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# Graph-theoretical approach to algorithmic construction of complex reaction networks

Yuliia Orlova



GRAPH-THEORETICAL APPROACH TO ALGORITHMIC CONSTRUCTION OF COMPLEX REACTION NETWORKS

Yuliia Orlova

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# Graph-theoretical approach to algorithmic construction of complex reaction networks

## ACADEMISCH PROEFSCHRIFT

ter verkrijging van de graad van doctor  
aan de Universiteit van Amsterdam,  
op gezag van de Rector Magnificus  
prof. dr. ir. K.I.J. Maex,  
ten overstaan van een door het College voor Promoties ingestelde commissie,  
in het openbaar te verdedigen in de Agnietenkapel  
op donderdag 24 september 2020, te 13.00 uur

door

**Yuliia Orlova**

geboren te Dniprodzerzhynsk

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Cover illustration: The cover depicts a fragment of "Almond Blossoms" painting by Vincent van Gogh, as well as an artistic representation of the fragments of the reaction network of triolein. The reaction network was reconstructed using the computational methodology introduced in this thesis.

Cover Design: Yuliia Orlova and Nataliia Cherneta

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