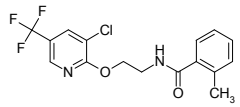
BIONET compounds –
A Key step ahead of the rest

Lotekber 20/2
Screening Collection Update

Key Organics
The right side of the Equation

12Z-5006	$C_{16}H_{14}ClF_3N_2O_2$	358.7504

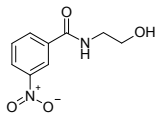


Heteroatoms	8.0000
Halogen atoms	4.0000
rotatable bonds	5.0000
H-bond acceptors	3.0000
H-bond donors	1.0000
LogP	4.4624

Melting_Point	LIST	comments
113 - 115	356	

N-(2-{[3-chloro-5-(trifluoromethyl)pyridin-2-yl]oxy}ethyl)-2-methylbenzamide

6X-5074	$C_9H_{10}N_2O_4$	210.1911

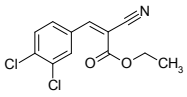


Heteroatoms	6.0000
Halogen atoms	0.0000
rotatable bonds	3.0000
H-bond acceptors	4.0000
H-bond donors	2.0000
LogP	0.6372

Melting_Point	LIST	comments
	356	

N-(2-hydroxyethyl)-3-nitrobenzamide

9N-915	$C_{12}H_9Cl_2NO_2$	270.1170

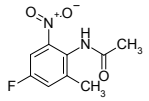


Heteroatoms	5.0000
Halogen atoms	2.0000
rotatable bonds	5.0000
H-bond acceptors	3.0000
H-bond donors	0.0000
LogP	3.2388

Melting_Point	LIST	comments
	356	

ethyl (2Z)-2-cyano-3-(3,4-dichlorophenyl)prop-2-enoate

AB-0824	$C_9H_9FN_2O_3$	212.1821

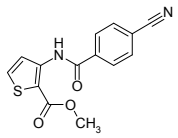


Heteroatoms	6.0000
Halogen atoms	1.0000
rotatable bonds	1.0000
H-bond acceptors	3.0000
H-bond donors	1.0000
LogP	1.4558

Melting_Point	LIST	comments
170 - 172		

N-(4-fluoro-2-methyl-6-nitrophenyl)acetamide

CF-0049	$C_{14}H_{10}N_2O_3S$	286.3114

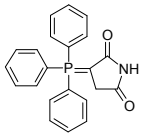


Heteroatoms	6.0000
Halogen atoms	0.0000
rotatable bonds	4.0000
H-bond acceptors	4.0000
H-bond donors	1.0000
LogP	1.6952

Melting_Point	LIST	comments
	356	

methyl 3-[(4-cyanobenzene)amido]thiophene-2-carboxylate

EG-0103	$C_{22}H_{18}NO_2P$	359.3681

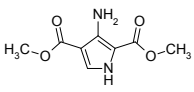


Heteroatoms	4.0000
Halogen atoms	0.0000
rotatable bonds	4.0000
H-bond acceptors	2.0000
H-bond donors	1.0000
LogP	

Melting_Point	LIST	comments

3-(triphenyl-$l^{5}-phosphanylidene)pyrrolidine- 2,5-dione

FG-0711	$C_8H_{10}N_2O_4$	198.1799

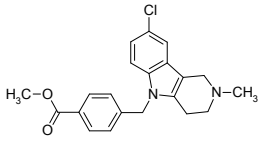


Heteroatoms	6.0000
Halogen atoms	0.0000
rotatable bonds	4.0000
H-bond acceptors	4.0000
H-bond donors	2.0000
LogP	-0.5054

Melting_Point	LIST	comments
165 - 166		

2,4-dimethyl 3-amino-1H-pyrrole-2,4-dicarboxylate

GG-0209	$C_{21}H_{21}ClN_2O_2$	368.8667

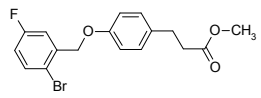


Heteroatoms	5.0000
Halogen atoms	1.0000
rotatable bonds	4.0000
H-bond acceptors	3.0000
H-bond donors	0.0000
LogP	3.5242

Melting_Point	LIST	comments
132 - 133		

methyl 4-({8-chloro-2-methyl-1H,2H,3H,4H,5H-pyrido[4,3-b]indol-5-yl}methyl)benzoate

