

Acetaldehyde-derived modifications on cytosolic human carbonic anhydrases

Acetaldehyde can generate modifications in several proteins, such as carbonic anhydrase (CA) II. In this study, we extended in vitro investigations on acetaldehyde adduct formation by focusing on the other human cytosolic CA enzymes I, III, VII, and XIII. High-resolution mass spectrometric analysis indicated that acetaldehyde most efficiently formed covalent adducts with CA II and XIII. The binding of up to 19 acetaldehydes in CA II is probably attributable to the high number of lysine residues (n=24) located mainly on the surface of the enzyme molecule. CA XIII formed more adducts (up to 25) than it contains lysine residues (n=16) in its primary structure. Acetaldehyde treatment induced only minor changes in CA catalytic activity in most cases. The present study provides the first evidence that acetaldehyde can bind to several cytosolic CA isozymes. The functional consequences of such modifications will be further investigated in vivo by using animal models.

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Multi-scaled biodata analysis and modelling (MultiBAM), School of Management (JKK), Ita-Suomen yliopisto, CNR-INO, Tampere University Hospital

Contributors: Bootorabi, F., Jänis, J., Hytönen, V. P., Valjakka, J., Kuuslahti, M., Vullo, D., Niemelä, O., Supuran, C. T., Parkkila, S.

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Scopus rating (2011): CiteScore 3 SJR 0.487 SNIP 0.818

Original language: English

ASJC Scopus subject areas: Drug Discovery, Pharmacology

Keywords: Acetaldehyde, Adduct, Alcohol, Mass spectrometry, Modification

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Source: Scopus

Source ID: 81355149286

Research output: Contribution to journal › Article › Scientific › peer-review

Alkylaminophenol induces G1/S phase cell cycle arrest in glioblastoma cells through p53 and cyclin-dependent kinase signaling pathway

Glioblastoma (GBM) is the most common type of malignant brain tumor in adults. We show here that small molecule 2-[(3,4-dihydroquinolin-1(2H)-yl)(p-tolyl)methyl]phenol (THTMP), a potential anticancer agent, increases the human glioblastoma cell death. Its mechanism of action and the interaction of selective signaling pathways remain elusive. Three structurally related phenolic compounds were tested in multiple glioma cell lines in which the potential activity of the compound, THTMP, was further validated and characterized. Upon prolonged exposure to THTMP, all glioma cell lines undergo p53 and cyclin-dependent kinase mediated cell death with the IC50 concentration of 26.5 and 75.4 μ M in LN229 and Snb19, respectively. We found that THTMP strongly inhibited cell growth in a dose and in time dependent manner. THTMP treatment led to G1/S cell cycle arrest and apoptosis induction of glioma cell lines. Furthermore, we identified 3,714 genes with significant changes at the transcriptional level in response to THTMP. Further, a transcriptional analysis (RNA-seq) revealed that THTMP targeted the p53 signaling pathway specific genes causing DNA damage and cell cycle arrest at G1/S phase explained by the decrease of cyclin-dependent kinase 1, cyclin A2, cyclin E1 and E2 in glioma cells. Consistently, THTMP induced the apoptosis by regulating the expression of Bcl-2 family genes and reactive oxygen species while it also changed the expression of several anti-apoptotic genes. These observations suggest that THTMP exerts proliferation activity inhibition and pro-apoptosis effects in glioma through affecting cell cycle arrest and intrinsic apoptosis signaling. Importantly, THTMP has more potential at inhibiting GBM cell proliferation compared to TMZ, the current chemotherapy treatment administered to GBM patients; thus, we propose that THTMP may be an alternative therapeutic option for glioblastoma.

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Research group: Molecular Signaling Lab, BioMediTech, Computing Sciences, Materials Science and Environmental Engineering, Research group: Computational Systems Biology, Research group: Predictive Society and

Data Analytics (PSDA)

Contributors: Doan, P., Musa, A., Candeias, N. R., Emmert-Streib, F., Yli-Harja, O., Kandhavelu, M.

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Publication information

Journal: FRONTIERS IN PHARMACOLOGY

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Ratings:

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ASJC Scopus subject areas: Pharmacology, Pharmacology (medical)

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<http://urn.fi/URN:NBN:fi:itty-201908282043>

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Source ID: 85068363943

Research output: Contribution to journal > Article > Scientific > peer-review

Indocyanine green: Photosensitizer or chromophore? Still a debate

Indocyanine green (ICG) is a water-soluble anionic tricarbo-cyanine dye developed during the Second World War that was first approved for clinical use in humans in 1956. The main features of ICG that make it suitable for bioimaging applications are its near infrared absorption and its fluorescence. Although ICG is mainly used for its fluorescence emission properties, it has also been hypothesized that it can serve as a photosensitizer for photodynamic therapy applications, eliciting cytotoxic effects both in vitro and in vivo when used in combination with light at wavelengths in the region of 800-830 nm. Moreover, ICG can be used for hyperthermia of enhanced-photocoagulation of blood vessels treatment. In this paper we have gathered all the available data concerning the use of ICG for different treatments.

General information

Publication status: Published

MoE publication type: A2 Review article in a scientific journal

Organisations: Frontier Photonics, CNRS Centre National de la Recherche Scientifique, INSERM U703, Lille University Hospital, CNRS 3049 Médicaments Photoactivables-Photochimiothérapie (PHOTOMED), GDR

Contributors: Giraudeau, C., Moussaron, A., Stallivieri, A., Mordon, S., Frochot, C.

Number of pages: 27

Pages: 1871-1897

Publication date: 2014

Peer-reviewed: Yes

Publication information

Journal: CURRENT MEDICINAL CHEMISTRY

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Issue number: 16

ISSN (Print): 0929-8673

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Scopus rating (2014): CiteScore 7.5 SJR 1.282 SNIP 1.202

Original language: English

ASJC Scopus subject areas: Molecular Medicine, Pharmacology, Medicine(all)

Keywords: Cytotoxic effects, Fluorescence, Hyperthermia, Indocyanine Green (ICG), Photodynamic therapy (PDT), Selective photocoagulation, Site-specific therapy

URLs:

<http://www.scopus.com/inward/record.url?scp=84899786456&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

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Research output: Contribution to journal > Review Article > Scientific > peer-review

Pulmonary toxicity of Fe₂O₃, ZnFe₂O₄, NiFe₂O₄ and NiZnFe₄O₈ nanomaterials: Inflammation and DNA strand breaks

Exposure to metal oxide nanomaterials potentially occurs at the workplace. We investigated the toxicity of two Fe-oxides: Fe₂O₃ nanoparticles and nanorods; and three MFe₂O₄ spinels: NiZnFe₄O₈, ZnFe₂O₄, and NiFe₂O₄ nanoparticles. Mice were dosed 14, 43 or 128 µg by intratracheal instillation. Recovery periods were 1, 3, or 28 days. Inflammation – neutrophil influx into bronchoalveolar lavage (BAL) fluid – occurred for Fe₂O₃ rods (1 day), ZnFe₂O₄ (1, 3 days), NiFe₂O₄ (1, 3, 28 days), Fe₂O₃ (28 days) and NiZnFe₄O₈ (28 days). Conversion of mass-dose into specific surface-area-dose showed that inflammation correlated with deposited surface area and consequently, all these nanomaterials belong to the so-called low-solubility, low-toxicity class. Increased levels of DNA strand breaks were observed for both Fe₂O₃ particles and rods, in BAL cells three days post-exposure. To our knowledge, this is, besides magnetite (Fe₃O₄), the first study of the pulmonary toxicity of MFe₂O₄ spinel nanomaterials.

