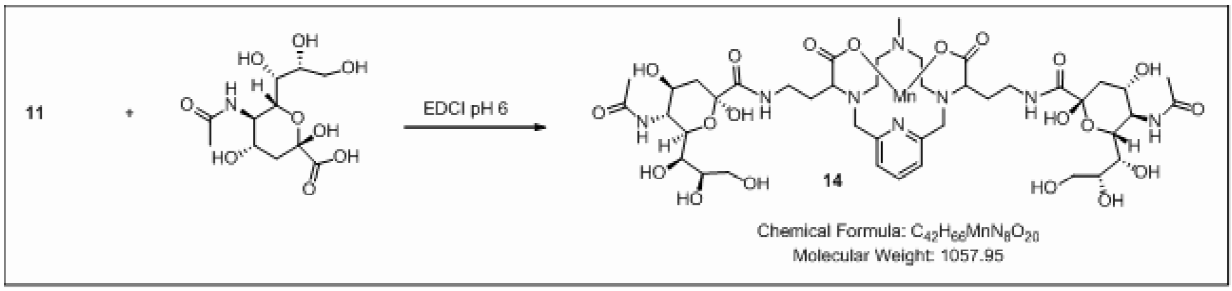
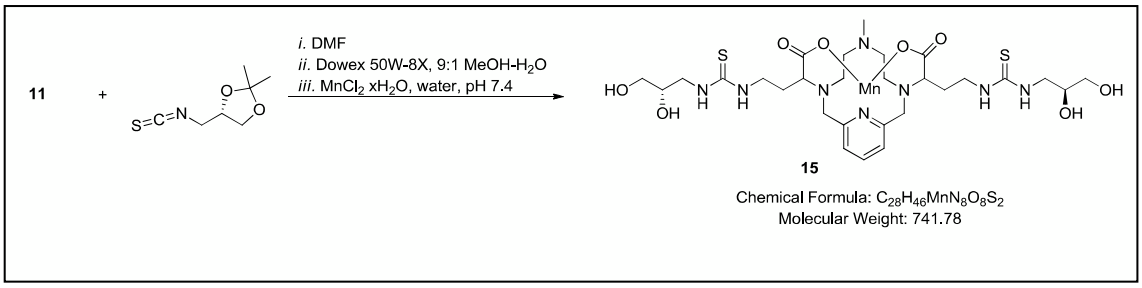
The desired compound **11** is further purified using reversed phase chromatography on C-18 functionalized silica gel and eluting with water-acetonitrile or water-methanol mixtures.

Synthesis of the conjugate **14**



The aminopyramine **13** is dissolved in water and *N*-acetylneuraminic acid (2.1 eq) and EDCI-HCl (2.1 eq) are added. The pH is adjusted to 6.5 with HCl and HOBt (0.4 eq) is then added. The pH of the resulting solution is maintained at approximately 6 while stirring for 16 h. Additional EDCI-HCl (1.1 eq) is then added, and the reaction pH is maintained at pH approximately 6 and is stirred for an additional 16 h. The solvent is removed in vacuo and the desired compound **14** is further purified using reversed phase chromatography on C-18 functionalized silica gel and eluting with water-acetonitrile or water-methanol mixtures.

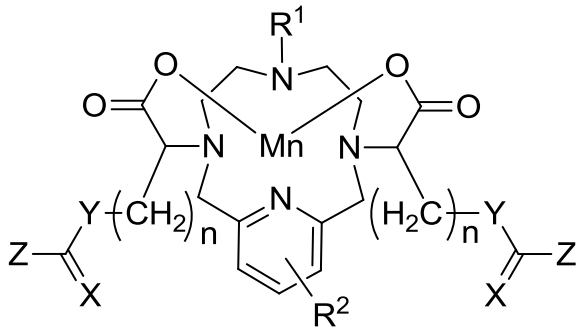
Synthesis of the conjugate **15**



A solution of (*S*)-4-(isothiocyanatomethyl)-2,2-dimethyl-1,3-dioxolane in DMF (2 equivalents) is added to the diamine **11** in DMF. The reaction mixture is stirred for several hours at room temperature and its progress is monitored using analytical chromatographic techniques. The addition of excess (*S*)-4-

Claims

1. A compound of Formula I or a salt or solvate thereof:



(I)

wherein:

X is O or S;

Y is O, S or Q-R^3 where Q is N or CH and R^3 is selected from the group comprising C_{1-20} hydroxyalkyl, C_{1-6} alkyl or hydrogen;

Z is O-L-R^4, S-L-R^4 or Q-R^3-(L-R^4) where Q and R^3 are as defined for Y and L is an optional linker selected from the groups comprising C_{1-6} alkylene, C_{1-6} hydroxyalkylene and a PEG linker, R^4 is selected from the group comprising C_{1-6} alkyl-R^5, C_{3-6} aryl-R^5, hydroxy, -O-C_{1-3} alkyl-R^5, sulfonyl, a 5-6-membered heterocyclic ring, a carbohydrate moiety, a chelate moiety, an amino acid moiety, wherein R^5 represents one or more optional substituents selected from hydroxy, amino, oxo, halo, C_{1-3} alkyl, sulfonamide or -C(=O)-NH-C_{1-6} hydroxyalkyl; or Z itself forms part of a carbohydrate moiety or a 5-6-membered heterocyclic ring;

