

Probing the Allosteric Role of the $\alpha 5$ Subunit of $\alpha 3\beta 4\alpha 5$ Nicotinic Acetylcholine Receptors by Functionally Selective Modulators and Ligands

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Supporting Information

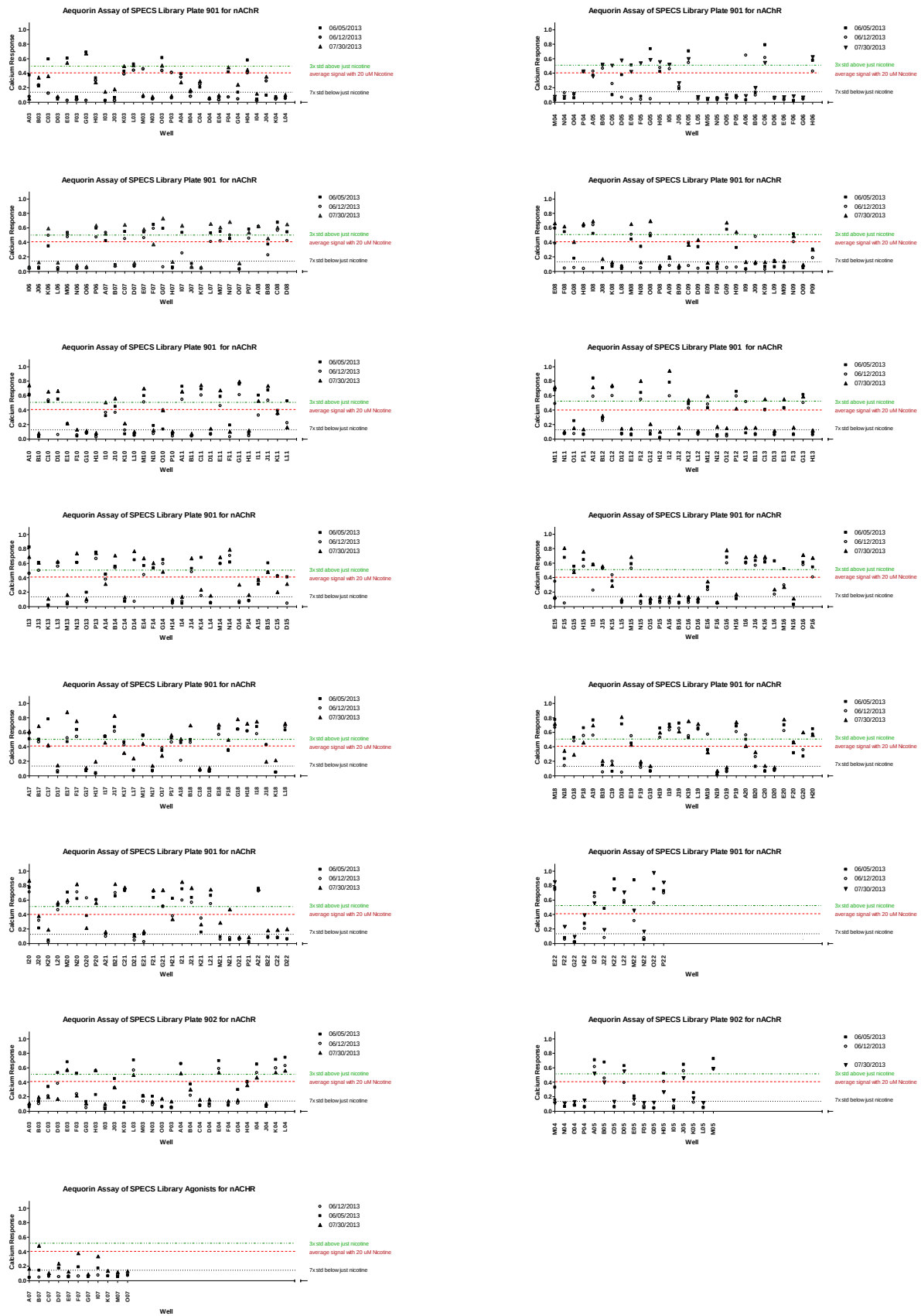
Supplemental Figure Legends and Figures

Supplemental Figure 1S. Primary Screen of the Directed Specs Chemicals Library against Cell Lines Expressing $\alpha 3\beta 4$, $\alpha 3\beta 4\alpha 5$ and $\alpha 3\beta 4\alpha 5D398N$ nAChRs – A. Three 96 well plate, single point antagonist assays were performed in permanent HEK-293 cell lines containing a distinct receptor. The cells were pre-incubated with 33 μM of a library compound for 15-30 minutes followed by the sequential addition of 20 μM nicotine to an individual well. Calcium response data were acquired on a Berthold LB940. Single point responses were calculated from three independent experiments and the results plotted per compound position in the daughter plate. The response to nicotine alone determined from eight control wells was used to calculate standard deviations in the calcium response. Lead compounds were identified as those that inhibited the calcium response to at least 7 standard deviations below cells treated with nicotine alone. Data were analyzed and plotted using GraphPad Prism 5.0. **B.** Compounds were binned based upon their effect on nicotine mediated calcium signaling relative to the mean nicotine calcium response (mr_n) and its standard deviation (std_n). An assignment of 0, 1, 2, 3, corresponded to a nicotine response in the presence of compound in the range ($mr_n \pm 3 std_n$), ($mr_n - 3std_n$ to $mr_n - 5std_n$), ($mr_n - 5std_n$ to $mr_n - 7std_n$), and less than ($mr_n - 7 std_n$) respectively. Values from the three experiments were averaged for each receptor type and the corresponding cell in the compound table for that receptor colored to enable response bias across receptors to

be easily appreciated. Positive modulators of the calcium signal above 3 standard deviation from the mean were assigned a value of -1.

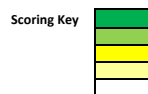
Supplemental Figure 2S. Screening of a Directed Library against Cell Lines Expressing $\alpha 3\beta 4$, $\alpha 3\beta 4\alpha 5$ and $\alpha 3\beta 4\alpha 5D398N$ nAChRs – Antagonist assays were performed as described for the remaining 22 of 38 compounds from the directed Specs Chemicals Library that were considered hits in the primary screen. Dose responses were calculated from triplicate wells in three independent experiments to determine the effects of compounds on inhibition of the whole cell calcium mediated nicotine (20 μ M) response in HEK-293 cell-lines permanently transfected with one of the nAChRs. Data were analyzed using GraphPad Prism 5.0 and the results are presented as 95% confidence intervals.

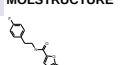
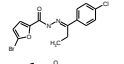
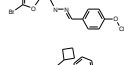
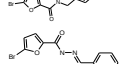
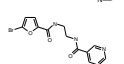
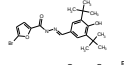
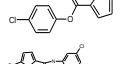
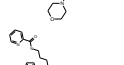
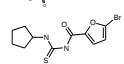
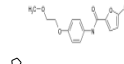
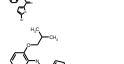
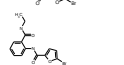
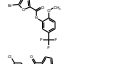
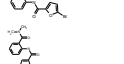
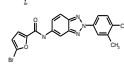
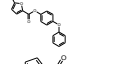
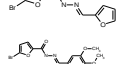
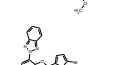
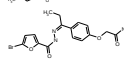
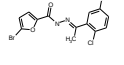
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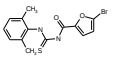
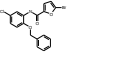
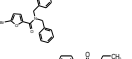
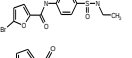
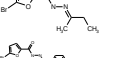
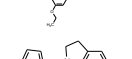
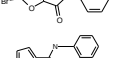
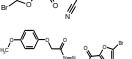
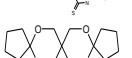
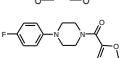
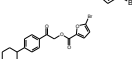
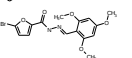
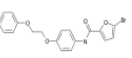
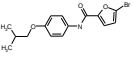
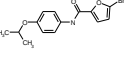
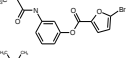
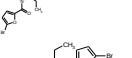
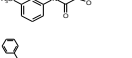
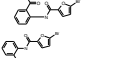
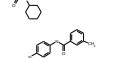
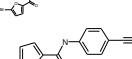
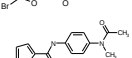
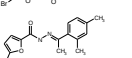
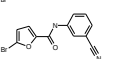
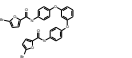
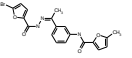
Supplemental Figure 1S

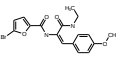
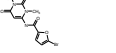
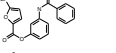
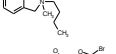
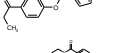
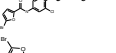
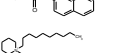
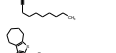
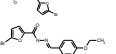
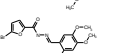
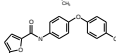
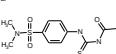
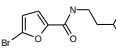
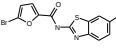
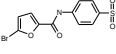
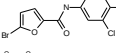
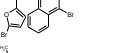
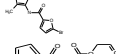
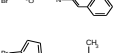
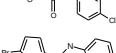
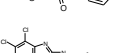
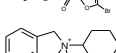
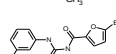
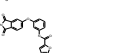
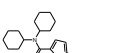
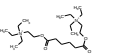
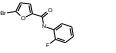
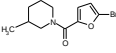
Supplemental Figure 15-B.
Aequorin Cell-base Calcium Screen of Nicotine Activation
N=3 for each receptor
Library Screened at 32 µM

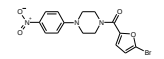
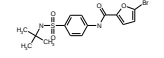
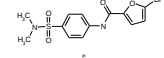
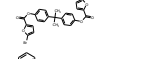
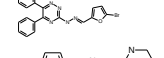
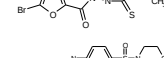
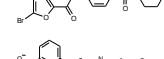
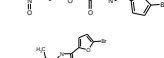
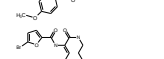
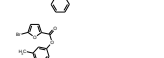
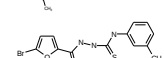
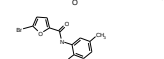
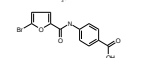
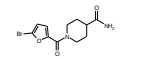
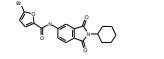
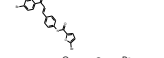
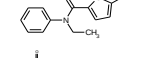
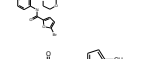
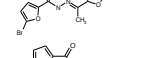
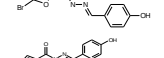
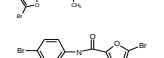
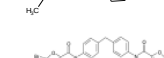
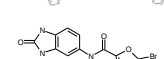
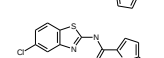
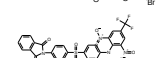
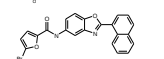
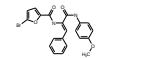
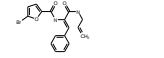


