Building your own AI models

M3. Real-world cases
26.09.2023

Ersilia

Three real-world datasets
— Open Source Mycetoma
— HDAC1 inhibitors
— ACE2-Spike PPI inhibitors

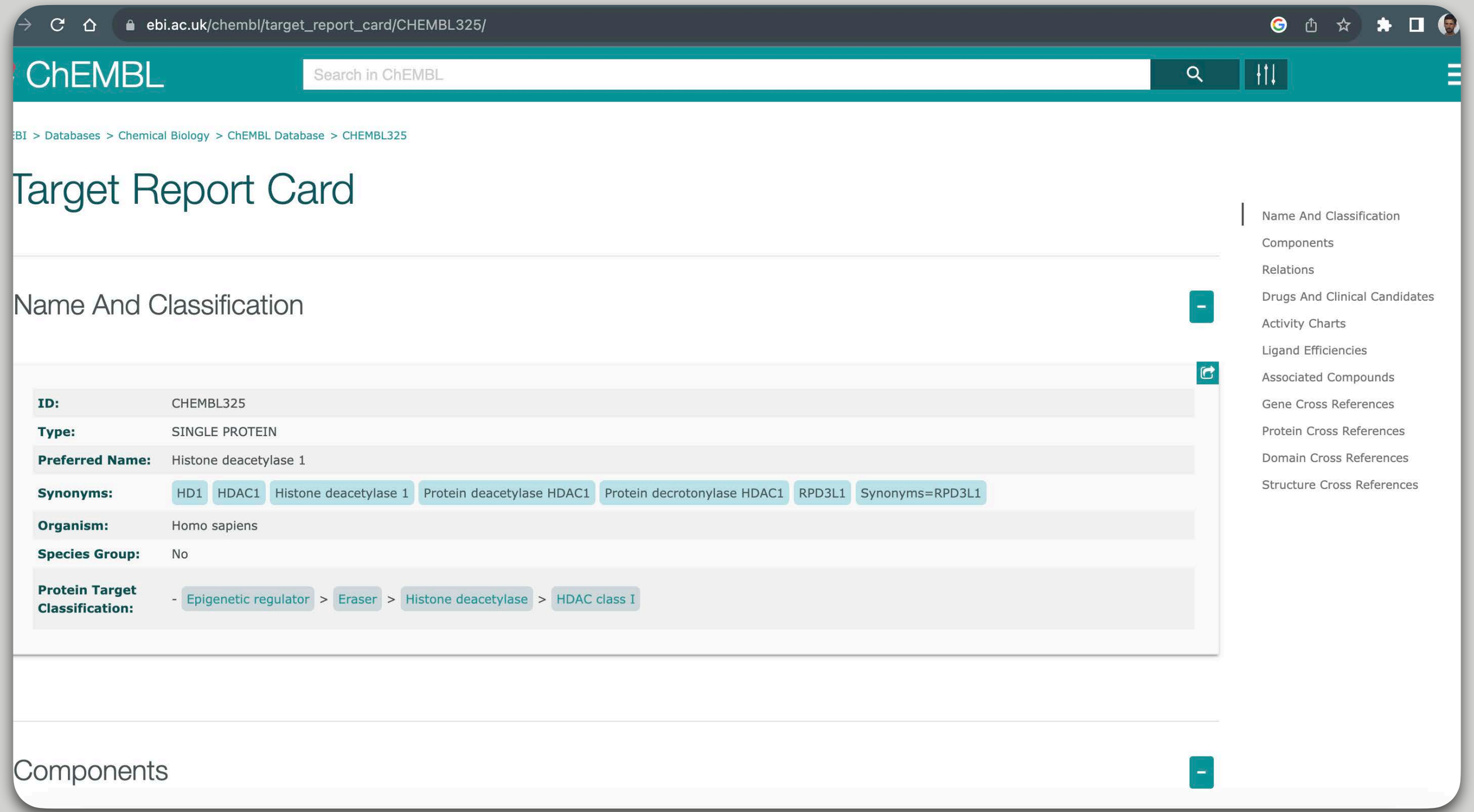
👩‍💻 Exercise

— Split in 3 groups.
— Understand the source of your data.
— Binarize the output variable.
— Divide your dataset into a training set and a test set.
— Train an AI model with LazyQSAR.
— Evaluate performance.
— Retrain model with full dataset and download it.

