

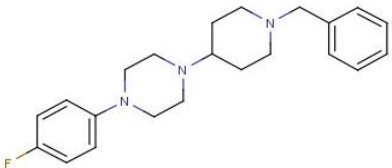
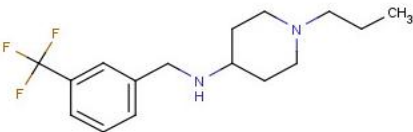
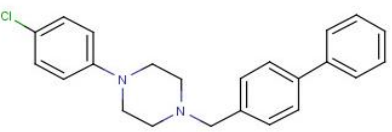
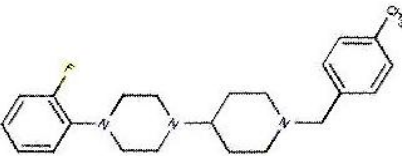
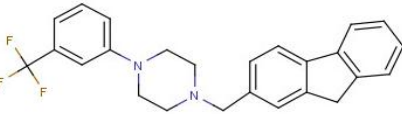
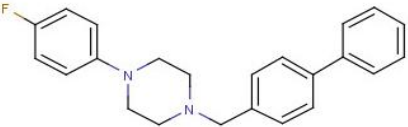
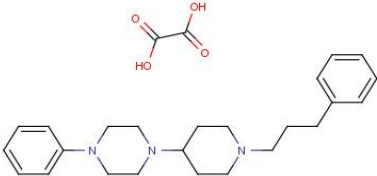
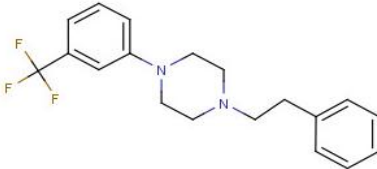
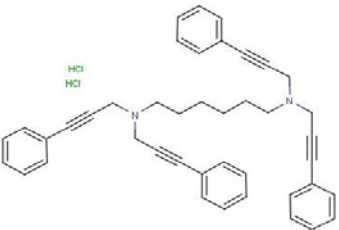
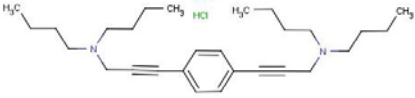
ID	structural formula	chemical formula	colored?	MW (g/ mol)	IUPAC name	MFR	Binding on Lipid II?	active against S.aureus	active against E.coli	cytotoxic for Caco II (C _{50%} survival)	cytotoxic for Jurkat (C _{50%} survival)	compound category	Nr.
5457685		C ₂₂ H ₂₈ F N ₃	no	353.5	1-(1-benzyl-4-piperidinyl)-4-(4-fluorophenyl)piperazine	Chem Bridge	No	No	No	No	?	A	1
5452876		C ₁₆ H ₂₃ F ₃ N ₂	no	300.4	1-propyl-N-[3-(trifluoromethyl)benzyl]-4-piperidinamine	Chem Bridge	No	No	No	No	?	A	2
5270046		C ₂₃ H ₂₃ Cl N ₂	no	362.9	1-(4-biphenylmethyl)-4-(4-chlorophenyl)piperazine	Chem Bridge	No	No	No	No	?	A	3
6711103		C ₂₃ H ₃₀ F N ₃	no	367.5	1-(2-fluorophenyl)-4-[1-(4-methylbenzyl)-4-piperidinyl]piperazine	Chem Bridge	No	No	No	No	?	A	4
5418391		C ₂₅ H ₂₃ F ₃ N ₂	no	408.5	1-(9H-fluoren-2-ylmethyl)-4-[3-(trifluoromethyl)phenyl]piperazine	Chem Bridge	No	No	No	Yes (159)	?	A	5

plate A

5267798		$C_{23} H_{23} F N_2$	no	346.4	1-(4-biphenylmethyl)-4-(4-fluorophenyl)piperazine	Chem Bridge	No	No	No	No	?	A	6
6785396		$C_{24} H_{33} N_3 \cdot C_2 H_2 O_4$	no	453.6	1-phenyl-4-[1-(3-phenylpropyl)-4-piperidinyl]piperazine oxalate	Chem Bridge	No	No	No	Yes (168)	?	A	7
5422765		$C_{19} H_{21} F_3 N_2$	no	334.4	1-(2-phenylethyl)-4-[3-(trifluoromethyl)phenyl]piperazine	Chem Bridge	Yes	No	No	Yes (130)	?	A*	8
5230300		$C_{42} H_{40} N_2 \cdot 2 Cl H$	no	645.7	N,N,N',N'-tetrakis(3-phenyl-2-propyn-1-yl)-1,6-hexanediamine dihydrochloride	Chem Bridge	No	No	No	No	?	A	9
5230313		$C_{28} H_{44} N_2 \cdot 2 Cl H$	no	481.6	3,3'-(1,4-phenylene) bis(N,N-dibutyl-2-propyn-1-amine) dihydrochloride	Chem Bridge	Yes	No	No	Yes (366)	?	A*	10

