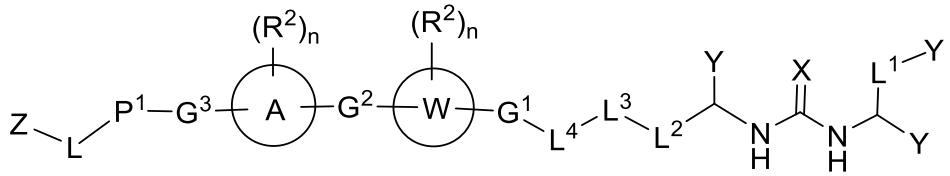
What is claimed is:

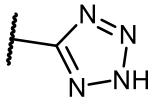
1. A compound of Formula (I):



(I),

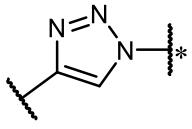
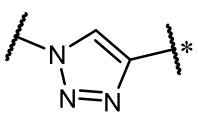
or a stereoisomer, a mixture of stereoisomers, a tautomer, or a pharmaceutically acceptable salt thereof, wherein:

X is O, S, or NH;

each Y is independently $-CO_2H$, $-SO_2H$, $-SO_3H$, $-OSO_3H$, $-PO_2H$, $-PO_3H_2$, $-OPO_3H_2$, or ;

L^1 is optionally substituted C_1-C_6 alkylene, wherein one or two $-CH_2-$ in the alkylene is independently optionally replaced by a -NHC(=O)-*, -C(=O)NH-*, -O-, -S-, $-S(=O)_2-$, -S(=O)-, -C(=O)-, -C(=O)O-*, -OC(=O)-*, or -NH-, wherein * refers to the direction toward the Y adjacent to L^1;

L^2 is optionally substituted C_1-C_6 alkylene, wherein one or two $-CH_2-$ in the alkylene is independently optionally replaced by -O-, -S-, C_3-C_6 cycloalkylene, C_3-C_6 cycloalkenylene, or 3 to 6-membered heterocyclylene;

L^3 is -(C=O)-NR^1-*, -NR^1-(C=O)-*, -C(=O)-, -O-, -S-, -S-S-, $-S-CH_2-S-$, -S(=O)-, $-S(O)_2-$, NR^1, -NR^1-(C=O)-NR^1-, -C(=O)-NR^1-C(=O)-, -OC(=O)-NR^1-*, -NR^1C(=O)O-*, -OC(=S)-NR^1-*, -NR^1C(=S)O-*, , , -(C=O)-(3- to 10-membered optionally substituted N-containing ring)-*, or -(3- to 10-membered optionally substituted N-containing ring)-(C=O)-*, wherein * refers to the direction toward L^2;

L^4 is optionally substituted C_1-C_6 alkylene;

G^1 is absent, -O-, -S-, -NR^4-, -NR^4-(C=O)-*, -(C=O)-NR^4-*, or optionally substituted C_2-C_6 alkylene, wherein one or more -CH_2- in the alkylene is independently replaced by a -O-, -S-, -$S(=O)_2$-, -S(=O)-, -C(=O)-, -C(=O)O-*, -OC(=O)-*, NR^4, -(C=O)-NR^4-*, or -NR^4-(C=O)-*, wherein * refers to the direction toward L^4;

G^2 and G^3 are each independently absent, -O-, -S-, -NR^1-, -NR^1-(C=O)-*, -(C=O)-NR^1-*, -NR^1-(C=S)-*, or optionally substituted C_1-C_6 alkylene, wherein one or more -CH_2- in the alkylene is independently optionally replaced by a -O-, -S-, -$S(=O)_2$-, -S(=O)-, -C(=O)-, -C(=O)O-*, -OC(=O)-*, NR^1, -(C=O)-NR^1-*, -NR^1-(C=O)-*, or -NR^1-(C=S)-*, wherein * refers to the direction toward G^1;

R^4 is H or optionally substituted C_1-C_6 alkyl; or R^4 and NR^1 of G^2 together with the intervening atoms form a 5 to 12-membered heterocyclyl ring;

P^1 is absent, NR^8, C_6-C_{10} aryl, 5 to 10-membered heteroaryl, C_3-C_{14} cycloalkyl, or 5 to 14-membered heterocyclyl; wherein the aryl, heteroaryl, cycloalkyl, and heterocyclyl are independently optionally substituted;

R^8 is independently H or optionally substituted C_1-C_6 alkyl;

Ring W is a 5 to 10-membered heteroaryl, C_3-C_8 cycloalkyl, C_3-C_8 cycloalkenyl, or 5 to 14-membered heterocyclyl;

Ring A is C_6-C_{10} aryl, 5 to 10-membered heteroaryl, C_3-C_{14} cycloalkyl, or 5 to 14-membered heterocyclyl;

each R^1 is independently H or optionally substituted C_1-C_6 alkyl;

each R^2 is independently OH, halogen, oxo, C_1-C_6 alkyl, -O-(C_1-C_6 alkyl), -S-(C_1-C_6 alkyl), -NH_2, -NH-(C_1-C_6 alkyl), or -N(C_1-C_6 alkyl)$_2$, wherein each alkyl is independently optionally substituted with one or more OH, oxo, or halogen;

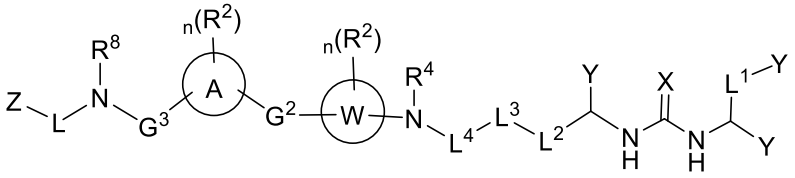
n is an integer from 0 to 6 as valency permits;

L is absent or a linker; and

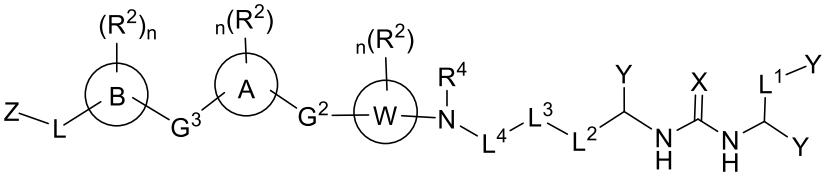
Z is a radioactive moiety, a chelating agent, a fluorescent dye, a contrast agent, a cytostatic or cytotoxic agent, a cytokine, an immunomodulatory molecule, an amphiphilic substance, a nucleic acid, a viral structural protein, a protein, or biotin.

2. The compound of claim 1, wherein G^1 is O or -NR^4-.

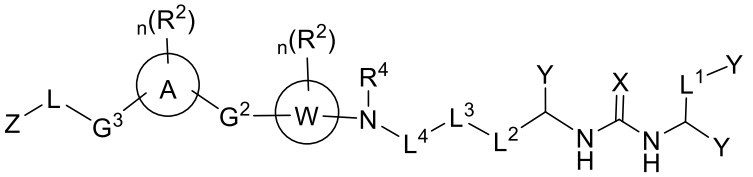
3. The compound of claim 1, which is a compound of Formula (II-A), (II-B), (II-C), or (II-D):



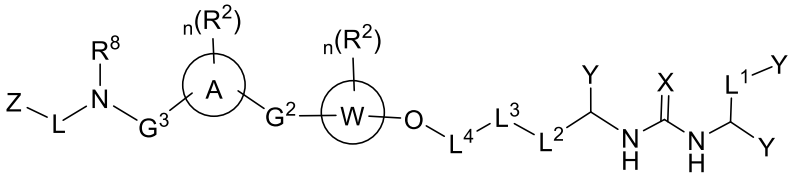
(II-A),



(II-B),



(II-C), or



(II-D),

or a stereoisomer, a mixture of stereoisomers, a tautomer, or a pharmaceutically acceptable salt thereof, wherein:

Ring B is C_6-C_{10} aryl, 5 to 10-membered heteroaryl, C_3-C_{14} cycloalkyl, or 5 to 14-membered heterocyclyl;

each instance of R^2 is independently OH, halogen, oxo, C_1-C_6 alkyl, -O-(C_1-C_6 alkyl), -S-(C_1-C_6 alkyl), -NH_2, -NH-(C_1-C_6 alkyl), or -N(C_1-C_6 alkyl)$_2$, wherein each alkyl is independently optionally substituted with one or more OH, oxo, or halogen; and

each instance of n is an integer from 0 to 6 as valency permits.

