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[54] **THIAZOLE BENZENESULFONAMIDES AS β3 AGONISTS FOR TREATMENT OF DIABETES AND OBESITY**

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Related U.S. Application Data

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[51] **Int. Cl.**[7] **C07D 417/10**; A61K 31/44

[52] **U.S. Cl.** **514/342**; 546/269.7; 546/256; 514/333

[58] **Field of Search** 514/342; 546/269.7

[56] **References Cited**

U.S. PATENT DOCUMENTS

5,451,677	9/1995	Fisher et al.	546/130
5,561,142	10/1996	Fisher et al.	514/312
5,705,515	1/1998	Fisher et al.	514/365

FOREIGN PATENT DOCUMENTS

0 091 749	10/1983	European Pat. Off. .
0 611 003	8/1994	European Pat. Off. .
WO 95/29159	11/1995	WIPO .

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[57] **ABSTRACT**

Thiazole substituted benzenesulfonamides are β_3 adrenergic receptor agonists with very little β_1 and β_2 adrenergic receptor activity and as such the compounds are capable of increasing lipolysis and energy expenditure in cells. The compounds thus have potent activity in the treatment of Type II diabetes and obesity. The compounds can also be used to lower triglyceride levels and cholesterol levels or raise high density lipoprotein levels or to decrease gut motility. In addition, the compounds can be used to reduced neurogenic inflammation or as antidepressant agents. The compounds are prepared by coupling an aminoalkylphenylsulfonamide with an appropriately substituted epoxide. Compositions and methods for the use of the compounds in the treatment of diabetes and obesity and for lowering triglyceride levels and cholesterol levels or raising high density lipoprotein levels or for decreasing gut motility are also disclosed.

10 Claims, No Drawings

THIAZOLE BENZENESULFONAMIDES AS β3 AGONISTS FOR TREATMENT OF DIABETES AND OBESITY

CROSS REFERENCE TO RELATED APPLICATIONS

This application is based on, and claims priority from, provisional application No. 60/036,760 filed Jan. 28, 1997.

BACKGROUND OF THE INVENTION

β-Adrenoceptors have been subclassified as β_1 and β_2 since 1967. Increased heart rate is the primary consequence of β_1-receptor stimulation, while bronchodilation and smooth muscle relaxation typically result from β_2 stimulation. Adipocyte lipolysis was initially thought to be solely a β_1-mediated process. However, more recent results indicate that the receptor mediating lipolysis is atypical in nature. These atypical receptors, later called β_3-adrenoceptors, are found on the cell surface of both white and brown adipocytes where their stimulation promotes both lipolysis (breakdown of fat) and energy expenditure.

Early developments in this area produced compounds with greater agonist activity for the stimulation of lipolysis (β_3 activity) than for stimulation of atrial rate (β_1) and tracheal relaxation (β_2). These early developments disclosed in Ainsworth et al., U.S. Pat. Nos. 4,478,849 and 4,396,627, were derivatives of phenylethanolamines.

Such selectivity for β_3-adrenoceptors could make compounds of this type potentially useful as antiobesity agents. In addition, these compounds have been reported to show antihyperglycemic effects in animal models of non-insulin-dependent diabetes mellitus.

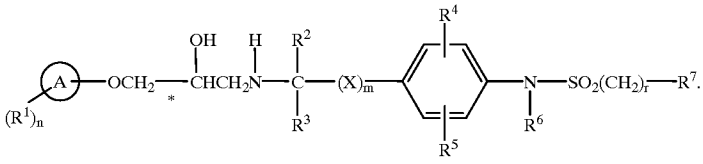
A major drawback in treatment of chronic diseases with β_3 agonists is the potential for stimulation of other β-receptors and subsequent side effects. The most likely of these include muscle tremor (β_2) and increased heart rate (β_1). Although these phenylethanolamine derivatives do possess some β_3 selectivity, side effects of this type have been observed in human volunteers. It is reasonable to expect that these side effects resulted from partial β_1 and/or β_2 agonism.

More recent developments in this area are disclosed in Ainsworth et al., U.S. Pat. No. 5,153,210, Caulkett et al., U.S. Pat. No. 4,999,377, Alig et al., U.S. Pat. No. 5,017,619, Lecount et al., European Patent 427480 and Bloom et al., European Patent 455006.