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Materials Science and Environmental Engineering, Research group: Materials Characterization, National Research Centre for the Working Environment (NRCWE), Member of the German Center for Lung Research (DZL), German Research Center for Environmental Health, National Institute of Occupational Health, Risø Campus

Contributors: Hadrup, N., Saber, A. T., Kyjovska, Z. O., Jacobsen, N. R., Vippola, M., Sarlin, E., Ding, Y., Schmid, O., Wallin, H., Jensen, K. A., Vogel, U.

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ASJC Scopus subject areas: Toxicology, Pharmacology, Health, Toxicology and Mutagenesis

Keywords: Iron, Metal oxides, Nanomaterial, Nickel, Pulmonary, Zinc

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Source: Scopus

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Research output: Contribution to journal › Article › Scientific › peer-review

Cell-based bioreporter assay coupled to HPLC micro-fractionation in the evaluation of antimicrobial properties of the basidiomycete fungus *Pycnoporus cinnabarinus*

Context Identification of bioactive components from complex natural product extracts can be a tedious process that aggravates the use of natural products in drug discovery campaigns. Objective This study presents a new approach for screening antimicrobial potential of natural product extracts by employing a bioreporter assay amenable to HPLC-based activity profiling. Materials and methods A library of 116 crude extracts was prepared from fungal culture filtrates by liquid-liquid extraction with ethyl acetate, lyophilised, and screened against *Escherichia coli* using TLC bioautography. Active extracts were studied further with a broth microdilution assay, which was, however, too insensitive for identifying the active microfractions after HPLC separation. Therefore, an assay based on bioluminescent *E. coli* K-12 (pTetLux1) strain was coupled with HPLC micro-fractionation. Results Preliminary screening yielded six fungal extracts with potential antimicrobial activity. A crude extract from a culture filtrate of the wood-rotting fungus, *Pycnoporus cinnabarinus* (Jacq.) P. Karst. (Polyporaceae), was selected for evaluating the functionality of the bioreporter assay in HPLC-based activity profiling. In the bioreporter assay, the IC₅₀ value for the crude extract was 0.10 mg/mL. By integrating the bioreporter assay with HPLC micro-fractionation, the antimicrobial activity was linked to LC-UV peak of a compound in the chromatogram of the extract. This compound was isolated and identified as a fungal pigment phlebiarubrone. Discussion and conclusion HPLC-based activity profiling using the bioreporter-based approach is a valuable tool for identifying antimicrobial compound(s) from complex crude extracts, and offers improved sensitivity and speed compared with traditional antimicrobial assays, such as the turbidimetric measurement.

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Chemistry and Bioengineering, Research group: Industrial Bioengineering and Applied Organic Chemistry, University of Helsinki, Universite de Geneve

Contributors: Järvinen, P., Nybond, S., Marcourt, L., Ferreira Queiroz, E., Wolfender, J. L., Mettälä, A., Karp, M., Vuorela, H., Vuorela, P., Hatakka, A., Tammela, P.

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Peer-reviewed: Yes

Publication information

Journal: Pharmaceutical Biology

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ISSN (Print): 1388-0209

Ratings:

Scopus rating (2016): CiteScore 2.7 SJR 0.575 SNIP 0.856

Original language: English

ASJC Scopus subject areas: Drug Discovery, Pharmacology, Pharmaceutical Science, Complementary and alternative medicine, Molecular Medicine

Keywords: Bioluminescent bacterial strain, Escherichia coli, Gram-negative bacteria, phlebiarubrone

DOIs:

10.3109/13880209.2015.1103754

Bibliographical note

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Source: Scopus

Source ID: 84958036747

Research output: Contribution to journal › Article › Scientific › peer-review

Use of insulin and insulin analogs and risk of cancer - systematic review and meta-analysis of observational studies

Background: An association of insulin use and risk of cancer has been reported but evidence is conflicting and methodological issues have been identified. Objective: To summarize results regarding insulin use and cancer risk by a systematic review and meta-analysis of cohort and case-control studies examining risk of cancer associated with insulin use in patients with diabetes. Data Sources: Systematic literature search in 5 databases: PubMed, Embase, Web of Science, Scopus and Cochrane Library. Study Eligibility Criteria (PICOS): Population: diabetes patients. Exposure: Users of any exogenous insulin. Comparison: Diabetes patients with or without use of antidiabetic drugs. Outcome: Any incident cancer. Study Design: Cohort and case-control studies. Results: 42 eligible studies examined risk of any cancer and 27 site-specific cancers. Results of individual studies were heterogeneous. Meta-analyses were significant for: Insulin vs No Insulin: Increased risk for pancreas, liver, kidney, stomach and respiratory cancer, decreased risk for prostate cancer. Insulin vs Non-Insulin Antidiabetics: Increased risk for any, pancreatic and colorectal cancer. Glargine vs Non-Glargine Insulin: Increased risk for breast cancer, decreased risk for colon cancer. Limitations: Few studies available for most cancer sites and exposure contrasts, and few assess effect of dose and duration of exposure. Methodological issues in several studies. Availability of confounders. Conclusions: Insulin use was associated with risk of cancer at several sites. Cautious interpretation of results is warranted as methodological issues and limitations in several of the included studies have been identified. Choice of study design may have a profound effect on estimated cancer risk.

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Prostate cancer research center (PCRC), Norwegian Institute of Public Health, Aalborg University, Aalborg University Hospital, Utrecht University, Netherlands Cancer Institute, Karolinska Institutet, University of Helsinki, Maastricht University

Contributors: Karlstad, Ø., Starup-Linde, J., Vestergaard, P., Hjellvik, V., Bazelier, M. T., Schmidt, M. K., Andersen, M., Auvinen, A., Haukka, J., Furu, K., de Vries, F., de Bruin, M. L.