4. The compound of any one of claims 1 to 3, wherein (i) L^4 is $-(CH_2)_{0-3}CH(R^3)(CH_2)_{0-3}-$, or R^4 is $-(CH_2)_{1-3}-R^{3a}$, wherein R^3 is C_1-C_{20} alkyl, C_2-C_{20} alkenyl, C_2-C_{20} alkynyl, C_3-C_8 cycloalkyl, or $-(CH_2)_{0-3}-R^{3a}$, wherein each R^{3a} independently is C_6-C_{20} aryl, C_3-C_{14} cycloalkyl, 3 to 14-membered heterocyclyl, or 5 to 20-membered heteroaryl, and wherein the alkyl, alkenyl, alkynyl, aryl, cycloalkyl, heterocyclyl, or heteroaryl in R^3 or R^{3a} is optionally substituted with one or more halogen, OH, C_1-C_6 alkyl, C_6-C_{10} aryl, C_6-C_{10} cycloalkyl, 5- to 10-membered heteroaryl, 3 to 8-membered heterocyclyl, C_6-C_{10} aryloxy, C_6-C_{10} cycloalkyloxy, or 5- to 10-membered heteroaryloxy;

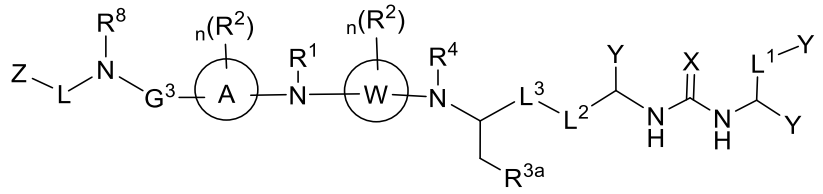
(ii) L^4 is $-(CH_2)_{0-3}CH(CH_2R^{3a})(CH_2)_{0-3}-$;

(iii) G^2 is NR^1 or O;

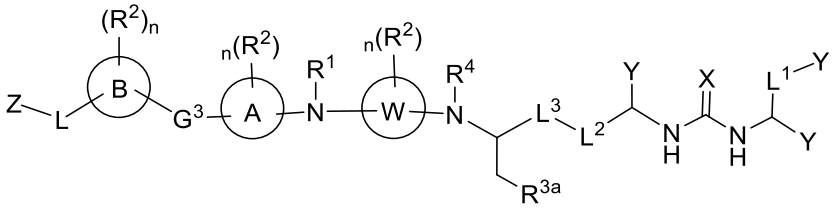
(iv) G^2 is absent or unsubstituted C_1-C_6 alkylene; or

(v) G^2 is C_1-C_6 alkylene, wherein one or two $-CH_2-$ in G^2 is replaced by a -O-, -S-, $-S(=O)_2-$, -S(=O)-, -C(=O)-, -C(=O)O-*, -OC(=O)-*, -NH-, -(C=O)-NH-*, -NH-(C=O)-*, or $-NR^1-(C=S)-$*, wherein * refers to the direction toward G^1.

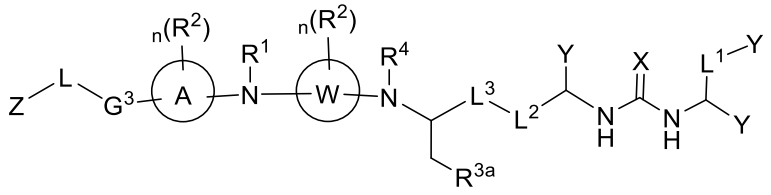
5. The compound of claim 1, which is a compound of Formula (III-A), (III-B), (III-C), (III-D), (III-E), (III-F), or (III-G):



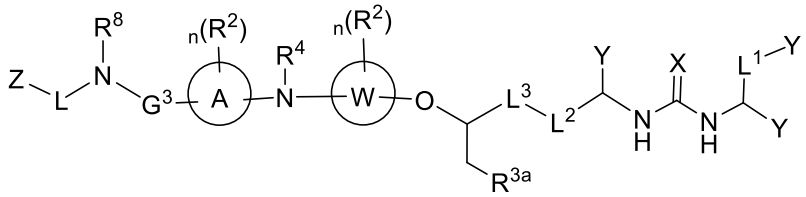
(III-A),



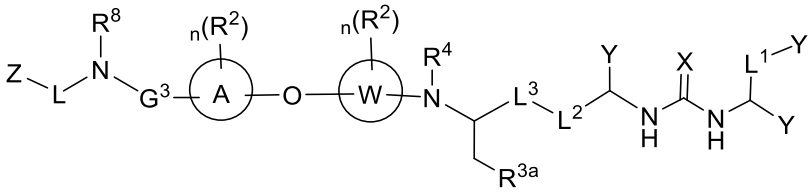
(III-B),



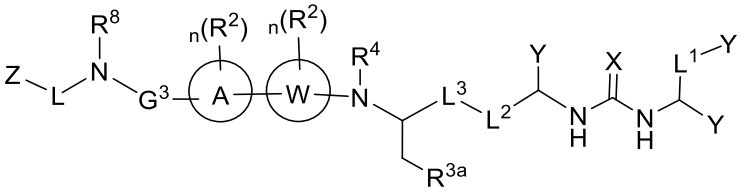
(III-C),



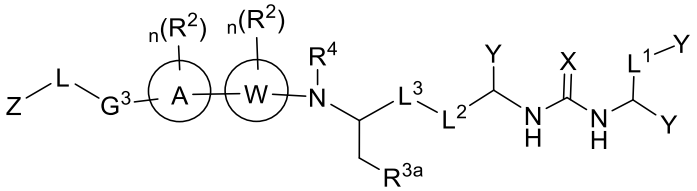
(III-D),



(III-E),



(III-F), or



(III-G),

or a stereoisomer, a mixture of stereoisomers, a tautomer, or a pharmaceutically acceptable salt thereof, wherein:

R^{3a} is C_6-C_{20} aryl, C_3-C_{14} cycloalkyl, 3 to 14-membered heterocyclyl, or 5 to 20-membered heteroaryl, and wherein the alkyl, alkenyl, alkynyl, aryl, cycloalkyl, heterocyclyl, or

heteroaryl in R^3 or R^{3a} is optionally substituted with one or more halogen, OH, C_1-C_6 alkyl, C_6-C_{10} aryl, C_6-C_{10} cycloalkyl, 5 to 10-membered heteroaryl, 3 to 8-membered heterocyclyl, C_6-C_{10} aryloxy, C_6-C_{10} cycloalkyloxy, or 5- to 10-membered heteroaryloxy.

