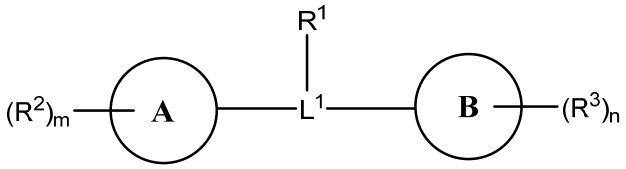
WHAT IS CLAIMED IS:

1. A compound of Formula I:



I

or a pharmaceutically acceptable salt thereof, wherein:

Ring **A** is selected from the group consisting of C_{6-10} aryl, 4-16 membered heterocycloalkyl, and 5-16 membered heteroaryl;

Ring **B** is selected from the group consisting of C_{6-10} aryl, 4-16 membered heterocycloalkyl, and 5-16 membered heteroaryl;

L^1 is selected from the group consisting of $NHC(O)L^2$, $NHC(O)\text{-}L^2\text{-}C(O)NH$, $L^2\text{-}NHC(O)\text{-}L^2$, $L^2\text{-}NHC(O)\text{-}L^2\text{-}NHC(O)$, and $L^2\text{-}NHC(O)\text{-}L^2\text{-}NHC(O)\text{-}L^2\text{-}$;

each L^2 is independently selected from the group consisting of C_{1-4} alkylene, C_{1-4} alkyleneoxy, and C_{1-4} alkenylene;

R^1 comprises a chelating group and a metal;

R^2 are R^3 are each independently selected from the group consisting of OR^a, $C(O)R^a$, and $OC(O)R^a$;

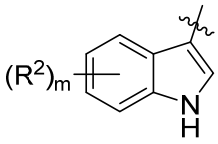
each R^a is independently selected from the group consisting of H and C_{1-4} alkyl;

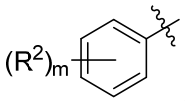
m is 0, 1, 2, 3, or 4; and

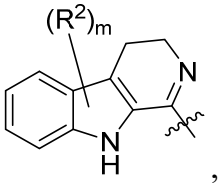
n is 0, 1, 2, 3, or 4.

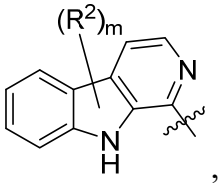
2. The compound of claim 1, or a pharmaceutically acceptable salt thereof, wherein Ring **A** is selected from the group consisting of phenyl, bicyclic 8-16 membered heterocycloalkyl, tricyclic 8-16 membered heterocycloalkyl, bicyclic 8-16 membered heteroaryl, and tricyclic 8-16 membered heteroaryl.

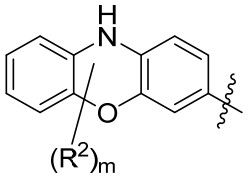
3. The compound of claim 1, or a pharmaceutically acceptable salt thereof, wherein Ring **A** is selected from the group consisting of:



,


,


,


, and


;
wherein ~~~~ indicates the bond between Ring **A** and L^1.

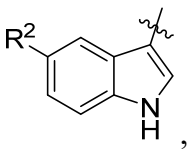
4. The compound of any one of claims 1 to 3, or a pharmaceutically acceptable salt thereof, wherein m is 1 or 2.

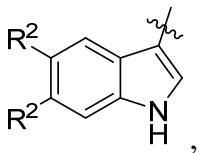
5. The compound of any one of claims 1 to 4, or a pharmaceutically acceptable salt thereof, wherein m is 1.

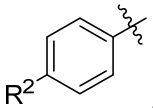
6. The compound of any one of claims 1 to 5, or a pharmaceutically acceptable salt thereof, wherein each R^2 is independently selected from the group consisting of OH, OCH_3, $C(O)CH_3$, and $OC(O)CH_3$.

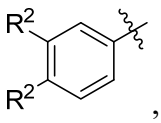
7. The compound of any one of claims 1 to 5, or a pharmaceutically acceptable salt thereof, wherein each R^2 is OH.