R^1 is C_{1-3} alkyl or -$(CH_2)_m$-Y^1-C(=X^1)-Z^1 wherein X^1, Y^1 and Z^1 are as defined for X, Y and Z and m is an integer from 2-5;

R^2 represents 0-3 substituents independently selected from the group comprising hydroxy, halo, amino, amido, C_{1-6} alkyl and C_{1-6} hydroxyalkyl; and,

each n is an integer from 0-15;

wherein the compound of Formula I comprises at least two hydroxy groups; and,

with the proviso that when Y is Q-R^3 where Q is CH, Z is not Q-R^3-(L-R^4) where Q is N.

2. The compound as defined in Claim 1 wherein X is O, Y is Q-R^3 wherein Q is N and Z is Q-R^3-(L-R^4) wherein Q is N.

3. The compound as defined in Claim 1 wherein X is S, Y is Q-R^3 wherein Q is N and Z is Q-R^3-(L-R^4) wherein Q is N.

4. The compound as defined in Claim 1 wherein X is O, either Y is O or Z is O-L-R^4 and when Y is not O it is Q-R^3 wherein Q is N and when Z is not O-L-R^4 it is Q-R^3-(L-R^4) wherein Q is N.

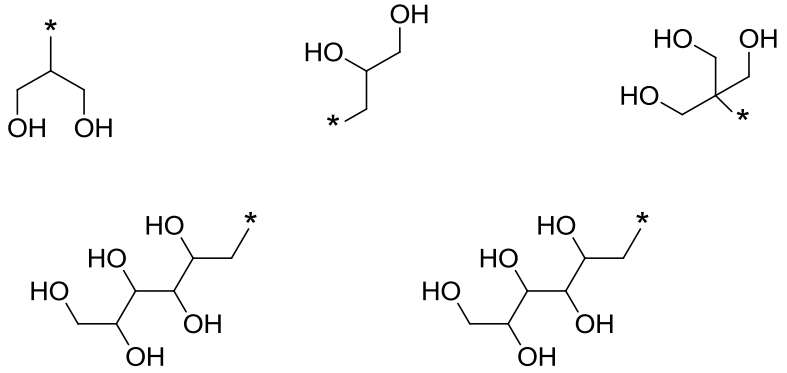
5. The compound as defined in Claim 1 wherein X is S, either Y is O or Z is O-L-R^4 and when Y is not O it is Q-R^3 wherein Q is N and when Z is not O it is Q-R^3-(L-R^4) wherein Q is N.

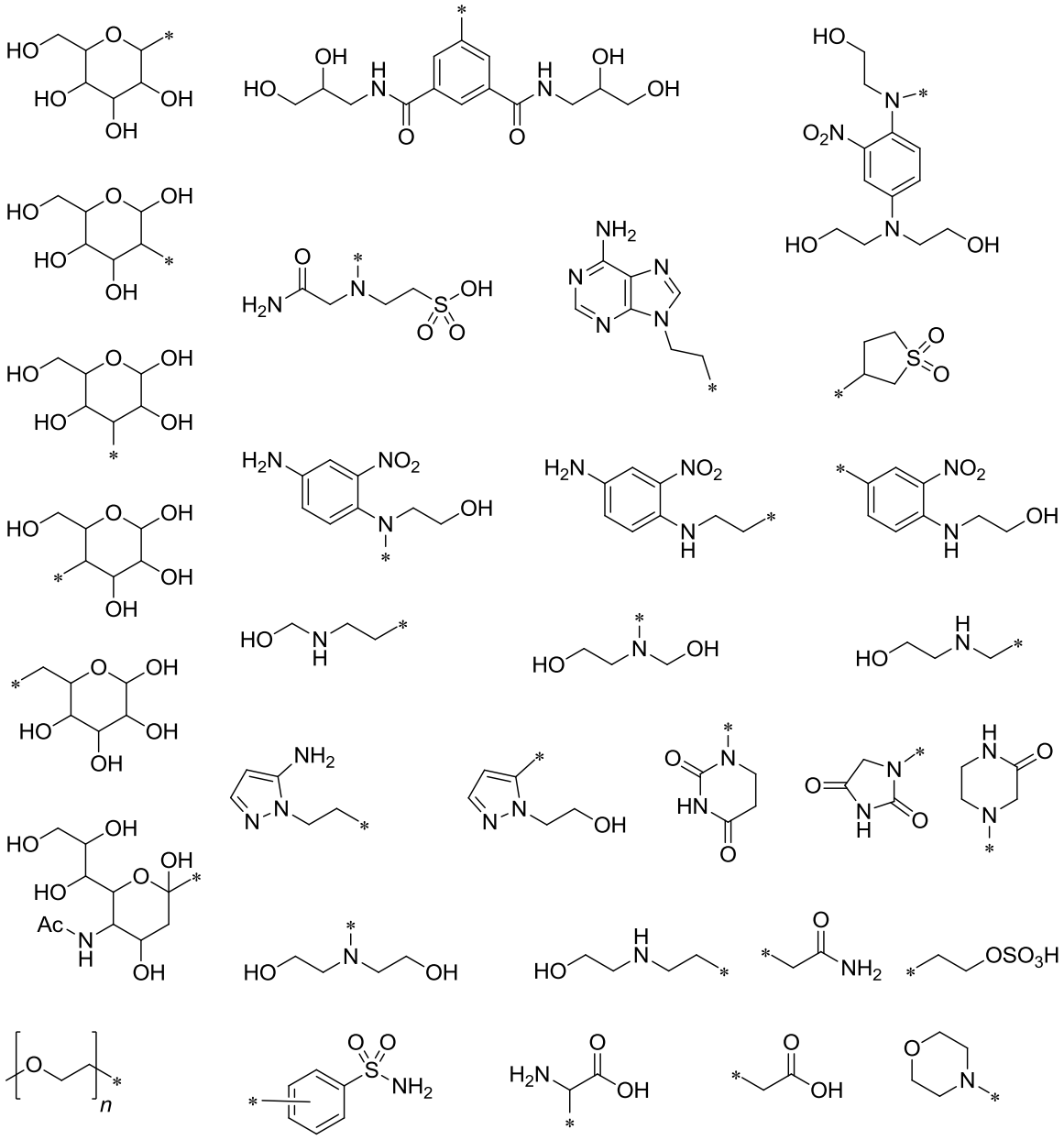
6. The compound as defined in Claim 1 wherein X is O, Y is Q-R^3 wherein Q is N and Z is Q-R^3-(L-R^4) wherein Q is CH.

