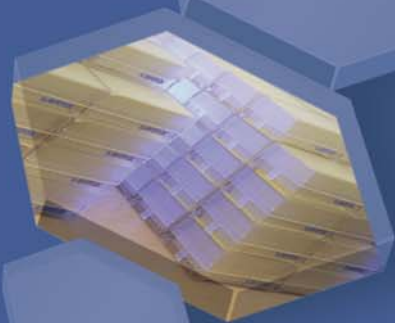


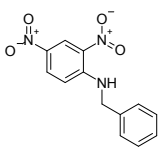


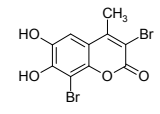
BIONET compounds –
A Key step ahead of the rest

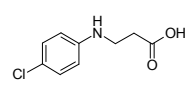


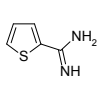
September 2012
Combined Screening and
Fragments
Collection Update

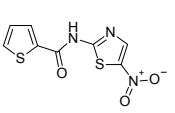
 **Key Organics**
The right side of the Equation

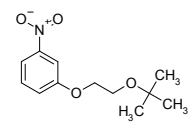
10F-368S	$C_{13}H_{11}N_3O_4$	273.2503	
		Heteroatoms	7.0000
		Halogen atoms	0.0000
		rotatable bonds	3.0000
		H-bond acceptors	4.0000
		H-bond donors	1.0000
		LogP	3.1610
		Melting_Point	Solid LIST 356
N-benzyl-2,4-dinitroaniline			

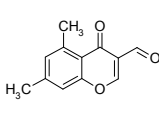
10X-0362	$C_{10}H_6Br_2O_4$	349.9649	
		Heteroatoms	6.0000
		Halogen atoms	2.0000
		rotatable bonds	0.0000
		H-bond acceptors	4.0000
		H-bond donors	2.0000
		LogP	2.3718
		Melting_Point	262 - 264 LIST 356
3,8-dibromo-6,7-dihydroxy-4-methyl-2H-chromen-2-one			

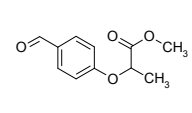
12C-002	$C_9H_{10}ClNO_2$	199.6386	
		Heteroatoms	3.0000
		Halogen atoms	1.0000
		rotatable bonds	4.0000
		H-bond acceptors	2.0000
		H-bond donors	2.0000
		LogP	1.7183
		Melting_Point	LIST 356
3-[(4-chlorophenyl)amino]propanoic acid			

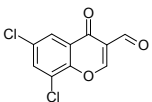
5L-0512	$C_5H_7ClN_2S$	162.6419	
		Heteroatoms	3.0000
		Halogen atoms	1.0000
		rotatable bonds	0.0000
		H-bond acceptors	1.0000
		H-bond donors	1.0000
		LogP	0.8234
		Melting_Point	Solid LIST 356
thiophene-2-carboximidamide hydrochloride			

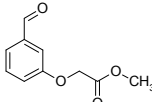
6N-021	$C_8H_5N_3O_3S_2$	255.2754	
		Heteroatoms	8.0000
		Halogen atoms	0.0000
		rotatable bonds	2.0000
		H-bond acceptors	4.0000
		H-bond donors	1.0000
		LogP	1.5974
		Melting_Point	Solid LIST 356
N-(5-nitro-1,3-thiazol-2-yl)thiophene-2-carboxamide			

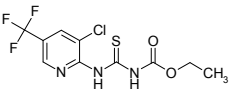
6W-0221	$C_{12}H_{17}NO_4$	239.2736	
		Heteroatoms	5.0000
		Halogen atoms	0.0000
		rotatable bonds	5.0000
		H-bond acceptors	4.0000
		H-bond donors	0.0000
		LogP	2.4165
		Melting_Point	Solid LIST 356
1-[2-(tert-butoxy)ethoxy]-3-nitrobenzene			

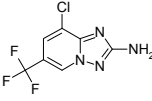
8C-118	$C_{12}H_{10}O_3$	202.2117	
		Heteroatoms	3.0000
		Halogen atoms	0.0000
		rotatable bonds	1.0000
		H-bond acceptors	3.0000
		H-bond donors	0.0000
		LogP	1.7412
		Melting_Point	LIST
5,7-dimethyl-4-oxo-4H-chromene-3-carbaldehyde			

