# Pharmaceutical Chemistry

## QSAR through the OCHEM portal


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# Introduction

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**Online chemical modeling environment (OCHEM): web platform for data storage, model development and publishing of chemical information**

The Online Chemical Modeling Environment is a web-based platform that aims to automate and simplify the typical steps required for QSAR modeling. The platform consists of two major subsystems: the database of experimental measurements and the modeling framework. A user-contributed database contains a set of tools for easy input, search and modification of thousands of records. The OCHEM database is based on the wiki principle and focuses primarily on the quality and verifiability of the data. The database is tightly integrated with the modeling framework, which supports all the steps required to create a predictive model: data search, calculation and selection of a vast variety of molecular descriptors, application of machine learning methods, validation, analysis of the model and assessment of the applicability domain. As compared to other similar systems, OCHEM is not intended to re-implement the existing tools or models but rather to invite the original authors to contribute their results, make them publicly available, share them with other users and to become members of the growing research community. Our intention is to make OCHEM a widely used platform to perform the QSPR/QSAR studies online and share it with other users on the Web. The ultimate goal of OCHEM is collecting all possible chemoinformatics tools within one simple, reliable and user-friendly resource. The OCHEM is free for web users and it is available online at http://www.ochem.eu

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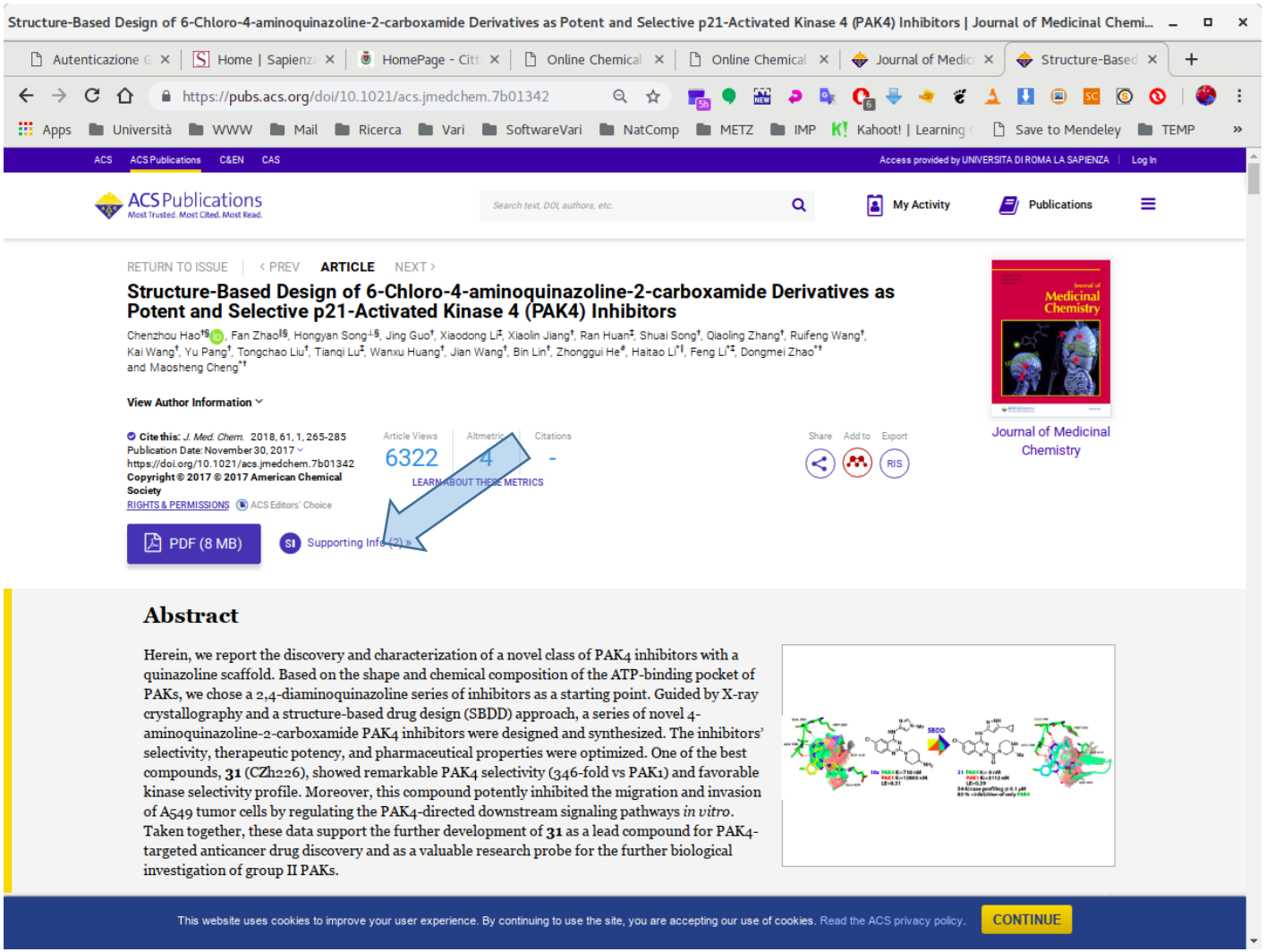
# Preparing the dataset



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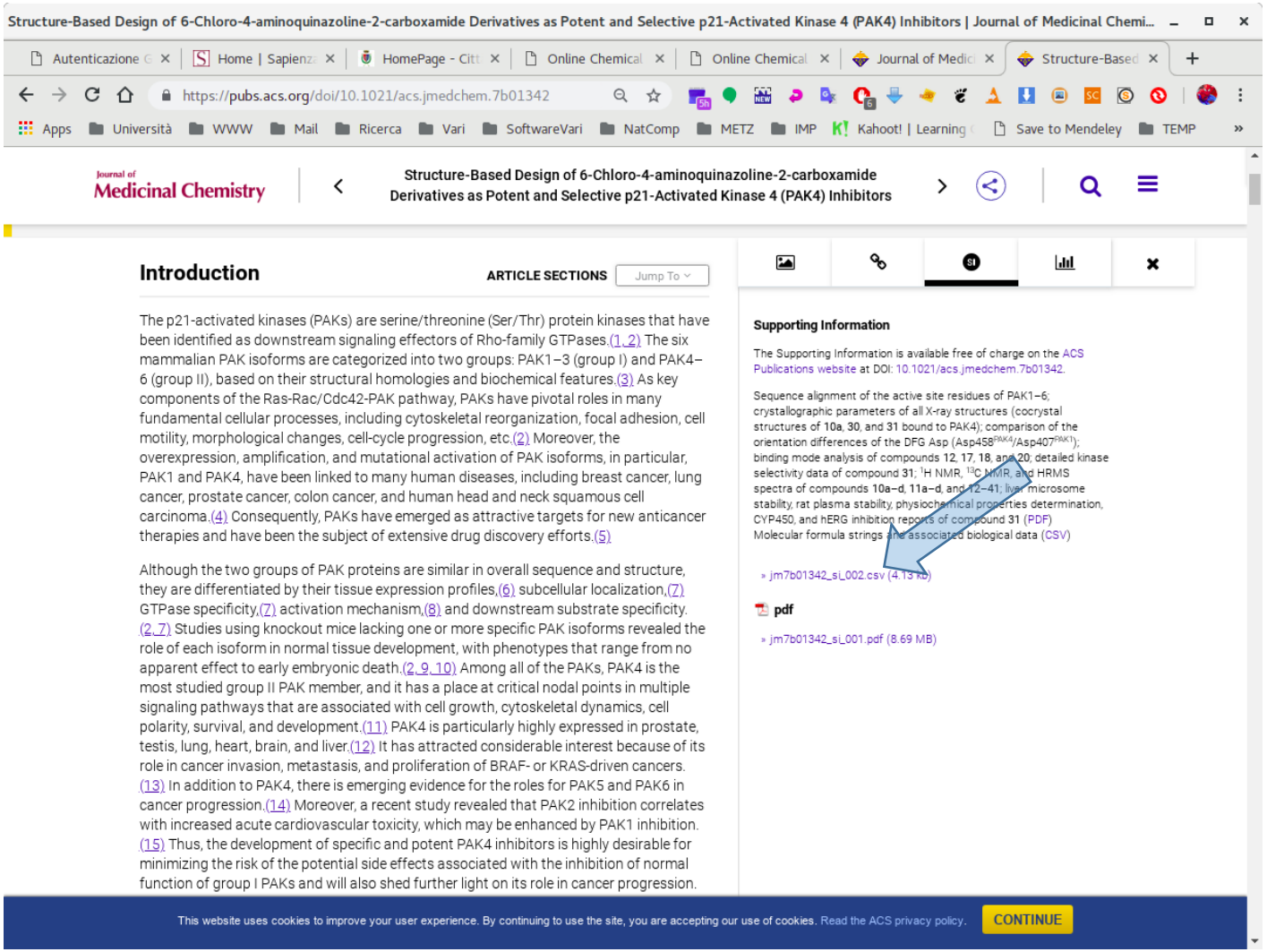

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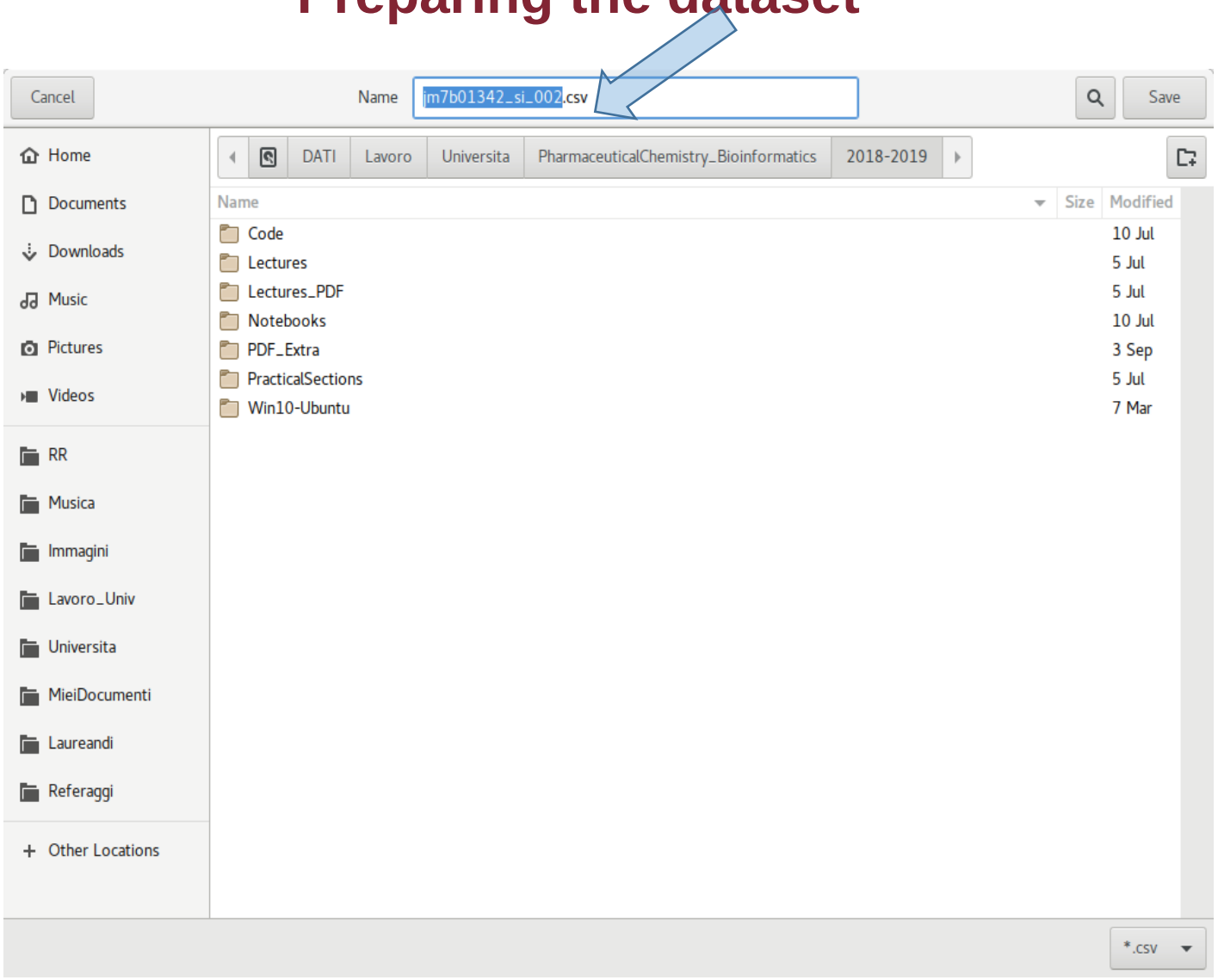

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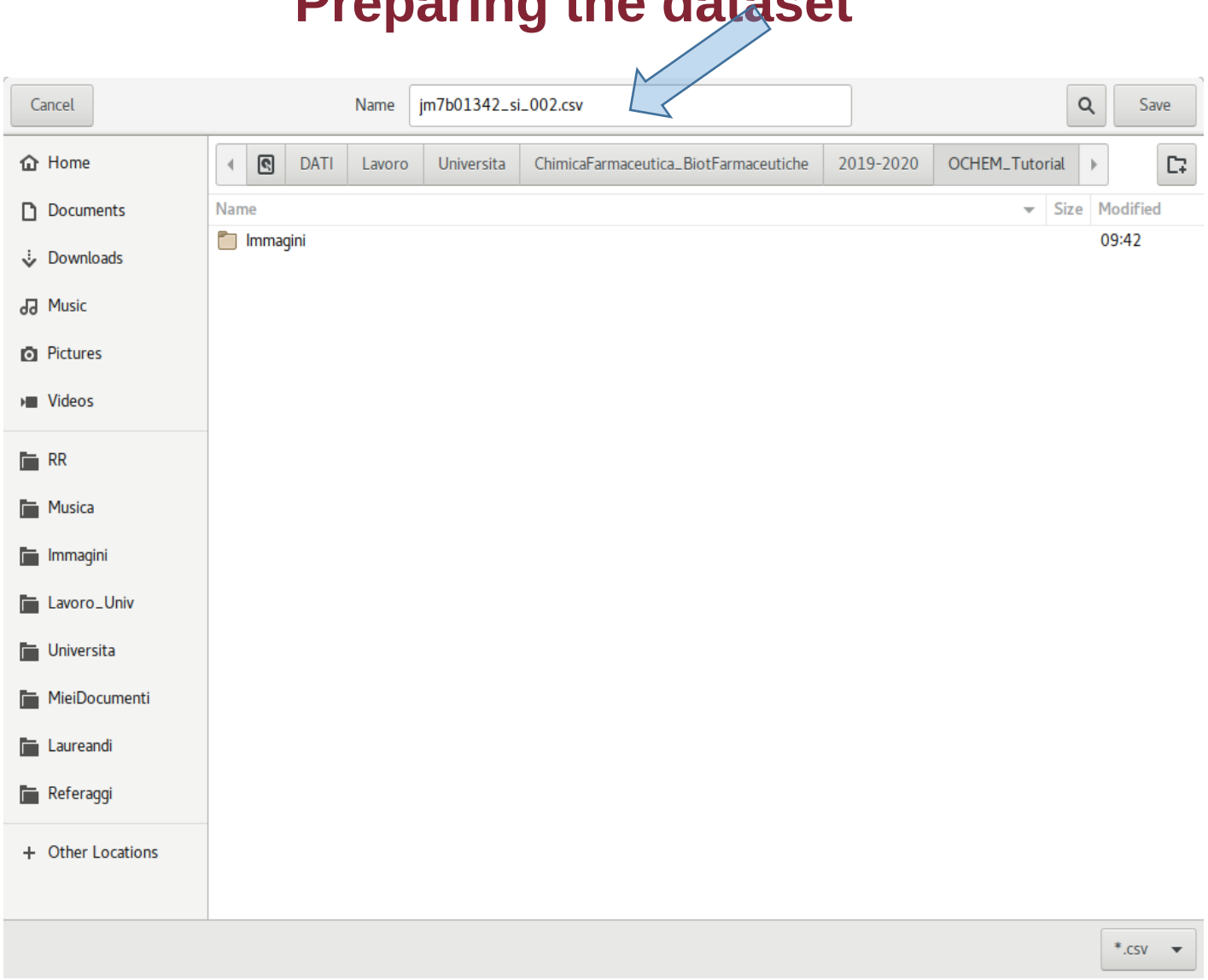

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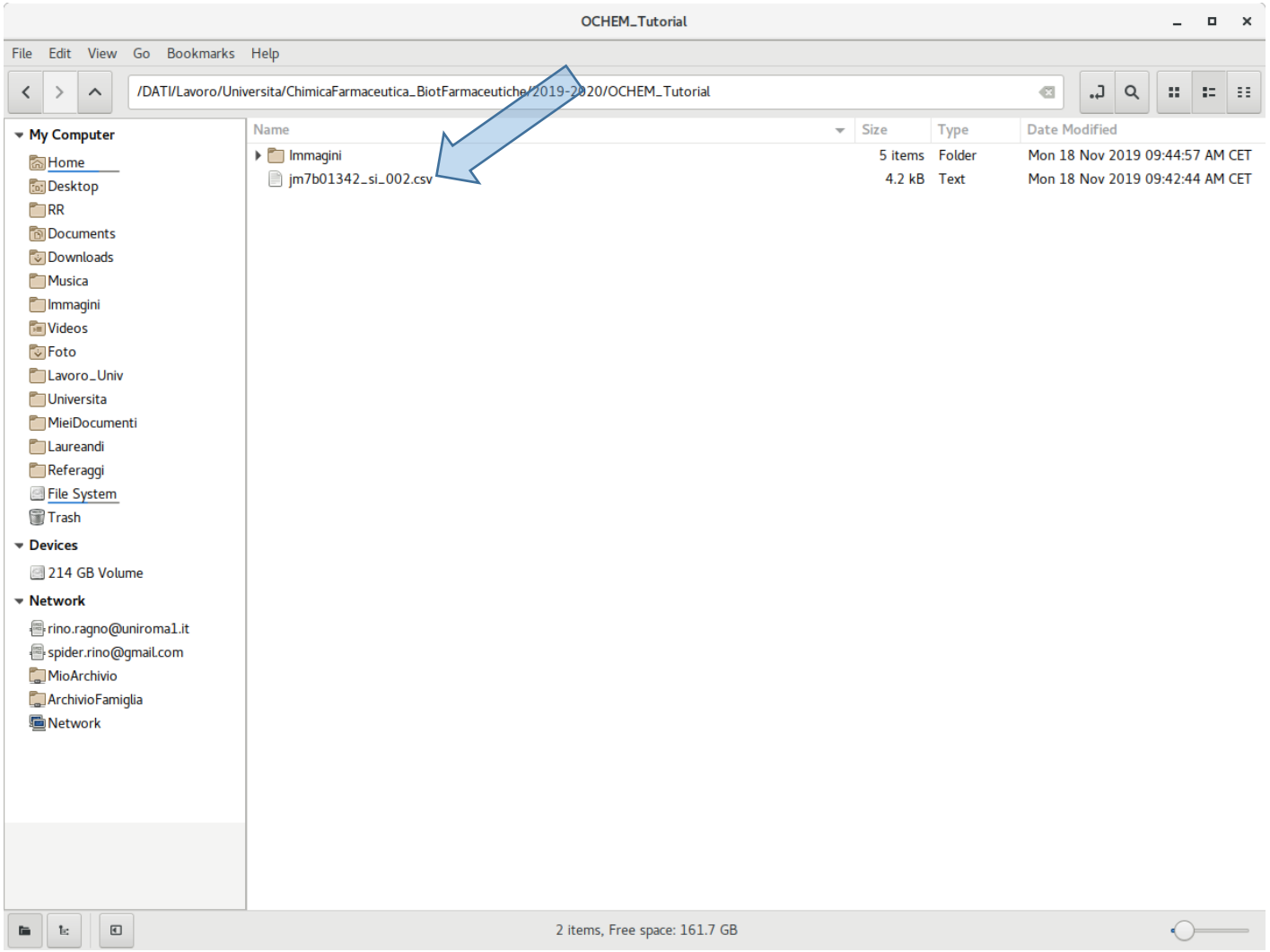

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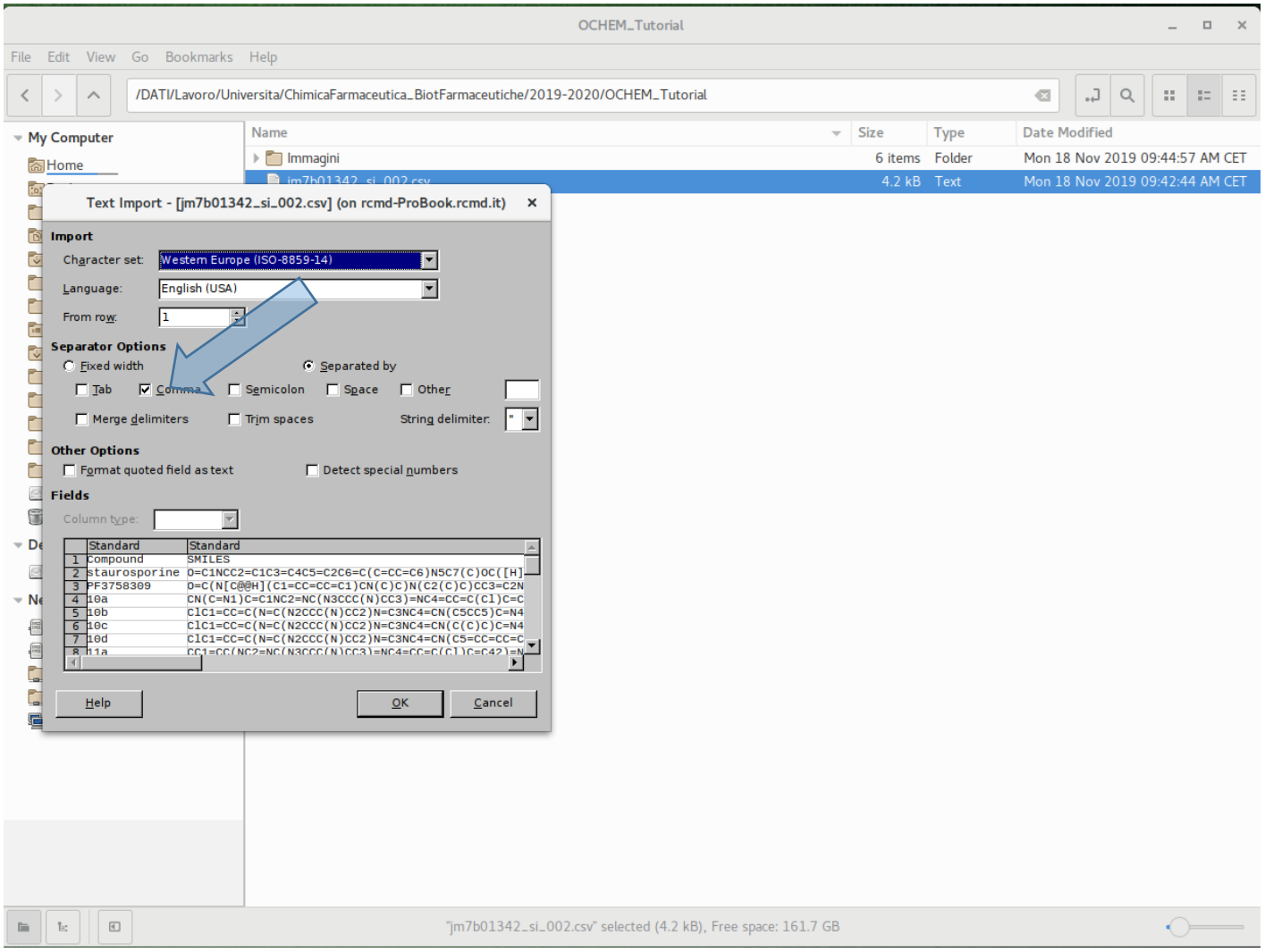

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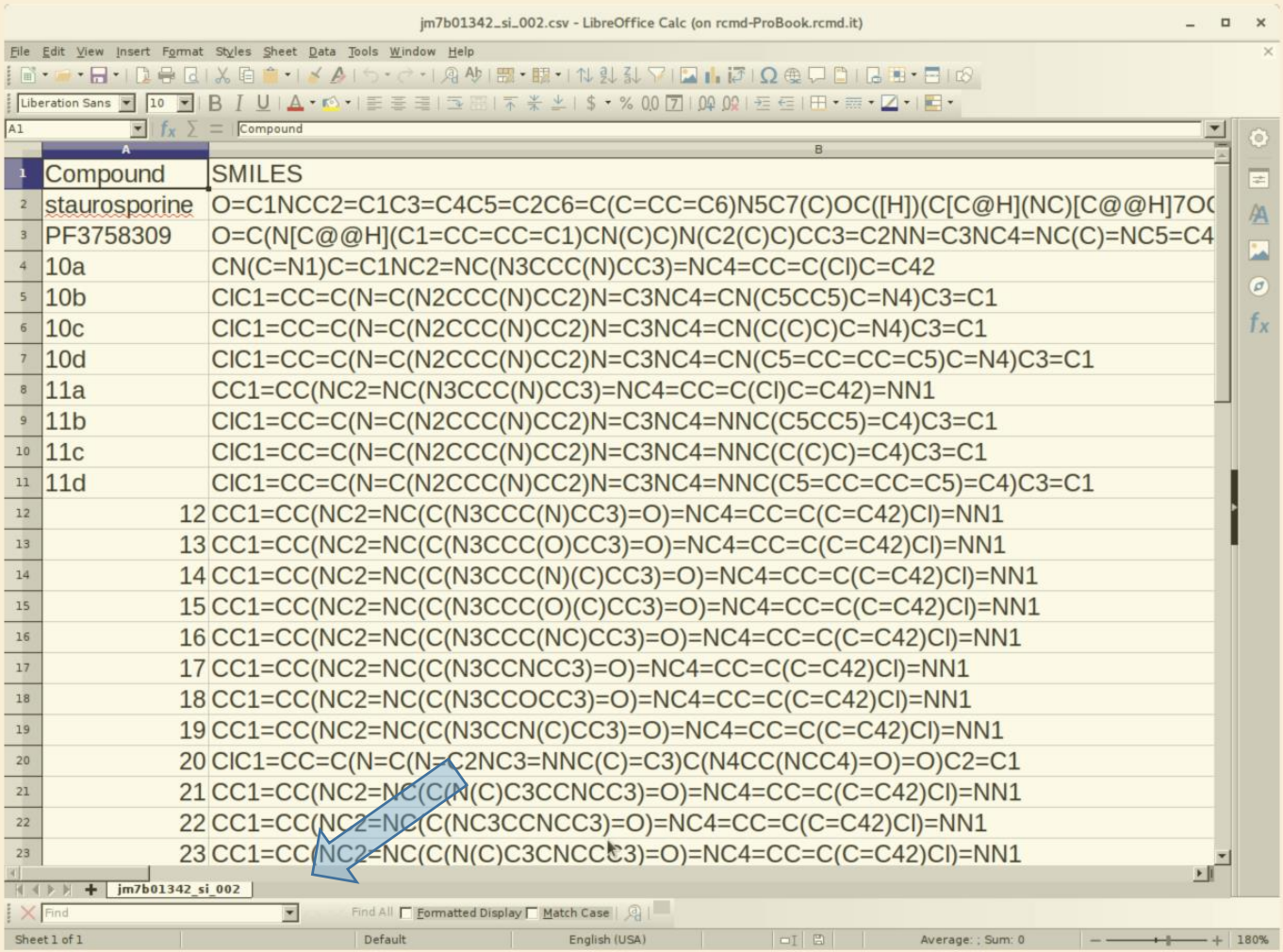
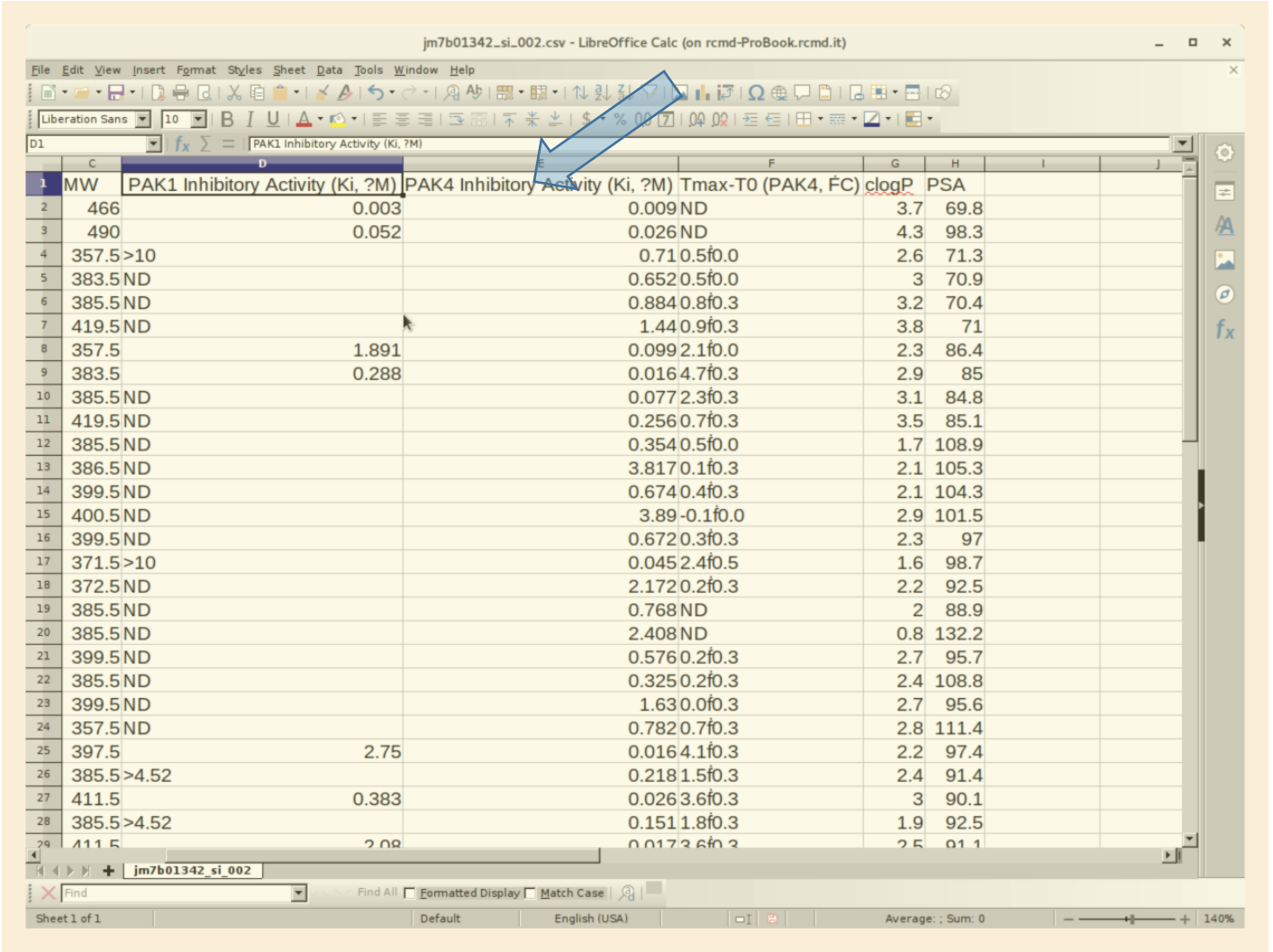


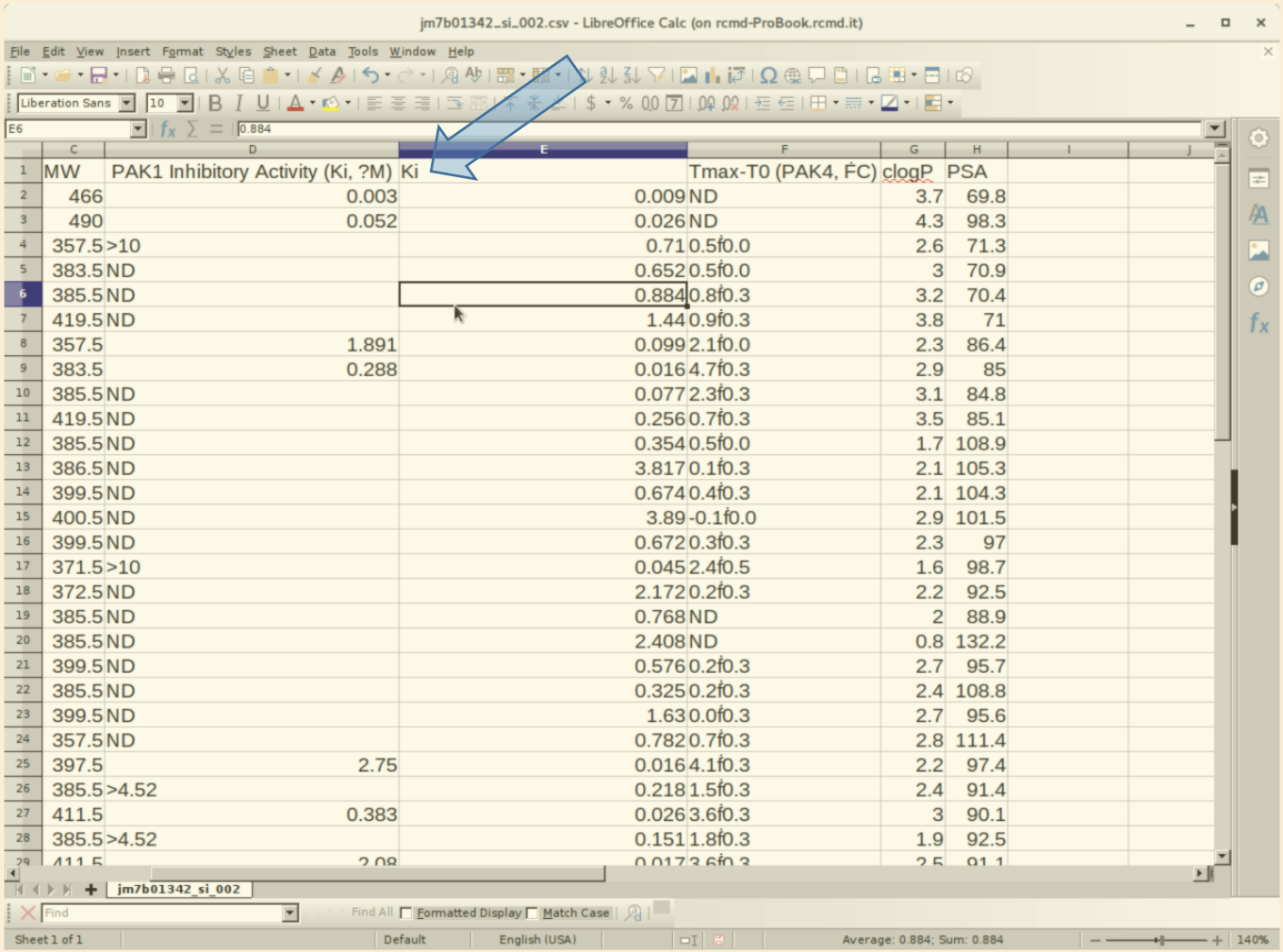

| | A | B |
|---|---|---|
| 1 | Compound | SMILES |
| 2 | staurosporine | O=C1NCC2=C1C3=C4C5=C2C6=C(C=CC=C6)N5C7(C)OC([H])(C[C@H](NC)[C@@H]7OC |
| 3 | PF3758309 | O=C(N[C@@H](C1=CC=CC=C1)CN(C)C)N(C2(C)C)CC3=C2NN=C3NC4=NC(C)=NC5=C4 |
| 4 | 10a | CN(C=N1)C=C1NC2=NC(N3CCC(N)CC3)=NC4=CC=C(Cl)C=C42 |
| 5 | 10b | ClC1=CC=C(N=C(N2CCC(N)CC2)N=C3NC4=CN(C5CC5)C=N4)C3=C1 |
| 6 | 10c | ClC1=CC=C(N=C(N2CCC(N)CC2)N=C3NC4=CN(C(C)C)C=N4)C3=C1 |
| 7 | 10d | ClC1=CC=C(N=C(N2CCC(N)CC2)N=C3NC4=CN(C5=CC=CC=C5)C=N4)C3=C1 |
| 8 | 11a | CC1=CC(NC2=NC(N3CCC(N)CC3)=NC4=CC=C(Cl)C=C42)=NN1 |
| 9 | 11b | ClC1=CC=C(N=C(N2CCC(N)CC2)N=C3NC4=NNC(C5CC5)=C4)C3=C1 |
| 10 | 11c | ClC1=CC=C(N=C(N2CCC(N)CC2)N=C3NC4=NNC(C(C)C)=C4)C3=C1 |
| 11 | 11d | ClC1=CC=C(N=C(N2CCC(N)CC2)N=C3NC4=NNC(C5=CC=CC=C5)=C4)C3=C1 |
| 12 | 12 | CC1=CC(NC2=NC(C(N3CCC(N)CC3)=O)=NC4=CC=C(C=C42)Cl)=NN1 |
| 13 | 13 | CC1=CC(NC2=NC(C(N3CCC(O)CC3)=O)=NC4=CC=C(C=C42)Cl)=NN1 |
| 14 | 14 | CC1=CC(NC2=NC(C(N3CCC(N)(C)CC3)=O)=NC4=CC=C(C=C42)Cl)=NN1 |
| 15 | 15 | CC1=CC(NC2=NC(C(N3CCC(O)(C)CC3)=O)=NC4=CC=C(C=C42)Cl)=NN1 |
| 16 | 16 | CC1=CC(NC2=NC(C(N3CCC(NC)CC3)=O)=NC4=CC=C(C=C42)Cl)=NN1 |
| 17 | 17 | CC1=CC(NC2=NC(C(N3CCNCC3)=O)=NC4=CC=C(C=C42)Cl)=NN1 |
| 18 | 18 | CC1=CC(NC2=NC(C(N3CCOCC3)=O)=NC4=CC=C(C=C42)Cl)=NN1 |
| 19 | 19 | CC1=CC(NC2=NC(C(N3CCN(C)CC3)=O)=NC4=CC=C(C=C42)Cl)=NN1 |
| 20 | 20 | ClC1=CC=C(N=C(N=C2NC3=NNC(C)=C3)C(N4CC(NCC4)=O)=O)C2=C1 |
| 21 | 21 | CC1=CC(NC2=NC(C(N(C)C3CCNCC3)=O)=NC4=CC=C(C=C42)Cl)=NN1 |
| 22 | 22 | CC1=CC(NC2=NC(C(NC3CCNCC3)=O)=NC4=CC=C(C=C42)Cl)=NN1 |
| 23 | 23 | CC1=CC(NC2=NC(C(N(C)C3CNCCC3)=O)=NC4=CC=C(C=C42)Cl)=NN1 |

# Preparing the dataset




| | C | D | E | F | G | H | I | J |
|---|---|---|---|---|---|---|---|---|
| 1 | MW | PAK1 Inhibitory Activity (Ki, ?M) | PAK4 Inhibitory Activity (Ki, ?M) | Tmax-T0 (PAK4, FC) | clogP | PSA | | |
| 2 | 466 | 0.003 | 0.009 | ND | 3.7 | 69.8 | | |
| 3 | 490 | 0.052 | 0.026 | ND | 4.3 | 98.3 | | |
| 4 | 357.5 | >10 | 0.71 | 0.5±0.0 | 2.6 | 71.3 | | |
| 5 | 383.5 | ND | 0.652 | 0.5±0.0 | 3 | 70.9 | | |
| 6 | 385.5 | ND | 0.884 | 0.8±0.3 | 3.2 | 70.4 | | |
| 7 | 419.5 | ND | 1.44 | 0.9±0.3 | 3.8 | 71 | | |
| 8 | 357.5 | 1.891 | 0.099 | 2.1±0.0 | 2.3 | 86.4 | | |
| 9 | 383.5 | 0.288 | 0.016 | 4.7±0.3 | 2.9 | 85 | | |
| 10 | 385.5 | ND | 0.077 | 2.3±0.3 | 3.1 | 84.8 | | |
| 11 | 419.5 | ND | 0.256 | 0.7±0.3 | 3.5 | 85.1 | | |
| 12 | 385.5 | ND | 0.354 | 0.5±0.0 | 1.7 | 108.9 | | |
| 13 | 386.5 | ND | 3.817 | 0.1±0.3 | 2.1 | 105.3 | | |
| 14 | 399.5 | ND | 0.674 | 0.4±0.3 | 2.1 | 104.3 | | |
| 15 | 400.5 | ND | 3.89 | -0.1±0.0 | 2.9 | 101.5 | | |
| 16 | 399.5 | ND | 0.672 | 0.3±0.3 | 2.3 | 97 | | |
| 17 | 371.5 | >10 | 0.045 | 2.4±0.5 | 1.6 | 98.7 | | |
| 18 | 372.5 | ND | 2.172 | 0.2±0.3 | 2.2 | 92.5 | | |
| 19 | 385.5 | ND | 0.768 | ND | 2 | 88.9 | | |
| 20 | 385.5 | ND | 2.408 | ND | 0.8 | 132.2 | | |
| 21 | 399.5 | ND | 0.576 | 0.2±0.3 | 2.7 | 95.7 | | |
| 22 | 385.5 | ND | 0.325 | 0.2±0.3 | 2.4 | 108.8 | | |
| 23 | 399.5 | ND | 1.63 | 0.0±0.3 | 2.7 | 95.6 | | |
| 24 | 357.5 | ND | 0.782 | 0.7±0.3 | 2.8 | 111.4 | | |
| 25 | 397.5 | 2.75 | 0.016 | 4.1±0.3 | 2.2 | 97.4 | | |
| 26 | 385.5 | >4.52 | 0.218 | 1.5±0.3 | 2.4 | 91.4 | | |
| 27 | 411.5 | 0.383 | 0.026 | 3.6±0.3 | 3 | 90.1 | | |
| 28 | 385.5 | >4.52 | 0.151 | 1.8±0.3 | 1.9 | 92.5 | | |
| 29 | 411.5 | 2.08 | 0.017 | 3.6±0.3 | 2.5 | 91.1 | | |

# Preparing the dataset




| | C | D | E | F | G | H |
|---|---|---|---|---|---|---|
| 1 | MW | PAK1 Inhibitory Activity (Ki, ?M) | Ki | Tmax-T0 (PAK4, ?C) | clogP | PSA |
| 2 | 466 | 0.003 | 0.009 | ND | 3.7 | 69.8 |
| 3 | 490 | 0.052 | 0.026 | ND | 4.3 | 98.3 |
| 4 | 357.5 | >10 | 0.71 | 0.5?0.0 | 2.6 | 71.3 |
| 5 | 383.5 | ND | 0.652 | 0.5?0.0 | 3 | 70.9 |
| 6 | 385.5 | ND | 0.884 | 0.8?0.3 | 3.2 | 70.4 |
| 7 | 419.5 | ND | 1.44 | 0.9?0.3 | 3.8 | 71 |
| 8 | 357.5 | 1.891 | 0.099 | 2.1?0.0 | 2.3 | 86.4 |
| 9 | 383.5 | 0.288 | 0.016 | 4.7?0.3 | 2.9 | 85 |
| 10 | 385.5 | ND | 0.077 | 2.3?0.3 | 3.1 | 84.8 |
| 11 | 419.5 | ND | 0.256 | 0.7?0.3 | 3.5 | 85.1 |
| 12 | 385.5 | ND | 0.354 | 0.5?0.0 | 1.7 | 108.9 |
| 13 | 386.5 | ND | 3.817 | 0.1?0.3 | 2.1 | 105.3 |
| 14 | 399.5 | ND | 0.674 | 0.4?0.3 | 2.1 | 104.3 |
| 15 | 400.5 | ND | 3.89 | -0.1?0.0 | 2.9 | 101.5 |
| 16 | 399.5 | ND | 0.672 | 0.3?0.3 | 2.3 | 97 |
| 17 | 371.5 | >10 | 0.045 | 2.4?0.5 | 1.6 | 98.7 |
| 18 | 372.5 | ND | 2.172 | 0.2?0.3 | 2.2 | 92.5 |
| 19 | 385.5 | ND | 0.768 | ND | 2 | 88.9 |
| 20 | 385.5 | ND | 2.408 | ND | 0.8 | 132.2 |
| 21 | 399.5 | ND | 0.576 | 0.2?0.3 | 2.7 | 95.7 |
| 22 | 385.5 | ND | 0.325 | 0.2?0.3 | 2.4 | 108.8 |
| 23 | 399.5 | ND | 1.63 | 0.0?0.3 | 2.7 | 95.6 |
| 24 | 357.5 | ND | 0.782 | 0.7?0.3 | 2.8 | 111.4 |
| 25 | 397.5 | 2.75 | 0.016 | 4.1?0.3 | 2.2 | 97.4 |
| 26 | 385.5 | >4.52 | 0.218 | 1.5?0.3 | 2.4 | 91.4 |
| 27 | 411.5 | 0.383 | 0.026 | 3.6?0.3 | 3 | 90.1 |
| 28 | 385.5 | >4.52 | 0.151 | 1.8?0.3 | 1.9 | 92.5 |
| 29 | 411.5 | 2.08 | 0.017 | 3.6?0.3 | 2.5 | 91.1 |