HG-0047	$C_{17}H_{16}BrFO_3$	367.2177

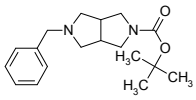


Heteroatoms	5.0000
Halogen atoms	2.0000
rotatable bonds	7.0000
H-bond acceptors	3.0000
H-bond donors	0.0000
LogP	4.5607

Melting_Point	LIST	comments
Oil		

methyl 3-{4-[(2-bromo-5-fluorophenyl)methoxy]phenyl}propanoate

HG-0052	$C_{18}H_{26}N_2O_2$	302.4201

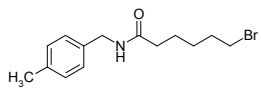


Heteroatoms	4.0000
Halogen atoms	0.0000
rotatable bonds	4.0000
H-bond acceptors	3.0000
H-bond donors	0.0000
LogP	2.3101

Melting_Point	LIST	comments
Oil		

tert-butyl 5-benzyl-octahydropyrrolo[3,4-c]pyrrole-2-carboxylate

HG-0216	$C_{14}H_{20}BrNO$	298.2256

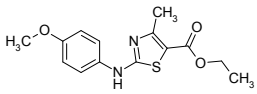


Heteroatoms	3.0000
Halogen atoms	1.0000
rotatable bonds	7.0000
H-bond acceptors	1.0000
H-bond donors	1.0000
LogP	3.3376

Melting_Point	LIST	comments
84 - 86		

6-bromo-N-[(4-methylphenyl)methyl]hexanamide

HG-0703	$C_{14}H_{16}N_2O_3S$	292.3592

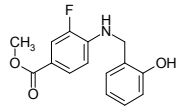


Heteroatoms	6.0000
Halogen atoms	0.0000
rotatable bonds	6.0000
H-bond acceptors	4.0000
H-bond donors	1.0000
LogP	2.5285

Melting_Point	LIST	comments
173 - 175 (dec.)		

ethyl 2-[(4-methoxyphenyl)amino]-4-methyl-1,3-thiazole-5-carboxylate

HG-0704	$C_{15}H_{14}FNO_3$	275.2821

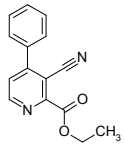


Heteroatoms	5.0000
Halogen atoms	1.0000
rotatable bonds	5.0000
H-bond acceptors	3.0000
H-bond donors	2.0000
LogP	2.8390

Melting_Point	LIST	comments
130 - 131		

methyl 3-fluoro-4-{[(2-hydroxyphenyl)methyl]amino}benzoate

KG-0709	$C_{15}H_{12}N_2O_2$	252.2751

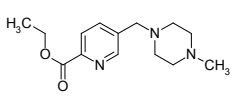


Heteroatoms	4.0000
Halogen atoms	0.0000
rotatable bonds	4.0000
H-bond acceptors	4.0000
H-bond donors	0.0000
LogP	2.7558

Melting_Point	LIST	comments
153 - 155		

ethyl 3-cyano-4-phenylpyridine-2-carboxylate

KG-0712	$C_{14}H_{21}N_3O_2$	263.3424

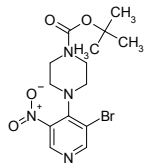


Heteroatoms	5.0000
Halogen atoms	0.0000
rotatable bonds	5.0000
H-bond acceptors	5.0000
H-bond donors	0.0000
LogP	0.8946

Melting_Point	LIST	comments
62 - 64		

ethyl 5-[(4-methylpiperazin-1-yl)methyl]pyridine-2-carboxylate

KG-0716	$C_{14}H_{19}BrN_4O_4$	387.2359

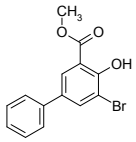


Heteroatoms	9.0000
Halogen atoms	1.0000
rotatable bonds	3.0000
H-bond acceptors	5.0000
H-bond donors	0.0000
LogP	2.3008

