



3PYChem

3rd Portuguese Young Chemists Meeting

Book of Highlights

9 – 11th May 2012

Departamento de Química e Bioquímica
Faculdade de Ciências da Universidade do Porto





3PYChem

3rd Portuguese Young Chemists Meeting

Book of Highlights

9 – 11th May 2012

**Departamento de Química e Bioquímica
Faculdade de Ciências da Universidade do Porto**

**3PYCheM
3rd
Portuguese
Young
Chemists
Meeting
2012**

Book of Highlights of the 3rd Portuguese Young Chemists Meeting

Editores

Ana Rodrigues
João Martins
Inês Rocha
Marisa Rocha

Montagem

Organizing committee

This book is a compilation of the highlights submitted by the authors for presentation at the meeting. There were introduced only minor editing alterations that do not change the scientific content.
The scientific content is sole the responsibility of the authors.

Sponsors



SCIENTIFIC COMMITTEE



Artur Silva

Universidade de Aveiro



Fernando Jorge Pina

*Faculdade de Ciências e Tecnologia,
Universidade Nova de Lisboa*



Hugh Burrows

Universidade de Coimbra



Joaquim Luís Faria

Faculdade de Engenharia, Universidade do Porto



Maria Fernanda Proença

Universidade do Minho



João Carlos Paiva

Faculdade de Ciências, Universidade do Porto



Maria João Ramos

Faculdade de Ciências, Universidade do Porto



Alexandre Quintanilha

*Instituto Ciências Biomédicas Abel Salazar,
Universidade do Porto*

ORGANIZING COMMITTEE

FCUP Young Chemists

Ana Rita Figueira

Inês Rocha

Marisa Rocha

Juliana Oliveira

Ana Sofia Rodrigues

João Martins

Inês Valente

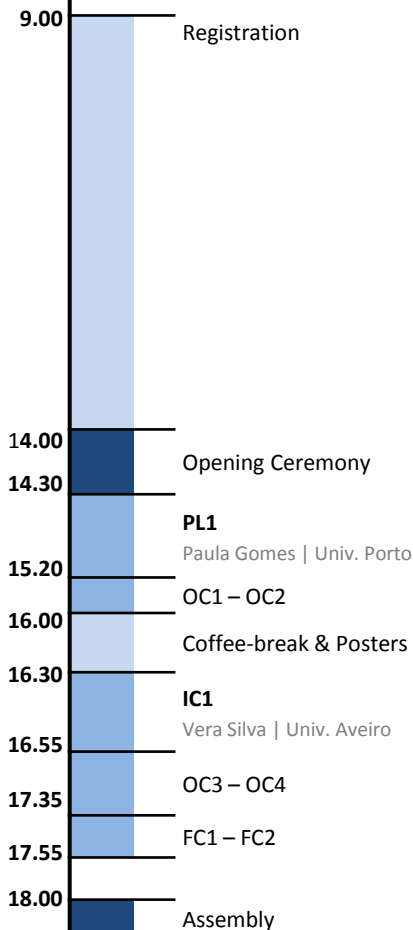
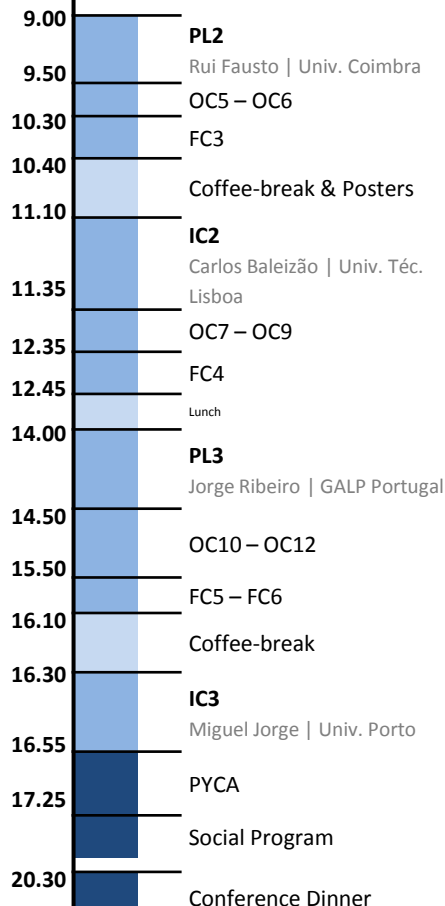
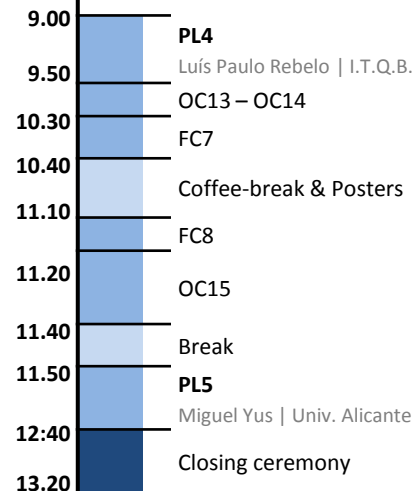
Joana Reis

Christiane Santos

André Barbosa

Member from Sociedade Portuguesa de Química

Leonardo Mendes

PROGRAM (Room A1)**Wednesday, May 9th****Thursday, May 10th****Friday, May 11th**

PL – Plenary Lectures

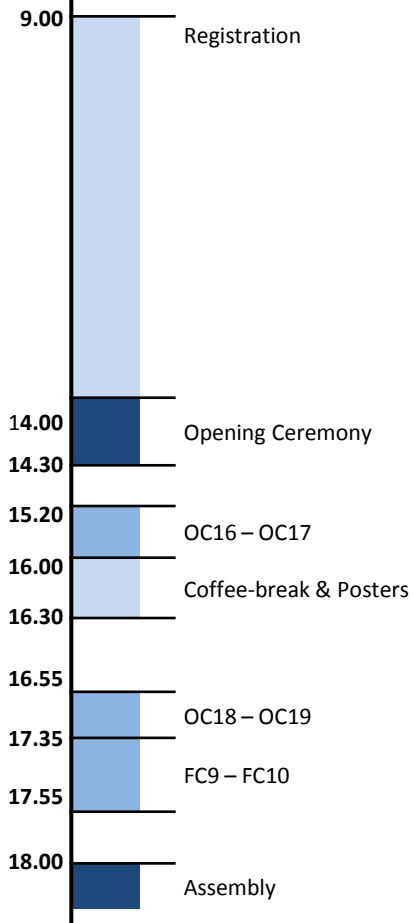
IC – Invited Lectures

OC – Oral communications

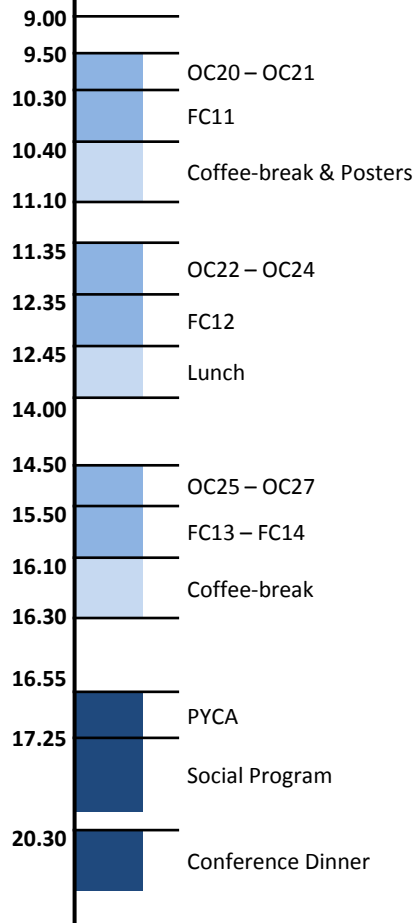
FC – Flash communications

PROGRAM (Room A2)

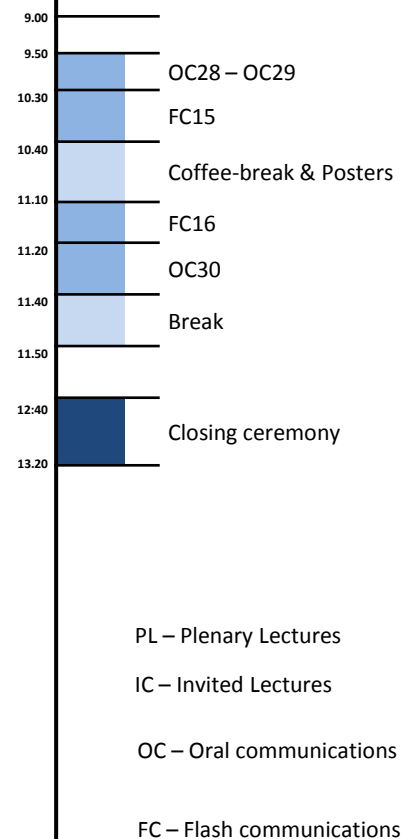
Wednesday, May 9th



Thursday, May 10th



Friday, May 11th



DETAILED PROGRAM**Wednesday, May 9th**

9:00	Registration	
14:00	Opening Ceremony	
14:30	PL1. Old drugs with new faces: chemical strategies to cover primaquine unpleasant traits while preserving its attractive antimalarial attributes	3
	<i>Room A1</i>	
	<u>Paula Gomes</u> , Nuno Vale and Joana Matos <i>Faculty of Science, University of Porto, Portugal</i>	
15:20	OC1. New chromene scaffolds for adenosine receptors: synthesis and pharmacology	13
	<i>Room A1</i>	
	<u>Marta Costa</u> , Filipe Areias, Marian Castro, Jose Brea, María I. Loza and Fernanda Proença <i>University of Minho, Portugal</i>	
	OC16. Photophysics of push-pull oxazolones derivatives with nonlinear optical properties	20
	<i>Room A2</i>	
	<u>Inês de F. A. Mariz</u> , Catarina Rodrigues, Ermelinda M. S. Maçôas, Carlos Afonso and José M. G. Martinho <i>Instituto Superior Técnico, Lisboa, Portugal</i>	
15:40	OC2. Marine biomaterials on the origin of biomedical applications	13
	<i>Room A1</i>	
	<u>Tiago H. Silva</u> , Joana Moreira-Silva, Lara L. Reys, Ana Rita C. Duarte, Simone S. Silva, Susana Fernandes-Silva, João F. Mano, Rui L. Reis <i>University of Minho, Braga / PT Government Associate Laboratory, Braga/Guimarães, Portugal</i>	
	OC17. New porphyrin materials for optoelectronic and PET applications	21
	<i>Room A2</i>	
	<u>Sara M. A. Pinto</u> , César A. Henriques, Carlos J. P. Monteiro, Ana V. C. Simões, Mário J. F. Calvete, Mariette M. Pereira and Hugh D. Burrows <i>Faculty of Science and Technology, University of Coimbra, Portugal</i>	
16:00	Coffee-break & Poster Session	
16:30	IC1. Development of synthetic methodologies for new biologically active heterocyclic compounds	9
	<i>Room A1</i>	
	<u>Vera L. M. Silva</u> , Artur M. S. Silva and José A. S. Cavaleiro <i>University of Aveiro, Portugal</i>	

Pg.

16:55	OC3. New synthetic approach towards the miharamycins sugar moiety	14
	<i>Room A1</i>	
	<u>Vasco Cachatra</u> , Andreia Almeida and Amélia P. Rauter <i>Faculty of Science, University of Lisbon, Portugal</i>	
	OC18. Clay materials for the storage and release of nitric oxide for therapeutic purposes	21
	<i>Room A2</i>	
	<u>Ana C. Fernandes</u> and M. L. Pinto, J. Pires <i>Faculty of Science, University of Lisbon, Portugal</i>	
17:15	OC4. Mechanochemistry: a new pathway for the synthesis of metallodrugs and metallopharmaceuticals	14
	<i>Room A1</i>	
	<u>Vânia André</u> and M. Teresa Duarte <i>Instituto Superior Técnico, Universidade Técnica de Lisboa, Portugal</i>	
	OC19. On the voltammetry of chalcones: trans-chalcone, cardamonin and xanthohumol	22
	<i>Room A2</i>	
	<u>Eliana M. Tavares</u> , Luís M. Gonçalves, José A. Rodrigues and Aquiles A. Barros <i>Faculty of Science, University of Porto, Portugal</i>	
17:35	FC1. Thermochemistry of 1-methylimidazolium nitrate	31
	<i>Room A1</i>	
	<u>Joana Vitorino</u> , C. E. S. Bernardes and M. E. Minas da Piedade <i>Faculty of Science, University of Lisbon, Portugal</i>	
	FC9. Application of the QuEChERS methodology for the determination of volatile phenols in beverages	35
	<i>Room A2</i>	
	<u>Inês M. Valente</u> , Christiane M. Santos, Manuela M. Moreira, José A. Rodrigues and Aquiles A. Barros <i>Faculty of Science, University of Porto, Portugal</i>	
17:45	FC2. On the synthesis of dehydropregnenolone derivatives: reactivity as diene/dienophile in the Diels Alder reaction	31
	<i>Room A1</i>	
	<u>Tiago E. B. Valadeiro</u> , Jorge A. R. Salvador, Sílvia Gramacho and M. Pineiro <i>University of Coimbra, Portugal</i>	
	FC10. Syngas production over M-Ni nanoparticles (M = Pr, Gd, Th and U)	35
	<i>Room A2</i>	
	<u>Ana C. Ferreira</u> , J.P. Leal and Joaquim B. Branco <i>Instituto Superior Técnico, Universidade Técnica de Lisboa / FCUL, Portugal</i>	
18:00	Assembly	
	<i>Room A1</i>	



DETAILED PROGRAM

Thursday, May 10th

9:00	PL2. Light induced reactions in cryogenic matrices	Room A1	Pg. 3
	<u>Rui Fausto</u> University of Coimbra, Portugal		
9:50	OC5. The Sulfur-shift: the activation mechanism of mononuclear Mo enzymes	Room A1	15
	<u>Nuno M. F. S. A. Cerveira</u> Faculty of Science, University of Porto, Portugal		
	OC20. Computational studies on the aspartic protease Renin	Room A2	22
	<u>Natércia F. Brás, Pedro A. Fernandes and Maria J. Ramos</u> Faculty of Science, University of Porto, Portugal		
10:10	OC6. Manganese porphyrins as catalysts in the oxidation of diclofenac	Room A1	15
	<u>Cláudia M. B. Neves, Mário M. Q. Simões, Isabel C. M. S. Santos, Filipe A. Almeida Paz, M. Graça P. M. S. Neves, Artur M. S. Silva and José A. S. Cavaleiro</u> University of Aveiro, Portugal		
	OC21. Ciprofloxacin and norfloxacin spectrophotometric determination in a fully automated multi-pumping flow system	Room A2	23
	<u>Maria H. R. Amorim, Karine L. Marques, João L. M. Santos and José L. F. C. Lima</u> Faculty of Pharmacy, University of Porto, Portugal		
10:30	FC3. Dicarboxylate recognition by two macrobicyclic receptors: selectivity for fumarate over maleate	Room A1	32
	<u>Pedro Mateus, Rita Delgado, Paula Brandão and Vítor Félix</u> Instituto de Tecnologia Química e Biológica, Portugal		
	FC11. Characterization and antibacterial studies of a copper(II) lomefloxacin ternary complex	Room A2	36
	<u>Patrícia Fernandes, Mariana Ferreira and Paula Gameiro</u> Faculty of Science, University of Porto, Portugal		
10:40	Coffee-break & Poster Session		
11:10	IC2. Perylenediimide based functional hybrid materials	Room A1	9
	<u>Carlos Baleizão</u> Instituto Superior Técnico, Universidade Técnica de Lisboa, Portugal		
11:35	OC7. Light-activated delivery of inorganic and organic phosphates: using metal nanoparticles for the release of caged compounds in aqueous media	Room A1	16
	<u>Artur J. Moro, Joana Sousa, João Rosa, P. V. Baptista and João C. Lima</u> Faculdade de Ciências e Tecnologia, Universidade Nova de Lisboa, Portugal		

	OC22. Efficient synthesis of new spiroisoxazoline oxindoles	Room A2	23
	<u>Carlos J. A. Ribeiro, Rui Moreira and Maria M. M. Santos</u> Faculty of Pharmacy, University of Lisbon, Portugal		
11:55	OC8. Encapsulation of resveratrol in lipid nanoparticles: formulation and characterization	Room A1	16
	<u>Ana Neves, M. Lúcio, J. L. F. C. Lima and S. Reis</u> Faculty of Pharmacy, University of Porto, Portugal		
	OC23. New composites based on polyoxometalates and porous MOFs as active catalysts for liquid phase oxidation	Room A2	24
	<u>Carlos M. Granadeiro, André D. S. Barbosa, Patrícia Silva, Filipe A. Almeida Paz, Baltazar de Castro, Salette S. Balula and Luís Cunha-Silva</u> Faculty of Science, University of Porto, Portugal		
12:15	OC9. Monitoring heavy metals in urban soils at lisbon	Room A1	17
	<u>Hugo F. Silva, Andrei Sadovski, Cristina Oliveira and Manuel J. Matos</u> Instituto Superior Engenharia de Lisboa, Portugal		
	OC24. Iron oxide/gold core/shell nanoparticles and screen printed carbon electrode for sensitive detection of salmonella typhimurium	Room A2	24
	<u>Maria Freitas, S. Viswanathan, M.B.P.P. Oliveira and C. Delerue-Matos</u> Faculty of Pharmacy, University of Porto, Portugal		
12:35	FC4. Effect of extraction conditions for chlorogenic acid determination in lamb's lettuce	Room A1	32
	<u>Fábio Oliveira, Manuela M. Moreira, Aquiles A. Barros and Luís F. Guido</u> Faculty of Science, University of Porto, Portugal		
	FC12. Conception of glycerophospholipid hydrated bilayer models through computational modeling	Room A2	36
	<u>João T. S. Coimbra, Sérgio F. Sousa, Pedro A. Fernandes, Maria Rangel, Maria J. Ramos</u> Faculty of Science, University of Porto, Portugal		
12:45	Lunch		
14:00	PL3. Collaborative R&D between GALP Energia and university as a factor to promote competitiveness	Room A1	4
	<u>Jorge Correia Ribeiro</u> Galp Energia, Portugal		
14:50	OC10. Dow human element, fostering an innovation culture	Room A1	17
	<u>Raquel Fortes</u> New Business Development Leader, Dow Europe GmbH, Switzerland		

15:10	OC25. e-lab: a didactic interactive experiment. An approach to the Boyle-Mariotte law <i>Room A1</i>	25
	<u>Sérgio Leal</u> , João P. Leal and Horácio Fernandes <i>Faculty of Science, University of Lisbon, Portugal</i>	
	OC11. Photoacoustic waves based technology using light absorbing thin films for transdermal drug delivery <i>Room A1</i>	18
15:30	<u>Gonçalo F. F. Sá</u> , Carlos Serpa and Luís G. Arnaut <i>University of Coimbra / LaserLeap Technologies, Coimbra, Portugal</i>	
	OC26. Dual complexation mode of cucurbit[7]uril and cationic surfactants <i>Room A2</i>	25
	<u>Márcia Pessêgo</u> , J. A. Moreira and L. García-Río <i>Universidad de Santiago de Compostela, Spain / Faculty of Science and Technology, University of Algarve, Portugal</i>	
15:50	OC12. Use of solid phase extraction in a sequential injection system for the determination of alkaline phosphatase activity in plant roots <i>Room A1</i>	18
	<u>Inês C. Santos</u> , Raquel B. R. Mesquita, Adriano A. Bordalo and António O. S. S. Rangel <i>Universidade Católica Portuguesa, Portugal</i>	
	OC27. The conducting polymer based electrochemical sensors and biosensors with autocatalytical stage and the description of their work <i>Room A2</i>	26
16:00	<u>Volodymyr V. Tkach</u> , Vasyli V. Nechyporuk, Petro I. Yagodynets' and Aline M. da Rocha <i>Chernivtsi National University, Ukraine</i>	
	FC5. Understanding the mechanism of resistance of HIV-1 RT to tenofovir <i>Room A1</i>	33
	<u>Rui M. Ramos</u> , Irina S. Moreira, Pedro A. Fernandes and Maria J. Ramos <i>Faculty of Science, University of Porto, Portugal</i>	
16:00	FC13. Synthesis of novel bipyrrrolic compounds with potential application in anion binding <i>Room A2</i>	37
	<u>Flávio Figueira</u> , Andreia F. S. Farinha, Augusto C. Tomé, José A. S. Cavaleiro and João P. C. Tomé <i>University of Aveiro, Portugal</i>	
	FC6. Mannosylated nanoparticles for targeted delivery of amphotericin B towards visceral leishmaniasis <i>Room A1</i>	33
16:00	<u>Daniela Barros</u> , A. Cordeiro-da-Silva and S. Costa-Lima <i>IBMC-INEB Infection and Immunity- Parasite Disease Group, Porto, Portugal</i>	
	FC14. On the complexation between bovine serum albumin and manganese porphyrin <i>Room A2</i>	37
	<u>Otávio A. Chaves</u> , Gonçalo F.F. Sá, Catarina S.H. Jesus, Carlos Serpa, L.G. Arnaut <i>Capes Foundation, Brazil / University of Coimbra, Portugal</i>	

16:30	Coffee-break	
	IC3. Molecular simulation of hybrid organic-inorganic nanoporous materials: synthesis and adsorption predictions <i>Room A1</i>	10
	<u>Miguel Jorge</u> , Ryusuke Futamura, Christophe Siquet and José R. B. Gomes <i>Faculty of Engineering, University of Porto, Portugal</i>	
16:55	PYCA <i>Room A1</i>	
	Social Program	
	Conference Dinner	

DETAILED PROGRAM

Friday, May 11th

		Pg.
9:00	PL4. Novel ionic liquids – New flexibility <i>Room A1</i>	4
	<u>Luís Paulo N. Rebelo</u> <i>Instituto de Tecnologia Química e Biológica, Universidade Nova de Lisboa, Portugal</i>	
	OC13. Preparation and characterization of ionic liquids based on thioflavin T <i>Room A1</i>	19
9:50	<u>Alexandra Costa</u> , Luís C. Branco and Isabel Marrucho <i>Faculdade de Ciências e Tecnologia, Universidade Nova de Lisboa, Portugal</i>	
	OC28. One-step three-component vs two-step two-component microwave assisted synthesis of 4,6-diaryldehydropyrimidinethiones <i>Room A2</i>	26
	<u>Tiago E. B. Valadeiro</u> , Bruno F. O. Nascimento and M. Pineiro <i>University of Coimbra, Portugal</i>	
10:10	OC14. PDLC devices that consume lower power and are environmentally friendly <i>Room A1</i>	19
	<u>Ana Mouquinho</u> and João Sotomayor <i>Faculdade de Ciências e Tecnologia, Universidade Nova de Lisboa, Portugal</i>	
	OC29. Molecular imprinted polymer on graphene nanosheets modified glassy carbon electrode for norfloxacin detection <i>Room A2</i>	27
	<u>Hélder da Silva</u> , Subramanian Viswanathan and Cristina Delerue-Matos <i>School of Engineering, ISEP, Polytechnic Institute of Porto, Portugal</i>	

10:30	FC7. The role of ionizable amino acid residues on peptide and protein folding: a time-resolved photoacoustic calorimetry experiment <i>Room A1</i>	34
	<u>Catarina S. H. Jesus</u> , Rui M. D. Nunes, Rui M. M. Brito, Luis G. Arnaut and Carlos Serpa <i>University of Coimbra, Portugal</i>	
	FC15. Halogen---Cyano group interaction: an energetic and structural analysis of monohalogenated benzonitrile isomers <i>Room A2</i>	38
	<u>Inês M. Rocha</u> and Manuel A.V. Ribeiro da Silva <i>Faculty of Science, University of Porto, Portugal</i>	
10:40	Coffee-break & Poster Session	
11:10	FC8. Chemistry at the university: an approach to science dissemination for youngsters <i>Room A1</i>	34
	<u>Daniel Ribeiro</u> and Maria D. M. C. Ribeiro da Silva <i>Faculty of Science, University of Porto, Portugal</i>	
	FC16. Structural and thermodynamic study of nonlinear polyphenyls <i>Room A2</i>	38
	<u>Ana S. M. C. Rodrigues</u> , Marisa A. A. Rocha, Lúcia R. Gomes, John L. Low and Luís M. N. B. F. Santos <i>Faculty of Science, University of Porto, Portugal</i>	
11:20	OC15. A GC-MS method for the simultaneous identification and quantification of amino acids, fatty acids and sterols in marine organisms <i>Room A1</i>	20
	<u>David M. Pereira</u> , Juliana Vinholes, Patrícia Valentão, Paula Guedes de Pinho, Natércia Teixeira and Paula B. Andrade <i>Faculty of Pharmacy, University of Porto, Portugal</i>	
	OC30. Gold(I)-catalyzed intermolecular (4 + 2) and (2 + 2) cycloadditions of allenamides <i>Room A2</i>	27
	<u>Hélio Faustino</u> , Fernando López and José L. Mascareñas <i>Universidad de Santiago de Compostela, Spain</i>	
11:40	Break	
11:50	PL5. Efficiency in chemistry: from hydrogen autotransfer to multicomponent catalysis <i>Room A1</i>	5
	<u>Miguel Yus</u> <i>Facultad de Ciencias, Universidad de Alicante, Spain</i>	
12:40	Closing Ceremony	

POSTER SESSION**Wednesday, May 9th**

		Pg.		
P11	Force field parameterization of cobalt-containing metalloproteins	46		
	Ana C. V. Cunha, Sérgio F. Sousa, Pedro A. Fernandes and Maria J. Ramos Faculty of Science, University of Porto, Portugal			
P12	Pressure waves generated by light-absorbing thin films	46		
	A. P. Marques, G. F. F. Sá, C. Serpa and L. G. Arnaut University of Coimbra, Portugal			
P13	Thermodynamic study of phase transitions in methyl esters of <i>ortho</i> -, <i>meta</i> - and <i>para</i> -aminobenzoic acids	47		
	Ana R. R. P. Almeida and M. J. S. Monte Faculty of Science, University of Porto, Portugal			
P14	Monovacant polyoxometalates @ MIL-101: synthesis and heterogeneous catalytic studies	47		
	André D. S. Barbosa, Filipe A. Almeida Paz, Baltazar de Castro, Salette S. Balula and Luís Cunha-Silva Faculty of Science, University of Porto, Portugal			
P15	Isolation and quantification of labdanolic acid from <i>Cistus ladaniferus</i>	48		
	André N. C. Martins, L. M. T. Frija, S. Simeonov and C. A. M. Afonso Faculdade de Farmácia da Universidade de Lisboa / Instituto Superior Técnico, Portugal			
P16	Application of geochemistry software to corrosion studies	48		
	A. B. Oliveira, A. C. Bastos, O. V. Karavai, A. A. Ferreira, M. L. Zheludkevich and M. G. S. Ferreira University of Aveiro, Portugal			
P17	Micro-electrochemical techniques to study localised corrosion	49		
	A. B. Oliveira, A. C. Bastos, O. V. Karavai, M. L. Zheludkevich and M. G. S. Ferreira University of Aveiro, Portugal			
P18	Approach to the synthesis of nucleoside inhibitors of butyrylcholinesterase	49		
	Andreia Almeida, Vasco Cachatra and Amélia P. Rauter Faculty of Science, University of Lisbon, Portugal			
P19	A green integrated biocatalytic system for the conversion of CO ₂ and vegetable oils into biodiesel	50		
	Andreia Pimenta, Pedro Vidinha and Susana Barreiros Faculdade de Ciências e Tecnologia, Universidade Nova de Lisboa, Portugal			
P20	Development of ionic liquids based on biological compounds	50		
	Andreia Forte, Luís C. Branco and César Laia Faculdade de Ciências e Tecnologia, Universidade Nova de Lisboa, Portugal			
P1	Synthesis of 9-methyl-6-methylamino-2-arylpyrimidines as potential new ligands to adenosine receptors	41		
	A. Brito, C. Correia, M. A. Carvalho and M. F. Proença University of Minho, Portugal			
P2	Chiral HPLC method for determination of the enantiomeric purity of new xanthone derivatives	41		
	Carla Fernandes, Alexandre Santos, Maria Elizabeth Tiritan, Carlos Afonso and Madalena Pinto Faculty of Pharmacy, University of Porto, Portugal			
P3	Synthesis of new pyrimido[5,4- <i>d</i>]pyrimidines derivatives as potential antitubercular agents	42		
	A. Gonçalves, A. Rocha, A. Brito, M. A. Carvalho and M. F. Proença University of Minho, Portugal			
P4	Biotransformation of primary aromatic amines by laccases	42		
	Ana Catarina Sousa, Lígia O. Martins and M. Paula Robalo Instituto Superior de Engenharia de Lisboa, Portugal			
P5	Phenol glycosylation catalysed by zeolite HY	43		
	Ana Assunção, Ana Jesus, Ana P. Carvalho and Amélia P. Rauter Faculty of Science, University of Lisbon, Portugal			
P6	Oxidative coupling of methane using nitrous oxide as oxidant over calcium-rare earth oxides nanoparticles	43		
	Ana C. Ferreira, J. P. Leal and Joaquim B. Branco Instituto Tecnológico e Nuclear, Universidade Técnica de Lisboa / FCUL, Portugal			
P7	Fluorescent labelling of valine with a new benzo[<i>a</i>]phenoxazinium chloride functionalized at the 2- and 5-positions	44		
	A. Daniela G. Firmino and M. Sameiro T. Gonçalves University of Minho, Portugal			
P8	Solvent-free microwave synthesis of 2-, 5- and 9-substituted benzo[<i>a</i>]phenoxazinium chlorides	44		
	A. Daniela G. Firmino and M. Sameiro T. Gonçalves University of Minho, Portugal			
P9	Thermochemical study of the some fluoronitrophenol isomers	45		
	Ana I. M. C. Lobo Ferreira and Manuel A.V. Ribeiro da Silva Faculty of Science, University of Porto, Portugal			
P10	Thermochemistry study of 2-methylbenzoxazole and 2-methylbenzothiazole	45		
	Ana L. R. Silva, A. Cimas and Maria D. M. C. Ribeiro da Silva Faculty of Science, University of Porto, Portugal			

