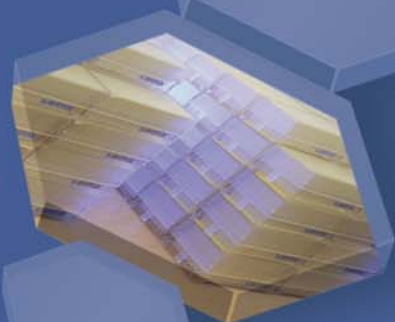


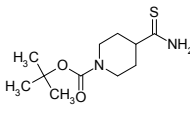


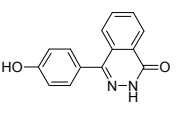
BIONET compounds –
A Key step ahead of the rest

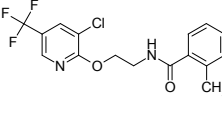



@ohember 2012
Combined Screening and
Fragments
Collection Update

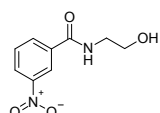
 **Key Organics**
The right side of the Equation

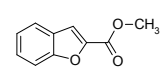
10N-311S	C ₁₁ H ₂₀ N ₂ O ₂ S	244.3583
		Heteroatoms
		Halogen atoms
		rotatable bonds
		H-bond acceptors
		H-bond donors
		LogP
		Melting_Point
comments		
tert-butyl 4-carbamothioylpiperidine-1-carboxylate		

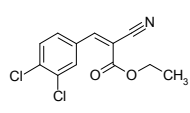
10Z-0807	C ₁₄ H ₁₀ N ₂ O ₂	238.2480
		Heteroatoms
		Halogen atoms
		rotatable bonds
		H-bond acceptors
		H-bond donors
		LogP
		Melting_Point
comments		
4-(4-hydroxyphenyl)-1,2-dihydrophthalazin-1-one		

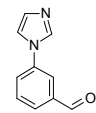
12Z-5006	C ₁₆ H ₁₄ ClF ₃ N ₂ O ₂	358.7504
		Heteroatoms
		Halogen atoms
		rotatable bonds
		H-bond acceptors
		H-bond donors
		LogP
		Melting_Point
comments		
N-(2-[[3-chloro-5-(trifluoromethyl)pyridin-2-yl]oxy]ethyl)-2-methylbenzamide		

5B-009	C ₈ H ₉ NS	151.2316
		Heteroatoms
		Halogen atoms
		rotatable bonds
		H-bond acceptors
		H-bond donors
		LogP
		Melting_Point
comments		
3,4-dihydro-2H-1,4-benzothiazine		

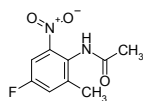
6X-5074	C ₉ H ₁₀ N ₂ O ₄	210.1911
		Heteroatoms
		Halogen atoms
		rotatable bonds
		H-bond acceptors
		H-bond donors
		LogP
		Melting_Point
comments		
N-(2-hydroxyethyl)-3-nitrobenzamide		

8R-0046	C ₁₀ H ₈ O ₃	176.1735
		Heteroatoms
		Halogen atoms
		rotatable bonds
		H-bond acceptors
		H-bond donors
		LogP
		Melting_Point
comments		
methyl 1-benzofuran-2-carboxylate		

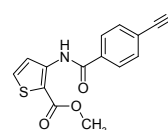
9N-915	C ₁₂ H ₉ Cl ₂ NO ₂	270.1170
		Heteroatoms
		Halogen atoms
		rotatable bonds
		H-bond acceptors
		H-bond donors
		LogP
		Melting_Point
comments		
ethyl (Z)-2-cyano-3-(3,4-dichlorophenyl)prop-2-enoate		

9P-759	C ₁₀ H ₈ N ₂ O	172.1881
		Heteroatoms
		Halogen atoms
		rotatable bonds
		H-bond acceptors
		H-bond donors
		LogP
		Melting_Point
comments		
3-(1H-imidazol-1-yl)benzaldehyde		

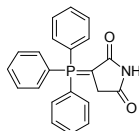
AB-0824	C ₉ H ₉ FN ₂ O ₃	212.1821	
			Heteroatoms 6.0000
			Halogen atoms 1.0000
			rotatable bonds 1.0000
			H-bond acceptors 3.0000
			H-bond donors 1.0000
			LogP 1.4558
Melting_Point	170 - 172	LIST	comments
N-(4-fluoro-2-methyl-6-nitrophenyl)acetamide			



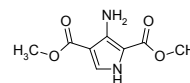
CF-0049	C ₁₄ H ₁₀ N ₂ O ₃ S	286.3114	
			Heteroatoms 6.0000
			Halogen atoms 0.0000
			rotatable bonds 4.0000
			H-bond acceptors 4.0000
			H-bond donors 1.0000
			LogP 1.6952
Melting_Point		LIST	356 comments
methyl 3-[(4-cyanobenzene)amido]thiophene-2-carboxylate			



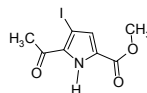
EG-0103	C ₂₂ H ₁₈ N ₂ O ₂ P	359.3681	
			Heteroatoms 4.0000
			Halogen atoms 0.0000
			rotatable bonds 4.0000
			H-bond acceptors 2.0000
			H-bond donors 1.0000
			LogP
Melting_Point		LIST	comments
3-(triphenyl-sil[5]-phosphanylidene)pyrrolidine-2,5-dione			



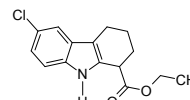
FG-0711	C ₈ H ₁₀ N ₂ O ₄	198.1799	
			Heteroatoms 6.0000
			Halogen atoms 0.0000
			rotatable bonds 4.0000
			H-bond acceptors 4.0000
			H-bond donors 2.0000
			LogP -0.5054
Melting_Point	165 - 166	LIST	comments
2,4-dimethyl 3-amino-1H-pyrrole-2,4-dicarboxylate			



