A Bioactive Saccharides Hydration 'Soulmate' Mechanism: Synergistic Intermolecular Hydrogen Bonding with (2,3-Dihydroxypropyl) Arginine HCl

NT-65

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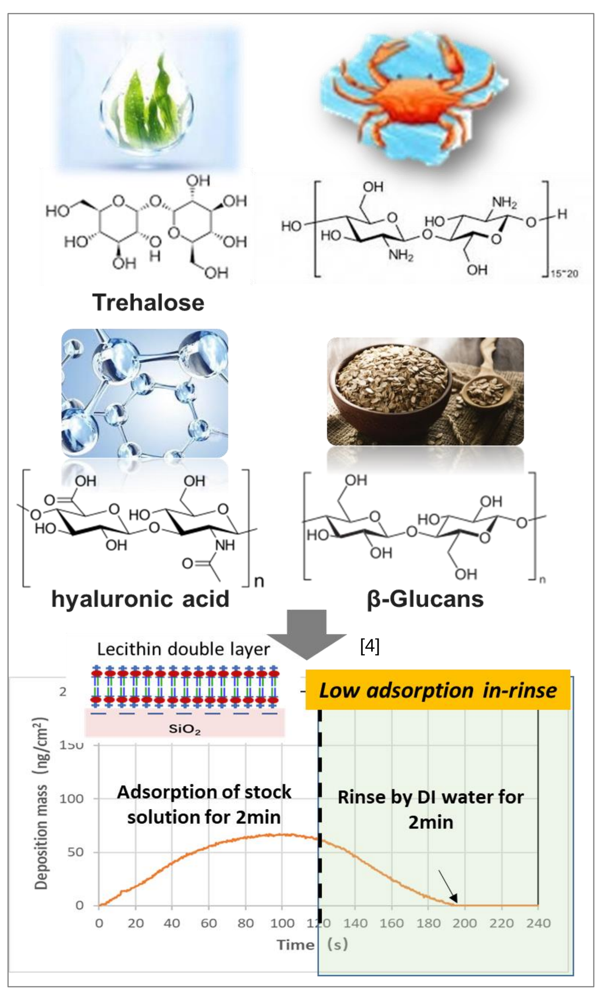
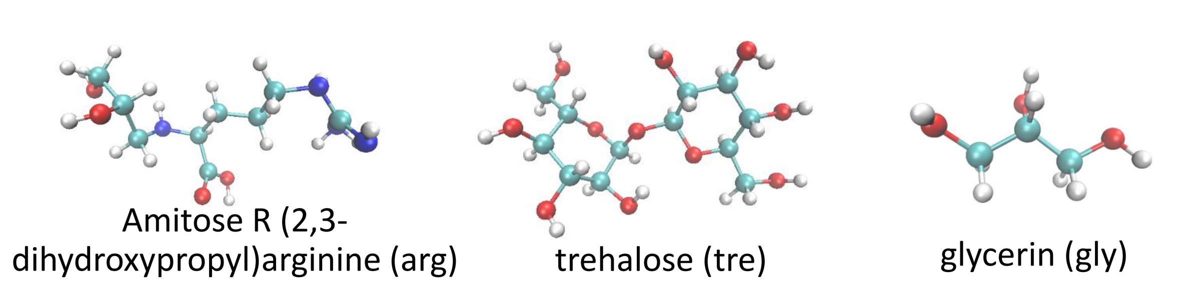
Introduction:

Long-lasting moisturization is an enduring hot topic of cosmetic research. Bioactive saccharides are rising stars in functional cosmetics particularly for hydrating products in China market due to their excellent biocompatibility, biodegradability and naturality (***McCranie and Bachmann, 2014; Miao J et al., 2020***). Improving the hydration properties of saccharides via bioactivity enhancement has been extensively studied. Yet, most approaches either involve sophisticated chemistry or lack of versatility towards universal applications (***Farinha and Freitas, 2020***). Deposition efficacy in rinsing, the inter-/intra-molecular and molecule/substrate interactions, together play a key role in hydration. Unfortunately, most bioactive saccharides are hydrophilic or negatively charged, causing low surface adsorptions upon rinse. For the first time we report a bioactive saccharides hydration 'soulmate' mechanism through a synergistic intermolecular hydrogen bonding with (2,3-dihydroxypropyl) arginine HCl to achieve enhanced 1) deposition efficacy, 2) long-lasting moisturization and 3) superior sensorial performance.



