

REVUE ROUMAINE DE CHIMIE (ROUMANIAN JOURNAL OF CHEMISTRY)

Tome 60, N^{os} 2-3

Février-Mars 2015

Professor Zeno SIMON

Rev. Roum. Chim., 2015, 60(2-3), 105-120

Alexandru T. BALABAN

To be or not to be ... aromatic?

Rev. Roum. Chim., 2015, 60(2-3), 121-140

Zeno SIMON

Octogenarian retrospective

Rev. Roum. Chim., 2015, 60(2-3), 141-149

PAPERS

Maria MRACEC and Mircea MRACEC

QSAR study of 4-hydroxybiphenyl derivatives active on ER β subtype

Statistical indices of the best regression are the following:

$n = 61$; $r^2 = 0.871$; $r^2_{adj} = 0.862$; $see = 0.238$;

$F(4,56) = 94.37$; $p < 0.00000$

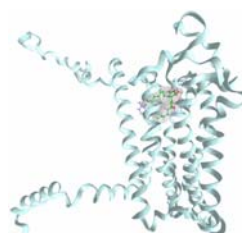
$q^2_{LOO} = 0.856$; $SDEP = 0.246$

Rev. Roum. Chim., 2015, 60(2-3), 151-160

Key words: 4-hydroxybiphenyl derivatives, QSAR, ER β subtype antagonist, AM1.

**Ana BOROTA, Alina BORA, Liliana HALIP,
Ramona CURPAN, Maria MRACEC and
Mircea MRACEC**

3D homology model of the human prostanoid receptor hEP3 and docking studies

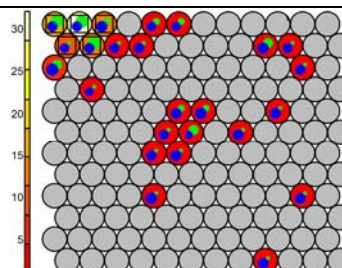


Rev. Roum. Chim., 2015, 60(2-3), 161-166

Key words: prostanoid EP3 receptor, prostaglandin PGE2, homology model, molecular docking.

**Sorin AVRAM, Stefana AVRAM,
Luminita CRISAN, Liliana PACUREANU,
Ludovic KURUNCZI and Alina BORA**

Self-organizing map classification model for the prediction of MEK1 inhibitors

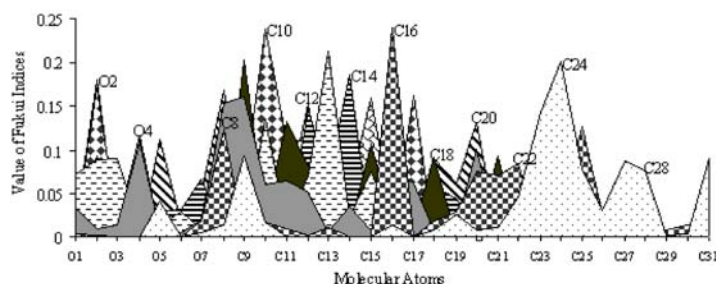


Rev. Roum. Chim., 2015, 60(2-3), 167-173

Key words: self-organizing map, MEK1, scaffold hopping, virtual screening, angiogenesis.

**Alina BORA, Sorin AVRAM,
Luminita CRISAN, Liliana HALIP,
Ramona CURPĂN, Liliana PACUREANU and
Ionel CIUCANU**

Theoretical investigations of quercetin and its analogues as anticancer agents

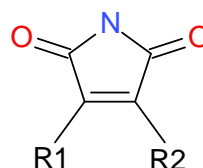


Key words: flavonoid, quercetin, electronic parameter, density functional theory, ADME.

Rev. Roum. Chim., 2015, 60(2-3), 175-181

**Luminita CRISAN, Sorin AVRAM,
Alina BORA, Ludovic KURUNCZI and
Liliana PACUREANU**

3D-QSAR study of maleimide analogues as glycogen synthase kinase-3 (GSK-3) inhibitors using CoMSIA approach

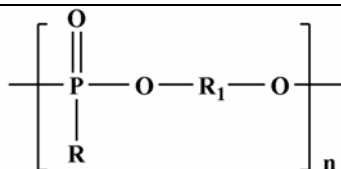


Key words: 3D QSAR, COMSIA, maleimide.

Rev. Roum. Chim., 2015, 60(2-3), 183-188

**Luminita CRISAN, Smaranda ILIESCU and
Simona FUNAR-TIMOFEI**

The investigation of structure-flammability relationships of polyphosphonates by PLS analysis

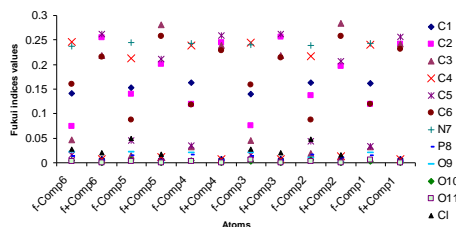


Key words: polyphosphonates, LOI, PLS, internal validation, external validation.