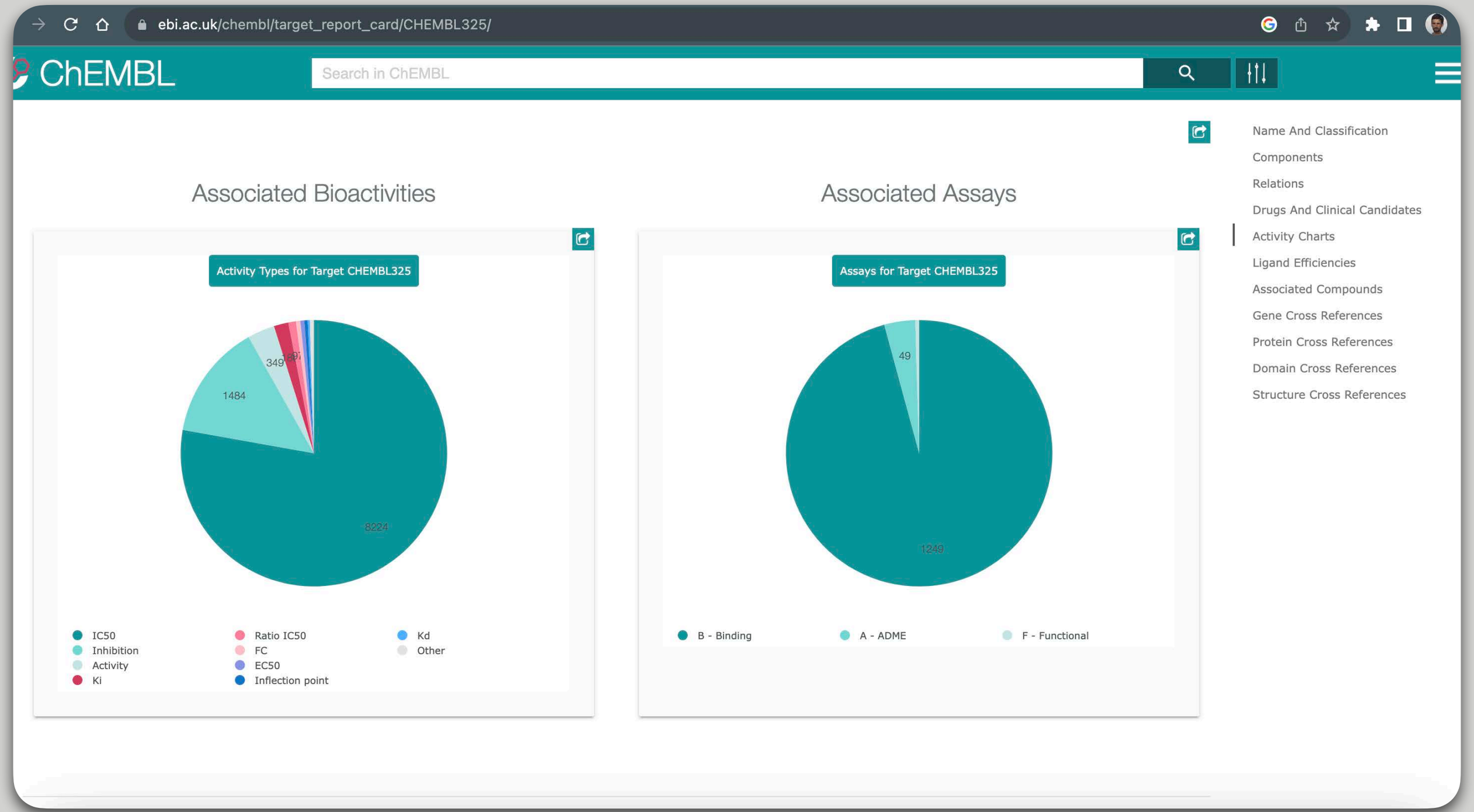
👩‍💻 Tomorrow: present your results!

🚀 Deployment in the Ersilia Model Hub!

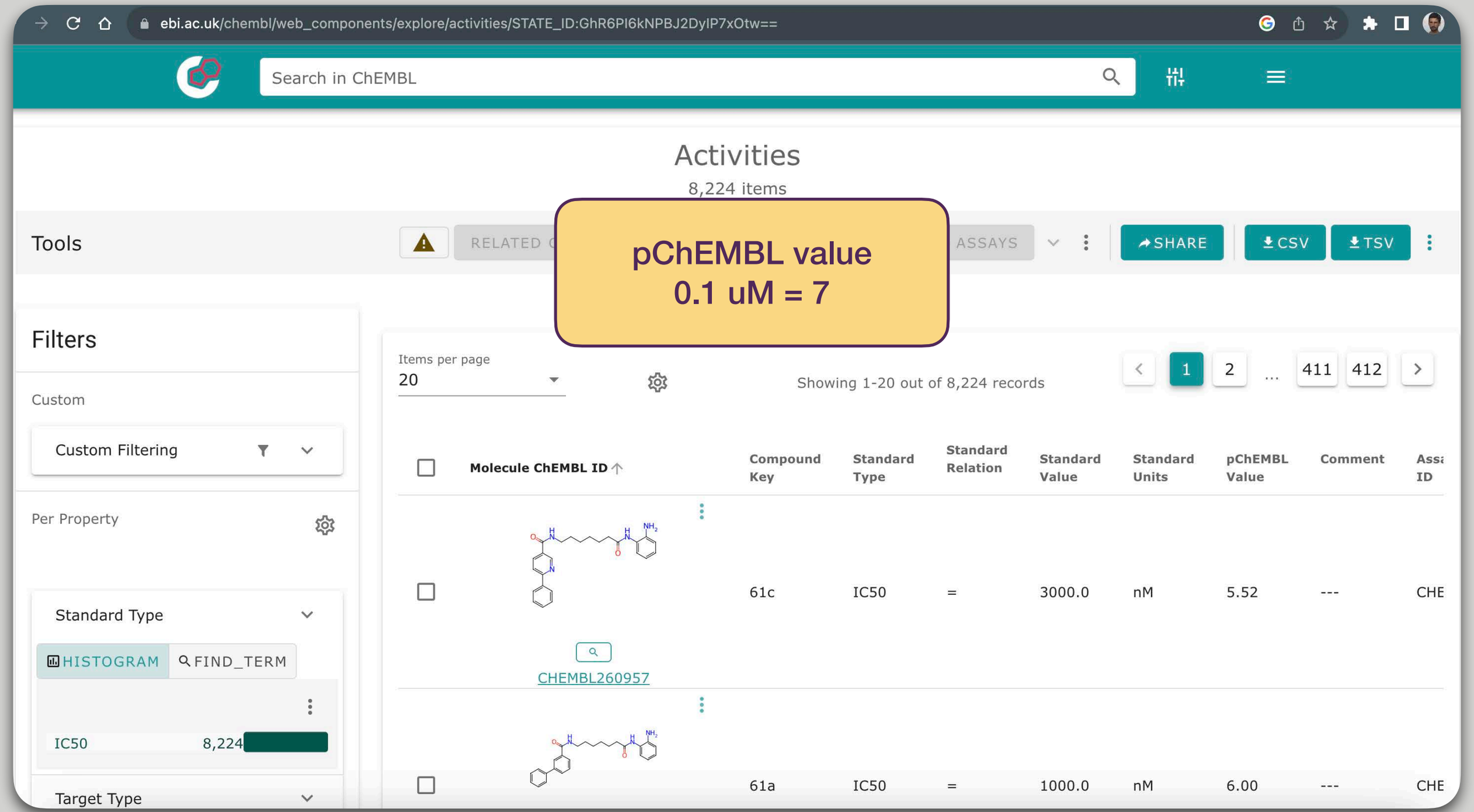
HDAC1 inhibitors from ChEMBL (target 325)