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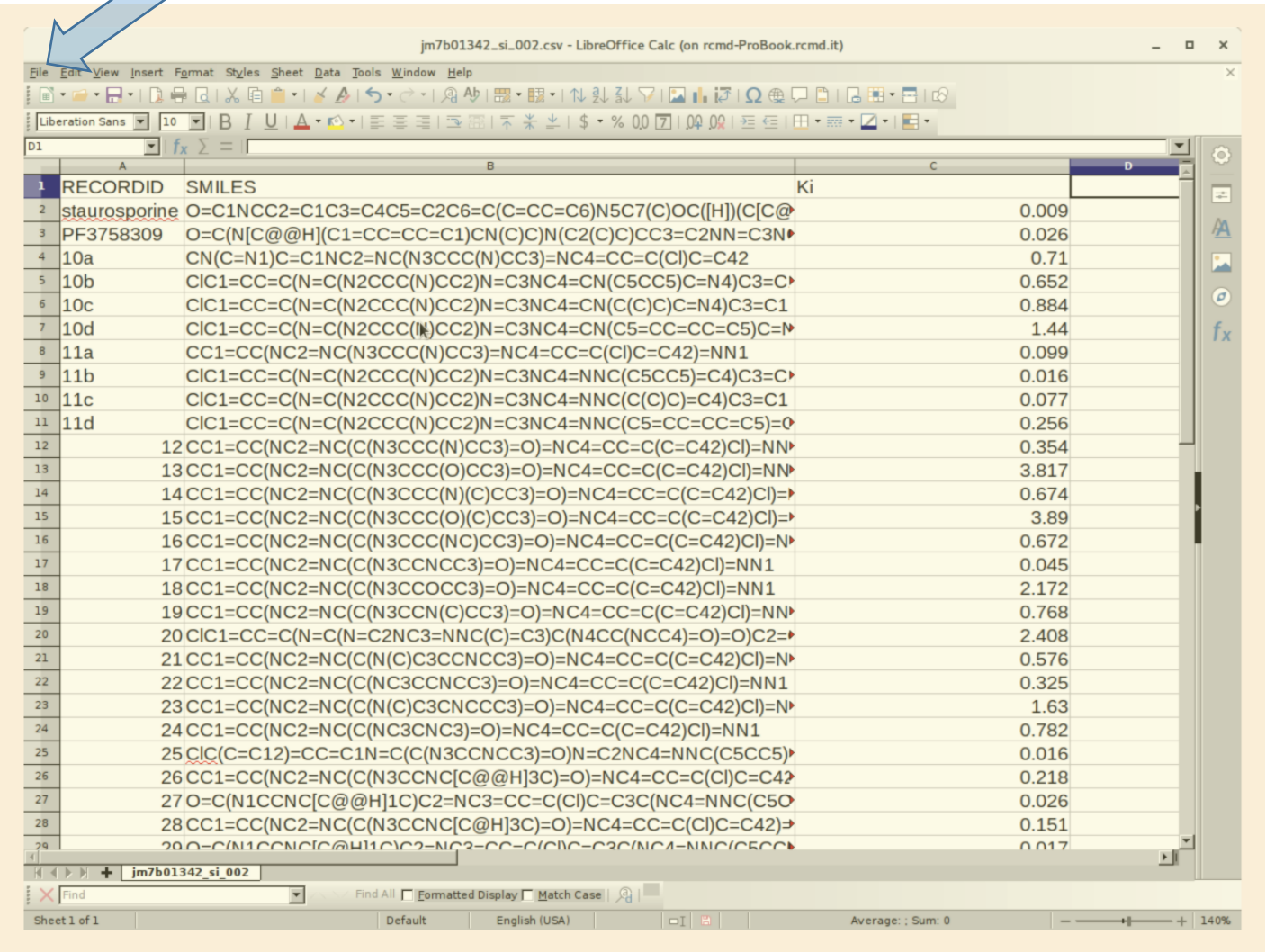


| | A | B | C | D |
|---|---|---|---|---|
| 1 | RECORDID | SMILES | Ki | |
| 2 | staurosporine | O=C1NCC2=C1C3=C4C5=C2C6=C(C=CC=C6)N5C7(C)OC([H])(C[C@ | 0.009 | |
| 3 | PF3758309 | O=C(N[C@@H](C1=CC=CC=C1)CN(C)C)N(C2(C)C)CC3=C2NN=C3N | 0.026 | |
| 4 | 10a | CN(C=N1)C=C1NC2=NC(N3CCC(N)CC3)=NC4=CC=C(Cl)C=C42 | 0.71 | |
| 5 | 10b | ClC1=CC=C(N=C(N2CCC(N)CC2)N=C3NC4=CN(C5CC5)C=N4)C3=C | 0.652 | |
| 6 | 10c | ClC1=CC=C(N=C(N2CCC(N)CC2)N=C3NC4=CN(C(C)C)C=N4)C3=C1 | 0.884 | |
| 7 | 10d | ClC1=CC=C(N=C(N2CCC(N)CC2)N=C3NC4=CN(C5=CC=CC=C5)C=N | 1.44 | |
| 8 | 11a | CC1=CC(NC2=NC(N3CCC(N)CC3)=NC4=CC=C(Cl)C=C42)=NN1 | 0.099 | |
| 9 | 11b | ClC1=CC=C(N=C(N2CCC(N)CC2)N=C3NC4=NNC(C5CC5)=C4)C3=C | 0.016 | |
| 10 | 11c | ClC1=CC=C(N=C(N2CCC(N)CC2)N=C3NC4=NNC(C(C)C)=C4)C3=C1 | 0.077 | |
| 11 | 11d | ClC1=CC=C(N=C(N2CCC(N)CC2)N=C3NC4=NNC(C5=CC=CC=C5)=C | 0.256 | |
| 12 | 12 | CC1=CC(NC2=NC(C(N3CCC(N)CC3)=O)=NC4=CC=C(C=C42)Cl)=NN | 0.354 | |
| 13 | 13 | CC1=CC(NC2=NC(C(N3CCC(O)CC3)=O)=NC4=CC=C(C=C42)Cl)=NN | 3.817 | |
| 14 | 14 | CC1=CC(NC2=NC(C(N3CCC(N)(C)CC3)=O)=NC4=CC=C(C=C42)Cl)= | 0.674 | |
| 15 | 15 | CC1=CC(NC2=NC(C(N3CCC(O)(C)CC3)=O)=NC4=CC=C(C=C42)Cl)= | 3.89 | |
| 16 | 16 | CC1=CC(NC2=NC(C(N3CCC(NC)CC3)=O)=NC4=CC=C(C=C42)Cl)=N | 0.672 | |
| 17 | 17 | CC1=CC(NC2=NC(C(N3CCNCC3)=O)=NC4=CC=C(C=C42)Cl)=NN1 | 0.045 | |
| 18 | 18 | CC1=CC(NC2=NC(C(N3CCOCC3)=O)=NC4=CC=C(C=C42)Cl)=NN1 | 2.172 | |
| 19 | 19 | CC1=CC(NC2=NC(C(N3CCN(C)CC3)=O)=NC4=CC=C(C=C42)Cl)=NN | 0.768 | |
| 20 | 20 | ClC1=CC=C(N=C(N=C2NC3=NNC(C)=C3)C(N4CC(NCC4)=O)=O)C2= | 2.408 | |
| 21 | 21 | CC1=CC(NC2=NC(C(N(C)C3CCNCC3)=O)=NC4=CC=C(C=C42)Cl)=N | 0.576 | |
| 22 | 22 | CC1=CC(NC2=NC(C(NC3CCNCC3)=O)=NC4=CC=C(C=C42)Cl)=NN1 | 0.325 | |
| 23 | 23 | CC1=CC(NC2=NC(C(N(C)C3CNCCC3)=O)=NC4=CC=C(C=C42)Cl)=N | 1.63 | |
| 24 | 24 | CC1=CC(NC2=NC(C(NC3CNC3)=O)=NC4=CC=C(C=C42)Cl)=NN1 | 0.782 | |
| 25 | 25 | ClC(C=C12)=CC=C1N=C(C(N3CCNCC3)=O)N=C2NC4=NNC(C5CC5) | 0.016 | |
| 26 | 26 | CC1=CC(NC2=NC(C(N3CCNC[C@@H]3C)=O)=NC4=CC=C(Cl)C=C42 | 0.218 | |
| 27 | 27 | O=C(N1CCNC[C@@H]1C)C2=NC3=CC=C(Cl)C=C3C(NC4=NNC(C5O | 0.026 | |
| 28 | 28 | CC1=CC(NC2=NC(C(N3CCNC[C@H]3C)=O)=NC4=CC=C(Cl)C=C42) | 0.151 | |
| 29 | | O=C(N1CCNC[C@H]1C)C2=NC3=CC=C(Cl)C=C3C(NC4=NNC(C5CC | 0.017 | |

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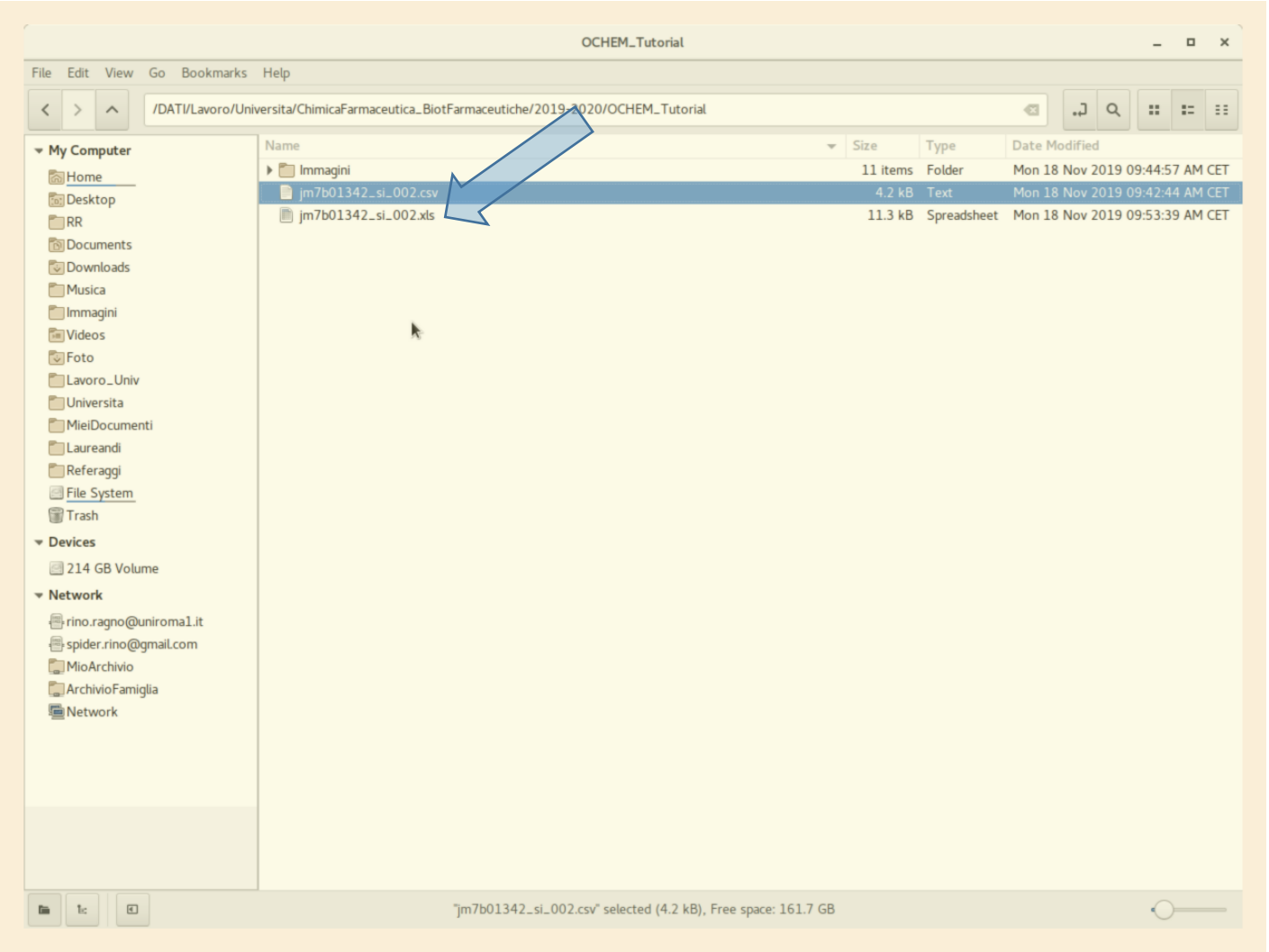

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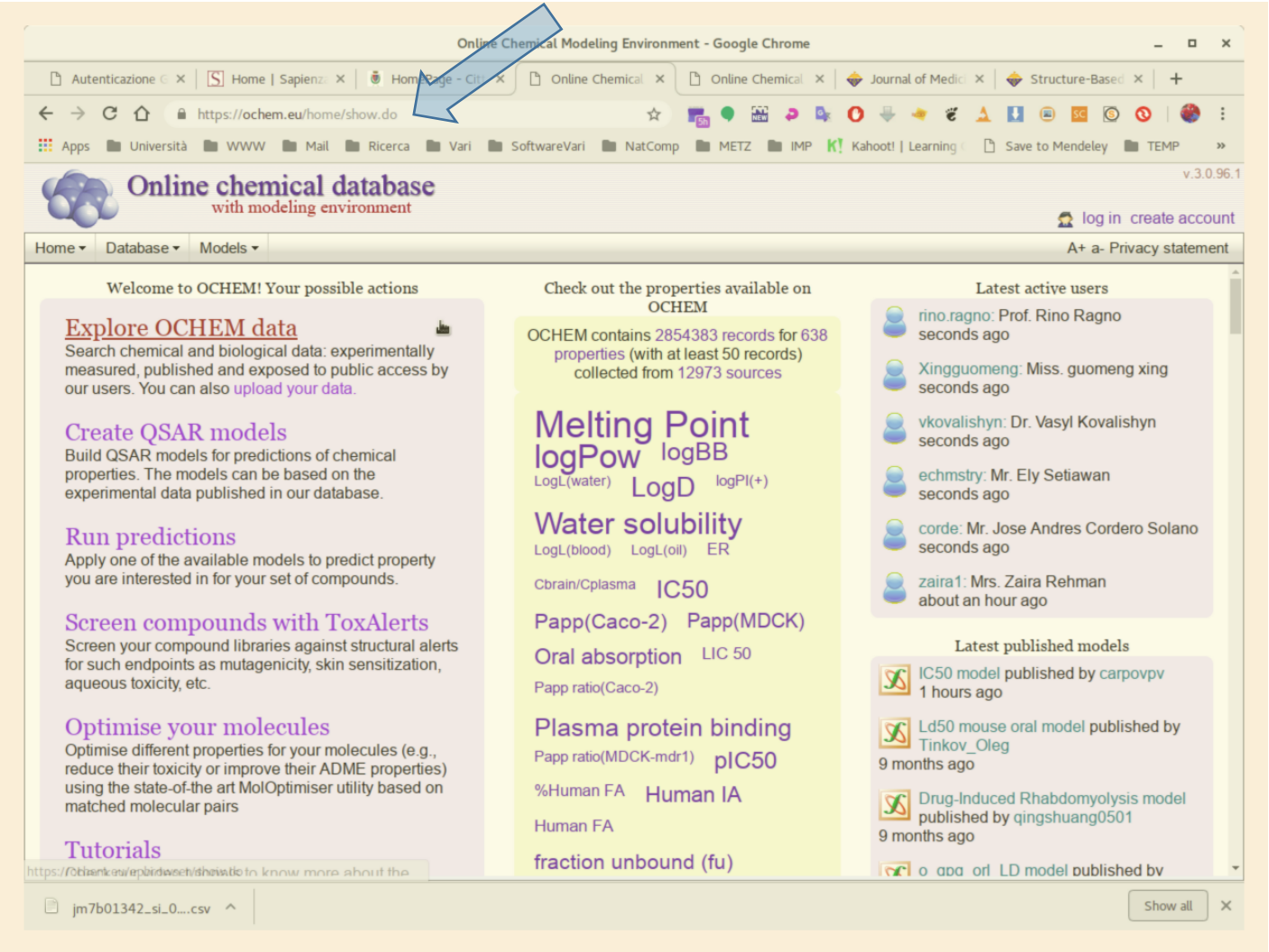

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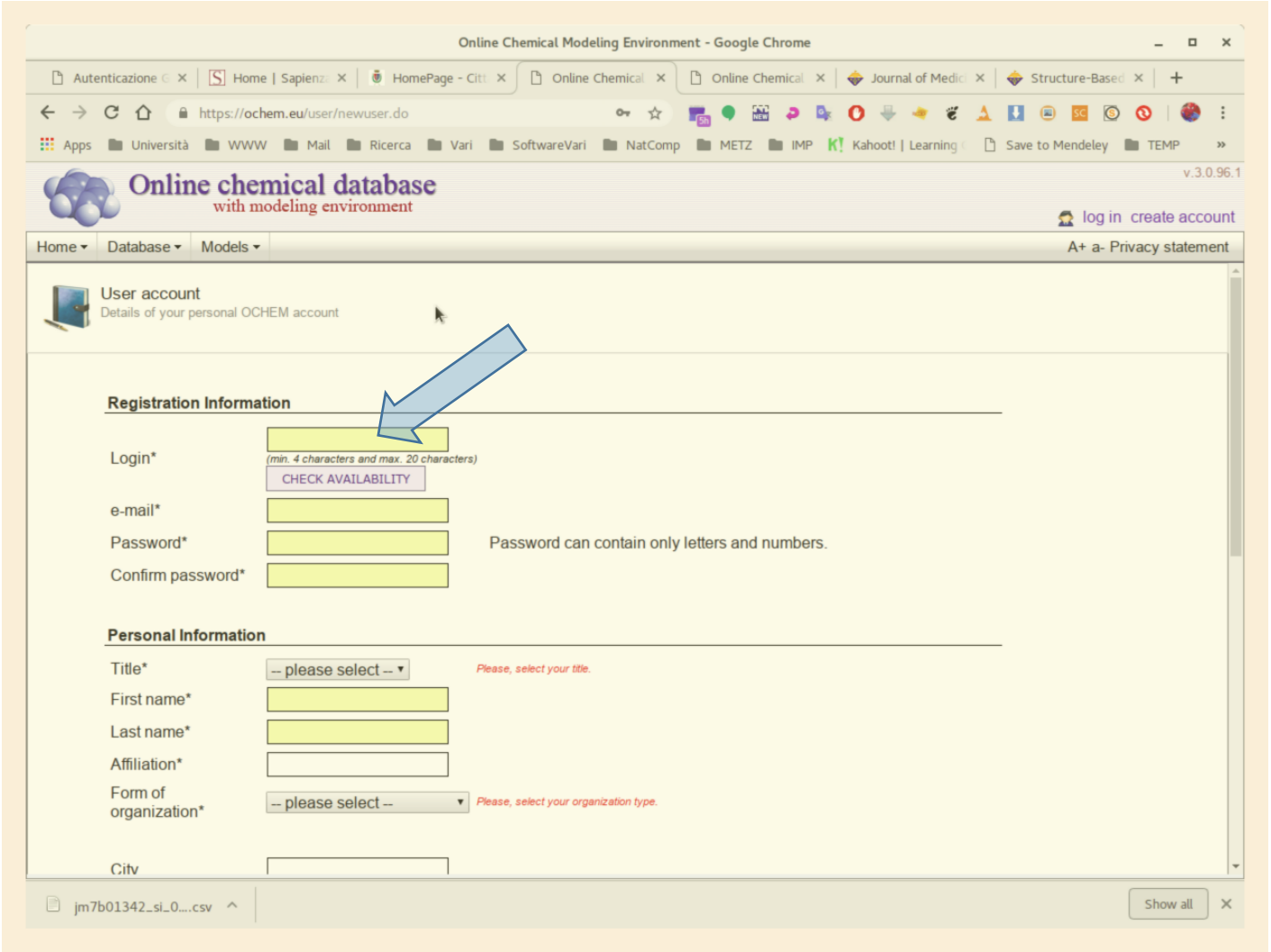

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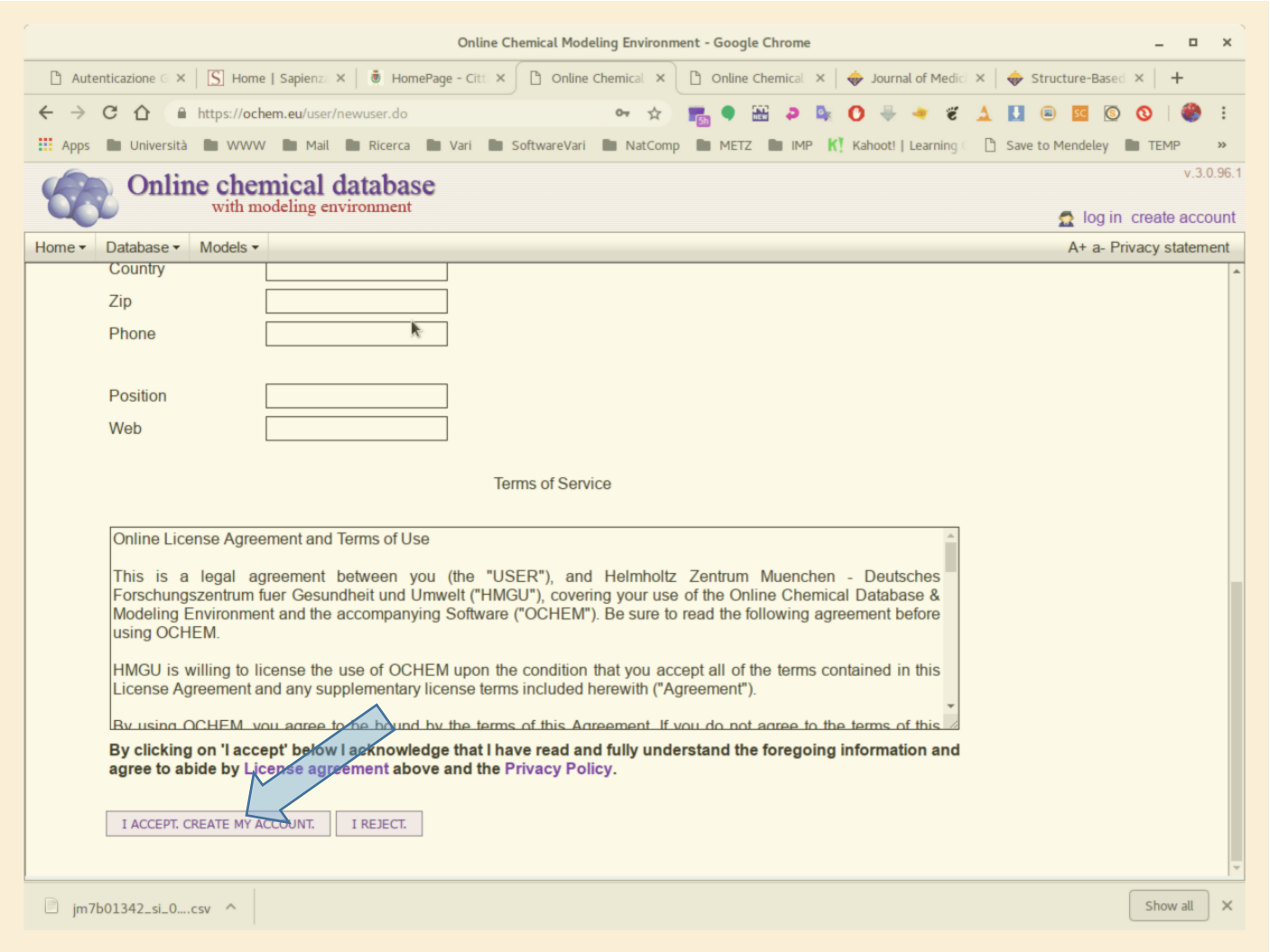

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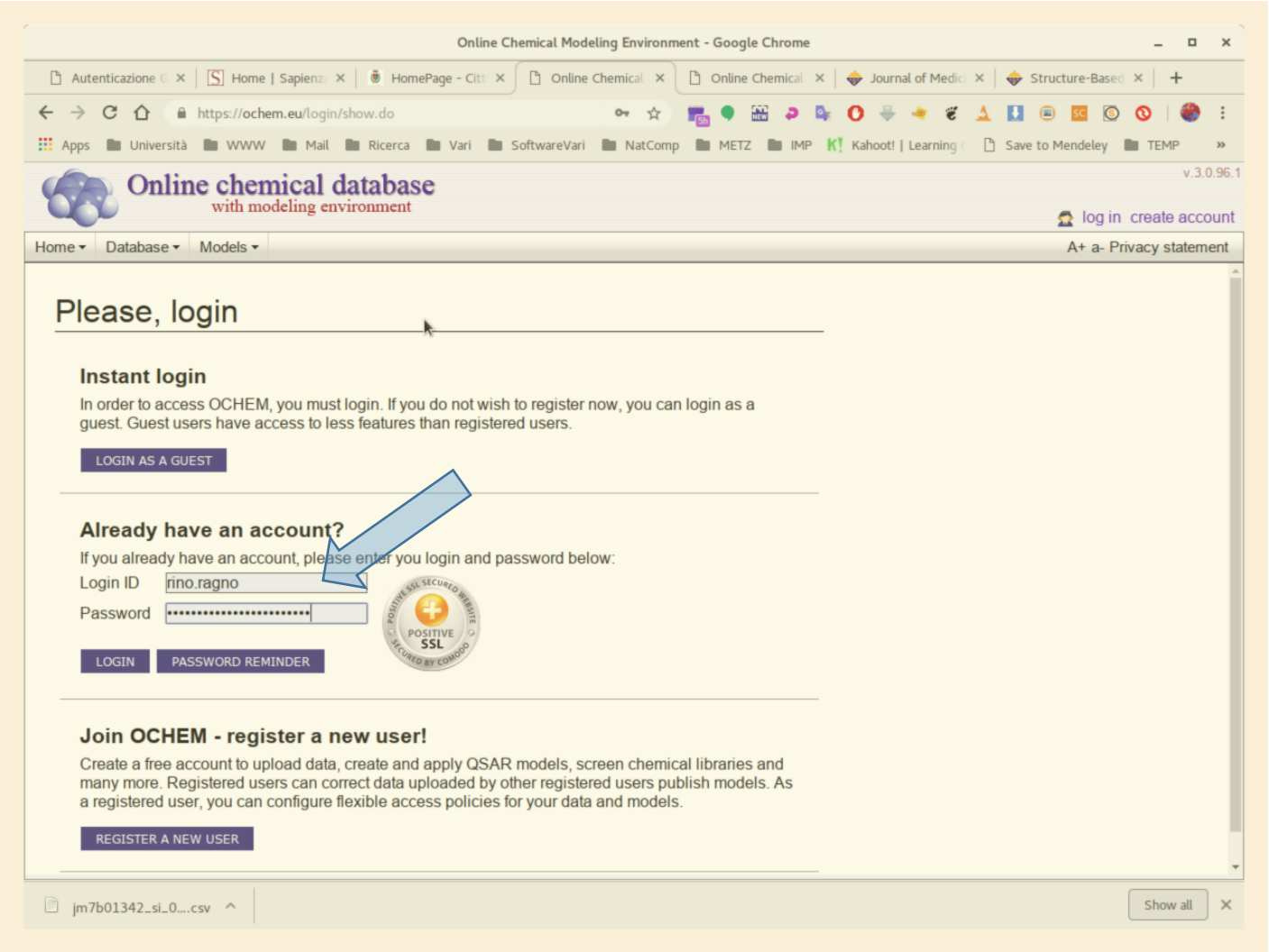

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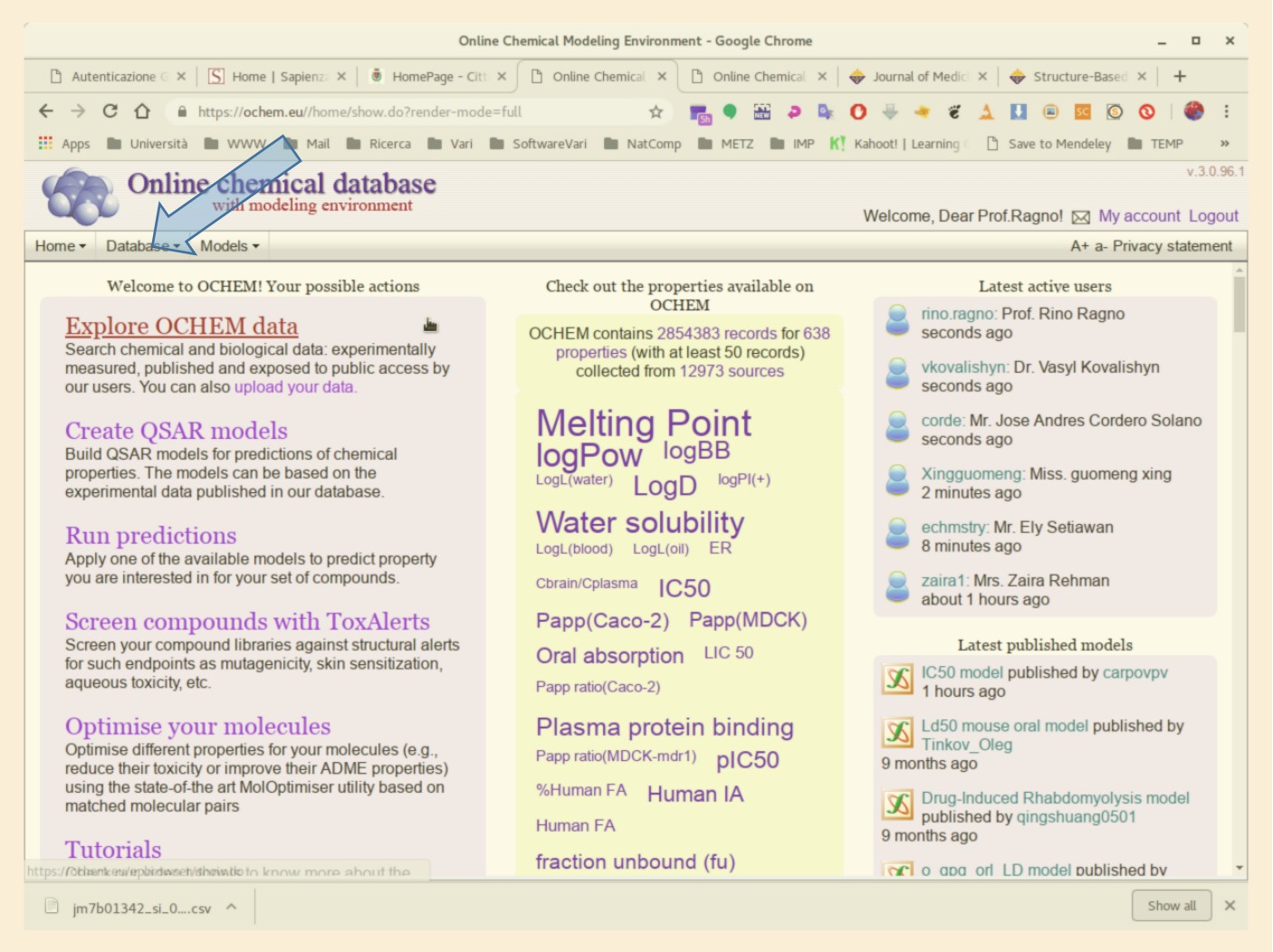

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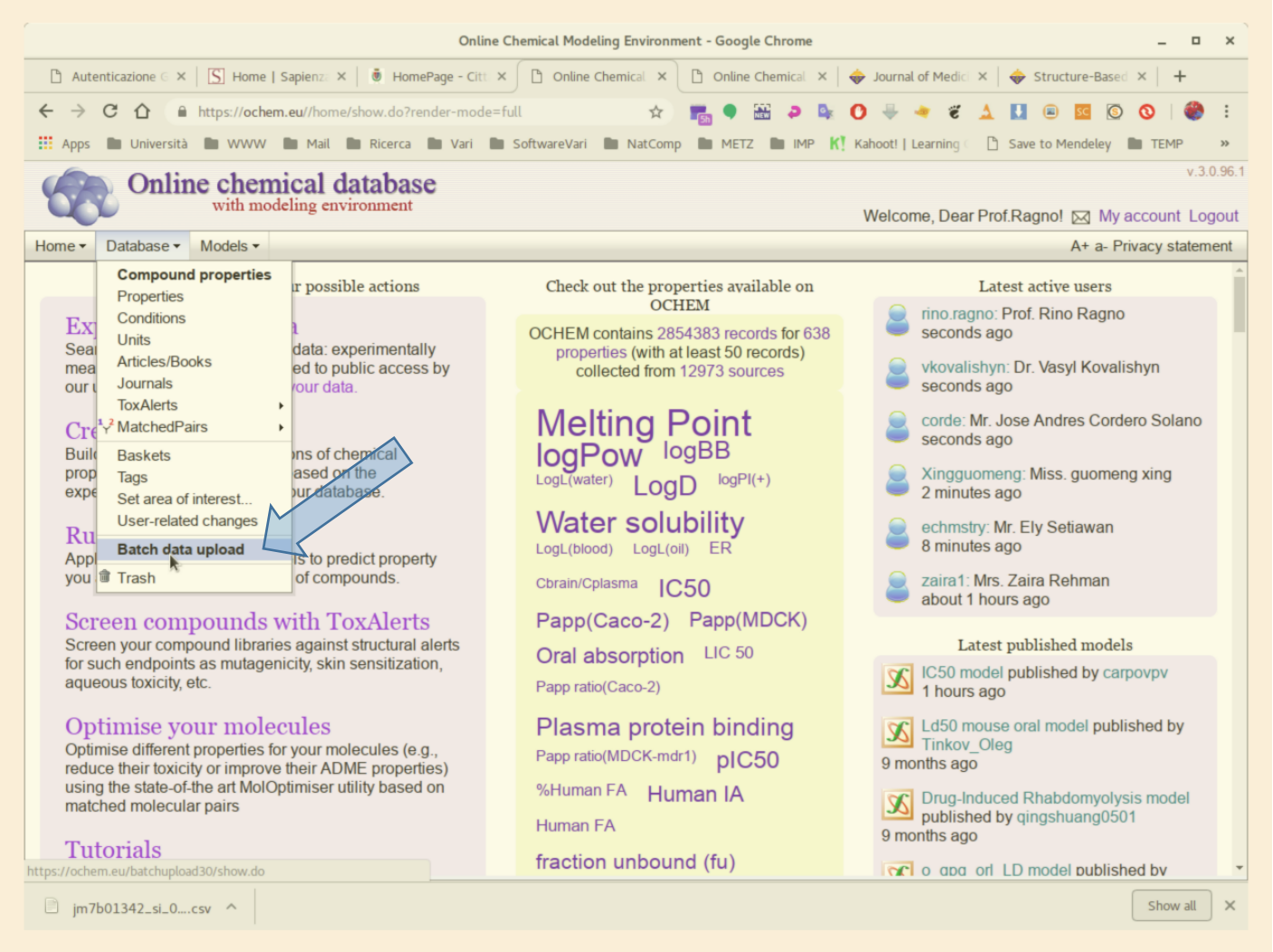

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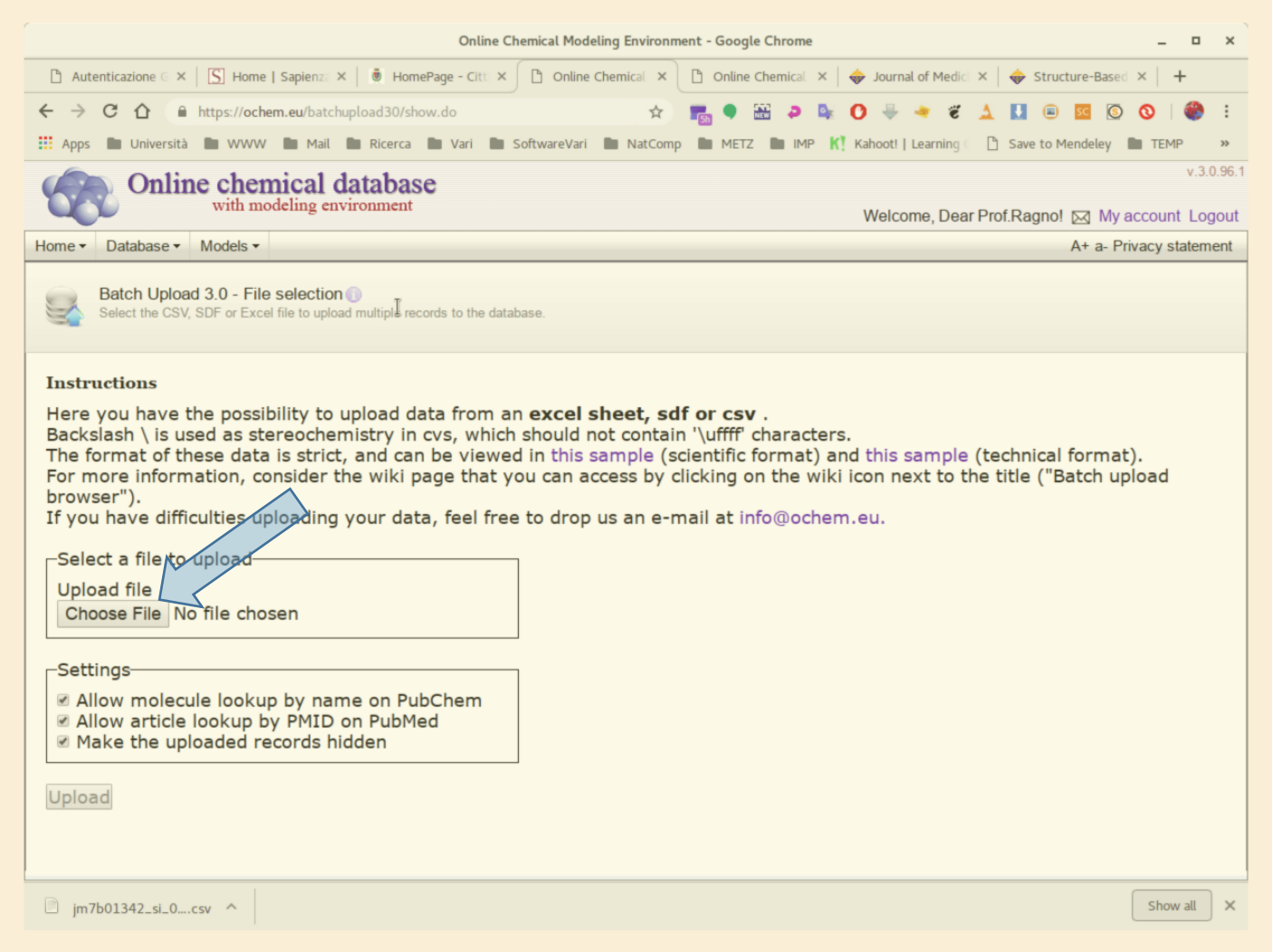

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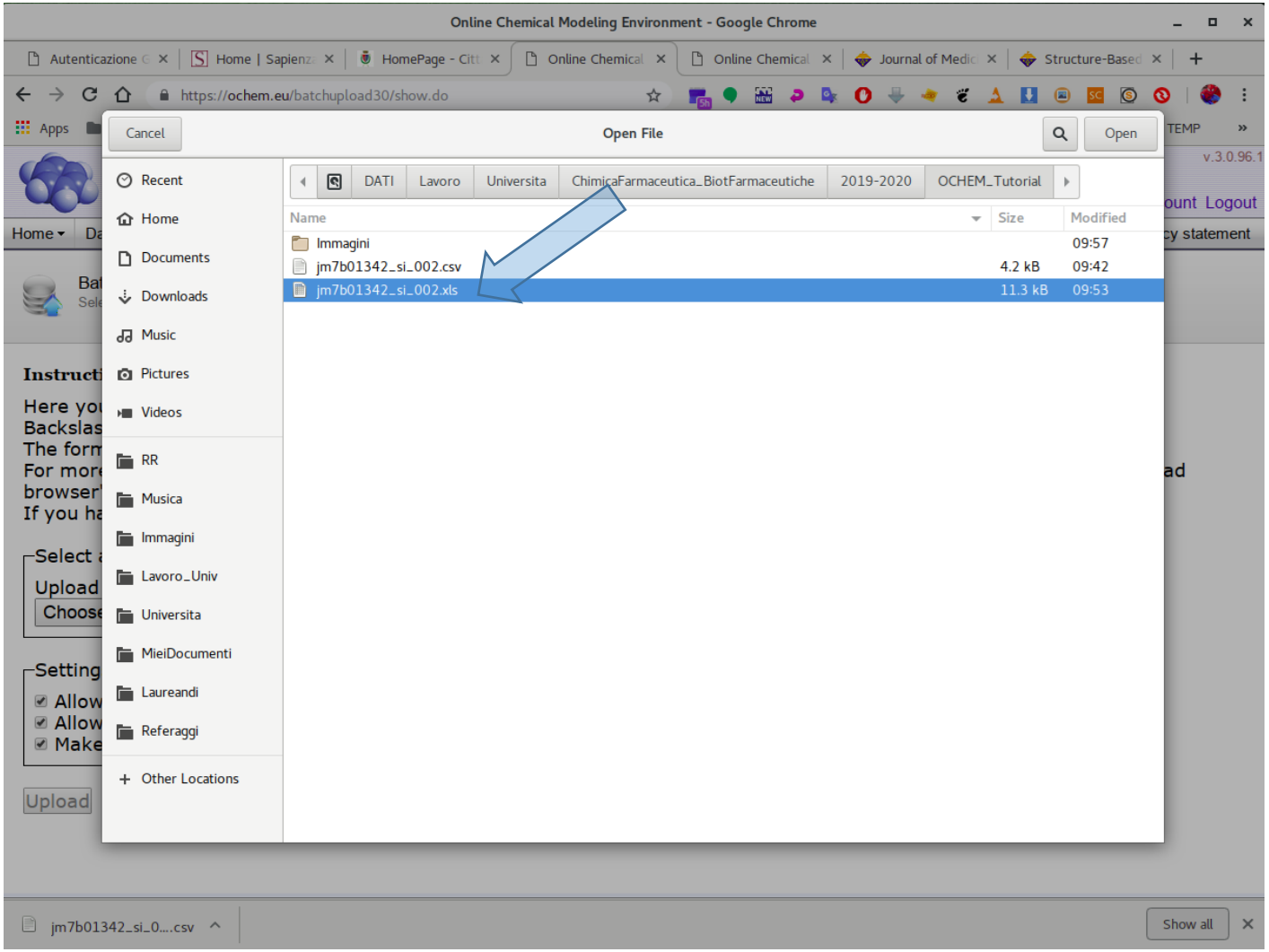

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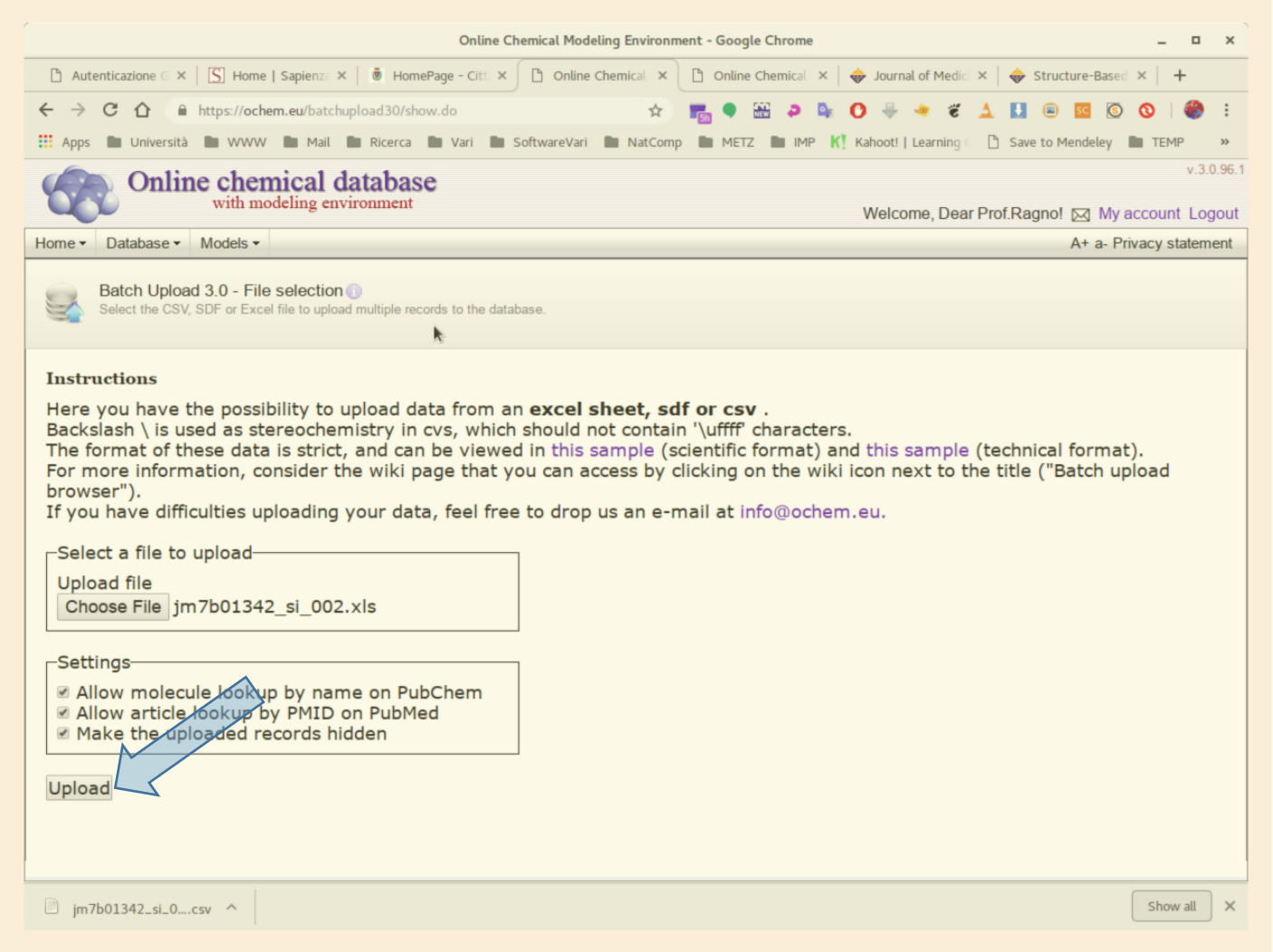