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Publication date: Dec 2013

Peer-reviewed: Yes

Publication information

Journal: CURRENT DRUG SAFETY

Volume: 8

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Ratings:

Scopus rating (2013): CiteScore 2.6 SJR 0.539 SNIP 0.612

Original language: English

ASJC Scopus subject areas: Pharmacology (medical), Toxicology, Pharmacology
Keywords: Cancer risk, Diabetes mellitus, Insulin, Meta-analysis, Neoplasm, Systematic review
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Source: Scopus

Source ID: 84891507550

Research output: Contribution to journal › Article › Scientific › peer-review

Coxsackievirus B3 VLPs purified by ion exchange chromatography elicit strong immune responses in mice

Coxsackievirus B3 (CVB3) is an important cause of acute and chronic viral myocarditis, and dilated cardiomyopathy (DCM). Although vaccination against CVB3 could significantly reduce the incidence of serious or fatal viral myocarditis and various other diseases associated with CVB3 infection, there is currently no vaccine or therapeutic reagent in clinical use. In this study, we contributed towards the development of a CVB3 vaccine by establishing an efficient and scalable ion exchange chromatography-based purification method for CVB3 virus and baculovirus-insect cell-expressed CVB3 virus-like particles (VLPs). This purification system is especially relevant for vaccine development and production on an industrial scale. The produced VLPs were characterized using a number of biophysical methods and exhibited excellent quality and high purity. Immunization of mice with VLPs elicited a strong immune response, demonstrating the excellent vaccine potential of these VLPs.

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Multi-scaled biodata analysis and modelling (MultiBAM), School of Management (JKK), Vactech Ltd., Pirkanmaan sairaanhoitopiiri, Jyväskylän yliopisto, Karolinska University Hospital

Contributors: Koho, T., Koivunen, M. R. L., Oikarinen, S., Kummola, L., Mäkinen, S., Mähönen, A. J., Siiofy-Khojine, A., Marjomäki, V., Kazmertsuk, A., Junttila, I., Kulomaa, M. S., Hyöty, H., Hytönen, V. P., Laitinen, O. H.

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Peer-reviewed: Yes

Publication information

Journal: ANTIVIRAL RESEARCH

Volume: 104

Issue number: 1

ISSN (Print): 0166-3542

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ASJC Scopus subject areas: Pharmacology, Virology

Keywords: CVB3, Ion exchange chromatography, VLP

DOIs:

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Research output: Contribution to journal › Article › Scientific › peer-review

Pectin and Mucin Enhance the Bioadhesion of Drug Loaded Nanofibrillated Cellulose Films

Purpose: Bioadhesion is an important property of biological membranes, that can be utilized in pharmaceutical and biomedical applications. In this study, we have fabricated mucoadhesive drug releasing films with bio-based, non-toxic and biodegradable polymers that do not require chemical modifications. Methods: Nanofibrillar cellulose and anionic type nanofibrillar cellulose were used as film forming materials with known mucoadhesive components mucin, pectin and chitosan as functional bioadhesion enhancers. Different polymer combinations were investigated to study the adhesiveness, solid state characteristics, film morphology, swelling, mechanical properties, drug release with the model compound metronidazole and in vitro cytotoxicity using TR146 cells to model buccal epithelium. Results: SEM revealed lamellar structures within the films, which had a thickness ranging 40–240 µm depending on the film polymer composition. All bioadhesive components were non-toxic and showed high adhesiveness. Rapid drug release was observed, as 60–80% of the total amount of metronidazole was released in 30 min depending on the film formulation. Conclusions: The liquid molding used was a straightforward and simple method to produce drug releasing highly mucoadhesive films, which could be utilized in treating local oral diseases, such as periodontitis. All materials used were natural biodegradable polymers from renewable sources, which are generally regarded as safe.

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Chemistry and Bioengineering, Research group: Chemistry & Advanced Materials, Aalto University, Università degli Studi di Padova, Italy, University of Helsinki, University of Helsinki

Contributors: Laurén, P., Paukkonen, H., Lipiäinen, T., Dong, Y., Oksanen, T., Rääkkönen, H., Ehlers, H., Laaksonen, P., Yliperttula, M., Laaksonen, T.

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Publication information

Journal: Pharmaceutical Research

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Article number: 145

ISSN (Print): 0724-8741

Ratings:

Scopus rating (2018): CiteScore 6.9 SJR 1.093 SNIP 1.131

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Keywords: bioadhesion, drug release, mucoadhesion, nanofibrillar cellulose, TR146

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DOIs:

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Source: Scopus

Source ID: 85047448577

Research output: [Contribution to journal](#) > [Article](#) > [Scientific](#) > [peer-review](#)

Neuroinformatics and Computational Modelling as Complementary Tools for Neurotoxicology Studies

Neuroinformatics is an area of science that aims to integrate neuroscience data and develop modern computational tools to increase our understanding of the functions of the nervous system in health and disease. Neuroinformatics tools include, among others, databases for storing and sharing data, repositories for managing documents and source code, and software tools for analysing, modelling and simulating signals and images. This MiniReview aims to present the state of the art in neuroinformatics and computational in silico modelling of neurobiological processes and neuroscientific phenomena as well as to discuss the use of in silico models in neurotoxicology research. In silico modelling can be considered a new, complementary tool in chemical design to predict potential neurotoxicity and in neurotoxicity testing to help clarify initial hypothesis obtained in in vitro and in vivo. Validated in silico models can be used to identify pharmacological targets, to help bridge in vitro and in vivo studies and, ultimately, to develop safer chemicals and efficient therapeutic strategies.

General information

Publication status: Published

MoE publication type: A2 Review article in a scientific journal

Organisations: Faculty of Biomedical Sciences and Engineering

Contributors: Linne, M.

Pages: 56-61

Publication date: Sep 2018

Peer-reviewed: Yes

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Publication information

Journal: Basic and Clinical Pharmacology and Toxicology

Volume: 123

Issue number: S5

ISSN (Print): 1742-7835

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Original language: English

ASJC Scopus subject areas: Toxicology, Pharmacology

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10.1111/bcpt.13075

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Source ID: 85052786993

Research output: Contribution to journal › Review Article › Scientific › peer-review

Resveratrol interferes with the aggregation of membrane-bound human-IAPP: A molecular dynamics study

Amyloid aggregation of islet amyloid polypeptide (IAPP) in pancreatic tissues is a typical feature of type 2 diabetes mellitus. Resveratrol, a natural product extensively studied for its wide range of biological effects, has been shown to inhibit IAPP aggregation. However, the mechanism by which resveratrol inhibits IAPP aggregation is still far from complete elucidation. Now, an increasing knowledge of the mechanism of amyloid toxicity shifts the target of research towards the development of compounds which can prevent amyloid-mediated membrane damage rather than merely inhibit fiber formation. In this study we used all atom molecular dynamics to investigate the interaction of resveratrol with full-length human IAPP in a negatively charged membrane environment. Our results show that the presence of resveratrol induces the formation of secondary structures (sheets and helices) by inserting in a hydrophobic pocket between the interaction surface of two IAPP molecules in aqueous solution. On the other hand, resveratrol significantly perturbs the interaction of IAPP with negatively charged membranes by anchoring specific hydrophobic regions (23FGA25 and 32VGS34) of the peptide and forming a stable 1:2 IAPP:resveratrol complex at the water/membrane interphase.