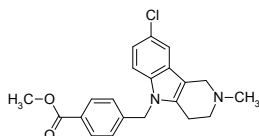
FG-0718	C ₈ H ₈ INO ₃	293.0623	
			Heteroatoms
			Halogen atoms 1.0000
			rotatable bonds 3.0000
			H-bond acceptors 3.0000
			H-bond donors 1.0000
			LogP 0.8778
Melting_Point	121 - 122	LIST	FRA021 comments
methyl 5-acetyl-4-iodo-1H-pyrrole-2-carboxylate			



GA-0859	C ₁₅ H ₁₆ ClNO ₂	277.7533	
			Heteroatoms
			Halogen atoms 1.0000
			rotatable bonds 3.0000
			H-bond acceptors 2.0000
			H-bond donors 1.0000
			LogP 3.0290
Melting_Point		LIST	356 comments
ethyl 6-chloro-2,3,4,9-tetrahydro-1H-carbazole-1-carboxylate			




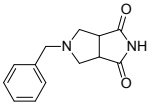
GG-0209	C ₂₁ H ₂₁ ClN ₂ O ₂	368.8667	
			Heteroatoms 5.0000
			Halogen atoms 1.0000
			rotatable bonds 4.0000
			H-bond acceptors 3.0000
			H-bond donors 0.0000
			LogP 3.5242
Melting_Point	132 - 133	LIST	comments
methyl 4-({8-chloro-2-methyl-1H,2H,3H,4H,5H-pyrido[4,3-b]indol-5-yl)methyl}benzoate			

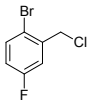


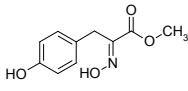
GG-0221	C ₉ H ₇ IN ₂	270.0739	
			Heteroatoms
			Halogen atoms 1.0000
			rotatable bonds 0.0000
			H-bond acceptors 1.0000
			H-bond donors 1.0000
			LogP 2.6102
Melting_Point	121 - 125	LIST	FRA021 comments
3-iodoquinolin-8-amine			

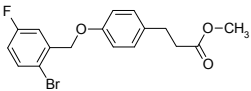


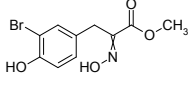
GG-0702	C ₆ H ₈ O ₃	128.1289		
			Heteroatoms	
			Halogen atoms	
			rotatable bonds	
			H-bond acceptors	
			H-bond donors	
			LogP	
			Melting_Point	Oil
1-acetylcyclopropane-1-carboxylic acid				

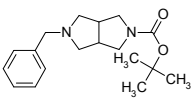
HG-0008	C ₁₃ H ₁₄ N ₂ O ₂	230.2687		
			Heteroatoms	
			Halogen atoms	
			rotatable bonds	
			H-bond acceptors	
			H-bond donors	
			LogP	
			Melting_Point	135 - 137
5-benzyl-octahydropyrrolo[3,4-c]pyrrole-1,3-dione				

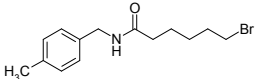
HG-0023	C ₇ H ₆ BrClF	223.4733		
			Heteroatoms	
			Halogen atoms	
			rotatable bonds	
			H-bond acceptors	
			H-bond donors	
			LogP	
			Melting_Point	Oil not distilled
1-bromo-2-(chloromethyl)-4-fluorobenzene				

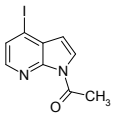
HG-0044	C ₁₀ H ₁₁ NO ₄	209.2035		
			Heteroatoms	
			Halogen atoms	
			rotatable bonds	
			H-bond acceptors	
			H-bond donors	
			LogP	
			Melting_Point	131 - 132
methyl (2E)-2-(N-hydroxyimino)-3-(4-hydroxyphenyl)propanoate				

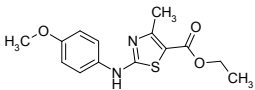
HG-0047	C ₁₇ H ₁₆ BrFO ₃	367.2177		
			Heteroatoms	
			Halogen atoms	
			rotatable bonds	
			H-bond acceptors	
			H-bond donors	
			LogP	
			Melting_Point	Oil
methyl 3-(4-[(2-bromo-5-fluorophenyl)methoxy]phenyl)propanoate				

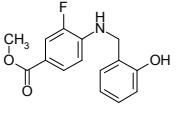
HG-0050	C ₁₀ H ₁₀ BrNO ₄	288.0995		
			Heteroatoms	
			Halogen atoms	
			rotatable bonds	
			H-bond acceptors	
			H-bond donors	
			LogP	
			Melting_Point	157 - 159
methyl 3-(3-bromo-4-hydroxyphenyl)-2-(hydroxyimino)-propanoate				

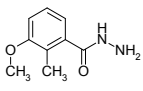
HG-0052	C ₁₈ H ₂₆ N ₂ O ₂	302.4201		
			Heteroatoms	
			Halogen atoms	
			rotatable bonds	
			H-bond acceptors	
			H-bond donors	
			LogP	
			Melting_Point	Oil
tert-butyl 5-benzyl-octahydropyrrolo[3,4-c]pyrrole-2-carboxylate				

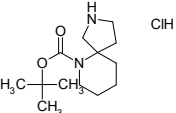
HG-0216	C ₁₄ H ₂₀ BrNO	298.2256		
			Heteroatoms	
			Halogen atoms	
			rotatable bonds	
			H-bond acceptors	
			H-bond donors	
			LogP	
			Melting_Point	84 - 86
6-bromo-N-[(4-methylphenyl)methyl]hexanamide				

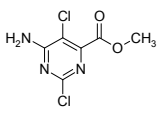
HG-0221	C ₉ H ₇ IN ₂ O	286.0733				
			Heteroatoms			
			Halogen atoms			
			rotatable bonds			
			H-bond acceptors			
			H-bond donors			
			LogP			
			Melting_Point	138 - 139	LIST	FRA021
			comments			4-iodo-1-acetyl-7-azaindole

