

Screening synthetic  
and natural  
compounds from  
MyOS Compounds  
List against mm55.

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# The Compounds



- 35 compounds in total
- Mostly natural/ perfume compounds + 4 drugs (3 antifungals and a bisphosphonate)
- Many oily compounds (15) and 6 powders made up with DMSO

- 36 compounds in total
- Synthetic, non-biological compounds
- All initially powders or oily compounds → made up with DMSO

## Orange Box Compounds – Natural + 4 drugs

Orange Box - Tube label	Compound Name - Series 7 - Natural/Perfume Compounds	MYOS Codes	Type
	1Honokiol	MYOS_00370_00_01	Powder
	4O-Propargyleugenol	MYOS_00368_00_01	Liquid (oily)
	5Isoeugenol	MYOS_00363_00_01	Liquid (oily)
	9O-Allyleugenol	MYOS_00367_00_01	Liquid (oily)
	11Bakuchiol	MYOS_00372_00_01	Liquid (oily)
	15Oxyoctaline formate	MYOS_00356_00_01	Liquid (oily)
	18ortho-Eugenol	MYOS_00364_00_01	Liquid (oily)
	20Ebanol	MYOS_00345_00_01	Liquid (oily)
	21Javanol	MYOS_00354_00_01	Liquid (oily)
	22Glycolierral	MYOS_00351_00_01	Liquid (oily)
	23Ambrettolide	MYOS_00342_00_01	Liquid (oily)
	29Magnolol	MYOS_00369_00_01	Powder
	30Okoumal	MYOS_00355_00_01	Liquid (oily)
	31Vetynal fine	MYOS_00362_00_01	Liquid (oily)
	32Climbazole	MYOS_00375_00_01	Powder
	33Zoledronic acid	MYOS_00376_00_01	Powder
	34Bifonazole	MYOS_00374_00_01	Powder
	35Clotrimazole	MYOS_00373_00_01	Powder
	2Silvial	MYOS_00358_00_01	Liquid
	3Folenox	MYOS_00349_00_01	Liquid
	6Dupical	MYOS_00344_00_01	Liquid
	7Florhydral	MYOS_00347_00_01	Liquid
	8Estragole	MYOS_00365_00_01	Liquid
	10O-Methyleugenol	MYOS_00366_00_01	Liquid
	12Isolongifolanone	MYOS_00352_00_01	Liquid
	13Spirogalbanone	MYOS_00360_00_01	Liquid
	14cis-Jasmone	MYOS_00353_00_01	Liquid
	16Spirambrene	MYOS_00359_00_01	Liquid
	17Verdoracine	MYOS_00361_00_01	Liquid
	19Givescone (isomers)	MYOS_00350_00_01	Liquid
	24Safranal	MYOS_00357_00_01	Liquid
	25Bisabolene	MYOS_00343_00_01	Liquid
	26Florocyclene (isomers)	MYOS_00348_00_01	Liquid
	27Ethyl safranate	MYOS_00346_00_01	Liquid
	28Cinnamonitrile	MYOS_00371_00_01	Liquid