P21	Topical drug delivery of lidocaine and diclofenac gels: Viscoelastic properties and <i>in vitro</i> skin distribution studies	51	P31	Breath analysis by optical fiber sensor for the diagnosis of human health	56
	Ângela Correia, Gonçalo F. F. Sá, Carlos Serpa and Luís G. Arnaut <i>University of Coimbra, Portugal</i>			Celine I. L. Justino, Lurdes I. B. Silva, Kátia R. Duarte, Ana C. Freitas, Teresa A. P. Rocha-Santos and Armando C. Duarte <i>University of Aveiro, Portugal</i>	
P22	Computational studies of Binol based phosphites and respective metal complexes at PM6 and DFT levels. Application in asymmetric hydrogenation of olefins.	51	P32	Determination of α-dicarbonyl compounds in foodstuff by HPLC-UV using gas-diffusion microextraction	56
	Ângela C. B. Neves, Rui M. B. Carrilho, Andreia F. Peixoto, Ana R. Almeida, Paulo E. Abreu, M. Calvete and Mariette M. Pereira <i>University of Coimbra, Portugal</i>			Christiane M. Santos, Inês M. Valente, José A. Rodrigues and Aquiles A. Barros <i>Faculty of Science, University of Porto, Portugal</i>	
P23	Gamma irradiation protects oleic acid from oxidation: an experiment in <i>Lactarius deliciosus</i> wild mushroom	52	P33	Synthesis of <i>N</i>-ethyl β,β-diaryldehydroalanine and <i>N</i>-ethylindole derivatives	57
	Ângela Fernandes, M. Beatriz P. P. Oliveira, Amílcar L. Antonio, Anabela Martins and Isabel C. F. R. Ferreira <i>Instituto Politécnico de Bragança / Faculdade de Farmácia da Universidade do Porto, Portugal</i>			Cláudia Barroso and Luís S. Monteiro <i>University of Minho, Portugal</i>	
P24	1,3-Dipolar cycloaddition of (2<i>R</i>,4<i>aR</i>,8<i>aS</i>)-2-phenyl-4,4a-dihydropyrano[3,2-<i>d</i>][1,3]dioxin-6(8<i>aH</i>)-one with aromatic diazomethyl compounds	52	P34	Magnetic core-shell nanoparticles as catalyst supports	57
	António Ribeiro, Cristina E. A. Sousa, M. José Alves and A. Gil Fortes <i>University of Minho, Portugal</i>			Cristina I. Fernandes, Pedro D. Vaz and Carla D. Nunes <i>Faculty of Science, University of Lisbon, Portugal</i>	
P25	An efficient synthetic approach to 6-triazolopurines	53	P35	Influence of different malt varieties on xanthohumol isomerization in pale and dark beers	58
	A. Rocha, M. A. Carvalho and M. F. Proença <i>University of Minho, Portugal</i>			Daniel O. Carvalho, Aquiles A. Barros and Luís F. Guido <i>Faculty of Science, University of Porto, Portugal</i>	
P26	A left-handed helical 3D metal-organic chiral framework derived from the decomposition of 3-amino-1<i>H</i>-1,2,4-triazole-5-carboxylic acid	53	P36	The PROFILES project as a way to provide continuous professional development of the science teachers	58
	Bing Liu, J. A. Fernandes, J. P. C. Tomé, F. A. Almeida Paz and L. Cunha-Silva <i>University of Aveiro / Faculty of Science, University of Porto, Portugal</i>			Daniel Ribeiro, Carla Morais and João Paiva <i>Faculty of Science, University of Porto, Portugal</i>	
P27	Synthesis of new porphyrin-phosphonate derivatives for MOFs construction	54	P37	Chemical composition and antimicrobial activity of <i>Salvia sclareoides</i> Brot. extracts	59
	Carla F. Pereira, João M. M. Rodrigues, Sérgio M. F. Vilela, Filipe A. Almeida Paz and João P. C. Tomé <i>University of Aveiro, Portugal</i>			Daniela Batista, Alice Martins, Isabel Branco, Catarina Dias, Ana Neves, Jorge Justino and Amélia P. Rauter <i>Faculty of Science, University of Lisbon, Portugal</i>	
P28	Application of an optimized ELISA assay in the assessment of 17β-estradiol levels in surface and waste waters from the Aveiro region (Portugal)	54	P38	Functionalized Fe₃O₄/SiO₂ core/shell particles: new sorbents for the magnetic removal of aqueous Hg(II)	59
	Carla P. Silva, Rudolf J. Schneider, Marta Otero and Valdemar I. Esteves <i>University of Aveiro, Portugal</i>			Daniela S. Tavares, C. B. Lopes, A. L. Daniel-da-Silva, A. C. Duarte, E. Pereira and T. Trindade <i>University of Aveiro, Portugal</i>	
P29	Computational studies of Cu-catalyzed addition of azides to iodoalkynes	55	P39	Application of ESI-MS/MS to the structural characterization of <i>Genista tenera</i> flavonoids and flavonoid glycosides	60
	Carlos E. P. Bernardo and Pedro J. Silva <i>University Fernando Pessoa, Portugal</i>			Diana Mendes, Alice Martins, Paulo J. Amorim Madeira, Humberto E. Ferreira, José Condeço, Inês Fernandes, João C.M. Bordado and Amélia P. Rauter <i>Faculty of Science, University of Lisbon, Portugal</i>	
P30	Screening of single-walled carbon nanotubes by optical fiber sensing	55	P40	ELISA application on EE2 water monitoring	60
	Celine I. L. Justino, Ana C. Freitas, Teresa A. P. Rocha-Santos and Armando C. Duarte <i>University of Aveiro, Portugal</i>			Diana L. D. Lima, Rudolf J. Schneider and Valdemar I. Esteves <i>University of Aveiro, Portugal</i>	

Thursday, May 10th

P60	Synthesis of new titanocene(IV) carboxylate complexes: an alternative chemotherapeutic treatment against cancer	70	P71	Young chemists at IJUP: opportunities for research training at U. Porto	76
	<u>Jesús Ceballos-Torres</u> , María J. Caballero-Rodríguez, Sanjiv Prashar, Reinhard Paschke, Dirk Steinborn, Goran N. Kaluđerović and Santiago Gómez-Ruiz <i>Universidad Rey Juan Carlos, Spain</i>			<u>Marcela A. Segundo</u> and Maria Rangel <i>Faculty of Pharmacy, University of Porto, Portugal</i>	
P61	Synthesis of new flavon-3-ols with potential antioxidant activity	71	P72	Characterisation of phenolic compounds from <i>Acacia melanoxylon</i> biomass extracts by capillary electrophoresis	76
	<u>Joana L. C. Sousa</u> and Artur M. S. Silva <i>University of Aveiro, Portugal</i>			<u>Márcia A. Ribeiro</u> , Alice I. Martins, Luísa B. Roseiro and Amélia P. Rauter <i>Faculty of Science, University of Lisbon, Portugal</i>	
P62	Development of a new library of novel and reversible MAO-B inhibitors based on the benzopyranic nucleus: an overview	71	P73	Interaction of 4-chromanone with double stranded DNA: a UV spectroscopy study	77
	<u>J. Reis</u> , A. Gaspar, F. Cagide, E. Uriarte, S. Alcaro, F. Ortuso and F. Borges <i>Faculty of Science, University of Porto, Portugal</i>			<u>Diana Sousa</u> and M. J. Sottomayor <i>Faculty of Science, University of Porto, Portugal</i>	
P63	Confinement effects over the energetic profile of a Menshutkin S_N2 reaction, a computational study	72	P74	2D NMR Studies of sesquiterpene lactones with potential antitumoral activity	77
	<u>J. M. Martins</u> and A. L. Magalhães <i>Faculty of Science, University of Porto, Portugal</i>			<u>Maria H. R. Amorim</u> , Rui M. Gil da Costa and Margarida M. S. M. Bastos <i>Engineering Faculty, University of Porto, Portugal</i>	
P64	Environmental and pharmaceutical applications of cyclodextrin-assisted molecular encapsulation	72	P75	High-resolution solid-state MAS NMR methods applied to structural studies of mammalian end-binding protein 3	78
	<u>José Dias</u> , Marta Martins, E. Manuela Garrido, Maria J. Sottomayor, Fernanda Borges and Jorge Garrido <i>Faculty of Science, University of Porto, Portugal</i>			<u>Mariana Sardo</u> , Luís Mafra, João Rocha, Beat H. Meier and Anja Böckmann <i>University of Aveiro, Portugal / Physical Chemistry, ETH-Zurich, Switzerland</i>	
P65	Thermodynamic study of two 9-substituted fluorene derivatives	73	P76	Electrocatalytic reduction of nitrate in water with mono and bimetallic catalysts supported on carbon nanotubes	78
	<u>Juliana A. S. A. Oliveira</u> , Maria M. Calvino, Manuel J. S. Monte and Maria D. M. C. Ribeiro da Silva <i>Faculty of Science, University of Porto, Portugal</i>			<u>M. Ferreira</u> , M. F. Pinto, I. C. Neves, A. M. Fonseca, O. S. G. P. Soares, M. F. R. Pereira, J. J. M. Órfão, J. L. Figueiredo and P. Parpot <i>University of Minho, Portugal</i>	
P66	Incorporation of polyfluorenes into poly(lactic acid) films for sensor and optoelectronics applications	73	P77	Polycyclic aromatic hydrocarbons extraction from digestive glands by microwave-assisted and solid phase extraction	79
	<u>L. Martelo</u> , A. Jiménez, A. J. M. Valente, H. D. Burrows, A. T. Marques, M. Förster, U. Scherf, M. Peltzer and S. M. Fonseca <i>University of Coimbra, Portugal / University of Alicante, Spain</i>			<u>Marta Oliveira</u> , Simone Moraes, Filipa Gomes, Maria J. Ramalhosa and Cristina Delerue-Matos <i>Instituto Superior de Engenharia do Porto, Portugal</i>	
P67	In situ oxalate formation from imidazole 4,5-dicarboxylic acid in ionothermal reactions	74	P78	Electrochemical techniques applied to the study of pesticide's photodegradation	79
	<u>Ling Xu</u> , Baltazar de Castro and Luís Cunha-Silva <i>Faculty of Science, University of Porto, Portugal</i>			Cátia Costa, <u>Marta Martins</u> , Jorge Garrido, Fernanda Borges and E. Manuela Garrido <i>Faculty of Science, University of Porto / School of Engineering, ISEP, Polytechnic Institute of Porto, Portugal</i>	
P68	Monitoring the production of biodiesel with real-time laser spectroscopy	74	P79	Impact of antioxidants on the oxidation stability of biodiesel	80
	<u>Luís A. B. De Boni</u> , Teresa M. R. Maria, M. M. Pereira and Isaac N. L. da Silva <i>University of Coimbra, Portugal / Pontifical Catholic University of Rio Grande do Sul, Brasil</i>			<u>Marta Martins</u> , E. Manuela Garrido, Fernanda Borges and Jorge Garrido <i>Faculty of Science, University of Porto / School of Engineering, ISEP, Polytechnic Institute of Porto, Portugal</i>	
P69	New insights about malvidin-3-glucoside-catechin dimeric compound	75	P80	Mo(II) catalysts in the epoxidation of cy8: the effect of temperature, solvent and oxidants	80
	<u>Luís Cruz</u> , Nuno Mateus and Victor de Freitas <i>Faculty of Science, University of Porto, Portugal</i>			<u>Marta S. Saraiva</u> , Carla D. Nunes and Maria José Calhorda <i>Faculty of Science, University of Lisbon, Portugal</i>	
P70	Electrochemical mineralization of oxalic acid at metallic catalyst based on carbon nanotubes	75			
	<u>M. F. Pinto</u> , M. Ferreira, I. C. Neves, A. M. Fonseca, O. S. G. P. Soares, J. J. M. Órfão, M. F. R. Pereira, J. L. Figueiredo and P. Parpot <i>University of Minho, Portugal</i>				

POSTER SESSION**Friday, May 11th**

		Pg.		
P81	Assessment of endpoint antioxidant capacity of red wines using a novel kinetic matching approach	81	<u>P. G. Rosado</u> , J. B. Branco, J. P. Ieal, L. M. Ferreira and J. J. H. Lancastre <i>Instituto Tecnológico e Nuclear, Instituto Superior Técnico, Universidade Técnica de Lisboa, Portugal</i>	
	<u>Miguel A. Maia</u> , Luís M. Magalhães, Luísa Barreiros, Salette Reis and Marcela A. Segundo <i>Faculty of Pharmacy, University of Porto, Portugal</i>		P92	Synthesis of 2-N-benzyl carboxamide derivates of 1-azafagomine
P82	A novel and efficient approach to 2-amino-6-cyanopurines	81	<u>Raquel Mendes</u> , Vera C. M. Duarte, A. Gil Fortes and M. José Alves <i>University of Minho, Portugal</i>	86
	<u>Nádia Senhorães</u> , Alice Dias, and M. Fernanda Proença <i>University of Minho, Portugal</i>		P93	One-pot method in the synthesis of diphosphonic-based lanthanide metal-organic frameworks
P83	A new and efficient synthesis of 3-amino[1,2,4]-triazoles	82	<u>Ricardo Mendes</u> , Sérgio M. F. Vilela, Patrícia Silva, José A. Fernandes and Filipe A. Almeida Paz <i>University of Aveiro, Portugal</i>	87
	<u>Nádia Senhorães</u> , Alice Dias and M. Fernanda Proença <i>University of Minho, Portugal</i>		P94	Stability of simvastatin under different atmospheric humidities
P84	The effect of conformational preorganization on the micellization of calixarene-based surfactants	82	<u>Ricardo G. Simões</u> , João F. Pinto and Manuel E. Minas da Piedade <i>University of Science, University of Lisboa, Portugal</i>	87
	<u>Nuno Basílio</u> , Luis García-Río and Manuel Martín-Pastor <i>Universidad de Santiago de Compostela, Spain</i>		P95	Enzymatic conversion of CO ₂ to methanol: a spectroscopic approach
P85	Primaquine peptidomimetic and organometallic derivatives against <i>Leishmania infantum</i>	83	<u>Rita Craveiro</u> , Pedro Vidinha and Susana Barreiros <i>Faculdade de Ciências e Tecnologia, Universidade Nova de Lisboa, Portugal</i>	88
	<u>Nuno Vale</u> , Sílvia V. Costa, Ana Tomás, Rui Moreira, Maria S. Gomes and Paula Gomes <i>Faculty of Science, University of Porto, Portugal</i>		P96	Setting a new biomolecular force-field: parameterizing manganese first coordination spheres from metalloproteins
P86	New oxysterol derivatives on <i>Opisthorchis viverrini</i>	83	<u>Rui P. P. Neves</u> , Sérgio F. Sousa, Pedro A. Fernandes and Maria J. Ramos <i>Faculty of Science, University of Porto, Portugal</i>	88
	<u>Nuno Vale</u> , Maria João Gouveia, Mónica Botelho, Paula Gomes, Paul Brindley and José M. C. da Costa <i>Faculty of Science, University of Porto, Portugal</i>		P97	Ionic liquids containing nitro and cyano groups
P87	Photophysic study of complexation between β -lapachone-3-sulfonic acid with bovine serum albumin (BSA)	84	<u>Sandra Dias</u> , Andreia Forte and Luís C. Branco <i>Faculdade de Ciências e Tecnologia, Universidade Nova de Lisboa, Portugal</i>	89
	<u>Otávio A.Chaves</u> , Eduardo Benes, Edgar Schaeffer, Bauer O. Bernardes, Aurélio B. B. Ferreira, Jose C. Netto-Ferreira and Dari C. Sobrinho <i>University of Coimbra, Portugal / Universidade Federal Rural do Rio de Janeiro, Brazil</i>		P98	Molecular fluorescence spectroscopy as a technique for the assessment of secondary organic aerosol formation during sampling of atmospheric particles
P88	Synthesis of alkyl glycosides with potential application as antimicrobial agents	84	<u>Sandra M. S. Freire</u> , Regina M. B. O. Duarte and Armando C. Duarte <i>University of Aveiro, Portugal</i>	89
	<u>Patrícia Serra</u> , Vasco Cachatra, Alice Martins and Amélia P. Rauter <i>Faculty of Science, University of Lisboa, Portugal</i>		P99	Interaction of 3,4-dihydroxyxanthone with double stranded DNA in water/ethanol solutions
P89	Pt and Ru complexes and porphyrins as sensitizers for dye-sensitized solar cells	85	<u>Sara Leirosa</u> , C. Sousa, M. J. Sottomayor and M. Pinto <i>Faculty of Science, University of Porto, Portugal</i>	90
	<u>Patricia Jesus</u> , Carlos J. P. Monteiro, Paul A. Scattergood, Julia A. Weinstein, Carlos Serpa, Mariette M. Pereira and Luis G. Arnaut <i>University of Coimbra, Portugal</i>		P100	Pedagogical material for the teaching of Organic Chemistry in the primary level
P90	Multi-residue method for the analysis of veterinary pharmaceutical compounds in sludge	85	<u>Sérgio Leal</u> and João P. Leal <i>Faculty of Science, University of Lisbon, Portugal</i>	90
	<u>Pedro N. Carvalho</u> , M. Clara P. Basto and C. Marisa R. Almeida <i>Faculty of Science, University of Porto, Portugal</i>			

P101	Novel lanthanide phosphonate MOFs: synthesis, crystal structures, photoluminescent and catalytic properties <u>Sérgio M. F. Vilela</u> , Duarte Ananias, Ana C. Gomes, Anabela A. Valente, Luís D. Carlos, José A. S. Cavaleiro, João Rocha, João P. C. Tomé and Filipe A. Almeida Paz <i>University of Aveiro, Portugal</i>	91	P111	Biosensor development for pirimicarb pesticide determination <u>Thiago M. B. F. Oliveira</u> , Simone Morais, Maria F. Barroso, Pedro de Lima-Neto, Adriana N. Correia, Maria B. P. P. Oliveira and Cristina Delerue-Matos <i>School of Engineering, ISEP, Polytechnic Institute of Porto, Portugal</i>	96
P102	The influence of microwave irradiation in the outcome of solid phase peptide synthesis <u>Silvia Maia</u> , Miguel A. Fernandez and Paula Gomes <i>Faculty of Science, University of Porto, Portugal</i>	91	P112	Transition metal substituted polyoxometalates: potentialities in oxidation by hydrogen peroxide <u>Tiago A. G. Duarte</u> , Ana C. Estrada, Isabel C. M. Santos, Mário M. Q. Simões, M. Graça P. M. S. Neves, Ana M. V. Cavaleiro and José A. S. Cavaleiro <i>University of Aveiro, Portugal</i>	96
P103	Bisphenol-A adsorption onto activated carbon. Langmuir and Freundlich isotherms and kinetics. <u>Sofia Amaro</u> and I. Macedo <i>University of Aveiro, Portugal</i>	92	P113	From 2-hydroxypyridine to 4(3H)-pyrimidinone: the role of aromaticity, hydrogen bonds and substituent effects in tautomeric equilibrium <u>Tiago L. P. Galvão</u> , Inês M. Rocha and Manuel A. V. Ribeiro da Silva <i>Faculty of Science, University of Porto, Portugal</i>	97
P104	Synthesis and evaluation of the biological activity of new flavonoid-porphyrin dyads <u>Sónia P. Lopes</u> , Diana C. G. A. Pinto, Maria A. F. Faustino, Artur M. S. Silva, Maria G. P. M. S. Neves and José A. S. Cavaleiro <i>University of Aveiro, Portugal</i>	92	P114	Fate of the antiepileptic drug carbamazepine at the water/soil interface <u>Vânia Calisto</u> and Valdemar I. Esteves <i>University of Aveiro, Portugal</i>	97
P105	Application of scientific computation in the chemistry education <u>Stéfano Araújo Novais</u> and Fabio da S. Miranda <i>Universidade Federal Fluminense, Rio de Janeiro, Brazil</i>	93	P115	Structural and thermophysical studies of 9-acridanone and 10-methyl-9-acridanone <u>Vera L. S. Freitas</u> , Paulo J. O. Ferreira and Maria D. M. C. Ribeiro da Silva <i>Faculty of Science, University of Porto, Portugal</i>	98
P106	Biocompatible fluorescence based temperature sensor <u>Suzete Almeida</u> , Sérgio Alves, José M. G. Martinho, José P. S. Farinha and Carlos Baleizão <i>Instituto Superior Técnico, Universidade Técnica de Lisboa, Portugal</i>	93	P116	Host:guest binding constant influenced by the host counterion <u>Vitor Francisco</u> , Nuno Basilio, and Luis Garcia-Rio <i>Universidad de Santiago de Compostela, Spain</i>	98
P107	Palladium/carbon catalyzed hydrogenolysis and hydrogenation of xanthene type fluorophores: a study by NMR <u>Tânia Moniz</u> , Carla Queirós, Ana M. G. Silva, Galya Ivanova, Baltazar de Castro and Maria Rangel <i>Instituto de Ciências Biomédicas de Abel Salazar, Portugal</i>	94	P117	The mathematical description for the electrochemical synthesis of heterocyclic compounds in galvanostatic mode <u>Volodymyr V. Tkach</u> , Vasyly V. Nechyporuk and Petro I. Yagodynets <i>Chernivtsi National University, Ukraine</i>	99
P108	Synthesis and anticancer activity of a selection of quercetin analogues and their precursors <u>T. A. Dias</u> , C. L. Duarte, M. F. Proença, C. F. Lima and C. Pereira-Wilson <i>University of Minho, Portugal</i>	94			
P109	Synthesis of new molecules with the 4H-chromen-4-ylidene scaffold <u>T. A. Dias</u> and M. F. Proença <i>University of Minho, Portugal</i>	95			
P110	Nutritional value of Senegalese sole (<i>Solea senegalensis</i> Kaup, 1858) fed with eco-friendly diets <u>Telmo J. R. Fernandes</u> , Sílvia D. Campos, Eduarda M. Cabral, Manuela Castro-Cunha, Luísa M. P. Valente and M. Beatriz P. P. Oliveira <i>Faculty of Pharmacy, University of Porto, Portugal</i>	95			

Plenary Lectures



OLD DRUGS WITH NEW FACES

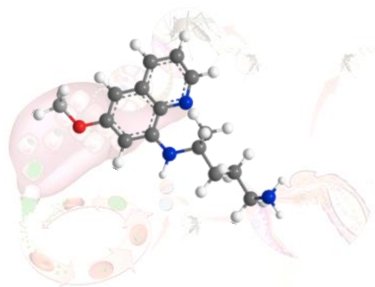
Chemical strategies to cover primaquine unpleasant traits while preserving its attractive antimalarial attributes

Paula Gomes*, Nuno Vale, Joana Matos

Faculdade de Ciências, Universidade do Porto, Portugal

*pgomes@fc.up.pt

PL1



- The World Health Organization estimates that there were 216 million new malaria cases worldwide in 2011, leading to the death of about 655 thousand people, 86% of which were children under five years old.
- Over six decades after its discovery, primaquine is still the only clinically available antimalarial capable of eliminating all exoerythrocytic forms of malaria parasites.
- Primaquine has low oral bioavailability and is hemotoxic, which precludes its use on the most vulnerable population: pregnant women and infants.
- Chemical approaches to reduce primaquine's undesirable features while conserving its antimalarial activity have been carried out.
- The novel peptidomimetic and organometallic derivatives of primaquine developed have revealed highly promising properties both concerning antimalarial activity and enzymatic stability.

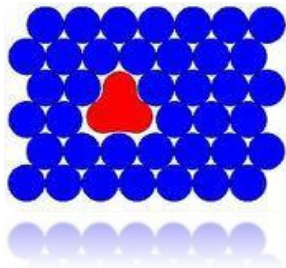
Light Induced Reactions in Cryogenic Matrices

Rui Fausto*

University of Coimbra, Portugal.

* rfausto@ci.uc.pt

PL2



- The fundamentals of the matrix isolation technique will be presented, and its main advantages in the study of chemical reactivity described.
- Examples of its use in the investigation of photochemical (UV-induced) and hot-vibrational chemistry (IR-induced) processes will be given and discussed.
- These examples will include conformational isomerizations, rearrangements, fragmentations and molecular aggregation.



PL3

Collaborative R&D Between GALP Energia and university as a factor to promote competitiveness

Jorge Correia Ribeiro*

Galp Energia, Portugal

**jorge.ribeiro@galpenergia.com*



- Collaborations between GALP Energia and academic community, under the EngIQ program.
- The interaction between industry and university plays an important role due to the high activity of this diverse competitive industrial sector.
- Aim to meet the technological requirements as well as, to train highly qualified professionals, to promote the fundamental and applied knowledge.
- Key factors for the technological and scientific based support of GALP Energia competitive strategy for the future.



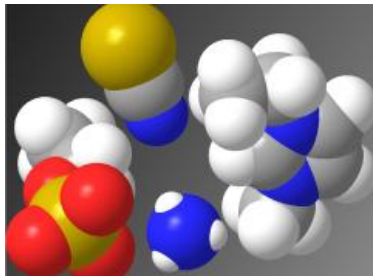
PL4

Novel Ionic Liquids – New Flexibility

Luís Paulo N. Rebelo*

Instituto de Tecnologia Química e Biológica, UNL, Portugal.

**luis.rebelo@itqb.unl.pt*

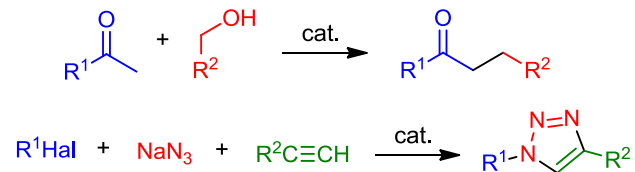


Efficiency in Chemistry: From Hydrogen Autotransfer to Multicomponent Catalysis

Miguel Yus*

Facultad de Ciencias, Universidad de Alicante, Spain

*yus@ua.es



- Ru- and Ni-catalyzed α -alkylation of methyl ketones with alcohols
- Ru-catalyzed Friedländer cyclization with alcohols
- Cu- and Ru-catalyzed monoalkylation of amines with alcohols
- Fe-catalyzed aza-Sakurai reaction
- Cu-catalyzed 'click' chemistry

Invited Communications

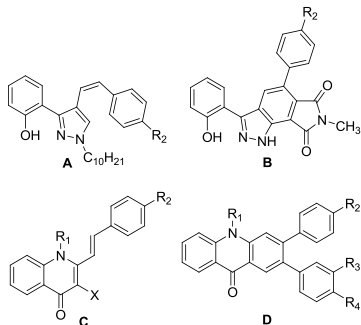


Development of synthetic methodologies for new biologically active heterocyclic compounds

Vera L. M. Silva*, Artur M. S. Silva and José A. S. Cavaleiro

University of Aveiro, Portugal

*verasilva@ua.pt



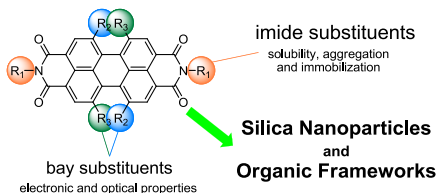
- An efficient methodology for the synthesis of a series of new (*Z*)- and (*E*)-3(5)-(2-hydroxyphenyl)-4-styrylpyrazoles (**A**) was developed.
- The alkylation of these pyrazoles with long alkyl chains bromides in basic medium afforded pyrazoles with affinity towards CB¹ cannabinoid receptors in the nanomolar range (**A**).
- Microwave irradiation under solvent-free conditions induces 1-acetyl-4-styryl-1*H*-pyrazoles to undergo Diels-Alder cycloaddition reactions with *N*-methyl or *N*-phenylmaleimide to give tetrahydroindazoles, which upon dehydrogenation gave indazoles in good yields and with high selectivities (**B**).
- New synthetic routes for the preparation of (*E*)-2-styrylquinolin-4(1*H*)-ones and (*E*)-1-methyl-2-styrylquinolin-4(1*H*)-ones were established (**C**).
- Two new efficient methodologies for the synthesis of 2,3-diarylacridin-9(10*H*)-ones were developed (**D**).

Perylenediimide based functional hybrid materials

Carlos Baleizão *

Instituto Superior Técnico, Universidade Técnica de Lisboa, Portugal

* carlos.baleizao@ist.utl.pt



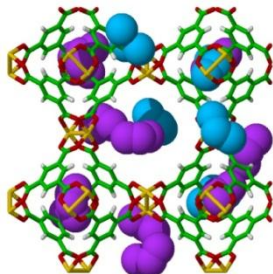
- Synthesis of new perylenediimide derivatives.
- Electronic properties tuned through the introduction of different substituents.
- Incorporation in silica nanostructures and organic frameworks.
- Application to imaging and solar cells.