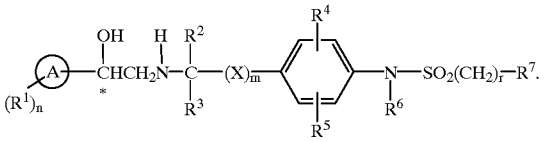
Even though these more recent developments purport to describe compounds with greater β_3 selectivity over the β_1 and β_2 activities, this selectivity was determined using rodents, in particular, rats as the test animal. Because even the most highly selective compounds, as determined by these assays, still show signs of side effects due to residual β_1 and β_2 agonist activity when the compounds are tested in humans, it has become apparent that the rodent is not a good model for predicting human β_3 selectivity.

Recently, assays have been developed which more accurately predict the effects that can be expected in humans. These assays utilize cloned human β_3 receptors which have been expressed in Chinese hamster ovary cells. See Emorine et al, *Science,* 1989, 245:1118–1121; Liggett, *Mol. Pharmacol.,* 1992, 42:634–637; and Grannemann et al., *Mol. Pharmacol.,* 1992, 42: 964–970. The agonist and antagonist effects of the various compounds on the cultivated cells provide an indication of the antiobesity and antidiabetic effects of the compounds in humans.

U.S. Pat. No. 5,451,677 discloses selective β3 agonists of the formula:



U.S. Pat. No. 5,561,142 published Nov. 2, 1995 discloses selective β3 agonists of the formula



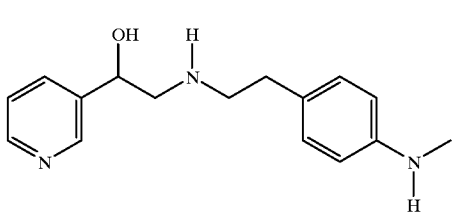
Compounds of the present invention that are within the generic disclosure of U.S. Pat. No. 5,561,142 represent a novel selection thereof.

SUMMARY OF THE INVENTION

The instant invention is concerned with thiazole substituted benzenesulfonamides which are useful as antiobesity and antidiabetic compounds. Thus, it is an object of this invention to describe such compounds. It is a further object to describe the specific preferred stereoisomers of the substituted sulfonamides. A still further object is to describe processes for the preparation of such compounds. Another object is to describe methods and compositions which use the compounds as the active ingredient thereof. Further objects will become apparent from reading the following description.

DESCRIPTION OF THE INVENTION

The present invention provides compounds having the formula I:



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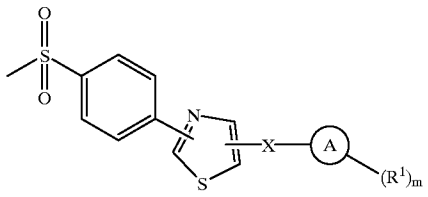

wherein

X is

(1) a bond,

(2) C_1–C_3 alkylene, optionally substituted with 1 or 2 groups selected from methyl and halogen,

(3) C_1–C_3 alkylene wherein said alkylene contains an oxygen, optionally substituted with 1 or 2 groups selected from methyl and halogen;

m is

0 to 5;

A is

(1) phenyl,

(2) a 5 or 6-membered heterocyclic ring with from 1 to 4 heteroatoms selected from oxygen, sulfur and nitrogen,

(3) a benzene ring fused to a C_5–C_{10} carbocyclic ring,

(4) a 5 or 6-membered heterocyclic ring with from 1 to 4 heteroatoms selected from oxygen, sulfur and nitrogen fused to a 5 or 6-membered heterocyclic ring with from 1 to 4 heteroatoms selected from oxygen, sulfur and nitrogen, or

(5) a 5 or 6-membered heterocyclic ring with from 1 to 4 heteroatoms selected from oxygen, sulfur and nitrogen fused to a C_5–C_{10} carbocyclic ring;

R^1 is

(1) C_1–C_{10} alkyl optionally substituted with up to 5 groups selected from

(a) hydroxy,

(b) halogen,

(c) cyano,

(d) QR^2,

(e) C_3–C_8 cycloalkyl,

(f) A optionally substituted with up to 5 groups selected from halogen, C_1–C_{10} alkyl and C_1–C_{10} alkoxy,