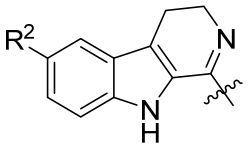
8. The compound of any one of claims 1, 6, and 7, or a pharmaceutically acceptable salt thereof, wherein Ring **A** is selected from the group consisting of:

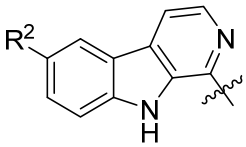


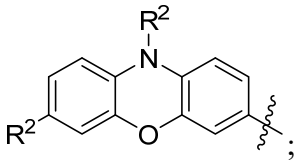
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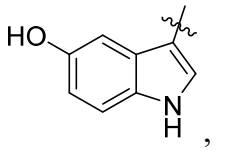
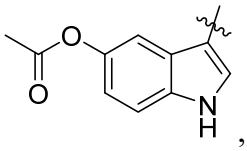
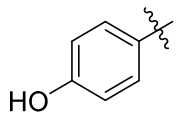
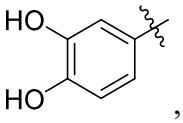
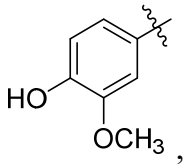
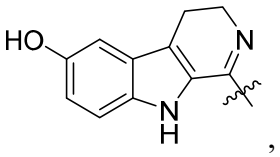
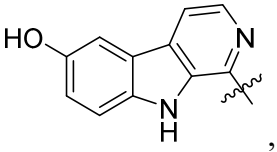
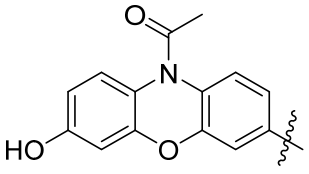
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and


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wherein ~~~~ indicates the bond between Ring **A** and L^1

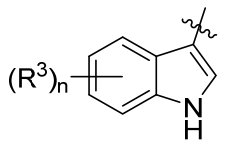
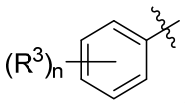
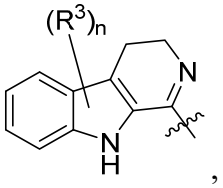
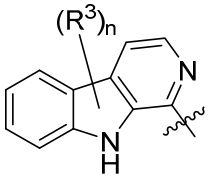
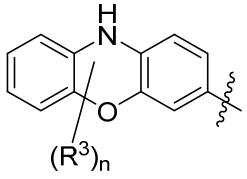
9. The compound of claim 1, or a pharmaceutically acceptable salt thereof, wherein Ring **A** is selected from the group consisting of:

wherein ~~~~ indicates the bond between Ring **A** and L^1.

10. The compound of any one of claims 1 to 9, or a pharmaceutically acceptable salt thereof, wherein Ring **B** is selected from the group consisting of phenyl, bicyclic 8-16 membered heterocycloalkyl, tricyclic 8-16 membered heterocycloalkyl, bicyclic 8-16 membered heteroaryl, and tricyclic 8-16 membered heteroaryl.

11. The compound of any one of claims 1 to 9, or a pharmaceutically acceptable salt thereof, wherein Ring **B** is selected from the group consisting of:

wherein ~~~~ indicates the bond between Ring **B** and L^1.

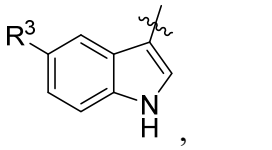
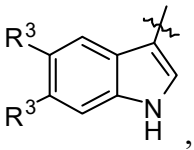
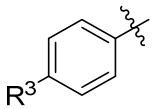
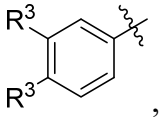
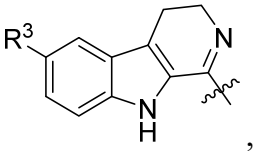
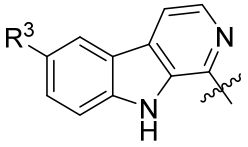
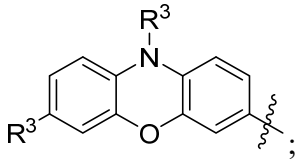
12. The compound of any one of claims 1 to 11, or a pharmaceutically acceptable salt thereof, wherein n is 1 or 2.

13. The compound of any one of claims 1 to 11, or a pharmaceutically acceptable salt thereof, wherein n is 1.

14. The compound of any one of claims 1 to 13, or a pharmaceutically acceptable salt thereof, wherein each R^3 is independently selected from the group consisting of OH, OCH_3, $C(O)CH_3$, and $OC(O)CH_3$.

