

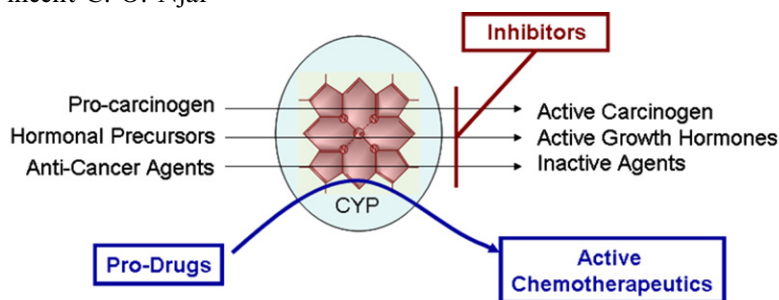
Contents

REVIEW

Targeting cytochrome P450 enzymes: A new approach in anti-cancer drug development

pp 5047–5060

Robert D. Bruno and Vincent C. O. Njar*



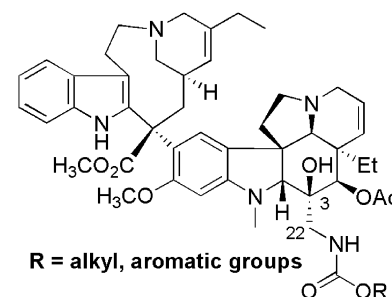
ARTICLES

Synthesis and structure–activity relationships study of novel anti-tumor carbamate anhydrovinblastine analogues

pp 5061–5075

Yong Shao, Hong Ding, Weidong Tang, Liguang Lou* and Lihong Hu*

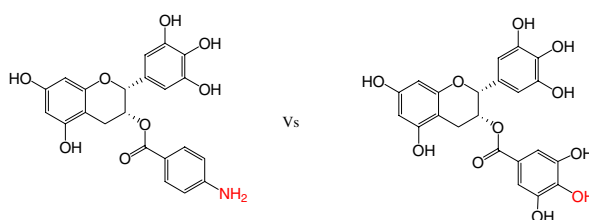
A new series of 3-demethoxycarbonyl-3-carbamate methyl anhydrovinblastine derivatives were synthesized and evaluated the cytotoxic activity in vitro against A549 and HeLa cell lines (IC_{50} : 38–609 nM and 6–387 nM, respectively). The SARs of this new series are reported.



A para-amino substituent on the D-ring of green tea polyphenol epigallocatechin-3-gallate as a novel proteasome inhibitor and cancer cell apoptosis inducer

pp 5076–5082

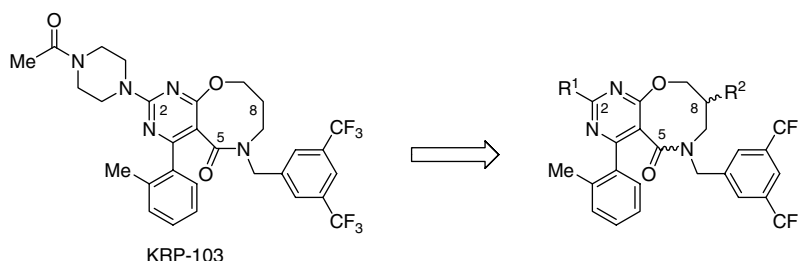
Kumi Osanai, Kristin R. Landis-Piwowar, Q. Ping Dou and Tak Hang Chan*



Analysis of crucial structural requirements of 2-substituted pyrimido[4,5-*b*][1,5]oxazocines as NK₁ receptor antagonist by axially chiral derivatives

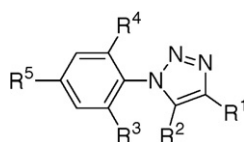
pp 5083–5089

Shigeki Seto* and Jun Asano


Synthesis, 3D-QSAR, and docking studies of 1-phenyl-1*H*-1,2,3-triazoles as selective antagonists for β_3 over $\alpha_1\beta_2\gamma_2$ GABA receptors