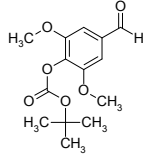
8P-065	$C_{11}H_{12}O_4$	208.2159	
		Heteroatoms	4.0000
		Halogen atoms	0.0000
		rotatable bonds	5.0000
		H-bond acceptors	4.0000
		H-bond donors	0.0000
		LogP	1.5804
		Melting_Point	oil LIST
methyl 2-(4-formylphenoxy)propanoate			

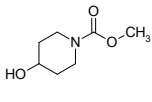
9C-091	C ₁₀ H ₄ Cl ₂ O ₃	243.0476	
			
		Heteroatoms	5.0000
		Halogen atoms	2.0000
		rotatable bonds	1.0000
		H-bond acceptors	3.0000
		H-bond donors	0.0000
		LogP	1.8428
Melting_Point	LIST	comments	
6,8-dichloro-4-oxo-4H-chromene-3-carbaldehyde			

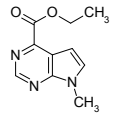
9P-009	C ₁₀ H ₁₀ O ₄	194.1888	
			
		Heteroatoms	4.0000
		Halogen atoms	0.0000
		rotatable bonds	5.0000
		H-bond acceptors	4.0000
		H-bond donors	0.0000
		LogP	1.0429
Melting_Point	LIST	comments	
methyl 2-(3-formylphenoxy)acetate			

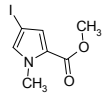
AG-0018	C ₁₀ H ₉ ClF ₃ N ₃ O ₂ S	327.7143	
			
		Heteroatoms	10.0000
		Halogen atoms	4.0000
		rotatable bonds	5.0000
		H-bond acceptors	4.0000
		H-bond donors	2.0000
		LogP	3.9101
Melting_Point	LIST	comments	
ethyl N-([3-chloro-5-(trifluoromethyl)pyridin-2-yl]carbamothioyl)carbamate			

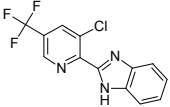
AG-0031	C ₇ H ₄ ClF ₃ N ₄	236.5849	
			
		Heteroatoms	4.0000
		Halogen atoms	0.0000
		rotatable bonds	2.0000
		H-bond acceptors	1.0000
		LogP	1.2116
Melting_Point	LIST	FRA021	comments
8-chloro-6-(trifluoromethyl)-[1,2,4]triazolo[1,5-a]pyridin-2-amine			

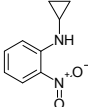
DG-0008	C ₁₄ H ₁₈ O ₆	282.2960	
			
		Heteroatoms	6.0000
		Halogen atoms	0.0000
		rotatable bonds	7.0000
		H-bond acceptors	6.0000
		H-bond donors	0.0000
		LogP	2.1747
Melting_Point	LIST	comments	
tert-butyl 4-formyl-2,6-dimethoxyphenyl carbonate			

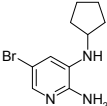
EG-0095	C ₇ H ₁₃ NO ₃	159.1866	
			
		Heteroatoms	0.0000
		Halogen atoms	0.0000
		rotatable bonds	1.0000
		H-bond acceptors	3.0000
		H-bond donors	1.0000
		LogP	-0.3605
Melting_Point	LIST	FRA021	comments
methyl 4-hydroxypiperidine-1-carboxylate			

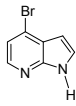
EG-0727	C ₁₀ H ₁₁ N ₃ O ₂	205.2181	
			
		Heteroatoms	5.0000
		Halogen atoms	0.0000
		rotatable bonds	3.0000
		H-bond acceptors	4.0000
		H-bond donors	0.0000
		LogP	1.3401
Melting_Point	85 - 87	LIST	comments
ethyl 7-methyl-7H-pyrrolo[2,3-d]pyrimidine-4-carboxylate			

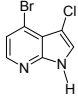
EG-0735	C ₇ H ₈ INO ₂	265.0517	
			
		Heteroatoms	1.0000
		Halogen atoms	2.0000
		rotatable bonds	2.0000
		H-bond acceptors	2.0000
		H-bond donors	0.0000
		LogP	2.0516
Melting_Point	65 - 67	LIST	FRA021
methyl 4-iodo-1-methyl-1H-pyrrole-2-carboxylate			


FG-0027	C ₁₃ H ₇ ClF ₃ N ₃	297.6690	
			Heteroatoms
			7.0000
			Halogen atoms
			4.0000
			rotatable bonds
			1.0000
			H-bond acceptors
2.0000			
H-bond donors			
1.0000			
LogP	4.0666		
Melting_Point	LIST	comments	
2-[3-chloro-5-(trifluoromethyl)pyridin-2-yl]-1H-1,3-benzodiazole			

