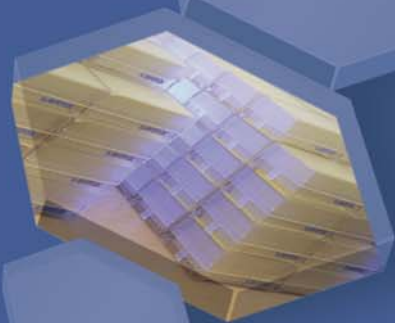





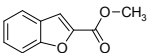
BIONET compounds –
A Key step ahead of the rest

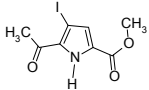


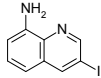
@ohember 20#2
Fragments Collection Update


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

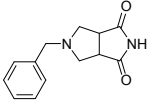
5B-009	C ₈ H ₉ NS	151.2316	
		Halogen atoms	0.0000
		rotatable bonds	0.0000
		H-bond acceptors	0.0000
		H-bond donors	1.0000
		LogP	1.3900
		Purity	>95%
		LogS	TPSA
3,4-dihydro-2H-1,4-benzothiazine			


8R-0046	C ₁₀ H ₈ O ₃	176.1735	
		Halogen atoms	0.0000
		rotatable bonds	2.0000
		H-bond acceptors	3.0000
		H-bond donors	0.0000
		LogP	1.4915
		Purity	>90%
		LogS	-3.36486
methyl 1-benzofuran-2-carboxylate			

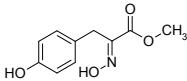
FG-0718	C ₈ H ₈ INO ₃	293.0623	
		Halogen atoms	1.0000
		rotatable bonds	3.0000
		H-bond acceptors	3.0000
		H-bond donors	1.0000
		LogP	0.8778
		Purity	>97%
		LogS	TPSA
methyl 5-acetyl-4-iodo-1H-pyrrole-2-carboxylate			

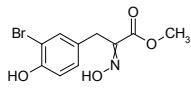
GG-0221	C ₉ H ₇ IN ₂	270.0739	
		Halogen atoms	1.0000
		rotatable bonds	0.0000
		H-bond acceptors	1.0000
		H-bond donors	1.0000
		LogP	2.6102
		Purity	>97%
		LogS	TPSA
3-iodoquinolin-8-amine			

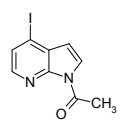
GG-0702	C ₆ H ₈ O ₃	128.1289	
		Halogen atoms	0.0000
		rotatable bonds	2.0000
		H-bond acceptors	3.0000
		H-bond donors	1.0000
		LogP	0.9622
		Purity	>95%
		LogS	TPSA
1-acetylcyclopropane-1-carboxylic acid			

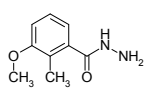
HG-0008	C ₁₃ H ₁₄ N ₂ O ₂	230.2687	
		Halogen atoms	0.0000
		rotatable bonds	2.0000
		H-bond acceptors	3.0000
		H-bond donors	1.0000
		LogP	0.5091
		Purity	>95%
		LogS	TPSA
5-benzyl-octahydropyrrolo[3,4-c]pyrrole-1,3-dione			

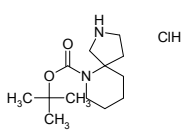
HG-0023	C ₇ H ₅ BrClF	223.4733	
		Halogen atoms	3.0000
		rotatable bonds	1.0000
		H-bond acceptors	0.0000
		H-bond donors	0.0000
		LogP	3.5893
		Purity	>95%
		LogS	TPSA
1-bromo-2-(chloromethyl)-4-fluorobenzene			

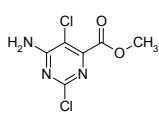
HG-0044	C ₁₀ H ₁₁ NO ₄	209.2035	
		Halogen atoms	0.0000
		rotatable bonds	5.0000
		H-bond acceptors	5.0000
		H-bond donors	2.0000
		LogP	1.6193
		Purity	>97%
		LogS	TPSA
methyl (2E)-2-(N-hydroxyimino)-3-(4-hydroxyphenyl)propanoate			

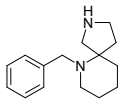
HG-0050	$C_{10}H_{10}BrNO_4$	288.0995
		Halogen atoms
		1.0000
		rotatable bonds
		5.0000
		H-bond acceptors
		5.0000
H-bond donors		
2.0000		
LogP	2.4111	
Purity	>97%	
LogS	TPSA	79.125
methyl 3-(3-bromo-4-hydroxyphenyl)-2-(hydroxyimino)-propanoate		

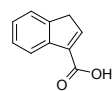
HG-0221	$C_9H_7IN_2O$	286.0733
		Halogen atoms
		1.0000
		rotatable bonds
		0.0000
		H-bond acceptors
		2.0000
H-bond donors		
0.0000		
LogP	2.9864	
Purity	>97%	
LogS	TPSA	34.897
4-iodo-1-acetyl-7-azaindole		

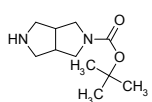
HG-0706	$C_9H_{12}N_2O_2$	180.2082
		Halogen atoms
		0.0000
		rotatable bonds
		2.0000
		H-bond acceptors
		3.0000
H-bond donors		
2.0000		
LogP	1.0819	
Purity	>97%	
LogS	TPSA	64.35
3-methoxy-2-methylbenzohydrazide		