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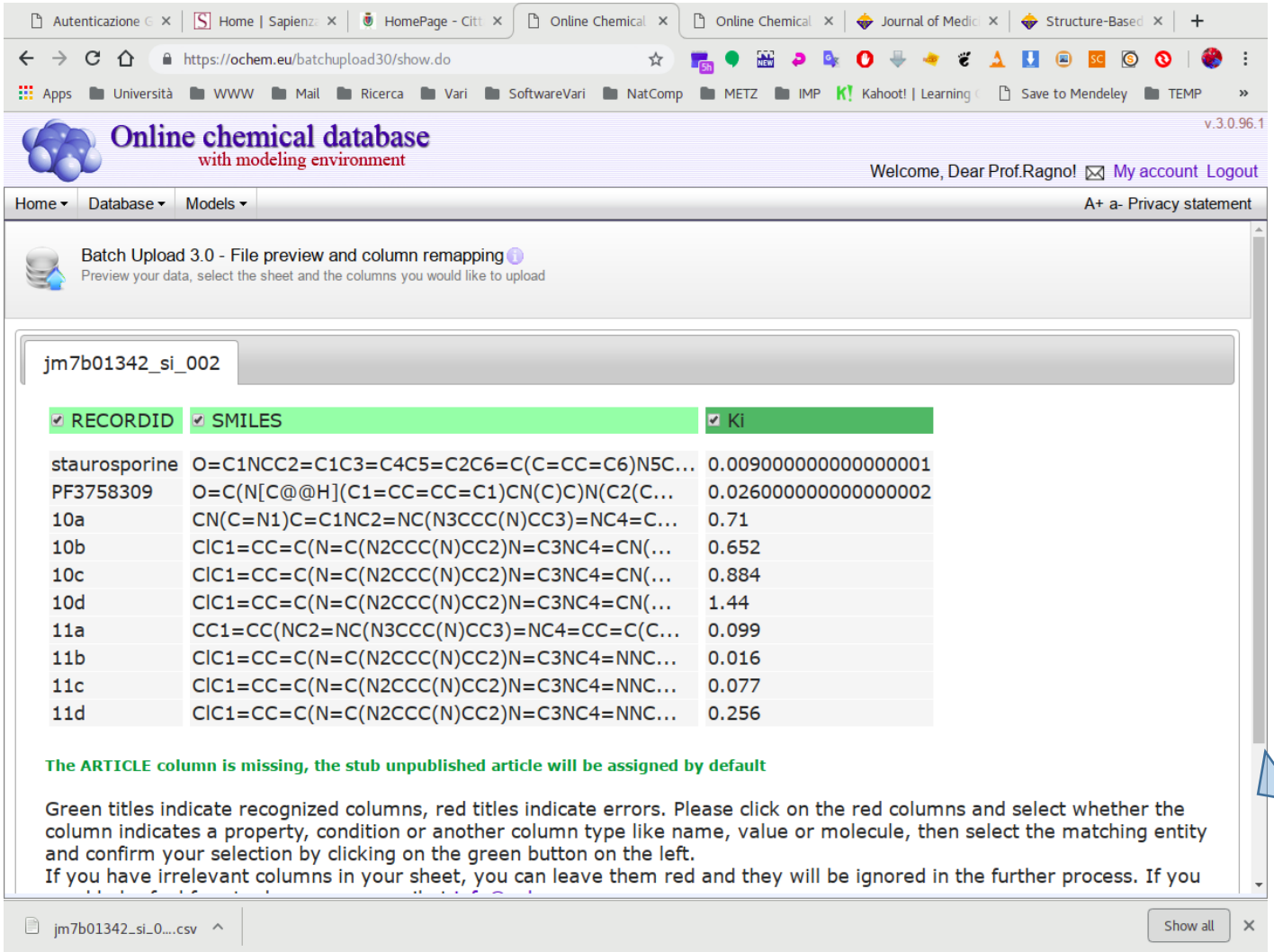
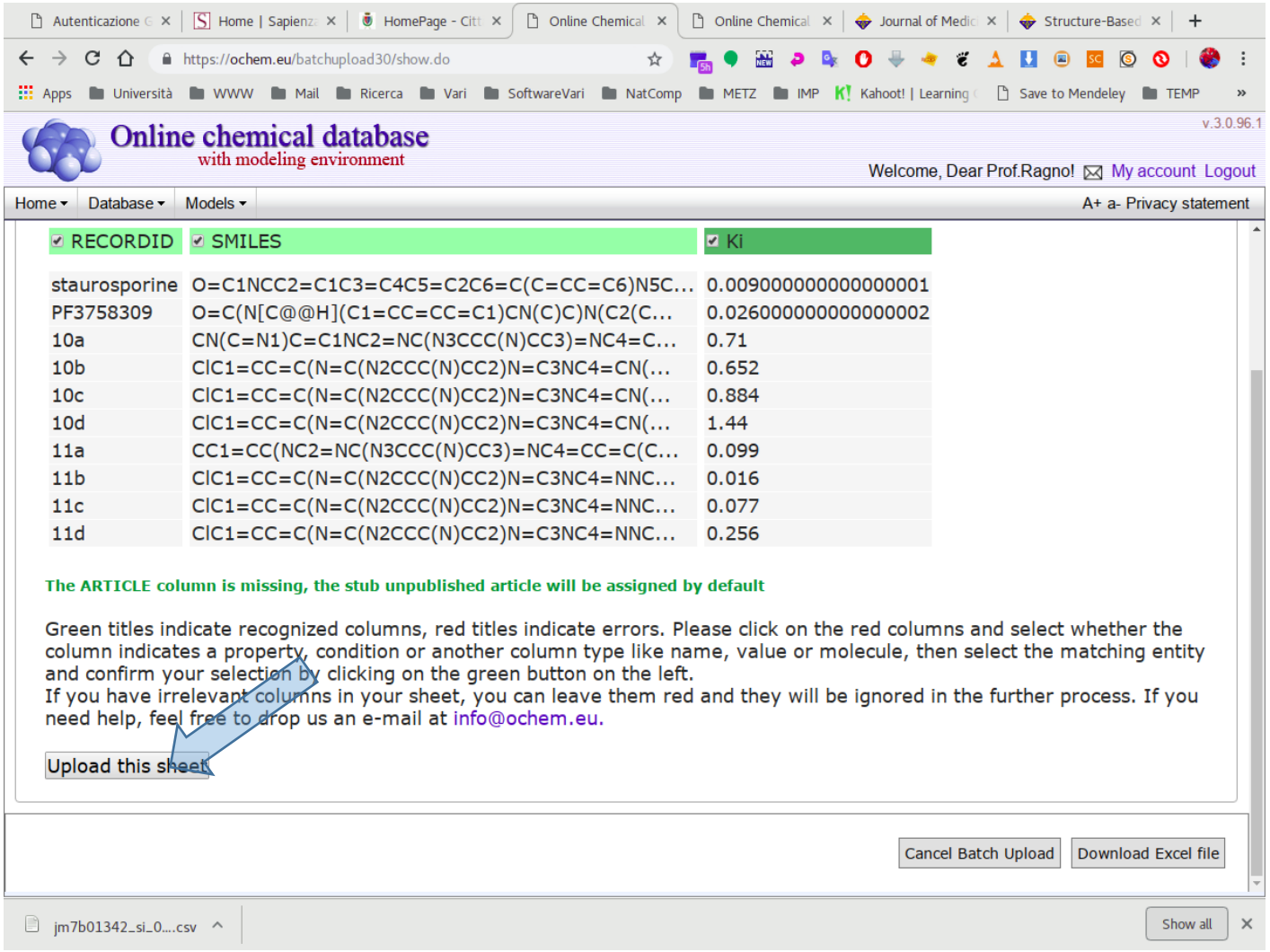
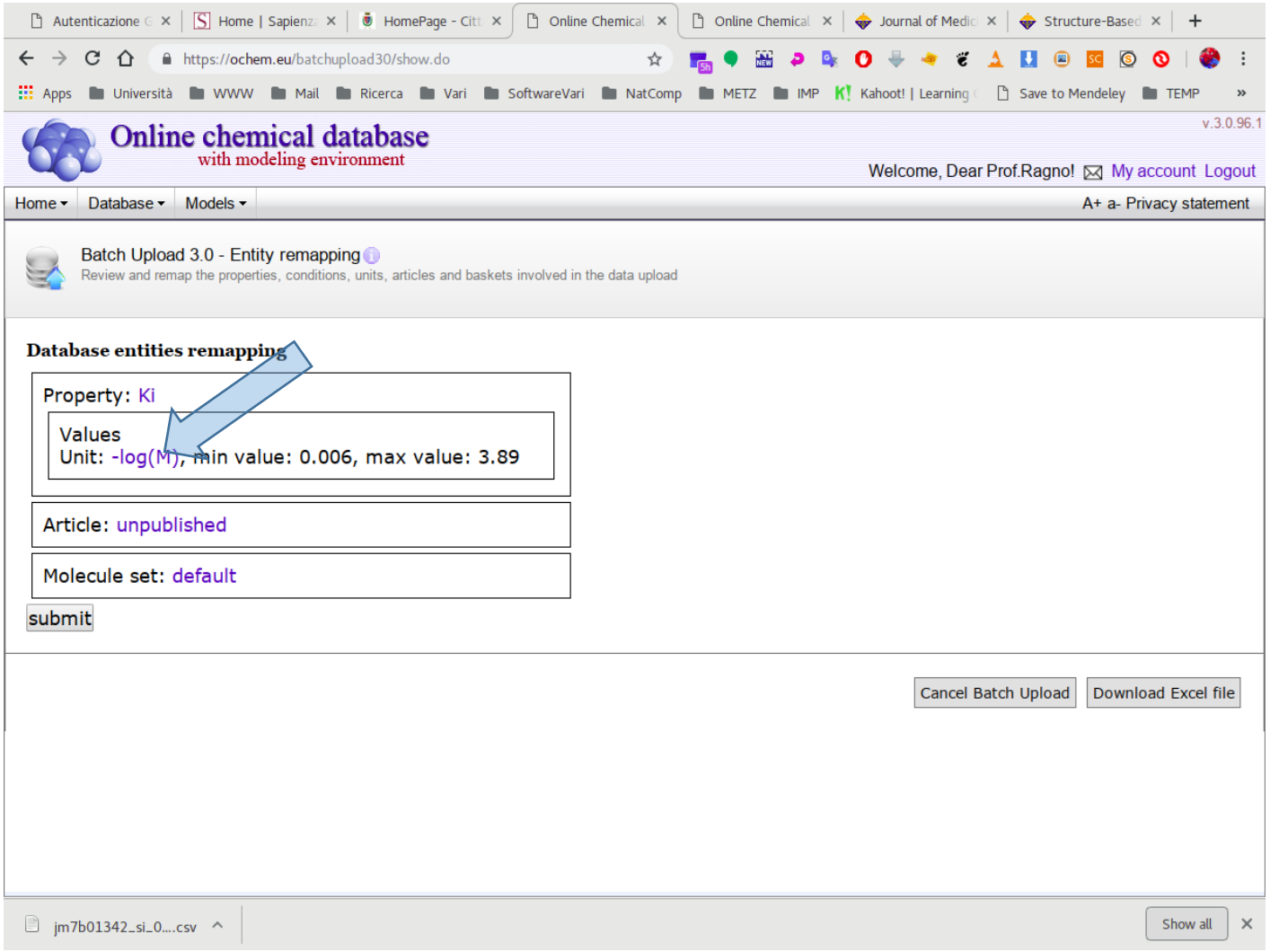


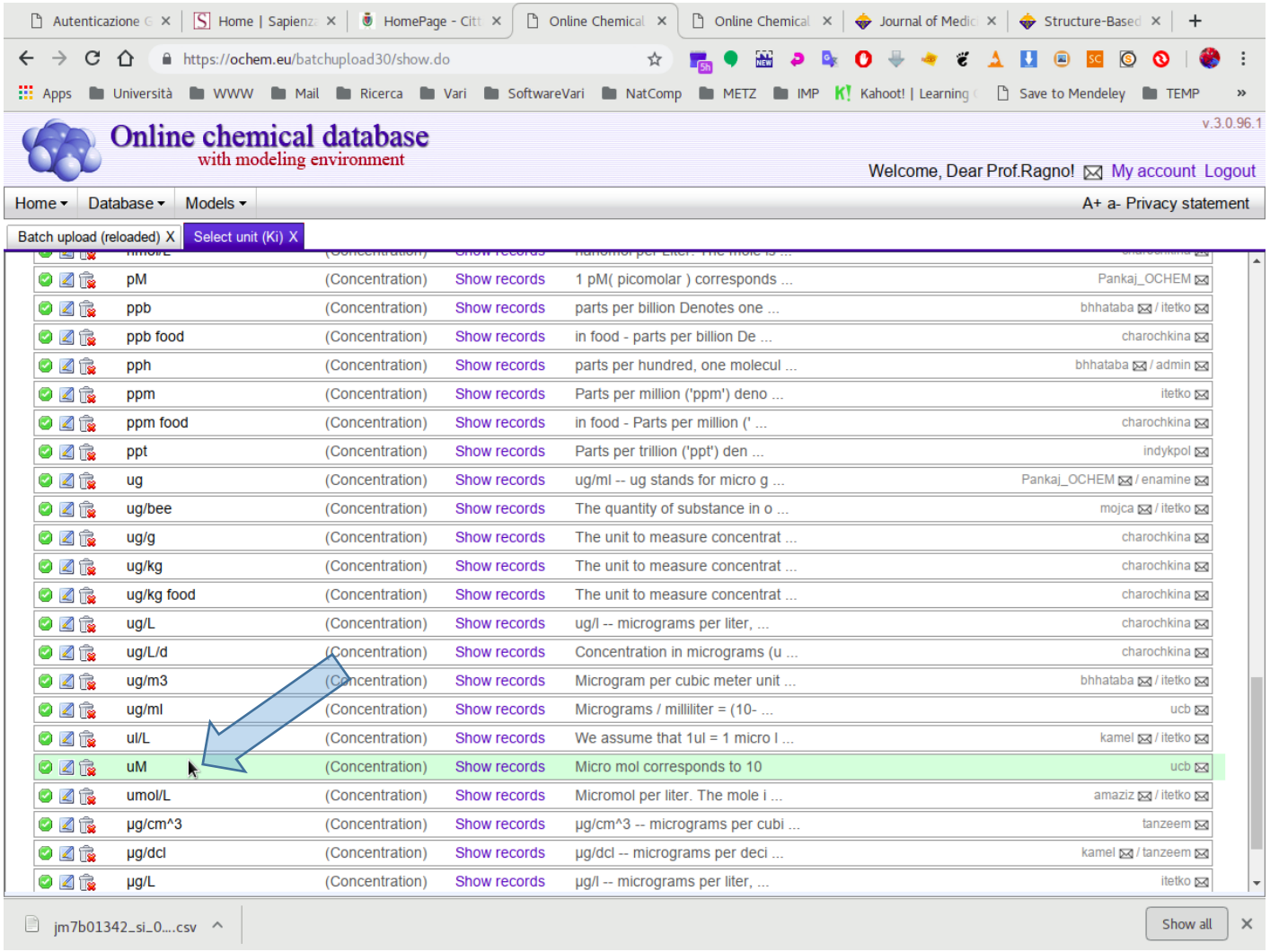
# Preparing the dataset



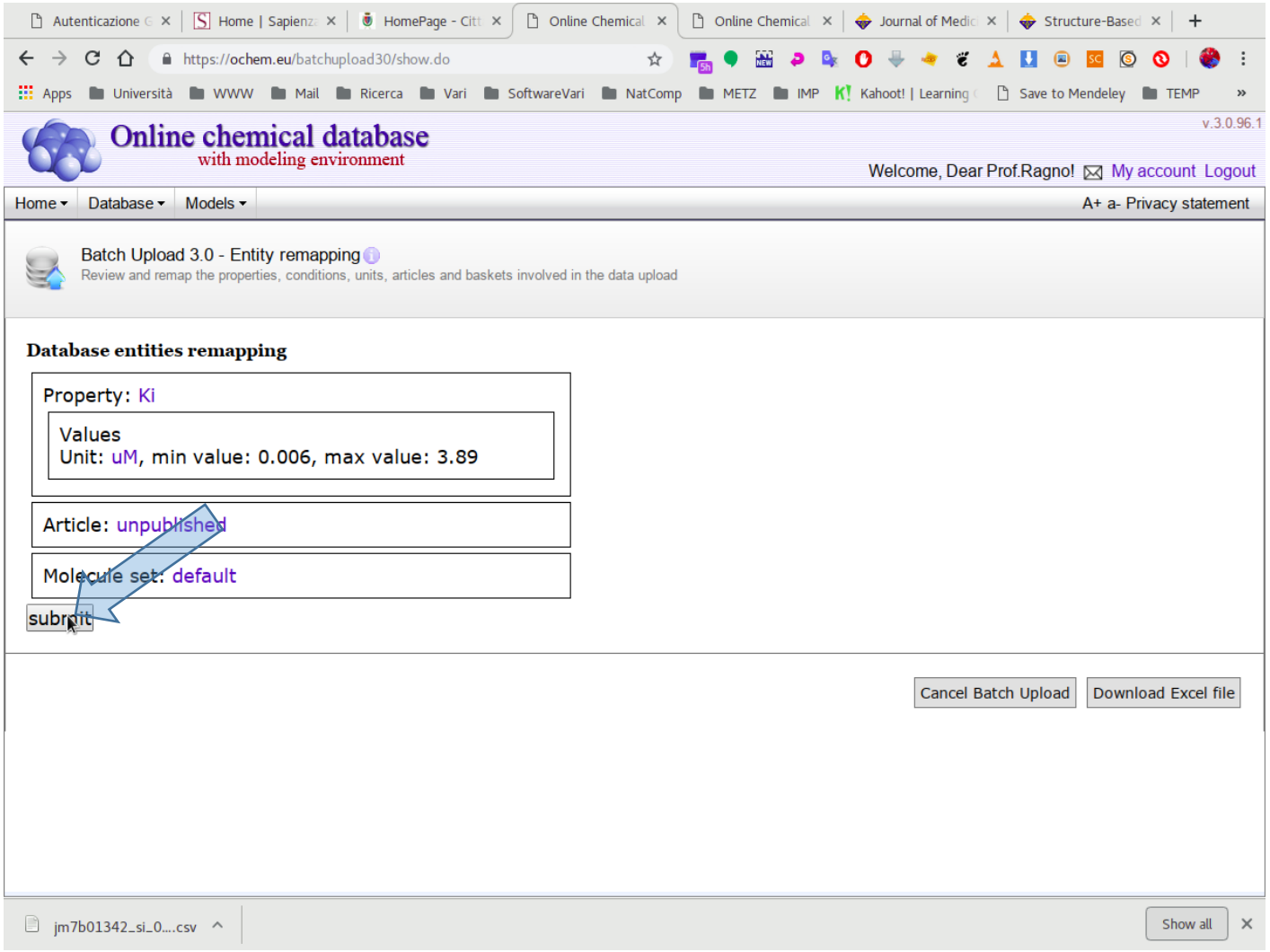
# Preparing the dataset



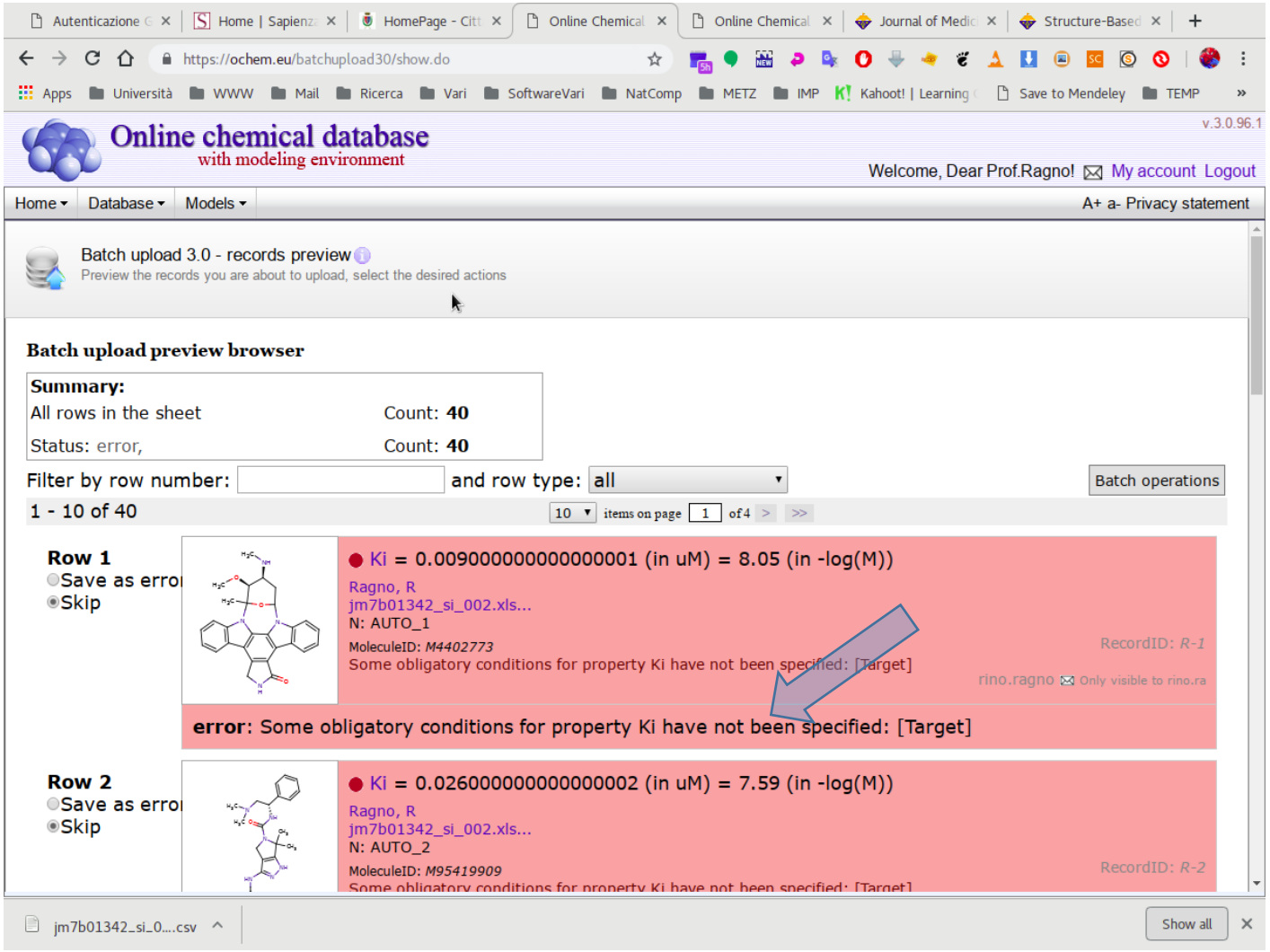
# Preparing the dataset



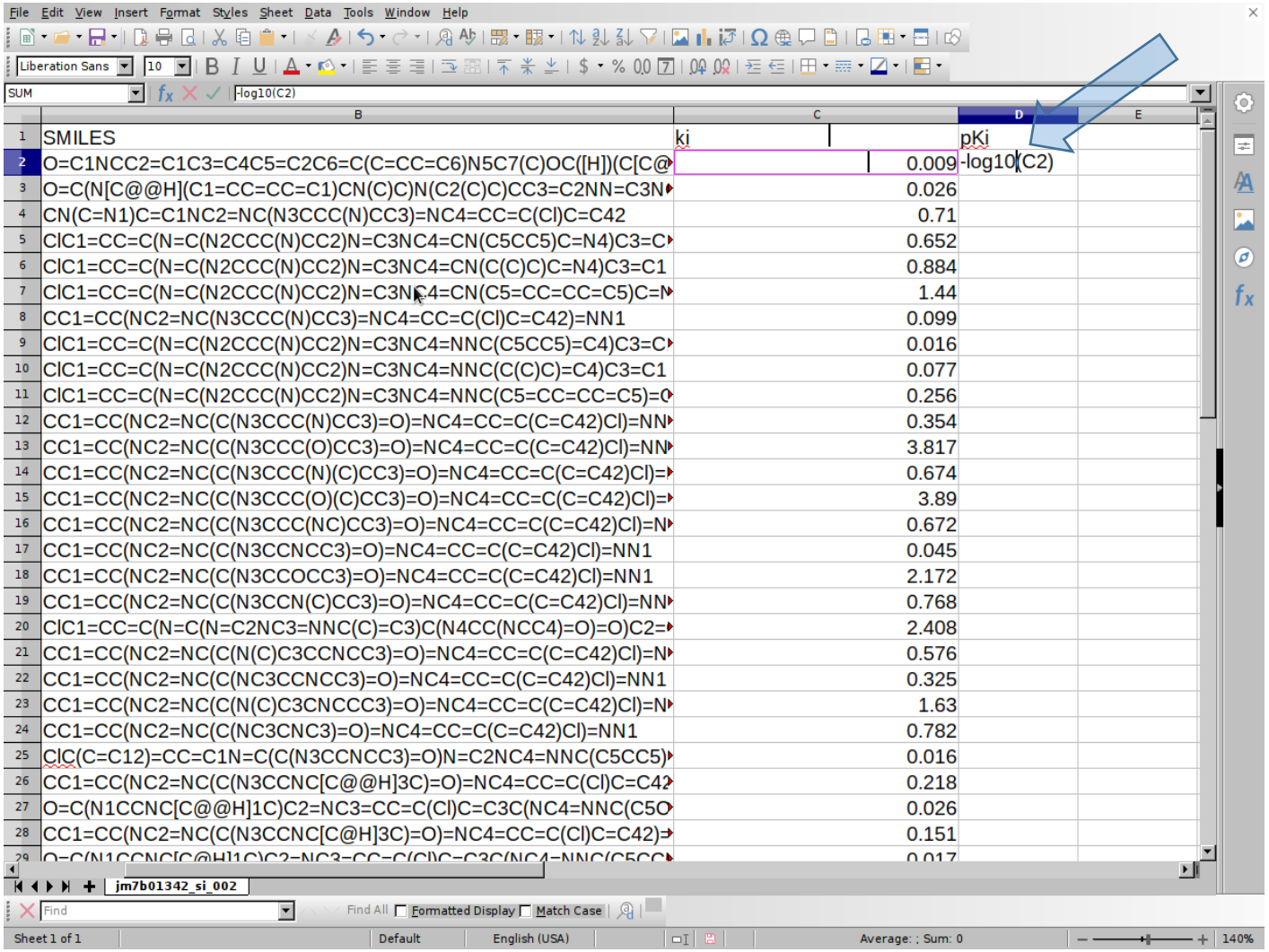
# Preparing the dataset



# Preparing the dataset

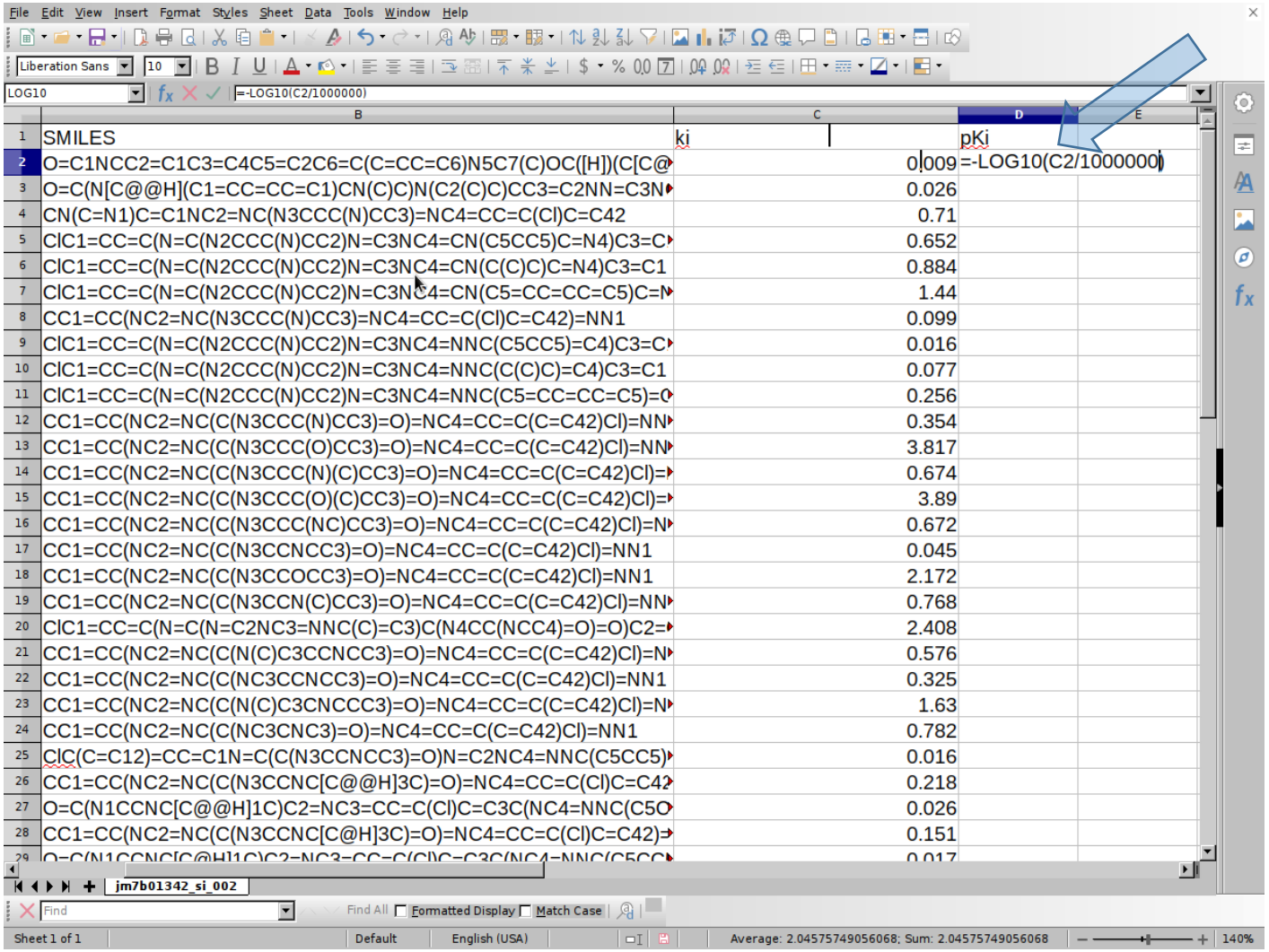


# Preparing the dataset



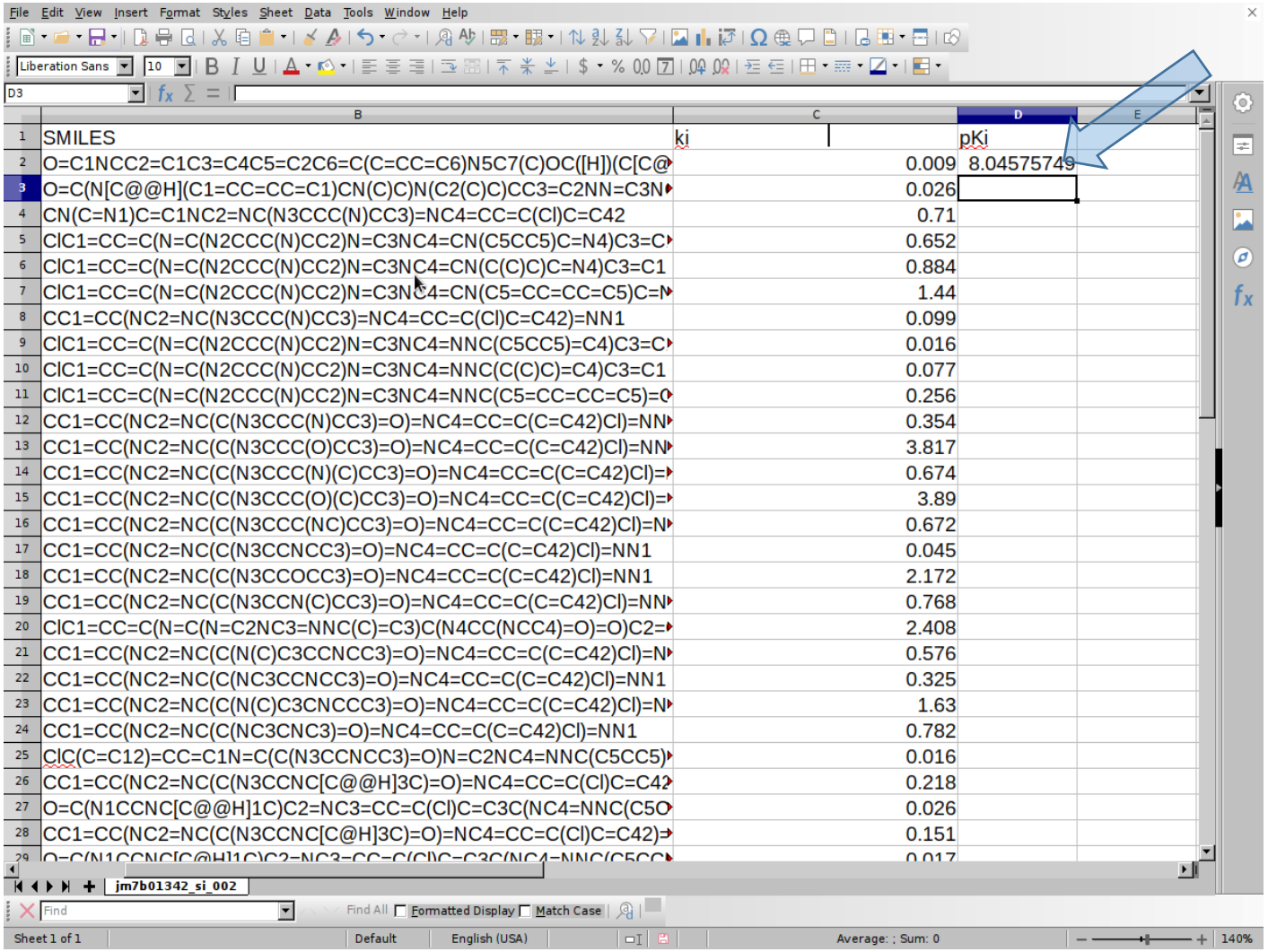

| | B | C | D | E |
|---|---|---|---|---|
| 1 | SMILES | ki | pKi | |
| 2 | O=C1NCC2=C1C3=C4C5=C2C6=C(C=CC=C6)N5C7(C)OC([H])(C[C@ | 0.009 | -log10(C2) | |
| 3 | O=C(N[C@@H](C1=CC=CC=C1)CN(C)C)N(C2(C)C)CC3=C2NN=C3N | 0.026 | | |
| 4 | CN(C=N1)C=C1NC2=NC(N3CCC(N)CC3)=NC4=CC=C(Cl)C=C42 | 0.71 | | |
| 5 | ClC1=CC=C(N=C(N2CCC(N)CC2)N=C3NC4=CN(C5CC5)C=N4)C3=C | 0.652 | | |
| 6 | ClC1=CC=C(N=C(N2CCC(N)CC2)N=C3NC4=CN(C(C)C)C=N4)C3=C1 | 0.884 | | |
| 7 | ClC1=CC=C(N=C(N2CCC(N)CC2)N=C3NC4=CN(C5=CC=CC=C5)C=N | 1.44 | | |
| 8 | CC1=CC(NC2=NC(N3CCC(N)CC3)=NC4=CC=C(Cl)C=C42)=NN1 | 0.099 | | |
| 9 | ClC1=CC=C(N=C(N2CCC(N)CC2)N=C3NC4=NNC(C5CC5)=C4)C3=C | 0.016 | | |
| 10 | ClC1=CC=C(N=C(N2CCC(N)CC2)N=C3NC4=NNC(C(C)C)=C4)C3=C1 | 0.077 | | |
| 11 | ClC1=CC=C(N=C(N2CCC(N)CC2)N=C3NC4=NNC(C5=CC=CC=C5)=C | 0.256 | | |
| 12 | CC1=CC(NC2=NC(C(N3CCC(N)CC3)=O)=NC4=CC=C(C=C42)Cl)=NN | 0.354 | | |
| 13 | CC1=CC(NC2=NC(C(N3CCC(O)CC3)=O)=NC4=CC=C(C=C42)Cl)=NN | 3.817 | | |
| 14 | CC1=CC(NC2=NC(C(N3CCC(N)(C)CC3)=O)=NC4=CC=C(C=C42)Cl)= | 0.674 | | |
| 15 | CC1=CC(NC2=NC(C(N3CCC(O)(C)CC3)=O)=NC4=CC=C(C=C42)Cl)= | 3.89 | | |
| 16 | CC1=CC(NC2=NC(C(N3CCC(NC)CC3)=O)=NC4=CC=C(C=C42)Cl)=N | 0.672 | | |
| 17 | CC1=CC(NC2=NC(C(N3CCNCC3)=O)=NC4=CC=C(C=C42)Cl)=NN1 | 0.045 | | |
| 18 | CC1=CC(NC2=NC(C(N3CCOCC3)=O)=NC4=CC=C(C=C42)Cl)=NN1 | 2.172 | | |
| 19 | CC1=CC(NC2=NC(C(N3CCN(C)CC3)=O)=NC4=CC=C(C=C42)Cl)=NN | 0.768 | | |
| 20 | ClC1=CC=C(N=C(N=C2NC3=NNC(C)=C3)C(N4CC(NCC4)=O)=O)C2= | 2.408 | | |
| 21 | CC1=CC(NC2=NC(C(N(C)C3CCNCC3)=O)=NC4=CC=C(C=C42)Cl)=N | 0.576 | | |
| 22 | CC1=CC(NC2=NC(C(NC3CCNCC3)=O)=NC4=CC=C(C=C42)Cl)=NN1 | 0.325 | | |
| 23 | CC1=CC(NC2=NC(C(N(C)C3CNCCC3)=O)=NC4=CC=C(C=C42)Cl)=N | 1.63 | | |
| 24 | CC1=CC(NC2=NC(C(NC3CNC3)=O)=NC4=CC=C(C=C42)Cl)=NN1 | 0.782 | | |
| 25 | ClC(C=C12)=CC=C1N=C(C(N3CCNCC3)=O)N=C2NC4=NNC(C5CC5) | 0.016 | | |
| 26 | CC1=CC(NC2=NC(C(N3CCNC[C@@H]3C)=O)=NC4=CC=C(Cl)C=C42 | 0.218 | | |
| 27 | O=C(N1CCNC[C@@H]1C)C2=NC3=CC=C(Cl)C=C3C(NC4=NNC(C5O | 0.026 | | |
| 28 | CC1=CC(NC2=NC(C(N3CCNC[C@H]3C)=O)=NC4=CC=C(Cl)C=C42) | 0.151 | | |
| 29 | O=C(N1CCNC[C@H]1C)C2=NC3=CC=C(Cl)C=C3C(NC4=NNC(C5CC | 0.017 | | |

# Preparing the dataset



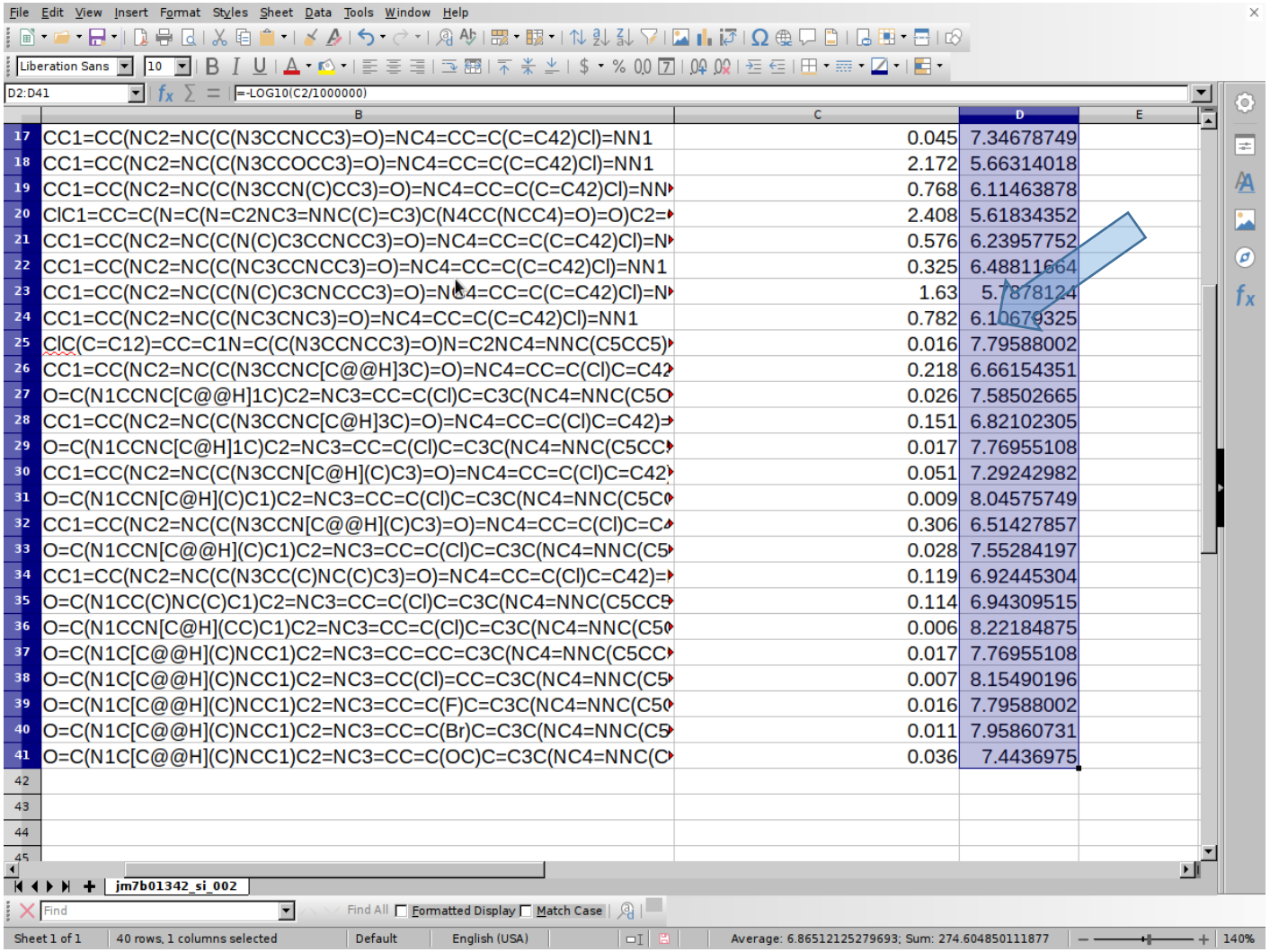

| | B | C | D | E |
|---|---|---|---|---|
| 1 | SMILES | ki | pKi | |
| 2 | O=C1NCC2=C1C3=C4C5=C2C6=C(C=CC=C6)N5C7(C)OC([H])(C[C@ | 0.009 | =-LOG10(C2/1000000) | |
| 3 | O=C(N[C@@H](C1=CC=CC=C1)CN(C)C)N(C2(C)C)CC3=C2NN=C3N | 0.026 | | |
| 4 | CN(C=N1)C=C1NC2=NC(N3CCC(N)CC3)=NC4=CC=C(Cl)C=C42 | 0.71 | | |
| 5 | ClC1=CC=C(N=C(N2CCC(N)CC2)N=C3NC4=CN(C5CC5)C=N4)C3=C | 0.652 | | |
| 6 | ClC1=CC=C(N=C(N2CCC(N)CC2)N=C3NC4=CN(C(C)C)C=N4)C3=C1 | 0.884 | | |
| 7 | ClC1=CC=C(N=C(N2CCC(N)CC2)N=C3NC4=CN(C5=CC=CC=C5)C=N | 1.44 | | |
| 8 | CC1=CC(NC2=NC(N3CCC(N)CC3)=NC4=CC=C(Cl)C=C42)=NN1 | 0.099 | | |
| 9 | ClC1=CC=C(N=C(N2CCC(N)CC2)N=C3NC4=NNC(C5CC5)=C4)C3=C | 0.016 | | |
| 10 | ClC1=CC=C(N=C(N2CCC(N)CC2)N=C3NC4=NNC(C(C)C)=C4)C3=C1 | 0.077 | | |
| 11 | ClC1=CC=C(N=C(N2CCC(N)CC2)N=C3NC4=NNC(C5=CC=CC=C5)=C | 0.256 | | |
| 12 | CC1=CC(NC2=NC(C(N3CCC(N)CC3)=O)=NC4=CC=C(C=C42)Cl)=NN | 0.354 | | |
| 13 | CC1=CC(NC2=NC(C(N3CCC(O)CC3)=O)=NC4=CC=C(C=C42)Cl)=NN | 3.817 | | |
| 14 | CC1=CC(NC2=NC(C(N3CCC(N)(C)CC3)=O)=NC4=CC=C(C=C42)Cl)= | 0.674 | | |
| 15 | CC1=CC(NC2=NC(C(N3CCC(O)(C)CC3)=O)=NC4=CC=C(C=C42)Cl)= | 3.89 | | |
| 16 | CC1=CC(NC2=NC(C(N3CCC(NC)CC3)=O)=NC4=CC=C(C=C42)Cl)=N | 0.672 | | |
| 17 | CC1=CC(NC2=NC(C(N3CCNCC3)=O)=NC4=CC=C(C=C42)Cl)=NN1 | 0.045 | | |
| 18 | CC1=CC(NC2=NC(C(N3CCOCC3)=O)=NC4=CC=C(C=C42)Cl)=NN1 | 2.172 | | |
| 19 | CC1=CC(NC2=NC(C(N3CCN(C)CC3)=O)=NC4=CC=C(C=C42)Cl)=NN | 0.768 | | |
| 20 | ClC1=CC=C(N=C(N=C2NC3=NNC(C)=C3)C(N4CC(NCC4)=O)=O)C2= | 2.408 | | |
| 21 | CC1=CC(NC2=NC(C(N(C)C3CCNCC3)=O)=NC4=CC=C(C=C42)Cl)=N | 0.576 | | |
| 22 | CC1=CC(NC2=NC(C(NC3CCNCC3)=O)=NC4=CC=C(C=C42)Cl)=NN1 | 0.325 | | |
| 23 | CC1=CC(NC2=NC(C(N(C)C3CNCCC3)=O)=NC4=CC=C(C=C42)Cl)=N | 1.63 | | |
| 24 | CC1=CC(NC2=NC(C(NC3CNC3)=O)=NC4=CC=C(C=C42)Cl)=NN1 | 0.782 | | |
| 25 | ClC(C=C12)=CC=C1N=C(C(N3CCNCC3)=O)N=C2NC4=NNC(C5CC5) | 0.016 | | |
| 26 | CC1=CC(NC2=NC(C(N3CCNC[C@@H]3C)=O)=NC4=CC=C(Cl)C=C42 | 0.218 | | |
| 27 | O=C(N1CCNC[C@@H]1C)C2=NC3=CC=C(Cl)C=C3C(NC4=NNC(C5O | 0.026 | | |
| 28 | CC1=CC(NC2=NC(C(N3CCNC[C@H]3C)=O)=NC4=CC=C(Cl)C=C42) | 0.151 | | |
| 29 | O=C(N1CCNC[C@H]1C)C2=NC3=CC=C(Cl)C=C3C(NC4=NNC(C5CC | 0.017 | | |