7. The compound as defined in Claim 1 wherein X is O, either Y is O or Z is O-L-R^4 and when Y is not O it is Q-R^3 wherein Q is CH and when Z is not O it is Q-R^3-(L-R^4) wherein Q is CH.

8. The compound as defined in any one of Claims 1-7 wherein each -L-R^4 is $C_{1\text{-}12}$ hydroxyalkyl.

9. The compound as defined in any one of Claims 1-8 wherein each -L-R^4 is independently selected from the group comprising:





wherein in each case the asterisk denotes the point of attachment to the rest of the compound of Formula I.

10. The compound as defined in any one of Claims 1-9 wherein each R^4 is the same.

11. The compound as defined in any one of Claims 1-10 wherein each R^3 is independently selected from the group comprising C_{1-3} alkyl or hydrogen.

12. The compound as defined in Claim 11 wherein each R^3 is C_{1-3} alkyl.

13. The compound as defined in Claim 11 wherein each R^3 is hydrogen.

14. The compound as defined in any one of Claims 1-13 wherein each R^3 is the same.

15. The compound as defined in any one of Claims 1-14 wherein each n is an integer from 1-6.

16. The compound as defined in any one of Claims 1-15 wherein m is 3.

17. The compound as defined in any one of Claims 1-16 wherein R^1 is C_{1-3} alkyl.

18. The compound as defined in any one of Claims 1-16 wherein R^1 is $-(CH_2)_m$-Y-C(=X)-Z wherein X, Y, Z and m are as defined in any one of Claims 1-16.

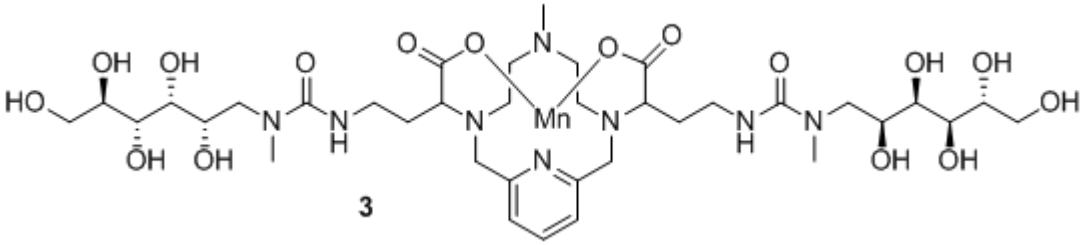
19. The compound as defined in any one of Claims 1-18 wherein R^2 represents 0 substituents.

20. The compound as defined in any one of Claims 1-18 wherein R^2 represents 2 hydroxy groups.

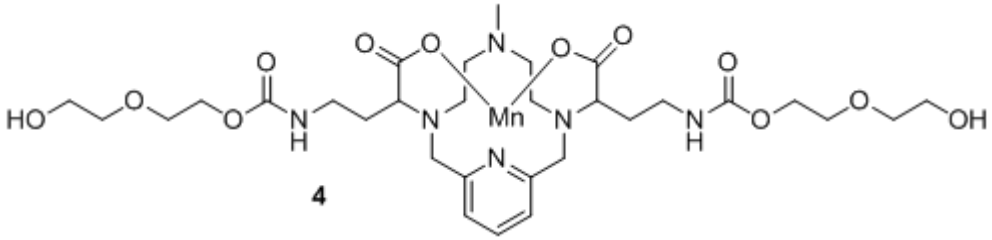
21. The compound as defined in Claim 20 wherein said hydroxyl groups are at the meta positions on the pyridyl ring.