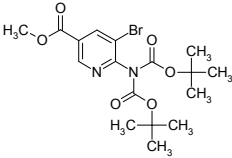
FG-0053	C ₉ H ₁₀ N ₂ O ₂	178.1923	
			Heteroatoms
			0.0000
			Halogen atoms
			0.0000
			rotatable bonds
			2.0000
			H-bond acceptors
2.0000			
H-bond donors			
1.0000			
LogP	1.8270		
Melting_Point	LIST	FRA021	comments
N-cyclopropyl-2-nitroaniline			


FG-0063	C ₁₀ H ₁₄ BrN ₃	256.1472	
			Heteroatoms
			1.0000
			Halogen atoms
			1.0000
			rotatable bonds
			2.0000
			H-bond acceptors
1.0000			
H-bond donors			
2.0000			
LogP	2.5262		
Melting_Point	56 - 58	LIST	FRA021
5-bromo-3-N-cyclopentylpyridine-2,3-diamine			

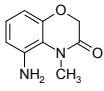
FG-0210	C ₇ H ₅ BrN ₂	197.0353	
			Heteroatoms
			1.0000
			Halogen atoms
			0.0000
			rotatable bonds
			0.0000
			H-bond acceptors
1.0000			
H-bond donors			
1.0000			
LogP	2.5227		
Melting_Point	176 - 177	LIST	FRA021
4-bromo-1H-pyrrolo[2,3-b]pyridine			

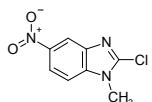
FG-0213	C ₇ H ₄ BrClN ₂	231.4803	
			Heteroatoms
			2.0000
			Halogen atoms
			0.0000
			rotatable bonds
			0.0000
			H-bond acceptors
1.0000			
H-bond donors			
1.0000			
LogP	3.0407		
Melting_Point	227 - 228	LIST	FRA021
4-bromo-3-chloro-1H-pyrrolo[2,3-b]pyridine			

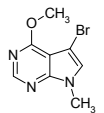
FG-0700	C ₆ H ₅ NO ₂	111.1011	
			Heteroatoms
			0.0000
			Halogen atoms
			0.0000
			rotatable bonds
			1.0000
			H-bond acceptors
3.0000			
H-bond donors			
1.0000			
LogP	0.5816		
Melting_Point	148 - 150	LIST	FRA021
1-cyanocyclopropane-1-carboxylic acid			

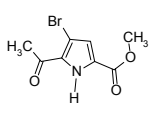
FG-0702	C ₁₇ H ₂₃ BrN ₂ O ₆	431.2867	
			Heteroatoms
			9.0000
			Halogen atoms
			1.0000
			rotatable bonds
			7.0000
			H-bond acceptors
7.0000			
H-bond donors			
0.0000			
LogP	4.1853		
Melting_Point	129 - 131	LIST	comments
methyl 6-[[bis(tert-butoxy)carbonyl]amino]-5-bromopyridine-3-carboxylate			

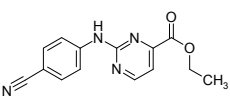
FG-0709	C ₆ H ₆ INO ₂	251.0246	
			Heteroatoms
			1.0000
			Halogen atoms
			1.0000
			rotatable bonds
			1.0000
			H-bond acceptors
2.0000			
H-bond donors			
1.0000			
LogP	2.0199		
Melting_Point	141 - 144	LIST	FRA021
4-iodo-1-methyl-1H-pyrrole-2-carboxylic acid			

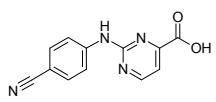
FG-0714	$C_9H_{10}N_2O_2$	178.1923	
			Heteroatoms
			Halogen atoms
			rotatable bonds
			H-bond acceptors
			H-bond donors
			LogP
			Melting_Point
5-amino-4-methyl-3,4-dihydro-2H-1,4-benzoxazin-3-one			

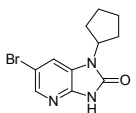
FG-0715	$C_8H_6ClN_3O_2$	211.6089	
			Heteroatoms
			Halogen atoms
			rotatable bonds
			H-bond acceptors
			H-bond donors
			LogP
			Melting_Point
2-chloro-1-methyl-5-nitro-1H-1,3-benzodiazole			

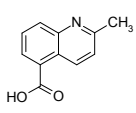
FG-0716	$C_8H_8BrN_3O$	242.0765	
			Heteroatoms
			Halogen atoms
			rotatable bonds
			H-bond acceptors
			H-bond donors
			LogP
			Melting_Point
5-bromo-4-methoxy-7-methyl-7H-pyrrolo[2,3-d]pyrimidine			