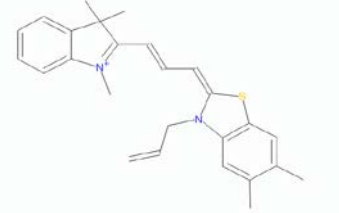
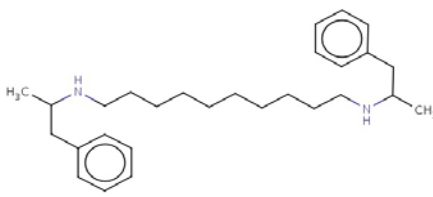
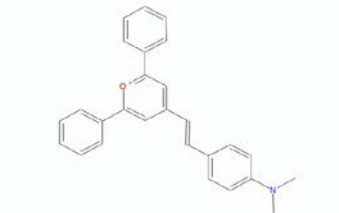
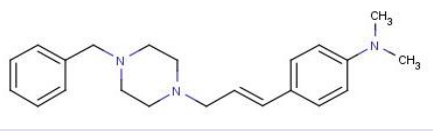
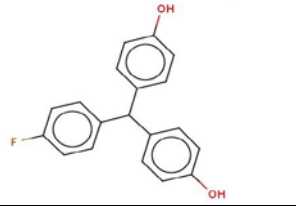
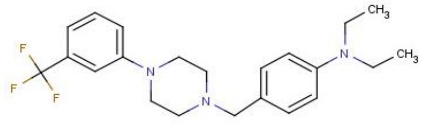
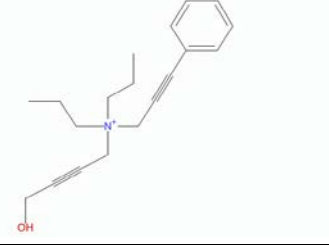
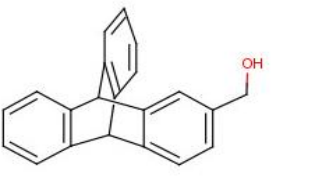
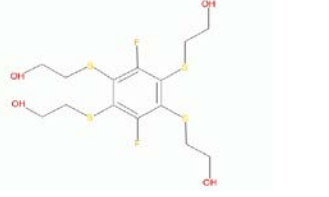
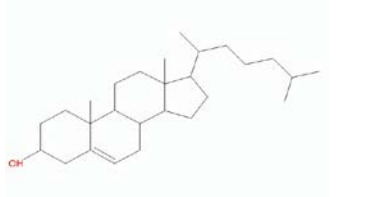
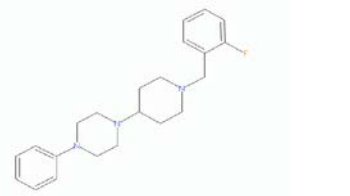
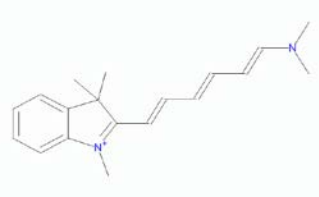

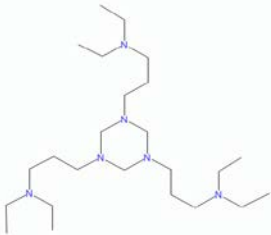
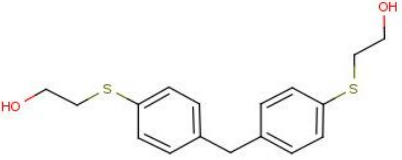
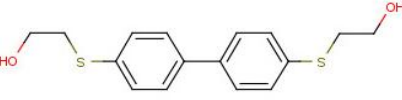
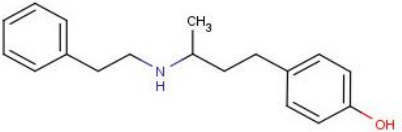
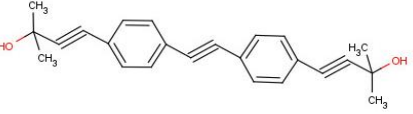
7771-0701		C ₂₆ H ₂₉ N ₂ S	yes	401.6	n/a	Chem Div	Yes	Yes (15.625)	Yes (31.25)	Yes (16,7)	?	B/C*	11
8006-3639		C ₂₈ H ₄₄ N ₂	no	408.7	n/a	Chem Div	No	Yes (125)	Yes (125)	Yes (3,6)	?	B	12
1499-1221		C ₂₇ H ₂₄ N O	yes	378.5	n/a	Chem Div	No	Yes (1.95)	Yes (125)	Yes (8,9)	?	B/C	13
5429346		C ₂₂ H ₂₉ N ₃	(yes)	335.5	4-[3-(4-benzyl-1-piperaziny)-1-propen-1-yl]-N,N-dimethylaniline	Chem Bridge	Yes	Yes (500)	No	Yes (131,9)	?	C*	14
0251-0215		C ₁₉ H ₁₅ F O ₂	no	294.3	n/a	Chem Div	No	Yes (125)	No	Yes (17,1)	?	B/C	15
5427129		C ₂₂ H ₂₈ F ₃ N ₃	no	391.5	N,N-diethyl-4-({4-[3-(trifluoromethyl)phenyl]-1-piperaziny)methyl} aniline	Chem Bridge	Yes	(No)	No	Yes (192,2)	?	A*	16