(g) $Q'COR^3$,

(h) $S(O)_nR^3$, where n is 0 to 2,

(i) $NR^2SO_2R^3$,

(j) $NR^2CO_2R^2$, and

(k) CO_2R^2,

(2) C_3–C_8 cycloalkyl,

(3) oxo,

(4) halogen,

(5) cyano,

(6) QR^2,

(7) $S(O)_nR^3$, where n is 0 to 2,

(8) $Q'COR^3$,

(9) $NR^2SO_2R^3$,

(10) $NR^2CO_2R^2$,

(11) A optionally substituted with up to 5 groups independently selected from

(a) R^2,

(b) QR^2,

(c) halogen, and

(d) oxo; or

(12) CO_2R^2;

R^2 is

(1) hydrogen,

(2) C_1–C_{10} alkyl optionally substituted with up to 5 groups selected from

(a) hydroxy,

(b) halogen,

(c) CO_2R^4,

(d) $S(O)_n$-C_1–C_{10} alkyl, where n is 0 to 2,

(e) C_3–C_8 cycloalkyl,

(f) C_1–C_{10} alkoxy, and

(g) A optionally substituted with up to 5 groups selected from halogen, C_1–C_{10} alkyl and C_1–C_{10} alkoxy,

(3) C_3–C_8 cycloalkyl, or

(4) A optionally substituted with up to 5 groups selected from

(a) halogen,

(b) nitro,

(c) oxo,

(d) NR^4R^4,

(e) C_1–C_{10} alkoxy,

(f) $S(O)_n$-C_1–C_{10} alkyl where n is 0 to 2, and

(g) C_1–C_{10} alkyl optionally substituted with up to 5 groups selected from hydroxy, halogen, CO_2R^4, $S(O)_n$-C_1–C_{10} alkyl, where n is 0 to 2, C_3–C_8 cycloalkyl, C_1–C_{10} alkoxy, and A optionally substituted with up to 5 groups selected from halogen, C_1–C_{10} alkyl and C_1–C_{10} alkoxy;

R^3 is

(1) R^2 or

(2) NR^2R^2;

$R^4$is

(1) H, or

(2) C_1–C_{10} alkyl;

Q is

(1) $N(R^2)$,

(2) O or

(3) S(O)n, and n is 0 to 2;

Q' is

(1) $N(R^2)$,

(2) O or

(3) a bond; or

a pharmaceutically acceptable salt thereof, or a prodrug thereof.

One subset of compounds of formula I provides compounds wherein

X is

(1) a bond,

(2) CH_2

(3) CH_2O, wherein C is attached to thiazole, and O is attached to A;

Another subset of compounds of formula I provides compounds wherein

R^1 is

(1) C_1–C_{10} alkyl optionally substituted with up to 5 halogens;

(2) halogen,

(3) QR^2,

(4) $Q'COR^3$,

(5) phenyl;

R^2 is

(1) hydrogen,

(2) C_1–C_{10} alkyl optionally substituted with up to 5 halogens;

R^3 is

(1) C_1–C_{10} alkyl; and

Q is

(1) O.

There is one subset of compounds of formula I wherein the thiazolyl moiety is attached to the benzenesulfonamide moiety via the carbon at the 2 position (C2) of the thiazole ring. There is another subset of compounds of formula I wherein the thiazolyl moiety is attached to X, or where X is a bond, directly to A via the carbon at the 2 position of the thiazole ring. Preferably, either the benzenesulfonamide moiety or X (or A, if X is a bond) is attached to the C2 of the thiazole ring, and the other to the C4 positions of the thiazole ring.

Another subset of compounds of formula I provides compounds wherein A is selected from phenyl, naphthyl, a 5 or 6-membered heterocyclic ring with from 1 to 4 heteroatoms selected from oxygen, sulfur and nitrogen fused to a benzene ring, and a 5 or 6-membered heterocyclic ring with from 1 to 4 heteroatoms selected from oxygen, sulfur and nitrogen. Preferably, A is selected from phenyl, naphthyl, thienyl, pyridinyl, benzothienyl, quinolinyl, indolyl, and benzofuranyl.