pp 5090–5104

Mohammad Sayed Alam, Jia Huang, Fumiyo Ozoe, Fumio Matsumura and Yoshihisa Ozoe*



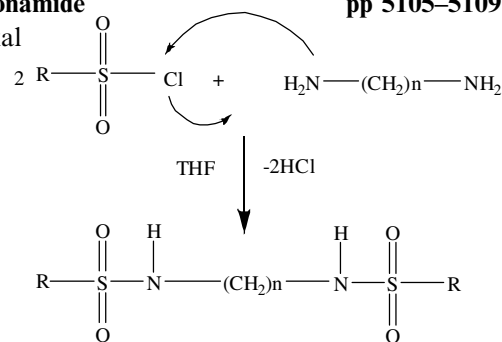
1-Phenyl-1*H*-1,2,3-triazoles showed higher affinity for human β_3 than for $\alpha_1\beta_2\gamma_2$ GABA receptors. 3D-QSAR and molecular docking studies revealed the favorable and unfavorable moieties of 1-phenyl-1*H*-1,2,3-triazole antagonists for high affinity and their putative binding site in the receptors.

Synthesis, characterization and antimicrobial activity of new aliphatic sulfonamide

pp 5105–5109

Neslihan Özbek, Hikmet Katircioğlu, Nurcan Karacan* and Tülay Baykal

Preparation of symmetric aliphatic sulfonamide.

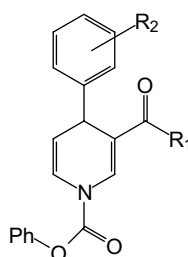


Preparation of symmetric aliphatic sulfonamide

Structure–activity relationships of novel *N*-acyloxy-1,4-dihydropyridines as *P*-glycoprotein inhibitors

pp 5110–5113

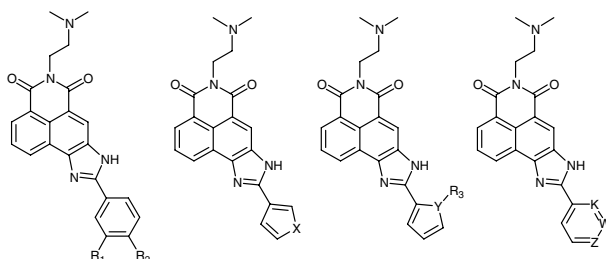
Burkhardt Voigt, Claudius Coburger, Josef Monár and Andreas Hilgeroth*



Molecular design, chemical synthesis, and biological evaluation of ‘4-1’ pentacyclic aryl/heteroaryl-imidazonaphthalimides

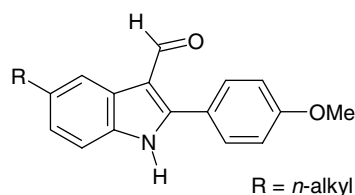
pp 5114–5121

Feng Li, Jingnan Cui,* Lianying Guo, Xuhong Qian,* Weimin Ren, Kewei Wang and Fengyu Liu

**Antimitotic activities of 2-phenylindole-3-carbaldehydes in human breast cancer cells**

pp 5122–5136

Doris Kaufmann, Michaela Pojarová, Susanne Vogel, Renate Liebl, Robert Gastpar, Dietmar Gross, Tsuyuki Nishino, Tobias Pfaller and Erwin von Angerer*

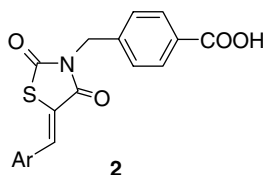


5-*n*-Alkyl-2-phenylindole-3-carbaldehydes strongly inhibit the growth of MDA-MB 231 breast cancer cells (IC_{50} : 5–20 nM) through interference with tubulin polymerization and subsequent cell cycle arrest in G_2/M phase.

5-Arylidene-2,4-thiazolidinediones as inhibitors of protein tyrosine phosphatases

pp 5137–5149

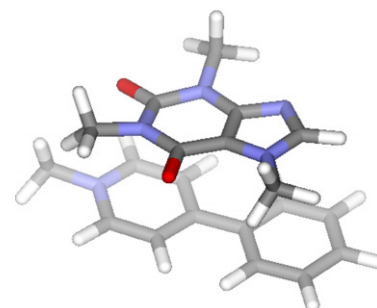
Rosanna Maccari,* Paolo Paoli, Rosaria Ottanà, Michela Jacomelli, Rosella Ciurleo, Giampaolo Manao, Theodora Steindl, Thierry Langer, Maria Gabriella Vigorita and Guido Camici