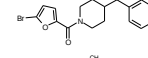
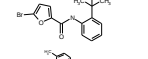
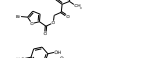
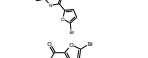
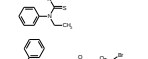
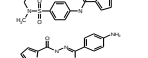
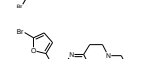
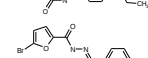
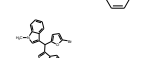
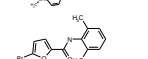
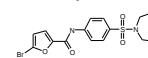
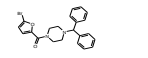
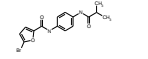
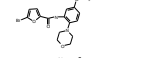
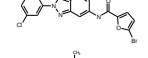
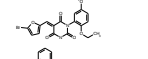
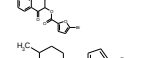
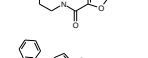
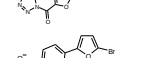
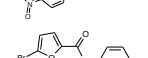
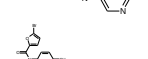
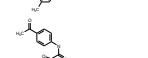
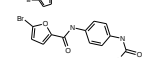
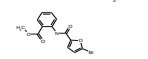
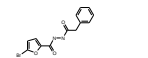
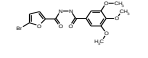
Specs ID-Number	Well	A3B4 (avg)	std	A3B4A5 wt (avg)	std	A3B4A5-D398N (avg)	std	MOLSTRUCTURE	NAME	MW	Formula
AK-968/41927491	A03	3.00	0.00	2.67	0.58	3.00	0.00		5-bromo-N-[2-(4-fluorophenyl)ethyl]-2-furamide	312.14	C13H11BrFN2O2
AK-968/37005227	A04	2.00	1.00	1.00	1.73	1.67	0.58		5-bromo-N-[1-(4-chlorophenyl)propylidene]-2-furohydrazide	355.62	C14H12BrClN2O2
AK-968/37005307	A05	1.67	1.15	1.00	1.73	2.00	1.00		5-bromo-N-(4-methoxybenzylidene)-2-furohydrazide	323.15	C13H11BrN2O3
AN-329/42239496	A06	2.00	1.73	2.67	0.58	2.00	1.73		N-benzyl-5-bromo-N-(cyclobutylmethyl)-2-furamide	348.24	C17H18BrN2O2
AK-968/37005275	A07	1.00	1.73	1.33	1.53	1.33	1.15		5-bromo-N-(pyridin-2-ylmethylene)-2-furohydrazide	294.11	C11H8BrN3O2
AO-365/43264267	A08	0.00	0.00	0.67	1.53	0.00	0.00		N-[2-[(5-bromo-2-furoyl)amino]ethyl]nicotinamide	338.16	C13H12BrN3O3
AK-968/41026442	A09	3.00	0.00	1.00	1.00	1.67	1.15		5-bromo-N'-(3,5-di-tert-butyl-4-hydroxybenzylidene)-2-furohydrazide	421.34	C20H25BrN2O3
AN-329/41675179	A10	-0.33	0.58	0.67	1.15	0.67	1.15		4-chlorophenyl 5-bromo-2-furoate	301.53	C11H6BrClO3
AN-465/42887956	A11	-0.33	0.58	0.00	0.00	0.67	0.58		5-bromo-N-[5-chloro-2-(4-morpholinyl)phenyl]-2-furamide	385.65	C15H14BrClN2O3
AO-365/43264266	A12	-0.33	0.58	0.67	0.58	0.00	1.00		N-[3-[(5-bromo-2-furoyl)amino]propyl]-2-pyridinecarboxamide	352.19	C14H14BrN3O3
AN-329/43386012	A13	2.00	1.73	1.67	1.53	2.67	0.58		N-(5-bromo-2-furoyl)-N'-cyclopentylthiourea	317.21	C11H13BrN2O2S
AN-329/43385519	A14	2.00	1.00	1.33	0.58	2.00	0.00		5-bromo-N-[4-(2-methoxyethoxy)phenyl]-2-furamide	340.18	C14H14BrN2O4
AN-329/43074311	A15	1.67	1.15	2.33	0.58	1.00	1.00		5-bromo-N-[2-(1-pyrrolidinylcarbonyl)phenyl]-2-furamide	363.21	C16H15BrN2O3
AN-329/43237088	A16	3.00	0.00	1.00	2.00	1.00	1.00		5-bromo-N-[2-[(2-furylmethyl)amino]carbonyl]phenyl]-2-furamide	389.21	C17H13BrN2O4
AN-329/43385404	A17	0.33	0.58	-0.33	0.58	0.33	1.15		5-bromo-N-(2-isobutoxyphenyl)-2-furamide	338.20	C15H16BrN2O3
AN-329/43341759	A18	1.67	1.53	1.67	1.15	0.67	0.58		5-bromo-N-[2-[(ethylamino)carbonyl]phenyl]-2-furamide	337.18	C14H13BrN2O3
AN-329/43341964	A19	-0.33	0.58	1.33	1.53	0.67	0.58		5-bromo-N-[2-methoxy-5-(trifluoromethyl)phenyl]-2-furamide	364.12	C13H9BrF3NO3
AN-329/43341946	A20	1.00	1.00	0.67	1.15	0.00	1.00		5-bromo-N-[5-chloro-2-(2-methoxyethoxy)phenyl]-2-furamide	374.62	C14H13BrClNO4
AN-329/43201204	A21	3.00	0.00	1.67	1.53	2.33	0.58		5-bromo-N-[2-(1-piperidinylcarbonyl)phenyl]-2-furamide	377.24	C17H17BrN2O3
AN-329/43341726	A22	-1.00	0.00	0.33	1.53	0.00	1.00		5-bromo-N-[2-[(dimethylamino)carbonyl]phenyl]-2-furamide	337.18	C14H13BrN2O3
AK-778/37026131	B03	2.00	1.00	0.33	0.58	1.00	1.00		5-bromo-N-[2-(3,4-dimethylphenyl)-2H-1,2,3-benzotriazol-5-yl]-2-furamide	411.26	C19H15BrN4O2
AF-399/33192038	B04	3.00	0.00	0.67	1.15	1.33	1.53		4-phenoxyphenyl 5-bromo-2-furoate	359.18	C17H11BrO4
AK-968/37005314	B05	0.33	0.58	0.33	0.58	0.67	0.58		5-bromo-N-(2-furylmethylene)-2-furohydrazide	283.08	C10H7BrN2O3
AK-968/37005281	B06	3.00	0.00	0.67	0.58	2.00	1.73		5-bromo-N'-(3,4,5-trimethoxybenzylidene)-2-furohydrazide	383.20	C15H15BrN2O5
AG-690/36518051	B07	3.00	0.00	2.33	0.58	3.00	0.00		2-(2H-1,2,3-benzotriazol-2-yl)-4-methylphenyl 5-bromo-2-furoate	398.22	C18H12BrN3O3
AK-968/41026429	B08	2.00	1.00	1.33	0.58	1.67	0.58		2-[4-[N-(5-bromo-2-furoyl)propanehydrazono]phenoxy]acetamide	394.23	C16H16BrN3O4
AK-968/41026443	B09	3.00	0.00	2.00	0.00	3.00	0.00		5-bromo-N'-[1-(2,5-dichlorophenyl)ethylidene]-2-furohydrazide	376.04	C13H9BrCl2N2O2

AN-465/42887955	B10	3.00	0.00	2.67	0.58	3.00	0.00		5-bromo-N-[3-chloro-2-(4-morpholinyl)phenyl]-2-furamide	385.65	C15H14BrClN2O3
AK-968/41927631	B11	3.00	0.00	3.00	0.00	3.00	0.00		5-bromo-N-(1,5-dimethylhexyl)-2-furamide	302.21	C13H20BrNO2
AN-329/40287115	B12	2.33	0.58	2.00	1.00	2.33	0.58		5-bromo-N-[3-((5-bromo-2-furoyl)amino)propyl]-2-furamide	420.06	C13H12Br2N2O4
AN-329/43386006	B13	3.00	0.00	3.00	0.00	3.00	0.00		N-(5-bromo-2-furoyl)-N'-(2-thienylmethyl)thiourea	345.24	C11H9BrN2O2S2
AN-329/40152489	B14	0.33	0.58	0.33	0.58	2.00	1.00		5-bromo-N,N-diethyl-2-furamide	246.11	C9H12BrNO2
AN-329/43074367	B15	0.00	0.00	1.00	0.00	0.67	0.58		N-[2-((allylamino)carbonyl)phenyl]-5-bromo-2-furamide	349.19	C15H13BrN2O3
AN-329/42943502	B16	3.00	0.00	1.33	1.15	1.00	1.00		5-bromo-N-[2-((2-phenylethyl)amino)carbonyl]phenyl]-2-furamide	413.27	C20H17BrN2O3
AN-329/43385411	B17	0.67	1.15	1.00	1.00	-0.33	0.58		5-bromo-N-[2-((methylamino)carbonyl)phenyl]-2-furamide	323.15	C13H11BrN2O3
AN-329/43341860	B18	0.67	1.15	0.67	1.15	0.00	1.00		1-(5-bromo-2-furoyl)-4-(2-furoyl)piperazine	353.17	C14H13BrN2O4
AN-329/43341952	B19	3.00	0.00	1.67	1.15	0.33	1.15		5-bromo-N-[4-chloro-2-(4-morpholinyl)phenyl]-2-furamide	385.65	C15H14BrClN2O3
AN-329/43341605	B20	2.00	1.00	2.00	0.00	2.00	1.00		2-(((5-bromo-2-furoyl)amino)carbothioylamino)-N-ethylbenzamide	396.27	C15H14BrN3O3S
AH-357/05675054	B21	-0.67	0.58	0.33	0.58	1.00	2.00		4-(methoxycarbonyl)phenyl 5-bromo-2-furoate	325.12	C13H9BrO5
AN-329/43341963	B22	3.00	0.00	0.00	0.00	0.00	1.00		5-bromo-N-(cyclohexylmethyl)-2-furamide	286.17	C12H16BrNO2
AG-690/11934028	C03	1.33	1.53	0.67	0.58	1.00	1.00		5-bromo-N-(2,4-dibromophenyl)-2-furamide	423.89	C11H6Br3NO2
AF-399/33192039	C04	2.33	0.58	0.00	0.00	0.33	0.58		4-benzoylphenyl 5-bromo-2-furoate	371.19	C18H11BrO4
AK-968/11367491	C05	1.67	1.53	1.00	0.00	1.33	1.53		5-bromo-N'-(4-methylbenzylidene)-2-furohydrazide	307.15	C13H11BrN2O2
AK-968/37005272	C06	-0.33	0.58	1.00	0.00	1.33	0.58		5-bromo-N'-(4-hydroxy-3,5-dimethoxybenzylidene)-2-furohydrazide	369.17	C14H13BrN2O5
AK-968/11367383	C07	0.33	0.58	0.67	0.58	0.33	0.58		5-bromo-N'-(3-ethoxy-2-hydroxybenzylidene)-2-furohydrazide	353.17	C14H13BrN2O4
AK-968/11369267	C08	0.00	0.00	0.00	0.00	0.67	1.15		1-(5-bromo-2-furoyl)-1H-benzimidazole	291.11	C12H7BrN2O2
AN-329/41692948	C09	2.33	1.15	0.00	0.00	0.00	0.00		2-bromo-4-chlorophenyl 5-bromo-2-furoate	380.42	C11H5Br2ClO3
AK-968/11369211	C10	0.33	0.58	0.00	0.00	-0.33	0.58		5-bromo-N-(4-pyridinylmethyl)-2-furamide	281.11	C11H9BrN2O2
AF-399/40769066	C11	-0.67	0.58	0.33	0.58	-0.33	0.58		N'-[(5-bromo-2-furyl)methylene]-3,5-bisnitrobenzohydrazide	383.12	C12H7BrN4O6
AK-968/41026853	C12	-0.67	0.58	0.00	0.00	-0.33	0.58		4-[2-(5-bromo-2-furoyl)hydrazino]-4-oxobutanoic acid	305.09	C9H9BrN2O5
AK-968/40097430	C13	1.33	1.53	2.00	0.00	2.00	0.00		N-(1,3-benzodioxol-5-yl)-5-bromo-2-furamide	310.11	C12H8BrNO4
AN-329/43385833	C14	3.00	0.00	1.67	1.15	0.67	1.15		3-(methoxycarbonyl)phenyl 5-bromo-2-furoate	325.12	C13H9BrO5
AN-329/43385512	C15	2.33	1.15	2.33	0.58	2.67	0.58		5-bromo-N-(4-butoxyphenyl)-2-furamide	338.20	C15H16BrNO3
AN-329/43385627	C16	3.00	0.00	1.33	1.15	2.67	0.58		5-bromo-N-[4-(isopentyl)oxy]phenyl]-2-furamide	352.23	C16H18BrNO3
AN-329/43385839	C17	0.33	1.15	2.00	0.00	2.00	1.00		N-[4-(allyloxy)phenyl]-5-bromo-2-furamide	322.16	C14H12BrNO3
AN-329/41830925	C18	3.00	0.00	2.67	0.58	2.67	0.58		2-isopropylphenyl 5-bromo-2-furoate	309.16	C14H13BrO3
AK-968/11369149	C19	3.00	0.00	2.33	0.58	3.00	0.00		5-bromo-N-cycloheptyl-2-furamide	286.17	C12H16BrNO2

