W.
 Modulation of bitter taste perception by a small molecule hTAS2R antagonist
Curr. Biol., 20(12): 1104-1109, 2010
- C 44.** Bohin MC., Roland WS., Gruppen H., Gouka RJ., van der Hijden HT., Dekker P., Smit G., Vincken JP.
 Evaluation of the bitter-masking potential of food proteins for EGCG by a cell-based human bitter taste receptor assay and binding studies
J. Agric. Food Chem., 61(42): 10010-10017, 2013
- C 45.** Yamazaki T., Narukawa M., Mochizuki M., Misaka T., Watanabe T.
 Activation of the hTAS2R14 human bitter-taste receptor by (-)-epigallocatechin gallate and (-)-epicatechin gallate
Biosci. Biotechnol. Biochem., 77(9): 1981-1983, 2013
- C 46.** Piccoli S., Suku E., Garonzi M., Giorgetti A.
 Genome-wide membrane protein structure prediction
Curr. Genomics, 14(5): 324-329, 2013
- C 47.** Tuleu C., Breitkreutz J.
 Educational paper: formulation-related issues in pediatric clinical pharmacology
Eur. J. Pediatr., 172(6): 717-720, 2013

- C 48.** Foster S.R., Porrello E.R., Purdue B., Chan H.W., Voigt A., Frenzel S., Hannan R.D., Moritz K.M., Simmons D.G., Molenaar P., Roura E., Boehm U., Meyerhof W., Thomas W.G.
 Expression, regulation and putative nutrient-sensing function of taste GPCRs in the heart
PLoS One, 8(5): e64579, 2013
- C 49.** Behrens M., Meyerhof W.
 Bitter taste receptor research comes of age: from characterization to modulation of TAS2Rs
Semin. Cell Dev. Biol., 24(3): 215-221, 2013
- C 50.** Sun-Waterhouse D., Wadhwa S.S.
 Industry-relevant approaches for minimising the bitterness of bioactive compounds in functional foods: a review
Food Bioprocess Tech., 6(3): 607-627, 2013
- C 51.** Born S., Levit A., Niv M.Y., Meyerhof W., Behrens M.
 The human bitter taste receptor TAS2R10 is tailored to accommodate numerous diverse ligands
J. Neurosci., 33(1): 201-213, 2013
- C 52.** Clark A.A., Liggett S.B., Munger S.D.
 Extraoral bitter taste receptors as mediators of off-target drug effects
FASEB J., 26(12): 4827-4831, 2012
- C 53.** Beck M., Jekle M., Becker T.
 Sodium chloride - sensory, preserving and technological impact on yeast-leavened products
Int. J. Food Sci. Tech., 47(9): 1798-1807, 2013
- T 25.** Margan D., Borota A., Mracec M., Mracec M.
 3D homology model of the human prostaglandin E2 receptor EP4 subtype
Rev.Roum.Chim., 57: 39-44, 2012
- C 54.** Konya V., Marsche G., Schuligoj R., Heinemann A.
 E-type prostanoid receptor 4 (EP4) in disease and therapy
Pharmacology & Therapeutics, 138: 485-502, 2013
- T 26.** Halip-Ostopovici L., Borota A., Mracec M., Curpan R., Gruia A., Mracec M.
 3D homology model of the alpha2A adrenergic receptor subtype
Rev.Roum.Chim., 54: 157-161, 2009
- C 55.** Kasetti Y., Bharatam P.V.
 Pharmacophoric features of drugs with guanylurea moiety:
J.Mol.Model., 19: 1865-1874, 2013
- T 27.** Curpan R.F., Simons P.C., Zhai D., Young S.M., Carter M.B., Bologa C.G., Oprea T.I., Satterthwait A.C., Reed J.C., Edwards B.S., Sklar L.A.
 High-throughput screen for the chemical inhibitors of antiapoptotic bcl-2 family proteins by multiplex flow cytometry
Assay Drug Dev. Technol., 9(5): 465-474, 2011
- C 56.** Buranda T., BasuRay S., Swanson S., Agola J., Bondu V., Wandinger-Ness A.
 Rapid parallel flow cytometry assays of active GTPases using effector beads
Anal Biochem., 442(2): 149-157, 2013
- C 57.** Sivakumar D., Gorai B., Sivaraman T.
 Screening efficient BH3-mimetics to hBcl-B by means of peptidodynmimetic method
Mol. Biosyst., 9(4): 700-712, 2013
- C 58.** Edwards B.S., Zhu J., Chen J., Carter M.B., Thal D.M., Tesmer J.J., Graves S..W., Sklar L.A.

Cluster cytometry for high-capacity bioanalysis
Cytometry A., 81(5): 419-429, 2012

T 28. Lewis-Wambi J.S., Kim H., Curpan R., Grigg R., Sarker M.A., Jordan V.C.
The selective estrogen receptor modulator bazedoxifene inhibits hormone-independent breast cancer cell growth and down-regulates estrogen receptor α and cyclin D1
Mol Pharmacol., 80(4): 610-620, 2011

C 59. Palacios S., de Villiers T.J., Nardone Fde C., Levine A.B., Williams R., Hines T., Mirkin S., Chines A.A.

Assessment of the safety of long-term bazedoxifene treatment on the reproductive tract in postmenopausal women with osteoporosis: results of a 7-year, randomized, placebo-controlled, phase 3 study

Maturitas., 76(1): 81-87, 2013

C 60. Segala G., de Medina P., Iuliano L., Zerbinati C., Paillasse M.R., Noguer E., Dalenc F., Payre B., Jordan V.C., Record M., Silvente-Poirot S., Poirot M.

5,6-Epoxy-cholesterols contribute to the anticancer pharmacology of tamoxifen in breast cancer cells

Biochem Pharmacol., 86(1): 175-189, 2013

C 61. Komm B.S., Mirkin S.

Evolution of the tissue selective estrogen complex (TSEC)

J. Cell Physiol., 228(7): 1423-1427, 2013

C 62. Mirkin S., Komm B.S., Pan K., Chines A.A.

Effects of bazedoxifene/conjugated estrogens on endometrial safety and bone in postmenopausal women

Climacteric., 16(3): 338-346, 2013

C 63. Wardell S.E., Nelson E.R., Chao C.A., McDonnell DP.

Bazedoxifene Exhibits Antiestrogenic Activity in Animal Models of Tamoxifen-Resistant Breast Cancer: Implications for Treatment of Advanced Disease

Clin. Cancer Res., 19(9): 2420-2431, 2013

C 64. Burris T.P., Solt L.A., Wang Y., Crumbley C., Banerjee S., Griffett K., Lundasen T., Hughes T., Kojetin D.J.

Nuclear receptors and their selective pharmacologic modulators

Pharmacol. Rev., 65(2): 710-778, 2013

C 65. Wright D.J., Earnhardt J.N., Perry R., Bailey S., Komm B., Minck D.R., Cukierski M.A.

Carcinogenicity and hormone studies with the tissue-selective estrogen receptor modulator bazedoxifene

J. Cell Physiol., 228(4), 724-733, 2013

C 66. Calaf Alsina J., Coronado Martín P.J.

Third generation selective estrogen receptor modulators benefits beyond bone: effects on breast

Med. Clin. (Barc.), 140(5): 217-222, 2013

C 67. Phillips T.A., Fabian C.J., Kimler B.F., Petroff B.K.

Assessment of RNA in human breast tissue sampled by random periareolar fine needle aspiration and ductal lavage and processed as fixed or frozen specimens

Reprod. Biol., 13(1): 75-81, 2013

C 68. Manavathi B., Dey O., Gajulapalli V.N., Bhatia R.S., Bugide S., Kumar R.

Derailed estrogen signaling and breast cancer: an authentic couple

Endocr. Rev., 34(1): 1-32, 2013

- C 69.** Hadji P.
The evolution of selective estrogen receptor modulators in osteoporosis therapy
Climacteric., 15(6): 513-523, 2013
- C 70.** Ethun KF, Wood CE, Register TC, Cline JM, Appt SE, Clarkson TB.
Effects of bazedoxifene acetate with and without conjugated equine estrogens on the breast of postmenopausal monkeys
Menopause, 19(11): 1242-1252, 2012
- C 71.** Jan R., Huang M., Lewis-Wambi J.
Loss of pigment epithelium-derived factor: a novel mechanism for the development of endocrine resistance in breast cancer
Breast Cancer Res., 14(6): R146, 2012
- T 29.** Maximov P.Y., Myers C.B., Curpan R.F., Lewis-Wambi J.S., Jordan V.C.
Structure-function relationships of estrogenic triphenylethylenes related to endoxifen and 4-hydroxytamoxifen
J. Med. Chem., 53(8): 3273-3283, 2010
- C 72.** Gryder B.E., Rood M.K., Johnson K.A., Patil V., Raftery E.D., Yao L.P., Rice M., Azizi B., Doyle D.F., Oyelere A.K.
Histone deacetylase inhibitors equipped with estrogen receptor modulation activity
J. Med. Chem., 56(14): 5782-5796, 2013
- C 73.** Leow M.L., Chin H.L., Yu P.S., Pasunooti K.K., Tay R.X., Zhang D., Yoon H.S., Liu X.W.
Benzofuran-based estrogen receptor α modulators as anti-cancer therapeutics: in silico and experimental studies
Curr. Med. Chem., 20(22): 2820-2837, 2013
- C 74.** Sengupta S., Obiorah I., Maximov P.Y., Curpan R., Jordan V.C.
Molecular mechanism of action of bisphenol and bisphenol A mediated by oestrogen receptor alpha in growth and apoptosis of breast cancer cells
Br. J. Pharmacol., 169(1): 167-178, 2013
- C 75.** Obiorah I., Jordan V.C.
Scientific rationale for postmenopause delay in the use of conjugated equine estrogens among postmenopausal women that causes reduction in breast cancer incidence and mortality
Menopause, 20(4): 372-382, 2013
- C 76.** Shahrokh K., Cheatham T.E. 3rd, Yost G.S.
Conformational dynamics of CYP3A4 demonstrate the important role of Arg212 coupled with the opening of ingress, egress and solvent channels to dehydrogenation of 4-hydroxy-tamoxifen
Biochim. Biophys. Acta., 1820(10): 1605-1617, 2012
- C 77.** Nelson D.J., Shagufta, Kumar R.
Characterization of a tamoxifen-tethered single-walled carbon nanotube conjugate by using NMR spectroscopy
Anal. Bioanal. Chem., 404(3): 771-776, 2012
- C 78.** Keely N.O., Zisterer D.M., Meegan M.J.
Design, Synthesis and Biochemical Evaluation of Estrogen Receptor Ligand Conjugates as Tumour Targeting Agents
Lett. Drug Des. Discov., 9(3): 295-304, 2012
- T 30.** Burai R., Ramesh C., Shorty M., Curpan R., Bologa C., Sklar L.A., Oprea T., Prossnitz E.R., Arterburn J.B.
Highly efficient synthesis and characterization of the GPR30-selective agonist G-1 and related tetrahydroquinoline analogs

Org. Biomol. Chem., 8(9): 2252-2259, 2010

C 79. Jang E.J., Seok Y.M., Arterburn J.B., Olatunji L.A., Kim I.K.

GPER-1 agonist G1 induces vasorelaxation through activation of epidermal growth factor receptor-dependent signalling pathway

J. Pharm. Pharmacol., 65(10): 1488-1499, 2013

C 80. Burai R., Ramesh C., Nayak T.K., Dennis M.K., Bryant B.K., Prossnitz E.R., Arterburn J.B.

Synthesis and characterization of tricarbonyl-Re/Tc(I) chelate probes targeting the G protein-coupled estrogen receptor GPER/GPR30

PLoS One, 7(10): e46861, 2012

C 81. Prakash M., Kesavan V.

Highly enantioselective synthesis of 2,3-dihydroquinazolinones through intramolecular amidation of imines

Org. Lett., 14(7): 1896-1899, 2012

T 31. Haynes M.K., Strouse J.J., Waller A., Leitao A., Curpan R.F., Bologa C., Oprea T.I., Prossnitz E.R., Edwards B.S., Sklar L.A., Thompson T.A.

Detection of intracellular granularity induction in prostate cancer cell lines by small molecules using the hypercyt (r) high-throughput flow cytometry system

J. Biomol. Screen., 14(6): 596-609, 2009

C 82. Edwards B.S., Zhu J., Chen J., Carter M.B., Thal D.M., Tesmer J.J., Graves S.W., Sklar L.A.

Cluster cytometry for high-capacity bioanalysis

Cytometry A., 81(5): 419-429, 2012

T 32. Taboureau O., Nielsen S.K., Audouze K., Weinhold N., Edsgård D., Roque F.S., Kouskoumvekaki I., Bora A., Curpan R., Jensen T.S., Brunak S., Oprea T.I.

ChemProt: a disease chemical biology database

Nucleic Acids Res., 39 (1): D367-D372, 2011

C 83. Audouze K., Brunak S., Grandjean P.

A computational approach to chemical etiologies of diabetes

Scientific Reports, 3, DOI: 10.1038/srep02712, 2013

C 84. Perot S., Regad L., Reynes C., Sperandio O., Miteva M.A., Villoutreix B.O., Camproux A.C.

Insights into an original pocket-ligand pair classification: a promising tool for ligand profile prediction

Plos One, 8(6): e63730, 2013

C 85. Cheng F., Li W., Liu G., Tang Y.

In silico ADMET prediction : recent advances, current challenges and future trends

Curr. Top Med. Chem., 13(11): 1273-1289, 2013

C 86. Csermely P., Korcsmaros T., Kiss H.J., London G., Nussinov R.

Structure and dynamics of molecular networks: A novel paradigm of drug discovery: A comprehensive review

Pharmacol Ther., 138(3): 333-408, 2013

C 87. Kell D.B., Goodacre R.

Metabolomics and systems pharmacology: why and how to model the human metabolic network for drug discovery

Drug Discov. Today, DOI: 10.1016/j.drudis.2013.07.014, 2013

C 88. Kell D.B.

Finding novel pharmaceuticals in the systems biology era using multiple effective drug targets, phenotypic screening and knowledge of transporters: where drug discovery went wrong and how to fix it

FEBS J., 280(23): 5957-5980, **2013**

C 89. Trosset J.Y., Vodovar N.

Structure-based target druggability assessment

Methods Mol. Biol., 986: 141-164, **2013**

C 90. Hekmat O., Munk S., Fogh L., Yadav R., Francavilla C., Horn H., Wurtz S.O., Schrohl A.S., Damsgaard B., Romer M.U., Belling K.C., Jensen N.F., Gromova I., Bekker-Jensen D.B., Moreira J.M., Jensen L.J., Gupta R., Lademann U., Brunner N., Olsen J.V., Stenvang J.

TIMP-1 increases expression and phosphorylation of proteins associated with drug resistance in breast cancer cells

J. Proteome Res., 12(9): 4136-4151, **2013**

C 91. Nicolaes G.A., Kulharia M., Voorberg J., Kaijen P.H., Wroblewska A., Wielders S., Schrijver R., Sperandio O., Villoutreix B.O.

Rational design of small molecules targeting the C2 domain of coagulation factor VIII

Blood., DOI: 10.1182/blood-2013-05-503227, **2013**

C 92. Mpangase P.T., Szolkiewicz M.J., le Grange M., Smit J.H., Burger P.B., Joubert F. Discovery-2: an interactive resource for the rational selection and comparison of putative drug target proteins in malaria.

Malar J., 12(116): 1-9, **2013**

C 93. Smith R.E., Tran K., Vocque R.H.

Network medicine and high throughput screening

Curr. Drug. Discov. Technol., 10(3): 182-194, **2013**

C 94. Seoane J.A., Lopez-Campos G., Dorado J., Martin-Sanchez F.

New approaches in data integration for systems chemical biology

Curr. Top. Med. Chem., 13(5): 591-601, **2013**

C 95. Thun C.-W.

Prediction of non-genotoxic hepatocarcinogenicity using chemical-protein interactions

Pattern Recognition in Bioinformatics (PRIB), LNBI, Springer-Verlag Berlin

Heidelberg, Ngom A. et al., Ed., 7986: 231-241, **2013**

C 96. Azmi A.S.

Adopting network pharmacology for cancer drug discovery

Curr. Drug. Discov. Technol., 10(2): 95-105, **2013**

C 97. Laverty H., Gunn M., Goldman M.

Improving R&D productivity of pharmaceutical companies through public-private partnership: experiences from the innovative medicines initiative

Expert Rev. Pharmacoecon. Outcomes Res., 12(5), 545-548, **2012**

C 98. Kim Kjærulff S., Wich L., Kringleum J., Jacobsen U.P., Kouskoumvekaki I.,

Audouze K., Lund O., Brunak S., Oprea T.I., Taboureau O.

ChemProt-2.0: visual navigation in a disease chemical biology database

Nucleic Acids Res., 41: D464-469, **2013**

T 33. Olah M., Mracec M., Ostropovici L., Rad R., Bora A., Hadaruga N., Olah I., Banda M., Simon Z., Mracec M., Oprea T.I.

WOMBAT: world of molecular bioactivity

Chemoinformatics in Drug Discovery, Wiley-VCH Verlag GmbH & Co. KGaA, Oprea, T.I. Ed., DOI: 10.1002/3527603743.ch9, Vol. 1, **2005**

C 99. Evers A., Hessler G., Wang Li-h., Werrel S., Monecke P., Matter H.

CROSS: an efficient workflow for reaction-driven rescaffolding and sidechain optimization using robust chemical reactions and available reagents

J. Med. Chem., 56(11): 4656–4670, **2013**

C 100. Percha B., Altman R.B.

- Informatics confronts drug-drug interactions
Trends Pharmacol. Sci., 34(3): 178-184, 2013
- C 101.** Wang L., Ma C., Wipf P., Liu H., Su W., Xie X.Q.
TargetHunter: an in silico target identification tool for predicting therapeutic potential of small organic molecules based on chemogenomic database
AAPS J., 15(2): 395-406, 2013
- C 102.** Carrieri A., Perez-Nueno V.I., Lentini G., Ritchie D.W.
Recent trends and future prospects in computational GPCR drug discovery: from virtual screening to polypharmacology
Curr. Top Med. Chem., 13(9): 1069-1097, 2013
- C 103.** Lavecchia A., Di Giovanni C.
Virtual screening strategies in drug discovery: a critical review
Curr. Med. Chem., 20(23): 2839-2860, 2013
- C 104.** Manallack D.T., Prankerd R.J., Nassta G.C., Ursu O., Oprea T.I., Chalmers D.K.
A chemogenomic analysis of ionization constants--implications for drug discovery
Chem. Med. Chem., 8(2): 242-255, 2013
- C 105.** Laufer R., Forrest B., Li S.W., Liu Y., Sampson P., Edwards L., Lang Y., Awrey D.E., Mao G., Plotnikova O., Leung G., Hodgson R., Beletskaya I., Mason J.M., Luo X., Wei X., Yao Y., Feher M., Ban F., Kiarash R., Green E., Mak T.W., Pan G., Pauls H.W.
The discovery of PLK4 inhibitors: (E)-3-((1H-indazol-6-yl)methylene)indolin-2-ones as novel antiproliferative agents
J. Med. Chem., 56(15): 6069–6087, 2013
- C 106.** Mavridis L., Mitchell J.B.
Predicting the protein targets for athletic performance-enhancing substances
J. Cheminform., 5(31):1-13, 2013
- C 107.** Tiikkainen P., Bellis L., Light Y., Franke L.
Estimating error rates in bioactivity databases
J. Chem. Inf. Model., 53(10): 2499–2505, 2013
- C 108.** Flachner B., Tomori T., Hajdu I., Dobi K., Lorincz Z., Cseh S., Dorman G.
Rapid in silico selection of an MCHR1 antagonists' focused library from multi-million compounds' repositories: biological evaluation
Med. Chem. Res., DOI 10.1007/s00044-013-0695-0, 2013
- T34.** Olah M., Rad R., Ostovici L., Bora A., Hadaruga N., Hadaruga D., Moldovan R., Fulias A., Mracec M., Oprea T.I.
WOMBAT and WOMBAT PK: Bioactivity Databases for Lead and Drug Discovery
Chemical Biology: From Small Molecules To Systems Biology And Drug Design, Wiley-VCH, Schreiber S.L., Kapoor T.M., Wees G. Editors, 1-3: 760-786, 2008
- C 109.** Kim Kjærulff S., Wich L., Kringleum J., Jacobsen U.P., Kouskoumvekaki I., Audouze K., Lund O., Brunak S., Oprea T.I., Taboureau O.
ChemProt-2.0: visual navigation in a disease chemical biology database
Nucleic Acids Res., 41: D464-469, 2013
- C 110.** Koutsoukas A., Lowe R., KalantarMotamedi Y., Mussa H.Y., Klaffke W., Mitchell J.B.O., Glen R.C., Bender A.
In silico target predictions: defining a benchmarking data set and comparison of performance of the multiclass naive bayes and parzen-rosenblatt window
J. Chem. Inf. Model., 53(8): 1957–1966, 2013
- C 111.** Petrone P.M., Wassermann A.M., Lounkine E., Kutchukian P., Simms B., Jenkins J., Selzer P., Glick M.
Biodiversity of small molecules: case study to demonstrate a new perspective in screening set selection
Drug Discov. Today, 18(s13–14): 674–680, 2013

C 112. Benet L.Z.

The role of BCS (biopharmaceutics classification system) and BDDCS (biopharmaceutics drug disposition classification system) in drug development

J. Pharm. Sci., 102(1): 34-42, 2013

C 113. Mathias S.L., Hines-Kay J., Yang J.J., Zahoransky-Kohalmi G., Bologa C.G., Ursu O., Oprea T.I.

The CARLSBAD database: a confederated database of chemical bioactivities

Database (Oxford), DOI: 10.1093/database/bat044, 2013

C 114. Liggi S., Drakakis G., Hendry A.E., Hanson K.M., Brewerton S.C, Wheeler G.N., Bodkin M.J., Evans D.A., Bender A.

Extensions to in silico bioactivity predictions using pathway annotations and differential pharmacology analysis: application to *xenopus laevis* phenotypic readouts

Mol. Inform., DOI: 10.1002/minf.201300102, 2013

C 115. Carrieri A., Perez-Nueno V.I., Lentini G., Ritchie D.W.

Recent trends and future prospects in computational GPCR drug discovery: from virtual screening to polypharmacology

Curr. Top Med. Chem., 13(9): 1069-1097, 2013

C 116. Yang K., Kock K., Sedykh A., Tropsha A., Brouwer K.L.

An updated review on drug-induced cholestasis: Mechanisms and investigation of physicochemical properties and pharmacokinetic parameters

J. Pharm. Sci., 102(9): 3037-3057, 2013.

C 117. Kooistra A.J., Leurs R., de Esch I.J., de Graaf C.

From three-dimensional GPCR structure to rational ligand discovery

Adv. Exp. Med. Biol., 796: 129-157, 2014

C 118. Hu Y., Bajorath J.

Compound promiscuity—what can we learn from current data?

Drug Discov. Today., 18(13-14): 644-50, 2013

C 119. Singla D., Dhanda S.K., Chauhan J.S., Bhardwaj A., Brahmachari S.K.

Open source software and web services for designing therapeutic molecules

Curr. Top Med. Chem., 13(10): 1172-1191, 2013

C 120. Hess S.

The emerging field of chemo- and pharmacoproteomics

Proteomics Clin Appl., 7(1-2): 171-180, 2013

T 35. Kurunczi L., Funar-Timofei S., Bora A., Seclaman E.

Application of the MTD-PLS method to heterocyclic dye-cellulose interactions

Int. J. Quant. Chem., 107 (11): 2057-2065, 2007

C 121. Schafer K.N., Cisek K., Huseby C.J., Chang E., Kuret J.

Structural determinants of Tau aggregation inhibitor potency

J. Biol. Chem., 288(45): 32599-32561, 2013

C 122. Luan F., Xu X., Liu H., Dias Soeiro Cordeiro M.N.

Review of quantitative structure-activity/property relationship studies of dyes: recent advances and perspectives

Coloration Technol. 129(3): 173-186, 2013.

T 36. Pacureanu L., Simon Z.