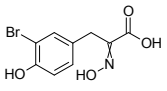
HG-0707	$C_{13}H_{25}ClN_2O_2$	276.8094
		Halogen atoms
		1.0000
		rotatable bonds
		3.0000
		H-bond acceptors
		3.0000
H-bond donors		
1.0000		
LogP	1.2481	
Purity	>95%	
LogS	TPSA	41.57
tert-butyl 2,6-diazaspiro[4.5]decane-6-carboxylate hydrochloride		

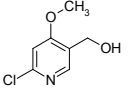
HG-0708	$C_6H_5Cl_2N_3O_2$	222.0317
		Halogen atoms
		2.0000
		rotatable bonds
		2.0000
		H-bond acceptors
		4.0000
H-bond donors		
1.0000		
LogP	1.3464	
Purity	>97%	
LogS	TPSA	78.112
methyl 6-amino-2,5-dichloropyrimidine-4-carboxylate		

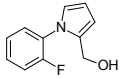
HG-0710	$C_{15}H_{22}N_2$	230.3560
		Halogen atoms
		0.0000
		rotatable bonds
		2.0000
		H-bond acceptors
		2.0000
H-bond donors		
1.0000		
LogP	1.9537	
Purity	>97%	
LogS	TPSA	15.265
6-benzyl-2,6-diazaspiro[4.5]decane		

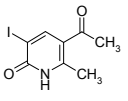
KG-0002	$C_{10}H_8O_2$	160.1741
		Halogen atoms
		0.0000
		rotatable bonds
		1.0000
		H-bond acceptors
		2.0000
H-bond donors		
1.0000		
LogP	1.9977	
Purity	>97%	
LogS	TPSA	37.299
1H-indene-3-carboxylic acid		

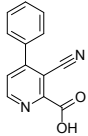
KG-0017	$C_{11}H_{20}N_2O_2$	212.2943
		Halogen atoms
		0.0000
		rotatable bonds
		2.0000
		H-bond acceptors
		3.0000
H-bond donors		
1.0000		
LogP	0.1721	
Purity	>97%	
LogS	TPSA	41.57
tert-butyl octahydropyrrolo[3,4-c]pyrrole-2-carboxylate		

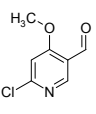
KG-0028	C ₉ H ₈ BrNO ₄	274.0724	
		Halogen atoms	1.0000
		rotatable bonds	4.0000
		H-bond acceptors	5.0000
		H-bond donors	3.0000
		LogP	2.3794
		Purity	>97%
LogS	TPSA	90.119	
3-(3-bromo-4-hydroxyphenyl)-2-(hydroxyimino)propanoic acid			

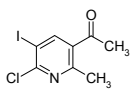
KG-0700	C ₇ H ₈ ClNO ₂	173.6003	
		Halogen atoms	1.0000
		rotatable bonds	2.0000
		H-bond acceptors	3.0000
		H-bond donors	1.0000
		LogP	0.8354
		Purity	>97%
LogS	TPSA	42.354	
(6-chloro-4-methoxypyridin-3-yl)methanol			

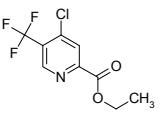
KG-0701	C ₁₁ H ₁₀ FNO	191.2069	
		Halogen atoms	1.0000
		rotatable bonds	2.0000
		H-bond acceptors	1.0000
		H-bond donors	1.0000
		LogP	2.5823
		Purity	>97%
LogS	TPSA	25.162	
[1-(2-fluorophenyl)-1H-pyrrrol-2-yl]methanol			

KG-0703	C ₈ H ₈ IINO ₂	277.0629	
		Halogen atoms	1.0000
		rotatable bonds	1.0000
		H-bond acceptors	2.0000
		H-bond donors	1.0000
		LogP	-0.8366
		Purity	>95%
LogS	TPSA	49.933	
5-acetyl-3-iodo-6-methyl-1,2-dihydropyridin-2-one			

KG-0710	C ₁₃ H ₈ N ₂ O ₂	224.2209	
		Halogen atoms	0.0000
		rotatable bonds	2.0000
		H-bond acceptors	4.0000
		H-bond donors	1.0000
		LogP	2.3816
		Purity	>97%
LogS	TPSA	73.983	
3-cyano-4-phenylpyridine-2-carboxylic acid			

KG-0711	C ₇ H ₆ ClNO ₂	171.5844	
		Halogen atoms	1.0000
		rotatable bonds	2.0000
		H-bond acceptors	3.0000
		H-bond donors	0.0000
		LogP	1.0462
		Purity	>97%
LogS	TPSA	39.197	
6-chloro-4-methoxypyridine-3-carbaldehyde			

KG-0713	C ₈ H ₇ ClINO	295.5085	
		Halogen atoms	2.0000
		rotatable bonds	1.0000
		H-bond acceptors	2.0000
		H-bond donors	0.0000
		LogP	2.8387
		Purity	>97%
LogS	TPSA	29.963	
1-(6-chloro-5-iodo-2-methylpyridin-3-yl)ethan-1-one			