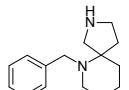
HG-0703	C ₁₄ H ₁₆ N ₂ O ₃ S	292.3592				
			Heteroatoms			
			Halogen atoms			
			rotatable bonds			
			H-bond acceptors			
			H-bond donors			
			LogP			
			Melting_Point	173 - 175 (dec.)	LIST	
			comments			ethyl 2-[(4-methoxyphenyl)amino]-4-methyl-1,3-thiazole-5-carboxylate


HG-0704	C ₁₅ H ₁₄ FN ₂ O ₃	275.2821				
			Heteroatoms			
			Halogen atoms			
			rotatable bonds			
			H-bond acceptors			
			H-bond donors			
			LogP			
			Melting_Point	130 - 131	LIST	
			comments			methyl 3-fluoro-4-[[[(2-hydroxyphenyl)methyl]amino]benzoate

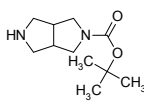
HG-0706	C ₉ H ₁₂ N ₂ O ₂	180.2082				
			Heteroatoms			
			Halogen atoms			
			rotatable bonds			
			H-bond acceptors			
			H-bond donors			
			LogP			
			Melting_Point	114 - 117	LIST	FRA021
			comments			3-methoxy-2-methylbenzohydrazide

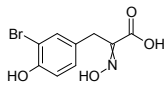
HG-0707	C ₁₃ H ₂₅ ClN ₂ O ₂	276.8094				
			Heteroatoms			
			Halogen atoms			
			rotatable bonds			
			H-bond acceptors			
			H-bond donors			
			LogP			
			Melting_Point	113 - 115	LIST	FRA021
			comments			tert-butyl 2,6-diazaspiro[4.5]decane-6-carboxylate hydrochloride

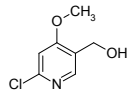
HG-0708	C ₆ H ₅ Cl ₂ N ₃ O ₂	222.0317				
			Heteroatoms			
			Halogen atoms			
			rotatable bonds			
			H-bond acceptors			
			H-bond donors			
			LogP			
			Melting_Point	168 - 170	LIST	FRA021
			comments			methyl 6-amino-2,5-dichloropyrimidine-4-carboxylate

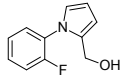
HG-0710	C ₁₅ H ₂₂ N ₂	230.3560				
			Heteroatoms			
			Halogen atoms			
			rotatable bonds			
			H-bond acceptors			
			H-bond donors			
			LogP			
			Melting_Point	Viscous oil	LIST	FRA021
			comments			6-benzyl-2,6-diazaspiro[4.5]decane

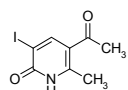
KG-0002	C ₁₀ H ₈ O ₂	160.1741				
			Heteroatoms			
			Halogen atoms			
			rotatable bonds			
			H-bond acceptors			
			H-bond donors			
			LogP			
			Melting_Point	158 - 160	LIST	FRA021
			comments			1H-indene-3-carboxylic acid

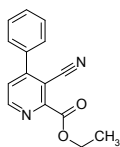
KG-0017	$C_{11}H_{20}N_2O_2$	212.2943	
			Heteroatoms
			Halogen atoms
			rotatable bonds
			H-bond acceptors
			H-bond donors
			LogP
			Melting_Point
tert-butyl octahydroindolizino[1,2-a]pyrrole-2-carboxylate			

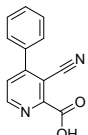
KG-0028	$C_9H_8BrNO_4$	274.0724	
			Heteroatoms
			Halogen atoms
			rotatable bonds
			H-bond acceptors
			H-bond donors
			LogP
			Melting_Point
3-(3-bromo-4-hydroxyphenyl)-2-(hydroxyimino)propanoic acid			


KG-0700	$C_7H_8ClNO_2$	173.6003	
			Heteroatoms
			Halogen atoms
			rotatable bonds
			H-bond acceptors
			H-bond donors
			LogP
			Melting_Point
(6-chloro-4-methoxypyridin-3-yl)methanol			

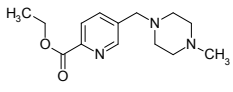
KG-0701	$C_{11}H_{10}FNO$	191.2069	
			Heteroatoms
			Halogen atoms
			rotatable bonds
			H-bond acceptors
			H-bond donors
			LogP
			Melting_Point
[1-(2-fluorophenyl)-1H-pyrrol-2-yl]methanol			

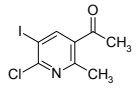
KG-0703	$C_8H_8INO_2$	277.0629	
			Heteroatoms
			Halogen atoms
			rotatable bonds
			H-bond acceptors
			H-bond donors
			LogP
			Melting_Point
5-acetyl-3-iodo-6-methyl-1,2-dihydropyridin-2-one			

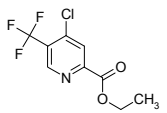
KG-0709	$C_{15}H_{12}N_2O_2$	252.2751	
			Heteroatoms
			Halogen atoms
			rotatable bonds
			H-bond acceptors
			H-bond donors
			LogP
			Melting_Point
ethyl 3-cyano-4-phenylpyridine-2-carboxylate			

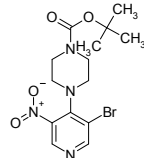
KG-0710	$C_{13}H_8N_2O_2$	224.2209	
			Heteroatoms
			Halogen atoms
			rotatable bonds
			H-bond acceptors
			H-bond donors
			LogP
			Melting_Point
3-cyano-4-phenylpyridine-2-carboxylic acid			

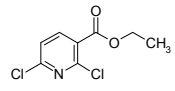
KG-0711	$C_7H_6ClNO_2$	171.5844	
			Heteroatoms
			Halogen atoms
			rotatable bonds
			H-bond acceptors
			H-bond donors
			LogP
			Melting_Point
6-chloro-4-methoxypyridine-3-carbaldehyde			

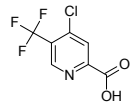
KG-0712	C ₁₄ H ₂₁ N ₃ O ₂	263.3424	
		Heteroatoms	5.0000
		Halogen atoms	0.0000
		rotatable bonds	5.0000
		H-bond acceptors	5.0000
		H-bond donors	0.0000
		LogP	0.8946
		Melting_Point	62 - 64
ethyl 5-[(4-methylpiperazin-1-yl)methyl]pyridine-2-carboxylate			