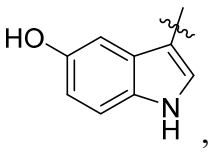
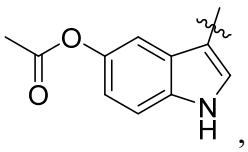
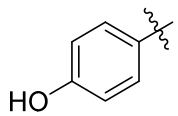
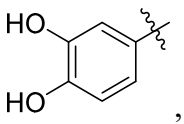
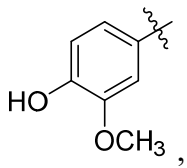
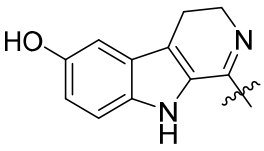
15. The compound of any one of claims 1 to 13, or a pharmaceutically acceptable salt thereof, wherein each R^3 is OH.

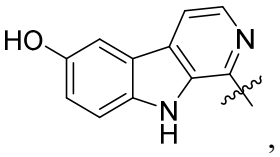
16. The compound of any one of claims 1 to 11, 14, and 15, or a pharmaceutically acceptable salt thereof, wherein Ring **B** is selected from the group consisting of:

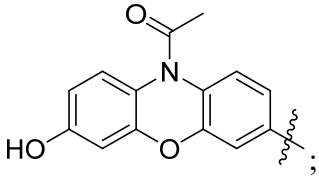






and ;

wherein ~~~~ indicates the bond between Ring **B** and L^1.

17. The compound of any one of claims 1 to 11, or a pharmaceutically acceptable salt thereof, wherein Ring **B** is selected from the group consisting of:



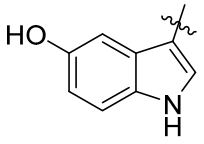
, and 

;
wherein ~~~~ indicates the bond between Ring **B** and L^1.

18. The compound of any one of claims 1 to 17, or a pharmaceutically acceptable salt thereof, wherein Ring **A** and Ring **B** are the same.

19. The compound of any one of claims 1 to 17, or a pharmaceutically acceptable salt thereof, wherein Ring **A** and Ring **B** are different.

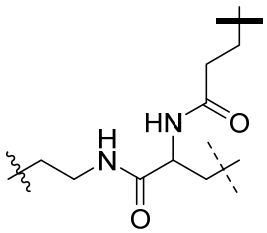
20. The compound of claim 1, or a pharmaceutically acceptable salt thereof,

wherein Ring **A** and Ring **B** are each 

.

21. The compound of any one of claims 1 to 20, or a pharmaceutically acceptable salt thereof, wherein L^1 is L^2-NHC(O)-L^2-NHC(O)-L^2-, and each L^2 is an independently selected C_{1-4} alkylene.

22. The compound of any one of claims 1 to 20, or a pharmaceutically acceptable salt thereof, wherein L^1 is:



wherein:

~~~~ indicates the bond between L^1 and Ring **A**;

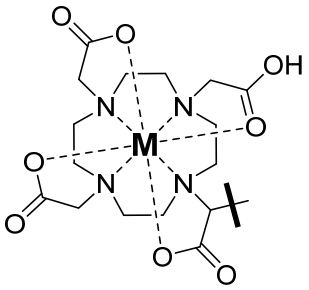
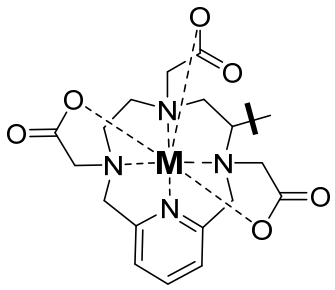
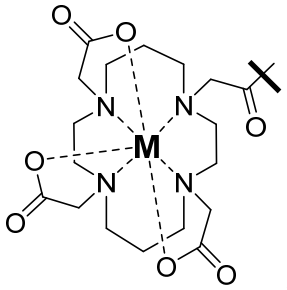
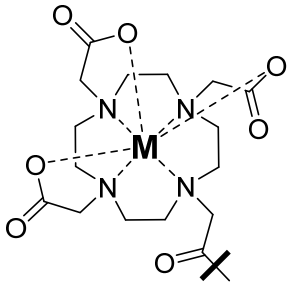
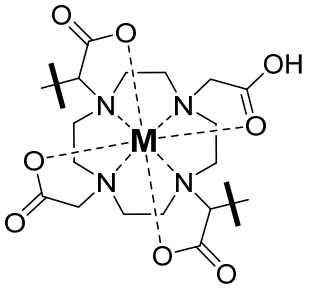
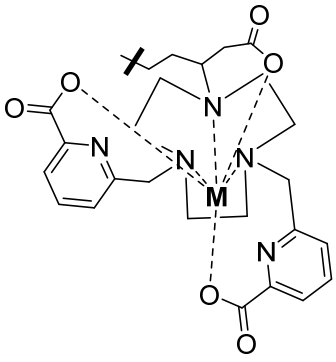
------ indicates the bond between L^1 and Ring **B**; and

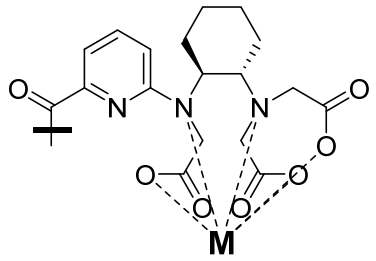
—— indicates the bond between L^1 and R^1.
~~~~