6. The compound of any one of claims 1 to 5, wherein (i) G^3 is absent or unsubstituted C_1-C_6 alkylene;

(ii) G^3 is C_1-C_6 alkylene, wherein one or more -CH_2- in G^3 is replaced by a -O-, -S-, -S(=O)$_2$-, -S(=O)-, -C(=O)-, -C(=O)O-*, -OC(=O)-*, -NH-, -(C=O)-NH-*, -NH-(C=O)-*, or -NR^1-(C=S)-*,wherein * refers to the direction toward G^1;

(iii) L^1 is unsubstituted C_1-C_6 alkylene, or C_1-C_6 alkylene substituted with one or more halogen;

(iv) L^1 is C_1-C_6 alkylene, and wherein one -CH_2- in L^1 is replaced by a -NHC(=O)-*, -C(=O)NH-*, -O-, -S-, -S(=O)$_2$-, or -S(=O)-, wherein * refers to the direction toward the Y adjacent to L^1; or

(v) L^1 is -CH_2-, -CH_2CH_2-, -$CH_2CH_2CH_2$-, -CH_2-NHC(=O)-, -CH_2CH_2-NHC(=O)-, -$CH_2CH_2CH_2$-NHC(=O)-, -CH(OH)-, -CHF-, -CF_2-, -$CH(CH_3)$-, -$C(CH_3)_2$-, -CH_2CH(OH)-, -CH_2CHF-, -CHFCH_2-, -CF_2CH_2-, -CH_2CF_2-, -CH(OH)CH_2-, -CH_2CH(OH)CH_2-, -CH_2CHFCH_2-, -$(CH_2)_2$CH(OH)-, -$(CH_2)_2$CHF-, -CH_2OCH_2-, -CH_2SCH_2-, -CH(OH)CH_2CH_2-, -$CH(CH_3)$-O-CH_2-, -$C(CH_3)_2$-O-CH_2-, -CH_2-O-$CH(CH_3)$-, -CH_2-O-$C(CH_3)_2$-, -CH_2-S(O)-CH_2-, -CH_2-S(O)$_2$-CH_2-, -$CH(CH_3)$-S-CH_2-, -$C(CH_3)_2$-S-CH_2-, -CH_2-S-$CH(CH_3)$-, -CH_2-S-$C(CH_3)_2$-, -$CH(CH_3)$-S(O)-CH_2-, -$C(CH_3)_2$-S(O)-CH_2-, -CH_2-S(O)-$CH(CH_3)$-, -CH_2-S(O)-$C(CH_3)_2$-, -$CH(CH_3)$-S(O)$_2$-CH_2-, -$C(CH_3)_2$-S(O)$_2$-CH_2-, -CH_2-S(O)$_2$-$CH(CH_3)$-, -CH_2-S(O)$_2$-$C(CH_3)_2$-, -C(=O)NH-CH_2-, -NHC(=O)-CH_2CH_2-, -C(=O)NH-$CH(CH_3)$-, -NHC(=O)-$CH_2CH_2CH_2$-, or -C(=O)NH-$C(CH_3)_2$-.

7. The compound of any one of claims 1 to 6, wherein (i) L^2 is a straight C_1-C_6 alkylene;

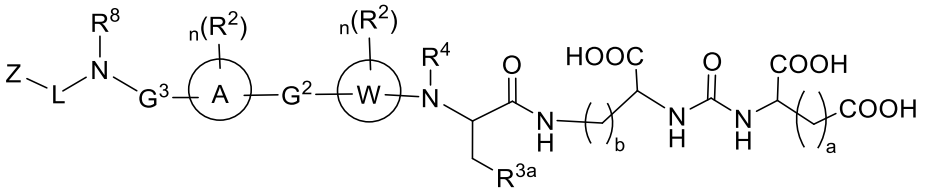
(ii) L^2 is -$CH_2CH_2CH_2CH_2$-;

(iii) L^3 is -(C=O)-NR^1-* or -NR^1-(C=O)-*, wherein * refers to the direction toward L^2;

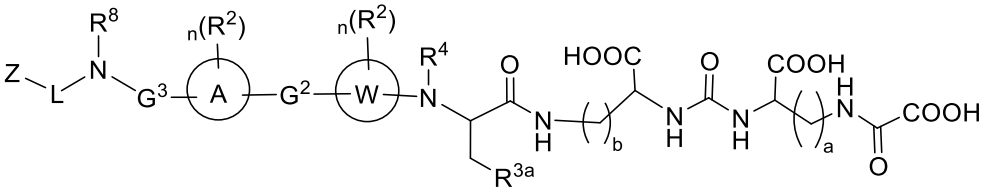
(iv) X is O; or

(v) all Y are COOH.

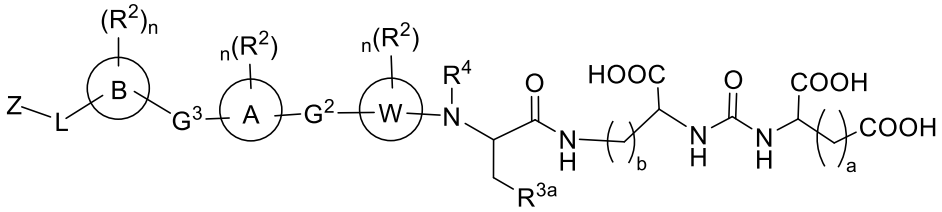
8. The compound of any one of claims 1 to 6, which is a compound of Formula (IV-A1), (IV-A2), (IV-B1), (IV-B2), (IV-C1), or (IV-C2):



