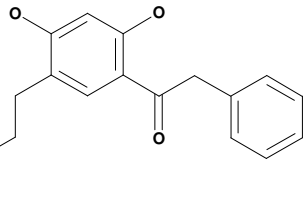
Article's title: DERIVATIVES OF PIPERAZINES AS POTENTIAL THERAPEUTIC AGENTS FOR ALZHEIMER'S DISEASE

Authors: Elena Popugaeva, Daria Chernyuk, Hua Zhang, Tatyana Y. Postnikova, Karina Pats, Elena Fedorova, Vladimir Poroikov, Aleksey V. Zaitsev, Ilya Bezprozvanny

Journal title: Molecular Pharmacology

Name of the supplemental file: List of analogues of TRPC6 agonists obtained from InterBioScreen ltd.

InterBioScreen Ltd. analogues of TRPC6 agonists

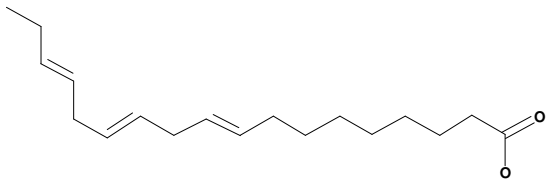


Analog ID: TRPC6-0001
Analog name: HYP-1
Similarity: 0.8281

ID:	Salt:	MW:
STOCK1N-01059		284.3583
Formula:	Comment:	Index:
$C_{18}H_{20}O_3$		RDNC

IUPAC Name: 1-(5-butyl-2,4-dihydroxyphenyl)-2-phenylethanone

H-Bond Donors:	H-Bond Acceptors:	Rotatable Bonds:	Rings:	TPSA:	CLogP:
2	3	6	2	57.5300	5.2140

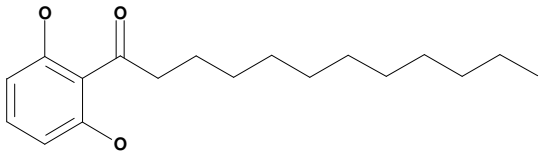


Analog ID: TRPC6-0013
Analog name: 20-HETE
Similarity: 0.8429

ID:	Salt:	MW:
STOCK1N-57379		278.4386
Formula:	Comment:	Index:
$C_{18}H_{30}O_2$		DNC

IUPAC Name: (9E,12E,15E)-octadeca-9,12,15-trienoic acid

H-Bond Donors:	H-Bond Acceptors:	Rotatable Bonds:	Rings:	TPSA:	CLogP:
1	2	13	0	37.3000	6.8180

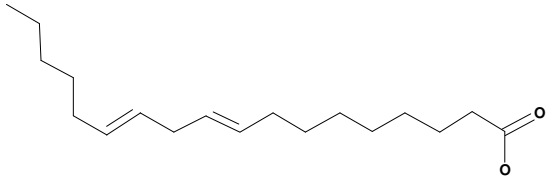


Analog ID: TRPC6-0003
Analog name: HYP-9
Similarity: 0.8293

ID:	Salt:	MW:
STOCK1N-66516		292.4221
Formula:	Comment:	Index:
$C_{18}H_{28}O_3$		RGNC

IUPAC Name: 1-(2,6-dihydroxyphenyl)dodecan-1-one

H-Bond Donors:	H-Bond Acceptors:	Rotatable Bonds:	Rings:	TPSA:	CLogP:
2	3	11	1	57.5300	6.7000

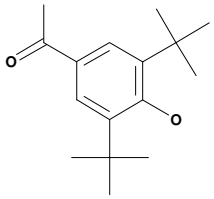


Analog ID: TRPC6-0013
Analog name: 20-HETE
Similarity: 0.8286

ID:	Salt:	MW:
STOCK1N-69973		280.4545
Formula:	Comment:	Index:
$C_{18}H_{32}O_2$		DNC

IUPAC Name: (9E,12E)-octadeca-9,12-dienoic acid

H-Bond Donors:	H-Bond Acceptors:	Rotatable Bonds:	Rings:	TPSA:	CLogP:
1	2	14	0	37.3000	7.3020

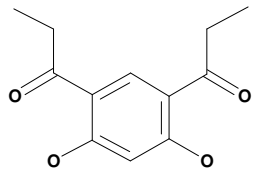


Analog ID: TRPC6-0001
Analog name: HYP-1
Similarity: 0.8000

ID:	Salt:	MW:
STOCK1S-52790		248.3685
Formula:	Comment:	Index:
$C_{16}H_{24}O_2$		SC

IUPAC Name: 1-(3,5-di-tert-butyl-4-hydroxyphenyl)ethanone

H-Bond Donors:	H-Bond Acceptors:	Rotatable Bonds:	Rings:	TPSA:	CLogP:
1	2	3	1	37.3000	4.9070

