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8th International PSU – UNS Bioscience Conference

Towards the SDG Challenges

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BOOK OF ABSTRACTS



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RESULTS:

Anisotropic lipophilicity was quantified with retention constants, R_M^0 obtained by applying thin-layer reversed-phase chromatography for 13 newly synthesized 1-aryl-3-methyl succinimide derivatives. All observed compounds are expected to have favorable Caco-2 permeability except compound 5 with carboxylic group which ionizes in physiological fluids. For all analyzed succinimide derivatives short absorption times are expected as well as high absorption rate. Statistically significant parabolic correlation ($r^2=0.447$, $p=0.021$) was determined between Caco-2 permeability (calculated with pkCSM software) and anisotropic lipophilicity. Moreover, statistically significant parabolic association ($r^2=0.710$, $p<0.001$) was obtained between absorption constant, k_a (i-lab 2.0 software) and experimentally determined anisotropic lipophilicity, RM_0 for the observed compounds. Finally, the percent of the absorbed molecules, %absorbed (pkCSM software) was influenced by anisotropic lipophilicity with statistical significance ($r^2=0.622$, $p=0.003$) and described with parabolic function.

CONCLUSIONS:

Lipophilicity is the key characteristic in transport processes, including intestinal absorption and membrane permeability of 1-aryl-3-methyl succinimide derivatives. The increment of lipophilicity of the 1-aryl-3-methyl succinimide core results in enhanced permeability, elevated absorption constants and enlarged bioavailability. However, the augmentation of the permeability through membranes and intestinal absorption as a result of increased lipophilicity is limited probably due to consequent solubility decrement of the studied compounds.

T3-P-11 Subchronic acrylamide treatment induces superoxide dismutase 1 expression in rat liver

Jelena Marković Filipović, Ivana Ivelja, Jelena Karan, Marko Miler, Verica Milošević⁴⁶,
Milica Matavulj⁴⁷

KEYWORDS: acrylamide; liver; superoxide dismutase 1

INTRODUCTION:

Acrylamide (AA) is a widely used chemical and an important monomer in various industrial and laboratory purposes. In addition, AA is formed in many types of fried and oven-baked foods during cooking. Considering proven neurotoxic, carcinogenic and mutagenic effects on living organisms, AA became a main topic of interest for many research groups.

OBJECTIVES:

The objective of our study was to determine whether acrylamide treatment affects superoxide dismutase 1 (SOD1) expression in rat liver.

METHOD / DESIGN:

Adult male Wistar rats were subchronically (three weeks) treated with 25 mg/kg or 50 mg/kg body weight (b.w.) of AA. Formalin-fixed paraffin-embedded liver tissue was cut into 5 μm thin sections and immunostained with anti-SOD1 antibody. The amount of SOD1 in immunostained sections was determined using Windows based ImageJ program (ImageJ, Version 1.50f). The optical density (OD) and stained percentage color area of immunolabeled SOD1 were measured.

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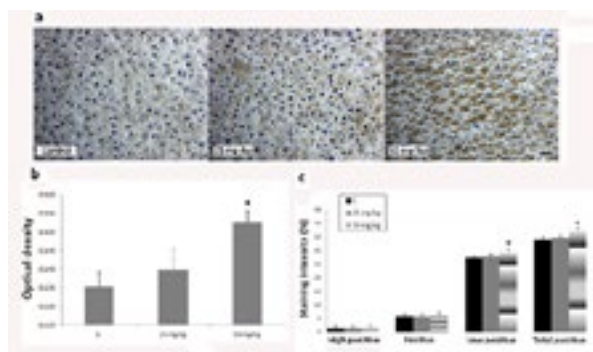
RESULTS:

Figure 1. Representative micrographs of superoxide dismutase 1 (SOD1) immunohistochemical staining in liver of control rats, rats treated with acrylamide (AA) in dose of 25 mg/kg b.w., and rats treated with acrylamide in dose of 50 mg/kg b.w. (a). Optical density of SOD1 immunopositive cells in control and AA-treated rats in doses of 25 mg/kg b.w. and 50 mg/kg b.w. (b). Percentage contribution of high positive, positive, low positive and total positive immunohistochemical staining of SOD1 in control and AA-treated rats in doses of 25 mg/kg b.w. and 50 mg/kg b.w. (c). Values in charts are means \pm SEM; $n = 10$, $*p < 0.05$. In statistical analysis AA-treated animals were compared with the control group.

CONCLUSIONS:

Immunostaining of SOD1 in liver of control rats showed weak cytoplasmic immunoreactivity in hepatocytes (Fig. 1a). AA application induced dose-dependent increase of immunostaining intensity (Fig. 1a). Significant increase of OD and percentage contribution of low positive and total positive cells of immunostained SOD1 was detected in group treated with AA in a dose of 50 mg/kg (Fig. 1b, c).

T3-P-12 Correlation between anisotropic lipophilicity and *in silico* predicted human distribution of 1-aryl-3-methyl succinimide derivatives

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KEYWORDS: lipophilicity; volume of distribution; plasma protein binding; *in silico*; drug design

INTRODUCTION:

Lipophilicity of drug candidates is used in quantitative structure–activity relationship (QSAR) studies, as molecular descriptor in ADME-tox predictions and as structural information about their biological effects. The distribution of drugs in the body depends mainly on their lipophilicity and their potential to bind to plasma proteins.

OBJECTIVES:

To analyze the influence of lipophilicity on the distribution of newly synthesized succinimide derivatives in the human body based on *in silico* predicted volume of distribution and affinity to bind to the plasma proteins.

METHOD / DESIGN:

Thirteen newly synthesized 1-aryl-3-methyl succinimide derivatives were studied by reversed chromatography and their anisotropic lipophilicity was determined. Precoated RP-18W/UV 254 plates (Macherey-Nagel GMBH and Co., Düren, Germany) was used as stationary phase while binary solutions of methanol and water with a varying volume fraction of organic solvent were applied as the mobile phase. The spots were detected at 254 nm with UV lamp. Software package i-lab 2.0 (<https://ilab.acdlabs.com/iLab2/>) was used for determining volume of distribution (Vd) while pkCSM (<http://biosig.unimelb.edu.au/pkcsml/>) was applied for predicting the volume of distribution in stationary state (Vdss) and the fraction of the drug unbound

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