## Blue Box Compounds – Synthetic

Blue Box	Compound Name	MYOS Codes	Type	PLATES number
	1 1,4-Naphthoquinone	MYOS_00377_00_01	Powder	A02
	2 1,2-Naphthoquinone	MYOS_00378_00_01	Powder	A03
	3 Plumbagin	MYOS_00379_00_01	Powder	A04
	4 Quinizarin	MYOS_00380_00_01	Powder	A05
	5 PyrCypPyr-4CF3	MYOS_00381_00_01	Powder	A06
	6 N-(4-fluorophenyl)-4-(pyridin-2-yl)thiazol-2-amine	MYOS_00315_00_01	Powder	A07
	7 4-(pyridin-2-yl)-N-(4-(trifluoromethyl)phenyl)thiazol-2-amine	MYOS_00316_00_01	Powder	A08
	8 4-(pyridin-2-yl)-N-(4-(trifluoromethyl)phenyl)thiazol-2-amine	MYOS_00317_00_01	Powder	A09
	9 N-(4-chloro-3-(trifluoromethyl)phenyl)-4-(pyridin-2-yl)thiazol-2-amine	MYOS_00318_00_01	Powder	A10
	10 N-(2-chloro-5-(trifluoromethyl)phenyl)-4-(pyridin-2-yl)thiazol-2-amine	MYOS_00319_00_01	Powder	A11
	11 N-(benzof[d][1,3]diox01-5-yl)-4-(pyridin-2-yl)thiazol-2-amine	MYOS_00320_00_01	Powder	B02
University College London Compounds	Compound Name	MYOS Codes	Type	PLATES number
	1 DM61-1	MYOS_00321_00_01	Liquid (oily)	B03
	2 DM62-1	MYOS_00322_00_01	Powder	B04
	3 DM63-1	MYOS_00323_00_01	Powder	B05
	4 DM65-1	MYOS_00324_00_01	Liquid (oily)	B06
	5 DM68-1	MYOS_00325_00_01	Powder?	B07
University of Otago Compounds	Label on vial	MYOS Codes	Type	PLATES number
	1 UO 15	DNDI0004039624	Powder (dry, solids)	B08
	2 UO 16	DNDI0004039625	Powder (dry, solids)	B09
	3 UO 17	DNDI0004039626	Powder (dry, solids)	B10
	4 UO 18	DNDI0004039627	Powder (dry, solids)	B11
	5 UO 19	DNDI0004039628	Powder (dry, solids)	C02
	6 UO 20	DNDI0004039629	Powder (dry, solids)	C03
	7 UO 21	DNDI0004039630	Powder (dry, solids)	C04
	8 UO 22	DNDI0004039631	Powder (dry, solids)	C05
	9 UO 23	DNDI0004039632	Powder (dry, solids)	C06
	10 UO 24	DNDI0004039633	Powder (dry, solids)	C07
	11 UO 25	DNDI0004039634	Powder (dry, solids)	C08
	12 UO 26	DNDI0004039635	Powder (dry, solids)	C09
	13 UO3051	DNDI0003949121	Powder (dry, solids)	C10
	14 UO30510	DNDI0003949124	Powder (dry, solids)	C11
	15 UO30511	DNDI0003949129	Powder (dry, solids)	D02
	16 UO30512	DNDI0003949130	Powder (dry, solids)	D03
	17 UO3053	DNDI0003949125	Powder (dry, solids)	D04
Compounds from Kymberly (Sydney)	Label on vial	MYOS Codes	Type	PLATES number
	1 KRS_038	MYOS_00307_00_01	Powder	D05
	2 KRS_039	MYOS_00308_00_01	Powder	D06
	3 KRS_040	MYOS_00309_00_01	Powder	D07

# Blue – Experiments at 100uM and 25uM

01

02

## Experiment Results

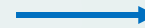
16 compounds to be tested at 120uL 100uM and 25uM concentrations to determine IC50