DFT Plus PCM Calculation for Pairing Specificity of Watson-Crick-Type Bases in Aqueous Solutions

Int. J. Quant. Chem. 110(6), 1295-1305, 2010.

- C 123.** Zhang Y.C., Liang J., Lian P., Han Y., Chen Y., Bai L., Wang Z., Liang J., Deng Z., Zhao Y.L.
Theoretical Study on Steric Effects of DNA Phosphorothioation: B-Helical Destabilization in Rp-Phosphorothioated DNA
J. Phys. Chem. B, 116(35), 10639-10648, **2012**.
- T 37.** Katritzky A.R., Pacureanu L.M., Slavov S.H., Dobchev D.A., Karelson M.
QSPR study of the first and second critical micelle concentrations of cationic surfactants
Comput. Chem. Eng. 33(1), 321-332, **2009**.
- C 124.** Olson M.A., Thompson J.R., Dawson T.J., Hernandez C.M., Messina M.S., O'Neal T.
Template-directed self-assembly by way of molecular recognition at the micellar-solvent interface: modulation of the critical micelle concentration
Org. Biomol. Chem. 11(38), 6483-6492, **2013**.
- C 125.** Taha A.A., Rahman H H.A., Ahmed A.M., Abouzeid F.M.
A Study of Factors Influencing on Dissolution Behavior of Copper in Orthophosphoric Acid Using Rotating Cylinder Electrode (RCE) and Rotating Disc Electrode (RDE)
Int. J. Electrochem. Sci. 8(7), 9041-9059, **2013**.
- C 126.** Tian F., Wu J., Huang N., Guo T., Mao C.
The critical aggregation concentration of peptide surfactants is predictable from dynamic hydrophobic property
SAR & QSAR Environ. Res. 24(2), 89-101, **2013**.
- C 127.** Zhu Zhi-Chen; Wang Qiang; Jia Qing-Zhu; Tang H.M., Ma P.S.
Quantitative Structure-Property Relationship of the Critical Micelle Concentration of Different Classes of Surfactants
Acta Phys.-Chim. Sin. 29(1), 30-34, **2013**.
- C 128.** Creton B., Nieto-Draghi C., Pannacci N.
Prediction of Surfactants' Properties using Multiscale Molecular Modeling Tools: A Review
Oil & Gas Science and Technology – Revue d'IFP Energies nouvelles 67(6), 969-982, **2012**.
- T 38.** Katritzky A.R., Pacureanu L.M., Slavov S.H., Dobchev D., Karelson M.
QSPR Study of Critical Micelle Concentrations of Nonionic Surfactants
Ind. & Eng. Chem. Res. 47(23), 9687-9695, **2008**.
- C 129.** Mattei, Michele; Kontogeorgis, Georgios M.; Gani, Rafiqul
Modeling of the Critical Micelle Concentration (CMC) of Nonionic Surfactants with an Extended Group-Contribution Method
Ind. & Eng. Chem. Res. 52(34), 12236-12246, **2013**.
- C 130.** Yu, Guangren; Wen, Lu; Zhao, Dachuan; Asumana C., Chen X.
QSPR study on the viscosity of bis(trifluoromethylsulfonyl)imide-based ionic liquids
J. Mol. Liq. 184, 51-59, **2013**.
- C 131.** Micellar and Interfacial Behavior of Cationic Benzalkonium Chloride and Nonionic Polyoxyethylene Alkyl Ether Based Mixed Surfactant Systems
Nandni, Durgesh; Mahajan, Rakesh Kumar
J. Surfactants Deterg. 16(4), 587-599, **2013**.
- C 132.** Tian F., Wu J., Huang N., Guo T., Mao C.
The critical aggregation concentration of peptide surfactants is predictable from dynamic hydrophobic property
SAR QSAR Environ. Res. 24(2), 89-101, **2013**.

- C 133.** Creton, B.; Nieto-Draghi, C.; Pannacci, N.
 Prediction of Surfactants' Properties using Multiscale Molecular Modeling Tools: A Review
Oil & Gas Science and Technology – Revue d'IFP Energies nouvelles 67(6), 969-982, 2012.
- T 39.** Katritzky, A.R.; Pacureanu, L., Dobchev, D., Karelson M.
 QSPR modeling of hyperpolarizabilities
J. Mol. Model. 13(9): 951-963, 2007
- C 134.** Shariati-Rad, M., Hasani M.
 Linear and nonlinear quantitative structure-property relationships modeling of charge-transfer complex formation of organic donors with iodine and iodine monochloride using partial least squares and radial basis function-partial least squares
J. Iran. Chem. Soc. 10(6), 1247-1256, 2013.
- C 135.** Alparone, A.
 Nonlinear optical properties of fluorobenzenes: A Time-Dependent Hartree-Fock study
Comput. Theor. Chem. 1013, 23-24, 2013.
- C 136.** Sousa, Ines J.; Ferreira, Maria-Jose U.; Molnar, Joseph; et al.
 QSAR studies of macrocyclic diterpenes with P-glycoprotein inhibitory activity
Eur. J. Pharm. Sci., 48(3), 542-553, 2013.
- C 137.** Alparone, A.
 Dipole (hyper)polarizabilities of fluorinated benzenes: An ab initio investigation
J. Fluorine Chem. 144, 94-101, 2012.
- T 40.** Katritzky A.R., Pacureanu L., Dobchev D.A., Karelson M.
 QSPR Study of Critical Micelle Concentration of Anionic Surfactants Using Computational Molecular Descriptors
J. Chem. Inf. Model., 47 (3):782–793, 2007
- C 138.** Roy K., Kabir H.
 QSPR with extended topochemical atom (ETA) indices: Exploring effects of hydrophobicity, branching and electronic parameters on logCMC values of anionic surfactants
Chem. Eng. Sci. 87, 141-151, 2013.
- C 139.** Zhu Zhi-Chen; Wang Qiang; Jia Qing-Zhu; Tang H.M., Ma P.S.
 Quantitative Structure-Property Relationship of the Critical Micelle Concentration of Different Classes of Surfactants
Acta Phys.-Chim. Sin. 29(1), 30-34, 2013.
- C 140.** Creton B., Nieto-Draghi C., Pannacci N.
 Prediction of Surfactants' Properties using Multiscale Molecular Modeling Tools: A Review
Oil & Gas Science and Technology – Revue d'IFP Energies nouvelles 67(6), 969-982, 2012.
- T 41.** Katritzky A.R., Pacureanu L., Slavov S., Dobchev D.A., Karelson M.
 QSAR study of antiplatelet agents
Bioorg. Med. Chem., 14(22): 7490-7500, 2006
- C 141.** Zhan S., Huang J., Shao Q. et al.
 Prediction of Microdialysis Relative Recovery of Flavone Derivatives Based on Molecular Descriptors
J. Braz. Chem. Soc., 23(11), 2035-2042, 2012.

T 42. Katritzky A.R., Pacureanu L., Dobchev D.A., Fara D.C., Duchowicz P.R., Karelson M.

QSAR Modeling of the Inhibition of Glycogen Synthase Kinase-3

Bioorg. Med. Chem., 14(14): 4987-5002, 2006.

C 142. Yu, Guangren; Wen, Lu; Zhao, Dachuan; Asumana C., Chen X.

QSPR study on the viscosity of bis(trifluoromethylsulfonyl)imide-based ionic liquids

J. Mol. Liq. 184, 51-59, 2013.

C 143. Long W., Zhang X.D., Wang H., Shen X., Si, H.Z., Fan S.J., Zhou Z.W., Liu P.X.
Prediction of Enhancement Effect of Nitroimidazoles on Irradiation by Gene Expression
Programming

Chem. Res. Chin. Univ. 29(3), 519-525, 2013.

T 43. Avram S., Pacureanu L.M., Seclaman E., Bora A., Kurunczi L.

PLS-DA-Docking optimized combined energetic terms (plsda-docet) protocol: a brief
evaluation

J. Chem. Inf. Model. 51(12), 3169-3179, 2011

C 144. Yuriev E., Ramsland P.A.

Latest developments in molecular docking: 2010–2011 in review

J. Mol. Recognit. 26(5), 215-239, 2013

T44: Fagadar-Cosma E., Cseh L., Badea V., Fagadar-Cosma G., Vlascici D.

Combinatorial synthesis and characterization of new asymmetric Porphyrins as potential
Photosensitizers in photodynamic therapy

Comb. Chem. High T. Scr. 10(6): 466-472, 2007

C145: Guo L., Fu L., Ferreira R.A.S., Carlos L.D., Yan B.

Photofunctional hybrid silica microspheres covalently functionalized with
metalloporphyrins

J. Solid State Chem. 194: 9-14, 2012

T45: Făgădar-Cosma E., Vlascici D., Făgădar-Cosma G., Bizerea O., Chiriac A.

The study of the electrochemical behaviour of metalo-porphyrins with Co(II) and Co(III).
Nitrite-selective electrode based on [5,10,15,20-tetraphenyl-21H, 23H-porphyrinato-N21,
N22, N23, N24] Co(III) chloride

Rev. Chim. 55(11): 882-885, 2004

C146: Poursaberi T., Ganjali M.R., Hassanasadi M.

A novel fluoride-selective electrode based on metalloporphyrin grafted-grapheneoxide

Talanta 101: 128-134, 2012

C147: Poursaberi T., Ghadernia S., Hassanasadi M., Torkestani K., Mirrahimi M.

Efficient separation of nitrite from aqueous solutions by grafting metalloporphyrin on
 Fe_3O_4 nanoparticles

J. Iran. Chem. Soc., 10(1): 13-20, 2013.

C148: Poursaberi T., Karimi M., Hassanasadi M., Sereshti H.

Magnetic removal of nitrate ions from aqueous solution using amino-silica coated
magnetic nanoparticles modified by oxovanadium(IV) porphyrin

J. Porphyr. Phthalocya. 17(5): 359-366 2013.

T46: Fagadar-Cosma E., Enache C., Tudose R., Armeanu I., Mosoarca E., Vlascici D., Costisor O.

UV-VIS and fluorescence spectra of meso-tetraphenylporphyrin and meso-tetrakis-(4-methoxyphenyl) porphyrin in THF and THF-water systems. The influence of pH.

Rev. Chim. 58(5): 451-455, 2007.

C149: Pinto S.M.A., Neves A.C.B., Calvete M.J.F., Abreu A.R., Rosado M.T.S., Costa T., Burrows H.D., Pereira M.M.

Metalloporphyrin triads: Synthesis and photochemical characterization

J. Photochem. Photobiol. A. 242: 59-66, 2012.

T47: Vlascici D., Pruneanu S., Olenic L., Pogacean F., Ostafe V., Chiriac V., Pica E.M., Bolundut L.C., Nica L., Fagadar-Cosma E.

Manganese(III) porphyrin-based potentiometric sensors for diclofenac assay in pharmaceutical preparations

Sensors 10(10): 8850-8864, 2010.

C150: Singh A.K., Bandi K.R., Upadhyay A., Jain A.K.

A comparative study on fabrication of Mn²⁺ selective polymeric membrane electrode and coated graphite electrode

Mater. Sci. Eng. C 33(2): 626-633, 2013

C151: Rada M., Bolundut L., Pica M., Zagrai M., Rada S., Culea E.

Mixed ionic-electronic conduction and electrochemical behavior of the lead and molybdenum ions in the lead-molybdate-germanate glasses

J. Non-Cryst. Solids 365(1): 105-111, 2013

C152: Lvova L., Di Natale C., Paolesse R.

Porphyrin-based chemical sensors and multisensor arrays operating in the liquid phase

Sensor. Actuat. B-Chem. 179: 21-31, 2013

T48: Fagadar-Cosma E., Mirica M.-C., Balcu I., Bucovicean C., Cretu C., Armeanu I., Fagadar-Cosma G.

Syntheses, spectroscopic and AFM characterization of some manganese porphyrins and their hybrid silica nanomaterials

Molecules 14(4): 1370-1388, 2009

C153: Lata B.S., Sudha Y.

Some Mn-III-porphyrins with de-polymerization activity toward humic acid

J. Coord. Chem. 65(19): 3492-3501 2012.

C154: Simandan I.D., Popescu M., Antohe S.

Stabilized langmuir layers based on silver stearate, carbon nanotubes and porphyrins additives for UV-sensor applications

Optoelectron. Adv. Mater. Rapid Comm. 6(11-12): 1164-1167, 2012

C155: Chung S.-G., Chang Y.-S., Choi J.-W., Baek K.-Y., Hong S.-W., Yun S.-T., Lee S.-H

Photocatalytic degradation of chlorophenols using star block copolymers: Removal efficiency, by-products and toxicity of catalyst

Chem. Eng. J. 215-216: 921-928, 2013

T49. Şimăndan I.D., Popescu M., Lorinczi A., Velea A., Fagadar-Cosma E.

Preparation and properties of barium stearate multilayers with carbon nanotubes, manganese porphyrin and silver nitrate

Digest J. Nanomater. Bios. 5(4): 1029-1033, 2010

C156: Simandan I.D., Popescu M., Antohe S.

Stabilized langmuir layers based on silver stearate, carbon nanotubes and porphyrins additives for UV-sensor applications

T50. Vlascici D., Fagadar-Cosma E., Popa I., Chiriac V., Gil-Agusti M.
A Novel Sensor for Monitoring of Iron(III) Ions Based on Porphyrins

Sensors 12(6): 8193-8203, 2012

C157. Lv Y., Cao M., Li J., Wang J.
A sensitive ratiometric fluorescent sensor for Zinc(II) with high selectivity
Sensors 13(3): 3131-3141, 2013

T51. Vlascici D., Cosma E.F., Pica E.M., Cosma V., Bizerea O., Mihailescu G., Olenic L.
Free base porphyrins as ionophores for heavy metal sensors

Sensors 8(8): 4995-5004, 2008

C158. Lvova L., Galloni P., Floris B., Lundström I., Paolesse R., Di Natale C.
A Ferrocene-porphyrin ligand for multi-transduction chemical sensor development

Sensors 13(5): 5841-5856, 2013

C159. Bajju G.D., Devi G., Katoch S., Bhagat M., Deepmala Ashu Kundan S., Anand S.K.
Synthesis, spectroscopic, and biological studies on new zirconium(IV) porphyrins with axial ligand

Bioinorg. Chem. Appl. 903616, 2013

T52. Grama S., Hurdic N., Fagadar-Cosma E., Vasile M., Tarabukina E., Fagadar-Cosma G.

Novel porphyrin-based polysiloxane micromaterial

Digest J. Nanomater. Bios. 4: 959-973, 2010

C160. Garg K., Singh A., Majumder C., Nayak S.K., Aswal D.K., Gupta S.K., Chattopadhyay S.

Room temperature ammonia sensor based on jaw like bis-porphyrin molecules

Org. Electron. phys. mater. appl. 14(4): 1189-1196, 2013

T53. Fagadar-Cosma E., Vlascici D., Fagadar-Cosma G.

Monomer and Sandwich Type Dimmer Complexes of Zr (IV) with Meso-tetraphenylporphyrin. Synthesis and Comparative IR, UV-vis and HPLC Behavior

Proceedings of the 12th Symposium on Analytical and Environmental Problems, Szeged, 25-29, 2005

C161. Bajju G.D., Devi G., Katoch S., Bhagat M., Deepmala Ashu Kundan S., Anand S.K.
Synthesis, spectroscopic, and biological studies on new zirconium(IV) porphyrins with axial ligand

Bioinorg. Chem. Appl. art. no. 903616, 2013

T54. Vlascici D., Bizerea-Spiridon O., Fagadar-Cosma E.

Metalloporphyrin Based Fluoride-selective Electrode

Proceedings of the 13th Symposium on Analytical and Environmental Problems, Szeged, 92-95, 2006

C162. Bajju G.D., Devi G., Katoch S., Bhagat M., Deepmala Ashu Kundan S., Anand S.K.
Synthesis, spectroscopic, and biological studies on new zirconium(IV) porphyrins with axial ligand

Bioinorg. Chem. Appl. art. no. 903616, 2013

T55. Fagadar-Cosma E., Enache C., Vlascici D., Fagadar-Cosma G., Vasile M., Bazylak G.

Novel nanomaterials based on 5,10,15,20-tetrakis(3,4-dimethoxyphenyl)-21H,23H-porphyrin entrapped in silica matrices

Mat. Res. Bull. 44(12):2186-2193, 2009

C163. RECENZIE ARTICOL

Biological Pigments: Advances in Research and Application: 2011 Edition
ScholarlyEditions, Atlanta, Georgia, SUA, 2012, ISBN 978-1-464-92212-1
www.ScholarlyEditions.com

T56. Popescu M., Simandan I.D., Sava F., Velea A., Fagadar-Cosma E.
Sensor of nitrogen dioxide based on single wall carbon nanotubes and manganese-porphyrin

Digest J. Nanomater. Bios. (3) 1253-1256, 2011

C164. Jahangirian H., Shah Ismail M.H., Jelas Haron M., Rafiee-Moghaddam R., Shameli K.

Hosseini S., Kalantari K., Soltaninejad S.

Synthesis and characterization of zeolite/Fe₃O₄ nanocomposite by green quick precipitation method

Digest J. Nanomater. Bios. 8 (4): 1405-1413 2013

T57. Lascu A., Sisu I., Bercean V., Lupea A.X., Caproiu M.T., Sisu E.
Mild and efficient method to obtain glycosyl sulfones of mercaptotriazole

Rev. Roum. Chim. 55(3): 205-210, 2010

C165. El-Ebary, N.M.A., El-Telbani, E.M., Swellem, R.H., Zeid, I.F., Nawwar, G.A.M.
Design, synthesis, crystal structure, and antimicrobial evaluation of novel pyrazolyl-1,3,5-oxadiazoles, pyrazolyl-1,2,4-triazoles and their related thioglycosides

Lett. Drug Des. Discov. 10(5): 444-452, 2013

T58. Sisu E., Neanu C., Sisu I., Lascu A., Caproiu M.T., Francisc P., Csunderlik C., Rusu V.

Pseudo-keramides and their derivatives. 1. Isopropylidene acetals of N-acetyl-N-methyl glucamine - Preliminary study

Rev. Chim. Buc. 53(11): 750-754, 2002

C166: Rafailă, M., Pascariu, M.-C., Gruia, A., Penescu, M., Purcarea, V.L., Medeleanu, M.,

Rusnac, L.-M., Davidescu, C.

GC-MS analysis of long chain mannofuranose derivatives as biocompatible surfactant precursors. Correlation between peak intensities and stability of corresponding fragments

Farmacia 61(1): 116-126, 2013

T59. Ilia G.

Phosphorus containing hydrogels

Polym. Advanced Techn. 20(9): 707-722, 2009.

C167. Ün Ş.S., Özcan E., Uslu A., Yokes F., Kılıç A.

Cyclotriphosphazene derivatives with three different chiral centres: Synthesis, characterization and investigation of their stereogenic properties

Polyhedron 62: 250-259, 2013.

T60. Vlase T., Vlase G., Doca N., Ilia G., Fulias A.

Coupled thermogravimetric-IR techniques and kinetic analysis by non-isothermal decomposition of Cd²⁺ and Co²⁺ vinyl-phosphonates.

J. Therm. Anal. Calorim. 97(2): 467-472, 2009.

C168. Fulias A., Vlase G., Grigorie C., Ledeți I., Albu P., Bilanin M., Vlase T.

Thermal behaviour studies of procaine and benzocaine: Part 1. Kinetic analysis of the active substances under non-isothermal conditions

J. Therm. Anal. Calorim. 113(1): 265-271, 2013.

C169. Fuliaş A., Vlase G., Vlase T., Soica C., Heghes A., Craina M., Ledeti I.

Comparative kinetic analysis on thermal degradation of some cephalosporins using TG and DSC data

Chem. Cent. J. 7(1): art. no. 70, 2013.

T61. Ilia G., Parvulescu V., Popa A., Iliescu S.

Organic-inorganic hybrids containing phosphonate groups obtained by sol-gel process

J. Optoelectron. Adv. M. 10(12): 3398-3402, 2008.

C170. Al-Othman A., Tremblay A.Y., Pell W., Letaief S., Liu Y., Peppley B.A., Ternan M.

A modified silicic acid (Si) and sulphuric acid (S)-ZrP/PTFE/glycerol composite membrane for high temperature direct hydrocarbon fuel cells

J. Power Sources 224: 158-167, 2013.

T62. Ilia G., Iliescu S., Popa A.

A new method for the synthesis of triaryl phosphates

Green Chem. 7(4): 217-218, 2005.

C171. Li X., Jia X., Li J.

Applications and process in the synthesis of triphenyl phosphate

Speciality Petrochem. 30(4): 83-86, 2013.

T63. Ilia G., Popa A., Iliescu S., Bora A., Dehelean G., Pascariu A.

Synthesis of mixed alkylphosphites and alkylphosphates

Phosphorus Sulfur 178(7): 1513-1519, 2003.

C172. Kotlarska J., Binnemans K., Dehaen W.

A convenient two-step synthesis of dialkylphosphate ionic liquids

Tetrahedron 69(47): 9947-9950, 2013.

T64. Ioitescu A., Vlase G., Vlase T., Ilia G., Doca N.

Synthesis and characterization of hydroxyapatite obtained from different organic precursors by sol-gel method

J. Therm. Anal. Calorim. 96(3): 937-942, 2009.

C173. Sadat-Shojaei M., Khorasani M-T., Dinpanah-Khoshdargi E.

Synthesis methods for nanosized hydroxyapatite with diverse structures

Acta Biomat. 9(8): 7591-7621, 2013.

T65. Ilia G., Drehe M.

Grafted 2-chloroethylphosphonic acid on inorganic supports used as flame retardant for unsaturated polyester resins

Fire Mater. 34(6): 271-283, 2010.

C174. Guerrero G., Alauzun J.G., Granier M., Laurencin D., Mutin PH.

Phosphonate coupling molecules for the control of surface/interface properties and the synthesis of nanomaterials

Dalton Trans. 42(35): 12569-12585, 2013.

T66. Ilia G., Macarie L., Balint E., Keglevich G.

Phase Transfer Catalysis in Phosphorus Chemistry

Cat. Rev. - Sci. Eng. 53(2): 152-198, 2011.

C175. Keglevich G., Gruen A., Balint E.
Microwave Irradiation and Phase Transfer Catalysis in C-, O- and N-Alkylation Reactions
Curr. Org. Synth. 10(5): 751-763, **2013**.

T67. Petric M., Grozav M., Ilia G.,
Boron phosphate flame-retardant for certain resins
Rev. Chim. 61(12):1183-1185, **2010**.

C176. Çakmakçı E., Güngör A.,
Preparation and characterization of flame retardant and proton conducting boron
phosphate/polyimide composites
Polym. Degrad. Stabil. 98 (5): 927-933, **2013**.

C177. Karacan I., Soy T.
Structure and properties of oxidatively stabilized viscose rayon fibers impregnated with
boric acid and phosphoric acid prior to carbonization and activation steps
J. Mater. Sci. 48(5): 2009-2021, **2013**.

T68. Micle A., Miklášova N., Varga R., Pascariu A., Pleșu N., Petric M., Ilia G.,
A versatile synthesis of a new bisiminophosphorane
Tetrahedron Lett. 50(40): 5622-5624, **2009**.