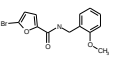
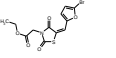
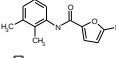
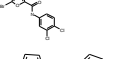
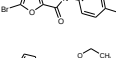
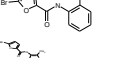
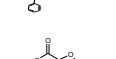
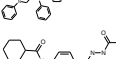
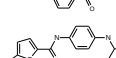
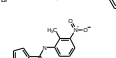
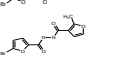
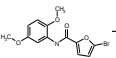
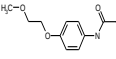
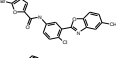
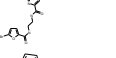
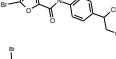
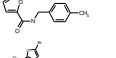
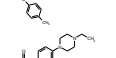
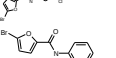
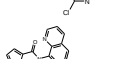
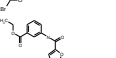
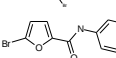
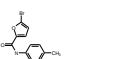
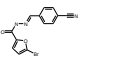
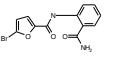
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AN-329/43341961	C21	-1.00	0.00	0.33	0.58	-0.33	0.58		N-[2-(benzyloxy)-5-chlorophenyl]-5-bromo-2-furamide	406.67	C18H13BrClNO3
AN-329/43337212	C22	3.00	0.00	2.33	1.15	2.67	0.58		5-bromo-N-cyclohexyl-N-methyl-2-furamide	286.17	C12H16BrNO2
AF-399/33192035	D03	3.00	0.00	1.33	0.58	1.67	1.15		N,N-dibenzyl-5-bromo-2-furamide	370.25	C19H16BrNO2
AN-329/40744097	D04	3.00	0.00	3.00	0.00	3.00	0.00		5-bromo-N-{4-[(diethylamino)sulfonyl]phenyl}-2-furamide	401.28	C15H17BrN2O4S
AK-968/11367293	D05	2.00	1.73	0.33	0.58	0.67	1.15		5-bromo-N'-(1-methylpropylidene)-2-furohydrazide	259.10	C9H11BrN2O2
AK-968/11367435	D06	3.00	0.00	2.67	0.58	3.00	0.00		5-bromo-N'-(2-ethoxybenzylidene)-2-furohydrazide	337.18	C14H13BrN2O3
AG-690/36465058	D07	3.00	0.00	1.67	0.58	1.67	1.53		1-(5-bromo-2-furoyl)indoline	292.13	C13H10BrNO2
AN-329/40744082	D08	0.67	0.58	0.67	0.58	0.33	0.58		5-bromo-N-(2-cyanophenyl)-2-furamide	291.11	C12H7BrN2O2
AN-329/41770440	D09	2.33	1.15	0.67	0.58	0.67	1.15		5-bromo-N-[(2-[(4-methoxyphenoxy)acetyl]hydrazino)carbothioyl]-2-furamide	428.26	C15H14BrN3O5S
AG-690/08791039	D10	1.33	1.53	0.33	0.58	-0.33	0.58		6,10,16,19-tetraoxatrispiro[4.2.2.4.2]nonadecane	268.36	C15H24O4
AK-968/12117231	D11	3.00	0.00	2.67	0.58	2.67	0.58		1-(5-bromo-2-furoyl)-4-(4-fluorophenyl)piperazine	353.19	C15H14BrFN2O2
AK-918/41206409	D12	3.00	0.00	1.00	1.00	1.67	1.53		2-(4-cyclohexylphenyl)-2-oxoethyl 5-bromo-2-furoate	391.26	C19H19BrO4
AK-968/40605655	D13	3.00	0.00	2.00	0.00	1.67	1.53		5-bromo-N'-(2,4,6-trimethoxybenzylidene)-2-furohydrazide	383.20	C15H15BrN2O5
AN-329/43385516	D14	0.67	2.08	0.67	0.58	0.33	1.53		5-bromo-N-[4-(2-phenoxyethoxy)phenyl]-2-furamide	402.25	C19H16BrNO4
AN-329/43385511	D15	2.67	0.58	2.33	0.58	2.67	0.58		5-bromo-N-(4-isobutoxyphenyl)-2-furamide	338.20	C15H16BrNO3
AN-329/43385624	D16	3.00	0.00	2.33	0.58	2.33	0.58		5-bromo-N-(4-isopropoxyphenyl)-2-furamide	324.18	C14H14BrNO3
AN-329/43385393	D17	3.00	0.00	2.33	0.58	3.00	0.00		3-(propionylamino)phenyl 5-bromo-2-furoate	338.16	C14H12BrNO4
AN-329/42724817	D18	3.00	0.00	1.33	1.15	2.33	0.58		2,3-dimethylphenyl 5-bromo-2-furoate	295.13	C13H11BrO3
AN-329/43197468	D19	0.33	2.31	0.00	0.00	-0.33	0.58		4-(5-bromo-2-furoyl)-3-ethyl-2-piperazinone	301.14	C11H13BrN2O3
AN-329/43341960	D20	3.00	0.00	2.33	0.58	2.33	1.15		5-bromo-N-ethyl-N-(3-methylphenyl)-2-furamide	308.18	C14H14BrNO2
AN-329/42955283	D21	3.00	0.00	1.67	1.53	0.33	0.58		N-[2-[(benzylamino)carbonyl]phenyl]-5-bromo-2-furamide	399.25	C19H15BrN2O3
AN-329/42613182	D22	3.00	0.00	1.67	0.58	0.33	0.58		5-bromo-N-[2-[(cyclohexylamino)carbonyl]phenyl]-2-furamide	391.27	C18H19BrN2O3
AG-670/11881016	E03	1.00	1.73	0.67	0.58	1.00	1.00		5-bromo-N-[4-[(3-methylbenzoyl)amino]phenyl]-2-furamide	399.25	C19H15BrN2O3
AN-329/40744080	E04	3.00	0.00	2.33	0.58	2.33	1.15		5-bromo-N-(4-cyanophenyl)-2-furamide	291.11	C12H7BrN2O2
AN-329/40744078	E05	1.67	1.15	1.67	0.58	1.67	0.58		N-[4-[acetyl(methyl)amino]phenyl]-5-bromo-2-furamide	337.18	C14H13BrN2O3
AK-968/11367331	E06	3.00	0.00	3.00	0.00	3.00	0.00		5-bromo-N'-[1-(2,4-dimethylphenyl)ethylidene]-2-furohydrazide	335.20	C15H15BrN2O2
AN-329/40744085	E07	0.33	0.58	0.67	0.58	0.00	0.00		5-bromo-N-(3-cyanophenyl)-2-furamide	291.11	C12H7BrN2O2
AG-690/10117038	E08	0.33	0.58	0.67	0.58	2.00	0.00		5-bromo-N-[4-{3-[4-[(5-bromo-2-furoyl)amino]phenoxy]phenoxy]phenyl]-2-furamide	638.27	C28H18Br2N2O6
AK-968/40707711	E09	3.00	0.00	3.00	0.00	3.00	0.00		N-[3-[N-(5-bromo-2-furoyl)ethanehydrazono]phenyl]-5-methyl-2-furamide	430.26	C19H16BrN3O4

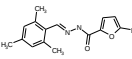
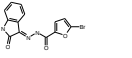
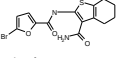
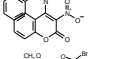
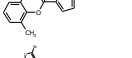
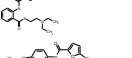
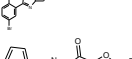
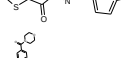
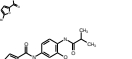
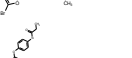
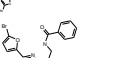
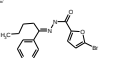
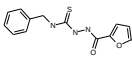
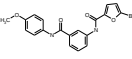
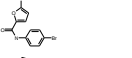
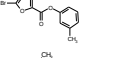
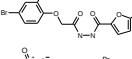
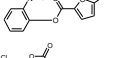
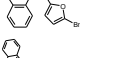
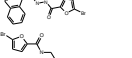
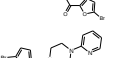
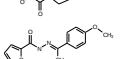
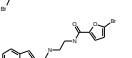
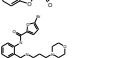
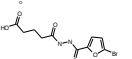
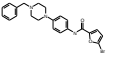
AL-281/15329053	E10	2.33	0.58	1.00	1.00	0.67	0.58		5-bromo-N-1-[(ethylamino)carbonyl]-2-(4-methoxyphenyl)vinyl-2-furamide	393.24	C17H17BrN2O4
AK-968/11986799	E11	0.00	0.00	0.33	0.58	0.00	0.00		5-bromo-N-(1,3-dimethyl-2,6-dioxo-1,2,3,6-tetrahydro-4-pyrimidinyl)-2-furamide	328.12	C11H10BrN3O4
AK-918/11684002	E12	3.00	0.00	2.00	0.00	1.67	1.53		3-(benzoylamino)phenyl 5-bromo-2-furoate	386.20	C18H12BrNO4
AL-281/41935321	E13	1.33	1.53	0.67	0.58	0.67	0.58		2-butyl-2-methyl-2,3-dihydro-1H-isindolium	190.31	C13H20N
AN-329/41690001	E14	0.00	0.00	0.33	0.58	-0.33	0.58		4-propionylphenyl 5-bromo-2-furoate	323.15	C14H11BrO4
AN-465/42000665	E15	2.33	1.15	3.00	0.00	2.33	0.58		N-[4-(4-benzoyl-1-piperazinyl)-3-chlorophenyl]-5-bromo-2-furamide	488.77	C22H19BrClN3O3
AG-205/08441024	E16	2.00	1.00	2.33	0.58	2.33	1.15		5-bromo-N-(2-naphthyl)-2-furamide	316.16	C15H10BrNO2
AK-968/40218701	E17	0.33	1.53	-0.33	0.58	-0.67	0.58		1-decyl-1-(2-undecynyl)piperidinium	376.70	C26H50N
AK-968/12163749	E18	0.00	0.00	0.33	0.58	0.00	0.00		N-[3-(aminocarbonyl)-5,6,7,8-tetrahydro-4H-cyclohepta[b]thien-2-yl]-5-bromo-2-furamide	383.27	C15H15BrN2O3S
AK-968/11369222	E19	1.33	1.53	2.00	1.00	1.33	1.53		5-bromo-N'-(4-ethoxy-3-methoxybenzylidene)-2-furohydrazide	367.20	C15H15BrN2O4
AK-968/11369088	E20	-0.67	0.58	0.00	0.00	0.67	1.15		5-bromo-N-(2,4,5-trimethoxybenzylidene)-2-furohydrazide	383.20	C15H15BrN2O5
AM-879/40769453	E21	3.00	0.00	3.00	0.00	2.67	0.58		5-bromo-N-[4-(4-chlorophenoxy)phenyl]-2-furamide	392.64	C17H11BrClNO3
AN-329/42260836	E22	-1.00	0.00	0.33	0.58	0.00	1.00		4-[[[(5-bromo-2-furoyl)amino]carbothioyl]amino]-N,N-dimethylbenzenesulfonamide	432.32	C14H14BrN3O4S2
AN-329/40744095	F03	3.00	0.00	2.67	0.58	2.67	0.58		5-bromo-N-[2-(1-cyclohexen-1-yl)ethyl]-2-furamide	298.18	C13H16BrNO2
AH-034/08461036	F04	2.00	1.73	1.00	0.00	0.33	0.58		5-bromo-N-(6-ethoxy-1,3-benzothiazol-2-yl)-2-furamide	367.22	C14H11BrN2O3S
AN-329/40744093	F05	2.00	1.73	1.67	0.58	1.33	1.53		5-bromo-N-[4-(1-pyrrolidinesulfonyl)phenyl]-2-furamide	399.27	C15H15BrN2O4S
AN-329/40744081	F06	3.00	0.00	3.00	0.00	3.00	0.00		5-bromo-N-(4-bromo-3-chlorophenyl)-2-furamide	379.44	C11H6Br2ClNO2
AG-670/11881010	F07	0.33	0.58	1.67	1.15	1.67	0.58		4-bromo-1-naphthyl 5-bromo-2-furoate	396.04	C15H8Br2O3
AK-968/40732327	F08	1.33	1.53	0.33	0.58	-0.33	0.58		5-bromo-N-(1-ethyl-3,5-dimethyl-1H-pyrazol-4-yl)-2-furamide	312.17	C12H14BrN3O2
AN-038/15563010	F09	3.00	0.00	2.00	0.00	2.67	0.58		allyl 2-[(5-bromo-2-furoyl)amino]-3-phenylacrylate	376.21	C17H14BrNO4
AO-081/41933640	F10	3.00	0.00	2.33	0.58	2.67	0.58		5-bromo-N-(4-chloro-2-methylphenyl)-2-furamide	314.57	C12H9BrClNO2
AK-968/11368924	F11	3.00	0.00	1.33	1.15	1.67	1.53		5-bromo-N-(4-isopropylphenyl)-2-furamide	308.18	C14H14BrNO2
AN-465/42769476	F12	-0.33	0.58	0.00	0.00	-0.33	0.58		5-bromo-N-(4,5-dichloro-1,3-benzothiazol-2-yl)-2-furamide	392.06	C12H5BrCl2N2O2S
AL-281/41935323	F13	3.00	0.00	2.00	0.00	3.00	0.00		2-cyclohexyl-2-methyl-2,3-dihydro-1H-isindolium	216.35	C15H22N
AN-329/41967579	F14	0.33	0.58	1.33	0.58	0.33	0.58		N-(5-bromo-2-furoyl)-N'-(3-methylphenyl)thiourea	339.21	C13H11BrN2O2S
AN-979/41972062	F15	0.33	2.31	1.00	1.00	-0.33	0.58		5-bromo-N-[3-[(1,3-dioxo-2,3-dihydro-1H-isindol-5-yl)oxy]phenyl]-2-furamide	427.21	C19H11BrN2O5
AK-968/11036034	F16	3.00	0.00	2.33	0.58	2.00	1.00		5-bromo-N,N-dicyclohexyl-2-furamide	354.29	C17H24BrNO2
AK-968/40208381	F17	-0.33	0.58	0.33	0.58	0.33	0.58		N,N,N-triethyl-2-[(6-oxo-6-[2-(triethylammonio)ethoxy]hexanoyl)oxy]ethanaminium	402.62	C22H46N2O4
AK-968/11368975	F18	1.33	1.53	0.33	0.58	0.33	0.58		5-bromo-N-(2-fluorophenyl)-2-furamide	284.09	C11H7BrFNO2
AK-968/11369249	F19	3.00	0.00	1.33	0.58	2.00	0.00		1-(5-bromo-2-furoyl)-3-methylpiperidine	272.14	C11H14BrNO2

