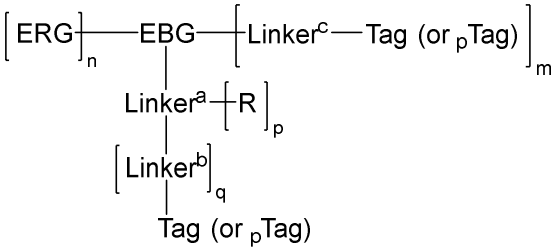
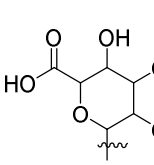
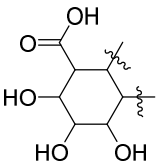
CLAIMS

1. A probe having a structure satisfying Formula II

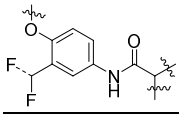


Formula II

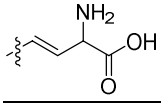
wherein

ERG, if present, is  ;  ; $S(O)_2OH$, or an anionic form thereof; $P(O)(OH)_2$, or an anionic form thereof; a halogen; or $-OPh-CH_2-ONO_2$;

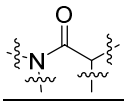
EBG has a structure satisfying a formula selected from Formulas IIA_{EBG}- IIJ_{EBG} ~~Formulas IIB_{EBG}~~



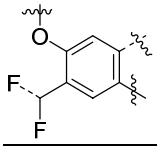
Formula IIA_{EBG};



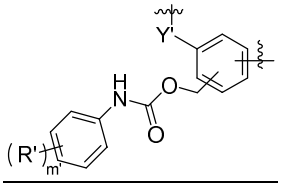
Formula IIB_{EBG};



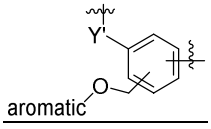
Formula IIC_{EBG};



Formula IID_{EBG};



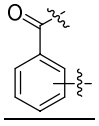
Formula IIE_{EBG};



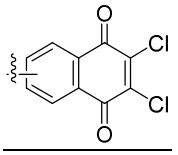
Formula IIF_{EBG};



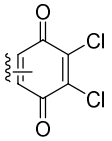
Formula IIG_{EBG};



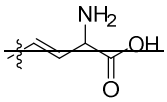
Formula IIH_{EBG};



Formula III_{EBG}; or



Formula IIJ_{EBG}



~~Formula IIB$_{EBG}$;~~

wherein Y is CH_3 or CF_3; Y' is O, NO_2, or -N=NR'', wherein R'' is a dye or other reporting moiety; and m' is an integer selected from 0 to 5; and R' is selected from aldehyde, ketone, ester, carboxylic acid, acyl, acyl halide, cyano, sulfonate, nitro, nitroso, quaternary amine, CF_3, alkyl halide, or combinations thereof;

Linker^a comprises an aliphatic group, a heteroaliphatic group, an aromatic group, an aliphatic-aromatic group, a heteroaliphatic-aromatic group, a heteroaromatic group, an aliphatic-heteroaromatic group, or a heteroaliphatic-heteroaromatic group;

each of Linker^b, and Linker^c, if present, independently comprises an aliphatic group, a heteroaliphatic group, an aromatic group, an aliphatic-aromatic group, a heteroaliphatic-aromatic group, a heteroaromatic group, an aliphatic-heteroaromatic group, or a heteroaliphatic-heteroaromatic group;

R, if present, is a group comprising a carbamate or a carbonate; and

each of n, m, p, and q independently is 0 or 1;

provided that one of the following applies:

(a) one or more Tags are present, and each Tag is independently a fluorophore, a binding partner of an affinity-based binding pair, a quantum dot, or a dye; or

(b) one or more $_p$Tags are present and each $_p$Tag is independently an azide or an alkyne

~~each Tag, if present, independently comprises a functional group or molecule capable of generating a detectable signal;~~

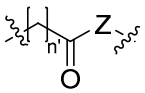
~~each $_p$Tag, which is present if a Tag is not present, independently comprises a clickable functional group; n and m are 0; and~~

~~each of p and q independently is 0 or 1~~.

