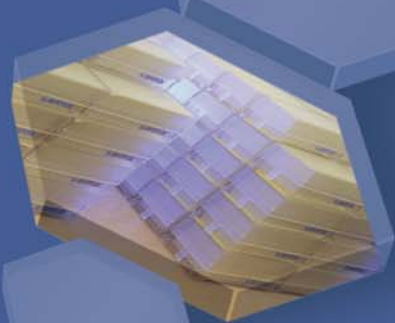




BIONET compounds –
A Key step ahead of the rest

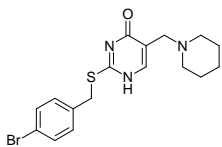


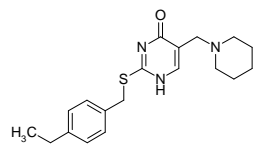
3 April 20#0
Screening Collection Update

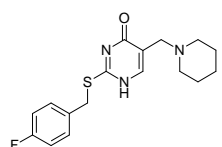


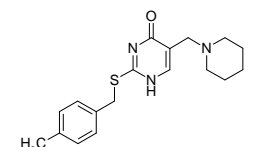
Key Organics

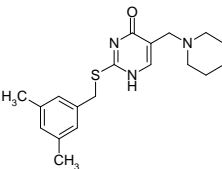
The right side of the Equation

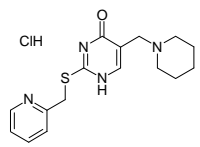
CB-0024	C ₁₇ H ₂₀ BrN ₃ OS	394.3365													
		<table border="1"> <tr><td>Heteroatoms</td><td>6.0000</td></tr> <tr><td>Halogen atoms</td><td>1.0000</td></tr> <tr><td>rotatable bonds</td><td>5.0000</td></tr> <tr><td>H-bond acceptors</td><td>3.0000</td></tr> <tr><td>H-bond donors</td><td>1.0000</td></tr> <tr><td>LogP</td><td>3.8914</td></tr> </table>	Heteroatoms	6.0000	Halogen atoms	1.0000	rotatable bonds	5.0000	H-bond acceptors	3.0000	H-bond donors	1.0000	LogP	3.8914	
Heteroatoms	6.0000														
Halogen atoms	1.0000														
rotatable bonds	5.0000														
H-bond acceptors	3.0000														
H-bond donors	1.0000														
LogP	3.8914														
Melting_Point	LIST	349	comments												
2-(((4-bromophenyl)methyl)sulfanyl)-5-(piperidin-1-ylmethyl)-1,4-dihydropyrimidin-4-one															

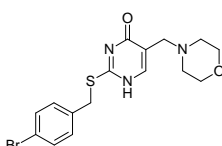
CB-0025	C ₁₉ H ₂₅ N ₃ OS	343.4946													
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Heteroatoms	5.0000														
Halogen atoms	0.0000														
rotatable bonds	6.0000														
H-bond acceptors	3.0000														
H-bond donors	1.0000														
LogP	3.9631														
Melting_Point	LIST	349	comments												
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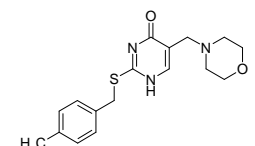
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Heteroatoms	6.0000														
Halogen atoms	1.0000														
rotatable bonds	5.0000														
H-bond acceptors	3.0000														
H-bond donors	1.0000														
LogP	3.2391														
Melting_Point	LIST	349	comments												
2-(((4-fluorophenyl)methyl)sulfanyl)-5-(piperidin-1-ylmethyl)-1,4-dihydropyrimidin-4-one															

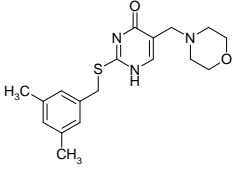
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Heteroatoms	5.0000														
Halogen atoms	0.0000														
rotatable bonds	5.0000														
H-bond acceptors	3.0000														
H-bond donors	1.0000														
LogP	3.5668														
Melting_Point	LIST	349	comments												
2-(((4-methylphenyl)methyl)sulfanyl)-5-(piperidin-1-ylmethyl)-1,4-dihydropyrimidin-4-one															