22. The compound as defined in any one of Claims 1-21 which comprises at least 4 hydroxy groups.

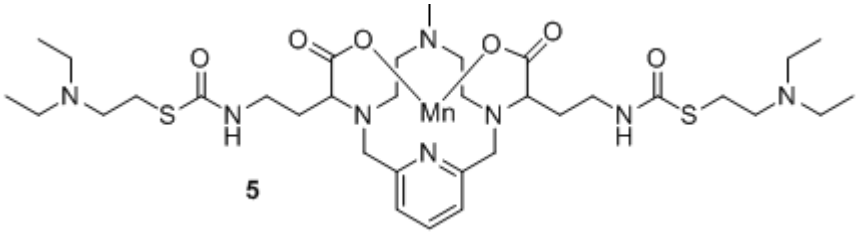
23. The compound as defined in Claim 1 which is selected from the following compounds:



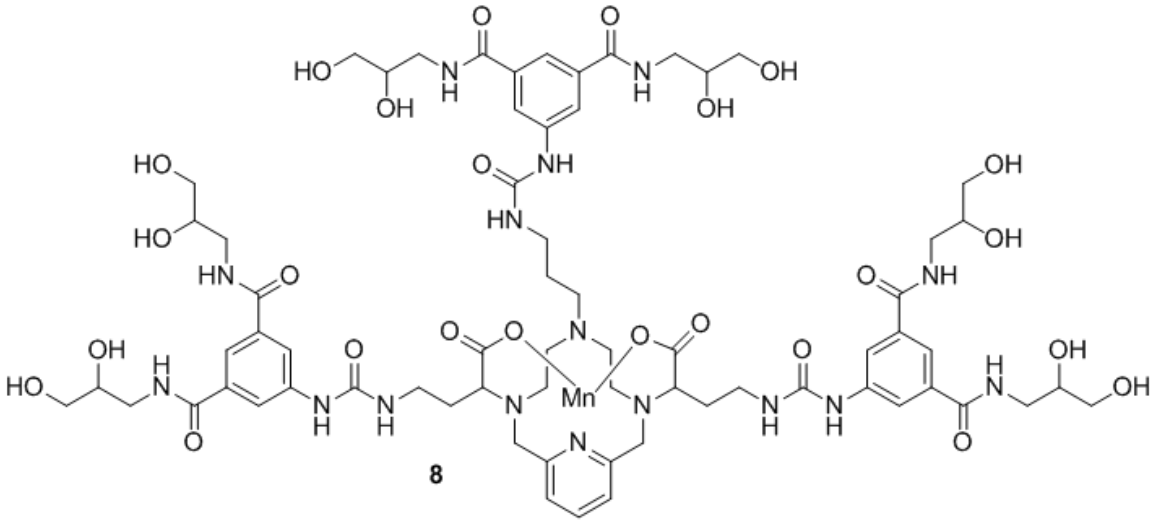
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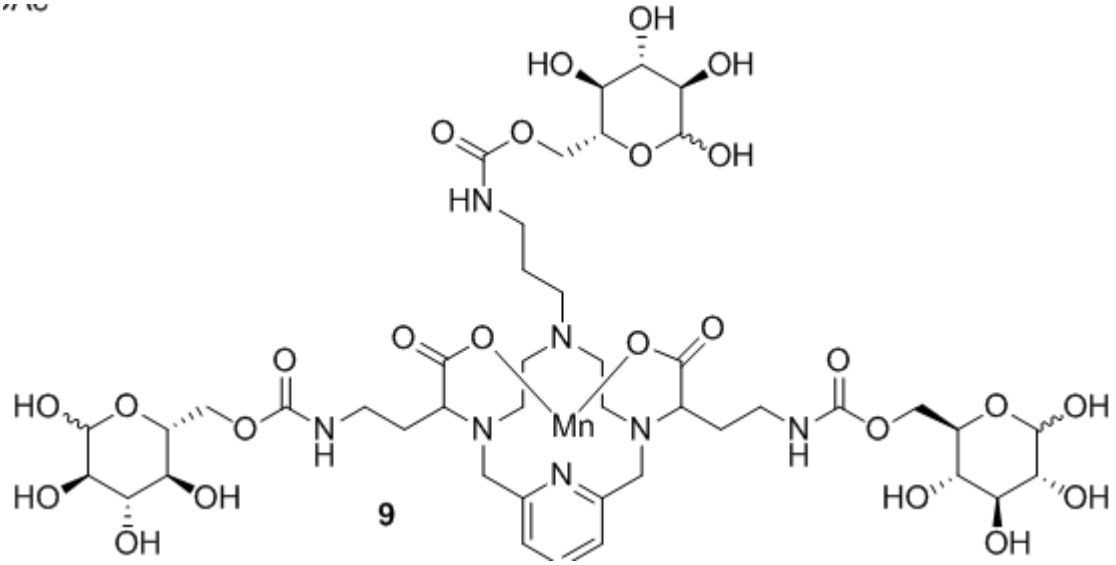
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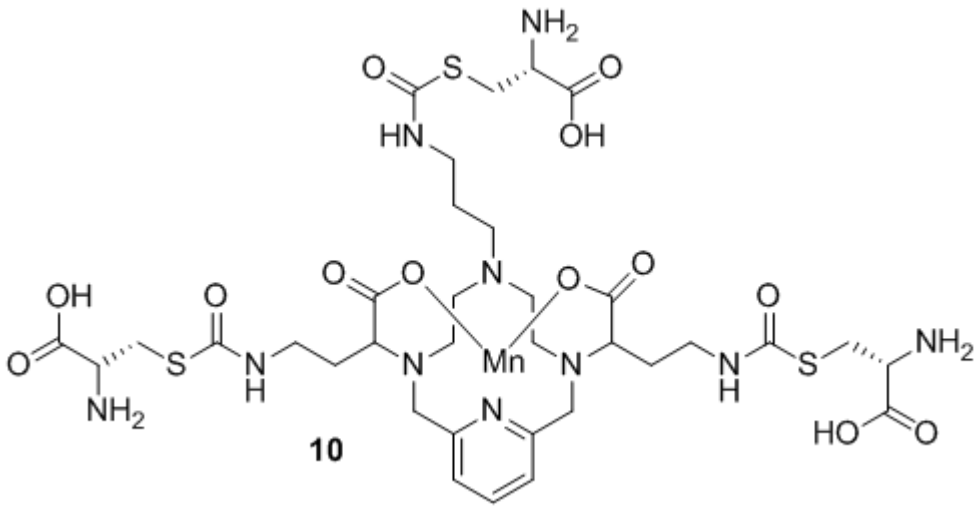
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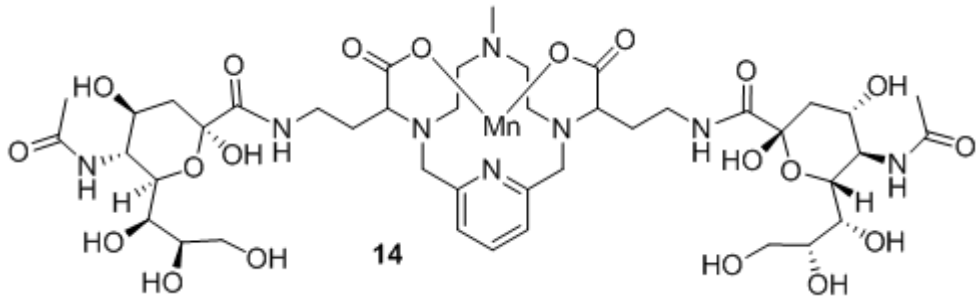
