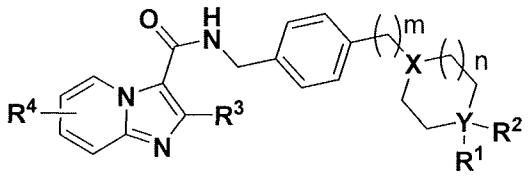
Claims

1. ____A compound having the general formula I:



I

wherein

X is CH or N;

Y is CH, O or N;

m is 0 or 1;

n is 0 or 1;

R^1 is, at each occurrence, independently selected from the group consisting of hydrogen, halogen, methyl, ethyl, t-butyl, phenyl, $-NC(O)R^5$, $-OR^5$, $-C(O)R^5$, $-C(O)OR^5$, any of which is optionally substituted with one or several members selected from the group consisting of halogen, C_1-C_3 alkyl, C_1-C_3 haloalkyl, methylhydroxyl, COOMe, C(O)H, COOH, OCH_3 and OCF_3;

R^2 is, at each occurrence, independently selected from the group consisting of hydrogen and hydroxyl;

R^3 is, at each occurrence, independently selected from the group consisting of methyl and ethyl;

R^4 is, at each occurrence, independently selected from the group consisting of hydrogen, halogen, methyl, -methoxy and $-CF_3$;

R^5 is, at each occurrence, independently selected from the group consisting of C_1-C_3 alkylhetorocycle, phenyl and benzyl, any of which is optionally substituted with one or several members selected from the group consisting of halogen, C_1-C_3 alkyl, C_1-C_3 haloalkyl, methylhydroxyl, COOMe, C(O)H, COOH, OCH_3 and OCF_3;

and pharmaceutically acceptable salts thereof;

wherein, if m is 0, n is 1, X is N, Y is O and R^3 is ethyl, then R^4 is not hydrogen, 6-chloro, 6-methyl, 6-methoxy, 6-bromo, 6-trifluoromethyl, 6-fluoro, 7-chloro, 7-methyl, 7-methoxy, 7-trifluoromethyl, 7-bromo, 8-fluoro, 8-trifluoromethyl, 8-methoxy, or 8-bromo;

wherein, if m is 0, n is 1, X is N and Y is C, R^1 is H, R^2 is H, R^3 is ethyl, then R^4 is not 6-chloro or 7-chloro;

wherein, if m is 0, n is 1, X is N and Y is N, R^1 is methyl, R^3 is ethyl, then R^4 is not 6-chloro or 7-chloro;

wherein, if m is 0, n is 1, X is N, Y is C, R^2 is hydroxyl, R^3 is ethyl and R^4 is 7-chloro, then R^1 is not hydrogen;

wherein, if m is 0, n is 1, X is N, Y is C, R^1 is OR^5, R^2 is hydrogen, R^3 is ethyl and R^5 is 4-fluorobenzyl, then R^4 is not 6-chloro or 7-chloro;

wherein, if m is 0, n is 1, X is N, Y is C, R^1 is OR^5, R^2 is hydrogen, R^3 is ethyl and R^5 is 4-chlorophenyl, then R^4 is not 6-chloro or 7-chloro;

wherein, if m is 0, n is 1, X is N, Y is C, R^1 is OR^5, R^2 is hydrogen, R^3 is ethyl and R^5 is 4-fluorophenyl, then R^4 is not 6-chloro or 7-chloro;

wherein, if m is 0, n is 1, X is N, Y is C, R^1 is OR^5, R^2 is hydrogen, R^3 is ethyl and R^5 is 4-(trifluoromethyl)phenyl, then R^4 is not 6-chloro or 7-chloro;

wherein, if m is 0, n is 1, X is N, Y is C, R^1 is OR^5, R^2 is hydrogen, R^3 is ethyl and R^5 is 4-(trifluoromethoxy)phenyl, then R^4 is not 6-chloro, 6-trifluoromethyl or 7-chloro;

wherein, if m is 0, n is 1, X is N, Y is C, R^1 is methyl, R^2 is hydrogen and R^3 is ethyl, then R^4 is not 6- chloro or 7-chloro;

wherein, if m is 0, n is 0, X is N, Y is C, R^1 is methyl, R^2 is hydrogen and R^3 is ethyl, then R^4 is not 6- chloro or 7-chloro;