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Physics, NEST Istituto Nanoscienze-CNR, Department of Chemical Sciences, University of Catania, Unità Organizzativa e di Supporto di Catania, Istituto di Biostrutture e Bioimmagini

Contributors: Lolicato, F., Raudino, A., Milardi, D., La Rosa, C.

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Pages: 876-881

Publication date: 6 Mar 2015

Peer-reviewed: Yes

Publication information

Journal: European Journal of Medicinal Chemistry

Volume: 92

ISSN (Print): 0223-5234

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ASJC Scopus subject areas: Drug Discovery, Organic Chemistry, Pharmacology

Keywords: Atomistic simulation, Membrane, Molecular dynamics, Resveratrol, Type II diabetes

DOIs:

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Source: Scopus

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Research output: Contribution to journal › Article › Scientific › peer-review

Elucidation of Compression-Induced Surface Crystallization in Amorphous Tablets Using Sum Frequency Generation (SFG) Microscopy

Purpose: To investigate the effect of compression on the crystallization behavior in amorphous tablets using sum frequency generation (SFG) microscopy imaging and more established analytical methods. Method: Tablets containing neat amorphous griseofulvin with/without excipients (silica, hydroxypropyl methylcellulose acetate succinate (HPMCAS), microcrystalline cellulose (MCC) and polyethylene glycol (PEG)) were prepared. They were analyzed upon preparation and storage using attenuated total reflectance Fourier transform infrared (ATR-FTIR) spectroscopy, scanning electron microscopy (SEM) and SFG microscopy. Results: Compression-induced crystallization occurred predominantly on the surface of the neat amorphous griseofulvin tablets, with minimal crystallinity being detected in the core of the tablets. The presence of various types of excipients was not able to mitigate the compression-induced surface crystallization of the amorphous griseofulvin tablets. However, the excipients affected the crystallization rate of amorphous griseofulvin in the core of the tablet upon compression and storage. Conclusions: SFG microscopy can be used in combination with ATR-FTIR spectroscopy and SEM to understand the crystallization behaviour of amorphous tablets upon compression and storage. When selecting excipients for amorphous formulations, it is important to consider the effect of the excipients on the physical stability of the amorphous formulations.

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Chemistry and Bioengineering, University of Helsinki, Division of Biopharmaceutical Sciences, Biomedicum Imaging Unit, FIN-00014 University of Helsinki

Contributors: Mah, P. T., Novakovic, D., Saarinen, J., van Landeghem, S., Peltonen, L., Laaksonen, T., Isomäki, A., Strachan, C. J.

Number of pages: 14

Pages: 957-970

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Early online date: 13 Oct 2016

Publication information

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ISSN (Print): 0724-8741

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Original language: English

ASJC Scopus subject areas: Biotechnology, Molecular Medicine, Pharmacology, Pharmaceutical Science, Organic Chemistry, Pharmacology (medical)

DOIs:

10.1007/s11095-016-2046-6

Source: Scopus

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Research output: Contribution to journal › Article › Scientific › peer-review

Unity is strength

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Frontier Photonics, Univ Lille Nord de France, Lille University Hospital - CHRU, St. Philibert Hospital

Contributors: Maunoury, V., Mordon, S., Bulois, P.

Number of pages: 2

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Publication date: Apr 2011

Peer-reviewed: Yes

Publication information

Journal: CHEMOTHERAPY

Volume: 57

Issue number: 2

ISSN (Print): 0009-3157

Ratings:

Scopus rating (2011): CiteScore 3.4 SJR 0.694 SNIP 0.866

Original language: English

ASJC Scopus subject areas: Pharmacology (medical), Oncology, Infectious Diseases, Pharmacology, Drug Discovery

DOIs:

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Research output: Contribution to journal › Letter › Scientific › peer-review

Comparative effects of high and low-dose simvastatin on prostate epithelial cells: The role of LDL

Epidemiological studies have linked statin use with a decreased risk of advanced prostate cancer and an improved recurrence-free survival after radical therapy. It is unclear, however, whether statins could have direct effects against prostate cancer in a clinical setting, as their growth-inhibiting effects on prostate cancer cells have been demonstrated at drug concentrations which exceed the level in plasma during standard clinical dosing. We compared responses to high-dose and therapeutic-dose simvastatin in normal and cancerous prostate epithelial cells. Simvastatin was more effective at inhibiting the growth of normal prostate epithelial cells than of cancer cells. At therapeutic 100 nM concentration simvastatin had a cytostatic effect on normal cells: apoptosis was only slightly induced, but a decrease in cell cycle activity and an increase in senescence were observed. At therapeutic concentrations, lipophilic simvastatin caused a stronger

growth inhibition than did hydrophilic rosuvastatin. In contrast, 10 μM simvastatin had a cytotoxic effect both on normal and cancer cells. Addition of LDL-cholesterol effectively reversed the cytostatic effect in all cell lines, but overcoming the cytotoxicity of 10 μM simvastatin required a combination of LDL-cholesterol and mevalonate. As LDL-cholesterol completely prevented the growth-inhibiting effect of therapeutic-dose simvastatin already at low, subphysiological concentrations it is unlikely that statins have direct effects on growth of prostate epithelial cells in vivo. Statins' possible benefits against prostate cancer could be due to systemic cholesterol-lowering, as suggested by epidemiological studies. Future clinical studies evaluating the effects of statins on prostate cancer prevention should monitor serum LDL and should probably administer statins at higher concentrations than those currently used in the treatment of hypercholesterolemia.

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Prostate cancer research center (PCRC), Central Finland Central Hospital, Tampere University Hospital

Contributors: Murtola, T. J., Syväälä, H., Pennanen, P., Bläuer, M., Solakivi, T., Ylikomi, T., Tammela, T. L. J.