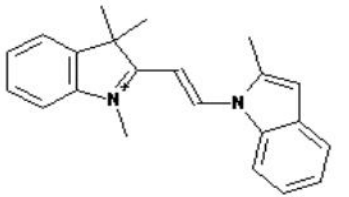
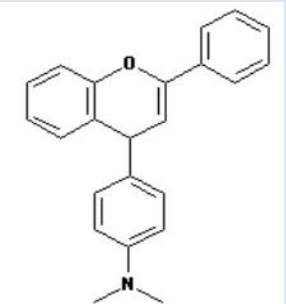
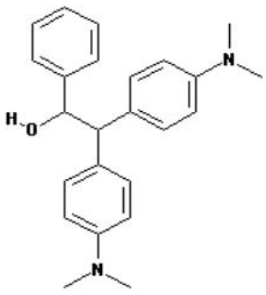
plate C

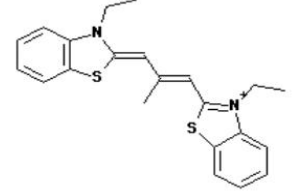
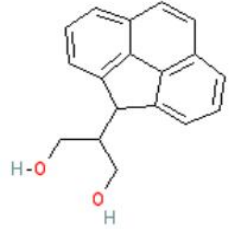
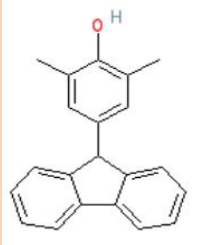
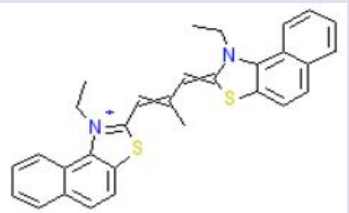
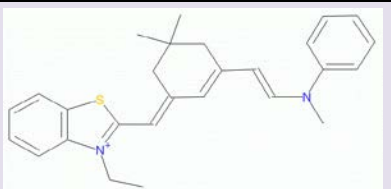
4636-0141		C ₁₉ H ₂₆ N O	no	284.4	(4-hydroxybut-2-yn-1-yl)(3-phenylprop-2-yn-1-yl)dipropylazanium	Chem Div	No	No	No	No	?	A	17
5100015		C ₂₁ H ₁₆ O	no	284.4	pentacyclo[6.6.6.0-2,7~.0-9,14~.0-15,20]-jicosa-2,4,6,9,11,13,15,17,19-nonaen-4-ylmethanol	Chem Bridge	No	Yes (500)	No	Yes (68)	?	B/C	18
0438-0367		C ₁₄ H ₂₀ F ₂ O ₄ S ₄	no	418.6	2-((2,5-difluoro-3,4,6-tris((2-hydroxyethyl)sulfanyl)phenyl)sulfanyl)ethan-1-ol	Chem Div	No	No	No	No	?	A	19
N050-0022		C ₂₇ H ₄₆ O	no	386.7	2,15-dimethyl-14-(6-methylheptan-2-yl)tetracyclo[8.7.0.0 ^{2,7} .0 ^{11,15}]heptadec-7-en-5-ol	Chem Div	No	No	No	Yes (122,9)	?	A	20
5607-0206		C ₂₂ H ₂₈ F N ₃	no	353.5	1-{1-[(2-fluorophenyl)methyl]piperidin-4-yl}-4-phenylpiperazine	Chem Div	No	No	No	No	?	A	21