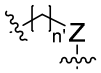
2. The probe of claim 1, wherein Linker^a is a linker group having a structure satisfying a formula selected from ~~one or more of~~ Formulas IIA$_{Linkera}$-IIH$_{Linkera}$



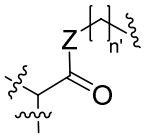
Formula IIA$_{linkera}$



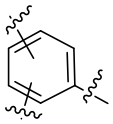
Formula IIB$_{linkera}$



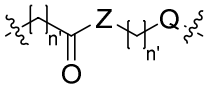
Formula IIC$_{linkera}$



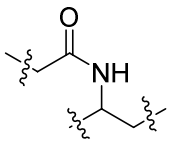
Formula IID$_{linkera}$



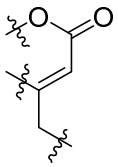
Formula IIE$_{linkera}$



Formula IIF$_{linkera}$



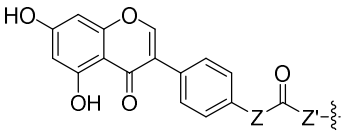
Formula IIG$_{linkera}$



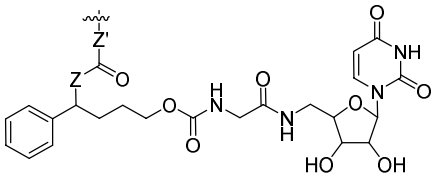
Formula IIH$_{linkera}$

wherein each n' independently is an integer ranging from 1 to 50; Z is oxygen or NR"', wherein R"' is hydrogen, aliphatic, or aromatic; and Q is carbon, oxygen or NR"', wherein R"' is hydrogen, aliphatic, or aromatic.

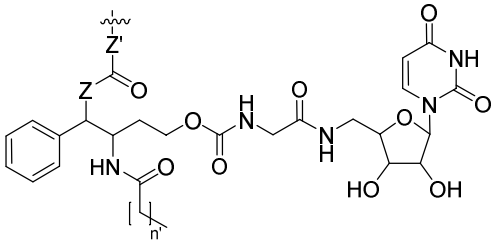
3. The probe of claim 1 or claim 2, wherein R is present and has a structure satisfying any one or more Formulas IIA$_R$- IID$_R$ ~~IIC$_R$~~



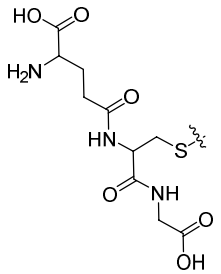
Formula IIA$_R$



Formula IIB$_R$



Formula IIC$_R$



Formula IID$_R$

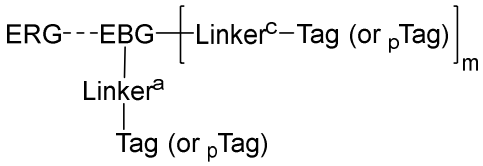
wherein Z and Z' independently are oxygen or NR"', wherein R"' is hydrogen, aliphatic, or aromatic; and n' is an integer ranging from 0 to 50.

~~4. The probe of any one of claims 1-3, wherein one or more Tags are present and wherein each Tag independently is a fluorophore, a binding partner of an affinity-based binding pair, a quantum dot, or a dye.~~

4~~5~~. The probe of claim 1~~4~~, wherein the one or more Tags independently are rhodamine, fluorescein, or biotin.

~~6. The probe of any one of claims 1-3, wherein one or more $_p$Tags are present and wherein each $_p$Tag independently is an azide or an alkyne.~~

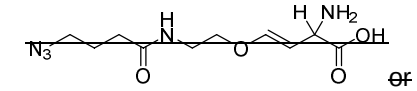
5~~7~~. The probe of claim 1, wherein the compound has a structure satisfying Formula IIIA

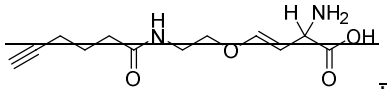


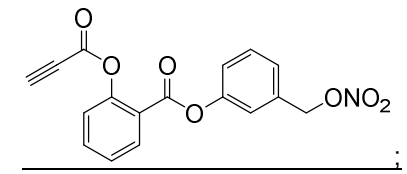
Formula IIIA.

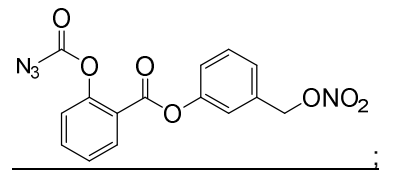
6~~8~~. The probe of claim 5~~7~~, wherein Linker^a is an ester group, an -O(CH$_2$)$_{n'}$NR'''C(O)(CH$_2$)$_{n'}$- group, or a -(CH$_2$)$_{n'}$- group, wherein each n' independently is an integer ranging from 1 to 20 and wherein R''' is hydrogen, aliphatic, or aromatic.