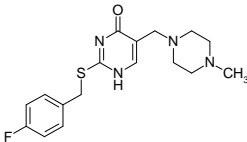
CB-0028	C ₁₉ H ₂₅ N ₃ OS	343.4946													
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Heteroatoms	5.0000														
Halogen atoms	0.0000														
rotatable bonds	5.0000														
H-bond acceptors	3.0000														
H-bond donors	1.0000														
LogP	4.0340														
Melting_Point	LIST	349	comments												
2-(((3,5-dimethylphenyl)methyl)sulfanyl)-5-(piperidin-1-ylmethyl)-1,4-dihydropyrimidin-4-one															

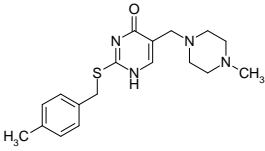
CB-0029	C ₁₆ H ₂₁ ClN ₄ OS	352.8890													
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Heteroatoms	7.0000														
Halogen atoms	1.0000														
rotatable bonds															
H-bond acceptors	4.0000														
H-bond donors	1.0000														
LogP	2.9602														
Melting_Point	LIST	349	comments												
5-(piperidin-1-ylmethyl)-2-((pyridin-2-ylmethyl)sulfanyl)-1,4-dihydropyrimidin-4-one hydrochloride															

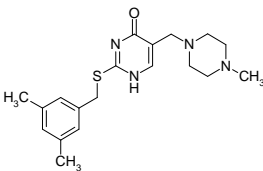
CB-0030	C ₁₆ H ₁₈ BrN ₃ O ₂ S	396.3088													
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Heteroatoms	7.0000														
Halogen atoms	1.0000														
rotatable bonds	5.0000														
H-bond acceptors	4.0000														
H-bond donors	1.0000														
LogP	2.8269														
Melting_Point	LIST	349	comments												
2-(((4-bromophenyl)methyl)sulfanyl)-5-(morpholin-4-ylmethyl)-1,4-dihydropyrimidin-4-one															

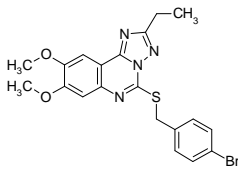
CB-0033	C ₁₇ H ₂₁ N ₃ O ₂ S	331.4398													
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Heteroatoms	6.0000														
Halogen atoms	0.0000														
rotatable bonds	5.0000														
H-bond acceptors	4.0000														
H-bond donors	1.0000														
LogP	2.5023														
Melting_Point	LIST	349	comments												
2-(((4-methylphenyl)methyl)sulfanyl)-5-(morpholin-4-ylmethyl)-1,4-dihydropyrimidin-4-one															

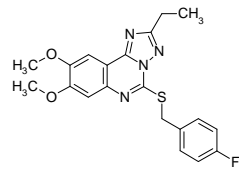
CB-0034	C ₁₈ H ₂₃ N ₃ O ₂ S	345.4669	
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		H-bond acceptors	4.0000
		H-bond donors	1.0000
		LogP	2.9695
Melting_Point	LIST	349	comments
2-(((3,5-dimethylphenyl)methyl)sulfanyl)-5-(morpholin-4-ylmethyl)-1,4-dihydropyrimidin-4-one			

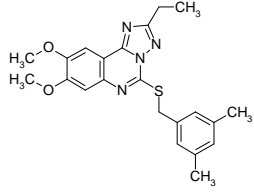
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		rotatable bonds	5.0000
		H-bond acceptors	4.0000
		H-bond donors	1.0000
		LogP	2.3185
Melting_Point	LIST	349	comments
2-(((4-fluorophenyl)methyl)sulfanyl)-5-((4-methylpiperazin-1-yl)methyl)-1,4-dihydropyrimidin-4-one			

