Pharmaceutical Chemistry

QSAR through the OCHEM portal

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Introduction

J Comput Aided Mol Des (2011) 25:533–554
DOI 10.1007/s10822-011-9440-2

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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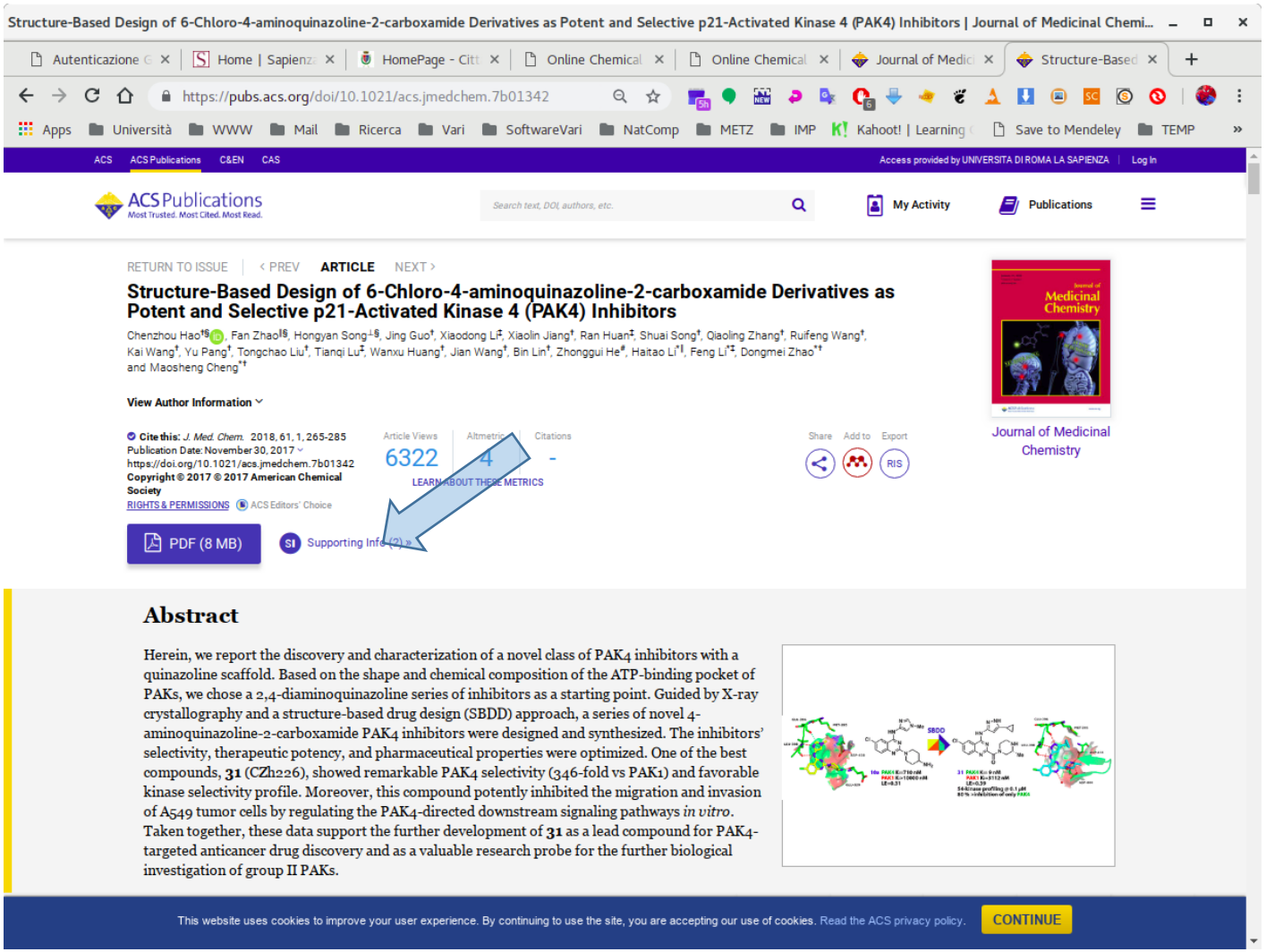
Preparing the dataset



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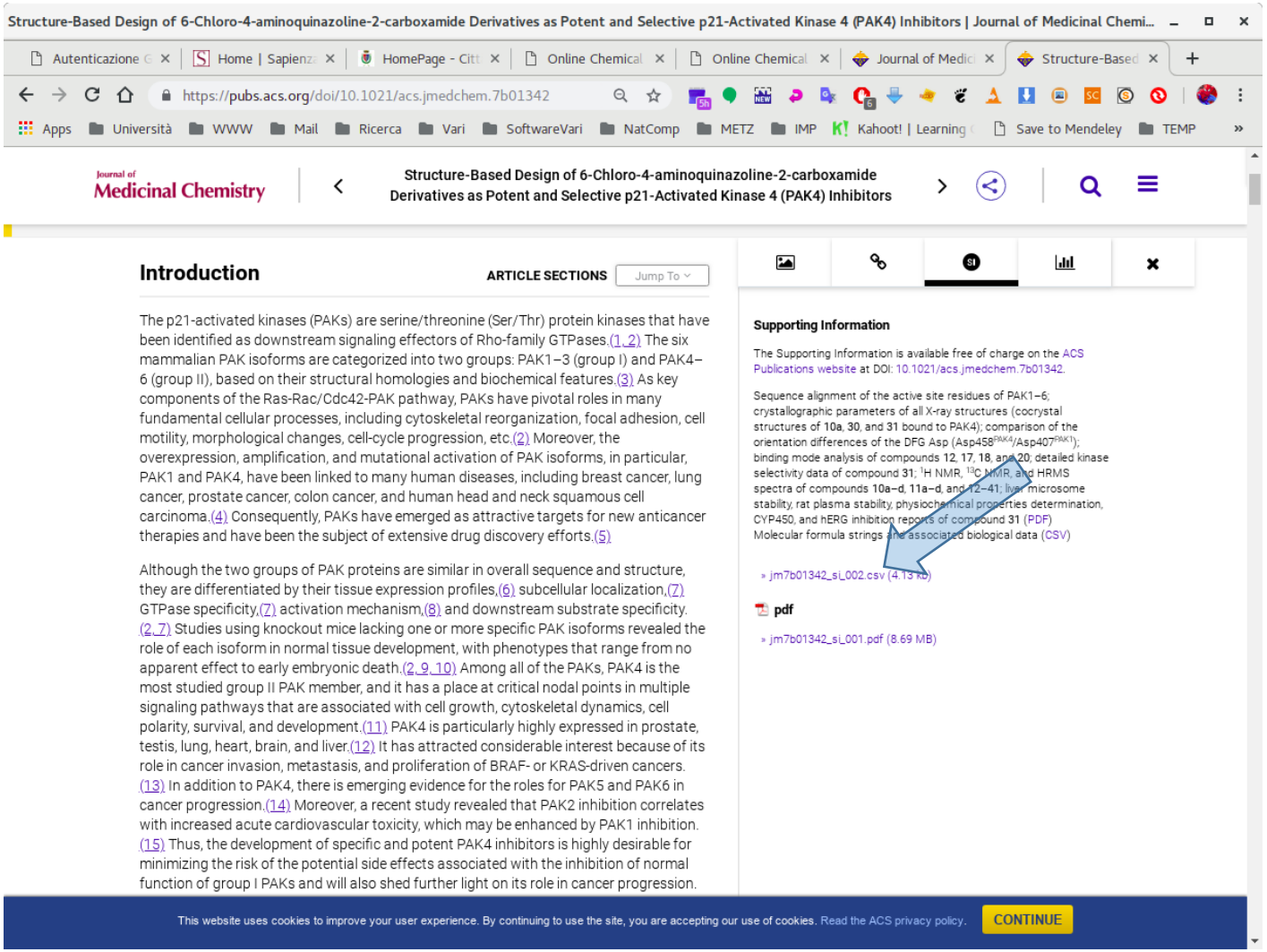

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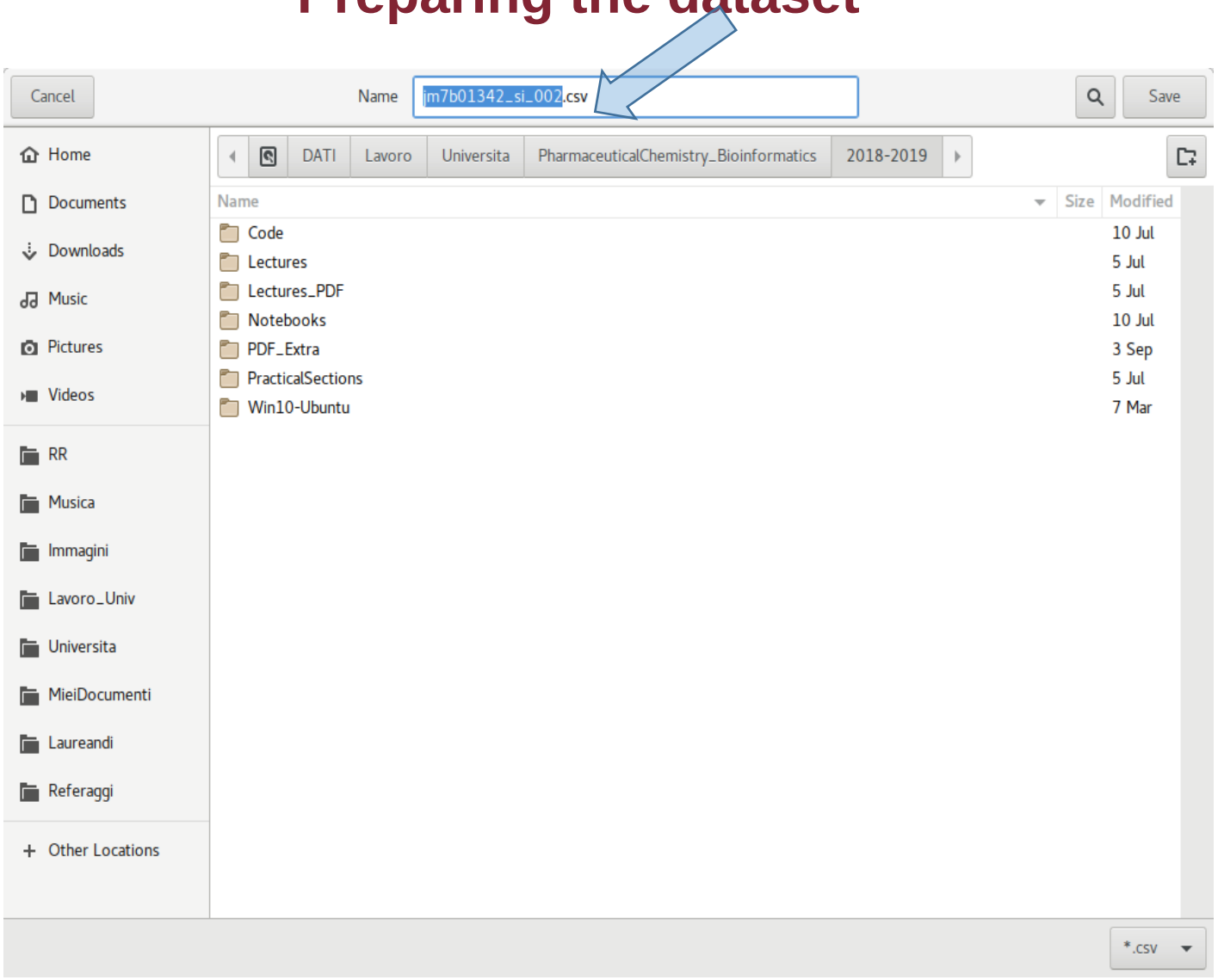

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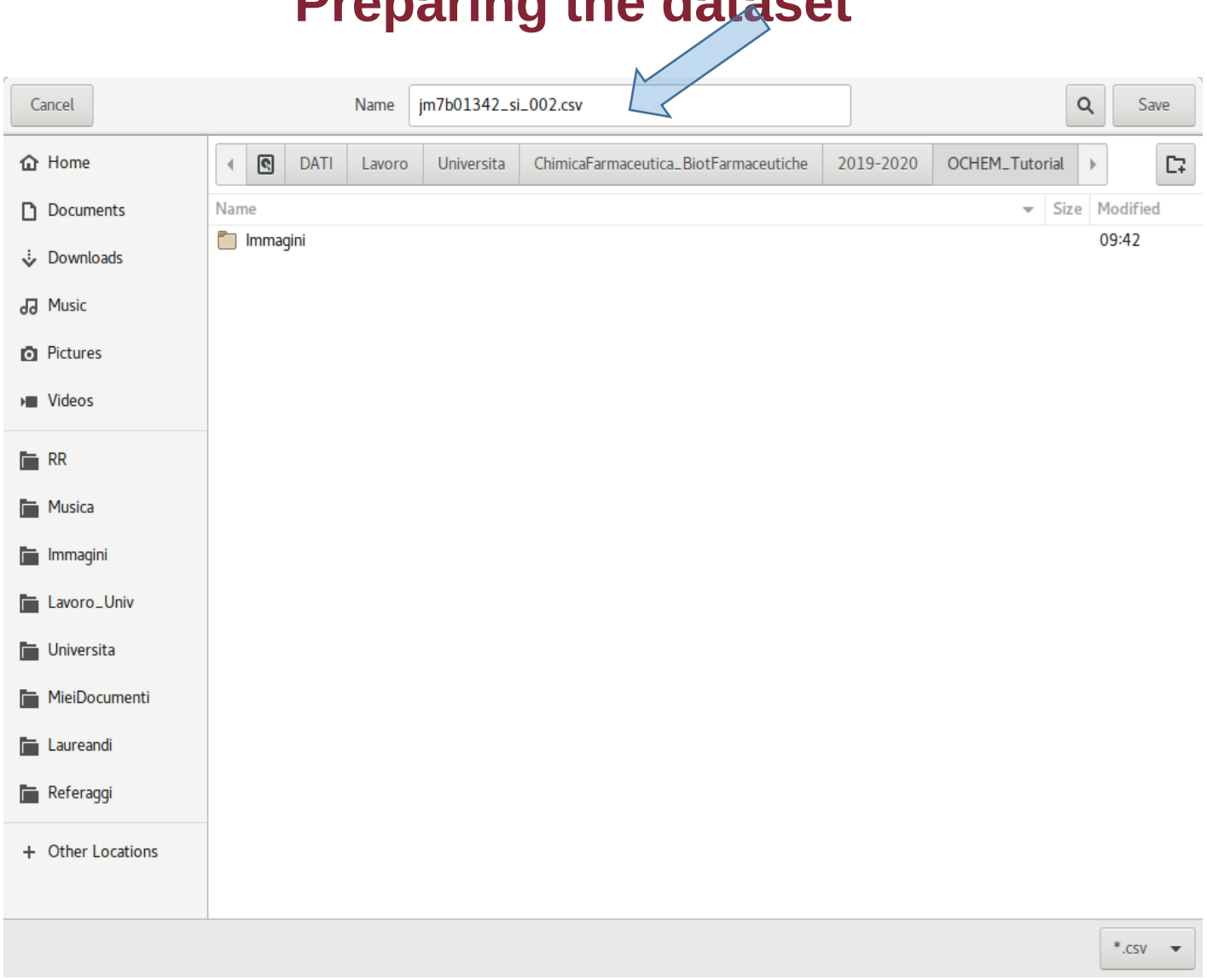

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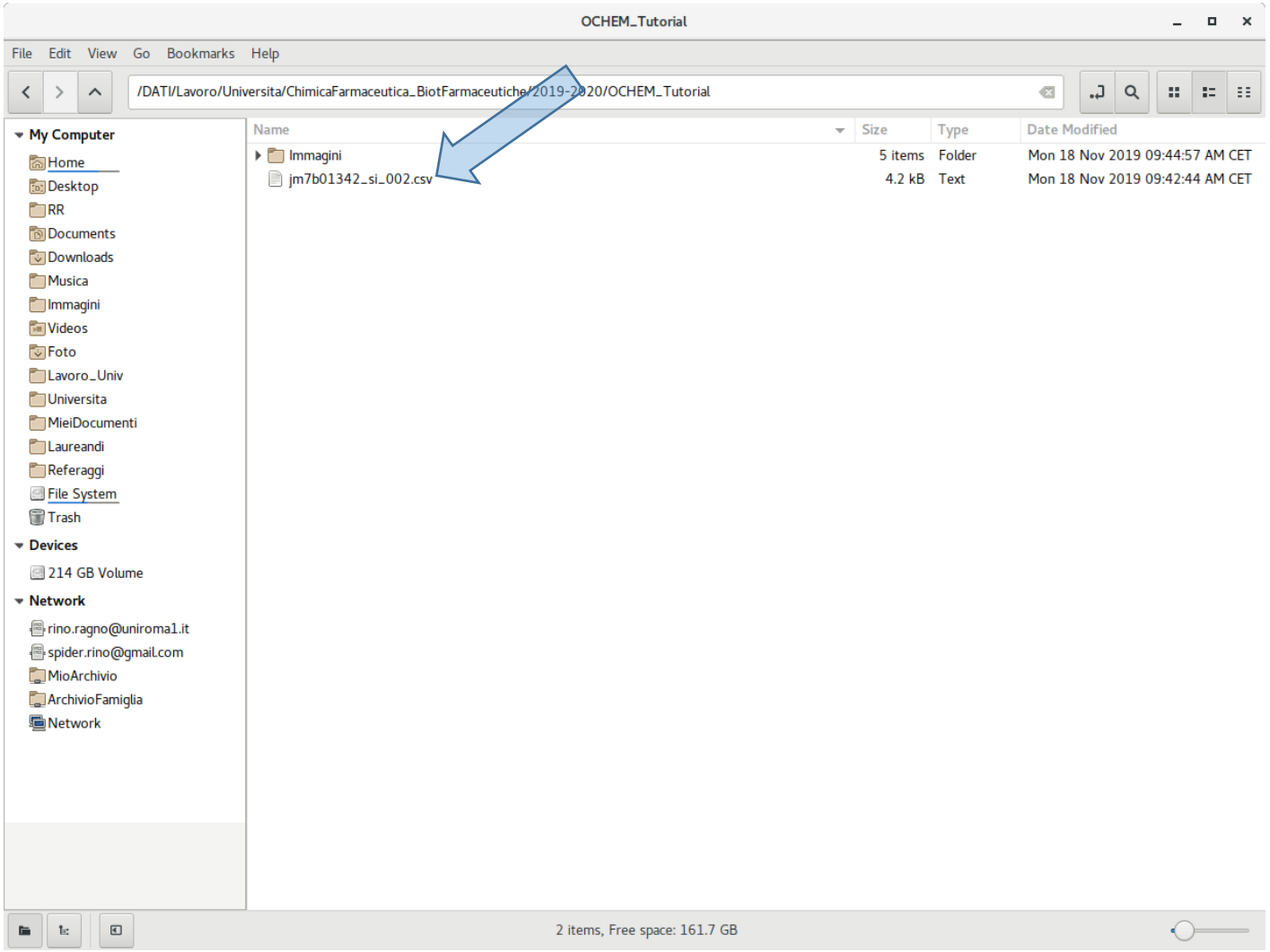

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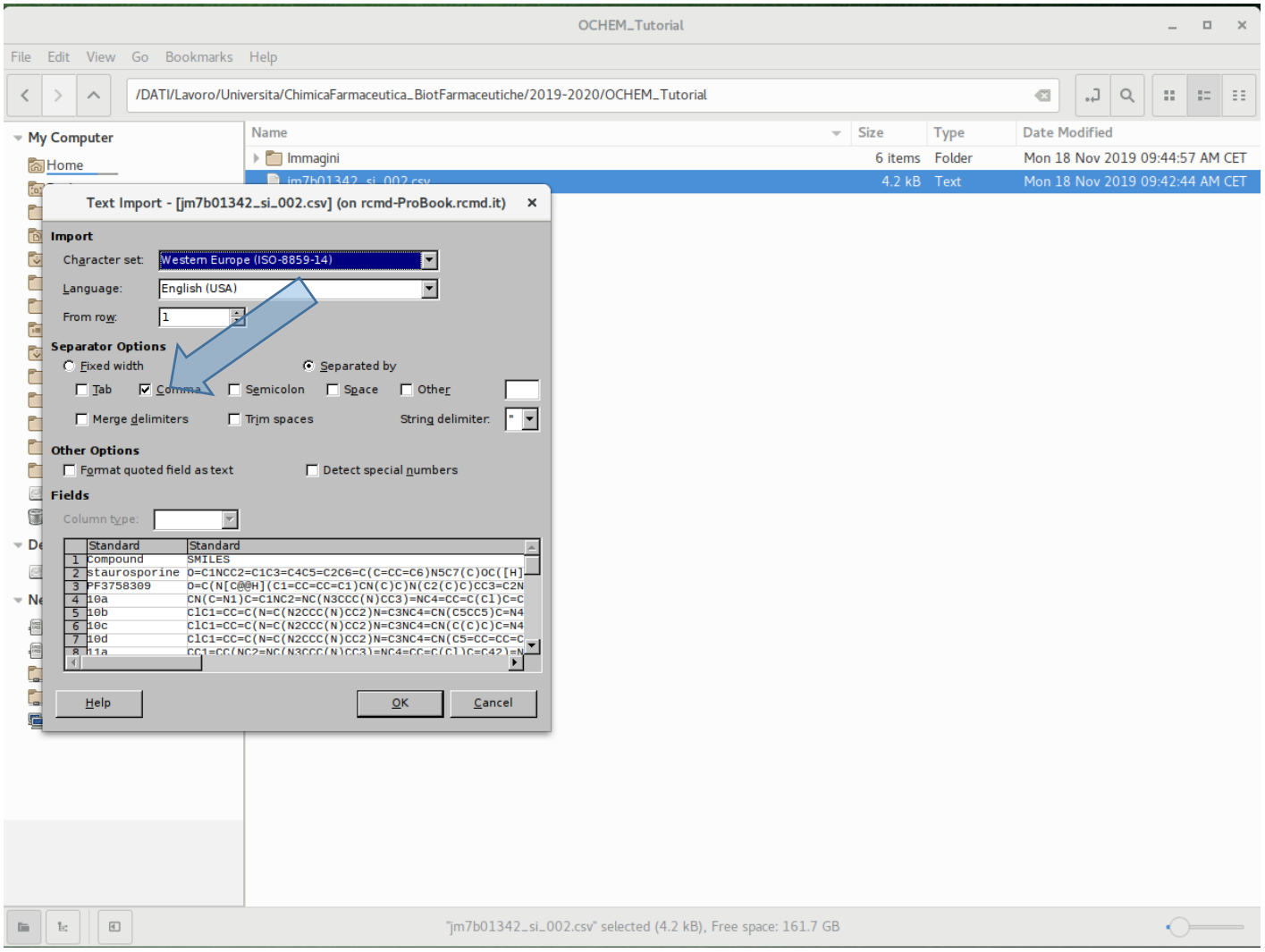

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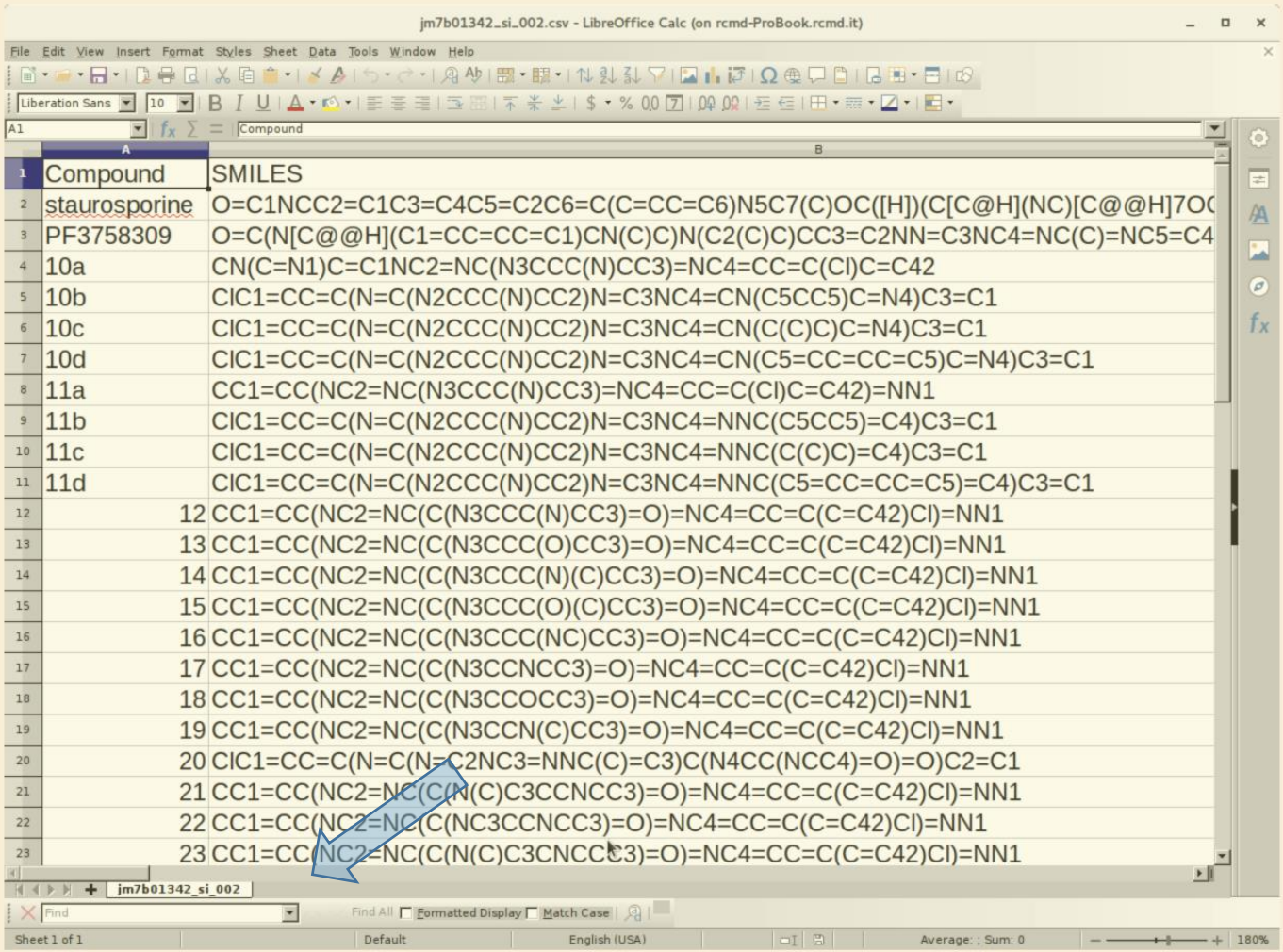

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1	Compound	SMILES
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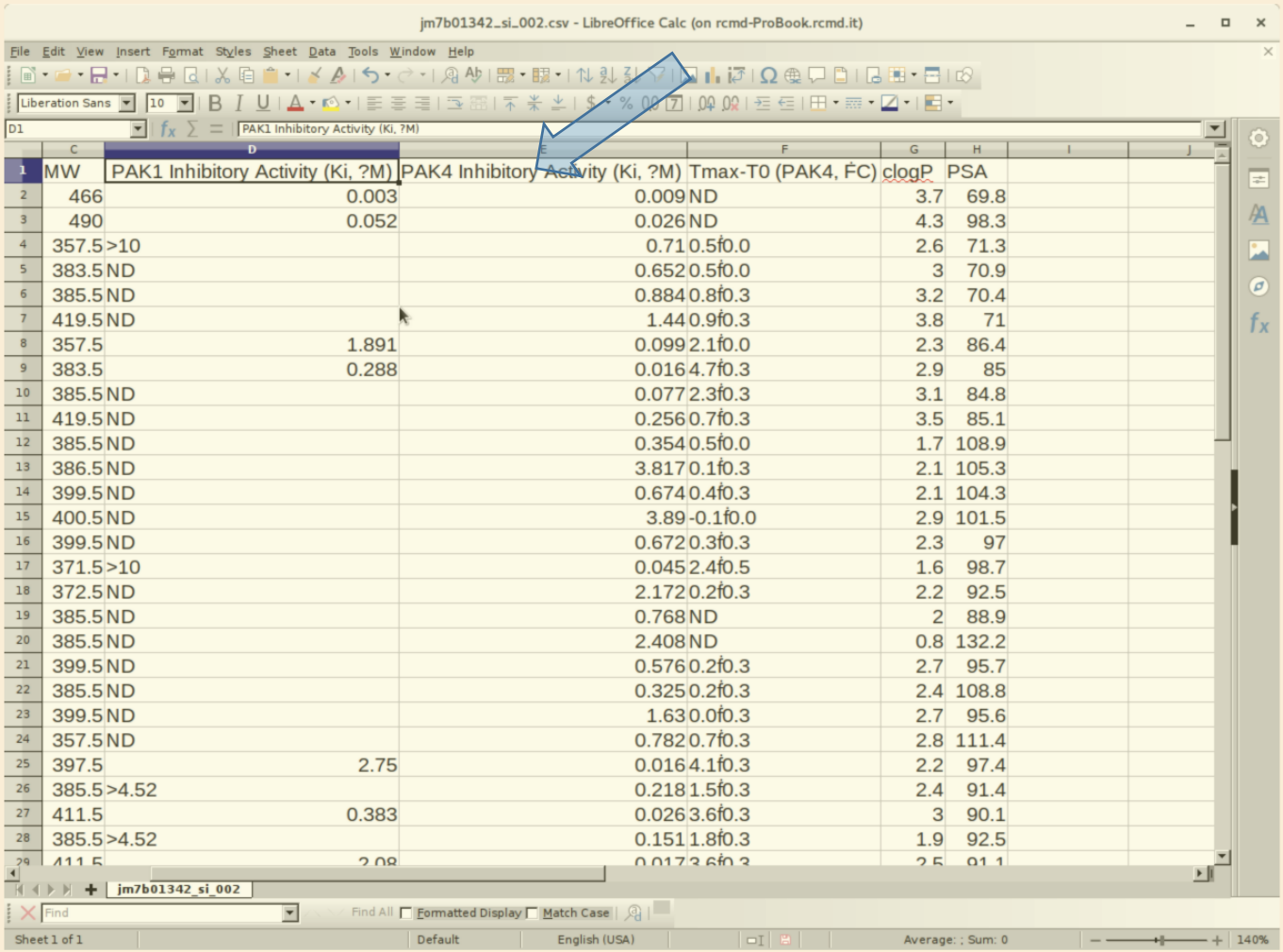
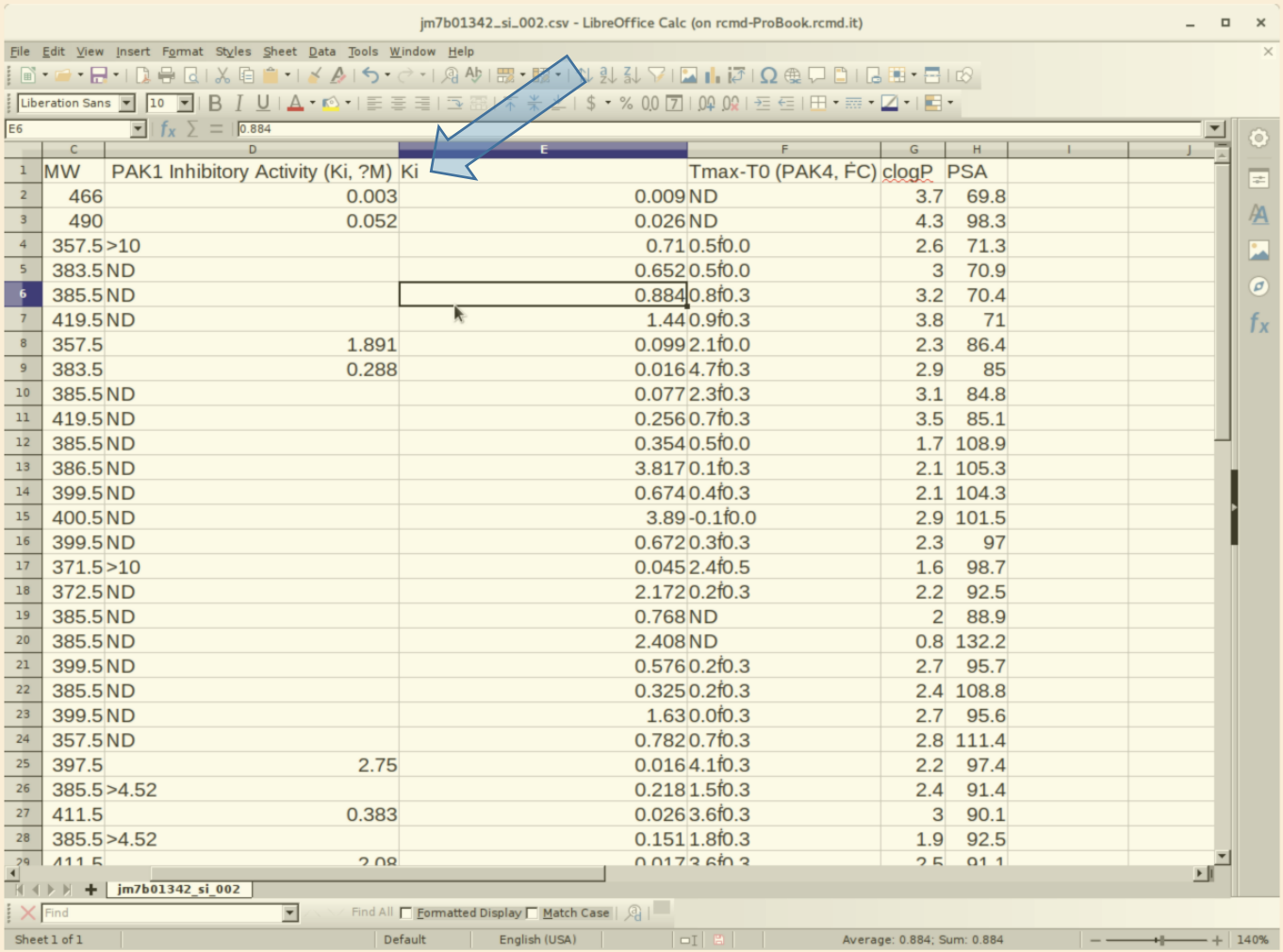
3	PF3758309	O=C(N[C@@H](C1=CC=CC=C1)CN(C)C)N(C2(C)C)CC3=C2NN=C3NC4=NC(C)=NC5=C4
4	10a	CN(C=N1)C=C1NC2=NC(N3CCC(N)CC3)=NC4=CC=C(Cl)C=C42
5	10b	ClC1=CC=C(N=C(N2CCC(N)CC2)N=C3NC4=CN(C5CC5)C=N4)C3=C1
6	10c	ClC1=CC=C(N=C(N2CCC(N)CC2)N=C3NC4=CN(C(C)C)C=N4)C3=C1
7	10d	ClC1=CC=C(N=C(N2CCC(N)CC2)N=C3NC4=CN(C5=CC=CC=C5)C=N4)C3=C1
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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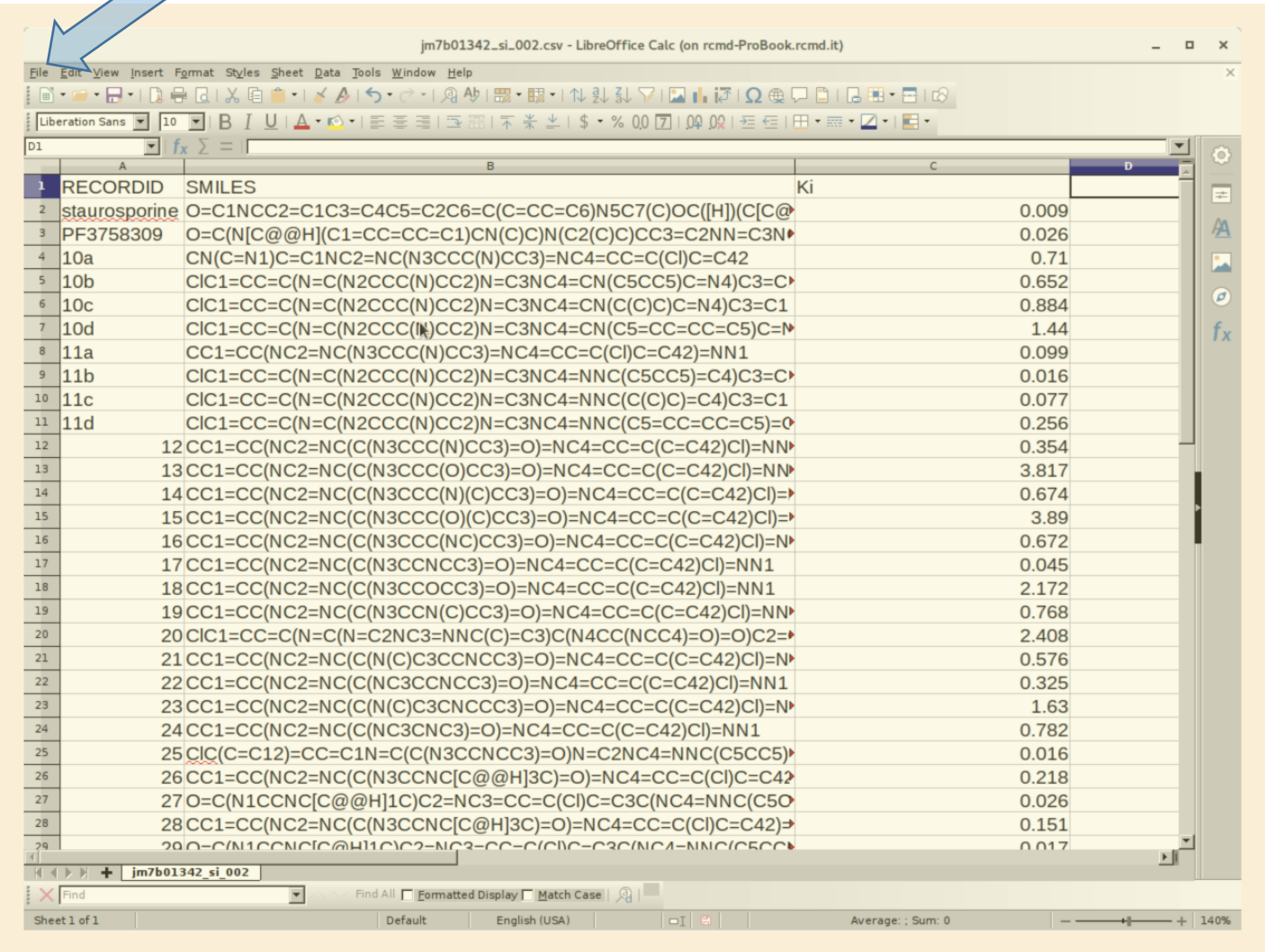
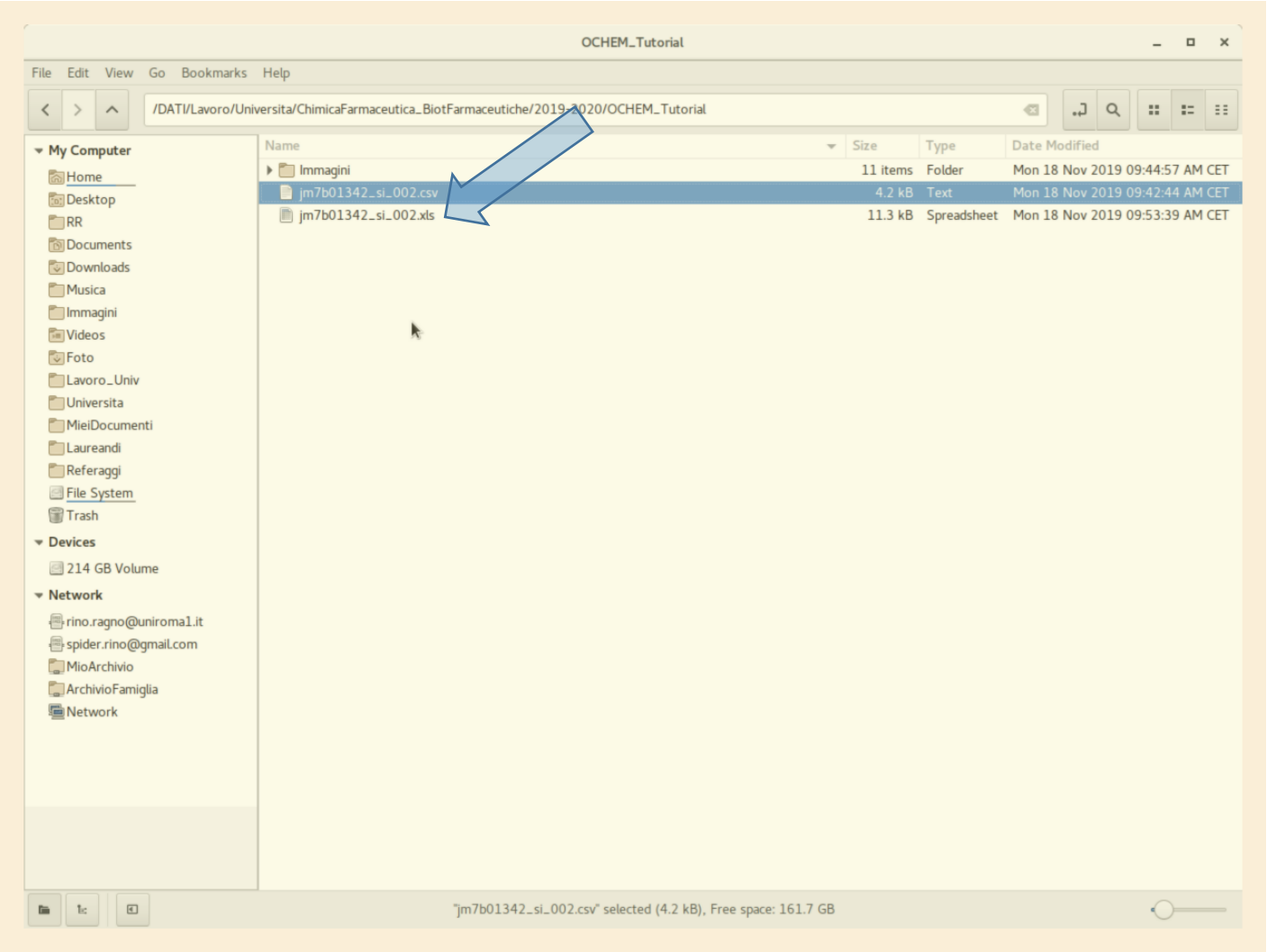