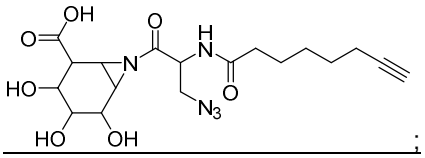
7~~9~~. A probe selected from

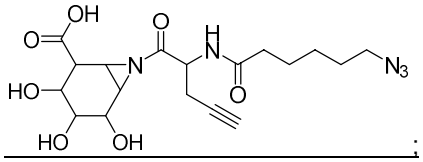

~~or~~

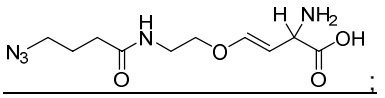

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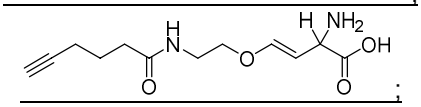

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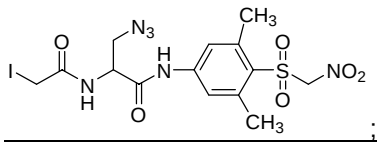

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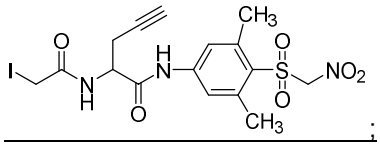

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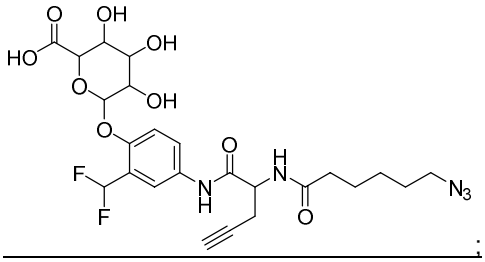

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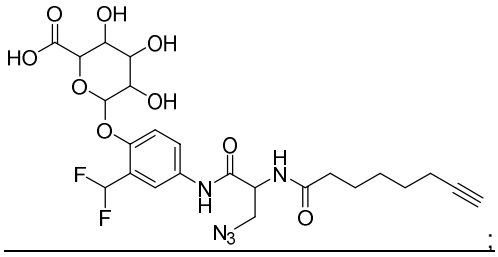
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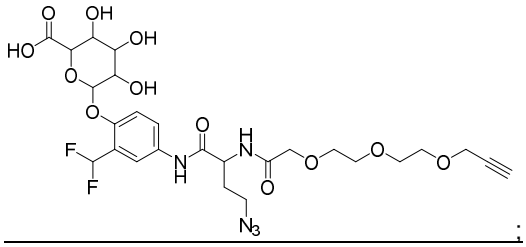
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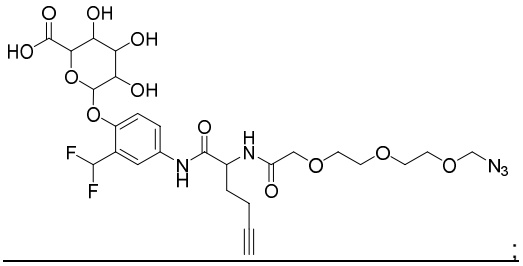
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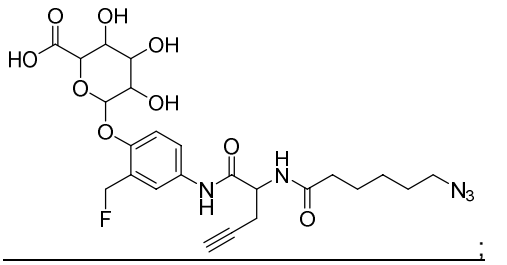
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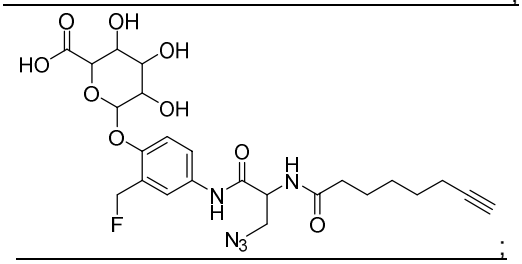
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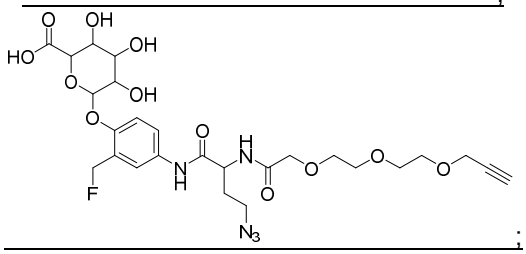
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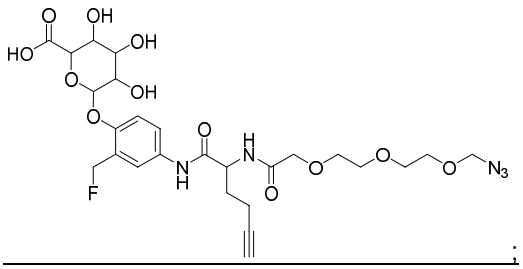
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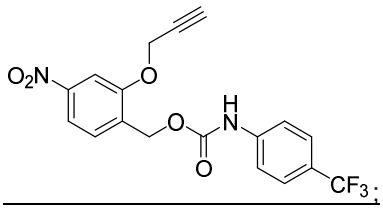
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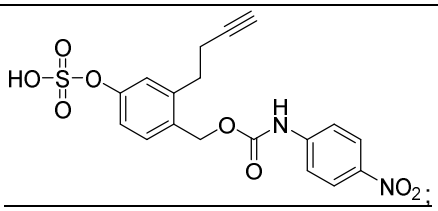
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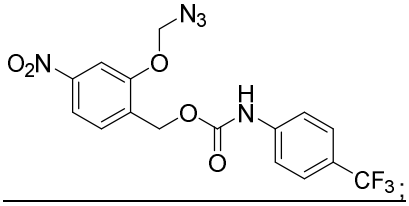
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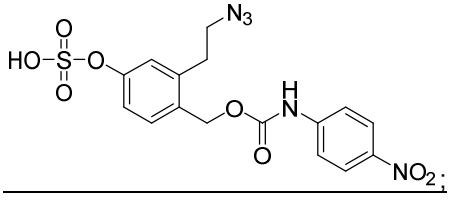
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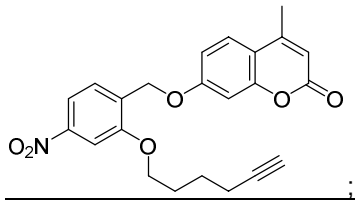
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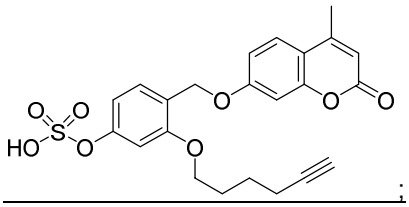