C178. Xu L., Yue F., Shi W. , Hui Y., Mi H., Ma F., Tian Y., Xie Z.
A type of novel fluorescent phosphinimine derivative: Catalyst-free simple synthesis and
optical properties
Dyes Pigments 99(3): 822-828, **2013**

T69. Chumakov Y.M., Smirnov, Y.A., Grozav M., Crisan, M., Bocelli G., Yakovenko
A.A., Lyubetsky D.
Hydrogen-bonding network in the organic salts of 4-nitrobenzoic acid
Cent. Eur. J. Chem. 4(3): 458-475, **2006**

C179. Kizas C.M., Papatriantafyllopoulou C., Pissas M., Sanakis Y., Javed
A., Tasiopoulos A.J., Lampropoulos C.
Synthesis, magnetic and spectroscopic characterization of a new Fe₇ cluster with a six-
pointed star topology
Polyhedron 64: 280-288, **2013**

T70. Hora S., Simu G., Rad R., Popa A., Milos M.
The utilization of some functionalized polymers containing captive dyes for the separation
of Cu(II) and Zn(II) ions from aqueous solutions
Rev. Chim. Buc. 55(12): 948-951, **2004**

C180. Al-Karam U.F., de Namor A.F.D., Derwish G.A.W., Al-Dujaili A.H.
Removal of chromium, copper, cadmium and lead ions from aqueous solutions by
diatomaceous earth
Environ. Eng. Manage. J., 11(4), 813-821, **2012**

C181. Abdulla N.I., Al-Haidary A.M.A., Al-Jeboori M.I., Zanganah F.H.H., Al-Azawi
S.R.F. Al-Dujaili A.H.
Kinetics and equilibrium Adsorption study of lead (II) onto low cost clays
Environ. Eng. Manage. J. 12(3): 483-491, **2013**

T71. Popa A., Muntean S.G., Paska O.M., Iliescu S., Ilia G., Zhang Z.
Resins containing α -hydroxyphosphonic acid groups used for adsorption of dyes from
wastewater
Polym. Bull., 66(3): 419-432, **2011**

C182. Davidescu, C.-M., Ciopec, M., Negrea, A., Popa, A., Lupa, L., Dragan, E.-S., Ardelean, R., Ilia G., Iliescu, S.

Synthesis, characterization, and Ni(II) ion sorption properties of poly(styrene-co-divinylbenzene) functionalized with aminophosphonic acid groups

Polym. Bull. 70(1): 277-291, **2013**

T72. Plesu N., Kellenberger A., Mihali M., Vaszilcsin N.

Effect of temperature on the electrochemical synthesis and properties of polyaniline films
J. Non-Cryst. Solids 356(20-22): 1081-1088, **2010**.

C183. Brancewicz E., Gradzka E., Winkler K.

Comparison of electrochemical properties of two-component C-60-Pd polymers formed under electrochemical conditions and by chemical synthesis

J. Solid State Electrochem. 17(4): 1233-1245, **2013**.

C184. Wei H., Zhu J., Wu S., Wei, S.Y., Guo Z.H.

Electrochromic polyaniline/graphite oxide nanocomposites with endured electrochemical energy storage

Polymer 54(7): 1820-1831, **2013**.

T73. Piticescu R.M., Buruiana T., Plesu N., Vasile E., Moldovan C., Fartat B., Rusti C.
Soft chemical methods integration with micro fabrication in developing new scaffolds for tissue engineering

Optoelectron Adv. Mat., 4(3): 401-406, **2010**

C185. Popescu L.M., Rusti C.F., Piticescu, R.M., Buruiana T., Valero T., Kintzios S.,
Synthesis and characterization of acid polyurethane-hydroxyapatite composites for biomedical applications

J. Compos Mater. 47(5): 603-612, **2013**

C186. Tardei C., Spataru M., Albu F.M., Stoleriu S., Ioncea A.

Fabrication and characterization of porous tri-calcium phosphate ceramic microspheres

Rom. J. Mat. 43(1): 41-47, **2013**

T74. Plesu N., Ilia G., Sfirloaga P., Iliescu S.

Organic-inorganic hybrids obtained by in situ polymerization of aniline in silica/phosphonate matrix

J. Mater Sci., 44 (23): 6437-6446, **2009**

C187. Kannusamy P., Sivalingam T.

Chitosan-ZnO/polyaniline hybrid composites: Polymerization of aniline with chitosan-ZnO for better thermal and electrical property

Polym. Degrad. Stability 98(5): 988-996, **2013**

T75. Vlase G., Vlase T., Doca N., Perta M., Ilia G., Plesu N.

Thermal behavior of a sol-gel system containing aniline and organic phosphonates

J. Therm. Anal. Calorim. 97(2): 473-478, **2009**

C188. Mohammad A, Inamuddin, Amin A, Naushad Mu, El-Desoky G E,
Nicotinic acid adsorption thermodynamics study on carboxymethyl cellulose Ce(IV)
molybdochosphate composite cation-exchanger

J. Therm. Anal. Calorim. 111(1): 831-838, **2013**

T76. Plesu N., Grozav I., Iliescu S., Ilia G.

Acrylic blends based on polyaniline. Factorial design

Synth. Met. 159(5-6): 501-507, **2009**

C189. Arujo J.R., Aamo C.B., Costa e Silva M.V, De Paoli M-A
Antistatic-reinforced biocomposites of polyamide-6 and polyaniline-coated curaua fibers prepared on a pilot plant scale
Polym. Composites 34(7): 1081-1090, **2013**

T77. Plesu N., Ilia G., Pascariu A., Vlase G.
Preparation, degradation of polyaniline doped with organic phosphorus acids and corrosion essays of poly aniline-acrylic blends
Synth. Met. 56(2-4): 230-238, **2006**

C190. Jaymand M.
Recent progress in chemical modification of polyaniline
Progress Polym. Sci. 38(9): 1287-1306, **2013**

C191. Zhang H.-M, Wang X.-H.
Eco-friendly water-borne conducting polyaniline
Chin. J. Polym. Sci. 31(6): 853-869, **2013**

C192. Bagheri H., Ayazi, Z., Naderi M.
Conductive polymer-based microextraction methods: A review
Anal.Chimica Acta 767: 1-13, **2013**

C193. Graillot A., Monge S., Faur C., Bouyer D., Robin J.J.
Synthesis by RAFT of innovative well-defined (co) polymers from a novel phosphorus-based acrylamide monomer
Polym. Chem., 4(3): 795-803, **2013**

T78. Plesu N., Kellenberger A., Vaszilcsin N., Manoviciu I.
Electrochemical polymerisation of aniline on skeleton nickel electrodes
Mol. Cryst. Liquid Cryst. 416: 127-135, **2004**.

C194. Abaci U., Guney H., Y., Kadiroglu U.
Morphological and electrochemical properties of PPy, PAni bilayer films and enhanced stability of their electrochromic devices (PPy/PAni-PEDOT, PAni/PPy-PEDOT)
Electrochim. Acta 96: 214-224, **2013**.

T79. Iliescu S., Avram E., Pascariu A., Plesu N., Popa A., Ilia G.
New technique for the synthesis of polyphosphoesters
Macromol. Res. 19(11): 1186-1191, **2011**

C195. Kaniappan K., Murugavel S., Chandrasekaran T., Thangaian D.
Synthesis and properties of few polyphosphonate derivatives containing photosensitive unsaturated keto group in the main chain
Macromol. Res. 21(10): 1045-1053, **2013**

T80. Iliescu S., Grozav I., Funar-Timofei S., Plesu N., Popa A., Ilia G.
Optimization of synthesis parameters in interfacial polycondensation using design of experiments
Polym. Bul. 64(3): 303-314, **2010**

C196. Jelmy E.J., Ramakrishnan S., Devanathan S. Rangarajan M., Kothurkar N, K.
Optimization of the conductivity and yield of chemically synthesized polyaniline using a design of experiments
J. Appl. Polym. Sci. 130(2): 1047-1057, **2013**

T81. Iliescu S., Pascariu A., Plesu N., Popa A., Macarie L., Ilia G.
Unconventional method used in synthesis of polyphosphoesters
Polym. Bull. 63: 485-495, **2009**

C197. Troev K.D.

Poly[alkylene (arylene) phosphate]s

Polyphosphoesters: chemistry and application, Elsevier, 129-261, **2012** (neraportata in 2012)

C198. Troev K.D.

Poly[alkylene (arylene) phosphate]s

Polyphosphoesters: chemistry and application, Elsevier, 263-320, **2012** (neraportata in 2012)

T82. Iliescu S., Ilia G., Pascariu A., Popa A., Plesu N.

Novel synthesis of phosphorus containing polymers under inverse phase transfer catalysis,
Polymer 47(19): 6509-6512, **2006**

C199. Troev K.D.

Poly[alkylene (arylene) phosphate]s

Polyphosphoesters: chemistry and application, Elsevier, 129-261, **2012** (neraportata in 2012)

T83. Funar-Timofei S., Kurunczi L, Iliescu S.

Structure-property study of some phosphorus-containing polymers by computational methods

Polym. Bull. 54(6): 443-449, **2005**

C200. Mallakpour S. Hatami M., Golmohammadi H.

QSPR prediction of thermal decomposition property of non-vinyl polymers having alpha-amino acids moieties

Polym. Bull. 70(2): 715-732, **2013**

T84. Iliescu S., Ilia G., Popa A.

Phase transfer catalysis in the synthesis of phosphorus-containing polymers

J. Serb. Chem. Soc. 70(7): 951-956, **2005**

C201. Troev K. D.

Poly[alkylene (arylene) phosphate]s

Polyphosphoesters: chemistry and application, Elsevier, 263-320, **2012** (neraportata in 2012)

T85. Iliescu S., Ilia G., Dehelean G., Popa A.

New polyphosphonates obtained by vapor-liquid interfacial polycondensation

Polym. Bull. 48: 451-458, **2002**

C202. Troev K.D.

Poly[alkylene (arylene) phosphate]s

Polyphosphoesters: chemistry and application, Elsevier, 268-328, **2012** (neraportata in 2012)

T86. Iliescu S., Ilia G., Popa A., Dehelean G., Macarie L., Pacureanu, L.

The study of the vapor-liquid interfacial polycondensation of the cyclohexylphosphonic dichloride with bisphenol A. The influence of temperature, reaction time, base concentration and molar ratio on yield inherent viscosity and molecular weight.

Polym. Bull. 46: 165-174, **2001**

C203. Troev K.D.

Poly[alkylene (arylene) phosphate]s

Polyphosphoesters: chemistry and application, Elsevier, 260-320, **2012** (neraportata in 2012)

- T87.** Ciopec M., Davidescu C. M., Negrea, A. I. Grozav, L. Lupa, P. Negrea, A. Popa Adsorption studies of Cr(III) ions from aqueous solutions by DEHPA impregnated onto Amberlite XAD7-Factorial design analysis
Chem. Eng. Res. Des. 90(10): 1660-1670, **2012**
- C204.** Ahmed M. A., Ali S. M., El-Dek S. I.
Magnetite-hematite nanoparticles prepared by green methods for heavy metal ions removal from water
Mat. Sci. Eng. B-Solid 178(10): 744-751, **2013**
- C205.** Hua C.J., Tao X.H., Xu G.H.
Preparation, characterization and adsorption properties of a novel 3-aminopropyltriethoxysilane functionalized sodium alginate porous membrane adsorbent for Cr(III) ions
J. Hard. Mater. 248: 285-294, **2013**
- T88.** Buruiana L.-I., Avram E. ; Popa A., Ioan S.
Electrical conductivity and optical properties of a new quaternized polysulfone
Polym. Bull. 68(6): 1641-1661, **2012**
- C206.** Dizman C., Tasdelen M.A., Yagci Y.
Recent advances in the preparation of functionalized polysulfones
Polym. Int. 62(7): 991-1007, **2013**
- T89.** Ciopec M., Davidescu C. M., Negrea A., Grozav I., Lupa L., Muntean C., Negrea P., Popa A. Statististical optimization of chromium ions adsorption on DEHPA-impregnated Amberlite XAD
Env. Eng. Manag. J. 11(3): 525-531, **2012**
- C207.** Modrogean C., Apostol D. Giani, Butucea O.D.
Kinetic study of hexavalent chromium removal from wastewaters by ion exchange
Env. Eng. Manag. J. 12(5): 929-935, **2013**
- C208.** Muntean C., Stoia M., Barvinschi P.
Synthesis of nanocrystalline ZnFe₂O₄ and its use for the removal of congo red from aqueous solutions
Env. Eng. Manag. J. 12(5), 959-967, **2013**
- T90.** Popa A., Avram E., Lisa G., Visa A., Iliescu S., Parvulescu V., Ilia G.
Crosslinked polysulfone obtained by Wittig-Horner reaction in biphasic system
Polym. Eng. Sci. 52(2): 352-359, **2012**
- C209.** Dizman C., Tasdelen, M.A., Yagci Y.
Recent advances in the preparation of functionalized polysulfones
Polym. Int. 62(7): 991-1007, **2013**
- C210.** Zhao Q., Sun Jie, Li Jinbo
Kinetics and mechanism of Horner-Wadsworth-Emmons reaction of weakly acidic phosphonate in solid-liquid phase-transfer catalysis system
Cat. Comm., 36: 98-103, **2013**
- T91.** Ciopec M., Lupa L., Negrea A., Davidescu C.M. Popa A., Negrea P., Motoc M., David D., Kaycsa D.
Kinetic and thermodynamic studies regarding Cu(II) ions removal from aqueous solution by poly(styrene-divinylbenzene)-supported aminophosphonic acids
Rev. Chim. 63(1): 49-53, **2012**
- C211.** Gavris G., Stoia M., Petrehele A.I.G.
Sodium Hypophosphite as Reduction Reagent for Copper Ions Recovery from Aqueous Solutions

Rev. Chim. 64(5): 519-523, 2013

C212. Zelinschi B.C., Dorohoi D.O.

In-vitro Release Study of (2-[(1-benzyl-4-piperidyl) methyl]-5,6-dimethoxy-2,3-dihydroinden-1-one) BPMDMDHI Included in the PVA Matrix

Rev. Chim. 63(8): 811-814, 2012

T92. Ciopec M., Davidescu C., Negrea A., Lupa L., Popa A., Negrea P.

Use of D2EHPA-impregnated XAD7 resin for the removal of Cd(II) and Zn(II) from aqueous solutions

Env. Eng. Manag. J. 10(10): 1597-1608, 2011

C213. Muntean C., Stoia M., Barvinschi P.

Synthesis of nanocrystalline ZnFe₂O₄ and its use for the removal of congo red from aqueous solutions

Env. Eng. Manag. J. 12(5): 959-967, 2013

T93. Negrea A., Ciopec M., Lupa L., Davidescu C., Popa A., Negrea P.

Removal of As-V by Fe-III-Loaded XAD7 Impregnated Resin Containing Di(2-ethylhexyl) Phosphoric Acid (DEHPA): Equilibrium, kinetic, and thermodynamic modeling studies

J. Chem. Eng. Data 56(10): 3830-3838, 2011

C214. Yu X., Tong S., Ge M.

Synthesis and characterization of multi-amino-functionalized cellulose for arsenic adsorption

Carbohydr. Polym. 92(1): 380-387, 2013

T94. Popa A., Davidescu C.-M., Negrea P., Ilia G., Demadis K.

Synthesis and characterization of phosphonate ester/phosphonic acid grafted styrene - Divinylbenzene copolymer microbeads and their utility in adsorption of divalent metal ions in aqueous solutions

Ind. Eng. Chem. Res. 47(6): 2010-2017, 2008

C215. Foti C., Giuffre O., Sammartano S.

Thermodynamics of HEDPA protonation in different media and complex formation with Mg²⁺ and Ca²⁺

J. Chem. Thermodyn. 66: 151-160, 2013

C216. Graillot A., Bouyer D., Monge S.

Sorption properties of a new thermosensitive copolymeric sorbent bearing phosphonic acid moieties in multi-component solution of cationic species

J. Hard. Mater. 260: 425-433 2013

C217. Ali S. W., Waqar F., Malik M. A.

Study on the synthesis of a macroporous ethylacrylate-divinylbenzene copolymer, its conversion into a bi-functional cation exchange resin and applications for extraction of toxic heavy metals from wastewater

J. Appl. Polym. Sci. 129(4): 2234-2243, 2013

C218. Bouyer D., Monge S.

Removal of nickel ions from aqueous solution by low energy-consuming sorption process involving thermosensitive copolymers with phosphonic acid groups Graillot A.,

J. Hard. Mater., 244: 507-515, 2013

C219. Abdouss M., Najafabadi S. A. H., Shoushtari A. M.

Preparation of ethanolamine modified micro and new nano acrylic fibers for ion adsorption

Ind. Text. 64(3): 129-135, 2013

- C220.** Graillot A., Monge S., Faur C.
Synthesis by RAFT of innovative well-defined (co) polymers from a novel phosphorus-based acrylamide monomer
Polym. Chem. 4(3): 795-803, 2013
- T95.** Popa A., Ilia G., Davidescu CM, Iliescu S., Plesu N., Pascariu A., Zhang Z.
Wittig-Horner reactions on styrene-divinylbenzene supports with benzaldehyde side-groups
Polym. Bull., 57(2): 189-197, 2006
- C221.** Zhao Q., Sun J., Li J.
Kinetics and mechanism of Horner-Wadsworth-Emmons reaction of weakly acidic phosphonate in solid-liquid phase-transfer catalysis system
Cat. Comm. 36: 98-103, 2013
- T96.** Popa A., Davidescu C.M., Trif R., Ilia G., Iliescu S., Dehelean G.
Study of quaternary 'onium' salts grafted on polymers: antibacterial activity of quaternary phosphonium salts grafted on 4 gel-type' styrene-divinylbenzene copolymers
React. Funct. Polym. 55(2): 151-158, 2003
- C222.** Garcia-Arguelles S., Concepcion Serrano M., Gutierrez M.C.
Deep Eutectic Solvent-Assisted Synthesis of Biodegradable Polyesters with Antibacterial Properties
Langmuir 29(30): 9525-9534, 2013
- C223.** Pugachev M.V., Shtyrlin N.V., Sysoeva L.P.
Synthesis and antibacterial activity of novel phosphonium salts on the basis of pyridoxine
Bioorgan. Med. Chem. 21(14): 4388-4395, 2013
- C224.** Guterman R., Berven B. M., Corkery T. C.
Fluorinated polymerizable phosphonium salts from PH3: Surface properties of photo-polymerized films
J. Polym. Sci. Pol. Chem. 51(13): 2782-2792, 2013
- C225.** Carmona-Ribeiro A.M., de Melo C., Dias L.
Cationic Antimicrobial Polymers and Their Assemblies
Internat. J. of Molec. Sci. 14(5): 9906-9946, 2013
- C226.** Chun L., Yuan L., Qiu-Yuan Z.
Preparation and antimicrobial activity of quaternary phosphonium modified epoxidized natural rubber
Mater. Lett. 93: 145-148, 2013
- T97.** Macarie L., Ilia G.
Poly(vinylphosphonic acid) and its derivatives
Prog. Polym. Sci. 35(8), 1078-1092, 2010
- C227.** Aslan A., Bozkurt A.
An investigation of proton conductivity of nanocomposite membranes based on sulfated nano-titania and polymer
Solid State Ionics 239: 21-27, 2013
- C228.** Chen R., Goldshtain J., Margel S
Synthesis and characterization of hydroxy-bisphosphonate micrometer-sized particles by dispersion polymerization of a new styrylbisphosphonate monomer
J. Polym. Sci. Part A-Polymer Chemistry 51(10): 2199-2207, 2013
- C229.** Gashti M.P., Almasian A.
UV radiation induced flame retardant cellulose fiber by using polyvinylphosphonic acid/carbon nanotube composite coating

Compos. Part B-Eng. 45(10): 282-289, **2013**

C230. Markova D., Opper K.L., Wagner M.

Synthesis of proton conducting phosphonic acid-functionalized polyolefins by the combination of ATRP and ADMET

Polym. Chem. 4(5): 1351-1363, **2013**

T98. Macarie L, Bandur G, Ilia G

Comparative study of the photoinitiating reactivity of the acylphosphonates and acylphosphine oxides

Rev. Roum. Chem. 52(4): 437-443, **2007**

C231. Ponikvar-Svet M., Zeiger D.N., Keating L.R.

Interplay of Thermochemistry and Structural Chemistry

Struct. Chem. 24(5): 1759-1779, **2013**

T99. Pascariu A., Ilia G., Bora A., Iliescu S., Popa A., Dehelean G., Pacureanu L.

Carbon-carbon double bond obtained by Wittig and Wittig-Horner reaction in phase transfer catalysis conditions

Cent. Eur. J.-Chem. 4: 491-542, **2003**

C232. Byrne P.A., Gilheany D.G.

The modern interpretation of the Wittig reaction mechanism

Chem. Soc. Rev. 42(16): 6670-6696, **2013**

T100. Pascariu A., liescu S., Popa A., Ilia G.

Polydentate phosphines

J. Organomet. Chem. 694(25): 3982-4000, **2009**

C233. Lee C.C., Huang H.C., Liu S.T., Liu Y.H, Peng S.M., Chen, J.T

Coordination chemistry and catalytic activity of ruthenium(II) complexes containing a phospha-macrocyclic ligand

Polyhedron 52: 1024-1029, **2013**

C234. Gusarova N.K., Kuimov V.A., Malysheva S.E., Belogorlova N.A., Albanov A.I.

One-pot synthesis of ultra-branched mixed tetradentate tripodal phosphines and phosphine chalcogenides

Tetrahedron 68(45): 9218-9225, **2012** (neraportata 2012)

T101. Ackermann M., Pascariu A., Hoecher T., Siehl H.-U., Berger S.

Electronic Properties of Furyl Substituents at Phosphorus and their Influence on ^{31}P NMR Chemical Shifts

J. Am. Chem. Soc. 128(26): 8434-8440, **2006**

C235. Rahaman A., Alam F.R., Ghosh S., Haukka M., Kabir S.E., Nordlander E., Hogarth G

Generation of sigma,pi-furyl and thiienyl ligands at di-iron centers via facile phosphorus-carbon bond cleavage: Synthesis and molecular structures of $[\text{Fe}-2(\text{CO})(6)(\mu\text{-eta}(1),\text{eta}(2)\text{-C}_4\text{H}_3\text{E})\{\mu\text{-P}(\text{C}_4\text{H}_3\text{E})_2\}]$ ($\text{E} = \text{O}, \text{S}$)

J. Organomet. Chem. 730: 123-131, **2013**

T102. Colodrero R.M.P., Cabeza A., Olivera-Pastor P., Choquesillo-Lazarte D., Garcia-Ruiz J.M., Turner A., Ilia G., Maranescu B., Aranda M.A.G

Divalent metal vinylphosphonate layered materials: Compositional variability, structural peculiarities, dehydration behavior, and photoluminescent properties

Inorg. Chem. 50(21): 11202-11211, **2011**

C236. Vilela S.M.F., Mendes R.F., Silva P., Fernandes J.A., Tome J.P.C., Paz F.A.A.

Structural Diversity of Lanthanum-Organic Frameworks Based on 1,4-Phenylene-bis(methylene)diphosphonic Acid

T103. Pascariu A., Mracec M., Berger S.

Dynamic NMR study of the oxaphosphetane complexation with lithium during the Wittig reaction

Int. J. Quant. Chem. 108(6): 1052-1058, 2008

C237. Liyasova M.S., Schopfer L.M., Kodani S., Lantz S.R., Casida J.E., Lockridge O. Newly Observed Spontaneous Activation of Ethepron as a Butyrylcholinesterase Inhibitor
Chem. Res. Toxicol. 26(3): 422-431, 2013

T104. Iliescu S., Grozav I., Funar-Timofei S., Plesu N., Popa A., Ilia G.

Optimization of synthesis parameters in interfacial polycondensation using design of experiments

Polym. Bull. 64(3): 303-314, 2010

C 238. Jelmy E. J., Ramakrishnan S., Devanathan, S., Rangarajan M., Kothurkar N, K. Optimization of the conductivity and yield of chemically synthesized polyaniline using a design of experiments

J. Appl. Polym. Sci. 130(2): 1047-1057, OCT 2013

T105. Mang X, Zeng X, Tang B, Liu F, Ungar G, Zhang R, Cseh L, Mehl GH Control of anisotropic self-assembly of gold nanoparticles coated with mesogens
J. Mater. Chem. 22 (22): 11101-11106, 2012

C239. Paczesny, J., Wójcik, M., Sozański, K., Nikiforov, K., Tschierske, C., Lehmann, A., Górecka, E., (...), Hołyst, R.