	A	B	C	D
1	RECORDID	SMILES	Ki	
2	staurosporine	O=C1NCC2=C1C3=C4C5=C2C6=C(C=CC=C6)N5C7(C)OC([H])(C[C@	0.009	
3	PF3758309	O=C(N[C@@H](C1=CC=CC=C1)CN(C)C)N(C2(C)C)CC3=C2NN=C3N	0.026	
4	10a	CN(C=N1)C=C1NC2=NC(N3CCC(N)CC3)=NC4=CC=C(Cl)C=C42	0.71	
5	10b	ClC1=CC=C(N=C(N2CCC(N)CC2)N=C3NC4=CN(C5CC5)C=N4)C3=C	0.652	
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	

Preparing the dataset



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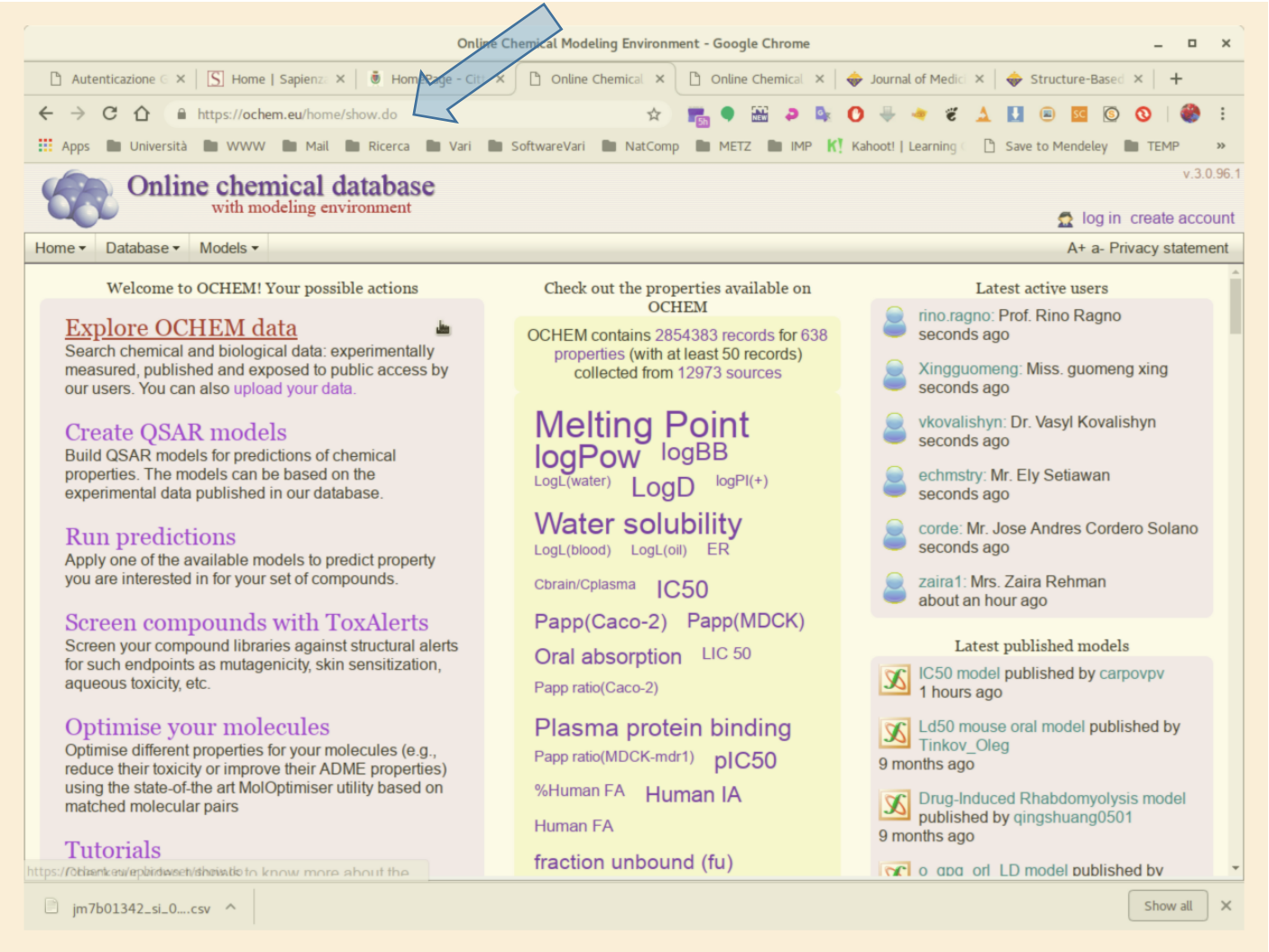

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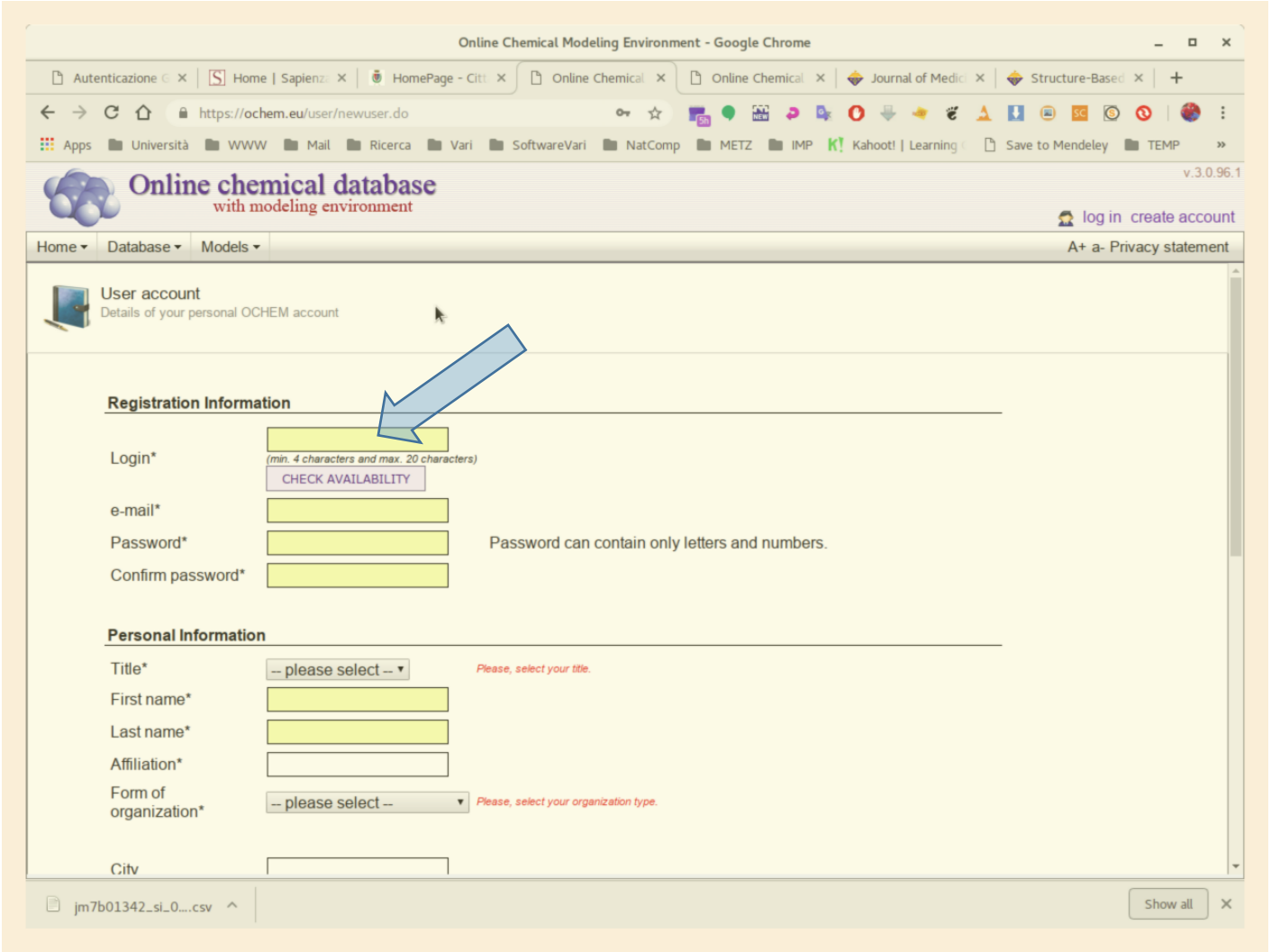

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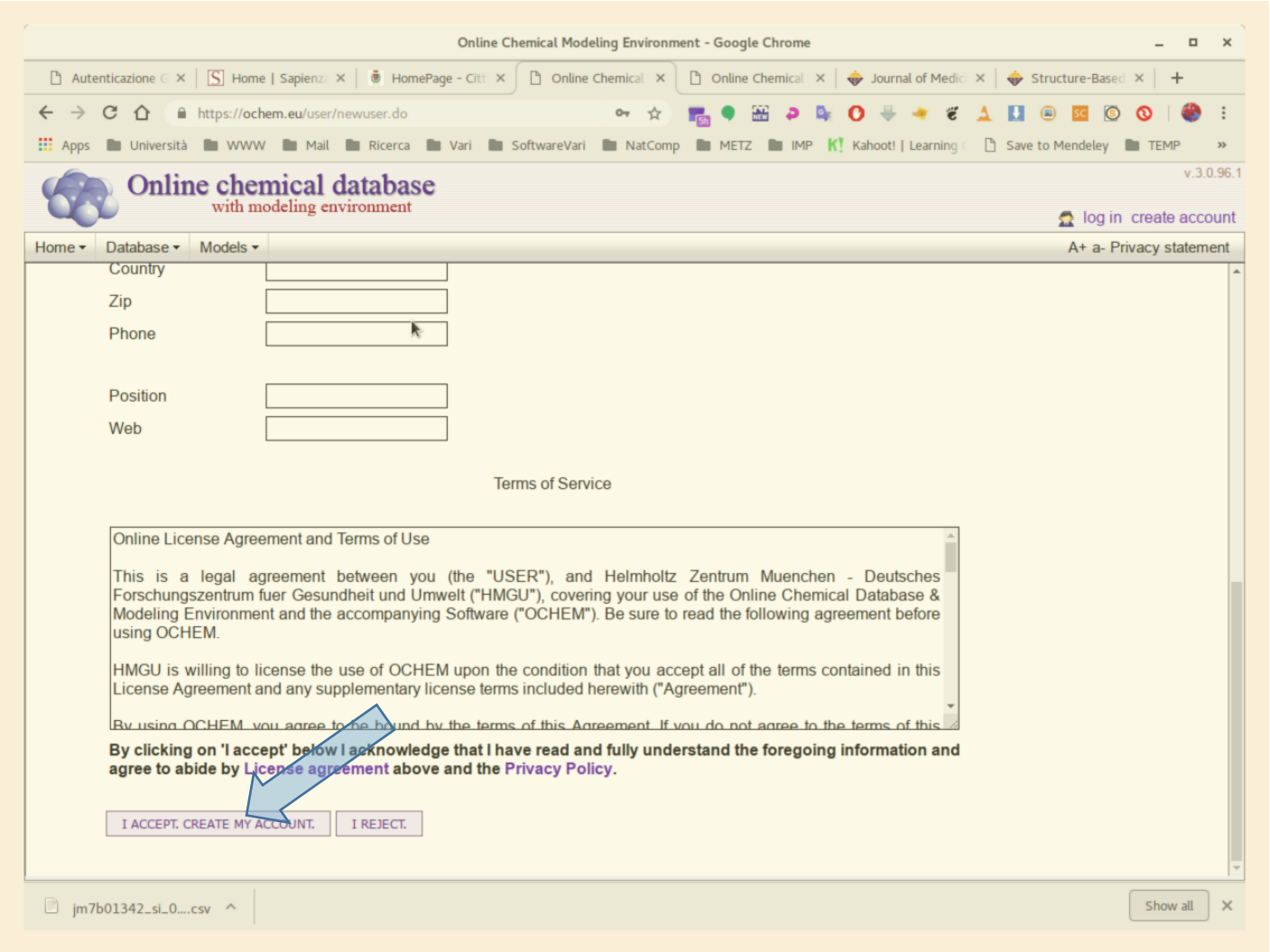

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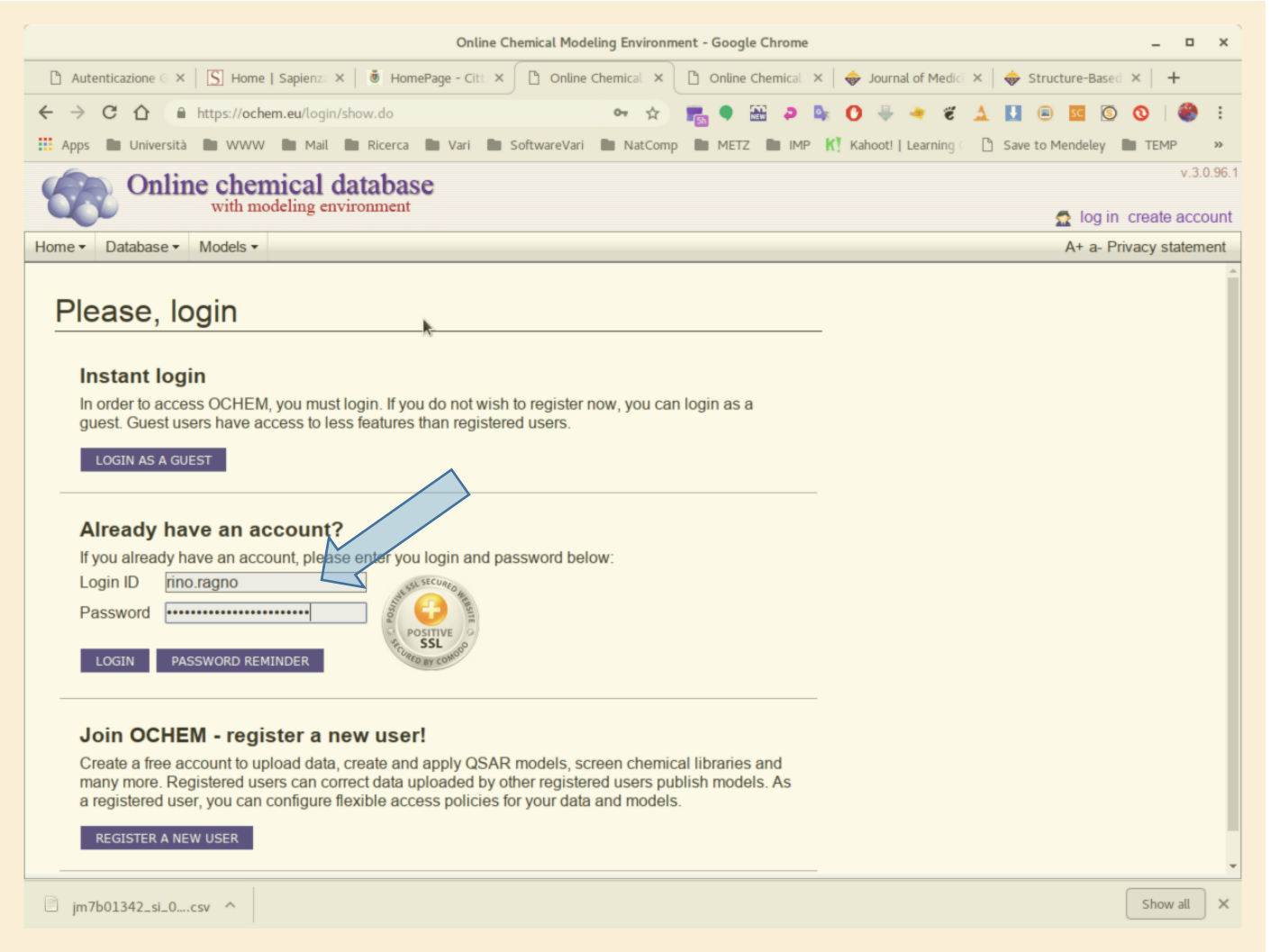

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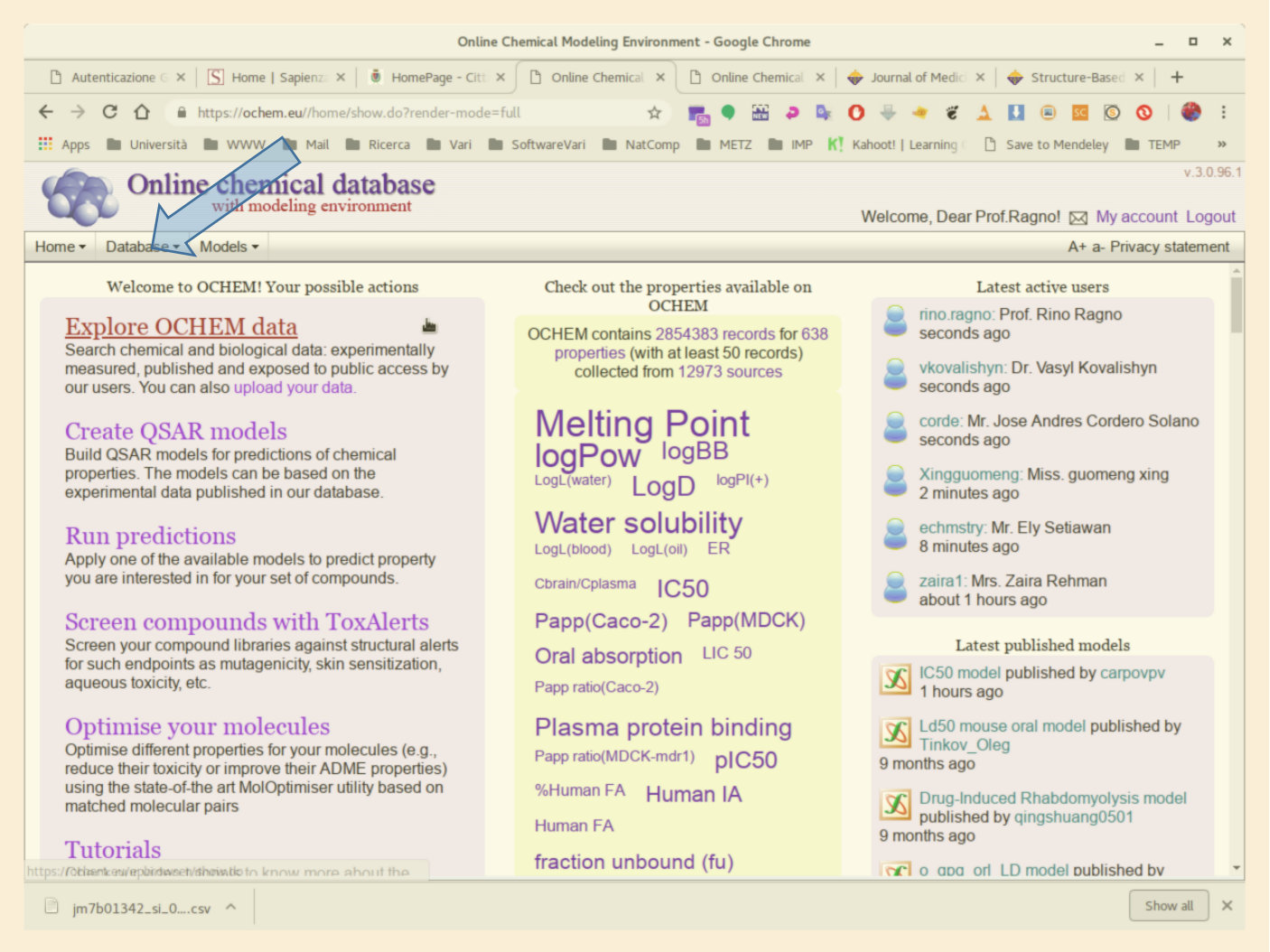

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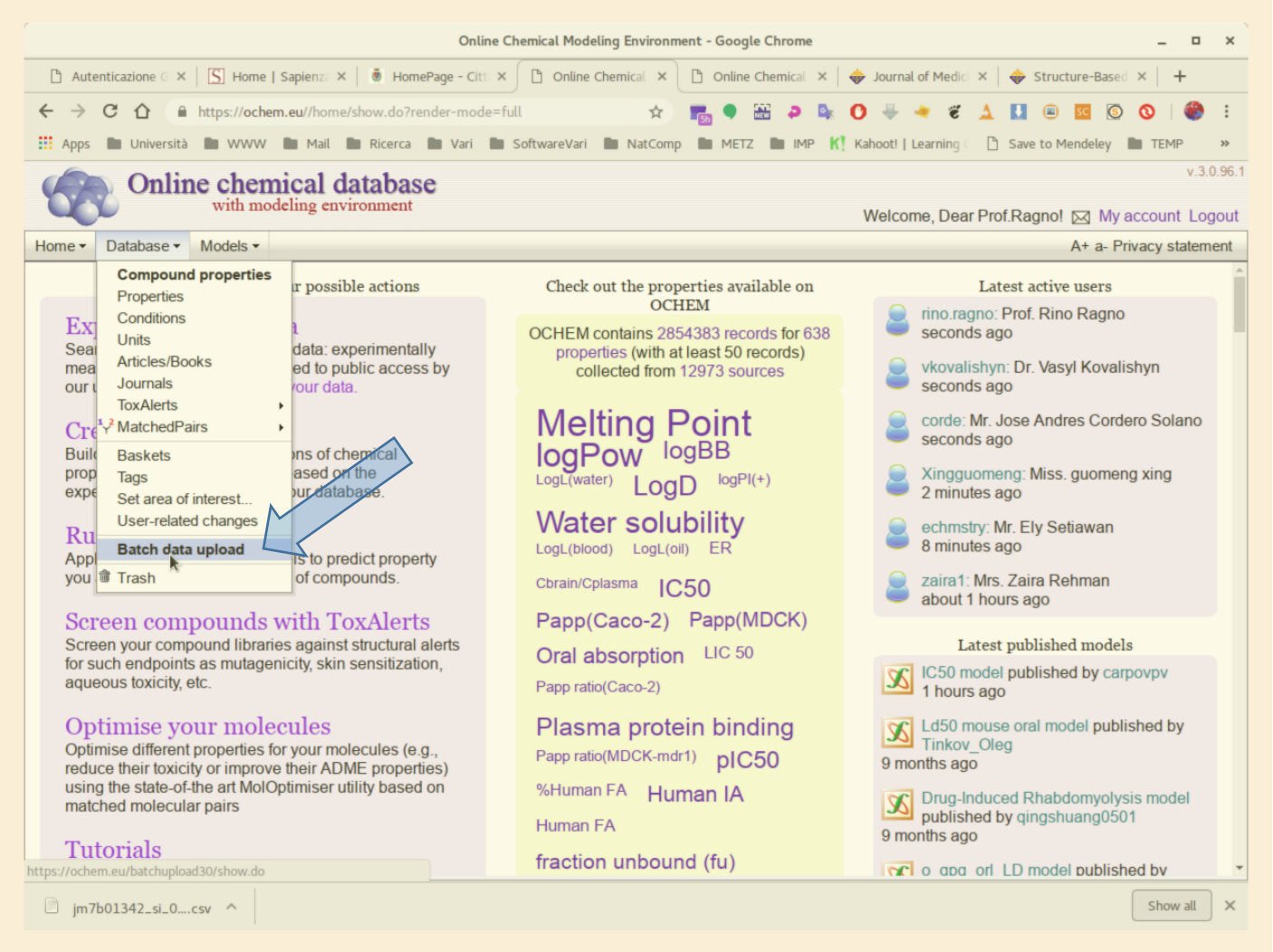

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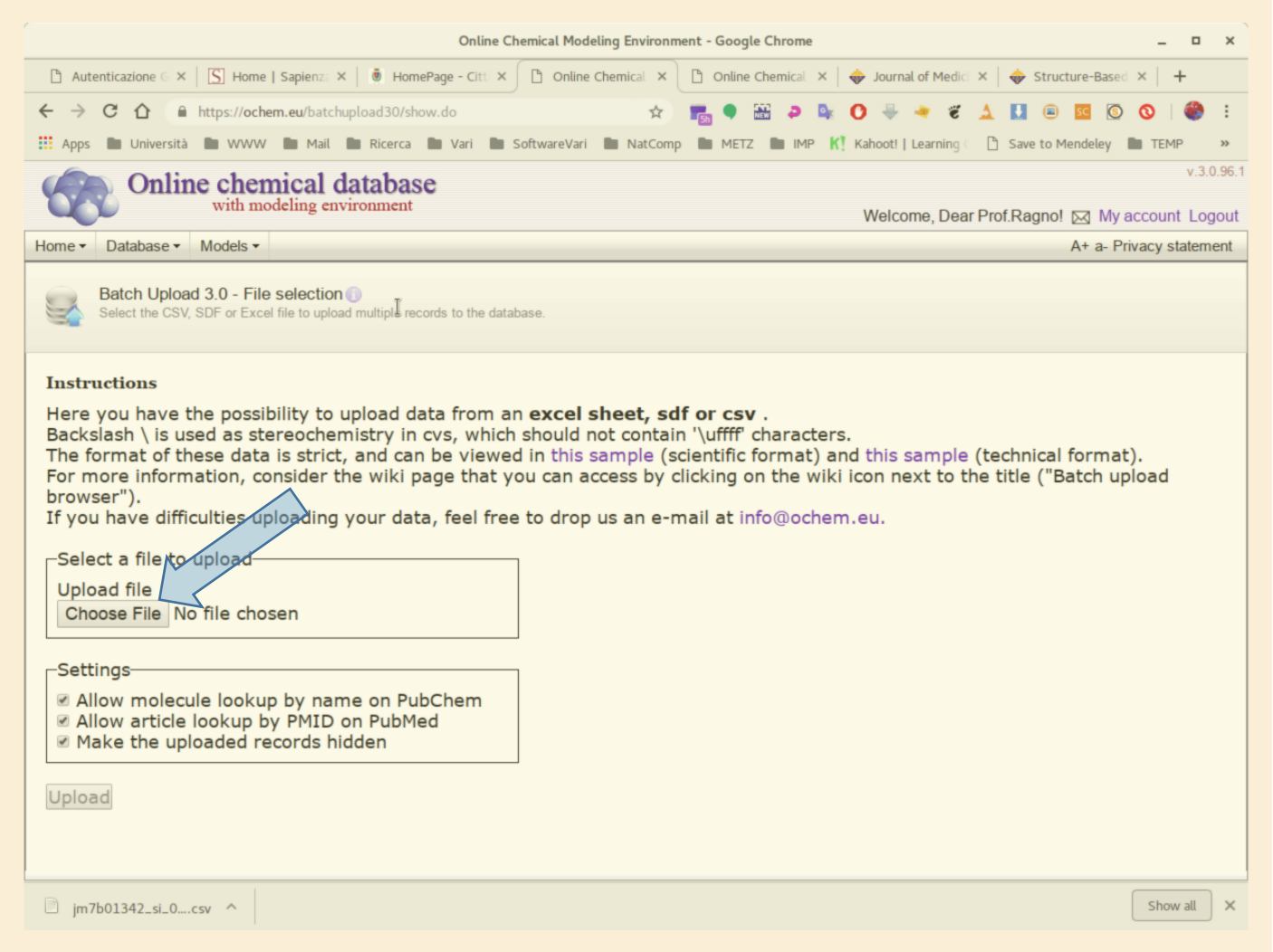

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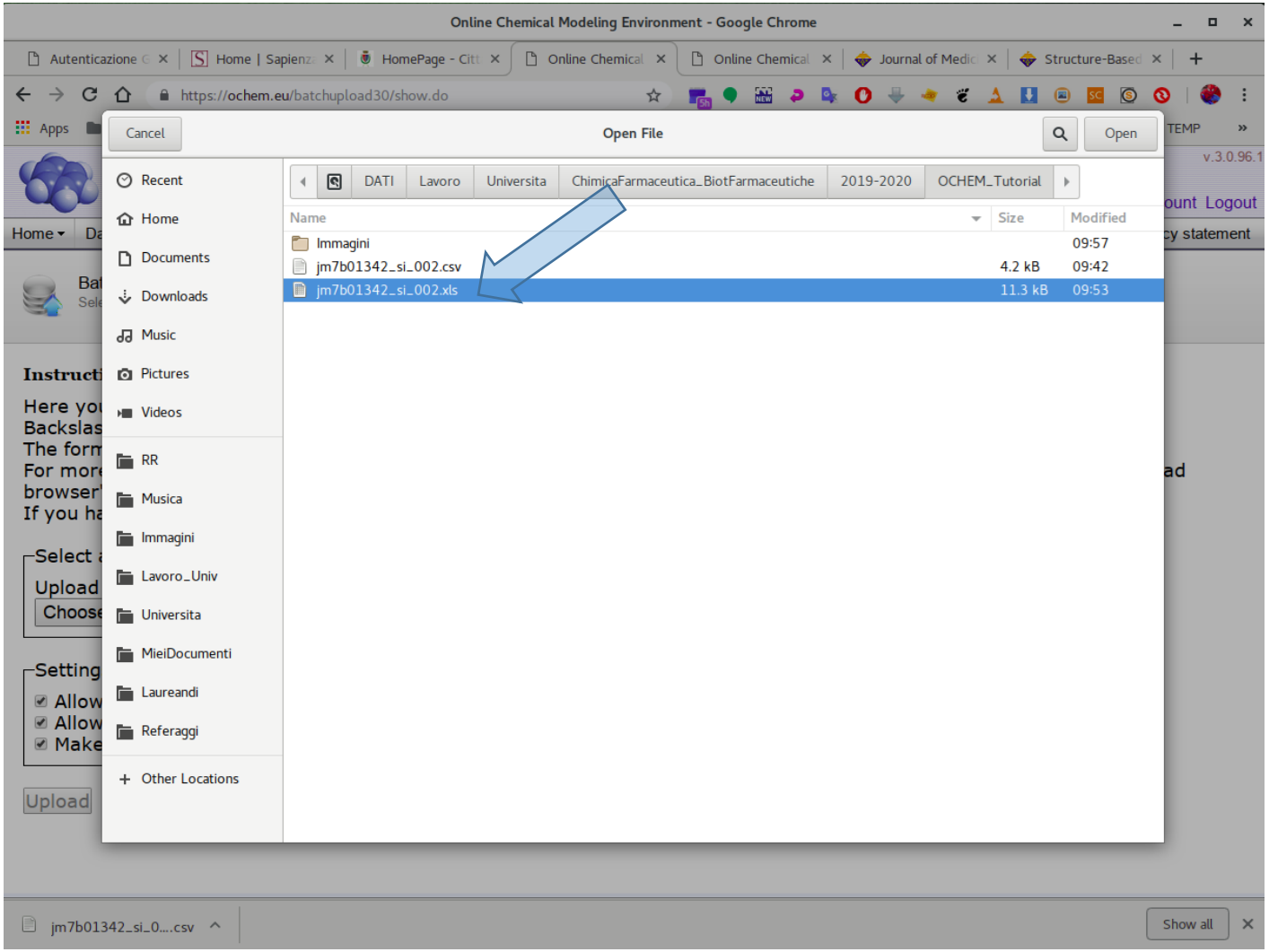

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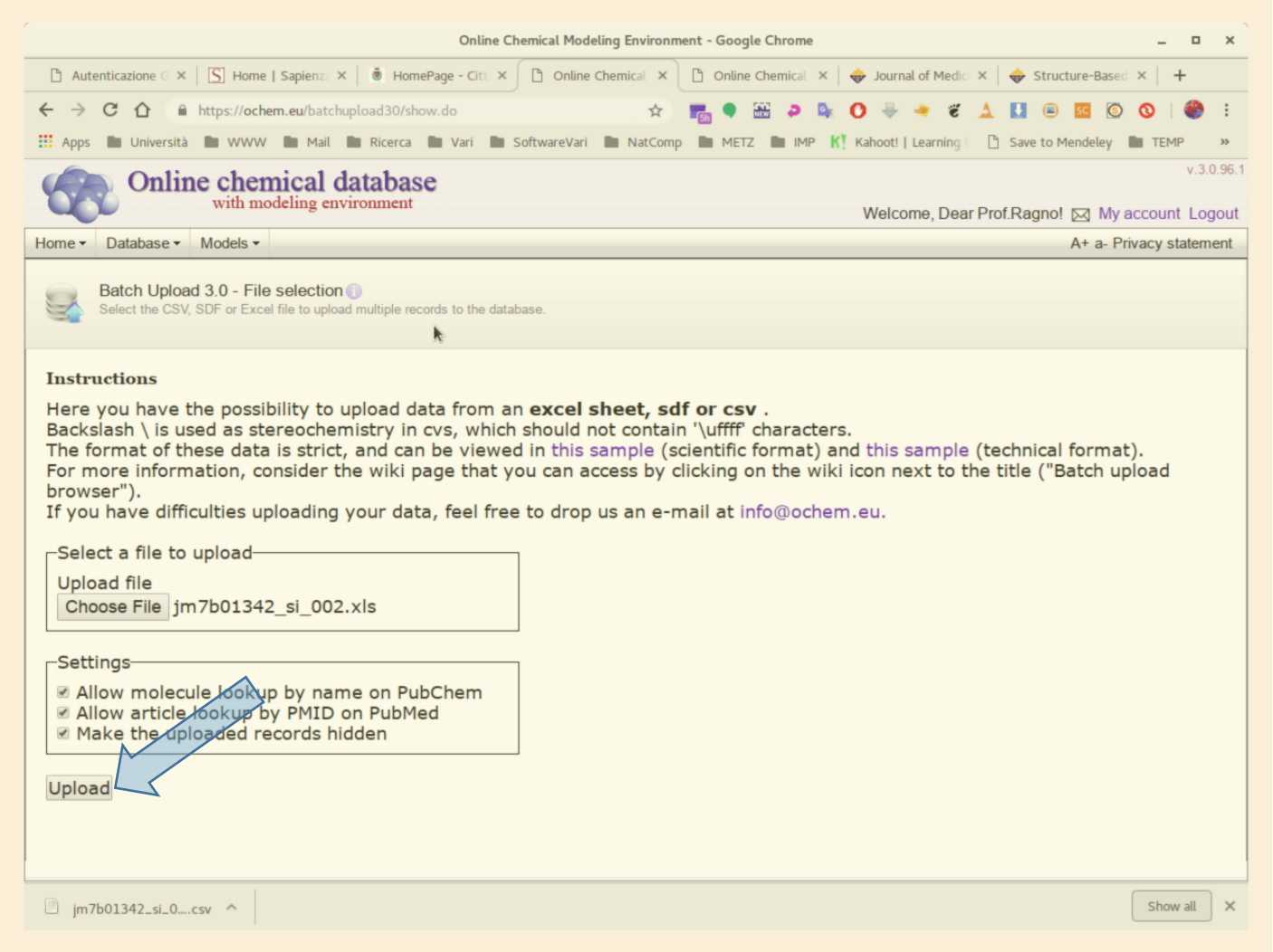

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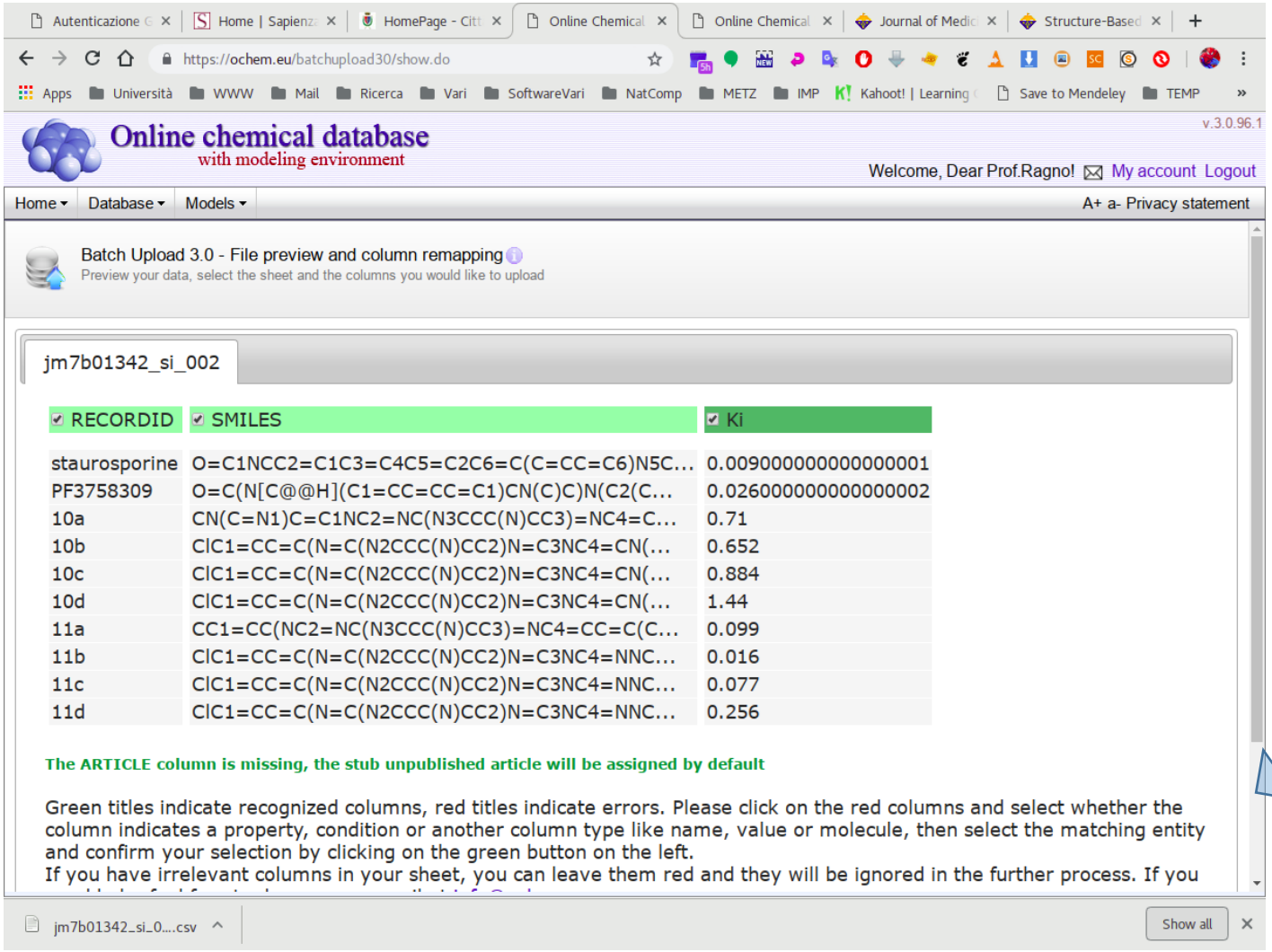