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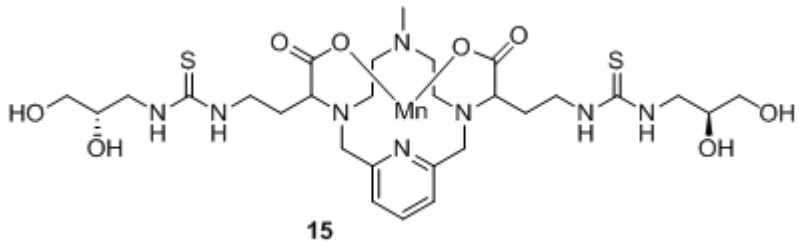
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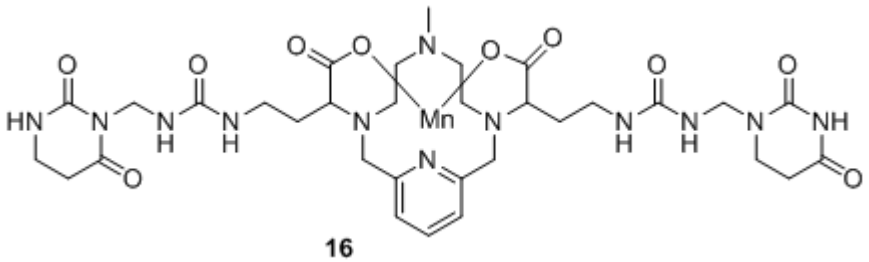
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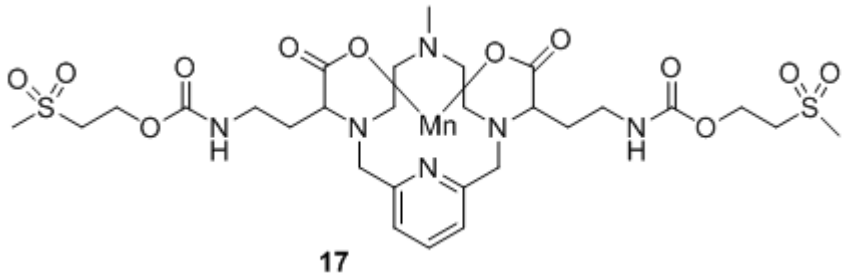
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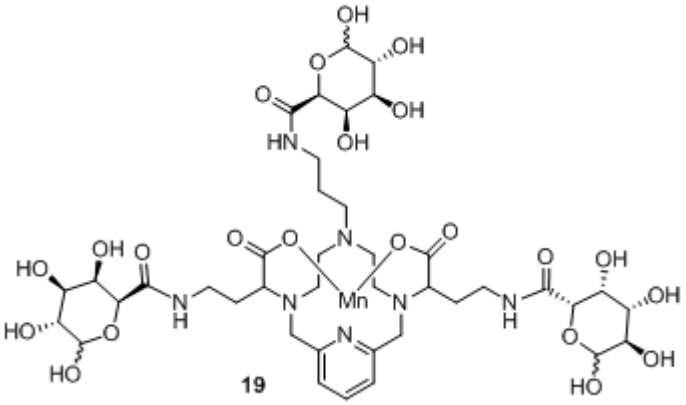
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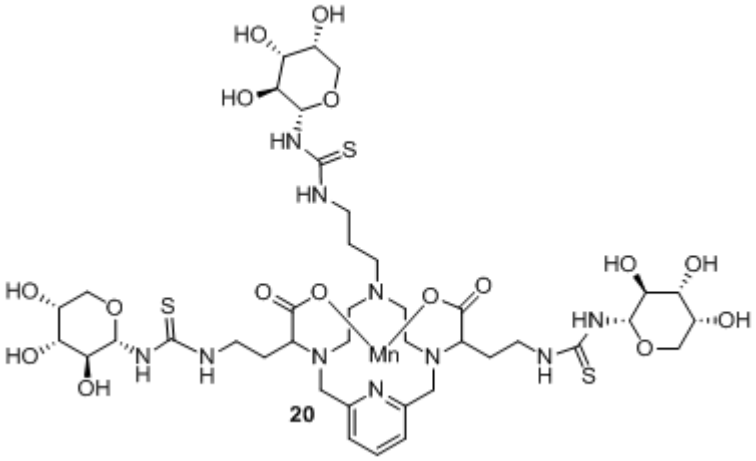
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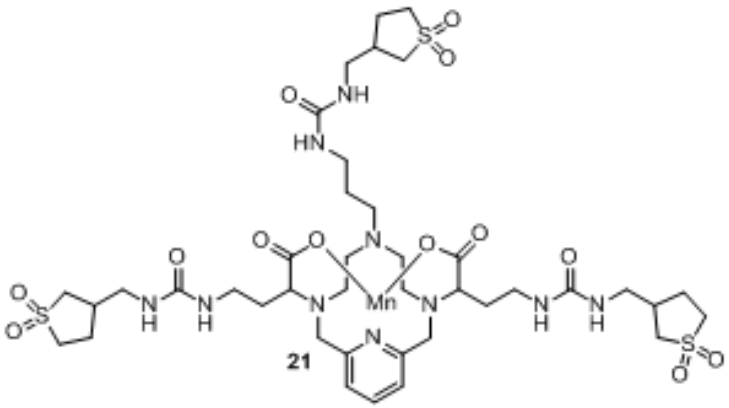