MYOS Codes	PLATES number	100uM Repea	100uM R2	100uM R3	25uM Repea	25uM R2	25uM R3	
MYOS_00377_00_01	A02	12.6066838	11.6487936	10.9721343	6.31362468	7.57372654	7.17226092	*
MYOS_00378_00_01	A03	22.60154242	17.3324397	17.5269158	14.0874036	11.0053619	9.35718809	*
MYOS_00379_00_01	A04	7.177377892	6.39410188	7.93223559	9.02827763	2.10455764	5.74730842	*
MYOS_00380_00_01	A05	80.47300771	67.6273458	90.5794807	52.3393316	42.5335121	47.640912	
MYOS_00381_00_01	A06	54.68380463	39.3163539	95.1393287	65.7892031	42.2117962	35.5763141	
MYOS_00315_00_01	A07	7.917737789	2.74798928	5.36732109	64.3084833	3.06970509	4.89233692	*
MYOS_00316_00_01	A08	50.36503856	40.2815013	44.1260291	61.7172237	30.308311	48.1158961	
MYOS_00317_00_01	A09	6.066838046	6.17962466	5.93730209	5.20308483	2.74798928	3.08739709	*
MYOS_00318_00_01	A10	52.9562982	78.8873995	75.7599747	58.1388175	38.3512064	31.3014566	
MYOS_00319_00_01	A11	99.35218509	105.053619	114.803673	95.403599	63.766756	119.743509	
MYOS_00320_00_01	B02	10.2622108	7.68096515	9.83217226	100.956298	70.308311	89.5345155	
MYOS Codes	PLATES number							
MYOS_00321_00_01 DM61-1	B03	9.5218509	3.49865952	6.31728942	9.5218509	0.06702413	5.55731476	*
MYOS_00322_00_01 DM62-1	B04	5.203084833	34.1689008	67.7802407	79.7326478	53.9008043	115.468651	
MYOS_00323_00_01 DM63-1	B05	77.01799486	52.9356568	60.0854972	95.5269923	48.4316354	54.0056998	
MYOS_00324_00_01 DM65-1	B06	45.55269923	39.3163539	45.6459785	94.7866324	44.0348525	59.9905003	
MYOS_00325_00_01 DM68-1	B07	44.81233933	45.7506702	96.659278	66.0359897	34.383378	56.9506016	
MYOS Codes	PLATES number							
DNDI0004039624	B08	43.8251928	29.9865952	38.6162128	31.8560411	16.7962466	34.531349	
DNDI0004039625	B09	40.37017995	33.2037534	35.5763141	92.1953728	45.8579088	50.2058265	
DNDI0004039626	B10	10.01542416	7.03753351	6.03229892	9.39845758	0.81769437	2.13742875	*
DNDI0004039627	B11	5.94344473	3.28418231	50.490817	9.5218509	1.3538874	4.22421925	*
DNDI0004039628	C02	3.969151671	4.14209115	6.88727042	70.1079692	67.30563	58.7555415	
DNDI0004039629	C03	4.709511568	2.21179625	5.84230526	74.1799486	62.4798928	54.8606713	
DNDI0004039630	C04	4.462724936	3.60589812	4.03736542	5.44987147	0.92493298	2.70740975	*
DNDI0004039631	C05	6.066838046	3.1769437	5.84230526	9.39845758	29.8793566	2.32742242	*
DNDI0004039632	C06	4.33933162	1.78284182	6.60227992	7.17737789	1.67560322	2.32742242	*
DNDI0004039633	C07	9.398457584	5.10723861	24.7466751	3.84575835	1.3538874	2.04243192	*
DNDI0004039634	C08	79.11568123	50.5764075	77.5649145	76.0308483	60.6568365	56.4756175	
DNDI0004039635	C09	50.61182519	45	33.2013933	101.573265	61.8364611	60.3704877	
DNDI0003949121	C10	5.573264781	3.49865952	5.55731476	106.879177	0.60321716	2.04243192	*
DNDI0003949124	C11	12.23650386	6.17962466	4.51234959	7.91773779	1.46112601	2.70740975	*
DNDI0003949129	D02	9.892030848	51.2198391	36.9062698	5.94344473	-0.4691689	2.23242559	*
DNDI0003949130	D03	3.969151671	1.24664879	8.21722609	1.25449871	-0.1474531	2.23242559	*
DNDI0003949125	D04	109.2236504	67.9490617	45.8359721	115.023136	4.963235	59.2305256	
MYOS Codes	PLATES number							
MYOS_00307_00_01	D05	70.97172237	60.0134048	102.359088	76.8946015	111.7647	93.3343889	
MYOS_00308_00_01	D06	76.89460154	61.8364611	65.880304	94.0462725	105.6985	81.7447752	
MYOS_00309_00_01	D07	90.22107969	41.461126	35.671311	109.100257	96.50735	70.8201393	