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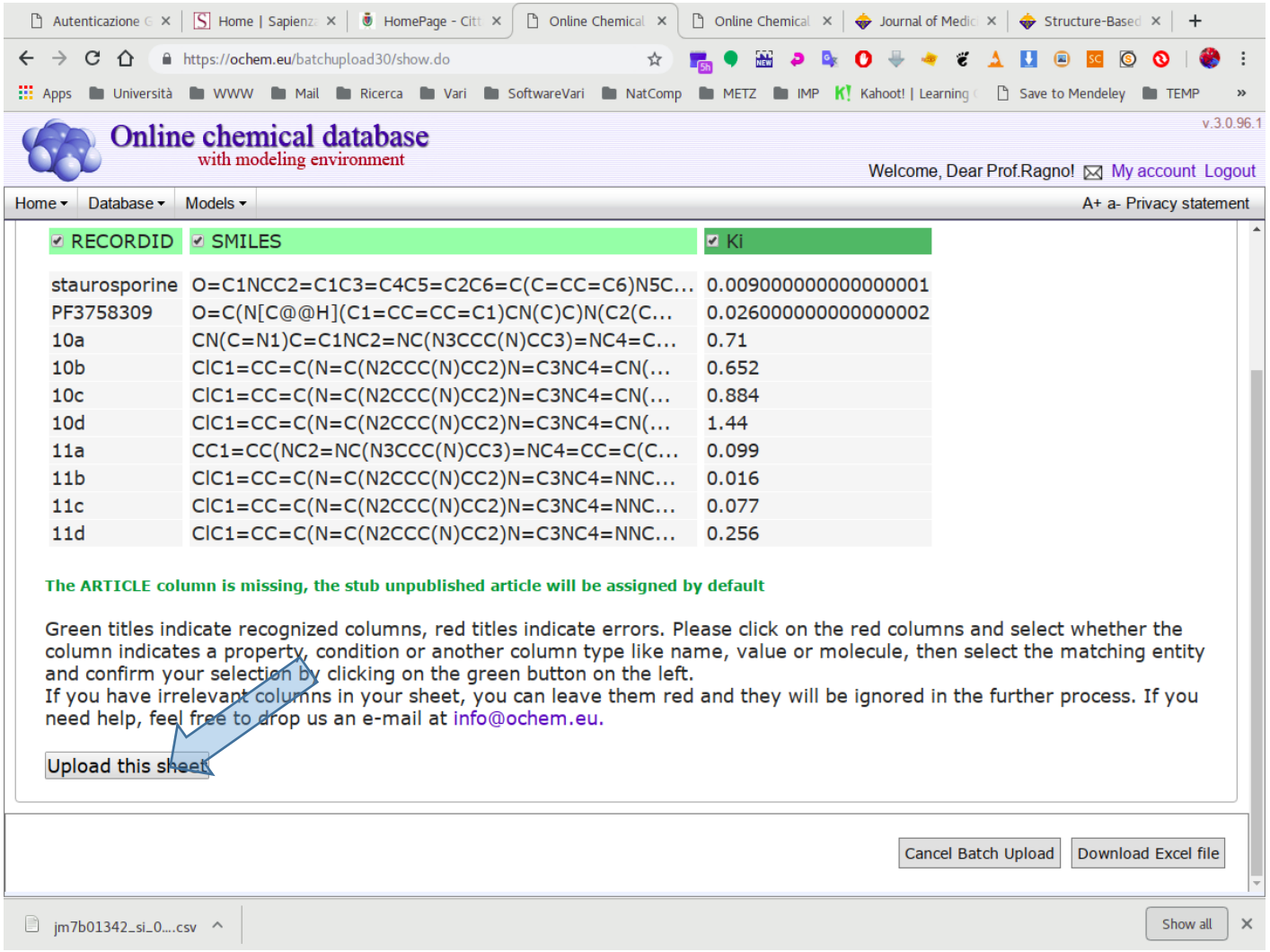

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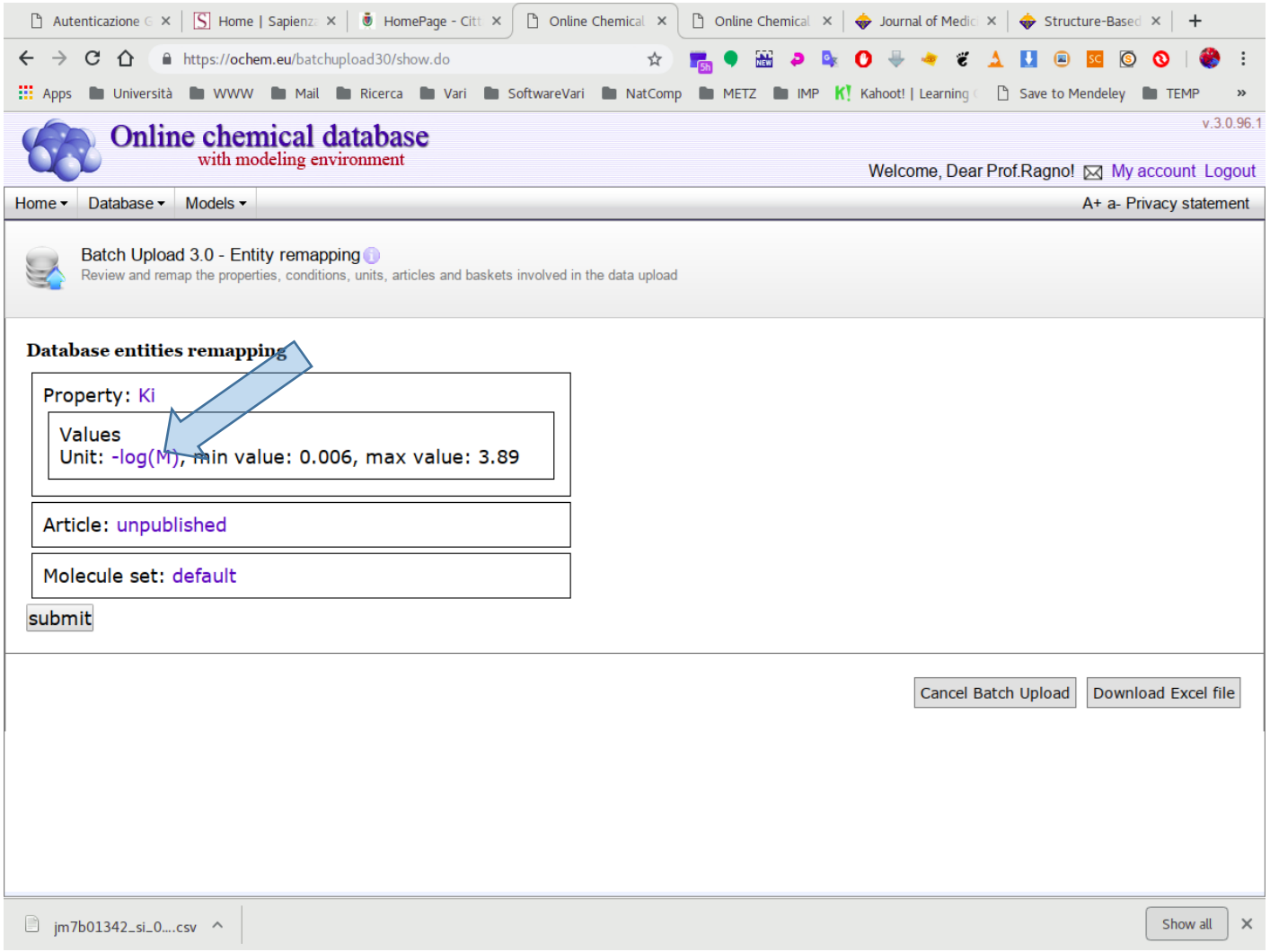

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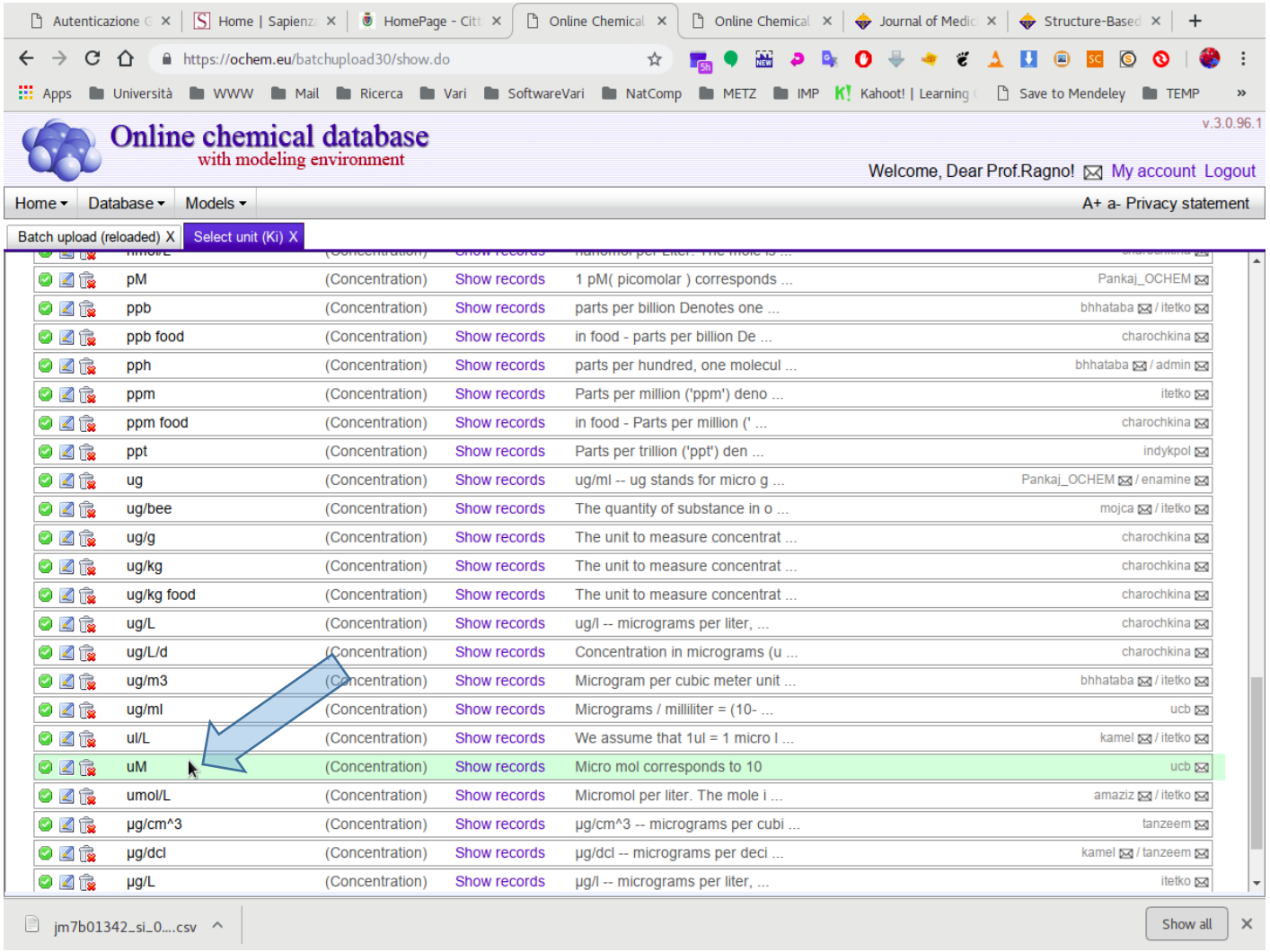

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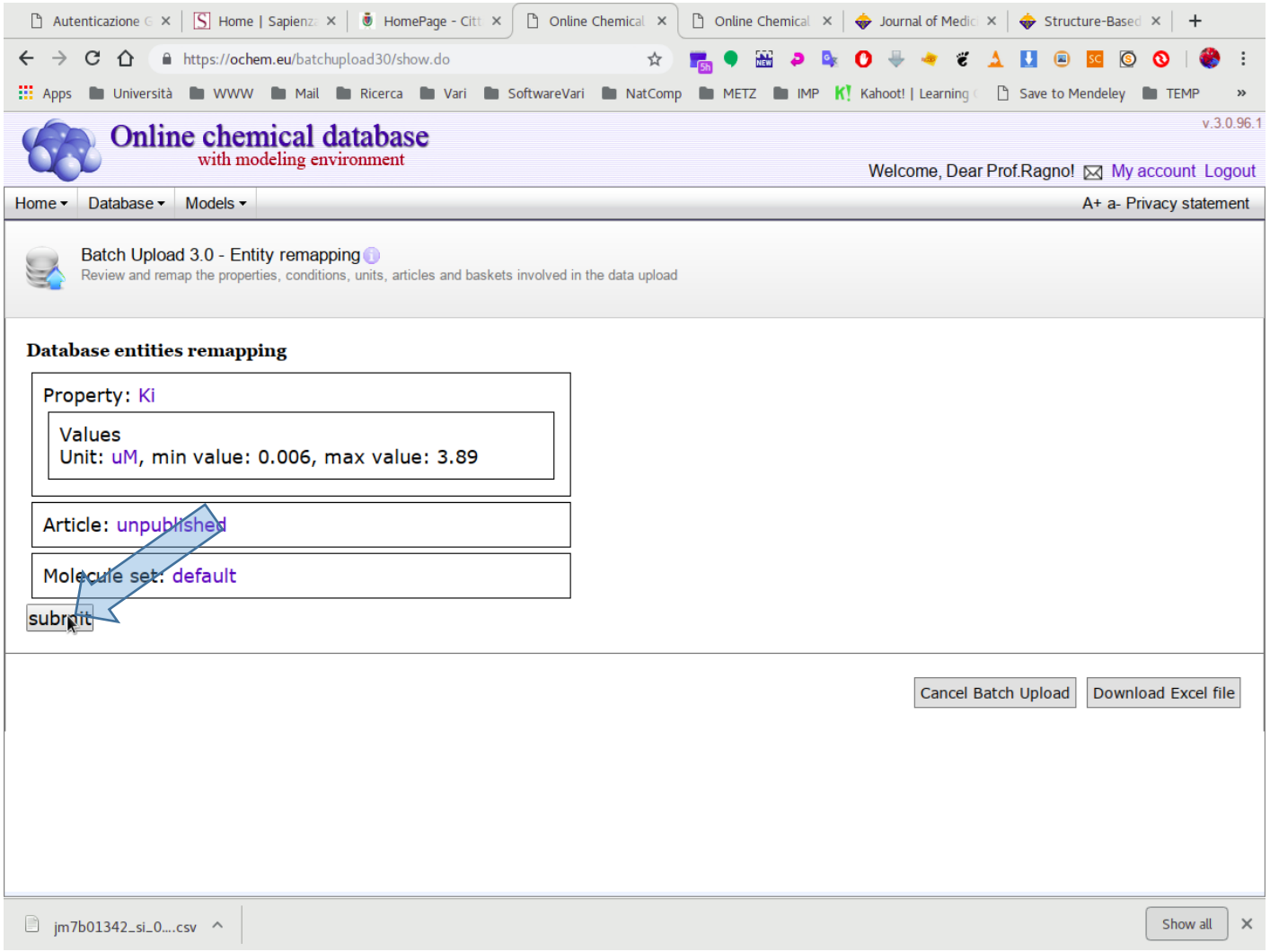
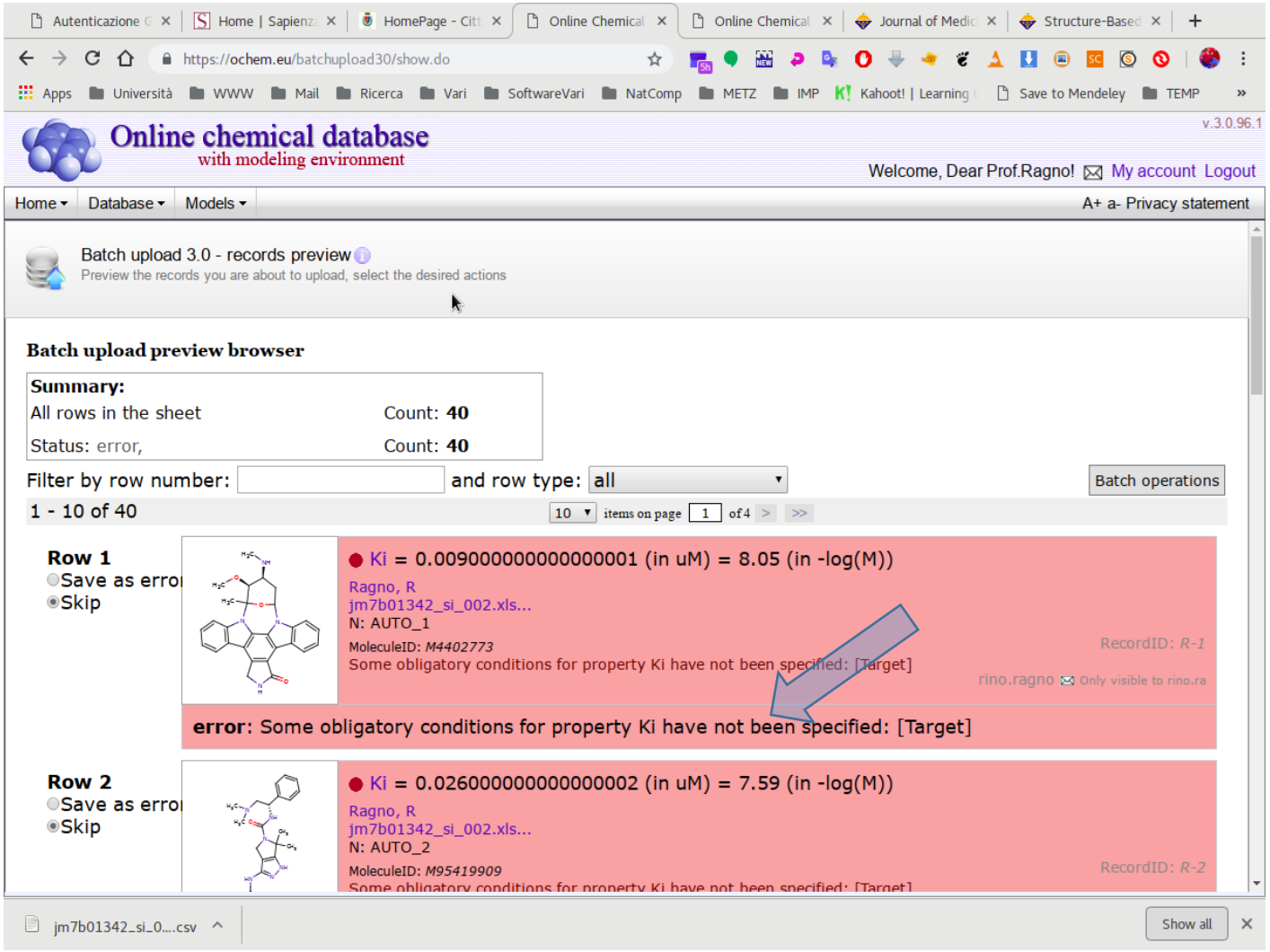
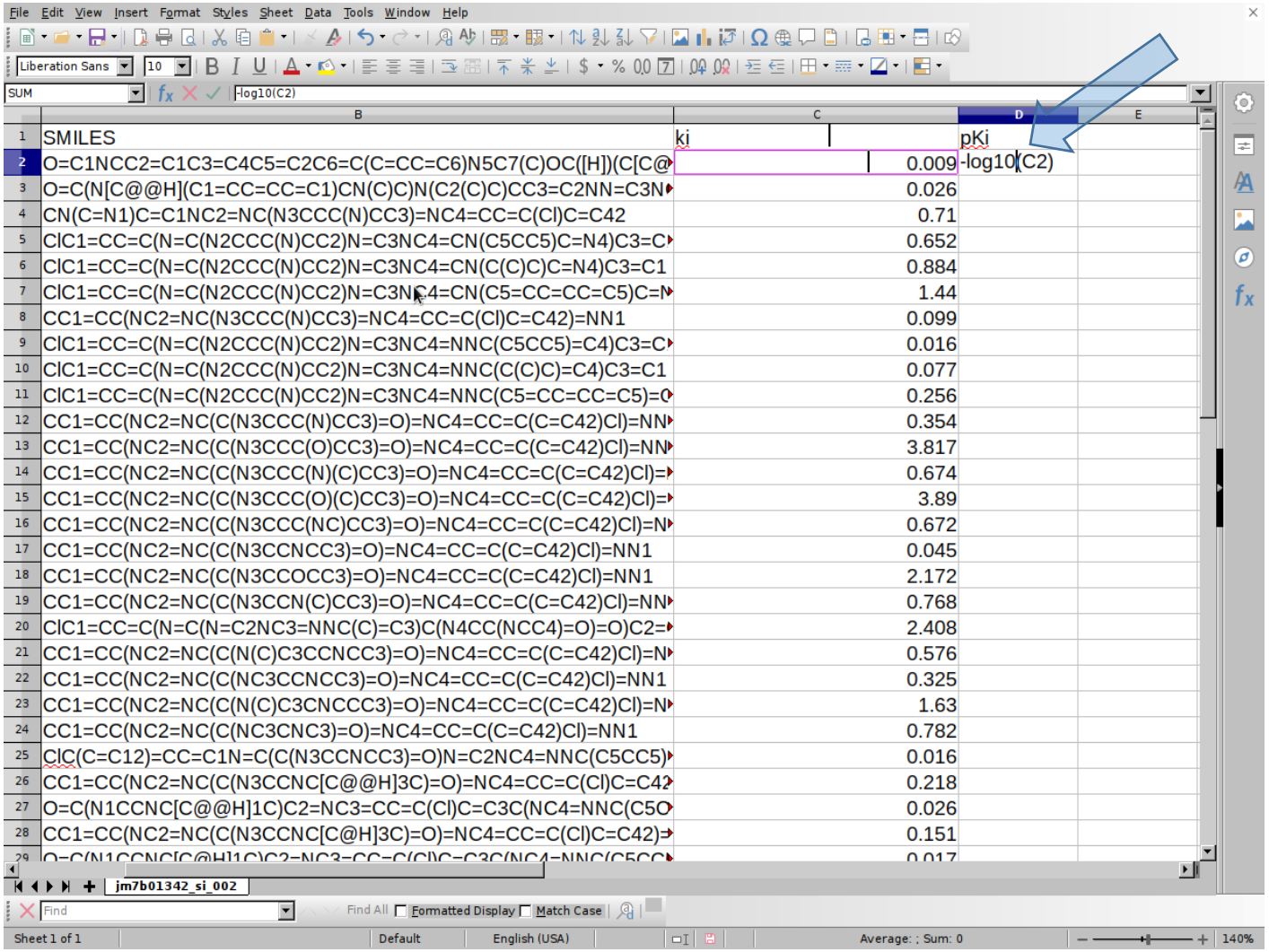


Preparing the dataset

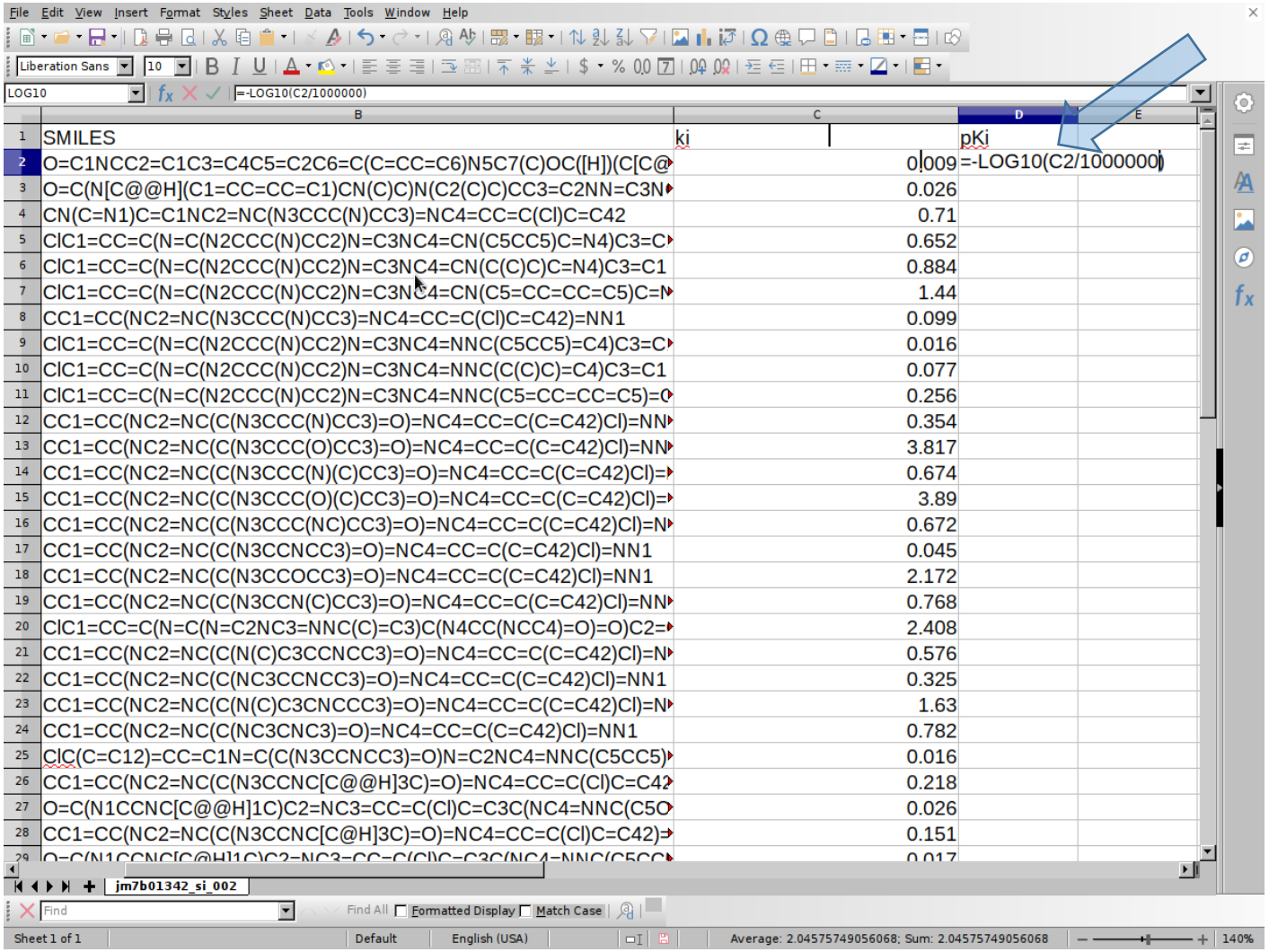


Preparing the dataset



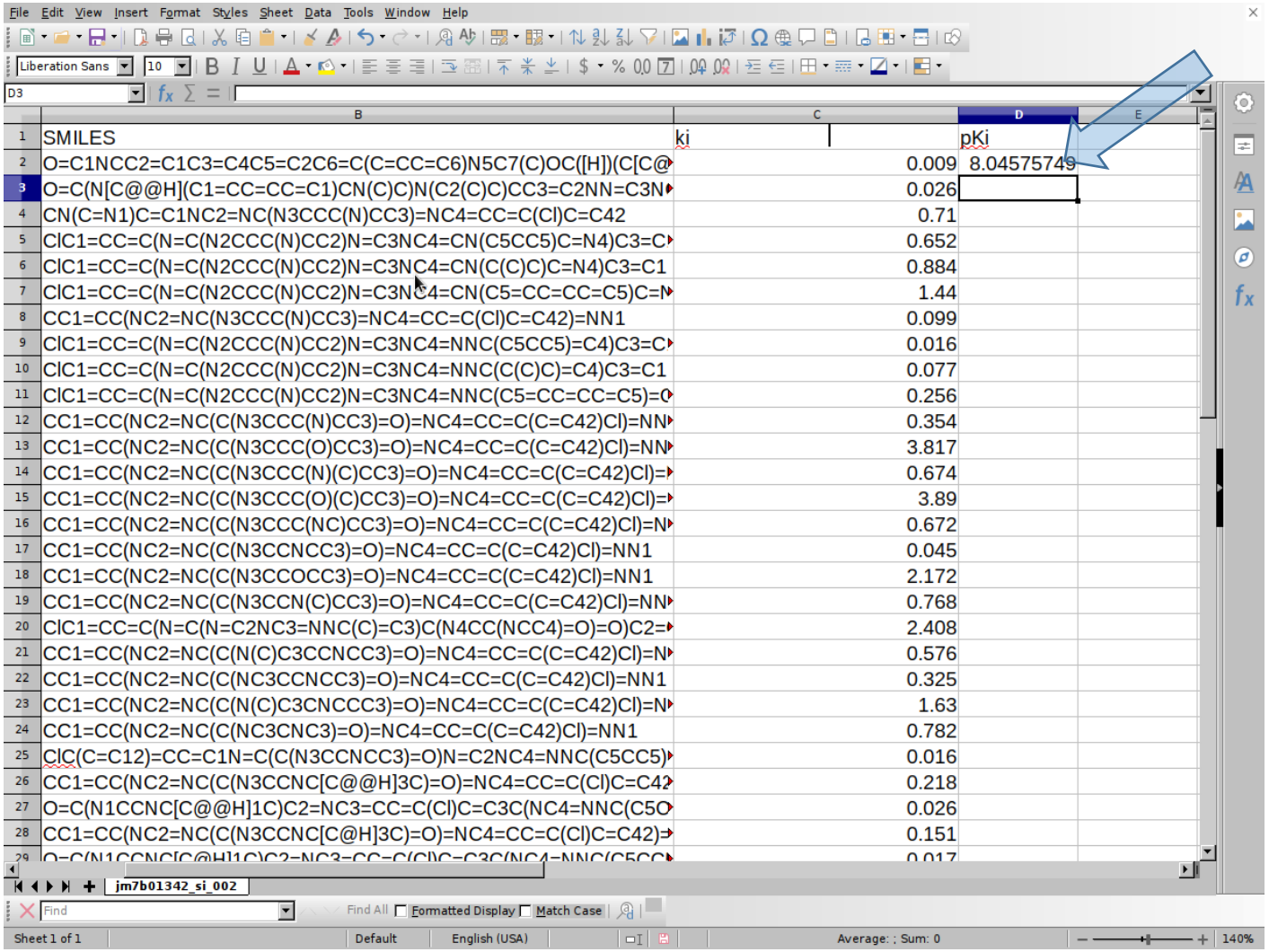
	B	C	D	E
1	SMILES	ki	pKi	
2	O=C1NCC2=C1C3=C4C5=C2C6=C(C=CC=C6)N5C7(C)OC([H])(C[C@	0.009	-log10(C2)	
3	O=C(N[C@@H](C1=CC=CC=C1)CN(C)C)N(C2(C)C)CC3=C2NN=C3N	0.026		
4	CN(C=N1)C=C1NC2=NC(N3CCC(N)CC3)=NC4=CC=C(Cl)C=C42	0.71		
5	ClC1=CC=C(N=C(N2CCC(N)CC2)N=C3NC4=CN(C5CC5)C=N4)C3=C	0.652		
6	ClC1=CC=C(N=C(N2CCC(N)CC2)N=C3NC4=CN(C(C)C)C=N4)C3=C1	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



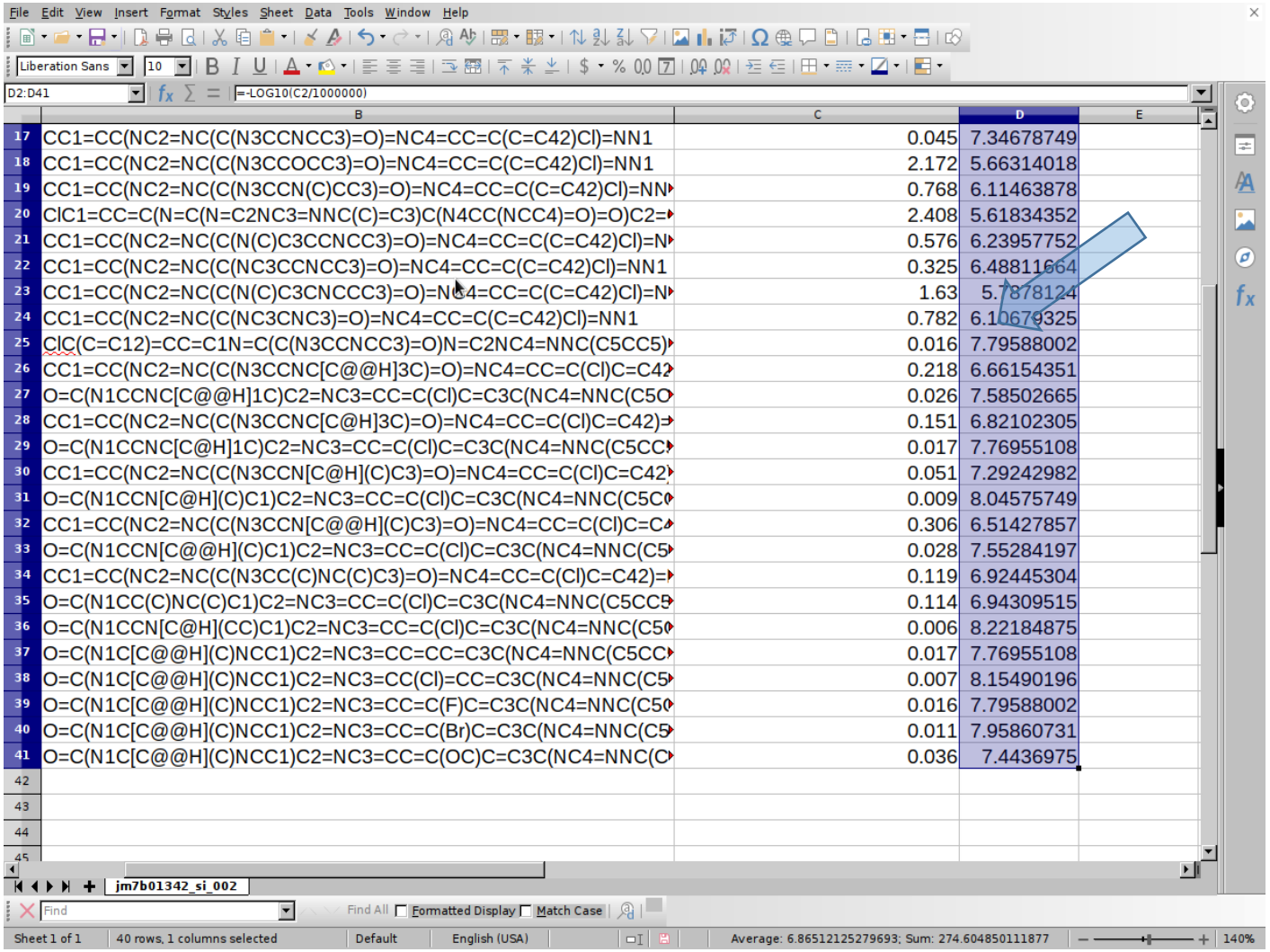
	B	C	D	E
1	SMILES	ki	pKi	
2	O=C1NCC2=C1C3=C4C5=C2C6=C(C=CC=C6)N5C7(C)OC([H])(C[C@	0.009	=-LOG10(C2/1000000)	
3	O=C(N[C@@H](C1=CC=CC=C1)CN(C)C)N(C2(C)C)CC3=C2NN=C3N	0.026		
4	CN(C=N1)C=C1NC2=NC(N3CCC(N)CC3)=NC4=CC=C(Cl)C=C42	0.71		
5	ClC1=CC=C(N=C(N2CCC(N)CC2)N=C3NC4=CN(C5CC5)C=N4)C3=C	0.652		
6	ClC1=CC=C(N=C(N2CCC(N)CC2)N=C3NC4=CN(C(C)C)C=N4)C3=C1	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



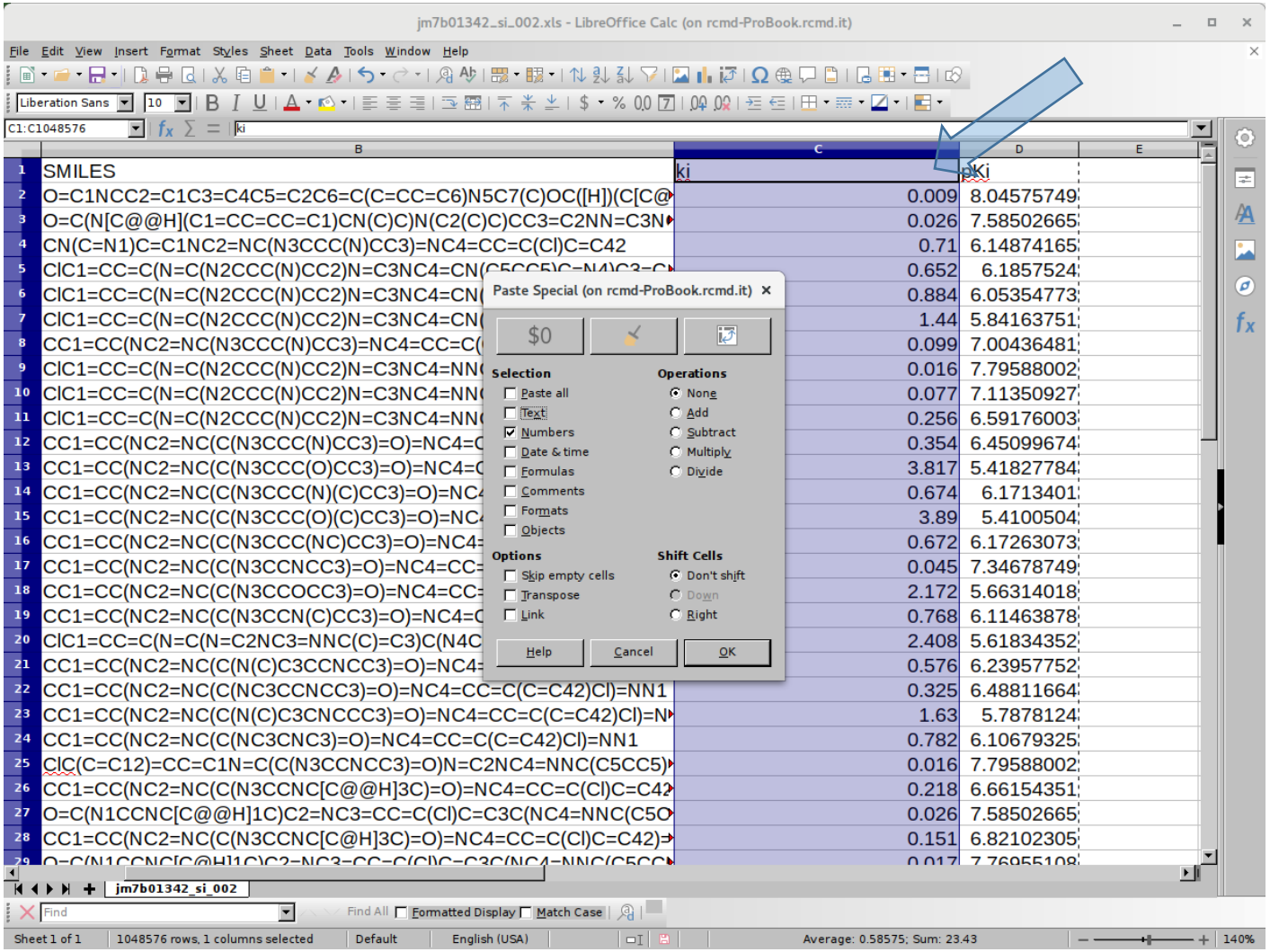
	B	C	D	E
1	SMILES	ki	pKi	
2	O=C1NCC2=C1C3=C4C5=C2C6=C(C=CC=C6)N5C7(C)OC([H])(C[C@	0.009	8.04575749	
3	O=C(N[C@@H](C1=CC=CC=C1)CN(C)C)N(C2(C)C)CC3=C2NN=C3N	0.026		
4	CN(C=N1)C=C1NC2=NC(N3CCC(N)CC3)=NC4=CC=C(Cl)C=C42	0.71		
5	ClC1=CC=C(N=C(N2CCC(N)CC2)N=C3NC4=CN(C5CC5)C=N4)C3=C	0.652		
6	ClC1=CC=C(N=C(N2CCC(N)CC2)N=C3NC4=CN(C(C)C)C=N4)C3=C1	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

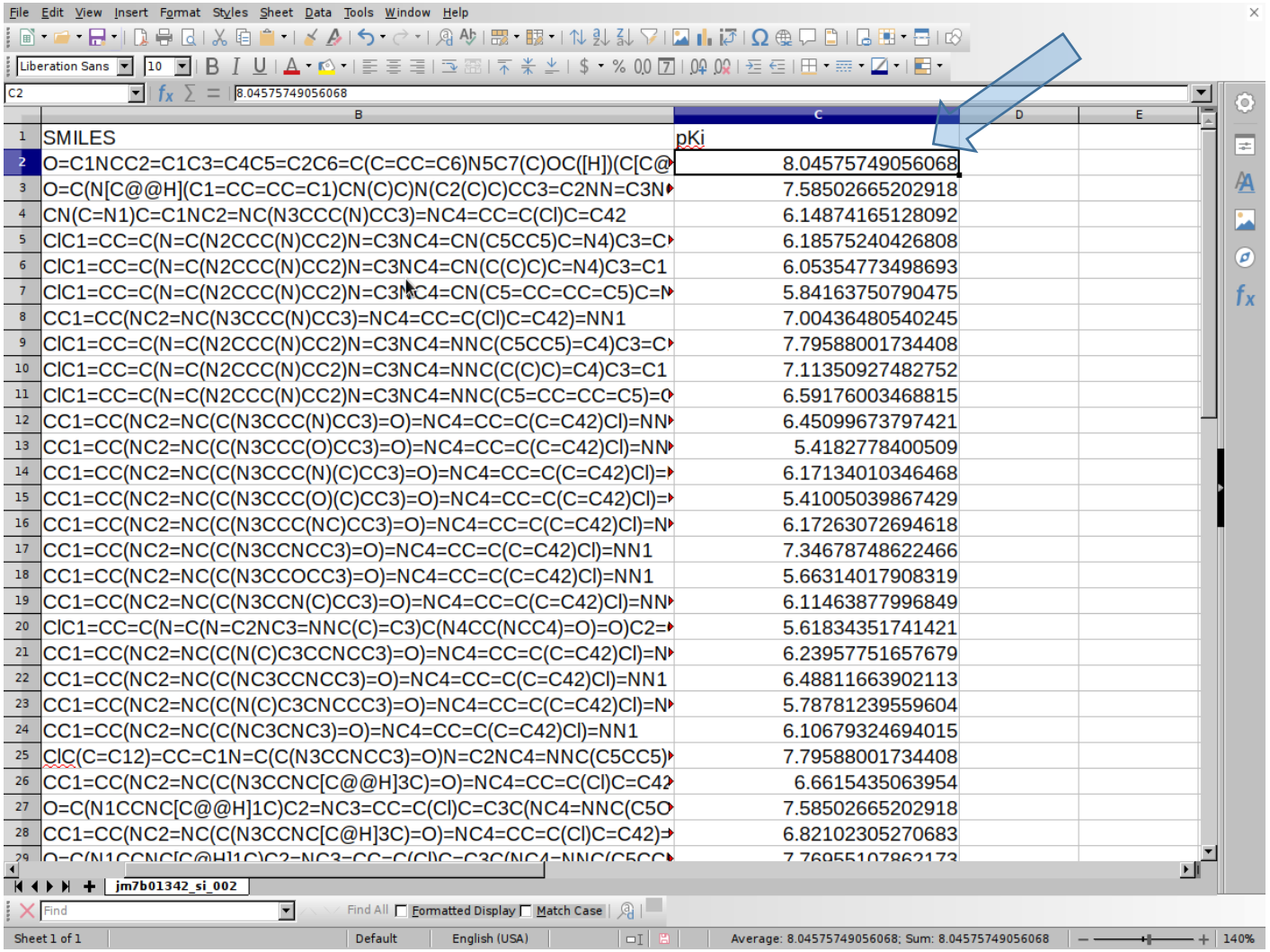


	B	C	D	E
17	CC1=CC(NC2=NC(C(N3CCNCC3)=O)=NC4=CC=C(C=C42)Cl)=NN1	0.045	7.34678749	
18	CC1=CC(NC2=NC(C(N3CCOCC3)=O)=NC4=CC=C(C=C42)Cl)=NN1	2.172	5.66314018	
19	CC1=CC(NC2=NC(C(N3CCN(C)CC3)=O)=NC4=CC=C(C=C42)Cl)=NN	0.768	6.11463878	
20	ClC1=CC=C(N=C(N=C2NC3=NNC(C)=C3)C(N4CC(NCC4)=O)=O)C2=	2.408	5.61834352	
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