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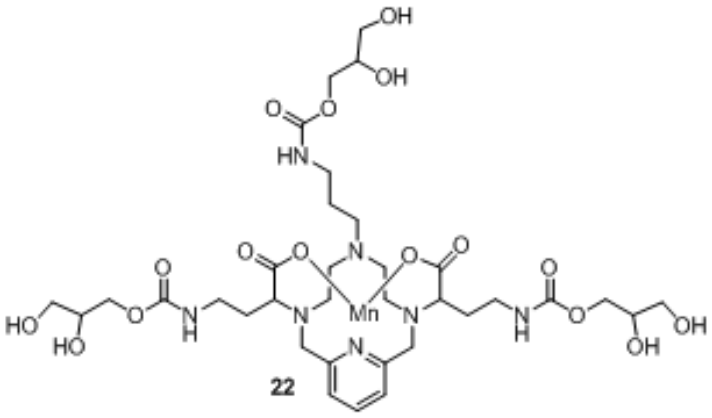


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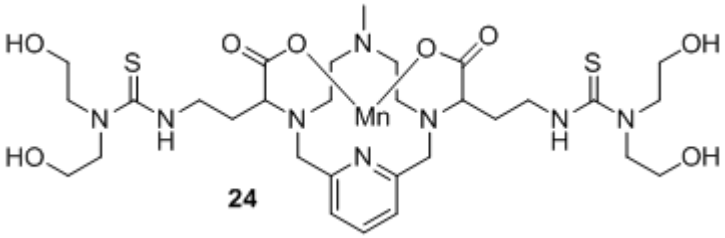
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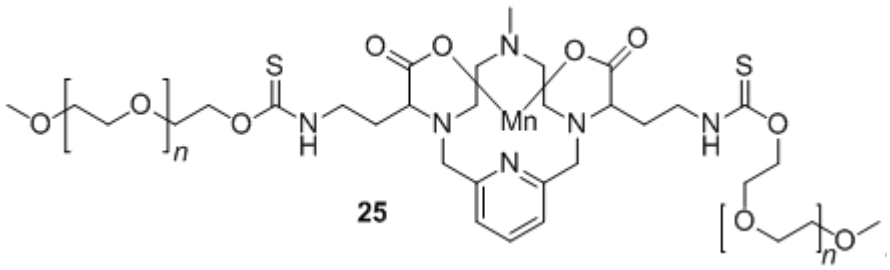
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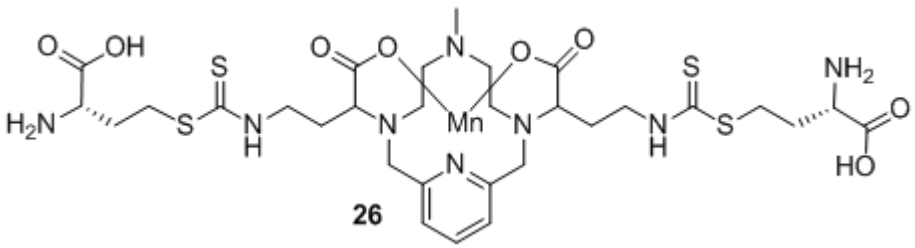