5400-0379		C ₁₉ H ₂₅ N ₂	yes	281.4	n/a	Chem Div	No	Yes (125)	No	Yes (55,8)	?	B/C	22
2729-1114		C ₁₇ H ₁₈ O S ₂	no	302.5	4-(7,8-dimethyl-3,5-dihydro-1H-2,4-benzodithiepin-3-yl) phenol	Chem Div	No	No	No	Yes (119,1)	?	A	23
000A-0859		C ₂₄ H ₅₄ N ₆	no	426.7	(3-{3,5-bis [3-(diethylamino)propyl]-1,3,5-triazinan-1-yl}propyl) diethylamine	Chem Div	Yes	Yes (500)	Yes (500)	Yes (418,6)	?	B*	24
5210734		C ₁₇ H ₂₀ O ₂ S ₂	no	320.5	2,2'-(methylenebis(4,1-phenylene)) diethanol	Chem Bridge	No	No	No	No	?	A	25
5230234		C ₁₆ H ₁₈ O ₂ S ₂	no	306.4	2,2'-(4,4'-biphenyldiyl)bis(thio) diethanol	Chem Bridge	No	No	No	No	?	A	26
5460400		C ₁₈ H ₂₃ NO	no	269.4	4-(3-((2-phenylethyl)amino)butyl) phenol	Chem Bridge	No	No	No	No	?	A	27
7191067		C ₂₄ H ₂₂ O ₂	no	342.4	4,4'-(1,2-ethynediyl)di-4,1-phenylene bis(2-methyl-3-butyn-2-ol)	Chem Bridge	No	No	No	No	?	A	28

pl

plate E (+ DMSO)

7411164		$C_{14}H_{20}F_2O_4$ S_4	no	418.6	2,2',2''- [[3,6-difluorobenzene- 1,2,4,5-tetrayl]tetrakis (thio)]tetraethanol	Chem Bridge	No	No	No	No	?	A	29
4431/1		$C_{22}H_{23}N_2$	No	315.4	1,3,3-trimethyl-2- (2-(2-methyl-1H-indol-1-yl) vinyl)-3H-1λ ⁵ -indole	NCI	No	Yes (250)	No	No	?	C	31
55870/1		$C_{23}H_{21}NO$	No	327.4	N,N-dimethyl-4- (2-phenyl-4H-chromen-4-yl) aniline	NCI	Yes	Yes (250)	No	Yes (25,9)	?	C*	32
35487/2		$C_{24}H_{28}N_2O$	No	360.5	2,2-bis (4-(dimethylamino)phenyl)- 1-phenylethanol	NCI	No	No	No	No	?	A	33

96932/4		C ₂₂ H ₂₃ N ₂ S ₂	Yes	379.6	3-ethyl-2-(3-(3-ethyl-1,3-benzothiazol-2(3H)-ylidene)-2-methyl-1-propenyl)-1,3λ ⁵ -benzothiazole	NCI	No	Yes (15,6)	Yes (15.625)	Yes (19)	?	B	34
625586/1		C ₁₈ H ₁₆ O ₂	No	264.3	2-(4H-cyclopenta[def]phenanthren-4-yl)-1,3-propanediol	NCI	No	No	No	Yes (83,8)	?	A	35
610995/1		C ₂₁ H ₁₈ O	No	286.4	4-(9H-fluoren-9-yl)-2,6-dimethylphenol	NCI	Yes	Yes (125)	No	Yes (9,2)	?	B/C*	36
290437/2		C ₃₀ H ₂₇ N ₂ S ₂	Yes	479.7	1-ethyl-2-(3-(1-ethylnaphtho[1,2-d][1,3]thiazol-2(1H)-ylidene)-2-methyl-1-propenyl)-1λ ⁵ -naphtho[1,2-d][1,3]thiazole	NCI	No	Yes (1,95)	Yes (31.35)	Yes (2,2)	?	B/C	37
4090-1978		C ₂₇ H ₃₁ N ₂ S	Yes	415.6	2-(((1E)-5,5-dimethyl-3-((E)-2-[methyl(phenyl)amino]ethenyl)cyclohex-2-en-1-ylidene)methyl)-3-ethyl-1,3-benzothiazol-3-ium	Chem Div	No	Yes (15,625)	Yes (62,5)	Yes (16,7)	?	B/C	38

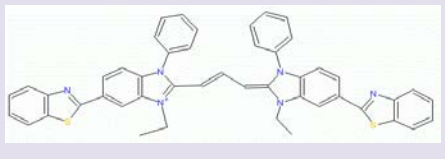

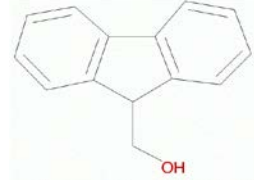
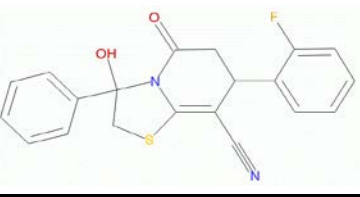
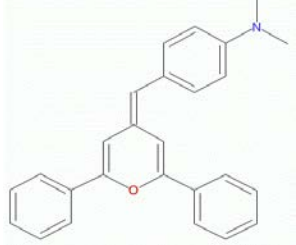
2332-1014		$C_{47}H_{37}N_6S_2$	Yes	750.0	n/a	Chem Div	No	Yes (62,5)	No	Yes (22,6)	?	B/C	39
4890-0291		$C_{26}H_{30}N_3O_2S$	Yes	432.6	n/a	Chem Div	No	Yes (7,81)	Yes (62,5)	Yes (10,7)	?	B/C	40
4121-0081		$C_{14}H_{12}O$	No	196.2	9H-fluoren-9-ylmethanol	Chem Div	No	No	No	Yes (201,8)	?	A	41
C611-0808		$C_{20}H_{15}FN_2O_2S$	No	366.4	n/a	Chem Div	No	No	No	No	?	A	42
3377-0105		$C_{26}H_{23}NO$	No	365.5	4-[(2,6-diphenyl-4H-pyran-4-ylidene)methyl]-N,N-dimethylaniline	Chem Div	No	Yes (500)	No	Yes (100,4)	?	A/B	43