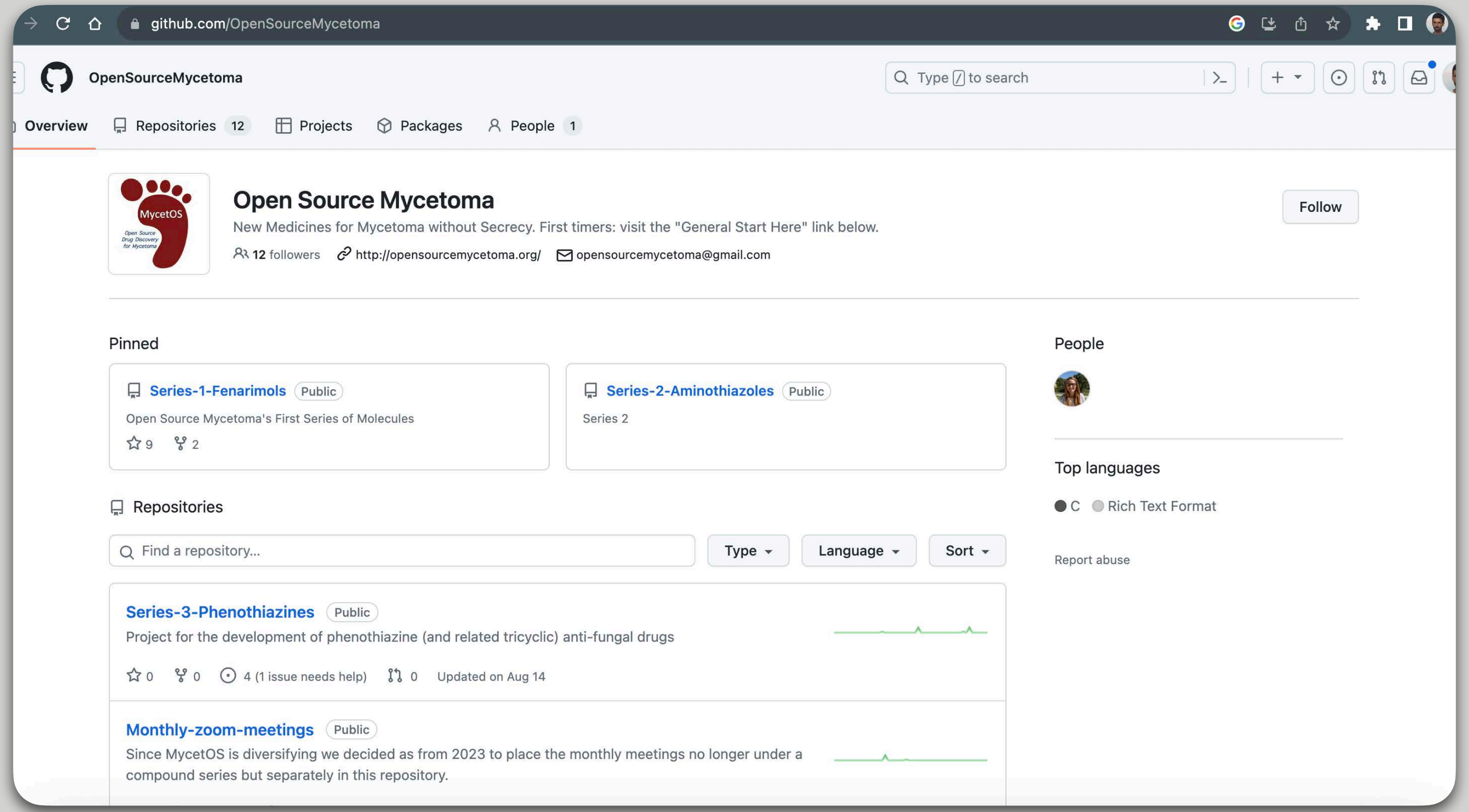
HDAC1 inhibitors from ChEMBL (target 325)