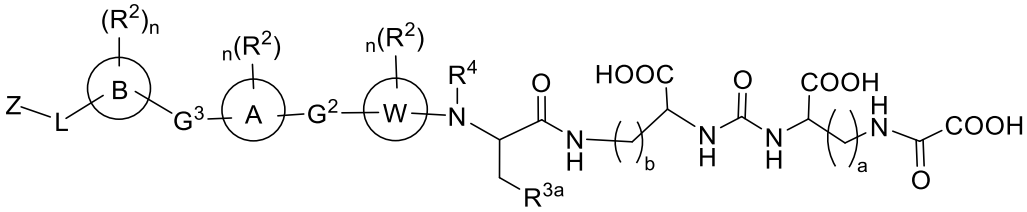
(IV-A1),



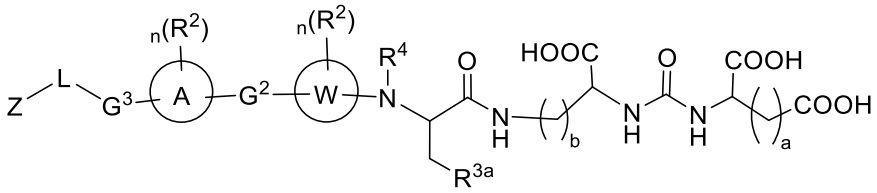
(IV-A2),



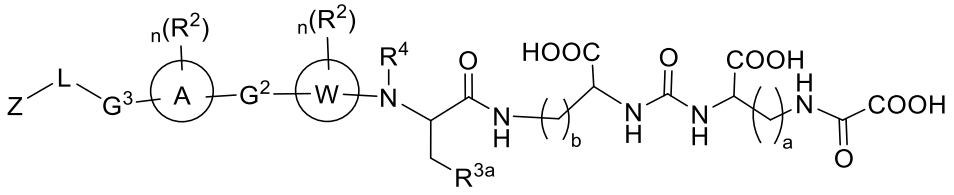
(IV-B1),



(IV-B2),



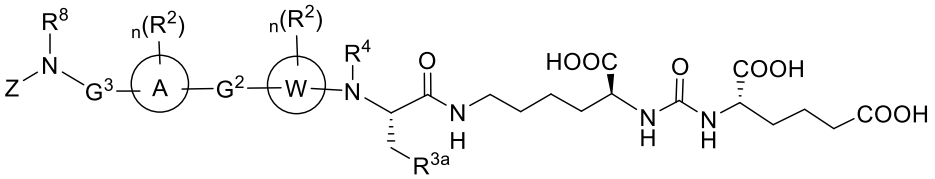
(IV-C1), or



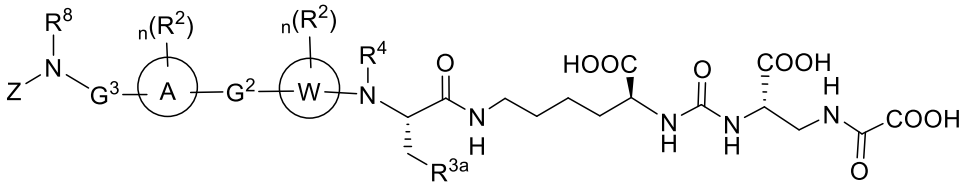
(IV-C2),

or a stereoisomer, a mixture of stereoisomers, a tautomer, or a pharmaceutically acceptable salt thereof, wherein a and b are each independently an integer from 1 to 5.

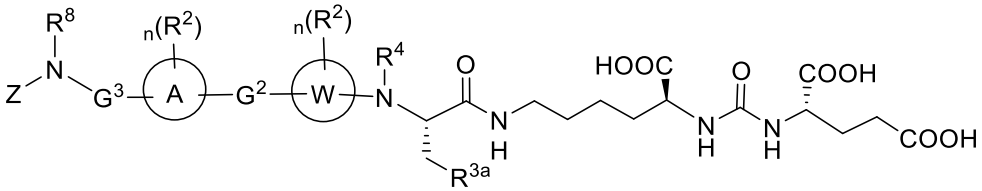
9. The compound of claim 8, which is a compound of Formula (V-A1), (V-A2), (V-A3), (V-B1), (V-B2), (V-B3), (V-C1), (V-C2), or (V-C3):



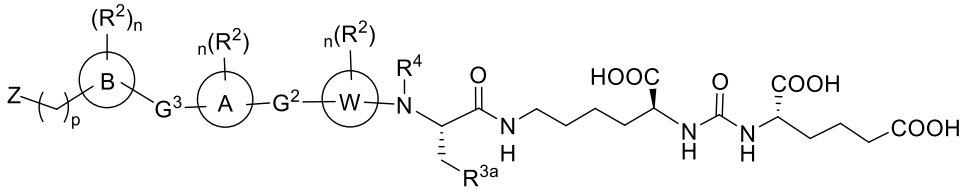
(V-A1),



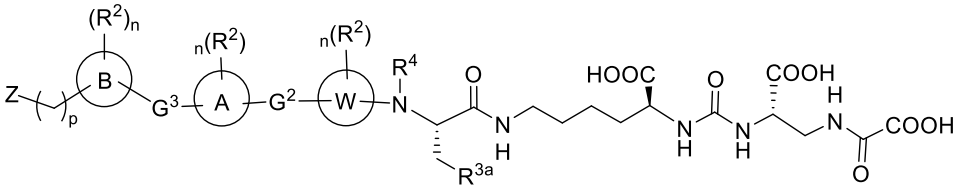
(V-A2),



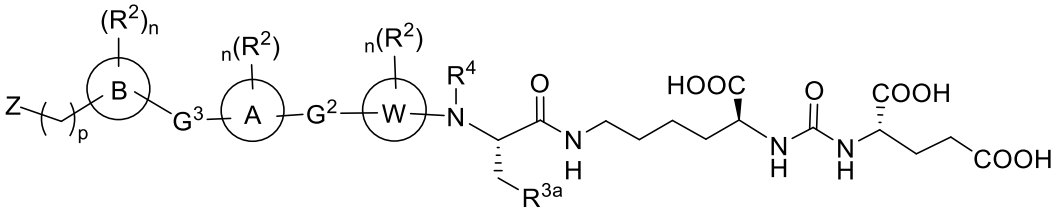
(V-A3),



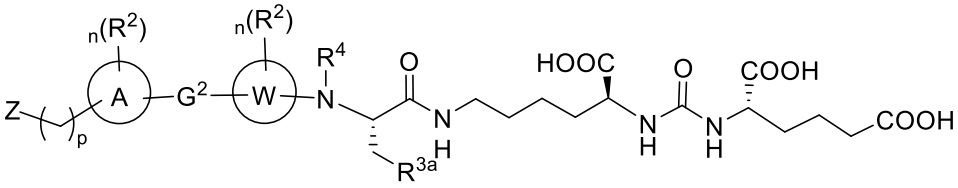
(V-B1),



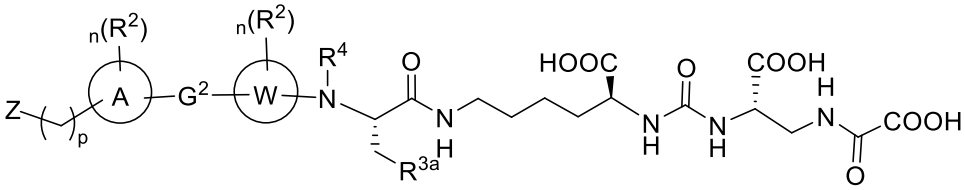
(V-B2),



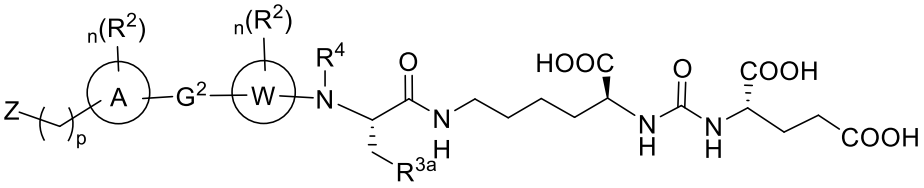
(V-B3),



(V-C1),



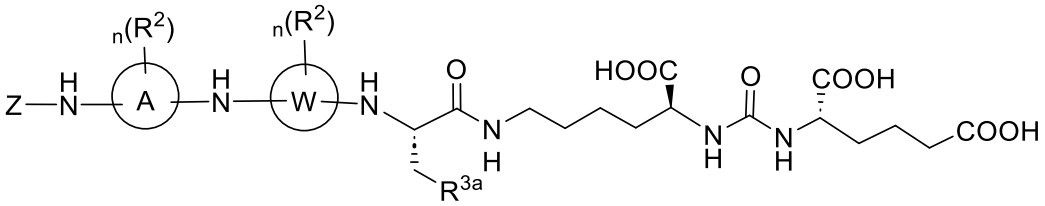
(V-C2), or



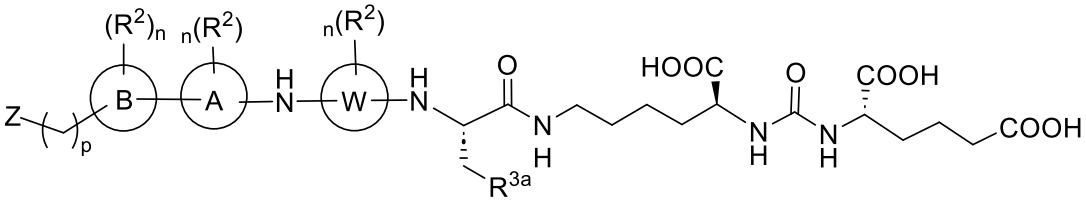
(V-C3),

or a stereoisomer, a mixture of stereoisomers, a tautomer, or a pharmaceutically acceptable salt thereof, wherein p is an integer from 0 to 6.