Number of pages: 5

Pages: 96-100

Publication date: 30 Dec 2011

Peer-reviewed: Yes

Publication information

Journal: European Journal of Pharmacology

Volume: 673

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ISSN (Print): 0014-2999

Ratings:

Scopus rating (2011): CiteScore 5.1 SJR 1.058 SNIP 1.069

Original language: English

ASJC Scopus subject areas: Pharmacology

Keywords: Cell cycle, Cell proliferation, Epithelial cell, Low-density lipoprotein, Prostate, Simvastatin

DOIs:

10.1016/j.ejphar.2011.10.022

URLs:

<http://www.scopus.com/inward/record.url?scp=81855207294&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 81855207294

Research output: Contribution to journal > Article > Scientific > peer-review

Seller's reputation and capacity on the illicit drug markets: 11-month study on the Finnish version of the Silk Road

Aims This 11-month study analyzed illicit drug sales on the anonymous Tor network, with a focus on investigating whether a seller's reputation and capacity increased daily drug sales. **Design and setting** The data were gathered from Silkkitie, the Finnish version of the Silk Road, by web crawling the site on a daily basis from (November 2014 to September 2015). The data include information on sellers ($n = 260$) and products ($n = 3823$). **Measurements** The measurements include the sellers' reputation, the sale amounts (in euros), the number of available products and the types of drugs sold. The sellers' capacity was measured using their full sales potential (in euros). **Fixed-effects regression models** were used to estimate the effects of sellers' reputation and capacity; these models were adjusted for the types of drugs sold. **Findings** Overall, illicit drug sales totalled over 2 million euros during the study, but many products were not sold at all, and sellers were active for only a short time on average (mean = 62.8 days). Among the products sold, stimulants were most widely purchased, followed by cannabis, MDMA, and psychedelics. A seller's reputation and capacity were both associated with drug sales. **Conclusion** The Tor network has enabled a transformation in drug sales. Due to the network's anonymity, the seller's reputation and capacity both have an impact on sales.

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Pervasive Computing, A-Clinic Foundation, University of Helsinki

Contributors: Nurmi, J., Kaskela, T., Perälä, J., Oksanen, A.

Number of pages: 7

Pages: 201-207

Publication date: 1 Sep 2017

Peer-reviewed: Yes

Publication information

Journal: DRUG AND ALCOHOL DEPENDENCE

Volume: 178

ISSN (Print): 0376-8716

Ratings:

Scopus rating (2017): CiteScore 5.7 SJR 1.715 SNIP 1.256

Original language: English

ASJC Scopus subject areas: Toxicology, Pharmacology, Psychiatry and Mental health, Pharmacology (medical)

Keywords: Anonymity, Cryptomarket, Illicit drugs, Internet, Longitudinal, Tor network, Web crawling

DOIs:

10.1016/j.drugalcdep.2017.05.018

Source: Scopus

Source ID: 85021047298

Research output: Contribution to journal > Article > Scientific > peer-review

In vitro characterization of arylhydrazones of active methylene derivatives

Arylhydrazones of active methylene compounds (AHAMCs) are potent chemotherapy agents for the cancer treatment. AHAMCs enhance the apoptotic cell death and antiproliferation properties in cancer cells. In this study, a series of AHAMCs, 13 compounds, was assayed for cytotoxicity, apoptosis, externalization of phosphatidylserine, heterogeneity and cellular calcium level changes. The in vitro cytotoxicity study against HEK293T cells suggests that AHAMCs have significant cytotoxic effect over the concentrations. Top 5 compounds, 5-(2-(2-hydroxyphenyl) hydrazono)pyrimidine-2,4,6(1H,3H,5H)-trione (5), 4-hydroxy-5-(2-(2,4,6-trioxo-tetrahydro-pyrimidin-5(6H) ylidene)hydrazinyl)benzene-1,3-disulfonic acid (6), 5-chloro-3-(2-(4,4-dimethyl-2,6-dioxocyclohexylidene)hydrazinyl)-2-hydroxybenzenesulfonic acid (8), 5-(2-(4,4-dimethyl-2,6-dioxocyclohexylidene)hydrazinyl)-4-hydroxybenzene-1,3-disulfonic acid (9) and 2-(2-sulfophenylhydrazo)malononitrile (10) were chosen for the pharmacodynamics study. Among these, compound 5 exhibited the better cytotoxic effect with the IC_{50} of 50.86 ± 2.5 mM. DNA cleavage study revealed that 5 induces cell death through apoptosis and shows more effects after 24 and/or 48 h. Independent validation of apoptosis by following the externalization of phosphatidylserine using Annexin-V is also in agreement with the potential activity of 5. Single cell image analysis of Annexin-V bound cells confirms the presence of mixture of early, mid and late apoptotic cells in the population of the cells treated with 5 and a decreased trend in cell-to-cell variation over the phase was also identified. Additionally, intracellular calcium level measurements identified the Ca^{2+} up-regulation in compound treated cells. A brief inspection of the effect of the compound 5 against multiple human brain astrocytoma cells showed a better cell growth inhibitory effect at micro molar level. These systematic studies provide insights in the development of novel AHAMCs compounds as potential cell growth inhibitors for cancer treatment.

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Faculty of Biomedical Sciences and Engineering, Research group: Computational Systems Biology, Peoples' Friendship University of Russia, Baku State University, Centro de Quimica Estrutural at Instituto Superior Tecnico

Contributors: Palanivel, S., Zhurina, A., Doan, P., Chandraseelan, J. G., Khandelwal, V. K. M., Zubkov, F. I., Mahmudov, K. T., Pombeiro, A. J., Yli-Harja, O., Kandhavelu, M.

Pages: 430-436

Publication date: 2018

Peer-reviewed: Yes

Publication information

Journal: Saudi Pharmaceutical Journal

Volume: 26

Issue number: 3

ISSN (Print): 1319-0164

Ratings:

Scopus rating (2018): CiteScore 4.7 SJR 0.67 SNIP 2.022

Original language: English

ASJC Scopus subject areas: Pharmacology, Pharmaceutical Science

Keywords: Apoptosis, Arylhydrazones of active methylene compounds, Chemotherapy, Cytotoxic effect, Glioma, Immortal cells, Single cell analysis

Electronic versions:

1-s2.0-S1319016417302268-main

DOIs:

10.1016/j.jsps.2017.12.018

URLs:

<http://urn.fi/URN:NBN:fi:tty-201803161382>

Source: Scopus

Source ID: 85039901326

Research output: Contribution to journal > Article > Scientific > peer-review

Anticancer activity of THMPP: Downregulation of PI3K/ S6K1 in breast cancer cell line

Breast cancer is the most common cancer that majorly affects female. The present study is focused on exploring the potential anticancer activity of 2-((1, 2, 3, 4-Tetrahydroquinolin-1-yl) (4 methoxyphenyl) methyl) phenol (THMPP), against human breast cancer. The mechanism of action, activation of specific signaling pathways, structural activity relationship and drug-likeness properties of THMPP remains elusive. Cell proliferation and viability assay, caspase enzyme activity, DNA fragmentation and FITC/Annexin V, AO/EtBr staining, RT-PCR, QSAR and ADME analysis were executed to understand the mode of action of the drug. The effect of THMPP on multiple breast cancer cell lines (MCF-7 and SkBr3), and non-tumorigenic cell line (H9C2) was assessed by MTT assay. THMPP at IC₅₀ concentration of 83.23 µM and 113.94 µM, induced cell death in MCF-7 and SkBr3 cells, respectively. Increased level of caspase-3 and -9, fragmentation of DNA, translocation of phosphatidylserine membrane and morphological changes in the cells confirmed the effect of THMPP in inducing the apoptosis. Gene expression analysis has shown that THMPP was able to downregulate the expression of PI3K/S6K1 genes, possibly via EGFR signaling pathway in both the cell lines, MCF-7 and SkBr3. Further, molecular docking also confirms the potential binding of THMPP with EGFR. QSAR and ADME analysis proved THMPP as an effective anti-breast cancer drug, exhibiting important pharmacological properties. Overall, the results suggest that THMPP induced cell death might be regulated by EGFR signaling pathway which augments THMPP being developed as a potential candidate for treating breast cancer.