plate 2

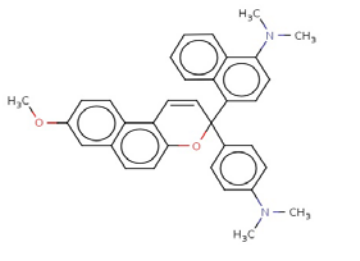
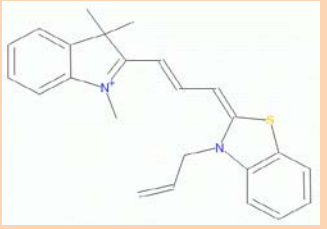
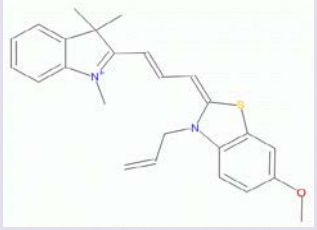
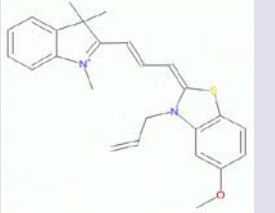
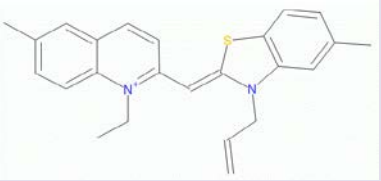
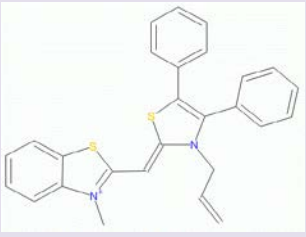
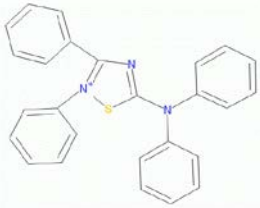
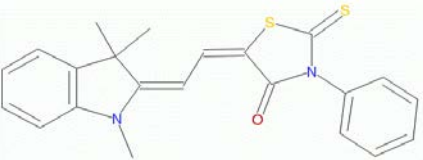
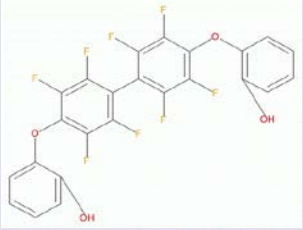
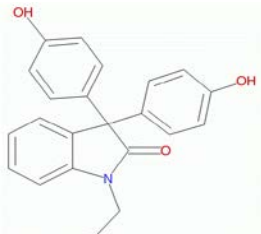
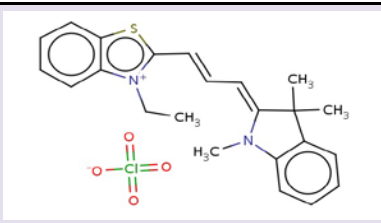
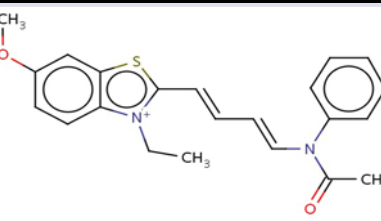
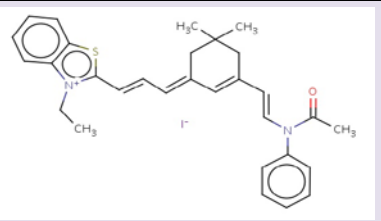
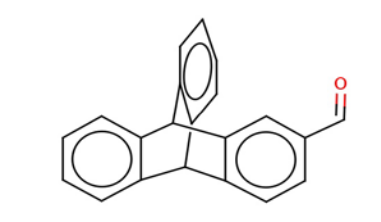
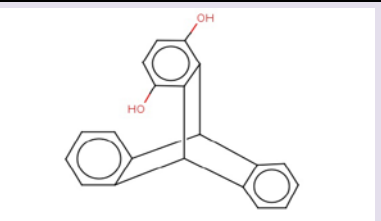
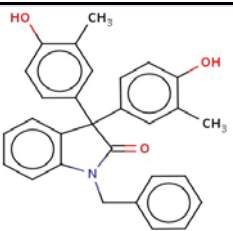
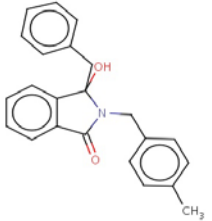
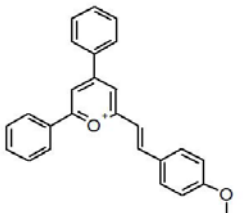
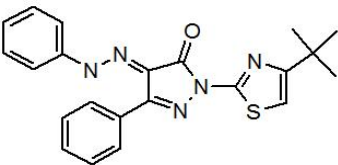
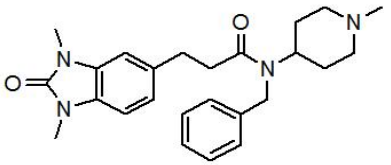
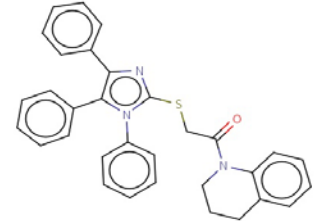
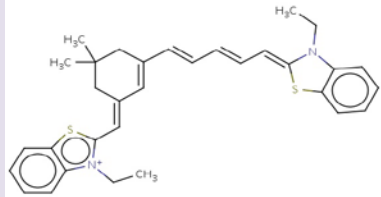
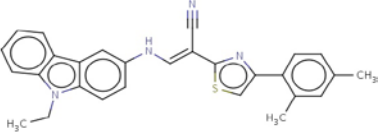
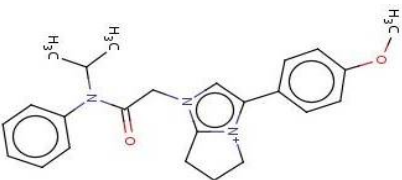
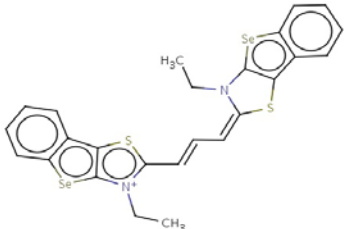
2331-0475		$C_{34}H_{32}N_2O_2$	No	500.6	n/a	Chem Div	No	No	No	No	?	A	44
7771-0699		$C_{24}H_{25}N_2S$	Yes	373.5	n/a	Chem Div	No	Yes (7,8)	Yes (125)	Yes (7,9)	?	B	45
7771-0716		$C_{25}H_{27}N_2O_S$	Yes	403.6	n/a	Chem Div	No	Yes (15,625)	Yes (125)	Yes (5,3)	?	B	46
7771-0700		$C_{25}H_{27}N_2O_S$	Yes	403.6	n/a	Chem Div	No	Yes (7,8)	Yes (62,5)	Yes (3,7)	?	B	47
7165-0606		$C_{24}H_{25}N_2S$	Yes	373.5	n/a	Chem Div	No	Yes (7,8)	Yes (31,25)	Yes (11,9)	?	B	48