Molecular Simulation of Hybrid Organic-Inorganic Nanoporous Materials: Synthesis and Adsorption Predictions

Miguel Jorge*, Ryusuke Futamura, Christophe Siquet and José R. B. Gomes

Faculdade de Engenharia, Universidade do Porto, Portugal

* mjorge@fe.up.pt



- Molecular Dynamics simulations of the synthesis of hybrid PMO materials were performed.
- Results clarify the role of inorganic and organic precursors in the formation of the material.
- Monte Carlo simulations of adsorption in hybrid MOF materials are also presented.
- A new approach combining quantum mechanical information and classical models was developed.
- Good predictions are obtained for olefin/paraffin separations using the new approach.

Oral Communications



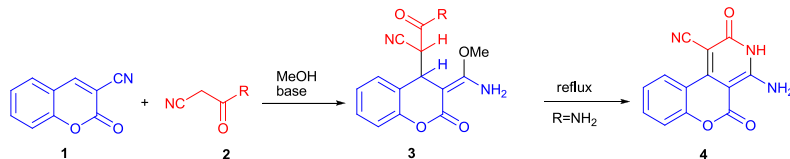
New chromene scaffolds for adenosine receptors: synthesis and pharmacology

Marta Costa*, Filipe Areias, Marian Castro, Jose Brea, María I. Loza and Fernanda Proença

University of Minho, Portugal

*martasilviacosta@gmail.com

OC1



- Adenosine receptors are distributed throughout the body, regulating different cellular functions and can be considered attractive targets for therapeutic agents.
- The interaction of chromene derivatives with adenosine receptors was never reported before.
- Novel chromene derivatives **3** and **4** were synthesized in a one-pot procedure.
- These new scaffolds proved to be active at adenosine receptors and several hits were identified with affinities in the submicromolar range.

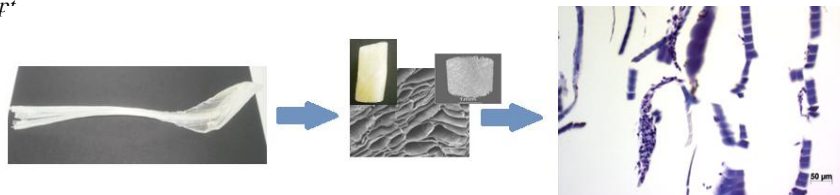
Marine biomaterials on the origin of biomedical applications

Tiago H. Silva*, Joana Moreira-Silva, Lara L. Reys, Ana Rita C. Duarte, Simone S. Silva, Susana Fernandes-Silva, João F. Mano, Rui L. Reis

University of Minho, Braga / PT Government Associate Laboratory, Braga/Guimarães, Portugal

*tiago.silva@dep.uminho.pt

OC2



- Valorization of marine resources by creating new marine biomaterials, further used on the development of biomedical applications.
- Chitosan produced from squid pens was used for the development of porous structures for engineering of bone and cartilage tissue.
- Polymeric structures for tissue engineering scaffolding were developed by cross-linking of collagen obtained from fish skins.
- Sustainable exploitation of natural marine resources.

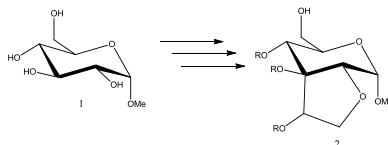


New Synthetic Approach towards the Miharamycins Sugar Moiety

Vasco Cachatra*, Andreia Almeida and Amélia Pilar Rauter

Universidade de Lisboa, Faculdade de Ciências, Portugal

*vasco_cachatra@hotmail.com



- Simple and stereoselective reactions for the synthesis of the miharamycins sugar moiety.
- Control of the configuration of isomers by the appropriate choice of solvent and/or protecting groups.
- Less toxic methodology then those reported to date.

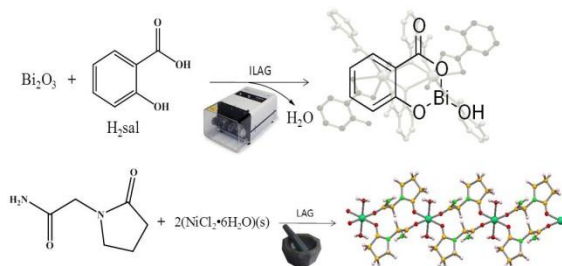


Mechanosynthesis: a new pathway for the synthesis of metallodrugs and metallopharmaceuticals

Vânia André* and M. Teresa Duarte

Instituto Superior Técnico, Universidade Técnica de Lisboa, Portugal

*vaniandre@ist.utl.pt



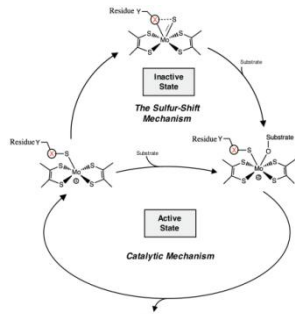
- Design and synthesis of metallodrugs and metallopharmaceutics
- Solution synthesis vs mechanochemical synthesis
- Rapid, efficient and selective synthesis of metallodrugs by ion- and liquid-assisted grinding (ILAG)
- Metallopharmaceuticals with improved properties
- Metallopharmaceuticals making use of the metal benefits
- Evaluation of the relevant properties (stability, temperature, RH, pH, time), solubility, dissolution, tableting of the new forms
- Structure-property relationships
- Intellectual property protection

The Sulfur-Shift: The activation mechanism of mononuclear Mo enzymes

Nuno M. F. S. A. Cerqueira*

Faculdade de Ciências, Universidade do Porto, Portugal.

*nscerque@fc.up.pt



Legend : X=S and Y=Cys. X=Se and Y=SeCys

- This mechanism unravels the enigmatic activation mechanism of mononuclear Mo enzymes.
- Provides an efficient mechanism to lower down the activation barriers for ligand exit or entrance processes.
- Allows to protect the metal site from other molecules that can potential destroy or inactive it, including the solvent.
- The mechanism is very similar to the popular carboxylate-shift mechanism found in other enzymes.
- These results suggest that enzymes containing metals in their active site may possess similar type of mechanisms and such trend might be more common in nature than we were expecting.

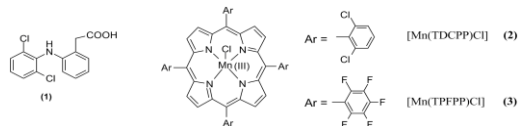
Manganese porphyrins as catalysts in the oxidation of diclofenac

Cláudia M. B. Neves*, Mário M. Q. Simões, Isabel C. M. S. Santos, Filipe A. A. Paz, M. Graça P. M. S. Neves,

Artur M. S. Silva and José A. S. Cavaleiro

University of Aveiro, Portugal

*claudianeves@ua.pt



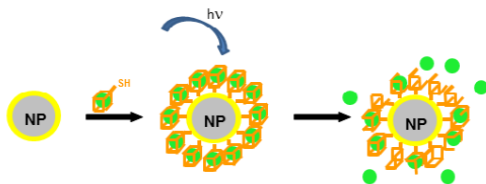
- Manganese(III) porphyrins were used as catalysts in the oxidation of diclofenac (**1**).
- Reactions were performed using diluted H_2O_2 , under normal atmosphere, in a mixture of acetonitrile/water at 30 °C.
- Different co-catalysts were used.
- Reactions were monitored by TLC and HPLC.
- The products were characterized by MS, 1D and 2D NMR studies and X-ray crystallography.

Light-activated delivery of inorganic and organic phosphates: using metal nanoparticles for the release of caged compounds in aqueous media

Artur J. Moro*, Joana Sousa, João Rosa, P. V. Baptista and João C. Lima

Faculdade de Ciências e Tecnologia, Universidade Nova de Lisboa, Portugal

* ajm12769@fct.unl.pt



- Synthesis of coumarins with a photocleavable group (phosphate or nucleotide) at position 4, bearing also a spacer chain (tetraethyleneglycol) with a terminal thiol group at position 7.
- Spectroscopic characterization of the synthesized compounds (UV-Vis absorption, fluorescence spectroscopy) and full description of the photochemical processes and photoproducts upon light irradiation (HPLC, LC-MS).
- Functionalization of metal nanoparticles (NPs) and evaluation of their influence on the previously described photochemistry per comparison.
- Application of the NPs in biological samples, e.g. for the control of RNA polymerization via light.

Encapsulation of resveratrol in lipid nanoparticles: formulation and characterization

Ana Neves, M. Lúcio, J. L. F. C. Lima and S. Reis

Faculdade de Farmácia, Universidade do Porto, Portugal

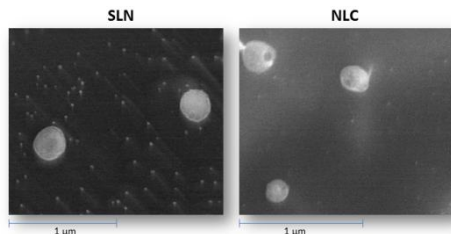


Figure 1: Cryo-SEM images of the nanoparticles.

- Development and characterization of lipid nanoparticles (SLN and NLC) loaded with resveratrol.
- Good encapsulation efficiency of around 70% and no significant differences between SLN and NLC.
- Low release of resveratrol over the time in storage conditions, only 10% corresponding to the non-encapsulated resveratrol.
- Stability also verified periodically by measurement of particle size and zeta potential.
- Novel biocompatible resveratrol nanodelivery systems applied as nutraceuticals to enhance its solubility, physical stability, and bioavailability.

Monitoring Heavy Metals in Urban Soils at Lisbon

Hugo F. Silva*, Andrei Sadovski, Cristina Oliveira, Manuel J. Matos

Instituto Superior Engenharia de Lisboa, Portugal

*hsilva@deq.isel.ipl.pt

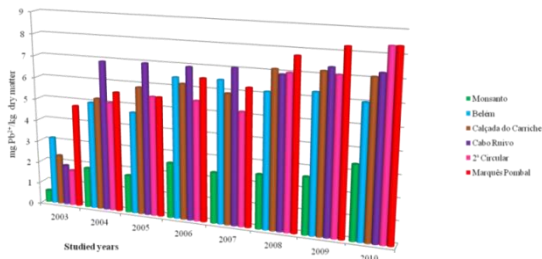


Figure 1: Levels of lead in Lisbon soils between 2003 and 2010

- Levels of metals have increased over the years, proving its accumulation in the soil;
- Lisbon almost without industry → Main source → Traffic;
- Most polluted sites → Marquês of Pombal and 2ª Circular → Higher traffic intensity.

Dow Human Element: Fostering an Innovation Culture

Raquel Fortes*

New Business Development Leader, Dow Europe GmbH, Switzerland



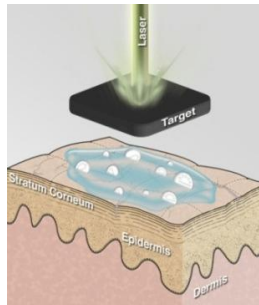
- New products and technologies are vital to the success and future prosperity of a modern corporation.
- Organizational culture is a fundamental element of sustained innovativeness and financial performance.
- Science requires immense creativity because the process that we are trying to address for tomorrow are not going to be obvious.
- At Dow we are constantly searching for how to use our fundamental knowledge of chemistry to solve these difficult problems.
- The one element that changes everything, it is the human element.

Photoacoustic Waves based Technology using Light Absorbing Thin Films for Transdermal Drug Delivery

Gonçalo F. F. Sá*, Carlos Serpa and Luís G. Arnaut

University of Coimbra / LaserLeap Technologies, Coimbra, Portugal

* gsa@ui.uc.pt



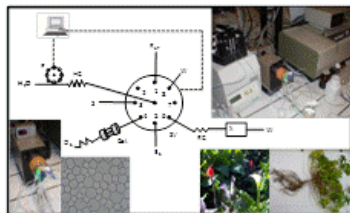
- Transdermal drug delivery facilitated with an active method based on photoacoustic waves.
- Thin films of polymers-calorimetric references or titanium dioxide-calorimetric references, but strongly absorbing.
- Production of pressure waves with short rise times (< 50 ns) with low optical power densities (40 MW/cm^2), but high amplitude peaks (12 atm).
- 3 times increase in TEWL if compared with non-treatment site and full recovery in one minute.
- Transdermal drug delivery of porphyrins, bacteriochlorins and GFP.

Use of solid phase extraction in a sequential injection system for the determination of alkaline phosphatase activity in plant roots

Inês C. Santos*, Raquel B. R. Mesquita, Adriano A. Bordalo and António O. S. S. Rangel

Universidade Católica Portuguesa, Porto, Portugal

* icsantos@porto.ucp.pt



- In-line solid phase extraction for enzyme pre concentration in a sequential injection system.
- Nitritotriacetic Acid (NTA) Superflow charged with Zn^{2+} to bind alkaline phosphatase.
- Significant reduction in reagent and sample consumption.
- Determination rate of 17 h^{-1} and detection limit of $0.025 \text{ unit cm}^{-3}$ were achieved.
- Successful determination in different types of root plants.

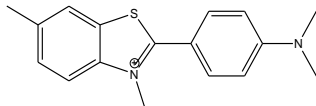
Preparation and Characterization of Ionic Liquids based on Thioflavin T

Alexandra Costa*, Luís C. Branco and Isabel Marrucho

Faculdade de Ciências e Tecnologia, UNL, Portugal

**alexandrampcosta@gmail.com*

OC13



- Thioflavin T is a basic yellow biological compound used as a dye to detect and quantify the amyloid fibrils.
- Recent studies showed that Room Temperature Ionic Liquids (RTILs) can effectively trigger amyloid fibril formation.
- Thioflavin T as an organic cation was combined with different anions such as bis(trifluoromethylsulfonyl)imide (NTf₂), docusate (AOT), trifluoromethanesulfonate (OTf) and dicyanamide (DCA) in order to prepare novel Ionic Liquids (ILs).
- Novel Thioflavin salts were characterized by NMR (¹H, ¹³C and ¹⁹F), FTIR and elemental analysis.
- Some physical-chemical and thermal properties were also evaluated in particular their rheological (viscosity), spectroscopic (UV-Vis and emission spectra) and calorimetric (melting point, glass transition and decomposition temperatures) behavior.

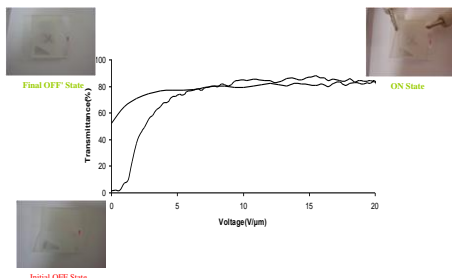
PDLC devices that consume lower power and are environmentally friendly

Ana Mouquinho* and João Sotomayor

Faculdade de Ciências e Tecnologia, Universidade Nova de Lisboa, Portugal

**a.mouquinho@campus.fct.unl.pt*

OC14



- We obtain for the initial OFF state that correspond to the transmittance of the initial opaque state (0%), the ON state to the transmittance upon applying electric field (80%) and for the final OFF' state after removal of the applied field (55%). The electric field required for this PDLC to reach 90% of its maximum transmittance was 4.85 V/μm.
- For this to happen there must be a weak force between LC molecules and the polymer surface (low anchoring effect)
- This effect can be used in memory devices, such as, write information in a digital way on a pixel (opaque or transparent state), read written information (evaluating the transmittance of the pixel), and erase the information just applying temperature.

A GC-MS method for the simultaneous identification and quantification of amino acids, fatty acids and sterols in marine organisms

David M. Pereira*, Juliana Vinholes, Patrícia Valentão, Paula Guedes de Pinho, Natércia Teixeira and Paula B. Andrade
Faculdade de Farmácia, Universidade do Porto, Portugal

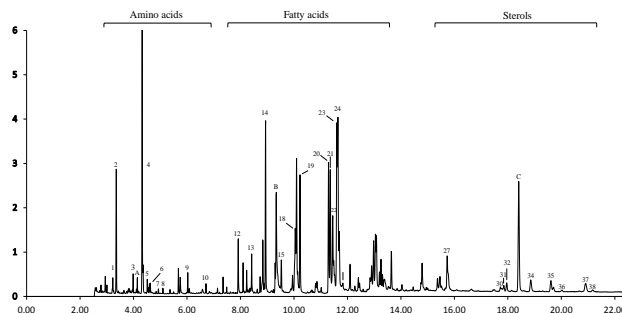
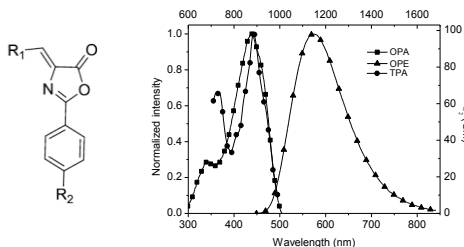


Figure 1: GC-MS profile of the equinoderm *Marthasterias glacialis* (spiny sea-star).

- A GC-MS method for detection and quantification of amino acids, fatty acids and sterols was developed.
- 40 compounds can be identified and quantified in a 20-minutes run.
- No hazardous solvents are used.
- This work can be used in metabolite screening of marine organisms for both the food and biomedical industry.

Photophysics of push-pull oxazolones derivatives with nonlinear optical properties

Inês de F. A. Mariz*, Catarina Rodrigues, Ermelinda M. S. Mações, Carlos Afonso and José M. G. Martinho
Instituto Superior Técnico, Lisboa, Portugal
*ines.mariz@ist.utl.pt



Oxazol-5-(4H)-ones (referred as oxazolones) are small and simple molecules with potential applications as labels in bioimage, and as nonlinear activated optical sensors.

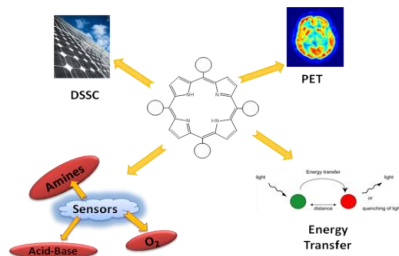
- A series of oxazolones (see Figure) with different electron donor and acceptor groups and the same active center have been synthesized and their linear and nonlinear properties analyzed.
- In general, these molecules have quite reasonable two-photon absorption cross-sections (up to 540 GM, 1 GM= 10⁻⁵⁰ cm²s) but low emission quantum yield due to non-radiative processes of different nature. By changing the electron donor group of the molecule we were able to obtain molecules with a two-photon absorption cross section around 320 GM and a high emission quantum yield (0.79).
- The performance of this optimized oxazolone can be compared with commercial available fluorophores used in bioimaging, which have at best two-photon absorption cross sections around 100-200 GM and quantum yields of 0.4-0.9.

New porphyrin materials for optoelectronic and PET applications

Sara M.A.Pinto*, César A. Henriques, Carlos J.P. Monteiro, Ana V.C. Simões, Mário J.F. Calvete, Mariette M. Pereira and Hugh D. Burrows

Faculdade de Ciências e Tecnologia, Universidade de Coimbra, Portugal

*smpinto@qui.uc.pt



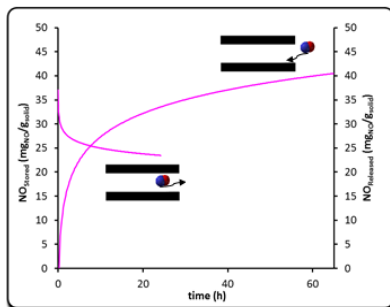
- New porphyrin triads were synthesised and tested as amine, acid-base and O₂ sensors.
- Modulation of melting points (to the range 70°C to 100°C) of porphyrins was induced by changing meso substitution.
- A library of new porphyrins for application in dye sensitized solar cells (DSSC) was obtained and photophysically characterized.
- Fluorine labelled radioactive porphyrins were synthesised for PET and in vivo tests are in progress.

Clay materials for the storage and release of nitric oxide for therapeutic purposes

Ana C. Fernandes* and M. L. Pinto, J. Pires

Faculty of Science, University of Lisbon, Portugal

*acfernandes@fc.ul.pt



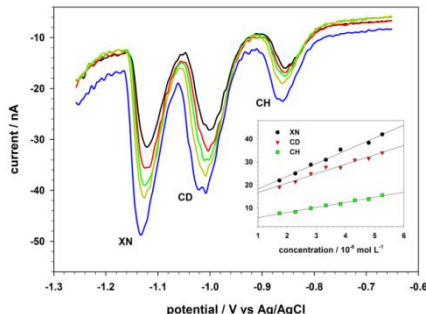
- NO used for medical purposes;
- Synthesis of clay adsorbent material for storage and subsequent controlled release of NO;
- Use of clay materials with cobalt ions in its structure to promote adsorption of NO;
- Clay materials have high surface area;
- CoClay-2 has a high storage capacity of NO.

On the voltammetry of chalcones: trans-calcone, cardamonin and xanthohumol

Eliana M. Tavares*, Luís M. Gonçalves, José A. Rodrigues and Aquiles A. Barros

Faculdade de Ciências, Universidade do Porto, Portugal

*elianartavares@gmail.com



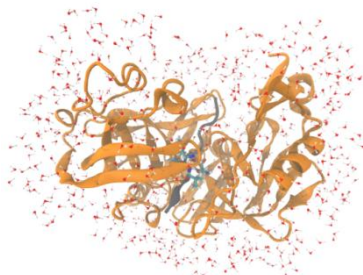
- Chalcones have important antioxidant and health promoting activities
- Chalcones are naturally present in plants and can be used in new food products and pharmaceutical formulations
- Cyclic voltammetry (CV) on a hanging mercury drop electrode (HMDE) was applied to study them
- The reduction of these chalcones seemed to be an overall irreversible process and a mixed adsorptive and diffusive response was obtained. Also, for major times of accumulation was showed a stagnation of the adsorptive effective
- Voltammetry is very sensible analysing chalcones, low LODs were obtained.

Computational studies on the aspartic protease Renin

Natércia F. Brás*, Pedro A. Fernandes and Maria J. Ramos

Faculdade de Ciências, Universidade do Porto, Portugal.

*nbras@fc.up.pt



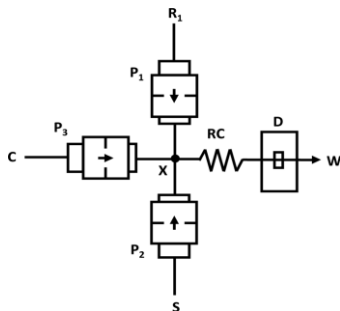
- Hybrid ONIOM method was performed to study the theoretical catalytic mechanism of human and mouse renin enzymes (REN).
- The gem-diol intermediate formation was found to be the rate-limiting step of REN mechanism of action.
- Differences in the amino acids surrounding the active site are responsible for the high specificity of each studied REN.
- Molecular Dynamics simulations and Alanine Scanning Mutagenesis studies were performed.
- Several flexible regions and specific amino acids that are crucial to an efficient REN activity were uncovered.
- All these results are preminent to future drug design studies.

Ciprofloxacin and norfloxacin spectrophotometric determination in a fully automated multi-pumping flow system

Maria H. R. Amorim*, Karine L. Marques, João L. M. Santos and José L. F. C. Lima

Faculty of Pharmacy, Porto University, Portugal.

*helenara@fe.up.pt



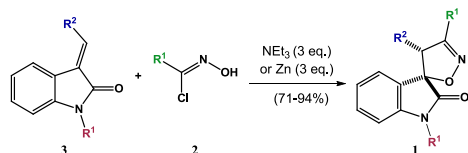
- A multi-pumping flow system was developed for the spectrophotometric determination of two fluoroquinolones
- A precise, sensitive, simple and reproducible methodology
- The procedure presents high flexibility and versatility
- The proposed procedure presents good figures of merit, namely lower detection limits.

Efficient Synthesis of new Spiroisoxazoline Oxindoles

Carlos J. A. Ribeiro*, Rui Moreira and Maria M. M. Santos

Faculty of Pharmacy, University of Lisbon, Portugal

*cjacribeiro@ff.ul.pt



1a R¹=Me, R²=CO₂Et, R³=CO₂Et;

1b R¹=Me, R²=CO₂Et, R³=Ph;

1c R¹=Me, R²=CO₂Me, R³=Ph;

1d R¹=H, R²=CO₂Et, R³=Ph;

1e R¹=H, R²=CO₂Me, R³=Ph;

1f R¹=Me, R²=CO₂Me, R³=CO₂Et;

1g R¹=H, R²=CO₂Et, R³=CO₂Et;

1h R¹=H, R²=CO₂Me, R³=CO₂Et;

1i R¹=H, R²=CO₂Et, R³=CO₂Me;

1j R¹=H, R²=CO₂Et, R³=pOMePh;

1k R¹=Me, R²=CO₂Et, R³=pOMePh;

- Spiroisoxazoline oxindoles were synthesized in yields up to 94% by 1,3-dipolar cycloaddition;
- It is the first time that Zn is used as dehydrochlorinating agent;
- The compounds obtained were always the spiro[indoline-3,5'-isoxazoline]-2-one regioisomer

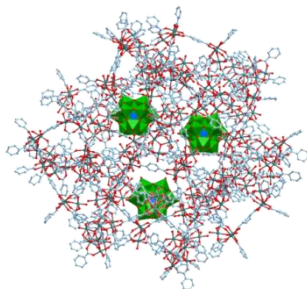
New composites based on polyoxometalates and porous MOFs as active catalysts for liquid phase oxidation

Carlos M. Granadeiro*, André D. S. Barbosa, Patrícia Silva, Filipe A. Almeida Paz, Baltazar de Castro,

Salete S. Balula and Luís Cunha-Silva

Faculty of Sciences, University of Porto, Portugal

*cgranadeiro@fc.up.pt



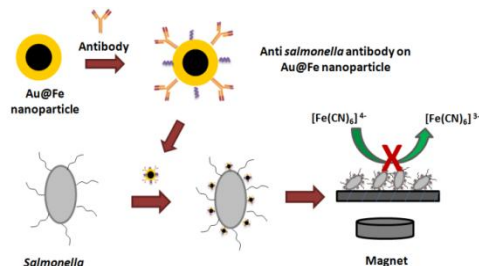
- Metal-organic frameworks (MOFs) are nowadays on the top of research as promising materials for catalytic applications.
- 3D structures of MOFs frequently originate the formation of porous materials with large, regular and accessible channels and cages.
- Large cavities of MOF materials can promote the confinement effect between different components of the catalytic reaction.
- Immobilization of active POMs into MOFs cavities open the opportunity to create new eco-sustainable catalytic systems.

Iron Oxide/Gold Core/Shell Nanoparticles and Screen printed carbon electrode for sensitive detection of *Salmonella typhimurium*

Maria Freitas, S. Viswanathan*, M.B.P.P. Oliveira and C. Delerue-Matos

Faculdade Farmácia, Universidade do Porto, Portugal

*rviswa@gmail.com



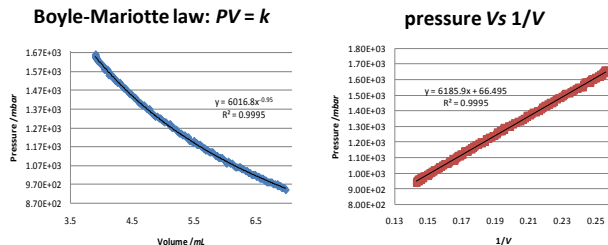
- Successful use of iron oxide/gold core/shell magnetic nanoparticles for salmonella detection is developed.
- Gold shell provides a perfect platform for the conjugation of antibody molecules.
- A magnetic property of nanoparticle was utilized to perform rapid detection of *Salmonella*.
- A screen-printed carbon electrode for *Salmonella* detection was tested successfully.

e-lab: a didactic interactive experiment. An approach to the Boyle-Mariotte law

Sérgio Leal*, João P. Leal and Horácio Fernandes

Faculty of Science, University of Lisbon, Portugal

*sergioleal20@gmail.com



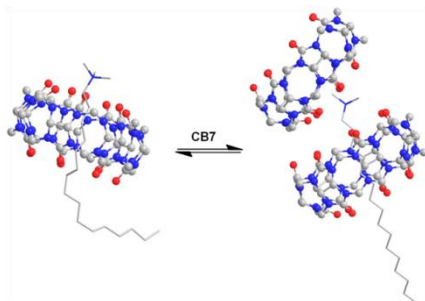
- Both graphs are from the same experience performed and have satisfactory results in verifying Boyle-Mariotte law.
- Graphs result from data directly obtained from e-lab and using a spreadsheet.
- The first graph is a numerical fit of the plot Pressure Vs Volume, to be used for advanced students (exponent not exactly -1).
- The second graph was obtained in MSExcel with the plot of the Pressure against the inverse of the Volume. Students can infer directly the inverse proportionality law.
- Students can easily deduce the law supported on the quality of the measurements obtained by them.

Dual complexation mode of Cucurbit[7]uril and cationic surfactants

Márcia Pessêgo*, J. A. Moreira and L. García-Río

Universidade de Santiago, Santiago de Compostela, Spain / Faculdade de Ciências e Tecnologia, Universidade do Algarve, Portugal

*cjacribeiro@ff.ul.pt



- CB7 molecules can form 1:1 and 2:1 with cationic surfactants.
- The $K_{1:1}$ is independent of the chain length of the surfactants.
- The $K_{2:1}$ presents a relationship with hydrophobic character of surfactants.
- In the 2:1 complex both hosts complex the trimethylammonium group of the surfactant.

