

**A Rapid Phenotypic Whole Cell Screening Approach for the Identification of Small Molecule Inhibitors that Counter Beta-lactamase Resistance in *Pseudomonas aeruginosa***

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**Short title:**

HTS Identification of AmpG Specific Small Molecule Inhibitors in *Pseudomonas aeruginosa*

Key words: Pseudomonas, AmpG, Gram negative bacteria

**α** Co-communicated with SJ

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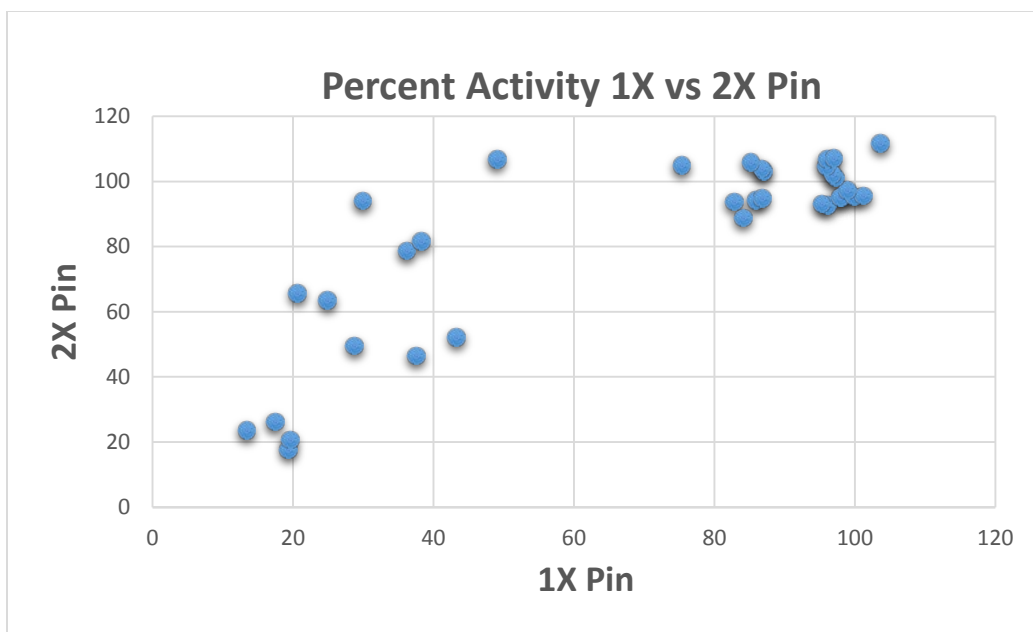
*Email: [spicert@scripps.edu](mailto:spicert@scripps.edu)*

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**Supplemental Section:**

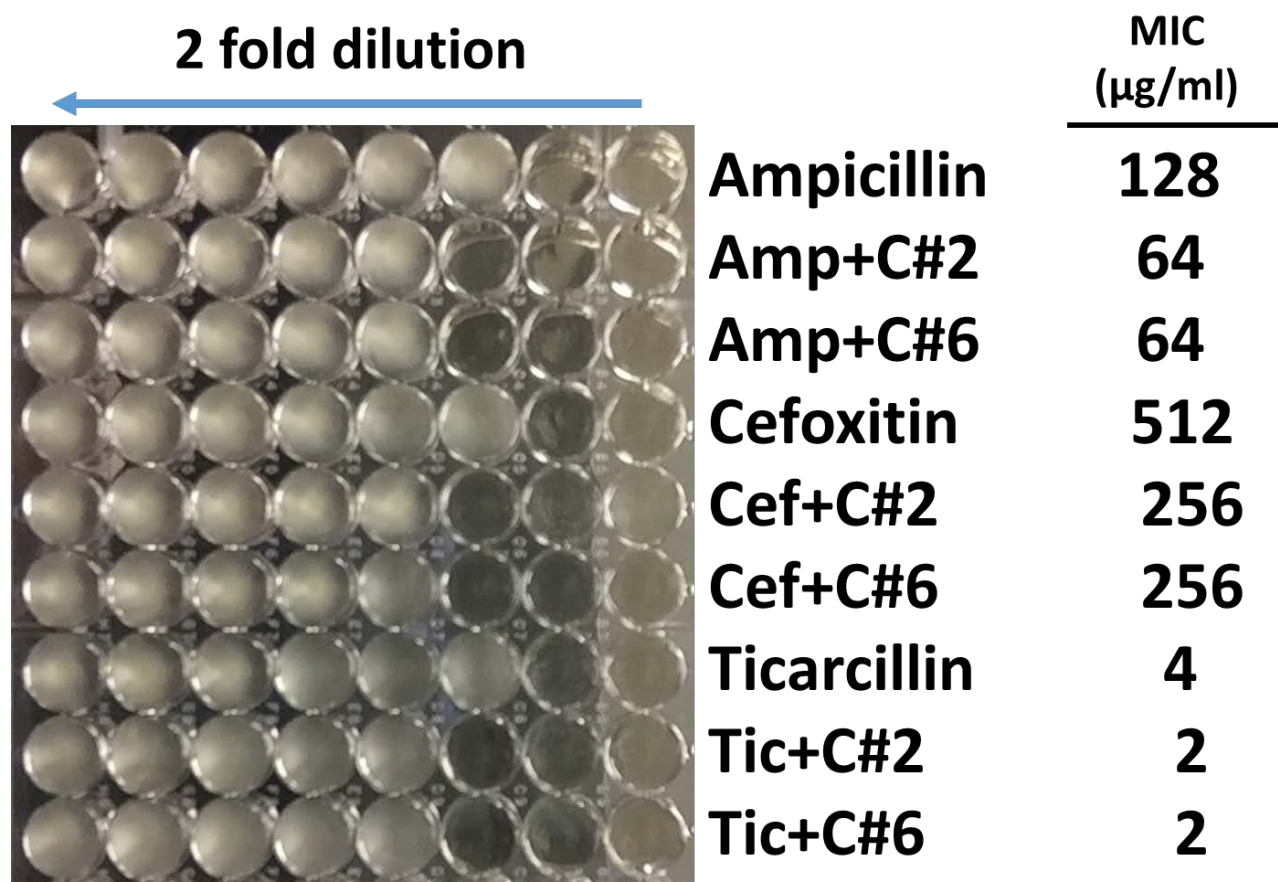
<u>Antibiotic</u>	<u>Expected MIC</u> <u>(ug/mL)</u>	<u>Scripps MIC</u> <u>(ug/mL)</u>	<u>S:B</u>	<u>Z'</u>
Ciprofloxacin	2	3	3.04	0.89
Erythromycin	64	100	2.92	0.9
Aztreonam	2	1.6	2.96	0.82

