



Universiteit  
Leiden

The Netherlands

## **Metabolomics of biofluids : from analytical tools to data interpretation**

Nevedomskaya, E.

### **Citation**

Nevedomskaya, E. (2011, November 23). *Metabolomics of biofluids : from analytical tools to data interpretation*. Retrieved from <https://hdl.handle.net/1887/18135>

Version: Corrected Publisher's Version

License: [Licence agreement concerning inclusion of doctoral thesis in the Institutional Repository of the University of Leiden](#)

Downloaded from: <https://hdl.handle.net/1887/18135>

**Note:** To cite this publication please use the final published version (if applicable).

# Metabolomics of biofluids: from analytical tools to data interpretation

Ekaterina Nevedomskaya

ISBN: 978-94-6182-038-9

The printing of this thesis was financially supported by:

Bruker BioSpin GmbH, Germany

Dionex Benelux B.V.

Beckman Coulter (Nederland) B.V.

Bruker Nederland B.V.

Cover: fragment of “To Touch The Grass - 1” by Anton Shirkin.

Printing: Off Page, Amsterdam

Copyright © 2011 by E. Nevedomskaya. All rights reserved. No part of this book may be reproduced, stored in a retrieval system or transmitted in any form or by any means, without prior permission of the author.

Metabolomics of biofluids:  
from analytical tools to data interpretation

**Proefschrift**

ter verkrijging van  
de graad van Doctor aan de Universiteit Leiden,  
op gezag van Rector Magnificus Prof. Mr. P.F. van der Heijden,  
volgens besluit van het College voor Promoties  
te verdedigen op woensdag 23 november 2011  
klokke 16:15 uur

door

**Ekaterina Nevedomskaya**

geboren te Moskou, Rusland in 1985

## PROMOTIECOMMISSIE

**Promotor:** Prof. dr. A.M. Deelder

**Co-promotor:** Dr. O.A. Mayboroda

**Overige leden:** Prof. dr. M.S. Gelfand  
*Institute for Information Transmission Problems RAS, Moscow, Russia*

Dr. H. Keun  
*Dept. of Surgery and Cancer, Faculty of Medicine, Imperial College,  
London, UK*

Prof. dr. T.W.J. Huizinga

Prof. dr. P. Slagboom

Prof. dr. J.T. van Dissel

Prof. dr. A.E. Gorbalenya

Моим родителям  
*(For my parents)*



## TABLE OF CONTENTS

<b>General Introduction</b>		9
<hr/>		
<b>PART I</b>	<b>Method development</b>	
<b>Chapter 1</b>	Gas chromatography/atmospheric pressure chemical ionization-time of flight mass spectrometry: analytical validation and applicability to metabolic profiling	23
<b>Chapter 2</b>	Alignment of capillary electrophoresis–mass spectrometry datasets using accurate mass information	47
<hr/>		
<b>PART II</b>	<b>Application to animal studies</b>	
<b>Chapter 3</b>	CE-MS for metabolic profiling of volume-limited urine samples: application to accelerated aging TTD mice	65
<b>Chapter 4</b>	Metabolic profiling of accelerated aging ERCC1 <sup>d/-</sup> mice	83
<hr/>		
<b>PART III</b>	<b>Application to human studies</b>	
<b>Chapter 5</b>	Integrating study design and clinical data into metabolic profiling of urinary tract infection	109
<b>Chapter 6</b>	Cross-platform analysis of longitudinal data in metabolomics	127
<hr/>		
<b>General discussion</b>		153
<hr/>		
<b>Summary</b>		161
<b>Nederlandse samenvatting</b>		165
<b>Acknowledgements</b>		171
<b>Curriculum vitae</b>		173
<b>List of publications</b>		174