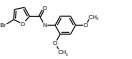
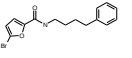
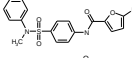
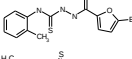
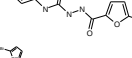
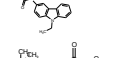
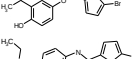
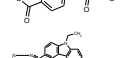
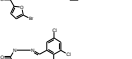
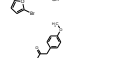
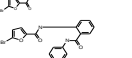
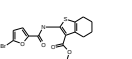
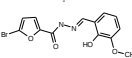
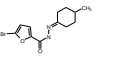
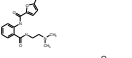
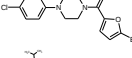
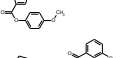
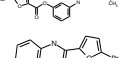
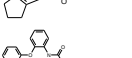
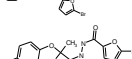
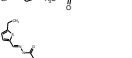
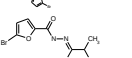
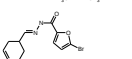
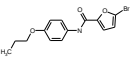
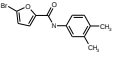
AK-968/11987447	F20	1.33	1.53	0.67	0.58	0.67	1.15		1-(5-bromo-2-furyl)-4-(4-nitrophenyl)piperazine	380.20	C15H14BrN3O4
AN-329/42174071	F21	-0.67	0.58	0.67	0.58	1.67	1.53		5-bromo-N-[4-((tert-butylamino)sulfonyl)phenyl]-2-furamide	401.28	C15H17BrN2O4S
AN-329/42260890	F22	2.67	0.58	2.00	0.00	2.00	0.00		5-bromo-N-[4-((dimethylamino)sulfonyl)phenyl]-2-furamide	373.23	C13H13BrN2O4S
AG-690/36518052	G03	0.67	2.08	0.33	0.58	0.33	0.58		4-(1-[4-((5-bromo-2-furyl)oxy)phenyl]-1-methylethyl)phenyl 5-bromo-2-furoate	574.23	C25H18Br2O6
AK-968/36945066	G04	2.67	0.58	0.67	0.58	0.67	1.15		5-bromo-2-furaldehyde (5,6-diphenyl-1,2,4-triazin-3-yl)hydrazide	420.27	C20H14BrN5O
AK-968/40730805	G05	0.67	2.08	0.00	0.00	0.00	0.00		2-(5-bromo-2-furyl)-N-ethylhydrazinecarbothioamide	292.16	C8H10BrN3O2S
AN-329/40744096	G06	3.00	0.00	0.67	1.15	1.33	1.53		5-bromo-N-[4-(4-morpholinesulfonyl)phenyl]-2-furamide	415.27	C15H15BrN2O5S
AG-205/11955495	G07	0.67	2.08	0.67	0.58	0.00	0.00		N'-[5-bromo-2-furyl)methylene]-2-[3-nitrophenoxy]acetohydrazide	368.15	C13H10BrN3O5
AK-968/15256132	G08	2.33	1.15	1.33	0.58	1.33	0.58		5-bromo-N-(4-methoxy-2-methylphenyl)-2-furamide	310.15	C13H12BrNO3
AL-281/15328027	G09	1.00	1.73	0.00	0.00	-0.33	0.58		5-bromo-N-(1-[(3-hydroxypropyl)amino]carbonyl)-2-phenylvinyl)-2-furamide	393.24	C17H17BrN2O4
AK-918/13010067	G10	3.00	0.00	2.00	0.00	1.67	1.53		3,5-dimethylphenyl 5-bromo-2-furoate	295.13	C13H11BrO3
AK-968/41926264	G11	-0.67	0.58	0.33	0.58	0.67	1.53		2-(5-bromo-2-furyl)-N-(3-methylphenyl)hydrazinecarbothioamide	354.23	C13H12BrN3O2S
AK-968/11368950	G12	3.00	0.00	1.67	0.58	2.33	0.58		5-bromo-N-(2,5-dimethylphenyl)-2-furamide	294.15	C13H12BrNO2
AN-652/11215871	G13	0.00	0.00	0.33	0.58	-0.33	0.58		4-[(5-bromo-2-furyl)amino]benzoic acid	310.11	C12H8BrNO4
AO-081/41933651	G14	0.00	0.00	0.33	0.58	-0.33	0.58		1-(5-bromo-2-furyl)-4-piperidinecarboxamide	301.14	C11H13BrN2O3
AN-979/42273817	G15	0.33	0.58	1.67	1.15	0.33	1.15		5-bromo-N-(2-cyclohexyl-1,3-dioxo-2,3-dihydro-1H-isindol-5-yl)-2-furamide	417.26	C19H17BrN2O4
AN-979/41971613	G16	-0.67	0.58	0.67	1.15	0.33	1.53		5-bromo-N-[4-[3-(4-bromophenyl)-3-oxo-1-propenyl]phenyl]-2-furamide	475.14	C20H13Br2NO3
AN-329/41583613	G17	3.00	0.00	1.00	1.00	1.67	1.53		5-bromo-N-ethyl-N-phenyl-2-furamide	294.15	C13H12BrNO2
AP-064/42710440	G18	-0.33	0.58	0.33	0.58	0.33	1.53		5-bromo-N-[2-(4-morpholinylcarbonyl)phenyl]-2-furamide	379.21	C16H15BrN2O4
AK-968/11367341	G19	3.00	0.00	2.00	0.00	2.67	0.58		5-bromo-N'-[1-(5-methyl-2-furyl)ethylidene]-2-furohydrazide	311.14	C12H11BrN2O3
AK-968/11367505	G20	1.33	1.53	1.00	0.00	0.33	0.58		5-bromo-N'-(4-hydroxybenzylidene)-2-furohydrazide	309.12	C12H9BrN2O3
AK-968/11368775	G21	0.00	1.00	0.33	0.58	-0.33	0.58		5-bromo-N'-[1-(4-hydroxyphenyl)ethylidene]-2-furohydrazide	323.15	C13H11BrN2O3
AP-970/41128478	G22	3.00	0.00	3.00	0.00	3.00	0.00		5-bromo-N-(4-bromo-3-methylphenyl)-2-furamide	359.02	C12H9Br2NO2
AK-968/36846007	H03	2.33	0.58	1.33	0.58	1.33	1.15		5-bromo-N-[4-[(5-bromo-2-furyl)amino]benzyl]phenyl)-2-furamide	544.20	C23H16Br2N2O4
AK-968/10816064	H04	0.67	0.58	1.00	0.00	1.33	1.15		5-bromo-N-(2-oxo-2,3-dihydro-1H-benzimidazol-5-yl)-2-furamide	322.12	C12H8BrN3O3
AP-970/43374655	H05	1.00	1.73	0.67	0.58	0.00	0.00		5-bromo-N-(5-chloro-1,3-benzothiazol-2-yl)-2-furamide	357.61	C12H6BrClN2O2S
AE-848/32002063	H06	0.33	0.58	0.67	0.58	0.33	0.58		2-[4-[(4-[2,6-bisnitro-4-(trifluoromethyl)anilino]phenyl)sulfonyl]phenyl]-1H-isindole-1,3(2H)-dione	612.50	C27H15F3N4O8S
AK-778/11467049	H07	3.00	0.00	1.67	0.58	2.67	0.58		5-bromo-N-[2-(1-naphthyl)-1,3-benzoxazol-5-yl]-2-furamide	433.26	C22H13BrN2O3
AL-281/15328031	H08	1.00	1.73	1.00	1.00	0.00	1.00		5-bromo-N-[1-[(4-methoxyanilino)carbonyl]-2-phenylvinyl]-2-furamide	441.28	C21H17BrN2O4
AL-281/15329083	H09	2.00	1.73	0.67	0.58	0.67	0.58		N-[1-[(allylamino)carbonyl]-2-phenylvinyl]-5-bromo-2-furamide	375.22	C17H15BrN2O3

AK-968/12096017	H10	3.00	0.00	2.00	1.00	2.33	1.15		5-bromo-N-(3-cyano-4,5,6,7,8,9-hexahydrocycloocta[b]thiophen-2-yl)-2-furamide	379.28	C16H15BrN2O2S
AN-329/43450212	H11	3.00	0.00	1.67	0.58	1.33	1.53		5-bromo-N-[2-(tetrahydro-2-furanylmethoxy)phenyl]-2-furamide	366.21	C16H16BrNO4
AK-968/41753486	H12	3.00	0.00	3.00	0.00	3.00	0.00		4-benzyl-1-(5-bromo-2-furoyl)piperidine	348.24	C17H18BrNO2
AO-081/41933655	H13	3.00	0.00	2.33	0.58	2.67	0.58		5-bromo-N-(2-tert-butylphenyl)-2-furamide	322.20	C15H16BrNO2
AK-918/42193422	H14	3.00	0.00	2.67	0.58	2.33	0.58		2-(2,5-dimethylphenyl)-2-oxoethyl 5-bromo-2-furoate	337.17	C15H13BrO4
AN-979/41971619	H15	-0.33	0.58	0.00	0.00	-0.33	0.58		5-bromo-N-(2-hydroxy-5-methylphenyl)-2-furamide	296.12	C12H10BrNO3
AN-329/41769822	H16	3.00	0.00	2.33	0.58	2.67	0.58		N'-(5-bromo-2-furoyl)-N-ethyl-N-phenylthiourea	353.24	C14H13BrN2O2S
AN-329/41473608	H17	3.00	0.00	2.33	0.58	2.67	0.58		N-(4-((benzyl(methyl)amino)sulfonyl)phenyl)-5-bromo-2-furamide	449.33	C19H17BrN2O4S
AK-968/11368711	H18	-0.33	0.58	0.33	0.58	0.33	0.58		N'-[1-(4-aminophenyl)ethylidene]-5-bromo-2-furohydrazide	322.16	C13H12BrN3O2
AK-968/11367296	H19	0.00	0.00	0.00	0.00	0.00	0.00		5-bromo-N'-(1-propylpiperidin-4-ylidene)-2-furohydrazide	328.21	C13H18BrN3O2
AK-968/11367481	H20	0.00	0.00	0.67	0.58	0.67	0.58		5-bromo-N'-(4-bromobenzylidene)-2-furohydrazide	372.02	C12H8Br2N2O2
AN-655/41148542	H21	0.67	0.58	1.00	0.00	0.67	1.15		3-((5-bromo-2-furyl)(1-methyl-1H-indol-3-yl)methyl)-1-methyl-1H-indole	419.32	C23H19BrN2O
AK-968/11368844	H22	2.00	1.00	1.67	0.58	1.00	1.00		5-bromo-N-(2,6-dimethylphenyl)-2-furamide	294.15	C13H12BrNO2
AN-329/40744090	I03	3.00	0.00	3.00	0.00	2.67	0.58		N-[4-(1-azepanylsulfonyl)phenyl]-5-bromo-2-furamide	427.32	C17H19BrN2O4S
AK-968/37005285	I04	3.00	0.00	2.67	0.58	2.67	0.58		1-benzhydryl-4-(5-bromo-2-furoyl)piperazine	425.33	C22H18BrN2O2
AP-970/4200640	I05	0.33	0.58	1.00	0.00	1.00	0.00		5-bromo-N-[4-(isobutylamino)phenyl]-2-furamide	351.20	C15H15BrN2O3
AP-970/43375295	I06	3.00	0.00	3.00	0.00	2.33	1.15		5-bromo-N-[5-methoxy-2-(4-morpholinyl)phenyl]-2-furamide	381.23	C16H17BrN2O4
AK-778/37120018	I07	1.00	1.00	0.67	0.58	0.00	0.00		5-bromo-N-[2-(3-chlorophenyl)-2H-1,2,3-benzotriazol-5-yl]-2-furamide	417.65	C17H10BrClN4O2
AM-879/15039155	I08	0.33	0.58	0.00	1.00	-0.33	0.58		5-((5-bromo-2-furyl)methylene)-1-(2,5-diethoxyphenyl)-2,4,6-(1H,3H,5H)-pyrimidinetrione	449.26	C19H17BrN2O6
AK-918/12623084	I09	3.00	0.00	2.33	0.58	1.00	1.73		2-oxo-1,2-diphenylethyl 5-bromo-2-furoate	385.22	C19H13BrO4
AK-968/11369236	I10	1.33	1.53	0.67	0.58	0.00	1.00		1-(5-bromo-2-furoyl)-4-methylpiperidine	272.14	C11H14BrNO2
AK-968/11367471	I11	0.33	0.58	0.67	0.58	0.00	0.00		1-(5-bromo-2-furoyl)-1H-1,2,3-benzotriazole	292.09	C11H6BrN3O2
AH-262/34397014	I12	-0.67	0.58	0.33	0.58	1.00	1.73		2-bromo-5-(4-nitrophenyl)furan	268.07	C10H6BrNO3
AH-034/07270026	I13	-0.33	0.58	0.33	0.58	0.00	1.00		5-bromo-N-(3-pyridinyl)-2-furamide	267.08	C10H7BrN2O2
AN-652/05699061	I14	3.00	0.00	2.00	0.00	2.67	0.58		5-bromo-N-(2,4-dimethylphenyl)-2-furamide	294.15	C13H12BrNO2
AN-652/05685026	I15	0.67	1.15	0.67	0.58	0.00	1.00		N-(4-acetylphenyl)-5-bromo-2-furamide	308.13	C13H10BrNO3
AN-652/05685029	I16	0.00	0.00	0.33	0.58	1.00	1.73		N-[4-(acetylamino)phenyl]-5-bromo-2-furamide	323.15	C13H11BrN2O3
AN-652/12689769	I17	0.67	0.58	0.67	0.58	0.33	0.58		methyl 2-((5-bromo-2-furoyl)amino)benzoate	324.13	C13H10BrNO4
AN-329/40744117	I18	-0.33	0.58	0.33	0.58	-0.33	0.58		5-bromo-N'-(phenylacetyl)-2-furohydrazide	323.15	C13H11BrN2O3
AN-329/40744129	I19	-0.33	0.58	0.00	0.00	-0.33	0.58		5-bromo-N'-(3,4,5-trimethoxybenzoyl)-2-furohydrazide	399.20	C15H15BrN2O6