Melting_Point	LIST	comments
106 - 107		

tert-butyl 4-(3-bromo-5-nitropyridin-4-yl)piperazine-1-carboxylate

LG-0018	$C_{14}H_{11}BrO_3$	307.1460

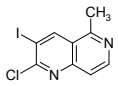


Heteroatoms	4.0000
Halogen atoms	1.0000
rotatable bonds	3.0000
H-bond acceptors	3.0000
H-bond donors	1.0000
LogP	3.9685

Melting_Point	LIST	comments

methyl 3-bromo-2-hydroxy-5-phenylbenzoate

LG-0719	$C_9H_6ClIN_2$	304.5190

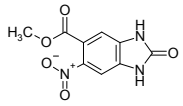


Heteroatoms	4.0000
Halogen atoms	2.0000
rotatable bonds	0.0000
H-bond acceptors	2.0000
H-bond donors	0.0000
LogP	4.0845

Melting_Point	LIST	comments
172 - 174		

2-chloro-3-iodo-5-methyl-1,6-naphthyridine

LG-0724	$C_9H_7N_3O_5$	237.1732

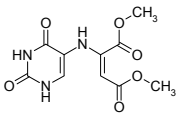


Heteroatoms	8.0000
Halogen atoms	0.0000
rotatable bonds	2.0000
H-bond acceptors	5.0000
H-bond donors	2.0000
LogP	-0.1602

Melting_Point	LIST	comments
>300		

methyl 6-nitro-2-oxo-2,3-dihydro-1H-1,3-benzodiazole-5-carboxylate

SS-4408	$C_{10}H_{11}N_3O_6$	269.2157

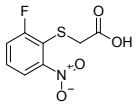


Heteroatoms	9.0000
Halogen atoms	0.0000
rotatable bonds	7.0000
H-bond acceptors	6.0000
H-bond donors	3.0000
LogP	-2.9017

Melting_Point	LIST	comments

2,4-dioxo-1,2,3,4-tetrahydro-pyrimidin-5-ylamino)-fumaric acid dimethyl ester

SS-4412	$C_8H_6FNO_4S$	231.2037

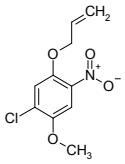


Heteroatoms	7.0000
Halogen atoms	1.0000
rotatable bonds	3.0000
H-bond acceptors	4.0000
H-bond donors	1.0000
LogP	1.7721

Melting_Point	LIST	comments

2-[(2-fluoro-6-nitrophenyl)sulfanyl]acetic acid

SS-4413	$C_{10}H_{10}ClNO_4$	243.6485

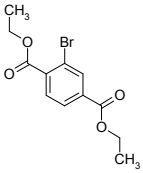


Heteroatoms	6.0000
Halogen atoms	1.0000
rotatable bonds	4.0000
H-bond acceptors	4.0000
H-bond donors	0.0000
LogP	2.7534

Melting_Point	LIST	comments

1-chloro-2-methoxy-4-nitro-5-(prop-2-en-1-yloxy)benzene

SS-4415	$C_{12}H_{13}BrO_4$	301.1390

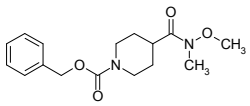


Heteroatoms	5.0000
Halogen atoms	1.0000
rotatable bonds	6.0000
H-bond acceptors	4.0000
H-bond donors	0.0000
LogP	2.9836

Melting_Point	LIST	comments
Oil		

1,4-diethyl 2-bromobenzene-1,4-dicarboxylate

SS-4416	$C_{16}H_{22}N_2O_4$	306.3647

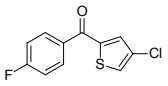


Heteroatoms	6.0000
Halogen atoms	0.0000
rotatable bonds	5.0000
H-bond acceptors	4.0000
H-bond donors	0.0000
LogP	1.8133

Melting_Point	LIST	comments
Oil		

benzyl 4-[methoxy(methyl)carbamoyl]piperidine-1-carboxylate

SS-4427	$C_{11}H_6ClFOS$	240.6853

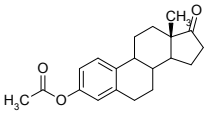


Heteroatoms	4.0000
Halogen atoms	2.0000
rotatable bonds	2.0000
H-bond acceptors	1.0000
H-bond donors	0.0000
LogP	3.2172