**Supplemental Table 1.** Susceptibility of PAO1 to well-studied antibiotics. PAO1 was cultured in the presence of varying concentrations of antibiotics and MIC values were compared to established values.



<b>Pearson r</b>	<b>0.8281</b>
<b>95% confidence interval</b>	<b>0.6804 to 0.9111</b>
<b>P value (two-tailed)</b>	<b>&lt; 0.0001</b>
<b>P value summary</b>	<b>***</b>
<b>Is the correlation significant?</b>	<b>Yes</b>
<b>R squared</b>	<b>0.6857</b>





















**Supplemental Figure 1.** PAO1 AmpG assay correlation plot – 1X vs 2X pinning. The relative activities of compounds for 17 matched plates were compared at single versus double pinning (10uM versus 20uM screening concentration).



**Supplemental Figure 2.** Synergy testing in PAO1 bacteria. 25µg/mL of test compound were tested in combination with or without antibiotics known to induce AmpC. This was the highest concentration of compound that was not found to be toxic to the bacteria by itself. In this case the antibiotics were serially diluted and added to a constant concentration of test compound, i.e. either compound #2 or #6 (C#2 or C#6) as listed in Table 3 of the main text. The MIC of each antibiotic by itself or in combination is shown. The presence of turbidity indicates bacterial growth which as shown when in combination yields a 2 fold improvement in the efficacy of the Amp=Ampicillin, Cef=Cefoxitin, Tic=Ticarcillin. This experiment was repeated and confirmed the results shown above for an N of 2 experiments.