**Impaired mutagenic activities of MPDP⁺ (1-methyl-4-phenyl-2,3-dihydropyridinium) and MPP⁺ (1-methyl-4-phenylpyridinium) due to their interactions with methylxanthines**

pp 5150–5157

Katarzyna Ulanowska, Jacek Piosik, Anna Gwizdek-Wisniewska and Grzegorz Węgrzyn*

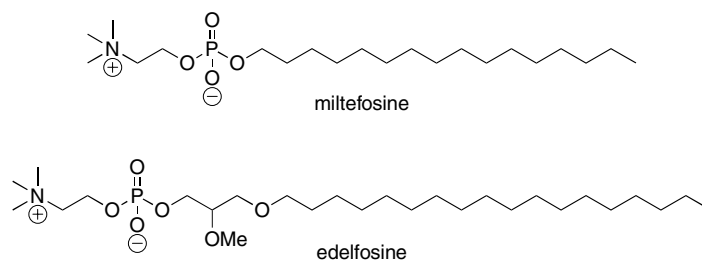
Formation of stacking complexes between MPDP⁺ or MPP⁺ and methylxanthines attenuate biological activities of these toxins.



Synthesis, antifungal and antimicrobial activity of alkylphospholipids

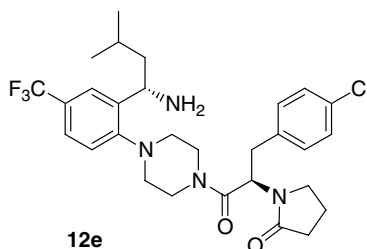
pp 5158–5165

Daniel Obando, Fred Widmer, Lesley C. Wright, Tania C. Sorrell and Katrina A. Jolliffe*

**Pyrrolidinones as orally bioavailable antagonists of the human melanocortin-4 receptor with anti-cachectic activity**

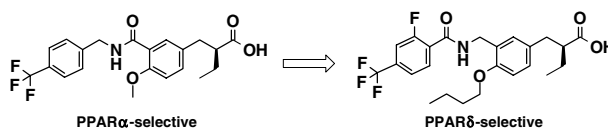
pp 5166–5176

Joe A. Tran, Fabio C. Tucci, Wanlong Jiang, Dragan Marinkovic, Caroline W. Chen, Melissa Arellano, Stacy Markison, Beth A. Fleck, Jenny Wen, Nicole S. White, Joseph Pontillo, John Saunders, Daniel Marks, Sam R. Hoare, Ajay Madan, Alan C. Foster and Chen Chen*

**Design, synthesis, and evaluation of potent, structurally novel peroxisome proliferator-activated receptor (PPAR) δ -selective agonists**

pp 5177–5190

Jun-ichi Kasuga, Izumi Nakagome, Atsushi Aoyama, Kumiko Sako, Michiyasu Ishizawa, Michitaka Ogura, Makoto Makishima, Shuichi Hirono, Yuichi Hashimoto and Hiroyuki Miyachi*

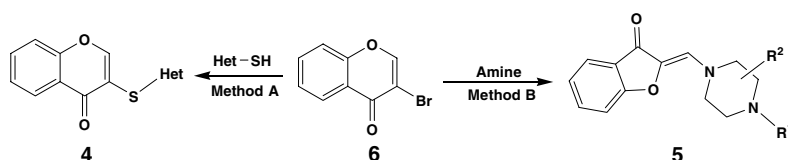


A series of 3-(4-alkoxyphenyl)propanoic acid derivatives was prepared as candidate peroxisome proliferator-activated receptor (PPAR) δ -selective agonists.

Design, syntheses, and antitumor activity of novel chromone and aurone derivatives

pp 5191–5197

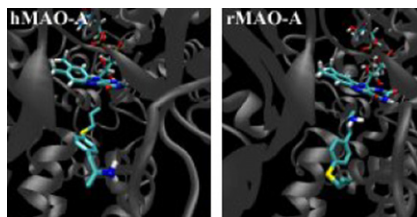
Wei Huang, Ming-Zhen Liu, Yan Li,* Ying Tan and Guang-Fu Yang*



Human and rat monoamine oxidase-A are differentially inhibited by (*S*)-4-alkylthioamphetamine derivatives: Insights from molecular modeling studies

pp 5198–5206

Angélica Fierro, Mauricio Osorio-Olivares, Bruce K. Cassels, Dale E. Edmondson, Silvia Sepúlveda-Boza and Miguel Reyes-Parada*