wherein, if m is 1, n is 1, X is N, Y is N, R^1 is 4-(butyramidomethyl)phenyl and R^3 is ethyl, then R^4 is not 7-chloro;

wherein, if m is 0, n is 1, X is N, Y is N, R^1 is 4-fluorophenyl and R^3 is ethyl, then R^4 is not hydrogen, 6-fluoro, 6-chloro, 6-methyl, 6-methoxy, 6-bromo, 7-bromo, 7-chloro, 7-methyl, 7-methoxy , 8-methoxy, 8-bromo or 8-fluoro;

wherein, if m is 0, n is 1, X is N, Y is N, R^1 is 4-(trifluoromethoxy)phenyl and R^3 is ethyl, then R^4 is not hydrogen, 6-chloro or 7-chloro;

wherein, if m is 0, n is 1, X is N, Y is C, R^1 is 4-fluorophenyl, R^2 is hydrogen and R^3 is ethyl, then R^4 is not hydrogen, 6-chloro or 7-chloro;

wherein, if m is 0, n is 1, X is N, Y is C, R^1 is 4-(trifluoromethoxy)phenyl, R^2 is hydrogen and R^3 is ethyl, then R^4 is not hydrogen, 6-chloro or 7-chloro;

wherein, if m is 0, n is 1, X is N, Y is C, R^1 is 4-chlorophenyl, R^2 is hydrogen and R^3 is ethyl, then R^4 is not 6-chloro or 7-chloro;

wherein, if m is 0, n is 1, X is N, Y is C, R^1 is 4-fluorophenyl, R^2 is hydroxy and R^3 is ethyl, then R^4 is not 6-chloro or 7-chloro;

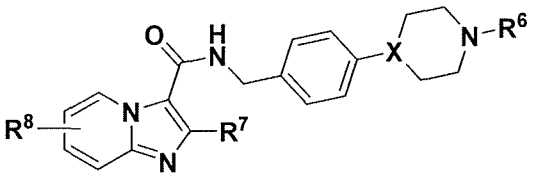
wherein, if m is 0, n is 1, X is N, Y is C, R^1 is phenyl, R^2 is hydroxy and R^3 is ethyl, then R^4 is not 7-chloro;

wherein, if m is 0, n is 1, X is N, Y is N, R^1 is phenyl and R^3 is ethyl, then R^4 is not 7-chloro.

2. ____The Compound according to claim 1, wherein m = 0.

3. ____The compound according to any of claims 1 and 2, wherein m = 0 and R^1 is, at each occurrence, independently selected from the group consisting of halogen, methyl, ethyl, t-butyl, phenyl, -NC(O)R^5, -OR^5, -C(O)R^5, -C(O)OR^5, any of which is optionally substituted with one or several members selected from the group consisting of halogen, C_1-C_3 alkyl, C_1-C_3 haloalkyl, methylhydroxyl, COOMe, C(O)H, COOH, OCH_3 and OCF_3.

4. ____A compound having the general formula II:



II

wherein

X is CH or N

R^6 is, at each occurrence, independently selected from the group consisting of phenyl and C(O)R^9 , any of which is optionally substituted with one or several members selected from the group consisting of halogen, C_1-C_3 alkyl, C_1-C_3 haloalkyl, methylhydroxyl, COOMe, C(O)H, COOH, OCH_3 and OCF_3;

R^7 is, at each occurrence, independently selected from the group consisting of methyl and ethyl;

R^8 is, at each occurrence, independently selected from the group consisting of hydrogen, halogen, methyl, -methoxy and $-CF_3$;

R^9 is, at each occurrence, independently selected from the group consisting of phenyl, benzyl, any of which is optionally substituted with one or several members selected from the group consisting of halogen, C_1-C_3 alkyl, C_1-C_3 haloalkyl, methylhydroxyl, COOMe, C(O)H, COOH, OCH_3 and OCF_3;

and pharmaceutically acceptable salts thereof;

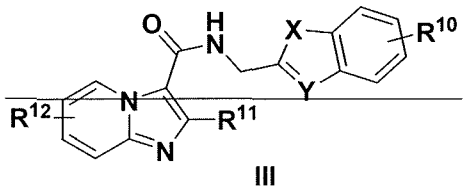
wherein, if X is N, R^6 is phenyl and R^7 is ethyl, then R^8 is not 7-chloro;

wherein, if X is N, R^6 is 4-fluorophenyl and R^7 is ethyl, then R^8 is not hydrogen, 6-fluoro, 6-chloro, 6-methyl, 6-methoxy, 6-bromo, 7-bromo, 7-chloro, 7-methyl, 7-methoxy , 8-methoxy, 8-bromo or 8-fluoro;

wherein, if X is N, R^6 is 4-(butyramidomethyl)phenyl and R^7 is ethyl, then R^8 is not 7-chloro;

wherein, if X is N, R^6 is 4-(trifluoromethoxy)phenyl and R^7 is ethyl, then R^8 is not hydrogen, 6-chloro or 7-chloro.