23. The compound of any one of claims 1 to 22, or a pharmaceutically acceptable salt thereof, wherein the metal of R^1 is selected from the group consisting of Gd^{3+}, Mn^{2+}, ^{68}Ga, ^{64}Cu, and ^{111}In.

24. The compound of any one of claims 1 to 22, or a pharmaceutically acceptable salt thereof, wherein the metal of R^1 is Gd^{3+}.

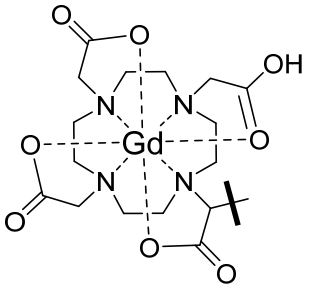
25. The compound of any one of claims 1 to 22, or a pharmaceutically acceptable salt thereof, wherein the chelating group of R^1 is selected from the group consisting of:


,

,

,

,

,

,

and  ;

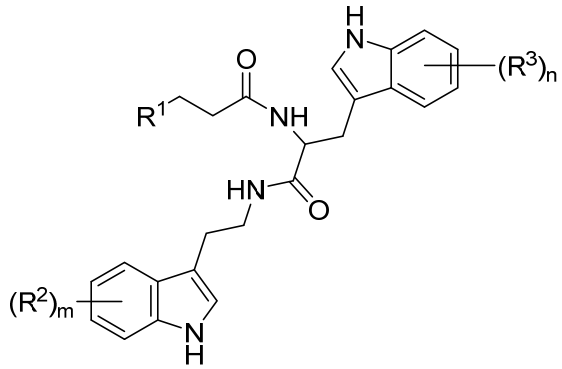
wherein **M** is the metal and — indicates the bond between R^1 and L^1.

26. The compound of any one of claims 1 to 22, or a pharmaceutically acceptable salt thereof, wherein R^1 is:

 ,

wherein — indicates the bond between R^1 and L^1.

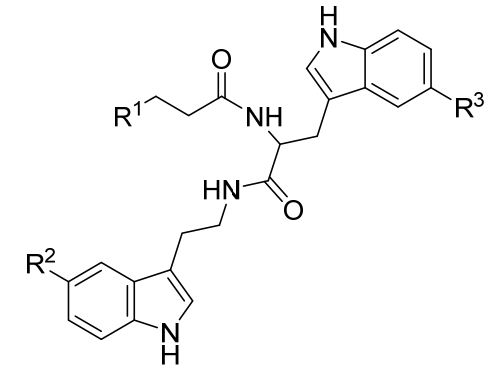
27. The compound of claim 1, or a pharmaceutically acceptable salt thereof, wherein the compound of Formula I is a compound of Formula II:



II

or a pharmaceutically acceptable salt thereof.

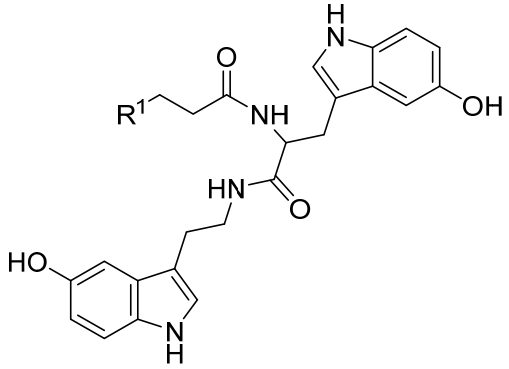
28. The compound of claim 1, or a pharmaceutically acceptable salt thereof, wherein the compound of Formula I is a compound of Formula III:



III

or a pharmaceutically acceptable salt thereof.