In a preferred embodiment of compounds of formula I

X is

(1) a bond,

(2) CH_2,

(3) CH_2O, wherein C is attached to thiazole, and O is attached to A;

m is

0 to 5;

A is

(1) phenyl,

(2) a 5 or 6-membered heterocyclic ring with from 1 to 4 heteroatoms selected from oxygen, sulfur and nitrogen,

(3) a benzene ring fused to a C_5–C_{10} carbocyclic ring,

(4) a 5 or 6-membered heterocyclic ring with from 1 to 4 heteroatoms selected from oxygen, sulfur and nitrogen fused to a 5 or 6-membered heterocyclic ring with from 1 to 4 heteroatoms selected from oxygen, sulfur and nitrogen, or

(5) a 5 or 6-membered heterocyclic ring with from 1 to 4 heteroatoms selected from oxygen, sulfur and nitrogen fused to a C_5–C_{10} carbocyclic ring;

R^1 is

(1) C_1–C_{10} alkyl optionally substituted with up to 5 halogens;

(2) halogen,

(3) QR^2,

(4) $Q'COR^3$,

(5) phenyl;

R^2 is

(1) hydrogen,

(2) C_1–C_{10} alkyl optionally substituted with up to 5 halogens;

R^3 is

(1) C_1–C_{10} alkyl; and

Q is

(1) O; or

a pharmaceutically acceptable salt thereof.

In a more preferred embodiment are compounds of formula I wherein

X is

(1) a bond,

(2) CH_2,

(3) CH_2O, wherein C is attached to thiazole, and O is attached to A;

m is

0 to 5;

A is

(1) phenyl,

(2) a 5 or 6-membered heterocyclic ring with from 1 to 4 heteroatoms selected from oxygen, sulfur and nitrogen,

(3) naphthyl, or

(4) a 5 or 6-membered heterocyclic ring with from 1 to 4 heteroatoms selected from oxygen, sulfur and nitrogen fused to a benzene ring;

R^1 is

(1) C_1–C_{10} alkyl optionally substituted with up to 5 halogens;

(2) halogen,

(3) QR^2,

(4) $Q'COR^3$,

(5) phenyl;

R^2 is

(1) hydrogen,

(2) C_1–C_{10} alkyl optionally substituted with up to 5 halogens;

R^3 is

(1) C_1–C_{10} alkyl; and

Q is

(1) O; and

either the benzenesulfonamide moiety or X (or A, if X is a bond) is attached to the C2 of the thiazole ring, and the other to the C4 positions of the thiazole ring; or

a pharmaceutically acceptable salt thereof.

Compounds of the present invention that are within the generic structure disclosed in U.S. Pat. No. 5,561,142 represent a novel selection thereof. The present compounds are potent β3 agonists, and have improved oral bioavailability in animals.

Representative antiobesity and antidiabetic compounds of the present invention include the following:

1. N-[4-[2-[[2-hydroxy-2-(3-pyridinyl)ethyl]amino]ethyl]phenyl]-4-[4-(2-naphthylmethyl)thiazol-2-yl]benzenesulfonamide;
2. N-[4-[2-[[2-hydroxy-2-(pyridin-3-yl)ethyl]amino]ethyl]phenyl]-4-[4-[4-(trifluoromethyl)phenyl]thiazol-2-yl]benzenesulfonamide;
3. N-[4-[2-[[2-hydroxy-2-(pyridin-3-yl)ethyl]amino]ethyl]phenyl]-4-[4-[4-(trifluoromethoxy)phenyl]thiazol-2-yl]benzenesulfonamide;
4. N-[4-[2-[[2-hydroxy-2-(pyridin-3-yl)ethyl]amino]ethyl]phenyl]-4-[4-(3,4-difluorophenylmethyl)thiazol-2-yl]benzenesulfonamide;
5. N-[4-[2-[[2-hydroxy-2-(pyridin-3-yl)ethyl]amino]ethyl]phenyl]-4-[4-(3-pyridyl)thiazol-2-yl]benzenesulfonamide;
6. N-[4-[2-[[2-hydroxy-2-(pyridin-3-yl)ethyl]amino]ethyl]phenyl]-4-[4-(4-fluorophenylmethyl)thiazol-2-yl]benzenesulfonamide;
7. N-[4-[2-[[2-hydroxy-2-(pyridin-3-yl)ethyl]amino]ethyl]phenyl]-4-[4-(3,4-difluorophenyl)thiazol-2-yl]benzenesulfonamide;
8. N-[4-[2-[[2-hydroxy-2-(pyridin-3-yl)ethyl]amino]ethyl]phenyl]-4-[4-[4-(trifluoromethyl)phenylmethyl]thiazol-2-yl]benzenesulfonamide;