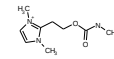
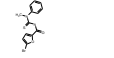
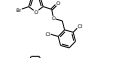
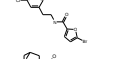
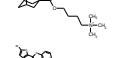
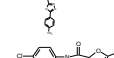
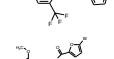
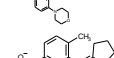
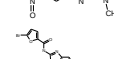
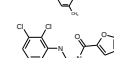
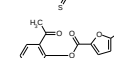
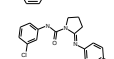
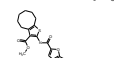
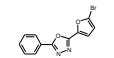
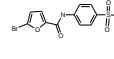
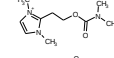
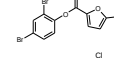
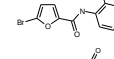
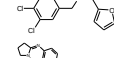
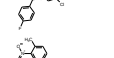
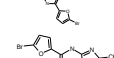
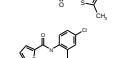
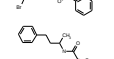
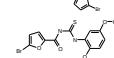
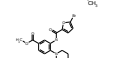
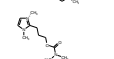
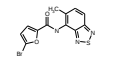
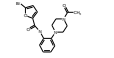
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AN-329/41574527	I21	-0.67	0.58	0.00	0.00	-0.33	1.15		N-(5-bromo-2-furyl)-N'-(3,5-dichlorophenyl)thiourea	394.08	C12H7BrCl2N2O2S
AK-968/11367319	I22	-0.33	0.58	0.00	0.00	-0.33	0.58		5-bromo-N'-[1-(4-pyridinyl)ethylidene]-2-furohydrazide	308.14	C12H10BrN3O2
AK-918/11939021	J03	3.00	0.00	1.67	1.15	2.33	0.58		5-bromo-N'-[2'-[(5-bromo-2-furyl)amino]1,1'-biphenyl-2-yl]-2-furamide	530.18	C22H14Br2N2O4
AK-968/37005269	J04	2.00	1.00	1.33	1.53	1.33	0.58		5-bromo-N'-[(5-methyl-2-thienyl)methylene]-2-furohydrazide	313.17	C11H9BrN2O2S
AG-205/36915291	J05	2.33	0.58	1.33	0.58	1.67	1.53		5-[(5-bromo-2-furyl)methylene]-3-phenyl-2-(phenylimino)-1,3-thiazolidin-4-one	425.31	C20H13BrN2O2S
AG-205/07929021	J06	3.00	0.00	2.00	1.00	2.33	1.15		N'-[(5-bromo-2-furyl)methylene]-2-(2,6-dibromo-4-methylphenoxy)acetohydrazide	494.97	C14H11Br3N2O3
AJ-292/41083297	J07	3.00	0.00	1.00	0.00	1.33	1.53		ethyl 2-[(5-bromo-2-furyl)amino]-5,5-dimethyl-4,7-dihydro-5H-thieno[2,3-c]pyran-3-carboxylate	428.30	C17H18BrN5O5S
AK-918/12623152	J08	3.00	0.00	2.33	0.58	2.33	0.58		2-(4-methoxyphenyl)-2-oxo-1-phenylethyl 5-bromo-2-furoate	415.24	C20H15BrO5
AN-465/42000087	J09	2.00	1.73	2.00	0.00	2.33	0.58		5-bromo-N-[4-(4-methyl-1-piperazinyl)phenyl]-2-furamide	364.24	C16H18BrN3O2
AK-968/11368867	J10	1.33	1.53	0.67	0.58	0.67	1.15		5-bromo-N-(2,4-difluorophenyl)-2-furamide	302.08	C11H6BrF2N2O2
AK-968/15603652	J11	-0.33	0.58	0.00	0.00	-0.33	0.58		5-bromo-N-[4-[N-(cyclopropylcarbonyl)ethanehydrazonoyl]phenyl]-2-furamide	390.24	C17H16BrN3O3
AK-968/41753488	J12	3.00	0.00	2.33	0.58	2.33	0.58		5-bromo-N'-[2-(4-methoxyphenyl)ethyl]-2-furamide	324.18	C14H14BrNO3
AH-034/07270022	J13	0.00	0.00	0.00	0.00	0.67	1.15		5-bromo-N-(5-methyl-1,3,4-thiadiazol-2-yl)-2-furamide	288.12	C8H6BrN3O2S
AK-968/14004393	J14	0.33	0.58	0.00	0.00	0.00	1.00		5-bromo-N-isopentyl-2-furamide	260.13	C10H14BrNO2
AG-690/36545058	J15	0.33	0.58	0.67	0.58	0.67	1.15		5-bromo-N-(1,3-thiazol-2-yl)-2-furamide	273.11	C8H5BrN2O2S
AN-652/11215872	J16	0.00	0.00	0.67	0.58	0.00	1.00		3-[(5-bromo-2-furyl)amino]benzoic acid	310.11	C12H8BrNO4
AN-652/41376266	J17	-0.33	0.58	0.33	0.58	-0.33	0.58		2-[(5-bromo-2-furyl)amino]benzoic acid	310.11	C12H8BrNO4
AN-329/40805545	J18	2.33	1.15	1.67	0.58	1.33	1.15		5-bromo-N'-[(2-bromo-4-methylphenoxy)acetyl]-2-furohydrazide	432.07	C14H12Br2N2O4
AN-329/41574511	J19	-0.33	0.58	0.33	0.58	0.00	1.00		N-(5-bromo-2-furyl)-N'-(2,4-dimethylphenyl)thiourea	353.24	C14H13BrN2O2S
AN-329/41559355	J20	1.67	1.15	1.00	0.00	0.33	0.58		5-bromo-N'-[[2-(thien-2-ylcarbonyl)hydrazino]carbonyl]-2-furamide	374.24	C11H8BrN3O3S2
AK-968/33942059	J21	-0.33	0.58	0.67	0.58	0.00	1.00		5-bromo-N-(2,5-dichlorophenyl)-2-furamide	334.99	C11H6BrCl2NO2
AN-329/43201735	J22	2.67	0.58	1.00	1.00	0.67	0.58		5-bromo-N-[2-[(tert-butylamino)carbonyl]phenyl]-2-furamide	365.23	C16H17BrN2O3
AG-205/33111049	K03	1.33	1.53	0.67	0.58	0.67	1.15		N'-[(5-bromo-2-furyl)methylene]-2-(3-bromophenoxy)acetohydrazide	402.04	C13H10Br2N2O3
AE-562/12222519	K04	3.00	0.00	2.67	0.58	2.67	0.58		5-(1,3-benzodioxol-5-ylmethyl)-4-methoxy-6,6-dimethyl-5,6,7,8-tetrahydro-6-ambda-5-[[1,3]dioxolo[4,5-g]isoquinoline	370.43	C21H24NOS
AG-205/36699005	K05	-0.33	0.58	0.00	0.00	0.67	0.58		2-(3,4-dichlorophenyl)-2-oxoethyl 5-bromo-2-furoate	378.01	C13H7BrCl2O4
AG-205/36710044	K06	1.00	1.73	0.67	0.58	0.33	0.58		4-[[[(5-bromo-2-furyl)methylene]amino]-4-azatricyclo[5.2.2.0-2,6]-undec-6-ene-3,5-dione	349.19	C15H13BrN2O3
AG-670/37139019	K07	3.00	0.00	1.00	1.00	1.67	1.53		3,4-dimethylphenyl 5-bromo-2-furoate	295.13	C13H11BrO3
AK-968/11368854	K08	3.00	0.00	2.33	0.58	2.67	0.58		5-bromo-N-(2-isopropylphenyl)-2-furamide	308.18	C14H14BrNO2
AK-968/11368900	K09	3.00	0.00	1.67	0.58	2.33	0.58		5-bromo-N-(3,5-dimethylphenyl)-2-furamide	294.15	C13H12BrNO2

AO-081/4193645	K10	2.67	0.58	2.33	0.58	1.67	0.58		5-bromo-N-(2-methoxybenzyl)-2-furamide	310.15	C13H12BrNO3
AM-879/40861516	K11	1.67	1.15	2.33	0.58	0.00	1.00		ethyl 5-[(5-bromo-2-furyl)methylene]-2,4-dioxo-1,3-thiazolidin-3-yl]acetate	360.19	C12H10BrNO5S
AK-968/10821006	K12	1.00	1.00	1.00	0.00	0.00	0.00		5-bromo-N-(2,3-dimethylphenyl)-2-furamide	294.15	C13H12BrNO2
AN-652/40052606	K13	3.00	0.00	2.67	0.58	2.67	0.58		5-bromo-N-(3,4-dichlorophenyl)-2-furamide	334.99	C11H6BrCl2NO2
AK-968/09820028	K14	1.33	2.08	2.33	0.58	0.67	1.15		5-bromo-N-(4-ethoxyphenyl)-2-furamide	310.15	C13H12BrNO3
AK-968/41753487	K15	1.67	1.53	1.33	0.58	0.67	0.58		5-bromo-N-(2-ethoxyphenyl)-2-furamide	310.15	C13H12BrNO3
AG-690/12764874	K16	0.00	0.00	0.00	0.00	-0.33	0.58		5-bromo-N-(1,5-dimethyl-3-oxo-2-phenyl-2,3-dihydro-1H-pyrazol-4-yl)-2-furamide	376.21	C16H14BrN3O3
AN-652/42568585	K17	1.67	0.58	0.67	0.58	1.33	1.15		phenyl 5-bromo-2-furoate	267.08	C11H7BrO3
AN-329/40744138	K18	2.67	0.58	1.67	0.58	1.67	1.53		5-bromo-N-[2-[(5-bromo-2-furoyl)anilino]ethyl]-N-phenyl-2-furamide	558.23	C24H18BrN2NO4
AN-329/41006856	K19	0.00	1.00	0.33	0.58	0.33	0.58		N-[4-[[2-(5-bromo-2-furoyl)hydrazino]carbonyl]phenyl]cyclohexanecarboxamide	434.29	C19H20BrN3O4
AN-329/40744079	K20	3.00	0.00	2.67	0.58	2.33	0.58		N-(4-anilinophenyl)-5-bromo-2-furamide	357.21	C17H13BrN2O2
AN-329/40744087	K21	2.00	1.00	1.00	0.00	1.33	0.58		5-bromo-N-[3-nitro-2-methylphenyl]-2-furamide	325.12	C12H9BrN2O4
AN-329/40744134	K22	-1.00	0.00	0.00	1.00	-0.33	0.58		5-bromo-N'-(2-methyl-3-furoyl)-2-furohydrazide	313.11	C11H9BrN2O4
AJ-292/11893076	L03	0.33	0.58	0.33	0.58	0.67	0.58		N-[1-(aminocarbonyl)-2-(1,3-benzodioxol-5-yl)vinyl]-5-bromo-2-furamide	379.17	C15H11BrN2O5
AK-968/10818020	L04	3.00	0.00	2.33	0.58	2.33	1.15		5-bromo-N-(2,5-dimethoxyphenyl)-2-furamide	326.15	C13H12BrNO4
AG-205/36696043	L05	3.00	0.00	2.67	0.58	2.67	0.58		2-oxo-2-phenylethyl 5-bromo-2-furoate	309.12	C13H9BrO4
AG-670/12032023	L06	3.00	0.00	1.67	0.58	2.00	1.00		5-bromo-N-[4-chloro-3-(5-methyl-1,3-benzoxazol-2-yl)phenyl]-2-furamide	431.68	C19H12BrClN2O3
AO-365/43264264	L07	0.67	0.58	0.33	0.58	0.00	1.00		N-[2-[(5-bromo-2-furoyl)amino]ethyl]-2-pyridinecarboxamide	338.16	C13H12BrN3O3
AK-968/11369020	L08	3.00	0.00	2.67	0.58	2.33	1.15		5-bromo-N-(4-sec-butylphenyl)-2-furamide	322.20	C15H16BrNO2
AK-968/11369112	L09	3.00	0.00	2.00	0.00	1.67	1.53		5-bromo-N-(4-methylbenzyl)-2-furamide	294.15	C13H12BrNO2
AN-652/42568552	L10	3.00	0.00	1.67	0.58	2.00	1.00		2-methoxyphenyl 5-bromo-2-furoate	297.11	C12H9BrO4
AH-262/08501053	L11	2.00	1.00	1.67	0.58	1.33	1.53		4-methylphenyl 5-bromo-2-furoate	281.11	C12H9BrO3
AP-970/42683306	L12	3.00	0.00	2.33	0.58	2.33	0.58		5-bromo-N-[3-chloro-4-(4-ethyl-1-piperazinyl)phenyl]-2-furamide	412.72	C17H19BrClN3O2
AN-652/40097422	L13	0.00	0.00	0.00	0.00	-0.33	0.58		5-bromo-N-(2-chloro-3-pyridinyl)-2-furamide	301.53	C10H6BrClN2O2
AN-652/40072434	L14	3.00	0.00	2.33	0.58	2.33	0.58		5-bromo-N-(8-quinolinyl)-2-furamide	317.14	C14H9BrN2O2
AN-652/42568556	L15	3.00	0.00	2.33	0.58	3.00	0.00		ethyl 3-[(5-bromo-2-furoyl)amino]benzoate	338.16	C14H12BrNO4
AN-652/40051821	L16	1.67	1.53	1.67	0.58	1.67	0.58		5-bromo-N-(4-chlorophenyl)-2-furamide	300.54	C11H7BrClNO2
AN-652/05699060	L17	2.67	0.58	1.33	1.15	1.67	1.53		5-bromo-N-(4-methylphenyl)-2-furamide	280.12	C12H10BrNO2
AN-329/40839978	L18	-0.67	0.58	-0.33	0.58	0.00	0.00		5-bromo-N'-(4-cyanobenzylidene)-2-furohydrazide	318.13	C13H8BrN3O2
AN-329/40744083	L19	0.00	0.00	0.00	0.00	-0.33	0.58		N-[2-(aminocarbonyl)phenyl]-5-bromo-2-furamide	309.12	C12H9BrN2O3