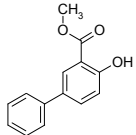
KG-0713	C ₈ H ₇ ClINO	295.5085	
		Heteroatoms	
		Halogen atoms	2.0000
		rotatable bonds	1.0000
		H-bond acceptors	2.0000
		H-bond donors	0.0000
		LogP	2.8387
Melting_Point	64 - 66	LIST	FRA021
1-(6-chloro-5-iodo-2-methylpyridin-3-yl)ethan-1-one			

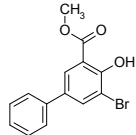
KG-0715	C ₉ H ₇ ClF ₃ NO ₂	253.6098	
		Heteroatoms	
		Halogen atoms	4.0000
		rotatable bonds	3.0000
		H-bond acceptors	3.0000
		H-bond donors	0.0000
		LogP	3.0721
		Melting_Point	47 - 49
ethyl 4-chloro-5-(trifluoromethyl)pyridine-2-carboxylate			

KG-0716	C ₁₄ H ₁₉ BrN ₄ O ₄	387.2359	
		Heteroatoms	9.0000
		Halogen atoms	1.0000
		rotatable bonds	3.0000
		H-bond acceptors	5.0000
		H-bond donors	0.0000
		LogP	2.3008
		Melting_Point	106 - 107
tert-butyl 4-(3-bromo-5-nitropyridin-4-yl)piperazine-1-carboxylate			

KG-0717	C ₈ H ₇ Cl ₂ NO ₂	220.0565	
		Heteroatoms	
		Halogen atoms	2.0000
		rotatable bonds	3.0000
		H-bond acceptors	3.0000
		H-bond donors	0.0000
		LogP	2.5847
		Melting_Point	50 - 51
ethyl 2,6-dichloropyridine-3-carboxylate			

KG-0719	C ₇ H ₃ ClF ₃ NO ₂	225.5557	
		Heteroatoms	
		Halogen atoms	4.0000
		rotatable bonds	1.0000
		H-bond acceptors	3.0000
		H-bond donors	1.0000
		LogP	2.6979
		Melting_Point	150
4-chloro-5-(trifluoromethyl)pyridine-2-carboxylic acid			

LG-0016	C ₁₄ H ₁₂ O ₃	228.2499	
		Heteroatoms	
		Halogen atoms	0.0000
		rotatable bonds	3.0000
		H-bond acceptors	3.0000
		H-bond donors	1.0000
		LogP	3.1767
		Melting_Point	
methyl 2-hydroxy-5-phenylbenzoate			

LG-0018	C ₁₄ H ₁₁ BrO ₃	307.1460	
		Heteroatoms	4.0000
		Halogen atoms	1.0000
		rotatable bonds	3.0000
		H-bond acceptors	3.0000
		H-bond donors	1.0000
		LogP	3.9685
		Melting_Point	
methyl 3-bromo-2-hydroxy-5-phenylbenzoate			

LG-0700	C ₉ H ₇ IN ₂ O	286.0733	
			Heteroatoms
			Halogen atoms
			1.0000
			rotatable bonds
			0.0000
			H-bond acceptors
			2.0000
			H-bond donors
			1.0000
			LogP
			1.6134
Melting_Point	260 - 263	LIST FRA021	comments
3-iodo-5-methyl-1,2-dihydro-1,6-naphthyridin-2-one			

LG-0705	C ₉ H ₉ BrO ₃	245.0743	
			Heteroatoms
			Halogen atoms
			1.0000
			rotatable bonds
			3.0000
			H-bond acceptors
			3.0000
			H-bond donors
			1.0000
			LogP
			2.6266
Melting_Point	48 - 50	LIST FRA021	comments
ethyl 5-bromo-2-hydroxybenzoate			

LG-0706	C ₁₀ H ₇ ClO ₃	210.6185	
			Heteroatoms
			Halogen atoms
			1.0000
			rotatable bonds
			2.0000
			H-bond acceptors
			3.0000
			H-bond donors
			0.0000
			LogP
			2.0095
Melting_Point	90 - 92	LIST FRA021	comments
methyl 4-chloro-1-benzofuran-2-carboxylate			

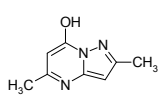
LG-0709	C ₇ H ₈ N ₄ O	164.1680	
			Heteroatoms
			Halogen atoms
			0.0000
			rotatable bonds
			1.0000
			H-bond acceptors
			4.0000
			H-bond donors
			1.0000
			LogP
			0.7708
Melting_Point	240 - 242	LIST FRA021	comments
4-amino-2-methoxy-6-methylpyrimidine-5-carbonitrile			

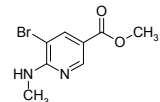
LG-0710	C ₉ H ₁₁ FN ₂ O	182.1992	
			Heteroatoms
			Halogen atoms
			1.0000
			rotatable bonds
			1.0000
			H-bond acceptors
			1.0000
			H-bond donors
			2.0000
			LogP
			0.7190
Melting_Point	144 - 145	LIST FRA021	comments
N-(2-amino-4-fluoro-6-methylphenyl)acetamide			

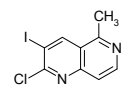
LG-0711	C ₉ H ₁₀ INO ₂	291.0899	
			Heteroatoms
			Halogen atoms
			1.0000
			rotatable bonds
			2.0000
			H-bond acceptors
			3.0000
			H-bond donors
			0.0000
			LogP
			2.3959
Melting_Point	111 - 112	LIST FRA021	comments
1-(5-iodo-6-methoxy-2-methylpyridin-3-yl)ethan-1-one			