~~5. A compound having the general formula III:~~



III

~~wherein~~

~~X is S, O or NR^{13}~~

~~Y is CH or N~~

~~R^{10} is, at each occurrence, independently selected from the group consisting of halogen and phenyl, any of which is optionally substituted;~~

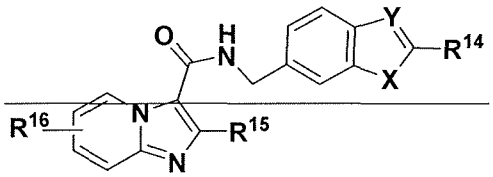
~~R^{11} is, at each occurrence, independently selected from the group consisting of methyl and ethyl;~~

~~R^{12} is, at each occurrence, independently selected from the group consisting of hydrogen, halogen, methyl, methoxy and CF_3;~~

~~R^{13} is, at each occurrence, independently selected from the group consisting of hydrogen, methyl and benzyl, any of which is optionally substituted;~~

~~and pharmaceutically acceptable salts thereof.~~

~~6. A compound having the general formula IV:~~



IV

~~wherein~~

~~X is S, O or NR^{17}~~

~~Y is CH or N~~

~~R^{14} is, at each occurrence, independently selected from the group consisting of hydrogen, C_1-C_3 alkyl, C_1-C_3 alkylheterocycle, phenyl, any of which is optionally substituted;~~

~~R^{15} is, at each occurrence, independently selected from the group consisting of methyl and ethyl;~~

~~R^{16} is, at each occurrence, independently selected from the group consisting of hydrogen, halogen, methyl, methoxy and CF_3;~~

~~R^{17} is, at each occurrence, independently selected from the group consisting of hydrogen, methyl and benzyl, any of which is optionally substituted;~~

~~and pharmaceutically acceptable salts thereof;~~

~~wherein, if X is NR^{17}, Y is N, R^{14} is 4-(trifluoromethoxy)phenyl, R^{15} is ethyl and R^{17} is hydrogen, then R^{16} is not 6-chloro or 7-chloro;~~

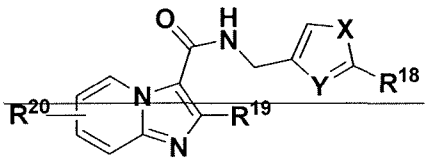
~~wherein, if X is NR^{17}, Y is N, R^{14} is morpholinomethyl, R^{15} is ethyl and R^{17} is hydrogen, then R^{16} is not 7-chloro;~~

~~wherein, if X is O, Y is N, R^{14} is 4-(trifluoromethoxy)phenyl, and R^{15} is ethyl, then R^{16} is not 6-chloro or 7-chloro;~~

~~wherein, if X is O, Y is N, R^{14} is 4-fluorophenyl, and R^{15} is ethyl, then R^{16} is not hydrogen, 6-chloro or 7-chloro;~~

~~wherein, if X is O, Y is N, R^{14} is cyclohexyl, and R^{15} is ethyl, then R^{16} is not 6-chloro or 7-chloro.~~

~~7. A compound having the general formula V:~~



V

~~wherein~~
~~X is S, O or NH~~
~~Y is CH or N~~

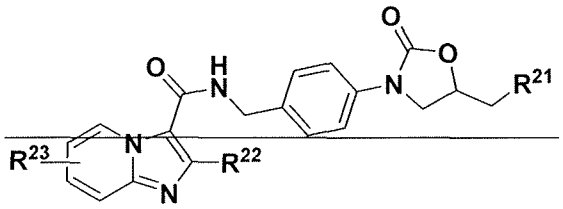
~~R^{18} is, at each occurrence, independently selected from the group consisting of C_1-C_3 alkylheterocycle, phenyl and benzyl, any of which is optionally substituted;~~

~~R^{19} is, at each occurrence, independently selected from the group consisting of methyl and ethyl;~~

