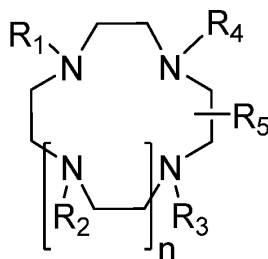


WHAT IS CLAIMED IS:

1. A compound having the structure of formula (I) below, or a metal complex thereof, or a pharmaceutically acceptable salt thereof:

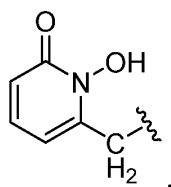


(I),

wherein

R_1 , R_2 , and R_3 each are, independently, -L-U, R_4 is -X-W, and R_5 is H, -L-U, or -X-W; or R_1 , R_2 , R_3 , and R_4 each are, independently, -L-U, and R_5 is -X-W; and

n is an integer of 0-3, when n is 0 and R_5 is H, R_1 , R_3 , and R_4 are not all equal to



wherein

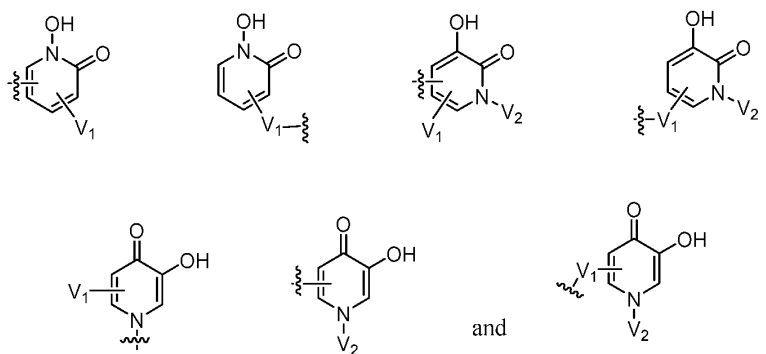
L is C=O or -CH(R)-, in which R is H, optionally substituted alkyl, optionally substituted heteroalkyl, or $-L^1-Z_1-L^2-Z_2-B$;

U is optionally substituted aryl, optionally substituted heteroaryl, optionally substituted carboxylic acid, or optionally substituted phosphonic acid; or -L-U is $-L^1-Z_1-L^2-Z_2-B$;

at least one of R_1 - R_3 has U as optionally substituted heteroaryl;

X is C=O or optionally substituted C_1 - C_3 alkylene; and

W is a donating moiety capable of coordinating to a radiometal, wherein the donating moiety is an optionally substituted hydroxypyridinone having the structure selected from the group consisting of



in which V_1 is deleted, fused aryl or heteroaryl, fused carbocycle or heterocycle, alkyl, ether, alcohol, acid, ester, amide, phosphonate or sulfonate; and V_2 is H, alkyl, or acyl, wherein

L^1 is bond, optionally substituted C_1 - C_6 alkylene, or optionally substituted C_1 - C_6 heteroalkylene;

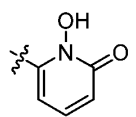
Z_1 is bond, $C=O(NR^4)$, $C=S(NR^4)$, $OC=O(NR^4)$, $NR^4C=O(O)$, $NR^4C=O(NR^4)$, $-CH_2PhC=O(NR^4)$, $-CH_2Ph(NR^4)C=O$, or $-CH_2Ph(NH)C=S(NR^4)$, each R^4 independently being H, optionally substituted C_1 - C_6 alkyl, optionally substituted C_1 - C_6 heteroalkyl, or optionally substituted aryl or heteroaryl;

L^2 is optionally substituted C_1 - C_{50} alkylene, or optionally substituted C_1 - C_{50} heteroalkylene, or C_5 - C_{20} polyethylene glycol;

Z_2 is $C=O$, $-NR'-(C=O)-$, or $-NR'-(C=O)-R''$, R' being H or C_1 - C_6 alkyl and R'' being C_1 - C_{20} alkylene, C_2 - C_{20} heteroalkylene, or arylene; and

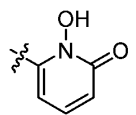
B is a therapeutic moiety, a targeting moiety, or cross-linking group.