plate 3

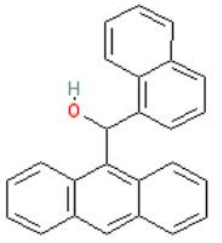
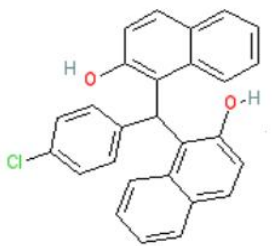
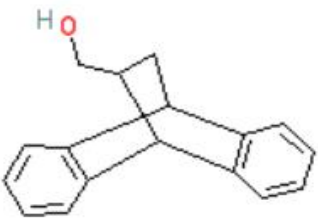
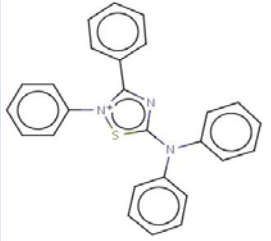
7165-0758		$C_{27}H_{23}N_2S_2$	No	439.6	n/a	Chem Div	No	Yes (7,8)	Yes (125)	Yes (6,7)	?	B	49
1492-0330		$C_{26}H_{20}N_3S$	No	406.5	5-(diphenylamino)-2,3-diphenyl-1,2,4,5-thiadiazol-2-ylum	Chem Div	Yes	No	No	Yes (101,2)	?	A*	50
2101-0102		$C_{22}H_{20}N_2O S_2$	Yes	392.5	(5E)-3-phenyl-2-sulfanylidene-5-[2-[(2E)-1,3,3-trimethyl-2,3-dihydro-1H-indol-2-ylidene]ethylidene]-1,3-thiazolidin-4-one	Chem Div	No	No	No	No	?	A	51
1611-0203		$C_{24}H_{10}F_8O_4$	No	514.3	2-[2,3,5,6-tetrafluoro-4-[2,3,5,6-tetrafluoro-4-(2-hydroxyphenoxy)phenyl]phenoxy]phenol	Chem Div	No	Yes (3,9)	No	Yes (4,2)	?		52
4896-3423		$C_{22}H_{19}NO_3$	No	345.4	1-ethyl-3,3-bis(4-hydroxyphenyl)-2,3-dihydro-1H-indol-2-one	Chem Div	No	No	No	Yes (72,1)	?	A	53