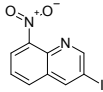
FG-0717	$C_8H_8BrNO_3$	246.0619	
			Heteroatoms
			Halogen atoms
			rotatable bonds
			H-bond acceptors
			H-bond donors
			LogP
			Melting_Point
methyl 5-acetyl-4-bromo-1H-pyrrole-2-carboxylate			


FG-0719	$C_{14}H_{12}N_4O_2$	268.2773	
			Heteroatoms
			Halogen atoms
			rotatable bonds
			H-bond acceptors
			H-bond donors
			LogP
			Melting_Point
ethyl 2-[(4-cyanophenyl)amino]pyrimidine-4-carboxylate			

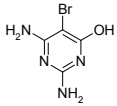
FG-0723	$C_{12}H_8N_4O_2$	240.2232	
			Heteroatoms
			Halogen atoms
			rotatable bonds
			H-bond acceptors
			H-bond donors
			LogP
			Melting_Point
2-[(4-cyanophenyl)amino]pyrimidine-4-carboxylic acid			

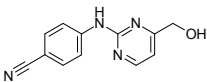
GG-0019	$C_{11}H_{12}BrN_3O$	282.1418	
			Heteroatoms
			Halogen atoms
			rotatable bonds
			H-bond acceptors
			H-bond donors
			LogP
			Melting_Point
6-bromo-1-cyclopentyl-1H,2H,3H-imidazo[4,5-b]pyridin-2-one			

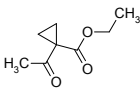
GG-0060	$C_{11}H_9NO_2$	187.1999	
			Heteroatoms
			Halogen atoms
			rotatable bonds
			H-bond acceptors
			H-bond donors
			LogP
			Melting_Point
2-methylquinoline-5-carboxylic acid			

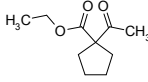
GG-0202	$C_9H_5N_2O_2$	300.0568													
		<table border="1"> <tr><td>Heteroatoms</td><td>5.0000</td></tr> <tr><td>Halogen atoms</td><td>1.0000</td></tr> <tr><td>rotatable bonds</td><td>0.0000</td></tr> <tr><td>H-bond acceptors</td><td>3.0000</td></tr> <tr><td>H-bond donors</td><td>0.0000</td></tr> <tr><td>LogP</td><td>3.8119</td></tr> </table>	Heteroatoms	5.0000	Halogen atoms	1.0000	rotatable bonds	0.0000	H-bond acceptors	3.0000	H-bond donors	0.0000	LogP	3.8119	
Heteroatoms	5.0000														
Halogen atoms	1.0000														
rotatable bonds	0.0000														
H-bond acceptors	3.0000														
H-bond donors	0.0000														
LogP	3.8119														
Melting_Point	120 - 121	LIST	comments												
3-iodo-8-nitroquinoline															


GG-0205	$C_7H_4BrIN_2$	322.9317													
		<table border="1"> <tr><td>Heteroatoms</td><td>2.0000</td></tr> <tr><td>Halogen atoms</td><td>2.0000</td></tr> <tr><td>rotatable bonds</td><td>0.0000</td></tr> <tr><td>H-bond acceptors</td><td>1.0000</td></tr> <tr><td>H-bond donors</td><td>1.0000</td></tr> <tr><td>LogP</td><td>3.7801</td></tr> </table>	Heteroatoms	2.0000	Halogen atoms	2.0000	rotatable bonds	0.0000	H-bond acceptors	1.0000	H-bond donors	1.0000	LogP	3.7801	
Heteroatoms	2.0000														
Halogen atoms	2.0000														
rotatable bonds	0.0000														
H-bond acceptors	1.0000														
H-bond donors	1.0000														
LogP	3.7801														
Melting_Point	222 - 224	LIST	FRA021 comments												
4-bromo-3-iodo-1H-pyrrolo[2,3-b]pyridine															


GG-0242	$C_4H_5BrN_4O$	205.0147													
		<table border="1"> <tr><td>Heteroatoms</td><td>4.0000</td></tr> <tr><td>Halogen atoms</td><td>1.0000</td></tr> <tr><td>rotatable bonds</td><td>0.0000</td></tr> <tr><td>H-bond acceptors</td><td>3.0000</td></tr> <tr><td>H-bond donors</td><td>3.0000</td></tr> <tr><td>LogP</td><td>0.9319</td></tr> </table>	Heteroatoms	4.0000	Halogen atoms	1.0000	rotatable bonds	0.0000	H-bond acceptors	3.0000	H-bond donors	3.0000	LogP	0.9319	
Heteroatoms	4.0000														
Halogen atoms	1.0000														
rotatable bonds	0.0000														
H-bond acceptors	3.0000														
H-bond donors	3.0000														
LogP	0.9319														
Melting_Point	256 - 257	LIST	FRA021 comments												
2,6-diamino-5-bromopyrimidin-4-ol															