# Preparing the dataset



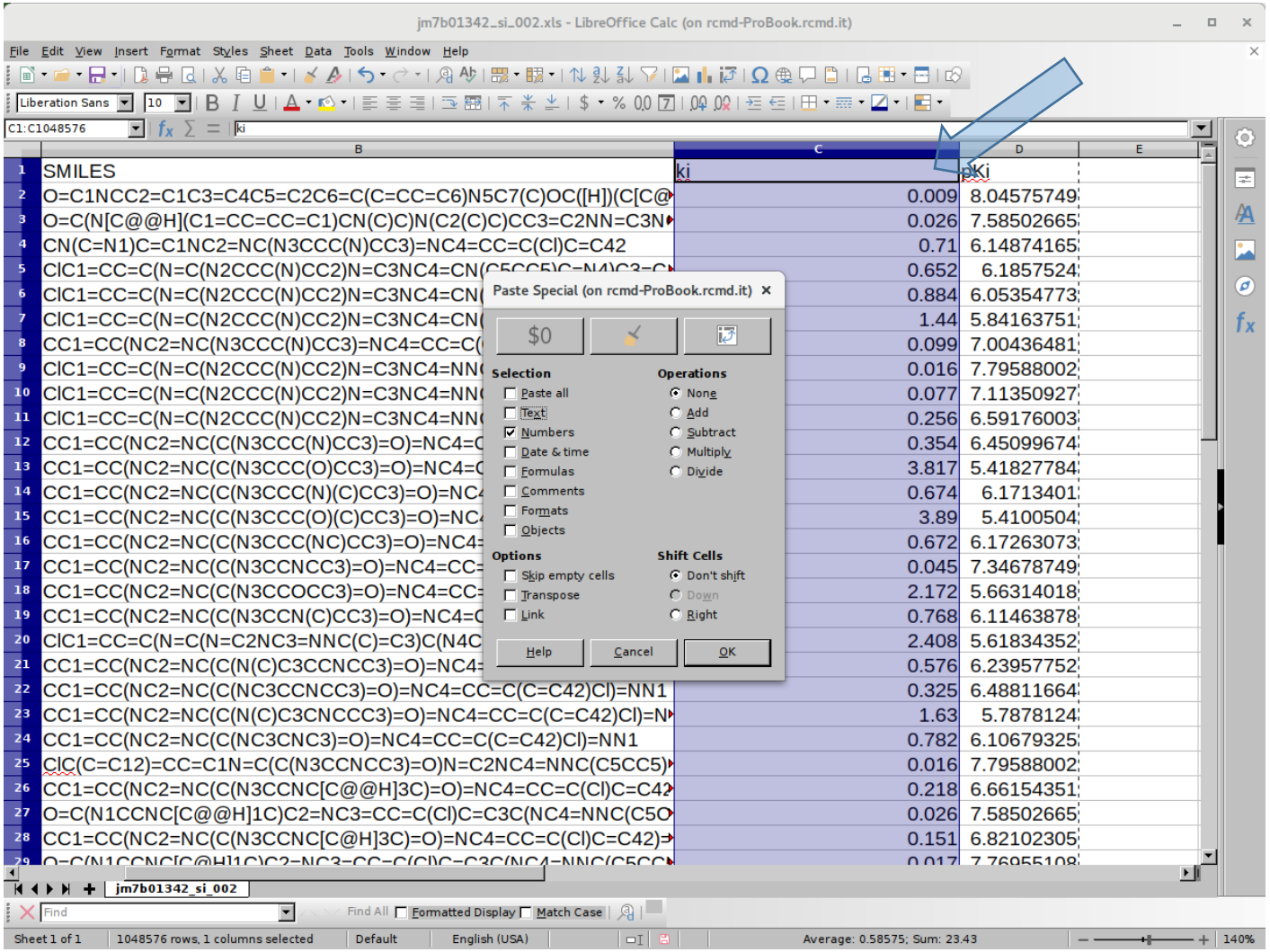
| | B | C | D | E |
|---|---|---|---|---|
| 1 | SMILES | ki | pKi | |
| 2 | O=C1NCC2=C1C3=C4C5=C2C6=C(C=CC=C6)N5C7(C)OC([H])(C[C@ | 0.009 | 8.04575749 | |
| 3 | O=C(N[C@@H](C1=CC=CC=C1)CN(C)C)N(C2(C)C)CC3=C2NN=C3N | 0.026 | | |
| 4 | CN(C=N1)C=C1NC2=NC(N3CCC(N)CC3)=NC4=CC=C(Cl)C=C42 | 0.71 | | |
| 5 | ClC1=CC=C(N=C(N2CCC(N)CC2)N=C3NC4=CN(C5CC5)C=N4)C3=C | 0.652 | | |
| 6 | ClC1=CC=C(N=C(N2CCC(N)CC2)N=C3NC4=CN(C(C)C)C=N4)C3=C1 | 0.884 | | |
| 7 | ClC1=CC=C(N=C(N2CCC(N)CC2)N=C3NC4=CN(C5=CC=CC=C5)C=N | 1.44 | | |
| 8 | CC1=CC(NC2=NC(N3CCC(N)CC3)=NC4=CC=C(Cl)C=C42)=NN1 | 0.099 | | |
| 9 | ClC1=CC=C(N=C(N2CCC(N)CC2)N=C3NC4=NNC(C5CC5)=C4)C3=C | 0.016 | | |
| 10 | ClC1=CC=C(N=C(N2CCC(N)CC2)N=C3NC4=NNC(C(C)C)=C4)C3=C1 | 0.077 | | |
| 11 | ClC1=CC=C(N=C(N2CCC(N)CC2)N=C3NC4=NNC(C5=CC=CC=C5)=O | 0.256 | | |
| 12 | CC1=CC(NC2=NC(C(N3CCC(N)CC3)=O)=NC4=CC=C(C=C42)Cl)=NN | 0.354 | | |
| 13 | CC1=CC(NC2=NC(C(N3CCC(O)CC3)=O)=NC4=CC=C(C=C42)Cl)=NN | 3.817 | | |
| 14 | CC1=CC(NC2=NC(C(N3CCC(N)(C)CC3)=O)=NC4=CC=C(C=C42)Cl)= | 0.674 | | |
| 15 | CC1=CC(NC2=NC(C(N3CCC(O)(C)CC3)=O)=NC4=CC=C(C=C42)Cl)= | 3.89 | | |
| 16 | CC1=CC(NC2=NC(C(N3CCC(NC)CC3)=O)=NC4=CC=C(C=C42)Cl)=N | 0.672 | | |
| 17 | CC1=CC(NC2=NC(C(N3CCNCC3)=O)=NC4=CC=C(C=C42)Cl)=NN1 | 0.045 | | |
| 18 | CC1=CC(NC2=NC(C(N3CCOCC3)=O)=NC4=CC=C(C=C42)Cl)=NN1 | 2.172 | | |
| 19 | CC1=CC(NC2=NC(C(N3CCN(C)CC3)=O)=NC4=CC=C(C=C42)Cl)=NN | 0.768 | | |
| 20 | ClC1=CC=C(N=C(N=C2NC3=NNC(C)=C3)C(N4CC(NCC4)=O)=O)C2= | 2.408 | | |
| 21 | CC1=CC(NC2=NC(C(N(C)C3CCNCC3)=O)=NC4=CC=C(C=C42)Cl)=N | 0.576 | | |
| 22 | CC1=CC(NC2=NC(C(NC3CCNCC3)=O)=NC4=CC=C(C=C42)Cl)=NN1 | 0.325 | | |
| 23 | CC1=CC(NC2=NC(C(N(C)C3CNCCC3)=O)=NC4=CC=C(C=C42)Cl)=N | 1.63 | | |
| 24 | CC1=CC(NC2=NC(C(NC3CNC3)=O)=NC4=CC=C(C=C42)Cl)=NN1 | 0.782 | | |
| 25 | ClC(C=C12)=CC=C1N=C(C(N3CCNCC3)=O)N=C2NC4=NNC(C5CC5)= | 0.016 | | |
| 26 | CC1=CC(NC2=NC(C(N3CCNC[C@@H]3C)=O)=NC4=CC=C(Cl)C=C42 | 0.218 | | |
| 27 | O=C(N1CCNC[C@@H]1C)C2=NC3=CC=C(Cl)C=C3C(NC4=NNC(C5C | 0.026 | | |
| 28 | CC1=CC(NC2=NC(C(N3CCNC[C@H]3C)=O)=NC4=CC=C(Cl)C=C42)= | 0.151 | | |
| 29 | O=C(N1CCNC[C@H]1C)C2=NC3=CC=C(Cl)C=C3C(NC4=NNC(C5CC | 0.017 | | |

# Preparing the dataset

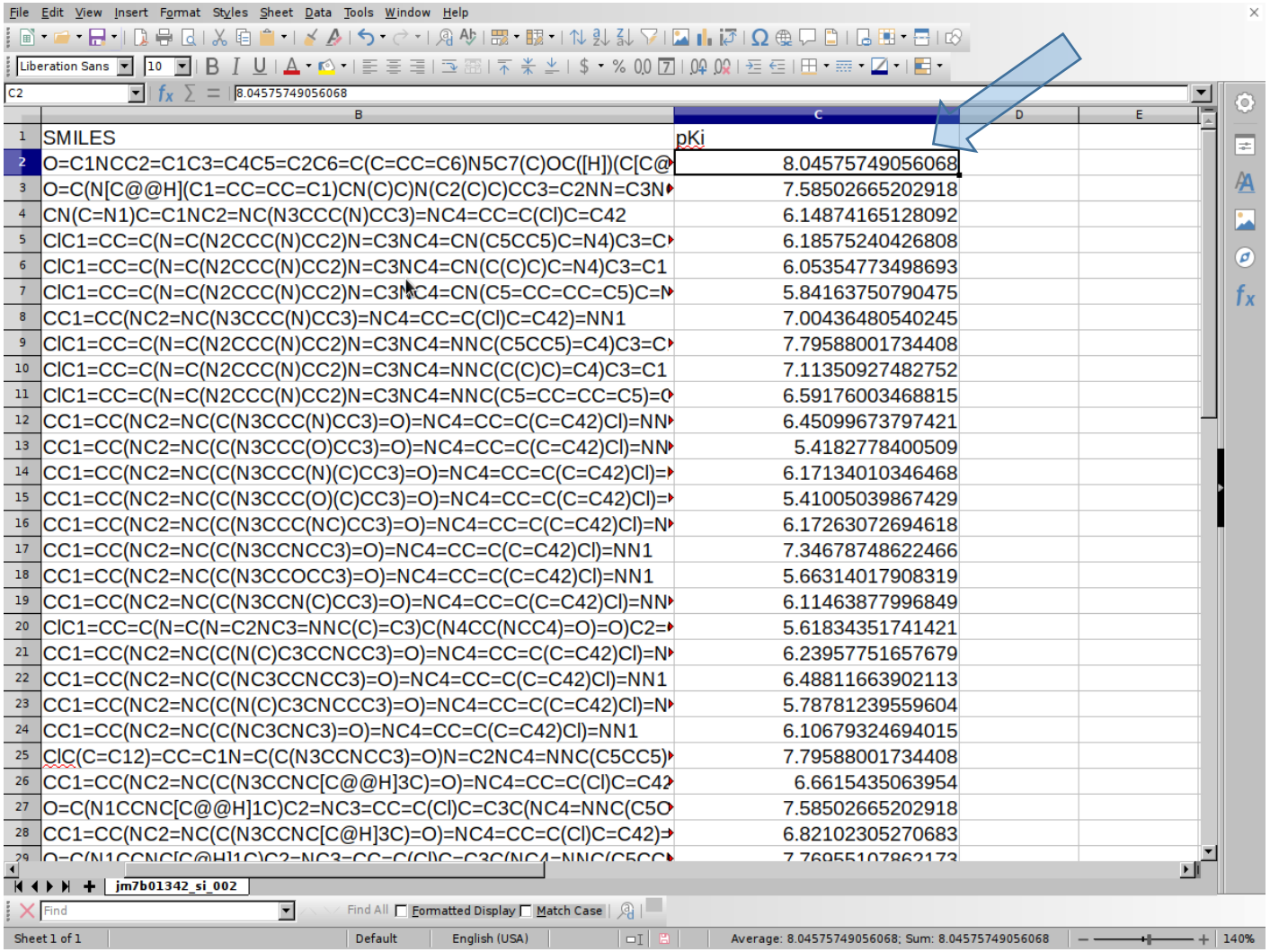



| | B | C | D | E |
|---|---|---|---|---|
| 17 | CC1=CC(NC2=NC(C(N3CCNCC3)=O)=NC4=CC=C(C=C42)Cl)=NN1 | 0.045 | 7.34678749 | |
| 18 | CC1=CC(NC2=NC(C(N3CCOCC3)=O)=NC4=CC=C(C=C42)Cl)=NN1 | 2.172 | 5.66314018 | |
| 19 | CC1=CC(NC2=NC(C(N3CCN(C)CC3)=O)=NC4=CC=C(C=C42)Cl)=NN | 0.768 | 6.11463878 | |
| 20 | ClC1=CC=C(N=C(N=C2NC3=NNC(C)=C3)C(N4CC(NCC4)=O)=O)C2= | 2.408 | 5.61834352 | |
| 21 | CC1=CC(NC2=NC(C(N(C)C3CCNCC3)=O)=NC4=CC=C(C=C42)Cl)=N | 0.576 | 6.23957752 | |
| 22 | CC1=CC(NC2=NC(C(NC3CCNCC3)=O)=NC4=CC=C(C=C42)Cl)=NN1 | 0.325 | 6.48811664 | |
| 23 | CC1=CC(NC2=NC(C(N(C)C3CNCCC3)=O)=NC4=CC=C(C=C42)Cl)=N | 1.63 | 5.7878124 | |
| 24 | CC1=CC(NC2=NC(C(NC3CNC3)=O)=NC4=CC=C(C=C42)Cl)=NN1 | 0.782 | 6.10679325 | |
| 25 | ClC(C=C12)=CC=C1N=C(C(N3CCNCC3)=O)N=C2NC4=NNC(C5CC5) | 0.016 | 7.79588002 | |
| 26 | CC1=CC(NC2=NC(C(N3CCNC[C@@H]3C)=O)=NC4=CC=C(Cl)C=C42 | 0.218 | 6.66154351 | |
| 27 | O=C(N1CCNC[C@@H]1C)C2=NC3=CC=C(Cl)C=C3C(NC4=NNC(C5O | 0.026 | 7.58502665 | |
| 28 | CC1=CC(NC2=NC(C(N3CCNC[C@H]3C)=O)=NC4=CC=C(Cl)C=C42)= | 0.151 | 6.82102305 | |
| 29 | O=C(N1CCNC[C@H]1C)C2=NC3=CC=C(Cl)C=C3C(NC4=NNC(C5CC | 0.017 | 7.76955108 | |
| 30 | CC1=CC(NC2=NC(C(N3CCN[C@H](C)C3)=O)=NC4=CC=C(Cl)C=C42 | 0.051 | 7.29242982 | |
| 31 | O=C(N1CCN[C@H](C)C1)C2=NC3=CC=C(Cl)C=C3C(NC4=NNC(C5C | 0.009 | 8.04575749 | |
| 32 | CC1=CC(NC2=NC(C(N3CCN[C@@H](C)C3)=O)=NC4=CC=C(Cl)C=C4 | 0.306 | 6.51427857 | |
| 33 | O=C(N1CCN[C@@H](C)C1)C2=NC3=CC=C(Cl)C=C3C(NC4=NNC(C5 | 0.028 | 7.55284197 | |
| 34 | CC1=CC(NC2=NC(C(N3CC(C)NC(C)C3)=O)=NC4=CC=C(Cl)C=C42)= | 0.119 | 6.92445304 | |
| 35 | O=C(N1CC(C)NC(C)C1)C2=NC3=CC=C(Cl)C=C3C(NC4=NNC(C5CC5 | 0.114 | 6.94309515 | |
| 36 | O=C(N1CCN[C@H](CC)C1)C2=NC3=CC=C(Cl)C=C3C(NC4=NNC(C5( | 0.006 | 8.22184875 | |
| 37 | O=C(N1C[C@@H](C)NCC1)C2=NC3=CC=CC=C3C(NC4=NNC(C5CC | 0.017 | 7.76955108 | |
| 38 | O=C(N1C[C@@H](C)NCC1)C2=NC3=CC(Cl)=CC=C3C(NC4=NNC(C5 | 0.007 | 8.15490196 | |
| 39 | O=C(N1C[C@@H](C)NCC1)C2=NC3=CC=C(F)C=C3C(NC4=NNC(C5( | 0.016 | 7.79588002 | |
| 40 | O=C(N1C[C@@H](C)NCC1)C2=NC3=CC=C(Br)C=C3C(NC4=NNC(C5 | 0.011 | 7.95860731 | |
| 41 | O=C(N1C[C@@H](C)NCC1)C2=NC3=CC=C(OC)C=C3C(NC4=NNC(C | 0.036 | 7.4436975 | |
| 42 | | | | |
| 43 | | | | |
| 44 | | | | |
| 45 | | | | |

# Preparing the dataset

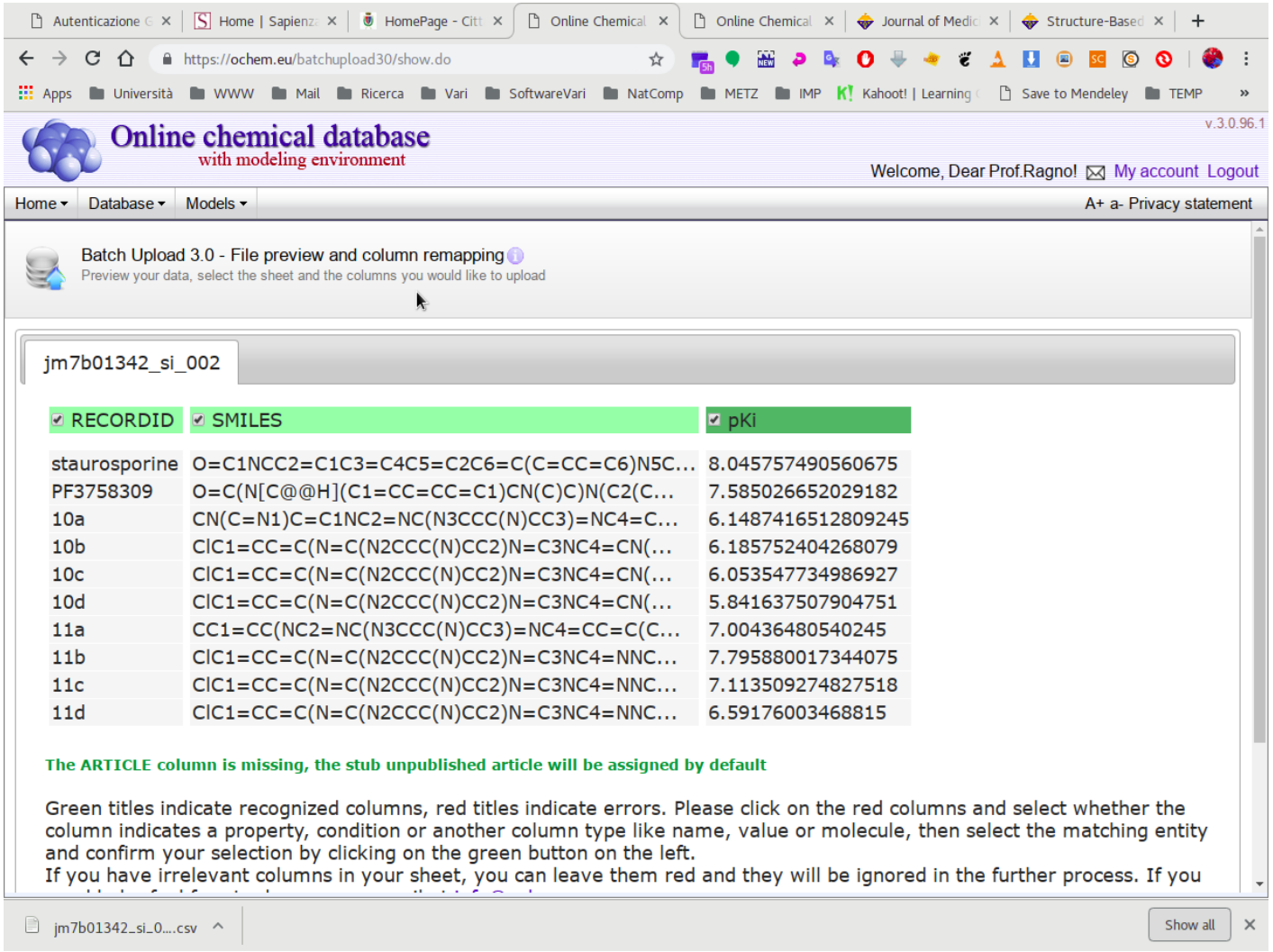


# Preparing the dataset




| | B | C | D | E |
|---|---|---|---|---|
| 1 | SMILES | pKi | | |
| 2 | O=C1NCC2=C1C3=C4C5=C2C6=C(C=CC=C6)N5C7(C)OC([H])(C[C@ | 8.04575749056068 | | |
| 3 | O=C(N[C@@H](C1=CC=CC=C1)CN(C)C)N(C2(C)C)CC3=C2NN=C3N | 7.58502665202918 | | |
| 4 | CN(C=N1)C=C1NC2=NC(N3CCC(N)CC3)=NC4=CC=C(Cl)C=C42 | 6.14874165128092 | | |
| 5 | ClC1=CC=C(N=C(N2CCC(N)CC2)N=C3NC4=CN(C5CC5)C=N4)C3=C | 6.18575240426808 | | |
| 6 | ClC1=CC=C(N=C(N2CCC(N)CC2)N=C3NC4=CN(C(C)C)C=N4)C3=C1 | 6.05354773498693 | | |
| 7 | ClC1=CC=C(N=C(N2CCC(N)CC2)N=C3NC4=CN(C5=CC=CC=C5)C=N | 5.84163750790475 | | |
| 8 | CC1=CC(NC2=NC(N3CCC(N)CC3)=NC4=CC=C(Cl)C=C42)=NN1 | 7.00436480540245 | | |
| 9 | ClC1=CC=C(N=C(N2CCC(N)CC2)N=C3NC4=NNC(C5CC5)=C4)C3=C | 7.79588001734408 | | |
| 10 | ClC1=CC=C(N=C(N2CCC(N)CC2)N=C3NC4=NNC(C(C)C)=C4)C3=C1 | 7.11350927482752 | | |
| 11 | ClC1=CC=C(N=C(N2CCC(N)CC2)N=C3NC4=NNC(C5=CC=CC=C5)=C | 6.59176003468815 | | |
| 12 | CC1=CC(NC2=NC(C(N3CCC(N)CC3)=O)=NC4=CC=C(C=C42)Cl)=NN | 6.45099673797421 | | |
| 13 | CC1=CC(NC2=NC(C(N3CCC(O)CC3)=O)=NC4=CC=C(C=C42)Cl)=NN | 5.4182778400509 | | |
| 14 | CC1=CC(NC2=NC(C(N3CCC(N)(C)CC3)=O)=NC4=CC=C(C=C42)Cl)= | 6.17134010346468 | | |
| 15 | CC1=CC(NC2=NC(C(N3CCC(O)(C)CC3)=O)=NC4=CC=C(C=C42)Cl)= | 5.41005039867429 | | |
| 16 | CC1=CC(NC2=NC(C(N3CCC(NC)CC3)=O)=NC4=CC=C(C=C42)Cl)=N | 6.17263072694618 | | |
| 17 | CC1=CC(NC2=NC(C(N3CCNCC3)=O)=NC4=CC=C(C=C42)Cl)=NN1 | 7.34678748622466 | | |
| 18 | CC1=CC(NC2=NC(C(N3CCOCC3)=O)=NC4=CC=C(C=C42)Cl)=NN1 | 5.66314017908319 | | |
| 19 | CC1=CC(NC2=NC(C(N3CCN(C)CC3)=O)=NC4=CC=C(C=C42)Cl)=NN | 6.11463877996849 | | |
| 20 | ClC1=CC=C(N=C(N=C2NC3=NNC(C)=C3)C(N4CC(NCC4)=O)=O)C2= | 5.61834351741421 | | |
| 21 | CC1=CC(NC2=NC(C(N(C)C3CCNCC3)=O)=NC4=CC=C(C=C42)Cl)=N | 6.23957751657679 | | |
| 22 | CC1=CC(NC2=NC(C(NC3CCNCC3)=O)=NC4=CC=C(C=C42)Cl)=NN1 | 6.48811663902113 | | |
| 23 | CC1=CC(NC2=NC(C(N(C)C3CNCCC3)=O)=NC4=CC=C(C=C42)Cl)=N | 5.78781239559604 | | |
| 24 | CC1=CC(NC2=NC(C(NC3CNC3)=O)=NC4=CC=C(C=C42)Cl)=NN1 | 6.10679324694015 | | |
| 25 | ClC(C=C12)=CC=C1N=C(C(N3CCNCC3)=O)N=C2NC4=NNC(C5CC5)= | 7.79588001734408 | | |
| 26 | CC1=CC(NC2=NC(C(N3CCNC[C@@H]3C)=O)=NC4=CC=C(Cl)C=C42 | 6.6615435063954 | | |
| 27 | O=C(N1CCNC[C@@H]1C)C2=NC3=CC=C(Cl)C=C3C(NC4=NNC(C5O | 7.58502665202918 | | |
| 28 | CC1=CC(NC2=NC(C(N3CCNC[C@H]3C)=O)=NC4=CC=C(Cl)C=C42)= | 6.82102305270683 | | |
| 29 | O=C(N1CCNC[C@H]1C)C2=NC3=CC=C(Cl)C=C3C(NC4=NNC(C5CC= | 7.76955107862173 | | |

# Preparing the dataset



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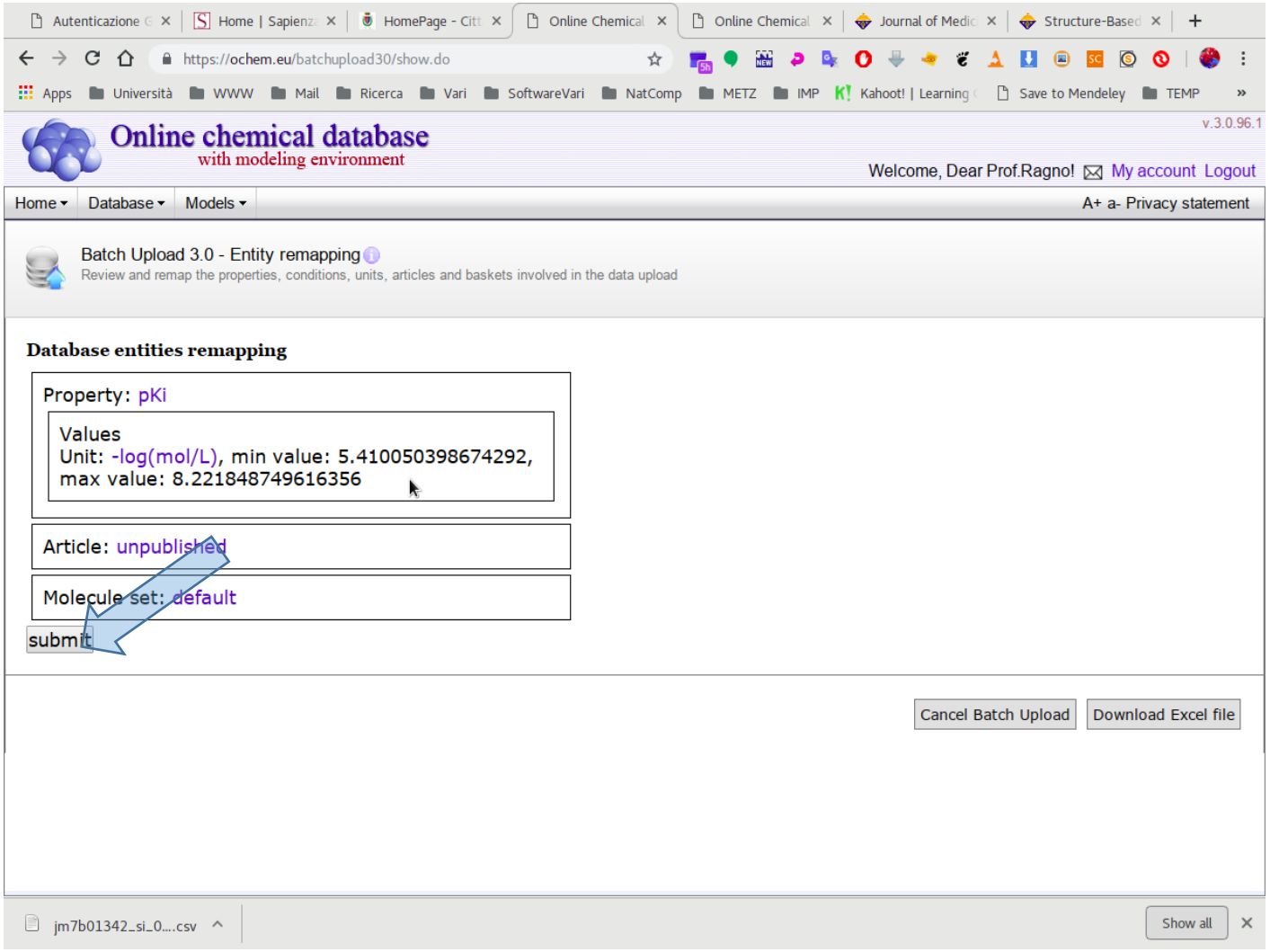

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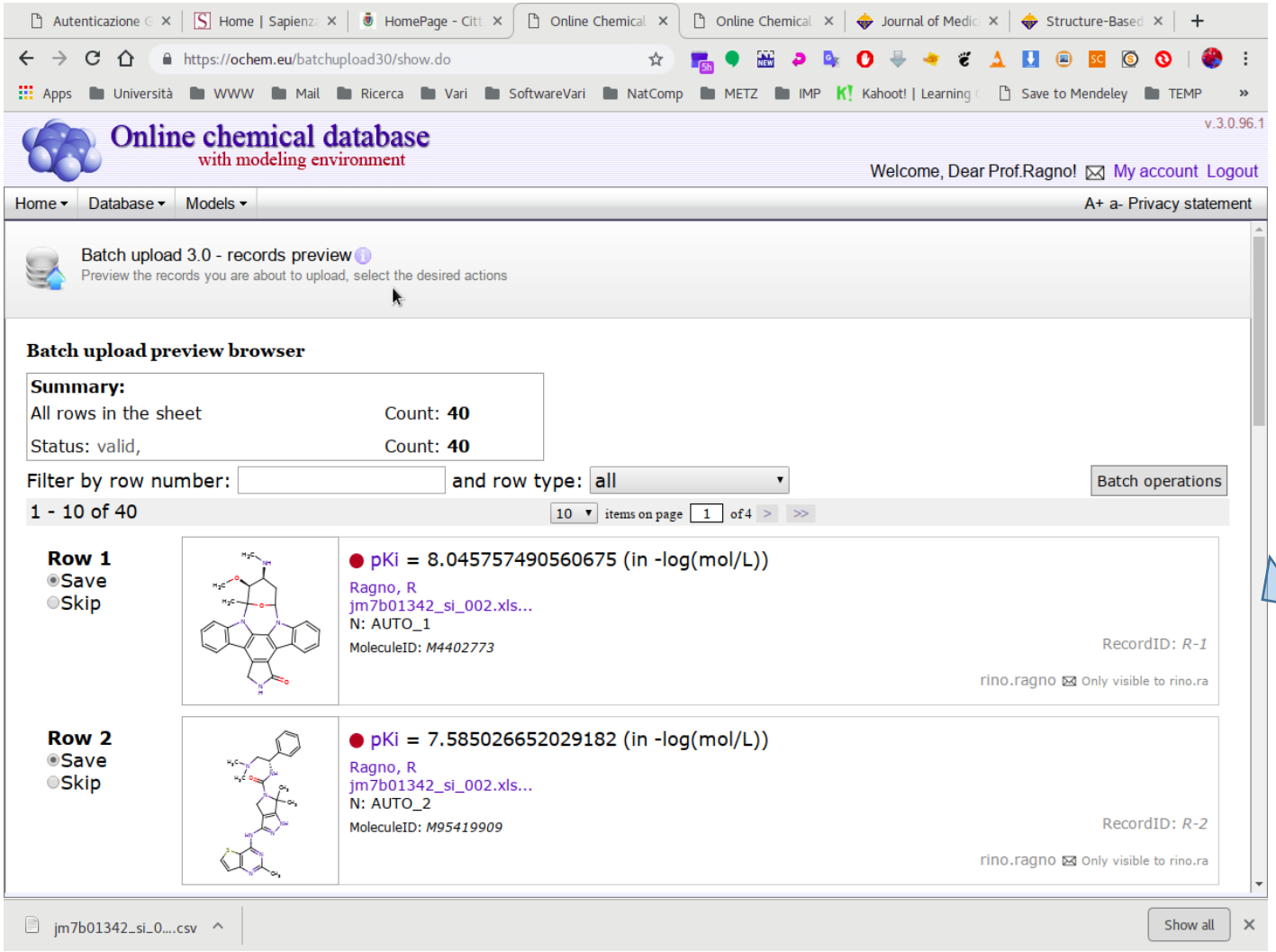

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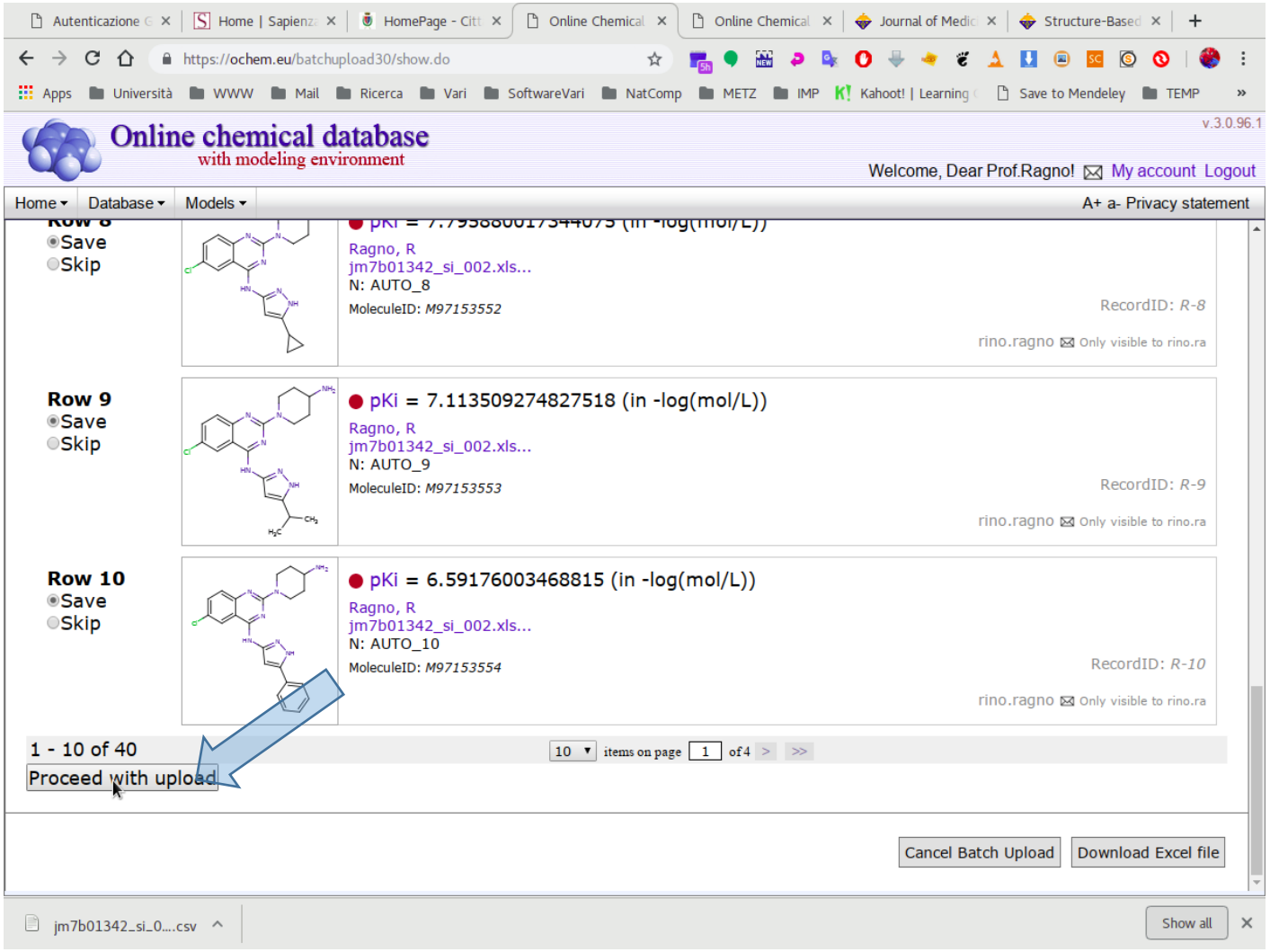

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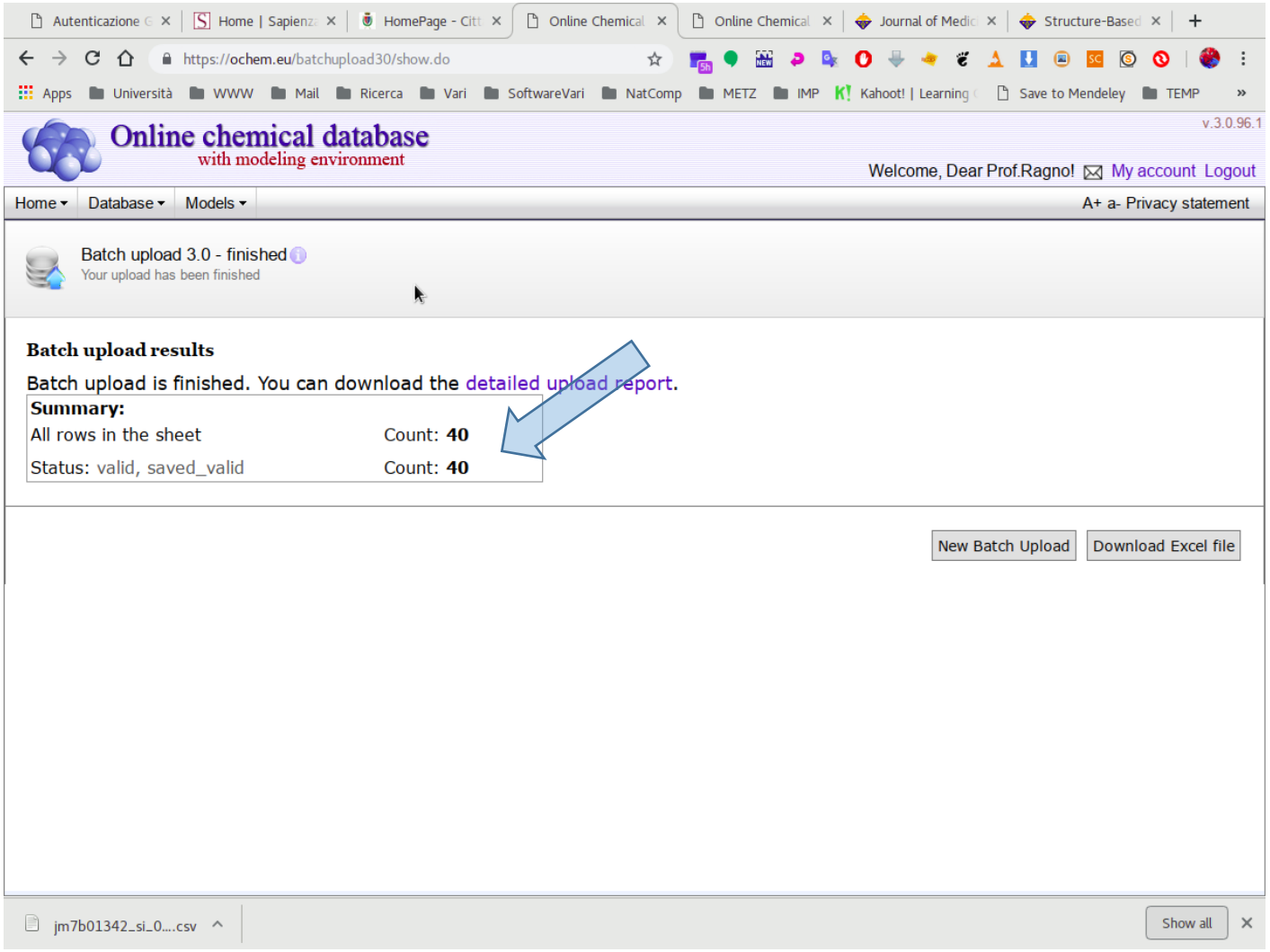

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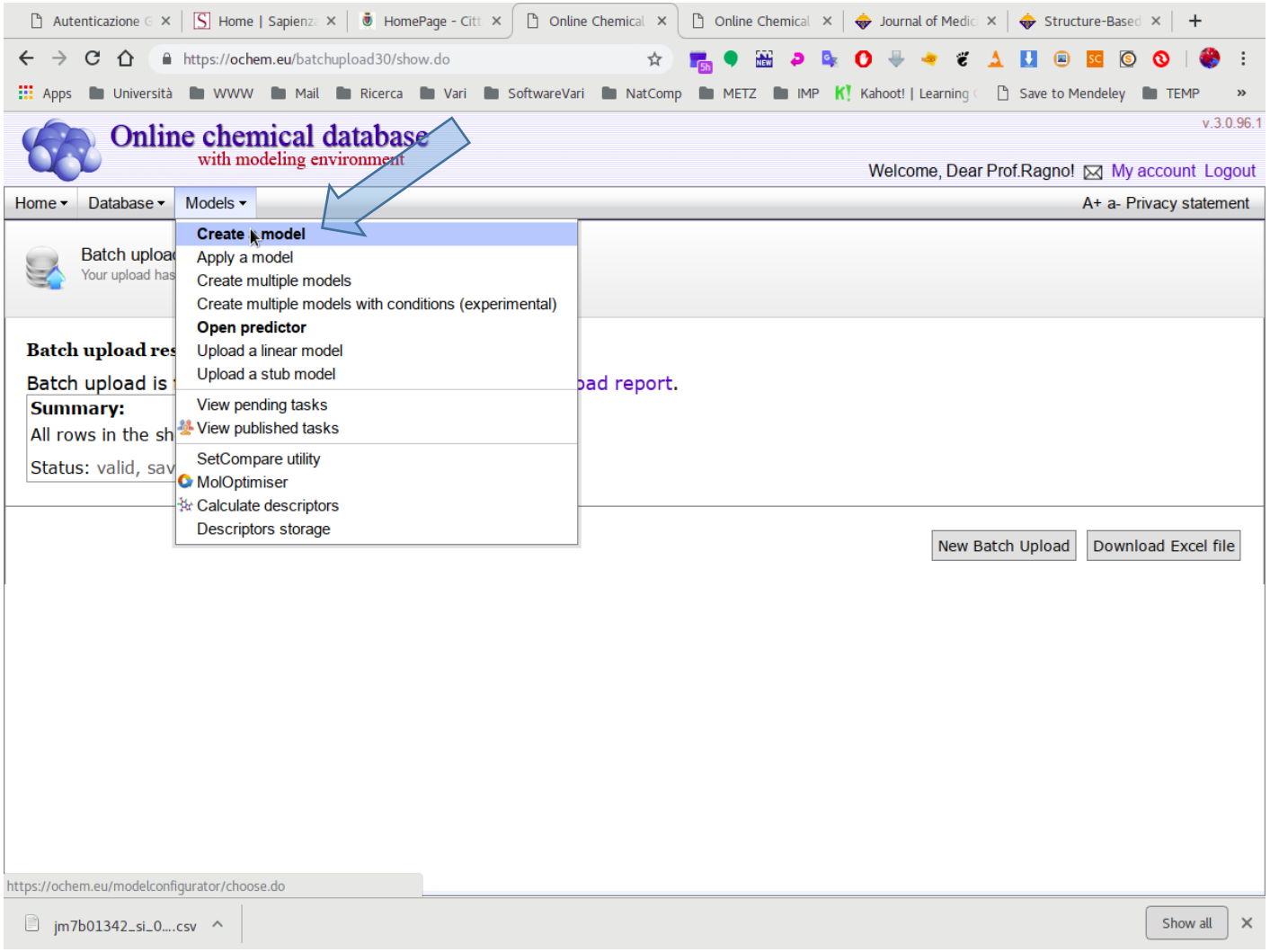