HDAC1 inhibitors from ChEMBL (target 325)



MycetOS, series 1
An open source project



MycetOS, series 1
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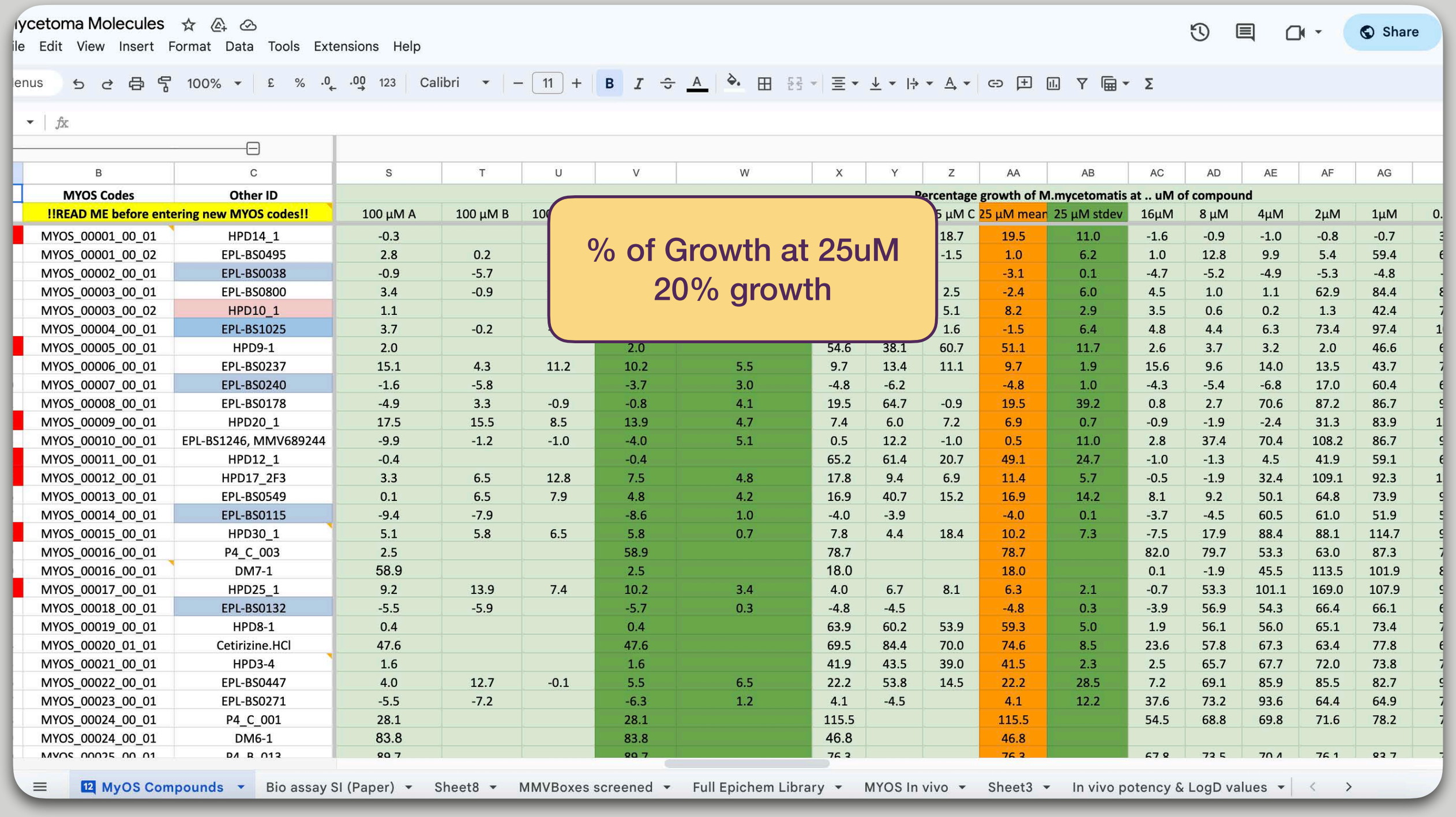
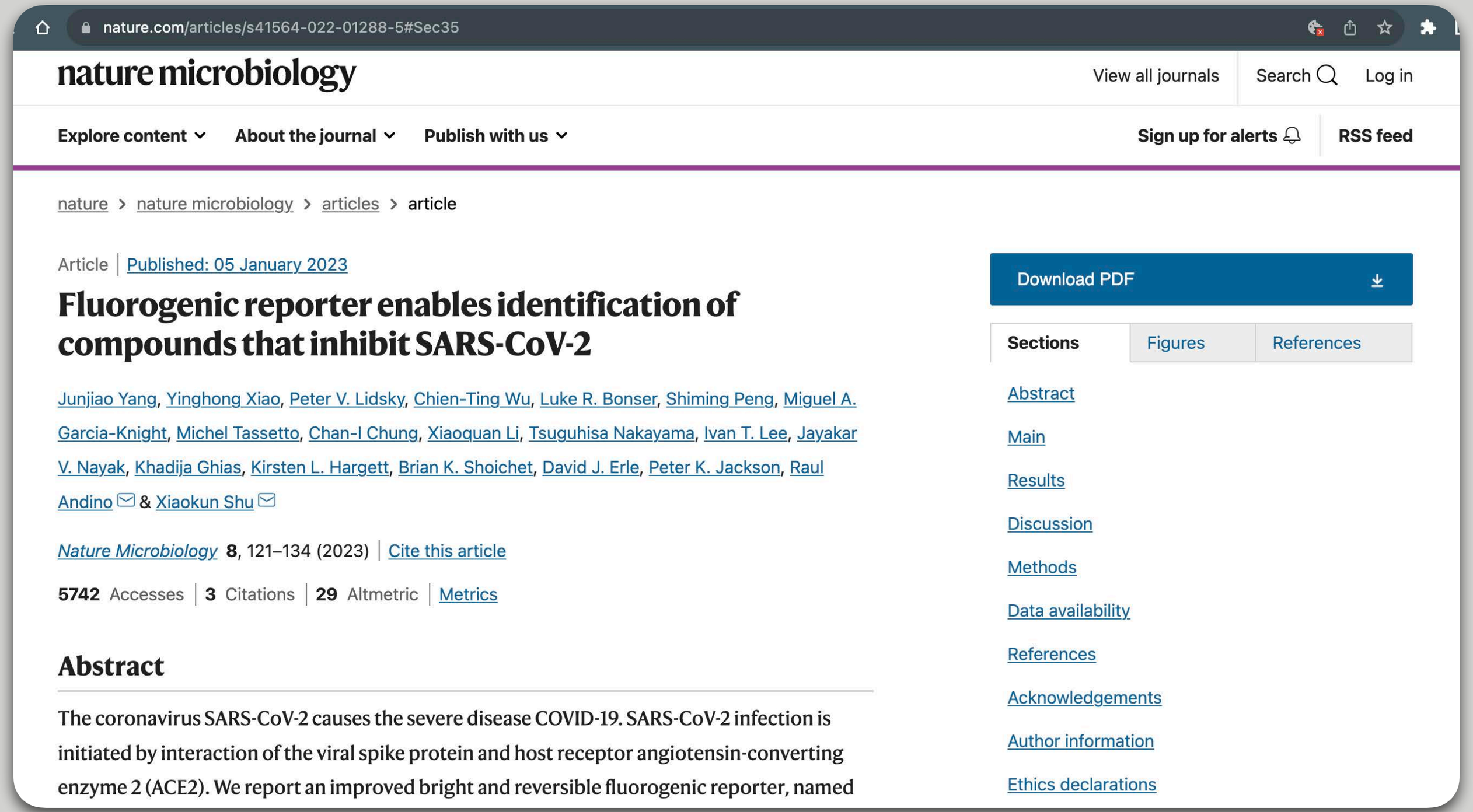


