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## Use of electrospray ionization mass spectrometry to study protein conformation and protein-protein interactions

Stephen J. Watt  
*University of Wollongong*

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# **Use of Electrospray Ionization Mass Spectrometry to Study Protein Conformation and Protein-Protein Interactions**

A thesis submitted in (partial) fulfilment of the  
requirements for the award of the degree

**Doctor of Philosophy**

**from**



**University of Wollongong**

**by**

**Stephen J. Watt**

Bachelor of Medicinal Chemistry (Honours)

**Department of Chemistry  
2005**

## **CERTIFICATION**

I, Stephen J. Watt, declare that this thesis, submitted in partial fulfilment of the requirements for the award of Doctor of Philosophy, in the Department of Chemistry, University of Wollongong, is wholly my own work unless otherwise referenced or acknowledged. The document has not been submitted for qualification at any other academic institution.

Stephen J. Watt

23<sup>th</sup> August 2005

*For my family*

## PUBLICATIONS

Watt, S.J., Oakley, A., Sheil, M.M., and Beck, J.L. (2005) Comparison of Negative and Positive Ion ESI Mass Spectra of Calmodulin and its Complex with Trifluoperazine. *Rapid Communications in Mass Spectrometry*, **19**, 2123-2130.

Williams, N.K., Liepinsh, E., Watt, S.J., Prosselkov, P., Matthews, J.M., Attard, P., Beck, J.L., Dixon N.E. and Otting G. (2005) Stabilization of Native Protein Fold by Intein-Mediated Covalent Cyclization, *Journal of Molecular Biology*, **346**, 1095-1108.

## ABSTRACT

*The polymerisation of a polypeptide chain from an encoded genetic sequence allows the formation of structured molecules, known as proteins. These are essential components for a range of processes including molecular recognition, DNA replication and enzymatic functions. In this thesis, the ability of electrospray ionization (ESI) mass spectrometry (MS) to be used as a tool to determine functional properties of proteins has been explored. The coupling of ESI-MS to hydrogen deuterium exchange has been used to show how restriction of the C- and N-termini by cyclization of the polypeptide backbone can affect the ability of a protein to sample unfolded or partially unfolded states. The development of appropriate methodologies for analysis of linear (uncyclized) and cyclized systems identified a slowing of the rate of unfolding due to cyclization. The implication for the unfolding processes of proteins are discussed. An increased thermal stability of the cyclized protein was also demonstrated. This property was used to analyse the ability of ESI-MS to identify changes in protein structure from shifts in ion distributions. Important observations regarding the polarity of ionization used in these experiments are highlighted.*

*The effect opposite polarity ionization has on the ability to detect conformational changes in proteins and interactions with small ligands was explored using the well-characterized calmodulin-calcium-antipsychotic drug system. Important considerations regarding the binding of metal ions to protein structures are discussed in relation to the ability to unequivocally identify a conformational transition in protein structure from ESI mass spectra. An inability to detect complexes of calcium loaded-calmodulin with the antipsychotic drug trifluoperazine in the negative ion mode was observed, a result believed to be due to the Coulombic repulsions between acidic residues of calmodulin.*

*Finally, the non-covalent complex and interactions of the E. coli helicase (DnaB) were probed by nanoESI-MS and MS/MS studies. Development of suitable conditions allowed for identification of a previously unresolved heptamer in addition to the expected hexamer. The interaction of DnaB with its loading partner DnaC and the possible roles of ATP and ADP in this interaction were also probed with findings being related to the biological functions of these proteins.*



## ACKNOWLEDGMENTS

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## ABBREVIATIONS

ADP	Adenosine-5'-diphosphate
AMP-PNP	Adenosine 5'-( $\beta,\gamma$ -imido)triphosphate

ATP	Adenosine-5'-triphosphate
ATP $\gamma$ S	Adenosine-5'-( $\gamma$ -thio)-triphosphate
AS	Aerospray
$\beta\gamma$ ATP	$\beta$ - $\gamma$ -methyleneadenosine-5'-triphosphate
BSA	Bovine serum albumin
CAD	Collisionally Activated Dissociation
CaM	Calmodulin
CD	Circular Dichroism
CI	Chemical Ionization
CRM	Charged Residue Model
CryoEM	Cryoelectron Micrograph
CSD	Charge State Distribution
DnaB-N	N-Terminal of DnaB
ds	Double Stranded
DSC	Differential Scanning Calorimetry
DTT	Dithiothreitol
EDTA	Ethylenediaminetetraacetic acid
EI	Electron Ionization
EH	Electrohydrodynamic
ESI	Electrospray Ionization
FIB	Fast Ion Bombardment
FAB	Fast Atom Bombardment
HDX	Hydrogen Deuterium Exchange
IEM	Ion Evaporation Model

IPA	Imipramine
ITC	Isothermal Titration Calorimetry
LD	Laser Desorption
MALDI	Matrix Assisted Laser Desorption Ionization
MHC	Major Histocompatibility Complexes
MS	Mass Spectrometry
$m/z$	Mass to Charge
NMR	Nuclear Magnetic Resonance
oa	Orthogonal Acceleration
OAc	Acetate
PD	Plasma Desorption
PDB	Protein Data Bank
Q-ToF	Quadrupole Time of Flight
ss	Single Stranded
SPR	Surface Plasmon Resonance
TFP	Trifluoperazine
ToF	Time-of-Flight
TS	Thermospray