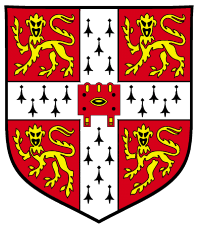

University of Cambridge
Department of Chemistry

This is the Thesis Title

This dissertation is submitted to the University of Cambridge
for the degree of Doctor of Philosophy

Jane Doe
Churchill College
June 2017

Declaration

The work described in this dissertation was carried out by the author in the Department of Chemistry at the University of Cambridge between October 2013 and June 2017. The contents are the original work of the author except where otherwise indicated and contain nothing that is the outcome of collaboration. The contents have not previously or concurrently been submitted for any other degree or qualification at the University of Cambridge or another institution. The number of words does not exceed 60000.

Jane Doe
June 2017

Acknowledgements

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for...

This is the Thesis Title

Jane Doe

Abstract

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Abbreviations

AMBER	assisted model building with energy refinement
CFA	Coulomb field approximation
CHARMM	chemistry at Harvard macromolecular mechanics
DNEB	doubly-nudged elastic band
DPS	discrete path sampling
FES	free energy surface
GB	Generalised Born
HEF	hybrid eigenvector-following
L-BFGS	limited-memory Broyden-Fletcher-Goldfarb-Shanno
MFET	mean first encounter time
MFPT	mean first passage time
MD	molecular dynamics
NGT	new graph transformation
PB	Poisson-Boltzmann
PDB	protein data bank
PE	potential energy
PES	potential energy surface
REMD	replica exchange molecular dynamics
RMSD	root-mean square distance
TZ1	tryptophan zipper (trpzip) 1
vdW	van der Waals

Publications

Chapter 3

J. Doe. *This is the title of your paper.* Journal of Some Chemistry **2014**, 6 (5), 1007–1045.

Chapter 4

insert title...

Chapter 5

insert title..

Other Publication(s)

I have also contributed to the following publication(s) during my PhD:
J. Doe. *Other title of paper.* Some Journal Name **2017**.

Contents

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1

Introduction

In 1951, Sanger and Tuppy's seminal work on the sequencing of insulin[1] transformed our understanding of protein structure.

References

[1] F. Sanger and H. Tuppy, *Biochem. J.*, **1951**, 49(4); 463.