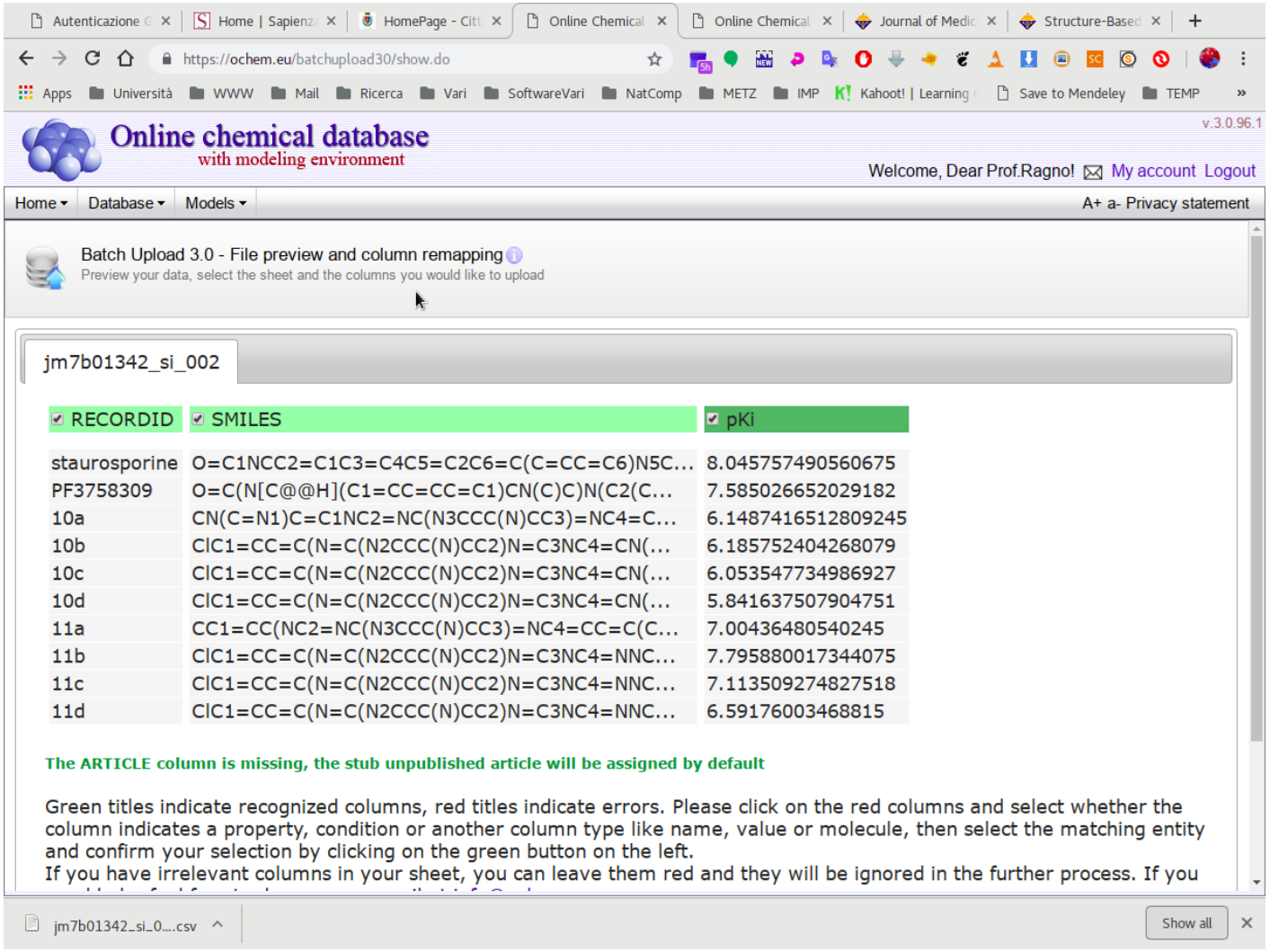


Preparing the dataset



	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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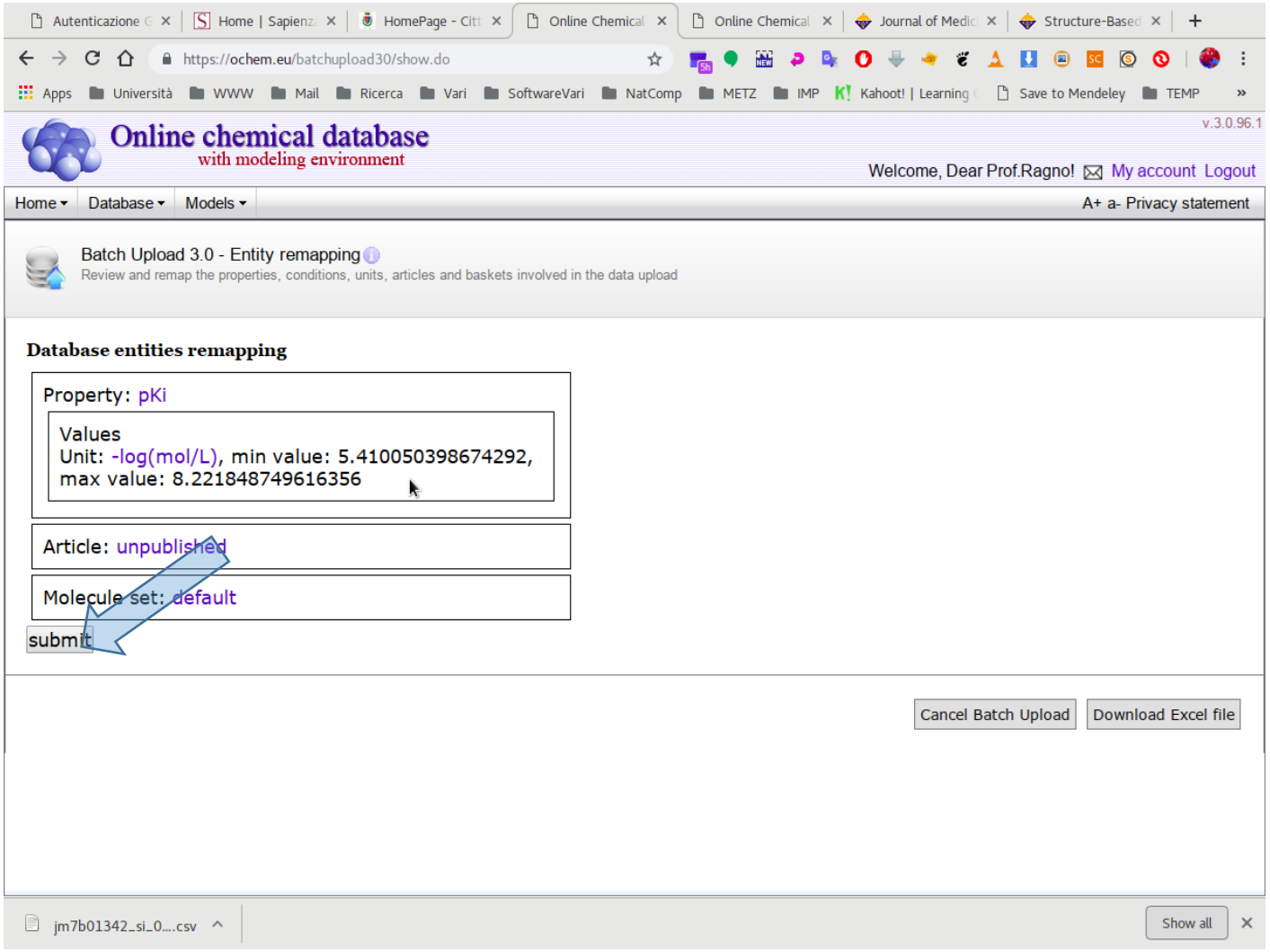

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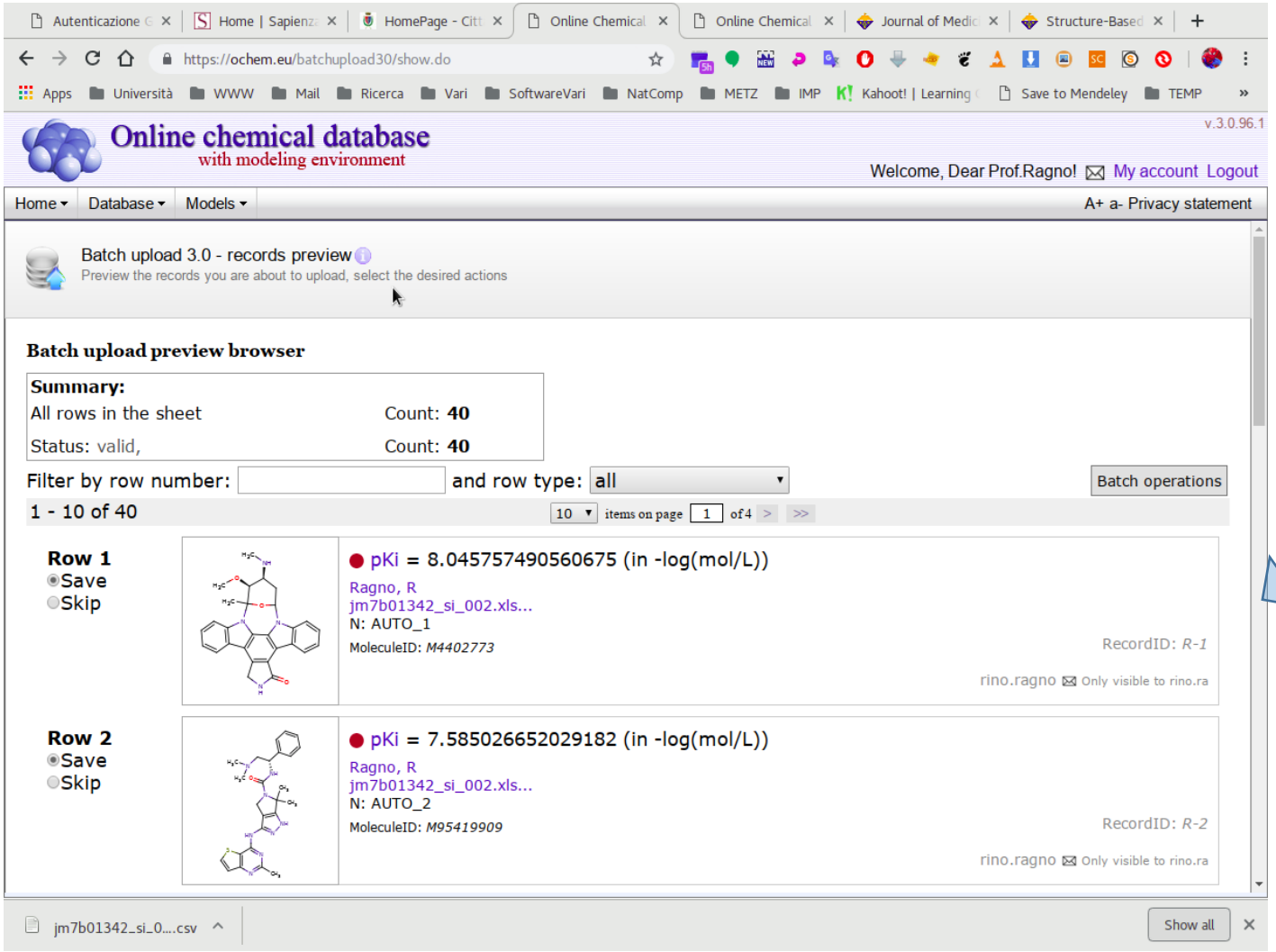

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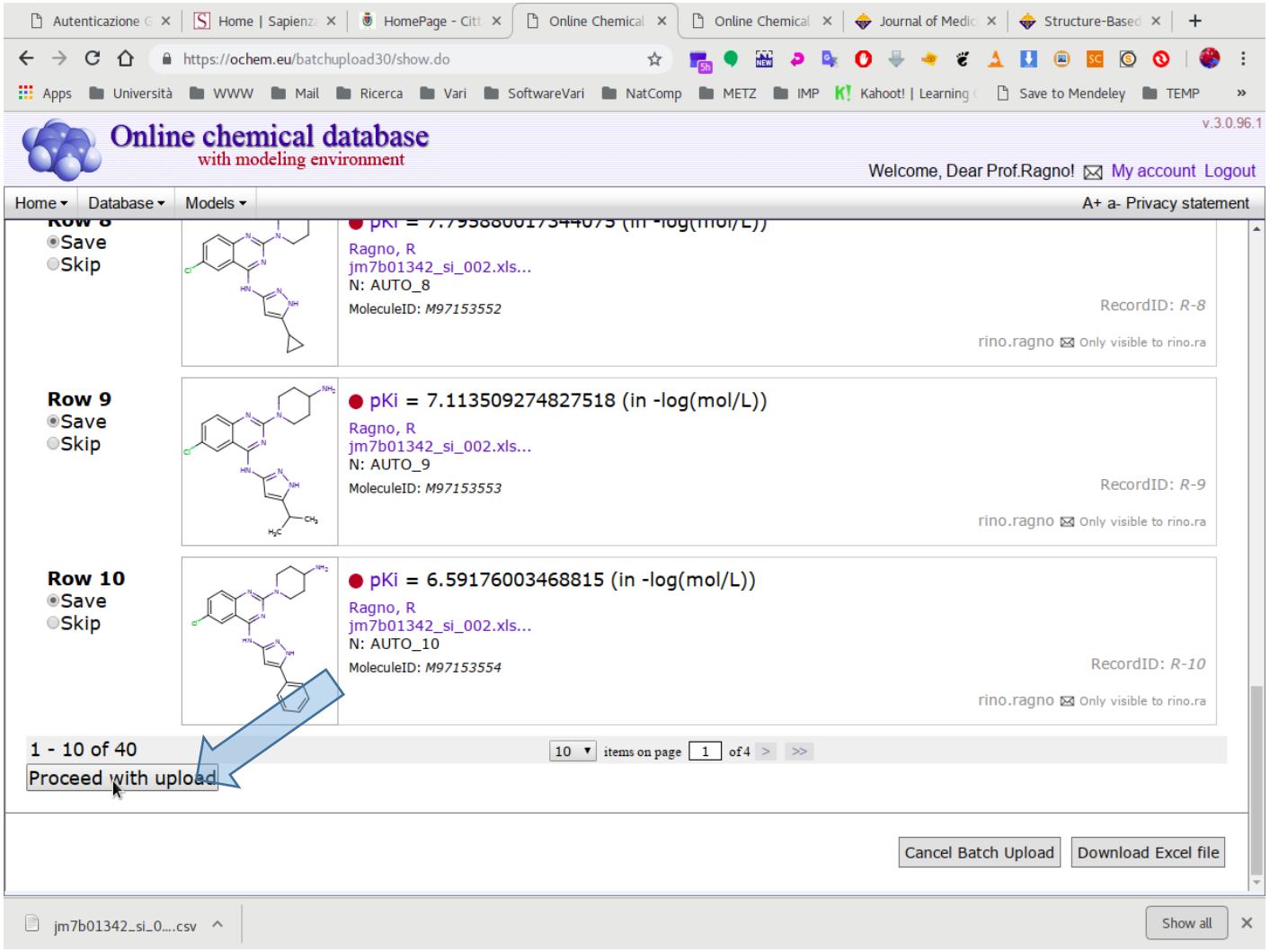

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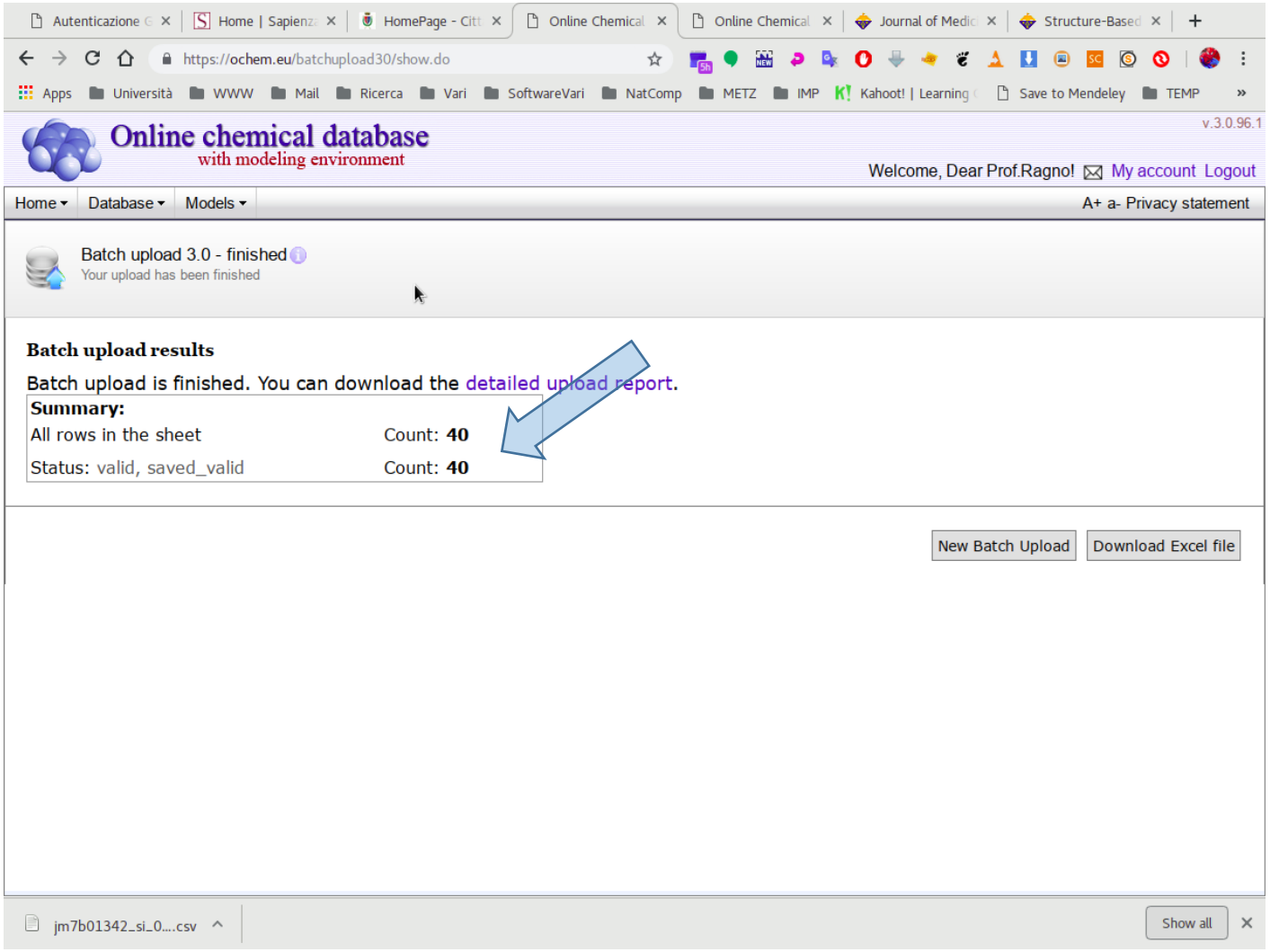

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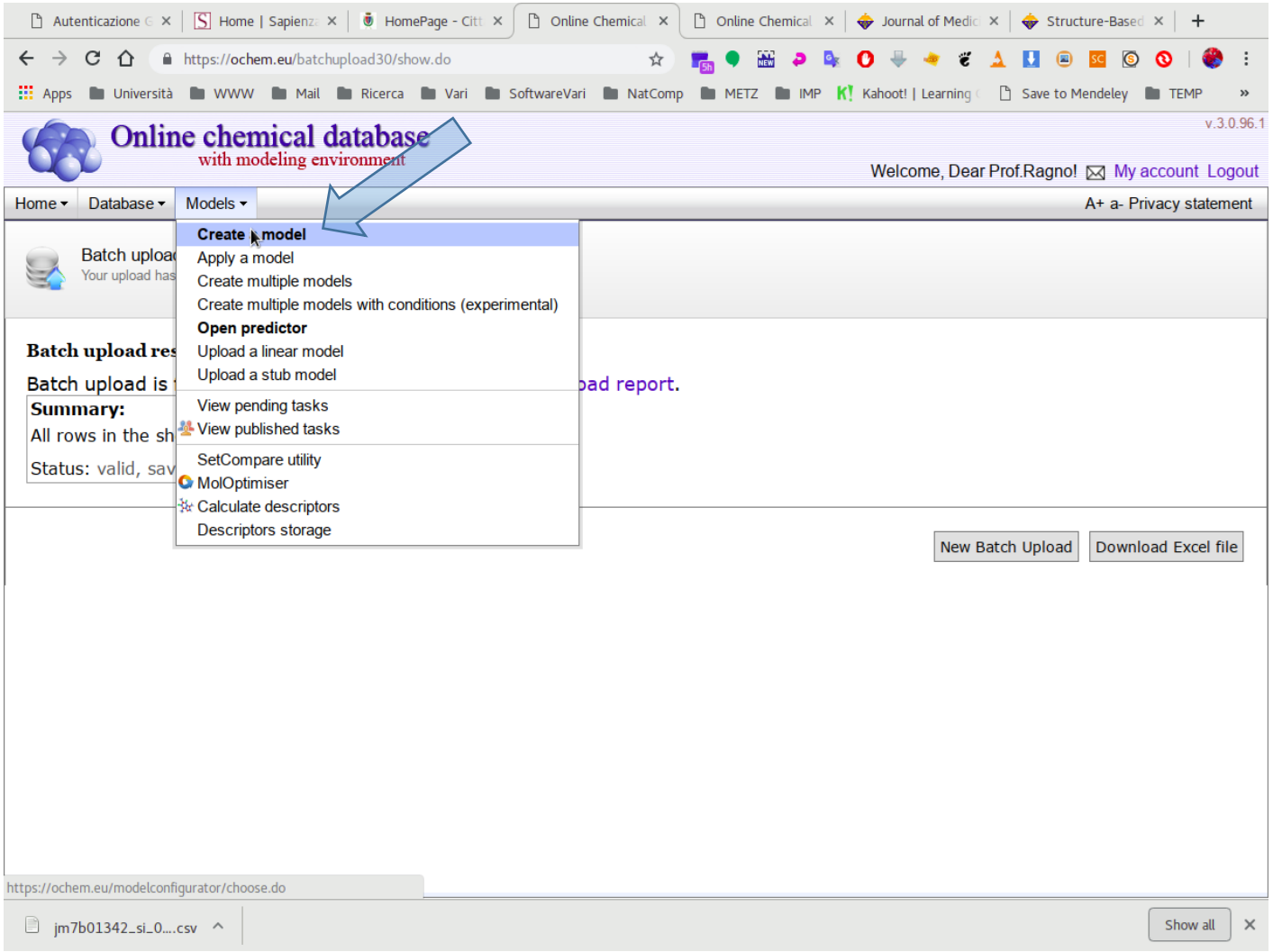

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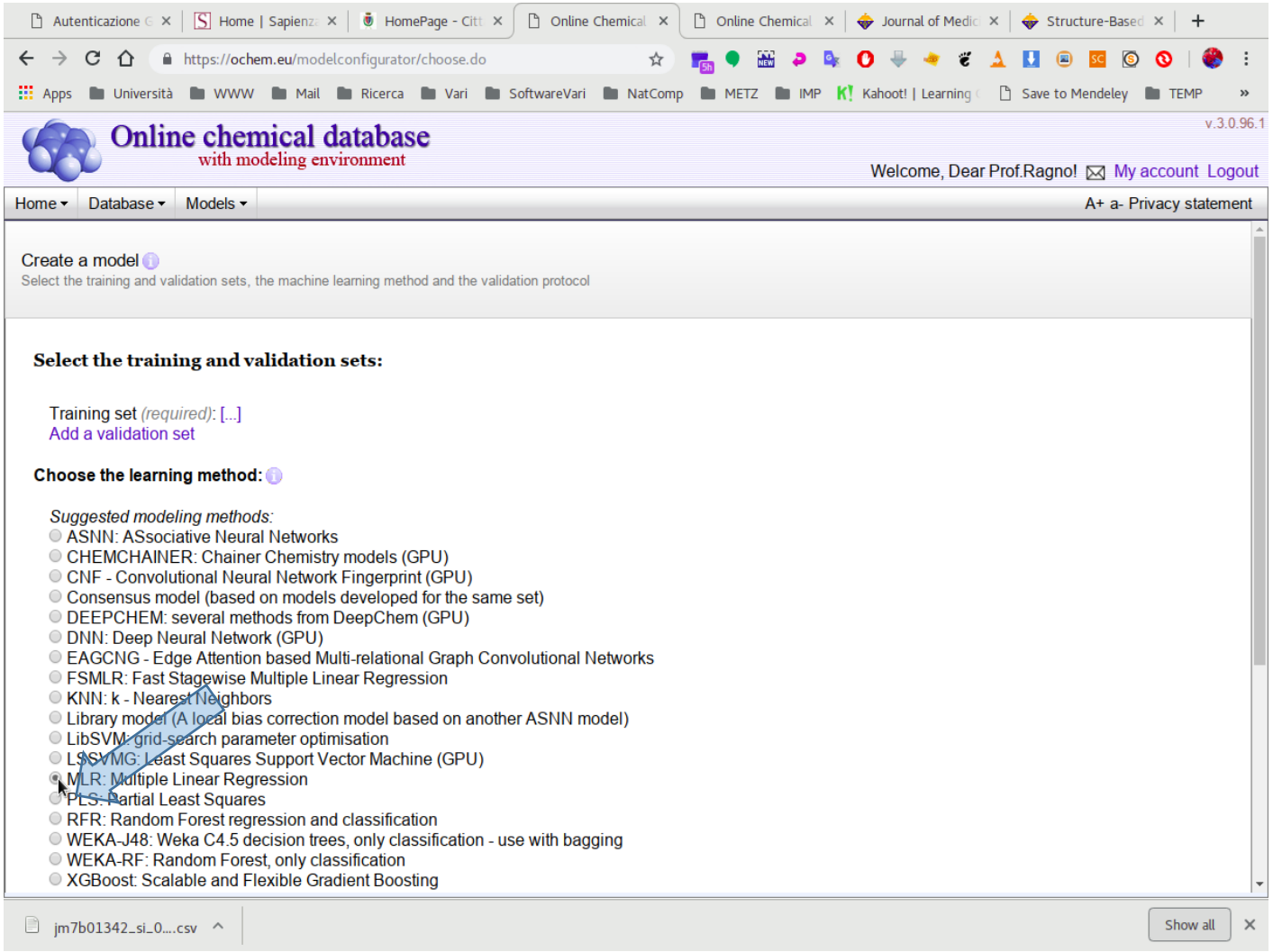

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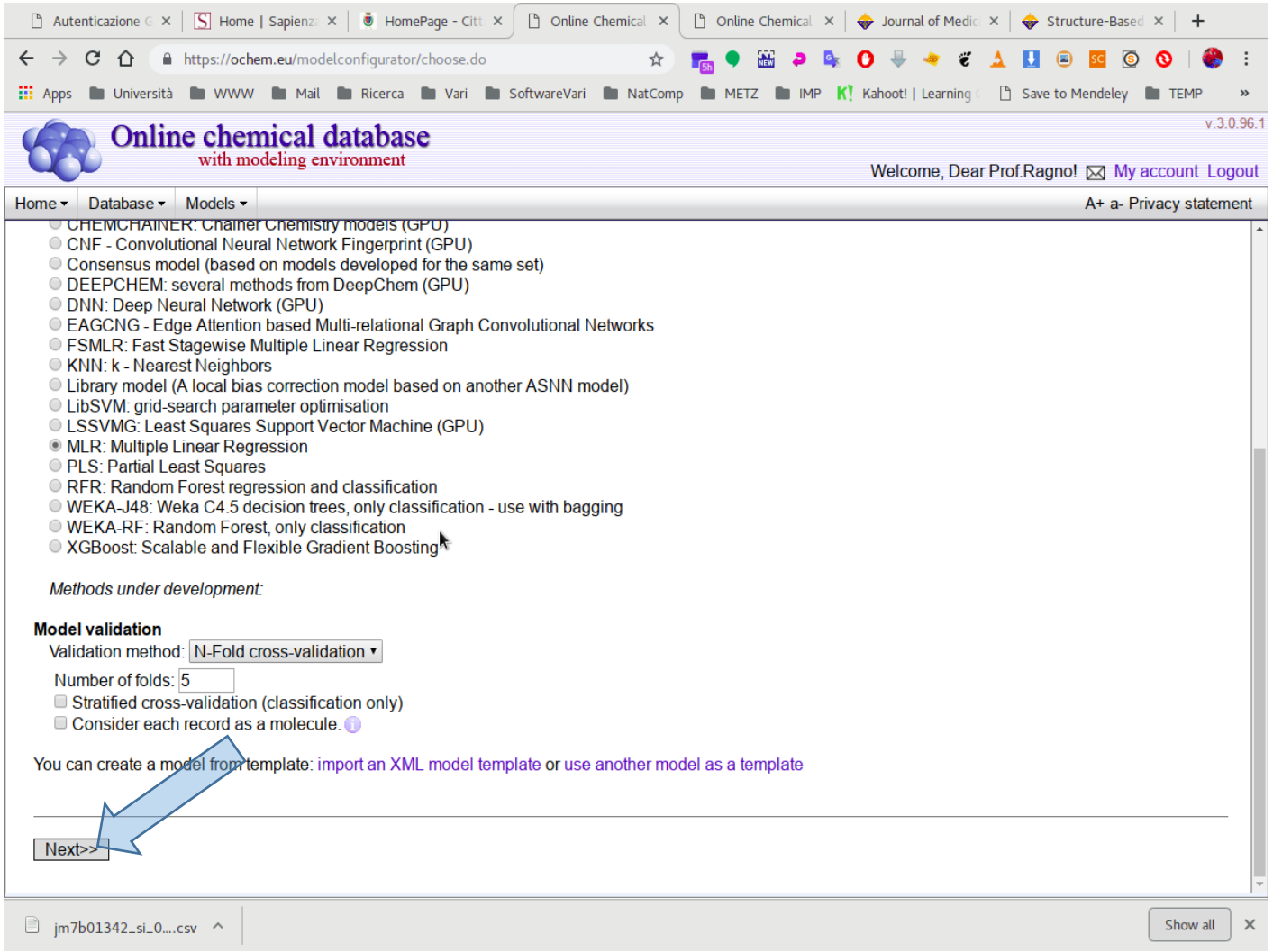

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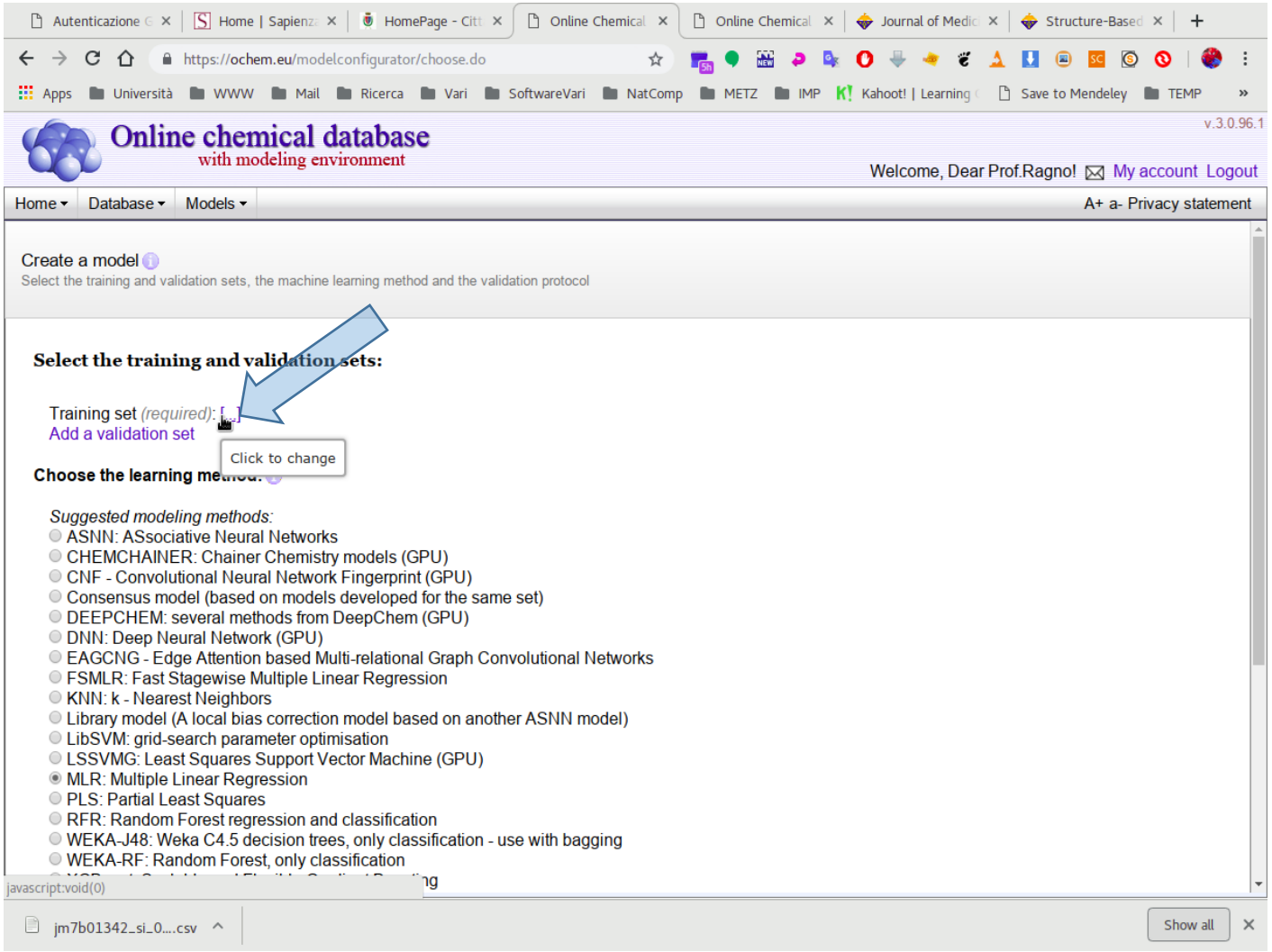

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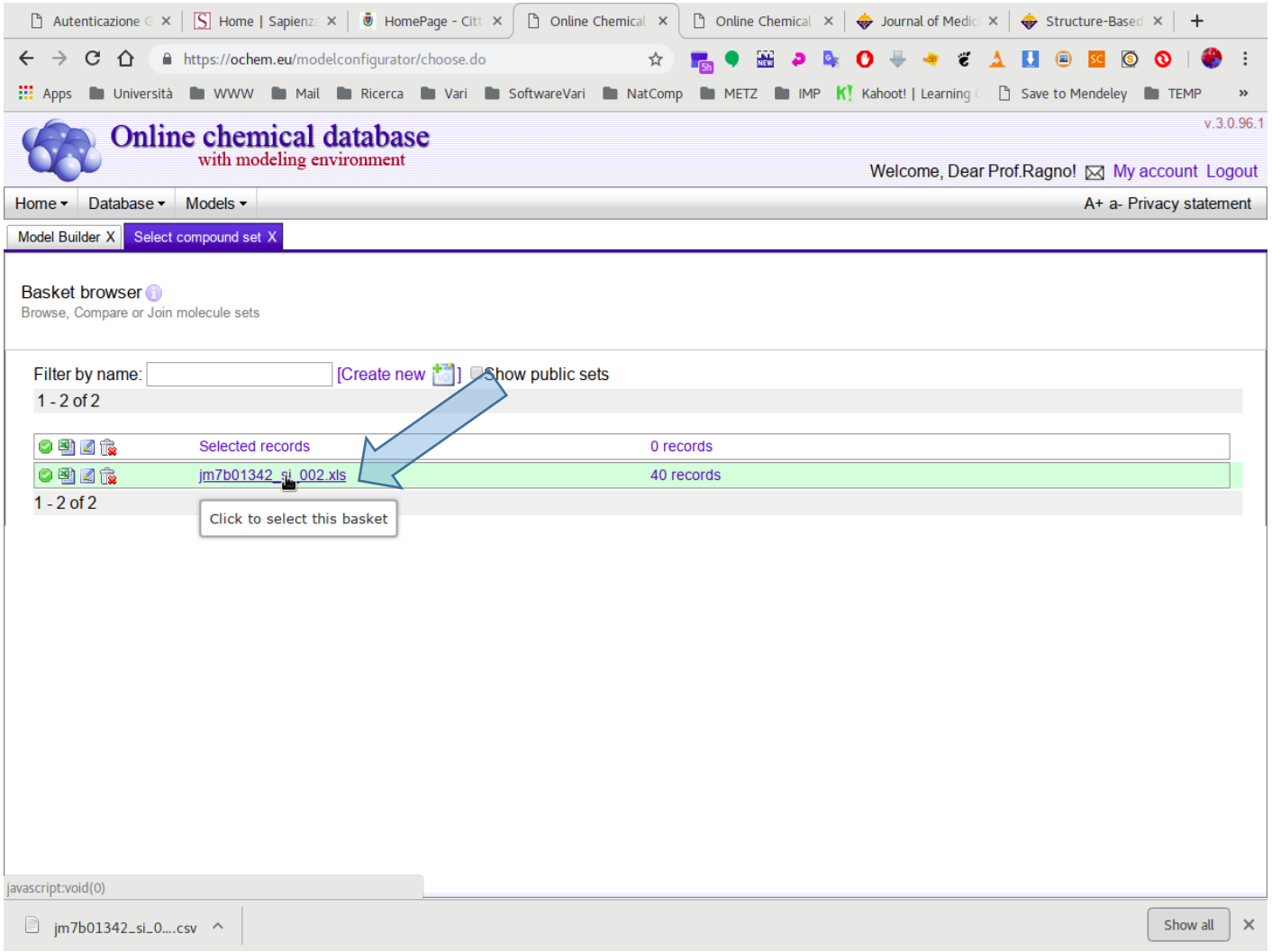