SampleID	Compound Information		Compound Descriptors							PAINS_A	PAINS_B	PAINS_C	Dose Response Curve	PAO1 PamC LUX LUMI						PAO1 LUX ABS			PAO1 ABS			No Fox ABS							
	Structure	Vendor Name	Vendor Catalog	Heavy Atom Count	H bond donors	H bond acceptors	Molecular Weight	logP	logD					Final EC50	Averaged Max % Response	StdDev Max % Response	Hill Slope	Ligand Efficiency	logP	logD	Final EC50	Averaged Max % Response	StdDev Max % Response	Final EC50	Averaged Max % Response	StdDev Max % Response	Hill Slope	Final EC50	Averaged Max % Response	StdDev Max % Response			
SR-010002786-1		ChemBridge	7826815	32	2	6	434.48	3.53	3.52					= 2.4E-9	52.27	35.41	1.58	0.38	####	5.10	>	45.7E-6	-2.9E+0	1.53	>	45.7E-6	2.40	3.83	>	45.7E-6	-223.7E-3	4.17	
SR-010007620-2		SigmaAldrich	R-2751	25	14	16	786.35	0.54	0.54					= 3.1E-6	96.71	0.32	2.92	0.31	####	4.96	=	27.3E-6	107.70	4.33	=	41.1E-6	89.78	9.90	18.29	=	42.2E-6	90.39	8.44
SR-050000238-3		BIOMOL	NP-223	11	1	4	154.12	#####	-0.38					= 6.5E-6	91.48	1.57	0.78	0.66	####	5.57	>	45.7E-6	22.66	10.69	=	34.8E-6	80.67	12.84	5.86	=	36.6E-6	67.93	13.14
SR-01001020782-1		Asinex	BAS 00244885	19	2	4	255.27	2.34	2.33			hizone_chemid_A(479)		= 10.4E-6	85.46	5.21	3.84	0.37	####	2.65	>	45.7E-6	14.35	3.00	>	45.7E-6	26.55	3.04	>	45.7E-6	21.34	6.29	
SR-01000827276-1		Sequoia Research Products Ltd.	SRP00850b	28	2	7	389.42	#####	-0.43					>	11.4E-6	9.79	16.34	0.25	####	5.37	=	11.4E-6	50.41	3.70	=	6.8E-6	58.30	6.97	5.56	=	7.1E-6	54.40	6.57
SR-050000070-1		MicroSource	01500492	85	18	18	1203.48	#####	-17.72					= 14.E-6	97.11	0.98	2.23	0.08	####	22.57	=	27.2E-6	107.51	6.96	>	15.2E-6	#####	0.85	>	15.2E-6	103.63	1.47	
SR-01000597499-6		Cayman Chemical	70610	20	3	5	270.24	2.71	1.95			catechol_A(92)		>	18.3E-6	25.47	10.62	0.33	####	2.79	>	18.3E-6	12.16	2.70	>	18.3E-6	15.74	4.37	>	18.3E-6	15.23	4.67	
SR-01000000495-5		Cayman Chemical	81025	27	2	6	368.38	4.12	4.12					>	18.3E-6	20.44	7.73	0.25	####	0.62	>	18.3E-6	9.23	3.27	>	18.3E-6	29.08	2.68	>	18.3E-6	26.99	1.71	
SR-01000946328-1		Cayman Chemical	10009986	29	0	6	396.43	4.42	4.41					>	18.3E-6	37.19	47.61	0.23	####	0.32	>	18.3E-6	9.46	2.41	>	18.3E-6	30.06	4.36	>	18.3E-6	27.01	2.66	
SR-01000588239-1		Deltagen	K839-0038	28	2	5	378.42	3.61	3.58			manmich_A(246)		= 21.2E-6	76.83	1.47	6.96	0.23	####	1.09	=	11.6E-6	75.58	4.55	=	22.1E-6	61.66	3.88	1.35	=	16.9E-6	58.01	3.59
SR-01000612324-5		BIOMOL	DL-498	25	1	7	363.41	0.83	-0.18					>	25.1E-6	20.91	7.86	0.26	####	4.78	>	25.1E-6	22.48	2.38	=	11.2E-6	#####	0.57	8.65	=	13.7E-6	94.51	5.86
SR-01000949932-1		Deltagen	4545-1561	32	1	6	468.81	5.22	5.17			ene_fwe_het_A(21)		>	29.3E-6	-9.5E+0	1.45	0.20	####	#####	>	29.3E-6	-1.3E+0	2.25	>	29.3E-6	5.49	6.84	>	29.3E-6	3.59	6.98	
SR-01000455070-1		Deltagen	3486-0184	24	2	5	326.35	3.10	3.07					>	34.5E-6	12.02	9.41	0.26	####	1.39	>	34.5E-6	14.34	0.67	>	34.5E-6	28.18	5.00	>	34.5E-6	27.09	2.07	
SR-01000569902-1		Deltagen	K784-0750	26	0	3	371.54	4.71	4.71					>	35.1E-6	-3.9E+0	3.92	0.24	####	#####	>	35.1E-6	2.06	0.94	>	35.1E-6	23.68	2.42	>	35.1E-6	19.36	5.20	
SR-01000548585-1		Deltagen	C093-0157	34	1	5	452.55	5.24	4.64					>	37.9E-6	17.82	12.25	0.18	####	#####	>	37.9E-6	0.21	3.81	>	37.9E-6	2.87	3.30	>	37.9E-6	-1.1E+0	3.19	
SR-01000407137-1		Deltagen	1773-0188	27	1	3	358.43	4.65	4.65					>	40.4E-6	-13.9E+0	3.52	0.23	####	#####	>	40.4E-6	-1.5E+0	0.11	>	40.4E-6	17.21	3.23	>	40.4E-6	11.93	4.86	
SR-01000536500-1		Deltagen	8012-5120	28	2	3	392.37	4.63	4.63					>	40.6E-6	-11.3E+0	11.64	0.22	####	#####	>	40.6E-6	-443.3E-3	5.65	>	40.6E-6	19.20	2.21	>	40.6E-6	13.44	2.81	
SR-0100021819-1		Deltagen	8008-9610	20	1	4	336.23	1.47	1.37					>	40.9E-6	22.51	10.95	0.31	####	3.02	>	40.9E-6	9.61	1.82	>	40.9E-6	17.37	2.23	>	40.9E-6	13.70	3.46	
SR-01000520919-1		Deltagen	8008-7873	24	1	3	387.28	3.20	3.20					>	42.2E-6	31.11	21.74	0.26	####	1.17	>	42.2E-6	4.21	4.57	>	42.2E-6	18.45	1.38	>	42.2E-6	8.50	9.41	