10. The compound of claim 8 or 9, which is a compound of Formula (V-A1') or (V-B1'):



(V-A1'), or



(V-B1'),

or a stereoisomer, a mixture of stereoisomers, a tautomer, or a pharmaceutically acceptable salt thereof, wherein p is an integer from 0 to 6.

11. The compound of any one of claims 1 to 10, wherein (i) Ring W is a 5 to 10-membered heteroaryl;

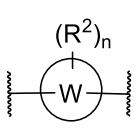
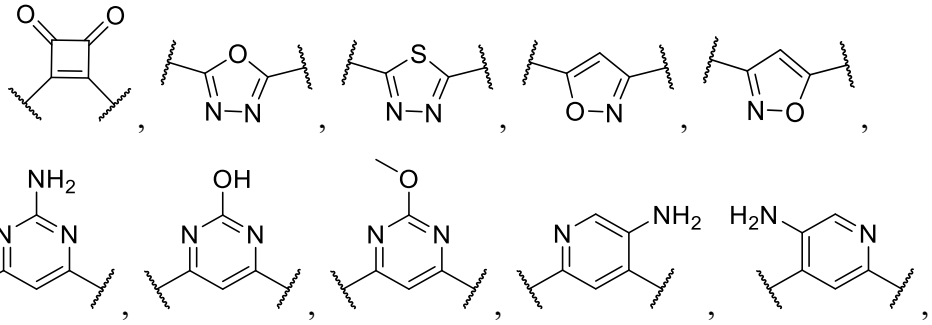
(ii) Ring W is a 5 or 6-membered nitrogen-containing heteroaryl;

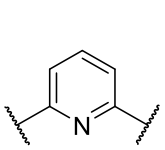
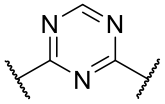
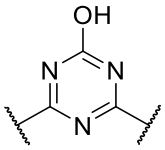
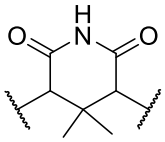
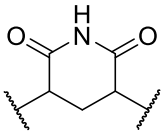
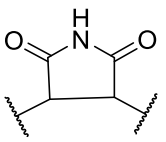
(iii) Ring W is a C_3-C_8 cycloalkenyl;

(iv) Ring W is cyclopropenyl, cyclobutenyl, cyclopentenyl, or cyclohexenyl;

(v) Ring W is a 5 to 8-membered heterocyclyl;

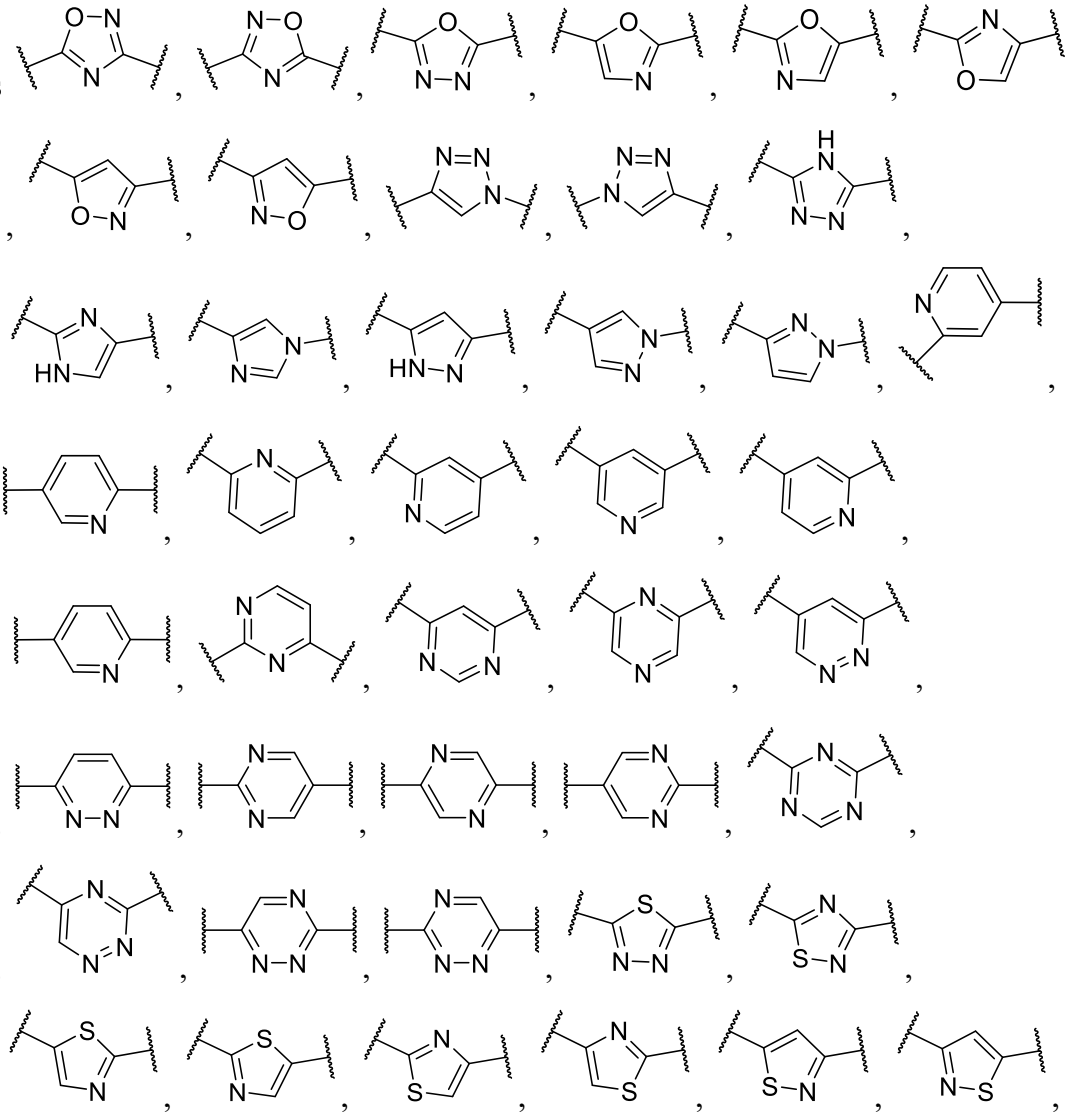
(vi) Ring W is a 5 or 6-membered nitrogen-containing heterocyclyl; or

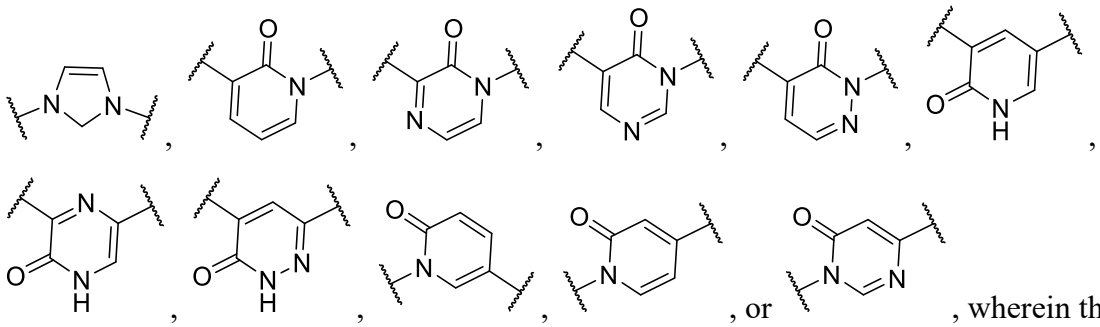
(vii)  is 






, or , wherein the attachment to the left is to the direction of Z.