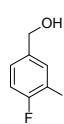
LG-0713	C ₁₂ H ₁₇ N ₃ O	219.2888	
			Heteroatoms
			Halogen atoms
			0.0000
			rotatable bonds
			0.0000
			H-bond acceptors
			2.0000
			H-bond donors
			2.0000
			LogP
			1.5797
Melting_Point	303 - 305	LIST FRA021	comments
7-methyl-2',3',4',6'-tetrahydrospiro[cyclohexane-1,1'-pyrazolo[3,4-b]pyridine]-3'-one			

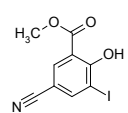
LG-0714	C ₉ H ₁₅ N ₃ O ₂	197.2388	
			Heteroatoms
			Halogen atoms
			0.0000
			rotatable bonds
			2.0000
			H-bond acceptors
			3.0000
			H-bond donors
			1.0000
			LogP
			1.6401
Melting_Point	137 - 139	LIST FRA021	comments
tert-butyl 5-amino-3-methyl-1H-pyrazole-1-carboxylate			

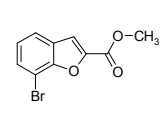
LG-0715	$C_8H_9N_3O$	163.1804	
			Heteroatoms
			Halogen atoms
			rotatable bonds
			H-bond acceptors
			H-bond donors
			LogP
			Melting_Point
2,5-dimethylpyrazolo[1,5-a]pyrimidin-7-ol			

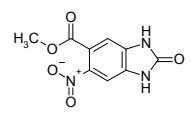
LG-0717	$C_8H_9BrN_2O_2$	245.0771	
			Heteroatoms
			Halogen atoms
			rotatable bonds
			H-bond acceptors
			H-bond donors
			LogP
			Melting_Point
methyl 5-bromo-6-(methylamino)pyridine-3-carboxylate			

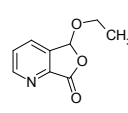
LG-0719	$C_9H_6ClIN_2$	304.5190	
			Heteroatoms
			Halogen atoms
			rotatable bonds
			H-bond acceptors
			H-bond donors
			LogP
			Melting_Point
2-chloro-3-iodo-5-methyl-1,6-naphthyridine			

LG-0720	C_7H_6FIO	252.0281	
			Heteroatoms
			Halogen atoms
			rotatable bonds
			H-bond acceptors
			H-bond donors
			LogP
			Melting_Point
(4-fluoro-3-iodophenyl)methanol			

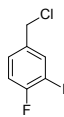
LG-0722	$C_9H_6INO_3$	303.0575	
			Heteroatoms
			Halogen atoms
			rotatable bonds
			H-bond acceptors
			H-bond donors
			LogP
			Melting_Point
methyl 5-cyano-2-hydroxy-3-iodobenzoate			

LG-0723	$C_{10}H_7BrO_3$	255.0695	
			Heteroatoms
			Halogen atoms
			rotatable bonds
			H-bond acceptors
			H-bond donors
			LogP
			Melting_Point
methyl 7-bromo-1-benzofuran-2-carboxylate			

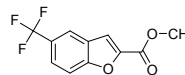
LG-0724	$C_9H_7N_3O_5$	237.1732	
			Heteroatoms
			Halogen atoms
			rotatable bonds
			H-bond acceptors
			H-bond donors
			LogP
			Melting_Point
methyl 6-nitro-2-oxo-2,3-dihydro-1H-1,3-benzodiazole-5-carboxylate			

LG-0727	$C_9H_9NO_3$	179.1770	
			Heteroatoms
			Halogen atoms
			rotatable bonds
			H-bond acceptors
			H-bond donors
			LogP
			Melting_Point
ethyl 3-formylpyridine-2-carboxylate			

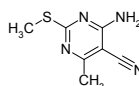
LG-0730	C ₇ H ₅ ClFI	270.4737	
			Heteroatoms
			Halogen atoms
			3.0000
			rotatable bonds
			1.0000
			H-bond acceptors
			0.0000
			H-bond donors
			0.0000
			LogP
			4.0549
Melting_Point	Oil	LIST FRA021	comments
4-(chloromethyl)-1-fluoro-2-iodobenzene			



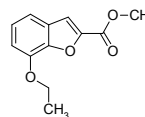
LG-0731	C ₁₁ H ₇ F ₃ O ₃	244.1718	
			Heteroatoms
			Halogen atoms
			3.0000
			rotatable bonds
			2.0000
			H-bond acceptors
			3.0000
			H-bond donors
			0.0000
			LogP
			2.3743
Melting_Point	97 - 100	LIST FRA021	comments
methyl 5-(trifluoromethyl)-1-benzofuran-2-carboxylate			



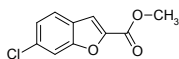
LG-0732	C ₇ H ₈ N ₄ S	180.2326	
			Heteroatoms
			Halogen atoms
			0.0000
			rotatable bonds
			1.0000
			H-bond acceptors
			3.0000
			H-bond donors
			1.0000
			LogP
			1.1141
Melting_Point	237 - 239	LIST FRA021	comments
4-amino-6-methyl-2-(methylsulfanyl)pyrimidine-5-carbonitrile			



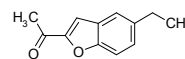
LG-0738	C ₁₂ H ₁₂ O ₄	220.2270	
			Heteroatoms
			Halogen atoms
			0.0000
			rotatable bonds
			4.0000
			H-bond acceptors
			4.0000
			H-bond donors
			0.0000
			LogP
			1.5813
Melting_Point	99 - 101	LIST FRA021	comments
methyl 7-ethoxy-1-benzofuran-2-carboxylate			



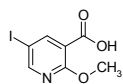
LG-0740	C ₁₀ H ₇ ClO ₃	210.6185	
			Heteroatoms
			Halogen atoms
			1.0000
			rotatable bonds
			2.0000
			H-bond acceptors
			3.0000
			H-bond donors
			0.0000
			LogP
			2.0095
Melting_Point	97 - 99	LIST FRA021	comments
methyl 6-chloro-1-benzofuran-2-carboxylate			



