บทความที่น่าสนใจประจำเดือน มีนาคม 2556

Title :	Stepwise MLR and PCR QSAR study of the pharmaceutical activities of antimalarial 3-hydroxypyridinone agents using B3LYP/6-311++G** descriptors
Author :	Lotfollah Saghaie, Hamidreza Sakhi, Hassan Sabzyan, Mohsen Shahlaei, Danial Shamshirian
Journal :	Medicinal Chemistry Research, April 2013, Volume 22, Issue 4, pp 1679-1688
Abstract :	The quantitative relationship between molecular properties and pharmaceutical activities of 19 antimalarial 3-hydroxypyridinones is studied using B3LYP/6-311++G** structural, electronic, and thermochemical characteristics. In this QSAR study, stepwise-multilinear regression (MLR) and principle component regression (PCR) are utilized based on volume, HOMO, nCrH2, and nHDon descriptors selected from a number of descriptor sets calculated and examined. The MLR coefficients are evaluated by cross-validation and external test sets methods. Regression coefficients of $R^2 = 0.882$ and $R^2 = 0.874$ are obtained, respectively, for the MLR and PCR predicted pIC50 values as referenced to their experimental values. Results of PCR predict the same trend for the predicted IC50 approving validity of the MLR results. Based on the present MLR and PCR analyses, pIC50 value is calculated for six candidate antimalarial drugs designed in this work, two of which are found to have promising antimalarial activity as high as that of the two best already synthesized and examined drugs.
Database :	SpringerLink

Title :	Synthesis, characterization, in vitro anticancer activity, and docking of Schiff bases of 4-amino-1,2-naphthoquinone
Author :	S. Shukla, R. S. Srivastava, S. K. Shrivastava, A. Sodhi, Pankaj Kumar
Journal :	Medicinal Chemistry Research, April 2013, Volume 22, Issue 4, pp 1604-1617
Abstract :	A series of Schiff bases of 4-amino-1,2-naphthoquinone were synthesized, purified, characterized, and evaluated for cytotoxicity against a panel of human cancer cell lines (Hep-G2, MG-63, and MCF-7). The cells were dosed with these Schiff bases at varying concentrations, and cell viability was measured by a 3-(4,5-dimethylthiazol-2-yl)-2,5-diphenyltetrazolium bromide (MTT) assay. Significant anticancer activities were observed in vitro for some members of the series and compounds 4-(3,4,5-trimethoxybenzylideneamino)naphthalene-1,2-dione (S10) as well as 4-(4-hydroxy-3-methoxybenzylideneamino)naphthalene-1,2-dione (S13) are active cytotoxic agents against different cancer cell lines with IC50 values in the range of 5.91–9.98 µM. The structures of synthesized compounds were established by spectroscopic (FT-IR, 1H NMR, 13C NMR) and elemental analysis. To study the molecular basis of interaction and affinity of binding of the target molecules, all the compounds were docked into the ATPase domain of Topoisomerase-II (TP-II) by using Schrödinger molecular modeling software package. Docking experiments showed a good correlation between their predicted glide scores and the observed IC50 values of synthesized compounds. Structure–activity relationships indicated that presence of electron donating groups on phenyl ring of Schiff bases enhances the activity but Schiff base with electron withdrawing substituents on phenyl ring shows diminished activity.
Database :	SpringerLink

Title :	[The Impact of a Ketogenic Diet and Liver Dysfunction on Serum Very Long-Chain Fatty Acids Levels](#)
Author :	T. J. Stradomska, M. Bachański, J. Pawłowska, M. Syczewska, A. Stolarczyk, A. Tylki-Szymańska
Journal :	Lipids, April 2013, Volume 48, Issue 4, pp 405-409
Abstract :	Peroxisomes play an essential role in mammalian cellular metabolism, particularly in oxidation fatty acid pathways. Serum very long-chain fatty acids (VLCFA), the main biochemical diagnostic parameters for peroxisomal disorders, were examined in 25 neurological patients with epilepsy on a ketogenic diet and 27 patients with liver dysfunction. The data show that patients on a ketogenic diet have increased levels of C22:0 and C24:0, but not C26:0, and normal C24:0/C22:0 and C26:0/C22:0. Patients with liver insufficiency showed a slightly elevated level of C26:0, a normal level of C24:0 and a decreased level of C22:0; thus in 21/27 the ratio of C24:0/C22:0 was increased and 15/27 the ratio of C26:0/C22:0 was increased.
Database :	SpringerLink