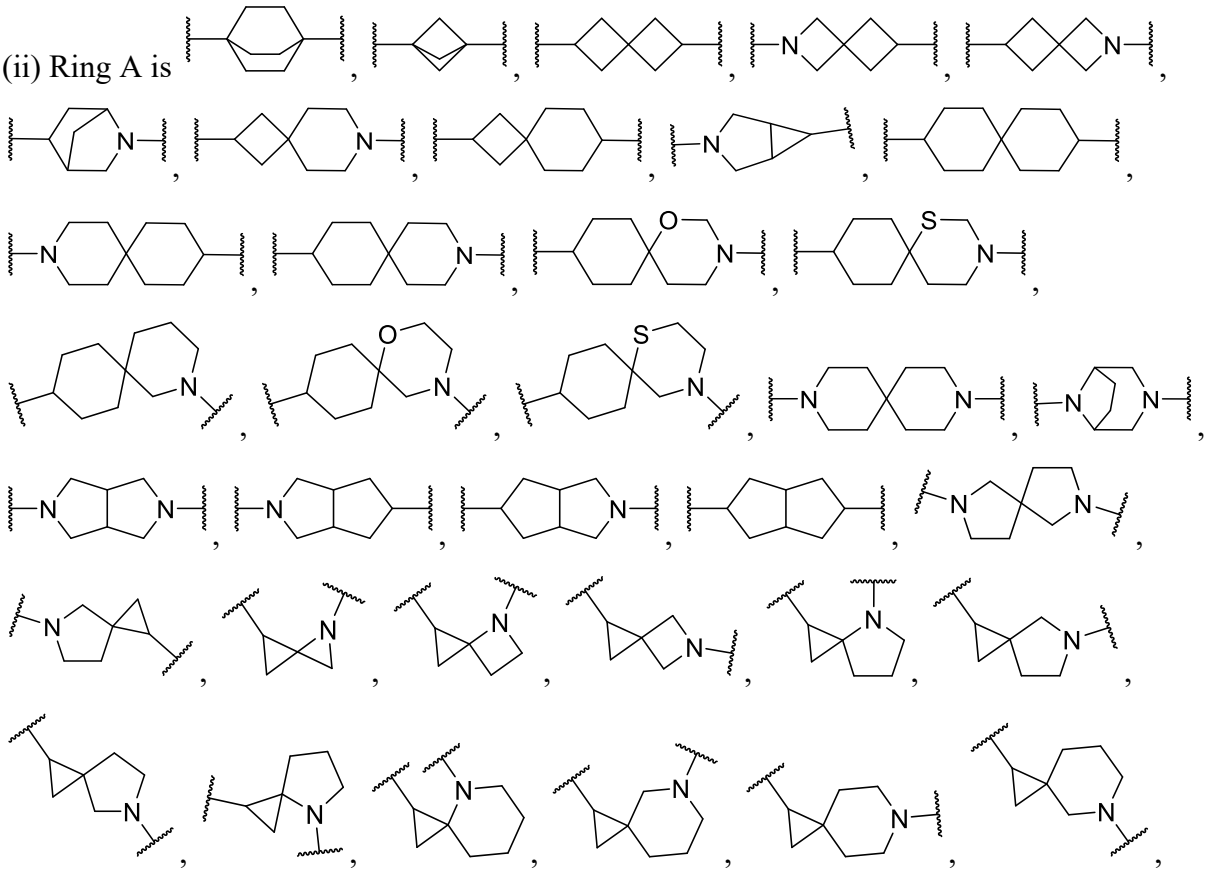
12. The compound of any one of claims 3 to 11, wherein (i) Ring B is a 5 or 6-membered heteroaryl;

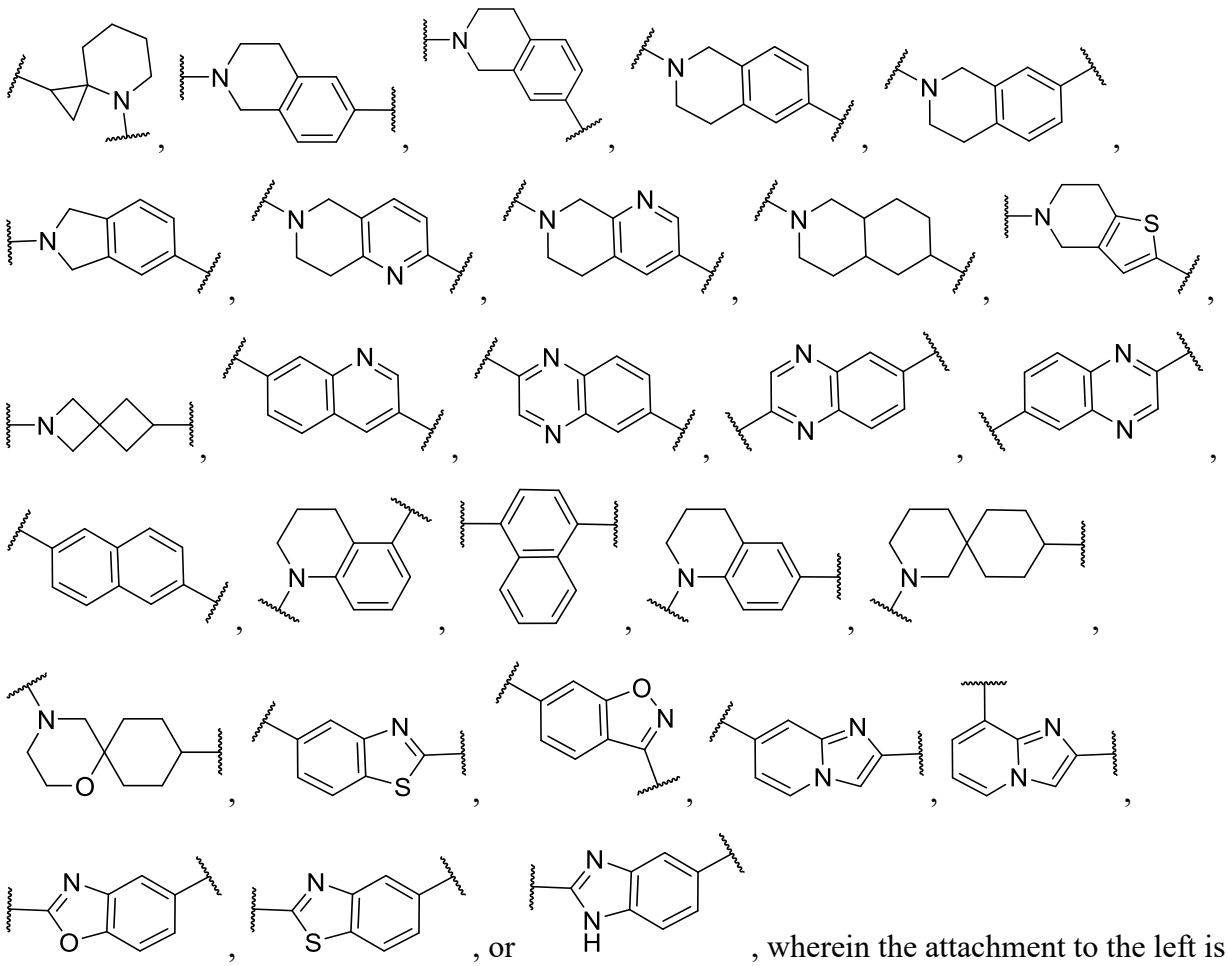
(ii) Ring B is a 5 or 6-membered nitrogen-containing heteroaryl; or

(iii) Ring B is 


, wherein the attachment to the left is to the direction of Z.