Materials & Methods:

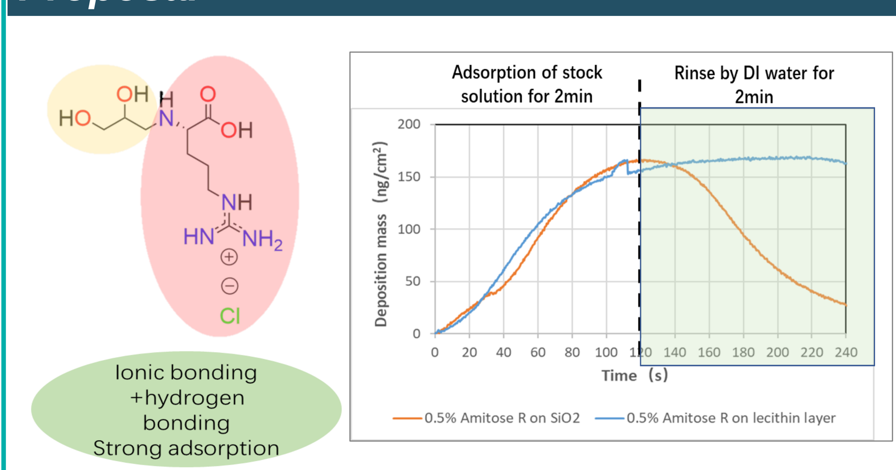
Major Model Materials



Composition	Acronym
1% trehalose	1% Tre
0.5% (2,3-dihydroxypropyl) arginine	0.5% Arg
0.5% glycerin	0.5% Gly
1% trehalose +0.5% (2,3-dihydroxypropyl) arginine	1% Tre+0.5% Arg
1% trehalose +0.5% glycerin	1% Tre+0.5% Gly

- (2,3-dihydroxypropyl) arginine HCl (Arg) is obtained from Seiwa Kasei Co., Ltd. (Osaka, Japan). Trehalose (Tre) is selected here as a model system of bioactive saccharide. Tre is obtained from Nagase (China) Co., Ltd. (Shanghai, China). Glycerin (Gly) is from Aladdin (AR, 99%).
- All simple solution mixtures are prepared with DI water at room temperature with magnetic stirring until fully dissolved. The samples are listed in Table 1.