KG-0715	C ₉ H ₇ ClF ₃ NO ₂	253.6098	
		Halogen atoms	4.0000
		rotatable bonds	3.0000
		H-bond acceptors	3.0000
		H-bond donors	0.0000
		LogP	3.0721
		Purity	>95%
LogS	TPSA	39.197	
ethyl 4-chloro-5-(trifluoromethyl)pyridine-2-carboxylate			

KG-0717	C ₈ H ₇ Cl ₂ NO ₂	220.0565	<table border="1"> <tr><td>Halogen atoms</td><td>2.0000</td></tr> <tr><td>rotatable bonds</td><td>3.0000</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>2.5847</td></tr> <tr><td>Purity</td><td>>95%</td></tr> </table>	Halogen atoms	2.0000	rotatable bonds	3.0000	H-bond acceptors	3.0000	H-bond donors	0.0000	LogP	2.5847	Purity	>95%
Halogen atoms	2.0000														
rotatable bonds	3.0000														
H-bond acceptors	3.0000														
H-bond donors	0.0000														
LogP	2.5847														
Purity	>95%														
LogS	TPSA	39.197													
ethyl 2,6-dichloropyridine-3-carboxylate															

KG-0719	C ₇ H ₃ ClF ₃ NO ₂	225.5557	<table border="1"> <tr><td>Halogen atoms</td><td>4.0000</td></tr> <tr><td>rotatable bonds</td><td>1.0000</td></tr> <tr><td>H-bond acceptors</td><td>3.0000</td></tr> <tr><td>H-bond donors</td><td>1.0000</td></tr> <tr><td>LogP</td><td>2.6979</td></tr> <tr><td>Purity</td><td>>97%</td></tr> </table>	Halogen atoms	4.0000	rotatable bonds	1.0000	H-bond acceptors	3.0000	H-bond donors	1.0000	LogP	2.6979	Purity	>97%
Halogen atoms	4.0000														
rotatable bonds	1.0000														
H-bond acceptors	3.0000														
H-bond donors	1.0000														
LogP	2.6979														
Purity	>97%														
LogS	TPSA	50.191													
4-chloro-5-(trifluoromethyl)pyridine-2-carboxylic acid															

LG-0700	C ₉ H ₇ IN ₂ O	286.0733	<table border="1"> <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>2.0000</td></tr> <tr><td>H-bond donors</td><td>1.0000</td></tr> <tr><td>LogP</td><td>1.6134</td></tr> <tr><td>Purity</td><td>>97%</td></tr> </table>	Halogen atoms	1.0000	rotatable bonds	0.0000	H-bond acceptors	2.0000	H-bond donors	1.0000	LogP	1.6134	Purity	>97%
Halogen atoms	1.0000														
rotatable bonds	0.0000														
H-bond acceptors	2.0000														
H-bond donors	1.0000														
LogP	1.6134														
Purity	>97%														
LogS	TPSA	45.754													
3-iodo-5-methyl-1,2-dihydro-1,6-naphthyridin-2-one															

LG-0705	C ₉ H ₉ BrO ₃	245.0743	<table border="1"> <tr><td>Halogen atoms</td><td>1.0000</td></tr> <tr><td>rotatable bonds</td><td>3.0000</td></tr> <tr><td>H-bond acceptors</td><td>3.0000</td></tr> <tr><td>H-bond donors</td><td>1.0000</td></tr> <tr><td>LogP</td><td>2.6266</td></tr> <tr><td>Purity</td><td>>97%</td></tr> </table>	Halogen atoms	1.0000	rotatable bonds	3.0000	H-bond acceptors	3.0000	H-bond donors	1.0000	LogP	2.6266	Purity	>97%
Halogen atoms	1.0000														
rotatable bonds	3.0000														
H-bond acceptors	3.0000														
H-bond donors	1.0000														
LogP	2.6266														
Purity	>97%														
LogS	TPSA	46.53													
ethyl 5-bromo-2-hydroxybenzoate															

LG-0706	C ₁₀ H ₇ ClO ₃	210.6185	<table border="1"> <tr><td>Halogen atoms</td><td>1.0000</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>0.0000</td></tr> <tr><td>LogP</td><td>2.0095</td></tr> <tr><td>Purity</td><td>>95%</td></tr> </table>	Halogen atoms	1.0000	rotatable bonds	2.0000	H-bond acceptors	3.0000	H-bond donors	0.0000	LogP	2.0095	Purity	>95%
Halogen atoms	1.0000														
rotatable bonds	2.0000														
H-bond acceptors	3.0000														
H-bond donors	0.0000														
LogP	2.0095														
Purity	>95%														
LogS	TPSA	39.445													
methyl 4-chloro-1-benzofuran-2-carboxylate															

LG-0709	C ₇ H ₈ N ₄ O	164.1680	<table border="1"> <tr><td>Halogen atoms</td><td>0.0000</td></tr> <tr><td>rotatable bonds</td><td>1.0000</td></tr> <tr><td>H-bond acceptors</td><td>4.0000</td></tr> <tr><td>H-bond donors</td><td>1.0000</td></tr> <tr><td>LogP</td><td>0.7708</td></tr> <tr><td>Purity</td><td>>97%</td></tr> </table>	Halogen atoms	0.0000	rotatable bonds	1.0000	H-bond acceptors	4.0000	H-bond donors	1.0000	LogP	0.7708	Purity	>97%
Halogen atoms	0.0000														
rotatable bonds	1.0000														
H-bond acceptors	4.0000														
H-bond donors	1.0000														
LogP	0.7708														
Purity	>97%														
LogS	TPSA	84.83													
4-amino-2-methoxy-6-methylpyrimidine-5-carbonitrile															