SR-01000139385-1	SR-05000002388-2	SR-01000095587-1	SR-0100016437-1	SR-0100027910-1	SR-0100025678-1	SR-01000849391-1	SR-0100037437-1	SR-01000289591-1	SR-01000106388-1	SR-01000246161-1	SR-0100028278-1	SR-0100029852-1	SR-01000274283-1	SR-0100006670-1	SR-01000019293-1	SR-01000296981-1	SR-0100011590-1	SR-0100050437-1		
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27	24	26	26	32	26	24	33	23	28	19	27	28	31	30	29	29	27	28	28	
2	1	2	1	2	1	1	0	4	0	2	1	2	2	3	1	2	2	2	1	
4	4	4	6	4	3	3	5	5	4	3	5	5	4	4	3	4	6	4	4	
359.40	319.40	345.37	364.42	447.55	412.85	347.26	438.43	316.28	401.57	285.40	380.41	399.46	411.41	425.50	411.52	417.50	368.38	404.52	385.45	
4.46	1.94	3.73	2.36	4.86	3.11	3.13	3.14	3.24	4.55	3.37	3.51	3.37	3.57	4.32	3.77	3.22	4.12	3.86	3.10	
4.37	1.71	3.70	2.36	4.59	3.11	3.13	3.14	3.19	4.55	3.01	3.05	3.36	3.57	4.24	3.77	3.21	4.12	3.86	3.10	
mamich_A(296) mamich_A(296) mamich_A(296)																				
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42.3E-6	43.7E-6	44.7E-6	45.1E-6	45.3E-6	45.7E-6	45.7E-6	45.7E-6	45.7E-6	45.7E-6	45.7E-6	45.7E-6	45.7E-6	45.7E-6	45.7E-6	45.7E-6	45.7E-6	45.7E-6	45.7E-6	45.7E-6	
3.74	53.10	73.15	2.01	19.61	-7.4E+0	6.89	21.04	10.38	3.47	11.68	-7.7E+0	-3.3E+0	5.58	-5.2E+0	18.91	-7.4E+0	35.44	15.13	0.12	
17.67	16.76	9.43	21.49	19.68	9.50	20.04	21.04	10.38	9.86	9.33	8.53	20.10	4.02	6.63	7.06	6.21	16.61	9.47	12.78	
0.23	0.25	0.23	0.23	0.19	0.23	0.25	0.18	0.26	0.22	0.32	0.23	0.22	0.20	0.20	0.21	0.21	0.23	0.22	0.22	
###	###	###	###	###	###	###	###	###	###	###	###	###	###	###	###	###	###	###	###	###
4E-3	2.65	0.65	1.99	###	1.23	1.21	1.20	1.15	###	1.33	1.30	0.98	0.77	0.10	0.57	1.13	0.22	0.48	1.24	
catechol_A(02) thiophene_amino C(7)																				
>	>	>	>	>	>	>	>	>	>	>	>	>	>	>	>	>	>	>	>	
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18.78	9.28	49.41	18.03	1.41	2.30	12.72	4.39	-873.1E-3	1.07	6.32	3.42	-1.2E+0	-2.2E+0	1.29	11.26	0.85	23.60	12.62	7.71	
4.09	0.88	4.98	2.88	4.82	3.24	5.61	1.68	1.00	19.32	2.25	0.56	6.23	3.10	3.20	0.91	2.47	3.45	1.62	5.86	
>	>	>	>	>	>	>	>	>	>	>	>	>	>	>	>	>	>	>	>	>
42.3E-6	45.7E-6	45.7E-6	45.1E-6	45.3E-6	45.7E-6	45.7E-6	45.7E-6	45.7E-6	45.7E-6	45.7E-6	45.7E-6	45.7E-6	45.7E-6	45.7E-6	45.7E-6	45.7E-6	45.7E-6	45.7E-6	45.7E-6	45.7E-6
26.43	9.40	47.53	20.62	6.95	17.92	23.71	11.35	13.63	16.19	31.20	15.36	23.66	22.47	14.14	29.74	14.46	34.96	30.68	24.32	
4.96	2.35	6.53	3.26	1.94	2.96	2.48	4.67	2.97	8.79	3.88	3.25	6.35	9.24	5.75	5.09	2.74	5.62	3.37	2.68	
>	>	>	>	>	>	>	>	>	>	>	>	>	>	>	>	>	>	>	>	>
42.3E-6	45.7E-6	45.7E-6	45.1E-6	45.3E-6	45.7E-6	45.7E-6	45.7E-6	45.7E-6	45.7E-6	45.7E-6	45.7E-6	45.7E-6	45.7E-6	45.7E-6	45.7E-6	45.7E-6	45.7E-6	45.7E-6	45.7E-6	45.7E-6
19.84	6.21	45.10	17.38	3.36	15.91	17.73	5.76	9.84	15.20	33.15	11.59	16.54	12.85	10.98	18.11	9.60	33.41	19.46	16.60	
1.86	4.33	2.99	1.74	3.19	2.76	5.85	2.73	1.68	6.65	6.33	1.25	3.13	6.03	9.34	8.79	7.54	3.33	7.26	1.96	

SF-0100023482-1	SF-01000289290-1	SF-01000254817-1	SF-01000295053-1	SF-01000106641-1	SF-01000271350-1	SF-01000099440-1	SF-01000115944-1	SF-01000348203-1	SF-01000296731-1	SF-0100032489-1	SF-01000135766-1	SF-0100031787-1	SF-01000199901-1	SF-01000333351-1	SF-0100044287-1	SF-01000106201-1	SF-01000285703-1	SF-01000235880-1	SF-01000324800-1	
																				