13. The compound of any one of claims 1 to 12, wherein (i) Ring A is a fused, bridged or spiro C_5-C_{12} cycloalkyl, a fused, bridged or spiro 5 to 12-membered heterocyclyl, a fused C_{10} aryl, or a fused 9 or 10-membered heteroaryl;

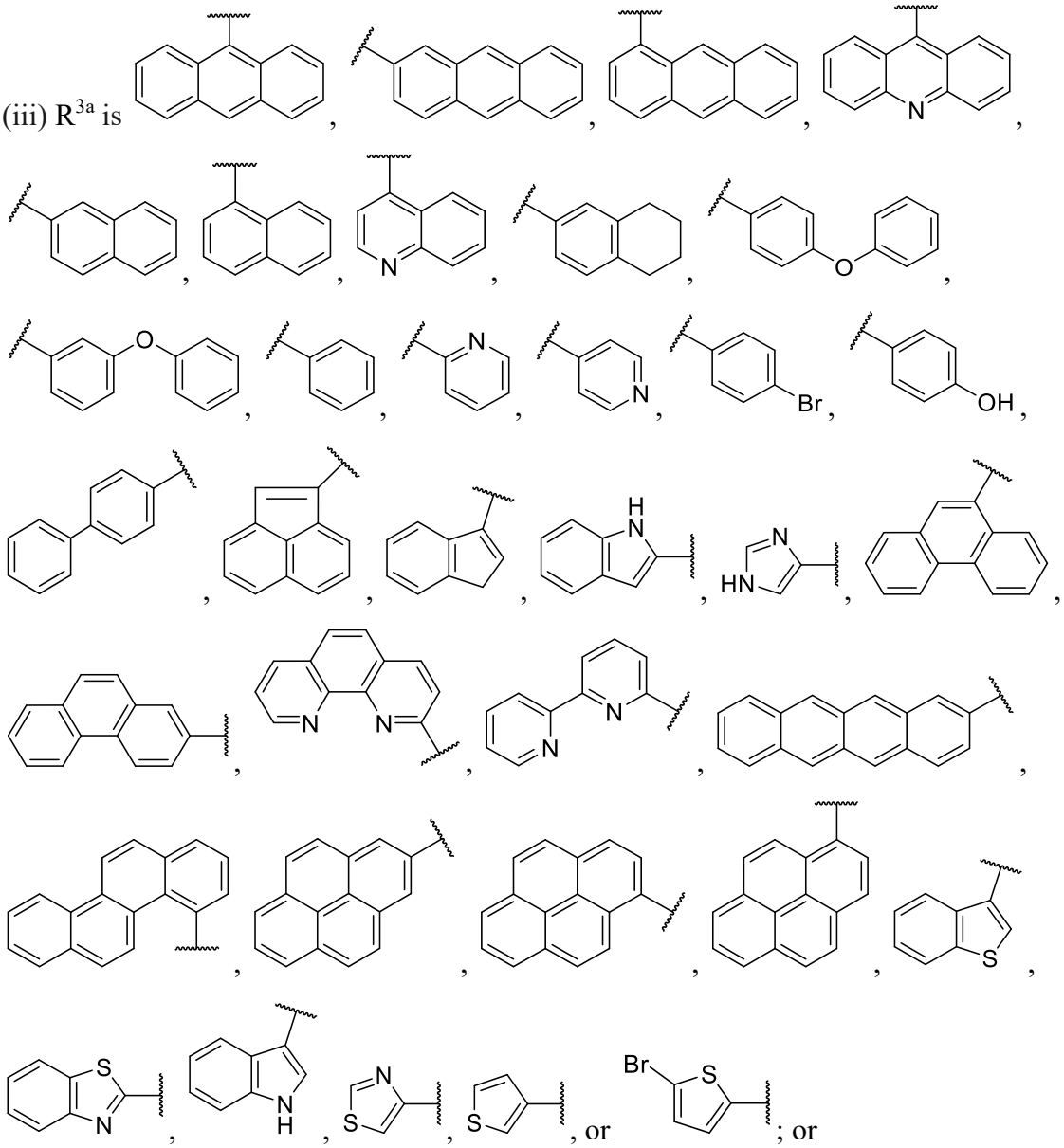
(ii) Ring A is 

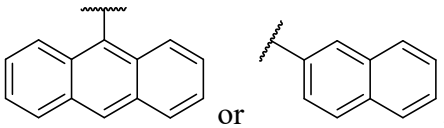

, wherein the attachment to the left is to the direction of Z; or

(iii) Ring A is a monocyclic C_3-C_8 cycloalkyl, or monocyclic 3 to 6-membered heterocyclyl.

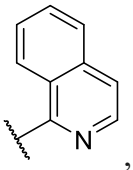
14. The compound of any one of claims 4 to 13, wherein (i) R^{3a} is a C_6-C_{20} aryl, 5 to 20-membered heteroaryl, or 3 to 14-membered heterocyclyl, wherein the aryl, heteroaryl and heterocyclyl are optionally substituted with one or more halogen, OH, C_1-C_6 alkyl, C_6-C_{10} aryl, C_6-C_{10} cycloalkyl, C_6-C_{10} aryloxy, or 3 to 8-membered heterocyclyl;

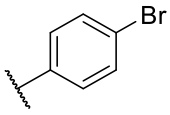
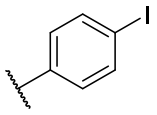
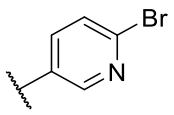
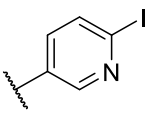
(ii) R^{3a} is phenyl, pyridyl, biphenyl, bipyridyl, anthracenyl, acridinyl, acenaphthylenyl, indenyl, phenanthrenyl, phenalenyl, triphenylenyl, naphthalenyl, tetracenyl, chrysenyl, or pyrenyl, wherein R^{3a} is optionally substituted with one or more halogen, OH, or C_1-C_6 alkyl;

(iii) R^{3a} is ; or

(iv) R^{3a} is .

15. The compound of any one of claims 1 to 14, wherein (i) R^1 is H;

(ii) R^1 is C_1-C_6 alkyl optionally substituted with one or more OH, halogen, oxo, ,

, , , or ;

(iii) R^4 is H;

(iv) R^4 and NR^1 of G^2 together with the intervening atoms form a 5 to 8-membered heterocyclyl ring;

(v) each R^2 is independently OH, oxo, halogen, NH_2, or C_1-C_6 alkyl; or

(vi) each n is independently 0, 1, or 2.