# Blue – Lower Concentrations

Plate Position	IC50 Repeat 1	IC50 Repeat 2	IC50 Repeat 3	Mean IC50
A02	9.73	11.74	8.647	9.1885
A03	8.4825	12.085	11.24	11.6625
A04	12.93	11.59	9.665	12.26
A07	>16	>16	>16	>16
A09	>16	14.695	13.075	13.885
<b>B03</b>	5.725	5.325	5.645	<b>5.565</b>
<b>B10</b>	3.22	5.003	4.8	<b>4.341</b>
B11	11.075	8.26	11.165	11.12
C04	>16	>16	7.63	>16
<b>C05</b>	2.58	0.9755	1.535	<b>1.69683333</b>
<b>C06</b>	8.12	0.8225	0.389	<b>3.1105</b>
<b>C07</b>	6.825	2.5025	8.11	<b>5.8125</b>
C10	>16	>16	>16	>16
<b>C11</b>	2.532	6.128	3.4725	<b>4.04416667</b>
D02	>16	>16	>16	>16
D03	15.86	13.87	12.24	13.99

**Six compounds** for  
MIC50 test



**Ten isolates:** mm55,  
I1, I3, I11, Peru72012,  
mm14, S01, P1, AL1,  
CBS247.48

# Orange – Experiments at 1% and 0.25%

01

02

Results

**Why might this be**

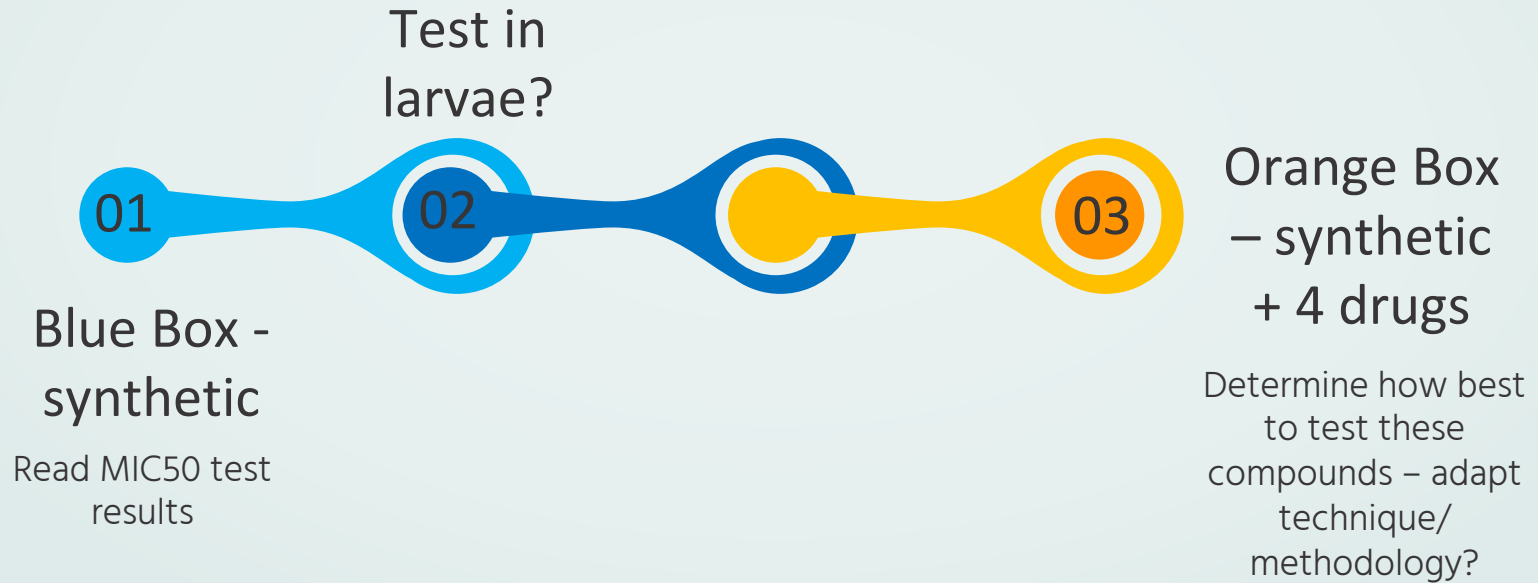
Yielded many  
(possibly too  
many) positive  
hits particularly at