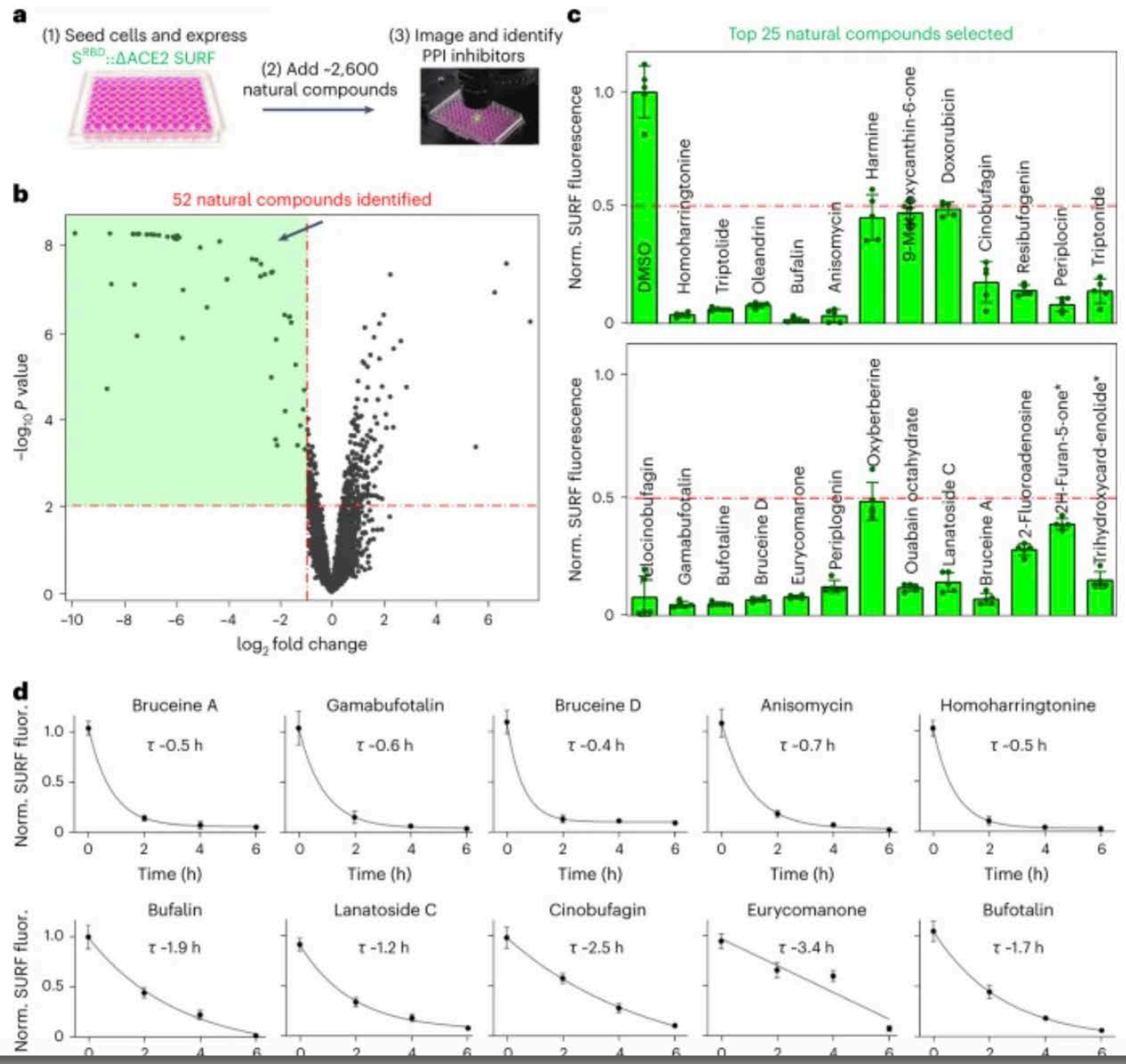
MYOS Codes	Other ID	100 µM A	100 µM B	100						25 µM mean	25 µM stdev	16µM	8 µM	4µM	2µM	1µM	0.
!!READ ME before entering new MYOS codes!!																	
									5 µM C								
MYOS_00001_00_01	HPD14_1	-0.3							18.7	19.5	11.0	-1.6	-0.9	-1.0	-0.8	-0.7	3
MYOS_00001_00_02	EPL-BS0495	2.8	0.2						-1.5	1.0	6.2	1.0	12.8	9.9	5.4	59.4	6
MYOS_00002_00_01	EPL-BS0038	-0.9	-5.7							-3.1	0.1	-4.7	-5.2	-4.9	-5.3	-4.8	-
MYOS_00003_00_01	EPL-BS0800	3.4	-0.9						2.5	-2.4	6.0	4.5	1.0	1.1	62.9	84.4	8
MYOS_00003_00_02	HPD10_1	1.1							5.1	8.2	2.9	3.5	0.6	0.2	1.3	42.4	7
MYOS_00004_00_01	EPL-BS1025	3.7	-0.2						1.6	-1.5	6.4	4.8	4.4	6.3	73.4	97.4	1
MYOS_00005_00_01	HPD9-1	2.0			2.0		54.6	38.1	60.7	51.1	11.7	2.6	3.7	3.2	2.0	46.6	6
MYOS_00006_00_01	EPL-BS0237	15.1	4.3	11.2	10.2	5.5	9.7	13.4	11.1	9.7	1.9	15.6	9.6	14.0	13.5	43.7	7
MYOS_00007_00_01	EPL-BS0240	-1.6	-5.8		-3.7	3.0	-4.8	-6.2		-4.8	1.0	-4.3	-5.4	-6.8	17.0	60.4	6
MYOS_00008_00_01	EPL-BS0178	-4.9	3.3	-0.9	-0.8	4.1	19.5	64.7	-0.9	19.5	39.2	0.8	2.7	70.6	87.2	86.7	9
MYOS_00009_00_01	HPD20_1	17.5	15.5	8.5	13.9	4.7	7.4	6.0	7.2	6.9	0.7	-0.9	-1.9	-2.4	31.3	83.9	1
MYOS_00010_00_01	EPL-BS1246, MMV689244	-9.9	-1.2	-1.0	-4.0	5.1	0.5	12.2	-1.0	0.5	11.0	2.8	37.4	70.4	108.2	86.7	9
MYOS_00011_00_01	HPD12_1	-0.4			-0.4		65.2	61.4	20.7	49.1	24.7	-1.0	-1.3	4.5	41.9	59.1	6