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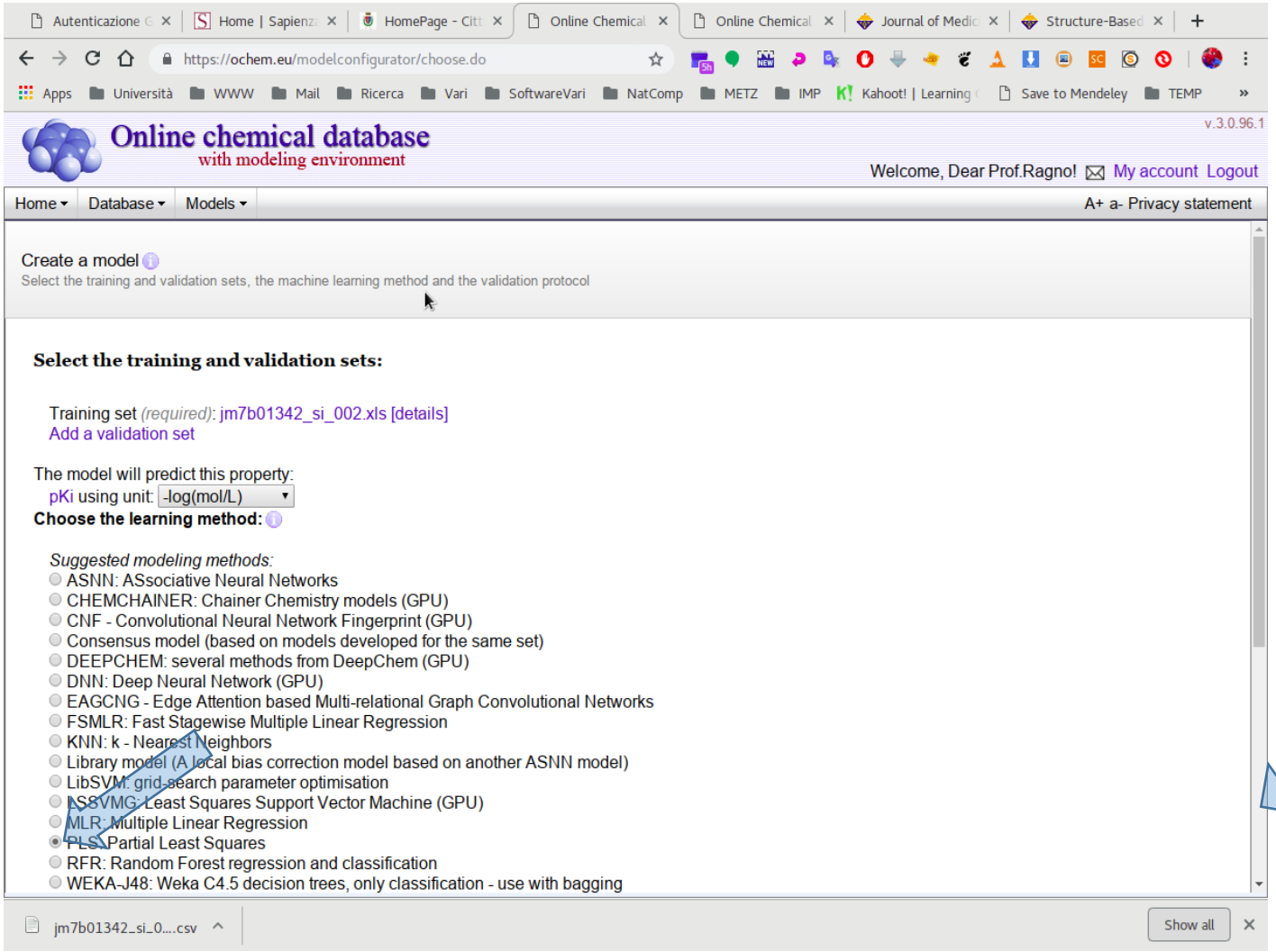

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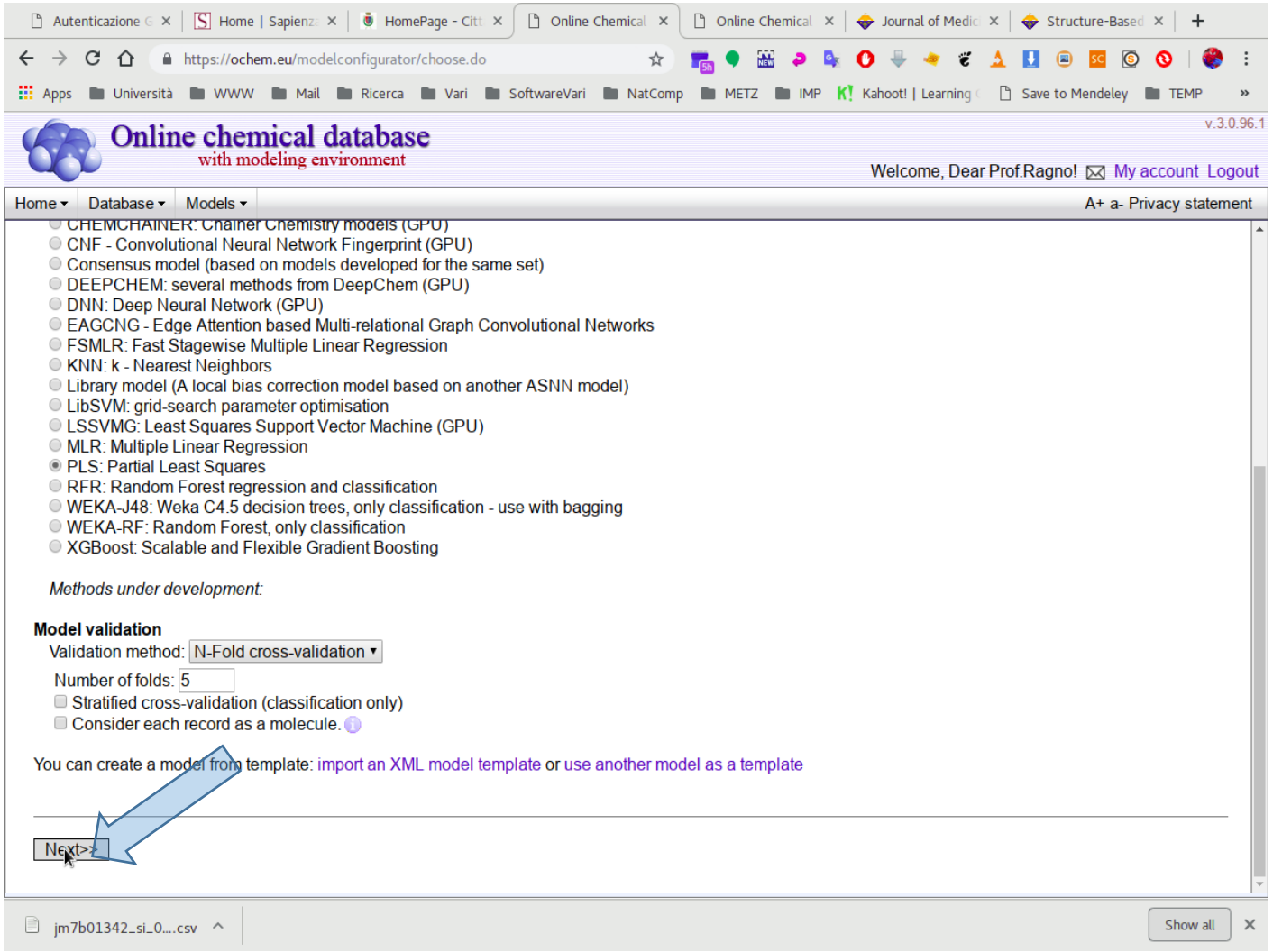

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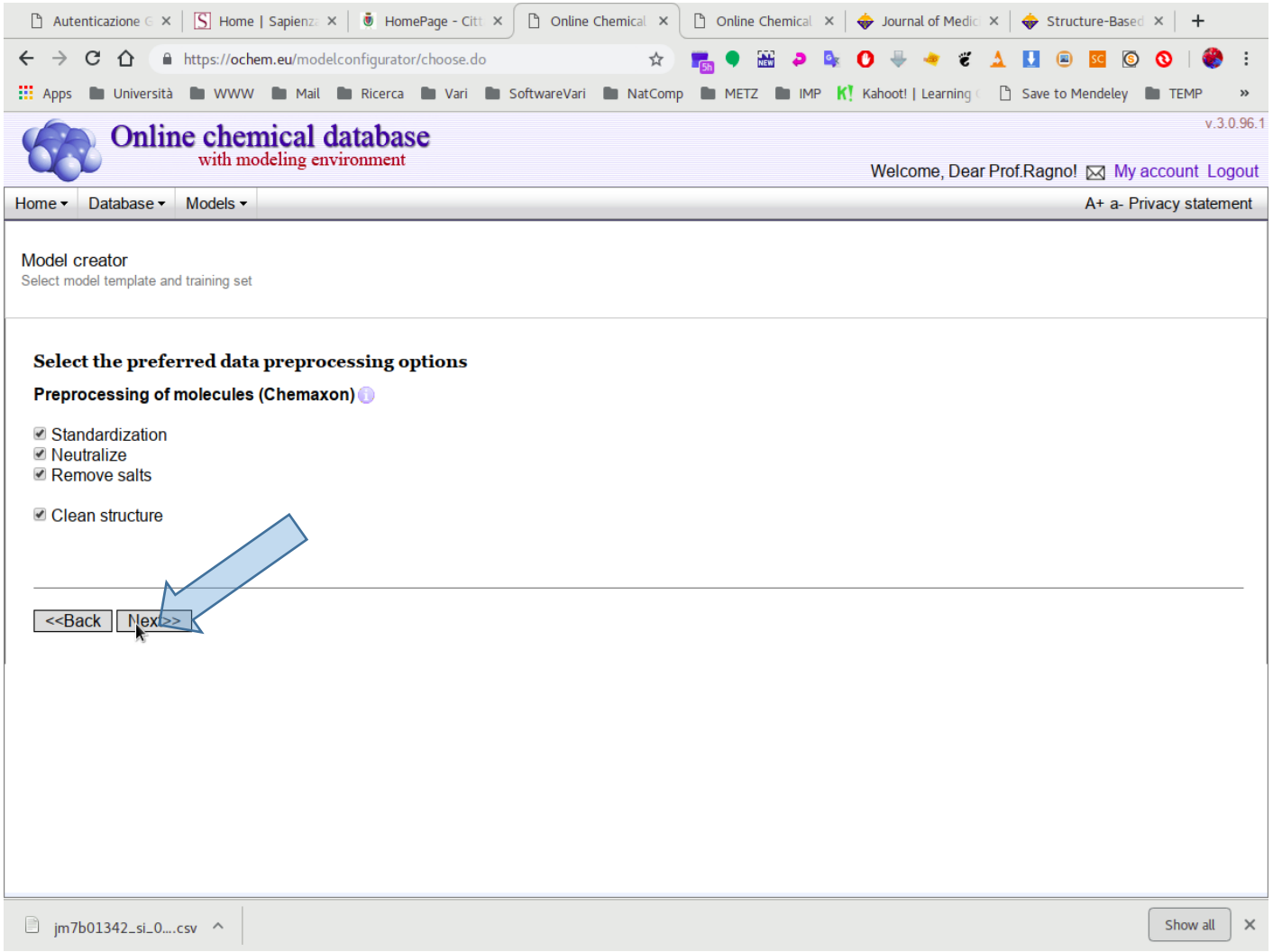

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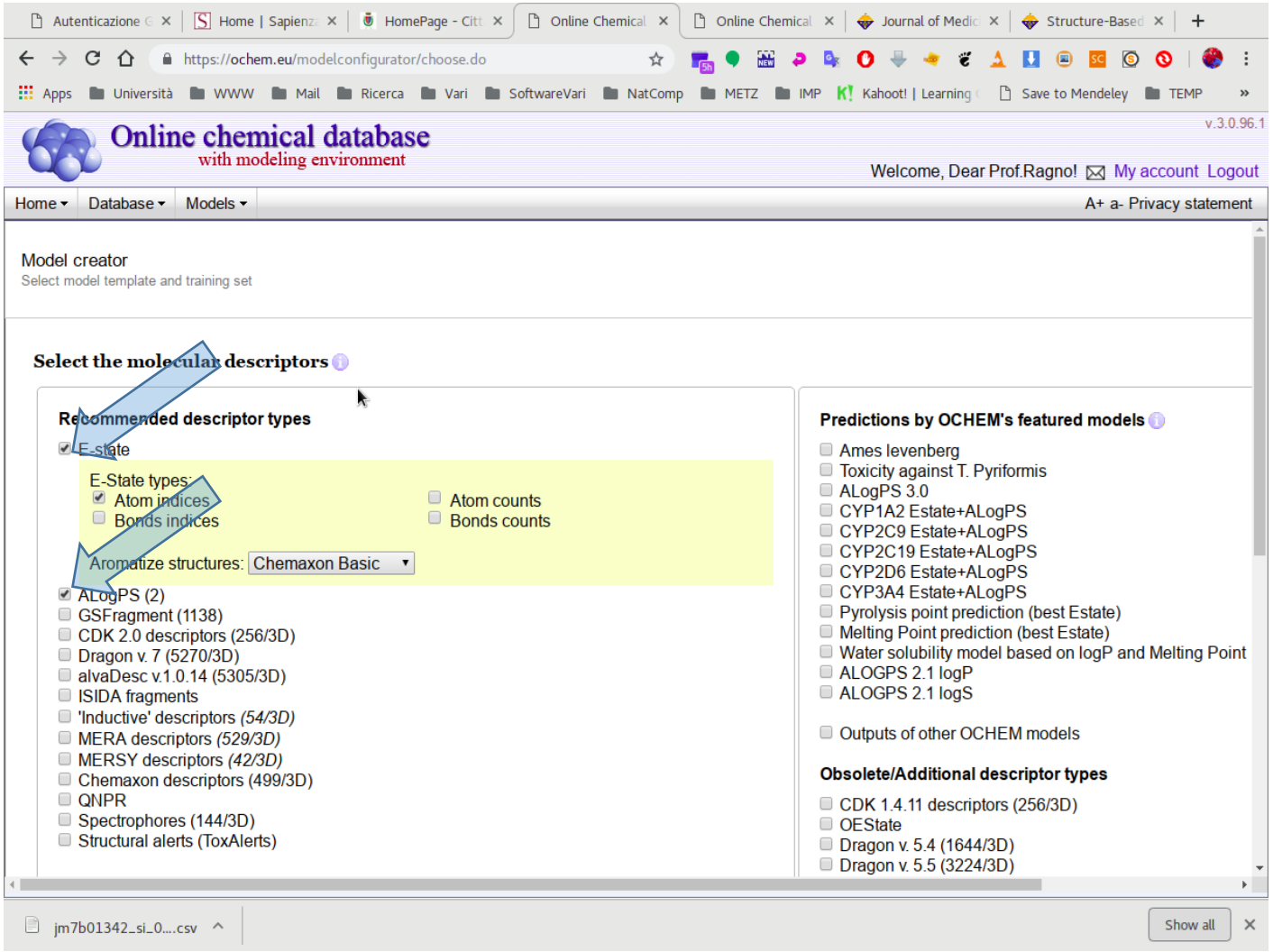

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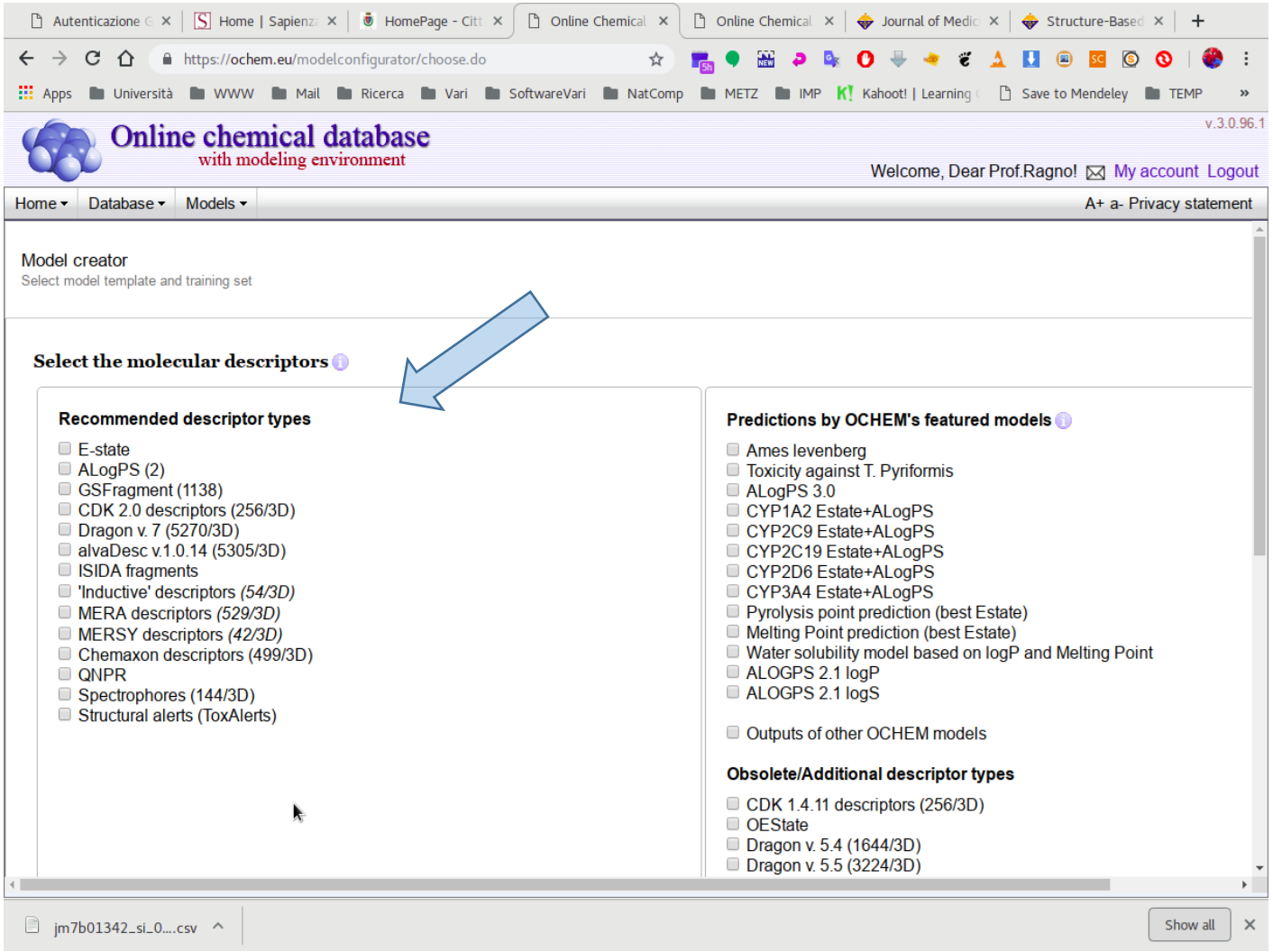

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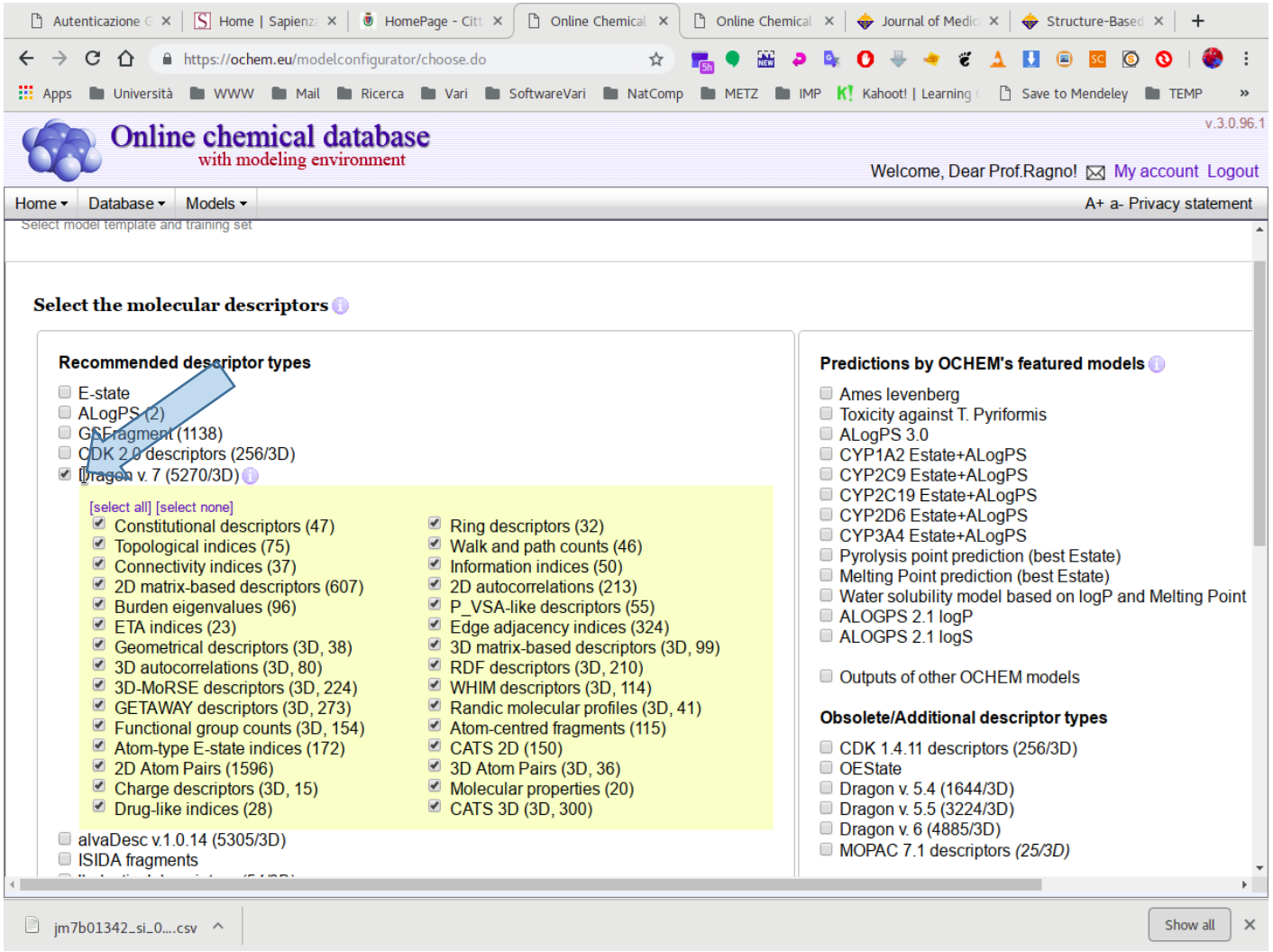

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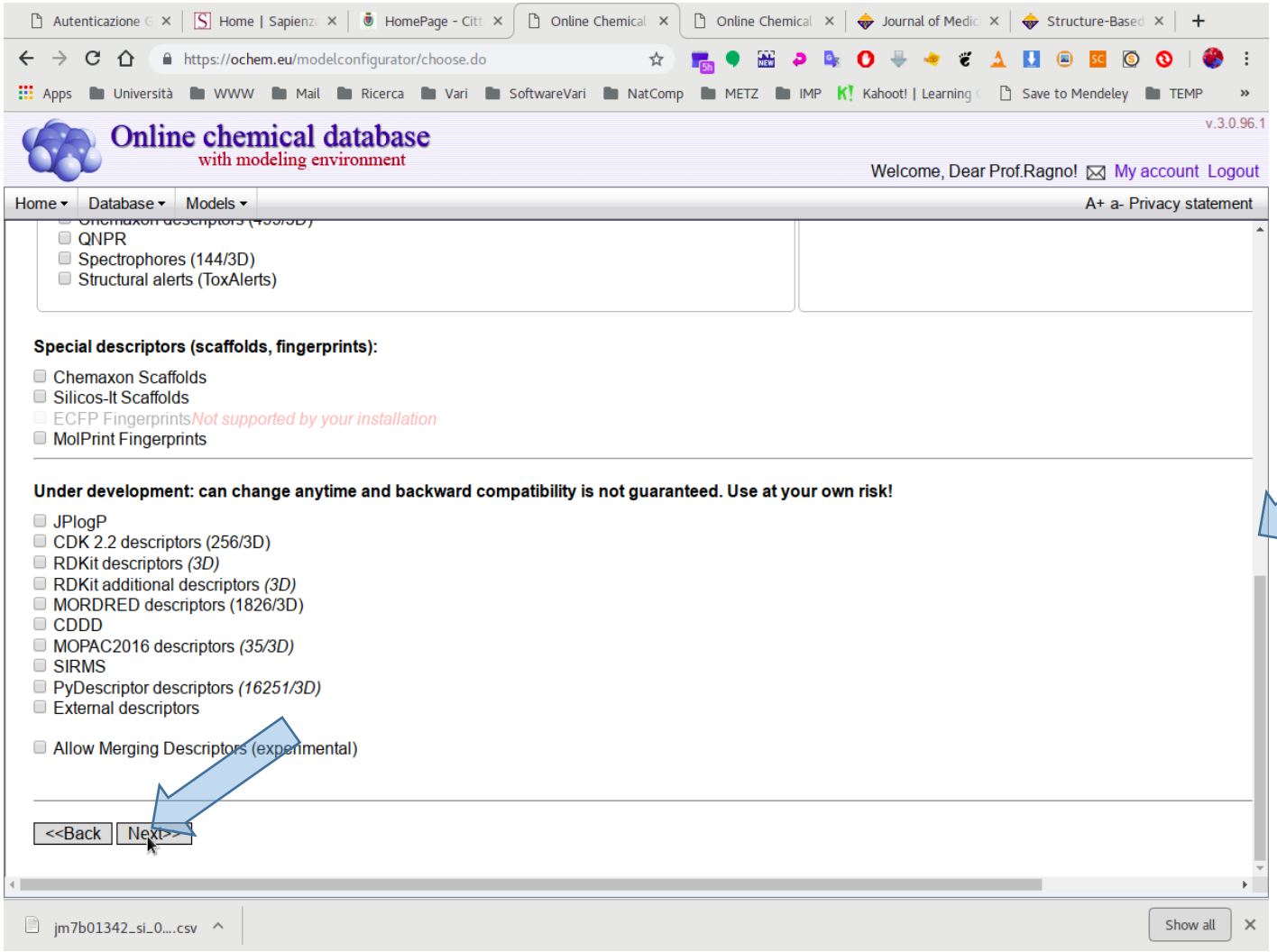

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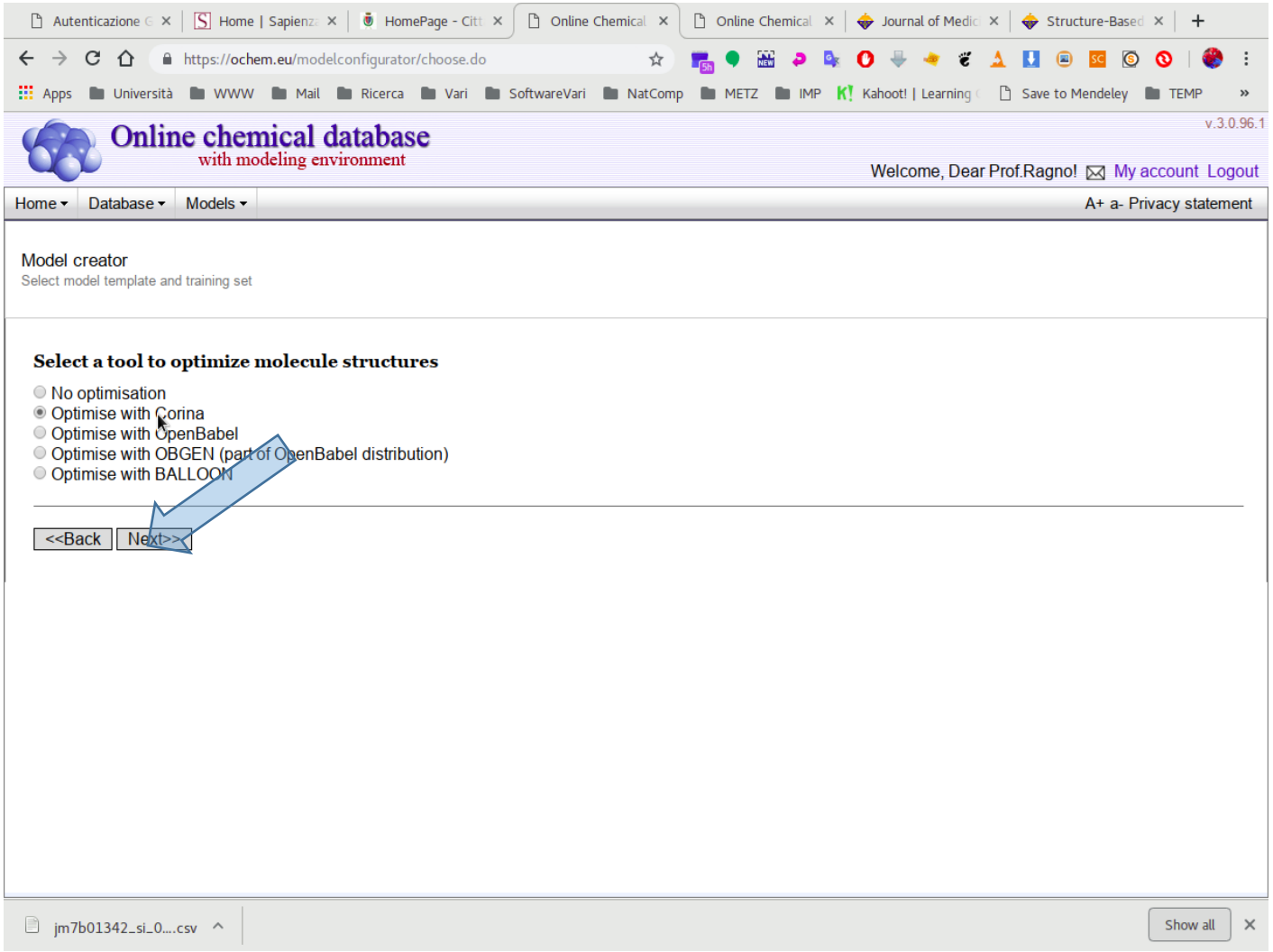

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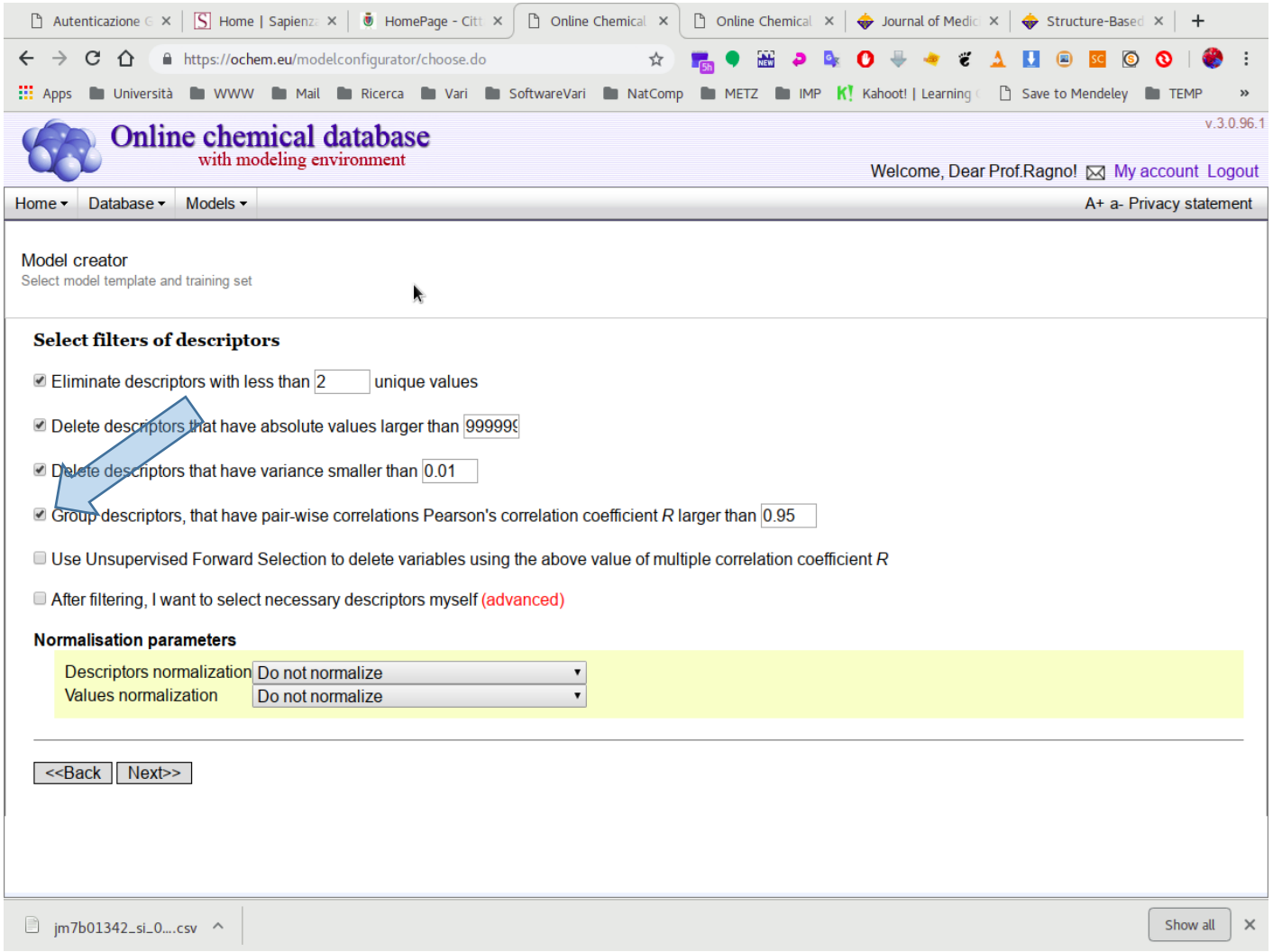

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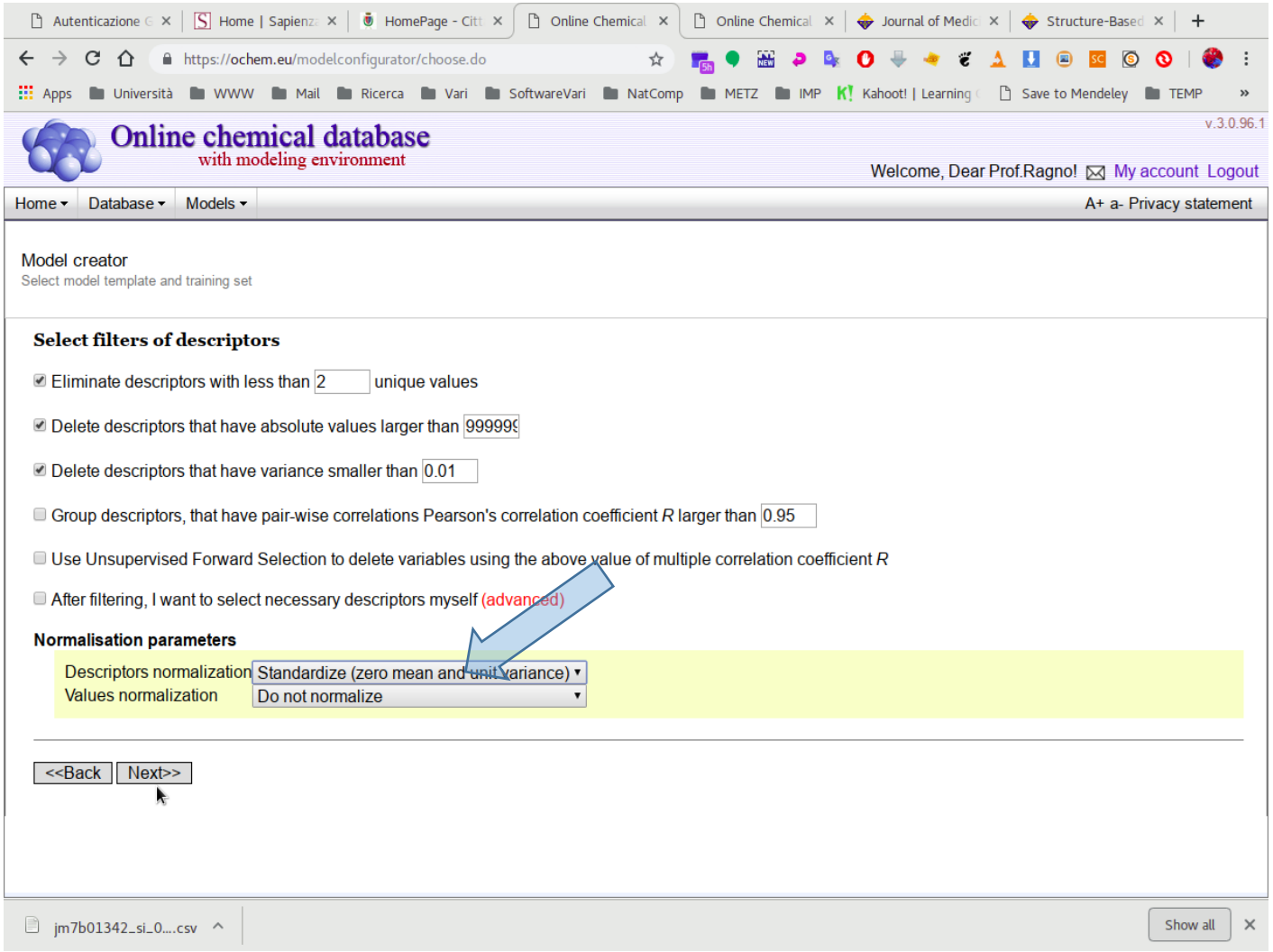

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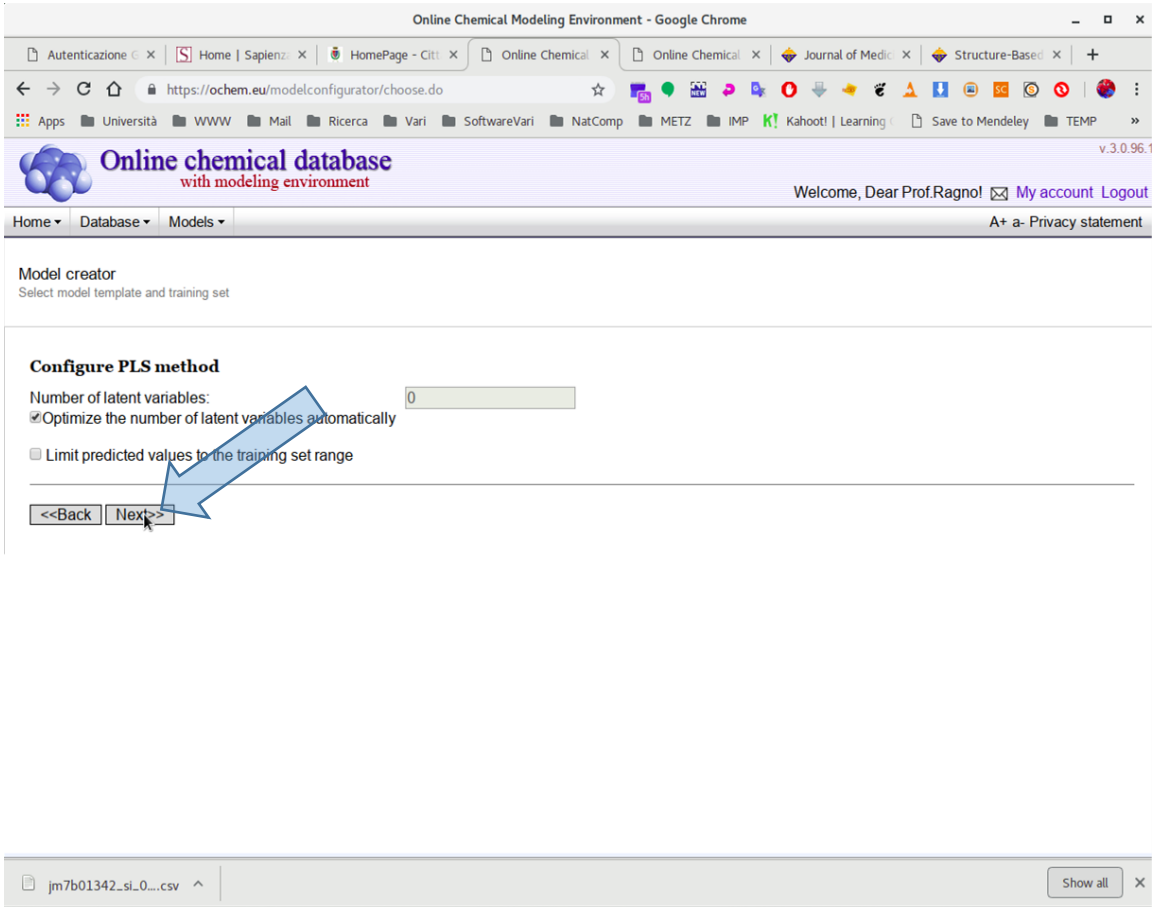