LG-0710	C ₉ H ₁₁ FN ₂ O	182.1992	<table border="1"> <tr><td>Halogen atoms</td><td>1.0000</td></tr> <tr><td>rotatable bonds</td><td>1.0000</td></tr> <tr><td>H-bond acceptors</td><td>1.0000</td></tr> <tr><td>H-bond donors</td><td>2.0000</td></tr> <tr><td>LogP</td><td>0.7190</td></tr> <tr><td>Purity</td><td>>95%</td></tr> </table>	Halogen atoms	1.0000	rotatable bonds	1.0000	H-bond acceptors	1.0000	H-bond donors	2.0000	LogP	0.7190	Purity	>95%
Halogen atoms	1.0000														
rotatable bonds	1.0000														
H-bond acceptors	1.0000														
H-bond donors	2.0000														
LogP	0.7190														
Purity	>95%														
LogS	TPSA	55.121													
N-(2-amino-4-fluoro-6-methylphenyl)acetamide															

LG-0711	C ₉ H ₁₀ INO ₂	291.0899	<table border="1"> <tr><td>Halogen atoms</td><td>1.0000</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>0.0000</td></tr> <tr><td>LogP</td><td>2.3959</td></tr> <tr><td>Purity</td><td>>97%</td></tr> </table>	Halogen atoms	1.0000	rotatable bonds	2.0000	H-bond acceptors	3.0000	H-bond donors	0.0000	LogP	2.3959	Purity	>97%
Halogen atoms	1.0000														
rotatable bonds	2.0000														
H-bond acceptors	3.0000														
H-bond donors	0.0000														
LogP	2.3959														
Purity	>97%														
LogS	TPSA	39.197													
1-(5-iodo-6-methoxy-2-methylpyridin-3-yl)ethan-1-one															

LG-0713	$C_{12}H_{17}N_3O$	219.2888	<table border="1"> <tr><td>Halogen atoms</td><td>0.0000</td></tr> <tr><td>rotatable bonds</td><td>0.0000</td></tr> <tr><td>H-bond acceptors</td><td>2.0000</td></tr> <tr><td>H-bond donors</td><td>2.0000</td></tr> <tr><td>LogP</td><td>1.5797</td></tr> <tr><td>Purity</td><td>>95%</td></tr> </table>	Halogen atoms	0.0000	rotatable bonds	0.0000	H-bond acceptors	2.0000	H-bond donors	2.0000	LogP	1.5797	Purity	>95%
Halogen atoms	0.0000														
rotatable bonds	0.0000														
H-bond acceptors	2.0000														
H-bond donors	2.0000														
LogP	1.5797														
Purity	>95%														
LogS			TPSA 57.781												
7-methyl-2',3',4',6'-tetrahydrospiro[cyclohexane-1,1'-pyrazolo[3,4-b]pyridine]-3'-one															

LG-0714	$C_9H_{15}N_3O_2$	197.2388	<table border="1"> <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>1.0000</td></tr> <tr><td>LogP</td><td>1.6401</td></tr> <tr><td>Purity</td><td>>95%</td></tr> </table>	Halogen atoms	0.0000	rotatable bonds	2.0000	H-bond acceptors	3.0000	H-bond donors	1.0000	LogP	1.6401	Purity	>95%
Halogen atoms	0.0000														
rotatable bonds	2.0000														
H-bond acceptors	3.0000														
H-bond donors	1.0000														
LogP	1.6401														
Purity	>95%														
LogS			TPSA 70.154												
tert-butyl 5-amino-3-methyl-1H-pyrazole-1-carboxylate															

LG-0715	$C_8H_9N_3O$	163.1804	<table border="1"> <tr><td>Halogen atoms</td><td>0.0000</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>1.0000</td></tr> <tr><td>LogP</td><td>1.1284</td></tr> <tr><td>Purity</td><td>>95%</td></tr> </table>	Halogen atoms	0.0000	rotatable bonds	0.0000	H-bond acceptors	3.0000	H-bond donors	1.0000	LogP	1.1284	Purity	>95%
Halogen atoms	0.0000														
rotatable bonds	0.0000														
H-bond acceptors	3.0000														
H-bond donors	1.0000														
LogP	1.1284														
Purity	>95%														
LogS			TPSA 50.427												
2,5-dimethylpyrazolo[1,5-a]pyrimidin-7-ol															