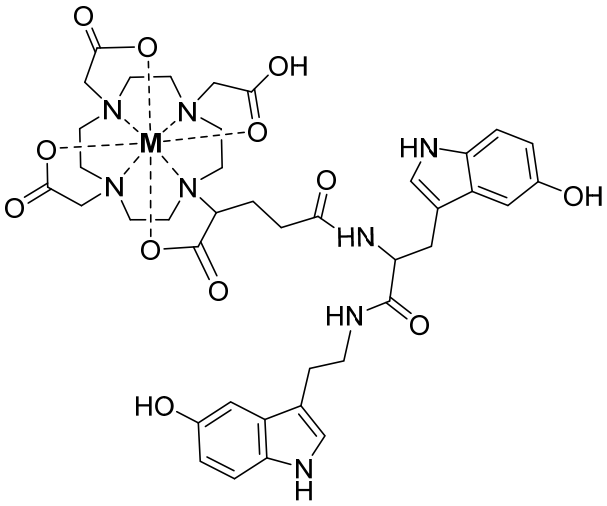
29. The compound of claim 1, or a pharmaceutically acceptable salt thereof, wherein the compound of Formula I is a compound of Formula IV:



IV

or a pharmaceutically acceptable salt thereof.

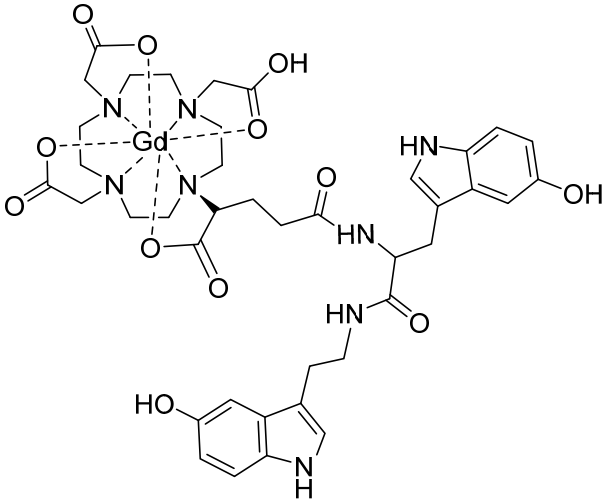
30. The compound of claim 1, or a pharmaceutically acceptable salt thereof, wherein the compound of Formula I is a compound of Formula Vb:



Vb,

or a pharmaceutically acceptable salt thereof, wherein **M** is the metal.

31. The compound of claim 1, which is:



or a pharmaceutically acceptable salt thereof.

32. A pharmaceutical composition comprising a compound of any one of claims 1 to 31, or a pharmaceutically acceptable salt thereof, and at least one pharmaceutically acceptable carrier.

33. A method of imaging a cell or tissue sample of a subject, wherein the subject had been administered a compound of any one of claims 1 to 31, or a pharmaceutically acceptable salt thereof, the method comprising:

~~i) administering to the subject a compound of any one of claims 1 to 31, or a pharmaceutically acceptable salt thereof;~~

ii~~i~~) waiting a time sufficient to allow the compound to accumulate at the cell or tissue sample; and

iii~~ii~~) imaging the cell or tissue sample with an imaging technique.

34. A method of imaging the liver of a subject, wherein the subject had been administered a compound of any one of claims 1 to 31, or a pharmaceutically acceptable salt thereof, the method comprising:

~~i) administering to the subject a compound of any one of claims 1 to 31, or a pharmaceutically acceptable salt thereof;~~

ii~~i~~) waiting a time sufficient to allow the compound to accumulate at the liver; and

iii~~ii~~) imaging a ~~the~~ cell or tissue sample of the liver with an imaging technique.

35. The method of claim 34, wherein the subject has been identified as having nonalcoholic steatohepatitis.

36. A method of diagnosing a disease or disorder associated with abnormal myeloperoxidase activity in a subject, wherein the subject had been administered a compound of any one of claims 1 to 31, or a pharmaceutically acceptable salt thereof, the method comprising:

~~i) administering to the subject a compound of any one of claims 1 to 31, or a pharmaceutically acceptable salt thereof;~~

ii~~i~~) waiting a time sufficient to allow the compound to accumulate at a cell or tissue site associated with the disease; and

iii~~ii~~) imaging the cell or tissue with an imaging technique.