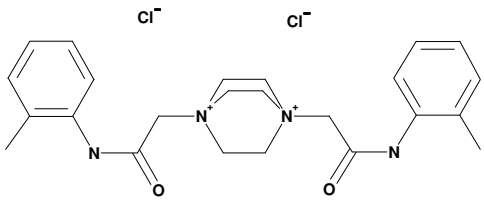


Analog ID: TRPC6-0001
Analog name: HYP-1
Similarity: 0.9182

ID:	Salt:	MW:
STOCK1S-64402		222.2430
Formula:	Comment:	Index:
$C_{12}H_{14}O_4$		RSC

IUPAC Name: 1,1'-(4,6-dihydroxy-1,3-phenylene)bis(propan-1-one)

H-Bond Donors:	H-Bond Acceptors:	Rotatable Bonds:	Rings:	TPSA:	CLogP:
2	4	4	1	74.6000	2.1780

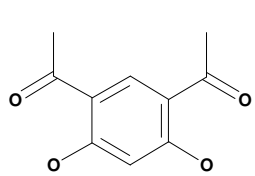


Analog ID: TRPC6-0005
Analog name: 871099
Similarity: 0.8160

ID:	Salt:	MW:
STOCK1S-95722	2 Cl-	479.4542
Formula:	Comment:	Index:
$C_{24}H_{32}Cl_2N_4O_2$		SC

IUPAC Name: 1,4-bis(2-oxo-2-(o-tolylamino)ethyl)-1,4-diazabicyclo[2.2.2]octane-1,4-diium chloride

H-Bond Donors:	H-Bond Acceptors:	Rotatable Bonds:	Rings:	TPSA:	CLogP:
2	6	8	4	58.2000	0.8700

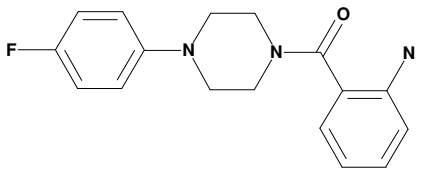


Analog ID: TRPC6-0001
Analog name: HYP-1
Similarity: 0.8000

ID:	Salt:	MW:
STOCK2S-10458		194.1888
Formula:	Comment:	Index:
$C_{10}H_{10}O_4$		RSC

IUPAC Name: 1,1'-(4,6-dihydroxy-1,3-phenylene)diethanone

H-Bond Donors:	H-Bond Acceptors:	Rotatable Bonds:	Rings:	TPSA:	CLogP:
2	4	2	1	74.6000	1.1200

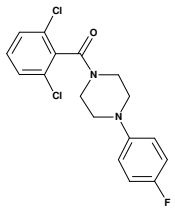


Analog ID: TRPC6-0004
Analog name: 830288
Similarity: 0.8060

ID:	Salt:	MW:
STOCK2S-48512		299.3509
Formula: $C_{17}H_{18}FN_3O$	Comment:	Index: SC

IUPAC Name: (2-aminophenyl)(4-(4-fluorophenyl)piperazin-1-yl)methanone

H-Bond Donors:	H-Bond Acceptors:	Rotatable Bonds:	Rings:	TPSA:	CLogP:
1	4	3	3	49.5700	2.3610

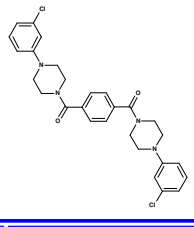


Analog ID: TRPC6-0004
Analog name: 830288
Similarity: 0.8488

ID:	Salt:	MW:
STOCK2S-60341		353.2263
Formula: $C_{17}H_{15}Cl_2FN_2O$	Comment:	Index: RSC

IUPAC Name: (2,6-dichlorophenyl)(4-(4-fluorophenyl)piperazin-1-yl)methanone

H-Bond Donors:	H-Bond Acceptors:	Rotatable Bonds:	Rings:	TPSA:	CLogP:
0	3	3	3	23.5500	4.6060

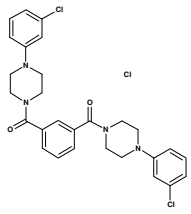


Analog ID: TRPC6-0004
Analog name: 830288
Similarity: 0.8350

ID:	Salt:	MW:
STOCK2S-62607		523.4670
Formula: $C_{28}H_{28}Cl_2N_4O_2$	Comment:	Index: SC

IUPAC Name: 1,4-phenylenebis((4-(3-chlorophenyl)piperazin-1-yl)methanone)

H-Bond Donors:	H-Bond Acceptors:	Rotatable Bonds:	Rings:	TPSA:	CLogP:
0	6	6	5	47.1000	5.4290