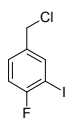
LG-0717	$C_8H_9BrN_2O_2$	245.0771	<table border="1"> <tr><td>Halogen atoms</td><td>1.0000</td></tr> <tr><td>rotatable bonds</td><td>3.0000</td></tr> <tr><td>H-bond acceptors</td><td>3.0000</td></tr> <tr><td>H-bond donors</td><td>1.0000</td></tr> <tr><td>LogP</td><td>1.3858</td></tr> <tr><td>Purity</td><td>>97%</td></tr> </table>	Halogen atoms	1.0000	rotatable bonds	3.0000	H-bond acceptors	3.0000	H-bond donors	1.0000	LogP	1.3858	Purity	>97%
Halogen atoms	1.0000														
rotatable bonds	3.0000														
H-bond acceptors	3.0000														
H-bond donors	1.0000														
LogP	1.3858														
Purity	>97%														
LogS			TPSA 51.224												
methyl 5-bromo-6-(methylamino)pyridine-3-carboxylate															

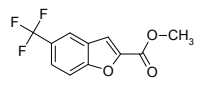
LG-0720	C_7H_6FIO	252.0281	<table border="1"> <tr><td>Halogen atoms</td><td>2.0000</td></tr> <tr><td>rotatable bonds</td><td>1.0000</td></tr> <tr><td>H-bond acceptors</td><td>1.0000</td></tr> <tr><td>H-bond donors</td><td>1.0000</td></tr> <tr><td>LogP</td><td>2.9082</td></tr> <tr><td>Purity</td><td>>95%</td></tr> </table>	Halogen atoms	2.0000	rotatable bonds	1.0000	H-bond acceptors	1.0000	H-bond donors	1.0000	LogP	2.9082	Purity	>95%
Halogen atoms	2.0000														
rotatable bonds	1.0000														
H-bond acceptors	1.0000														
H-bond donors	1.0000														
LogP	2.9082														
Purity	>95%														
LogS			TPSA 20.228												
(4-fluoro-3-iodophenyl)methanol															

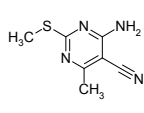
LG-0722	$C_9H_6INO_3$	303.0575	<table border="1"> <tr><td>Halogen atoms</td><td>1.0000</td></tr> <tr><td>rotatable bonds</td><td>2.0000</td></tr> <tr><td>H-bond acceptors</td><td>4.0000</td></tr> <tr><td>H-bond donors</td><td>1.0000</td></tr> <tr><td>LogP</td><td>2.6147</td></tr> <tr><td>Purity</td><td>>95%</td></tr> </table>	Halogen atoms	1.0000	rotatable bonds	2.0000	H-bond acceptors	4.0000	H-bond donors	1.0000	LogP	2.6147	Purity	>95%
Halogen atoms	1.0000														
rotatable bonds	2.0000														
H-bond acceptors	4.0000														
H-bond donors	1.0000														
LogP	2.6147														
Purity	>95%														
LogS			TPSA 70.325												
methyl 5-cyano-2-hydroxy-3-iodobenzoate															

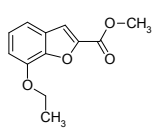
LG-0723	$C_{10}H_7BrO_3$	255.0695	<table border="1"> <tr><td>Halogen atoms</td><td>1.0000</td></tr> <tr><td>rotatable bonds</td><td>2.0000</td></tr> <tr><td>H-bond acceptors</td><td>3.0000</td></tr> <tr><td>H-bond donors</td><td>0.0000</td></tr> <tr><td>LogP</td><td>2.2833</td></tr> <tr><td>Purity</td><td>>90%</td></tr> </table>	Halogen atoms	1.0000	rotatable bonds	2.0000	H-bond acceptors	3.0000	H-bond donors	0.0000	LogP	2.2833	Purity	>90%
Halogen atoms	1.0000														
rotatable bonds	2.0000														
H-bond acceptors	3.0000														
H-bond donors	0.0000														
LogP	2.2833														
Purity	>90%														
LogS			TPSA 39.445												
methyl 7-bromo-1-benzofuran-2-carboxylate															

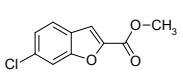
LG-0727	$C_9H_9NO_3$	179.1770	<table border="1"> <tr><td>Halogen atoms</td><td>0.0000</td></tr> <tr><td>rotatable bonds</td><td>2.0000</td></tr> <tr><td>H-bond acceptors</td><td>4.0000</td></tr> <tr><td>H-bond donors</td><td>0.0000</td></tr> <tr><td>LogP</td><td>1.5741</td></tr> <tr><td>Purity</td><td>>97%</td></tr> </table>	Halogen atoms	0.0000	rotatable bonds	2.0000	H-bond acceptors	4.0000	H-bond donors	0.0000	LogP	1.5741	Purity	>97%
Halogen atoms	0.0000														
rotatable bonds	2.0000														
H-bond acceptors	4.0000														
H-bond donors	0.0000														
LogP	1.5741														
Purity	>97%														
LogS			TPSA 48.431												
ethyl 3-formylpyridine-2-carboxylate															

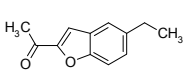
LG-0730	C ₇ H ₅ ClFI	270.4737	
		Halogen atoms	3.0000
		rotatable bonds	1.0000
		H-bond acceptors	0.0000
		H-bond donors	0.0000
		LogP	4.0549
		Purity	>95%
LogS	TPSA	0	
4-(chloromethyl)-1-fluoro-2-iodobenzene			