~~R^{20} is, at each occurrence, independently selected from the group consisting of hydrogen, halogen, methyl, -methoxy and CF_3;~~

~~and pharmaceutically acceptable salts thereof.~~

~~8. A compound having the general formula VI:~~



VI

~~wherein~~

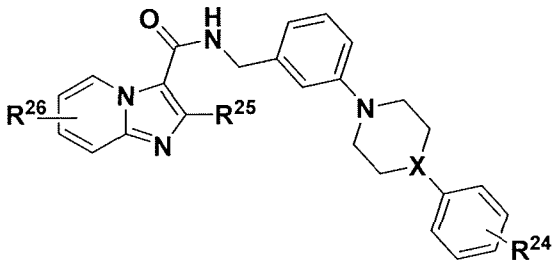
~~R^{21} is, at each occurrence, independently selected from the group consisting of phenyl and O-phenyl, any of which is optionally substituted;~~

~~R^{22} is, at each occurrence, independently selected from the group consisting of methyl and ethyl;~~

~~R^{23} is, at each occurrence, independently selected from the group consisting of hydrogen, halogen, methyl, methoxy and CF_3;~~

~~and pharmaceutically acceptable salts thereof.~~

~~9~~5. ___A compound having the general formula VII:



VII

wherein

X is CH or N

R^{24} is, at each occurrence, independently selected from the group consisting of hydrogen, halogen, C_1-C_2 alkyl, -methoxy, $-CF_3$ and $-OCF_3$;

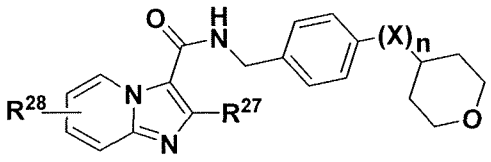
R^{25} is, at each occurrence, independently selected from the group consisting of methyl and

ethyl;

R^{26} is, at each occurrence, independently selected from the group consisting of hydrogen, halogen, methyl, –methoxy and $–CF_3$;

and pharmaceutically acceptable salts thereof.

~~106~~. A compound having the general formula VIII:



VIII

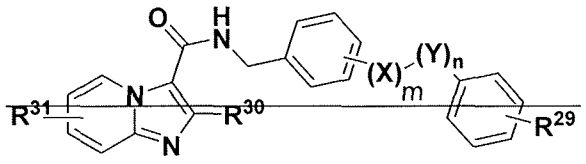
wherein
X is CH_2 or NH
n is 0 or 1

R^{27} is, at each occurrence, independently selected from the group consisting of methyl and ethyl;

R^{28} is, at each occurrence, independently selected from the group consisting of hydrogen, halogen, methyl, -methoxy and $–CF_3$;

and pharmaceutically acceptable salts thereof.

~~11. A compound having the general formula IX:~~



IX

~~wherein~~
~~X is CH_2, NR^{32}, O, C(O)NH or HC=CH~~
~~Y is CH_2, or C(O)NH,~~
~~m is 0 or 1~~

~~n is 0 or 1~~

~~R^{29} is, at each occurrence, independently selected from the group consisting of hydrogen, halogens, C_1-C_2 alkyl, -methoxy, COOH, CF_3 and OCF_3;~~

~~R^{30} is, at each occurrence, independently selected from the group consisting of methyl and ethyl;~~

~~R^{31} is, at each occurrence, independently selected from the group consisting of hydrogen, halogens, methyl, -methoxy and CF_3;~~

~~R^{32} is, at each occurrence, independently selected from the group consisting of hydrogen and methyl;~~

~~and pharmaceutically acceptable salts thereof;~~

~~wherein, if X is *para*-O, m is 1, n is 0, R^{29} is hydrogen and R^{30} is methyl, then R^{31} is not hydrogen;~~

~~wherein, if X is *para*-C, m is 0, n is 0, R^{29} is hydrogen and R^{30} is methyl, then R^{31} is not hydrogen, 6-chloro or 7-chloro;~~

~~wherein, if X is *para*-C, m is 0, n is 0, R^{29} is hydrogen and R^{30} is ethyl, then R^{31} is not hydrogen, 6-chloro or 6-methyl;~~

~~wherein, if X is *para*-O, m is 1, n is 0, R^{29} is hydrogen and R^{30} is ethyl, then R^{31} is not hydrogen, 6-methyl or 6-chloro;~~