Title :	[Public health intelligence and the detection of potential pandemics](#)
Author :	Martin French, Eric Mykhalovskiy
Journal :	Sociology of Health & Illness, February 2013, Volume 35, Issue 2, pages 174–187
Abstract :	This article considers contemporary developments in public health intelligence (PHI), especially their focus on health events of pandemic potential. It argues that the sociological study of PHI can yield important insights for the sociology of pandemics. PHI aims to detect health events as (or even before) they unfold. Whilst its apparatuses envelope traditional public health activities, such as epidemiological surveillance, they increasingly extend to non-traditional public health activities such as data-mining in electronically mediated social networks. With a focus on non-traditional PHI activities, the article first situates the study of PHI in relation to the sociology of public health. It then discusses the conceptualisation and actualisation of pandemics, reflecting on how public health professionals and organisations must equip themselves with diverse allies in order to realise the claims they make about pandemic phenomena. Finally, using the analytic tools of actor-network theory, sites for future empirical research that can contribute to the sociology of pandemics are suggested.
Database :	Wiley Online Library

Title :	[Stem cell microencapsulation for phenotypic control, bioprocessing, and transplantation](#)
Author :	Jenna L. Wilson, Todd C. McDevitt
Journal :	Biotechnology and Bioengineering, Volume 110, March 2013, Issue 3, pages 667–682
Abstract :	Cell microencapsulation has been utilized for decades as a means to shield cells from the external environment while simultaneously permitting transport of oxygen, nutrients, and secretory molecules. In designing cell therapies, donor primary cells are often difficult to obtain and expand to appropriate numbers, rendering stem cells an attractive alternative due to their capacities for self-renewal, differentiation, and trophic factor secretion. Microencapsulation of stem cells offers several benefits, namely the creation of a defined microenvironment which can be designed to modulate stem cell phenotype, protection from

	hydrodynamic forces and prevention of agglomeration during expansion in suspension bioreactors, and a means to transplant cells behind a semi-permeable barrier, allowing for molecular secretion while avoiding immune reaction. This review will provide an overview of relevant microencapsulation processes and characterization in the context of maintaining stem cell potency, directing differentiation, investigating scalable production methods, and transplanting stem cells for clinically relevant disorders.
Database :	Wiley Online Library

Title :	Glutamine effects on brain growth in very preterm children in the first year of life
Author :	Jorrit F. de Kieviet, Pieter J. Vuijk, et al.
Journal :	Clinical Nutrition, In Press, Available online 4 April 2013
Abstract :	Background & Aims: Glutamine supplementation in the neonatal period has been associated with increased brain structure volumes at school-age in very preterm children. The aim of this study was to clarify the emergence and specificity of differences in brain structure volumes, using growth trajectories of head circumference, weight, and length.
Database :	ScienceDirect

Title :	Breast Cancer Screening: The Paradigm Shifts (Finally)
Author :	Robert G. Stern
Journal :	The American Journal of Medicine, In Press: Available online 3 April 2013
Abstract :	The seemingly endless and often overwrought debate about the utility of screening mammography may finally be drawing to a close. We may at last be moving beyond the standard paradigm of mass screening by mammography alone, which has had, at best, marginal success in most developed countries, to a tailored approach using a variety of methodologies that take into account pertinent patient characteristics.
Database :	ScienceDirect

Title :	Determination of Sodium Hyaluronate in pharmaceutical formulations by HPLC-UV
Author :	K. Ruckmani, Saleem Z. Shaikh, Pavne Khalil, M.S. Muneera, O.A Thusleem
Journal :	Journal of Pharmaceutical Analysis, In Press, Available online 14 March 2013
Abstract :	"A liquid chromatography (HPLC) method with UV detection was developed for determination of sodium hyaluronate in pharmaceutical formulation. Sodium hyaluronate is a polymer of disaccharides, composed of D-glucuronic acid and D-N-acetylglucosamine, linked via alternating β-1, 4 and β-1, 3 glycosidic bonds. Being a polymer compound it lacks a UV absorbing chromophore. In the absence of a UV absorbing chromophore and highly polar nature of compound, the analysis becomes a major challenge. To overcome these problems a novel method for the determination of sodium hyaluronate was developed and validated based on size exclusion liquid chromatography (SEC) with UV detection. An isocratic mobile phase consisting of buffer 0.05 M potassium dihydrogen