2. The compound of claim 1, wherein W is



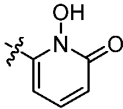
3. The compound of claim 1, wherein X is C_1 - C_3 alkylene.

4. The compound of claim 3, wherein W is



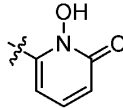
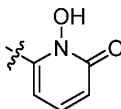
and X is CH_2 .

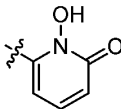
5. The compound of claim 1, wherein n is 1.

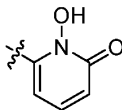
6. The compound of claim 5, wherein W is  and X is CH₂.

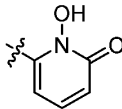
7. The compound of claim 1, wherein R₁, R₂, and R₃ each are, independently, -L-U, in which L is -CH(R)-, R being H.

8. The compound of claim 7, wherein U is optionally substituted heteroaryl or optionally substituted carboxylic acid.

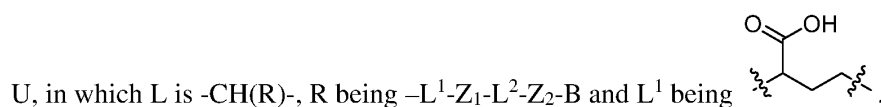
9. The compound of claim 8, wherein U is  or CO₂H, and at least one of R₁-R₃ has U as .

10. The compound of claim 7, wherein at least one of R₁-R₃ has U as .

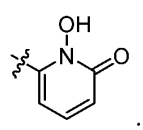
11. The compound of claim 7, wherein each of R₁-R₃ has U as .

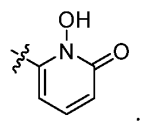
12. The compound of claim 11, wherein W is  and X is CH₂.

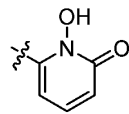
13. The compound of claim 1, wherein R_1 , R_2 , and R_3 each are, independently, -L-



14. The compound of claim 13, wherein L^2 is C_5 - C_{20} polyethylene glycol and Z_2 is $-NR'-(C=O)-R''$, R' being H and R'' being arylene.

15. The compound of claim 13, wherein at least one of R_1 - R_3 has U as .

16. The compound of claim 3, wherein each of R_1 - R_3 has U as .

17. The compound of claim 16, wherein W is  and X is CH_2 .

18. The compound of claim 13, wherein B is a therapeutic moiety or targeting moiety.

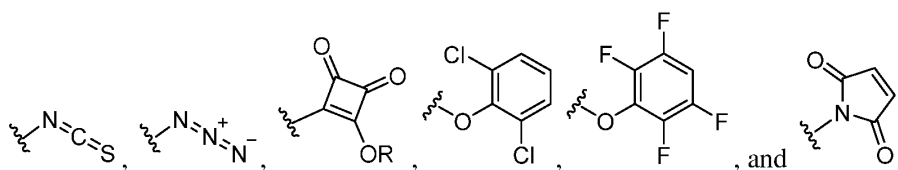
19. The compound of claim 18, wherein the therapeutic moiety or targeting moiety is an antibody, or an antigen-binding fragment thereof.

20. The compound of claim 19, wherein the antibody, or an antigen-binding fragment thereof, specifically binds IGF-1R.

21. The compound of claim 13, wherein B is a cross-linking group selected from the group consisting of an amino-reactive cross-linking group, a methionine-reactive cross-linking group, and a thiol-reactive cross-linking group.

22. The compound of claim 21, wherein the cross-linking group comprises an activated ester, an imidate, anhydride, thiol, disulfide, maleimide, azide, alkyne, strained alkyne, strained alkene, halogen, sulfonate, haloacetyl, amine, hydrazide, diazirine, phosphine, tetrazine, isothiocyanate, or oxaziridine, in which the activated ester is a hydroxysuccinimide ester, 2,3,5,6-tetrafluorophenol ester, 2,6-dichlorophenol ester or a 4-nitrophenol ester.