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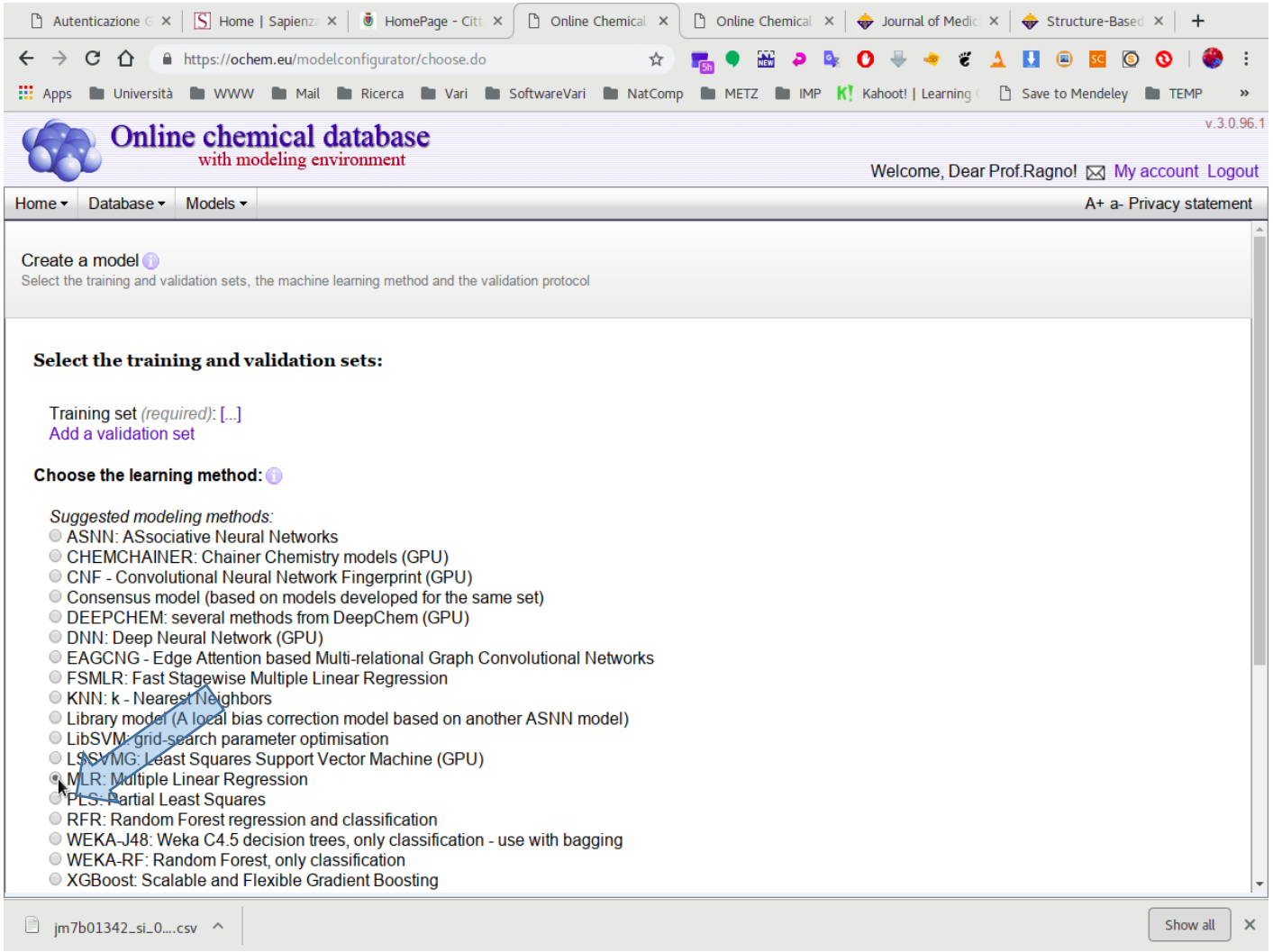

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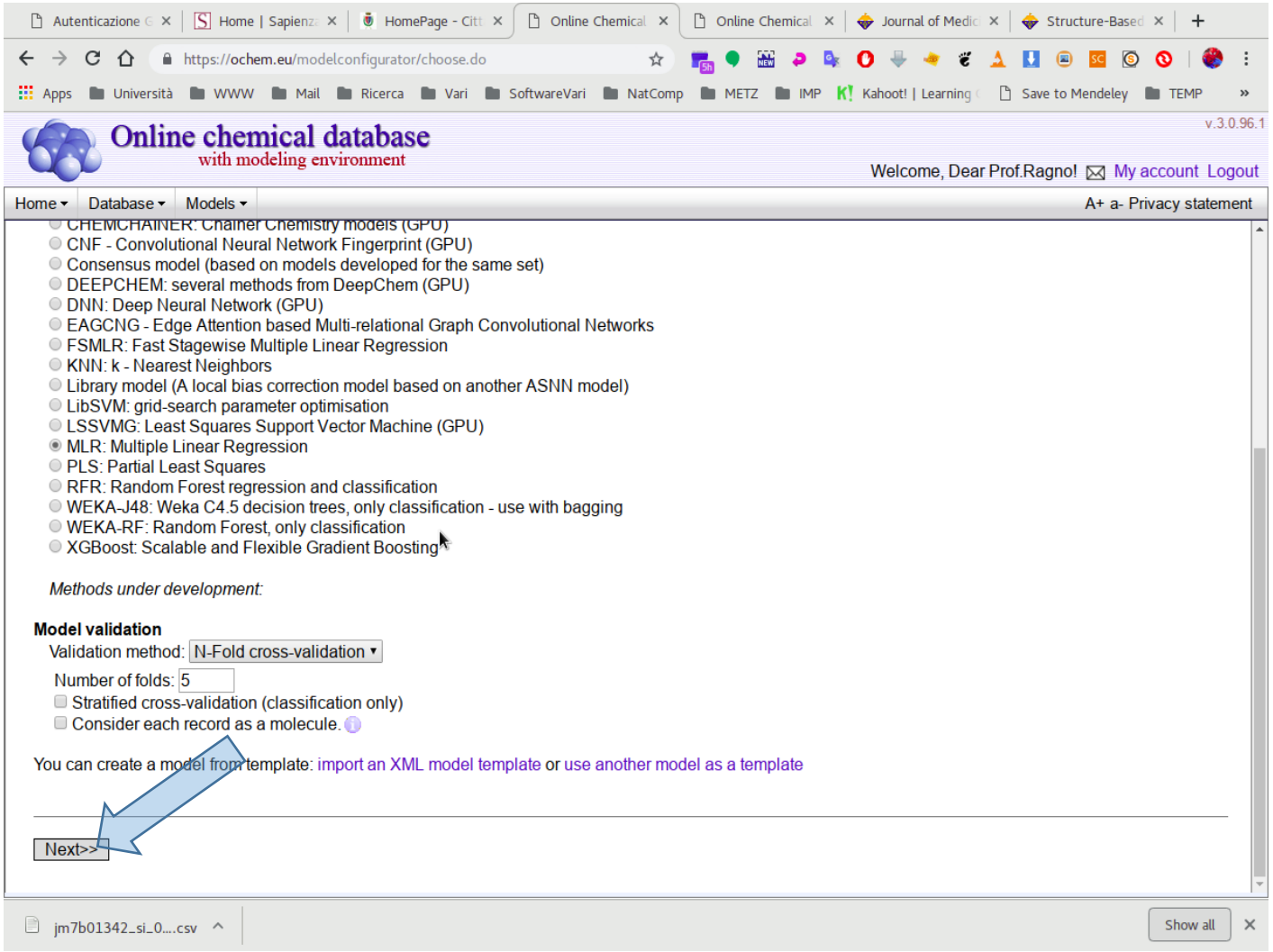

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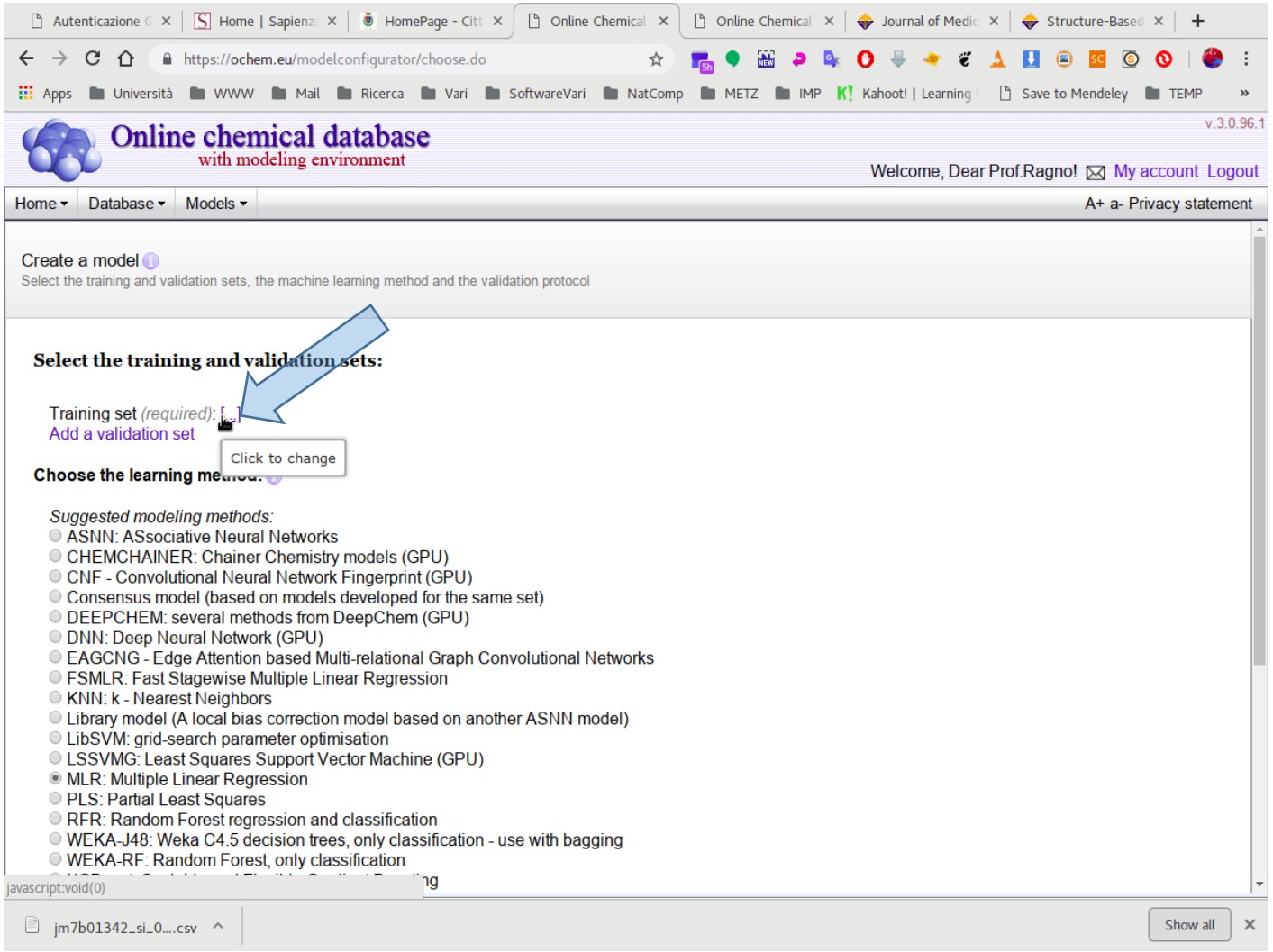

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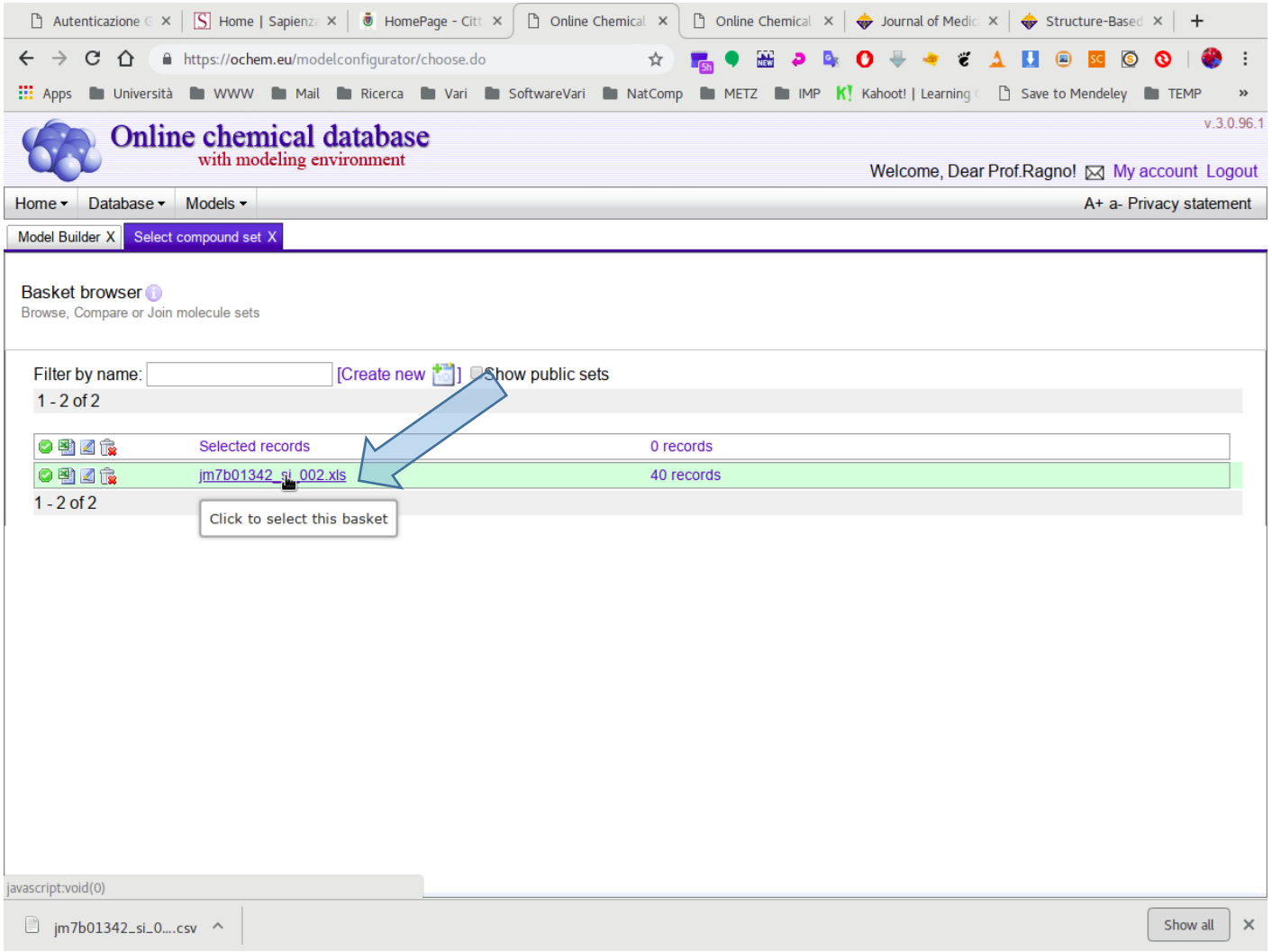

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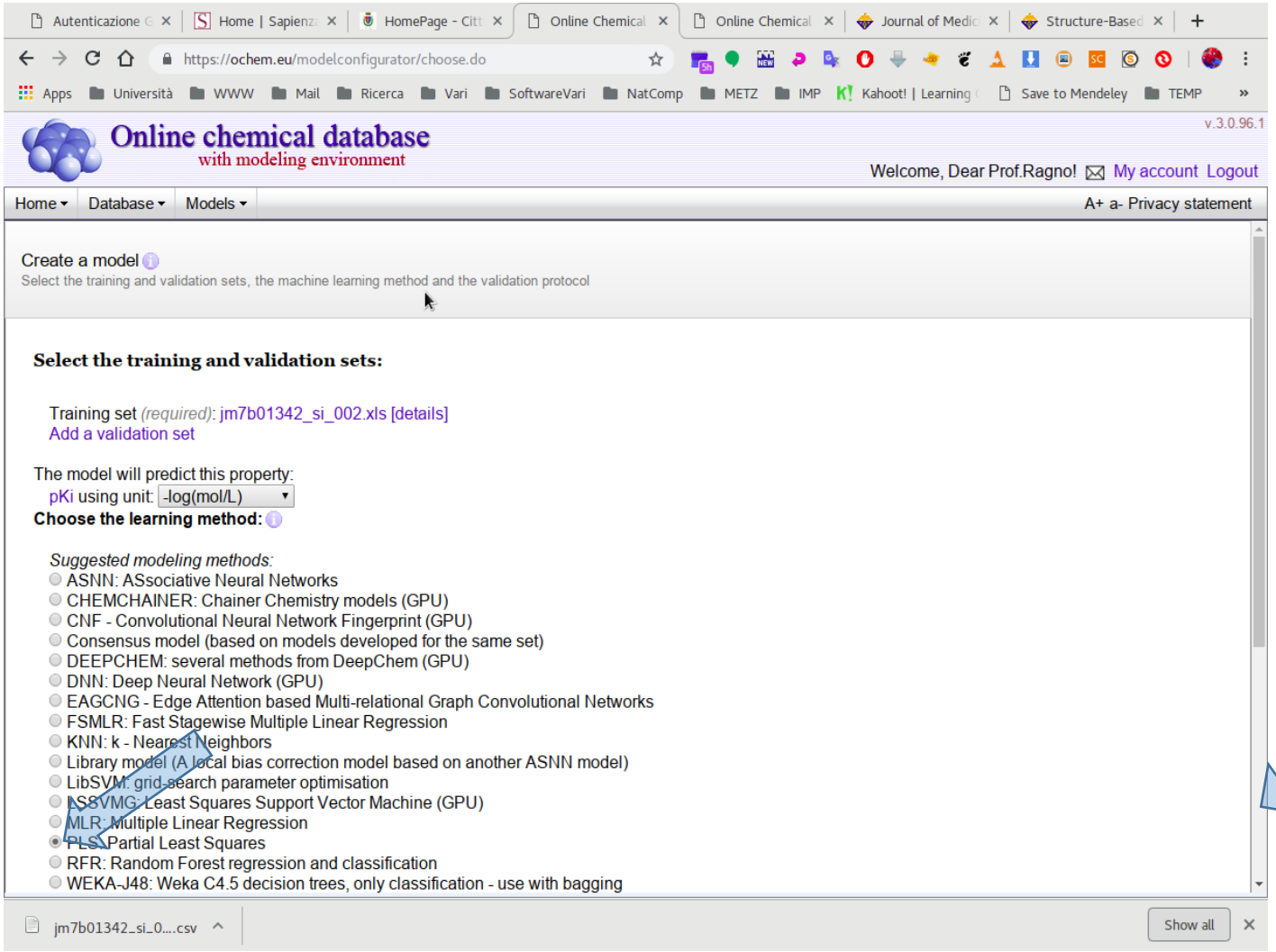

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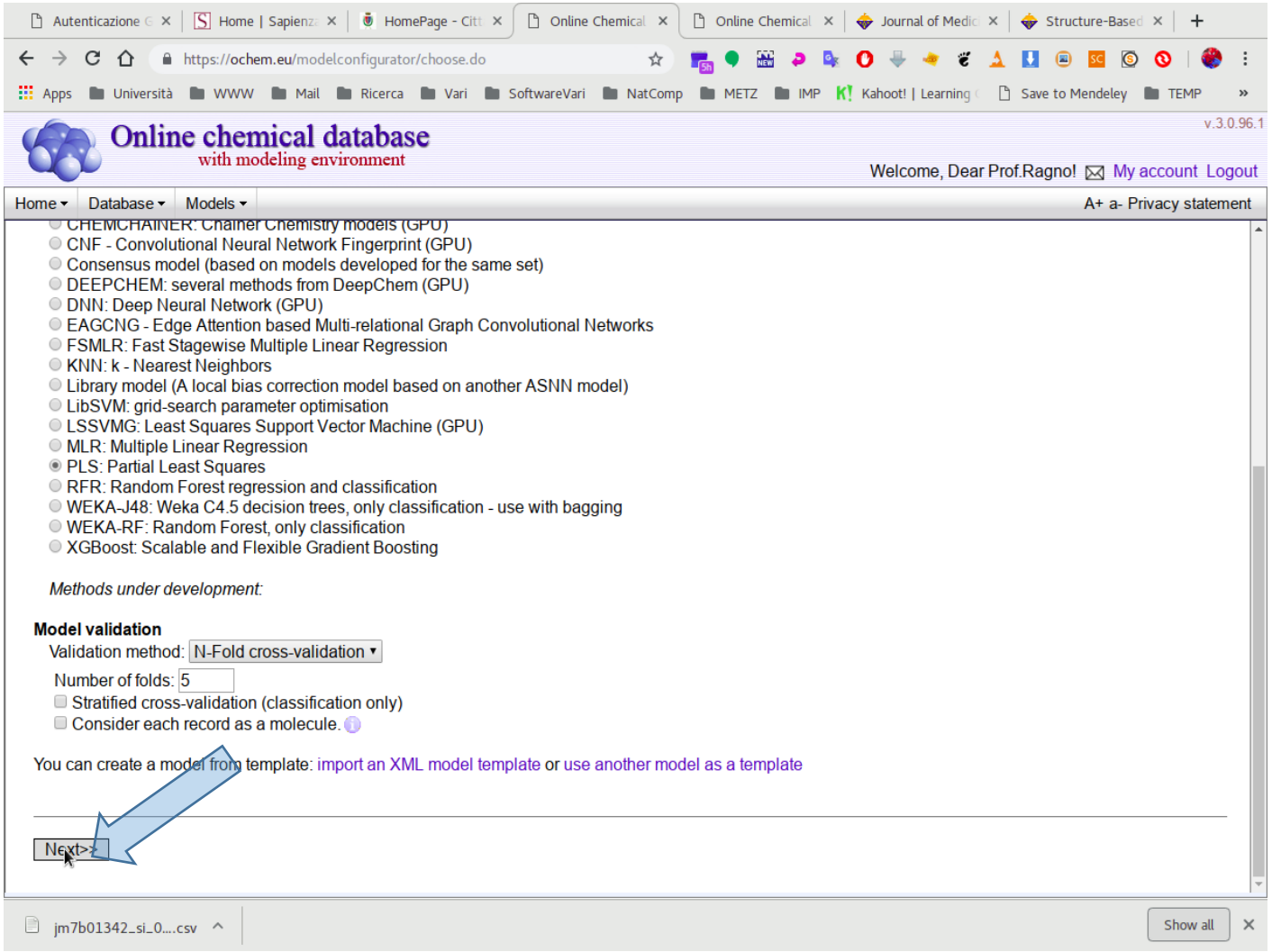

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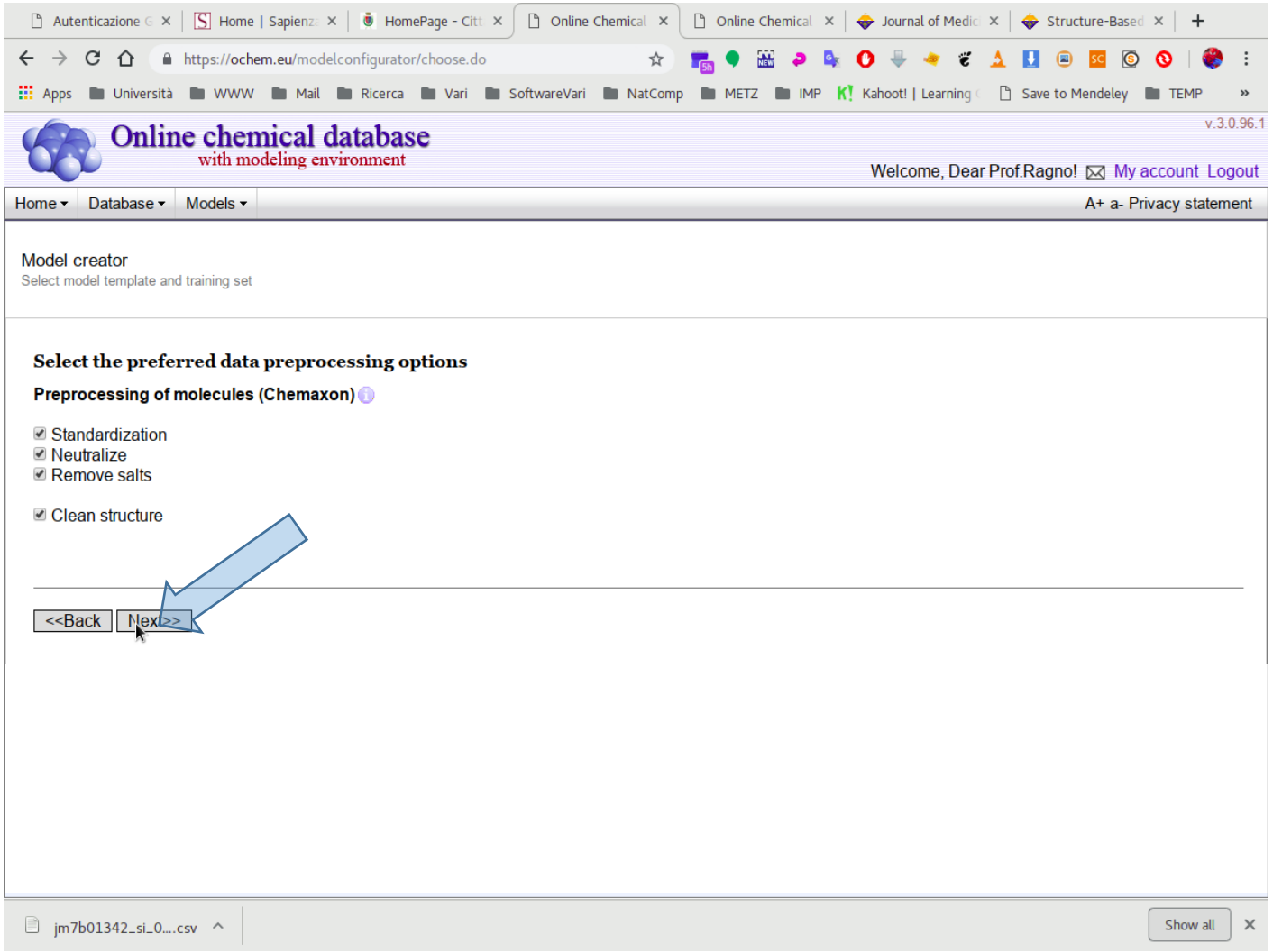

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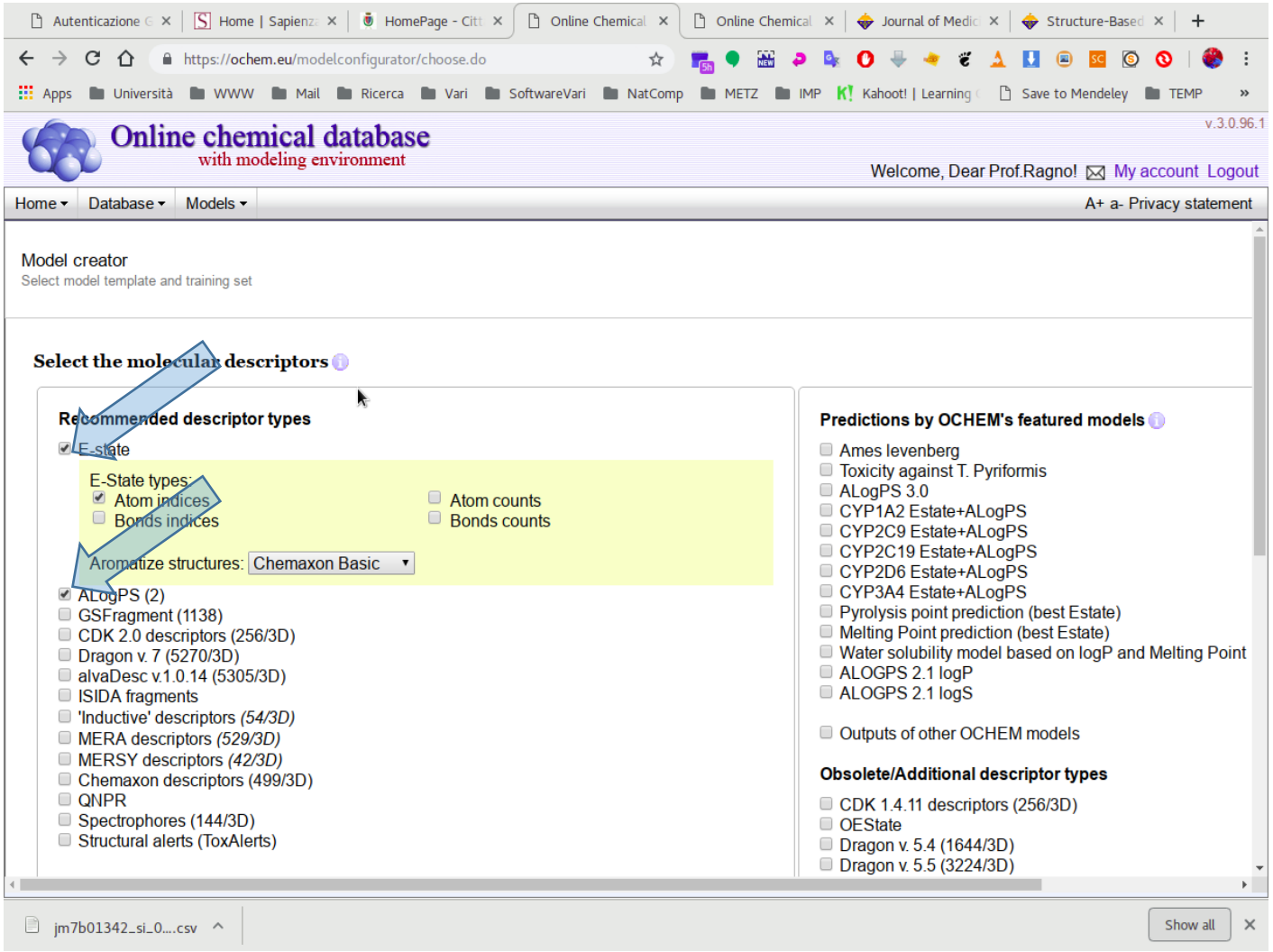

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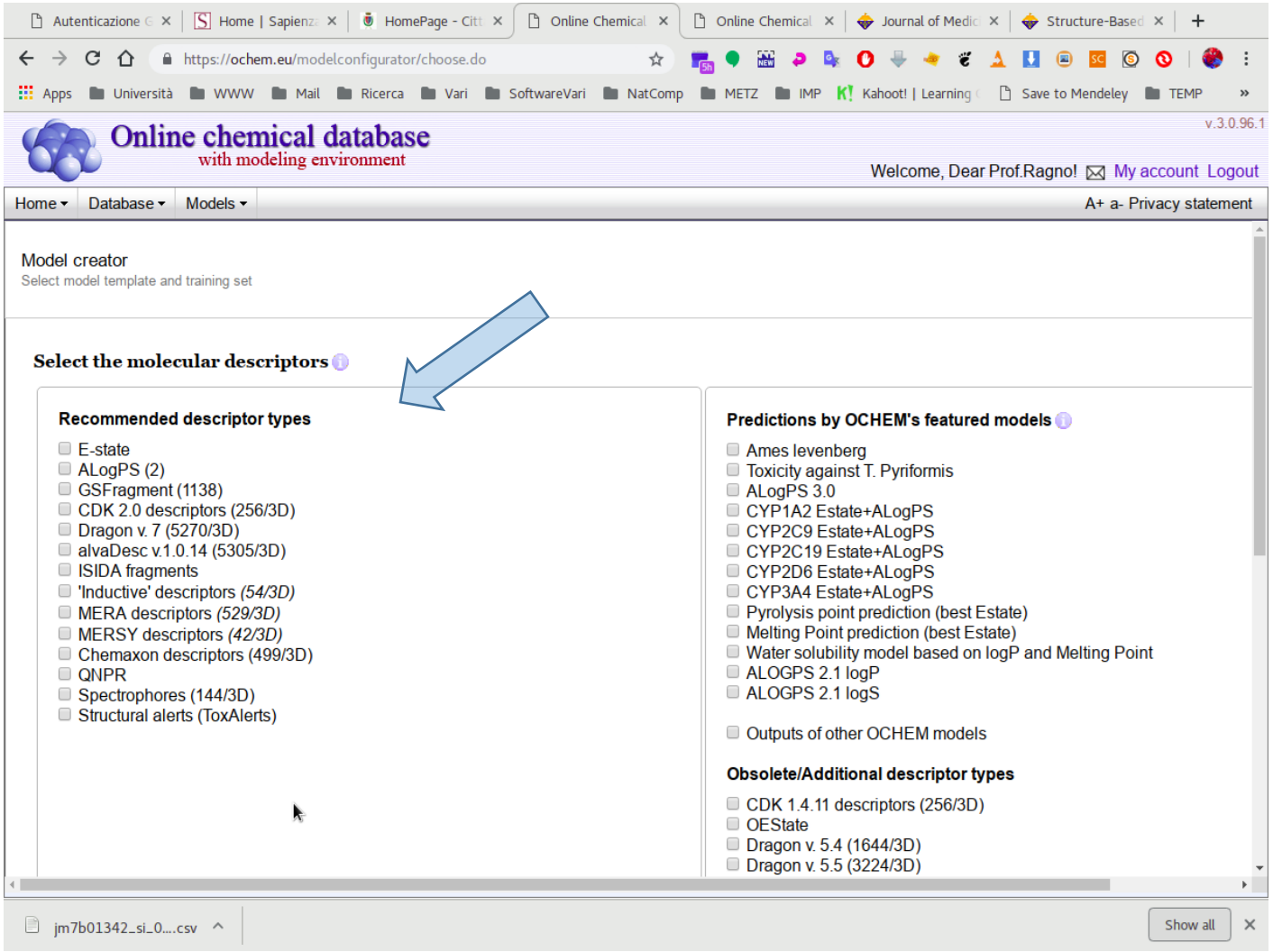

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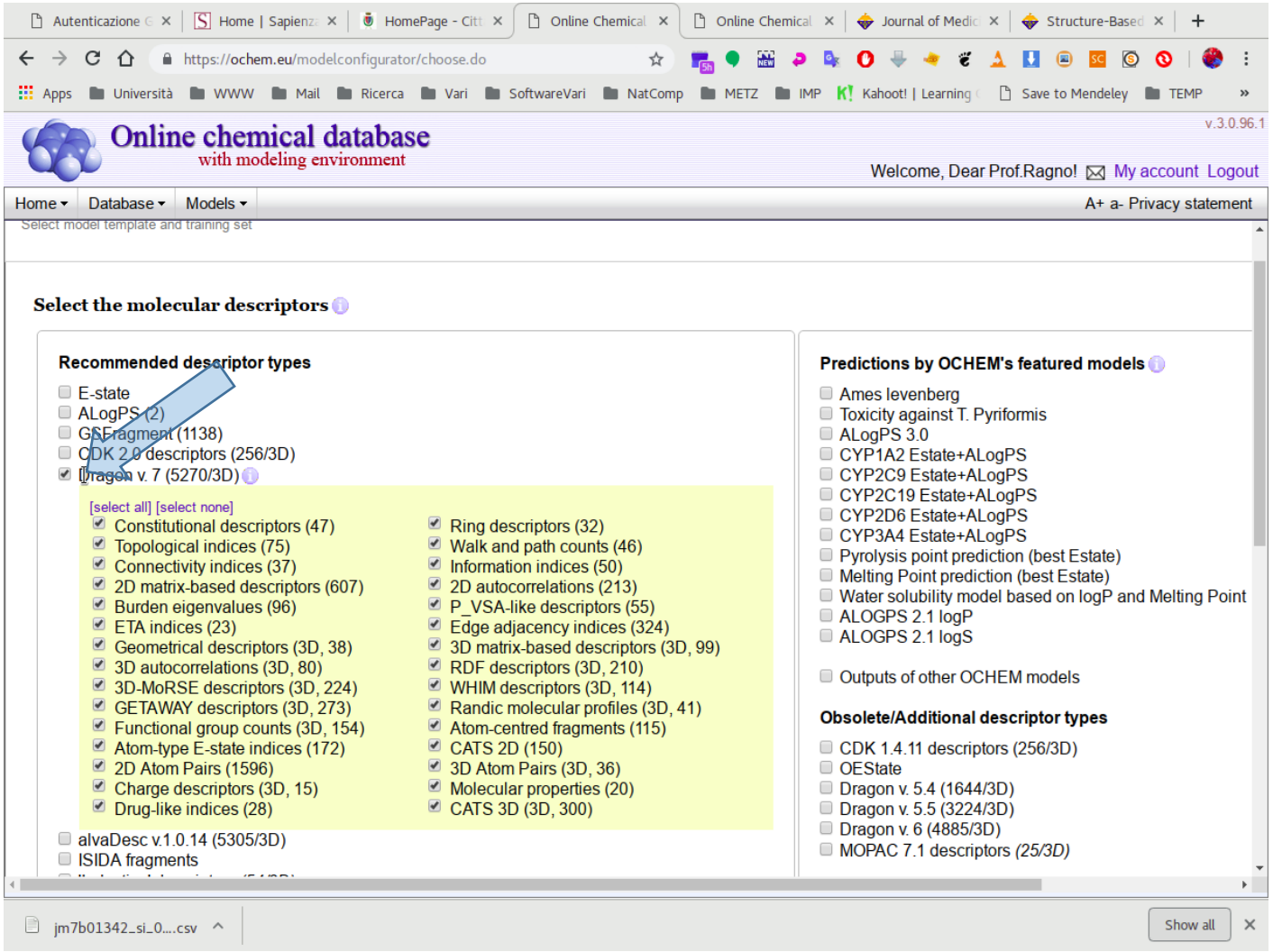

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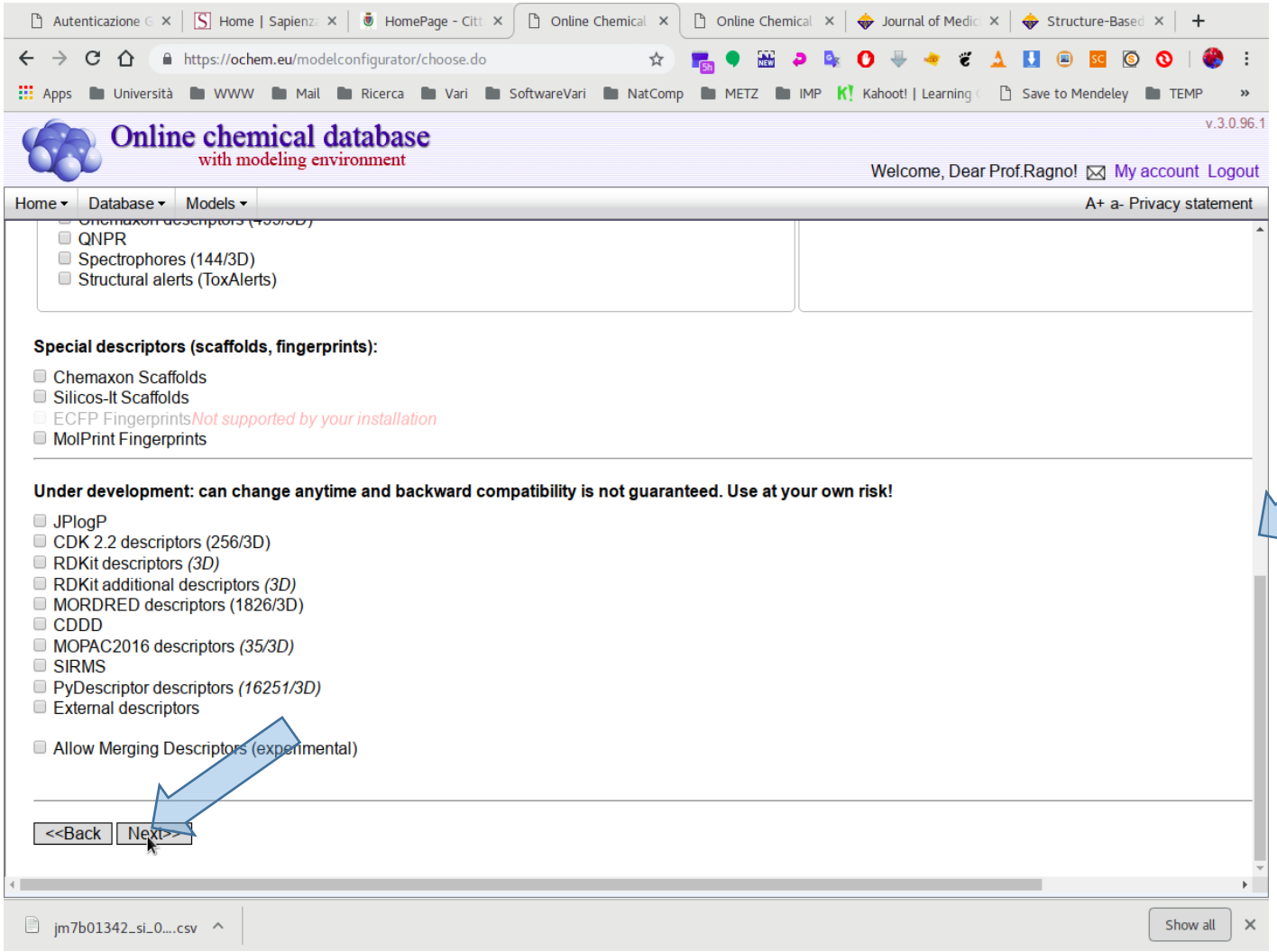

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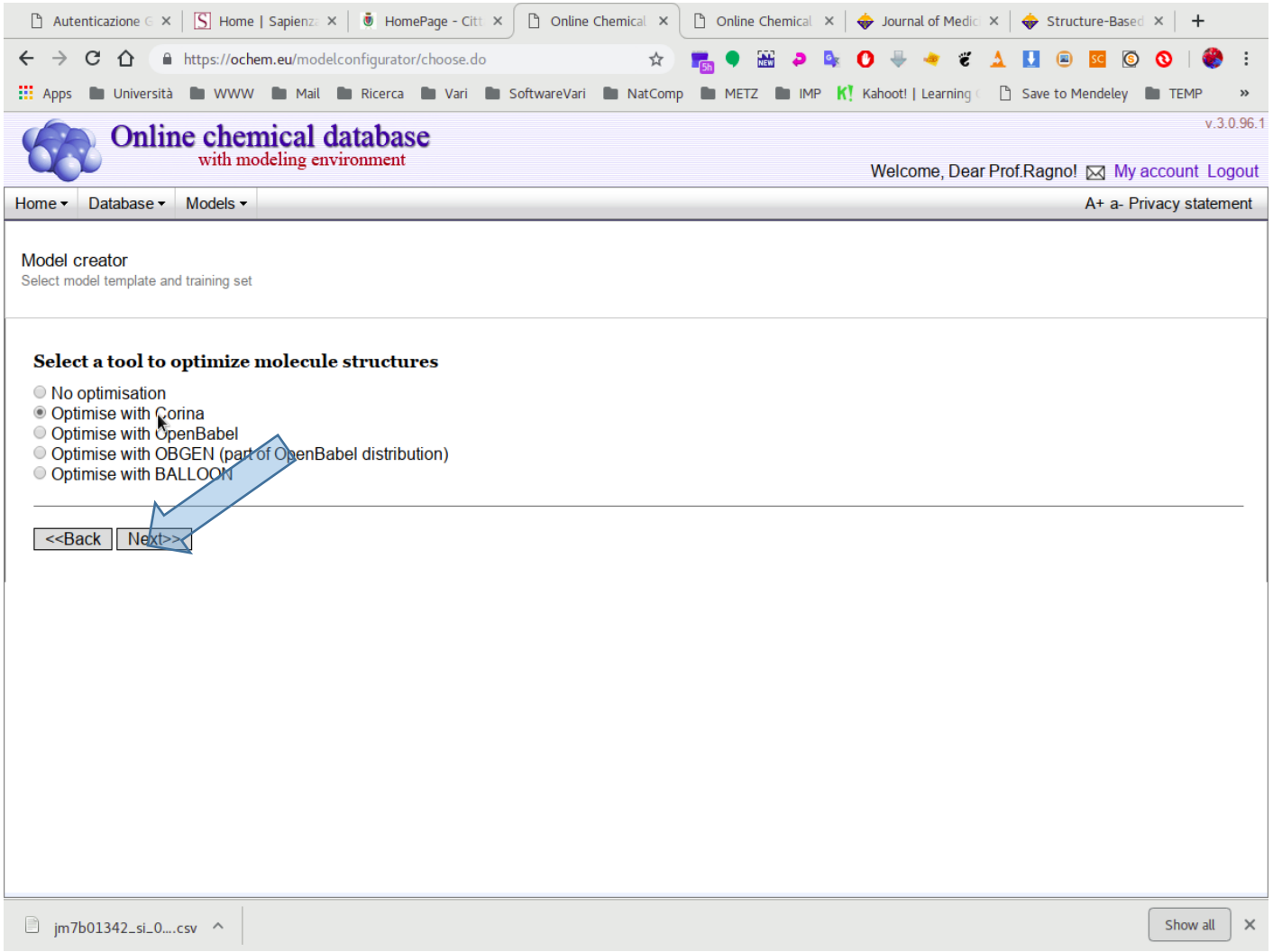