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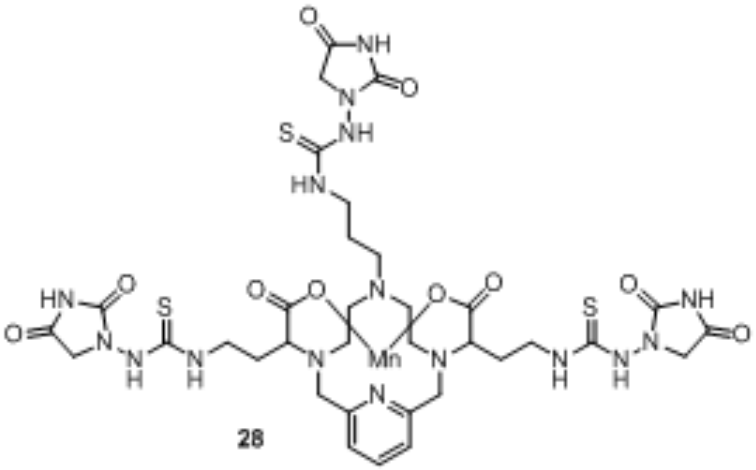
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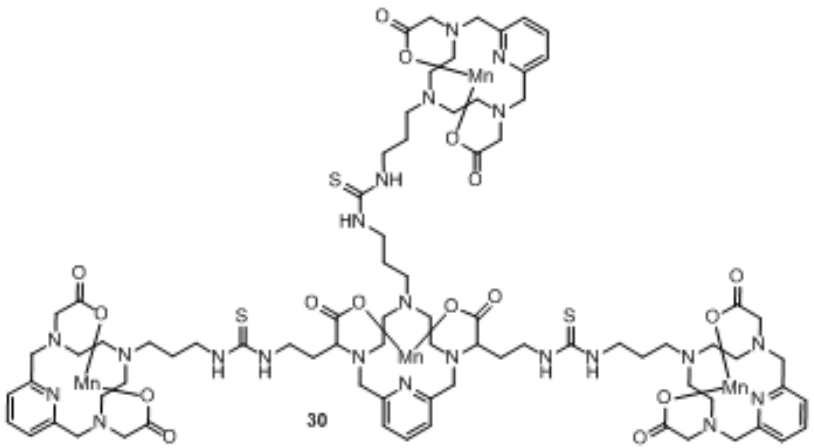
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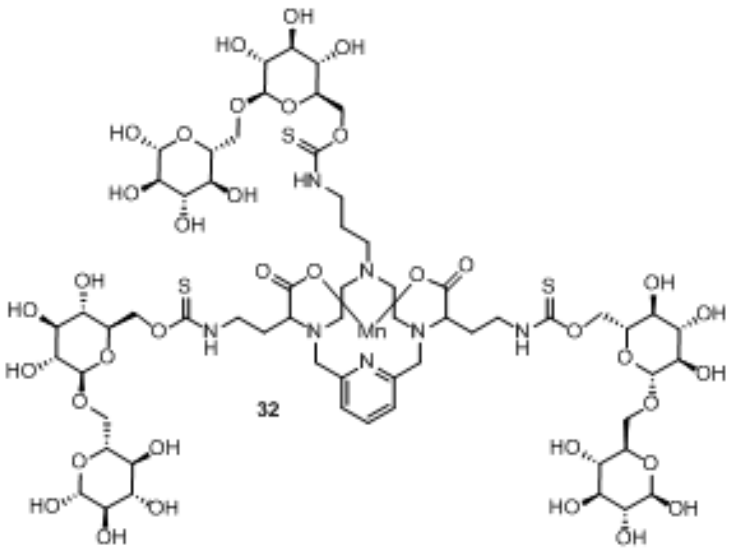
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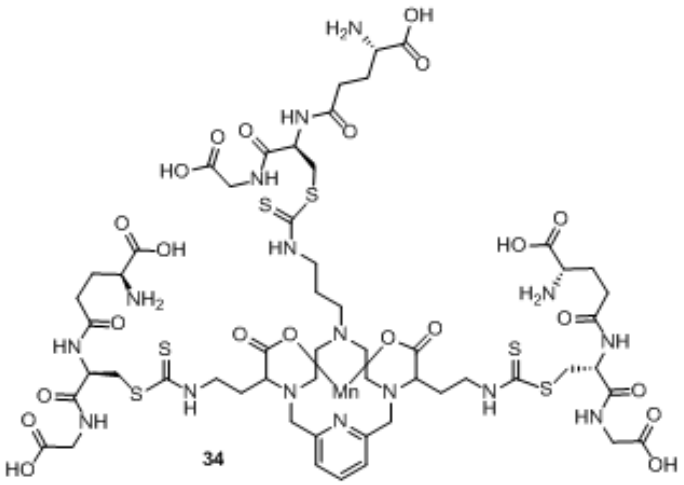