23. The compound of claim 22, wherein the cross-linking group is selected from the group consisting of:



24. The compound of claim 1, wherein the compound comprises a metal complex that contains a metal selected from the group consisting of Bi, Pb, Y, Mn, Cr, Fe, Co, Zn, Ni, In, Ga, Cu, Re, Sm, a lanthanide, and an actinide.

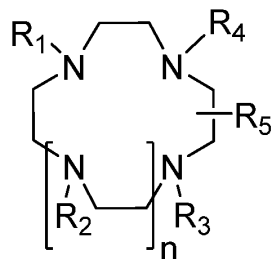
25. The compound of claim 1, wherein the compound comprises a metal complex that contains a radionuclide selected from the group consisting of ^{89}Zr , ^{47}Sc , ^{55}Co , ^{60}Cu , ^{61}Cu , ^{62}Cu , ^{64}Cu , ^{67}Cu , ^{66}Ga , ^{67}Ga , ^{68}Ga , ^{82}Rb , ^{86}Y , ^{87}Y , ^{90}Y , ^{97}Ru , ^{105}Rh , ^{109}Pd , ^{111}In , $^{117\text{m}}\text{Sn}$, ^{149}Pm , ^{52}Mn , ^{149}Tb , ^{152}Tb , ^{153}Sm , ^{177}Lu , ^{186}Re , ^{188}Re , ^{199}Au , ^{201}Tl , ^{203}Pb , ^{212}Pb , ^{212}Bi , ^{213}Bi , ^{225}Ac , ^{223}Ra and ^{227}Th .

26. The compound of claim 25, wherein the radionuclide is ^{89}Zr , ^{111}In , or ^{225}Ac .

27. A pharmaceutical composition comprising a compound of claim 1 and a pharmaceutically acceptable carrier.

28. A method of treating an immunoregulatory abnormality in a subject in need thereof, the method comprising administering to said subject a compound of claim 1 in an amount effective for treating said immunoregulatory abnormality.

29. A compound having the structure of formula (I) below, or a metal complex thereof, or a pharmaceutically acceptable salt thereof:



(I),

wherein

R_1 , R_2 , and R_3 each are, independently, $-L-U$, R_4 is $-X-W$, and R_5 is H, $-L-U$, or $-X-W$; or R_1 , R_2 , R_3 , and R_4 each are, independently, $-L-U$, and R_5 is $-X-W$; and

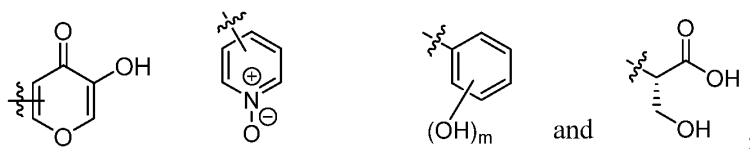
n is an integer of 0-3,

wherein

L is optionally substituted C_{1-3} alkylene;

U is optionally substituted carboxylic acid or optionally substituted phosphonic acid;

W is a donating moiety capable of coordinating to a radiometal, in which the donating moiety is an optionally substituted hydroxypyridinone or a moiety selected from the group consisting of



m is an integer of 1-3; and

X is $-L^1-Z_1-L^2-N(R)-(C=O)-$, in which R is H, optionally substituted alkyl, optionally substituted heteroalkyl, or $-L^3-Z_2-B$,

wherein

L^1 and L^2 each are, independently, bond, optionally substituted C_1-C_6 alkylene, or optionally substituted C_1-C_6 heteroalkylene;

L^3 is optionally substituted C_1-C_{50} alkylene, or optionally substituted C_1-C_{50} heteroalkylene, or C_5-C_{20} polyethylene glycol;