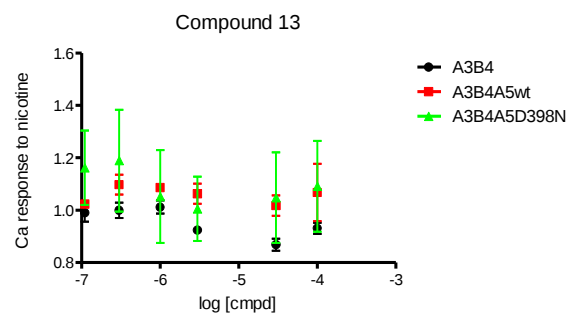
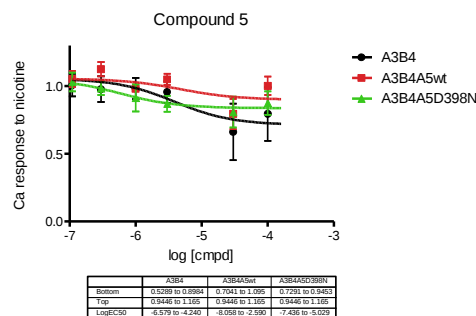
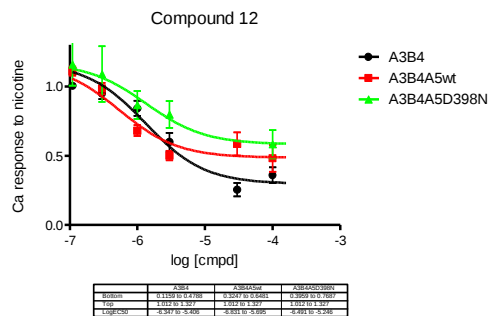
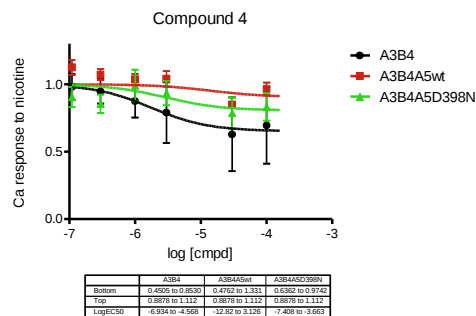
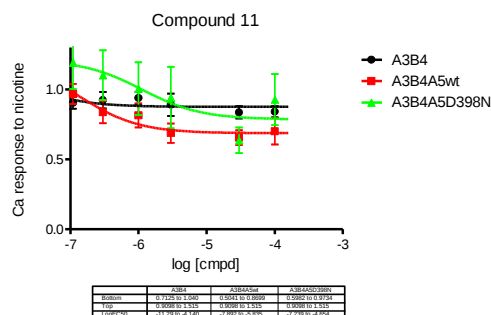
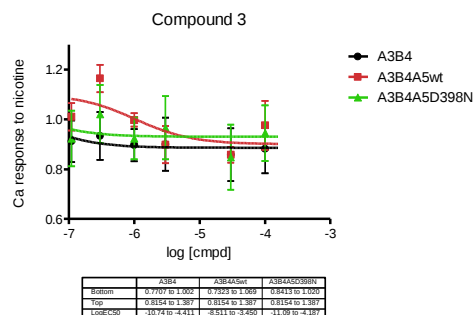
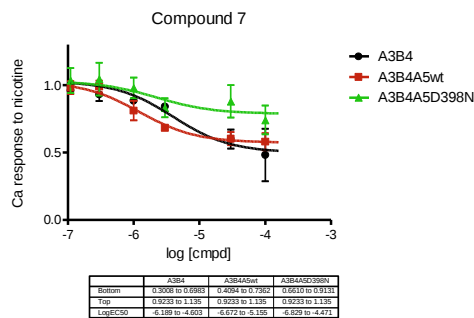
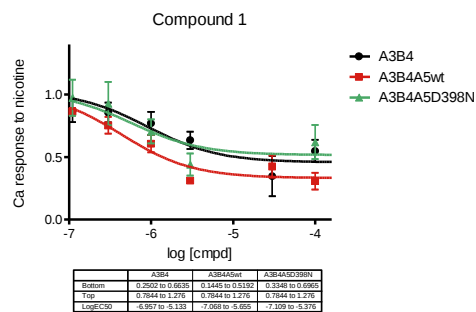
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AN-329/40254006	L21	-0.33	0.58	0.33	0.58	-0.33	0.58		5-bromo-N'-(2-oxo-1,2-dihydro-3H-indol-3-ylidene)-2-furohydrazide	334.13	C13H8BrN3O3
AN-329/40744089	L22	0.33	0.58	0.67	0.58	0.00	1.00		N-[3-(aminocarbonyl)-4,5,6,7-tetrahydro-1-benzothien-2-yl]-5-bromo-2-furamide	369.24	C14H13BrN2O3S
AH-034/32475045	M03	2.00	1.73	0.33	0.58	1.00	1.73		4-(benzylamino)-3-nitro-2H-chromen-2-one	296.29	C16H12N2O4
AN-329/41830836	M04	3.00	0.00	0.67	0.58	2.67	0.58		2,6-dimethylphenyl 5-bromo-2-furoate	295.13	C13H11BrO3
AO-365/43402738	M05	3.00	0.00	2.67	0.58	2.67	0.58		5-bromo-N'-[2-((2-(diethylamino)ethylamino)carbonyl)phenyl]-2-furamide	408.30	C18H22BrN3O3
AK-778/11811017	M06	0.33	0.58	0.67	0.58	-0.33	0.58		5-bromo-N'-[2-(5-bromo-2-chlorophenyl)-1,3-benzoxazol-5-yl]-2-furamide	496.55	C18H9Br2ClN2O3
AN-329/11658808	M07	0.67	0.58	0.67	0.58	0.67	0.58		5-bromo-N'-(2-thienylcarbonyl)-2-furohydrazide	315.15	C10H7BrN2O3S
AN-329/43449025	M08	1.00	1.73	0.33	0.58	0.00	0.00		5-bromo-N'-[3-(4-morpholinylcarbonyl)phenyl]-2-furamide	379.21	C16H15BrN2O4
AG-670/42111674	M09	3.00	0.00	2.33	0.58	2.67	0.58		5-bromo-N'-[4-(isobutylamino)-3-methoxyphenyl]-2-furamide	381.23	C16H17BrN2O4
AN-329/43449686	M10	0.00	0.00	0.33	0.58	-0.33	0.58		4-(propionylamino)phenyl 5-bromo-2-furoate	338.16	C14H12BrNO4
AF-399/40769063	M11	-0.33	0.58	0.33	0.58	0.00	1.00		N-[2-{2-[(5-bromo-2-furyl)methylene]hydrazino}-2-oxoethyl]benzamide	350.17	C14H12BrN3O3
AN-329/43448985	M12	1.00	1.73	0.33	0.58	0.33	0.58		5-bromo-N'-[3-[(isopropylamino)carbonyl]phenyl]-2-furamide	351.20	C15H15BrN2O3
AK-968/40605757	M13	3.00	0.00	1.67	0.58	1.33	1.53		5-bromo-N'-(1-phenylpentylidene)-2-furohydrazide	349.23	C16H17BrN2O2
AK-968/41924375	M14	0.00	0.00	0.67	1.15	0.00	1.00		N-benzyl-2-(5-bromo-2-furyl)hydrazinecarbothioamide	354.23	C13H12BrN3O2S
AG-690/10280046	M15	0.00	0.00	0.33	0.58	1.67	1.15		5-bromo-N'-[3-[(4-methoxyanilino)carbonyl]phenyl]-2-furamide	415.25	C19H15BrN2O4
AN-652/05699057	M16	1.67	0.58	1.67	0.58	2.00	1.00		5-bromo-N-(4-bromophenyl)-2-furamide	344.99	C11H7Br2NO2
AN-652/34351048	M17	0.67	0.58	1.00	0.00	0.00	1.00		3-methylphenyl 5-bromo-2-furoate	281.11	C12H9BrO3
AN-329/41558674	M18	-1.00	0.00	0.00	0.00	-0.33	0.58		5-bromo-N'-[(4-bromo-2-methylphenoxy)acetyl]-2-furohydrazide	432.07	C14H12Br2N2O4
AN-329/41306889	M19	1.33	1.53	0.67	1.15	0.33	0.58		2-nitrophenyl 5-bromo-2-furoate	312.08	C11H6BrNO5
AN-329/41306942	M20	-0.33	0.58	0.33	0.58	0.00	1.00		2-chlorophenyl 5-bromo-2-furoate	301.53	C11H6BrClO3
AN-329/40256100	M21	2.67	0.58	2.33	0.58	1.33	0.58		N'-(9-anthrylmethylene)-5-bromo-2-furohydrazide	393.24	C20H13BrN2O2
AN-329/40287114	M22	0.33	1.15	1.33	0.58	1.00	1.00		5-bromo-N'-[2-[(5-bromo-2-furyl)amino]ethyl]-2-furamide	406.03	C12H10Br2N2O4
AO-081/41933654	N03	3.00	0.00	2.00	0.00	2.33	1.15		1-(5-bromo-2-furyl)-4-(2-pyridinyl)piperazine	336.19	C14H14BrN3O2
AK-968/37005249	N04	3.00	0.00	0.67	1.53	2.00	1.73		5-bromo-N'-(1-(4-methoxyphenyl)ethylidene)-2-furohydrazide	337.18	C14H13BrN2O3
AO-365/43403333	N05	3.00	0.00	3.00	0.00	3.00	0.00		N-[2-[(5-bromo-2-furyl)amino]ethyl]-1-benzofuran-2-carboxamide	377.20	C16H13BrN2O4
AO-365/43402633	N06	3.00	0.00	2.33	0.58	2.33	1.15		5-bromo-N'-[3-[(3-(4-morpholinyl)propylamino)carbonyl]phenyl]-2-furamide	436.31	C19H22BrN3O4
AK-968/41026852	N07	1.00	1.73	0.00	0.00	0.00	1.00		5-[2-(5-bromo-2-furyl)hydrazino]-5-oxopentanoic acid	319.11	C10H11BrN2O5
AN-329/43448963	N08	3.00	0.00	2.00	0.00	2.00	1.00		5-bromo-N'-[3-(sec-butylamino)carbonyl]phenyl]-2-furamide	365.23	C16H17BrN2O3
AG-670/42112028	N09	0.67	0.58	1.33	0.58	0.67	0.58		N-[4-(4-benzyl-1-piperazinyl)phenyl]-5-bromo-2-furamide	440.34	C22H22BrN3O2