The conducting polymer based electrochemical sensors and biosensors with autocatalytical stage and the description of their work

Volodymyr V. Tkach*, Vasyl V. Nechyporuk, Petro I. Yagodynets and Aline M. da Rocha

Chernivtsi National University, Ukraine

**nightwatcher2401@gmail.com*

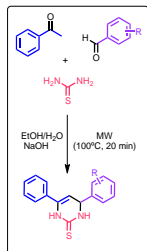
- The work of the electrochemical conducting-polymer based sensors and biosensors with autocatalytical stage was described mathematically. The corresponding model was analyzed by linear stability theory and bifurcational analysis
- The linear stability analysis showed, that the region of the best response of the sensor (corresponding to the linear relation between the electrochemical parameter and analyte concentration) is limited by the critical value of diffusional parameter κ , which is defined by other parameters' values.
- The oscillatory instability in this system can be caused by the influence of electrochemical oxidation of the reduced form of the analyte to the double electrical layer (DEL) on the second stage and also by the autocatalytic scenario of the reaction on the first stage.
- The monotonic instability in this system, also known as steady-state multiplicity, occurs in the critical value of the diffusional parameter κ . It corresponds to the N-shaped fragment of the voltamperogram. In this point the system exists in the multiplicity of stationary states, choosing only one of them. It destroys after changing the conditions.
- This model is also capable to describe the processes of the conducting polymer modification, related with the sensing systems.

One-step three-component vs two-step two-component microwave assisted synthesis of 4,6-diaryldehydropyrimidinthiones

Tiago E. B. Valadeiro, Bruno F. O. Nascimento and M. Pineiro*

Coimbra Univeristy, Portugal

**mpineiro@qui.uc.pt*



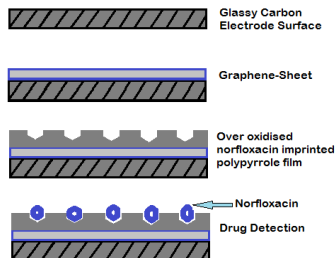
- The three-component reaction of benzaldehyde, acetophenone and thiourea using Lewis acids such as ZnI_2 or FeCl_3 as catalysts under microwave irradiation do not afford the desired 4,6-diaryldihydropyrimidinthiones.
- Base-mediated three-component reaction of arylaldehydes, acetophenone and thiourea afford, after recrystallization of the reaction product, 4,6-diaryldihydropyrimidinthiones with yields up to 45%.
- Two-step one-pot base-mediated reaction: benzaldehyde and acetophenone microwave assisted condensation followed by addition of thiourea afford, after recrystallization, 15% of 4,6-diphenyldihydropyrimidinthione.
- Base-mediated two-component two-pot reaction: benzaldehyde and acetophenone condensation under conventional heating conditions followed by condensation with thiourea under microwave irradiation afford, after recrystallization, 4,6-diphenyldihydropyrimidinthione with 86% yield.
- Base-mediated two-component reaction 1,3-diarylpentenones (previously prepared under conventional heating conditions) and thiourea afford, after recrystallization of the reaction product, 4,6-diaryldihydropyrimidinthiones in 80-86%.
- NMR- ^1H and GC-MS evidence of the formation of condensation products of 1,3-diarylpentenone and acetaldehyde explain the differences on the reaction yields obtained in the two presented methodologies and allow to refine the three-component reaction conditions in order to increase the reaction yields above 50%

Molecular Imprinted Polymer on Graphene Nanosheets Modified Glassy Carbon Electrode for Norfloxacin detection

Hélder da Silva, Subramanian Viswanathan*, and Cristina Delerue-Matos

Instituto Superior de Engenharia do Porto, Portugal

* rsviswa@gmail.com



- Fabrication of graphene nanosheet-modified glassy carbon electrode
- Direct electrochemical synthesis of norfloxacin imprinted over oxidised polypyrrole film.
- Voltammetric determination of norfloxacin using imprinted polymer sensor.
- Detection norfloxacin from spiked human urine samples.

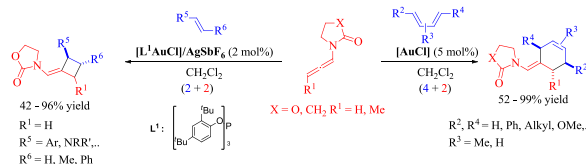
Gold(I)-catalyzed intermolecular (4 + 2) and (2 + 2) cycloadditions of allenamides

Hélio Faustino*, Fernando López and José L. Mascareñas

Universidad de Santiago de Compostela. Santiago de Compostela, Spain

* heliofaus@hotmail.com

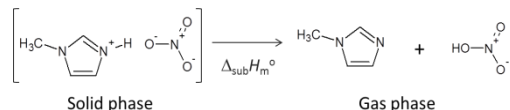
Allenamides work as efficient two-carbon partners in a variety of intermolecular gold-catalyzed (4 + 2) or (2 + 2) cycloadditions to dienes or alkenes, respectively:



- These transformations represent a simple and practical entry to highly substituted cyclohexenic and cyclobutanic derivatives and take place with high regio- and stereocontrol.
- Complete diastereoselectivity is achieved when a chiral allenamide is employed in the (4 + 2) cycloaddition.
- Different mechanistic scenarios are discussed in the basis of the type of products and trapped reaction intermediates.
- One of the very few examples of intermolecular gold catalyzed cycloadditions.

Flash Communications





* *mpineiro@qui.uc.pt*

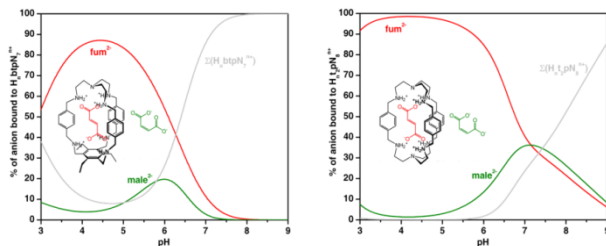


Dicarboxylate recognition by two macrobicyclic receptors: selectivity for fumarate over maleate

Pedro Mateus*, Rita Delgado, Paula Brandão and Vítor Félix

Instituto de Tecnologia Química e Biológica, Portugal

*pmateus@itqb.unl.pt



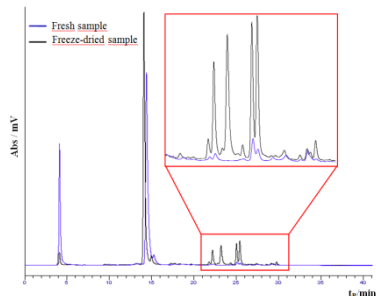
- Two ditopic polyamine macrobicyclic compounds were studied as receptors for the recognition of dicarboxylate anions of varying chain length in aqueous solution.
- Both compounds are able to form stable associations with the dianionic substrates in competitive aqueous solution.
- The receptors show unprecedented selectivity for fumarate over other dicarboxylate competitors, including its *cis* isomer maleate.
- The selectivity pattern is identical in both cases.
- The more rigid and lipophilic compound shows lower affinity for the substrates.

Effect of extraction conditions for chlorogenic acid determination in lamb's lettuce

Fábio Oliveira*, Manuela M. Moreira, Aquiles A. Barros and Luís F. Guido

Faculdade de Ciências, Universidade do Porto, Porto, Portugal

*c0809115@fc.up.pt



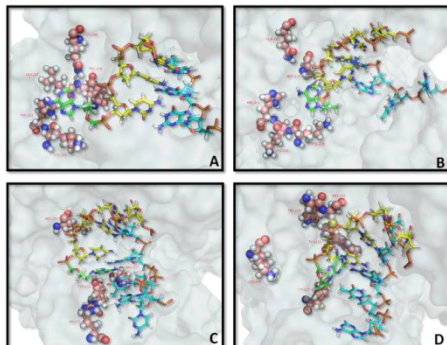
- Lamb's lettuce is an important source of antioxidant compounds, namely CGA.
- An ultrasound extraction of CGA was applied to fresh and freeze-dried samples.
- The influence of extraction pH on the recovery of CGA was evaluated.
- Both samples (fresh and freeze-dried) extracted at low pH (2 and 3.5) achieved the highest CGA content.
- Some differences were detected between fresh and freeze-dried extracts, namely in the compounds extracts.

Understanding the mechanism of resistance of HIV-1 RT to Tenofovir

Rui M. Ramos*, Irina S. Moreira, Pedro A. Fernandes and Maria J. Ramos

Faculty of Sciences, University of Porto, Portugal

*ramos.ruimiguel@gmail.com



- TDF adopts two different conformations at the P-site, in which the adenine base of TDF is flipped by 180° from the first conformation (1T03A / 1T03B).
- Molecular dynamics simulations of both complexes were performed.
- Various conformations of TDF were detected and analyzed.
- TDF has the propensity to acquire a more stable 1T03B conformation due to strong TDF/DNA contacts.
- Flexibility shown by TDF at the P-site prevents the retrotranslocation to the N-site, reducing excision rate.

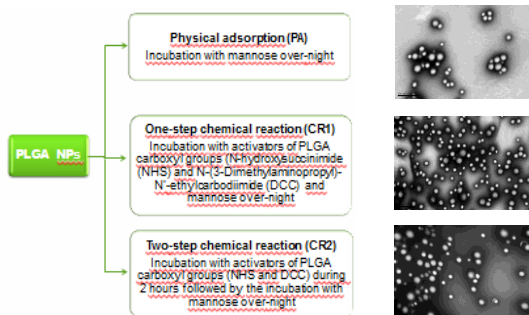
Figure 1: Representation of the protein-DNA interactions made by the tenofovir complex at the active site. A – 1T03A (A); B – 1T03A (C); C – 1T03B (D); D – 1T03B (E); Tenofovir (green/magenta), primer strand (yellow), template strand (cyan), amino acid residues (sphere representation).

Mannosylated nanoparticles for targeted delivery of amphotericin B towards visceral leishmaniasis

Daniela Barros, A. Cordeiro-da-Silva and S. Costa-Lima *

IBMC-INEB Infection and Immunity- Parasite Disease Group, Porto, Portugal

* slima@ibmc.up.pt



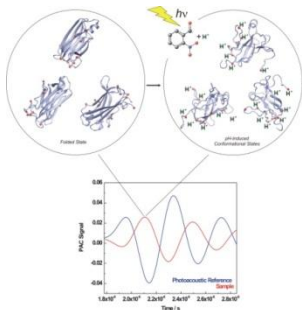
- The NPs, in particular the ones that are prepared by one-step chemical reaction, present low polydispersity ($<0,1$).
- TEM photographs revealed that M-PLGA NPs prepared by physical adsorption and one-step chemical reaction were spherical in shape, whereas the ones that were prepared by two-step chemical reaction present an “oval” shape.
- Mannose in M-PLGA NPs prepared by two-step chemical reaction is capable of interacting, in a greater extent, with the lectin receptors than the ones that are prepared by physical adsorption and one-step chemical reaction.
- The nanoformulations don't present cytotoxicity against THP1 differentiated macrophages and do not have any inhibitory activity on intracellular *L. infantum* amastigotes up to 2 mg/ml in polymer.

The Role of Ionizable Amino Acid Residues on Peptide and Protein Folding: a Time-Resolved Photoacoustic Calorimetry Experiment

Catarina S. H. Jesus*, Rui M. D. Nunes, Rui M. M. Brito, Luis G. Arnaut and Carlos Serpa

University of Coimbra, Portugal

**catarina.jesus@student.qui.uc.pt*



- The structural volume changes and the rate constants can be determined as a function of sample concentration using a two-temperature methodology to analyse the photoacoustic waveforms.
- In the multi-temperature method, the sample concentration is fixed and it is possible to determine the enthalpic changes, activation energies, volume changes and rate constants associated with each process within the detection range of time-resolved photoacoustics.
- Upon excitation at 355nm, occurs a release of protons by *o*NBA that induces a fast pH jump. Both in the presence and in the absence of other solutes, this fast release of protons is accompanied by a fast contraction (lifetime <10ns).
- For the protonation of aspartic acid and glutamic acid free in solution, is detected a volume expansion that is related with the charge neutralization of the carboxylic group. However, the protonation of the imidazole ring of histidine, that induces a positive charge formation, is accompanied by a small volume contraction.
- Preliminary studies on the conformational dynamics of the α -helical peptide show that the unfolding promoted by the protonation of the aspartic acid involved in a salt-bridge on the native structure is associated with a volume contraction.

Chemistry at the university: an approach to science dissemination for youngsters

Daniel Ribeiro* and Maria D. M. C. Ribeiro da Silva

Faculty of Sciences, University of Porto, Portugal.

**danieltiago.ribeiro@gmail.com*



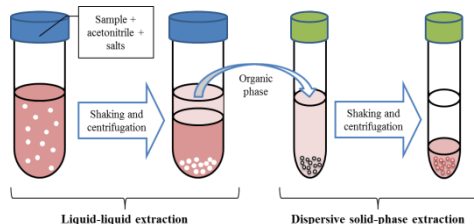
- The young students have better prospects with the implementation of this kind of projects.
- These activities enhance the interest for chemistry.
- With these projects, students can assess the academic environment.
- Students can solidify knowledge in various scientific areas, sharing the participation on their activities.

Application of the QuEChERS methodology for the determination of volatile phenols in beverages

Inês M. Valente*, Christiane M. Santos, Manuela M. Moreira, José A. Rodrigues and Aquiles A. Barros

Faculdade de Ciências, Universidade do Porto, Portugal.

**inesmariavalete@sapo.pt*



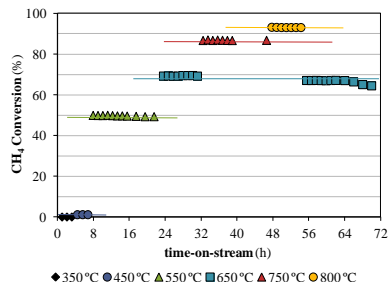
- QuEChERS is mainly used for analysis of pesticides in solid samples.
- In this work QuEChERS was applied to the analysis of volatile phenols in beverages.
- Beer, wine and fruit juice samples were analysed.
- 4-ethylphenol and 4ethylguaicol were the phenols present at higher concentrations.

Syngas Production over M-Ni nanoparticles (M = Pr, Gd, Th and U)

Ana C. Ferreira*, J.P. Leal and Joaquim B. Branco

Instituto Superior Técnico, Universidade Técnica de Lisboa / FCUL, Portugal

**acferreira@itn.pt*



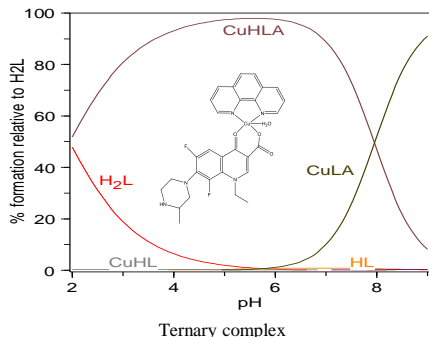
- The bimetallic oxides compounds were synthesized by modified sol-gel methods to obtain nanoparticles (<50nm).
- The bimetallic oxides were studied for partial oxidation of methane from 350°C at 800°C.
- The results of bimetallic oxides with lanthanides and actinides are comparable with commercial catalysts as 5%Rh/Al₂O₃ and 5%Pt/Al₂O₃.
- All catalysts are stable at the same experimental conditions.
- The selectivities to H₂ and CO were higher, with H₂/CO ratio of 2.

Characterization and antibacterial studies of a copper(II) lomefloxacin ternary complex

Patrícia Fernandes*, Mariana Ferreira and Paula Gameiro

Faculdade de Ciências, Universidade do Porto, Portugal

*up05030308@alunos.fc.up.pt



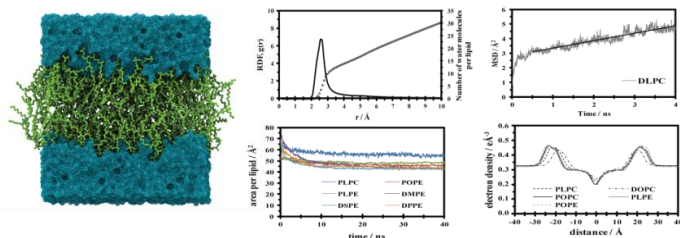
- Solution behavior of Cu(II):lmx complexes with and without 1, 10-phenanthroline was studied.
- Under physiological conditions (μM range, pH 7.4) only Cu(II):lmx:phen complexes are stable.
- MIC determinations very important to conclude about the possible use of the ternary complex as a metalloantibiotics.
- MICs for porin-deficient *E. coli* strains will allow confirmation of the entry pathway of these compounds.
- Interaction of lomefloxacin and Cu(II):lmx:phen complex with liposomes will allow us to try to understand the uptake mechanism of these compounds at a molecular level.

Conception of glycerophospholipid hydrated bilayer models through computational modeling

João T. S. Coimbra*, Sérgio F. Sousa, Pedro A. Fernandes, Maria Rangel, and Maria J. Ramos

Faculdade de Ciências, Universidade do Porto, Portugal

*jts.coimbra@gmail.com



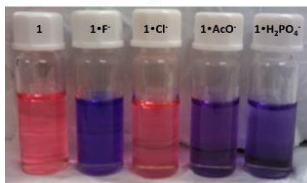
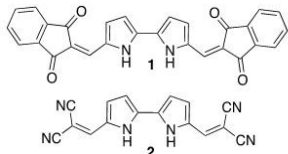
- Conception of 12 membrane models through Molecular Dynamics (MD) simulations, consistent with the General-AMBER Force Field (GAFF).
- Structural and dynamic validation of the glycerophospholipid bilayer models.
- Validation of the Molecular Dynamics simulation protocol.
- Parameters reproduce stable bilayer models.
- Volume per lipid quantity, coefficients for lateral diffusion of glycerophospholipids, and DOPC system in good agreement with experimental data.

Synthesis of novel bipyrrolic compounds with potential application in anion binding

Flávio Figueira*, Andreia F. S. Farinha, Augusto C. Tomé, José A. S. Cavaleiro and João P.C. Tomé

University of Aveiro, Portugal

*ffigueira@ua.pt



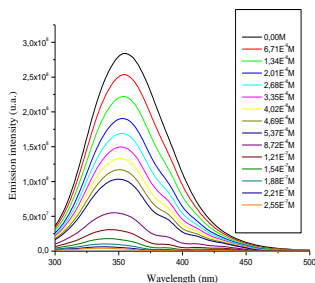
- Pyrrole derivatives **1** and **2**, based on a bipyrrolic skeleton, have been synthesized and fully characterized.
- Receptors **1** and **2** are easy to make selective receptors for different anions.
- Association constants of **1** (M^{-1}) with various anionic guest species at 25 °C has been achieved in DMSO with the addition of Anions as their tetrabutylammonium salts.
- Derivative **1** has shown to be an effective anion receptor in DMSO solutions and has the ability to selectively recognize and sense anionic analytes using the naked eye.

On the Complexation between Bovine Serum Albumin and Manganese Porphyrin

Otávio Augusto Chaves*, Gonçalo F. F. Sá, Catarina S. H. Jesus, Carlos Serpa and Luis G. Arnaut

Capes Foundation, Ministry of Education of Brazil, Brazil / University of Coimbra, Portugal

*otavio_ufrjr@hotmail.com



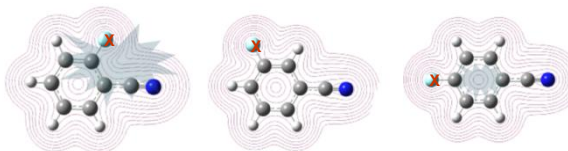
- Photophysics of the interaction between the porphyrin MnTPPS, with solution of BSA buffered with PBS (pH=7.4).
- The interaction was based on the fluorescence spectroscopy and photoacoustic calorimetry at temperatures of 276K, 279K, 281K, 283K, 288K and 293K.
- High K_a value indicates that the bond BSA-MnTPPS is strong.
- The negative value of ΔG° , shows the spontaneity binding and the positive value of ΔS° shows that the type of interaction between the porphyrin and BSA is hydrophobic.
- Time resolved photoacoustic calorimetry may provide new insights on the heat release mechanism and possible alterations in the BSA stability and/or in the protein-porphyrin interaction.

Halogen...Cyano group interaction: an energetic and structural analysis of monohalogenated benzonitrile isomers

Inês M. Rocha* and Manuel A.V. Ribeiro da Silva

Faculdade de Ciências, Universidade do Porto, Portugal

**inesmrocha@gmail.com*



X = F, Cl, Br and I

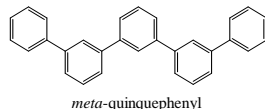
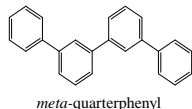
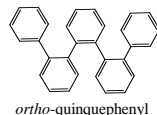
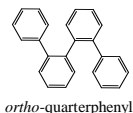
- The present work is dedicated to the study of the interaction of the halogen atoms with the cyano group of the benzonitrile;
- An energetic study was performed using experimental techniques: the rotating-bomb combustion calorimetry and the Knudsen effusion mass-loss technique or Calvet microcalorimetry;
- The experimental study was complemented with a computational study based on several methodologies such as NICS, NBO and Mulliken population analysis.

Structural and Thermodynamic Study of Nonlinear Polyphenyls

Ana S. M. C. Rodrigues*, Marisa A. A. Rocha, Lúgia R. Gomes, John L. Low, Luís M. N. B. F. Santos

Faculdade de Ciências, Universidade do Porto, Portugal

**anasofiaconde@gmail.com*



- Synthesis of polyphenyls compounds by Suzuki-Miyaura method.
- Single crystal X-ray characterization.
- Thermophysical properties at $T=298.15\text{K}$: T_{fusion} , $\Delta_{\text{cr}}^{\text{l}}H_{\text{m}}^{\circ}(T_{\text{fus}})$, $\Delta_{\text{cr}}^{\text{l}}S_{\text{m}}^{\circ}(T_{\text{fus}})$, $C_{p,m}^{\circ}(T_{\text{fus}})$, $\Delta_{\text{cr}}^{\text{g}}H_{\text{m}}^{\circ}$.
- Thermochemical properties at $T=298.15\text{K}$: $\Delta_{\text{f}}H_{\text{m}}^{\circ}(\text{cr})$, $\Delta_{\text{f}}H_{\text{m}}^{\circ}(\text{g})$
- Odd/even effect in fusion equilibrium and gaseous phase energetics of the *ortho* series.

Poster Communications



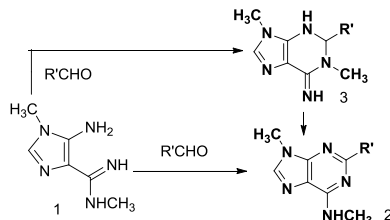
Synthesis of 9-methyl-6-methylamino-2-arylpurines as potential new ligands to adenosine receptors

A. Brito*, C. Correia, M. A. Carvalho and M. F. Proença

University of Minho, Portugal

*alexandra.m.brito@hotmail.com

P1



- Adenosine receptors are important therapeutic targets.
- Purine structure 2 was identified as new ligand to adenosine receptors.
- The reaction of 5-amino-4-cyanoformimidoyl-9-methylimidazole 1 with aldehydes leads to mixtures of dihydropurine 3, as kinetic product, and purine 2.
- The target compounds 2 were obtained under thermodynamic conditions.

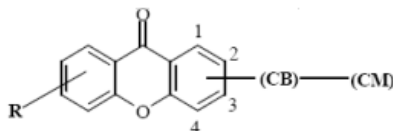
Chiral HPLC method for determination of the enantiomeric purity of new xanthone derivatives

Carla Fernandes, Alexandre Santos, Maria Elizabeth Tiritan, Carlos Afonso and Madalena Pinto*

Faculdade de Farmácia, Universidade do Porto, Portugal.

*madalena@ff.up.pt

P2



CXD

R: Functional Group

CB: Chemical Bridge

CM: Chiral Moiety

- HPLC enantioseparation of ten chiral xanthone derivatives (CXDs) was performed.
- Multimodal elution conditions were evaluated on four polysaccharide-based columns.
- All the CXDs were enantioseparated with high enantioselectivity and resolution.
- The best resolution was achieved on the amylose tris-3,5-dimethylphenylcarbamate coated onto APS-Nucleosil column under polar organic elution conditions.
- Enantiomeric purity of chiral xanthone enantiomers was generally higher than 99 %.



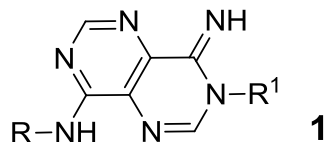
P3

Synthesis of new Pyrimido[5,4-*d*]pyrimidines derivatives as potential antitubercular agents

A. Gonçalves*, A. Rocha, A. Brito, M. A. Carvalho and M. F. Proença

University of Minho, Portugal

*ana.alex.goncalves@gmail.com



- Tuberculosis affects much of the world population.
- Appearance of resistant strains to actual antibiotics leads to an urgent demand for new and more effective anti-TB drugs
- Pyrimido[5,4-*d*]pyrimidine structure identified as a new class of antitubercular compounds.
- Synthesis and characterization of new derivatives of pyrimido[5,4-*d*]pyrimidines **1** with lipophilic groups as substituents R and R¹.



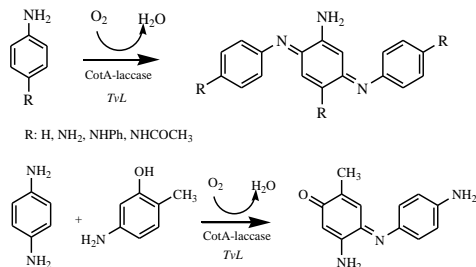
P4

Biotransformation of primary aromatic amines by laccases

Ana Catarina Sousa, Lúcia O. Martins and M. Paula Robalo*

Instituto Superior de Engenharia de Lisboa, Portugal / Instituto Superior Técnico, Portugal,

*mprobalo@deq.isel.ipl.pt



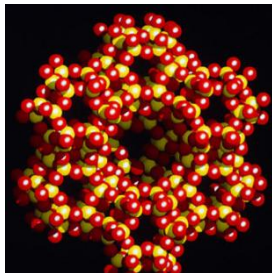
- Biotransformation of *p*-substituted primary aromatic amines using two different laccases as catalysts.
- The oxidation of the studied substrates is dependent on the electronic nature of the *p*-substituent of the aromatic ring.
- Kinetic parameters were determinate for CotA-laccase oxidation of several substrates and experimental conditions were optimized for each enzyme/substrate system.
- Both laccases catalysed the substrates biotransformation leading to diaminated quinoneimine dimers and trimers identified by 1D and 2D NMR techniques.
- CotA-laccase showed the higher conversion yields in pH range 6-8.

Phenol glycosylation catalysed by zeolite HY

Ana Assunção*, Ana Jesus, Ana P. Carvalho and Amélia P. Rauter

Faculdade de Ciências da Universidade de Lisboa, Portugal

*anacatarina.10@gmail.com



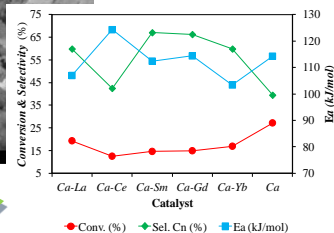
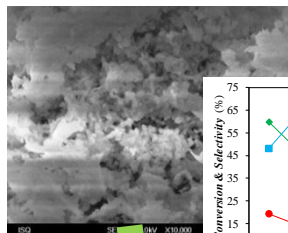
- Glycosylation of phenolic using zeolites HY.
- This reaction presents higher selectivity, is eco-friendly and with some aglycone has good yields.
- The crystallinity of the zeolite remains unchanged throughout the reaction.

Oxidative coupling of methane using nitrous oxide as oxidant over calcium-rare earth oxides nanoparticles

Ana C. Ferreira*, J.P.Leal and Joaquim B. Branco

Instituto Tecnológico e Nuclear, Instituto Superior Técnico, Universidade Técnica de Lisboa / FCUL, Portugal

*acferreira@itn.pt



- Synthesis of calcium-rare earth nanoparticles using sol-gel techniques.
- The calcium-rare-earth oxides were studied for oxidative coupling of methane from 650- 800°C with nitrous oxide as oxidant.
- Higher production of C2 hydrocarbons (ethane and ethylene).
- Relation of acid/basicity of catalysts with selectivity to C2 hydrocarbons.



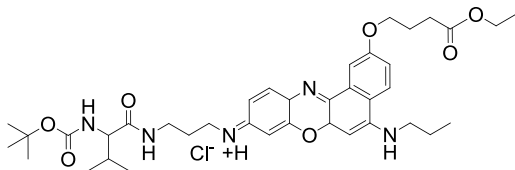
P7

Fluorescent labelling of valine with a new benzo[*a*]phenoxazininium chloride functionalized at the 2- and 5-positions

A. Daniela G. Firmino*, M. Sameiro and T. Gonçalves

University of Minho, Portugal

*daniela_firmino1@msn.com



- A new benzo[*a*]phenoxazininium dye possessing the ester and amine groups as terminals in 2- and 5-positions of the polycyclic system was synthesised.
- This cationic dye displayed absorption maxima (λ_{abs}) in ethanol, in physiologically simulated conditions and distilled water in the 610-620 nm range.
- It is highly fluorescent and showed a maximum emission wavelength (λ_{em}) between 642 and 646 nm.
- The covalent labelling of valine was carried and the resulting bioconjugate displayed superior λ_{abs} and λ_{em} regarding the label and was also highly fluorescent.