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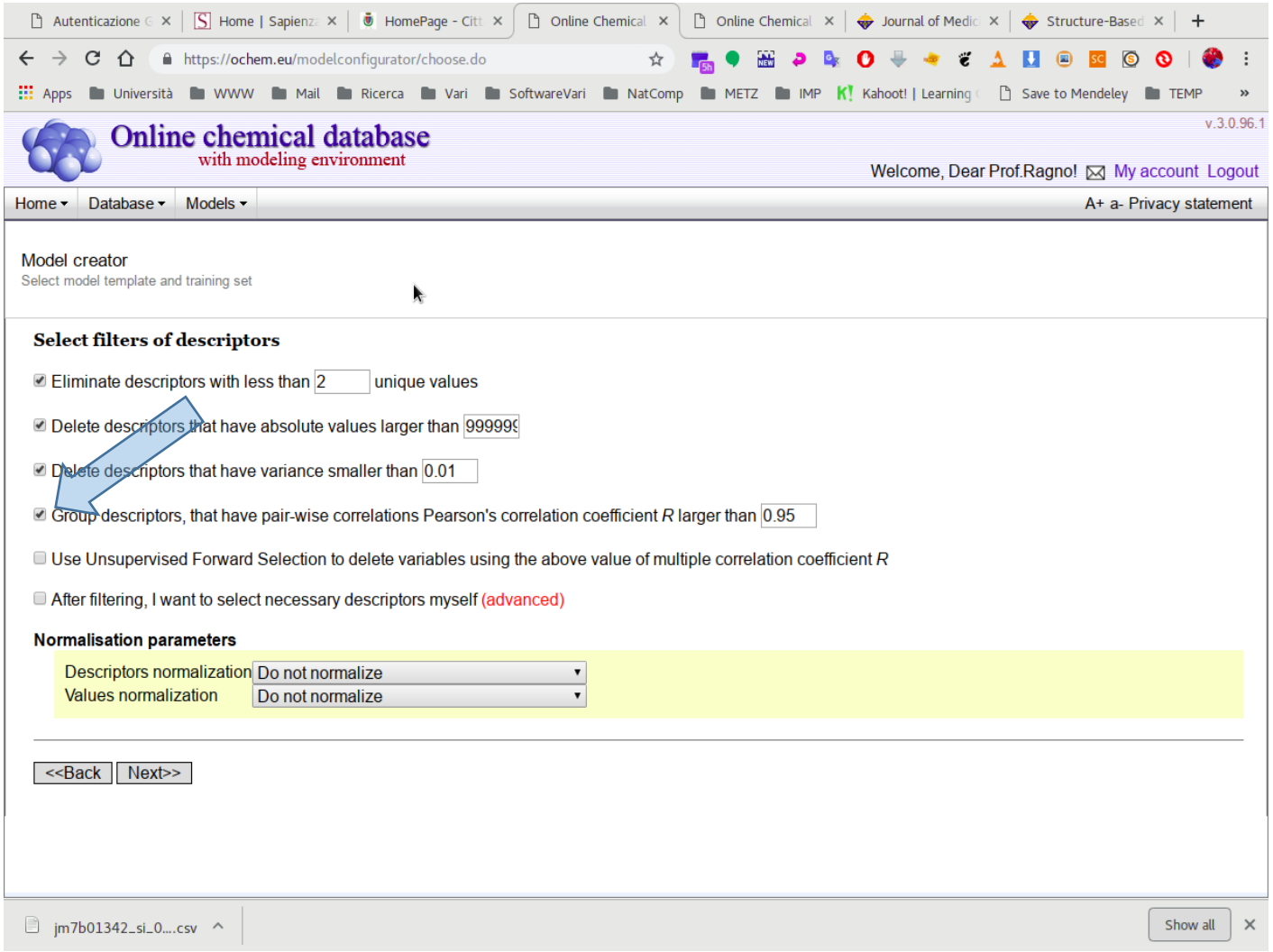

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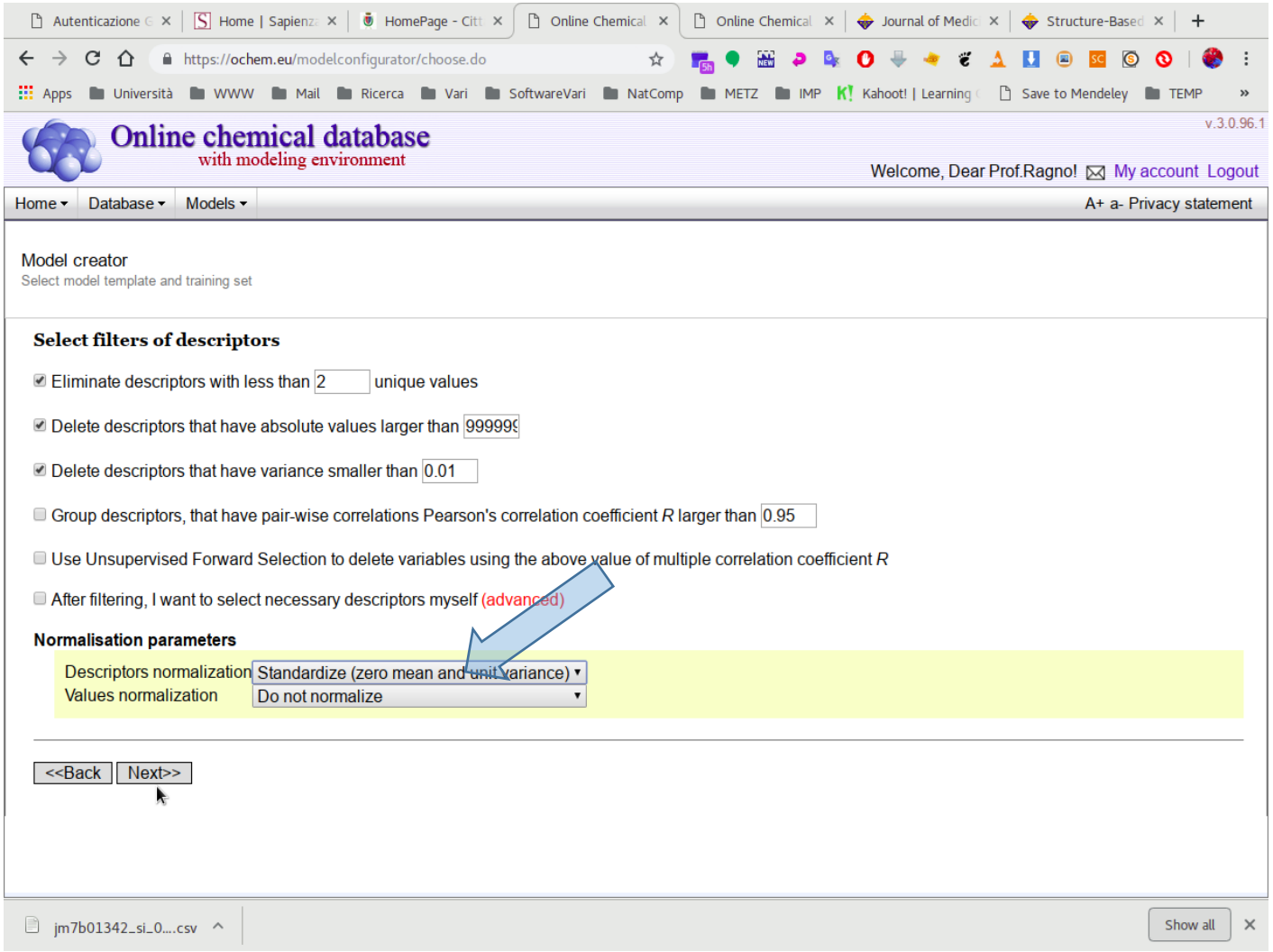

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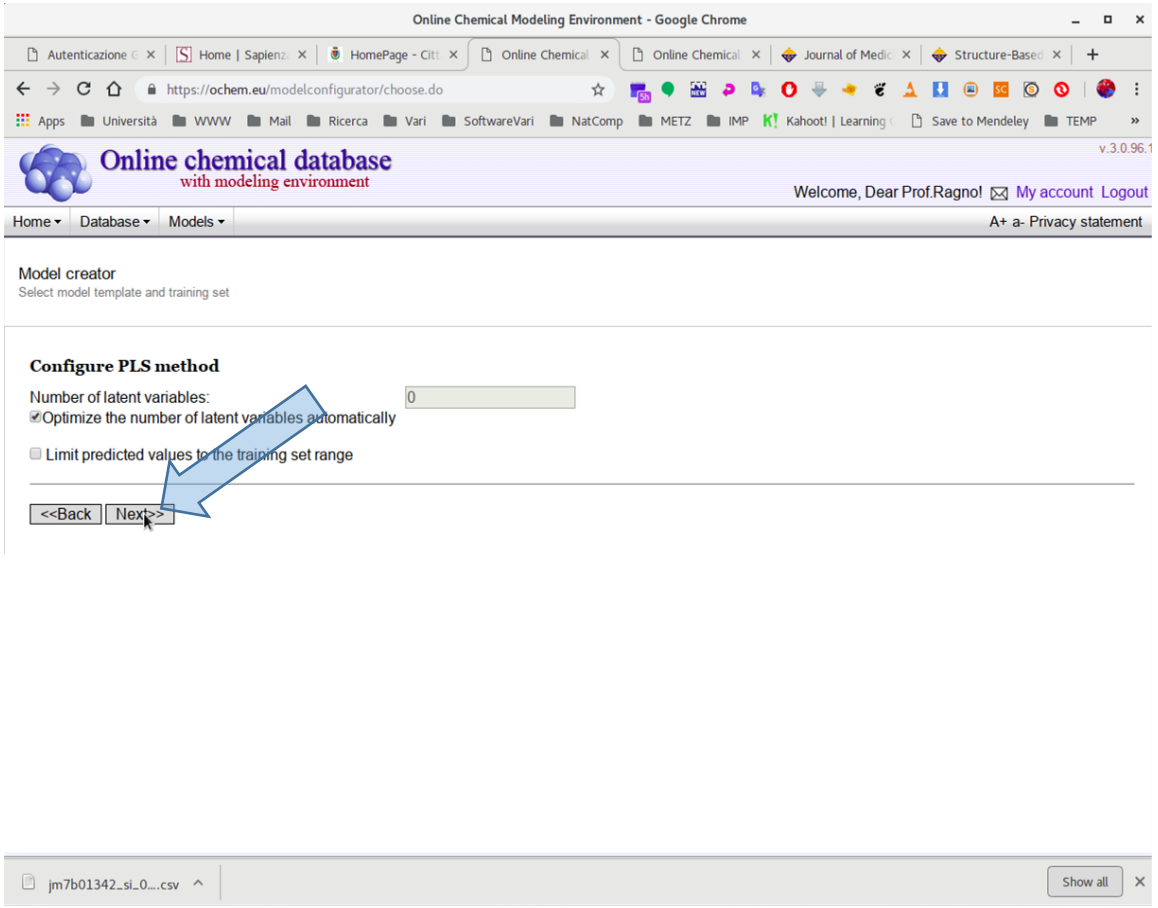

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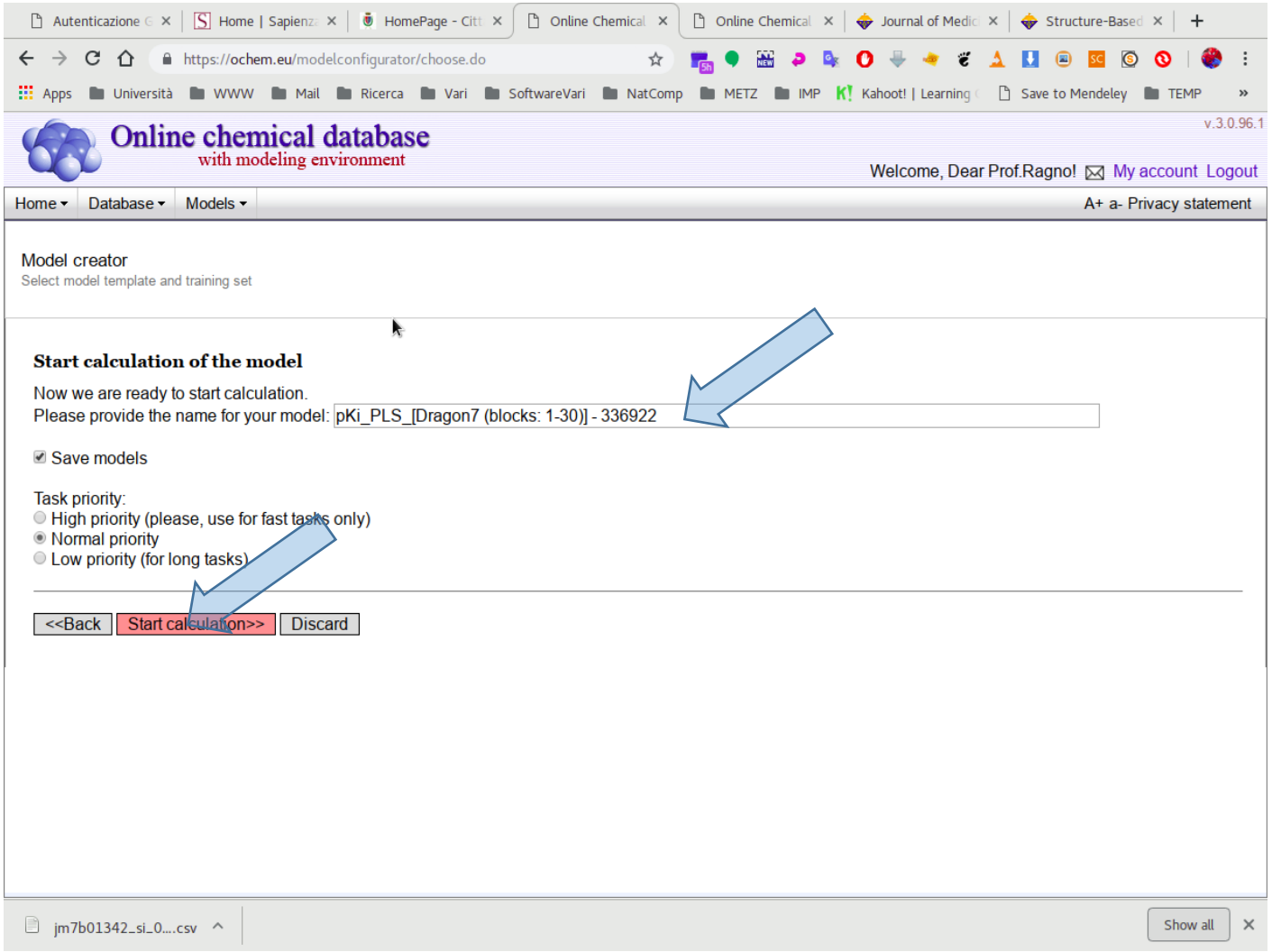

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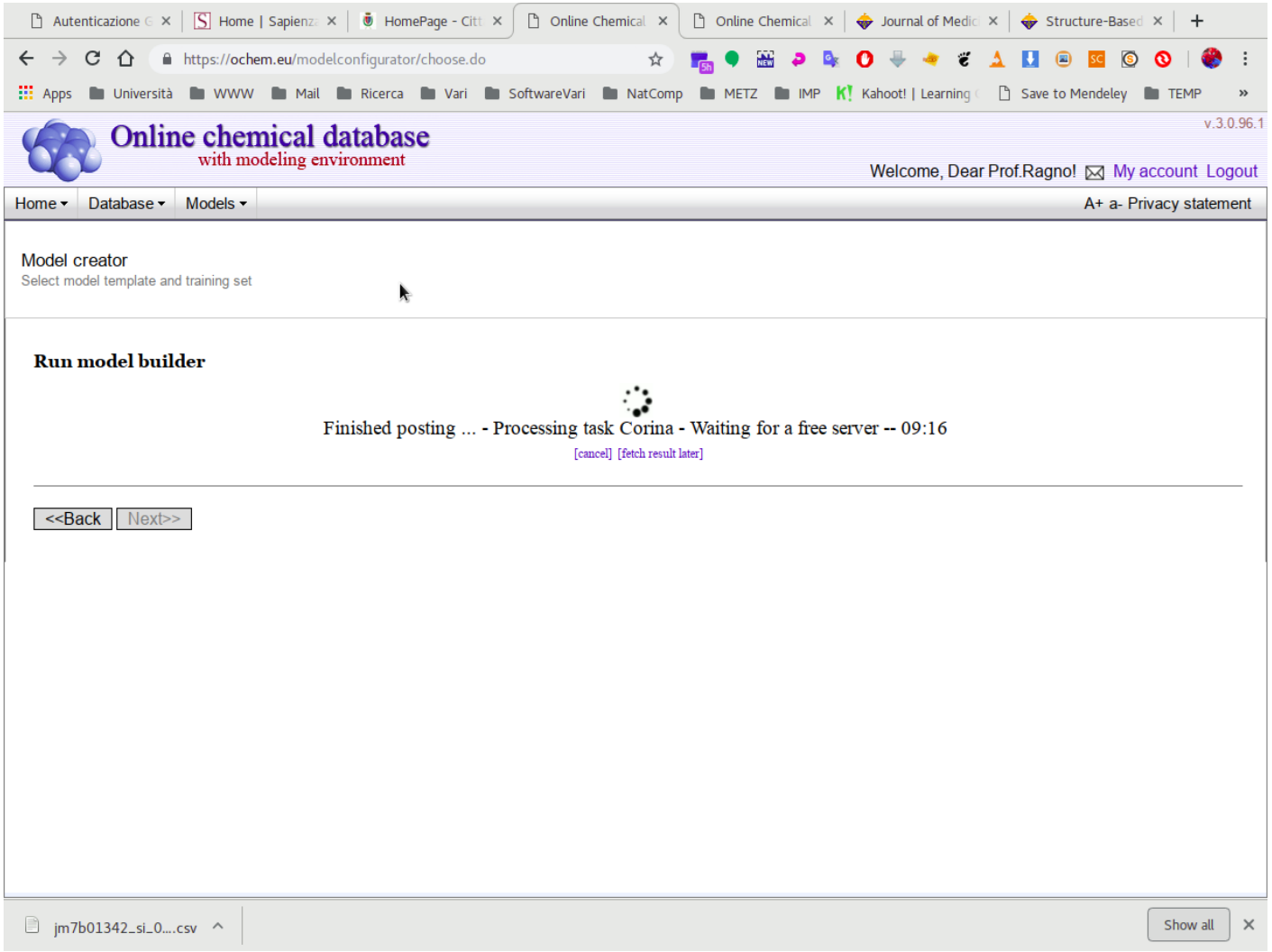

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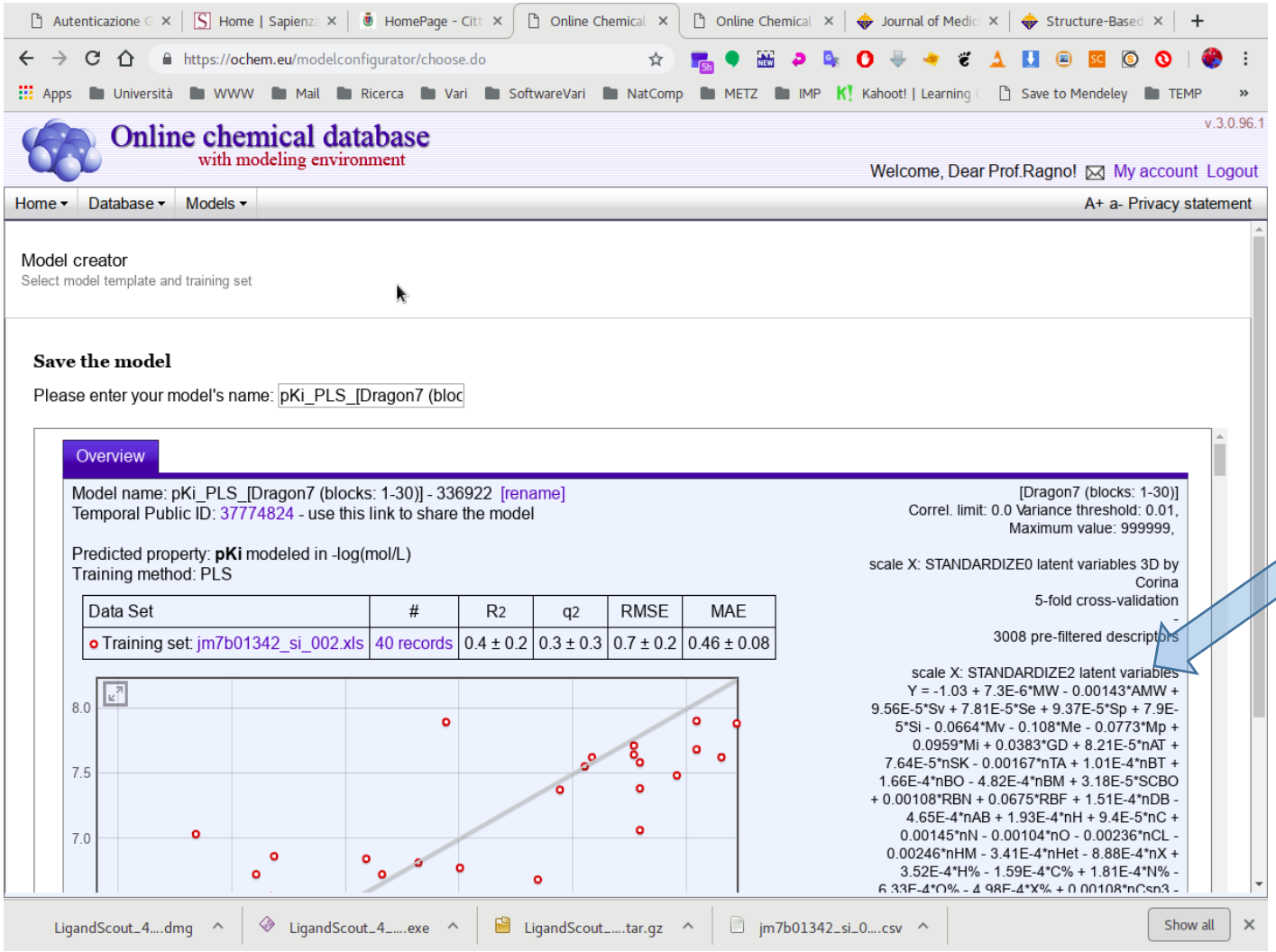

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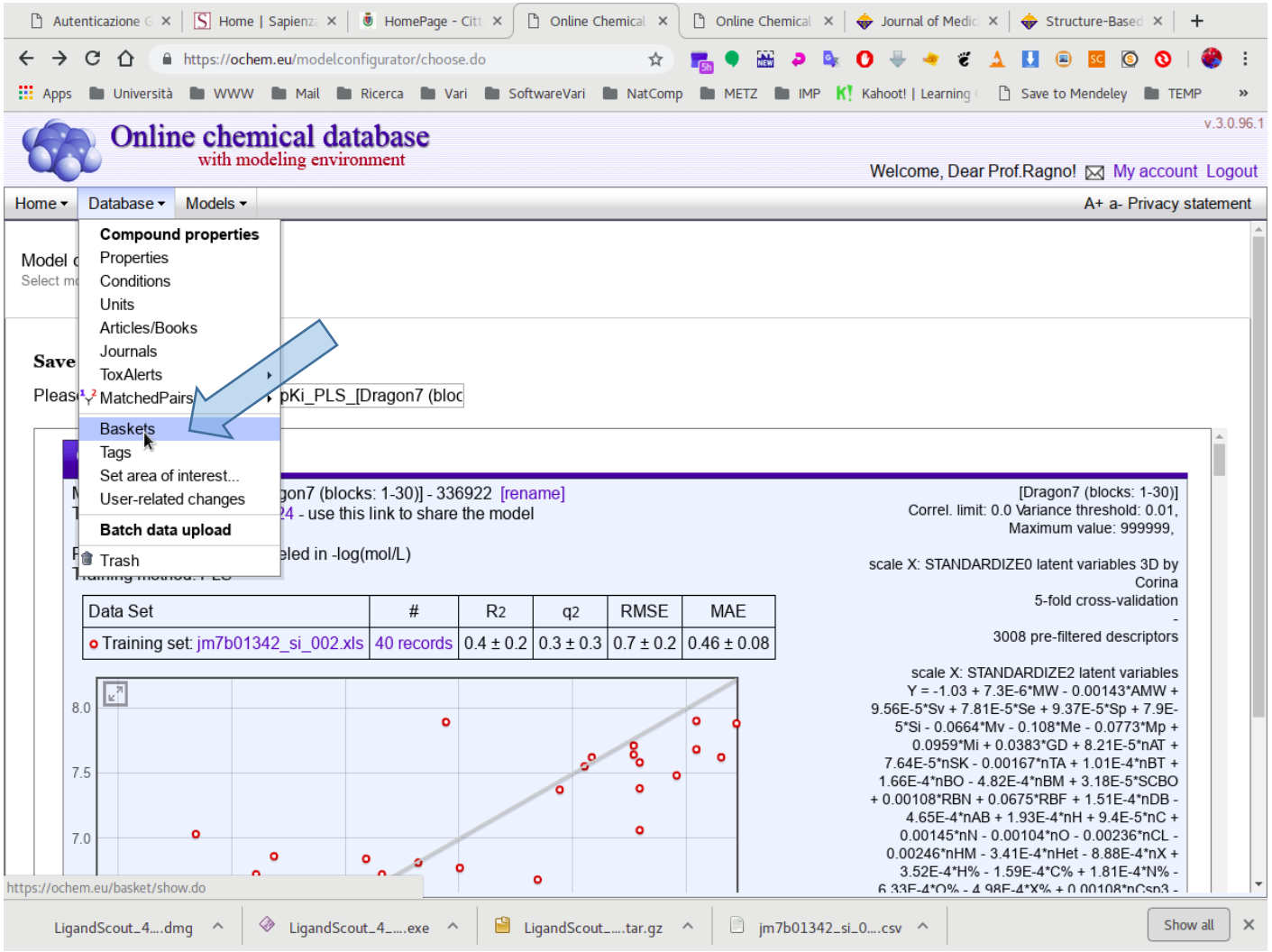

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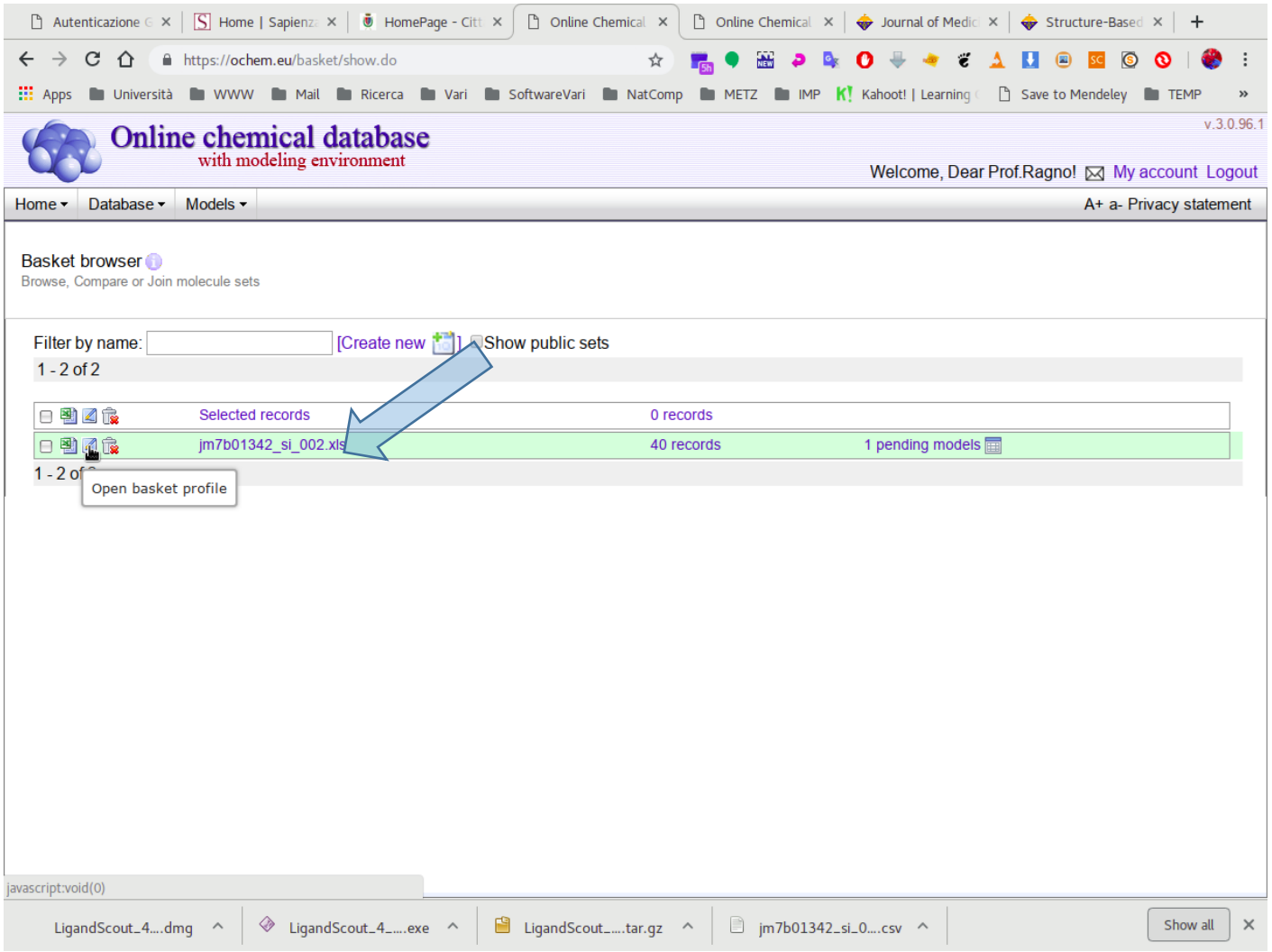

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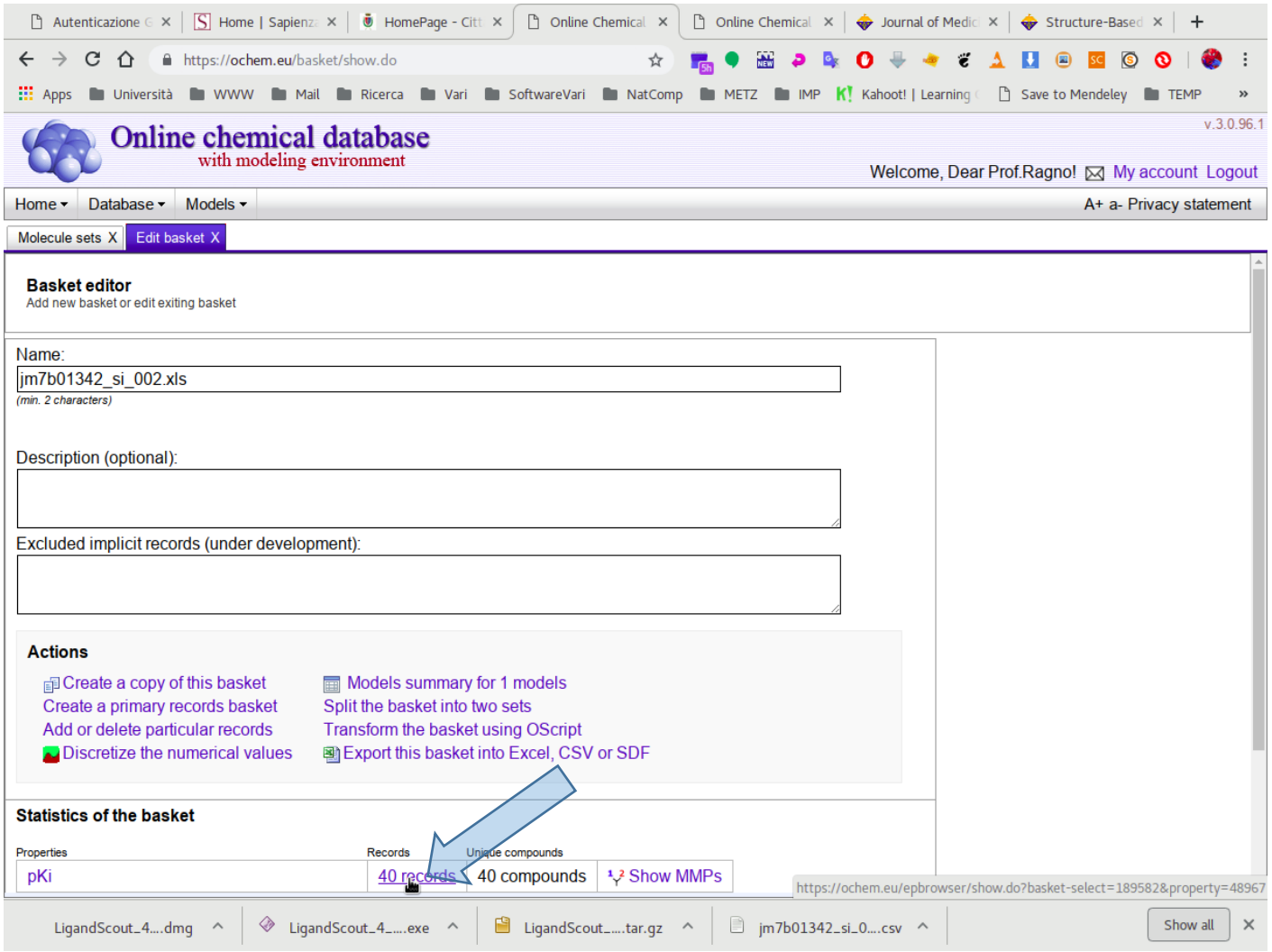

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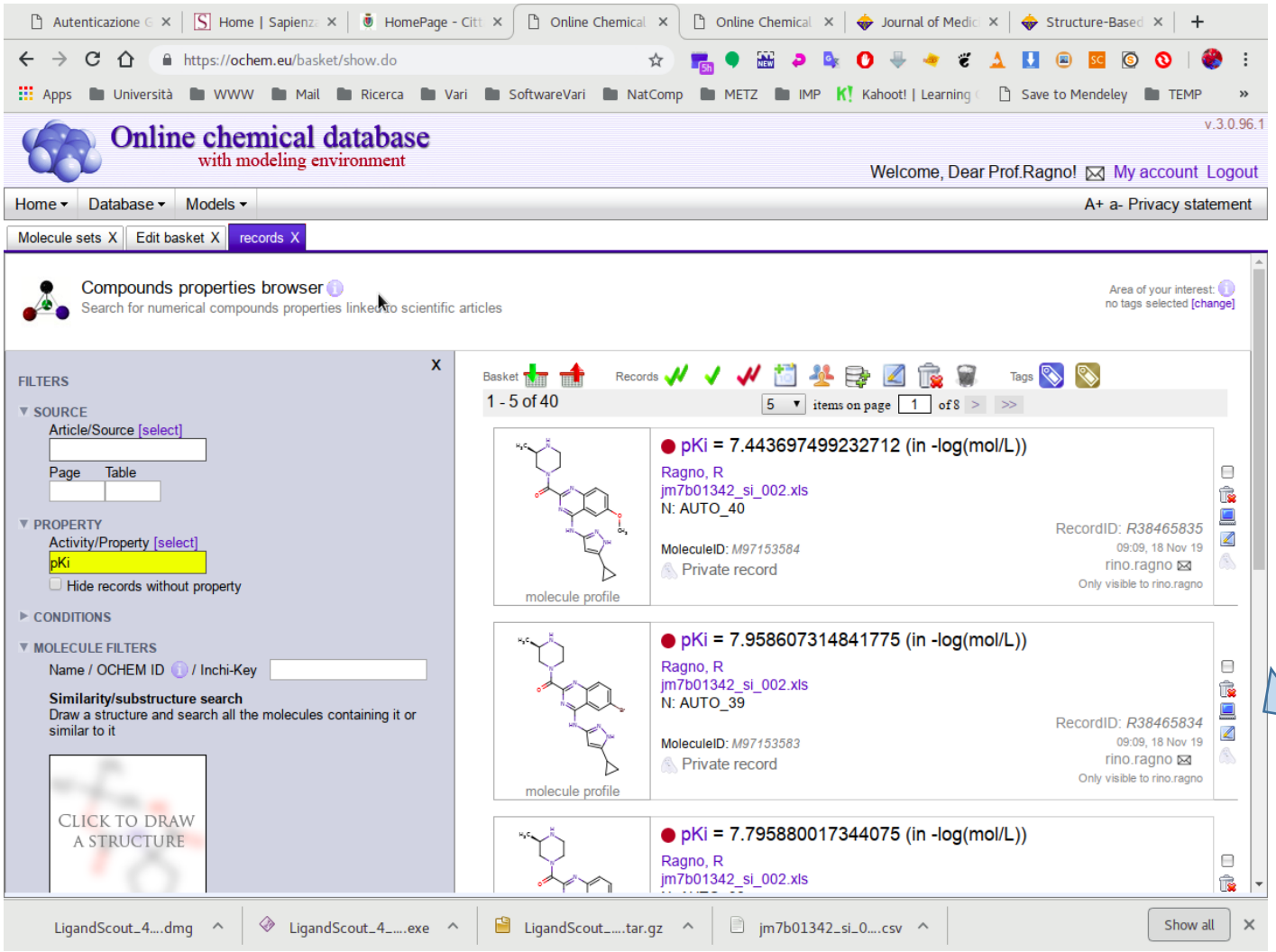

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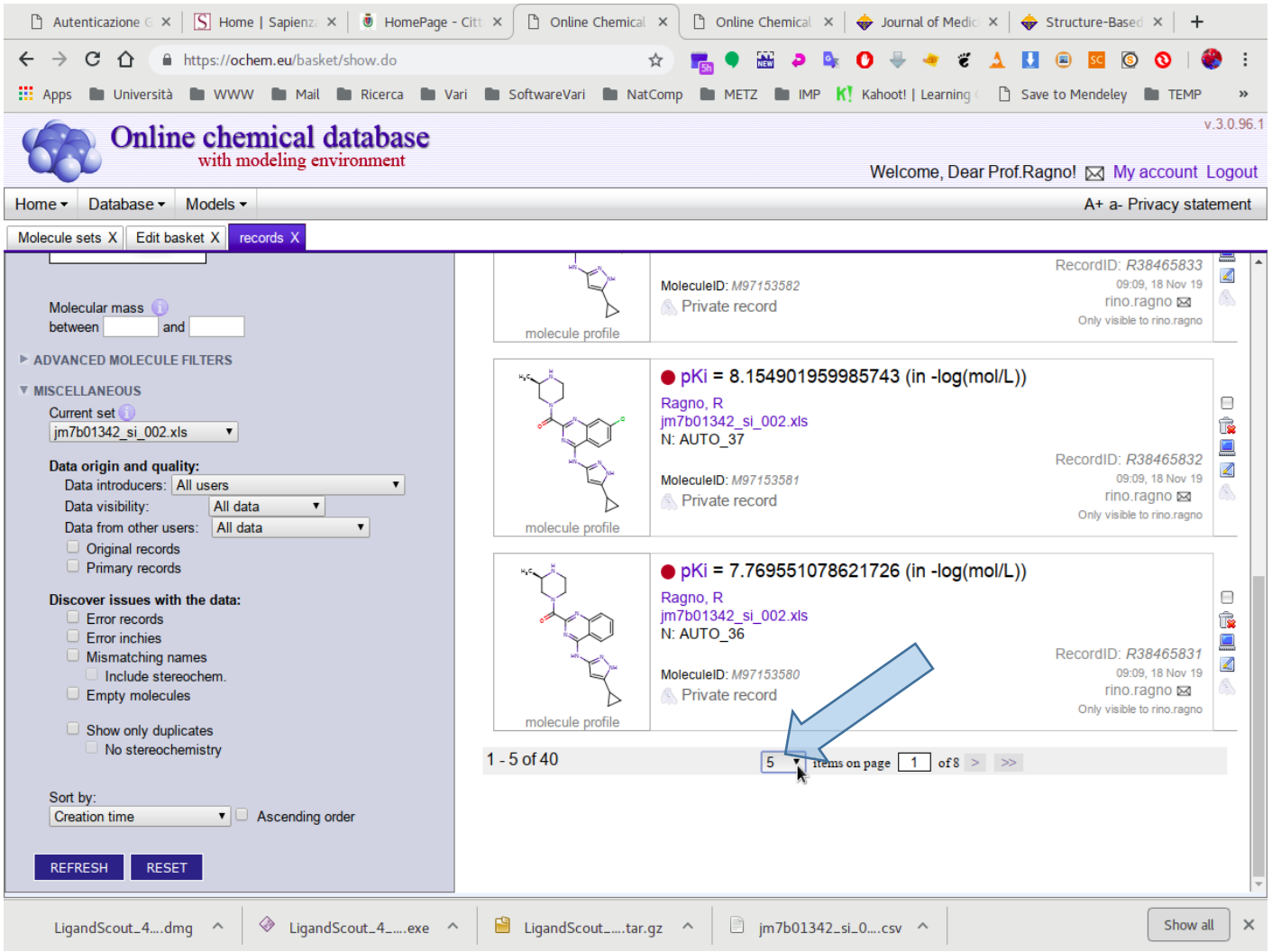

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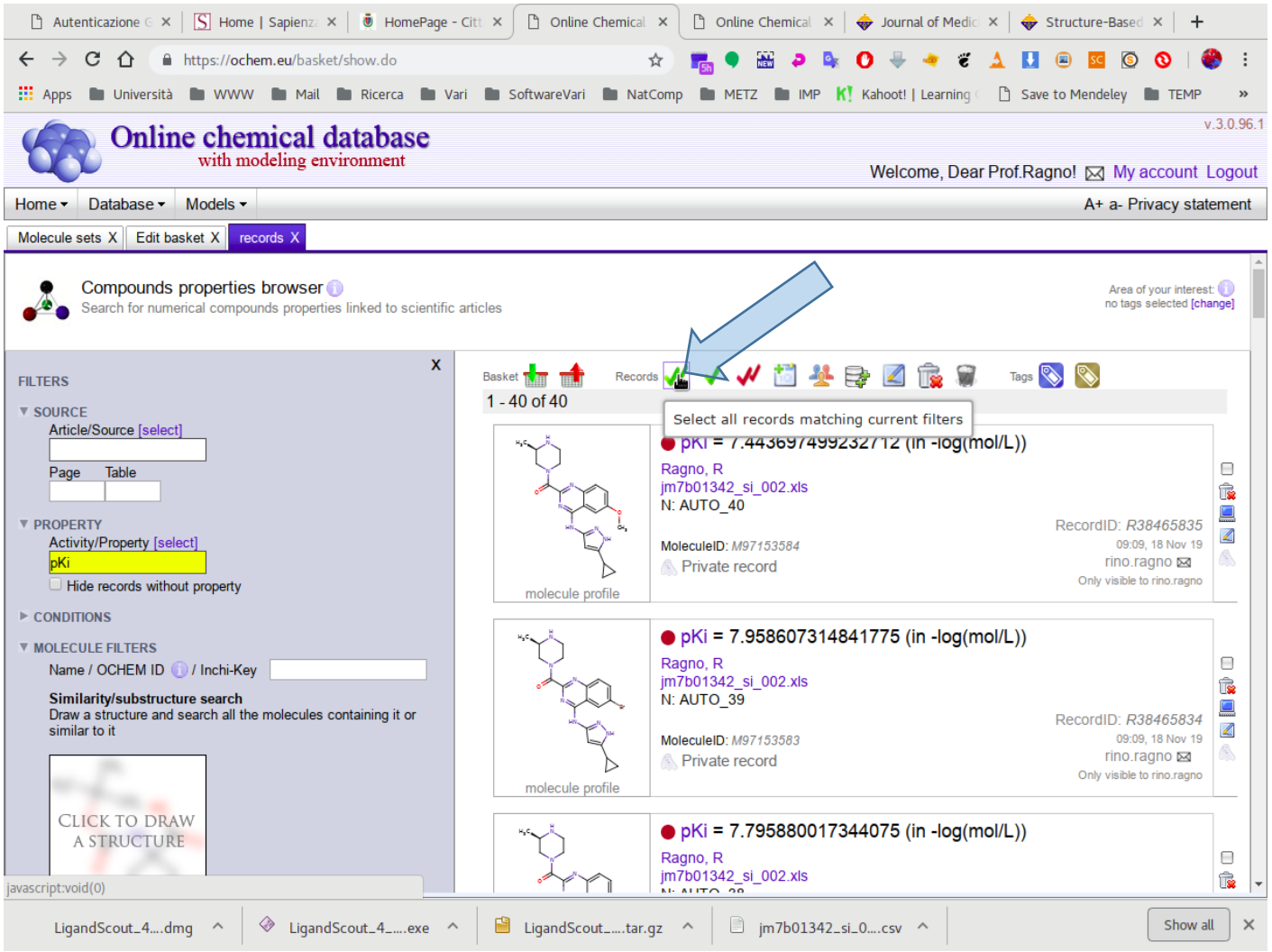

