

tetrahedron have been obtained, and X-ray crystallography has been used for characterization. As a proof of concept, metal-containing porphyrins, specifically Fe(III) meso-Tetra(4-sulfonatophenyl) porphine chloride, have been implemented for testing of the encapsulation of a metal-containing molecule inside of the DNA cage. Upon reduction of the metal through coordination of two orthogonally oriented peptides covalently attached to the DNA tetrahedron which contain terminal histidine residues, iron (III) becomes EPR active and the assembly can be analyzed electrochemically. Upon assembly of the complete metal-containing center (both porphyrin molecule and aOEC), x-ray crystallography, EPR, and electrochemistry will be used to test functionality in the stable DNA framework.

3241-Pos Board B102

Formation and Characterization of DNA-Concatemers

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Self-assembly is a spontaneous process in which small objects could combine to form larger and more complex constructs. Here we present experiments on how to use two sequence-designed single stranded nucleotideoligos (50 bases) to form fairly long (>500 base pairs) double stranded DNA concatemers by hybridization due to the recognition of complementary bases on the two strands. To optimize the construction of long DNA concatemers, the incubation conditions have been varied, such as oligo concentration, salt concentration, hybridization time and presence of congesting agents as poly vinyl alcohol. Formed concatemers were characterized by gel-electrophoresis and Atomic Force Microscopy (AFM) to investigate the size and shape distribution.

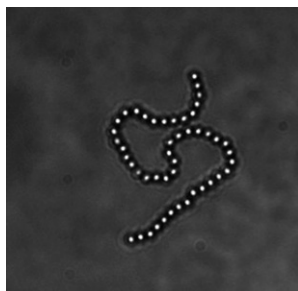
3242-Pos Board B103

DNA-Linked Magnetic Particles: A Model Macromolecule

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We have recently formed novel colloidal "polymers" by utilizing a magnetic field to align and DNA to cross-link paramagnetic colloidal particles into chain structures. Depending on the length of DNA used during linking, these chains have distinct properties, such as variations in elasticity. Combined with the magnetic properties of the particles, they can be used as model systems to study biopolymer dynamics at the micron scale. I will discuss a how to utilize and optimize experimental parameters to synthesize more stable and reliable colloidal models of biomolecular assemblies.



3243-Pos Board B104

A Multiscale Approach to RNA 3D Structure Prediction

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One of the key issues in the theoretical prediction of RNA stability and structure is how to predict the loop free energy. Experimental results have shown strong sequence-dependence of the loop free energy. However, most currently available models only account for the loop length-dependence of the loop free energy. We recently developed a three-bead coarse-grained model to generate the three-dimensional conformations for RNA hairpin loops. Based on the pseudo-torsion angles for the coarse-grained structures, we can extract a set of pseudo-torsion angle-based statistical potential parameters from the known structures. The statistical potential parameters enable folding predictions of the low-energy coarse-grained 3D structures from the sequence. Further molecular dynamics computations for an ensemble of decoy conformations about the predicted coarse-grained structures lead to the final all-atom structures. A notable advantage of the approach is the use of the statistical potential for evaluating

the loop free energies and guiding the search for the low-energy coarse-grained structures from the sequence.

3244-Pos Board B105

Biochemical Studies of a Long Noncoding RNA Involved in Breast Cancer Biology

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Long non-coding RNAs, a significant fraction of the transcriptome in higher eukaryotes, are emerging as key players in many rapidly growing areas of biology, including embryonic stem cell differentiation, brain function, subcellular compartmentalization, chromatin remodeling and cancer biology. We report one of the first biochemical characterizations of a long ncRNA, which coactivates sex hormone nuclear receptors and is strongly associated with breast cancer. This was the first RNA proven to act as a regulatory non-coding RNA and to code for a protein. To date, eleven variant transcripts of the long ncRNA have been identified. We study three: 1) a noncoding isoform, 2) a coding isoform, and 3) an intron-comprising noncoding transcript, which is alternatively spliced and possesses a partial intron insertion. To assess the secondary structures of the selected RNAs and map their overall structural organization, we employ chemical probing tools at select experimental conditions.

3245-Pos Board B106

Functional Non-Coding RNA Coding Vascular Epigenetics: Chance and Necessity in Adaptation Reactions

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OBJECTIVE: Noncoding ncRNAs, the main RNA transcript fraction, were investigated in epigenetic vascular [angiogenic/arteriogenic] phenotype biology. Background: From same genotype [twins, clones, polyphenisms], different phenotypes may result from coded genetic [Mendelian] information and epigenetic [non-Mendelian] reactions; e.g. normal, functionally efficient, organized and abnormal, inefficient, mess-chaotic [tumor] tissues. The genetic code was deciphered. Epigenetic reaction principles [episcruption, ~"overscription"] including posttranslational modifications are still debated whether just being chance reactions or coded [necessity, algorithms]. **METHODS:** Ann.N.Y. Acad.Sci. **1022:**163-184,2004; **1137:**316-342,2008; Biophys.J. **98:**659a,2010; **96:**62a,2009. **RESULTS:** Angiotropin-related functional fncRNAs were isolated and sequenced from endothelial cells and macrophages following chance reactions by environmental chemical and physical factors. In focus were extrinsic metabolic, hypoxia and mechanosensitive [shear stress] factors and ncRNA-riboswitch regulation of hypoxia-inducible, Krueppel, inositol:NADP-epimerase- and NADPH-oxidase-associated transcription factors. fncRNAs are non-Mendelian spliced, modified, edited, redox- and metalloregulated, 5'-end-phosphorylated small hairpin bioaptamers [<200 n]. Modified bases/nucleosides are e.g. isoguanine/isoguanosine/crotonoside, adenine/adenosine-N1-oxide of 151Da base families. Biosynthetically, these result from Fenton-type redox-OH*-radical RNA modification by environmental factors [hypoxia, metal ions, reductones/vitamins]. By 5'-CUG-3'-hairpin loops, fncRNAs regulate phenotypic adaptation to environmental needs by complementary interaction with defined conserved homologous helix-nucleating Mendelian consensus domains shared in epigenetic regulator proteins. Unrelated sequences/conformations and precursors without modifications showed no function. **CONCLUSIONS:** The results suggest novel mechanisms and therapeutic targets for metabolically and hemodynamically switched vascular adaptation [angiogenesis/arteriogenesis], like collateral safeguard circulation [form follows function]. For epigenetic imprinting and inheritance, extrinsically induced chance and heuristic reactions in algorithmic [necessity] processes include sequences of finite instructions in which probabilistic randomness may be incorporated. Although molecular self-organization of some final phenotype patterns seemingly may reflect Fibonacci relations [golden ratio], beyond instructions, chance *and* necessity spatiotemporal relations generate non-Mendelian fncRNA diversity for best fitting codes in interactions with Mendelian biomolecules and influence how selection impinges on [transient] phenotypes.