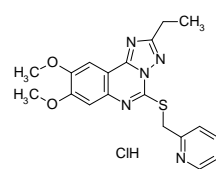
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		rotatable bonds	5.0000
		H-bond acceptors	4.0000
		H-bond donors	1.0000
		LogP	2.6462
Melting_Point	LIST	349	comments
2-(((4-methylphenyl)methyl)sulfanyl)-5-((4-methylpiperazin-1-yl)methyl)-1,4-dihydropyrimidin-4-one			

CB-0046	C ₁₉ H ₂₆ N ₄ OS	358.5093	
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		Halogen atoms	0.0000
		rotatable bonds	5.0000
		H-bond acceptors	4.0000
		H-bond donors	1.0000
		LogP	3.1134
Melting_Point	LIST	349	comments
2-(((3,5-dimethylphenyl)methyl)sulfanyl)-5-((4-methylpiperazin-1-yl)methyl)-1,4-dihydropyrimidin-4-one			

CB-0048	C ₂₀ H ₁₉ BrN ₄ O ₂ S	459.3680	
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		Halogen atoms	1.0000
		rotatable bonds	6.0000
		H-bond acceptors	5.0000
		H-bond donors	0.0000
		LogP	5.7363
Melting_Point	LIST	349	comments
5-(((4-bromophenyl)methyl)sulfanyl)-2-ethyl-8,9-dimethoxy-[1,2,4]triazolo[1,5-c]quinazoline			

CB-0050	C ₂₀ H ₁₉ FN ₄ O ₂ S	398.4624	
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		Halogen atoms	1.0000
		rotatable bonds	6.0000
		H-bond acceptors	5.0000
		H-bond donors	0.0000
		LogP	5.0840
Melting_Point	LIST	349	comments
2-ethyl-5-(((4-fluorophenyl)methyl)sulfanyl)-8,9-dimethoxy-[1,2,4]triazolo[1,5-c]quinazoline			

CB-0052	C ₂₂ H ₂₄ N ₄ O ₂ S	408.5262	
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		rotatable bonds	6.0000
		H-bond acceptors	5.0000
		H-bond donors	0.0000
		LogP	5.8789
Melting_Point	LIST	349	comments
5-(((3,5-dimethylphenyl)methyl)sulfanyl)-2-ethyl-8,9-dimethoxy-[1,2,4]triazolo[1,5-c]quinazoline			

CB-0053	C ₁₉ H ₂₀ ClN ₅ O ₂ S	417.9206	
		Heteroatoms	9.0000
		Halogen atoms	1.0000
		rotatable bonds	6.0000
		H-bond acceptors	6.0000
		H-bond donors	0.0000
		LogP	4.8051
Melting_Point	LIST	349	comments
2-(((2-ethyl-8,9-dimethoxy-[1,2,4]triazolo[1,5-c]quinazolin-5-yl)sulfanyl)methyl)pyridine hydrochloride			

CB-0058	C ₁₇ H ₁₇ ClN ₄ O ₂	344.8036	
			Heteroatoms 7.0000
			Halogen atoms 1.0000
			rotatable bonds 6.0000
			H-bond acceptors 4.0000
			H-bond donors 1.0000
			LogP 2.6309
Melting_Point	LIST	349	comments
ethyl 4-[[[4-chlorophenyl)methyl]amino]-1-methyl-1H-pyrazolo[3,4-b]pyridine-5-carboxylate			

CB-0060	C ₁₈ H ₂₀ N ₄ O ₂	324.3857	
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			Halogen atoms 0.0000
			rotatable bonds 6.0000
			H-bond acceptors 4.0000
			H-bond donors 1.0000
			LogP 2.5801
Melting_Point	LIST	349	comments
ethyl 1-methyl-4-[[[4-methylphenyl)methyl]amino]-1H-pyrazolo[3,4-b]pyridine-5-carboxylate			

CB-0062	C ₁₅ H ₁₆ N ₄ O ₂ S	316.3844	
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			Halogen atoms 0.0000
			rotatable bonds 6.0000
			H-bond acceptors 4.0000
			H-bond donors 1.0000
			LogP 1.4046
Melting_Point	LIST	350	comments
ethyl 1-methyl-4-[[[thiophen-2-yl)methyl]amino]-1H-pyrazolo[3,4-b]pyridine-5-carboxylate			

