



## Assignment Sheet 3

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### A.3.1: Line Notations

1. CC3(C)SC2C(/N=C(O)\C1(N)CCCCC1)C(=O)N2C3C(=O)O; also called cyclacillin.<sup>1</sup>
2. O=C1CC2(CCCC2)CC(=O)N1CCCCN3CCN(CC3)c4ncccc4 is drawn below in Figure 1. The molecule is most likely buspirone.<sup>2</sup>
3. InChI=1S/C7H10N2O2S/c1-3-11-7(10)9-5-4-8(2)6(9)12/h4-5H,3H2,1-2H3 is drawn below in Figure 1. The structure is most likely carbimazole.<sup>3</sup>

### A.3.2: SMILES generator

List of used packages for the implementation:

- rdkit v.2020.09.1.0

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<sup>1</sup><https://go.drugbank.com/drugs/DB01000>

<sup>2</sup><https://go.drugbank.com/drugs/DB00490>

<sup>3</sup><https://go.drugbank.com/drugs/DB01000>

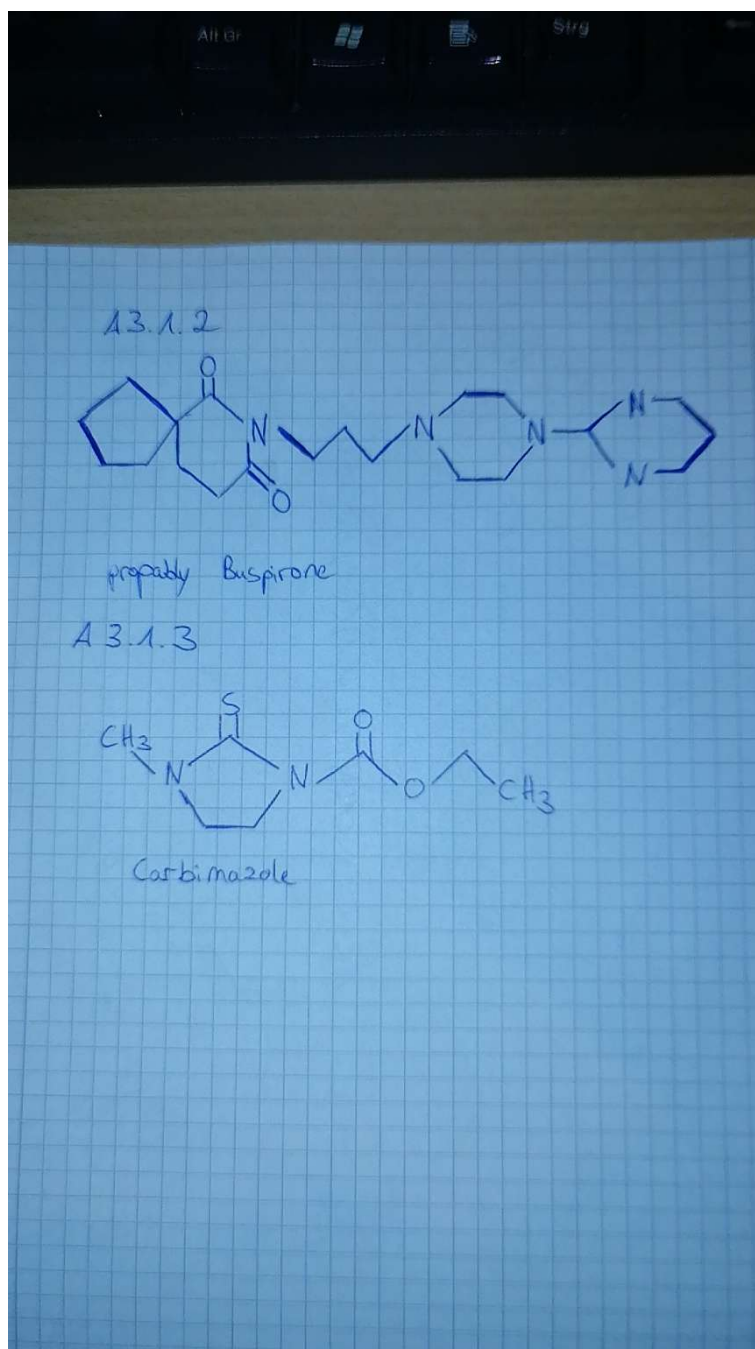


Figure 1: Drawn molecules of the subtasks 2 and 3.