Abstract Acceptance

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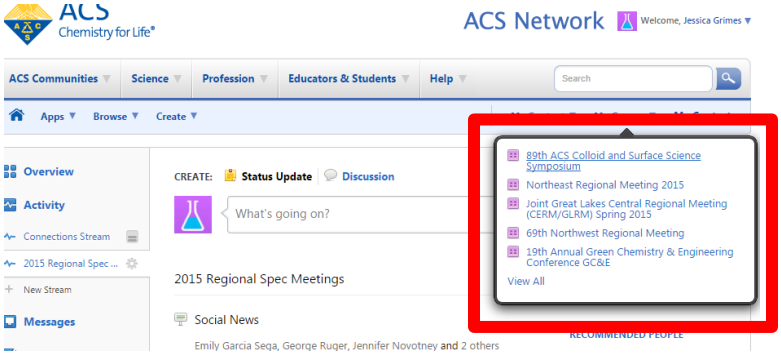

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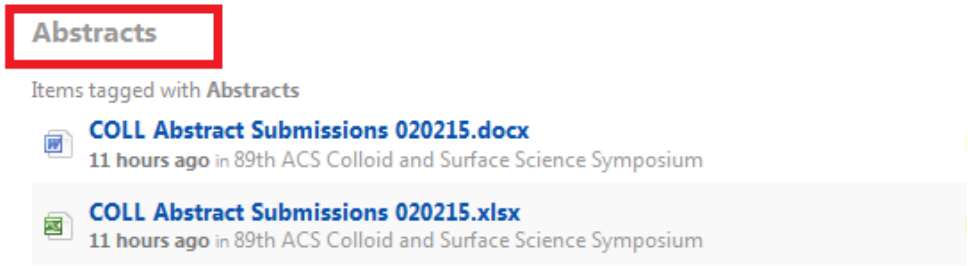

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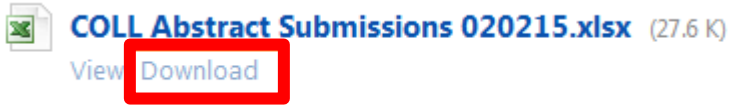

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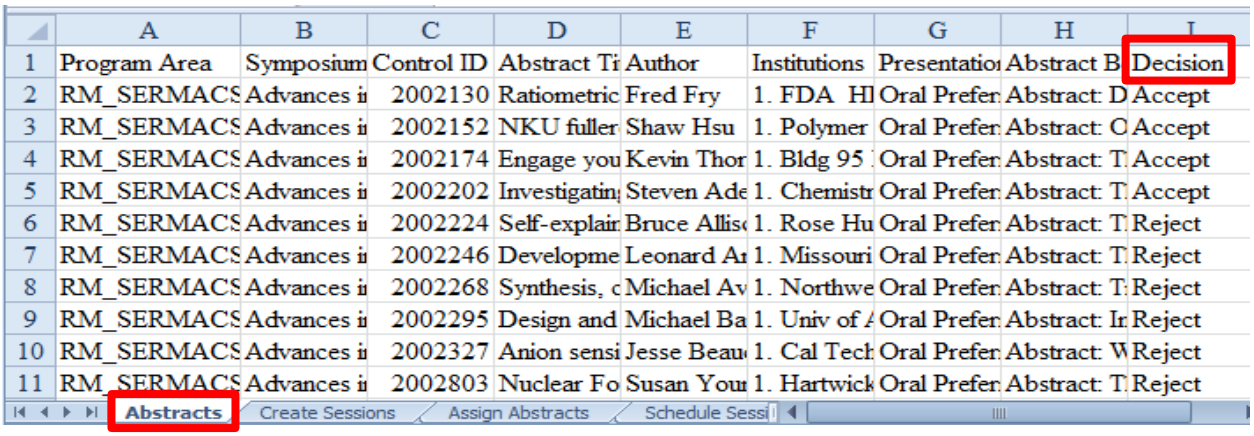

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CONTROL ID: 2194676

TITLE: Self-assembly of linear peptide analogs and their interaction with lipid bilayers using MD simulations

PRESENTER: Brian Novak

INSTITUTIONS (ALL): 1. Louisiana State University, Baton Rouge, LA, United States.

PRESENTATION TYPE: Oral Preferred

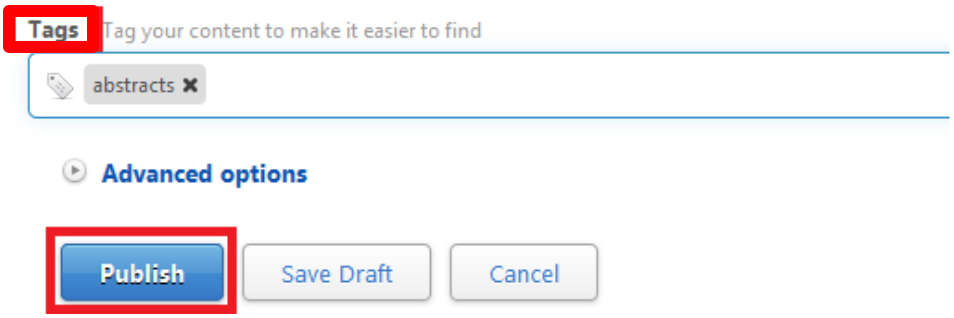
ABSTRACT BODY:

Abstract: The self-assembly and DPPC bilayer interaction of cationic linear peptide analogs (LPAs) with the formula Lys-NH$(CH_2)_n$ CO-Arg-NH$(CH_2)_n$CO-Arg with n varying from 4 to 13 has been studied using molecular dynamics simulations. These LPAs were designed to deliver an anionic phosphopeptide into cells, and experimental work on n = 4, 7, and 11 LPAs[1-3] showed that: (i) LPAs induced changes in lipid phase behavior, (ii) the n = 11 LPAs caused the most structural changes to and leakage from DPPC, DPPC/DPPG, and DPPC/DPPS liposomes, and (iii) only the n = 11 LPAs were taken up by cells to a significant amount. Self-assembly of n = 11 LPAs in solution was also observed, and may be related to their activity. Our simulations showed that stable LPAs micelles formed in aqueous solution (0.1 M LPAs) for n > 7, LPAs in those micelles had increased β-sheet type structure consistent with experimental results, and that micelles with more than 8 molecules were cylindrical. The equilibrium depth of single LPAs in a DPPC bilayer increased with increasing n up to n = 8, but remained almost constant for n > 8. A 5 molecule, n = 11 LPA micelle sank into an 85% DPPC/15% DPPS bilayer, but remained intact and did not cause major disruption to the bilayer within about 350 ns. We will also present results of the behavior of n = 11 LPAs added to a DPPC bilayer one at a time.

[1] A. Gupta *et al.*, Eur. Biophys. J. Biophy. **40**, 727 (2011).
[2] G. F. Ye *et al.*, Colloids Surf., B **76**, 76 (2010).
[3] G. F. Ye *et al.*, J. Med. Chem. **50**, 3604 (2007).

CONTACT (COUNTRY ONLY): United States

7. Save the workbook.
8. Upload the MS Excel workbook into the network group.
9. Tag the uploaded workbook with “abstracts”.



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