Rev. Roum. Chim., 2015, 60(2-3), 189-195

**Mihaela PETRIC, Manuela CRISAN,
Luminita CRISAN and Gheorghe ILIA**

Synthesis and theoretical study on some new phosphoramidates

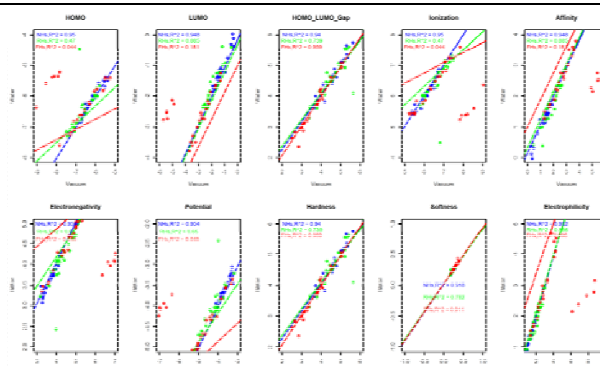


Key words: phosphoramidates, liquid-liquid system, liquid-solid system, HOMO-LUMO, Fukui indices.

Rev. Roum. Chim., 2015, 60(2-3), 197-203

**Ramona CURPĂN, Sorin AVRAM,
Liliana HALIP and Cristian BOLOGA**

Biological promiscuity of HTS hits evaluated via chemical reactivity descriptors

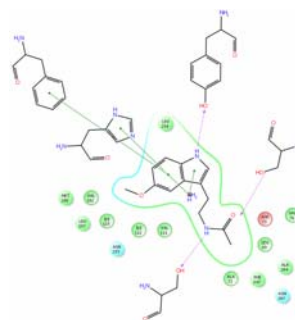


Rev. Roum. Chim., 2015, 60(2-3), 205-211

Key words: promiscuity, frequent hitters, HTS, reactivity descriptors, DFT.

Liliana HALIP, Ramona CURPĂN,
Ana BOROTA and Alina BORA

Insight the binding site of human melatonin
MTR1A receptor



Rev. Roum. Chim., 2015, 60(2-3), 213-218

Key words: melatonin receptor, MTR1A, comparative modeling, molecular docking.

Cristian G. BOLOGA, Oleg URSU,
Liliana HALIP, Ramona CURPĂN and
Tudor I. OPREA

Chemical and biological descriptor integration
improves computational modeling of *in vivo* rat
toxicity

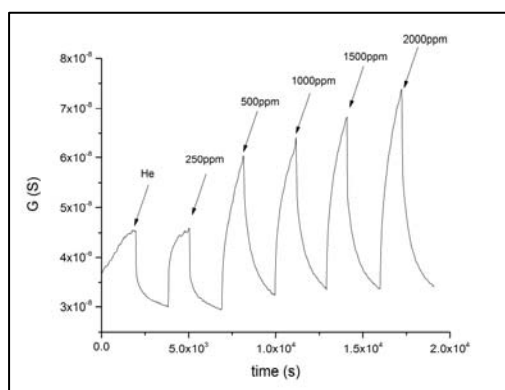
Molecular fragments favoring lower toxicities		Molecular fragments favoring higher toxicities	
	LD ₅₀ = 3300 mg/kg		LD ₅₀ = 160 mg/kg
	LD ₅₀ = 10000 mg/kg		LD ₅₀ = 10.5 mg/kg

Rev. Roum. Chim., 2015, 60(2-3), 219-226

Key words: QSAR, PLS, toxicity, computational toxicology, rat LD₅₀, HTS, biological descriptors.

Paul CHESLER, Cristian HORNOIU,
Veronica BRATAN, Cornel MUNTEANU,
Mariuca GARTNER and Niculae I. IONESCU

Carbon monoxide sensing properties of TiO₂

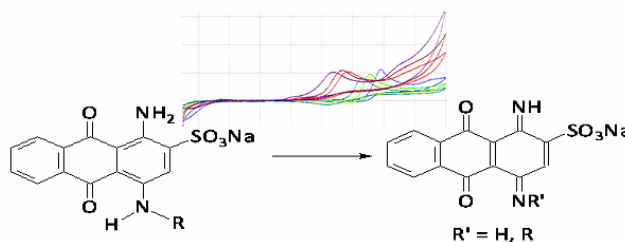


Rev. Roum. Chim., 2015, 60(2-3), 227-232

Key words: CO sensor, TiO₂, SEM, XRD, mechanism.