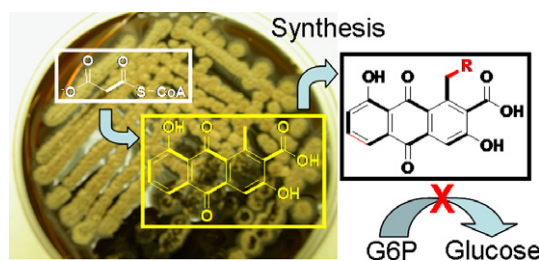


Amphetamine derivatives differentially inhibit human or rat MAO-A and exhibit different binding modes into the active site of both enzymes.

Structure–activity relationships of semisynthetic mumbaistatin analogs

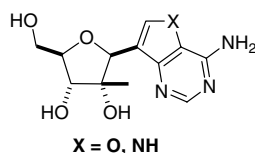
pp 5207–5218

Taek Soon Lee, Abhirup Das and Chaitan Khosla*

**Synthesis and HCV inhibitory properties of 9-deaza- and 7,9-dideaza-7-oxa-2'-*C*-methyladenosine**

pp 5219–5229

Gabor Butora,* David B. Olsen, Steven S. Carroll, Daniel R. McMasters, Christoph Schmitt, Joseph F. Leone, Mark Stahlhut, Christine Burlein and Malcolm MacCoss

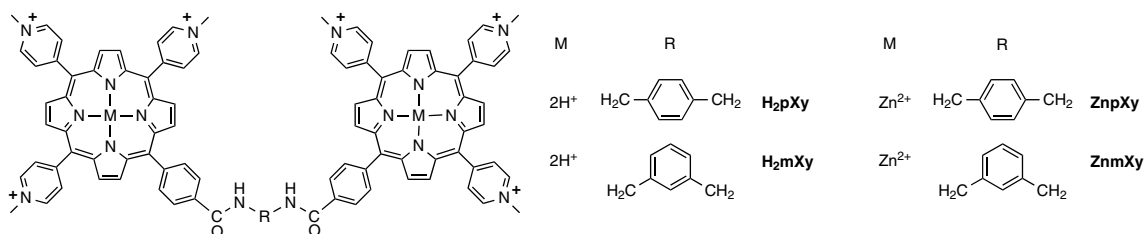


2'-*C*-Methyl analogs of 7-oxa- and 7-aza-7,9-dideazadenosines were synthesized and their metabolic stability as well as antiviral (HCV) properties evaluated.

Synthetic control of interchromophoric interaction in cationic bis-porphyrins toward efficient DNA photocleavage and singlet oxygen production in aqueous solution

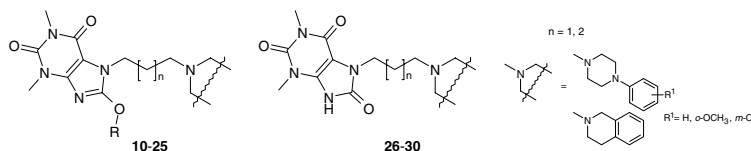
pp 5230–5238

Yoshinobu Ishikawa,* Naoki Yamakawa and Tadayuki Uno*



7-Arylpiperazinylalkyl and 7-tetrahydroisoquinolylalkyl derivatives of 8-alkoxy-purine-2,6-dione and some of their purine-2,6,8-trione analogs as 5-HT_{1A}, 5-HT_{2A}, and 5-HT₇ serotonin receptor ligands pp 5239–5250

Grażyna Chłoń-Rzepa, Paweł Żmudzki, Paweł Zajdel, Andrzej J. Bojarski, Beata Duszyńska, Agnieszka Nikiforuk, Ewa Tatarczyńska and Maciej Pawłowski*



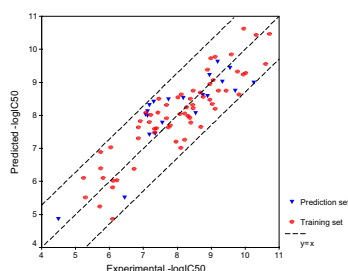
A series of new arylpiperazinylalkyl and tetrahydroisoquinolylalkyl analogs of 8-alkoxy-1,3-dimethyl-3,7-dihydro-purine-2,6-dione (**10–25**) and 1,3-dimethyl-7,9-dihydro-3H-purine-2,6,8-trione (**26–30**) were synthesized and their 5-HT_{1A}, 5-HT_{2A}, and 5-HT₇ receptor affinities were determined. Selected compound was evaluated in behavioral models of depression and anxiety.