5660386		$C_{23}H_{25}ClN_2O_4S$	Yes	461.0	3-ethyl-2-[(1E)-3-[(2Z)-1,3,3-trimethyl-2,3-dihydro-1H-indol-2-ylidene]prop-1-en-1-yl]-1,3-benzothiazol-3-ium perchlorate	Chem Bridge	No	Yes (7,8)	Yes (125)	Yes (5,6)	?		54
STK 874226		$C_{22}H_{23}N_2O_2S$	Yes	379.5	2-[(1E,3E)-4-[acetyl(phenyl)amino]buta-1,3-dien-1-yl]-3-ethyl-6-methoxy-1,3-benzothiazol-3-ium	VitasM Lab	No	Yes (125)	Yes (250)	No	?		55
5119716		$C_{30}H_{33}IN_2OS$	Yes	596.6	2-[(1E)-3-[(1E)-5,5-dimethyl-3-[(E)-2-(N-phenylacetamido)ethenyl]cyclohex-2-en-1-ylidene]prop-1-en-1-yl]-3-ethyl-1,3-benzothiazol-3-ium iodide	Chem Bridge	No	Yes (125)	No	Yes (52,7)	?		56
5100004		$C_{21}H_{14}O$	No	282.3	pentacyclo[6.6.6.0 ^{2,7} .0 ^{9,14} .0 ^{15,20}]jicosa-2,4,6,9,11,13,15,17,19-nonaene-4-carbaldehyde	Chem Bridge	No	No	No	No	?	A	57
5190620		$C_{20}H_{14}O_2$	(Yes)	286.3	pentacyclo[6.6.6.0 ^{2,7} .0 ^{9,14} .0 ^{15,20}]jicosa-2(7),3,5,9,11,13,15,17,19-nonaene-3,6-diol	Chem Bridge	No	Yes (62,5)	No	Yes (3,7)	?		58

5142587		C ₂₉ H ₂₅ N O ₃	No	435.5	1-benzyl-3,3-bis(4-hydroxy-3-methylphenyl)-2,3-dihydro-1H-indol-2-one	Chem Bridge	No	Yes (15,625)	No	Yes (4,4)	?		59
7832238		C ₂₃ H ₂₁ N O ₂	No	343.4	3-benzyl-3-hydroxy-2-[(4-methylphenyl)methyl]-2,3-dihydro-1H-isoindol-1-one	Chem Bridge	No	No	No	No	?	A	60
BAS 00138032		C ₂₆ H ₂₁ O ₂	Yes	365.4	2-[2-(4-methoxy-phenyl)-vinyl]-4,6-diphenyl-pyranilium	Asinex	No	No	No	No	?	A	61
BAS 00691248		C ₂₂ H ₂₁ N ₅ O S	Yes	403.5	2-(4-tert-butyl-thiazol-2-yl)-5-phenyl-4-(phenyl-hydrazono)-2,4-dihydro-pyrazol-3-one	Asinex	No	No	No	No	?	A	62
SYN 22879441		C ₂₅ H ₃₂ N ₄ O ₂	No	420.6	N-Benzyl-3-(1,3-dimethyl-2-oxo-2,3-dihydro-1H-benzoimidazol-5-yl)-N-(1-methyl-piperidin-4-yl)-propionamide	Asinex	No	No	No	No	?	A	63

ST 4098270		$C_{32}H_{27}N_3O$ S	No	501.7	1-(1,2,3,4-tetrahydroquinolin-1-yl)-2-[(1,4,5-triphenyl-1H-imidazol-2-yl)sulfanyl]ethan-1-one	Tim Tec	No	No	No	No	?	A	64
STK 792971		$C_{32}H_{35}N_2S_2$	Yes	511.8	3-ethyl-2-[(E)-{3-[(1E,3E,5Z)-5-(3-ethyl-1,3-benzothiazol-2(3H)-ylidene)penta-1,3-dien-1-yl]-5,5-dimethylcyclohex-2-en-1-ylidene)methyl]-1,3-benzothiazol-3-ium	VitasM Lab	No	Yes (62,5)	No	No	?	C	65
STK 537076		$C_{28}H_{24}N_4S$	No	448.6	(2E)-2-[4-(2,4-dimethylphenyl)-1,3-thiazol-2-yl]-3-[(9-ethyl-9H-carbazol-3-yl)amino]prop-2-enitrile	VitasM Lab	No	No	No	Yes (240)	?	A	66
STL05007 2		$C_{24}H_{28}N_3$ O_2	No	390.5	3-(4-methoxyphenyl)-1-(2-oxo-2-phenylpropan-2-ylamino)ethyl-1,5,6,7-tetrahydropyrrolo[1,2-a]imidazol-4-ium	VitasM Lab	No	No	No	Yes (340)	?	A	67
STK 368153		$C_{25}H_{21}N_2S_2$ Se_2	Yes	571.5	3-ethyl-2-[(1E,3E)-3-(3-ethyl[1]benzoselenopheno[2,3-d][1,3]thiazol-2(3H)-ylidene)prop-1-en-1-yl][1]benzoselenopheno[2,3-d][1,3]thiazol-3-ium	VitasM Lab	Yes	Yes (7,8)	Yes (7,8)	Yes (9,6)	?	B*	68