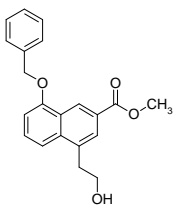
CB-0063	C ₁₇ H ₁₆ Cl ₂ N ₄ O ₂	379.2487	
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			rotatable bonds 6.0000
			H-bond acceptors 4.0000
			H-bond donors 1.0000
			LogP 3.1489
Melting_Point	LIST	350	comments
ethyl 4-[[[2,4-dichlorophenyl)methyl]amino]-1-methyl-1H-pyrazolo[3,4-b]pyridine-5-carboxylate			

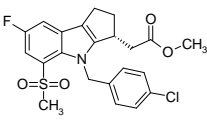
CB-0072	C ₂₀ H ₁₈ Cl ₂ N ₄ O ₂ S	449.3621	
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			rotatable bonds 6.0000
			H-bond acceptors 5.0000
			H-bond donors 0.0000
			LogP 5.9805
Melting_Point	LIST	350	comments
5-[[[3,4-dichlorophenyl)methyl]sulfanyl]-2-ethyl-8,9-dimethoxy-[1,2,4]triazolo[1,5-c]quinazoline			

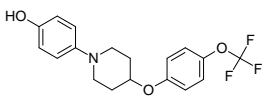
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			Halogen atoms 2.0000
			rotatable bonds 6.0000
			H-bond acceptors 5.0000
			H-bond donors 0.0000
			LogP 5.6020
Melting_Point	LIST	350	comments
5-[[[2-chloro-6-fluorophenyl)methyl]sulfanyl]-2-ethyl-8,9-dimethoxy-[1,2,4]triazolo[1,5-c]quinazolin e			


CB-0075	C ₂₁ H ₂₂ N ₄ O ₂ S	394.4991	
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			Halogen atoms 0.0000
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			H-bond acceptors 5.0000
			H-bond donors 0.0000
			LogP 5.1962
Melting_Point	LIST	350	comments
2-ethyl-8,9-dimethoxy-5-[[[2-phenylethyl]sulfanyl]-[1,2,4]triazolo[1,5-c]quinazoline			

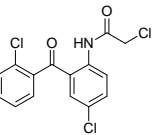
SS-3167	C ₁₄ H ₁₀ ClNO	243.6949	
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			H-bond acceptors 1.0000
			H-bond donors 1.0000
			LogP 3.2204
Melting_Point	LIST	350	comments
11-chloro-5,11-dihydro-6H-dibenzo[b,e]azepin-6-one			

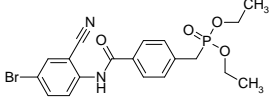
SS-3176	C ₂₁ H ₂₀ O ₄	336.3911	
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	Melting_Point	LIST 350	comments
	methyl 8-(benzyloxy)-4-(2-hydroxyethyl)-2-naphthoate		

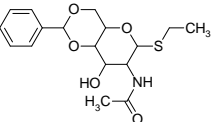
SS-3179	C ₂₂ H ₂₁ ClFNO ₄ S	449.9324	
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	Halogen atoms	2.0000	
	rotatable bonds	6.0000	
	H-bond acceptors	4.0000	
	H-bond donors	0.0000	
	LogP	3.6899	
	Melting_Point	LIST 350	comments
	methyl 2-[(3R)-4-(4-chlorobenzyl)-7-fluoro-5-(methylsulfonyl)-1,2,3,4-tetrahydrocyclopenta[b]indol-3-yl]acetate		

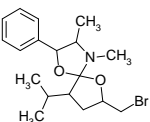
SS-3227	C ₁₈ H ₁₈ F ₃ NO ₃	353.3443	
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	Halogen atoms	3.0000	
	rotatable bonds	4.0000	
	H-bond acceptors	3.0000	
	H-bond donors	1.0000	
	LogP	4.6599	
	Melting_Point	LIST 350	comments
	4-[4-[4-(trifluoromethoxy)phenoxy]piperidino]benzenol		