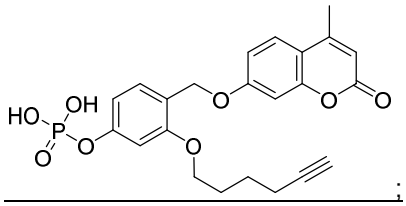
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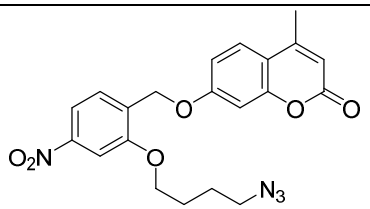


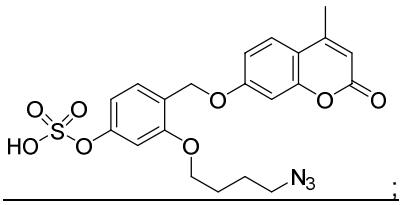
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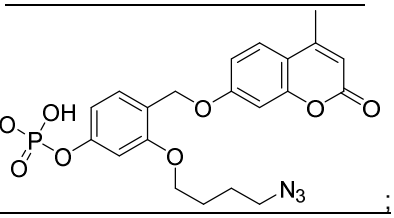

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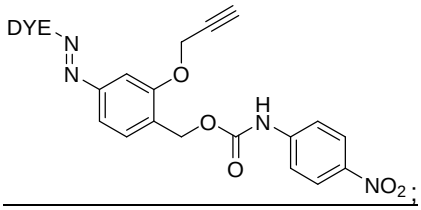

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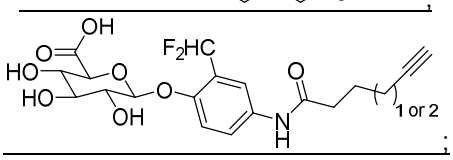

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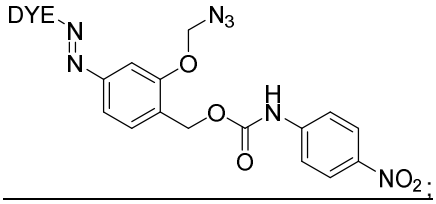