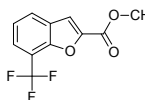
LG-0743	C ₁₂ H ₁₂ O ₂	188.2282	
			Heteroatoms
			Halogen atoms
			0.0000
			rotatable bonds
			2.0000
			H-bond acceptors
			2.0000
			H-bond donors
			0.0000
			LogP
			1.9334
Melting_Point	Oil	LIST FRA021	comments
1-(5-ethyl-1-benzofuran-2-yl)ethan-1-one			

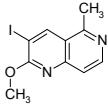


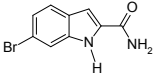
LG-0744	C ₇ H ₆ INO ₃	279.0352	
			Heteroatoms
			Halogen atoms
			1.0000
			rotatable bonds
			2.0000
			H-bond acceptors
			4.0000
			H-bond donors
			1.0000
			LogP
			2.6013
Melting_Point	194 - 196	LIST FRA021	comments
5-iodo-2-methoxypyridine-3-carboxylic acid			




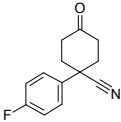
LG-0745	C ₁₁ H ₇ F ₃ O ₃	244.1718	
			Heteroatoms
			Halogen atoms
			3.0000
			rotatable bonds
			2.0000
			H-bond acceptors
			3.0000
			H-bond donors
			0.0000
			LogP
			2.3743
Melting_Point	51 - 53	LIST FRA021	comments
methyl 7-(trifluoromethyl)-1-benzofuran-2-carboxylate			

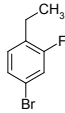


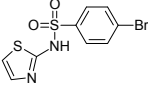
LG-0747	$C_{10}H_9IN_2O$	300.1004	
			Heteroatoms
			Halogen atoms
			rotatable bonds
			H-bond acceptors
			H-bond donors
			LogP
			Melting_Point
3-iodo-2-methoxy-5-methyl-1,6-naphthyridine			

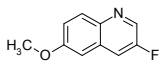
LG-0748	$C_9H_7BrN_2O$	239.0729	
			Heteroatoms
			Halogen atoms
			rotatable bonds
			H-bond acceptors
			H-bond donors
			LogP
			Melting_Point
6-bromo-1H-indole-2-carboxamide			

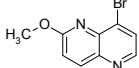
NE-0702	$C_6H_7ClN_4$	158.5913	
			Heteroatoms
			Halogen atoms
			rotatable bonds
			H-bond acceptors
			H-bond donors
			LogP
			Melting_Point
pyrimidine-2-carboximidamide hydrochloride			

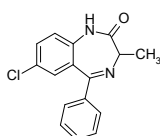
SS-3591	$C_{13}H_{12}FNO$	217.2451	
			Heteroatoms
			Halogen atoms
			rotatable bonds
			H-bond acceptors
			H-bond donors
			LogP
			Melting_Point
1-(4-fluorophenyl)-4-oxocyclohexanecarbonitrile			

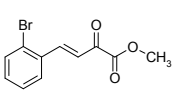
SS-3619	C_8H_8BrF	203.0554	
			Heteroatoms
			Halogen atoms
			rotatable bonds
			H-bond acceptors
			H-bond donors
			LogP
			Melting_Point
4-bromo-1-ethyl-2-fluorobenzene			

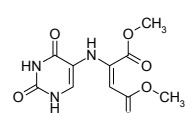
SS-4400	$C_9H_7BrN_2O_2S_2$	319.2003	
			Heteroatoms
			Halogen atoms
			rotatable bonds
			H-bond acceptors
			H-bond donors
			LogP
			Melting_Point
4-bromo-N-(1,3-thiazol-2-yl)benzene-1-sulfonamide			

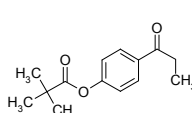
SS-4402	$C_{10}H_8FNO$	177.1798	
			Heteroatoms
			Halogen atoms
			rotatable bonds
			H-bond acceptors
			H-bond donors
			LogP
			Melting_Point
3-fluoro-6-methoxyquinoline			

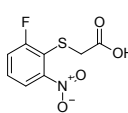
SS-4403	$C_9H_7BrN_2O$	239.0729	
			Heteroatoms
			Halogen atoms
			rotatable bonds
			H-bond acceptors
			H-bond donors
			LogP
			Melting_Point
8-bromo-2-methoxy-1,5-naphthyridine			

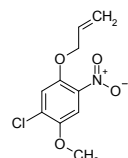
SS-4406	C ₁₆ H ₁₃ ClN ₂ O	284.7478	
			Heteroatoms
			Halogen atoms
			rotatable bonds
			H-bond acceptors
			H-bond donors
			LogP
			Melting_Point
7-chloro-3-methyl-5-phenyl-2,3-dihydro-1H-1,4-benzodiazepin-2-one			

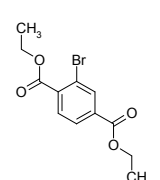
SS-4407	C ₁₁ H ₉ BrO ₃	269.0966	
			Heteroatoms
			Halogen atoms
			rotatable bonds
			H-bond acceptors
			H-bond donors
			LogP
			Melting_Point
methyl (3E)-4-(2-bromophenyl)-2-oxobut-3-enoate			

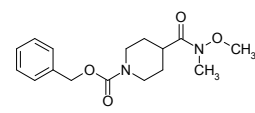
SS-4408	C ₁₀ H ₁₁ N ₃ O ₆	269.2157	
			Heteroatoms
			Halogen atoms
			rotatable bonds
			H-bond acceptors
			H-bond donors
			LogP
			Melting_Point
2,4-dioxo-1,2,3,4-tetrahydro-pyrimidin-5-ylamino-fumaric acid dimethyl ester			

SS-4410	C ₁₄ H ₁₈ O ₃	234.2978	
			Heteroatoms
			Halogen atoms
			rotatable bonds
			H-bond acceptors
			H-bond donors
			LogP
			Melting_Point
4-propanoylphenyl 2,2-dimethylpropanoate			