SS-3253	C ₈ H ₄ Br ₂ S ₂	324.0571	
	Heteroatoms	4.0000	
	Halogen atoms	2.0000	
	rotatable bonds	1.0000	
	H-bond acceptors	0.0000	
	H-bond donors	0.0000	
	LogP	3.8980	
	Melting_Point	LIST 350	comments
	3-bromo-2-(3-bromothiophen-2-yl)thiophene		

SS-3265	C ₁₅ H ₁₀ Cl ₃ NO ₂	342.6114	
	Heteroatoms	6.0000	
	Halogen atoms	3.0000	
	rotatable bonds	4.0000	
	H-bond acceptors	2.0000	
	H-bond donors	1.0000	
	LogP	3.7440	
	Melting_Point	LIST 350	comments
	2-chloro-N-[4-chloro-2-(2-chlorobenzoyl)phenyl]acetamide		

SS-3273	C ₁₉ H ₂₀ BrN ₂ O ₄ P	451.2600	
	Heteroatoms	8.0000	
	Halogen atoms	1.0000	
	rotatable bonds	8.0000	
	H-bond acceptors	5.0000	
	H-bond donors	1.0000	
	LogP	3.8563	
	Melting_Point	LIST 350	comments
	diethyl 4-[(4-bromo-2-cyanoanilino)carbonyl]benzylphosphonate		

SS-3302	C ₁₇ H ₂₃ NO ₅ S	353.4406	
	Heteroatoms	7.0000	
	Halogen atoms	0.0000	
	rotatable bonds	4.0000	
	H-bond acceptors	5.0000	
	H-bond donors	2.0000	
	LogP	1.2751	
	Melting_Point	LIST 350	comments
	N-[6-(ethylsulfanyl)-8-hydroxy-2-phenylhexahydroprano[3,2-d][1,3]dioxin-7-yl]acetamide		

SS-3309	C ₁₈ H ₂₆ BrNO ₂	368.3174	
	Heteroatoms	4.0000	
	Halogen atoms	1.0000	
	rotatable bonds	3.0000	
	H-bond acceptors	3.0000	
	H-bond donors	0.0000	
	LogP	5.1070	
	Melting_Point	LIST 350	comments
	7-(bromomethyl)-9-isopropyl-3,4-dimethyl-2-phenyl-1,6-dioxo-4-azaspiro[4.4]nonane		

SS-3339	C ₁₈ H ₁₈ BrNO ₂	360.2537	
			Heteroatoms 4.0000
			Halogen atoms 1.0000
			rotatable bonds 6.0000
			H-bond acceptors 2.0000
			H-bond donors 1.0000
			LogP 3.9442
Melting_Point	LIST	350	comments
9H-fluoren-9-ylmethyl N-(3-bromopropyl)carbamate			

SS-3348	C ₁₅ H ₃₀ O ₅ Si	318.4894	
			Heteroatoms 6.0000
			Halogen atoms 0.0000
			rotatable bonds 8.0000
			H-bond acceptors 5.0000
			H-bond donors 0.0000
			LogP
Melting_Point	LIST	350	comments
methyl 3-[[tert-butyl(dimethyl)silyl]oxy]-2-(tetrahydro-2H-pyran-2-yloxy)propanoate			

SS-3378	C ₂₅ H ₂₆ O ₂	358.4848	
			Heteroatoms 2.0000
			Halogen atoms 0.0000
			rotatable bonds 3.0000
			H-bond acceptors 2.0000
			H-bond donors 0.0000
			LogP 5.4857
Melting_Point	LIST	350	comments
(13S)-3-(benzyloxy)-13-methyl-6,7,8,9,11,12,13,14-octahydro-17H-cyclopenta[a]phenanthren-17-one			

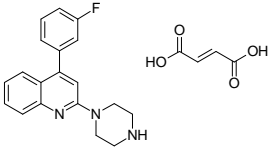
SS-3396	C ₅ H ₅ KO ₃	152.1958	
			Heteroatoms 4.0000
			Halogen atoms 0.0000
			rotatable bonds
			H-bond acceptors 3.0000
			H-bond donors 0.0000
			LogP
Melting_Point	LIST	350	comments
potassium 2-cyclopropyl-2-oxoacetate			