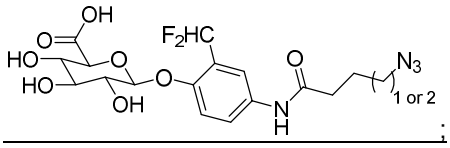

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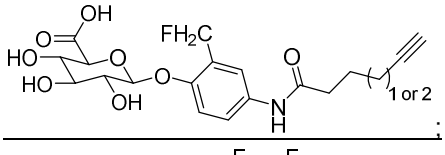

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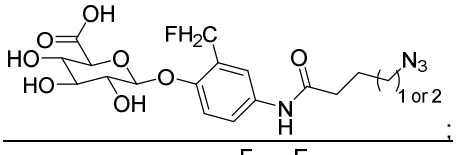

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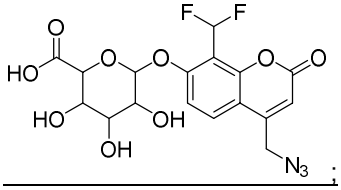

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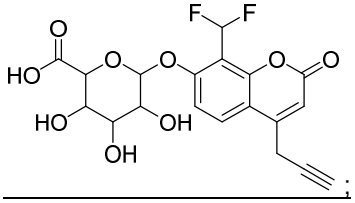

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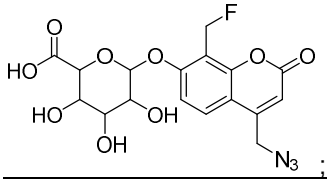

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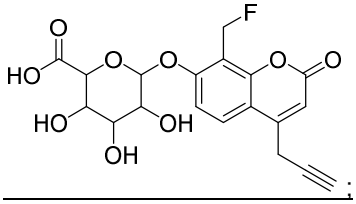

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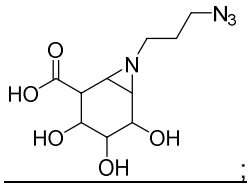

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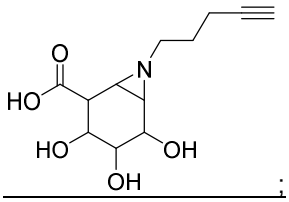

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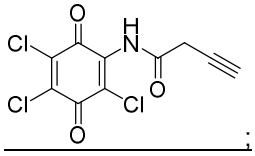

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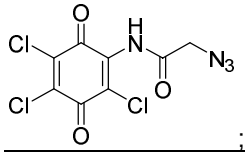

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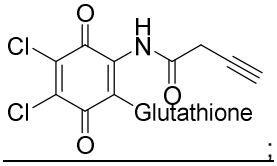

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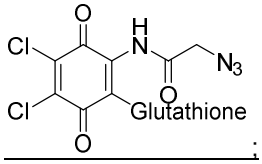

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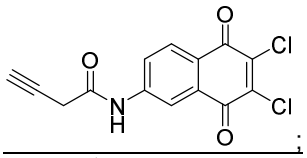

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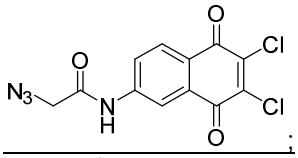

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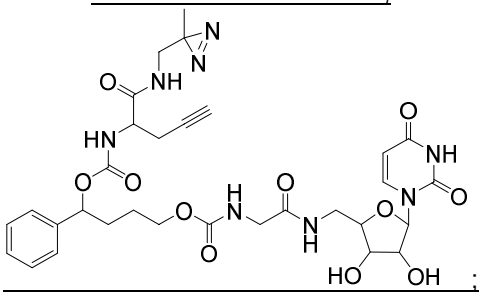

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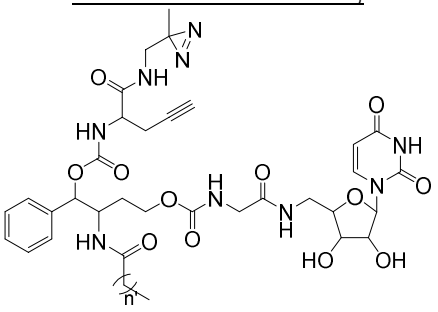

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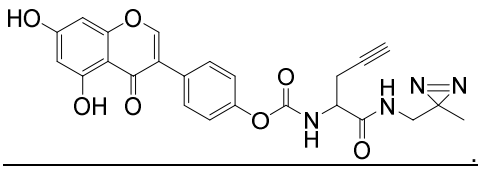

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;


wherein n' is 0 to 50; or


.

