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LIQUID CRYSTAL FORMATION BY BASE-PAIRING AND DUPLEX STACKING OF MONONUCLEOSIDE TRIPHOSPHATES IN AQUEOUS SOLUTION

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Introduction: Nucleic acid (NA) oligomers as short as 4 base pairs can carry out the self-assembly steps of duplexing, end-to-end aggregation of duplexes, and condensation of aggregates to form columnar liquid crystal phases. In such phases the molecules, self-selected because of their complementarity, create a fluid structural and chemical environment in which oligomer ligation into longer polymers can be strongly promoted [1]. This ligation represents an autocatalytic step in a positive feedback loop in which the liquid crystal structure selects, organizes and polymerizes molecules, thereby enhancing its own stability. Such a scenario has been proposed as a mechanism for the appearance of sequence-directed assembly in early life, and for providing polymer feedstock to the RNA world [2]. However, starting from even few-base oligomers is problematical, because such families of molecules are already highly selected. Any realistic scenario must start from pools of simpler and more diverse molecular species. In this paper we demonstrate that mixtures of single nucleobase species in aqueous solution can order into liquid crystal phases in which the key elements of base-pairing of nucleosides, columnar stacking of base-pairs, and of complementarity-dependent selection are operative. We observe for the first time duplex columnar liquid crystal order in aqueous solution of dATP/dTTP and dGTP/dCTP at high concentrations (~700mg/mL) and low temperature (5°C) [Figure 1]. Liquid crystal phases were not observed in mixtures containing only individual triphophates and were observed in mixtures containing all four dNTPs. These observations set the stage for exploration of ligation reactions involving formation of natural phophodiester bonds by pyrophosphate elimination.

References: [1] Fraccia TP et al. (2015) *Nature Communications* 6:6424, DOI:10.1038/ncomms7424. [2] Fraccia TP et al. (2015) Origins of Life and Evolution of Biospheres **45**, (1-2), 51-68 DOI: 10.1007/s11084-015-9438-1

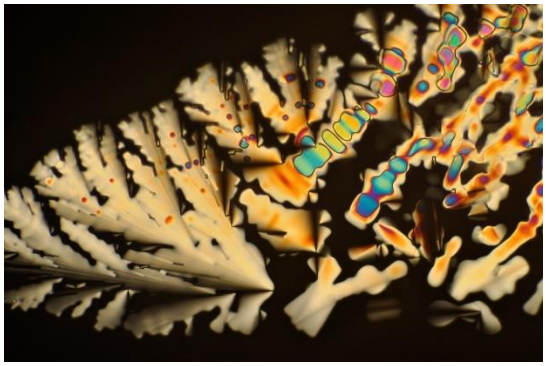

Figure 1- Polarized light microscopic image of dATP/dTTP aqueous mixture columnar fan textures.

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