QSAR study of selective ligands for the thyroid hormone receptor β

pp 5251–5261

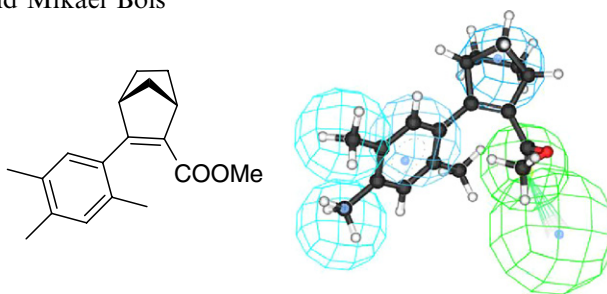
Huanxiang Liu and Paola Gramatica*



Predicted $-\log IC_{50}$ values versus experimental values for training set and prediction set (Two side lines express the confidence interval of 95%).

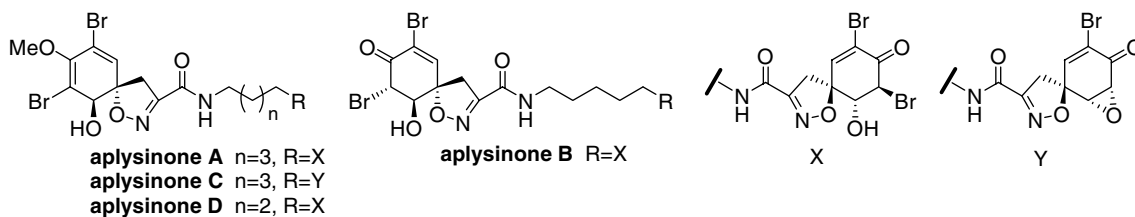
QSAR studies and pharmacophore identification for arylsubstituted cycloalkenecarboxylic acid methyl esters with affinity for the human dopamine transporter pp 5262–5274

Helena S. Christensen, Søren V. Boye, Jacob Thinggaard, Steffen Sinning, Ove Wiborg, Birgit Schiøtt* and Mikael Bols*



Cytotoxic dibromotyrosine-derived metabolites from the sponge *Aplysina gerardogreeni* pp 5275–5282

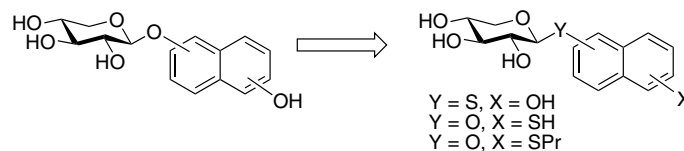
Claudia J. Hernández-Guerrero, Eva Zubía,* María J. Ortega and J. Luis Carballo



Effects of oxygen–sulfur substitution on glycosaminoglycan-priming naphthoxylosides

pp 5283–5299

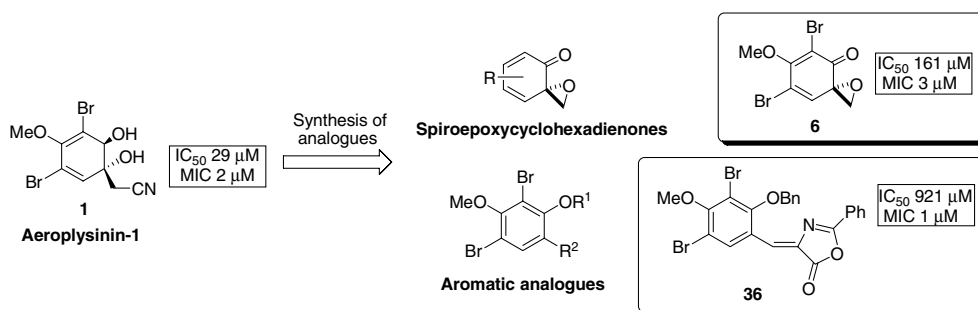
Mårten Jacobsson, Katrin Mani and Ulf Ellervik*