16. The compound of any one of claims 1 to 15, wherein (i) L is absent;

(ii) L is a linker;

(iii) L comprises or is an optionally substituted C_1-C_{12} alkylene, wherein one or more -CH_2- in the alkylene is independently optionally replaced by a -NHC(=O)-*, -C(=O)NH-*, -NHC(=S)-*, -C(=S)NH-*, -O-, -S-, -$S(=O)_2$-, -S(=O)-, -C(=O)-, -C(=O)O-*, -OC(=O)-*, or -NH-, wherein * refers to the direction toward P^1; or

(iv) L is -$(CH_2)_{1-6}$-;

17. The compound of any one of claims 1 to 16, wherein Z is a radioactive moiety; optionally wherein:

(i) the radioactive moiety is a fluorescent isotope, a radioisotope, or a radioactive drug;

(ii) the radioactive moiety is selected from the group consisting of alpha radiation emitting isotopes, beta radiation emitting isotopes, gamma radiation emitting isotopes, Auger electron emitting isotopes, X-ray emitting isotopes, and fluorescence emitting isotopes;

(iii) the radioactive moiety is a complex formed by a radioisotope of a metal cation and a chelating agent;

(iv) the radioactive moiety is a complex formed by a cation of ^{177}Lu, Al^{18}F, ^{203}Pb, ^{212}Pb, ^{51}Cr, ^{67}Ga, ^{68}Ga, ^{89}Zr, ^{111}In, ^{99m}Tc, ^{139}La, ^{140}La, ^{175}Yb, ^{153}Sm, ^{166}Ho, ^{88}Y, ^{90}Y, ^{149}Pm, ^{165}Dy, ^{169}Er, ^{47}Sc, ^{142}Pr, ^{159}Gd, ^{212}Bi, ^{213}Bi, ^{97}Ru, ^{109}Pd, ^{105}Rh, ^{101m}Rh, ^{119}Sb, ^{128}Ba, ^{197}Hg, ^{151}Eu, ^{153}Eu, ^{169}Eu, ^{201}Tl, ^{64}Cu, ^{67}Cu, ^{188}Re, ^{186}Re, ^{198}Au, ^{225}Ac, ^{227}Th, or ^{199}Ag and a chelating agent in Table 1;

(v) the radioactive moiety is a metal-chelating moiety of: ^{177}Lu-DOTA, ^{177}Lu-DOTAGA, ^{68}Ga-DOTA, ^{90}Y-DOTA, Al^{18}F-NOTA, ^{203}Pb-TCMC, ^{212}Pb-PSC, ^{203}Pb-PSC, ^{212}Pb-TCMC, ^{64}Cu-DOTA, or ^{225}Ac-DOTA; or

(vi) the radioactive moiety comprises ^{11}C, ^{18}F, ^{72}As, ^{72}Se, ^{123}I, ^{124}I, ^{131}I, or ^{211}At.

18. The compound of any one of claims 1 to 16, wherein Z is a fluorescent dye or a contrast agent; optionally wherein:

(i) the fluorescent dye is a Xanthene, an Acridine, an Oxazine, a Cyanine, a Styryl dye, a Coumarin, a Porphine, a Metal-Ligand-Complex, a Fluorescent protein, Nanocrystals, a Perylene, a Boron-dipyrromethene, or a Phthalocyanine, or a conjugate or combination thereof; or (ii) the contrast agent comprises a paramagnetic agent.

19. The compound of any one of claims 1 to 16, wherein Z is a chelating agent; optionally wherein:

(i) the chelating agent is a tetradentate chelating agent, a hexadentate chelating agent, or an octadentate chelating agent;

(ii) the chelating agent comprises an optionally substituted 8 to 20-membered nitrogen-containing heterocyclyl;

(iii) the chelating agent is a chelating moiety of: 1,4,7,10-tetraazacyclododecane-N,N',N,N'- tetra acetic acid (DOTA), ethylenediaminetetraacetic acid (EDTA), 1,4,7-triazacyclononane-l,4,7-triacetic acid (NOTA), 1,4,7,10-tetraazacyclododecane-1-(glutaric acid)-4,7,10-triacetic acid (DOTAGA), 2-[4,7,10-tris(2-amino-2-oxoethyl)-1,4,7,10-

tetrazacyclododec-1-yl]acetamide (TCMC), triethylenetetramine (TETA), iminodiacetic acid, diethylenetriamine-N,N,N',N',N''-penta acetic acid (DTPA), bis-(carboxymethyl imidazole)glycine, or 6-hydrazinopyridine-3-carboxylic acid (HYNIC); or

(iv) the chelating agent is a chelating agent in Table 1.

20. A compound in Table 2 or Table 2A, or a stereoisomer, a mixture of stereoisomers, a tautomer, or a pharmaceutically acceptable salt thereof.

21. A complex formed by a compound of any one of claims 1 to 16, 19, and 20 and a metal cation; optionally wherein:

(i) the metal cation is a cation of Cr, Ga, In, Tc, Re, La, Yb, Sm, Ho, Y, Pm, Dy, Er, Lu, Sc, Pr, Gd, Bi, Ru, Pd, Rh, Sb, Ba, Hg, Eu, Tl, Pb, Cu, Re, Au, Ac, Th, or Ag;

(ii) the metal cation is a cation of ^{51}Cr, ^{67}Ga, ^{68}Ga, ^{89}Zr, ^{111}In, ^{99m}Tc, ^{186}Re, ^{188}Re, ^{139}La, ^{140}La, ^{175}Yb, ^{153}Sm, ^{166}Ho, ^{88}Y, ^{90}Y, ^{149}Pm, ^{165}Dy, ^{169}Er, ^{177}Lu, ^{47}Sc, ^{142}Pr, ^{159}Gd, ^{212}Bi, ^{213}Bi, ^{97}Ru, ^{109}Pd, ^{105}Rh, ^{101m}Rh, ^{119}Sb, ^{128}Ba, ^{197}Hg, ^{151}Eu, ^{153}Eu, ^{169}Eu, ^{201}Tl, ^{203}Pb, ^{212}Pb, ^{64}Cu, ^{67}Cu, ^{198}Au, ^{225}Ac, ^{227}Th, or ^{199}Ag; or

(iii) the metal cation is $^{177}Lu^{3+}$, $^{68}Ga^{3+}$, $^{111}In^{3+}$, $^{99m}Tc^{4+}$, $^{90}Y^{3+}$, $^{203}Pb^{2+}$, $^{212}Pb^{2+}$, $^{64}Cu^{2+}$, or $^{225}Ac^{3+}$.

22. A complex in Table 3, or a stereoisomer, a mixture of stereoisomers, a tautomer, or a pharmaceutically acceptable salt thereof.

23. A pharmaceutical composition comprising a compound of any one of claims 1 to 20 or a complex of claim 21 or 22, and a pharmaceutically acceptable excipient.

24. Use of a compound of any one of claims 1 to 20, a complex of claim 21 or 22, or a pharmaceutical composition of claim 23 in the manufacture of a medicament for treating or diagnosing a prostate-specific membrane antigen (PSMA) positive cancer in a subject in need thereof; optionally wherein:

the cancer is prostate cancer, renal cancer, breast cancer, thyroid cancer, gastric cancer, colorectal cancer, bladder cancer, pancreatic cancer, lung cancer, liver cancer, brain tumor,

melanoma, neuroendocrine tumor, ovarian cancer, adenoid cystic carcinoma, salivary duct carcinoma, or sarcoma.

25. The use of claim 24, wherein the cancer is prostate cancer.

26. Use of a compound of any one of claims 1 to 20, a complex of claim 21 or 22, or a pharmaceutical composition of claim 23 in the manufacture of a medicament for detecting cells or tissues expressing prostate-specific membrane antigen (PSMA), wherein the detecting comprises (i) contacting the PSMA-expressing cells or tissues with the compound, complex, or pharmaceutical composition and (ii) applying one or more imaging method to detect the cells or tissues; optionally wherein:

(a) the imaging method comprises positron emission tomography (PET), single-photon emission computed tomography (SPECT), magnetic resonance imaging (MRI), computed tomography (CT), scintigraphy imaging, luminescence imaging, or fluorescence imaging, or a combination thereof;

(b) the PSMA-expressing cells or tissues comprise prostate cells or tissues, spleen cells or tissues, or kidney cells or tissues; or

(c) the detecting is performed *in vivo*, *ex vivo*, or *in vitro*.