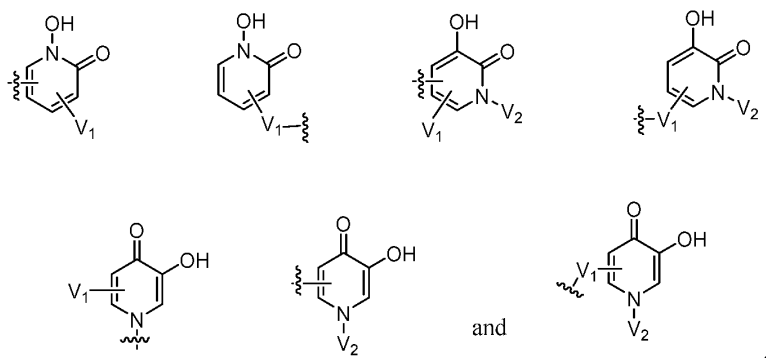
Z_1 is bond, $C=O(NR^4)$, $C=S(NR^4)$, $OC=O(NR^4)$, $NR^4C=O(O)$, $NR^4C=O(NR^4)$, $-CH_2PhC=O(NR^4)$, $-CH_2Ph(NR^4)C=O$, or $-CH_2Ph(NH)C=S(NR^4)$, each R^4 independently

being H, optionally substituted C₁-C₆ alkyl, optionally substituted C₁-C₆ heteroalkyl, or optionally substituted aryl or heteroaryl;

Z₂ is C=O, -NR'-(C=O)-, or -NR'-(C=O)-R'', R' being H or C₁-C₆ alkyl and R'' being C₁-C₂₀ alkylene, C₂-C₂₀ heteroalkylene, or arylene; and

B is a therapeutic moiety, a targeting moiety, or cross-linking group.

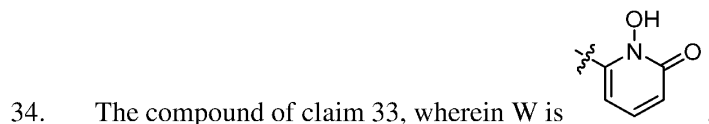
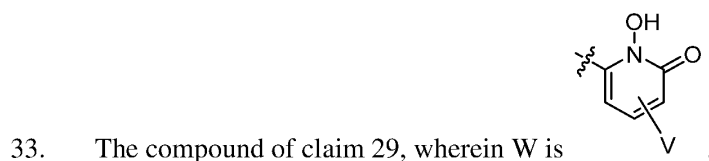
30. The compound of claim 29, wherein W is an optionally substituted hydroxypyridinone, having the structure selected from the group consisting of



in which V₁ is deleted, fused aryl or heteroaryl, fused carbocycle or heterocycle, alkyl, ether, alcohol, acid, ester, amide, phosphonate or sulfonate; and V₂ is H, alkyl, or acyl.

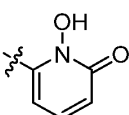
31. The compound of claim 29, wherein R₁, R₂, and R₃ each are, independently, -L-U, in which L is optionally substituted C₁ alkylene and U is -CO₂H.

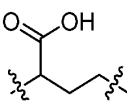
32. The compound of claim 31, wherein L is CH₂.



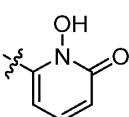
35. The compound of claim 29, wherein n is 1.

36. The compound of claim 35, wherein each of R_1 , R_2 , and R_3 is -L-U, in which L is CH_2 and U is $-CO_2H$.

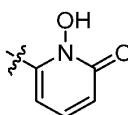
37. The compound of claim 35, wherein W is .

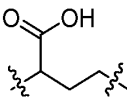
38. The compound of claim 29, wherein X is $-L^1-Z_1-L^2-N(R)-(C=O)-$, in which L^1 is , and R is H.

39. The compound of claim 38, wherein each of R_1 , R_2 , and R_3 is -L-U, in which L is CH_2 and U is $-CO_2H$.

40. The compound of claim 38, wherein W is .

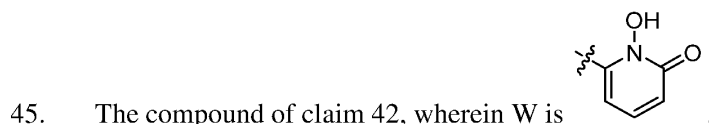
41. The compound of claim 38, wherein each of R_1 , R_2 , and R_3 is -L-U, in which L

is CH_2 and U is $-CO_2H$; and W is .

