Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

Hydrogen Bonding Motifs in MutSaphla and their response to binding damaged DNA LACRA NEGUREANU, FREDDIE SALSBURY, Wake Forest University — Over the past decade, there has been a growing interest in studying the binding of damaged DNA to the MutSalpha protein complex. This protein complex, the Msh2/Msh6 complex in humans, is the initial complex that binds mismatched DNA and other DNA defects that occur during replication. This complex has also been shown to bind at least some types of damaged DNA. As a result of this interest, multiple studies have contrasted the interactions of MutSalpha with its normal mismatched substrate and with the interactions of MutsSalpha to DNA damaged by the chemotherapeutic cisplatin. To complement these studies, we examined the interaction between MutSalpha and DNA damaged by carboplatin via all-atom molecular dynamics simulations. These simulations provide evidence for different hydrogen bonding interactions at the protein/DNA and protein/protein interface. The hydrogen bonding motifs found are broadly similar to those found in binding to the adduct from cis-platin, but have distinct differences. These subtle differences may play a role in the way the different damages are signaled by MutS.

Freddie Salsbury
Wake Forest University

Date submitted: 28 Nov 2012 Electronic form version 1.4