Florentina Daniela MUNTEANU,
Andreia SANISLAV and
Michaela Dina STANESCU

Coupled electrochemical and enzymatic
degradation of two anthraquinone dyes

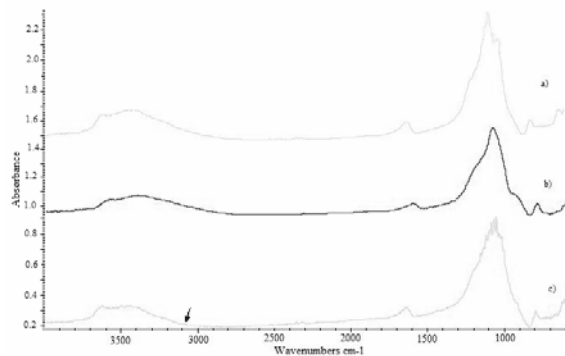


Rev. Roum. Chim., 2015, 60(2-3), 233-239

Key words: electrochemical oxidation, aminoanthraquinone dyes, Laccase, Michaelis-Menten kinetics.

Claudia COBZARU, Adriana MARINOIU and Corina CERNATESCU

Sorption of vitamin C on acid modified clinoptilolite

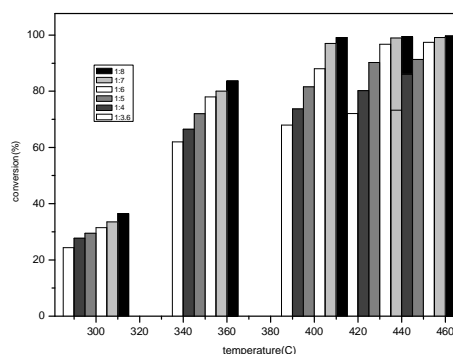


Rev. Roum. Chim., 2015, 60(2-3), 241-247

Key words: native tuff, modified clinoptilolite, vitamin C, sorption process.

Adriana MARINOIU, Claudia COBZARU, Mircea RACEANU, Mihai VARLAM, Elena CARCADEA, Corina CERNATESCU and Ioan STEFANESCU

Carbon dioxide conversion to methane over supported nickel base catalysts

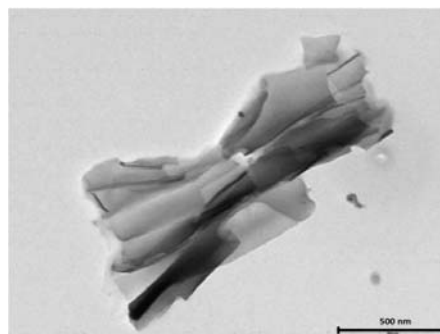


Rev. Roum. Chim., 2015, 60(2-3), 249-256

Key words: nickel base catalysts, carbon dioxide hydrogenation, CO₂ conversion.

Boldizsár NAGY, Carmen MÂNZATU, Anamaria TÖRÖK, Cerasella INDOLEAN, Andrada MÁICĂNEANU, Szende TONK and Cornelia MAJDIK

Isotherm and thermodynamic studies of Cd(II) removal process using chemically modified lignocellulosic adsorbent

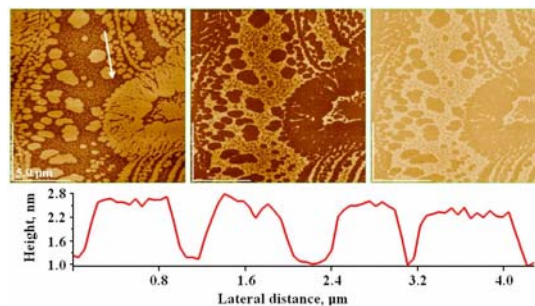


Rev. Roum. Chim., 2015, 60(2-3), 257-264

Key words: sawdust, cadmium, chemical treatment, isotherms, thermodynamics.

Petre T. FRANGOPOL, David Allan CADENHEAD, Gheorghe TOMOAI, Aurora MOCANU and Maria TOMOAI-COTISEL

The effect of procaine on lipid domains investigated by contact mode atomic force microscopy

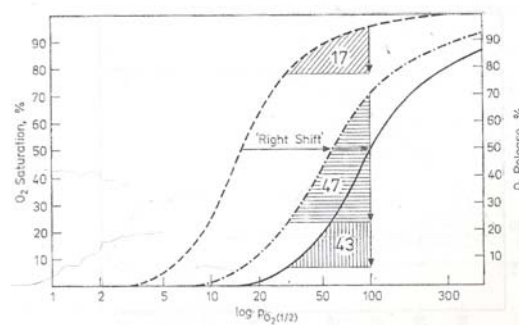


Rev. Roum. Chim., 2015, 60(2-3), 265-273

Key words: lipid domains, DPPC, procaine, LB-monolayers, cm-AFM.

Claude NICOLAU

Modulation of oxygen release by red blood cells:
physiological and therapeutic perspectives



Rev. Roum. Chim., 2015, 60(2-3), 275-282

Key words: oxygen transport, hemoglobin, oxygen-affinity, allosteric effectors, cardiac output.