Self-assembly of gold nanoparticles into 2D arrays induced by bolaamphiphilic ligands

J. Phys. Chem. C 117 (45): 24056-24062, 2013

C240. Lewandowski W, Constantin D, Walicka K, Pociecha D, Mieczkowski J, Górecka E Smectic mesophases of functionalized silver and gold nanoparticles with anisotropic plasmonic properties

Chem. Comm. 49 (71):7845-7847, 2013

C241. Tschierske, C

Development of structural complexity by liquid-crystal self-assembly

Angewandte Chem. – Int. Ed. 52 (34): 8828-8878, 2013

C242. Liu Y, Song F, Zhang J, Lv Z, Liu J, Yu Y, Zhao H, Wang H

Tunable local surface plasmon resonance in liquid-crystal-coated Ag nanoparticles

Phys. Lett. A. 377 (16-17): 1199-1204, 2013

C243. Scharf T, Dintinger J, Tang BJ, Mehl GH, Zeng X, Ungar G, Mühlig S, (...), Rockstuhl C

Liquid crystal plasmonic metamaterials

Proceedings of SPIE - The International Society for Optical Engineering 8642 , art. no. 86420J, 2013

C244 Thiruvengadathan R, Korampally V, Ghosh A, Chanda N, Gangopadhyay K, Gangopadhyay S

Nanomaterial processing using self-assembly-bottom-up chemical and biological approaches

Rep. Prog. Phys. 76 (6): no. 066501, 2013

C245. Orlandi S, Zannoni C

Phase organization of mesogen-decorated spherical nanoparticles

Mol. Cryst. Liq. Cryst. 573 (1): 1-9, 2013

C246. Dintinger J, Tang BJ, Zeng X, Liu F, Kienzler T, Mehl GH, Ungar G, Scharf T A self-organized anisotropic liquid-crystal plasmonic metamaterial

Adv. Mater. 25 (14): 1999-2004, 2013

- C247.** Lewandowski W, Jatczak K, Pociecha D, Mieczkowski J
 Control of gold nanoparticle superlattice properties via mesogenic ligand architecture
Langmuir 29 (10): 3404-3410, **2013**
- C248.** Pucci A, Willinger MG, Liu F, Zeng X, Rebuttini V, Clavel G, Bai X, Pinna N
 One-step synthesis and self-assembly of metal oxide nanoparticles into 3D superlattices
ACS Nano 6 (5): 4382-4391, **2012**
- T106.** Lysenko D, Ouskova E, Ksondzik S, Reshetnyak V, Cseh L, Mehl GH, Reznikov Y
 Light-induced changes of the refractive indices in a colloid of gold nanoparticles in a nematic liquid crystal
Eur. Phys. J. E, 35 (5), art. no. 33, **2012**
- C249.** Uklein A, Vasko AA, Ouskova EV, Brodyn MS, Gayvoronsky VY
 Nonlinear optical properties of new photosensitive smart materials based on nematic liquid crystal with H-bonded dye-polymer complex
Optics Comm., 296: 79-83, **2013**
- T107.** Ouskova E, Lysenko D, Ksondzik S, Cseh L, Mehl GH, Reshetnyak V, Reznikov Yu
 Strong cubic optical nonlinearity of gold nanoparticles suspension in nematic liquid crystal
Mol. Cryst. Liq. Cryst., 545: 123-132, **2011**
- C250.** Lyashchova A, Fedorenko D, Garbovskiy Y, Klimusheva G, Mirnaya T, Asaula V
 Strong thermal optical nonlinearity caused by CdSe nanoparticles synthesised in smectic ionic liquid crystal
Liq. Cryst. 40 (10): 1377-1382, **2013**
- T108.** Zeng X, Liu F, Fowler AG, Ungar G, Cseh L, Mehl GH, Macdonald JE
 3D ordered gold strings by coating nanoparticles with mesogens
Adv. Mater. 21 (17): 1746-1750, **2009**
- C251.** Wei WB, Chen K, Ge GL
 Electrostatically controlled nematic and smectic assembly of gold nanorods
Chem. Res. Chinese Univ. 29 (5): 929-933, **2013**
- C252.** Lewandowski W, Constantin D, Walicka K, Pociecha D, Mieczkowski J, Górecka E
 Smectic mesophases of functionalized silver and gold nanoparticles with anisotropic plasmonic properties
Chem. Comm. 49 (71): 7845-7847, **2013**
- C253.** Scheeler SP, Mühlig S, Rockstuhl C, Hasan SB, Ullrich S, Neubrech F, Kudera S, Pacholski C
 Plasmon coupling in self-assembled gold nanoparticle-based honeycomb islands
J. Phys. Chem. C 117 (36): 18634-18641, **2013**
- C254.** Kumaraswamy G, Sharma KP
 Polymer and colloidal inclusions in lyotropic lamellar and hexagonal surfactant mesophases
Adv. Planar Lipid Bilayers and Liposomes 18: 181-208, **2013**
- C255.** Tschierske C
 Development of structural complexity by liquid-crystal self-assembly
Angewandte Chem. – Int. Ed. 52 (34): 8828-8878, **2013**
- C256.** Yannopapas V
 Fluctuational-electrodynamics calculations of the van der waals potential in nanoparticle superlattices
J. Phys. Chem. C 117 (29): 15342-15346, **2013**
- C257.** Dalmaschio CJ, Da Silveira Firmiano EG, Pinheiro AN, Sobrinho DG, Farias De Moura A, Leite ER

Nanocrystals self-assembled in superlattices directed by the solvent-organic capping interaction

Nanoscale 5 (12): 5602-5610, **2013**

C258. Scharf T, Dintinger J, Tang BJ, Mehl GH, Zeng X, Ungar G, Mühlig S, Rockstuhl C
Liquid crystal plasmonic metamaterials

Proceedings of SPIE - The International Society for Optical Engineering 8642, art. no. 86420J, **2013**

C259. Dintinger J, Tang BJ, Zeng X, Liu F, Kienzler T, Mehl GH, Ungar G, Scharf T
A self-organized anisotropic liquid-crystal plasmonic metamaterial

Adv. Mater. 25 (14): 1999-2004, **2013**

C260. Umadevi S, Feng X, Hegmann T

Large area self-assembly of nematic liquid-crystal-functionalized gold nanorods

Adv. Functional Mater. 23 (11): 1393-1403, **2013**

C261. Lewandowski W, Jatczak K, Pociecha D, Mieczkowski J

Control of gold nanoparticle superlattice properties via mesogenic ligand architecture

Langmuir 29 (10): 3404-3410, **2013**

C262. Yannopapas V, Fytas N, Kyrimi V, Kallos E, Vanakaras AG, Photinos DJ

Light scattering by a metallic nanoparticle coated with a nematic liquid crystal

Phys. Status Solidi A, 210 (2): 335-340, **2013**

C263. Droulias S, Yannopapas V

Broad-band giant circular dichroism in metamaterials of twisted chains of metallic nanoparticles

J. Phys. Chem. C, 117 (2): 1130-1135, **2013**

T109. Zeng X, Cseh L, Mehl GH, Ungar G

Testing the triple network structure of the cubic Im $\bar{3}$ m (I) phase by isomorphous replacement and model refinement

J. Mater. Chem., 18 (25): 2953-2961, **2008**

C264. Tan X, Kong L, Dai H, Cheng X, Liu F, Tschiesske C

Triblock polyphiles through click chemistry: Self-assembled thermotropic cubic phases formed by micellar and monolayer vesicular aggregates

Chem. – Eur. J. 19 (48): pp. 16303-16313, **2013**

C265. Dai H, Yang X, Tan X, Su F, Cheng X, Liu F, Tschiesske C

Liquid crystalline 2-thienyl-4,6-diamino-1,3,5-triazines exhibiting Im $\bar{3}$ m and Pm $\bar{3}$ n micellar cubic phases in an inverted sequence

Chem. Comm. 49 (90): 10617-10619, **2013**

C266. Tschiesske C

Development of structural complexity by liquid-crystal self-assembly

Angewandte Chem. – Int. Ed. 52 (34): 8828-8878, **2013**

T110. Fagadar-Cosma E, Cseh L, Badea V, Fagadar-Cosma G, Vlascici D
Combinatorial synthesis and characterization of new asymmetric porphyrins as potential photosensitizers in photodynamic therapy

Combinatorial Chem. High Throughput Screening, 10 (6): 466-472, **2007**

C267. Iordache S, Cristescu R, Popescu AC, Popescu CE, Dorcioman G, Mihailescu IN, Ciucu AA, Chrisey DB

Functionalized porphyrin conjugate thin films deposited by matrix assisted pulsed laser evaporation

Appl. Surface Sci. 278: 207-210, **2013**

- T111.** Cseh L, Mehl GH
 Structure-property relationships in nematic gold nanoparticles
J. Mater. Chem. 17 (4): 311-315, **2007**
- C268.** Scharf T, Dintinger J, Tang BJ, Mehl GH, Zeng X, Ungar G, Mühlig S, Rockstuhl
 Liquid crystal plasmonic metamaterials
Proceedings of SPIE - The International Society for Optical Engineering 8642 , art. no. 86420J, **2013**
- C269.** Orlandi S, Zannoni C
 Phase organization of mesogen-decorated spherical nanoparticles
Mol. Cryst. Liq. Cryst. 573 (1): 1-9, **2013**
- C270.** Dintinger J, Tang BJ, Zeng X, Liu F, Kienzler T, Mehl GH, Ungar G, Scharf T
 A self-organized anisotropic liquid-crystal plasmonic metamaterial
Adv. Mater. 25 (14): 1999-2004, **2013**
- C271.** Knoppe S, Bürgi T
 Chiroptical properties of intrinsically chiral thiolate-protected gold clusters
Chimia 67 (4): 236-239, **2013**
- C272.** Li B, Zhang J, Wang S, Li W, Wu L
 Nematic ion-clustomesogens from surfactant-encapsulated polyoxometalate assemblies
Eur. J. Inorg. Chem. 10-11: 1869-1875, **2013**
- C273.** Wolska JM, Pociecha D, Mieczkowski J, Gorecka E
 Gold nanoparticles with flexible mesogenic grafting layers
Soft Matter 9 (11): 3005-3008, **2013**
- C274.** Neeraj K, Raina K
 Nickel nanoparticles doped ferroelectric liquid crystal composites
Opt. Mater. 35 (3): 531-535, **2013**
- T112.** Cseh L., Mehl G.H.
 The design and investigation of room temperature thermotropic nematic gold nanoparticles
J. Am. Chem. Soc. 128 (41): 13376-13377, **2006**
- C275.** Beqa L, Deschamps D, Perrio S, Gaumont AC, Knoppe S, Bürgi T
 Ligand exchange reaction on Au₃₈(SR)₂₄, separation of Au₃₈(SR)₂₃(SR')₁ regioisomers, and migration of thiolates
J. Phys. Chem. C 117 (41): 21619-21625, **2013**
- C276.** Knoppe S, Bürgi T
 The fate of Au₂₅(SR)₁₈ clusters upon ligand exchange with binaphthyl-dithiol: Interstaple binding vs. decomposition
Phys. Chem. 15 (38): 15816-15820, **2013**
- C277.** Prodanov MF, Pogorelova NV, Kryshtal AP, Klymchenko AS, Mely Y, Semynozhenko VP, Krivoshey AI, Vashchenko VV
 Thermodynamically stable dispersions of quantum dots in a nematic liquid crystal
Langmuir 29 (30): 9301-9309, **2013**
- C278.** Yannopapas V
 Fluctuational-electrodynamics calculations of the van der waals potential in nanoparticle superlattices
J. Phys. Chem. C 117 (29): 15342-15346, **2013**
- C279.** Knoppe S, Michalet S, Bürgi T
 Stabilization of thiolate-protected gold clusters against thermal inversion: Diastereomeric Au₃₈(SCH₂CH₂Ph)₂₄-2 x(R -BINAS)x
J. Phys. Chem. C 117 (29): 15354-15361, **2013**
- C280.** Scharf T, Dintinger J, Tang BJ, Mehl GH, Zeng X, Ungar G, Mühlig S, Rockstuhl
 Liquid crystal plasmonic metamaterials

Proceedings of SPIE - The International Society for Optical Engineering 8642, art. no. 86420J 2013

C281. Orlandi S, Zannoni C

Phase organization of mesogen-decorated spherical nanoparticles

Mol. Cryst. Liq. Cryst. 573 (1): pp. 1-9, 2013

C282. Dintinger J, Tang BJ, Zeng X, Liu F, Kienzler T, Mehl GH, Ungar G, Scharf T

A self-organized anisotropic liquid-crystal plasmonic metamaterial

Adv. Mater. 25 (14): 1999-2004, 2013

C283. Knoppe, S., Bürgi, T.

Chiroptical properties of intrinsically chiral thiolate-protected gold clusters

Chimia 67 (4) , pp. 236-239, 2013

C284. Li B, Zhang J, Wang S, Li W, Wu L

Nematic ion-clustomesogens from surfactant-encapsulated polyoxometalate assemblies

Eur. J. Inorg. Chem. 10-11: 1869-1875, 2013

C285. Umadevi S, Feng X, Hegmann T

Large area self-assembly of nematic liquid-crystal-functionalized gold nanorods

Adv. Functional Mater. 23 (11): 1393-1403, 2013

C286. Lewandowski W, Jatczak K, Pociecha D, Mieczkowski J

Control of gold nanoparticle superlattice properties via mesogenic ligand architecture

Langmuir 29 (10): 3404-3410, 2013

C287. Yannopapas V, Fytas N, Kyrimi V, Kallos E, Vanakaras AG, Photinos DJ

Light scattering by a metallic nanoparticle coated with a nematic liquid crystal

Phys. Status Solidi A, 210 (2): 335-340, 2013

C288. Droulias S, Yannopapas V

Broad-band giant circular dichroism in metamaterials of twisted chains of metallic nanoparticles

J. Phys. Chem. C 117 (2): 1130-1135, 2013

C289. Vardanyan KK, Sita DM, Walton RD, Saidel WM, Jones KM

Cyanobiphenyl liquid crystal composites with gold nanoparticles

RSC Advances 3 (1): 259-273, 2013

T113. Cseh L, Csunderlik C, Pantenburg I, Meyer G, Costisor O

Synthesis, crystal structure, and spectral properties of a Cobalt(II) complex with N-salicylidene-p-toluidine

Zeitschrift fur Anorganische und Allgemeine Chemie, 629 (6): 985-988, 2003

C290. Zhao ZG, Kodaira T, Nagai N, Hakuta Y, Bando KK, Takashima H, Mizukami F
Self-standing microporous films of arrayed alumina nano-fibers including Schiff base molecules: Effect of the environment around the molecules on their photo-luminescence

J. Mater. Chem. 22 (19): 9738-9744, 2012

T114. Stefan LM, Pana AM, Bandur G, Martin P, Popa M, Rusnac LM

Thermal analysis of new glycopolymers derived from monosaccharides

J. Therm. Anal. Calorimetry, 111 (1): 789-797, 2013

C291. Yilmaz, G., Becer, C.R.

Precision glycopolymers and their interactions with lectins

Eur. Polym. J. 49 (10): 3046-3051 2013

T115. Stefan LM, Pana AM, Pascariu MC, Sisu E, Bandur G, Rusnac LM

Synthesis and characterization of a new methacrylic glycomonomer

Turk. J. Chem., 35 (5): 757-767, 2011

C292. Rafailă M, Pascariu MC, Gruiu A, Penescu M, Purcarea VL, Medeleanu M, Rusnac LM, Davidescu C

GC-MS analysis of long chain mannofuranose derivatives as biocompatible surfactant precursors. Correlation between peak intensities and stability of corresponding fragments
Farmacia 61 (1): 116-126, 2013

C293. Pascariu MC, Rusnac LM, Macsim AM
Tethered glycoderivatives with unsaturated spacer: Synthesis and characterization
Synth. Comm. 42 (17): 2503-2511, 2012

T116. Pana AM, Rusnac LM, Bandur G, Deleanu C, Balan M, Silion M
Synthesis and characterization of new glycopolymers based on monosaccharides and maleic anhydride II. Mannose derivatives
Mater. Plast., 47 (3): 299-305, 2010.

C294. Pascariu MC, Rusnac LM, Macsim AM
Tethered glycoderivatives with unsaturated spacer: Synthesis and characterization
Synth. Comm. 42 (17): 2503-2511, 2012

C295. Rusu LC, Ardelean L, Podariu AC, Matei C, Tampa M
Allergenic potential evaluation of acrylic resins from the complete prostheses
Mater. Plast. 49 (2): 133-134, 2012

C296. Podariu AC, Ardelean L, Jumanca D, Galuscan A, Rusu LC
Determining the amount of volatile organic phase in PMMA dentures
Rev. Chim 63 (7): 720-721, 2012

T117. Pana AM, Rusnac LM, Bandur G, Sisu E, Badea V, Silion M
Synthesis and characterization of new glycopolymers based on monosaccharides and maleic anhydride I. Glucose derivatives
Mater. Plast., 47 (1) , pp. 28-34, 2010

C297. Pascariu MC, Rusnac LM, Macsim AM
Tethered glycoderivatives with unsaturated spacer: Synthesis and characterization *Synth. Comm.* 42 (17): 2503-2511, 2012

T118. Popovici M., Gich M., Niznansky D., Roig A., Savii C., Casas L., Molins E., Zaveta K.,

Enache C., Sort J., Brion S., Chouteau G., Nogues J.
Optimized synthesis of the elusive epsilon-Fe₂O₃ phase via sol-gel chemistry
Chem Mater, 16(25), 5542-5548, DEC 2004

C298: Ohkoshi, Shin-ichi, Tokoro, Hiroko
Hard Magnetic Ferrite: epsilon-Fe₂O₃
B Chem Soc Jpn, 86 (8), 897-907, AUG 2013

C299: Namai Asuka, Yoshihiro Marie, Umeda Sayaka, Yoshida Takayuki, Miyazaki Tatsuro
The synthesis of rhodium substituted epsilon-iron oxide exhibiting super high frequency natural resonance
J Mater Chem, 1 (34), 5200-5206, 2013

T119. Popovici M., Gich M., Roig A., Casas L., Molins E., Savii C., Becherescu D., Sort J., Suriñach S., Muñoz J., Baró MD., Nogués J.
Ultraporous single phase iron oxide-silica nanostructured aerogels from ferrous precursors
Langmuir, 20 (4), 1425-1429, FEB 2004

C300: Luo Fengzuan, Shao Zaidong, Zhang Ying, Xuan Cheng
Synthesis of paramagnetic iron incorporated silica aerogels by ambient pressure drying
Mater Chem Phys, 142 (1), 113-118, OCT 2013

- T120.** Caizer C., Popovici M., Savii C.
 Spherical (Zn delta Ni1-delta Fe₂O₄)(gamma) nanoparticles in an amorphous (SiO₂)(1-gamma) matrix, prepared with the sol-gel method
Acta Mater., 51 (12), 3607-3616, JUL 2003
- C301.** Gawas UB, Verenkar VMS
 Synthesis, thermo-analytical and IR spectral studies of hydrazinated mixed metal carboxylates: A single source precursor to nanosize mixed metal oxides
Thermochim Acta, 556, 41-46, MAR 2013
- T121.** Caizer C., Savii C., Popovici M.
 Magnetic behaviour of iron oxide nanoparticles dispersed in a silica matrix
Mat Sci Eng B-Solid, 97 (2), 129-134, JAN 2003
- C302.** Espinosa A, Muñoz-Noval A, García-Hernández M, Serrano A, Jiménez de Morena J, Figuerola A, Quarta A, Pellegrino T, Wilhelm C, García MA
 Magnetic properties of iron oxide nanoparticles prepared by seeded-growth route
J Nanopart Res., 15 (4), APR 2013
- T122.** Savii C., Popovici M., Enache C., Subrt J., Niznansky D., Bakardzieva S., Caizer C., Hrianci I.
 Fe₂O₃-SiO₂ composites obtained by sol-gel synthesis
Solid State Ionics, 151(1-4), 219-227, NOV 2002
- C303.** Ciriminna R, Fidalgo A, Pandarus V, Béland F, Ilharco LM, Pagliaro M
 The Sol-Gel Route to Advanced Silica-Based Materials and Recent Applications
Chem Rev., 113 (8), 6592-6620, AUG 2013
- T123.** Putz M.V., Lazea M, Putz A.M., Duda-Seiman C.
 Introducing Catastrophe-QSAR. Application on Modeling Molecular Mechanisms of Pyridinone Derivative-Type HIV Non-Nucleoside Reverse Transcriptase Inhibitors
Int J Mol Sci., 12(12), 9533-9569, DEC 2011
- C304.** Milicevic A, Raos N
 Theoretical Model for the Prediction of the Stability of Co²⁺, Ni²⁺, Cu²⁺, Zn²⁺, and Cd²⁺ mono-complexes with monocarboxylic acids based on (3)chi(nu) connectivity index
Acta Chim Slov., 60 (1), 120-123, 2013
- T124.** Putz M.V., Putz A.M., Lazea M., Chiriac A.
 Spectral vs.statistic approach of structure-activity relationship. Application on ecotoxicity of aliphatic amines
J Theor Comput Chem., 8 (6), 1235-1251, DEC 2009
- C305.** Lazea M, Saitos Z, Chiriac A
 Qsar studies of some metal ions toxicity
J Environ Prot Ecol., 14 (2), 699-706, 2013
- T125.** Putz M.V., Putz A.M., Lazea M., Ienciu L., Chiriac A.
 Quantum-SAR Extension of the Spectral-SAR Algorithm. Application to Polyphenolic Anticancer Bioactivity
Int J Mol Sci., 10 (3), 1193-1214, MAR 2009
- C306.** Khaled, K F, El-Sherik AM
 Using Molecular Dynamics Simulations and Genetic Function Approximation to Model Corrosion Inhibition of Iron in Chloride Solutions
Int J Electrochem Sc., 8 (7), 10022-10043, JUL 2013
- C307.** Chakraborty A, Pan S, Chattaraj PK.
 Biological Activity and Toxicity: A Conceptual DFT Approach

Book Editor(s): Putz MV, Mingos DMP
Applications of density functional theory to biological and bioinorganic chemistry
Struct Bond, 150, 143-179, 2013

T126. Putz M.V., Putz (Lacrama) A.M.

Spectral-sar: old wine in new bottle

Stud Univ Babes-Bol, 53 (2), 73-81, 2008

C308. Chakraborty A, Pan S, Chattaraj PK

Biological Activity and Toxicity: A Conceptual DFT Approach

Book Editor(s): Putz MV, Mingos DMP

Applications of density functional theory to biological and bioinorganic chemistry

Struct Bond, 150, 143-179, 2013

T127. Banica R., Nyari T., Sasca V.

$Zn_{2x}(CuIn)_{1-x}S_2$ photocatalysts synthesis by a hydrothermal process using H_4EDTA as complexing agent,

International Journal of Hydrogen Energy, 37 (21), pp. 16489-16497, 2012.

C309. Baniasadi, E., Dincer, I., Naterer, G.F., Measured effects of light intensity and catalyst concentration on photocatalytic hydrogen and oxygen production with zinc sulfide suspensions

International Journal of Hydrogen Energy 38 (22), pp. 9158-9168, 2013

C310. Zamfirescu, C. Quantum efficiency modeling and system scaling-up analysis of water splitting with $Cd_{1-x}ZnxS$ solid-solution photocatalyst.

Chem. Eng. Sci., JUN 28 2013.

C311. Zhang, Kai. Metal sulphide semiconductors for photocatalytic hydrogen production

Catal. Sci. Technol., 2013

T128. Sasca V., Avram L., Verdes O., Popa A.

The n-butyl amine TPD measurement of Bronsted acidity for solid catalysts by simultaneous TG/DTG-DTA

Appl. Surf. Sci. 256 5533-5538 2010

C312. Luz, Geraldo E., Jr. Determination of SBA-15 acidity through n-butyl amine TPD: a theoretical and experimental study.

J. Mater. Sci., OCT 2013

T129. Stefanescu M., Sasca V., Bîrzescu M.

The thermal behavior of the homopolymeric glyoxilates complex combinations with Cu(II), respectively Cr(III),

J. Thermal.Anal.Cal., 2003, 72, 515-524

C313. Stefanescu, O.

Preparation of $CuFe_2O_4/SiO_2$ nanocomposite starting from Cu(II)-Fe(III) carboxylates embedded in hybrid silica gels.