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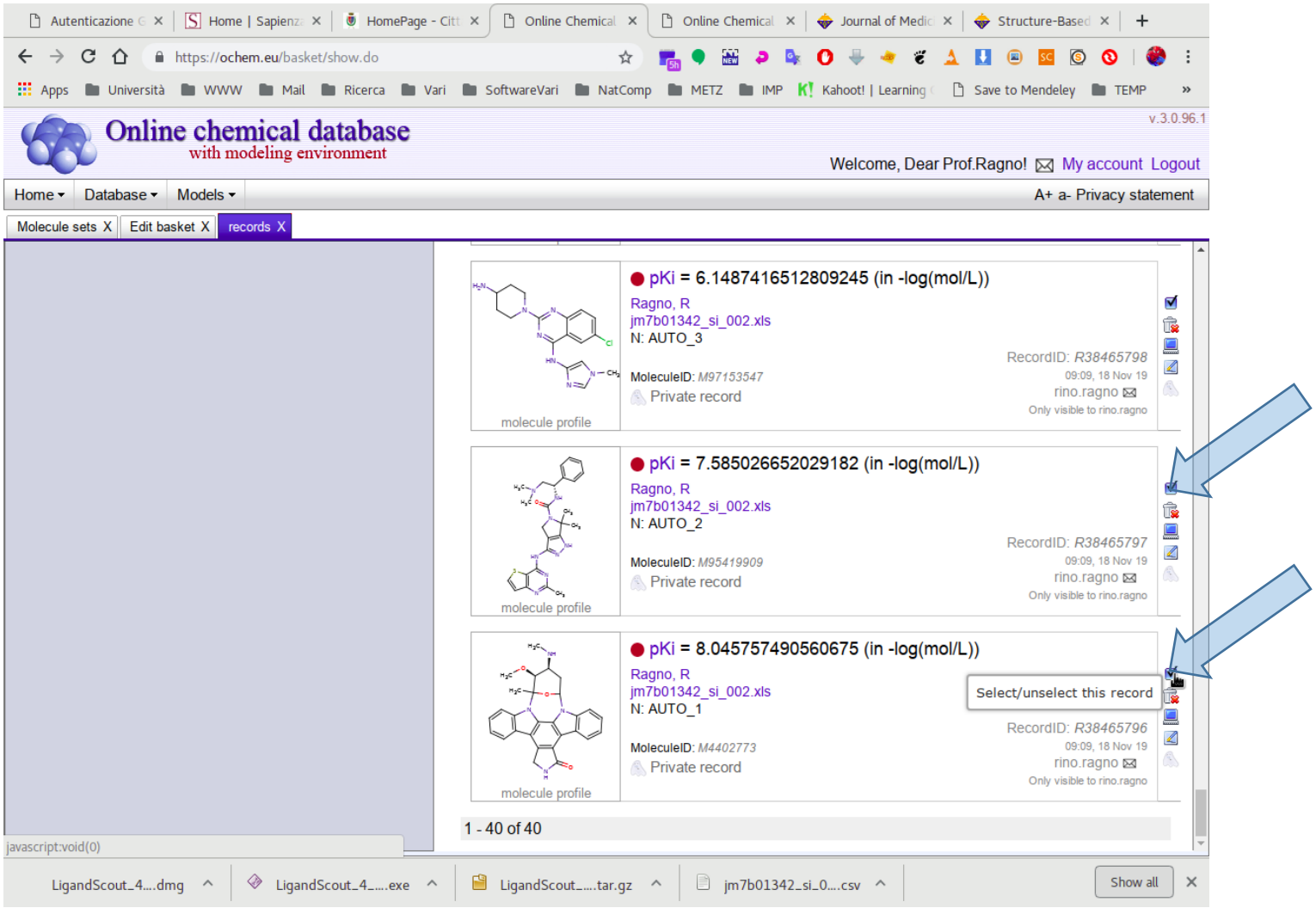

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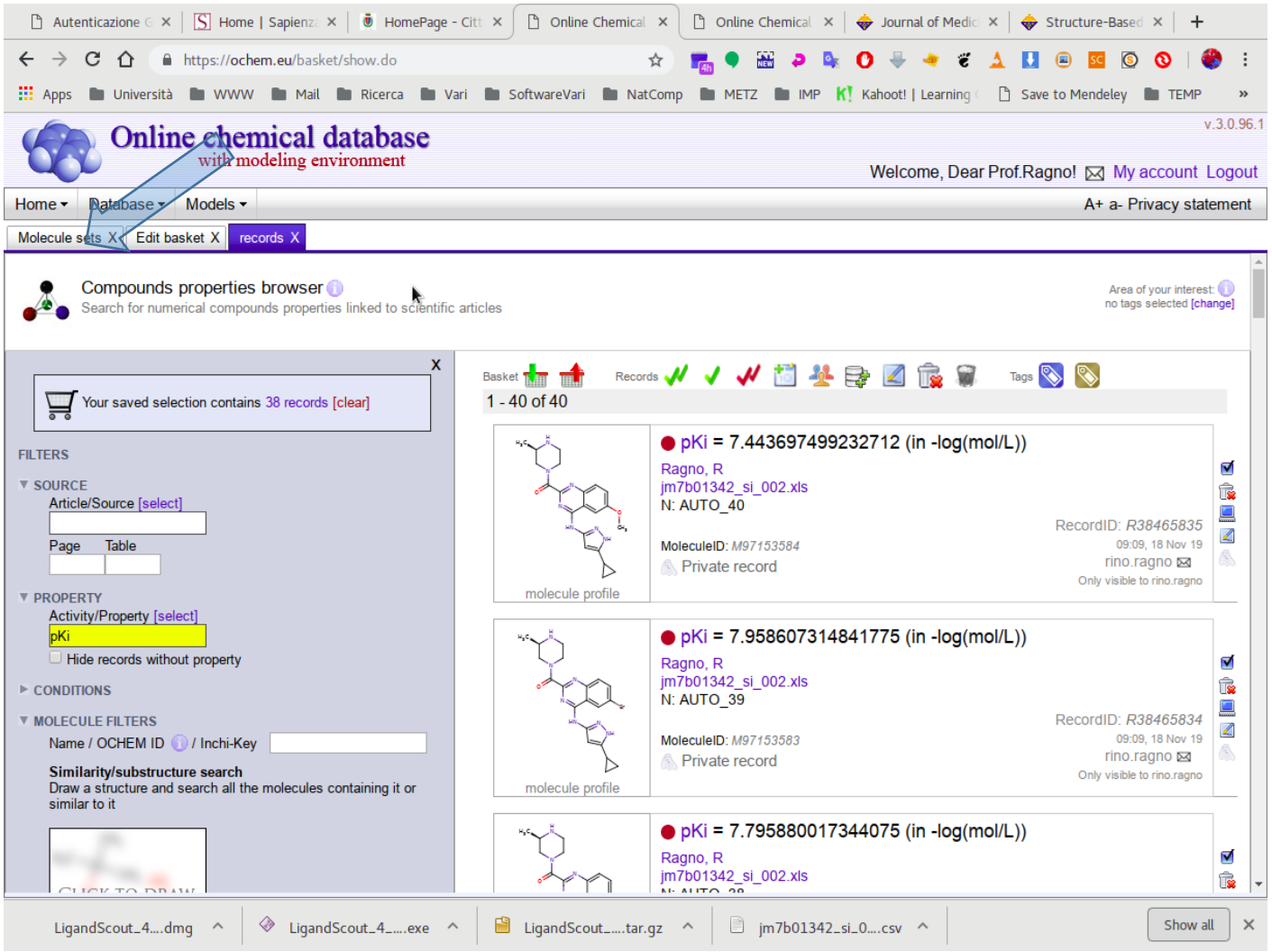

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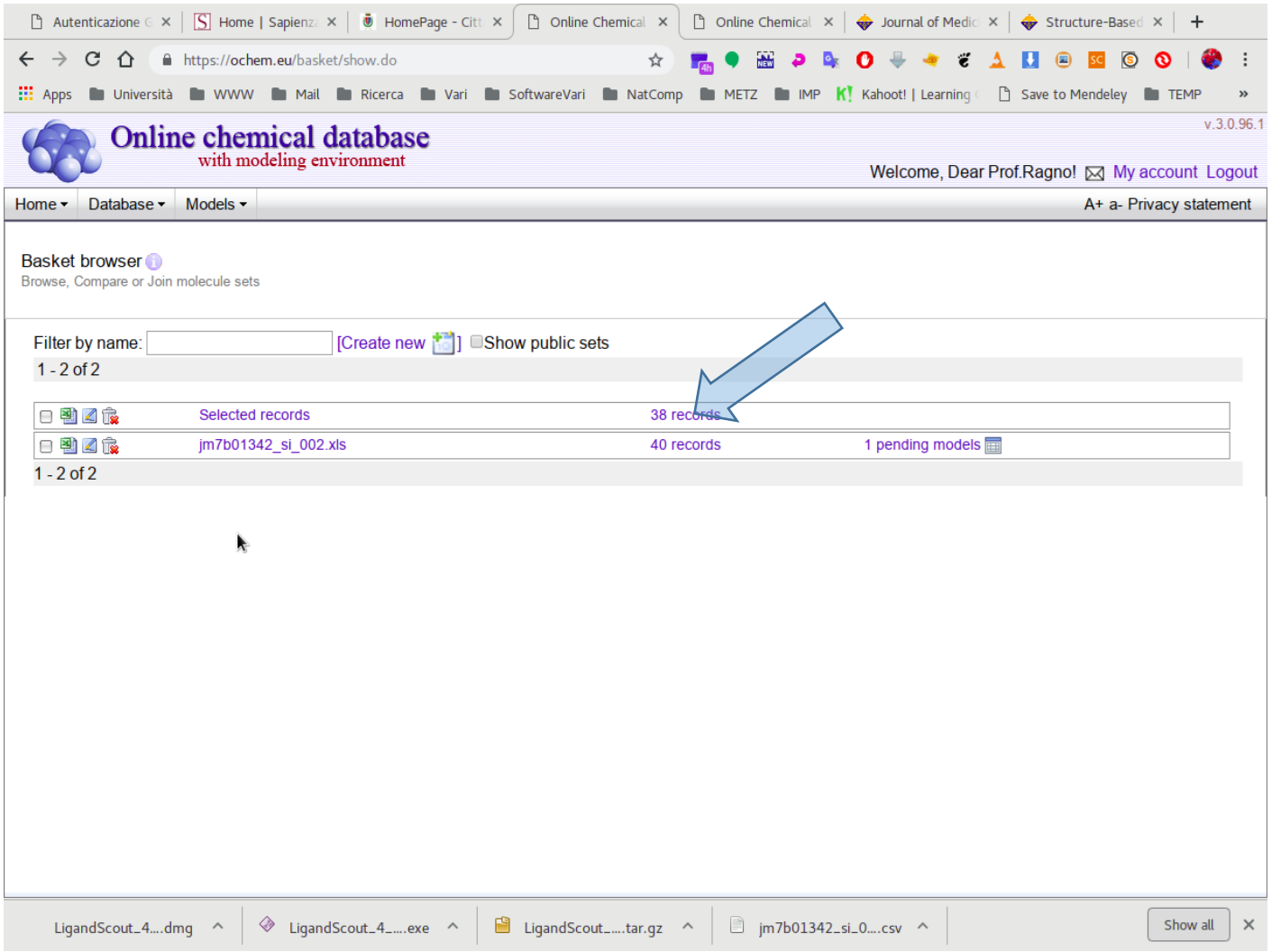

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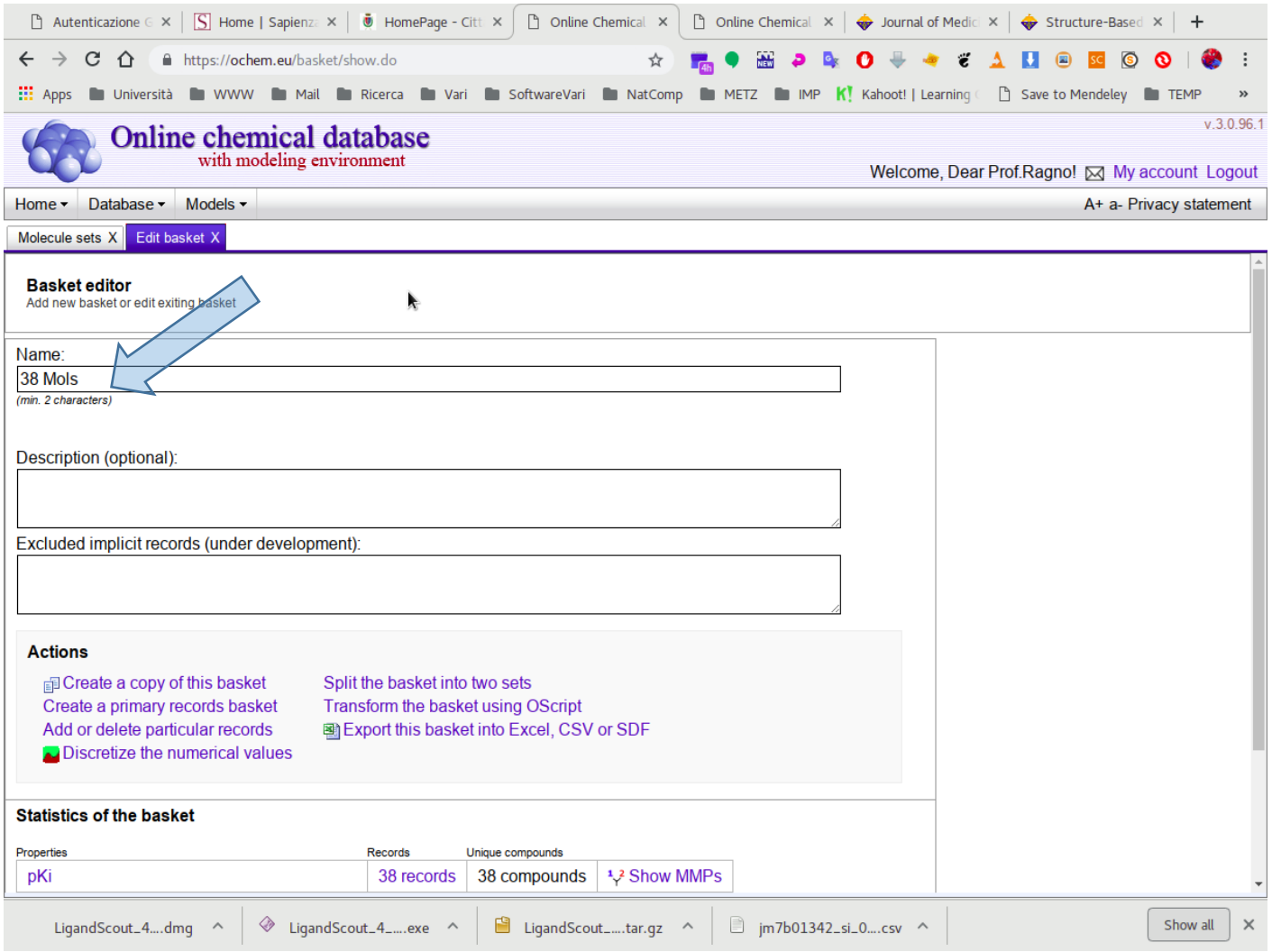

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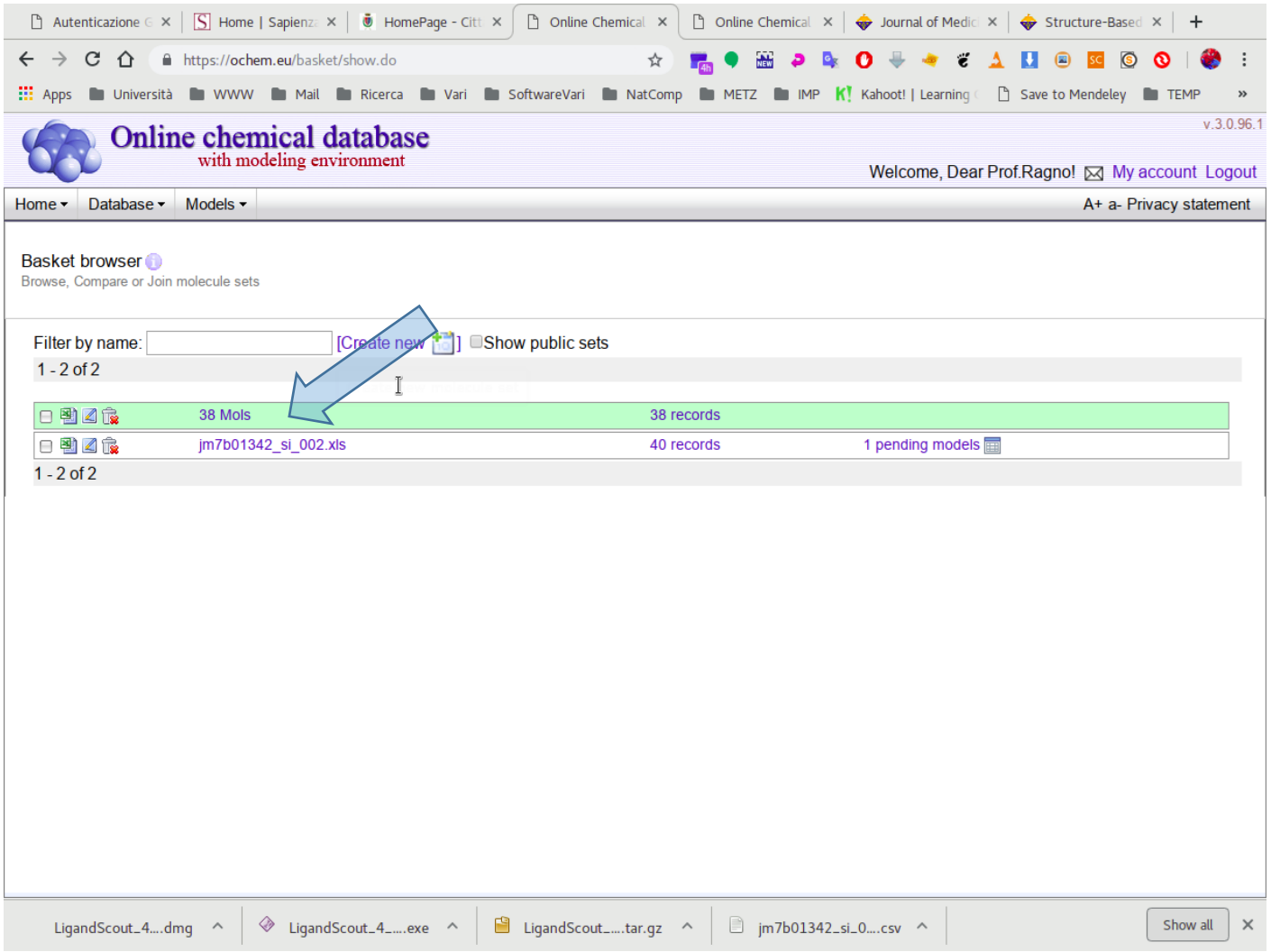

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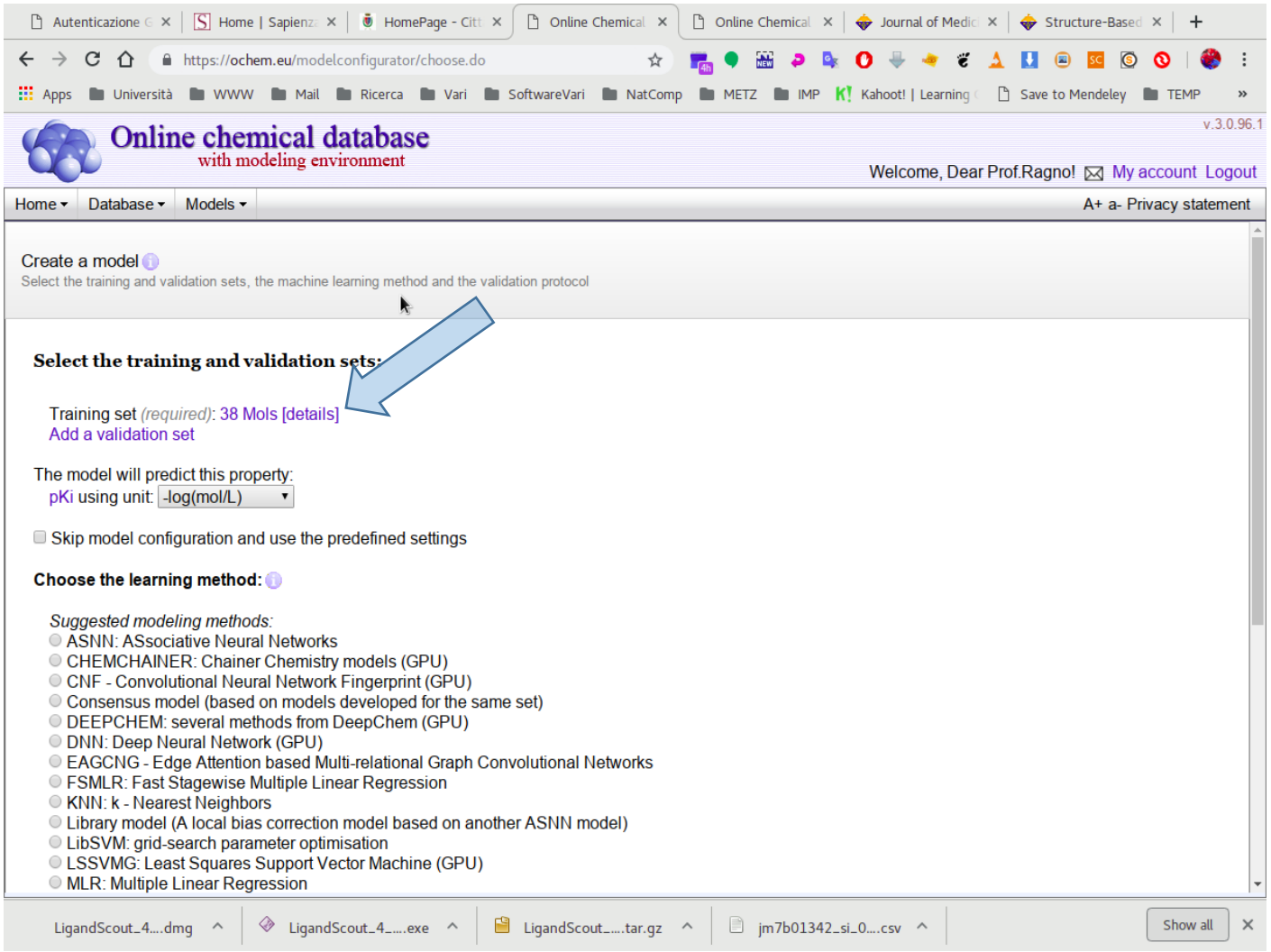

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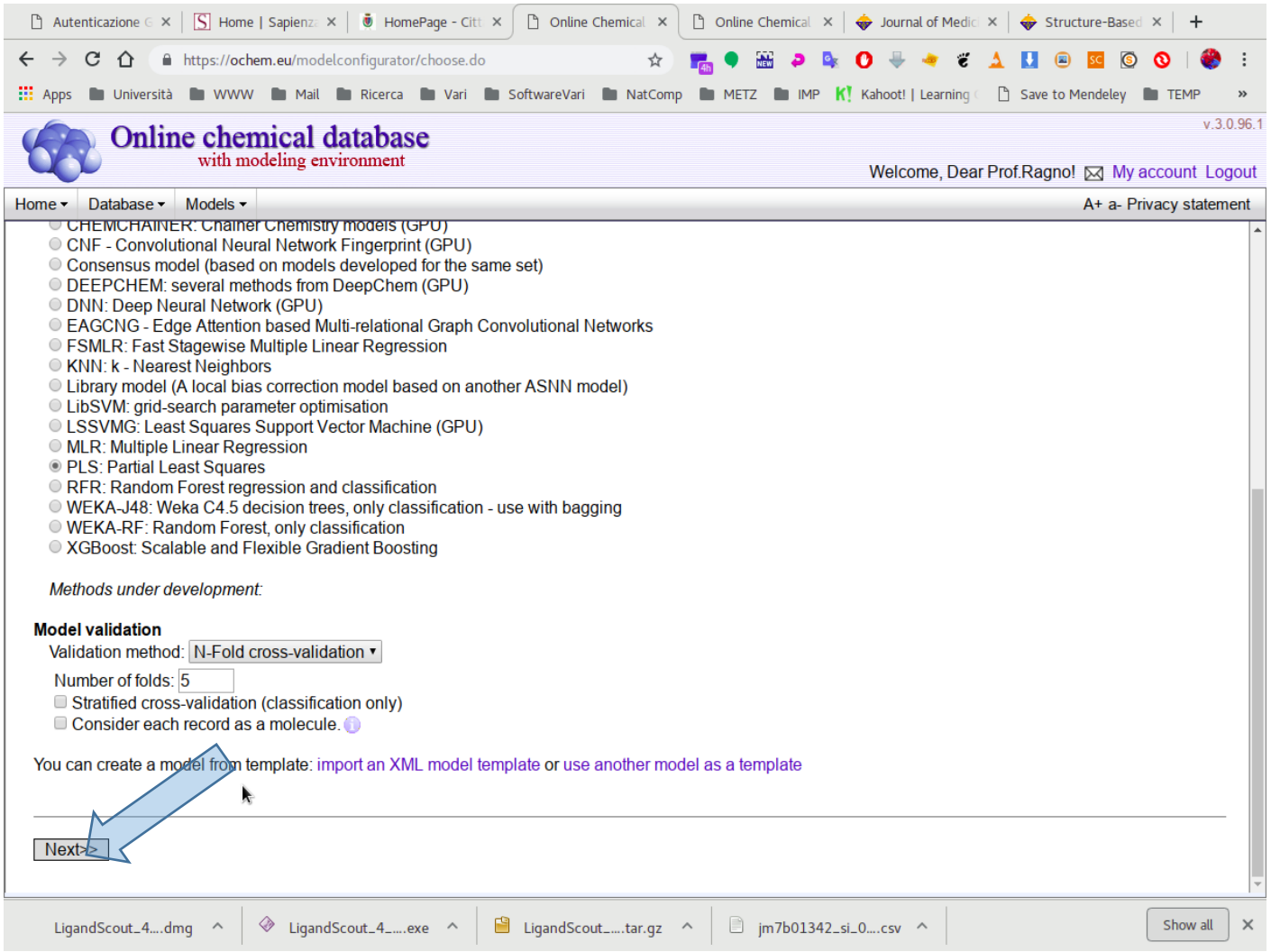

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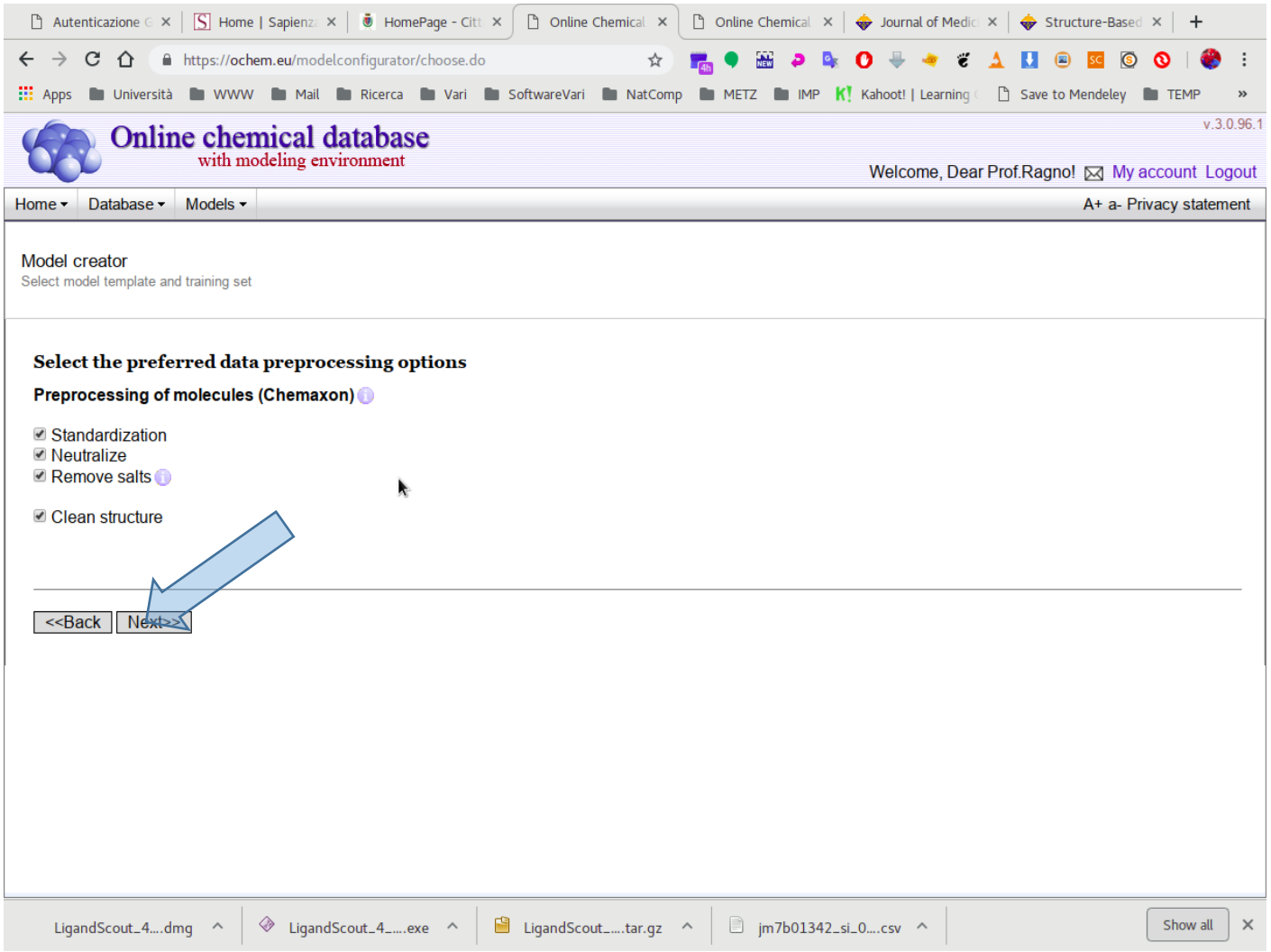

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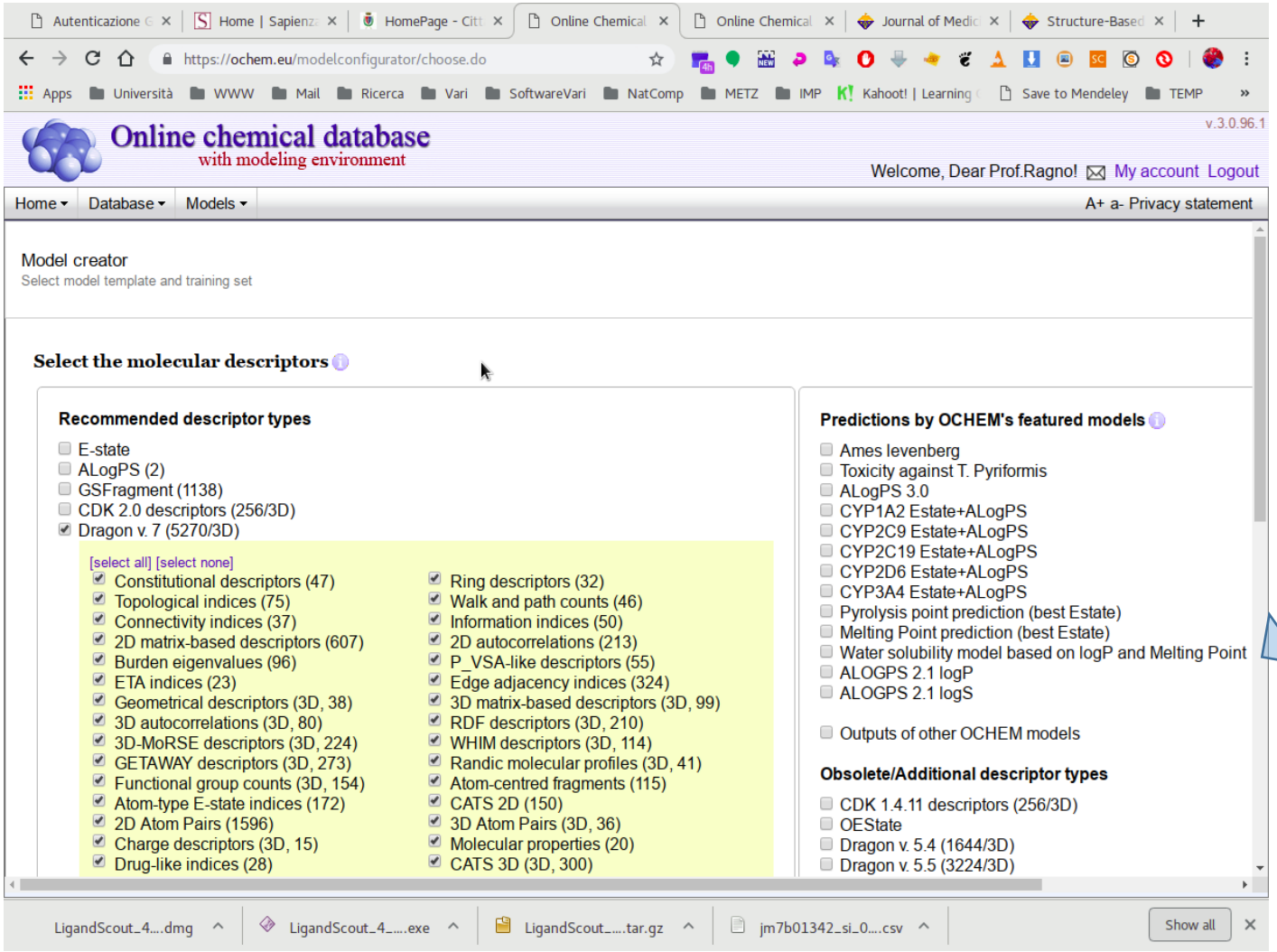

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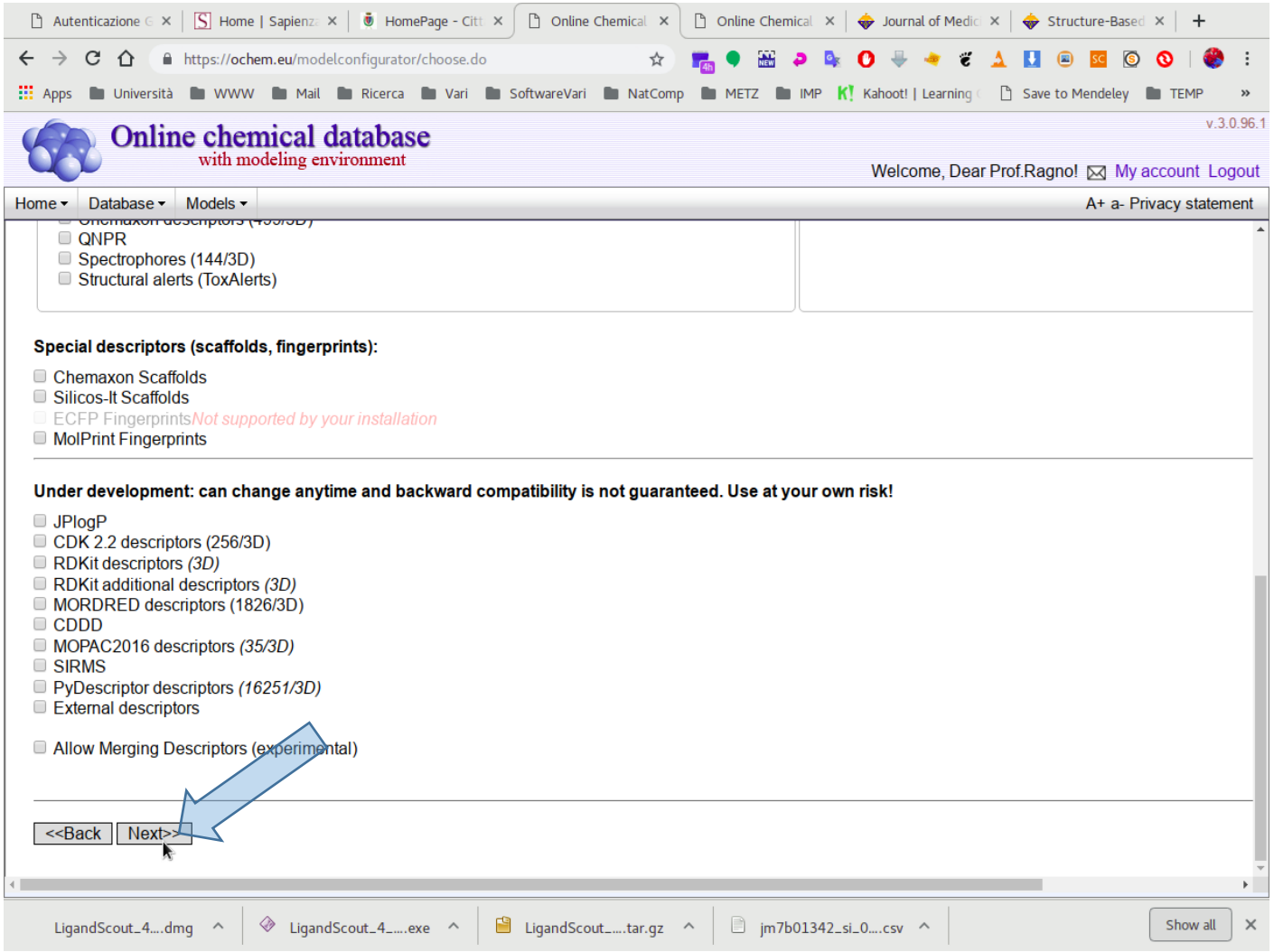

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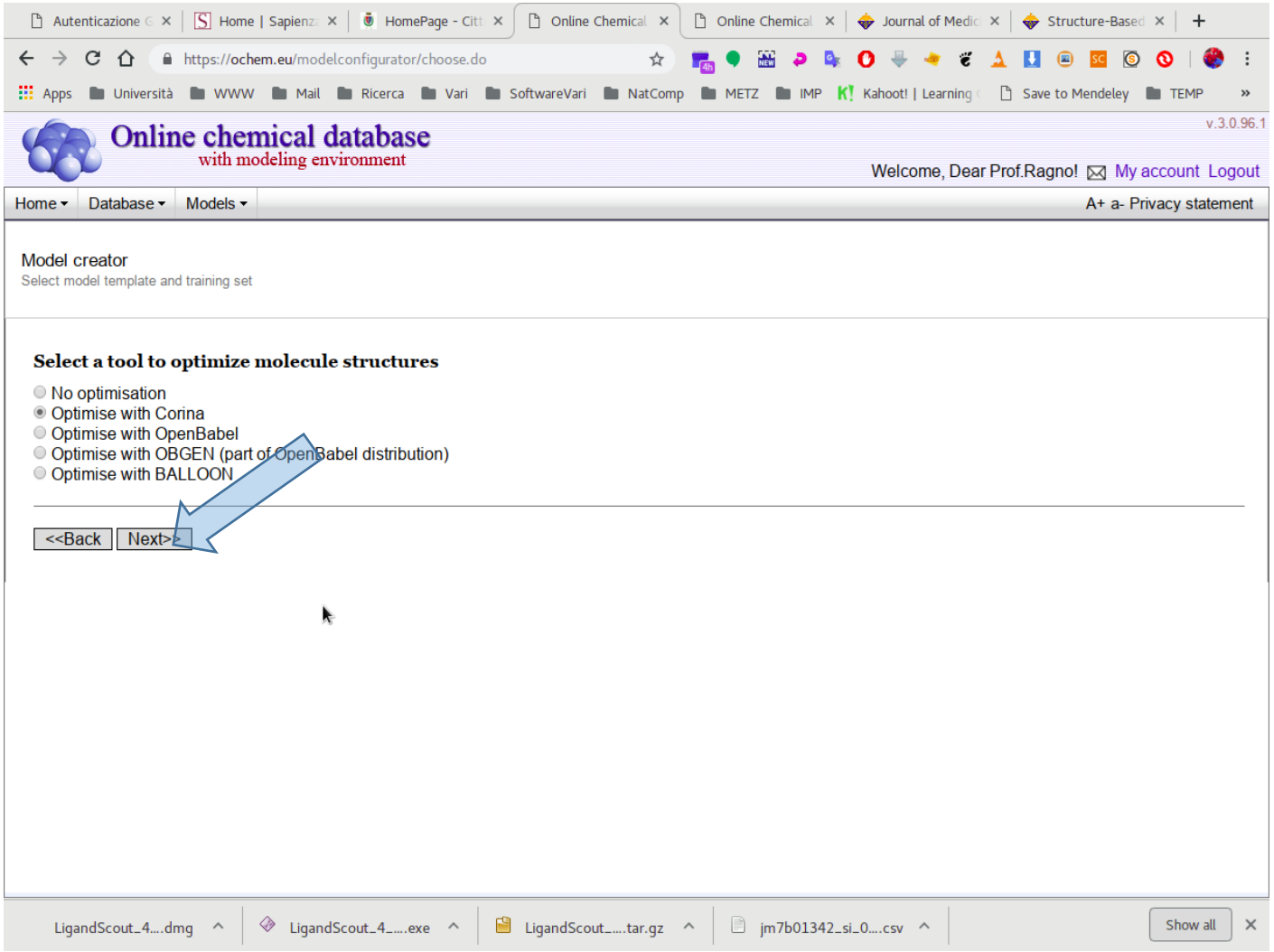

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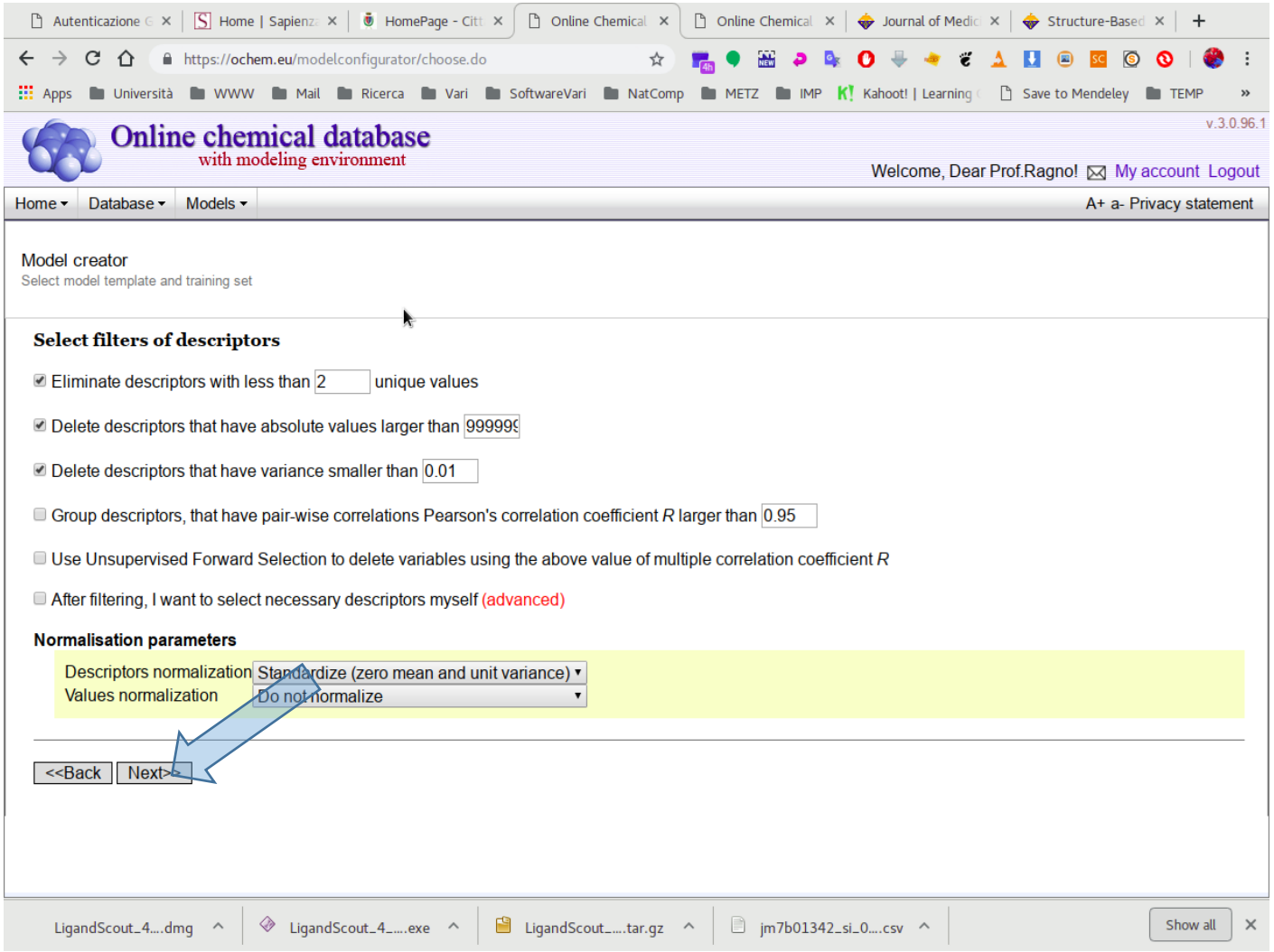