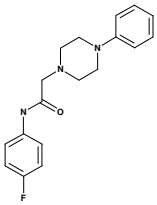


Analog ID: TRPC6-0004
Analog name: 830288
Similarity: 0.8186

ID:	Salt:	MW:
STOCK2S-63514	HCl	559.9279
Formula: $C_{28}H_{29}Cl_3N_4O_2$	Comment:	Index: SC

IUPAC Name: 1,3-phenylenebis((4-(3-chlorophenyl)piperazin-1-yl)methanone) hydrochloride

H-Bond Donors:	H-Bond Acceptors:	Rotatable Bonds:	Rings:	TPSA:	CLogP:
0	6	6	5	47.1000	5.4290

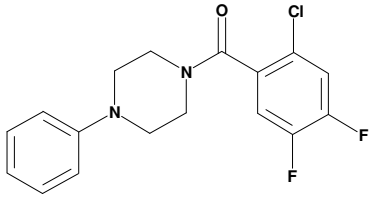


Analog ID: TRPC6-0006
Analog name: 880395
Similarity: 0.8232

ID:	Salt:	MW:
STOCK3S-16264		313.3780
Formula: $C_{18}H_{20}FN_3O$	Comment:	Index: SC

IUPAC Name: N-(4-fluorophenyl)-2-(4-phenylpiperazin-1-yl)acetamide

H-Bond Donors:	H-Bond Acceptors:	Rotatable Bonds:	Rings:	TPSA:	CLogP:
1	4	5	3	35.5800	3.6850

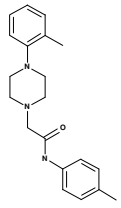


Analog ID: TRPC6-0004
Analog name: 830288
Similarity: 0.8702

ID:	Salt:	MW:
STOCK3S-26021		336.7717
Formula: $C_{17}H_{15}ClF_2N_2O$	Comment:	Index: SC

IUPAC Name: (2-chloro-4,5-difluorophenyl)(4-phenylpiperazin-1-yl)methanone

H-Bond Donors:	H-Bond Acceptors:	Rotatable Bonds:	Rings:	TPSA:	CLogP:
0	3	3	3	23.5500	3.8040

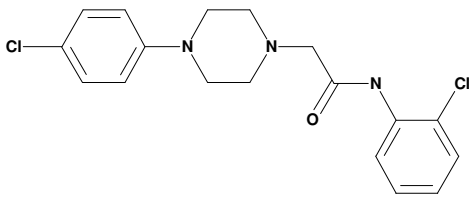


Analog ID: TRPC6-0005
Analog name: 871099
Similarity: 0.8232

ID:	Salt:	MW:
STOCK3S-29732		323.4418
Formula: $C_{20}H_{25}N_3O$	Comment:	Index: SC

IUPAC Name: N-(p-tolyl)-2-(4-(o-tolyl)piperazin-1-yl)acetamide

H-Bond Donors:	H-Bond Acceptors:	Rotatable Bonds:	Rings:	TPSA:	CLogP:
1	4	5	3	35.5800	4.2820

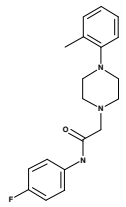


Analog ID: TRPC6-0005
Analog name: 871099
Similarity: 0.8650

ID:	Salt:	MW:
STOCK3S-46766		364.2776
Formula: $C_{18}H_{19}Cl_2N_3O$	Comment:	Index: SC

IUPAC Name: N-(2-chlorophenyl)-2-(4-(4-chlorophenyl)piperazin-1-yl)acetamide

H-Bond Donors:	H-Bond Acceptors:	Rotatable Bonds:	Rings:	TPSA:	CLogP:
1	4	5	3	35.5800	4.2240

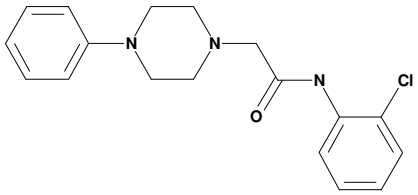


Analog ID: TRPC6-0006
Analog name: 880395
Similarity: 0.9024

ID:	Salt:	MW:
STOCK3S-50741		327.4051
Formula: $C_{19}H_{22}FN_3O$	Comment:	Index: SC

IUPAC Name: N-(4-fluorophenyl)-2-(4-(o-tolyl)piperazin-1-yl)acetamide

H-Bond Donors:	H-Bond Acceptors:	Rotatable Bonds:	Rings:	TPSA:	CLogP:
1	4	5	3	35.5800	4.1190

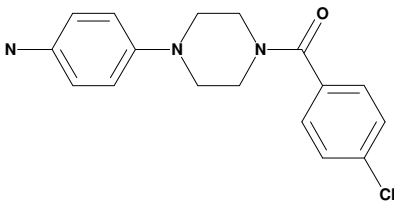


Analog ID: TRPC6-0005
Analog name: 871099
Similarity: 0.8812

ID:	Salt:	MW:
STOCK3S-51164		329.8326
Formula: $C_{18}H_{20}ClN_3O$	Comment:	Index: SC