37. The method of claim 36, wherein the method further comprises imaging the subject prior to step i).

38. A method of imaging myeloperoxidase activity in a cell, the method comprising:

i) contacting the cell with a compound of any one of claims 1 to 31, or a pharmaceutically acceptable salt thereof; and

ii) imaging the cell with an imaging technique.

39. A method of detecting myeloperoxidase activity in a cell or tissue sample, the method comprising:

i) contacting the cell or tissue sample with a compound of any one of claims 1 to 31, or a pharmaceutically acceptable salt thereof; and

ii) imaging the cell or tissue sample with an imaging technique.

40. A method of detecting myeloperoxidase activity in a subject, wherein the subject had been administered with a compound of any one of claims 1 to 31, or a pharmaceutically acceptable salt thereof, the method comprising:

~~i) administering to the subject a compound of any one of claims 1 to 31, or a pharmaceutically acceptable salt thereof; and~~

i~~i~~) imaging the subject with an imaging technique.

41. A method of monitoring treatment of a disease or disorder associated with abnormal myeloperoxidase activity in a subject, wherein the subject had been administered a compound of any one of claims 1 to 31, or a pharmaceutically acceptable salt thereof, the method comprising:

~~i) administering to the subject a compound of any one of claims 1 to 31, or a pharmaceutically acceptable salt thereof;~~

i~~i~~) imaging the subject with an imaging technique;

~~iii) administering to the subject a therapeutically effective amount of a therapeutic compound to treat the disease or disorder;~~

ii~~iv~~) imaging ~~the~~ cell or tissue in the subject with an imaging technique, wherein the subject had been further administered with a therapeutically effective amount of a therapeutic compound to treat the disease or disorder; and

iii~~v~~) comparing the image of step i) and the image of step ii~~iv~~).

42. The method of claim 41, wherein ~~the method further comprises administering to the subject~~ a compound of any one of claims 1 to 31, or a pharmaceutically acceptable salt thereof is to be additionally administered after the subject had been administered the therapeutic compound~~, after the administering of step iii)~~ and prior to the imaging of step ii~~iv~~).

43. The method of any one of claims 33 to 42, wherein the imaging technique is selected from the group consisting of magnetic resonance imaging and nuclear imaging.

44. The method of any one of claims 36, 37, and 41 to 43, wherein the disease or disorder associated with abnormal myeloperoxidase activity is selected from the group consisting of nonalcoholic steatohepatitis, a cancer, a rheumatic disease, an infectious disease, a disease of the central nervous system, a cardiovascular disorder, an autoimmune disorder, and inflammation associated with one or more of a cancer, a rheumatic disease, an infectious disease, disease of the central nervous system, cardiovascular disorder, and autoimmune disorder.

45. The method of claim 44, wherein the disease of the central nervous system is selected from the group consisting of Alzheimer's disease, stroke, epilepsy, Parkinson's disease, a neurodegenerative disease, and inflammation associated with one or more of Alzheimer's disease, stroke, epilepsy, Parkinson's disease, and neurodegenerative disease.

46. The method of claim 44, wherein the cardiovascular disorder is selected from the group consisting of atherosclerosis, myocardial infarction, atrial fibrillation, vasculitis, and inflammation associated with one or more of atherosclerosis, myocardial infarction, atrial fibrillation, and vasculitis.

47. The method of claim 44, wherein the autoimmune disorder is selected from the group consisting of multiple sclerosis, meningitis, encephalitis, and inflammation associated with one or more of multiple sclerosis, meningitis, and encephalitis.

48. The method of claim 44, wherein the cancer is selected from the group consisting of bladder cancer, breast cancer, carcinoma, cervical cancer, colorectal cancer, endometrial cancer, glioma, cancer of the head and neck, liver cancer, lung cancer, melanoma, ovarian cancer, pancreatic cancer, prostate cancer, renal cancer, skin cancer, stomach cancer, testicular cancer, leukemia, and thyroid cancer.

49. The method of claim 44, wherein the cancer is a solid tumor.

50. The method of claim 44, wherein the rheumatic disease is selected from the group consisting of rheumatoid arthritis, osteoarthritis, and inflammatory arthritis.

51. The method of claim 50, wherein the inflammatory arthritis is selected from the group consisting of gout and calcium pyrophosphate deposition disease (CPPD).

52. The method of claim 44, wherein the infectious disease is selected from the group consisting of a fungal disease and a bacterial disease.

53. The method of claim 44, wherein the disease or disorder associated with abnormal myeloperoxidase activity is nonalcoholic steatohepatitis.