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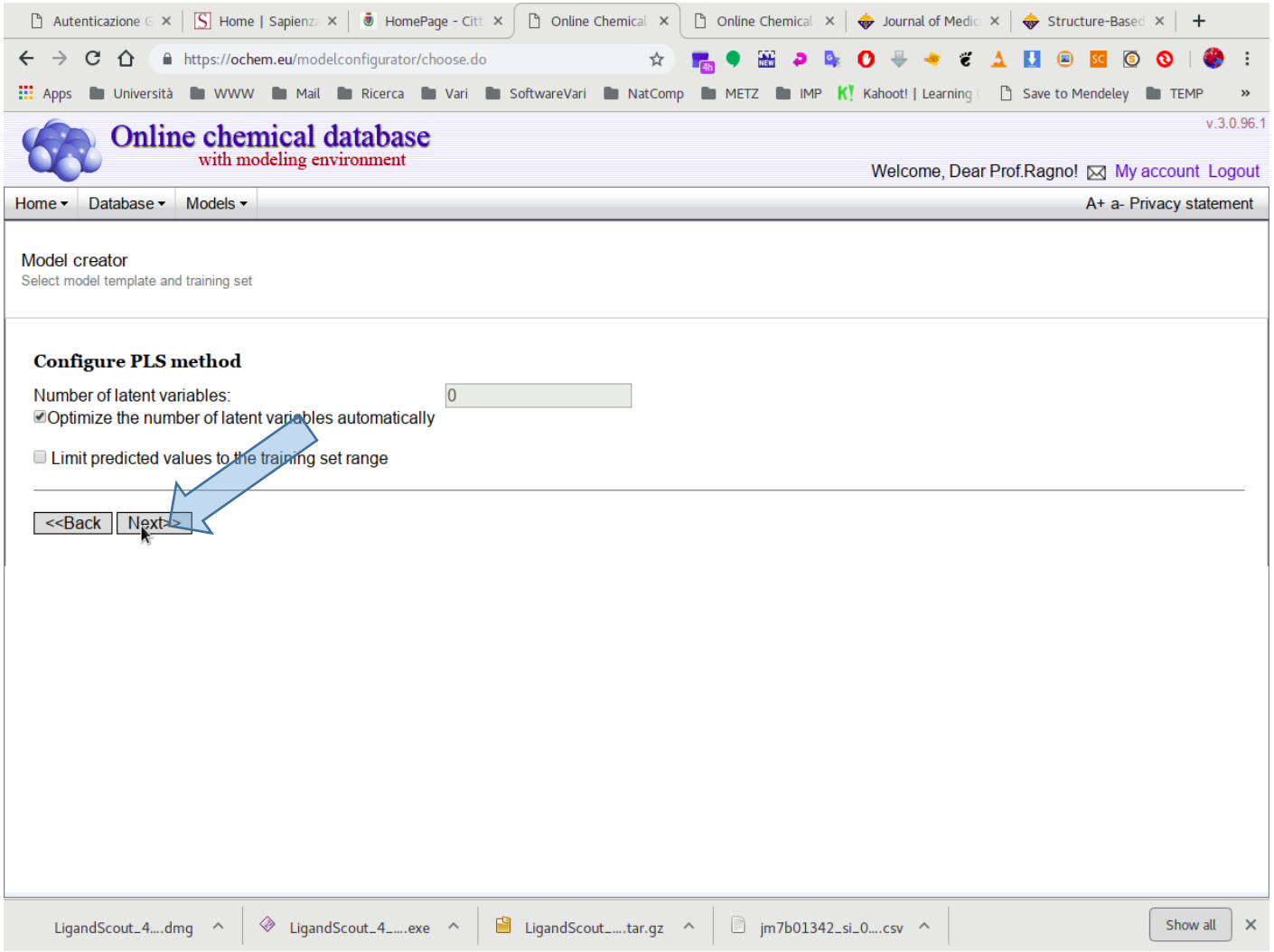

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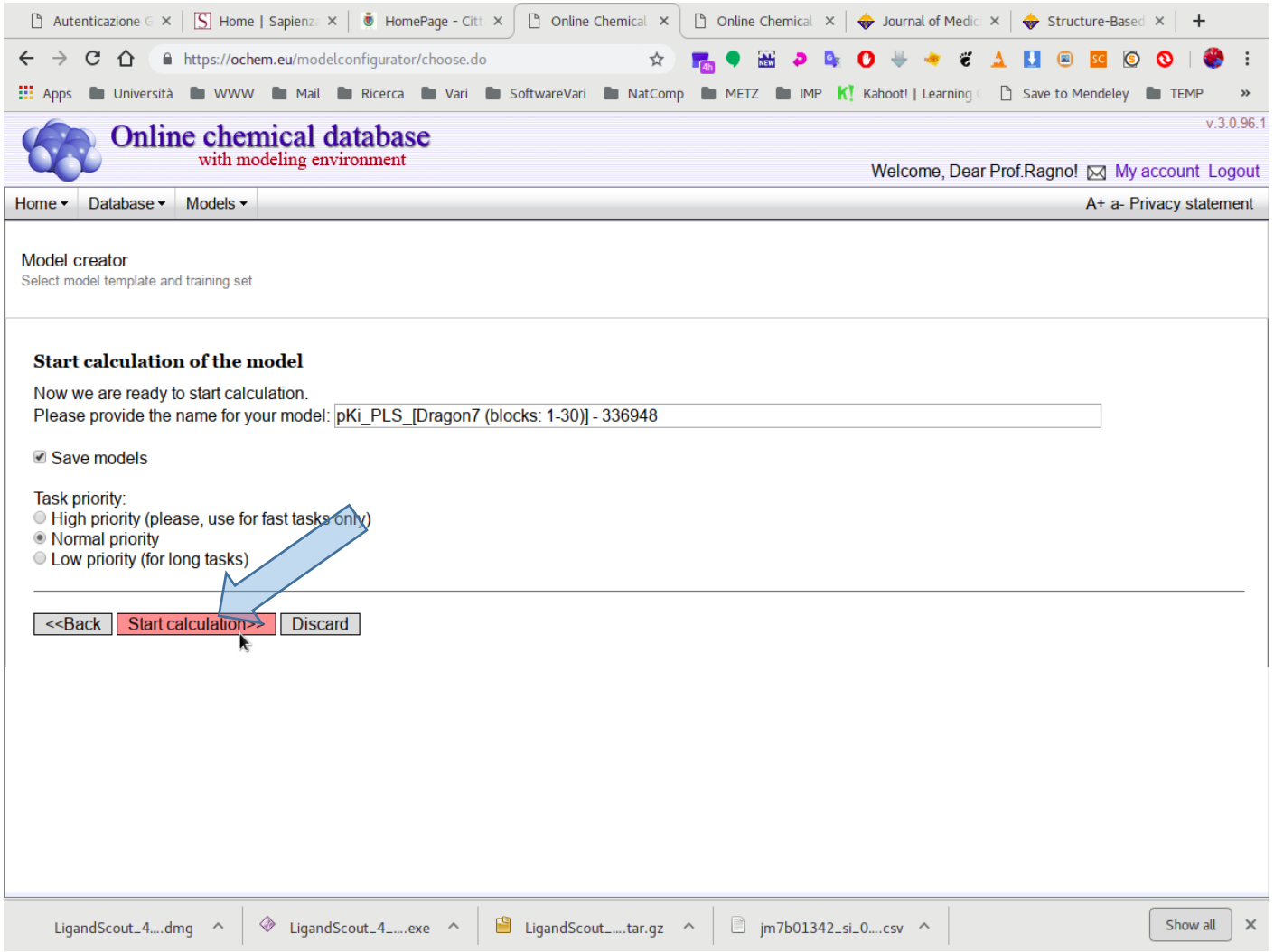
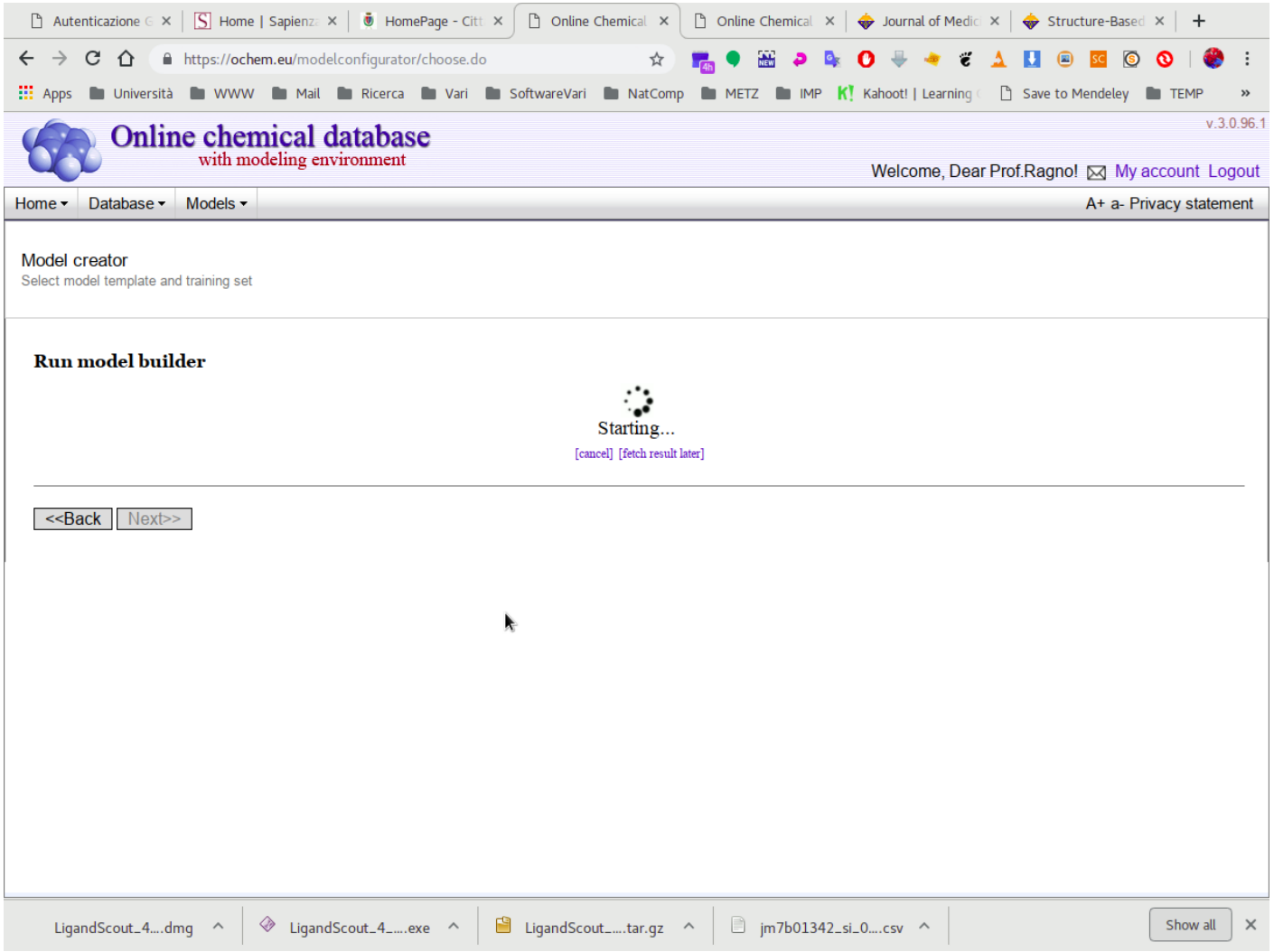


# Preparing the dataset



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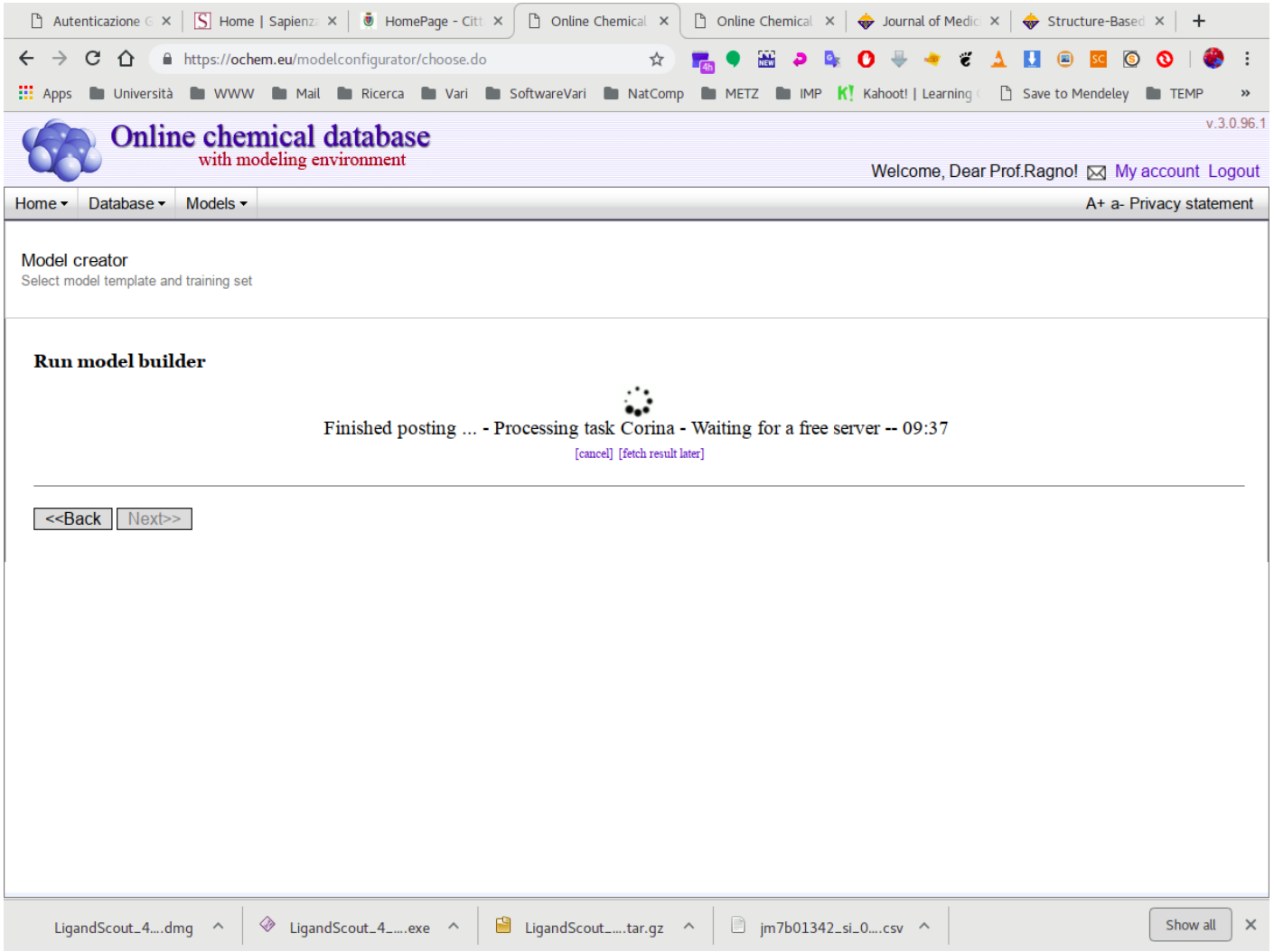

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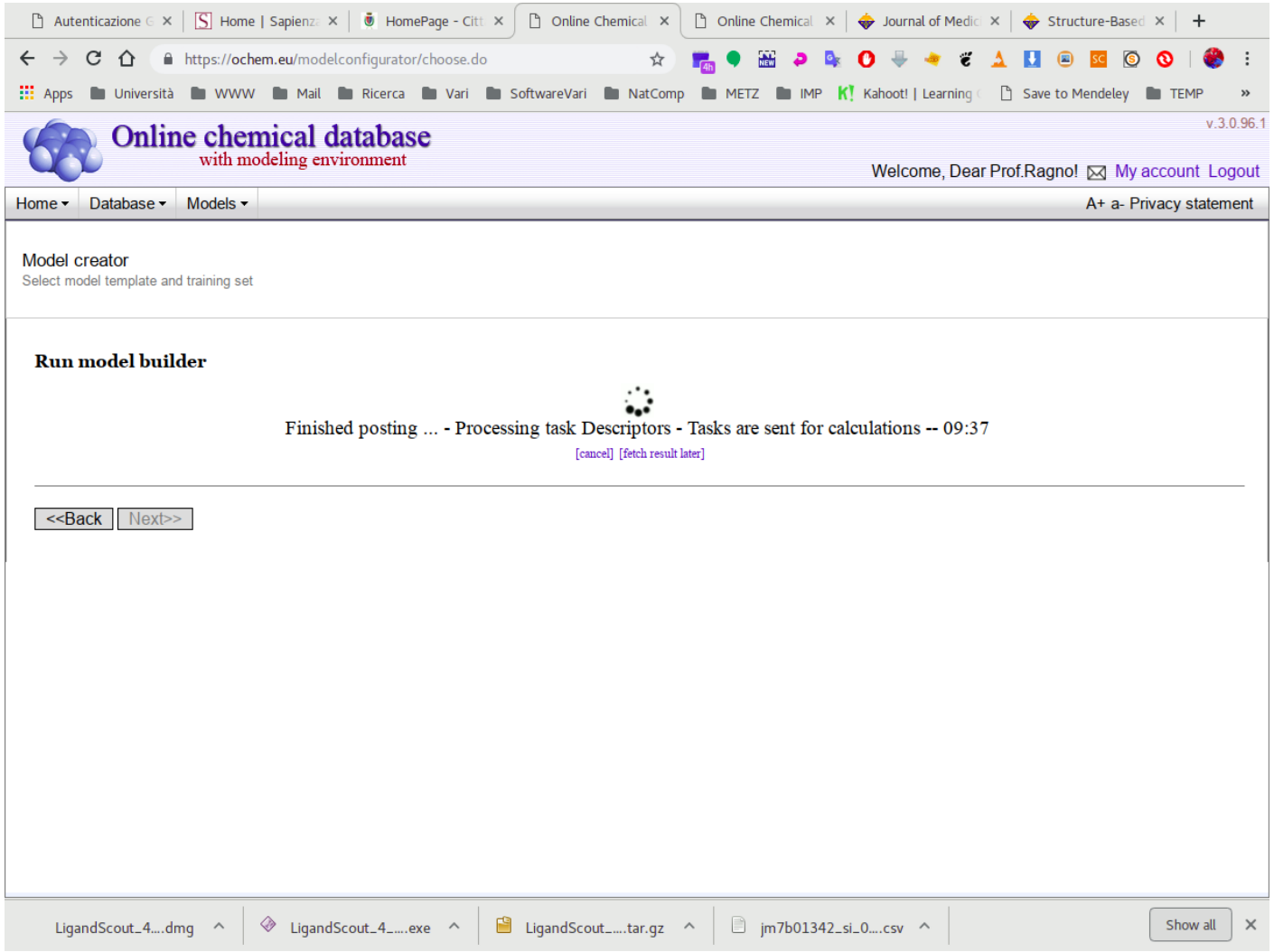

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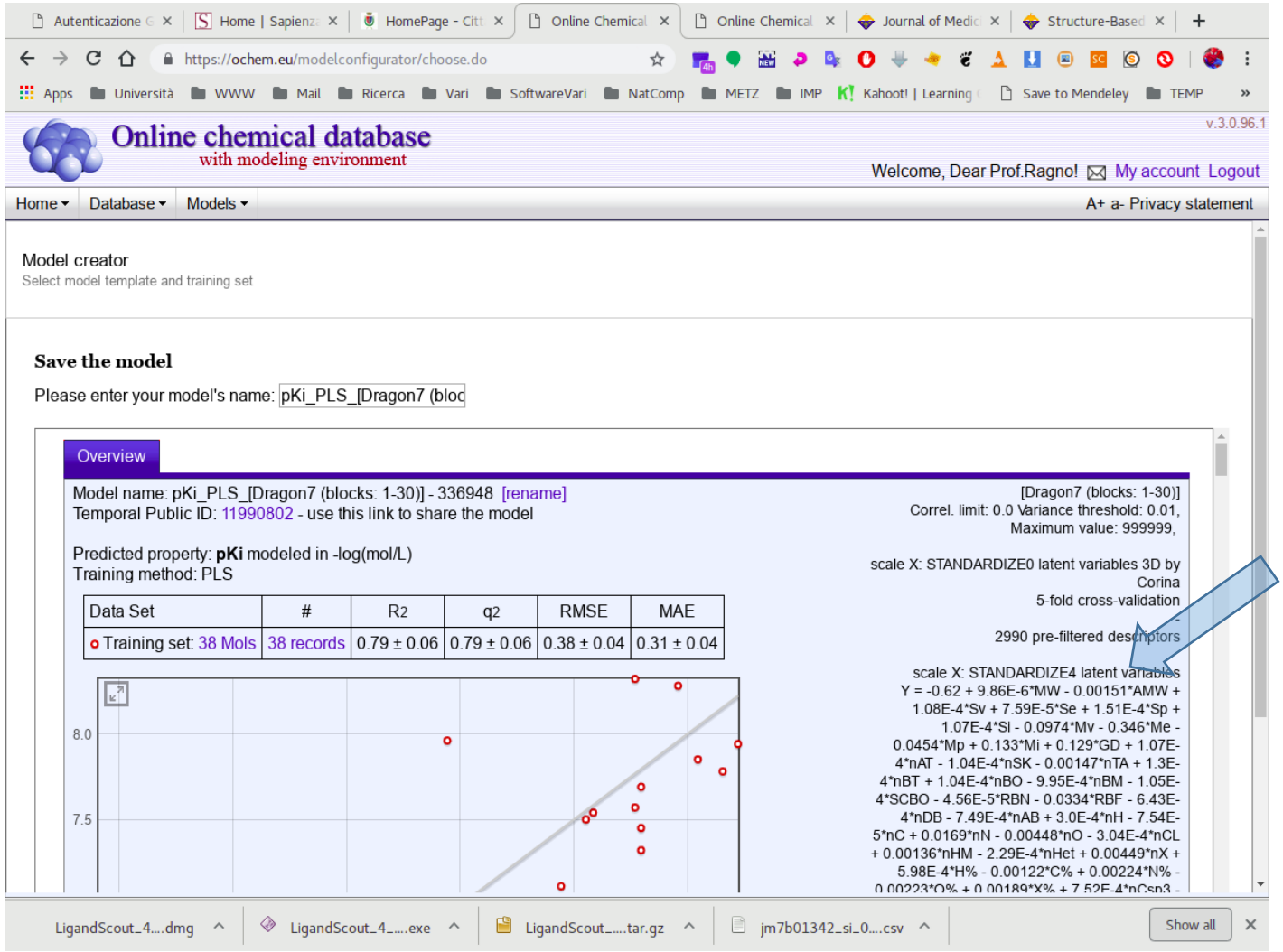

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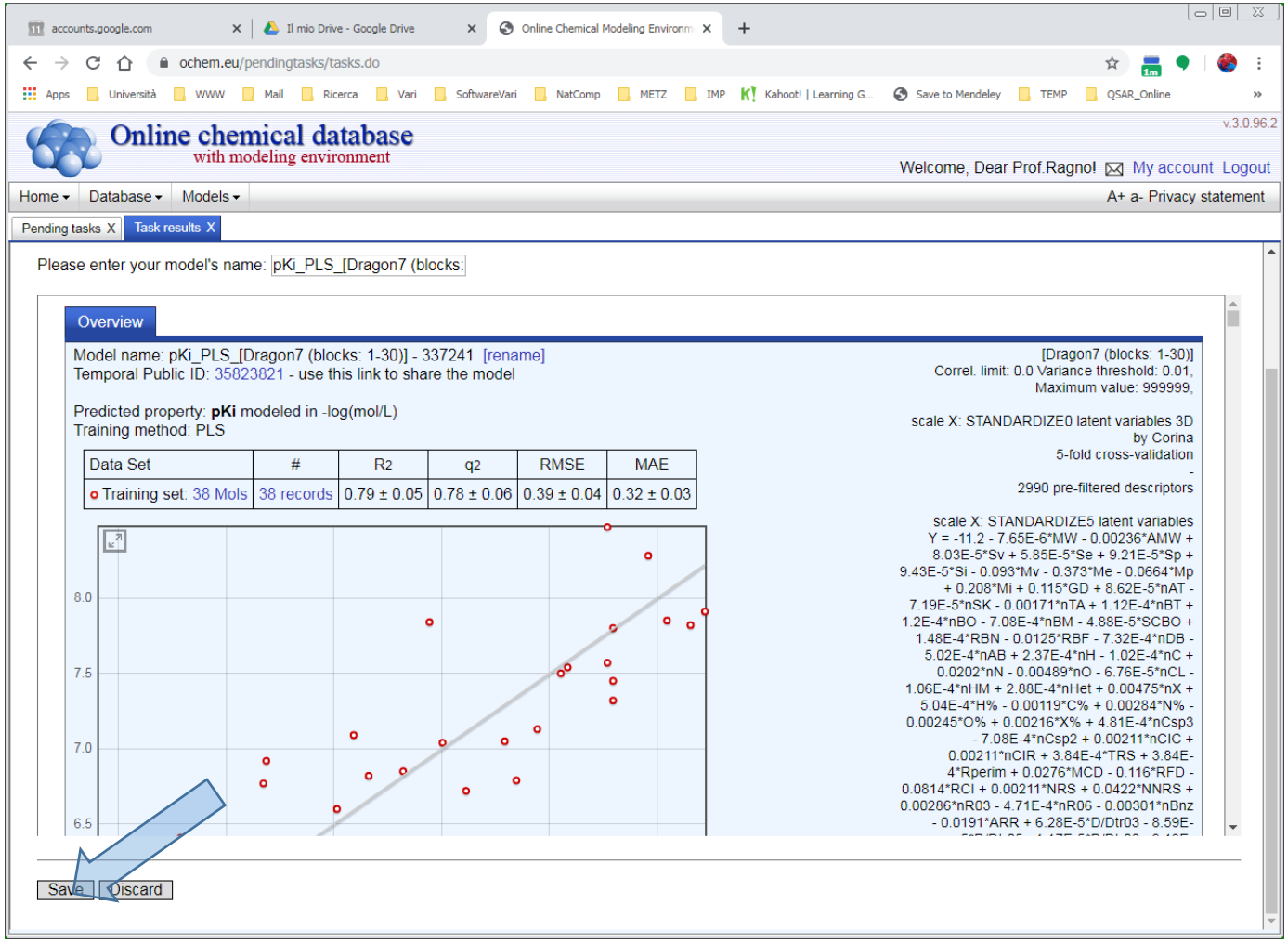

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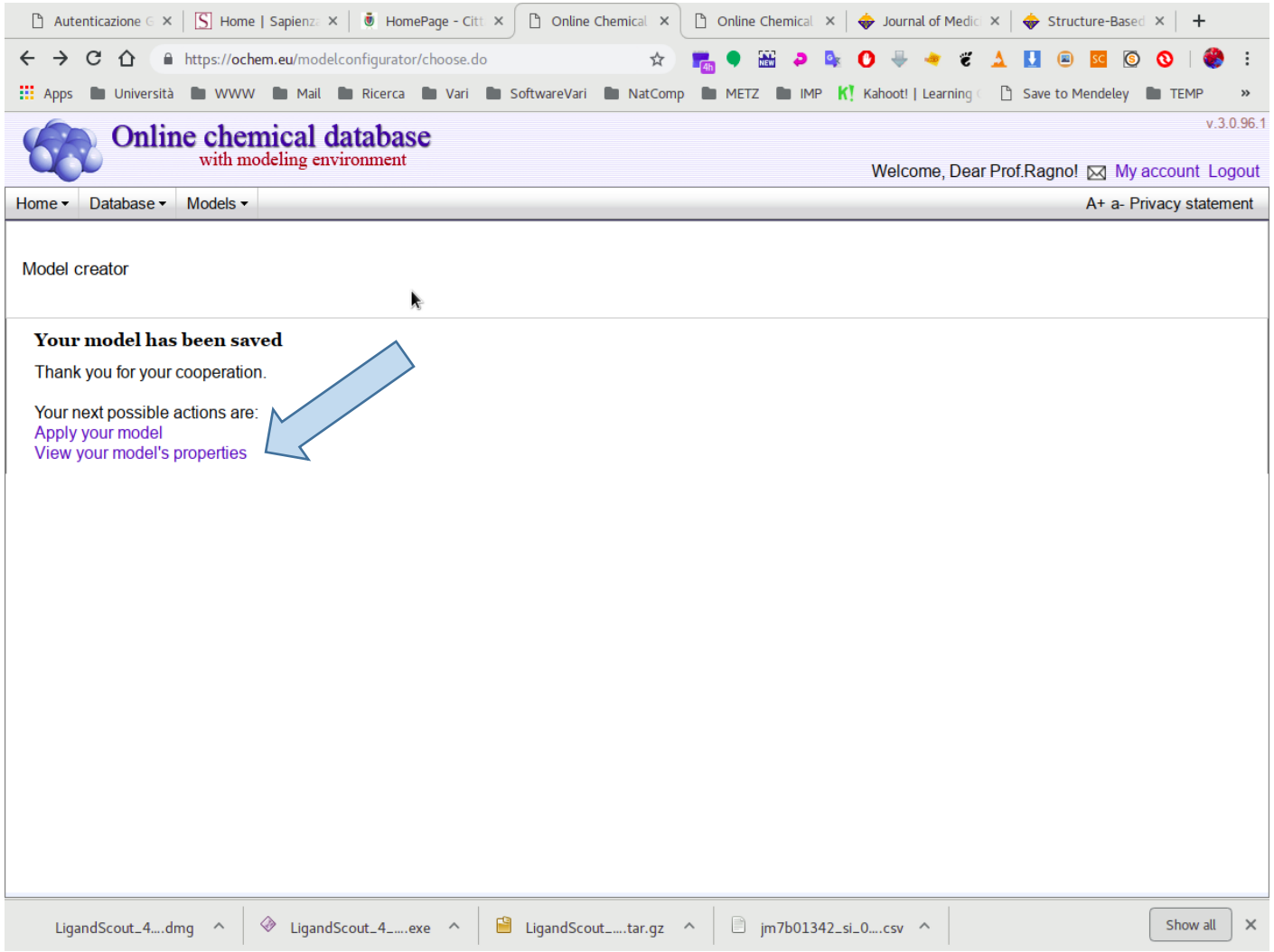

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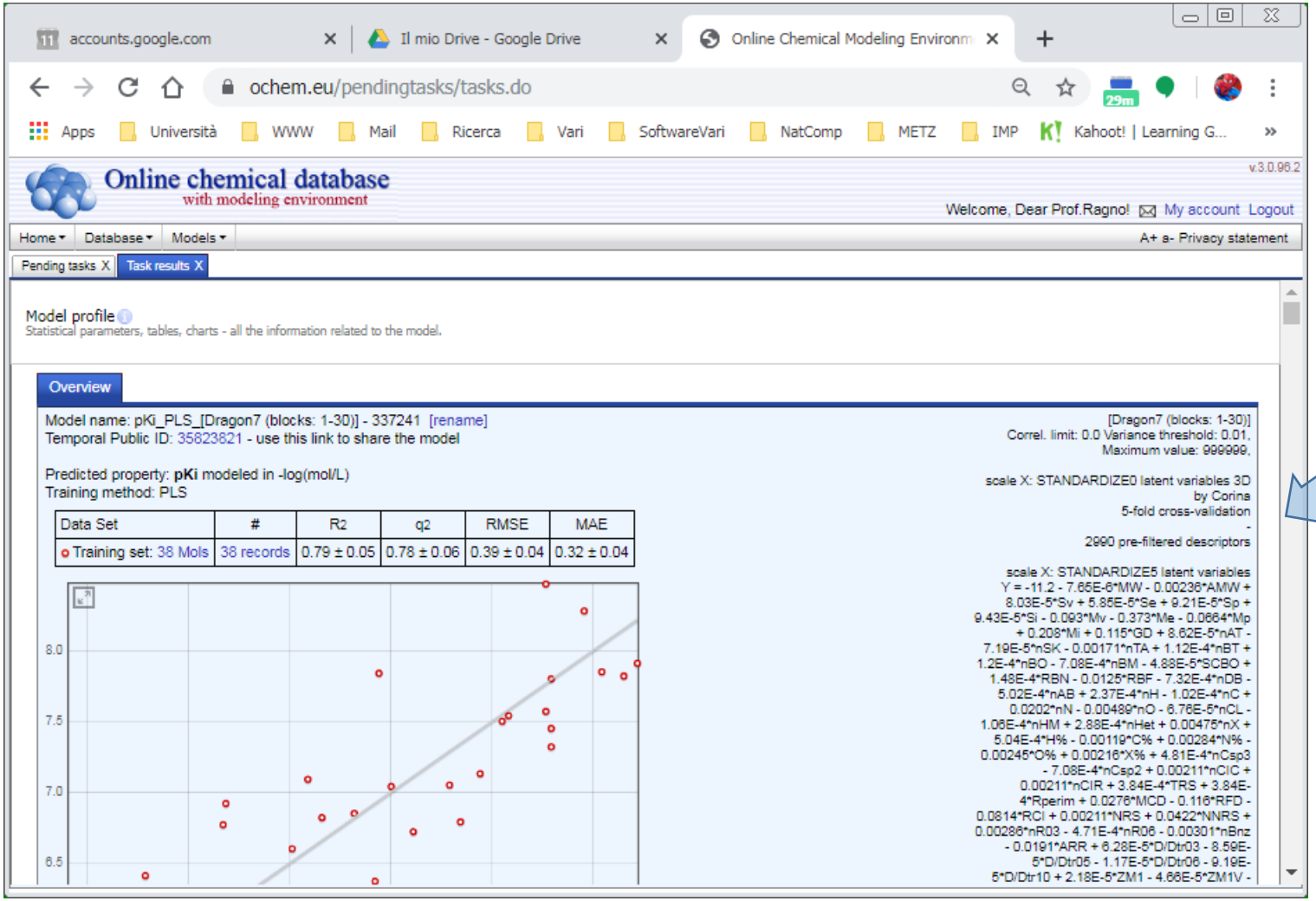

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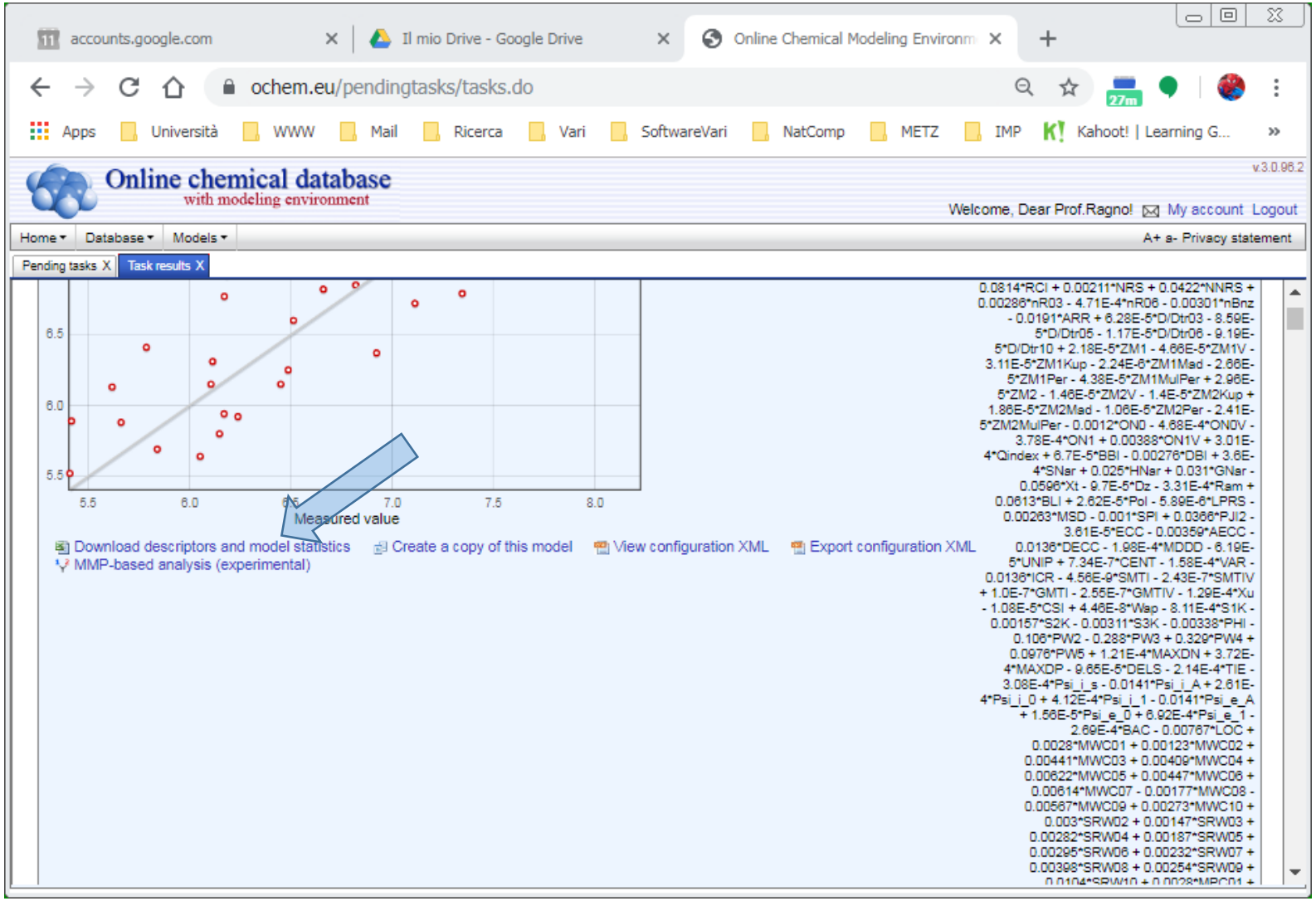

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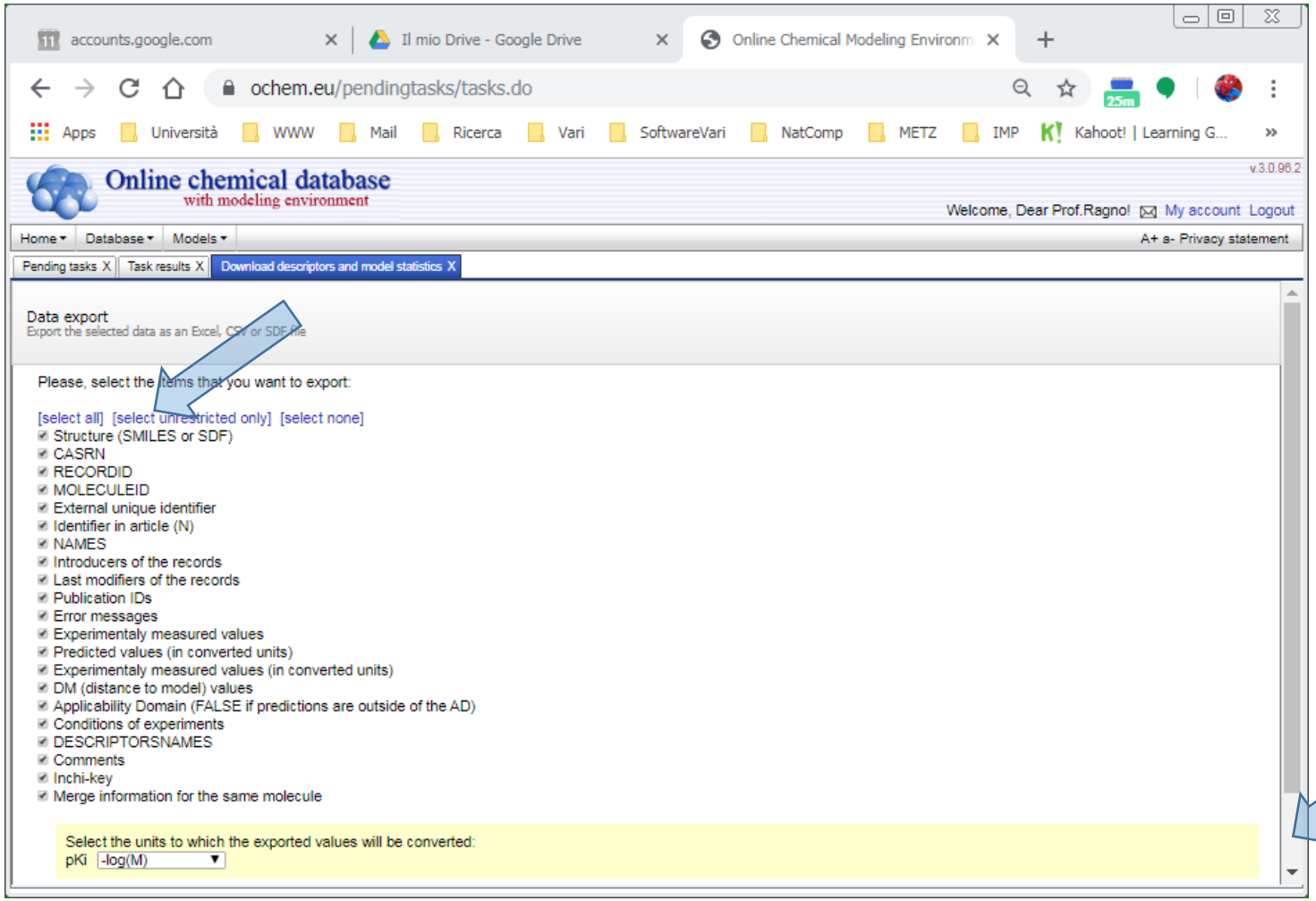

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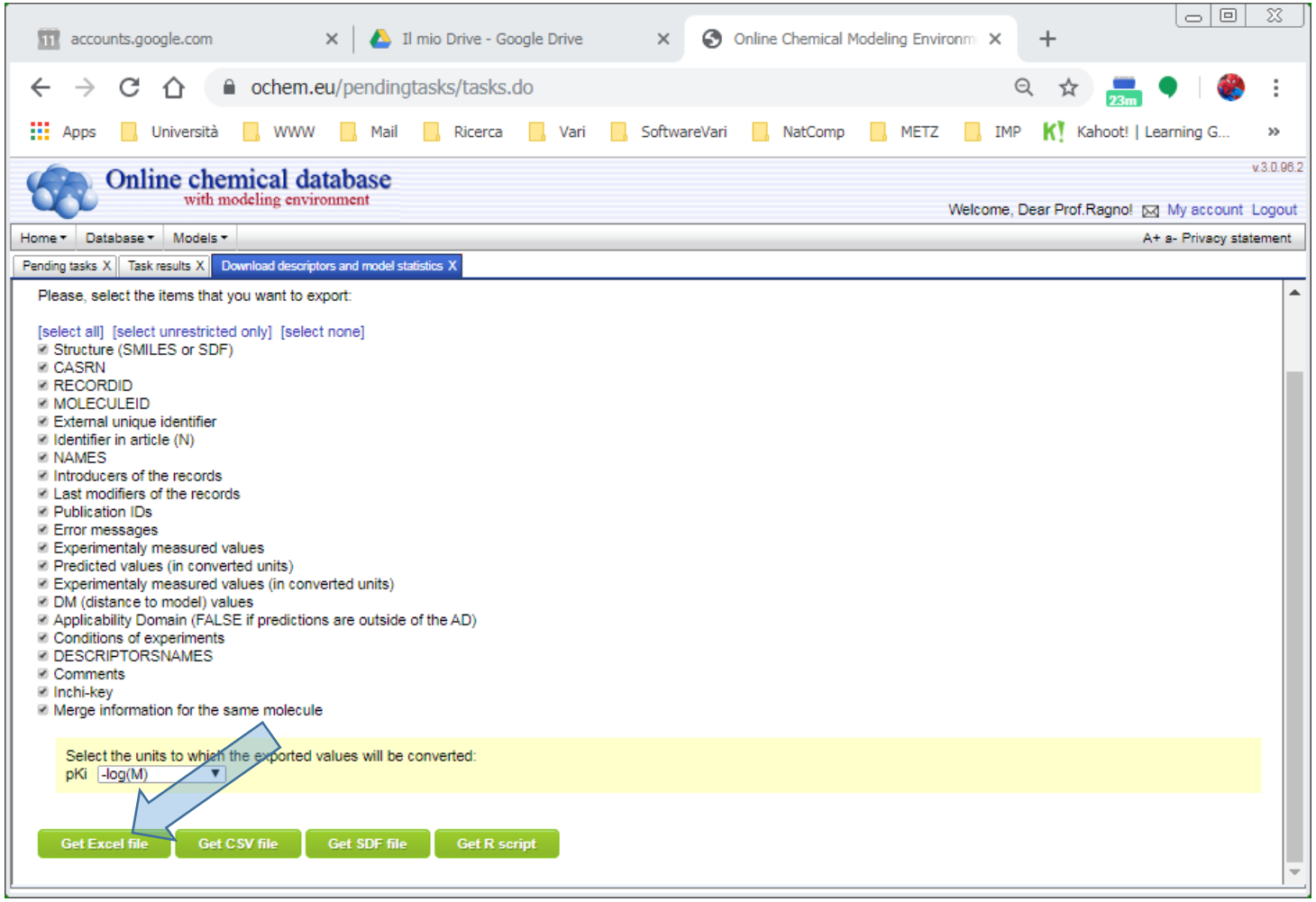

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