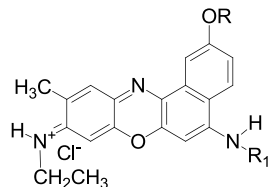
P8

Solvent-free microwave synthesis of 2-, 5- and 9-substituted benzo[*a*]phenoxazininium chlorides

A. Daniela G. Firmino*, M. Sameiro and T. Gonçalves

University of Minho, Portugal

*daniela_firmino1@msn.com



R, R¹ = H, (CH₂)₂CH₃, (CH₂)₃CO₃CH₂CH₃,
(CH₂)₃CO₃H, (CH₂)₃NH₂

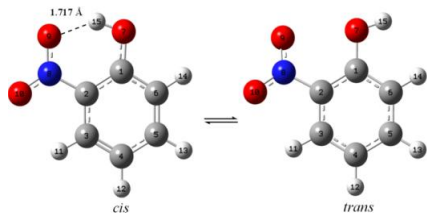
- The synthesis of benzo[*a*]phenoxazininium chlorides by the condensation of the suitable nitrosophenol with 5-aminonaphthalen-2-ol and its *N*- or/and *O*-alkylated derivatives was carried out using microwave irradiation (MW).
- The solvent-free conditions, silica gel as a solid support, revealed more efficiency than in the presence of DMF as solvent.
- Time reduction was from 9 to 140 times when compared to conventional heating, with good to excellent yields.

Thermochemical Study of the Some Fluoronitrophenol Isomers

Ana I.M.C. Lobo Ferreira* and Manuel A.V. Ribeiro da Silva

Faculty of Science of University of Porto, Portugal.

*ana.ferreira@fc.up.pt



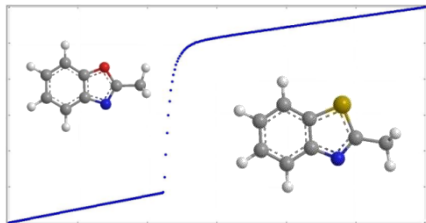
- Standard molar enthalpies of formation in the condensed and gas phase of 3-fluoro-6-nitrophenol and 4-fluoro-2-nitrophenol were determined. Vapor pressures at different temperatures, were measured using the Knudsen mass loss effusion technique.
- The experimental results for the energetics in the gaseous phase were compared with the ones obtained by computational calculations at the G3MP2//B3LYP level.
- Most stable conformation of the four fluorine substituted 2-nitrophenols. *cis* / *trans* isomerization were evaluated.
- The influence of the fluorine atom in the strength of the internal hydrogen bond of the four fluoro-*ortho*-nitrophenol isomers, were assessed.
- Determination O–H bond dissociation enthalpies.

Thermochemistry study of 2-methylbenzoxazole and 2-methylbenzothiazole

Ana L. R. Silva*, A. Cimas and Maria D. M. C. Ribeiro da Silva

Faculty of Science, University of Porto, Portugal

*ana.luisa@alunos.fc.up.pt



- Combustion calorimetry and high temperature Calvet microcalorimetry were used on the measurements of thermochemical properties.
- The standard molar enthalpies of formation, in gaseous state, of benzoxazole and benzothiazole methyl derivatives are presented.
- Contribution to the establishment of correlations between energetic and structural characteristics of heterocyclic molecules.
- The enthalpic effect of the methylation on the oxygenated ring is more significant than in the sulfured ring.



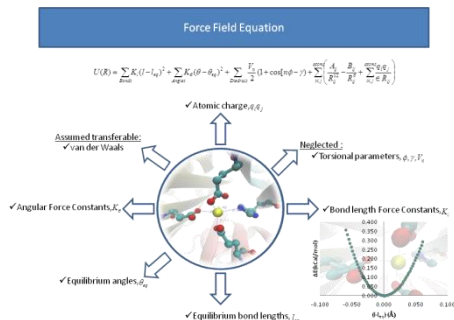
P11

Force Field Parameterization of Cobalt-containing Metalloproteins

Ana C. V. Cunha*, Sérgio F. Sousa, Pedro A. Fernandes and Maria J. Ramos

Faculdade de Ciências, Universidade do Porto, Portugal

*carvalhovicentecunha@gmail.com



- Optimization of the selected models using DFT (B3LYP) and Force constants calculated with B3LYP/SDD:6-31G(d), with RESP charges derived at the B3LYP/6-311G++(3df,3pd) level.
- Results of the Potential Energy Surface along linear transit scans (PES-SCAN) have the form of a second degree polynomial equation.
- The angular and force constants vary according to the amino acid type and metallic center geometry
- A database containing these molecular mechanical parameters for use with popular molecular dynamics codes is currently in preparation



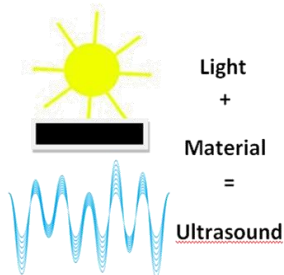
P12

Pressure Waves Generated by Light-Absorbing Thin Films

A. P. Marques, G. F. F. Sá, C. Serpa and L. G. Arnaut

University of Coimbra, Portugal

*amarques@qui.uc.pt



- Ultrasound generated by laser pulse irradiation of suitable materials can permeabilize biological barriers and enhance drug delivery to or through the skin.
- Materials capable of absorbing a laser pulse and generate a high-intensity ultrasound pressure wave were developed.
- Amaranth, new coccine and MnTPP are good dyes to make homogeneous thin films unlike allura red and brilliant blue.
- MnTPP films generate pressure waves whose intensity and frequency depends on the thickness and absorbance of the films.

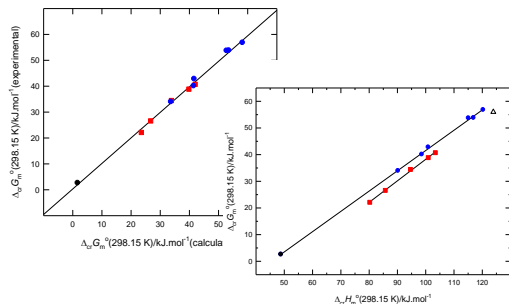
Thermodynamic study of phase transitions in methyl esters of *ortho*-, *meta*- and *para*- aminobenzoic acids

Ana R. R. P. Almeida* and M.J.S. Monte

Faculty of Science of University of Porto, Portugal.

*ana.figueira@fc.up.pt

P13



- Accurate values of enthalpies of sublimation, vaporization and fusion were derived.
- The enthalpy of intermolecular $\text{NH}\cdots\text{O}$ hydrogen bond in methyl *p*-aminobenzoate was determined.
- The volatility of the methyl benzoates was compared with the volatility of the parent acids.
- A correlation involving the temperature of fusion and the enthalpy and Gibbs energy of sublimation of benzene, methyl benzoates and benzoic acids was derived

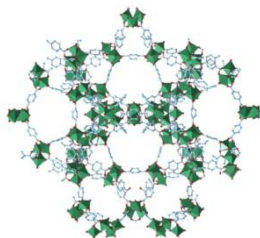
Monovacant polyoxometalates @ MIL-101: synthesis and heterogeneous catalytic studies

André D. S. Barbosa*, Filipe A. Almeida Paz, Baltazar de Castro, Salette S. Balula and Luís Cunha-Silva

Faculty of Science of University of Porto, Portugal

* andredbarbosa@gmail.com

P14



- Metal-organic framework (MOF) materials are formed by metal centers interconnected by organic molecules, leading to infinite one-, two- or three dimensional networks.
- Porous MIL-101, chromium(III) terephthalate, was prepared by hydrothermal synthesis using terephthalic acid and chromium(III) nitrate nonahydrate.
- MIL-101 as used as solid support for the preparation of heterogeneous catalysts.
- $\text{K}_7[\text{PW}_{11}\text{O}_{39}]\cdot n(\text{H}_2\text{O})$ (PW_{11}) and $\text{K}_8[\text{SiW}_{11}\text{O}_{39}]\cdot m(\text{H}_2\text{O})$ (SiW_{11}) were immobilized in the porous MIL-101 leading to two novel composite materials, $\text{PW}_{11}@\text{MIL-101}$ and $\text{SiW}_{11}@\text{MIL-101}$
- All materials were characterized by FTIR spectroscopy, powder XRD and SEM/EDS.
- Catalytic performance was ascertained for the two composite materials in the oxidation reaction of geraniol, using hydrogen peroxide as oxidant.



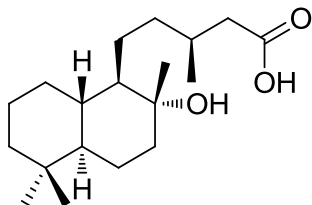
P15

Isolation and quantification of labdanolic acid from *Cistus ladaniferus*

André N. C. Martins*, L. M. T. Frija, S. Simeonov and C. A. M. Afonso

Faculdade de Farmacia da Universidade de Lisboa / Instituto Superior Técnico, Portugal

*andremartins@ff.ul.pt



- Extraction of a natural product;
- Creation of an analytical method for the quantification of Labdanolic acid;
- Quantification of labdanolic acid in *Cistus ladaniferus* during a year.



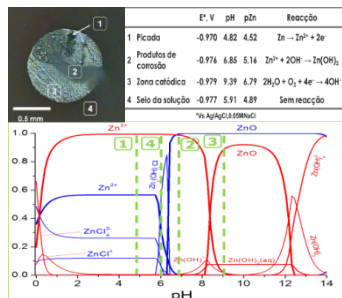
P16

Application of geochemistry software to corrosion studies

A. B. Oliveira*, A. C. Bastos, O. V. Karavai, A. A. Ferreira, M. L. Zheludkevich and M. G. S. Ferreira

Universidade de Aveiro, Aveiro, Portugal

*arboliveira@ua.pt



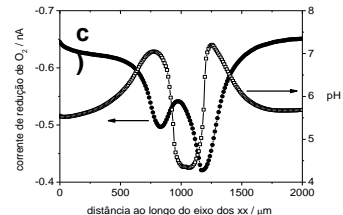
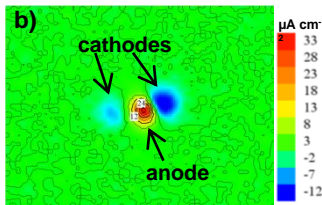
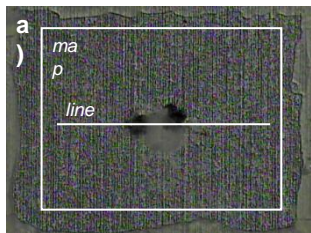
- Experimental characterization of the corrosion a pure zinc disc electrode through potentiometric microelectrodes (figure on the left).
- Computation of speciation diagrams of zinc in aqueous solution.
- Coperison of experimental and computed data.
- Kinetic study on the influence of pH for the oxidation of Fe^{2+} to Fe^3 .

Micro-electrochemical techniques to study localised corrosion

A. B. Oliveira*, A. C. Bastos, O. V. Karavai, M. L. Zheludkevich and M. G. S. Ferreira

Universidade de Aveiro, Portugal

*arboliveira@ua.pt



- Application of micro-electrochemical techniques for the study of localized corrosion.
- Combination of different information from various techniques for the illustration of the overall process (metal ion concentration, dissolved oxygen, pH).

Approach to the synthesis of nucleoside inhibitors of butyrylcholinesterase

Andreia Almeida*, Vasco Cachatra and Amélia P. Rauter

Faculdade de Ciências da Universidade de Lisboa, Portugal

*afilpalmeida14@gmail.com



- The nucleoside has a bicyclic sugar moiety
- The reactions involved in the sugar moiety synthesis include regioselective protection, oxidation, Wittig reaction, cyclization and reduction.
- The nucleoside is a selective inhibitor of butyrylcholinesterase, an enzyme that plays an important role in Alzheimer's disease.



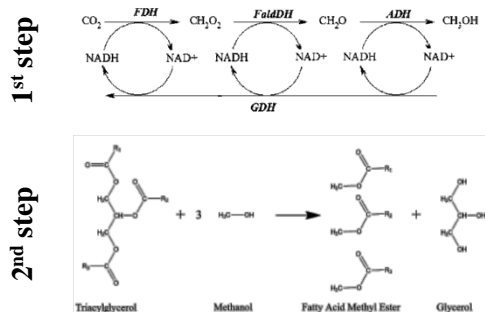
P19

A green integrated biocatalytic system for the conversion of CO₂ and vegetable oils into biodiesel

Andreia Pimenta, Pedro Vidinha* and Susana Barreiros

Faculdade de Ciências e Tecnologia, Universidade Nova de Lisboa, Portugal

*pm.gomes@fct.unl.pt



- Implementation of a experimental apparatus;
- Production of methanol from CO₂ by enzymatic reduction;
- Integration of common cooking oil in the system for transesterification with methanol (catalyzed by immobilized *Candida Antarctica* lipase B - Novozym 435);
- Analysis of the product by *Gas Chromatography*;
- Determination of the amount of Biodiesel produced.



P20

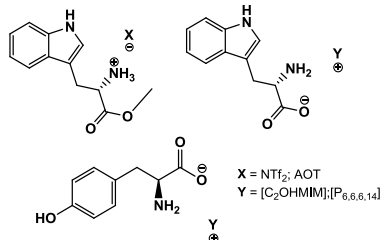
Development of Ionic Liquids based on biological compounds

Andreia Forte*, Luís C. Branco and César Laia

Faculdade de Ciências e Tecnologia da Universidade Nova de Lisboa, Portugal

*p110533@campus.fct.unl.pt

Tryptophan and Tyrosine ILs



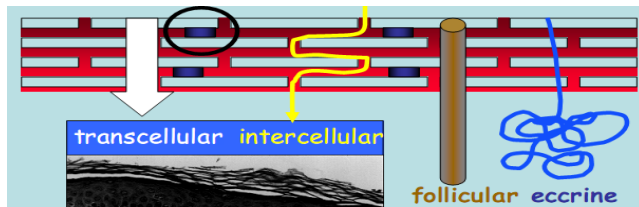
- Development of Ionic Liquids (ILs) based on L-tryptophan and L-tyrosine derivatives as biological units.
- L-tryptophan methyl ester as organic cation and L-tryptophan and L-tyrosine as organic anions were combined with appropriate counter-ions selected according their toxicity as well as hydrophobicity behavior.
- All novel ILs were characterized by NMR, FTIR and elemental analysis in order to check their expected structure and purity.
- Some physical (density, viscosity and solubility) and thermal (melting point, glass transition temperature T_g and decomposition temperature) properties will be evaluated.
- Partition coefficient studies using water-octanol systems have been performed through UV / Vis and fluorescence spectroscopy measurements.

Topical drug delivery of Lidocaine and Diclofenac Gels – Viscoelastic Properties and *in vitro* skin distribution studies

Ângela Correia^{*}, Gonçalo F.F. Sá, Carlos Serpa and Luís G. Arnaut

University of Coimbra, Portugal

*angela_c_3@hotmail.com



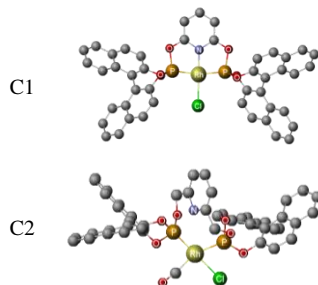
- Determination of the mechanical and viscoelastic properties using TPA and rheology.
- In vitro skin distribution studies using Franz Cells and quantification by HPLC.
- Selection of the best vehicles to topical drug delivery of lidocaine and diclofenac.

Computational studies of Binol based phosphites and respective metal complexes at PM6 and DFT levels. Application in asymmetric hydrogenation of olefins.

Ângela C. B. Neves^{*}, Rui M. B. Carrilho, Andreia F. Peixoto, Ana R. Almeida, Paulo E. Abreu, M. Calvete and Mariette M. Pereira

Universidade de Coimbra, Portugal

*angela.neves@live.com.pt



- The lowest energy structures of BINOL based C_3 -symmetric monophosphite, pyridine-*bis*-BINOL-phosphite ditopic ligands like and some of their rhodium complexes were optimized through semiempirical PM6 and DFT methods.
- Slight differences in the ligand structure resulted in rhodium complexes with different geometries, **C1** and **C2**.
- Great influence of the ligand structure in the catalytic activity of dimethyl itaconate hydrogenation was observed.
- Enantiomeric excess up to 62% was achieved.
- Complex **C2** (PP-rhodium coordination) is the more active complex, while the more stable **C1** (PNP-rhodium coordination) is the less active.



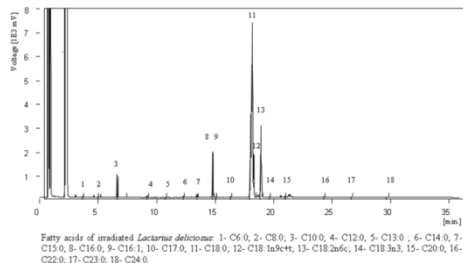
P23

Gamma irradiation protects oleic acid from oxidation: an experiment in *Lactarius deliciosus* wild mushroom

Ângela Fernandes, M. Beatriz P. P. Oliveira, Amílcar L. Antonio, Anabela Martins and Isabel C. F. R. Ferreira*

Instituto Politécnico de Bragança / Faculdade de Farmácia da Universidade do Porto, Portugal.

*iferreira@ipb.pt



- Control and irradiated *L. deliciosus* samples revealed identical fatty acid profiles.
- Control sample showed a lower C18:1n9c content after 8 days of storage.
- Sample irradiated with 0.5 kGy maintained C18:1n9c content until day 8.
- Irradiation protected fatty acids from oxidation.
- Irradiation could be an alternative to extend the life of mushrooms.



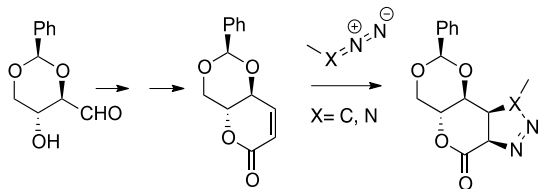
P24

1,3-Dipolar Cycloaddition of (2*R*,4*aR*,8*aS*)-2-phenyl-4,4a-dihydropyrano[3,2-*d*][1,3]dioxin-6(8*aH*)-one with Aromatic Diazomethyl Compounds

António Ribeiro, Cristina E. A. Sousa, M. José Alves and A. Gil Fortes

Universidade do Minho, Portugal

*antonio.manuel.p.ribeiro@gmail.com



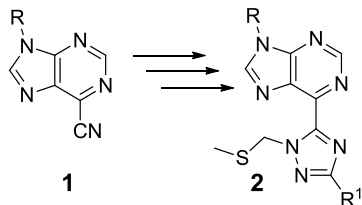
- Derivative of D-erythrose was used as dipolarophile in 1,3-dipolar cycloaddition.
- Reactions with alkyl azides and diazomethyl compounds were totally *regio*- and *stereo*-selective.

An efficient synthetic approach to 6-triazolopurines

A. Rocha, M.A. Carvalho*, and M. F. Proença

Universidade do Minho, Portugal

*mac@quimica.uminho.pt



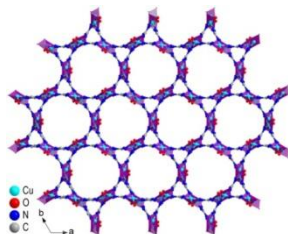
- In the last decade, tuberculosis (TB) has resurfaced as a significant threat to public health.
- New-anti TB drugs are crucial to control resistant strains (MDR-TB and XDR-TB).
- 9-aryl-purines were identified as a new class of anti-TB agents.
- Synthesis and characterization of new 9-aryl-6-triazolopurines.

A left-handed helical 3D metal-organic chiral framework derived from the decomposition of 3-amino-1H-1,2,4-triazole-5-carboxylic acid

Bing Liu*, J. A. Fernandes, J. P. C. Tomé, F. A. Almeida Paz and L. Cunha-Silva,

University of Aveiro / Faculty of Science of University of Porto, Portugal

*bing.liu@fc.up.pt



- A novel 3D metal-organic chiral framework, $[\text{Cu}(\text{atr})(\text{OH})] \cdot 3\text{H}_2\text{O}$ (Hatr = 3-Amino-1H-1,2,4-triazole), was isolated in hydrothermal condition, whose formation involves in the decarboxylation of 3-Amino-1H-1,2,4-triazole-5-carboxylic acid.
- The skeleton of the chiral MOF contains left-handed helices which are originated by the growth of a foundational repeating neutral unit $[\text{Cu}(\text{atr})(\text{OH})]$.
- Regarding Cu center and atr⁻ moiety both as 3-connected nodes, the topology of the overall structure is a uninodal 5-connected $(3^3.4.6^3.7^3)$ network.



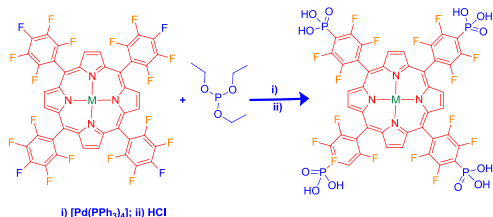
P27

Synthesis of new porphyrin-phosphonate derivatives for MOFs construction

Carla F. Pereira*, João M. M. Rodrigues, Sérgio M. F. Vilela, Filipe A. Almeida Paz and João P. C. Tomé

University of Aveiro, Portugal

*carlafpereira@ua.pt



- Synthesis of porphyrin macrocycles with multi-phosphonate groups.
- Porphyrin complexation with catalytic active metals.
- Porphyrin-phosphonate ligands for MOFs construction and evaluation of the catalytic activity.



P28

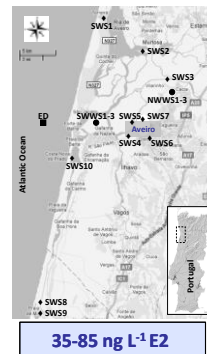
Application of an optimized ELISA assay in the assessment of 17 β -estradiol levels in surface and waste waters from the Aveiro region (Portugal)

Carla P. Silva*, Rudolf J. Schneider, Marta Otero and Valdemar I. Esteves

University of Aveiro, Portugal

*patricia.silva@ua.pt

- Estrogen 17 β -estradiol (E2) is an endocrine disrupting compound.
- Main sources of E2 in the environment are sewage discharge and disposal of animal wastes.
- Enzyme linked immunosorbent assay (ELISA) is a rapid, simple and cost-effective analytic method, with detection limits in the ng L⁻¹ range.
- An ELISA procedure was optimized to avoid matrix effects, achieving a quantification limit of 30 ng L⁻¹.
- Surface and waste waters from the Aveiro region (Portugal) were analysed without any sample pre-treatment and E2 concentrations between 35 and 85 ng L⁻¹ were determined.

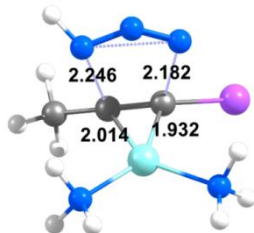


Computational studies of Cu-catalyzed addition of azides to iodoalkynes

Carlos E. P. Bernardo and Pedro J. Silva*

Universidade Fernando Pessoa, Portugal

*pedros@ufp.edu.pt



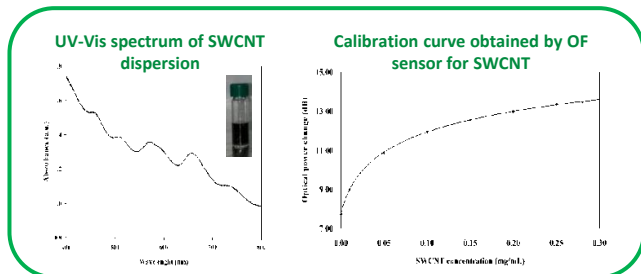
- A large variety of mechanisms for the Cu(I)-catalyzed addition of azides to iodoalkynes was studied with density-functional methods.
- The mechanisms proposed in the literature are *slower* than the uncatalyzed reaction.
- Reaction instead proceeds directly through azide attack on the Cu(I)-activated iodoalkyne.
- The computations correctly describe the experimentally observed regiochemistry and also explain the effects of alkyne and azide substituents on the reaction rates.

Screening of single-walled carbon nanotubes by optical fiber sensing

Celine I. L. Justino*, Ana C. Freitas, Teresa A. P. Rocha-Santos and Armando C. Duarte

University of Aveiro, Portugal

*celinejustino@ua.pt



- This work consists in the development of an optical fiber (OF) methodology to screen single walled carbon nanotubes (SWCNT) in solutions.
- The developed methodology has a compact design and requires low volume of sample.
- The results obtained with the OF system are comparable with a standard methodology based on UV-Vis spectroscopy.

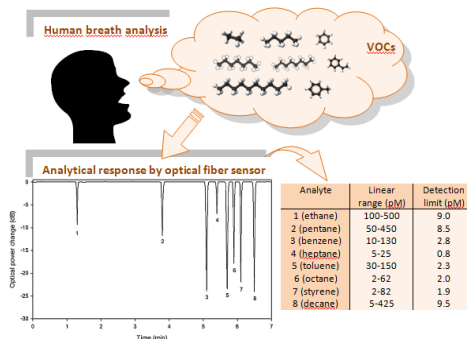
**P31**

Breath analysis by optical fiber sensor for the diagnosis of human health

Celine I. L. Justino*, Lurdes I. B. Silva, Kátia R. Duarte, Ana C. Freitas, Teresa A. P. Rocha-Santos, and Armando C. Duarte

University of Aveiro, Portugal

*celinejustino@ua.pt



- An optical fiber (OF) sensor was used for the determination of volatile organic compounds (VOCs) from human breath.
- Adequate analytical performance was obtained with the OF sensor in terms of stability, linearity, accuracy, and detection limits.
- The developed system provides near real-time responses, low instrumentation costs, and simple and fast breath sampling.
- Analytical signals for the eight tested analytes were comparable with responses of a reference method (GC-MS).

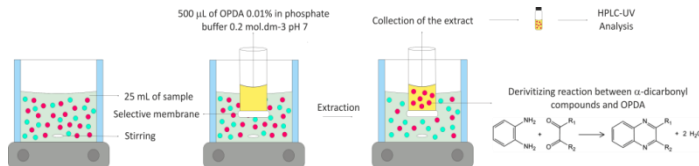
**P32**

Determination of α -dicarbonyl compounds in foodstuff by HPLC-UV using gas-diffusion microextraction

Christiane M. Santos*, Inês M. Valente, José A. Rodrigues and Aquiles A. Barros

Faculdade de Ciências da Universidade do Porto, Portugal.

*christiane.mello.santos@gmail.com



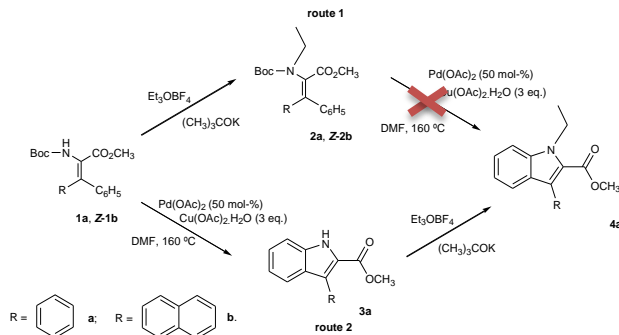
- The α -dicarbonyl compounds play an important role in the aroma of many fermented foods and beverages.
- Methylglyoxal is a toxic compound with effective anti-bacterial properties.
- Gas-diffusion microextraction was used to analyze α -dicarbonyl compounds.
- Methylglyoxal was found in samples in concentrations varying from 244.2 mg/L to 1.86 mg/L.

Synthesis of *N*-ethyl β,β -diaryldehydroalanine and *N*-ethylindole derivatives

Cláudia Barroso* and Luís S. Monteiro

University of Minho, Portugal.

*claudia_ventura@live.com.pt



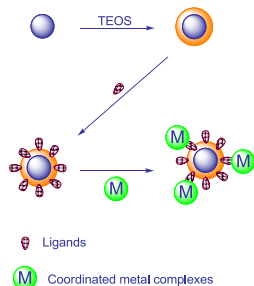
- *N*-Alkylation of dehydroamino acid derivatives using triethyloxonium tetrafluoroborate (Et_3OBF_4) as alkylating agent.
- Metal-assisted C-N intramolecular cyclization of β,β -diaryldehydroamino acid derivatives to give indole derivatives.
- Synthesis of *N*-ethylindole derivatives involving alkylation and metal-assisted C-N intramolecular cyclization via 2 strategies.
- The route in which alkylation occurs prior to C-N intramolecular cyclization was unsuccessful.
- The route consisting of C-N intramolecular cyclization followed by alkylation, was successful with an overall yield of 58%.

Magnetic core-shell nanoparticles as catalyst supports

Cristina I. Fernandes*, Pedro D. Vaz and Carla D. Nunes

Faculdade de Ciências da Universidade de Lisboa, Portugal

*csilvafernandes@gmail.com



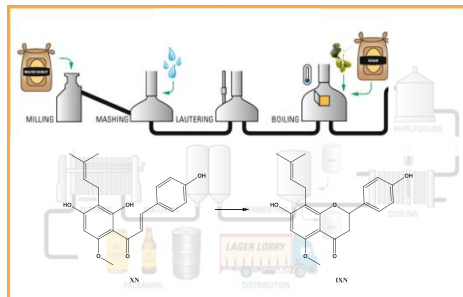
- Magnetic nanoparticles with Mo active catalyst were successfully prepared.
- The resulting catalysts were very efficient and selective in olefin epoxidation.
- It also is a good C=C bond oxidative cleavage catalyst.
- It is easily recovered from reaction medium.