ChemBridge	ChemBridge	ChemBridge	ChemDiv	ChemDiv	ChemBridge	ChemDiv	ChemDiv	ChemDiv	ChemBridge	ChemDiv	ChemDiv	ChemDiv	ChemBridge	ChemBridge	ChemBridge	ChemDiv	ChemDiv	ChemBridge	ChemBridge	
6475864	7935659	7314826	7959388	0991-0004	7722941	C756-0152	7706-0015	ASN 06577716	6167610	BAS 09668359	C753-1930	ASN 08245352	5231551	AEM 10396833	K784-7981	C753-1665	7916720	6495558	BAS 11099827	
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1	1	3	2	1	2	1	1	1	1	2	2	1	2	1	1	2	1	1	2	
4	3	4	3	4	3	3	4	5	3	6	3	6	6	5	3	3	4	4	3	
437.73	443.32	416.53	397.55	357.42	326.22	398.56	319.40	420.82	402.89	264.37	410.51	302.33	398.91	410.53	336.43	408.51	417.26	441.34	313.78	
3.14	3.95	4.10	2.74	3.76	3.62	3.27	1.95	3.08	3.59	2.76	3.40	0.75	3.80	3.19	3.28	2.31	2.96	3.64	3.49	
3.14	3.95	1.29	2.72	3.69	1.94	3.27	1.74	3.08	3.59	2.20	3.40	0.75	3.80	3.19	3.47	3.28	2.31	2.96	3.49	
indol_3yl_alk(461)	indol_3yl_alk(461)	indol_3yl_alk(461)	indol_3yl_alk(461)	indol_3yl_alk(461)	indol_3yl_alk(461)	indol_3yl_alk(461)	indol_3yl_alk(461)	indol_3yl_alk(461)	indol_3yl_alk(461)	indol_3yl_alk(461)	indol_3yl_alk(461)	indol_3yl_alk(461)	indol_3yl_alk(461)	indol_3yl_alk(461)	indol_3yl_alk(461)	indol_3yl_alk(461)	indol_3yl_alk(461)	indol_3yl_alk(461)	indol_3yl_alk(461)	manmch_A(296)
> 45.7E-6	> 45.7E-6	> 45.7E-6	> 45.7E-6	> 45.7E-6	> 45.7E-6	> 45.7E-6	> 45.7E-6	> 45.7E-6	> 45.7E-6	> 45.7E-6	> 45.7E-6	> 45.7E-6	> 45.7E-6	> 45.7E-6	> 45.7E-6	> 45.7E-6	> 45.7E-6	> 45.7E-6	> 45.7E-6	> 45.7E-6
10.94	19.63	-5.3E+0	7.52	20.48	-3.9E+0	-6.2E+0	45.74	-9.8E+0	10.20	17.49	3.90	-6.9E+0	25.39	0.14	0.12	21.21	4.85	1.69	10.94	
12.51	17.66	5.63	17.44	13.42	13.64	9.31	48.00	13.69	5.75	17.17	19.07	11.41	8.80	19.19	9.49	17.19	8.69	4.59	12.51	
0.28	0.20	0.21	0.21	0.25	0.29	0.22	0.25	0.21	0.23	0.32	0.20	0.28	0.23	0.21	0.24	0.20	0.23	0.23	0.28	
###	###	###	###	###	###	###	###	###	###	###	###	###	###	###	###	###	###	###	###	###
0.85	0.39	3.05	1.62	0.65	2.40	1.07	2.60	1.26	0.75	2.14	0.95	3.59	0.54	1.15	0.87	1.06	2.03	1.38	0.85	
> 45.7E-6	> 45.7E-6	> 45.7E-6	> 45.7E-6	> 45.7E-6	> 45.7E-6	> 45.7E-6	> 45.7E-6	> 45.7E-6	> 45.7E-6	> 45.7E-6	> 45.7E-6	> 45.7E-6	> 45.7E-6	> 45.7E-6	> 45.7E-6	> 45.7E-6	> 45.7E-6	> 45.7E-6	> 45.7E-6	> 45.7E-6
7.66	1.13	4.62	0.25	8.31	-1.1E+0	1.14	16.98	6.68	4.97	34.36	5.36	27.95	2.77	3.82	9.70	11.12	0.06	2.86	7.66	
7.92	1.13	3.28	3.88	2.37	4.32	3.72	1.73	3.18	1.97	10.37	6.02	11.08	2.17	1.96	7.75	2.11	2.02	2.64	7.92	
> 45.7E-6	> 45.7E-6	> 45.7E-6	> 45.7E-6	> 45.7E-6	> 45.7E-6	> 45.7E-6	> 45.7E-6	> 45.7E-6	> 45.7E-6	> 45.7E-6	> 45.7E-6	> 45.7E-6	> 45.7E-6	> 45.7E-6	> 45.7E-6	> 45.7E-6	> 45.7E-6	> 45.7E-6	> 45.7E-6	> 45.7E-6
6.89	11.04	25.99	5.60	13.91	19.06	17.17	18.42	13.65	30.90	28.05	22.31	12.46	15.54	20.64	29.45	19.12	15.37	20.95	6.89	
1.48	3.07	4.64	4.68	3.71	15.04	8.00	3.21	3.69	3.24	4.29	1.42	0.35	2.28	3.19	3.51	3.51	2.64	16.04	1.48	
> 45.7E-6	> 45.7E-6	> 45.7E-6	> 45.7E-6	> 45.7E-6	> 45.7E-6	> 45.7E-6	> 45.7E-6	> 45.7E-6	> 45.7E-6	> 45.7E-6	> 45.7E-6	> 45.7E-6	> 45.7E-6	> 45.7E-6	> 45.7E-6	> 45.7E-6	> 45.7E-6	> 45.7E-6	> 45.7E-6	> 45.7E-6
10.46	11.04	20.81	4.28	12.75	8.20	13.37	11.15	6.40	22.40	25.75	16.88	5.07	12.33	13.06	24.24	22.75	12.32	20.06	10.46	
0.60	1.06	1.06	4.17	0.85	19.65	6.37	6.48	3.49	2.16	5.40	1.95	3.16	5.87	3.51	3.06	5.95	0.75	12.87	0.60	












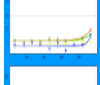
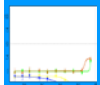