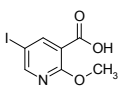
LG-0731	C ₁₁ H ₇ F ₃ O ₃	244.1718	
		Halogen atoms	3.0000
		rotatable bonds	2.0000
		H-bond acceptors	3.0000
		H-bond donors	0.0000
		LogP	2.3743
		Purity	>95%
LogS	TPSA	39.445	
methyl 5-(trifluoromethyl)-1-benzofuran-2-carboxylate			

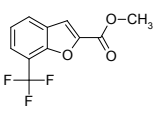
LG-0732	C ₇ H ₈ N ₄ S	180.2326	
		Halogen atoms	0.0000
		rotatable bonds	1.0000
		H-bond acceptors	3.0000
		H-bond donors	1.0000
		LogP	1.1141
		Purity	>97%
LogS	TPSA	75.599	
4-amino-6-methyl-2-(methylsulfanyl)pyrimidine-5-carbonitrile			

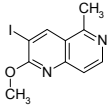
LG-0738	C ₁₂ H ₁₂ O ₄	220.2270	
		Halogen atoms	0.0000
		rotatable bonds	4.0000
		H-bond acceptors	4.0000
		H-bond donors	0.0000
		LogP	1.5813
		Purity	>97%
LogS	TPSA	48.679	
methyl 7-ethoxy-1-benzofuran-2-carboxylate			

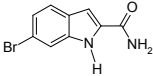
LG-0740	C ₁₀ H ₇ ClO ₃	210.6185	
		Halogen atoms	1.0000
		rotatable bonds	2.0000
		H-bond acceptors	3.0000
		H-bond donors	0.0000
		LogP	2.0095
		Purity	>97%
LogS	TPSA	39.445	
methyl 6-chloro-1-benzofuran-2-carboxylate			

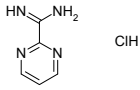
LG-0743	C ₁₂ H ₁₂ O ₂	188.2282	
		Halogen atoms	0.0000
		rotatable bonds	2.0000
		H-bond acceptors	2.0000
		H-bond donors	0.0000
		LogP	1.9334
		Purity	>97%
LogS	TPSA	30.211	
1-(5-ethyl-1-benzofuran-2-yl)ethan-1-one			

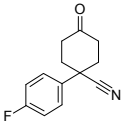
LG-0744	C ₇ H ₆ INO ₃	279.0352	
		Halogen atoms	1.0000
		rotatable bonds	2.0000
		H-bond acceptors	4.0000
		H-bond donors	1.0000
		LogP	2.6013
		Purity	>97%
LogS	TPSA	59.425	
5-iodo-2-methoxypyridine-3-carboxylic acid			

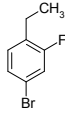
LG-0745	C ₁₁ H ₇ F ₃ O ₃	244.1718	
		Halogen atoms	3.0000
		rotatable bonds	2.0000
		H-bond acceptors	3.0000
		H-bond donors	0.0000
		LogP	2.3743
		Purity	>95%
LogS	TPSA	39.445	
methyl 7-(trifluoromethyl)-1-benzofuran-2-carboxylate			

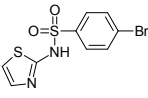
LG-0747	C ₁₀ H ₉ IN ₂ O	300.1004	
		Halogen atoms	1.0000
		rotatable bonds	1.0000
		H-bond acceptors	3.0000
		H-bond donors	0.0000
		LogP	3.6417
		Purity	>97%
LogS	TPSA	35.018	
3-iodo-2-methoxy-5-methyl-1,6-naphthyridine			

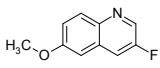
LG-0748	C ₉ H ₇ BrN ₂ O	239.0729	
		Halogen atoms	1.0000
		rotatable bonds	1.0000
		H-bond acceptors	1.0000
		H-bond donors	2.0000
		LogP	1.2094
		Purity	90%
LogS	TPSA	58.885	
6-bromo-1H-indole-2-carboxamide			

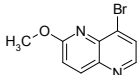
NE-0702	C ₆ H ₇ ClN ₄	158.5913	
		Halogen atoms	1.0000
		rotatable bonds	
		H-bond acceptors	3.0000
		H-bond donors	1.0000
		LogP	0.2382
		Purity	>95%
LogS	TPSA	75.659	
pyrimidine-2-carboximidamide hydrochloride			

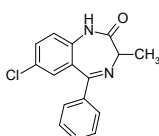
SS-3591	C ₁₃ H ₁₂ FNO	217.2451	
		Halogen atoms	1.0000
		rotatable bonds	1.0000
		H-bond acceptors	2.0000
		H-bond donors	0.0000
		LogP	3.0462
		Purity	>95%
LogS	TPSA	40.863	
1-(4-fluorophenyl)-4-oxocyclohexanecarbonitrile			

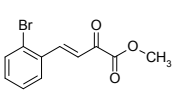
SS-3619	C ₈ H ₈ BrF	203.0554	
		Halogen atoms	2.0000
		rotatable bonds	1.0000
		H-bond acceptors	0.0000
		H-bond donors	0.0000
		LogP	3.8414
		Purity	>95%
LogS	TPSA	0	
4-bromo-1-ethyl-2-fluorobenzene			

