

entry: 3FN3) was chosen for modeling. Multiple alignment process was carried out on the selected sequences by ClustalX2 (protein weight matrix: BLOSUM series). Model building was performed in the program MODELLER9v5 using model-ligand algorithm and models at various refinement levels were generated. Finally the refined structures were minimized under molecular mechanic AMBER method (RMS gradient = 0.5) in HyperChem7.5. All models were validated using the program ERRAT and PROCHECK at UCLA.

Results: The best 3D model had an Errat score of 94%. In the modelled protein all of the glycosyl-linked residues (Asn 83, 91, 138, 157 and 166) are situated in the external region of the 3D structure with steric flexibility of their side chains.

Conclusion: Our modeling supports the data which indicates that vOX2 has two Ig-like domains, located between residue 9 to 120, and 130–160, respectively and the integrin-binding motif, RGD, at residues 190–193 is exposed.

Keywords: KSHV, vOX2, Bioinformatic, 3-D modelling, Protein modelling

doi:10.1016/j.clinbiochem.2011.08.1034

Oral – [A-10-998-1]

Surface proteins, potential drug target for antiviral therapy against Nipah virus and in silico drug design

Rafiqur Rahman^a, S.M. Mahbubur Rashid^a, Manzur Sayeem^a, Istiaq Sharif^a, Kawsar Sharif^b

^aDepartment of Genetic Engineering and Biotechnology, University of Dhaka, Dhaka-1000, Bangladesh

^bDepartment of Pharmacy, North South University, Dhaka, Bangladesh

E-mail addresses: rafiqurrahman41@yahoo.com (R. Rahman), suzandu@gmail.com (S.M.M. Rashid), imsayeem@gmail.com (M. Sayeem), istiaq.sharif@ymail.com (I. Sharif), kawsar4@gmail.com (K. Sharif)

Introduction: Nipah virus being one of the most devastating new varieties in the paramyxoviridae family, started affecting various parts of Bangladesh and neighboring India causing around 106 fatalities. As there is no known cure for Nipah virus infection, it is thought to be a serious threat as bioweapon. We are proposing an in silico based drug by docking strategy and inhibition against the surface proteins of Nipah virus.

Materials and methods: We retrieved the protein sequence of the peptide from the patented source active against influenza virus and the NiV surface protein sequence from NCBI database. The 3D structure of both the proteins was predicted using CPH-model 3 Server. Molecular docking was done of the peptides in their PDB format using PatchDock.

Results: Our process involved docking strategy of our target peptide as an inhibitor against binding site of NiV surface proteins with a docking score above 8000 which is even in case of proposed antiviral activity against hemagglutinin only 5000 indicating as even a better inhibitor for NiV surface proteins.

Conclusion: Our particular therapeutic peptide affective in inhibiting influenza viral replication, the peptide binds to the proteins of Nipah virus with high precision and in a case hits a score over 8000! The energy change of the reactions was impressive. So the computational data supports the peptide as inhibitor of Nipah virus surface proteins.

Keywords: Nipah virus (NiV), Docking, In silico, NCBI, Patchdock, Surface proteins

doi:10.1016/j.clinbiochem.2011.08.1035

Trace Elements in Health and Disease

Oral – [A-10-6-2]

Determining the effects of two essential trace elements on polymerization of human amylin hormone

Seyyed Mehdi Mirhashemi

Biochemistry and Nutrition Department, Faculty of Medicine, Kashan University of Medical Sciences, Kashan, Iran

E-mail address: mirhashemi@kaums.ac.ir (S.M. Mirhashemi)

Introduction: Amyloid beta-sheets observed in diabetes are cytotoxic and may have a prominent role in beta-cell dysfunction. In this research, the effects of iron and copper as two essential trace elements on amylin polymerization were studied in vitro.

Materials and methods: Human amylin peptide and other chemicals were purchased from Sigma-Aldrich Company. Peptide stock solution was prepared by adding 1 ml dimethyl sulfoxide, sonicating at room temperature for 15 min. Stock solution (1 mg/ml) was diluted to a final concentration of 8 µM with PBS, pH: 7.4. Diluted solution was divided into three groups so that each group had six samples. Iron and copper with concentration of 8 µM were prepared in the two separate groups. The samples without the elements were selected as controls. All samples were incubated at 37 °C for 120 h with shaking. To monitor the peptide polymerization, Thioflavin T (ThT) assay was performed. ThT fluorescence measurements were recorded in a fluorescence spectrometer. The results have shown as Mean ± SEM. Means comparison was carried out using t-test and differences are statistically significant at p < 0.05.