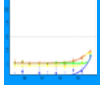
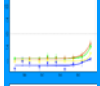



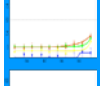
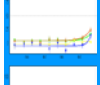
SR	Chemical Structure	Source	PubChem ID	Count	Score	Score	Score	Score	Score	Score	Score	Score	Score	Score	Score	Score	Score	Score							
SF-0100028569-1		ChemBridge	6990311	21	1	3	311.44	3.77	3.77		> 45.7E-6	-4.3E+0	4.49	0.29	###	0.57	> 45.7E-6	4.52	3.34	> 45.7E-6	23.35	2.34	> 45.7E-6	18.81	0.46
SF-01000348318-1		Asinex	ASN 07274721	25	1	4	338.45	3.78	3.78		> 45.7E-6	-15.5E+0	11.25	0.24	###	0.56	> 45.7E-6	3.26	2.05	> 45.7E-6	14.88	2.48	> 45.7E-6	12.92	4.69
SF-01000317422-1		Asinex	BAS 00127549	22	0	2	290.36	4.49	4.49		> 45.7E-6	6.52	6.18	0.28	###	#####	> 45.7E-6	15.84	1.12	> 45.7E-6	36.70	3.57	> 45.7E-6	31.10	6.07
SF-0100027206-1		ChemBridge	7749545	25	1	5	334.41	4.94	4.94		> 45.7E-6	11.90	9.09	0.24	###	#####	> 45.7E-6	9.57	2.44	> 45.7E-6	23.54	4.49	> 45.7E-6	20.81	1.84
SF-01000353698-1		Asinex	AST 06571411	28	1	5	396.87	4.43	4.43		> 45.7E-6	2.60	8.03	0.22	###	#####	> 45.7E-6	4.81	3.88	> 45.7E-6	25.79	4.01	> 45.7E-6	11.63	8.01
SF-01000287779-1		ChemBridge	7928910	25	1	3	433.27	3.05	3.05		> 45.7E-6	24.90	17.84	0.24	###	1.29	> 45.7E-6	32.13	5.14	> 45.7E-6	32.23	6.03	> 45.7E-6	27.90	3.37
SF-01000212925-1		ChemDiv	C527-0741	28	1	3	402.55	3.34	3.32		> 45.7E-6	6.08	16.85	0.22	###	1.02	> 45.7E-6	3.00	3.01	> 45.7E-6	19.44	0.39	> 45.7E-6	16.88	1.18
SF-01000106178-1		ChemDiv	C753-1629	29	2	3	390.52	3.36	3.36		> 45.7E-6	14.49	16.33	0.21	###	0.98	> 45.7E-6	3.70	4.81	> 45.7E-6	25.34	3.22	> 45.7E-6	20.89	4.82
SF-01000004532		SigmaAldrich	T2320	31	1	3	481.33	4.77	4.49		> 45.7E-6	4.32	10.57	0.20	###	#####	> 45.7E-6	5.79	4.12	> 45.7E-6	15.67	5.44	> 45.7E-6	11.52	3.44
SF-01000289313-1		ChemBridge	6224766	24	1	3	431.73	3.37	3.37		> 45.7E-6	23.71	26.37	0.25	###	0.97	> 45.7E-6	0.41	1.79	> 45.7E-6	20.40	5.73	> 45.7E-6	11.08	2.56
SF-01000258231-1		ChemBridge	6074033	25	0	5	412.25	3.17	3.17		> 45.7E-6	9.37	17.98	0.24	###	1.17	> 45.7E-6	3.36	2.93	> 45.7E-6	7.57	1.54	> 45.7E-6	3.91	0.87
SF-01000226450-1		ChemBridge	6058084	24	4	6	326.39	4.68	4.25		> 45.7E-6	-974.1E-3	13.97	0.25	###	0.09	> 45.7E-6	2.75	2.46	> 45.7E-6	24.54	3.72	> 45.7E-6	22.23	1.80
SF-01000001375		MicroSource	01503934	27	1	5	403.97	3.69	2.82		> 45.7E-6	10.17	16.66	0.23	###	1.52	> 45.7E-6	-2.8E+0	3.85	> 45.7E-6	23.28	3.64	> 45.7E-6	20.61	1.61
SF-01000233672-1		ChemBridge	6400918	24	0	3	360.90	3.99	3.99		> 45.7E-6	-2.9E+0	8.27	0.25	###	0.35	> 45.7E-6	0.13	1.77	> 45.7E-6	20.00	7.08	> 45.7E-6	13.93	7.58
SF-0100026096-1		ChemBridge	7377356	24	0	3	330.46	3.96	3.96		> 45.7E-6	-4.1E+0	5.62	0.25	###	0.38	> 45.7E-6	-416.8E-3	4.00	> 45.7E-6	23.17	5.05	> 45.7E-6	17.76	9.67
SF-01000153722-1		ChemDiv	D014-0048	23	1	4	314.42	1.99	1.74		> 45.7E-6	3.60	5.25	0.26	###	2.60	> 45.7E-6	13.01	2.39	> 45.7E-6	18.46	7.31	> 45.7E-6	11.04	10.39
SF-0100018322-1		Asinex	BAS 03386064	26	1	4	370.37	4.22	4.20		> 45.7E-6	11.82	6.33	0.23	###	0.14	> 45.7E-6	10.03	2.07	> 45.7E-6	33.63	6.23	> 45.7E-6	29.33	5.16
SF-01000113297-1		ChemDiv	6018-0225	24	1	7	330.34	2.61	2.61		> 45.7E-6	16.60	16.40	0.25	###	1.73	> 45.7E-6	2.21	5.77	> 45.7E-6	3.60	2.01	> 45.7E-6	3.46	1.55
SF-01000233335-1		ChemBridge	6469056	31	1	5	448.58	3.81	3.81		> 45.7E-6	-1.6E+0	12.42	0.20	###	0.53	> 45.7E-6	2.62	3.45	> 45.7E-6	11.30	3.67	> 45.7E-6	8.60	6.02
SF-0100028569-1		ChemBridge	7937271	28	1	5	416.37	1.98	1.98		> 45.7E-6	36.05	13.89	0.22	###	2.36	> 45.7E-6	14.08	13.77	> 45.7E-6	28.15	3.21	> 45.7E-6	15.65	15.38