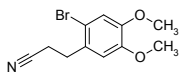
SS-4412	C ₈ H ₆ FNO ₄ S	231.2037	
			Heteroatoms
			Halogen atoms
			rotatable bonds
			H-bond acceptors
			H-bond donors
			LogP
			Melting_Point
2-[(2-fluoro-6-nitrophenyl)sulfanyl]acetic acid			

SS-4413	C ₁₀ H ₁₀ ClNO ₄	243.6485	
			Heteroatoms
			Halogen atoms
			rotatable bonds
			H-bond acceptors
			H-bond donors
			LogP
			Melting_Point
1-chloro-2-methoxy-4-nitro-5-(prop-2-en-1-yloxy)benzene			

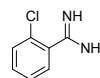
SS-4415	C ₁₂ H ₁₃ BrO ₄	301.1390	
			Heteroatoms
			Halogen atoms
			rotatable bonds
			H-bond acceptors
			H-bond donors
			LogP
			Melting_Point
1,4-diethyl 2-bromobenzene-1,4-dicarboxylate			

SS-4416	C ₁₆ H ₂₂ N ₂ O ₄	306.3647	
			Heteroatoms
			Halogen atoms
			rotatable bonds
			H-bond acceptors
			H-bond donors
			LogP
			Melting_Point
benzyl 4-[methoxy(methyl)carbamoyl]piperidine-1-carboxylate			

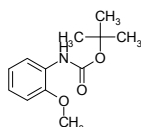
SS-4417	C ₁₁ H ₁₂ BrNO ₂	270.1278	
			Heteroatoms
			Halogen atoms
			1.0000
			rotatable bonds
			4.0000
			H-bond acceptors
			3.0000
			H-bond donors
			0.0000
			LogP
			2.5268
Melting_Point	LIST	FRA021	comments
3-(2-bromo-4,5-dimethoxyphenyl)propanenitrile			



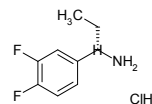
SS-4420	C ₇ H ₇ ClN ₂	154.6002	
			Heteroatoms
			Halogen atoms
			1.0000
			rotatable bonds
			1.0000
			H-bond acceptors
			1.0000
			H-bond donors
			1.0000
			LogP
			1.7412
Melting_Point	78 - 79	LIST	FRA021
2-chlorobenzenecarboximidamide			



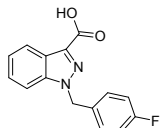
SS-4421	C ₁₂ H ₁₇ NO ₃	223.2742	
			Heteroatoms
			Halogen atoms
			0.0000
			rotatable bonds
			4.0000
			H-bond acceptors
			3.0000
			H-bond donors
			1.0000
			LogP
			2.1019
Melting_Point	Oil	LIST	FRA021
tert-butyl N-(2-methoxyphenyl)carbamate			



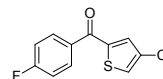
SS-4425	C ₉ H ₁₂ ClF ₂ N	207.6525	
			Heteroatoms
			Halogen atoms
			3.0000
			rotatable bonds
			1.0000
			H-bond acceptors
			1.0000
			H-bond donors
			1.0000
			LogP
			2.6330
Melting_Point		LIST	FRA021
(1S)-1-(3,4-difluorophenyl)propan-1-amine hydrochloride			



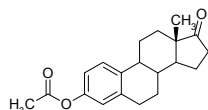
SS-4426	C ₁₅ H ₁₁ FN ₂ O ₂	270.2655	
			Heteroatoms
			Halogen atoms
			1.0000
			rotatable bonds
			3.0000
			H-bond acceptors
			3.0000
			H-bond donors
			1.0000
			LogP
			3.4005
Melting_Point		LIST	FRA021
1-[(4-fluorophenyl)methyl]-1H-indazole-3-carboxylic acid			



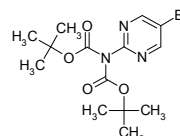
SS-4427	C ₁₁ H ₆ ClFOS	240.6853	
			Heteroatoms
			4.0000
			Halogen atoms
			2.0000
			rotatable bonds
			2.0000
			H-bond acceptors
			1.0000
			H-bond donors
			0.0000
			LogP
			3.2172
Melting_Point		LIST	
(4-chlorothiophen-2-yl)(4-fluorophenyl)methanone			

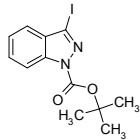


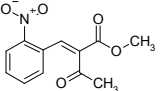
SS-4431	C ₂₀ H ₂₄ O ₃	312.4125	
			Heteroatoms
			3.0000
			Halogen atoms
			0.0000
			rotatable bonds
			2.0000
			H-bond acceptors
			3.0000
			H-bond donors
			0.0000
			LogP
			4.3186
Melting_Point		LIST	
Estrone acetate			

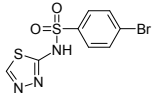


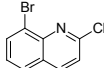
SS-4436	C ₁₄ H ₂₀ BrN ₃ O ₄	374.2372	
			Heteroatoms
			8.0000
			Halogen atoms
			1.0000
			rotatable bonds
			5.0000
			H-bond acceptors
			6.0000
			H-bond donors
			0.0000
			LogP
			3.6156
Melting_Point		LIST	
tert-butyl N-(5-bromopyrimidin-2-yl)-N-[(tert-butoxy)carbonyl]carbamate			

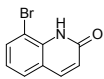


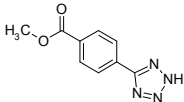
SS-4437	C ₁₂ H ₁₃ N ₂ O ₂	344.1540	
			Heteroatoms
			5.0000
			Halogen atoms
			1.0000
			rotatable bonds
			2.0000
			H-bond acceptors
3.0000			
H-bond donors			
0.0000			
LogP	3.7854		
Melting_Point	LIST	comments	
tert-butyl 3-iodo-1H-indazole-1-carboxylate			

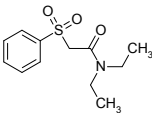
SS-4438	C ₁₂ H ₁₁ NO ₅	249.2252	
			Heteroatoms
			6.0000
			Halogen atoms
			0.0000
			rotatable bonds
			5.0000
			H-bond acceptors
5.0000			
H-bond donors			
0.0000			
LogP	1.2574		
Melting_Point	LIST	comments	
methyl 2-(2-nitrobenzylidene)acetoacetate			