phosphate, pH adjusted to 7.0 using potassium hydroxide (10%) was used. Chromatography was carried out at 25 °C on a BioSep SEC S2000, 300×7.8 mm column. The detection was carried out using variable wavelength UV-vis detector set at 205 nm. The compounds were eluted isocratically at a steady flow rate of 1.0 mL/min. Sodium hyaluronate retention time was about 4.9 minutes with an asymmetry factor of1.93. A calibration curve was obtained from 1 to 38 g mL−1 (r>0.9998). Within-day % RSD was 1.0 and between-day % RSD was 1.10. Specificity/ selectivity experiments revealed the absence of interference from excipients, recovery from spiked samples for sodium hyaluronate was99–102. The developed method was applied to the determination of sodium hyaluronate in pharmaceutical drug substance and product."

Database :	ScienceDirect

Title :	[Intracellular Aggregation of Multimodal Silica Nanoparticles for Ultrasound-Guided Stem Cell Implantation,](#)
Author :	Jesse V. Jokerst, Christine Khademi and Sanjiv S. Gambhir
Journal :	Science Translational Medicine, March 2013, Vol. 5, Issue 177, p. 177ra35
Abstract :	The promises of cardiac stem cell therapy have yet to be fully realized, in part because of poor survival and engraftment efficacy of implanted cells. Cells die after implantation owing to ischemia, inflammation, immune response, as well as mis-injection or implantation into fibrotic tissue. Imaging tools can help implant cells in areas of the heart most receptive to stem cell therapy and monitor the efficacy of treatment by reporting the viability, location, and number of implanted stem cells. We describe a multimodal, silica-based nanoparticle that can be used for cell sorting (fluorescence), real-time guided cell implantation ultrasound, and high-resolution, long-term monitoring by magnetic resonance imaging (MRI). The nanoparticle agent increased the ultrasound and MRI contrast of labeled human mesenchymal stem cells (hMSCs) 700 and 200% versus unlabeled cells, respectively, and allowed cell imaging in animal models for 13 days after implantation. The agent had no significant impact on hMSC cell metabolic activity, proliferation, or pluripotency, and it increased the production of many paracrine factors implicated in cardiac repair. Electron microscopy and ultrasound imaging suggest that the mechanism of action is in vivo aggregation of the 300-nm silica nanoparticles into larger silica frameworks that amplify the ultrasound backscatter. The detection limit in cardiac tissue was 250,000 hMSCs via MRI and 70,000 via ultrasound. This ultrasound-guided cell delivery and multimodal optical/ultrasound/MRI intracardiac cell-tracking platform could improve cell therapy in the clinic by minimizing misdelivery or implantation into fibrotic tissue.
Database :	American Association for the Advancement of Science (AAAS)

Title :	[Autobiographical memory in multiple sclerosis patients: Assessment and cognitive facilitation](#)
Author :	A. Ernst, F. Blanc, V. Voltzenlogel, J. de Seze, B. Chauvin & L. Manning
Journal :	Neuropsychological Rehabilitation: An International Journal, 2013, Volume 23, Issue 2, pages 161-181
Abstract :	The multifocal nature of lesions in multiple sclerosis hints at the occurrence of autobiographical memory (AbM) impairment. However, the dearth of studies on AbM in multiple sclerosis is noticeable, notwithstanding the importance of AbM in everyday life. In the first section of this study, 25 multiple sclerosis patients and 35 controls underwent a detailed episodic AbM assessment. Results obtained by

	means of ANOVA suggested an AbM retrieval deficit in every patient. That pattern of performance paved the way for the second section of the study, in which we followed up 10 out of the 25 patients. Our objective was to assess the effectiveness of a cognitive facilitation programme designed to alleviate AbM retrieval deficits, based on the key role of mental visual imagery on AbM. Statistical group analyses by means of ANOVA and individual analyses using the χ^2 test showed significant differences in AbM test results, in post-facilitation relative to pre-facilitation training, in all 10 patients. Moreover, the patients' comments showed that the positive effects were transferred in their daily life functioning. We would like to suggest that the facilitation programme efficiently enhanced the process of self-centred mental visual imagery, which might have compensated for poor retrieval of personal memories by providing better access to visual details and detailed visual scenes of personal recollections.
Database :	Taylor & Francis Online Journals

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