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POSTERS

Table of Contents

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* Each poster has been given a unique number beginning with the letter P; the next part relates to the session in which the poster will be presented.

P.01 Molecular mechanism of inflammation-related diseases
P.02 DNA variation
P.03 Cardiovascular diseases
P.04 Intracellular ion channels and transporters
P.05 RNA processing
P.06 Signal transduction
P.07 Mitochondria and signaling
P.08 DNA architecture
P.09 RNA transcription
P.10 DNA editing and modification
P.11 RNA transport and translation
P.12 Single cell analysis and imaging
P.13 Calcium and ROS signalling
P.14 Sulfur metabolism and cellular regulation
P.15 Molecular neurobiology
P.16 RNA turnover
P.17 Cytoskeleton and molecular mechanisms of motility
P.18 Rare diseases
P.19 Signaling in brain cancer
P.20 Synthetic biopolymers for biomedicine
P.21 Integrative approaches to structural and synthetic biology
P.22 Induced pluripotent cells
P.23 Long noncoding RNA
P.24 Neurodegeneration
P.25 Cell therapy and regenerative medicine
P.26 Small noncoding RNA
P.27 Proteins: structure, disorder and dynamics
P.28 Plant biotechnology
P.29 Natural networks and systems
P.30 RNA in pathogenesis and therapy
P.31 Molecular biology of aging
P.32 Plant–environment interaction
P.33 Synthetic networks and systems
P.34 Multicomponent complexes
P.35 Cell signaling in tumor biology
P.36 Bionanotechnology
P.37 Epigenetics and protein glycosylation
P.38 Genome editing (CRISPR)
P.39 Proteomic technologies
P.40 Education, training, and career planning in molecular life sciences
P.41 General topics – various

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P-20-022
Fluorescence and circular dichroism spectroscopy studies of interactions between interferon α2b and yeast oligoribonucleotides

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RNA-based drugs can bind epigenetic regulators and transcriptional proteins and affect their activity. Using fluorescence quenching we determined dissociation constants for interactions of yeast oligoribonucleotides (ORNs), their Na^+ salts (ORNsNa), and complex with D-mannitol (ORNs-D-M) with Interferon α2b – a key protein of the antiviral cell defense mechanism. Using ORD CD we analyzed conformational changes of the protein. Mass spectrometric analysis showed that the dominant fraction consisted of RNA oligomers of 4–7 nucleotides in length. The analysis of IFN secondary structure changes was made by external service (Bestsel). For INF/ORNs-D-M the dissociation constant Kd=6,96±1.019 μM was found, while those for IFN/ORNs and INF/ORNsNa Kd=5.38±0.423 μM and Kd=9,64 ±2.259 μM, respectively, were noted. The analysis of IFN secondary structure showed 27.2% of α-helix (α-h), 26.9% of antiparallel β-stand (aβ-s), 0% of parallel β-stand (pβ-s), 9% of β-turn and 39.9% of random coil (r.c.) Upon addition of ORNs we observed 0% α-h, 33.3% aβ-s, 0% pβ-s, 21.2% β-turn and 45.5%, r.c., so one can note an increase in β-turn content compared to the native protein. Addition of ORNs-D-M gave 0.8% α-h, 54.4% aβ-s, 30.4% pβ-s, 5.6% β-turn and 8.9% r.c., so increase in aβ-s contents was found. On the other hand, addition of ORNsNa led to 1.5% α-h, 44.4% aβ-s, 42.8% pβ-s, 0% β-turn and 11.3% r.c. (increase in aβ-s and pβ-s content). CONCLUSIONS: ORNs and ORNs-D-M interact with IFN more strongly than ORNsNa. The observed effects of different forms of ORNs on the secondary structure of INF can be explained by involvement of various binding sites.

Integrative approaches to structural and synthetic biology

P-21-001
Validation of a new gas chromatography-mass spectrometry (GC-MS) method to evaluate aromatase activity

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Estrone (E_1) and Estradiol (E_2) are steroidal molecules with regulatory functions in normal breast and in estrogen-receptor positive (ER^+) breast cancers. These estrogens are converted from the androgens, androstenedione (A) and testosterone (T), through an aromatization process catalysed by the enzyme aromatase. Thus, aromatase inhibitors (AIs) are considered the first-line treatment for ER^+ breast cancers. Currently, the screening of new potent AIs is performed trough a radiometric assay, in human placental microsomes, that relies on the quantification of tritiated water resultant from the conversion of a radiolabelled substrate, [1β-^{3}H] androstenedione. As this method is expensive and not environmental-friendly, we aimed to develop a new simple and fast GC-MS method to quantify A and E_1, and consequently, determine aromatase activity. Method performance was evaluated through linearity, limit of detection (LOD), limit of quantification (LOQ), precision and accuracy. The method showed good linearity with a coefficient of determination (r^2) of 0.9884 and 0.9974, for A and E_1, respectively. LOD were 3 nM and 1.5 nM while LOQs were 10 nM and 5 nM, for A and E_1, respectively. The relative standard deviation (%RSD) of the intra- and inter-day precision were lower than 18% and the extraction efficiency was higher than 65%, for both hormones. Moreover, the dose-responses curves for Exemestane, Anastrozole and Letrozole, the AIs used in clinic, were compared to the ones obtained by the radiometric assay, being the rate of inhibition similar in both methods. Therefore, this new GC-MS method is sensitive and precise for the simultaneous quantification of androgens and estrogens and suitable to estimate aromatase activity. Tiago Augusto thanks Fundação para a Ciência e Tecnologia (FCT) for PhD grant (BD/128333/2017) funded by FCT PhD i3DU Programme. Sara C. Cunha acknowledges FCT for the IF/01616/2015 contract. *The authors marked with an asterisk equally contributed to the work.

P-21-002
Investigation of dipeptides binding to double-stranded DNA using molecular modeling and docking

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Peptides are promising drug candidates due to its high chemical diversity, selectivity, broad range of targets, low toxicity and accumulation in tissues than that of small drug like organic compounds. It is known that DNA is a target for many ligands of different chemical nature, including globular proteins, low molecular weight organic compounds and metal ions. However, there are only a few crystal structures of DNA complexes with short peptides in PDB. This is particularly surprising given large number of known interactions of short peptides with globular proteins used by living cell in the course of evolution. In this work we systematically analyzed ability of dipeptides (all possible combinations of the 20 standard amino acids) to bind with all possible combinations of tetra-nucleotides in central part of double-stranded DNA in classic B-form using molecular docking (ICM-Pro, Molsoft LLC) and molecular dynamics (AMBER, University of California). Totally 108800 DNA complexes of dipeptides with free and blocked N- and C-termini were analyzed. Our results indicate that vast majority of dipeptides showed no abilities of DNA binding. As can be expected the most preferable DNA binders are positively charged peptides containing Arg+ and Lys+, although with very low selectivity. However, we also were able to identify dipeptides capable of selective binding with only one or two DNA sequence motifs. These results were confirmed by MD simulations of the low energy complexes in a periodic water box. We present complete maps of dipeptide-DNA interactions including structural features essential for DNA binding. It was found that N- and C-terminal blocking groups significantly increase selectivity of the dipeptide binding to DNA indicating potentially much higher DNA binding selectivity of tri- and tetra-peptides. These findings may improve our understanding of mechanisms of interactions of short peptides with DNA that may have both theoretical and practical significance.