Antiangiogenic versus cytotoxic activity in analogues of aeroplysinin-1

pp 5300–5315

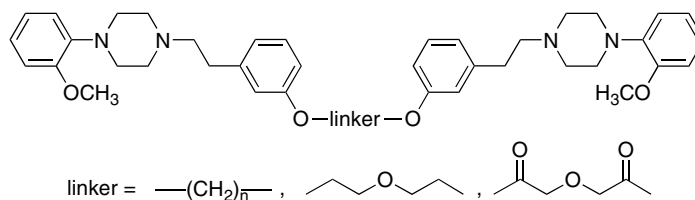
Rubén Córdoba,* Nélida Salvador Tormo, Antonio Fernández Medarde and Joaquín Plumet*



Bivalent ligand approach on 4-[2-(3-methoxyphenyl)ethyl]-1-(2-methoxyphenyl)piperazine: Synthesis and binding affinities for 5-HT₇ and 5-HT_{1A} receptors

pp 5316–5321

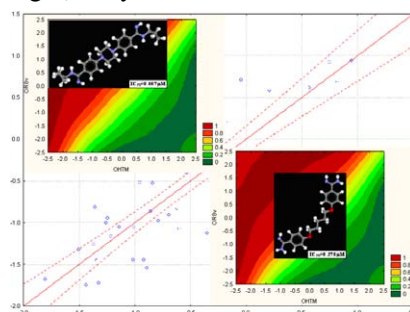
Marcello Leopoldo,* Enza Lacivita, Nicola A. Colabufo, Mauro Niso, Francesco Berardi and Roberto Perrone



Computational modeling tools for the design of potent antimalarial bisbenzamides: Overcoming the antimalarial potential of pentamidine

pp 5322–5339

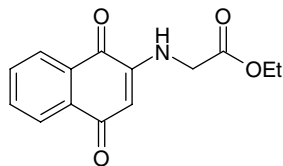
Maykel Cruz-Monteagudo, Fernanda Borges, Maykel Perez González* and M. Natália Dias Soeiro Cordeiro*



The 1,4-naphthoquinone scaffold in the design of cysteine protease inhibitors

pp 5340–5350

Cláudia Valente, Rui Moreira,* Rita C. Guedes, Jim Iley,* Mohammed Jaffar and Kenneth T. Douglas

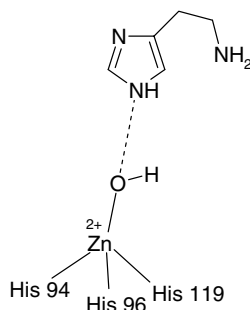


1,4-Naphthoquinone derivatives were found to be irreversible inhibitors for papain and bovine spleen cathepsin B. The chemical reactivity of the compounds towards cysteine as a model thiol is dependent on the naphthoquinone LUMO energy, whereas papain inactivation is not.

Carbonic anhydrase activators: The first activation study of the human secretory isoform VI with amino acids and amines

pp 5351–5357

Isao Nishimori, Saburo Onishi, Daniela Vullo, Alessio Innocenti, Andrea Scozzafava and Claudiu T. Supuran*

**OTHER CONTENTS****Bioorganic & Medicinal Chemistry Reviews and Perspectives**
Summary of instructions to authorspp 5358–5360
p I

*Corresponding author

i* Supplementary data available via ScienceDirect

COVER

L-Phenylalanine is a good activator of carbonic anhydrase (CA) isozymes II and VI. The figure shows the activator bound to CA II ($K_A = 13$ nM), as determined by X-ray crystallography. In CA VI all amino acid involved in the binding of the activator are the same as for CA II, except Asn67 which is Gln67. This leads to a diminished affinity of the activator for the enzyme active site ($K_A = 1.23$ μ M) [Nishimori, I.; Onishi, S.; Vullo, D.; Innocenti, A.; Scozzafava, A.; Supuran, C. T. *Bioorg. Med. Chem.* **2007**, *15*, 5351–5357].

Indexed/Abstracted in: Beilstein, Biochemistry & Biophysics Citation Index, CANCERLIT, Chemical Abstracts, Chemistry Citation Index, Current Awareness in Biological Sciences/BIODATA, Current Contents: Life Sciences, EMBASE/Excerpta Medica, MEDLINE, PASCAL, Research Alert, Science Citation Index, SciSearch, TOXFILE



ELSEVIER

ISSN 0968-0896