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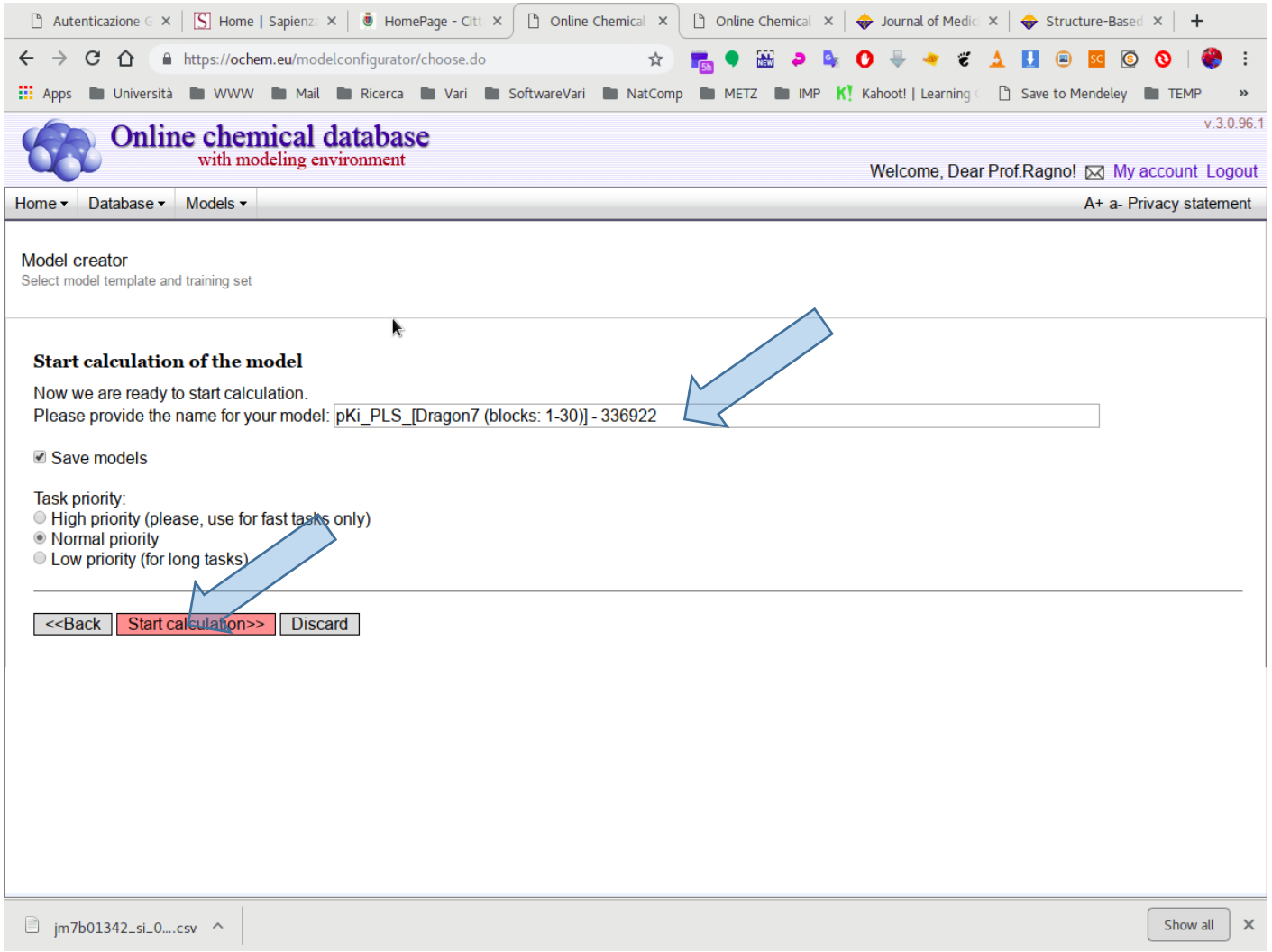

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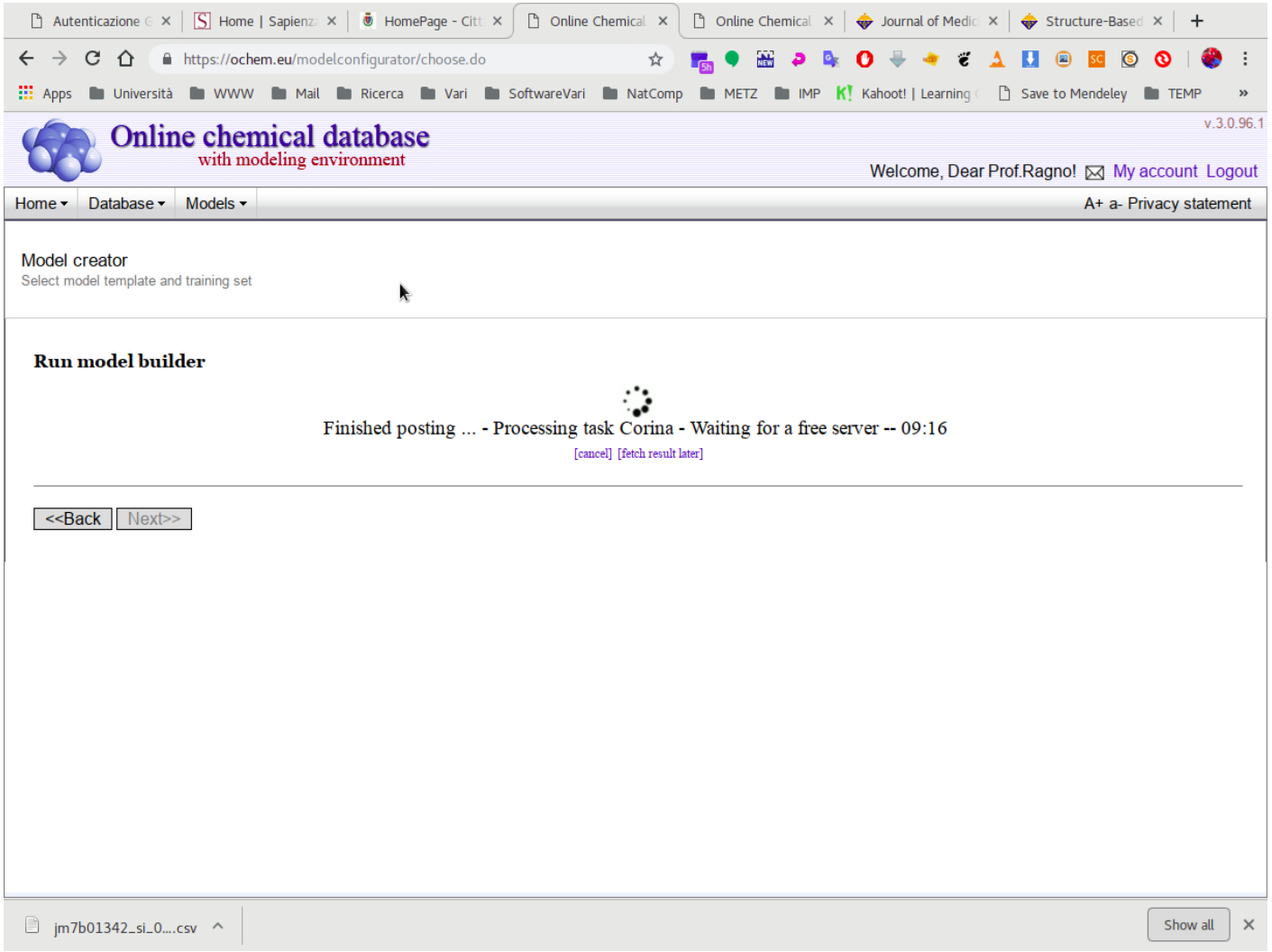

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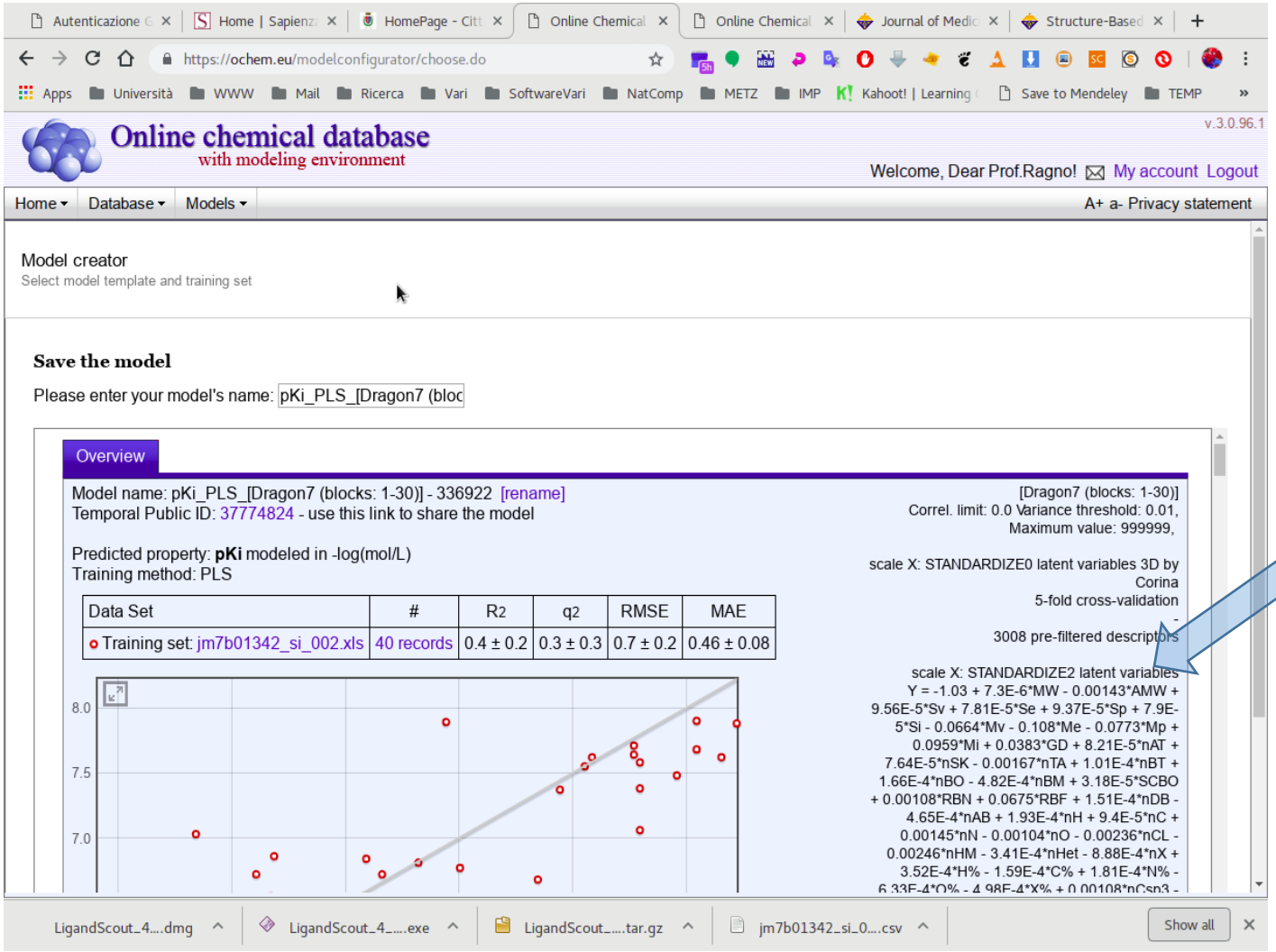

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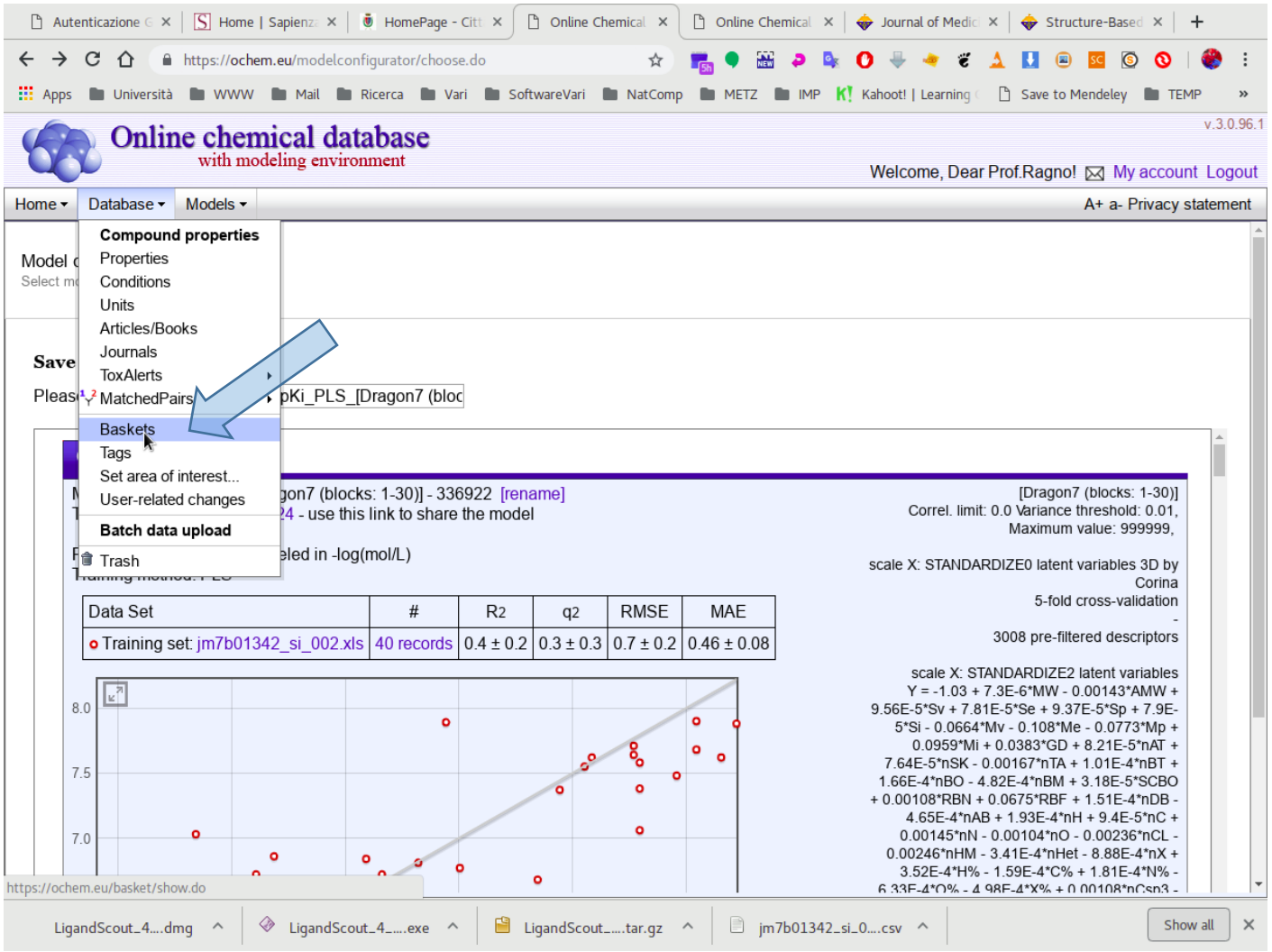

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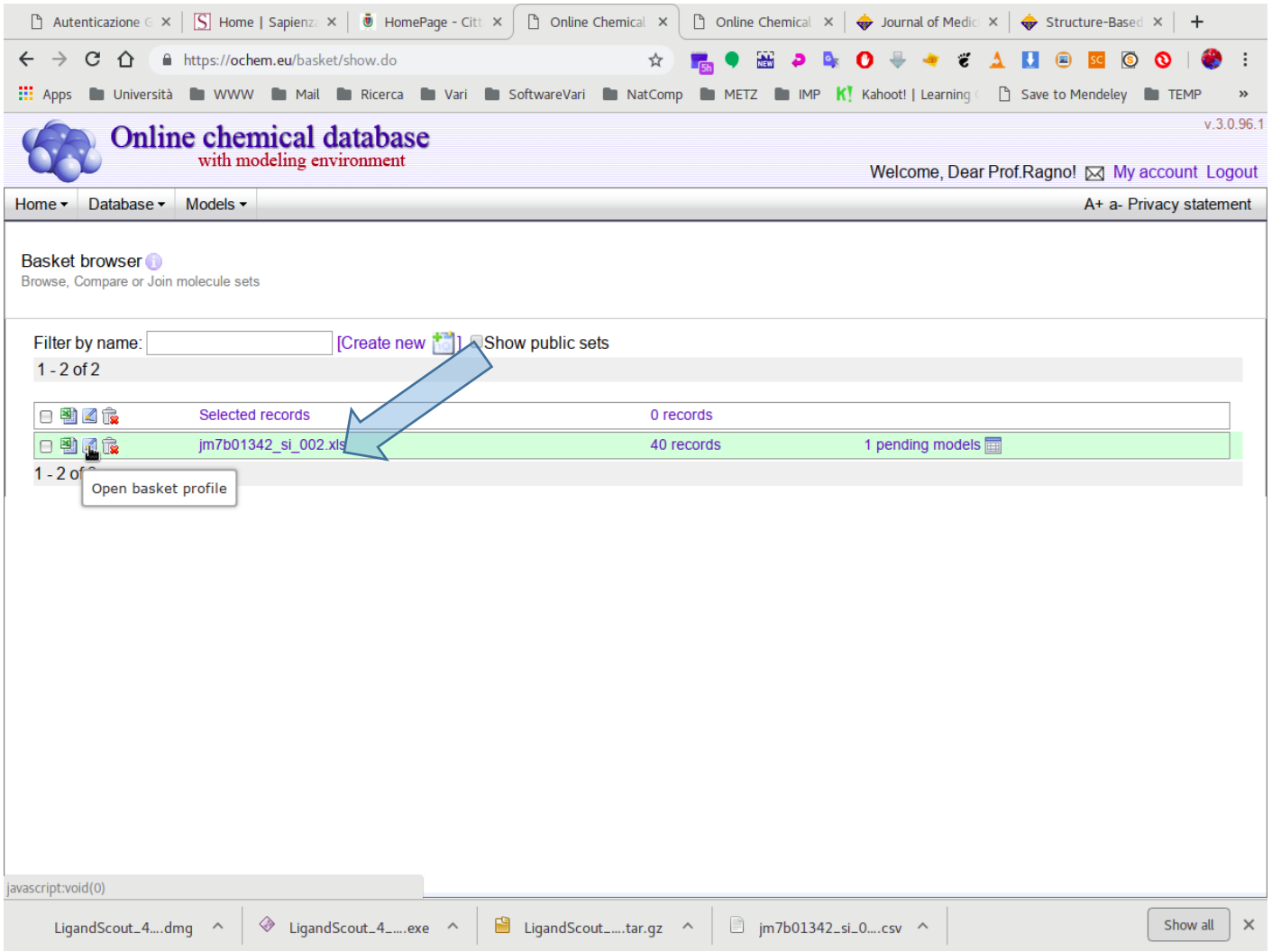

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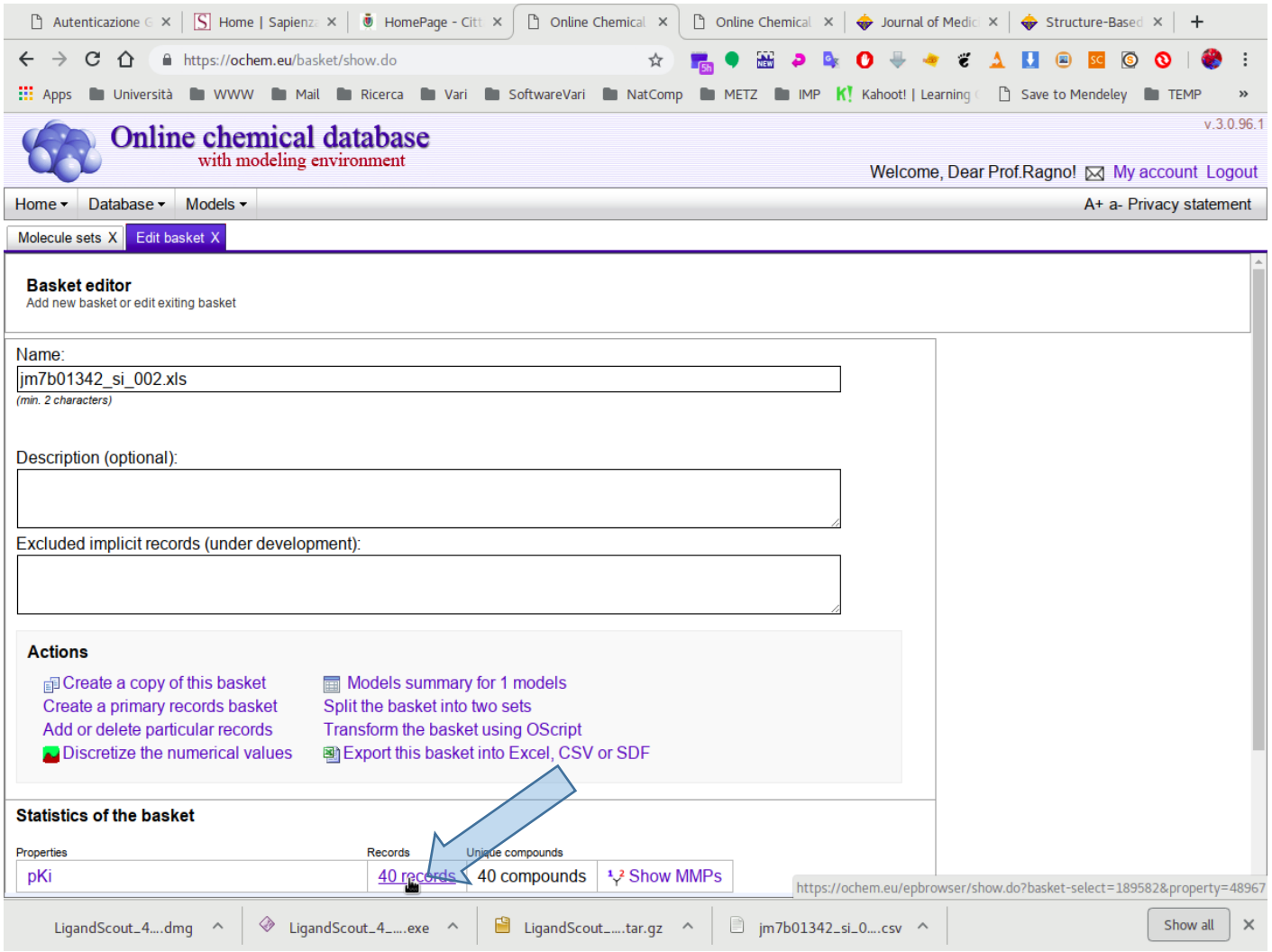

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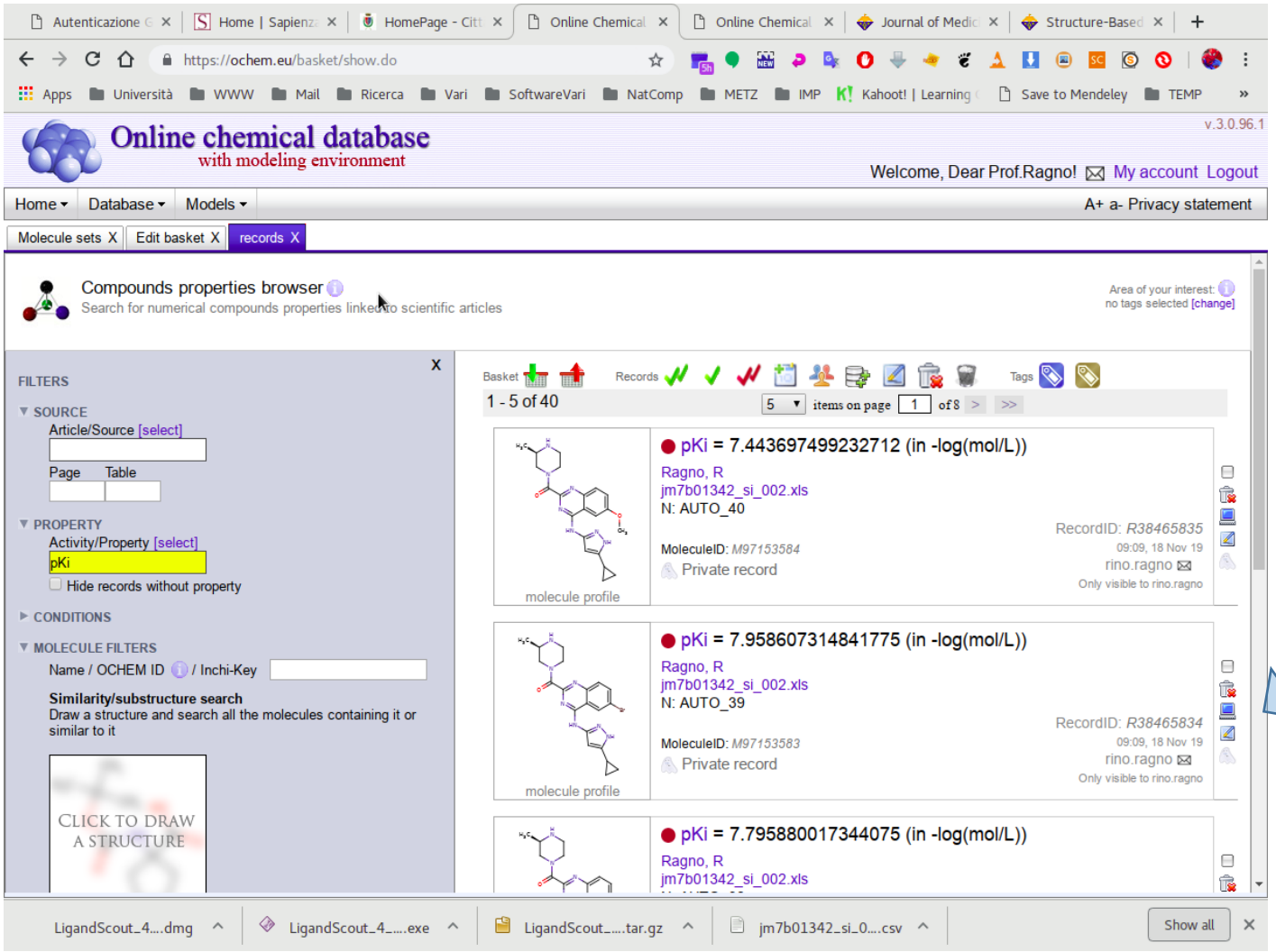

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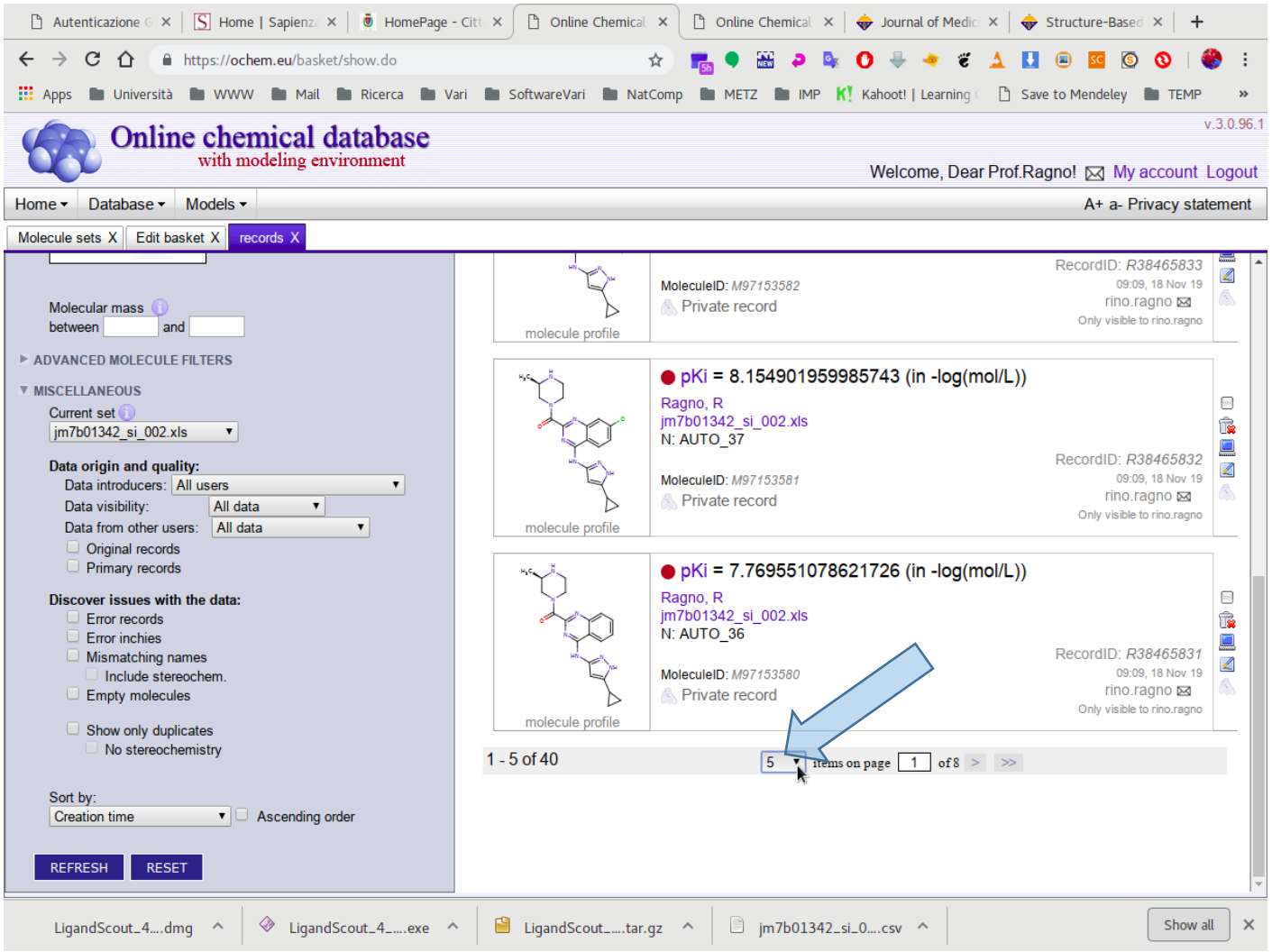

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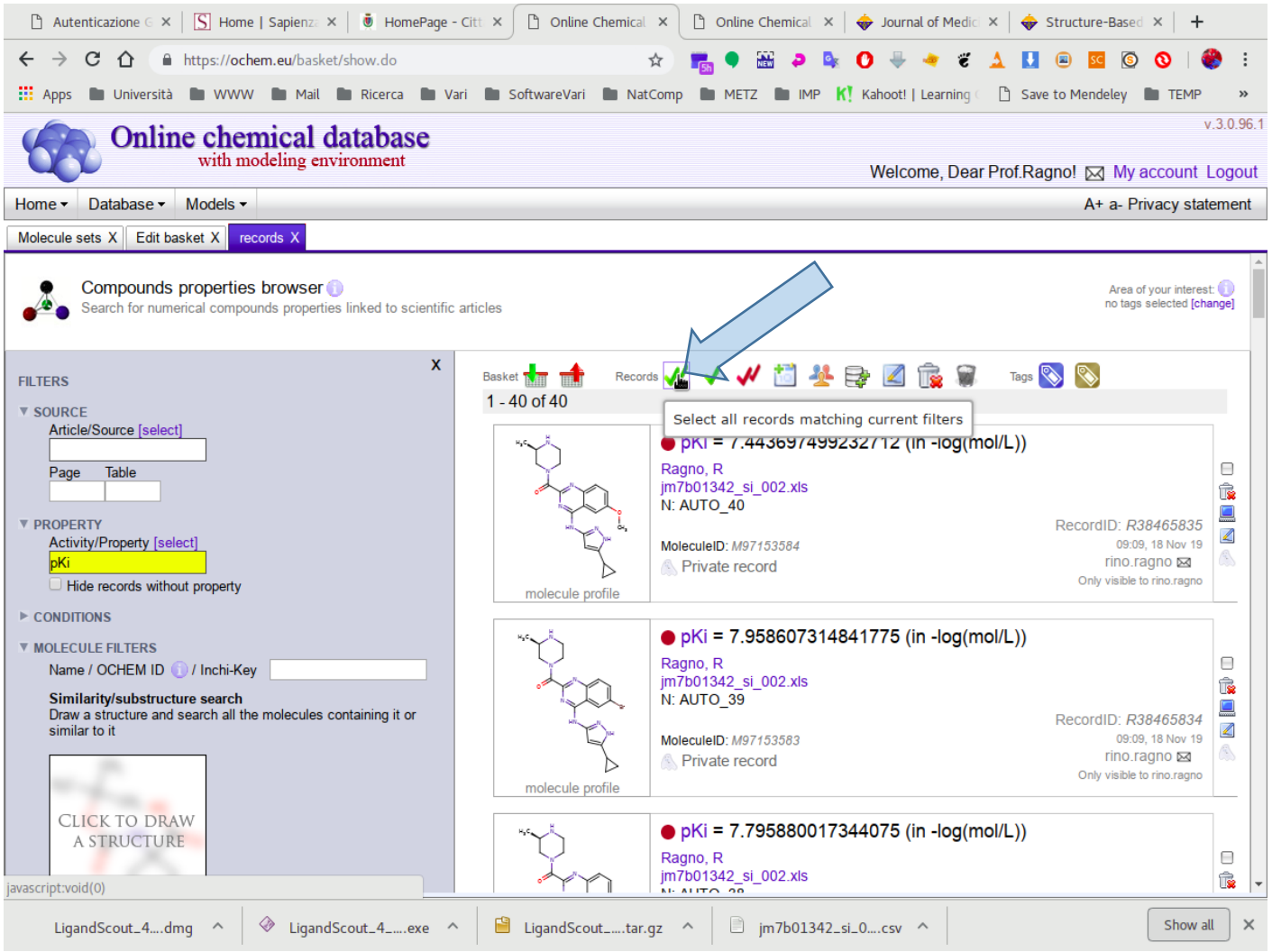

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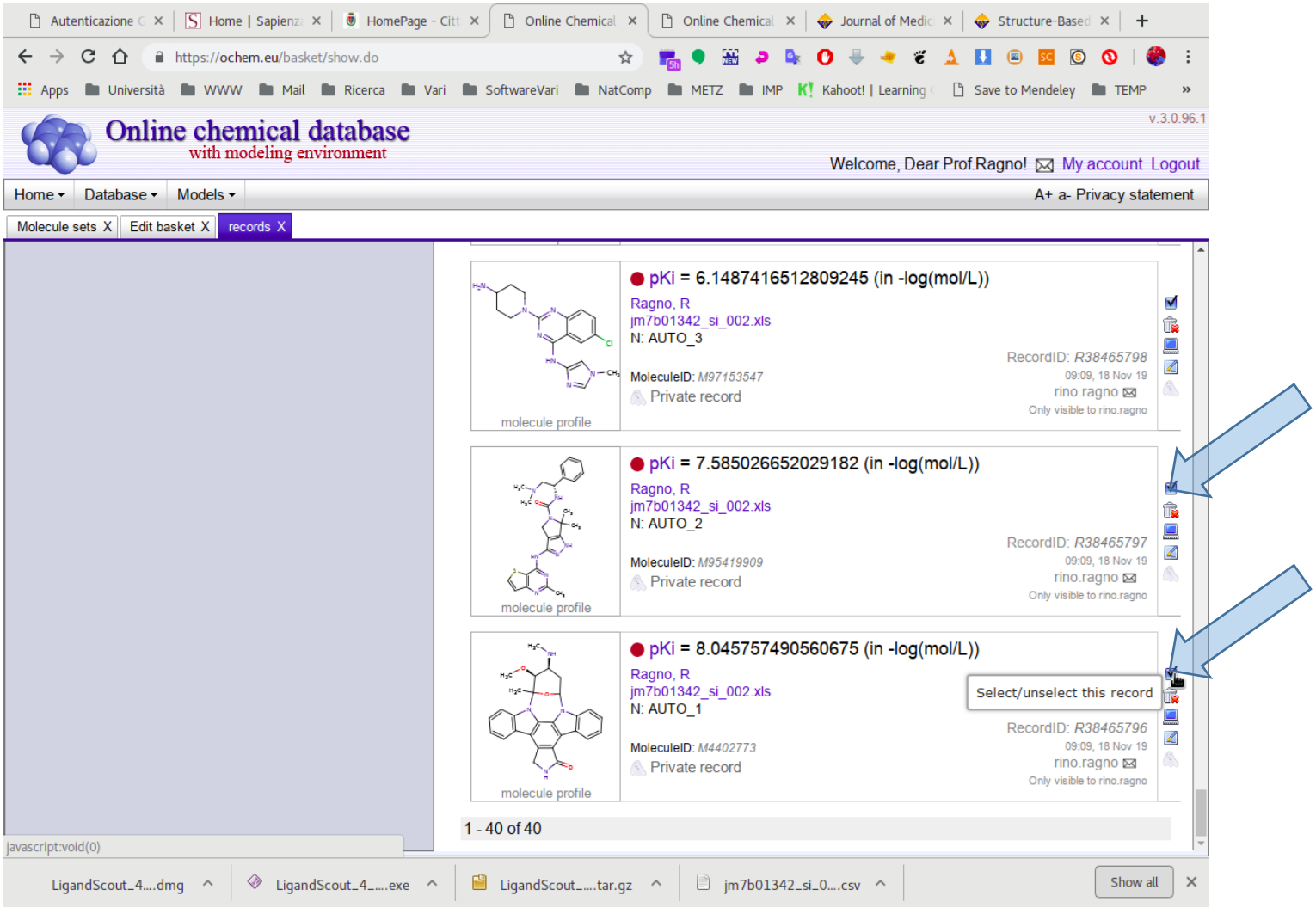

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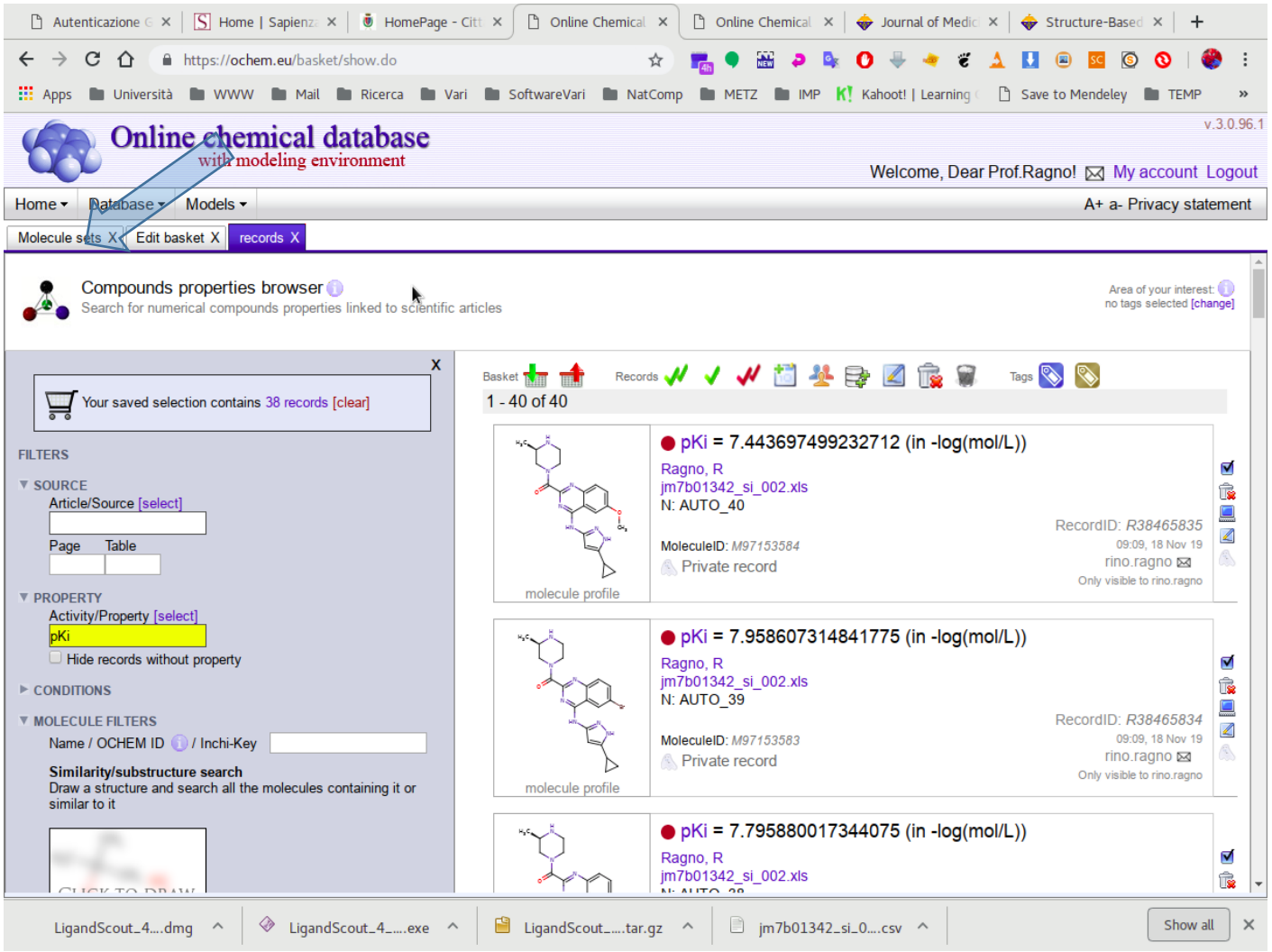