IUPAC Name: N-(2-chlorophenyl)-2-(4-phenylpiperazin-1-yl)acetamide

H-Bond Donors:	H-Bond Acceptors:	Rotatable Bonds:	Rings:	TPSA:	CLogP:
1	4	5	3	35.5800	3.4050

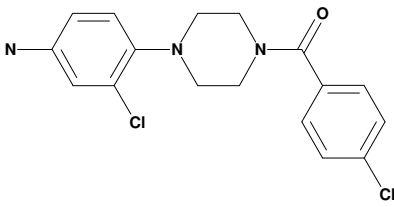


Analog ID: TRPC6-0004
Analog name: 830288
Similarity: 0.8141

ID:	Salt:	MW:
STOCK3S-96022		315.8055
Formula: $C_{17}H_{18}ClN_3O$	Comment:	Index: SC

IUPAC Name: (4-(4-aminophenyl)piperazin-1-yl)(4-chlorophenyl)methanone

H-Bond Donors:	H-Bond Acceptors:	Rotatable Bonds:	Rings:	TPSA:	CLogP:
1	4	3	3	49.5700	2.3260

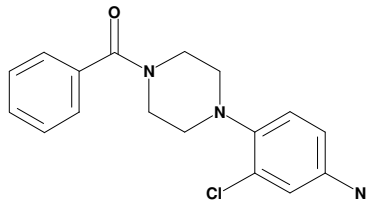


Analog ID: TRPC6-0004
Analog name: 830288
Similarity: 0.8039

ID:	Salt:	MW:
STOCK4S-05400		350.2505
Formula: $C_{17}H_{17}Cl_2N_3O$	Comment:	Index: SC

IUPAC Name: (4-(4-amino-2-chlorophenyl)piperazin-1-yl)(4-chlorophenyl)methanone

H-Bond Donors:	H-Bond Acceptors:	Rotatable Bonds:	Rings:	TPSA:	CLogP:
1	4	3	3	49.5700	3.3700

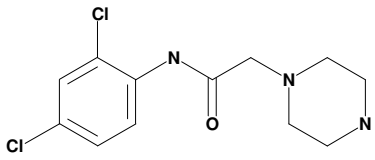


Analog ID: TRPC6-0004
Analog name: 830288
Similarity: 0.8109

ID:	Salt:	MW:
STOCK4S-10000		315.8055
Formula: $C_{17}H_{18}ClN_3O$	Comment:	Index: SC

IUPAC Name: (4-(4-amino-2-chlorophenyl)piperazin-1-yl)(phenyl)methanone

H-Bond Donors:	H-Bond Acceptors:	Rotatable Bonds:	Rings:	TPSA:	CLogP:
1	4	3	3	49.5700	2.5810

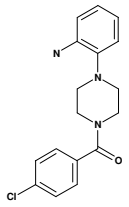


Analog ID: TRPC6-0005
Analog name: 871099
Similarity: 0.8133

ID:	Salt:	MW:
STOCK5S-58883		288.1789
Formula: $C_{12}H_{15}Cl_2N_3O$	Comment:	Index: SC

IUPAC Name: N-(2,4-dichlorophenyl)-2-(piperazin-1-yl)acetamide

H-Bond Donors:	H-Bond Acceptors:	Rotatable Bonds:	Rings:	TPSA:	CLogP:
2	4	4	2	44.3700	1.8110

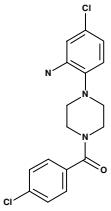


Analog ID: TRPC6-0004
Analog name: 830288
Similarity: 0.8141

ID:	Salt:	MW:
STOCK6S-09122		315.8055
Formula: $C_{17}H_{18}ClN_3O$	Comment:	Index: SC

IUPAC Name: (4-(2-aminophenyl)piperazin-1-yl)(4-chlorophenyl)methanone

H-Bond Donors:	H-Bond Acceptors:	Rotatable Bonds:	Rings:	TPSA:	CLogP:
1	4	3	3	49.5700	2.3260



Analog ID: TRPC6-0004
Analog name: 830288
Similarity: 0.8119

ID:	Salt:	MW:
STOCK6S-14276		350.2505
Formula: $C_{17}H_{17}Cl_2N_3O$	Comment:	Index: SC

IUPAC Name: (4-(2-amino-4-chlorophenyl)piperazin-1-yl)(4-chlorophenyl)methanone

H-Bond Donors:	H-Bond Acceptors:	Rotatable Bonds:	Rings:	TPSA:	CLogP:
1	4	3	3	49.5700	3.3700