indol\_3yl\_alk(461)

mannich\_A(296)



SR-0100004522-1	SR-01000024217-1	SR-01000017424-1	SR-01000015792-1	SR-01000006671-1	SR-01000047932-1	SR-01000265381	SR-0100026533-1	SR-01000401381	SR-0100024762-1	SR-0100088054-1	SR-01000253940-1	SR-0100025817-1	SR-0100028155-1	SR-01000910344-1	SR-0100032617-1	SR-01000139653-1	SR-01000925275-1	SR-01000323393-1		
Eramine	Life Chemicals	Life Chemicals	Life Chemicals	Life Chemicals	ChemDiv	ChemBridge	ChemBridge	ChemBridge	ChemBridge	ChemDiv	ChemBridge	ChemBridge	ChemBridge	Life Chemicals	Asinex	ChemDiv	Life Chemicals	Asinex		
T0518-5204	F2597-0101	F1854-0019	F2031-0666	F0526-1308	7790-1092	7960672	6061526	7567236	ASN 05551942	5786784	7188000	7184581	7914038	F5041-0268	BAS 09668346	E002-0538	F5832-0261	BAS 00782554		
30	27	28	23	31	22	23	26	21	27	27	25	27	26	24	20	27	26	24		
0	1	4	5	2	3	2	3	1	0	6	1	0	3	6	1	2	1	3		
7	4	3	3.54	4.90	3.20	3.82	3.72	3.40	3.65	2.37	3.56	3.77	4.10	1.02	3.27	5.05	3.73	1.42		
1.70	3.64	3.67	3.54	4.64	2.45	3.80	3.70	3.40	3.65	-0.40	3.56	3.77	4.09	1.02	2.79	5.05	3.73	1.20		
429.45	410.46	392.47	314.36	435.54	314.36	329.42	347.41	395.19	386.92	371.43	380.89	364.40	375.85	345.42	276.38	399.43	377.47	321.29		
1.70	3.66	3.68	3.54	4.90	3.20	3.82	3.72	3.40	3.65	2.37	3.56	3.77	4.09	1.02	3.27	5.05	3.73	1.42		
1.20	1.20	1.20	1.20	1.20	1.20	1.20	1.20	1.20	1.20	1.20	1.20	1.20	1.20	1.20	1.20	1.20	1.20	1.20	1.20	
4.79	4.79	4.79	4.79	4.79	4.79	4.79	4.79	4.79	4.79	4.79	4.79	4.79	4.79	4.79	4.79	4.79	4.79	4.79	4.79	
>	>	>	>	>	>	>	>	>	>	>	>	>	>	>	>	>	>	>	>	
45.7E-6	45.7E-6	45.7E-6	45.7E-6	45.7E-6	45.7E-6	45.7E-6	45.7E-6	45.7E-6	45.7E-6	45.7E-6	45.7E-6	45.7E-6	45.7E-6	45.7E-6	45.7E-6	45.7E-6	45.7E-6	45.7E-6	45.7E-6	
24.06	-2.3E+0	15.82	15.09	18.62	28.67	15.09	34.86	0.01	15.82	7.22	4.29	-16.1E+0	4.32	-1.9E+0	22.83	1.95	11.53	13.45	0.25	
13.45	11.53	10.31	15.09	15.25	13.63	15.09	34.17	16.19	10.31	11.99	12.01	6.09	18.85	15.08	14.92	16.28	11.53	13.45	0.25	
0.25	0.26	0.22	0.26	0.20	0.28	0.26	0.23	0.29	0.23	0.23	0.24	0.23	0.23	0.25	0.30	0.23	0.23	0.25	0.25	
###	###	###	###	###	###	###	###	###	###	###	###	###	###	###	###	###	###	###	###	###
3.14	0.79	0.66	0.79	###	1.89	0.54	0.64	0.94	0.69	4.74	0.78	0.57	0.25	3.32	1.55	###	0.61	3.14	3.14	
>	>	>	>	>	>	>	>	>	>	>	>	>	>	>	>	>	>	>	>	>
45.7E-6	46.5E-6	46.5E-6	46.5E-6	46.4E-6	45.7E-6	45.7E-6	45.7E-6	45.7E-6	45.7E-6	45.7E-6	45.7E-6	45.7E-6	45.7E-6	45.7E-6	45.7E-6	45.7E-6	45.7E-6	45.7E-6	45.7E-6	45.7E-6
17.47	3.21	7.13	3.21	-2.2E+0	10.74	1.96	35.27	-2.1E+0	-1.6E+0	0.46	12.85	1.08	0.24	28.70	17.00	15.77	2.89	17.47	4.05	
4.05	2.75	4.42	2.75	1.49	3.63	3.45	2.78	3.32	3.28	5.03	3.86	3.64	3.75	2.33	4.25	1.12	3.20	4.05	4.05	
>	>	>	>	>	>	>	>	>	>	>	>	>	>	>	>	>	>	>	>	>
45.7E-6	46.5E-6	46.5E-6	46.5E-6	46.4E-6	45.7E-6	45.7E-6	45.7E-6	45.7E-6	45.7E-6	45.7E-6	45.7E-6	45.7E-6	45.7E-6	45.7E-6	45.7E-6	45.7E-6	45.7E-6	45.7E-6	45.7E-6	45.7E-6
21.84	26.26	19.75	26.26	6.74	10.77	17.20	17.39	10.83	8.29	4.21	32.70	14.10	18.48	30.09	30.62	31.26	26.04	21.84	21.84	21.84
1.19	3.41	2.64	3.41	2.87	5.53	1.43	19.87	1.49	2.34	2.06	2.37	3.93	0.90	4.52	7.88	3.03	1.84	1.19	1.19	1.19
>	>	>	>	>	>	>	>	>	>	>	>	>	>	>	>	>	>	>	>	>
45.7E-6	46.5E-6	46.5E-6	46.5E-6	46.4E-6	45.7E-6	45.7E-6	45.7E-6	45.7E-6	45.7E-6	45.7E-6	45.7E-6	45.7E-6	45.7E-6	45.7E-6	45.7E-6	45.7E-6	45.7E-6	45.7E-6	45.7E-6	45.7E-6
16.84	14.71	16.74	14.71	3.89	5.82	9.47	21.58	3.43	5.58	3.84	21.91	8.00	16.28	26.47	28.38	23.97	18.99	16.84	16.84	16.84
1.62	7.20	0.99	7.20	2.42	5.18	4.45	4.47	0.17	3.94	3.31	2.80	8.98	2.05	1.82	3.08	2.84	6.90	1.62	1.62	1.62