Influence of different malt varieties on xanthohumul isomerization in pale and dark beers

Daniel O. Carvalho*, Aquiles A. Barros and Luís F. Guido

Faculdade de Ciências da Universidade do Porto, Portugal

**danielcarvalho.21@gmail.com*



- XN was largely converted into IXN in pale and caramel malt wort.
- Roasted malt inhibits XN isomerization, resulting in high levels of XN in the final wort.
- Melanoidin content is higher for roasted malts.
- The total polyphenol content is 5-fold higher for roasted malt, as well as the content of flavano-3-ols and proanthocyanidins.

The PROFILES project as a way to provide continuous professional development of the science teachers

Daniel Ribeiro*, Carla Morais and João Paiva

Faculty of Sciences of University of Porto, Portugal.

**danieltiago.ribeiro@gmail.com*

PROFILES

Professional Reflection Oriented Focus on Inquiry-based Learning and Education through Science

- There are indicators that suggest that students do not like science, as it is taught in European schools.
- It is essential that teachers develop a self-critical spirit on his school activity – in order to achieve the ultimate goal of teacher ownership.
- The PROFILES project aims to provide professional, methodological and self-reflexivity competences to science teachers.
- The project was implemented through an action of teacher training which was attended by about 30 chemistry teachers.
- It is possible to establish a link between society and science, influencing the ways of teaching and educating through science.

Chemical composition and antimicrobial activity of *Salvia sclareoides* Brot. extracts

Daniela Batista*, Alice Martins, Isabel Branco, Catarina Dias, Ana Neves, Jorge Justino and Amélia P. Rauter

Faculdade de Ciências da Universidade de Lisboa, Portugal

*daniadbatista@gmail.com



- Study of *Salvia sclareoides*, an aromatic herb native to Portugal with high potential for the prevention of neurodegenerative diseases.
- The phytochemical study of this plant revealed a high content of phenolics and terpenoid type compounds.
- The antimicrobial activity of six *S. sclareoides* extracts was tested with seven pathogenic bacteria and five pathogenic fungi, and evaluated by the paper disk diffusion method.
- The dichloromethane, acetone and methanol extracts caused significant inhibition on *Enterococcus faecalis* and *Listeria monocytogenes* and on the fungus *Botrytis cinerea*.

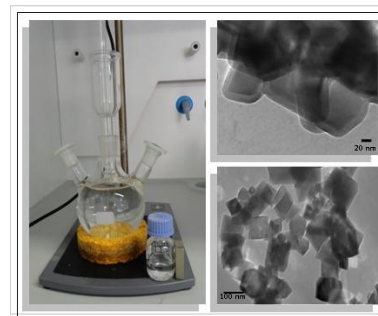
Functionalized Fe₃O₄/SiO₂ core/shell particles: new sorbents for the magnetic removal of aqueous Hg(II)

Daniela S. Tavares*, C. B. Lopes, A. L. Daniel-da-Silva, A. C. Duarte, E. Pereira and T. Trindade

University of Aveiro, Portugal

*danielatavares@ua.pt

- Sorbents based on dithiocarbamate functionalized particles exhibiting high affinity for Hg(II).
- Easy magnetic removal of Hg(II) loaded sorbents from water.
- High removal efficiency (>99%) with low amount of particles (6 mg/L) from seawater and river water.



Application of ESI-MS/MS to the structural characterization of *Genista tenera* flavonoids and flavonoid glycosides

Diana Mendes*, Alice Martins, Paulo J. Amorim Madeira, Humberto E. Ferreira, José Condeço, Inês Fernandes,

João C.M. Bordado and Amélia P. Rauter

Faculdade de Ciências da Universidade de Lisboa, Portugal

*digmendes85@gmail.com



Genista tenera

- Study of *Genista tenera*, a medicinal plant used in folk medicine to control diabetes.
- Mass spectrometry structural characterization of *G. tenera* aqueous extracts.
- Flavones, isoflavones, and glycosylated flavonoids were detected in the lyophilized aqueous extract by electrospray tandem mass spectrometry (ESI-MS/MS) in the negative and positive ion modes.

ELISA application on EE2 water monitoring

Diana L.D. Lima*, Rudolf J. Schneider and Valdemar I. Esteves

University of Aveiro, Portugal.

*diana.lima@ua.pt



7 groundwater samples

↓
< LOD



11 surface water samples

↓
< LOD



6 samples from 2 STP

↓
From 33 to 91 ng L⁻¹

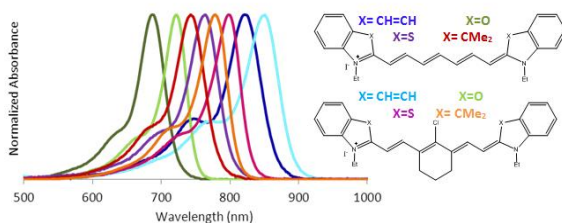
- The analytical working range for EE2 quantification obtained was between 0.03 and 40 mg L⁻¹.
- An increase of humic acid concentration lead to flattened calibration curves and the sigmoidal shape tended to be lost.
- The organic matter interference was overcome in the presence of BSA buffer 1% (w/v) incubated together with the standard and samples.
- EE2 was detected in North and South STP (only after primary treatment).
- No EE2 was detected in ground and surface water samples.

Photochemical properties of rigidified and non-rigidified heptamethine cyanine dyes in solution and adsorbed onto polymers

Diana P. Ferreira^{*}, Luís F. Vieira Ferreira, A. S. Oliveira, Lucinda V. Reis, Paulo F. Santos, Susana S. Ramos and Paulo Almeida

Instituto Superior Técnico da Universidade Técnica de Lisboa, Portugal.

**diana.ferreira@ist.utl.pt*



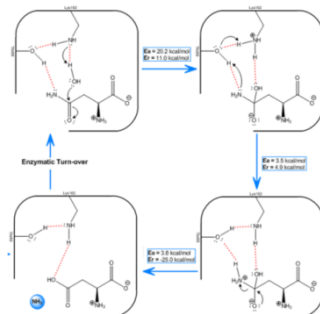
- Near infrared (NIR) fluorescence imaging
- Organic NIR fluorescent dyes, more precisely heptamethine cyanines
- Comparison of the non-rigidified dyes with the respective rigidified molecules
- High fluorescence quantum yields and fluorescence lifetimes
- Determination of singlet oxygen quantum yield of formation
- Microcrystalline cellulose and chitosan

Unveiling the Catalytic Mechanism of L-asparaginase II using Computational Methods

D.S. Gesto^{*}, N.M.F.S.A. Cerqueira, P.A. Fernandes and M.J. Ramos

Faculdade de Ciências da Universidade do Porto, Portugal.

**dianagesto@gmail.com*



- Using QM/QM hybrid methods, namely ONIOM, we were able to evaluate the reaction mechanism of the enzyme L-asparaginase.
- The reaction catalyzed by the enzyme consists of three steps, in which the first one is the rate-limiting step.
- The catalytic residues of L-asparaginase are Thr89 and Lys162. There is also a catalytic water molecule in the active site, which is needed for the reaction.
- The activation barrier is 20.2 kcal/mol and the energy of reaction amounts to -9.0 kcal/mol.
- We were able to identify and characterize all intermediates and transition states in terms of structure and energy.
- Despite what is described in the literature, we did not find a favorable mechanism in which there is the formation of an acyl-enzyme intermediate, formed between the substrate and Thr12.



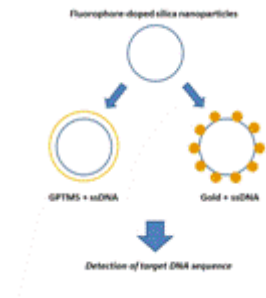
P43

Preparation of Multifunctional Fluorophore-Doped Silica Nanoparticles for Genetic Detection Applications

Diogo Ferreira^{*}, Cristina Neves, Pedro Quaresma, Craig Medforth, Eulália Pereira, Pedro V. Baptista and Peter Eaton

Faculdade de Ciências da Universidade do Porto, Portugal.

^{*}dmrferreira@gmail.com



- A new bioconjugate for sensors consisting of rhodamine-B isothiocyanate-doped silica nanoparticles with ssDNA on the surface was synthesized.
- Binding of ssDNA to the nanoparticles was achieved by using 3-glycidylpropyltrimethoxysilane (GPTMS) as a linker.
- A gold-decorated version was also synthesized by a deposition-precipitation method.
- The nanoparticles were characterized by UV-Vis spectroscopy, fluorimetry, TEM, ¹H NMR and light scattering-based zeta potential and size measurements.



P44

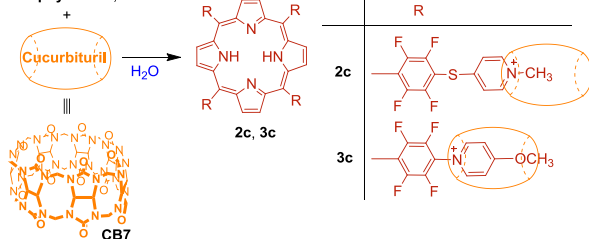
Pyridinium porphyrins and their host-guest interactions with cucurbituril macrocycles

Dora C. S. Costa^{*}, Vânia F. Pais, Artur M. S. Silva, José A. S. Cavaleiro, Uwe Pischel and João P. C. Tomé

University of Aveiro, Portugal.

^{*}doracosta@ua.pt

Porphyrins 2b, 3b



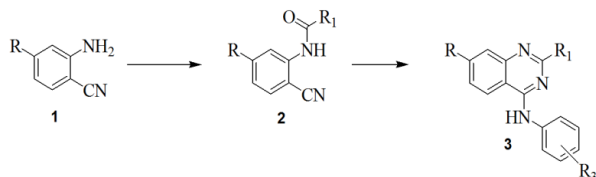
- TPPF₂₀ functionalization by thio- and hydroxy-pyridine
- Cationization of both groups
- Spectroscopic characterization
- Supramolecular complexes with cucurbituril CB7.

The reaction of anthranilonitrile with carbonyl compounds: a convenient synthesis of fused quinazolines

Elina Marinho* and M. Fernanda Proença

University of Minho, Portugal

*ElinaMarinho@sapo.pt



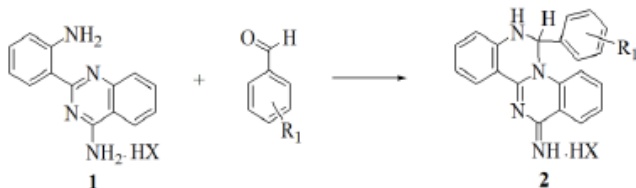
- The quinazoline ring system is present in a wide range of biologically active compounds.
- Anthranilonitrile is often used as the starting material in the preparation of quinazoline derivatives.
- New substituted 4-phenylaminoquinazolines were prepared from anthranilonitrile, active carbonyl compounds and primary aromatic amines.

Synthesis of dihydroquinazolines by microwave irradiation

Elina Marinho* and M. Fernanda Proença

University of Minho, Portugal

*ElinaMarinho@sapo.pt



- Most of the synthetic methods reported in the literature for the preparation of quinazoline derivatives are time consuming and lead to poor yields of the product.
- Microwave assisted synthesis have already demonstrated to be widely successful in the organic chemistry field.
- Dihydroquinazolines were prepared in excellent yield from the reaction of 2-(2-aminophenyl)quinazolin-4-amine and aromatic aldehydes.
- The reaction was performed under conventional heating conditions and under microwave irradiation.

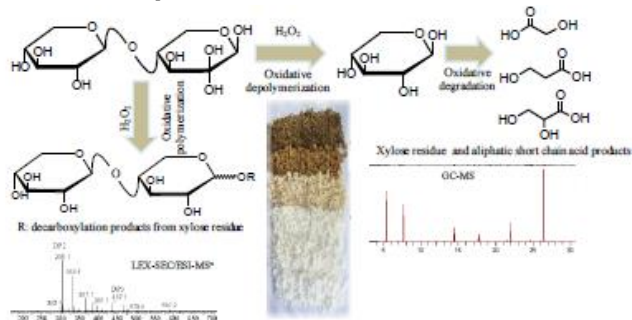
P47

Mimicking bleaching reactions in cellulosic pulp: oxidation of xylo-oligosaccharides by alkaline hydrogen peroxide

Elisabete V. da Costa*, Ana S. P. Moreira, Maria R. Domingues and Dmitry V. Evtuguin

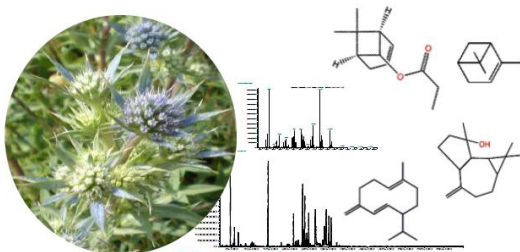
University of Aveiro, Portugal

*elisabetecosta@ua.pt



Composition of the volatile oil of *Eryngium dilatatum* Lam.

Eunice Fernandes*, Lígia Salgueiro and Carlos Cavaleiro
 Faculdade de Farmácia da Universidade de Coimbra, Portugal
 *nixesilva@hotmail.com



The volatile extract from *Eryngium dilatatum* (Apiaceae) was studied for the first time.

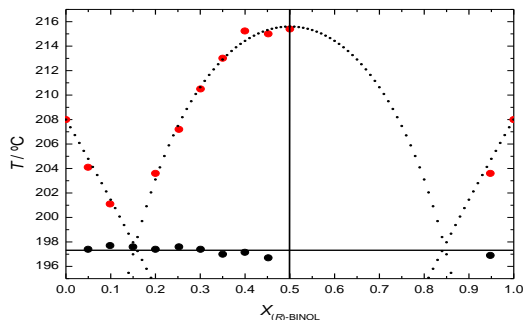
A combined methodology of gas chromatography and gas chromatography / mass spectroscopy was used for analysis.

Sesquiterpene fraction is dominant (57.5%), chiefly composed by germacrene D (10.3%), bicyclogermacrene (8.1%), spathulenol (5.9%) and α -cadinol (5.7%).

Z-Chrysantenyl acetate (11.1%) is the major monoterpene.

The Solid - Liquid Phase Diagram for BINOL Enantiomer Mixtures

Fabio A. Marins*, Teresa M. R. Maria, João Canotilho, M. M. Pereira and M. Ermelinda S. Eusébio
 University of Coimbra, Portugal
 *fabinhomarins@hotmail.com



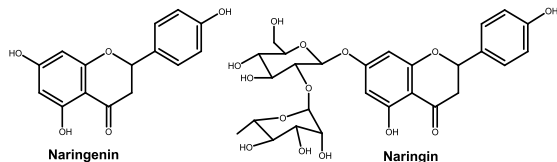
- The detailed solid – liquid phase diagram was established.
- The two eutectic mixtures have composition $X_{(R)-BINOL} = 0.155$ and 0.845 , $T_E = (197.3 \pm 0.6)^\circ\text{C}$.
- The equation $i = (T_{\text{fus,R}} - T_E) / (T_{\text{fus,A}} - T_E) = 1.7$ (> 1.5), which may be used to predict racemic compound formation, is fulfilled.
- The diagram is well described by the superposition of the Schroeder-van Laar and Prigogine-Defay equations.

**P51****Regioselective modification of natural polyphenols and their glycosides through enzyme catalyzed reactions**

Filipa Barradas, Margaux Matias, M. Manuel Silva* and Jorge A. R. Salvador

Faculdade de Farmácia da Universidade de Coimbra, Portugal

*msilva@ff.uc.pt



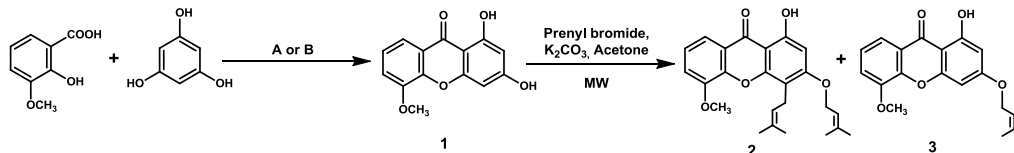
- Regioselective modification of polyphenolic compounds and their glycosides using lipases as catalysts.
- The influence of the type of enzyme, the nature of the reaction (transesterification of alcoholysis), the solvent and the structure of the substrates on regioselectivity is discussed.
- Diverse monoacyl and monoalcohol derivatives were isolated in high yields.
- Further synthetic modification of these compounds by chemical synthesis is under investigation aiming to obtain novel bioactive compounds.

**P52****Prenylated xanthonic derivatives: an inspiration for synthesis of new inhibitors of growth of human tumor cell lines**

F. Oliveira, R. Castanheiro*, M. Pinto and J. A. R. Salvador

Centro de Química Medicinal da Universidade do Porto (CEQUIMED-UP), Portugal.

* raquelc@ff.up.pt



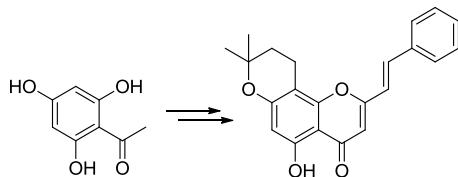
- Concerning 1,3-dihydroxy-5-methoxyxanthone (1), the best yield was obtained through the application of classic Grover, Shah and Shah reaction (A) rather than with the use of Eaton's reagent (B).
- In the reaction of 1,3-dihydroxy-5-methoxyxanthone (1) with prenyl bromide under microwave irradiation, prenylated xanthones 2 and 3, were obtained in different yields, being the 3-mono-oxiprenylated xanthone (3) the major product.

Synthesis of prenylated (*E*)-2-styrylchromones

Frederico R. Baptista, Diana C. G. A. Pinto, Artur M. S. Silva* and José A. S. Cavaleiro

University of Aveiro, Portugal

*artur.silva@ua.pt



- Direct C-prenylation of 2,4,6-trihydroxyacetophenone.
- Synthesis of the (*E*)-5,7-dimethoxy-8,8-dimethyl-2-styryl-9,10-dihydropyrano[2,3-*f*]chromen-4(8*H*)-one by the Baker-Venkataraman method.
- Deprotection and formation of a fused dihydropyran ring.

Solid-phase peptide synthesis of bombesin analogs bearing unnatural amino acids with fluorescent and metal-chelating properties

Gonalo M. A. Ribeiro, Sílvia Maia, M. Manuela M. Raposo, Susana P. G. Costa and Paula Gomes*

University of Minho / Faculdade de Ci ncias da Universidade do Porto, Portugal;

*pgomes@fc.up.pt



- Bombesin is a natural antimicrobial peptide, secreted by the skin of the asian frog *Bombesia orientalis*, which has interesting tumor-seeking properties.
- Bombesin analogs, bearing unnatural fluorescent and metal-chelating aminoacids, were synthesized by solid-phase methodologies.
- The Bombesin analogs were evaluated as chemosensors for the interaction with biologically important alkaline, alkaline-earth and transition metallic cations.
- Spectrofluorometric titrations were carried out in acetonitrile to evaluate their ability to respond, *via* changes in the fluorescence spectra, to the presence of the cations.



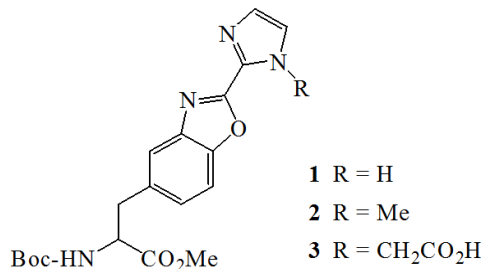
P55

Synthetic unnatural amino acids as fluorimetric probes for metallic cations

Gonalo M. A. Ribeiro, Ctia Esteves, M. Manuela M. Raposo and Susana P. G. Costa *

University of Minho, Portugal

*spc@quimica.uminho.pt



- The synthesis of benzoxazolyl-alanines **1-3** bearing an imidazolyl moiety with different substituents was accomplished.
- The new unnatural amino acids were evaluated as chemosensors for the interaction with biologically important alkaline, alkaline-earth and transition metallic cations.
- Spectrofluorometric titrations were carried out in acetonitrile to evaluate their ability to respond, *via* changes in the fluorescence spectra, to the presence of the cations.
- ¹H NMR titrations of amino acid **3** were also performed.



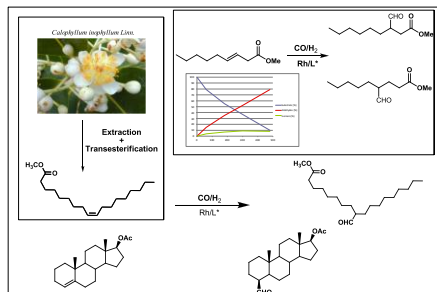
P56

Rhodium-Phosphinite Catalyzed Hydroformylation of Natural Products

Gonalo N. Costa,* Rui M. B. Carrilho, Juvncio C. Ruas, Artur R. Abreu, M. Jos S. M. Moreno, Mariette M. Pereira

Faculdade de Cincias e Tecnologia da Universidade de Coimbra, Portugal

*gnascosta@gmail.com



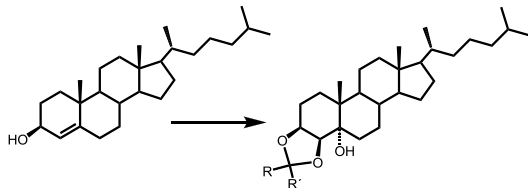
- Efficient and clean two-step synthesis of a family of BINOL based bulky monophosphite ligands
- Remarkable catalytic activity was observed in the hydroformylation of hindered olefins, like natural oils and steroids
- Significant effect of the ether substituent R at the ligand was observed in catalytic activity and chemoselectivity

Cytotoxic oxysterols: synthesis and biological evaluation of ketal derivatives

Hélia Jeremias, João F. S. Carvalho, M. Manuel Cruz Silva and M. Luisa Sá e Melo*

Universidade de Coimbra, Portugal

*samelo@ff.uc.pt



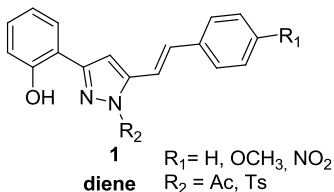
- Oxysterols exert a wide range of biological effects, including cytotoxicity against cancer cell lines, being therefore interesting starting molecules for drug discovery and development.
- We have synthesised several polyhydroxylated derivatives of cholesterol and their ketal counterparts aiming to evaluate the effect of these structural modifications on selective cytotoxicity, by in vitro studies in cancer and non cancer cell lines.
- A method to synthesize ketals from allylic alcohols is reported and a library of 3,4-ketals and 6,7-ketals was prepared.
- The compounds synthesized exhibited antiproliferative activity in a low micromolar range.

3(5)-(2-Hydroxyphenyl)-5(3)-styryl-1H-pyrazoles: synthesis and reactivity studies on Diels-Alder transformations

Inês C. S. Cardoso*, Vera L. M. Silva*, Artur M. S. Silva and José A. S. Cavaleiro

University of Aveiro, Portugal

*inescamoiana@ua.pt; verasilva@ua.pt



- An efficient methodology for the synthesis of 3(5)-(2-hydroxyphenyl)-5-styryl-1H-pyrazoles **1** was developed.
- The acetylation of pyrazoles **1** is not regioselective giving a mixture of the corresponding mono- and diacetylated pyrazoles.
- Microwave irradiation under solvent-free conditions induces 1-acetyl-5-styryl-1H-pyrazole to undergo Diels-Alder cycloaddition reaction with *N*-methylmaleimide to give the desired cycloadduct in moderate yield.



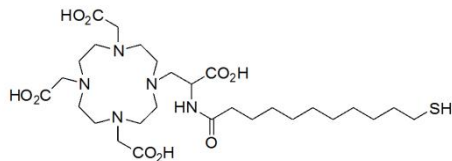
P59

Gold nanoparticles functionalized with Gd^{3+} chelates as high relaxivity Contrast Agents for Magnetic Resonance Imaging

Janaína Gonçalves*, Paula M. Ferreira, Carlos F. G. C. Geraldês, Lothar Helm and José A. Martins

University of Minho, Portugal.

*janainag23@gmail.com



DO3A-N-(α -11-mercaptoundecanamido)propionate (**1**)

- The synthesis of a novel w-tiol derivatized metal chelator and its Gd^{3+} complex was achieved;
- The cmc of the complex was determined (2,003 mM);
- The complex DO3A-N-(11-mercaptoundecanamide)aminopropionate is very stable
- The gold nanoparticles are very stable in high temperature, and a range of pH(2-7);



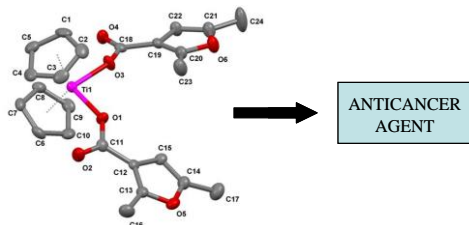
P60

Synthesis of new titanocene(IV) carboxylate complexes: An alternative chemotherapeutic treatment against cancer

Jesús Ceballos-Torres*, María J. Caballero-Rodríguez, Sanjiv Prashar, Reinhard Paschke, Dirk Steinborn, Goran N. Kaluderović and Santiago Gómez-Ruiz

Universidad Rey Juan Carlos, Spain.

*jesus.cebillos@urjc.es



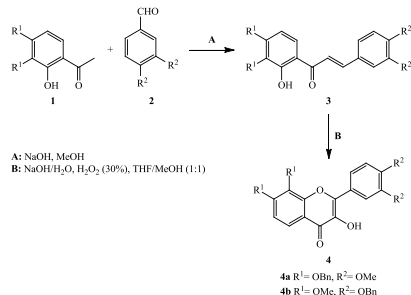
- New titanocene(IV) complexes containing different carboxylate ligands have been synthesized.
- Complexes have been tested against the tumour cell line A2780 (ovarian carcinoma), showing notable cytotoxicity in comparison with $[Ti(\eta^5-C_5H_5)_2Cl_2]$.
- A study of the interaction of some of the complexes with DNA (probably one of the biological target-molecules of the titanocene derivatives) has been monitored by UV-visible spectroscopy.

Synthesis of new flavon-3-ols with potential antioxidant activity

Joana L. C. Sousa* and Artur M. S. Silva*

University of Aveiro, Portugal

*joanasousa@ua.pt, artur.silva@ua.pt



- New 3-hydroxyflavone derivatives were synthesized.
- It was used a two-step synthetic route based on well-known reactions.
- The 3-hydroxyflavones prepared will be studied as potential antioxidant compounds.

Development of a new library of novel and reversible MAO-B inhibitors based on the benzopyranic nucleus: an overview

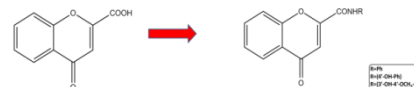
J. Reis*, A. Gaspar, F. Cagide, E. Uriarte, S. Alcaro, F. Ortuso and F. Borges

Faculty of Sciences of University of Porto, Portugal.

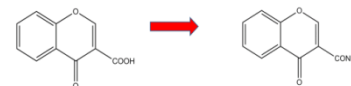
*jocostareis@gmail.com

- Chromone is a valid scaffold for the design of potent, selective and reversible MAO inhibitors.
- Chromones with substituents in position 3 of γ -pyrone nucleus operate as *h*MAO-B selective inhibitors.
- The SAR study allow to conclude that the type of substituent on the aromatic ring of the chromone amide side chain is crucial for the modulation of the efficacy *vs* selectivity of the novel MAO-B inhibitors.
- The introduction of halogen (chloro/iodo), methyl or hydroxy substituents in *para* position of the exocyclic aromatic ring of the 3-carboxamide chromone improve the potency and selectivity towards MAO-B.
- Preliminary studies performed so far reveal that 3-carboxamide chromone behave as quasi-reversible MAO-B inhibitors

2-carboxamide chromone derivatives



3-carboxamide chromone derivatives





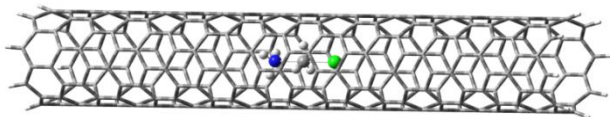
P63

Confinement effects over the energetic profile of a Menshutkin SN2 reaction, a computational study

J. M. Martins and A. L. Magalhães*

Faculty of Sciences of University of Porto, Portugal

*almagalh@fc.up.pt



- S_N2 reaction confined inside carbon nanotubes.
- Computational study using an ONIOM QM/QM approach.
- Able to successfully predict reaction path energies and conformation changes.
- Confinement inside CNTs lowers the reaction energy barrier compared to reaction in vacuum.
- Different nanotube structure differently affects the energy profile of the reaction.



