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POSTERS

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P-20-012
Peptide-protein conjugation in the context of targeted therapy: modeling and experiment

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Bioconjugation techniques are widely used in the area of imaging, drug delivery, mapping of protein interactions, etc. One particularly intriguing line of research is development of irreversible inhibitors for use in targeted therapy, including covalent peptidic ligands. In this context, it should be useful to develop a modeling technique to assess the feasibility of covalent binding and to predict possible changes in target protein structure in response to ligand binding. To develop such computational technique, we have chosen the model system reported by Yu et al. which consists of N-terminal SH3 domain from adapter protein Grb2 and its Sos1-derived peptide ligand containing non-native C-terminal residue (chloroacetyl lysine, X'). Using NMR spectroscopy, mass-spectrometry and other techniques, we have shown that the modified peptide initially binds to its target non-covalently before reacting with the proximal cysteine C32 at the binding site. We profiled the pH dependence of this reaction, demonstrating that it proceeds via the thiolate anion. Based on these experimental observations, we have designed an MD-based protocol to model the conjugation of Sos1X' with Grb2 N-SH3. Specifically, we have derived a set of force-field parameters necessary to model the non-native reactive amino acid, chloroacetyl lysine, as well as the resulting thioether linkage. We have also devised a procedure to model the formation of covalent bond while avoiding any significant perturbations to the macroscopic MD parameters. A series of MD simulations with the net length of 10 μs led to high-quality atomic models of Grb2 N-SH3 / Sos1X' conjugates. These models have been successfully validated using the experimental NMR chemical shift data. We believe that the new methodology presented in this report will help to develop new covalent peptide inhibitors targeted toward cell-surface receptors implicated in human diseases. This research was supported by RSF grant 15-14-20038. *The authors marked with an asterisk equally contributed to the work.

P-20-013
New chromogenic and fluorogenic substrates of glutamine specific peptidases

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Proteins with high content of Gln residues are often resistant to hydrolysis. For instance, complete hydrolysis of prolamins – major proteins of cereal seeds – is a problem due to repeated sequences with Pro- and Gln-rich motifs. Hydrolysis of prolamines in the human stomach "stops" at the step of large peptides. Some of these peptides are toxic to people predisposed to autoimmune disease of the gastrointestinal tract – celiac disease. Currently no drugs are available against this disease. Patients are prescribed to life-long refusal of food containing wheat, rye and barley. Treatment of celiac disease may be achieved by enzyme therapy using postglutamine-cleaving peptidases (PGCP). PGCP may also be used in processing of food raw materials for gluten-free foods. However, most of the known enzymes including human and mammalian digestive enzymes do not cleave Gln-rich peptides. The search for new PGCP is difficult because they are rare, but the key problem is the lack of reliable and sensitive compounds suitable for screening and detection of PGCP. The aim of this work was to create selective and effective Gln-containing substrates for different PGCP, including cysteine peptidases of the papain C1 family. General formula of synthesized substrates is Glp-Phe-Gln↓B, where B = pNA, AMC. Synthesis of the substrates was performed by fragment condensation. Hydrolysis of the obtained substrates was studied by plant enzymes papain, bromelain, ficin, lysosomal mammalian cathepsins B and L, and digestive cathepsin L of an insect stored product pest Tribolium castaneum. All tested substrates were cleaved by all cysteine peptidases. The important advantage of the proposed substrates to the commercially available Arg-containing substrates is the selectivity for the cysteine peptidases, and the ability to differentially test the activity of cysteine peptidases in complex multi-component natural mixtures. This work was supported by RFBR grants 17-54-61008 Egypt_a and 18-04-01221_a.

P-20-014
Human adipose-derived stem cells behaviour and cytoskeleton development in contact with electrospun fibrous gelatin materials enriched with magnetic nanoparticles

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Magnetic nanoparticles (MNPs) are currently used as bioactive cues for therapy in nanotechnology and medicine. Recently, incorporating MNPs in different polymeric materials designed for tissue engineering (TE) generated better biocompatibility and positive cell response in contact with the composites. Here, we tested electrospun fibrous biocomposites, based on fish gelatin, loaded with 1–2% MNPs exposed or not to a static magnetic field (FG_MNPs) for biocompatibility and potential to support cell adhesion, namely focal adhesions formation. Fibers were crosslinked with ethanolic glutaraldehyde to prevent dissolution in culture media. Fibers morphology and the homogenous distribution of MNPs within the fibers was shown in electron microscopy. After seeding human adipose-derived stem cells (hASCs) on FG_MNPs substrates, MTT and LDH assays were performed, together with confocal microscopy to visualize live and dead cell population. Additionally, immunolabeling for β-tubulin and paxillin, together with phalloidin-FITC staining were used to study in depth cell attachment to the substrates. No significant cytotoxic effect was reported for all tested compositions. Better cell viability and proliferation were found in contact with FG_MNPs 2%, as compared to FG control and composites with lower MNPs-content. Cell attachment was enhanced in the presence of MNPs, suggested by better developed F-actin

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