~~10. A method, comprising:~~

~~exposing a subject or a sample to a probe according to any one of claims 1-9 for a time sufficient to allow the probe to bind to an enzyme involved in xenobiotic metabolism such that a probe-enzyme conjugate is formed; and~~

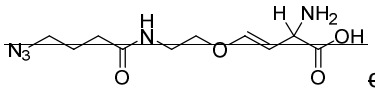
~~analyzing the probe-enzyme conjugate using a fluorescent detection technique, a colorimetric detection technique, a mass spectrometry technique, or a combination thereof.~~

~~11. The method of claim 10, further comprising exposing the probe-enzyme conjugate to a Tag-containing compound to form a probe-enzyme conjugate comprising a Tag moiety.~~

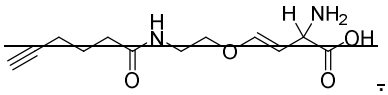
~~12. The method of claim 10 or 11, further comprising exposing the probe to a light source.~~

~~13. The method of any one of claims 10-12, further comprising extracting a subject sample from the subject and analyzing the subject sample using a fluorescent detection technique, a colorimetric detection technique, a mass spectrometry technique, or a combination thereof.~~

~~14. The method of any one of claims 10-13, wherein the probe is selected from~~



~~or~~



.

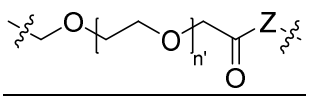
~~15. An assay platform, comprising:~~

~~a substrate; and~~

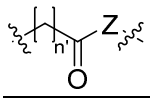
~~a probe according to any one of claims 1-9, wherein the probe is covalently bound to the substrate.~~

8. The probe of claim 1, wherein Linker^{b} is present and comprises a -$(CH_2)_{n'}$- group, wherein n' is an integer ranging from 1 to 50; an amide group; or a combination thereof.

9. The probe of claim 1, wherein Linker^{c} is present and has a structure satisfying Formula $IIA_{Linkerc}$ or Formula $IIB_{Linkerc}$



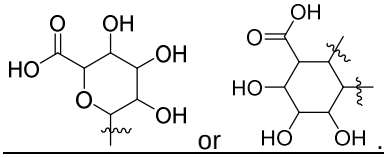
Formula $IIA_{Linkerc}$



Formula $IIB_{Linkerc}$

wherein n' is an integer ranging from 0 to 50; and Z is oxygen or NR'", wherein R"' is hydrogen, aliphatic, or aromatic.

10. The probe of claim 5, wherein the ERG is present and is iodo; -OPh-CH_2-ONO_2;

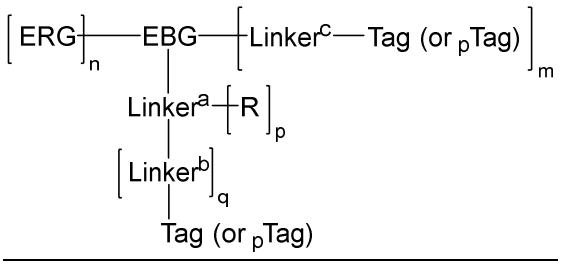


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11. The probe of claim 5, wherein m is 1 and Linker^{c} is an -NR"'C(O)$(CH_2)_{n'}$- group or an –NR"'C(O)$CH_2[O(CH_2)_2]_{n'}OCH_2$- group, wherein each n' independently is an integer ranging from 1 to 20 and wherein R"' is hydrogen, aliphatic, or aromatic.

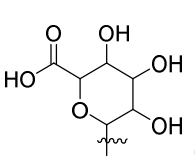
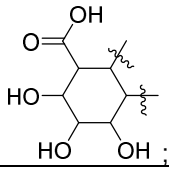
12. The probe of claim 5, wherein m is 1.

13. A probe having a structure satisfying Formula II

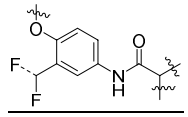


Formula II

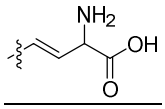
wherein

ERG is  or  ;

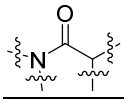
EBG has a structure satisfying a formula selected from



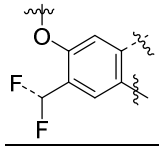
Formula IIA$_{EBG}$;



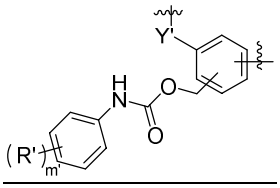
Formula IIB$_{EBG}$;



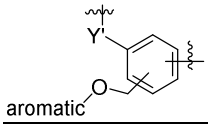
Formula IIC$_{EBG}$;



Formula IID$_{EBG}$;



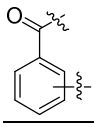
Formula IIE$_{EBG}$



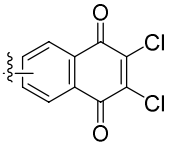
Formula IIF$_{EBG}$



Formula IIG$_{EBG}$;