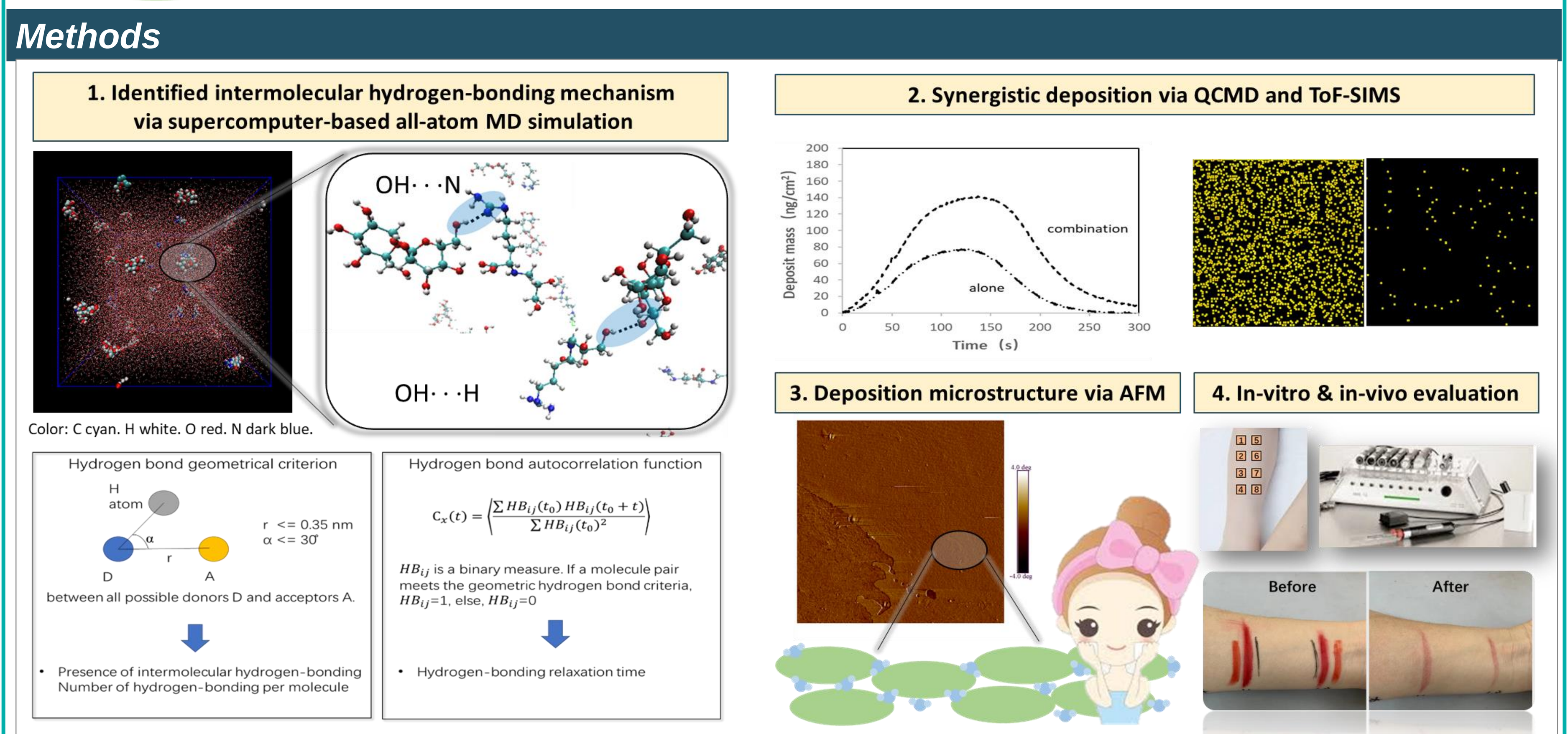
Proposal



What if combining the benefits of Arg and Tre?