42. The compound of claim 29, wherein X is $-L^1-Z_1-L^2-N(R)-(C=O)-$, in which L^1 is , and R is $-L^3-Z_2-B$.

43. The compound of claim 42, wherein L^3 is C_5 - C_{20} polyethylene glycol and Z_2 is $-NR'-(C=O)-R''$, R' being H and R'' being arylene.

44. The compound of claim 42, wherein each of R_1 , R_2 , and R_3 is -L-U, in which L is CH_2 and U is $-CO_2H$.



46. The compound of claim 45, wherein each of R_1 , R_2 , and R_3 is -L-U, in which L is CH_2 and U is $-CO_2H$; L^3 is C_5 - C_{20} polyethylene glycol; and Z_2 is $-NR'-(C=O)-R''$, R' being H and R'' being arylene.

47. The compound of claim 42, wherein B is a therapeutic moiety or targeting moiety.

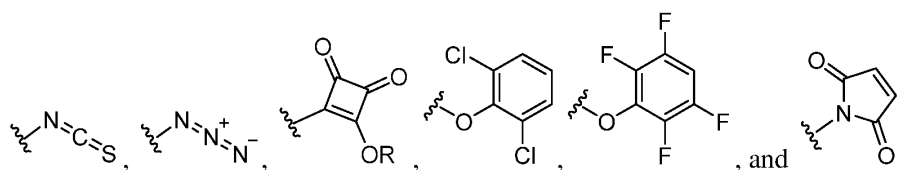
48. The compound of claim 47, wherein the therapeutic moiety or targeting moiety is an antibody, or an antigen-binding fragment thereof.

49. The compound of claim 48, wherein the antibody, or an antigen-binding fragment thereof, specifically binds insulin-like growth factor-1 receptor (IGF-1R).

50. The compound of claim 42, wherein B is a cross-linking group selected from the group consisting of an amino-reactive cross-linking group, a methionine-reactive cross-linking group, and a thiol-reactive cross-linking group.

51. The compound of claim 50, wherein the cross-linking group comprises an activated ester, an imidate, anhydride, thiol, disulfide, maleimide, azide, alkyne, strained alkyne, strained alkene, halogen, sulfonate, haloacetyl, amine, hydrazide, diazirine, phosphine, tetrazine, isothiocyanate, or oxaziridine, in which the activated ester is a hydroxysuccinimide ester, 2,3,5,6-tetrafluorophenol ester, 2,6-dichlorophenol ester or a 4-nitrophenol ester.

52. The compound of claim 51, wherein the cross-linking group is selected from the group consisting of:



53. The compound of claim 29, wherein the compound comprises a metal complex that contains a metal selected from the group consisting of Bi, Pb, Y, Mn, Cr, Fe, Co, Zn, Ni, In, Ga, Cu, Re, Sm, a lanthanide, and an actinide.

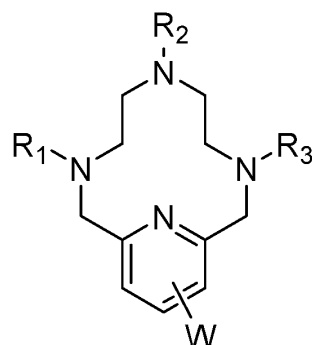
54. The compound of claim 29, wherein the compound comprises a metal complex that contains a radionuclide selected from the group consisting of ^{89}Zr , ^{47}Sc , ^{55}Co , ^{60}Cu , ^{61}Cu , ^{62}Cu , ^{64}Cu , ^{67}Cu , ^{66}Ga , ^{67}Ga , ^{68}Ga , ^{82}Rb , ^{86}Y , ^{87}Y , ^{90}Y , ^{97}Ru , ^{105}Rh , ^{109}Pd , ^{111}In , $^{117\text{m}}\text{Sn}$, ^{149}Pm , ^{52}Mn , ^{149}Tb , ^{152}Tb , ^{153}Sm , ^{177}Lu , ^{186}Re , ^{188}Re , ^{199}Au , ^{201}Tl , ^{203}Pb , ^{212}Pb , ^{212}Bi , ^{213}Bi , ^{225}Ac , ^{223}Ra and ^{227}Th .