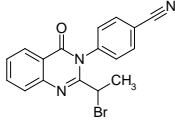
SS-3397	C ₈ H ₉ N ₃ O ₃	195.1792	
			Heteroatoms 6.0000
			Halogen atoms 0.0000
			rotatable bonds 0.0000
			H-bond acceptors 4.0000
			H-bond donors 2.0000
			LogP -2.3436
Melting_Point	LIST	350	comments
3H-imidazo[4,5-b]pyridin-4-ium-4-olate; acetic acid			

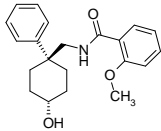
SS-3399	C ₁₅ H ₁₅ N ₇ O ₂	325.3325	
			Heteroatoms 9.0000
			Halogen atoms 0.0000
			rotatable bonds 4.0000
			H-bond acceptors 6.0000
			H-bond donors 3.0000
			LogP 1.0349
Melting_Point	LIST	350	comments
4-[[[2,4-diamino-6-pteridyl]methyl](methyl)amino]benzenecarboxylic acid			

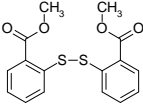
SS-3414	C ₂₁ H ₂₆ F ₂ O ₄ S	412.4998	
			Heteroatoms 7.0000
			Halogen atoms 2.0000
			rotatable bonds 1.0000
			H-bond acceptors 4.0000
			H-bond donors 3.0000
			LogP 1.6507
Melting_Point	LIST	350	comments
(6S,9R,10S,11S,13S,16R,17R)-6,9-difluoro-11,17-dihydroxy-10,13,16-trimethyl-3-oxo-6,7,8,9,10,11,12,13,14,15,16,17-dodecahydro-3H-cyclopenta[a]phenanthrene-17-carboxylic S-acid			

SS-3417	C ₁₈ H ₂₃ NO ₂	285.3895	
			Heteroatoms 3.0000
			Halogen atoms 0.0000
			rotatable bonds 1.0000
			H-bond acceptors 3.0000
			H-bond donors 0.0000
			LogP 2.5116
Melting_Point	LIST	350	comments
(1R,9S,14S)-6-methoxy-15-methyl-15-azatetracyclo[7.5.3.0-3,8-0-9,14-]heptadeca-3,5,7-trien-2-one			

SS-3433	$C_{23}H_{22}FN_3O_4$	423.4479	
		Heteroatoms	
		8.0000	
		Halogen atoms	
		1.0000	
		rotatable bonds	
		5.0000	
		H-bond acceptors	
6.0000			
H-bond donors			
3.0000			
LogP	3.9330		
Melting_Point	LIST	350	comments
4-(3-fluorophenyl)-2-piperazinoquinoline			

SS-3463	$C_{17}H_{12}BrN_3O$	354.2087	
		Heteroatoms	
		5.0000	
		Halogen atoms	
		1.0000	
		rotatable bonds	
		2.0000	
		H-bond acceptors	
3.0000			
H-bond donors			
0.0000			
LogP	3.9165		
Melting_Point	LIST	350	comments
4-[2-(1-bromoethyl)-4-oxo-3(4H)-quinazoliny]benzenecarbonitrile			

SS-3468	$C_{21}H_{25}NO_3$	339.4383	
		Heteroatoms	
		4.0000	
		Halogen atoms	
		0.0000	
		rotatable bonds	
		5.0000	
		H-bond acceptors	
3.0000			
H-bond donors			
2.0000			
LogP	3.4375		
Melting_Point	LIST	350	comments
Achiral center(s)			

SS-3470	$C_{16}H_{14}O_4S_2$	334.4156	
		Heteroatoms	
		6.0000	
		Halogen atoms	
		0.0000	
		rotatable bonds	
		7.0000	
		H-bond acceptors	
4.0000			
H-bond donors			
0.0000			
LogP	3.8936		
Melting_Point	LIST	350	comments
methyl 2-[[2-(methoxycarbonyl)phenyl]disulfanyl]benzenecarboxylate			