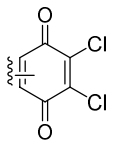


Formula IIH$_{EBG}$;



Formula III$_{EBG}$;

or



Formula IIJ$_{EBG}$

wherein Y' is O; m' is an integer selected from 0 to 5; and each occurrence of R' is independently selected from aldehyde, ketone, ester, carboxylic acid, acyl, acyl halide, cyano, sulfonate, nitro, nitroso, quaternary amine, CF_3, alkyl halide, or combinations thereof;

Linker^a comprises an aliphatic group, a heteroaliphatic group, an aromatic group, an aliphatic-aromatic group, a heteroaliphatic-aromatic group, a heteroaromatic group, an aliphatic-heteroaromatic group, or a heteroaliphatic-heteroaromatic group;

each of Linker^b, and Linker^c, if present, independently comprises an aliphatic group, a heteroaliphatic group, an aromatic group, an aliphatic-aromatic group, a heteroaliphatic-aromatic group, a heteroaromatic group, an aliphatic-heteroaromatic group, or a heteroaliphatic-heteroaromatic group;

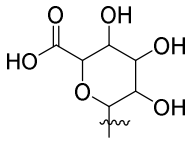
R, if present, is a group comprising a carbamate or a carbonate;

each of n, m, p, and q independently is 0 or 1; and

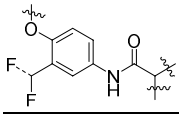
provided that one of the following applies:

(a) one or more Tags are present, and each Tag is independently a fluorophore, a binding partner of an affinity-based binding pair, a quantum dot, or a dye; or

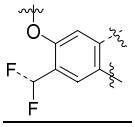
(b) one or more $_p$Tags are present, and each $_p$Tag is independently an azide or an alkyne.

14. The probe of claim 13, wherein the ERG is .

15. The probe of claim 13, wherein the EBG has a structure satisfying a formula selected form

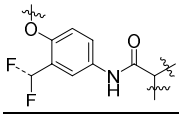


Formula IIA$_{EBG}$; or



Formula IID$_{EBG}$.

16. The probe of claim 13, wherein the EBG has a structure satisfying a formula of



Formula IIA$_{EBG}$.

17. The probe of claim 13, wherein Linker^b and R are absent and wherein q and m are 0.

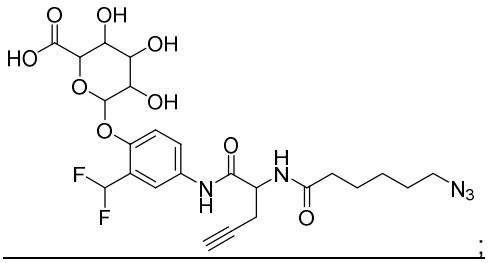
18. The probe of claim 13, wherein Linker^a is an -O(CH$_2$)$_{n'}$NR'''C(O)(CH$_2$)$_{n'}$- group, or a -(CH$_2$)$_{n'}$- group, wherein each n' independently is an integer ranging from 1 to 20 and wherein R''' is hydrogen, aliphatic, or aromatic.

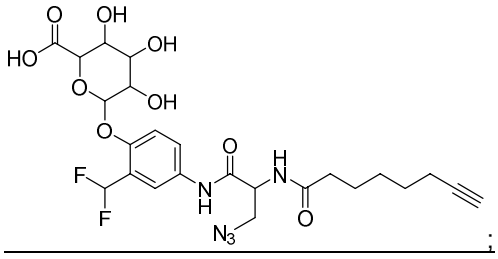
19. The probe of claim 13, wherein the one or more Tags are present.

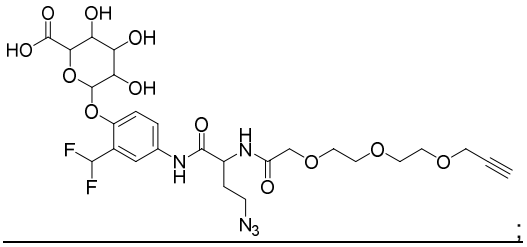
20. The probe of claim 13, wherein the one or more $_p$Tags are present.

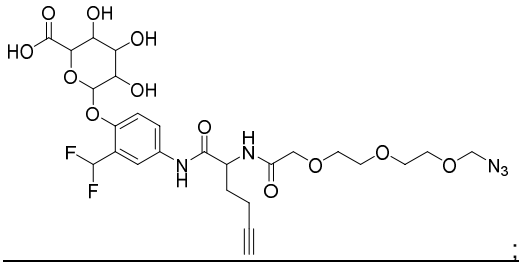
21. The probe of claim 13, wherein n is 1.