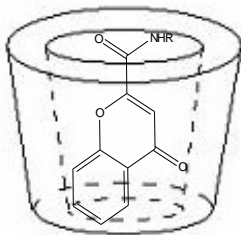
P64

Environmental and pharmaceutical applications of cyclodextrin-assisted molecular encapsulation

José Dias, Marta Martins, E. Manuela Garrido, Maria J. Sottomayor, Fernanda Borges and Jorge Garrido*

Faculty of Sciences of University of Porto, Portugal

*jgg@isep.ipp.pt



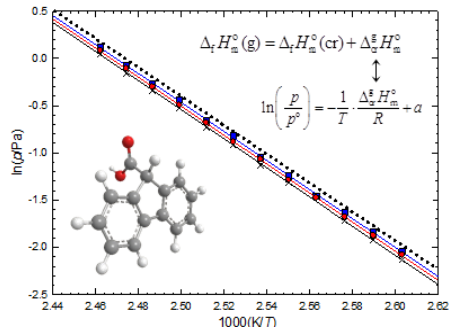
- Molecular encapsulation by cyclodextrins
- Physicochemical properties of the inclusion complexes
- Enhanced aqueous solubility and chemical stability of various compounds
- Application in pharmaceutical and environmental area

Thermodynamic study of two 9-substituted fluorene derivatives

Juliana A. S. A. Oliveira*, Maria M. Calvino, Manuel J. S. Monte and Maria D. M. C. Ribeiro da Silva

Faculdade de Ciências, Universidade do Porto, Portugal

*juliana.oliveira@fc.up.pt



- Thermodynamic study of fluorene-9-methanol and fluorene-9-carboxylic acid:
- Standard molar enthalpies of formation, in the crystalline phase, were determined by static bomb combustion calorimetry.
- Standard molar enthalpies of sublimation were derived from the sublimation vapour pressures, determined by a static apparatus and a Knudsen effusion apparatus.
- Standard ($p^\circ = 0.1$ MPa) molar enthalpies of formation, in the gaseous phase, at $T = 298.15$ K, were calculated from the previous parameters.
- Estimation of the enthalpic increments associated to the insertion of different functional groups (OH and COOH) to the fluorene molecule.
- The volatility study of the solid phase, interpreted in terms of molecular structure, allows inferring on the thermal stability of the referred compounds.

Incorporation of polyfluorenes into poly(lactic acid) films for sensor and optoelectronics applications

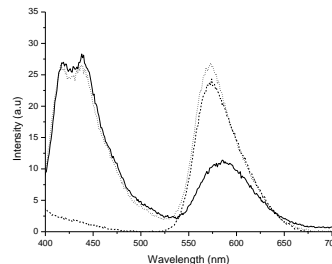
L. Martelo*, A. Jiménez, A. J. M. Valente, H. D. Burrows, A. T. Marques, M. Förster,

U. Scherf, M. Peltzer and S. M. Fonseca

University of Coimbra, Portugal / University of Alicante, Spain

*liliana.martelo@hotmail.com

- The films obtained were thin, optically transparent, luminescent, flexible and exhibiting good thermal and photochemical stability.
- Ratiometric luminescence sensing is possible by inclusion of a phosphorescent ruthenium (II) complex.
- In the presence of the $\text{Ru}(\text{bpy})_3^{2+}$ quenching of the fluorescence of PBS-PFP is observed (see Figure) and accompanied by the appearance of a new emission band with a maxima at 600 nm, corresponding to the phosphorescence of the $\text{Ru}(\text{bpy})_3^{2+}$, consistent with energy transfer from the polyelectrolyte to the ruthenium (II) complex.
- Excellent oxygen permeability, with an increase in OTR but maintaining physical and chemical properties.
- They are shown to be good candidate for ratiometric sensing studies.



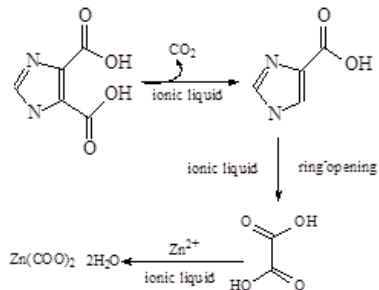
Fluorescence spectra of PLA + 10 wt % of C207/6 + 1089 ppm of PBS-PFP in relation between the $\text{Ru}(\text{bpy})_3^{2+}$ of: 1:0.75 (solid line), 1:1 (dashed line) and 1:1.25 (dotted line).

In situ oxalate formation from imidazole 4,5-dicarboxylic acid in ionothermal reactions

Ling Xu*, Baltazar de Castro and Luís Cunha-Silva

Faculty of Sciences, University of Porto, Portugal

*ling.xu@fc.up.pt



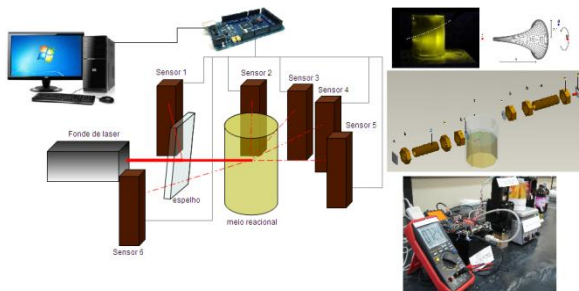
- Ionothermal synthesis is an emerging method for the preparation of new materials
- In situ formation of Ox²⁻ was confirmed by the preparation of the crystalline product Zn(Ox)·2H₂O (Ox²⁻ = C₂O₄²⁻), in various 1-alkyl-3-methylimidazolium bromides ILs.
- The formation of Ox²⁻ involves with the decarboxylation and open-ring of imidazole 4,5-dicarboxylic acid (H₂ImDC), assisted by the IL environment.
- The decomposition of H₂ImDC under ionothermal conditions was observed for the first time.

Monitoring the production of biodiesel with real-time laser spectroscopy

Luis A. B. De Boni*, Teresa M. R. Maria, M. M. Pereira and Isaac N. L. da Silva

University of Coimbra, Portugal / Pontifical Catholic University of Rio Grande do Sul, Porto Alegre, Brasil

*labdeboni@gmail.com



The prototype shows:

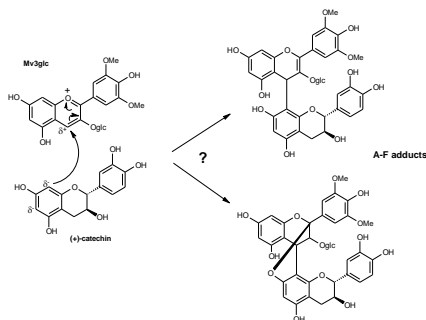
- Real-time monitoring of the reaction.
- Easy interpretation of the graphical interface.
- Improves of the reaction time.
- Reduction of the energy intake.
- Reduction of the generation of co-products and waste.
- Raises the profitability of the process.

New insights about malvidin-3-glucoside-catechin dimeric compound

Luís Cruz*, Nuno Mateus and Victor de Freitas

Faculdade de Ciências, Universidade do Porto, Portugal.

*luís.cruz@fc.up.pt



- Anthocyanins (A) and flavanols (F) are the main flavonoid compounds responsible for color and flavor of red wines, respectively.
- These compounds are very reactive during wine processing and ageing giving rise to a large number of new compounds.
- The characterization and formation pathway of F-A adducts in wines is well documented in the literature while the A-F pigments formation mechanisms are not totally elucidated.
- A-F adducts were never isolated in sufficient quantities from wines or model solutions to proceed to full structural elucidation and follow their evolution.
- This work aims to bring new insights about the reaction between malvidin-3-glucoside and (+)-catechin in order to clarify the dimeric A-F flavene structure and follow its evolution.

Electrochemical mineralization of oxalic acid at metallic catalyst based on carbon nanotubes

M.F. Pinto, M. Ferreira, I.C. Neves, A.M. Fonseca, O.S.G.P. Soares, J.J.M. Órfão, M.F.R. Pereira, J.L. Figueiredo and P. Parpot*

Universidade do Minho, Braga, Portugal.

* parpot@quimica.uminho.pt

- The electrochemical mineralization of oxalic acid was carried out in 0.10 M NaCl and 0.5 M NaOH media on CNT and metal modified electrodes with high yields;
- Higher current efficiencies were obtained in 0.10 M NaCl. The oxidation reactions take place in this case by the electrogeneration of active chlorine species;
- Among the catalysts tested, Ru-Cu/CNT showed the best performance for the mineralization of oxalic acid.



P71

Young chemists at IJUP: opportunities for research training at U.Porto

Marcela A. Segundo * and Maria Rangel

Faculdade de Farmácia, Universidade do Porto, Portugal.

*mseguno@ff.up.pt



- IJUP is the designation chosen to identify all initiatives for promoting the participation of young students in research activities at U.Porto.
- Five IJUP meetings have been held yearly since 2008.
- Participation of students from chemical sciences has been significant, accounting for 10-24% of oral presentations and 21-47% of poster communications presented in each meeting.



P72

Characterisation of phenolic compounds from *Acacia melanoxylon* biomass extracts by capillary electrophoresis

Márcia A. Ribeiro, Alice I. Martins, Luísa B. Roseiro* and Amélia P. Rauter

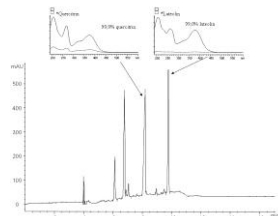
Universidade de Lisboa, Faculdade de Ciências, Portugal

*luisa.roseiro@lneg.pt

A. melanoxylon biomass



CE profile of diethyl ether extract of *A. melanoxylon*



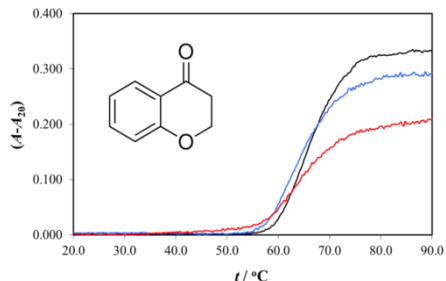
- *Acacia* species are the most prolific invaders in France, Italy, Spain and Portugal, especially in conservation areas.
- Biomasses of *Acacia* species are residues from forest activities that could be promising sources of added-value compounds.
- Aerial biomass of *Acacia melanoxylon* was subject to solvent extraction and CC purification in order to obtain phenolic-rich fractions.
- Phenolic fractions of *Acacia melanoxylon* were characterised by capillary electrophoresis, revealing different phenolics with industrial interest.
- *Acacia melanoxylon* biomass (leaves and stems) are rich in quercitrin, a common antioxidant flavonoid found in vegetables, among others.

Interaction of 4-chromanone with double stranded DNA. An UV spectroscopy study

Diana Sousa and M. J. Sottomayor*

Faculdade de Ciências, Universidade do Porto, Portugal

**mjsotto@fc.up.pt*



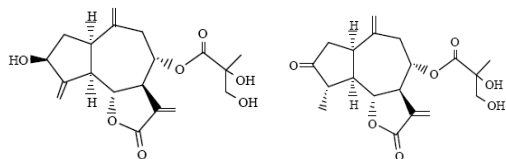
- The interaction of 4-chromanone with double stranded DNA was studied by UV spectroscopy.
- The results evidence a noteworthy interaction of 4-chromanone with DNA.
- The concentration of 4-chromanone has a pronounced effect on the characteristics of DNA thermal denaturation.

2D NMR Studies of sesquiterpene lactones with potential antitumoral activitie

Maria H. R. Amorim*, Rui M. Gil da Costa and Margarida M. S. M. Bastos

Engineering Faculty (FEUP), University of Porto, Portugal.

**helenara@fe.up.pt*



- Two guaianolide-type sesquiterpene lactones were structurally elucidated
- ^1H NMR, ^{13}C NMR Broad Band (BB) and ^{13}C NMR Distortionless Enhanced Polarization Transfer (DEPT) studies were performed for skeletal elucidation
- COSY, HMQC and HMBC were performed for the establishment of carbon-hydrogen correlation

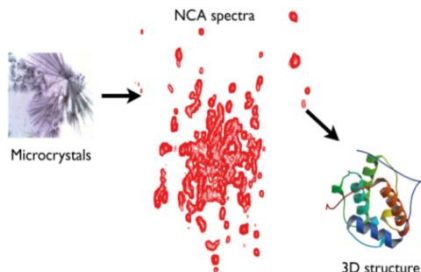
P75

High-resolution solid-state MAS NMR methods applied to structural studies of mammalian end-binding protein 3

Mariana Sardo^{*}, Luis Mafra, João Rocha, Beat H. Meier and Anja Böckmann

University of Aveiro, Portugal / Physical Chemistry, ETH-Zurich, 8093 Zurich, Switzerland

**msardo@ua.pt*



- Solid-state NMR studies of the mammalian EB3 protein in view of the further development of high-resolution structure determination methods.
- ^{13}C and ^{15}N uniformly labeled EB3 expressed and purified from E. Coli host strains.
- Two-dimensional homonuclear (^{13}C - ^{13}C DARR) and heteronuclear (^{15}N - ^{13}C NCA, NCO) spectra as well as three-dimensional NCACO, NCOCA, CANCO and NCACB are presented for assignment purposes.
- EB3 is a good crystalline model system, revealing sufficient resolution and sensitivity to continue further with structural studies.

P76

Electrocatalytic reduction of nitrate in water with mono and bimetallic catalysts supported on carbon nanotubes

M. Ferreira, M. F. Pinto, I. C. Neves, A. M. Fonseca, O. S. G. P. Soares, M. F. R. Pereira, J. J. M. Órfão, J. L. Figueiredo and P. Parpot^{*}

Universidade do Minho, Braga, Portugal

**parpot@quimica.uminho.pt*

- Electrocatalytic reduction of nitrate was carried out in aqueous medium on monometallic (Pd and Pt) and bimetallic (Pd-Cu, Pt-Cu and Ru-Cu) catalysts supported on carbon nanotubes with high yields.
- Concerning the electrocatalytic reduction of nitrate, besides nitrogen, nitrite and ammonia appears as by-product.
- Bimetallic catalysts showed better performance for the reduction of nitrate in comparison with monometallic catalysts.

Polycyclic aromatic hydrocarbons extraction from digestive glands by microwave-assisted and solid phase extraction

Marta Oliveira*, Simone Morais, Filipa Gomes, Maria J. Ramalhosa and Cristina Delerue-Matos

Instituto Superior de Engenharia do Porto, Portugal

*martamadalen@gmail.com



- Polycyclic aromatic hydrocarbons are one of the priority environmental pollutants due to their extremely hazardous properties to human health.
- Polycyclic aromatic hydrocarbons quantification in digestive glands was based on MAE-SPE-LC-FLD-PAD.
- The optimal operational parameters were found to be for MAE: 20 minutes at 110 °C with 20 mL of acetonitrile, 1 g of sample and medium stirring speed, and for SPE the application of a Sep-Pak® Plus Silica cartridge 55-105 µm with a pore size of 125 Å.

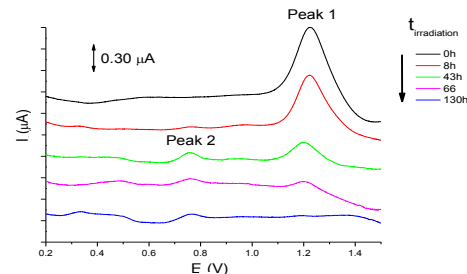
Electrochemical techniques applied to the study of pesticide's photodegradation

Cátia Costa, Marta Martins, Jorge Garrido, Fernanda Borges and E. Manuela Garrido*

Faculty of Sciences, University of Porto / School of Engineering, ISEP, Polytechnic Institute of Porto, Portugal

*emg@isep.ipp.pt

- Environmental impact of pesticides.
- Photodegradation of pesticides in environment.
- Electrochemical determination of pesticides and its photodegradation products.
- Development of new methodologies for simultaneous determination of pesticides and its by-products.



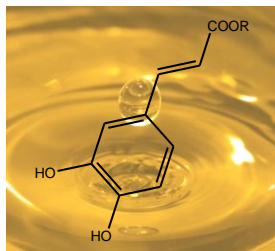
**P79**

Impact of antioxidants on the oxidation stability of biodiesel

Marta Martins, E. Manuela Garrido, Fernanda Borges and Jorge Garrido*

Faculty of Sciences, University of Porto / School of Engineering, ISEP, Polytechnic Institute of Porto, Portugal

**jg@isep.ipp.pt*



- Oxidation stability is important for the biodiesel quality.
- Oxidation of biodiesel can be prevented by using antioxidants.
- Effect on phenolic antioxidant additives on biodiesel.
- The effectiveness of antioxidants at improving the oxidation stability is highlighted.

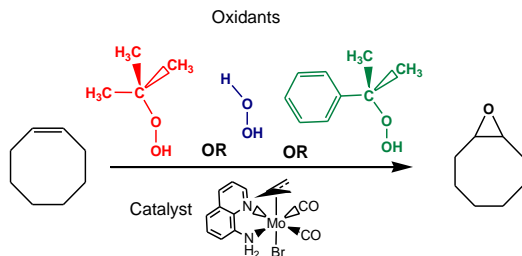
**P80**

Mo(II) catalysts in the epoxidation of cy8: the effect of temperature, solvent and oxidants

Marta S. Saraiva, Carla D. Nunes* and Maria José Calhorda

Faculdade de Ciências, Universidade de Lisboa, Portugal

mssaraiva@fc.ul.pt



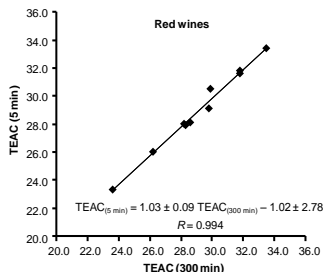
- Mo(II) complexes catalyze the epoxidation of cis-cyclooctene.
- Reaction conditions were changed to check how to achieve optimal conditions.
- Higher temperature leads to higher substrate conversion.
- The same conversion is obtained in the absence of solvent.
- Cumene hydroperoxide leads to the highest conversions, followed by TBHP and hydrogen peroxide.
- The catalytic conversion is achieved with an almost stoichiometric amount of oxidant (compared to 2:1)

Assessment of endpoint antioxidant capacity of red wines using a novel kinetic matching approach

Miguel A. Maia*, Luís M. Magalhães, Luísa Barreiros, Salette Reis and Marcela A. Segundo

Faculdade de Farmácia, Universidade do Porto, Portugal

*miguelmaia2@gmail.com



- A novel kinetic matching approach is proposed to foster rapid assessment of total (endpoint) antioxidant capacity of food samples.
- By selecting a compound with an oxidation kinetic profile similar to that shown by sample it is not necessary to achieve endpoint conditions.
- The analysis time (60 to 300 min at endpoint conditions) was reduced to <10 min for F-C, CUPRAC, DPPH[•] and ABTS^{•+} assays.
- The antioxidant values obtained with the kinetic matching standard were converted to a common standard, providing an universal way for expression of results.
- The antioxidant values estimated by the kinetic matching approach after 5 min were similar to those obtained by time-consuming endpoint approach (figure 1).

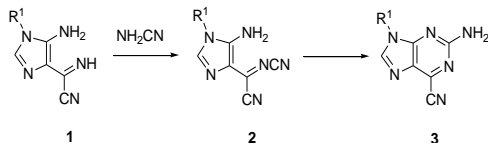
Figure 1: Relationship between the Trolox equivalents antioxidant capacity (TEAC, mM) obtained by the kinetic matching approach (5 min) and those obtained by the endpoint approach (300 min) for ABTS^{•+} assay regarding red wines from Portuguese vintages

A novel and efficient approach to 2-amino-6-cyanopurines

Nádia Senhorães*, Alice Dias, and M. Fernanda Proença

Universidade do Minho, Braga, Portugal

*nadiarodrigues85@gmail.com



- Tuberculosis remains a deadly disease, being the greatest single infection worldwide.
- Compounds containing the purine ring were identified as a new class of promising antimicrobial agents.
- A new and efficient method to the synthesis of 2-amino-6-cyanopurines was developed.
- These compounds will be tested as antituberculosis agents.

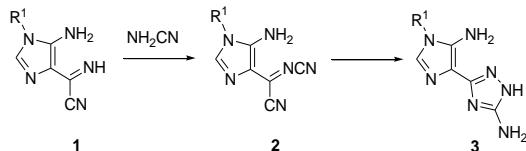
**P83**

A new and efficient synthesis of 3-amino[1,2,4]-Triazoles

Nádia Senhorães^{*}, Alice Dias and M. Fernanda Proença

Universidade do Minho, Braga, Portugal

**nadiarodrigues85@gmail.com*



- 1,2,4-Triazole derivatives are present in a wide range of biologically active molecules.
- A new and efficient method to the synthesis of 5-amino[1,2,4]-triazoles was developed.
- These novel 1,2,4-triazoles will be submitted to biological assays.

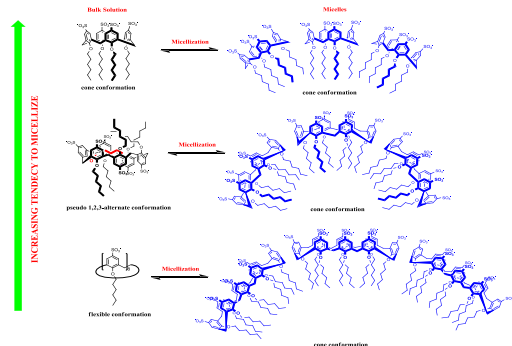
**P84**

The Effect of Conformational Preorganization on the Micellization of Calixarene-Based Surfactants

Nuno Basilio^{*}, Luis García-Río and Manuel Martín-Pastor

Universidad de Santiago, Santiago de Compostela, Spain.

**nuno.basilio@usc.es*



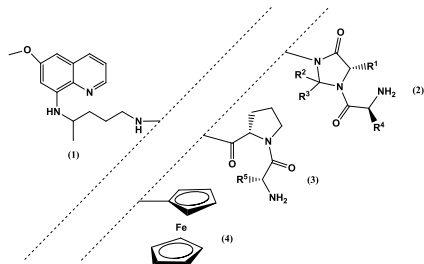
- The cone conformation is ideal for the formation of globular micelles.
- Calix[6 and 8]arenes undergo an aggregation induced structural reorganization into the cone conformation.
- Calix[4]arenes preorganized into the cone conformation show a higher tendency to self-aggregate.
- The preorganization effect is related with both the enthalpy and entropy of the process.

Primaquine peptidomimetic and organometallic derivatives against *Leishmania infantum*

Nuno Vale^{*}, Sílvia Vale Costa, Ana Tomás, Rui Moreira, Maria Salomé Gomes and Paula Gomes

Faculdade de Ciências da Universidade do Porto, Portugal

*nuno.vale@fc.up.pt



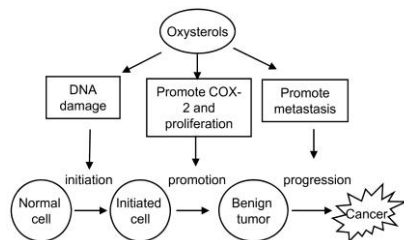
- Primaquine (**1**), an anti-malarial 8-aminoquinoline, displays activity against *Leishmania* spp.
- However, primaquine exhibits hemotoxicity and low oral bioavailability due to oxidative deamination of its aliphatic chain.
- We have previously developed peptidomimetic (**2** and **3**) and organometallic (**4**) derivatives of primaquine with higher resistance to proteolytic degradation and oxidative deamination.
- These new derivatives presented significant activity against primaquine-sensitive pathogens like *Plasmodium* or *Pneumocystis*.
- Some derivatives have an interesting anti-leishmanial profile with very low toxicity for host cells.

New oxysterol derivatives on *Opisthorchis viverrini*

Nuno Vale^{*}, Maria João Gouveia, Mónica Botelho, Paula Gomes, Paul Brindley and José Manuel Correia da Costa

Faculdade de Ciências da Universidade do Porto, Portugal

*nuno.vale@fc.up.pt



- *Opisthorchis viverrini* can develop mitogenic substances into excretory/secretory products that may play an important role in promoting the genesis of cholangiocarcinoma.
- Certain oxysterols, which are metabolic oxidation products of cholesterol, have been shown to be mutagenic and genotoxic.
- Oxysterols possess pro-oxidative and pro-inflammatory properties which can contribute to carcinogenesis.
- We developed a liquid chromatography with tandem mass spectrometry (LC-MS/MS) method to identify oxysterols in *Opisthorchis viverrini* samples.
- Results obtained allowed detecting bile acid conjugates with guanine which possibly underlie *Ov*-promoted DNA damage, and eventual correlations between oxysterols and various types of *Ov*-associated cancer.

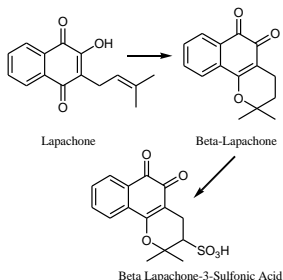


P87 Photophysics study of complexation between β -Lapachone-3-Sulfonic Acid with Bovine Serum Albumin (BSA)

Otávio Augusto Chaves*, Eduardo Benes, Edgar Schaeffer, Bauer de Oliveira Bernardes, Aurélio B.B. Ferreira and Jose Carlos Netto-Ferreira, Darí Cesarin Sobrinho

University of Coimbra, Portugal / ICE-Universidade Federal Rural do Rio de Janeiro-Seropédica – Seropédica/RJ - Brazil

* otavio_ufrj@hotmail.com



- This work aims to study the photophysics interaction between the bioactive molecule of β -lapachone-3-sulfonic acid with a solution of BSA buffered with PBS, pH=7.4. by UV-Visible, fluorescence and circular dichroism spectroscopies.
- Using the Stern-Volmer equation, and the Van't Hoff equation, obtain the value of K_{sv} , K_q , ΔG° , ΔH° and ΔS° at temperatures 288K, 293K and 298K.
- The high value of the rate constant of fluorescence quenching, indicate that the process of fluorescence quenching of the BSA is static.
- The negative value of ΔG° , shows the spontaneity of the bind and de positive value of ΔH° indicate that the interaction is endothermic.
- The circular dichroism spectra indicate that with the acid addition influence the ellipticity of albumin, showing a decrease of two bands, 208 nm and 222 nm. This proves complex formation between BL3SA and BSA.



P88 Synthesis of alkyl glycosides with potential application as antimicrobial agents

Patrícia Serra*, Vasco Cachatra, Alice Martins and Amélia P. Rauter

Universidade de Lisboa, Faculdade de Ciências, Portugal

* patriciafaserra@gmail.com



- Synthesis of a new series of compounds structurally related to 2-deoxy glycosides.
- Investigation and improvement of the synthetic methods.
- Search for original structures leading to a new antimicrobial mechanism of action.

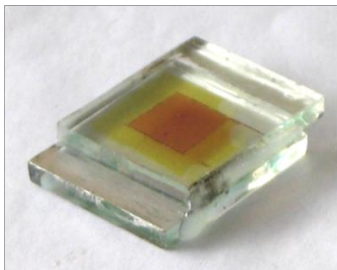
Pt and Ru Complexes and Porphyrins as Sensitizers for Dye-Sensitized Solar Cells

Patricia Jesus^{*}, Carlos J. P. Monteiro, Paul A Scattergood, Julia A. Weinstein, Carlos Serpa,

Mariette M. Pereira and Luis G. Arnaut

University of Coimbra, Portugal

**patricia_m.jesus@hotmail.com*



- The results obtained for these dyes are compared with the performance of DSSC prepared with ruthenium polypyridyl dyes.
- Porphyrins and platinum complexes used in this study show good adsorption onto TiO₂ thin films.
- The porphyrins adsorption kinetics and surface covering yield onto TiO₂ films depends on the number and position of the anchoring groups.

Multi-residue method for the analysis of veterinary pharmaceutical compounds in sludge

Pedro N. Carvalho^{*}, M. Clara P. Basto and C. Marisa R. Almeida

Faculdade de Ciências, Universidade do Porto, Portugal

**pedro.carvalho@fc.up.pt*

- Pharmaceutical compounds are currently labeled as emerging contaminants.
- Veterinary drugs are still poorly studied in terms of pathways, release rates and effects on the environment.
- The large variety of compounds and matrices pose difficult analytical challenges.
- A methodology for the simultaneous determination of five commonly used veterinary pharmaceuticals, in sludge samples is being developed.
- Ultrasonic solvent extraction followed by solid-phase extraction and HPLC-DAD was applied.

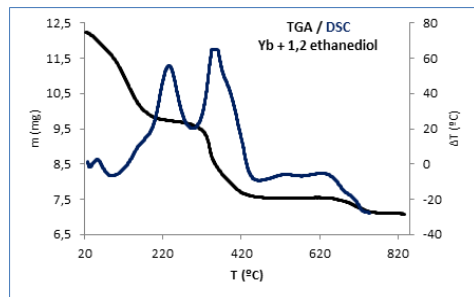


P91 Synthesis and Characterization of Novel Alkaline and Lanthanide Metal Alkoxides

P. G. Rosado*, J. B. Branco, J. P. leal, L. M. Ferreira and J. J. H. Lancastre

Instituto Tecnológico e Nuclear, Instituto Superior Técnico, Universidade Técnica de Lisboa, Portugal.

**pedrorosado@itm.pt*



- Ytterbium alkoxide was obtained by ammonia solution synthesis.
- Alkaline alkoxides were obtained by direct reaction of the metal with the diol in solution.
- The resulting compounds are very sensible to moisture and O₂.
- TGA, DSC, elemental analysis, X-ray and IR spectroscopy were used for the characterization of the resulting compounds.