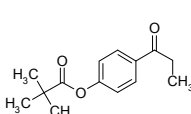
SS-4400	C ₉ H ₇ BrN ₂ O ₂ S ₂	319.2003	
		Halogen atoms	1.0000
		rotatable bonds	3.0000
		H-bond acceptors	3.0000
		H-bond donors	1.0000
		LogP	2.8873
		Purity	>97%
LogS	TPSA	59.061	
4-bromo-N-(1,3-thiazol-2-yl)benzene-1-sulfonamide			

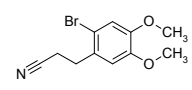
SS-4402	C ₁₀ H ₈ FNO	177.1798	
		Halogen atoms	1.0000
		rotatable bonds	1.0000
		H-bond acceptors	2.0000
		H-bond donors	0.0000
		LogP	2.0228
		Purity	>97%
LogS	TPSA	22.126	
3-fluoro-6-methoxyquinoline			


SS-4403	C ₉ H ₇ BrN ₂ O	239.0729	
		Halogen atoms	1.0000
		rotatable bonds	1.0000
		H-bond acceptors	3.0000
		H-bond donors	0.0000
		LogP	2.4609
		Purity	>95%
LogS	TPSA	35.018	
8-bromo-2-methoxy-1,5-naphthyridine			

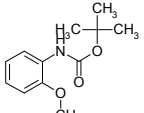
SS-4406	C ₁₆ H ₁₃ ClN ₂ O	284.7478
		Halogen atoms 1.0000
		rotatable bonds 1.0000
		H-bond acceptors 2.0000
		H-bond donors 1.0000
		LogP 3.3001
		Purity >97%
LogS	TPSA	41.462
7-chloro-3-methyl-5-phenyl-2,3-dihydro-1H-1,4-benzodiazepin-2-one		

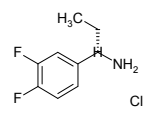
SS-4407	C ₁₁ H ₉ BrO ₃	269.0966
		Halogen atoms 1.0000
		rotatable bonds 5.0000
		H-bond acceptors 3.0000
		H-bond donors 0.0000
		LogP 2.5135
		Purity >95%
LogS	TPSA	43.376
methyl (3E)-4-(2-bromophenyl)-2-oxobut-3-enoate		

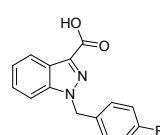
SS-4410	C ₁₄ H ₁₈ O ₃	234.2978
		Halogen atoms 0.0000
		rotatable bonds 5.0000
		H-bond acceptors 3.0000
		H-bond donors 0.0000
		LogP 3.3379
		Purity >97%
LogS	TPSA	234.295
4-propanoylphenyl 2,2-dimethylpropanoate		

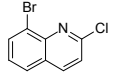
SS-4417	C ₁₁ H ₁₂ BrNO ₂	270.1278
		Halogen atoms 1.0000
		rotatable bonds 4.0000
		H-bond acceptors 3.0000
		H-bond donors 0.0000
		LogP 2.5268
		Purity >97%
LogS	TPSA	42.26
3-(2-bromo-4,5-dimethoxyphenyl)propanenitrile		

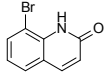
SS-4420	C ₇ H ₇ ClN ₂	154.6002
		Halogen atoms 1.0000
		rotatable bonds 1.0000
		H-bond acceptors 1.0000
		H-bond donors 1.0000
		LogP 1.7412
		Purity >97%
LogS	TPSA	49.875
2-chlorobenzene-carboximidamide		

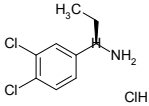
SS-4421	C ₁₂ H ₁₇ NO ₃	223.2742
		Halogen atoms 0.0000
		rotatable bonds 4.0000
		H-bond acceptors 3.0000
		H-bond donors 1.0000
		LogP 2.1019
		Purity >97%
LogS	TPSA	47.566
tert-butyl N-(2-methoxyphenyl)carbamate		

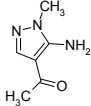
SS-4425	C ₉ H ₁₂ ClF ₂ N	207.6525
		Halogen atoms 3.0000
		rotatable bonds
		H-bond acceptors 1.0000
		H-bond donors 1.0000
		LogP 2.6330
		Purity >97%
LogS	TPSA	26.023
(1S)-1-(3,4-difluorophenyl)propan-1-amine hydrochloride		

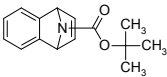
SS-4426	C ₁₅ H ₁₁ FN ₂ O ₂	270.2655
		Halogen atoms 1.0000
		rotatable bonds 3.0000
		H-bond acceptors 3.0000
		H-bond donors 1.0000
		LogP 3.4005
		Purity >97%
LogS	TPSA	55.125
1-[(4-fluorophenyl)methyl]-1H-indazole-3-carboxylic acid		


SS-4441	C ₉ H ₆ BrClN	242.5039	
		Halogen atoms	2.0000
		rotatable bonds	0.0000
		H-bond acceptors	1.0000
		H-bond donors	0.0000
		LogP	3.8165
		Purity	>97%
		LogS	TPSA
8-bromo-2-chloroquinoline			

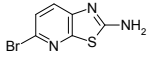
SS-4442	C ₉ H ₆ BrNO	224.0583	
		Halogen atoms	1.0000
		rotatable bonds	0.0000
		H-bond acceptors	1.0000
		H-bond donors	1.0000
		LogP	1.9616
		Purity	>97%
		LogS	TPSA
8-bromo-1,2-dihydroquinolin-2-one			