plate

179415/1		$C_{25}H_{18}O$	No	334.4	9-anthryl(1-naphthyl)methanol	NCI	Yes	Yes (3,9)	No	No	?	C*	69
363003/1		$C_{27}H_{19}ClO_2$	No	410.9	n/a	NCI	Yes	Yes (3,9)	No	Yes (3,5)	?	B/C*	70
55266/1		$C_{17}H_{16}O$	No	236.3	n/a	NCI	Yes	No	No	Yes (208,6)	?	A*	71
1492-0330		$C_{26}H_{20}N_3S$	No	406.5	5-(diphenylamino)-2,3-diphenyl-1,2,4-thiadiazol-2-ylum	Chem Div	Yes	Yes (125)	No	Yes (143,3)	?	B/C*	72

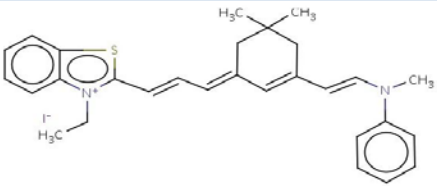
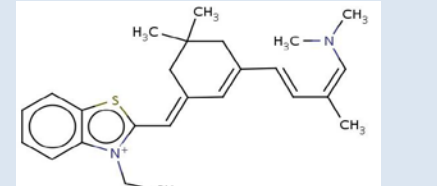
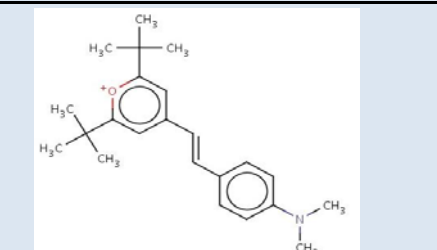
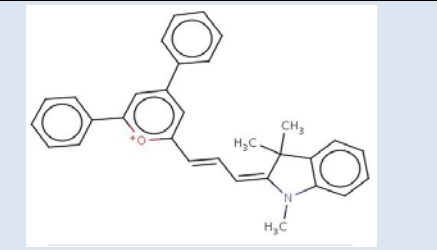
5107930		$C_{29}H_{33}IN_2S$	Yes	568.6	2-[(1E)-3-[(1E)-5,5-dimethyl-3-[(E)-2-[methyl(phenyl)amino]ethenylidene]prop-1-en-1-yl]-3-ethyl-1,3-benzothiazol-3-ium iodide	Chem Bridge	Yes	Yes (31,25)	Yes (125)	Yes (27,9)	?	B/C*	73
4090-1979		$C_{25}H_{33}N_2S$	Yes	393.6	n/a	Chem Div	Yes	Yes (62,5)	No	Yes (46,2)	?	B/C*	74
1493-0289		$C_{23}H_{32}NO$	Yes	338.5	2,6-di-tert-butyl-4-[(E)-2-[4-(dimethylamino)phenyl]ethenyl]-1H-pyran-1-ium	Chem Div	Yes	Yes (3,9)	Yes (125)	Yes (6,8)	?	B/C*	75
BAS 0012753 8		$C_{31}H_{28}NO$	Yes	430.6	2,4-diphenyl-6-[(1E)-3-[(2E)-1,3,3-trimethyl-2,3-dihydro-1H-indol-2-ylidene]prop-1-en-1-yl]-1H-pyran-1-ium	Asinex	Yes	Yes (1,95)	Yes (7,8)	Yes (2,7)	?	B/C*	76
All concentrations are in μM													total amount 75 + DMSO

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*Compound category	
A	<p>Not effective compound</p> <p>Not active against S.aureus Not active or active against E.coli Not toxic or toxic for tested cell lines</p>
B	<p>Effective but not specific</p> <p>Highly active against S.aureus Highly active against E.coli Toxic for tested cell lines</p>
C	<p>Effective and specific, antibiotic candidate</p> <p>Highly active against S.aureus less active against E.coli Not (strong) toxic for tested cell lines</p>
*	Lipid II binding

IC_{100%} Inhibitory concentration on which 100% killing of bacteria occurred, determined by no bacterial regrowth after exposure to the compound