KU Leuven
Group Biomedical Sciences
Faculty of Pharmaceutical Sciences
Department Pharmaceutical and Pharmacological Sciences
Laboratory of Medicinal Chemistry
Rega Institute for Medical Research



MOLECULAR MODELING TOOLS TO IMPROVE AND EXPAND COMPUTATIONAL RESEARCH ON SYNTHETIC NUCLEIC ACIDS

Jérôme RIHON

Promotor Eveline Lescrinier
Co-Promotor Vitor Bernardes Pinheiro

Co-Promotor Matheus Froeyen
Chair Jef Rozenski
Jury member Kalyan Das

Jury member Joost Schymkowitz

Dissertation presented in partial fulfilment of the requirements for the degree of Doctor in Pharmaceutical Sciences

KU Leuven
Groep Biomedische Wetenschappen
Faculteit Farmaceutische Wetenschappen
Departement Farmaceutische en Farmacologische Wetenschappen
Laboratorium van Medicinale Chemie
Rega Instituut voor Medisch Onderzoek



MOLECULAIRE MODELING TOOLS TER BEVORDERING EN UITBREIDING VAN COMPUTATIONEEL ONDERZOEK OP SYNTHETISCHE NUCLEÏNEZUREN

Jérôme RIHON

Promotor Eveline Lescrinier
Co-Promotor Vitor Bernardes Pinheiro

Co-Promotor Matheus Froeyen
Chair Jef Rozenski
Jury member Kalyan Das

Jury member Joost Schymkowitz

Proefschrift voorgedragen tot het behalen van de graad van Doctor in de Farmaceutische Wetenschappen

CONTENTS

1. Structural insights into the Morpholino Nucleic Acid/RNA duplex using the new XNA builder Ducque in
a molecular modeling pipeline.
1.1. Introduction
1.1.1. Welcome to the thesis
1.2. Methods
1.3. Result & Discussion
1.4. Conclusion
2. The puckers toolkit to calculation puckers values of biomolecular monomers

STRUCTURAL INSIGHTS INTO THE MORPHOLINO NUCLEIC ACID/RNA DUPLEX USING THE NEW XNA BUILDER DUCQUE IN A MOLECULAR MODELING PIPELINE.

1.1. Introduction

Welcome to the thesis

Lorem ipsum dolor sit amet, consectetur adipiscing elit, sed do eiusmod tempor incididunt ut labore et dolore magnam aliquam quaerat voluptatem. Ut enim aeque doleamus animo, cum corpore dolemus, fieri tamen permagna accessio potest, si aliquod aeternum et infinitum impendere malum nobis opinemur. Quod idem licet transferre in voluptatem, ut. I did a thing here!

1.2. Methods

Lorem ipsum dolor sit amet, consectetur adipiscing elit, sed do eiusmod tempor incididunt ut labore et dolore magnam aliquam quaerat voluptatem. Ut enim aeque doleamus animo, cum corpore dolemus, fieri tamen permagna accessio potest, si aliquod aeternum et infinitum impendere malum nobis opinemur. Quod idem licet transferre in voluptatem, ut.

1.3. Result & Discussion

Lorem ipsum dolor sit amet, consectetur adipiscing elit, sed do eiusmod tempor incididunt ut labore et dolore magnam aliquam quaerat voluptatem. Ut enim aeque doleamus animo, cum corpore dolemus, fieri tamen permagna accessio potest, si aliquod aeternum et infinitum impendere malum nobis opinemur. Quod idem licet transferre in voluptatem, ut.

1.4. Conclusion

Lorem ipsum dolor sit amet, consectetur adipiscing elit, sed do eiusmod tempor incididunt ut labore et dolore magnam aliquam quaerat voluptatem. Ut enim aeque doleamus animo, cum corpore dolemus, fieri tamen permagna accessio potest, si aliquod aeternum et infinitum impendere malum nobis opinemur. Quod idem licet transferre in voluptatem, ut.

THE *PUCKE.RS* TOOLKIT TO CALCULATION PUCK-ERS VALUES OF BIOMOLECULAR MONOMERS.