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Path-metadynamics: A computational study of conformational transitions in proteins

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Path-Metadynamics

A computational study of conformational transitions in proteins

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University of Amsterdam

Path-Metadynamics

A computational study of conformational transitions in proteins

ACADEMISCH PROEFSCHRIFT

ter verkrijging van de graad van doctor
aan de Universiteit van Amsterdam
op gezag van de Rector Magnificus
prof. dr. D.C. van den Boom
ten overstaan van een door het college voor promoties
ingestelde commissie,
in het openbaar te verdedigen in de Agnietenkapel

op vrijdag 15 november, te 10.00 uur

door

Grisell Díaz Leines
geboren te Mexico-Stad, Mexico

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Faculteit der Natuurwetenschappen, Wiskunde en Informatica

To Jetze Sikkema, my parents, Sergio and Gloria,
and my brother Sergio ...

'Logic will get you from A to B. Imagination will take you everywhere.'
Albert Einstein

*Hay hombres que luchan un día y son buenos.
Hay otros que luchan un año y son mejores.
Hay quienes luchan muchos años y son muy buenos.
Pero hay los que luchan toda la vida.
Esos son los imprescindibles.*
Bertolt Brecht