GG-0701	$C_{12}H_{10}N_4O$	226.2397													
		<table border="1"> <tr><td>Heteroatoms</td><td>4.0000</td></tr> <tr><td>Halogen atoms</td><td>0.0000</td></tr> <tr><td>rotatable bonds</td><td>3.0000</td></tr> <tr><td>H-bond acceptors</td><td>4.0000</td></tr> <tr><td>H-bond donors</td><td>2.0000</td></tr> <tr><td>LogP</td><td>1.4348</td></tr> </table>	Heteroatoms	4.0000	Halogen atoms	0.0000	rotatable bonds	3.0000	H-bond acceptors	4.0000	H-bond donors	2.0000	LogP	1.4348	
Heteroatoms	4.0000														
Halogen atoms	0.0000														
rotatable bonds	3.0000														
H-bond acceptors	4.0000														
H-bond donors	2.0000														
LogP	1.4348														
Melting_Point	172 - 174	LIST	FRA021 comments												
4-[[4-(hydroxymethyl)pyrimidin-2-yl]amino]benzonitrile															

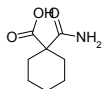
GG-0703	$C_8H_{12}O_3$	156.1830													
		<table border="1"> <tr><td>Heteroatoms</td><td>3.0000</td></tr> <tr><td>Halogen atoms</td><td>0.0000</td></tr> <tr><td>rotatable bonds</td><td>4.0000</td></tr> <tr><td>H-bond acceptors</td><td>3.0000</td></tr> <tr><td>H-bond donors</td><td>0.0000</td></tr> <tr><td>LogP</td><td>1.3364</td></tr> </table>	Heteroatoms	3.0000	Halogen atoms	0.0000	rotatable bonds	4.0000	H-bond acceptors	3.0000	H-bond donors	0.0000	LogP	1.3364	
Heteroatoms	3.0000														
Halogen atoms	0.0000														
rotatable bonds	4.0000														
H-bond acceptors	3.0000														
H-bond donors	0.0000														
LogP	1.3364														
Melting_Point		LIST	FRA021 comments												
ethyl 1-acetylcyclopropane-1-carboxylate															

GG-0704	$C_{10}H_{16}O_3$	184.2372													
		<table border="1"> <tr><td>Heteroatoms</td><td>3.0000</td></tr> <tr><td>Halogen atoms</td><td>0.0000</td></tr> <tr><td>rotatable bonds</td><td>4.0000</td></tr> <tr><td>H-bond acceptors</td><td>3.0000</td></tr> <tr><td>H-bond donors</td><td>0.0000</td></tr> <tr><td>LogP</td><td>2.1290</td></tr> </table>	Heteroatoms	3.0000	Halogen atoms	0.0000	rotatable bonds	4.0000	H-bond acceptors	3.0000	H-bond donors	0.0000	LogP	2.1290	
Heteroatoms	3.0000														
Halogen atoms	0.0000														
rotatable bonds	4.0000														
H-bond acceptors	3.0000														
H-bond donors	0.0000														
LogP	2.1290														
Melting_Point		LIST	FRA021 comments												
ethyl 1-acetylcyclopentane-1-carboxylate															

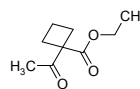
GG-0707	$C_7H_{11}NO_3$	157.1706													
		<table border="1"> <tr><td>Heteroatoms</td><td>4.0000</td></tr> <tr><td>Halogen atoms</td><td>0.0000</td></tr> <tr><td>rotatable bonds</td><td>2.0000</td></tr> <tr><td>H-bond acceptors</td><td>3.0000</td></tr> <tr><td>H-bond donors</td><td>2.0000</td></tr> <tr><td>LogP</td><td>0.3428</td></tr> </table>	Heteroatoms	4.0000	Halogen atoms	0.0000	rotatable bonds	2.0000	H-bond acceptors	3.0000	H-bond donors	2.0000	LogP	0.3428	
Heteroatoms	4.0000														
Halogen atoms	0.0000														
rotatable bonds	2.0000														
H-bond acceptors	3.0000														
H-bond donors	2.0000														
LogP	0.3428														
Melting_Point	165 - 170	LIST	FRA021 comments												
1-carbamoylcyclopentane-1-carboxylic acid															

