



Cheminformatics

Winter Semester 2022/23

Institute for Bioinformatics and Medical Informatics

Assignment Sheet 4

Author: Stephan Liu

A.4.1: SMARTS

A.4.2: Morgans Algorithm

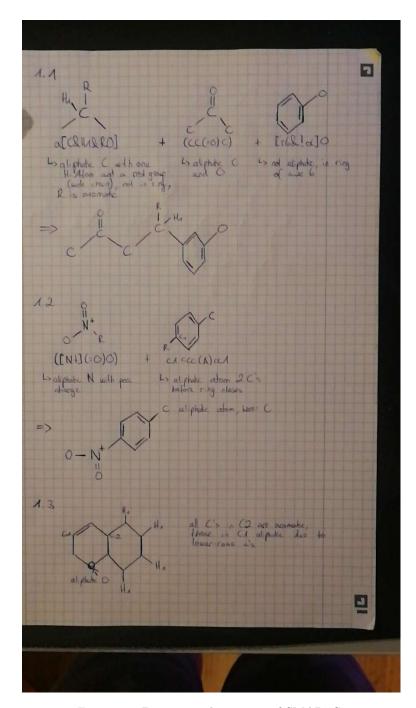


Figure 1: 2D structural patterns of SMARTS.

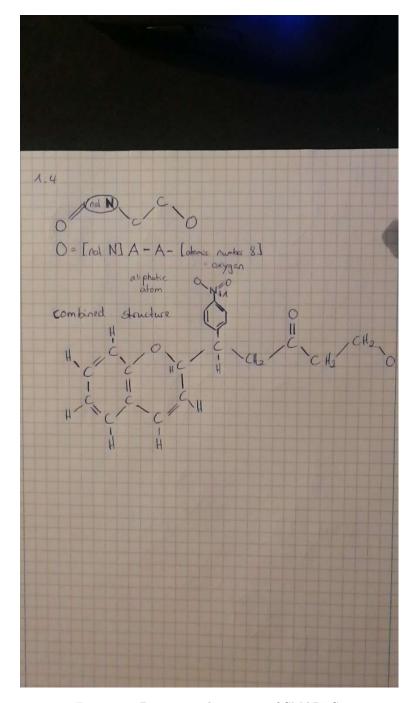


Figure 2: 2D structural patterns of SMARTS.

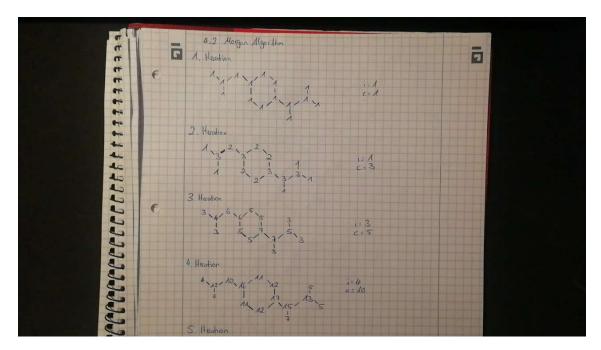


Figure 3: Morgan's Algorithm solved by hand.

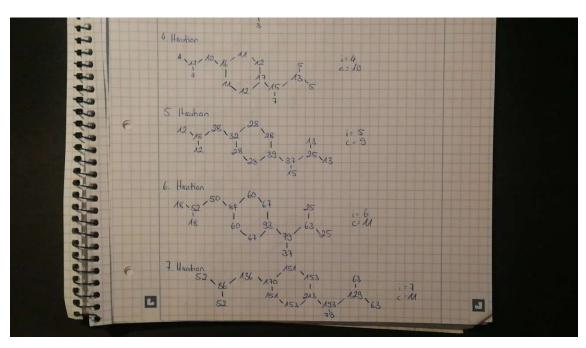


Figure 4: Morgan's Algorithm solved by hand.

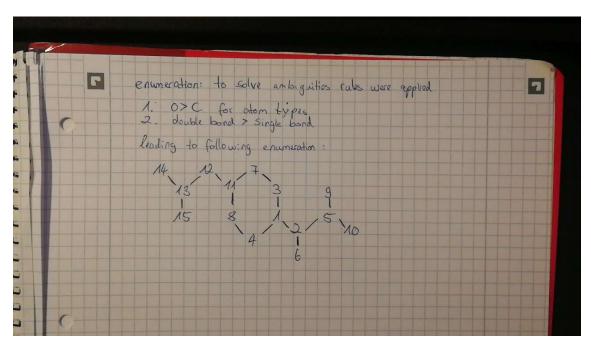


Figure 5: Enumeration of the Morgan's Algorithm.