MYOS_00012_00_01	HPD17_2F3	3.3	6.5	12.8	7.5	4.8	17.8	9.4	6.9	11.4	5.7	-0.5	-1.9	32.4	109.1	92.3	1
MYOS_00013_00_01	EPL-BS0549	0.1	6.5	7.9	4.8	4.2	16.9	40.7	15.2	16.9	14.2	8.1	9.2	50.1	64.8	73.9	9
MYOS_00014_00_01	EPL-BS0115	-9.4	-7.9		-8.6	1.0	-4.0	-3.9		-4.0	0.1	-3.7	-4.5	60.5	61.0	51.9	5
MYOS_00015_00_01	HPD30_1	5.1	5.8	6.5	5.8	0.7	7.8	4.4	18.4	10.2	7.3	-7.5	17.9	88.4	88.1	114.7	9
MYOS_00016_00_01	P4_C_003	2.5			58.9		78.7			78.7		82.0	79.7	53.3	63.0	87.3	7
MYOS_00016_00_01	DM7-1	58.9			2.5		18.0			18.0		0.1	-1.9	45.5	113.5	101.9	8
MYOS_00017_00_01	HPD25_1	9.2	13.9	7.4	10.2	3.4	4.0	6.7	8.1	6.3	2.1	-0.7	53.3	101.1	169.0	107.9	9
MYOS_00018_00_01	EPL-BS0132	-5.5	-5.9		-5.7	0.3	-4.8	-4.5		-4.8	0.3	-3.9	56.9	54.3	66.4	66.1	6
MYOS_00019_00_01	HPD8-1	0.4			0.4		63.9	60.2	53.9	59.3	5.0	1.9	56.1	56.0	65.1	73.4	7
MYOS_00020_01_01	Cetirizine.HCl	47.6			47.6		69.5	84.4	70.0	74.6	8.5	23.6	57.8	67.3	63.4	77.8	6
MYOS_00021_00_01	HPD3-4	1.6			1.6		41.9	43.5	39.0	41.5	2.3	2.5	65.7	67.7	72.0	73.8	7
MYOS_00022_00_01	EPL-BS0447	4.0	12.7	-0.1	5.5	6.5	22.2	53.8	14.5	22.2	28.5	7.2	69.1	85.9	85.5	82.7	9
MYOS_00023_00_01	EPL-BS0271	-5.5	-7.2		-6.3	1.2	4.1	-4.5		4.1	12.2	37.6	73.2	93.6	64.4	64.9	7
MYOS_00024_00_01	P4_C_001	28.1			28.1		115.5			115.5		54.5	68.8	69.8	71.6	78.2	7
MYOS_00024_00_01	DM6-1	83.8			83.8		46.8			46.8							
MYOS_00025_00_01	P4_B_013	89.7			89.7		76.3			76.3		67.8	73.5	70.4	76.1	83.7	7