J. Thermal.Anal.Cal., SEP 2013.

C314. Barvinschi, Paul.

Evaluation of cation influence on the formation of $M(II)Cr_2O_4$ during the thermal decomposition of mixed carboxylate type precursors.

J. Thermal.Anal.Cal., APR 2013

T130. Stefanescu M., Sasca V., Birzescu M.,

Studies on thermal decomposition of heteropolymeric glyoxilates of Cr(III) and Cu(II),

J. Thermal.Anal., 1999, 56, 579-586

- C315.** Li, Xinwei. In situ PMMA-templating preparation and excellent catalytic performance of Co₃O₄/3DOM La_{0.6}SrO₄CoO₃ for toluene combustion.
Appl. Catal.A-General, MAY 10 2013.
- C316.** Barvinschi, Paul. Evaluation of cation influence on the formation of M(II)Cr₂O₄ during the thermal decomposition of mixed carboxylate type precursors.
J. Thermal.Anal.Cal., APR 2013
- T131.** Sasca V., Verdeş O., Avram L., Popa A., Barvinschi P. , Mracec M. Non-isothermal Kinetic Study of the Constitutional Water Loss from 12-Tungstophosphoric Acid and Some of its Acidic Cesium Salts
Rev.Roum.Chim., 2011 56 (5), 501-516
- C317.** Xiao, Yanxin. Development of cesium phosphotungstate salt and chitosan composit membrane for direct methanol fuel cells.
Carbohydrate Polym., OCT 15 2013.
- T 132.** Popa A., Sasca V., Holclajtner-Antunovic I. The influence of surface coverage on textural, structural and catalytic properties of cesium salts of 12-molybdophosphoric acid supported on SBA-15 mesoporous silica
Micropor. Mesopor. Mater., 156: 127-137, 2012
- C 318.** Lei J., Chen L., Yang P., Du X., Yan X. Oxidative desulfurization of diesel fuel by mesoporous phosphotungstic acid/SiO₂: The effect of preparation methods on catalytic performance
J. Porous. Mat. 20 (5): 1379-1385, OCT 2013
- C319.** Ahmed A.I., Samra S.E., El-Hakam S.A., Khder A.S., El-Shenawy H.Z., El-Yazeed W.S.A. Characterization of 12-molybdophosphoric acid supported on mesoporous silica MCM-41 an its catalytic performance in the synthesis of hydroquinone diacetate
Appl. Surf. Sci. 282: 217-225, OCT 2013
- C320.** El-Naggar M.R., Aglan R.F., Sayed M.S. Direct incorporation method for the synthesis of molybdophosphate/MCM-41 silica composite: Adsorption study of heavy metals from aqueous solutions
J. Environ. Chem. Eng., 1 (3): 516-525 2013
- C321.** Zhao H., Zeng L., Li Y., Liu C., Hou B., Wu D., Feng N., Yu N Polyoxometalate-based ionic complexes immobilized in mesoporous silicas prepared via a one-pot procedure: Efficient and reusable catalysts for H₂O₂-mediated alcohol oxidations in aqueous media
Micropor. Mesopor. Mater. 172: 67-76, MAY 2013
- T133.** Popa A., Sasca V., Kis E.E., Marinkovic-Nedycin R., Bokorov M.T., Halasz J. Structure and texture of some keggin type heteropolyacids supported on silica and titania
J. Optoelectron. Adv. M., 7 (6): 3169-3177, 2005
- C322.** Krishnamurthy N., Palanichamy M., Chellamani A. Liquid Phase Depolymerization of Neyveli Lignite Over Phosphotungstic Acid
Asian J. Chem. 25 (13): 7437-7440,,OCT 2013
- T134.** Popa A., Plesu N., Sasca V., Kis E.E., Marinkovic-Nedycin R. Physicochemical features of polyaniline supported heteropolyacids
J. Optoelectron. Adv. M., 8 (5):1944-1950, 2006
- C323.** Liu, H., Wang, Y., Gou, X., Qi, T., Yang, J., Ding, Y. Three-dimensional graphene/polyaniline composite material for high-performance supercapacitor applications
Mater. Sci. Eng. B: Solid-State Mater. Adv. Tech. 178 (5): 293-298, MAR 2013

- T135.** Holclajtner-Antunovic I., Bajuk-Bogdanovic D., Popa A., Uskokovic-Markovic S. Spectroscopic identification of molecular species of 12-tungstophosphoric acid in methanol/water solutions
Inorg. Chim. Acta, 383: 26-32, **2012**
- C324.** Chen G., Zhou Y., Zhao P., Long Z., Wang J. Mesostructured dihydroxy-functionalized guanidinium-based polyoxometalate with enhanced heterogeneous catalytic activity in epoxidation
ChemPlusChem 78 (6): 561-569, IUN **2013**
- C325.** Wang, Y., Liu, S., Liu, Z., Yang, J., Hu, X. Study on the interactions of antiemetic drugs and 12-tungstophosphoric acid by absorption and resonance Rayleigh scattering spectra and their analytical applications
Spectrochim. Acta A 105: 612-617, **2013**
- C326.** Tessonniere J.-P., Goubert-Renaudin S., Alia S., Yan Y., Barteau M.A. Structure, stability, and electronic interactions of polyoxometalates on functionalized graphene sheets
Langmuir 29 (1): 393-402, IAN **2013**
- T136.** Magda A., Pode R., Muntean C., Medeleanu M., Popa A. Synthesis and characterization of ammonium phosphate fertilizers with boron
J. Serb. Chem. Soc., 75 (7): 951-963, **2010**
- C327.** Churikov A.V., Ivanishchev A.V., Ushakov A.V., Gamayunova I.M., Leenson I.A. Thermodynamics of LiFePO₄ solid-phase synthesis using iron(II) oxalate and ammonium dihydropophosphate as precursors
J. Chem. Eng. Data, 58 (6): 1747-1759, IUN **2013**
- T137.** Stefanescu M., Stoia M., Stefanescu O., Popa A., Simon M., Ionescu C. The interaction between TEOS and some polyols: Thermal analysis and FTIR
J. Therm. Anal. Calorim., 88 (1): 19 - 26, **2007**
- C328.** Pronin I.A., Goryacheva M.V. Principles of structure formation and synthesis models produced by the sol-gel method SiO₂-MexOy nanocomposites
Surf. Coat. Tech., 235: 835 - 840, **2013**
- T138.** Putz M.V., Lazea M., Putz A.M., Duda-Seiman C. Introducing Catastrophe-QSAR. Application on Modeling Molecular Mechanisms of Pyridinone Derivative-Type HIV Non-Nucleoside Reverse Transcriptase Inhibitors
Int J Mol Sci, 12(12), 9533-9569, DEC **2011**
- C329.** Milicevic A., Raos N Theoretical Model for the Prediction of the Stability of Co²⁺, Ni²⁺, Cu²⁺, Zn²⁺, and Cd²⁺ mono-complexes with monocarboxylic acids based on (3)chi(nu) connectivity index
Acta Chim Slov, 60 (1), 120-123, **2013**
- T139.** Putz M.V., Putz A.M., Lazea M., Chiriac A. Spectral vs.statistic approach of structure-activity relationship. Application on ecotoxicity of aliphatic amines
J Theor Comput Chem, 8 (6), 1235-1251, DEC **2009**
- C330.** Lazea M., Saitos Z., Chiriac A Qsar studies of some metal ions toxicity
J Environ Prot Ecol, 14 (2), 699-706, **2013**

- T140.** Putz M.V., Putz A.M., Lazea M., Ienciu L., Chiriac A.
 Quantum-SAR Extension of the Spectral-SAR Algorithm. Application to Polyphenolic
 Anticancer Bioactivity
Int J Mol Sci, 10 (3), 1193-1214, MAR 2009
- C331.** Khaled, K F, El-Sherik AM
 Using Molecular Dynamics Simulations and Genetic Function Approximation to Model
 Corrosion Inhibition of Iron in Chloride Solutions
Int J Electrochem Sc, 8 (7), 10022-10043, JUL 2013
- C332.** Chakraborty A, Pan S, Chattaraj PK.
 Biological Activity and Toxicity: A Conceptual DFT Approach
 Book Editor(s): Putz MV, Mingos DMP
 Applications of density functional theory to biological and bioinorganic chemistry
Struct Bond, 150, 143-179, 2013
- C333.** Sun Na-Bo, Shi, Yan-Xia, Liu Xing-Hai, Ma Yi, Tan Cheng-Xia, Weng Jian-Quan,
 Jin Jian-Zhong, Li Bao-Ju
 Design, Synthesis, Antifungal Activities and 3D-QSAR of New *N,N'*-Diacylhydrazines
 Containing 2,4-Dichlorophenoxy Moiety
Int J Mol Sci, 14, 21741-21756, 2013
- T141.** Putz M.V., Putz (Lacrama) A.M.
 Spectral-sar: old wine in new bottle
Stud Univ Babes-Bol, 53 (2), 73-81, 2008
- C334.** Chakraborty A, Pan S, Chattaraj PK
 Biological Activity and Toxicity: A Conceptual DFT Approach
 Book Editor(s): Putz MV, Mingos DMP
 Applications of density functional theory to biological and bioinorganic chemistry
Struct Bond, 150, 143-179, 2013
- T142.** Putz M.V., Lacrama A.M., Ostafe V.
 Full Analytic Progress Curves of the Enzymic Reactions in Vitro
Int J Mol Sci, 7, 469-484, 2006
- C335.** Theillet FX, Rose HM, Liokatis S; Binolfi A, Thongwichian R, Stuiver M, Selenko
 Site-specific NMR mapping and time-resolved monitoring of serine and threonine
 phosphorylation in reconstituted kinase reactions and mammalian cell extracts
Nature Protocols, 8 (7), 1416-1432, 2013
- C335.** Golicnik, Marko
 Die Kinetik der Invertinwirkung' of L. Michaelis and ML Menten Revisited After 100
 Years: Closed Form Solutions of Genuine Invertase-Reaction Dynamics
Match-commun Math Co, 70 (1), 63-72, 2013
- T143.** Duda-Seiman C., Duda-Seiman D., Dragoş D., Medeleanu M., Careja V., Putz
 M.V.,
 Lacrama A.M., Chiriac A., Nuțiu R., Ciubotariu D.
 Design of anti-HIV Ligands by means of minimal topological difference (MTD) method
Int J Mol Sci, 7 (11), 537-555, NOV 2006
- C336.** Bolboaca SD, Jaentschi L
 The Effect of Leverage and/or Influential on Structure-Activity Relationships
Com Chem High T Scr, 16 (4), 288-297, 2013
- C336.** Chakraborty A, Pan S, Chattaraj PK
 Biological Activity and Toxicity: A Conceptual DFT Approach
 Book Editor(s): Putz MV, Mingos DMP
 Applications of density functional theory to biological and bioinorganic chemistry

T144. Putz M.V., Lacrama A.M.

Introducing Spectral structure activity relationship (S-SAR) analysis. Application to ecotoxicology

Int J Mol Sci, 8, 363-391, 2007

C337. Ying-Ting L

A tandem regression-outlier analysis of a ligand cellular system for key structural modifications around ligand binding

Journal Of Cheminformatics, 5 (21) , 2013

C338. Pei J F, Cai CZ, Zhu YM

Modeling And Predicting The Glass Transition Temperature Of Vinyl Polymers By Using Hybrid Pso-Svr Method

J Theor Comput Chem, 12 (3), 1350002, 2013

C339. Chakraborty A, Pan S, Chattaraj PK

Biological Activity and Toxicity: A Conceptual DFT Approach

Book Editor(s): Putz MV, Mingos DMP

Applications of density functional theory to biological and bioinorganic chemistry

Struct Bond, 150, 143-179, 2013

C340. Wu XY, Wan SH, Zhang JJ

Three Dimensional Quantitative Structure-Activity Relationship of 5H-Pyrido[4,3-b]indol-4 carboxamide JAK2 Inhibitors

Int J Mol Sci, 14 (6), 12037-12053, 2013

T145. Lacrama A.M., Putz M.V., Ostafe V.

A Spectral-SAR model for the anionic-cationic interaction in ionic liquids: Application to Vibrio fischeri ecotoxicity

Int J Mol Sci, 8, 842-863, 2007

C341. Ying-Ting L

A tandem regression-outlier analysis of a ligand cellular system for key structural modifications around ligand binding

Journal Of Cheminformatics, 5 (21) , 2013

C342. Chakraborty A, Pan S, Chattaraj PK

Biological Activity and Toxicity: A Conceptual DFT Approach

Book Editor(s): Putz MV, Mingos DMP

Applications of density functional theory to biological and bioinorganic chemistry

Struct Bond, 150, 143-179, 2013

C343. Wu XY, Wan SH, Zhang JJ

Three Dimensional Quantitative Structure-Activity Relationship of 5H-Pyrido[4,3-b]indol-4 carboxamide JAK2 Inhibitors

Int J Mol Sci, 14 (6), 12037-12053, 2013

T146. Putz M.V., Ionascu C; Putz A.M., Ostafe V.

Alert-QSAR. Implications for Electrophilic Theory of Chemical Carcinogenesis

Int J Mol Sci, 12 (8), 5098-5134, 2011

C344. Sun Na-Bo, Shi, Yan-Xia, Liu Xing-Hai, Ma Yi, Tan Cheng-Xia, Weng Jian-Quan, Jin Jian-Zhong, Li Bao-Ju

Design, Synthesis, Antifungal Activities and 3D-QSAR of New *N,N'*-Diacylhydrazines Containing 2,4-Dichlorophenoxy Moiety

Int J Mol Sci, 14, 21741-21756, 2013

- T147.** Putz M.V., Putz A.M., Barou R.
 Spectral-SAR realization of OECD-QSAR principles
Internat. J. Chem. Modeling, 3, 173–190, **2011**
- C345.** Sun Na-Bo, Shi, Yan-Xia, Liu Xing-Hai, Ma Yi, Tan Cheng-Xia, Weng Jian-Quan, Jin Jian-Zhong, Li Bao-Ju
 Design, Synthesis, Antifungal Activities and 3D-QSAR of New *N,N'*-Diacylhydrazines Containing 2,4-Dichlorophenoxy Moiety
Int J Mol Sci, 14, 21741-21756, **2013**
- T148.** Stefan LM, Pana AM, Bandur G, Martin P, Popa M, Rusnac LM
 Thermal analysis of new glycopolymers derived from monosaccharides
J. Therm. Anal. Calorimetry, 111 (1): 789-797, **2013**
- C346.** Yilmaz, G., Becer, C.R.
 Precisio8n glycopolymers and their interactions with lectins
Eur. Polym. J. 49 (10): 3046-3051 **2013**
- T149.** Stefan LM, Pana AM, Pascariu MC, Sisu E, Bandur G, Rusnac LM
 Synthesis and characterization of a new methacrylic glycomonomer
Turk. J. Chem., 35 (5): 757-767, **2011**
- C347.** Rafailă M, Pascariu MC, Gruia A, Penescu M, Purcarea VL, Medeleanu M, Rusnac LM, Davidescu C
 GC-MS analysis of long chain mannofuranose derivatives as biocompatible surfactant precursors. Correlation between peak intensities and stability of corresponding fragments
Farmacia 61 (1): 116-126, **2013**
- C348.** Pascariu MC, Rusnac LM, Macsim AM
 Tethered glycoderivatives with unsaturated spacer: Synthesis and characterization
Synth. Comm. 42 (17): 2503-2511, **2012**
- T150.** Pana AM, Rusnac LM, Bandur G, Deleanu C, Balan M, Silion M
 Synthesis and characterization of new glycopolymers based on monosaccharides and maleic anhydride II. Mannose derivatives
Mater. Plast., 47 (3): 299-305, **2010**.
- C349.** Pascariu MC, Rusnac LM, Macsim AM
 Tethered glycoderivatives with unsaturated spacer: Synthesis and characterization
Synth. Comm. 42 (17): 2503-2511, **2012**
- C350.** Rusu LC, Ardelean L, Podariu AC, Matei C, Tampa M
 Allergenic potential evaluation of acrylic resins from the complete prostheses
Mater. Plast. 49 (2): 133-134, **2012**
- C351.** Podariu AC, Ardelean L, Jumanca D, Galuscan A, Rusu LC
 Determining the amount of volatile organic phase in PMMA dentures
Rev. Chim 63 (7): 720-721, **2012**
- T151.** Pana AM, Rusnac LM, Bandur G, Sisu E, Badea V, Silion M
 Synthesis and characterization of new glycopolymers based on monosaccharides and maleic anhydride I. Glucose derivatives
Mater. Plast., 47 (1) , pp. 28-34, **2010**
- C352.** Pascariu MC, Rusnac LM, Macsim AM
 Tethered glycoderivatives with unsaturated spacer: Synthesis and characterization *Synth. Comm.* 42 (17): 2503-2511, **2012**

TOTAL: 352*0.5 = **176**

Anexa 4.20

Factor de impact cumulat conform *Web of Science* (Thomson Reuters)³
FI×(N_{ic}/N_a)

1.	M. Goodarzi, S. Funar-Timofei, Y. Vander Heyden Towards better understanding of feature selection/reduction techniques for QSAR models <i>TrAC-Trend. Anal. Chem.</i>, 42, 49-63, 2013	6.273x(1/3)	2.091
2.	Margan D., Ilia G., Borota A., Mracec M. Conformational analysis of prostaglandin E2. II <i>Rev.Roum.Chim.</i>, 57, 449-456, 2012	0.418x(2/4)	0.209
3.	Halip L., Gruia A.T., Borota A., Mracec M., Curpan R.F., Mracec M. 3D homology model of the alpha(2C)-adrenergic receptor subtype <i>Rev.Roum.Chim.</i>, 57, 763-768, 2012	0.418x(4/6)	0.279
4.	Liliana Ostopovici-Halip, Ramona Rad-Curpan, Modeling of ligand binding to dopamine D2 receptor, <i>J.Serb. Chem. Soc.</i> (2013) doi: 10.2298/JSC130208046O	0.912x(2/2)	0.912
5.	Crisan L., Pacureanu L., Bora A., Avram S., Kurunczi L., Implementation of PLS discriminant analysis to rank indirubin derivatives against decoys, <i>Cent. Eur. J. Chem.</i>, 11(10), 1644-1656, 2013	1.167x(4/5)	0.934
6.	Crisan L., Pacureanu L., Avram S., Bora A., Avram S., Kurunczi L., Shape-based similarity and PLS analysis of maleimide derivatives, <i>J. Enz. Inhib. Med. Chem.</i>, DOI:10.3109/14756366.2013.833196, 2013	1.495x(4/6)	0.997
7.	Avram S.I., Crisan L., Bora A., Pacureanu L.M., Avram S., Kurunczi L. Retrospective group fusion similarity search based on eROCE evaluation metric, <i>Bioorg. Med. Chem.</i>, 21(5), 1268-1278, 2013	2.903x(4/5)	2.322
8.	Ivan D., Funar-Timofei S., Medeleanu M., Mracec M., Mracec M. Formation Enthalpy for conformers of (3s,5s,6s)-6-Acetylaminopenicillanic Acid calculated by the PM6 and PM7 semiempirical MO Methods, <i>Rev. Roum. Chim.</i>, 58(4-5),463-472, 2013.	0.331x(3/5)	0.199
9.	Tarabukina E., Fagadar-Cosma E., Enache C., Zakharova N., Birdeanu M. Molecular Properties and Aggregation of Porphyrin Modified Polysiloxane in Solutions <i>J. Macromol. Sci. Phys.</i> 52(8): 1077-1091, 2013	0.807x(2/5)	0.323
10.	Vlascici D., Popa I., Chiriac V.A., Fagadar-Cosma G., Popovici H., Fagadar-Cosma E. Potentiometric detection and removal of copper using	1.31x(1/6)	0.218

	porphyrins <i>Chem. Centr. J.</i> 7(1): 111, 2013		
11.	Iordache S., Cristescu R., Popescu A.C., Popescu C.E., Dorcioman G., Mihailescu I.N, Ciucu A.A., Balan A., Stamatin I., Fagadar-Cosma E., Chrisey D.B. Functionalized porphyrin conjugate thin films deposited BZ matrix assisted pulsed laser evaporation <i>Appl. Surf. Sci.</i> 278: 207-210, 2013	2.112x(1/11)	0.192
12.	Bîrdeanu M., Bîrdeanu A.-V., Gruia A.S., Fagadar-Cosma E., Avram C.N. Synthesis and characterization of Zn ₃ Ta ₂ O ₈ nanomaterials by hydrothermal method <i>J. Alloy. Compd.</i> 573: 53–57, 2013	2.390x(1/5)	0.478
13.	Press release FP7-Project Fagadar-Cosma E., Gil-Agusti M. SOMABAT- Development of novel solid materials for high power Li polymer batteries (SOMABAT) recyclability of components-press release <i>Rev. Chim. Buc.</i> 63(10): 2 pag. 2012	0.538x(1 /2)	0.269
14.	Creangă I., Făgădar-Cosma G., Palade A., Lascu A., Enache C., Birdeanu M., Făgădar-Cosma E. New hybrid silver colloid-A ₃ B porphyrin complex exhibiting wide band absorption <i>Digest J. Nanomater. Bios.</i> 8(2): 561-572, 2013	1.092x(5/7)	0.780
15.	Palade A., Fagadar-Cosma G., Lascu A. Creanga I., Birdeanu M., Făgădar-Cosma E. New porphyrin-based spectrometric sensor for Ag ⁰ detection <i>Digest J. Nanomater. Bios.</i> 8(3): 1013-1022, 2013	1.092x(3 /3)	1.092
16.	Birdeanu M, Birdeanu A.V., Fagadar-Cosma E., Enache C., Miron I., Grozescu I. Structural, morphological, optical and thermal properties of the ZnTa ₂ O ₆ nanomaterials obtained by solid state method <i>Digest J. Nanomater. Bios.</i> 8(1): 263-272, 2013	1.092x(2/6)	0.364
17.	Ilia G., Crasmareanu E., Pascut D., Darabantă L., Simulescu V. The use of mass spectrometry in obstetric and gynecology <i>Cent. Eur. J. Chem.</i> 11(5): 645-654, 2013	1.167x(3/5)	0.700
18.	Balint E., Tajti A., Drahos L., Ilia G., Keglevich G. Alcoholysis of dialkyl phosphites under microwave conditions <i>Curr. Org. Chem.</i> 17(5): 555-562, 2013	3.434x(1/5)	0.687
19.	Petric M., Crisan L., Crisan M., Micle A., Maranescu B., Ilia G. Synthesis and QSRR Study for a Series of Phosphoramidic Acid Derivatives <i>Heteroatom Chem.</i> 24(2): 138 -145, 2013.	1.577x(4/6)	1.051
20.	Margan D. Borota A., Ilia G., Mracec M. Conformational Analysis for prostglandin E2II <i>Rev. Roum. Chim.</i> 57(4-5): 449-456, 2012	0.331x(3/4)	0.248