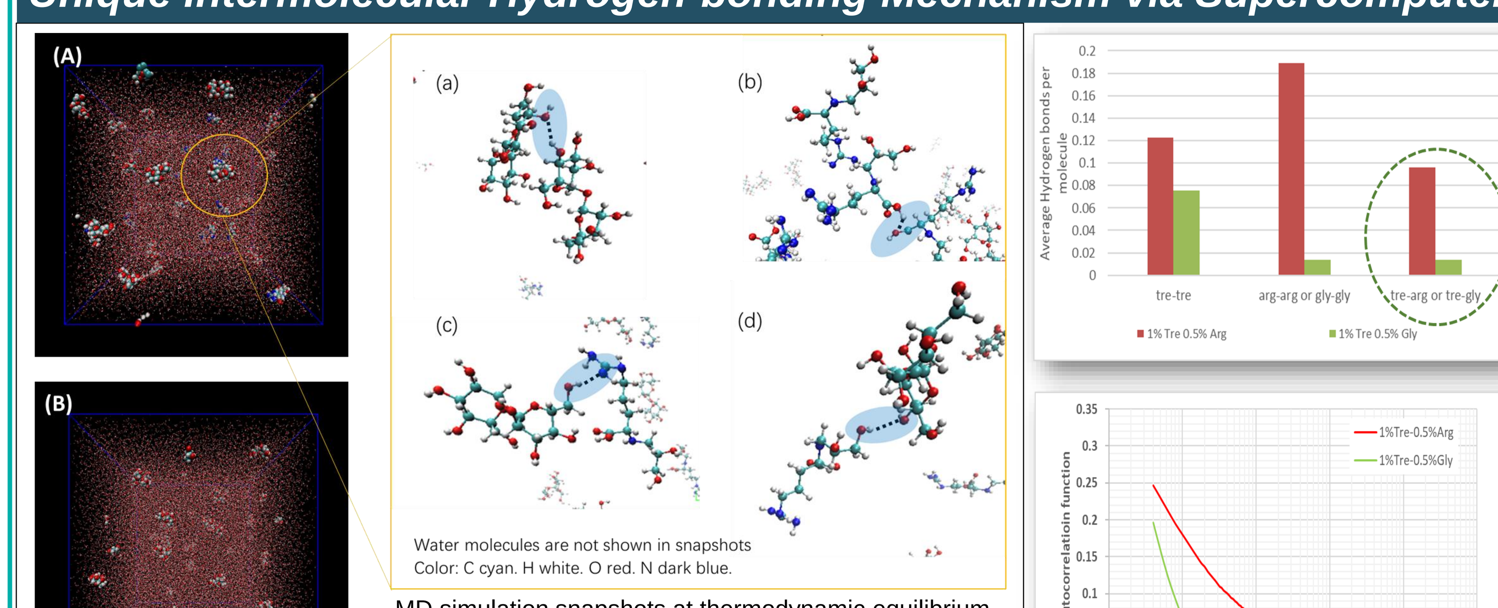
(2,3-dihydroxypropyl) arginine bearing both hydroxyl and amine groups can create a strong hydrogen-bonding network with trehalose. Such positively charged hydrogen-bonding "complexes" can further interact strongly with negatively charged surfaces (skin, hair, scalp) through strong electrostatic interactions.

Methods



Results & Discussion:

Unique Intermolecular Hydrogen-bonding Mechanism via Supercomputer MD Simulation

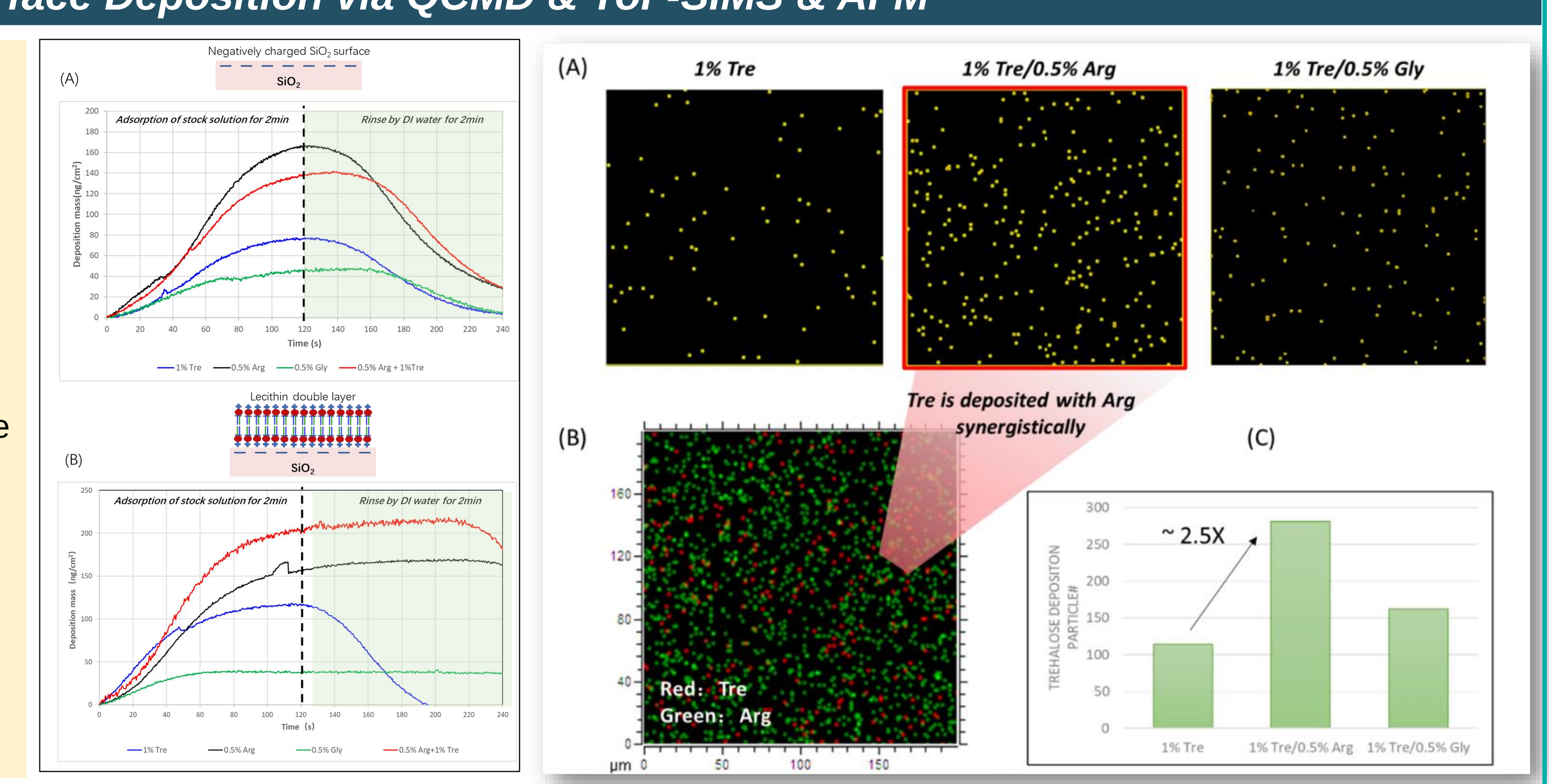


MD simulation snapshots at thermodynamic equilibrium state for (A) 0.5% Arg+1% Tre four types of intermolecular hydrogen bound (a)Tre-Tre OH· · ·H, (b)Arg-Arg OH· · ·H, (c)Tre-Arg OH· · ·N, (d)Tre-Arg OH· · ·H

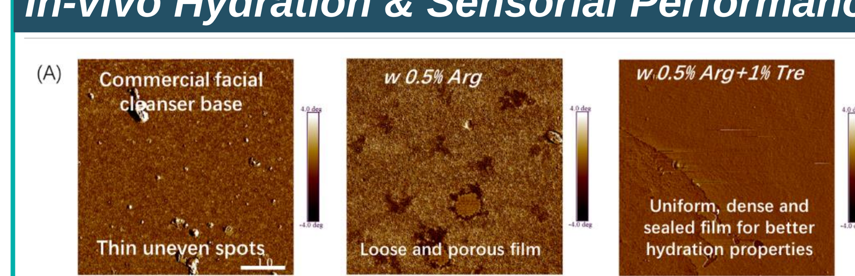
All-atom MD simulation confirmed the presence of strong intermolecular hydrogen bonding between Tre and Arg. By contrast, regular Gly molecule does not show any specific hydrogen-bonding interaction with Tre, suggesting the uniqueness of the intermolecular hydrogen-bonding interactions between Arg and Tre.