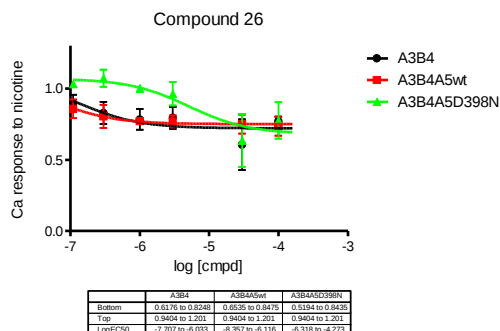
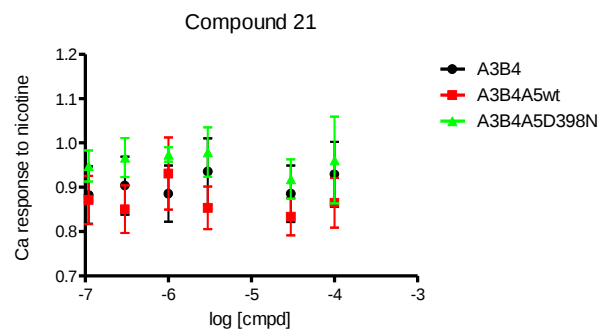
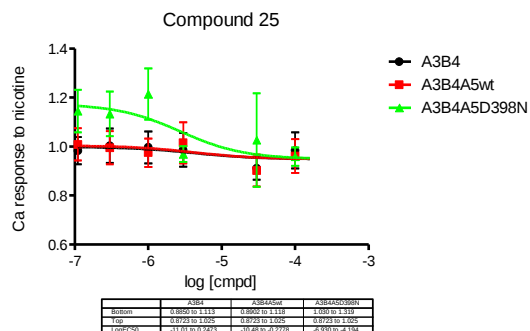
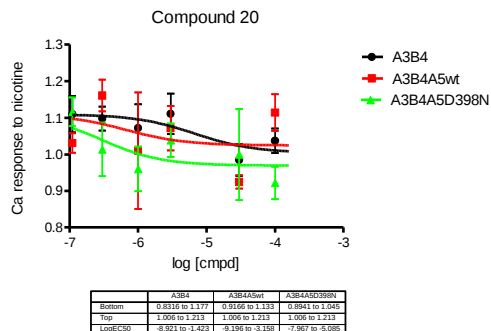
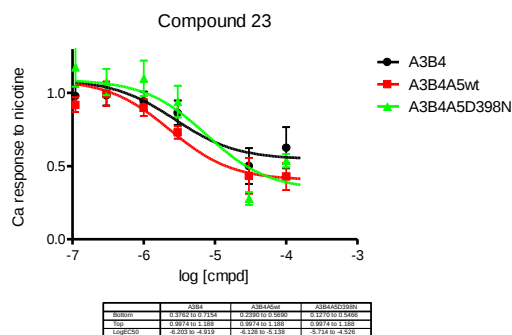
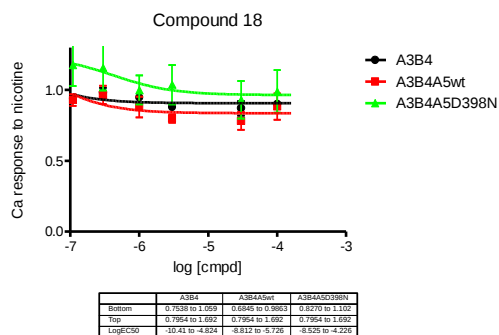
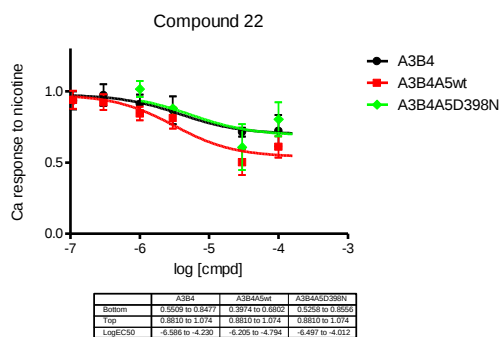
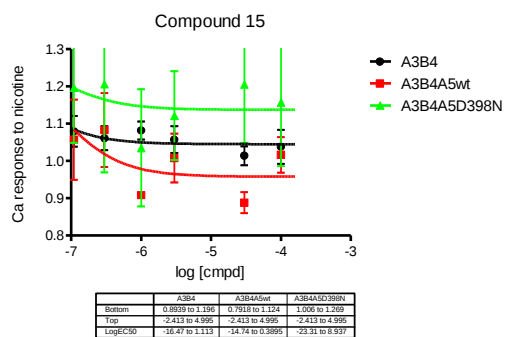
AK-968/1136890	N10	3.00	0.00	2.33	0.58	2.33	0.58		5-bromo-N-(2,4-dimethoxyphenyl)-2-furamide	326.15	C13H12BrNO4
AK-968/11369090	N11	3.00	0.00	2.33	0.58	2.67	0.58		5-bromo-N-(4-phenylbutyl)-2-furamide	322.20	C15H16BrNO2
AN-329/42613149	N12	3.00	0.00	2.33	0.58	2.67	0.58		5-bromo-N-([4-((methylamino)sulfonyl)phenyl]phenyl)-2-furamide	435.30	C18H15BrN2O4S
AK-968/41924353	N13	-0.33	0.58	0.00	0.00	1.00	1.00		2-(5-bromo-2-furoyl)-N-(2-methylphenyl)hydrazinecarbothioamide	354.23	C13H12BrN3O2S
AK-968/41924264	N14	-0.67	0.58	0.00	0.00	-0.33	0.58		N-allyl-2-(5-bromo-2-furoyl)hydrazinecarbothioamide	304.17	C9H10BrN3O2S
AN-652/09829029	N15	3.00	0.00	2.33	0.58	2.00	1.00		5-bromo-N-(9-ethyl-9H-carbazol-3-yl)-2-furamide	383.25	C19H15BrN2O2
AN-652/4256554	N16	3.00	0.00	2.33	0.58	1.67	1.53		3-tert-butyl-4-hydroxyphenyl 5-bromo-2-furoate	339.19	C15H15BrO4
AG-690/12886226	N17	3.00	0.00	2.33	0.58	2.33	0.58		ethyl 4-[(5-bromo-2-furoyl)amino]benzoate	338.16	C14H12BrNO4
AN-329/40839974	N18	2.33	1.15	1.33	0.58	1.00	0.00		5-bromo-N'-[(9-ethyl-9H-carbazol-3-yl)methylene]-2-furohydrazide	410.27	C20H16BrN3O2
AN-329/40839980	N19	3.00	0.00	1.33	1.53	1.33	1.53		5-bromo-N'-(3,5-dichloro-2-hydroxybenzylidene)-2-furohydrazide	378.01	C12H7BrCl2N2O3
AN-329/40744111	N20	-0.67	0.58	0.00	1.00	-0.33	0.58		5-bromo-N'-[(4-methoxyphenyl)acetyl]-2-furohydrazide	353.17	C14H13BrN2O4
AN-329/40744084	N21	2.00	1.73	1.00	0.00	-0.33	0.58		N-[2-(anilinoacetyl)phenyl]-5-bromo-2-furamide	385.22	C18H13BrN2O3
AN-329/40744088	N22	3.00	0.00	1.33	0.58	0.33	0.58		methyl 2-[(5-bromo-2-furoyl)amino]-4,5,6,7-tetrahydro-1-benzothiophene-3-carboxylate	384.25	C15H14BrNO4S
AK-968/37005293	O03	0.00	0.00	0.00	0.00	0.33	0.58		5-bromo-N'-(2-hydroxy-3-methoxybenzylidene)-2-furohydrazide	339.15	C13H11BrN2O4
AK-968/37005214	O04	3.00	0.00	0.67	1.53	1.00	1.00		5-bromo-N'-(4-methylcyclohexylidene)-2-furohydrazide	299.17	C12H15BrN2O2
AN-329/43449026	O05	3.00	0.00	2.33	0.58	2.33	1.15		5-bromo-N-[3-[(diethylamino)carbonyl]phenyl]-2-furamide	365.23	C16H17BrN2O3
AO-365/43402993	O06	3.00	0.00	2.33	0.58	2.67	0.58		5-bromo-N-[2-[(2-(dimethylamino)ethyl)amino]carbonyl]phenyl]-2-furamide	380.24	C16H18BrN3O3
AK-968/11987233	O07	3.00	0.00	2.33	0.58	2.67	0.58		1-(5-bromo-2-furoyl)-4-(4-chlorophenyl)piperazine	369.65	C15H14BrClN2O2
AN-329/43448928	O08	0.67	1.15	1.33	0.58	0.00	0.00		5-bromo-N-(4-[(3-methylbutanoyl)amino]phenyl)-2-furamide	365.23	C16H17BrN2O3
AN-329/43449021	O09	3.00	0.00	2.33	0.58	2.67	0.58		5-bromo-N-(3-[(2-furylmethyl)amino]carbonyl]phenyl)-2-furamide	389.21	C17H13BrN2O4
AN-329/05699054	O10	1.67	1.15	1.00	0.00	1.33	1.53		4-methoxyphenyl 5-bromo-2-furoate	297.11	C12H9BrO4
AK-918/12440572	O11	3.00	0.00	2.33	0.58	2.67	0.58		3-[(3-methoxybenzoyl)amino]phenyl 5-bromo-2-furoate	416.23	C19H14BrNO5
AK-968/14003142	O12	3.00	0.00	2.33	0.58	2.33	0.58		5-bromo-N-(2,3-dihydro-1H-inden-5-yl)-2-furamide	306.16	C14H12BrNO2
AK-968/41927440	O13	3.00	0.00	2.33	0.58	2.33	0.58		5-bromo-N-(2-phenoxyphenyl)-2-furamide	358.19	C17H12BrNO3
AK-968/41922148	O14	2.67	0.58	1.33	0.58	2.33	0.58		5-bromo-N'-[2-(4-chlorophenoxy)-2-methylpropanoyl]-2-furohydrazide	401.65	C15H14BrClN2O4
AK-968/40307670	O15	3.00	0.00	2.33	0.58	2.33	0.58		5-bromo-N'-[(5-ethyl-2-thienyl)methylene]-2-furohydrazide	327.20	C12H11BrN2O2S
AK-968/11368442	O16	0.00	0.00	0.00	0.00	-0.33	0.58		5-bromo-N'-(1,2-dimethylpropylidene)-2-furohydrazide	273.13	C10H13BrN2O2
AK-968/40386583	O17	2.00	1.00	0.67	0.58	1.67	0.58		5-bromo-N'-(3-cyclohexen-1-yl)methylene)-2-furohydrazide	297.15	C12H13BrN2O2
AN-329/43385616	O18	1.00	1.00	1.67	0.58	1.00	1.00		5-bromo-N-(4-propoxyphenyl)-2-furamide	324.18	C14H14BrNO3
AN-329/33948023	O19	3.00	0.00	1.67	0.58	2.00	1.00		5-bromo-N-(3,4-dimethylphenyl)-2-furamide	294.15	C13H12BrNO2

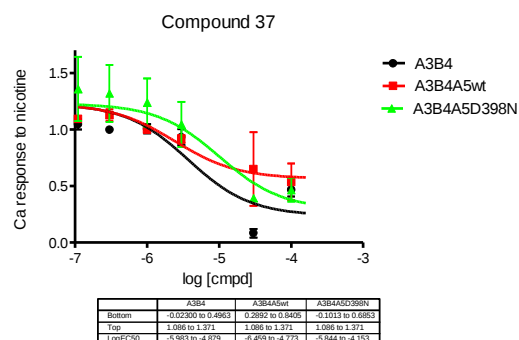
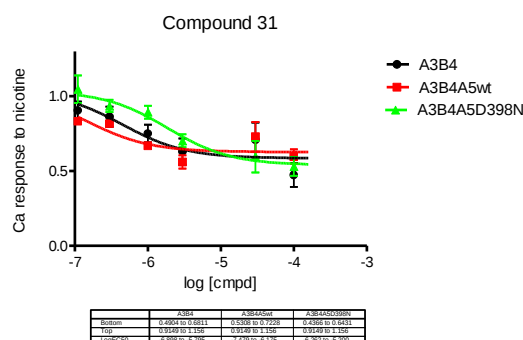
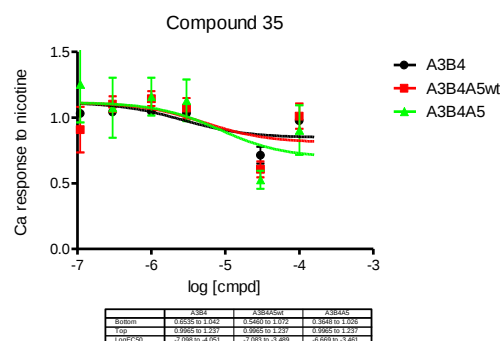
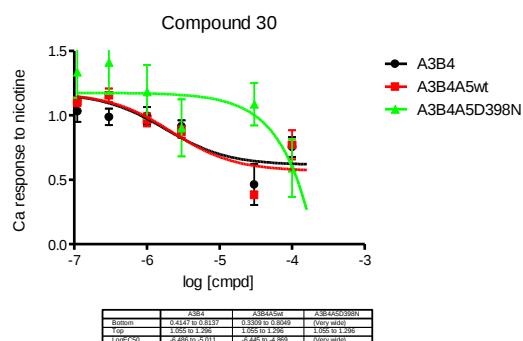
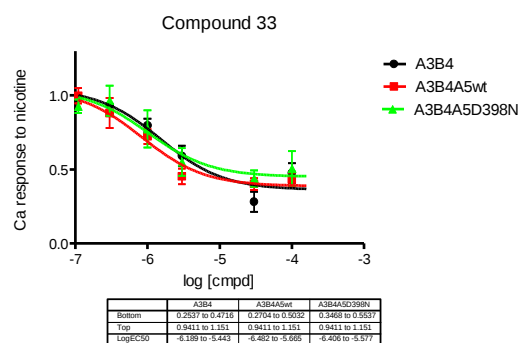
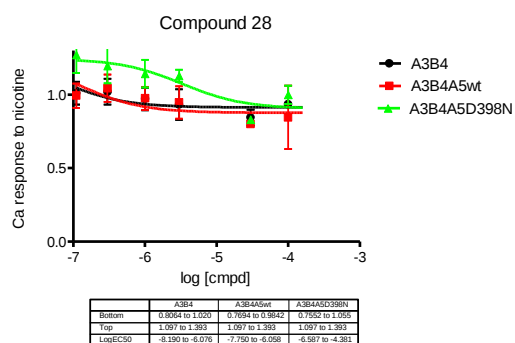
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AN-329/12864804	O21	3.00	0.00	2.33	0.58	2.33	1.15		5-bromo-N-mesityl-2-furamide	308.18	C14H14BrNO2
AN-329/40744086	O22	-0.67	0.58	0.67	0.58	-0.67	0.58		5-bromo-N-[5-nitro-2-methoxyphenyl]-2-furamide	341.12	C12H9BrN2O5
AN-329/40744092	P03	2.33	1.15	1.00	1.73	1.00	1.73		5-bromo-N-[4-(1-piperidinylsulfonyl)phenyl]-2-furamide	413.29	C16H17BrN2O4S
AK-968/11367284	P04	1.67	1.15	0.00	1.00	0.67	0.58		5-bromo-N'-cycloheptylidene-2-furohydrazide	299.17	C12H15BrN2O2
AN-329/43450127	P05	3.00	0.00	2.00	1.00	2.67	0.58		N-[2-(allyloxy)phenyl]-5-bromo-2-furamide	322.16	C14H12BrNO3
AG-670/13188026	P06	0.00	0.00	0.00	0.00	-0.33	0.58		5-bromo-N-[2-(4-bromophenyl)-2H-1,2,3-benzotriazol-5-yl]-2-furamide	462.10	C17H10Br2N4O2
AG-690/11571991	P07	0.00	0.00	0.67	0.58	0.00	0.00		1-(5-bromo-2-furoyl)-3,5-bis(4-bromophenyl)-4,5-dihydro-1H-pyrazole	553.05	C20H13Br3N2O2
AN-329/43449024	P08	3.00	0.00	2.00	1.00	1.67	0.58		N-[4-(1-azepanylcarbonyl)phenyl]-5-bromo-2-furamide	391.27	C18H19BrN2O3
AN-329/43449028	P09	2.67	0.58	2.00	1.00	1.67	0.58		5-bromo-N-[4-[(diethylamino)carbonyl]phenyl]-2-furamide	365.23	C16H17BrN2O3
AN-329/43450214	P10	3.00	0.00	2.00	1.00	2.33	1.15		5-bromo-N-(2-isopropoxyphenyl)-2-furamide	324.18	C14H14BrNO3
AN-329/43449645	P11	3.00	0.00	1.67	0.58	2.00	1.00		5-bromo-N-(2-butoxyphenyl)-2-furamide	338.20	C15H16BrNO3
AG-690/12763583	P12	0.33	0.58	0.00	0.00	-0.33	0.58		5-bromo-N-(3-pyridinylmethyl)-2-furamide	281.11	C11H9BrN2O2
AK-968/41923758	P13	-1.00	0.00	0.00	0.00	-0.33	0.58		2-(5-bromo-2-furoyl)-N-isobutylhydrazinecarbothioamide	320.21	C10H14BrN3O2S
AG-205/07808008	P14	3.00	0.00	1.33	1.15	1.67	1.53		5-bromo-N-[2-chloro-5-(trifluoromethyl)phenyl]-2-furamide	368.54	C12H6BrClF3NO2
AK-968/11367377	P15	3.00	0.00	1.67	0.58	2.33	0.58		N'-(bicyclo[2.2.1]hept-2-ylmethylene)-5-bromo-2-furohydrazide	311.18	C13H15BrN2O2
AK-968/12122023	P16	0.67	0.58	0.00	0.00	0.00	0.00		5-bromo-N-butyl-2-furamide	246.11	C9H12BrNO2
AK-968/40279810	P17	0.33	0.58	0.33	0.58	0.67	0.58		5-bromo-N'-(1-isopropyl-4-piperidinylidene)-2-furohydrazide	328.21	C13H18BrN3O2
AN-329/10830053	P18	0.33	0.58	0.33	0.58	-0.33	0.58		N-[4-(aminocarbonyl)phenyl]-5-bromo-2-furamide	309.12	C12H9BrN2O3
AN-329/09830049	P19	-0.67	0.58	-0.67	0.58	-0.33	0.58		5-bromo-N'-(3-nitrobenzoyl)-2-furohydrazide	354.12	C12H8BrN3O5
AK-968/11368956	P20	0.00	0.00	1.00	1.00	1.33	1.53		N'-(4-benzyloxy)benzylidene)-5-bromo-2-furohydrazide	399.25	C19H15BrN2O3
AN-329/12974430	P21	3.00	0.00	2.33	0.58	2.33	0.58		propyl 4-[(5-bromo-2-furoyl)amino]benzoate	352.19	C15H14BrNO4
AN-329/40744124	P22	-1.00	0.00	-0.33	0.58	0.00	0.00		N-benzyl-4-[2-(5-bromo-2-furoyl)hydrazino]-4-oxobutanamide	394.23	C16H16BrN3O4
AE-641/30156032	A03	3.00	0.00	2.00	1.00	2.67	0.58		8-[2-[(diphenylacetyl)oxy]ethyl]-2-isopropyl-8-methyl-1,3-dioxo-2-aza-8-azoniaspiro[4.5]decane	463.60	C28H35N2O4
AA-516/30054006	A04	0.33	0.58	0.67	0.58	0.00	0.00		methyl 5-bromo-2-furoate	205.01	C6H5BrO3
AK-968/41728420	A05	0.00	1.00	0.67	0.58	0.33	0.58		5-bromo-N-(6-chloro-1,3-benzothiazol-2-yl)-2-furamide	357.61	C12H6BrClN2O2S
AE-641/30177001	A07	3.00	0.00	2.33	0.58	2.67	0.58		N,N,4-trimethyl-5,6-diphenyl-1-hexanamine	295.47	C21H29N
AN-329/41933649	B03	3.00	0.00	1.33	0.58	2.67	0.58		5-bromo-N-methyl-N-phenyl-2-furamide	280.12	C12H10BrNO2
AN-329/42667829	B04	3.00	0.00	0.67	0.58	0.00	0.00		N-(5-bromo-2-furoyl)-N'-(2-ethoxyphenyl)thiourea	369.24	C14H13BrN2O3S
AK-968/41925804	B05	1.33	1.15	0.67	0.58	0.67	0.58		5-bromo-N-(5-methyl-2-pyridinyl)-2-furamide	281.11	C11H9BrN2O2