GG-0709	$C_5H_7NO_3$	129.1164													
		<table border="1"> <tr><td>Heteroatoms</td><td>4.0000</td></tr> <tr><td>Halogen atoms</td><td>0.0000</td></tr> <tr><td>rotatable bonds</td><td>2.0000</td></tr> <tr><td>H-bond acceptors</td><td>3.0000</td></tr> <tr><td>H-bond donors</td><td>2.0000</td></tr> <tr><td>LogP</td><td>-0.4498</td></tr> </table>	Heteroatoms	4.0000	Halogen atoms	0.0000	rotatable bonds	2.0000	H-bond acceptors	3.0000	H-bond donors	2.0000	LogP	-0.4498	
Heteroatoms	4.0000														
Halogen atoms	0.0000														
rotatable bonds	2.0000														
H-bond acceptors	3.0000														
H-bond donors	2.0000														
LogP	-0.4498														
Melting_Point	186 - 188	LIST	FRA021 comments												
1-carbamoylcyclopropane-1-carboxylic acid															

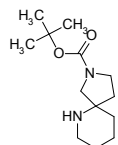
GG-0710	$C_8H_{13}NO_3$	171.1977	
			Heteroatoms
			Halogen atoms
			0.0000
			rotatable bonds
			2.0000
			H-bond acceptors
			3.0000
			H-bond donors
			2.0000
			LogP
			0.7391
Melting_Point	155 - 157	LIST	FRA021
comments			
1-carbamoylcyclohexane-1-carboxylic acid			



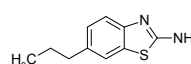
GG-0714	$C_9H_{14}O_3$	170.2101	
			Heteroatoms
			Halogen atoms
			0.0000
			rotatable bonds
			4.0000
			H-bond acceptors
			3.0000
			H-bond donors
			0.0000
			LogP
			1.7327
Melting_Point		LIST	FRA021
			Oil
comments			
ethyl 1-acetylcyclobutane-1-carboxylate			



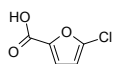
GG-0718	$C_{13}H_{24}N_2O_2$	240.3484	
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			Halogen atoms
			0.0000
			rotatable bonds
			2.0000
			H-bond acceptors
			3.0000
			H-bond donors
			1.0000
			LogP
			0.9396
Melting_Point		LIST	FRA021
			Oil
comments			
tert-butyl 2,6-diazaspiro[4.5]decane-2-carboxylate			



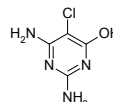
HG-0005	$C_{10}H_{12}N_2S$	192.2845	
			Heteroatoms
			Halogen atoms
			0.0000
			rotatable bonds
			2.0000
			H-bond acceptors
			1.0000
			H-bond donors
			1.0000
			LogP
			2.8248
Melting_Point		LIST	356
comments			
6-propyl-1,3-benzothiazol-2-amine			



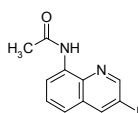
HG-0015	$C_6H_3ClO_3$	146.5309	
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			Halogen atoms
			1.0000
			rotatable bonds
			1.0000
			H-bond acceptors
			3.0000
			H-bond donors
			1.0000
			LogP
			0.8262
Melting_Point		LIST	
comments			
5-chlorofuran-2-carboxylic acid			



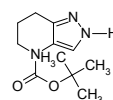
HG-0204	$C_4H_5ClN_4O$	160.5637	
			Heteroatoms
			6.0000
			Halogen atoms
			1.0000
			rotatable bonds
			0.0000
			H-bond acceptors
			3.0000
			H-bond donors
			3.0000
			LogP
			0.6581
Melting_Point	316 - 318	LIST	
comments			
2,6-diamino-5-chloropyrimidin-4-ol			

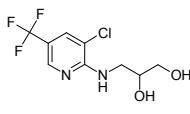


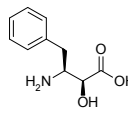
HG-0213	$C_{11}H_9IN_2O$	312.1116	
			Heteroatoms
			Halogen atoms
			1.0000
			rotatable bonds
			1.0000
			H-bond acceptors
			2.0000
			H-bond donors
			1.0000
			LogP
			2.2423
Melting_Point	127 - 135	LIST	FRA021
comments			
N-(3-iodoquinolin-8-yl)acetamide			