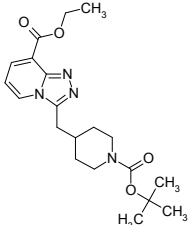
SS-4440	C ₈ H ₆ BrN ₃ O ₂ S ₂	320.1879	
			Heteroatoms
			8.0000
			Halogen atoms
			1.0000
			rotatable bonds
			3.0000
			H-bond acceptors
4.0000			
H-bond donors			
1.0000			
LogP	1.9817		
Melting_Point	LIST	comments	
4-bromo-N-(1,3,4-thiadiazol-2-yl)benzene-1-sulfonamide			

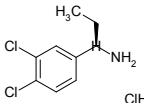
SS-4441	C ₉ H ₅ BrClN	242.5039	
			Heteroatoms
			2.0000
			Halogen atoms
			2.0000
			rotatable bonds
			0.0000
			H-bond acceptors
1.0000			
H-bond donors			
0.0000			
LogP	3.8165		
Melting_Point	LIST	FRA021	comments
8-bromo-2-chloroquinoline			

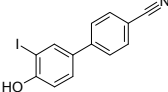
SS-4442	C ₉ H ₆ BrNO	224.0583	
			Heteroatoms
			1.0000
			Halogen atoms
			0.0000
			rotatable bonds
			1.0000
			H-bond acceptors
1.0000			
H-bond donors			
1.0000			
LogP	1.9616		
Melting_Point	LIST	FRA021	comments
8-bromo-1,2-dihydroquinolin-2-one			

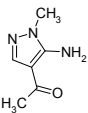
SS-4444	C ₉ H ₈ N ₄ O ₂	204.1897	
			Heteroatoms
			6.0000
			Halogen atoms
			0.0000
			rotatable bonds
			3.0000
			H-bond acceptors
5.0000			
H-bond donors			
1.0000			
LogP	1.5228		
Melting_Point	LIST	comments	
methyl 4-(2H-1,2,3,4-tetrazol-5-yl)benzoate			

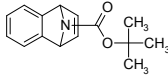
SS-4446	C ₁₂ H ₁₇ NO ₃ S	255.3382	
			Heteroatoms
			5.0000
			Halogen atoms
			0.0000
			rotatable bonds
			5.0000
			H-bond acceptors
3.0000			
H-bond donors			
0.0000			
LogP	1.0466		
Melting_Point	LIST	comments	
2-(benzenesulfonyl)-N,N-diethylacetamide			


SS-4447	C ₂₀ H ₂₈ N ₄ O ₄	388.4706	
			Heteroatoms
			8.0000
			Halogen atoms
			0.0000
			rotatable bonds
			7.0000
			H-bond acceptors
6.0000			
H-bond donors			
0.0000			
LogP	2.1808		
Melting_Point	LIST	comments	
tert-butyl 4-[[8-(ethoxycarbonyl)-[1,2,4]triazolo[4,3-a]pyridin-3-yl]methyl]piperidine-1-carboxylate			

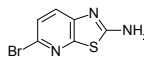
SS-4449	C ₉ H ₁₂ Cl ₃ N	240.5617	
		Heteroatoms	
		Halogen atoms	
		rotatable bonds	
		H-bond acceptors	
		H-bond donors	
		LogP	
		Melting_Point	LIST
(1R)-1-(3,4-dichlorophenyl)propan-1-amine hydrochloride			

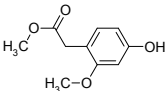
SS-4452	C ₁₃ H ₈ INO	321.1192
		Heteroatoms
		Halogen atoms
		rotatable bonds
		H-bond acceptors
		H-bond donors
		LogP
		Melting_Point
4-(4-hydroxy-3-iodophenyl)benzonitrile		

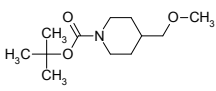
SS-4454	C ₆ H ₉ N ₃ O	139.1581	
		Heteroatoms	
		Halogen atoms	
		rotatable bonds	
		H-bond acceptors	
		H-bond donors	
		LogP	
		Melting_Point	LIST
1-(5-amino-1-methyl-1H-pyrazol-4-yl)ethan-1-one			

SS-4455	C ₁₅ H ₁₇ NO ₂	243.3082	
		Heteroatoms	
		Halogen atoms	
		rotatable bonds	
		H-bond acceptors	
		H-bond donors	
		LogP	
		Melting_Point	LIST
tert-butyl 11-azatricyclo[6.2.1.0 ^{2,7}]undeca-2,4,6,9-tetraene-11-carboxylate			

SS-4457	C ₄ H ₅ N ₃ O	111.1040	
		Heteroatoms	
		Halogen atoms	
		rotatable bonds	
		H-bond acceptors	
		H-bond donors	
		LogP	
		Melting_Point	LIST
6-methyl-1,2,4-triazin-5-ol			

SS-4460	C ₆ H ₄ BrN ₃ S	230.0869	
		Heteroatoms	
		Halogen atoms	
		rotatable bonds	
		H-bond acceptors	
		H-bond donors	
		LogP	
		Melting_Point	LIST
5-bromo-[1,3]thiazolo[5,4-b]pyridin-2-amine			

SS-4464	C ₁₀ H ₁₂ O ₄	196.2047	
		Heteroatoms	
		Halogen atoms	
		rotatable bonds	
		H-bond acceptors	
		H-bond donors	
		LogP	
		Melting_Point	LIST
methyl 2-(4-hydroxy-2-methoxyphenyl)acetate			

SS-4465	C ₁₂ H ₂₃ NO ₃	229.3220	
		Heteroatoms	
		Halogen atoms	
		rotatable bonds	
		H-bond acceptors	
		H-bond donors	
		LogP	
		Melting_Point	LIST
tert-butyl 4-(methoxymethyl)piperidine-1-carboxylate			