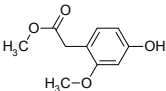
SS-4449	C ₉ H ₁₂ Cl ₃ N	240.5617	
		Halogen atoms	3.0000
		rotatable bonds	
		H-bond acceptors	1.0000
		H-bond donors	1.0000
		LogP	3.3900
		Purity	>97%
		LogS	TPSA
(1R)-1-(3,4-dichlorophenyl)propan-1-amine hydrochloride			

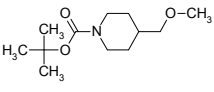
SS-4454	C ₆ H ₉ N ₃ O	139.1581	
		Halogen atoms	0.0000
		rotatable bonds	1.0000
		H-bond acceptors	2.0000
		H-bond donors	1.0000
		LogP	-0.9115
		Purity	>97%
		LogS	TPSA
1-(5-amino-1-methyl-1H-pyrazol-4-yl)ethan-1-one			

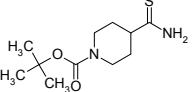
SS-4455	C ₁₅ H ₁₇ NO ₂	243.3082	
		Halogen atoms	0.0000
		rotatable bonds	2.0000
		H-bond acceptors	2.0000
		H-bond donors	0.0000
		LogP	2.9218
		Purity	>97%
		LogS	TPSA
tert-butyl 11-azatricyclo[6.2.1.0 ^{2,7}]undeca-2,4,6,9-tetraene-11-carboxylate			

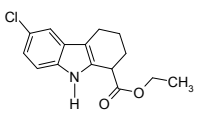
SS-4457	C ₄ H ₅ N ₃ O	111.1040	
		Halogen atoms	0.0000
		rotatable bonds	0.0000
		H-bond acceptors	4.0000
		H-bond donors	1.0000
		LogP	0.7025
		Purity	>97%
		LogS	TPSA
6-methyl-1,2,4-triazin-5-ol			

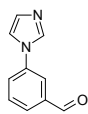
SS-4460	C ₆ H ₄ BrN ₃ S	230.0869	
		Halogen atoms	1.0000
		rotatable bonds	0.0000
		H-bond acceptors	2.0000
		H-bond donors	1.0000
		LogP	2.2005
		Purity	>97%
		LogS	TPSA
5-bromo-[1,3]thiazolo[5,4-b]pyridin-2-amine			

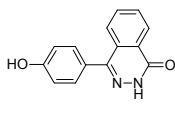
SS-4464	C ₁₀ H ₁₂ O ₄	196.2047	
		Halogen atoms	0.0000
		rotatable bonds	4.0000
		H-bond acceptors	4.0000
		H-bond donors	1.0000
		LogP	1.1721
		Purity	>97%
		LogS	TPSA
methyl 2-(4-hydroxy-2-methoxyphenyl)acetate			

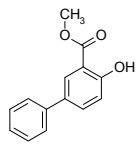
SS-4465	$C_{12}H_{23}NO_3$	229.3220	
		Halogen atoms	0.0000
		rotatable bonds	4.0000
		H-bond acceptors	3.0000
		H-bond donors	0.0000
		LogP	1.1753
		Purity	>95%
LogS	TPSA	38.777	
tert-butyl 4-(methoxymethyl)piperidine-1-carboxylate			

10N-311S	$C_{11}H_{20}N_2O_2S$	244.3583	
		Halogen atoms	0.0000
		rotatable bonds	3.0000
		H-bond acceptors	3.0000
		H-bond donors	1.0000
		LogP	1.0120
		Purity	
LogS	TPSA		
tert-butyl 4-carbamothioylpiperidine-1-carboxylate			

GA-0859	$C_{15}H_{16}ClNO_2$	277.7533	
		Halogen atoms	1.0000
		rotatable bonds	3.0000
		H-bond acceptors	2.0000
		H-bond donors	1.0000
		LogP	3.0290
		Purity	
LogS	TPSA		
ethyl 6-chloro-2,3,4,9-tetrahydro-1H-carbazole-1-carboxylate			

9P-759	$C_{10}H_8N_2O$	172.1881	
		Halogen atoms	0.0000
		rotatable bonds	2.0000
		H-bond acceptors	2.0000
		H-bond donors	0.0000
		LogP	2.0534
		Purity	
LogS	TPSA		
3-(1H-imidazol-1-yl)benzaldehyde			

10Z-0807	$C_{14}H_{10}N_2O_2$	238.2480	
		Halogen atoms	0.0000
		rotatable bonds	1.0000
		H-bond acceptors	3.0000
		H-bond donors	2.0000
		LogP	2.6407
		Purity	
LogS	TPSA		
4-(4-hydroxyphenyl)-1,2-dihydrophthalazin-1-one			

LG-0016	$C_{14}H_{12}O_3$	228.2499	
		Halogen atoms	0.0000
		rotatable bonds	3.0000
		H-bond acceptors	3.0000
		H-bond donors	1.0000
		LogP	3.1767
		Purity	
LogS	TPSA		
methyl 2-hydroxy-5-phenylbenzoate			