~~wherein, if X is *para*-C, m is 0, n is 0, R^{30} is ethyl and R^{31} is 6-chloro, then R^{29} is not 2-chloro, 4-chloro, 2-methyl, 3-methyl, 2-trifluoromethyl or 4-methyl;~~

~~wherein, if X is *para*-C, m is 0, n is 0, R^{30} is ethyl, R^{31} is 7-chloro, then R^{29} is not hydrogen, 2-chloro, 4-chloro, 2-methyl, 3-methyl, 4-methyl, 4-fluoro, 4-methoxy, 4-trifluoromethoxy, 4-trifluoromethyl or 2-trifluoromethyl;~~

~~wherein, if X is *para*-O, m is 1, n is 0, R^{29} is 4-trifluoromethoxy and R^{30} is ethyl, then R^{31} is not hydrogen, 6-chloro or 7-chloro, 6-fluoro, 6-bromo, 6-methyl, 7-methyl or 8-fluoro;~~

~~wherein, if X is *para*-O, m is 1, n is 0, R^{29} is 4-fluoro and R^{30} is ethyl, then R^{31} is not 6-chloro, 6-bromo or 7-chloro;~~

~~wherein, if X is *para*-O, m is 1, n is 0, R^{29} is 4-chloro and R^{30} is ethyl, then R^{31} is not 6-chloro or 7-chloro;~~

~~wherein, if X is *para*-N, Y is C, m is 1, R^{29} is 4-trifluoromethoxy, R^{30} is ethyl, R^{31} is 7-chloro and R^{32} is hydrogen, then n is not 0 or 1;~~

~~wherein, if X is *para*-O, Y is C, m is 1, n is 1, R^{29} is 4-trifluoromethoxy and R^{30} is ethyl, then R^{31} is not hydrogen, 6-chloro, 6-fluoro, 6-bormo or 7-chloro;~~

~~wherein, if X is *para*-O, Y is C, m is 1, n is 1, R^{29} is 4-fluoro and R^{30} is ethyl, then R^{31} is not 6-chloro or 7-chloro;~~

~~wherein, if X is *meta*-C, m is 0, n is 0, R^{30} is ethyl and R^{31} is 7-chloro, then R^{29} is not 4-trifluoromethoxy;~~

~~wherein, if X is *para*-N, Y is C, m is 1, n is 1, R^{29} is 4-trifluoromethoxy, R^{30} is ethyl and R^{31} is hydrogen, then R^{32} is not methyl.~~

~~12~~7. __The compound according to any of claims 1-~~11~~6, having one of the formulae 1-350 as shown in Tables 1 and 2, preferably one of the formulae 1-21, 23-24, 26, 28-33, 35-57, 59-77, 79-83, 85-87, 90-98, 100-102, 106-111, 113-116 118-124, 126-128, 130-142, 144-150, 153, 155-167, 169-184, 186-188, 190-197, 199, 201, 203-208, 210-211, 213-214, 216, 218-

231, 233, 235-246, 252-254, 256-259, 261, 267-270, 273, 279-280, 284-303, 307-316, 319-328, 333-338, 340-350 as shown in Tables 1 and 2.

~~13~~8. The compound according to any of claims 1 – ~~12~~7, having one of the formulae 55, 171, 175 and 325 as shown in Tables 1 and 2,

and pharmaceutically acceptable salts thereof.

~~14~~9. The compound according to any of claims 1 – ~~13~~8, for use in the treatment of a bacterial infection.

~~15~~10. The compound according to claim ~~14~~9, wherein said bacterial infection is Tuberculosis.

~~16~~11. A pharmaceutical composition comprising a compound according to any of claims 1 – ~~15~~10, and a pharmaceutically acceptable carrier.

~~17~~12. Use of a compound according to any of claims 1 – ~~15~~ 10 or a pharmaceutical composition according to claim 16 in the manufacture of a medicament for the treatment of a bacterial infection, in particular Tuberculosis, in a human subject in need thereof.

~~18. A compound that competitively inhibits the specific binding of a compound according to any of claims 1 – 15.~~

~~19. Use of a compound, which compound is characterized by an ability to competitively inhibit the specific binding of a compound according to any of claims 1 – 15 or a pharmaceutical composition according to claim 18, to its target protein, in the manufacture of a medicament for the treatment of a bacterial infection, in particular Tuberculosis, in a human subject in need thereof.~~