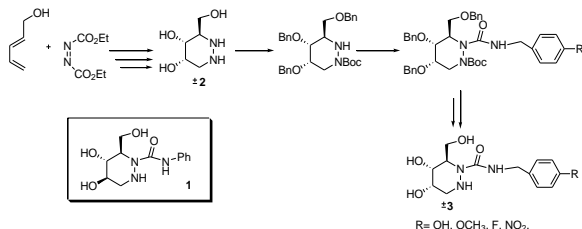


P92 Synthesis of 2-N-Benzyl Carboxamide Derivates of 1-Azafagomine

Raquel Mendes*, Vera C.M. Duarte, A. Gil Fortes and M. José Alves

Universidade do Minho, Braga, Portugal.

**tec.raquelmendes@hotmail.com*



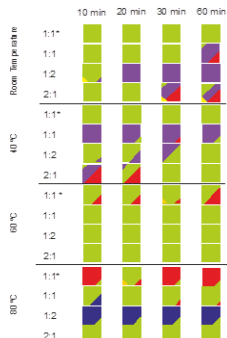
- The molecular modelling studies predicted a higher inhibitory activity for some derivatives of 1-azafagomine **2**.
- Synthesis of new 1-N-phenyl carboxamide derivatives of 1-azafagomine **1** was carried out.
- Glucosidase inhibition tests will be performed on final products (**3**)

One-Pot Method in the Synthesis of Diposphonic-Based Lanthanide Metal-Organic Frameworks

Ricardo Mendes*, Sérgio M. F. Vilela, Patrícia Silva, José A. Fernandes and Filipe A. Almeida Paz

University of Aveiro, Portugal

*rfmendes@ua.pt



- By varying the reaction conditions, four distinct materials were discovered (as represented by distinct colors in the diagram)
- Two phases (green and purple) can also be isolated using microwave-assisted synthesis.
- Two phases (red and blue) are only present in the mixtures with at least one of the previous phases
- The four distinct phases exhibit different crystal morphologies
- For each phase, the crystal morphology remains the same for different experimental conditions and methods (microwave and hydrothermal method).
- All the samples are highly crystalline with crystal sizes in the micrometer range.

Figure 1: Diagram of the obtained phases using the one-pot method. The colors red, blue, green and purple are indicative of different phases. The color orange indicates the presence of the organic ligand as a small contaminant.

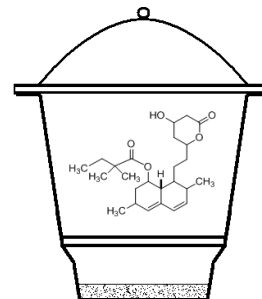
Stability of Simvastatin Under Different Atmospheric Humidities

Ricardo G. Simões*, João F. Pinto and Manuel E. Minas da Piedade

Faculdade de Ciências e Universidade de Lisboa, Portugal.

*rasimoes@fc.ul.pt

- The stability of simvastatin under different atmospheric humidities was evaluated.
- The samples were placed for 2 months in desiccators with 11%, 52%, and 93% humidities.
- Differential scanning calorimetry (DSC) runs were performed after 1, 2, 5, 7, 15, 30, and 60 days.
- No phase changes, water absorption, or significant variations of peak positions were observed.
- Simvastatin is stable throughout the experimental conditions.





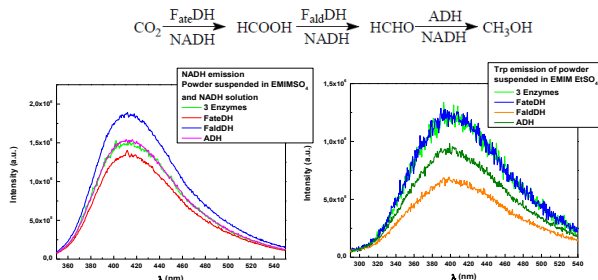
P95

Enzymatic conversion of CO₂ to Methanol. A Spectroscopic Approach

Rita Craveiro, Pedro Vidinha* and Susana Barreiros

Faculdade de Ciências e Tecnologia, Universidade Nova de Lisboa, Portugal

*pm.gomes@fct.unl.pt



- Enzymatic conversion of CO₂ to methanol is important in the production of raw materials for alternative fuels. This is possible to achieve, using three distinct dehydrogenases which are NADH dependent.
- The enzymes were immobilized in silica sol-gel matrices, in order to optimize methanol production. Ionic liquid [EMIM][EtSO₄] was also used as a solvent.
- Spectroscopic studies were carried out, namely fluorescence and 2D NMR spectroscopy.
- The results will help to understand and optimize the CO₂ solubilization in the medium, in order to enhance the methanol production.



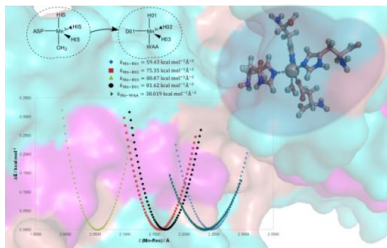
P96

Setting a New Biomolecular Force-Field: Parameterizing Manganese First Coordination Spheres from Metalloproteins

Rui P. P. Neves*, Sérgio F. Sousa, Pedro A. Fernandes and Maria J. Ramos

Faculdade de Ciências da Universidade do Porto, Portugal

*rppneves@gmail.com



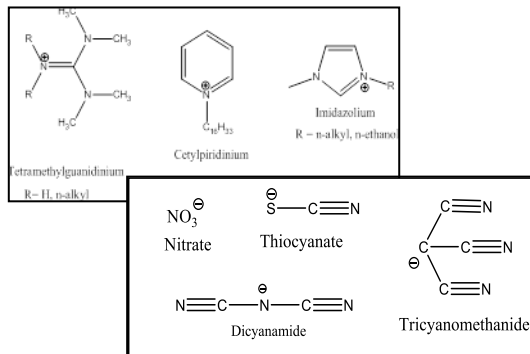
- The study of biologically relevant manganese centers was pursued using the B3LYP hybrid functional within the DFT methodology, with a hybrid basis set, 6-31G(d,p)/SDD, during geometry optimization and bond/angle scanning;
- Bond and angle force constants were determined using the harmonic potential approximation, with the least squares method, for each of the individual bond and angle stretching between ligands and metallic center (residues not involved in angle and bond stretching were kept frozen during the scan process);
- RESP methodology based on the Merz-Kollman scheme was used for atomic charge calculations, from single-point charge calculus with 6-311++G(3df,3dp) and tight SCF convergence criteria;
- Van der Waals parameters were obtained from literature and assumed transferable;
- Validation of the parameters developed was assured by molecular dynamics simulations.

Ionic Liquids containing nitro and cyano groups

Sandra Dias*, Andreia Forte and Luís C. Branco

Faculdade de Ciências e Tecnologia, Universidade Nova de Lisboa, Portugal

*sid17586@campus.fct.unl.pt



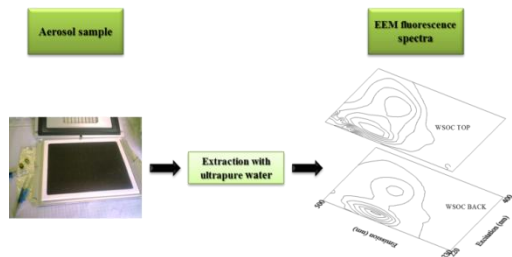
- Novel energetic materials based on ionic liquids (ILs);
- Energetic salts offer many advantages over conventional energetic molecular compounds;
- Different energetic ILs or molten salts based on tetramethylguanidinium [TMG], cetylpyridinium [C16pyr] and methylimidazolium [MIM] as nitrogen-rich organic cations were combined with thiocyanate [SCN], nitrate [NO₃], dicyanamide [DCA] and tricyanomethanide [TCM] as anions.
- Functionalized TMG cations were developed by the reaction with an adequate halo-alkyl compound;
- All energetic salts will be characterized by NMR, FTIR and Elemental analysis;
- Calorimetric (determination of melting point and glass transition temperatures) and Solubility studies will be also performed.

Molecular fluorescence spectroscopy as a technique for the assessment of secondary organic aerosol formation during sampling of atmospheric particles

Sandra M.S. Freire[†], Regina M.B.O. Duarte, and Armando C. Duarte

University of Aveiro, Portugal

*sandra.freire@ua.pt



- Secondary organic aerosols (SOA) can be formed *in situ* by chemical reactions and gas-to-particle conversion of volatile organic compounds.
- Atmospheric aerosol samples were collected following a tandem quartz fiber filters methodology.
- The assessment of SOA formation was screened by EEM and synchronous fluorescence spectroscopy of the aqueous extracts.
- Results suggest the likely occurrence of SOA formation during aerosol sampling.

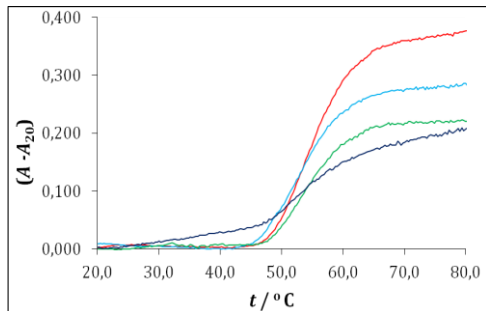
**P99**

Interaction of 3,4-dihydroxyxanthone with double stranded DNA in water/ethanol solutions

Sara Leirosa, C. Sousa, M. J. Sottomayor* and M. Pinto

Faculdade de Ciências, Universidade do Porto, Portugal

**mjsotto@fc.up.pt*



- The interaction of 3,4-dihydroxyxanthone with double stranded DNA was studied by UV spectroscopy, in water/ethanol solutions.
- 3,4-dihydroxyxanthone has a noteworthy effect on the stability of the double helix.
- The results suggest that 3,4-dihydroxyxanthone can intercalate into the base pairs of DNA.

**P100**

Pedagogical material for the teaching of Organic Chemistry in the primary level

Sérgio Leal* and João P. Leal

Faculdade de Ciências e Universidade de Lisboa, Portugal

**sergioleal20@gmail.com*

- Preliminary results indicate that students change their opinions after classes taught with different approaches. However, the main negative causes for the learning of Organic Chemistry remain: students' lack of commitment and the use, by teachers, of the same strategy to teach various contents.
- Students clearly prefer experimental lessons with an interactive component, especially after having experienced this type of class.
- Confirming previous findings, it seems that the use of technologies and laboratory work can make students more motivated and interested on Chemistry.

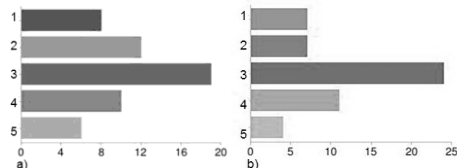


Figure 1: Answer to the question:

“Do you have difficulty in understanding aspects of Organic Chemistry?”

1- Not at all or very little ; 2 – Little ; 3 – Reasonably ; 4 – Fairly or very;
5 – Do not know

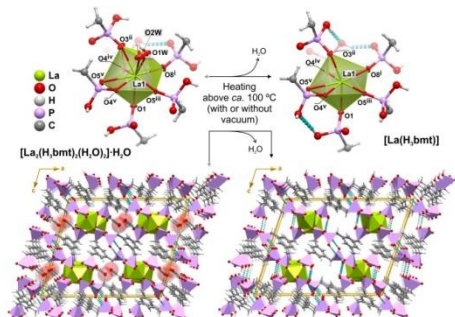
a) Before class was delivered ; b) After class

Novel lanthanide phosphonate MOFs: synthesis, crystal structures, photoluminescent and catalytic properties

Sérgio M. F. Vilela^{*}, Duarte Ananias, Ana C. Gomes, Anabela A. Valente, Luís D. Carlos, José A. S. Cavaleiro, João Rocha, João P. C. Tomé and Filipe A. Almeida Paz
University of Aveiro, Portugal

^{*}sergiovilela83@ua.pt

P101



- Isotypical 3D lanthanide-organic frameworks, formulated as $[\text{Ln}_2(\text{H}_3\text{bmt})_2(\text{H}_2\text{O})_2 \cdot \text{H}_2\text{O}]$ [where $\text{Ln}^{3+} = \text{La}^{3+}$ (1), Ce^{3+} (2), Pr^{3+} (3), Nd^{3+} (4), $(\text{La}_{0.95}\text{Eu}_{0.05})^{3+}$ (5) and $(\text{La}_{0.95}\text{Tb}_{0.05})^{3+}$ (6)], were prepared using typical hydrothermal conditions.
- Water molecules of 1 were easily removed by heating, obtaining its dehydrated form $[\text{Ln}(\text{H}_3\text{bmt})]$ (1-dehyd).
- Despite the removal of all water molecules, 1-dehyd retains crystallinity and the framework topology of 1.
- Photoluminescent studies showed that the dehydration of 5 promotes a drastic increase of the quantum efficiency.
- Compound 1 shows recyclability and excellent selectivity towards 2-methoxy-2-phenylethanol in the ring opening of styrene oxide.

The influence of microwave irradiation in the outcome of solid phase peptide synthesis

Sílvia Maia, Miguel Ángel, Fernandez and Paula Gomes^{*}

Faculdade de Ciências da Universidade do Porto, Portugal

^{*}pgomes@fc.up.pt

P102



Conventional SPPS

MW-assisted SPPS

- Study of the influence of microwave irradiation (MW) on the outcome of the solid-phase peptide synthesis (SPPS).
- Synthesis of the antimicrobial peptide, human lactoferrin (1-11), GRRRRSVQWCA, by conventional and MW-assisted SPPS, using a classic Fmoc/tBu SPPS orthogonal protection scheme.
- The crude peptides were analyzed and compared in terms of yield and purity degree.
- MW-SPPS yielded higher amounts of purer peptide.
- MW-SPPS allowed the synthesis to reach completion in 9 hours whereas 4 days were needed to complete the synthesis by the conventional approach.

Bisphenol-A adsorption onto activated carbon. Langmuir and Freundlich isotherms and kinetics

Sofia Amaro* and I. Macedo

University of Aveiro, Portugal

*sofia.amaro@ua.pt

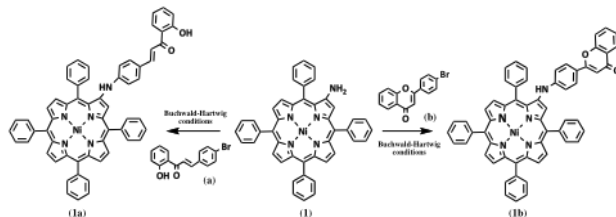
- Preparation of activated carbon from walnut shell with ZnCl_2 activation and carbonization under N_2 atmosphere.
- Study of adsorption kinetics: first, second and pseudo-second order models are used.
- Study of adsorption isotherms: fit to Langmuir and Freundlich models.
- First order kinetics and Langmuir isotherm models fit best to the experimental results.
- Comparison of adsorption performance of walnutshell-based activated carbon with data in literature.

Synthesis and evaluation of the biological activity of new flavonoid-porphyrin dyads

Sónia P. Lopes, Diana C. G. A. Pinto*, Maria A. F. Faustino, Artur M. S. Silva, Maria G. P. M. S. Neves and José A. S. Cavaleiro

University of Aveiro, Portugal

*diana@ua.pt



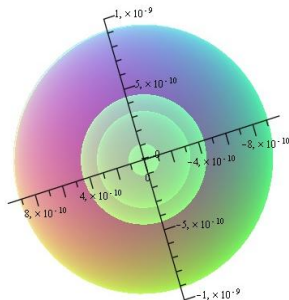
- Dyads **1a** and **1b** were obtained in good yields.
- Experimental synthesis conditions will be discussed.
- NMR characterization confirmed the proposed structures.
- Dyads DNA intercalating activity was evaluated.

Application of Scientific Computation in the Chemistry Education

Stéfano Araújo Novais* and Fabio da Silva Miranda

Universidade Federal Fluminense, Niterói, Rio de Janeiro, Brazil.

*stefano_novais@id.uff.br



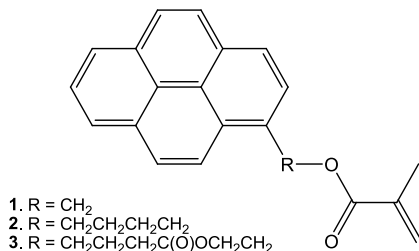
- The utilization of scientific computation provides a differential formation for the chemistry student.
- Mathematical softwares, like MAPLE, may generate a better and dynamic view from the atomic orbitals surfaces.
- Multiplication of the wave functions, radial and angular, give us the Ψ wave function. With MAPLE, we can plot it and analyse the characteristics of the atomic orbital surface.
- It's also possible to analyse the radial and the angular wave function separately, as the radial distribution function.
- With easy commands, the professor can select the content required for your classes, depending on the level of the class.

Biocompatible fluorescence based temperature sensor

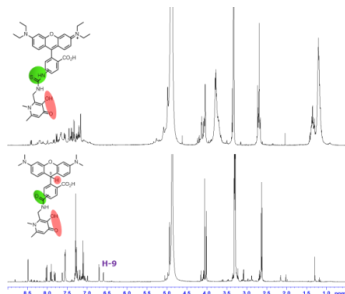
Suzete Almeida*, Sérgio Alves, José M. G. Martinho, José P. S. Farinha and Carlos Baleizão

Instituto Superior Técnico, Universidade Técnica de Lisboa, Portugal

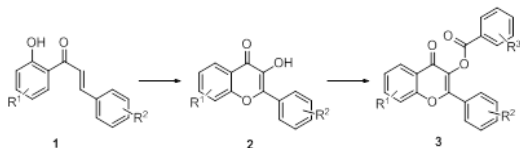
suzetcv@hotmail.com



- Synthesis of different pyrene derivatives bearing methacrylates groups.
- Preparation of water-soluble thermoresponsive biocompatible copolymers via ATRP.
- The monomers are based in (ethylene oxide)methacrylate co-monomers, and the polymer was labeled with pyrene.
- The lower critical solution temperature (LCST) can be tuned by adjusting the ratio of the two monomers.
- The collapse/expansion of the polymer chains changes the pyrene excimer-to-monomer intensity ratio.

**P107****Palladium/ carbon catalyzed hydrogenolysis and hydrogenation of xanthene type fluorophores:****A study by NMR**Tânia Moniz^{*}, Carla Queirós, Ana M. G. Silva, Galya Ivanova, Baltazar de Castro and Maria Rangel*Instituto de Ciências Biomédicas de Abel Salazar, Portugal.***tania.moniz@alunos.fc.up.pt*

- Synthesis and characterization of novel xanthene ligands containing a 3-hydroxy-4-pyridinone or a catechol chelating unit for use as chemosensors and iron (III) chelators.
- Synthesis of these ligands involves the coupling reaction of the xanthene fluorescent platform with the chelating unit, followed by the removal of the protecting groups.
- Deprotection step was performed by dissolution of the protected ligand in a mixture of methanol/HCl and placed under a hydrogen atmosphere over 10% Pd/C.
- The process is in agreement with green chemistry principles as a more ecofriendly methodology.
- NMR spectroscopy revealed that in deprotection conditions the benzyl groups are successfully removed but in some cases it was also observed the reduction of the double bond at position 9 of the xanthene ring, more or less favoured, depending on substituent groups introduced in the periphery of the ring.

**P108****Synthesis and anticancer activity of a selection oquercetin analogues and their precursors**T. A. Dias^{*}, C. L. Duarte, M. F. Proença, C. F. Lima and C. Pereira-Wilson*University of Minho, Braga, Portugal***pg16461@alunos.uminho.pt*

- The flavonoid core is present in many natural products and is associated to a broad range of biological activities.
- Quercetin, a widely studied polyphenolic compound also shows diverse biological activities, including anticancer effects.
- Different chalcones, flavanols and derivatives were prepared in a straightforward route, from commercially available starting materials.
- A selection of compounds was tested for their anticancer activity.

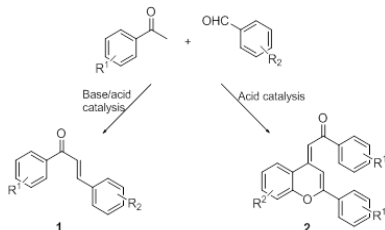
Synthesis of new molecules with the 4*H*-chromen-4-ylidene scaffold

T. A. Dias* and M. F. Proença

University of Minho, Braga, Portugal

*pg16461@alunos.uminho.pt

P109



- Compounds with the chromene scaffold usually display important pharmacological properties.
- Only a few reports are known on the association of the chromene moiety to a 4-methylene substituent.
- Several chalcones were prepared from polyphenolic aldehydes and acetophenone, with acid catalysis.
- A new 4*H*-chromen-4-ylidene structure was isolated from the reaction of acetophenone and salicylaldehydes under appropriate reaction conditions.

Nutritional value of Senegalese sole (*Solea senegalensis* Kaup, 1858) fed with eco-friendly diets

Telmo J. R. Fernandes, Sílvia D. Campos, Eduarda M. Cabral, Manuela Castro-Cunha, Luísa M. P. Valente and

M. Beatriz P. P. Oliveira

Faculdade de Farmácia, Universidade do Porto, Portugal

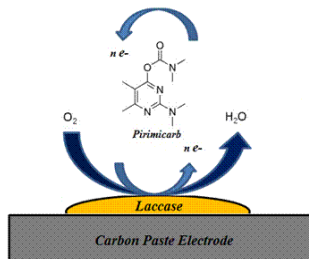
*beatoliv@ff.up.pt

P110

- A fishmeal based diet (FM) was compared to isonitrogenous and isoenergetic diets containing **increasing levels** of a blend of **plant protein (PP) sources**, (50, 75 and 100% PP) in order to evaluate possible alterations on **lipid content** and **fatty acid profile**.
- Concerning muscle and skin tissues, total lipids were similar among the different diets while regarding liver its fat content was significantly higher ($P < 0.05$) in PP50 (25.59%) and PP100 (28.57%) groups.
- Fatty acid profiles, achieved by GC-FID technique, were significantly affected by the different levels of PP sources, mainly in liver: PP50 showed higher levels of Saturated Fatty Acids (34.77%), Monounsaturated Fatty Acids (46.35%), DHA/EPA ratio (15.62) and reduced contents of Polyunsaturated Fatty Acids (16.40%). No major alterations were found in muscle fatty acid profile.
- In conclusion, senegalese sole can reach the market size with blends of plant protein up to 75% incorporation level without compromising muscle lipid content and fatty acid profile.

P111 Biosensor development for pirimicarb pesticide determination

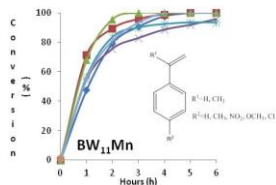
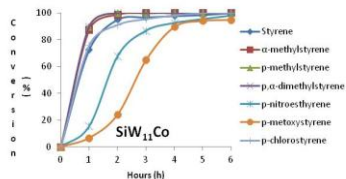
Thiago M. B. F. Oliveira*, Simone Morais, Maria F. Barroso, Pedro de Lima-Neto, Adriana N. Correia, Maria B. P. P. Oliveira and Cristina Delerue-Matos
 Instituto Superior de Engenharia do Porto, Portugal
 *thiagomielle@yahoo.com.br



- The selected sensing element of the developed biosensor is laccase, a copper oxidoreductase enzyme which is a highly specific bioreceptor for phenolic compounds.
- A carbon paste electrode was used as the working electrode.
- Quantification is based on the inhibition of the catalysis reaction performed by laccase.

P112 Transition Metal Substituted Polyoxometalates: Potentialities in Oxidation by Hydrogen Peroxide

Tiago A.G. Duarte*, Ana C. Estrada, Isabel C.M. Santos, Mário M.Q. Simões, M. Graça P.M.S. Neves, Ana M.V. Cavaleiro and José A.S. Cavaleiro
 University of Aveiro, Portugal
 *a39903@ua.pt



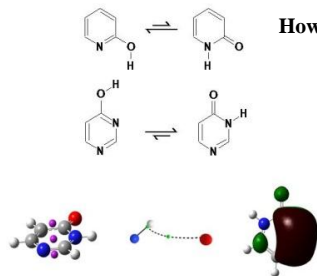
- The oxidation of styrene and styrene derivatives was performed in the presence of several polyoxometalates with H_2O_2 ;
- The best catalysts were $BW_{11}Mn$ and $SiW_{11}Co$, for all the substrates;
- After 1 h of reaction, the substrates with an α -methyl group were almost completely oxidized;
- The carbon-carbon double bond cleavage was always the main oxidation pathway.

From 2-hydroxypyridine to 4(3*H*)-pyrimidinone: The role of aromaticity, hydrogen bonds and substituent effects in tautomeric equilibrium

Tiago L.P. Galvão*, Inês M. Rocha and Manuel A.V. Riveiro da Silva

Faculty of Science, University of Porto, Portugal.

*tlpgalvao@gmail.com



How to control the gaseous-phase keto-enol tautomeric equilibrium of pyridine and pyrimidine derivatives?

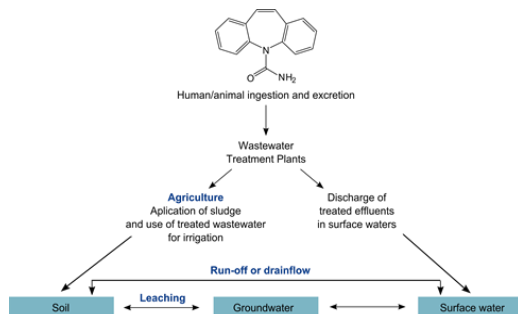
- Molecular energetics: gaseous-phase tautomeric equilibrium and thermodynamic changes of appropriate reactions.
- NICS: aromaticity.
- QTAIM: intramolecular hydrogen bonds.
- NBO analysis: electronic delocalization.
- The conclusions obtained for these model systems allow to understand the keto-enol tautomeric equilibrium in nitrogen rings and justify the tautomeric preference in pyrimidine nucleobases.

Fate of the antiepileptic drug carbamazepine at the water/soil interface

Vânia Calisto* and Valdemar I. Esteves

University of Aveiro, Aveiro, Portugal

*vania.calisto@ua.pt



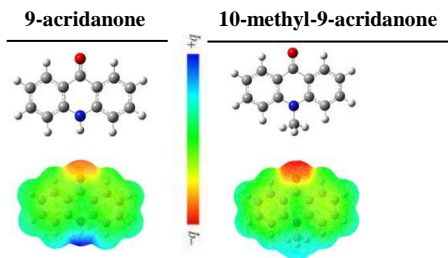
- The adsorption behavior of carbamazepine onto agricultural soils is dependent on the type of fertilization.
- Carbamazepine is not extensively sorbed onto agricultural soils.
- Contaminated soils may be a potential source of carbamazepine into ground and surface waters by run-off and leaching.
- Environmental risks involving the application of WWTP's effluents and sludge for agricultural purposes should be investigated.

Structural and thermophysical studies of 9-acridanone and 10-methyl-9-acridanone

Vera L. S. Freitas*, Paulo J. O. Ferreira and Maria D. M. C. Ribeiro da Silva

Faculdade de Ciências, Universidade do Porto, Portugal

*vera.freitas@fc.up.pt



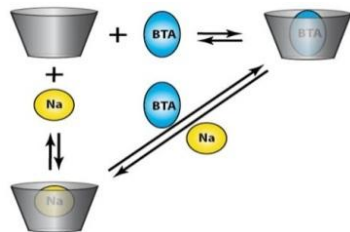
- Experimental and computational studies of 9-acridanone and 10-methyl-9-acridanone.
- Determination of the enthalpy of sublimation of acridanones, using the Calvet microcalorimetry technique.
- Heat capacity of gaseous acridanone molecules derived from statistical thermodynamics, using the vibrational frequencies determined from DFT calculations (B3LYP/6-31G(d)).
- Geometrical parameters of the isolated acridanone structures optimized at the B3LYP/6-31G(d) level of theory.
- Electrostatic potential map of acridanones from total self consistent field density, based on Natural Bond Orbital (NBO) theory.

Host: guest binding constant influenced by the host counterion

Vitor Francisco*, Nuno Basilio and Luis Garcia-Rio

Universidad de Santiago, Santiago de Compostela, Spain.

*francisco.vms@gmail.com



- In absence of added salts and at neutral pH, the cavity of *p*-sulfonatocalix[4]arene (SC4) fully binds an Na⁺ counterion.
- ITC experiments have been done to measure the binding constant between SC4 and BTA
- The binding constant for the complexation of BTA by SC4 depends on the concentration of the host
- Is necessary to extrapolate the binding constants to zero calixarene concentration in order to get the true equilibrium constant.

The mathematical description for the electrochemical synthesis of heterocyclic compounds in galvanostatic mode

Volodymyr V. Tkach^{*}, Vasyl V. Nechyporuk and Petro I. Yagodynets

Chernivtsi National University, Ukraine

**nightwatcher2401@gmail.com*

- The galvanostatic electropolymerization of heterocyclic compounds can be described mathematically with the three-dimensioned model
- The mathematical model for this system can be analyzed by using the linear stability theory and bifurcation analysis
- The steady-state stability region in this system is limited by the critical of diffusion parameter κ , which depends on the other parameters' values. It can be shown that the steady-state in this system will be stable in cause of the distraction between the adsorbed particles.
- The oscillatory instability, observed during the galvanostatic polymerization of heterocyclic compounds is caused by attraction between the adsorbed particles and the influences of the electropolymerization to the double electric layer (DEL).
- The voltamperogram of this synthesis gains its N-shaped form in the conditions of monotonic instability, which occurs when the diffusion parameter κ gains its critical value.