Melting_Point	LIST	comments

(4-chlorothiophen-2-yl)(4-fluorophenyl)methanone

SS-4431	$C_{20}H_{24}O_3$	312.4125

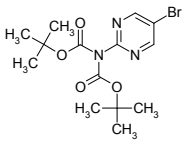


Heteroatoms	3.0000
Halogen atoms	0.0000
rotatable bonds	2.0000
H-bond acceptors	3.0000
H-bond donors	0.0000
LogP	4.3186

Melting_Point	LIST	comments

Estrone acetate

SS-4436	$C_{14}H_{20}BrN_3O_4$	374.2372

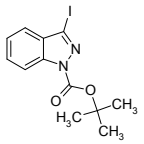


Heteroatoms	8.0000
Halogen atoms	1.0000
rotatable bonds	5.0000
H-bond acceptors	6.0000
H-bond donors	0.0000
LogP	3.6156

Melting_Point	LIST	comments

tert-butyl N-(5-bromopyrimidin-2-yl)-N-[(tert-butoxy)carbonyl]carbamate

SS-4437	$C_{12}H_{13}IN_2O_2$	344.1540

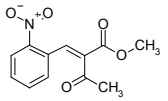


Heteroatoms	5.0000
Halogen atoms	1.0000
rotatable bonds	2.0000
H-bond acceptors	3.0000
H-bond donors	0.0000
LogP	3.7854

Melting_Point	LIST	comments

tert-butyl 3-iodo-1H-indazole-1-carboxylate

SS-4438	$C_{12}H_{11}NO_5$	249.2252

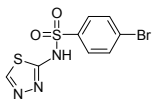


Heteroatoms	6.0000
Halogen atoms	0.0000
rotatable bonds	5.0000
H-bond acceptors	5.0000
H-bond donors	0.0000
LogP	1.2574

Melting_Point	LIST	comments

methyl 2-(2-nitrobenzylidene)acetoacetate

SS-4440	$C_8H_6BrN_3O_2S_2$	320.1879

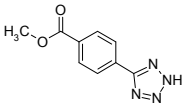


Heteroatoms	8.0000
Halogen atoms	1.0000
rotatable bonds	3.0000
H-bond acceptors	4.0000
H-bond donors	1.0000
LogP	1.9817

Melting_Point	LIST	comments

4-bromo-N-(1,3,4-thiadiazol-2-yl)benzene-1-sulfonamide

SS-4444	$C_9H_8N_4O_2$	204.1897

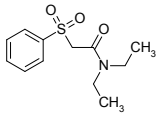


Heteroatoms	6.0000
Halogen atoms	0.0000
rotatable bonds	3.0000
H-bond acceptors	5.0000
H-bond donors	1.0000
LogP	1.5228

Melting_Point	LIST	comments

methyl 4-(2H-1,2,3,4-tetrazol-5-yl)benzoate

SS-4446	$C_{12}H_{17}NO_3S$	255.3382

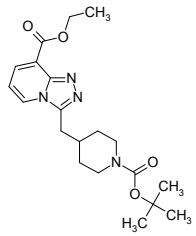


Heteroatoms	5.0000
Halogen atoms	0.0000
rotatable bonds	5.0000
H-bond acceptors	3.0000
H-bond donors	0.0000
LogP	1.0466

Melting_Point	LIST	comments

2-(benzenesulfonyl)-N,N-diethylacetamide

SS-4447	$C_{20}H_{28}N_4O_4$	388.4706

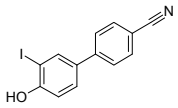


Heteroatoms	8.0000
Halogen atoms	0.0000
rotatable bonds	7.0000
H-bond acceptors	6.0000
H-bond donors	0.0000
LogP	2.1808

Melting_Point	LIST	comments

tert-butyl 4-{[8-(ethoxycarbonyl)-[1,2,4]triazolo[4,3-a]pyridin-3-yl]methyl}piperidine-1-carboxylate

SS-4452	$C_{13}H_8INO$	321.1192



Heteroatoms	3.0000
Halogen atoms	1.0000
rotatable bonds	1.0000
H-bond acceptors	2.0000
H-bond donors	1.0000
LogP	4.5690

Melting_Point	LIST	comments

4-(4-hydroxy-3-iodophenyl)benzonitrile