Results: The results indicated that ThT fluorescence for control was 32.55 ± 0.51 while these values for iron and copper groups were 36.71 ± 0.44 and 27.70 ± 0.48, respectively.

Conclusion: This research expressed that compared to controls, iron stimulated amylin polymerization while copper had inhibitory effect on formation of beta-amyloid sheet, significantly (p < 0.05). It may be concluded that toxic effects of amylin precipitation on pancreatic beta-cells should be increased by iron toxicity and reduced by copper supplementations.

Keywords: Amylin, Diabetes, Trace elements, Polymerization

doi:10.1016/j.clinbiochem.2011.08.1036

Oral – [A-10-28-2]

Effect of excess iodine on immune system; An in-vitro study

Ghollam-Reza Moshtaghi-Kashanian, Mohammad Hassannejad

Kerman University of Medical Sciences, Kerman, Iran

E-mail addresses: moshtaghikashanian@hotmail.com (G.-R. Moshtaghi-Kashanian), cb1360@gmail.com (M. Hassannejad)

Introduction: While iodine is an essential element for the synthesis of thyroid hormones, epidemiological studies showed consumption of iodine leads to autoimmune thyroid diseases, with unknown mechanism. Previous studies showed disturbance in the circulating cytokines could lead to autoimmune diseases. To determine the role of iodine in cytokine production and development of thyroid autoimmune diseases, whole blood was stimulated with NaI (10 mM) and I2 (0.5 mM).

Materials and methods: After evaluation of laboratory results of 25 healthy middle age female (age 40–45 years), 10 subject who had matching results were selected. Ten ml of sterile heparinized peripheral blood was collected for each subject and immediately divided to 6 groups (control, NaI stimulated, I2 stimulated and matching groups in presence of standard stimulators (LPS 1 µg/ml & PHA 10 µg/ml). Three identical sets were setup to investigate the

cytokine production at 24, 48, and 72 hours. All samples were incubated in cell culture incubator (95% O₂ and 5% CO₂) and after elapse of appropriated time, plasma were separated from each well and kept at -70 °C till the time of cytokines (IL-4, IL-10, INF- γ and TGF- β 1) analysis.

Results: Statistical analysis of data showed NaI could decrease ($P < 0.02$) the production of TGF- β 1 at all time points, while it did not affect the level of other cytokines. On the other hands, I2 significantly decreased the level of IL-4 and IL-10 ($P < 0.01$). In presence of LPS/PHA, NaI also reduced the production of IL-10 ($P < 0.02$), while I2 decreased the level of IL-4 as well as IL-10 ($P < 0.01$).

Conclusion: For the first time the results of the study indicated high levels of NaI and I2 may reduce the level of protective cytokines in circulation. Finally, since neither thyroid hormones nor thyroid gland had role in this process, it may be conclude high consumption of iodine could leads to imbalance cytokine production in blood and initiation autoimmune thyroid.

Keywords: Autoimmune thyroid diseases, High iodine intake NaI, I2, TGF-beta, INF-gama, IL-4 and IL-10

doi:10.1016/j.clinbiochem.2011.08.1037

Oral – [A-10-92-1]

Comparing of lead level in breast milk and cow's milk

Ahmadshah Farhat^a, Ashraf Mohammadzadeh^b, Mahdi Balalimood^c, Habibollah Esmaily^b, Motavali Haghi Simin^b

^aNeonatal Research Center, School of medicine, University of Medical Sciences, Mashhad, Iran

^bMashhad, University of Medical Sciences

^cMedical Toxicology Research Center, Mashhad, University of Medical Science

E-mail addresses: farhata@mums.ac.ir (A. Farhat), mohamadzadeha@mums.ac.ir (A. Mohammadzadeh), BalalimoodM@mums.ac.ir (M. Balalimood), EsmailyH@mums.ac.ir (H. Esmaily), nrc@mums.ac.ir (M.H. Simin)

Introduction: Lead has many applications and its toxic effect can pollute the environment. Also, it is very dangerous for embryo and children under 7. Regarding the high level of lead in children's and mothers' blood in Mashhad, we investigate the amount of lead in mother's milk which is main nutrient of the newborn and cow milk which has an important role in under-seven-children's nutrition.