9. N-[4-[2-[[2-hydroxy-2-(pyridin-3-yl)ethyl]amino]ethyl]phenyl]-4-[4-(2-pyridyl)thiazol-2-yl]benzenesulfonamide;
10. N-[4-[2-[[2-hydroxy-2-(pyridin-3-yl)ethyl]amino]ethyl]phenyl]-4-[4-[1-(2-phenyl)ethyl]thiazol-2-yl]benzenesulfonamide;
11. N-[4-[2-[[2-hydroxy-2-(pyridin-3-yl)ethyl]amino]ethyl]phenyl]-4-[4-(4-fluorophenyl)thiazol-2-yl]benzenesulfonamide;
12. N-[4-[2-[[2-hydroxy-2-(pyridin-3-yl)ethyl]amino]ethyl]phenyl]-4-[4-(2-naphthyl)thiazol-2-yl]benzenesulfonamide;
13. N-[4-[2-[[2-hydroxy-2-(pyridin-3-yl)ethyl]amino]ethyl]phenyl]-4-[4-(3,4,5-trifluorophenyl)thiazol-2-yl]benzenesulfonamide;
14. N-[4-[2-[[2-hydroxy-2-(pyridin-3-yl)ethyl]amino]ethyl]phenyl]-4-[4-(4-hexylphenyl)thiazol-2-yl]benzenesulfonamide;
15. N-[4-[2-[[2-hydroxy-2-(pyridin-3-yl)ethyl]amino]ethyl]phenyl]-4-[4-[4-(trifluoromethoxy)phenylmethyl]thiazol-2-yl]benzenesulfonamide;
16. N-[4-[2-[[2-hydroxy-2-(pyridin-3-yl)ethyl]amino]ethyl]phenyl]-4-[4-[4-(trifluoromethoxy)phenoxymethyl]thiazol-2-yl]benzenesulfonamide;
17. N-[4-[2-[[2-hydroxy-2-(pyridin-3-yl)ethyl]amino]ethyl]phenyl]-4-[4-(2-benzo[b]thienyl)thiazol-2-yl]benzenesulfonamide;
18. N-[4-[2-[[2-hydroxy-2-(pyridin-3-yl)ethyl]amino]ethyl]phenyl]-4-[4-(3-quinolinyl)thiazol-2-yl]benzenesulfonamide;
19. N-[4-[2-[[2-hydroxy-2-(pyridin-3-yl)ethyl]amino]ethyl]phenyl]-4-[4-(6-quinolinyl)thiazol-2-yl]benzenesulfonamide;
20. N-[4-[2-[[2-hydroxy-2-(pyridin-3-yl)ethyl]amino]ethyl]phenyl]-4-[4-(2-benzo[b]furyl)thiazol-2-yl]benzenesulfonamide;
21. N-[4-[2-[[2-hydroxy-2-(pyridin-3-yl)ethyl]amino]ethyl]phenyl]-4-[4-(3-indolyl)thiazol-2-yl]benzenesulfonamide;
22. N-[4-[2-[[2-hydroxy-2-(pyridin-3-yl)ethyl]amino]ethyl]phenyl]-4-[4-(2,4-difluorophenyl)thiazol-2-yl]benzenesulfonamide;
23. N-[4-[2-[[2-hydroxy-2-(pyridin-3-yl)ethyl]amino]ethyl]phenyl]-4-[4-(3,5-difluorophenyl)thiazol-2-yl]benzenesulfonamide;
24. N-[4-[2-[[2-hydroxy-2-(pyridin-3-yl)ethyl]amino]ethyl]phenyl]-4-[4-[4-(1,1-dimethylethyl)phenyl]thiazol-2-yl]benzenesulfonamide;
25. N-[4-[2-[[2-hydroxy-2-(pyridin-3-yl)ethyl]amino]ethyl]phenyl]-4-[4-(2,3-difluorophenyl)thiazol-2-yl]benzenesulfonamide;
26. N-[4-[2-[[2-hydroxy-2-(pyridin-3-yl)ethyl]amino]ethyl]phenyl]-4-[4-[3-(trifluoromethyl)phenyl]thiazol-2-yl]benzenesulfonamide;
27. N-[4-[2-[[2-hydroxy-2-(pyridin-3-yl)ethyl]amino]ethyl]phenyl]-4-[4-[4-(difluoromethyl)phenyl]thiazol-2-yl]benzenesulfonamide;
28. N-[4-[2-[[2-hydroxy-2-(pyridin-3-yl)ethyl]amino]ethyl]phenyl]-4-[4-(2,4-dichlorophenyl)thiazol-2-yl]benzenesulfonamide;