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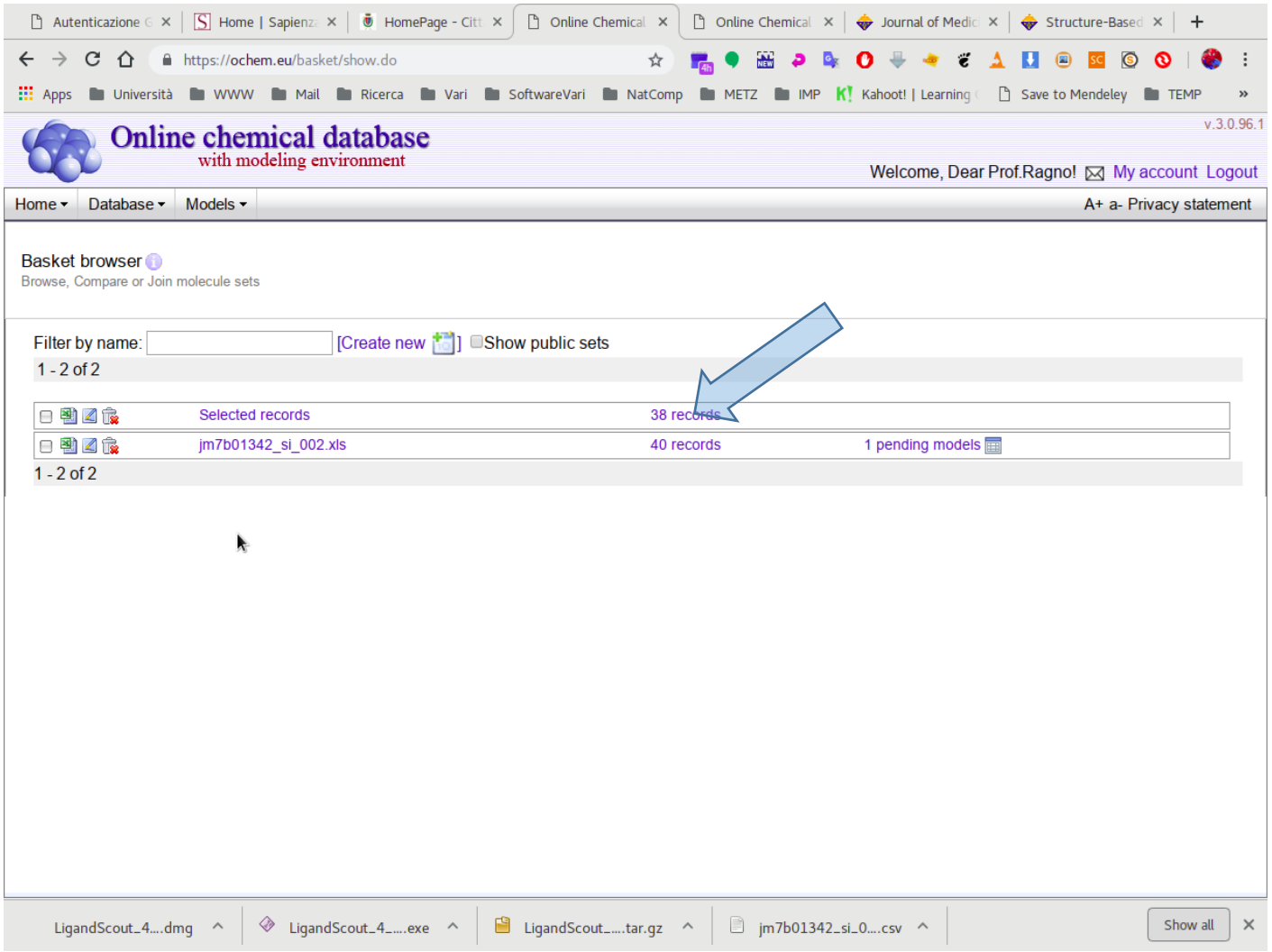

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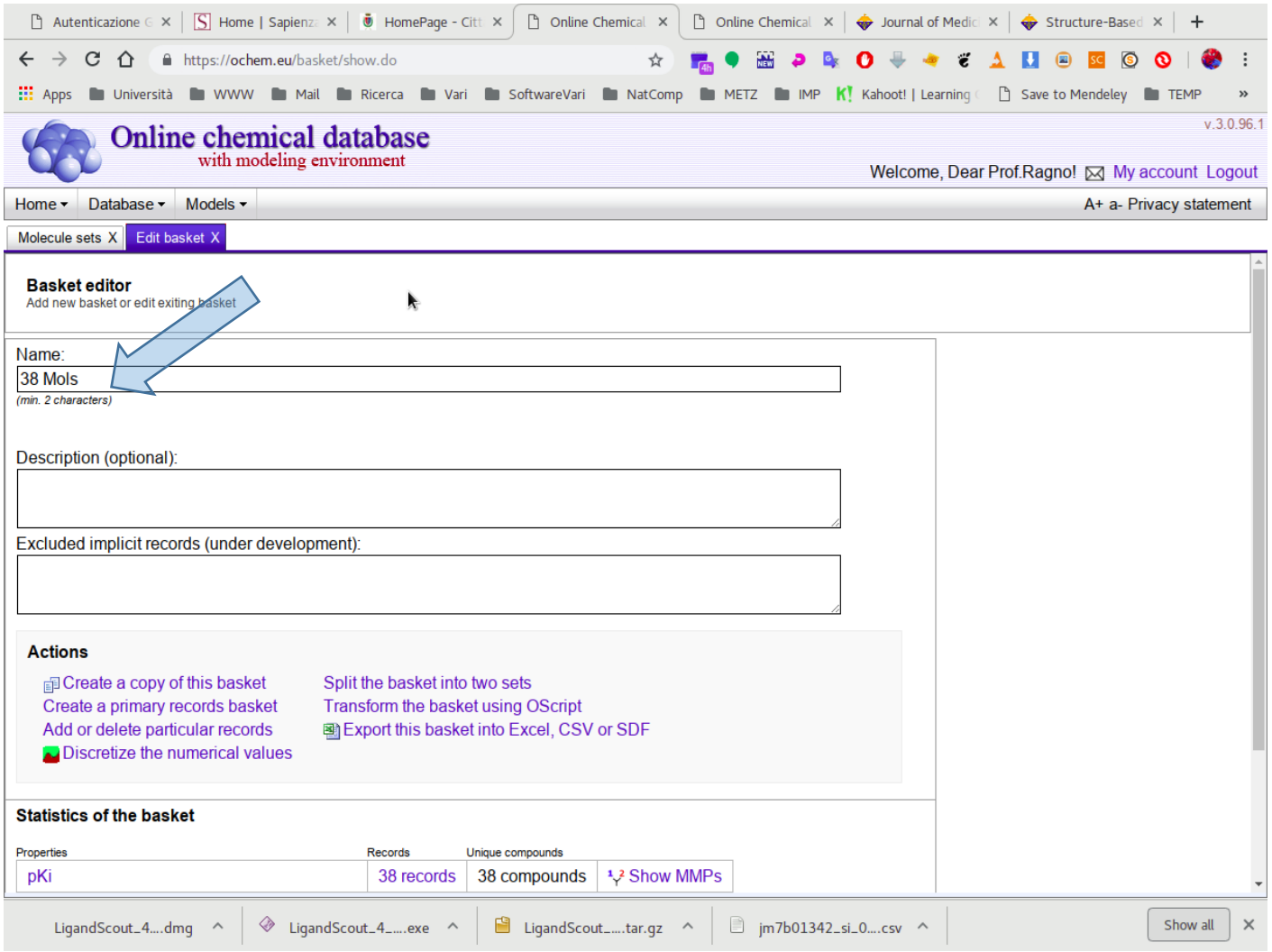

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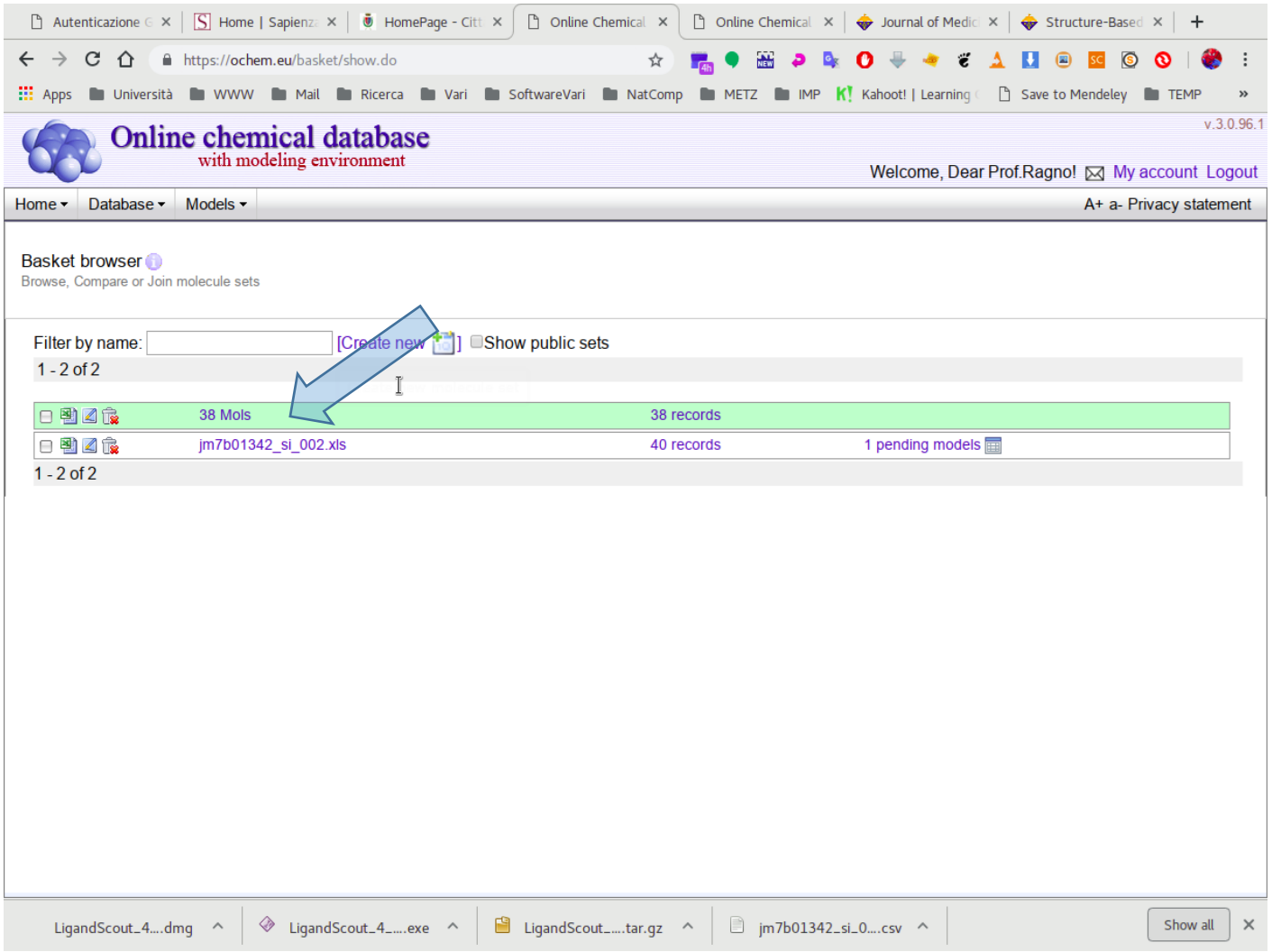

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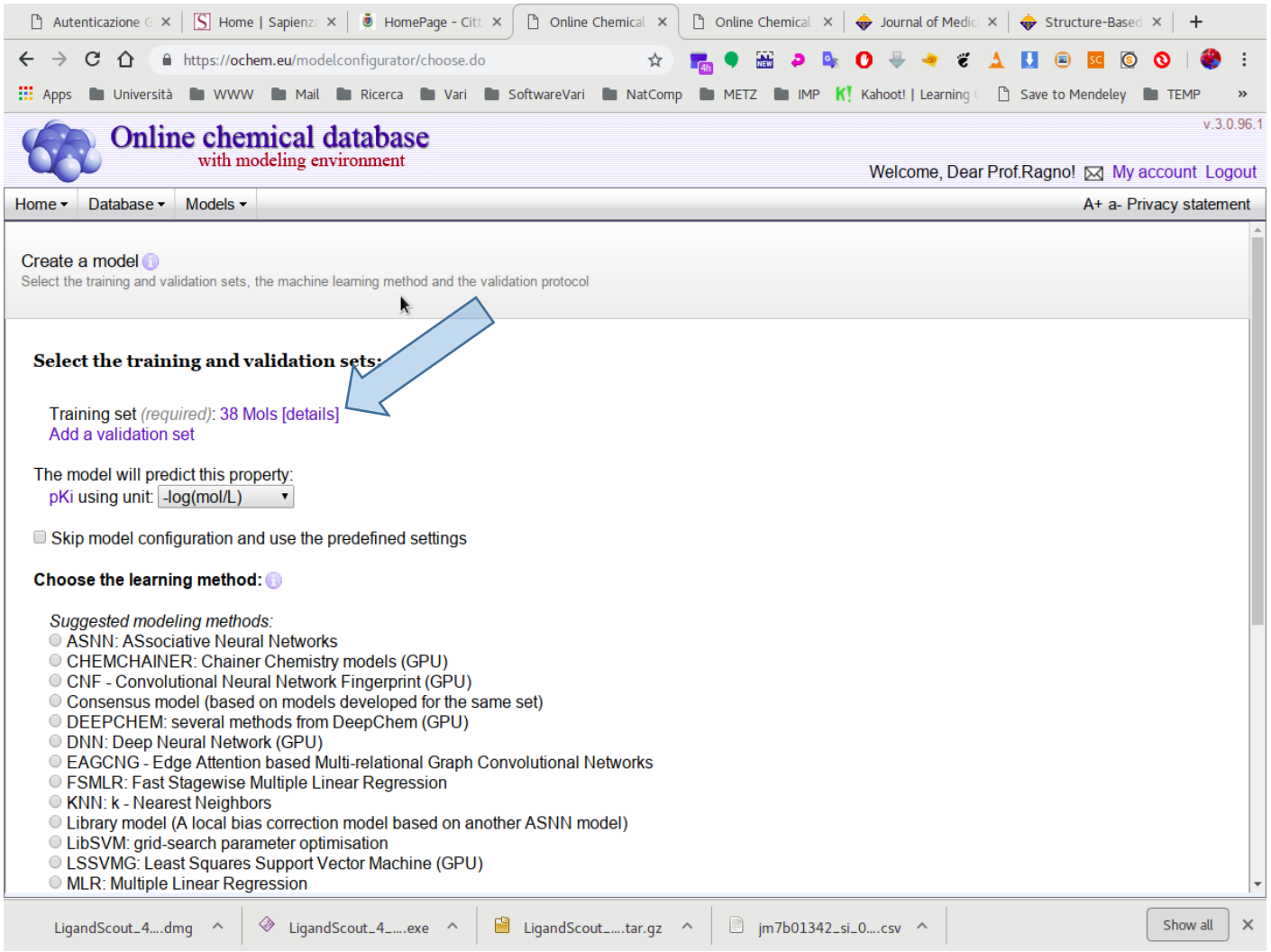

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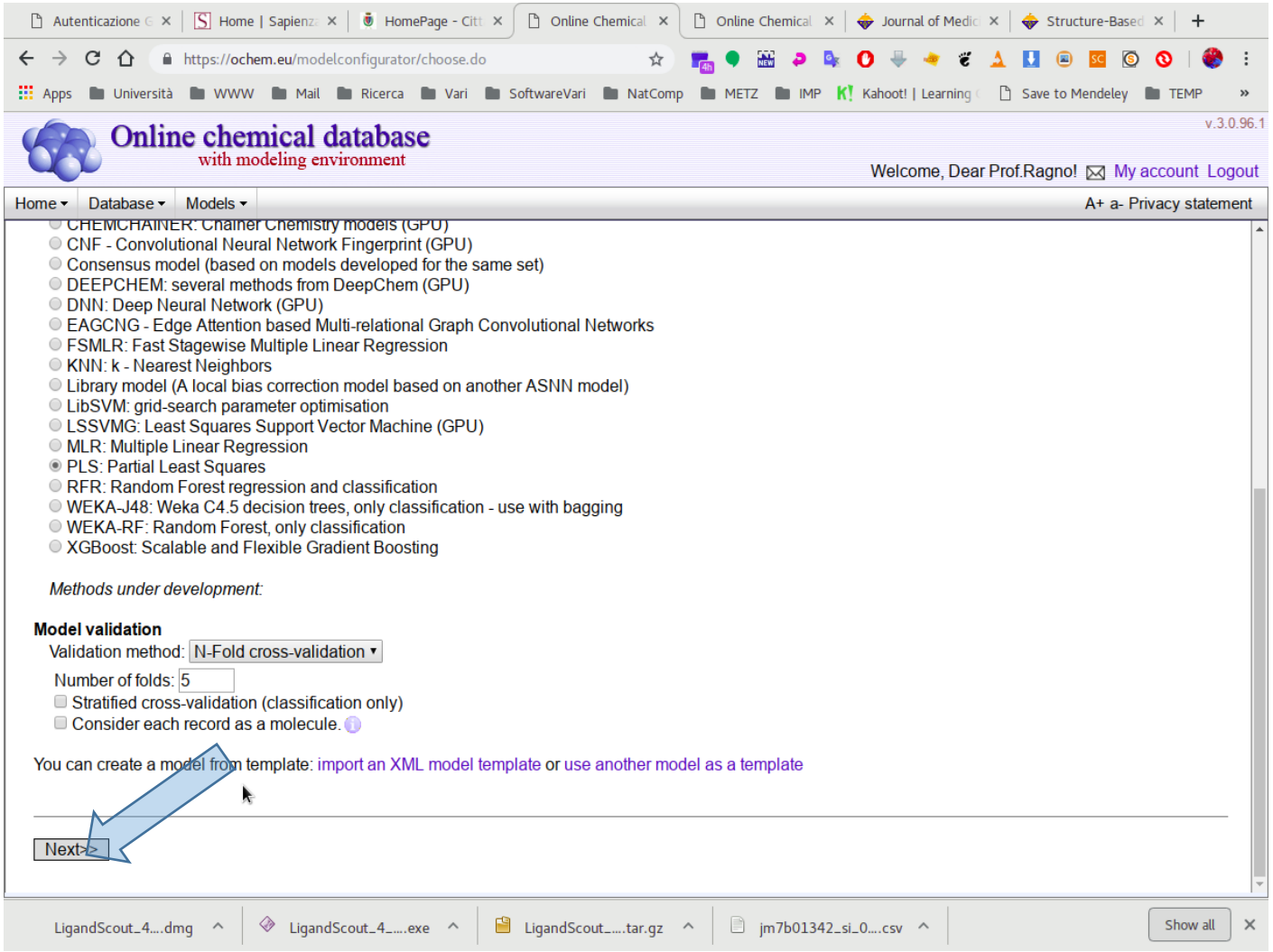

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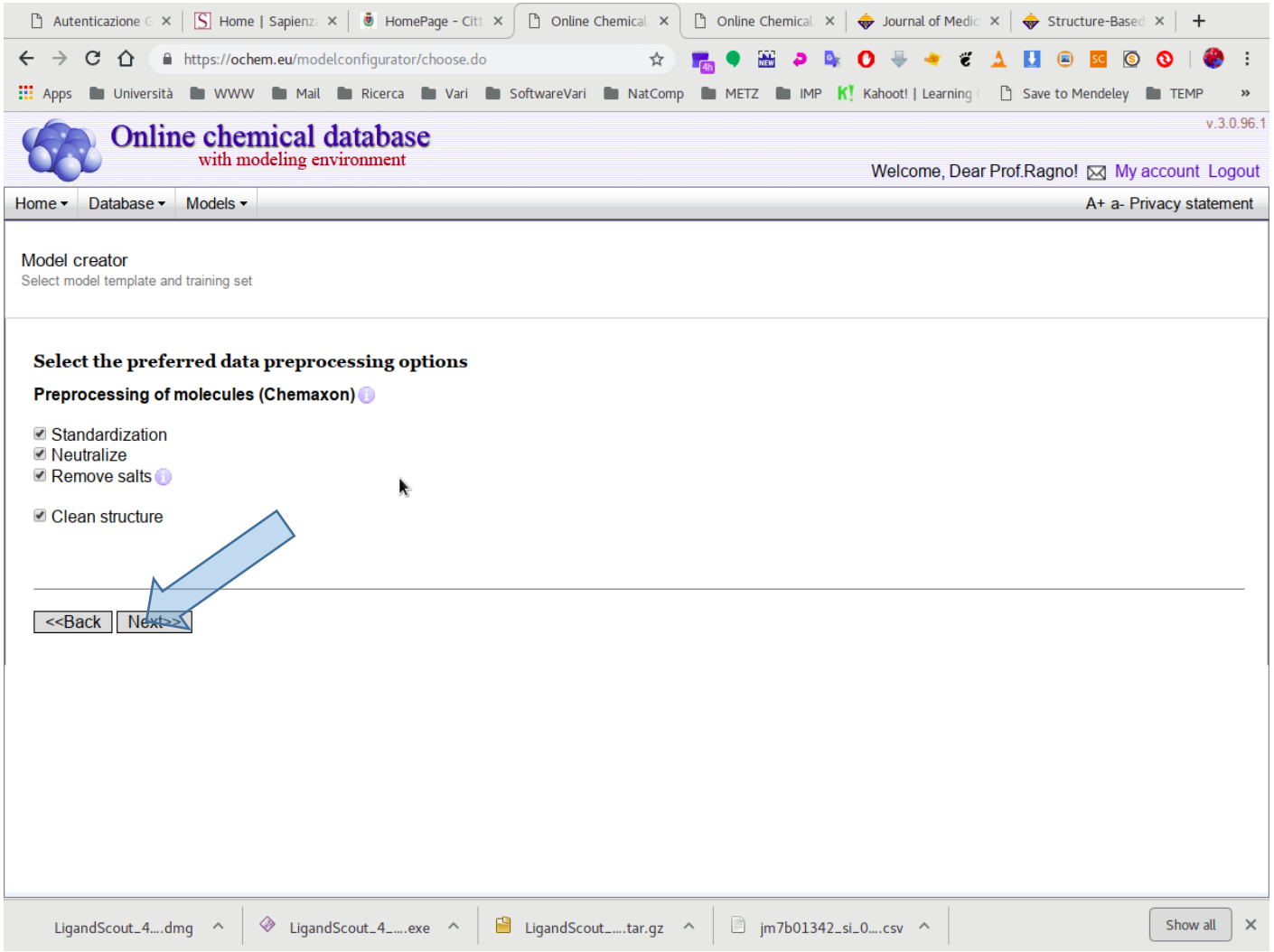

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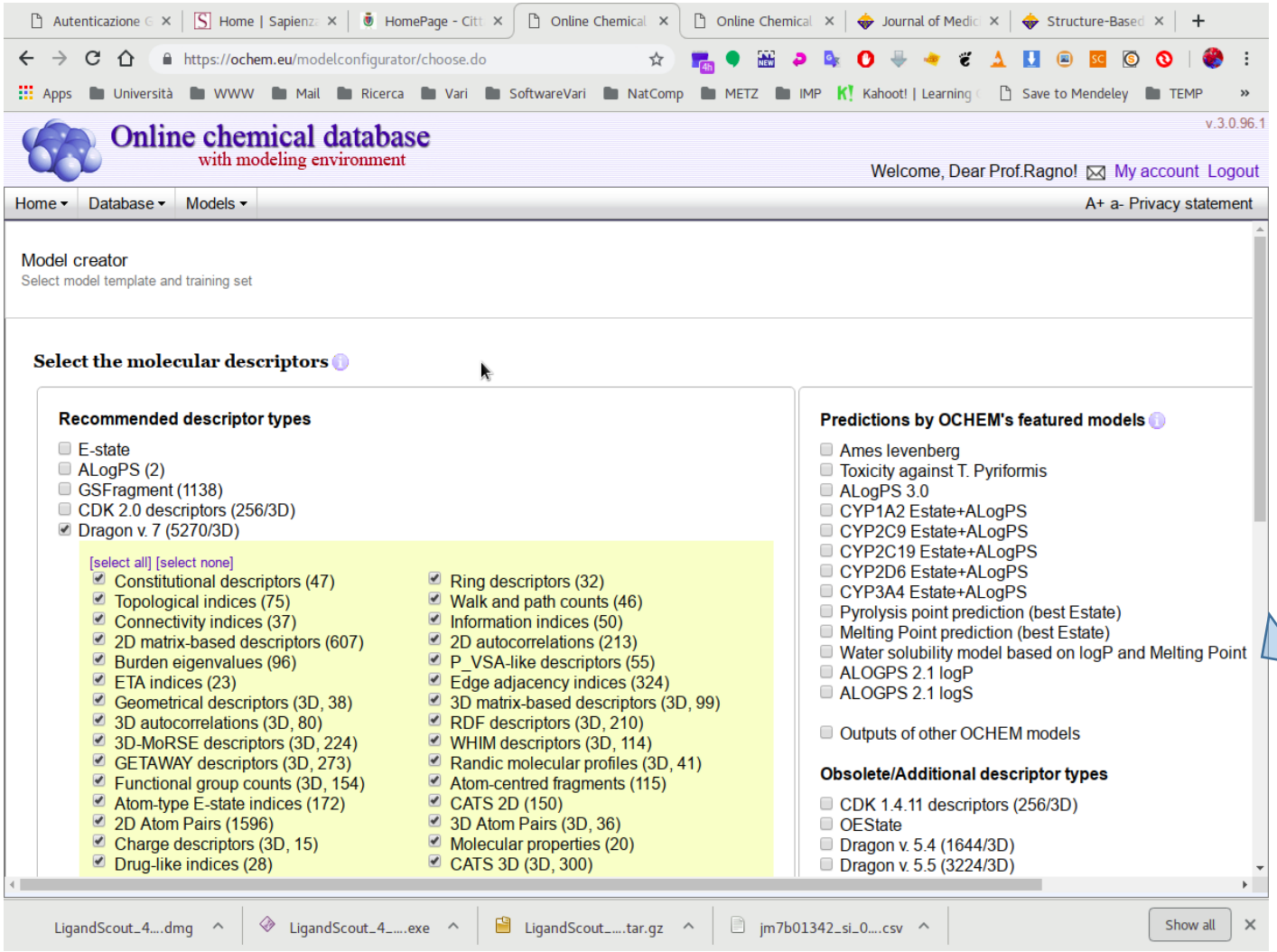

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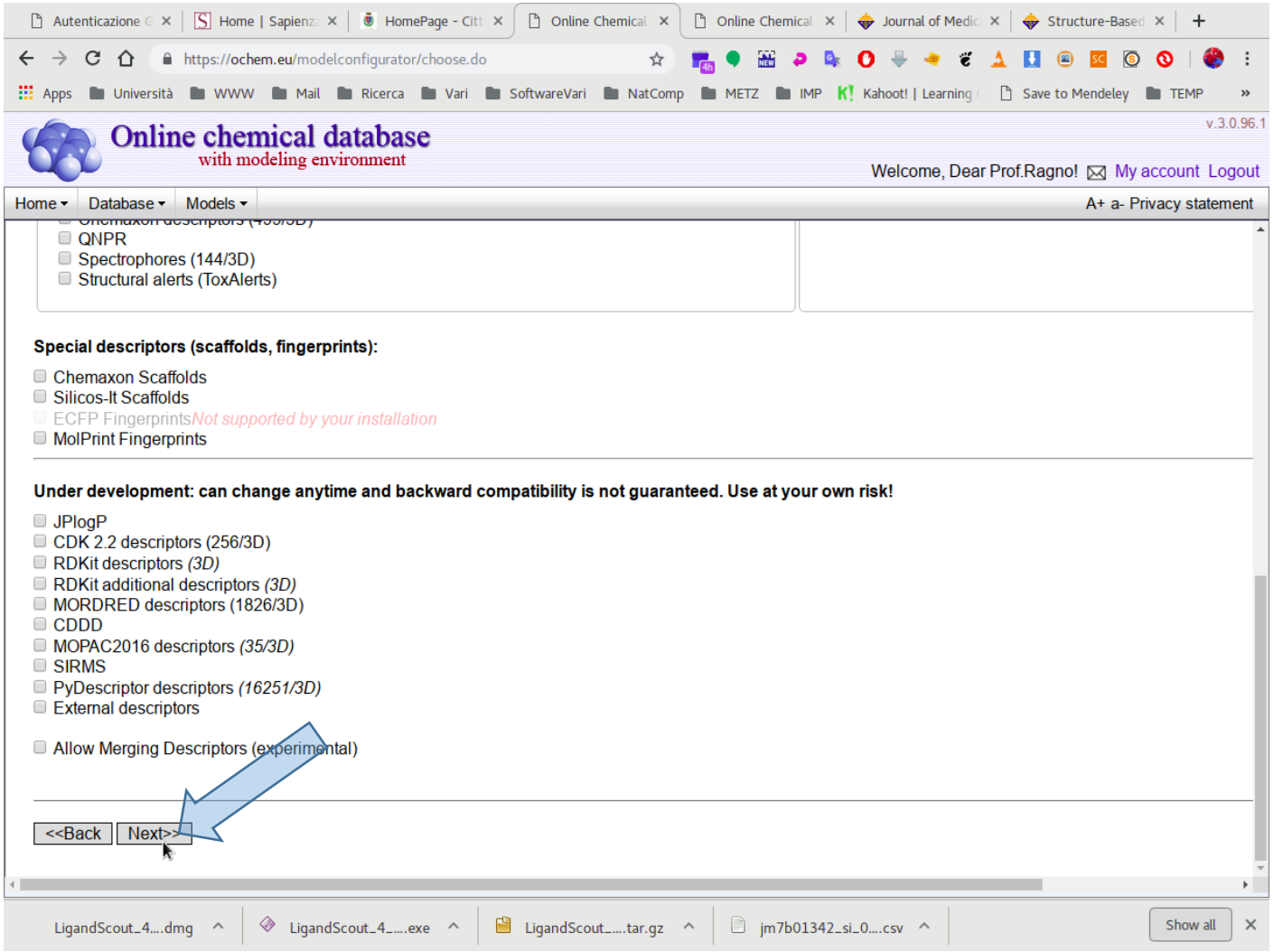

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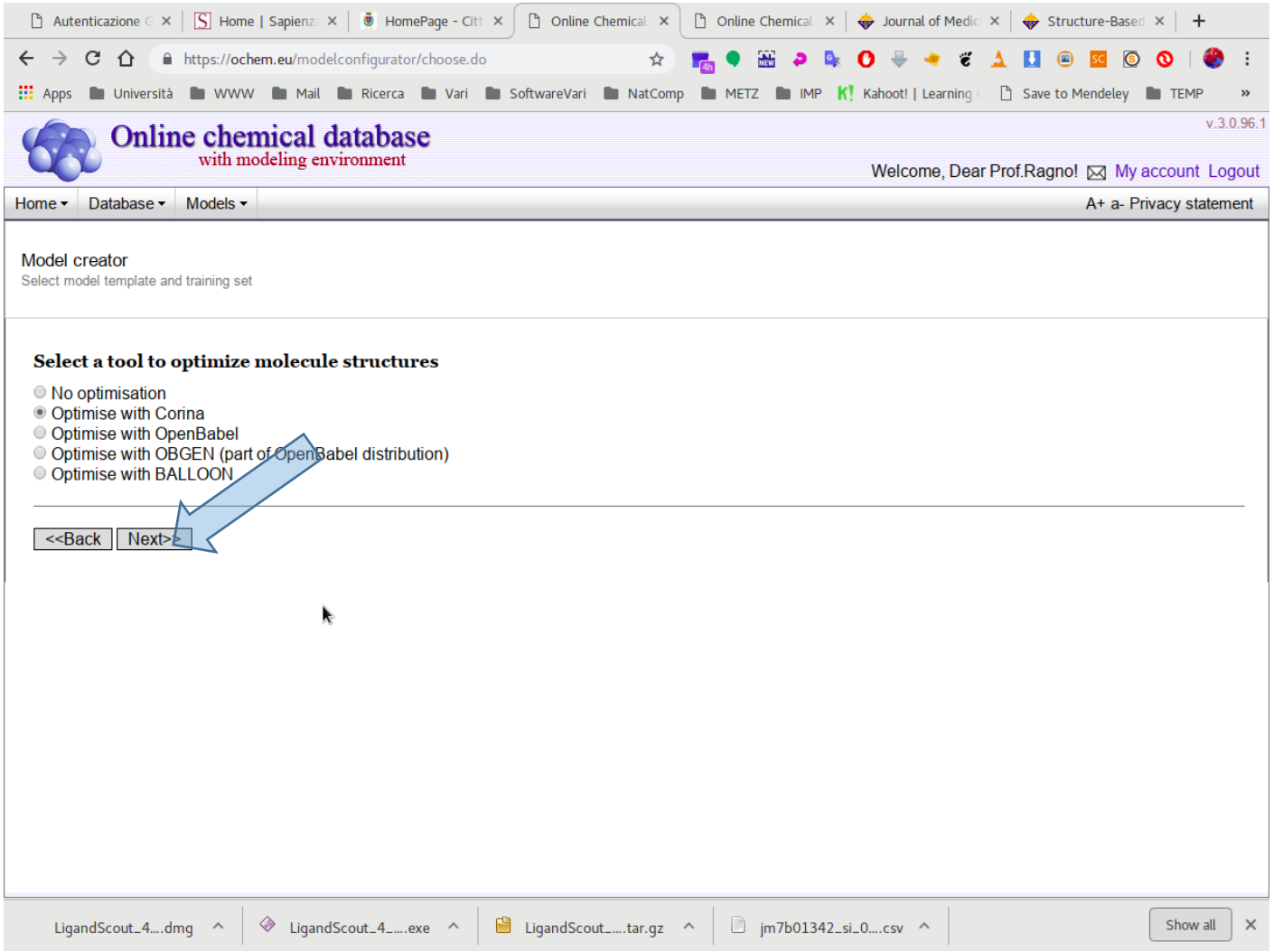

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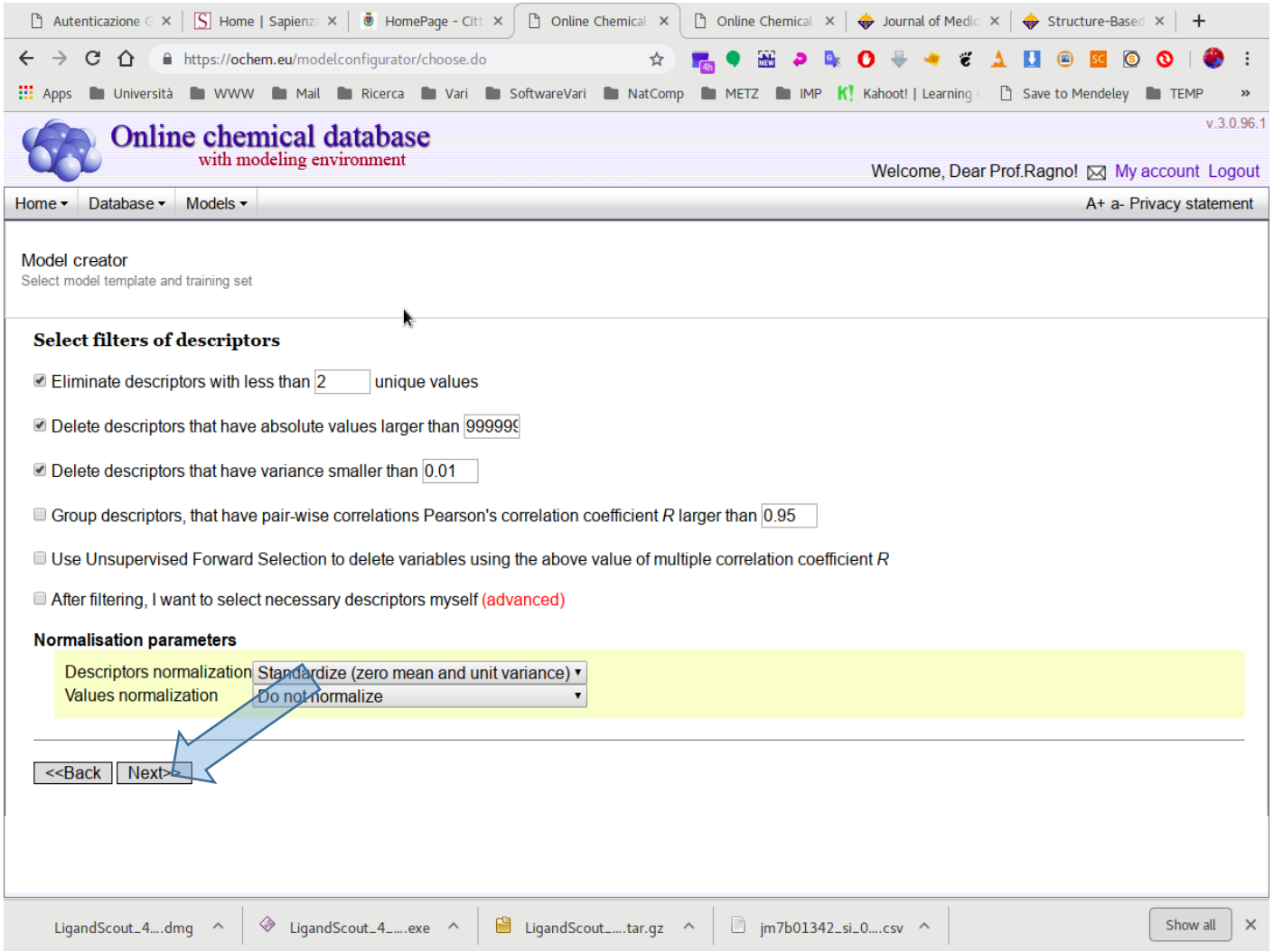

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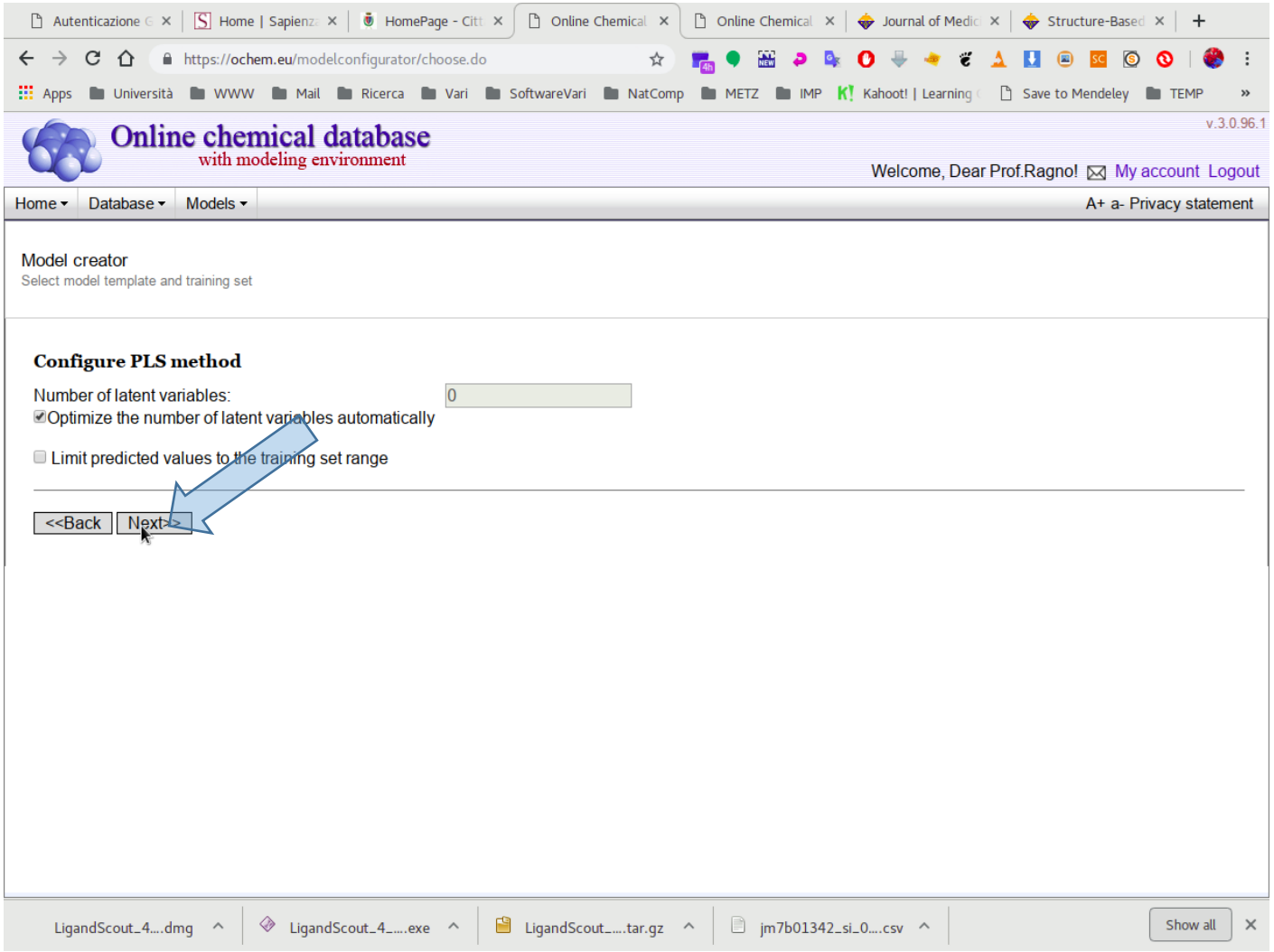