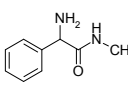


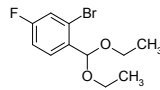
LF-0076	$C_{11}H_{17}N_3O_2$	223.2770	
			Heteroatoms
			Halogen atoms
			0.0000
			rotatable bonds
			2.0000
			H-bond acceptors
			3.0000
			H-bond donors
			1.0000
			LogP
			1.5610
Melting_Point	101 - 103	LIST	FRA021
comments			
tert-butyl 2H,4H,5H,6H,7H-pyrazolo[4,3-b]pyridine-4-carboxylate			

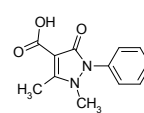


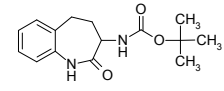
MF-0049	C ₉ H ₁₀ ClF ₃ N ₂ O ₂	270.6404	
			Heteroatoms
			8.0000
			Halogen atoms
			4.0000
			rotatable bonds
			4.0000
			H-bond acceptors
3.0000			
H-bond donors			
3.0000			
LogP	1.9140		
Melting_Point	LIST	oil	comments
3-[[3-chloro-5-(trifluoromethyl)pyridin-2-yl]amino]propane-1,2-diol			

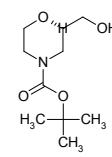
SS-3011	C ₁₀ H ₁₃ NO ₃	195.2200	
			Heteroatoms
			4.0000
			Halogen atoms
			0.0000
			rotatable bonds
			4.0000
			H-bond acceptors
4.0000			
H-bond donors			
3.0000			
LogP	0.7798		
Melting_Point	LIST	FRA021	comments
(2S,3S)-3-amino-2-hydroxy-4-phenylbutanoic acid			

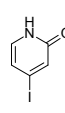
SS-3472	C ₉ H ₁₂ N ₂ O	164.2088	
			Heteroatoms
			0.0000
			Halogen atoms
			0.0000
			rotatable bonds
			2.0000
			H-bond acceptors
2.0000			
H-bond donors			
2.0000			
LogP	0.2823		
Melting_Point	LIST	Oil	FRA021
2-amino-N-methyl-2-phenylacetamide			

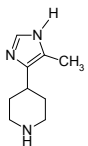
SS-3534	C ₁₁ H ₁₄ BrFO ₂	277.1354	
			Heteroatoms
			4.0000
			Halogen atoms
			2.0000
			rotatable bonds
			5.0000
			H-bond acceptors
2.0000			
H-bond donors			
0.0000			
LogP	3.5787		
Melting_Point	LIST	Oil	comments
2-bromo-1-(diethoxymethyl)-4-fluorobenzene			

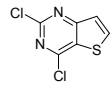
SS-3597	C ₁₂ H ₁₂ N ₂ O ₃	232.2410	
			Heteroatoms
			0.0000
			Halogen atoms
			0.0000
			rotatable bonds
			2.0000
			H-bond acceptors
3.0000			
H-bond donors			
1.0000			
LogP			
Melting_Point	LIST	FRA021	comments
1,5-dimethyl-3-oxo-2-phenyl-2,3-dihydro-1H-pyrazole-4-carboxylic acid			

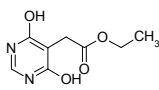
SS-3682	C ₁₅ H ₂₀ N ₂ O ₃	276.3383	
			Heteroatoms
			5.0000
			Halogen atoms
			0.0000
			rotatable bonds
			3.0000
			H-bond acceptors
3.0000			
H-bond donors			
2.0000			
LogP	1.8511		
Melting_Point	LIST		comments
tert-butyl N-(2-oxo-2,3,4,5-tetrahydro-1H-1-benzazepin-3-yl)carbamate			

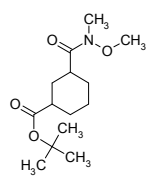
SS-4340	C ₁₀ H ₁₉ NO ₄	217.2672	
			Heteroatoms
			0.0000
			Halogen atoms
			0.0000
			rotatable bonds
			3.0000
			H-bond acceptors
4.0000			
H-bond donors			
1.0000			
LogP	0.2043		
Melting_Point	LIST	FRA021	comments
tert-butyl (2S)-2-(hydroxymethyl)morpholine-4-carboxylate			

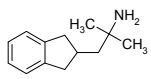
SS-4341	C ₅ H ₄ INO	220.9981	
			Heteroatoms
			1.0000
			Halogen atoms
			1.0000
			rotatable bonds
			0.0000
			H-bond acceptors
1.0000			
H-bond donors			
1.0000			
LogP	0.4813		
Melting_Point	LIST	FRA021	comments
4-iodo-1,2-dihydropyridin-2-one			