AQ-776/42801681	B07	1.33	1.53	0.67	0.58	0.67	1.15		2-(1,3-dimethyl-1H-imidazol-3-ium-2-yl)ethyl methylcarbamate	198.25	C9H16N3O2
AN-329/42581112	C03	3.00	0.00	1.67	0.58	2.33	0.58		N'-(5-bromo-2-furoyl)-N-methyl-N-phenylthiourea	339.21	C13H11BrN2O2S
AK-918/42409778	C04	3.00	0.00	0.33	0.58	0.00	0.00		2,6-dichlorobenzyl 5-bromo-2-furoate	350.00	C12H7BrCl2O3
AK-968/41925801	C05	3.00	0.00	1.67	1.53	3.00	0.00		5-bromo-N-[2-(3-chlorophenyl)ethyl]-2-furamide	328.60	C13H11BrClNO2
AG-690/15427908	C07	3.00	0.00	2.00	1.00	2.67	0.58		4-[(1-adamantylcarbonyloxy)-N,N,N-trimethyl-1-butanaminium	294.46	C18H32NO2
AN-979/42723369	D03	2.33	1.15	1.33	1.53	1.67	1.15		5-bromo-N-[3-{5-(4-methylphenyl)-1,3,4-oxadiazol-2-yl}phenyl]-2-furamide	424.26	C20H14BrN3O3
AN-652/41072564	D04	3.00	0.00	2.00	1.00	1.67	1.53		5-bromo-N-[4-chloro-2-(trifluoromethyl)phenyl]-2-furamide	368.54	C12H6BrClF3NO2
AP-970/43375149	D05	1.33	1.53	0.00	0.00	0.67	1.15		methyl 3-[(5-bromo-2-furoyl)amino]-4-(4-morpholinyl)benzoate	409.24	C17H17BrN2O5
AE-473/30080042	D07	2.67	0.58	1.33	0.58	1.67	0.58		2-[(5-nitro-2-methylphenyl)imino]-1-methylpyrrolidine	233.27	C12H15N3O2
AH-034/07270029	E03	-0.33	0.58	0.00	0.00	1.00	0.00		5-bromo-N-(6-methyl-1,3-benzothiazol-2-yl)-2-furamide	337.20	C13H9BrN2O2S
AN-329/42295052	E04	0.00	1.00	0.00	0.00	1.00	0.00		N-(5-bromo-2-furoyl)-N'-(2,3-dichlorophenyl)thiourea	394.08	C12H7BrCl2N2O2S
AN-329/41689899	E05	3.00	0.00	2.67	0.58	2.33	0.58		2-acetylphenyl 5-bromo-2-furoate	309.12	C13H9BrO4
AG-664/42183910	E07	3.00	0.00	2.00	1.00	2.00	1.00		N-(3-chlorophenyl)-2-[(4-chlorophenyl)imino]-1-pyrrolidinecarboxamide	348.23	C17H15Cl2N3O
AK-968/4125901	F03	2.33	1.15	0.00	0.00	0.33	0.58		methyl 2-[(5-bromo-2-furoyl)amino]-4,5,6,7,8,9-hexahydrocycloocta[b]thiophene-3-carboxylate	412.31	C17H18BrNO4S
AN-329/42344165	F04	3.00	0.00	1.67	0.58	1.33	0.58		2-(5-bromo-2-furyl)-5-phenyl-1,3,4-oxadiazole	291.11	C12H7BrN2O2
AN-329/42548417	F05	3.00	0.00	2.00	1.00	2.67	0.58		5-bromo-N-[4-[(4-methyl-1-piperazinyl)sulfonyl]phenyl]-2-furamide	428.31	C16H18BrN3O4S
AQ-776/42801680	F07	2.67	0.58	1.33	0.58	1.00	1.00		2-(1,3-dimethyl-1H-imidazol-3-ium-2-yl)ethyl dimethylcarbamate	212.27	C10H18N3O2
AN-652/42568584	G03	3.00	0.00	0.00	0.00	1.00	1.00		2,4-dibromophenyl 5-bromo-2-furoate	424.87	C11H5Br3O3
AN-652/40051836	G04	3.00	0.00	1.67	1.15	1.67	0.58		5-bromo-N-(2,3-dichlorophenyl)-2-furamide	334.99	C11H6BrCl2NO2
AK-968/41925309	G05	3.00	0.00	2.00	1.00	2.33	1.15		5-bromo-N-(3,4-dichlorobenzyl)-2-furamide	349.01	C12H8BrCl2NO2
AG-664/42183909	G07	3.00	0.00	2.00	1.00	2.67	0.58		N-(4-chlorophenyl)-N-[1-(4-fluorobenzoyl)-2-pyrrolidinylidene]amine	316.77	C17H14ClFN2O
AK-968/12865274	H03	1.00	1.73	1.33	1.53	2.33	0.58		5-bromo-N-[3-nitro-4-methylphenyl]-2-furamide	325.12	C12H9BrN2O4
AK-968/41753492	H04	2.33	0.58	1.33	1.15	2.00	1.00		5-bromo-N-(4,5-dimethyl-1,3-thiazol-2-yl)-2-furamide	301.16	C10H9BrN2O2S
AN-652/41482755	H05	2.00	1.00	1.67	0.58	2.33	0.58		N-(2-benzoyl-4-chlorophenyl)-5-bromo-2-furamide	404.65	C18H11BrClNO3
AK-968/41927264	I03	3.00	0.00	2.00	1.00	3.00	0.00		5-bromo-N-(1-methyl-3-phenylpropyl)-2-furamide	322.20	C15H16BrNO2
AN-329/41574537	I04	0.67	0.58	0.67	0.58	0.67	0.58		N-(5-bromo-2-furoyl)-N'-(2,5-dimethoxyphenyl)thiourea	385.24	C14H13BrN2O4S
AP-970/43268313	I05	3.00	0.00	2.00	1.00	3.00	0.00		methyl 3-[(5-bromo-2-furoyl)amino]-4-(4-methyl-1-piperazinyl)benzoate	422.28	C18H20BrN3O4
AQ-776/42801591	I07	2.00	1.00	1.67	1.15	1.33	0.58		3-(1,3-dimethyl-1H-imidazol-3-ium-2-yl)propyl dimethylcarbamate	226.30	C11H20N3O2
AN-465/14962022	J03	2.67	0.58	1.00	1.73	1.33	1.15		5-bromo-N-(5-methyl-2,1,3-benzothiadiazol-4-yl)-2-furamide	338.18	C12H8BrN3O2S
AP-970/43375832	J04	3.00	0.00	1.33	0.58	2.00	1.00		N-[2-(4-acetyl-1-piperazinyl)phenyl]-5-bromo-2-furamide	392.26	C17H18BrN3O3

AN-465/42769709	J05	0.33	0.58	0.33	0.58	0.67	0.58		5-bromo-N-(4-chloro-1,3-benzothiazol-2-yl)-2-furamide	357.61	C12H6BrClN2O2S
AK-968/10831035	K03	3.00	0.00	1.67	1.53	1.00	1.73		5-bromo-N-(2-methoxy-5-methylphenyl)-2-furamide	310.15	C13H12BrNO3
AK-968/41925681	K04	0.00	1.00	0.00	0.00	0.33	0.58		5-bromo-N-(5-nitro-2-pyridinyl)-2-furamide	312.08	C10H6BrN3O4
AN-329/41340294	K05	3.00	0.00	1.00	1.73	1.00	1.00		N-(5-bromo-2-furoyl)-N'-(2-methoxyphenyl)thiourea	355.21	C13H11BrN2O3S
AQ-344/43100284	K07	3.00	0.00	1.67	0.58	2.67	0.58		2,3-diphenyl-1,2,3,3a,4,9b-hexahydrochromeno[4,3-b]pyrrole	327.43	C23H21NO
AN-329/42607833	L03	0.00	1.00	0.33	0.58	1.00	0.00		methyl 2-(((5-bromo-2-furoyl)amino)carbothioyl)amino)benzoate	383.22	C14H11BrN2O4S
AN-329/42504596	L04	0.00	1.00	0.33	0.58	0.00	0.00		5-bromo-N-[(4-methyl-1-piperazinyl)carbothioyl]-2-furamide	332.22	C11H14BrN3O2S
AK-968/41925615	L05	3.00	0.00	2.00	1.00	2.67	0.58		1-(5-bromo-2-furoyl)-4-(3-(trifluoromethyl)phenyl)piperazine	403.20	C16H14BrF3N2O2
AE-641/30115025	M03	3.00	0.00	1.67	1.15	2.67	0.58		1-[2-(acetyloxyethyl)-4-[4,4-bis(4-fluorophenyl)butyl]-1,4-dimethylpiperazinium	446.59	C26H36F2N2O2
AA-516/31409048	M04	3.00	0.00	0.00	0.00	0.33	0.58		4-chloro-2-iodo-3,5-dimethylphenyl 5-bromo-2-furoate	455.48	C13H9BrClIO3
AK-968/11369181	M05	-0.33	0.58	0.00	0.00	0.33	0.58		5-bromo-N-(tetrahydro-2-furanylmethyl)-2-furamide	274.12	C10H12BrNO3
AE-848/31926026	M07	3.00	0.00	1.33	0.58	2.67	0.58		N-[2-(dimethylamino)-4-quinolinyl]-N-(1-methyl-2-pyrrolidinylidene)amine	268.36	C16H20N4
AK-918/40864607	N03	3.00	0.00	-0.33	0.58	0.67	0.58		4-benzylphenyl 5-bromo-2-furoate	357.21	C18H13BrO3
AK-918/41945284	N04	3.00	0.00	2.00	1.00	2.33	1.15		4-chlorobenzyl 5-bromo-2-furoate	315.55	C12H8BrClO3
AQ-390/40898049	O03	3.00	0.00	2.33	0.58	2.33	1.15		N-[3-(1,3-benzothiazol-2-ylsulfanyl)-4-hydroxyphenyl]-2,5-dichlorobenzenesulfonamide	483.42	C19H12Cl2N2O3S3
AP-970/42252102	O04	3.00	0.00	0.33	0.58	0.33	0.58		5-bromo-N-[6-methyl-2-(1-naphthyl)-2H-1,2,3-benzotriazol-5-yl]-2-furamide	447.29	C22H15BrN4O2
AH-262/36795022	O07	3.00	0.00	1.67	1.15	2.33	1.15		N-(3,4-dihydro-2(1H)-quinolinylidene)-N-(4-methylphenyl)amine	236.32	C16H16N2
AN-329/41921591	P03	3.00	0.00	0.67	1.15	2.67	0.58		5-bromo-N-[4-[(ethylamino)sulfonyl]phenyl]-2-furamide	449.33	C19H17BrN2O4S
AN-329/41574560	P04	3.00	0.00	0.33	0.58	1.00	1.00		N-(5-bromo-2-furoyl)-N'-[2-(1-cyclohexen-1-yl)ethyl]thiourea	357.27	C14H17BrN2O2S







Supplemental Figure 2S