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: BioMediTech, Research group: Molecular Signaling Lab, Department of Biotechnology, Lady Doak College, Institute for Systems Biology, Seattle, Washington, USA, Institute of Biosciences and Medical Technology

Contributors: Palanivel, S., Murugesan, A., Yli-Harja, O., Kandhavelu, M.

Number of pages: 9

Pages: 495-503

Publication date: 1 Apr 2020

Peer-reviewed: Yes

Publication information

Journal: Saudi Pharmaceutical Journal

Volume: 28

Issue number: 4

ISSN (Print): 1319-0164

Original language: English

ASJC Scopus subject areas: Pharmacology, Pharmaceutical Science

Keywords: ADME, Apoptosis, Docking, EGFR, Gene expression, QSAR, Tetrahydroquinoline

Electronic versions:

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DOIs:

10.1016/j.jsps.2020.02.015

URLs:

<http://urn.fi/URN:NBN:fi:tuni-202006236194>

Source: Scopus

Source ID: 85082417780

Research output: Contribution to journal › Article › Scientific › peer-review

Antiproliferative and apoptotic effects of indole derivative, N-(2-hydroxy-5-nitrophenyl (4'-methylphenyl) methyl) indoline in breast cancer cells

Indoline derivatives functions as an inhibitors of epidermal growth factor receptor (EGFR) with the anticancer potential against various cancers. We aim to investigate anti-breast cancer effects and mechanism of action of novel indoline derivatives. Molecular docking of seven indoline derivates with EGFR revealed, N-(2-hydroxy-5-nitrophenyl (4'-methylphenyl) methyl) indoline (HNPMI) as the top lead compound. RT-PCR analysis showed the downregulation of PI3K/S6K1 genes in breast cancer cells through the activation of EGFR with HNPMI. This compound found to have higher cytotoxicity than Cyclophosphamide, with the IC₅₀ of 64.10 µM in MCF-7 and 119.99 µM in SkBr3 cells. HNPMI significantly reduced the cell proliferation of MCF-7 and SkBr3 cells, without affecting non-cancerous cells, H9C2. Induction of apoptosis was analyzed by Caspase-3 and -9, DNA fragmentation, AO/EtBr staining and flow cytometry assays. A fold change of 0.218- and 0.098- for caspase-3 and 0.478- and 0.269- for caspase-9 in MCF7 and SkBr3 cells was observed, respectively. Caspase mediated apoptosis caused DNA fragmentation in breast cancer cells upon HNPMI treatment. The structural elucidation of HNPMI by QSAR model and ADME-Tox suggests, a bi-molecular interaction of HNPMI-EGFR which is related to antiproliferative and apoptotic activity. The data concludes that, HNPMI-induced the apoptosis via EGFR signaling pathway in breast cancer cells. Thus, HNPMI might serve as a scaffold for developing a potential anti-breast cancer therapeutic agent.

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: BioMediTech, Institute of Biosciences and Medical Technology, Department of Biotechnology, Lady Doak College, University of Witwatersrand, Institute for Systems Biology, Seattle, Washington, USA

Contributors: Palanivel, S., Murugesan, A., Subramanian, K., Yli-Harja, O., Kandhavelu, M.

Publication date: 15 Aug 2020

Peer-reviewed: Yes

Publication information

Journal: European Journal of Pharmacology

Volume: 881

Article number: 173195

ISSN (Print): 0014-2999

Original language: English

ASJC Scopus subject areas: Pharmacology

Keywords: ADME, Apoptosis, Docking, EGFR, Gene expression, Indoline derivatives, QSAR

DOIs:

10.1016/j.ejphar.2020.173195

Source: Scopus

Source ID: 85086163282

Research output: Contribution to journal > Article > Scientific > peer-review

Reversible biofunctionalization of surfaces with a switchable mutant of avidin

Label-free biosensors detect binding of prey molecules ("analytes") to immobile bait molecules on the sensing surface. Numerous methods are available for immobilization of bait molecules. A convenient option is binding of biotinylated bait molecules to streptavidin-functionalized surfaces, or to biotinylated surfaces via biotin-avidin-biotin bridges. The goal of this study was to find a rapid method for reversible immobilization of biotinylated bait molecules on biotinylated sensor chips. The task was to establish a biotin-avidin-biotin bridge which was easily cleaved when desired, yet perfectly stable under a wide range of measurement conditions. The problem was solved with the avidin mutant M96H which contains extra histidine residues at the subunit-subunit interfaces. This mutant was bound to a mixed self-assembled monolayer (SAM) containing biotin residues on 20% of the oligo(ethylene glycol)-terminated SAM components. Various biotinylated bait molecules were bound on top of the immobilized avidin mutant. The biotin-avidin-biotin bridge was stable at pH ≥ 3 , and it was insensitive to sodium dodecyl sulfate (SDS) at neutral pH. Only the combination of citric acid (2.5%, pH 2) and SDS (0.25%) caused instantaneous cleavage of the biotin-avidin-biotin bridge. As a consequence, the biotinylated bait molecules could be immobilized and removed as often as desired, the only limit being the time span for reproducible chip function when kept in buffer (2-3 weeks at 25 C). As expected, the high isoelectric pH (pI) of the avidin mutant caused nonspecific adsorption of proteins. This problem was solved by acetylation of avidin (to pI <5), or by optimization of SAM formation and passivation with biotin-BSA and BSA.

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Multi-scaled biodata analysis and modelling (MultiBAM), Johannes Kepler University, Fimlab Laboratories Ltd, University of Salzburg, University of Basel, University of South Bohemia, Goethe-University Frankfurt

Contributors: Pollheimer, P., Taskinen, B., Scherfler, A., Gusenkov, S., Creus, M., Wiesauer, P., Zauner, D., Schöfberger, W., Schwarzinger, C., Ebner, A., Tampé, R., Stutz, H., Hytönen, V. P., Gruber, H. J.