ACE2-Spike protein-protein interaction

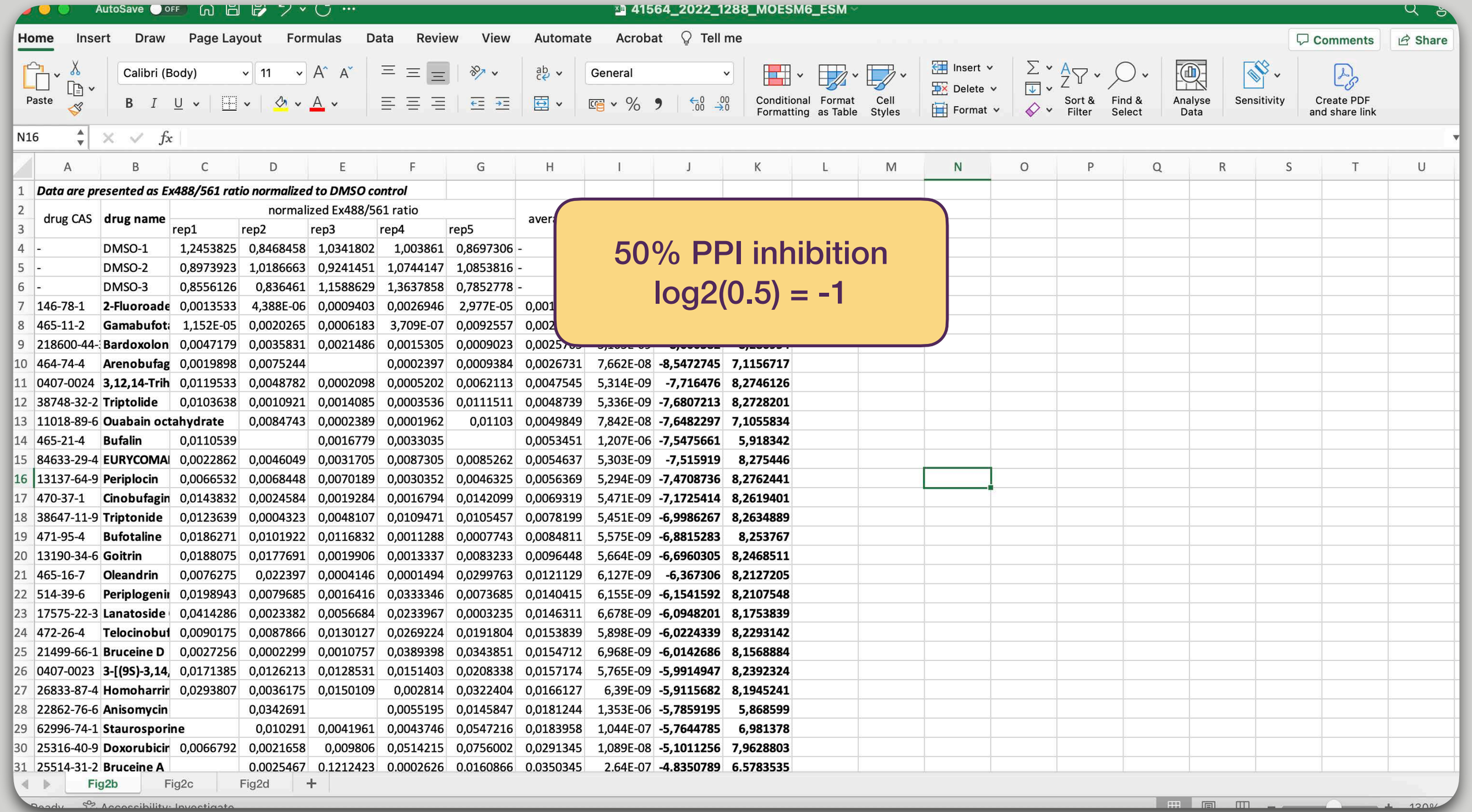


ACE2-Spike protein-protein interaction

Fig. 2: HPS of natural compounds that inhibit spike and ACE2 interaction.



