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AND COMPUTER SCIENCE

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# Computational Synthesis Planning Using Big Data

Computational Syntese planlægning ved hjælp af big data

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*Author:*  
Henrik Schulz

*Supervisors:*  
Daniel Merkle



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**Abstract**

**Resumé**

## **1 Preface**

## **2 Introduction**

### **Problem formulation**

## **3 Preliminaries**

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kkkk [1]

kkk [2]

kkkk [3]

## **4 Dynamic Approach**

## **5 Nielsens Algorithm**

k [4]

## **6 Konklusion**

## Books

- [1] R. W. Hoffmann, *Elements of Synthesis Planning*. Springer Berlin Heidelberg, 2009.

## Articles

- [2] S. Szymkuc, E. P. Gajewska, T. Klucznik, K. Molga, P. Dittwald, M. Startek, M. Bajczyk, and B. A. Grzybowski, “Computer-assisted synthetic planning: The end of the beginning”, *Angewandte Chemie International Edition*, no. 55, pp. 5904–5937, 2016.
- [3] R. Fagerberg, C. Flamm, R. Kianian, D. Merkle, and P. F. Stadler, “Finding the k best synthesis plans”, 2017, Unpublished Article.
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## Other

- [5] C. G. Lützen and D. F. Johansen, “A computational and mathematical approach to synthesis planning”, Master’s thesis, University of Southern Denmark, 2015.

## **7    Appendiks**