**What I did next?**

- Tested compounds at 0.0625% and 0.015625% – in process of analysing these results

Orange Box - Tube label	1% Repeat 1	1% R2	1% R3		0.25% Repea	0.25% R2	0.25% R3
1	33.5140018	29.8938013	23.64624		15.4923216	31.1591474	10.6094042
4	15.0180668	19.0479777	15.3624172		56.7524842	12.1789561	9.11560007
5	69.2411924	98.0417263	87.7440163		18.33785	50.1393387	34.1028688
9	25.2935863	21.7594336	18.7574266		5.69105691	19.4095052	8.97979969
11	35.4110208	35.4974768	38.3126804		18.495935	19.9517963	17.1278221
15	33.6720867	47.6086465	39.3990833		13.5953026	19.5902689	16.3130199
18	65.7633243	66.9503653	40.7570871		27.1906052	37.3051141	26.3622475
20	56.4363144	39.6550426	23.64624		18.0216802	19.0479777	19.7080292
21	44.4218609	40.3780975	30.0288576		17.2312556	15.9749944	10.4736038
22	22.4480578	16.6980493	14.547615		8.37850045	19.2287414	9.11560007
23	13.7533875	80.1461173	124.545918		5.84914182	92.0765233	12.2390087
29	29.403794	22.6632522	23.7820404		12.3306233	14.890412	10.7452045
30	14.5438121	18.1441591	17.2636225		4.26829268	12.7212473	5.58479036
31	21.4995483	23.7478346	18.4858258		6.95573622	12.902011	9.11560007
32	21.3414634	20.6748512	23.3746393		11.3821138	8.38291783	8.30079783
33	27.66486	41.4626798	24.0536411		13.1210479	12.2635384	12.2390087
34	46.6350497	38.9319876	38.9916822		32.2493225	31.5206749	12.7822102
35	37.6242096	8.02139037	27.7202512		14.2276423	20.1325601	15.0908165
2	11.6982836	10.1905551	19.8438296		20.5510388	19.2287414	12.6464098
3	14.3857272	16.878813	10.7452045		6.16531165	9.10597273	107.570871
6	25.9259259	27.0015817	14.1402139		16.1246612	30.4360925	17.9426243
7	14.2276423	19.0479777	10.6094042		3.3197832	7.84062665	4.362587
8	18.1797651	20.6748512	14.2760143		4.74254743	8.38291783	4.76998812
10	11.8563686	13.4443022	10.8810049		3.00361337	4.76764329	5.04158886
12	14.701897	17.0595767	9.93040231		6.95573622	4.58687957	5.44898998
13	22.131888	20.6748512	11.9674079		5.37488708	13.6250659	5.72059073
14	24.028907	32.062966	14.8192158		4.58446251	6.93680801	4.09098625
16	16.2827462	19.5902689	10.8810049		2.84552846	8.56368155	6.26379223
17	12.1725384	18.867214	16.8562214		5.37488708	6.03298938	4.90578849
19	9.64317977	14.5288845	12.6464098		3.3197832	7.5604429	4.63418774
24	19.9186992	27.7246366	10.4736038		5.05871725	7.65986292	5.17738924
25	17.2312556	21.3979062	13.5970124		9.64317977	15.0711757	8.70819895
26	11.2240289	15.9749944	8.4365982		8.53658537	5.67146193	4.22678662
27	13.4372177	18.6864503	11.5600068		5.37488708	8.38291783	7.89339671
28	7.11382114	15.0711757	9.93040231		9.16892502	4.76764329	4.22678662

# Next Steps





# THANKS

Do you have any questions?

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