**Crystal Molecular Dynamics**

**by**

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**And**

**Graduate Program in Computational Biology and Molecular Biophysics**

**Written under the direction of**

**Prof. David A. Case**

**And**

**Prof. Darrin M. York**

**And approved by**

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**New Brunswick, New Jersey**

**August, 2015**

# Abstract of the dissertation

**Crystal Molecular Dynamics**

**By Paweł A. Janowski**

**Dissertation Director**

**David A. Case Ph.D and Darrin M. York Ph.D**

Blah Blah Blah

# Acknowledgements

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# Abbreviations used

MD – Molecular dynamics;

BX – Biomolecular crystallography;

# Chapter 1. Introduction

My PhD research

## Biomolecular Crystallography

### What is crystallography

Blah blah

### Theory

Blah blah

### Refinement

Blah blah

* 1. Molecular Dynamics

### What is Molcular Dynamics?

Blah blah

### Theory

Blah blah

### Molecular Dynamics of Crystals

Blah blah

## Goals and overview

Blah blah

# Chapter 2. Developing molecular dynamics of crystals.

## Fav8 1

Blah blah

## Fav8 2

Blah blah

## 4lzt

Blah blah

## DNA/RNA

Blah blah

# Chapter 3. Applications of molecular dynamics of crystals

## Hairpin

Blah blah

## RnaseA

Blah blah

# Chapter 4: Improved crystallographic methods through crystal molecular dynamics

## AFITT

Blah blah

## Phenix-Amber

Blah blah