Number of pages: 13

Pages: 1656-1668

Publication date: 16 Oct 2013

Peer-reviewed: Yes

Publication information

Journal: Bioconjugate Chemistry

Volume: 24

Issue number: 10

ISSN (Print): 1043-1802

Ratings:

Scopus rating (2013): CiteScore 9.1 SJR 2.02 SNIP 1.201

Original language: English

ASJC Scopus subject areas: Biotechnology, Bioengineering, Organic Chemistry, Pharmaceutical Science, Biomedical Engineering, Pharmacology

DOIs:

10.1021/bc400087e

URLs:

<http://www.scopus.com/inward/record.url?scp=84886070072&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 84886070072

Research output: Contribution to journal > Article > Scientific > peer-review

Neuroprotective effect of RO-20-1724-a phosphodiesterase4 inhibitor against intracerebroventricular streptozotocin induced cognitive deficit and oxidative stress in rats

Cyclic nucleotides viz cGMP and cAMP are known to play an important role in learning and memory processes. Enhancement of cyclic nucleotide signalling through inhibition of phosphodiesterases (PDEs) has been reported to be beneficial in several neurodegenerative disorders associated with cognitive decline. The present study was undertaken to investigate the effect of RO-20-1724-a PDE4 inhibitor on streptozotocin (STZ) induced experimental sporadic dementia of Alzheimer's type. The STZ was injected twice intracerebroventricularly (3 mg/kg i.c.v.) on alternate days (day 1 and day 3) in rats. The STZ injected rats were treated with RO-20-1724 (125, 250 and 500 µg/kg i.p.) for 21 days following first i.c.v. STZ administration. Learning and memory in rats were assessed by passive avoidance [PA (days 14 and 15)] and Morris water maze [MWM (days 17, 18, 19, 20 and 21)] following first i.c.v. STZ administration. On day 22 rat cerebral homogenate was used for all the biochemical estimations. The pharmacological inhibition of PDE4 by RO-20-1724 significantly attenuated STZ induced cognitive deficit and oxidative stress. RO-20-1724 was found to not only improve learning and memory in MWM and PA paradigms but also restore STZ induced elevation in cholinesterase activity. Further, RO-20-1724 significantly reduced malondialdehyde and nitrite levels, and restored the glutathione levels indicating attenuation of oxidative stress. Current data complement previous studies by providing evidence for a subset of cognition enhancing effects after PDE4 inhibition. The observed beneficial effects of RO-20-1724 in spatial memory may be due to its ability to restore cholinergic functions and possibly through its antioxidant mechanisms.

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Computational Science X (CompX), Neuropharmacology Div., ISF College of Pharmacy

Contributors: Sharma, V., Bala, A., Deshmukh, R., Bedi, K. L., Sharma, P. L.

Number of pages: 7

Pages: 239-245

Publication date: Apr 2012

Peer-reviewed: Yes

Publication information

Journal: PHARMACOLOGY BIOCHEMISTRY AND BEHAVIOR

Volume: 101

Issue number: 2

ISSN (Print): 0091-3057

Ratings:

Scopus rating (2012): CiteScore 4.7 SJR 1.197 SNIP 0.913

Original language: English

ASJC Scopus subject areas: Biochemistry, Clinical Biochemistry, Pharmacology, Toxicology, Behavioral Neuroscience, Biological Psychiatry

Keywords: Alzheimer's disease, Cognitive dysfunction, Oxidative stress, Phosphodiesterase4, RO-20-1724, Streptozotocin

DOIs:

10.1016/j.pbb.2012.01.004

URLs:

<http://www.scopus.com/inward/record.url?scp=84857569798&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 84857569798

Research output: Contribution to journal > Article > Scientific > peer-review

Evaluation of *Caesalpinia pulcherrima* Linn. for anti-inflammatory and antiulcer activities

Objective: To evaluate the ethanolic and aqueous extracts of aerial parts of *Caesalpinia pulcherrima* (Linn.) Sw. for anti-inflammatory and antiulcer activities. Materials and Methods: Anti-inflammatory action of the ethanolic and aqueous extracts of *C. pulcherrima* (100 and 200 mg/kg b.w.) (CPE and CPA) were evaluated by cotton pellet granuloma models. Pylorus ligation and aspirin induced ulcer models were employed for evaluating antiulcer activity for both the extracts. Ulcerogenic potential of CP was also evaluated. Result: The ethanolic and aqueous extracts of *C. pulcherrima* significantly decreased (P

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Computational Science X (CompX), Department of Pharmacology, K.L.E. Society's College of Pharmacy
Contributors: Sharma, V., Rajani, G.
Number of pages: 4
Pages: 168-171
Publication date: Apr 2011
Peer-reviewed: Yes

Publication information

Journal: INDIAN JOURNAL OF PHARMACOLOGY

Volume: 43

Issue number: 2

ISSN (Print): 0253-7613

Ratings:

Scopus rating (2011): CiteScore 1.2 SJR 0.309 SNIP 0.776

Original language: English

ASJC Scopus subject areas: Pharmacology, Pharmacology (medical)

Keywords: Anti-inflammatory, antiulcer, Caesalpinia pulcherrima (Linn.) sw

DOIs:

10.4103/0253-7613.77354

URLs:

<http://www.scopus.com/inward/record.url?scp=79957552659&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 79957552659

Research output: Contribution to journal › Article › Scientific › peer-review

CARING (CAncer Risk and INSulin analogues): The association of diabetes mellitus and cancer risk with focus on possible determinants - a systematic review and a meta-analysis

Background: Patients suffering from diabetes mellitus (DM) may experience an increased risk of cancer; however, it is not certain whether this effect is due to diabetes per se. Objective: To examine the association between DM and cancers by a systematic review and meta-analysis according to the PRISMA guidelines. Data Sources: The systematic literature search includes Medline at PubMed, Embase, Cinahl, Bibliotek.dk, Cochrane library, Web of Science and SveMed+ with the search terms: "Diabetes mellitus", "Neoplasms", and "Risk of cancer". Study Eligibility Criteria: The included studies compared the risk of cancer in diabetic patients versus non-diabetic patients. All types of observational study designs were included. Results: Diabetes patients were at a substantially increased risk of liver (RR=2.1), and pancreas (RR=2.2) cancer. Modestly elevated significant risks were also found for ovary (RR=1.2), breast (RR=1.1), cervix (RR=1.3), endometrial (RR=1.4), several digestive tract (RR=1.1-1.5), kidney (RR=1.4), and bladder cancer (RR=1.1). The findings were similar for men and women, and unrelated to study design. Meta-regression analyses showed limited effect modification of body mass index, and possible effect modification of age, gender, with some influence of study characteristics (population source, cancer- and diabetes ascertainment). Limitations: Publication bias seemed to be present. Only published data were used in the analyses. Conclusions: The systematic review and meta-analysis confirm the previous results of increased cancer risk in diabetes and extend this to additional cancer sites. Physicians in contact with patients with diabetes should be aware that diabetes patients are at an increased risk of cancer.