21.	Crasmareanu E., Simulescu V., Ilia G. Synthesis by Reversed Phase Transfer Catalysis and Characterization of Naphthol AS-D pigment <i>J. Chem.</i> . Article ID 545374, 2013 .	0.484x(3/3)	0.484
22.	Crisan M., Bouros P., Chumakov Y., Petric M., Ilia G. Supramolecular assembly and ab initio quantum chemical calculations of 2-hydroxyethylammonium salts of para-substituted benzoic acids <i>Cryst. Growth Des.</i> 13(1): 143-154, 2013	4.689x(3/5)	2.813
23.	Grad M.E., Simu G.M., Muntean S.G., Ilia G. Synthesis, characterization and colour determination using CIELAB colour space of stilbene dyes, <i>J. Iran. Chem. Soc.</i> 10(4): 807-816, 2013	2.072x(3/4)	1.554
24.	Muntean S.G., Paska O.M., Coseri S., Simu G.M., Grad M.E., Ilia G. Evaluation of a functionalized copolymer as adsorbent on direct dyes removal process: kinetics and equilibrium studies <i>J. Appl. Polym. Sci.</i> 127(6): 4409-4421, 2013	1.395x(4/6)	0.930
25.	Pacurariu C., Mihoc G., Popa A., Muntean S.G., Ianos R. Adsorption of phenol and p-chlorophenol from aqueous solutions on poly (styrene-co-divinylbenzene) functionalized materials, <i>Chem. Eng. J.</i> 222: 218–227, 2013	3.461x(2/5)	1.384
26.	Plesu N., Kellenberger A., Taranu I., Taranu B.O., Popa I. Impedimetric detection of dopamine on poly(3-aminophenylboronic acid) modified skeleton nickel electrodes <i>React. Functional Polym.</i> 73(5): 772-778, 2013	2.505x(1/5)	0.501
27.	Kellenberger A., Plesu N., Tara-Lunga Mihali M., Vasziicsin N. Synthesis of polyaniline nanostructures by electrochemical deposition on niobium, <i>Polymer</i> 54(13): 3166-3174, 2013	3.379x(2/4)	1.690
28.	Iliescu S., Zubizarreta L., Plesu N., Macarie L., Popa,A., Ilia G. Polymers containing phosphorus groups and polyethers: from synthesis to application <i>Chem. Cent. J.</i> 6: 132, 2012 (neraportata in 2012)	1.312x(5/6)	1.093
29.	Buruiana L.-I., Avram E., Popa A., Stoica I., Ioan S. Influence of triphenylphosphonium pendant groups on the rheological and morphological properties of new quaternized polysulfone <i>J. Appl. Polym. Sci.</i> 129(4): 1752-1762, 2013	1.395x(1/5)	0.279
30.	Ciopec M., Davidescu C.- M., Negrea A., Lupa L., Popa A., Muntean C., R. Ardelean, G. Ilia Synthesis, characterization, and adsorption behavior of aminophosphinic grafted on poly(styrene-Co-divinylbenzene) for divalent metal ions in aqueous solutions <i>Polym. Eng. Sci.</i> 53(5): 1117-1124, 2013	1.243x(2/8)	0.311

31.	Parvulescu V., Niculescu V., Ene R., Popa A., Mureseanu M., Ene, C. D., Andruh M. Supported monocationic copper(II) complexes obtained by coordination with dialkylphosphonate groups on styrene-divinylbenzene copolymer as catalysts for oxidation of organic compounds <i>J. of Molec. Catalysis A-Chemical</i> , 366: 275-281, 2013	3.187x(1/7)	0.455
32.	Davidescu C.-M., Ciopec M., Negrea A., Popa A., Lupa L., Dragan E.-S., Ardelean R., Ilia G., Iliescu S. Synthesis, characterization, and Ni(II) ion sorption properties of poly(styrene-co-divinylbenzene) functionalized with aminophosphonic acid groups, <i>Polym. Bull.</i> 70(1): 277-291, 2013	1.332x(3/9)	0.444
33.	Visa A., Maranescu B., Bucur A., Iliescu S., Demadis K. Synthesis and Characterization of a Novel Phosphonate Metal Organic Framework Starting from Copper Salts <i>Phosphorus Sulfur DOI: 10.1080/10426507.2013.843004</i> , 2013	0.601x(3/5)	0.361
34.	Holclajtner-Antunovic I.D., Popa A., Bajuk-Bogdanovic D.V., Mentus S., Nedic Vasiljevic B.M., Uskokovic-Markovic S.M , Synthesis and characterization of acid silver salts of 12-tungstophosphoric acid, <i>Inorg. Chim. Acta</i> , 407, 197–203, 2013	1.899x(1/6)	0.317
35.	Popa A., Sasca V., Verdes O., Barvinschi P., Holclajtner-Antunović I. Acidic and neutral cesium salts of 12-molybdophosphoric acid supported on SBA-15 mesoporous silica. The influence of Cs concentration and surface coverage on textural and structural properties, <i>Mater. Res. Bull.</i> , 50, 312-322, 2014	1.913x(3/5)	1.148
36.	Vlad-Oros B., Dascalu D., Dudas Z., Popovici H., Preda G., Ostafer V. Equilibrium and Kinetics Studies Regarding the Adsorption of Copper (II) Ions by various types of Chitosan Beads <i>Dig. J. Nanomater. Bios.</i> , 8(3), 917 – 927, 2013	1.092x(1/6)	0.182
37.	Sasca V., Verdes O., Avram L., Popa A., Erdohelyi A., Oszko A., The $Cs_xH_{3-x}PW_{12}O_{40}$ catalysts microstructure model, <i>Appl Catal A: Gen</i> 451 50–57 2013	3,410x(4/6)	2.273
38.	Sasca V., Popa A., Band-gap energy of heteropoly compounds containing Keggin polyanion- $[PV_xMo_{12-x}O_{40}]^{-(3+x)}$ relates to counter-cations and temperature studied by UV-VIS diffuse reflectance spectroscopy <i>J Appl Phys</i> , 114, 133503(1-7) 2013	2,210x(2/2)	2.210
39.	Sasca V., Verdes O., Avram L., Popa A., Thermal decomposition of Pd doped 12-tungstophosphoric acid and some of its cesium salts <i>Rev Roum Chim</i> 58(4-5) 451-461 2013	0,331x(4/4)	0.331

40.	Putz M.V., Putz A.M. DFT Chemical Reactivity Driven by Biological Activity: Applications for the Toxicological Fate of Chlorinated PAHs. <i>Str. Bond.</i> , 150 (2013) 181–232; DOI: 10.1007/978-3-642- 32750-6_6;	4.068)×(1/2)	2.034
TOTAL			35.139

Anexa 4.21

O carte apărută într-o editură consacrată din țară

- 1 Ilia G., Fagadar-Cosma E., Iliescu S., Macarie L., Plesu N., Fagadar-Cosma G., Popa A.
Solid polymer electrolites for batteries
Editura Mirton, Timisoara, ISBN 978-973-52-1396-1, 230 pag., **2013.** 7x(6/7) 6

TOTAL: 6

Anexa 4.22

O carte editată într-o editură consacrată din țară⁷

Anexa 4.23

Un articol apărut într-o revistă recunoscută de CNCS (B+) sau indexată într-o bază internațională de date (BDI)

Anexa 4.24

O conferință invitată/plenară/keynote prezentată la o manifestare științifică internațională

1. Făgădar-Cosma E., speaker invitat video-conferință:
Research Trends and the Elsevier Labs presents: “The Individual and Scholarly Network - a two-part seminar on Building Networks and Evaluating Network Relationships”
January 22, 2013
2. Făgădar-Cosma E., speaker invitat video-conferință:
“Collaboration and Communication regarding EU Research programmes. Challenges
Elsevier –Invitation Innovation Explorers, <https://elsevier.comunispace.com/>
3. Făgădar-Cosma E.
Conferință: “Porphyrins. Optoelectrical applications”
13th Edition of Academic Days Timisoara - New trends and strategies in the chemistry of advanced materials with relevance in biological systems, technique and environmental protection, Timișoara, România, 22, Ed. Art Press, ISSN: 2065-0760, 2013.

TOTAL: 10*3=30

Anexa 4.25

O conferință invitată/plenară/*keynote* prezentată la o manifestare științifică națională

Anexa 4.26

O comunicare orală prezentată la o manifestare științifică internațională

$$5 \times (N_{ic}/N_a)$$

1.	Pacureanu L.M., Bora A., Crisan L., Avram S., Ivan D., Neanu C. Theoretical work beyond imagination CDK's inhibitors selectivity versus optimal off-target effect <i>13th Edition of Timisoara's Academic Days, New Trends and Strategies in the Chemistry of Advanced materials with relevance in Biological Systems, technique and Environmental Protection, Chemistry</i> , 13-14 June 2013, 48, P26, Timișoara, Romania.	5×(6/6)	5.000
2.	Taranu B.-O., Fagadar-Cosma E., Popa I., Fagadar-Cosma G., Vlascici D., Birdeanu M. I., Taranu I. Preliminary studies on glassy carbon electrode modified with a novel functionalized A ₃ B porphyrin. Application as potentiometric cation sensor <i>Proceedings of the 19th International Symposium on Analytical and Environmental Problems</i> , 23 September 2013, Szeged (Hungary), 80-83, ISBN 978-963-315-141-9	5×(1/7)	0.714
3.	Cristescu R., Popescu A., Popescu C., Mihailescu I.N., Ciucu A.A., Balan A., Iordache S., Stamatin I., Fagadar-Cosma E., Chrisey D.B. Novel meso-phenyl unsymmetrical substituted porphyrin thin films deposited by MAPLE <i>E-MRS 2013 SPRING MEETING Congress Center - Strasbourg, France, Symposium O: Synthesis, processing and characterization of nanoscale multi functional oxide films IV, Technical sessions: May 27-31, 2013</i>	5×(1/10)	0.500
4.	Făgădar-Cosma E., Vlascici D., Pică E.M., Costișor O., Cosma V., Olenic L., Bizerea O. Procedure for obtaining of a highly selective potentiometric sensor for silver ion detection based on porphyrin ionophore <i>EuroInvent 2013 European Exhibition of Creativity and Innovation</i> , 9-11 mai 2013, Iasi, Romania, ISBN: 978-973-703-891-3, Editura Universitatii Al.I. Cuza Iasi, 137, 2013	5×(2/7)	1.429
5.	Dudás Z., Enache C., Savii C. Low temperature willemite luminescent properties enhanced by activators <i>13th Edition Timisoara's Academic Days, Chemistry</i> , June 13-14 2013, Timisoara, Romania	5×(3/3)	5.000
6.	Dudás Z., Enache C., Fábián M., Lazău R., Savii C. Rare-Earth co-Dopant Effect upon the Structure of Sol-Gel Derived Inorganic Luminophores <i>Conference for Young Scientist in Ceramics -The Tenth Students' Meeting, SM-2013</i> November 6-9, 2013, pp. 49, Novi Sad, Serbia	5×(2/5)	2.000
7.	Sorescu S-L, Ianasi C., Stefanescu M.	5x(2/3)	3.333

	Synthesis of Fe2O3/SiO2 nanocomposites from Fe(III) carboxylate precursors inside hybrid silica gels, <i>Conference for Young Scientist in Ceramics -The Tenth Students' Meeting, SM-2013</i> , November 6-9, 2013, pp. 83, Novi Sad, Serbia		
8.	Sasca V. Z., Verdes O., Popa A., Furcă M., Barbu M., Ethanol dehydration on $H_{3-x}Cs_xPW_{12}O_{40}$ and Pd doped catalysts, <i>International Symposium of the Romanian Catalysis Society, Cluj-Napoca, Romania, May 29-31, 2013</i> , p.47-48	5x(5/5)	5.000
9.	Sasca V. Z., Verdes O., Furca M., Popa A. Thermogravimetric standard method used to the determination of the kinetic parameters for decomposition of heteropoly acidic catalysts and their thermal endurance calculation. <i>The 19th Symposium on Analytical and Environmental Problems, Szeged, 23 Septembrie 2013</i>	5x(4/4)	5.000
10.	Sasca V., Verdes O., Popa A. Study on TPD of basic substances by thermogravimetry for Bronsted acidity determination from solid catalysts <i>Timisoara's Academic Days XIIIth, New trends and strategies in the chemistry of advanced materials with relevance in biological systems, technique and environmental protection, Timișoara, 13- 14 June, 2013</i> , p. 87.	5x(3/3)	5.000
11.	Verdeş O., Sasca V., Popa A., Barbu M., Furca M. L., Oszko A., Catalytic activity of Pd doped $Cs_xH_{3-x}PW_{12}O_{40}$ in relation with its microstructure <i>Timisoara's Academic Days XIIIth, New trends and strategies in the chemistry of advanced materials with relevance in biological systems, technique and environmental protection, Timișoara, 13-14 June, 2013</i> , p. 122.	5x(5/6)	4.167
12.	Furca M. L., Barbu M., Verdeş O., Popa A., Sasca V., Catalytic activity of Ni doped $Cs_xH_{3-x}PW_{12}O_{40}$ for ethanol conversion <i>Timisoara's Academic Days XIIIth, New trends and strategies in the chemistry of advanced materials with relevance in biological systems, technique and environmental protection, Timișoara, 13-14 June, 2013</i> , p. 135.	5x(5/5)	5.000
13.	Popa A., Sasca V., Verdes O., Furca, Barbu M.L. UV-Vis DRS studies of some supported catalysts <i>Timisoara's Academic Days XIIIth, New trends and strategies in the chemistry of advanced materials with relevance in biological systems, technique and environmental protection, Timișoara, 13-14 June, 2013</i> , p. 106.	5x(5/5)	5.000
14.	Barbu M., Furca M., Sasca V. Preparation and characterization of $CS_xH_{3-x}PW_{12}O_{40}$ doped with Ni <i>Timisoara's Academic Days XIIIth, New trends and strategies in the chemistry of advanced materials with relevance in biological systems, technique and environmental protection, Timișoara, 13-14 June, 2013</i> , p. 131.	5x(3/3)	5.000
	TOTAL		52.143

Anexa 4.27

O comunicare orală prezentată la o manifestare științifică națională

Anexa 5.1

Un grant câștigat de către institut/centru de la organizații internaționale

1. Proiect SOMABAT -FP7, Nr. 266090/2010-11-09

Denumire proiect: Development of novel solid materials for high power Li polymer bateries (SOMABAT). Recyclability of components.

Responsabil Proiect ICT (PARTENER 5) Eugenia Fagadar-Cosma

Valoare proiect: **78794 Eur**

Durata contractului: 3 ani

6

2. FP7 EU-OPENSCREEN -European Infrastructure of Open Screening Platforms for Chemical Biology Grant nr.261861, Preparatory PhaseFonduri acordate: **4400 Eur.**

Institutul de Chimie Timisoara - reprezentant national.

Director proiect: Dr. Liliana Pacureanu

2

3. Proiect CEI (Central European Initiative)

Denumire Proiect: Fostering scientific cooperation in CEI countries through research and training in renewable energies and nanophysics

Coordonator : UNESCO Chair at Horia Hulubei Foundation, <http://www.unescocchair-hhf.ro/>

Director Proiect : Victor Barsan

Responsabili Proiect: Laura Tugulea, Stefan Antohe, Eugenia Fagadar-Cosma (intra muros expert), Radu Lungu, Sandica Manole

Valoare proiect: **43200 EUR**

Durata contractului: 1 an (mai 2013/mai 2014).

4

Total: 12

Anexa 5.2

Un grant câștigat de către institut/centru de la organisme naționale 2013

In calitate de coordonator

1. Grant CNCSIS PD nr. 174/2010: Reactivitatea chimică – cauza majoră de rezultate false în testarea biologică de capacitate ridicată?

Diretor de proiect: Dr. Curpă Ramona

Valoare totală grant: **63.000 RON/2013**

Durata: 4 ani (2010-2014)

2

2. Grant CNCSIS PD nr. 119/2010: Noi strategii de identificare a compușilor farmacologic activi pe receptorii cuplați cu proteine G (GPCR) orfani

Diretor de proiect: Dr. Halip Liliana

Valoare totală grant: **170.000 RON/2013**

Durata: 4 ani (2010-2014)

3

3. Proiect PNII Capacitati-Modul III-SOMABAT Nr. 128EU/28 iunie 2011

Cofinanțare la PROIECTUL de Colaborare EU-FP7

Denumire proiect: Dezvoltarea de noi materiale solide pentru baterii Li-polimerice (SOMABAT) cu putere mare. Reciclarea componentelor

Diretor de proiect: Eugenia Fagadar-Cosma

Valoare proiect: **73849 lei/2013**

Durata contractului: 2011-2013

2

4. Proiect PN 09-450102, Program Nucleu INCDFM Institutul Național de Cercetare – Dezvoltare pentru Fizica Materialelor și Institutul de Chimie Timișoara

Titlul proiectului: Prepararea și caracterizarea materialelor cu dimensionalitate redusă pentru confeționarea de senzori

Diretor de proiect: Mihai Popescu

Titlu fază **2013**: Straturi Langmuir-Blodgett depuse pe stearat de Ba cu metalo-porfirine și nanotuburi de carbon. Senzori rezistivi.

Parteneri: Eugenia Făgădar-Cosma (Institutul de Chimie Timișoara)

-

In calitate de partener

5. Grant PN-II-RU-TE-2011-3-92: Contract de finanțare nr. 81/05.11.2011; Retele metal organice fosfonice: complexitatea si diversitatea structurilor si a aplicatiilor

Diretor de proiect: Dr. Visa Aurelia

Valoare totală grant: **215671 RON/2013**

Durata: 3 ani (2011-2014)

3

Colaborare bilaterală

6. Contract nr. 669/2013 România Ungaria 2013-2014; Modul III

Institutul de Chimie Timisoara Cordonator: Dr. Ing. Ilia Gheorghe

Universitatea Tehnica si Economica Budapesta: Cordonator: Prof Keglevich Gyorgy

Valoare totală grant: **13500 RON/2013**

Durata: 20 luni (2013-2014)

2

Total: 12

Anexa 5.3

Un contract extrabugetar obținut de către institut/centru de la organizații internaționale sau naționale

1 Contract Nr. 1159/25.08.2008, Act Aditional Nr. 2/19.01.2010 - S.C. SYSTRONICS S.R.L, Ing. Milos Mihai – 3695.20 RON	0.5
2. Contract nr. 547/1997, Act Adițional 891/01. 09. 2004 Tema: Monitorizarea calităților fizice și chimice ale unor organe de asamblare din oțeluri speciale. Beneficiar S. C. Notabil Pek SRL, Timișoara; Valoare: 9972.55 RON	1
3. Contract participațiupe nr. 1098/1997, Act adițional nr. 1/2004 Tema: Materiale avansate cu proprietăți optice și magnetice speciale Beneficiar: MOBIFON, Timișoara; Valoare: 101925.75 RON	3
4. Contract participațiupe SC UNDERGROUND SRL, nr. 1154/1997; Valoare: 30624 RON	2
5. Contract participatiune nr. 1338/1998-SC Teletim SRC, Valoare: 22968 RON	2
6. Consiliu Județean Timis; Centrul de Cultura si Arta al Județului Timis; contract nr.849/22.05.2013 Tema: sustinere Simpozion <i>Timisoara's Academic Days, 13th Edition, New trends and strategies in the chemistry of advanced materials with relevance in biological systems, technique and environmental protection</i> , 13-14 Iun., Timișoara, România, 2013 Valoare: 7000 RON	1
7. Contract de colaborare cu ISIM Tema: prestari servicii Valoare: 2000 RON	0.5
8. Ministerul Educației Naționale (MEN) – ANCS; contract nr. 21/28.05.2013 Tema: sustinere Simpozion <i>Timisoara's Academic Days, 13th Edition, New trends and strategies in the chemistry of advanced materials with relevance in biological systems, technique and environmental protection</i> , 13-14 Iun., Timișoara, România, 2013 Valoare: 2000 RON	0.5

Total: 10.5

Anexa 5.4

O manifestare științifică (congres, conferință, simpozion) sau școală de vară internațională organizată de institut

A. Simpozion

1. Simpozion: "*13th EDITION OF ACADEMIC DAYS TIMISOARA - New trends and strategies in the chemistry of advanced materials with relevance in biological systems, technique and environmental protection*", June 13-14, 2013, Timisoara, Romania.

10

B. Organizare de Workshop -

C. Manifestari Stiintifice la care ICT este co-organizator.

2. Asociatia de Cercetare Multidisciplinara pentru Zona de Vest, Romania – Ungaria – Serbia, ACMV, Al XV-lea Simpozion International “Tinerii si Cercetarea Multidisciplinara” ISYPMR – Timisoara 14-15 nov. 2013

10

Total: 20

Anexa 5.5

**O manifestare științifică (congres, conferință, simpozion) sau școală de vară națională
organizată de institut**

Anexa 6.1
Un brevet acordat

Anexa 6.2
Un brevet aplicat

Anexa 6.3
Un brevet citat în *Web of Science* (Thomson Reuters)

Anexa 6.4

**Produse și tehnologii rezultate din activități de cercetare bazate pe omologări sau
inovații proprii (produs vândut, sume încasate)**

Anexa 6.5
Un laborator de cercetare-dezvoltare acreditat

Anexa 6.6
Studii de impact si servicii comandate de un beneficiar

1. Dr. Curpăń Ramona - Reactivitatea chimică – cauza majoră de rezultate false în testarea biologică de capacitate ridicată?

Grant PN-II-RU-PD-2010; Contract de finanțare PD_502, nr. 174/2010 încheiat între UEFISCDI și Institutul de Chimie Timișoara al Academiei Române

2. Dr. Liliana Halip - Noi strategii de identificare a compușilor farmacologic activi pe receptori cuplați cu proteine G (GPCR) orfani

Grant PN-II-RU-PD-2010; Contract de finanțare PD_500, nr. 119/05.08.2010 încheiat între UEFISCDI și Institutul de Chimie Timișoara al Academiei Române

3. Făgădar-Cosma Eugenia - Dezvoltarea de noi materiale solide pentru baterii Li-polimerice (SOMABAT) cu putere mare. Reciclarea componentelor

Proiect PNII Capacități-Modul III-SOMABAT Nr. 128EU/28 iunie 2011; Cofinanțare la PROIECTUL de Colaborare EU-FP7

4. Făgădar-Cosma Eugenia - Prepararea și caracterizarea materialelor cu dimensionalitate redusă pentru confecționarea de senzori'

Titlu fază 2013: Straturi Langmuir-Blodgett depuse pe stearat de Ba cu metalo-porfirine și nanotuburi de carbon. Senzori rezistivi

Proiectul PN 09-450102, Program Nucleu INCDFM Institutul Național de Cercetare – Dezvoltare pentru Fizica Materialelor și Institutul de Chimie Timișoara

5. Dr. Visa Aurelia - Retele metal organice fosfonice: complexitatea și diversitatea structurilor și a aplicațiilor

Grant PN-II-RU-TE-2011-3-92; Contract de finanțare nr. 81/05.11.2011 încheiat între UEFISCDI și Institutul de Chimie Timișoara al Academiei Române

6. Dr. Ramona Tudose - Evaluarea activitatii antitumorale și antivirale a unor noi combinatii complexe continand elemente 3d și acizi biliari, baze Schiff și baze Mannich. Institutul de Morfologie, Patologie și Antropologie Experimentală și Muzeu al Academiei Bulgară de Științe din Sofia

7. Dr. Savii Cecilia - Sinteza și caracterizarea unor nanomateriale chimic active

Academia de Științe a Republicii Cehe, Institutul de Chimie Anorganica, Departamentul de Chimia Stării Solide și Compuși de Intercalare, Praga, Republica Cehe

8. Dr. Popa Alexandru - Heteropoliajizi cu structura Keggin folositi în cataliza eterogenă Universitatea din Belgrad, Facultatea de de Chimie Fizică și la Departamentul de Cataliză și Inginerie chimică din cadrul Institutului de Chimie Tehnologie și Metalurgie, Localitatea Belgrad, Serbia

9. Milos Mihai - Studii perspective privind determinarea continutului de oligoelemente în produse biologice. Metode preparative în spectroscopia de absorbtie atomica.

Beneficiar: Proiect Nr. 2/2010, cod CNCIS ID-PCCE-140 din cadrul Programului PNCDI-II-IDEI, Aplicatii ale compusilor metalelor - Metallomics - 2010-2013.

