# EXPLORATION OF THE BIOMACROMOLECULAR INTERACTIONS OF AN INTERPENETRATING PROTEO-SACCHARIDE HYDROGEL NETWORK AT THE MUCOSAL INTERFACE

[1]Felix Mashingaidze, [1]Yahya E. Choonara, [1]Pradeep Kumar, [1]Lisa C. du Toit, [2]Vinesh Maharaj, [3]Eckhart Buchmann, [4]Valence M. K. [1]Ndesendo, Viness Pillay

[1]University of the Witwatersrand, Faculty of Health Sciences, Department of Pharmacy and Pharmacology, 7 York Road,

Parktown, 2193, Johannesburg, South Africa

[2]Council for Scientific and Industrial Research, Department of Biosciences, Meiring Naud_e Road, Brummeria,

Pretoria, South Africa

[3]University of the Witwatersrand, Faculty of Health Sciences, Department of Obstetrics and Gynecology, 7 York Road,

Parktown, 2193, Johannesburg, South Africa

[4]St. John's University of Tanzania, School of Pharmacy and Pharmaceutical Sciences, Dodoma, Tanzania

Received 13 September 2012; revised 1 February 2013; accepted 5 February 2013
Published online in Wiley Online Library (wileyonlinelibrary.com). DOI: 10.1002/jbm.a.34664

**Abstract:**

The relationship between mucin (MUC) and pectin (PEC) was explored in an attempt to understand the biomacro - molecular interactions that occur at mucosal surfaces when mucus membranes are exposed to PEC-based materials. These interactions were explored through techniques, such as attenuated total reflection Fourier transform infrared (ATR-FTIR) spectroscopy, SEM imagery of lyophilized MUC–PEC blends, thermodynamic analysis, rheology investigations, and in silico static lattice atomistic simulations using a molecular mechanics energy relationships (MMER) approach. Three types of PEC that had different degrees of esterification and degrees of amidation were investigated at different MUC–PEC mass ratios (1:0, 1:1, 1:4, 1:9, and 0:1). The effect PEG 400 and Ca2 þ in the MUC–PEC interactions were also studied. ATR-FTIR spectroscopy revealed broadening and strengthening of FTIR peaks at 3363cmÿ1 and between 3000–3650cmÿ1 due to stretching vibrations of the –OH, –COOH groups on MUC and PEC as well as the –N–H group on MUC. This suggested significant intra- and inter-molecular H-bonding. Morphologically,

MUC-rich scaffolds were porous, thin, and multidirectional compared with the smooth, rigid, and unidirectional PEC-rich scaffolds. The Flory–Huggins interaction parameter (v12) for all MUC–PEC mass ratios was negative, thus confirming MUC–PEC miscibility and interactions. UV absorbance increased with increasing relative concentration of PEC in the aqueous MUC–PEC dispersions. Furthermore, rheology investigations demonstrated synergistic enhancement in viscosity (g) and dynamic moduli upon the addition of PEG 400 and Ca2 þ . MMER analysis revealed several key MUC–PEC interacttions that corroborated well with the experimental data. Notably, higher esterification and larger mass ratios of PEC yielded greater MUC–PEC interactions. VC 2013 Wiley Periodicals, Inc. J Biomed Mater Res Part A: 00A:000–000, 2013.