Materials and methods: This study was a cross sectional that 5-10 ml of 120 mothers' milk after the 7th day of milking who took their newborn to Imam Reza neonatal clinic and cow milk distributed in Mashhad markets (from 6 factories, n = 18) were collected. The lead level of the collected samples was measured in toxicology department of the same hospital after digestion with atomic absorption spectrophotometry method. The questionnaire contained age, height and weight of the newborn, weight, age, education status and the occupation of the mother and father's education and income and the pregnancy age. The data were analyzed by spss independent t-test, one-way ANOVA correlation methods.

Results: The mean level of the lead in mothers' milk was 36.28 ± 7.48 $\mu\text{g/l}$ and for cow milk was 16.27 ± 4.67 which their difference was significant ($P < 0.001$). The relationship between the residual area of the parents and lead level was significant ($P < 0.001$) and the pregnancy age with lead level was also significant ($P = 0.037$) but it was insignificant with other factors.

Conclusion: The lead level of mothers' milk is more than cow milk. The less level of the lead in cow milk can be due to the living situation of the cows in not polluted places or their physiological factors or the production procedures of the milk, which needs more

investigation. The lead level of mothers' milk in rural areas is less than urban areas ($P < 0.001$). The reverse correlation between lead level and pregnancy age may show the effect of lead on preterm labor.

Keywords: Mother's milk, Cow's milk, Lead

doi:10.1016/j.clinbiochem.2011.08.1038

Oral – [A-10-173-2]

Relationship between low birth weight neonate and some micronutrients

Ashraf Mohammadzadeh^a, Ahmadsha Farhat^a, Nayere Khadem^b, Mohammad Reza Parizadeh Seyed^b, Mohammad Khajedaluae^b

^aNeonatal Research Center, School of Medicine, University of Medical Sciences, Mashhad, Iran

^bWoman's Health Research Center, School of medicine, Mashhad, University of Medical Sciences

E-mail addresses: mohamadzadeha@mums.ac.ir (A. Mohammadzadeh), farhata@mums.ac.ir (A. Farhat), KhademN@mums.ac.ir (N. Khadem), ParizadehMR@mums.ac.ir (M.R. Parizadeh Seyed), KhajedaluaeM@mums.ac.ir (M. Khajedaluae)

Introduction: Trace element deficiencies have been documented to play an important role in determination of the fetal outcome. It has been reported that the pregnant women in developing countries consume diets with a lower density of minerals and vitamins. The aim of study was to determine serum selenium, copper and zinc concentration in pregnant women and risk of low birth weight (<2500 g) in their newborns.

Material and methods: We conducted a case-control study on women who delivered low birth weight infants (Cases), and women with normal birth weight infants (Controls). We collected blood samples from all women within 24 hours after delivery, and assessed the concentration of selenium, copper and zinc using atomic absorption spectroscopy (AAS). Then compared serum concentration values between two groups. Multiple linear regression analysis was performed to control of potential confounding variables.

Results: A total of 117 mothers were studied, of them 65 Cases with a low birth weight infants (1845 ± 472 g) and 52 Controls (birth weight = 3166 ± 435 g). Mothers in the Cases and Controls groups did not differ in age (24 ± 4 vs. 24.7 ± 5.4 years), body mass index (23.4 ± 3.4 vs. 22.9 ± 3.2), and socioeconomic or demographic factors. Maternal selenium concentration ($\mu\text{g/l}$) did not differ between Cases and Controls; 118.8 ± 24.5 $\mu\text{g/l}$ vs. 122.5 ± 29.3 $\mu\text{g/l}$ respectively ($P > 0.05$). Maternal selenium did not differ between premature and full term deliveries. It also did not differ when newborns were small for their gestational or not. Maternal copper concentration ($\mu\text{g/dl}$) did not differ between Cases and Controls; 1158.35 ± 299.57 $\mu\text{g/dl}$ vs. 1187.11 ± 249.59 $\mu\text{g/dl}$ respectively ($P = 0.58$). Maternal copper did not differ between premature and full term deliveries. It also did not differ when newborns were small for their gestational or not ($P = 0.29$). Maternal zinc concentration differ between control and case; 753.34 ± 15 $\mu\text{g/l}$ vs. 654.76 ± 12 $\mu\text{g/l}$ respectively ($P < 0.01$) maternal zinc differ between preterm and full term delivery ($P < 0.001$).

Conclusion: Maternal selenium and copper concentration has no impact on neonatal birth weight or premature deliveries but zinc deficiency has effect on low birth weight delivery.

Keywords: Maternal serum selenium, Copper and zinc, Low birth weight, Normal birth weight

doi:10.1016/j.clinbiochem.2011.08.1039