ACE2-Spike protein-protein interaction



	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q	R	S	T	U
1	***Data are presented as Ex488/561 ratio normalized to DMSO control***																				
2	drug CAS	**drug name**	normalized Ex488/561 ratio					aver													
3			rep1	rep2	rep3	rep4	rep5														
4	-	DMSO-1	1,2453825	0,8468458	1,0341802	1,003861	0,8697306	-													
5	-	DMSO-2	0,8973923	1,0186663	0,9241451	1,0744147	1,0853816	-													
6	-	DMSO-3	0,8556126	0,836461	1,1588629	1,3637858	0,7852778	-													
7	146-78-1	**2-Fluoroade**	0,0013533	4,388E-06	0,0009403	0,0026946	2,977E-05	0,001													
8	465-11-2	**Gamabufot**	1,152E-05	0,0020265	0,0006183	3,709E-07	0,0092557	0,002													
9	218600-44-	**Bardoxolon**	0,0047179	0,0035831	0,0021486	0,0015305	0,0009023	0,0025													
10	464-74-4	**Arenobufag**	0,0019898	0,0075244		0,0002397	0,0009384	0,0026731	7,662E-08	**-8,5472745**	**7,1156717**										
11	0407-0024	**3,12,14-Trih**	0,0119533	0,0048782	0,0002098	0,0005202	0,0062113	0,0047545	5,314E-09	**-7,716476**	**8,2746126**										
12	38748-32-2	**Triptolide**	0,0103638	0,0010921	0,0014085	0,0003536	0,0111511	0,0048739	5,336E-09	**-7,6807213**	**8,2728201**										
13	11018-89-6	**Ouabain octahydrate**	0,0084743	0,0002389	0,0001962	0,01103	0,0049849	7,842E-08	**-7,6482297**	**7,1055834**											
14	465-21-4	**Bufalin**	0,0110539		0,0016779	0,0033035		0,0053451	1,207E-06	**-7,5475661**	**5,918342**										
15	84633-29-4	**EURYCOMA**	0,0022862	0,0046049	0,0031705	0,0087305	0,0085262	0,0054637	5,303E-09	**-7,515919**	**8,275446**										
16	13137-64-9	**Periplocin**	0,0066532	0,0068448	0,0070189	0,0030352	0,0046325	0,0056369	5,294E-09	**-7,4708736**	**8,2762441**										
17	470-37-1	**Cinobufagin**	0,0143832	0,0024584	0,0019284	0,0016794	0,0142099	0,0069319	5,471E-09	**-7,1725414**	**8,2619401**										
18	38647-11-9	**Triptonide**	0,0123639	0,0004323	0,0048107	0,0109471	0,0105457	0,0078199	5,451E-09	**-6,9986267**	**8,2634889**										
19	471-95-4	**Bufotaline**	0,0186271	0,0101922	0,0116832	0,0011288	0,0007743	0,0084811	5,575E-09	**-6,8815283**	**8,253767**										
20	13190-34-6	**Goitrin**	0,0188075	0,0177691	0,0019906	0,0013337	0,0083233	0,0096448	5,664E-09	**-6,6960305**	**8,2468511**										
21	465-16-7	**Oleandrin**	0,0076275	0,022397	0,0004146	0,0001494	0,0299763	0,0121129	6,127E-09	**-6,367306**	**8,2127205**										
22	514-39-6	**Periplogeni**	0,0198943	0,0079685	0,0016416	0,0333346	0,0073685	0,0140415	6,155E-09	**-6,1541592**	**8,2107548**										
23	17575-22-3	**Lanatoside**	0,0414286	0,0023382	0,0056684	0,0233967	0,0003235	0,0146311	6,678E-09	**-6,0948201**	**8,1753839**										
24	472-26-4	**Telocinobuf**	0,0090175	0,0087866	0,0130127	0,0269224	0,0191804	0,0153839	5,898E-09	**-6,0224339**	**8,2293142**										
25	21499-66-1	**Bruceine D**	0,0027256	0,0002299	0,0010757	0,0389398	0,0343851	0,0154712	6,968E-09	**-6,0142686**	**8,1568884**										
26	0407-0023	**3-[(9S)-3,14,**	0,0171385	0,0126213	0,0128531	0,0151403	0,0208338	0,0157174	5,765E-09	**-5,9914947**	**8,2392324**										
27	26833-87-4	**Homoharrir**	0,0293807	0,0036175	0,0150109	0,002814	0,0322404	0,0166127	6,39E-09	**-5,9115682**	**8,1945241**										
28	22862-76-6	**Anisomycin**		0,0342691		0,0055195	0,0145847	0,0181244	1,353E-06	**-5,7859195**	**5,868599**										
29	62996-74-1	**Staurosporine**		0,010291	0,0041961	0,0043746	0,0547216	0,0183958	1,044E-07	**-5,7644785**	**6,981378**										
30	25316-40-9	**Doxorubicir**	0,0066792	0,0021658	0,009806	0,0514215	0,0756002	0,0291345	1,089E-08	**-5,1011256**	**7,9628803**										
31	25514-31-2	**Bruceine A**		0,0025467	0,1212423	0,0002626	0,0160866	0,0350345	2,64E-07	**-4,8350789**	**6,5783535**										

Let’s get started!
— Work on your Colab notebook
— Prepare a presentation