Synergistic Surface Deposition via QCMD & ToF-SIMS & AFM

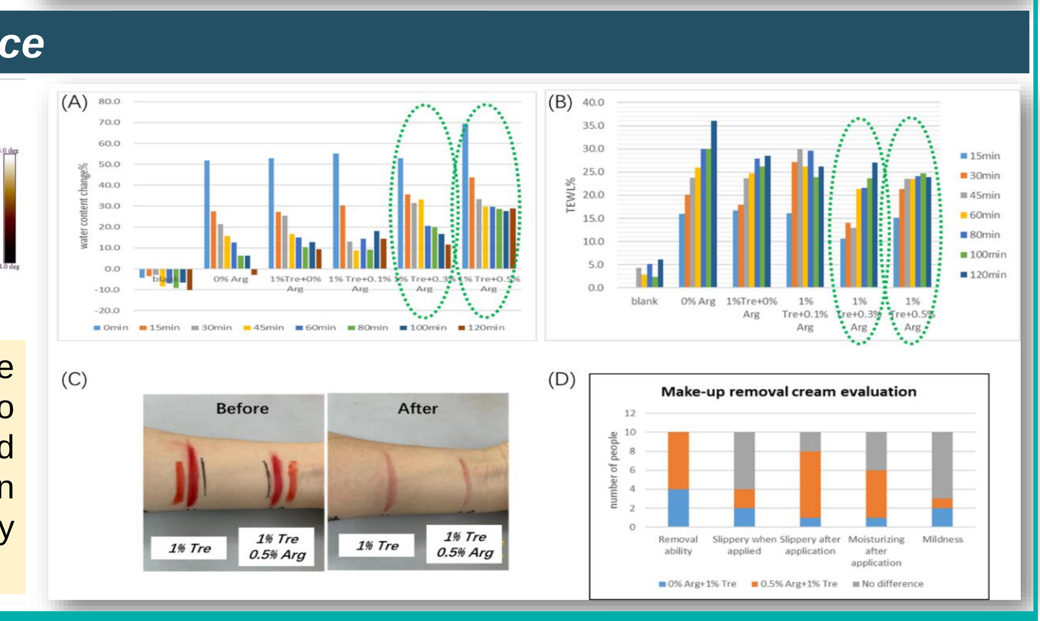
QCMD, ToF-SIMS & AFM further confirm that the synergistic hydrogen-bonding and additional ionic-bonding induced by Arg lead to a significant improvement in deposition (~2.5 time of improvement) of Trehalose on various model substrates in-rinse, especially on the skin mimicking lecithin double layer surface.



In-vivo Hydration & Sensorial Performance



Hydration performance & sensorial evaluations were carried out with at least 10 volunteers. The in vivo results are quite consistent with all the theoretical and in vitro studies performed. Long-lasting moisturization and good sensorial performance are achieved by combining the Arg and Tre at various concentrations.



Conclusions:

- We report a synergistic 'soulmate' intermolecular hydrogen-bonding mechanism of bioactive saccharides and (2,3-dihydroxypropyl) arginine HCl to achieve enhanced 1) deposition efficacy, 2) long-lasting moisturization, and 3) sensorial performance.
- Such 'soulmate' mechanism is simple (i.e., no complicated biochemistry involved) and versatile (i.e., plenty choices of hydrogen-bonding pairs), and can easily scaled up for industrial applications. This study provides a new pathway for improved cosmetic performance using bioactive saccharides, especially in rinse-off cosmetics.

Aknowledgments:

- The authors are grateful to Mr. Lihua Dai, Mr. Hailong Zhao, and Mr. Zhijun Xu (Jiangxi Chufu Cosmetics Co., Ltd.) for providing test samples and support.
- Thanks to Prof. Yan Huang (Fuzhou University) for helping QCMD measurements and Prof. Naisheng Jiang (University of Science and Technology Beijing) for helping AFM measurements.

References:

1. McCranie E, and Bachmann B (2014), Bioactive Oligosaccharide Natural Products. Nat Prod Rep. 31:1026-1042.
2. Miao J et al. (2020), Isolation, structural characterization and bioactivities of polysaccharides and its derivatives from Auricularia-A review. International Journal of Biological Macromolecules 150:102-113.
3. Farinha I, Freitas F (2020), Chemically modified chitin, chitosan, and chitinous polymers as biomaterials. Handbook of Chitin and Chitosan 3:43-69.
4. Adsorption and rinse-off behavior were studied via QCM-D: ①DI water rinse to baseline---②Stock solution of 1% trehalose adsorption for 2min---③DI water rinse for 2min.

More Interesting Findings Coming!