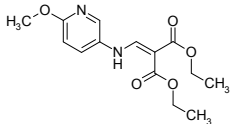
SS-4342	$C_9H_{17}Cl_2N_3$	238.1619	
			Heteroatoms
			Halogen atoms
			rotatable bonds
			H-bond acceptors
			H-bond donors
			LogP
			Melting_Point
4-(5-methyl-1H-imidazol-4-yl)piperidine dihydrochloride			

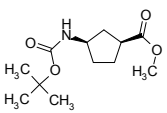
SS-4343	$C_6H_2Cl_2N_2S$	205.0662	
			Heteroatoms
			Halogen atoms
			rotatable bonds
			H-bond acceptors
			H-bond donors
			LogP
			Melting_Point
2,4-dichlorothieno[3,2-d]pyrimidine			

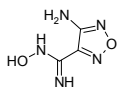
SS-4344	$C_8H_{10}N_2O_4$	198.1799	
			Heteroatoms
			Halogen atoms
			rotatable bonds
			H-bond acceptors
			H-bond donors
			LogP
			Melting_Point
ethyl 2-(4,6-dihydroxypyrimidin-5-yl)acetate			

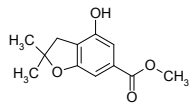
SS-4345	$C_{14}H_{25}NO_4$	271.3596	
			Heteroatoms
			Halogen atoms
			rotatable bonds
			H-bond acceptors
			H-bond donors
			LogP
			Melting_Point
tert-butyl 3-[methoxy(methyl)carbamoyl]cyclohexane-1-carboxylate			

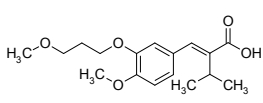
SS-4347	$C_{13}H_{20}ClN$	225.7641	
			Heteroatoms
			Halogen atoms
			rotatable bonds
			H-bond acceptors
			H-bond donors
			LogP
			Melting_Point
1-(2,3-dihydro-1H-inden-2-yl)-2-methylpropan-2-amine hydrochloride			

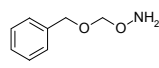
SS-4359	$C_{14}H_{18}N_2O_5$	294.3100	
			Heteroatoms
			Halogen atoms
			rotatable bonds
			H-bond acceptors
			H-bond donors
			LogP
			Melting_Point
Diethyl 2-[[6-methoxypyridin-3-yl]amino]methylene]malonate			

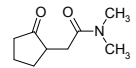
SS-4386	$C_{12}H_{21}NO_4$	243.3055	
			Heteroatoms
			Halogen atoms
			rotatable bonds
			H-bond acceptors
			H-bond donors
			LogP
			Melting_Point
(1S,3R)-methyl 3-[(tert-butoxycarbonyl)amino]cyclopentanecarboxylate			

SS-4387	$C_3H_5N_5O_2$	143.1056	
			Heteroatoms
			Halogen atoms
			rotatable bonds
			H-bond acceptors
			H-bond donors
			LogP
			Melting_Point
4-amino-N-hydroxy-1,2,5-oxadiazole-3-carboximidamide			

SS-4388	C ₁₂ H ₁₄ O ₄	222.2430	
			Heteroatoms
			Halogen atoms
			rotatable bonds
			H-bond acceptors
			H-bond donors
			LogP
			Melting_Point
methyl 4-hydroxy-2,2-dimethyl-2,3-dihydro-1-benzofuran-6-carboxylate			

SS-4390	C ₁₇ H ₂₄ O ₅	308.3778	
			Heteroatoms
			Halogen atoms
			rotatable bonds
			H-bond acceptors
			H-bond donors
			LogP
			Melting_Point
(2E)-2-[[4-methoxy-3-(3-methoxypropoxy)phenyl]methylidene]-3-methylbutanoic acid			

SS-4393	C ₈ H ₁₁ NO ₂	153.1824	
			Heteroatoms
			Halogen atoms
			rotatable bonds
			H-bond acceptors
			H-bond donors
			LogP
			Melting_Point
O-[(benzyloxy)methyl]hydroxylamine			

SS-4395	C ₉ H ₁₅ NO ₂	169.2254	
			Heteroatoms
			Halogen atoms
			rotatable bonds
			H-bond acceptors
			H-bond donors
			LogP
			Melting_Point
N,N-dimethyl-2-(2-oxocyclopentyl)acetamide			