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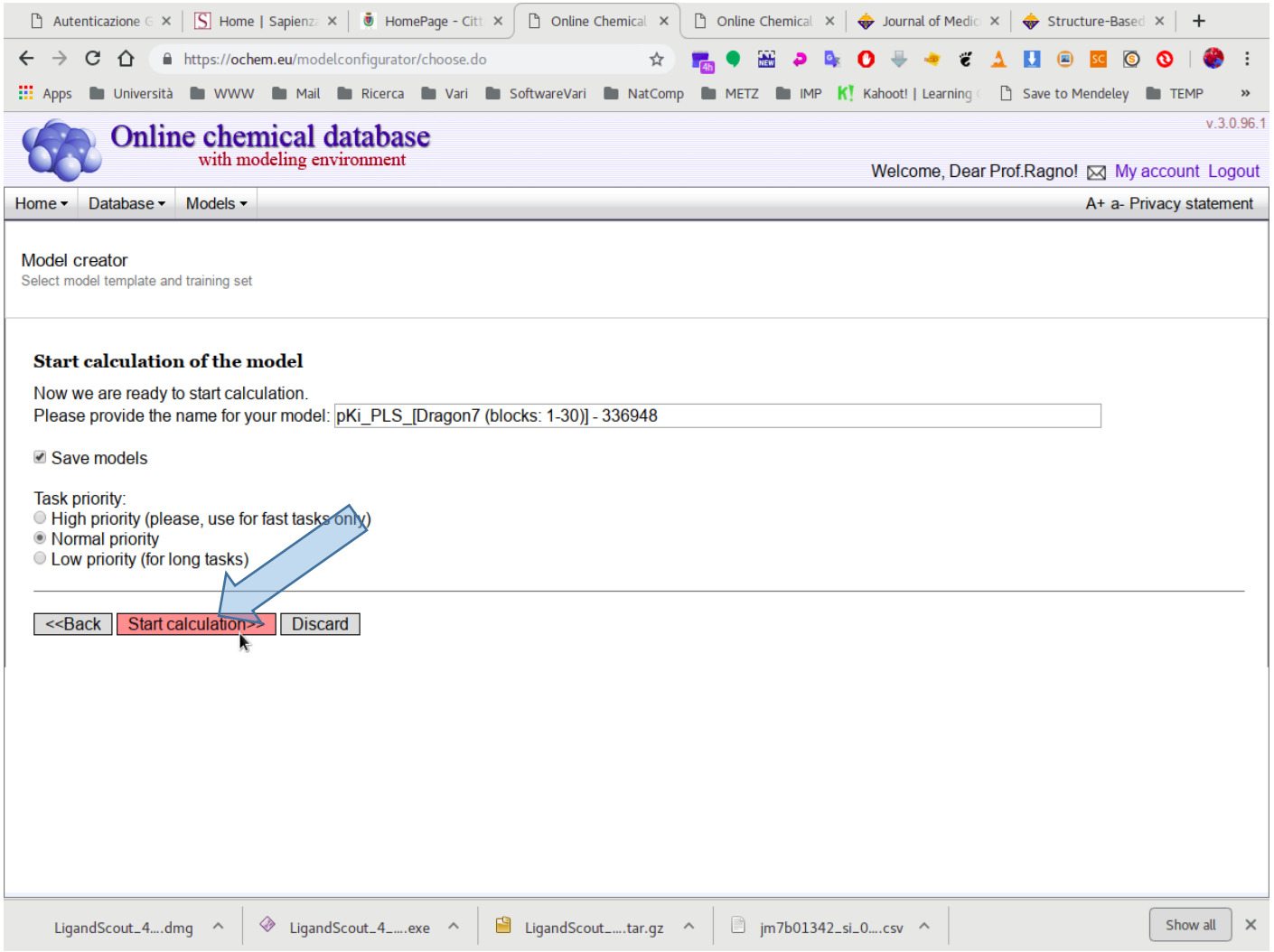

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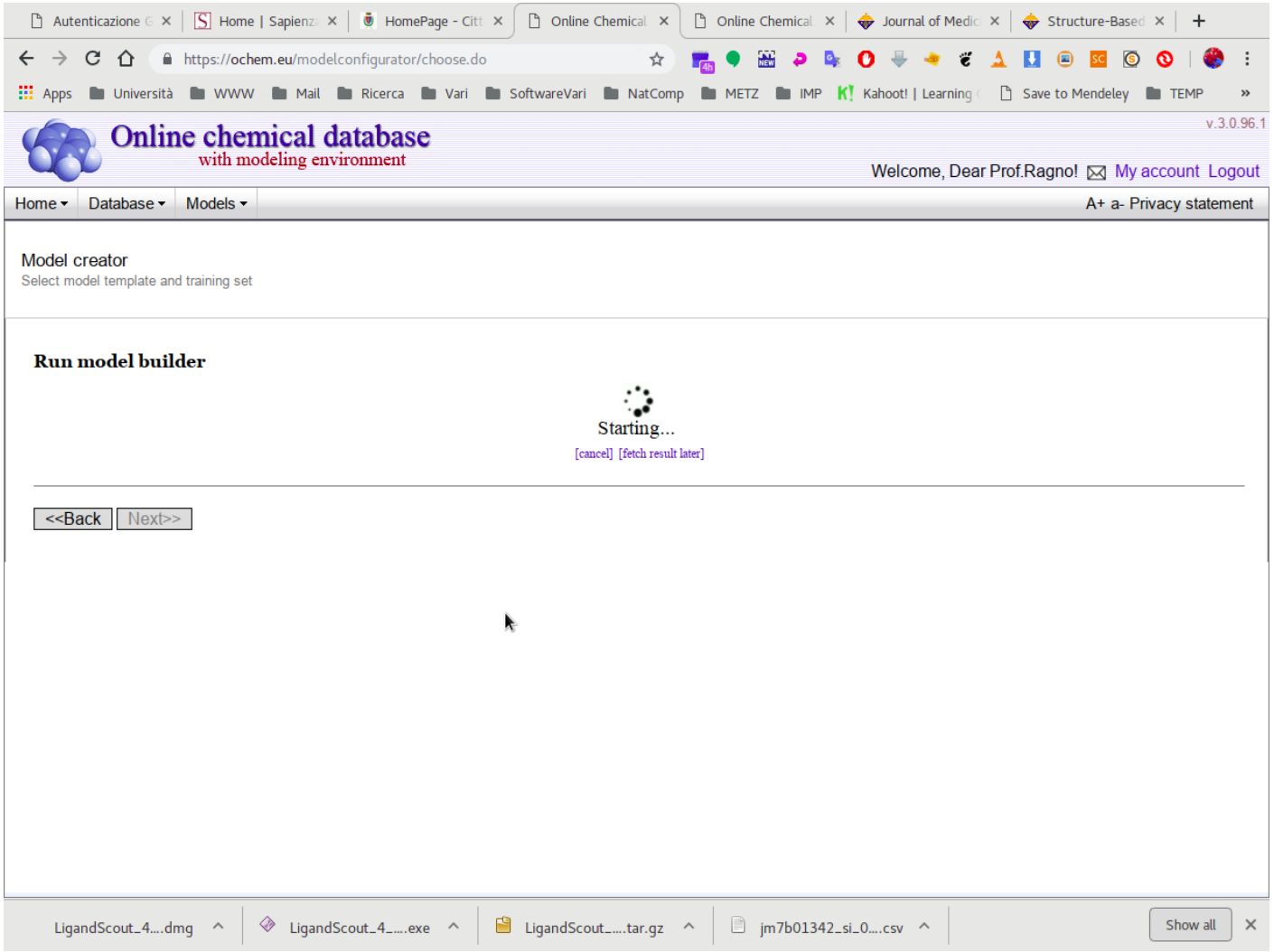

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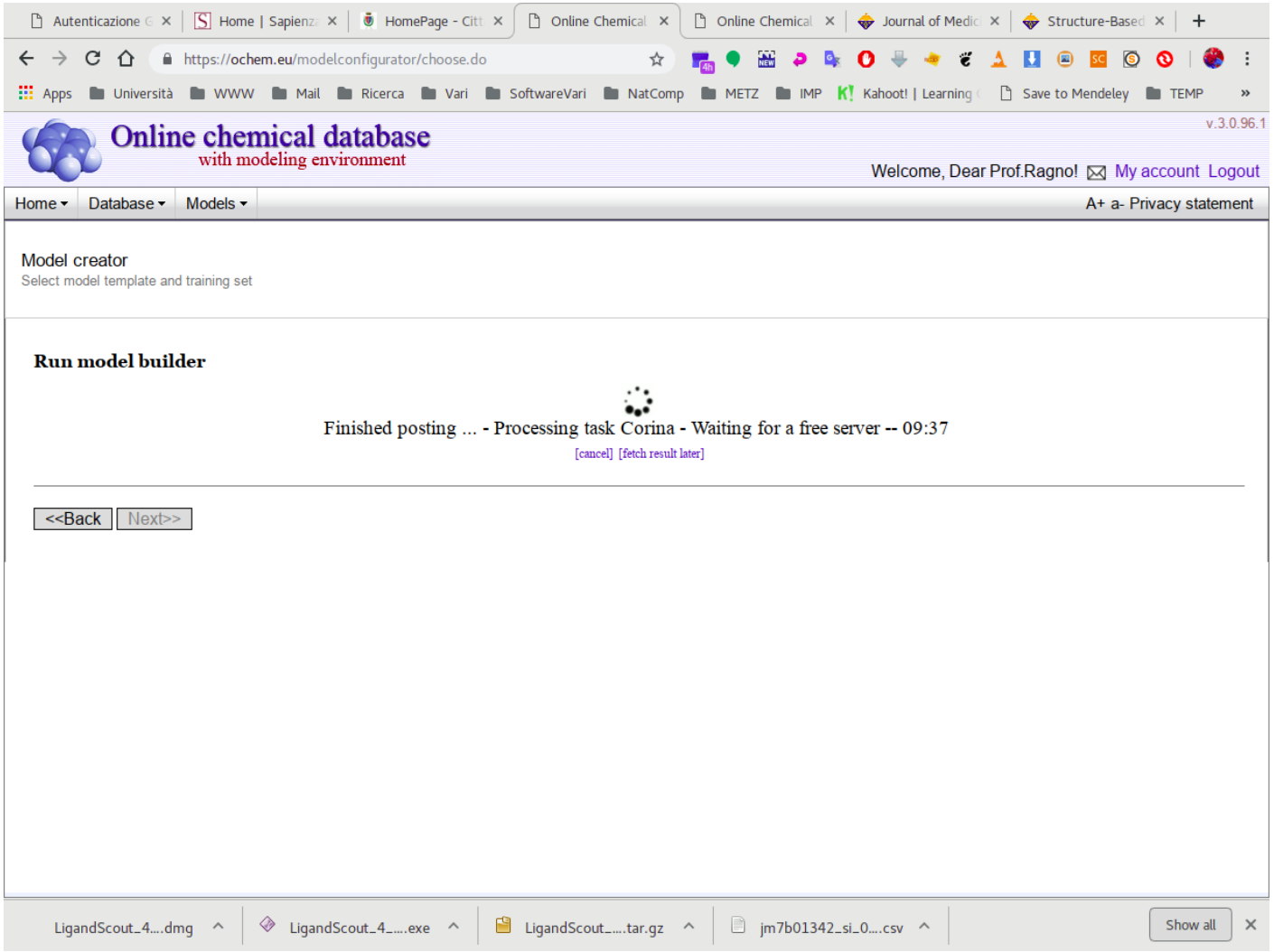

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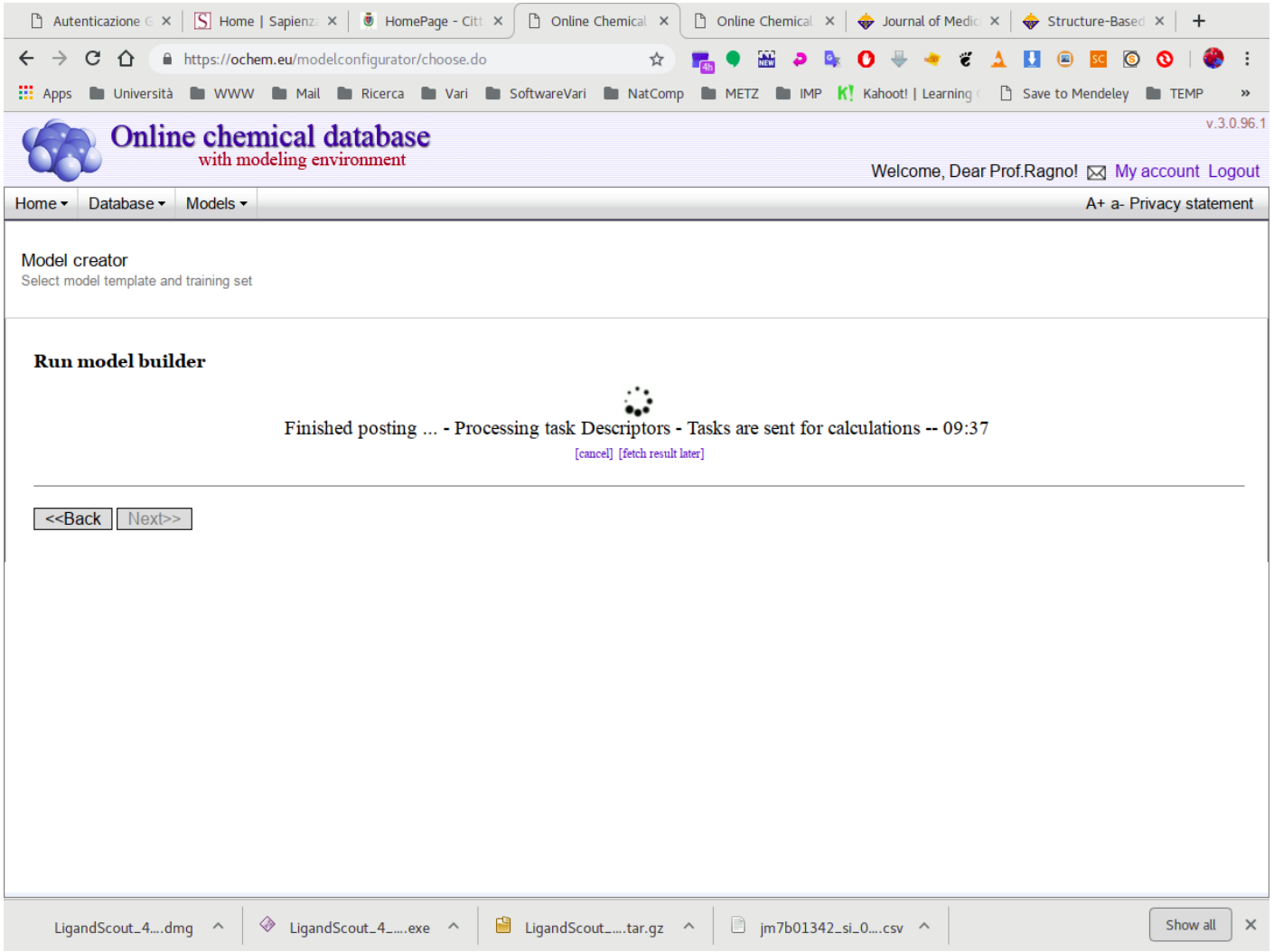

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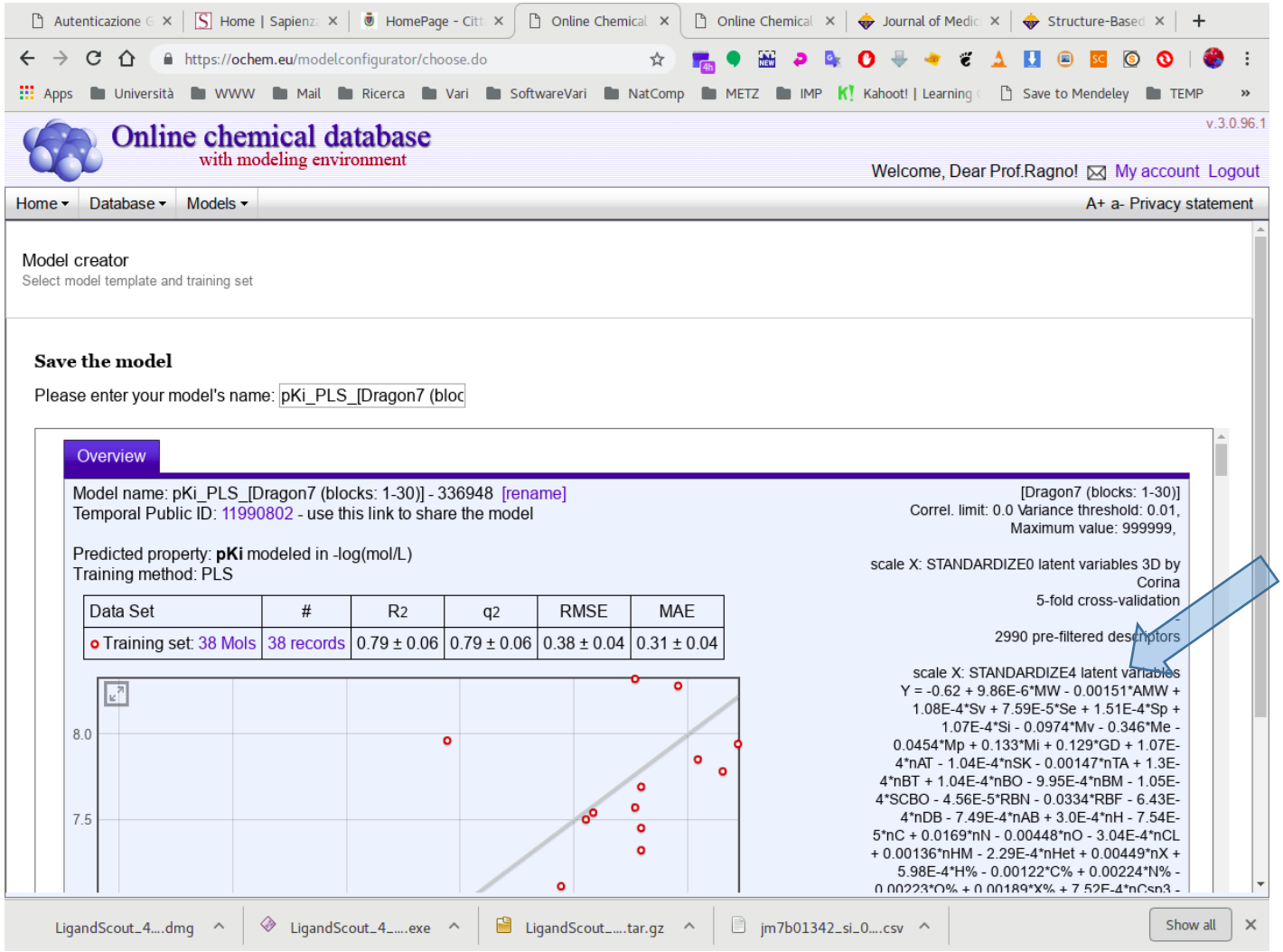

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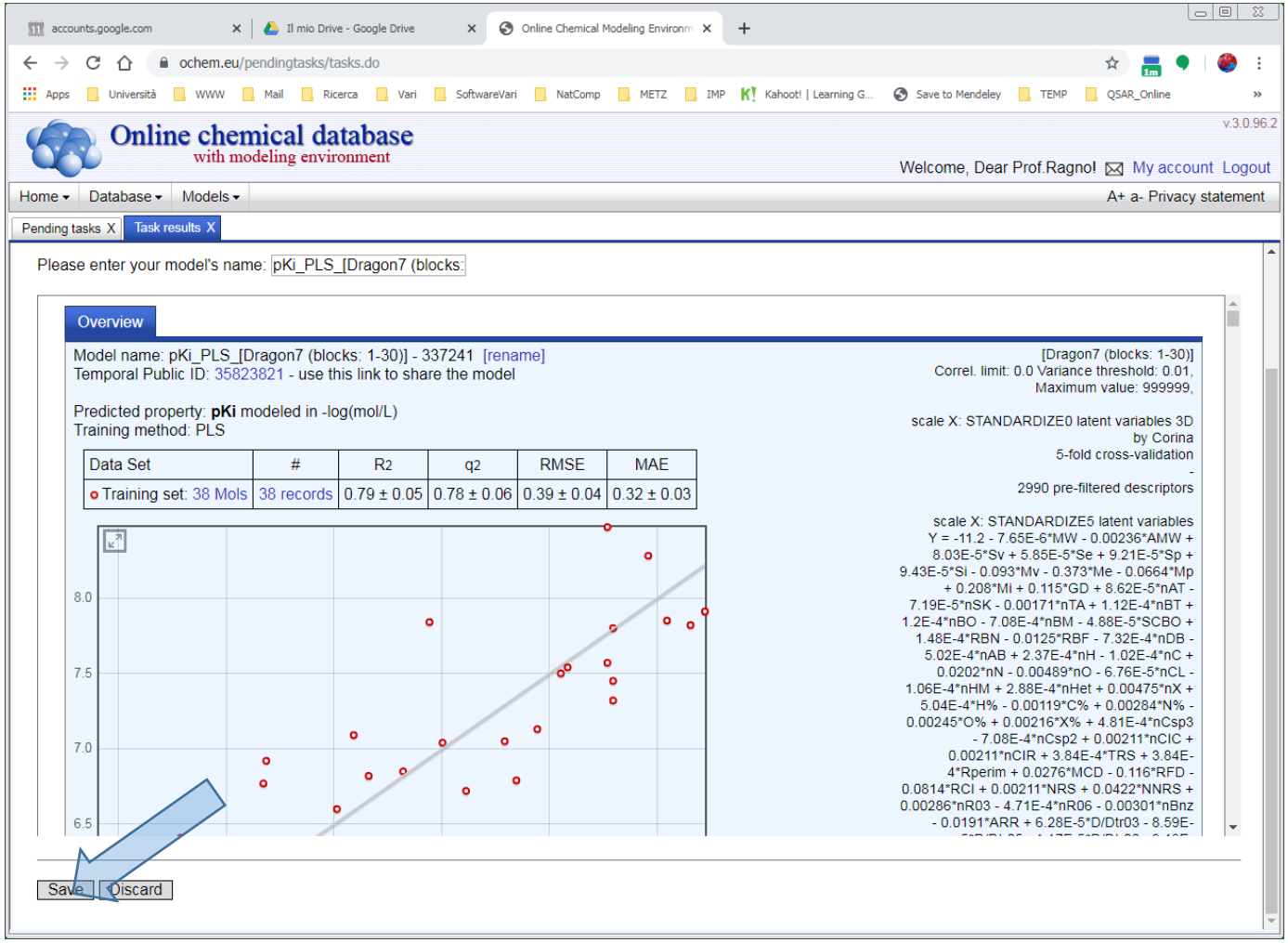

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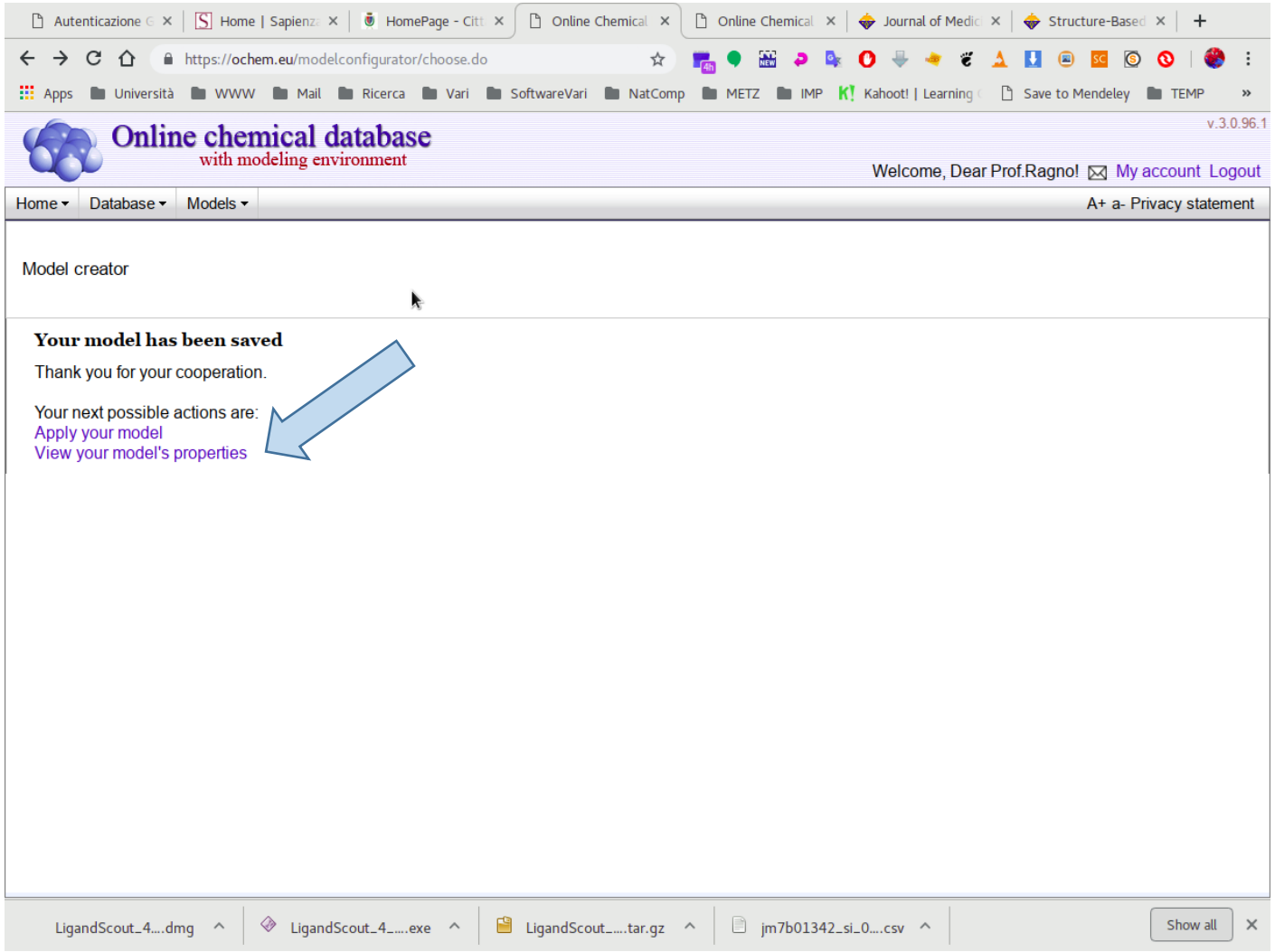

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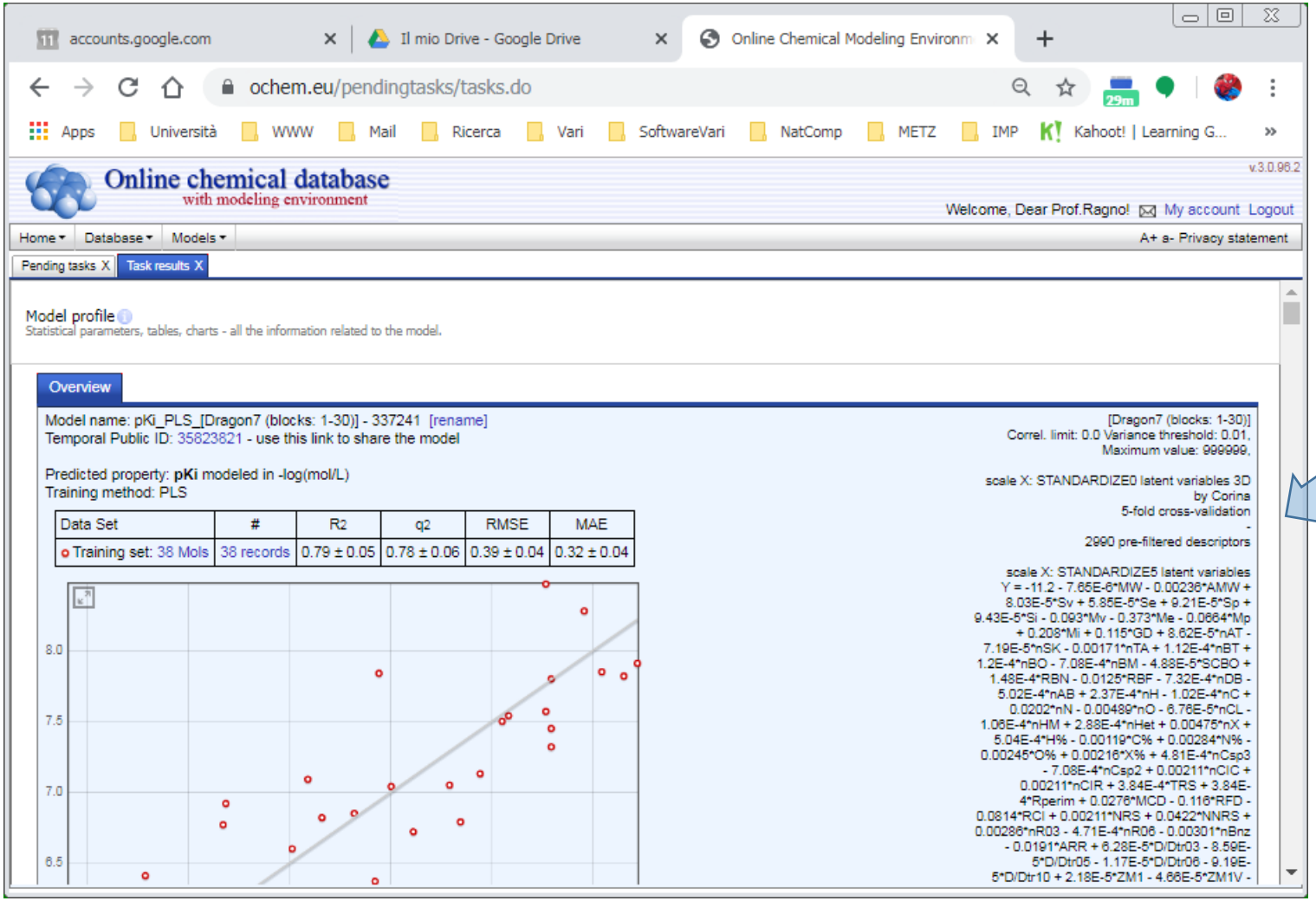

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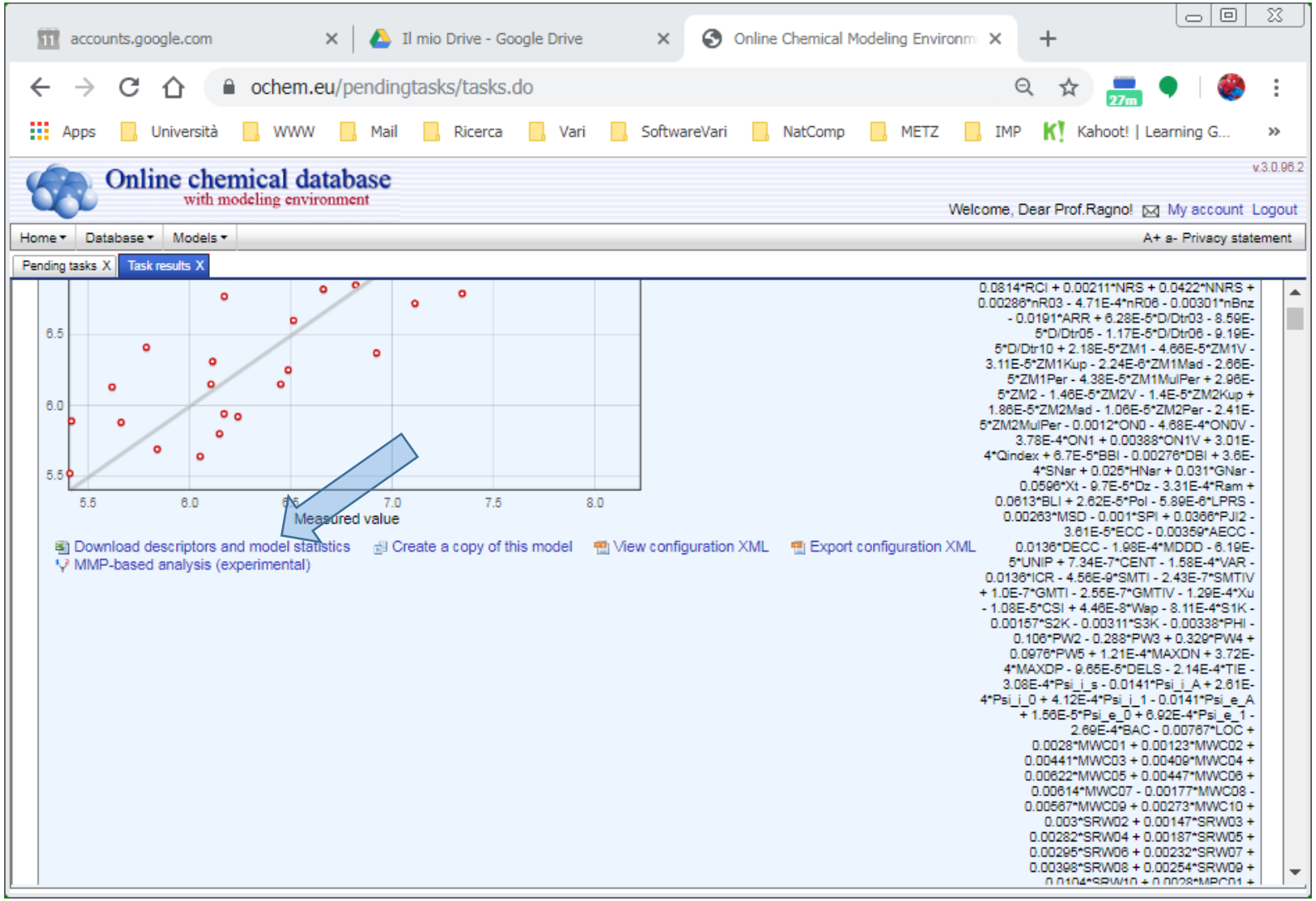

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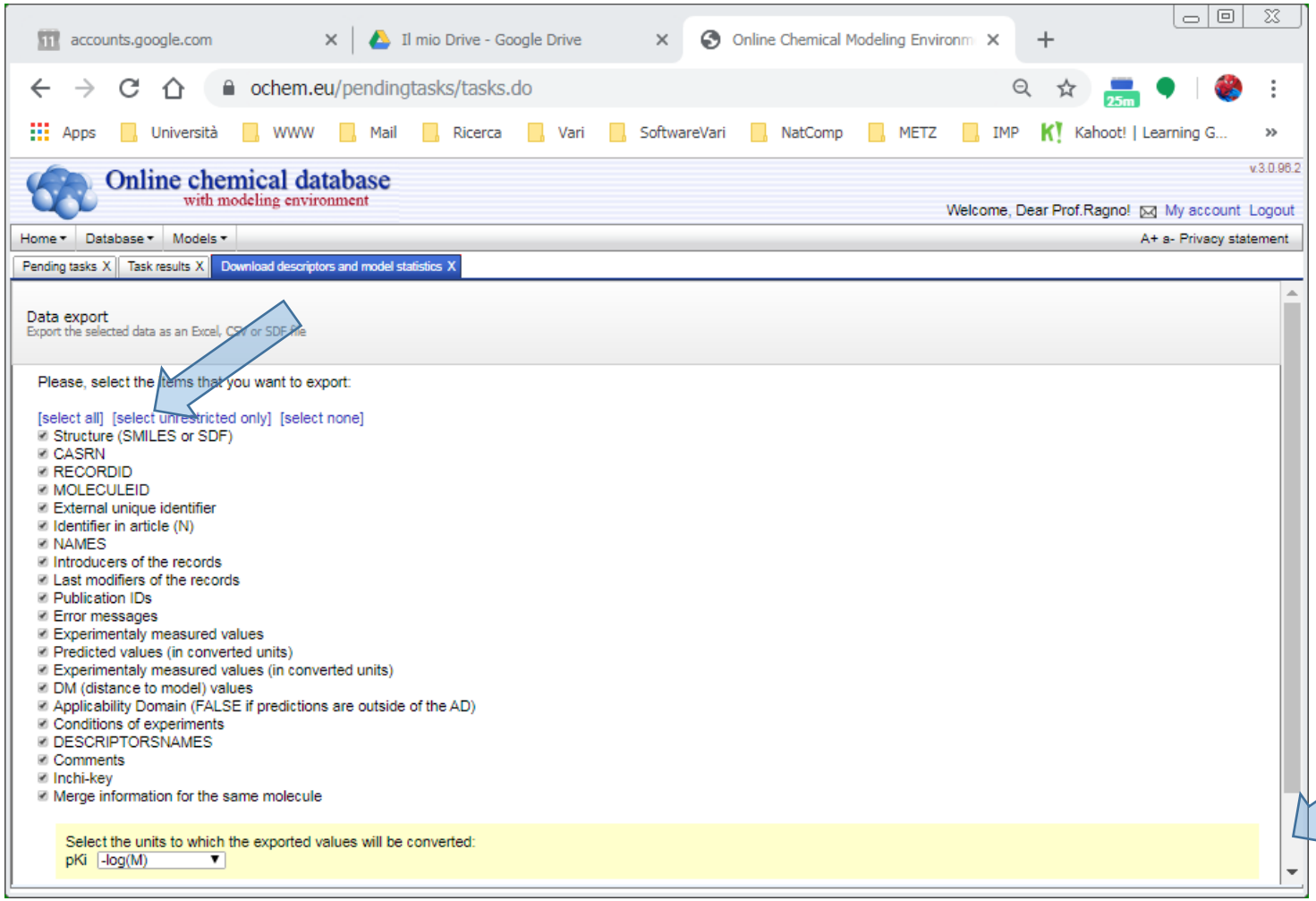

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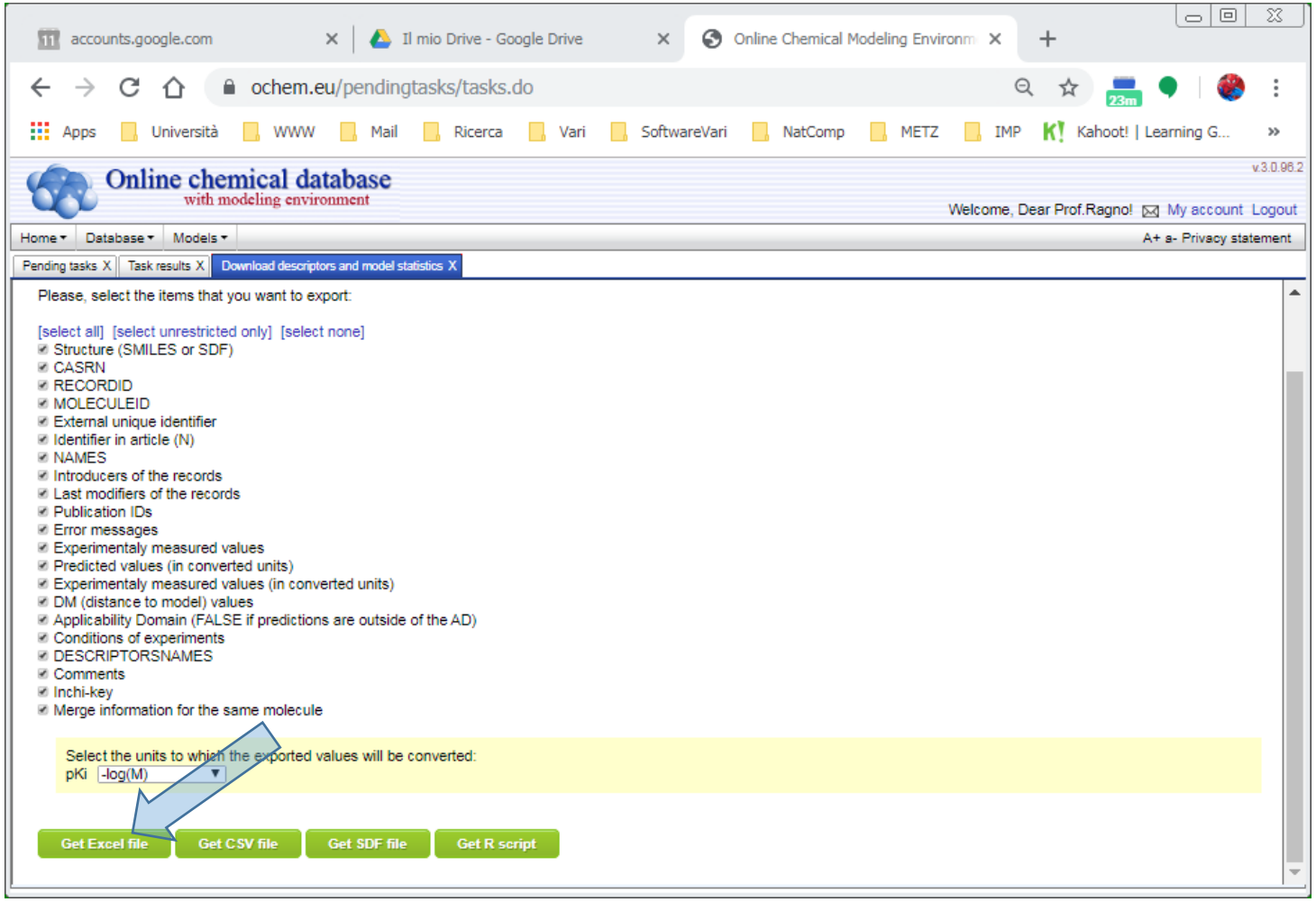

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