10. Milos Mihai - Optimizarea metodelor de analiza a otelurilor prin spectroscopie de absorbtie atomica. Beneficiar: S.C. SYSTRONICS S.R.L
11. Sasca Viorel - Proiectarea de catalizatori cu înaltă eficiență pentru conversia etanolului prin cercetare comună complementară; Proiect HURO/0901/090/2.2.2, Program de Cooperare Transfrontalieră Ungaria-Romania (CBC Phare Programme) 2007-2013.
12. Milos Mihai - Monitorizarea calităților fizice și chimice ale unor organe de asamblare din oțeluri speciale. Contract nr. 547/1997, Act Adițional 891/01. 09. 2004; Beneficiar S. C. Notabil Pek SRL
13. Tema: Materiale avansate cu proprietăți optice și magnetice speciale; Contract participație nr. 1098/1997, Act adițional nr. 1/2004; Beneficiar: MOBIFON.
14. Tema: Obținerea unor doze solutii de reactivi chimici si pentru atac metalografic pe probe sudate si nesudate tip A, B, C, D, E si F conform cu lista de reactivi CR 12361; Beneficiar: ISIM.
15. Dr. Savii Cecilia - Tema: Magnetita micrometrica, monocristalina, monodispersa, functionalizata, cu comportament superparamagnetic pentru uz in imagistica gastrointestinala, ca agent de contrast de tip MRI T2. Coordonator: Institutul C&D pentru Electrochimie si Materie Condensata, Timisoara
16. Dr. Savii Cecilia - Tema: Acoperiri rezistente la eroziune-coroziune obținute prin tehnologii inovative de pulverizare termică cu aplicare în medii apoase; Coordonator: Universitatea Politehnica din Timișoara
17. Dr. Ramona Tudose: Acoperirea implanturilor medicale cu straturi compozite biocompatibile depuse prin tehnici de pulverizare moderne; Beneficiar: Universitatea Politehnica din Timisoara.
18. Dr. Cseh Liliana: Recuperarea avansata a produselor utile din deseurile de catalizatori uzati; Beneficiar Pro Air Clean

Total: $18 \times 5 = 90$

Anexa 7.1
Institutul/centrul are dreptul de a conduce doctorate

1. INSTITUTUL DE CHIMIE TIMIȘOARA AL ACADEMIEI ROMÂNE (ICT)

Total: 20

Anexa 7.2
Conducători de doctorat care activează în institut

1. Prof. Dr. Zeno Simon, M.C. al Academiei Romane
2. Prof. Dr. Ludovic Kurunczi
3. Prof. Dr. Mircea Mracec
4. Dr. Otilia Costișor
5. Dr. Eugenia Lenuța Făgădar-Cosma

Total 5*20=100

**Anexa 7.3
Doctoranzi**

Doctoranzi angajati ai institutului

1. Creanga C. Maria-Ionela
2. Palade I. Anca-Maria
3. Ianăși M. Cătălin
4. Crețu V. Daniela Carmen
5. Bucovicean C. Carmen Maria
6. Mosoarca C. Elena Maria

Doctoranzi externi

1. Uderscu-Milosan V. Lucretia Paula
2. Țăranu I. Bogdan Ovidiu
3. Haidu I. Daniela
4. Oprescu I. Raul
5. Popa D. Iuliana
6. Gruia G. Alexandra Teodora
7. Mocanu P. Liviu Lucian
8. Olariu C. V. Tudor
9. Marius Mioc
10. Bogdan Dragos

Total doctoranzi : $6+10=16$

Punctaj : $16*10=\mathbf{160}$

Anexa 7.4
Post-Doctoranzi

1. Dr. Dudás Zoltán

Titlu: Luminophores and superparamagnetic composites, advanced optic and magnetic micro- and nano-materials with tunable structure, morphology and composition.

Institutia: Hungary, Budapest, Wigner Research Centre for Physics, Department of Neutron Spectroscopy

Durata: 3 ani, 01.10.2013-01.10.2016

Coordonator: Dr. János Füzi

10

2. Dr. Simulescu Vasile

Proiect: Excellent young researchers at BUT

Titlul temei: Research on delivery systems focusing on the physical chemistry of biopolymers and biocolloids

Institutia: Materials Research Centre, Faculty of Chemistry, Brno University of Technology, Brno, Czech Republic

Coordonator: Prof. Miloslav Pekar

10

3.Dr. Pana Ana-Maria

Proiect: Polimeri biodegradabili pe baza de carbohidrati / Materiale performante

Institutia:Universitatea Tehnica "Gheorghe Asachi" Iasi, Facultatea de Inginerie Chimica si Protectia Mediului

Coordonator: Prof dr.ing. dr.h.c. Marcel Popa

Durata: 01.03.2011 - 28.02.2013

10

Total: 30

Anexa 7.5

Cercetator angajat în institut/centru care a obținut titlul de doctor în perioada de evaluare

1. Avram Iancu Sorin
2. Furca Liliana Marinela
3. Barbu Mirela

TOTAL: 30

Anexa 8.1
Un membru în colectivul de redacție al unei reviste naționale/internationale

1. Făgădar-Cosma E. - ***Der Chemica Sinica*** www.pelagiaresearchlibrary.com (ISSN No 0976 – 8505) din anul 2010
2. Făgădar-Cosma E. - ***Advances in Applied Science Research***
www.pelagiaresearchlibrary.com (ISSN No 0976 – 8610) din anul 2010
3. Făgădar-Cosma E. - ***The Open Chemical and Biomedical Methods Journal***
<http://www.benthamscience.com/open/tocbmj/EBM.htm> (ISSN: 1875-0389) Bentham Science Publishers Ltd.
4. Făgădar-Cosma E. - ***Journal of Advanced Scientific Research***
<http://www.sciensage.info/jasr/editorial-board.php> (ISSN: 0976-9595)
5. Făgădar-Cosma E. - ***European Journal of Experimental Biology***,
<http://pelagiaresearchlibrary.com/european-journal-of-experimental-biology/index.html>
6. Făgădar-Cosma E. - ***American Journal of Organic Chemistry***
<http://journal.sapub.org/AJOC>, Scientific & Academic Publishing (<http://www.sapub.org/>), USA (ISSN: 2163-1271)
7. Făgădar-Cosma E. -***Chemical Sensors Journal***, Simplex Academic Publishers
www.simplex-academic-publishers.com
8. Făgădar-Cosma E. - ***The Science***, VA 22201, 703.778.3080
9. Făgădar-Cosma E. - ***American Journal of Nanoscience and Nanotechnology***,
<http://www.sciencepublishinggroup.com/j/NANO>
10. Făgădar-Cosma Eugenia - ***Annals of West University of Timisoara***
11. Ilia Gheorghe - ***Current Green Chemistry***, <http://www.benthamscience.com/cgc>
12. Ilia Gheorghe - ***American Journal of Polymer Science***,
<http://www.sapub.org/journal/aimsandscope.aspx?journalid=1019>
13. Simon Zeno - Revue Roumaine de Chimie
14. Costișor Otilia - Material Science Research Publ. Oriental Scientific , Publishing Company ISSN 0973-3469

TOTAL: 20*14 = **280**

Anexa 8.2

Un membru în conducerea unei organizații internaționale de specialitate

1. Fagadar-Cosma E. este membru (expert) în Comisia: Risk Assessment & Advisory Structure of Scientific Committees and Experts, EUROPEAN COMMISSION, Health systems and products; **e-Health and Health Technology Assessment**, Scrisoare de numire: Ref. Ares(2013)1262115 - 23/05/2013

TOTAL: 20

Anexa 8.3
Un membru al Academiei Române

1. Prof. Simon Zeno - Membru Corespondent al Academiei Române

TOTAL: 50

Anexa 8.4
Cercetător cu un indice Hirsch peste 8

1. Dr. Simona Funar-Timofei 12
2. Dr. Făgădar-Cosma Eugenia 8
3. Dr. Ilia Gheorghe 9
4. Dr. Iliescu Smaranda 8
5. Dr. Popa Adriana 9
6. Dr. Visa Aurelia 8

TOTAL: $20 \times 6 = 120$

Anexa 8.5
**Un membru de onoare (*fellow, senior*) al unei societăți științifice
naționale/internăționale**

1. Făgădar-Cosma E. este numită Senior Editor: Chemical Sensors (September 2012 to August 2013- application for 2013/2014) Section: New Materials Developments Academic Publishers Website: www.simplex-academic-publishers.com

TOTAL: 20

Anexa 8.6
Un premiu al Academiei Române

Anexa 8.7

Un premiu (distincție) al unei societăți științifice naționale obținut printr-un proces de selecție

1. Diploma și Medalia Petru Poni

Patent no. RO 123.447/30.05.2012

Făgădar-Cosma E., Vlascici D., Pică E.M., Costișor O., Cosma V., Olenic L., Bizerea O.
Procedure for obtaining of a highly selective potentiometric sensor for silver ion detection
based on porphyrin ionophore

Salonul National de Inventica Chim-Invent 2013, Academia Romana, Institutul De
Chimie Macromoleculară “Petru Poni”, 3-5 iulie 2013 Iasi, Romania.

TOTAL: 10

Anexa 8.8

Un premiu (distincție) al unei societăți științifice internaționale obținut printr-un proces de selecție

1. Diplomă și Medalie de AUR

Patent no. RO 123.447/30.05.2012

Făgădar-Cosma E., Vlascici D., Pică E.M., Costișor O., Cosma V., Olenic L., Bizerea O.
Procedure for obtaining of a highly selective potentiometric sensor for silver ion detection
based on porphyrin ionophore

5th European Exhibition of Creativity and Innovation, 9-11 May 2013, Iași, Catalog

Editura Universității Alexandru Ioan Cuza, Iași, ISBN: 978-973-703-891-3, 137 Editor:
Andrei-Victor Sandu.

2. Diplomă și Medalie de AUR

Patent no. RO 123.447/30.05.2012

Eugenia Făgădar-Cosma, Dana Vlascici, Elena Maria Pică, Otilia Costișor, Viorica Cosma,
Liliana Olenic, Otilia Bizerea

Procedure for obtaining of a highly selective potentiometric sensor for silver ion detection
based on porphyrin ionophore

Salonul Internațional al Cercetării, Inovării și Inventiilor "Pro Invent" Cluj-Napoca,
România, Ediția a XI-a, 19 - 23 martie 2013

3. Bianca Maranescu - premiu la postere oferit de editura RSC, jurnalul PCCP cu lucrarea:
Ni – vinyl phosphonate electrical properties, 44th IUPAC World Chemistry Congress,
Istanbul, Turcia, 11-16 August 2013, p. 1202

TOTAL: 40*3 = 120

Lucrări publicate ca rezumat la conferințe, congrese și simpozioane internaționale – Postere

1. Tăraru B., Popa I., Făgădar-Cosma E.

Electrochemical studies on novel functionalized A3B porphyrin

Timisoara's Academic Days, 13th Edition, New trends and strategies in the chemistry of advanced materials with relevance in biological systems, technique and environmental protection, 13-14 Iun., Timișoara, România, 2013, 36. (ISSN: 2065-0760)

2. Popa I., Tăraru B., Făgădar-Cosma E., Tăraru I.

Corrosion inhibition of carbon steel by 5,10,15,20-tetra(4-methylphenyl)-21h,23h-porphine cobalt (II), in acid media

Timisoara's Academic Days, 13th Edition, New trends and strategies in the chemistry of advanced materials with relevance in biological systems, technique and environmental protection, 13-14 Iun., Timișoara, România, 2013, 39. (ISSN: 2065-0760)

3. Șișu I., Ghiulai R., Lascu A., Șerb A., Capitan F., Pascariu M.-C., Rusnac L.-M., Șișu E.

Mass spectrometry analysis of maltodextrin-lactones

Timisoara's Academic Days, 13th Edition, New trends and strategies in the chemistry of advanced materials with relevance in biological systems, technique and environmental protection, 13-14 Iun., Timișoara, România, 2013, 62. (ISSN: 2065-0760)

4. Lascu A., Creanga I., Palade A., Fagadar-Cosma E.

Synthesis and spectroscopic characterization of Fe(III)-meso-tetra-(3-hydroxyphenyl) porphyrinate chloride

Timisoara's Academic Days, 13th Edition, New trends and strategies in the chemistry of advanced materials with relevance in biological systems, technique and environmental protection, 13-14 Iun., Timișoara, România, 2013, 57. (ISSN: 2065-0760)

5. Palade A., Făgădar-Cosma G., Lascu A., Creangă I., Birdeanu M., Bârsan V., Făgădar-Cosma E.

New porphyrin -based spectrophotometric sensor for Ag⁺ detection

Solar Energy for World Peace, August 17-19, 2013 Istanbul / Turkey, Book of Abstracts, Abstract: 0399, pag 266

6. Creangă I., Palade A., Lascu A., Făgădar-Cosma E.
Obtaining of silver colloid-A₃B porphyrin complex
Timisoara's Academic Days, 13th Edition, New trends and strategies in the chemistry of advanced materials with relevance in biological systems, technique and environmental protection, 13-14 Iun., Timișoara, România, **2013**, 61. (ISSN: 2065-0760)
7. Palade A., Lascu A., Creanga I., Fagadar-Cosma E.
Spectrophotometric sensor for Ag⁰ detection based on porphyrin
Timisoara's Academic Days, 13th Edition, New trends and strategies in the chemistry of advanced materials with relevance in biological systems, technique and environmental protection, 13-14 Iun., Timișoara, România, **2013**, 64. (ISSN: 2065-0760)
8. Petric M., Crisan L., Crisan M., Micle A., Maranescu B., Ilia G.
PLS study of phosphoramidic acid derivatives based on molecular descriptors,
Timisoara's Academic Days, 13th Edition, New trends and strategies in the chemistry of advanced materials with relevance in biological systems, technique and environmental protection, 13-14 Iun., Timișoara, România, **2013**, 66. (ISSN: 2065-0760)
9. Crisan M., Bouros P., Chumakov Y., Petric M., Ilia G.
Synthesis, crystal structure and biological activity of 2-hydroxyethylammonium salt of *para*-hydroxybenzoic acid
Timisoara's Academic Days, 13th Edition, New trends and strategies in the chemistry of advanced materials with relevance in biological systems, technique and environmental protection, 13-14 Iun., Timișoara, România, **2013**, 59. (ISSN: 2065-0760)
10. Kellenberger A., Plesu N., Taranu I., Taranu B. O., Popa I.
Nonoxidative impedimetric sensor based on poly(3-aminophenylboronic acid) modified skeleton nickel electrodes for dopamine detection
Fourth Regional Symposium on Electrochemistry South East Europe, 26-30 May, **2013**, Ljubljana, Slovenia, 43. ISBN 978-961-6104-23-4.
11. Kellenberger A., Plesu N., Taranu I., Taranu B. O., Popa I.
Eis assays of poly(3-aminophenylboronic acid) films on platinum electrodes,
Fourth Regional Symposium on Electrochemistry South East Europe, **2013**, 26-30 May, Ljubljana, Slovenia, 80, ISBN 978-961-6104-23-4.
12. Iliescu S., Visa A., Macarie L., Popa A., Maranescu B., Ilia G.
Polyphosphoesters obtained by inverse phase transfer catalysis
Timisoara's Academic Days, 13th Edition, New trends and strategies in the chemistry of advanced materials with relevance in biological systems, technique and environmental protection, 13-14 Iun., Timișoara, România, **2013**, 61. (ISSN: 2065-0760)

13. Ene R., Popa A., Parvulescu V.

Immobilized Cu(II) and Mn(II) complexes as catalysts for oxidation of hydrocarbons. Comparative study of polymer support functions

The International Symposium of The Romanian Catalysis Society, Cluj Napoca, Romania, May 29-31, **2013**, 102-103

14. Davidescu C.-M., Ardelean R., Popa A., Ilia G., Iliescu S.

Poly(styrene-co-divinylbenzene) functionalized with isopropylaminophosphonic acid used for removal of phenol compounds from aqueous solutions

13th Edition of Timisoara's Academic Days, Chemistry, Timisoara, Romania, June 13-14, **2013**, 44

15. Ene R., Filip M., Popa A., Mureseanu M., Parvulescu V.

Hybrid catalysts with Cu(II) and Mn(II) complexes obtained by functionalization of polymeric organic and inorganic supports

International Conference of Physical Chemistry - ROMPHYSCHM 15, Bucuresti, 1-13 sept. **2013**, 166

16. Buruiana L.-I., Avram E., Petreus O., Popa A., Ioan S.

Structure / antithrombogenic properties relationship of new phosphorus-modified polysulfones

18th International Conference on Chemistry and Chemical Engineering, Septembrie, 4-7, **2013**, Sinaia, Romania, S4-68,

17. Buruiana L.I., Avram E., Popa A., Ioan S.

Pseudoplastic behaviour of quaternized polysulfone/poly(vinylidene fluoride) blends, with implications in cellular engineering

International Conference of Physical Chemistry - ROMPHYSCHM 15, Bucuresti, 1-13 sept. **2013**, 48

18. Macarie L., Plesu N., Iliescu S., Ilia G.

Synthesis and characterization of copolymers of epoxyacrylate and 1-vinylimidazole
Timisoara's Academic Days, 13th Edition, New trends and strategies in the chemistry of advanced materials with relevance in biological systems, technique and environmental protection, *13-14 Iun., Timișoara, România, 2013, 110-113 (ISSN: 2065-0760)*

19. Visa A., Maranescu B., Bucur A.

Phosphonate Metal Organic Framework Synthesis For Diverse Applications

Timisoara's Academic Days, 13th Edition, New trends and strategies in the chemistry of advanced materials with relevance in biological systems, technique and environmental protection, 13-14 Iun., Timișoara, România, **2013**, 49

20. Maranescu B., Visa A., Simulescu V.

Synthesis And Characterization Of New Unsaturated Layered Metal Phosphonates

Timisoara's Academic Days, 13th Edition, New trends and strategies in the chemistry of advanced materials with relevance in biological systems, technique and environmental protection, 13-14 Iun., Timișoara, România, **2013**, 55

21. Visa A., Maranescu B., Bucur A.

Studies on the salts effect on crystallinity of phosphonate metal organic framework

44th IUPAC World Chemistry Congress, Istanbul, Turcia, 11-16 August **2013**, 906

22. Visa A., Maranescu B., Mracec M.

Structural properties analyses of phosphonate metal organic framework

44th IUPAC World Chemistry Congress, Istanbul, Turcia, 11-16 August **2013**, 1513

23. Maranescu B., Visa A.

Styryl phosphonic acid as precursor for new metal organic framework

44th IUPAC World Chemistry Congress, Istanbul, Turcia, 11-16 August **2013**, 1198

24. Maranescu B., Maranescu V., Visa A.

Ni–vinyl phosphonate electrical properties

44th IUPAC World Chemistry Congress, Istanbul, Turcia, 11-16 August **2013**, 1202

25. Maranescu B., Visa A.

A study on the effect of synthesis parameters of a new divalent metal phosphonate

International Conference of Physical Chemistry Romphschem 15, Bucharest, Romania, 11-13 September **2013**, 122

26. Visa A., Maranescu B., Mracec M.

Electronic Properties of Cu²⁺ vinylphosphonate Estimated by PM3 Semiempirical Method

International Conference of Physical Chemistry Romphschem 15, Bucharest, Romania, 11-13 September **2013**, 37

27. Cretu C., Tudose R., Cseh L., Dudas Z., Salifoglou A., Costisor O.

The crystal structures and fluorescence properties of a schiff base ligand and its novel homo-dinuclear Zn(II) complex

Timisoara's Academic Days, 13th Edition, New trends and strategies in the chemistry of advanced materials with relevance in biological systems, technique and environmental protection, 13-14 Iun., Timișoara, România, 2013, 40

28. Cretu C., Cseh L., Badea V., Zeng X., Tang B.J., Mehl G.H., Costisor O.

Synthesis and liquid crystalline properties of two new Schiff base ligands

Timisoara's Academic Days, 13th Edition, New trends and strategies in the chemistry of advanced materials with relevance in biological systems, technique and environmental protection, 13-14 Iun., Timișoara, România, 2013, 47

29. Bucovicean-Bereczki C.M., Cseh L., Tudose R., Salifoglou A., Costisor O.

The single-crystal x-ray diffraction analysis of the Schiff base N, N'-bis[3(4-dodecyloxy-benzylideneamino)-propyl]-piperazine and the infrared spectra study on its stability as ligand by complexation reactions.

Timisoara's Academic Days, 13th Edition, New trends and strategies in the chemistry of advanced materials with relevance in biological systems, technique and environmental protection, 13-14 Iun., Timișoara, România, 2013, 50

30. Pană A.M., Cseh L., Badea V., Costișor O.

pH-dependent photochromic behavior of a curcumin analogue

Timisoara's Academic Days, 13th Edition, New trends and strategies in the chemistry of advanced materials with relevance in biological systems, technique and environmental protection, 13-14 Iun., Timișoara, România, 2013, 53

31. Tudose R., Dudas Z., Costisor O.

Spectroscopic studies of mono- and binuclear complexes of Zn(II), Cu(II) and La(III) containing N,N'-bis-(antipyryl-methylen)-piperazine as a ligand

Timisoara's Academic Days, 13th Edition, New trends and strategies in the chemistry of advanced materials with relevance in biological systems, technique and environmental protection, 13-14 Iun., Timișoara, România, 2013, 130

32. Borota A., Halip L., Bora A., Ivan D., Neanu C.,

Pharmacophore models for histamine H3 receptor agonists

Timisoara's Academic Days, 13th Edition, New trends and strategies in the chemistry of advanced materials with relevance in biological systems, technique and environmental protection, 13-14 Iun., Timișoara, România, 2013, p.63, Timisoara, Romania, (Electronic vol. ISSN:2065-0760

33. Ostopovici-Halip L., Rad-Curpan R., Borota A.,

G-protein coupled receptor pharmacophore validation and analysis

Timisoara's Academic Days, 13th Edition, New trends and strategies in the chemistry of advanced materials with relevance in biological systems, technique and environmental protection, 13-14 Iun., Timișoara, România, 2013, p.65, Timisoara, Romania, (Electronic vol. ISSN:2065-07603

34. Ostopovici-Halip L., Bologa C. Innovative solutions for G-protein coupled receptors deorphanization

Timisoara's Academic Days, 13th Edition, New trends and strategies in the chemistry of advanced materials with relevance in biological systems, technique and environmental protection, 13-14 Iun., Timișoara, România, 2013, p. 58.

35. Ostopovici-Halip C., Bologa C. Key molecular features of the orphan G-protein coupled receptor (oGPCR).

Timisoara's Academic Days, 13th Edition, New trends and strategies in the chemistry of advanced materials with relevance in biological systems, technique and environmental protection, 13-14 Iun., Timișoara, România, 2013, p. 38.

36. Ostopovici-Halip L., Bologa C. Structurally conserved motifs in pharmacologically relevant class B and C G-protein-coupled receptors (GPCR), *44th IUPAC World Chemistry Congress*, 11-16 August 2013, Istanbul, Turcia.p.1307

37. Ostopovici-Halip L., Bologa C. A potential strategy for GPCR de-orphanization
44th IUPAC World Chemistry Congress, 11-16 August 2013, Istanbul, Turcia. p.1308

38. Ostopovici-Halip L, Bologa C.

Template Structure Selection for Homology Modeling of Class A Orphan G-protein Coupled Receptors

International Conference of Physical Chemistry ROMPHYSCHM 15, 11-13 September 2013, Bucharest, Romania. p34

39. Ostopovici-Halip L., Bologa C. Template Structure Selection for Homology Modeling of Class A Orphan G-protein Coupled Receptors *International Conference of Physical Chemistry ROMPHYSCHM* 15, 11-13 September 2013, Bucharest, Romania. p34

40. Bora A., Crisan L., Avram S., Neanu C., Pacureanu L.

Preliminary molecular docking study of 2-phenyl-chroman-4-one derivatives against cyclin dependent kinases

Timisoara's Academic Days, 13th Edition, New trends and strategies in the chemistry of advanced materials with relevance in biological systems, technique and environmental protection, 13-14 Iun., Timișoara, România, 2013, P50

41. Crisan L., Pacureanu L., Bora A., Avram S., Ivan D., Neanu C., Kurunczi L.

Preliminary PLS study of 38 benzofuran-3-yl-(indol-3-yl) maleimide and 18 4-azaindolyl-indolyl-maleimide derivatives using DRAGON and MOPAC descriptors

Timisoara's Academic Days, 13th Edition, New trends and strategies in the chemistry of advanced materials with relevance in biological systems, technique and environmental protection, 13-14 Iun., Timișoara, România, 2013, P54

42. Ivan D., Crisan L., Pacureanu L.,
3D-similarity analysis of HIV1- reverse transcriptase inhibitors
Timisoara's Academic Days, 13th Edition, New trends and strategies in the chemistry of advanced materials with relevance in biological systems, technique and environmental protection, 13-14 Iun., Timișoara, România, 2013, P55
43. Neanu C., Avram S., Borota A., Bora A., Crisan L., Pacureanu L.,
Mapping representative protein structures for Glycogen Synthase Kinase-3
Timisoara's Academic Days, 13th Edition, New trends and strategies in the chemistry of advanced materials with relevance in biological systems, technique and environmental protection, 13-14 Iun., Timișoara, România, 2013, P43
44. Pascariu M.C., Gruia A., Neanu C., Rafaila M., Rusnac L.M., Sisu E.N.V.,
Structure determination of sugar mono- and diacetal derivatives through GC-EI-MS combined with computational chemistry,
Timisoara's Academic Days, 13th Edition, New trends and strategies in the chemistry of advanced materials with relevance in biological systems, technique and environmental protection, 13-14 Iun., Timișoara, România, 2013, pag.56, P60
45. Avram S.I., Crisan L., Bora A., Pacureanu L.M., Avram S., Kurunczi L.
Prediction of Promiscuous Flavonoid-Related Compounds In High-Throughput Screenings
Timisoara's Academic Days, 13th Edition, New trends and strategies in the chemistry of advanced materials with relevance in biological systems, technique and environmental protection, 13-14 Iun., Timișoara, România, 2013, 48, P26
46. Pacureanu L.M., Bora A., Crisan L., Avram S., Ivan D., Neanu C.
Theoretical work beyond imagination CDK's inhibitors selectivity versus optimal off-target effect
Timisoara's Academic Days, 13th Edition, New trends and strategies in the chemistry of advanced materials with relevance in biological systems, technique and environmental protection, 13-14 Iun., Timișoara, România, 2013, 48, P26
47. Funar-Timofei S., Simu G., Ionescu D., Chicu S. A.
Sudan I structure study by molecular mechanics and quantum semiempirical methods
Timisoara's Academic Days, 13th Edition, New trends and strategies in the chemistry of advanced materials with relevance in biological systems, technique and environmental protection, 13-14 Iun., Timișoara, România, 2013, pag. 30, (poster).
48. Ostopovici-Halip L., Bora A., Rad-Curpăń R., Funar-Timofei S.
General aspects of CDK5 inhibition: II. 3-methyl triazoles attached to cyclohexyl thiophene
Timisoara's Academic Days, 13th Edition, New trends and strategies in the chemistry of advanced materials with relevance in biological systems, technique and environmental protection, 13-14 Iun., Timișoara, România, 2013, pag. 42, (poster).