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Prostate cancer research center (PCRC), Aalborg University, Norwegian Institute of Public Health, Aalborg University Hospital, Netherlands Cancer Institute, Utrecht University, Karolinska Institutet, University of Helsinki

Contributors: Starup-Linde, J., Karlstad, Ø., Eriksen, S. A., Vestergaard, P., Bronsveld, H. K., de Vries, F., Andersen, M., Auvinen, A., Haukka, J., Hjellvik, V., Bazelier, M. T., de Boer, A., Furu, K., De Bruin, M. L.

Number of pages: 37

Pages: 296-332

Publication date: Dec 2013

Peer-reviewed: Yes

Publication information

Journal: CURRENT DRUG SAFETY

Volume: 8

Issue number: 5

ISSN (Print): 1574-8863

Ratings:

Scopus rating (2013): CiteScore 2.6 SJR 0.539 SNIP 0.612

Original language: English

ASJC Scopus subject areas: Pharmacology (medical), Toxicology, Pharmacology

Keywords: Cancer risk, Diabetes mellitus, Meta-analysis, Neoplasm, Systematic review

URLs:

<http://www.scopus.com/inward/record.url?scp=84891552505&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 84891552505

Research output: Contribution to journal > Article > Scientific > peer-review

Switchavidin: Reversible biotin-avidin-biotin bridges with high affinity and specificity

Switchavidin is a chicken avidin mutant displaying reversible binding to biotin, an improved binding affinity toward conjugated biotin, and low nonspecific binding due to reduced surface charge. These properties make switchavidin an optimal tool in biosensor applications for the reversible immobilization of biotinylated proteins on biotinylated sensor surfaces. Furthermore, switchavidin opens novel possibilities for patterning, purification, and labeling. (Graph Presented).

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Integrated Technologies for Tissue Engineering Research (ITTE), Multi-scaled biodata analysis and modelling (MultiBAM), Fimlab Laboratories Ltd, Johannes Kepler University, Tampere University Hospital

Contributors: Taskinen, B., Zauner, D., Lehtonen, S. I., Koskinen, M., Thomson, C., Kähkönen, N., Kukkurainen, S., Määttä, J. A. E., Ihalainen, T. O., Kulomaa, M. S., Gruber, H. J., Hytönen, V. P.

Number of pages: 11

Pages: 2233-2243

Publication date: 17 Dec 2014

Peer-reviewed: Yes

Publication information

Journal: Bioconjugate Chemistry

Volume: 25

Issue number: 12

ISSN (Print): 1043-1802

Ratings:

Scopus rating (2014): CiteScore 8.7 SJR 1.711 SNIP 1.164

Original language: English

ASJC Scopus subject areas: Biotechnology, Bioengineering, Organic Chemistry, Pharmaceutical Science, Biomedical Engineering, Pharmacology, Medicine(all)

DOIs:

10.1021/bc500462w

URLs:

<http://www.scopus.com/inward/record.url?scp=84918539954&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 84918539954

Research output: Contribution to journal > Article > Scientific > peer-review

Role of the acyl groups in carbohydrate chains in cytotoxic properties of olivomycin A

A series of olivomycin A derivatives containing different combinations of the acyl residues in the carbohydrate chains was obtained. The formation of complexes of Mg²⁺-coordinated dimers of these compounds with double-stranded DNA was studied using spectral methods such as absorption, fluorescence and circular dichroism (CD) spectral analyses. There was a good correlation of the values of binding constants of complexes (antibiotic) 2 Mg²⁺-DNA, the quantum yields of fluorescence and changes of the induced CD spectra with topoisomerase I inhibition and cytotoxicity. We demonstrate that the presence of the acyl groups in the saccharide residues of olivomycin A derivatives is absolutely necessary for a high cytotoxic potency of these antibiotics. On the basis of the experimental results and quantum chemical calculations, we presume that the acyl residue in the 4-O-position in the A-sugar residue is involved, to the most part, in the antibiotic-antibiotic interactions in the (olivomycin) 2 Mg²⁺ dimers, whereas the O-acyl group in E-olivomycoside residue largely participates in the formation of the (olivomycin) 2 Mg²⁺-DNA complexes.

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Frontier Photonics, Russian Academy of Medical Sciences, Emanuel' Institute of Biochemical Physics, Russian Academy of Sciences, N.N. Blokhin Russian Cancer Research Center, Russian Academy of Medical Sciences

Contributors: Tevyashova, A. N., Durandin, N. A., Vinogradov, A. M., Zbarsky, V. B., Reznikova, M. I., Dezhenkova, L. G., Bykov, E. E., Olsufyeva, E. N., Kuzmin, V. A., Shtil, A. A., Preobrazhenskaya, M. N.

Number of pages: 8

Pages: 523-530

Publication date: Sep 2013

Peer-reviewed: Yes

Publication information

Journal: JOURNAL OF ANTIBIOTICS

Volume: 66

Issue number: 9

ISSN (Print): 0021-8820

Ratings:

Scopus rating (2013): CiteScore 3.7 SJR 0.712 SNIP 0.886

Original language: English

ASJC Scopus subject areas: Pharmacology, Drug Discovery

Keywords: Aureolic acid antibiotics, Cytotoxicity, Olivomycin A, Quantum chemical calculations, Spectroscopy, Structure-activity relationships, Topoisomerase I inhibitors

DOIs:

10.1038/ja.2013.39

URLs:

<http://www.scopus.com/inward/record.url?scp=84884999183&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 84884999183

Research output: Contribution to journal › Article › Scientific › peer-review

Solid-phase bromination and Suzuki coupling of 2-carboxyindoles

As part of an ongoing lead discovery project we have developed a convenient method for the modification and substitution of indole moieties at the 3-position. Selective bromination of three different 2-carboxyindoles was followed by Suzuki cross-coupling with aryl and heteroaryl boronic acids on a Merrifield resin solid-phase. After column chromatography, yields of the 3- substituted indoles ranged from 42-98%.

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: University of Helsinki, Department of Pharmacy

Contributors: Tois, J., Franzén, R., Aitio, O., Laakso, I., Huuskonen, J., Taskinen, J.

Number of pages: 4

Pages: 521-524

Publication date: 2001

Peer-reviewed: Yes

Publication information

Journal: Combinatorial Chemistry and High Throughput Screening

Volume: 4

Issue number: 6

ISSN (Print): 1386-2073

Ratings:

Scopus rating (2001): SJR 0.78 SNIP 0.872

Original language: English

ASJC Scopus subject areas: Clinical Biochemistry, Chemistry (miscellaneous), Pharmacology

DOIs:

10.2174/1386207013330887

URLs:

<http://www.scopus.com/inward/record.url?scp=0034861953&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 0034861953

Research output: Contribution to journal › Article › Scientific › peer-review