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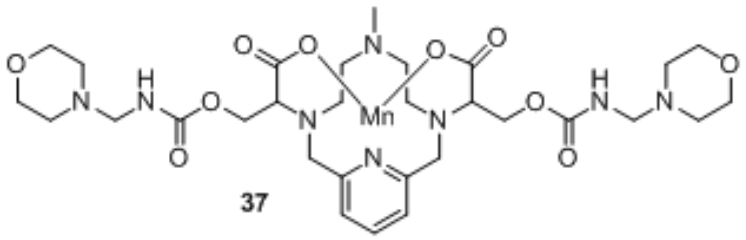


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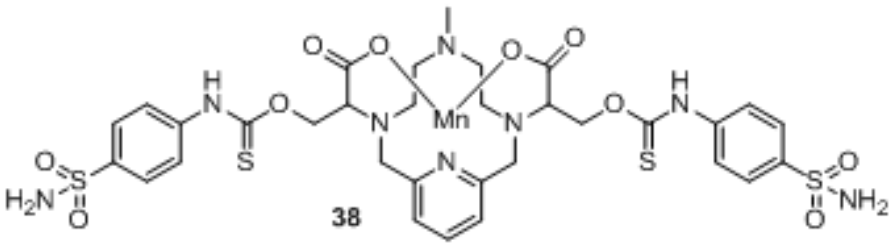
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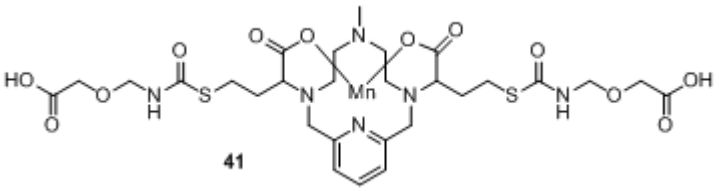
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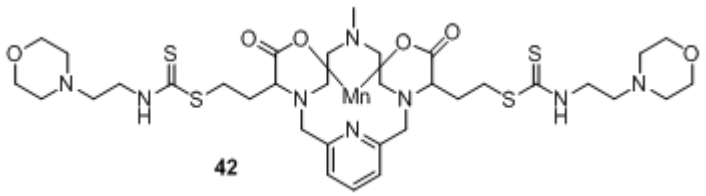
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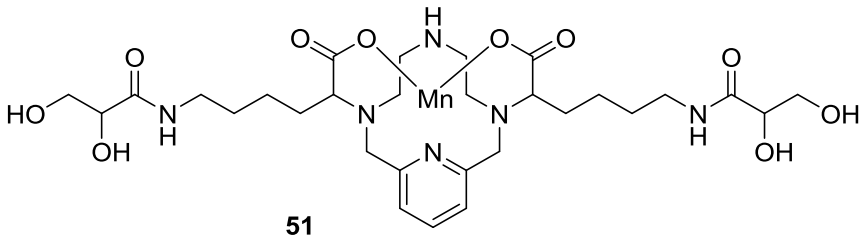
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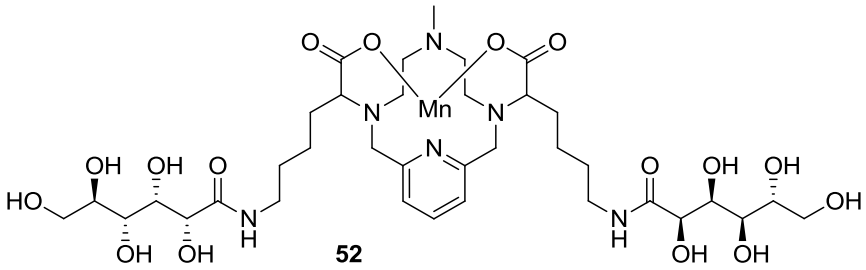
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24. The compound of Formula I as defined in any one of Claims 1-23 which is either a racemic mixture or diastereomerically pure.

25. A pharmaceutical composition comprising the compound of Formula I as defined in any one of Claims 1-24 together with a biocompatible carrier in a form suitable for mammalian administration.

26. The pharmaceutical composition as defined in Claim 25 further comprising one or more pharmaceutically-acceptable excipients.

27. The pharmaceutical composition as defined in Claim 26 wherein said pharmaceutically-acceptable excipients are selected from buffering agents, stabilizers, antioxidants, osmolality adjusting agents, pH adjusting agents, excess cheland and weak complexes of physiologically tolerable ions.

28. A method comprising:

(i) administration to a subject of the compound of Formula I as defined in any one of Claims 1-24 or the pharmaceutical composition as defined in any one of Claims 25-27;

(ii) detection of magnetic resonance (MR) signals from said subject or parts of said subject in which said compound has distributed;

(iii) generation of MR images and/or MR spectra from said detected signals.

29. The compound of Formula I as defined in any one of Claims 1-24 for use in the method as defined in Claim 28.