SR-01000526704-1	SR-01000533315-1	SR-01000394877-1	SR-0100006628-1	SR-0100026567-1	SR-0100047931-1	SR-0100068951-1	SR-0100047241-1	SR-01000479551-1	SR-0100052656-1	SR-0100050581-1
										
Enamine	Enamine	Enamine	Enamine	Enamine	Enamine	Enamine	Enamine	Enamine	Enamine	Enamine
TS316067	0828-0243	0806-2387	8009-9257	8009-9018	70520-4474	TS362953	4161-1755	8009-9016	TS316067	TS316067
23	20	21	18	19	31	26	26	21	23	23
1	1	0	1	1	2	0	2	1	1	1
2	3	2	3	3	4	3	3	3	2	2
347.40	268.31	290.75	262.73	276.76	442.90	371.86	357.58	304.81	347.40	347.40
3.88	4.55	5.12	1.65	2.14	2.29	3.65	4.57	2.88	3.88	3.88
3.88	4.55	5.12	1.60	2.10	2.29	3.65	0.70	2.71	3.88	3.88
										
> 47.3E-6	> 51.2E-6	> 51.8E-6	> 52.3E-6	> 49.7E-6	> 49.5E-6	> 49.1E-6	> 47.8E-6	> 47.5E-6	> 47.3E-6	> 47.3E-6
13.22	-9.9E+0	3.45	-1.6E+0	12.80	2.80	-112.9E-3	8.55	-10.2E+0	13.22	13.22
4.59	4.20	18.47	6.76	5.23	1.87	13.26	15.89	16.16	4.59	4.59
0.26	0.30	0.29	0.33	0.32	0.19	0.23	0.23	0.29	0.26	0.26
###	####	####	###	###	###	###	###	###	###	###
0.45	####	####	2.68	2.21	2.01	0.65	3.62	1.61	0.45	0.45
> 47.3E-6	> 51.2E-6	> 51.8E-6	> 52.3E-6	> 49.7E-6	> 49.5E-6	> 49.1E-6	> 47.8E-6	> 47.5E-6	> 47.3E-6	> 47.3E-6
5.09	-8.1E+0	23.33	23.74	19.93	14.06	-448.1E-3	10.70	10.33	5.09	5.09
1.13	4.06	4.66	7.22	4.12	8.50	3.61	3.77	1.98	1.13	1.13
> 47.3E-6	> 51.2E-6	> 51.8E-6	> 52.3E-6	> 49.7E-6	> 49.5E-6	> 49.1E-6	> 47.8E-6	> 47.5E-6	> 47.3E-6	> 47.3E-6
24.60	22.87	39.76	24.26	23.72	33.18	26.06	29.38	21.05	24.60	24.60
3.53	2.76	3.03	7.21	3.87	4.16	5.70	11.20	3.59	3.53	3.53
> 47.3E-6	> 51.2E-6	> 51.8E-6	> 52.3E-6	> 49.7E-6	> 49.5E-6	> 49.1E-6	> 47.8E-6	> 47.5E-6	> 47.3E-6	> 47.3E-6
16.20	18.58	39.30	21.45	17.00	26.64	19.24	32.99	16.50	16.20	16.20
1.32	5.02	1.29	1.21	2.38	4.44	1.95	3.58	2.00	1.32	1.32