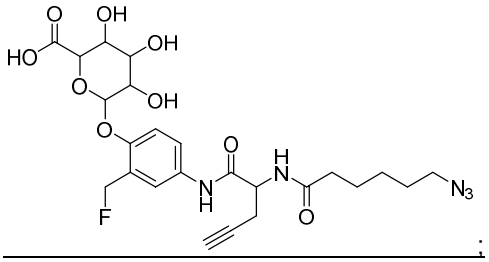
22. A probe selected from:

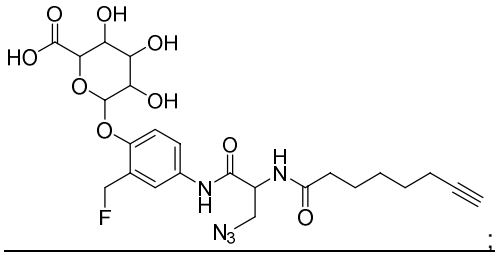

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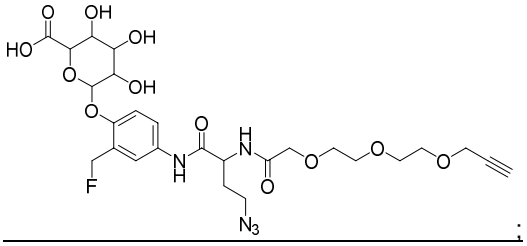

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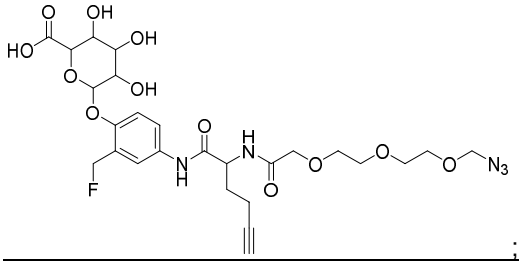

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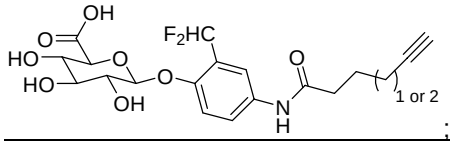

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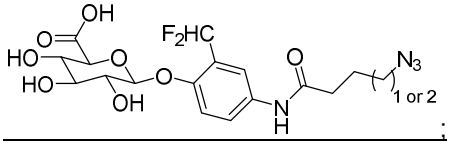

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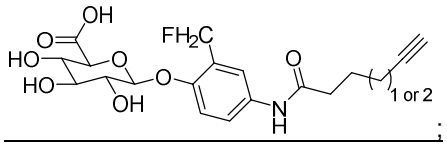

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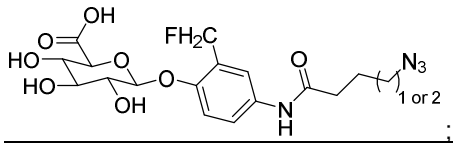


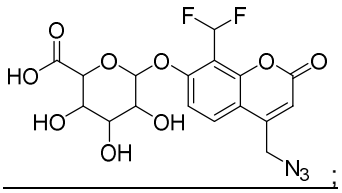
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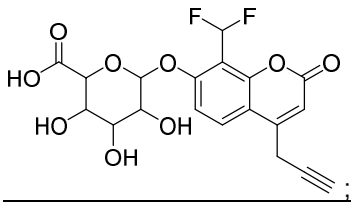


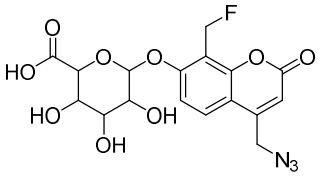
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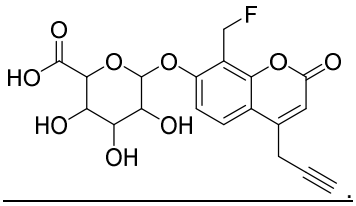

OH
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HO
HO
O
OH
FH2C
O
N
H
1 or 2
;


OH
O
HO
HO
O
OH
FH2C
O
N
H
N3
1 or 2
;


F
F
O
HO
O
O
HO
OH
OH
O
O
N3
;


F
F
O
HO
O
O
HO
OH
OH
O
O
;


F
O
HO
O
O
HO
OH
OH
O
O
N3
; or


F
O
HO
O
O
HO
OH
OH
O
O
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