55. The compound of claim 54, wherein the radionuclide is ^{89}Zr , ^{111}In , or ^{225}Ac .

56. A pharmaceutical composition comprising a compound of claim 29 and a pharmaceutically acceptable carrier.

57. A method of treating an immunoregulatory abnormality in a subject in need thereof, the method comprising administering to said subject a compound of claim 29 in an amount effective for treating said immunoregulatory abnormality.

58. A compound having the structure of formula (II) below, or a metal complex thereof, or a pharmaceutically acceptable salt thereof:



(II),

wherein

R_1 , R_2 , and R_3 each are, independently, $-L-U$, and W is H or $-L^1-Z_1-L^2-Z_2-B$,

wherein

L is $C=O$ or $-CH(R)-$, in which R is H , optionally substituted alkyl, optionally substituted heteroalkyl, or $-L^1-Z_1-L^2-Z_2-B$;

U is optionally substituted aryl, optionally substituted heteroaryl, optionally substituted carboxylic acid, or optionally substituted phosphonic acid; or $-L-U$ is $-L^1-Z_1-L^2-Z_2-B$;

at least one of R_1 - R_3 has U as optionally substituted heteroaryl;

wherein

L^1 is bond, optionally substituted C_1 - C_6 alkylene, or optionally substituted C_1 - C_6 heteroalkylene;

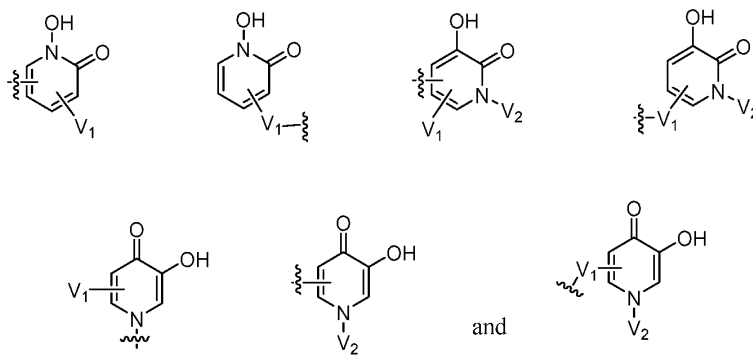
Z_1 is bond, $C=O(NR^4)$, $C=S(NR^4)$, $OC=O(NR^4)$, $NR^4C=O(O)$, $NR^4C=O(NR^4)$, $-CH_2PhC=O(NR^4)$, $-CH_2Ph(NR^4)C=O$, or $-CH_2Ph(NH)C=S(NR^4)$, each R^4 independently being H , optionally substituted C_1 - C_6 alkyl, optionally substituted C_1 - C_6 heteroalkyl, or optionally substituted aryl or heteroaryl;

L^2 is optionally substituted C_1 - C_{50} alkylene, or optionally substituted C_1 - C_{50} heteroalkylene, or C_5 - C_{20} polyethylene glycol;

Z_2 is $C=O$, $-NR'-(C=O)-$, or $-NR'-(C=O)-R''$, R' being H or C_1 - C_6 alkyl and R'' being C_1 - C_{20} alkylene, C_2 - C_{20} heteroalkylene, or arylene; and

B is a therapeutic moiety, a targeting moiety, or cross-linking group.

59. The compound of claim 58, wherein U is a donating moiety capable of coordinating to a radiometal, wherein the donating moiety is an optionally substituted hydroxypyridinone having the structure selected from the group consisting of



in which V₁ is deleted, fused aryl or heteroaryl, fused carbocycle or heterocycle, alkyl, ether, alcohol, acid, ester, amide, phosphonate or sulfonate; and V₂ is H, alkyl, or acyl.

60. A pharmaceutical composition comprising a compound of claim 58 and a pharmaceutically acceptable carrier.

61. A method of treating an immunoregulatory abnormality in a subject in need thereof, the method comprising administering to said subject a compound of claim 58 in an amount effective for treating said immunoregulatory abnormality.