49. Funar-Timofei S., Halip L., Borota A., Bora A.
Quantitative Structure-Activity Study of Some Cyclin-Dependent Kinase 5/P25 Inhibitors
Timisoara's Academic Days, 13th Edition, New trends and strategies in the chemistry of advanced materials with relevance in biological systems, technique and environmental protection, 13-14 Iun., Timișoara, România, 2013, pag. 46, poster.
50. Bora A., Ostopovici-Halip L., Curpăn R., Funar-Timofei S.
Identification of Novel Antitubercular Agents - Still a Challenge for the Scientist
Timisoara's Academic Days, 13th Edition, New trends and strategies in the chemistry of advanced materials with relevance in biological systems, technique and environmental protection, 13-14 Iun., Timișoara, România, 2013, pag. 52, poster.
51. Funar-Timofei S., Halip L., Bora A.
Comparative Study of a Thiosemicarbazone Derivative Structure by Advanced Quantum-Chemical Approaches
Timisoara's Academic Days, 13th Edition, New trends and strategies in the chemistry of advanced materials with relevance in biological systems, technique and environmental protection, 13-14 Iun., Timișoara, România, 2013, pag. 54, poster.
52. Bora A., Borota A., Ostopovici-Halip L., Funar-Timofei S.
General Aspects of CDK5 Inhibition: I. Triazoles Derivatives Substituted with Thiophene Rings
Timisoara's Academic Days, 13th Edition, New trends and strategies in the chemistry of advanced materials with relevance in biological systems, technique and environmental protection, 13-14 Iun., Timișoara, România, 2013, pag. 60, poster.

Lucrari publicate in reviste fara factor de impact

1. Suzuki T., Rad-Curpăń R., Ostopovici-Halip L., Goodarzi M., Saeys W., Funar-Timofei S.

Modeling of Thienyl Triazoles CDK5/P25 Inhibitors by Accessible Computational Methods

J. Toyo Univ., Natural Sci., 57, 123-138, **2013** (ISSN: 0372-0330)

2. Suzuki T., Funar-Timofei S., Iliescu S.

Structure-Flammability Relationships Study of Some Polyphosphonates

J. Univ., Natural Sci., 57, 109-121, **2013** (ISSN: 0372-0330)

MANIFESTARI STIINTIFICE 2013

A. MANIFESTARI STIINTIFICE ORGANIZATE DE INSTITUTUL DE CHIMIE TIMISOARA AL ACADEMIEI ROMANE

1. SIMPOZION - „Zilele Academice Timișene – Noi tendințe și strategii în chimia materialelor avansate, cu relevanță în sisteme biologice, tehnică și protecția mediului”
– ediția a XIII-a; 13-14 iunie 2013

Finantare:

Consiliu Judetean Timis:	7000 lei
ANCS.....	2000 lei
Finantare din surse proprii:	8000 lei
TOTAL:.....	17000 lei

Număr comunicări prezentate: **96**

- 15 conferințe (lecții invitate)
- 7 prezentari extinse
- 14 prezentări orale
- 60 de postere

Număr participanți : **145**

- 112 din țară
- 33 din străinătate

B. MANIFESTARI STIINTIFICE la care ICT este co-organizator.

1. Asociația de Cercetare Multidisciplinara pentru Zona de Vest, Romania – Ungaria – Serbia, ACMV, Al XV-lea Simpozion International “Tinerii si Cercetarea Multidisciplinara” ISYPMR – Timisoara 14-15 nov. 2013

SITUAȚIE CENTRALIZATOARE
privind doctoratul la
INSTITUTUL DE CHIMIE TIMIȘOARA AL ACADEMIEI ROMANE
2013

1. Doctoranzi:

- 6 interni
- 10 externi

2. Conducatori doctorat:

- Dr. Chim. Costișor Otilia
- Dr. Ing. Făgădar-Cosma Eugenia
- Prof. Dr. Simon Zeno, MCA
- Prof. Dr. Kurunczi Ludovic - Universitatea de Farmacie Timisoara
- Prof. Dr. Mracec Mircea - pensionat

3. S-au sustinut:

- referate - 7
- examene - 6
- teze 3

Director

Dr. Otilia Costisor

Secretar Stiintific

Dr. Ramona Tudose

**Recenzori/referenti
la publicatii si teze de doctorat**

1. Savii C. - *Mat. Res. Bull.*, Elsevier, 4 prezente
2. Savii C. - *Czech Science Foundation*, 3 prezente
3. Savii C. - *EU funded network : M-ERA.NET*, call 2013; call topics: 3. Composite Technology and 4. Materials for Health; 1 prezenta;
4. Savii C. - *International Evaluation Panel for JICAM Programme, Nanotechnology*, la solicitarea : Portuguese Foundation for Science and Technology; 3 prezente
5. Sasca V. – *Appl. Catalysis A: General* -1 prezenta
6. Sasca V. – *J. Mater. Sci.*-1 prezenta
7. Tudose R. – *J. Serbian Chem. Soc.*, - 1 prezenta
8. Popa Al. - *Mat. Res. Bull.*, Elsevier, - 2 prezente
9. Popa Al. – *Appl. Surf. Sci.*, - 2 prezente
10. Popa Al. – *Talanta* - 1 prezente
11. Funar-Timofei S. - *African J. Microbiology Res.* – 1 prezență
12. Funar-Timofei S. – *Canadian J. Chem.* - 1 prezență
13. Funar-Timofei S. – *Desalination Water Treatment* – 1 prezență
14. Funar-Timofei S. – *Dyes and Pigments* – 1 prezență
15. Funar-Timofei S. – *Food and Chemical Toxicology* – 1 prezență
16. Funar-Timofei S. – *J. Mexican Chem. Soc.* – 1 prezență
17. Funar-Timofei S. – *Separation Sci. Technol.*– 1 prezență
18. Liliana Ostopovici-Halip – *J. Bioinfor. Sequence Anal.* - 1 prezență
19. Liliana Ostopovici-Halip – *J. Computer Sci. System Biol.* - 1 prezență
20. Alina Bora – *J. Inhibition Med. Chem.* - 1 prezență
21. Fagadar-Cosma E. - *Arabian Journal of Chemistry*, Elsevier 3 prezente
22. Fagadar-Cosma E. - *Materials Research Bulletin*, Elsevier 1 prezenta
23. Fagadar-Cosma E. - *Materials Chemistry and Physics*, Elsevier 4 prezente
24. Fagadar-Cosma E. - *Colloids and Surfaces A: Physicochemical and Engineering Aspects* Elsevier 3 prezente
25. Fagadar-Cosma E. - *Journal of Solid State Chemistry*, Elsevier 1 prezenta
26. Fagadar-Cosma E. - *American Chemical Science Journal*, 1 prezenta
27. Fagadar-Cosma E. - *SciKnow*, 1 prezenta
28. Fagadar-Cosma E. - *Chinese Journal of Chemistry*, Wiley 1 prezenta
29. Fagadar-Cosma E. - *Combinatorial Chemistry & High Throughput Screening*, BSP 1 prezenta
30. Fagadar-Cosma E. *Bioinorganic Chemistry and Applications*, Hindawi 1 prezenta
31. Fagadar-Cosma E. - *Journal of Electroanalytical Chemistry*, Elsevier 2 prezente
32. Ilia G. - *Current Organic Chemistry*, Benthamscience 2 prezente
33. Ilia G. - *Current Green Chemistry*, Benthamscience 4 prezente
34. Ilia G. - *Letters in Organic Chemistry*, Benthamscience 1 prezente
35. Ilia G. - *Oomics Publishing Group/ACR*, Omicsonline 1 prezente
36. Ilia G. - *Journal of Applied Polymer Science*, Wiley 4 prezente
37. Ilia G. - *Journal of Colloid and Interface Science*, Elsevier 1 prezenta
38. Ilia G. - *Journal of Hazardous Materials*, Elsevier 1 prezenta
39. Ilia G. - *Journal of Inorganic and Organometallic Polymers and Material*, Springer 1 prezenta
40. Ilia G. - *Journal of Thermal Analysis and Calorimetry*, Springer 1 prezenta
41. Ilia G. - *Journal of Magnetism and Magnetic Materials*, Elsevier 1 prezenta
42. Ilia G. - *British Journal of Applied Science & Technology*, Sciencedomain 1 prezenta
43. Ilia G. - *American Journal of Polymer Science*, Sapub 1 prezente

44. Ilia G. - *Industrial & Engineering Chemistry Research*, Pubs.ACS.org 1 prezenta
45. Ilia G. - *Heteroatom Chemistry*, Wiley 1 prezenta
46. Muntean S.G. - *Journal of Materials Chemistry A*, RSC, 2 prezențe
47. Plesu N. - *Annals of West University of Timisoara* Ed. Universitatii de Vest Timisoara, 1 prezenta
48. Plesu N. - *Synthetic Metals*, Elsevier, 1 prezenta
49. Savii C. – 4 teze
50. Costisor Otilia 5 teze

COOPERARI STIINTIFICE

a. Schimburi interacademice

1. Institutul de Morfologie, Patologie si Antropologie Experimentalala si Muzeu al Academiei Bulgare de Stiinte din Sofia

Tematica de cercetare: „Evaluation of antitumor and antiviral activities of newly coordination compound of bile acids, Schiff and Mannich type bases with 3d metal ions.

2. Academia de Stiinte a Republicii Cehe, Institutul de Chimie Anorganica, Departamentul de Chimia Starii Solide si Compusi de Intercalare, Praga, Republica Ceha
Tematica de cercetare: „Sinteză și caracterizarea unor nanomateriale chimic active”.

3. Universitatea din Belgrad, Facultatea de de Chimie Fizică și la Departamentul de Cataliză și Inginerie chimică din cadrul Institutului de Chimie Tehnologie și Metalurgie, Localitatea Belgrad, Serbia

Tematica de cercetare: Heteropoliacizi cu structura Keggin folositi în cataliza eterogenă

b. Colaborari internationale bilaterale

4. Institution of Russian Academy of Sciences, Institute of Macromolecular Compounds Russian Academy of Sciences, Saint-Petersburg, RUSSIA

Elena Tarabukina, PhD, Coordinator, Senior researcher, Laboratory of molecular physics of polymers

Tematica de cercetare: Synthesis, characterisation and investigation of structure and properties in solutions of porphyrin based compounds using methods of molecular hydrodynamics and optics (sedimentation and diffusion analysis, viscometry, dynamic and static light scattering).

Institute of Chemistry Timisoara of Romanian Academy, Group Dr. Eugenia Fagadar-Cosma (Organic Chemistry Laboratory)

5. Kiev National University of Technologies & Design, Kiev, Ucraina

Group of Professor Viacheslav Barsukov (Department of Electrochemical Power Engineering & Chemistry)

Tematica de cercetare: Synthesis, diagnostic and electrochemical characterization of advanced nanomaterials for intersectorial applications, based on metalloporphyrins and their applications as electrocatalytic active materials for oxygen reduction. Self-assembling and self-organization.

In the frame of scientific collaboration programs encouraged by *EU-PROJECT MINOS EURONET” Cooperation in research in an enlarged Europe”*

6. Colaborare bilaterală Romania Ungaria 2013-2014

Contract nr. 669/2013

Institutul de Chimie Timisoara - Universitatea Tehnica si Economica Budapestă

Coordonator: Dr. Ing. Gheorghe Ilia

Coordonator: prof Gyorgy Keglevich

c. Colaborari cu universitati si institute internationale:

7. Institute of Applied Synthetic Chemistry, Universitatea Tehnica Viena, Austria, prof. Wolfgang Linert.
Tema: Combinatii polinucleare precursori pentru sisteme supramoleculare si materiale avansate.
8. Institute fuer Anorganische Chemie, Universitatea Koeln, Germania, Prof. G. Meyer.
Tema: Relatii structura - proprietati ale combinatiilor polinucleare cintinand liganzi de tip baze Mannich.
9. Universitatea Hull, Departamentul de Chimie, Anglia, prof. Georg Mehl.
Tema: Compozisi cu proprietati multifunctionale: cristalin-lichide, fotocromice si luminescenta.
10. Kiev National University of Technologies & Design, Kiev, Ucraina
Group of Professor Viacheslav Barsukov (Department of Electrochemical Power Engineering & Chemistry)
11. Nicolaus Copernicus University, Faculty of Pharmacy, Collegium Medicum, Bydgoszcz, Poland, DSc Grzegorz Bazylak (Department of Pharmacobiology & Molecular Nutrition).
12. University of Mexico School of Medicine, Albuquerque, USA (Prof. Dr. Tudor I. Oprea, Dr. Cristian G. Bologa)
13. Universitatea, Karl-Franzens' Graz, Institutul de Chimie Organică, Graz, Austria (Prof. dr. Walter M.F. Fabian)
14. Natural Science Laboratory, Toyo University, Tokyo, Japonia (Prof. dr. Takahiro Suzuki)
15. Acord de cooperare cu Cape Peninsula University of Technology, Faculty of Applied Science, Department of Chemistry, Cape Town, Africa de Sud, (Prof. T.N. van der Walt)
16. Universitatea Leipzig, Institut fur Analitische Chimie. (Prof. dr. Stefan Bergher)
17. Nankai University, Institute of Polymer Chemistry, R.P. China. (Prof. Dr. Zhang Zhengpu)
18. University of Crete, Department of Chemistry, Grecia (Prof. Dr. Konstantinos D. Demadis)
19. Inst. Chim. Anorg. Rez, Ac.Siintę Republica Cehă;UACHR.Cz
20. Fac Tehnol.Univ. Novi-Sad, Serbia

d. Colaborari cu universitati si institute nationale:

21. Universitatea de Medicină și Farmacie Victor Babeș Timișoara, Facultatea de Farmacie (Prof. dr. Kurunczi Ludovic, Conf. dr. Șeclăman Edward, Dr. Daniela Ionescu)
22. Univ. de Vest Timișoara- Prof. Nicolae Doca, Conf. Titus Vlase
23. Institutul National de Electrochimie și Materiale Condensate Timișoara (INMCD) (Dr.Ing. Ioan Tăranu, Dr. Ing. Paula Sfarloagă)
24. Universitatea "Politehnica" Timisoara, Facultatea de Chimie Industrială și Ingineria Mediului (Dr.Ing. Simona Popa, Dr.Ing. Andrea Kellenberger, Dr.Ing. Geza Bandur, Dr.Ing. Nicolae Vaszilcsin, Dr.chim Narcis Duteanu, dr. ing. Bercean Vasile, Prof. dr. Davidescu C.M., Prof. dr. Pacurariu C., Prof. dr. Negrea P., Sef Luc. Negrea A.)
25. Azur Timisoara, Subsidiary of ICC Industries Inc. New York, U. S. A. (Ing. Adriana Miulescu)
26. U.S.A.M.V. "Banat" Timisoara, Facultatea de Medicina Veterinara, laboratorul Disciplinei de Microbiologie : Prof. dr. Radu Trif, Conf. dr. Ileana Nichita; Facultatea de Tehnologia Produselor Alimentare: Conf. dr. Butnariu Monica.
27. Institutul de Chimie Fizica "Ilie Murgulescu" Bucuresti- Dr. Viorică Parvulescu

28. Institutul National pentru Cercetare-Dezvoltare a Tehnologiilor Izotopice si Moleculare Cluj Napoca (NIRDIMT)- Dr. Nicolae Aldea
29. Institutul de Chimie Macromoleculară „Petru Poni” Iasi (Dr.Ing. Sergiu Coșeri, Dr.Ing. Violeta Neagu, Dr.Ing. George Nistor)
30. Universitatea "Aurel Vlaicu" Arad, Facultatea de Inginerie Alimentară, Turism și Protecția mediului (Dr.Ing. Michaela Dina Stănescu)
31. Institutul Național de Cercetare Dezvoltare pentru Chimie și Petrochimie –ICECHIM, București (Dr.Ing. Valentin Rădițoiu, Dr.Ing. Luminița Wagner)
32. Universitatea Politehnica Bucuresti, Facultatea de Chimie Aplicată și Știința Materialelor (Dr.Ing. Stefan Tomas)
33. Institutul National de Metale rare si neferoase Bucuresti (INMR) (Dr.Ing. Roxana Mioara Piticescu)
34. Institutul de Fizica Cluj-Napoca

Personalitati din strainatate care au vizitat si sustinut conferinte la ICT 2013

1. Alexandrova R. Institute of Experimental Morphology, Pathology and Anthropology with Museum, Bulgarian Academy of Sciences, Bulgaria
2. Almasy L. Institute for Solid State Physics and Optics of the Hungarian Academy of Sciences, Budapest.
3. Andonova-Lilova B. Institute of Experimental Morphology, Pathology and Anthropology with Museum, Bulgarian Academy of Sciences, Bulgaria
4. Balogh R. MTA-SZTE Bioinorganic Chemistry Research Group at Department of Inorganic and Analytical Chemistry, University of Szeged, Hungary
5. Bologa C.G. Department of Internal Medicine, University of New Mexico Health Sciences Center, Albuquerque, NM
6. Borsos K. MTA-SZTE Bioinorganic Chemistry Research Group at Department of Inorganic and Analytical Chemistry, University of Szeged, Hungary
7. Cotarca L. Head of Research & Industrial Development, ZaCh spa - Zambon Chemicals, Italy
8. Czene A. MTA-SZTE Bioinorganic Chemistry Research Group, Department of Inorganic and Analytical Chemistry, University of Szeged, Hungary
9. Dyakova L. Institute of Neurobiology, Bulgarian Academy of Sciences, Sofia, Bulgaria
10. Endreffy E. Department of Pediatrics, Albert Szent-Györgyi Medical Center, University of Szeged, Hungary
11. Faigl F. Research Group for Organic Chemical Technology, University of Technology and Economics, Budapest, Budapest, Hungary
12. Fogassy E. Department of Organic Chemistry and Technology, University of Technology and Economics, Budapest
13. Georgieva M. Institute of Molecular Biology, Sofia, Bulgaria
14. Gyurcsik B. MTA-SZTE Bioinorganic Chemistry Research Group, Department of Inorganic and Analytical Chemistry, University of Szeged, Hungary
15. Hey-Hawkins E. Institute of Inorganic Chemistry
Faculty of Chemistry and Mineralogy,
Universität Leipzig, Germany
16. Jancsó A. MTA-SZTE Bioinorganic Chemistry Research Group at Department of Inorganic and Analytical Chemistry, University of Szeged, Hungary
17. Kalfin R. Institute of Neurobiology, Bulgarian Academy of Sciences, Sofia, Bulgaria
18. Labadi I. University of Szeged, Department of Inorganic and Analytical Chemistry, Hungary
19. Laczkó L. University of Szeged, Department of Inorganic and Analytical Chemistry, Hungary

20. Laguna A. Departamento de Química Inorgánica. Instituto de Síntesis Química y Catálisis Homogénea. Universidad de Zaragoza, Spain
21. Mehl G.H. Department of Chemistry, University of Hull, Hull, UK
22. Miloshev G. Institute of Molecular Biology, Sofia, Bulgaria
23. Németh E. MTA-SZTE Bioinorganic Chemistry Research Group, Department of Inorganic and Analytical Chemistry, University of Szeged, Hungary
24. Niznansky D. Department of Inorganic Chemistry; Charles University in Prague; Faculty of Science; Praha; Czech Republic
25. Oszko A. Institute of Physical Chemistry and Material Science-University of Szeged
26. Palovics E. Research Group for Organic Chemical Technology, University of Technology and Economics, Budapest, Hungary
27. Plocek J. Institute of Inorganic Chemistry, v.v.i., Academy of Sciences of the CR, Czech Republic
28. Salifoglou A. Department of Chemical Engineering, Aristotle University of Thessaloniki, Greece
29. Szekely N. Institute for Solid State Physics and Optics of the Hungarian Academy of Sciences , Budapest
30. Szeleczky Z. Department of Organic Chemistry and Technology, University of Technology and Economics, Budapest
31. Zeng X. The University of Sheffield, Department of Materials Science and Engineering, Sheffield, UK
32. Zhivkova T. Institute of Experimental Morphology, Pathology and Anthropology with Museum, Bulgarian Academy of Sciences, Bulgaria
33. Zóka I. G. MTA-SZTE Bioinorganic Chemistry Research Group, Department of Inorganic and Analytical Chemistry, University of Szeged, Hungary

Prestigiul ICT **Note suplimentare**

Vizibilitatea ICT :

1. Relatii internationale:
 - Schimburi interacademice: Republicile Rusă, Ceha, Sârba, si Ungaria și Bulgaria
 - Programul COPBIL: Bulgaria
 - Colaborari bilaterale: Austria, Anglia, Italia, Franta, Germania, Ungaria.
2. Colaborari cu institutii de invatamant superior din tara si institute ale Academiei Române - 29
3. Cercetatori ai ICT sunt experti evaluatori pentru:
 - Programme europene:
 - Costisor Otilia :
 - FP 7 : Membru in comitetul managerial al proiectului COST CM0802 "Phoscinet"
 - Fagadar-Cosma Eugenia -FP 7:
 - INNOVATION Programme si EUREKA
 - National Excelence Programs for EU integration (since 2005)
 - Savii Cecilia : - FP 7 'Nanosciences, Nanotechnologies,Materials and New Production Technologies", FP7-NMP-2012-LARGE-6.
 - Programele nationale de cercetare dezvoltare ale altor țări:
 - Savii Cecilia - expert evaluator si referent la : Czech Science Foundation (GA CR), (2010 – 2013); Grantové Agentura České Republiky
 - Comisii de doctorat ale universitatilor din strainatate:
Costisor Otilia – Universitatea Cairo – Facultatea de stiinte.
4. Cercetatori ICT fac parte din comisii de doctorat: 6
5. 12 Cercetatori au fost referenti: 82 prezențe
6. Personalități din țara si strainatate au vizitat institutul si au ținut conferinte si prezentari orale: 28
7. Cercetatori ai ICT fac parte din comisii ale MEC(ex. CNATDCU): 1