29. N-[4-[2-[[2-hydroxy-2-(pyridin-3-yl)ethyl]amino]ethyl]phenyl]-4-[4-[2-(trifluoromethyl)phenyl]thiazol-2-yl]benzenesulfonamide;
30. N-[4-[2-[[2-hydroxy-2-(pyridin-3-yl)ethyl]amino]ethyl]phenyl]-4-[4-[2-fluoro-4-(trifluoromethyl)phenyl]thiazol-2-yl]benzenesulfonamide;
31. N-[4-[2-[[2-hydroxy-2-(pyridin-3-yl)ethyl]amino]ethyl]phenyl]-4-[4-[4-fluoro-2-(trifluoromethyl)phenyl]thiazol-2-yl]benzenesulfonamide;
32. N-[4-[2-[[2-hydroxy-2-(pyridin-3-yl)ethyl]amino]ethyl]phenyl]-4-[4-[2,4-bis(trifluoromethyl)phenyl]thiazol-2-yl]benzenesulfonamide;
33. N-[4-[2-[[2-Hydroxy-2-(pyridin-3-yl)ethyl]amino]ethyl]phenyl]-4-[5-(4-fluorophenyl)thiazol-2-yl]benzenesulfonamide;
34. N-[4-[2-[[2-Hydroxy-2-(pyridin-3-yl)ethyl]amino]ethyl]phenyl]-4-[2-(4-trifluoromethylphenyl)thiazol-4-yl]benzenesulfonamide;
35. N-[4-[2-[[2-Hydroxy-2-(pyridin-3-yl)ethyl]amino]ethyl]phenyl]-4-[2-(4-trifluoromethylphenyl)thiazol-5-yl]benzenesulfonamide;
36. N-[4-[2-[[2-hydroxy-2-(pyridin-3-yl)ethyl]amino]ethyl]phenyl]-4-[4-(4-phenylphenyl)thiazol-2-yl]benzenesulfonamide;
37. N-[4-[2-[[2-hydroxy-2-(pyridin-3-yl)ethyl]amino]ethyl]phenyl]-4-[4-(3,4-dihydroxyphenyl)thiazol-2-yl]benzenesulfonamide;
38. N-[4-[2-[[2-hydroxy-2-(pyridin-3-yl)ethyl]amino]ethyl]phenyl]-4-[4-(4-hydroxyphenyl)thiazol-2-yl]benzenesulfonamide;
39. N-[4-[2-[[2-hydroxy-2-(pyridin-3-yl)ethyl]amino]ethyl]phenyl]-4-[4-(4-acetoxyphenyl)thiazol-2-yl]benzenesulfonamide;
40. N-[4-[2-[[2-hydroxy-2-(pyridin-3-yl)ethyl]amino]ethyl]phenyl]-4-[4-(4-acetamidophenyl)thiazol-2-yl]benzenesulfonamide;
41. N-[4-[2-[[2-hydroxy-2-(pyridin-3-yl)ethyl]amino]ethyl]phenyl]-4-[2-(4-trifluoromethoxyphenyl)thiazol-4-yl]benzenesulfonamide.

The compounds of the instant invention all have at least one asymmetric center as noted by the asterisk in structural Formula I. Additional asymmetric centers may be present on the molecule. Each such asymmetric center will produce two optical isomers and it is intended that all such optical isomers, as separated, pure or partially purified optical isomers or racemic mixtures thereof, be included within the ambit of the instant invention. In the case of the asymmetric center represented by the asterisk in Formula I, it has been found that the compound in which the hydroxy substituent is above the plane of the structure, as seen in Formula Ic, is more active and thus more preferred over the compound in which the hydroxy substituent is below the plane of the structure.

The following stereospecific structure represents the preferred stereoisomers of the instant invention:

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